NMR Database of Lignin and Cell Wall Model Compounds

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This database was designed to provide a coherent, single source of NMR data of lignin and other plant cell wall model compounds. The database exists in several different formats: a FileMaker Pro© database for cross-platform use, an Adobe© pdf cross-platform file for viewing and printing, and a hardcopy version derived from the FileMaker Pro database. FileMaker Pro and pdf versions are available for downloading over the internet from the Dairy Forage Research Center (DFRC) web site:

http://www.dfrc.ars.usda.gov
(under the Software section)

A hardcopy version is available by request from the authors at the Forest Products Laboratory, but users are encouraged to print their own version. The use of trade or firm names in this publication is for reader information and does not imply endorsement by the US Department of Agriculture of any product or service.

In general ^{13}C NMR data was collected in three common deuterated solvents (acetone, chloroform and dimethyl sulfoxide) for each compound. We used the center line of the solvent peaks as our reference, 2.04 and 29.83 ppm for acetone-d_6, 7.24 and 77.00 for $CDCl_3$ and 2.49 and 39.50 ppm for DMSO-d_6. The ^1H NMR data early on was reported for only one solvent. A standard set of acquisition parameters was used to acquire and process the spectra to keep the data as uniform and constant as possible. The samples were run at ambient temperature, about 298° K.

Those compounds with an index number less than 1000 were run on a Bruker 250 MHz spectrometer at FPL and those compounds with an index number between 1000 and 10,000 were run at the DFRC on a Bruker 360 MHz instrument. The order of the compounds in the database reflects their arrival at the spectrometer rather than a preordained plan. The inclusion of analogous series of structures with small structural differences allows calculation of substituent effects that are invaluable for chemical shift predictions of structures not included in the database.

The chemical shift assignments for most of the compounds were made by comparison with other compounds, literature values, and in some cases using the standard set of 1D and 2D NMR experiments. Every effort was made to correctly assign the chemical shifts; however, limited time and resources precluded confirming the shifts for many of the compounds. The shifts are reported to the second decimal place only to distinguish very close shifts; comparisons between spectra are practical only within ± 0.1 ppm. The authors would greatly appreciate learning of any corrections on suspect assignments.
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The compounds themselves came from many sources — in-house collections, syntheses and donations from other researchers for which we are grateful. The source of the compounds is often given in the "Notes" field along with other pertinent data.

This database was originally intended as an aid for the assignment of chemical shifts for wood and plant lignin NMR spectra. The trivial names used throughout are well known to wood chemists as is the numbering system. We have attempted to include more formal chemical names for many of the compounds and these were obtained using Beilstein's Autonom© program. The chemical names for the larger 3 and 4 ring models became so cumbersome that the authors employed an abbreviated system to identify both the moieties involved as well as the linkages between the moieties. Examples of the naming, numbering and linking conventions used are given below.

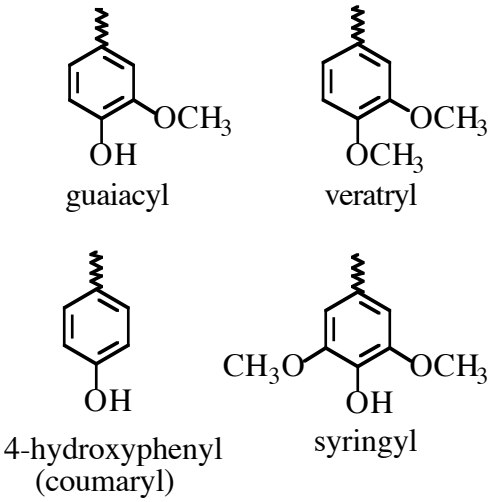
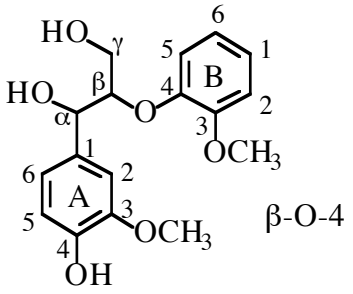


Fig. 1 Trivial names for substituents at the 3,4 and 5 positions on the aromatic ring.

The naming of the larger oligomer lignin models uses a combination of upper case letters to describe the ring structure and lower case letters and numbers to describe the type of linkage between the rings.

Table 2. Terminology of Abbreviated Structural Entities

Entity	Abbreviation
guaiacyl ring	G
syringyl ring	S
coumaryl ring	H
α–O–4 linkage	a
β–O–4 linkage	b
β–5 (phenylcoumaran)	c
β–1 linkage	b1
β–β (resinol)	r
5-5 (biphenyl)	5,5
coniferyl alcohol end unit	CA
sinapyl alcohol end unit	SA
p-coumaryl alcohol end unit	HA
ferulic acid end unit	FA
erythro	*e*
threo	*t*



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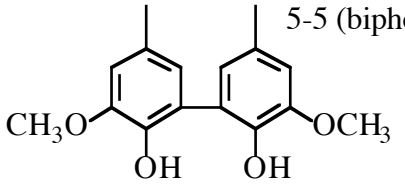

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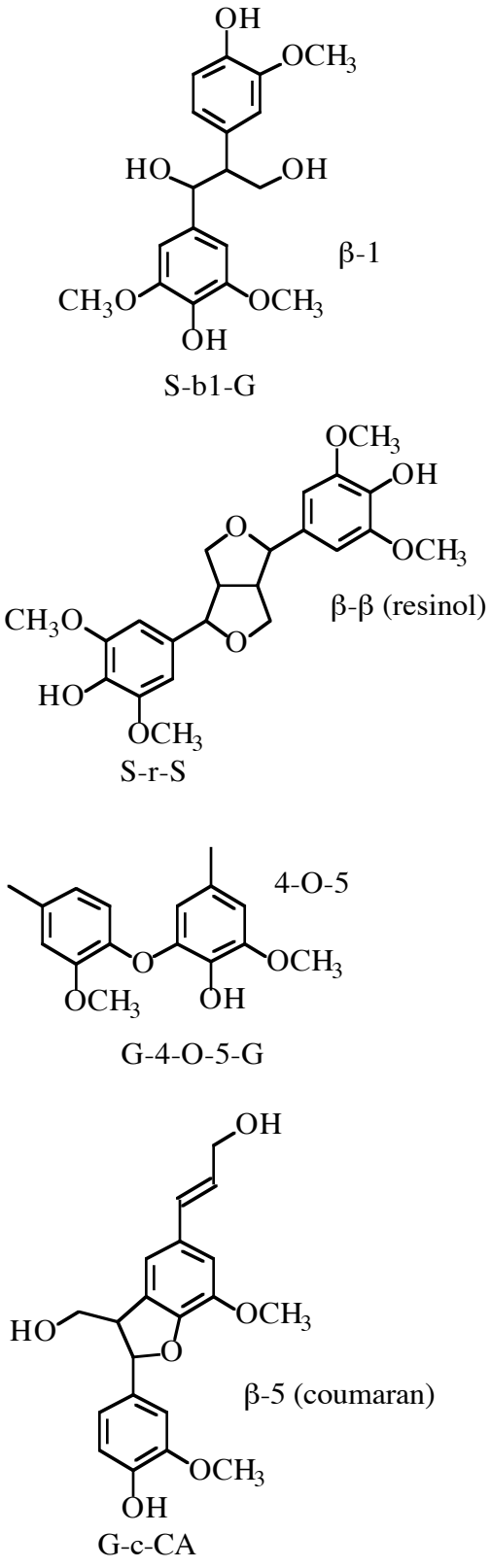

Fig. 2 Examples of linkages and abbreviated names.

With this convention the name FA-5,5-FA would represent a diferulic acid biphenyl structure. The trimer CA-a-G-b-CA would be a guaiacyl unit with two coniferyl alcohol end groups etherified at the α- and β-positions.

The structure index is arranged based upon the number of rings in the structure. Where possible the structures are also arranged by ring type such as guaiacyl, syringyl etc. The number under the structure refers to the index number at the top of the data sheet. An asterisk after a number indicates the acetylated analog of that compound. In some cases only the acetylated compound is included.

We hope to continue adding to and improving this database. Regular updates will be made to the database to keep the online sources current. This database was written and prepared for the most part by U.S. Government employees on official time, and it is therefore in the public domain and not subject to copyright. Please feel free to contact the authors with suggestions or questions.

The authors gratefully acknowledge the many generous contributions made by others at both labs towards this database; Foremost Larry Landucci for compounds, patience, assignments and encouragment. William Landucci for software development, Martin Wesolowski and Kolby Hirth, NMR spectroscopists, and the frequent donation of compounds from Mike Mozuch, Noritsugu Terashima, Stéphane Quideau, Rich Helm, Fachuang Lu, Hoon Kim, Jamie Milhaupt and Susana Luque. The authors also acknowledge partial support of the National Research Initiative Competitive Grants Program/USDA (Wood Section), award #94-03465.

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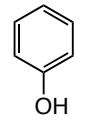

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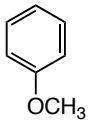

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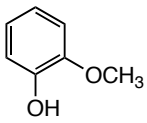

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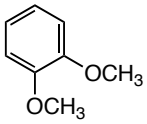

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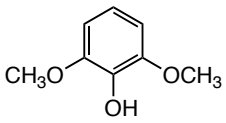

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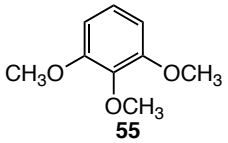

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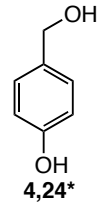

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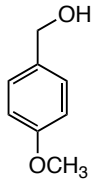

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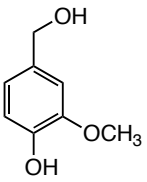

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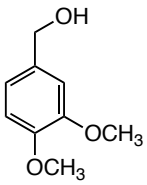

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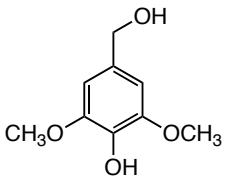

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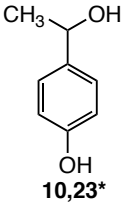

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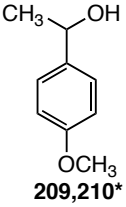

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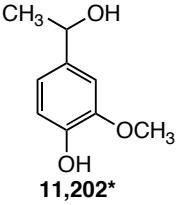

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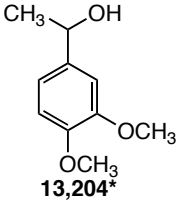

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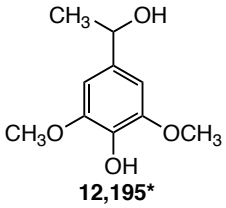

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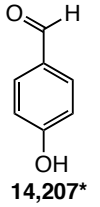

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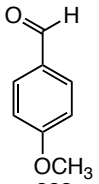

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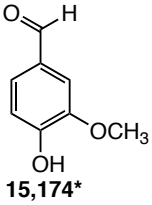

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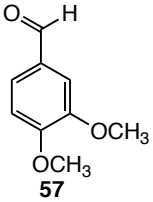

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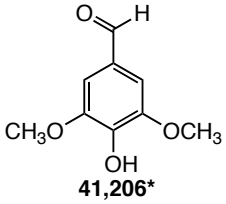

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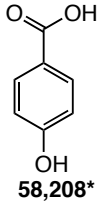

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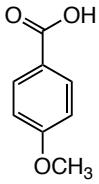

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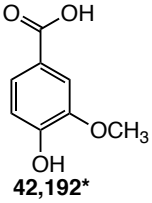

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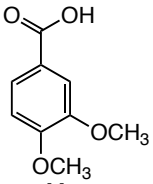

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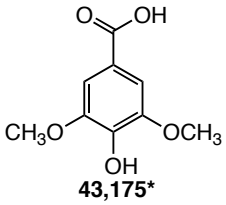

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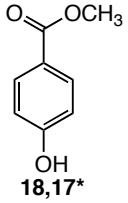

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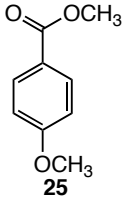

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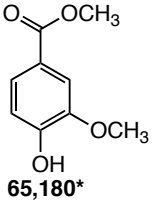

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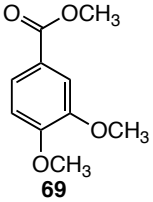

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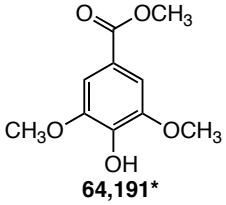

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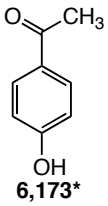

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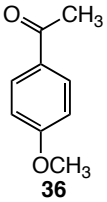

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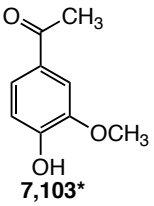

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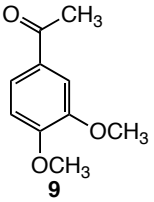

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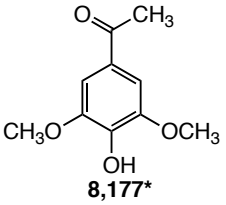

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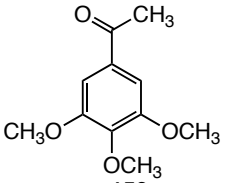

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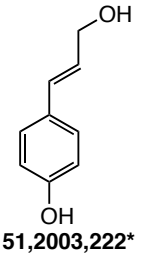
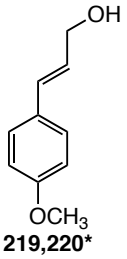
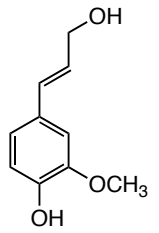
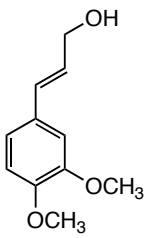
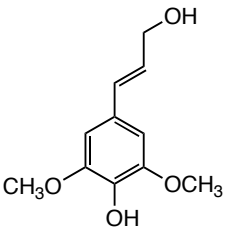
Monomers ctd

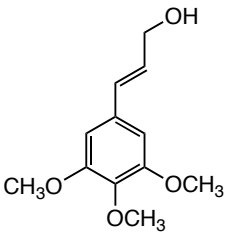

151,2003,222*

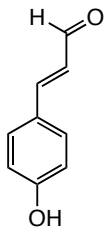

219,220*

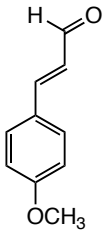

87,2001,142*, cis 231


145,159*


2002,211*


302


152,223*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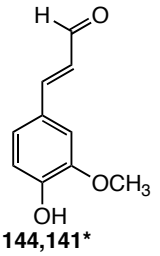
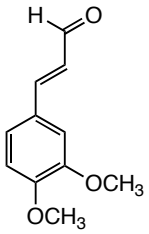
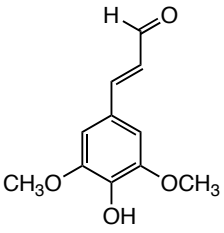
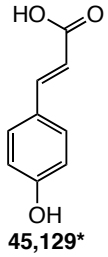
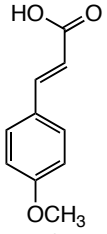
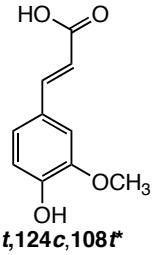

144,141*

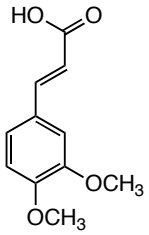

150

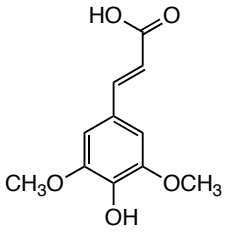

153,155*

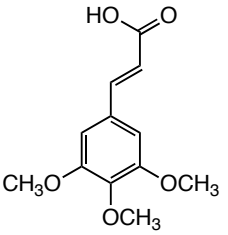

45,129*

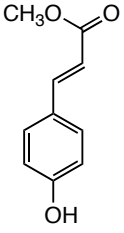

49

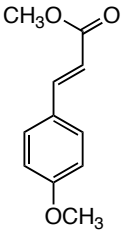

48*t*,124*c*,108*t*


47


46,178*


63


61,148*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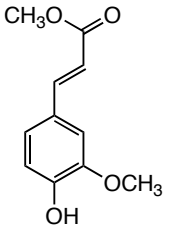
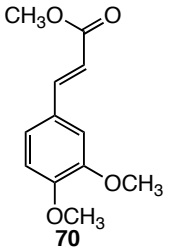

68,149*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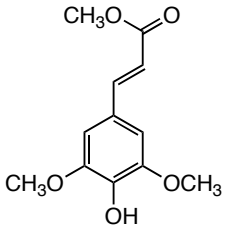
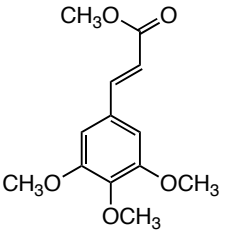
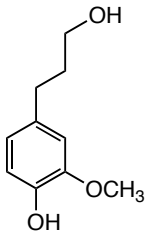
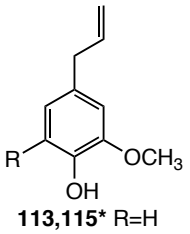
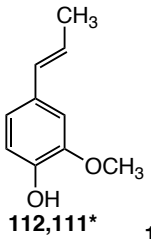

60,196*

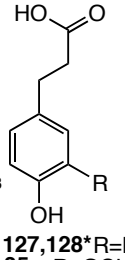

62

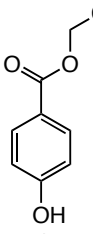
Misc. Monomers

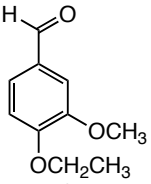

279, 280*

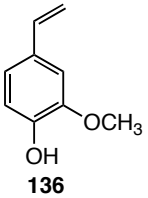

113,115* R=H
114,116* R=OCH$_3$

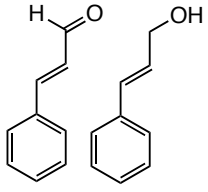

112,111*

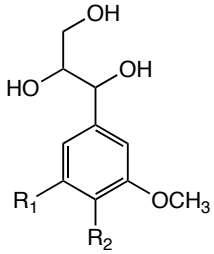

127,128* R=H
35 R=OCH$_3$

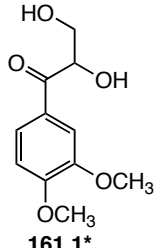

94

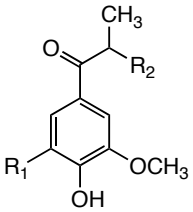

167

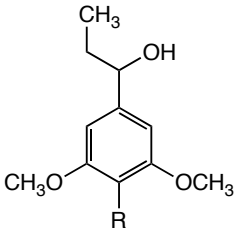

136

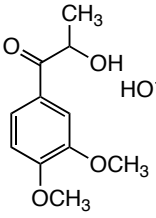

96 **95**

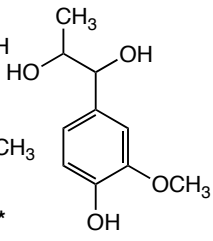

240* R_1=H R_2=OH
272*,285 R_1=OCH$_3$ R_2=OH
160 R_1=H, R_2=OCH$_3$

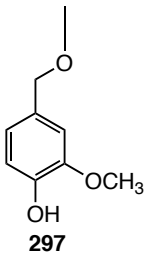

161,1*


130 R_1=OCH$_3$, R_2=OAc
264, 265* R_1=H, R_2=OH

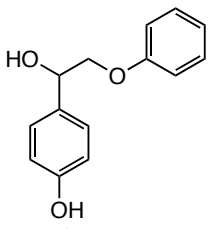

290, 294* R=OH
292, 296* R=OCH$_3$

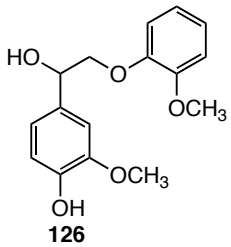

291, 295*

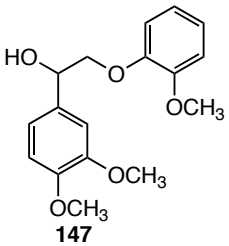

293

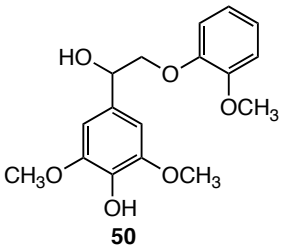

297

b-O-4 Dimers, 2-Carbon Sidechain


125


126


147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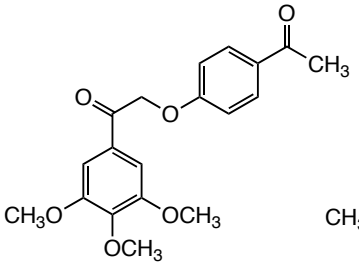
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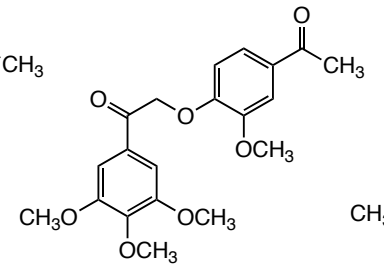
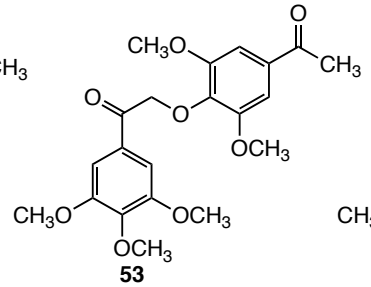

52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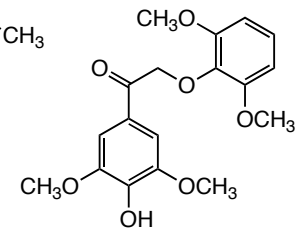
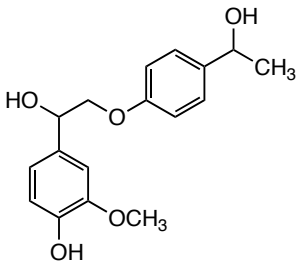
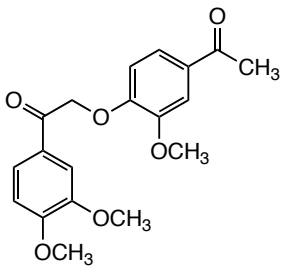

22,26*


132,138*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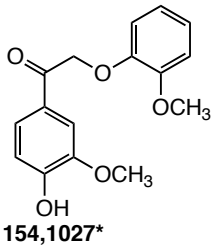
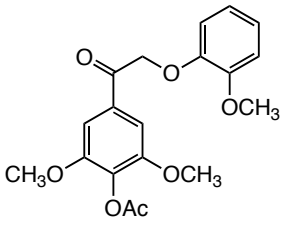
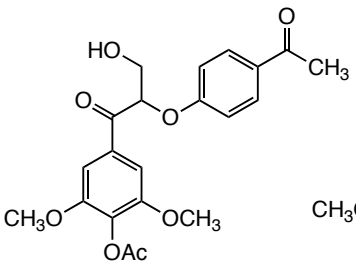
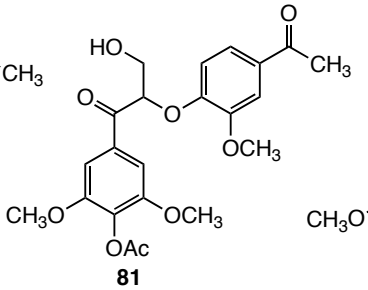
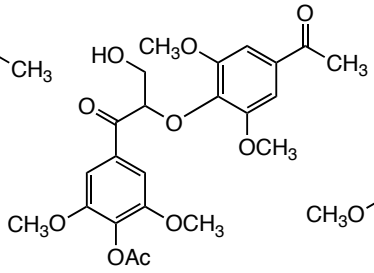

154,1027*

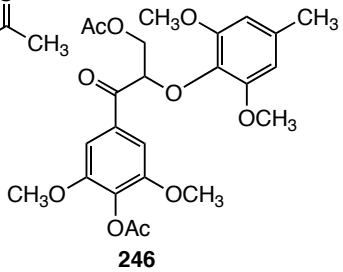

27

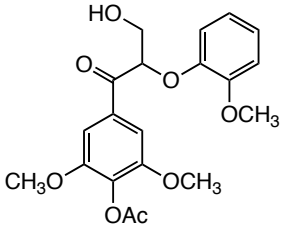
b-O-4 Dimers, 3-Carbon Sidechain, a-C=O

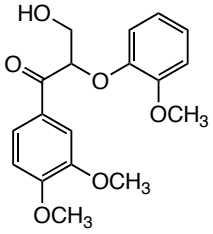

80

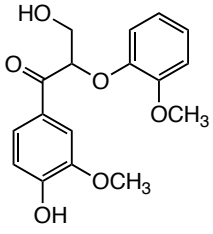

81

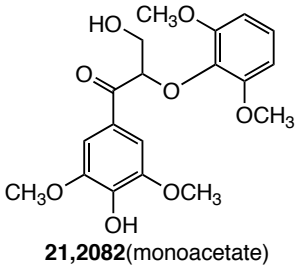

79


246

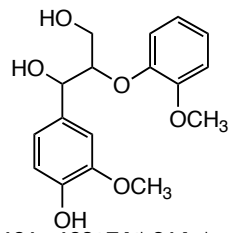

92,2067


110,163*

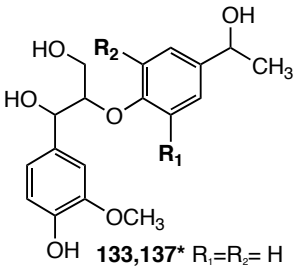

106,162*,1028(monoacetate)


21,2082(monoacetate)

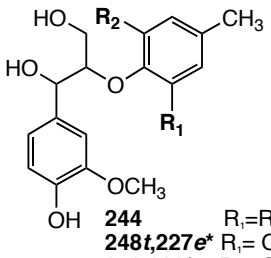
b-O-4 Dimers, 3-Carbon Sidechain



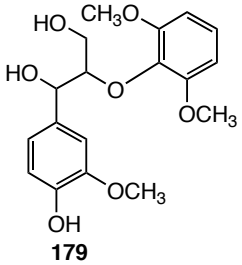
101*e*,102*t*,74*t,214*e**
(**1029t,1030e** a,g Ac'd)



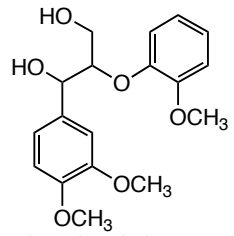
133,137* R_1=R_2= H
131,140* R_1= OCH_3, R_2= H
134,139* R_1= OCH_3, R_2= OCH_3



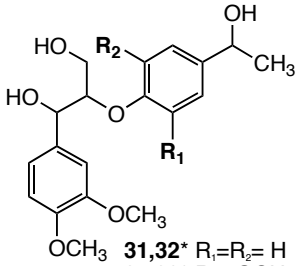
244 R_1=R_2= H
248*t*,227*e* R_1= OCH_3, R_2= H
242,232* R_1= OCH_3, R_2= OCH_3



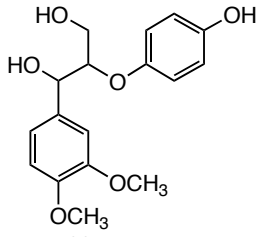
179



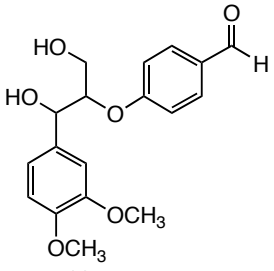
104*t*,105*e*,3*e*



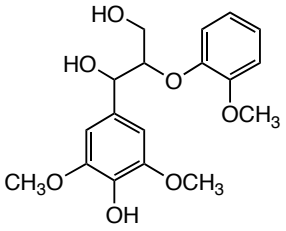
31,32* R_1=R_2= H
34,33* R_1= OCH_3, R_2= H
2,29* R_1= OCH_3, R_2= OCH_3



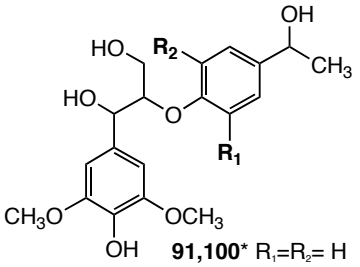
166



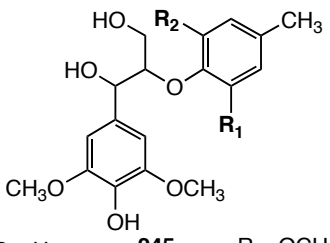
168



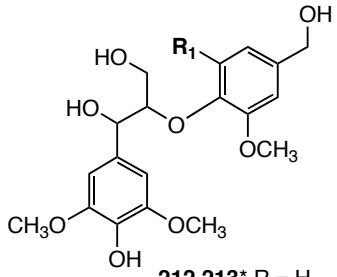
90,99*



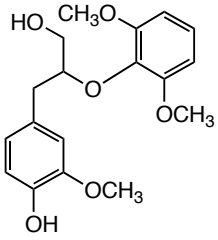
91,100* R_1=R_2= H
88,97* R_1= OCH_3, R_2= H
89,98* R_1= OCH_3, R_2= OCH_3



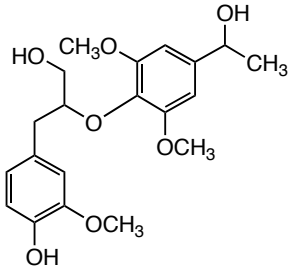
245 R_1= OCH_3, R_2= H
243,230* R_1= OCH_3, R_2= OCH_3



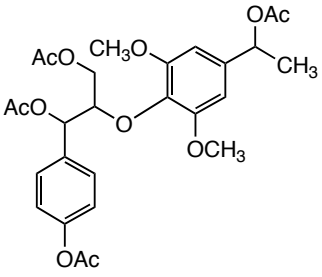
212,213* R_1= H
229* R_1= OCH_3



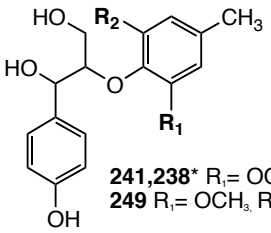
217,218*



135

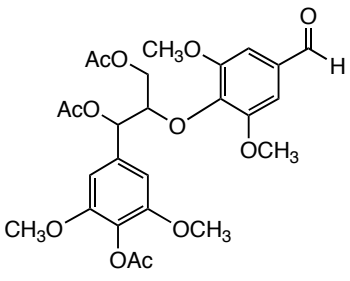


225

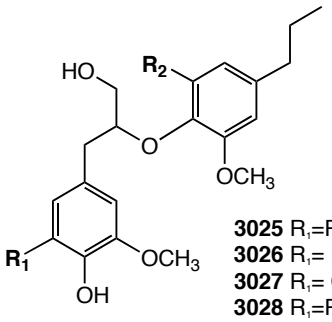


241,238* R_1= OCH_3 R_2=H
249 R_1= OCH_3, R_2=H

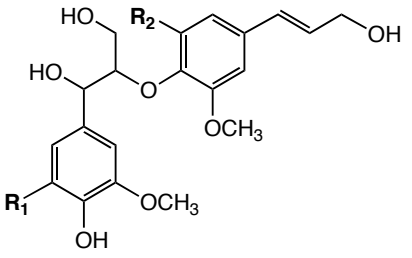
268*e*,269*t*,270*e,271*t**** R_1=R_2=H



228

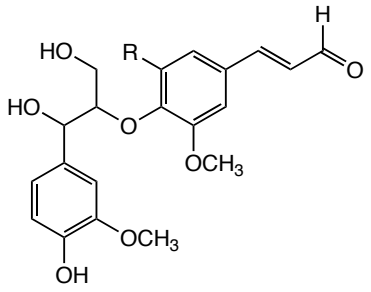


3025 R_1=R_2= H
3026 R_1= H, R_2= OCH_3
3027 R_1= OCH_3, R_2= H
3028 R_1=R_2= OCH_3

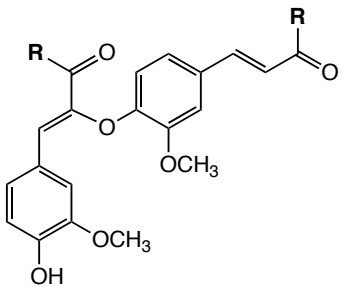


2013*t*,2014*e*,2012*e,2011*t**,3008*t**** R_1=R_2= H
3067,188* R_1= H, R_2= OCH_3
186* R_1= OCH_3, R_2= H
185* R_1=R_2= OCH_3

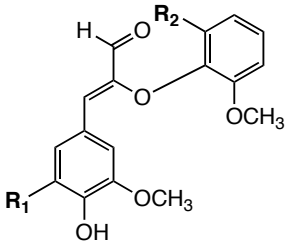
More b-O-4 Dimers, 3-Carbon Sidechain



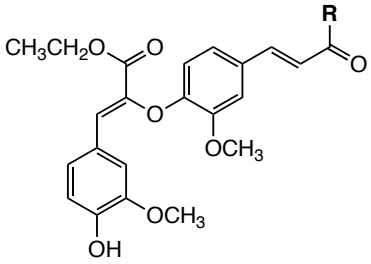
3010*t**, **3011*e**** R = H
3071 R = OCH_3 (with only g-Ac)



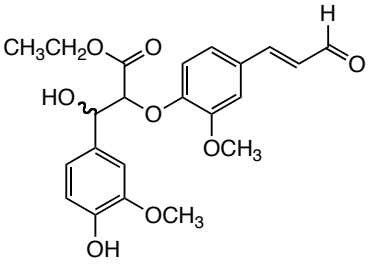
3031 R = H
2040 R = OH



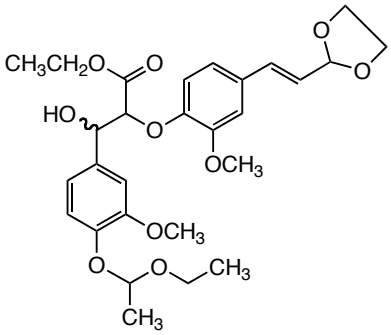
3034, **3035*** R_1,R_2 = H
3036, **3037*** R_1 = OCH_3, R_2 = H
3038, **3039*** R_1 = H, R_2 = OCH_3
3040, **3041*** R_1, R_2 = OCH_3



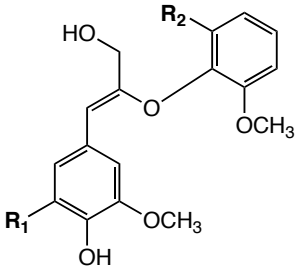
2041 R = OCH_3
2042 R = H



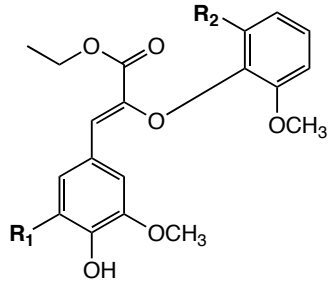
2043*e*,2044*t*



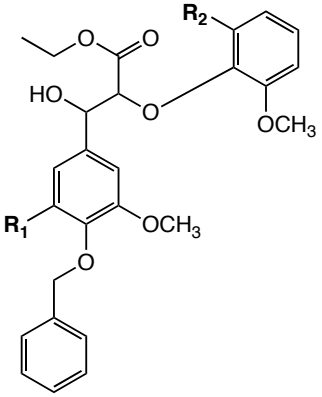
2045*e*,2046*t*



3053, R1 = H, R2 = OCH3
3057, R1 = OCH3, R2 = H

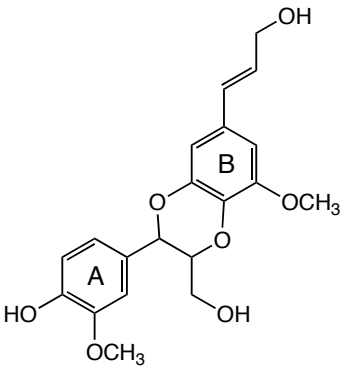


3052, R_1=H, R_2=OCH_3
3056, R_1=OCH_3, R_2=H

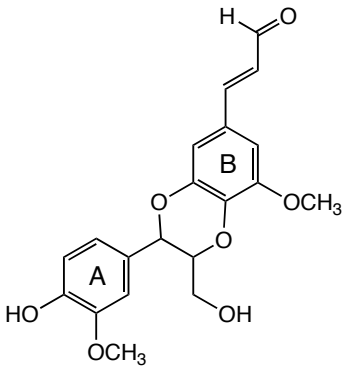


3050, 3051 isomers R_1=H, R_2=OCH_3
3054, 3055 isomers R_1=OCH_3, R_2=H

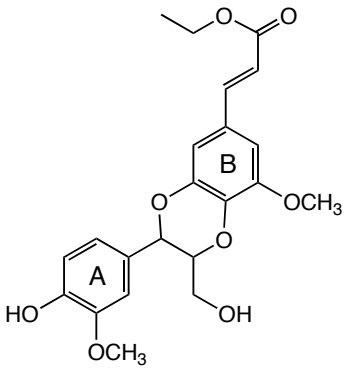
5-Hyroxyconiferyl alcohol b-O-4 Dimers, 3-Carbon Sidechain



3068



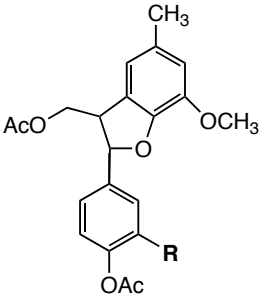
3069



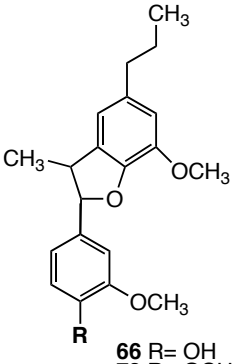
3070

X

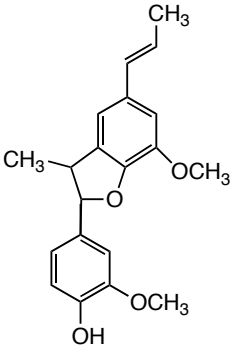
b-5 Dimers



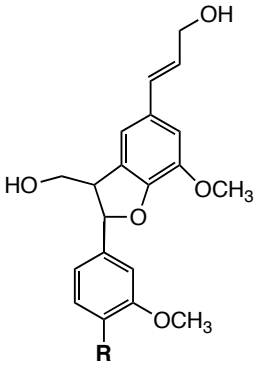
239 R= H
234 R= OCH_3



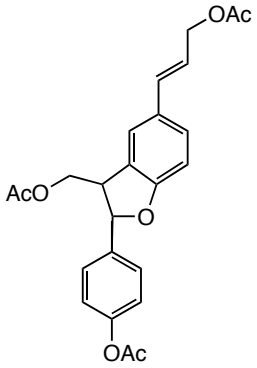
66 R= OH
73 R= OCH_3



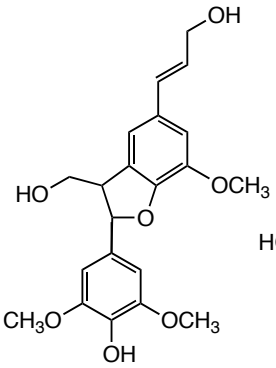
67



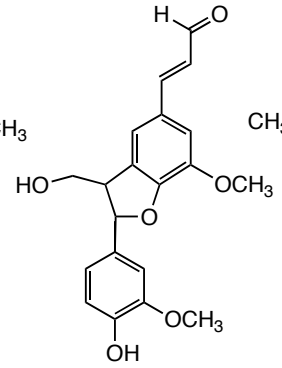
2004,2005* R= OH
2051,221* R= OCH_3



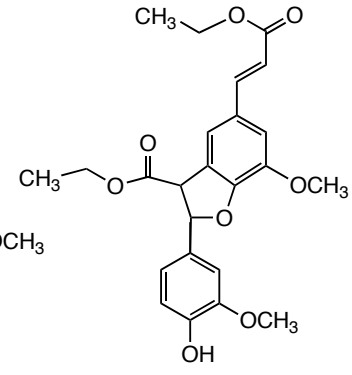
267



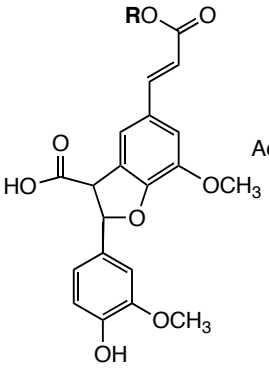
3063,187*



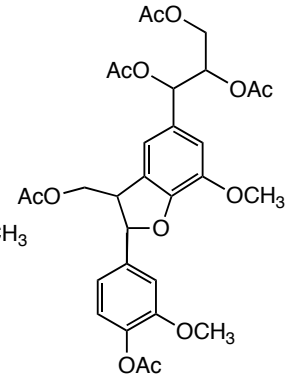
2021



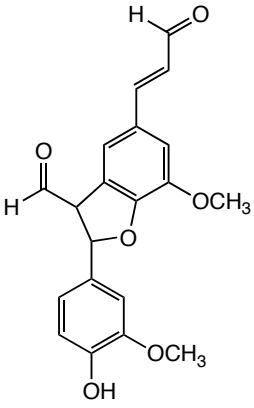
2006



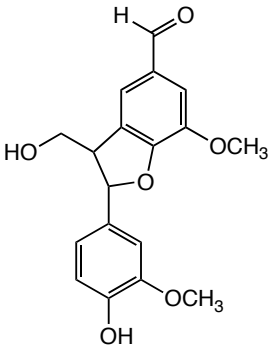
2018 R= H
2052 R= Et



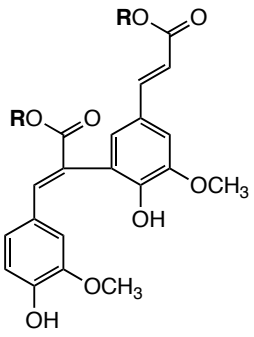
262



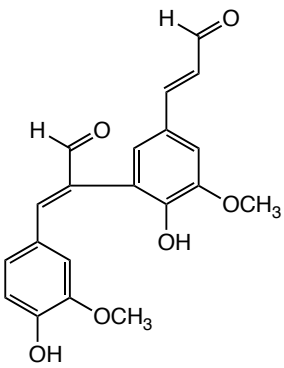
3059



3061

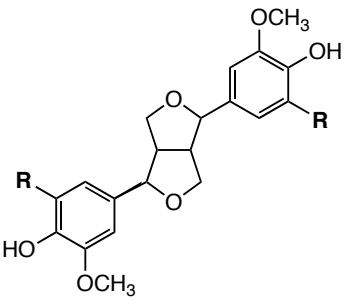


2054 R= H
2019 R= Et

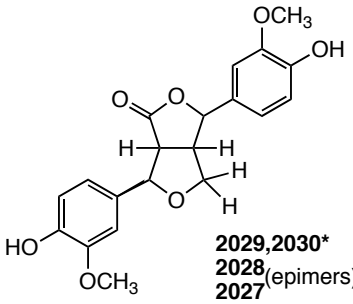


3030

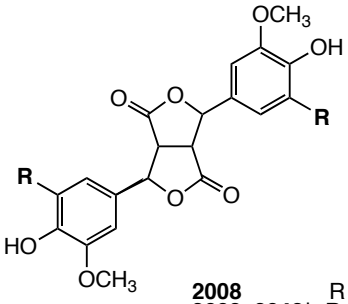
b-b Dimers



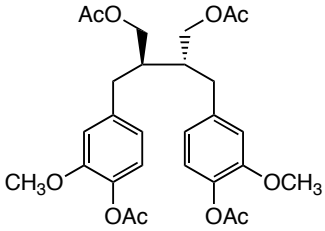
2020,109* R = H
117,123* R = OCH_3



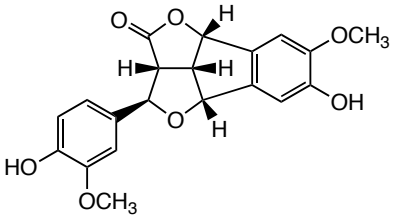
2029,2030*
2028(epimers)
2027



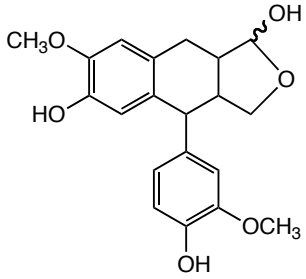
2008 R = H
3002, 3042* R = OCH_3



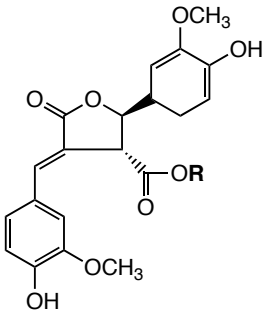
2070



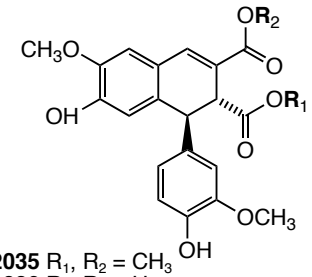
2026



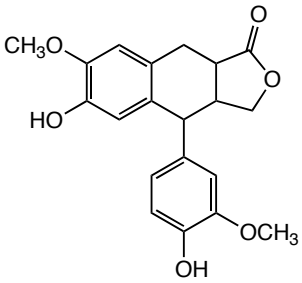
3014, 3015 isomers



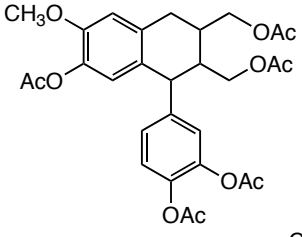
2033 R = H
2034 R = OCH_3



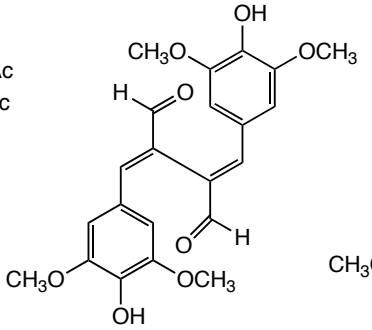
2035 R_1, R_2 = CH_3
2036 R_1, R_2 = H
2062 R_1 = CH_3, R_2 = H



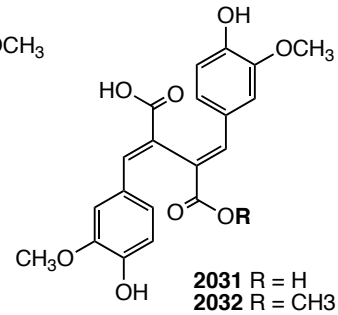
3017, 3016*



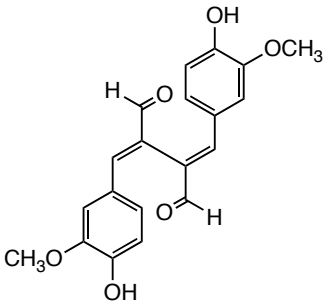
2069,3018



3060

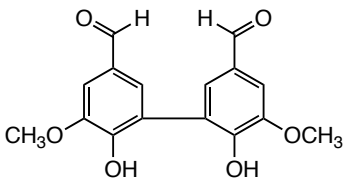


2031 R = H
2032 R = CH3

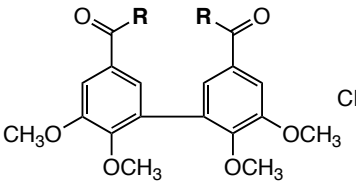


3032

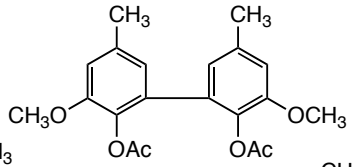
5-5 Dimers



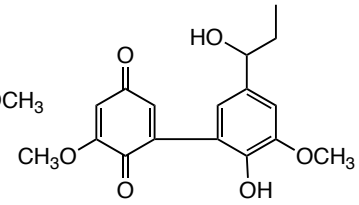
28



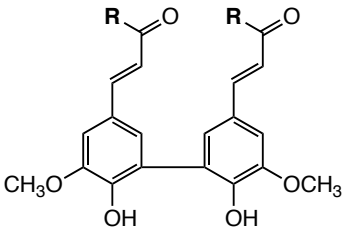
71 R = H
72 R = OH



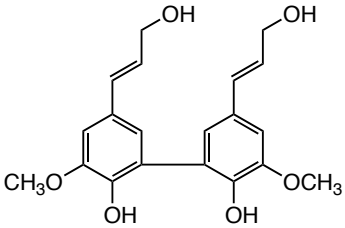
247



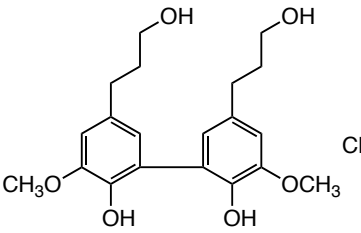
275, 276*



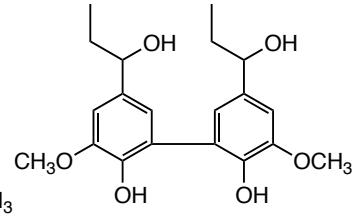
3033 R = H
2056 R = OH
2057 R = OCH_2CH_3



2058

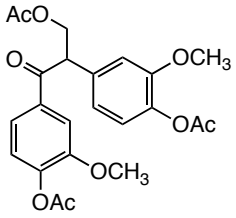


259, 260*

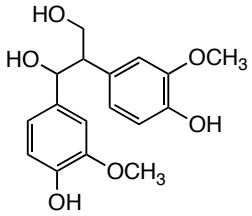


281, 282*

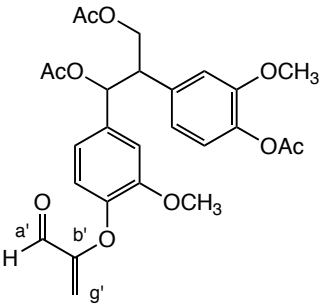
b-1 Dimers



233

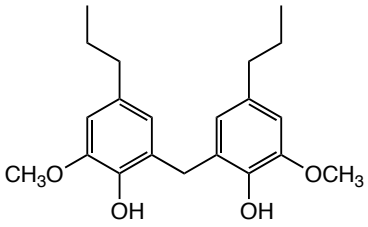


171, 3004*e*
172*, **3005*f****, **3006*e****



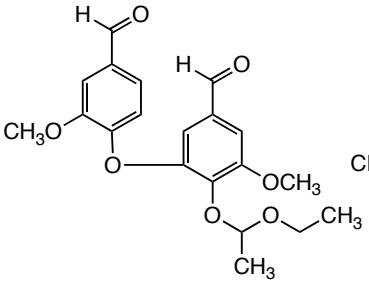
3007*e*

Biphenyl methane Dimer

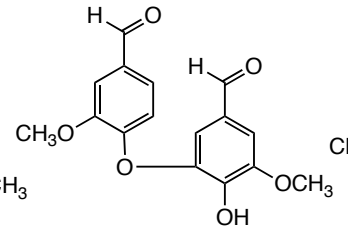


283

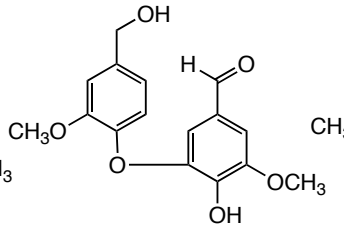
5-O-4 Dimers



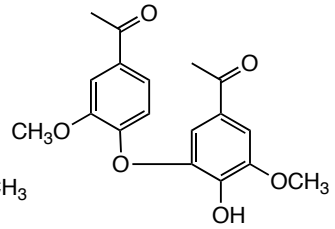
2037



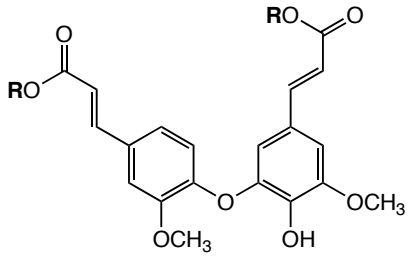
2038



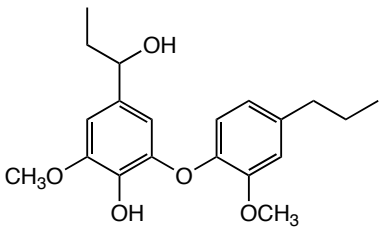
2039



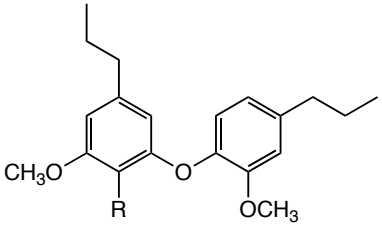
300



3003 R = H
3001 R = CH_2CH_3

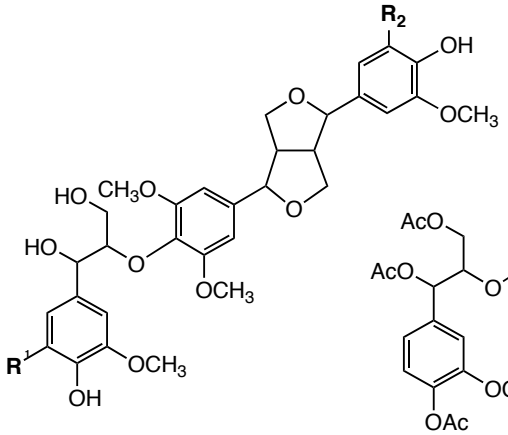


273, 274*

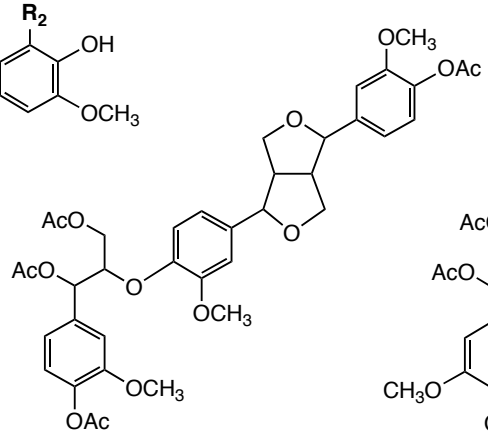


286 R=OCH_3

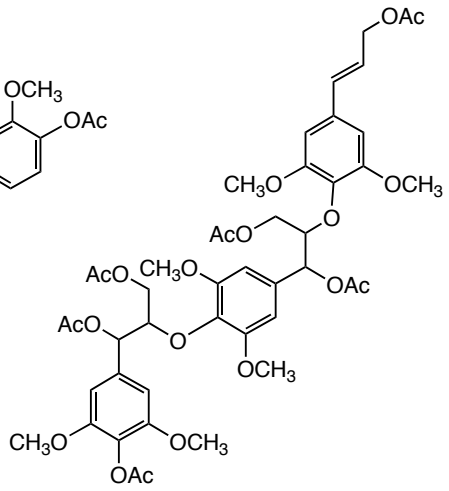
Trimers



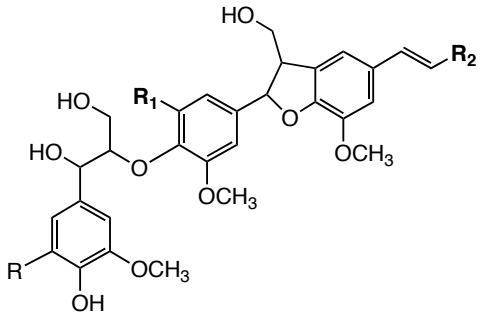
183,184* R_1 = H, R_2= OCH_3 **, G-b-S-r-S**
198,199* R_1R_2 = OCH_3 **, S-b-S-r-S**
3064 R_1R_2 = H, **G-b-S-r-G**



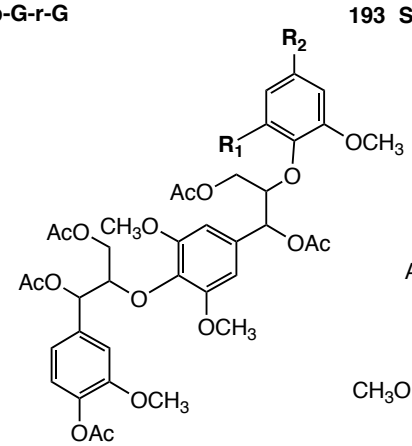
263 G-b-G-r-G



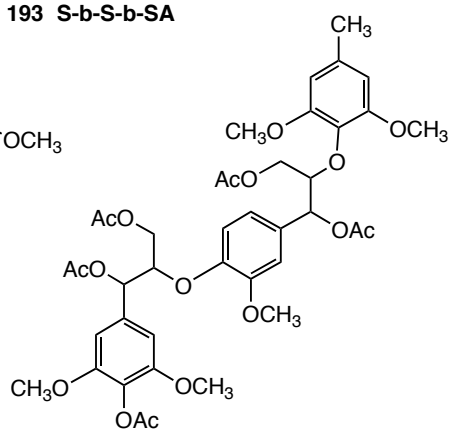
193 S-b-S-b-SA



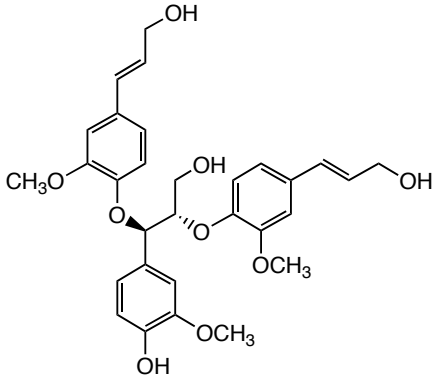
181,182* R = H, R_1 = OCH_3, R_2= CH_2OH **G-b-S-c-CA**
216* R = H, R_1 = H, R_2= CH_2OH **G-b-G-c-CA**
3065 R = H, R_1 = OCH_3, R_2=CHO **G-b-G-c-CAld**
3072 R = OCH_3, R_1 = H, R_2= CH_2OH **S-b-G-c-CA**



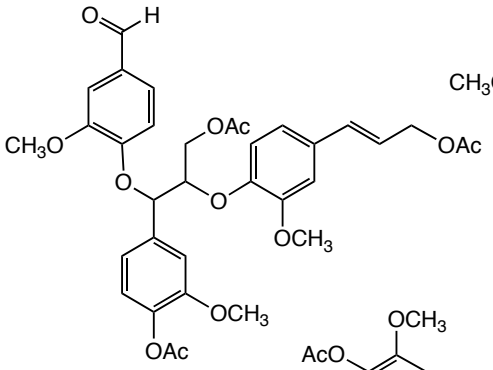
226 R_1 = R_2 = H **G-b-S-b-G**
250 R_1 = OCH_3 R_2 = CH_3 **G-b-S-b-S**



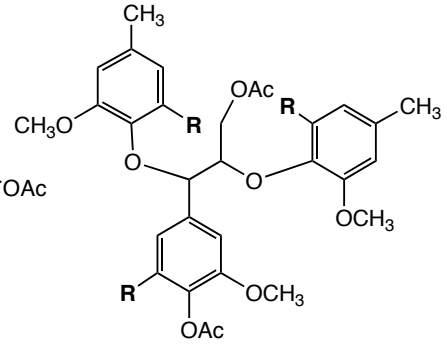
261 S-b-G-S



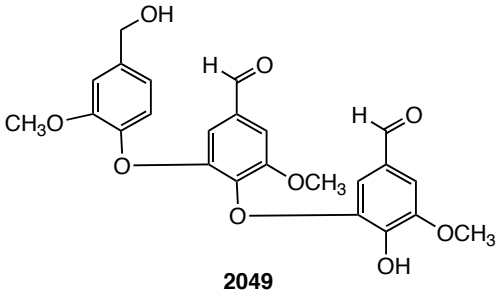
2015e,2022e* **CA-a-G-b-CA**



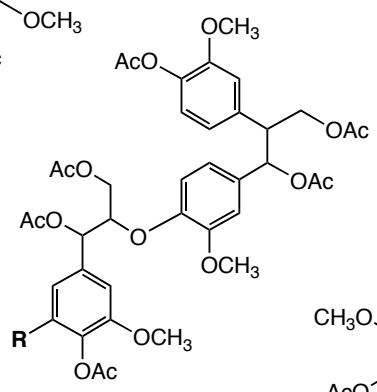
258



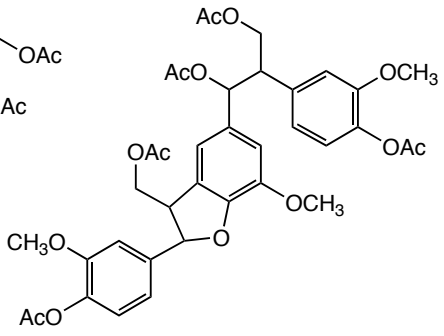
237 R = H G-a-G-b-G
266 R = OCH3 S-a-S-b-S



2049

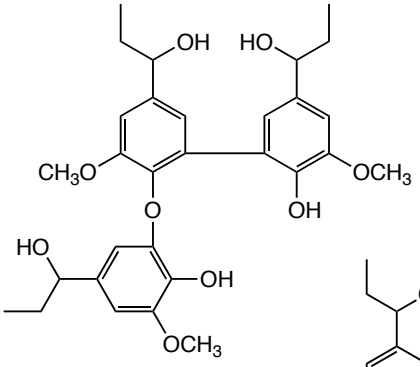


236, 3013 R = H **G-b-G-b1-G**
235 R = OCH_3 **S-b-G-b1-G**

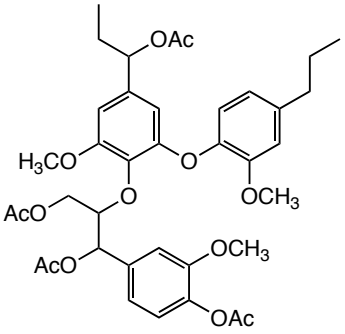


3012

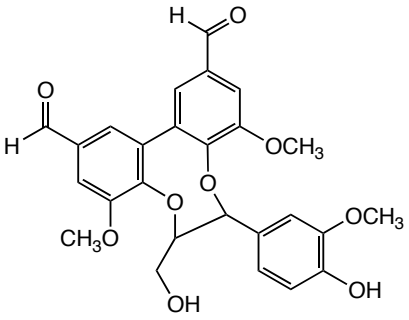
Trimers Cont'd



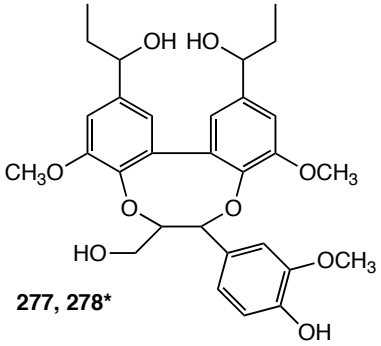
284, 289*



299

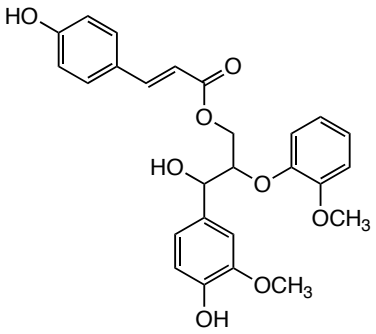


3062



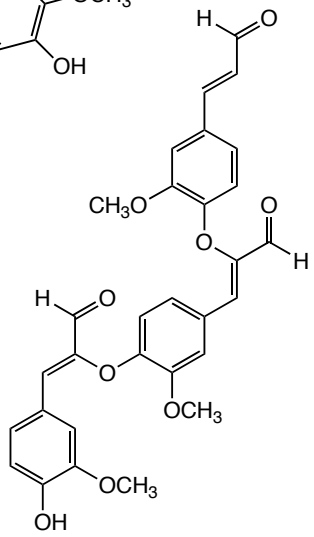
277, 278*

Trimers Containing Ferulic or Coumaric Acid

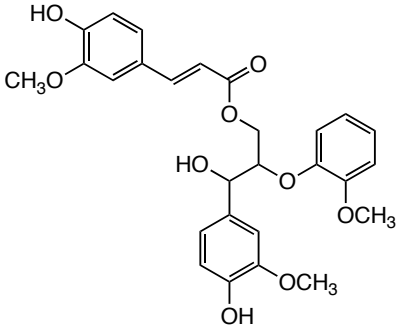


1015*t*,1016*e*,1019*t* *,1020*e* *,82*t* *,83*e* *

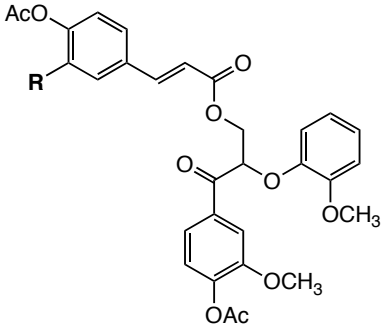
1011*t*,1012*e* (diacetates, phenolic)



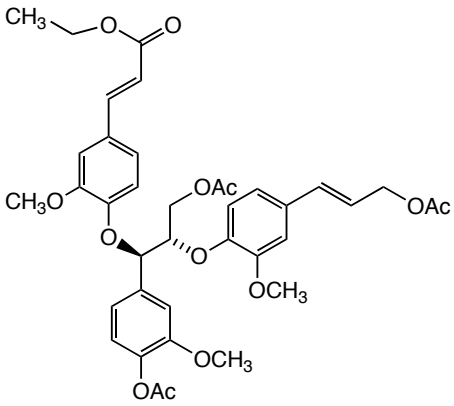
3058



1017*t*,1018*e*,1021*t* *,1022*e* *,76*e,75*t* ***
1013*t*,1014*e* (diacetates, phenolic)

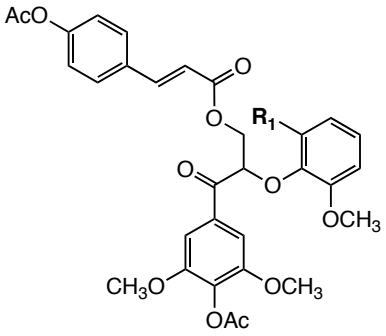


1009 R = H
1010 R = OCH_3

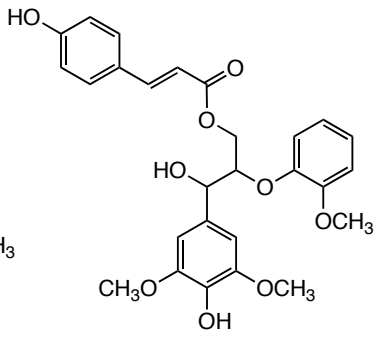


2016

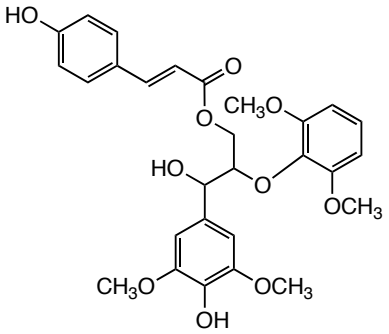
More Trimers Containing Ferulic, Coumaric or *p*-OH-Benzoic Acid



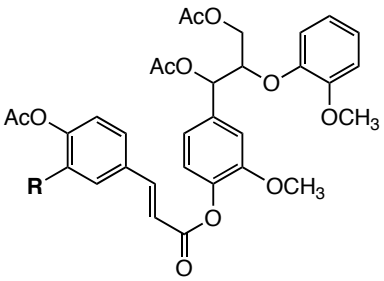
2066 R = H
2081 R = OCH_3



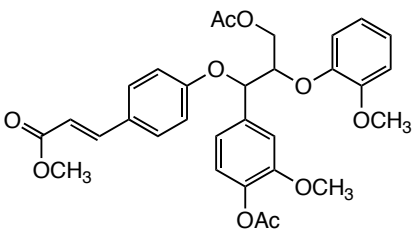
2076*t*, 2078*e*
2075*t,2077*e***
2068*e*, (diacetate, phenolic)



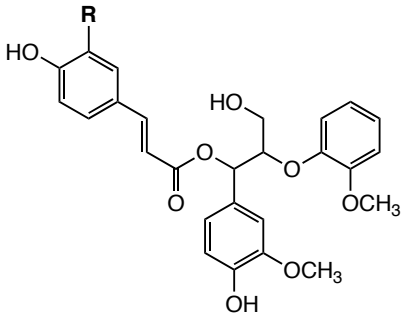
2071*t*, **2072*e***, **2073*t****, **2074*e****
2079*t*, 2080*e* (diacetate, phenolics)



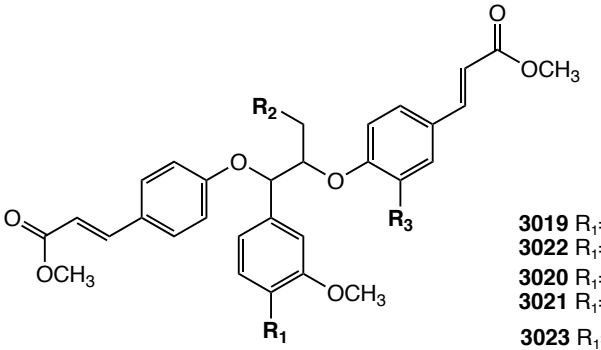
1023*t*,1024*e* R = H
1025*t*,1026*e*,84*e* R = OCH_3



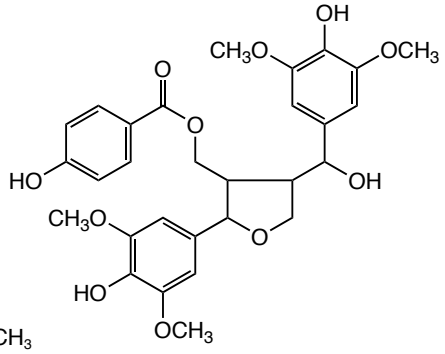
85, 86



1001*t*,1002*e*,1005*t* *,1006*e* *,78*t* *,77*e* * R = H
1003*t*,1004*e*,1007*t* *,1008*e* * R = OCH_3

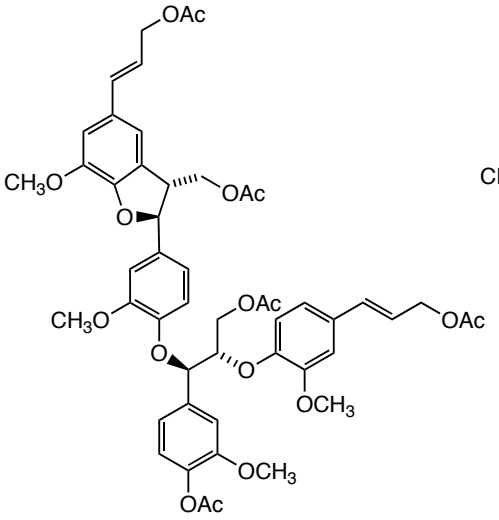


3019 R_1=R_2= OH, R_3= H
3022 R_1=R_2= OH, R_3= OCH_3
3020 R_1= OCH_3, R_2= OH, R_3= H
3021 R_1= OCH_3, R_2= OAc, R_3= H
3023 R_1= OCH_3, R_2= OH, R_3= OCH_3
3024 R_1= OCH_3, R_2= OAc, R_3= OCH_3

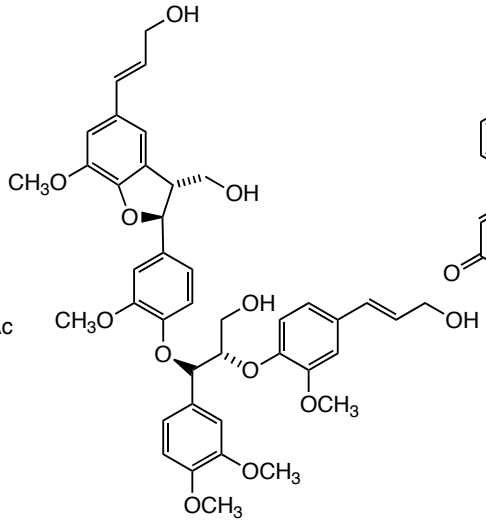


3066

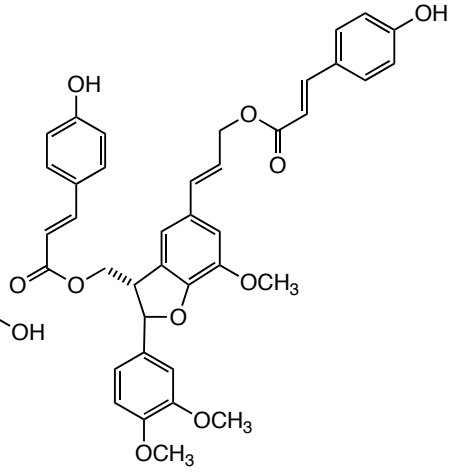
Tetramers



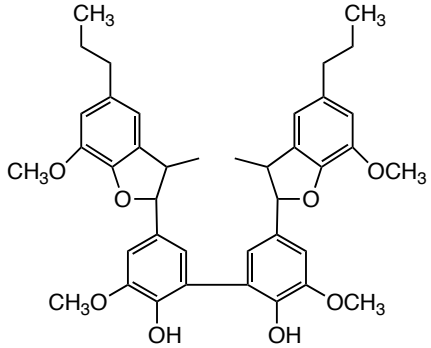
2023*e*



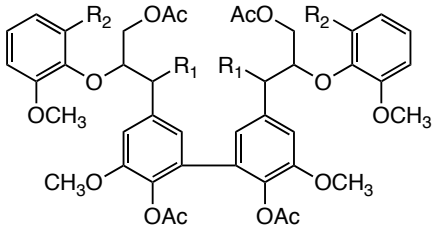
2017*e*,2024*t**



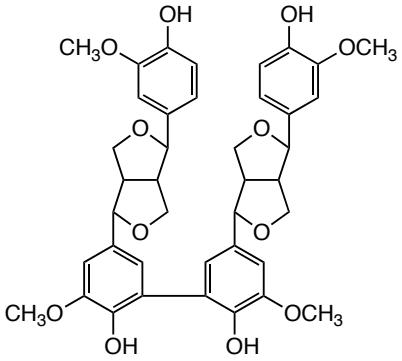
2060,2061*



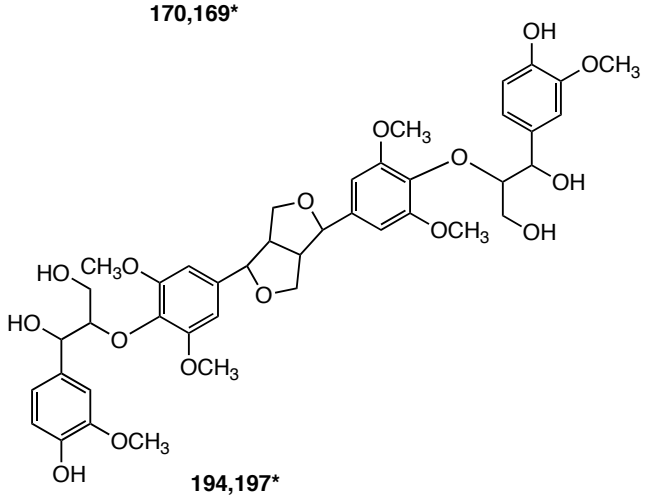
170,169*



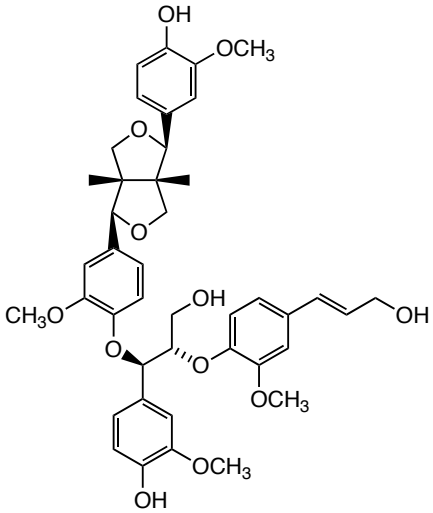
224 R_1 = H, R_2 = OCH_3
3009 R_1 = OAc, R_2 = H



164,165*

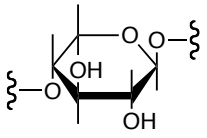


194,197*

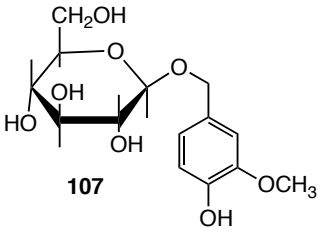


2025*e* ,2059*

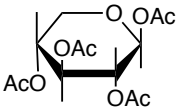
Misc. Compounds



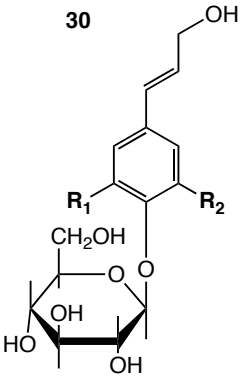
30



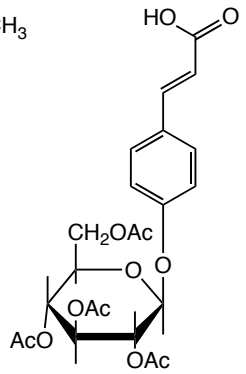
107



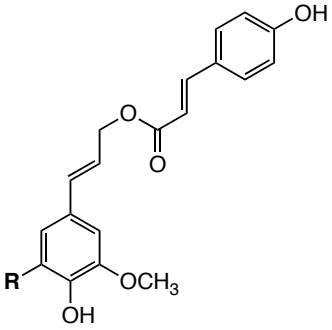
122, *a* &*b*



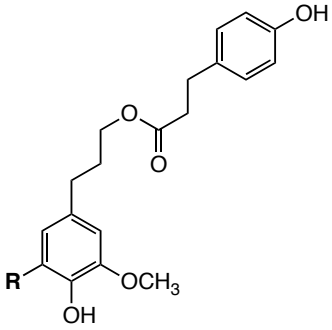
157 R_1, R_2 = H
118,120* R_1 = H, R_2 = OCH_3
119,121* R_1, R_2 = OCH_3



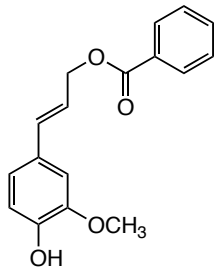
158*



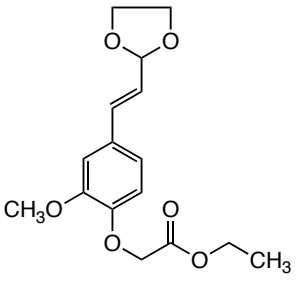
2009 R = H
2065 R = OCH_3



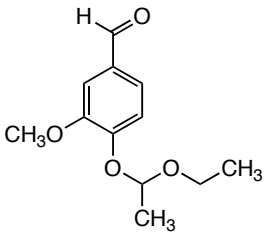
2063 R = H
2064 R = OCH_3



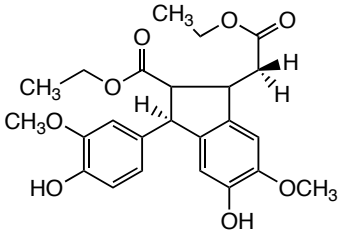
2010



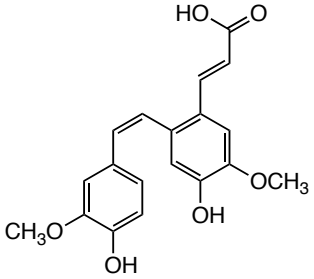
2047



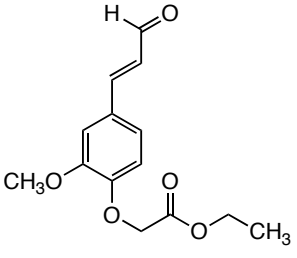
2048



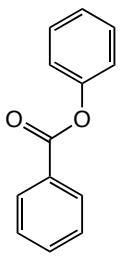
2050



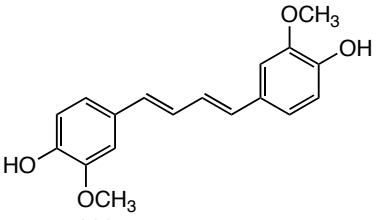
2053



2055

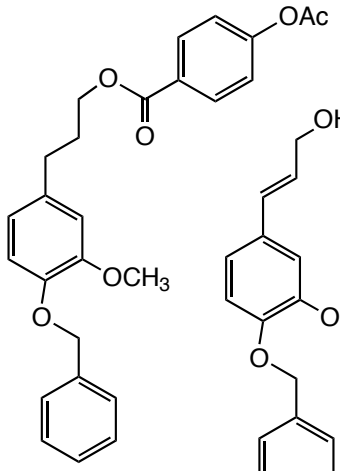


93



2007

Misc. Compounds



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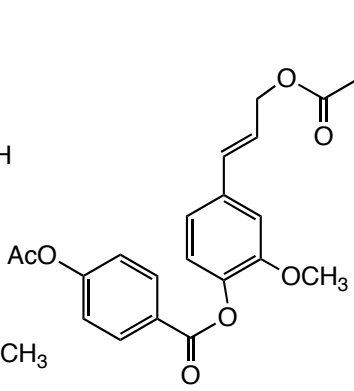
252



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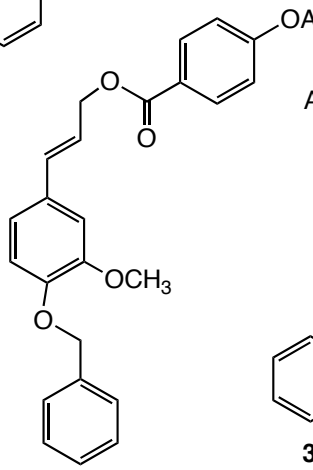

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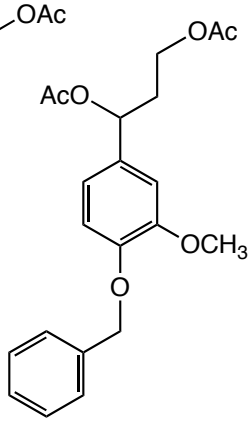

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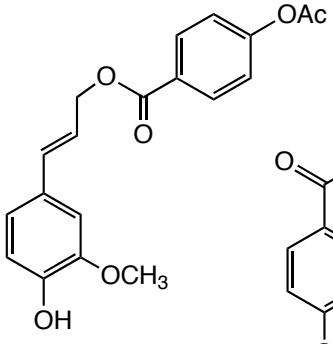

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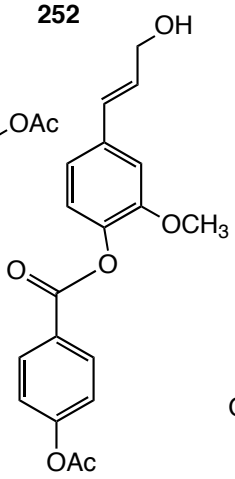

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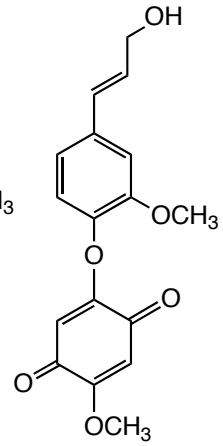

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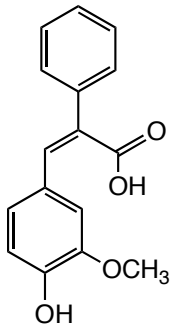

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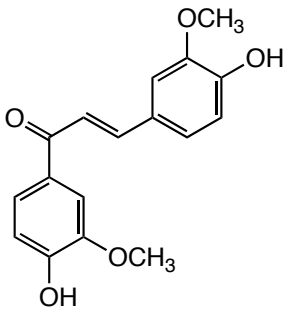

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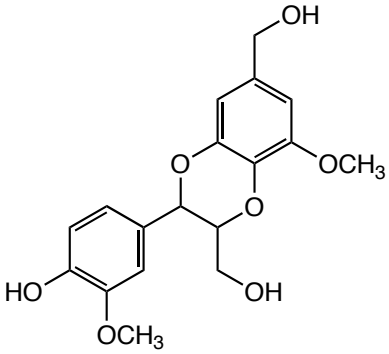

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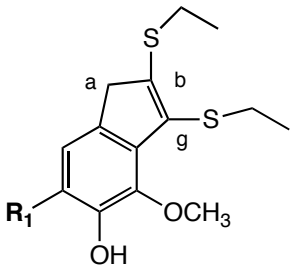
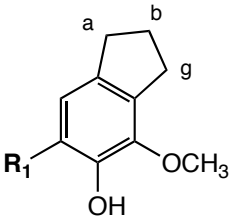
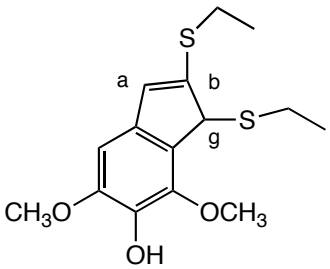


3046 R_1 = OCH$_3$
3049 R_1 = H

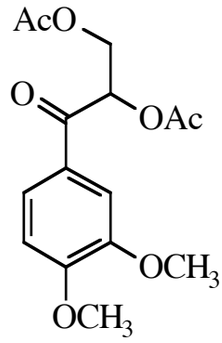


3045 R_1 = OCH$_3$
3048 R_1 = H



3047

Compound Number 1



2,3-Diacetoxypropioveratrone

2,3-diacetoxy-3',4'-dimethoxypropiophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.08		
Ac Me	2.19		
OMe	3.95		
OMe	3.95		
γ1	4.25	dd	12.1, 7.9
γ2	4.68	dd	12.1, 3.1
β	6.18	dd	7.9, 3.1
A2	7.56	d	8.4
A5	6.93	dd	2.0
A6	7.71	dd	8.4, 2.0

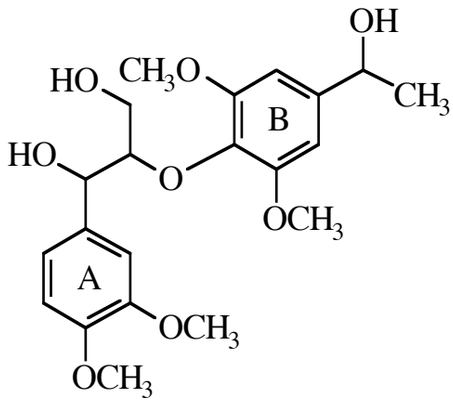
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.67	74	20.49	72	20.30	88
Ac Me	20.72	71	20.58	64	20.42	87
OMe	56.05	98	56.11	98	55.51	95
OMe	56.15	97	56.25	100	55.77	100
γ	63.22	84	63.64	96	62.60	71
β	72.99	98	74.14	96	73.28	85
2	110.32	100	111.60	91	110.35	78
5	110.64	91	111.66	92	111.03	84
6	123.33	98	123.85	98	123.02	88
1	127.41	55	128.35	38	126.67	77
3	149.31	41	150.31	30	148.72	71
4	154.16	40	155.21	30	153.72	63
Ac C=O	170.21	48	170.35	32	169.61	67
Ac C=O	170.75	36	170.88	32	170.03	56
α	191.52	48	192.03	36	191.18	66

Notes:

M. Mozuch #36/46/Ac
21 mg

Compound Number 2



threo

1-(3,4-Dimethoxyphenyl)-2-[4-(1-hydroxyethyl)-2,6-dimethoxy phenoxy]propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.45	d	6.4
OMe	3.85	s	
OMe	3.85	s	
OMe	3.87	s	
OMe	3.89	s	
B α	4.81	q	6.4
α	5.02	d	8.7
B2,6	6.63	s	
A2	6.9	m	
A5	6.83	d	8.7
A6	6.9	m	

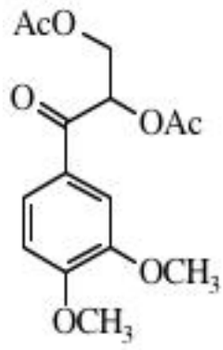
Notes:

S. Ralph III-12
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.45	34	26.23	49	25.86	44
OMe	55.87	100	55.97	58	55.31	52
OMe	55.87	100	56.03	51	55.43	53
B OMe	56.08	99	56.44	100	55.80	100
B OMe	56.08	99	56.44	100	55.80	100
γ	60.48	29	61.26	38	60.13	25
B α	70.11	43	69.93	51	68.17	43
α	73.98	39	73.89	45	71.36	32
β	88.94	37	89.58	47	87.10	31
B2	102.25	67	103.30	84	102.50	55
B6	102.25	67	103.30	84	102.50	55
A2	110.28	36	111.78	38	110.60	32
A5	111.02	41	112.18	47	111.08	32
A6	119.80	34	120.22	42	118.84	34
A1	132.56	38	134.74	32	134.53	63
B1	134.08	24	135.39	18	134.53	63
B4	143.04	30	144.54	29	143.01	37
A4	148.73	29	149.58	22	147.64	31
A3	148.90	29	149.86	25	148.03	34
B3	152.84	61	153.52	48	152.20	65
B5	152.84	61	153.52	48	152.20	65

Compound Number 1



2,3-Diacetoxypropioveratrone

2,3-diacetoxy-3',4'-dimethoxypropiophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.08		
Ac Me	2.19		
OMe	3.95		
OMe	3.95		
γ1	4.25	dd	12.1, 7.9
γ2	4.68	dd	12.1, 3.1
β	6.18	dd	7.9, 3.1
A2	7.56	d	8.4
A5	6.93	dd	2.0
A6	7.71	dd	8.4, 2.0

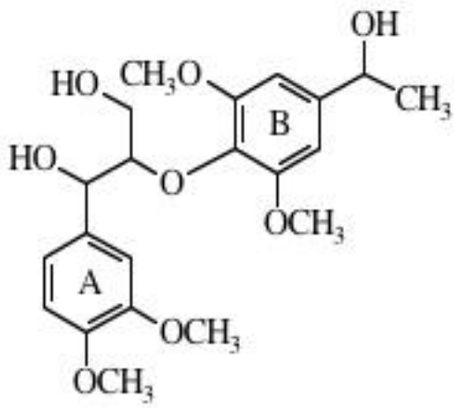
Notes:

M. Mozuch #36/46/Ac
21 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.67	74	20.49	72	20.30	88
Ac Me	20.72	71	20.58	64	20.42	87
OMe	56.05	98	56.11	98	55.51	95
OMe	56.15	97	56.25	100	55.77	100
γ	63.22	84	63.64	96	62.60	71
β	72.99	98	74.14	96	73.28	85
2	110.32	100	111.60	91	110.35	78
5	110.64	91	111.66	92	111.03	84
6	123.33	98	123.85	98	123.02	88
1	127.41	55	128.35	38	126.67	77
3	149.31	41	150.31	30	148.72	71
4	154.16	40	155.21	30	153.72	63
Ac C=O	170.21	48	170.35	32	169.61	67
Ac C=O	170.75	36	170.88	32	170.03	56
α	191.52	48	192.03	36	191.18	66

Compound Number 2



threo

1-(3,4-Dimethoxyphenyl)-2-[4-(1-hydroxyethyl)-2,6-dimethoxy phenoxy]propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.45	d	6.4
OMe	3.85	s	
OMe	3.85	s	
OMe	3.87	s	
OMe	3.89	s	
B α	4.81	q	6.4
α	5.02	d	8.7
B2,6	6.63	s	
A2	6.9	m	
A5	6.83	d	8.7
A6	6.9	m	

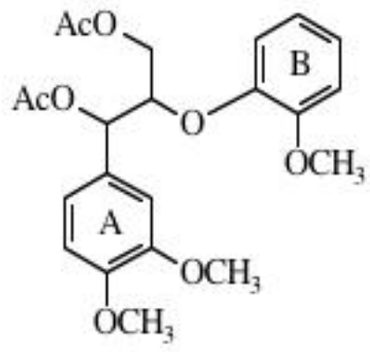
Notes:

S. Ralph III-12
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.45	34	26.23	49	25.86	44
OMe	55.87	100	55.97	58	55.31	52
OMe	55.87	100	56.03	51	55.43	53
B OMe	56.08	99	56.44	100	55.80	100
B OMe	56.08	99	56.44	100	55.80	100
γ	60.48	29	61.26	38	60.13	25
B α	70.11	43	69.93	51	68.17	43
α	73.98	39	73.89	45	71.36	32
β	88.94	37	89.58	47	87.10	31
B2	102.25	67	103.30	84	102.50	55
B6	102.25	67	103.30	84	102.50	55
A2	110.28	36	111.78	38	110.60	32
A5	111.02	41	112.18	47	111.08	32
A6	119.80	34	120.22	42	118.84	34
A1	132.56	38	134.74	32	134.53	63
B1	134.08	24	135.39	18	134.53	63
B4	143.04	30	144.54	29	143.01	37
A4	148.73	29	149.58	22	147.64	31
A3	148.90	29	149.86	25	148.03	34
B3	152.84	61	153.52	48	152.20	65
B5	152.84	61	153.52	48	152.20	65

Compound Number 3



erythro

Veratrylglycerol-β-guaiacyl ether diacetate

1,3-diacetoxy-1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy) propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.03	s	
Ac Me	2.07	s	
OMe	3.79	s	
OMe	3.83	s	
OMe	3.86	s	
γ1	4.23	dd	11.0, 4.0
γ2	4.43	dd	11.9, 5.9
α	6.03	d	5.3
β	4.71	m	

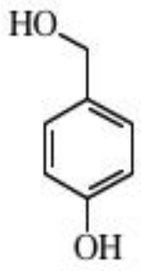
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.78	34	20.61	38	20.41	22
Ac Me	21.05	38	20.89	40	20.65	27
OMe	55.78	55	56.02	63	55.38	100
OMe	55.88	100	56.08	57	55.38	100
OMe	55.88	100	56.15	54	55.54	64
γ	62.82	38	63.23	44	62.10	33
α	74.12	42	74.77	49	73.35	17
β	80.10	45	80.28	48	78.39	41
A2	110.86	51	112.24	100	110.87	20
A5	110.89	45	112.24	100	111.27	39
B2	112.55	44	113.68	57	112.80	39
B5	119.18	46	119.51	52	117.70	36
A6	120.08	44	120.79	54	119.63	38
B6	120.93	48	121.56	57	120.62	62
B1	123.41	46	123.82	64	122.70	41
A1	128.98	30	130.15	31	128.71	58
B4	147.32	24	148.36	20	146.74	50
A4	148.84	26	150.10	23	148.43	52
A3	149.09	25	150.29	19	148.65	47
B3	151.04	22	151.93	20	150.27	56
Ac C=O	169.67	24	169.85	23	169.18	45
Ac C=O	170.75	21	170.71	20	170.00	45

Notes:

L. Landucci
51mg
threo data in acetone
γ 63.8 α 75.7 β 80.8

Compound Number 4



p-Hydroxybenzyl alcohol
4-hydroxybenzyl alcohol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α	4.62	s	
3,5	6.82	m	
2,6	7.22	m	

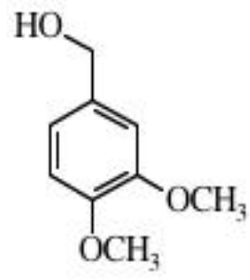
Notes:

J. Ralph: JR A91.11
50mg
Not very soluble in CDCL3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α			64.54	34	62.68	43
3			115.69	99	114.66	100
5			115.69	99	114.66	100
2			129.05	100	127.92	100
6			129.05	100	127.92	100
1			133.96	13	132.61	31
4			157.23	18	156.03	35

Compound Number 5



3,4-Dimethoxybenzyl alcohol

3,4-dimethoxybenzyl alcohol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.85	s	
OMe	3.85	s	
α	4.56	s	
2	6.82	m	
5	6.86	m	
6	6.86	m	

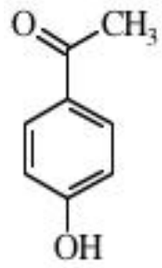
Notes:

J. Ralph: JR A91.14
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.78	100	55.93	100	55.27	100
OMe	55.90	84	56.11	97	55.47	94
α	65.04	79	64.58	70	62.79	88
2	110.45	86	111.69	82	110.51	74
5	111.04	96	112.54	88	111.48	73
6	119.33	95	119.62	78	118.50	81
1	133.66	38	135.95	21	135.03	58
4	148.43	25	149.32	16	147.60	36
3	149.00	27	150.19	18	148.54	41

Compound Number 6



p-Hydroxyacetophenone
4-hydroxyacetophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	2.60	s	
3,5	7.92	m	8.8
2,6	7.00	m	8.8

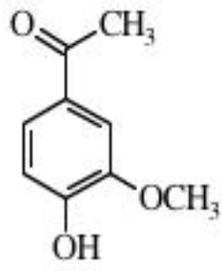
Notes:

J.Ralph: JR A95.11
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	26.28	51	26.25	39	26.16	39
3	115.66	100	115.89	98	115.11	100
5	115.66	100	115.89	98	115.11	100
1	129.16	17	130.38	11	128.56	23
2	131.35	97	131.48	100	130.64	91
6	131.35	97	131.48	100	130.64	91
4	161.90	19	162.54	20	161.98	35
α	199.32	12	196.40	93	195.89	21

Compound Number 7



Acetovanillone

4-hydroxy-3-methoxyacetophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	2.56	s	
OMe	3.91	s	
2	7.53	m	
5	6.95	d	8.7
6	7.53	m	

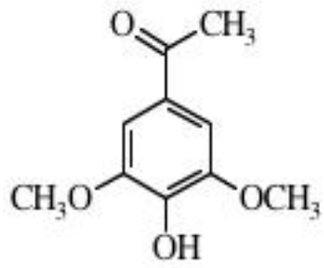
Notes:

J. Ralph: JR A95.12
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	26.16	82	26.22	74	26.14	77
OMe	56.01	81	56.17	91	55.52	92
2	109.89	62	111.40	65	111.04	76
5	113.97	85	115.26	85	114.85	100
6	124.06	100	124.22	100	123.34	98
1	130.02	20	130.65	22	128.84	59
3	146.77	29	148.16	23	147.45	61
4	150.66	34	152.12	28	151.65	82
α	197.14	23	196.30	19	195.98	57

Compound Number 8



Acetosyringone

3,5-dimethoxy-4-hydroxyacetophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	2.57	s	
OMe	3.94	s	
OMe	3.94	s	
2,6	7.24	s	

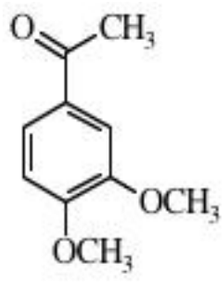
Notes:

J. Ralph: JR A95.13
46mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	26.21	44	26.30	41	26.22	45
OMe	56.45	100	56.63	100	56.02	100
OMe	56.45	100	56.63	100	56.02	100
2	105.81	90	106.97	84	106.13	84
6	105.81	90	106.97	84	106.13	84
1	128.21	22	129.13	16	127.33	29
4	139.89	21	141.75	16	140.86	29
3	146.79	41	148.29	34	147.44	65
5	146.79	41	148.29	34	147.44	65
α	196.64	16	196.31	14	196.06	30

Compound Number 9



Acetoveratrone

3,4-dimethoxyacetophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	2.56	s	
OMe	3.93	s	
OMe	3.94	s	
2	7.52	d	2.0
5	6.90	d	8.4
6	7.57	dd	8.4, 2.0

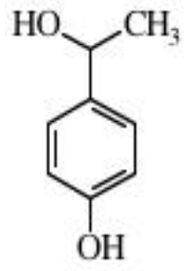
Notes:

J. Ralph: JR A95.14
55mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	26.17	63	26.25	72	26.23	78
OMe	55.95	92	55.96	91	55.43	100
OMe	56.04	100	56.10	100	55.68	90
2	109.99	86	111.17	56	110.17	91
5	110.09	70	111.30	77	110.74	87
6	123.27	95	123.73	94	123.04	98
1	130.48	30	131.24	17	129.88	55
3	148.99	26	150.00	17	148.55	41
4	153.30	27	154.38	17	153.06	43
α	196.70	23	196.34	17	196.22	33

Compound Number 10



1-(4-Hydroxyphenyl)ethanol

1-(4-hydroxyphenyl)ethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	1.48	d	6.5
α	4.85	q	6.5
3,5	6.81	m	8.6
2,6	7.25	m	8.6

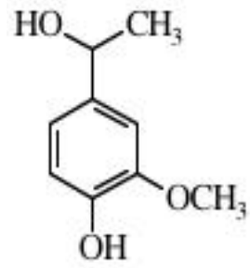
Notes:

J. Ralph: JR A97.11
34mg Almost insoluble in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β			26.10	54	25.83	91
α			69.61	28	67.70	101
3	115.28	100	115.55	89	114.54	180
5	115.28	100	115.55	89	114.54	180
2	126.91	95	127.31	100	126.31	180
6	126.91	95	127.31	100	126.31	180
1			138.90	12	137.56	61
4			156.98	15	155.86	75

Compound Number 11



Apocynol

1-(4-hydroxy-3-methoxyphenyl)ethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β Me	1.46	d	
OMe	3.87	s	
α	4.81	q	6.5
5	6.81	m	
2	6.91	m	
6	6.84	m	

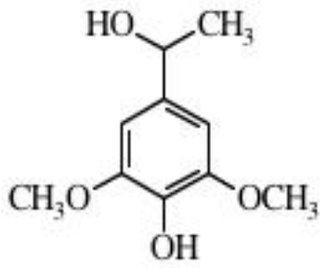
Notes:

J. Ralph: JR A97.12

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	25.07	95	26.22	87	25.88	78
OMe	55.88	99	56.09	87	55.42	98
α	70.30	89	69.81	78	67.89	100
2	108.05	80	109.76	76	109.54	71
5	114.20	94	115.21	87	114.80	82
6	118.31	100	118.65	100	117.47	77
1	137.91	40	139.67	31	138.35	64
4	144.96	32	146.13	31	144.98	69
3	146.62	33	147.97	22	147.11	52

Compound Number 12



1-(4-Hydroxy-3,5-dimethoxyphenyl)ethanol

1-(4-hydroxy-3,5-dimethoxyphenyl)ethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	1.46	d	6.4
OMe	3.85	s	
OMe	3.85	s	
α	4.79	q	6.4
2,6	6.58		

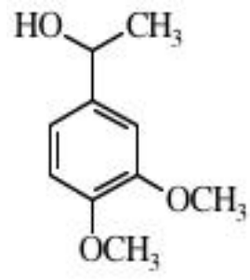
Notes:

J. Ralph: JR A97.13

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	25.22	52	26.28	45	25.94	56
OMe	56.25	100	56.49	100	55.79	100
OMe	56.25	100	56.49	100	55.79	100
α	70.50	51	70.07	43	68.16	62
2	102.15	94	103.61	87	102.65	85
6	102.15	94	103.61	87	102.65	85
1	133.90	22	135.46	14	133.93	35
4	137.22	32	138.70	20	137.53	39
3	147.01	43	148.36	24	147.56	75
5	147.01	43	148.36	24	147.56	75

Compound Number 13



1-(3,4-Dimethoxyphenyl)ethanol

1-(3,4-dimethoxyphenyl)ethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	1.46	d	6.4
OMe	3.85	s	
OMe	3.87	s	
α	4.81	q	6.4
5	6.82		
6	6.85		
2	6.92	d	1.7

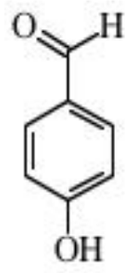
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	25.12	99	26.25	92	25.92	88
OMe	55.80	94	55.99	100	55.29	99
OMe	55.91	87	56.15	89	55.48	94
α	70.08	94	69.72	86	67.82	100
2	108.68	67	110.38	59	109.24	72
5	110.98	78	112.56	62	111.43	82
6	117.50	100	118.18	95	117.10	85
1	138.65	40	140.97	19	139.99	62
4	148.26	27	149.17	14	147.40	39
3	148.99	28	150.14	11	148.43	45

Notes:

J. Ralph: JR A97.14

Compound Number 14



p-Hydroxybenzaldehyde
4-hydroxybenzaldehyde

^{1}H (chloroform)

Atom	H Shifts	Mult	J
3,5	7.00	m	8.6
2,6	7.82	m	8.6
α	9.85	s	
<u>acetone</u>			
3,5	7.00		
2,6	7.79		
α	9.84		
OH	9.40		

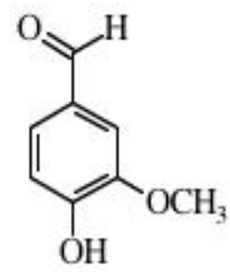
Notes:

J. Ralph: JR A87.11
52mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3	116.01	100	116.62	100	115.80	100
5	116.01	100	116.62	100	115.80	100
1	129.81	14	130.34	11	128.40	25
2	132.54	97	132.77	85	132.04	83
6	132.54	97	132.77	85	132.04	83
4	161.65	19	163.80	15	163.28	31
α	191.28	39	191.02	35	190.80	42

Compound Number 15



Vanillin

4-hydroxy-3-methoxybenzaldehyde

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.92	s	
2	7.41	m	
5	7.04	d	8.6
6	7.44	m	
α	9.81	s	
acetone			
OMe	3.91	s	
2	7.46	d	1.8
5	7.00	d	8.6
6	7.43	m	
α	9.81	s	
OH	8.30	bs	

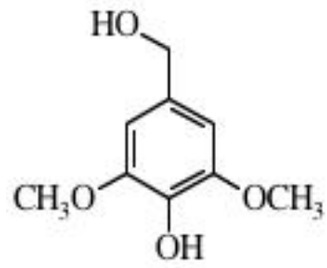
Notes:

J. Ralph: JR A87.12
66mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.07	100	56.24	100	55.52	100
2	109.02	50	110.82	72	110.63	69
5	114.59	67	115.87	97	115.36	100
6	127.57	89	126.98	83	126.04	81
1	129.70	22	130.62	29	128.70	64
3	147.34	20	148.86	23	148.12	53
4	151.99	20	153.45	32	153.00	61
α	191.16	47	191.07	85	190.89	82

Compound Number 16



Syringyl alcohol

4-hydroxy-3,5-dimethoxybenzyl alcohol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.88		
OMe	3.88		
α	4.60	s	
2,6	6.60	s	
acetone			
OMe	3.79	s	
OMe	3.79	s	
OH-α	4.07	bt	
α	4.50	bd	
2,6	6.63	s	
ph-OH	7.08	bs	

Notes:

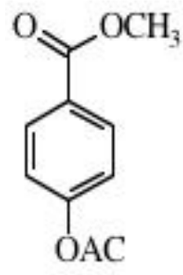
J. Ralph: JR A91.13

20mg Almost insoluble in acetone.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.29	100	56.54	100	55.77	100
OMe	56.29	100	56.54	100	55.77	100
α	65.68	39	64.98	26	63.09	40
2	103.88	82	105.08	75	103.91	72
6	103.88	82	105.08	75	103.91	72
1	132.06	21	133.80	12	132.48	26
4	134.19	15	135.75	9	134.03	26
3	147.10	35	148.54	23	147.67	52
5	147.10	35	148.54	23	147.67	52

Compound Number 17



Methyl 4-acetoxybenzoate

4-acetoxybenzoic acid methyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.30	s	
OMe	3.90	s	
3,5	7.16	m	8.9
2,6	8.06	m	8.9

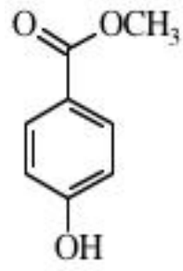
Notes:

L. Landucci
53mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.12	29	20.97	37	20.82	50
OMe	52.16	38	52.37	44	52.13	50
3	121.60	94	122.82	100	122.21	92
5	121.60	94	122.82	100	122.21	92
1	127.70	14	128.46	13	127.08	21
2	131.14	100	131.60	100	130.70	100
6	131.14	100	131.60	100	130.70	100
4	154.30	14	155.56	14	154.20	25
α	166.25	10	166.47	11	165.49	17
Ac C=0	168.79	11	169.23	11	168.72	20

Compound Number 18



Methyl 4-hydroxybenzoate
4-hydroxybenzoic acid methyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.90	s	
3,5	6.89	m	8.9
2,6	7.95	m	8.9

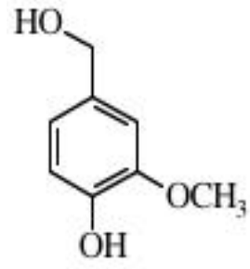
Notes:

Aldrich
62mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	52.12	43	51.86	29	51.55	32
3	115.31	97	116.00	100	115.31	100
5	115.31	97	116.00	100	115.31	100
1	122.22	15	122.33	12	120.29	15
2	131.97	100	132.37	83	131.40	100
6	131.97	100	132.37	83	131.40	100
4	160.36	23	162.58	25	161.97	24
α	167.53	10	167.07	5	166.05	14

Compound Number 19



4-Hydroxy-3-methoxybenzyl alcohol

4-hydroxy-3-methoxybenzyl alcohol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.89	s	
α	4.60	s	

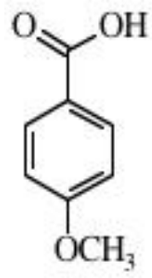
Notes:

Aldrich
54mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.90	100	56.11	100	55.38	100
α	65.44	79	64.76	76	62.93	95
2	109.94	90	111.37	78	110.91	72
5	114.27	92	115.37	87	114.93	83
6	120.22	100	120.29	95	119.00	93
1	132.93	31	134.62	33	133.37	62
4	145.26	33	146.37	31	145.17	64
3	146.65	23	148.10	25	147.24	49

Compound Number 20



p-Anisic acid

4-methoxybenzoic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.89	s	
3,5	6.96	m	9.0
2,6	8.07	m	9.0

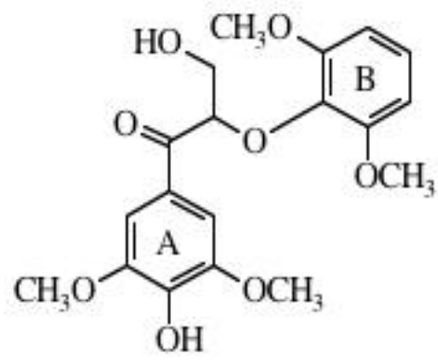
Notes:

Aldrich
52mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.48	45	55.86	46	55.36	51
3	113.75	97	114.50	88	113.74	99
5	113.75	97	114.50	88	113.74	99
1	121.67	11	123.67	12	122.97	22
2	132.35	100	132.48	100	131.32	100
6	132.35	100	132.48	100	131.32	100
4	164.04	18	164.39	13	162.80	26
α	171.45	16	167.54	13	167.00	29

Compound Number 21



2-(2,6-Dimethoxyphenoxy)-3-hydroxy-1-(4-hydroxy-3,5-dimethoxyphenyl)propan-1-one

^1H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.74	s	
OMe	3.92	s	
β	5.10	dd	6.4, 2.7
A2,6	7.42	s	
B2,6	6.59	d	8.4
B1	7.03	t	8.4

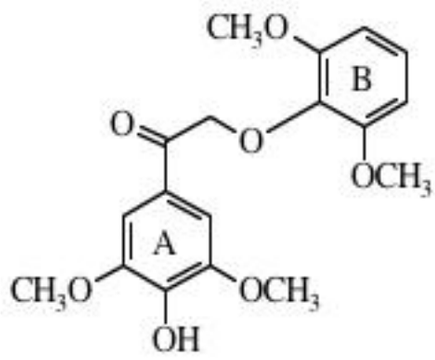
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.97	100	56.35	92	55.73	100
OMe	55.97	100	56.35	92	55.73	100
OMe	56.49	86	56.71	100	55.97	98
OMe	56.49	86	56.71	100	55.97	98
γ	63.48	39	63.66	47	61.95	34
β	87.16	48	86.21	51	82.80	31
B2	105.27	88	106.32	91	105.46	81
B6	105.27	88	106.32	91	105.46	81
A2	106.35	82	107.69	63	106.56	63
A6	106.35	82	107.69	63	106.56	63
B1	124.34	49	124.78	46	123.51	37
A1	126.98	30	127.86	23	126.22	35
B4	136.46	18	137.37	10	135.80	27
A4	140.05	29	141.99	14	140.92	37
A3	146.79	58	148.31	37	147.30	68
A5	146.79	58	148.31	37	147.30	68
B3	152.73	49	153.86	38	152.43	73
B5	152.73	49	153.86	38	152.43	73
α	194.84	28	195.15	20	194.71	35

Notes:

Has acetyl piperidine in sample.
J. Ralph JRA127.P1
27mg γ - protons coupled to OH's, shifts not determined.

