

## NMR Database of Lignin and Cell Wall Model Compounds

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This database was created and is administered as a cooperative effort between the US Forest Products Laboratory and the US Dairy Forage Research Center. It was designed to provide a coherent, single source of NMR data of lignin model compounds as well as compounds modeling similar structures in grasses and other forage plants. The database exists in four different formats: an interactive HyperCard<sup>©</sup> stack for the Macintosh<sup>®</sup> computer, a FileMaker Pro<sup>©</sup> database for cross-platform use, an Adobe<sup>©</sup> pdf cross-platform file for viewing and printing, and a hardcopy version derived from the FileMaker Pro database. The first three versions are available for downloading over the internet from the Dairy Forage Research Center web site:

<http://www.dfrc.ars.usda.gov>

The hardcopy is available by request from the authors at the Forest Products Laboratory. The use of trade or firm names in this publication is for reader information and does

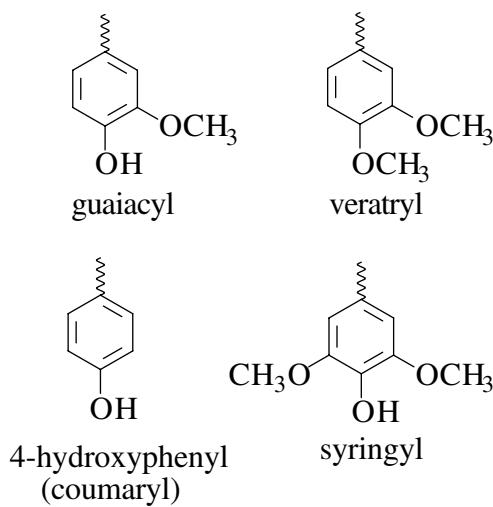
not imply endorsement by the US Dept. of Agriculture of any product or service.

In general <sup>13</sup>C NMR data was collected in three common deuterated solvents (acetone, chloroform and dimethyl sulfoxide) for each compound. The <sup>1</sup>H NMR data was reported for 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. 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. Search routines for the software versions allow grouping the compounds with similar traits, whereas the structure index is most useful for the hardcopy version. The inclusion of many 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 other NMR experiments such as long and short range C-H correlations, COSY and DEPT. 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 however comparisons between spectra are practical only within  $\pm 0.1$  ppm. The authors would greatly appreciate any corrections on misassignments.

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. The intensities of the individual chemical shift signals are used for the line plots generated by the HyperCard program but they are also useful in the hardcopy version for comparison with spectra.

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.

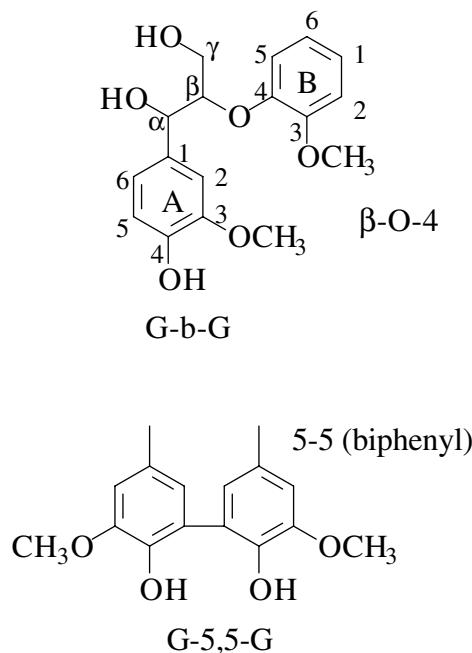


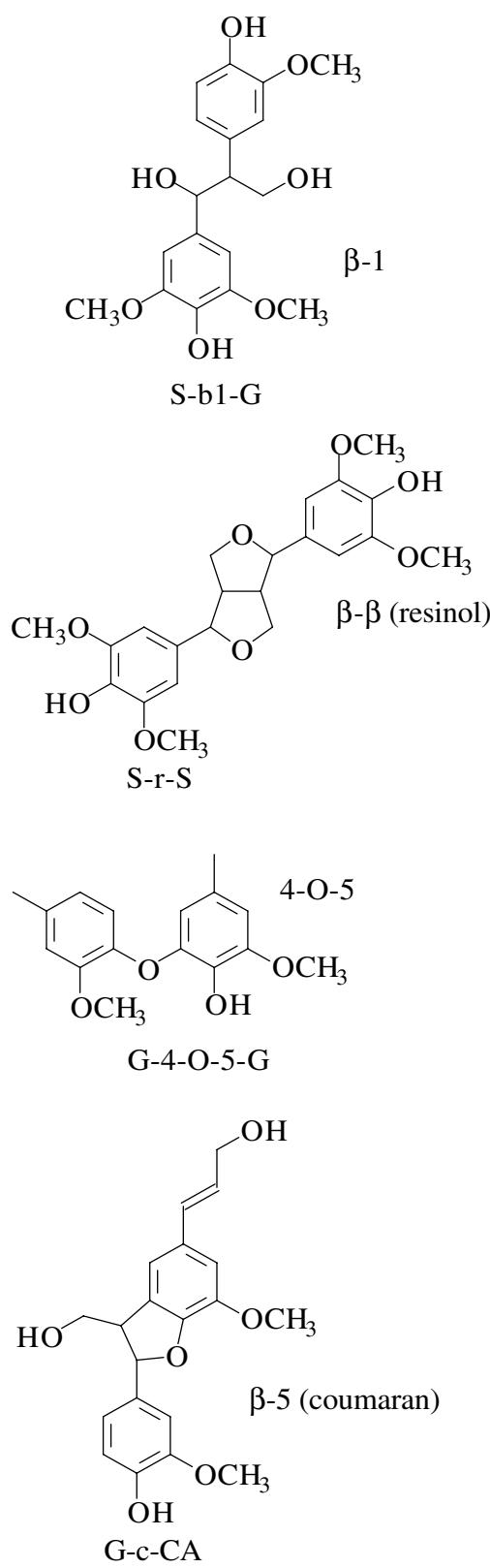
**Fig. 1** Trivial names for substituents at the 3,4 and 5 positions on the aromatic ring.

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**

<u>Entity</u>	<u>Abbreviation</u>
guaiacyl ring	G
syringyl ring	S
coumaryl ring	H
$\alpha$ -O-4 linkage	a
$\beta$ -O-4 linkage	b
$\beta$ -5 (phenylcoumaran)	c
$\beta$ -1 linkage	b1
$\beta$ - $\beta$ (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
<i>erythro</i>	e
<i>threo</i>	t





**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 alpha and beta 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. We will also make every effort to keep those researchers with hardcopy versions supplied with more pages. This database was written and prepared 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.

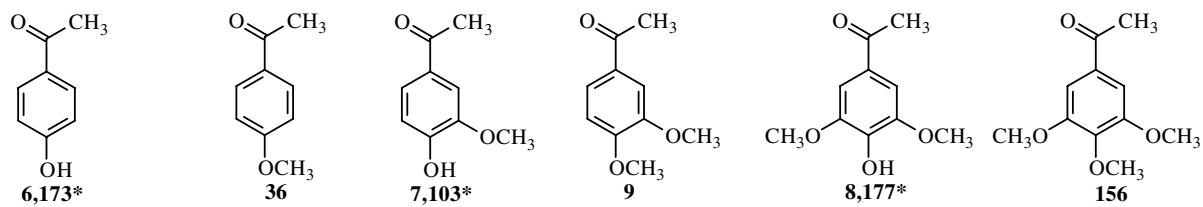
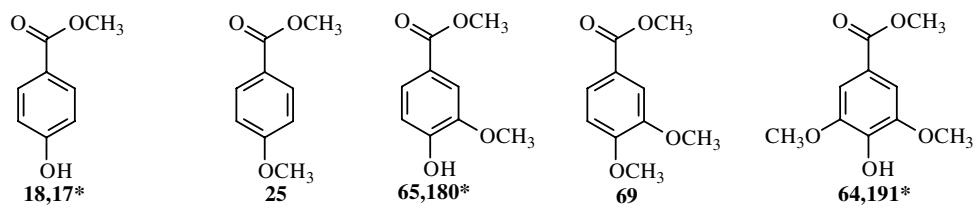
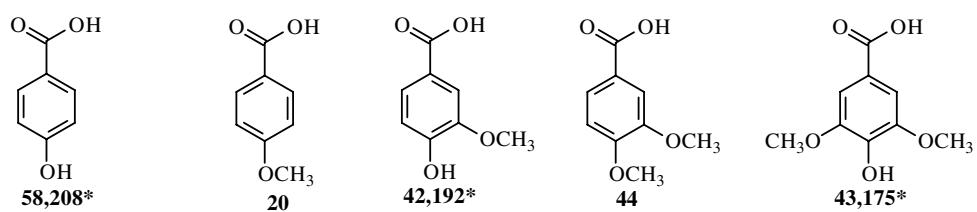
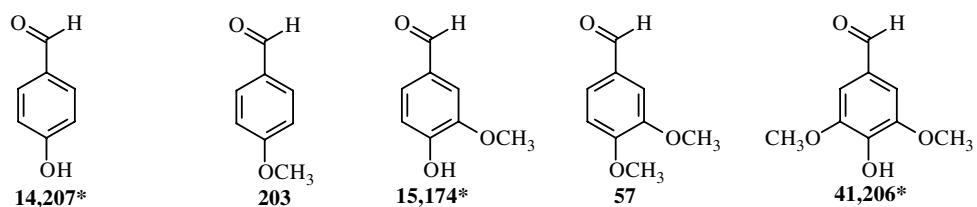
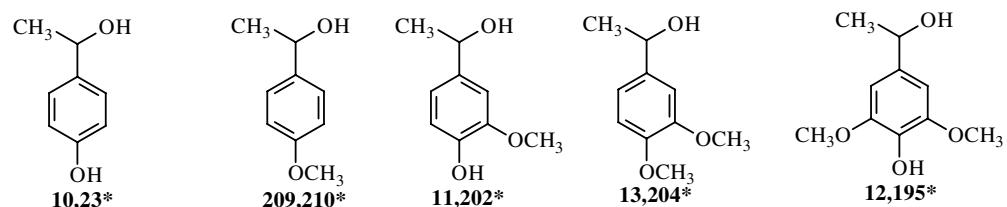
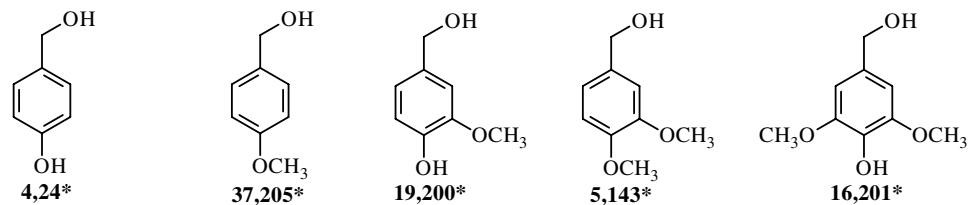
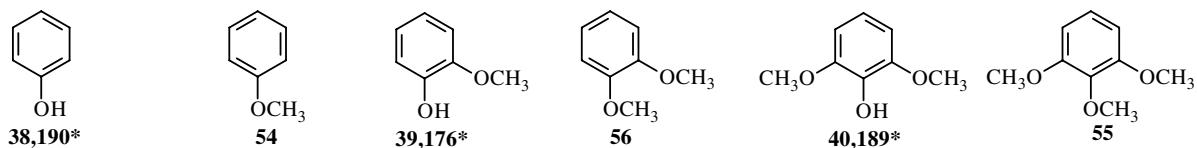
The authors gratefully acknowledge the many generous contributions made by others at both labs towards this database; William Landucci for software development, Martin Wesolowski and Kolby Hirth, NMR spectroscopists, and the frequent donation of compounds from Mike Mozuch, Noritsugu Terashima, Stéphane 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.