Compound Number 22



2-(2,6-Dimethoxyphenoxy)-1-(4-hydroxy-3,5-dimethoxy phenyl)ethanone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.82	s	
OMe	3.94	s	
β	5.11	s	
A2,6	7.43	s	
B2,6	6.59	d	8.4
B1	7.03	t	8.4

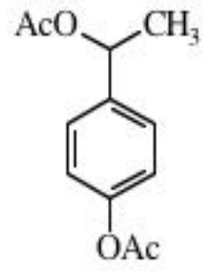
Notes:

J. Ralph JRA127.P2
23mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B OMe	56.09	100	56.42	100	55.82	100
B OMe	56.09	100	56.42	100	55.82	100
A OMe	56.48	98	56.72	94	56.03	98
A OMe	56.48	98	56.72	94	56.03	98
β	75.45	41	75.90	47	74.39	30
B2	105.33	89	106.47	98	105.52	80
B6	105.33	89	106.47	98	105.52	80
A2	106.07	84	107.45	97	105.97	63
A6	106.07	84	107.45	97	105.97	63
B1	124.20	48	124.87	53	123.84	35
A1	126.68	25	127.09	19	124.92	34
B4	136.48	11	137.55	11	135.85	21
A4	139.89	22	142.15	13	141.14	33
A3	146.74	48	148.39	27	147.50	71
A5	146.74	48	148.39	27	147.50	71
B3	153.30	42	154.43	32	152.85	61
B5	153.30	42	154.43	32	152.85	61
α	193.61	24	193.69	23	192.75	29

Compound Number 23



Hydroxyphenylethanol diacetate

1-acetoxy-1-(4-acetoxyphenyl)ethane

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.24	s	
β	1.48	d	6.6
α	5.84	q	6.6
3,5	7.09	m	8.6
2,6	7.40	m	8.6

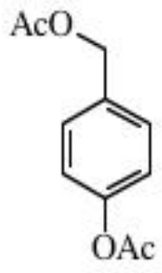
Notes:

J. Ralph JRA93.5
22mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.10	33	20.91	39	20.74	45
Ac Me	21.30	28	21.08	31	20.89	40
β	22.14	41	22.48	55	21.95	46
α	71.68	42	72.03	51	71.01	53
3	121.57	100	122.53	99	121.70	100
5	121.57	100	122.53	99	121.70	100
2	127.31	100	127.84	100	126.99	96
6	127.31	100	127.84	100	126.99	96
1	139.18	18	140.39	18	139.13	31
4	150.16	15	151.29	14	149.79	25
A4 Ac C=O	169.41	14	169.58	14	169.11	16
α Ac C=O	170.21	13	170.16	11	169.54	15

Compound Number 24



p-Hydroxybenzyl alcohol diacetate

4-acetoxybenzyl acetate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.08	s	
Ac Me	2.29	s	
α	5.08	s	
3,5	7.08	m	8.6
2,6	7.37	m	

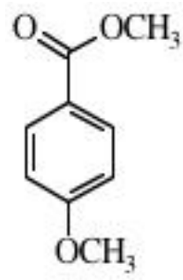
Notes:

S. Ralph SRIII-20
52mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.95	24	20.76	25	20.62	32
Ac Me	21.08	31	20.92	35	20.75	40
α	65.58	38	65.80	40	64.83	37
3	121.70	100	122.59	100	121.78	94
5	121.70	100	122.59	100	121.78	94
2	129.50	97	130.02	93	129.25	100
6	129.50	97	130.02	93	129.25	100
1	133.56	22	134.84	18	133.67	29
4	150.53	16	151.60	12	150.15	21
A4 Ac C=O	169.31	15	169.53	7	169.08	18
α Ac C=O	170.72	11	170.77	6	170.14	12

Compound Number 25



Methyl-p-anisate
methyl 4-methoxybenzoate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
4 OMe	3.83	s	
α OMe	3.86	s	
3,5	6.89	m	8.8
2,6	7.99	m	8.8

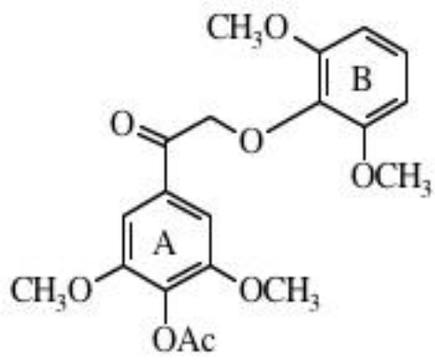
Notes:

S. Ralph SRIII-21
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
4 OMe	51.82	31	51.94	32	51.73	48
α OMe	55.39	41	55.83	50	55.45	44
3	113.59	100	114.51	98	113.95	100
5	113.59	100	114.51	98	113.95	100
1	122.60	10	123.36	9	121.88	16
2	131.57	81	132.12	100	131.20	93
6	131.57	81	132.12	100	131.20	93
4	163.33	13	164.35	11	163.12	18
α	166.82	8	166.84	6	165.88	14

Compound Number 26



1-(4-acetoxy-3,5-dimethoxyphenyl)-2-(2,6-dmethoxyphenoxy) ethanone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Aχ Mε	2.34	s	
B OMε	3.80	s	
A OMε	3.87	s	
β	5.13	s	
A2,6	7.40	s	
B2,6	6.58	d	8.4
B1	7.02	t	8.4

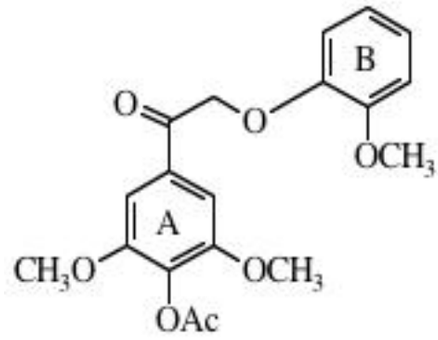
Notes:

J. Ralph GV 49.1
25mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.42	37	20.23	35	20.02	40
B OMe	56.08	93	56.44	100	55.82	100
B OMe	56.08	93	56.44	100	55.82	100
A OMe	56.37	100	56.71	98	56.18	100
A OMe	56.37	100	56.71	98	56.18	100
β	75.54	39	75.99	39	74.59	32
B2	105.35	90	106.34	94	104.87	80
B6	105.35	90	106.34	94	104.87	80
A2	105.54	90	106.50	96	105.53	94
A6	105.54	90	106.50	96	105.53	94
B1	124.26	49	124.95	50	123.88	45
A1	133.12	30	133.94	7	132.10	24
A4	133.12	30	134.21	19	132.64	38
B4	136.45	14	137.50	11	135.81	28
A3	152.26	52	153.30	33	151.80	72
A5	152.26	52	153.30	33	151.80	72
B3	153.27	43	154.36	31	152.74	69
B5	153.27	43	154.36	31	152.74	69
Ac C=0	168.11	23	168.15	16	167.60	32
α	194.03	28	194.58	24	193.75	40

Compound Number 27



1-(4-acetoxy-3,5-dimethoxyphenyl)-2-(2-methoxyphenoxy) ethanone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.35	s	
B OMe	3.87	s	
A OMe	3.87	s	
β	5.26	s	
A2,6	7.34	s	

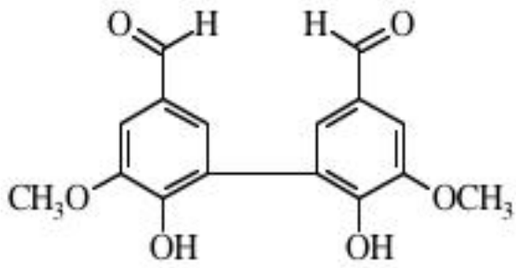
Notes:

J. Ralph GV 35.1
25mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.41	41	20.23	36	20.03	47
B OMe	55.85	47	56.25	48	55.51	60
A OMe	56.34	100	56.73	92	56.24	100
A OMe	56.34	100	56.73	92	56.24	100
β	72.53	35	72.65	40	70.85	32
A2	105.25	84	105.90	100	104.78	84
A6	105.25	84	105.90	100	104.78	84
B2	112.26	48	113.68	56	112.48	44
B5	114.95	49	115.73	48	113.80	39
B6	120.89	51	121.56	56	120.45	48
B1	122.64	49	122.80	56	121.37	43
A1	133.41	12	134.14	8	132.32	17
A4	132.58	27	133.81	20	132.38	39
B3	147.37	16	148.96	16	147.33	34
B4	149.79	17	150.90	16	148.96	29
A3	152.41	49	153.45	36	151.90	74
A5	152.41	49	153.45	36	151.90	74
Ac C=0	168.06	20	168.14	20	167.59	35
α	193.77	25	194.35	20	193.70	42

Compound Number 28



Dehydrodivanillin

6,6'-Dihydroxy-5,5'-dimethoxybiphenyl-3,3'-dicarbaldehyde

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.94	s	
2	7.44	s	
6	7.44	s	
α	9.81	s	
Acetone			
OMe	3.95	s	
2	7.42	d	J = 1.84
6	7.55	d	J = 1.84
α	9.84	s	

^{13}C

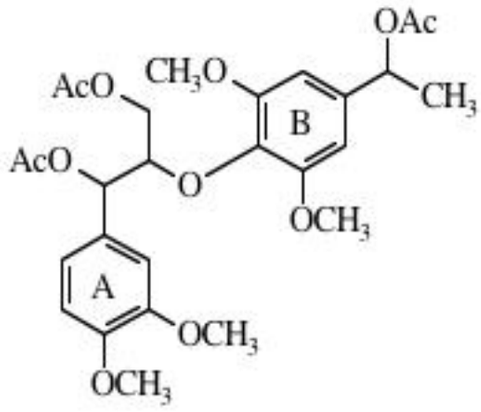
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe					55.94	100
2					109.08	53
6					124.54	47
5					127.61	75
1					128.05	53
4					148.12	59
3					152.93	16
α					190.97	72

Notes:

J. Ralph KM 77.1

25mg contains impurities As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 29



threo

Veratrylglycerol-β-syringol ether triacetate

1,3-diacetoxy-1-(3,4-dimethoxyphenyl)-2-(4-(1-acetoxyethyl)-2,6-dimethoxyphenoxy)propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	1.92	s	
Ac Me	2.00	s	
Ac Me	2.07	s	
B β	1.51	d	6.6
OMe	3.86	s	
OMe	3.86	s	
B OMe	3.80	s	
γ1	-	-	
γ2	4.29	dd	11.7, 3.6
B α	5.79	q	6.6
α	6.11	d	7.1
β	4.59	m	
B2,6	6.55	s	
A2	6.94	m	
A5	6.81	d	8.8
A6	6.95	m	

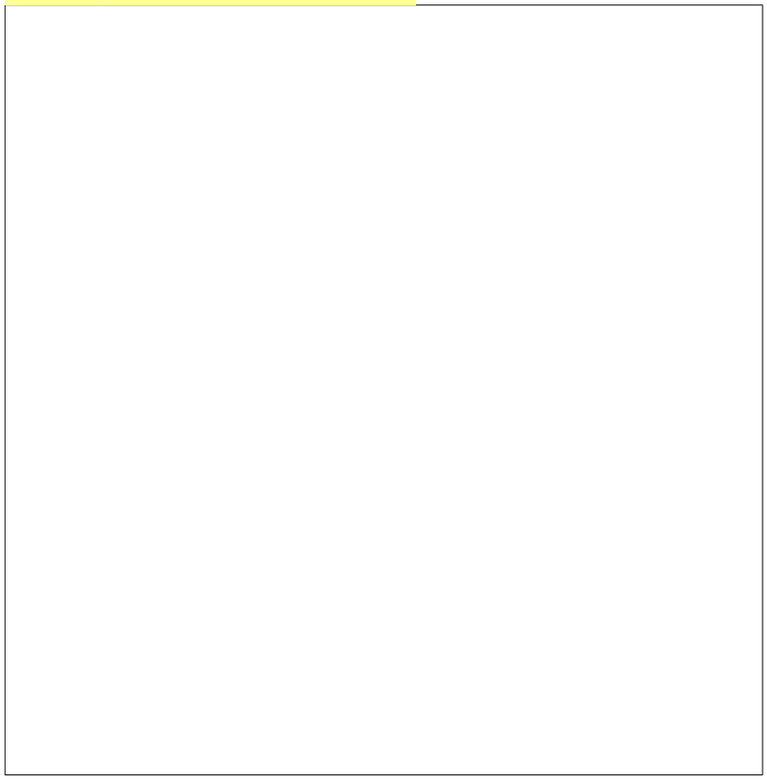
Notes:

S. Ralph III-14
65mg sample has impurities
γ1 proton hidden by OMe's

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.75	41	20.62	51	20.36	40
Ac Me	21.01	32	20.96	52	20.62	35
Ac Me	21.34	34	21.14	41	20.96	38
B β	22.22	34	22.58	52	22.03	27
A OMe	55.88	63	56.02	71	55.43	52
A OMe	55.97	61	56.02	71	55.50	58
B OMe	56.08	100	56.33	100	55.80	100
B OMe	56.08	100	56.33	100	55.80	100
γ	63.84	26	64.43	48	63.36	21
B α	72.38	29	72.70	49	71.70	33
α	76.01	45	76.69	51	75.65	22
β	80.76	46	81.52	52	80.30	26
B2	103.29	77	103.91	86	102.90	50
B6	103.29	77	103.91	86	102.90	50
A2	110.70	28	112.03	44	110.80	29
A5	111.02	45	112.31	51	111.51	31
A6	119.92	49	120.59	48	119.58	30
A1	129.64	40	130.68	32	129.28	39
B1	136.22	14	137.06	19	135.43	22
B4	137.37	41	138.53	25	137.28	33
A3	148.89	35	150.05	29	148.53	46
A4	149.10	33	150.25	22	148.74	38
B3	152.88	60	153.68	51	152.27	66
B5	152.88	60	153.68	51	152.27	66
Ac C=0	169.76	22	169.78	25	169.11	37
Ac C=O	170.15	24	170.14	19	169.52	34
Ac C=O	170.57	31	170.59	24	169.89	40

Compound Number 30



Xylan

Xylan,Birch

^{1}H (DMSO)

Atom	H Shifts	Mult	J

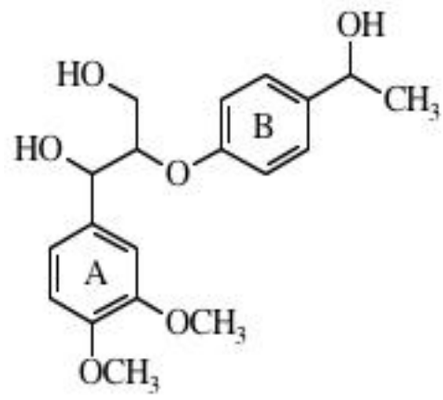
Notes:

IPC Xylan 79-7
60mg 147- Quantitative run 148- Run at 363K
shifts at 58.94 and 101.14 are for end groups

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
					58.94	35
					63.09	73
					72.56	96
					73.83	92
					75.40	92
					101.14	54
					101.65	100

Compound Number 31



threo

1-(3,4-Dimethoxyphenyl)-2-[4-(1-hydroxyethyl) phenoxy] propane-1,3-diol

^{1}H (DMSO)

Atom	H Shifts	Mult	J
B β	1.28	d	
OMe	3.71	s	
OMe	3.71	s	
α	5.36	d	5.1

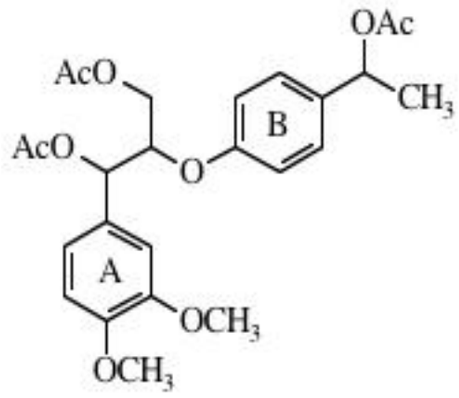
Notes:

S. Ralph SR111-7 28mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.03	34	26.15	33	25.81	39
OMe	55.88	88	55.99	41	55.30	44
OMe	55.88	88	56.04	41	55.40	44
γ	61.06	32	61.60	37	59.92	24
B α	69.74	34	69.48	33	67.57	44
α	73.47	27	73.18	41	70.77	41
β	82.92	34	84.04	41	82.98	34
A2	110.00	34	111.73	37	110.57	41
A5	111.00	34	112.18	33	111.17	34
B3	116.35	88	116.61	90	115.34	93
B5	116.35	88	116.61	90	115.34	93
A6	119.26	41	119.84	43	118.62	39
B2	126.84	100	127.14	100	126.15	100
B6	126.84	100	127.14	100	126.15	100
A1	132.46	27	135.41	24	134.78	44
B1	139.26	29	140.44	20	139.27	29
A3	148.81	27	149.53	12	147.69	29
A4	148.98	29	149.91	12	148.13	29
B4	157.45	29	158.87	20	157.62	49
erythro isomer						
γ	61.46		61.94		59.92	
α	73.88		73.81		71.37	
β	82.00		83.67		82.98	

Compound Number 32



threo

1,3-diacetoxy-1-(3,4-dimethoxyphenyl)-2-[4-(1-acetoxyethyl) phenoxy] propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.03	s	
Ac Me	2.03	s	
Ac Me	2.05	s	
B β	1.51	d	6.6
OMe	3.87	s	
OMe	3.87	s	
γ1	4.00	dd	11.8, 6.2
γ2	4.24	dd	11.9, 4.0
B α	5.84	q	6.6
α	6.02	d	6.6
β	4.70	m	

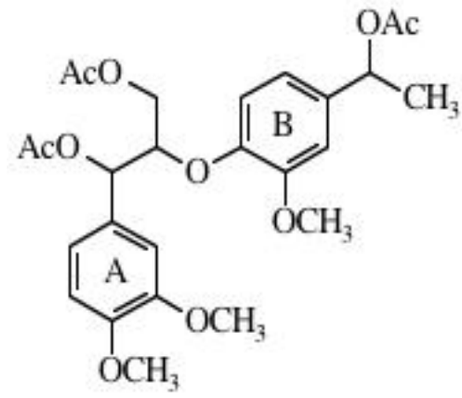
Notes:

S. Ralph SR III-17AC
28mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.69	35	20.56	26	20.38	67
Ac Me	21.04	43	20.89	34	20.64	64
Ac Me	21.35	39	21.13	28	20.93	69
B β	22.01	38	22.35	38	21.78	51
OMe	55.91	58	56.06	54	55.41	82
OMe	55.99	49	56.17	56	55.51	72
γ	62.91	42	63.46	30	62.32	28
B α	71.86	22	72.17	38	71.14	49
α	74.34	20	75.35	34	74.25	41
β	78.43	41	79.30	34	77.67	39
A2	110.51	38	112.16	33	110.85	41
A5	111.20	42	112.54	38	111.52	38
B3	116.40	84	117.10	67	115.98	100
B5	116.40	84	117.10	67	115.98	100
A6	119.92	39	120.84	49	119.82	41
B2	127.62	100	128.22	100	127.29	95
B6	127.62	100	128.22	100	127.29	95
A1	128.58	32	130.00	25	128.62	44
B1	135.13	27	136.10	20	134.59	44
A3	149.10	27	150.34	18	148.60	46
A4	149.41	23	150.61	16	148.87	44
B4	158.17	20	159.27	20	157.76	41
Ac C=0	169.81	26	169.90	16	169.28	41
Ac C=O	170.27	18	170.11	16	169.51	46
Ac C=O	170.55	24	170.58	16	169.92	38
erythro isomer:						
γ	62.59		63.11		61.88	
α	73.95		74.41		72.92	
β	78.43		78.93		76.96	

Compound Number 33



threo

1,3-diacetoxy-1-(3,4-dimethoxyphenyl)-2-[4-(1-acetoxyethyl)-2-methoxyphenoxy] propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.00	s	
Ac Me	2.02	s	
Ac Me	2.06	s	
B β	1.52	d	6.5
OMe	3.85	s	
OMe	3.86	s	
OMe	3.87	s	
γ2	4.27	dd	11.9, 4.0
γ1	3.99	dd	11.9, 5.8
B α	4.82	q	6.5
α	6.07	d	6.7
β	4.63	m	

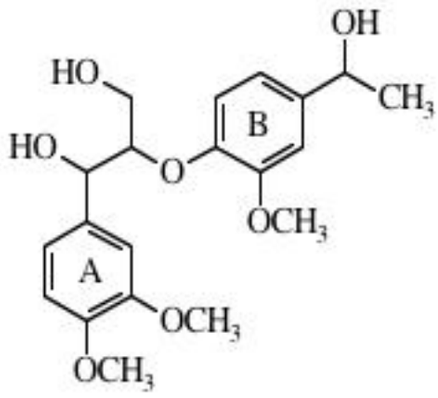
Notes:

S. Ralph SR III-15AC
35mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.71	40	20.59	64	20.36	70
Ac Me	21.05	41	20.95	52	20.64	55
Ac Me	21.35	45	21.14	48	20.94	77
B β	22.09	44	22.45	70	21.87	45
OMe	55.91	97	56.06	100	55.41	100
OMe	55.95	100	56.14	76	55.46	57
OMe	55.95	100	56.32	79	55.66	68
γ	63.26	32	63.80	61	62.61	29
B α	72.06	41	72.39	76	71.36	54
α	74.87	33	75.67	64	74.54	36
β	80.44	40	80.88	70	79.23	36
B2	110.58	35	111.79	70	110.64	34
A2	110.75	29	112.17	64	110.84	38
A5	111.12	41	112.49	73	111.48	39
B5	118.23	40	118.74	67	117.02	39
B6	118.66	47	119.19	76	118.08	43
A6	119.88	42	120.73	76	119.74	39
A1	128.93	45	130.22	55	128.75	45
B1	136.59	31	137.61	45	135.92	36
B4	147.72	18	148.68	36	147.12	36
A3	149.04	29	150.28	33	148.57	46
A4	149.30	27	150.51	39	148.83	43
B3	150.65	23	151.56	30	149.86	38
Ac C=O	170.54	26	169.88	30	169.22	39
Ac C=O	170.23	21	170.14	30	169.52	41
Ac C=O	169.76	27	170.59	36	169.91	45
erythro isomer:						
γ	62.74		63.25		62.04	
α	74.08		74.76		73.25	
β	79.98		80.23		78.29	

Compound Number 34



threo

1-(3,4-dimethoxyphenyl)-2-[4-(1-hydroxyethyl)-2-methoxy phenoxy] propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.46	d	6.4
OMe	3.86	s	
OMe	3.86	s	
OMe	3.86	s	
B α	4.83	q	6.4
α	4.94	d	7.7
β	4.01	m	
γ1	3.46	mm	
γ2	3.60	dd	

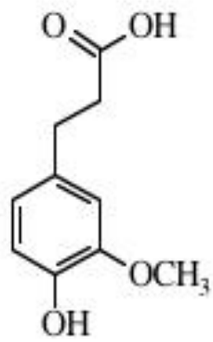
Notes:

S. Ralph SR III-15
28mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.22	35	26.10	95	25.83	91
OMe	55.92	100	55.93	100	55.20	92
OMe	55.92	100	56.01	90	55.41	83
OMe	55.92	100	56.17	88	55.52	100
γ	61.08	28	61.68	67	59.96	55
B α	69.98	38	69.66	90	67.79	86
α	73.84	32	73.62	67	70.72	50
β	89.01	19	88.12	52	84.56	38
B2	109.33	28	110.46	60	109.79	44
A2	110.03	32	111.67	67	110.65	47
A5	111.10	38	112.14	71	111.08	71
B5	118.40	32	118.58	64	115.57	35
B6	119.56	34	119.22	52	117.24	62
A6	120.22	17	119.99	69	118.59	56
A1	132.23	26	134.87	40	134.50	58
B1	141.94	21	142.61	33	140.50	61
B4	146.76	21	148.03	36	146.78	56
A3	148.90	22	149.54	33	147.68	55
A4	149.08	25	149.87	36	148.07	79
B3	151.00	15	151.20	33	149.33	64
erythro isomer:						
γ	60.82		61.68		59.96	
α	72.78		73.62		71.51	
b	87.01		86.50		83.82	

Compound Number 35



Dihydroferulic Acid

3-(4-hydroxy-3-methoxyphenyl)propanoic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α	2.64	t	7.4
β	2.88	t	7.4
OMe	3.84	s	
2	6.71	m	
5	6.82	d	7.6
6	6.69	m	

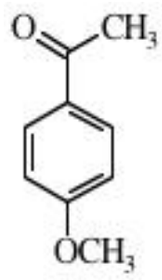
Notes:

J. Obst
35mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	30.38	96	31.24	100	30.00	93
β	36.01	88	36.38	95	35.68	100
OMe	55.92	96	56.22	94	55.52	96
2	111.10	96	112.81	91	112.52	82
5	114.52	100	115.64	85	115.25	98
6	120.89	95	121.47	93	120.21	95
1	132.15	44	133.23	36	131.62	67
4	144.16	51	145.76	36	144.68	73
3	146.55	37	148.17	25	147.34	60
γ	178.88	40	174.26	18	173.77	61

Compound Number 36



4-Methoxyacetophenone

4-methoxyacetophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	2.53	s	
OMe	3.85	s	
3,5	6.90	m	8.8
2,6	7.90	m	8.8

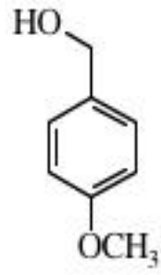
Notes:

Aldrich
57mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	26.28	30	26.33	31	26.29	34
OMe	55.43	60	55.85	47	55.44	50
3	113.68	86	114.45	95	113.75	100
5	113.68	86	114.45	95	113.75	100
1	130.35	15	131.28	12	129.89	18
2	130.55	100	131.18	100	130.40	97
6	130.55	100	131.18	100	130.40	97
4	163.48	11	164.31	11	163.06	20
α	196.62	12	196.23	8	196.14	14

Compound Number 37



p-Methoxybenzyl alcohol
4-methoxybenzyl alcohol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.75	s	
α	4.51	s	
3,5	6.86	m	8.7
2,6	7.20	m	8.7

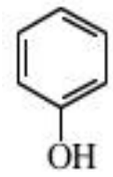
Notes:

Aldrich
65mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.23	49	55.39	58	54.94	56
α	64.68	35	64.34	45	62.59	46
3	113.87	**100**	114.27	**100**	113.40	**100**
5	113.87	100	114.27	100	113.40	100
2	128.56	97	128.82	92	127.86	99
6	128.56	97	128.82	92	127.86	99
1	133.21	16	135.23	13	134.49	27
4	159.05	13	159.64	12	158.14	19

Compound Number 38



Phenol

phenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
3,5	6.84	m	
1	6.93	m	
2,6	7.22	m	

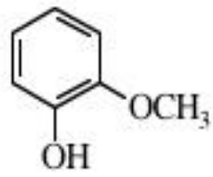
Notes:

Aldrich JR 85-11
54mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3	115.41	100	116.03	100	115.18	100
5	115.41	100	116.03	100	115.18	100
1	120.89	47	120.13	54	118.70	49
2	129.71	85	130.16	94	129.26	89
6	129.71	85	130.16	94	129.26	89
4	155.25	18	158.16	15	157.29	23

Compound Number 39



Guaiacol
2-methoxyphenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.83	s	
OH	5.72	s	

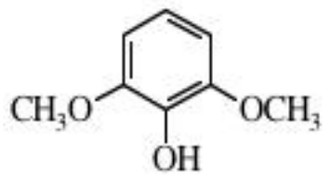
Notes:

Aldrich JR A85.12
54mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.86	100	56.16	94	55.47	99
2	110.81	95	112.48	99	112.30	97
5	114.60	83	115.84	94	115.51	85
1	120.15	94	120.39	100	119.09	91
6	121.47	85	121.94	92	120.83	100
3	145.70	21	147.48	21	146.52	49
4	146.63	17	148.33	19	147.59	37

Compound Number 40



Syringol

2,6-dimethoxyphenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.86	s	
OMe	3.86	s	
2,6	6.56	d	8.1
1	6.78	t	8.1

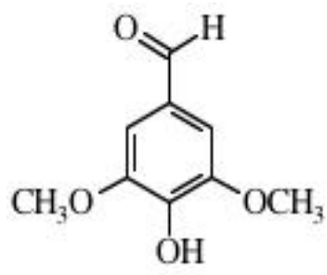
Notes:

Aldrich JR A 85.13
56mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.27	100	56.55	100	55.89	100
OMe	56.27	100	56.55	100	55.89	100
2	105.03	100	106.57	100	105.70	95
6	105.03	100	106.57	100	105.70	95
1	119.06	49	119.16	44	118.06	42
4	134.97	12	137.08	8	135.70	21
3	147.31	23	148.86	16	148.16	39
5	147.31	23	148.86	16	148.16	39

Compound Number 41



Syringaldehyde

3,5-dimethoxy-4-hydroxybenzaldehyde

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.95	s	
2,6	7.15	s	
α	9.81	s	
acetone			
OMe	3.91	s	
2,6	7.23	s	
α	9.81	s	
OH	8.20	bs	

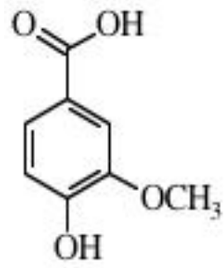
Notes:

J. Ralph JRA87.13
62mg
Poor solubility

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.48	100	56.64	100	56.02	100
OMe	56.48	100	56.64	100	56.02	100
2	106.81	80	107.74	80	107.05	67
6	106.81	80	107.74	80	107.05	67
1	128.34	24	129.02	19	127.14	34
4	141.03	20	142.92	15	142.11	28
3	147.44	30	148.94	25	148.09	56
5	147.44	30	148.94	25	148.09	56
α	190.79	52	191.05	45	190.99	38

Compound Number 42



Vanillic acid

4-hydroxy-3-methoxy benzoic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.96	s	
2	7.59	d	1.9
5	6.97	d	8.3
6	7.72	dd	8.3, 1.9

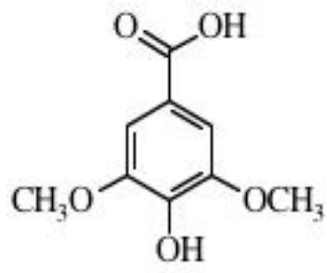
Notes:

J. Ralph JRA89.12
55mg
not very soluble in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.28	95	55.50	100
2			113.46	87	112.73	83
5			115.43	87	115.00	84
1			122.70	33	121.62	52
6			124.90	100	123.46	83
3			147.96	31	147.17	71
4			152.03	28	151.05	69
α			167.84	33	167.16	53

Compound Number 43



Syringic acid

3,5-dimethoxy-4-hydroxybenzoic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.96	s	
2,6	7.40	s	

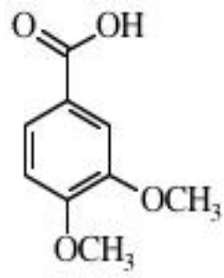
Notes:

J. Ralph JRA 89-13
55mg not very soluble in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.66	98	55.92	100
OMe			56.66	98	55.92	100
2			108.20	100	106.85	82
6			108.20	100	106.85	82
1			121.40	19	120.32	29
4			141.61	14	140.17	43
3			148.30	29	147.37	81
5			148.30	29	147.37	81
α			167.68	19	167.14	38

Compound Number 44



Veratric acid

3,4-dimethoxybenzoic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.94	s	
OMe	3.95	s	
2	7.60	d	1.9
5	6.92	d	8.5
6	7.78	dd	8.5, 1.9

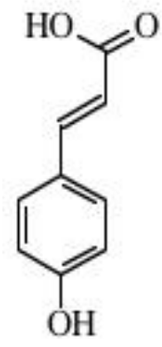
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.02	100	56.08	100	55.41	100
OMe	56.06	86	56.12	91	55.58	93
2	110.36	87	111.64	81	110.93	85
5	112.38	87	113.34	72	111.93	73
1	121.77	46	123.64	25	122.98	43
6	124.61	94	124.42	78	123.16	85
3	148.72	56	149.89	22	148.30	54
4	153.78	46	154.37	19	152.60	42
α	172.08	50	167.53	28	167.08	55

Notes:

J. Ralph JRA 89-14
55mg

Compound Number 45



trans

p-Coumaric acid

4-hydroxycinnamic acid

^{1}H (DMSO)

Atom	H Shifts	Mult	J
α	7.54	d	16.0
3,5	6.83	d	8.6
2,6	7.53	d	8.6
β	6.32	d	16.0

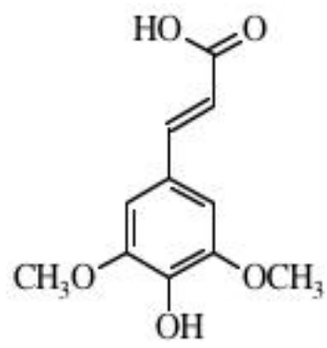
Notes:

Fluka
60mg
*not soluble in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β			115.51	45	115.30	38
3			116.66	100	115.72	100
5			116.66	100	115.72	100
1			126.95	22	125.24	34
2			130.90	91	129.98	99
6			130.90	91	129.98	99
α			145.95	45	144.11	43
4			160.49	26	159.54	43
γ			169.03	19	167.90	39

Compound Number 46



trans

Sinapinic acid

3,5-dimethoxy-4-hydroxycinnamic acid

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.83	s	
2,6	7.00	s	
α	7.50	d	15.9
β	6.44	d	15.9

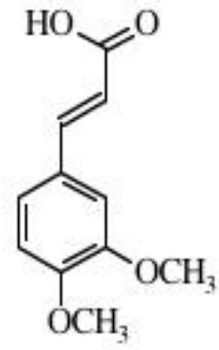
Notes:

Lancaster Synthesis
60mg *not very soluble in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.68	100	56.04	100
OMe			56.68	100	56.04	100
2			106.84	100	106.04	74
6			106.84	100	106.04	74
β			116.20	50	116.03	37
1			126.19	22	124.59	38
4			139.43	22	138.05	38
α			146.23	58	144.74	39
3			148.90	44	148.00	79
5			148.90	44	148.00	79
γ			168.26	28	167.90	45

Compound Number 47



trans

3,4-Dimethoxycinnamic acid

3,4-dimethoxycinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.92	s	
OMe	3.92	s	
2	7.08	d	2.0
5	6.88	d	8.3
6	7.14	dd	8.3, 2.0
α	7.73	d	15.9
β	6.33	d	15.9

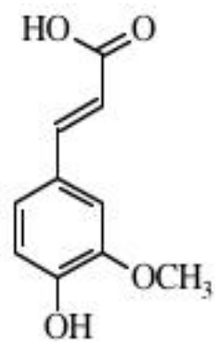
Notes:

K & K Labs
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.92	98	56.08	90	55.49	94
OMe	55.99	92	56.13	100	55.56	100
2	109.88	94	111.20	84	110.35	74
5	111.09	96	112.40	82	111.50	71
β	114.94	94	116.60	80	116.68	75
6	123.10	100	123.43	94	122.53	76
1	127.08	72	128.31	39	127.05	72
α	146.95	91	145.64	90	144.08	71
3	149.31	53	150.61	29	148.97	68
4	151.56	47	152.48	27	150.77	55
γ	172.53	77	168.11	27	167.83	71

Compound Number 48



trans

Ferulic acid

4-hydroxy-3-methoxycinnamic acid

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.84	s	
2	7.29	d	1.9
5	6.83	d	8.2
6	7.10	dd	8.2,1.9
α	7.53	d	15.9
β	6.39	d	15.9

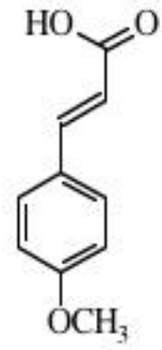
Notes:

Aldrich
60mg not very soluble in CDCl3 Note: .0238 was run in d4-MeOH.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.28	98	55.64	100
2			111.30	95	111.14	74
β			115.77	87	115.52	77
5			116.00	90	115.60	73
6			123.80	98	122.72	76
1			127.38	51	125.76	62
α			146.16	100	144.44	71
3			148.64	46	147.87	79
4			149.97	51	149.04	81
γ			168.88	60	167.93	76
d4-MeOH	56.44					
	111.71					
	115.89					
	116.46					
	123.94					
	127.77					
	146.89					
	149.30					
	150.43					
	170.93					

Compound Number 49



trans

4-Methoxycinnamic acid

4-methoxycinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.85	s	
3,5	6.92	m	8.8
α	7.75	d	15.9
2,6	7.51	m	8.8
β	6.32	d	15.9

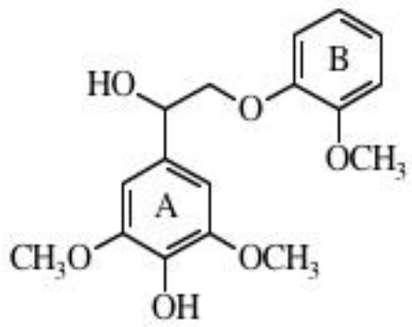
Notes:

Aldrich
66mg not CDCl3 soluble

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			55.68	51	55.22	52
3			115.14	100	114.30	97
5			115.14	100	114.30	97
β			116.52	44	116.51	41
1			128.02	18	126.82	29
2			130.58	98	129.84	100
6			130.58	98	129.84	100
α			145.19	53	143.65	42
4			162.41	16	160.90	28
γ			168.11	22	167.78	35

Compound Number 50



Syringylglycol-β-guaiacyl ether

1-(3,5-dimethoxy-4-hydroxyphenyl)-2-(2-methoxyphenoxy) ethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B OMe	3.85	s	
A OMe	3.87	s	
α	5.00	dd	9.9, 3.0
β1	3.94	t	9.9
β2	4.14	dd	9.9, 3.0
A2,6	6.66	s	

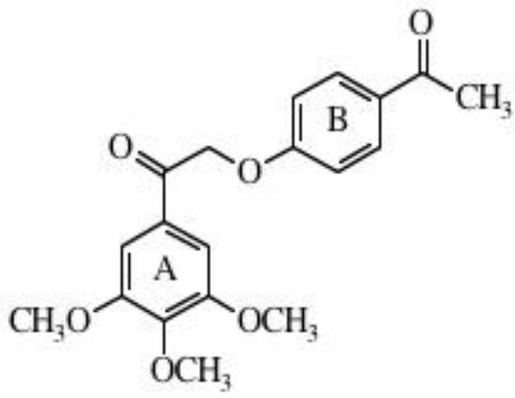
Notes:

S. Ralph SG 100mg
33mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B OMe	55.84	50	56.24	49	55.41	52
A OMe	56.32	100	56.58	100	55.81	100
A OMe	56.32	100	56.58	100	55.81	100
α	72.47	54	72.85	51	70.97	47
β	76.39	48	76.15	45	73.98	38
A2	103.11	96	104.79	84	103.73	79
A6	103.11	96	104.79	84	103.73	79
B2	112.06	52	113.44	45	112.25	42
B5	115.96	50	115.52	38	113.40	38
B6	121.12	51	121.76	55	120.66	48
B1	122.50	56	122.29	55	120.79	47
A1	130.84	36	133.07	27	132.54	40
A4	134.46	31	136.13	24	134.51	36
A3	147.12	56	148.46	51	147.57	77
A5	147.12	56	148.46	51	147.57	77
B3	148.06	27	149.62	22	148.11	33
B4	150.11	23	150.84	18	148.94	37

Compound Number 51



2-(4-Acetylphenoxy)-1-(3,4,5-trimethoxyphenyl)ethanone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	2.54	s	
A3,5 OMe	3.92	s	
A4 OMe	3.94	s	
β	5.32	s	
A2,6	7.26	s	
B3,5	6.96	m	8.9
B2,6	7.92	m	8.9

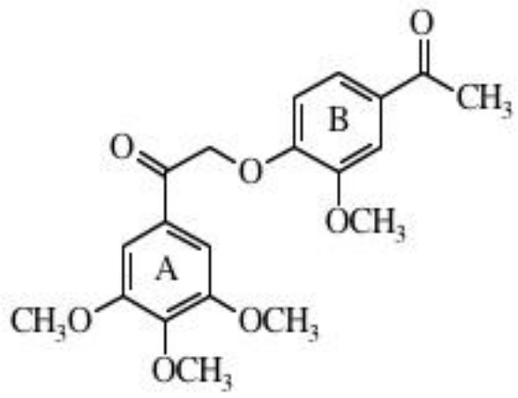
Notes:

L. Landucci LLL XVII 9A
26mg contains trace impurity

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	26.34	46	26.37	43	26.34	60
A3 OMe	56.42	86	56.68	88	56.12	100
A5 OMe	56.42	86	56.68	88	56.12	100
A4 OMe	61.00	35	60.72	33	60.12	52
β	70.62	35	71.10	37	70.11	37
A2	105.84	81	106.60	90	105.47	87
A6	105.84	81	106.60	90	105.47	87
B3	114.44	94	115.27	96	114.45	97
B5	114.44	94	115.27	96	114.45	97
A1	129.36	26	130.72	20	129.38	38
B2	130.62	100	131.11	100	130.26	92
B6	130.62	100	131.11	100	130.26	92
B1	131.16	26	131.70	20	130.11	37
A4	143.65	12	144.27	10	142.41	25
A3	153.32	57	154.41	41	152.88	77
A5	153.32	57	154.41	41	152.88	77
B4	161.77	28	163.09	22	161.79	40
α	192.49	32	193.05	24	192.70	37
B α	196.55	19	196.23	16	196.12	35

Compound Number 52



2-(4-Acetyl-2-methoxyphenoxy)-1-(3,4,5-trimethoxyphenyl) ethanone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	2.54	s	
B OMe	3.95	s	
A3,5 OMe	3.92	s	
A4 OMe	3.93	s	
β	5.39	s	
A2,6	7.47	s	
B2	7.63	d	1.9
B5	6.80	d	8.3
B6	7.52	dd	8.3, 1.9

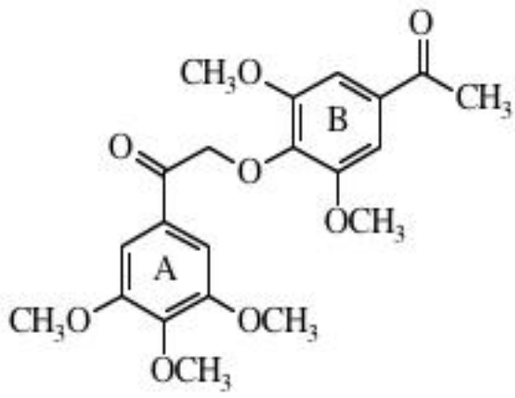
Notes:

L. Landucci LLL XVII 9c
28.5mg trace impurity present

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	26.23	55	26.30	53	26.25	49
B OMe	56.01	53	56.28	51	55.58	56
A3 OMe	56.32	100	56.64	100	56.12	100
A5 OMe	56.32	100	56.64	100	56.12	100
A4 OMe	60.96	47	60.70	33	60.13	49
β	71.57	32	71.84	42	70.48	28
A2	105.79	92	106.70	93	105.57	74
A6	105.79	92	106.70	93	105.57	74
B2	110.85	43	112.10	45	110.84	36
B5	112.27	43	113.40	48	112.24	38
B6	122.87	53	123.39	52	122.56	41
A1	129.33	28	130.74	25	129.40	36
B1	131.48	33	131.98	21	130.24	36
A4	143.44	17	144.21	12	142.45	23
B3	149.31	30	150.23	21	148.52	44
B4	151.49	27	152.98	18	151.61	44
A3	153.23	55	154.34	45	152.85	85
A5	153.23	55	154.34	45	152.85	85
α	192.68	25	193.34	22	192.76	36
Bα	196.64	25	196.32	19	196.19	36

Compound Number 53



2-(4-Acetyl-2,6-dimethoxyphenoxy)-1-(3,4,5-trimethoxyphenyl) ethanone□□

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	2.59	s	
A3,5 OMe	3.92	s	
B3,5 OMe	3.88	s	
A4 OMe	3.91	s	
β	5.29	s	
A2,6	7.31	s	
B2,6	7.22	s	

Notes:

L. Landucci LLL XVII 9d
37mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	26.43	26	26.55	43	26.52	47
A3 OMe	56.33	100	56.61	100	56.04	100
A5 OMe	56.33	100	56.61	100	56.04	100
B3 OMe	56.33	100	56.66	75	56.09	95
B5 OMe	56.33	100	56.66	75	56.09	95
A4 OMe	60.94	22	60.67	32	60.08	43
β	74.82	22	75.43	45	74.15	28
A2	105.87	100	106.81	86	105.52	70
A6	105.87	100	106.81	86	105.52	70
B2	105.87	100	106.95	91	105.84	70
B6	105.87	100	106.95	91	105.84	70
A1	129.99	15	131.21	20	129.69	30
B1	132.67	15	133.62	19	132.05	33
B4	140.75	10	141.68	13	140.24	27
A4	142.94	8	143.88	10	142.15	20
B3	152.53	33	153.61	38	152.04	65
B5	152.53	33	153.61	38	152.04	65
A3	153.12	33	154.23	36	152.80	70
A5	153.12	33	154.23	36	152.80	70
α	193.28	15	193.81	22	193.11	35
B α	196.71	14	196.70	19	196.61	28

Compound Number 54

Anisole

Methoxybenzene

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.77	s	
3,5,1	6.90	m	
2,6	7.27	m	

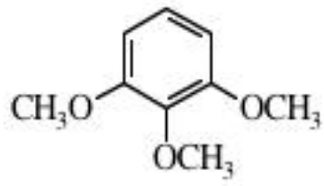
Notes:

Aldrich
40mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.08	70	55.28	73	54.86	54
3	113.92	100	114.62	98	113.84	99
5	113.92	100	114.62	98	113.84	99
1	120.64	61	121.19	64	120.39	43
2	129.52	100	130.14	100	129.39	100
6	129.52	100	130.14	100	129.39	100
4	159.60	12	160.63	14	159.24	10

Compound Number 55



1,2,3-trimethoxybenzene

^{1}H (chloroform)

Atom	H Shifts	Mult	J
3,5 OMe	3.85	s	
4 OMe	3.85	s	
2,6	6.57	d	8.3
1	6.98	t	8.3

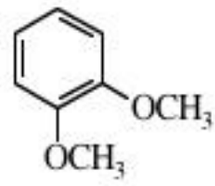
Notes:

Aldrich
40mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3 OMe	56.09	100	56.35	91	55.77	100
5 OMe	56.09	100	56.35	91	55.77	100
4 OMe	60.80	38	60.43	38	59.90	48
2	105.34	88	106.54	100	105.56	95
6	105.34	88	106.54	100	105.56	95
1	123.61	51	124.30	42	123.57	49
4	138.27	8	139.52	8	137.69	10
3	153.56	23	154.67	19	153.16	33
5	153.56	23	154.67	19	153.16	33

Compound Number 56



Veratrole

1,2-dimethoxybenzene

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.86	s	
2,5	6.89	m	
1,6	6.89	m	

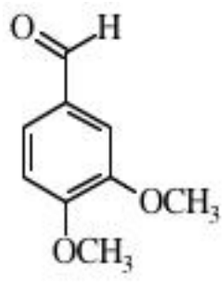
Notes:

Aldrich
40mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.80	100	56.01	100	55.38	100
OMe	55.80	100	56.01	100	55.38	100
2	111.44	76	113.02	89	111.98	99
5	111.44	76	113.02	89	111.98	99
1	120.85	83	121.60	86	120.67	100
6	120.85	83	121.60	86	120.67	100
3	149.08	16	150.50	17	148.88	29
4	149.08	16	150.50	17	148.88	29

Compound Number 57



Veratraldehyde
3,4-dimethoxybenzaldehyde

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.94	s	
OMe	3.97	s	
2	7.41	d	1.8
5	6.98	d	8.2
6	7.46	dd	8.2, 1.8
α	9.85	s	

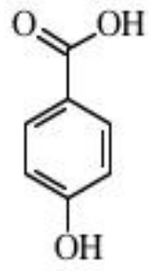
Notes:

Aldrich
40mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.00	100	56.07	100	55.47	100
OMe	56.17	93	56.29	91	55.82	85
2	109.05	65	110.31	80	109.46	66
5	110.46	88	111.85	91	111.22	83
6	126.77	79	126.72	94	126.00	79
1	130.19	37	131.21	27	129.65	49
3	149.66	21	150.77	20	149.17	38
4	154.51	25	155.63	16	154.18	37
α	190.78	70	191.16	79	191.21	84

Compound Number 58



4-hydroxybenzoic acid

^{1}H (DMSO)

Atom	H Shifts	Mult	J
3,5	6.85	m	8.8
2,6	7.83	m	8.8

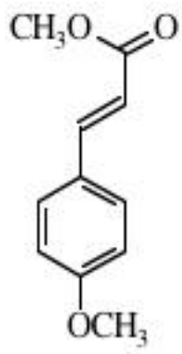
Notes:

Aldrich
40mg *CDCl3 insoluble

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3			115.99	94	115.06	100
5			115.99	94	115.06	100
1			122.43	14	121.35	27
2			132.78	100	131.47	87
6			132.78	100	131.47	87
4			162.65	21	161.55	39
α			168.24	20	167.11	33

Compound Number 59



methyl (4-methoxy)cinnamate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ OMe	3.79	s	
4 OMe	3.82	s	
2,6	7.46	m	8.8
α	7.65	d	16.0
3,5	6.89	m	8.8
β	6.31	d	16.0

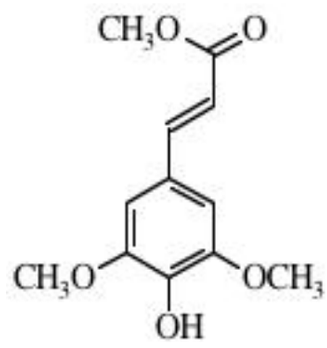
Notes:

J. Ralph PS 137x1
95mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ OMe	51.50	45	51.58	43	51.23	37
4 OMe	55.32	43	55.70	47	55.28	47
3	114.34	98	115.14	98	114.36	**100**
5	114.34	98	115.14	98	114.36	100
β	115.30	41	115.96	43	115.09	51
1	127.14	21	127.84	17	126.65	36
2	129.71	**100**	130.63	**100**	130.08	89
6	129.71	100	130.63	100	130.08	89
α	144.49	49	145.04	45	144.28	45
4	161.42	17	162.42	14	161.17	32
γ	167.68	18	167.81	15	166.90	23

Compound Number 60



trans

Methyl Sinapate

methyl (3,5-dimethoxy-4-hydroxy)cinnamate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ OMe	3.79	s	
3,5 OMe	3.90	s	
2,6	6.76	s	
α	7.60	d	15.9
β	6.30	d	15.9

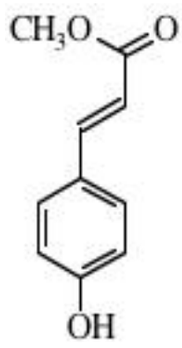
Notes:

J. Ralph JRPS 135x1
52mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ OMe	51.60	45	51.46	24	51.13	51
3 OMe	56.34	100	56.68	88	56.06	100
5 OMe	56.34	100	56.68	88	56.06	100
2	105.17	86	106.83	100	106.26	85
6	105.17	86	106.83	100	106.26	85
β	115.50	47	115.73	47	114.58	42
1	125.85	30	126.08	22	124.34	43
4	137.30	28	139.46	19	138.36	37
α	145.15	52	145.99	38	145.32	43
3	147.29	53	148.88	43	148.00	82
5	147.29	53	148.88	43	148.00	82
γ	167.58	25	167.78	11	166.98	32

Compound Number 61



trans

Methyl p-Coumarate

methyl 4-hydroxycinnamate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ OMe	3.80	s	
α	7.64	d	16.0
3,5	6.86	m	8.7
2,6	7.42	m	8.7
β	6.28	d	16.0

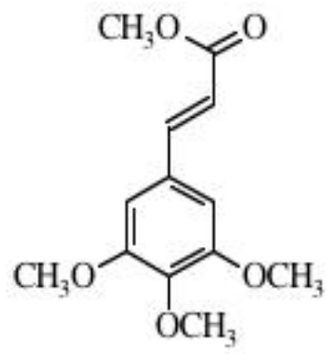
Notes:

J. Ralph JRPS 133.2x1
68mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ OMe	51.71	38	51.49	41	51.13	44
β	114.98	36	115.22	40	113.90	44
3	115.95	91	116.64	100	115.78	99
5	115.95	91	116.64	100	115.78	99
1	126.98	21	126.90	20	125.07	35
2	130.00	100	130.82	94	130.21	100
6	130.00	100	130.82	94	130.21	100
α	144.89	38	145.33	46	144.69	51
4	158.12	24	160.45	28	159.87	46
γ	168.18	14	167.87	14	166.99	30

Compound Number 62



trans

methyl (3,4,5-trimethoxy)cinnamate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ OMe	3.74	s	
3,5 OMe	3.82	s	
4 OMe	3.82	s	
2,6	6.70	s	
α	7.54	d	
β	6.29	d	15.9

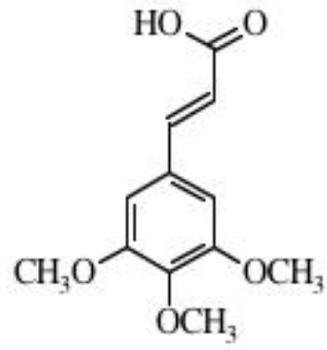
Notes:

J. Ralph JRPS 139x1
92mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ OMe	51.61	43	51.57	41	51.31	48
3 OMe	56.15	100	56.45	100	56.02	100
5 OMe	56.15	100	56.45	100	56.02	100
4 OMe	60.89	39	60.58	42	60.06	46
2	105.36	90	106.58	84	105.99	84
6	105.36	90	106.58	84	105.99	84
β	117.04	46	117.70	50	117.06	46
1	129.90	33	130.70	28	129.61	36
4	140.24	16	141.27	11	139.61	19
α	144.81	52	145.45	49	144.75	45
3	153.46	53	154.51	42	153.11	42
5	153.46	53	154.51	42	153.11	42
γ	167.29	25	167.51	22	166.78	34

Compound Number 63



trans

3,4,5-trimethoxy cinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
3,5 OMe	3.89	s	
4 OMe	3.89	s	
2,6	6.78	s	
α	7.70	d	15.9
β	6.36	d	15.9

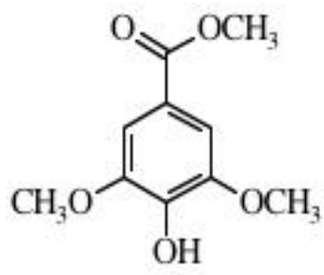
Notes:

Aldrich
100mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3 OMe	56.19	100	56.49	100	55.98	100
5 OMe	56.19	100	56.49	100	55.98	100
4 OMe	60.96	35	60.60	43	60.05	69
2	105.67	81	106.62	87	105.77	80
6	105.67	81	106.62	87	105.77	80
b	116.55	44	118.15	55	118.51	49
1	129.52	39	130.83	30	129.87	48
4	140.62	18	141.24	12	139.38	27
α	147.02	42	145.87	46	144.14	53
3	153.48	76	154.54	47	153.10	91
5	153.48	76	154.54	47	153.10	91
γ	172.46	32	168.33	28	167.72	52

Compound Number 64



Syringic acid methyl ester
methyl (4-hydroxy-3,5-dimethoxy)benzoate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α OMe	3.89	s	
3,5 OMe	3.90	s	
2,6	7.31	s	

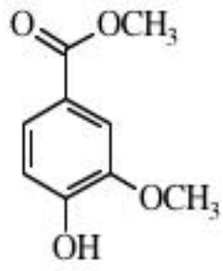
Notes:

J. Ralph JRPS 7x1
93.3mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α OMe	52.07	47	52.11	47	51.78	50
3 OMe	56.41	100	56.67	98	56.04	100
5 OMe	56.41	100	56.67	98	56.04	100
2	106.80	99	107.87	100	106.82	82
6	106.80	99	107.87	100	106.82	82
1	120.96	24	121.07	22	119.28	34
4	139.49	27	141.65	25	140.72	37
3	146.78	54	148.33	46	147.58	66
5	146.78	54	148.33	46	147.58	66
α	166.92	18	167.16	15	166.10	29

Compound Number 65



Vanillic acid methyl ester
methyl (3-methoxy-4-hydroxy)benzoate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α OMe	3.88	s	
4 OMe	3.88	s	
2	7.53	d	1.8
5	6.93	d	8.3
6	7.62	dd	8.3, 1.8

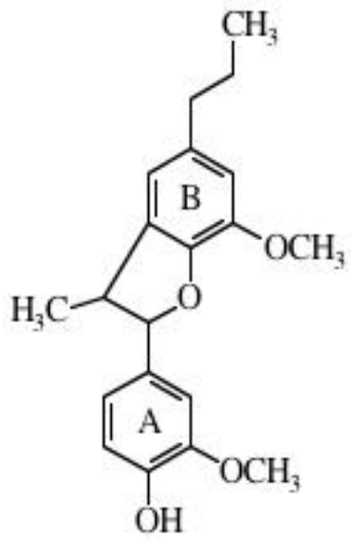
Notes:

J. Ralph JRPS 3.1
101mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α OMe	52.02	83	52.00	79	51.64	89
4 OMe	56.07	100	56.29	91	55.60	100
2	111.98	81	113.20	89	112.54	80
5	114.33	91	115.58	89	115.19	96
1	122.13	37	122.43	38	120.52	53
6	124.23	98	124.53	100	123.44	88
3	146.41	34	148.08	29	147.36	64
4	150.29	45	152.14	46	151.53	78
α	167.12	24	167.15	23	166.06	46

Compound Number 66



Dihydrodehydrodiisoeugenol

2-Methoxy-4-(7-methoxy-3-methyl-5-propyl-2,3-dihydro benzofuran-2-yl)phenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B γ	0.96	t	7.3
γ	1.36	d	6.8
B β	1.64	m	7.3
B α	2.55	t	7.3
β	3.44	dd	9.6,6.8
OMe	3.86	s	
OMe	3.87	s	
α	5.07	d	9.6
B2	6.59	s	
B6	6.62	s	
A5	6.89	m	
A6	6.89	m	
A2	6.99	s	

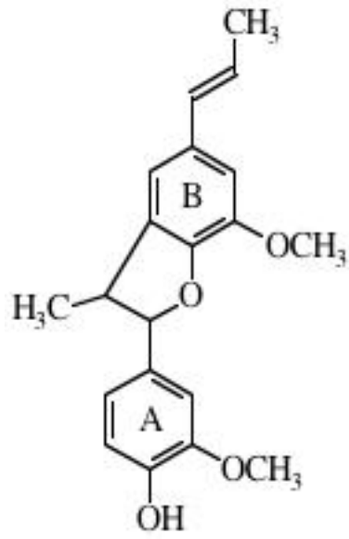
Notes:

J. Ralph JRL 109x2
44mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ	13.90	80	14.08	88	13.65	85
γ	17.44	72	17.83	88	17.17	81
B β	25.07	84	25.74	97	24.52	94
B α	38.09	71	38.54	79	37.27	77
β	45.81	85	46.43	91	44.71	74
OMe	55.99	100	56.28	100	55.59	100
OMe	55.99	100	56.41	97	55.64	100
α	93.61	66	93.80	94	92.37	70
A2	109.04	72	110.69	85	110.56	66
B2	111.91	65	113.63	76	112.24	57
A5	114.11	63	115.55	76	115.20	66
B6	115.46	74	116.39	85	115.35	68
A6	119.94	76	120.22	91	119.25	74
A1	132.28	52	133.03	53	130.82	77
B5	132.98	45	134.12	44	132.91	68
B1	136.29	45	136.62	59	135.32	64
B4	143.86	44	144.78	41	143.30	64
A4	145.41	24	146.59	32	144.93	45
B3	145.77	43	147.52	44	146.67	77
A3	146.71	35	148.39	38	147.59	77

Compound Number 67



Dehydrodiisoeugenol

2-Methoxy-4-(7-methoxy-3-methyl-5-propenyl-2,3-dihydro benzofuran-2-yl) phenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ	1.37	d	6.8
B γ	1.87	dd	5.3, 1.2
β	3.44	dt	9.4, 6.8
OMe	3.85	s	
OMe	3.88	s	
α	5.09	d	9.4
B β	6.11	dq	15.8, 5.3
B α	6.36	dq	15.8, 1.2
B2	6.76	s	
B6	6.78	s	
A5	6.88	m	
A6	6.80	m	
A2	6.97	s	

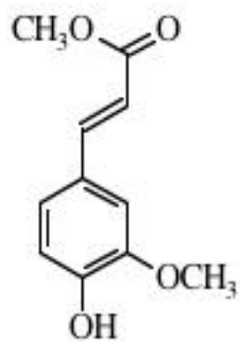
Notes:

J. Ralph JRKM 67-1
150mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	17.60	43	17.86	89	17.25	72
B γ	18.34	41	18.42	93	18.06	78
β	45.62	52	46.21	100	44.51	60
OMe	55.97	100	56.25	93	55.59	100
OMe	55.97	100	56.33	81	55.61	95
α	93.76	47	93.96	84	92.55	60
A2	108.97	48	110.66	86	109.74	50
B2	109.40	41	111.06	77	110.58	58
A5	113.36	46	114.30	87	113.29	58
B6	114.14	47	115.55	84	115.23	55
A6	119.91	47	120.21	93	119.25	60
B β	123.41	47	123.22	97	122.60	60
B α	130.98	51	132.05	93	130.68	52
A1	132.11	26	132.81	67	130.93	65
B5	132.22	34	132.83	61	131.39	62
B1	133.30	32	134.43	54	133.30	65
B4	144.15	28	145.03	26	143.61	60
A4	145.82	31	147.53	53	146.07	45
B3	146.62	30	147.72	20	146.71	55
A3	146.71	32	148.36	44	147.59	60

Compound Number 68



trans

Methyl ferulate

methyl 4-hydroxy-3-methoxycinnamate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ OMe	3.79	s	
3 OMe	3.89	s	
2	7.31	d	1.8
α	7.61	d	15.9
5	6.90	d	8.1
6	7.05	dd	8.1, 1.8
β	6.28	d	15.9

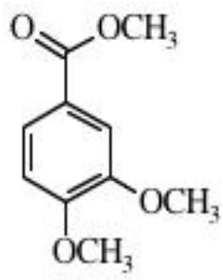
Notes:

J. Ralph JRKM 85.1
54mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ OMe	51.60	80	51.47	86	51.12	90
3 OMe	55.93	90	56.32	100	55.68	100
2	109.56	92	111.34	98	111.32	71
β	114.86	96	115.51	100	114.19	72
5	115.09	85	116.03	98	115.54	81
6	123.00	100	123.78	88	122.99	81
1	126.92	58	127.38	50	125.56	66
α	145.03	92	145.65	96	145.02	78
3	146.89	51	148.66	44	147.92	65
4	148.11	58	149.99	50	149.38	72
γ	167.80	47	167.82	40	167.02	62

Compound Number 69



Methylveratrate

methyl 3,4-dimethoxybenzoate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α OMe	3.89	s	
OMe	3.93	s	
OMe	3.93	s	
2	7.54	d	1.9
5	6.88	d	8.4
6	7.67	dd	8.4, 1.9

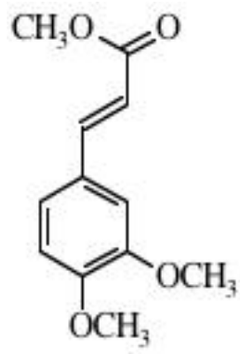
Notes:

J. Ralph JRPS 5.1
55mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α OMe	51.93	45	52.00	68	51.79	86
OMe	55.99	100	56.10	100	55.50	100
OMe	55.99	100	56.10	100	55.66	94
2	110.32	45	111.65	75	111.07	86
5	112.05	46	112.99	70	111.70	82
1	122.71	16	123.37	25	121.84	51
6	123.58	49	124.08	77	123.13	93
3	148.65	17	149.90	23	148.46	51
4	153.00	16	154.38	19	152.98	43
α	166.82	14	166.92	19	165.96	35

Compound Number 70



trans

methyl 3,4-dimethoxycinnamate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ OMe	3.79	s	
OMe	3.90	s	
OMe	3.90	s	
2	7.04	d	1.9
5	6.86	d	8.2
6	7.09	dd	8.2, 1.9
α	7.63	d	15.9
β	6.30	d	15.9

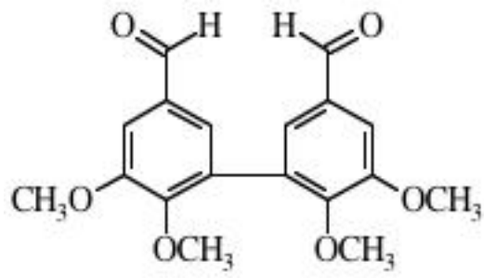
Notes:

J. Ralph JRPS 21x1
52mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ OMe	51.55	79	51.50	77	51.20	96
3 OMe	55.89	92	56.07	100	55.52	97
4 OMe	55.96	100	56.12	96	55.59	100
2	109.77	79	111.23	88	110.49	77
5	111.12	84	112.38	88	111.51	83
β	115.53	78	116.15	89	115.26	83
6	122.56	81	123.46	93	122.81	89
1	127.41	56	128.19	43	126.85	68
α	144.74	85	145.41	88	144.67	80
3	149.27	40	150.59	32	149.00	61
4	151.18	41	152.54	32	151.02	58
γ	167.58	49	167.71	39	166.92	61

Compound Number 71



Dehydrodiveratraldehyde

5,6,5',6'-Tetramethoxybiphenyl-3,3'-dicarbaldehyde

^{1}H (chloroform)

Atom	H Shifts	Mult	J
4 OMe	3.77	s	
3 OMe	3.99	s	
2	7.51	d	1.9
6	7.40	d	1.9
α	9.91	s	
acetone			
4 OMe	3.75	s	
3 OMe	4.01	s	
2	7.58	d	
6	7.44	d	
α	9.96	s	

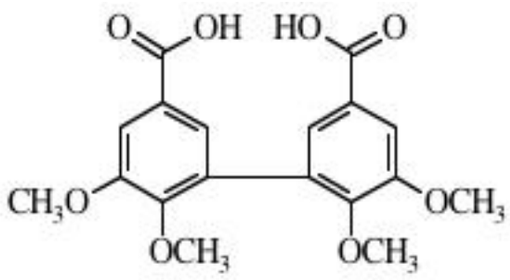
Notes:

Obst
38 mg contains impurity
As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3 OMe	56.05	100	56.40	90	55.94	100
4 OMe	60.95	79	60.98	73	60.36	93
2	110.43	86	111.92	90	111.39	63
6	127.51	83	127.15	97	125.97	74
5	131.76	48	133.01	33	131.52	58
1	132.06	60	133.21	47	131.76	82
4	152.36	35	153.02	23	151.50	44
3	153.37	50	154.27	40	152.82	72
α	190.87	100	191.51	100	191.60	75

Compound Number 72



Dehydrodiveratric acid

5,6,5',6'-Tetramethoxybiphenyl-3,3'-dicarboxylic acid

^{1}H (DMSO)

Atom	H Shifts	Mult	J
3 OMe	3.64	s	
4 OMe	3.93	s	
2	7.42	d	1.9
6	7.71	d	1.9

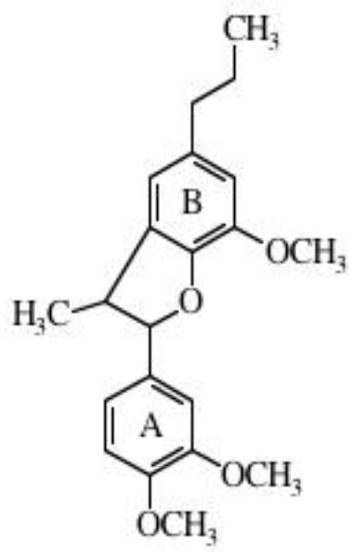
Notes:

Obst 35 mg
* only soluble in DMSO * aldehyde impurity
As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3 OMe					55.81	98
4 OMe					60.19	100
2					112.91	48
6					124.10	65
1					125.84	73
5					131.27	62
4					150.04	67
3					152.11	94
α					166.72	60

Compound Number 73



2-(3,4-Dimethoxyphenyl)-7-methoxy-3-methyl-5-propyl-2,3-dihydrobenzofuran

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B γ	0.96	t	7.3
γ	1.37	d	6.8
B β	1.64	h	7.3
B α	2.55	t	7.3
β	4.45	dq	9.6, 6.8
OMe	3.86	s	
OMe	3.87	s	
OMe	3.88	s	
α	5.09	d	9.6
B2	6.59	s	
B6	6.62	s	
A5	6.83	d	8.2
A6	6.96	dd	8.2, 1.9
A2	7.00	dd	1.9

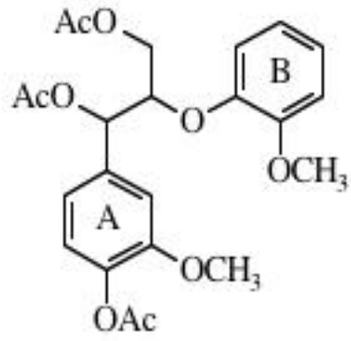
Notes:

Obst
45mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ	13.90	65	14.08	55	13.66	88
γ	17.47	63	17.90	55	17.18	75
B β	25.06	67	25.74	63	24.53	81
B α	38.09	63	38.53	62	37.28	69
β	45.77	60	46.47	55	44.87	68
OMe	55.92	100	56.12	100	55.47	100
OMe	55.92	100	56.12	100	55.47	100
OMe	56.00	62	56.41	60	55.66	76
α	93.48	61	93.58	62	92.11	62
A2	109.62	57	111.03	53	110.01	60
A5	110.88	58	112.57	58	111.58	60
B2	111.90	56	113.62	53	112.28	51
B6	115.44	52	116.40	55	115.37	60
A6	119.22	63	119.68	55	118.85	64
B5	132.90	25	134.07	33	132.49	55
A1	132.95	44	134.25	33	132.86	57
B1	136.30	38	136.69	32	135.46	61
B4	143.87	32	144.80	28	143.34	54
B3	145.42	25	146.57	18	144.92	37
A3	149.10	33	150.40	22	148.83	93
A4	149.16	32	150.49	23	148.83	93

Compound Number 74



threo

Guaiacylglycerol-β-guaiacyl ether triacetate

1-(4-acetoxy-3-methoxyphenyl)-1,3-diacetoxy-2-(2-methoxy phenoxy)propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	1.99	s	
Ac Me	2.05	s	
Ac Me	2.29	s	
OMe	3.80	s	
OMe	3.81	s	
γ1	4.06	dd	11.9, 5.7
γ2	4.32	dd	11.9, 4.5
α	6.12	d	6.3
β	4.63	m	

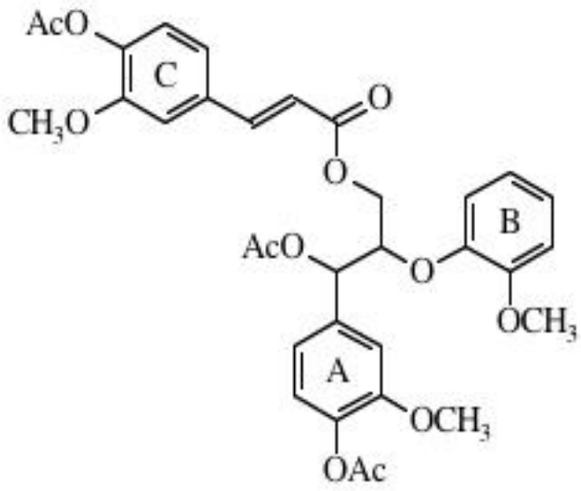
Notes:

R. Helm RFH5C
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.63	86	20.45	89	20.28	94
Ac Me	20.68	78	20.58	84	20.35	100
Ac Me	21.02	88	20.91	61	20.63	82
OMe	55.81	100	56.21	92	55.54	100
OMe	55.96	94	56.30	100	55.76	91
γ	63.09	75	63.58	79	62.47	52
α	74.52	86	75.37	87	74.28	67
β	80.26	87	80.68	87	79.05	67
A2	111.75	86	112.66	87	111.62	64
B2	112.58	90	113.76	79	112.75	76
B5	118.79	91	119.22	95	117.47	73
A6	119.58	84	120.27	95	119.36	64
B6	121.00	90	121.66	87	120.64	76
A5	122.79	78	123.52	79	122.57	58
B1	123.31	91	123.75	87	122.62	58
A1	135.35	68	136.66	61	135.40	79
A4	139.93	49	140.88	37	139.19	58
B4	147.96	54	149.05	37	147.54	61
B3	150.84	54	151.81	39	150.13	73
A3	151.12	55	152.18	47	150.67	73
A4 Ac C=O	168.71	48	168.83	34	168.31	58
α Ac C=O	169.65	49	169.94	39	169.30	61
γ Ac C=O	170.52	51	170.62	42	169.89	67

Compound Number 75



threo

3-(4-Acetoxy-3-methoxyphenyl) acrylic acid 3-acetoxy- 3- (4- acetoxy -3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.28	s	
Ac Me	2.31	s	
Ac Me	2.07	s	
OMe	3.80	s	
OMe	3.80	s	
OMe	3.87	s	
γ1	4.20	dd	11.9, 5.2
γ2	4.42	dd	11.9, 4.2
β	4.70	m	
α	6.20	d	6.5
C β	6.35	d	15.9
C α	7.54	d	15.9

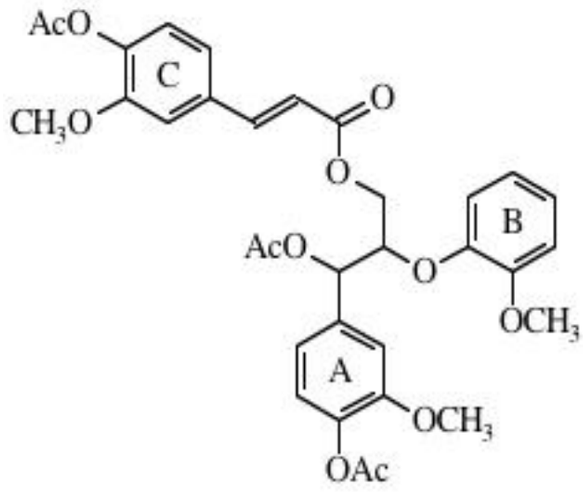
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.61	93	20.46	100	20.30	100
Ac Me	20.61	93	20.46	100	20.30	100
Ac Me	21.06	42	20.95	48	20.67	58
OMe	55.80	53	56.21	54	55.55	67
OMe	55.95	100	56.29	54	55.75	62
OMe	55.95	100	56.41	54	55.96	71
γ	63.35	28	63.94	39	62.87	21
α	74.64	35	75.54	39	74.44	33
β	80.51	37	80.85	41	79.20	33
C2	111.27	37	112.46	50	111.68	33
A2	111.74	35	112.70	43	111.86	46
B2	112.54	44	113.74	43	112.75	50
C β	117.58	35	118.62	48	117.53	54
B5	119.01	44	119.32	52	117.68	54
A6	119.55	40	120.29	43	119.38	33
B6	120.99	51	121.67	50	120.66	58
C6	121.44	44	122.25	46	121.62	46
A5	122.85	35	123.57	46	122.58	42
B1	123.23	49	123.78	48	122.67	38
C5	123.35	40	124.08	61	123.15	58
C1	133.16	30	134.09	30	132.81	46
A1	135.34	33	136.65	30	135.41	46
A4	139.93	26	140.91	26	139.21	50
C4	141.61	28	142.73	26	141.10	42
C α	144.62	42	145.16	48	144.30	42
B4	147.96	33	149.08	26	147.57	46
B3	150.93	33	151.87	26	150.16	46
A3	151.14	30	152.20	28	150.68	50
C3	151.42	40	152.64	35	151.13	54
C γ	166.24	28	166.62	35	165.74	50
Ac C=O	168.67	37	168.75	35	168.22	54
Ac C=O	168.70	33	168.82	26	168.29	50
Ac C=O	169.70	33	169.99	28	169.34	46

Notes:

R. Helm RFH101D1
40mg Vinyl C's at 124.08 and 145.16 in acetone. In CDCl3 123.23 and 144.62
Acetone 1H data in J. Ag. Food Chem. 41(4) 570-576, 1993

Compound Number 76



erythro

3-(4-Acetoxy-3-methoxyphenyl) acrylic acid 3-acetoxy- 3-(4- acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.32	s	
Ac Me	2.29	s	
Ac Me	2.10	s	
OMe	3.77	s	
OMe	3.82	s	
OMe	3.87	s	
γ1	4.44	dd	11.9, 4.2
γ2	4.53	dd	11.9, 5.3
β	4.75	m	
α	6.14	d	5.5
C β	6.35	d	16.0
C α	7.54	d	16.0

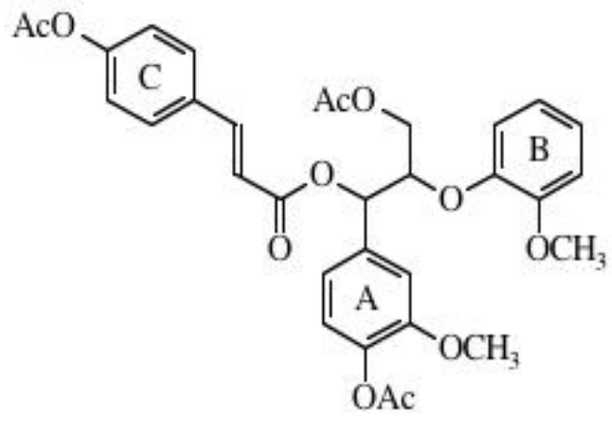
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.64	70	20.46	100	20.32	100
Ac Me	20.64	70	20.46	100	20.32	100
Ac Me	21.05	41	20.90	42	20.66	44
OMe	55.81	48	56.22	48	55.60	76
OMe	55.96	100	56.30	56	55.73	42
OMe	55.96	100	56.41	62	55.97	62
γ	62.88	30	63.34	36	62.26	31
α	73.96	31	74.72	42	73.28	30
β	80.46	38	80.52	44	78.58	41
C2	111.31	38	112.47	46	111.72	23
A2	112.05	33	112.77	46	111.86	34
B2	112.63	39	113.80	46	112.91	58
C β	117.70	36	118.62	40	117.70	41
B5	119.74	75	119.97	50	118.08	54
A6	119.74	75	120.44	44	119.41	32
B6	121.00	45	121.65	48	120.67	54
C6	121.44	38	122.22	48	121.60	31
A5	122.60	38	123.37	44	122.50	44
B1	123.23	44	124.09	86	122.90	44
C5	123.66	42	124.09	86	123.16	55
C1	133.22	31	134.09	32	132.80	56
A1	135.53	34	136.71	38	135.37	52
A4	139.80	30	140.79	28	139.11	44
C4	141.58	20	142.74	20	141.11	49
C α	144.61	34	145.13	48	144.28	48
B4	147.23	33	148.30	30	146.70	61
B3	151.00	30	152.11	36	150.38	38
A3	151.20	34	152.11	32	150.58	61
C3	151.42	31	152.65	32	151.16	39
C γ	166.40	34	166.64	32	165.77	45
Ac C=O	168.68	31	168.75	32	168.20	34
Ac C=O	168.75	28	168.86	28	168.31	45
Ac C=O	169.50	23	169.89	28	169.20	35

Notes:

R. Helm RFH101D2
30mg Vinyl C's at 124.09 and 145.13 in acetone
Acetone 1H data in J. Ag. Food Chem. 41(4) 570-576, 1993

Compound Number 77



erythro

3-(4-Acetoxyphenyl) acrylic acid 3-acetoxy-1-(4-acetoxy- 3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.02	s	
Ac Me	2.28	s	
Ac Me	2.30	s	
OMe	3.77	s	
OMe	3.81	s	
γ1	4.32	dd	11.9, 4.3
γ2	4.48	dd	11.9, 5.9
β	4.77	m	
α	6.20	d	5.0
C β	6.44	d	16.0
C2,6	7.13	m	8.6
C3,5	7.53	m	8.6
C α	7.65	d	16.0

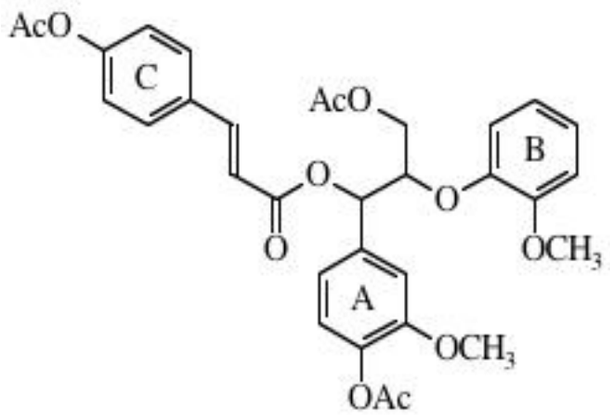
Notes:

R. Helm RFH119D1
47mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.64	64	20.46	67	20.30	71
Ac Me	20.75	57	20.62	48	20.39	77
Ac Me	21.09	60	20.95	48	20.79	68
OMe	55.82	55	56.24	60	55.61	74
OMe	55.94	64	56.31	54	55.74	74
γ	62.73	34	63.16	38	62.06	29
α	74.12	45	74.97	44	73.50	39
β	80.25	40	80.43	46	78.57	35
A2	111.88	45	112.82	42	111.73	42
B2	112.68	51	113.82	48	112.91	55
C β	117.66	47	118.65	40	117.55	48
B5	119.58	49	119.87	48	118.04	48
A6	119.66	47	120.45	46	119.31	39
B6	121.02	53	121.67	48	120.68	45
C3	122.15	91	123.20	100	122.31	100
C5	122.15	91	123.20	100	122.31	100
A5	122.60	43	123.38	44	122.52	42
B1	123.63	47	124.06	46	122.89	45
C2	129.31	100	130.25	92	129.65	97
C6	129.31	100	130.25	92	129.65	97
C1	131.91	34	132.79	35	131.49	48
A1	135.38	43	136.60	38	135.32	48
A4	139.78	34	140.82	27	139.12	48
C α	144.58	43	145.09	46	144.32	42
B4	147.18	36	148.38	25	146.76	52
B3	151.01	36	152.04	29	150.34	39
A3	151.15	38	152.11	29	150.57	35
C4	152.28	36	153.54	29	152.10	45
C γ	165.33	40	165.76	29	164.86	52
Ac C=O	168.74	32	168.85	29	168.32	55
Ac C=O	168.99	32	169.36	33	168.82	52
Ac C=O	170.72	36	170.71	31	169.95	55

Compound Number 78



threo

3-(4-Acetoxyphenyl)□acrylic acid 3-acetoxy-1-(4-acetoxy- 3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.28	s	
Ac Me	2.30	s	
OMe	3.77	s	
OMe	3.82	s	
γ1	4.14	dd	11.9, 5.8
γ2	4.36	dd	11.9, 4.4
β	4.72	m	
α	6.23	d	6.4
C β	6.37	d	16.0
C2.6	7.12	m	8.6
C3.5	7.49	m	8.6
C α	7.55	d	16.0

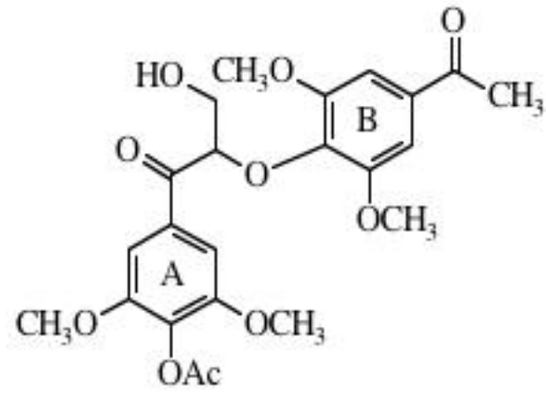
Notes:

R. Helm RFH119D2
44mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.64	56	20.44	44	20.29	78
Ac Me	20.72	56	20.60	34	20.38	74
Ac Me	21.10	51	20.95	47	20.78	63
OMe	55.77	59	56.17	59	55.53	85
OMe	55.97	59	56.31	51	55.80	74
γ	63.26	36	63.69	30	62.58	33
α	74.96	46	75.78	40	74.61	41
β	80.52	39	80.86	44	79.18	37
A2	111.71	43	112.73	34	111.71	41
B2	112.47	51	113.68	38	112.71	56
C β	117.78	49	118.73	43	117.56	56
B5	118.91	46	119.33	42	117.63	52
A6	119.49	43	120.27	45	119.36	37
B6	120.96	54	121.62	38	120.62	52
C3	122.14	90	123.16	100	122.28	100
C5	122.14	90	123.16	100	122.28	100
A5	122.84	38	123.56	38	122.57	52
B1	123.30	46	123.75	34	122.69	48
C2	129.26	100	130.15	69	129.56	93
C6	129.26	100	132.78	26	129.56	93
C1	131.96	39	132.78	26	131.50	56
A1	135.41	36	136.68	29	135.44	48
A4	139.94	38	140.94	23	139.25	52
C α	144.34	43	144.86	29	144.10	44
B4	148.08	38	149.10	26	147.56	59
B3	150.89	34	151.87	21	150.17	56
A3	151.14	36	152.21	21	150.69	44
C4	152.23	30	153.47	29	152.04	44
C γ	165.46	33	165.84	14	165.03	52
Ac C=O	168.70	30	168.77	19	168.27	37
Ac C=O	169.02	33	169.32	14	168.81	44
Ac C=O	170.56	30	170.62	22	169.90	48

Compound Number 79



1-(4-acetoxy-3,5-dimethoxyphenyl)-2-(4-acetyl-2,6-dimethoxy phenoxy) -3-hydroxypropan-1-one

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.35	s	
B β	2.58	s	
A3,5 OMe	3.81	s	
B3,5 OMe	3.86	s	
β	5.22	dd	7.2, 3.3
A2,6	7.36	s	
B2,6	7.21	s	

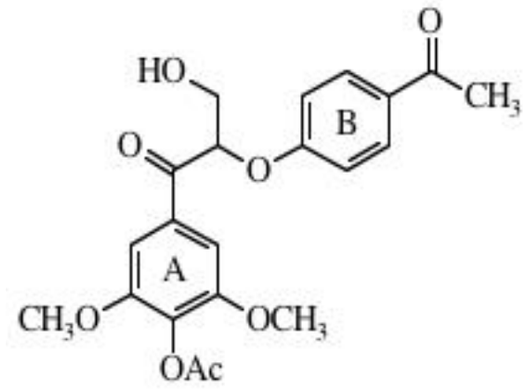
Notes:

SR III - 39
45mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.41	49	20.22	50	20.06	54
B β	26.41	57	26.54	50	26.48	53
OMe	56.24	100	56.56	82	56.01	100
OMe	56.24	100	56.56	82	56.01	100
OMe	56.39	89	56.70	100	56.18	89
OMe	56.39	89	56.70	100	56.18	89
γ	63.36	33	63.67	32	62.39	37
β	87.06	36	86.08	39	83.67	32
A2	105.72	94	106.52	84	105.44	67
A6	105.72	94	106.52	84	105.44	67
B2	105.75	76	106.62	90	105.85	70
B6	105.75	76	106.62	90	105.85	70
A1	133.17	27	133.66	27	131.79	39
A4	133.27	48	133.80	11	132.05	25
B1	133.27	48	134.87	23	133.69	37
B4	140.52	21	141.29	16	140.22	28
A3	152.33	68	153.21	94	151.62	68
A5	152.33	68	153.21	94	151.62	68
B3	152.36	70	153.21	94	151.71	79
B5	152.36	70	153.21	94	151.71	79
Ac C=O	168.05	27	168.15	21	167.60	33
B α	194.74	29	195.71	23	195.27	35
α	196.50	24	196.65	21	196.51	35

Compound Number 80



1-(4-acetoxy-3,5-dimethoxyphenyl)-2-(4-acetylphenoxy)-3-hydroxypropan-1-one

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.34	s	
B β	2.51	s	
A3,5 OMe	3.82	s	
γ	4.19	m	
β	5.60	dd	5.8, 4.2
A2,6	7.32	s	
B3,5	6.90	m	8.9
B2,6	7.87	m	8.9

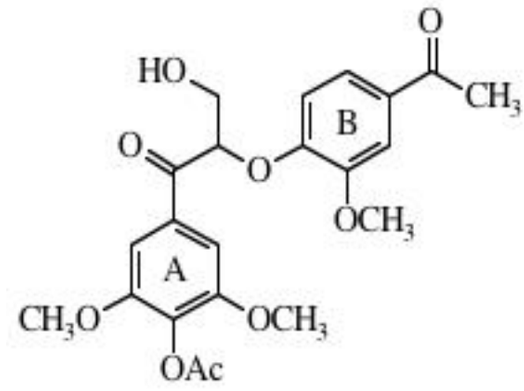
Notes:

SR III - 37
40mg
B2,6 and A1 shifts changes places in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.40	49	20.21	46	20.05	51
B β	26.33	56	26.34	50	26.28	53
OMe	56.36	100	56.76	100	56.31	100
OMe	56.36	100	56.76	100	56.31	100
γ	63.32	38	63.94	37	62.41	29
β	81.33	49	82.26	40	80.64	32
A2	105.67	89	106.40	90	105.42	64
A6	105.67	89	106.40	90	105.42	64
B3	114.83	85	115.68	96	114.78	73
B5	114.83	85	115.68	96	114.78	73
B2	130.78	92	131.20	87	130.36	66
B6	130.78	92	131.20	87	130.36	66
A1	131.38	33	131.80	23	130.19	37
B1	132.25	31	133.97	29	132.74	34
A4	133.87	18	134.34	12	132.55	24
A3	152.55	60	153.47	46	151.98	64
A5	152.55	60	153.47	46	151.98	64
B4	161.00	33	162.44	27	161.22	41
Ac C=O	168.06	24	168.11	19	167.62	34
B α	194.60	29	195.47	19	194.76	34
α	196.64	31	196.21	17	196.08	31

Compound Number 81



1-(4-acetoxy-3,5-dimethoxyphenyl)-2-(4-acetoxy-2-methoxy phenoxy)-3-hydroxypropan-1-one

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.34	s	
B β	2.53	s	
B3 OMe	3.89	s	
A3,5 OMe	3.85	s	
γ	4.17	d	5.1
β	5.53	t	5.1
A2,6	7.38	s	
B2	7.53	d	2.0
B5	6.82	d	8.4
B6	7.45	dd	8.4, 2.0

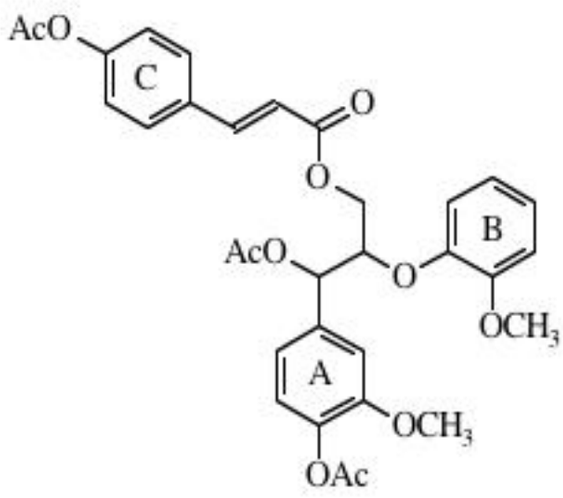
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.39	38	20.21	45	20.05	38
B β	26.23	67	26.30	55	26.23	71
B OMe	55.91	56	56.28	45	55.55	41
A OMe	56.32	59	56.69	100	56.22	100
A OMe	56.32	59	56.69	100	56.22	100
γ	63.47	27	63.91	42	62.32	32
β	83.63	38	83.76	50	81.51	46
A2	105.80	100	106.56	92	105.45	66
A6	105.80	100	106.56	92	105.45	66
B2	111.17	40	112.34	45	111.05	46
B5	114.89	33	114.72	45	113.02	56
B6	123.01	41	123.46	53	122.65	41
A1	132.23	35	132.37	21	130.46	47
B1	132.38	37	134.04	21	132.75	51
A4	133.75	16	134.22	11	132.46	21
B3	149.76	33	150.40	21	148.67	47
B4	150.76	16	152.27	21	150.96	50
A3	152.47	57	153.35	45	151.87	54
A5	152.47	57	153.35	45	151.87	54
Ac C=O	168.00	16	168.08	24	167.57	24
B α	194.85	17	195.94	24	195.02	50
α	196.57	21	196.27	21	196.14	41

Notes:

SR III - 38
17mg
B1 and A4 switch places in DMSO A4 has very low intensity and is easy to follow

Compound Number 82



threo

4-Acetoxycinnamic acid 3-acetoxy-3-(4-acetoxy- 3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.07	s	
Ac Me	2.28	s	
Ac Me	2.30	s	
OMe	3.79	s	
OMe	3.80	s	
γ1	4.23	dd	11.9, 5.8
γ2	4.42	dd	11.9, 4.2
β	4.72	m	
α	6.19	d	6.3
C β	6.34	d	16.0
C2,6	7.12	m	8.6
C3,5	7.51	m	8.6
C α	7.55	d	16.0

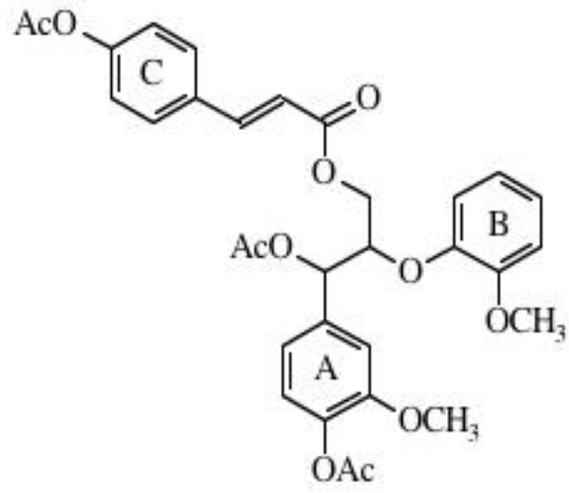
Notes:

R. Helm RFH87D1
36.6mg
129.85 and 129.57 for Bα and C2,6 change places in DMSO see 1019

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.63	38	20.46	38	20.29	45
Ac Me	21.07	55	20.95	89	20.67	52
Ac Me	21.10	60	20.95	89	20.78	57
OMe	55.81	49	56.21	52	55.55	67
OMe	55.95	44	56.28	52	55.75	52
γ	63.39	28	63.93	33	62.86	21
α	74.62	36	75.53	21	74.43	33
β	80.50	36	80.88	41	79.25	33
A2	111.78	33	112.71	38	111.70	31
B2	112.55	42	113.75	42	112.76	45
C β	117.58	39	118.56	41	117.51	40
B5	118.98	47	119.36	47	117.59	50
A6	119.56	35	120.30	34	119.38	29
B6	121.01	43	121.68	51	120.66	48
C3	122.13	100	123.17	100	122.29	100
C5	122.13	100	123.17	100	122.29	100
A5	122.84	36	123.56	36	122.59	40
B1	123.35	41	123.78	48	129.85	17
C2	129.30	83	130.20	82	129.57	90
C6	129.30	83	130.20	82	129.57	90
C1	131.95	35	132.78	29	131.49	43
A1	135.36	34	136.67	30	135.43	40
A4	139.94	32	140.90	18	139.21	40
C α	144.22	44	144.71	42	143.87	40
B4	148.00	30	149.10	27	147.59	50
B3	150.92	30	151.88	21	150.18	43
A3	151.14	28	152.20	23	150.67	36
C4	152.23	27	153.48	27	152.04	40
C γ	166.28	32	166.56	30	165.66	40
Ac C=O	168.70	25	168.81	22	168.28	33
Ac C=O	169.02	32	169.35	36	168.83	45
Ac C=O	169.68	25	169.96	22	169.32	40

Compound Number 83



erythro

4-Acetoxycinnamic acid 3-acetoxy-3-(4-acetoxy- 3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.10	s	
Ac Me	2.29	s	
Ac Me	2.30	s	
OMe	3.76	s	
OMe	3.81	s	
γ1	4.47	dd	11.9, 4.2
γ2	4.75	dd	11.9, 5.6
β	4.75	m	
α	6.14	d	5.4
C β	6.35	d	16.0
C α	7.56	d	16.0

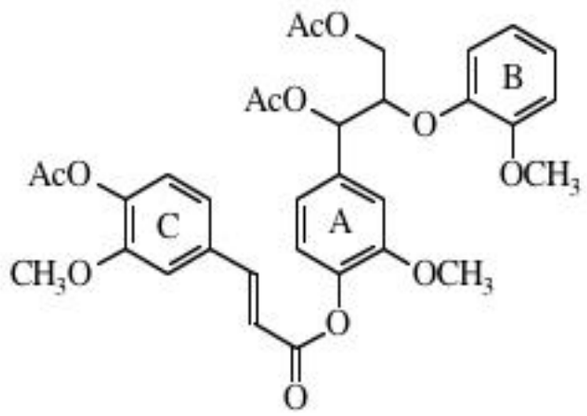
Notes:

Rich Helm RFH87D2
38.6mg
see 1020

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.65	50	20.47	40	20.29	65
Ac Me	21.03	50	20.90	42	20.63	58
Ac Me	21.10	51	20.95	50	20.78	62
OMe	55.80	49	56.21	50	55.58	69
OMe	55.94	54	56.28	48	55.70	58
γ	62.93	32	63.34	34	62.26	23
α	74.01	39	74.73	42	73.28	35
β	80.43	44	80.54	36	78.58	31
A2	112.04	39	112.78	36	111.71	42
B2	112.64	40	113.79	46	112.89	46
C β	117.67	46	118.54	44	117.46	46
B5	119.73	71	120.01	44	118.09	46
A6	119.73	71	120.44	44	119.39	35
B6	121.01	44	121.64	48	120.65	46
C3	122.11	100	123.17	100	122.29	100
C5	122.11	100	123.17	100	122.29	100
A5	122.59	42	123.35	42	122.48	42
B1	123.66	46	124.09	44	122.89	46
C2	129.30	90	130.18	98	129.54	96
C6	129.30	90	130.18	98	129.54	96
C1	132.00	31	132.77	46	131.46	35
A1	135.53	39	136.71	30	135.36	46
A4	139.80	33	140.78	34	139.08	46
C α	144.19	43	144.68	38	143.85	46
B4	147.25	29	148.31	22	146.69	46
B3	151.00	35	152.10	46	150.35	42
A3	151.19	33	152.10	46	150.55	50
C4	152.21	24	153.48	22	152.02	38
C γ	166.42	33	166.57	30	165.67	46
Ac C=O	168.74	25	168.84	24	168.32	46
Ac C=O	169.02	31	169.35	26	168.84	50
Ac C=O	169.50	35	169.87	24	169.21	46

Compound Number 84



erythro

3-(4-Acetoxy-3-methoxyphenyl)acrylic acid 4-[1,3-diacetoxy-2-(2-methoxyphenoxy)propyl]phenyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.03	s	
Ac Me	2.10	s	
Ac Me	2.32	s	
OMe	3.79	s	
OMe	3.82	s	
OMe	3.86	s	
γ1	4.27	dd	11.9, 4.0
γ2	4.47	dd	11.9, 5.6
β	4.69	m	
α	6.11	d	5.4
C β	6.60	d	15.9
C α	7.80	d	15.9

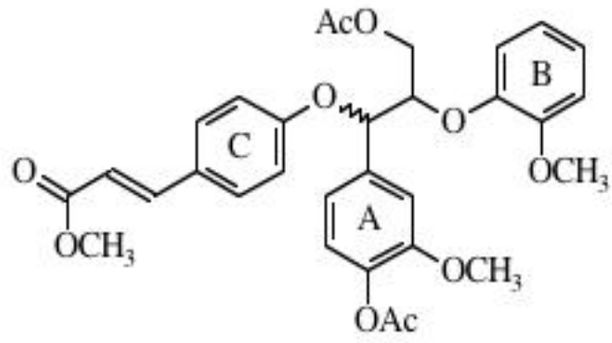
Notes:

R. Helm RFH9D
39.4mg
see 1026

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.62	77	20.47	92	20.31	81
Ac Me	20.76	68	20.61	79	20.37	88
Ac Me	21.01	70	20.87	74	20.60	81
OMe	55.81	85	56.21	100	55.58	100
OMe	55.94	79	56.28	89	55.72	75
OMe	56.00	100	56.44	89	55.98	100
γ	62.59	57	63.00	68	61.89	44
α	73.84	57	74.61	74	73.17	50
β	80.22	57	80.32	71	78.40	44
C2	111.41	68	112.60	74	111.69	44
A2	112.04	57	112.79	61	112.13	56
B2	112.68	64	113.81	87	112.90	69
C β	117.16	57	118.04	71	117.09	50
B5	119.55	68	119.82	84	117.96	69
A6	119.75	55	120.45	71	119.36	44
B6	121.01	64	121.63	95	120.64	75
C6	121.54	68	122.47	79	121.90	56
A5	122.67	55	123.42	66	122.54	44
B1	123.33	68	124.04	84	122.87	56
C5	123.63	60	124.16	82	123.18	62
C1	133.17	49	134.02	63	132.77	50
A1	135.48	45	136.73	50	135.40	50
A4	139.77	40	140.70	39	139.03	50
C4	141.78	40	142.96	34	141.30	50
C α	145.85	57	146.39	66	145.79	50
B4	147.18	47	148.26	39	146.63	69
B3	151.10	57	152.04	50	150.32	62
A3	151.14	51	152.17	55	150.63	62
C3	151.49	53	152.73	61	151.17	62
C γ	164.57	42	164.96	50	164.22	50
Ac C=O	168.64	51	168.74	58	168.21	56
Ac C=O	169.50	40	169.86	50	169.20	56
Ac C=O	170.74	38	170.70	42	169.96	69

Compound Number 85



3-{4-[3-Acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxy phenoxy)propoxy]phenyl}acrylic acid methyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	1.95	s	
Ac Me	2.27	s	
OMe	3.71	s	
OMe	3.76	s	
OMe	3.77	s	
γ	4.61	m	
β	4.46	m	
α	5.51	d	5.0
C β	6.27	d	16.0
C3,5	6.88	m	8.7
C2,6	7.39	m	8.7
C α	7.59	d	16.0

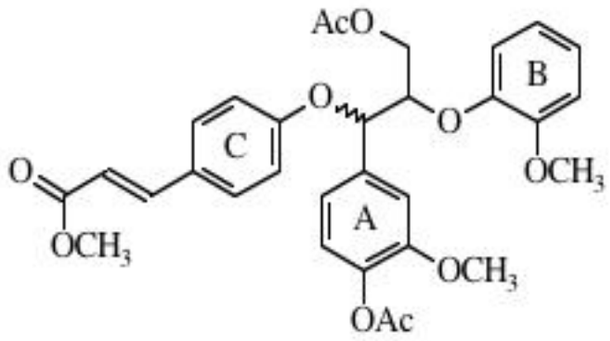
Notes:

R. Helm RFH111D1
39.0 mg
Isomer of 86

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.62	54	20.45	55	20.29	77
Ac Me	20.72	51	20.60	48	20.39	71
C γ OMe	51.54	49	51.52	52	51.19	71
OMe	55.72	56	56.17	61	55.53	87
OMe	55.96	52	56.27	61	55.70	81
γ	62.79	41	63.18	42	62.20	39
α	78.84	44	79.69	52	77.75	45
β	82.13	43	81.73	48	79.67	48
A2	110.95	47	112.62	48	111.97	45
B2	112.61	48	113.79	55	112.85	61
C β	115.75	48	116.52	52	115.50	52
C3	116.22	100	117.18	100	116.08	94
C5	116.22	100	117.18	100	116.08	94
B5	119.05	44	119.93	55	117.78	58
A6	119.92	54	120.27	45	119.39	45
B6	121.05	48	121.63	55	120.62	61
A5	122.86	49	123.50	52	122.52	45
B1	123.75	44	123.99	48	122.69	45
C1	127.82	47	128.60	35	127.21	58
C2	129.63	95	130.56	94	129.96	100
C6	129.63	95	130.56	94	129.96	100
A1	136.23	46	137.03	42	135.78	55
A4	139.65	32	140.73	26	139.00	58
C α	144.26	44	144.77	55	143.99	52
B4	147.06	34	148.41	29	146.95	61
B3	151.23	35	152.04	29	150.26	65
A3	151.32	34	152.26	32	150.58	58
C4	159.48	34	160.44	32	158.88	61
A γ C=O	167.59	32	167.59	29	166.74	65
A4 C=O	168.70	30	168.78	29	168.24	42
C γ	170.74	39	170.69	32	169.98	65

Compound Number 86



3-{4-[3-Acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxy phenoxy)propoxy]phenyl}acrylic acid methyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	1.99	s	
Ac Me	2.28	s	
C γ OMe	3.75	s	
OMe	3.77	s	
OMe	3.79	s	
γ1	4.13	dd	11.8, 5.9
γ2	4.42	dd	11.7, 4.3
β	4.68	m	
α	5.51	d	5.3
C β	6.27	d	16.0
C2,6	7.37	m	8.7
C α	7.59	d	16.0

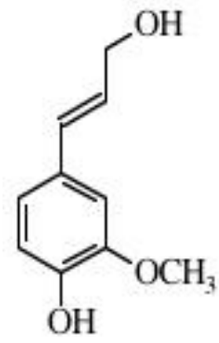
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.62	62	20.45	50	20.28	92
Ac Me	20.72	55	20.59	50	20.36	84
C γ OMe	51.53	51	51.52	55	51.17	72
OMe	55.69	55	56.14	50	55.45	92
OMe	55.96	59	56.30	52	55.74	80
γ	63.32	37	63.70	36	62.55	36
α	79.79	43	80.57	43	78.99	44
β	81.51	43	81.71	48	79.91	44
A2	111.00	45	112.61	48	111.77	44
B2	112.43	53	113.68	52	112.70	60
C β	115.68	51	116.43	40	115.36	52
C3	116.25	99	117.12	95	116.02	100
C5	116.25	99	117.12	95	116.02	100
B5	119.13	46	119.33	48	117.27	56
A6	119.23	50	120.27	48	119.42	44
B6	120.95	55	121.61	45	120.58	64
A5	122.93	46	123.67	64	122.35	44
B1	123.40	49	123.67	64	122.70	44
C1	127.72	38	128.47	43	127.02	60
C2	129.58	100	130.52	100	129.90	100
C6	128.58	100	130.52	43	129.90	100
A1	135.56	42	136.80	43	135.66	56
A4	139.86	29	140.88	26	139.12	52
C α	144.28	50	144.80	48	144.02	52
B4	148.03	33	149.21	29	147.68	56
B3	150.94	29	151.85	29	150.07	56
A3	151.42	33	152.37	26	150.75	52
C4	159.50	39	160.59	31	159.19	60
C γ C=O	167.60	39	167.60	29	166.74	64
A4 C=O	168.64	28	168.76	29	168.21	52
A γ	170.50	33	170.62	24	169.91	60

Notes:

Rich Helm RFH111D2
35mg
Isomer of 85

Compound Number 87



trans

Coniferyl alcohol

4-hydroxy-3-methoxy cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ OH	3.78	t	5.6
OMe	3.86	s	
γ's	4.18	td	5.5, 1.5
β	6.22	dt	15.9, 5.5
α	6.49	dt	15.9, 15
5	6.76	d	8.1
6	6.84	dd	8.1,1.9
2	7.04	d	1.9
4 OH	7.63	s	

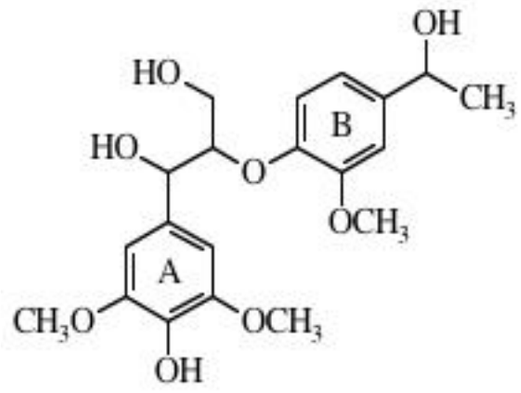
Notes:

Aldrich
30mg
Proton data from 360 MHz spectrum in acetone..S.Q.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.88	100	56.20	100	55.47	100
γ	63.71	87	63.42	80	61.63	86
2	108.52	80	110.06	76	109.66	84
5	114.57	93	115.76	83	115.36	86
6	120.25	87	120.60	91	119.30	86
β	126.22	90	128.07	78	127.38	91
1	129.30	45	130.26	41	128.41	67
α	131.24	82	130.45	72	128.87	81
4	145.63	46	147.14	41	146.06	67
3	146.75	38	148.41	30	147.60	63

Compound Number 88



threo

1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[4-(1-hydroxyethyl)-2-methoxyphenoxy]propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B β	1.38	d	6.4
B OMe	3.87	s	
A3,5 OMe	3.80	s	
α OH	4.50	d	3.9
A2,6	6.77	s	

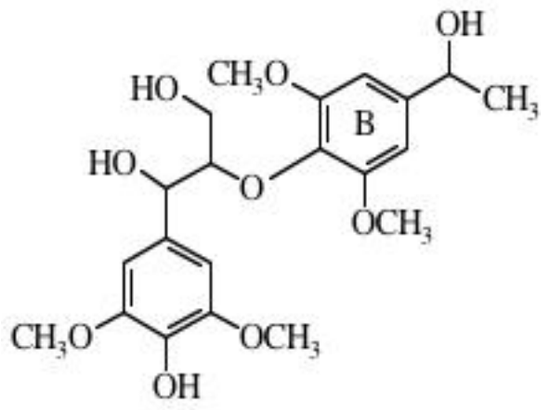
Notes:

S Ralph SRIII-43
30mg Small amount of 4 Ac present.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.24	37	26.23	47	25.84	70
B OMe	55.87	47	56.27	59	55.44	69
A OMe	56.33	100	56.59	100	55.73	100
A OMe	56.33	100	56.59	100	55.73	100
γ	61.04	28	61.94	34	59.99	26
B α	69.95	48	69.73	54	67.80	63
α	74.12	33	74.05	46	70.87	28
β	89.03	30	88.50	32	84.39	21
A2	103.79	66	105.36	95	104.06	53
A6	103.79	66	105.36	95	104.06	53
B2	109.30	36	110.58	39	109.65	27
B5	118.40	35	118.65	44	115.29	27
B6	120.27	22	119.45	34	117.20	36
A1	130.71	28	132.80	22	131.93	34
A4	134.56	25	136.12	20	134.24	29
B1	142.02	29	142.85	6	140.36	31
B4	146.66	25	148.27	29	146.73	33
A3	147.09	52	148.38	43	147.30	73
A5	147.09	52	148.38	43	147.30	73
B3	150.99	18	151.38	21	149.23	37

Compound Number 89



threo

1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[4-(1-hydroxyethyl)-2,6-dimethoxyphenoxy]propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B β	1.39	d	6.4
A3,5 OMe	3.80	s	
B3,5 OMe	3.89	s	
B α	4.81	m	
α	4.97	dd	7.3, 2.9
B2,5	6.77	s	
A2,6	6.76	s	
γ 2	3.31	m	
B α OH	4.27	d	4.1
α OH	4.44	d	2.9

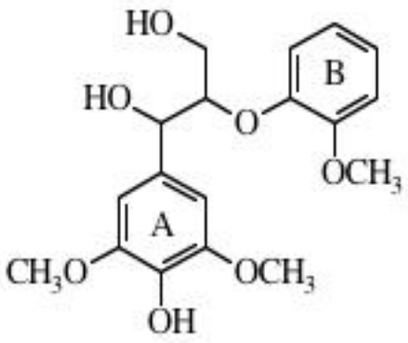
Notes:

S Ralph SRIII-44
30mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.43	37	26.27	45	25.84	28
OMe	56.12	94	56.50	100	55.80	100
OMe	56.12	94	56.50	100	55.80	100
OMe	56.31	100	56.57	95	55.80	100
OMe	56.31	100	56.57	95	55.80	100
γ	60.48	31	61.41	29	60.15	12
B α	70.21	43	69.98	41	68.09	26
α	74.34	37	74.22	36	71.54	16
β	88.97	37	89.69	36	87.11	16
B2	102.27	75	103.41	87	102.49	32
B6	102.27	75	103.41	87	102.49	32
A2	104.04	70	105.46	72	104.14	30
A6	104.04	70	105.46	72	104.14	30
A1	130.99	33	132.60	25	131.97	17
B1	134.10	21	135.54	12	134.22	15
A4	134.46	31	136.11	21	134.50	17
B4	142.94	32	144.61	26	142.91	17
A3	147.02	56	148.30	36	147.25	36
A5	147.02	56	148.30	36	147.25	36
B3	152.88	56	153.58	42	152.14	35
B5	152.88	56	153.58	42	152.14	35

Compound Number 90



threo

Syringylglycerol-β-guaiacyl ether

1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxyphenoxy) propane -1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B OMe	3.86	s	
A3,5 OMe	3.79	s	
α	4.88	dd	6.0, 3.7
β	4.22	m	
α OH	4.49	d	3.7
A2,6	6.86	s	

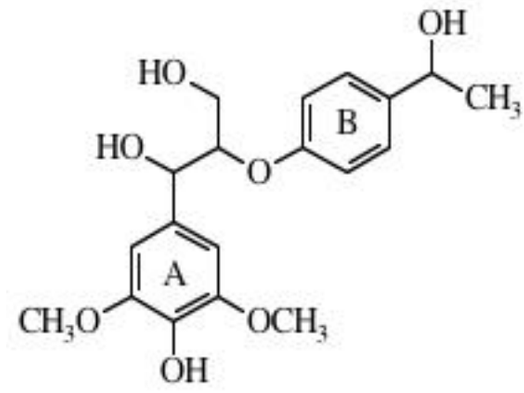
Notes:

S. Ralph SRIII-45
30mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B OMe	55.88	56	56.24	62	55.45	75
A OMe	56.32	100	56.54	100	55.72	100
A OMe	56.32	100	56.54	100	55.72	100
γ	61.02	37	61.89	40	60.01	18
α	74.16	39	73.97	40	70.88	36
β	89.22	34	88.19	46	84.03	32
A2	103.81	64	105.28	74	104.07	59
A6	103.81	64	105.28	74	104.07	59
B2	112.16	50	113.27	39	112.38	51
B5	120.86	40	119.66	4	115.52	33
B6	121.67	53	121.91	52	120.58	51
B1	124.17	40	123.30	56	120.90	37
A1	130.71	24	132.72	23	131.89	39
A4	134.57	19	136.07	16	134.26	30
A3	147.10	49	148.34	36	147.31	72
A5	147.10	49	148.34	36	147.31	72
B4	147.58	17	149.60	18	148.18	26
B3	151.22	23	151.65	15	149.55	33

Compound Number 91



1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[4-(1-hydroxy ethyl)phenoxy]propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B β	1.35	d	6.4
A3,5 OMe	3.79	s	
A2,6	6.77	s	
B2,6	7.23	m	8.6

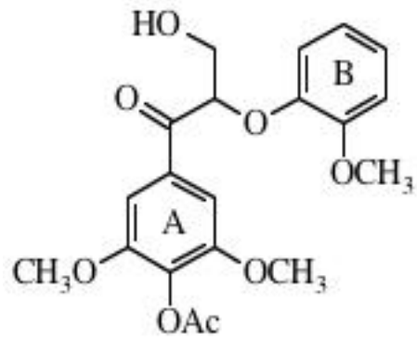
Notes:

S. Ralph SRIII-46
20mg contains 4-AC impurity.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.07	39	26.17	58	25.81	88
A OMe	56.34	**100**	56.58	94	55.82	**100**
A OMe	56.34	100	56.58	94	55.82	100
γ	61.14	30	61.73	32	60.01	27
B α	69.75	42	69.50	58	67.57	73
α	73.85	28	73.54	34	71.09	33
β	82.97	24	84.14	32	83.01	33
A2	103.70	52	105.27	64	104.12	58
A6	103.70	52	105.27	64	104.12	58
B3	116.34	64	116.64	**100**	115.34	100
B5	116.34	64	116.64	100	115.34	100
B2	126.84	84	127.15	90	126.13	85
B6	126.84	84	127.15	90	126.13	85
A1	130.90	23	133.23	26	132.31	39
A4	134.56	23	136.00	14	134.31	30
B1	139.33	23	140.47	20	139.21	39
A3	147.07	44	148.32	44	147.36	76
A5	147.07	44	148.32	44	147.36	76
B4	157.42	19	158.98	18	157.69	42

Compound Number 92



1-(4-acetoxy-3,5-dimethoxyphenyl)-3-hydroxy-2-(2-methoxy phenoxy)propan-1-one

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.34	s	
B OMe	3.82	s	
A3,5 OMe	3.83	s	
γ	4.09	d	5.2
β	5.38	t	5.2
A2,6	7.36	s	

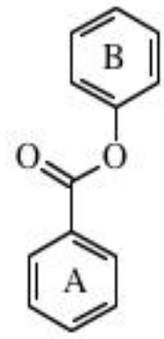
Notes:

S. Ralph SRIII-40
30mg *A1 + A4 switch around in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.41	54	20.21	44	20.04	65
B OMe	55.73	54	56.07	49	55.39	60
A OMe	56.29	100	56.60	100	56.12	100
A OMe	56.29	100	56.60	100	56.12	100
γ	63.39	40	63.88	21	62.35	38
β	84.41	47	84.02	36	81.59	32
A2	105.84	87	106.50	82	105.38	68
A6	105.84	87	106.50	82	105.38	68
B2	112.33	49	113.57	41	112.64	38
B5	117.86	42	116.84	29	114.73	32
B6	121.23	50	121.57	53	120.49	48
B1	123.61	42	123.15	40	121.67	38
A4	133.42	12	133.93	7	132.25	20
A1	132.81	28	134.31	18	132.99	37
B4	146.71	23	148.17	16	146.73	35
B3	150.24	26	150.90	16	149.13	33
A3	152.32	48	153.19	34	151.75	77
A5	152.32	48	153.19	34	151.75	77
Ac C=O	168.06	20	168.10	17	167.58	32
α	195.72	22	196.70	20	195.86	35

Compound Number 93



Phenyl benzoate

Benzoic acid phenyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
A2,6	8.21	m	8.3

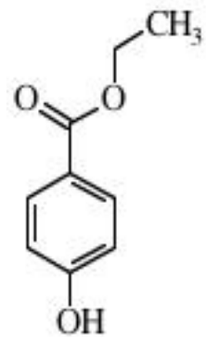
Notes:

Aldrich
60mg
Al changes position in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3	121.70	90	122.61	89	121.85	85
B5	121.70	90	122.61	89	121.85	85
B1	125.84	52	126.51	51	125.92	43
A2	128.54	100	129.47	100	128.88	100
A6	128.54	100	129.47	100	128.88	100
B2	129.45	100	130.15	96	129.50	100
B6	129.45	100	130.15	96	129.50	100
A1	129.57	15	130.42	19	128.94	25
A3	130.13	95	130.60	98	129.72	99
A5	130.13	95	130.60	98	129.72	99
A4	133.53	48	134.39	54	133.93	42
B4	150.96	12	151.99	14	150.62	27
α	165.11	9	165.32	9	164.51	15

Compound Number 94



Ethyl 4-hydroxybenzoate

ethyl 4-hydroxybenzoate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
CH3	1.39	t	7.1
CH2	4.36	q	7.1
A3,5	6.91	m	8.8
A2,6	7.95	m	8.8

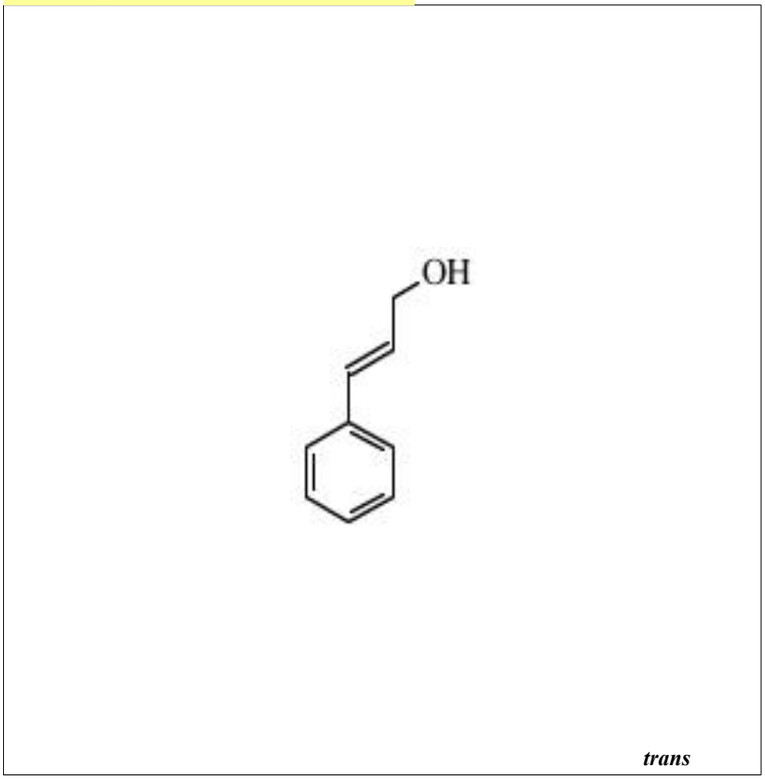
Notes:

Aldrich
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	14.30	46	14.63	47	14.24	53
CH2	61.13	44	60.84	42	60.04	44
3	115.34	100	115.92	100	115.27	91
5	115.34	100	115.92	100	115.27	91
1	122.13	21	122.69	10	120.61	20
2	131.94	90	132.30	90	131.35	100
6	131.94	90	132.30	90	131.35	100
4	160.74	26	162.44	22	161.93	40
α	167.45	17	166.49	10	165.56	21

Compound Number 95



trans

Cinnamyl alcohol

(E)-3-phenyl-2-propen-1-ol(E)-cinnamyl alcohol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ	4.25	dd	5.6, 1.1
β	6.30	dt	15.9, 5.6
α	6.54	dt	15.9, 1.1

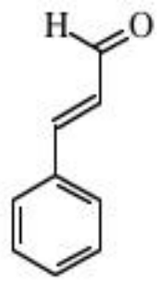
Notes:

Fluka
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	63.39	41	63.12	52	61.50	42
2	126.40	72	126.98	100	126.05	88
6	126.40	72	126.98	100	126.05	88
β	127.57	41	127.93	51	127.08	48
3	128.52	100	129.25	95	128.49	100
5	128.52	100	129.25	95	128.49	100
4	128.52	100	129.90	42	128.37	40
α	130.86	34	130.90	49	130.72	47
1	136.66	13	138.08	14	136.87	18

Compound Number 96



trans

Cinnamaldehyde

(E)-3-phenyl-2-propenal(E)-cinnamaldehyde

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	6.69	dd	16.0, 7.7
α	7.50	d	16.0
γ	9.68	d	7.7

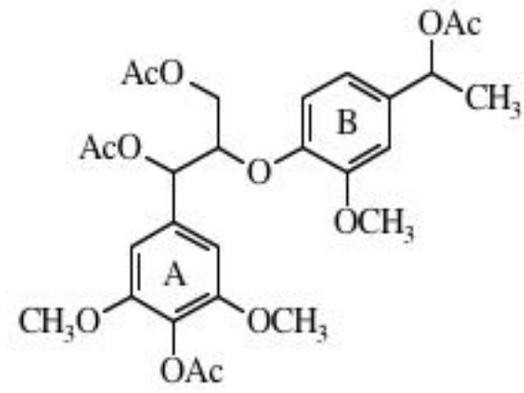
Notes:

Fluka
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
2	128.45	100	129.30	91	128.69	100
6	128.45	100	129.30	91	128.69	100
4	128.45	100	129.40	48	128.50	48
3	129.04	92	129.81	100	129.02	96
5	129.04	92	129.81	100	129.02	96
β	131.20	41	131.78	55	131.13	48
1	133.96	12	135.19	12	134.07	23
α	152.66	21	153.19	32	153.00	35
γ	193.54	25	193.96	30	194.19	32

Compound Number 97



threo

1-(4-acetoxy-3,5-dimethoxyphenyl)-1,3-diacetoxy-2-[4-(1-acetoxyethyl)-2-methoxyphenoxy]

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.00	s	
Ac Me	2.06	s	
Ac Me	2.07	s	
Ac Me	2.32	s	
B β	1.52	d	6.6
B OMe	3.83	s	
A3,5 OMe	3.81	s	
γ1	4.07	dd	11.8, 5.7
γ2	4.32	dd	11.8, 4.6
β	4.60	m	
B α	5.82	q	6.6
α	6.08	d	6.2
A2,6	6.67	s	

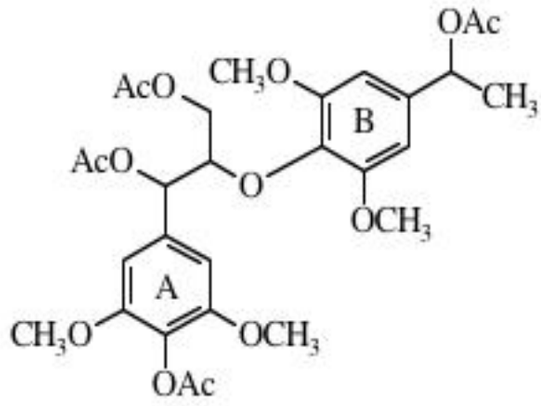
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.42	42	20.23	49	20.04	58
Ac Me	20.70	32	20.62	46	20.37	67
Ac Me	21.04	37	20.93	40	20.63	50
Ac Me	21.35	42	21.15	44	20.93	67
B β	22.08	34	22.46	40	21.87	42
B OMe	55.88	50	56.29	59	55.61	54
A OMe	56.21	100	56.52	100	55.96	100
A OMe	56.21	100	56.52	100	55.96	100
γ	62.98	21	63.58	37	62.42	25
B α	72.06	26	72.40	48	71.35	42
α	74.65	24	75.64	41	74.54	29
β	80.12	24	80.68	33	79.08	29
A2	104.09	55	104.93	81	103.91	33
A6	104.09	55	104.93	81	103.91	33
B2	110.64	18	111.71	32	110.55	21
B5	118.22	24	118.71	30	117.03	33
B6	118.65	26	119.18	43	118.05	42
A4	128.83	18	129.65	10	127.78	21
A1	134.71	32	136.12	32	134.92	38
B1	136.72	26	137.72	24	136.00	33
B4	147.53	16	148.51	22	146.99	42
B3	150.58	32	151.52	25	149.82	42
A3	152.17	53	153.14	51	151.52	75
A5	152.17	53	153.14	51	151.52	75
A4 Ac C=O	168.47	26	168.40	21	167.88	33
α Ac C=O	169.66	18	169.96	19	169.32	33
B αAc C=O	170.27	24	170.17	17	169.52	38
γAc C=O	170.55	26	170.65	19	169.92	33

Notes:

S. Ralph SRIII-43
40mg
ca 90% threo

Compound Number 98



threo

1-(4-acetoxy-3,5-dimethoxyphenyl)-1,3-diacetoxy-2-[4-(1-acetoxyethyl)-2,6-dimethoxyphenoxy]propane

^1H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.07	s	
Ac Me	2.08	s	
Ac Me	2.32	s	
B β	1.52	d	6.6
OMe	3.78	s	
OMe	3.80	s	
γ1	3.94	dd	11.8, 7.3
γ2	4.36	dd	11.8, 4.5
β	4.54	m	
B α	5.79	q	6.6
α	6.12	d	6.1
B2,6	6.55	s	
A2,6	6.70	s	

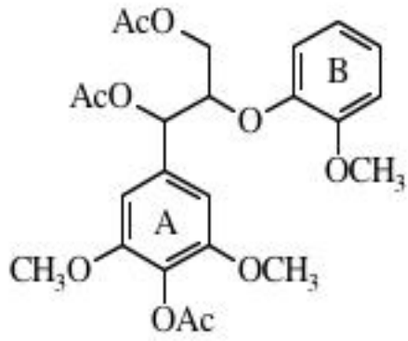
Notes:

S. Ralph SRIII-44
131mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.42	47	20.23	40	20.06	49
Ac Me	20.72	42	20.63	35	20.37	46
Ac Me	21.02	31	20.92	31	20.62	35
Ac Me	21.33	36	21.14	41	20.95	57
Bβ	22.25	31	22.56	29	22.02	32
OMe	56.02	96	56.36	91	55.78	100
OMe	56.02	96	56.36	91	55.78	100
OMe	56.21	100	56.45	100	55.98	95
OMe	56.21	100	56.45	100	55.98	95
γ	63.53	18	64.18	32	63.22	22
B α	72.35	25	72.68	35	71.72	37
α	75.61	31	76.62	26	75.73	18
β	80.64	35	81.44	33	80.27	23
B2	103.14	46	103.92	55	102.85	38
B6	103.14	46	103.92	55	102.85	38
A2	104.18	46	104.78	57	103.76	49
A6	104.18	46	104.78	57	103.76	49
A4	128.64	14	129.42	9	127.75	11
A1	135.46	28	136.61	29	135.39	32
B1	135.95	11	136.96	17	135.48	35
B4	137.57	32	138.68	26	137.40	35
A3	151.98	61	152.94	49	151.52	65
A5	151.98	61	152.94	49	151.52	65
B3	152.87	38	153.69	49	152.27	66
B5	152.87	38	153.69	49	152.27	66
A4 Ac C=O	168.49	19	168.37	20	167.93	29
α Ac C=O	169.70	15	169.80	22	169.27	35
B αAc C=O	170.16	19	170.11	20	169.56	40
γ Ac C=O	170.50	25	170.56	19	169.95	40

Compound Number 99



threo

1-(4-acetoxy-3,5-dimethoxyphenyl)-1,3-diacetoxy-2-(2-methoxy phenoxy)propane

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.97	s	
Ac Me	2.02	s	
Ac Me	2.21	s	
A3,5 OMe	3.80	s	
OMe	3.81	s	
γ1	4.04	dd	11.9, 5.6
γ2	4.26	dd	11.9, 4.2
β	4.79	m	
α	6.08	d	6.5
A2,6	6.85	s	
B1	6.97	m	8.2, 8.1, 1.3
B2	6.99	m	8.2, 1.0
B5	7.04	m	8.0, 1.3
B6	6.87	m	8.0, 8.1, 1.0

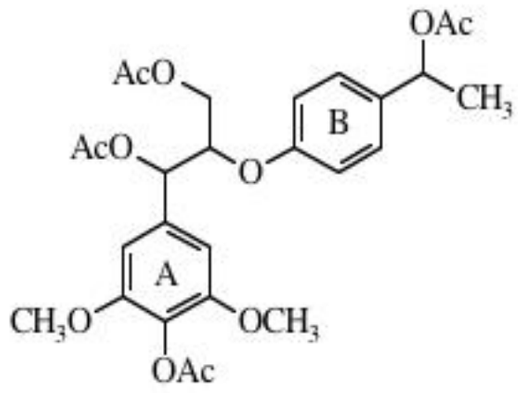
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.42	48	20.24	56	20.05	68
Ac Me	20.71	36	20.62	48	20.39	50
Ac Me	21.05	40	20.94	44	20.65	47
B OMe	55.77	54	56.20	63	55.52	59
OMe	56.20	100	56.52	100	55.97	100
OMe	56.20	100	56.52	100	55.97	100
γ	63.08	32	63.60	43	62.48	26
α	74.77	35	75.67	43	74.58	35
b	80.23	36	80.64	48	79.00	35
A2	104.08	61	104.93	81	103.92	62
A6	104.08	61	104.93	81	103.92	62
B2	112.48	34	113.71	44	112.69	41
B5	118.61	40	119.04	43	117.31	41
B6	120.98	41	121.66	48	120.63	53
B1	123.28	42	123.68	44	122.49	35
A4	128.79	10	129.65	10	127.81	21
A1	134.80	31	136.18	27	134.99	41
B4	147.92	20	149.06	17	147.54	38
B3	150.76	20	151.75	21	150.06	35
A3	152.16	50	153.14	41	151.56	74
A5	152.16	50	153.14	41	151.56	74
A4 Ac C=O	168.47	21	168.41	29	167.89	29
α Ac C=O	169.68	20	169.97	17	169.34	26
γ Ac C=O	170.55	19	170.66	19	169.94	29

Notes:

S. Ralph SRIII-45
55mg ca 80% threo
*CS assignments for overlapping 1H patterns A2,6 and B1,B2,B5 and B6 from deconvolution and simulation spectra, MacNuts, Acorn NMR Inc.