# Structure Index

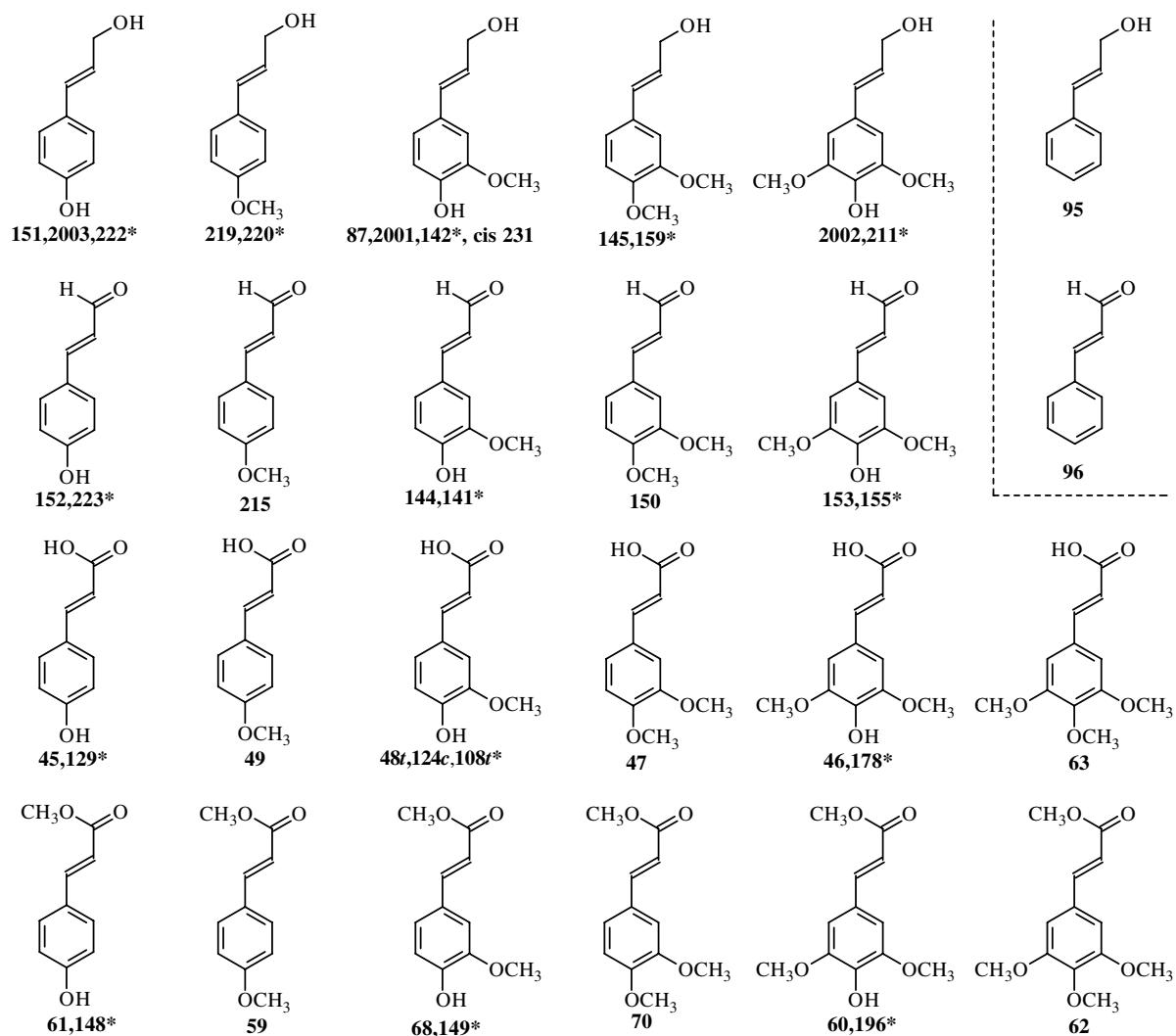
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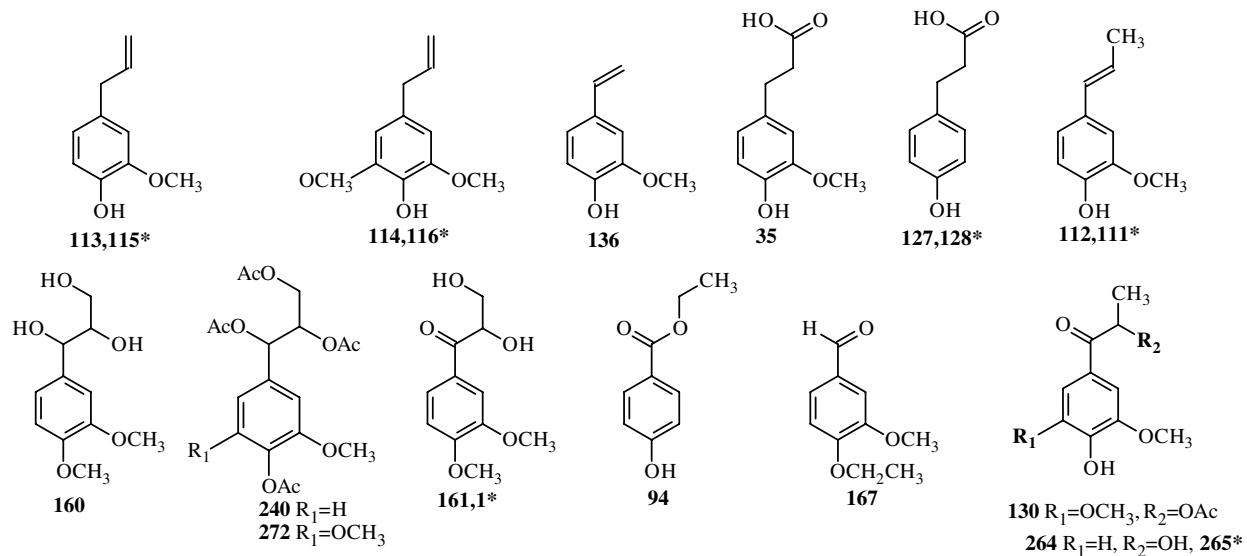
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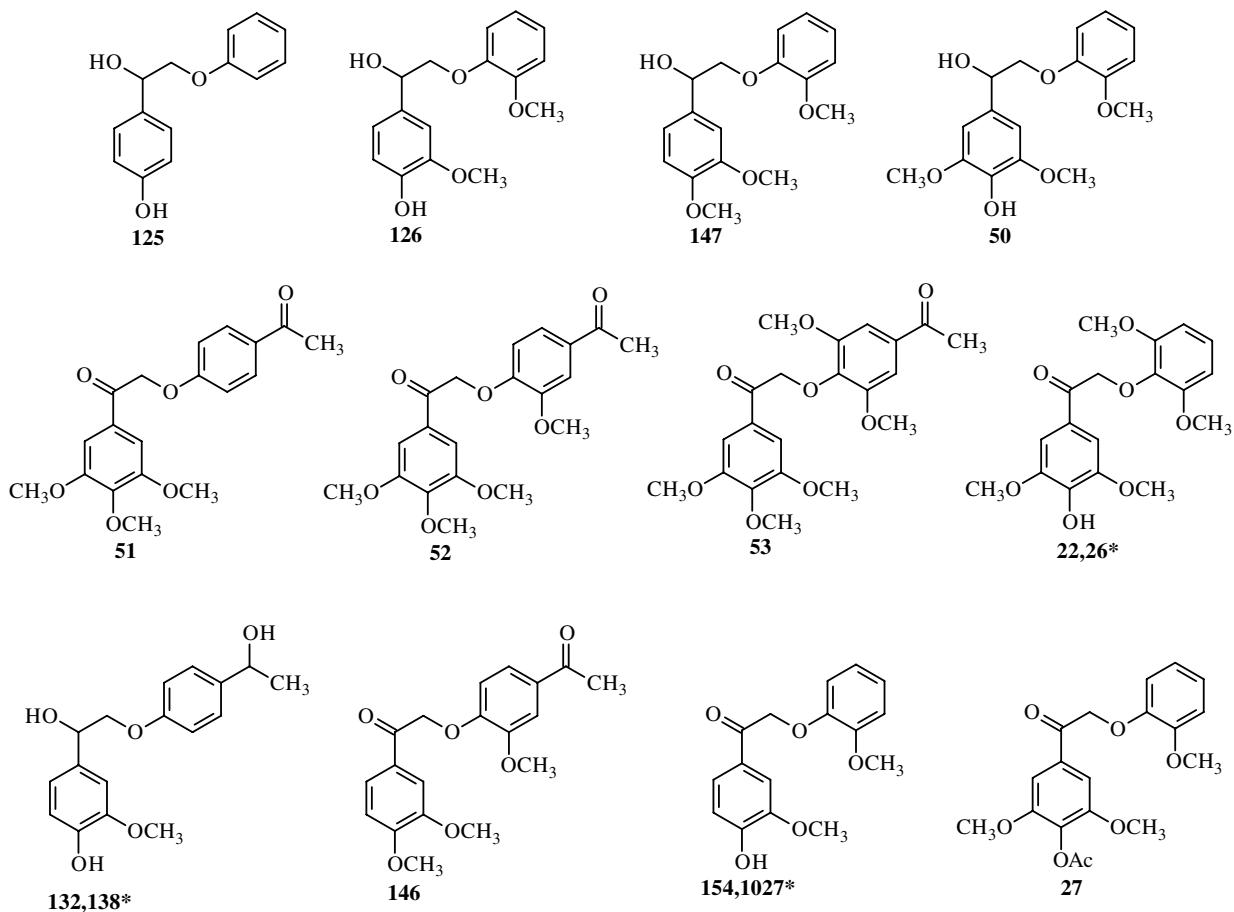
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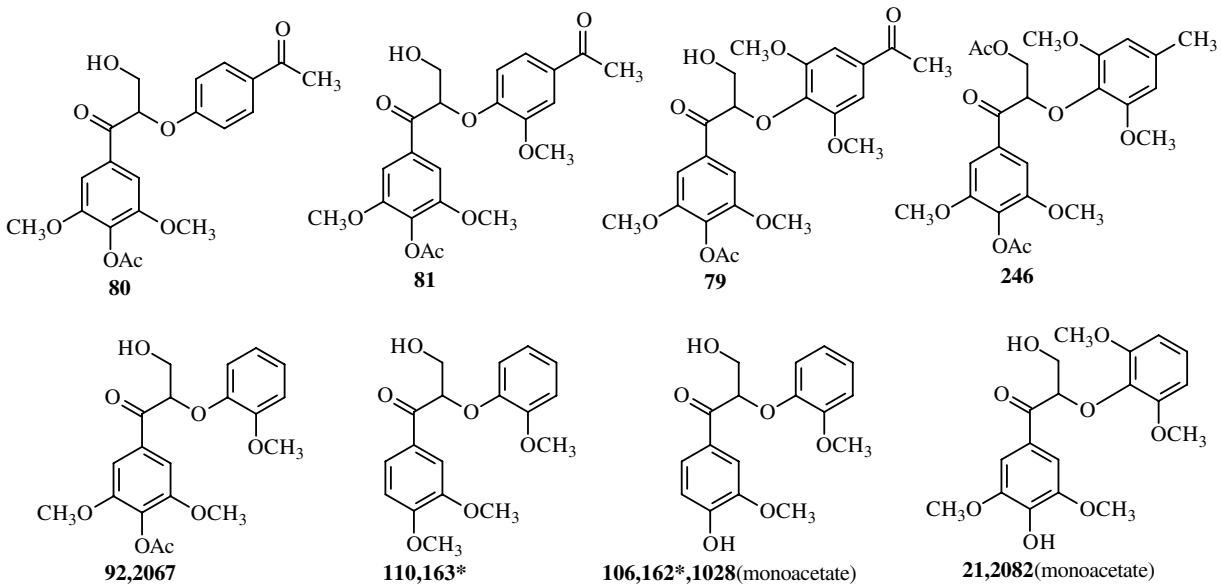
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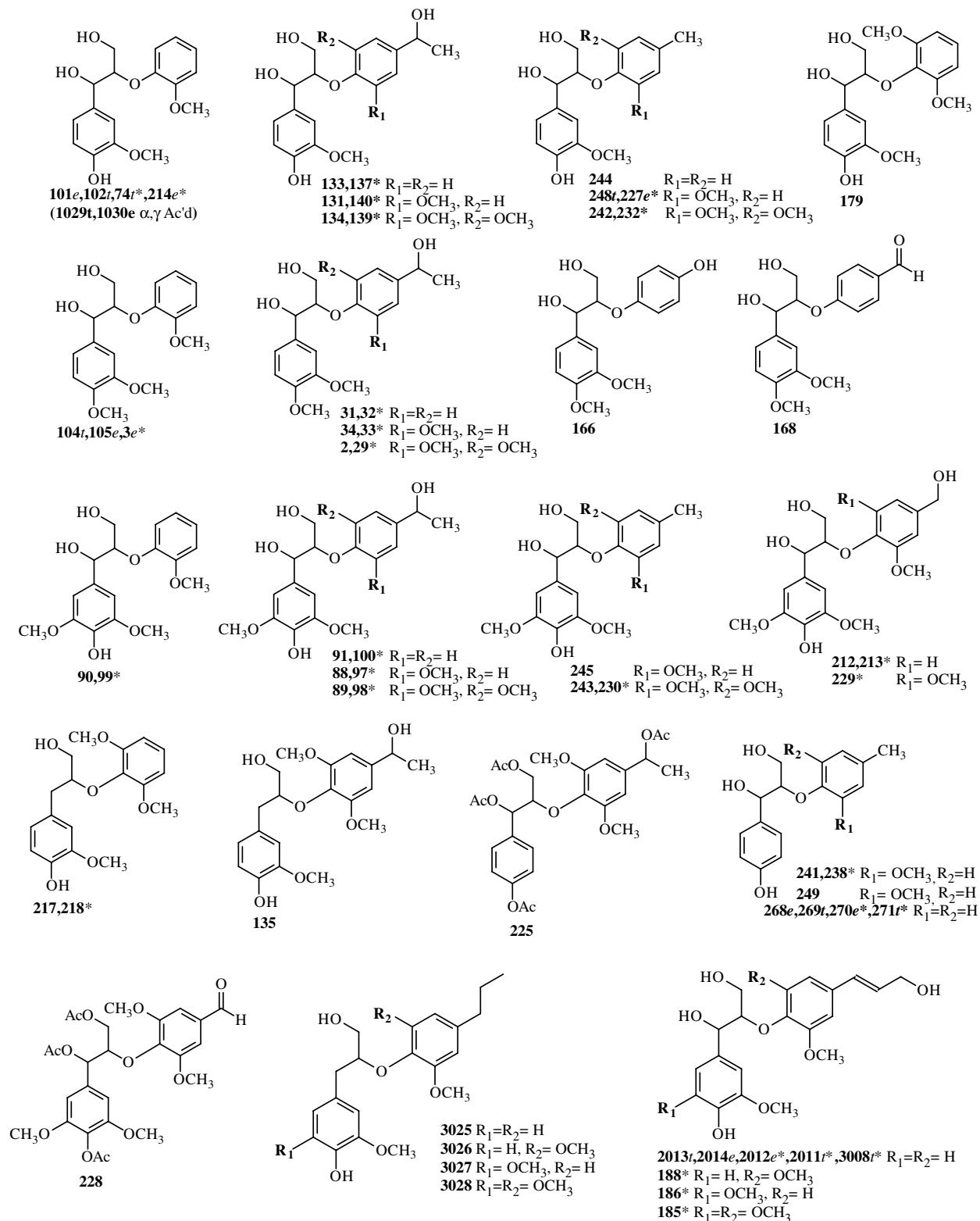
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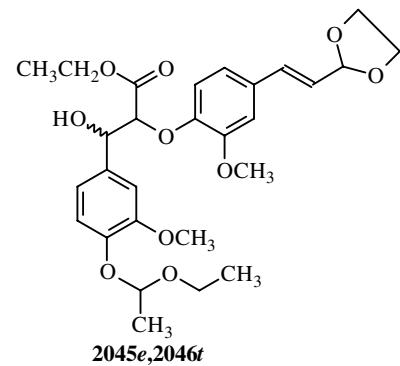
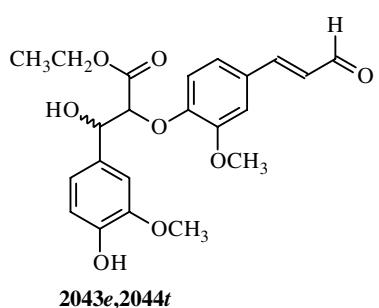
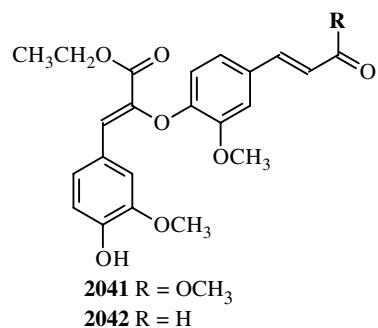
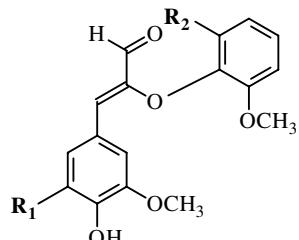
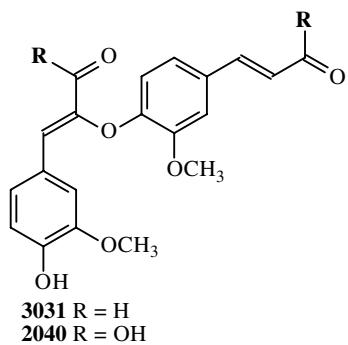
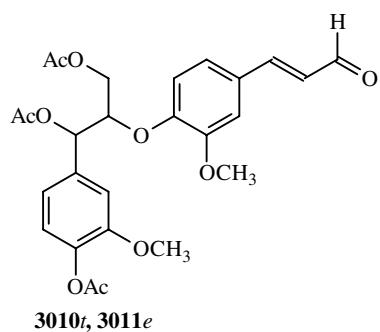
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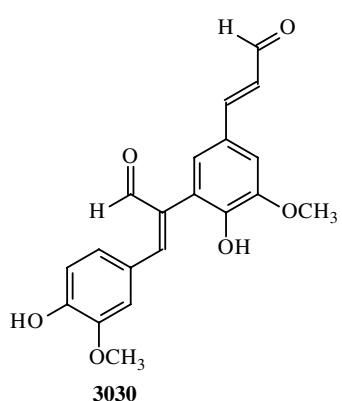
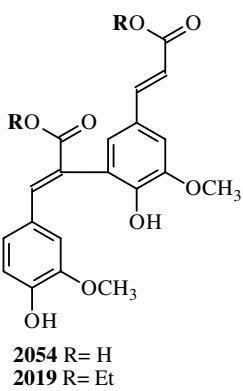
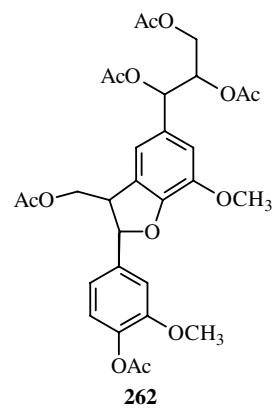
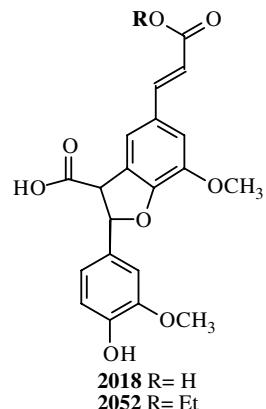
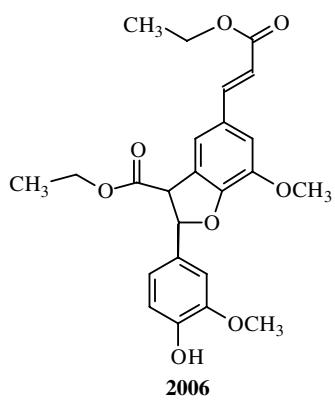
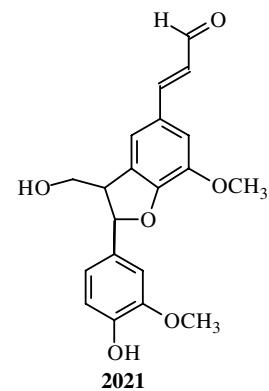
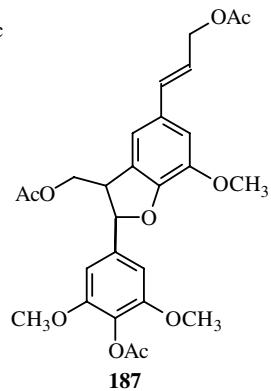
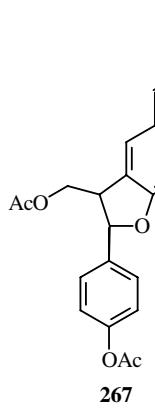
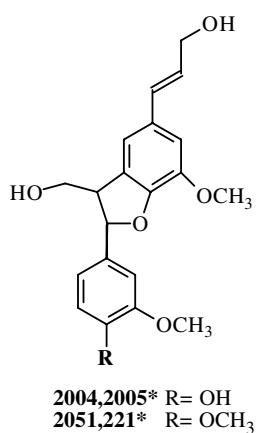
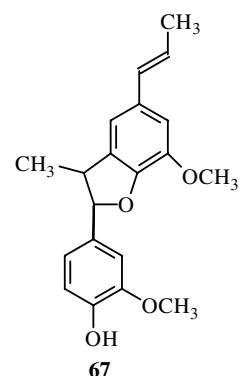
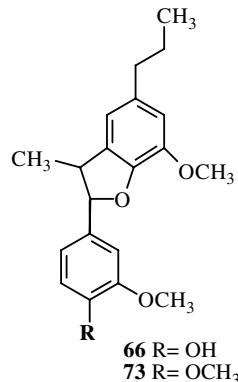
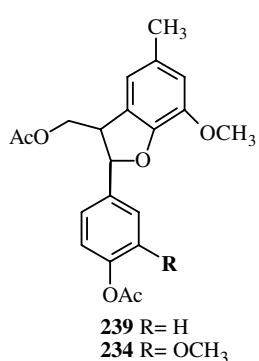
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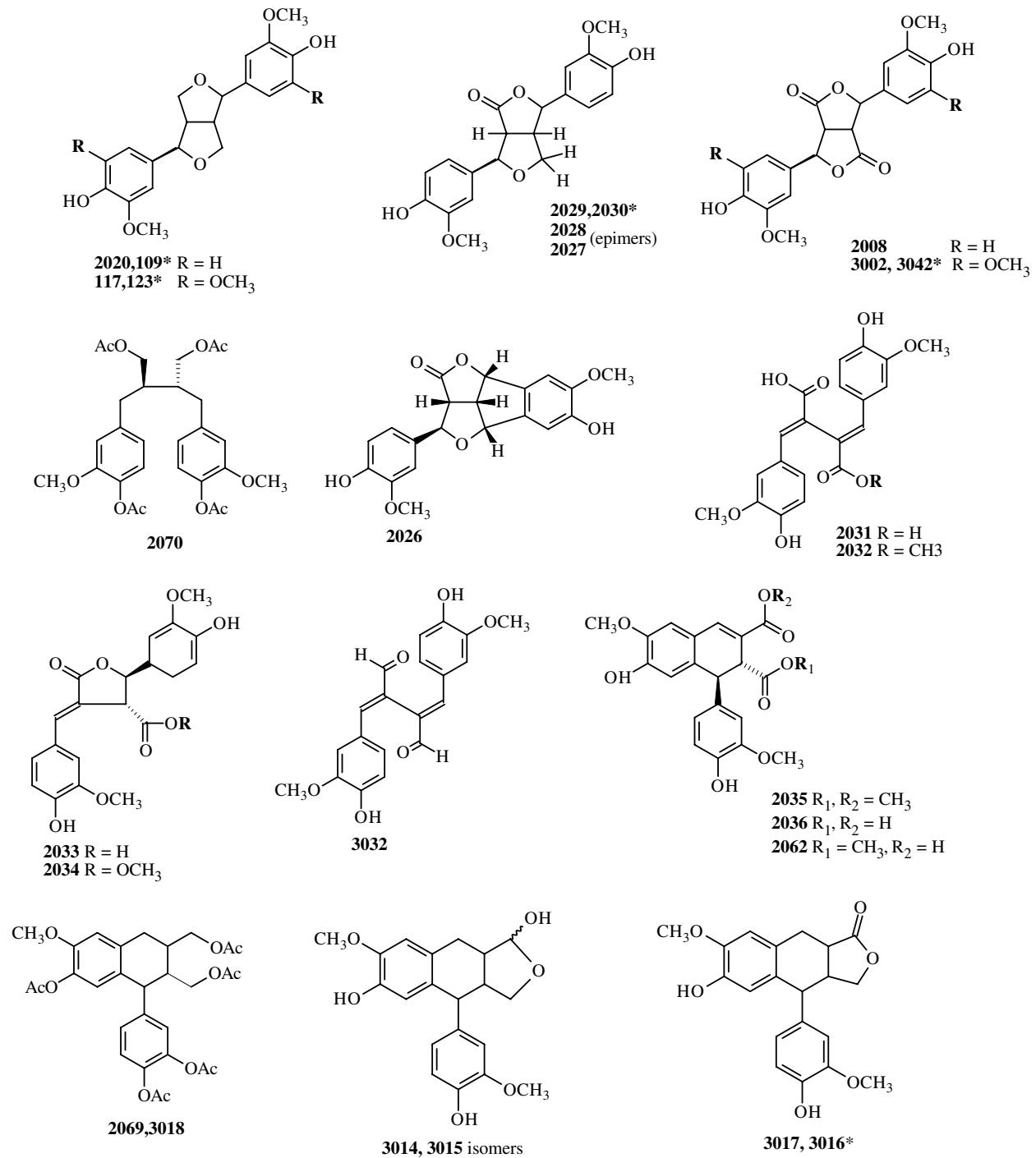
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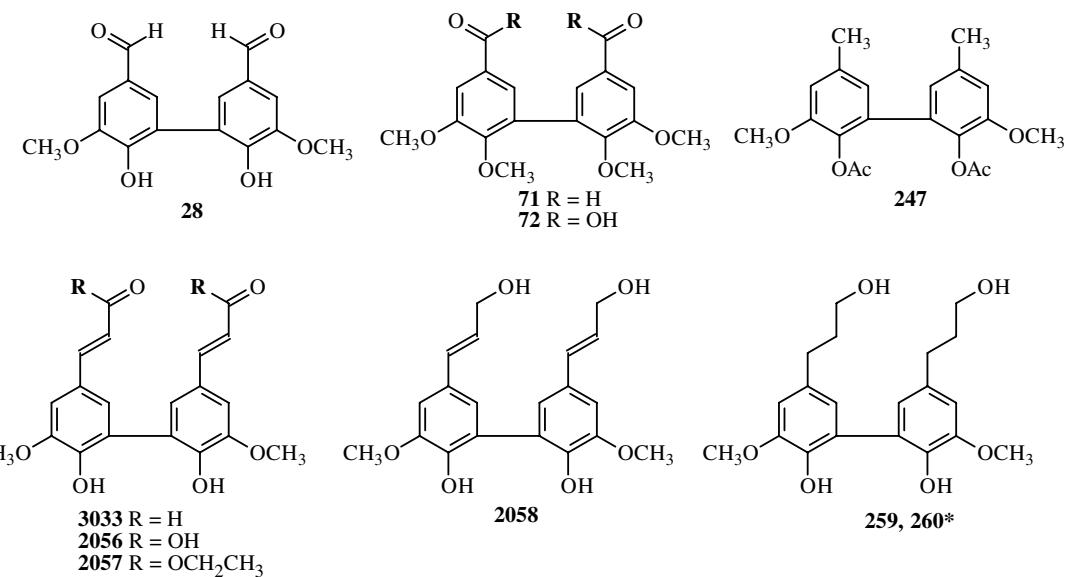
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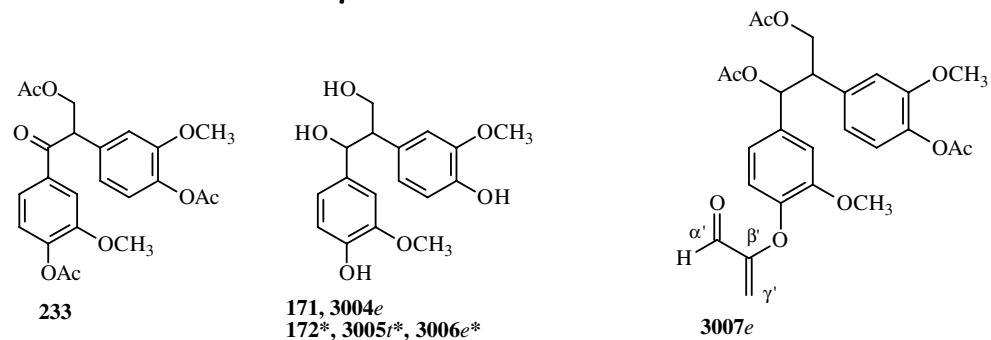
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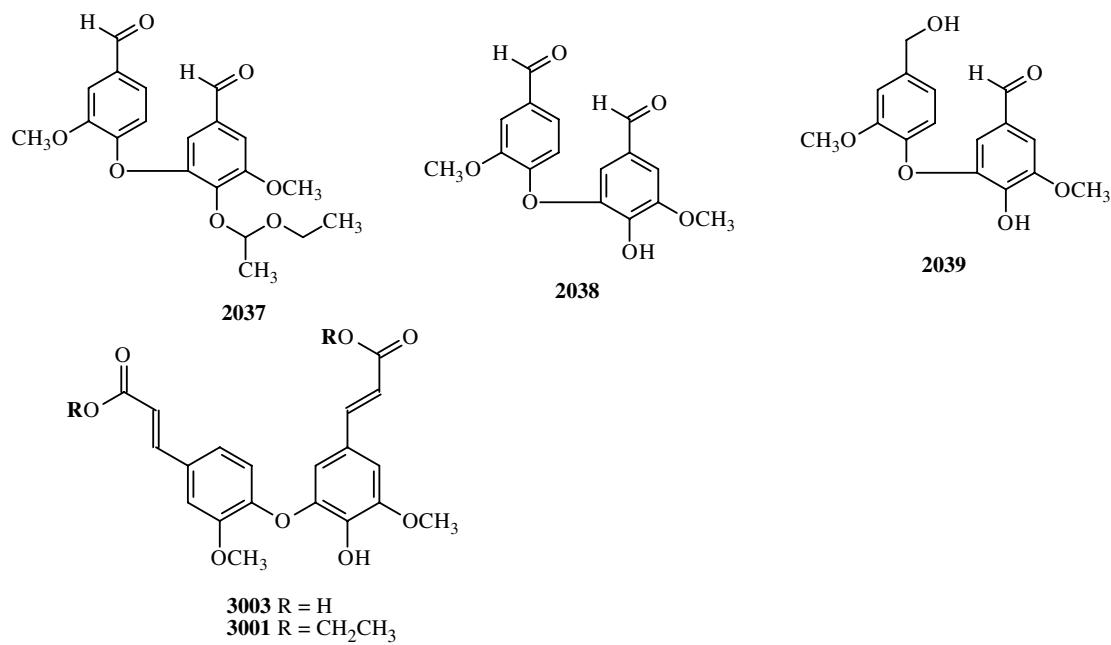
### 5-5 Dimers

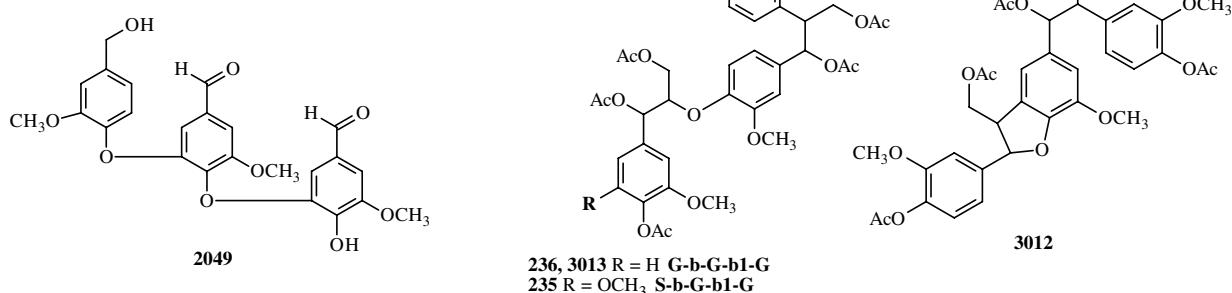
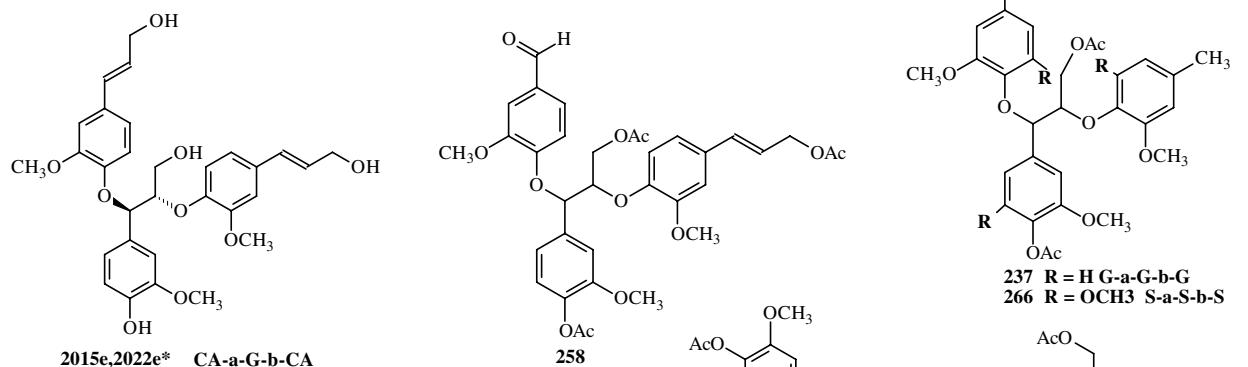
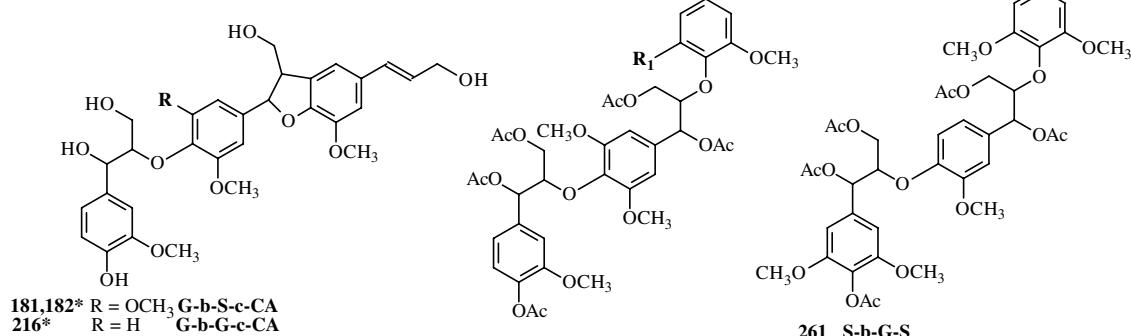
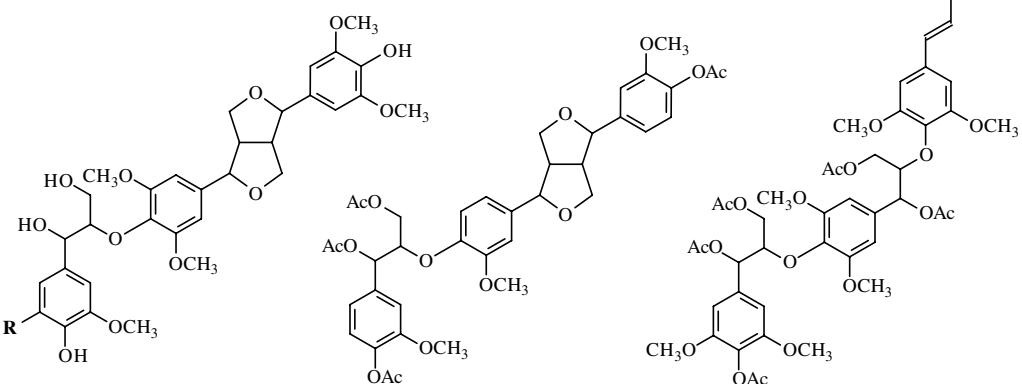


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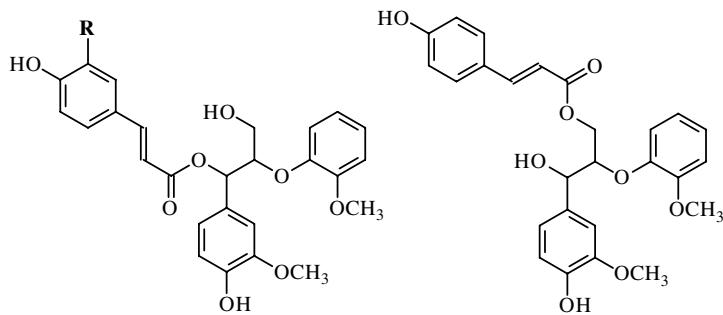


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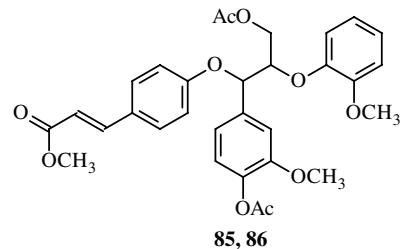
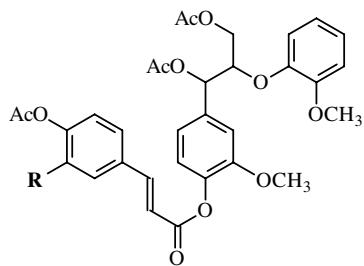
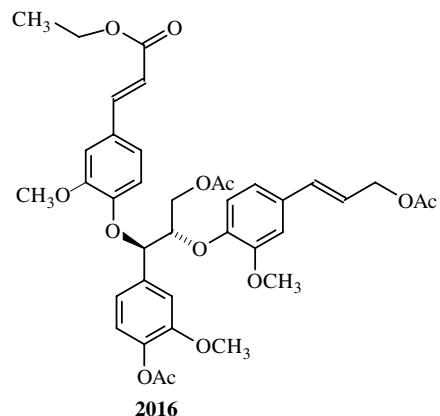
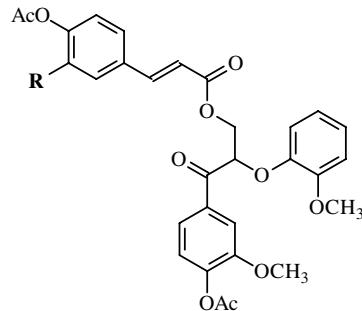
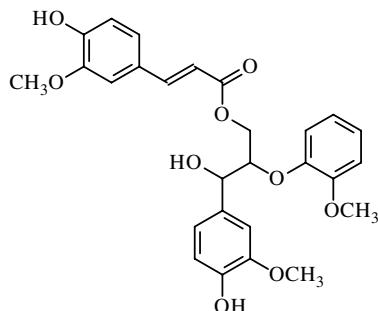


**Trimers**

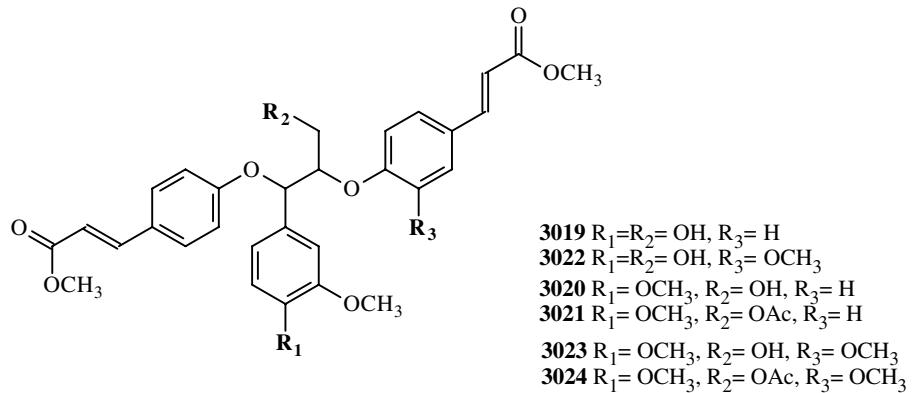
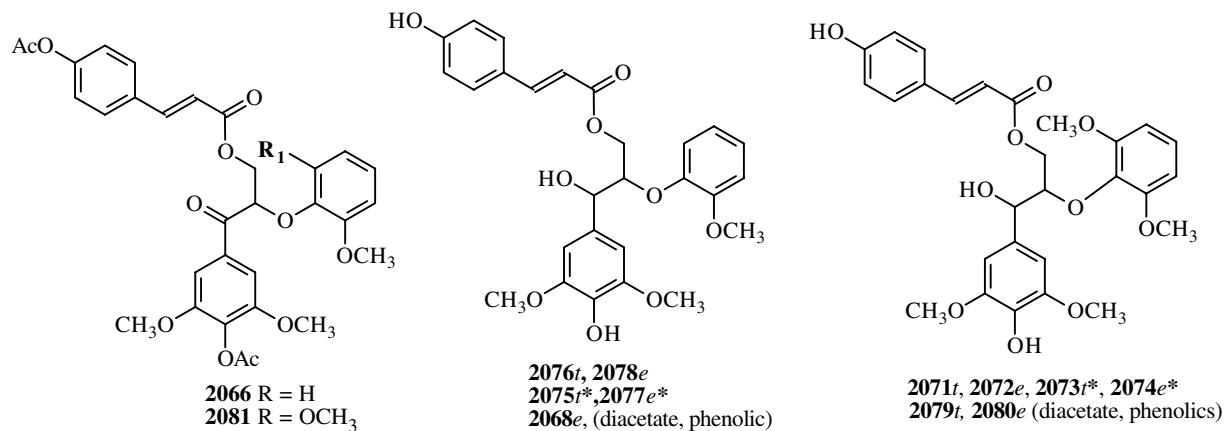
## Trimmers Containing Ferulic or Coumaric Acid



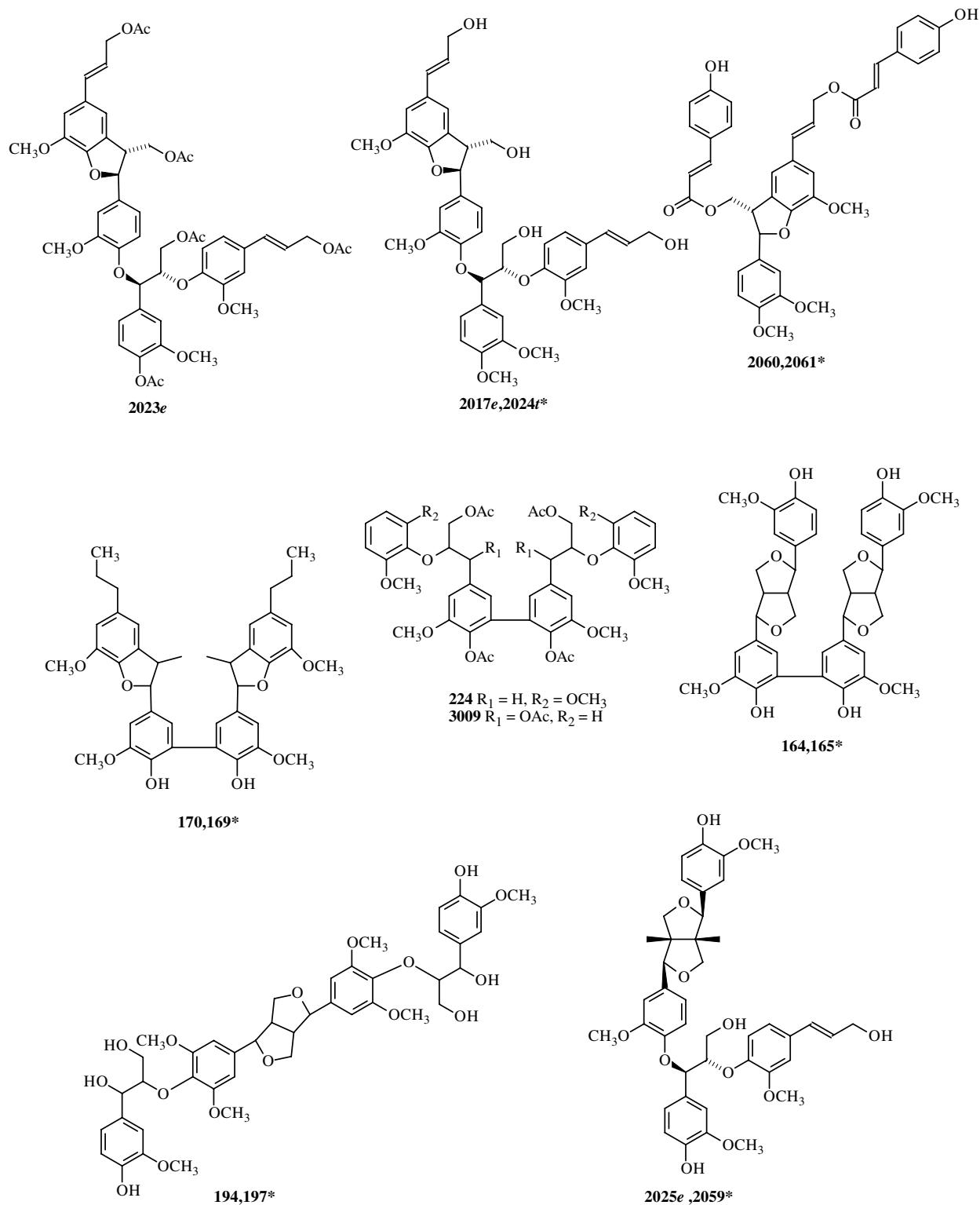
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1011*t*,1012*e* (diacetates, phenolic)**



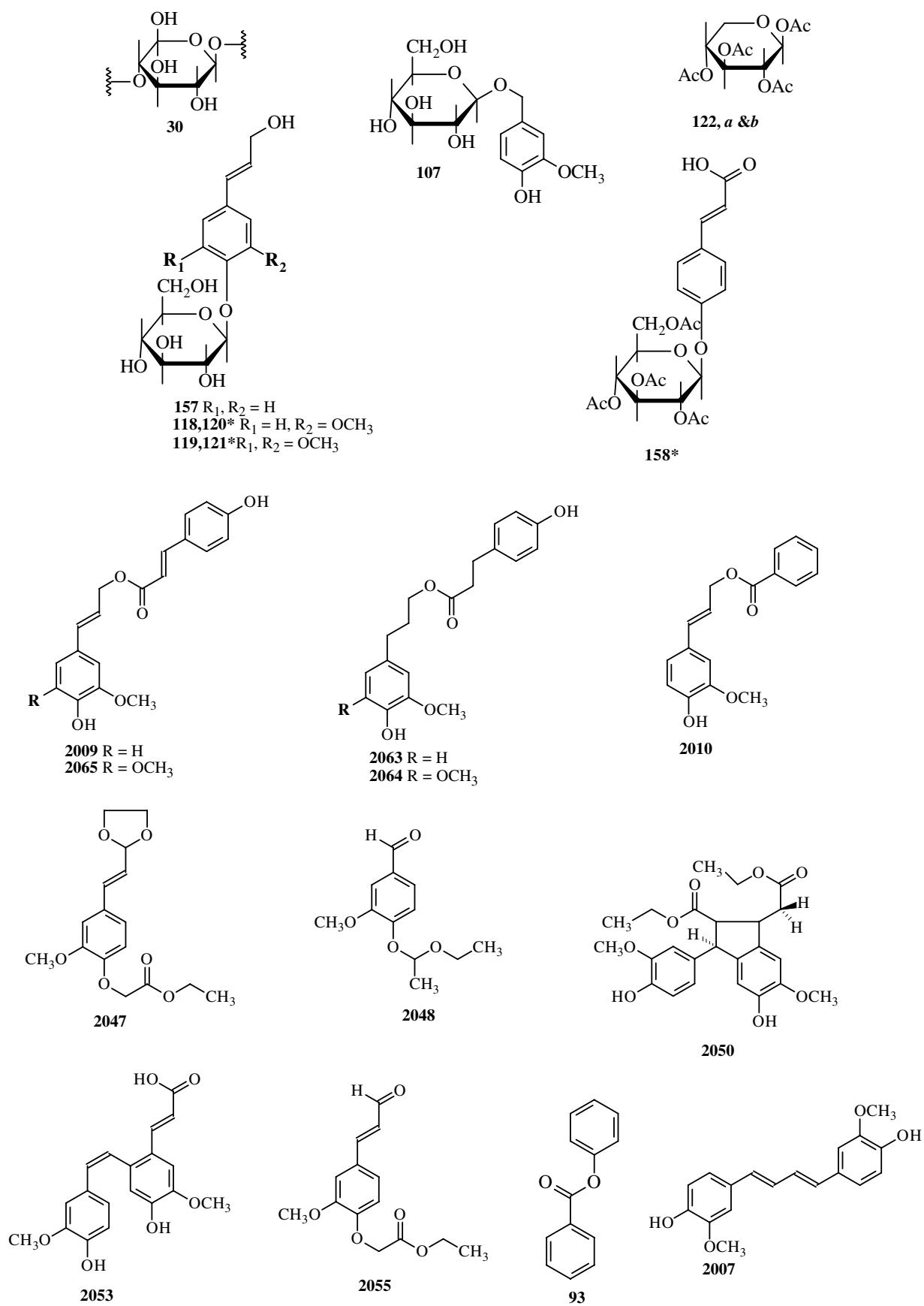
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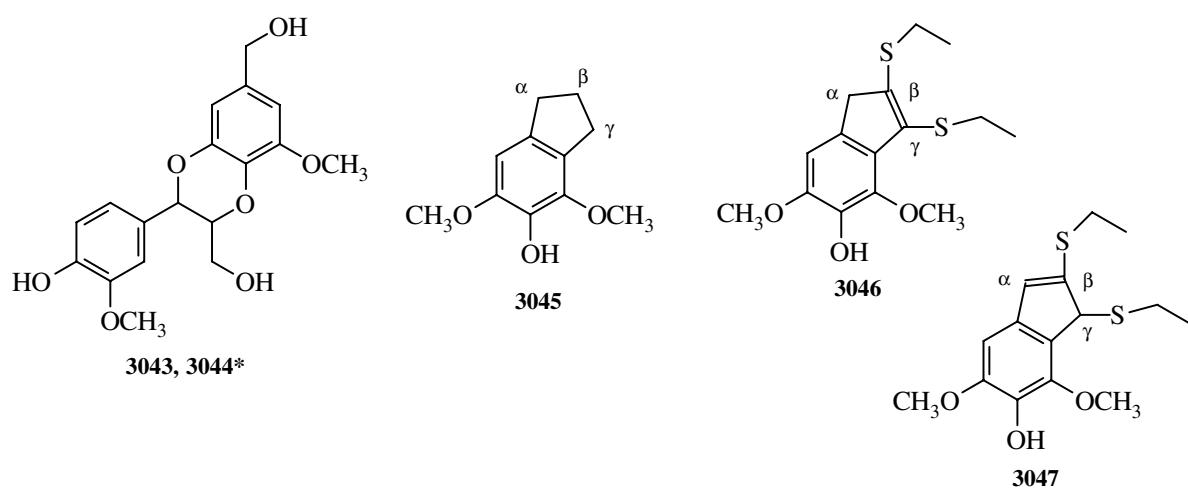
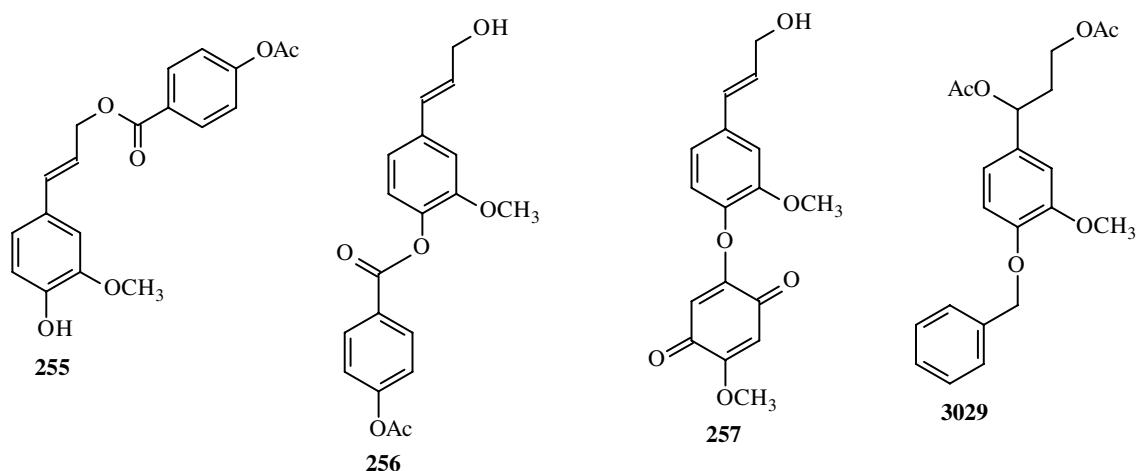
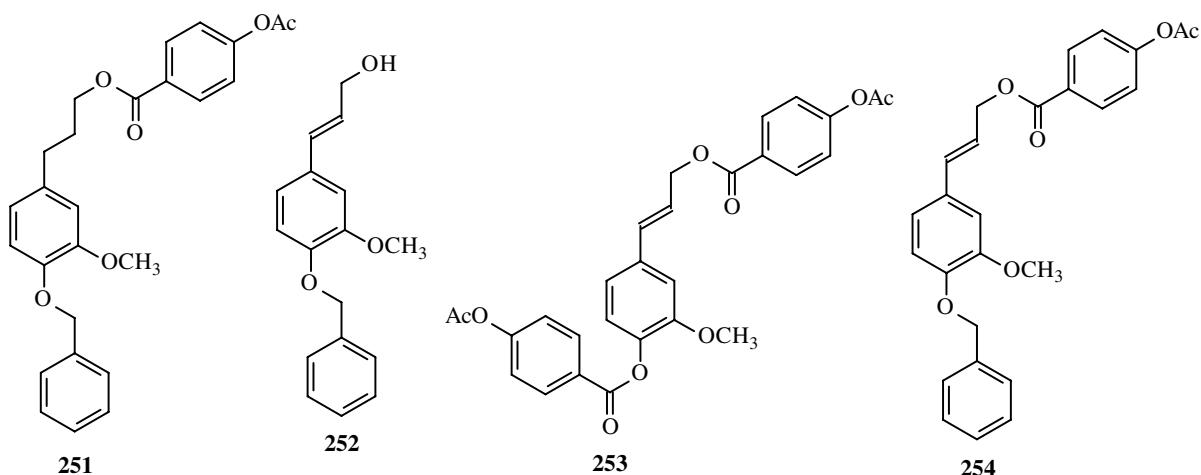


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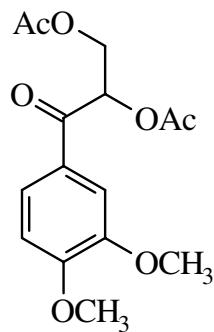
## Misc. Compounds



**Misc. Compounds**

**Compound Number** 1

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

**2,3-Diacetoxypipoveratrone**

**2,3-diacetoxyl-3',4'-dimethoxypropiophenone**

<sup>1</sup>H (chloroform)

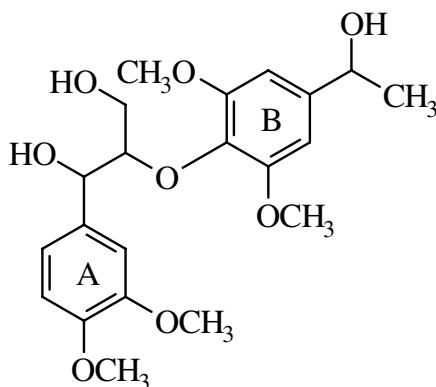
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Ac Me	2.08		
Ac Me	2.19		
OMe	3.95		
OMe	3.95		
γ1	4.25	dd	12.1, 7.9
γ2	4.68	dd	12.1, 3.1
β	6.18	dd	7.9, 3.1
A2	7.56	d	8.4
A5	6.93	dd	2.0
A6	7.71	dd	8.4, 2.0

**Notes:**

M. Mozuch #36/46/Ac  
21 mg

Compound Number 2

<sup>13</sup>C



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

<sup>1</sup>H (chloroform)

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

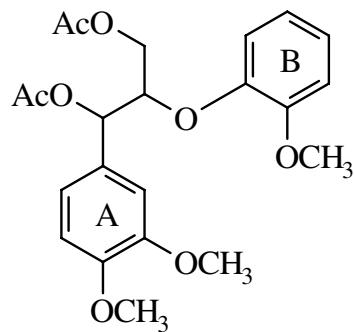
**Notes:**

S. Ralph III-12  
60mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$	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
$\gamma$	60.48	29	61.26	38	60.13	25
B $\alpha$	70.11	43	69.93	51	68.17	43
$\alpha$	73.98	39	73.89	45	71.36	32
$\beta$	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

<sup>13</sup>C



*erythro*

**Veratrylglycerol- $\beta$ -guaiacyl ether diacetate**  
1,3-diacetoxy-1-(3,4-dimethoxyphenyl)-2-(2-methoxyphenoxy)  
propane

<sup>1</sup>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	
$\gamma^1$	4.23	dd	11.0, 4.0
$\gamma^2$	4.43	dd	11.9, 5.9
$\alpha$	6.03	d	5.3
$\beta$	4.71	m	

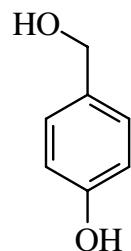
**Notes:**

L. Landucci  
51mg  
threo data  
in acetone  
 $\gamma$  63.8  
 $\alpha$  75.7  
 $\beta$  80.8

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\gamma$	62.82	38	63.23	44	62.10	33
$\alpha$	74.12	42	74.77	49	73.35	17
$\beta$	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

Compound Number 4

<sup>13</sup>C



p-Hydroxybenzyl alcohol  
4-hydroxybenzyl alcohol

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
$\alpha$	4.62	s	
3,5	6.82	m	
2,6	7.22	m	

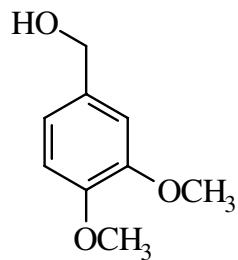
Notes:

J. Ralph: JR A91.11  
50mg  
Not very soluble in CDCl<sub>3</sub>

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
$\alpha$			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

<sup>13</sup>C



**3,4-Dimethoxybenzyl alcohol**  
**3,4-dimethoxybenzyl alcohol**

<sup>1</sup>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	

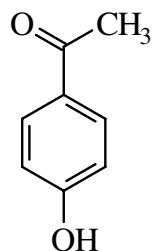
**Notes:**

J. Ralph: JR A91.14  
50mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C



**p-Hydroxyacetophenone**  
**4-hydroxyacetophenone**

<sup>1</sup>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

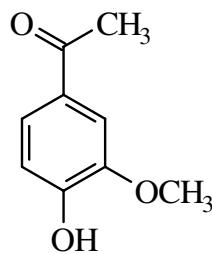
**Notes:**

J.Ralph: JR A95.11  
50mg

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



**Acetovanillone**  
**4-hydroxy-3-methoxyacetophenone**

<sup>1</sup>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	

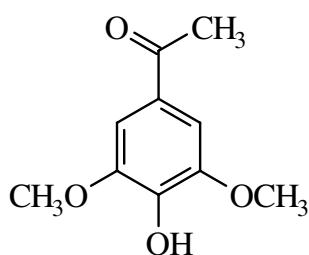
**Notes:**

J. Ralph: JR A95.12  
50mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C



**Acetosyringone**  
**3,5-dimethoxy-4-hydroxyacetophenone**

<sup>1</sup>H (chloroform)

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

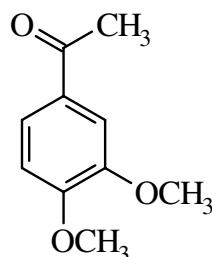
**Notes:**

J. Ralph: JR A95.13  
46mg

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



**Acetoveratrone  
3,4-dimethoxyacetophenone**

**<sup>1</sup>H** (chloroform)

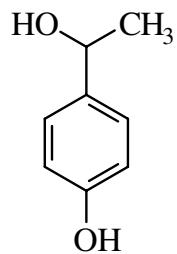
Atom	H Shifts	Mult	J
β	2.56	s	
OMe	3.93	s	
OMe	3.94	s	
2	7.52	d	2.0
5	6.90	d	8.4
6	7.57	dd	8.4, 2.0

**Notes:**

J. Ralph: JR A95.14  
55mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C

**1-(4-Hydroxyphenyl)ethanol**  
**1-(4-hydroxyphenyl)ethanol**

**<sup>1</sup>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

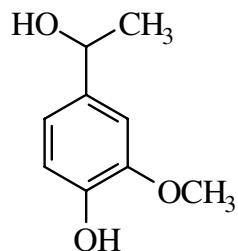
**Notes:**

J. Ralph: JR A97.11  
 34mg Almost insoluble in CDCl<sub>3</sub>

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



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

<sup>1</sup>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	

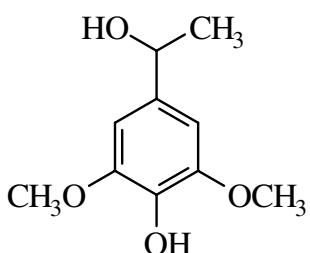
**Notes:**

J. Ralph: JR A97.12

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C



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

<sup>1</sup>H (chloroform)

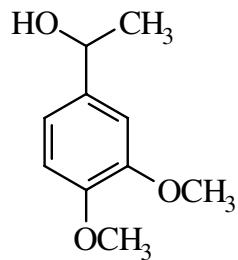
Atom	H Shifts	Mult	J
β	1.46	d	6.4
OMe	3.85	s	
OMe	3.85	s	
α	4.79	q	6.4
2,6	6.58		

Notes:

J. Ralph: JR A97.13

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C

**1-(3,4-Dimethoxyphenyl)ethanol**  
**1-(3,4-dimethoxyphenyl)ethanol**

<sup>1</sup>H (chloroform)

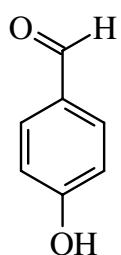
Atom	H Shifts	Mult	J
β	1.46	d	6.4
OMe	3.85	s	
OMe	3.87	s	
α	4.81	q	6.4
5	6.82		
6	6.85		
2	6.92	d	1.7

**Notes:**

J. Ralph: JR A97.14

Compound Number 14

<sup>13</sup>C



p-Hydroxybenzaldehyde  
4-hydroxybenzaldehyde

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
3,5	7.00	m	8.6
2,6	7.82	m	8.6
$\alpha$	9.85	s	

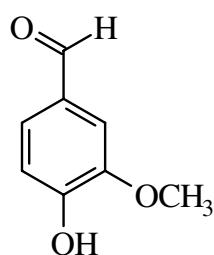
**Notes:**

J. Ralph: JR A87.11  
52mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\alpha$	191.28	39	191.02	35	190.80	42

**Compound Number**    **15**

**<sup>13</sup>C**



**Vanillin**  
**4-hydroxy-3-methoxybenzaldehyde**

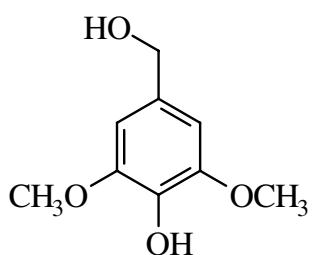
**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
OMe	3.92	s	
2	7.41	m	
5	7.04	d	8.6
6	7.44	m	
$\alpha$	9.81	s	

**Notes:**

J. Ralph: JR A87.12  
66mg

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\alpha$	191.16	47	191.07	85	190.89	82



**Syringyl alcohol**  
**4-hydroxy-3,5-dimethoxybenzyl alcohol**

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.88		
OMe	3.88		
$\alpha$	4.60	s	
2,6	6.60	s	

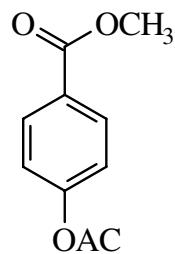
**Notes:**

J. Ralph: JR A91.13  
 20mg Almost insoluble in acetone.

Atom	CDCl <sub>3</sub>		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
$\alpha$	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**

**<sup>13</sup>C**



**Methyl 4-acetoxybenzoate**  
**4-acetoxybenzoic acid methyl ester**

**<sup>1</sup>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

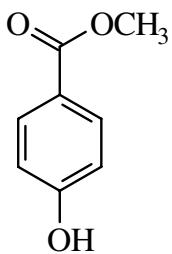
**Notes:**

L. Landucci  
53mg

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\alpha$	166.25	10	166.47	11	165.49	17
Ac C=O	168.79	11	169.23	11	168.72	20

Compound Number 18

<sup>13</sup>C



Methyl 4-hydroxybenzoate  
4-hydroxybenzoic acid methyl ester

<sup>1</sup>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

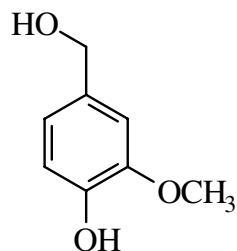
Notes:

Aldrich  
62mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\alpha$	167.53	10	167.07	5	166.05	14

**Compound Number**    **19**

**<sup>13</sup>C**



**4-Hydroxy-3-methoxybenzyl alcohol**  
**4-hydroxy-3-methoxybenzyl alcohol**

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
OMe	3.89	s	
$\alpha$	4.60	s	

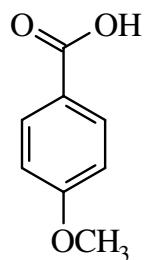
**Notes:**

Aldrich  
54mg

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
OMe	55.90	100	56.11	100	55.38	100
$\alpha$	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

<sup>13</sup>C



**p-Anisic acid**  
**4-methoxybenzoic acid**

<sup>1</sup>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

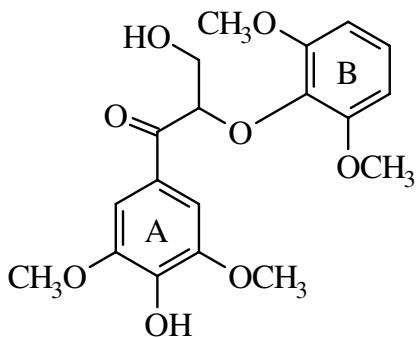
**Notes:**

Aldrich  
52mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\alpha$	171.45	16	167.54	13	167.00	29

Compound Number 21

<sup>13</sup>C



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

<sup>1</sup>H (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

**Notes:**

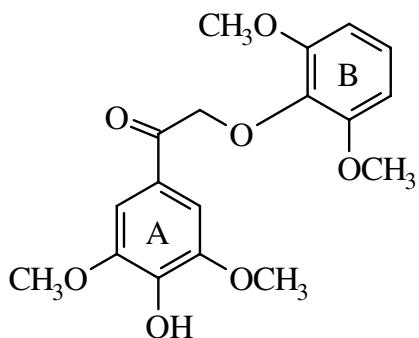
Has acetyl piperidine in sample.