Compound Number 100



threo

1-(4-acetoxy-3,5-dimethoxyphenyl)-1,3-diacetoxy-2-[4-(1-acetoxyethyl)phenoxy] propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	1.99	s	
Ac Me	2.05	s	
Ac Me	2.05	s	
Ac Me	2.32	s	
B β	1.51	d	6.6
A3,5 OMe	3.80	s	
γ1	4.06	dd	11.8, 6.1
γ2	4.25	dd	11.8,-
β	4.69	m	
B α	5.83	q	6.6
α	6.03	d	6.3
A2,6	6.63	s	
B3,5	6.89	m	7.8
B2,6	7.28	m	7.8

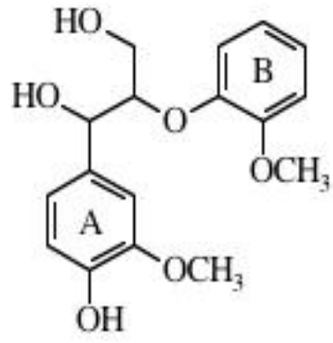
Notes:

S. Ralph SRIII-46
24mg
CDCl3 spectrum poor

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.43	33	20.23	49	20.04	66
Ac Me	20.68	40	20.60	38	20.38	69
Ac Me	21.03	45	20.89	47	20.62	59
Ac Me	21.36	48	21.15	40	20.92	72
B β	22.01	36	22.36	36	21.76	50
OMe	56.25	100	56.58	89	56.01	100
OMe	56.25	100	56.58	89	56.01	100
γ	62.67	33	63.31	33	62.15	25
B α	71.85	45	72.19	40	71.12	22
α	74.24	21	75.45	36	74.32	28
β	78.17	26	79.23	22	77.60	25
A2	104.09	76	105.05	89	104.00	62
A6	104.09	76	105.05	89	104.00	62
B3	116.32	60	117.12	49	116.00	84
B5	116.32	60	117.12	49	116.00	84
B2	127.67	88	128.29	100	127.28	78
B6	127.67	88	128.29	100	127.28	78
A4	128.95	5	129.80	4	127.83	5
B1	134.35	31	135.98	27	134.66	56
A1	135.26	29	136.24	24	134.81	59
A3	152.28	52	153.25	47	151.57	72
A5	152.28	52	153.25	47	151.57	72
B4	158.02	19	159.20	18	157.68	34
A4 Ac C=O	168.44	21	168.39	22	167.86	28
α Ac C=O	169.69	24	170.02	20	169.37	38
B α Ac C=O	170.30	21	170.19	13	169.52	41
γ Ac C=O	170.56	24	170.68	20	169.94	31

Compound Number 101



erythro

Guaiacylglycerol-β-guaiacyl ether

1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propan-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.84	s	
α	4.95	d	4.8
β	4.16	m	

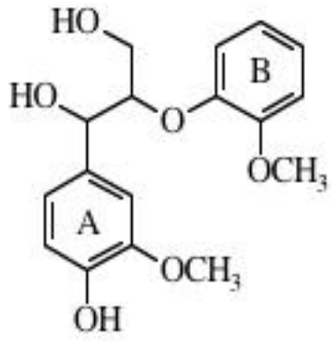
Notes:

J. Ralph JRB 178.3
30mg
J. Ralph Holzforschung 42(1988) p273-5

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.86	82	56.20	97	55.35	100
OMe	55.94	100	56.27	100	55.52	84
γ	60.75	76	61.81	81	60.04	59
α	72.78	76	73.82	81	71.60	72
β	87.02	75	86.72	100	83.67	66
A2	108.81	71	111.38	94	111.35	62
B2	112.19	75	113.50	81	112.60	69
A5	114.31	84	115.12	90	114.48	66
B5	119.07	73	119.70	90	115.86	59
A6	120.57	75	120.45	94	119.43	66
B6	121.59	90	121.85	100	120.56	78
B1	124.00	80	123.32	100	120.89	69
A1	131.95	51	134.23	55	133.15	69
A4	145.09	49	146.61	42	145.35	78
A3	146.64	45	147.93	39	146.86	72
B4	146.89	35	149.04	35	148.00	62
B3	151.40	39	151.96	35	149.68	56

Compound Number 102



threo

Guaiacylglycerol-β-guaiacyl ether

1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.86	s	
OMe	3.90	s	
α	4.96	d	8.0
β	4.02	m	

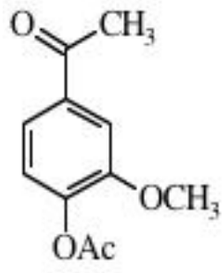
Notes:

J. Ralph JRGV 135.X1
21mg
J. Ralph Holzforschung 42(1988) p.273-5

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.91	92	56.21	96	55.33	97
OMe	55.97	100	56.31	100	55.53	100
γ	61.06	72	61.90	75	60.02	59
α	74.00	80	73.93	84	70.90	69
β	89.45	72	88.58	84	84.37	62
A2	109.46	86	111.41	96	110.96	66
B2	112.18	88	113.40	86	112.50	66
A5	114.35	88	115.21	78	114.57	62
B5	120.25	88	120.06	90	115.79	62
A6	120.98	75	120.57	88	118.92	62
B6	121.69	94	121.95	80	120.60	76
B1	124.21	85	123.44	88	120.96	69
A1	131.51	46	133.81	43	132.86	76
A4	145.59	48	146.82	39	145.33	79
A3	146.68	42	148.00	29	146.89	66
B4	147.63	35	149.70	31	148.32	59
B3	151.27	38	151.80	29	149.62	59

Compound Number 103



Acetylated acetovanillone
4-acetoxy-3-methoxyacetophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.59	s	
β	2.33	s	
OMe	3.88	s	
2	7.59	d	1.9
5	7.12	d	8.1
6	7.54	dd	8.1, 1.9

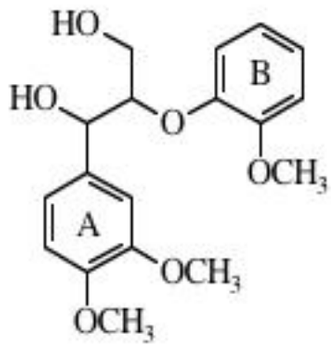
Notes:

IPC
45mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.61	65	20.46	64	20.29	83
β	26.49	81	26.63	84	26.62	88
OMe	56.05	100	56.37	97	55.88	100
2	111.51	97	112.44	97	111.62	77
6	121.94	88	122.38	93	121.56	83
5	122.80	95	123.77	100	123.02	84
1	135.96	37	136.93	30	135.62	51
4	143.87	26	144.80	21	143.21	35
3	151.41	33	152.40	24	150.92	41
Ac C=O	168.46	30	168.64	26	168.12	44
α	196.91	30	196.89	29	196.88	40

Compound Number 104



threo

Veratrylglycerol-β-guaiacyl ether

1-(3,4-Dimethoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.82	s	
OMe	3.83	s	
OMe	3.84	s	
α	4.96	d	5.0
β	4.15	m	

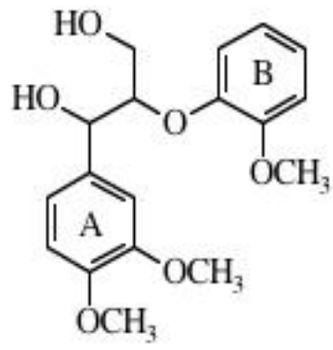
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.84	76	56.03	100	55.22	72
OMe	55.88	100	56.11	97	55.42	82
OMe	55.88	100	56.27	94	55.52	100
γ	61.04	16	61.70	60	60.02	48
α	73.77	16	73.64	74	70.77	18
β	88.82	14	87.92	28	84.26	20
A2	110.05	15	111.89	67	110.67	20
A5	111.07	45	112.29	74	111.13	53
B2	112.21	43	113.36	31	112.52	23
A6	119.55	15	120.03	72	115.84	23
B5	120.52	15	119.56	32	118.62	22
B6	121.61	19	121.83	34	120.56	32
B1	123.93	17	123.30	66	120.95	23
A1	132.38	12	135.01	16	134.47	22
B4	147.65	10	148.92	25	147.72	27
A4	148.83	12	149.67	15	147.98	43
A3	149.04	12	149.96	32	148.25	20
B3	151.07	11	151.61	10	149.67	23

Notes:

LL Landucci
75mg Shifts reported are for threo isomer-
minor isomer of this mixture, see 105 also

Compound Number 105



erythro

Veratrylglycerol-β-guaiacyl ether

1-(3,4-Dimethoxyphenyl)-2-(2-methoxyphenoxy)-propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.85	s	
OMe	3.85	s	
OMe	3.85	s	
α	4.99	d	4.8
β	4.17	m	
γ1	3.69	m	
γ2	3.92	m	
A2	6.90	m	
A6	6.99	m	
acetone			
OMe	3.76		
OMe	3.77		
OMe	3.81		
α	4.91		
β	4.29		
γ1	3.67		
γ2	3.81		
A2	7.11	d	2.1
A6	6.86	d	8.45

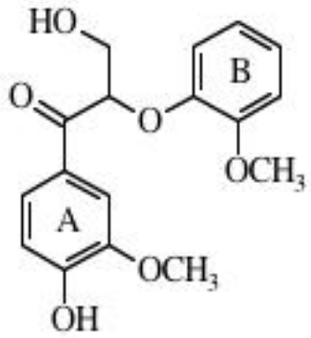
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.87	73	56.07	87	55.23	92
OMe	55.91	100	56.15	87	55.44	100
OMe	55.91	100	56.30	95	55.54	97
γ	60.81	46	61.79	30	60.03	61
α	72.75	50	73.75	36	71.54	69
β	87.10	50	86.58	74	83.62	67
A2	109.41	46	111.97	80	111.03	72
A5	111.08	50	112.35	84	111.14	75
B2	112.21	53	113.55	84	112.61	75
A6	118.49	50	120.06	100	115.95	72
B5	120.68	50	119.64	85	119.18	67
B6	121.58	48	121.86	87	120.56	81
B1	124.02	45	123.32	87	120.95	72
A1	132.70	37	135.50	31	134.79	69
B4	146.96	26	149.03	31	147.76	56
A4	148.48	26	149.63	31	147.99	61
A3	149.02	27	150.04	34	148.10	67
B3	151.47	26	151.96	31	149.72	53

Notes:

LL Landucci
30mg alpha OH proton 4.55 in acetone

Compound Number 106



Erone

3-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxy phenoxy)-propan-1-one

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.87	s	
γ	4.08	d	5.1
β	5.43	t	5.1

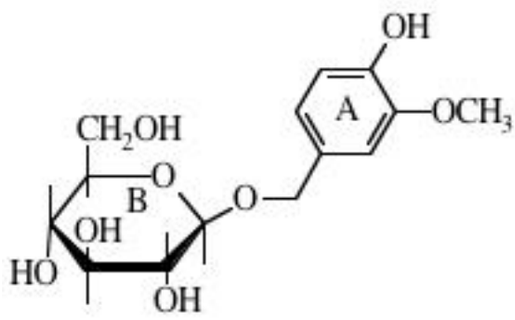
Notes:

S. Ralph
45mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.82	100	56.20	97	55.46	96
OMe	56.02	96	56.24	100	55.50	100
γ	63.70	72	64.11	41	62.52	55
β	83.94	88	83.69	82	81.32	61
A2	110.88	87	112.48	73	111.71	56
B2	112.35	89	113.65	85	112.67	60
A5	114.21	87	115.50	82	114.48	57
B5	117.56	79	116.70	81	114.98	55
B6	121.18	92	121.57	88	120.48	66
B1	123.26	88	122.94	82	121.47	60
A6	124.16	88	124.66	86	123.51	54
A1	127.68	56	128.72	42	126.79	52
B4	146.91	55	148.29	36	146.94	56
A3	146.95	59	148.36	41	147.49	61
B3	150.12	42	150.86	27	149.13	54
A4	151.28	62	152.76	41	152.22	68
α	194.91	52	195.64	42	194.69	50

Compound Number 107



Vanillyl-β-D-Glucoside

2-(4-Hydroxy-3-methoxybenzyloxy)-6-hydroxymethyl tetrahydropyran-3,4,5-triol

^{1}H Not run

Atom	H Shifts	Mult	J

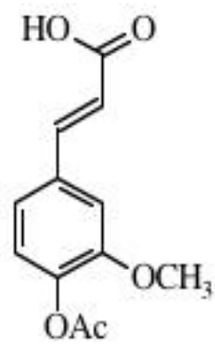
Notes:

M.Mozuch 88/71/1
20mg not soluble in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.30	100	55.46	100
B6			63.00	76	61.09	57
B4			70.98	76	69.40	61
B2			71.74	90	70.09	86
B5			74.90	86	73.40	93
α			77.48	84	76.66	89
B3			78.02	88	76.82	86
B1			102.70	79	101.52	82
A2			112.81	88	112.29	82
A5			115.41	87	114.90	82
A6			121.77	87	120.50	79
A1			130.28	50	128.57	79
A3			147.00	46	145.80	75
A4			148.21	33	147.25	71

Compound Number 108



Acetylated ferulic acid
4-acetoxy-3-methoxycinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.33	s	
OMe	3.88	s	
α	7.04	d	15.9
β	6.41	d	15.9

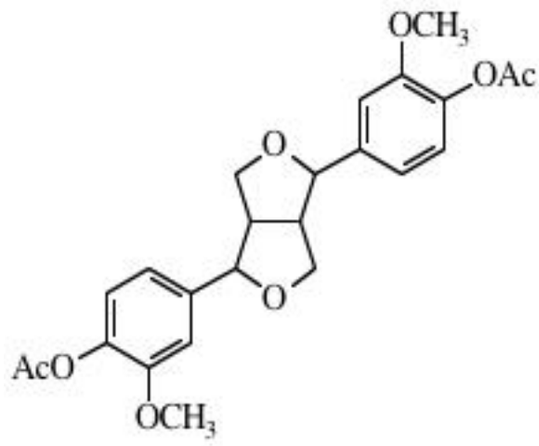
Notes:

R. Helm RFH 83F1
50mg not suluble in CDCL3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.48	86	20.29	98
OMe			56.42	96	55.90	100
2			112.48	80	111.79	76
β			119.48	76	119.47	80
6			122.03	91	121.20	84
5			124.11	100	123.10	82
1			134.38	39	133.19	64
4			142.62	26	140.77	56
α			144.79	89	143.23	80
3			152.71	34	151.09	64
Ac C=O			167.70	41	167.50	78
γ			168.78	36	168.29	66

Compound Number 109



Pinoresinol diacetate

Acetic acid 4-[4-(4-acetoxy-3-methoxyphenyl) tetrahydrofuro[3,4-c] furan-1-yl]-2-methoxyphenyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.30	s	
OMe	3.83	s	
β	3.08	m	
γ1	3.92	dd	9.0, 3.2
γ2	4.27	dd	9.0, 6.8
α	4.78	d	3.9
6	6.88	dd	8.1, 1.4
2	6.99	m	
5	7.00	m	

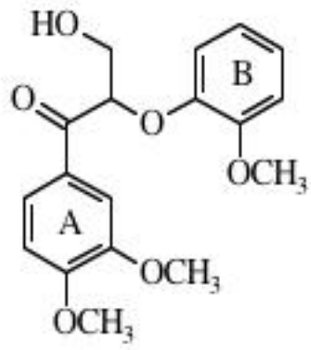
Notes:

J. Pew
As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.62	86	20.48	76	20.28	85
β	54.36	94	55.42	92	53.75	85
OMe	55.92	100	56.23	100	55.67	100
γ	71.95	86	72.58	79	71.24	78
α	85.50	93	86.22	92	84.64	80
2	109.91	87	111.12	81	110.33	78
6	117.92	88	118.63	84	117.78	76
5	122.74	77	123.46	83	122.50	83
4	139.13	37	140.15	27	138.42	51
1	140.11	61	141.80	43	140.41	71
3	151.23	48	152.28	35	150.70	66
Ac C=O	168.99	42	168.98	25	168.44	58

Compound Number 110



Veratrone

1-(3,4-Dimethoxyphenyl)-3-hydroxy-2-(2-methoxyphenoxy) propan-1-one

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.84	s	
OMe	3.90	s	
OMe	3.93	s	
γ	4.08	m	
β	5.42	t	5.2
A2	7.61	d	2.0
A6	7.76	dd	8.4, 2.0

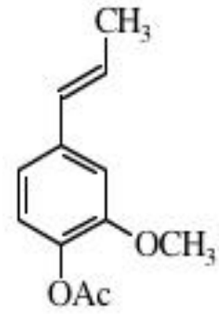
Notes:

LL Landucci
34mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.82	94	56.05	59	55.39	84
OMe	55.97	100	56.05	59	55.46	100
OMe	56.10	100	56.21	100	55.70	87
γ	63.73	77	64.11	52	62.47	68
β	84.31	89	83.88	65	81.38	71
A2	110.17	81	111.53	56	110.75	68
A5	111.04	83	112.23	57	110.87	71
B2	112.35	89	113.74	67	112.68	71
B5	117.96	74	116.95	61	114.58	71
B6	121.17	85	121.59	69	120.48	74
B1	123.40	94	123.04	65	121.56	74
A6	123.63	77	124.28	56	123.24	65
A1	128.10	42	129.44	28	127.88	61
B4	146.97	34	148.43	20	146.88	52
A3	149.20	47	150.07	22	148.50	65
B3	150.30	38	151.01	20	149.14	55
A4	153.95	40	154.89	22	153.40	58
α	195.04	49	195.92	26	195.14	55

Compound Number 111



acetylated isoeugenol

1-(3-methoxy-4-acetoxyphenyl)-1-propene

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ	1.85	dd	6.35, 1.4
Ac Me	2.28	s	
OMe	3.81	s	
β	6.17	dq	15.7, 6.35
α	6.35	dd	15.7, 1.4

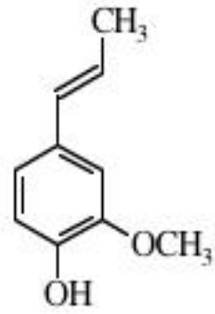
Notes:

J. Ralph JRPS115.1
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	18.37	91	18.45	81	18.11	94
Ac Me	20.62	73	20.45	68	20.32	86
OMe	55.77	100	56.10	100	55.64	100
2	109.69	77	110.54	89	109.73	95
6	118.36	96	118.90	97	117.99	100
5	122.65	85	123.53	97	122.68	92
β	126.01	85	126.34	94	125.80	79
α	130.48	87	131.36	94	130.24	92
1	137.06	41	137.70	35	136.44	71
4	138.65	25	139.88	21	138.24	46
3	151.02	31	152.26	24	150.86	52
Ac C=O	169.04	32	168.95	23	168.46	40

Compound Number 112



Isoeugenol

1-(3-methoxy-4-hydroxyphenyl)-1-propene

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ	1.83	dd	6..5, 1.6
OMe	3.84	s	
β	6.05	dq	15.7, 6.5
α	6.30	dd	15.7, 1.6

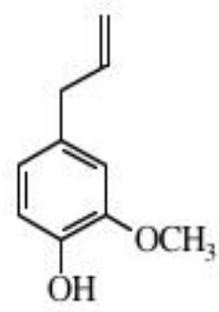
Notes:

Aldrich
50mg contains an impurity

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	18.30	86	18.38	88	18.05	98
OMe	55.82	100	56.13	100	55.50	100
2	108.01	81	109.64	83	109.41	87
5	114.43	95	115.66	89	115.41	91
6	119.30	98	119.89	100	118.78	95
β	123.34	86	122.97	89	121.98	95
1	130.66	42	130.93	30	129.11	56
α	130.78	96	131.86	85	130.87	88
4	144.79	44	146.61	37	145.80	72
3	146.61	26	148.28	27	147.64	61

Compound Number 113



Eugenol

4-Allyl-2-methoxyphenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α	3.30	d	6.6
OMe	3.84	s	
γ	5.04	m	
β	5.94	ddt	6.6
5	6.83	d	8.5

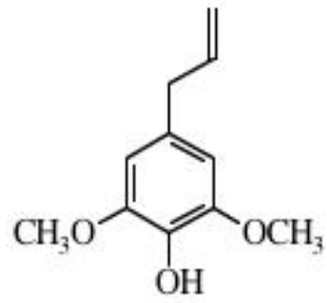
Notes:

Aldrich
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	39.88	84	40.32	90	39.08	99
OMe	55.86	100	56.16	100	55.49	100
2	111.17	94	112.83	81	112.58	82
γ	114.31	98	115.31	71	115.11	82
5	115.46	86	115.61	93	115.35	100
6	121.19	96	121.66	86	120.48	76
1	131.90	36	132.07	27	130.39	56
β	137.83	72	139.05	68	138.13	82
4	143.93	32	145.68	32	144.72	63
3	146.47	27	148.13	25	147.43	50

Compound Number 114



4-Allyl-2,6-dimethoxyphenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α	3.30	d	6.7
OMe	3.85	s	
2,6	6.40	s	
γ1	5.04	m	
β	5.94	ddt	16.8, 10.2, 6.7

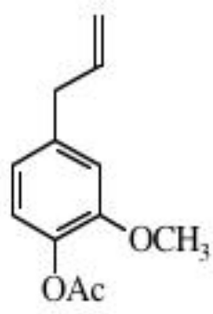
Notes:

Aldrich 50mg Extraneous peaks
around 106 and 119

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	40.31	49	40.73	53	39.53	66
OMe	56.26	97	56.58	99	55.89	100
OMe	56.26	97	56.58	99	55.89	100
2	105.26	100	106.83	100	105.83	83
6	105.26	100	106.83	100	105.83	83
γ	115.65	46	115.42	45	115.26	48
1	131.06	23	131.13	19	129.63	30
4	133.10	16	135.19	15	133.81	28
β	137.60	43	138.95	36	137.98	47
3	147.03	36	148.60	28	147.93	54
5	147.03	36	148.60	28	147.93	54

Compound Number 115



acetylated eugenol

1-(3-methoxy-4-acetoxyphenyl)-2-propene

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.29	s	
α	3.36	d	6.7
OMe	3.80	s	
2			
γ	5.07	m	
β	5.95	ddt	16.8, 10.2, 6.7
A6	6.75	m	
A2	6.77	m	
A5	6.94	d	7.9

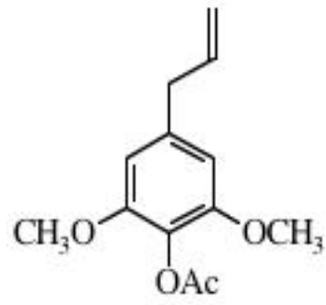
Notes:

J. Ralph JRC91.1
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.64	76	20.45	73	20.30	69
α	40.08	100	40.51	100	39.26	100
OMe	55.81	89	56.08	100	55.57	81
2	112.76	89	113.66	87	112.82	67
γ	116.12	76	116.03	79	115.87	68
5	120.66	100	121.10	92	120.15	76
6	122.51	100	123.37	92	122.48	68
β	137.03	78	138.32	69	137.34	68
4	138.05	24	139.24	21	137.53	31
1	138.98	43	139.72	37	138.66	43
3	150.89	28	152.10	25	150.61	33
Ac C=O	169.12	32	168.95	25	168.47	33

Compound Number 116



1-(3,5-dimethoxy-4-acetoxyphenyl)-2-propene

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.31	s	
α	3.34	d	6.7
OMe	3.79	s	
2,6	6.43	s	
γ	5.09	m	
β	5.95	ddt	16.8, 10.1, 6.7

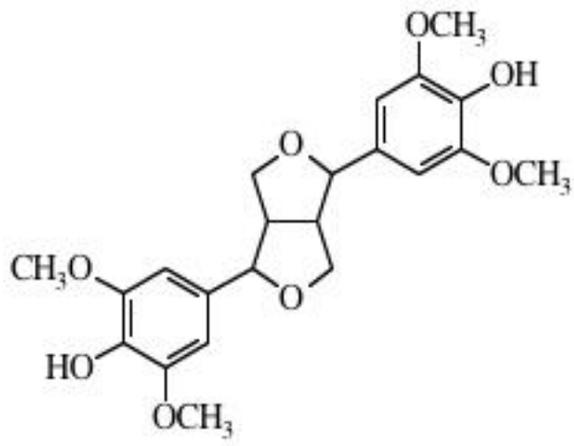
Notes:

J. Ralph JRPS143.1
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.43	40	20.24	38	20.09	52
α	40.64	45	41.06	47	39.89	100
OMe	56.07	100	56.32	94	55.80	97
OMe	56.07	100	56.32	94	55.80	97
2	105.16	88	105.93	100	105.01	88
6	105.16	88	105.93	100	105.01	88
γ	116.22	39	116.11	44	115.97	47
4	126.99	8	128.10	6	126.33	12
β	136.90	38	138.24	37	137.27	47
1	138.52	25	139.32	20	138.31	35
3	151.97	34	153.06	25	151.58	57
5	151.97	34	153.06	25	151.58	57
Ac C=O	168.81	13	168.56	15	168.06	27

Compound Number 117



Syringylresinol

3,3',5,5'-tetramethoxy-7,9',7',9-diepoxylignan-4,4'-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	4.28	m	
OMe	3.90	s	
γ2	4.28	m	
α	4.73	d	4.3
2,6	6.58	s	

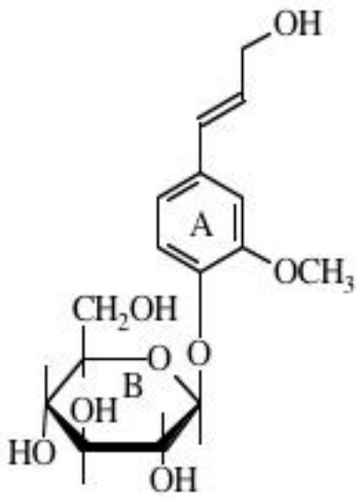
Notes:

IPC - Pearl
14mg
As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	54.38	49	55.33	61	53.59	39
OMe	56.41	100	56.69	100	55.95	100
OMe	56.41	100	56.69	100	55.95	100
γ	71.83	47	72.37	57	70.99	41
α	86.08	44	86.81	54	85.26	41
2	102.78	79	104.52	100	103.59	78
6	102.78	79	104.52	100	103.59	78
1	132.13	29	133.24	26	131.36	35
4	134.38	25	136.23	17	134.81	33
3	147.19	50	148.69	26	147.82	69
5	147.19	50	148.69	26	147.82	69

Compound Number 118



Coniferin
4-(3-hydroxy-1-propenyl)-2-methoxyphenyl-β-D-glucopyranoside

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.78	s	
γ1,γ2	4.10	dd	5.03
β	6.28	dt	15.9,5.0
α	6.47	d	15.9
A2	7.06	d	1.8
A5	7.02	d	8.4
A6	6.89	dd	8.4,1.8
B1	4.89	d	7.3
B2,3,4,5	3.34-3.18	nr	
B6 α	3.46	m	
B6 β	3.67	ddd	
B6 OH	4.54	t	5.7
γ OH	4.83	t	5.6

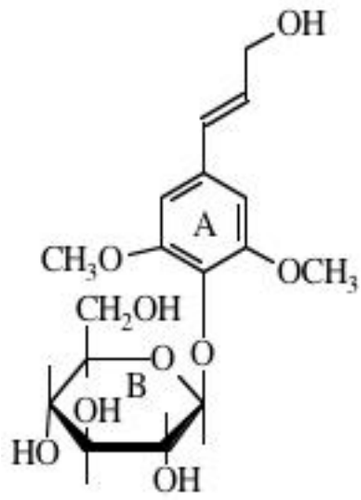
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe					55.57	100
B6					60.60	49
γ					61.51	88
B4					69.60	68
B2					73.12	68
B5					76.76	67
B3					76.91	70
B1					100.00	65
A2					109.84	56
A5					115.25	58
A6					118.89	63
α					128.31	79
β					128.87	70
A1					130.95	70
A4					145.89	67
A3					148.94	70

Notes:

IPC - Pearl
53mg only soluble in DMSO
Terashima, Ralph, Landucci, Holzforschung, 50(1995)p. 151-155

Compound Number 119



Syringin

4-(3-hydroxy-1-propenyl)-2,6-dimethoxy- β-D-glucopyranoside

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.77	s	
γ1	4.11	dd	5.0
β	6.63	dt	15.9,4.7
α	6.47	d	15.9
A2,6	6.73	s	
B1	4.91	d	4.8
B2,3,4,5	3.18-3.04	nr	
B6 α	3.4	m	
B6 β	3.59	ddd	
B6 OH	4.29	t	5.4
γ OH	4.85	t	5.5

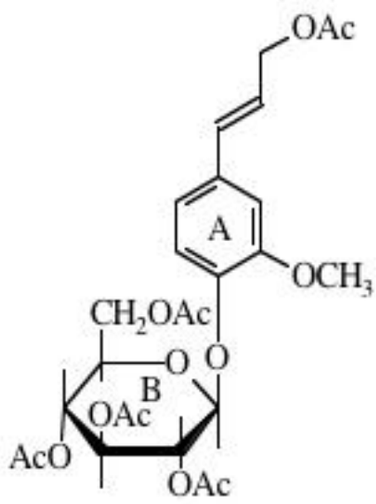
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe					56.27	100
OMe					56.27	100
B6					60.82	29
γ					61.37	45
B4					69.86	37
B2					74.09	37
B5					76.45	37
B3					77.08	37
B1					102.51	35
A2					104.39	62
A6					104.39	62
α					128.35	37
β					130.05	37
A1					132.52	35
A4					133.80	26
A3					152.60	77
A5					152.60	77

Notes:

IPC - Pearl
50mgonly soluble in DMSO
Terashima, Ralph, Landucci, Holzforschung, 50(1995)p. 151-155

Compound Number 120



Coniferin acetate

4-(3-hydroxy-1-propenyl)-2-methoxy pheny-l β-D-glycopyranoside pentaacetate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.03		
Ac Me	2.03		
Ac Me	2.07		
Ac Me	2.07		
Ac Me	2.09		
OMe	3.80	s	
γ	4.70	d	6.4
β	6.20	dt	15.8, 6.3
α	6.59	d	15.8
A6	6.89	bd	8.2
A2	6.94	bs	
A5	7.07	d	8.2

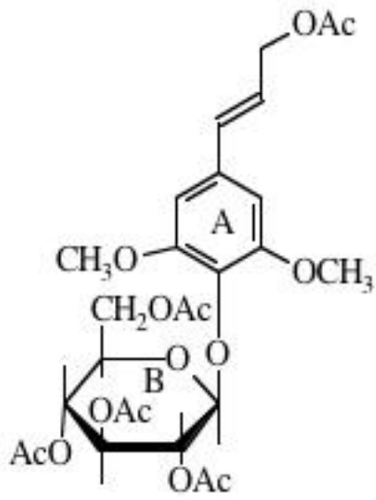
Notes:

S. Ralph III-58
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.60	100	20.51	50	20.23	75
Ac Me	20.60	100	20.59	100	20.28	100
Ac Me	20.60	100	20.59	100	20.30	100
Ac Me	20.66	66	20.59	100	20.41	77
Ac Me	20.95	46	20.78	43	20.65	92
OMe	56.07	57	56.47	50	55.90	77
B6	61.97	38	62.69	36	61.66	33
γ	64.93	52	65.23	45	64.32	67
B4	68.46	47	69.33	43	68.15	46
B2	71.24	47	71.96	39	70.77	48
B5	72.02	45	72.56	41	70.86	52
B3	72.61	48	73.23	38	71.92	46
B1	100.67	47	100.79	48	98.76	46
A2	110.58	44	111.55	38	110.61	52
A5	119.57	46	119.77	37	118.05	46
A6	119.93	48	120.26	40	119.34	54
β	122.83	56	123.86	44	123.02	58
A1	133.02	37	133.63	30	132.14	54
α	133.58	48	133.82	40	132.67	60
A4	146.09	32	147.19	26	145.66	56
A3	150.69	38	151.44	26	149.91	58
Ac C=O	169.26	34	169.58	24	168.91	50
Ac C=O	169.36	32	169.96	25	169.24	52
Ac C=O	170.15	34	170.22	28	169.49	56
Ac C=O	170.47	34	170.58	26	169.90	58
Ac C=O	170.71	22	170.69	16	170.07	44

Compound Number 121



Syringin acetate

4-(3-hydroxy-1-propenyl)-2,6-dimethoxy phenyl-β-D-glucopyranoside penta acetate

^1H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.03	s	
Ac Me	2.03	s	
Ac Me	2.03	s	
Ac Me	2.03	s	
Ac Me	2.09	s	
OMe	3.84	s	
γ	4.71	d	6.4
β	6.22	dt	16.8, 6.4
α	6.57	d	16.8
A2,6	6.61	s	

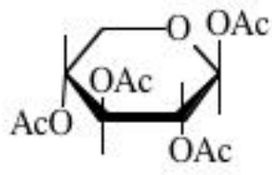
Notes:

S. Ralph III - 58
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.60	52	20.56	100	20.25	51
Ac Me	20.68	100	20.56	100	20.36	75
Ac Me	20.68	100	20.56	100	20.36	75
Ac Me	20.68	100	20.67	49	20.36	75
Ac Me	20.95	39	20.77	43	20.64	54
OMe	56.32	89	56.69	97	56.13	100
OMe	56.32	89	56.69	97	56.13	100
B6	62.35	32	62.91	40	61.82	25
γ	64.84	41	65.14	49	64.19	42
B4	68.56	36	69.47	48	68.26	31
B2	71.99	42	72.51	46	70.73	31
B5	72.08	42	72.81	48	71.54	31
B3	73.11	40	73.61	48	72.14	29
B1	101.21	36	101.69	43	100.48	31
A2	104.09	72	105.10	89	104.09	56
A6	104.09	72	105.10	89	104.09	56
β	123.30	39	124.38	46	123.74	36
A1	133.11	31	134.02	33	132.79	56
α	133.86	42	134.11	41	132.79	56
A4	134.56	23	135.38	19	133.87	32
A3	153.07	63	154.06	54	152.68	68
A5	153.07	63	154.06	54	152.68	68
Ac C=O	169.25	29	169.59	22	168.94	34
Ac C=O	169.41	30	169.94	24	169.24	36
Ac C=O	170.31	30	170.24	29	169.48	31
Ac C=O	170.51	25	170.48	24	169.81	37
Ac C=O	170.75	20	170.64	17	170.04	32

Compound Number 122



α + β Xylose Acetate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.02	s	
Ac Me	2.049	s	
Ac Me	2.049	s	
Ac Me	2.052	s	
Ac Me	2.052	s	
Ac Me	2.06	s	
Ac Me	2.11	s	
Ac Me	2.17	s	

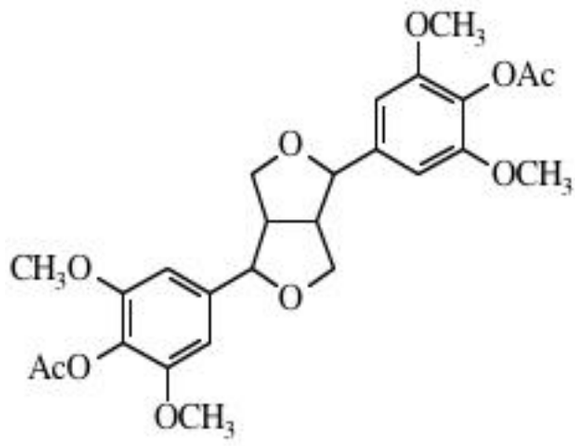
Notes:

S. Ralph III - 58
50mg mixture of α + β

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.42	62	20.35	59	20.21	43
Ac Me	20.54	40	20.46	43	20.25	54
Ac Me	20.60	83	20.51	71	20.34	100
Ac Me	20.60	83	20.55	100	20.34	100
Ac Me	20.66	88	20.55	100	20.34	100
Ac Me	20.66	88	20.55	100	20.34	100
Ac Me	20.74	41	20.65	70	20.44	62
Ac Me	20.79	55	20.65	70	20.52	49
5	60.65	49	61.12	57	60.05	32
5	62.76	31	63.14	35	62.01	18
4	68.35	32	69.09	41	67.99	41
4	68.67	53	69.22	59	68.10	28
3	69.39	100	69.87	63	68.83	41
3	69.39	100	70.24	67	68.93	41
2	69.53	38	70.30	48	69.36	25
2	70.97	34	71.54	37	70.52	23
1	89.26	54	89.76	56	88.60	38
1	92.05	31	92.67	41	91.49	24
Ac C=O	168.92	37	169.35	17	168.78	19
Ac C=O	168.92	37	169.53	21	169.02	43
Ac C=O	169.22	18	169.66	17	169.02	43
Ac C=O	169.65	31	170.01	17	169.36	24
Ac C=O	169.68	35	170.10	23	169.41	33
Ac C=O	169.68	35	170.19	40	169.49	24
Ac C=O	169.75	23	170.22	36	169.54	33
Ac C=O	170.02	27	170.22	36	169.58	37

Compound Number 123



Syringylresinol diacetate

Acetic acid 4-[4-(4-acetoxy-3,5-dimethoxyphenyl) tetrahydrofuro[3,4-c] furan-1-yl]-2,6-dimethoxyphenyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.33	s	
β	3.09	m	
OMe	3.83	s	
γ1	3.95	dd	9.1, 3.3
γ2	4.31	dd	9.1, 6.7
α	4.77	d	4.1
A2,6	6.59	s	

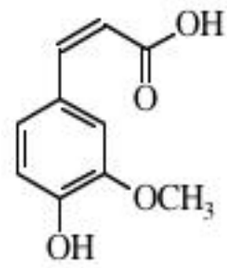
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.46	42	20.26	52	20.07	44
β	54.42	41	55.41	58	53.72	41
OMe	56.23	100	56.46	98	55.90	100
OMe	56.23	100	56.46	98	55.90	100
γ	72.11	47	72.71	54	71.38	36
α	85.85	47	86.51	56	84.93	34
2	102.29	85	103.30	100	102.44	63
6	102.29	85	103.30	100	102.44	63
1	128.06	12	128.91	8	127.04	19
4	139.63	30	141.41	31	140.03	31
3	152.30	50	153.23	44	151.60	68
5	152.30	50	153.23	44	151.60	68
Ac C=O	168.76	23	168.59	15	168.01	29

Notes:

S. Ralph III - 58
20mg
As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 124



cis

cis - Ferulic Acid

(Z)-4-hydroxy-3-methoxycinnamic acid

^{1}H (methanol)

Atom	H Shifts	Mult	J
OMe	3.85	s	
β	5.77	d	12.9
α	6.80	d	12.9
5	6.76	d	8.0
6	7.09	dd	8.1, 2.0
2	7.70	d	2.0

Notes:

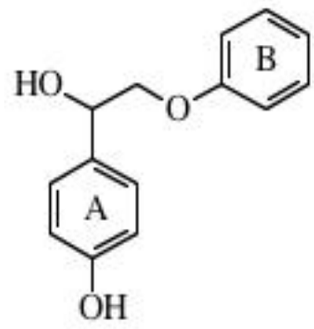
J. Obst

25mg Thanks to Rong Ji et.al, Chemosphere (2005) 1169-1181 for noting the miss assignment of C6 and Cβ

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.93	100	56.16	97	55.38	100
2	113.15	87	114.99	89	114.30	80
5	113.98	89	115.23	100	114.78	75
β	115.50	87	116.82	97	116.77	69
6	126.17	80	126.51	100	124.78	82
1	126.79	44	127.80	36	126.09	57
α	145.97	38	144.40	89	141.90	70
3	146.36	76	147.60	31	146.72	52
4	147.50	51	149.04	39	147.90	41
γ	171.34	44	167.85	31	167.54	51

Compound Number 125



1-(4-hydroxyphenyl)-2-phenoxyethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α	5.05	dd	8.3, 3.6
β	4.05	m	

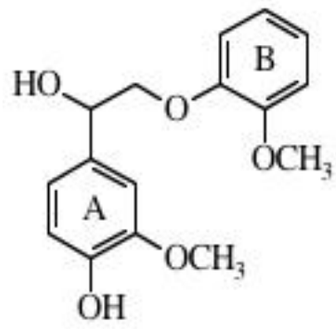
Notes:

JR C37.1
52mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	72.31	43	72.42	41	70.55	44
β	73.25	49	74.32	50	73.07	39
B3	114.73	93	115.43	90	114.49	100
B5	114.73	93	115.43	90	114.49	100
A3	115.51	98	115.76	88	114.74	92
A5	115.51	98	115.76	88	114.74	92
B1	121.33	51	121.37	46	120.38	42
A2	127.80	98	128.39	95	127.42	85
A6	127.80	98	128.39	95	127.42	85
B2	129.55	100	130.12	100	129.32	94
B6	129.55	100	130.12	100	129.32	94
A1	131.68	20	133.53	22	132.63	25
A4	155.77	28	157.61	22	156.54	38
B4	158.41	20	159.84	15	158.52	29

Compound Number 126



1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)ethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.88	s	
OMe	3.89	s	
α	5.02	dd	9.3, 3.0
β1	3.93	dd	10.0, 9.3
β2	4.15	dd	10.0, 3.0

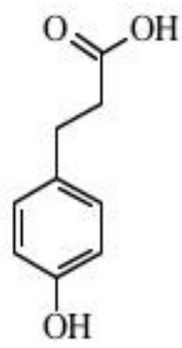
Notes:

JR 145.2
62mg * 76.50 shift in CDCL3
falls under solvent peak.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.90	87	56.28	95	55.52	100
OMe	55.97	87	56.35	92	55.52	100
α	72.20	67	72.71	70	70.81	61
β	76.50	100	76.32	95	74.15	51
A2	108.87	70	111.01	95	110.75	52
B2	112.16	77	113.67	88	112.51	52
A5	114.26	77	115.37	82	113.75	49
B5	116.21	73	115.93	75	114.92	57
A6	119.37	77	119.89	95	118.67	55
B6	121.13	77	121.83	100	120.74	66
B1	122.58	73	122.45	90	120.92	60
A1	131.61	33	134.17	35	133.46	47
A4	145.46	30	146.84	30	145.66	52
A3	146.68	27	148.12	22	147.21	44
B3	148.10	23	149.74	25	148.23	43
B4	150.26	20	151.06	18	149.10	38

Compound Number 127



Dihydrocoumaric acid

3-(4-hydroxyphenyl)propionic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	2.63	t	7.0
α	2.88	t	7.0
3,5	6.77	m	8.6
2,6	7.06	m	8.6

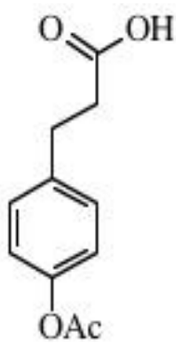
Notes:

IPC Pearl Coll.
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	29.94	53	30.68	43	29.58	43
β	35.75	40	36.33	46	35.70	41
3	115.46	92	115.99	100	115.04	93
5	115.46	92	115.99	100	115.04	93
2	129.36	100	130.00	79	129.00	100
6	129.36	100	130.00	79	129.00	100
1	132.10	14	132.54	17	130.92	34
4	154.55	22	156.42	18	155.46	34
γ	176.90	5	174.68	10	173.81	27

Compound Number 128



acetylated dihydrocoumaric acid

3-(4-acetoxyphenyl)propionic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
β	2.67	t	7.3
α	2.92	t	7.3
2,6	6.99	m	8.5
3,5	7.19	m	8.5

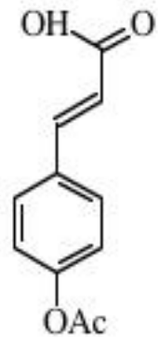
Notes:

IPC Pearl Coll.
60mg Contains unacetylated cmpd also

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.06	39	20.91	39	20.73	45
α	29.96	51	30.80	53	29.68	46
β	35.48	46	35.80	55	35.14	36
3	121.56	100	122.37	86	121.47	100
5	121.56	100	122.37	86	121.47	100
2	129.24	100	129.94	100	129.09	94
6	129.24	100	129.94	100	129.09	94
1	137.78	27	139.24	20	138.29	29
4	149.17	19	150.24	14	148.70	25
Ac C=O	169.78	14	169.65	13	169.14	23
γ	178.63	20	174.18	17	173.60	24

Compound Number 129



trans

acetylated coumaric acid

(E)-4-acetoxycinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.31	s	
β	6.41	d	16.0
3,5	7.15	m	8.6
2,6	7.57	m	8.6
α	7.75	d	16.0

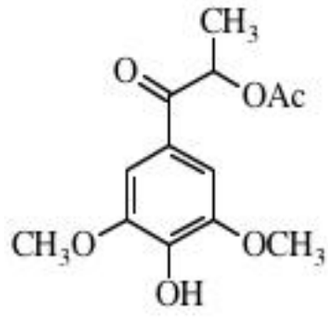
Notes:

IPC Pearl coll.
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.12	45	20.96	43	20.76	54
β	117.38	47	119.32	50	119.29	38
3	122.22	100	123.19	100	122.28	98
5	122.22	100	123.19	100	122.28	98
2	129.48	100	130.07	95	129.32	100
6	129.48	100	130.07	95	129.32	100
1	131.82	26	133.04	19	131.89	38
α	145.80	42	144.44	43	142.88	43
4	152.50	24	153.41	17	151.80	31
Ac C=O	168.98	21	167.68	21	167.48	30
γ	171.14	13	169.39	14	168.92	26

Compound Number 130



2-acetoxy-1-(4-hydroxy-3,5-dimethoxyphenyl)propan-1-one

^{1}H (chloroform)

Atom	H Shifts	Mult	J
γ	1.53	d	7.0
Ac Me	2.15	s	
OMe	3.94	s	
β	5.96	q	7.0
2,6	7.24	s	

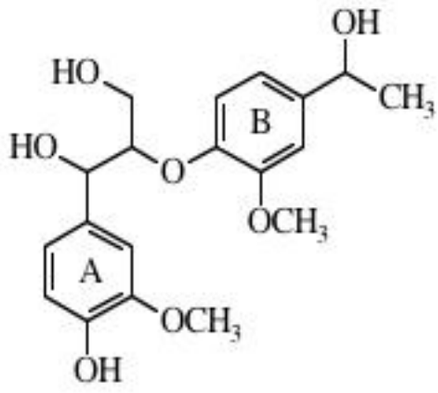
Notes:

IPC Pearl coll.
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	17.44	41	17.77	43	17.43	51
Ac Me	20.78	29	20.63	38	20.40	43
OMe	56.57	100	56.85	100	56.22	100
OMe	56.57	100	56.85	100	56.22	100
β	70.94	47	71.98	48	71.15	40
2	106.12	84	107.38	98	106.43	76
6	106.12	84	107.38	98	106.43	76
1	125.83	16	126.17	13	124.02	31
4	140.42	13	142.41	7	141.67	29
3	147.02	30	148.59	18	147.75	57
5	147.02	30	148.59	18	147.75	57
Ac C=O	170.45	13	170.42	13	169.70	29
α	195.11	16	195.30	15	194.63	29

Compound Number 131



threo

1-(4-hydroxy-3-methoxyphenyl)-2-[4-(1-hydroxyethyl)-2-methoxyphenoxy]propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.46	d	6.4
OMe	3.84	s	
OMe	3.86	s	
B α	4.82	q	6.4
α	4.92	d	7.7
A5	7.03	d	8.2

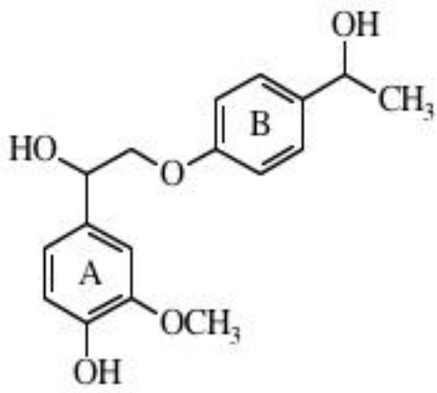
Notes:

S. Ralph SRIII-62-1
35mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.20	68	26.21	66	25.80	90
OMe	55.90	86	56.24	85	55.35	67
OMe	55.98	100	56.31	100	55.52	87
γ	61.09	46	61.89	61	60.02	49
B α	70.01	73	69.74	80	67.78	85
α	73.93	59	73.95	63	70.91	38
β	89.03	51	88.72	51	84.74	36
B2	109.35	54	110.67	58	109.79	36
A2	109.54	57	111.45	76	110.98	38
A5	114.42	59	115.24	64	114.57	49
B5	118.41	62	118.70	64	115.62	38
B6	120.17	65	119.68	68	117.24	49
A6	120.23	49	120.59	71	118.93	44
A1	131.56	38	133.85	34	132.89	54
B1	141.90	43	142.92	41	140.44	38
A4	145.57	51	146.83	41	145.31	59
A3	146.72	54	148.04	29	146.87	100
B4	146.78	35	148.31	31	146.87	100
B3	150.99	35	151.45	31	149.31	46
erythro isomer:						
γ	60.8		61.9		60.0	
α	72.8		73.8		71.6	
β	86.9		86.9		83.9	
A1	132.0		134.3		133.2	

Compound Number 132



1-(4-hydroxy-3-methoxyphenyl)-2-[4-(1-hydroxyethyl)-2-methoxyphenoxy]ethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.46	d	6.4
OMe	3.90	s	
β1	3.96	dd	9.7, 8.6
β2	4.06	dd	9.7, 3.5
B α	4.84	q	6.4
α	5.03	dd	8.6, 3.5

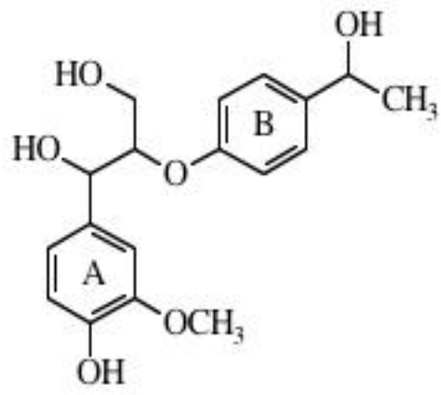
Notes:

S. Ralph SRIII-63-1
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.05	40	26.20	40	25.83	54
OMe	55.98	52	56.27	50	55.50	62
B α	69.91	44	69.50	39	67.52	62
α	72.43	50	72.65	46	70.68	46
β	73.58	44	74.65	48	73.22	38
A2	108.82	44	110.89	39	110.55	35
B3	114.64	87	115.07	84	113.95	96
B5	114.64	87	115.07	84	113.95	96
A5	114.37	56	115.42	38	114.88	46
A6	119.33	52	119.88	41	118.63	42
B2	126.73	100	127.27	100	126.28	100
B6	126.73	100	127.27	100	126.28	100
A1	131.66	25	134.30	21	133.30	37
B1	138.66	23	140.41	21	139.30	37
A4	145.57	25	146.86	21	145.60	40
A3	146.70	25	148.16	15	147.17	38
B4	157.81	23	158.80	18	157.19	38

Compound Number 133



major

1-(4-hydroxy-3-methoxyphenyl)-2-[4-(1-hydroxyethyl)phenoxy]-propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.47	d	6.4
OMe	3.87	s	
β	4.37	m	
Bα	4.85	q	6.4
α	4.96	d	6.7

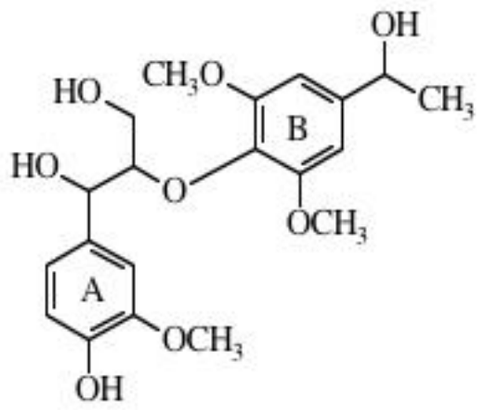
Notes:

S. Ralph SRIII-63-3
70mg
2:1 isomeric mixture,

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.08	49	26.07	52	25.78	64
OMe	56.00	72	56.22	53	55.45	49
γ	61.24	34	61.69	34	60.00	27
B α	69.86	64	69.52	52	67.60	62
α	73.94	43	73.38	36	70.95	24
β	83.28	45	84.16	38	83.14	29
A2	109.42	45	111.37	45	110.90	22
A5	114.38	47	115.19	48	114.68	33
B3	116.47	91	116.69	81	115.39	78
B5	116.47	91	116.69	81	115.39	78
A6	119.99	49	120.34	42	118.96	29
B2	126.88	100	127.14	100	126.14	100
B6	126.88	100	127.14	100	126.14	100
A1	131.60	26	134.18	25	133.19	36
B1	139.39	26	140.38	31	139.20	44
A4	145.68	19	146.63	25	145.33	42
A3	146.72	17	147.92	25	146.93	40
B4	157.50	21	158.92	23	157.71	33
minor isomer shifts						
γ	61.54		62.04		60.11	
α	74.04		73.99		71.50	
β	82.09		83.75		83.14	
B3,5	116.54		116.81		115.54	
A6	119.33		120.47		119.37	
B2,6	126.78		127.10		126.07	
A1	132.35		134.44		133.32	
B4	157.06		158.55		157.41	

Compound Number 134



threo

1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(1-hydroxyethyl)-2,6-dimethoxyphenoxy]propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.47	d	6.4
A OMe	3.86	s	
B OMe's	3.89	s	
B α	4.83	q	6.4
α	5.00	d	8.8
B2,6	6.63	s	
A2	6.95	s	
A5	6.85	d	8.3
A6	6.91	dd	8.3, 1.7

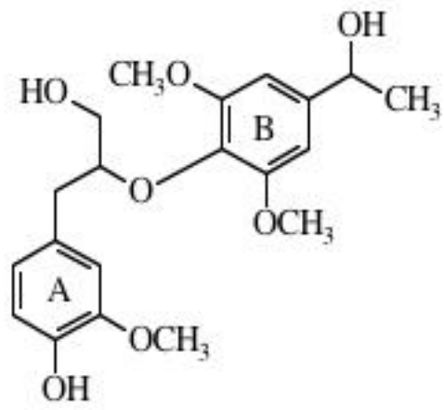
Notes:

S. Ralph SRIII-64-1
35mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.39	37	26.27	42	25.81	51
A OMe	55.96	45	56.23	49	55.46	51
B OMe	56.14	**100**	56.54	**100**	55.80	**100**
B OMe	56.14	100	56.54	100	55.80	100
γ	60.55	30	61.35	41	60.09	27
B α	70.29	39	70.01	44	68.07	56
α	74.10	35	74.10	42	71.48	34
β	89.00	35	89.82	40	87.20	37
B2	102.32	69	103.48	87	102.53	63
B6	102.32	69	103.48	87	102.53	63
A2	109.90	36	111.51	41	110.97	24
A5	114.36	37	115.24	54	114.56	32
A6	120.34	38	120.75	48	119.14	37
A1	131.89	26	133.67	26	132.82	39
B1	134.26	15	135.57	13	134.56	24
B4	142.80	23	144.64	26	142.88	41
A4	145.44	29	146.79	24	145.23	39
A3	146.56	30	147.95	25	146.77	37
B3	152.91	50	153.64	45	152.13	73
B5	152.91	50	153.64	45	152.13	73

Compound Number 135



3-(4-hydroxy-3-methoxyphenyl)-2-[4-(1-hydroxyethyl)-2,6-dimethoxyphenoxy]propan-1-ol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.47	d	6.4
α1	2.97	dd	13.6, 8.8
α2	3.20	dd	13.6, 5.4
B OMe	3.85	s	
A OMe	3.83	s	
B α	4.82	q	6.4
β	4.18	m	
B2,6	6.61	s	
A6	6.74	dd	8.0, 1.9
A2	6.80	d	1.9
A5	6.82	d	8.0

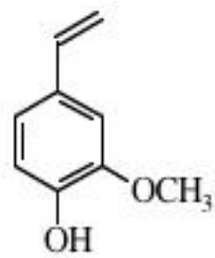
Notes:

S. Ralph SRIII-64-2
30mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	25.30	35	26.26	45	25.81	54
α	37.32	36	38.03	45	36.77	26
A OMe	55.94	58	56.23	48	55.46	49
B OMe	56.11	100	56.44	100	55.74	100
B OMe	56.11	100	56.44	100	55.74	100
γ	62.31	34	62.84	36	61.58	26
B α	70.42	35	70.04	39	68.13	51
β	84.52	42	85.30	48	83.40	36
B2	102.45	62	103.53	66	102.50	56
B6	102.45	62	103.53	66	102.50	56
A2	112.31	37	113.93	38	113.55	31
A5	114.27	46	115.51	48	115.01	36
A6	122.10	37	122.80	46	121.57	38
A1	130.13	25	130.80	25	129.24	38
B1	134.64	14	135.57	11	133.95	21
B4	142.09	19	144.15	14	142.83	38
A4	144.07	25	145.80	14	144.55	36
A3	146.38	20	148.04	18	147.03	36
B3	153.29	46	154.08	39	152.61	74
B5	153.29	46	154.08	39	152.61	74

Compound Number 136



Vinyl guaiacol
2-methoxy-4-vinylphenol
4-vinylguaiacol

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.84	s	
β1	5.04	dd	10.9, 1.1
β2	5.62	dd	17.6, 1.1
α	6.63	dd	17.6, 10.9
A5	6.78	d	8.1
A6	6.90	dd	8.1, 1.9
A2	7.07	d	1.9

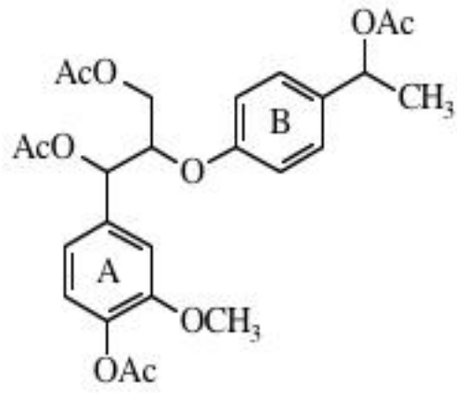
Notes:

J. Ralph
30mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.86	100	56.17	83	55.52	77
2	108.14	51	109.85	50	109.61	47
β	111.38	78	111.09	100	110.81	73
5	114.40	85	115.69	42	115.34	74
6	120.03	88	120.58	86	119.46	93
1	130.26	24	130.59	22	128.77	44
α	136.62	78	137.70	86	136.63	100
A4	145.64	20	147.55	9	146.68	43
A3	146.63	22	148.38	14	147.64	37

Compound Number 137



threo

1,3-diacetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-[4-(1-acetoxyethyl)phenoxy] propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	1.98	s	
Ac Me	2.05	s	
Ac Me	2.05	s	
Ac Me	2.29	s	
B β	1.51	d	6.6
OMe	3.81	s	
γ1	4.04	dd	11.8, 6.1
γ2	4.27	dd	11.8, 3.8
B α	5.83	q	6.6
α	6.07	d	6.3
β	4.69	m	
erythro			
B β	1.50	d	6.6
α	6.03	d	5.2
B α	5.82	q	6.6

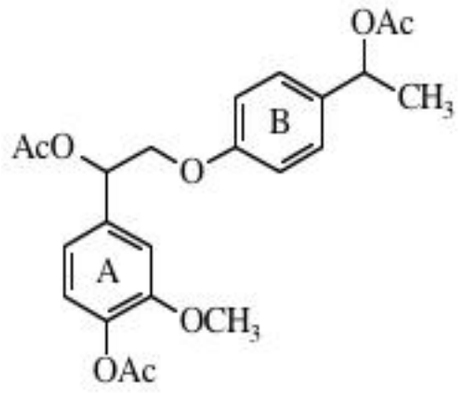
Notes:

S. Ralph SRIII-65-A 52mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.62	65	20.45	52	20.28	**100**
Ac Me	20.62	65	20.56	35	20.36	93
Ac Me	20.98	54	20.86	39	20.61	81
Ac Me	21.34	50	21.14	41	20.92	100
B β	22.00	44	22.34	38	21.78	64
OMe	55.98	65	56.31	42	55.82	69
γ	62.64	36	63.24	28	62.16	31
B α	71.85	49	72.17	27	71.14	57
α	74.00	36	75.07	32	74.00	40
β	78.08	25	79.10	22	77.57	36
A2	111.64	32	112.61	32	111.65	45
B5	116.31	68	117.08	51	116.01	98
B3	116.31	68	117.08	51	116.01	98
A6	119.60	40	120.37	43	119.45	40
A5	122.96	39	123.63	32	122.71	45
B2	127.66	**100**	128.27	**100**	127.30	100
B6	127.66	100	128.27	100	127.30	100
B1	134.86	32	136.20	18	134.71	40
A1	135.22	24	136.39	22	135.25	48
A4	140.05	18	140.97	14	139.25	36
A3	151.20	22	152.25	18	150.73	45
B4	157.97	17	159.12	19	157.69	40
A4 Ac C=O	168.71	20	168.81	18	168.30	43
Ac C=O	169.69	19	169.99	14	169.35	45
Ac C=O	170.29	18	170.18	14	169.51	48
Ac C=O	170.55	22	170.65	14	169.82	45
erythro isomer:						
γ	62.32		62.88		61.73	
B α	71.85		72.17		71.14	
α	73.62		74.21		72.81	
β	78.40		78.86		76.99	
B4	157.58		158.59		157.03	

Compound Number 138



1-Acetoxy-1-(4-acetoxy-3-methoxyphenyl)2-[4-(1-acetoxyethyl) phenoxy] ethane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.04	s	
Ac Me	2.11	s	
Ac Me	2.31	s	
Bβ	1.51	d	6.6
OMe	3.85	s	
β1	4.13	dd	10.4, 3.9
β2	4.25	dd	10.4, 7.8
B α	5.83	q	6.6
α	6.12	dd	7.8, 3.9
B3,5	6.86	m	8.7
B2,6	7.28	m	8.7

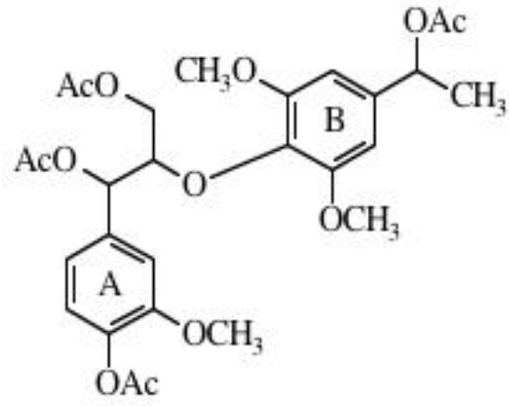
Notes:

S. Ralph SRIII-65-B
14mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.65	52	20.45	46	20.28	68
Ac Me	21.12	46	20.94	42	20.73	64
Ac Me	21.37	40	21.13	36	20.92	64
B β	21.98	52	22.35	50	21.78	64
OMe	55.98	59	56.30	52	55.79	64
β	70.49	43	71.18	44	69.76	36
B α	71.92	43	72.20	47	71.13	56
α	73.52	43	74.21	47	73.01	48
A2	111.26	39	112.20	42	111.34	40
B3	114.72	87	115.45	100	114.55	100
B5	114.72	87	115.45	100	114.55	100
A6	119.09	52	119.70	43	118.71	44
A5	122.95	53	123.61	44	122.66	52
B2	127.62	100	128.27	88	127.29	100
B6	127.62	100	128.27	88	127.29	100
B1	134.50	29	135.58	24	134.09	40
A1	135.85	30	137.17	24	135.84	44
A4	139.90	16	140.87	13	139.09	32
A3	151.20	27	152.28	20	150.69	36
B4	158.09	25	159.08	20	157.55	44
A4 Ac C=O	168.88	20	168.84	8	168.38	36
Ac C=O	169.98	20	170.13	14	169.49	36
Ac C=O	170.30	16	170.13	14	169.58	32

Compound Number 139



threo

G-β-S5

1,3-diacetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-[4-(1-acetoxy ethyl)-2,6-dimethoxyphenoxy] propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	1.99	s	
Ac Me	2.06	s	
Ac Me	2.07	s	
Ac Me	2.30	s	
B β	1.51	d	6.6
A OMe	3.82	s	
B OMe	3.77	s	
γ1	3.95	dd	11.8, 3.2
γ2	4.34	dd	11.8, 4.7
β	4.54	m	
B α	5.79	q	6.6
α	6.15	d	6.3
B2,6	6.54	s	
A2	7.08	bs	
A5	6.99	m	
A6	6.99	m	

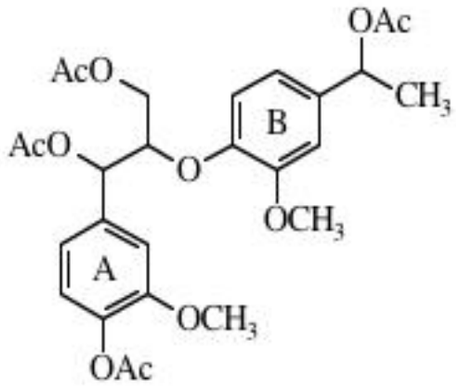
Notes:

S. Ralph SRIII-65-C 51mg
erythro shifts from SRVII 138BB in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.64	46	20.45	53	20.30	46
Ac Me	20.70	41	20.58	43	20.60	26
Ac Me	21.00	29	20.92	38	20.95	37
Ac Me	21.34	36	21.14	43	22.01	19
B β	22.23	25	22.57	32	22.06	19
A OMe	55.99	65	56.28	57	55.78	100
B OMe	56.02	100	56.39	100	55.78	100
B OMe	56.02	100	56.39	100	55.78	100
γ	63.48	18	64.17	42	63.14	13
B α	72.38	29	72.71	48	71.70	23
α	75.25	36	76.25	32	75.28	13
β	80.59	35	81.38	42	80.11	18
B2	103.21	47	104.01	68	102.88	32
B6	103.21	47	104.01	68	102.88	32
A2	111.92	21	112.64	38	111.53	15
A6	119.65	39	120.24	50	119.25	21
A5	122.51	39	123.34	48	122.53	19
A1	135.96	26	136.92	17	135.25	19
B1	135.96	26	137.14	30	135.84	25
B4	137.54	22	138.78	32	137.44	24
A4	139.72	21	140.71	18	139.08	21
A3	150.91	26	152.02	27	150.58	26
B3	152.91	43	153.79	50	152.30	45
B5	152.91	43	153.79	50	152.30	45
A4 Ac C=O	168.80	19	168.86	20	168.37	19
Ac C=O	169.71	12	169.85	23	169.25	20
Ac C=O	170.19	15	170.16	20	169.56	20
Ac C=O	170.54	19	170.57	22	169.89	22
erythro isomer						
γ			63.28			
Bα			72.68			
α			75.06			
β			81.26			
B2,6			103.91			
2			112.17			
6			119.99			
5			123.36			

Compound Number 140



threo

1,3-diacetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-[4-(1-acetoxy ethyl)-2-methoxyphenoxy] propane

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B β	1.51	d	6.6
Ac Me	1.99	s	
Ac Me	2.06	s	
Ac Me	2.065	s	
Ac Me	2.30	s	
OMe	3.82	s	
OMe	3.83	s	
γ1	4.04	dd	11.9, 5.6
γ2	4.30	dd	11.9, 4.6
β	4.61	m	
B α	5.82	q	6.6
α	6.11	d	6.3

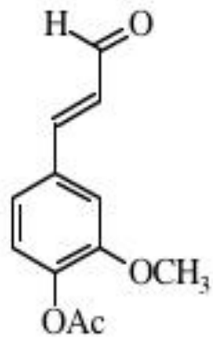
Notes:

S. Ralph SRIII-65-D
44mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.64	89	20.45	51	20.28	92
Ac Me	20.68	71	20.58	47	20.35	100
Ac Me	21.01	63	20.91	38	20.62	74
Ac Me	21.35	64	21.15	53	20.94	87
B β	22.09	57	22.45	39	21.89	58
OMe	55.92	100	56.29	100	55.66	84
OMe	55.97	86	56.29	100	55.78	71
γ	62.99	41	63.55	37	62.43	32
B α	72.06	57	72.39	46	71.37	71
α	74.41	41	75.34	39	74.26	39
β	80.14	41	80.68	39	79.10	45
B2	110.74	29	111.76	26	110.64	37
A2	111.74	46	112.64	32	111.62	45
B5	118.35	43	118.85	28	117.18	50
B6	118.67	56	119.19	43	118.09	61
A6	119.57	64	120.28	44	119.38	50
A5	122.80	60	123.51	41	122.63	47
A1	135.24	53	136.60	37	135.36	55
B1	136.76	43	137.78	22	136.11	53
A4	139.94	39	140.88	17	139.21	47
B4	147.53	24	148.48	17	147.00	50
B3	150.65	36	151.57	20	149.92	63
A3	151.12	43	152.18	21	150.68	55
A4 Ac C=O	168.74	37	168.82	16	168.32	42
Ac C=O	169.66	29	169.94	14	169.31	47
Ac C=O	170.25	27	170.16	14	169.53	47
Ac C=O	170.53	31	170.62	18	169.91	53
erythro isomer						
γ	63.0		62.5		61.8	
α	73.7		74.5		73.1	
β	80.1		80.2		78.3	
B4	146.7		147.7		146.1	

Compound Number 141



acetylated coniferylaldehyde
4-acetoxy-3-methoxycinnamaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.25	s	
OMe	3.89	s	
β	6.79	dd	15.9, 7.7
5	7.15	d	8.1
6	7.29	d	8.1, 1.9
2	7.49	d	1.9
α	7.64	d	15.9
γ	9.69	d	7.7

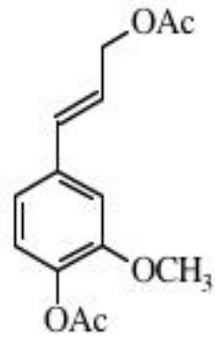
Notes:

S. Ralph SRIII-76B
30mg
in acetone 3 & α switch places

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.57	57	20.43	62	20.28	86
OMe	55.98	95	56.44	91	55.99	91
2	111.55	67	112.65	62	112.08	62
6	121.82	78	122.68	71	122.04	71
5	123.49	100	124.25	100	123.32	93
β	128.74	89	129.68	98	128.72	100
1	132.97	45	134.17	38	133.00	69
4	142.30	20	143.22	18	141.55	34
3	151.66	26	152.77	24	151.22	48
α	151.74	52	152.55	51	152.29	52
Ac C=O	168.52	21	168.72	16	168.19	34
γ	193.27	50	193.89	49	194.17	60

Compound Number 142



acetylated coniferyl alcohol

4-acetoxy-3-methoxycinnamylacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me Ac Me	2.04 2.23	s s	
OMe	3.8	s	
γ	4.69	dd	
β	6.36	dt	
α	6.68	dt	
5	7.01	m	
6	7.01	m	
2	7.21	s	

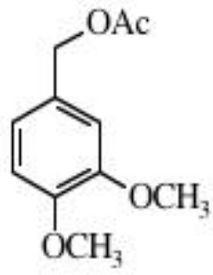
Notes:

M.Mozuch 177/95 47mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me Ac Me	20.59 20.92	75 56	20.45 20.76	72 48	20.27 20.60	98 76
OMe	55.88	100	56.24	91	55.75	96
γ	64.84	84	65.13	82	64.12	96
2	110.34	73	111.23	51	110.41	80
6	119.37	92	119.92	100	118.99	100
5	122.88	97	123.74	96	122.83	98
β	123.61	90	124.90	93	124.16	100
α	133.52	97	133.62	97	132.29	100
1	135.30	43	136.26	39	134.97	62
4	139.76	21	140.82	18	139.08	40
3	151.21	35	152.43	25	150.94	56
A4 Ac C=O γ Ac C=O	168.83 170.68	30 21	168.89 170.69	22 16	168.37 170.02	49 33

Compound Number 143



Acetylated veratryl alcohol
3,4-dimethoxybenzylacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
OMe	3.79	s	
OMe	3.80	s	
α	5.00	s	
5	6.91	m	
6	6.91	m	
2	6.98	s	

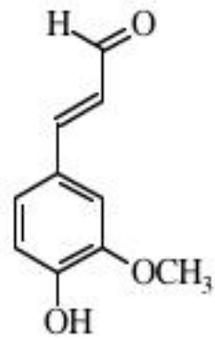
Notes:

M.Mozuch 177/95 48mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.03	36	20.83	33	20.66	57
OMe	55.96	**100**	56.18	**100**	55.50	**100**
OMe	55.96	100	56.18	100	55.50	100
α	66.38	58	66.53	62	65.47	82
2	111.27	50	112.76	36	111.70	54
5	112.06	52	113.50	38	112.34	61
6	121.33	66	121.90	68	120.88	84
1	128.60	24	129.99	15	128.45	36
3	149.14	18	150.38	13	148.66	30
4	149.26	17	150.45	11	148.75	28
Ac C=O	170.82	12	170.85	10	170.15	25

Compound Number 144



coniferaldehyde

4-hydroxy-3-methoxycinnamaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.93	s	
β	6.67	dd	15.8, 7.8
5	6.92	d	8.2
6	7.21	dd	8.2, 2.0
2	7.38	d	2.0
α	7.57	d	15.8
γ	9.64	d	7.8

Notes:

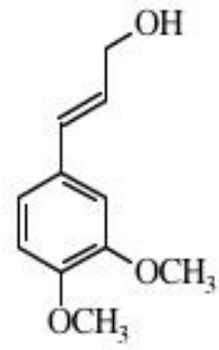
Aldrich 40mg

Note: In DMSO β and 1 are coincident

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.05	100	56.41	92	55.74	63
2	109.75	90	111.66	70	111.59	44
5	115.06	93	116.21	100	115.68	59
6	124.03	92	124.68	78	123.86	56
β	126.35	95	127.03	92	125.69	100
1	126.66	38	127.46	32	125.69	100
4	147.11	33	148.83	27	148.02	37
3	149.12	43	150.78	35	150.15	39
α	153.16	57	153.89	57	153.83	46
γ	193.62	95	193.78	65	193.84	50

Compound Number 145



3,4-dimethoxycinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.79	s	
OMe	3.82	s	
γ	4.20	dd	5.4, 1.5
β	6.26	dt	15.9, 5.4
α	6.49	dt	15.9, 1.5
5	6.88	m	
6	6.89	m	
2	7.06	d	1.7

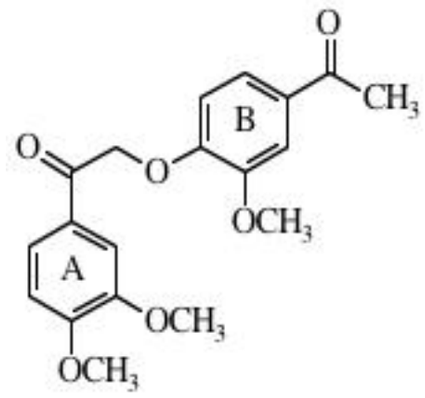
Notes:

M.Mozuch 199/16 25mg
Note: only 8 mg was used for DMSO spec.
and 1 and α switch places in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.87	100	56.12	100	55.50	100
OMe	55.95	97	56.18	90	55.55	86
γ	63.76	71	63.34	57	61.63	81
2	109.14	53	110.59	47	109.33	58
5	111.34	58	112.92	56	111.91	58
6	119.69	97	120.24	89	119.16	81
β	126.65	77	128.90	85	128.53	81
α	131.09	94	130.14	89	128.60	91
1	129.87	33	131.40	23	129.94	47
3	149.01	21	150.10	16	148.36	93
4	149.14	23	150.55	15	148.91	40

Compound Number 146



2-(4-Acetyl-2-methoxyphenoxy)-1-(3,4-dimethoxyphenyl) ethanone

^{1}H (acetone)

Atom	H Shifts	Mult	J
B β	2.50	s	
OMe	3.87	s	
OMe	3.89	s	
OMe	3.90	s	
β	5.56	s	
B5	6.94	d	8.9
A5	7.07	d	8.4
A6	7.75	dd	8.4, 1.9

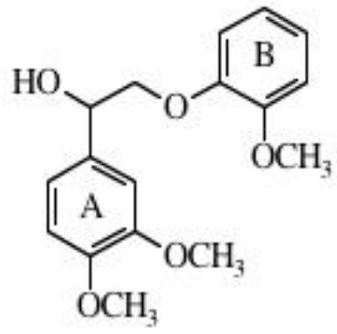
Notes:

LLL XVII -19A

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	26.16	54	26.29	56	26.22	60
OMe	56.03	77	56.21	86	55.59	96
OMe	56.10	100	56.30	100	55.63	96
OMe	56.10	100	56.36	82	55.78	80
β	71.39	48	71.71	61	70.30	56
A2	110.30	55	111.63	46	110.32	51
A5	110.54	43	111.77	68	110.92	51
B2	111.10	43	112.29	45	111.03	64
B5	112.57	38	113.55	48	112.28	56
B6	122.74	62	123.45	83	122.58	100
A6	122.85	67	123.54	90	122.58	100
A1	127.58	22	128.67	23	127.08	44
B1	131.52	26	132.02	24	130.24	40
A3	149.40	29	150.32	32	148.54	44
B3	149.40	29	150.32	32	148.69	47
B4	151.79	22	153.19	25	151.73	40
A4	154.14	23	155.19	24	153.61	38
α	192.22	29	192.90	24	192.24	44
B α	196.56	23	196.36	20	196.17	33

Compound Number 147



1-(3,4-Dimethoxyphenyl)-2-(2-methoxyphenoxy)ethanol

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.78	s	
OMe	3.82	s	
OMe	3.82	s	
β1	4.0	dd	9.9, 7.7
β2	4.07	dd	9.9, 4.2
α	4.98	m	
A2	7.14	d	1.9

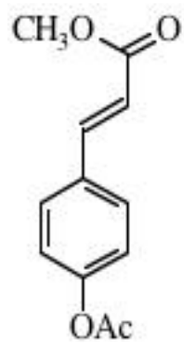
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.93	100	56.13	83	55.38	51
OMe	55.93	100	56.26	100	55.57	100
OMe	56.01	77	56.36	63	55.57	98
α	72.17	67	72.59	67	70.68	47
β	76.53	67	76.22	76	74.07	40
A2	109.67	41	111.63	59	110.48	36
A5	111.28	44	112.77	66	111.56	37
B2	112.21	45	113.67	64	112.55	37
B5	116.28	45	115.82	57	113.79	33
A6	118.67	64	119.44	100	118.32	48
B6	121.15	67	121.86	71	120.73	52
B1	122.61	67	122.43	84	120.94	47
A1	132.36	23	135.50	33	135.11	35
B3	148.14	17	149.71	29	147.99	25
A3	148.89	21	149.71	29	148.20	26
A4	149.23	20	149.84	29	148.46	29
B4	150.30	17	150.30	29	149.11	22

Notes:

LLL V-59B
β-carbon in CDCl3 was observed as shoulder on solvent.
Very limited solubility in acetone; DEPT was run in DMSO.

Compound Number 148



acetylated methyl coumarate
methyl 4-acetoxycinnamate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
OMe	3.75	s	
β	6.51	d	16.0
3,5	7.18	m	8.7
α	7.67	d	16.0
2,6	7.69	m	8.7

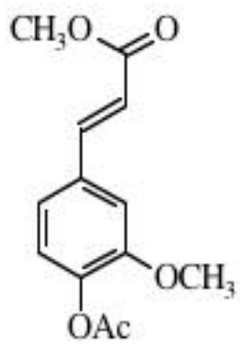
Notes:

J. Ralph P.S. 169.1
50mg
contains 30% unacetylated

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.02	100	20.93	40	20.79	47
OMe	51.66	11	51.70	45	51.70	47
β	118.04	11	118.75	48	118.75	45
3	122.23	25	123.10	100	122.30	100
5	122.23	25	123.10	100	122.30	100
2	129.24	24	130.02	100	129.50	100
6	129.24	24	130.02	100	129.50	100
1	132.13	9	132.81	40	131.70	36
α	143.80	12	144.21	48	143.49	47
4	152.31	4	153.34	18	152.06	26
γ	167.31	4	167.36	17	166.56	26
Ac C=O	169.05	4	169.36	17	168.84	26

Compound Number 149



acetylated methyl ferulate
methyl 4-acetoxy-3-methoxycinnamate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.25	s	
γ OMe	3.74	s	
OMe	3.86	s	
β	6.54	d	16.0
5	7.09	d	8.1
6	7.23	dd	8.1, 1.7
2	7.41	d	1.7
α	7.64	d	16.0

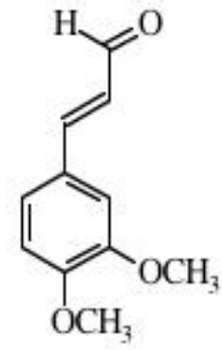
Notes:

J. Ralph P.S. 171.1

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.54	68	20.46	70	20.28	100
γ OMe	51.62	73	51.69	85	51.34	83
OMe	55.94	100	56.44	100	55.95	96
2	111.52	71	112.59	78	112.01	71
β	118.13	85	118.95	85	118.05	96
6	120.20	87	122.04	89	121.37	83
5	123.30	98	124.12	100	123.11	88
1	133.41	47	134.25	33	132.92	67
4	141.66	27	142.73	22	140.98	42
α	144.12	85	144.68	100	143.81	92
3	151.57	37	152.72	30	151.10	58
γ	167.15	32	167.41	33	166.52	58
Ac C=O	168.59	27	168.76	26	168.19	46

Compound Number 150



3,4-dimethoxy cinnamaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.88	s	
OMe	3.90	s	
β	6.70	dd	15.8, 7.7
5	7.05	d	8.3
6	7.28	dd	8.3, 7.0
2	7.38	d	7.0
α	7.62	d	15.8
γ	9.67	d	7.7

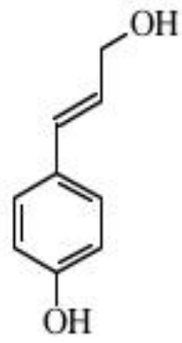
Notes:

S. Ralph SRIII-81
50mg
DMSO nmr 20mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.01	**100**	56.26	**100**	55.51	**100**
OMe	56.06	95	56.32	100	55.51	100
2	110.20	49	111.66	58	110.58	42
5	111.32	63	112.61	72	111.55	58
6	123.41	80	124.30	82	123.50	61
β	126.78	81	127.57	91	126.42	67
1	127.17	34	128.28	31	126.80	42
3	149.52	20	150.73	15	148.93	30
4	152.11	17	153.24	18	151.53	30
α	152.71	51	153.64	58	153.27	45
γ	193.39	56	193.83	62	193.81	55

Compound Number 151



p-Coumaryl alcohol
4-hydroxycinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	4.20	bd	5.2
β	6.21	dt	15.8, 5.5
α	6.51	bd	15.9
3,5	6.80	m	8.7
2,6	7.31	m	8.7

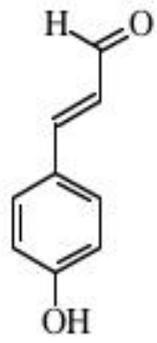
Notes:

S. Ralph
36mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ			63.47	36	61.66	36
3			116.19	100	115.28	96
5			116.19	100	115.28	96
β			127.67	41	127.06	42
2			128.33	89	127.27	100
6			128.33	89	127.27	100
1			129.73	14	127.86	27
α			130.29	42	128.64	45
4			157.78	22	156.70	29

Compound Number 152



p-Coumaraldehyde
4-hydroxy cinnamaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	6.62	dd	15.8, 7.7
3,5	6.94	m	8.7
α	7.58	d	15.8
2,6	7.61	m	8.7
γ	9.64	d	7.7

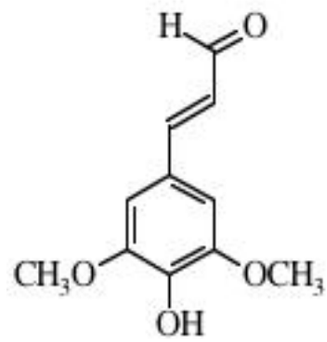
Notes:

S. Ralph
35mg
order of β & 1 are reversed in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3			116.84	96	115.88	97
5			116.84	96	115.88	97
1			126.73	46	125.34	51
β			126.96	15	125.15	29
2			131.48	100	130.81	100
6			131.48	100	130.81	100
α			153.64	37	153.50	37
4			161.24	19	160.49	31
γ			193.81	40	193.80	46

Compound Number 153



Sinapaldehyde

3,4-dimethoxy-4-hydroxycinnamaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.90	s	
β	6.69	dd	15.8, 7.7
2,6	7.08	s	
α	7.55	d	15.8
γ	9.63	d	7.7

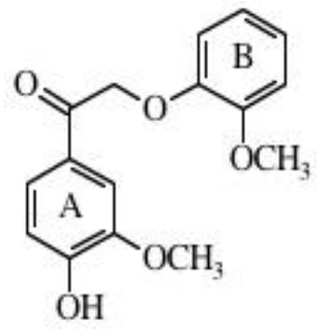
Notes:

S. Ralph
25mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.45	100	56.76	100	56.08	100
OMe	56.45	100	56.76	100	56.08	100
2	105.73	80	107.39	81	106.71	77
6	105.73	80	107.39	81	106.71	77
1	125.62	22	126.15	18	124.40	26
β	126.81	50	127.28	51	126.03	46
4	138.24	15	140.26	6	139.13	14
3	147.44	32	149.02	23	148.02	43
5	147.44	32	149.02	23	148.02	43
α	153.09	32	154.22	38	154.12	37
γ	193.32	35	193.70	26	193.75	40

Compound Number 154



1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)- ethanone

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.92	s	
β	5.36	s	

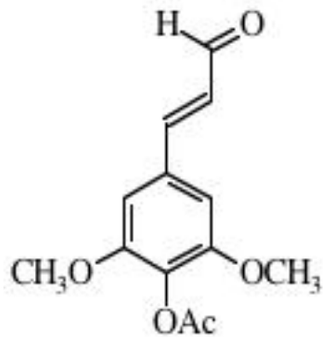
Notes:

S. Ralph

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.95	96	56.26	100	55.54	83
OMe	56.12	100	56.26	100	55.62	100
β	72.08	67	72.42	51	70.46	58
A2	110.31	74	111.84	57	111.21	58
B2	112.31	63	113.68	46	112.50	58
A5	114.06	93	115.42	57	113.70	58
B5	114.88	56	115.71	43	115.00	83
B6	120.86	93	121.48	69	120.46	100
B1	122.38	96	122.55	66	121.19	83
A6	123.41	85	123.94	71	122.79	83
A1	127.62	37	128.24	23	126.18	58
A3	146.86	33	148.30	20	147.56	92
B3	147.69	22	149.14	17	147.56	92
B4	149.82	26	150.86	14	148.96	42
A4	151.02	48	152.69	17	152.18	67
α	193.17	37	193.27	23	192.60	42

Compound Number 155



Acetylated sinapaldehyde

4-acetoxy-3,5-dimethoxycinnamaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.26	s	
OMe	3.87	s	
β	6.81	dd	15.9, 7.6
2,6	7.12	s	
α	7.61	d	15.9
γ	9.68	d	7.6

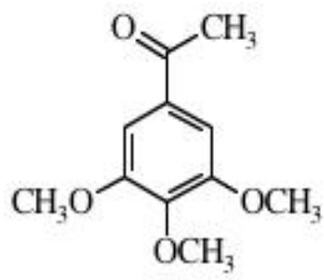
Notes:

Pearl Coll.
40mg
α and 3,5 change places in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.39	43	20.23	40	20.05	50
OMe	56.25	100	56.68	100	56.20	100
OMe	56.25	100	56.68	100	56.20	100
2	105.13	86	106.26	88	105.63	84
6	105.13	86	106.26	88	105.63	84
β	128.79	52	129.80	48	128.93	47
1	131.23	9	132.01	8	130.20	13
4	132.30	26	133.55	22	132.39	39
α	152.20	34	153.08	36	15277	66
3	152.63	47	153.64	33	152.05	37
5	152.63	47	153.64	33	152.05	37
Ac C=O	168.30	17	168.37	15	167.76	24
γ	193.25	36	193.94	36	194.18	39

Compound Number 156



3,4,5-Trimethoxyacetophenone

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	2.56	s	
4 OMe	3.80	s	
3,5 OMe	3.89	s	
2,6	7.29	s	

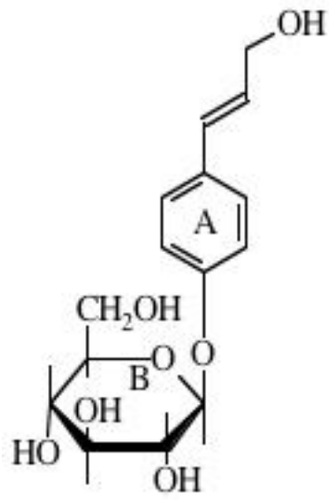
Notes:

Aldrich
48mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	26.39	43	26.52	47	26.50	51
OMe	56.34	100	56.57	100	56.01	100
OMe	56.34	100	56.57	100	56.01	100
4 OMe	60.91	41	60.64	44	60.07	47
2	106.00	75	106.85	80	105.80	87
6	106.00	75	106.85	80	105.80	87
1	132.49	23	133.51	19	132.18	30
4	142.77	9	143.62	8	141.91	11
3	153.08	41	154.16	33	152.68	60
5	153.08	41	154.16	33	152.68	60
α	196.79	16	196.76	15	196.70	17

Compound Number 157



p-Gluco cinnamyl alcohol

4-(3-hydroxy-1-propenyl)phenyl-β-D-glucopyranoside

^{1}H (DMSO)

Atom	H Shifts	Mult	J
γ	4.09	dd	5.2
β	6.24	dt	15.9, 5.0
α	6.49	bd	16.0
A3,5	6.98	d	8.7
A2,6	7.35	d	8.7
B1	4.84	d	7.3
B2,3,4,5	3.36-3.14	nr	
B6 α	3.46	m	11.7,6.0
B6 β	3.70	ddd	11.7
B6 OH	4.58	t	5.7
γOH	4.83	t	5.4

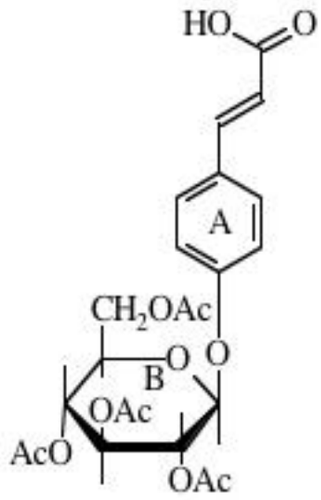
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B6					60.63	36
γ					61.49	45
B4					69.64	45
B2					73.14	41
B5					76.51	41
B3					76.94	50
B1					100.32	41
A3					116.23	91
A5					116.23	91
A2					127.02	100
A6					127.02	100
α					127.97	50
β					128.71	45
A1					130.58	36
A4					156.62	41

Notes:

N. Terashima
15mg only DMSO soluble
Terashima, Ralph, Landucci, Holzforschung, 50(1995)p. 151-155

Compound Number 158



acetylated p-gluco cinnamic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	6.44	d	16.0
A3,5	7.13	d	8.8
α	7.64	d	8.7
A2,6	7.68	d	15.7

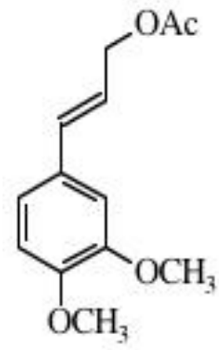
Notes:

N. Terashima
22mg
β + 3,5 switch places in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.58	100	18.86	100	20.22	91
Ac Me	20.58	100	18.86	100	20.22	91
Ac Me	20.58	100	20.52	70	20.28	81
Ac Me	20.58	100	20.58	70	20.37	66
B6	61.97	32	62.73	47	61.52	41
B4	68.29	42	69.29	43	67.96	47
B2	71.17	42	71.96	43	70.60	47
B5	72.23	45	72.75	43	70.84	53
B3	72.68	48	73.33	47	71.86	44
B1	98.55	39	98.86	40	96.67	44
A3	117.18	90	117.81	87	116.48	100
A5	117.18	90	117.81	87	116.48	100
β	116.31	42	117.96	47	117.80	47
A1	129.38	29	130.39	23	128.98	41
A2	129.90	81	130.60	83	129.76	100
A6	129.90	81	130.60	83	129.76	100
α	145.76	39	144.67	40	143.05	53
4	158.52	29	159.39	33	157.60	38
γ	169.25	29	167.83	27	167.50	41
Ac C=O	169.39	32	169.71	23	168.95	44
Ac C=O	170.20	29	170.02	27	169.17	44
Ac C=O	170.51	29	170.29	27	169.44	38
Ac C=O	171.26	26	170.62	27	169.82	47

Compound Number 159



3,4-dimethoxycinnamyl acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.02	s	
OMe	3.79	s	
OMe	3.82	s	
γ	4.65	dd	6.5, 1.3
β	6.22	dt	15.9, 6.4
α	6.61	bd	15.9
5	6.89	d	8.3
6	6.95	dd	8.3, 1.9
2	7.10	q	1.9

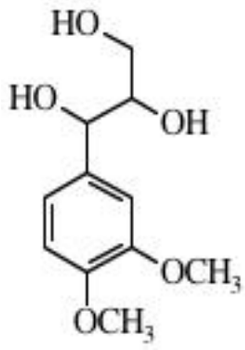
Notes:

S. Ralph 15mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.01	60	20.79	44	20.64	47
OMe	55.88	100	56.08	100	55.41	100
OMe	55.94	100	56.08	100	55.41	100
γ	65.25	87	65.48	59	64.43	47
2	109.07	60	110.48	40	109.28	33
5	111.20	67	112.67	46	111.63	37
6	120.03	87	120.78	58	119.73	50
β	121.19	100	122.28	58	121.37	50
1	129.34	47	130.37	24	128.81	30
α	134.28	87	134.54	58	133.25	43
3	149.14	33	150.54	19	148.83	43
4	149.31	40	150.62	17	148.83	43
Ac C=O	170.84	27	170.72	15	170.05	20

Compound Number 160



Veratryl glycerol
1-(3,4-dimethoxyphenyl)glycerol

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.77	s	
OMe	3.78	s	
γ1	3.36	dd	
γ2	3.48	dd	
β	3.62	m	
α	4.58	d	
5	6.86	m	
6	6.86	m	
2	7.00	bs	

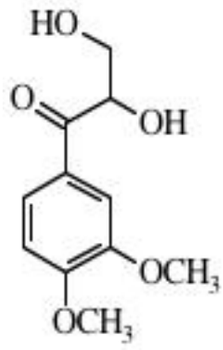
Notes:

M. Mozuch 2mg
No DEPT run and not run in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.98	100	56.10	94		
OMe	55.98	100	56.20	94		
γ	63.41	50	63.98	100		
β	74.87	47	74.70	88		
α	75.81	53	77.21	88		
2	109.71	33	111.82	62		
5	111.25	33	112.54	69		
6	119.04	50	119.91	88		
1	133.04	27	136.24	56		
3	149.08	23	149.70	31		
4	149.28	27	150.16	31		

Compound Number 161



1-(3,4-dimethoxyphenyl)-2,3-dihydroxypropan-1-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.89	s	
OMe	3.92	s	
β	5.13	m	
5	7.08	d	8.4
2	7.55	d	2.0
6	7.71	dd	2.0, 8.4

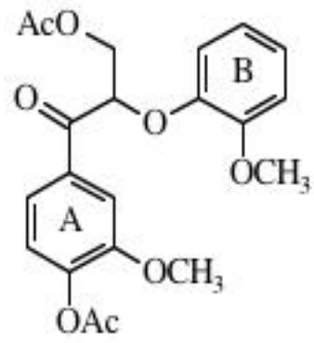
Notes:

M. Mozuch 17 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.11	100	56.20	72		
OMe	56.21	100	56.28	76		
γ	65.95	93	66.30	100		
β	74.17	93	75.28	90		
2	110.34	79	111.64	76		
5	110.77	71	112.03	48		
6	123.46	100	124.23	86		
1	126.55	43	128.45	24		
3	149.52	50	150.28	28		
4	154.42	36	155.09	28		
α	197.65	50	199.22	41		

Compound Number 162



Erone diacetate

3-acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxy phenoxy)propan-1-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.98	s	
Ac Me	2.27	s	
OMe	3.76	s	
OMe	3.88	s	
γ1	4.49	dd	6.5, 11.9
γ2	4.65	dd	3.9, 11.9
β	5.84	dd	3.9, 6.5
A2,6	7.81	m	
A5	7.23	d	8.8

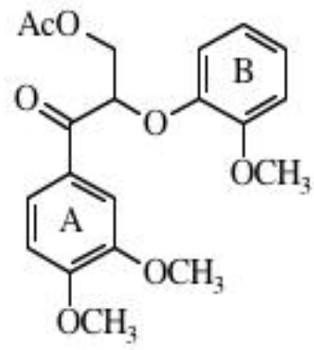
Notes:

L.Landucci 30 mg
Not run in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.62	100	20.48	100		
Ac Me	20.75	65	20.64	70		
OMe	55.75	75	56.16	79		
OMe	56.08	85	56.46	85		
γ	64.36	70	64.66	70		
β	80.58	60	80.50	67		
A2	112.73	85	113.45	66		
B2	112.73	85	113.93	64		
B5	118.53	65	118.58	56		
B6	121.04	80	121.67	74		
A6	122.34	70	122.81	67		
B1	122.97	75	124.04	89		
A5	123.66	80	124.04	89		
A1	133.67	40	134.87	39		
A4	144.38	30	145.35	20		
B4	146.82	25	147.86	33		
B3	150.43	35	151.40	25		
A3	151.47	35	152.50	39		
A4 Ac C=O	168.30	35	168.58	28		
γ Ac C=O	170.82	30	170.90	28		
α	194.59	40	195.10	31		

Compound Number 163



Veratrone acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.98	s	
OMe	3.77	s	
OMe	3.85	s	
OMe	3.89	s	
γ1	4.47	dd	6.8, 11.9
γ2	4.62	dd	3.9, 11.9
β	5.81	dd	3.9
A5	7.06	d	8.5
A2	7.66	d	2.0
A6	7.84	dd	2.0, 8.4

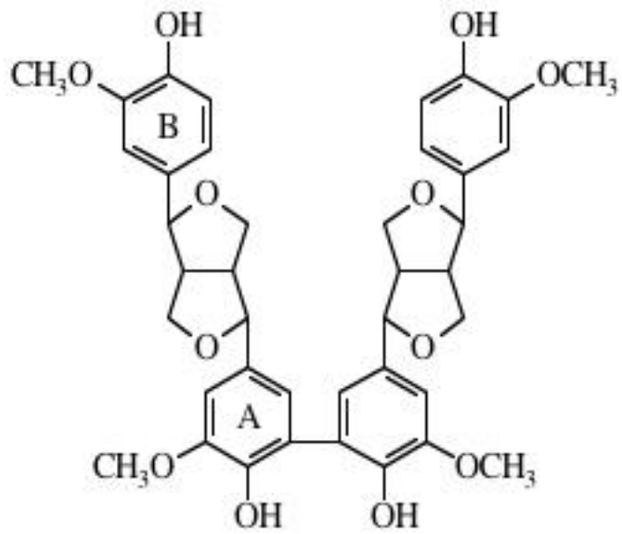
Notes:

L.Landucci
35 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.78	84	20.64	64	20.44	95
OMe	55.79	100	56.05	82	55.40	93
OMe	55.96	95	56.17	100	55.53	100
OMe	56.07	93	56.22	96	55.74	90
γ	64.62	86	64.85	79	63.60	67
β	80.28	89	80.00	82	79.08	67
A2	110.22	82	111.59	82	110.70	74
A5	111.10	84	112.06	82	110.98	76
B2	112.67	88	113.85	86	112.88	76
B5	118.05	88	117.99	79	115.61	74
B6	120.96	93	121.57	89	120.53	83
A6	123.33	89	123.69	82	122.28	79
B1	123.76	95	124.27	86	123.23	79
A1	128.04	47	128.96	39	127.29	57
B4	146.92	37	147.95	32	146.33	55
A3	149.04	46	150.13	36	148.58	55
B3	150.32	39	151.25	32	149.37	55
A4	153.88	44	155.11	36	153.67	57
Ac C=O	170.84	42	170.89	32	170.00	55
α	194.05	46	194.24	39	193.22	62

Compound Number 164



Pinoresinol biphenyl

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.82	s	
OMe	3.87	s	
A,B γ2	4.21	dd	6.8, 9.0
A,B α	4.67	d	4.5

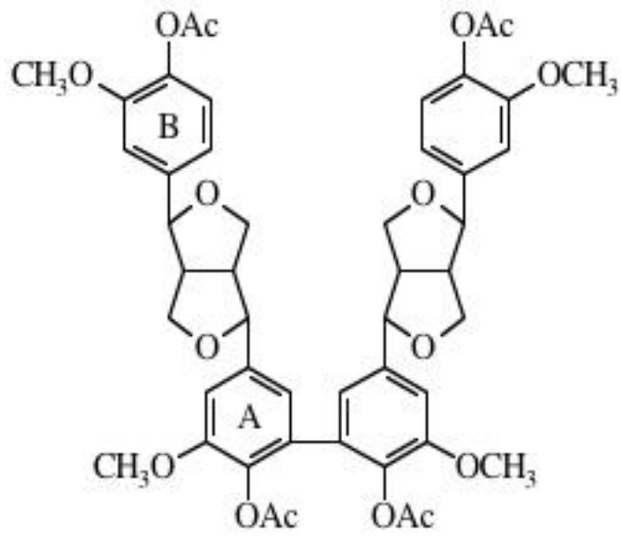
Notes:

J.Pew
15 mg
As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A β	54.13	81	55.26	100	53.60	93
Bβ	54.18	81	55.26	100	53.60	93
OMe	55.97	100	56.25	69	55.57	100
OMe	56.22	91	56.48	83	55.90	77
A γ	71.66	62	72.19	60	70.86	53
B γ	71.82	62	72.33	59	70.98	51
A α	85.82	72	86.67	93	85.14	66
Bα	85.93	72	86.67	93	85.21	56
A2	108.17	47	109.38	49	108.61	34
B2	108.64	74	110.58	57	110.39	77
B5	114.28	77	115.51	58	115.08	73
B6	118.98	72	119.62	62	118.60	68
A6	120.93	51	121.96	51	120.90	36
A5	124.06	34	125.96	23	125.44	26
A1	132.82	55	133.50	41	131.28	44
B1	132.82	55	134.17	31	132.16	47
A4	142.31	47	144.01	28	142.96	38
B4	145.26	51	146.82	35	145.85	54
B3	146.73	47	148.28	33	147.46	65
A3	147.40	45	148.68	38	147.63	41

Compound Number 165



Pinoresinol biphenyl acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.00	s	
Ac Me	2.21	s	
OMe	3.80	s	
OMe	3.84	s	
A,B β	3.14	m	
A,B γ2	4.28	m	
A,Bα	4.80	m	

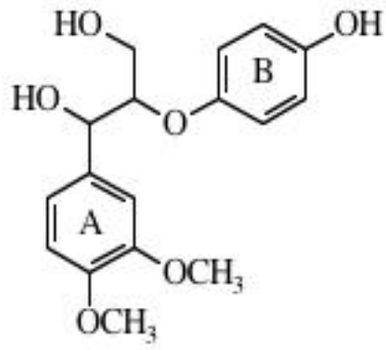
Notes:

J. Pew
7 mg intensities for some peaks are irregular
As this compound has a plane of symmetrythe shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.47	65	20.42	77	20.19	66
Ac Me	20.67	55	20.49	92	21.16	100
A β	54.28	65	55.40	86	54.57	74
B β	54.37	52	55.40	86	54.57	74
OMe	55.96	73	56.22	71	56.52	99
OMe	56.17	85	56.47	64	56.82	66
A γ	71.95	66	72.62	100	72.09	69
B γ	72.05	45	72.62	100	72.09	69
A α	85.49	100	86.17	72	85.32	47
B α	85.49	100	86.17	72	85.42	63
A2	109.40	41	110.55	41	110.80	20
B2	109.89	46	111.09	55	111.18	61
B6	117.96	54	118.62	53	118.63	65
A6	119.79	50	120.26	38	119.80	22
B5	122.76	58	123.47	60	123.36	63
A5	131.38	32	132.09	26	131.16	33
A4	136.93	18	137.76	20	136.84	31
B4	139.13	28	140.12	20	139.23	42
A1	139.40	28	141.07	31	140.59	43
B1	140.02	29	141.80	35	141.24	41
A3	151.24	31	152.27	34	151.52	55
B3	151.51	35	152.59	38	151.86	48
A Ac C=O	168.71	25	168.83	26	168.93	26
B Ac C=O	169.08	26	169.02	34	169.32	51

Compound Number 166



1-(3,4-dimethoxyphenyl)-2-(4-hydroxyphenoxy)propan-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.49	dd	5.2, 11.3
OMe	3.77	s	
OMe	3.77	s	
β	4.26	m	
α	4.95	d	5.0

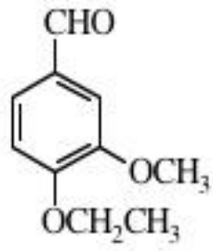
Notes:

M. Mozuch
40 mg
not very soluble in CDCl3, not run in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.03	61		
OMe			56.09	63		
γ			61.58	40		
α			73.29	40		
β			85.37	48		
A2			111.84	46		
A5			112.30	54		
B2			116.42	100		
B6			116.42	100		
B3			118.70	100		
B5			118.70	100		
A6			119.90	46		
A1			135.53	27		
A3			149.56	22		
A4			149.97	25		
B1			152.52	27		
B4			153.12	19		
minor isomer						
γ			61.96			
α			73.94			
β			85.17			

Compound Number 167



Ethyl vanillin

^{1}H (acetone)

Atom	H Shifts	Mult	J
Me	1.42	t	7.0
OMe	3.89	s	
CH2	4.15	q	7.0
5	7.08	d	8.2
2	7.41	d	1.9
6	7.49	dd	1.9, 8.2
α	9.85	s	

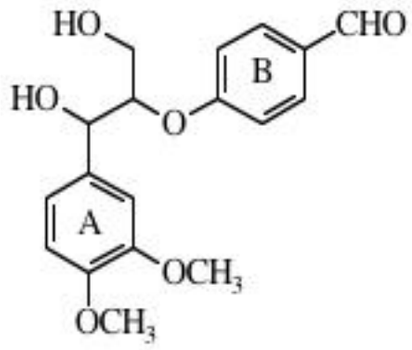
Notes:

M. Mozuch
40 mg
Not run in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Me	14.38	87	14.92	75		
OMe	55.77	100	56.00	100		
CH2	64.39	88	65.02	83		
2	108.97	59	110.36	79		
5	111.07	73	112.52	93		
6	126.53	65	126.65	70		
1	129.69	33	130.98	30		
3	149.51	23	150.72	20		
4	153.71	24	154.88	20		
α	190.60	73	191.06	72		

Compound Number 168



1-(3,4-dimethoxyphenyl)-2-(4-carboxymethylphenoxy) propan-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.82	s	
β	4.54	m	
α	4.99	d	5.6
B 2,6	7.72	m	
B α	9.78	s	

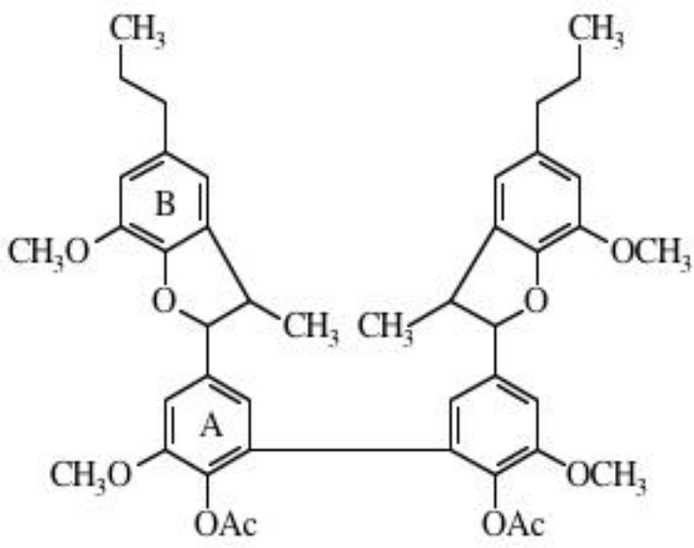
Notes:

S. Kawai
50 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.87	100	56.03	91		
γ	61.71	37	62.00	39		
α	74.04	41	73.55	36		
β	81.49	38	83.70	38		
A2	109.66	38	111.84	44		
A5	111.06	41	112.22	45		
B3	116.00	84	116.94	100		
B5	116.00	84	116.94	100		
A6	119.16	37	120.09	36		
A1	130.24	27	130.89	27		
B2	131.94	77	132.18	80		
B6	131.94	77	132.18	80		
B1	132.82	33	135.16	23		
A3	148.82	19	149.63	17		
A4	149.00	26	149.93	19		
B4	162.93	28	164.83	20		
B α	190.78	31	191.01	47		
Minor isomer						
γ	61.37					
α	73.62					
β	82.58					

Compound Number 169



Phenylcoumaran biphenyl acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.92	t	7.3
γ	1.41	d	6.8
B β	1.60	m	7.5
Ac Me	2.02	s	
B α	2.51	m	7.3
β	3.42	m	
OMe	3.82	s	
OMe	3.85	s	
α	5.18	d	8.7
B2	6.63	s	
B6	6.69	s	
A2	6.96	d	1.8
A6	7.25	d	1.9

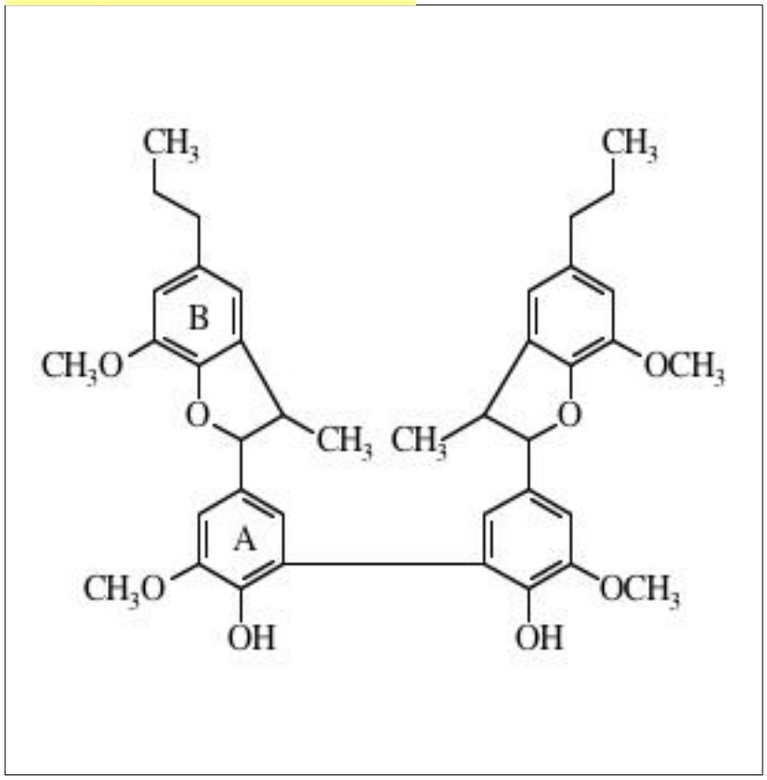
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ	13.75	**100**	14.10	97	13.71	**100**
γ	17.71	75	18.49	74	17.81	57
Ac Me	20.26	77	20.30	67	19.96	49
B β	24.92	85	25.73	64	24.56	83
B α	37.91	82	38.53	86	37.29	60
β	45.76	73	46.82	61	45.26	49
OMe	55.85	88	56.43	**100**	55.66	79
OMe	56.00	81	56.48	93	56.04	64
α	92.66	66	92.74	74	91.15	43
B2	109.60	40	110.63	68	110.13	38
A2	111.74	52	113.65	69	112.29	40
B6	115.33	68	116.42	81	115.42	45
A6	120.42	38	120.46	56	119.24	23
A1	130.96	45	132.00	46	130.33	45
B1	132.48	62	133.69	68	132.47	51
A5	136.36	59	137.00	47	135.76	53
A4	137.28	33	138.28	29	136.61	36
B5	138.51	62	140.22	46	138.84	47
B3	143.69	55	144.86	31	143.40	53
A3	145.07	40	146.36	29	144.73	43
B4	151.39	56	152.72	49	151.24	47
Ac C=O	168.36	26	168.66	28	168.02	26

Notes:

J. Pew
50 mg
As this compound has a plane of symmetrythe shifts for the other half are identical.

Compound Number 170



Phenyl coumaran biphenyl

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ	13.91	100	14.10	100	13.77	100
γ	17.48	70	17.87	78	17.28	76
B β	25.08	84	25.79	100	24.62	84
B α	38.07	84	38.54	93	37.32	64
β	45.68	79	46.48	74	44.80	50
OMe	56.00	80	56.40	89	55.66	84
OMe	56.20	85	56.50	93	55.94	68
α	93.52	72	93.84	81	92.39	48
B2	108.42	49	109.38	63	108.67	32
A2	111.83	54	113.57	70	112.19	46
B6	115.44	69	116.40	81	115.42	52
A6	122.01	61	122.57	74	121.57	36
A5	123.90	48	125.82	33	125.33	42
B1	132.15	64	132.38	48	129.98	46
A1	132.96	57	134.15	56	132.94	56
B5	136.28	62	136.65	48	135.41	58
B3	142.71	56	144.74	56	143.32	58
A4	143.82	49	144.79	56	143.78	48
A3	145.34	33	146.58	30	144.91	48
B4	147.41	52	148.76	56	147.74	50

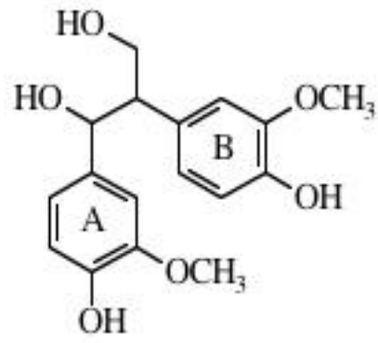
^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.92	t	7.3
γ	1.37	d	6.8
B β	1.61	h	7.4
B α	2.52	t	7.4
β	3.44	m	
OMe	3.80	s	
OMe	3.89	s	
α	5.09	d	9.4
B2	6.63	s	
B6	6.68	s	
A2	7.02	d	1.8
A6	7.11	d	1.9

Notes:

J. Pew
30 mg
As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 171



1,2-diguaiacylpropane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.67	s	
OMe	3.72	s	
β	2.94	m	
α	5.02	d	

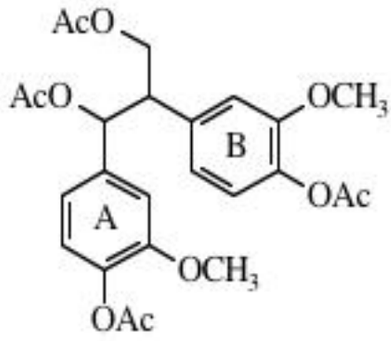
Notes:

S. Ralph
15 mg
β higher ppm than OMe's in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	55.60	46	56.46	85	54.69	74
OMe	55.90	100	56.05	90	54.87	100
OMe	55.90	100	56.15	100	55.06	95
γ	64.25	49	64.42	78	62.20	60
α	75.78	51	74.86	70	71.96	67
A2	109.06	54	111.18	72	110.27	71
B2	111.80	51	114.18	72	113.46	74
A5	113.98	56	114.82	92	113.98	90
B5	114.58	51	115.01	88	114.03	81
A6	119.70	51	119.92	82	118.13	74
B6	121.54	51	123.00	82	121.32	71
B1	130.29	27	132.17	52	130.96	69
A1	133.99	32	136.59	60	135.49	71
B4	144.97	32	145.91	42	144.13	74
A4	145.32	29	146.12	45	144.36	64
B3	146.53	27	147.54	52	146.05	69
A3	146.63	27	147.60	45	146.24	67

Compound Number 172



1,2-diguaiacylpropane-1,3-diol tetraacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.93	s	
Ac Me	1.98	s	
Ac Me	2.21	s	
Ac Me	2.22	s	
β	3.52	m	
γ1	4.21	dd	6.6, 11.0
γ2	4.38	dd	6.8, 11.3
α	6.18	d	6.6

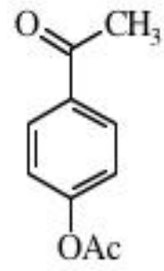
Notes:

S. Ralph
15 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.63	92	20.45	68	20.28	82
Ac Me	20.63	92	20.45	68	20.28	82
Ac Me	20.79	48	20.67	43	20.44	56
Ac Me	20.96	49	20.84	46	20.53	63
β	50.09	43	50.97	48	49.08	35
OMe	55.88	100	56.20	100	55.60	100
OMe	55.88	100	56.20	100	55.60	100
γ	64.02	42	64.86	42	63.94	28
α	74.87	42	75.56	46	74.49	35
A2	111.24	41	112.07	43	111.00	28
B2	113.32	46	114.49	42	113.38	37
A6	119.13	11	119.71	49	118.69	39
B6	120.98	47	121.91	48	120.71	39
B5	122.46	52	123.12	58	122.15	41
A5	122.58	47	123.29	51	122.38	34
B1	135.77	33	137.41	29	136.55	34
A1	136.91	33	138.70	26	137.52	35
B4	139.04	21	140.02	17	138.15	32
A4	139.58	21	140.48	17	138.71	32
B3	150.71	27	151.78	22	150.14	39
A3	150.86	24	151.97	20	150.40	34
Ac C=O	168.76	28	168.88	23	168.32	42
Ac C=O	168.84	27	168.94	22	168.32	42
α Ac C=O	169.63	26	169.64	20	169.19	32
γAc C=O	170.74	26	170.74	20	169.98	35
Minor isomer						
β			50.70			
γ			64.71			
α			76.50			

Compound Number 173



4-acetoxy-acetophenone

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.28	s	
β	2.57	s	
3	7.24	d	8.9
2	8.02	d	8.9

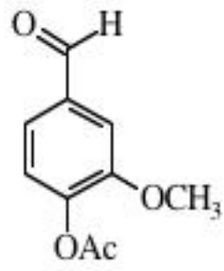
Notes:

Jamie Milhaupt
JR-JMA 29.1
50 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.11	39	20.98	40	20.51	47
β	26.55	41	20.64	45	26.62	46
3	121.75	92	122.75	100	122.02	93
5	121.75	92	122.75	100	122.02	93
2	129.91	100	130.53	94	129.78	100
6	129.91	100	130.53	94	129.78	100
1	134.72	15	135.65	11	134.39	23
4	154.35	15	155.43	11	154.08	22
Ac C=O	168.78	15	169.27	13	168.73	19
α	196.75	13	196.80	11	196.75	15

Compound Number 174



Vanillin acetate

4-formyl-2-methoxy phenyl acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
OMe	3.91	s	
2	7.57	d	0.8
5	7.29	d	7.8
6	7.55	dd	7.8, 0.8
α	9.97	s	

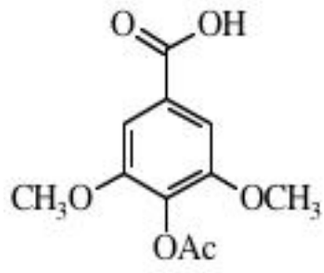
Notes:

Jamie Milhaupt
JR-JMA 23.1
50mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.58	72	20.45	62	20.29	90
OMe	56.06	100	56.46	86	55.96	100
2	110.92	85	112.31	79	111.84	90
6	123.40	98	124.39	100	123.46	90
5	124.59	87	124.44	100	123.63	100
1	135.23	40	136.43	25	135.00	51
4	144.93	24	145.83	18	144.19	34
3	151.96	30	153.03	20	151.50	41
Ac C=O	168.26	28	168.57	18	168.01	41
α	190.97	92	191.76	71	191.87	95

Compound Number 175



Syringic Acid Acetate

4-acetoxy-3,5-dimethoxy benzoic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
OMe	3.88	s	
2,6	7.37	s	

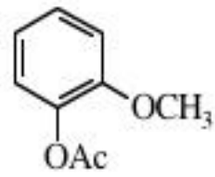
Notes:

Jamie Milhaupt
JR-JMA 25.1
25 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.43	47	20.23	43	19.93	50
OMe	56.34	100	56.65	98	55.92	100
OMe	56.34	100	56.65	98	55.92	100
2	106.90	100	107.12	100	105.72	83
6	106.90	100	107.12	100	105.72	83
1	127.15	12	129.34	17	128.72	33
4	133.37	14	133.63	12	131.44	17
3	152.19	57	153.21	33	151.48	63
5	152.19	57	153.21	33	151.48	63
α	168.17	27	166.97	21	166.44	35
Ac C=O	171.25	20	168.18	19	167.52	30

Compound Number 176



Guaiacol acetate
2-methoxyphenyl acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.22	s	
OMe	3.79	s	
2	6.93	m	
5	7.20	m	
1	7.05	m	
6	7.05	m	

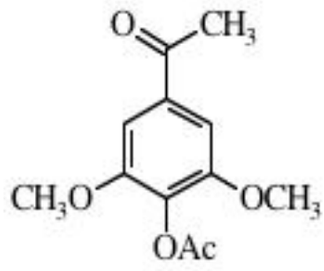
Notes:

Jamie Milhaupt
JR-JMA 27.1
54 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.64	64	20.48	68	20.21	84
OMe	55.78	100	56.12	95	55.62	96
2	112.39	93	113.41	94	112.74	99
5	120.72	97	121.30	100	120.47	100
1	122.78	95	123.66	98	122.76	97
6	126.86	95	127.50	97	126.79	93
4	139.75	19	141.01	15	139.33	28
3	151.10	22	152.36	19	150.87	35
Ac C=O	168.99	21	168.93	17	168.43	34

Compound Number 177



Acetosyringone acetate

4-acetoxy-3,5-dimethoxy acetophenone

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.25	s	
β	2.58	s	
OMe	3.87	s	
2,6	7.31	s	

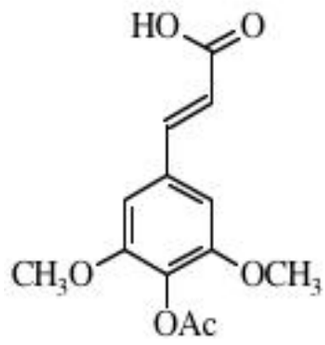
Notes:

Jamie Milhaupt
JR-JMA 31.1
50 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.41	43	20.23	40	20.86	50
β	26.50	44	26.68	47	27.47	50
OMe	52.28	100	56.66	100	56.94	100
OMe	56.28	100	56.66	100	56.94	100
2	105.10	94	105.89	100	105.79	88
6	105.10	94	105.89	100	105.79	88
4	132.81	9	133.70	6	132.75	13
1	135.11	23	136.19	13	135.69	31
3	152.20	40	153.28	26	152.56	57
5	152.20	40	153.28	26	156.56	57
Ac C=O	168.14	17	168.21	13	168.43	27
α	196.75	17	196.92	13	197.64	28

Compound Number 178



Sinapic acid acetate

4-acetoxy-3,5-dimethoxy cinnamic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac OMe	2.29	s	
OMe	3.86	s	
2,6	7.13	s	
β	6.66	d	5.9
α	7.79	d	5.9

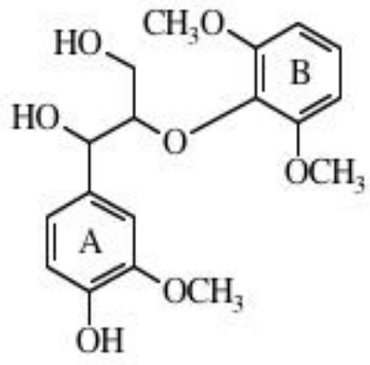
Notes:

20 mg
sample has a minor impurity

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.41	51	20.23	48	20.03	60
OMe	56.27	100	56.66	100	56.20	100
OMe	56.27	100	56.66	100	56.20	100
2	105.19	87	106.42	100	105.93	68
6	105.19	87	106.42	100	105.93	68
b	116.92	41	117.90	48	117.16	38
4	131.30	11	132.15	10	130.30	19
1	131.93	31	132.95	25	131.78	34
α	148.34	44	149.06	45	148.37	34
3	152.60	57	153.60	40	151.97	66
5	152.60	57	153.60	40	151.97	66
γ	162.19	25	163.11	15	162.61	28
Ac C=O	168.33	25	168.35	20	167.74	32

Compound Number 179



threo

Guaiacylglycerol-β-syringyl ether

1-(4-hydroxy-3-methoxyphenyl)-2-(2,6-dimethoxyphenoxy) propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.29	m	
γ2	3.64	m	
α	5.00	dd	7.5, 2.6
β	3.51	m	
B2	6.73	d	8.4
A2	7.07	d	1.8
A5	6.78	d	8.0
A6	6.92	dd	8.0, 1.8
B1	7.04	t	8.4
A4	7.46	s	
α OH	4.36	dd	2.6, 1.1

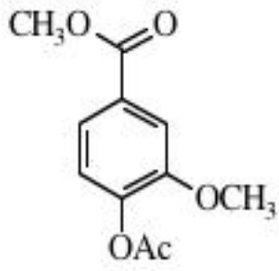
Notes:

S. Lemke SLI 75B
17.7mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.97	58	56.23	37	55.45	49
OMe	56.16	100	56.58	100	55.85	100
OMe	56.16	100	56.58	100	55.85	100
γ	60.49	42	61.31	46	60.08	31
α	74.13	45	74.07	44	71.40	39
β	89.06	47	89.76	51	86.96	34
B2	105.36	98	106.53	93	105.64	72
B6	105.36	98	106.53	93	105.64	72
A2	109.91	44	111.51	46	110.93	36
A5	114.33	45	115.23	49	114.55	39
A6	120.40	47	120.76	53	119.10	37
B1	124.50	47	124.90	53	123.26	39
A1	132.00	26	133.71	23	132.86	36
B4	135.38	15	137.16	11	136.18	22
A4	145.46	27	146.81	23	145.20	36
A3	146.58	24	147.95	18	146.76	33
B3	153.26	35	154.19	35	152.69	58
B5	153.26	35	154.19	35	152.69	58
erythro isomer						
γ	60.59		60.94		59.71	
α	72.52		73.35		72.04	
β	87.03		87.83		86.12	

Compound Number 180



4-acetoxy-3-methoxy methyl benzoate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
α OMe	3.89	s	
OMe	3.88	s	
2	7.65	d	1.9
5	7.18	d	8.0
6	7.63	dd	8.0, 1.9

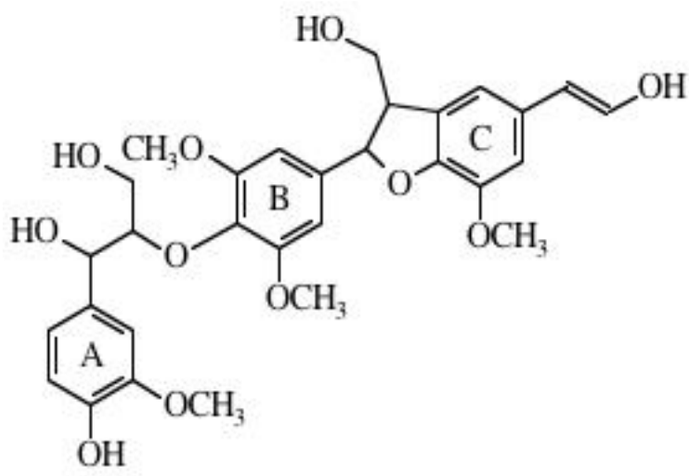
Notes:

Jamie Milhaupt
JR-JMA 43.1
50 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.61	73	20.45	72	20.33	96
α OMe	52.26	77	52.45	74	52.60	91
OMe	56.07	96	56.40	100	55.95	91
2	113.44	88	113.96	82	112.96	77
6	122.60	93	123.05	88	122.06	100
5	122.78	100	123.85	88	123.24	93
1	128.82	34	129.67	30	128.32	52
4	143.64	22	144.81	20	143.28	41
3	151.07	28	152.30	24	150.93	49
α	166.33	33	166.53	20	165.56	46
Ac C=O	168.43	29	168.59	22	168.14	46

Compound Number 181



G-b-S-c-CA

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.82	s	
OMe	3.84	s	
OMe	3.89	s	
α	5.00	m	
B α	5.62	d	6.5
B2,6	6.83	s	
C β	6.25	dt	15.8, 5.4
C α	6.54	d	15.9

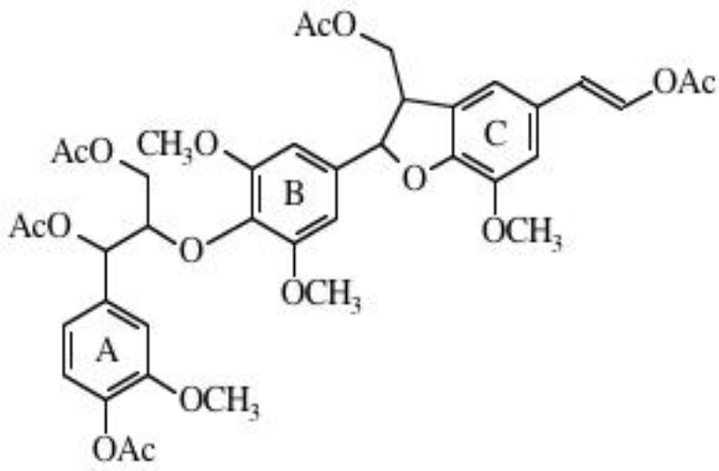
Notes:

S. Luque SLL 11C
7mg Assignments from 360 MHz exps in acetone. Spectrum in CDCl3 weak 3's,4's, and 1's uncertain Landucci, Luque and Ralph, J. Wood Chem. Tech., 15 (4), 493-513 (1995)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	53.94	48	54.91	35	52.93	27
OMe	56.10	86	56.24	61	55.42	55
OMe	56.10	86	56.50	52	55.90	73
OMe	56.34	80	56.61	100	55.71	100
OMe	56.34	80	56.61	100	55.71	100
γ	60.66	33	60.97	38	59.64	24
C γ	63.81	28	63.36	41	61.52	31
B γ	64.21	16	64.62	34	62.71	28
α	72.64	20	73.37	41	71.98	33
β	87.19	29	87.87	38	86.14	31
B α	88.18	15	88.36	28	86.93	19
B2	103.26	45	104.10	66	103.24	40
B6	103.26	45	104.10	66	103.24	40
A2	108.53	29	110.89	41	110.81	39
C2	110.67	21	111.89	31	110.88	39
A5	114.29	40	115.20	42	114.56	30
C6	114.89	33	116.06	35	114.82	22
A6	118.84	30	120.01	39	119.19	21
C β	126.87	23	128.57	35	128.02	22
C5	130.15	13	130.15	15	128.78	24
C α	131.51	27	130.40	35	129.22	21
C1	131.34	31	132.20	18	130.63	19
A1	131.34	31	133.73	18	133.15	27
B1	134.75	13	136.10	8	134.79	15
B4	137.86	25	139.09	14	136.59	21
C3	144.57	12	145.22	11	143.59	25
A4	144.94	23	146.44	20	145.18	31
A3	146.71	17	147.97	17	146.86	36
C4	148.76	10	148.82	7	146.86	36
B3	153.53	39	154.26	30	152.60	43
B5	153.53	100	154.26	30	152.60	43

Compound Number 182



G-b-S-c-CA (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.16	dd	11.9, 4.0
C γ	4.65	dd	6.5, 1.2
α	6.06	d	4.5
β	4.73	m	
B α	5.54	d	7.1
B2,6	6.76	s	
C2	7.14	m	
Cβ	6.24	dt	15.8, 6.5
C α	6.64	d	15.9

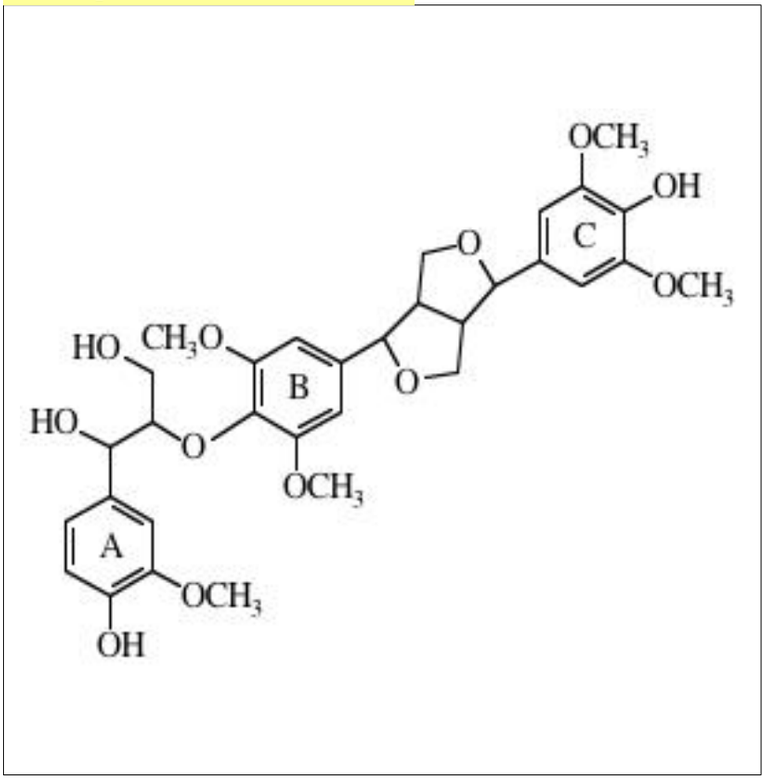
Notes:

L. Landucci SR VII-9,
8mg Assignments in d6-acetone based on 360MHz cosy df br HMBC and HMQC exps. Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.68	56	20.49	56	20.33	80
Ac Me	2078	52	20.61	51	20.31	80
Ac Me	20.85	49	20.77	58	20.55	43
Ac Me	21.07	56	20.82	64	20.67	50
Ac Me	21.07	56	20.93	54	20.71	51
B β	50.51	30	51.32	36	49.37	22
OMe	55.96	48	56.28	56	55.73	53
OMe	56.10	100	56.45	100	55.82	100
OMe	56.10	100	56.45	100	55.82	100
OMe	56.10	100	56.51	78	55.82	100
γ	62.64	24	63.29	26	62.06	15
C γ	65.19	39	65.51	40	64.51	35
B γ	65.33	28	65.96	36	64.76	21
α	74.00	26	75.03	32	73.68	18
β	80.95	21	81.37	33	79.94	22
Bα	88.55	28	88.86	32	87.60	21
B2	103.08	57	103.94	65	103.13	39
B6	103.08	57	103.94	65	103.13	39
C2	110.72	26	112.19	29	111.07	24
A2	111.50	29	112.30	42	111.07	24
C6	115.33	29	116.33	36	115.24	20
A6	119.18	24	120.01	35	118.79	22
C β	121.37	33	122.30	35	121.41	25
A5	122.44	31	123.29	44	122.54	25
C5	127.52	24	129.08	24	127.99	25
C1	130.74	23	131.60	23	130.13	27
C α	134.28	31	134.70	35	133.48	27
B4	135.16	11	136.15	12	134.30	23
A1	136.12	16	137.09	22	135.63	22
B1	136.62	24	138.02	26	136.41	23
A4	139.51	21	140.56	21	138.89	22
C3	144.46	23	145.41	22	143.89	24
C4	148.19	17	149.31	14	147.55	19
A3	150.86	21	152.03	23	150.57	27
B3	153.38	47	154.19	45	152.65	47
B5	153.38	47	154.19	45	152.65	47
Ac C=O	168.88	21	168.97	21	168.44	25
Ac C=O	169.50	22	169.95	28	169.32	25
Ac C=O	170.71	24	170.70	24	169.94	28
Ac C=O	170.85	37	170.79	23	170.12	23
Ac C=O	170.85	37	170.98	24	170.25	30

Compound Number 183



G-b-S-r-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
B β	3.11	m	
C β	3.11	m	
γ 2	3.44	dd	72.0, 3.4
β	4.17	m	
C γ	4.22	m	
B γ	4.22	m	
C α	4.67	d	4.0
B α	4.73	d	4.0
α	4.98	d	3.4
B2	6.76	s	
C2	6.67	s	
A2	7.03	s	

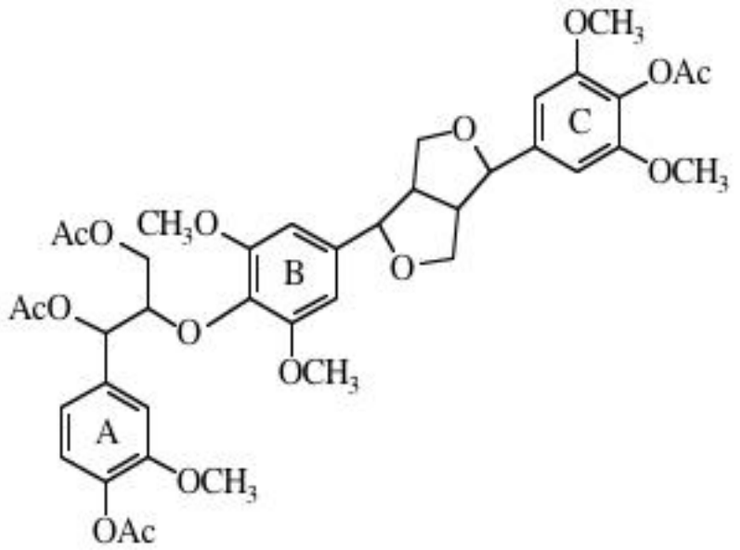
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	54.32	27	55.23	32	53.61	22
C β	54.48	26	55.39	36	53.76	27
OMe	56.00	66	56.28	54	55.53	53
OMe	56.27	80	56.60	100	55.99	100
OMe	56.27	80	56.60	100	55.99	100
OMe	56.44	62	56.67	79	55.99	100
OMe	56.44	62	56.67	79	55.99	100
γ	60.57	36	60.97	34	59.84	22
C γ	71.76	22	72.38	33	71.13	22
B γ	72.08	25	72.57	33	71.27	25
α	72.56	29	73.38	39	72.12	27
B α	85.98	41	86.57	41	85.12	33
C α	85.98	41	86.72	30	85.32	23
β	87.03	27	87.78	42	86.14	32
B2	102.88	100	104.09	70	103.29	46
B6	102.88	100	104.09	70	103.29	46
C2	102.88	100	104.50	55	103.68	51
C6	102.88	100	104.50	55	103.67	51
A2	108.61	34	110.93	38	110.96	28
A5	114.28	39	115.21	41	114.65	28
A6	118.80	33	120.04	39	119.36	28
C1	131.37	22	133.10	18	131.38	22
A1	131.91	18	133.74	20	133.26	23
B1	134.36	14	135.67	17	134.77	20
C4	134.52	15	136.20	16	134.89	20
B4	137.80	19	139.05	24	136.89	23
A3	144.94	28	146.43	29	145.32	35
A4	146.71	27	147.96	28	146.96	34
C3	147.29	33	148.67	33	147.90	44
C5	147.29	33	148.67	33	147.90	44
B3	153.45	44	154.15	47	152.61	47
B5	153.45	44	154.15	47	152.61	47

Notes:

S. Lugue SR VII 9
34mg Assignments in d6-acetone based on 360MHz HMBC and HMQC exps
Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)

Compound Number 184



G-b-S-r-S (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C γ1	3.90	dd	
γ 1	4.18	ddd	11.9, 4.1, 1.8
B,Cγ2	4.27	dd	
γ2	4.39	ddd	11.8, 5.9, 0.8
B α	4.72	d	4.4
C α	4.76	d	4.4
α	6.05	dd	4.7, 2.6
B2,6	6.68	s	
C2,6	6.74	s	
A6	6.96	dd	8.1, 1.8
A2	7.14	d	1.8
A5	7.01	d	7.4

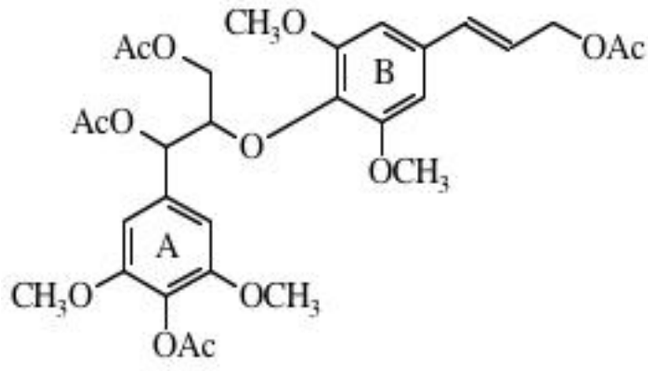
Notes:

L. Landucci XXI 36
40mg Assign'ts in d6-acetone based on the HMBC exp't H assign'ts for 360 MHz spectra Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.32	42	20.24	33	20.11	45
Ac Me	20.51	46	20.48	63	20.31	81
Ac Me	20.63	46	20.61	52	20.31	81
Ac Me	20.93	46	20.94	56	20.66	45
B β	54.16	25	55.33	30	53.67	39
C β	54.33	35	55.43	33	53.81	35
OMe	55.79	44	56.26	57	55.69	45
OMe	55.96	89	56.38	90	55.78	100
OMe	55.96	89	56.38	90	55.78	100
OMe	56.09	100	56.46	100	55.94	97
OMe	56.09	100	56.46	100	55.94	97
γ	62.50	26	63.29	36	62.10	26
B γ	71.87	25	72.65	53	71.36	45
C γ	71.98	25	72.65	53	71.36	45
α	73.82	21	75.05	30	73.72	23
β	80.62	21	81.28	22	79.86	16
B α	85.63	33	86.45	31	84.92	32
C α	85.77	30	86.54	33	85.06	32
C2	102.12	75	103.23	55	102.44	68
C6	102.12	75	103.23	55	102.44	68
B2	102.64	51	103.73	54	102.80	42
B6	102.64	51	103.73	54	102.80	42
A2	111.37	28	112.21	34	110.95	23
A6	119.09	26	120.04	25	118.80	16
A5	122.26	33	123.26	37	122.49	23
C4	127.87	14	128.85	8	127.06	19
B4	134.41	18	135.48	13	133.63	23
A1	135.97	18	137.12	18	135.71	19
B1	137.13	26	138.89	17	137.53	32
A4	139.35	26	140.54	21	138.86	26
C1	139.58	28	141.44	17	140.14	35
A3	150.68	26	152.00	23	150.53	29
C3	152.16	49	153.21	31	151.64	68
C5	152.16	49	153.21	31	151.64	68
B3	153.19	49	154.04	37	152.54	48
B5	153.19	49	154.04	37	152.54	48
Ac C=O	168.64	25	168.61	15	168.08	29
Ac C=O	168.72	26	168.94	29	168.41	29
Ac C=O	169.36	28	169.92	30	169.31	35
Ac C=O	170.70	28	170.67	31	169.94	35

Compound Number 185



S-b-SA (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	3.81	s	
Ac Me	3.85	s	
γ2	4.19	dd	11.8, 4.1
γ1	4.43	dd	11.8, 6.1
B γ	4.68	dd	7.4, 1.2
α	6.07	d	4.2
β	4.74	dt	6.1, 4.2
A6 or B6	3.78	s	
A2 or B2	6.80	s	
B β	6.33	dt	15.8, 6.3
B α	6.63	d	16.0

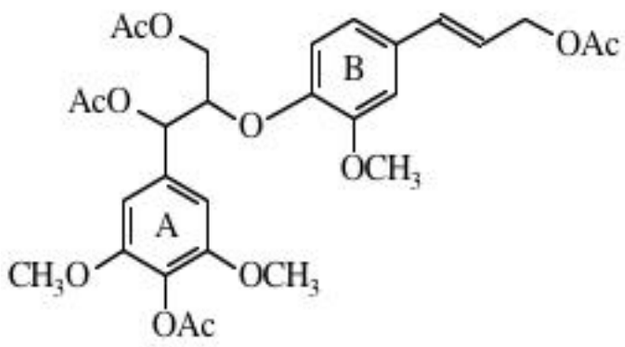
Notes:

S. Ralph SRVII 15A
67mg Landucci, Luque and Ralph, J. Wood Chem. Tech.15(4), 493-513 (1995)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.46	43	20.26	49	20.04	47
Ac Me	20.76	43	20.63	47	20.29	52
Ac Me	20.99	43	20.80	44	20.62	75
Ac Me	21.07	47	20.93	47	20.62	75
OMe	56.02	96	56.39	100	55.73	100
OMe	56.02	96	56.39	100	55.73	100
OMe	56.17	100	56.49	96	55.86	91
OMe	56.17	100	56.49	96	55.84	91
γ	62.76	34	63.28	40	62.07	26
B γ	64.92	43	65.25	48	64.16	40
α	74.25	35	75.29	41	73.84	91
β	80.93	37	81.56	42	79.98	91
A2	103.69	65	104.52	77	103.20	55
A6	103.69	65	104.52	77	103.20	55
B2	103.95	57	104.60	78	103.53	58
B6	103.95	57	104.60	78	103.53	58
B β	122.95	35	124.09	44	123.32	35
A4	128.49	11	129.32	11	127.47	19
B1	132.41	31	133.30	26	131.88	29
Bα	134.07	38	134.36	48	132.96	37
A1	135.37	18	136.46	17	134.40	28
B4	135.53	30	136.62	28	135.19	31
A3	151.93	51	153.02	43	151.44	64
A5	151.93	51	153.02	43	151.44	64
B3	153.22	53	154.14	49	152.58	62
B5	153.22	53	154.14	49	152.58	62
Ac C=O	168.57	18	168.51	22	167.91	26
Ac C=O	169.57	24	169.95	25	169.24	31
Ac C=O	170.82	27	170.68	26	169.86	35
Ac C=O	170.82	27	170.74	20	170.00	26

Compound Number 186



S-b-CA (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.86	s	
OMe	3.81	s	
γ1	4.38	dd	11.9, 5.9
γ2	4.26	dd	11.9, 4.1
B γ	4.68	dd	6.4, 1.2
β	4.89	m	
α	6.05	d	5.1
B β	6.30	dt	15.8, 6.4
B α	6.63	d	15.9
A2,6	6.87	s	
B2	7.15	d	1.6

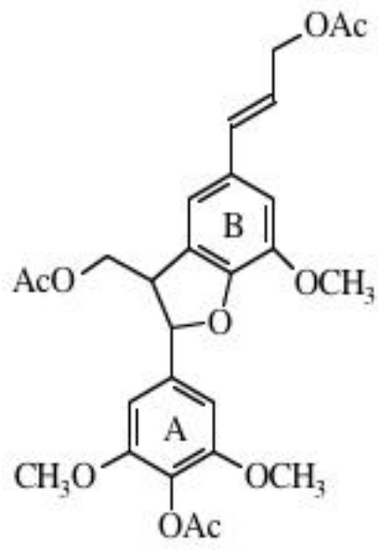
Notes:

S. Ralph SR VII 16D
15mg Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.54	34	20.25	45	20.04	45
Ac Me	20.86	37	20.64	43	20.38	52
Ac Me	21.12	46	20.80	41	20.63	75
Ac Me	21.12	46	20.89	47	20.63	75
OMe	55.91	57	56.29	54	55.61	56
OMe	56.29	100	56.54	100	55.90	100
OMe	56.29	100	56.54	100	55.90	100
γ	62.73	37	63.09	43	61.88	29
B γ	56.15	43	65.36	52	64.31	45
α	74.05	46	74.78	46	73.20	35
β	80.21	37	80.17	43	78.01	32
A2	104.52	83	105.14	81	103.94	65
A6	104.52	83	105.14	81	103.94	65
B2	110.41	43	111.40	45	110.26	33
B5	119.04	43	119.16	44	117.14	37
B6	119.89	46	120.49	40	119.43	39
B β	122.36	49	123.52	48	122.30	40
A4	128.85	14	129.61	11	127.66	23
B1	131.93	31	132.56	27	130.71	31
B α	133.90	43	134.13	48	132.84	40
A1	134.82	31	136.11	26	134.78	32
B4	147.37	29	148.33	22	146.56	31
B3	151.06	29	151.92	21	150.11	33
A3	152.13	60	153.06	38	151.38	65
A5	152.13	60	153.06	38	151.38	65
Ac C=O	168.59	23	168.46	21	167.90	31
Ac C=O	169.55	31	169.89	22	169.18	32
Ac C=O	170.84	26	170.75	29	169.96	36
Ac C=O	170.90	23	170.75	29	170.03	29

Compound Number 187



S-c-CA (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.48	dd	11.1, 5.5
γ2	4.37	dd	11.1, 7.3
B γ	4.67	d	6.4
α	5.59	d	7.1
B β	6.25	dt	15.9, 6.4
B α	6.65	d	15.9
A2	6.84	s	
B2 or B6	7.05	s	
B2 or B6	7.07	s	

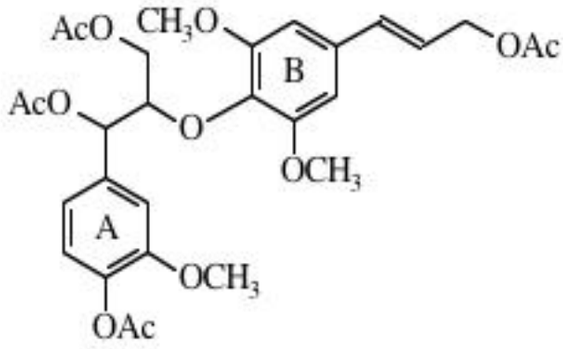
Notes:

S. Ralph SR VII 21C
8mg
Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.53	45	20.25	30	20.13	46
Ac Me	20.92	43	20.74	30	20.57	52
Ac Me	21.11	42	20.82	30	20.73	54
β	50.62	47	51.37	32	49.37	34
OMe	56.18	58	56.54	100	55.84	55
OMe	56.31	100	56.54	100	56.00	100
OMe	56.31	100	56.54	100	56.00	100
B γ	65.26	53	65.50	35	64.51	48
γ	65.43	42	65.96	34	64.47	34
α	88.44	42	88.76	31	87.46	37
A2	102.65	81	103.51	62	102.86	73
A6	102.65	81	103.51	62	102.86	73
B2	110.87	43	112.38	31	111.11	33
B6	115.42	45	116.34	31	115.24	34
B β	121.44	47	122.36	31	121.46	39
B5	127.51	34	129.03	15	127.98	36
A4	128.68	13	129.52	6	127.74	18
B1	130.85	34	131.70	16	130.22	36
B α	134.33	47	134.67	31	133.46	37
A1	135.97	36	140.50	18	138.92	34
B3	144.53	30	145.55	15	143.90	34
B4	148.26	21	149.28	10	147.49	25
A3	152.43	53	153.40	27	151.77	69
A5	152.43	53	153.40	27	151.77	69
Ac C=O	168.69	25	168.57	12	168.02	28
Ac C=O	170.79	30	170.75	8	170.13	28
Ac C=O	170.93	15	170.94	8	170.28	37

Compound Number 188



G-b-SA acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.84	s	
γ1	4.42	dd	11.8, 6.0
γ2	4.18	dd	11.8, 4.1
B γ	4.69	dd	6.2, 1.1
α	6.08	d	4.3
B2,6	6.80	s	
B β	6.33	dt	15.9, 6.2
B α	6.64	d	16.0

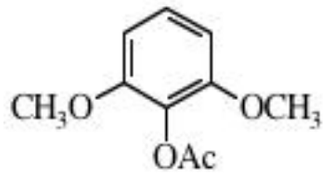
Notes:

S. Ralph SR VII - 17A
16mg
Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.72	55	20.49	55	20.35	100
Ac Me	20.81	48	20.61	51	20.35	100
Ac Me	21.06	49	20.81	47	20.70	79
Ac Me	21.02	57	20.94	54	20.70	79
OMe	55.99	58	56.31	64	55.73	62
OMe	56.07	100	56.44	100	55.82	96
OMe	56.07	100	56.44	100	55.82	96
γ	62.74	32	63.24	43	62.05	27
B γ	65.00	39	65.26	49	64.24	37
α	74.09	35	75.07	38	73.67	29
β	81.03	36	81.57	39	80.04	29
B2	103.76	67	104.71	84	103.62	60
B6	103.76	67	104.71	84	103.62	60
A2	111.56	32	111.46	47	110.92	28
A6	119.24	33	119.94	39	118.72	28
A5	122.51	36	123.34	46	122.58	43
B β	122.97	41	124.14	45	123.43	34
B1	132.46	28	133.39	25	132.02	28
B α	134.16	36	134.40	41	133.02	35
A1	135.38	14	136.46	16	134.36	24
B4	136.11	26	137.14	28	135.66	27
A4	139.56	19	140.60	14	138.88	24
A3	150.91	22	152.10	22	150.59	29
B3	153.29	45	154.23	39	152.69	52
B5	153.29	45	154.23	39	152.69	52
Ac C=O	168.92	19	168.94	18	168.45	27
Ac C=O	169.55	26	169.92	24	169.33	33
Ac C=O	170.88	38	170.66	22	169.95	36
Ac C=O	170.88	38	170.66	22	170.10	27

Compound Number 189



2,6-dimethoxyphenol acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.22	s	
OMe	3.37	s	
2,6	6.69	d	8.5
1	7.13	t	8.5

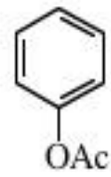
Notes:

Jamie Milhaupt
JR-JMA 35.1
40mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.45	36	20.27	35	20.12	47
OMe	56.12	100	56.40	100	55.89	96
OMe	56.12	100	56.40	100	55.89	96
2	104.91	90	105.77	95	105.00	100
6	104.91	90	105.77	95	105.00	100
1	126.23	47	126.92	53	126.23	53
4	128.85	5	129.94	5	128.11	9
3	152.34	24	153.43	22	151.90	42
5	152.34	24	153.43	22	151.90	42
Ac C=O	168.71	11	168.56	10	168.04	19

Compound Number 190



phenol acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.23	s	
3,5	7.12	m	
1	7.22	m	
2,6	7.40	m	

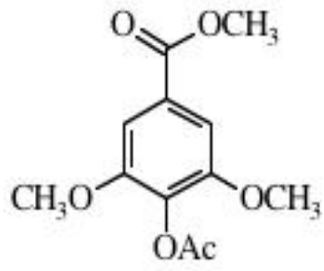
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.12	33	20.94	36	20.75	47
3	121.58	89	122.57	97	121.70	100
5	121.58	89	122.57	97	121.70	100
1	125.82	50	126.36	57	125.63	59
2	129.42	100	130.09	100	129.35	100
6	129.42	100	130.09	100	129.35	100
4	150.74	10	151.96	10	150.44	16
Ac C=O	169.48	10	169.61	10	169.05	14

Notes:

Jamie Milhaupt
JR-JMA 55
54mg

Compound Number 191



methyl (4-acetoxy-3,5-dimethoxy) benzoate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.26	s	
α OMe	3.88	s	
OMe	3.87	s	
2,6	7.33	s	

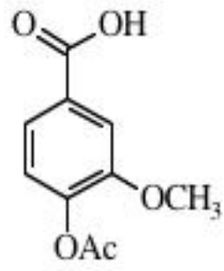
Notes:

Jamie Milhaupt
JR-JMA 41.1
40mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.40	42	20.22	43	20.06	48
α OMe	52.34	45	52.57	45	52.36	49
OMe	56.32	100	56.68	96	56.17	100
OMe	56.32	100	56.68	96	56.17	100
2	106.34	95	106.87	100	105.79	90
6	106.34	95	106.87	100	105.79	90
1	128.10	21	129.04	17	127.70	29
4	132.63	9	133.69	8	131.96	10
3	152.10	39	153.27	26	151.81	58
5	152.10	39	153.27	26	151.81	58
α	166.37	16	166.61	11	165.75	25
Ac C=O	168.14	17	168.17	13	167.67	26

Compound Number 192



4-acetoxy-3-methoxy benzoic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.28	s	
OMe	3.90	s	
2	7.70	s	
6	7.67	dd	7.6, 1.8
5	7.19	dd	7.7, 1.0

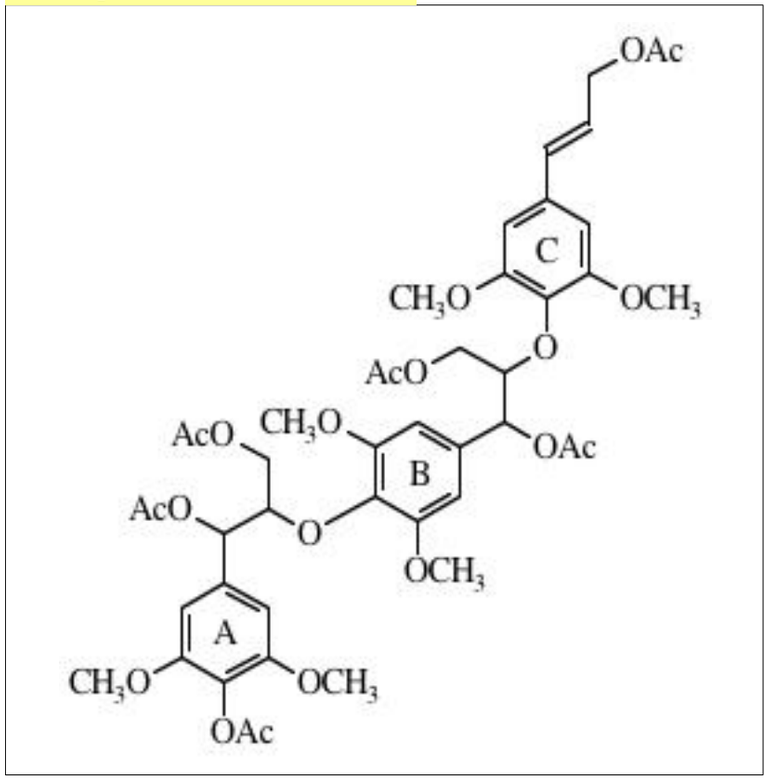
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.65	91	20.46	82	20.37	88
OMe	56.12	100	56.40	99	55.90	100
2	113.38	93	114.25	90	113.18	84
6	122.98	96	123.31	100	122.16	90
5	123.46	91	123.80	100	123.05	85
1	128.00	44	129.96	30	129.58	52
4	144.43	40	144.79	22	142.98	46
3	151.20	53	152.26	27	150.82	56
α	168.52	51	167.04	37	166.66	59
Ac C=O	171.37	56	168.65	37	168.21	54

Notes:

Jamie Milhaupt
JR-JMA 39.1
41mg 2D short range XH corr confirms assignment of 5 and 6.