J. Ralph JRA127.P1

27mg

γ - protons coupled to OH's, shifts not determined.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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



Atom	CDCl <sub>3</sub>		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

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

### <sup>1</sup>H (chloroform)

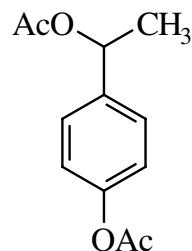
Atom	H Shifts	Mult	J
OMe	3.82	s	
OMe	3.94	s	
β	5.11	s	
A2,6	7.43	s	
B2,6	6.59	d	8.4
B1	7.03	t	8.4

### Notes:

J. Ralph JRA127.P2  
23mg

Compound Number 23

<sup>13</sup>C



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

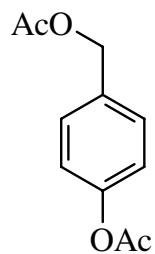
Atom	$\text{CDCl}_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.10	33	20.91	39	20.74	45
Ac Me	21.30	28	21.08	31	20.89	40
$\beta$	22.14	41	22.48	55	21.95	46
$\alpha$	71.68	42	72.03	51	71.01	53
3	121.57	100	122.53	99	121.70	100
5	121.57	100	122.53	99	121.70	100
2	127.31	100	127.84	100	126.99	96
6	127.31	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
$\alpha$ Ac C=O	170.21	13	170.16	11	169.54	15

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.24	s	
$\beta$	1.48	d	6.6
$\alpha$	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



**p-Hydroxybenzyl alcohol diacetate**  
**4-acetoxybenzyl acetate**

<sup>1</sup>H (chloroform)

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

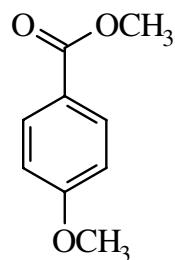
**Notes:**

S. Ralph SRIII-20  
52mg

Atom	CDCl <sub>3</sub>		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
$\alpha$	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
$\alpha$ Ac C=O	170.72	11	170.77	6	170.14	12

Compound Number 25

<sup>13</sup>C



Methyl-p-anisate  
methyl 4-methoxybenzoate

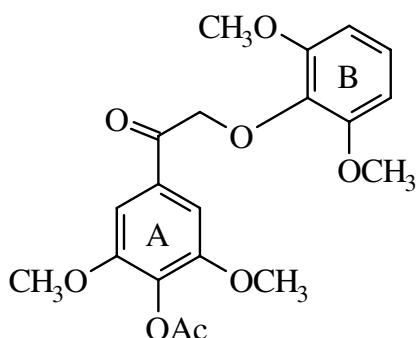
<sup>1</sup>H (chloroform)

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

Notes:

S. Ralph SRIII-21  
50mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
4 OMe	51.82	31	51.94	32	51.73	48
$\alpha$ 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
$\alpha$	166.82	8	166.84	6	165.88	14



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

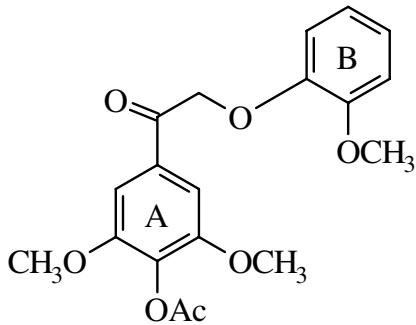
**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
A <sub>η</sub> Me	2.34	s	
B OM <sub>ε</sub>	3.80	s	
A OM <sub>ε</sub>	3.87	s	
β	5.13	s	
A <sub>2,6</sub>	7.40	s	
B <sub>2,6</sub>	6.58	d	8.4
B1	7.02	t	8.4

**Notes:**

J. Ralph GV 49.1  
25mg

Atom	CDCl <sub>3</sub>		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=O	168.11	23	168.15	16	167.60	32
α	194.03	28	194.58	24	193.75	40



Atom	$\text{CDCl}_3$		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
$\beta$	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
$\alpha$	193.77	25	194.35	20	193.70	42

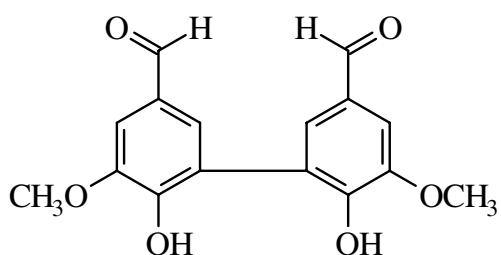
1-(4-acetoxy-3,5-dimethoxyphenyl)-2-(2-methoxyphenoxy)ethanone

<sup>1</sup>H (chloroform)

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

Notes:

J. Ralph GV 35.1  
25mg



Atom	CDCl <sub>3</sub>		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

**Dehydrodivanillin****6,6'-Dihydroxy-5,5'-dimethoxybiphenyl-3,3'-dicarbaldehyde****<sup>1</sup>H (DMSO)**

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

**Notes:**

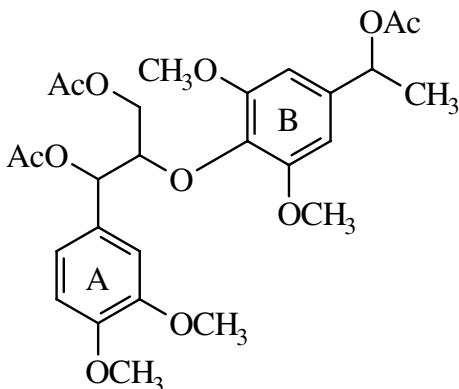
J. Ralph KM 77.1

25mg

contains impurities

As this compound has a plane of symmetry

The shifts for the other half are identical.



**Veratrylglycerol- $\beta$ -syringol ether triacetate**  
**1,3-diacetoxy-1-(3,4-dimethoxyphenyl)-2-(4-(1-acetoxyethyl)-**  
**2,6-dimethoxyphenoxy)propane**

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	1.92	s	
Ac Me	2.00	s	
Ac Me	2.07	s	
B $\beta$	1.51	d	
OMe	3.86	s	
OMe	3.86	s	
B OMe	3.80	s	
$\gamma^1$	-	-	
$\gamma^2$	4.29	dd	11.7, 3.6
B $\alpha$	5.79	q	6.6
$\alpha$	6.11	d	7.1
$\beta$	4.59	m	
B2,6	6.55	s	
A2	6.94	m	
A5	6.81	d	
A6	6.95	m	8.8

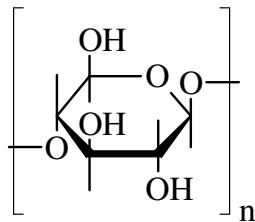
**Notes:**

S. Ralph III-14  
 65mg sample has impurities  
 $\gamma^1$  proton hidden by OMe's

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\beta$	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
$\gamma$	63.84	26	64.43	48	63.36	21
B $\alpha$	72.38	29	72.70	49	71.70	33
$\alpha$	76.01	45	76.69	51	75.65	22
$\beta$	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=O	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

<sup>13</sup>C



Xylan  
Xylan,Birch

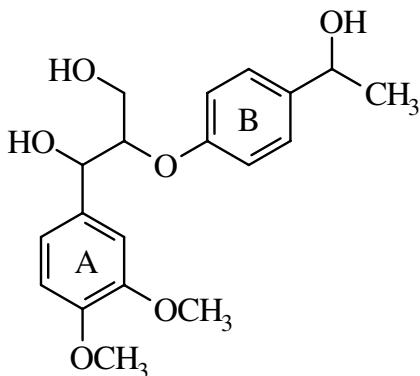
<sup>1</sup>H (DMSO)

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

Atom	<sup>CDCl</sup> <sub>3</sub>		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



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

<sup>1</sup>H (DMSO)

Atom	H Shifts	Mult	J
B $\beta$	1.28	d	
OMe	3.71	s	
OMe	3.71	s	
$\alpha$	5.36	d	5.1

**Notes:**

S. Ralph SR111-7

28mg

shifts for minor erythro isomer:

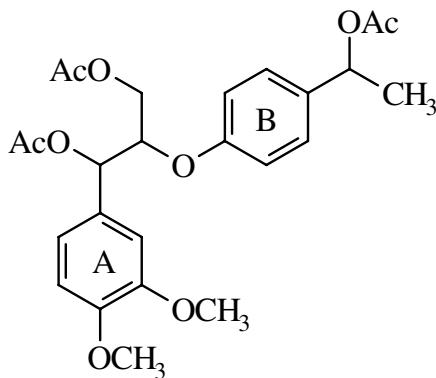
C A D

$\gamma$  61.46, 61.94, 59.92

$\alpha$  73.88, 73.81, 71.37

$\beta$  82.00, 83.67, 82.98

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$	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
$\gamma$	61.06	32	61.60	37	59.92	24
B $\alpha$	69.74	34	69.48	33	67.57	44
$\alpha$	73.47	27	73.18	41	70.77	41
$\beta$	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

*threo*

**1,3-diacetoxymethyl-2-[4-(1-acetoxyethyl)phenoxy]propane**

### <sup>1</sup>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	
γ <sup>1</sup>	4.00	dd	11.8, 6.2
γ <sup>2</sup>	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

shifts for minor erythro isomer:

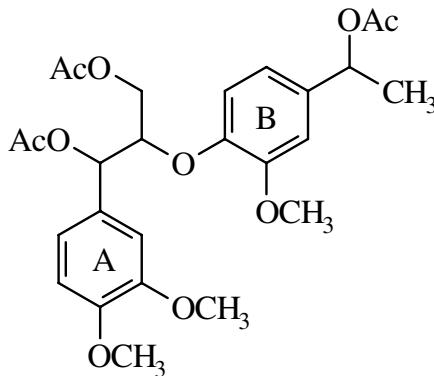
C A D

γ 62.59, 63.11, 61.88

α 73.95, 74.41, 72.92

β 78.43, 78.93, 76.96

Atom	CDCl <sub>3</sub>		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



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

**<sup>1</sup>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

Shifts for minor isomer:

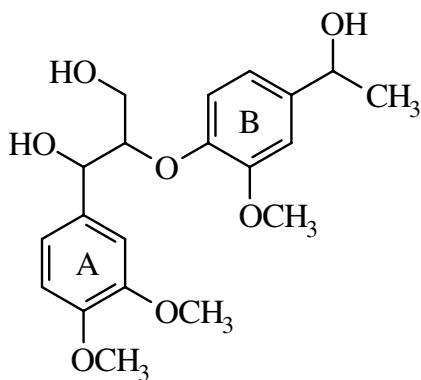
C A D

γ 62.74, 63.25, 62.04

α 74.08, 74.76, 73.25

β 79.98, 80.23, 78.29

Atom	CDCl <sub>3</sub>		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

*threo*

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$	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
$\gamma$	61.08	28	61.68	67	59.96	55
B $\alpha$	69.98	38	69.66	90	67.79	86
$\alpha$	73.84	32	73.62	67	70.72	50
$\beta$	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

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

### <sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
B $\beta$	1.46	d	6.4
OMe	3.86	s	
OMe	3.86	s	
OMe	3.86	s	
B $\alpha$	4.83	q	
$\alpha$	4.94	d	7.7
$\beta$	4.01	m	
$\gamma$ 1	3.46	mm	
$\gamma$ 2	3.60	dd	

### Notes:

S. Ralph SR III-15

28mg

shifts for minor isomer:

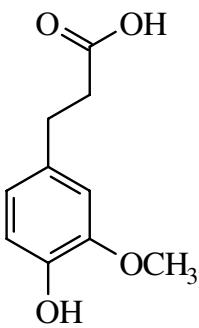
C A D

 $\gamma$  60.82, 61.68, 59.96 $\alpha$  72.78, 73.62, 71.51

b 87.01, 86.50, 83.82

**Compound Number**    **35**

**<sup>13</sup>C**



Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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

**Dihydroferulic Acid**

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

**<sup>1</sup>H** (chloroform)

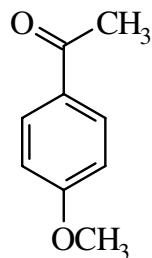
Atom	H Shifts	Mult	J
α	2.64	t	7.4
b	2.88	t	7.4
OMe	3.84	s	
2	6.71	m	
5	6.82	d	7.6
6	6.69	m	

**Notes:**

J. Obst  
35mg

Compound Number 36

<sup>13</sup>C



**4-Methoxyacetophenone**  
**4-methoxyacetophenone**

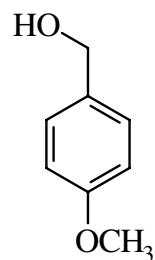
**<sup>1</sup>H** (chloroform)

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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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



**p-Methoxybenzyl alcohol**  
**4-methoxybenzyl alcohol**

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.75	s	
α	4.51	s	
3,5	6.86	m	87
2,6	7.20	m	87

**Notes:**

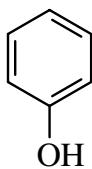
Aldrich  
65mg

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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



**Phenol**  
**phenol**

<sup>1</sup>H (chloroform)

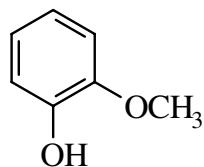
Atom	H Shifts	Mult	J
3,5	6.84	m	
1	6.93	m	
2,6	7.22	m	

**Notes:**

Aldrich JR 85-11  
54mg

Compound Number 39

<sup>13</sup>C



**Guaiacol**  
**2-methoxyphenol**

<sup>1</sup>H (chloroform)

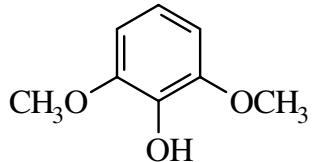
Atom	H Shifts	Mult	J
OMe	3.83	s	
OH	5.72	s	

**Notes:**

Aldrich JR A85.12  
54mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

Syringol  
2,6-dimethoxyphenol

<sup>1</sup>H (chloroform)

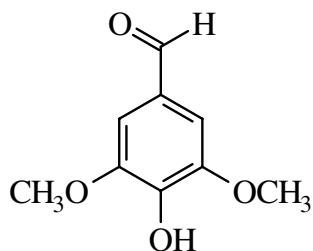
Atom	H Shifts	Mult	J
OMe	3.86	s	
OMe	3.86	s	
2,6	6.56	d	8.1
1	6.78	t	8.1

## Notes:

Aldrich JR A 85.13  
56mg

Compound Number 41

<sup>13</sup>C



Syringaldehyde  
3,5-dimethoxy-4-hydroxybenzaldehyde

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.95	s	
2,6	7.15	s	
$\alpha$	9.81	s	

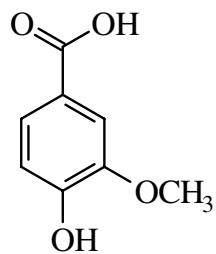
Notes:

J. Ralph JRA87.13  
62mg  
Poor solubility

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\alpha$	190.79	52	191.05	45	190.99	38

Compound Number 42

<sup>13</sup>C



**Vanilllic acid**  
**4-hydroxy-3-methoxy benzoic acid**

**<sup>1</sup>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

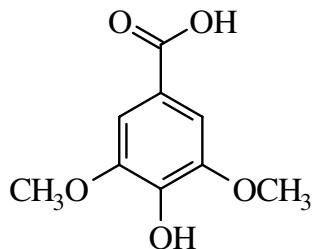
55mg

not very soluble in CDCl<sub>3</sub>

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



Syringic acid  
3,5-dimethoxy-4-hydroxybenzoic acid

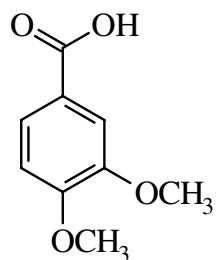
<sup>1</sup>H (chloroform)

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 CDCl<sub>3</sub>

Atom	CDCl <sub>3</sub>		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



**Veratric acid**  
**3,4-dimethoxybenzoic acid**

<sup>1</sup>H (chloroform)

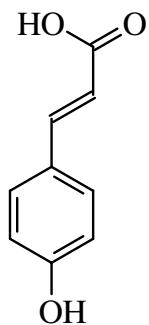
Atom	H Shifts	Mult	J
OMe	3.94	s	
OMe	3.95	s	
2	7.60	d	1.9
5	6.92	d	8.5
6	7.78	dd	8.5, 1.9

**Notes:**

J. Ralph JRA 89-14  
55mg

Atom	CDCl <sub>3</sub>		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
$\alpha$	172.08	50	167.53	28	167.08	55

## Compound Number 45

<sup>13</sup>C

**p-Coumaric acid**  
**4-hydroxycinnamic acid**

<sup>1</sup>H (DMSO)

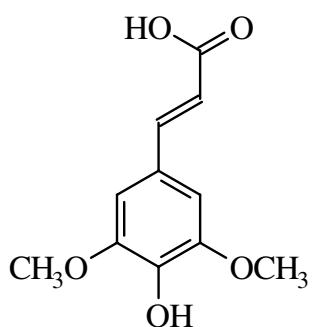
Atom	H Shifts	Mult	J
$\alpha$	7.54	d	16.0
3,5	6.83	d	8.6
2,6	7.53	d	8.6
$\beta$	6.32	d	16.0

**Notes:**

Fluka  
60mg  
\*not soluble in CDCl<sub>3</sub>

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
$\beta$			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
$\alpha$			145.95	45	144.11	43
4			160.49	26	159.54	43
$\gamma$			169.03	19	167.90	39

## Compound Number 46

<sup>13</sup>C

**Sinapinic acid**  
**3,5-dimethoxy-4-hydroxycinnamic acid**

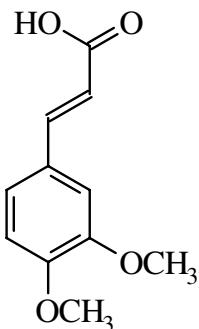
<sup>1</sup>H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.83	s	
2,6	7.00	s	
$\alpha$	7.50	d	15.9
$\beta$	6.44	d	15.9

**Notes:**

Lancaster Synthesis  
 60mg \*not very soluble in CDCl<sub>3</sub>

Atom	CDCl <sub>3</sub>		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
$\beta$			116.20	50	116.03	37
1			126.19	22	124.59	38
4			139.43	22	138.05	38
$\alpha$			146.23	58	144.74	39
3			148.90	44	148.00	79
5			148.90	44	148.00	79
$\gamma$			168.26	28	167.90	45



**3,4-Dimethoxycinnamic acid**  
**3,4-dimethoxycinnamic acid**

<sup>1</sup>H (chloroform)

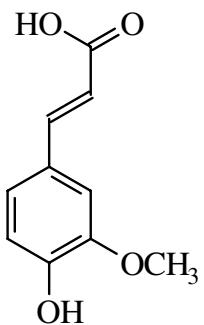
Atom	H Shifts	Mult	J
OMe	3.92	s	
OMe	3.92	s	
2	7.08	d	2.0
5	6.88	d	8.3
6	7.14	dd	8.3, 2.0
$\alpha$	7.73	d	15.9
$\beta$	6.33	d	15.9

**Notes:**

K & K Labs  
60mg

Atom	CDCl <sub>3</sub>		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
$\beta$	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
$\alpha$	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
$\gamma$	172.53	77	168.11	27	167.83	71

## Compound Number 48

<sup>13</sup>C*trans*

**Ferulic acid**  
**4-hydroxy-3-methoxycinnamic acid**

<sup>1</sup>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
$\alpha$	7.53	d	15.9
$\beta$	6.39	d	15.9

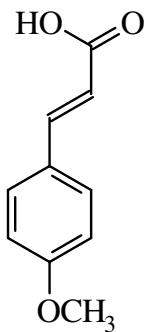
**Notes:**

Aldrich  
60mg not very soluble in CDCl<sub>3</sub>  
Note: .0238 was run in d4-MeOH.  
56.44, 111.71, 115.89, 116.46, 123.94  
127.77, 146.89, 149.30, 150.43, 170.93

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.28	98	55.64	100
2			111.30	95	111.14	74
$\beta$			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
$\alpha$			146.16	100	144.44	71
3			148.64	46	147.87	79
4			149.97	51	149.04	81
$\gamma$			168.88	60	167.93	76

Compound Number 49

<sup>13</sup>C



*trans*

**4-Methoxycinnamic acid**  
**4-methoxycinnamic acid**

<sup>1</sup>H (chloroform)

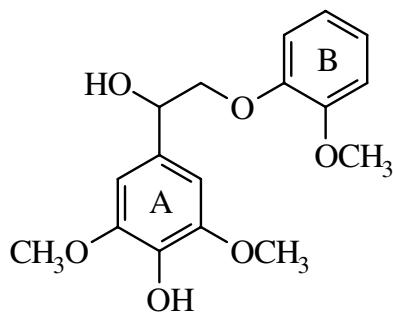
Atom	H Shifts	Mult	J
OMe	3.85	s	
3,5	6.92	m	8.8
$\alpha$	7.75	d	15.9
2,6	7.51	m	8.8
$\beta$	6.32	d	15.9

**Notes:**

Aldrich  
66mg not CDCl<sub>3</sub> soluble

Compound Number 50

<sup>13</sup>C



Syringylglycol- $\beta$ -guaiacyl ether  
1-(3,5-dimethoxy-4-hydroxyphenyl)-2-(2-methoxyphenoxy)  
ethanol

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
B OMe	3.85	s	
A OMe	3.87	s	
$\alpha$	5.00	dd	9.9, 3.0
$\beta 1$	3.94	t	9.9
$\beta 2$	4.14	dd	9.9, 3.0
A2,6	6.66		

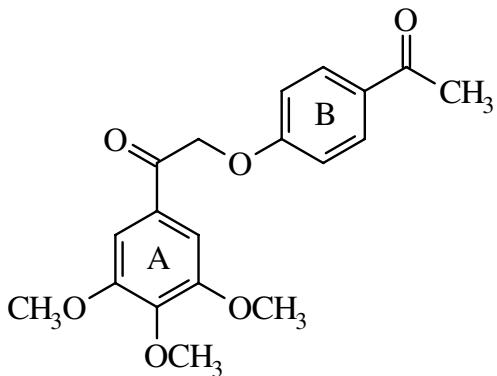
Notes:

S. Ralph SG 100mg  
33mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\alpha$	72.47	54	72.85	51	70.97	47
$\beta$	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**

**<sup>13</sup>C**



Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
B $\beta$	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
$\beta$	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
$\alpha$	192.49	32	193.05	24	192.70	37
B $\alpha$	196.55	19	196.23	16	196.12	35

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

**<sup>1</sup>H** (chloroform)

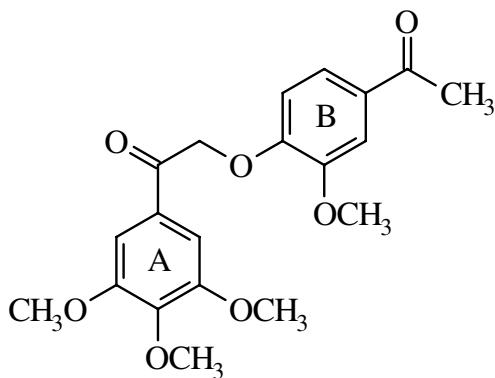
Atom	H Shifts	Mult	J
B $\beta$	2.54	s	
A3,5 OMe	3.92	s	
A4 OMe	3.94	s	
$\beta$	5.32	s	
A2,6	7.26	s	
B3,5	6.96	m	8.9
B2,6	7.92	m	8.9

**Notes:**

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

Compound Number 52

<sup>13</sup>C



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

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
B $\beta$	2.54	s	
B OMe	3.95	s	
A3,5 OMe	3.92	s	
A4 OMe	3.93	s	
$\beta$	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

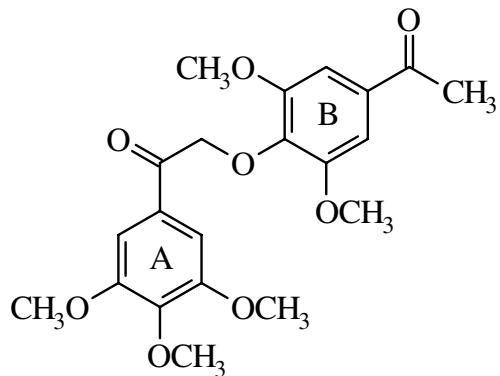
Notes:

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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$	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
$\beta$	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
$\alpha$	192.68	25	193.34	22	192.76	36
B $\alpha$	196.64	25	196.32	19	196.19	36

Compound Number 53

<sup>13</sup>C



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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$	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
$\beta$	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
$\alpha$	193.28	15	193.81	22	193.11	35
B $\alpha$	196.71	14	196.70	19	196.61	28

<sup>1</sup>H (chloroform)

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

Notes:

L. Landucci LLL XVII 9d  
37mg

Compound Number 54

<sup>13</sup>C

**Anisole**  
**Methoxybenzene**

**<sup>1</sup>H** (chloroform)

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

**Notes:**

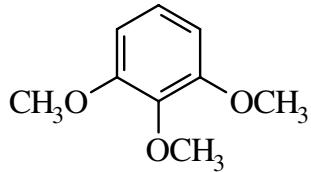
Aldrich  
40mg

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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



1,2,3-trimethoxybenzene

<sup>1</sup>H (chloroform)

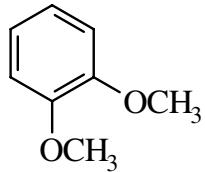
Atom	H Shifts	Mult	J
3,5 OMe	3.85	s	
4 OMe	3.85	s	
2,6	6.57	d	8.3
1	6.98	t	8.3

Notes:

Aldrich  
40mg

Compound Number 56

<sup>13</sup>C



**Veratrole**  
**1,2-dimethoxybenzene**

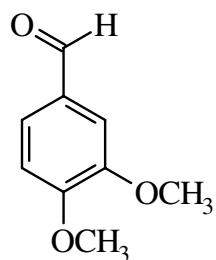
<sup>1</sup>H (chloroform)

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

**Notes:**

Aldrich  
40mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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



**Veratraldehyde**  
**3,4-dimethoxybenzaldehyde**

**<sup>1</sup>H** (chloroform)

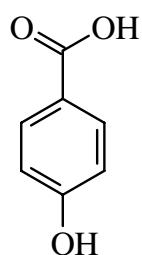
Atom	H Shifts	Mult	J
OMe	3.94	s	
OMe	3.97	s	
2	7.41	d	1.8
5	6.98	d	8.2
6	7.46	dd	8.2, 1.8
$\alpha$	9.85	s	

**Notes:**

Aldrich  
40mg

Compound Number 58

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

4-hydroxybenzoic acid

### <sup>1</sup>H (DMSO)

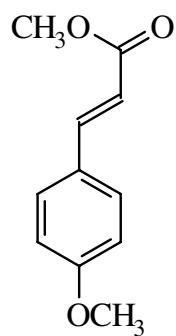
Atom	H Shifts	Mult	J
3,5	6.85	m	8.8
2,6	7.83	m	8.8

### Notes:

Aldrich  
40mg      \*CDCl<sub>3</sub> insoluble

Compound Number 59

<sup>13</sup>C



methyl (4-methoxy)cinnamate

<sup>1</sup>H (chloroform)

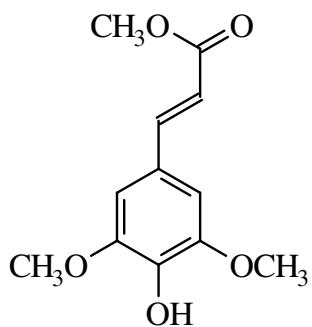
Atom	H Shifts	Mult	J
$\gamma$ OMe	3.79	s	
4 OMe	3.82	s	
2,6	7.46	m	88
$\alpha$	7.65	d	160
3,5	6.89	m	88
$\beta$	6.31	d	160

Notes:

J. Ralph PS 137x1  
95mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
$\gamma$ 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	<b>100</b>
5	114.34	98	115.14	98	114.36	100
$\beta$	115.30	41	115.96	43	115.09	51
1	127.14	21	127.84	17	126.65	36
2	129.71	<b>100</b>	130.63	<b>100</b>	130.08	89
6	129.71	100	130.63	100	130.08	89
$\alpha$	144.49	49	145.04	45	144.28	45
4	161.42	17	162.42	14	161.17	32
$\gamma$	167.68	18	167.81	15	166.90	23

Compound Number 60

<sup>13</sup>C

**Methyl Sinapate**  
methyl (3,5-dimethoxy-4-hydroxy)cinnamate

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
γOMe	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

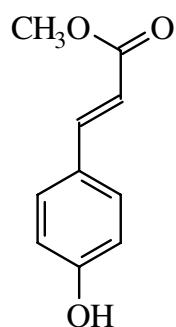
**Notes:**

J. Ralph JRPS 135x1  
52mg

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
γOMe	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

<sup>13</sup>C



*trans*

Methyl p-Coumarate  
methyl 4-hydroxycinnamate

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
γOMe	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

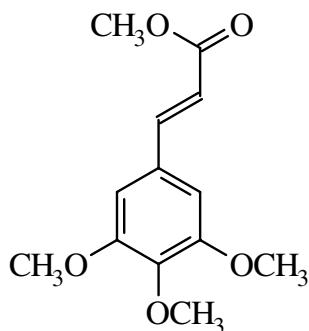
Notes:

J. Ralph JRPS 133.2x1  
68mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
γOMe	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

<sup>13</sup>C



*trans*

methyl (3,4,5-trimethoxy)cinnamate

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
γOMe	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

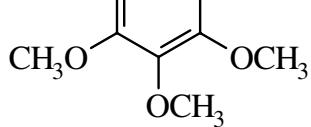
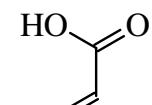
Notes:

J. Ralph JRPS 139x1  
92mg

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
γOMe	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**

**<sup>13</sup>C**



*trans*

**3,4,5-trimethoxy cinnamic acid**

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
3,5 OMe	3.89	s	
4 OMe	3.89	s	
2,6	6.78	s	
$\alpha$	7.70	d	15.9
$\beta$	6.36	d	15.9

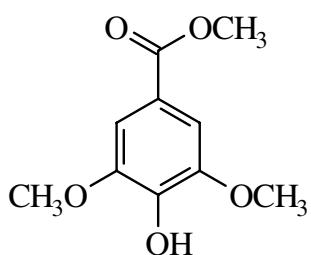
**Notes:**

Aldrich  
100mg

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\alpha$	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
$\gamma$	172.46	32	168.33	28	167.72	52

Compound Number 64

<sup>13</sup>C



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

<sup>1</sup>H (chloroform)

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

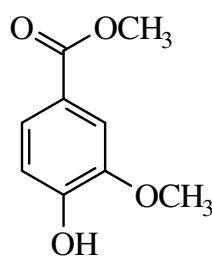
Notes:

J. Ralph JRPS 7x1  
93.3mg

Atom	CDCl <sub>3</sub>		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**

**<sup>13</sup>C**



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

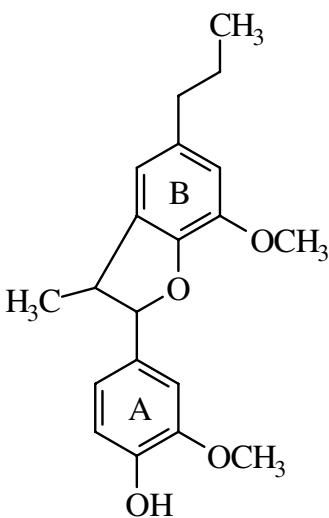
**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
$\alpha$ 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

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
$\alpha$ 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
$\alpha$	167.12	24	167.15	23	166.06	46



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\gamma$	13.90	80	14.08	88	13.65	85
$\gamma$	17.44	72	17.83	88	17.17	81
B $\beta$	25.07	84	25.74	97	24.52	94
B $\alpha$	38.09	71	38.54	79	37.27	77
$\beta$	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
$\alpha$	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

**Dihydrodehydrodiisoeugenol**

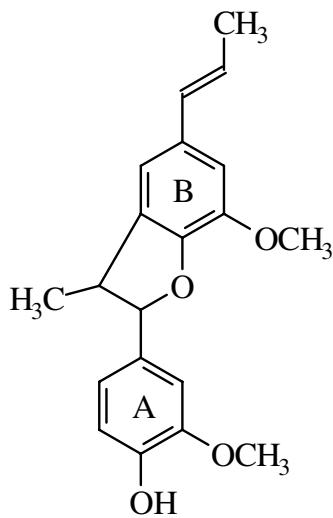
**2-Methoxy-4-(7-methoxy-3-methyl-5-propyl-2,3-dihydrobenzofuran-2-yl)phenol**

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
B $\gamma$	0.96	t	7.3
$\gamma$	1.36	d	6.8
B $\beta$	1.64	h	7.3
B $\alpha$	2.55	t	7.3
$\beta$	3.44	dd	9.6,6.8
OMe	3.86	s	
OMe	3.87	s	
$\alpha$	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

**Dehydrodiisoeugenol**

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

**<sup>1</sup>H** (chloroform)

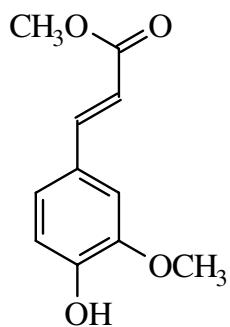
Atom	H Shifts	Mult	J
$\gamma$	1.37	d	6.8
B $\gamma$	1.87	dd	5.3, 1.2
$\beta$	3.44	dt	9.4, 6.8
OMe	3.85	s	
OMe	3.88	s	
$\alpha$	5.09	d	9.4
B $\beta$	6.11	dq	15.8, 5.3
B $\alpha$	6.36	dq	15.8, 1.2
B2	6.76	s	
B6	6.78	s	
A5	6.88	m	
A6	6.80	m	
A2	6.97	s	

**Notes:**

J. Ralph JRKM 67-1  
150mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
$\gamma$	17.60	43	17.86	89	17.25	72
B $\gamma$	18.34	41	18.42	93	18.06	78
$\beta$	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
$\alpha$	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 $\beta$	123.41	47	123.22	97	122.60	60
B $\alpha$	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

<sup>13</sup>C*trans*

**Methyl ferulate**  
methyl 4-hydroxy-3-methoxycinnamate

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
3 OMe	3.79	s	
$\gamma$ OMe	3.89	s	
2	7.31	d	1.8
$\alpha$	7.61	d	15.9
5	6.90	d	8.1
6	7.05	dd	8.1, 1.8
$\beta$	6.28	d	15.9

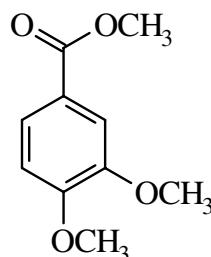
**Notes:**

J. Ralph JRKM 85.1  
54mg

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
$\gamma$ 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
$\beta$	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
$\alpha$	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
$\gamma$	167.80	47	167.82	40	167.02	62

**Compound Number      69**

**<sup>13</sup>C**



**Methylveratrate**  
**methyl 3,4-dimethoxybenzoate**

**<sup>1</sup>H** (chloroform)

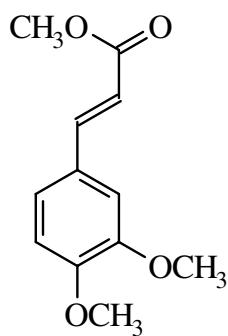
Atom	H Shifts	Mult	J
$\alpha$ OMe	3.89	s	
OMe	3.93	s	
OMe	3.93	s	
2	7.54	d	1.9
5	6.88	d	8.4
6	7.67	dd	8.4, 1.9

**Notes:**

J. Ralph JRPS 5.1  
55mg

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
$\alpha$ 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
$\alpha$	166.82	14	166.92	19	165.96	35

Compound Number 70

<sup>13</sup>C*trans*

methyl 3,4-dimethoxycinnamate

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
$\gamma$ 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
$\alpha$	7.63	d	15.9
$\beta$	6.30	d	15.9

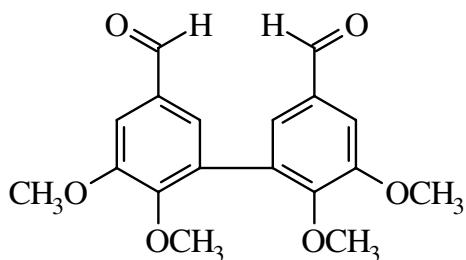
## Notes:

J. Ralph JRPS 21x1  
52mg

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
$\gamma$ 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
$\beta$	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
$\alpha$	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
$\gamma$	167.58	49	167.71	39	166.92	61

**Compound Number**    71

<sup>13</sup>C



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

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
3 OMe	3.77	s	
4 OMe	3.99	s	
2	7.51	d	1.9
6	7.40	d	1.9
$\alpha$	9.91	s	

**Notes:**

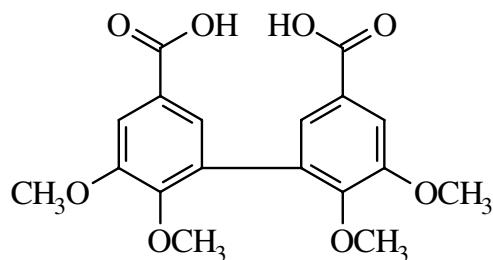
Obst

38 mg contains impurity

As this compound has a plane of symmetry

The shifts for the other half are identical.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
3	152.36	35	153.02	23	151.50	44
4	153.37	50	154.27	40	152.82	72
$\alpha$	190.87	100	191.51	100	191.60	75

**Dehydrodiveratic acid****5,6,5',6'-Tetramethoxybiphenyl-3,3'-dicarboxylic acid****<sup>1</sup>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

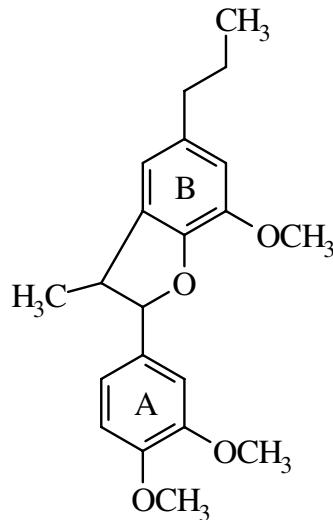
\* only soluble in DMSO

\* aldehyde impurity

As this compound has a plane of symmetry

The shifts for the other half are identical.

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
3					150.04	67
4					152.11	94
α					166.72	60



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\gamma$	13.90	65	14.08	55	13.66	88
$\gamma$	17.47	63	17.90	55	17.18	75
B $\beta$	25.06	67	25.74	63	24.53	81
B $\alpha$	38.09	63	38.53	62	37.28	69
$\beta$	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
$\alpha$	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

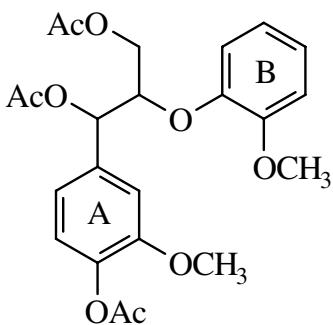
2-(3,4-Dimethoxyphenyl)-7-methoxy-3-methyl-5-propyl-2,3-dihydrobenzofuran

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
B $\gamma$	0.96	t	7.3
$\gamma$	1.37	d	6.8
B $\beta$	1.64	h	7.3
B $\alpha$	2.55	t	7.3
$\beta$	4.45	dq	9.6, 6.8
OMe	3.86	s	
OMe	3.87	s	
OMe	3.88	s	
$\alpha$	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

*threo*

**Guaiacylglycerol- $\beta$ -guaiacyl ether triacetate**  
**1-(4-acetoxy-3-methoxyphenyl)-1,3-diacetoxyl-2-(2-methoxy**  
**phenoxy)propane**

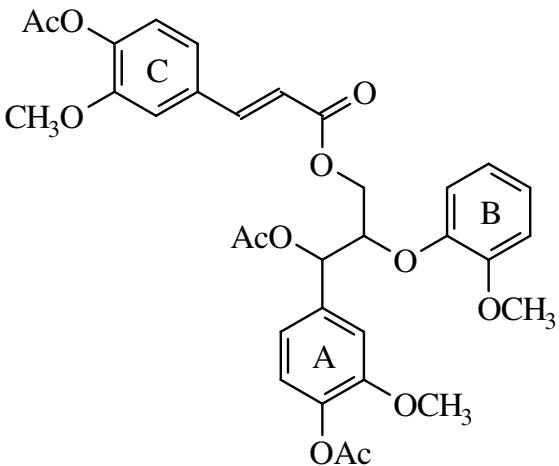
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.63	86	20.45	89	20.28	94
Ac Me	20.68	78	20.58	84	20.35	100
Ac Me	21.02	88	20.91	61	20.63	82
OMe	55.81	100	56.21	92	55.54	100
OMe	55.96	94	56.30	100	55.76	91
$\gamma$	63.09	75	63.58	79	62.47	52
$\alpha$	74.52	86	75.37	87	74.28	67
$\beta$	80.26	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
$\alpha$ Ac C=O	169.65	49	169.94	39	169.30	61
$\gamma$ Ac C=O	170.52	51	170.62	42	169.89	67

**<sup>1</sup>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	
$\gamma$ 1	4.06	dd	11.9, 5.7
$\gamma$ 2	4.32	dd	11.9, 4.5
$\alpha$	6.12	d	6.3
$\beta$	4.63	m	

**Notes:**

R. Helm RFH5C  
 50mg

*threo*

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

<sup>1</sup>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	
$\gamma_1$	4.20	dd	11.9, 5.2
$\gamma_2$	4.42	dd	11.9, 4.2
$\beta$	4.70	m	
$\alpha$	6.20	d	6.5
$C\beta$	6.35	d	15.9
$C\alpha$	7.54	d	15.9

**Notes:**

R. Helm RFH101D1

40mg

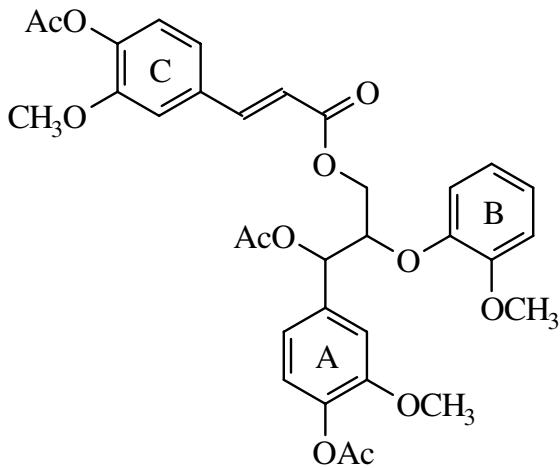
Vinyl C's at 124.08 and 145.16 in acetone.

In CDCl<sub>3</sub> 123.23 and 144.62

Acetone 1H data in J. Ag. Food Chem. 41(4)

570-576, 1993

Atom	CDCl <sub>3</sub>		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
$\gamma$	63.35	28	63.94	39	62.87	21
$\alpha$	74.64	35	75.54	39	74.44	33
$\beta$	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
$C\beta$	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
$C\alpha$	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
$C\gamma$	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

*erythro*

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

### <sup>1</sup>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	
$\gamma_1$	4.44	dd	11.9, 4.2
$\gamma_2$	4.53	dd	11.9, 5.3
$\beta$	4.75	m	
$\alpha$	6.14	d	5.5
$C\beta$	6.35	d	16.0
$C\alpha$	7.54	d	16.0

### Notes:

R. Helm RFH101D2

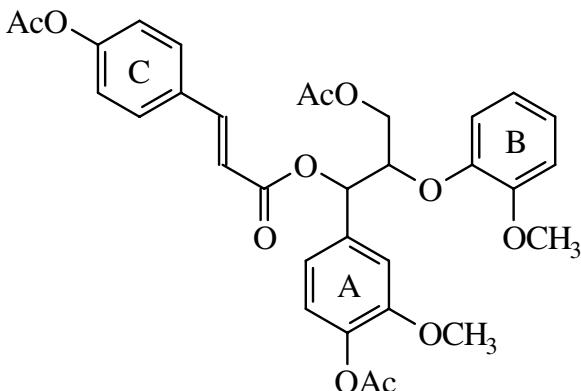
30mg

Vinyl C's at 124.09 and 145.13 in acetone

Acetone 1H data in J. Ag. Food Chem. 41(4)

570-576, 1993

Atom	CDCl <sub>3</sub>		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
$\gamma$	62.88	30	63.34	36	62.26	31
$\alpha$	73.96	31	74.72	42	73.28	30
$\beta$	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 $\beta$	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 $\alpha$	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 $\gamma$	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

*erythro*

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

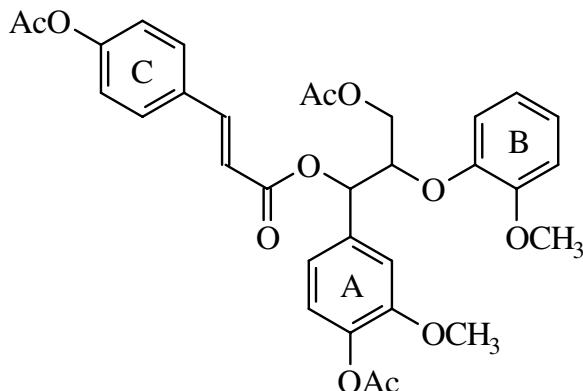
**<sup>1</sup>H** (chloroform)

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	
$\gamma_1$	4.32	dd	11.9, 4.3
$\gamma_2$	4.48	dd	11.9, 5.9
$\beta$	4.77	m	
$\alpha$	6.20	d	5.0
C $\beta$	6.44	d	16.0
C <sub>2,6</sub>	7.13	m	8.6
C <sub>3,5</sub>	7.53	m	8.6
C $\alpha$	7.65	d	16.0

**Notes:**

R. Helm RFH119D1  
47mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\gamma$	62.73	34	63.16	38	62.06	29
$\alpha$	74.12	45	74.97	44	73.50	39
$\beta$	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 $\beta$	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 $\alpha$	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 $\gamma$	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



threo

Atom	CDCl <sub>3</sub>		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
Cβ	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
Cα	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
Cγ	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

<sup>1</sup>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	
γ2	4.36	dd	11.9, 4.4
β	4.72	m	
α	6.23	d	6.4
Cβ	6.37	d	16.0
C2.6	7.12	m	8.6
C3.5	7.49	m	8.6
Cα	7.55	d	16.0

## Notes:

R. Helm RFH119D2  
44mg

**Compound Number 79**

<sup>13</sup>C

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**1-(4-acetoxy-3,5-dimethoxyphenyl)-2-(4-acetyl-2,6-dimethoxyphenoxy)-3-hydroxypropan-1-one**

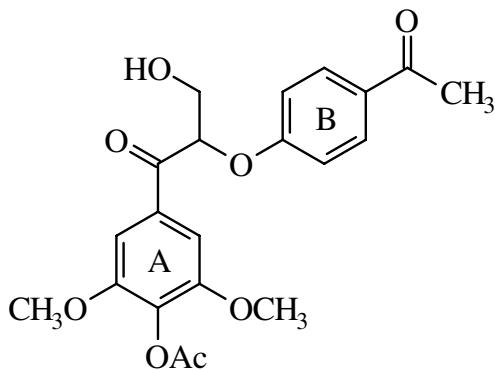
**<sup>1</sup>H** (chloroform)

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

**Notes:**

SR III - 39  
45mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.41	49	20.22	50	20.06	54
B $\beta$	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
$\gamma$	63.36	33	63.67	32	62.39	37
$\beta$	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 $\alpha$	194.74	29	195.71	23	195.27	35
$\alpha$	196.50	24	196.65	21	196.51	35



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

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.34	s	
B $\beta$	2.51	s	
A3,5 OMe	3.82	s	
$\gamma$	4.19	m	
$\beta$	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

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.40	49	20.21	46	20.05	51
B $\beta$	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
$\gamma$	63.32	38	63.94	37	62.41	29
$\beta$	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 $\alpha$	194.60	29	195.47	19	194.76	34
$\alpha$	196.64	31	196.21	17	196.08	31

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

**<sup>1</sup>H** (chloroform)

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

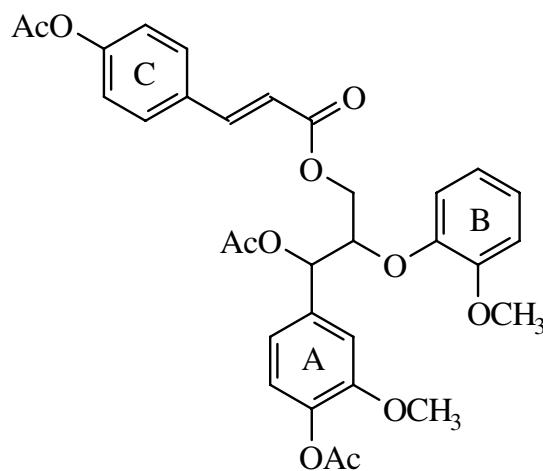
**Notes:**

SR III - 38

17mg

B1 and A4 switch places in DMSO A4 has very low intensity and is easy to follow

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.39	38	20.21	45	20.05	38
B $\beta$	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
$\gamma$	63.47	27	63.91	42	62.32	32
$\beta$	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 $\alpha$	194.85	17	195.94	24	195.02	50
$\alpha$	196.57	21	196.27	21	196.14	41

*threo*

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

### <sup>1</sup>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	
$\gamma_1$	4.23	dd	11.9, 5.8
$\gamma_2$	4.42	dd	11.9, 4.2
$\beta$	4.72	m	
$\alpha$	6.19	d	6.3
C $\beta$	6.34	d	16.0
C2,6	7.12	m	8.6
C3,5	7.51	m	8.6
C $\alpha$	7.55	d	16.0