Compound Number 193



S-b-S-b-SA (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
A,B γ2	4.14	m	
A,B γ1	4.40	m	
C γ	4.70	d	11.2
A,B α	6.06,6.03	d	4.0
C β	6.33	dt	15.6

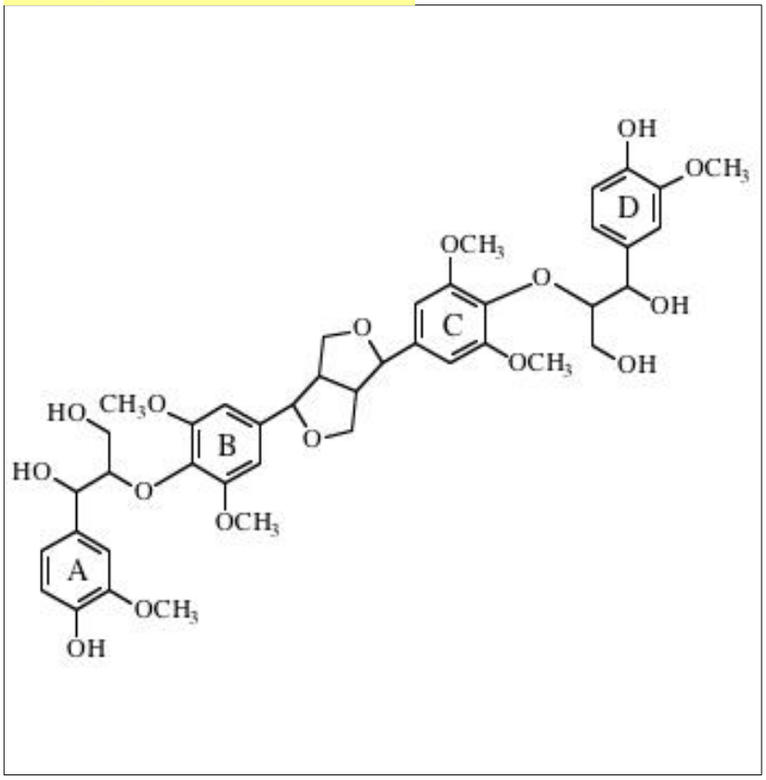
Notes:

L.Landucci
LLL XIV 148BA
10 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.53	70	20.26	41	20.04	50
Ac Me	20.53	70	20.26	41	20.04	50
Ac Me	20.85	56	20.67	27	20.21	33
Ac Me	20.85	56	20.80	21	20.30	35
Ac Me	21.15	73	20.95	46	20.61	70
Ac Me	21.15	73	20.95	46	20.61	70
OMe	56.12	100	56.46	100	55.72	100
OMe	56.12	100	56.46	100	55.72	100
OMe	56.26	100	56.46	100	55.72	100
OMe	56.26	100	56.46	100	55.72	100
OMe	56.26	100	56.46	100	55.85	92
OMe	56.26	100	56.46	100	55.85	92
γ	62.88	33	63.44	22	62.22	26
B γ	62.88	33	63.44	22	62.22	26
C γ	65.00	22	65.26	17	64.16	19
α	74.35	23	75.43	32	73.97	20
B α	74.50	23	75.43	32	73.97	20
β	80.89	33	81.42	14	79.89	17
B β	80.89	33	81.56	14	79.89	17
A2	103.81	41	104.67	49	103.35	46
A6	103.81	41	104.67	49	103.35	46
B2	104.10	44	104.67	49	103.35	46
B6	104.10	44	104.67	49	103.35	46
C2	104.33	35	104.96	20	103.53	30
C6	104.33	35	104.96	20	103.53	30
C β	123.04	17	124.09	12	123.29	13
A4	128.54	11	129.36	7	127.48	15
C1	132.45	11	133.25	9	131.80	11
B1	133.24	16	134.06	9	132.46	8
C α	134.12	18	134.38	12	132.95	15
C4	135.40	10	136.54	9	134.25	9
A1	135.63	12	136.60	9	134.45	7
B4	135.81	13	136.64	9	135.16	13
A3	151.96	42	153.01	26	151.40	43
A5	151.96	42	153.01	26	151.40	43
B3	153.08	29	153.88	21	152.29	34
B5	153.08	29	153.88	21	152.29	34
C3	153.29	33	154.16	19	152.54	26
C5	153.29	33	154.16	19	152.54	26
A4 Ac C=O	168.68	15	168.50	18	167.89	24
Ac C=O	169.52	18	169.95	28	169.23	33
Ac C=O	169.66	19	169.95	28	169.23	33
Ac C=O	170.79	17	170.67	23	169.83	39
Ac C=O	170.94	27	170.67	23	169.83	39
Ac C=O	170.94	27	170.67	23	169.98	12

Compound Number 194



G-b-S-r-S-b-G

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B,C β	54.48	30	55.37	40	53.56	31
OMe	56.00	80	56.26	70	55.41	69
OMe	56.27	**100**	56.62	**100**	55.89	**100**
OMe	56.27	100	56.62	100	55.89	100
A,D γ	60.56	43	60.97	34	59.73	25
B,C γ	72.01	27	72.64	38	71.21	25
A,D α	72.55	32	73.38	36	72.00	25
B,C α	85.86	25	86.53	40	84.97	25
A,D β	87.08	30	87.84	45	86.05	19
B,C 2	102.82	68	104.12	74	103.22	50
B,C 6	102.82	68	104.12	74	103.22	50
A,D 2	108.45	36	110.93	40	110.85	25
A,D 5	114.19	41	115.19	49	114.54	25
A,D 6	118.75	43	120.05	38	119.24	25
A,D 1	131.31	25	133.77	19	133.18	25
B,C 1	134.41	16	135.74	17	134.69	25
B,C 4	137.63	23	139.00	21	136.68	25
A,D 4	144.89	30	146.45	26	145.20	38
A,D 3	146.64	32	147.96	26	146.85	38
B,C 3	153.49	50	154.20	47	152.50	56
B,C 5	153.49	50	154.20	47	152.50	56

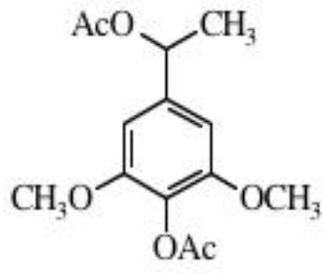
^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.87	s	
A,D γ2	3.71	dd	12.0, 3.4
A,D α	4.98	d	3.2
B,C α	4.75	d	2.3
B,C 2,6	6.77	s	
A,D 2	7.04	d	1.6

Notes:

S. Luque 12E
8 mg Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)
As this compound has a plane of symmetrythe shifts for the other half are identical.

Compound Number 195



1-(4-acetoxy-3,5-dimethoxyphenyl)-1-acetoxy ethane

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.04	s	
Ac Me	2.22	s	
β	1.49	d	6.6
OMe	3.80	s	
α	5.80	q	6.6
2,6	6.74	s	

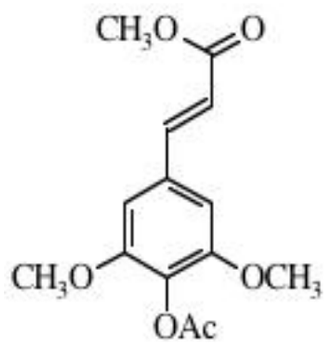
Notes:

J. Milhaupt
A 51
41mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.47	43	20.24	41	20.03	53
Ac Me	21.36	36	21.12	38	20.90	51
β	22.24	47	22.62	52	22.02	50
OMe	56.17	100	56.44	97	56.89	100
OMe	56.17	100	56.44	97	56.89	100
α	72.28	51	72.64	52	71.58	51
2	102.94	87	103.51	100	102.54	82
6	102.94	87	103.51	100	102.54	82
4	128.24	8	129.11	6	127.25	14
1	140.03	27	141.50	23	140.23	36
3	152.12	39	153.16	29	151.57	56
5	152.12	39	153.16	29	151.57	56
Ac C=O	168.69	18	168.52	14	168.00	28
α Ac C=O	170.15	15	170.16	14	169.54	26

Compound Number 196



Acetylated Sinapic acid methyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.25	s	
γ OMe	3.75	s	
OMe	3.87	s	
2,6	7.08	s	
β	6.58	d	16.0
α	7.62	d	16.1

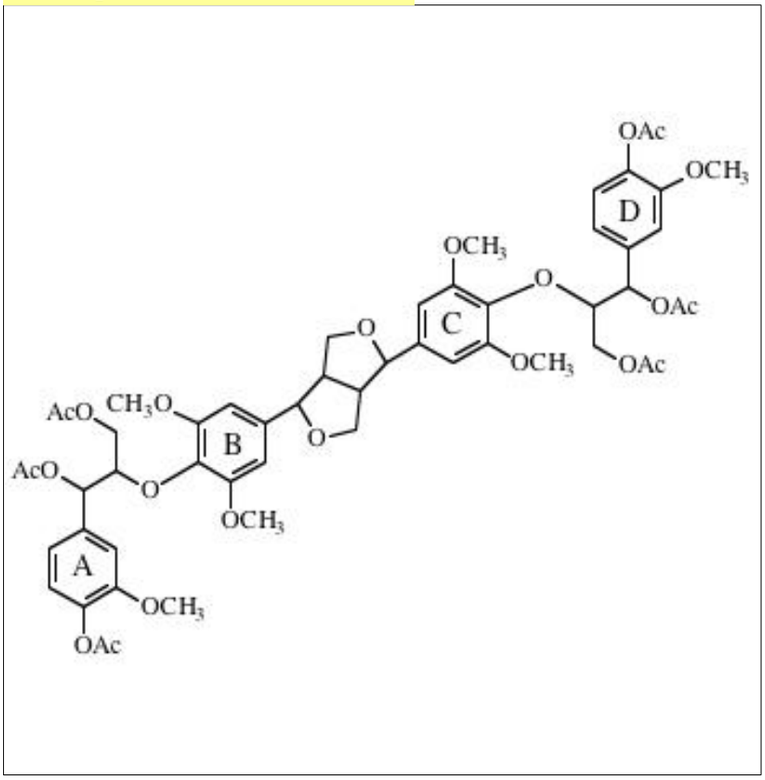
Notes:

J. Milhaupt
A 45
47mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.36	45	20.23	39	20.00	49
γ OMe	51.68	45	51.70	48	51.34	47
OMe	56.12	100	56.61	95	56.08	100
OMe	56.12	100	56.61	95	56.08	100
2	104.65	100	105.83	100	105.24	88
6	104.65	100	105.83	100	105.24	88
β	118.05	52	118.97	46	118.18	47
4	130.40	10	131.45	7	129.60	17
1	132.64	29	133.56	26	132.30	38
α	144.51	51	145.15	52	144.26	45
3	152.38	49	153.53	38	151.90	63
5	152.38	49	153.53	38	151.90	63
γ	167.11	24	167.44	18	166.57	30
Ac C=O	168.39	22	168.38	16	167.83	29

Compound Number 197



G-b-S-r-S-b-G (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C β	3.10	m	
OMe	3.80	s	
OMe	3.82	s	
B γ1	3.91	m	
A γ2	4.16	m	
B γ2	4.25	m	
A γ2	4.40	dd	
Aβ	4.68	m	
B,C α	4.72	m	
A,D α	6.06	m	
B,C 2,6	6.69	s	
A 6	6.96	dd	
A 5	7.02	d	
A 2	7.15	s	

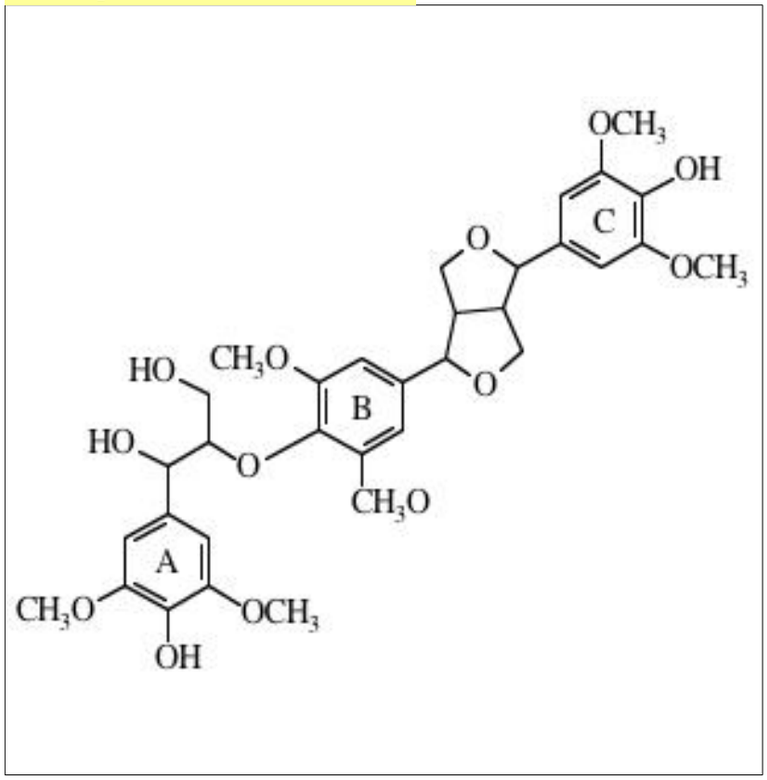
Notes:

S. Luque SLL 13F, 11 mg
1H data from 360 MHz spectrum. The β-O-4 units are erythro,
Landucci, Luque and Ralph J. Wood Chem. Tech., 15(4), 493-513 (1995) As this compound has a plane of symmetry,the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.74	83	20.48	80	20.27	86
Ac Me	20.83	69	20.61	62	20.27	86
Ac Me	21.14	59	20.94	64	20.61	43
B,C β	54.45	22	55.38	31	53.65	22
A,D OMe	56.00	72	56.26	69	55.63	66
B,C OMe	56.18	100	56.39	100	55.73	100
B,C OMe	56.18	100	56.39	100	55.73	100
A,D γ	62.78	28	63.27	33	62.02	18
B,C γ	72.06	13	72.60	33	71.24	21
A,D α	74.01	26	75.04	31	73.64	17
A,D β	80.87	25	81.30	24	79.83	20
B,C α	85.94	23	86.52	31	84.93	19
B,C 2	102.86	48	103.71	58	102.69	31
B,C 6	102.86	48	103.71	58	102.69	31
A,D 2	111.58	27	112.20	33	110.85	16
A,D 6	119.27	28	120.03	24	118.72	16
A,D 5	122.48	29	123.25	36	122.43	18
B,C 4	134.60	12	135.47	11	133.51	14
A,D 1	136.19	16	137.15	18	135.61	15
B,C 1	137.35	16	138.96	20	137.50	14
A,D 4	139.56	22	140.54	22	138.79	17
A,D 3	150.90	20	152.01	22	150.46	21
B,C 3	153.42	43	154.05	44	152.46	34
B,C 5	153.42	43	154.05	44	152.46	34
4 Ac C=O	168.92	28	168.92	33	168.35	32
αAc C=O	169.56	23	169.90	27	169.24	31
γAc C=O	170.91	28	170.65	33	169.87	29

Compound Number 198



S-b-S-r-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C β	3.12	m	
OMe	3.80	s	
OMe	3.82	s	
OMe	3.88	s	
B α	4.68	d	4.0
C α	4.74	d	4.0
α	4.99	m	
B 2,6	6.69	s	
C 2,6	6.71	s	
A 2,6	6.78	s	

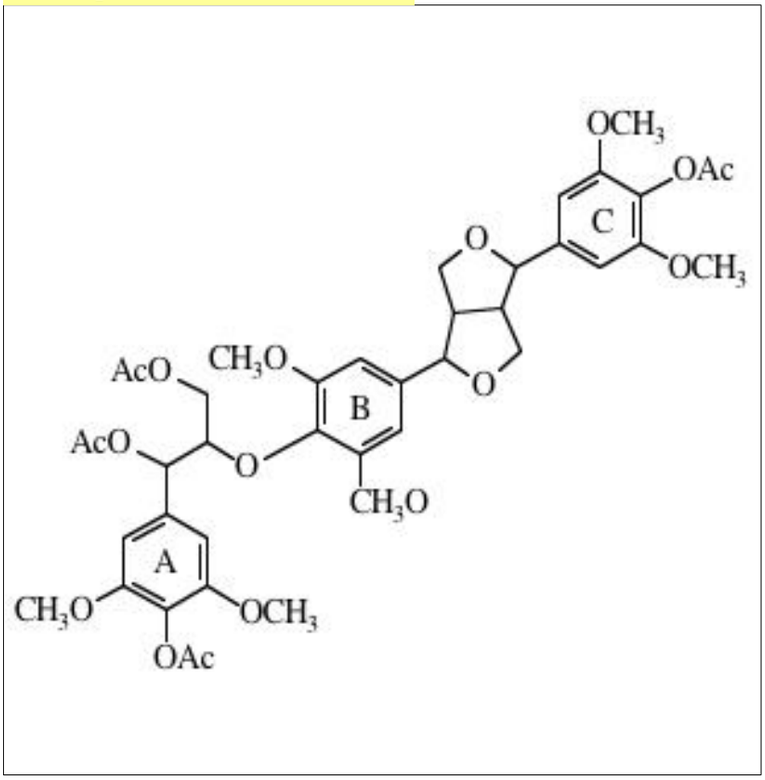
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	54.43	27	55.27	19	53.59	20
C β	54.57	21	55.42	19	53.73	20
OMe	56.34	68	56.63	100	55.88	76
OMe	56.34	68	56.63	100	55.88	76
OMe	56.45	100	56.63	100	56.01	100
OMe	56.45	100	56.63	100	56.01	100
OMe	56.49	88	56.63	100	56.01	100
OMe	56.49	88	56.63	100	56.01	100
γ	60.65	27	61.03	17	59.90	14
C γ	71.80	18	72.40	21	71.10	18
B γ	72.17	16	72.61	20	71.26	21
α	72.77	14	73.63	17	72.38	20
B α	86.01	23	86.61	20	85.10	20
C α	86.01	23	86.73	21	85.30	22
β	87.24	18	87.87	17	86.20	21
B2	102.69	45	104.10	36	103.28	33
B6	102.69	45	104.10	36	103.28	33
C2	102.84	64	104.51	43	103.65	46
C6	102.84	64	104.51	43	103.65	46
A2	102.94	50	104.91	40	104.29	37
A6	102.94	50	104.91	40	104.29	37
A1	130.46	11	132.73	11	131.36	21
C1	132.00	16	133.13	13	132.42	18
B1	134.05	18	135.86	13	134.42	21
A4	134.51	21	135.86	13	134.86	26
C4	134.51	21	136.23	10	134.86	26
B4	137.91	18	139.07	13	136.79	13
A3	147.15	43	148.38	26	147.40	39
A5	147.15	43	148.38	26	147.40	39
C3	147.29	36	148.68	21	147.88	45
C5	147.29	36	148.68	21	147.88	45
B3	153.55	36	154.16	20	152.55	33
B5	153.55	36	154.16	20	152.55	33

Notes:

S. Luque SLL I 12E
10 mg A4 was coincident with other shifts, the assignments were inferred from other models and peak heights.
Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)

Compound Number 199



S-b-S-r-S (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C β	3.11	m	
B α	4.73	d	
C α	4.76	d	
α	6.05	m	
2,6	6.70	s	
2,6	6.76	s	

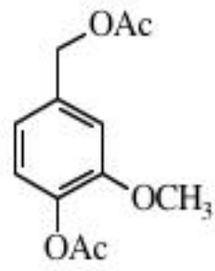
Notes:

S. Luque SLL 13F
15mg
Landucci, Luque and Ralph, J. Wood Chem. Tech., 15(4), 493-513 (1995)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.53	52	20.26	49	20.06	45
Ac Me	20.53	52	20.26	49	20.06	45
Ac Me	20.86	31	20.63	26	20.29	32
Ac Me	21.16	30	20.94	26	20.63	34
B β	54.39	17	55.33	20	53.61	23
Cβ	54.52	23	55.44	23	53.85	23
OMe	56.17	65	56.38	64	55.72	68
OMe	56.17	65	56.38	64	55.72	68
OMe	56.23	88	56.46	100	55.87	100
OMe	56.23	88	56.46	100	55.87	100
OMe	56.29	100	56.46	100	55.87	100
OMe	56.29	100	56.46	100	55.87	100
γ	62.81	18	63.41	19	62.16	13
C γ	72.07	21	72.66	44	71.31	34
B γ	72.19	21	72.66	44	71.31	34
α	74.25	16	75.33	15	73.92	13
β	80.78	15	81.29	11	79.76	12
B α	85.82	21	86.45	25	84.85	19
C α	85.98	20	86.56	20	85.00	18
C2	102.30	48	103.23	47	102.36	44
C6	102.30	48	103.23	47	102.36	44
B2	102.84	32	103.71	35	102.70	26
B6	102.84	32	103.71	35	102.70	26
A2	104.07	41	104.68	34	103.30	26
A6	104.07	41	104.68	34	103.30	26
C1	128.05	7	128.85	7	126.98	9
A4	128.51	11	129.34	7	127.45	12
B4	134.67	13	135.61	9	133.69	12
A1	135.66	11	136.65	10	135.21	12
B1	137.27	13	138.83	12	137.38	14
C4	139.74	16	141.45	15	140.08	18
A3	151.92	33	152.95	20	151.38	32
A5	151.92	33	152.95	20	151.38	32
C3	152.34	31	153.22	24	151.58	39
C5	152.34	31	153.22	24	151.58	39
B3	153.35	25	153.98	22	152.41	26
B5	153.35	25	153.98	22	152.41	26
Ac C=O	168.63	18	168.48	15	167.91	22
Ac C=O	168.85	16	168.58	15	168.02	19
Ac C=O	169.53	16	169.91	14	169.26	19
Ac C=O	170.94	16	170.76	15	169.89	19

Compound Number 200



Vanillyl alcohol diacetate

4-hydroxy-3-methoxybenzyl alcohol diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.04	s	
Ac Me	2.23	s	
OMe	3.80	s	
α	5.06	s	
6	6.96	dd	8.1,1.8
5	7.03	d	8.0
2	7.11	d	1.7

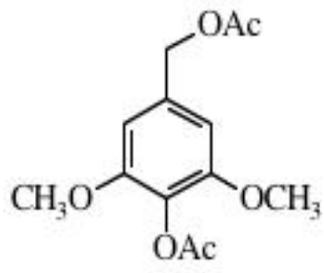
Notes:

S. Ralph
35mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.57	76	20.45	75	20.25	97
Ac Me	20.93	59	20.78	55	20.59	78
OMe	55.84	100	56.20	92	55.68	100
α	65.86	91	66.10	99	65.10	90
2	112.50	91	113.32	83	112.58	92
6	120.67	89	121.04	96	120.16	92
5	122.77	95	123.57	100	122.67	89
1	134.80	45	136.23	37	134.99	64
4	139.62	26	140.64	20	138.97	43
3	151.07	33	152.19	24	150.69	52
4 Ac C=O	168.84	29	168.93	24	168.42	49
α Ac C=O	170.66	23	170.79	19	170.15	36

Compound Number 201



Syringyl alcohol diacetate

3,5-dimethoxy-4-hydroxy benzyl alcohol diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.06	s	
Ac Me	2.22	s	
OMe	3.80	s	
α	5.05	s	
2,6	6.76	s	

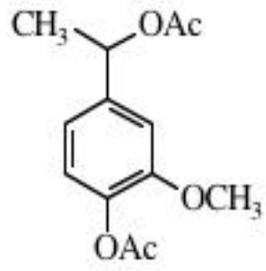
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.47	59	20.23	49	20.05	62
Ac Me	21.05	31	20.79	27	20.63	42
OMe	56.21	100	56.46	100	55.91	100
OMe	56.21	100	56.46	100	55.91	100
α	66.37	48	66.46	44	65.45	42
2	105.13	89	105.67	93	104.84	80
6	105.13	89	105.67	93	401.84	80
4	128.58	7	129.43	6	127.57	12
1	134.42	21	135.77	19	134.49	32
3	152.21	39	153.19	27	151.59	53
5	152.21	39	153.19	27	151.59	53
4 Ac C=O	168.67	16	168.50	12	167.97	28
α Ac C=O	170.77	12	170.80	9	170.14	17

Notes:

J. Milhaupt A 53
35 mg
Sample has impurity

Compound Number 202



1-(4-acetoxy-3-methoxyphenyl)-1-acetoxyethane

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.49	d	6.6
Ac Me	2.03	s	
Ac Me	2.22	s	
OMe	3.82	s	
α	5.83	q	6.6
6	6.95	dd	8.1,1.8
5	7.02	d	8.1
2	7.11	d	1.8

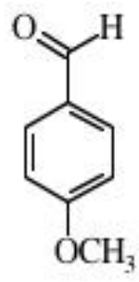
Notes:

J. Milhaupt
A 49.1
35mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.69	79	20.47	79	20.28	96
Ac Me	21.37	65	21.12	64	20.90	87
β	22.21	91	22.57	86	22.00	87
OMe	55.93	100	56.21	88	55.70	100
α	71.96	89	72.31	91	71.26	96
2	110.60	88	111.30	78	110.46	82
6	118.44	95	118.73	98	117.74	87
5	122.75	89	123.51	100	122.60	96
1	139.33	26	140.32	17	138.62	42
4	140.52	44	141.88	36	140.60	58
3	151.05	31	152.18	24	150.66	42
4 Ac C=O	169.01	31	168.95	22	168.44	49
α Ac C=O	170.21	30	170.17	19	169.55	42

Compound Number 203



4-methoxy benzaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.89	s	
3,5	7.08	d	8.8
2,6	7.85	d	8.8
α	9.86	s	

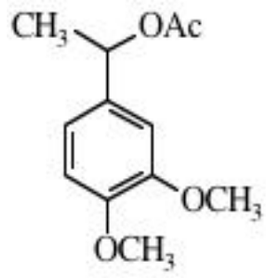
Notes:

Aldrich
60mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.51	51	56.03	58	55.51	38
3	114.26	100	115.16	100	114.35	87
5	114.26	100	115.16	100	114.35	87
1	129.90	14	131.11	11	129.57	18
2	131.88	97	132.43	90	131.65	100
6	131.88	97	132.43	90	131.65	100
4	164.55	14	165.44	11	164.10	18
α	190.68	45	191.09	42	191.01	51

Compound Number 204



1-(3,4-dimethoxyphenyl)-1-acetoxyethane

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.47	d	6.6
Ac Me	2.00	s	
OMe	3.78	s	
OMe	3.81	s	
α	5.78	q	6.6
5,6	6.90	m	
2	6.97	s	

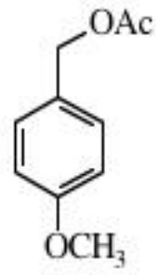
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.39	39	21.18	38	20.93	62
β	21.99	55	22.41	57	21.82	72
OMe	55.91	100	56.13	100	55.43	100
OMe	55.91	100	56.13	100	55.43	100
α	72.20	51	72.51	54	71.42	73
2	109.69	46	111.16	43	109.93	67
5	111.06	49	112.63	46	111.57	70
6	118.64	53	119.25	54	118.12	70
1	134.19	24	135.54	17	134.02	45
4	148.76	16	150.01	12	148.32	35
3	148.96	18	150.29	12	148.58	36
Ac C=O	170.29	15	170.21	13	169.51	31

Notes:

J. Milhaupt
A 141
38mg

Compound Number 205



4-methoxybenzyl alcohol acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.00	s	
OMe	3.78	s	
α	5.01	s	
3,5	6.91	d	8.7
2,6	7.31	d	8.7

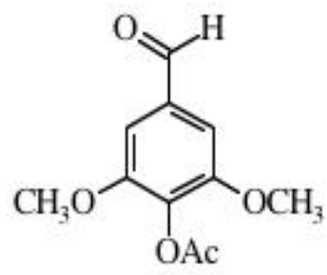
Notes:

J. Milhaupt
A 139
56mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.01	32	20.85	33	20.61	36
OMe	55.23	51	55.53	61	54.98	50
α	66.07	53	66.25	57	65.18	45
3	113.94	100	114.60	100	113.70	100
5	113.94	100	114.60	100	113.70	100
1	128.10	17	129.43	14	128.03	24
2	130.08	99	130.78	100	129.85	98
6	130.08	99	130.78	100	129.85	98
4	159.65	14	160.57	12	159.07	13
Ac C=O	170.85	11	170.85	10	170.13	13

Compound Number 206



Syringaldehyde acetate

3,5-dimethoxy-4-acetoxy-benzaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.28	s	
OMe	3.90	s	
2,6	7.28	s	
α	9.93	s	

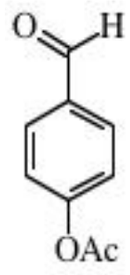
Notes:

J. Milhaupt
A 147
42mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.41	39	20.21	37	20.01	50
OMe	56.35	100	56.72	100	56.20	100
OMe	56.35	100	56.72	100	56.20	100
2	106.09	92	106.72	84	106.00	92
6	106.09	92	106.72	84	106.00	92
4	133.82	7	134.60	5	132.83	12
1	134.36	22	135.62	10	134.20	34
3	152.88	32	153.91	22	152.35	51
5	152.88	32	153.91	22	152.35	51
Ac C=O	168.01	14	168.15	11	167.58	23
α	191.00	45	191.82	31	191.89	48

Compound Number 207



4-Acetoxy benzaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.30	s	
3,5	7.35	d	8.6
2,6	7.97	d	8.6
α	10.01	s	

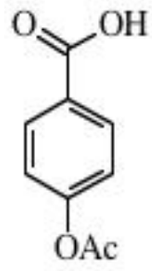
Notes:

J. milhaupt
137.5
42mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.06	39	20.98	39	20.78	42
3	122.32	100	123.43	100	122.63	98
5	122.32	100	123.43	100	122.63	98
2	131.12	92	131.68	100	130.85	100
6	131.12	92	131.68	100	130.95	100
1	133.93	16	135.13	13	133.75	19
4	155.30	12	156.42	11	154.99	16
Ac C=O	168.62	12	169.27	9	168.64	16
α	190.88	38	191.83	34	191.84	42

Compound Number 208



4-Acetoxy benzoic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.29	s	
3,5	7.26	d	8.8
2,6	8.08	d	8.8

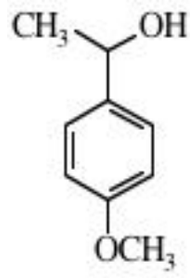
Notes:

J. Milhaupt
27mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.25	48	20.98	48	20.80	48
3	121.84	100	122.76	95	121.96	100
5	121.84	100	122.76	95	121.96	100
1	126.96	20	128.81	15	128.31	21
2	131.95	96	131.91	100	130.78	99
6	131.95	96	131.91	100	130.78	99
4	155.09	26	155.55	18	153.86	25
α	168.89	22	167.00	17	166.55	20
Ac C=O	171.38	13	169.28	15	168.75	25

Compound Number 209



4-Methoxy benzyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.37	d	6.5
OMe	3.76	s	
α	4.79	m	
3,5	6.86	d	8.7
2,6	7.29	d	8.6

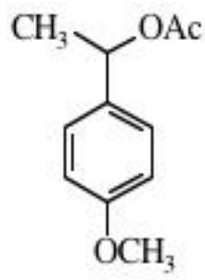
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	25.04	52	26.20	54	25.89	15
OMe	55.27	48	55.43	62	54.92	15
α	69.84	44	69.50	42	67.60	15
3	113.82	91	114.20	100	113.25	100
5	113.82	91	114.20	100	113.25	100
2	126.67	100	127.27	92	126.34	100
6	126.67	100	127.27	92	126.34	100
1	138.12	17	140.18	11	139.34	7
4	158.90	14	159.49	13	157.90	6

Notes:

J. Milhaupt
JMA 145
42mg

Compound Number 210



1-(4-acetoxyphenyl)-1-acetoxy ethane

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.46	d	6.6
Ac Me	1.98	s	
OMe	3.78	s	
α	5.79	q	6.6
3,5	6.90	d	8.8
2,6	7.30	d	8.8

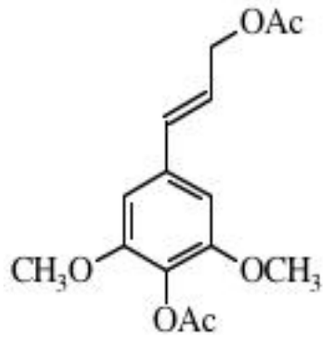
Notes:

J. Milhaupt
JMA 149
23mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.44	35	21.16	34	20.92	44
β	22.01	56	22.35	57	21.76	51
OMe	55.32	48	55.51	44	54.98	46
α	72.06	47	72.28	46	71.18	48
3	113.90	100	114.52	100	113.63	100
5	113.90	100	114.52	100	113.63	100
2	127.64	100	128.26	92	127.28	100
6	127.64	100	128.26	92	127.28	100
1	133.82	19	134.94	15	133.52	25
4	159.34	13	160.22	11	158.69	20
Ac C=O	170.38	12	170.20	10	169.49	19

Compound Number 211



Sinapyl alcohol diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.04	s	
Ac Me	2.22	s	
OMe	3.82	s	
γ	4.69	dd	6.2, 1.2
2,6	6.84	s	
β	6.38	dt	15.8, 6.2
α	6.66	d	15.9

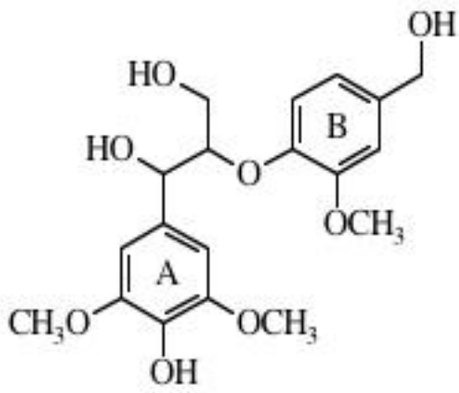
Notes:

J.Milhaupt
JMA 111
20mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.51	46	20.26	44	20.05	49
Ac Me	21.05	33	20.79	33	20.62	45
OMe	56.21	100	56.47	100	55.90	100
OMe	56.21	100	56.47	100	55.90	100
γ	64.90	50	65.13	51	64.06	45
2	103.38	88	104.18	93	103.22	78
6	103.38	88	104.18	93	103.22	78
β	123.71	49	124.99	44	124.32	41
4	128.75	8	129.68	5	127.69	14
α	134.01	49	134.04	44	132.55	42
1	134.71	26	135.67	17	134.33	30
3	152.28	42	153.36	32	151.73	58
5	152.28	42	153.36	32	151.73	58
4 Ac C=O	168.71	21	168.51	16	167395	25
γ Ac C=O	170.85	14	170.72	9	170.01	20

Compound Number 212



Syringylgycerol-β-vanillyl alcohol ether
1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[4-(1-hydroxymethyl)-2-methoxyphenoxy]propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.80	s	
B OMe	3.86	s	
γ1	3.50	m	
γ2	3.69	m	
β	4.18	m	
B α	4.56	d	5.6
α	4.87	m	
A 2,6	6.78	s	
6	6.84	dd	8.2,2.0
2	7.03	d	1.9
5	7.12	d	8.2

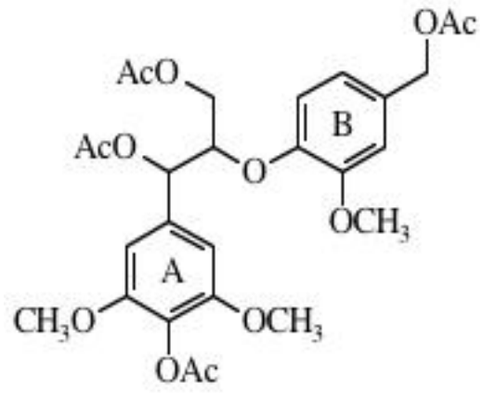
Notes:

T. Duch
I-57
25mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B OMe	55.90	54	56.28	59	55.44	70
A OMe	56.34	100	56.60	100	55.74	100
A OMe	56.34	100	56.60	100	55.74	100
γ	61.05	44	61.95	41	60.00	51
Bα	64.87	54	64.54	46	62.74	68
α	74.16	47	74.06	51	70.88	57
β	89.20	45	88.56	49	84.44	54
A2	103.82	73	105.41	94	104.13	76
A6	103.82	73	105.41	94	104.13	76
B2	110.98	48	111.95	51	110.97	57
B5	119.98	49	119.60	52	115.43	54
B6	120.50	45	120.02	48	118.58	57
A1	130.66	32	132.82	32	131.93	54
A4	134.61	29	136.17	32	134.31	46
B1	137.06	29	137.97	28	135.45	49
B4	146.93	38	148.42	49	146.93	46
A3	147.10	51	148.50	30	147.34	70
A5	147.10	51	148.50	30	147.34	70
B3	151.16	27	151.54	27	149.39	49

Compound Number 213



Syringylgycerol-β-vanillyl alcohol ether tetra-acetate
1-(4-acetoxy-3,5-dimethoxyphenyl)-1,3-diacetoxy-2-[4-(1-acetoxymethyl)-2-methoxyphenoxy]

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.98	s	
Ac Me	2.03	s	
Ac Me	2.09	s	
A4 Ac Me	2.21	s	
A OMe	3.80	s	
B OMe	3.83	s	
γ1	4.05	s	12.3,5.9
γ2	4.27	s	11.9,4.0
β	4.81	s	
B α	5.02	s	
α	6.08	d	6.5
A 2,6	6.86	s	
B6	6.91	dd	8.3,1.8
B5	7.03	d	8.4
B2	7.05	d	1.6

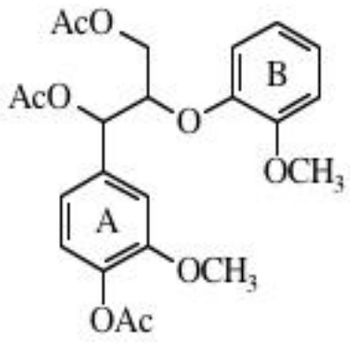
Notes:

T.Duch
I-55
40 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.36	45	20.24	51	20.03	66
Ac Me	20.64	57	20.63	75	20.38	62
Ac Me	20.97	68	20.83	45	20.65	**100**
Ac Me	20.97	68	20.95	50	20.65	100
B OMe	55.80	34	56.31	60	55.60	66
A OMe	56.14	**100**	56.55	**100**	55.98	100
A OMe	56.14	100	56.55	100	55.98	100
γ	62.91	27	63.59	46	63.37	48
B α	66.08	66	66.35	57	65.28	57
α	74.57	50	75.64	50	74.48	53
β	80.14	48	80.72	55	79.02	53
A2	104.02	89	105.13	99	103.94	90
A6	104.02	89	105.13	99	103.94	90
B2	112.70	52	113.94	59	112.86	60
B5	118.12	48	118.67	55	116.91	60
B6	121.15	52	121.77	56	120.69	62
A4	128.79	20	129.70	22	127.92	52
B1	130.88	36	132.09	30	130.30	57
A1	134.63	39	136.18	37	134.92	57
B4	147.90	34	148.97	29	147.38	55
B3	150.60	36	151.57	34	149.79	59
A3	152.14	61	153.21	57	151.55	78
A5	152.14	61	153.21	57	151.55	78
A4 Ac C=O	168.42	30	168.46	30	167.88	50
α Ac C=O	169.60	32	170.02	34	169.32	57
γ Ac C=O	170.48	34	170.72	24	167.94	59
Bα Ac C=O	170.79	25	170.88	24	170.15	40

Compound Number 214



erythro

Guaiacylglycerol-β-guaiacyl ether acetate
1-(4-acetoxy-3-methoxyphenyl)-1,3-diacetoxy-2-(2-methoxy phenoxy)propane

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.94	s	
Ac Me	2.08	s	
Ac Me	2.23	s	
OMe	3.81	s	
OMe	3.83	s	
γ1	4.22	dd	11.9,4.2
γ2	4.39	dd	11.9,5.8
β	4.83	m	
α	6.09	d	5.0

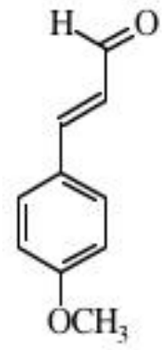
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.57	**100**	20.46	84	20.22	**100**
Ac Me	20.66	66	20.59	69	20.29	100
Ac Me	20.93	71	20.86	57	20.53	73
OMe	55.78	91	56.26	**100**	55.54	81
OMe	55.90	85	56.32	100	55.66	81
γ	62.55	57	63.03	55	61.84	44
α	73.79	60	74.63	55	73.10	49
β	80.15	71	80.37	59	78.36	47
A2	112.02	54	112.83	55	111.61	58
B2	112.70	61	113.90	62	112.89	51
B5	119.51	79	119.88	59	117.93	51
A6	119.71	56	120.46	59	119.28	59
B6	120.98	86	121.68	69	120.61	71
A5	122.52	60	123.36	61	122.43	58
B1	123.58	59	124.08	60	122.83	49
A1	135.41	32	136.71	41	135.30	44
A4	139.80	22	140.85	21	139.05	32
B4	147.18	21	148.33	18	146.61	29
B3	150.97	24	152.11	32	150.30	31
A3	151.11	24	152.11	32	150.52	34
Ac C=O	168.69	26	168.89	26	168.31	36
Ac C=O	169.44	26	169.89	25	169.16	37
Ac C=O	170.68	23	170.74	20	169.94	27

Notes:

S. Ralph
Mixture is 65/35 erythro/threo
35mg

Compound Number 215



p-Methoxy cinnamaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.86	s	
β	6.65	dd	15.9,7.7
3,5	7.02	d	8.9
α	7.60	d	15.9
2,6	7.68	d	8.9
γ	9.66	d	7.7

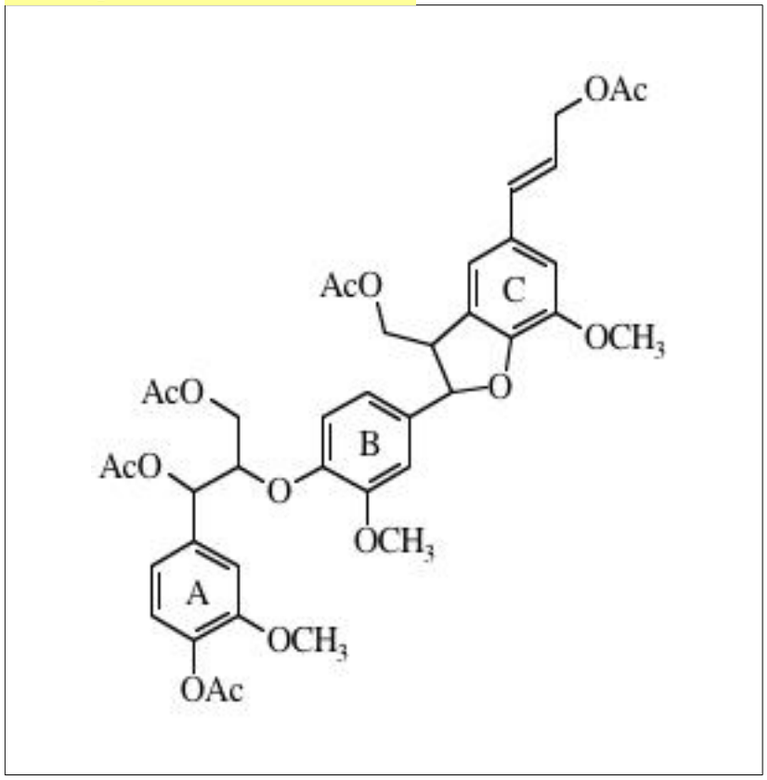
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.34	46	55.81	52	55.35	43
3	114.48	**100**	115.35	**100**	114.51	**100**
5	114.48	100	115.35	100	114.51	100
β	126.33	46	127.37	47	126.31	51
1	126.67	22	127.91	16	126.69	23
2	130.28	92	131.26	95	130.65	98
6	130.28	92	131.26	95	130.65	98
α	152.72	44	153.22	41	153.10	40
4	162.13	15	163.08	11	161.75	20
γ	193.66	46	193.81	44	194.00	43

Notes:

Pew Collection
50 mg

Compound Number 216



G-b-G-c-CA (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
C γAc Me	1.93	s	
A,Bγ Ac Me	2.04	s	
A α Ac Me	2.06	s	
A4 Ac Me	2.21	s	
B β	3.75	m	
A,B OMe	3.81	s	
C OMe	3.89	s	
A γ1	4.22	dd	4.1,12.0
Aγ2	4.36	dd	5.9,12.0
B γ1	4.32	dd	7.6,11.1
B γ2	4.43	dd	5.4,11.1
C γ	4.65	dd	1.3,6.5
β	4.86	m	
B α	5.55	d	6.8
α	6.05	d	5.2
C β	6.23	dt	6.5,15.8
C α	6.64	d	15.8
B6	6.91	dd	2.0,8.3
B5	7.00	d	8.3
B2	7.07	d	2.0
A2	7.23	m	

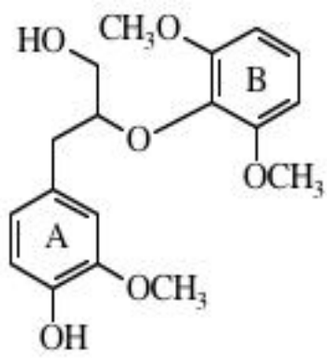
Notes:

S.Ralph
VII-70A
Assignments in acetone are based on
360MHZ HMBC and HMQC expts.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.63	111	20.45	104	20.32	97
A αAc Me	20.74	107	20.60	88	20.40	84
B γAC Me	20.79	99	20.68	92	20.51	68
C γAc Me	20.96	141	20.80	86	20.62	73
A γAc Me	21.00	141	20.86	86	20.70	73
B β	50.37	59	51.24	65	49.34	25
OMe	55.88	100	56.28	130	55.71	125
OMe	55.91	121	56.28	130	55.71	125
OMe	56.00	69	56.28	130	55.71	125
γ	62.45	46	63.04	65	61.85	33
C γ	65.18	76	65.49	100	64.49	50
B γ	65.29	43	65.95	73	64.76	31
α	73.66	40	74.48	71	73.01	32
β	80.25	57	80.30	105	78.30	31
B α	88.23	41	88.54	59	87.17	29
B2	110.28	86	111.50	76	110.74	16
C2	110.60	67	112.17	95	110.93	28
A2	111.88	81	112.71	69	111.62	29
C6	115.31	75	116.33	85	115.26	27
B6	118.69	45	119.14	56	117.49	21
B5	119.18	76	119.41	77	118.30	15
A6	119.60	67	120.45	92	119.33	37
C β	121.24	80	122.23	100	121.34	40
A5	122.59	79	123.33	99	122.50	35
C5	127.49	58	129.01	72	127.89	25
C1	130.60	72	131.53	90	130.04	32
C α	134.30	94	134.71	111	133.49	35
A1	135.30	42	136.60	68	135.05	20
B1	135.80	53	137.06	50	135.26	28
A4	139.75	65	140.78	70	139.06	39
C3	144.41	66	145.39	78	143.84	38
B4	147.19	42	148.14	59	146.54	23
C4	148.20	51	149.31	53	147.53	29
B3	150.96	71	151.95	72	150.16	28
A3	151.19	71	152.08	71	150.54	49
A4 C=O	168.80	48	168.92	67	168.43	47
A αC=O	169.49	56	169.89	68	169.26	46
C γC=O	170.74	75	170.77	107	170.04	61
B γC=O	170.76	92	170.95	94	170.15	41
A γC=O	170.88	59	170.95	94	170.28	47

Compound Number 217



3-(4-hydroxy-3-methoxyphenyl)-2-[2,6-dimethoxyphenoxy] propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	3.03	dd	13.6,5.4
γ	3.50	m	
A OMe	3.82	s	
B OMe	3.83	s	
β	4.17	m	
B 2,6	6.69	d	8.4
A 5,6	6.74	m	
A2	6.90	s	
B1	7.01	dd	8.8
Ar OH	7.39	s	

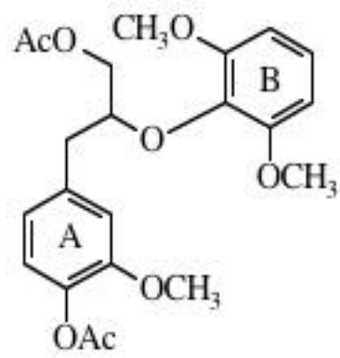
Notes:

T. Duch
TDI-143, 39mg
Assignments in acetone are based on
HMBC and HMQC expts.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	37.30	43	37.97	23	36.86	22
OMe	55.90	61	56.19	27	55.52	34
OMe	56.09	91	56.45	40	55.86	61
OMe	56.09	91	56.45	40	55.86	61
γ	62.21	37	62.78	20	61.69	22
β	84.48	45	85.29	24	83.46	31
B2	105.42	83	106.49	38	105.65	36
B6	105.42	83	106.49	38	105.65	36
A2	112.31	44	113.89	22	113.58	29
A5	114.28	45	115.52	22	115.11	31
A6	122.09	43	122.81	24	121.68	30
B1	123.95	46	124.51	24	123.41	31
A1	130.13	30	130.76	17	129.32	26
B4	135.66	21	137.09	13	135.65	22
A4	144.12	28	145.71	15	144.64	25
A3	146.44	27	148.05	15	147.15	25
B3	153.60	41	154.61	18	153.29	38
B5	153.60	41	154.61	18	153.29	38

Compound Number 218



Acetic acid 3-(4-acetoxy-3-methoxyphenyl)-2-[2,6-dimethoxy phenoxy] propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	3.06	t	11.5,6.5
B OMe	3.76	s	
OMe	3.79	s	
γ	4.11	d	4.8
β	4.51	m	
B 2,6	6.64	d	8.3
A6	6.86	dd	8.0,1.8
A5	6.95	d	8.2
B1	6.98	dd	8.2,8.0
A2	7.07	d	1.8

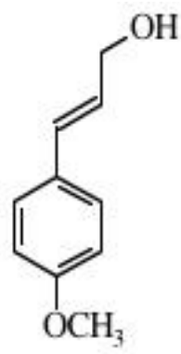
Notes:

T. Duch TDI-143 Ac'd,
32mg Assignments in acetone are based on HMBC and HMQC expts.
A1,B4, and A4 are too close to positively identify.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.70	42	20.49	44	20.37	38
Ac Me	20.85	31	20.65	35	20.46	38
α	38.26	31	38.82	33	37.51	23
OMe	55.97	76	56.12	40	55.60	35
OMe	55.97	76	56.30	77	55.74	53
OMe	55.97	76	56.30	77	55.74	53
γ	65.35	31	65.72	33	64.78	22
β	80.49	35	80.86	33	79.44	25
B2	105.20	68	106.29	59	105.39	42
B6	105.20	68	106.29	59	105.39	42
A2	113.95	33	114.77	32	113.76	25
A6	121.64	39	122.34	33	121.30	23
A5	122.30	36	123.12	38	122.27	27
B1	123.92	34	124.53	36	123.74	26
B4	135.89	18	137.12	17	137.28	18
A1	137.13	28	137.89	22	136.71	23
A4	138.26	21	139.37	17	137.69	19
A3	150.69	23	151.85	20	150.35	21
B3	153.66	35	154.65	26	153.16	32
B5	153.66	35	154.65	26	153.16	32
Ac C=O	169.17	22	169.08	21	168.60	21
γ Ac C=O	170.92	22	170.80	18	170.16	21

Compound Number 219



trans

p-Methoxy coumaryl alcohol
4-methoxy cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.76 (3.78)	s	
γ	4.20 (4.25)	bs	
β	6.24 (6.19)	dt	15.9, 5.4
α	6.53 (6.52)	d	15.9
3,5	6.86 (6.83)	d	8.7
2,6	7.33 (7.28)	d	8.7

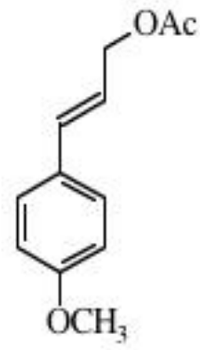
Notes:

S.Ralph 55mg
SRVIII-45
CDCl3 1H shifts in ( )'s

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.30	45	55.48	37	55.00	26
γ	63.76	42	63.36	33	61.62	33
3	113.99	78	114.73	67	113.96	62
5	113.99	78	114.73	67	113.96	62
2	127.69	82	128.24	67	127.27	66
6	127.69	82	128.24	67	127.27	66
β	126.43	44	128.61	33	128.20	43
α	130.82	32	129.76	34	128.27	32
1	129.57	14	130.78	9	129.51	15
4	159.32	12	160.05	8	158.57	13

Compound Number 220



trans

p-Methoxy coumaryl alcohol acetate
4-methoxy cinnamyl alcohol acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
OMe	3.78	s	
γ	4.65	dd	6.4,1.2
β	6.19	dt	15.7, 6.4
3,5	6.89	d	8.8
2,6	7.38	d	8.8

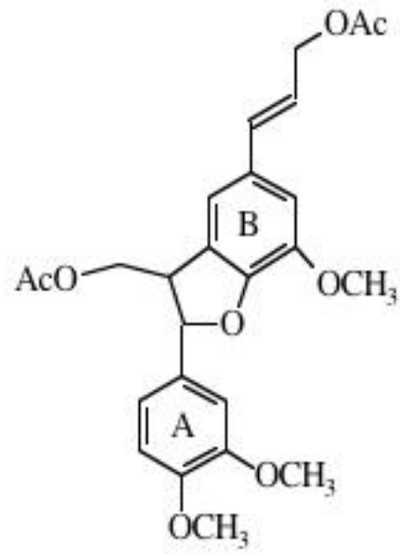
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.07	27	20.82	19	20.64	21
OMe	55.35	48	55.59	31	55.05	26
γ	65.39	46	65.52	32	64.48	26
3	114.13	86	114.91	55	114.02	50
5	114.13	86	114.91	55	114.02	50
β	121.00	40	122.21	33	121.17	25
2	127.94	85	128.69	65	127.74	53
6	127.94	85	128.69	65	127.74	53
1	130.17	11	130.80	7	129.86	7
α	134.10	41	134.32	28	133.00	24
4	159.73	13	160.71	5	159.13	10
Ac C=O	170.90	10	170.77	6	170.07	8

Notes:

S.Ralph
30mg
gHSQC, gHMBC Acetone shifts confirmed

Compound Number 221



V-c-CA

4-methoxy phenyl coumaran diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.00	s	
Ac Me	2.02	s	
OMe	3.79	s	
OMe	3.80	s	
OMe	3.88	s	
γ1	4.38	dd	11.1, 7.4
γ2	4.43	dd	11.1, 5.6
Bγ	4.66	dd	7.4, 0.9
Aα	5.54	d	7.0
Bβ	6.23	dt	15.8, 6.4
Bα	6.64	d	15.9

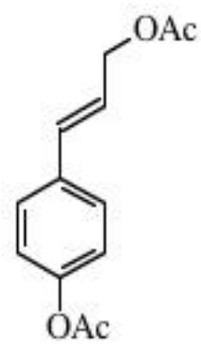
Notes:

S.Ralph 51mg
SRVII-104
HMBC and HMQC in acetone
gamma's and A3 and A4 are very close and may be switched

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.78	29	20.70	26	20.50	29
Ac Me	20.99	25	20.83	20	20.67	27
β	50.32	29	51.16	38	49.36	21
OMe	55.97	62	56.20	50	55.53	47
OMe	55.97	62	56.20	50	55.53	47
OMe	56.08	34	56.48	28	55.75	29
Bγ	65.19	31	65.52	29	64.51	27
γ	65.35	29	65.96	29	64.77	19
α	88.61	28	88.84	27	87.44	22
A2	109.39	30	110.95	26	109.96	23
B2	110.81	27	112.29	25	111.05	19
A5	111.21	30	112.77	26	111.76	24
B6	115.35	28	116.35	28	115.29	21
A6	118.78	31	119.35	28	118.47	25
Bβ	121.22	30	122.21	28	121.34	23
B5	127.76	13	129.18	13	128.06	20
B1	130.56	14	131.46	15	130.03	20
A1	132.94	18	134.53	14	132.88	20
Bα	134.35	29	134.75	28	133.55	22
B3	144.45	17	145.40	13	143.90	17
B4	148.35	11	149.40	8	147.67	12
A3	149.30	26	150.48	11	148.87	30
A4	149.30	26	150.55	10	148.87	30
Ac C=O	170.73	16	170.79	7	170.12	14
Ac C=O	170.73	10	170.94	12	170.26	20

Compound Number 222



trans

4-hydroxy cinnamyl alcohol diacetate

Coumaryl alcohol acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	2.03	s	
4 Ac Me	2.24	s	
γ	4.69	dd	6.2, 1.3
β	6.32	dt	16.0, 6.2
α	6.69	d	16.0
3,5	7.08	d	8.6
2,6	7.47	d	8.6

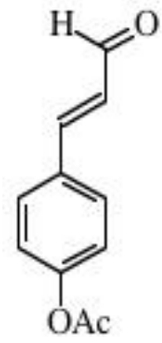
Notes:

S.Ralph 37mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ Ac Me	20.98	31	20.78	27	20.63	30
4 Ac Me	21.12	47	20.96	38	20.86	40
γ	64.95	39	65.17	36	64.18	28
3	121.79	78	122.85	62	121.97	58
5	121.79	78	122.85	62	121.97	58
β	123.58	36	124.89	31	123.97	28
2	127.62	75	128.29	65	127.43	57
6	127.62	75	128.29	65	127.43	57
α	133.19	36	133.28	30	132.05	28
1	134.08	13	134.99	13	133.64	15
4	150.52	12	151.70	9	150.13	13
4 Ac C=O	169.32	14	169.55	10	169.03	13
γ Ac C=O	170.78	10	170.74	8	170.07	9

Compound Number 223



trans

4-acetoxy cinnamaldehyde

Coumaryl aldehyde acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
β	6.73	dd	16.0, 7.6
3,5	7.22	d	8.6
α	7.66	d	16.0
2,6	7.76	d	8.5
γ	9.70	d	7.6

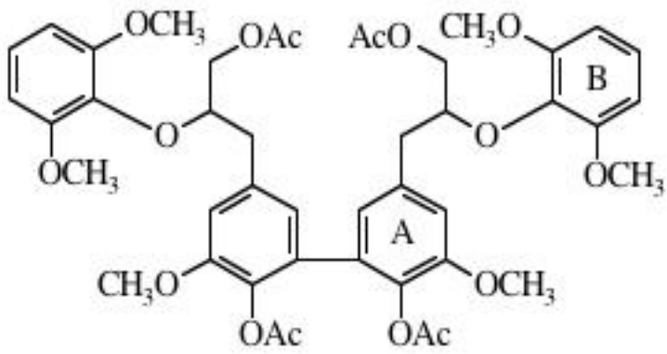
Notes:

S.Ralph
27mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.11	70	20.98	25	20.65	45
3	122.43	125	123.40	64	122.33	100
5	122.43	125	123.40	64	122.33	100
β	128.73	86	129.60	27	128.41	47
2	129.70	125	130.60	62	129.81	98
6	129.70	125	130.60	62	129.81	98
1	131.75	27	132.91	10	131.59	20
α	151.44	72	152.21	25	151.73	44
4	152.90	25	154.01	9	152.41	18
Ac C=O	168.97	22	169.40	6	168.70	17
γ	193.44	65	193.95	26	193.97	49

Compound Number 224



S-b-G-5,5-G-b-S (α = CH2)

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.93	s	
Ac Me	1.99	s	
α	3.07	m	
OMe	3.74	s	
OMe	3.82	s	
γ	4.14	d	4.8
β	4.51	bt	4.9
B2,6	6.62	d	8.4
A6	6.76	s	
A2	7.09	d	1.4

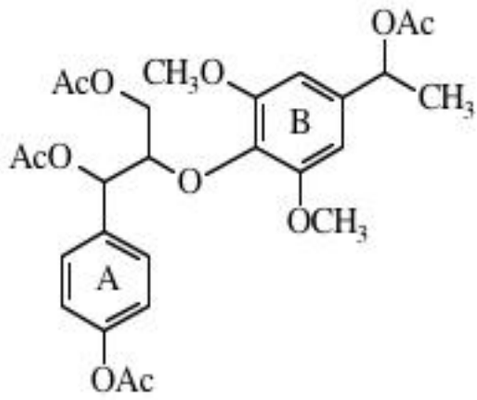
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.34	30	20.32	18	19.88	34
Ac Me	20.80	37	20.68	20	20.35	59
α	38.29	24	38.90	15	37.58	22
OMe	56.00	91	56.33	71	55.71	120
OMe	56.00	91	56.33	71	55.71	120
OMe	56.00	91	56.33	71	55.84	40
γ	65.26	25	65.69	17	64.70	28
β	80.43	28	80.91	18	79.49	31
B2	105.31	68	106.27	40	105.42	81
B6	105.31	68	106.27	40	105.42	81
A2	113.43	24	114.11	14	113.29	20
A6	128.48	23	124.07	11	122.66	20
B1	123.92	32	124.57	14	123.70	36
A5	131.10	18	131.92	8	130.30	23
B4	136.00	15	137.04	17	135.36	31
A1	136.19	29	137.04	17	135.42	31
A4	136.19	29	137.04	17	135.84	29
A3	151.02	20	152.12	12	150.67	26
B3	153.17	42	154.64	22	153.17	69
B5	153.17	42	154.64	22	153.17	69
4 Ac C=O	168.68	8	168.80	6	167.98	19
γ Ac C=O	170.82	19	170.80	10	170.02	35

Notes:

S.Ralph SRVII 109D
44mg
2D HMBC in CDCL3A4and A1 identical chemical shift and B4 very close
As compound has a plane of symmetry thru A5 only half the shifts are reported

Compound Number 225



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H-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bβ	1.47	d	6.6
Ac Me	1.84	s	
Ac Me	2.03	s	
Ac Me	2.12	s	
A4 Ac Me	2.25	s	
OMe	3.79	s	
γ1	4.15	dd	11.9, 4.2
γ2	4.38	dd	11.9, 5.9
β	4.69	m	
Bα	5.78	q	6.6
α	6.07	d	4.6
B2,6	6.68	s	
A3,5	7.11	d	8.5
A2,6	7.45	d	8.5

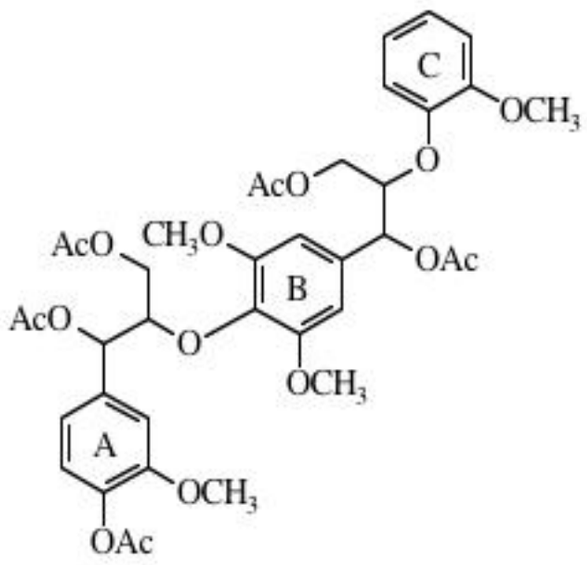
Notes:

S.Ralph
SRVII-139E3 18mg
gHMQC and gHMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.78	39	20.55	18	20.22	27
Ac Me	20.12	40	20.95	31	20.60	28
Ac Me	21.19	47	20.95	31	20.74	32
Ac Me	21.44	36	21.16	18	20.95	28
Bβ	22.26	34	22.60	21	21.99	25
OMe	56.08	78	56.38	44	55.75	54
OMe	56.08	78	56.38	44	55.75	54
γ	62.66	26	63.19	18	61.94	15
Bα	72.38	36	72.68	17	71.59	22
α	73.94	29	74.90	15	73.49	15
β	80.88	20	81.26	13	79.79	16
B2	103.29	67	103.98	38	102.85	39
B6	103.29	67	103.98	38	102.85	39
A3	121.36	57	122.33	37	121.56	45
A5	121.36	57	122.33	37	121.56	45
A2	128.06	42	128.89	30	128.72	37
A6	128.06	42	128.89	30	128.72	37
A1	134.69	14	135.64	7	134.26	10
B4	134.96	19	135.84	17	135.05	15
B1	137.91	21	139.17	11	137.40	15
A4	150.37	19	151.53	8	149.96	14
B3	153.22	40	154.08	17	152.52	29
B5	153.22	40	154.08	17	152.52	29
A4 Ac C=O	169.36	17	169.61	7	169.08	19
Aα Ac C=O	169.62	16	169.93	9	169.08	19
Bα Ac C=O	170.29	17	170.21	6	169.55	18
Aγ Ac C=O	170.29	17	170.66	10	169.90	19

Compound Number 226



threo

G-bt-S-bt-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.84		
γ Ac Me	1.98		
α Ac Me	2.00		
αAc Me	2.10		
A4 Ac Me	2.22		
OMe	3.80		
γ	4.03	m	
γ1,γ2	4.22	m	
γ	4.41	dd	11.8, 6.05
Aβ	4.71	m	
Bβ	4.79	m	
A,Bα	6.07	bd	6.31
B2,6	6.79	d	2.8

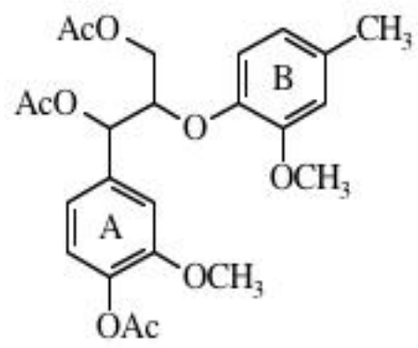
Notes:

S.Ralph SRVII-140C2
30mg
gHSQC and gHMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ Ac Me	20.69	44	20.48	99	20.28	55
γAc Me	20.75	50	20.58	96	20.28	55
α Ac Me	20.79	43	20.67	96	22.41	41
αAc Me	21.09	70	20.92	103	22.41	50
4 Ac Me	21.09	70	20.96	116	20.65	50
OMe	55.80	44	56.19	115	55.48	45
OMe	55.90	44	56.24	119	55.62	43
OMe	56.04	71	56.43	127	55.78	66
OMe	56.04	71	56.43	127	55.78	66
Aγ	62.74	27	63.36	63	62.19	22
Bγ	63.16	28	63.72	71	62.56	21
Aα	73.99	29	75.07	69	73.74	25
Bα	74.87	28	75.71	54	74.60	19
Bβ	80.36	18	80.76	69	79.15	24
Aβ	80.78	21	81.38	70	79.94	23
B2	104.30	51	105.27	125	104.13	43
B6	104.30	51	105.27	125	104.13	43
A2	111.60	16	112.26	47	110.95	21
C2	112.49	33	113.68	75	112.61	34
C5	118.50	37	118.95	60	117.23	23
A6	119.24	19	120.01	60	118.78	23
C6	120.98	31	121.66	81	120.60	34
A5	122.37	25	123.26	78	122.46	43
C1	123.24	30	123.61	89	122.46	43
B1	132.59	12	133.70	37	132.42	17
B4	135.35	10	136.40	19	134.48	16
A1	136.03	16	137.04	41	135.59	18
A4	139.49	16	140.53	33	138.85	21
C4	148.00	16	149.14	34	147.58	21
C3	150.77	25	151.74	37	150.03	22
A3	150.77	25	152.01	35	150.53	21
B3	153.14	27	153.96	68	152.43	37
B5	153.14	27	153.96	68	152.43	37
A4 Ac C=O	168.84	17	168.95	37	168.40	20
α Ac C=O	169.49	18	169.92	49	169.29	26
α Ac C=O	169.76	17	169.99	49	169.29	36
γ Ac C=O	170.51	20	170.61	60	169.92	39
γAc C=O	170.82	19	170.61	60	169.92	39

Compound Number 227



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G-b-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.94	s	
Ac Me	2.08	s	
Bα	2.22	s	
Ac Me	2.25	s	
OMe	3.79	s	
OMe	3.83	s	
γ1	4.20	dd	11.9, 4.2
γ2	4.37	dd	11.9, 5.8
β	4.74	m	
α	6.06	d	5.0
B6	6.65	bd	8.1
B2	6.82	bs	
B5	6.85	d	8.2
A5,6	7.04	m	
A2	7.23	s	
γ1 isomer	3.99		
γ2 isomer	4.25		
α isomer	6.10		

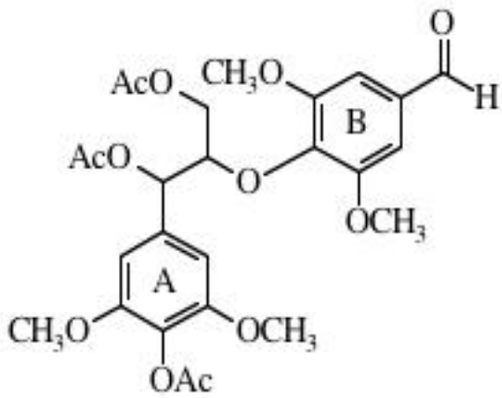
Notes:

S.Ralph
SRVII-141-1 31mg
gHSQC and gHMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.61	66	20.47	61	20.31	30
Ac Me	20.74	48	20.62	51	20.40	30
Ac Me	20.99	48	20.89	45	20.62	42
Bα	21.09	58	21.07	45	20.68	20
OMe	55.70	74	56.14	62	55.47	23
OMe	55.89	57	56.27	55	55.69	20
γ	62.48	43	62.95	45	61.80	12
α	73.70	45	74.58	44	73.10	17
β	80.57	59	80.63	45	78.71	19
A2	111.84	46	112.63	67	111.50	21
B2	113.49	46	114.61	50	113.60	15
B5	119.54	63	120.07	44	118.21	15
A6	119.69	49	120.30	51	119.17	17
B6	121.21	53	121.85	54	120.77	23
A5	122.55	46	123.36	45	122.50	14
B1	133.53	27	133.79	20	132.26	17
A1	135.62	28	136.82	27	135.45	17
A4	139.69	20	140.73	14	138.98	12
B4	144.76	22	145.94	15	144.24	13
B3	150.86	24	151.83	15	150.12	16
A3	150.95	25	152.11	17	150.53	15
A4 Ac C=O	168.79	23	168.92	18	168.41	14
α Ac C=O	169.50	24	169.91	17	169.26	14
γAc C=O	170.78	22	170.76	15	170.03	12
threo isomer						
γ	63.04		63.58			
α	74.54		75.38			
β	80.59		80.98			

Compound Number 228



S-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.87	s	
α Ac Me	2.14	s	
A4 Ac Me	2.22	s	
OMe	3.82	s	
OMe	3.95	s	
γ 1	4.22	dd	11.9, 3.8
γ 2	4.47	dd	11.9, 6.2
β	4.95	dt	6.6, 4.2
α	6.09	d	4.2
A 2,6	6.81	s	
B 2,6	7.25	s	
Bα	9.90	s	

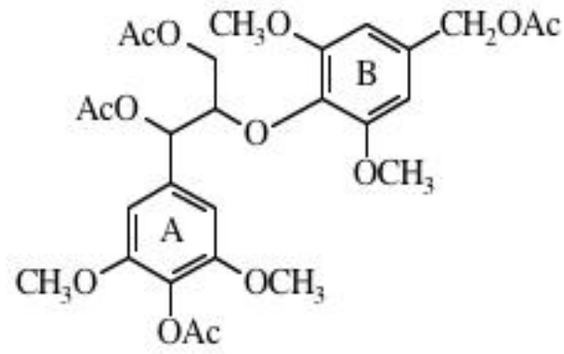
Notes:

L.Landucci LLL XXII-134C
35mg
gHSQC and gHMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.44	21	20.24	147	20.09	45
α AcMe	20.70	15	20.58	108	20.31	34
γ Ac Me	21.04	13	20.89	98	20.63	37
A OMe	56.18	49	56.50	270	55.93	79
A OMe	56.18	49	56.50	270	55.93	79
B OMe	56.18	49	56.58	279	55.99	87
B OMe	56.18	49	56.58	279	55.99	87
γ	62.90	11	63.40	96	62.26	18
α	74.17	12	75.17	93	73.81	22
β	80.87	12	81.67	98	80.21	20
A2	104.07	22	104.61	181	103.39	37
A6	104.07	22	104.61	181	103.39	37
B2	106.50	24	107.18	183	106.37	42
B6	106.50	24	107.18	183	106.37	42
A4	128.61	3	129.41	21	127.60	10
B1	132.08	8	133.26	54	131.82	18
A1	135.04	9	136.27	53	134.94	20
B4	140.89	4	141.81	28	140.06	16
A3	151.95	15	153.06	86	151.54	43
A5	151.95	15	153.06	86	151.54	43
B3	153.46	14	154.43	86	152.95	46
B5	153.46	14	154.43	86	152.95	46
A4 Ac C=O	168.60	7	168.52	48	168.03	21
α Ac C=O	169.46	9	169.94	50	169.35	25
γ Ac C=O	170.76	6	170.66	46	169.96	23
Bα	191.01	12	191.69	98	191.82	22

Compound Number 229



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S-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.86	s	
BαAc Me	2.05	s	
a Ac Me	2.14	s	
A4 Ac Me	2.22	s	
OMe	3.81	s	
OMe	3.82	s	
γ1	4.18	dd	11.9, 4.2
γ2	4.43	dd	11.9, 6.0
β	4.74	dt	6.2, 4.2
Bα	5.02	s	
α	6.08	d	4.3
B 2,6	6.71	s	
A 2,6	6.78	s	

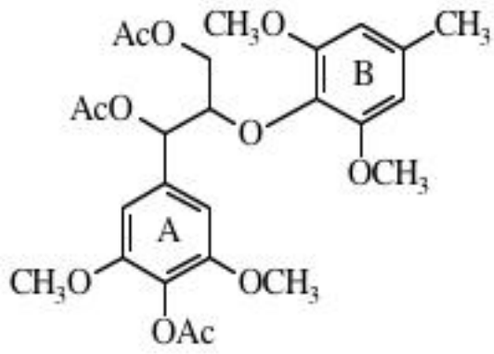
Notes:

S.Ralph SRIX-17D
18mg
gHSQC and gHMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.48	137	20.35	42	20.06	54
γ Ac Me	20.77	88	20.71	29	20.29	40
Bα Ac Me	21.06	92	20.93	20	20.64	52
α Ac Me	21.10	106	21.04	30	20.66	51
OMe	56.05	178	56.50	58	55.74	70
OMe	56.05	178	56.50	58	55.74	70
OMe	56.17	239	56.58	79	55.88	88
OMe	56.17	239	56.58	79	55.88	88
γ	62.73	71	63.42	23	62.09	18
Bα	66.45	67	66.71	22	65.58	27
α	74.19	75	75.41	23	73.88	24
β	80.79	65	81.55	25	79.96	22
A2	103.92	127	104.61	43	103.18	38
A6	103.92	127	104.61	43	103.18	38
B2	105.47	132	106.29	42	105.20	40
B6	105.47	132	106.29	42	105.20	40
A4	128.44	21	129.41	4	127.45	12
B1	132.02	49	133.40	11	131.90	19
B4	135.09	29	136.29	8	134.12	17
A1	135.59	48	136.76	13	135.26	18
A3	151.90	89	153.12	25	151.47	52
A5	151.90	89	153.12	25	151.47	52
B3	153.19	77	154.13	20	152.47	38
B5	153.19	77	154.13	20	152.47	38
A4 Ac C=O	168.64	44	168.64	13	168.10	26
α Ac C=O	169.54	43	170.09	13	169.35	28
γAc C=O	170.84	27	170.81	12	169.97	27
BαAc C =O	170.92	34	170.97	6	170.20	16

Compound Number 230



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S-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.87	s	
αAc Me	2.14	s	
A4 Ac Me	2.22	s	
Bα	2.27	s	
OMe	3.78	s	
OMe	3.81	s	
γ1	4.18	dd	11.9, 4.4
γ2	4.40	dd	11.9, 6.2
β	4.66	dt	5.8, 4.4
α	6.06	d	4.4
B 2,6	6.49	s	
A 2,6	6.76	s	

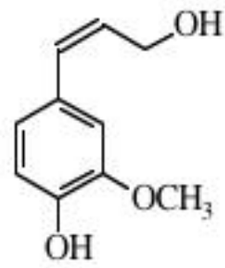
Notes:

S.Ralph SRIX-17E
40mg threo isomer shifts from SRIX-104D
gHSQC and gHMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.43	29	20.24	41	20.04	79
γ Ac Me	20.76	23	20.62	28	20.30	63
αAc Me	21.06	21	20.93	27	20.61	61
Bα	21.82	21	21.76	28	21.32	56
OMe	55.90	45	56.25	63	55.57	117
OMe	55.91	45	56.25	63	55.57	117
OMe	56.12	49	56.46	82	55.84	126
OMe	56.12	49	56.46	82	55.84	126
γ	62.69	18	63.22	29	62.00	32
α	74.20	17	75.33	29	73.88	37
β	80.80	19	81.45	31	79.94	38
A2	103.81	36	104.43	54	103.08	70
A6	103.81	36	104.43	54	103.08	70
B2	105.95	34	106.85	60	105.77	82
B6	105.95	34	106.85	60	105.77	82
A4	128.33	5	129.25	6	127.39	20
B4	132.79	6	134.15	9	132.12	29
B1	134.13	13	134.52	16	133.35	37
A1	135.77	13	136.80	17	135.39	38
A3	151.86	21	153.01	27	151.45	73
A5	151.86	21	153.01	27	151.45	73
B3	152.87	22	153.84	29	152.27	71
B5	152.87	22	153.84	29	152.27	71
A4 Ac C=O	168.62	10	168.54	14	167.99	35
α Ac C=O	169.54	11	169.98	15	169.33	42
γ Ac C=O	170.94	9	170.72	13	169.95	41
threo isomer						
γ	63.53		64.13			
α	75.60		76.58			
β	80.87		81.65			

Compound Number 231



cis

cis-coniferyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.83	s	
γ	4.41	d	5.8
β	5.73	dt	11.9, 6.2
α	6.39	d	11.7
6	6.72	dd	8.2, 2.0
5	6.82	d	8.2
2	6.87	d	2.0
CDCl3	CDCl3		
OMe	3.89	s	
γ	4.44	dd	6.4, 1.4
β	5.79	dt	11.5, 6.6
α	6.49	d	11.9
6	6.74	dd	8.2, 1.8
5	6.78	d	1.8
2	6.89	d	8.2

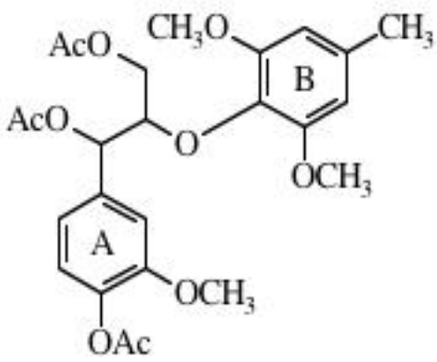
Notes:

J.Ralph
10mg
gHSQC and gHMBC in acetone
gHSQC in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.97	23	56.13	91	55.47	96
γ	59.75	21	59.73	77	58.16	86
2	111.53	20	113.19	82	112.84	81
5	114.33	21	115.55	82	115.15	79
6	122.25	22	122.78	86	121.56	83
1	129.04	6	129.73	26	128.06	46
α	129.51	20	130.19	82	128.62	82
β	131.10	20	131.44	82	130.95	75
4	145.17	7	146.69	29	145.74	50
3	146.38	5	147.93	22	147.13	39

Compound Number 232



erythro

G-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.85	s	
Ac Me	2.12	s	
Ac Me	2.22	s	
Bα	2.27	s	
B OMe	3.76	s	
A OMe	3.82	s	
γ1	4.16	dd	11.8, 4.4
γ2	4.43	dd	11.7, 5.8
β	4.67	dt	5.8, 4.2
α	6.10	d	4.2
B 2,6	6.51	s	
A6	6.99	dd	8.3, 1.8
A5	7.06	d	8.2
A2	7.18	d	1.8

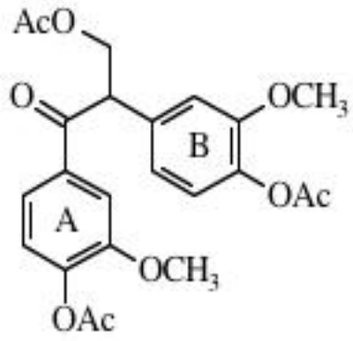
Notes:

S.Ralph SRIX-43G
55 mg
HSQC and HMBC in d6-DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.67	211	20.46	138	20.34	166
Ac Me	20.78	188	20.59	116	20.34	166
Ac Me	21.09	174	20.92	119	20.67	97
Bα	21.87	170	21.77	111	21.40	85
OMe	55.94	494	56.25	329	55.66	200
OMe	55.94	494	56.25	329	55.66	200
OMe	55.94	494	56.25	329	55.70	135
γ	62.64	157	63.10	122	61.98	59
α	74.02	160	75.04	125	73.72	66
β	80.92	173	81.40	126	80.03	68
B2	106.02	314	106.87	224	105.90	140
B6	106.02	314	106.87	224	105.90	140
A2	111.46	150	112.07	101	110.83	64
A6	119.10	157	119.81	115	118.66	65
A5	122.43	179	123.29	122	122.61	71
B4	132.81	59	134.03	33	132.13	47
B1	134.16	112	134.56	65	133.51	62
A1	136.35	118	137.26	75	135.87	63
A4	139.44	72	140.56	40	138.86	50
A3	150.84	88	152.02	53	150.63	60
B3	152.96	183	153.86	104	152.42	128
B5	152.96	183	153.86	104	152.42	128
A4 Ac C=O	168.91	75	168.94	50	168.51	56
α Ac C=O	169.56	85	169.93	56	169.39	57
γ Ac C=O	170.92	79	170.67	50	170.03	64

Compound Number 233



G-b1-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.93	s	
Ac Me	2.20	s	
Ac Me	2.24	s	
OMe	3.81	s	
OMe	3.96	s	
γ1	4.33	dd	10.5, 5.8
γ2	4.76	dd	10.5, 8.5
β	5.19	dd	8.5, 5.7
B6	6.98	dd	8.0, 2.0
B5	7.03	d	8.0
A5	7.16	d	8.2
B2	7.22	d	1.8
A6	7.73	d	6.2, 1.8
A2	7.77	d	1.8

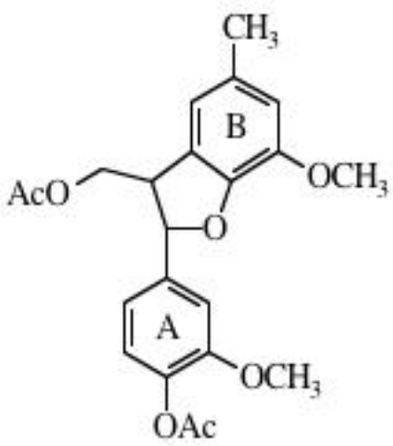
Notes:

S.Lempke I-31
HSQC and HMBC in d6-acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.67	47	20.43	46	20.32	24
Ac Me	20.67	47	20.43	46	20.32	24
Ac Me	20.92	21	20.66	20	20.55	9
β	52.08	21	52.37	21	50.52	8
OMe	56.03	49	56.29	27	55.80	11
OMe	56.03	49	56.40	28	55.95	13
γ	65.58	19	65.94	21	64.74	6
A2	111.99	21	113.14	23	112.35	8
B2	112.32	22	113.66	23	112.95	8
A6	120.95	124	121.30	24	120.26	8
B6	122.22	23	122.88	23	122.14	8
A5	122.94	25	123.95	24	123.28	16
B5	123.54	22	124.21	24	123.28	16
B1	133.94	15	135.54	14	134.26	7
A1	135.02	13	135.77	11	134.42	8
B4	139.64	10	140.53	8	138.79	6
A4	144.13	11	145.10	8	143.59	6
B3	151.54	12	152.52	11	151.11	13
A3	151.72	11	152.70	10	151.11	13
A4 Ac C=O	168.46	11	168.58	9	138.10	7
B4 Ac C=O	168.83	10	168.87	10	168.41	7
γ Ac C=O	170.89	11	170.75	10	170.10	6
α	195.95	13	196.63	11	195.91	7

Compound Number 234



G-c-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.22	s	
Bα	2.26	s	
β	3.74	m	
A OMe	3.80	s	
B OMe	3.83	s	
γ1	4.29	dd	11.1, 8.0
γ2	4.42	dd	10.9, 5.6
α	5.55	d	6.6
B6	6.70	s	
B2	6.73	s	
A6	6.99	dd	8.2, 1.8
A5	7.05	d	8.2
A2	7.18	d	1.8

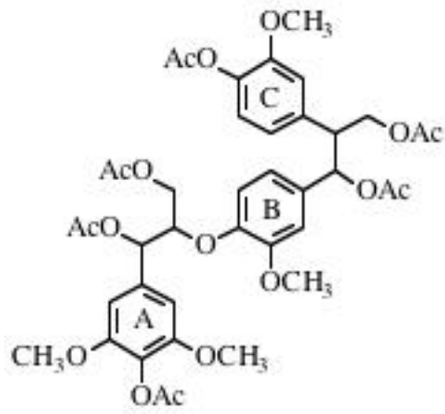
Notes:

S.Ralph
SRIX-46E
31mg
HSQC and HMBC in d6-acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.51	39	20.47	41	20.33	117
Ac Me	21.67	34	20.70	35	20.54	121
Bα	22.13	31	21.18	32	20.80	111
β	51.63	37	51.65	42	49.82	89
OMe	56.77	45	56.23	41	55.66	118
OMe	56.77	46	56.41	40	55.73	129
γ	66.49	38	66.19	44	65.03	75
α	88.49	38	87.85	43	86.41	80
A2	110.89	34	111.02	40	110.39	85
B2	114.11	29	114.79	32	113.50	57
B6	117.76	38	117.92	40	116.90	84
A6	119.09	38	118.61	44	117.81	97
A5	123.68	39	123.72	43	122.87	89
B5	127.71	20	128.29	17	127.22	72
B1	132.29	21	131.92	20	130.68	78
A4	140.42	11	140.61	10	138.98	52
A1	140.73	22	141.40	22	139.88	77
B3	144.89	16	145.00	13	143.48	71
B4	146.62	9	146.96	10	145.26	44
A3	152.09	16	152.36	13	150.83	66
A4 Ac C=O	169.81	13	168.97	13	168.47	51
γ Ac C=O	171.66	15	170.96	14	170.29	66

Compound Number 235



S-b-G-b1-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.89	s	
Ac Me	1.90	s	
Ac Me	2.04	s	
Ac Me	2.17	s	
Ac Me	2.18	s	
Bβ	3.46	m	
OMe	3.69	s	
OMe	3.72	s	
OMe	3.75	s	
OMe	3.76	s	
Bγ1	4.22	m	
Aγ1	4.31	m	
Bγ2	4.36	m	
Aγ2	4.38	m	
Aβ	4.82	m	
Aα	5.99	d	5.8
Bα	6.08	d	7.2
A2,6	6.80	s	
C2	6.97	s	

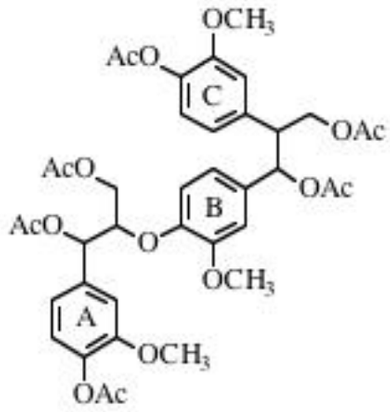
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γAc Me	20.19	26	20.25	39	19.99	106
γAc Me	20.39	24	20.49	37	20.24	118
α Ac Me	20.52	24	20.63	37	20.30	108
α Ac Me	20.56	25	20.68	37	20.38	99
4 Ac Me	20.73	27	20.87	51	20.50	133
4 Ac Me	20.76	27	20.87	51	20.50	133
Bβ	49.86	9	50.93	17	49.21	40
OMe	55.59	24	56.22	68	55.54	97
OMe	55.67	25	56.22	68	55.59	125
OMe	55.97	49	56.51	71	55.87	179
OMe	55.97	49	56.51	71	55.87	179
Aγ	62.37	10	63.07	20	61.95	41
Bγ	64.04	14	65.02	19	64.07	36
Aα	73.74	15	74.77	22	73.39	46
Bα	74.82	13	75.66	22	74.62	42
Aβ	79.64	8	79.97	19	78.10	25
A2	104.20	19	105.11	37	104.04	93
A6	104.20	19	105.11	37	104.04	93
B2	111.11	11	112.37	18	111.22	33
C2	112.95	16	114.30	22	113.27	57
B5	118.27	10	118.61	11	116.86	19
B6	119.26	12	120.13	19	119.06	40
C6	120.99	16	122.06	20	120.84	56
C5	122.25	20	123.12	25	122.10	59
A4	128.50	6	129.52	8	127.83	40
B1	133.19	10	134.59	9	133.00	25
A1	134.81	9	136.05	12	134.76	33
C1	136.11	10	137.79	13	136.85	47
C4	138.85	10	139.98	13	138.27	48
B4	146.81	5	147.93	7	146.40	37
B3	150.44	9	151.43	9	149.76	33
C3	150.59	12	151.80	17	150.26	65
A3	151.84	24	153.01	31	151.47	120
A5	151.84	24	153.01	31	151.47	120
A4 Ac C=O	168.23	8	168.49	16	167.81	59
C4 Ac C=O	168.61	10	168.98	15	168.27	53
α Ac C=O	169.27	12	169.93	29	169.07	57
α Ac C=O	169.50	8	169.93	29	169.12	68
γ Ac C=O	170.42	11	170.74	19	169.89	111
γ Ac C=O	170.50	12	170.77	21	169.89	111

Notes:

S. Ralph SRIX-44D6
70mg HSQC and HMBC in d6-acetone
Bβ,Aβ,A2,A6,B5,B1,A1,and B4 appear as split signals
The shift reported is the average.

Compound Number 236



G-b-G-b1-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.95	s	
α Ac Me	2.07	s	
4 Ac Me	2.15	s	
Bβ	3.50	m	
OMe	3.74	s	
OMe	3.78	s	
OMe	3.83	s	
Bγ 1	4.21	m	
Aγ 1	4.27	m	
Bγ 2	4.33	m	
Aγ 2	4.37	m	
Aβ	4.85	m	
Aα	6.06	d	5.0
Bα	6.13	d	7.0
B2	6.81	s	
B,C 6	6.82	m	
B,C 5	6.96	m	
C2	7.02	d	
A 5,6	7.05	m	
A2	7.25, 7.26		2 signals

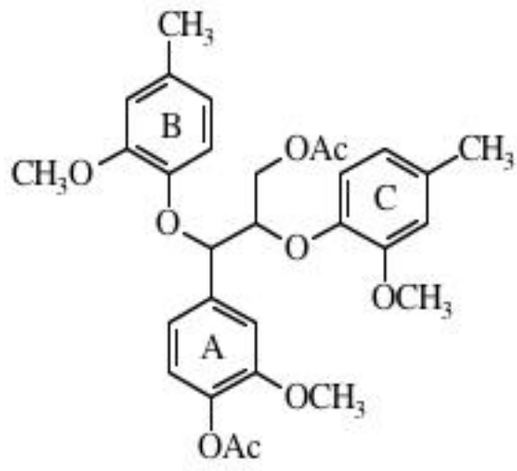
Notes:

SRIX-47C2
21 mg
Bβ,Aβ,A2,B5,B1,B4 appear assplit signals, the shift reported is the average.
HSQC and HMBC in d6-acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ Ac Me	20.69	44	20.49	90	20.35	99
γ Ac Me	20.69	44	20.49	90	20.35	99
α Ac Me	20.78	24	20.62	53	20.35	99
α Ac Me	20.85	25	20.69	55	20.50	53
4 Ac Me	21.03	33	20.87	84	20.61	88
4 Ac Me	21.03	33	20.87	84	20.61	88
Bβ	50.07	6	50.96	24	49.13	22
OMe	55.83	21	56.25	96	55.63	45
OMe	55.94	33	56.25	96	55.68	67
OMe	55.97	35	56.30	77	55.72	62
Aγ	62.52	12	63.04	29	61.94	20
Bγ	64.29	14	65.05	32	64.17	20
Aα	73.72	15	74.55	30	73.14	22
Bα	75.07	12	75.70	26	74.68	21
Aβ	80.01	7	80.16	34	78.15	17
B2	111.36	14	112.43	31	111.27	19
A2	111.98	8	112.78	22	111.68	20
C2	113.12	15	114.34	37	113.32	28
B5	118.74	11	118.93	17	116.97	11
B6	119.48	15	120.14	35	119.12	24
A6	119.73	11	120.46	34	119.40	26
C6	121.22	15	122.10	28	120.89	26
C5	122.50	19	123.13	41	122.19	28
A5	122.62	18	123.36	37	122.51	27
B1	133.41	7	134.76	13	133.13	15
A1	135.34	4	136.60	16	135.26	20
C1	136.29	5	137.84	16	137.02	25
C4	139.06	9	140.02	17	138.21	27
A4	139.82	9	140.80	15	139.10	25
B4	147.00	5	147.92	9	146.35	18
B3	150.75	11	151.55	15	149.81	21
C3	150.80	14	151.83	22	150.26	31
A3	151.02	10	152.11	17	150.57	24
4 Ac C=O	168.84	10	168.92	21	168.46	39
4 Ac C=O	168.90	12	168.98	24	168.46	39
α Ac C=O	169.55	10	169.93	29	169.23	33
α Ac C=O	169.78	10	169.93	29	169.28	32
γ Ac C=O	170.74	11	170.75	31	170.06	55
γ Ac C=O	170.80	11	170.75	31	170.06	55

Compound Number 237



G-a-G-b-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.90	s	
Ac Me	2.20	s	
B or C α	2.20	s	
B or C α	2.24	s	
OMe	3.75	s	
OMe	3.79	s	
OMe	3.83	s	
γ1	4.43	dd	11.7, 3.8
γ2	4.54	dd	11.7, 5.8
β	4.74	m	
α	5.55	d	5.4
C6	6.53	dd	8.2, 1.6
B6	6.61	dd	8.0, 1.4
C5	6.76	d	
B,C 2	6.78	s	
B5	6.83	d	8.0
A5	6.98	d	8.0
A6	7.05	dd	8.0, 1.8
A2	7.33	d	1.8

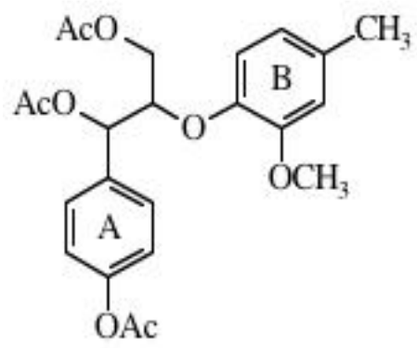
Notes:

SRIX-46DB
33mg
HSQC and HMBC in d6-acetone
Shifts for B and C α's,2's and 6's were too close to assign with confidence

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.69	24	20.46	29	20.34	129
Ac Me	20.82	24	20.65	27	20.44	134
Cα	21.05	23	20.96	28	20.56	136
Bα	21.12	23	21.05	28	20.61	136
OMe	55.71	25	56.11	33	55.48	131
OMe	55.96	49	56.19	36	55.63	193
OMe	55.96	49	56.28	32	55.63	193
γ	63.56	21	65.62	30	62.46	86
α	80.41	21	81.09	24	79.08	93
β	82.44	21	82.14	32	80.19	98
A2	111.53	21	112.70	21	111.79	86
B2	113.37	28	114.51	34	113.58	190
C2	113.41	27	114.54	29	113.58	190
C5	116.77	21	117.73	24	116.22	109
B5	119.45	24	119.80	31	117.84	118
A6	119.72	23	120.54	29	119.51	88
B6	121.01	24	121.64	30	120.67	117
C6	121.21	25	121.80	30	120.77	125
A5	122.36	22	123.13	30	122.30	87
C1	131.97	15	132.54	14	131.23	93
B1	133.11	15	133.32	15	131.83	89
A1	138.62	16	138.11	17	136.70	93
A4	139.42	10	140.48	9	138.81	79
C4	145.22	12	146.01	10	144.25	89
B4	145.32	12	146.37	11	144.77	88
C3	149.95	12	151.12	11	149.52	85
B3	150.79	12	151.69	11	150.00	86
A3	151.02	13	152.03	14	150.45	89
A4 Ac C=O	168.85	11	168.89	10	168.39	65
γ Ac C=O	170.91	12	170.81	12	170.13	70

Compound Number 238



erythro

H-b–G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.92	s	
α Ac Me	2.07	s	
A4 Ac Me	2.24	s	
Bα	2.25	s	
OMe	3.77	s	
γ1	4.17	dd	11.9, 4.4
γ2	4.37	dd	11.9, 5.6
β	4.69	m	
α	6.06	d	5.0
B6	6.64	m	
B 2,5	6.85	m	
A 3,5	7.12	m	
A 2,6	7.50	m	

Notes:

SRIX-51D-C

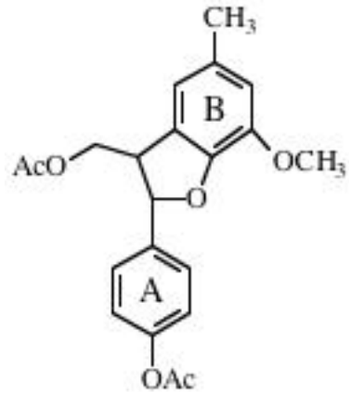
13mg HMBC,HSQC,selective INEPT in acetone

^{1}H in acetone (threo isomer) γ1 3.96, dd J = 11.8,5.6 γ2 4.24, dd J = 11.8,4.2
α 6.12,d J = 6.8

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γAc Me	20.82	21	20.59	46	20.34	66
α Ac Me	21.06	21	20.88	45	20.58	94
A4 Ac Me	21.18	47	20.95	88	20.58	94
Bα	21.18	47	21.07	48	20.73	78
OMe	55.79	28	56.13	57	55.46	58
γ	62.48	18	62.84	45	61.67	32
α	73.67	19	74.43	46	72.93	37
β	80.80	21	80.84	46	78.98	37
B2	113.60	20	114.65	47	113.64	42
B5	120.09	19	120.44	46	118.60	42
B6	121.27	25	121.85	60	120.77	51
A3	121.53	41	122.41	96	121.56	83
A5	121.53	41	122.41	96	121.56	83
A2	128.41	39	129.25	86	128.13	77
A6	128.41	39	129.25	86	128.13	77
B1	133.72	10	133.96	20	132.43	32
A1	134.44	12	135.53	23	134.05	34
B4	144.75	8	145.86	14	144.14	30
A4	150.59	9	151.71	20	150.11	28
B3	151.03	8	151.95	17	150.23	35
A4 Ac C=O	169.29	10	169.57	20	169.05	32
α Ac C=O	169.60	10	169.90	17	169.21	31
γ Ac C=O	170.87	9	170.73	16	169.97	30
minor isomer						
γ	63.10		63.56		62.38	
α	74.53		75.24		74.03	
β	80.73		81.06		79.39	

Compound Number 239



H-c-G

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γAc Me	20.89	25	20.68	53	20.48	26
A4 Ac Me	21.21	36	20.95	77	20.73	56
Bα	21.35	33	21.18	49	20.73	56
β	50.94	21	51.78	54	49.85	19
OMe	56.11	30	56.38	43	55.56	19
γ	65.83	22	66.29	57	65.02	20
α	87.46	21	87.57	53	85.95	20
B2	113.35	23	114.79	52	113.40	18
B6	117.04	23	118.02	51	116.88	21
A3	121.81	53	122.82	112	121.90	46
A5	121.81	53	122.82	112	121.90	46
A2	127.10	45	127.64	107	126.83	47
A6	127.10	45	127.64	107	126.83	47
B5	128.30	9	128.12	26	127.67	8
B1	131.59	12	131.95	21	130.59	14
A1	138.76	10	140.15	22	138.55	16
B3	144.09	7	145.03	14	143.38	11
B4	145.86	5	146.96	11	145.14	7
A4	150.54	9	151.66	16	150.07	11
A4 Ac C=O	169.44	10	169.62	19	169.08	17
γ Ac C=O	170.88	9	170.94	18	170.21	12

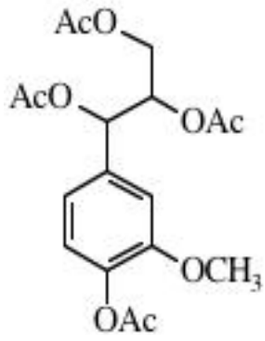
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	2.00	s	
A4 Ac Me	2.24	s	
Bα	2.26	s	
β	3.73	m	
OMe	3.83	s	
γ1	4.27	dd	10.9, 8.0
γ2	4.41	dd	10.9, 5.6
α	5.58	d	6.4
B2	6.70	bs	
B6	6.73	bs	
A3,5	7.11	d	8.5
A2,6	7.44	d	8.5

Notes:

SRIX-53E 2mg
HSQC and HMBC in acetone

Compound Number 240



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.98	s	
Ac Me	1.99	s	
Ac Me	2.08	s	
Ac Me	2.22	s	
OMe	3.83	s	
γ1	3.90	dd	11.9, 6.2
γ2	4.24	dd	11.9, 4.0
β	5.42	m	
α	5.97	d	6.6
6	7.00	dd	8.2, 1.6
5	7.06	d	8.2
2	7.17	d	1.6

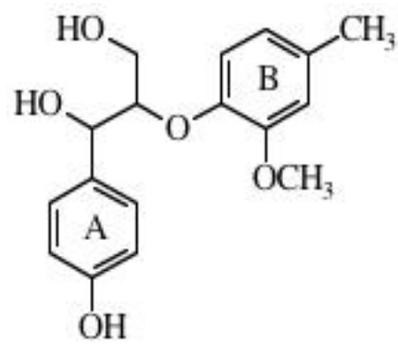
Notes:

SRIX-69E
7mg
gHSQCand gHMBC d6-acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.67	167	20.44	216	20.36	57
Ac Me	20.67	167	20.52	182	20.41	54
Ac Me	20.80	126	20.66	173	20.46	47
Ac Me	20.96	111	20.79	172	20.66	41
OMe	56.02	134	56.34	192	55.84	41
γ	62.11	93	62.81	156	61.93	24
β	72.22	95	72.92	167	71.68	27
α	73.43	96	74.15	151	72.90	25
2	111.30	106	112.29	169	111.25	27
6	119.75	102	120.15	161	119.00	26
5	123.10	104	123.72	155	122.81	29
1	134.70	62	136.28	74	135.20	22
4	140.20	36	140.98	45	139.19	21
3	151.37	41	152.30	54	150.72	22
4 Ac C=O	168.77	40	168.95	61	168.40	22
α Ac C=O	169.65	39	170.08	70	169.44	39
β Ac C=O	170.04	44	170.30	63	169.44	39
γAc C=O	170.43	40	170.73	66	169.97	22
minor isomer						
γ			62.31			
β			72.92			
α			73.53			

Compound Number 241



threo

H-b-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
B α	2.27	s	
γ2	3.43	m	
γ1	3.64	m	
OMe	3.85	s	
β	4.03	m	
α	4.83	dd	6.9, 3.2
B6	6.66	m	
A3,5	6.79	d	8.7
B2	6.85	d	2.0
B5	7.07	d	8.0
A2,6	7.28	d	8.7
A4 OH	8.26	s	

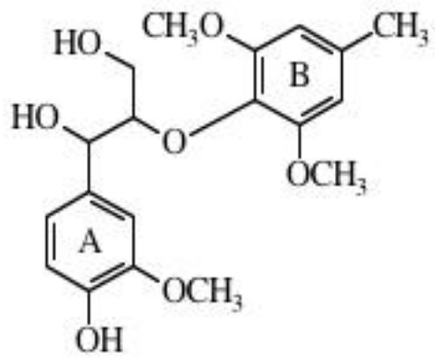
Notes:

SRIX-84
35mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B α	21.16	16	21.08	21	20.51	31
OMe	55.81	19	56.24	28	55.55	37
γ	60.79	11	61.73	22	60.00	17
α	73.72	13	73.84	21	70.94	19
β	89.12	14	89.41	22	85.34	20
B2	113.07	17	114.18	19	113.46	25
A3	115.53	31	115.62	46	114.35	44
A5	115.53	31	115.62	46	114.35	44
B5	120.78	19	120.73	23	116.69	24
B6	121.96	16	122.21	25	120.75	31
A2	128.42	28	129.10	45	127.75	47
A6	128.42	28	129.10	45	127.75	47
A1	131.29	6	133.16	10	130.38	20
B1	133.99	11	133.35	11	132.21	17
B4	145.21	7	147.33	7	146.17	17
B3	150.97	8	151.67	5	149.60	17
A4	156.37	9	157.63	11	156.19	20
erythro isomer						
γ	60.79		61.64		59.89	
α	72.72		73.55		71.41	
β	87.06		87.53		84.57	

Compound Number 242



threo

G-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
B α	2.29	s	
γ1	3.28	dd	12.5, 3.2
γ2	3.64	dd	12.6, 3.6
OMe	3.80	s	
β	3.88	m	
OMe	3.85	s	
α	5.00	d	7.6
B2,6	6.55	s	
A5	6.79	d	8.34
A6	6.92	dd	8.3, 1.8
A2	7.07	d	1.8

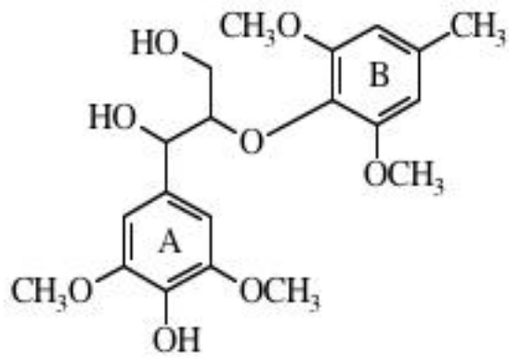
Notes:

SRIX-86B,C
40 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B α	21.99	36	21.77	39	21.31	74
OMe	56.01	58	56.16	46	55.48	93
OMe	56.14	111	56.46	86	55.82	168
OMe	56.14	111	56.46	86	55.82	168
γ	60.51	30	61.19	35	60.11	29
α	74.20	32	74.08	38	71.53	37
β	89.20	33	89.83	37	87.29	41
B2	106.10	95	107.09	76	106.28	100
B6	106.10	95	107.09	76	106.28	100
A2	109.92	33	111.45	36	111.01	44
A5	114.36	37	115.22	43	114.62	43
A6	120.47	34	120.73	38	119.22	47
A1	132.06	18	133.60	22	132.79	44
B4	133.04	10	134.65	14	132.90	34
B1	134.67	23	134.82	22	133.80	27
A4	145.46	17	146.75	24	145.29	33
A3	146.58	16	147.90	19	146.83	32
B3	152.75	29	153.60	34	152.27	59
B5	152.75	29	153.60	34	152.27	59
erythro isomer						
γ	60.63		60.86		59.57	
α	72.49		73.26		71.93	
β	87.13		87.90		86.11	

Compound Number 243



threo

S-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
B α	2.29	s	
OMe	3.80	s	
OMe	3.86	s	
α	4.99	d	6.8
A2,6	6.54	s	
B2,6	6.77	s	
A4 OH	7.08	s	

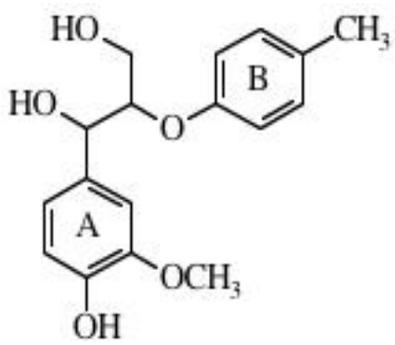
Notes:

SRIX-88SSB
54mg B1,B4,A4,A1
gHSQC, gHMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B α	21.85	42	21.78	78	21.31	91
OMe	56.02	94	56.48	173	55.88	252
OMe	56.02	94	56.48	173	55.88	252
OMe	56.25	94	56.56	175	55.90	266
OMe	56.25	94	56.56	175	55.90	266
γ	60.37	33	61.31	47	60.18	49
α	74.33	39	74.29	52	71.59	62
β	89.04	40	89.56	62	87.18	61
A2	104.04	77	105.39	150	104.30	124
A6	104.04	77	105.39	150	104.30	124
B2	105.99	87	107.05	169	106.34	155
B6	105.99	87	107.05	169	106.34	155
A1	131.04	27	132.54	37	132.13	59
B1	132.90	18	134.55	28	132.88	57
B4	134.43	26	134.78	47	133.92	46
A4	134.58	28	136.00	35	134.32	43
A3	146.99	54	148.23	68	147.37	112
A5	146.99	54	148.23	68	147.37	112
B3	152.63	46	153.52	74	152.34	113
B5	152.63	46	153.52	74	152.34	113
erythro isomer						
γ	60.50		61.23			
a	72.50		73.43			
β	87.03		86.32			

Compound Number 244



threo

G-b-H

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.22	s	
OMe	3.79	s	
γ1	3.54	m	
γ2	3.78	m	
β	4.39	m	
α	4.94	m	
A5	6.77	d	8.2
A2	7.08	bs	
A4 OH	7.44	s	

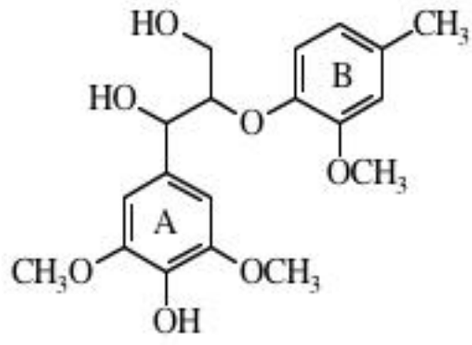
Notes:

SRIX-88GHB
36mg A1 and B1 may be interchanged
gHSQC, gHMBC in acetone and CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bα	20.53	27	20.46	42	20.05	125
OMe	55.98	34	56.20	49	55.49	119
γ	61.11	18	61.67	36	60.04	63
α	73.81	20	73.36	36	70.92	75
β	83.38	21	84.30	36	83.25	74
A2	109.56	21	111.36	48	110.95	79
A5	114.43	24	115.17	43	114.73	83
B3	116.57	47	117.08	79	115.88	199
B5	116.57	47	117.08	79	115.88	199
A6	120.00	21	120.36	40	119.01	80
B2	130.18	49	130.47	89	129.55	210
B6	130.18	49	130.47	89	129.55	210
B1	131.43	13	130.55	30	128.97	83
A1	131.76	14	134.24	20	133.25	66
A4	145.59	14	146.66	19	145.41	67
A3	146.75	13	147.93	17	146.99	68
B4	155.98	11	157.98	15	156.93	67
erythro isomer						
γ	61.44		62.03		60.17	
α	73.94		74.03		71.55	
b	81.22		83.98		83.37	

Compound Number 245



threo

S-b-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.25	s	
γ1	3.48	m	
A OMe	3.78	s	
B OMe	3.84	s	
γ2	4.10	m	
β	4.48	d	3.8
α	4.85	dd	3.6, 6.4
B6	6.65	m	
A2,6	6.76	s	
B2	6.83	d	1.8
B5	7.04	d	8.2

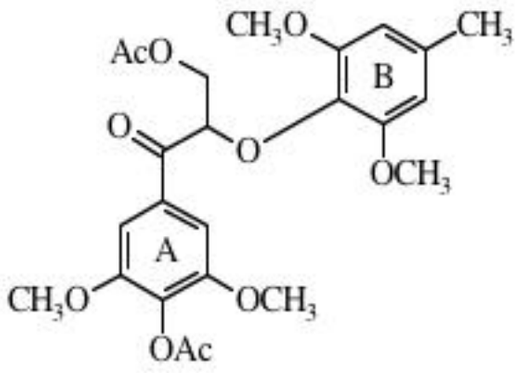
Notes:

SRIX-95BR
HSQC and HMBC in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bα	21.73	21	21.06	41	20.57	38
B OMe	55.85	24	56.26	49	55.50	46
A OMe	56.34	48	56.60	97	55.80	77
A OMe	56.34	48	56.60	97	55.80	77
γ	60.99	15	61.89	40	60.05	27
α	74.18	19	74.05	42	70.90	28
β	89.51	21	88.73	45	84.58	27
A2	103.86	39	105.41	95	104.15	56
A6	103.86	39	105.41	95	104.15	56
B2	113.06	23	114.20	45	113.34	33
B5	120.90	22	120.10	45	115.95	31
B6	121.96	22	122.19	48	120.76	34
A1	130.82	12	132.84	23	130.21	25
B1	134.17	14	133.10	22	132.00	27
A4	134.58	10	136.15	18	134.33	25
B4	145.25	10	147.36	18	145.98	25
A3	147.12	23	148.40	38	147.39	52
A5	147.12	23	148.40	38	147.39	52
B3	150.93	11	151.50	18	149.46	25
erythro shifts						
γ	60.76		61.75		59.94	
α	72.87		73.98		71.90	
β	87.70		87.09		83.97	

Compound Number 246



^{1}H (acetone)

Atom	H Shifts	Mult	J
A4 Ac Me	1.90	s	
Bα	2.08	s	
γ Ac Me	2.26	s	
B OMe	3.70	s	
A OMe	3.85	s	
γ	4.49	m	
β	5.50	t	5.4
B2,6	6.47	s	
A2,6	7.49	s	

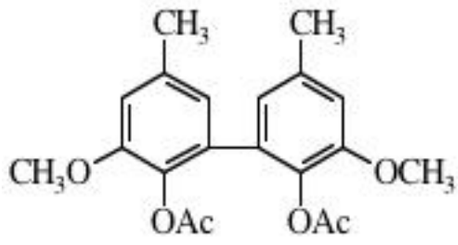
Notes:

SRTSII-131-Ac 12mg
A2,6 and B2,6 ; A1 and B1 switch in DMSO
HSQC and HMBC in Acetone, CDCl3 and DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.43	25	20.22	129	20.08	149
γ Ac Me	20.75	21	20.60	113	20.42	139
Bα	21.82	20	21.73	109	21.32	130
B OMe	55.86	49	56.19	268	55.65	293
B OMe	55.86	49	56.19	268	55.65	293
A OMe	56.29	48	56.60	249	56.12	272
A OMe	56.29	48	56.60	249	56.12	272
γ	64.15	22	64.34	117	63.26	88
β	81.65	24	81.24	119	79.70	97
B2	105.93	48	106.75	280	105.93	196
B6	105.93	48	106.75	280	105.93	196
A2	106.25	46	106.80	283	105.58	191
A6	106.25	46	106.80	283	105.58	191
A4	133.03	6	133.82	33	132.20	40
B4	133.50	15	134.25	35	132.74	68
A1	133.57	14	134.72	63	133.61	100
B1	134.31	14	134.88	67	133.33	102
A3	152.09	25	153.11	110	151.75	193
A5	152.09	25	153.11	110	151.75	193
B3	152.49	24	153.51	107	152.05	180
B5	152.49	24	153.51	107	152.05	180
A4 Ac C=O	168.14	11	168.20	55	167.79	81
γ Ac C=O	170.75	11	170.73	52	170.03	99
α	194.84	13	195.23	57	194.40	87

Compound Number 247



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.54	24	20.36	84	20.10	63
α	21.51	24	21.32	82	20.87	64
OMe	56.08	36	56.28	114	55.83	67
2	112.75	23	113.52	98	112.90	55
6	123.17	27	123.44	95	122.22	48
5	131.30	9	132.13	29	130.49	34
4	135.39	4	136.48	58	134.74	21
1	136.02	14	136.48	58	135.52	46
3	150.95	12	152.17	31	150.64	38
Ac C=O	168.96	9	168.67	21	168.00	26

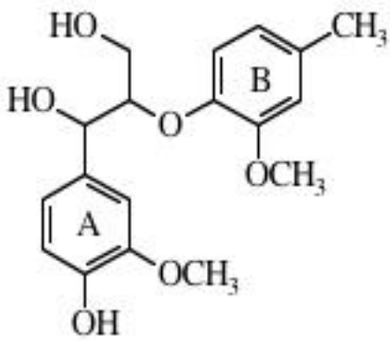
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.00	s	
α	2.33	s	
OMe	3.81	s	
6	6.60	bdd	2.0, 0.8
2	6.92	bd	1.6

Notes:

LLL-XXIII-76DA
37mg
As this dimer contains a plane of symmetry the CSs are reported for one unit.