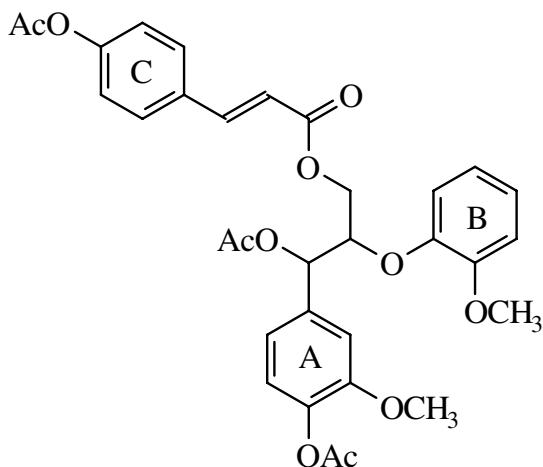
### Notes:

R. Helm RFH87D1

36.6mg

129.85 and 129.57 for B $\alpha$  and C2,6  
change places in DMSO see 1019

Atom	CDCl <sub>3</sub>		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
$\gamma$	63.39	28	63.93	33	62.86	21
$\alpha$	74.62	36	75.53	21	74.43	33
$\beta$	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 $\beta$	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 $\alpha$	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 $\gamma$	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

*erythro*

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

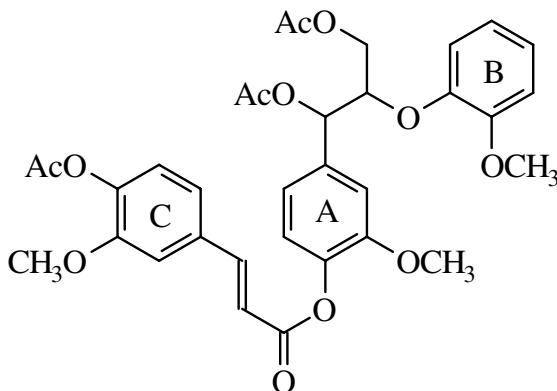
**<sup>1</sup>H** (chloroform)

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

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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



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

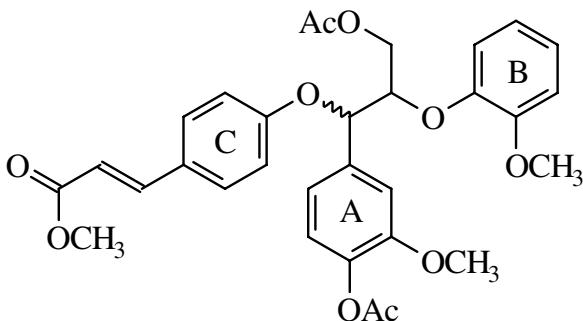
**<sup>1</sup>H** (chloroform)

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
Cβ	6.60	d	15.9
Cα	7.80	d	15.9

**Notes:**

R. Helm RFH9D  
39.4mg  
see 1026

Atom	CDCl <sub>3</sub>		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
Cβ	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
Cα	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
Cγ	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



3-[4-[3-Acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propoxy]phenyl]acrylic acid methyl ester

<sup>1</sup>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

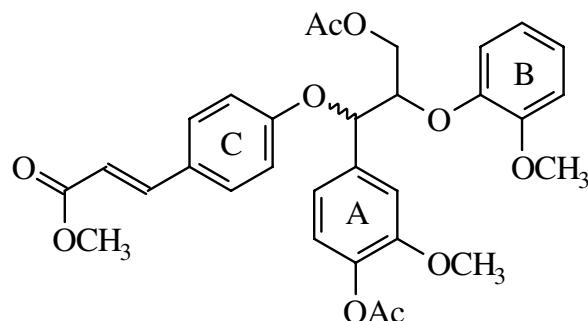
Notes:

R. Helm RFH111D1

39.0 mg

Isomer of 86

Atom	CDCl <sub>3</sub>		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



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

<sup>1</sup>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

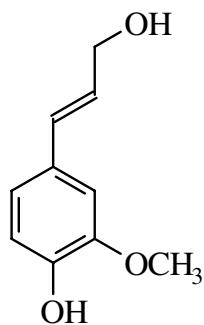
Notes:

Rich Helm RFH111D2

35mg

Isomer of 85

Atom	CDCl <sub>3</sub>		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
A γ C=O	167.60	39	167.60	29	166.74	64
A4 C=O	168.64	28	168.76	29	168.21	52
C γ	170.50	33	170.62	24	169.91	60

*trans*

Coniferyl alcohol

4-hydroxy-3-methoxy cinnamyl alcohol

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
γ OH	3.78	t	56
OMe	3.86	s	
γ's	4.18	td	55,15
β	6.22	dt	159,55
α	6.49	dt	159,15
5	6.76	d	81
6	6.84	dd	81,19
2	7.04	d	19
4 OH	7.63	s	

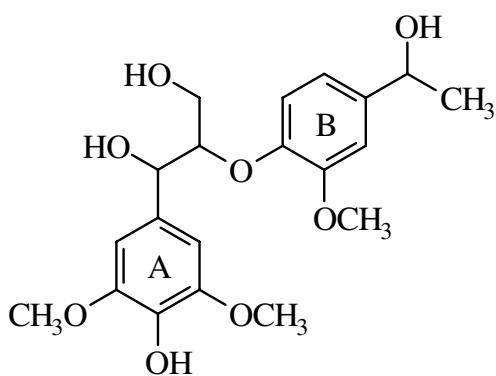
## Notes:

Aldrich

30mg

Proton data from 360 MHz spectrum in acetone..S.Q.

Atom	CDCl <sub>3</sub>		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

*threo*

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$	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
$\gamma$	61.04	28	61.94	34	59.99	26
B $\alpha$	69.95	48	69.73	54	67.80	63
$\alpha$	74.12	33	74.05	46	70.87	28
$\beta$	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

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

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\beta$	1.38	d	6.4
B OMe	3.87	s	
A3,5 OMe	3.80	s	
$\alpha$ OH	4.50	d	3.9
A2,6	6.77	s	

### Notes:

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

**Compound Number      89**

 <i>threo</i>
------------------

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

**<sup>1</sup>H (acetone)**

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

**Notes:**

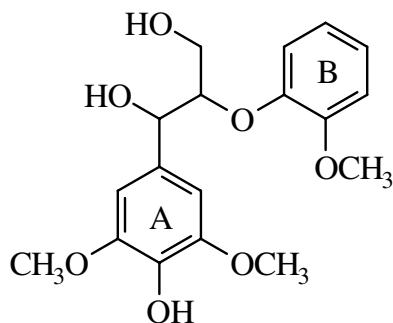
S Ralph SRIII-44  
30mg

**<sup>13</sup>C**

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
B $\beta$	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
$\gamma$	60.48	31	61.41	29	60.15	12
B $\alpha$	70.21	43	69.98	41	68.09	26
$\alpha$	74.34	37	74.22	36	71.54	16
$\beta$	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

<sup>13</sup>C



*threo*

**Syringylglycerol- $\beta$ -guaiacyl ether**

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

### <sup>1</sup>H (acetone)

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

**Notes:**

S. Ralph SRIII-45  
30mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\gamma$	61.02	37	61.89	40	60.01	18
$\alpha$	74.16	39	73.97	40	70.88	36
$\beta$	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

<sup>13</sup>C

|--|--|

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$	25.07	39	26.17	58	25.81	88
A OMe	56.34	<b>100</b>	56.58	94	55.82	<b>100</b>
A OMe	56.34	100	56.58	94	55.82	100
$\gamma$	61.14	30	61.73	32	60.01	27
B $\alpha$	69.75	42	69.50	58	67.57	73
$\alpha$	73.85	28	73.54	34	71.09	33
$\beta$	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	<b>100</b>	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

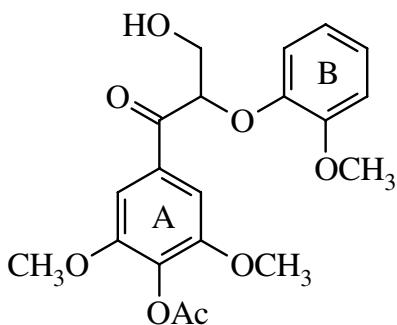
**1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[4-(1-hydroxyethyl)phenoxy]propane-1,3-diol**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B $\beta$	1.35	d	64
A3,5 OMe	3.79	s	
A2,6	6.77	s	
B2,6	7.23	m	86

**Notes:**

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



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

**<sup>1</sup>H** (chloroform)

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

**Notes:**

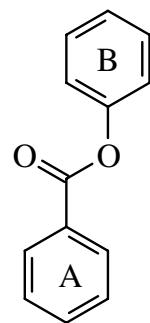
S. Ralph SRIII-40

30mg \*A1 + A4 switch around in CDCl<sub>3</sub>

Atom	CDCl <sub>3</sub>		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
$\gamma$	63.39	40	63.88	21	62.35	38
$\beta$	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
$\alpha$	195.72	22	196.70	20	195.86	35

Compound Number 93

<sup>13</sup>C



**Phenyl benzoate**  
**Benzoic acid phenyl ester**

<sup>1</sup>H (chloroform)

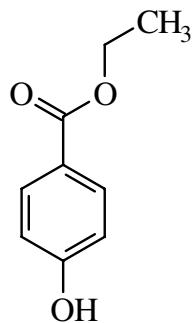
Atom	H Shifts	Mult	J
A2,6	8.21	m	8.3

**Notes:**

Aldrich  
60mg  
Al changes position in DMSO

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\alpha$	165.11	9	165.32	9	164.51	15

Compound Number 94

<sup>13</sup>C

**Ethyl 4-hydroxybenzoate**  
**ethyl 4-hydroxybenzoate**

<sup>1</sup>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

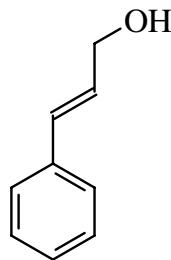
**Notes:**

Aldrich  
60mg

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



*trans*

Cinnamyl alcohol

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

<sup>1</sup>H (chloroform)

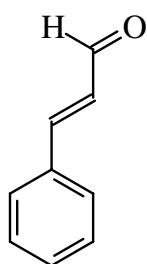
Atom	H Shifts	Mult	J
γ	4.25	dd	5.6, 1.1
β	6.30	dt	15.9, 5.6
α	6.54	dt	15.9, 1.1

**Notes:**

Fluka  
60mg

Compound Number 96

<sup>13</sup>C



*trans*

Cinnamaldehyde

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

<sup>1</sup>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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

 <i>threo</i>	
------------------	--

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>1</sup>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	
α	6.08	d	6.2
A2,6	6.67	s	

## Notes:

S. Ralph SRIII-43

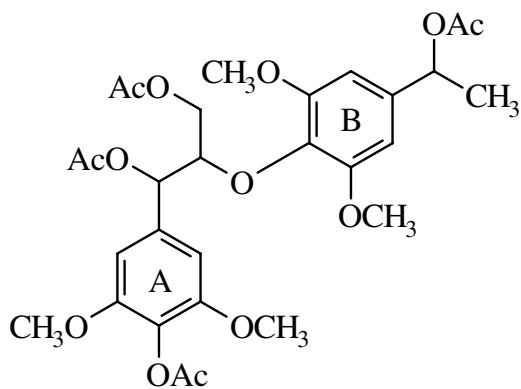
40mg

ca 90% threo

\*

**Compound Number      98**

<sup>13</sup>C



*threo*

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

**<sup>1</sup>H** (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

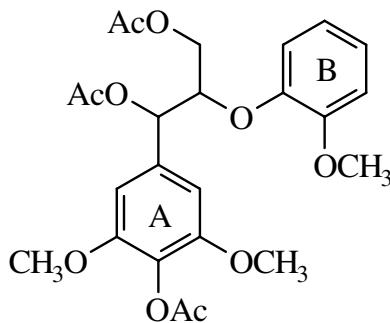
131mg

\*

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
B β	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**

**<sup>13</sup>C**



*threo*

**1-(4-acetoxy-3,5-dimethoxyphenyl)-1,3-diacetoxymethyl-2-(2-methoxyphenoxy)propane**

**<sup>1</sup>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	
$\gamma_1$	4.04	dd	11.9, 5.6
$\gamma_2$	4.26	dd	11.9, 4.2
$\beta$	4.79	m	
$\alpha$	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

**Notes:**

S. Ralph SRIII-45

55mg

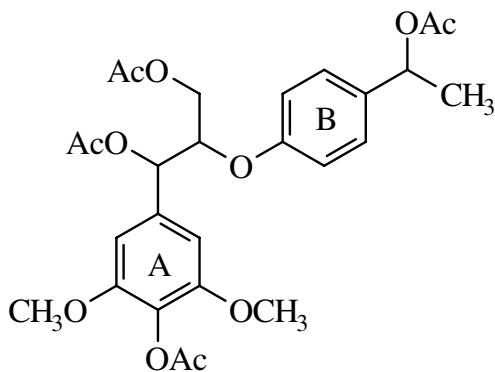
ca 80% threo

\*Chemical shift assignments for overlapping 1H patterns A2,6 and B1,B2,B5 and B6 were made with the assistance of deconvolution spectra obtained with MacNuts, Acorn NMR Inc. All patterns were complex multiplets (non-1st order) J's and CS's determined from simulation files

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\gamma$	63.08	32	63.60	43	62.48	26
$\alpha$	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
$\alpha$ Ac C=O	169.68	20	169.97	17	169.34	26
$\gamma$ Ac C=O	170.55	19	170.66	19	169.94	29

**Compound Number 100**

**<sup>13</sup>C**



*threo*

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

**<sup>1</sup>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

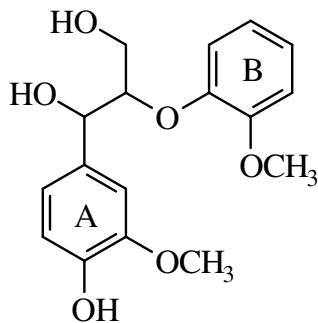
24mg

CDCl<sub>3</sub> spectrum poor

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



*erythro*

Guaiacylglycerol- $\beta$ -guaiacyl ether

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

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.84	s	
$\alpha$	4.95	d	
$\beta$	4.16	m	4.8

**Notes:**

J. Ralph JRB 178.3

30mg

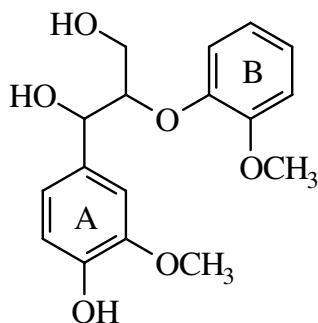
J. Ralph Holzforschung

42(1988) p273-5

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\gamma$	60.75	76	61.81	81	60.04	59
$\alpha$	72.78	76	73.82	81	71.60	72
$\beta$	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

<sup>13</sup>C



*threo*

**Guaiacylglycerol- $\beta$ -guaiacyl ether**

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

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
OMe	3.86	s	
OMe	3.90	s	
$\alpha$	4.96	d	
$\beta$	4.02	m	8.0

**Notes:**

J. Ralph JRGV 135.X1

21mg

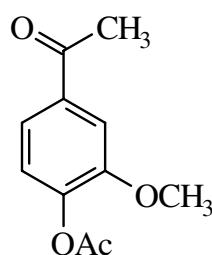
J. Ralph Holzforschung

42(1988) p.273-5

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\gamma$	61.06	72	61.90	75	60.02	59
$\alpha$	74.00	80	73.93	84	70.90	69
$\beta$	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

<sup>13</sup>C



**Acetylated acetovanillone  
4-acetoxy-3-methoxyacetophenone**

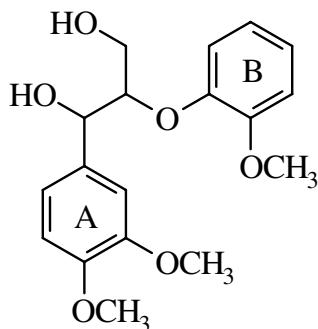
Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.61	65	20.46	64	20.29	83
β	26.49	81	26.63	84	26.62	88
OMe	56.05	100	56.37	97	55.88	100
2	111.51	97	112.44	97	111.62	77
6	121.94	88	122.38	93	121.56	83
5	122.80	95	123.77	100	123.02	84
1	135.96	37	136.93	30	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

**<sup>1</sup>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

*threo***Veratrylglycerol- $\beta$ -guaiacyl ether**

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

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
OMe	3.82	s	
OMe	3.83	s	
OMe	3.84	s	
$\alpha$	4.96	d	5.0
$\beta$	4.15	m	

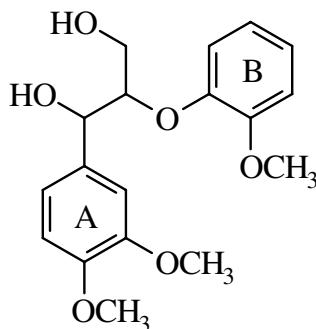
**Notes:**

LL Landucci

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

Atom	CDCl <sub>3</sub>		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
$\gamma$	61.04	16	61.70	60	60.02	48
$\alpha$	73.77	16	73.64	74	70.77	18
$\beta$	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	119.56	32	115.84	23
B5	120.52	15	120.03	72	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
A3	148.83	12	149.67	15	147.98	43
A4	149.04	12	149.96	32	148.25	20
B3	151.07	11	151.61	10	149.67	23

Compound Number 105

<sup>13</sup>C

**Veratrylglycerol- $\beta$ -guaiaetyl ether**  
**1-(3,4-Dimethoxyphenyl)-2-(2-methoxyphenoxy)-propane-**  
**1,3-diol**

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
OMe	3.85	s	
OMe	3.85	s	
OMe	3.85	s	
$\alpha$	4.96	d	4.8
$\beta$	4.16	m	
A2	7.6	d	1.8
A6	7.67	dd	8.4, 1.8

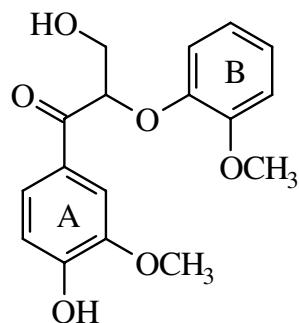
**Notes:**

LL Landucci  
30mg

Atom	CDCl <sub>3</sub>		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
$\gamma$	60.81	46	61.79	30	60.03	61
$\alpha$	72.75	50	73.75	36	71.54	69
$\beta$	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
B5	118.49	50	119.64	85	115.95	72
A6	120.68	50	120.06	100	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

Compound Number 106

<sup>13</sup>C



Atom	CDCl <sub>3</sub>		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

### Erone

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

### <sup>1</sup>H (chloroform)

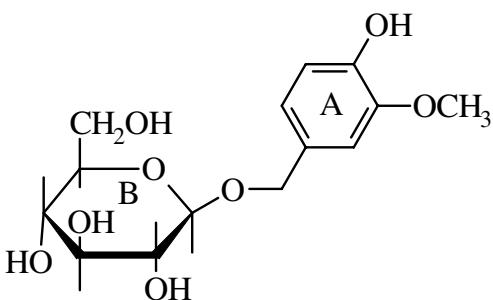
Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.87	s	
γ	4.08	d	5.1
β	5.43	t	5.1

### Notes:

S. Ralph  
45mg

Compound Number 107

<sup>13</sup>C



**Vanillyl- $\beta$ -D-Glucoside**  
2-(4-Hydroxy-3-methoxybenzyloxy)-6-hydroxymethyl  
tetrahydropyran-3,4,5-triol

<sup>1</sup>H Not run

Atom	H Shifts	Mult	J

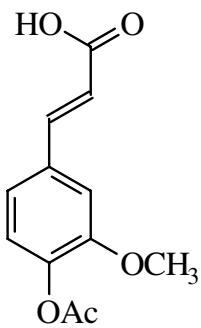
**Notes:**

M.Mozuch 88/71/1  
20mg not soluble in CDCl<sub>3</sub>

Atom	CDCl <sub>3</sub>		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
$\alpha$			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

<sup>13</sup>C



**Acetylated ferulic acid  
4-acetoxy-3-methoxycinnamic acid**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>1</sup>H (chloroform)

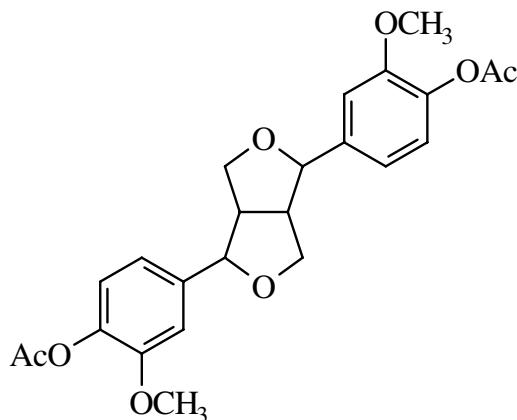
Atom	H Shifts	Mult	J
Ac Me	2.33	s	
OMe	3.88	s	
α	7.04	d	15.9
β	6.41	d	15.9

**Notes:**

R. Helm RFH 83F1  
50mg not soluble in CDCl<sub>3</sub>

**Compound Number** 109

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

**Pinoresinol diacetate**

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

**<sup>1</sup>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:**

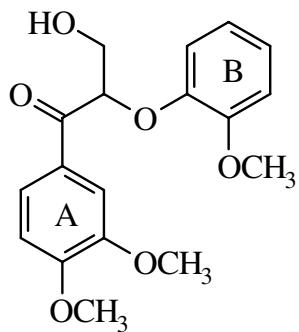
J. Pew

As this compound has a plane of symmetry

The shifts for the other half are identical.

Compound Number 110

<sup>13</sup>C



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

<sup>1</sup>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

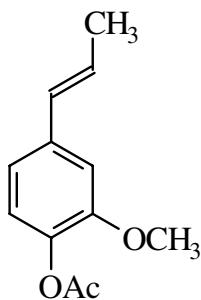
**Notes:**

LL Landucci  
34mg

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



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

<sup>1</sup>H (chloroform)

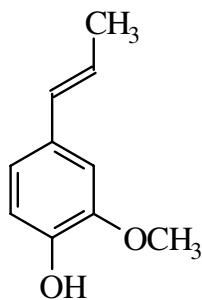
Atom	H Shifts	Mult	J
γ	1.85	dd	6.35, 1.4
Ac Me	2.28	s	
OMe	3.81	s	
β	6.17	dq	15.7, 6.35
α	6.35	dd	15.7, 1.4

Notes:

J. Ralph JRPS115.1  
50mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

**Isoeugenol****1-(3-methoxy-4-hydroxyphenyl)-1-propene****<sup>1</sup>H** (chloroform)

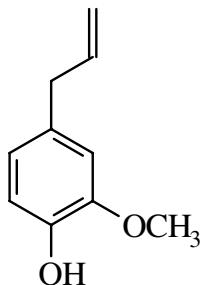
Atom	H Shifts	Mult	J
γ	1.83	dd	6..5, 1.6
OMe	3.84	s	
β	6.05	dq	15.7, 6.5
α	6.30	dd	15.7, 1.6

**Notes:**

Aldrich  
 50mg contains an impurity

**Compound Number 113**

<sup>13</sup>C



**Eugenol**  
**4-Allyl-2-methoxyphenol**

<sup>1</sup>H (chloroform)

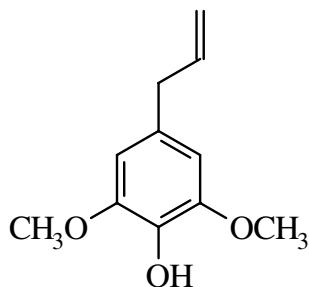
Atom	H Shifts	Mult	J
$\alpha$	3.30	d	6.6
OMe	3.84	s	
$\gamma$	5.04	m	
$\beta$	5.94	ddt	6.6
5	6.83	d	8.5

**Notes:**

Aldrich  
50mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
$\alpha$	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
$\gamma$	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
$\beta$	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

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

## 4-Allyl-2,6-dimethoxyphenol

<sup>1</sup>H (chloroform)

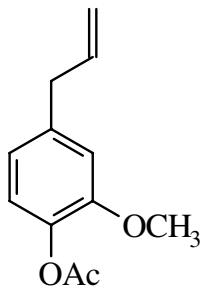
Atom	H Shifts	Mult	J
α	3.30	d	6.7
OMe	3.85	s	
2,6	6.40	s	
γ	5.04	m	
β	5.94	ddt	16.8, 10.2, 6.7

## Notes:

Aldrich 50mg Extraneous peaks around 106 and 119

Compound Number 115

<sup>13</sup>C



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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

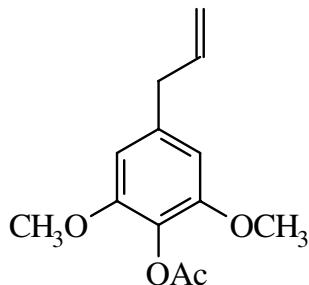
<sup>1</sup>H (chloroform)

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

## Compound Number 116

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

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

<sup>1</sup>H (chloroform)

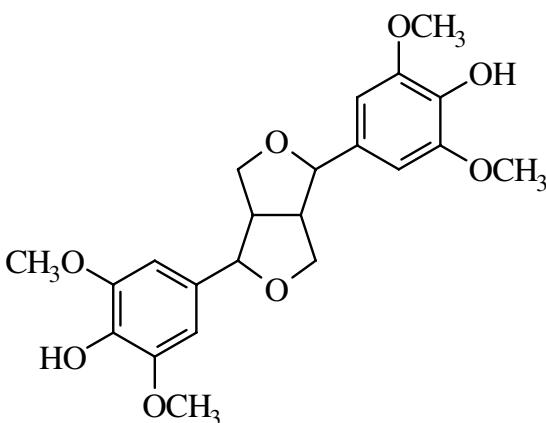
Atom	H Shifts	Mult	J
Ac Me	2.31	s	
α	3.34	d	6.7
OMe	3.79	s	
2,6	6.43	s	
γ	5.09	m	
β	5.95	ddt	16.8, 10.1, 6.7