Compound Number 248



threo

G-b-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.27	s	
γ1	3.51	m	
γ2	3.68	m	
OMe	3.81	s	
OMe	3.85	s	
β	4.07	m	
α	4.88	d	6.0
B6	6.66	bd	7.3
B5	6.87	bd	8.0
A4 OH	7.37	s	

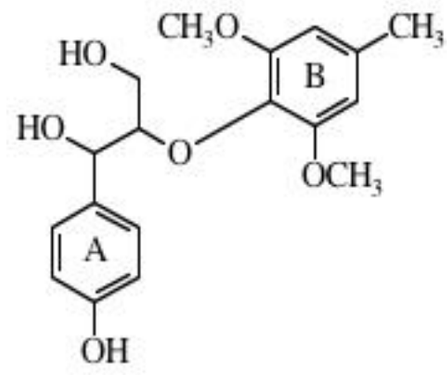
Notes:

SRIX-98 27mg
B5 and A6 may be switched
HSQC and HMBC in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bα	21.21	31	21.06	36	20.63	80
OMe	55.85	39	56.19	44	55.45	79
OMe	55.93	41	56.26	54	55.58	93
γ	60.96	17	61.82	26	60.10	47
α	73.96	24	73.95	28	70.96	52
β	89.52	23	88.90	33	84.95	44
A2	109.59	28	111.40	34	111.05	54
B2	113.05	32	114.17	36	113.43	52
A5	114.39	28	115.23	37	114.69	56
B5	120.22	30	120.23	37	116.28	48
A6	120.87	28	120.57	38	119.04	56
B6	121.94	33	122.19	41	120.84	71
A1	131.64	15	133.16	19	130.36	49
B1	134.08	18	133.82	16	133.01	52
B4	145.31	14	146.80	16	145.44	57
A4	145.58	15	147.82	14	146.13	44
A3	146.75	15	148.02	16	147.00	53
B3	150.86	13	151.47	12	149.57	45
erythro isomer						
γ	60.69		61.69		59.97	
α	72.71		73.78		71.72	
β	87.33		87.08		84.21	

Compound Number 249



threo

H-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.28	s	
γ1	3.21	dd	12.3, 3.2
γ2	3.60	dd	12.3, 3.2
β	3.82	m	
OMe	3.85	s	
α	4.98	d	7.8
B2,6	6.55	s	
A3,5	6.78	d	8.5
A2,6	7.27	d	8.5
CDCl3	CDCl3		
Bα	2.36		
γ1	3.32		
γ2	3.57		
β	3.87		
OMe	3.90		
α	5.03		
B2,6	6.47		
A3,5	6.72		
A2,6	7.26		

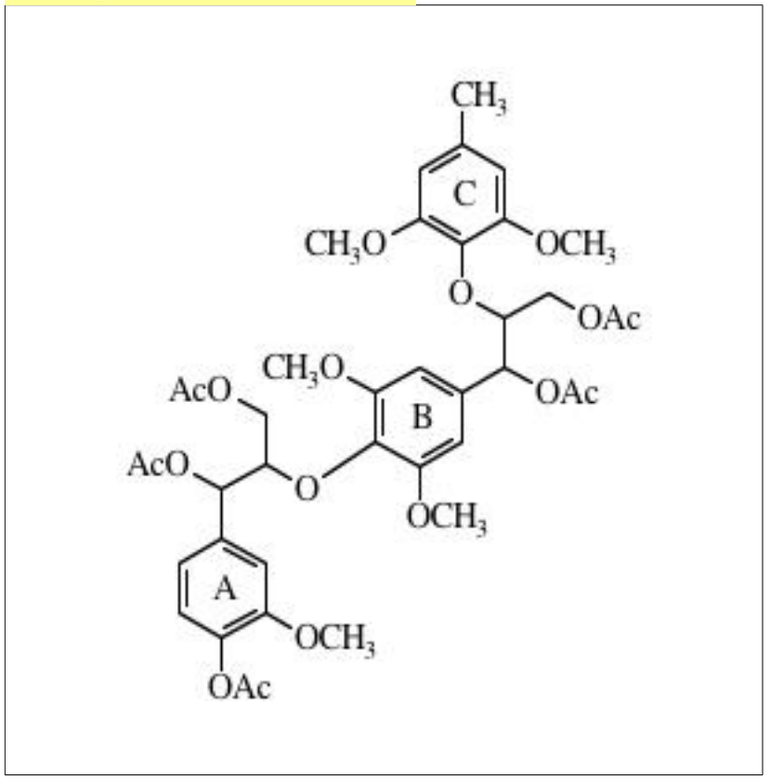
Notes:

SRIX-101B 21mg
HSQC acetone
HSQC & HMBC CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bα	22.01	25	21.78	21	21.34	35
OMe	56.19	58	56.48	50	55.86	77
OMe	56.19	58	56.48	50	55.86	77
γ	60.50	18	61.06	21	60.08	23
α	74.10	23	73.95	22	71.53	27
β	89.14	23	89.98	23	87.36	28
B2	106.16	48	107.12	42	106.33	57
B6	106.16	48	107.12	42	106.33	57
A3	115.56	48	115.58	48	114.37	59
A5	115.56	48	115.58	48	114.37	59
A2	128.75	45	129.22	46	127.88	61
A6	128.75	45	129.22	46	127.88	61
A1	131.26	17	133.06	10	132.21	23
B4	133.02	11	134.67	7	132.86	24
B1	134.77	15	134.84	10	133.93	17
B3	152.69	27	153.67	15	152.32	42
B5	152.69	27	153.67	15	152.32	42
A4	156.28	18	157.68	12	156.23	26
erythro isomer						
γ	60.6		60.8			
α	72.4		73.1			
β	87.0		87.8			

Compound Number 250



G-b-S-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.84	d	1.6
α Ac Me	1.93	d	1.4
γ Ac Me	2.00	d	3.0
αAc Me	2.11	d	1.0
A4 Ac Me	2.21	s	
Cα	2.28	s	
OMe	3.77	s	
OMe	3.79	s	
OMe	3.81	s	
Bγ 1	3.83	m	
Aγ 1	4.16	dd	11.7, 4.2
Bγ 2	4.22	ddd	11.7, 3.8, 1.8
Aγ 2	4.40	dd	11.7, 6.0
Bβ	4.52	m	
Aβ	4.70	m	
Aα	6.06	d	overlapping
Bα	6.06	d	overlapping
C2,6	6.49	s	
B2,6	6.74	d	
A5,6	7.00	m	1.6
A2	7.16	d	1.4

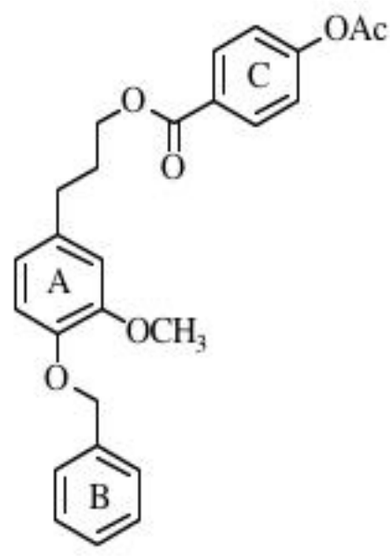
Notes:

SRIX-105 30mg
Order of Ac Me changes in CDCl3
HSQC and HMBC in CDCl3 and d6-acetone The first β-O-4 linkage appears to be erythro and the second linkage appears to be threo.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.85	47	20.48	55	20.27	35
γ Ac Me	20.67	46	20.59	48	20.35	47
γ Ac Me	20.73	41	20.74	41	20.48	36
α Ac Me	21.08	75	20.93	53	20.67	41
α Ac Me	21.08	75	21.02	48	20.73	40
Cα	21.85	39	21.74	47	21.37	35
B OMe	55.99	109	56.32	91	55.71	115
B OMe	55.99	109	56.32	91	55.71	115
C OMe	55.99	109	56.45	123	55.71	115
C OMe	55.99	109	56.45	123	55.71	115
A OMe	56.07	84	56.86	104	55.85	72
Aγ	62.76	21	63.39	39	62.25	19
Bγ	63.74	25	64.30	36	63.20	15
Aα	74.06	23	75.15	44	73.83	22
Bα	75.99	29	76.75	28	75.77	13
Aβ	80.89	57	81.45	34	80.00	17
Bβ	80.89	57	81.76	28	80.50	15
B2	104.44	53	105.27	79	104.01	36
B6	104.44	53	105.27	79	104.01	36
C2	106.05	70	106.99	89	105.89	53
C6	106.05	70	106.99	89	105.89	53
A2	111.60	17	112.30	33	111.04	21
A6	119.23	24	120.02	25	118.85	13
A5	122.42	33	123.30	41	122.57	21
C1	133.37	20	134.17	27	133.02	39
B1	133.74	25	134.36	27	133.02	39
C4	134.40	18	135.56	14	133.79	13
B4	135.22	11	136.33	18	134.35	20
A1	136.15	25	137.10	24	135.67	19
A4	139.50	19	140.57	20	138.92	23
A3	150.85	23	152.05	25	150.59	27
C3	152.65	41	153.67	49	152.13	48
C5	152.65	41	153.67	49	152.13	48
B3	153.06	41	153.91	53	152.43	42
B5	153.06	41	153.91	53	152.43	42
A4 Ac C=O	168.89	20	168.96	23	168.49	26
α Ac C=O	169.55	23	169.90	29	169.29	28
α Ac C=O	169.85	21	169.95	34	169.38	29
γ Ac C=O	170.54	21	170.69	45	169.99	34
γAc C=O	170.88	21	170.69	45	169.99	34

Compound Number 251



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			21.00	21		
β			31.15	12		
α			32.42	15		
OMe			56.13	18		
γ			64.98	14		
Bα			71.56	11		
A2			113.72	12		
A5			115.39	11		
A6			121.14	12		
C3			122.79	36		
C5			122.79	36		
B2			128.40	33		
B6			128.40	33		
B4			128.40	33		
C1			128.72	6		
B3			129.11	23		
B5			129.11	23		
C2			131.62	29		
C6			131.62	29		
A1			135.56	6		
B1			138.76	4		
A4			147.68	4		
A3			150.88	4		
C4			155.53	7		
Cα			166.03	4		
Ac C=O			169.26	8		

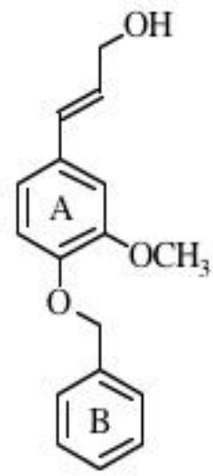
^{1}H (acetone)

Atom	H Shifts	Mult	J
β	2.08	s	
Ac Me	2.28	d	< 1.0
α	2.74	bt	8.0
OMe	3.79	s	
γ	4.31	bt	6.4
Bα	5.05	s	
A6	6.75	m	
A2,5	6.91	m	
C3,5	7.25	d	8.5
B3,4,5	7.35	m	
B2,6	7.47	bd	7.4
C2,6	8.05	d	8.5

Notes:

L.Landucci XXIII-143 39mg.
HSQC and HMBC in acetone d-6

Compound Number 252



^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.84	s	
γ	4.19	dd	5.4, 1.4
Bα	5.09	s	
β	6.26	dt	16.1, 5.4
α	6.52	dt	9.9, 1.7
A6	6.88	dd	8.3, 2.0
A5	6.96	d	8.3
A2	7.08	d	2.0
B2-6	7.3-7.5	m	

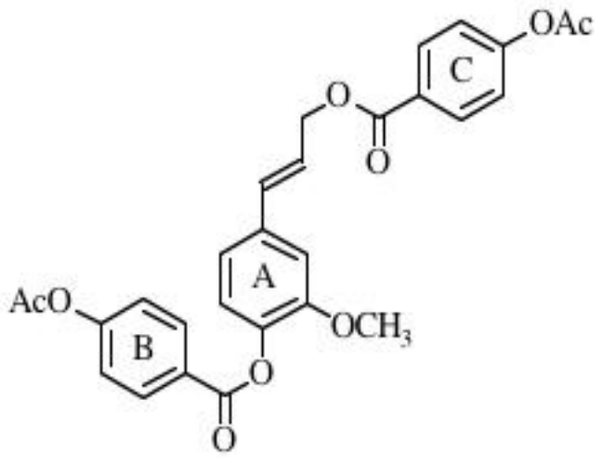
Notes:

L.Landucci XXIII-127G 48 mg
HSQC and HMBC in acetone d-6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.16	34		
γ			63.26	17		
Bα			71.47	30		
A2			110.73	29		
A5			115.12	28		
A6			120.11	32		
B2			128.46	61		
B6			128.46	61		
B4			128.54	38		
B3			129.19	77		
B5			129.19	77		
β			129.19	77		
α			130.01	31		
A1			131.94	13		
B1			138.60	13		
A4			148.98	7		
A3			151.02	10		

Compound Number 253



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.29	s	
Ac Me	2.31	s	
OMe	3.84	s	
γ	5.00	bd	6.0
β	6.55	dt	16.0, 6.0
α	6.85	bd	16.0
A6	7.13	dd	8.3, 1.8
A5	7.20	d	8.3
C3,5	7.28	d	8.7
A2	7.33	bs	
B3,5	7.35	d	8.7
C2,6	8.11	d	8.7
B2,6	8.21	d	8.7

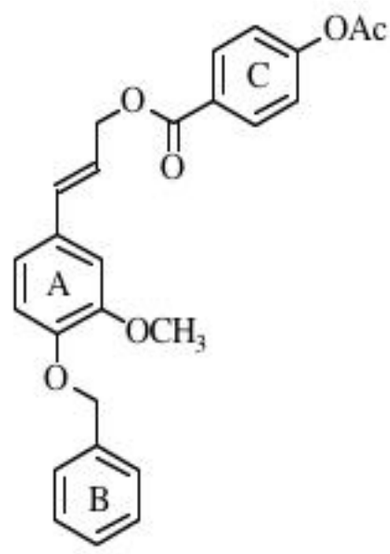
Notes:

L.Landucci XXIII-114B 16 mg
HSQC and HMBC in acetone d-6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.98	39		
Ac Me			20.98	39		
OMe			56.30	32		
γ			66.01	22		
A2			111.31	21		
A6			120.16	17		
C3			122.93	45		
C5			122.93	45		
B3			123.16	48		
B5			123.16	48		
A5			123.95	23		
β			124.89	21		
B1			127.72	8		
C1			128.57	7		
C2			131.77	48		
C6			131.77	48		
B2			132.34	46		
B6			132.34	46		
α			134.01	23		
A1			136.55	15		
A4			140.81	14		
A3			152.54	16		
C4			155.72	11		
B4			156.13	15		
Bα			164.23	4		
Cα			165.84	6		
Ac C=O			169.29	19		
Ac C=O			169.29	19		

Compound Number 254



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.28	s	
OMe	3.85	s	
γ	4.95	dd	6.4, 1.3
Bα	5.10	s	
β	6.38	dt	15.9, 6.4
α	6.74	d	15.9
A5,6	6.97	m	
A2	7.16	bs	
C3,5	7.26	d	8.7
B3,4,5	7.31-7.41	m	
B2,6	7.47	bd	7.4
C2,6	8.09	d	8.7

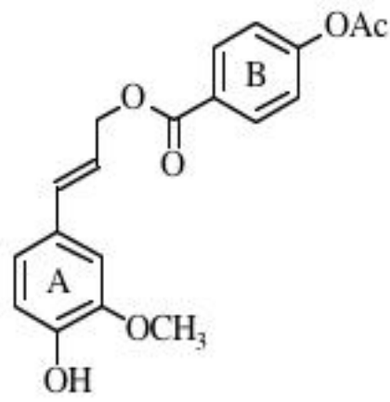
Notes:

L.Landucci XXIII-129B 57mg
HSQC and HMBC in acetone d-6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			21.00	39		
OMe			56.31	30		
γ			66.34	34		
Ba			71.53	26		
A2			111.16	18		
A5			115.17	18		
A6			120.82	37		
β			122.39	34		
C3			122.83	78		
C5			122.83	78		
B2			128.45	78		
B6			128.45	78		
B4			128.57	38		
C1			128.69	14		
B3			129.20	68		
B5			129.20	68		
A1			131.00	14		
C2			131.74	73		
C6			131.74	73		
α			134.95	36		
B1			138.49	15		
A4			149.70	13		
A3			151.13	12		
C4			155.68	13		
Cα			165.93	13		
Ac C=O			169.25	13		

Compound Number 255



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.98	32		
OMe			56.24	28		
γ			66.47	28		
A2			110.24	23		
A5			115.83	22		
A6			121.33	47		
β			121.33	47		
B3			122.90	62		
B5			122.90	62		
B1			128.70	9		
A1			129.35	10		
B2			131.73	62		
B6			131.73	62		
α			135.40	26		
A4			147.91	11		
A3			148.55	6		
B4			155.68	9		
Bα			165.90	8		
Ac C=O			169.29	11		

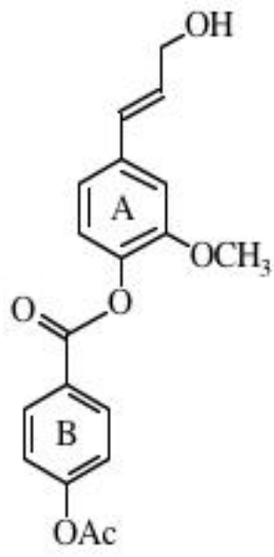
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.28	s	
OMe	3.86	s	
γ	4.94	dd	6.6, 1.2
β	6.33	dt	16.0, 6.6
α	6.72	d	16.0
A5	6.79	d	8.3
A6	6.93	dd	8.3, 2.1
A2	7.14	d	2.1
B3,5	7.27	d	8.9
B2,6	8.09	d	8.9

Notes:

L.Landucci XXIII-114D2 8mg
HSQC and HMBC in acetone d-6

Compound Number 256



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.31	s	
OMe	3.84	s	
OH	3.90	t	
γ	4.25	dt	5.2, 1.4
β	6.43	dt	15.9, 5.2
α	6.64	d	15.9
A6	7.05	dd	8.3, 1.9
A5	7.15	d	8.3
A2	7.23	d	1.9
B3,5	7.34	d	8.9
B2,6	8.20	d	8.9

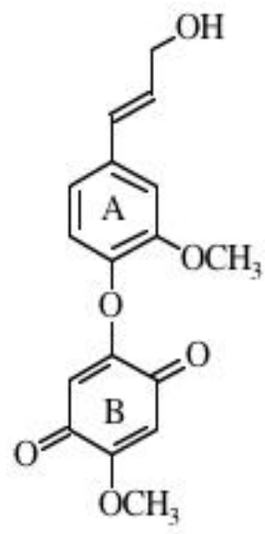
Notes:

L.Landucci XXIII-114D1 4mg
HSQC and HMBC in acetone d-6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.99	35		
OMe			56.22	39		
γ			63.10	29		
A2			111.04	37		
A6			119.58	36		
B3			123.15	76		
B5			123.15	76		
A5			123.81	38		
B1			127.80	16		
α			129.30	36		
β			131.61	37		
B2			132.32	73		
B6			132.32	73		
A1			137.50	17		
A4			140.16	11		
A3			152.44	16		
B4			156.10	13		
Bα			164.29	8		
Ac C=O			169.30	13		

Compound Number 257



^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.85	s	
B OMe	3.86	s	
γ	4.24	bs	
B2	5.40	s	
B5	6.02	s	
β	6.44	dt	15.9, 5.0
α	6.63	dt	16.1, 1.7
A5,6	7.09	m	
A2	7.27	bs	

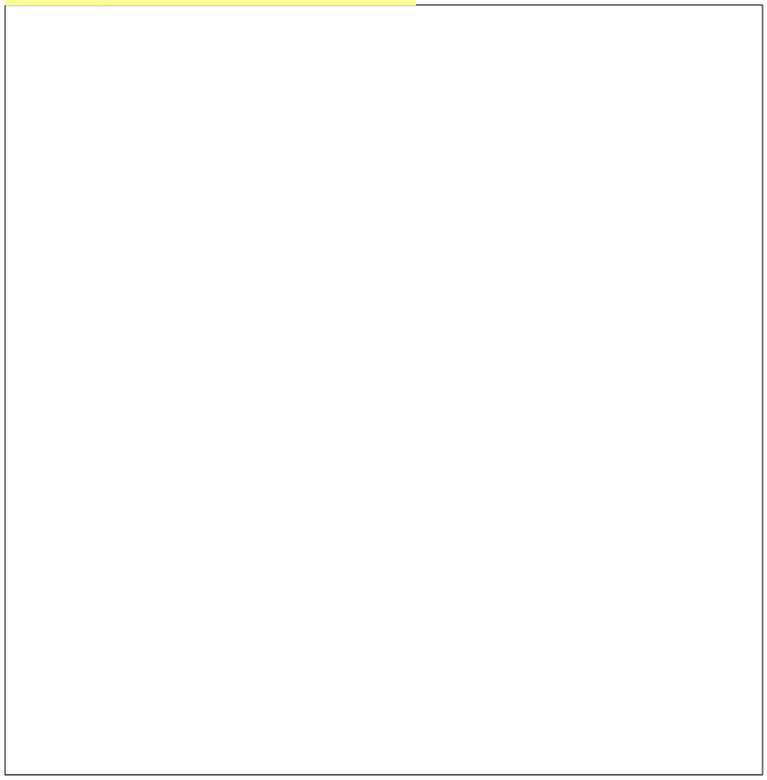
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A OMe			56.27	26		
B OMe			57.07	27		
γ			62.98	26		
B2			106.32	28		
B5			108.77	26		
A2			111.75	24		
A6			120.19	27		
A5			122.94	27		
α			128.91	24		
β			132.31	26		
A1			138.15	13		
A4			140.96	6		
A3			151.65	9		
B6			159.23	6		
B3			160.39	9		
B4			181.63	9		
B1			182.05	7		

Notes:

L.Landucci XXIII-93CC 17mg
HSQC and HMBC in acetone d-6

Compound Number 258



Vanillin-a-G-b-CA

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me's	1.91, 2.03, 2.07	s's	
OMe	3.81	s	
OMe	3.83	s	
OMe	3.97	s	
γ1	4.45	dd	11.9, 4.0
γ2	4.56	dd	11.9, 5.8
Bγ	4.67	dd	6.4, 1.2
β	4.91	m	
α	5.84	d	5.2
Bβ	6.27	dt	15.9, 6.4
Bα	6.63	d	15.9
B6	6.93	dd	8.2, 1.6
B5	7.01	d	8.3
A5	7.03	d	8.2
A6	7.14	dd	8.2, 1.8
B2	7.15	d	2.0
C5	7.15	d	8.3
A2	7.36	d	2.4
C6	7.39	dd	8.2, 1.8
C2	7.46	d	1.8
Cα	9.81	s	

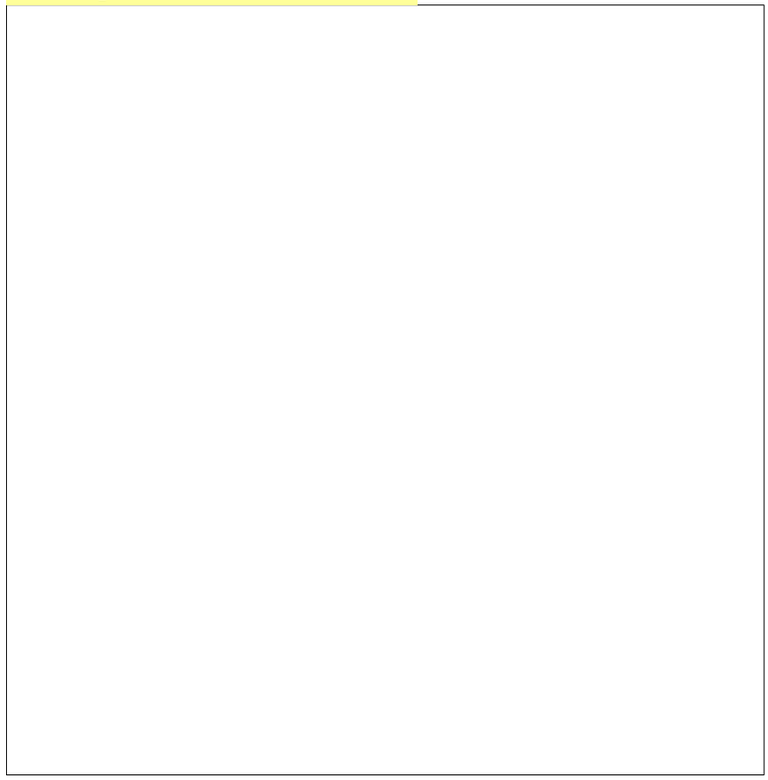
Notes:

SRIX-116E 3mg
gHSQC and gHMBC in acetone
proton CS's for A6,C5 and A2 determined by simulation (Acorn MacNuts)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.74	32	20.46	29		
γAc Me	20.82	31	20.62	27		
BγAc Me	21.10	19	20.80	22		
OMe	55.84	28	56.24	36		
OMe	56.09	38	56.29	31		
OMe	56.13	42	56.51	31		
γ	63.12	23	63.32	26		
Bγ	65.17	25	65.38	29		
α	79.98	23	80.55	26		
β	82.11	23	81.82	27		
B2	109.93	24	111.36	51		
C2	110.29	24	111.36	51		
A2	111.14	23	112.68	26		
C5	114.77	21	115.94	27		
B5	119.31	22	119.62	26		
A6	119.46	26	120.33	27		
B6	119.93	24	120.53	28		
Bβ	122.39	22	123.35	27		
A5	122.94	25	123.53	27		
C6	126.32	22	126.04	26		
C1	130.99	14	132.08	14		
B1	132.03	13	132.61	14		
Bα	133.93	21	134.20	25		
A1	136.05	16	136.78	17		
A4	139.89	12	140.85	11		
B4	147.31	12	148.54	12		
C3	150.68	13	151.58	12		
A3	151.13	11	152.02	12		
B3	151.43	12	152.28	12		
C4	152.81	11	153.36	12		
A4 Ac C=O	168.86	11	168.87	11		
γAc C=O	170.82	12	170.77	18		
γAc C=O	170.95	10	170.77	18		
Cα	190.96	25	191.26	30		

Compound Number 259



dihydrodiconiferyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.81	m	
α	2.64	m	
γ	3.58	t	6.6
OMe	3.85	s	
6	6.72	d	2.1
2	6.82	d	2.0

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	31.94	37	32.53	33	31.34	34
β	34.45	35	35.75	31	34.59	39
OMe	56.20	52	56.42	45	55.85	63
γ	62.38	34	61.85	22	60.24	48
2	110.71	32	111.75	31	110.77	28
6	123.04	40	123.94	32	122.73	32
5	124.52	13	126.47	11	125.89	18
1	133.76	16	134.15	19	132.26	30
4	140.83	17	142.49	13	141.36	24
3	147.33	18	148.64	14	147.61	20

Notes:

L.Landucci
XXIII-52H 25 mg
As this dimer contains a plane of symmetry the CSs are reported for one unit.

Compound Number 260

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.39	32	20.46	44	19.99	11
Ac Me	20.91	27	20.78	37	20.56	12
α	30.30	19	30.99	28	29.58	8
β	32.15	19	32.61	33	31.32	7
OMe	56.02	34	56.34	44	55.79	10
γ	63.72	21	64.04	30	63.10	9
2	111.95	13	112.93	21	112.16	4
6	122.27	15	122.80	19	121.46	4
5	131.36	8	132.20	9	130.51	4
4	135.76	7	136.81	8	135.09	4
1	139.28	10	140.33	12	139.20	4
3	151.13	11	152.37	14	150.82	5
4 Ac C=O	168.76	8	168.76	12	167.98	4
γ Ac C=O	171.08	9	171.00	11	170.25	5

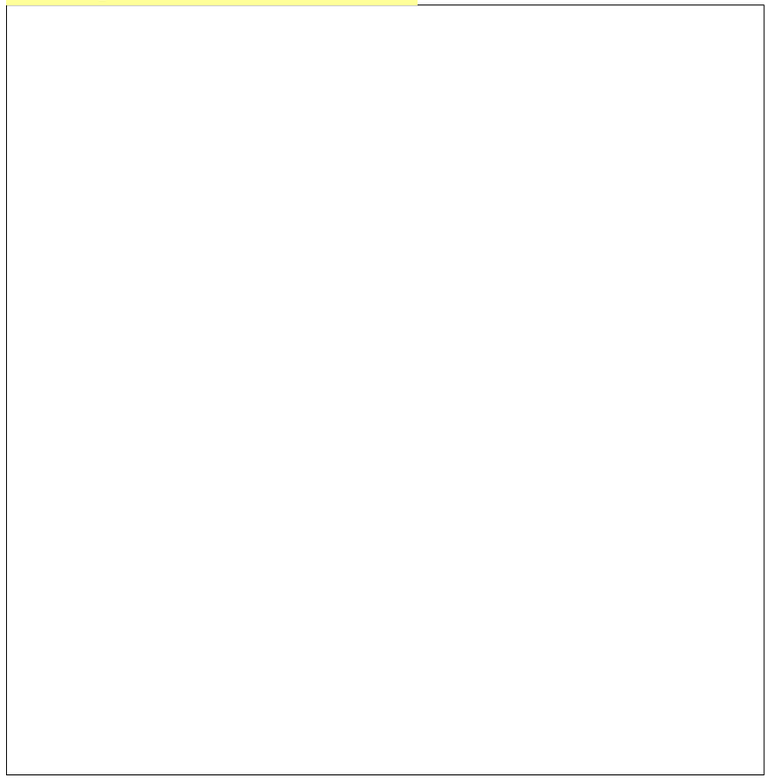
^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.97	m	
Ac Me	1.98	s	
Ac Me	2.01	s	
α	2.70	bt	8.0
OMe	3.83	s	
γ	4.07	t	6.4
6	6.66	d	1.8
2	6.99	d	1.8

Notes:

L.Landucci
XXIII-146ACH
As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 261



S-b(t)-G-b(e)-S5

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.88	s	
γ Ac Me	1.97	s	
α Ac Me	2.01	d	
αAc Me	2.12	d	
A4 Ac Me	2.21	s	
Cα	2.27	s	
OMe's	3.77, 3.80, 3.84	s's	
Aγ 1	4.05	dd	11.9, 5.4
Bγ 1	4.13	dd	11.5, 3.2
Aγ 2	4.26	m	
Bγ 2	4.39	m	
Bβ	4.65	m	
Aβ	4.81	m	
Bα	6.01	d	4.2
Aα	6.08	d	6.6
C 2,6	6.48	s	
A 2,6	6.85	s	
B6	6.90	m	
B5	7.02	d	8.3
B2	7.06	m	

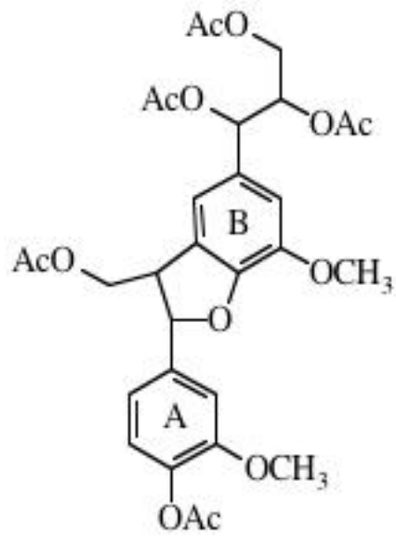
Notes:

S.Ralph
SRIX-115BAc 30 mg CS's indicate A-threo-B-erythro-C
gHSQC and gHMBC in acetone, some signals split due to isomers

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.48	32	20.24	46	20.05	27
γ Ac Me	20.75	26	20.64	81	20.35	38
γ Ac Me	20.84	35	20.64	81	20.35	38
α Ac Me	21.08	26	20.96	68	20.62	37
αAc Me	21.14	29	20.96	68	20.62	37
Cα	21.90	31	21.77	51	21.35	24
OMe	55.97	70	56.28	125	55.61	66
OMe	55.97	70	56.28	125	55.61	66
OMe	55.97	70	56.28	125	55.61	66
OMe	56.28	61	56.28	125	55.98	38
OMe	56.28	61	56.55	84	55.98	38
Bγ	62.82	15	63.35	26	62.12	15
Aγ	63.09	15	63.63	19	62.46	12
Bα	74.33	19	75.22	27	73.76	14
Aα	74.48	18	75.68	27	74.59	10
Aβ	80.20	18	80.65	15	78.96	10
Bβ	80.84	21	81.16	33	79.94	16
A2	104.16	30	104.97	46	103.97	23
A6	104.16	30	104.97	46	103.97	23
C2	106.09	50	106.92	88	105.87	41
C6	106.09	50	106.92	88	105.87	41
B2	111.59	10	112.49	16	110.87	9
B5	118.00	16	118.39	13	116.75	7
B6	119.52	18	120.29	16	118.89	10
A4	128.90	9	129.69	12	127.84	9
B1	132.33	8	132.98	10	131.07	6
C4	132.90	10	134.16	13	132.16	8
C1	134.14	15	134.48	20	133.32	14
A1	134.78	15	136.15	19	134.92	12
B4	147.69	8	148.70	14	147.19	8
B3	150.46	8	151.38	14	149.68	8
A3	152.26	28	153.20	35	151.58	22
A5	152.26	28	153.20	35	151.58	22
C3	152.98	35	153.88	48	152.34	29
C5	152.98	35	153.88	48	152.34	29
A4 Ac C=O	168.52	14	168.45	18	167.91	11
α Ac C=O	169.75	16	169.96	27	169.26	17
αAc C=O	169.79	12	170.01	27	169.33	17
γ Ac C=O	170.62	14	170.70	32	169.94	25
γ Ac C=O	170.91	14	170.70	32	169.94	25

Compound Number 262



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.98	m	
Ac Me	2.00	m	
Ac Me	2.03	s	
Ac Me	2.04	s	
A4 Ac Me	2.21	s	
Aβ	3.78	m	
A OMe	3.79	s	
B γ1	3.82	m	
B OMe	3.87	s	
B γ2	4.17	m	
Aγ	4.38	m	
Bβ	5.38	m	
Aα	5.61	d	6.8
Bα	5.92	dd	7.2, 2.8
B2,6,A6	6.99	m	
A5	7.04	d	8.2
A2	7.18	bs	

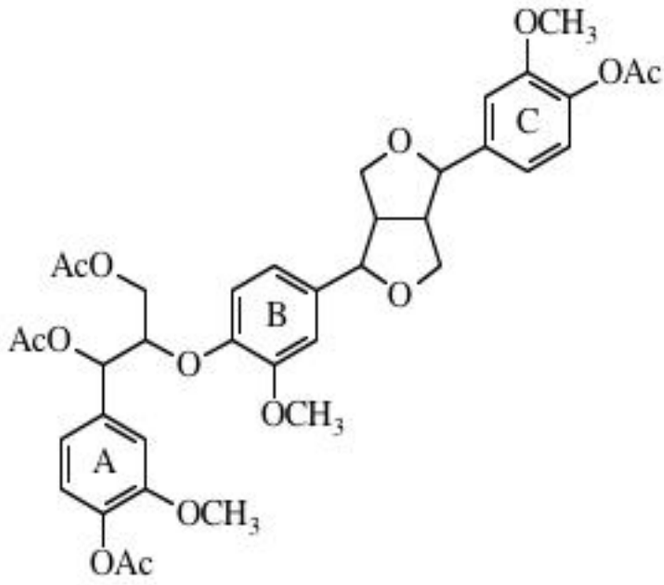
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.76	82	20.47	67		
Ac Me	20.76	82	20.56	56		
Ac Me	20.76	82	20.73	60		
Ac Me	20.85	68	20.73	64		
A4 Ac Me	21.07	46	20.89	49		
Aβ	50.64	23	51.45	43		
A OMe	56.02	42	56.29	62		
B OMe	56.26	38	56.59	52		
Bγ	62.36	23	63.00	38		
Aγ	64.98	13	65.79	19		
Bβ	72.47	22	73.27	36		
Bα	73.95	17	74.55	17		
Aα	88.20	22	88.40	27		
A2	110.13	21	111.11	28		
B2	111.74	13	113.19	20		
B6	115.87	13	116.84	20		
A6	118.40	19	118.78	27		
A5	122.97	31	123.80	54		
B5	127.58	14	128.83	13		
B1	129.80	14	131.06	14		
A1	139.29	11	140.82	14		
A4	139.84	10	140.92	15		
B3	144.61	10	145.31	9		
B4	148.54	7	149.38	7		
A3	151.39	15	152.46	21		
A4 Ac C=O	168.96	15	168.96	24		
Bα Ac C=O	169.87	14	170.01	17		
Bβ Ac C=O	170.10	15	170.26	17		
Bγ Ac C=O	170.45	15	170.63	20		
Aγ Ac C=O	170.75	18	170.95	23		

Notes:

SRVII-91D 8mg HSQC and HMBC in acetone and CDCl3
A1 and A4 tentative assignments, some signals split due to isomers

Compound Number 263



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
C4 Ac Me			20.48	71		
A4 Ac Me			20.48	71		
Aα Ac Me			20.63	29		
Aγ Ac Me			20.89	17		
Bβ			55.27	23		
Cβ			55.41	23		
OMe			56.21	41		
OMe			56.26	38		
OMe			56.28	19		
Aγ			63.03	14		
Bγ			72.50	40		
Cγ			72.62	40		
Aα			74.54	13		
Aβ			80.31	15		
Bα			86.17	42		
Cα			86.17	42		
C2			111.08	32		
B2			111.58	18		
A2			112.74	16		
C6			118.61	16		
B5			119.03	17		
B6			119.42	10		
A6			120.48	10		
A5			123.33	14		
C5			123.47	14		
A1			136.69	12		
B1			136.69	12		
C4			140.12	13		
A4			141.08	14		
C1			141.88	15		
B4			147.48	7		
B3			151.88	7		
C3			152.27	21		
A3			152.27	21		
A4 Ac C=O			168.92	14		
C4 Ac C=O			169.05	20		
AαAc C=O			169.91	7		
Aγ Ac C=O			170.77	7		
threo isomer						
Aγ			63.58			
Aα			75.33			
Aβ			80.74			

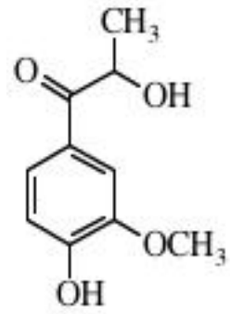
^{1}H (acetone)

Atom	H Shifts	Mult	J

Notes:

SRVII-143D 13 mg
Erythro isomer shirts reported
sample contains small amt of 5,5 resinol tetramer.

Compound Number 264



alpha,4-dihydroxy-3-methoxypropiophenone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.35	d	6.8
OMe	3.91	s	
β-OH	4.10	d	6.4
β	5.13	m	
5	6.94	d	8.2
2	7.57	d	2.0
6	7.60	dd	8.2, 2.0
4-OH	8.61	bs	
CDCl3			
γ	1.46	d	6.6
OMe	3.96	s	
β	5.13	m	
4-OH	6.61	bs	
5	6.98	d	8.2
6	7.48	dd	8.2, 2.0
2	7.54	d	2.0

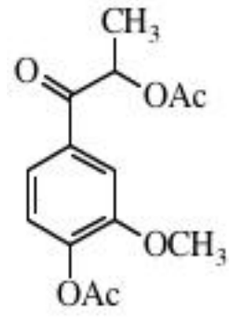
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	22.91	48	22.69	58	21.17	37
OMe	56.19	50	56.33	68	55.57	36
β	68.89	46	69.42	50	68.10	30
2	110.64	47	112.20	56	111.74	23
5	114.30	48	115.60	68	114.89	34
6	124.08	49	124.65	75	123.51	35
1	125.91	15	127.08	17	126.15	20
3	147.10	15	148.48	18	147.48	21
4	151.41	19	152.84	24	151.73	25
α	200.75	16	201.10	18	199.72	20

Notes:

FPL - Pearl collection
25 mg
HSQC and HMBC in acetone

Compound Number 265



alpha,4-diacetoxy-3-methoxypropiophenone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.48	d	7.0
β Ac Me	2.06	s	
4 Ac Me	2.27	s	
OMe	3.90	s	
β	6.00	q	7.0
5	7.23	d	8.0
2	7.64	O/Lap	
6	7.66	O/Lap	
CDCl3			
γ	1.53	d	7.0
βAc Me	2.14	s	
4 Ac Me	2.33	s	
OMe	3.89	s	
β	3.93	q	7.0
5	7.14	d	8.1
6	7.55	dd	8.1, 2.0
2	7.59	d	2.0

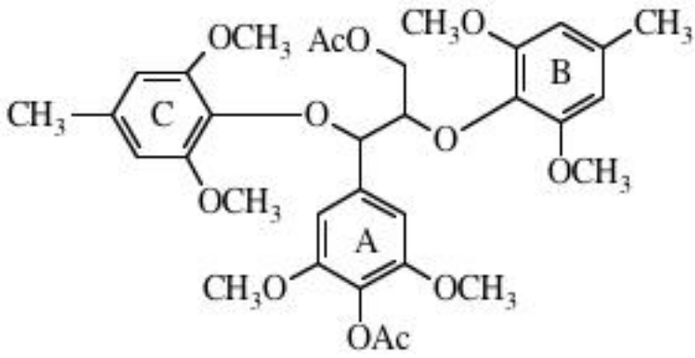
Notes:

FPL - Pearl Collection
25 mg
HSQC and HMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	17.16	63	17.41	76	16.90	26
β Ac Me	20.56	55	20.47	61	20.26	49
4 Ac Me	20.66	57	20.54	62	20.26	49
OMe	56.02	67	56.46	82	55.94	27
β	71.23	61	72.21	69	71.26	23
2	112.09	62	112.79	71	111.85	21
6	121.55	66	122.34	73	121.56	22
5	122.97	66	124.10	76	123.32	23
1	133.03	25	134.07	23	132.46	14
4	144.22	19	145.25	17	143.69	12
3	151.66	24	152.72	21	151.23	14
4 Ac C=O	168.31	22	168.62	22	168.02	11
β Ac C=O	170.32	23	170.54	22	169.74	13
α	195.65	23	196.21	24	195.52	13

Compound Number 266



S-a-S-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.83 (1.95)	s	
A4 Ac Me	2.17 (2.30)	s	
C α	2.18 (2.24)	s	
B α	2.22 (2.23)	s	
B OMe	3.69 (3.58)	s	
A/C OMe	3.73 (3.67)	s	
C/A OMe	3.74 (3.71)	s	
γ1	4.53 (4.64)	dd	11.7, 2.8
γ2	4.63 (4.72)	m	
β	4.73 (4.72)	m	
α	5.72 (5.60)	d	6.2
C 2,6	6.37 (6.26)	s	
B 2,6	6.40 6.25)	s	
A 2,6	6.81 (6.76)	s	

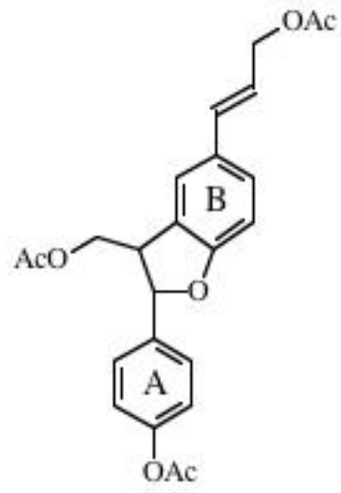
Notes:

SRIX-138A2
3mg 1H CDCl3 shifts in ( )s
HSQC and HMBC in acetone. A and C OMe shifts may be switched, B and C CH3's may be switchd

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.56	34	20.27	37	20.05	13
γ Ac Me	20.87	36	20.69	29	20.30	13
B α	21.76	35	21.61	31	21.18	12
C α	21.82	42	21.68	30	21.25	13
B OMe	55.87	79	56.27	86	55.46	25
B OMe	55.87	79	56.27	86	55.46	25
A OMe	55.96	93	56.35	94	55.62	32
A OMe	55.96	93	56.35	94	55.62	32
C OMe	56.12	86	56.39	90	55.67	29
C OMe	56.12	86	56.39	90	55.67	29
γ	64.44	30	64.64	33	62.98	8
β	81.52	31	82.68	36	80.92	9
α	81.89	34	83.16	37	81.36	8
A2	105.52	65	105.94	69	104.49	17
A6	105.52	65	105.94	69	104.49	17
B2	105.81	69	107.01	72	105.74	20
B6	105.81	69	107.01	72	105.74	20
C2	106.22	67	107.26	69	106.08	18
C6	106.22	67	107.26	69	106.08	18
A4	128.10	8	129.11	7	127.23	5
C1	133.01	20	133.61	19	132.21	6
B1	133.48	27	133.87	15	132.47	8
C4	133.48	27	134.38	10	132.72	10
B4	133.62	18	135.03	8	132.75	10
A1	138.02	20	138.47	20	136.90	7
A3	150.94	35	152.21	27	150.59	15
A5	150.94	35	152.21	27	150.59	15
C3	152.47	33	153.62	30	151.95	16
C5	152.47	33	153.62	30	151.95	16
B3	152.87	34	153.87	30	152.22	16
B5	152.87	34	153.87	30	152.22	16
A4 Ac C=O	168.75	18	168.52	13	167.91	7
γ Ac C=O	168.75	16	170.78	16	167.91	8

Compound Number 267



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.89	40	20.67	29		
Ac Me	21.11	34	20.81	23		
Ac Me	21.19	58	20.94	41		
β	50.26	40	51.06	30		
Bγ	65.35	42	65.51	33		
Aγ	65.68	40	66.10	31		
α	87.22	40	87.85	32		
B3	109.86	40	110.20	29		
Bβ	121.03	41	122.13	33		
A3	121.98	94	122.88	58		
A5	121.98	94	122.88	58		
B6	122.89	38	123.88	30		
A2	126.89	88	127.70	55		
A6	126.89	88	127.70	55		
B5	126.49	23	127.98	14		
B2	128.55	42	129.19	29		
B1	129.87	21	130.82	14		
Bα	134.16	38	134.43	30		
A1	138.63	19	139.84	12		
A4	150.64	15	151.77	12		
B4	159.85	14	160.77	10		
A4 C=O	169.44	17	169.62	13		
Bγ C=O	170.96	12	170.77	8		
AγC=O	170.84	20	170.94	13		

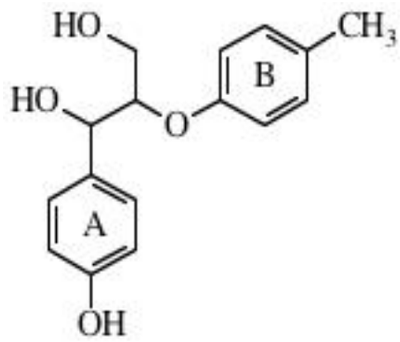
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.00 (2.07)	s	
Ac Me	2.01 (2.10)	s	
Ac Me	2.24(2.30)	s	
β	3.74 (3.70)	m	
γ1	4.34 (4.29)	dd	11.1, 7.8
γ2	4.46 (4.46)	dd	11.1, 5.4
Bγ	4.66 (4.71)	dd	6.4, 1.4
α	5.64 (5.54)	d	6.4
Bβ	6.23 (6.14)	dt	15.9, 6.4
Bα	6.66 (6.61)	d	15.9
B3	6.85 (6.85)	d	8.3
A 3,5	7.13 (7.09)	d	8.5
B2	7.33 (7.27)	dd	8.3, 2.0
A 2,6	7.45 (7.27)	d	8.5
B6	7.45 (7.37)		

Notes:

LLL XXV-17A-E 11mg
1H CDCl3 shifts in ( )s
Note: B5 and Bγ C=O move in CDCl3 to lower ppm relative to acetone shifts
HSQC and HMBC run in Acetone

Compound Number 268



erythro

H-b-H5e

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bα	20.58	58	20.45	28	20.07	43
γ	61.32	34	61.90	22	60.07	26
α	73.89	35	73.81	20	71.36	26
β	82.25	40	84.15	27	83.58	27
A3	115.52	83	115.50	64	114.46	64
A5	115.52	83	115.50	64	114.46	64
B3	116.79	90	117.33	49	116.22	64
B5	116.79	90	117.33	49	116.22	64
A2	127.71	81	128.89	80	128.01	58
A6	127.71	81	128.89	80	128.01	58
B2	130.18	98	130.44	60	129.52	68
B6	130.18	98	130.44	60	129.52	68
B1	131.41	27	130.61	14	129.03	26
A1	132.13	27	133.98	11	132.76	22
A4	155.78	28	157.43	13	156.25	30
B4	155.53	23	157.65	8	156.67	20

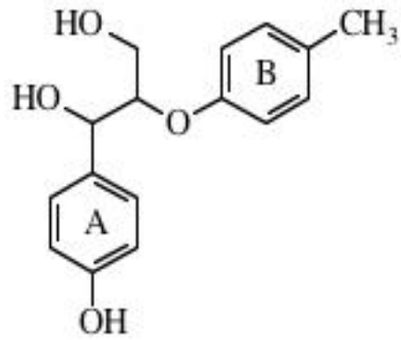
^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.19	s	
γ1	3.77	dd	11.7, 4.4
γ2	3.85	dd	11.7, 5.2
β	4.34	m	
α	4.89	d	5.6
A,B 3,5	6.78		
B 2,6	6.99		8.5
A 2,6	7.28		8.5
CDCl3			
Bα	2.25	s	
γ1	3.80	dd	11.9, 4.0
γ2	3.90	dd	11.9, 4.4
β	4.28	m	
α	4.98	d	5.2
A,B 3,5	6.74		
A 2,6	7.02	d	8.3
B 2,6	7.20	d	8.3

Notes:

S. Ralph SRIX-62
24mg, 70% erythro
A4 and B4 switch in CDCl3, B1 falls between A and B 2,6 in DMSO
HSQC and HMBC in all solvents

Compound Number 269



threo

H-b-H5t

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.21	s	
γ1	3.48	dd	11.5, 5.4
γ2	3.78	dd	11.5, 4.2
β	4.35	m	
α	4.94	d	5.2
A 3,5	6.78		
B 3,5	6.87		
B 2,6	7.02		
A 2,6	7.27		
CDCl3			
Bα	2.25	s	
γ1	3.46	dd	12.1, 3.8
γ2	3.73	dd	12.1, 4.0
β	4.28	m	
α	4.91	d	6.8
A 3,5	6.72		
B 3,5	6.84		
A 2,6	7.01		
B 2,6	7.18		

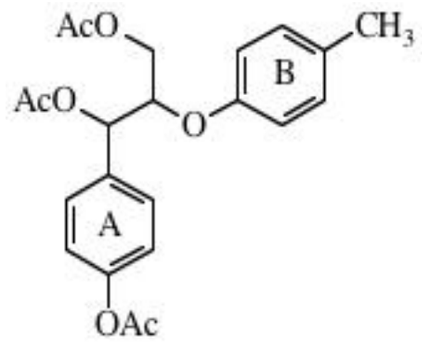
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bα	20.53	44	20.46	28	20.05	45
γ	60.95	27	61.54	24	59.99	18
α	73.64	26	73.15	19	70.79	25
β	83.32	28	84.43	25	83.41	27
A3	115.61	68	115.52	63	114.45	62
A5	115.61	68	115.52	63	114.45	62
B3	116.64	79	117.15	47	115.96	71
B5	116.64	79	117.15	47	115.96	71
A2	128.38	66	128.87	75	127.68	63
A6	128.38	66	128.87	75	127.68	63
B2	130.19	87	130.47	61	129.55	74
B6	130.19	87	130.47	61	129.55	74
B1	131.17	20	130.56	16	128.99	28
A1	131.42	25	133.58	13	132.50	19
A4	155.95	20	157.51	15	156.22	24
B4	156.21	26	159.00	10	156.95	20

Notes:

SRIX-62 20mg
75% threo, HSQC and HMBC in DMSO
B1 falls between A and B 2,6 in DMSO
A4 and B4 may be switched in CDCl3

Compound Number 270



erythro

H-b-H5e

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bα	20.31	64	20.49	46	20.04	42
Aγ Ac Me	20.50	52	20.58	41	20.40	42
Aα Ac Me	20.77	67	20.86	41	20.63	42
A4 Ac Me	20.88	74	20.94	52	20.77	48
γ	62.15	49	62.86	36	61.77	21
α	73.33	50	74.12	34	72.74	24
β	78.69	53	79.27	52	77.41	23
B3	116.76	103	117.56	68	116.37	61
B5	116.76	103	117.56	68	116.37	61
A3	121.44	110	122.49	74	121.66	52
A5	121.44	110	122.49	74	121.66	52
A2	128.30	133	129.31	92	128.31	54
A6	128.30	133	129.31	92	128.31	54
B2	129.88	148	130.74	107	130.33	71
B6	129.88	148	130.74	107	130.33	71
B1	131.39	25	131.85	12	130.51	21
A1	133.83	30	135.33	18	134.09	24
A4	150.54	23	151.79	12	150.23	19
B4	155.77	22	157.04	12	155.46	19
A4 Ac C=O	168.99	22	169.53	16	169.05	19
α Ac C=O	169.31	22	169.86	11	169.21	19
γ Ac C=O	170.48	20	170.76	11	170.04	18

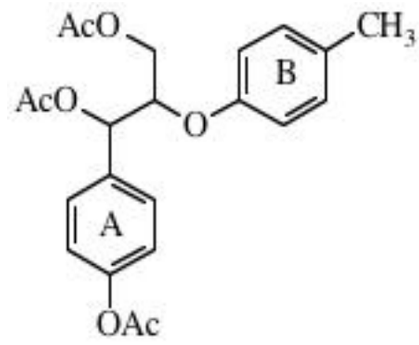
^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ Ac Me	1.94 (2.02)	s	
Aα Ac Me	2.06 (2.09)	s	
Bα	2.23 (2.28)	s	
A4 Ac Me	2.23 (2.28)	s	
γ1	4.23 (4.20)	dd	11.9, 4.2
γ2	4.34 (4.37)	dd	11.9, 6.0
β	4.83 (4.66)	m	
α	6.04 (6.04)	d	5.4
B 3,5	6.85 (6.77)	m	
B 2,6	7.08 (7.07)	m	
A 3,5	7.08 (7.07)	m	
A 2,6	7.51 (7.42)	d	8.7

Notes:

SRIX-62 25mg
1H CDCl3 shifts in ( )s
70% erythro
HSQC and HMBC in acetone

Compound Number 271



threo

H-b-H5t

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ Ac Me	1.94 (1.98)	s	
Aα Ac Me	2.01 (2.05)	s	
Bα	2.24 (2.28)	s	
A4 Ac Me	2.24 (2.28)	s	
γ1	4.01 (4.00)	dd	11.9, 5.8
γ2	4.23(4.26)	dd	11.9, 4.2
β	4.83 (4.64)	m	
α	6.10 (6.09)	d	6.4
B 3,5	6.90 (6.85)		
B 2,6	7.10 (7.07)		
A 3,5	7.10 (7.07)		
A 2,6	7.51 (7.42)	d	8.5

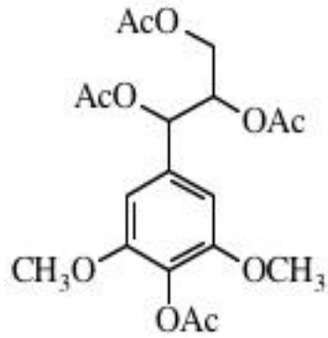
Notes:

SRIX-62 25mg
75% threo
1H CDCl3 shifts in ( )s

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bα	20.49	65	20.49	59	20.03	
Aγ Ac Me	20.64	54	20.55	54	20.39	
Aα Ac Me	20.97	65	20.88	57	20.64	
A4 Ac Me	21.08	75	20.94	72	20.77	
γ	62.68	56	63.27	53	62.23	
α	73.94	55	74.88	55	73.77	
β	78.49	64	79.27	76	77.74	
B3	116.48	124	117.24	104	116.09	
B5	116.48	124	117.24	104	116.09	
A3	121.78	118	122.67	109	121.81	
A5	121.78	118	122.67	109	121.81	
A2	128.47	141	129.33	124	128.37	
A6	128.47	141	129.33	124	128.37	
B2	130.04	154	130.74	137	129.81	
B6	130.04	154	130.74	137	129.81	
B1	131.37	29	131.66	22	130.33	
A1	133.81	33	135.22	25	134.04	
A4	150.84	28	151.94	21	150.36	
B4	156.33	24	157.59	20	156.12	
A4 Ac C=O	169.15	21	169.52	21	169.04	
α Ac C=O	169.73	24	170.04	19	169.41	
γ Ac C=O	170.57	24	170.68	17	169.98	

Compound Number 272



^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.99	s	
β Ac Me	2.01	s	
α Ac Me	2.08	s	
A4 Ac Me	2.21	s	
OMe	3.81	s	
γ1	3.91	dd	12.1, 6.2
γ2	4.23	dd	12.1, 3.8
β	5.41	m	
α	5.95	d	6.8
2,6	6.80	s	
CdCl3			
γ Ac Me	2.06	s	
β Ac Me	2.08	s	
α Ac Me	2.10	s	
A4 Ac Me	2.33	s	
OMe	3.83	s	
γ1	3.83		hidden
γ2	4.26	dd	12.1, 3.6
β	5.42	m	
α	5.92	d	7.6
2,6	6.61	s	

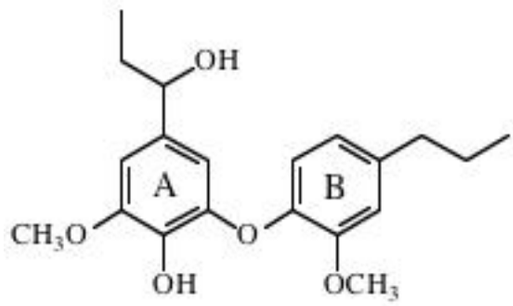
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.48	82	20.23	94	20.08	33
γ Ac Me	20.72	56	20.55	73	20.39	31
β Ac Me	20.85	74	20.71	80	20.46	29
α Ac Me	21.01	71	20.83	81	20.65	33
OMe	56.31	166	56.58	179	56.03	62
OMe	56.31	166	56.58	179	56.03	62
γ	62.17	45	62.85	65	61.92	14
β	72.24	46	72.99	73	71.73	16
α	73.78	47	74.45	60	73.17	16
2	104.05	97	104.76	125	103.59	33
6	104.05	97	104.76	125	103.59	33
4	129.13	9	129.79	8	127.83	8
1	134.19	30	135.85	28	134.79	15
3	152.45	45	153.30	48	151.64	29
5	152.45	45	153.30	48	151.64	29
A4 Ac C=O	168.51	20	168.42	22	167.93	13
α Ac C=O	169.67	22	170.00	23	169.43	23
β Ac C=O	170.09	24	170.21	22	169.43	23
γ Ac C=O	170.43	19	170.65	21	169.95	11
minor isomer						
γ	61.42		62.34			
β	72.48		72.99			
α	73.03		73.76			
2, 6	103.75		104.67			
1	134.19		135.63			
3, 5	152.27		153.19			

Notes:

L. Landucci XXII-138D7 19mg
2:1 mix of isomers

Compound Number 273



G-5-O-4-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	0.83	t	J = 7.3
Bγ	0.93	t	J = 7.3
Aβ,Bβ	1.62	m	
Bα	2.56	bt	J = 7.6
OMe	3.81	s	
OMe	3.86	s	
Aα	4.39	bt	J = 6.1
A6	6.45	d	J = 1.5
B6	6.70	dd	J = 8.1, 1.5
B5	6.75	d	J = 8.1
A2	6.76	d	J = 1.5
B2	6.94	d	J = 1.5
A4-OH	7.39	s	

^{13}C

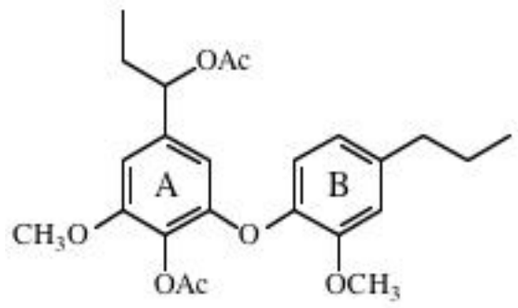
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Aγ	10.16	38	10.48	51	10.06	40
Bγ	13.85	47	14.05	49	13.68	40
Bβ	24.61	37	25.41	47	24.15	39
Aβ	31.83	34	33.20	43	32.05	30
Bα	37.87	37	38.33	50	38.50	34
B OMe	55.95	36	56.27	49	55.57	37
A OMe	56.29	34	56.56	49	55.91	37
Aα	75.94	30	75.40	27	73.36	30
A2	104.43	33	105.66	47	104.81	27
A6	109.38	34	109.81	49	108.57	28
B2	112.88	34	114.27	49	113.19	28
B5	119.57	33	119.64	48	118.00	29
B6	120.77	35	121.35	50	120.25	31
A4	136.18	12	137.28	9	135.77	23
A1	135.83	18	137.69	23	136.52	24
B1	139.42	17	139.25	21	137.60	24
B4	143.63	10	145.23	18	143.69	20
A5	144.59	11	145.44	18	144.24	20
A3	148.01	13	149.29	18	148.46	22
B3	150.27	13	151.45	20	149.79	21

Proton shifts in CDCl3	CDCl3 ppm	mult	CDCl3 J =
Aγ	0.86	t	7.6
Bγ	0.95	t	7.6
Aβ,Bβ	1.67	m	
Bα	2.56	bt	7.6
OMe	3.85	s	
OMe	3.91	s	
Aα	4.43	bt	6.6
A6	6.53	d	1.8
A2,B6	6.69	m	
B2	6.79	d	2.0
B5	6.88	d	8.1

Notes:

FPL Collection 11mg
Both A5 and A1 change order in CDCl3 compared to acetone-d6
B4 and A4 assignments taken from 2D in CDCl3
gHSQC and gHMBC in all solvents

Compound Number 274



G-5-O-4-G diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	0.82	t	J = 7.3
Bγ	0.93	t	J = 7.3
Bβ	1.64	m	
Aβ	1.73	m	
Aα Ac Me	1.96	s	
A4 Ac Me	2.18	s	
Bα	2.58	bt	J = 7.3
B OMe	3.76	s	
A OMe	3.84	s	
Aα	5.48	m	
A6	6.32	m	overlapped
B6	6.75	m	overlapped
A2	6.77	m	overlapped
B5	6.84	d	J = 8.1
B2	6.96	d	J = 1.7

^{13}C

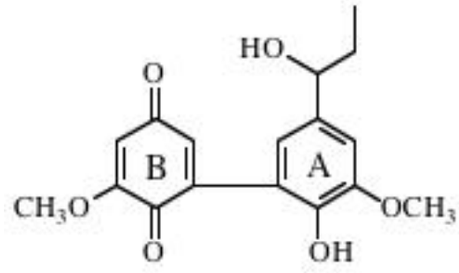
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Aγ	9.90	37	10.12	63	9.75	35
Bγ	13.81	36	14.00	64	13.63	32
A4 Ac Me	20.42	33	20.22	54	20.09	32
Aα Ac Me	21.19	31	20.94	50	20.78	31
Bβ	24.62	37	25.36	64	24.14	34
Aβ	29.31	36	30.11	60	28.91	27
Bα	37.87	36	38.36	64	37.05	31
B OMe	55.98	36	56.18	61	55.64	36
A OMe	56.22	36	56.56	63	56.17	30
Aα	76.92	35	77.23	60	76.07	22
A2	104.58	33	104.97	58	104.20	19
A6	108.53	33	107.93	58	106.52	25
B2	113.11	34	114.36	59	113.48	23
B6	120.49	34	121.58	64	120.55	25
B5	120.86	37	121.73	67	120.68	26
A4	129.59	8	129.57	8	128.30	11
A1	138.79	20	140.24	30	139.23	22
B1	139.73	18	141.00	28	139.90	22
B4	142.84	13	143.37	17	141.62	20
A5	150.39	14	151.63	19	150.02	16
B3	150.72	14	152.15	21	150.66	11
A3	152.46	15	153.60	20	152.18	17
A4 Ac C=O	168.48	12	168.46	19	168.05	19
Aα Ac C=O	170.26	15	170.25	19	169.76	17

Proton shifts in CDCl3	CDCl3		CDCl3
Aγ	0.84	t	J = 7.6
Bγ	0.95	t	J = 7.6
Bβ	1.65	m	
Aβ	1.76	m	
Aα Ac Me	2.03	s	
A4 Ac Me	2.24	s	
Bα	2.57	bt	J = 7.6
B OMe	3.80	s	
A OMe	3.85	s	
Aα	5.52	bt	J = 6.8
A6	6.38	d	J = 1.7
A2	6.63	d	J = 2.0
B6	6.69	dd	2.0, 8.1
B2	6.78	d	J = 1.7
B5	6.84	d	J = 8.1

Notes:

FPL Collection 6 mg
gHSQC and gHMBC in CDCl3 and acetone-d6
A4 upon acetylation appears as cluster of signals
in acetone-d6 B5 and B6 too close to assign definitively

Compound Number 275



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	10.21	28	10.64	45	10.30	29
β	31.90	24	33.21	38	32.03	24
B OMe	56.19	24	56.46	45	55.87	28
A OMe	56.39	28	56.84	44	56.57	27
α	75.72	22	75.40	30	73.45	26
B2	107.16	26	107.77	42	107.06	23
A2	109.43	25	110.91	43	110.48	20
A5	118.56	14	120.61	63	120.06	22
A6	120.19	26	120.61	63	119.35	22
B6	135.42	26	135.34	38	134.11	20
A1	136.30	19	138.14	32	136.85	23
A4	143.07	16	144.12	24	144.04	14
B5	142.53	14	144.79	24	142.84	19
A3	146.78	17	148.08	25	147.29	18
B3	159.02	15	160.27	26	159.09	18
B4	180.27	12	180.63	19	179.87	3
B1	187.51	17	188.03	25	187.39	16

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.91	t	J = 7.4
β	1.70	m	
A OMe	3.88	s	
B OMe	3.89	s	
α	4.50	bt	J = 6.4
B2	6.07	d	J = 2.2
B6	6.69	d	J = 2.2
A6	6.77	d	J = 1.7
A2	7.07	d	J = 1.7
A4-OH	7.76	s	
CDCl3			
γ	0.93	t	J = 7.6
β	1.76	m	
B OMe	3.86	s	
A OMe	3.93	s	
α	4.54	bt	J = 6.9
α OH	5.93		
B2	5.98	d	J = 2.2
A6	6.74	bd	J = 1.2
B6	6.83	d	J = 2.2
A2	6.98	bd	J = 1.2

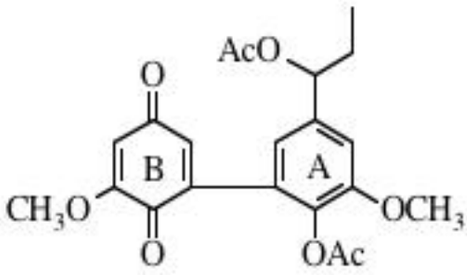
Proton shifts in DMSO

γ	0.82	t	J = 7.1
β	1.58	m	
OMe	3.80	s	
α	4.33	m	
α OH	5.06	d	J = 3.9
B2	6.14	d	J = 1.7
B6	6.61	d	J = 1.7
A6	6.64	s	
A2	6.96	s	
A4-OH	8.81	s	

Notes:

FPL Collection SRX-84 5 mg
gHSQC and gHMBC in all solvents, A5 is coincident with A6 in acetone-d6
B5 and A4 change order in CDCl3, A6 and A5 change order in DMSO
A and B OMe not definitively assigned in 13C DMSO-d6

Compound Number 276



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	10.06	60	10.22	29	9.84	13
A4 Ac Me	20.56	55	20.31	27	20.13	13
Aα Ac Me	21.28	55	21.02	26	20.88	15
β	29.33	61	30.13	01	28.85	9
A OMe	56.26	61	56.55	39	56.15	9
B OMe	56.53	59	56.91	28	56.60	9
α	77.29	60	77.01	27	75.82	6
B2	107.40	54	108.00	27	107.33	7
A2	112.23	50	112.42	26	111.63	6
A6	120.36	51	120.65	27	119.58	7
A5	126.86	46	128.45	9	127.00	5
B6	135.67	51	135.94	28	134.85	7
A4	137.30	27	138.05	5	136.35	3
A1	139.15	54	140.40	16	139.08	7
B5	141.95	39	142.79	9	141.15	5
A3	151.44	49	152.38	13	150.83	5
B3	158.88	47	159.98	10	158.74	4
A4 Ac C=O	168.19	46	168.42	10	167.88	6
Aα Ac C=O	170.44	46	170.38	10	169.95	8
B4	179.90	41	180.40	7	179.51	3
B1	186.98	45	187.46	11	186.80	5

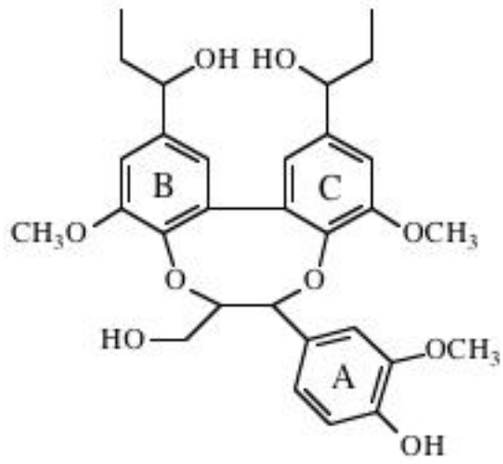
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.91	t	J = 7.3
β	1.88	m	
Aα Ac Me	2.06	s	
A4 Ac Me	2.11	s	
A OMe	3.87	s	
B OMe	3.89	s	
α	5.68	t	J = 6.9
B2	6.10	d	J = 2.2
B6	6.59	d	J = 2.2
A6	6.94	d	J = 1.7
A2	7.19	d	J = 1.7
CDCl3			
γ	0.93		
β	1.86		
Aα Ac Me	2.10		
A4 Ac Me	2.18		
A OMe	3.86		
α	5.66	t	J = 6.9
B2	5.99	d	J = 2.5
B6	6.70	d	J = 2.5
A6	6.81	d	J = 2.2
A2	7.00	d	J = 2.0

Notes:

FPL Collection SRX-84 5 mg
beta carbon shift taken from DEPT-135, obscured by solvent in 13C acetone-d6
Compound began to degrade after being taken up in CDCl3, shifts taken from mixture with unknown for CDCl3 and DMSO-d6

Compound Number 277



dibenzodioxicin

^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C γ	0.96	m	
B,C β	1.75	m	
Aγ1	3.48	m	
Aγ2	3.70	m	
OMe	3.77	s	
OMe	3.83	s	
OMe	3.92	s	
A β	4.03	m	
B,C α	4.60	m	
Aα	4.77	d	J = 10.0
A5	6.84	d	J = 8.1
A6	6.89	dd	J = 8.1, 1.7
C6	6.96	m	
A2	7.01	d	J = 1.7
B6	7.05	m	
C2	7.06, 7.08	d's	J = 2.0
B2	7.14, 7.16	d's	J = 2.0

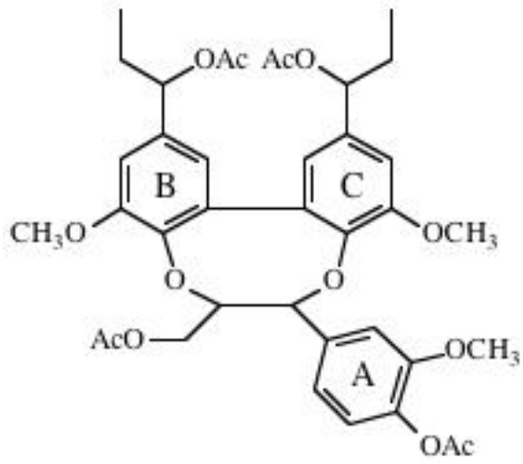
Notes:

SRVII-81 16mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B or C γ	10.34	97	10.71	60	10.39	32
B or C γ	10.38	97	10.77	60	10.49	31
B or C β	31.88	41	33.23	45	32.11	34
B or C β	32.08	48	33.30	45	32.11	34
OMe	55.78	108	56.06	50	55.54	31
A OMe	55.85	105	56.29	75	55.69	39
OMe	56.00	105	56.33	90	55.80	35
Aγ	62.97	47	62.97	32	60.66	16
B or C α	75.84	63	75.52	51	73.63	32
B or C α	75.84	63	75.52	51	73.63	32
Aα	84.82	38	85.18	29	83.34	13
A β	86.93	39	87.71	27	85.57	13
B2	108.86	23	110.17	19	109.45	16
C2	109.47	54	110.55	22	109.57	15
A2	109.47	54	111.94	38	111.82	18
A5	114.41	52	115.56	42	115.14	22
C6	118.92	41	119.26	31	117.93	21
B6	119.35	22	119.57	20	117.93	21
A6	120.90	52	121.33	41	120.11	17
A1	130.01	45	131.38	30	129.59	13
C5	133.19	15	133.24	14	131.87	10
B5	132.12	23	133.91	11	132.08	7
C1	141.36	21	143.38	18	142.41	12
B1	141.74	20	143.72	16	142.41	12
B4	144.75	22	145.95	16	144.87	9
C4	145.98	56	146.73	21	145.04	9
A4	145.98	56	147.43	35	146.31	20
A3	146.80	45	148.16	34	147.18	19
B3	151.72	22	152.75	15	151.68	21
C3	152.24	38	153.15	30	151.68	21
Proton shifts in CDCl3						
B,C γ	0.97					
B,C β	1.81					
Aγ	3.55					
OMe	3.76					
OMe	3.84					
OMe	3.92					
A β	4.14					
A,B,C α	4.59					
DMSO						
B,C γ	0.90					
B,C β	1.66					
Aγ1	3.22					
Aγ2	3.86					
A β	3.84					
B,C α	4.47					
Aα	4.81					

Compound Number 278



^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C γ	0.93	m	
B,C β	1.91	m	
γAc Me	1.91	s	
B,C α AcMe	2.07	s	
A4 Ac Me	2.24	s	
OMe	3.79	s	
OMe	3.94	s	
γ1	4.05	dd	J = 12.0, 3.4
β	4.30	m	
γ2	4.43	dd	J = 12.0, 3.4
α	4.93	d	J = 10.0
B,C α	5.71	m	
A5,A,B,C6	7.00-7.06	m	from HSQC
B or C 2	7.09	m	from HSQC
B or C 2	7.13	m	from HSQC
A2	7.17	m	from HSQC

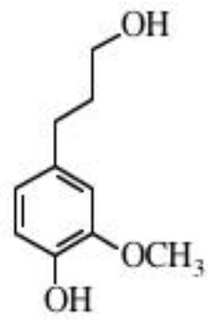
Notes:

SRVII-81Ac
gHSQC and gHMBC in d6-acetone and CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bγ	10.19	90	10.43	66	10.02	40
Cγ	10.19	90	10.43	66	10.02	40
A4 Ac Me	20.74	98	20.50	71	20.36	42
AαAc Me	20.84	75	20.58	61	20.42	37
B Ac Me	21.40	85	21.10	63	20.90	34
C Ac Me	21.40	85	21.10	63	20.90	34
B or C β	29.28	31	30.08	20	28.75	26
B or C β	29.38	33	30.43	18	29.22	23
OMe	56.10	84	56.19	53	55.74	55
OMe	56.17	70	56.32	77	55.94	61
OMe	56.22	84	56.38	62	56.02	47
Aγ	63.93	41	64.33	33	63.14	28
B or Cα	77.26	24	77.49	31	76.34	32
B or Cα	77.51	24	77.62	30	76.39	32
A β	82.76	24	83.41	25	81.80	17
Aα	84.45	25	85.33	27	84.06	21
B or C2	110.27	20	110.79	15	109.96	18
B or C2	111.03	20	111.19	14	110.43	16
A2	111.51	32	112.78	34	112.08	26
B or C6	119.26	14	119.35	12	118.00	10
B or C6	119.74	14	120.00	16	118.71	12
A6	119.91	49	120.74	33	119.98	26
A5	122.76	43	123.46	39	122.61	35
B or C5	132.63	23	133.22	13	131.58	10
B or C5	132.63	23	133.42	13	131.77	14
A1	137.13	45	138.06	20	136.45	29
B or C1	137.28	26	138.57	14	137.33	15
B or C1	137.28	26	138.75	14	137.60	12
A4	139.95	39	140.80	22	139.23	34
B4	146.17	18	146.86	14	145.13	17
C4	146.57	16	147.24	13	145.55	22
A3	151.32	33	152.14	27	150.63	39
B or C3	152.32	27	153.35	22	151.98	19
B or C3	152.52	36	153.53	19	152.16	20
A4 Ac C=O	168.84	46	168.94	33	168.47	43
BorCAcC=O	170.48	27	170.45	28	169.89	44
BorCAcC=O	170.58	26	170.45	28	169.92	44
Aγ Ac C=O	170.76	44	170.74	30	170.07	50
Proton shifts in CDCl3	CDCl3					
B,C γ	0.94					
B,C β	1.88					
Ac Me	1.97					
Ac Me	2.08					
Ac Me	2.12					
Ac Me	2.30					
OMe	3.74					
OMe	3.82					
OMe	3.90					
γ1	4.08					
β	4.14					
γ2	4.49					
α	4.85					
B,C α	5.70					
aromatic H	6.87-7.05					

Compound Number 279



dihydro-coniferyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.78 (1.86)	m	
α	2.60 (2.63)	bt	J = 8.0
γ	3.55 (3.67)	bt	J = 5.4
OMe	3.82 (3.86)	s	
6	6.64 (6.68)	dd	J = 8.1, 1.7
5	6.73 (6.70)	d	J = 8.1
2	6.81 (6.81)	d	J = 1.7
DMSO			
β	1.66		
α	2.48		
γ	3.40		
OMe	3.73		
γ OH	4.40		
6	6.55		
5	6.65		
2	6.72		
phenolic OH	8.60		

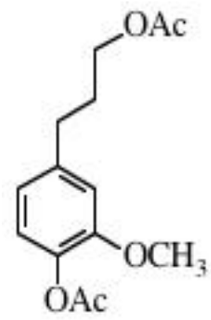
Notes:

J. Ralph 16 mg
gHSQC, gHMBC in d6-acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	31.72	24	32.44	33	32.62	26
β	34.43	24	35.85	27	35.99	26
OMe	55.84	25	56.21	31	56.95	30
γ	62.22	25	61.83	28	61.58	28
2	111.03	22	112.87	28	113.96	24
5	114.27	25	115.59	30	116.67	26
6	120.90	24	121.55	32	121.71	26
1	133.70	11	134.61	14	134.38	19
4	143.72	12	145.47	14	145.77	20
3	146.43	10	148.17	10	148.77	17

Compound Number 280



dihydro-coniferyl alcohol diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.94	m	
γ Ac Me	1.99	s	
A4 Ac Me	2.21	s	
α	2.68	bt	J = 7.8
OMe	3.79	s	
γ	4.05	t	J = 6.6
6	6.78	dd	J = 8.1, 1.7
5	6.94	d	J = 8.1
2	6.97	d	J = 1.7
CDCl3			
β	1.95	m	
γ Ac Me	2.05	s	
A4 Ac Me	2.29	s	
α	2.67	bt	J = 7.8
OMe	3.81	s	
γ	4.10	t	J = 6.6
6	6.75	bdd	8.1, 1.5
2	6.78	bs	
5	6.93	d	J = 8.1

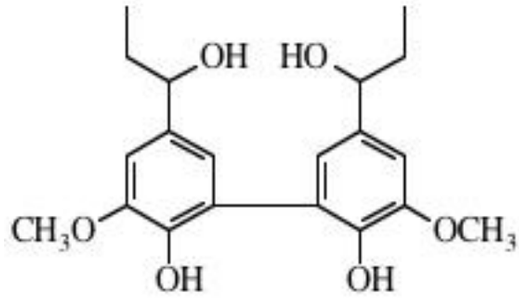
Notes:

JRalph 25mg
gHSQC, gHMBC in d6-acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.49	65	20.79	36	20.31	46
γ Ac Me	20.78	52	20.50	44	20.61	47
β	30.02	80	31.08	50	29.67	45
α	32.03	79	32.63	54	31.34	41
OMe	55.68	81	56.14	52	55.59	48
γ	63.63	79	64.10	54	63.21	48
2	112.45	61	113.63	46	112.76	42
6	120.30	83	121.05	54	120.06	44
5	122.43	79	123.39	52	122.41	46
4	137.84	25	139.17	14	137.45	25
1	140.06	47	141.27	27	140.14	33
3	150.77	36	152.14	18	150.60	32
A4 Ac C=O	169.01	27	169.07	18	168.56	29
γAc C=O	170.94	23	171.00	15	170.38	25

Compound Number 281



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	10.40	45	10.70	52	10.33	36
β	31.89	39	33.21	44	32.06	25
OMe	56.22	49	56.43	60	55.81	37
α	76.08	39	75.70	30	73.71	21
2	108.03	35	109.18	39	108.28	17
6	121.13	36	121.81	43	120.58	19
5	124.15	20	126.11	15	125.54	16
1	136.76	32	138.09	31	136.43	22
4	142.08	22	143.38	16	142.10	18
3	147.47	25	148.56	22	147.36	21

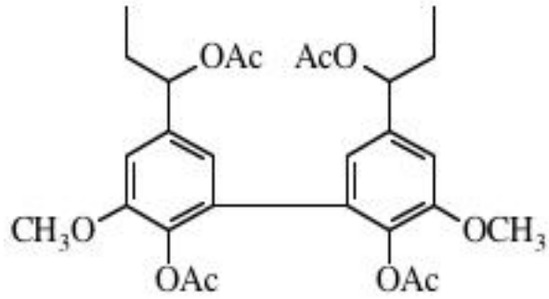
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.91	t	J = 7.3
β	1.71	m	
OMe	3.88	s	
α	4.50	t	J = 6.36
6	6.85	d	J = 2.0
2	6.99	d	J = 2.0
CDCl3			
γ	0.93	t	J = 7.3
β	1.79	m	
OMe	3.92	s	
α	4.54	t	J = 6.36
6	6.87	d	J = 2.0
2	6.93	d	J = 2.0
DMSO			
γ	0.84	t	J = 7.34
β	1.60	m	
OMe	3.81	s	
α	4.34	bs	
α OH	4.98	s	
6	6.66	d	J = 1.71
2	6.87	d	J = 1.71
4-OH	8.20	s	

Notes:

FPL Collection 10 mg
Compound has plane of symmetry

Compound Number 282



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	10.01	46	10.27	61	9.81	41
4 Ac Me	20.37	55	20.33	71	19.99	52
α Ac Me	21.23	43	21.04	63	20.82	42
β	29.46	34	30.20	70	28.90	30
OMe	56.10	48	56.46	66	56.04	40
α	76.86	49	77.29	56	76.03	30
2	110.14	29	110.87	44	110.20	19
6	120.24	19	120.41	24	118.88	13
5	131.15	20	131.87	26	130.12	22
4	137.00	14	137.91	17	136.15	18
1	138.66	21	140.04	31	138.82	23
3	151.37	24	152.64	38	151.14	27
Ac C=O	168.76	15	168.99	18	168.33	14
α Ac C=O	170.36	25	170.46	35	169.84	30

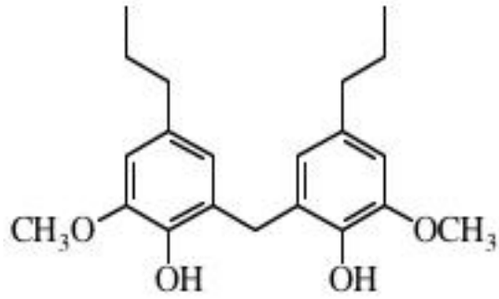
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.91 (0.86)	t	J = 7.34
β	1.87 (1.81)	m	
4 Ac Me	2.03 (2.02)	s	
α Ac Me	2.07 (2.07)	s	
OMe	3.87 (3.81)	s	
α	5.63 (5.58)	t	J = 6.6
6	6.79 (6.67)	bs	
2	7.11 (7.11)	bs	
CDCl3			
γ	0.90	t	J = 7.34
β	1.85	m	
4 Ac Me	2.08	s	
α Ac Me	2.09	s	
OMe	3.86	s	
α	5.63	t	J = 6.7
6	6.81	d	J = 1.7
2	6.90	d	J = 1.7

Notes:

FPL Collection 8mg
1H DMSO shifts in ( )s. Compound has plane of symmetry
beta shifts in acetone taken from DEPT 135 spectrum
g-HSQC, g-HMBC all solvents

Compound Number 283



biphenyl methane

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.87 (0.91)	t	J = 7.34
β	1.53 (1.57)	m	J = 7.34
α	2.41 (2.46)	dd	J = 7.34
OMe	3.79 (3.85)	s	
CH2	3.94 (3.93)	bs	
6	6.57 (6.55)	bd	J = 1.71
2	6.63 (6.61)	bd	J = 1.71
OH	7.23 (6.00)	bs	
DMSO			
γ	0.82	t	J = 7.34
β	1.47	m	J = 7.34
α	2.35	bt	
OMe	3.75	s	
CH2	3.74	s	
6	6.37	bd	J = 1.71
2	6.59	bd	J = 1.71
OH	8.22	s	

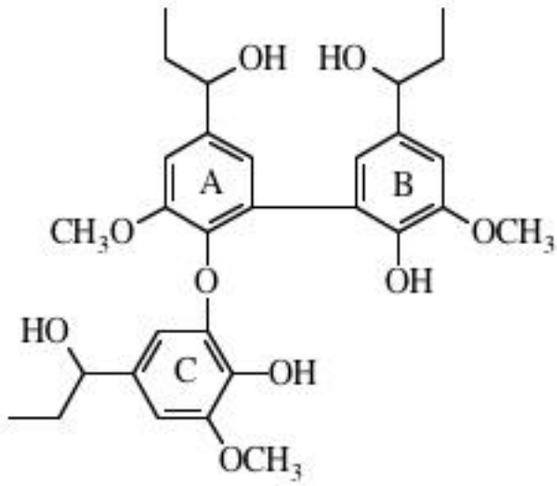
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	13.78	39	14.04	47	13.59	23
β	24.79	32	25.57	45	24.34	20
CH2	29.39	20	29.56	34	28.74	10
α	27.80	38	38.42	49	37.10	21
OMe	55.93	43	56.27	49	55.73	23
2	109.14	39	110.18	37	109.62	17
6	122.36	33	123.13	45	121.77	18
5	126.13	22	127.59	31	127.08	17
1	134.02	18	133.74	31	132.02	18
4	141.01	13	142.84	30	141.72	14
3	146.41	21	147.75	29	147.05	15

Notes:

FPL Collection 20 mg
1H CDCl3 shifts in ( )s. Plane of symmetry runs through molecule
CH2 shift obscured by solvent in acetone, taken from Dept 135
2 and 6 switch places in 1H in CDCl3

Compound Number 284



^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C γ	0.76	m	
A γ	0.96	t	
B,C β	1.53	m	
A β	1.74	m	
OMe	3.75	s	
OMe	3.81	s	
C α	4.23 (4.25)	t	J = 6.36
B α	4.35 (4.40)	t	J = 6.36
A α	4.60 (4.63)	t	J = 6.36
C6	6.18 (6.14)	d	J = 1.7
C2	6.52 (6.41)	bd	J = 1.7
B6	6.75 (6.76)	d	J = 1.7
B2	6.86 (6.78)	d	J = 1.7
A6	6.98 (6.97)	d	J = 1.7
A2	7.11 (7.04)	d	J = 1.7

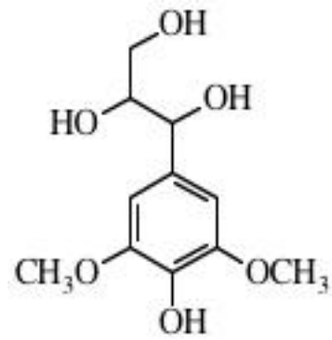
Notes:

FPL Collection 5 mg
1H--CDCl3 shifts in ( )s. g-HSQC and g-HMBC all solvents
Obscured 1H shifts taken from g-HSQC in CDCl3
A1 and B4 may switch order in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	10.15	84	10.51	64	9.95	46
γ	10.25	100	10.59	74	10.06	39
γ	10.30	88	10.59	74	10.26	43
B β	31.42	59	32.97	45	32.06	61
C β	31.48	69	33.11	44	32.06	61
A β	32.00	66	33.27	56	32.06	61
OMe	56.15	108	55.34	81	55.68	60
OMe	56.15	108	55.34	81	55.74	51
OMe	56.30	75	56.52	43	55.83	65
A α	75.80	74	75.42	46	73.51	40
B α	75.80	74	75.57	45	73.60	39
C α	76.02	56	75.66	40	73.66	35
C2	103.82	17	104.50	32	103.06	16
C6	106.66	17	106.31	30	104.51	20
B2	108.03	27	109.13	31	108.35	17
A2	109.45	47	110.37	36	109.50	20
B6	120.98	35	121.58	36	120.18	19
A6	121.20	35	122.17	46	121.16	17
B5	123.38	11	124.87	13	124.13	18
A5	132.06	14	133.71	16	132.72	16
C4	134.74	16	135.37	14	133.50	24
C1	135.22	20	136.74	19	135.41	18
B1	136.04	15	137.33	26	135.91	21
A4	141.12	6	141.12	9	139.14	14
B4	142.24	22	143.44	17	142.18	17
A1	142.01	20	143.71	19	142.47	23
C5	145.59	13	147.29	19	146.54	19
B3	146.79	22	148.14	23	147.28	19
C3	147.44	21	148.53	16	147.59	23
A3	152.39	19	153.21	17	151.70	18
1H--DMSO						
B,C γ	0.66					
A γ	0.88					
B,C β	1.40					
Aβ	1.65					
B,C α	4.13					
A α	4.45					
C6	6.02					
C2	6.45					
B6	6.59					
B2	6.82					
A6	6.88					
A2	7.04					
C4 OH	7.93					
B4 OH	8.14					

Compound Number 285



α-(4-hydroxy-3,5-dimethoxyphenyl)-glycerol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	3.63	d	J = 6.11
β	3.72	m	
OMe	3.81	s	
α	4.60	d	J = 6.11
2,6	6.71	s	
4 OH	7.09	bs	
CDCl3			
γ	3.77		
β	3.81		
OMe	3.91		
α	4.77		
2,6	6.64		
DMSO			
γ	3.42		
β	3.49		
OMe	3.72		
α	4.34		
2,6	6.58		

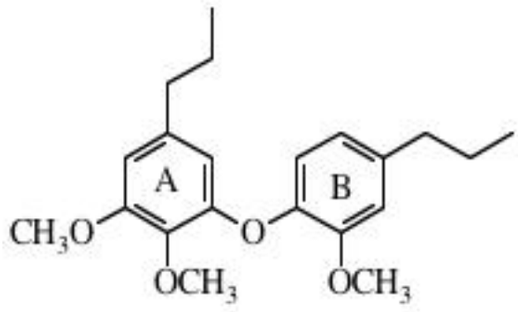
Notes:

FPL Collection 20 mg
Marginally soluble in CDCl3 and acetone-d6, g-HSQC and g-HMBC in all solvents
1H shifts for β and γ taken from HSQC in DMSO
β and α 13C shifts change order in DMSO (HSQC data)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.40	47	56.60	13	55.99	49
OMe	56.40	47	56.60	13	55.99	49
γ	63.24	19	64.24	6	63.10	20
β	74.69	20	76.26	9	75.49	20
α	75.99	22	76.26	9	74.24	20
2	103.03	42	105.32	12	104.72	39
6	103.03	42	105.32	12	104.72	39
1	131.60	10	133.98	4	133.58	18
4	134.57	10	135.90	3	134.31	19
3	147.28	20	148.32	7	147.42	34
5	147.28	20	148.32	7	147.42	34

Compound Number 286



^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	0.85	t	7.3
Bγ	0.93	t	7.3
Aβ	1.52	m	7.3
Bβ	1.64	m	7.3
Aα	2.41	bt	7.3
Bα	2.57	bt	7.3
A4 OMe	3.74	s	
B3 OMe	3.78	s	
A3 OMe	3.83	s	
A6	6.17	d	2.0
A2	6.58	d	2.0
B6	6.72	dd	1.7, 8.1
B5	6.78	d	8.1
B2	6.95	d	1.7

Notes:

SRX-110

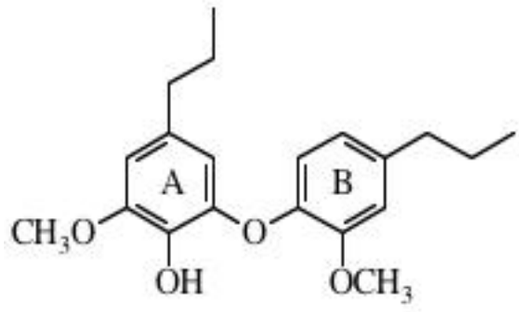
12 mg

α,β,γ and B3, A5 are too close to assign with certainty
HSCQ and HMBC all solvents

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Aγ	13.67	29	13.93	10	13.54	38
Bγ	13.78	32	14.04	11	13.70	36
Aβ	24.42	28	25.26	10	24.08	33
Bβ	24.57	32	25.39	11	24.18	34
Bα	37.80	35	38.36	12	37.08	33
Aα	37.99	29	38.58	10	37.28	30
OMe	55.95	33	56.24	10	55.70	31
OMe	56.04	30	56.38	10	55.88	31
A4 OMe	60.94	22	60.67	7	60.21	26
A2	107.18	27	108.19	10	107.36	25
A6	111.16	27	111.12	10	109.83	26
B2	113.01	23	114.37	9	113.43	27
B5	119.20	27	120.54	10	119.39	28
B6	120.55	28	121.41	10	120.50	28
A4	137.70	5	138.59	2	136.89	11
A1	138.19	15	138.86	4	137.90	20
B1	138.63	14	139.80	4	138.71	20
B4	143.82	9	144.64	3	142.89	17
B3	150.37	9	151.82	3	150.31	34
A5	150.48	10	151.94	3	150.31	34
A3	153.27	10	154.67	3	153.26	18
1H-CDCl3						
γ	0.88					
γ	0.95					
Aβ	1.55					
Bβ	1.65					
Aα	2.43					
Bα	2.56					
B3 OMe	3.83					
A 3,4 OMe	3.87					
A6	6.26					
A2	6.47					
B6	6.68					
B 2,5	6.79					
1H-DMSO						
γ	0.82					
γ	0.90					
β	1.47					
β	1.60					
Aα	2.37					
Bα	2.53					
A4 OMe	3.67					
B3 OMe	3.73					
A3 OMe	3.79					
A6	6.09					
A2	6.58					
B6	6.70					
B5	6.75					
B2	6.94					

Compound Number 287



4-O-5

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.85	t	7.3
γ	0.98	t	7.3
A β	1.52	m	7.3
B β	1.62	m	7.3
A α	2.41	bt	7.3
B α	2.55	bt	7.3
B OMe	3.80	s	
A OMe	3.83	s	
A6	6.25	d	2.0
A2	6.58	d	2.0
B6	6.69	dd	1.7, 8.3
B5	6.74	d	8.3
B2	6.92	d	1.7

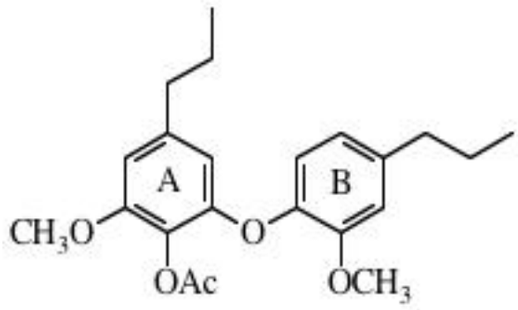
Notes:

FPL Collection
12 mg
A5 and B4 may be switched in acetone but confirmed in CDCl3 by 4-OH correlation to A5

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	13.49	63	13.91	38	13.48	31
γ	13.63	61	14.04	39	13.67	32
β	24.44	72	25.42	53	24.17	59
β	24.47	73	25.42	53	24.17	59
α	37.67	120	38.34	60	36.96	37
α	37.67	120	38.34	60	36.98	39
OMe	55.81	63	56.28	37	55.57	28
OMe	56.04	59	56.57	36	55.90	29
A2	107.05	57	108.23	36	107.39	23
A6	111.46	58	112.07	37	110.95	23
B2	112.75	60	114.27	34	113.17	24
B5	119.17	30	119.60	34	117.84	24
B6	120.53	61	121.37	33	120.27	25
A1	133.56	24	133.80	21	132.29	20
A4	134.79	20	136.58	10	135.22	19
B1	138.87	29	139.23	18	137.53	19
B4	143.84	19	145.27	14	143.77	16
A5	144.28	18	145.58	12	144.34	18
A3	147.59	20	149.43	13	148.71	19
B3	150.10	22	151.43	16	149.71	18
^{1}H CDCl3						
γ	0.80					
γ	0.86					
A β	1.47					
B β	1.56					
A α	2.35					
B α	2.47					
B OMe	3.78					
A OMe	3.80					
4 OH	5.94					
A6	6.30					
A2	6.41					
B6	6.60					
B5	6.71					
B2	6.78					
^{1}H DMSO						
γ	0.80					
γ	0.87					
A β	1.45					
B β	1.57					
A α	2.34					
B α	2.49					
B OMe	3.74					
A OMe	3.76					
A6	6.11					
A2	6.53					
B6	6.57					
B5	6.64					
B2	6.89					
4 OH	8.39					

Compound Number 288



4-O-5

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.86	t	7.3
Bγ	0.93	t	7.3
A β	1.53	m	7.3
B β	1.64	m	7.3
Ac Me	2.20	s	
A α	2.45	bt	7.3
B α	2.57	bt	7.3
B OMe	3.77	s	
A OMe	3.81	s	
A6	6.18	d	1.7
A2	6.63	d	1.7
B6	6.73	dd	2.0, 8.3
B5	6.82	d	8.3
B2	6.96	d	2.0

Notes:

SRX-110BAc

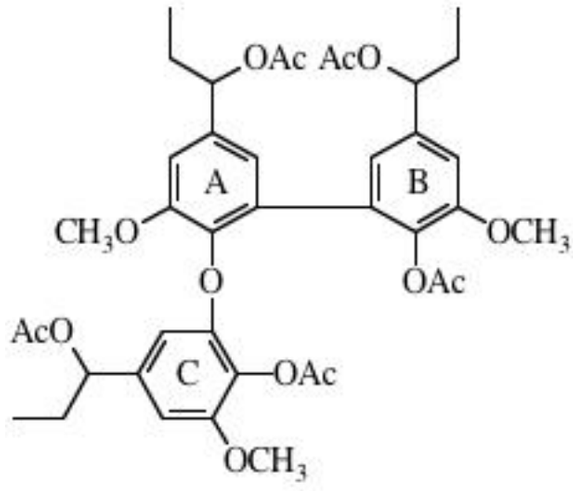
12 mg

α, β, γ shifts are too close to assign with absolute certainty
B2 and B5 change order in CDCl3 1H

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A γ	13.73	43	13.94	34	13.52	40
B γ	13.78	38	14.02	32	13.61	40
Ac Me	20.39	32	20.25	27	20.05	36
A β	24.33	38	25.22	31	24.00	36
B β	24.57	37	25.37	33	24.09	38
B α	37.83	36	38.37	32	37.03	32
A α	38.23	37	38.73	32	37.36	32
B OMe	56.08	62	56.24	30	55.63	37
A OMe	56.08	62	56.44	32	55.96	36
A2	106.59	36	107.26	31	106.58	26
A6	110.36	36	110.24	30	108.99	26
B2	113.16	35	114.39	28	113.39	28
B5	120.40	36	121.55	63	120.23	30
B6	120.82	36	121.55	63	120.53	21
A4	128.18	9	129.04	5	127.29	15
B1	139.36	20	140.62	14	139.39	16
A1	141.02	21	141.66	15	140.63	28
B4	143.25	15	143.86	9	142.07	22
A5	150.12	16	151.45	9	149.76	23
B3	150.73	17	152.14	11	150.53	25
A3	152.11	17	153.44	10	151.94	25
OAc C=O	168.70	14	168.57	9	168.04	19
1H--CDCl3						
γ	0.89					
γ	0.95					
A β	1.55					
B β	1.65					
Ac Me	2.24					
A α	2.45					
B α	2.56					
B OMe	3.82					
A OMe	3.82					
A6	6.25					
A2	6.49					
B6	6.68					
B2	6.78					
B5	6.85					
1H--DMSO						
γ	0.81					
γ	0.88					
A β	1.47					
B β	1.58					
Ac Me	2.15					
A α	2.39					
B α	2.51					
B OMe	3.70					
A OMe	3.74					
A6	6.09					
A2	6.62					
B6	6.69					
B5	6.74					
B2	6.92					

Compound Number 289



^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.78		
γ	0.82		
B γ	0.91		
A,C β	1.73		
B β	1.88		
AcMe Cα	1.95		
AcMe Aα	2.04		
AcMe Bα	2.05		
AcMe B4	2.10		
AcMe C4	2.16		
OMe	3.73		
OMe	3.76		
OMe	3.81		
Cα	5.46		
Aα	5.55		
Bα	5.65		
C6	6.20		
C2	6.64		
B6	6.81		
A6	6.83		
A2	6.99		
B2	7.13		

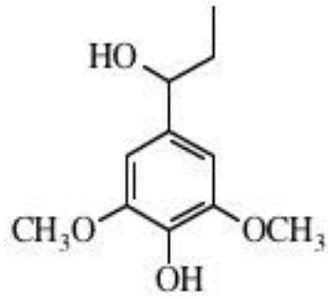
Notes:

FPL Collection 2 mg
COSY, HSQC and HMBC in acetone at 600MHz
1H in CDCl3 some shifts taken from HSQC and HMBC
Aromatic carbon shifts in DMSO are weak, no 2D spectra in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	9.79	39	10.19	65	9.57	63
γ	9.85	35	10.19	65	9.57	63
γ	9.90	40	10.19	65	9.57	63
C4AcMe	20.21	32	20.18	27	19.77	27
B4AcMe	20.32	26	20.18	27	19.88	23
AαAcMe	21.12	25	20.46	20	20.59	18
CαAcMe	21.16	36	21.25	40	20.68	27
BαAcMe	21.22	29	21.36	27	20.80	29
β	28.94	17	29.77	20	28.50	22
β	29.21	12	29.97	20	28.68	15
B β	29.46	25	30.18	20	28.84	24
OMe	56.00	46	56.38	46	55.89	34
OMe	56.00	46	56.38	46	55.89	34
OMe	56.07	32	56.65	32	55.89	34
α	76.83	27	77.28	35	75.94	37
α	76.88	27	77.28	35	75.94	37
α	76.88	27	77.28	35	75.94	37
C2	103.60	8	104.30	12	103.38	8
C6	105.82	11	106.11	10	106.53	8
A2	110.40	16	110.99	14	110.12	8
B2	110.70	15	111.63	12	110.88	11
B6	120.30	12	119.42	12	119.39	6
A6	120.78	14	120.81	15	119.64	15
C4	128.02	3	128.90	7	127.11	7
A5	130.86	8	131.83	8	130.23	8
B5	131.77	12	133.47	6	130.83	6
A4	136.95	6	137.91	7	136.20	10
B1	137.84	7	139.40	10	138.03	10
A1	138.16	16	139.65	13	138.31	15
C1	138.16	16	139.65	13	138.50	10
B4	140.05	6	140.78	8	138.96	9
C5	150.42	8	151.59	10	149.99	4
A3	151.11	9	152.36	9	150.84	13
B3	152.20	20	153.33	14	151.80	14
C3	152.20	20	153.33	14	151.80	14
C4AcC=O	167.92	8	167.62	7	167.29	8
B4AcC=O	168.77	9	169.09	8	168.23	9
AαAcC=O	170.30	12	169.09	9	169.71	18
CαAcC=O	170.40	17	170.37	12	169.71	18
BαAcC=O	170.40	17	170.50	15	169.71	18
1H CDCl3	1H				1H	
γ	0.72				0.71	
γ	0.79				0.78	
B γ	0.89				0.86	
β	1.72				1.67	
β	1.72				1.67	
B β	1.86				1.84	
AcMe Cα	1.99				1.92	
AcMe Aα	2.07				|	
AcMe Bα	2.10				|	
AcMe B4	2.16				|	
AcMe C4	2.21				2.15	
OMe	3.71				3.67	
OMe	3.74				3.72	
OMe	3.79				3.76	
Cα	5.45				5.42	
Aα	5.54				5.49	
Bα	5.63				5.61	
C6	6.13				6.03	
C2	6.46				6.62	
B6	6.82				6.70	
A6	6.76				6.70	
A2	6.81				6.99	
B2	6.87				7.13	

Compound Number 290



1-(3,5-dimethoxy-4-hydroxy)-propanol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.87	t	7.3
β	1.66	m	
OMe	3.79	s	
α	4.44	bt	6.4
2,6	6.63	s	
4 OH	6.99	s	
<u>CDCl3</u>			
γ	0.91		
β	1.75		
OMe	3.88		
α	4.50		
2,6	6.57		
<u>DMSO</u>			
γ	0.79		
β	1.56		
OMe	3.72		
α	4.30		
2,6	6.54		
4 OH	8.08		

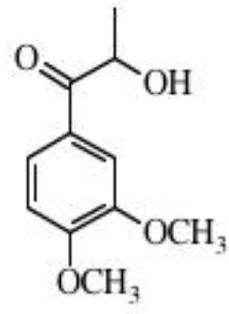
Notes:

FPL Collection
22 mg
HSQC and HMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	10.19	27	10.61	47	10.32	25
β	31.87	27	33.24	36	32.16	21
OMe	56.23	57	56.59	93	55.95	48
OMe	56.23	57	56.59	93	55.95	48
α	76.20	24	75.81	29	73.92	20
2	102.60	45	104.32	87	103.33	35
6	102.60	45	104.32	87	103.33	35
4	133.91	11	135.66	11	134.10	14
1	135.87	16	137.56	22	136.44	17
3	146.91	23	148.41	25	147.65	31
5	146.91	23	148.41	25	147.65	31

Compound Number 291



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	22.77	60	22.59	67	21.09	67
OMe	55.97	68	56.14	89	55.54	63
OMe	56.06	60	56.24	81	55.75	62
β	68.78	57	69.53	46	68.31	62
5	110.13	59	111.62	80	110.89	105
2	110.68	52	111.95	77	110.89	105
6	123.32	62	124.22	81	123.31	68
1	126.16	8	127.80	9	127.38	15
3	149.25	8	150.30	9	148.61	12
4	153.96	7	155.01	7	153.11	10
α	200.73	10	201.30	8	200.09	15

^{1}H (acetone)

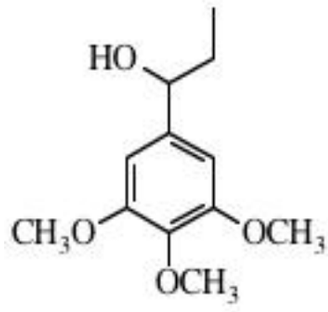
Atom	H Shifts	Mult	J
γ	1.35	d	6.85
OMe	3.87	s	
OMe	3.90	s	
β	5.14	q	6.85
5	7.06	d	8.6
2	7.54	d	2.0
6	7.68	dd	8.6, 2.0
CDCl3			
γ	1.43		
OMe	3.92		
OMe	3.93		
β	5.10		
5	6.89		
2	7.49		
6	7.49		

1H--DMSO	
γ	1.27
OMe	3.81
OMe	3.84
β	5.05
β OH	5.21
5	7.06
2	7.48
6	7.69

Notes:

SRX-115G 26 mg
HSQC in acetone and CDCl3, HMBC in acetone
HSQC shows that C2 is downfield of C5 for acetone and CDCl3
C2 = C5 in DMSO

Compound Number 292



1-(3,4,5-trimethoxyphenyl)-1-propanol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.89	t	7.3
β	1.67	m	
4 OMe	3.68	s	
OMe	3.79	s	
α	4.12	d	4.0
α OH	4.48	bt	6.4
2,6	6.65	s	
CDCl3			
γ	0.93		
β	1.76		
4 OMe	3.82		
OMe	3.86		
α	4.52		
2,6	6.58		
DMSO			
γ	0.81		
β	1.56		
4 OMe	3.60		
OMe	3.73		
α	4.35		
αOH	5.08		
2,6	6.59		

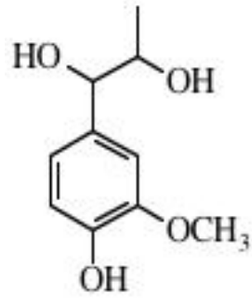
Notes:

SRX-115S
39 mg
HSQC and HMBC in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	10.06	46	10.58	79	10.29	90
β	31.84	66	33.20	83	32.08	91
OMe	55.86	97	56.32	142	55.78	183
OMe	55.86	97	56.32	142	55.78	183
4 OMe	60.57	24	60.44	38	59.98	60
α	75.80	34	75.69	55	73.81	92
2	102.68	113	104.06	144	103.00	179
6	102.68	113	104.06	144	103.00	179
4	136.84	3	137.95	3	136.05	9
1	140.60	9	142.75	12	142.09	30
3	152.96	16	154.08	14	152.55	38
5	152.96	16	154.08	14	152.55	38

Compound Number 293



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
major						
γ	18.34	55	18.08	82	18.42	41
OMe	56.83	67	56.20	74	55.56	52
β	72.25	46	72.03	65	70.67	38
α	78.37	49	78.15	66	76.83	40
2	110.18	52	111.20	70	111.04	30
5	115.09	53	115.09	70	114.65	34
6	120.61	54	120.32	74	119.26	36
1	133.49	10	134.95	14	134.56	22
4	146.17	10	146.39	11	145.16	20
3	147.55	7	147.81	8	146.97	16
minor isomer						
γ	19.67	19	19.30	33	19.00	16
OMe	56.83	67	56.20	74	55.56	52
β	73.15	19	72.68	25	70.89	16
α	80.27	17	79.80	26	77.79	14
2	110.12	25	111.27	34	111.12	15
5	115.16	26	115.21	31	114.76	17
6	120.90	22	120.66	29	119.50	14
1	134.08	4	134.90	9	133.98	10
4	146.40	4	146.77	4	145.46	9
3	147.61	4	148.02	4	147.04	9

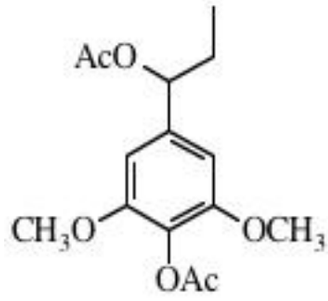
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.02 (0.92)	d	6.4
β	3.81 (3.69)	m	
OMe	3.80 (3.80)	s	
α	4.45 (4.20)	d	5.1 (7.3)
5	6.73 (6.73)	d	8.1
6	6.77 (6.77)	dd	8.1, 1.7
2	6.98 (6.95)	d	1.7
<u>CDCl3</u>			
γ	1.03 (0.96)		
β	3.87 (3.74)		
OMe	3.81 (3.81)		
α	4.49 (4.20)		
<u>DMSO</u>			
γ	0.93 (0.77)		
β	3.56 (3.56)		
OMe	3.69 (3.69)		
α	4.20 (4.09)		
5,6	6.64 (6.64)		
2	6.83 (6.81)		

Notes:

FPL Collection 20 mg
g-HSQC and g-HMBC in d6-acetone
2 isomers ^{1}H minor shifts and j's in ( )

Compound Number 294



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	10.01	40	10.29	66	9.93	59
4 Ac Me	20.41	32	20.26	47	20.14	57
α Ac Me	21.20	26	21.04	37	20.90	54
β	29.30	50	30.13	112	28.96	50
OMe	56.10	88	56.45	135	55.98	116
OMe	56.10	88	56.45	135	55.98	116
α	77.26	49	77.61	71	76.49	52
2	103.29	97	103.86	121	102.85	93
6	103.29	97	103.86	121	102.85	93
4	128.18	3	129.21	3	127.27	11
1	138.92	11	140.45	14	139.33	38
3	152.01	17	153.13	14	151.60	55
5	152.01	17	153.13	14	151.60	55
4 Ac C=O	168.65	6	168.55	10	168.14	27
α Ac C=O	170.25	5	170.39	8	169.89	24

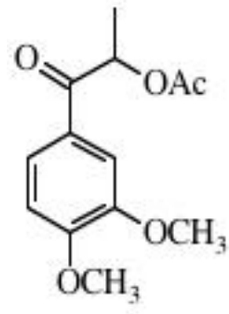
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.88	t	7.3
β	1.83	m	
α Ac Me	2.05	s	
4 Ac Me	2.21	s	
OMe	3.80	s	
α	5.61	dd	7.3
2,6	6.71	s	
CDCl3			
γ	0.91		
β	1.85		
Ac Me	2.09		
Ac Me	2.33		
OMe	3.82		
α	5.62		
2,6	6.58		
DMSO			
γ	0.85		
β	1.80		
Ac Me	2.07		
Ac Me	2.22		
OMe	3.74		
α	5.56		
2,6	6.68		

Notes:

SRX-115SSMAc
19 mg
C4 has very long T1, D1 set to 6 sec.