## Notes:

J. Ralph JRPS143.1  
50mg

**Compound Number 117**

<sup>13</sup>C



**Syringylresinol**

<sup>1</sup>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

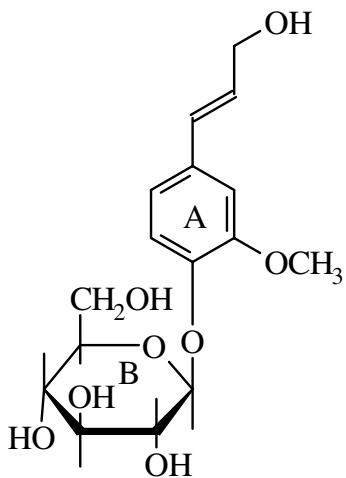
As this compound has a plane of symmetry

The shifts for the other half are identical.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C



Coniferin  
4-(3-hydroxy-1-propenyl)-2-methoxyphenyl-  
 $\beta$ -D-glucopyranoside

<sup>1</sup>H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.78	s	
$\gamma$ 1, $\gamma$ 2	4.10	dd	5.03
$\beta$	6.28	dt	15.9,5.0
$\alpha$	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 $\alpha$	3.46	m	
B6 $\beta$	3.67	ddd	
B6 OH	4.54	t	5.7
$\gamma$ OH	4.83	t	5.6

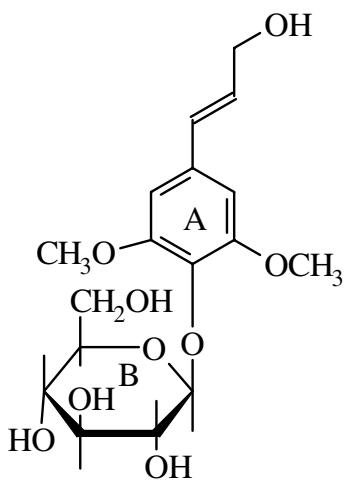
Notes:

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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
OMe					55.57	100
B6					60.60	49
$\gamma$					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
$\alpha$					128.31	79
$\beta$					128.87	70
A1					130.95	70
A4					145.89	67
A3					148.94	70

Compound Number 119

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
OMe					56.27	100
OMe					56.27	100
B6					60.82	29
$\gamma$					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
$\alpha$					128.35	37
$\beta$					130.05	37
A1					132.52	35
A4					133.80	26
A3					152.60	77
A5					152.60	77

Syringin

4-(3-hydroxy-1-propenyl)-2,6-dimethoxy-  $\beta$ -D-glucopyranoside

<sup>1</sup>H (DMSO)

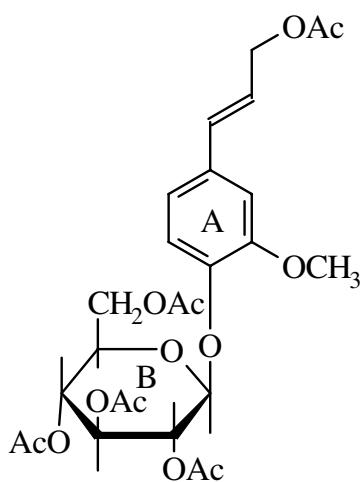
Atom	H Shifts	Mult	J
OMe	3.77	s	
$\gamma^l$	4.11	dd	5.0
$\beta$	6.63	dt	15.9,4.7
$\alpha$	6.47	d	15.9
A2,6	6.73	s	
B1	4.91	d	4.8
B2,3,4,5	3.18-3.04	nr	
B6 $\alpha$	3.4	m	
B6 $\beta$	3.59	ddd	
B6 OH	4.29	t	5.4
$\gamma$ OH	4.85	t	5.5

**Notes:**

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

Compound Number 120

<sup>13</sup>C



Coniferin acetate  
4-(3-hydroxy-1-propenyl)-2-methoxy phenyl-  
β-D-glycopyranoside pentaacetate

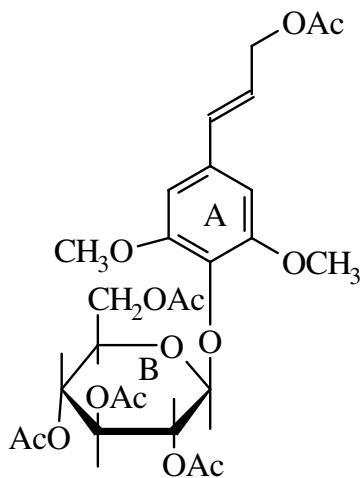
<sup>1</sup>H (chloroform)

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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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



**Syringin acetate**  
**4-(3-hydroxy-1-propenyl)-2,6-dimethoxy**  
**phenyl- $\beta$ -D-glucopyranoside penta acetate**

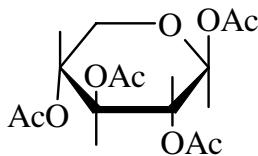
<sup>1</sup>H (chloroform)

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	
$\gamma$	4.71	d	6.4
$\beta$	6.22	dt	16.8, 6.4
$\alpha$	6.57	d	16.8
A2,6	6.61	s	

**Notes:**

S. Ralph III - 58  
50mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\gamma$	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
$\alpha$	123.30	39	124.38	46	123.74	36
A1	133.11	31	134.02	33	132.79	56
$\beta$	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

 $\alpha + \beta$  Xylose Acetate

Atom	CDCl <sub>3</sub>		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

<sup>1</sup>H (chloroform)

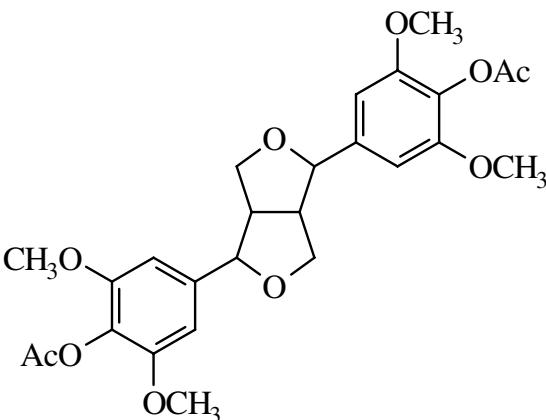
Atom	H Shifts	Mult	J
Ac Me	2.02	s	
Ac Me	2.049	s	
Ac Me	2.049	s	
Ac Me	2.052	s	
Ac Me	2.052	s	
Ac Me	2.06	s	
Ac Me	2.11	s	
Ac Me	2.17	s	

## Notes:

S. Ralph III - 58  
50mg mixture of  $\alpha + \beta$

**Compound Number** 123

<sup>13</sup>C



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

<sup>1</sup>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	

**Notes:**

S. Ralph III - 58

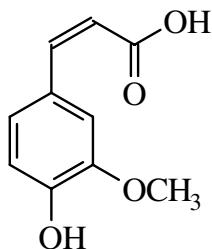
20mg

As this compound has a plane of symmetry

The shifts for the other half are identical.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

Compound Number 124

<sup>13</sup>C*cis*

**cis - Ferulic Acid**  
**(Z)-4-hydroxy-3-methoxycinnamic acid**

**<sup>1</sup>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

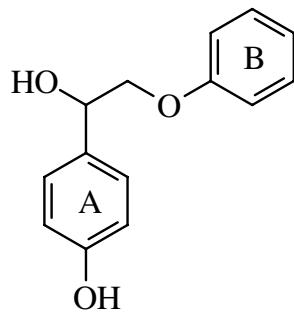
**Notes:**

J. Obst  
 25mg 617 is a 13C in d4-MeOH.  
 A Dept was run & marked on 617  
 not saved.

Atom	CDCl <sub>3</sub>		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
6	115.50	87	116.82	97	116.77	69
β	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**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

**1-(4-hydroxyphenyl)-2-phenoxyethanol**

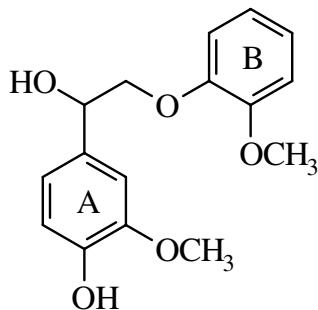
**<sup>1</sup>H (chloroform)**

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

**Notes:**

JR C37.1  
52mg

## Compound Number 126

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

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

<sup>1</sup>H (chloroform)

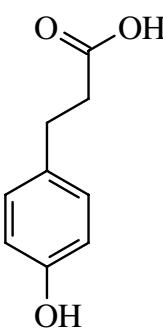
Atom	H Shifts	Mult	J
OMe	3.88	s	
OMe	3.89	s	
α	5.02	dd	9.3, 3.0
β1	3.93	dd	10.0, 9.3
β2	4.15	dd	10.0, 3.0

## Notes:

JR 145.2  
62mg \* 76.50 shift in CDCl<sub>3</sub>  
falls under solvent peak.

Compound Number 127

<sup>13</sup>C



Dihydrocoumaric acid  
3-(4-hydroxyphenyl)propionic acid

<sup>1</sup>H (chloroform)

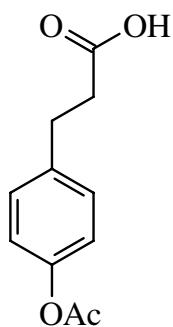
Atom	H Shifts	Mult	J
β	2.63	t	7.0
α	2.88	t	7.0
3,5	6.77	m	8.6
2,6	7.06	m	8.6

**Notes:**

IPC Pearl Coll.  
60mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C

**acetylated dihydrocoumaric acid  
3-(4-acetoxyphenyl)propionic acid**

<sup>1</sup>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:**

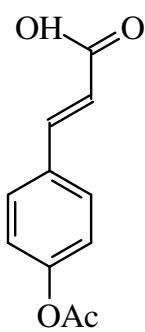
IPC Pearl Coll.

60mg Contains unacetylated cmpd also

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



*trans*

acetylated coumaric acid  
(E)-4-acetoxy cinnamic acid

<sup>1</sup>H (chloroform)

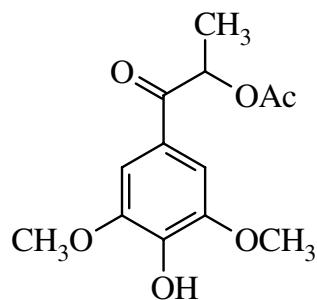
Atom	H Shifts	Mult	J
Ac Me	2.31	s	
β	6.41	d	16.0
3,5	7.15	m	8.6
2,6	7.57	m	8.6
α	7.75	d	16.0

Notes:

IPC Pearl coll.  
60mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

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

<sup>1</sup>H (chloroform)

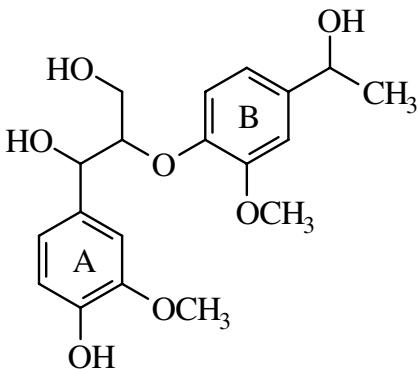
Atom	H Shifts	Mult	J
γ	1.53	d	7.0
Ac Me	2.15	s	
OMe	3.94	s	
β	5.96	q	7.0
2,6	7.24	s	

## Notes:

IPC Pearl coll.  
60mg

**Compound Number 131**

**<sup>13</sup>C**



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$	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
$\gamma$	61.09	46	61.89	61	60.02	49
B $\alpha$	70.01	73	69.74	80	67.78	85
$\alpha$	73.93	59	73.95	63	70.91	38
$\beta$	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

*threo*

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

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
B $\beta$	1.46	d	6.4
OMe	3.84	s	
OMe	3.86	s	
B $\alpha$	4.82	q	6.4
$\alpha$	4.92	d	7.7
A5	7.03	d	8.2

**Notes:**

S. Ralph SRIII-62-1

35mg

erythro data

C A D

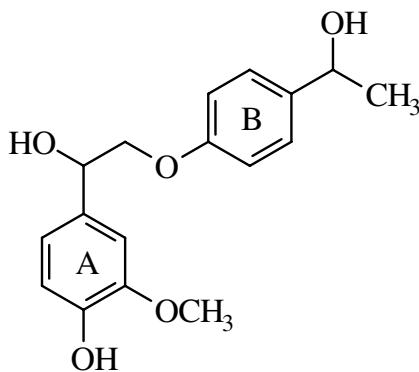
$\gamma$  60.8 61.9 60.0

$\alpha$  72.8 73.8 71.6

$\beta$  86.9 86.9 83.9

A1 132.0 134.3 133.2

## Compound Number 132

<sup>13</sup>C

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

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
B $\beta$	1.46	d	6.4
OMe	3.90	s	
$\beta$ 1	3.96	dd	9.7, 8.6
$\beta$ 2	4.06	dd	9.7, 3.5
B $\alpha$	4.84	q	6.4
$\alpha$	5.03	dd	8.6, 3.5

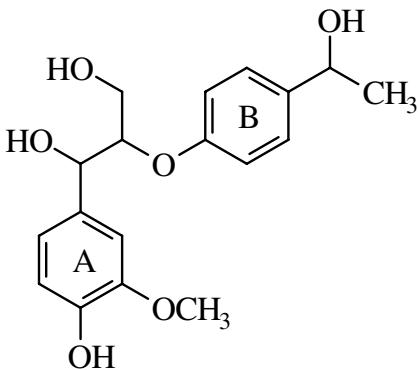
**Notes:**

S. Ralph SRIII-63-1  
50mg

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$	25.05	40	26.20	40	25.83	54
OMe	55.98	52	56.27	50	55.50	62
B $\alpha$	69.91	44	69.50	39	67.52	62
$\alpha$	72.43	50	72.65	46	70.68	46
$\beta$	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

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$	25.08	49	26.07	52	25.78	64
OMe	56.00	72	56.22	53	55.45	49
$\gamma$	61.24	34	61.69	34	60.00	27
B $\alpha$	69.86	64	69.52	52	67.60	62
$\alpha$	73.94	43	73.38	36	70.95	24
$\beta$	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

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

<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
B $\beta$	1.47	d	6.4
OMe	3.87	s	
$\beta$	4.37	m	
B $\alpha$	4.85	q	
$\alpha$	4.96	d	6.4
			6.7

Notes:

S. Ralph SRIII-63-3

70mg

2:1 isomeric mixture, minor isomer shifts

$\gamma$  61.54, 62.04, 60.11

a 74.04, 73.99, 71.50

$\beta$  82.09, 83.75, 83.14

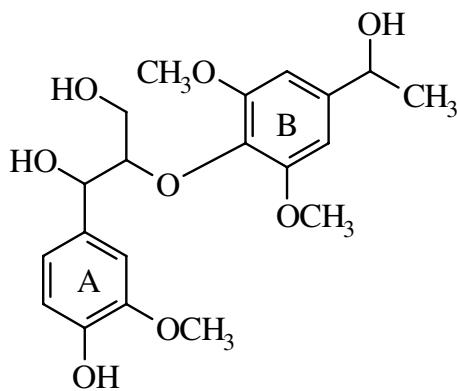
B3,5 116.54, 116.81, 115.54

A6 119.33, 120.47, 119.37

B2,6 126.78, 127.10, 126.07

Compound Number 134

<sup>13</sup>C



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$	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
$\gamma$	60.55	30	61.35	41	60.09	27
B $\alpha$	70.29	39	70.01	44	68.07	56
$\alpha$	74.10	35	74.10	42	71.48	34
$\beta$	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

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

### <sup>1</sup>H (chloroform)

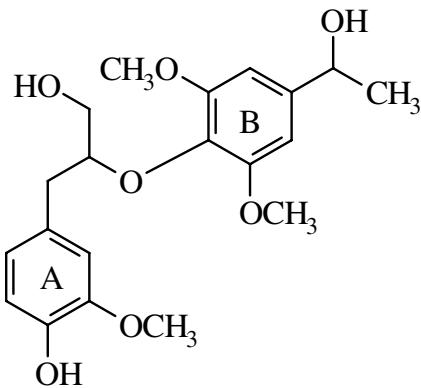
Atom	H Shifts	Mult	J
B $\beta$	1.47	d	6.4
A OMe	3.86	s	
B OMe s	3.89	s	
B $\alpha$	4.83	q	6.4
$\alpha$	5.00	d	8.8
B2,6	6.63	s	
A2	6.95	s	
A5	6.85	d	8.3
A6	6.91	dd	8.3,1.7

### Notes:

S. Ralph SRIII-64-1  
35mg

Compound Number 135

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$	25.30	35	26.26	45	25.81	54
$\alpha$	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
$\gamma$	62.31	34	62.84	36	61.58	26
B $\alpha$	70.42	35	70.04	39	68.13	51
$\beta$	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

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

<sup>1</sup>H (chloroform)

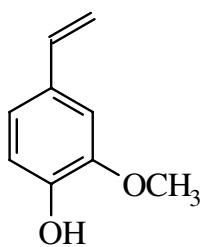
Atom	H Shifts	Mult	J
B $\beta$	1.47	d	6.4
$\alpha$ 1	2.97	dd	13.6, 8.8
$\alpha$ 2	3.20	dd	13.6, 5.4
B OMe	3.85	s	
A OMe	3.83	s	
B $\alpha$	4.82	q	6.4
$\beta$	4.18	m	
B2,6	6.61	s	
A6	6.74	dd	8.0, 1.9
A2	6.80	d	1.9
A5	6.82	d	8.0

Notes:

S. Ralph SRIII-64-2  
30mg

Compound Number 136

<sup>13</sup>C



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

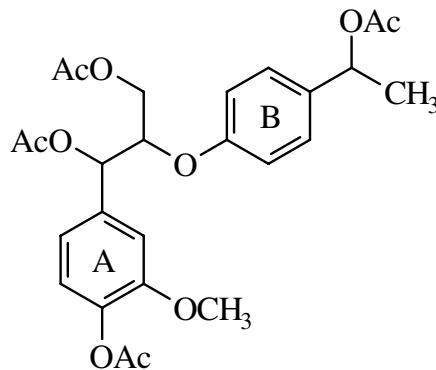
<sup>1</sup>H (acetone)

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

Atom	CDCl <sub>3</sub>		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



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

<sup>1</sup>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	66
OMe	3.81	s	
γ1	4.04	dd	118,61
γ2	4.27	dd	118,38
B α	5.83	q	66
α	6.07	d	63
β	4.69	m	
<u>erythro</u>			
B β	1.50	d	66
α	6.03	d	52
B α	5.82	q	66

**Notes:**

S. Ralph SRIII-65-A 52mg

erythro C13 and 1H data

γ 62.32, 62.88, 61.73

B α 71.85, 72.17, 71.14

α 73.62, 74.21, 72.81

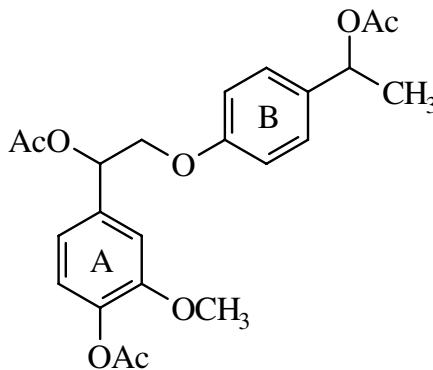
β 78.40, 78.86, 76.99

B4 157.58, 158.59, 157.03

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.62	65	20.45	52	20.28	<b>100</b>
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	<b>100</b>	128.27	<b>100</b>	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

**Compound Number 138**

**<sup>13</sup>C**



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

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.04	s	
Ac Me	2.11	s	
Ac Me	2.31	s	
B $\beta$	1.51	d	6.6
OMe	3.85	s	
$\beta$ 1	4.13	dd	10.4, 3.9
$\beta$ 2	4.25	dd	10.4, 7.8
B $\alpha$	5.83	q	6.6
$\alpha$	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

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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 $\beta$	21.98	52	22.35	50	21.78	64
OMe	55.98	59	56.30	52	55.79	64
$\beta$	70.49	43	71.18	44	69.76	36
B $\alpha$	71.92	43	72.20	47	71.13	56
$\alpha$	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
A5	119.09	52	119.70	43	118.71	44
A6	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
A 4Ac 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**

<sup>13</sup>C

|--|--|

**G- $\beta$ -S5**

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

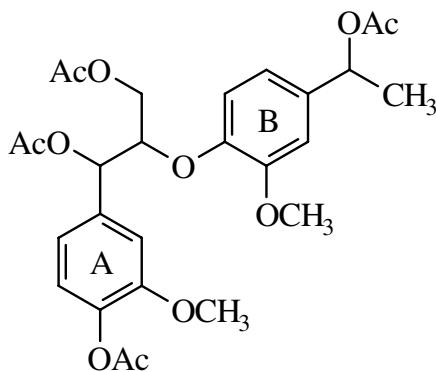
**<sup>1</sup>H** (chloroform)

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 $\beta$	1.51	d	6.6
A OMe	3.82	s	
B OMe	3.77	s	
$\gamma$ 1	3.95	dd	11.8, 3.2
$\gamma$ 2	4.34	dd	11.8, 4.7
$\beta$	4.54	m	
B $\alpha$	5.79	q	6.6
$\alpha$	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  
 $\gamma$  63.28 B2,6 103.91  
 $\text{Ba}$  72.68 2 112.17  
 $\alpha$  75.06 6 119.99  
 $\beta$  81.26 5 123.36

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\beta$	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
$\gamma$	63.48	18	64.17	42	63.14	13
B $\alpha$	72.38	29	72.71	48	71.70	23
$\alpha$	75.25	36	76.25	32	75.28	13
$\beta$	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

*threo*

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

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
B $\beta$	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	
$\gamma$ 1	4.04	dd	11.9, 5.6
$\gamma$ 2	4.30	dd	11.9, 4.6
$\beta$	4.61	m	
B $\alpha$	5.82	q	6.6
$\alpha$	6.11	d	6.3

**Notes:**

S. Ralph SRIII-65-D

44mg

erythro data

$\gamma$  63.0 62.5 61.8

$\alpha$  73.7 74.5 73.1

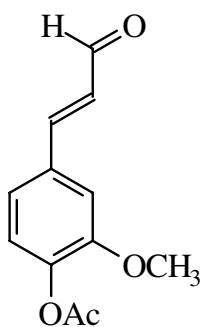
$\beta$  80.1 80.2 78.3

B4 146.7 147.7 146.1

Atom	CDCl <sub>3</sub>		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 $\beta$	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
$\gamma$	62.99	41	63.55	37	62.43	32
B $\alpha$	72.06	57	72.39	46	71.37	71
$\alpha$	74.41	41	75.34	39	74.26	39
$\beta$	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

Compound Number 141

<sup>13</sup>C



acetylated coniferylaldehyde  
4-acetoxy-3-methoxycinnamaldehyde

<sup>1</sup>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
	9.69	d	7.7

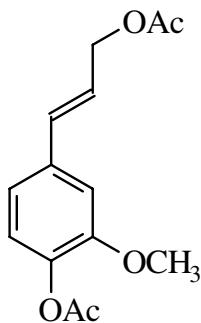
Notes:

S. Ralph SRIII-76B  
30mg

in acetone 3 & α switch places

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C

**acetylated coniferyl alcohol**  
**4-acetoxy-3-methoxycinnamylacetate**

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.59	75	20.45	72	20.27	98
Ac Me	20.92	56	20.76	48	20.60	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	168.83	30	168.89	22	168.37	49
γAc C=O	170.68	21	170.69	16	170.02	33

### <sup>1</sup>H (acetone)

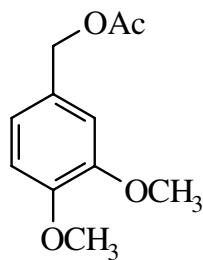
Atom	H Shifts	Mult	J
Ac Me	2.04	s	
Ac Me	2.23	s	
OMe	3.8	s	
γ	4.69	dd	
β	6.36	dt	
α	6.68	dt	
5	7.01	m	
6	7.01	m	
2	7.21	s	

### Notes:

M.Mozuch 177/95 47mg

Compound Number 143

<sup>13</sup>C



Acetylated veratryl alcohol  
3,4-dimethoxybenzylacetate

Atom	<sup>CDCl<sub>3</sub></sup>		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
$\alpha$	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

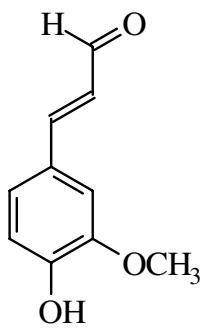
### <sup>1</sup>H (acetone)

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

### Notes:

M.Mozuch 177/95 48mg

## Compound Number 144

<sup>13</sup>C

**coniferaldehyde**  
**4-hydroxy-3-methoxycinnamaldehyde**

<sup>1</sup>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

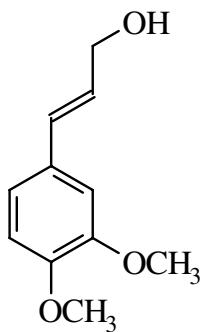
**Notes:**

Aldrich 40mg

Note: In DMSO β and 1 are coincident

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

3,4-dimethoxycinnamyl alcohol

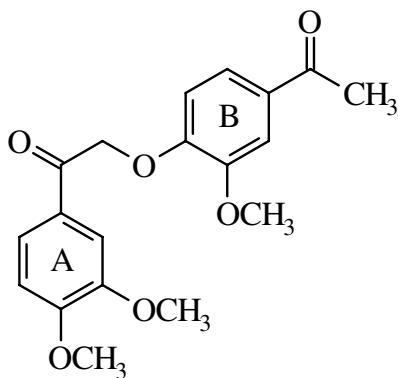
<sup>1</sup>H (acetone)

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 CDCl<sub>3</sub>



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

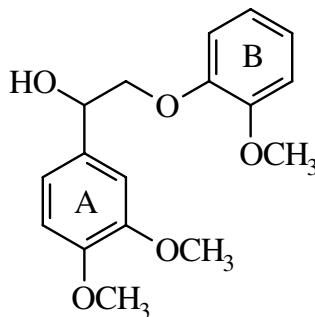
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\beta$	2.50	s	
OMe	3.87	s	
OMe	3.89	s	
OMe	3.90	s	
$\beta$	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

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$	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
$\beta$	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
$\alpha$	192.22	29	192.90	24	192.24	44
B $\alpha$	196.56	23	196.36	20	196.17	33



Atom	CDCl <sub>3</sub>		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

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

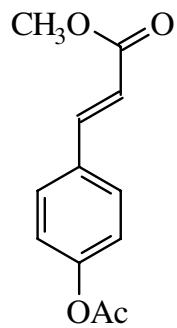
<sup>1</sup>H (acetone)

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

## Notes:

LLL V-59B  
 β-carbon in CDCl<sub>3</sub> was observed as shoulder on solvent.