Compound Number 295



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	17.40	60	17.70	61	17.32	48
AcMe	20.69	42	20.60	38	20.42	38
OMe	55.92	68	56.12	65	55.55	46
OMe	56.03	59	56.25	58	55.80	43
β	70.95	57	71.98	53	71.13	45
5	110.10	58	111.66	75	110.45	37
2	110.66	56	111.69	75	111.05	44
6	122.92	61	123.75	61	123.08	44
1	127.29	14	128.23	10	126.48	11
3	149.23	10	150.39	8	148.83	10
4	153.70	10	154.98	8	153.57	10
Ac C=O	170.35	11	170.47	7	169.78	10
α	195.21	12	195.54	7	194.95	11

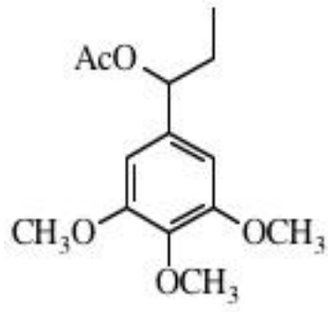
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.46	d	6.85
AcMe	2.05	s	
3 OMe	3.86	s	
4 OMe	3.90	s	
β	5.97	q	6.85
5	7.06	d	8.6
2	7.50	d	2.0
6	7.67	dd	8.6, 2.0
CDCl3			
γ	1.53		
AcMe	2.15		
OMe	3.93, 3.96		
β	5.96		
5	6.91		
2	7.52		
6	7.59		
DMSO			
γ	1.40		
AcMe	2.06		
OMe	3.81, 3.85		
β	5.99		
5	7.08		
2	7.43		
6	7.68		

Notes:

SRX-115GAc
12 mg
g-HSQC and g-HMBC in d6-acetone

Compound Number 296



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	9.92	60	10.30	53	9.90	46
α Ac Me	21.13	38	21.05	29	20.89	32
β	29.20	59	30.13	53	28.90	42
3 OMe	55.98	120	56.43	96	55.86	83
5 OMe	55.98	120	56.43	96	55.86	83
4 OMe	60.63	38	60.45	31	59.91	29
α	77.41	63	77.75	49	76.60	44
2	103.58	117	104.71	76	103.49	77
6	103.58	117	104.71	76	103.49	77
1	136.12	18	137.56	11	136.39	16
4	137.45	5	138.71	4	136.85	4
3	153.08	24	154.32	14	152.80	20
5	153.08	24	154.32	14	152.80	20
α Ac C=O	170.26	10	170.37	6	169.83	9

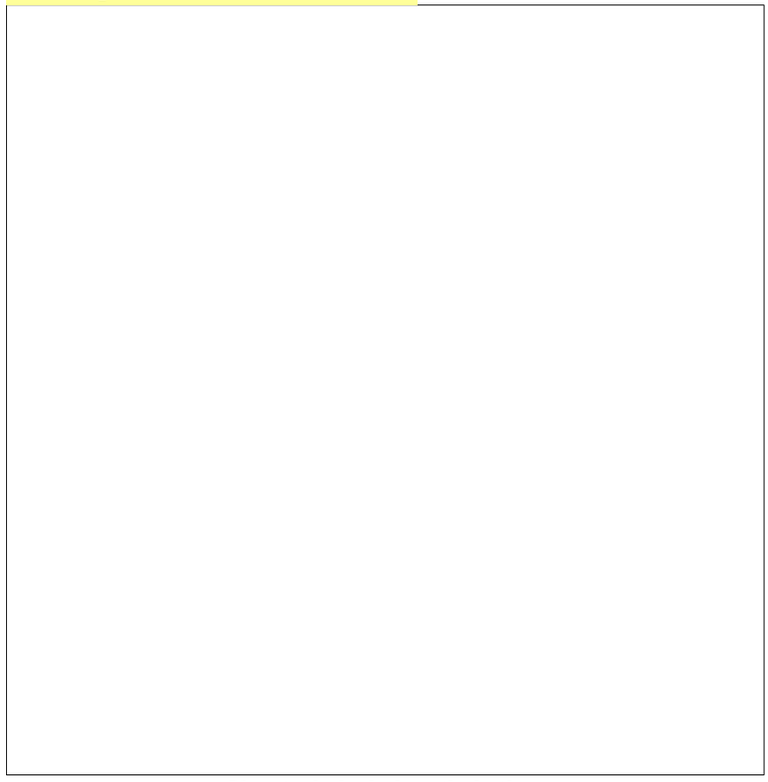
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.86	t	7.3
β	1.82	m	
α Ac Me	2.03	s	
4 OMe	3.69	s	
3,5 OMe	3.81	s	
α	5.56	bt	6.6
2,6	6.64	s	
CDCl3			
γ	0.90		
β	1.85		
α Ac Me	2.09		
4 OMe	3.83		
3,5 OMe	3.87		
α	5.59		
2,6	6.55		
DMSO			
γ	0.82		
β	1.77		
α Ac Me	2.05		
4 OMe	3.63		
3,5 OMe	3.76		
α	5.52		
2,6	6.60		

Notes:

SRX-115SAc
29mg
g-HMBC in d6-acetone

Compound Number 297



Veratryl alcohol methyl ether

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.80	61	56.03	58	55.37	126
OMe	55.89	57	56.12	56	55.46	117
α OMe	57.86	27	57.74	28	57.15	60
α	74.61	44	74.86	45	73.55	106
2 or 5	110.84	49	112.49	47	111.45	141
5 or 2	110.99	49	112.60	46	111.50	146
6	120.29	51	120.95	48	120.03	128
1	130.73	7	132.16	8	130.65	19
3 or 4	148.58	4	149.89	5	148.23	12
4 or 3	149.02	4	150.34	5	148.64	13

^{1}H (acetone)

Atom	H Shifts	Mult	J
α OMe	3.27	s	
OMe	3.78	s	
OMe	3.79	s	
α-CH_2	4.33	s	
6	6.83	dd	8.1, 2.0
5	6.89	d	8.1
2	6.91	d	2.0
CDCl3			
α-CH_2	4.37		
5	6.81		
6	6.85		
2	6.87		
DMSO			
α-CH_2	4.31		
6	6.83		
2	6.89		
5	6.90		

Notes:

S. Ralph
Carbon pairs 2 & 5 and 3 & 4 are to close for definitive assignment

Compound Number 298

3-Methoxy-4-hydroxy stilbene carboxylic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.38	s	
A2	6.50	d	2.0
A5	6.71	d	8.1
A6	6.80	dd	8.1, 2.0
B 2,6	7.27	m	
B4	7.36	m	
B 3,5	7.43	m	
α	7.80	s	
CDCl3			
A2	6.41		
A5	6.77		
A6	6.83		
B 2,6	7.29		
B4, B 3,5	7.37, 7.41		
α	7.87		
DMSO			
A2	6.41		
A5	6.64		
A6	6.66		
B 2,6	7.19		
B4, B 3,5	7.35, 7.41		
α	7.66		

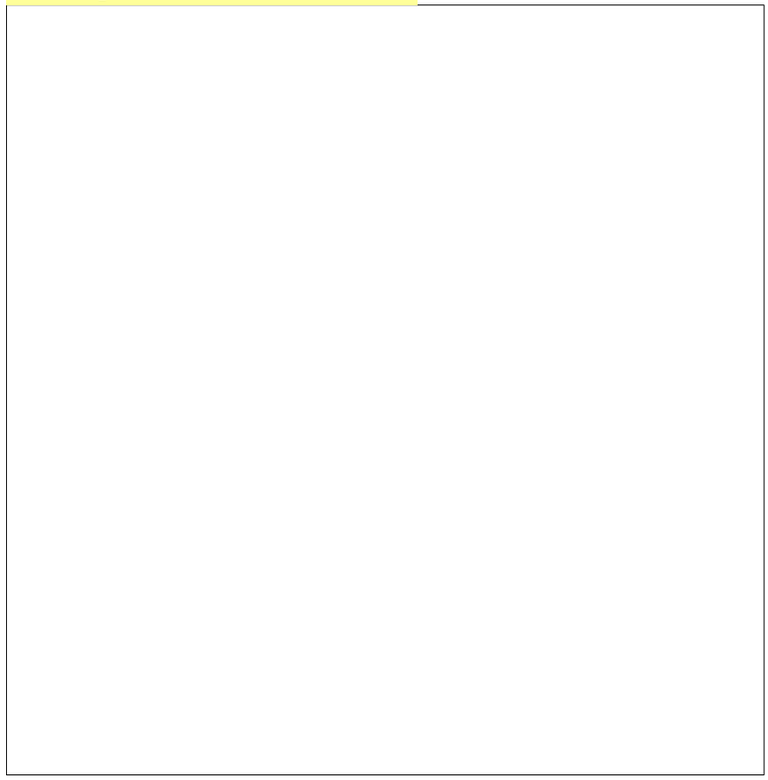
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.25	29	55.42	31	54.61	36
A2	112.07	36	113.60	30	113.05	29
A5	114.19	37	115.58	34	115.11	29
A6	126.78	41	126.69	34	125.35	30
A1	126.73	14	127.30	7	125.35	20
B4	127.90	39	128.25	34	127.28	30
B3	128.91	75	129.48	64	128.59	63
B5	128.91	75	129.48	64	128.59	63
β	128.91	75	130.55	7	129.64	9
B2	130.03	73	130.81	65	129.66	76
B6	130.03	73	130.81	65	129.66	76
B1	136.18	8	138.15	5	137.15	15
α	142.49	30	141.18	30	139.52	25
A3	145.76	7	147.68	5	146.88	14
A4	147.37	11	148.91	8	148.05	18
γ	172.08	6	169.12	7	168.58	16

Notes:

FPL - Pearl Collection
30 mg, beta under B3,5 shift from APT experiment, HSQC and HMBC all solvents
Some 1H shifts taken from HSBC expt.s

Compound Number 299



beta-O-4, 5-O-4 trimer

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	0.79 (0.79)	t	7.3
Bγ	0.94 (0.97)	t	7.3
Bβ--Aβ	1.6-1.75 (1.66-1.76)	m	
Cγ Ac Me	1.78 (1.86)	d	1.0
Aα Ac Me	1.93 (2.01)	s	
Cα Ac Me	2.08 (2.10)	s	
C4 Ac Me	2.20 (2.28)	s	
Bα	2.60 (2.59)	m	
C OMe	3.70 (3.69)	d	2.2
B OMe	3.74 (3.72)	s	
A OMe	3.82 (3.76)	s	
Cγ1	4.21 (4.26)	dd	4.2, 11.7
Cγ2	4.41 (4.47)	dd	5.9, 11.7
Cβ	4.98 (4.90)	m	
Aα	5.44 (5.44)	t	7.3
Cα	6.13 (6.14)	d	4.4
A6	6.24 (6.27)	bs	
A2	6.69 (6.52)	bs	
B6	6.80 (6.70)	dd	2.0, 8.1
B5	6.90 (6.80)	d	8.1
C6	6.97 (6.92)		
C5	6.98 (6.91)		
B2	6.99 (6.77)		
C2	7.15 (7.02)	bs	

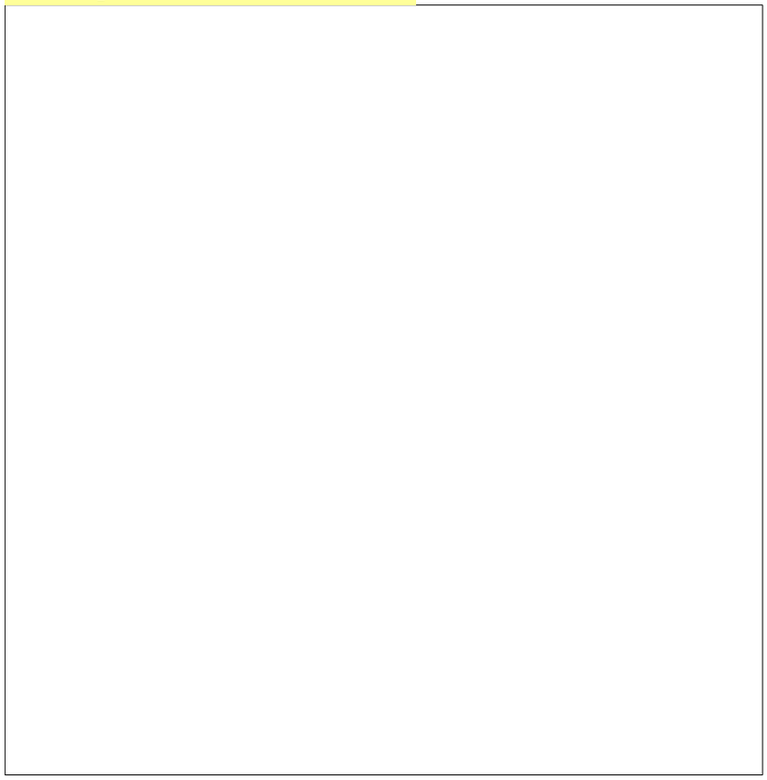
Notes:

SR X 125D1-2
B5 and B6 change order in CDCl3
1H shifts in CDCl3 in ( )s after acetone shift
C6, C5 and B2 shifts from HSQC

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Aγ	9.83	64	10.08	43		
Bγ	13.85	53	14.04	38		
C4 Ac Me	20.68	89	20.46	55		
Cγ Ac Me	20.68	89	20.53	32		
α Ac Me	21.03	55	20.89	44		
α Ac Me	21.19	51	20.95	41		
Bβ	24.63	79	25.38	55		
Aβ	29.27	76	30.02	98		
Bα	37.89	87	38.39	62		
OMe	55.63	70	56.11	62		
OMe	55.75	82	56.11	62		
A OMe	56.01	83	56.42	49		
Cγ	62.77	56	63.39	55		
Cα	74.22	75	75.20	37		
Aα	77.03	68	77.30	51		
Cβ	80.66	55	81.27	41		
A2	104.53	55	105.23	39		
A6	108.03	39	107.60	26		
C2	111.51	44	112.18	46		
B2	112.97	58	114.27	62		
C6	119.46	62	120.06	55		
B6	120.75	57	121.57	57		
B5	120.43	81	121.75	31		
C5	122.30	75	123.25	58		
A4	135.88	39	136.38	6		
C1	136.35	38	136.94	12		
A1	136.35	38	137.60	8		
C4	139.38	28	140.66	4		
B1	139.64	31	140.90	10		
B4	142.32	24	143.02	5		
B3	150.58	27	152.04	17		
C3	150.78	31	152.04	17		
A5	150.98	32	152.12	8		
A3	153.40	32	154.40	10		
C4 Ac C=O	168.98	29	168.91	9		
Cα Ac C=O	169.67	32	169.96	8		
Aα Ac C=O	170.28	32	170.17	7		
Cγ Ac C=O	170.93	30	170.66	7		

Compound Number 300



5-O-4 diacetovanillone

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aβ	2.49 (2.48)	s	
Bβ	2.53 (2.56)	s	
OMe	3.93 (3.95)	s	
OMe	3.95 (3.99)	s	
B5	6.78 (6.85)	d	8.3
A6	7.30 (7.28)	d	2.0
A2	7.47 (7.41)	d	2.0
B6	7.56 (7.49)	dd	8.3, 2.0
B2	7.64 (7.63)	d	2.0
DMSO			
Aβ	2.49		
Bβ	2.55		
OMe	3.90		
OMe	3.92		
B5	6.67		
A6	7.25		
A2	7.42		
B6	7.54		
B2	7.59		
A4-OH	10.00		

^{13}C

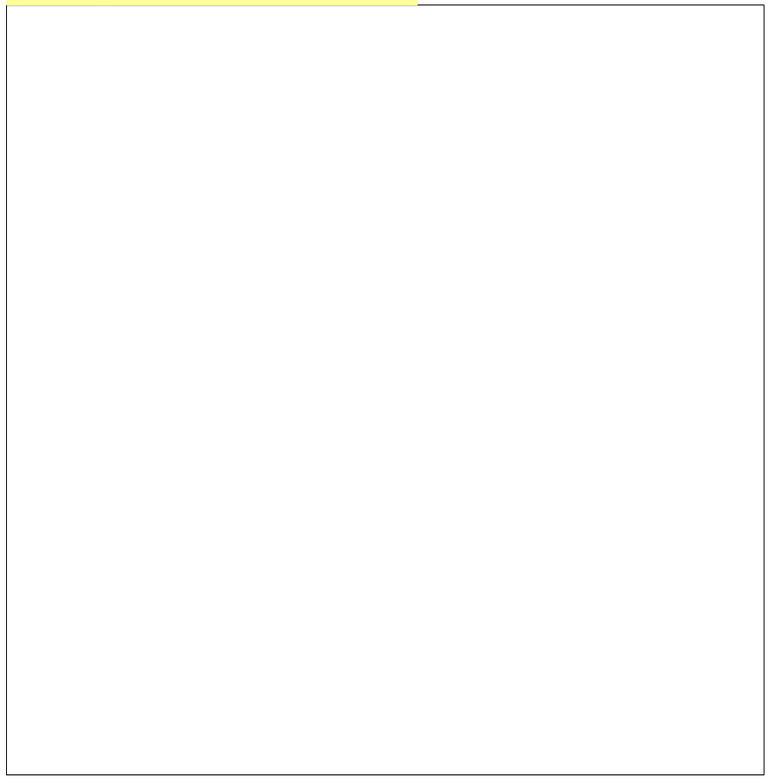
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Aβ	25.92	49	26.33	44	26.32	55
Bβ	26.09	46	26.47	43	26.51	44
B OMe	56.17	68	56.36	49	55.79	49
A OMe	56.50	66	56.76	49	56.23	47
A2	107.30	65	108.56	45	108.09	35
B2	112.30	47	112.68	44	111.65	34
A6	114.80	61	115.45	47	114.62	34
B5	116.82	47	116.80	44	115.44	34
B6	122.48	75	123.22	47	122.51	38
A1	129.24	16	129.73	13	127.91	26
B1	133.33	9	133.65	12	132.01	18
A5	142.21	6	143.16	8	141.97	15
A4	142.41	10	144.09	7	143.37	19
A3	148.16	10	149.67	9	148.83	17
B3	150.08	9	150.73	9	149.09	20
B4	150.43	10	151.69	8	150.44	14
Aα	195.70	10	195.93	11	195.87	18
Bα	196.37	9	196.55	10	196.50	17

Notes:

SRX-146C

A4-OH has strong HMBC correlations in DMSO to A3,4 ,5

Compound Number 301



guaiacyl chalcone

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.93 (3.87)	bs	
B5	6.83 (6.83)	d	8.3
A5	6.93 (6.97)	d	8.3
B6	7.29 (7.28)	dd	1.7, 8.3
B2	7.49 (7.49)	d	1.7
A2	7.61 (7.61)	d	1.7
γ	7.63 (7.63)	d	15.4
β	7.76 (7.76)	d	15.4
A6	7.80 (7.80)	dd	1.7, 8.3
CDCl3			
OMe	3.93	s	
OMe	3.95	s	
5	6.93	d	8.3
5	6.97	d	8.3
B2	7.10	d	1.96
B6	7.20	dd	1.96, 8.3
β	7.37	d	15.4
A2	7.61	d	obscured
A6	7.62	dd	obscured
γ	7.73	d	15.4

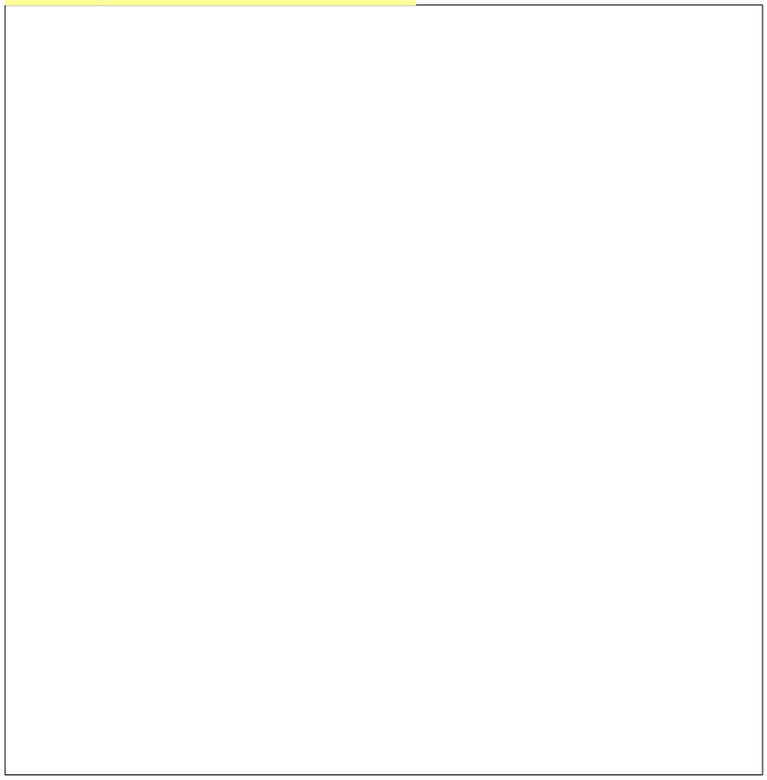
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.99	108	56.34	45	55.70	45
OMe	56.09	122	56.40	42	55.84	45
B2	110.07	126	111.95	50	111.79	26
A2	110.50	125	112.05	49	111.57	25
A5	113.71	121	115.36	35	114.92	31
B5	114.85	126	116.14	33	115.60	33
β	119.25	122	119.87	47	118.71	33
6	123.13	130	124.15	56	123.55	32
6	123.49	146	124.21	54	123.70	35
B1	127.62	18	128.33	7	126.51	25
A1	131.22	12	131.84	7	129.85	21
γ	144.33	122	144.36	47	143.60	36
A3	146.79	15	148.54	5	147.78	17
B3	146.85	15	148.74	4	147.96	17
B4	148.12	20	150.10	5	149.41	23
A4	150.21	22	152.17	4	151.66	22
α	188.62	13	187.90	7	187.02	19

Notes:

FPL collection
A2 and B2 change order in DMSO
1H DMSO chemical shifts in ( )'s
13C C6 shift assignments not confirmed, also C5s in CDCl3

Compound Number 302



3,4,5-trimethoxy cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
4 OMe	3.69 (3.81)	s	
3,5 OMe	3.82 (3.83)	s	
OH	3.89	t	5.4
γ	4.21 (4.28)	dt	1.5, 5.4
β	6.32 (6.24)	dt	15.9, 5.2
α	6.53 (6.50)	bt	15.9, 1.5
2,6	6.72 (6.57)	s	
DMSO			
4 OMe	3.64		
3,5 OMe	3.78		
γ	4.10		
β	6.33		
α	6.47		
2,6	6.72		

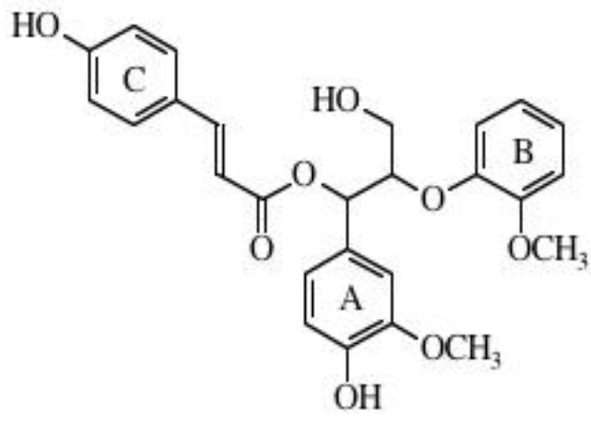
Notes:

S. Ralph

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
3 OMe	55.99	145	56.33	140	55.78	70
5 OMe	55.99	145	56.33	140	55.78	70
4 OMe	60.85	45	60.53	37	59.99	28
γ	63.47	70	63.17	67	61.43	31
2	103.47	109	104.55	146	103.43	60
6	103.47	109	104.55	146	103.43	60
α	128.04	70	130.11	71	128.55	31
β	130.92	66	130.32	66	130.16	31
1	132.40	16	133.87	11	132.65	17
4	137.78	4	138.76	3	136.83	6
3	153.22	26	154.41	22	152.94	26
5	153.22	26	154.41	22	152.94	26

Compound Number 1001



threo

3-(4-Hydroxyphenyl)acrylic acid3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.51	dd	7.2, 5.3
γ2	3.68	dd	7.2, 3.7
β	4.58	m	
α	6.16	d	7.3
C β	6.30	d	16.0
C α	7.51	d	15.6

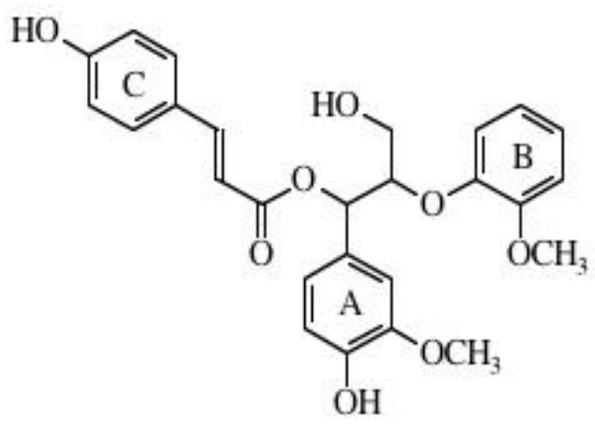
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.25			
OMe			56.31			
γ			61.76			
α			75.88			
β			85.20			
A2			112.04			
B2			113.58			
A5			115.58			
C β			115.81			
C3			116.64			
C5			116.64			
B5			119.36			
A6			121.23			
B6			121.78			
B1			123.24			
C1			127.04			
A1			130.16			
C2			130.91			
C6			130.91			
C α			145.39			
A4			147.48			
A3			148.18			
B4			149.82			
B3			151.87			
C4			160.48			
C γ			166.51			

Compound Number 1002



erythro

3-(4-Hydroxyphenyl)acrylicacid 3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.68	dd	11.7, 4.8
γ2	3.79	dd	11.8, 5.7
β	4.66	m	
α	6.12	d	4.8
C β	6.35	d	16.0
C α	7.56	d	16.0

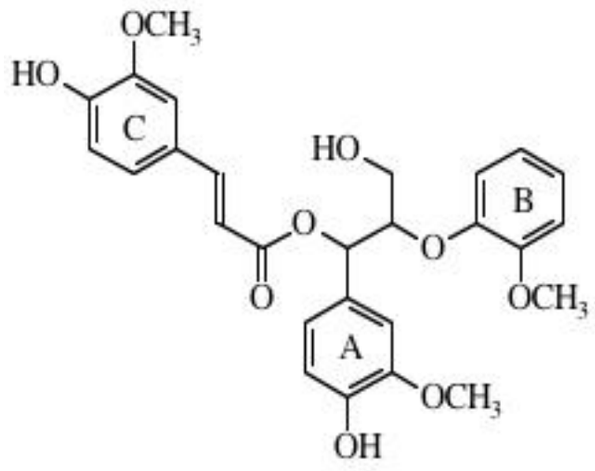
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.29			
OMe			56.29			
γ			61.49			
α			75.08			
β			84.09			
A2			112.57			
B2			113.67			
A5			115.21			
C β			115.62			
C3			116.67			
C5			116.67			
B5			119.18			
B6			121.75			
A6			121.79			
B1			123.31			
C1			126.97			
A1			129.64			
C2			130.96			
C6			130.96			
C α			145.65			
A4			147.35			
A3			147.99			
B4			149.22			
B3			151.86			
C4			160.59			
C γ			166.32			

Compound Number 1003



threo

3-(4-Hydroxy-3-methoxyphenyl)acrylicacid3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.52	dd	11.9, 5 .3
γ2	3.69	dd	11.9, 3.8
β	4.58	m	
α	6.16	d	2.3
C β	6.34	d	15.9
C α	7.49	d	15.9

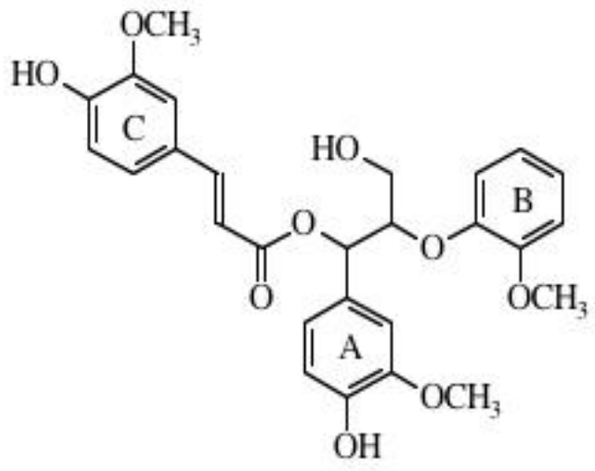
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.22			
OMe			56.31			
OMe			56.31			
γ			61.74			
α			75.87			
β			85.13			
C2			111.26			
A2			112.04			
B2			113.54			
A5			115.59			
C β			115.99			
C5			116.03			
B5			119.25			
A6			121.20			
B6			121.76			
B1			123.21			
C6			123.91			
C1			127.44			
A1			130.15			
C α			145.77			
A4			147.50			
A3			148.19			
C3			148.70			
B4			149.78			
C4			150.02			
B3			151.82			
C γ			166.55			

Compound Number 1004



erythro

3-(4-Hydroxy-3-methoxyphenyl)acrylic acid3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ 1	3.60	dd	11.7, 4.8
γ 2	3.79	dd	11.5, 5.8
β	4.67	m	
α	6.13	d	4.8
C β	6.39	d	15.9
C α	7.55	d	15.9

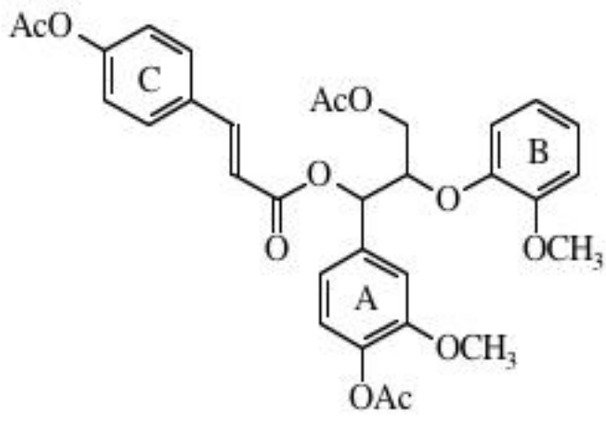
Notes:

R. Helm
CDCl3 column is D2O/Acetone-d6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
	Acet /D2O					
OMe	56.30		56.28			
OMe	56.31		56.30			
OMe	56.33		56.32			
γ	61.38		61.48			
α	75.10		75.09			
β	84.00		84.02			
C2	111.32		111.29			
A2	112.64		112.60			
B2	113.68		113.66			
A5	115.17		115.22			
Cβ	115.84		115.83			
C5	116.01		116.04			
B5	119.07		119.10			
B6	121.77		121.96			
A6	121.82		121.80			
B1	123.28		123.30			
C6	124.00		123.99			
C1	127.40		127.40			
A1	129.62		129.63			
C α	146.02		146.02			
A4	147.32		147.36			
A3	147.97		147.98			
C3	148.72		148.71			
B4	149.23		149.19			
C4	150.08		150.09			
B3	151.85		151.84			
C γ	166.35		166.34			

Compound Number 1005



threo

3-(4-Acetoxyphenyl)acrylic acid 3-acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.08	dd	11.9, 5.6
γ2	4.31	dd	11.9, 4.1
β	4.89	m	
α	6.24	d	6.6
C β	6.52	d	16.0
C α	7.63	d	16.0

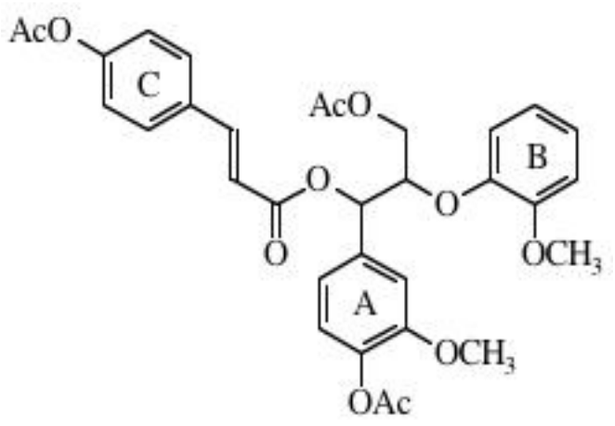
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.44			
Ac Me			20.60			
Ac Me			20.94			
OMe			56.16			
OMe			56.32			
γ			63.70			
α			75.81			
β			80.87			
A2			112.71			
B2			113.66			
Cβ			118.76			
B5			119.33			
A6			120.31			
B6			121.65			
C3			123.21			
C5			123.21			
A5			123.61			
B1			123.78			
C2			130.22			
C6			130.22			
C1			132.82			
A1			136.74			
A4			140.95			
C α			144.91			
B4			149.12			
B3			151.89			
A3			152.24			
C4			153.52			
C γ			165.90			
Ac C=O			168.86			
Ac C=O			169.42			
Ac C=O			170.69			

Compound Number 1006



erythro

3-(4-Acetoxyphenyl) acrylic acid 3-acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ 1	4.29	dd	11.9, 4.4
γ2	4.41	dd	11.9, 6.1
β	4.93	m	
α	6.22	d	4.7
C β	6.61	d	16.1
C α	7.71	d	16.1

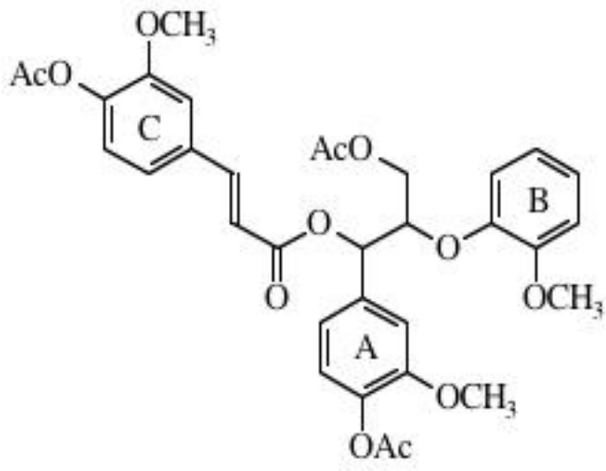
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.45			
Ac Me			20.61			
Ac Me			20.94			
OMe			56.22			
OMe			56.30			
γ			63.16			
α			74.96			
β			80.44			
A2			112.79			
B2			113.80			
C β			118.67			
B5			119.89			
A6			120.45			
B6			121.68			
C3			123.24			
C5			123.24			
A5			123.40			
B1			124.08			
C2			130.28			
C6			130.28			
C1			132.82			
A1			136.63			
A4			140.83			
C α			145.12			
B4			148.39			
B3			152.06			
A3			152.14			
C4			153.58			
C γ			165.79			
Ac C=O			168.89			
Ac C=O			169.42			
Ac C=O			170.75			

Compound Number 1007



threo

3-(4-Acetoxy-3-methoxyphenyl) acrylic acid 3-acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.09	dd	11.9, 5.6
γ2	4.30	dd	11.9, 4.1
β	4.89	m	
α	6.24	d	6.5
C β	6.56	d	
C α	7.60	d	15.8

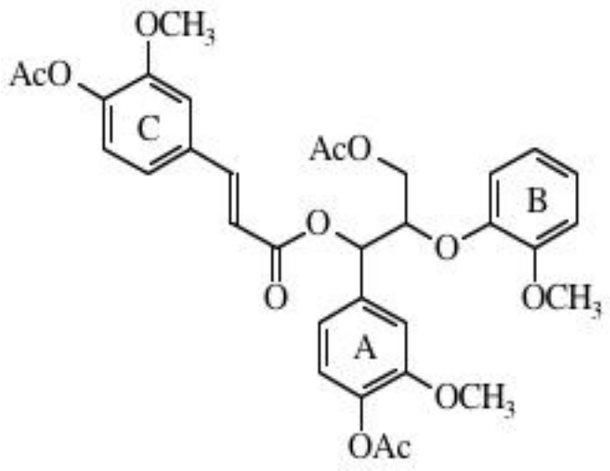
Notes:

R. Helm
16mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.44			
Ac Me			20.44			
Ac Me			20.60			
OMe			56.16			
OMe			56.32			
OMe			56.40			
γ			63.70			
α			75.82			
β			80.88			
C2			112.42			
A2			112.72			
B2			113.65			
C β			118.85			
B5			119.30			
A6			120.30			
B6			121.65			
C6			122.27			
A5			123.61			
B1			123.77			
C5			124.12			
C1			134.15			
A1			136.77			
A4			140.95			
C4			142.76			
C α			145.36			
B4			149.13			
B3			151.88			
A3			152.24			
C3			152.67			
C γ			165.96			
Ac C=O			168.79			
Ac C=O			168.86			
Ac C=O			170.69			

Compound Number 1008



erythro

3-(4-Acetoxy-3-methoxyphenyl) acrylic acid 3-acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.28	dd	11.8, 4.4
γ2	4.40	dd	11.8, 6.1
β	4.96	m	
α	6.22	d	4.7
C α	6.65	d	16.0
C β	7.68	d	16.0

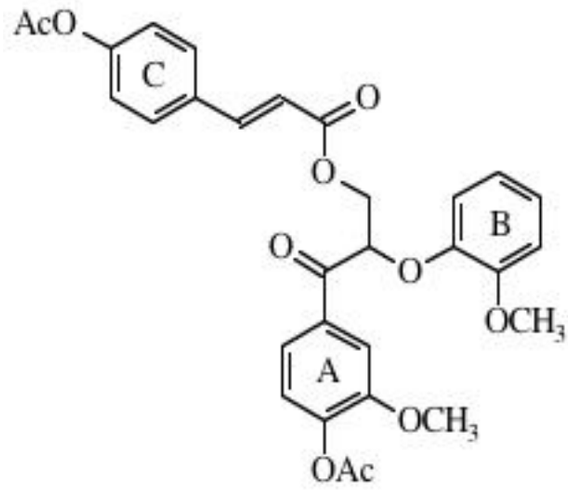
Notes:

R. Helm
19mg
Acetone run at 300 K

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.44			
Ac Me			20.44			
Ac Me			20.61			
OMe			56.22			
OMe			56.30			
OMe			56.41			
γ			63.16			
α			74.97			
β			80.39			
C2			112.46			
A2			112.79			
B2			113.79			
C β			118.75			
B5			119.85			
A6			120.43			
B6			121.68			
C6			122.35			
A5			123.41			
B1			124.08			
C5			124.14			
C1			134.13			
A1			136.61			
A4			140.83			
C4			142.82			
C α			145.57			
B4			148.37			
B3			152.05			
A3			152.14			
C3			152.69			
C γ			165.89			
Ac C=O			168.79			
Ac C=O			168.90			
Ac C=O			170.76			

Compound Number 1009



3-(4-Acetoxyphenyl) acrylic acid 3-(4-acetoxy-3- methoxyphenyl)-2-(2-methoxyphenoxy)-3-oxopropyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.62	dd	12.0, 6.5
γ2	4.81	dd	12.0, 3.8
β	5.91	dd	6.5, 3.8
C β	6.48	d	16.0
C α	7.60	d	16.0

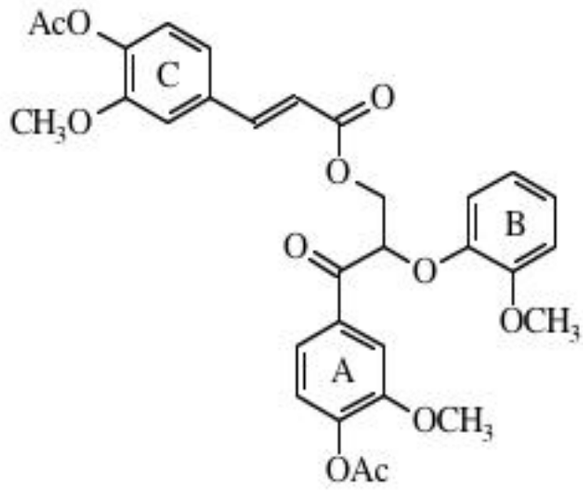
Notes:

R. Helm
25.5mg
acetone-d6 at 300 K

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.45			
Ac Me			20.94			
OMe			56.10			
OMe			56.42			
γ			64.97			
β			80.56			
A2			113.46			
B2			113.84			
C β			118.32			
B5			118.69			
B6			121.64			
A6			122.88			
C3			123.24			
C5			123.24			
A5			124.02			
B1			124.07			
C2			130.27			
C6			130.27			
C1			132.68			
A1			134.86			
C α			145.09			
A4			145.34			
B4			147.84			
B3			151.42			
A3			152.49			
C4			153.58			
C γ			166.76			
Ac C=O			168.58			
Ac C=O			169.42			
α			195.13			

Compound Number 1010



3-(4-Acetoxy-3-methoxyphenyl) acrylic acid 3-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)-3-oxopropyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.61	dd	12.0, 6.5
γ2	4.81	dd	12.0, 3.8
β	5.91	dd	6.5, 3.8
Cβ	6.52	d	16.0
C α	7.58	d	16.0

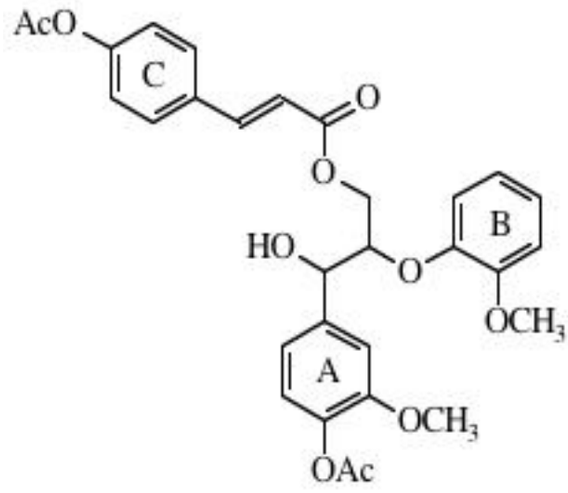
Notes:

R. Helm
25mg
300k, acetone-d6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.44			
Ac Me			20.44			
OMe			56.10			
OMe			56.40			
OMe			56.43			
γ			64.93			
β			80.54			
C2			112.41			
A2			113.48			
B2			113.83			
C β			118.44			
B5			118.62			
B6			121.64			
C6			122.35			
A6			122.87			
A5			124.03			
B1			124.06			
C5			124.15			
C1			134.01			
A1			134.85			
C4			142.83			
A4			145.35			
C α			145.50			
B4			147.82			
B3			151.40			
A3			152.50			
C3			152.69			
C γ			166.81			
Ac C=O			168.58			
Ac C=O			168.80			
α			195.11			

Compound Number 1011



threo

3-(4-Acetoxyphenyl) acrylic acid 3-(4-acetoxy-3-methoxy phenyl)-3-hydroxy-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	5.08	d	4.3
α OH	4.75		
β	4.64	m	
γ1	4.17	dd	11.9, 6.3
γ2	4.44	dd	11.9, 3.7
C β	6.46	d	16.1
C α	7.54	d	16.0

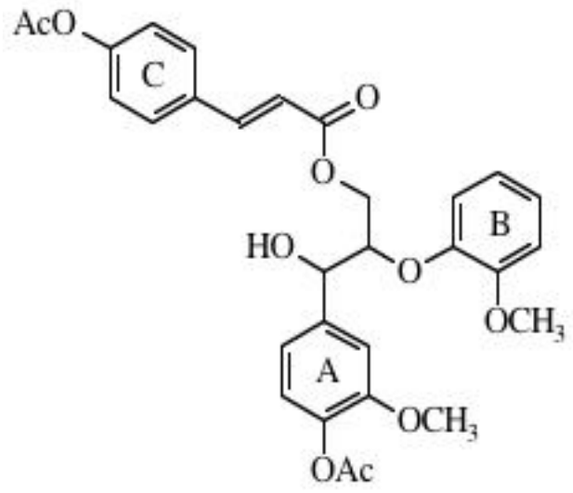
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ			64.28			
α			73.58			
β			83.80			
C β			118.73			
C α			144.57			
C γ			166.68			

Compound Number 1012



erythro

3-(4-Acetoxyphenyl) acrylic acid 3-(4-acetoxy-3-methoxy phenyl)-3-hydroxy-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	5.09	d	4.4
α OH	4.80		
β	4.70	m	
γ1	4.45	dd	11.8, 3.7
γ2	4.52	dd	11.8, 6.3
C β	6.41	d	16.1
C α	7.50	d	16.1

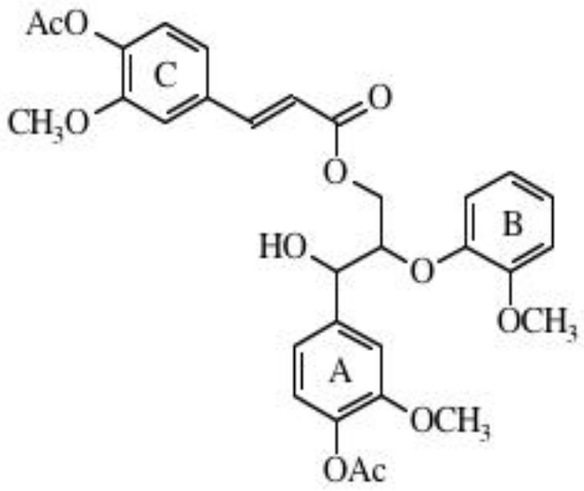
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ			63.95			
α			73.16			
β			83.22			
C β			118.83			
C α			144.36			
C γ			166.79			

Compound Number 1013



threo

3-(4-Acetoxy-3-methoxyphenyl) acrylic acid 3-(4-acetoxy-3-methoxyphenyl)-3-hydroxy-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	5.08	d	4.2
α OH	4.75		
β	4.64	m	
γ1	4.17	dd	11.9, 6.2
γ2	4.44	dd	11.9, 3.7
Cβ	6.49	d	16.0
C α	7.51	d	16.0

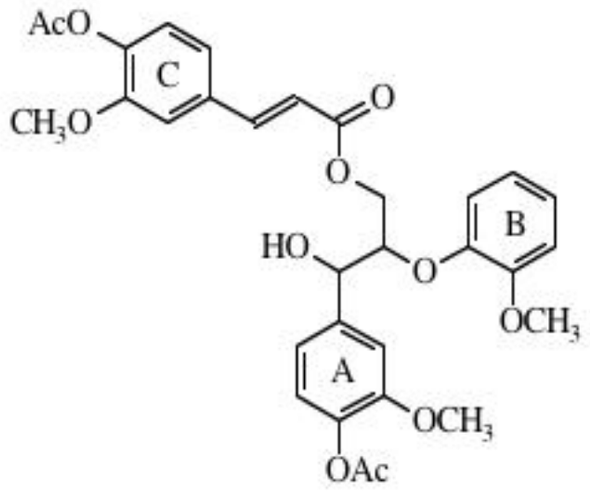
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ			64.27			
α			73.56			
β			83.73			
C β			118.81			
C α			144.94			
C γ			166.72			

Compound Number 1014



erythro

3-(4-Acetoxy-3-methoxyphenyl) acrylic acid 3-(4-acetoxy-3-methoxyphenyl)-3-hydroxy-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	5.08	d	4.4
α OH	4.79		
β	4.70	m	
γ1	4.45	dd	11.8, 3.7
γ2	4.58	dd	11.8, 6.2
C β	6.44	d	16.0
C α	7.47	d	16.0

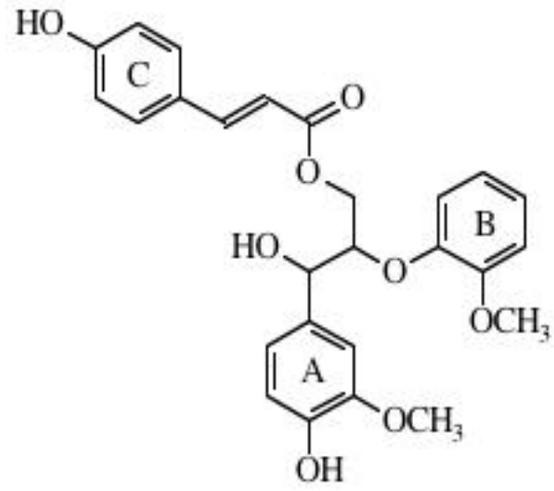
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ			63.93			
α			73.14			
β			83.18			
C β			118.91			
C α			144.79			
C γ			166.83			

Notes:

R. Helm

Compound Number 1015



threo

3-(4-Hydroxyphenyl) acrylic acid 3-hydroxy-3-(4- hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.10	dd	12.0, 6.2
γ2	4.36	dd	12.0, 3.5
β	4.56	m	
α OH	4.59	d	3.9
α	4.97	dd	6.2, 3.9
C β	6.29	d	16.0
C α	7.47	d	16.0

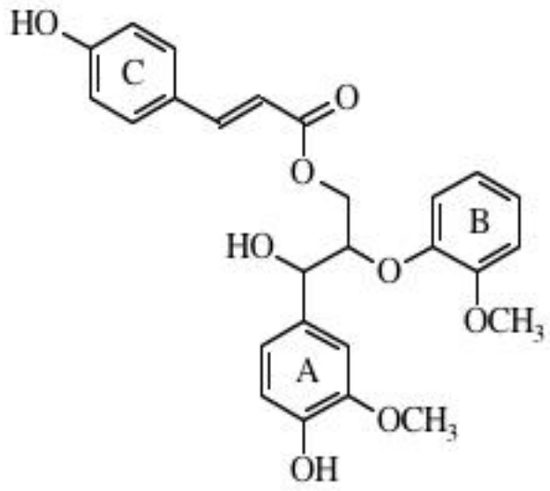
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.19			
OMe			56.25			
γ			64.18			
α			73.95			
β			84.52			
A2			111.46			
B2			113.59			
C β			115.22			
A5			115.34			
C3			116.66			
C5			116.66			
B5			119.42			
A6			120.56			
B6			121.81			
B1			123.55			
C1			126.89			
C2			130.94			
C6			130.94			
A1			133.16			
C α			145.57			
A4			147.02			
A3			148.09			
B4			149.36			
B3			151.79			
C4			160.63			
C γ			167.15			

Compound Number 1016



erythro

3-(4-Hydroxyphenyl) acrylic acid 3-hydroxy-3-(4- hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.39	dd	11.8, 3.6
γ2	4.46	dd	11.8, 6.6
β	4.66	m	
α	4.91	d	4.9
C β	6.24	d	16.0
C α	7.42	d	16.0

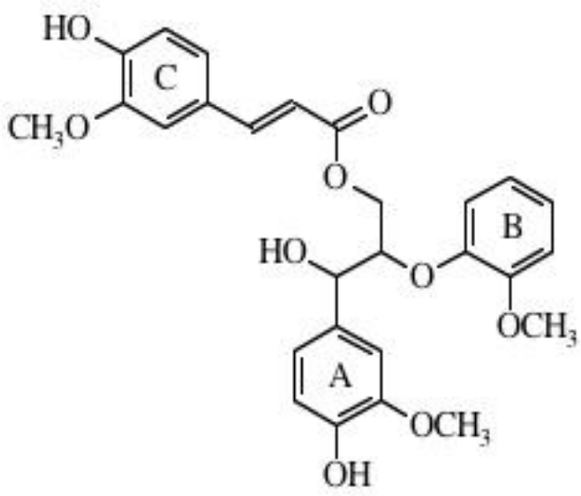
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.20			
OMe			56.22			
γ			63.98			
α			73.28			
β			83.54			
A2			111.20			
B2			113.64			
C β			115.24			
A5			115.34			
C3			116.64			
C5			116.64			
B5			119.67			
A6			120.32			
B6			121.71			
B1			123.51			
C1			126.91			
C2			130.88			
C6			130.88			
A1			133.59			
C α			145.39			
A4			146.72			
A3			148.02			
B4			148.86			
B3			152.02			
C4			160.52			
C γ			167.28			

Compound Number 1017



threo

3-(4-Hydroxy-3-methoxyphenyl) acrylic acid 3-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	4.96	d	6.3
β	4.56	m	
γ2	4.36	dd	12.0, 3.5
γ1	4.10	dd	12.0, 6.2
C β	6.33	d	16.0
C α	7.45	d	16.0

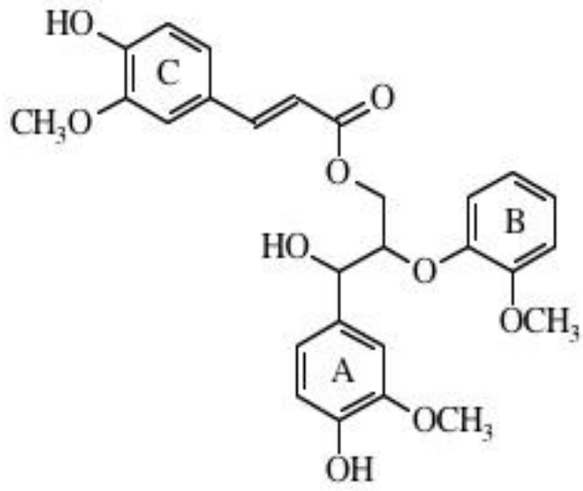
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.20			
OMe			56.26			
OMe			56.32			
γ			64.16			
α			73.94			
β			84.48			
C2			111.37			
A2			111.46			
B2			113.60			
A5			115.33			
C β			115.47			
C5			116.05			
B5			119.39			
A6			120.56			
B6			121.81			
B1			123.54			
C6			123.90			
C1			127.35			
A1			133.16			
C α			145.91			
A4			147.01			
A3			148.08			
C3			148.71			
B4			149.36			
C4			150.09			
B3			151.80			
C γ			167.14			

Notes:

R. Helm

Compound Number 1018



erythro

3-(4-Hydroxy-3-methoxyphenyl) acrylic acid 3-hydroxy-3-(4-□ hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.40	dd	3.7,
γ2	4.46	dd	6.7,
β	4.66	m	
α	4.97	d	4.9
C α	6.28	d	15.9
C β	7.40	d	15.9

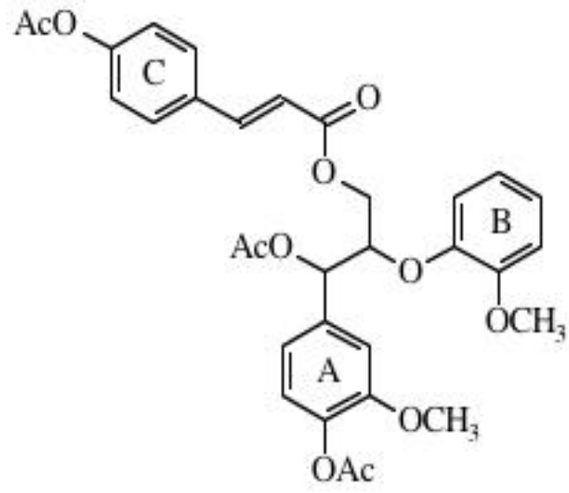
Notes:

R. Helm
27mg
300K, acetone-d6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.23			
OMe			56.23			
OMe			56.31			
γ			63.94			
α			73.26			
β			83.57			
A2			111.21			
C2			111.29			
B2			113.66			
A5			115.25			
C β			115.59			
C5			116.03			
B5			119.63			
A6			120.31			
B6			121.73			
B1			123.49			
C6			123.86			
C1			127.37			
A1			133.63			
C α			145.74			
A4			146.74			
A3			148.05			
C3			148.70			
B4			148.86			
C4			150.04			
B3			152.04			
C γ			167.28			

Compound Number 1019



threo

3-(4-acetoxyphenyl) acrylic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.17	dd	5.6,
γ2	4.40	dd	4.0,
β	4.88	m	
α	6.18	d	6.5
C β	6.51	d	16.0
C α	7.57	d	16.1

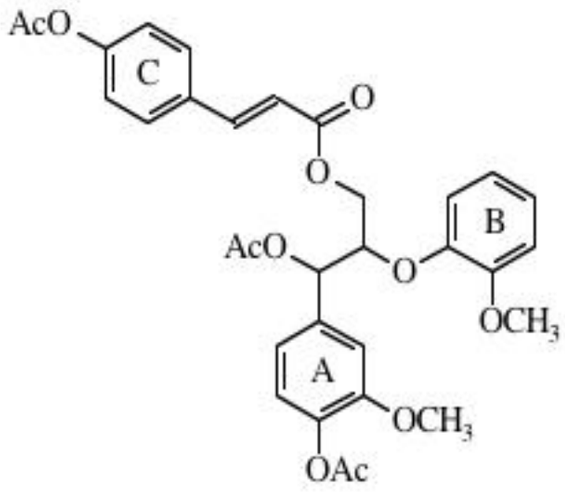
Notes:

R. Helm
18mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.45			
Ac Me			20.94			
Ac Me			20.94			
OMe			56.20			
OMe			56.28			
γ			63.94			
α			75.54			
β			80.89			
A2			112.70			
B2			113.73			
C β			118.57			
B5			119.36			
A6			120.32			
B6			121.69			
C3			123.21			
C5			123.21			
A5			123.59			
B1			123.81			
C2			130.25			
C6			130.25			
C1			132.81			
A1			136.71			
A4			140.91			
C α			144.75			
B4			149.12			
B3			151.90			
A3			152.22			
C4			153.52			
C γ			166.61			
Ac C=O			168.87			
Ac C=O			169.43			
Ac C=O			170.02			

Compound Number 1020



erythro

3-(4-acetoxyphenyl) acrylic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.40	dd	11.9, 4.2
γ2	4.48	dd	11.9, 5.9
β	4.92	m	
α	6.13	d	5.1
C β	6.45	d	16.0
C α	7.56	d	16.1

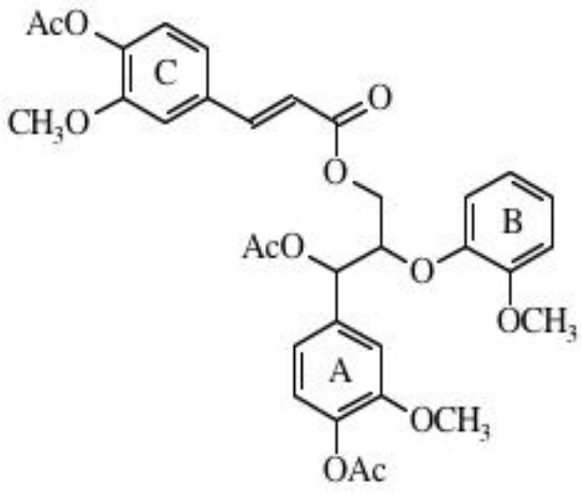
Notes:

R. Helm

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.46			
Ac Me			20.89			
Ac Me			20.94			
OMe			56.19			
OMe			56.26			
γ			63.33			
α			74.71			
β			80.52			
A2			112.74			
B2			113.76			
C β			118.54			
B5			119.99			
A6			120.44			
B6			121.64			
C3			123.20			
C5			123.20			
A5			123.37			
B1			124.10			
C2			130.21			
C6			130.21			
C1			132.78			
A1			136.73			
A4			140.77			
C α			144.71			
B4			148.30			
B3			152.09			
A3			152.11			
C4			153.49			
C γ			166.60			
Ac C=O			168.89			
Ac C=O			169.41			
Ac C=O			169.92			

Compound Number 1021



threo

3-(4-acetoxyphenyl) acrylic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.16	dd	12.0, 5.6
γ2	4.40	dd	12.0, 3.9
β	4.88	m	
α	6.18	d	6.6
C β	6.55	d	16.0
C α	7.54	d	16.0

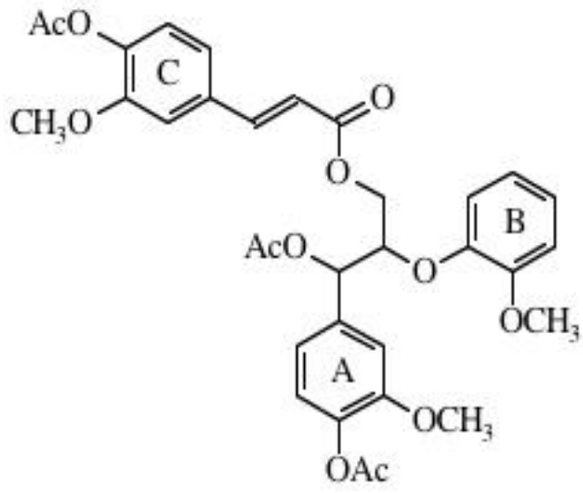
Notes:

R. Helm
18.5mg
300K

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.45			
Ac Me			20.45			
Ac Me			20.95			
OMe			56.20			
OMe			56.29			
OMe			56.42			
γ			63.96			
α			75.57			
β			80.88			
C2			112.45			
A2			112.69			
B2			113.73			
C β			118.64			
B5			119.33			
A6			120.32			
B6			121.69			
C6			122.30			
A5			123.60			
B1			123.80			
C5			124.12			
C1			134.13			
A1			136.69			
A4			140.92			
C4			142.76			
C α			145.20			
B4			149.10			
B3			151.89			
A3			152.23			
C3			152.68			
C γ			166.68			
Ac C=O			168.82			
Ac C=O			168.89			
Ac C=O			170.05			

Compound Number 1022



erythro

3-(4-acetoxyphenyl) acrylic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.40	dd	11.9, 4.2
γ2	4.49	dd	11.9, 5.9
β	4.92	m	
α	6.13	d	5.1
C β	6.48	d	16.0
C α	7.53	d	16.0

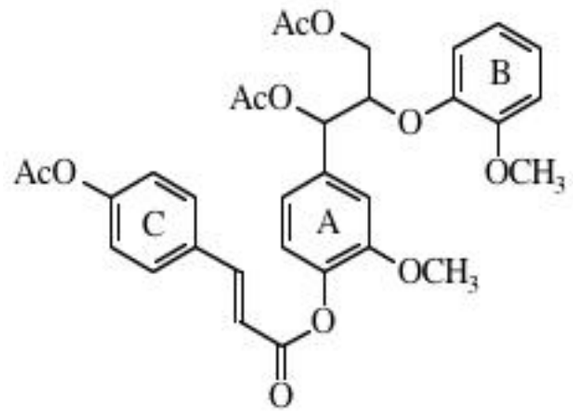
Notes:

R. Helm
18.5mg
300K

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.45			
Ac Me			20.45			
Ac Me			20.89			
OMe			56.19			
OMe			56.28			
OMe			56.40			
γ			63.33			
α			74.70			
β			80.50			
C2			112.44			
A2			112.74			
B2			113.77			
C β			118.63			
B5			119.97			
A6			120.44			
B6			121.65			
C6			122.25			
A5			123.38			
B1			124.41			
C5			124.41			
C1			134.11			
A1			136.73			
A4			140.79			
C4			142.74			
C α			145.16			
B4			148.30			
B3			152.10			
A3			152.12			
C3			152.67			
C γ			166.67			
Ac C=O			168.80			
Ac C=O			168.90			
Ac C=O			169.94			

Compound Number 1023



threo

3-(4-acetoxyphenyl) acrylic acid 4-[1,3-diacetoxy-2- (2-methoxyphenoxy) propyl] phenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
C α	7.84	d	16.1
C β	6.74	d	16.1
α	6.14	d	6.5
β	4.81	m	
γ1	4.28	dd	11.9, 4.2
γ 2	4.04	dd	11.9, 5.6

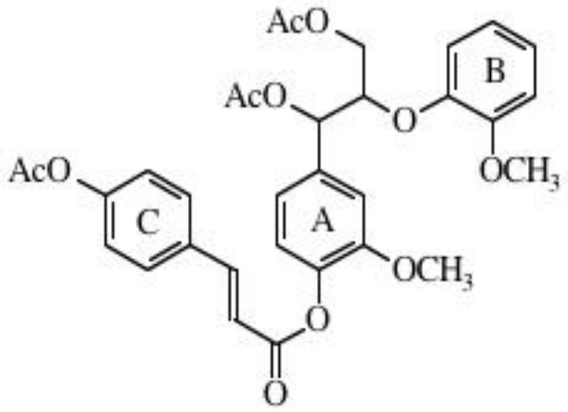
Notes:

R. Helm
20.6mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.59			
Ac Me			20.92			
Ac Me			20.96			
OMe			56.30			
OMe			56.20			
γ			63.60			
α			75.40			
β			80.70			
A2			112.70			
B2			113.74			
C β			117.92			
B5			119.23			
A6			120.34			
B6			121.68			
C3			123.31			
C5			123.31			
A5			123.64			
B1			123.72			
C2			130.44			
C6			130.44			
C1			132.72			
A1			136.78			
A4			140.83			
C α			146.05			
B4			149.08			
B3			151.84			
A3			152.30			
C4			153.74			
C γ			164.91			
Ac C=O			169.42			
Ac C=O			170.01			
Ac C=O			170.68			

Compound Number 1024



erythro

3-(4-acetoxyphenyl) acrylic acid 4-[1,3-diacetoxy-2- (2-methoxyphenoxy) propyl] phenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
C α	7.84	d	15.7
C β	6.74	d	16.1
α	6.10	d	5.1
β	4.85	m	
γ1	4.39	dd	11.9, 5.9
γ2	4.24	dd	11.9, 4.2

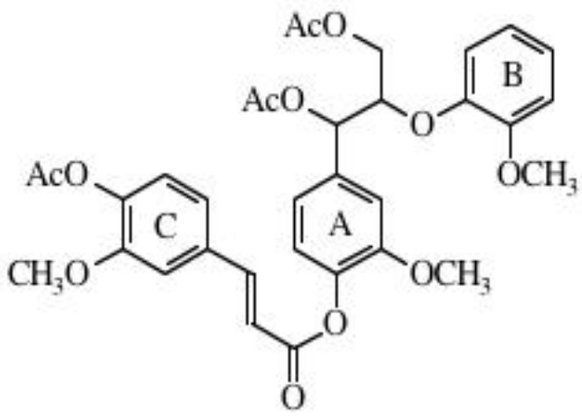
Notes:

R. Helm
25mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.61			
Ac Me			20.87			
Ac Me			20.96			
OMe			56.20			
OMe			56.28			
γ			63.00			
α			74.60			
β			80.32			
A2			112.77			
B2			113.79			
C β			117.95			
B5			119.82			
A6			120.45			
B6			121.64			
C3			123.31			
C5			123.31			
A5			123.45			
B1			124.06			
C2			130.44			
C6			130.44			
C1			132.73			
A1			136.78			
A4			140.71			
C α			146.02			
B4			148.27			
B3			152.06			
A3			152.19			
C4			153.74			
C γ			164.95			
Ac C=O			169.42			
Ac C=O			169.92			
Ac C=O			170.76			

Compound Number 1025



threo

3-(4-acetoxy-3-methoxyphenyl) acrylic acid 4-[1,3-diacetoxy-2-(2-methoxyphenoxy) propyl] phenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
C α	7.81	d	15.9
C β	6.77	d	16.0
α	6.14	d	6.5
β	4.81	m	
γ1	4.28	dd	11.9, 4.2
γ2	4.04	dd	11.9, 5.6

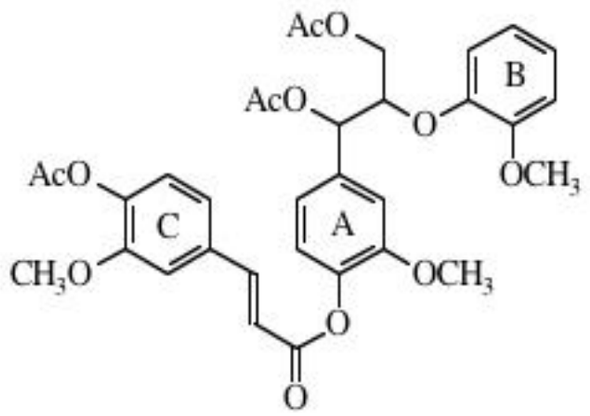
Notes:

R. Helm
20.6mg
std conditions

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.46			
Ac Me			20.59			
Ac Me			20.93			
OMe			56.20			
OMe			56.30			
OMe			56.44			
γ			63.61			
α			75.40			
β			80.70			
C2			112.61			
A2			112.70			
B2			113.75			
C β			118.03			
B5			119.23			
A6			120.34			
B6			121.68			
C6			122.52			
A5			123.64			
B1			123.72			
C5			124.20			
C1			134.04			
A1			136.77			
A4			140.83			
C4			142.98			
C α			146.46			
B4			149.08			
B3			151.84			
A3			152.30			
C3			152.76			
C γ			164.97			
Ac C=O			168.79			
Ac C=O			170.01			
Ac C=O			170.69			

Compound Number 1026



erythro

3-(4-acetoxy-3-methoxyphenyl) acrylic acid 4-[1,3-diacetoxy-2-(2-methoxyphenoxy) propyl] phenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
C α	7.81	d	15.8
C β	6.78	d	16.0
α	6.10	d	5.1
β	4.85	m	
γ1	4.39	dd	11.9, 5.6
γ2	4.24	dd	11.9, 4.2

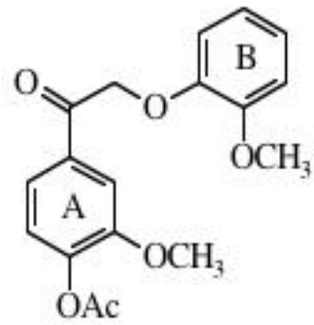
Notes:

R. Helm
20.9mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.46			
Ac Me			20.60			
Ac Me			20.86			
OMe			56.20			
OMe			56.27			
OMe			56.44			
γ			63.00			
α			74.60			
β			80.32			
C2			112.60			
A2			112.77			
B2			113.79			
C β			118.06			
B5			119.82			
A6			120.45			
B6			121.64			
C6			122.52			
A5			123.44			
B1			124.06			
C5			124.20			
C1			134.04			
A1			136.77			
A4			140.70			
C4			142.97			
C α			146.44			
B4			148.27			
B3			152.06			
A3			152.19			
C3			152.76			
C γ			165.00			
Ac C=O			168.80			
Ac C=O			169.92			
Ac C=O			170.76			

Compound Number 1027



Acetic acid 2-methoxy-4-[2-(2-methoxyphenoxy) acetyl] phenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	5.43		

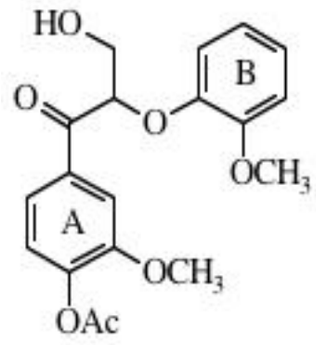
Notes:

R. Helm
crystalline

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.44			
OMe			56.21			
OMe			56.44			
β			72.50			
A2			112.66			
B2			113.63			
B5			115.72			
B6			121.54			
A6			122.13			
B1			122.79			
A5			123.99			
A1			134.59			
A4			145.22			
B4			148.97			
B3			150.88			
A3			152.58			
Ac C=O			168.63			
α			194.31			

Compound Number 1028



Acetic acid 4-[3-hydroxy-2-(2-methoxyphenoxy) propionyl]-2-methoxy phenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	5.55		
γ's	4.09		

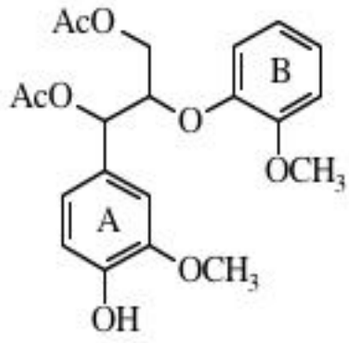
Notes:

R. Helm
20mg
300K acetone-d6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.44			
OMe			56.12			
OMe			56.35			
γ			63.90			
β			84.22			
A2			113.43			
B2			113.73			
B5			117.45			
B6			121.60			
A6			122.81			
B1			123.34			
A5			123.80			
A1			135.27			
A4			145.05			
B4			148.29			
B3			151.13			
A3			152.36			
Ac C=O			168.60			
α			196.80			

Compound Number 1029



threo

Acetic acid 3-acetoxy-3-(4-hydroxy-3-methoxyphenyl) -2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	6.04	d	7.13
β	4.77	m	
γ1	4.21	dd	11.9, 3.6
γ2	3.95	dd	11.9, 5.6

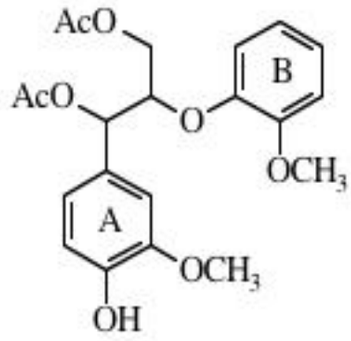
Notes:

R. Helm
19.6mg
acetone-d6

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.58			
Ac Me			20.97			
OMe			56.21			
OMe			56.30			
γ			63.86			
α			75.87			
β			80.99			
A2			111.89			
B2			113.77			
A5			115.64			
B5			119.13			
A6			121.19			
B6			121.67			
B1			123.57			
A1			129.17			
A4			147.71			
A3			148.26			
B4			149.31			
B3			151.83			
Ac C=O			169.95			
Ac C=O			170.66			

Compound Number 1030



erythro

Acetic acid 3-acetoxy-3-(4-hydroxy-3-methoxyphenyl) -2-(2-methoxyphenoxy) propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	5.99	d	4.99
β	4.81	m	
γ1	4.34	dd	11.9, 6.2
γ2	3.98	dd	11.9, 4.0

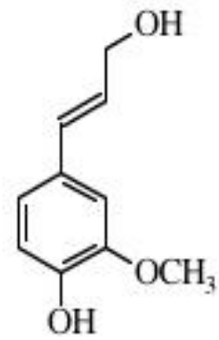
Notes:

R. Helm
15mg
std conditions

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.60			
Ac Me			20.90			
OMe			56.20			
OMe			56.29			
γ			63.30			
α			74.89			
β			80.40			
A2			112.01			
B2			113.78			
A5			115.41			
B5			119.56			
A6			121.28			
B6			121.61			
B1			123.83			
A1			129.07			
A4			147.53			
A3			148.15			
B4			148.49			
B3			152.00			
Ac C=O			169.90			
Ac C=O			170.75			

Compound Number 2001



trans

coniferyl alcohol

4-hydroxy-3-methoxy cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ OH	3.78	t	5.65
OMe	3.85	s	
γ	4.18	td	1.5, 5.6
β	6.22	dt	15.9, 5.5
α	6.49	dt	15.9, 1.5
	□	□	
5	6.76	d	8.1
6	6.84	dd	8.1, 1.9
2	7.04	d	1.9
Ar OH	7.63	s	

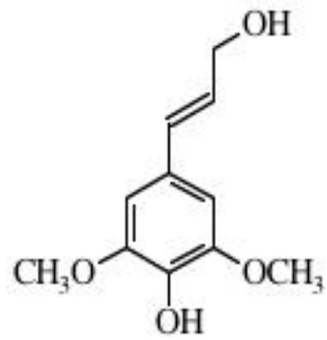
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.78	100	56.09	92	55.56	100
γ	63.66	67	63.37	100	61.73	64
2	108.40	59	109.91	71	109.72	67
5	114.48	69	115.73	99	115.47	68
6	120.18	81	120.55	100	119.43	70
β	126.05	92	127.96	90	127.49	65
1	129.18	48	130.16	40	128.52	52
α	131.23	80	130.41	97	129.00	69
4	145.51	53	147.07	45	146.17	54
3	146.64	31	148.36	34	147.72	55

Notes:

S. Quideau
Assignments confirmed in all three solvents
JAFC 1992-40(7), 1108-1110

Compound Number 2002



sinapyl alcohol

4-hydroxy-3,5-dimethoxy cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ OH	3.88	t	5.65
OMe	3.82	s	
γ	4.20	td	5.6, 1.5
β	6.24	dt	15.8, 5.5
α	6.48	dt	15.8, 1.5
2,6	6.71	s	
4 OH	7.30	s	

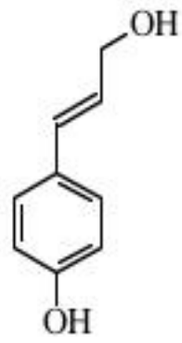
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.27	100	56.48	39	55.92	100
OMe	56.27	100	56.48	39	55.92	100
γ	63.76	52	63.33	21	61.62	42
2	103.35	94	104.65	32	103.79	76
6	103.35	94	104.65	32	103.79	76
β	126.58	49	128.27	19	127.89	41
1	128.22	22	128.99	10	127.40	28
α	131.50	50	130.62	100	129.17	42
4	134.80	20	136.52	8	135.17	14
3	147.13	41	148.71	16	148.01	50
5	147.13	41	148.71	16	148.01	50

Notes:

S. Quideau
Note A1 and β change places in DMSO. Assignments confirmed in CDCl3 and Acetone. JAFC 1992-40(7), 1108-1110

Compound Number 2003



p-coumaryl alcohol

4-hydroxy-cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ OH	3.85	t	5.65
g's	4.19	td	5.6, 1.6
β	6.19	dt	15.9, 5.6
α	6.50	dt	15.9, 1.6
3,5	6.78	m	
2,6	7.25	m	
4 OH	8.40	s	

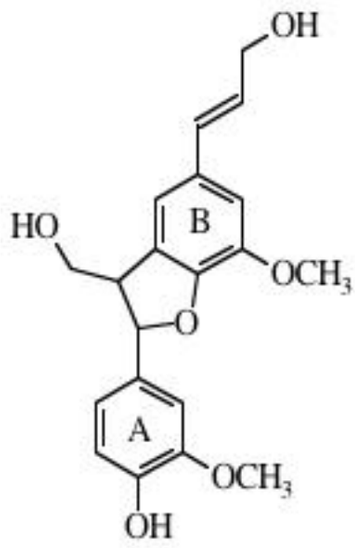
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ	63.79	46	63.41	41	61.72	49
3	115.50	100	116.15	84	115.37	85
5	115.50	100	116.15	84	115.37	85
β	125.74	46	127.71	42	127.15	50
2	127.73	98	128.33	100	127.38	100
6	127.73	98	128.33	100	127.38	100
1	128.90	24	129.68	18	127.92	27
α	131.08	48	130.13	44	128.70	50
4	156.12	31	157.76	18	156.80	27

Notes:

S. Quideau
JAFC-1992-40(7), 1108-1110

Compound Number 2004



4-[3-Hydroxymethyl-5-(3-hydroxypropenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-2-methoxyphenol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.53	br q	
γ + γ OH	3.78-3.88	m	
A3 OMe	3.81	s	
B3 OMe	3.85	s	
B γ OH	4.16	t	5.0
B γ	4.19	td	5.2, 1.5
α	5.56	d	6.5
B β	6.23	dt	15.8, 5.5
B α	6.52	dt	15.8, 1.5
A5	6.80	d	8.1
A6	6.87	ddd	8.1, 2.0, 0.5
B2	6.94	br s	
B6	6.97	br s	
A2	7.03	d	2.0
A4 OH	7.73	br s	

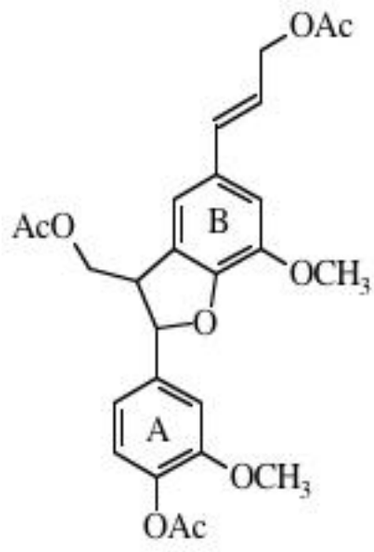
Notes:

S. Quideau-Ag2O oxidation of coniferyl alcohol.
Assignments confirmed in acetone.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	53.53	70	54.73	73	53.02	41
A OMe	55.99	97	56.26	94	55.68	46
B OMe	56.01	100	56.38	100	55.73	100
B γ	63.83	89	63.39	79	61.70	77
γ	64.00	72	64.60	68	62.98	32
α	88.24	72	88.51	100	87.26	45
A2	108.75	73	110.48	99	110.37	59
B2	110.54	73	111.72	85	110.37	59
A5	114.33	78	115.67	60	115.00	38
B6	114.78	72	116.08	97	115.37	52
A6	119.43	75	119.57	99	118.58	55
B β	126.45	70	128.33	85	128.02	46
B5	128.09	50	130.40	59	129.52	48
B α	131.33	80	130.54	100	129.04	73
B1	130.87	47	131.91	54	130.56	78
A1	132.87	49	134.36	55	132.39	69
B3	144.47	42	145.14	50	143.72	70
A4	145.74	52	147.27	26	146.42	87
A3	146.68	44	148.36	32	147.13	56
B4	148.38	28	148.84	32	147.60	78

Compound Number 2005



Acetic acid 4-[3-acetoxymethyl-5-(3-acetoxypropenyl)- 7-methoxy-2,3-dihydrobenzofuran-2-yl]-2-methoxyphenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	2.0	s	
B γ Ac Me	2.01	s	
A4 Ac Me	2.22	s	
β	3.78	m	
A3 OMe	3.79	s	
B3 OMe	3.88	s	
γ1	4.34	dd	11.1, 7.6
γ2	4.46	dd	11.1, 5.4
B γ	4.66	dd	6.5, 1.3
α	5.61	d	6.7
Bβ	6.24	dt	15.8, 6.5
B α	6.63	dt	15.8, 1.3
A6	7.0	br dd	8.1, 1.8
B6	7.03	br s	
B2	7.049	br s	
A5	7.054	d	8.1
A2	7.18	d	1.8

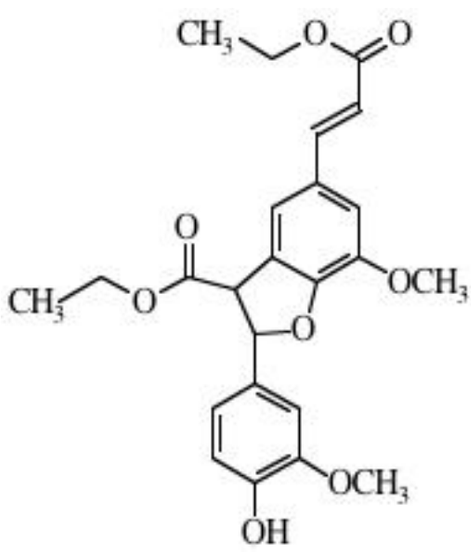
Notes:

S.Quideau-Ag2O oxidation of coniferyl alcohol + acetylation. Assignments confirmed in CDCl3 and acetone
A1 and A4 switch places in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.51	91	20.43	94	20.41	68
γAc Me	20.68	81	20.67	92	20.61	78
BγAc Me	20.90	84	20.78	77	20.79	84
β	50.36	71	51.33	85	49.53	46
A OMe	55.79	100	56.24	97	55.84	100
B OMe	55.92	95	56.41	92	55.84	100
Bγ	65.06	83	65.47	100	64.57	60
γ	65.22	61	65.96	75	64.90	37
α	87.91	72	88.34	89	87.01	47
A2	109.84	77	111.07	88	110.59	50
B2	110.56	60	112.20	79	111.08	35
B6	115.23	69	116.32	76	115.36	40
A6	118.08	78	118.67	90	118.00	50
B β	121.16	72	122.30	86	121.53	45
A5	122.79	79	123.76	94	123.01	50
B5	127.21	63	128.82	61	127.84	50
B1	130.59	60	131.65	58	130.28	47
B α	134.13	76	134.64	87	133.52	47
A4	139.56	46	140.70	38	139.14	40
A1	139.30	58	140.99	54	139.59	46
B3	144.30	56	145.39	53	143.96	47
B4	148.03	39	149.21	37	147.55	35
A3	151.16	57	152.38	44	150.92	53
A4 Ac C=O	168.82	52	168.98	44	168.60	42
γ C=O	170.63	53	170.97	43	170.41	51
B γ C=O	170.76	43	170.80	32	170.27	44

Compound Number 2006



5-(2-Ethoxycarbonylvinyl)-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-2,3-dihydrobenzofuran-3-carboxylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.27	t	7.1
CH3	1.27	t	7.1
A3 OMe	3.82	s	
B3 OMe	3.91	s	
CH2	4.18	q	7.1
CH2	4.25	m	
β	4.43	d	8.0
α	6.03	d	8.0
B β	6.41	d	15.9
A5	6.84	d	8.1
A6	6.91	dd	8.1, 1.9
A2	7.08	d	1.9
B6	7.27	br s	
B2	7.31	br s	
B α	7.62	d	15.9
A4 OH	7.87	s	

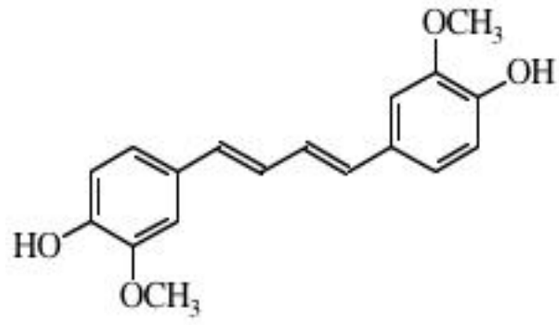
Notes:

S. Quideau-Ag2O oxidation of ethyl ferulate.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A CH3	14.24	95	14.48	94	14.12	100
B CH3	14.31	96	14.63	92	14.32	91
β	55.54	77	56.06	88	54.33	42
A OMe	55.98	100	56.31	98	55.78	96
B OMe	56.08	94	56.49	100	56.04	78
A CH2	61.83	87	62.20	89	61.49	80
B CH2	60.37	85	60.56	89	59.99	67
α	87.46	80	88.34	89	87.36	45
A2	108.74	90	110.74	79	110.86	59
B2	111.93	71	113.30	83	112.55	37
A5	114.49	95	115.82	64	115.48	57
B β	115.93	78	116.69	87	115.84	45
B6	117.86	75	118.91	90	118.31	41
A6	119.44	93	120.18	91	119.41	58
B5	125.85	65	127.41	57	126.35	53
B1	128.61	70	129.46	59	128.23	53
A1	131.44	67	132.10	42	129.97	57
B α	144.50	77	145.22	85	144.66	43
B3	144.69	63	145.82	50	147.83	66
A3	146.69	63	148.56	35	144.44	60
A4	146.03	65	147.97	34	149.50	47
B4	149.90	42	150.99	34	147.19	59
B γ	167.18	58	167.28	53	166.65	57
γ	170.20	64	171.10	53	170.42	65

Compound Number 2007



trans

1,4-bis-(4-hydroxy-3-methoxypheny)l-1,3-butadiene

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.87	s	
α	6.56	m	
A5	6.78	d	8.1
β, A6	6.85-6.92	m	
A2	7.12	d	1.9
Ar OH	7.71	s	

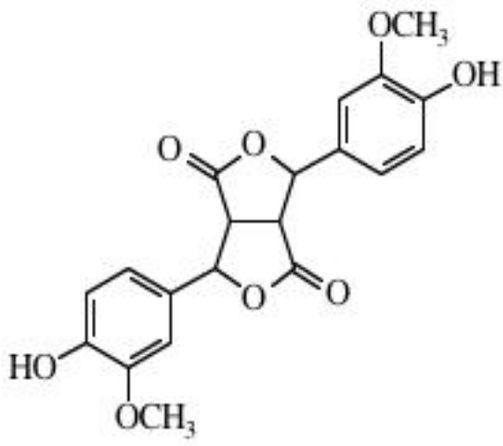
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.89	100	56.21	100	55.55	100
2	107.95	90	109.76	84	109.38	61
5	114.55	90	115.96	77	115.55	57
6	120.29	93	120.95	96	119.81	67
β	127.35	87	128.07	85	126.90	49
1	130.25	48	130.81	41	128.96	35
α	131.72	88	132.49	80	131.37	59
4	145.45	57	147.41	44	146.43	45
3	146.69	53	148.60	42	147.80	52

Notes:

S. Quideau
From LiBH4 red. of dilactone
As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 2008



dilactone from ferulic acid

3,6-Bis-(4-hydroxy-3-methoxyphenyl) tetrahydrofuro [3,4-c] furan-1,4-dione

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.85	s	
β	4.09	t	1.0
α	5.77	br s	
5	6.86	d	8.2
6	6.92	dd	8.2, 1.8
2	7.05	d	1.8
4 OH	7.90	s	

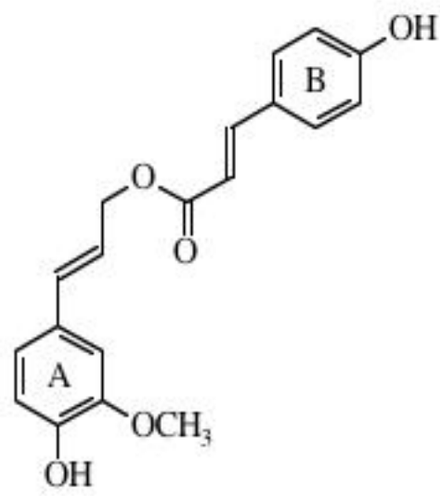
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	48.39	83	49.11	95	48.11	83
OMe	56.13	95	56.39	95	55.81	74
α	81.90	86	83.22	94	82.06	75
2	107.52	100	110.40	88	110.64	98
5	114.98	92	116.00	81	115.46	85
6	117.41	92	119.57	100	119.22	100
1	129.81	52	130.82	49	129.00	73
4	146.35	53	148.17	42	147.36	70
3	147.06	47	148.72	36	147.88	85
γ	174.94	48	175.99	48	175.40	75

Notes:

S. Quideau
As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 2009



coniferyl p-coumarate

3-(4-Hydroxyphenyl) acrylic acid 3-(4-hydroxy-3-methoxyphenyl) llyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.86	s	
γ	4.78	dd	6.5, 1.3
β	6.25	dt	15.8, 6.5
B β	6.37	d	15.9
α	6.65	dt	15.8, 1.3
A5	6.79	d	8.1
B3,5	6.88	m	
A6	6.91	dd	8.1, 2.0
A2	7.11	d	2.0
B2,6	7.54	m	
B α	7.63	d	15.9
ArOH	7.76	s	
ArOH	9.03	s	

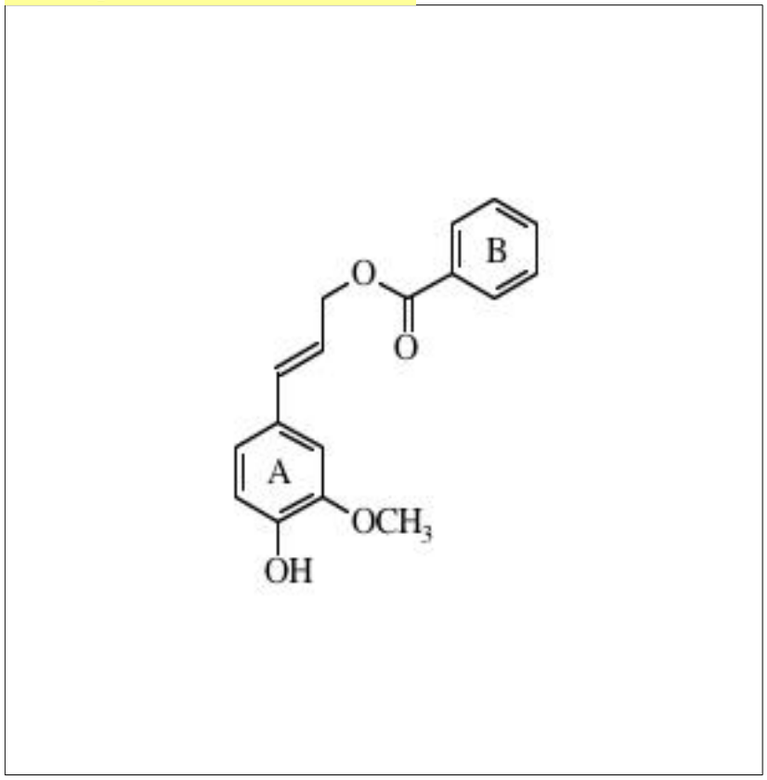
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.87	55	56.20	47	55.61	77
γ	65.35	43	65.49	55	64.62	34
A2	108.44	51	110.20	47	109.91	52
B β	114.45	53	115.45	43	114.13	44
A5	114.98	47	115.83	40	115.46	51
B3	115.93	100	116.68	67	115.81	96
B5	115.93	100	116.68	67	115.81	96
A6	120.62	54	121.19	46	120.12	53
β	120.89	52	121.72	44	120.61	49
B1	126.81	32	126.90	24	125.12	38
A1	128.83	30	129.39	22	127.59	43
B2	130.00	96	130.91	100	130.37	100
B6	130.00	96	130.91	100	130.37	100
α	134.43	50	134.90	45	133.9	49
Bα	145.07	41	145.49	43	144.90	43
A4	145.84	32	147.80	22	146.87	39
A3	146.63	31	148.53	17	147.79	47
B4	158.26	32	160.65	17	159.89	37
B γ	167.57	28	167.27	23	166.46	40

Compound Number 2010



coniferyl benzoate

3-Phenyl-acrylic acid 3-(4-hydroxy-3-methoxyphenyl)allyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.86	s	
γ	4.94	dd	6.5, 1.3
β	6.34	dt	15.8, 6.5
α	6.72	dt	15.8, 1.3
A5	6.80	d	8.1
A6	6.93	dd	8.1, 2.0
A2	7.14	d	2.0
B3,5	7.50	m	
B4	7.62	m	
B2,6	8.03 - 8.06	m	
ArOH	7.76	s	

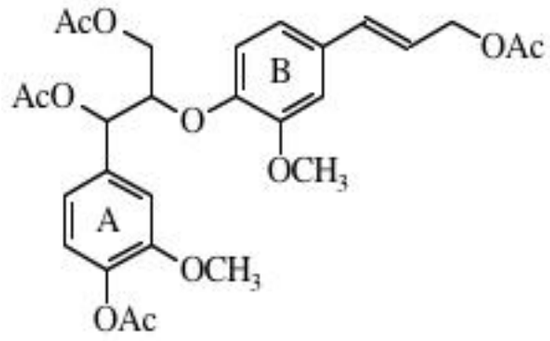
Notes:

S. Quideau
isolated from gum s.am

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.86	43	56.21	59	55.61	58
γ	65.74	45	66.35	60	65.55	45
A2	108.39	41	110.25	57	109.96	46
A5	114.44	40	115.84	43	115.45	44
A6	120.64	43	121.29	64	120.23	80
β	120.81	44	121.32	64	120.23	80
B3	128.32	95	129.37	100	128.82	96
B5	128.32	95	129.37	100	128.82	96
A1	128.76	21	129.31	100	127.52	30
B2	129.61	100	130.17	94	129.20	100
B6	129.61	100	130.17	94	129.20	100
B1	130.24	13	131.30	17	129.78	24
B4	132.93	45	133.86	59	133.39	50
α	134.50	44	135.34	60	134.29	50
A3	146.63	20	148.54	18	147.79	36
A4	145.91	23	147.89	18	146.93	31
B α C=O	166.46	16	166.58	16	165.62	25

Compound Number 2011



threo

Guaiacylglycerol-β-coniferyl ether peracetate

^{1}H (acetone)

Atom	H Shifts	Mult	J

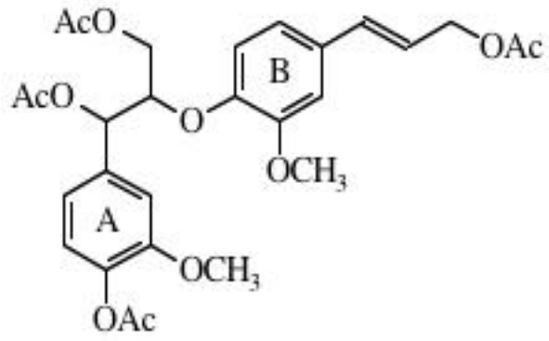
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.63		20.44		20.38	
α Ac Me	20.68		20.58		20.46	
γAc Me	20.99		20.78		20.75	
Bγ Ac Me	21.02		20.91		20.72	
A3 OMe	55.81		56.24		55.67	
B3 OMe	55.93		56.29		55.84	
γ	63.02		63.56		62.49	
B γ	65.08		65.36		64.45	
α	74.40		75.32		74.28	
β	80.19		80.56		78.95	
B2	110.17		111.31		110.22	
A2	111.66		112.64		111.65	
B5	118.31		118.74		116.99	
A6	119.54		120.30		119.46	
B6	119.82		120.54		119.56	
Bβ	122.13		123.26		122.35	
A5	122.83		123.56		122.74	
B1	131.54		132.35		130.64	
B α	133.87		134.16			
					132.99	
A1	135.18		136.61		135.40	
A4	139.92		140.92		139.23	
B4	148.02		149.09		147.56	
B3	150.71		151.75		150.09	
A3	151.12		152.22		150.73	
A4 Ac C=O	168.76		168.89		168.48	
αAc C=O	169.65		170.00		169.45	
γAc C=O	170.54		170.68		170.05	
BγAc C=O	170.84		170.77		170.21	

Compound Number 2012



erythro

Guaiacyl glycerol-β-coniferyl ether peracetate

Acetic acid 4-{1,3-diacetoxy-2-[4-(3-acetoxypropenyl)-2-methoxyphenoxy] propyl}-2-methoxyphenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.93	s	
B γ Ac Me	2.02	s	
α Ac Me	2.07	s	
A4 Ac Me	2.21	s	
A3 OMe	3.82	s	
B3 OMe	3.85	s	
γ1	4.22	dd	11.9, 4.1
γ2	4.36	dd	11.9, 5.9
B γ	4.66	dd	6.4, 1.4
β	4.85	m	
α	6.06	d	5.1
B β	6.26	dt	15.9, 6.4
B α	6.62	dt	15.9, 1.4
B6	6.93	dd	8.3, 2.0
B5	6.97	d	8.3
A5	7.02	d	8.1
A6	7.05	dd	8.1, 1.8
B2	7.13	d	2.0
A2	7.25	d	1.8

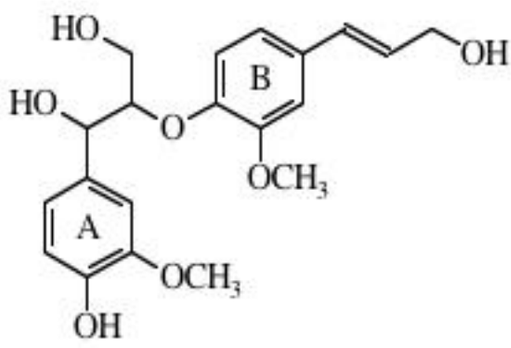
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.64		20.45	87	20.39	
α Ac Me	20.74		20.59	92	20.47	
γ Ac Me	20.99		20.77	86	20.69	
B γ Ac Me	20.99		20.85	90	20.75	
A3 OMe	55.80		56.25	100	55.72	
B3 OMe	55.91		56.27	100	55.78	
γ	62.53		62.98	71	61.92	
B γ	65.07		65.34	93	64.43	
α	73.70		74.49	83	73.07	
β	80.17		80.27	88	78.29	
B2	110.24		111.38	86	110.40	
A2	111.94		112.73	76	111.69	
B5	119.11		119.36	82	117.51	
A6	119.65		120.39	80	119.37	
B6	119.80		120.48	80	119.56	
B β	122.23		123.37	97	122.48	
A5	122.60		123.35	97	122.58	
B1	131.86		132.63	49	130.93	
B α	133.85		134.12	82	132.96	
A1	135.28		136.59	63	135.34	
A4	139.78		140.79	38	139.11	
B4	147.23		148.27	44	146.63	
B3	150.98		151.98	46	150.32	
A3	151.02		152.11	46	150.60	
A4 Ac C=O	168.80		168.90	38	168.51	
α Ac C=O	169.49		169.88	45	169.33	
γ Ac C=O	170.76		170.74	77	170.12	
B γ Ac C=O	170.83		170.74	77	170.21	

Compound Number 2013



threo

Guaiacylglycerol-β-coniferyl ether

1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxypropenyl)-2-methoxyphenoxy]propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.48	dd	11.9, 5.7
γ2	3.67	dd	11.9, 3.7
A,B γ OH	3.80-3.90		
A3 OMe	3.80	s	
B3 OMe	3.88	s	
B γ	4.20	br dd	5.3, 1.6
β	4.20	m	
α OH	4.45	d	3.9
α	4.87	br d	5.5
B β	6.28	dt	15.9, 5.4
B α	6.52	dt	15.9, 1.6
A5	6.76	d	8.1
A,B 6	6.88-6.91	m	
A2	7.08	d	1.9
B2	7.09	d	1.9
B5	7.11	d	8.4
A4 OH	7.50	br s	

^{13}C

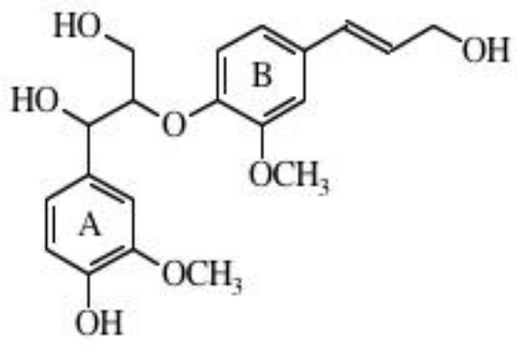
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe	55.97	83	56.19	100	55.44	75
B3 OMe	56.03	100	56.31	90	55.83	69
γ	61.21	22	61.88	60	60.16	50
B γ	63.56	57	63.25	100	61.65	100
α	74.07	21	73.83	50	71.01	35
β	89.47	54	88.37	80	84.36	36
B2	108.94	44	110.85	50	109.84	42
A2	110.00	68	111.42	40	111.05	38
A5	114.37	32	115.21	30	114.71	39
B5	120.15	63	119.57	90	115.53	42
B6	120.29	55	120.31	60	119.05	29
A6	120.83	53	120.54	80	119.10	51
B β	128.24	67	129.63	70	128.58	83
B α	130.53	67	129.85	90	128.60	83
B1	131.55	19	132.96	40	130.18	46
A1	133.15	28	133.82	40	132.97	43
A4	144.75	26	146.83	30	145.46	64
A3	145.71	16	148.03	30	147.03	48
B4	147.47	33	149.15	40	147.88	42
B3	151.33	35	151.69	40	149.70	25

Notes:

S. Quideau

α (e/t) and γ shifts (e/t) interchange from sample to sample, probably due to H-exchange of OH's in d6-acetone. CDCl3 and DMSO shifts not substantiated.

Compound Number 2014



erythro

Guaiacylglycerol-β-coniferyl ether

1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxypropenyl)-2-methoxyphenoxy]propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.69	dd	11.8, 4.0
γ2	3.81	dd	11.8, 6.2
A,B γ OH	3.80-3.90		
A3 OMe	3.80	s	
B3 OMe	3.84	s	
B γ	4.19	br dd	5.4, 1.6
β	4.29	m	
α OH	4.57	d	4.6
α	4.89	br d	5.2
B β	6.26	dt	15.9, 5.4
B α	6.50	dt	15.9, 1.6
A5	6.75	d	8.1
A,B6	6.86-6.89	m	
B5	6.91	d	1.9
B2	7.05	d	1.9
A2	7.10	d	8.4
A4 OH	7.47	br s	

^{13}C

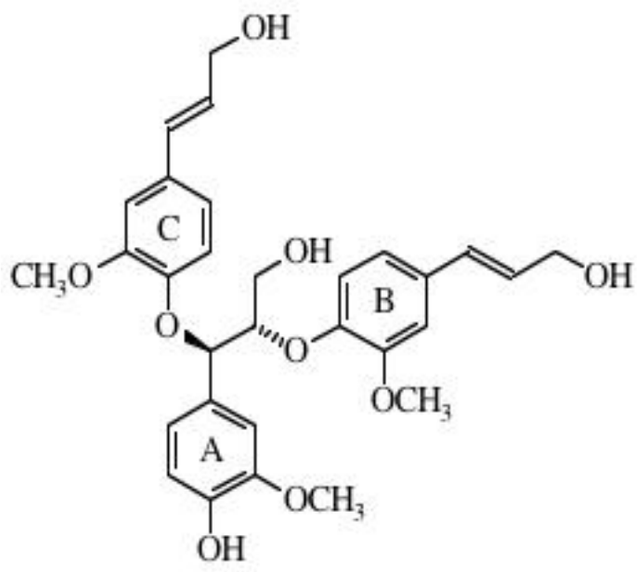
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe	55.97	84	56.21	100	55.64	100
B3 OMe	56.03	100	56.29	100	55.64	100
γ	60.87	16	61.82	60	60.16	92
B γ	63.56	58	63.25	99	61.65	92
α	72.96	11	73.81	70	71.67	24
β	87.34	43	86.63	49	83.75	23
B2	108.82	44	110.99	87	109.93	29
A2	110.05	68	111.44	92	111.47	24
A5	114.37	32	115.13	43	114.60	26
B5	119.14	42	119.27	58	115.60	38
B6	120.09	45	120.23	62	119.05	27
A6	120.79	54	120.46	86	119.54	27
B β	128.19	63	129.54	55	128.52	34
B α	130.56	61	129.87	92	128.60	78
B1	131.86	10	132.84	35	130.08	34
A1	133.11	34	134.24	35	133.23	28
A4	143.98	20	146.65	21	145.46	60
A3	145.27	14	147.96	27	147.00	40
B4	146.75	25	148.55	29	147.60	29
B3	151.62	22	151.88	31	149.75	44

Notes:

S. Quideau

α (e/t) and γ shifts (e/t) interchange from sample to sample, probably due to H-exchange of OH's in d6-acetone. CDCl3 and DMSO shifts not substantiated.

Compound Number 2015



erythro

Guaiacylglycerol-α,β-bis-coniferyl ether

4-{3-Hydroxy-1,2-bis-[4-(3-hydroxypropenyl)-2-methoxy phenoxy]propyl}-2-methoxyphenol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.46	d	5.5
A β	4.56	m	
A γ1	3.81□	dd	11.7, 7.1
A γ2	3.93	dd	11.7, 4.1

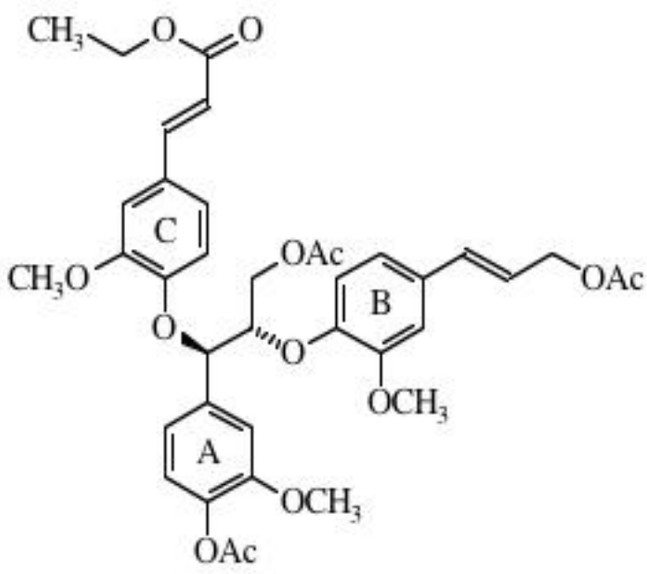
Notes:

S. Quideau Shifts for α and β's and A,B,C 1's change places in CDCl3 and DMSO
S. Quideau, and J. Ralph, A biomimetic route to lignin model compounds via silver (I) oxide oxidation. 2. NMR characterization of non-cyclic benzyl aryl ethers, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe	55.76	82	56.18	83	55.41	88
B3 OMe	55.85	92	56.20	83	55.61	100
C3 OMe	55.93	100	56.32	76	55.80	100
γ	62.17	40	61.75	46	59.74	31
B γ	63.56	61	63.25	100	61.52	71
C γ	63.63	64	63.25	100	61.58	72
α	81.68	52	81.15	49	79.01	39
β	85.42	56	85.31	57	82.53	40
C2	109.38	61	110.74	50	109.93	62
B2	109.54	56	110.93	51	109.93	62
A2	109.77	62	112.11	53	111.91	41
A5	114.26	54	115.23	46	114.74	31
C5	115.94	57	117.02	54	115.71	48
B5	119.13	58	119.04	59	116.15	41
C6	119.49	64	119.90	67	118.87	58
B6	119.74	61	120.15	66	119.00	53
A6	120.33	55	121.49	57	120.34	35
C β	127.10	68	129.22	56	128.32	72
B β	127.60	70	129.45	61	128.47	58
B α	130.59	62	129.85	100	130.49	79
C α	130.79	62	129.85	100	130.49	79
A1	130.43	49	130.39	41	128.24	40
C1	130.85	66	132.05	38	128.71	58
B1	132.09	45	132.74	41	128.82	58
A4	145.49	50	147.18	32	146.07	45
C4	146.64	47	147.77	33	146.27	58
A3	146.85	44	148.10	31	147.11	45
B4	147.08	45	148.61	36	147.36	58
C3	149.80	47	151.17	41	149.73	61
B3	150.81	46	151.71	40	149.80	61

Compound Number 2016



erythro

3-(4-{3-Acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-[4-(3-acetoxypropenyl)-2-methoxyphenoxy]propoxy}-3-methoxyphenyl) acrylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.45	dd	11.8, 3.8
γ2	4.53	dd	11.9, 6.0
B γ	4.66	dd	6.4, 1.3
β	4.88	m	
α	5.71	d	5.3
B β	6.25	dt	15.8, 6.4
C β	6.39	d	15.9
B α	6.61	dt	15.8, 1.3
C α	7.53	d	15.9

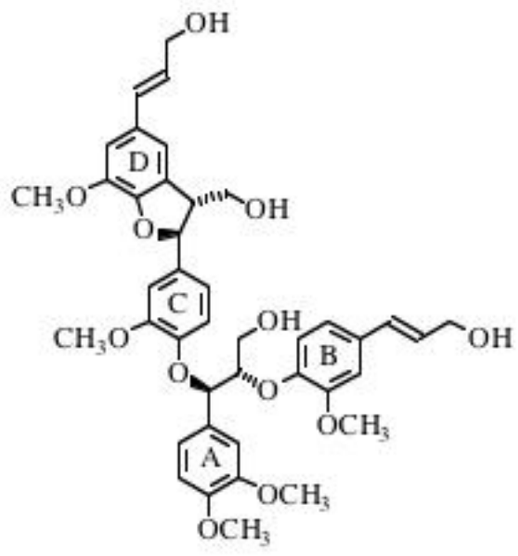
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Me	14.33	90	14.57	85	14.19	73
A4 Ac Me	20.65	94	20.43	100	20.33	77
γ Ac Me	20.74	84	20.60	62	20.43	81
B γAc Me	21.00	88	20.77	100	20.71	100
A OMe	55.73	61	56.16	92	55.67	97
B OMe	55.96	82	56.20	62	55.80	54
C OMe	55.98	100	56.44	62	55.95	61
CH2	60.39	75	60.56	62	59.79	53
γ	63.22	44	63.41	38	62.33	24
B γ	65.09	87	65.37	54	64.41	59
α	79.99	42	80.47	38	78.45	27
β	81.98	50	81.70	46	79.57	33
B2	110.14	72	111.19	38	110.22	37
C2	110.73	65	111.92	38	111.40	41
A2	111.17	48	112.80	46	111.89	38
C5	115.87	54	116.69	38	115.28	34
C β	116.51	47	117.15	46	116.25	39
B5	119.10	58	119.28	69	117.18	40
A6	119.34	42	120.33	54	119.35	28
B6	119.82	62	120.47	62	119.50	45
C6	122.08	75	122.57	62	122.33	39
B β	122.15	75	123.17	69	122.24	43
A5	122.66	68	123.36	46	122.49	25
C1	128.62	52	129.41	46	127.56	39
B1	131.71	50	132.37	46	130.59	43
B α	133.90	79	134.18	69	133.00	53
A1	136.48	56	137.19	31	135.93	31
A4	139.64	57	140.63	46	138.94	51
C α	144.28	58	144.96	46	144.23	42
B4	147.35	39	148.51	23	146.96	50
C4	149.33	52	150.06	31	148.42	47
C3	150.23	53	151.36	46	149.75	44
B3	150.96	55	151.86	23	150.12	53
A3	151.20	43	152.12	38	150.49	38
C γ C=O	167.13	52	167.23	69	166.40	53
A4 Ac C=O	168.78	48	168.90	54	168.36	44
γAc C=O	170.77	27	170.81	31	170.09	48
B γ Ac C=O	170.86	55	170.82	69	170.14	54

Notes:

S. Quideau Shifts substantiated in d6-acetone but not CDCL3 or DMSO. γ and Bγ Ac C=O shifts may be interchanged S. Quideau, and J. Ralph, A biomimetic route to lignin model compounds via silver (I) oxide oxidation. 2. NMR characterization of non-cyclic benzyl aryl ethers, Holzforschung, 1994, 48(2), 124-132.

Compound Number 2017



erythro

Veratryglycerol-α-dehydrodiconifyl-β-con.ether

^{1}H Acetone/D2O

Atom	H Shifts	Mult	J
A α	5.48	d	5.8
A β	4.62	m	
A γ1	3.80□	dd	11.9, 6.5
A γ2	3.91	dd	11.9, 4.9
C α	5.51	d	5.8
C β	3.43	m	
C γ1	3.69□	s	
C γ2	3.80	s	

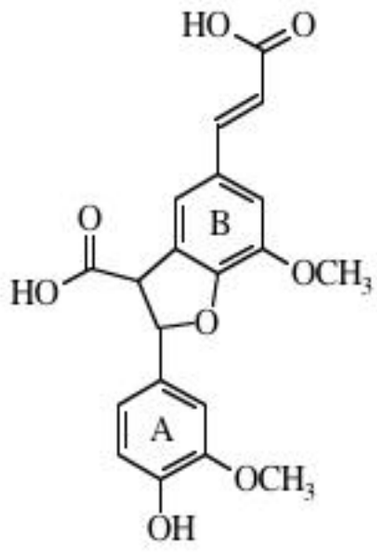
Notes:

S. Quideau Run only in Acetone:D2O (9:1) S. Quideau, and J. Ralph,, Holzforschung, 1994, 48(2), 124-132. Note: Two erythro isomers!! Resolvable pairs are:80.10, 80.05 54.28, 54.21 136.08, 136.05 110.98, 110.89 147.31, 147.30 116.41, 116.42 118.42, 118.40

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
			Note*			
C β			54.28	30		
A3 OMe			55.83	100		
A4 OMe			55.80	72		
B OMe			56.09	100		
D OMe			56.20	100		
C OMe			56.33	86		
γ			61.20	46		
B γ			62.77	94		
D γ			62.85	50		
C γ			64.18	52		
α			80.10	29		
β			83.86	46		
C α			87.80	55		
B2			110.71	66		
C2			110.98	29		
D2			111.35	46		
A5			111.67	44		
A2			112.04	47		
D6			115.96	59		
C5			116.41	24		
B5			117.55	49		
C6			118.42	49		
B6			119.99	64		
A6			120.96	36		
D β			127.73	65		
B β			128.64	64		
B α			130.02	85		
D5			129.64	33		
D α			130.57	39		
A1			130.94	39		
D1			131.83	53		
B1			132.11	46		
C1			136.08	24		
D3			144.75	61		
C4			147.31	25		
B4			147.98	48		
D4			148.27	24		
A3			149.45	53		
A4			149.48	53		
C3			150.58	50		
B3			150.83	50		

Compound Number 2018



beta-5-dehydrodiferulic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	6.05	d	7.8
β	4.39	d	7.8
A2	7.08	d	2.0
A5	6.83	d	8.1
A6	6.91	dd	8.1, 2.0
A3 OMe	3.83	s	
B α	7.62	d	15.9
B β	6.39	d	15.9
B2	7.29	br s	
B6	7.33	br s	
B3 OMe	3.91	s	

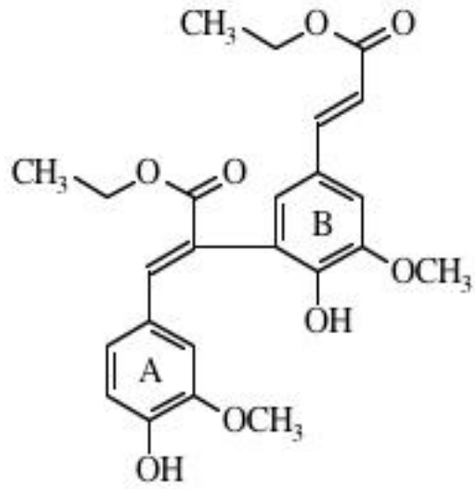
Notes:

S. Quideau
B α changes in CDCl3
JCS Perkin 1, 3485-98 (1994)
Cmpd 13

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe	56.03	55	56.31	82	55.61	80
B3 OMe	56.15	47	56.49	70	55.85	80
β	53.76	46	56.22	100	55.10	20
α	87.53	24	88.56	49	87.72	29
A2	108.77	93	110.72	57	110.61	70
B2	112.26	18	113.34	41	112.10	38
A5	114.53	20	115.78	57	115.30	61
B β	114.91	79	116.75	42	116.43	100
B6	118.63	26	118.95	42	117.93	49
A6	119.49	100	120.08	60	119.50	73
B5	125.93	24	128.05	35	127.82	43
B1	128.29	26	129.38	34	130.69	24
A1	131.44	29	132.49	31	137.46	15
B α	146.74	46	145.59	41	144.09	49
B3	144.71	80	145.73	34	144.19	49
A4	146.06	30	147.81	30	146.79	31
A3	146.74	46	148.53	31	147.60	60
B4	150.32	28	150.96	24	149.16	49
B γ	171.34	28	168.18	42	167.79	49
γ	173.67	31	172.55	38	171.66	42

Compound Number 2019



3-(4-Hydroxy-3-methoxyphenyl)-2-[2-hydroxy-3-methoxy-5-(2-propoxycarbonylvinyl)phenyl] acrylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.21	t	7.1
CH3	1.24	t	7.1
A3 OMe	3.44	s	
B3 OMe	3.96	s	
CH2	4.16	q	7.1
CH2	4.17	q	7.1
B β	6.38	d	15.9
A2	6.696	d	2.1
A5	6.702	d	8.2
A6	6.83	dd	8.2, 2.1
B6	7.00	d	2.0
B2	7.38	d	2.0
B α	7.56	d	15.9
A α	7.76	s	

Notes:

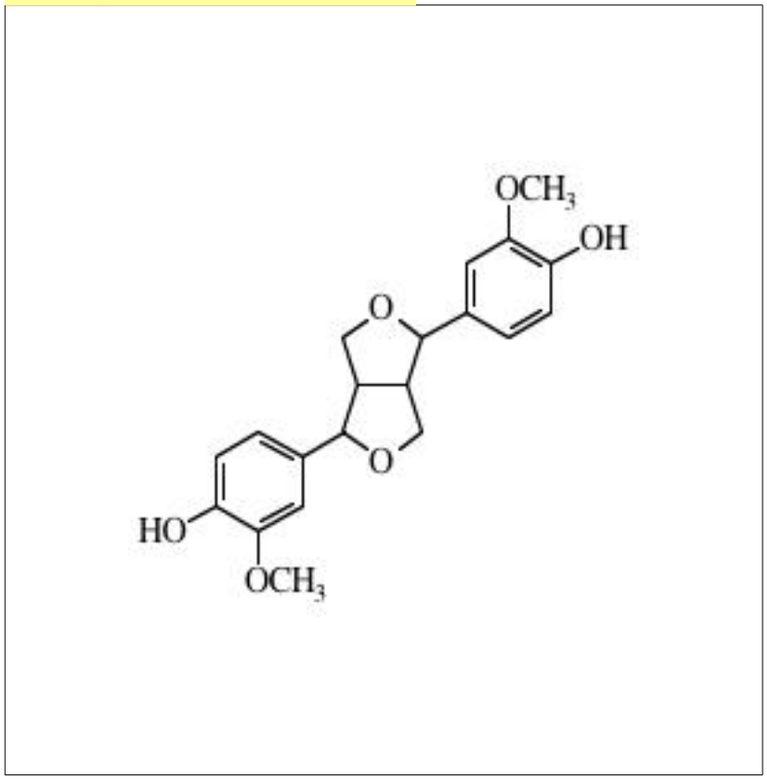
S. Quideau

B5,B6 and A6 switch in acetone and DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	14.28	100	14.61	100	14.14	100
CH3	14.28	100	14.62	100	14.16	94
A3 OMe	55.24	74	55.51	81	54.66	78
B3 OMe	56.12	72	56.58	88	56.05	74
CH2	60.35	71	60.47	79	59.62	64
CH2	61.09	69	61.05	74	60.15	61
B2	108.68	58	110.25	76	110.05	38
A2	111.57	61	113.28	81	112.92	48
A5	114.29	65	115.63	81	115.02	45
B β	116.00	63	116.31	76	115.17	50
β	123.29	41	124.92	38	123.97	44
B5	124.76	43	126.56	45	125.09	45
B6	124.82	62	125.71	76	124.61	42
A6	125.82	61	126.37	81	125.16	48
B1	126.81	48	127.31	50	125.56	51
A1	126.94	50	127.58	50	125.66	49
α	141.45	53	141.37	71	140.11	39
B α	144.30	60	145.25	74	144.49	42
A3	145.86	45	147.87	45	147.02	58
B4	146.05	44	148.03	43	147.11	46
A4	147.11	51	148.99	52	148.16	52
B3	147.31	44	149.10	45	148.23	59
B γ	167.11	43	167.29	40	166.44	52
γ	167.46	34	167.77	33	166.83	43

Compound Number 2020



Pinoresinol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.08	m	
γ1	3.80	dd	9.1, 3.8
OMe	3.83	s	
γ 2	4.19	dd	9.0, 7.0
α	4.66	d	4.25
A5	6.78	d	8.1
A6	6.83	dd	8.1, 1.8
A2	6.98	d	1..8
Ar OH	7.48	s	

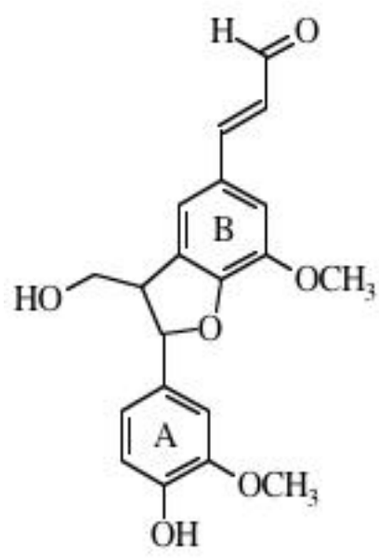
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	54.15	98	55.23	86	53.59	72
OMe	55.94	98	56.24	93	55.62	100
γ	71.66	98	72.20	88	70.91	70
α	85.86	98	86.62	83	85.17	72
2	108.60	95	110.60	80	110.43	72
5	114.27	93	115.52	69	115.15	73
6	118.95	100	119.59	100	118.64	75
1	132.91	51	134.17	46	132.26	61
4	145.24	59	146.86	47	145.91	66
3	146.70	48	148.32	32	147.53	66

Notes:

S. Quideau
As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 2021



erythro

3-[2-(4-Hydroxy-3-methoxyphenyl)-3-hydroxymethyl-7-methoxy-2,3-dihydrobenzofuran-5-yl] prop-2-enal

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.61	br q	
A3 OMe	3.82	s	
B3 OMe	3.91	s	
γ	3.87-3.91	m	
α	5.65	d	6.6
B β	6.65	dd	15.8, 7.7
A5	6.81	d	8.1
A6	6.88	dd	8.1, 2.0
A2	7.04	d	2.0
B2	7.29	bro	
B6	7.32	bro	
B α	7.59	d	15.8
B γ	9.63	d	7.7

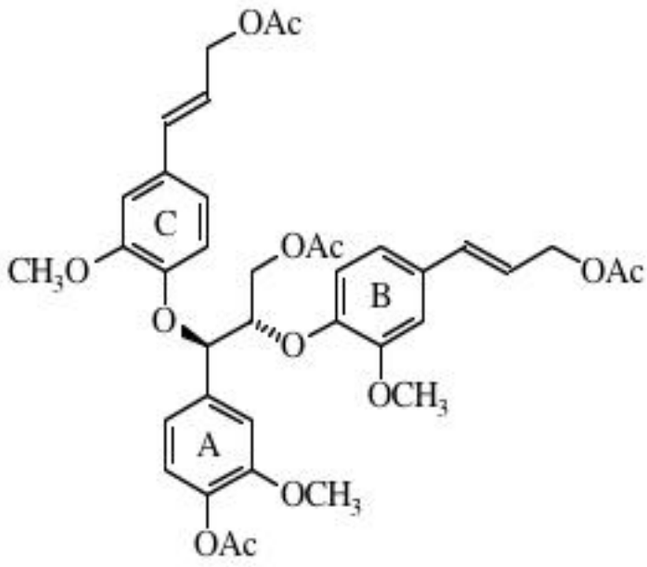
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β			54.25	59		
A3 OMe			56.29	100		
B3 OMe			56.46	81		
γ			64.32	54		
α			89.39	82		
A2			110.59	94		
B2			113.56	67		
A5			115.76	61		
B6			119.64	85		
A6			119.73	83		
B β			127.14	76		
B5			129.00	59		
B1			131.24	41		
A1			133.75	40		
B3			145.65	41		
A4			147.55	31		
A3			148.46	23		
B4			152.41	22		
B α			154.10	77		
B γ			193.77	87		

Compound Number 2022



erythro

Guaiacylglycerol-α,β-bis coniferyl ether acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.62		
A β	4.87		
A γ1	4.45		
A γ2	4.53		

Notes:

S. Quideau

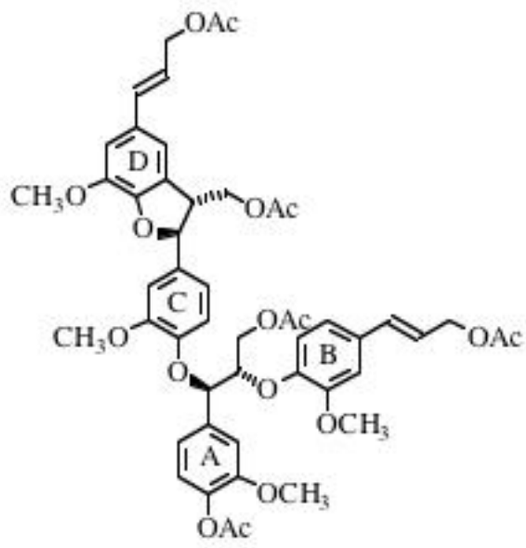
α and β of B and C can interchange in CDCl3

S. Quideau, and J. Ralph, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.63	45	20.44	57	20.33	87
γ Ac Me	20.73	40	20.62	57	20.42	87
C γ Ac Me	20.98	100	20.76	58	20.70	92
B γAc Me	20.98	77	20.78	55		
					20.70	92
A3 OMe	55.73	37	56.23	100	55.59	89
B3 OMe	55.91	44	56.23	100	55.64	89
C3 OMe	55.94	44	56.39	100	55.78	94
γ	63.37	20	63.56	28	62.39	31
C γ	65.08	35	65.37	55	64.39	100
B γ	65.12	41	65.37	55	64.39	100
α	80.17	25	80.85	31	78.68	38
β	81.92	24	81.74	36	79.56	31
C2	109.94	29	111.16	36	110.15	52
B2	110.11	29	111.32	41	110.21	52
A2	111.29	25	112.74	35	111.87	38
C5	116.41	28	117.41	35	115.81	52
B5	118.92	28	119.23	44	117.06	48
C6	119.49	26	120.45	51	119.43	70
B6	119.77	37	120.50	51	119.48	70
A6	119.79	37	120.51	51	119.50	70
C β	121.69	31	122.99	44	122.12	58
B β	122.03	31	123.18	47	122.19	59
A5	122.50	26	123.26	39	122.38	31
C1	130.61	24	131.73	38	130.12	45
B1	131.55	24	132.34	41	130.51	50
C α	133.92	32	134.22	91	133.00	76
B α	134.02	35	134.22	91	133.00	76
A1	136.80	24	137.52	40	136.19	57
A4	139.53	21	140.65	26	138.88	49
C4	147.45	26	148.20	39	146.38	48
B4	147.47	26	148.66	29	146.99	54
C3	150.18	25	151.43	40	149.75	49
B3	150.90	23	151.91	40	150.09	58
A3	151.09	22	152.12	32	150.45	52
A4 Ac C=O	168.76	23	168.85	35	168.34	50
A γ Ac C=O	170.76	29	170.72	32	170.07	73
D γ Ac C=O	170.83	29	170.74	32	170.10	73
C γ Ac C=O	170.83	29	170.77	40	170.12	73

Compound Number 2023



erythro

Guaiacylglycerol-α-dehydrodiconiferyl-bis-ether peracetate diastereomeric mixture

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.62	d	5.4
A β	4.88	m	
A γ1	4.46	dt	11.9, 3.8
A γ2	4.53	dt	11.9, 5.8
C α	5.49	d	6.9
C β	3.72	s	
C γ1	4.28	dd	11.1, 7.5
C γ2	4.40	dd	11.1, 5.4

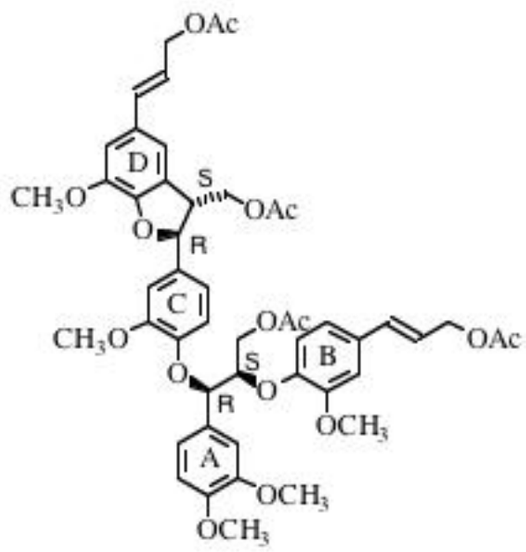
Notes:

S. Quideau
S. Quideau
S. Quideau, and J. Ralph, A biomimetic route to lignin model compounds via silver (I) oxide oxidation. 2. NMR characterization of non-cyclic benzyl aryl ethers, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.52	88	20.43	97	20.32	
A γAc Me	20.61	88	20.61	89	20.42	
C γ Ac Me	20.74	100	20.65	89	20.48	
B γ Ac Me	20.98	89	20.78	95	20.70	
D γ Ac Me	20.98	89	20.78	95	20.70	
OMe			56.39	78		
OMe			56.31	77		
OMe			56.17	100		
OMe			56.15	100		
C β	50.25	35	51.04	49	49.16	
γ	63.36	35	63.52	50	62.38	
B γ	65.06	84	65.36	85	64.40	
D γ	65.16	84	65.48	35	64.49	
C γ	65.28	43	65.84	55	68.42	
α	80.13	34	80.73	42	78.62	
β	81.87	47	81.63	48	79.49	
C α	88.38	30	88.61	38	87.25	
B2	110.09	75	111.17	30	110.20	
C2	110.17	75	111.36	57	110.74	
D2	110.61	55	112.02	30	110.93	
A2	111.33	32	112.69	45	111.89	
D6	115.31	39	116.24	32	115.24	
C5	116.39	41	117.29	31	115.76	
C6	118.64	29	119.11	31	118.35	
B5	118.89	62	119.11	31	117.00	
A6	119.51	38	120.45	81	119.43	
B6	119.77	70	120.46	81	119.49	
D β	121.13	60	122.13	66	121.31	
B β	122.01	67	123.10	74	122.18	
A5	122.47	52	123.24	57	122.38	
D5	127.53	32	128.99	42	127.93	
D1	130.49	41	131.41	48	129.99	
B1	131.52	45	132.23	49	130.48	
B α	133.90	69	134.20	74	133.00	
D α	134.31	65	134.69	74	133.50	
C1	134.49	65	135.94	27	134.13	
A1	136.76	39	137.49	28	136.18	
A4	139.52	43	140.56	47	138.88	
D3	144.36	42	145.32	44	143.83	
C4	147.36	45	147.96	37	146.31	
B4	147.45	45	148.56	46	146.95	
D4	148.22	27	149.22	46	147.51	
C3	150.35	27	151.33	30	149.63	
B3	150.87	47	151.82	55	150.07	
A3	151.06	36	152.05	46	150.44	
A4 Ac C=O	168.72		168.84		168.33	
B γ Ac C=O	170.74		170.74		170.12	
D γ Ac C=O	170.74		170.74		170.12	
A γ Ac C=O	170.80		170.76		170.12	
C γ Ac C=O	170.83		170.90		170.23	

Compound Number 2024



threo

Veratrylglycerol-α-dehydrodiconiferyl-β-coniferyl-bis-ether peracetate, diastereomeric mixture

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.54	d	5.2
A β	4.87	s	
A γ1	4.44	td	11.8, 3.7
A γ2	4.52	td	11.8, 6.2
C α	5.48	d	6.9
C β	3.70	s	
C γ1	4.28	dt	11.1, 7.5
C γ2	4.39	dt	11.1, 5.5

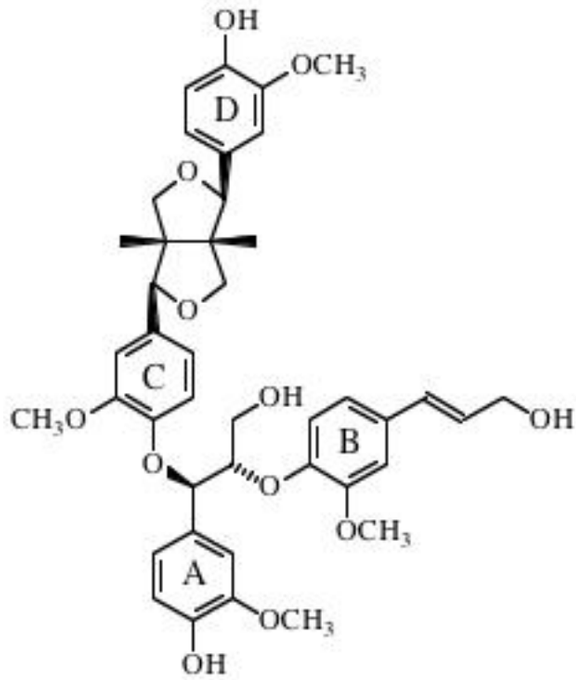
Notes:

S. Quideau
A3 and A4, C and D OMe's, and B and D γ's can be interchanged in all solvents Shifts are confirmed for Acetone
S. Quideau, and J. Ralph, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A γ Ac Me	20.75	72	20.64	98	20.45	97
C γAc Me	20.75	72	20.64	98	20.45	97
B γ Ac Me	20.98	100	20.79	98	20.70	97
D γAc Me	20.98	100	20.79	98	20.70	97
A4 OMe	55.75	89	55.97	94	55.33	99
A3 OMe	55.82	94	56.06	100	55.59	99
B3 OMe	55.86	94	56.22	100	55.70	99
C3 OMe	56.06	64	56.38	85	55.79	99
D3 OMe	55.97					
C β	50.18	28	51.08	39	49.16	54
γ	63.67	28	63.86	52	62.64	40
B γ	65.09	79	65.38	98	64.41	100
D γ	65.17	87	65.49	98	64.50	100
C γ	65.28	50	65.90	59	64.71	49
α	80.14	33	80.89	46	78.77	29
β	81.80	31	81.73	53	79.57	38
C α	88.43	28	88.65	44	87.28	52
B2	110.02	56	111.28	81	110.17	63
C2	110.33	29	111.45	39	110.63	29
D2	110.17	43	112.16	69	110.93	58
A5	110.56	56	112.22	69	111.25	45
A2	110.79	42	112.31	69	111.12	32
D6	115.29	38	116.31	52	115.24	46
C5	116.53	23	117.46	29	115.95	26
B5	118.47	51	118.91	48	116.79	46
C6	118.59	51	119.11	40	118.27	28
B6	119.73	57	120.48	73	119.49	66
A6	119.95	57	120.98	28	119.81	25
D β	121.16	48	122.19	76	121.32	61
B β	121.91	47	123.04	65	122.09	58
D5	127.57	30	129.06	38	127.93	53
A1	130.18	24	130.90	28	129.46	30
D1	130.49	32	131.46	49	129.99	58
B1	131.24	36	132.08	40	130.30	51
B α	133.94	58	134.26	75	133.03	76
C 1	134.12	38	135.74	28	133.92	39
D α	134.32	64	134.71	81	133.51	67
D3	144.37	43	145.37	49	143.83	63
C4	147.38	28	148.11	32	146.38	34
B4	147.71	33	148.83	40	147.12	51
D4	148.21	35	149.29	40	147.51	51
A3	148.83	32	150.20	44	148.37	51
A4	148.93	31	150.23	44	148.48	48
C3	150.39	25	151.42	31	149.69	33
B3	150.78	37	151.81	47	150.02	58
D γ Ac C=O	170.70		170.76		170.05	
B γ Ac C=O	170.77		170.76		170.10	
A γ Ac C=O	170.82		170.79		170.13	
C γ Ac C=O	170.85		170.90		170.23	

Compound Number 2025



erythro

Guaiacylglycerol-α-pinoresinol-β-coniferyl-bis-ether diastereomeric mixture

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.45	d	5.6
A β	4.55	m	
A γ1	3.82	dd	11.5, 6.5
A γ2	3.92	dd	11.5, 5.2
C α	4.63		
C β	3.04		
C γ1	3.77		
C γ2	4.17		

Notes:

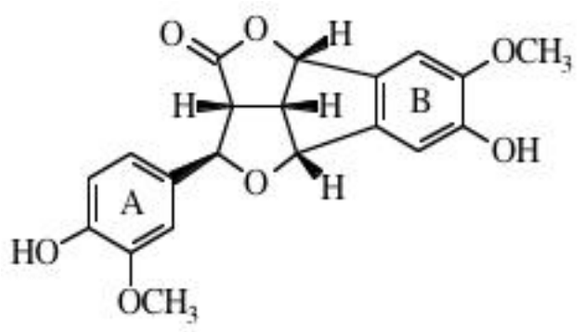
S. Quideau Only run in acetone

S. Quideau, and J. Ralph, A biomimetic route to lignin model compounds via silver (I) oxide oxidation. 2. NMR characterization of non-cyclic benzyl aryl ethers, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
D β			55.15	100		
C β			55.15	100		
D3 OMe			56.22	75		
A3 OMe			56.25	75		
B3 OMe			56.25	74		
C3 OMe			56.44	52		
γ			61.82	28		
B γ			63.27	44		
D γ			72.23	71		
C γ			72.23	71		
α			81.21	28		
β			85.38	36		
C α			86.37	51		
D α			86.58	36		
D2			110.59	52		
B2			111.05	43		
C2			111.43	22		
A2			112.21	19		
A5			115.28	32		
D5			115.50	45		
C5			116.83	24		
C6			118.96	20		
B5			119.06	43		
D6			119.61	61		
B6			120.17	42		
A6			121.53	23		
B β			129.50	37		
B α			129.88	42		
A1			130.53	27		
B1			132.78	33		
D1			134.10	32		
C1			136.29	22		
D4			146.85	26		
A4			147.24	12		
C4			147.61	23		
A3			148.15	16		
D3			148.30	22		
C3			151.12	17		
B3			151.75	21		

Compound Number 2026



11-hydroxy-(4-hydroxy-3methoxyphenyl)-10-methoxy-3a,4,6,6a-tetrahydro 3H-3,4-benzenofuro [3,4-c]f uran-1-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.36	dd	10.7, 6.4
B β	4.24	dddd	10.6, 7.5, 6.9, 0.6
α	4.72	dquin	6.3, 0.6
B α	5.73	br d	
B γ	5.60	dq	

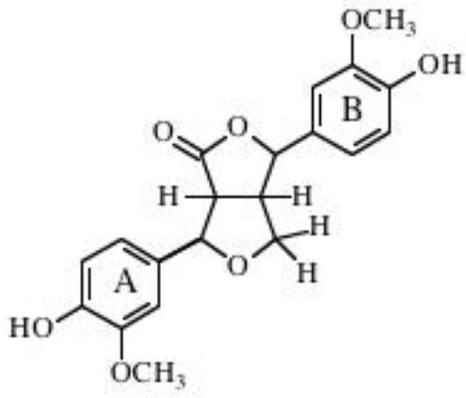
Notes:

S. Quideau
Ref: S. Quideau and John Ralph. J. Chem Soc. Perkin Trans. 1 1993 - issue 6 - 653 -659.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	50.40	100	51.13	86	49.78	54
β	53.87	88	54.58	81	53.16	50
B3 OMe	56.14	90	56.38	94	55.67	99
A3 OMe	55.95	93	56.25	92	55.58	100
α	82.38	87	84.18	90	83.14	62
B α	83.33	88	84.22	100	83.27	58
B γ	85.74	91	86.62	87	85.15	61
B2	106.87	84	108.57	78	108.24	50
A2	108.61	91	110.78	90	110.60	65
B5	110.88	83	112.10	66	111.46	54
A5	114.39	87	115.56	72	115.12	66
A6	118.82	90	119.80	90	118.98	65
A1	131.09	40	132.41	41	130.35	58
B1	132.06	37	133.24	34	131.52	63
B6	133.95	37	135.28	43	133.78	51
A4	145.52	40	147.28	35	146.38	65
A3	146.60	42	148.30	33	147.50	60
B4	148.42	40	150.03	42	149.01	63
B3	148.69	44	150.43	29	149.63	57
γ	176.43	43	177.32	46	176.86	65

Compound Number 2027



4-cis-8-trans-bis (4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo [3-3-0] octan-2-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.63	t	8.8
B β	3.35	ddd	9.0, 6.6, 4.6
α	5.05	br d	8.6
B α	5.23	br d	6.6
B γ cis	3.88	dd	9.5, 4.8
B γ trans	4.28	br d	9.5

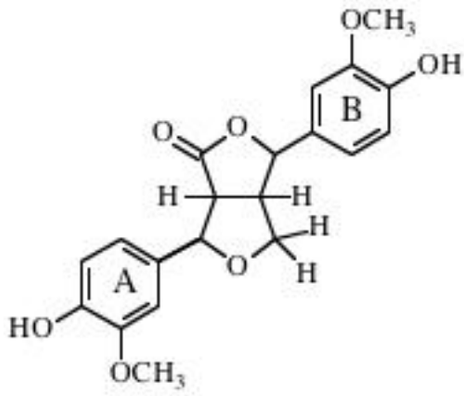
Notes:

S. Quideau
S. Quideau and John Ralph. J. Chem. Soc. Perkin Trans. 1 1993 issue 6 653-659.
Cmpd 14

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	51.31	89	52.02	97	50.42	58
β	51.67	91	52.43	93	51.54	73
A3 OMe	55.97	92	56.28	94	55.81	100
B3 OMe	56.11	100	56.35	93	55.91	61
B γ	71.63	91	72.08	87	71.06	58
α	84.00	93	84.43	95	83.07	54
B α	85.65	90	86.32	89	85.45	61
B2	107.89	96	110.68	96	110.88	60
A2	108.78	92	111.21	89	110.96	67
A5	114.43	99	115.39	76	115.28	55
B5	114.59	97	115.80	86	115.54	68
B6	118.83	100	120.06	100	119.27	68
A6	119.65	98	120.32	93	119.48	97
A1	127.88	46	129.78	49	128.41	54
B1	131.26	48	132.60	53	130.80	61
A4	145.81	60	147.15	35	146.24	57
B4	146.15	58	147.82	38	147.03	65
A3	146.60	46	147.99	35	147.35	71
B3	146.99	43	148.62	42	147.96	84
γ	174.51	30	174.93	38	174.99	62

Compound Number 2028



4-trans-8-cis-bis(4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo [3-3-0] octan-2-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.65	dd	8.7, 2.6
B β	3.71	m	
γ	5.16	br d	2.6
B α	5.82	br d	5.9
B γ cis	3.80	m	
B γ trans	3.47	dd	9.2, 6.7

Notes:

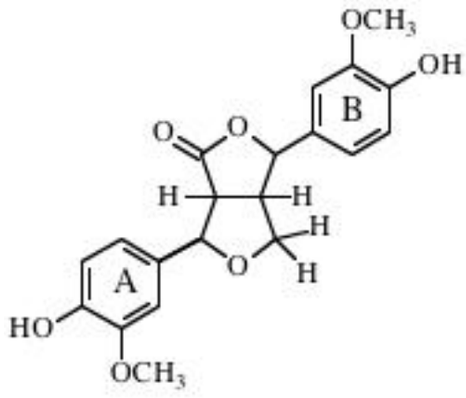
S. Quideau

S. Quideau and J. Ralph. J. Chem Soc . Perkin Trans. 1 1993 (6) 653-659

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	45.43	90	46.14	77		
β	54.80	99	55.35	78		
A3 OMe	56.00	82	56.26	100		
B3 OMe	56.13	93	56.34	82		
B γ	68.66	86	69.98	78		
B γ	80.37	89	81.09	78		
γ	83.70	88	84.56	81		
B2	107.47	85	109.50	73		
A2	108.17	91	110.24	74		
A5	114.41	100	115.65	37		
B5	114.65	82	115.87	42		
B6	117.76	88	118.57	74		
A6	118.11	97	119.17	85		
B1	127.90	53	129.22	36		
A1	132.46	44	133.48	41		
A4	145.33	63	147.10	17		
B4	145.56	45	147.24	19		
A3	146.67	44	148.39	14		
B3	146.80	49	148.54	15		
γ	177.07	54	177.77	38		

Compound Number 2029



3,6-bis(4-hydroxy-3-methoxyphenyl)-tetrahydro-furo[3,4-c]furan-1-one

4-cis-8-cis-bis (4-hydroxy-3-methoxyphenyl)-3,7-dioxabicylclo [3-3-0] octan-2-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.65	ddd	9.2, 3.7, 0.5
B β	3.39	ddddd	9.2, 7.0, 4.6, 3.6, 0.6
α	5.20	dquin	3.7, 0.6
B α	5.39	br d	3.6
B γ cis	4.30	ddd	9.4, 7.0, 0.5
B γ trans	4.02	ddt	9.4, 4.6, 0.5

Notes:

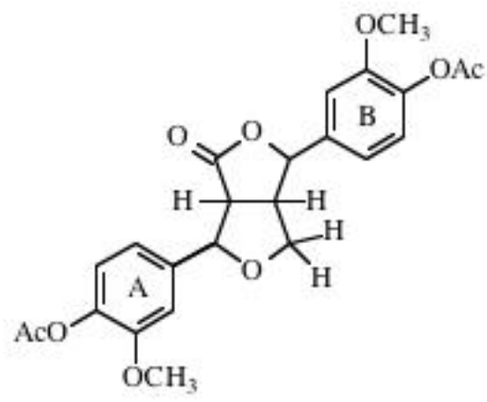
S. Quideau

S.Quideau and J. Ralph. J. Chem. Soc. Perkin Trans. 1 1993 (6) 653-659.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β	49.99	84	50.38	93	48.62	69
β	53.31	89	53.71	86	52.32	72
A3 OMe	56.02	88	50.26	99	55.61	100
B3 OMe	56.08	92	50.34	93	55.71	98
B γ	72.70	90	73.44	96	72.15	66
α	83.38	75	84.43	90	82.91	77
B α	84.59	91	85.78	92	84.83	73
A2	107.77	100	110.35	96	110.30	78
B2	108.11	87	110.45	97	110.54	77
A5	114.42	88	115.64	73	115.16	68
B5	114.71	85	115.87	71	115.34	66
A6	118.02	95	119.30	100	118.50	85
B6	118.40	99	119.66	95	118.88	78
B1	131.11	41	132.47	47	130.58	61
A1	132.31	41	133.17	47	131.08	57
A4	145.34	44	147.12	22	146.19	37
B4	146.07	46	147.80	26	146.85	47
A3	146.73	40	148.35	28	147.55	61
B3	146.94	47	148.63	30	147.73	59
γ	176.92	54	177.72	39	177.14	67

Compound Number 2030



4-cis-8-cis-bis (4-hydroxy-3-methoxyphenyl)-3,7-dioxabicylclo [3-3-0] octan-2-one diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.72	ddd	9.25, 3.8, 0.5
B β	3.45	ddddd	9.15, 7.1, 4.8, 3.0, 0.6
B γ trans	4.12	ddt	9.5, 4.8, 0.5
B γ cis	4.39	ddd	9.5, 7.1, 0.5
B α	5.52	br d	3.6
α	5.29	dquin	3.8, 0.6

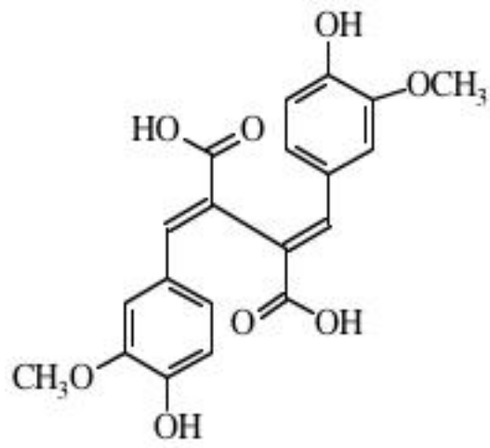
Notes:

S. Quideau
Ralph, Helm, Quideau. J. Chem. Soc. Perkin Trans. 1 1992 2971-2980

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.61	98	20.45	100	20.39	
Ac Me	20.63	98	20.45	100	20.39	
B β	49.89	84	50.33	76	48.62	
β	53.14	95	53.59	76	52.19	
A3 OMe	55.99	92	56.24	76	55.82	
B3 OMe	56.06	100	56.35	75	55.95	
B γ	72.80	90	73.72	81	72.51	
α	82.99	80	84.01	82	82.49	
B α	83.89	88	84.93	78	83.93	
A2	109.13	86	110.86	82	110.37	
B2	109.35	86	111.05	77	110.69	
A6	117.14	90	118.40	81	117.87	
B6	117.22	86	118.53	83	118.00	
A5	122.98	95	123.65	79	122.80	
B5	123.38	97	123.96	82	123.07	
B1	138.04	53	139.95	39	138.71	
A4	139.26	41	140.40	27	138.80	
A1	139.32	40	140.68	43	139.21	
B4	139.96	36	140.96	23	139.30	
A3	151.35	48	152.38	30	150.88	
B3	151.66	54	152.62	28	151.05	
Ac C=O	169.04	48	168.98	28	168.57	
Ac C=O	168.90	50	168.94	28	168.53	
γ	176.66	54	177.49	36	176.98	

Compound Number 2031



4,4'-dihydroxy-3,3'-dimethoxy-β,β'-bicinnamic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.74	s	
5	6.78	d	8.2
6	7.11	dd	8.2, 2.0
2	7.31	d	2.0
α	7.83	s	

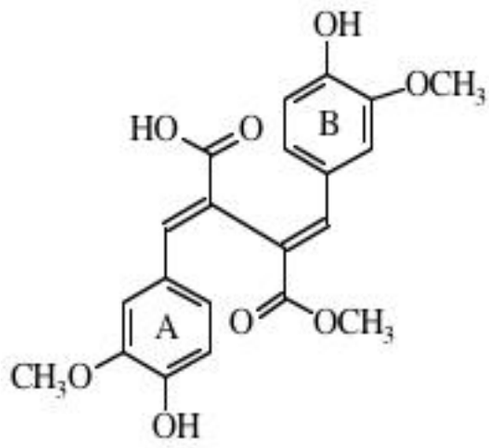
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.05	100	55.28	100
2			113.51	91	113.23	60
5			115.93	57	115.47	59
6			125.60	95	124.11	67
β			126.15	24	125.12	15
1			127.94	57	126.13	62
α			142.26	59	140.40	18
3			148.19	31	147.29	77
4			149.25	24	148.37	61
γ			168.46	28	168.06	40

Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 18
As this compound has a plane of symmetry only one set of shifts are reported.

Compound Number 2032



γ'-methoxy-4,4'-dihydroxy-3,3'-dimethoxy-β,β'-bicinnamic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.66	s	
A3 OMe	3.72	s	
B3 OMe	3.73	s	
A,B 5	6.78	d	8.2
B6	7.11	dd	8.3, 2.0
A6	7.09	dd	8.3, 2.0
A2	7.25	d	2.0
B2	7.30	d	2.0
B α	7.81	s	
α	7.84	s	

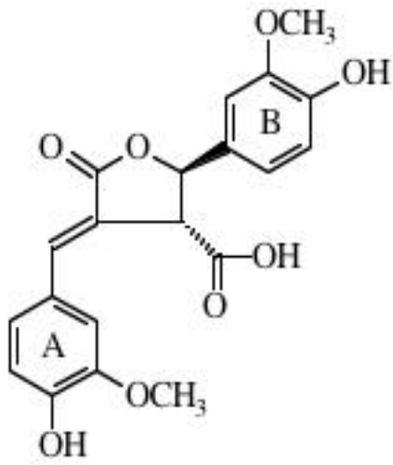
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B gOMe			52.28	54		
B3 OMe			56.04	100		
A3 OMe			56.04	100		
A2			113.40	56		
B2			113.54	59		
A5			115.95	58		
B5			115.97	59		
A6			125.60	56		
β			125.67	56		
Bβ			125.67	56		
B6			125.73	66		
A1			127.78	36		
B1			127.81	36		
B α			142.36	51		
α			142.47	44		
B3			148.19	33		
A3			148.20	33		
A4			149.32	27		
B4			149.37	21		
Bγ			168.22	27		
γ			168.53	19		

Compound Number 2033



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β			54.03	56	52.64	49
A3 OMe			56.27	100	55.54	90
B3 OMe			56.27	100	55.67	100
B α			81.24	66	80.17	48
B2			110.17	72	110.31	63
A2			113.95	67	113.67	53
B5			116.04	58	115.61	58
A5			116.20	57	115.70	58
B6			119.17	66	118.21	65
β			120.45	37	119.08	68
A1			126.54	68	124.72	57
A6			126.58	68	125.56	50
B1			132.37	42	130.42	62
α			140.46	59	139.48	42
B4			147.97	30	147.07	59
A3			148.54	29	147.72	67
B3			148.63	30	147.76	67
A4			150.20	34	149.54	51
γ			171.66	23	171.02	55
B γ			172.12	34	171.72	76

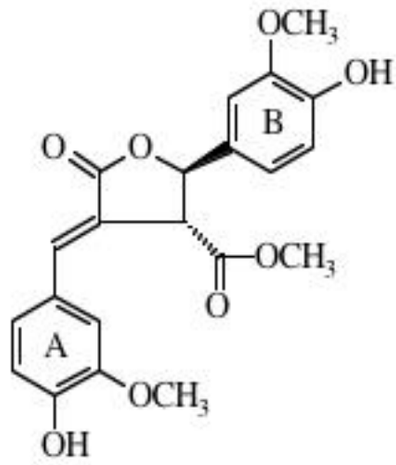
^{1}H (acetone)

Atom	H Shifts	Mult	J
B3 OMe	3.81	s	
A3 OMe	3.87	s	
B β	4.30	t	2.5
B α	5.75	d	2.8
B 5,6	6.82	m	
A5	6.89	d	8.2
B2	6.98	br s	
A6	7.21	dd	8.2, 2.0
A2	7.37	d	2.0
α	7.61	d	2.1

Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 12b (R=H)

Compound Number 2034



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γOMe	52.98	51	53.16	82	51.98	56
B β	53.49	50	53.78	89	52.75	74
B3 OMe	55.97	100	56.23	100	55.46	88
A3 OMe	55.97	100	56.26	100	55.62	100
B α	80.22	52	80.97	87	79.74	54
B2	107.65	56	110.12	89	110.26	63
A2	112.04	50	113.78	88	113.48	52
B5	114.78	62	116.04	89	115.53	47
A5	114.92	51	116.24	89	115.68	42
B6	118.22	54	119.23	93	118.26	67
β	118.38	38	120.03	52	118.34	41
A1	125.66	38	126.38	63	124.48	45
A6	125.59	51	126.42	93	125.44	50
B1	131.08	35	132.08	52	130.02	47
α	141.06	45	140.75	81	139.93	48
B4	146.12	37	147.99	56	147.11	33
A3	146.77	32	148.52	48	147.69	49
B3	146.89	33	148.61	48	147.71	50
A4	148.39	41	150.24	58	149.62	41
γ	170.77	38	171.45	33	170.53	68
B γ	171.23	26	171.56	52	170.70	48

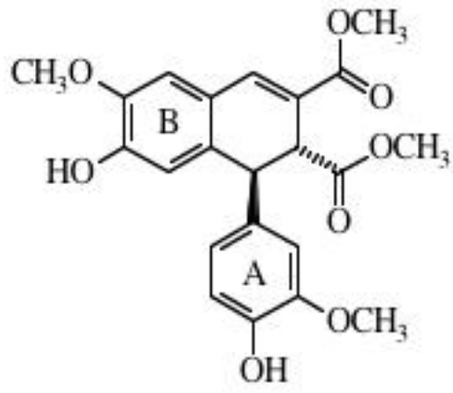
^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.73	s	
B3 OMe	3.81	s	
A3 OMe	3.88	s	
B β	4.39	t	2.6
B α	5.72	d	3.0
B 5,6	6.79 - 6.85	m	
A5	6.9	d	8.2
B2	6.97	br d	1.5
A6	7.17	dd	8.2, 2.0
A2	7.28	d	2.0
α	7.62	d	2.1

Notes:

S. Quideau

Compound Number 2035



Dimethyl 7-hydroxy-6-methoxy-1-(4-hydroxy-3-methoxy phenyl)-trans-1,2-dihydronaphtlalene-2,3-dicarboxylate

^{1}H (acetone)

Atom	H Shifts	Mult	J
A γ OMe	3.56	s	
B γ OMe	3.68	s	
A3 OMe	3.75	s	
B3 OMe	3.88	s	
β	3.94	d	3.0
α	4.53	d	3.0
A6	6.39	dd	8.2, 2.0
A5	6.65	d	8.2
B5	6.66	s	
A2	6.76	d	2.0
B2	7.10	s	
B α	7.65	s	

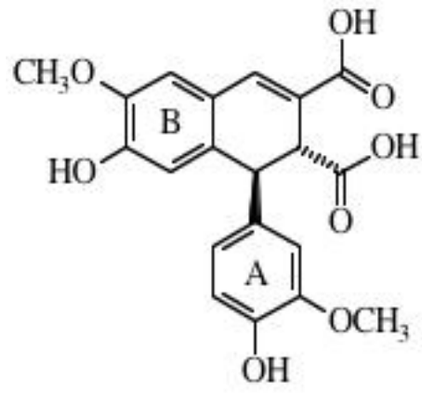
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α	45.60	82	46.33	92	44.69	53
β	47.20	81	48.09	92	46.74	48
B γ OMe	51.87	96	51.87	94	51.67	77
A γOMe	52.40	93	52.34	88	52.11	84
A3 OMe	55.83	100	56.21	99	55.62	100
B3 OMe	56.03	96	56.38	96	55.74	92
A2	110.12	91	112.03	100	111.65	66
B2	111.21	82	113.27	91	113.25	53
A5	114.17	90	115.59	98	115.24	64
B5	115.58	86	116.85	93	116.06	47
A6	120.35	89	120.83	98	119.48	61
B β	122.37	57	122.96	53	120.89	55
B1	123.85	58	124.37	58	122.47	48
B6	131.19	60	132.09	54	130.74	50
A1	134.28	61	135.31	59	133.56	54
B α	137.74	77	138.45	87	137.92	50
A4	144.42	69	146.29	58	145.31	66
B3	145.78	59	147.63	53	146.72	55
A3	146.40	60	148.20	53	147.39	64
B4	147.69	72	149.68	65	148.88	66
B γ	167.10	47	167.49	44	166.52	59
γ	172.93	60	173.17	58	172.31	69

Compound Number 2036



β-β-coupled dehydrodiferulic acid

7-hydroxy-6-methoxy-1-(4-hydroxy-3-methoxyphenyl)-trans-1,2-dihydronapthlalene-2,3-dicarboxylic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.74	s	
B3 OMe	3.86	s	
β	3.88	d	1.8
α	4.61	br d	1.8
A6	6.42	dd	8.2, 2.0
A5	6.64	d	8.2
B5	6.71	s	
A2	6.79	d	2.0
B2	7.04	s	
B α	7.60	s	

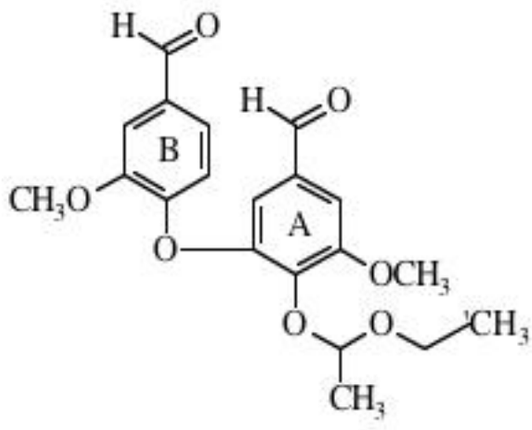
Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 19
Not very soluble in CDCl3

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α			46.00	72	44.25	35
β			48.08	43	47.80	13
A3 OMe			56.19	100	55.59	100
B3 OMe			56.39	99	55.76	87
A2			111.98	88	111.57	63
B2			113.06	75	112.63	37
A5			115.48	73	115.13	60
B5			116.92	65	116.23	45
A6			120.67	90	119.30	61
B β			124.34	19	123.07	43
B1			124.64	53	124.67	5
B6			132.35	48	130.85	42
A1			136.12	39	134.50	5
B α			137.58	44	135.09	18
A4			146.06	33	145.04	47
B3			147.48	46	146.46	42
A3			148.10	44	147.28	51
B4			149.29	38	147.99	29
B γ			169.32	14	169.23	9
γ			173.62	31	173.27	51

Compound Number 2037



^{1}H (acetone)

Atom	H Shifts	Mult	J
'CH3	1.08	t	7.05
CH3	1.38	d	5.1
CH2	3.56 -3.89	m	
OMe	3.95	s	
OMe	3.99	s	
CH	5.53	q	5.1
B5	7.04	d	8.1
A6	7.11	d	1.8
A2	7.42	d	1.8
B6	7.53	dd	8.1
B2	7.62	d	1.9
α	9.85	s	
B α	9.95	s	

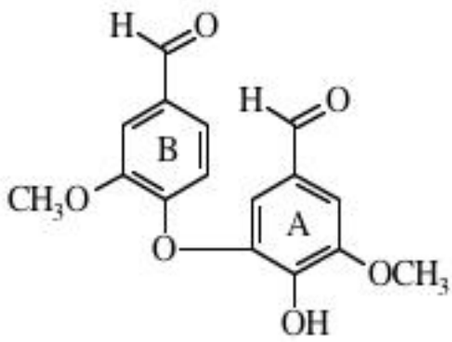
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
'CH3			15.45	91		
CH3			21.28	90		
B OMe			56.43	100		
A OMe			56.66	95		
CH2			63.26	83		
CH			104.47	91		
A2			108.94	81		
B2			112.46	83		
A6			114.45	80		
B5			119.32	89		
B6			125.46	84		
B1			133.26	46		
A1			134.22	44		
A4			143.42	26		
A3			150.68	31		
B3			151.42	33		
B4			151.95	33		
A5			155.59	36		
α			191.23	94		
B α			191.48	96		

Compound Number 2038



4-0-5-coupled dehydrodivanillin

3-{3-[4-(2-carboxyvinyl)-2-methoxy-phenoxy]-4-hydroxy-5-methoxy-phenyl} acrylic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
B OMe	3.95	s	
A OMe	3.98	s	
B5	6.94	d	8.2
A6	7.22	d	1.8
A2	7.40	d	1.8
B6	7.48	dd	8.2, 2.0
B2	7.58	d	2.0
α	9.80	s	
B α	9.92	s	

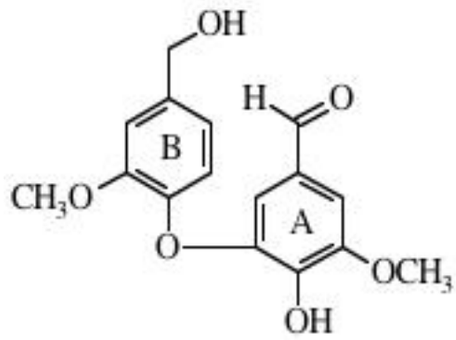
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3 OMe	56.07	100	56.41	100	55.85	100
A3 OMe	56.56	100	56.80	97	56.24	100
A2	106.80	68	108.48	66	108.09	51
B2	110.85	85	112.26	85	111.60	63
A6	116.92	67	116.99	61	116.27	86
B5	117.31	90	117.63	93	116.31	85
B6	125.55	90	125.55	88	124.80	68
A1	128.69	57	129.54	47	127.64	70
B1	132.76	54	133.56	47	131.84	69
A5	142.55	37	143.79	30	142.52	72
A4	143.30	44	145.22	36	144.52	56
A3	148.60	46	150.37	39	149.47	67
B3	150.61	45	151.49	36	149.82	78
B4	151.08	39	152.48	32	151.24	64
α	190.05	96	190.75	9	190.84	39
B α	190.84	100	191.43	97	191.57	27

Compound Number 2039



4-0-5 coupled dehydrovanillin / vanillyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B3 OMe	3.79	s	
A3 OMe	3.95	s	
B α	4.63	s	
A6	6.91	d	1.8
B 5,6	6.94 - 6.97	m	
B2	7.16	br d	
A2	7.27	d	1.8
α	9.71	s	

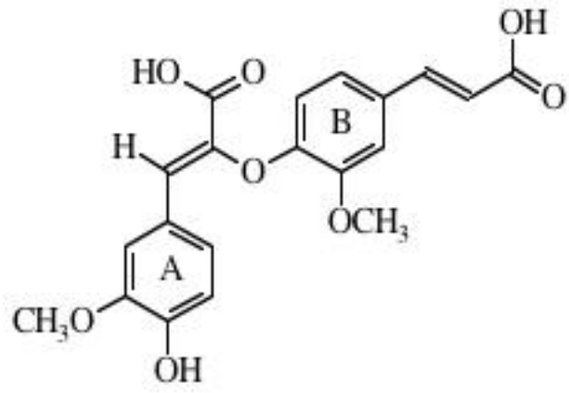
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3 OMe	55.94	58	56.19	94	55.61	100
A3 OMe	56.47	97	56.73	99	56.15	97
B α	64.91	88	64.34	35	62.59	90
A2	106.40	62	107.98	55	107.74	52
B2	111.55	97	112.52	98	111.09	34
A6	114.09	60	112.62	54	111.54	75
B6	119.49	100	119.78	100	118.81	81
B5	120.46	99	121.17	94	119.98	60
A1	128.30	59	129.00	48	127.04	46
B1	138.45	60	140.84	41	139.77	57
A4	142.58	48	143.92	31	142.63	42
B4	143.95	44	144.30	32	143.03	30
A5	145.16	42	146.98	31	145.90	43
A3	148.45	43	149.86	31	148.93	42
B3	150.87	48	152.00	34	150.45	71
α	190.44	83	190.91	92	190.97	67

Compound Number 2040



^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.73	s	
B3 OMe	4.00	s	
B β	6.43	d	15.9
A5	6.82	d	8.2
B5	6.83	d	8.3
B6	7.13	dd	8.3, 2.0
A6	7.23	dd	8.2, 2.0
α	7.42	s	
B2	7.44	d	2.0
A2	7.52	d	2.0
B α	7.59	d	15.9

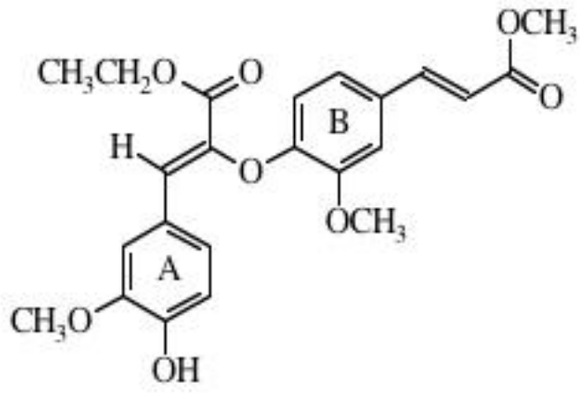
Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 15

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe			55.92	100	55.09	100
B3 OMe			56.47	91	55.86	85
B2			112.39	80	111.55	38
A2			113.77	83	112.98	41
B5			114.39	79	113.30	45
A5			115.96	70	115.53	36
B β			117.50	77	117.52	57
B6			122.92	82	122.02	42
A1			125.31	54	123.44	44
A6			126.06	80	124.62	39
α			128.49	63	127.09	34
B1			130.10	56	128.74	52
β			138.28	27	137.01	44
B α			145.25	77	143.71	46
A3			148.30	46	147.24	50
B4			148.90	40	147.42	47
A4			149.46	37	148.59	89
B3			150.23	52	148.59	88
γ			164.51	13	164.11	56
B γ			167.91	22	167.70	72

Compound Number 2041



^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.21	t	7.1
B γ OMe	3.71	s	
A3 OMe	3.73	s	
B3 OMe	3.99	s	
CH2	4.17	q	7.1
B β	6.45	d	16.0
B5	6.79	d	8.3
A5	6.81	d	8.3,
B6	7.12	dd	8.3, 2.0
A6	7.22	dd	8.3, 2.0
α	7.37	s	
B2	7.44	d	2.0
A2	7.49	d	2.0
B α	7.59	d	16.0
Ar OH	8.12	br s	

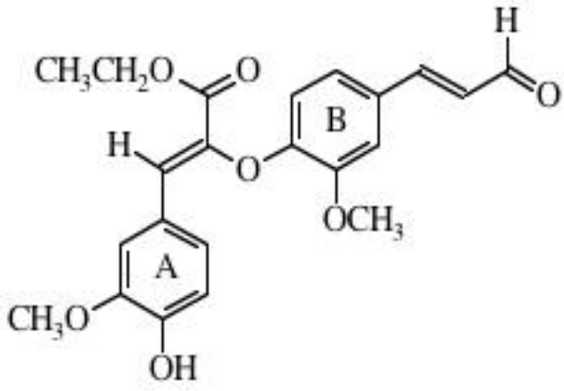
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	14.14	95	14.47	100	14.05	100
B γ OMe	51.65	83	51.58	78	51.32	62
A3 OMe	55.59	100	55.92	93	55.11	75
B3 OMe	56.21	97	56.49	90	55.93	59
CH2	61.42	92	61.72	74	60.96	61
B2	111.24	83	112.45	70	111.79	41
A2	112.03	97	113.78	70	113.17	34
B5	114.14	89	114.53	71	113.46	35
A5	114.47	87	115.99	70	115.57	26
B β	116.32	82	117.10	71	116.29	42
B6	122.12	80	122.92	78	122.27	46
A1	124.74	55	125.19	9	123.18	32
A6	125.54	84	126.03	71	124.79	35
α	127.80	71	128.05	10	127.43	49
B1	129.31	60	130.09	45	128.78	39
β	137.73	51	138.39	42	136.44	41
B α	144.42	90	145.02	72	144.23	42
A3	146.43	53	148.29	40	147.27	33
B4	147.44	67	148.89	35	147.43	26
A4	147.80	47	149.48	40	148.67	46
B3	149.16	59	150.24	43	148.67	46
γ	163.41	43	163.75	32	162.67	33
B γ	167.50	62	167.63	47	166.80	48

Notes:

S. Quideau
Toward β-O-4 dehydro diferulic acid
(steryl ether, Z isomer)

Compound Number 2042



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	14.06	98	14.48	12	14.05	100
B3 OMe	56.15	100	56.55	13	55.97	10
A3 OMe	55.47	94	55.94	16	55.11	73
CH2	61.37	91	61.76	92	60.99	74
B2	111.31	78	112.58	93	111.82	49
A2	112.06	80	113.81	91	113.35	53
B5	114.11	78	114.66	93	113.44	53
A5	114.57	79	116.03	82	115.59	40
B6	122.87	82	123.76	99	123.13	9
A1	124.41	62	125.16	54	123.13	83
A6	125.42	77	126.08	53	124.85	52
B β	127.19	85	128.29	100	128.89	65
α	127.90	75	128.16	100	127.35	55
B1	128.83	62	130.13	54	127.53	39
β	137.35	57	138.31	43	136.34	45
A3	146.51	57	148.31	43	147.45	41
A4	147.59	61	149.53	51	147.90	48
B4	148.54	52	149.58	46	148.78	59
B3	149.21	61	150.38	50	148.86	60
B α	152.33	80	153.18	96	152.98	57
γ	163.19	48	163.70	38	162.62	49
B γ	193.42	91	193.89	99	194.19	72

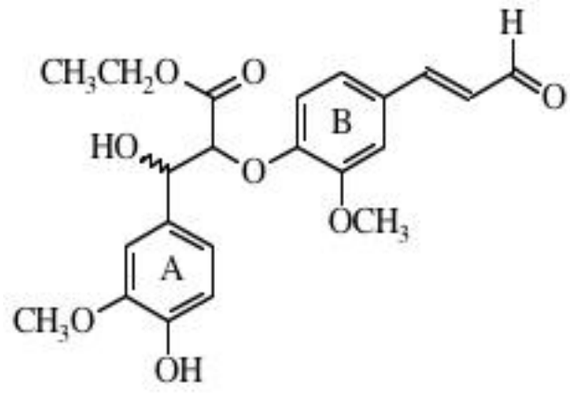
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.21	t	7.1
A3 OMe	3.73	s	
B3 OMe	4.00	s	
CH2	4.21	q	7.1
B β	6.70	dd	15.9, 7.7
A5	6.81	d	8.3
B5	6.83	d	8.3
B6	7.18	dd	8.3, 2.0
A6	7.23	ddd	8.3, 2.0, 0.4
α	7.38	s	
A2	7.49	d	2.0
B2	7.50	d	2.0
B α	7.58	d	15.9
B γ	9.65	d	7.7
Ar OH	8.14	s	

Notes:

S. Quideau
Toward β-O-4 dehydro diferulic acid(steryl ether, Z isomer)

Compound Number 2043



erythro

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	13.86	97				
OMe	55.72	100				
OMe	55.78	98				
CH2	61.33	84				
α	73.70	69				
β	82.29	71				
A2	109.63	73				
B2	111.09	72				
A5	113.93	71				
B5	115.99	71				
A6	119.80	73				
B6	122.72	82				
B β	127.15	81				
B1	128.79	80				
A1	130.89	64				
A3	145.48	70				
A4	146.36	58				
B3	149.72	54				
B4	150.11	59				
B α	152.38	74				
γ	168.80	64				
B γ	193.53	90				

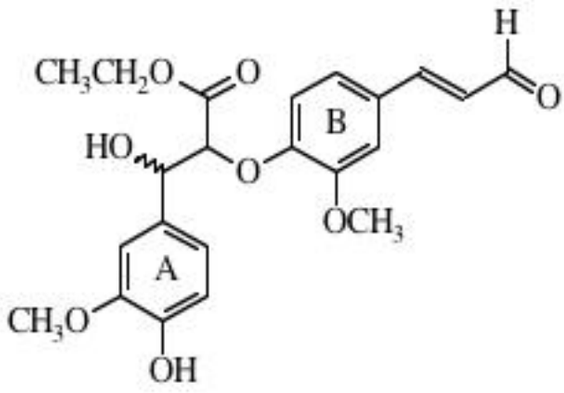
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.16	t	7.2
OMe	3.85	s	
OMe	3.86	s	
CH2	4.15	q	7.1
β	4.81	d	5.4
a	5.16	d	5.4
B β	6.58	dd	15.8, 7.7
B α	7.37	d	15.8
B γ	9.61	d	7.7
Ar OH	6.07		

Notes:

S. Quideau Compds 2043 and 2044 were run as a mixture and the different isomers were assigned. Relative intensities reflect the spectrum of the mixture.e isomer for synthesis of β-O-4 dehydro diferulic acid

Compound Number 2044



threo

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	13.73	100				
OMe	55.67	33				
OMe	55.82	34				
CH3	61.28	28				
α	74.49	14				
β	83.43	15				
A2	109.51	16				
B2	110.98	16				
A5	114.02	17				
B5	115.56	15				
A6	119.91	16				
B6	122.72	82				
B β	127.19	29				
B1	128.79	80				
A1	129.94	13				
A3	145.73	15				
A4	146.55	13				
B3	149.74	18				
B4	149.92	13				
B α	152.32	17				
γ	168.73	27				
B γ	193.53	90				

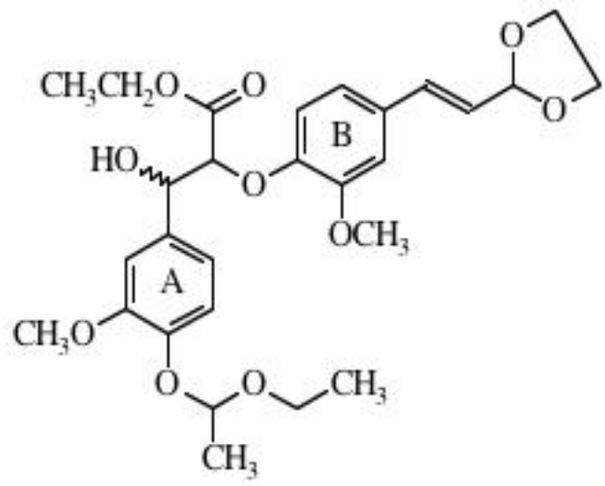
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.08	t	7.2
OMe	3.85	s	
OMe	3.87	s	
CH2	4.04-4.11	m	
β	4.67	d	6.2
α	5.10	d	6.2
B β	6.59	dd	15.8, 7.7
B α	7.38	d	15.8
B γ	9.62	d	7.7
Ar OH	6.10		

Notes:

S.Quideau Compounds 2043 and 2044 were run as a mixture and the different isomers were assigned. Relative intensities reflect the spectrum of the mixture. threo isomer for synthesis of β-O-4 dehydro diferulic acid

Compound Number 2045



erythro

^{1}H (chloroform)

Atom	H Shifts	Mult	J
CH3	1.47	d	5.1
β *t*	4.56	d	6.6
β *e*	4.72	d	5.4
α *t*	5.06	br d	6.3
α *e*	5.13	br s	
A 4 CH	5.32	q	5.2
B γ	5.36	d	6.0
B β	6.03	dd	15.9, 6.0
B α	6.66	d	16.0

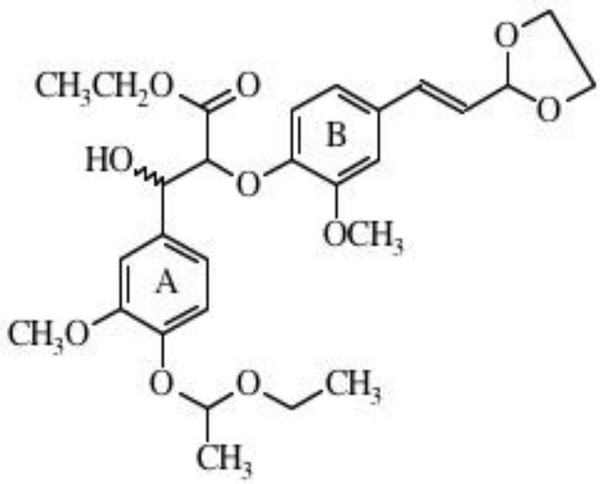
Notes:

S. Quideau
intermediate toward β--O-4 dehydro
diferulic acid

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A γ CH3	13.82	47				
CH3	14.93	57				
CH3	20.10	36				
OMe	55.54	54				
OMe	55.63	37				
4 CH2	61.01	50				
A CH2	61.84	32				
B CH2	64.82	100				
B CH2	64.82	100				
α	73.57	33				
β	83.09	25				
	100.92	35				
	103.59	57				
	110.04	40				
	110.76	27				
	117.40	27				
	118.63	31				
	119.09	34				
	120.07	43				
	124.08	43				
	131.25	30				
	133.82	18				
	133.84	18				
	134.08	44				
	145.39	16				
	147.22	21				
	150.12	9				
	150.40	31				
γ	169.03	35				

Compound Number 2046



threo

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	4.56	d	6.6
α	5.06	br d	6.3

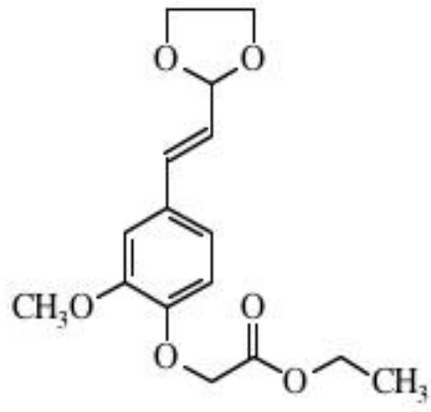
Notes:

S. Quideau
intermediate toward b--O-4 dehydro diferulic acid

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	-					
CH3	-					
CH3	-					
OMe	55.59	100				
OMe	55.59	100				
CH2	61.86	55				
CH2						
CH2	74.51	22				
α	84.39	21				
β	100.94	61				
	109.98	12				
	110.69	48				
	116.92	14				
	118.70	55				
	124.14	74				
	132.73	12				
	134.06	62				
	145.67	17				
	147.26	24				
	149.92	16				
	150.00	56				

Compound Number 2047



^{1}H (chloroform)

Atom	H Shifts	Mult	J
CH3	1.26	t	7.1
OMe	3.87	s	
CH2	3.90-4.05	m	
CH2	4.24	q	7.1
CH2	4.67	s	
γ	5.39	d	6.1
β	6.05	dd	15.9, 6.1
α	6.69	d	15.9
5	6.76	d	8.3
6	6.90	dd	8.3, 2.0
2	6.99	d	2.0

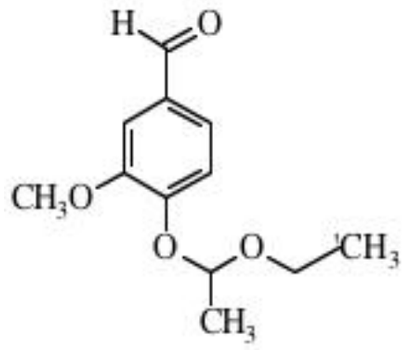
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	14.09	100				
OMe	55.84	72				
CH2	61.27	63				
CH2	65.01	94				
CH2	65.01	94				
CH2	66.42	60				
γ	103.90	71				
2	109.88	67				
5	113.88	67				
6	120.14	66				
β	123.75	68				
α	130.39	39				
1	134.47	66				
3	147.58	31				
4	149.56	34				
C=O	168.78	30				

Notes:

S. Quideau
For synthesis of b--O-4 dehydro diferulic acid

Compound Number 2048



^{1}H (chloroform)

Atom	H Shifts	Mult	J
'CH3	1.21	t	7.1
CH3	1.58	d	5.3
CH2	3.50-3.85	m	
OMe	3.92	s	
CH	5.54	q	5.3
Aromatics	7.21-7.43		
α	9.87	s	

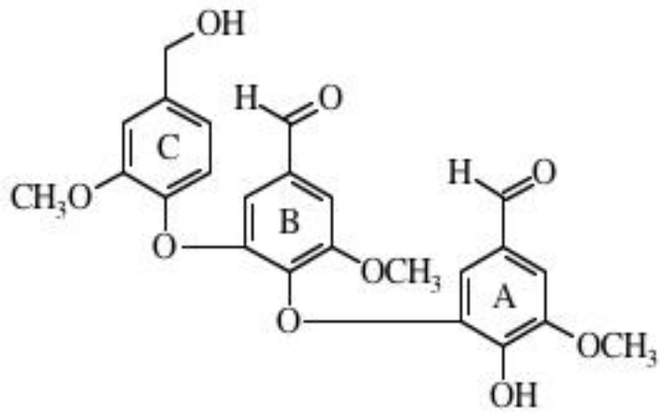
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
'CH3	15.03	85				
CH3	19.95	98				
OMe	55.90	94				
CH2	61.72	85				
CH	100.61	92				
2	109.81	79				
5	116.59	100				
6	126.06	81				
1	130.97	47				
3	150.78	37				
4	151.64	37				
α	190.89	91				

Notes:

S. Quideau
Intermediate for synthesis of β--O-4 dehydro diferulic acid

Compound Number 2049



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
C3 OMe			56.07	100		
A3 OMe			56.75	97		
B3 OMe			56.89	90		
C α			64.25	33		
B2			108.03	70		
A2			108.40	50		
B6			109.92	67		
A6			110.17	50		
C2			112.36	40		
C6			119.76	93		
C5			122.66	87		
A1			128.73	37		
B1			134.75	53		
B4			138.25	20		
C1			142.09	47		
C4			142.49	37		
A4			143.04	33		
A5			147.16	27		
A3			149.70	30		
C3			152.34	37		
B5			153.71	33		
B3			155.04	47		
α			191.02	55		
B α			191.69	55		

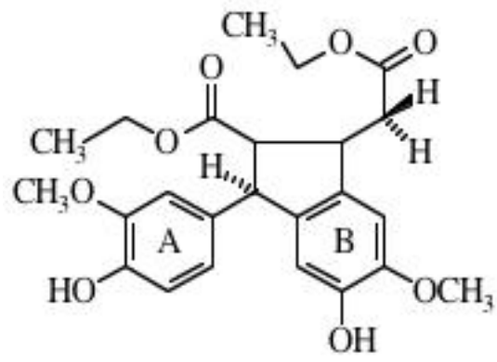
^{1}H (acetone)

Atom	H Shifts	Mult	J
C3 OMe	3.72	s	
B3 OMe	3.90	s	
A3 OMe	3.94	s	
C α	4.62	s	
B6	6.88	d	1.7
C6	6.94	dd	8.1, 1.7
C5	7.00	d	8.1
A6	7.01	d	1.7
C2	7.14	d	1.7
A2	7.26	d	1.7
B2	7.40	d	1.7
α	9.74	s	
B α	9.86	s	

Notes:

S. Quideau
5-O-4 trimer

Compound Number 2050



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A CH3	14.19	93	14.52	91	13.97	100
B CH3	14.22	88	14.47	89	14.07	100
B β	36.90	57	37.50	80	36.41	44
B α	42.15	75	43.06	85	41.74	54
α	51.31	66	52.35	80	50.93	46
A3 OMe	55.93	100	56.23	99	55.56	74
B3 OMe	56.10	99	56.39	100	55.64	97
β	58.66	67	59.09	87	56.96	53
B CH2	60.47	80	60.79	84	59.94	88
A CH2	60.63	78	60.95	84	60.07	76
B2	106.61	68	108.23	75	107.86	45
B5	110.87	80	112..04	82	111.25	42
A2	110.99	77	112.60	93	112.08	41
A5	114.29	91	115.76	92	115.32	45
A6	121.39	75	121.75	96	120.35	48
A1	134.34	58	135.02	55	133.25	53
B1	135.12	43	□135.58	50	133.61	46
B6	137.10	49	137.90	47	136.47	49
A4	144.54	63	146.45	56	145.36	53
B4	145.61	60	147.43	57	146.34	58
B3	146.04	52	147.92	46	147.08	52
A3	146.50	59	148.37	48	147.51	55
B γ	172.30	54	172.45	58	171.45	77
γ	172.43	55	173.00	61	172.10	61

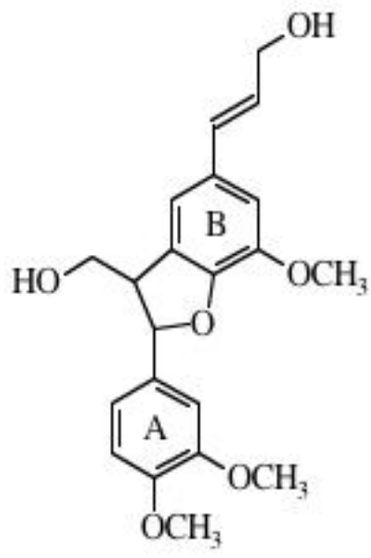
^{1}H (acetone)

Atom	H Shifts	Mult	J
B β1	2.43	dd	16.0, 8.0
B β2	2.61	dd	16.0, 7.0
β	3.43	dd	9.85, 8.20
B α	3.90	brq	8.0
α	4.56	d	10.1

Notes:

S. Quideau
Sterochemistry determined from NOESY experiments
αβ-/α6 model

Compound Number 2051



4-[3-Hydroxymethyl-5-(3-hydroxypropenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-1,2-dimethoxyphenyl

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.52	br q	
A3 OMe	3.77	s	
A4 OMe	3.78	s	
B3 OMe	3.86	s	
γ 's	3.80-3.92	m	
B γ OH	4.14	t	5.50
B γ	4.19	td	5.7, 1.7
α	5.58	d	6.4
B β	6.23	dt	15.8, 5.5
B α	6.52	dt	15.8, 1.7
A5	6.91	d	8.1
A,B6 + B2	6.94-9.67	m	
A2	7.03	d	1.8

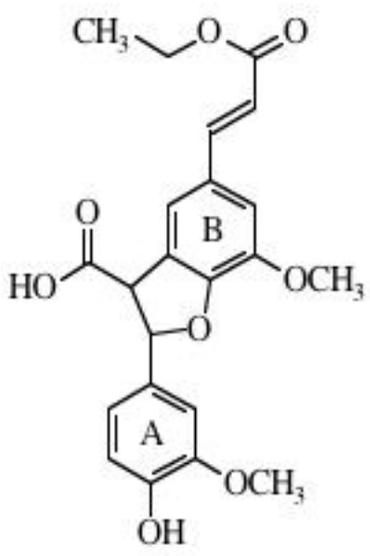
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β			54.81	63		
A3 OMe			56.12	100		
A4 OMe			56.12	95		
B3 OMe			56.39	84		
B γ			63.38	71		
γ			64.65	61		
α			88.34	71		
A2			110.84	79		
B2			111.74	72		
A5			112.67	84		
B6			116.08	73		
A6			119.02	83		
B β			128.42	69		
B5			130.30	41		
B α			130.49	74		
B1			132.00	54		
A1			135.59	45		
B3			145.18	38		
B4			148.93	26		
A4			150.15	30		
A3			150.45	31		

Notes:

S. Quideau
veratryl phenylcoumaran

Compound Number 2052



^{1}H (acetone)

Atom	H Shifts	Mult	J
β	4.37	br d	7.8
α	6.06	d	7.9
B β	6.38	d	15.9
B α	7.60	d	15.9

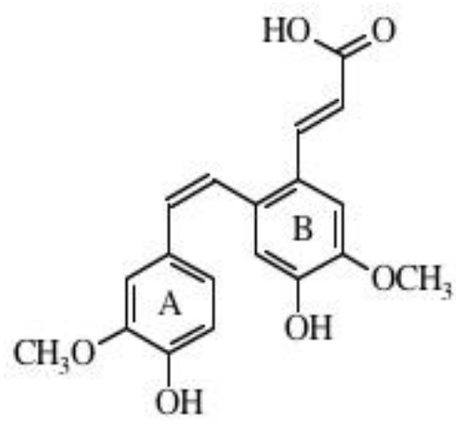
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3			14.63	85		
β			55.43	46		
A3 OMe			56.30	97		
B3 OMe			56.47	100		
CH2			60.51	79		
α			88.70	59		
A2			110.70	79		
B2			113.20	68		
A5			115.72	91		
B β			116.46	76		
B6			119.08	69		
A6			120.05	86		
B5			128.35	32		
B1			129.20	54		
A1			132.64	52		
B α			145.36	76		
B3			145.70	53		
A4			147.70	38		
A3			148.47	44		
B4			151.03	34		
B γ			167.31	60		
γ			172.24	20		

Compound Number 2053



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe			56.25	100		
B3 OMe			56.56	80		
B2			109.15	74		
A2			110.16	83		
A5			115.99	83		
B β			116.50	76		
β			120.61	78		
B6			120.84	74		
A6			121.14	88		
B5			125.47	48		
B1			126.98	56		
α			130.68	81		
A1			130.90	58		
B α			146.00	69		
B4			146.96	50		
A4			147.61	55		
A3			148.61	46		
B3			148.83	54		
B γ			168.22	47		

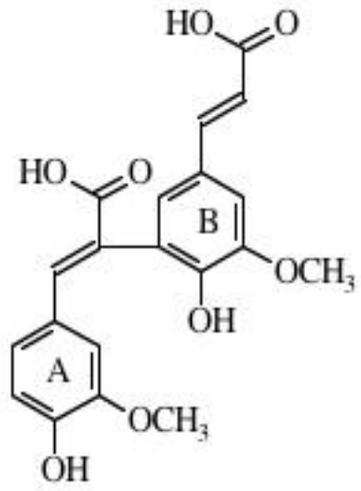
^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.91	s	
B3 OMe	3.95	s	
B β	6.44	d	15.9
A5	6.83	d	8.1
A6	7.05	dd	8.1, 2.0
A2	7.22	d	2.0
B2	7.23	d	1.9
α	7.31	dd	16.5, 7.38
β	7.33	dd	16.5, 7.38
B6	7.54	d	1.9
B α	7.63	d	15.9

Notes:

S. Quideau

Compound Number 2054



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe			55.48	100	54.62	100
B3 OMe			56.55	95	56.06	90
B2			110.27	67	109.76	36
A2			113.26	78	112.79	47
A5			115.63	74	115.63	47
B β			116.23	67	115.92	48
B5			125.14	40	124.57	42
B6			125.60	71	124.38	42
β			126.34	57	125.90	67
A6			126.36	80	124.95	48
B1			127.26	62	125.66	49
A1			127.58	62	125.88	67
α			141.81	62	139.75	34
B α			145.80	66	144.28	43
A3			147.86	54	145.82	32
B4			148.01	43	147.00	64
A4			148.98	50	148.05	65
B3			149.10	53	148.12	46
B γ			168.56	41	167.86	80
γ			169.15	36	168.38	68

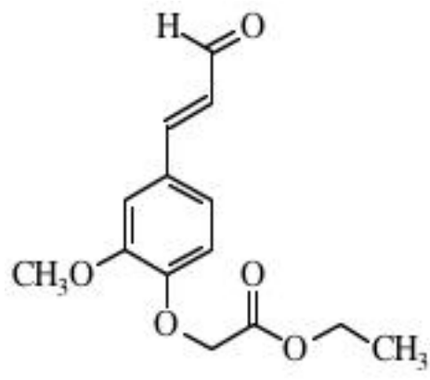
^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.45	s	
B3 OMe	3.95	s	
B β	6.38	d	15.4
A5	6.71	d	8.2
A2	6.73	d	1.9
A6	6.85	dd	8.2, 2.0
B6	7.03	d	1.9
B2	7.37	d	1.9
B α	7.60	d	15.9
α	7.81	s	

Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 14
Not soluble in CDCl3

Compound Number 2055



^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.25	t	7.1
OMe	3.89	s	
CH2	4.23	q	7.1
CH2	4.69	s	
β	6.57	dd	15.8, 7.7
5	6.78	d	7.9
2,6	7.06-7.08	m	
α	7.36	d	15.8
γ	9.62	d	7.7

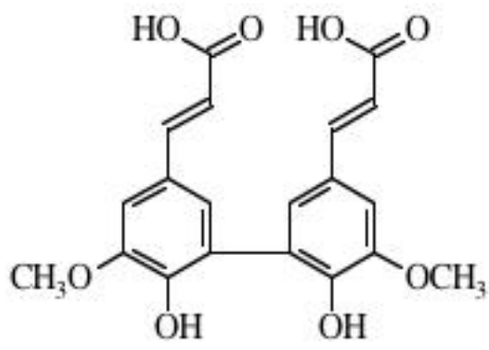
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	14.06	91				
OMe	55.95	97				
CH2	61.44	86				
CH2	65.99	88				
2	110.77	93				
5	113.40	94				
6	122.75	97				
α	127.17	99				
1	128.31	54				
3	149.74	46				
4	149.96	40				
β	152.36	84				
C=O	168.25	44				
γ	193.41	100				

Notes:

S. Quideau
intermediate for systhesis of β-O-4 dehydro diferulic acid

Compound Number 2056



5-5, Dehydrodiferulic Acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.97	s	
β	6.42	d	15.4
6	7.21	d	2.0
2	7.35	d	2.0
α	7.64	d	15.9

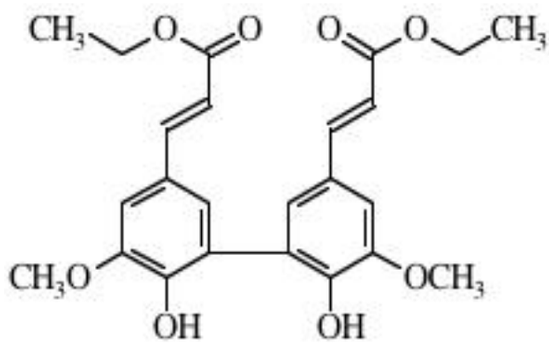
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.52	100	56.04	55
2			109.97	89	109.44	56
β			116.28	94	115.82	64
5			125.62	54	125.20	60
6			126.07	96	125.05	60
1			126.60	64	124.83	74
α			145.89	100	144.56	55
4			147.38	40	146.43	71
3			148.92	58	147.90	99
γ			168.36	59	167.94	100

Notes:

S. Quideau JCS Perkin 1, 3485-98 (1994) Cmpd 16
Note chemical shift differences of 5,6,1 between solvents. Shifts were verified in both solvents As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 2057



5-5 Dehydrodiferulate diethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.26	t	7.1
CH2	4.18	q	7.1
OMe	3.97	s	
β	6.43	d	15.9
6	7.20	d	2.0
2	7.36	d	2.0
α	7.62	d	15.9

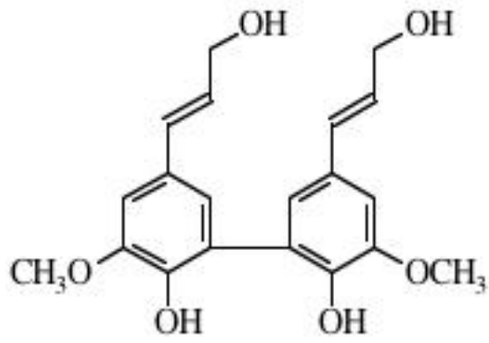
Notes:

S. Quideau
As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	14.31	100	14.64		14.22	
OMe	56.17	84	56.56		56.03	
CH2	60.34	79	60.46		59.63	
2	108.78	61	109.95		109.47	
β	116.21	71	116.23		114.70	
5	123.59	34	125.59		125.20	
6	124.81	68	126.22		125.35	
1	126.73	51	126.64		124.58	
α	144.46	70	145.58		144.98	
4	145.10	37	147.47		146.84	
3	147.27	46	148.93		147.94	
γ	167.14	47	167.39		166.59	

Compound Number 2058



5,5 Dehydrodiconiferyl Alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.89	s	
γ	4.21	br d	5.4
β	6.26	dt	15.8, 5..5
α	6.54	dt	15.8, 1.6
A6	6.92	d	2.0
A2	7.06	d	2.0
ArOH	7.42	s	

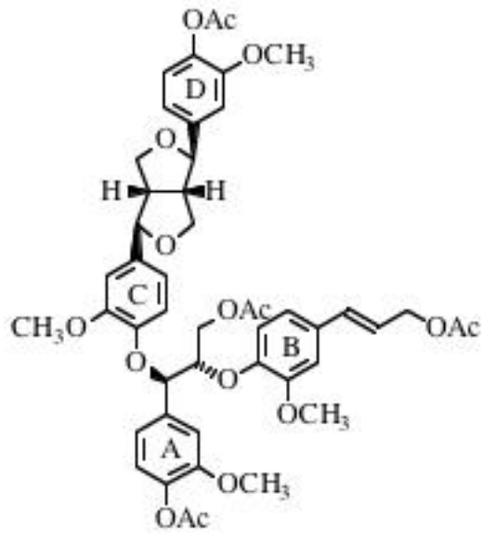
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.52	100		
γ			63.49	68		
2			108.97	69		
6			123.16	79		
5			126.15	21		
β			128.53	71		
1			129.69	45		
α			130.57	80		
4			144.53	26		
3			148.87	27		

Notes:

S. Quideau Run only in acetone, no HMBC run. Assignment of quatenary carbons based on shift assignments of diacid/diester parents. Poor solubility on CDCl3... sample degraded, no DMSO data.As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 2059



Guaiacylglycerol-α-pinoresinol-β-coniferyl-bis-ether (Ac'd)

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	5.60	d	5.6
β	4.86	m	
γ1	4.45	dd	11.9, 3.8
γ2	4.53	dd	11.9, 5.9
C α	4.66	s	
C α	3.06	m	
C γ1	3.83	m	
C γ2	4.17	m	
D α	4.74	d	4.5
D γ	4.23	m	

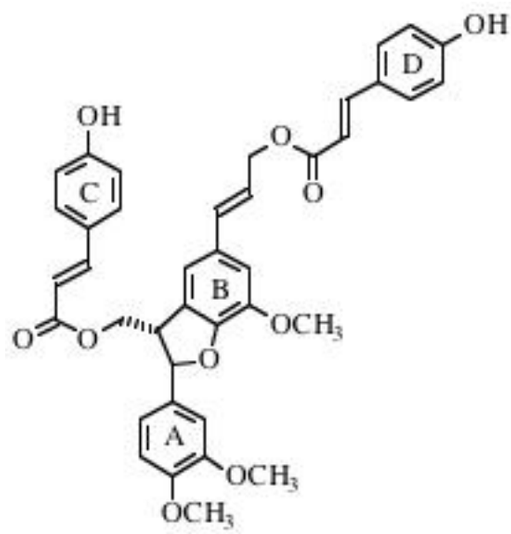
Notes:

S.Quideau
not substantiated in CDCl3 & d6 DMSO
Peracetate/diastereomeric mixture

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.59	99	20.45	99	20.35	99
Ac Me	20.59	99	20.45	99	20.35	99
Ac Me	20.70	70	20.62	50	20.43	49
Ac Me	20.93	70	20.78	70	20.70	49
C β	53.91	66	55.11	64	53.49	61
B β	54.39	74	55.36	60	53.74	63
A3 OMe	55.82	70	56.19	100	55.59	74
B3 OMe	55.95	100	56.23	100	55.65	74
D3 OMe	55.95	100	56.23	100	55.71	100
C3 OMe	56.11	56	56.40	100	55.79	100
A γ	63.45	36	63.62	40	62.44	36
B γ	65.05	69	65.38	59	64.40	61
C γ	71.88	70	72.37	48	71.07	52
D γ	71.88	70	72.48	48	71.18	52
A α	80.34	43	80.88	30	78.69	33
A β	81.87	43	81.73	43	79.56	32
D α	85.53	51	86.20	51	84.67	47
C α	85.64	45	86.27	51	84.75	47
D2	110.01	89	111.07	74	110.38	44
B2	110.35	59	111.31	74	110.20	82
C2	110.39	59	111.47	54	110.71	82
A2	111.55	35	112.77	28	111.89	34
C5	116.58	30	117.29	29	115.64	37
D6	117.93	79	118.62	71	116.96	41
C6	118.19	31	118.90	29	118.18	76
B5	118.87	39	119.11	51	117.83	76
A6	119.65	59	120.51	75	119.43	52
B6	119.65	59	120.51	75	119.43	52
B β	122.08	57	123.14	55	122.17	43
A5	122.45	49	123.25	79	122.37	86
D5	122.73	76	123.43	79	122.55	86
B1	131.55	40	132.27	34	130.46	33
B α	133.93	59	134.23	57	133.01	51
C1	135.13	35	136.85	25	135.21	29
A1	136.93	35	137.72	39	136.37	31
D4	139.19	29	140.08	31	138.42	17
A4	139.62	37	140.62	31	138.86	30
D1	140.23	44	141.84	44	140.50	33
C4	146.94	22	147.42	23	145.70	19
B4	147.63	30	148.67	30	147.00	21
C3	150.46	29	151.27	19	149.61	17
B3	150.93	39	151.86	36	150.06	24
A3	151.12	39	152.10	31	150.43	24
D3	151.27	39	152.24	34	150.72	22
A4 AcC=O	168.71	30	168.90	35	168.36	27
D4 AcC=O	168.98	40	169.05	35	168.54	25
B γ AcC=O	170.68	36	170.78	40	170.08	25
A γ AcC=O	170.76	36	170.81	40	170.12	25

Compound Number 2060



^{1}H (acetone)

Atom	H Shifts	Mult	J
A3,4 OMe	3.77	s	
β	3.85	m	
B3 OMe	3.88	s	
γ1	4.45	dd	11.1, 7.6
γ2	4.58	dd	11.1, 5.4
B γ	4.78	dd	6.5, 1.2
a	5.61	d	7.1
B β	6.31	dt	15.8, 6.5
D β	6.33	d	15.9
C β	6.37	d	15.9
B α	6.70	dt	15.8, 1.2
C,D 3,5	6.88	m	
A5	6.93	d	8.3
A6	7.00	d	8.3, 2.0
A,B 2	7.07	br d	2.0
B6	7.11	br s	
D 2,6	7.51	m	
C 2,6	7.54	m	
C α	7.63	d	15.9
D α	7.53	d	15.9

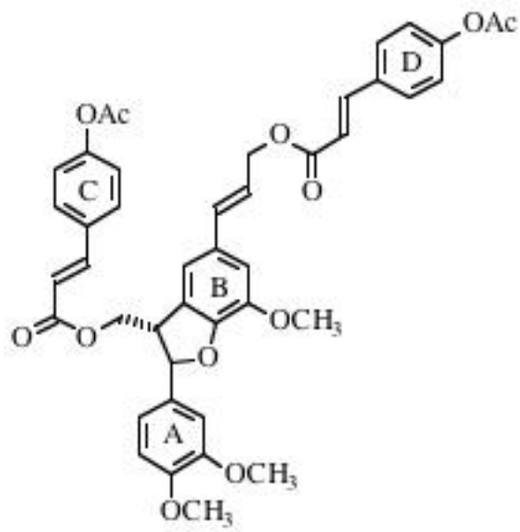
Notes:

S. Quideau
C3,4,5 and D3,4,5 Can be interchanged
not substantiated in CDCl3 & DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	50.40	30	51.33	39	49.47	15
A3 OMe	55.90	100	56.09	56	55.48	57
A4 OMe	55.90	100	56.13	32	55.76	22
B3 OMe	56.03	33	56.41	55	55.82	55
B γ	65.19	31	65.42	40	64.46	21
γ	65.38	25	65.92	33	64.80	12
α	88.86	34	89.15	42	87.87	20
A2	109.31	41	110.93	47	110.01	29
B2	110.67	26	112.25	33	111.03	11
A5	111.06	42	112.65	50	111.67	28
D β	114.53	39	115.08	51	113.68	21
C β	115.14	43	115.49	51	114.05	32
B6	115.39	32	116.36	40	115.31	16
D3	115.93	96	116.68	100	115.77	100
D5	115.83	96	116.68	100	115.77	100
C3	115.96	96	116.70	100	115.77	100
C5	115.96	96	116.70	100	115.77	100
A6	118.91	43	119.44	52	118.66	28
B β	121.37	36	122.40	41	121.56	18
D1	126.75	29	126.85	33	124.94	24
C1	126.98	29	126.97	37	125.08	29
B5	127.79	35	129.21	36	128.08	22
C2	130.00	34	130.94	100	130.34	100
C6	130.00	34	130.94	100	130.34	100
D2	130.06	97	131.02	100	130.34	100
D6	130.06	97	131.02	100	130.34	100
B1	130.62	34	131.51	27	130.06	24
A1	132.86	33	134.52	34	133.61	18
B α	134.27	36	134.78	44	132.79	29
B3	144.40	33	145.42	36	143.91	22
C α	144.94	40	145.50	50	144.89	29
D α	145.40	37	145.91	45	145.13	23
B4	148.27	26	149.42	25	147.65	23
A3	149.14	38	150.43	25	148.72	36
A4	149.17	38	150.51	28	148.81	21
D4	158.05	31	160.61	25	159.87	34
C4	158.23	31	160.71	25	159.94	27
C γ	167.20	34	167.23	38	166.38	5
D γ	167.37	29	167.23	38	166.38	14

Compound Number 2061



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.26	s	
A3,4 OMe	3.76	s	
B3 OMe	3.88	s	
β	~3.88	m	
γ1	4.48	dd	11.1, 7.5
γ2	4.61	dd	11.1, 5.4
B γ	4.81	dd	6.5, 1.3
α	5.61	d	7.2
B β	6.32	dt	15.8, 6.5
A5	6.43	d	8.3
D β	6.50	d	16.0
Cβ	6.54	d	16.0
B α	6.71	dt	15.8, 1.2
A6	7.00	dd	8.2, 2.0
A2	7.08	d	2.0
B2	7.08	br s	
B6	7.11	br s	
C,D 3,5	7.16-7.21	m	
D 2,6	7.68	m	
C α	7.70	d	16.0
C 2,6	7.72	m	

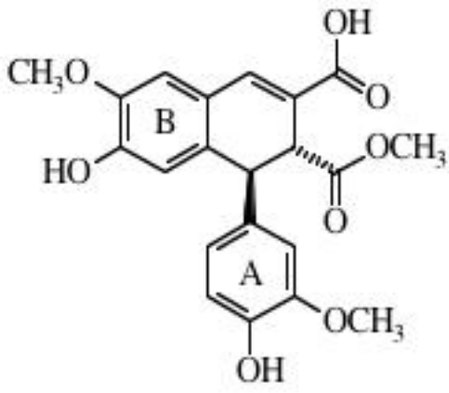
Notes:

S. Quideau
C4,D4 and Cg,Dg Can be interchanged
Not substantiated in CDCl3 & DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
C4 AcMe	21.08	85	20.94	91	20.76	100
D4 AcMe	21.08	85	20.94	91	20.76	100
β	50.45	30	51.21	31	49.36	32
A3 OMe	55.97	52	56.08	46	55.50	95
A4 OMe	56.00	47	56.14	31	55.50	95
B3 OMe	56.13	47	56.41	42	55.76	85
B γ	65.31	30	65.71	32	64.66	31
γ	65.56	23	66.15	23	64.98	26
α	88.94	35	89.17	34	87.72	31
A2	109.53	32	110.97	38	110.11	48
B2	110.96	25	112.28	26	111.18	30
A5	111.26	40	112.63	39	111.77	48
B6	115.41	30	116.35	30	115.30	32
D β	117.59	37	118.61	41	117.65	49
C β	118.21	41	119.01	41	118.01	57
A6	118.94	42	119.53	38	118.65	49
B β	121.34	34	122.17	31	121.32	33
D3	122.14	100	123.23	100	122.24	96
D5	122.14	100	123.23	100	122.24	96
C3	122.19	100	123.23	100	122.28	96
C5	122.19	100	123.23	100	122.28	96
B5	127.79	27	129.17	27	128.02	47
C2	129.21	57	130.16	96	129.49	44
C6	129.21	57	130.16	96	129.49	44
D2	129.42	24	130.21	93	129.53	96
D6	129.42	24	130.21	93	129.53	96
B1	130.66	26	131.47	26	130.01	41
D1	131.92	23	132.77	25	131.47	47
C1	132.16	23	132.91	25	131.62	46
A1	132.96	28	134.41	28	132.74	41
B α	134.47	31	134.99	31	133.72	41
C α	143.91	40	144.43	39	143.59	24
D α	144.39	37	144.79	37	143.81	55
B3	144.53	24	145.42	26	143.87	47
B4	148.45	18	149.44	19	147.67	32
A3	149.36	30	150.45	25	148.81	45
C4	152.21	17	153.46	21	151.99	47
D4	152.36	17	153.53	21	152.03	47
C γ	166.47	30	166.80	48	165.84	45
D γ	166.61	23	166.80	48	165.87	45
C4 C=O	168.97	30	169.45	34	168.87	52
D4 C=O	169.01	30	169.45	34	168.87	52

Compound Number 2062



Methyl 7-hydroxy-5-methoxy-1-(4-hydroxy-3-methoxyphenyl)- trans -1,1-dihydronapthalene-3-carboxylic Acid 2-carboxylate

^{1}H (acetone)

Atom	H Shifts	Mult	J
A γ OMe	3.55	s	
A3 OMe	3.74	s	
B3 OMe	3.87	s	
β	3.96	d	3.1
α	4.51	d	3.1
A6	6.43	dd	8.3, 1.9
A5	6.657	d	8.3
B5	6.661	s	
A2	6.77	d	2.0
B2	7.06	s	
B α	7.66	s	

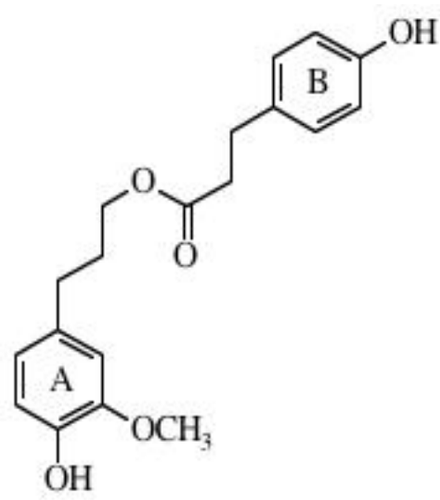
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α			46.46	87		
β			48.06	64		
A g OMe			52.25	96		
A3 OMe			56.18	95		
B3 OMe			56.36	95		
A2			112.01	95		
B2			113.11	87		
A5			115.52	72		
B5			116.75	64		
A6			120.82	100		
B β			123.97	24		
B1			124.58	64		
B6			132.08	64		
A1			135.45	73		
B α			138.07	56		
A4			146.14	35		
B3			147.51	48		
A3			148.11	48		
B4			149.34	35		
B γ			168.80	12		
A γ			173.44	63		

Compound Number 2063



Dihydroconiferyl 4-hydroxydihydrocinnamate

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.86	m	
α	2.55	t	7.4
B β	2.56	t	7.6
B α	2.82	t	7.6
OMe	3.80	s	
γ	4.03	t	6.5
A6	6.61	dd	8.0, 2.0
A5	6.73	d	7.9
B 3,5	6.75	m	
A2	6.79	d	2.0
B 2,6	7.06	m	
ArOH	7.86	s	
ArOH	8.10	s	

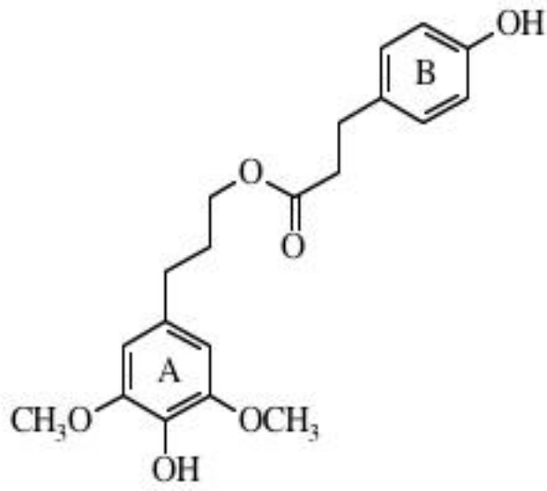
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B α	30.11	46	30.75	47	29.49	37
β	30.40	42	31.33	47	29.95	38
α	31.75	44	32.24	47	30.91	36
B β	36.17	45	36.69	49	35.47	39
OMe	55.87	47	56.16	45	55.48	47
γ	63.85	44	64.03	48	63.13	35
A2	110.96	48	112.73	49	112.43	40
A5	114.28	47	115.62	45	115.28	92
B3	115.31	99	116.00	89	115.03	39
B5	115.31	99	116.00	89	115.03	39
A6	120.93	51	121.55	51	120.30	43
B2	129.37	100	130.05	100	129.04	100
B6	129.37	100	130.05	100	129.04	100
B1	132.46	25	132.38	23	130.50	30
A1	133.09	28	133.55	25	131.83	33
A4	143.76	25	146.58	22	144.53	35
A3	146.40	23	148.16	17	147.38	31
B4	154.13	26	156.57	22	155.55	33
B γ	173.26	24	173.09	21	172.32	34

Compound Number 2064



Dihydrosinapyl dihydro-p-coumarate

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.87	m	
α	2.55	t	7.6
B β	2.56	t	7.5
B α	2.82	t	7.6
OMe	3.79	s	
γ	4.03	t	6.5
A 2,6	6.48	s	
B 3,5	6.74	m	
A4 OH	6.89	s	
B 2,6	7.06	m	
B4 OH	8.08	s	

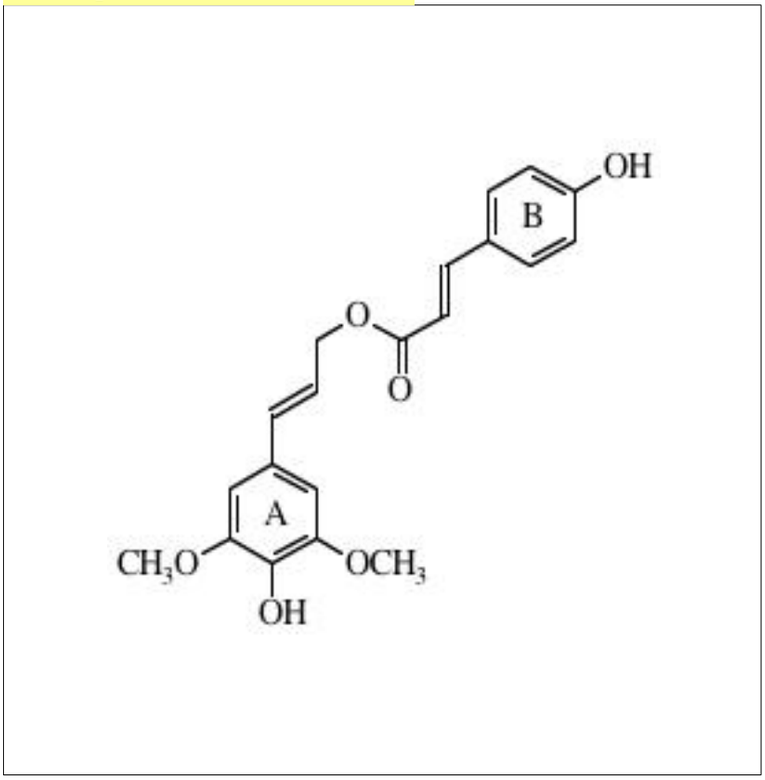
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B α	30.11	48	30.77	49	29.49	36
β	30.41	44	31.31	48	29.90	37
α	32.26	46	32.71	47	31.41	32
B β	36.17	46	36.71	49	35.46	36
OMe	56.27	96	56.57	92	55.87	100
OMe	56.27	96	56.57	92	55.87	100
γ	63.82	48	64.04	49	63.15	33
A2	105.03	94	106.69	90	105.63	69
A6	105.03	94	106.69	90	105.63	69
B3	115.32	95	116.01	92	115.02	81
B5	115.32	95	116.01	92	115.02	81
B2	129.34	100	130.07	100	129.03	91
B6	129.34	100	130.07	100	129.03	91
B1	132.28	31	132.40	26	130.50	25
A1	132.36	24	132.59	27	131.04	27
A4	132.93	26	135.07	23	133.55	25
A3	146.93	50	148.62	43	147.85	53
A5	146.93	50	148.62	43	147.85	53
B4	154.19	28	156.61	25	155.55	28
B γ	173.21	29	173.08	26	172.32	30

Compound Number 2065



Sinapyl p-coumarate

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.84	s	
γ	4.78	dd	6.5, 1.3
β	6.28	dt	15.8, 6.5
B β	6.38	d	15.9
α	6.64	dt	15.8, 1.3
A 2,6	6.79	s	
B 3,5	6.89	m	
B 2,6	7.55	m	
B α	7.63	d	15.9

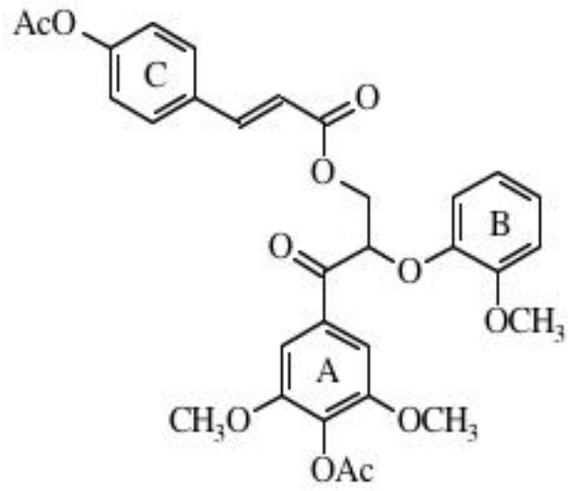
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.28	100	56.61	91	55.97	100
OMe	56.28	100	56.61	91	55.97	100
γ	65.15	43	65.42	43	64.50	23
A2	103.55	89	105.16	91	104.20	64
A6	103.55	89	105.16	91	104.20	64
B β	115.15	45	115.52	45	114.08	38
B3	115.92	93	116.70	100	115.78	64
B5	115.92	93	116.70	100	115.78	64
β	121.44	44	122.07	48	121.06	28
B1	126.98	28	126.99	24	125.08	25
A1	127.84	27	128.22	25	126.47	26
B2	129.98	94	130.95	99	130.34	73
B6	129.98	94	130.95	99	130.34	73
α	134.53	44	135.14	47	134.03	30
A4	135.03	28	137.27	22	135.80	26
B α	144.91	39	145.45	45	144.88	36
A3	147.10	59	148.84	49	148.04	64
A5	147.10	59	148.84	49	148.04	64
B4	158.06	32	160.62	27	159.87	25
B γ	167.32	26	167.22	23	166.40	24

Compound Number 2066



2-(4-Acetoxy-3,5-dimethoxybenzoyl)-2-(2-methoxyphenoxy) ethyl 4-acetoxycinnamate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.26	s	
Ac Me	2.26	s	
B3 OMe	3.75	s	
OMe	3.86	s	
γ1	4.60	dd	12.0, 6.8
γ2	4.86	dd	12.0, 3.6
β	5.96	dd	6.8, 3.6
C α	6.50	d	16.0
B6	6.83	ddd	7.9, 8.8, 2.5
B 1,2,5	6.98	m	
C 3,5	7.18	m	
A 2,6	7.56	s	
C β	7.62	d	16.0
C 2,6	7.69	m	

Notes:

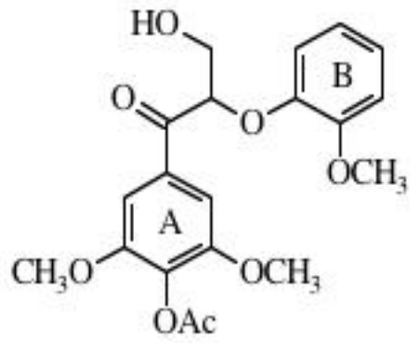
S. Quideau

B5 and C β can be interchanged

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac	20.41	52	20.21	45	20.08	56
Ac	21.10	51	20.94	45	20.83	50
B3 OMe	55.71	52	56.12	49	55.55	63
OMe	56.34	93	56.68	89	56.21	100
OMe	56.34	93	56.68	89	56.21	100
γ	64.70	31	65.07	36	63.82	20
β	80.76	41	80.41	44	78.23	28
A2	105.93	76	106.52	84	105.47	52
A6	105.93	76	106.52	84	105.47	52
B2	112.59	49	113.82	47	112.95	34
B5	117.42	43	118.33	50	116.01	35
C β	118.35	48	118.38	51	117.39	41
B6	121.03	47	121.64	47	120.63	40
C3	122.18	100	123.24	100	122.38	90
C5	122.18	100	123.24	100	122.38	90
B1	123.60	45	12334	8	122.55	32
C2	129.32	96	130.27	91	129.69	87
C6	129.32	96	130.27	91	129.69	87
C1	131.84	31	132.66	8	131.49	34
A1	132.66	30	133.94	26	132.49	34
A4	133.39	20	134.24	27	132.55	30
C α	144.59	42	145.13	13	144.28	36
B4	146.72	31	147.84	42	146.32	37
B3	150.37	29	151.34	24	149.51	39
A3	152.28	63	153.40	22	151.95	76
A5	152.28	63	153.40	22	151.95	76
C4	152.36	31	153.59	49	152.13	34
C γ	166.62	35	166.84	23	165.85	33
Ac C=O	168.05	29	168.13	26	167.63	37
Ac C=O	169.08	29	169.41	22	168.94	42
α	194.44	33	194.92	24	194.02	35

Compound Number 2067



1(4-acetoxy-3,5-dimethoxyphenyl)-3-hydroxy-2-(2-methoxy phenoxy)propanone

^{1}H (acetone)

Atom	H Shifts	Mult	J
B3 OMe	3.77	s	
OMe	3.85	s	
γ	4.10	dd	6.2, 5.0
γ OH	4.28	t	6.2
β	5.56	t	5.0
A 2,6	7.49	s	
B6	6.80	m	
B 1,5	6.41	m	
B2	6.96	m	

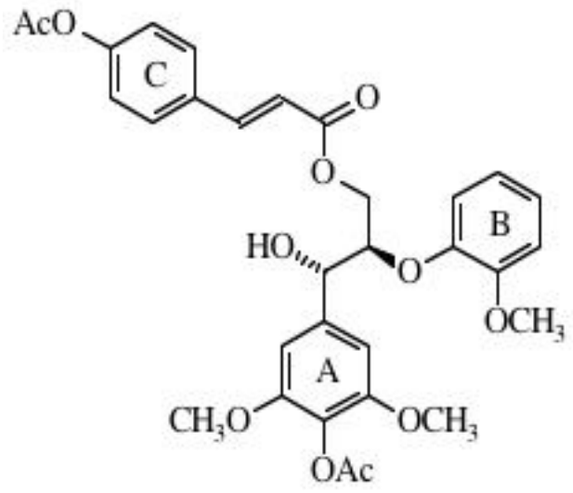
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.20	46		
B3 OMe			56.11	48		
OMe			56.62	94		
OMe			56.62	94		
γ			63.90	47		
β			84.04	50		
A2			106.56	100		
A6			106.56	100		
B2			113.67	50		
B5			117.03	46		
B6			121.61	53		
B1			123.24	53		
A4			133.99	13		
A1			134.39	25		
B4			148.26	21		
B3			151.03	21		
A3			153.25	48		
A5			153.25	48		
Ac C=O			168.15	24		
α			196.77	26		

Compound Number 2068



erythro

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac	2.20	s	
Ac	2.26	s	
OMe	3.78	s	
B3 OMe	3.81	s	
γ1	4.47	dd	11.9, 3.9
γ2	4.52	dd	11.9, 6.1
β	4.73	m	
α OH	4.78	d	4.5
α	5.07	br t	4.8
C β	6.41	d	16.0
B6	6.84	ddd	7.9, 6.4, 2.7
A 2,6	6.88	s	
B 1,2	6.95	m	
B5	7.04	br dd	1.4
C 3,5	7.17	m	
C α	7.51	d	16.0
C 2,6	7.66	m	

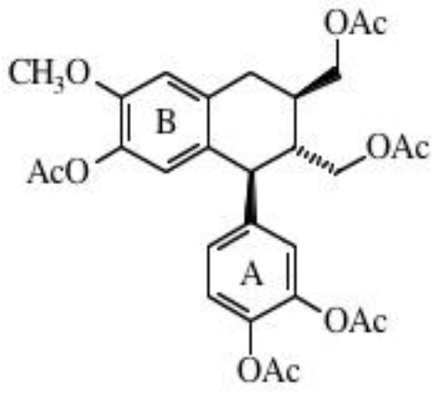
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac			20.25	50		
Ac			20.94	51		
B3 OMe			56.21	45		
OMe			56.39	94		
OMe			56.39	94		
γ			64.01	31		
α			73.49	40		
β			83.04	40		
A2			104.37	75		
A6			104.37	75		
B2			113.66	46		
C β			118.84	42		
B5			119.77	46		
B6			121.73	47		
C3			123.18	100		
C5			123.18	100		
B1			123.67	43		
A4			128.89	15		
C2			130.15	94		
C6			130.15	94		
C1			132.86	28		
A1			140.77	30		
C α			144.38	42		
B4			148.69	25		
B3			152.04	25		
A3			152.89	52		
A5			152.89	52		
C4			153.43	24		
C γ			166.80	28		
Ac C=O			168.58	21		
Ac C=O			169.43	30		

Compound Number 2069



Isotaxiresinol

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.00	s	
Ac Me	2.01	s	
Ac Me	2.10	s	
β	2.14	m	
Ac Me	2.22	s	
Ac Me	2.24	s	
B β	2.26	m	
B α	2.90	m	
A3 OMe	3.78	s	
γ1	3.90	dd	11.7, 3.5
α	4.06	br d	10.2
Bγ1	4.11	dd	11.2, 6.0
γ2	4.12	dd	11.7, 3.5
B γ2	4.22	dd	11.2, 4.4
B5	6.34	d	0.9
B2	6.88	br s	
A2	7.04	d	2.1
A6	7.10	dd	8.3, 4.1
A5	7.14	d	8.3

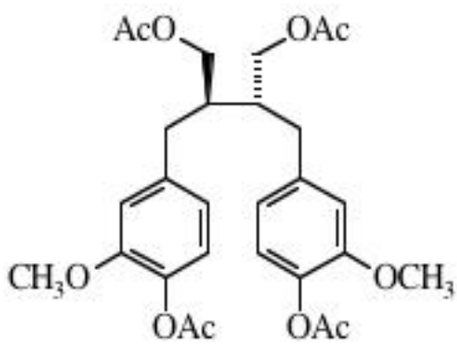
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 Ac Me			20.36	85		
A4 Ac Me			20.45	100		
B4 Ac Me			20.50	88		
Ac Me			20.60	83		
Ac Me			20.72	86		
B α			33.50	67		
B β			36.27	82		
β			44.34	80		
α			47.51	80		
OMe			56.18	96		
γ			63.57	65		
B γ			66.69	72		
B2			112.97	74		
B5			124.12	74		
A5			124.36	82		
A2			124.92	78		
A6			127.98	79		
B6			131.84	54		
B1			135.41	55		
B4			139.26	46		
A4			142.08	41		
A3			143.41	42		
A1			144.19	58		
B3			150.55	44		
A4 Ac C=O			168.52	46		
B4 Ac C=O			168.63	46		
A3 Ac C=O			168.92	45		
Ac C=O			171.04	58		
Ac C=O			171.05	55		

Notes:

S. Quideau
Diaxial configuration on 6-membered ring --Trans 7,8
Natural occuring isomer is (+), i.e. 7S.8R, 8R'

Compound Number 2070



Seco-isolariciresinol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	2.00	s	
4 Ac Me	2.21	s	
β	2.22	m	
α1	2.70	dd	13.9, 7.9
α2	2.83	dd	13.8, 6.7
A3 OMe	3.74	s	
γ1	4.03	dd	11.4, 5.5
γ2	4.25	dd	11.4, 6.1
A6	6.70	dd	8.0, 1.95
A2	6.87	d	1.92
A5	6.92	d	8.0

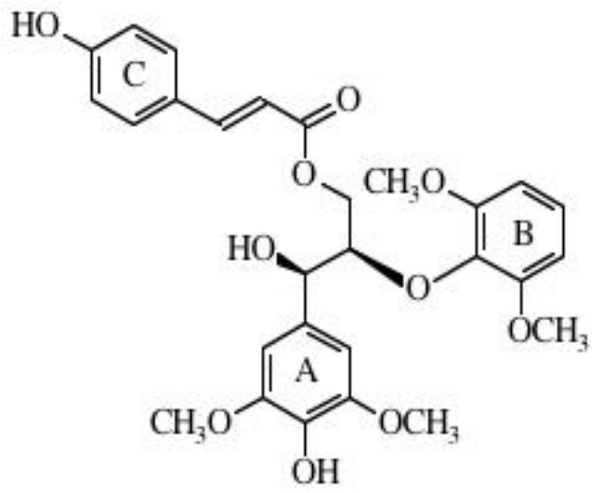
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
4 Ac Me			20.47	100		
γ AcMe			20.83	84		
α			35.51	64		
β			40.81	77		
γ			64.67	68		
2			114.00	79		
6			121.67	80		
5			123.32	80		
4			139.14	45		
1			140.00	1		
3			152.01	50		
4 Ac C=O			169.04	46		
γAc C=O			171.04	52		

Notes:

S. Quideau
natural occuring isomer (-), i.e. 8R, 8R'
As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 2071



threo

^{1}H (acetone)

Atom	H Shifts	Mult	J
A 3,5 OMe	3.76	s	
B 3,5 OMe	3.83	s	
γ1	4.06	dd	11.9, 4.2
β	4.27	ddd	7.3, 4.2, 3.1
γ2	4.45	dd	12.0, 3.2
α	5.00	br d	7.1
α OH	4.60	d	3.2
C β	6.33	d	16.0
B 2,6	6.68	d	8.4
A 2,1	6.67	d	0.3
C 3,5	6.89	m	
B1	7.01	dd	8.7, 8.1
C α	7.48	d	16.0
C 2,6	7.53	m	

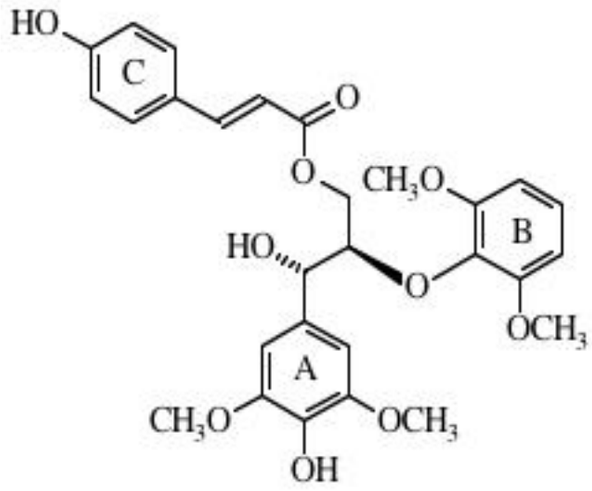
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B OMe	56.01	54	56.44	81	55.78	26
B OMe	56.01	54	56.44	81	55.78	26
A OMe	56.25	56	56.59	49	55.93	100
A OMe	56.25	56	56.59	49	55.93	100
γ	63.92	23	64.78	28	64.09	8
α	74.66	35	74.81	35	72.17	17
β	87.07	29	86.87	38	83.84	17
A2	103.75	78	105.39	72	104.32	36
A6	103.75	78	105.39	72	104.32	36
B2	105.16	98	106.35	100	105.58	51
B6	105.16	98	106.35	100	105.58	51
C β	114.87	38	115.52	42	114.12	36
C3	115.97	96	116.68	95	115.82	74
C5	115.97	96	116.68	95	115.82	74
B1	124.30	44	124.72	40	123.62	22
C1	126.83	32	126.97	44	125.07	25
C2	129.98	100	130.92	91	130.21	54
C6	129.98	100	130.92	91	130.21	54
A1	130.58	41	132.00	30	131.16	26
A4	134.50	38	136.27	24	134.63	32
B4	136.62	33	137.85	20	136.12	28
C α	144.86	44	145.28	41	144.38	13
A3	146.99	79	148.38	53	147.49	40
A5	146.99	79	148.38	53	147.49	40
B3	152.93	71	154.03	51	152.97	63
B5	152.93	71	154.03	51	152.97	63
C4	158.23	37	160.58	32	159.80	24
C γ	167.12	23	167.12	27	166.25	32

Compound Number 2072



erythro

^{1}H (acetone)

Atom	H Shifts	Mult	J
A 3,5 OMe	3.79	s	
B 3,5 OMe	3.82	s	
γ1	4.23	dd	11.8, 3.4
γ2	4.45	dd	11.8, 7.3
β	4.58	m	
α OH	4.697	d	3.9
α	4.96	br m	
C β	6.15	d	16.0
B 2,6	6.68	d	8.4
A 2,6	6.71	d	0.7
C 3,5	6.84	m	
B1	7.01	dd	8.6, 8.2
C α	7.33	d	16.0
C 2,6	7.46	m	

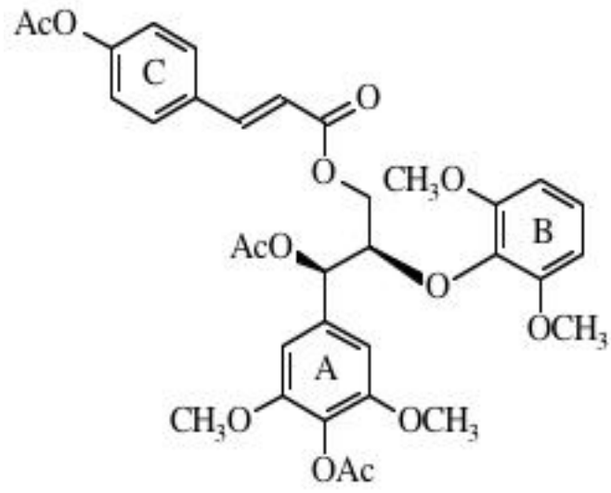
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B OMe	56.20	92	56.48	78	55.77	76
B OMe	56.20	92	56.48	78	55.77	76
A OMe	56.33	89	56.60	76	55.92	100
A OMe	56.33	89	56.60	76	55.92	100
γ	62.59	30	63.57	31	63.38	19
α	71.90	36	73.19	40	72.62	27
β	83.18	41	84.40	42	83.51	28
A2	102.78	85	104.59	88	103.77	62
A6	102.78	85	104.59	88	103.77	62
B2	105.36	92	106.34	96	105.32	69
B6	105.36	92	106.34	96	105.32	69
C β	115.19	46	115.73	46	114.12	42
C3	115.91	97	116.65	45	115.81	87
C5	115.91	97	116.65	45	115.81	87
B1	124.44	44	124.75	37	123.40	31
C1	126.85	36	127.03	32	125.03	37
C2	129.88	100	130.82	100	130.11	83
C6	129.88	100	130.82	100	130.11	83
A1	129.75	32	131.66	28	132.10	29
A4	133.91	29	135.91	24	134.45	32
B4	134.69	30	136.59	24	135.92	36
C α	144.58	44	144.99	47	144.16	37
A3	147.00	69	148.49	57	147.63	67
A5	147.00	69	148.49	57	147.63	67
B3	153.69	70	154.53	57	152.89	84
B5	153.69	70	154.53	57	152.89	84
C4	158.15	35	160.43	34	159.74	32
C γ	167.29	37	167.16	32	166.27	38

Compound Number 2073



threo

^{1}H (acetone)

Atom	H Shifts	Mult	J
α Ac Me	1.97	s	
Ac Me	2.02	s	
Ac Me	2.27	s	
OMe	3.78	s	
OMe	3.79	s	
γ1	4.07	dd	11.9, 4.7
γ2	4.41	dd	11.9, 3.8
β	4.68	ddd	6.8, 4.7, 3.8
α	6.18	d	6.8
C β	6.56	d	16.0
B 2,6	6.66	d	8.4
A 2,6	6.86	br s	
B1	6.99	t	8.4
C 3,5	7.19	m	
C α	7.55	d	16.0
C 2,6	7.72	m	

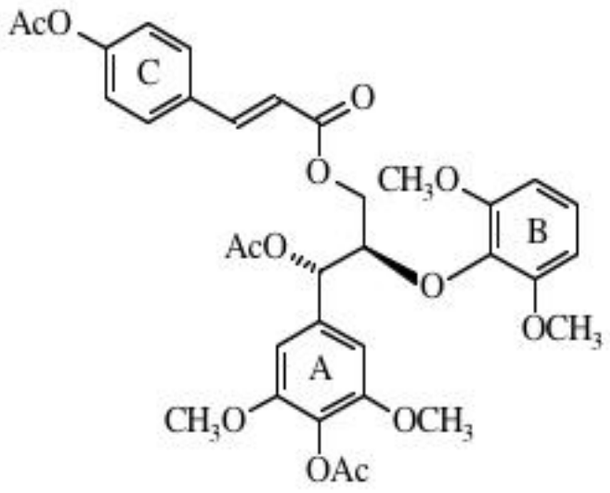
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.36	49	20.23	47	20.15	54
Ac Me	21.02	83	20.95	73	20.75	47
α Ac Me	21.02	83	20.95	73	20.88	52
OMe	55.89	**100**	56.35	72	55.80	77
OMe	55.89	100	56.35	72	55.80	77
OMe	56.13	78	56.49	73	56.01	56
OMe	56.13	78	56.49	73	56.01	56
γ	64.01	22	64.66	25	63.72	10
α	75.63	30	76.79	34	75.97	16
β	80.86	29	81.83	32	80.62	18
A2	104.10	51	104.92	61	103.89	34
A6	104.10	51	104.92	61	103.89	34
B2	105.09	69	106.22	77	105.29	70
B6	105.09	69	106.22	77	105.29	70
C β	117.75	34	118.88	38	117.82	27
C3	122.09	79	123.20	**100**	122.43	**100**
C5	122.09	79	123.20	100	122.43	100
B1	123.74	31	124.47	37	123.68	22
A4	128.57	18	129.54	14	127.74	25
C2	129.19	96	130.22	88	129.68	67
C6	129.19	96	130.22	88	129.68	67
C1	131.92	26	132.90	24	131.66	31
B4	135.42	30	136.76	36	135.61	27
A1	136.56	24	137.85	20	136.15	31
C α	143.86	33	144.48	39	143.76	29
A3	151.94	55	153.07	53	151.55	74
A5	151.94	55	153.07	53	151.55	74
C4	152.10	24	153.46	24	152.09	30
B3	153.14	53	154.19	53	152.69	66
B5	153.14	53	154.19	53	152.69	66
C γ	166.24	27	166.62	26	165.86	32
Ac C=O	168.45	25	168.46	21	168.06	28
Ac C=O	169.05	41	169.45	29	169.06	38
Ac C=O	169.68	27	169.93	27	169.44	30

Compound Number 2074



erythro

^{1}H (acetone)

Atom	H Shifts	Mult	J
α Ac Me	2.15	s	
Ac Me	2.21	s	
Ac Me	2.26	s	
B 3,5 OMe	3.79	s	
A 3,5 OMe	3.81	s	
γ1	4.36	dd	11.9, 4.0
γ2	4.53	dd	11.9, 6.2
β	4.80	dt	6.2, 4.0
α	6.14	d	4.2
C β	6.35	d	16.0
B 2,6	6.65	d	8.4
A 2,6	6.83	br s	
B1	6.99	t(dd)	8.4
C 3,5	7.18	m	
C α	7.44	d	16.0
C 2,6	7.66	m	

Notes:

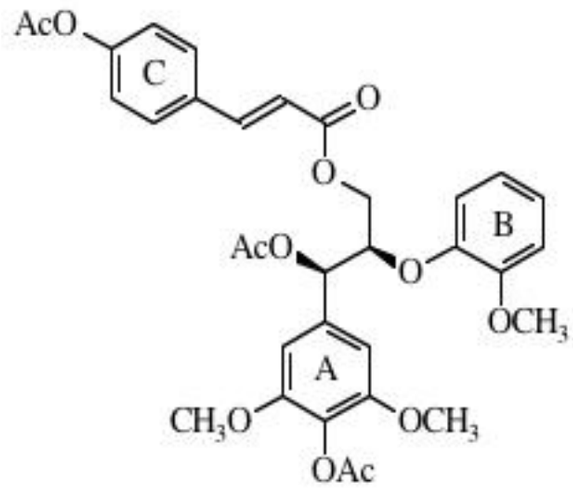
S. Quideau

B3,5 OMe and A3,5 OMe can be interchanged

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.36	57	20.24	42	20.15	61
α Ac Me	21.02	86	20.95	71	20.76	54
Ac Me	21.02	86	20.95	71	20.87	53
B OMe	55.87	100	56.32	80	55.78	100
B OMe	55.87	100	56.32	80	55.78	100
A OMe	56.07	100	56.47	79	55.97	88
A OMe	56.07	100	56.47	79	55.97	88
γ	63.13	25	63.73	28	62.64	15
α	74.50	34	75.58	37	74.23	26
β	80.92	35	81.67	38	80.19	26
A2	103.93	65	104.60	84	103.45	55
A6	103.93	65	104.60	84	103.45	55
B2	105.05	75	106.12	83	105.27	69
B6	105.05	75	106.12	83	105.27	69
C β	117.84	41	118.80	42	117.70	36
C3	122.03	87	123.19	100	122.43	99
C5	122.03	87	123.19	100	122.43	99
B1	124.00	3	124.72	43	124.00	29
A4	128.37	21	129.35	15	127.59	31
C2	129.19	94	130.15	90	129.57	82
C6	129.19	94	130.15	90	129.57	82
C1	131.98	31	132.85	26	131.56	33
B4	135.39	27	136.69	34	134.77	39
A1	135.73	33	136.77	21	135.43	34
C α	143.73	39	144.29	41	143.54	36
A3	151.84	62	153.06	55	151.58	85
A5	151.84	62	153.06	55	151.58	85
C4	152.04	29	153.44	23	152.06	36
B3	153.32	66	154.34	56	152.85	94
B5	153.32	66	154.34	56	152.85	94
C γ	166.42	32	166.52	27	165.70	36
Ac C=O	168.49	30	168.51	25	168.10	40
Ac C=O	169.04	35	169.44	27	169.05	45
Ac C=O	169.43	30	170.00	26	169.49	39

Compound Number 2075



threo

γ-p-coumaroylated syringylglycerol-β04-guaiacol ether (Ac'd)

^{1}H (acetone)

Atom	H Shifts	Mult	J
α Ac Me	2.04	s	
Ac Me	2.20	s	
Ac Me	2.27	s	
B OMe	3.79	s	
A 3,5 OMe	3.81	s	
γ1	4.19	dd	12.0, 5.5
γ2	4.39	dd	11.9, 3.9
β	4.88	ddd	6.6, 5.5
α	6.15	d	6.6
C β	6.54	d	16.0
B6	6.87	m	
A 2,6	6.88	br s	
B 1,2	6.93 - 7.00	m	
B5	7.08 - 7.10	m	
C 3,5	7.19	m	
C α	7.58	d	16.0
C 2,6	7.71	m	

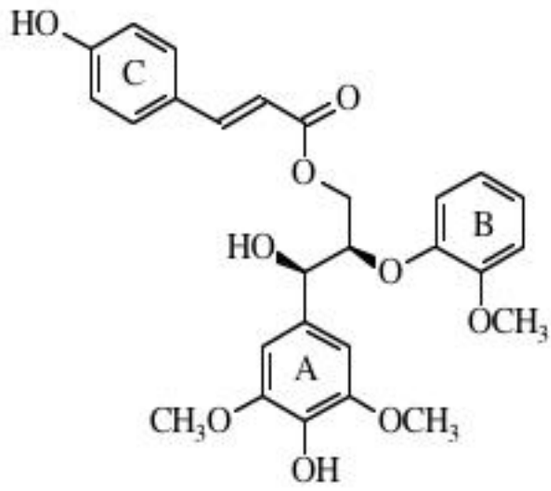
Notes:

S. Quideau
Not run in DMSO

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.42		20.23	25		
Ac Me	21.10		20.94	40		
αAc Me	21.10		20.94	40		
B3 OMe	35.77		56.21	30		
OMe	56.20		56.51	51		
OMe	56.20		56.51	51		
γ	63.39		63.97	14		
α	74.88		75.92	20		
β	80.50		80.89	19		
A2	104.09		105.00	41		
A6	104.09		105.00	41		
B2	112.45		113.74	31		
C β	117.52		118.62	24		
B5	118.85		119.25	26		
B6	121.00		121.70	27		
C3	122.14		123.22	100		
C5	122.14		123.22	100		
B1	123.34		123.75	24		
A4	128.81		129.70	7		
C2	129.31		130.26	56		
C6	129.31		130.26	56		
C1	131.91		132.83	15		
A1	134.81		136.23	17		
C α	144.25		144.78	25		
B4	147.99		149.16	13		
B3	150.86		151.87	13		
A3	152.01		153.21	29		
A5	152.01		153.21	29		
C4	152.20		153.53	18		
C γ	166.32		166.64	19		
Ac C=O	168.47		168.43	14		
Ac C=O	169.09		169.43	22		
Ac C=O	169.71		170.03	14		

Compound Number 2076



threo

γ-p-coumaroylated syringylglycerol-β04-guaiacyl ether

^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.79	s	
B3 OMe	3.84	s	
γ1	4.11	dd	12.0, 6.2
γ2	4.36	dd	12.0, 3.4
β	4.57	td	6.1, 3.4
α	4.96	(br)d	5.9
C β	6.31	d	16.0
A 2,6	6.82	d	0.4
B6	6.85-6.90	m	
C 3,5	6.88	m	
B 1,2	6.94-7.01	m	
B5	7.15	dd	7.9, 1.5
C α	7.48	d	16.0
C 2,6	7.51	m	

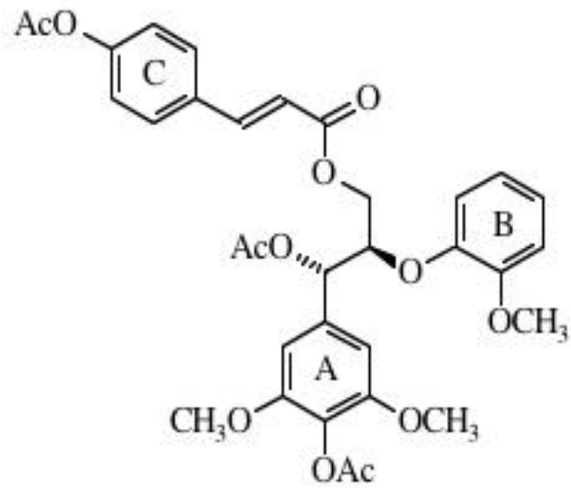
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3 OMe	55.82	50	56.27	38	55.60	54
OMe	56.31	91	56.59	74	55.88	95
OMe	56.31	91	56.59	74	55.88	95
γ	63.19	29	64.23	31	63.47	15
α	74.70	39	74.11	32	71.53	31
β	86.09	36	84.42	41	81.02	29
A2	103.82	80	105.41	85	104.24	68
A6	103.82	80	105.41	85	104.24	68
B2	112.19	50	113.60	48	112.70	46
C β	114.66	44	115.30	46	113.86	43
C3	115.95	99	116.68	99	115.78	100
C5	115.95	99	116.68	99	116.25	100
B5	120.53	49	119.33	50	116.25	54
B6	121.45	50	121.82	51	120.71	47
B1	124.12	52	123.52	47	121.71	35
C1	126.89	33	126.96	30	125.00	48
C2	130.04	100	130.97	100	130.30	95
C6	130.04	100	130.97	100	131.30	95
A1	130.29	34	132.11	25	131.22	36
A4	134.73	36	136.36	18	134.67	53
C α	145.18	44	145.57	46	144.84	35
A3	147.11	68	148.47	45	147.58	99
A5	147.11	68	148.47	45	147.58	99
B4	147.91	32	149.37	24	147.86	46
B3	150.91	32	151.80	23	149.91	55
C4	158.08	36	160.60	30	159.87	41
C γ	166.86	36	167.15	29	166.38	52

Compound Number 2077



erythro

γ-p-coumaroylated syringylglycerol-β04-guiacol ether (Ac'd)

^{1}H (acetone)

Atom	H Shifts	Mult	J
α Ac Me	2.09	s	
Ac Me	2.21	s	
Ac Me	2.26	s	
B3 OMe	3.81	s	
A OMe	3.81	s	
γ1	4.43	dd	11.9, 4.3
γ2	4.49	dd	11.9, 5.8
β	4.94	m	
α	6.12	d	5.1
C β	6.45	d	16.0
B6	6.85	m	
A 2,6	6.89	d	0.4
B 1,2	6.95-7.00	m	
B5	7.03-7.06	m	
C 3,5	7.19	m	
C α	7.57	d	16.0
C 2,6	7.69	m	

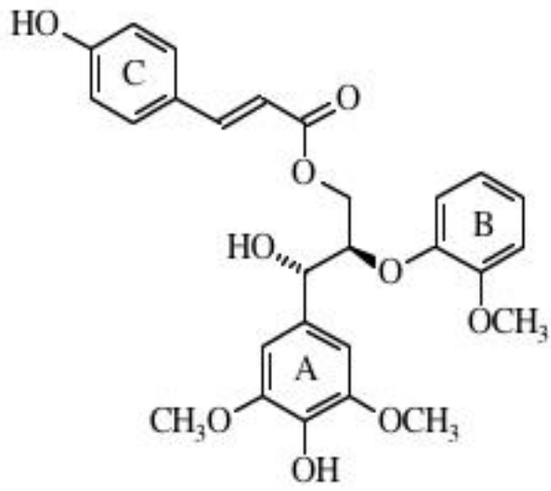
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.40	51	20.24	43	20.12	50
α Ac Me	21.01	47	20.90	37	20.70	51
Ac Me	21.06	58	20.94	47	20.84	54
B3 OMe	55.73	52	56.20	47	55.61	58
A OMe	56.14	93	56.50	82	55.97	99
A OMe	56.14	93	56.50	82	55.97	99
γ	62.98	27	63.41	27	62.35	18
α	74.17	35	74.99	35	73.53	29
β	80.31	36	80.38	34	78.34	24
A2	104.43	73	105.14	70	104.10	53
A6	104.43	73	105.14	70	104.10	53
B2	112.51	43	113.75	43	112.88	43
C β	117.59	43	118.57	40	117.53	40
B5	119.50	43	119.79	41	117.81	42
B6	120.95	45	121.65	42	120.69	45
C3	122.09	95	123.21	100	122.38	100
C5	122.09	95	123.21	100	122.38	100
B1	123.58	41	124.02	38	122.81	34
A4	128.67	20	129.57	13	127.73	27
C2	129.28	100	130.22	83	129.63	86
C6	129.28	100	130.22	83	129.63	86
C1	131.93	30	132.79	24	131.51	33
A1	134.92	31	136.25	26	134.99	32
C α	144.23	41	144.74	38	143.94	39
B4	147.24	31	148.36	22	146.75	36
B3	151.07	32	152.03	21	150.27	41
A3	151.98	61	153.07	45	151.48	70
A5	151.98	61	153.07	45	151.48	70
C4	152.16	29	153.51	21	152.08	36
C γ	166.44	30	166.63	26	165.76	33
Ac C=O	168.49	28	168.48	21	168.01	33
Ac C=O	169.06	33	169.43	25	168.97	37
α Ac C=O	169.48	27	169.95	21	169.34	30

Compound Number 2078



erythro

γ-p-coumaroylated syringylglycerol-β04-guaiacyl ether

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.80	s	
B3 OMe	3.81	s	
γ1	4.41	dd	11.8, 3.8
γ2	4.47	dd	11.8, 6.4
β	4.68	ddd	6.4, 5.0, 3.8
α	4.98	br d	4.9
C β	6.25	d	16.0
A 2,6	6.81	brs	
B6	6.83	m	
C 3,5	6.87	m	
B 1,2	6.91-6.96	m	
B5	7.05	br dd	7.8, 1.5
C α	7.44	d	16.0
C 2,6	7.48	m	

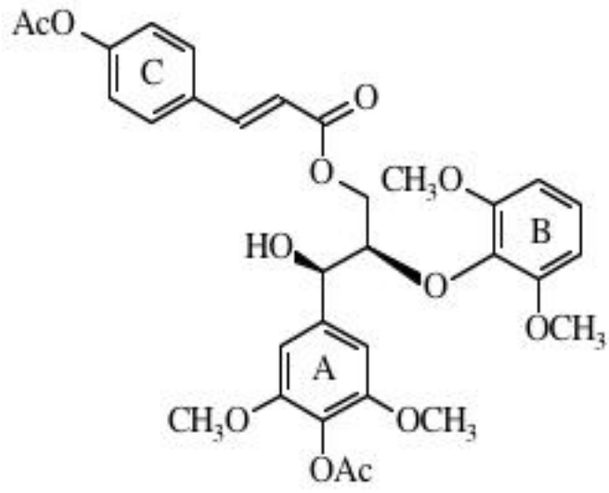
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3 OMe	55.83	53	56.23	48	55.54	
OMe	56.29	100	56.60	89	55.90	
OMe	56.29	100	56.60	89	55.90	
γ	62.70	30	64.04	33	63.29	
α	72.39	33	73.51	35	71.77	
β	84.23	40	83.41	42	80.92	
A2	103.13	84	105.23	84	104.38	
A6	103.13	84	105.23	84	104.38	
B2	112.22	49	113.63	47	112.74	
C β	114.40	46	115.37	45	113.93	
C3	115.95	99	116.67	100	115.75	
C5	115.95	99	116.67	100	115.75	
B5	120.53	49	119.55	48	116.89	
B6	121.46	54	121.72	48	120.62	
B1	124.03	46	123.46	45	121.83	
C1	126.44	36	126.92	28	124.99	
C2	129.98	99	130.90	94	130.24	
C6	129.98	99	130.90	94	130.24	
A1	130.16	37	132.59	31	132.05	
A4	134.15	37	136.12	26	134.61	
C α	145.25	44	145.42	43	144.71	
A3	147.00	60	148.42	51	147.52	
A5	147.00	60	148.42	51	147.52	
B4	147.02	39	148.91	24	147.52	
B3	151.42	35	152.00	22	150.03	
C4	158.68	38	160.58	31	159.82	
C γ	167.39	39	167.28	28	166.41	

Compound Number 2079



threo

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.19	s	
Ac Me	2.27	s	
A OMe	3.75	s	
B OMe	3.82	s	
γ1	4.16	dd	11.9, 4.6
β	4.38	ddd	6.3, 4.5, 3.6
γ2	4.50	dd	11.9, 3.6
α	5.07	br d	6.4
C β	6.47	d	16.0
B 2,6	6.68	d	8.4
A 2,6	6.87	br s	
B1	7.01	t	8.4
C 3,5	7.19	m	
C α	7.63	d	16.0
C 2,6	7.70	m	

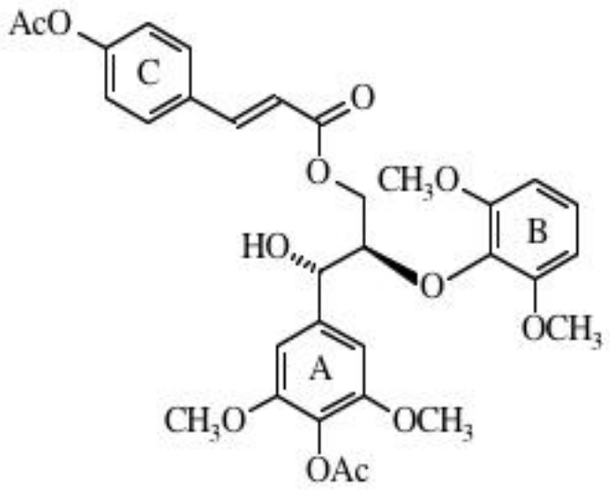
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.25	53		
Ac Me			21.06	53		
A OMe			56.36	83		
A OMe			56.36	83		
B OMe			56.45	81		
B OMe			56.45	81		
γ			64.93	30		
α			74.56	23		
β			85.88	37		
A2			104.48	69		
A6			104.48	69		
B2			106.35	88		
B6			106.35	88		
C β			118.98	40		
C3			123.19	100		
C5			123.19	100		
B1			124.80	43		
A4			128.98	14		
C2			130.17	91		
C6			130.17	91		
C1			132.93	39		
B4			137.65	21		
A1			140.28	21		
C α			144.26	40		
A3			152.82	53		
A5			152.82	53		
C4			153.43	24		
B3			154.07	54		
B5			154.07	54		
C γ			166.65	26		
Ac C=O			168.54	25		
Ac C=O			169.45	36		

Compound Number 2080



erythro

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.19	s	
Ac Me	2.26	s	
A OMe	3.78	s	
B OMe	3.83	s	
γ1	4.30	dd	11.7, 3.8
γ2	4.51	dd	11.7, 6.9
β	4.62	m	
α	5.05	br t	3.7
C β	6.34	d	16.0
B 2,6	6.09	d	8.4
A 2,6	6.82	br s	
B1	7.03	t	8.4
C 3,5	7.17	m	
C α	7.44	d	16.0
C 2,6	7.66	m	

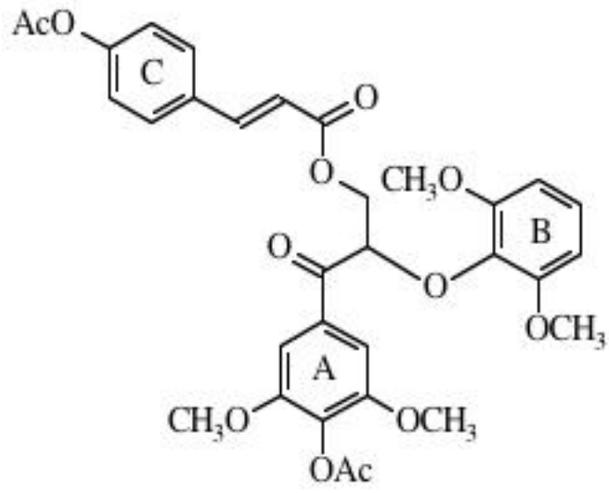
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.26	47		
Ac Me			20.94	54		
A OMe			56.38	86		
A OMe			56.38	86		
B OMe			56.48	97		
B OMe			56.48	97		
γ			63.67	31		
α			73.30	37		
β			84.07	39		
A2			103.76	82		
A6			103.76	82		
B2			106.31	88		
B6			106.31	88		
C β			119.10	44		
C3			123.16	100		
C5			123.16	100		
B1			124.83	43		
A4			128.69	14		
C2			130.11	89		
C6			130.11	89		
C1			132.93	29		
B4			136.57	21		
A1			140.05	25		
C α			144.00	42		
A3			152.94	48		
A5			152.94	48		
C4			153.36	21		
B3			154.51	52		
B5			154.51	52		
C γ			166.71	28		
Ac C=O			168.59	23		
Ac C=O			169.45	27		

Compound Number 2081



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.26	s	
Ac Me	2.28	s	
B OMe	3.72	s	
A OMe	3.85	s	
γ1	4.63	dd	11.7, 6.2
γ2	4.74	dd	11.7, 4.6
β	5.69	dd	6.2, 4.6
C β	6.39	d	16.0
B 2,6	6.64	d	8.4
B1	6.49	t	8.4
C 3,5	7.17	m	
C α	7.50	d	16.0
A 2,6	7.58	br s	
C 2,6	7.64	m	

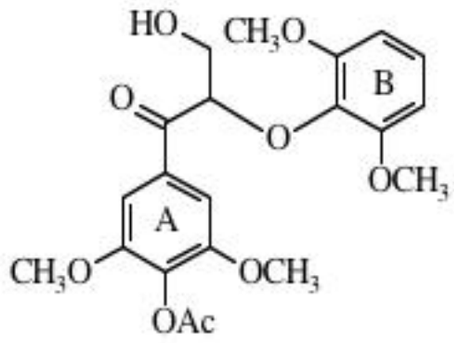
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.40	42	20.23		20.12	47
Ac Me	21.08	40	20.95		20.85	40
B OMe	55.88	85	56.31		55.80	100
B OMe	55.88	85	56.31		55.80	100
A OMe	56.28	82	56.67		56.20	92
A OMe	56.28	82	56.67		56.20	92
γ	64.49	27	64.90		63.77	17
β	81.85	38	81.50		79.82	26
B2	105.11	91	106.18		105.39	63
B6	105.11	91	106.18		105.39	63
A2	106.37	82	106.93		105.86	49
A6	106.37	82	106.93		105.86	49
C β	117.67	43	118.55		117.57	33
C3	122.15	100	123.25		122.45	76
C5	122.15	100	123.25		122.45	76
B1	124.23	46	124.99		124.07	28
C2	129.21	97	130.19		129.61	71
C6	129.21	97	130.19		129.61	71
C1	131.90	33	132.72		131.48	32
A4	133.05	19	133.96		132.28	26
A1	133.49	35	134.72		133.31	33
B4	135.68	24	136.63		135.12	32
C α	144.02	44	144.62		143.83	32
A3	152.08	69	153.20		151.80	69
A5	152.08	69	153.20		151.80	69
C4	152.16	28	153.52		152.11	31
B3	153.03	65	154.07		152.53	70
B5	153.03	65	154.07		152.53	70
C γ	166.34	33	166.55		165.73	32
Ac C=O	168.06	29	168.19		167.72	33
Ac C=O	169.08	29	169.43		169.02	32
α	194.81	33	195.26		184.38	31

Compound Number 2082



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
B OMe	3.73	s	
A OMe	3.86	s	
γ + γ OH	3.90-3.98	m	
β	5.22	dd	5.7, 4.5
B 2,6	6.67	d	8.4
B1	7.02	dd t	8.6, 8.2, 8.4
A 2,6	7.48	s	

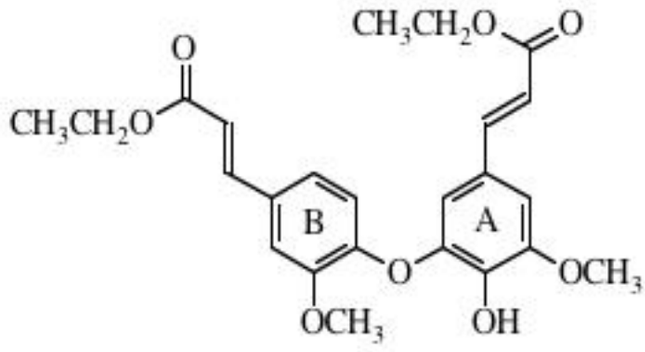
Notes:

S.Quideau

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.21	51		
B OMe			56.28	100		
B OMe			56.28	100		
A OMe			56.61	97		
A OMe			56.61	97		
γ			63.35	42		
β			86.41	48		
B2			106.22	97		
B6			106.22	97		
A2			106.51	91		
A6			106.51	91		
B1			124.92	47		
A4			133.59	14		
A1			135.01	29		
B4			137.01	20		
A3			153.06	51		
A5			153.06	51		
B3			153.77	50		
B5			153.77	50		
Ac C=O			168.18	22		
α			196.25	27		

Compound Number 3001



4-O-5 dehydrodiethylferulate

3-{3-[4-(2-ethoxycarbonyl-vinyl)-2-methoxy-phenoxy]-4-hydroxy-5-methoxy-phenyl}acrylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
A CH3	1.24	t	7.1
B CH3	1.27	t	7.1
B3 OMe	3.93	s	
A3 OMe	3.96	s	
A CH2	4.16	q	7.1
B CH2	4.19	q	7.1
A β	6.36	d	15.9
B β	6.48	d	15.95
B5	6.81	d	8.3
A6	6.89	d	1.9
B6	7.17	dd	8.7, 2.0
A2	7.22	d	1.9
B2	7.46	d	2.0
A α	7.53	d	15.9
B α	7.62	d	15.95

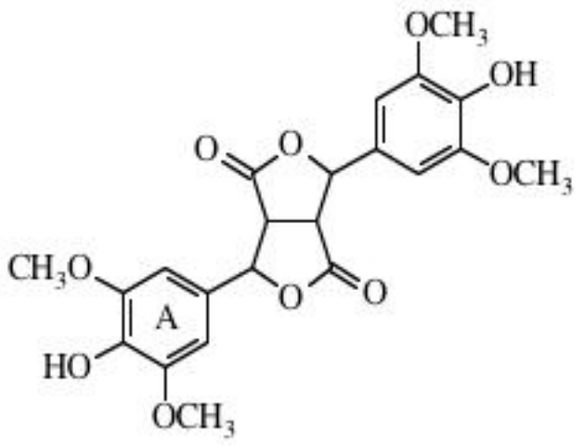
Notes:

jrf107.P1 /1 (H1), /2 (C13), /3 (Dept135)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A CH3			14.60	100		
B CH3			14.60	92		
B3 OMe			56.41	89		
A3 OMe			56.77	82		
A CH2			60.53	71		
B CH2			60.64	72		
A2			107.99	69		
B2			112.66	78		
A6			114.45	73		
A β			116.99	76		
B β			117.93	80		
B5			118.36	69		
B6			122.84	78		
A1			126.67	56		
B1			131.04	53		
A4			141.41	19		
A5			144.45	40		
B α			144.81	75		
A α			144.94	73		
B4			149.35	39		
A3			150.12	34		
B3			151.41	43		
B γ			167.15	53		
A γ			167.16	56		

Compound Number 3002



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β			49.06			
OMe			56.77			
OMe			56.77			
α			83.39			
2			104.31			
6			104.31			
4			129.87			
1			137.51			
3			149.04			
5			149.04			
g			176.05			

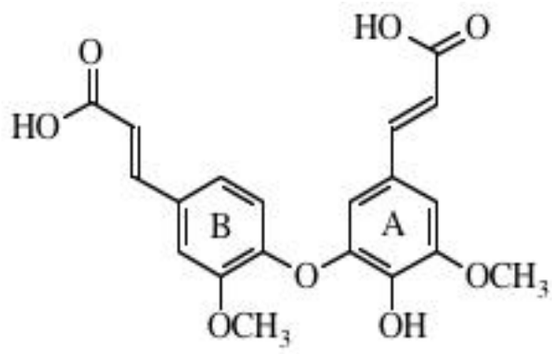
^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.83	s	
β	4.11	s	
α	5.95	s	
2,6	6.73	s	
OH	7.42	s	

Notes:

FLJ144
As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 3003



4-O-5 dehydrodiferulic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
B3 OMe	3.58	s	
A3 OMe	3.88	s	
A β	6.36	d	15.9
B β	6.47	d	15.95
B5	6.82	d	8.3
A6	6.90	d	1.9
B6	7.22	dd	8.3, 2.0
A2	7.22	d	1.9
B2	7.45	d	2.0
A α	7.54	d	15.9
B α	7.63	d	15.95
DMSO			
B3 OMe	3.85		
A3 OMe	3.86		
A β	6.35		
B β	6.47		
B5	6.59		
A6	6.85		
B6	7.12		
A2	7.20		
B2	7.43		
A α	7.42		
B α	7.51		
	7.51		

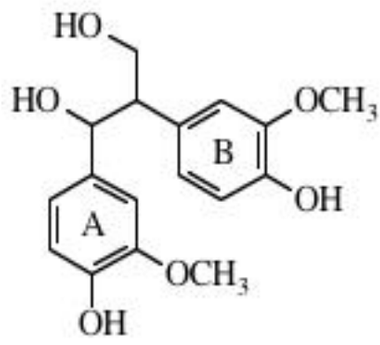
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3 OMe			56.40	94	55.85	100
A3 OMe			56.76	100	56.24	93
A2			108.03	70	107.58	32
B2			112.7	75	111.86	39
A6			114.46	79	114.05	46
A β			117.00	75	116.96	25
B β			117.95	76	118.00	21
B5			118.33	79	116.34	43
B6			122.80	79	121.91	46
A1			126.71	63	125.22	61
B1			131.06	63	129.43	54
A4			141.38	46	140.35	64
A5			144.44	54	142.94	64
A α			145.23	76	143.81	36
B α			145.38	73	143.63	29
B4			149.34	56	148.05	64
A3			150.12	56	149.28	71
B3			151.38	58	149.56	79
B γ			168.02	62	167.82	61
A γ			168.05	66	167.82	61

Notes:

Acetone: jrf117 /2 (C13) and /1 (H1) DMSO: jrf127.c7/2 Not soluble in chloroform
1H NMR (DMSO-d6) d: 3.85 (B3-OMe), 3.86 (A3-OMe),6.35 (A8), 6.47 (B8), 6.59 (B5), 6.85 (A6), 7.12 (B6), 7.20 (A2), 7.43 (B2), 7.42 (A7), 7.51 (B7)
JCS Perkin 1, 3485-98 (1994) Cmpd 17

Compound Number 3004



erythro

1,2-diguaiacylpropane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	2.93	m	
γ1	3.72	m	
γ2	3.87	m	
α	5.02	bd	
B6	6.60	bd	
B5	6.66	dd	
A5	6.68	d	8.1
A6	6.68	m	
A2	6.71	m	
B2	6.74	d	1.9

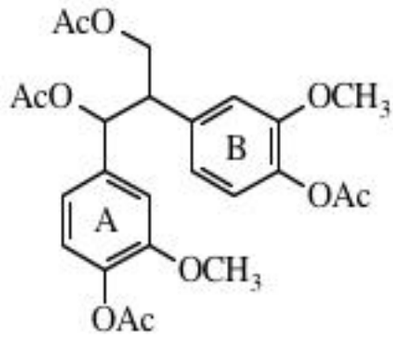
Notes:

jrlz 15
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			55.85	100		
OMe			55.95	100		
β			56.31	45		
γ			64.21	38		
α			74.66	57		
A2			111.01	99		
B2			114.00	99		
A5			114.81	35		
B5			115.00	36		
A6			119.95	95		
B6			123.05	95		
B1			132.24	64		
A1			136.67	38		
B4			145.96	16		
A4			146.17	16		
B3			147.56	18		
A3			147.63	16		

Compound Number 3005



threo

Acetic acid3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.93	s	
α Ac Me	2.09	s	
Ac Me	2.18	s	
Ac Me	2.19	s	
β	3.56	m	
OMe	3.67	s	
OMe	3.71	s	
γ1	4.38	dd	11.2, 5.2
γ2	4.54	dd	11.2, 7.2
α	6.02	d	8.2
B6	6.77	ddd	8.1, 2.0, 0.3
A2	6.79	bd	1.9
A6	6.82	ddd	8.1, 1.9, 0.5
B2	6.85	bd	1.9
B5	6.90	d	8.1
A5	6.91	d	8.1

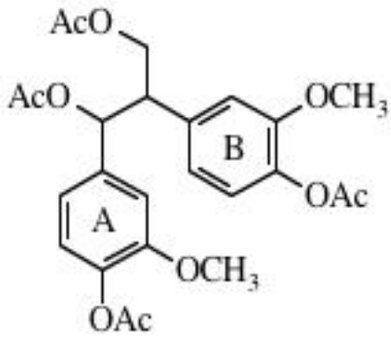
Notes:

jrlz9.1
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.41	96		
Ac Me			20.44	93		
Ac Me			20.72	81		
Ac Me			21.01	92		
β			50.71	78		
OMe			56.18	91		
OMe			56.21	100		
γ			64.71	68		
α			76.50	75		
A2			112.51	80		
B2			114.33	76		
A6			119.77	80		
B6			121.85	84		
A5			123.14	82		
B5			123.22	84		
B1			137.82	60		
A1			138.39	54		
B4			139.96	36		
A4			140.35	38		
B3			151.76	41		
A3			151.85	45		
Ac C=O			168.84	45		
Ac C=O			168.88	40		
α Ac C=O			170.01	47		
γ Ac C=O			170.81	43		

Compound Number 3006



erythro

Acetic acid3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.92	s	
α Ac Me	1.97	s	
Ac Me	2.20	s	
Ac Me	2.21	s	
β	3.50	m	6.7
OMe	3.69	s	
OMe	3.73	s	
γ1	4.20	dd	11.2, 6.7
γ2	4.37	dd	11.2, 6.8
α	6.16	d	6.6
B6	6.84	ddd	8.1, 1.9, 0.3
A2	6.84	bd	1.8
A6	6.87	ddd	8.1, 1.8, 0.5
B2	6.92	bd	1.9
B5	6.96	d	8.1
A5	6.98	d	8.1

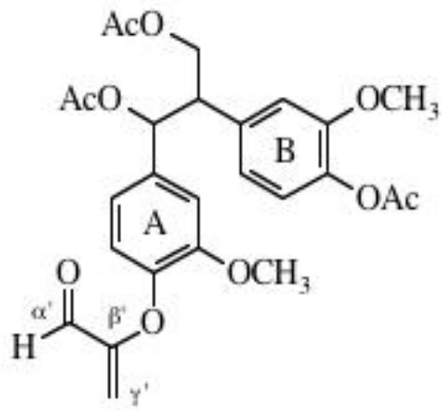
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.43	98		
Ac Me			20.46	100		
Ac Me			20.65	83		
Ac Me			20.83	85		
β			50.98	76		
OMe			56.20	97		
OMe			56.22	92		
γ			64.86	65		
α			75.56	75		
A2			112.09	74		
B2			114.52	75		
A6			119.73	76		
B6			121.93	75		
B5			123.13	78		
A5			123.30	84		
B1			137.43	50		
A1			138.72	50		
B4			140.05	40		
A4			140.51	39		
B3			151.80	46		
A3			152.00	49		
Ac C=O			168.89	41		
Ac C=O			168.95	38		
α Ac C=O			169.94	46		
γ Ac C=O			170.74	46		

Notes:

jrlz11.1
Liming Zhang, isolate from mild acidolysis
1H data at 600 MHz

Compound Number 3007



erythro

Acetic acid 3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.94	s	
α Ac Me	2.00	s	
Ar Ac Me	2.07	s	
β	3.50	m	
OMe	3.69	s	
OMe	3.76	s	
γ1	4.22	dd	11.2, 6.8
γ2	4.38	dd	11.2, 6.8
γ1'	5.00	d	2.8
γ2'	5.38	d	2.8
α	6.19	d	6.4
B6	6.81	dd	8.1, 1.6
A2	6.88	bd	
A6	6.89	dd	7.3, 1.5
B5	6.94	d	8.1
A5	6.97		
A2	6.99		
a'	9.45		

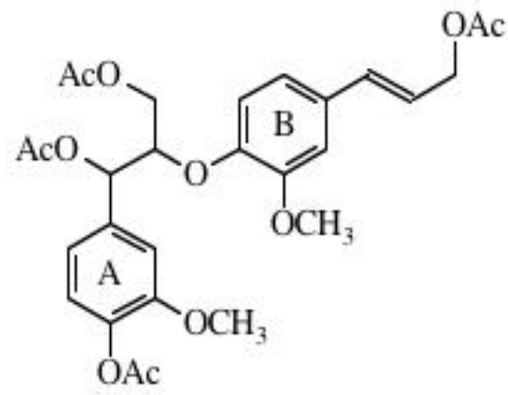
Notes:

jrlz 13
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.60	114	20.43	58		
Ac Me	20.79	80	20.66	51		
Ac Me	20.96	67	20.83	54		
β	50.13	61	51.07	41		
OMe	55.85	120	56.12	66		
OMe	55.85	120	56.22	66		
γ	63.96	49	64.82	42		
α	74.76	68	75.38	40		
γ'	107.76	51	108.01	34		
A2	111.65	73	122.68	40		
B2	113.15	58	114.44	41		
A6	119.35	65	120.17	43		
B6	121.12	65	122.12	48		
A5	121.61	68	122.14	31		
B5	122.45	79	123.16	52		
B1	135.71	51	137.41	27		
A1	136.32	58	138.17	29		
B4	139.10	43	140.07	19		
A4	142.55	43	143.24	18		
B3	150.75	68	151.76	25		
A3	150.75	68	151.81	27		
β'	157.84	60	159.33	25		
B4 Ac C=O	168.79	29	168.91	21		
α Ac C=O	169.70	52	169.94	23		
γAc C=O	170.69	65	170.71	24		
α'	186.74	93	187.55	45		

Compound Number 3008



threo

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-[4-(3-acetoxypropenyl)-2-methoxyyphenoxy]propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.95	s	
B γ Ac Me	2.01	s	
α Ac Me	2.02	s	
A4 Ac Me	2.21	s	
OMe	3.82	s	
OMe	3.85	s	
γ1	4.02	dd	11.9, 5.7
γ2	4.25	dd	11.9, 4.1
B γ	4.66	dd	6.4, 1.3
β	4.81	m	
α	6.10	d	6.4
B β	6.26	dt	15.9, 6.4
B α	6.63	bdt	15.9
B6	6.95	dd	8.3, 2.0
B5	7.00	d	8.3
A5	7.03	d	8.2
A6	7.09	dd	8.2, 1.7
B2	7.14	d	1.9
A2	7.22	d	1.6

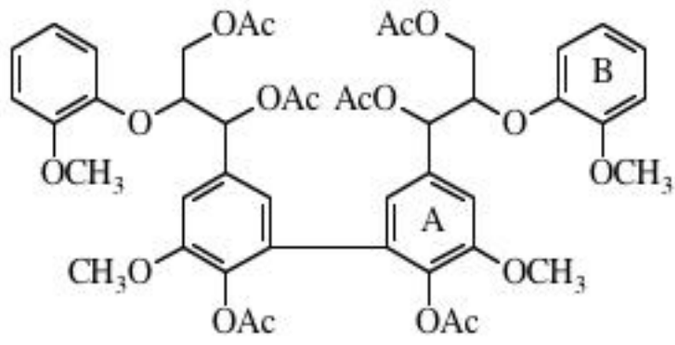
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.41	56		
Ac Me			20.55	58		
Ac Me			20.75	45		
Ac Me			20.89	50		
OMe			56.23	56		
OMe			56.27	56		
γ			63.54	44		
B γ			65.33	57		
α			75.29	56		
β			80.62	57		
B2			111.30	58		
A2			112.63	47		
B5			118.73	57		
A6			120.28	44		
B6			120.52	44		
B β			123.25	57		
A5			123.54	51		
B1			132.34	32		
B α			134.14	54		
A1			136359	31		
A4			140.90	22		
B4			149.08	26		
B3			151.74	23		
A3			152.21	22		
A4 Ac C=O			168.85	26		
α Ac C=O			169.95	30		
γ Ac C=O			170.64	23		
B γ Ac C=O			170.64	23		

Notes:

jrlz 35
Liming Zhang, isolate from mild acidolysis

Compound Number 3009



threo

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.77	s	
OMe	3.85	s	
γ1	4.09	m	
γ2	4.29	m	
β	4.78	m	
α	6.08	d	
A6,B6	6.80-6.90	m	
B1	6.96	m	
B2	6.99	m	
B5	7.02	m	
A2	7.26	m	

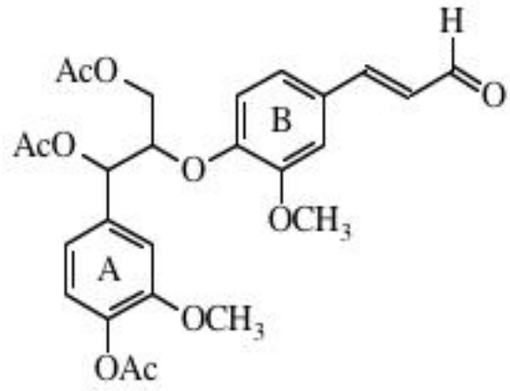
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.26	69		
Ac Me			20.61	112		
Ac Me			20.93	77		
OMe			56.17	86		
OMe			56.52	78		
γ			63.51	56		
α			75.31	34		
β			80.70	52		
A2			111.90	41		
B2			113.72	65		
B5			119.41	42		
A6			121.64	101		
B6			121.68	101		
B1			123.87	55		
A5			131.91	25		
A1			135.93	45		
A4			138.48	18		
B4			148.99	46		
B3			151.87	35		
A3			152.58	32		
4 Ac C=O			168.88	11		
α Ac C=O			170.09	39		
γ Ac C=O			170.71	36		
erythro isomer						
γ			62.95			
α			74.59			
β			80344			
B5			120.09			
B1			124.19			
A5			131.70			
A4			138.36			
B4			148.19			
B3			152.11			

Notes:

J.Ralph jrf79.5
As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 3010



threo

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-[2-methoxy-4-(3-oxopropenyl)phenoxy]propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.08	s	
Ac Me	2.21	s	
OMe	3.82	s	
OMe	3.91	s	
γ 1	4.07	dd	12.0, 5.8
γ 2	4.28	dd	12.0, 4.1
β	4.96	m	
α	6.11	d	6.4
Bβ	6.70	dd	15.9, 7.7
A5	7.03	d	8.1
A6	7.08	dd	8.5, 1.4
B5	7.15	d	8.4
A2	7.24	bd	
B6	7.25	dd	8.8, 1.7
B2	7.40	d	1.8
B α	7.59	d	16.0
B γ	9.66	d	7.6

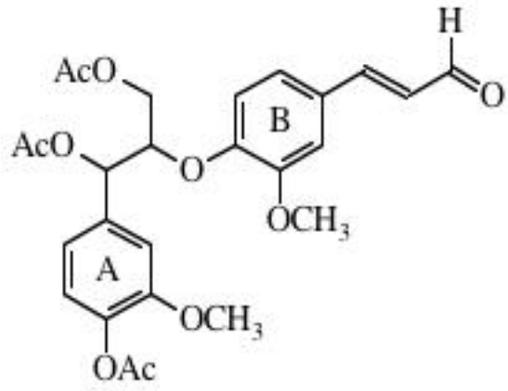
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
g Ac Me	20.60	80	20.43	39		
a Ac Me	20.68	45	20.57	24		
A4 Ac Me	20.94	60	20.88	20		
OMe	55.90	71	56.30	39		
OMe	55.98	85	56.41	25		
γ	62.81	25	63.45	25		
α	74.14	28	75.19	25		
β	79.67	30	80.26	24		
B2	111.28	31	112.56	27		
A2	111.58	35	112.66	31		
B5	117.36	31	117.85	32		
A6	119.48	38	120.34	28		
A5	122.71	32	123.61	24		
B6	122.89	32	123.76	31		
B β	127.40	34	128.23	27		
B1	128.88	22	129.89	14		
A1	134.87	24	136.40	18		
A4	140.01	19	140.99	15		
B4	150.72	24	151.73	22		
B3	150.68	24	151.73	22		
A3	151.16	23	152.26	16		
B α	152.26	45	153.29	26		
A4 Ac C=O	168.72	23	168.87	17		
α Ac C=O	169.41	24	169.85	15		
γ Ac C=O	170.48	24	170.66	15		
B γ	193.43	58	193.61	32		

Notes:

jrlz 29 1mg
Liming Zhang, isolate from mild acidolysis
see 3011 some shifts taken from isomer mix

Compound Number 3011



erythro

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-[2-methoxy-4-(3-oxopropenyl)phenoxy]propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me			
Ac Me			
Ac Me			
OMe	3.82	s	
OMe	3.90	s	
γ 1	4.27	m	
γ 2	4.37	m	
β	4.99	m	
α	6.07	d	5.2
B β	6.79	dd	15.9, 7.7
A5	7.02	d	8.1
A6	7.07	m	
B5	7.11	d	8.3
A2	7.23	m	
B6	7.27	d	1.8
B2	7.38	d	2.0
B α	7.58	d	15.9
B γ	9.65	d	7.7

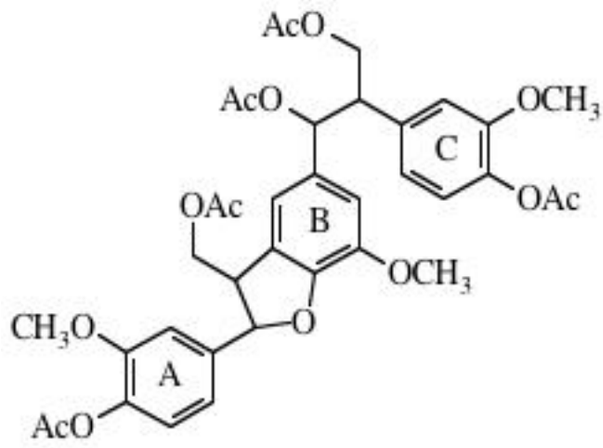
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ Ac Me	20.60	80	20.65	73		
α Ac Me	20.68	45	20.79	45		
A4 Ac Me	20.94	60	21.10	38		
OMe	55.87	71	56.51	53		
OMe	55.90	85	56.65	39		
γ	62.44	25	63.19	30		
α	73.55	28	74.57	27		
β	79.56	27	80.02	31		
B2	111.38	32	112.85	32		
A2	112.00	28	113.08	33		
B5	117.93	29	118.49	32		
A6	119.76	29	120.75	33		
A5	122.61	29	123.50	37		
B6	122.81	29	123.91	36		
B β	127.47	34	128.53	33		
B1	129.10	22	130.22	19		
A1	134.80	22	136.48	21		
A4	139.90	17	141.11	15		
B4	150.02	18	151.22	16		
B3	150.95	22	152.12	20		
A3	151.00	22	152.35	16		
B α	152.26	45	153.45	32		
A4 Ac C=O	168.74	23	169.09	23		
α Ac C=O	169.57	22	170.07	20		
γ Ac C=O	170.65	22	170.88	20		
B γ	193.43	58	194.10	66		

Notes:

jrlz41
Liming Zhang, isolate from mild acidolysis
CS's taken from isomer mix spectrum

Compound Number 3012



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β *t*			50.64			
B β *t*			50.67			
B β *e*			50.90			
B β *e*			50.95			
A β			50.95			
A β			51.23			
A β			51.26			
B γ *t*			64.74			
B γ *e*			64.85			
B γ *e*			64.89			
A γ			65.55			
A γ			65.63			
A γ			65.85			
B α *e*			75.75			
B α *e*			75.76			
B α *t*			76.56			
B α *t*			76.62			
α			87.91			
α			88.03			
α			88.04			

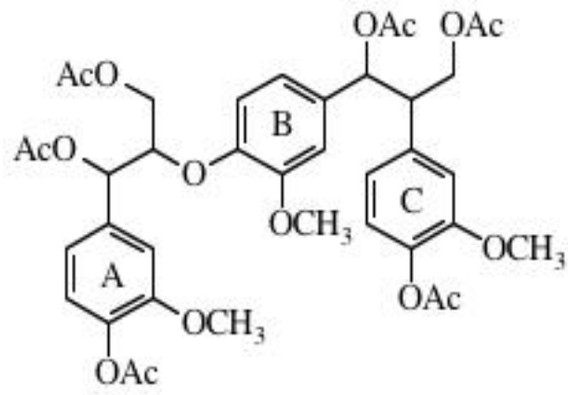
^{1}H (acetone)

Atom	H Shifts	Mult	J

Notes:

jrlz 19 15mg Liming Zhang, isolate from mild acidolysis. Due to the complexity of the model and the number of isomers present only the side chains chemical shifts have been assigned. The A side chain is a single isomer and the B chain is both erythro and threo giving 4 isomers.

Compound Number 3013



threo

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-{4-[1,3 -diacetoxy-2-(4-acetoxy-3-methoxyphenyl)propyl]-2-methoxyphenoxy}

^{1}H (acetone)

Atom	H Shifts	Mult	J

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B β *t*			50.37			
B β *t*			50.46			
B β *e*			50.71			
B β *e*			50.75			
γ			63.37			
B γ *t*			64.74			
B γ *t*			64.75			
B γ *e*			64.84			
B γ *e*			64.86			
α			75.13			
α			75.35			
α			75.19			
B α *e*			75.47			
B α *e*			75.53			
B α *t*			76.30			
B α *t*			76.35			
β			80.34			
β			80.36			
β			80.42			

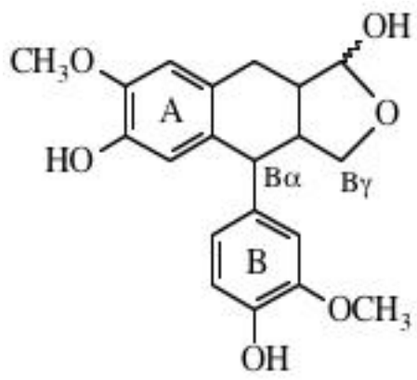
Notes:

jrlz 7 and jrlz 17 Liming Zhang - isolate from mild acidolysis.

threo β-O-4/threo+erythro β-1

Due to the complexity of the model and the number of isomers present only the side chains chemical shifts have been assigned.

Compound Number 3014



4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-1,3,3a,4,9,9a-hexahydronaphtho[2,3-c]furan-1,6-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A β	1.98	m	
B β	2.54	m	
A α1	2.84	m	
A α2	3.00	m	
B γ1	3.47	dd	10.0, 8.0
B α	3.64	d	12.2
B γ2	3.77	m	
OMe	3.77	s	
OMe	3.80	s	
A γ OH	4.99	d	4.3
A γ	5.40	d	4.3
A5	6.22	d	0.9
B6	6.63	dd	8.0, 2.0
A2	6.72	s	
B2	6.74	d	2.0
B5	6.77	d	8.0
A4 OH	7.17	s	
B4 OH	7.39	s	

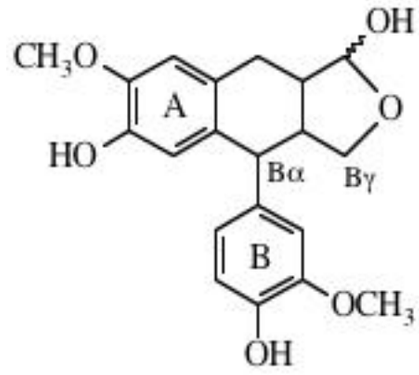
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α			29.84	55		
B β			46.24	56		
β			47.00	30		
B α			51.09	62		
OMe			55.96	79		
OMe			56.05	86		
B γ			72.06	57		
γ			98.75	34		
B2			112.38	29		
A2			112.84	57		
B5			115.51	32		
A5			116.17	35		
B6			121.75	42		
A1			128.34	44		
A6			133.42	39		
B1			137.28	38		
A4			145.11	19		
B4			145.93	17		
A3			146.61	21		
B3			148.24	20		

Notes:

jrlz5, mixture of 2 isomers in ca. 2:1 ratio.
Data for major isomer
Liming Zhang, isolate from mild acidolysis

Compound Number 3015



4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-1,3,3a,4,9,9a-hexahydronaphtho[2,3-c]furan-1,6-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A β	1.98	m	
B β	2.28	m	
A α1	2.80	m	
A α2	3.00	m	
B γ 1,2	3.64	m	
B α	3.72	bd	11.4
OMe	3.77	s	
OMe	3.80	s	
A γ	5.18	d	6.2
A γOH	5.28	d	
A5	6.55	d	
B6	6.62	dd	10.1, 2.0
A2	6.72	s	
B2	6.74	d	2.0
B5	6.77	d	8.0
A4 OH	7.17	s	
B4 OH	7.39	s	

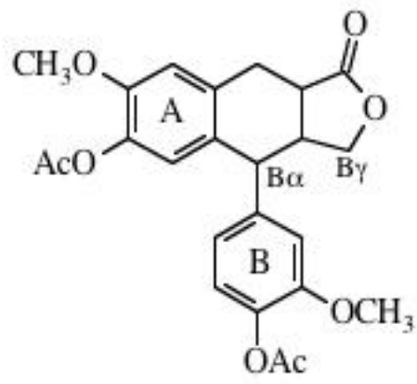
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α			31.98	22		
Bβ			49.88	48		
β			49.88	48		
B α			50.12	18		
OMe			55.96	79		
OMe			56.05	86		
Bγ			70.96	23		
γ			104.08	14		
B2			112.28	29		
A2			112.79	27		
B5			115.51	32		
A5			116.28	14		
B6			121.75	42		
A1			127.93	18		
A6			133.38	17		
B1			136.75	14		
A4			145.31	9		
B4			145.95	11		
A3			146.63	11		
B3			148.20	9		

Notes:

jrlz5, mixture of 2 isomers in ca. 2:1 ratio.
Data for minor isomer
Liming Zhang, isolate from mild acidolysis

Compound Number 3016



Acetic acid 4-(4-acetoxy-3-methoxyphenyl)-7-methoxy-1-oxo-1,3,3a,4,9,9a-hexahydroanphtho[2,3-c]furan-6-yl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.13	s	
Ac Me	2.23	s	
B β	2.75	m	
A β	2.78	m	
A α1	2.98	m	
A α2	3.18	dd	16.0, 5.0
OMe	3.75	s	
OMe	3.81	s	
B α	4.16	m	
B γ	4.16	m	
A5	6.44	s	
B6	6.83	dd	8.1, 1.9
B2	6.96	d	1.9
A2	6.98	s	
B5	7.03	d	8.1

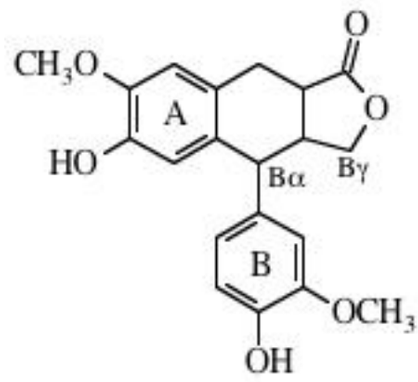
Notes:

jrlz25
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.53	82	20.36	48		
Ac Me	20.63	86	20.48	50		
α	29.57	49	30.12	23		
β	41.66	83	41.87	48		
B β	47.44	74	47.65	47		
Bα	49.93	71	50.09	45		
OMe	55.87	92	56.20	84		
OMe	55.93	103	56.20	84		
B γ	71.60	63	71.85	44		
B2	111.77	22	113.40	17		
A2	112.98	80	114.00	42		
B6	120.61	36	121.45	19		
B5	123.20	50	123.86	45		
A5	123.70	78	124.12	50		
A6	130.39	57	132.09	27		
A1	133.59	48	134.97	27		
A4	138.36	45	139.27	23		
B4	139.08	30	140.00	21		
B1	140.74	56	142.52	35		
A3	149.92	54	150.80	25		
B3	151.59	34	152.59	19		
Ac C=O	168.90	53	168.75	21		
Ac C=O	169.03	36	168.75	21		
γ	176.43	60	176.77	26		

Compound Number 3017



6-Hydroxy-4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-3a,4,9,9a-tetrahydro-3H-naphtho[2,3-c]furan-1-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
B β	2.67	m	
A β	2.67	m	
A α	3.07	dd	16.2, 4.5
OMe	3.78	s	
OMe	3.82	s	
B α	3.95	bd	9.5
B γ	4.10	m	
A5	6.26	d	0.9
B6	6.69	dd	8.0, 2.0
A2	6.79	s	
B2	6.80	d	2.0
B5	6.80	d	8.0

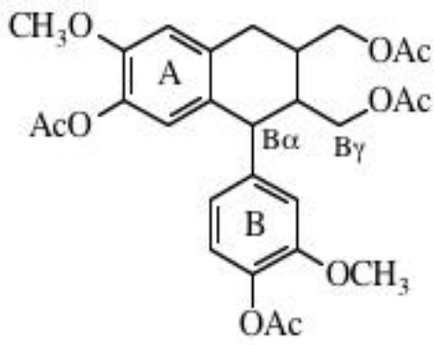
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
α			29.73	66		
β			41.98	80		
B β			47.61	75		
B α			49.95	70		
OMe			55.99	80		
OMe			56.03	85		
B γ			71.78	66		
B2			112.25	18		
A2			112.93	67		
B5			115.61	23		
A5			116.23	26		
B6			121.92	30		
A1			126.77	51		
A6			132.87	42		
B1			135.09	45		
A4			145.61	14		
B4			146.29	12		
A3			146.89	19		
B3			148.42	17		
γ			177.15	42		

Notes:

jrlz33
Liming Zhang, isolate from mild acidolysis

Compound Number 3018



Acetic acid 8-(4-acetoxy-3-methoxyphenyl)-6,7-bis-acetoxy methyl-3-methoxy-5,6,7,8-tetrahydronaphthalen-2-yl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.02	s	
Ac Me	2.11	s	
Ac Me	2.22	s	
Bβ	2.16	m	
β	2.29	m	
α	2.92	m	
OMe	3.74	s	
OMe	3.78	s	
B γ1	3.92	dd	11.7, 3.6
B α	4.02	d	10.5
B γ2	4.09	m	
A γ1	4.11	m	
A γ2	4.23	dd	11.1, 5.3
A5	6.34	bs	
B6	6.74	dd	8.1, 2.0
A2	6.87	s	
B2	6.92	d	2.0
B5	6.99	d	8.1

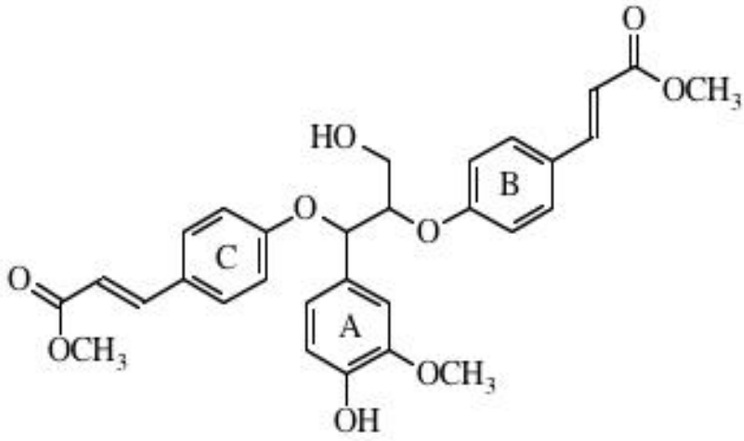
Notes:

jrlz27
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.56	67	20.36	54		
Ac Me	20.65	67	20.47	51		
Ac Me	20.77	67	20.69	51		
Ac Me	20.82	93	20.72	51		
α	33.02	45	33.53	33		
β	35.13	58	36.29	44		
B β	43.44	56	44.25	43		
B α	47.22	50	47.98	39		
OMe	55.83	65	56.17	45		
OMe	55.91	77	56.19	45		
B γ	63.04	48	63.57	37		
γ	66.20	46	66.74	40		
A2	111.81	65	112.90	50		
B2	113.17	42	114.53	46		
B6	121.52	55	121.11	57		
B5	122.81	53	123.64	44		
A5	123.71	53	124.16	40		
A6	131.13	46	132.26	26		
A1	134.05	38	135.25	31		
A4	138.03	34	139.17	19		
B4	138.03	34	139.63	26		
B1	142.77	46	144.24	23		
A3	149.35	43	150.46	20		
B3	151.16	41	152.28	22		
Ac C=O	168.91	26	168.93	23		
Ac C=O	169.11	25	168.96	23		
Ac C=O	170.80	41	171.06	31		
Ac C=O	170.97	49	171.06	31		

Compound Number 3019



erythro

3-(4-{3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2[4-(2-methoxy carbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.70	s	
C γ OMe	3.71	s	
A3 OMe	3.78	s	
γ 's	3.95	m	5.8
γ OH	4.16	t	5.8
β	4.88	m	
α	5.60	d	5.5
C β	6.34	d	16.0
B β	6.37	d	16.0
A5	6.79	d	8.1
A6	7.00	m	
C2,6	6.97	m	8.8
B2,6	7.02	m	8.8
A2	7.12	d	1.9
C3,5	7.50	m	8.6
B3,5	7.54	m	8.6
C α	7.55	d	16.0
B α	7.59	d	16.0

Notes:

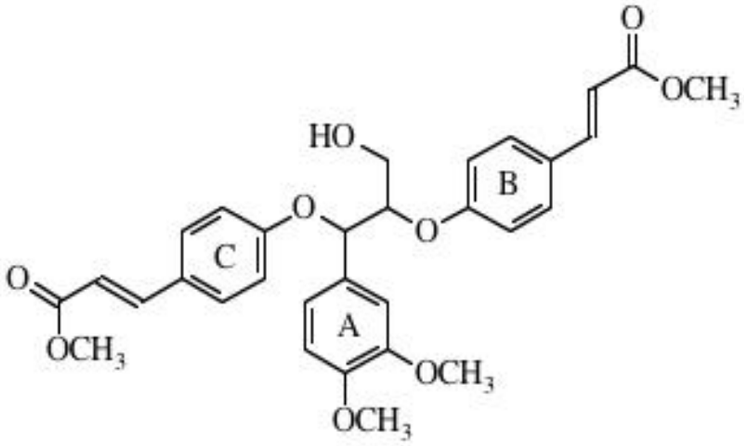
jrf101.C9-12

Authenticated assignments in acetone.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
C γ OMe	51.55	54	51.52	51	51.27	59
B γ OMe	51.59	50	51.53	51	55.63	66
A3 OMe	55.92	65	56.26	58	55.80	22
γ	61.43	27	61.42	24	59.79	15
α	78.70	35	79.32	34	77.75	18
β	81.89	35	82.67	32	81.24	18
A2	109.26	33	112.00	35	111.78	17
A5	114.48	35	115.55	24	115.29	27
B β	115.68	41	116.15	45	115.13	37
C β	115.86	45	116.25	42	115.13	37
C2	116.24	87	117.23	86	116.20	50
C6	116.24	87	117.23	86	116.20	50
B2	116.54	93	117.34	92	116.24	64
B6	116.54	93	117.34	92	116.24	64
A6	120.21	33	121.43	34	120.28	19
C1	127.73	38	128.19	42	126.74	44
B1	128.00	38	128.22	43	126.86	43
A1	128.67	45	129.37	38	127.73	40
B3	129.57	84	130.46	86	129.93	100
B5	129.57	84	130.46	86	129.93	100
C3	129.61	100	130.48	100	129.93	100
C5	129.61	100	130.48	100	129.93	100
C α	144.12	43	144.87	39	144.16	24
B α	144.23	38	144.94	43	144.26	29
A4	145.72	49	147.35	22	146.29	41
A3	146.78	45	148.23	25	147.31	52
C4	159.14	41	160.49	45	159.17	43
B4	159.81	42	161.67	44	160.5	53
C γ	167.62	44	167.67	40	166.86	55
B γ	167.63	48	167.72	39	166.92	56

Compound Number 3020



erythro

3-(4-{1-(3,4-dimethoxyphenyl)-3-hydroxy-2[4-(2-methoxy-carbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.693	s	
C γ OMe	3.711	s	
A4 OMe	3.732	s	
A3 OMe	3.752	s	
γ 's	3.954	m	5.9, *
γ OH	4.157	t	5.9
β	4.881	m	5.5, 4.9
α	5.603	d	5.5
C β	6.335	d	16.0
B β	6.363	d	16.0
A5	6.876	d	8.2
C2,6	6.973	m	8.8
B2,6	7.015	m	8.7
A6	7.047	dd	8.2, 1.9
A2	7.126	d	1.9
C3,5	7.515	m	8.8
B3,5	7.550	m	8.7
C α	7.543	d	16.0
B α	7.582	d	16.0

Notes:

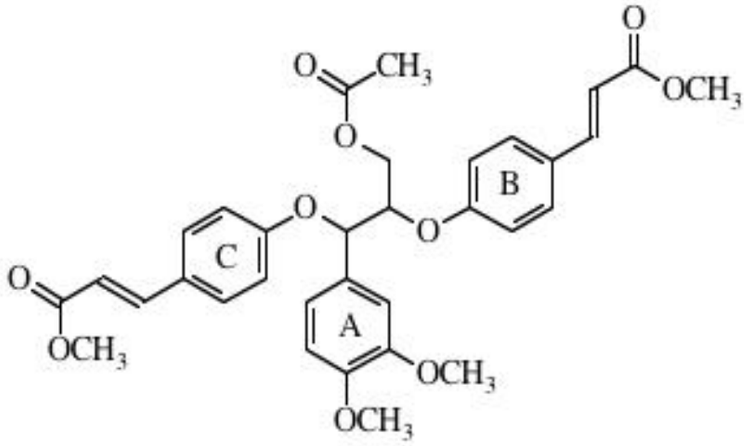
jrf119.C2

assignments not authenticated - from #3019

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
C γ OMe			51.52	38		
B γ OMe			51.52	38		
A4 OMe			55.97	40		
A3 OMe			56.12	40		
γ			61.38	20		
α			79.21	34		
β			82.64	34		
A2			112.38	32		
A5			112.47	28		
B β			116.21	40		
C β			116.33	34		
C2			117.26	86		
C6			117.26	86		
B2			117.38	98		
B6			117.38	98		
A6			121.02	38		
C1			128.26	30		
B1			128.32	32		
B3			130.51	100		
B5			130.51	100		
C3			130.52	94		
C5			130.52	94		
A1			130.56	32		
C α			144.87	38		
B α			144.96	40		
A4			150.25	32		
A3			150.26	28		
C4			160.50	30		
B4			161.69	32		
C γ			167.66	30		
B γ			167.72	28		

Compound Number 3021



erythro

3-(4-{3-carboxyoxy-1-(3,4-dimethoxyphenyl)-2-[4-(2-methoxy carbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.920	s	
B γ OMe	3.694	s	
C γ OMe	3.712	s	
A4 OMe	3.736	s	
A3 OMe	3.759	s	
γ 1	4.460	dd	11.9, 6.2
γ 2	4.507	dd	11.9, 3.8
β	5.084	m	6.2, 5.8, 3.8
α	5.629	d	5.8
C β	6.343	d	16.0
B β	6.378	d	16.0
A5	6.888	d	8.3
C2,6	6.992	m	8.7
B2,6	7.018	m	8.7
A6	7.073	dd	8.3, 2.0
A2	7.161	d	2.0
C3,5	7.527	m	8.7
B3,5	7.570	m	8.7
Cα	7.548	d	16.0
Bα	7.584	d	16.0

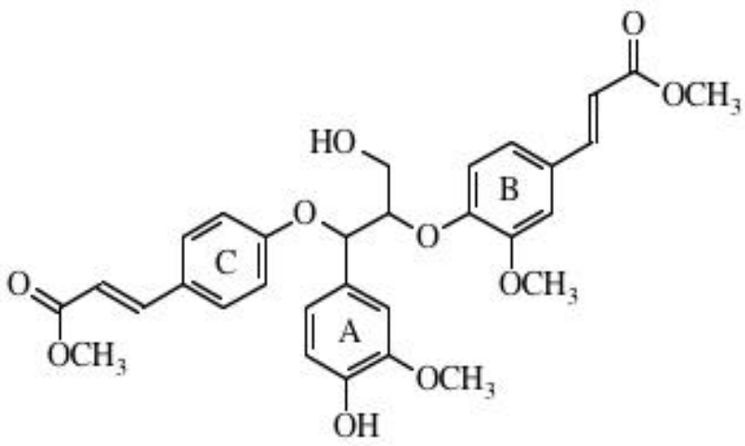
Notes:

jrf137
assignments not authenticated - from #3019/3020
A4 vs A3 OMe may be switched

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ Ac Me			20.58	53		
C γ OMe			51.54	53		
B γ OMe			51.57	47		
A4 OMe			55.97	53		
A3 OMe			56.14	55		
γ			63.49	34		
α			79.32	39		
β			79.81	39		
A2			112.17	42		
A5			112.47	42		
B β			116.49	45		
C β			116.55	47		
C2			117.27	95		
C6			117.27	95		
B2			117.41	97		
B6			117.41	97		
A6			120.88	39		
C1			128.55	24		
B1			128.74	24		
A1			130.09	34		
B3			130.53	100		
B5			130.53	100		
C3			130.61	97		
C5			130.61	97		
C α			144.81	82		
B α			144.81	82		
A4			150.38	26		
A3			150.43	24		
C4			160.24	26		
B4			161.18	26		
C γ			167.66	29		
B γ			167.69	26		
γ Ac C=O			170.79	24		

Compound Number 3022



erythro

3-(4-{3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-[2-methoxy-4-(2-methoxycarbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.696	s	
C γ OMe	3.720	s	
A3 OMe	3.804	s	
B3 OMe	3.853	s	
γ 's	3.95	m	
β	4.791	m	-
α	5.621	d	5.3
C β	6.330	d	16.0
B β	6.417	d	16.0
A5	6.798	d	8.2
C2,6	6.978	m	8.8
A6	7.013	dd	8.2, 1.9
B5	7.065	d	8.3
B6	7.123	dd	8.3, 1.9
A2	7.205	d	1.9
B2	7.283	d	1.9
C3,5	7.493	d	8.8
C α	7.554	d	16.0
B α	7.584	d	16.0

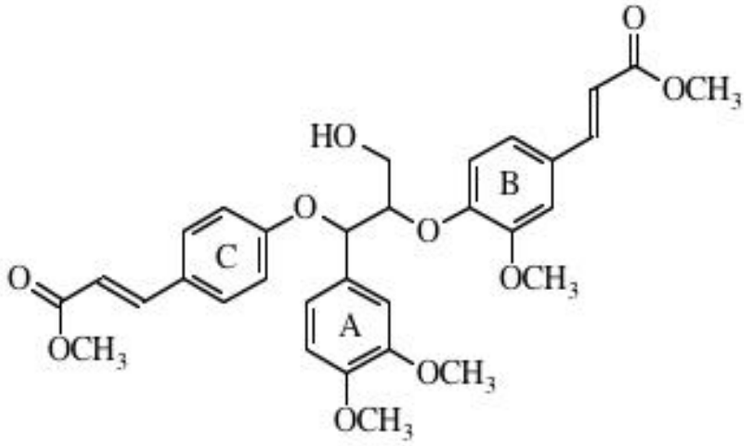
Notes:

jrf103.C12-25
fully authenticated in acetone

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ OMe	51.55	57	51.52	59	51.27	89
C γ OMe	51.66	56	51.56	56	51.28	82
A3 OMe	55.83	69	56.22	69	55.48	99
B3 OMe	55.96	69	56.32	66	55.79	100
γ	61.29	31	61.31	30	59.66	28
α	78.46	42	79.44	41	77.95	34
β	86.25	42	84.21	42	81.84	34
B2	110.87	46	112.14	49	111.43	40
A2	109.37	42	112.21	41	112.01	34
A5	114.49	44	115.38	38	114.89	36
C β	115.62	47	116.16	52	115.16	44
B β	116.77	48	116.59	51	115.24	49
C2	116.28	100	117.23	98	116.22	92
C6	116.28	100	117.23	98	116.22	92
B5	120.21	43	117.54	48	115.45	47
A6	119.50	47	121.53	41	120.44	34
B6	122.14	48	123.04	49	122.48	44
C1	127.67	39	128.13	41	126.79	62
B1	129.92	39	129.21	44	127.27	65
A1	129.32	43	129.39	46	127.54	60
C3	129.57	97	130.42	100	129.91	90
C5	129.57	97	130.42	100	129.91	90
C α	144.21	46	144.89	48	144.18	46
B α	144.28	47	145.23	48	144.61	44
A4	145.68	46	147.29	37	146.27	65
A3	146.78	42	148.17	38	147.24	74
B4	149.40	42	151.24	43	149.76	79
B3	151.14	46	151.54	46	150.11	69
C4	159.30	43	160.57	43	159.25	63
C γ	167.39	45	167.68	44	166.86	76
B γ	167.64	44	167.71	46	166.95	71

Compound Number 3023



erythro

3-(4-{1-(3,4-dimethoxyphenyl)-3-hydroxy-2-[2-methoxy-4-(2-methoxycarbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.693	s	
C γ OMe	3.715	s	
A3 OMe	3.741	s	
A4 OMe	3.773	s	
B3 OMe	3.865	s	
γ *	*	*	-
β	4.787	m	-
α	5.640	d	5.3
C β	6.337	d	16.0
B β	6.416	d	16.0
A5	6.871	d	8.3
C2,6	6.981	m	8.8
A6	7.067	dd	8.3, 1.9
B5	7.068	d	8.3
B6	7.134	dd	8.3, 1.9
A2	7.200	d	1.9
B2	7.302	d	1.9
C3,5	7.517	d	8.8
C α	7.537	d	16.0
B α	7.573	d	16.0

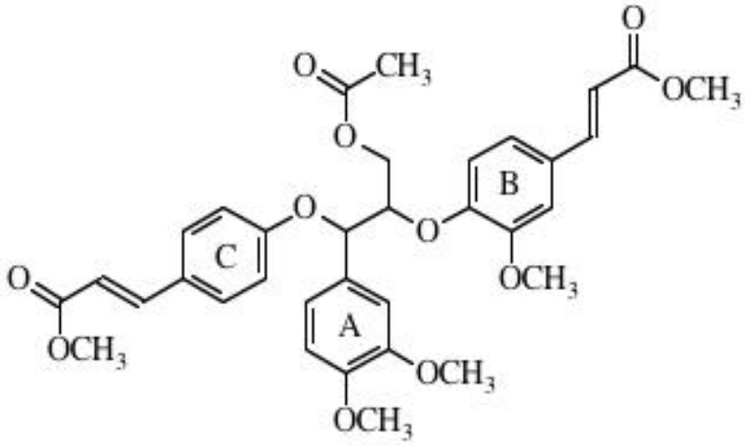
Notes:

jrf121.C5-7
assignments not authenticated - from #3022 and 3020
A4 vs A3 OMe may be switched
*γ and γ-OH protons buried, C-H correlations not run.

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ OMe			51.52	53		
C γ OMe			51.55	45		
A4 OMe			55.98	50		
A3 OMe			56.07	50		
B3 OMe			56.37	50		
γ			61.29	23		
α			79.37	37		
β			84.19	32		
B2			112.19	42		
B5			112.24	40		
A2			112.70	37		
C β			116.27	42		
B β			116.67	42		
C2			117.29	97		
C6			117.29	97		
B5			117.60	42		
A6			121.14	39		
B6			123.10	42		
C1			128.25	27		
B1			129.30	31		
C3			130.49	100		
C5			130.49	100		
A1			130.59	31		
C α			144.91	42		
B α			145.25	40		
A4			150.20	26		
A3			150.23	27		
B4			151.31	24		
B3			151.65	27		
C4			160.63	27		
C γ			167.68	27		
B γ			167.71	26		

Compound Number 3024



erythro

3-(4-{3-carboxyoxy-1-(3,4-dimethoxyphenyl)-2-[2-methoxy-4-(2-methoxycarbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.920	s	
B γ OMe	3.695	s	
C γ OMe	3.716	s	
A3 OMe	3.745	s	
A4 OMe	3.775	s	
B3 OMe	3.877	s	
γ1	4.428	dd	11.9, 3.8
γ2	4.487	dd	11.9, 6.2
β	4.988	m	6.2, 5.3, 3.8
α	5.659	d	5.3
C β	6.345	d	16.0
B β	6.431	d	16.0
A5	6.888	d	8.3
C2,6	6.995	m	8.8
B5	7.051	m	8.3
A6	7.066	dd	8.3, 2.0, 0.4
B6	7.143	dd	8.3, 2.0, 0.4
A2	7.190	d	2.0
B2	7.323	d	2.0
C3,5	7.527	m	8.8
C α	7.553	d	16.0
B α	7.576	d	16.0

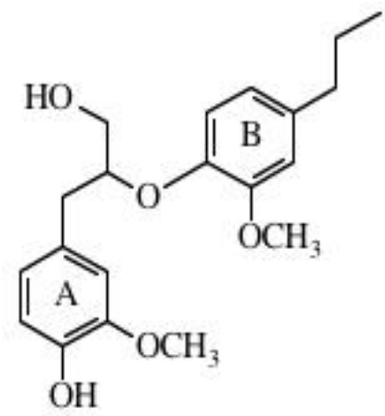
Notes:

jrf139
assignments not authenticated - from #3023 and 3021
A4 vs A3 OMe may be switched
Note γ's, J's switch from #3021!!

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
g Ac Me			20.61	46		
B γ OMe			51.54	54		
C γOMe			51.58	46		
A4 OMe			55.99	50		
A3 OMe			56.09	52		
B3 OMe			56.35	50		
γ			63.49	30		
α			79.62	37		
β			81.21	35		
A2			112.24	33		
B5			112.38	76		
B2			112.38	76		
C β			116.42	37		
B β			116.98	39		
C2			117.28	91		
C6			117.28	91		
B5			118.21	39		
A6			120.82	35		
B6			122.93	39		
C1			128.46	30		
B1			129.89	26		
A1			130.14	30		
C3			130.52	100		
C5			130.52	100		
C α			144.85	41		
B α			145.14	41		
A4			150.33	28		
A3			150.37	28		
B4			150.72	26		
B3			151.80	30		
C4			160.44	28		
C γ			167.67	35		
B γ			167.67	35		
γ OAc C=O			170.79	30		

Compound Number 3025



3-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxy-4-propylphenoxy)propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.895	t	7.3
B β	1.585	m	
B α	2.492	m	
α1	2.91	m	
α2	2.94	m	
γ	3.59	m	
γ OH	3.731	t	6.1
OMe	3.786	s	
OMe	3.802	s	
β	4.308	m	
B6	6.646	ddt	8.1, 2.1, 0.6
A5	6.72	m	
A6	6.72	m	
B2	6.816	d	2.1
B5	6.827	d	8.1
A2	6.918	m	
Ar OH	7.333	s	

Notes:

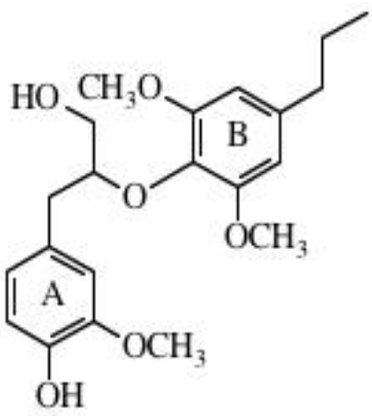
jrbha69

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ	13.77	80	14.01	79	13.75	86
B β	24.58	100	25.39	89	24.29	96
α	37.37	61	37.74	66	36.52	61
B α	37.76	66	38.22	69	36.97	89
OMe	55.76	42	56.15	33	55.49	100
OMe	55.89	42	56.20	34	55.58	86
γ	63.41	67	63.38	44	61.82	57
β	85.32	60	83.67	54	80.83	50
B2	112.16	93	113.85	87	112.89	61
A2	112.32	86	113.99	73	113.64	61
A5	114.34	98	115.49	71	115.19	64
B5	119.95	86	118.72	80	115.70	79
B6	121.00	88	121.37	100	120.21	64
A6	122.08	94	122.83	91	121.63	57
A1	129.75	62	130.58	52	129.16	82
B1	138.23	58	137.46	53	135.30	75
A4	144.20	61	145.88	39	144.79	71
B4	145.33	52	146.82	41	145.45	68
A3	146.44	54	148.05	34	147.26	71
B3	150.88	54	151.63	42	149.69	71

1H	CDCl3	DMSO
B γ	0.915	0.856
B β	1.594	1.531
B α	2.504	2.46
α1	2.866	2.733
α2	3.040	2.831
γ1	3.574	
γ2	3.656	
γ OH		4.761
OMe	3.823	3.680
OMe	3.841	3.703
β	4.160	4.265
Ar-OH	5.611	8.70

Compound Number 3026



2-(2,6-dimethoxy-4-propylphenoxy)-3-(4-hydroxy-3-methoxyphenyl)propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.917	t	7.3
B β	1.619	m	
B α	2.523	dd	
α1	2.941	dd	13.6, 8.2
α2	3.077	dd	13.6, 5.4
γ1	3.392	m	12.0, 4.1
γ2	3.483	m	12.0, 3.4
γ OH	3.5	m	
A OMe	3.809	s	
B OMe	3.817	s	
β	4.128	m	
B2,6	6.540	s	
A6	6.711	dd	8.0, 1.8
A5	6.740	dd	8.0, 0.4
A2	6.892	d	1.8
Ar OH	7.349	s	

Notes:

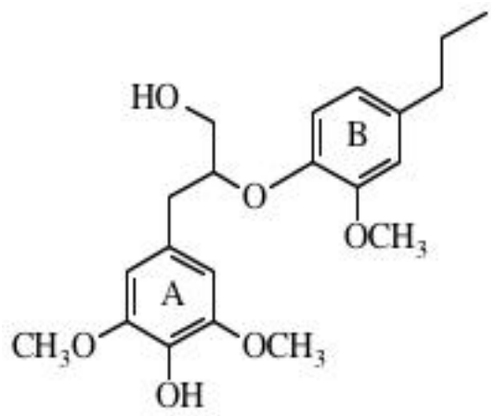
jrbha61
Hγ's are perfect dd's after adding D2O to acetone - otherwise complex multiplets; J's are from D2O exchanged spectra. All spectra ref'd to solvent, Acetone 2.04, 29.8 CDCl3 7.24, 77.0, DMSO 2.49, 39.5

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ	13.76	64	14.06	44	13.73	55
B β	24.51	86	25.30	47	24.10	57
α	37.28	48	38.00	38	36.86	27
B α	38.39	50	38.91	38	37.64	37
A OMe	55.81	35	56.17	19	55.51	50
B OMe	55.97	62	56.41	35	55.81	100
γ	62.17	45	62.77	28	61.65	29
β	84.36	48	85.24	32	83.39	28
B2	105.42	92	106.55	100	105.58	55
B6	105.42	92	106.55	100	105.58	55
A2	112.20	79	113.87	44	113.58	38
A5	114.15	68	115.50	47	115.06	36
A6	122.03	74	122.78	50	121.64	35
A1	130.19	49	130.81	35	129.36	42
B4	133.40	39	134.92	22	133.46	33
B1	138.77	55	139.25	33	137.62	41
A4	143.99	47	145.78	28	144.60	43
A3	146.31	40	148.03	24	147.11	38
B3	152.99	100	154.09	56	152.76	82
B5	152.99	100	154.09	56	152.76	82

1H	CDCl3	DMSO
B γ	0.928	0.886
B β	1.614	1.573
B α	2.513	2.753
α1	2.966	2.871
α2	3.192	~3.35?
γ1	3.418	~3.35?
γ2	3.54	~3.35?
γ OH	3.56	~3.35?
A OMe	3.805	3.697
B OMe	3.831	3.708
β	4.150	4.068
B2,6	6.392	6.465
A6	6.745	6.583
A5	6.809	6.641
A2	6.796	6.763
Ar OH	5.698	8.634

Compound Number 3027



3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxy-4-propylphenoxy)propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.894	t	7.4
B β	1.585	m	
B α	2.491	m	
α1	2.85	dd	13.9, 6.2
α2	2.922	dd	13.9, 6.1
γ	3.602	m	
γ OH	3.734	t	
A OMe	3.770	s	
B OMe	3.806	s	
β	4.335	m	
A2,6	6.596	s	
B6	6.646	ddt	8.2, 2.1, 0.6
B2	6.817	d	2.1
B5	6.833	d	8.2
Ar OH	6.940		

Notes:

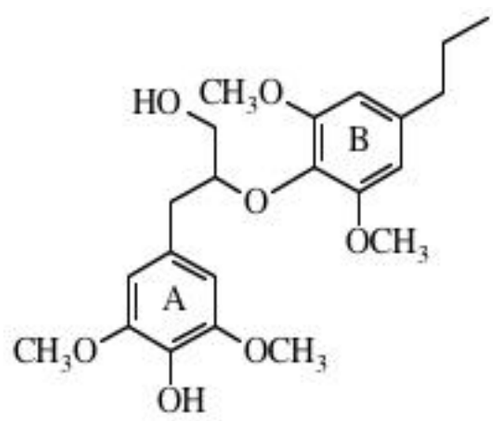
jrbha67

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ	13.77	63	14.01	45	13.67	66
B β	24.57	84	25.40	49	24.22	75
A α	37.76	53	38.21	41	36.90	59
B α	37.94	48	38.23	45	36.90	59
B OMe	55.77	31	56.19	19	55.47	62
A OMe	56.28	53	56.56	33	55.82	97
γ	63.47	53	63.46	22	61.84	28
β	85.35	48	83.47	31	80.56	38
A2	106.13	100	107.93	100	106.83	50
A6	106.13	100	107.93	100	106.83	50
B2	112.30	67	113.81	50	112.74	41
B5	120.04	70	118.54	45	115.44	47
B6	121.03	69	121.36	58	120.11	41
A1	128.98	60	129.59	27	128.24	47
A4	133.32	52	135.34	20	133.78	56
B1	138.31	52	137.38	28	135.09	44
B4	145.32	51	146.85	22	145.41	44
A3	146.97	95	148.48	35	147.64	100
A5	146.97	95	148.48	35	147.64	100
B3	150.89	52	151.57	22	149.53	47

1H	CDCl3	DMSO
B γ	0.910	0.86
B β	1.589	1.54
B α	2.499	2.45
α1	2.856	2.74
α2	3.032	2.84
γ1	3.578	
γ2	3.655	
γ OH		4.75
A OMe	3.831	3.68
B OMe	3.841	3.71
β	4.160	4.30
A2,6	6.478	6.49
B6	6.628	6.62
B2	6.697	6.76
B5	6.651	6.83
Ar OH	8.03	8.03

Compound Number 3028



3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2,5-dimethoxy-4-propylphenoxy)propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.917	t	7.4
B β	1.620	m	
B α	2.525	m	
α1	2.925	dd	13.6, 8.1
α2	3.074	dd	13.6, 5.3
γ1	3.402	m	12.0, 4.1
γ2	3.486	m	12.0, 3.6
γ OH	3.47	m	
A OMe	3.793	s	
B OMe	3.825	s	
β	4.142	m	
B2,6	6.544	s	
A2,6	6.573	s	
Ar OH	6.949	s	

Notes:

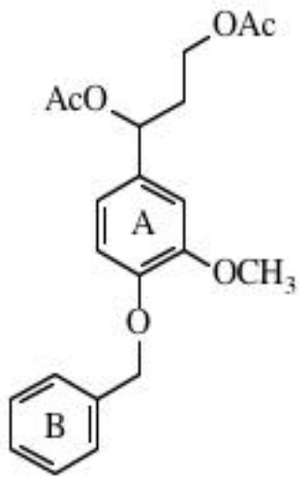
jrbha63 Hγ's are dd's after adding D2O to acetone - otherwise complex multiplets; J's are from D2O exchanged spectra. In acetone: Many peaks were split with a 2:1 ratio. Aα 38.38 & 38.50, Bα 38.80 & 38.93, A1 129.69 & 129.86, B4 134.94 & 134.97, A4 135.24 & 135.28, B1 139.10 & 139.26 , A3/5 148.44 & 148.49, B3/5 154.07 & 154.12

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B γ	13.70	37	14.06	100	13.82	49
B β	24.47	100	25.30	82	24.18	48
α	37.65	39	38.38	45	37.35	25
B α	38.24	47	38.80	45	37.60	27
A OMe	55.96	90	56.43	72	55.91	100
B OMe	56.19	86	56.58	76	55.97	96
γ	62.19	51	62.93	49	61.88	27
β	84.19	49	85.20	56	83.32	23
B2	105.42	37	106.57	59	105.67	11
B6	105.42	37	106.57	59	105.67	11
A2	106.12	35	107.83	55	106.89	10
A6	106.12	35	107.83	55	106.89	10
A1	129.21	49	129.69	38	128.54	30
B4	133.07	29	134.94	14	133.46	24
A4	133.28	28	135.24	16	133.70	28
B1	138.64	43	139.10	38	137.61	25
A3	146.75	55	148.44	45	147.65	48
A5	146.75	55	148.44	45	147.65	48
B3	152.92	79	154.07	54	152.79	52
B5	152.92	79	154.07	54	152.79	52

1H	CDCl3	DMSO
B γ	0.917	0.879
B β	1.592	1.562
B α	2.489	2.45
α1	2.950	2.756
α2	3.175	2.868
γ1	3.408	
γ2	3.542	
γ OH	3.47	4.334?
A OMe	3.798	3.692
B OMe	3.829	3.696
β	4.152	4.103
B2,6	6.386	6.449
A2,6	6.498	6.462
Ar OH	5.493	8.044

Compound Number 3029



1-(4-benzyloxy-3-methoxyphenyl)-propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.99	s	
α Ac Me	2.03	s	
β	2.18	m	
OMe	3.83	s	
γ	4.08	m	
B α	5.09	s	
α	5.85	dd	8.2, 5.7
A6	6.91	dd	8.3, 2.0
A5	6.99	d	8.3
A2	7.04	d	2.0
Bz H's	7.28-7.51	m	

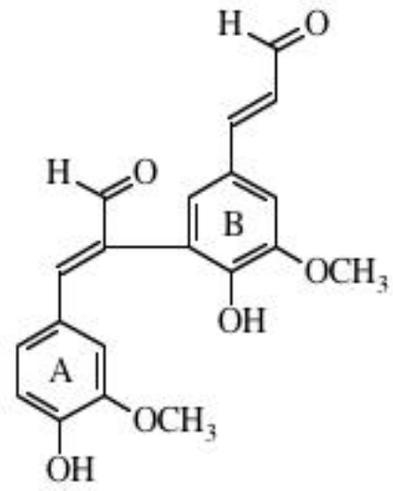
Notes:

JRHKC25

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ Ac Me			20.70			
α Ac Me			21.01			
β			35.78			
OMe			56.16			
γ			61.20			
B α			71.26			
α			73.17			
A2			111.49			
A5			114.64			
A6			119.58			
B3			128.28			
B5			128.28			
B2			129.09			
B6			129.09			
B4			128.45			
A1			134.19			
B1			138.33			
A4			149.02			
A3			150.68			
α Ac C=O			170.17			
γ Ac C=O			170.80			

Compound Number 3030



beta-[5-(2-formylvinyl)-2-hydroxy-3-methoxyphenyl] coniferyl aldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.47	s	
B3 OMe	3.96	s	
B β	6.66	dd	15.8, 7.8
A5	6.77	d	8.3
A2	6.87	d	2.0
A6	6.98	dd	8.3, 2.0
B6	7.01	d	2.0
B2	7.44	d	2.0
A α	7.57	s	
B α	7.57	d	15.8
OH	8.43	s	
B γ	9.61	d	7.8
A γ	9.69	s	

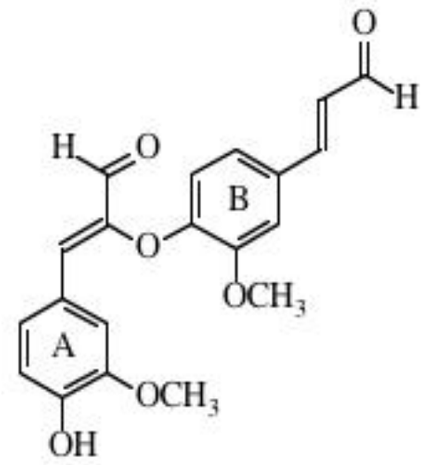
Notes:

JRHKB117 (Higuchi)
13mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe			55.55			
B3 OMe			56.63			
B2			110.61			
A2			113.56			
A5			115.95			
A β			123.15			
B6			126.36			
A6			126.92			
B β			127.29			
A1			127.38			
B1			127.44			
B5			136.33			
A3			148.13			
B4			148.59			
A3			149.30			
B4			150.16			
A α			151.36			
B α			153.79			
A γ			193.43			
B γ			193.96			

Compound Number 3031



beta-[4-(2-formylvinyl)-2-methoxyphenoxy] coniferyl aldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J

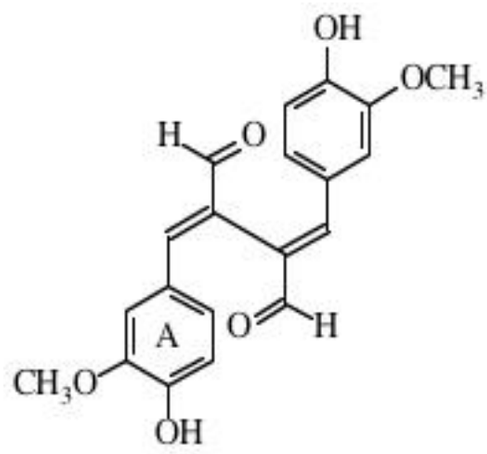
Notes:

JRHKB119 (Higuchi)
4 mg

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3 OMe			56.01			
A3 OMe			56.52			
B2			112.55			
A2			113.98			
B5			115.25			
A5			116.25			
B6			123.63			
A1			125.31			
A6			126.80			
B β			128.32			
B1			130.20			
A α			138.21			
A β			147.70			
B3			148.48			
B4			148.90			
A3			150.37			
A4			150.56			
B α			153.15			
A γ			197.48			
B γ			193.85			

Compound Number 3032



2,3-diformyl-1,4-bis(4-hydroxy-3-methoxyphenyl) buta-1,3-diene

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.70	s	
5	6.82	d	8.31
6	7.21	dd	8.31, 2.15
2	7.28	d	2.15
α	7.78	s	
OH	8.29	s	
γ	9.66	s	

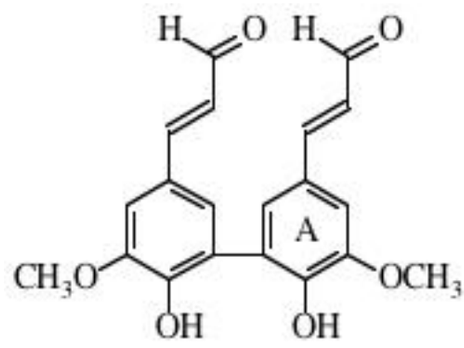
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.11			
2			113.71			
5			116.24			
6			126.25			
1			127.47			
β			134.42			
3			148.41			
4			150.51			
α			152.83			
γ			192.74			

Notes:

JRHKb121 11mg
Higuchi
As this dimer contains a plane of symmetry the CSs are reported for one unit.

Compound Number 3033



5,5'-bis-coniferyl aldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.95	s	
β	6.68	dd	15.84, 7.84
6	7.27	s	2.0
2	7.36	s	2.0
α	7.59	s	15.84
γ	9.65	s	7.84

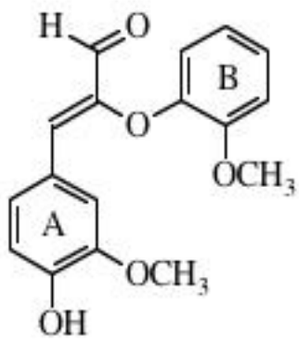
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.52			
2			110.00			
1			126.05			
5			126.13			
β			126.81			
6			127.10			
3			149.42			
4			149.63			
α			154.40			
γ			193.92			

Notes:

JRHKb123 37mg
Higuchi
As this dimer contains a plane of symmetry the CSs are reported for one unit.

Compound Number 3034



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe			55.84			
B3 OMe			56.17			
B2			113.51			
A2			113.82			
B5			114.85			
A5			116.07			
B6			121.34			
B1			123.35			
A1			125.49			
A6			126.57			
α			137.82			
B4			146.22			
β			148.09			
A3			148.30			
B3			149.89			
A4			150.20			
γ			187.90			

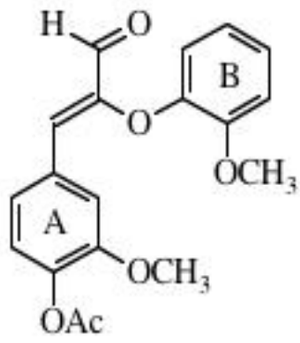
^{1}H (acetone)

Atom	H Shifts	Mult	J
A4 OMe	3.73	s	
B3 OMe	3.88	s	
B5	6.72	dd	8.0, 2.0
B6	6.76	ddd	8.2, 7.1, 2.0
A5	6.87	d	8.3
B1	6.95	ddd	8.2, 7.1, 2.0
B2	7.05	dd	8.2, 2.0
α	7.26	s	
A6	7.33	dd	8.3, 2.0
A2	7.59	d	2.0
γ	9.50	s	

Notes:

HKc63.4

Compound Number 3035



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.41			
A3 OMe			55.97			
B3 OMe			56.20			
B2			113.62			
A2			114.66			
B5			115.56			
B6			121.39			
B1			123.83			
A5			124.06			
A6			124.53			
A1			132.33			
α			135.40			
A4			142.47			
B4			146.01			
β			149.94			
B3			150.01			
A3			152.27			
Ac C=O			168.73			
γ			188.21			

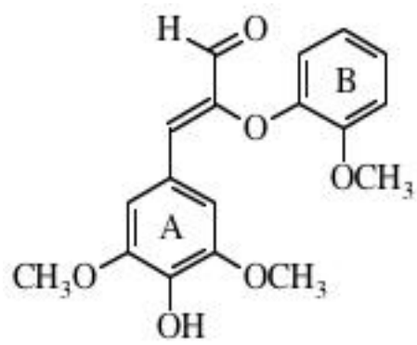
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.23	s	
A3 OMe	3.73	s	
B3 OMe	3.87	s	
B5	6.79	m	
B6	6.79	m	
B1	6.97	m	
B2	7.06	bd	7.8
A5	7.11	d	8.3
α	7.30	s	
A6	7.45	dd	8.3, 2.0
A2	7.68	d	2.0
γ	9.55	s	

Notes:

HKc 63.4Ac

Compound Number 3036



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3 OMe			56.11			
A3 OMe			56.31			
A5 OMe			56.31			
A2			109.27			
A6			109.27			
B2			113.39			
B5			114.53			
B6			121.32			
B1			123.27			
A1			124.05			
α			138.23			
A4			139.74			
B4			146.16			
β			148.15			
A3			148.57			
A5			148.57			
B3			149.76			
γ			187.91			

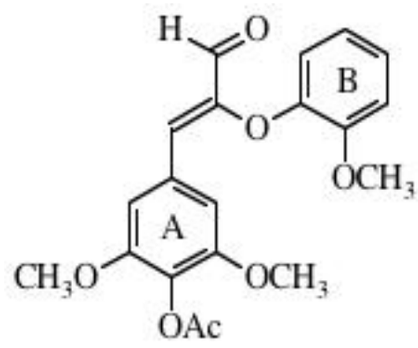
^{1}H (acetone)

Atom	H Shifts	Mult	J
A3,5 OMe	3.74	s	
B3 OMe	3.88	s	
B5	6.70	dd	8.2, 1.7
B6	6.76	ddd	8.2, 7.2, 1.5
B1	6.94	ddd	8.2, 7.2, 1.7
B2	7.05	dd	8.2, 1.5
A2,6	7.24	s	
α	7.26	s	
γ	9.51	s	

Notes:

HKd 59.1

Compound Number 3037



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.21	s	
A3,5 OMe	3.73	s	
B3 OMe	3.88	s	
B5	6.76	dd	8.2, 2.4
B6	6.77	ddd	8.2, 6.5, 1.4
B1	6.97	ddd	8.2, 6.5, 2.4
B2	7.06	dd	8.2, 1.4
A2,6	7.29	s	
α	7.31	s	
γ	9.57	s	

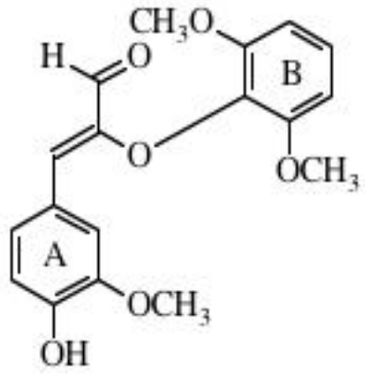
Notes:

HKd 59.1 Ac

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.17			
B3 OMe			56.14			
A3 OMe			56.29			
A5 OMe			56.29			
A2			108.10			
A6			108.10			
B2			113.48			
B5			115.07			
B6			121.37			
B1			123.68			
A1			131.35			
A4			131.53			
α			136.12			
B4			145.97			
b			149.81			
B3			149.84			
A3			153.20			
A5			153.20			
Ac C=O			168.30			
γ			188.26			

Compound Number 3038



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe			56.07			
B3 OMe			56.53			
B5 OMe			56.53			
B2			106.40			
B6			106.40			
A2			114.55			
A5			115.95			
B1			124.17			
A6			125.77			
A1			126.72			
α			129.06			
B4			135.22			
A3			148.04			
A4			149.05			
β			150.82			
B3			152.47			
B5			152.47			
γ			186.64			

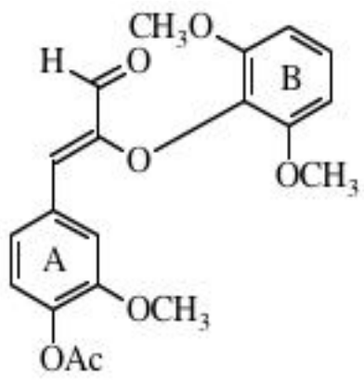
^{1}H (acetone)

Atom	H Shifts	Mult	J
B3,5 OMe	3.74	s	
A3 OMe	3.81	s	
α	6.64	s	
B2,6	6.65	d	8.2
A5	6.88	d	8.3
B1	6.99	dd	8.2, 7.6
A6	7.45	dd	8.3, 2.0
A2	7.60	d	2.0
γ	9.25	s	

Notes:

HKd 23.3

Compound Number 3039



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.45			
A3 OMe			56.09			
B3 OMe			56.52			
B5 OMe			56.52			
B2			106.29			
B6			106.29			
A2			115.15			
A5			123.78			
A6			124.04			
B1			124.53			
α			126.73			
A1			133.43			
B4			134.81			
A4			141.52			
A3			152.04			
β			152.11			
B3			152.41			
B5			152.41			
Ac C=O			168.85			
γ			187.00			

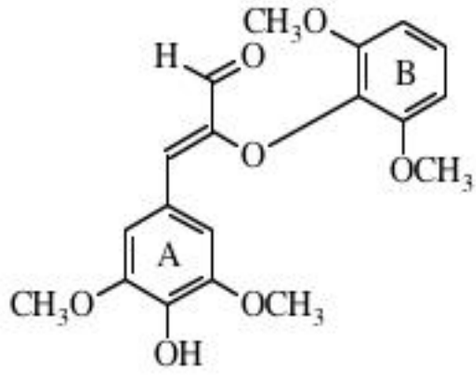
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.24	s	
B3,5 OMe	3.75	s	
A3 OMe	3.80	s	
B2,6	6.67	d	8.3
α	6.71	s	
B1	7.01	dd	8.3, 7.9
A5	7.11	d	8.2
A6	7.54	dd	8.2, 1.9
A2	7.68	d	1.9
γ	9.32	s	

Notes:

HKd 23.3 Ac

Compound Number 3040



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3 OMe			56.51			
A5 OMe			56.51			
B3 OMe			56.59			
B5 OMe			56.59			
B2			106.50			
B6			106.50			
A2			109.41			
A6			109.41			
B1			124.18			
A1			125.37			
α			129.08			
B4			135.21			
A4			138.72			
A3			148.44			
A5			148.44			
β			150.91			
B3			152.46			
B5			152.46			
γ			186.60			

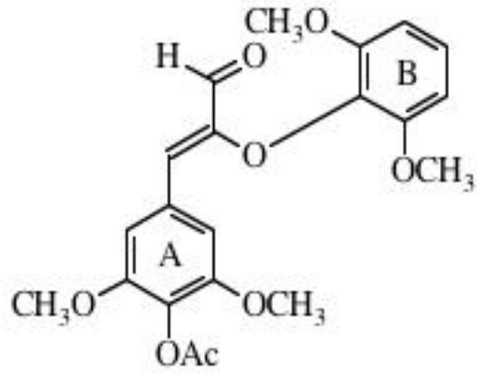
^{1}H (acetone)

Atom	H Shifts	Mult	J
B3,5 OMe	3.75	s	
A3,5 OMe	3.80	s	
α	6.63	s	
	6.66	d	8.3
B2,6	6.99	t	8.3
B1	7.31	s	
A2,6	9.25	s	
γ			

Notes:

HKd 63.1

Compound Number 3041



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.23	s	
A3,5 OMe	3.77	s	
B3,5 OMe	3.78	s	
B2,6	6.67	d	8.3
α	6.69	s	
B1	7.01	dd	8.6, 8.2
A2,6	7.34	s	
γ	9.32	s	

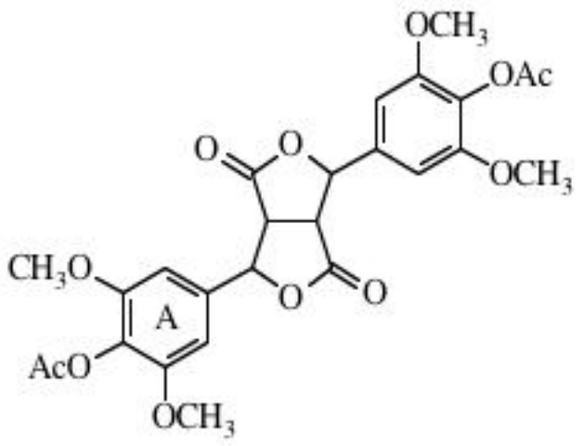
Notes:

HKd 63.1 Ac

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.22			
B3 OMe			56.35			
B5 OMe			56.35			
A3 OMe			56.56			
A5 OMe			56.56			
B2			106.37			
B6			106.37			
A2			108.07			
A6			108.07			
B1			124.51			
α			126.81			
A4			130.47			
A1			132.69			
B4			134.76			
β			152.09			
B3			152.35			
B5			152.35			
A3			153.01			
A5			153.01			
Ac C=O			168.43			
γ			186.95			

Compound Number 3042



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.18			
β			48.76			
3 OMe			55.56			
5 OMe			55.56			
α			82.61			
2			103.05			
6			103.05			
4			129.76			
1			137.84			
3			153.54			
5			153.54			
Ac C=O			168.50			
γ			175.77			

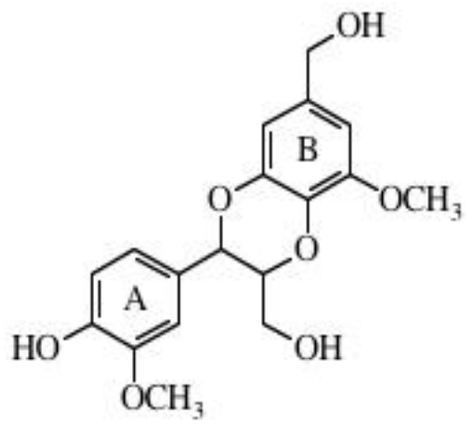
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.23	s	
OMe	3.81	s	
β	4.20	s	
α	5.86	s	
2,6	6.81	s	

Notes:

FLj 144
As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 3043



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3 OMe			56.26	98		
A3 OMe			56.32	105		
γ			61.83	53		
Bα			64.61	63		
α			76.97	93		
β			79.30	91		
B2			104.10	84		
B6			108.55	97		
A2			111.90	89		
A5			115.70	52		
A6			121.49	98		
A1			129.50	54		
B4			133.24	25		
B1			135.46	40		
B5			145.19	39		
A4			147.92	26		
A3			148.44	24		
B3			149.84	49		

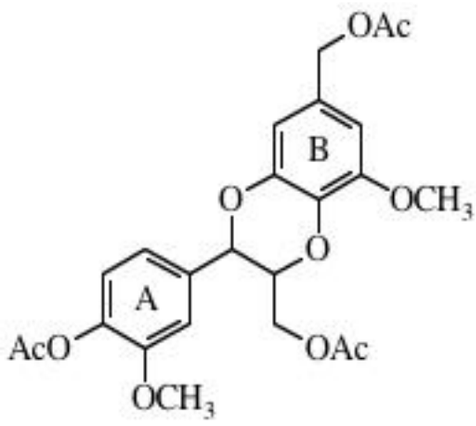
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.47	m	
γ2	3.76	m	
B3 OMe	3.81	s	
A3 OMe	3.85	s	
β	3.99	ddd	7.9, 3.9, 2.5
Bα	4.49	m	
α	4.95	d	7.9
B6	6.53	ddd	1.8, 0.75, 0.75
B2	6.60	d	1.8
A5	6.86	d	8.1
A6	6.94	ddd	8.1, 1.9, 0.5
A2	7.09	d	1.9
A4 OH	7.80	s	

Notes:

F. Lu
flm11

Compound Number 3044



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me			20.45	18		
γ Ac Me			20.49	18		
Bα Ac Me			20.81	12		
A3 OMe			56.36	18		
B3 OMe			56.44	18		
γ			63.36	14		
Bα			66.36	17		
β			75.97	16		
α			77.01	16		
B2			106.08	14		
B6			110.41	15		
A2			112.77	15		
A6			120.75	16		
A5			123.88	16		
B1			129.92	9		
B4			133.65	8		
A1			136.00	10		
A4			141.45	7		
B5			144.92	9		
B3			149.98	8		
A3			152.57	9		
A4 Ac C=O			168.86	9		
γ Ac C=O			170.62	8		
Bα Ac C=O			170.83	5		

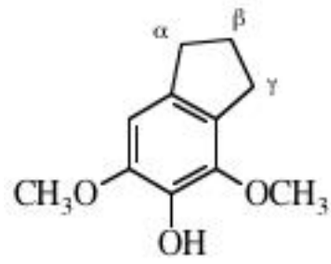
^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα Ac Me	1.99	s	
γ Ac Me	2.03	s	
A4 Ac Me	2.24	s	
B3 OMe	3.83	s	
A3 OMe	3.84	s	
γ1	4.02	dd	12.4, 4.3
γ2	4.28	dd	12.4, 3.4
β	4.40	ddd	7.7, 4.3, 3.4
Bα	4.98	s	
α	5.04	d	7.7
B6	6.61	d	1.9
B2	6.66	d	1.9
A6	7.08	dd	8.1, 1.7
A5	7.11	d	8.1
A2	7.26	d	1.7

Notes:

F. Lu
flm11Ac

Compound Number 3045



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β			26.11			
γ			30.33			
α			33.51			
5 OMe			56.73			
3 OMe			59.83			
6			104.24			
2			128.60			
1			134.89			
4			138.17			
3			144.71			
5			148.47			

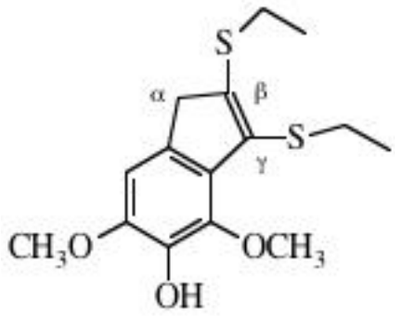
^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.98	quint	7.2
α	2.78	br t	7.2
γ	2.83	br t	7.2
5 OMe	3.77	s	
3 OMe	3.79	s	
6	6.58	s	
Benzene			
β	1.86	quin	7.37
α	2.71	td	7.37, 0.66
γ	2.86	t	7.37
5 OMe	3.28	s	
3 OMe	3.75	s	
6	6.32	s	

Notes:

HKE-11
Raney nickel reaction of hke5.5

Compound Number 3046



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ S-CH3			15.11			
β S-CH3			15.41			
β S-CH2			26.33			
γ S-CH2			29.12			
α			41.68			
5 OMe			56.91			
3 OMe			62.30			
6			105.00			
γ			126.93			
2			131.50			
1			133.78			
3			104.04			
4			141.58			
5			147.06			
β			148.43			

^{1}H (acetone)

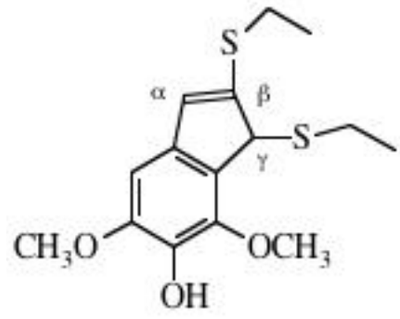
Atom	H Shifts	Mult	J
γ S-CH3	1.15	t	7.37
β S-CH3	1.30	t	7.37
γ S-CH2	2.89	q	7.37
β S-CH2	2.95	q	7.37
α	3.58	d	0.92
5 OMe	3.82	s	
3 OMe	3.85	s	
6	6.87	br t	0.92

Notes:

hke 5.4.1

Thioacidolysis product of β-O-4 (S-G) aldehyde dimer

Compound Number 3047



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ S-CH3			14.39			
β S-CH3			14.45			
γ S-CH2			22.23			
β S-CH2			26.80			
γ			52.56			
5 OMe			56.71			
3 OMe			60.09			
6			100.11			
α			124.89			
2			128.89			
1			135.82			
4			137.70			
β			145.14			
3			145.23			
5			149.46			

^{1}H (acetone)

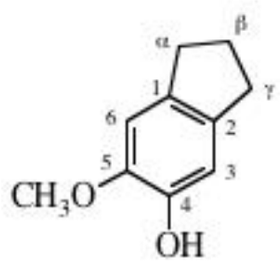
Atom	H Shifts	Mult	J
γ S-CH3	1.00	t	7.5
β S-CH3	1.33	t	7.37
γ S-CH2	2.22,2.04	dq, dq	12.1, 7.5
β S-CH2	2.94	q	7.37
5 OMe	3.82	s	
3 OMe	3.96	s	
γ	4.39	d	1.18
α	6.38	d	1.18
6	6.63	s	

Notes:

hke 5.5

Thioacidolysis product of γ-O-4 (S-G) aldehyde dimer

Compound Number 3048



6-methoxy-indan-5-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.99	quint	7.63
α	2.74	t	7.63
γ	2.76	t	7.63
OMe	3.79	s	
3	6.66	s	
6	6.78	s	

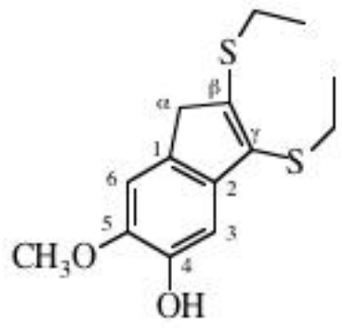
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β			26.45			
α			33.13			
γ			33.25			
OMe			56.48			
6			108.74			
3			111.56			
1			135.00			
2			136.73			
4			146.11			
5			147.01			

Notes:

hke87
Desulfurized (Raney-nickle Rxn)
thioacidolysis product of β-O-4 (G-S) aldehyde model compound

Compound Number 3049



2,3-bis-ethylsulfanyl-6-methoxy-1H-inden-5-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ S CH3	1.67	t	7.37
β S CH3	1.31	t	7.37
γ S CH2	2.81	q	7.37
β S CH2	2.99	q	7.37
α	3.58	d	0.79
OMe	3.83	s	
3	6.87	s	
6	7.06	br t	0.79

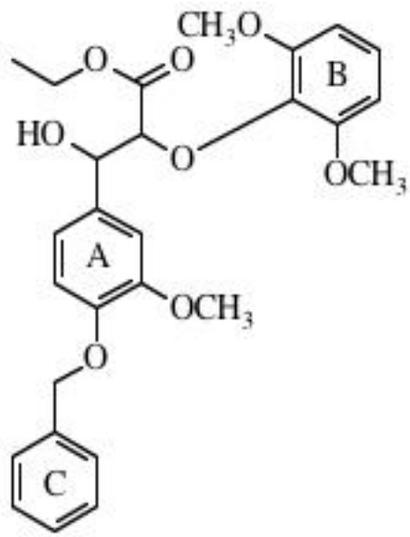
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β S CH3			15.47			
γ S CH3			15.74			
β S CH2			23.65			
γ S CH2			27.70			
α			41.57			
OMe			56.83			
4			106.37			
6			109.01			
γ			128.64			
1			133.31			
2			140.13			
5			146.09			
4			146.91			
β			148.16			

Notes:

hke83.3
Thioacidolysis product of β-O-4 (G-S) aldehyde dimer model.

Compound Number 3050



^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.09	t	7.10
B OMe	3.75	s	
A OMe	3.82	s	
CH2	4.04	m	
β	4.68	d	5.39
α	4.96	d	5.39
C α	5.09	s	
B 2,6	6.64	d	8.16
A6	6.92	dd	8.29, 1.71
A5	6.96	d	8.29
B1	6.99	t	8.16
A2	7.17	d	1.71
C 3,4,5	7.27-7.40	m	
C 2,6	7.37	br d	7.37

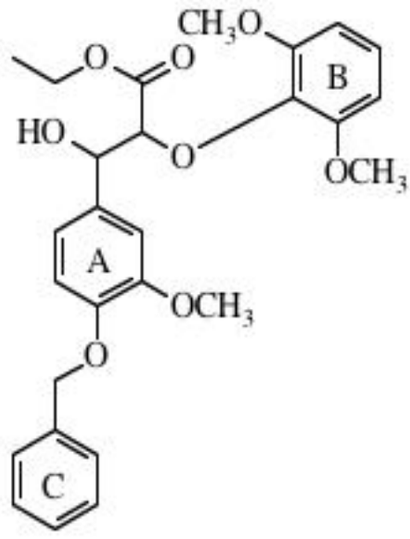
Notes:

hkd79.2C
possibly erythro

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3			14.41			
A OMe			56.13			
B OMe			56.44			
B OMe			56.44			
CH2			60.69			
C α			71.37			
α			74.31			
β			86.14			
B2			106.37			
B6			106.37			
A2			112.31			
A5			114.41			
A6			120.34			
B1			124.73			
C2			128.31			
C6			128.31			
C4			128.41			
C3			129.09			
C5			129.09			
A1			134.57			
B4			137.19			
C1			138.62			
A4			148.71			
A3			150.33			
B3			153.64			
B5			153.64			
γ			169.44			

Compound Number 3051



^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	0.99	t	7.23
A OMe	3.79	s	
B OMe	3.82	s	
CH2	3.95	m	
β	4.02	d	8.42
α	4.84	d	8.42
C α	5.09	s	
B 2,6	6.71	d	8.5
A6	6.81	dd	8.29, 1.97
A5	6.94	d	8.29
A2	6.99	d	1.97
B1	7.05	t	8.55
C 3,4,5	7.29-7.39	m	
C 2,6	7.46	br d	7.37

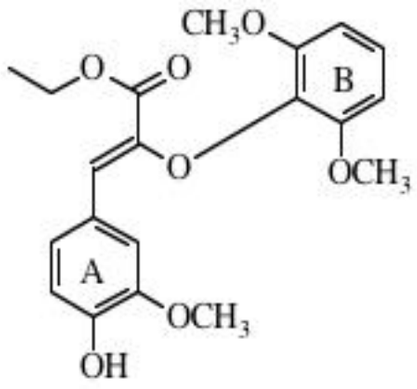
Notes:

hkd79.2Ex
possibly threo

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3			14.30			
A OMe			56.15			
B OMe			56.42			
B OMe			56.42			
CH2			60.68			
C α			71.38			
α			76.04			
β			90.35			
B2			106.26			
B6			106.26			
A2			112.09			
A5			114.61			
A6			120.46			
B1			125.18			
C2			128.33			
C6			128.33			
C4			128.44			
C3			129.11			
C5			129.11			
A1			132.51			
B4			138.07			
C1			138.56			
A4			149.17			
A3			150.62			
B3			153.39			
B5			153.39			
γ			169.49			

Compound Number 3052



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3			14.35			
A OMe			56.09			
B OMe			56.79			
B OMe			56.79			
CH2			61.05			
B2			107.08			
B6			107.08			
A2			114.38			
A5			115.74			
α			119.07			
B1			123.37			
A6			125.09			
A1			126.76			
B4			136.27			
β			143.08			
A3			148.01			
A4			148.10			
B3			152.01			
B5			152.01			
γ			163.74			

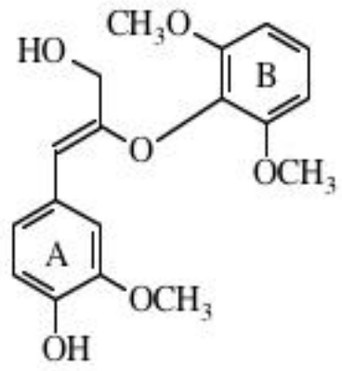
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.11	t	7.10
B OMe	3.74	s	
A OMe	3.76	s	
CH2	4.06	q	7.10
B 2,6	6.67	d	8.68
α	6.79	s	
A5	6.82	d	8.29
B1	6.94	t	8.68
A6	7.29	dd	8.29, 1.84
A2	7.52	d	1.84

Notes:

hkd 17.2.1.3

Compound Number 3053



^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.76	s	
B OMe	3.77	s	
γ	3.97	br s	
α	5.75	br s	
B 2,6	6.68	d	8.42
A5	6.79	d	8.29
B1	7.07	t	8.42
A6	7.18	dd	8.29, 1.84
A2	7.46	d	1.84

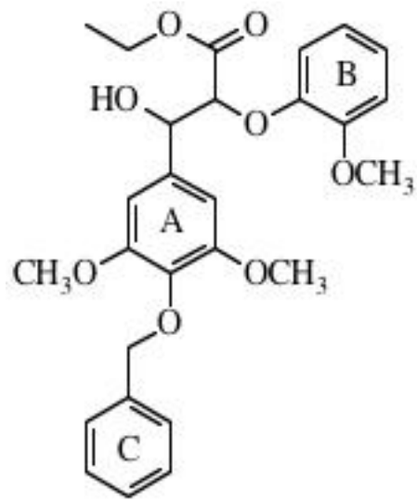
Notes:

hkd87

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
1H data only						

Compound Number 3054



^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.08	t	7.1
B OMe	3.80	s	
A OMe	3.82	s	
CH2	4.04	m	7.1
β	4.72	d	5.52
Cα	4.93	s	
α	5.08	d	5.52
A 2,6	6.83	s	
B 5,6	6.77-6.85	m	
B 1,2	6.90-7.00	m	
C 3,4,5	7.24-7.38	m	
C 2,6	7.50	br d	7.37

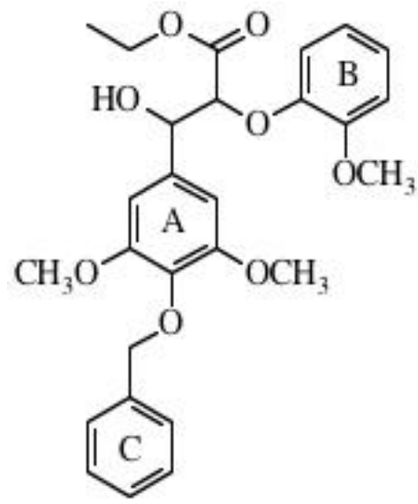
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3			14.35			
B OMe			56.36			
A OMe			56.44			
A OMe			56.44			
CH2			61.29			
C α			75.06			
α			75.59			
β			84.38			
A2			105.44			
A6			105.44			
B2			113.87			
B5			117.25			
B6			121.61			
B1			123.44			
C4			128.31			
C3			128.76			
C5			128.76			
C2			128.82			
C6			128.82			
A1			136.70			
A4			137.61			
C1			139.47			
B4			148.70			
B3			151.03			
A3			154.17			
A5			154.17			
γ			169.85			

Notes:

hkd35.2.1.2
possibly erythro (see 3055)
separated by cyclohexane:EtOAc:Acetic Acid (100:50:1)

Compound Number 3055



^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.19	t	7.10
B OMe	3.77	s	
A OMe	3.83	s	
CH2	4.16	q	7.10
β	4.70	d	6.71
C α	4.94	s	
α	5.07	d	6.71
B 5,6	6.79	m	
A 2,6	6.90	s	
B 1,2	6.90-6.97	m	
C 3,4,5	7.24-7.37	m	
C 2,6	7.5	br d	7.37

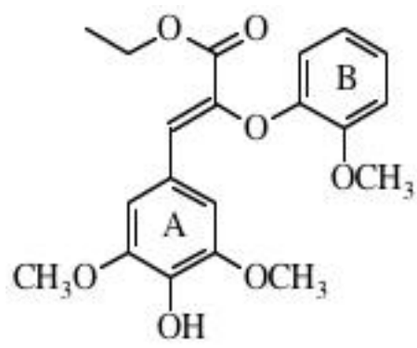
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3			14.16			
B OMe			56.28			
A OMe			56.40			
A OMe			56.40			
CH2			61.28			
α			74.84			
C α			75.04			
β			83.40			
A2			105.51			
A6			105.51			
B2			113.77			
B5			116.96			
B6			121.52			
B1			123.43			
C4			128.28			
C3			128.73			
C5			128.73			
C2			128.80			
C6			128.80			
A4			137.51			
A1			137.79			
C1			139.50			
B4			148.35			
B3			151.08			
A3			154.04			
A5			154.04			
γ			170.25			

Notes:

hkd35.2.1.1
Possible threo (see 3054)
separated by cyclohexane:EtOAc:Acetic Acid (100:50:1)

Compound Number 3056



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3			14.19			
B OMe			56.30			
A OMe			56.37			
A OMe			56.37			
CH2			61.58			
A2			109.09			
A6			109.09			
B2			113.72			
B5			114.15			
B6			121.49			
B1			123.24			
A1			124.12			
α			127.99			
β			138.78			
A4			138.94			
B4			146.94			
A3			148.50			
A5			148.50			
B3			149.87			
γ			164.06			

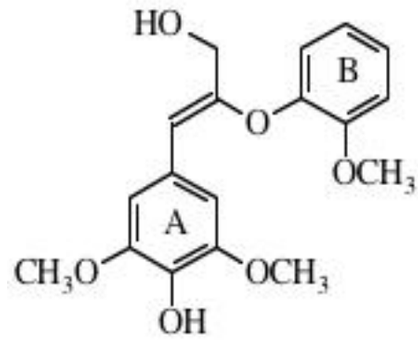
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.21	t	7.10
A OMe	3.73	s	
B OMe	3.90	s	
CH2	4.20	q	7.10
B5	6.72	dd	8.02, 1.58
B6	6.79	ddd	8.02, 7.37, 1.58
B1	6.94	ddd	8.02, 7.37, 1.58
B2	7.06	dd	8.02, 1.58
A 2,6	7.16	s	
α	7.33	s	

Notes:

hkd91.1.2

Compound Number 3057



^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.67	s	
B OMe	3.90	s	
γ	4.15	br s	
α	6.21	br s	
A 2,6	6.90	s	
B 1,2,5,6	6.75-7.05	m	
A4 OH	8.00	s	

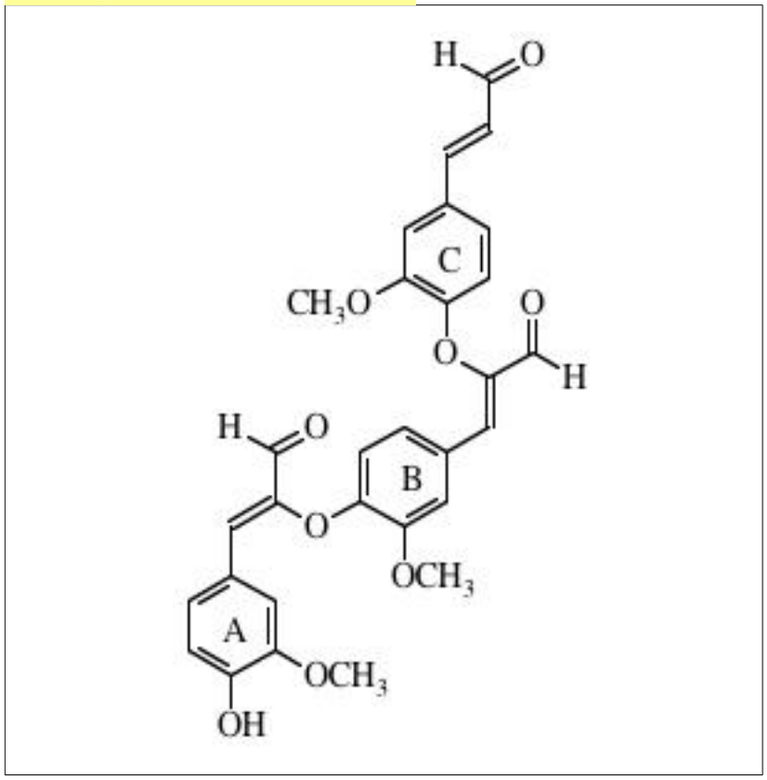
Notes:

hkd57.4
1H Data only

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
1H data only						

Compound Number 3058



^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.69	s	
B OMe	3.83	s	
C OMe	3.98	s	
C β	6.70	dd	15.92, 7.65
B5	6.79	d	8.29
C5	6.82	d	8.29
A5	6.85	d	8.29
C6	7.15	dd	8.29, 1.97
B6	7.28	dd	8.29, 1.97
A6	7.30	dd	8.29, 1.97
A α	7.30	s	
B α	7.33	s	
C2	7.48	d	1.97
A2	7.52	d	1.97
C α	7.58	d	15.92
B2	7.67	d	1.97
A OH	8.37	bs	
Aγ	9.48	s	
Bγ	9.53	s	
Cγ	9.65	d	7.65

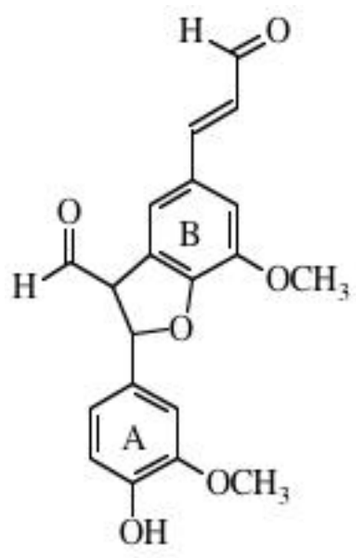
Notes:

hkc43.4.1

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A OMe			55.93			
B OMe			56.14			
C OMe			56.50			
C2			112.55			
A2			113.95			
B2			114.87			
B5			115.18			
C5			115.42			
A5			116.26			
C6			123.59			
A1			125.21			
B6			125.59			
A6			126.78			
B1			128.03			
Cβ			128.38			
C1			130.35			
Bα			137.15			
Aα			138.31			
Aβ			147.52			
A3			148.46			
B4			148.47			
Bβ			148.51			
C4			148.72			
B3			149.91			
C3			150.35			
A4			150.58			
Cα			153.13			
Aγ			187.43			
Bγ			187.65			
Cγ			193.91			

Compound Number 3059



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A OMe			56.31			
B OMe			56.54			
β			62.91			
α			85.24			
A2			110.66			
B2			114.27			
A5			115.93			
B6			119.49			
A6			119.81			
B5			125.79			
Bβ			127.69			
B1			129.66			
A1			132.18			
B3			146.01			
A3			147.91			
A4			148.57			
B4			151.77			
Bα			153.45			
Bγ			193.83			
γ			197.57			

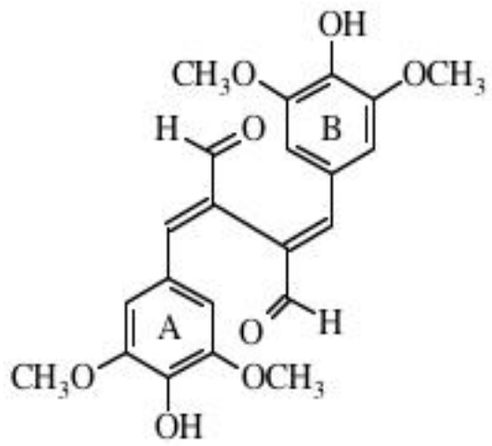
^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.82	s	
B OMe	3.92	s	
β	4.50	d	6.5
α	6.20	d	6.5
B β	6.70	dd	15.78, 7.76
A5	6.84	d	8.16
A6	6.90	dd	8.16, 1.84
A2	7.06	d	1.84
B2	7.38	s	
B6	7.43	s	
B α	7.61	d	15.78
A OH	8.29	s	
B γ	9.64	d	7.76
A γ	9.94	s	

Notes:

hkf69.2.2
Fll73.12

Compound Number 3060



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.54			
2			109.07			
6			109.07			
1			126.05			
β			134.78			
4			140.10			
3			148.71			
5			148.71			
α			152.98			
γ			192.70			

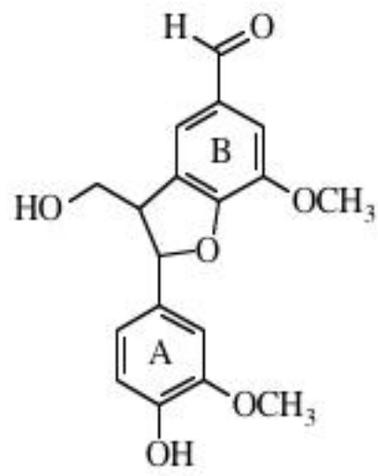
^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.72	s	
2,6	7.02	s	
α	7.79	s	
OH	7.94	bs	
γ	9.67	s	

Notes:

hkf7-1
This compound has a plane of symmetry and so the signals are reported for only one half.

Compound Number 3061



^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
β			53.84			
A OMe			56.30			
B OMe			56.37			
γ			64.22			
α			89.87			
A2			110.65			
B2			113.44			
A5			115.79			
A6			119.82			
B6			121.43			
B5			131.19			
B1			132.40			
A1			133.42			
B3			145.81			
A4			147.67			
A3			148.49			
B4			154.87			
B α			190.90			

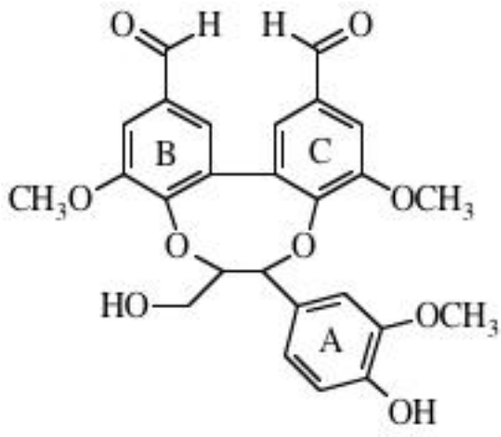
^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.67	bq	
A OMe	3.82	s	
B OMe	3.92	s	
γ	3.92	m	
α	5.69	d	6.84
A5	6.81	d	8.16
A6	6.88	dd	8.16, 1.97
A2	7.05	d	1.97
B2	7.42	d	1.45
B6	7.53	dd	1.45. 0.92
A OH	7.65	bs	
B α	9.82	s	

Notes:

hkf75.322

Compound Number 3062



^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.48	m	
γ2	3.95	m	
A OMe	3.82	s	
C OMe	3.91	s	
B OMe	4.03	s	
β	4.18	m	
α	5.05	d	10.14
A5	6.84	d	8.16
A6	6.93	dd	8.16, 1.97
A2	7.05	d	1.97
C2	7.56	d	1.84
B2	7.65	d	1.84
C6	7.70	d	1.84
B6	7.74	d	1.84
C α	10.02	s	
B α	10.06	s	

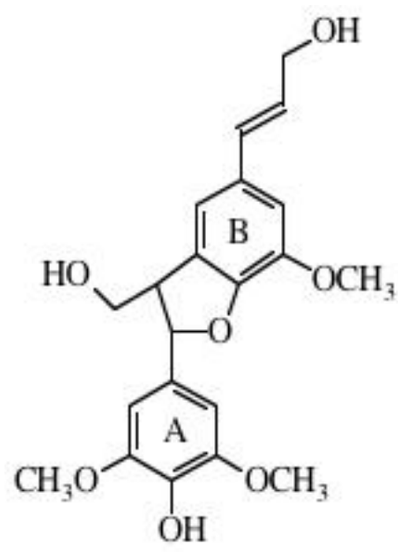
Notes:

hkf83.2.1 (6 mg)

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
C OMe			56.32			
A OMe			56.37			
B OMe			56.62			
γ			62.29			
α			85.11			
β			87.48			
B2			111.71			
C2			111.88			
A2			112.08			
A5			115.64			
A6			121.57			
C6			125.15			
B6			125.32			
A1			130.25			
B5			133.27			
C5			133.72			
B1			134.42			
C1			134.56			
A4			147.73			
A3			148.23			
B4			152.46			
C4			152.81			
B3			154.23			
C3			154.39			
Cα			191.66			
Bα			191.71			

Compound Number 3063



Simulanol, S-(8-5)-G

4-[3-hydroxy-5-(3-hydroxy-propenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-2,6-dimethoxy-phenol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.79	s	
B OMe	3.86	s	
Aβ	3.54	m	
Bγ	4.19	td	J = 5.52, 1.58
Aα	5.54	d	J = 6.71
Bβ	6.23	dt	J = 15.92, 5.52
Bα	6.52	dt	J = 15.92, 1.58
A 2,6	6.74	s	
B2	6.84	s	
B6	6.97	s	
A4-OH	7.19	s	

^{13}C

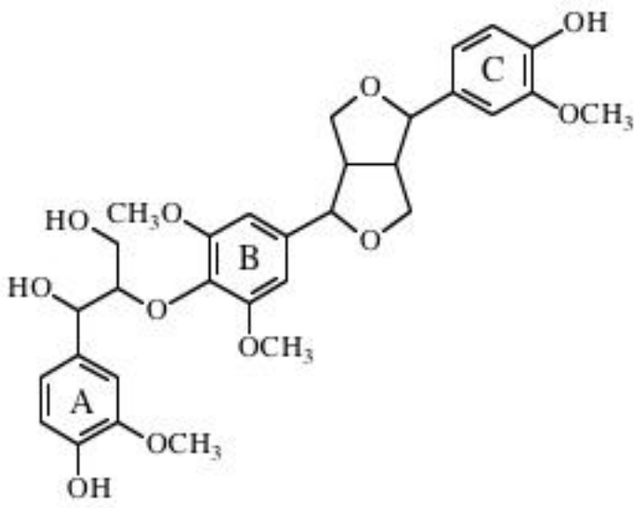
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Aβ			54.78			
B OMe			56.44			
B OMe			56.44			
A OMe			56.67			
Bγ			63.39			
Aγ			64.52			
Aα			88.74			
A2			104.55			
A6			104.55			
B2			111.80			
B6			116.07			
Bβ			128.38			
B5			130.47			
Bα			130.52			
B1			131.95			
A1			133.30			
A4			136.68			
B3			145.16			
A3			148.74			
A5			148.74			
B4			148.95			

Notes:

hkh 99.14 Morreel #6

Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W.Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

Compound Number 3064



threo

buddlenol E, G-(8-O-4)-S-(8-8)-G

1-(4-hydroxy-3-methoxy-phenyl)-2-{4-[4-(4-hydroxy-3-methoxy-phenyl)-tetrahydro-furo[3,4c]furan-1-yl]-2,6-dimethoxy-phenoxy}-

^{1}H (acetone)

Atom	H Shifts	Mult	J
Cβ +Bβ	3.10	m	
Aγ1	3.43	m	
Aγ2	3.84	m	
Cγ2 + Bγ2	3.86	m	
Aβ	4.15	m	
Cγ1 + Bγ1	4.24	m	
Cα	4.68	d	J = 4.34
Bα	4.73	d	J = 4.34
Aα	4.97	m	
B 2,6	6.76	s	
C2	6.98	d	J = 1.84
A2	7.03	d	J = 1.84
A4-OH	7.37	s	
C4-OH	7.49	s	

^{13}C

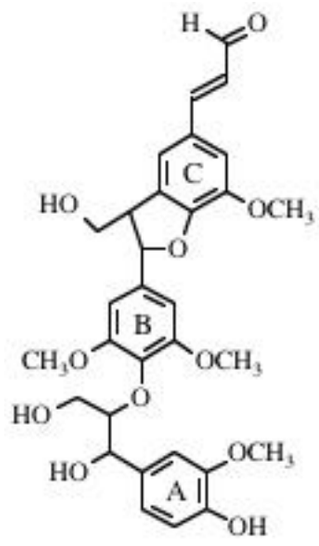
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Cβ			55.15			
Bβ			55.46			
OMe			56.24			
B OMe			56.59			
B OMe			56.59			
OMe			56.70			
Aγ			60.98			
Cγ			72.30			
Bγ			72.54			
Aα			73.38			
Bα			86.57			
Cα			86.60			
Aβ			87.86			
B2			104.12			
B6			104.12			
C2			110.62			
A2			110.92			
A5			115.20			
C5			115.54			
C6			119.60			
A6			120.04			
C1			133.77			
B1			133.80			
A1			134.10			
C4			135.72			
B4			139.10			
A3			146.47			
C3			146.90			
A4			147.98			
B3			154.20			
B5			154.20			

Notes:

hkh 99.6 Morreel #22

Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W. Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

Compound Number 3065



threo

buddlenol A, G-(t8-O-4)-S-(8-5)-G'

3-(2-{4-[2-hydroxy-3-methoxy-phenyl)1-hydroxymethyl-ethoxy]-3.5-dimethoxy-phenyl}-3-hydroxymethyl-7-methoxy-2,3-

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.82	s	
B OMe	3.84	s	
OMe	3.94	s	
Aα	4.97	t	J = 4.47
Bα	5.70	d	J = 6.45
Cβ	6.66	dd	J = 15.78, 7.63
A5	6.76	d	J = 8.02
A6	6.83	dd	J = 8.02, 1.84
B 2,6	6.83	s	
A2	7.03	d	J =1.84
Cα	7.59	d	J = 15.78
Cγ	9.64	d	J = 7.63

Notes:

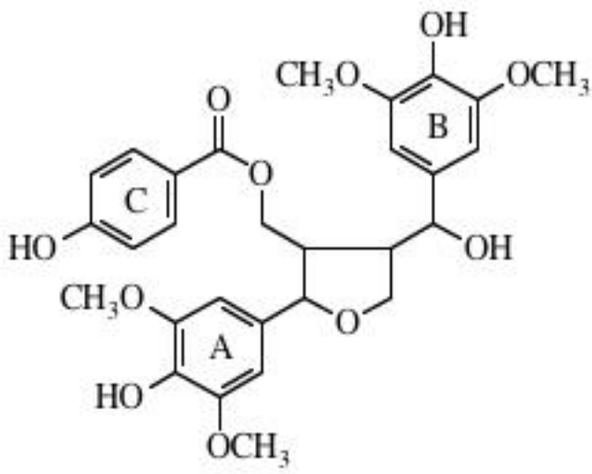
hkh 19.1t Morreel #23

Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W.Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
PROTON data only						

Compound Number 3066



SP-(8,8)-S

tetrahydro-α4,2-bis-(4-hydroxy-3,5-dimethoxyphenyl) α-3O-(4-hydroxybenzoyl)-3,4-furandimethanol

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aβ	2.55	m	
OMe	3.74	s	
OMe	3.78	s	
Bβ	3.99	m	
Bγ	4.14	m	
Aγ1	4.41	m	
Aγ2	4.68	m	
Aα	4.90	d	J = 6.3
Bα	4.96	d	J = 5.0
A2,6	6.66	s	
B2,6	6.72	s	
C3,5	6.87	m	
C2,6	7.77	m	

^{13}C

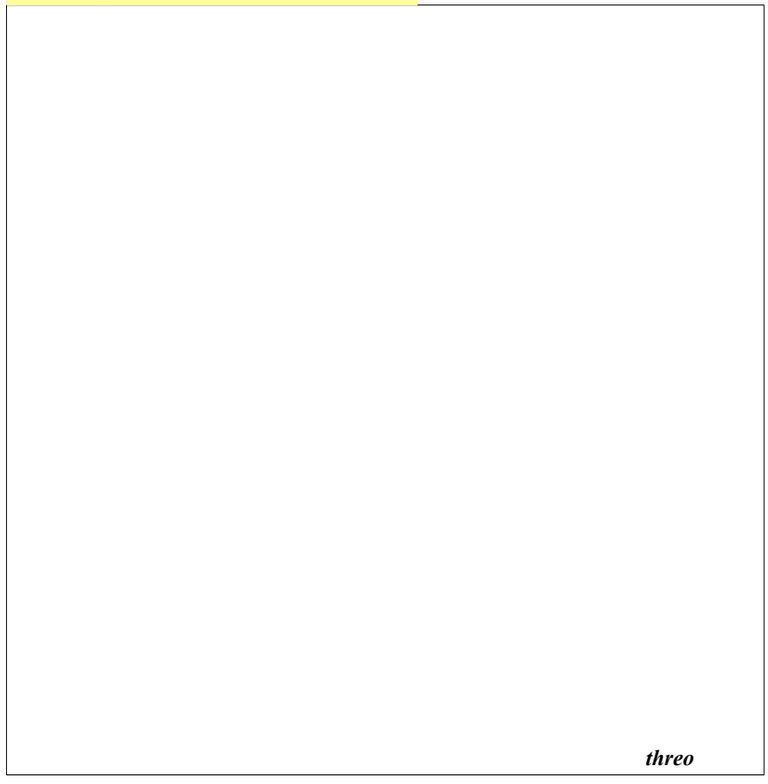
Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bβ			48.37			
Aβ			49.80			
OMe			56.50			
OMe			56.50			
OMe			56.50			
OMe			56.50			
Aγ			63.99			
Bγ			69.95			
Bα			72.59			
Aα			85.34			
A2			104.45			
A6			104.45			
B2			104.53			
B6			104.53			
C3			115.98			
C5			115.98			
C1			122.40			
C2			132.45			
C6			132.45			
A1			134.49			
B1			134.91			
A4			136.01			
B4			136.01			
A3			148.54			
A5			148.54			
B3			148.54			
B5			148.54			
C4			162.56			
Cα			166.43			

Notes:

Fln 117 Morreel #19

Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

Compound Number 3067



threo

G-(8-O-4)-S

***threo*-1-(4-hydroxy-3-methoxy-phenyl)-2-[2,6 dimethoxy-phenoxy-4-(3-**

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	3.39	m	-
A3 OMe	3.83	s	
B3 OMe	3.87	s	
Bγ	4.21	m	-
Aα–OH	4.33	d	J = 3.8
Aα	4.96	dd	J = 6.8, 8.4
Bβ	6.37	dt	J = 15.8, 5.1
Bα	6.54	d	J = 15.8
A5	6.76	d	J = 8.2
B2/6	6.79	s	
A6	6.82	dd	J = 8.2, 1.3
A2	7.03	d	J = 1.3
A4-OH	7.33	br s	

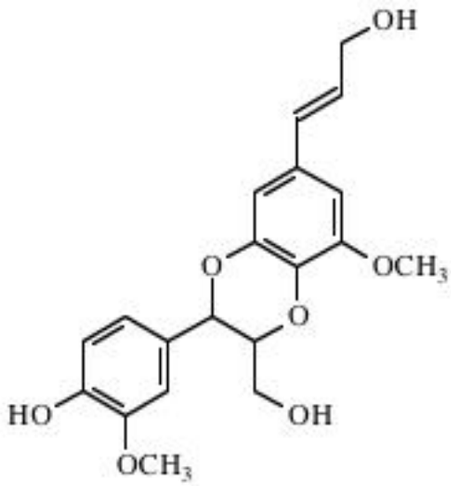
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
PROTON data only						

Notes:

HKh83.5, FLl112 Compound #8, Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W. Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549 See compound #118 for peracetate

Compound Number 3068



trans

G-(8-O-4)-5H [nocomtol]

4-[3-hydroxymethyl-7-(E)-(3-hydroxypropenyl)-5-methoxy-2,3-dihydro-benzo[1,4]dioxin-2-yl]-2-methoxyphenol

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ1	3.50	m	-
Aγ2	3.76	m	-
B3 OMe	3.85	s	
A3 OMe	3.85	s	
Aβ	4.05	m	-
Bγ	4.20	dd	J = 5.4, 1.6
Aα	4.96	d	J = 7.9
Bα	6.26	dt	J = 15.9, 5.4
Bβ	6.47	dt	J = 15.9, 1.6
B6	6.68	d	J = 1.8
A5	6.87	d	J = 8.1
A6	6.95	dd	J = 8.1, 1.8
A2	7.10	d	J = 1.8

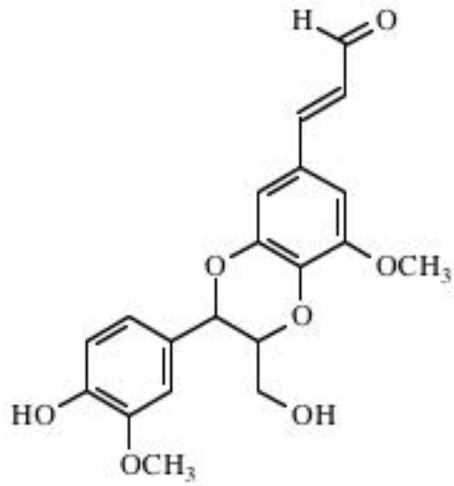
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
B3-OMe			56.2			
A3-OMe			56.2			
Aγ			61.9			
Bγ			63.6			
Aα			76.7			
Aβ			79.3			
B2			103.2			
B6			108.5			
A2			111.7			
A5			115.7			
A6			121.4			
Bβ			129.0			
A1			129.1			
Bα			130.1			
B1			130.3			
B4			133.7			
B5			145.2			
A4			147.8			
A3			148.3			
B3			149.8			

Notes:

FLm08 Cmpd 1a:Phenolic profiling of caffeic acid O-methyltransferase-deficient poplar reveals novel benzodioxane oligolignols. K. Morreel, J. Ralph, F. Lu, G. Goeminne, R. Busson, P. Herdewijn, J.L. Goeman, J. Van der Eycken, W. Boerjan and E. Messens. Plant Physiology, 136(4), 4023-4036 (2004).

Compound Number 3069



trans

G-(8-O-4)-5H′ [nocomtal]

(2E)-3-[3-(4-hydroxy-3-methoxy-phenyl)-2(hydroxymethyl)-8-methoxy-2,3-dihydro-1,4-benzodioxin-6-yl]acrylaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ1	3.53	m	-
Aγ2	3.82	m	-
A3 OMe	3.86	s	
B3 OMe	3.91	s	
Aβ	4.14	ddd	J = 8.0, 3.8, 2.6
Aα	5.01	d	J = 8.0
Bβ	6.67	dd	J = 15.8, 7.6
A5	6.88	d	J = 8.0
B6	6.92	dd	J = 2.0, 0.4
A6	6.97	ddd	J = 8.0, 2.0, 0.4
B2	7.02	d	J = 2.0
A2	7.12	d	J = 2.0
Bα	7.53	d	J = 15.8
A4-OH	7.59	bs	-
Bγ	9.64	d	7.6

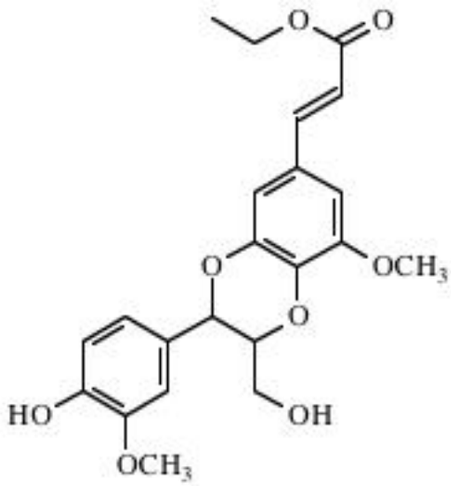
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A3-OMe			56.4			
B3-OMe			56.5			
Aγ			61.6			
Aα			77.0			
Aβ			79.8			
B2			105.5			
B6			111.9			
A2			112.0			
A5			115.8			
A6			121.6			
B1			127.5			
Bβ			128.0			
A1			128.9			
Bα			137.4			
B5			145.6			
A3			148.1			
A4			148.5			
B3			150.4			
B4			153.7			
Bγ			193.8			

Notes:

FLn55 Cmpd 3:Phenolic profiling of caffeic acid O-methyltransferase-deficient poplar reveals novel benzodioxane oligolignols. K. Morreel, J. Ralph, F. Lu, G. Goeminne, R. Busson, P. Herdewijn, J.L. Goeman, J. Van der Eycken, W. Boerjan and E. Messens. Plant Physiology, 136(4), 4023-4036 (2004).

Compound Number 3070



trans

G-(8-O-4)-5H″

3-[3-(4-hydroxy-4-methoxyphenyl)-2-hydroxymethyl-8-methoxy-2,3-dihydrobenzo[1,4] dioxin-6-yl]-acrylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Me	1.25	t	J = 7.1
Aγ1	3.50	m	-
Aγ2	3.83	m	-
B3 OMe	3.85	s	
A3 OMe	3.92	s	
Aβ	4.09	m	-
CH2	4.17	q	J = 7.1
Aα	4.98	d	J = 8.0
Bβ	6.40	d	J = 15.9
B6	6.85	d	J = 1.5
A5	6.88	d	J = 8.1
B2	6.95	d	J = 1.5
A6	6.96	dd	J = 8.1, 1.8
A2	7.10	d	J = 1.8
Bα	7.54	d	J = 15.9

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Me			14.6			
B3-OMe			56.2			
A3-OMe			56.3			
Aγ			61.6			
CH2			61.6			
Aα			76.9			
Aβ			79.5			
B2			104.7			
B6			111.1			
A2			111.7			
A5			115.7			
Bβ			117.0			
A6			121.4			
B1			127.4			
A1			128.8			
B4			136.4			
Bα			145.2			
B5			145.3			
A4			147.8			
B3			148.3			
A3			150.1			
Bγ			167.2			

Notes:

FL1111 Cmpd c:Phenolic profiling of caffeic acid O-methyltransferase-deficient poplar reveals novel benzodioxane oligolignols. K. Morreel, J. Ralph, F. Lu, G. Goeminne, R. Busson, P. Herdewijn, J.L. Goeman, J. Van der Eycken, W. Boerjan and E. Messens. Plant Physiology, 136(4), 4023-4036 (2004).

Compound Number 3071

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.84	s	-
A3/5 OMe	3.80	s	-
B3/5 OMe	3.94	s	-
γ1	4.12	dd	J = 11.9, 3.2
γ2	4.39	dd	J - 11.9, 7.4
β	4.62	m	-
α	4.94	dd	J = 6.7, 4.0
A2/6	6.70	s	-
Bβ	6.77	dd	J = 15.8, 7.6
B2/6	7.12	s	-
Bα	7.61	d	J = 15.8
Bγ	9.67	d	J = 7.6

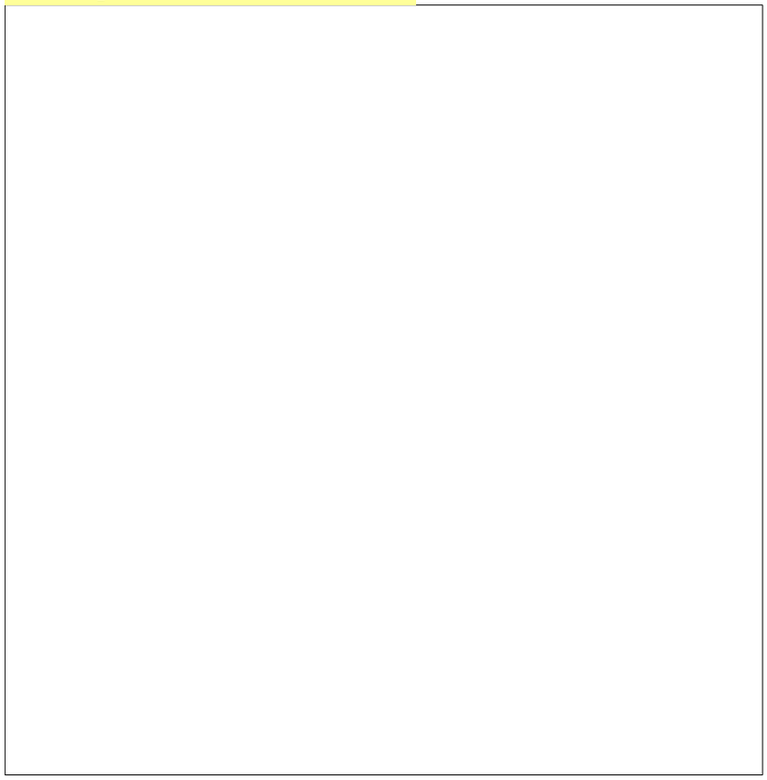
^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
γ Ac Me			20.66			
A3 OMe			56.62			
B3 OMe			56.73			
γ			63.59			
α			73.31			
β			84.56			
A2/6			104.65			
B2/6			106.94			
Bβ			129.11			
B1			131.09			
A1			131.65			
A4			136.04			
B4			139.26			
A3/5			148.51			
Bα			153.45			
B3/5			154.57			
γ Ac C=O			167.76			
Bγ			193.90			

Notes:

HKj51T6.7 Cmpd #9, Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W. Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549 Note the single γ-acetate!

Compound Number 3072



S-(8-O-4)-G-(8-5)-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bβ	3.51	m	
Aγ1	3.51	m	
Aγ2	3.71	m	
Bγ	3.85	m	
OMε	3.77	s	
OMε	3.86	s	
OMε	3.94	s	
Cγ	4.19	dd	J = 5.5, 1.3
Aβt	4.24	m	
Aβe	4.32	m	
Aα	4.86	d	J = 5.9
Bα	5.59	d	J = 6.5
Cβ	6.23	dt	J = 15.9, 5.5
Cα	6.51	d	J = 15.9
A 2,6	6.76	s	

^{13}C

Atom	$CDCl_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Bβ			54.8			
OMe			56.35			
OMe			56.39			
OMe			56.58			
Aγ			61.86			
Cγ			63.26			
Bγ			64.58			
Aα			73.84			
Aβe			86.32			
Aβt			88.03			
Bα			88.24			
A2/6			105.36			
C2/6			111.14			
B2/5/6			119.33			
Cβ			128.42			
Cα			130.48			

Notes:

HKf145, mixture of isomers Morreel #39 Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W. Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549