Very limited solubility in acetone; DEPT was run in DMSO.



**acetylated methyl coumarate  
methyl 4-acetoxy cinnamate**

<sup>1</sup>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

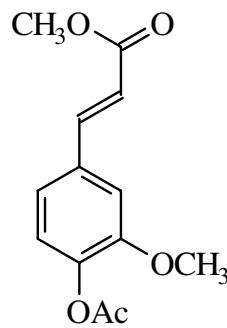
**Notes:**

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

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C



acetylated methyl ferulate  
methyl 4-acetoxy-3-methoxycinnamate

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.54	68	20.46	70	20.28	100
$\gamma$ 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
$\beta$	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
$\alpha$	144.12	85	144.68	100	143.81	92
3	151.57	37	152.72	30	151.10	58
Ac C=O	167.15	32	167.41	33	166.52	58
$\gamma$	168.59	27	168.76	26	168.19	46

### <sup>1</sup>H (acetone)

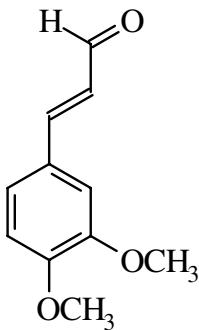
Atom	H Shifts	Mult	J
Ac Me	2.25	s	
$\gamma$ OMe	3.74	s	
OMe	3.86	s	
$\beta$	6.54	d	16.0
5	7.09	d	8.1
6	7.23	dd	8.1, 1.7
2	7.41	d	1.7
$\alpha$	7.64	d	16.0

### Notes:

J. Ralph P.S. 171.1

Compound Number 150

<sup>13</sup>C



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	56.01	<b>100</b>	56.26	<b>100</b>	55.51	<b>100</b>
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

3,4-dimethoxy cinnamaldehyde

<sup>1</sup>H (acetone)

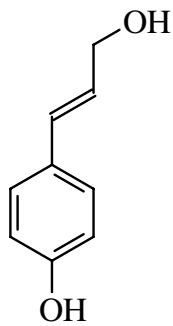
Atom	H Shifts	Mult	J
OMe	3.88	s	
OMe	3.90	s	
β	6.70	dd	158
5	7.05	d	83
6	7.28	dd	83,20
2	7.38	d	158,77
α	7.62	d	20
γ	9.67	d	77

Notes:

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

Compound Number 151

<sup>13</sup>C



p-Coumaryl alcohol  
4-hydroxycinnamyl alcohol

<sup>1</sup>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

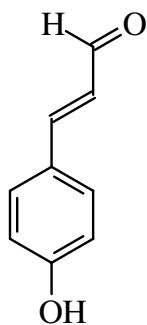
Notes:

S. Ralph  
36mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C



p-Coumaraldehyde  
4-hydroxy cinnamaldehyde

<sup>1</sup>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

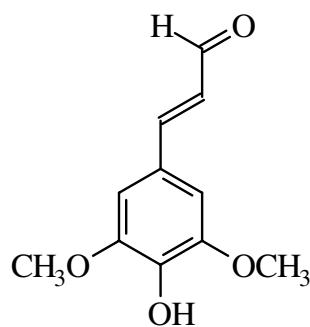
Notes:

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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C



**Sinapaldehyde**  
**3,4-dimethoxy-4-hydroxycinnamaldehyde**

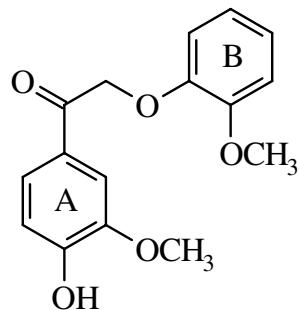
<sup>1</sup>H (acetone)

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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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



Atom	CDCl <sub>3</sub>		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

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

<sup>1</sup>H (acetone)

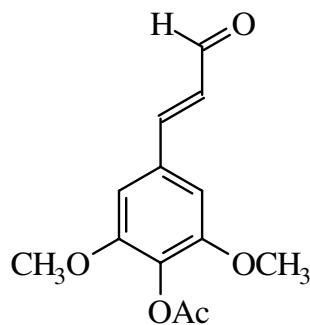
Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.92	s	
β	5.36	s	

## Notes:

S. Ralph

**Compound Number 155**

<sup>13</sup>C



**Acetylated sinapaldehyde  
4-acetoxy-3,5-dimethoxycinnamaldehyde**

<sup>1</sup>H (acetone)

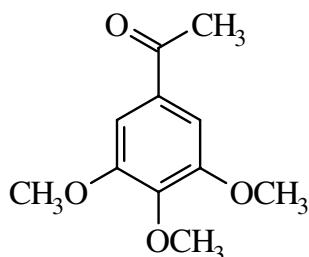
Atom	H Shifts	Mult	J
Ac Me	2.26	s	
OMe	3.87	s	
β	6.81	dd	15.9, 7.6
2,6	7.12	s	
α	7.61	d	15.9
γ	9.68	d	7.6

**Notes:**

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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C

3,4,5-Trimethoxyacetophenone

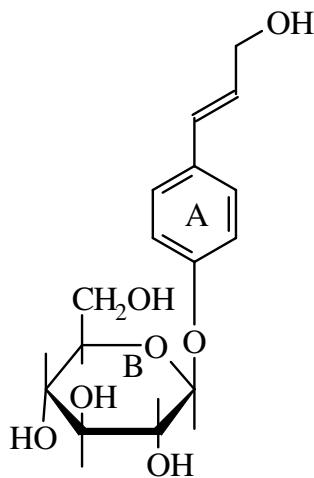
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
β	26.39	43	26.52	47	26.50	51
OMe	56.34	100	56.57	100	56.01	100
OMe	56.34	100	56.57	100	56.01	100
4 OMe	60.91	41	60.64	44	60.07	47
2	106.00	75	106.85	80	105.80	87
6	106.00	75	106.85	80	105.80	87
1	132.49	23	133.51	19	132.18	30
4	142.77	9	143.62	8	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

<sup>1</sup>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



**p-Gluco cinnamyl alcohol  
4-(3-hydroxy-1-propenyl)phenyl- $\beta$ -D-glucopyranoside**

<sup>1</sup>H (DMSO)

Atom	H Shifts	Mult	J
$\gamma$	4.09	dd	5.2
$\beta$	6.24	dt	15.9, 5.0
$\alpha$	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 $\alpha$	3.46	m	11.7,6.0
B6 $\beta$	3.70	ddd	11.7
B6 OH	4.58	t	5.7
$\gamma$ OH	4.83	t	5.4

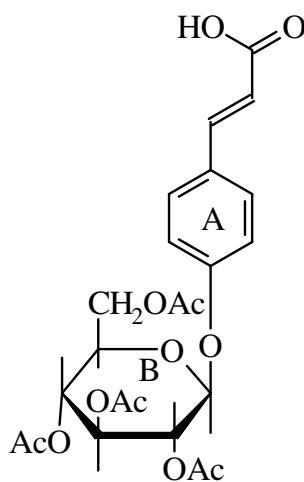
**Notes:**

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

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B6					60.63	36
$\gamma$					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
$\alpha$					127.97	50
$\beta$					128.71	45
A1					130.58	36
A4					156.62	41

Compound Number 158

<sup>13</sup>C



acetylated p-gluco cinnamic acid

Atom	CDCl <sub>3</sub>		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
$\beta$	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
$\alpha$	145.76	39	144.67	40	143.05	53
4	158.52	29	159.39	33	157.60	38
$\gamma$	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

<sup>1</sup>H (acetone)

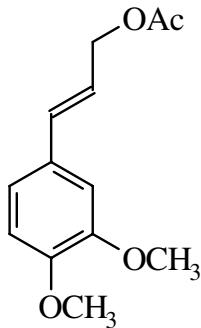
Atom	H Shifts	Mult	J
$\beta$	6.44	d	16.0
A3,5	7.13	d	8.8
$\alpha$	7.64	d	8.7
A2,6	7.68	d	15.7

Notes:

N. Terashima  
22mg  
 $\beta + 3,5$  switch places in CDCl<sub>3</sub>

**Compound Number 159**

<sup>13</sup>C



3,4-dimethoxycinnamyl acetate

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

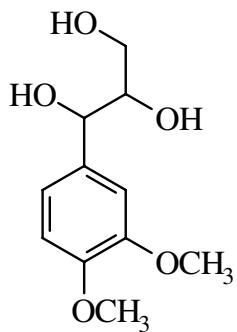
<sup>1</sup>H (acetone)

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

Compound Number 160

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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		

<sup>1</sup>H (acetone)

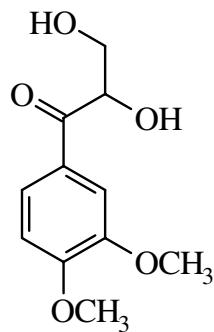
Atom	H Shifts	Mult	J
OMe	3.77	s	
OMe	3.78	s	
γ1	3.36	dd	
γ2	3.48	dd	
β	3.62	m	
α	4.58	d	
5	6.86	m	
6	6.86	m	
2	7.00	bs	

## Notes:

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

Compound Number 161

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		

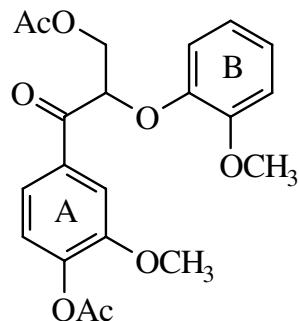
1-(3,4-dimethoxyphenyl)-2,3-dihydroxypropan-1-one

<sup>1</sup>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

**Erone diacetate**

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

**<sup>1</sup>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	
$\gamma^1$	4.49	dd	6.5, 11.9
$\gamma^2$	4.65	dd	3.9, 11.9
$\beta$	5.84	dd	3.9, 6.5
A2,6	7.81	m	
A5	7.23	d	8.8

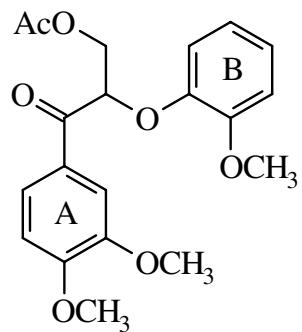
**Notes:**

L.Landucci 30 mg  
Not run in DMSO

Atom	CDCl <sub>3</sub>		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		
$\gamma$	64.36	70	64.66	70		
$\beta$	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		
$\gamma$ Ac C=O	170.82	30	170.90	28		
$\alpha$	194.59	40	195.10	31		

Compound Number 163

<sup>13</sup>C



Veratrone acetate

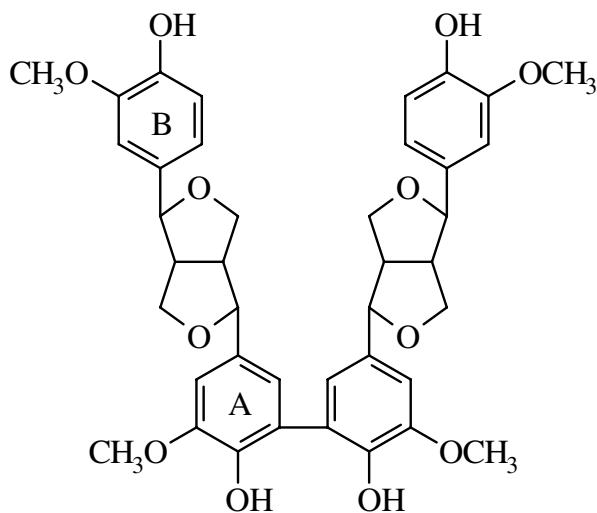
Atom	<i>CDCl</i> <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.78	84	20.64	64	20.44	95
OMe	55.79	100	56.05	82	55.40	93
OMe	55.96	95	56.17	100	55.53	100
OMe	56.07	93	56.22	96	55.74	90
γ	64.62	86	64.85	79	63.60	67
β	80.28	89	80.00	82	79.08	67
A2	110.22	82	111.59	82	110.70	74
A5	111.10	84	112.06	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

### <sup>1</sup>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



Pinoresinol biphenyl

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
A $\beta$	54.13	81	55.26	100	53.60	93
B $\beta$	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 $\gamma$	71.66	62	72.19	60	70.86	53
B $\gamma$	71.82	62	72.33	59	70.98	51
A $\alpha$	85.82	72	86.67	93	85.14	66
B $\alpha$	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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
OMe	3.82	s	
OMe	3.87	s	
A,B $\gamma$ 2	4.21	dd	6.8, 9.0
A,B $\alpha$	4.67	d	4.5

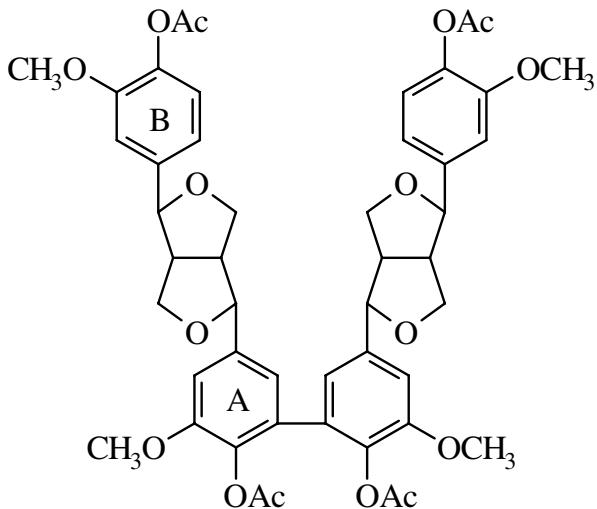
## Notes:

J.Pew

15 mg

As this compound has a plane of symmetry

The shifts for the other half are identical.



Pinoresinol biphenyl acetate

Atom	CDCl <sub>3</sub>		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 $\beta$	54.28	65	55.40	86	54.57	74
B $\beta$	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 $\gamma$	71.95	66	72.62	100	72.09	69
B $\gamma$	72.05	45	72.62	100	72.09	69
A $\alpha$	85.49	100	86.17	72	85.32	47
B $\alpha$	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

<sup>1</sup>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 $\beta$	3.14	m	
A,B $\gamma$	4.28	m	
A,B $\alpha$	4.80	m	

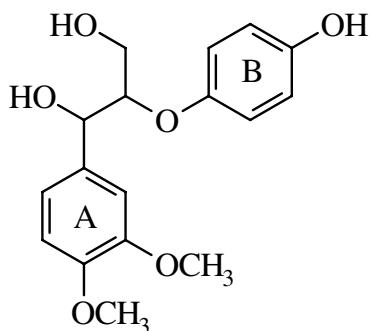
## Notes:

J. Pew

7 mg intensities for some peaks are irregular

As this compound has a plane of symmetry

The shifts for the other half are identical.



Atom	CDCl <sub>3</sub>		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		

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

### <sup>1</sup>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

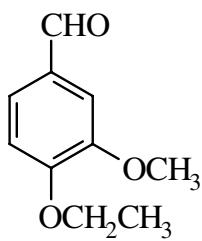
### Notes:

M. Mozuch

40 mg not very soluble in CDCl<sub>3</sub>, not run  
in DMSO, minor isomer shifts: γ 61.96,  
α 73.94, β 85.17 in acetone.

Compound Number 167

<sup>13</sup>C



Ethyl vanillin

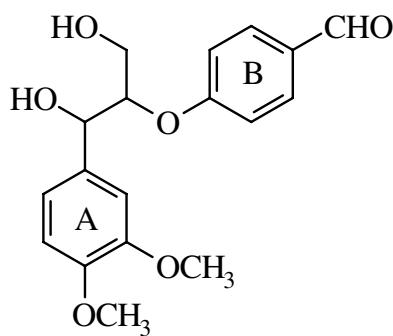
Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Me	14.38	87	14.92	75		
OMe	55.77	100	56.00	100		
CH2	64.39	88	65.02	83		
2	108.97	59	110.36	79		
5	111.07	73	112.52	93		
6	126.53	65	126.65	70		
1	129.69	33	130.98	30		
3	149.51	23	150.72	20		
4	153.71	24	154.88	20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

### <sup>1</sup>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
$\alpha$	9.85	s	

### Notes:

M. Mozuch  
40 mg  
Not run in DMSO



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

**<sup>1</sup>H** (chloroform)

Atom	H Shifts	Mult	J
OMe	3.82	s	
$\beta$	4.54	m	
$\alpha$	4.99	d	5.6
B 2,6	7.72	m	
B $\alpha$	9.78	s	

**Notes:**

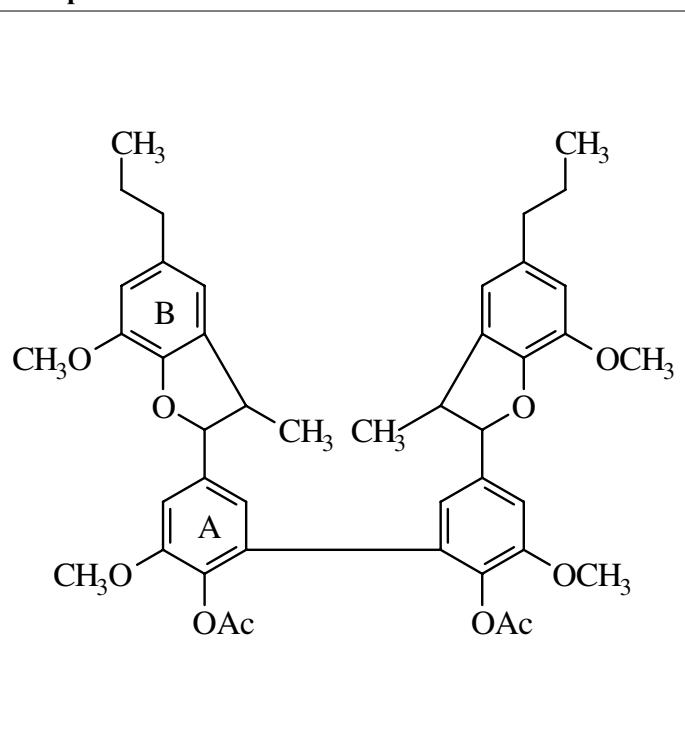
S. Kawai  
50 mg

Minor isomer:  $\gamma$  61.37,  $\alpha$  73.62,  $\beta$  82.58 in  
 $\text{CDCl}_3$

Atom	$\text{CDCl}_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe	55.87	100	56.03	91		
$\gamma$	61.71	37	62.00	39		
$\alpha$	74.04	41	73.55	36		
$\beta$	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 $\alpha$	190.78	31	191.01	47		

**Compound Number 169**

<sup>13</sup>C



**Phenylcoumaran biphenyl acetate**

Atom	<sup>13</sup> CDCl <sub>3</sub>		<sup>13</sup> CAcetone		<sup>13</sup> CDMSO	
	CS	i	CS	i	CS	i
B $\gamma$	13.75	<b>100</b>	14.10	97	13.71	<b>100</b>
$\gamma$	17.71	75	18.49	74	17.81	57
Ac Me	20.26	77	20.30	67	19.96	49
B $\beta$	24.92	85	25.73	64	24.56	83
B $\alpha$	37.91	82	38.53	86	37.29	60
$\beta$	45.76	73	46.82	61	45.26	49
OMe	55.85	88	56.43	<b>100</b>	55.66	79
OMe	56.00	81	56.48	93	56.04	64
$\alpha$	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

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B $\gamma$	0.92	t	73
$\gamma$	1.41	d	68
B $\beta$	1.60	m	75
Ac Me	2.02	s	
B $\alpha$	2.51	m	73
$\beta$	3.42	m	
OMe	3.82	s	
OMe	3.85	s	
$\alpha$	5.18	d	87
B2	6.63	s	
B6	6.69	s	
A2	6.96	d	18
A6	7.25	d	19

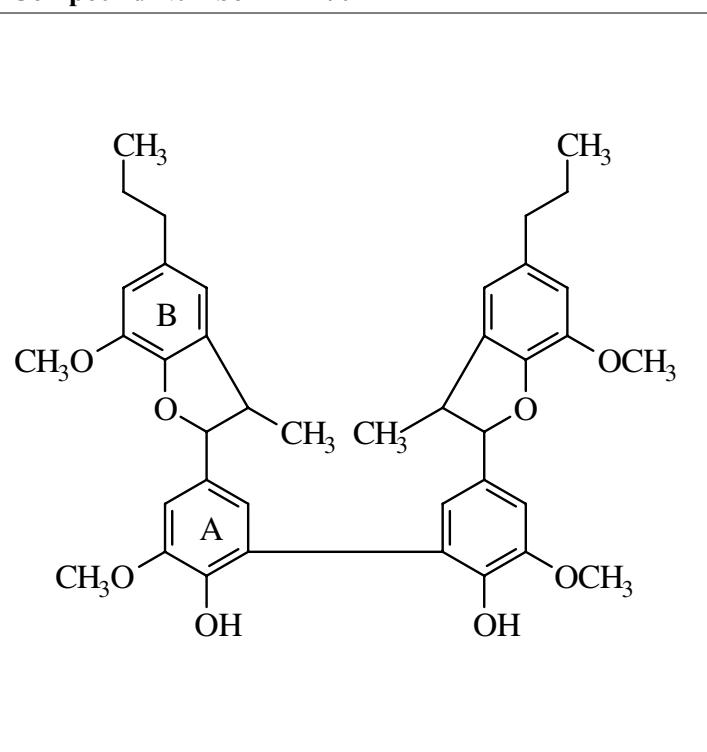
**Notes:**

J. Pew

50 mg

As this compound has a plane of symmetry

The shifts for the other half are identical.



Phenyl coumaran biphenyl

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\gamma$	13.91	100	14.10	100	13.77	100
$\gamma$	17.48	70	17.87	78	17.28	76
B $\beta$	25.08	84	25.79	100	24.62	84
B $\alpha$	38.07	84	38.54	93	37.32	64
$\beta$	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
$\alpha$	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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\gamma$	0.92	t	7.3
$\gamma$	1.37	d	6.8
B $\beta$	1.61	h	7.4
B $\alpha$	2.52	t	7.4
$\beta$	3.44	m	
OMe	3.80	s	
OMe	3.89	s	
$\alpha\alpha$	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

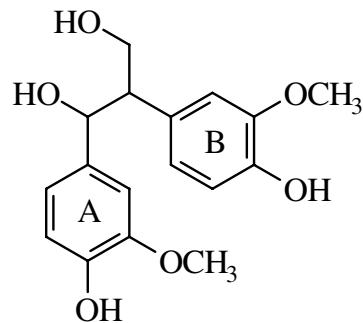
## Notes:

J. Pew

30 mg

As this compound has a plane of symmetry

The shifts for the other half are identical.



Atom	CDCl <sub>3</sub>		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

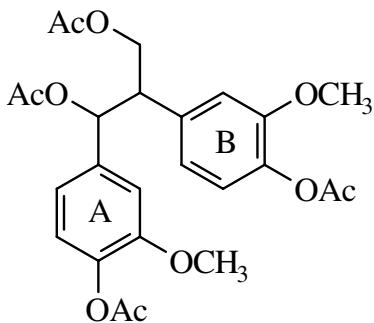
## 1,2-diguaiacylpropane-1,3-diol

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
OMe	3.67	s	
OMe	3.72	s	
β	3.94	m	
α	5.02	d	

## Notes:

S. Ralph  
15 mg  
β shifts above OME's in acetone



1,2-diguaiaicylpropane-1,3-diol tetraacetate

Atom	CDCl <sub>3</sub>		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
γ Ac C=O	170.74	26	170.74	20	169.98	35

<sup>1</sup>H (acetone)

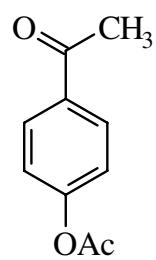
Atom	H Shifts	Mult	J
Ac Me	1.93	s	
Ac Me	1.98	s	
Ac Me	2.21	s	
Ac Me	2.22	s	
β	3.52	m	
γ1	4.21	dd	6.6, 11.0
γ2	4.38	dd	6.8, 11.3
α	6.18	d	6.6

## Notes:

S. Ralph  
15 mg

Minor isomer in d6-acetone  
β 50.70, γ 64.71, α 76.50

Compound Number 173

<sup>13</sup>C

Atom	$\text{CDCl}_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	21.11	39	20.98	40	20.51	47
$\beta$	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
$\alpha$	196.75	13	196.80	11	196.75	15

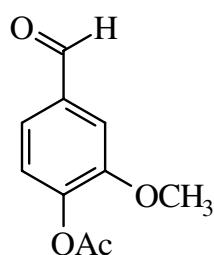
**4-acetoxy-acetophenone****<sup>1</sup>H (acetone)**

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

**Notes:**

Jamie Milhaupt  
JR-JMA 29.1  
50 mg

Compound Number 174

<sup>13</sup>C

**Vanillin acetate**  
**4-formyl-2-methoxy phenyl acetate**

<sup>1</sup>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
$\alpha$	9.97	s	

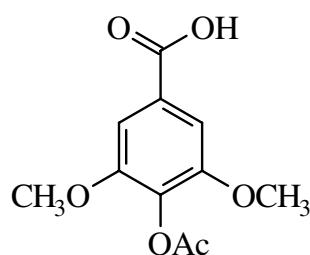
**Notes:**

Jamie Milhaupt  
 JR-JMA 23.1  
 50mg

Atom	CDCl <sub>3</sub>		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
$\alpha$	190.97	92	191.76	71	191.87	95

Compound Number 175

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

Syringic Acid Acetate  
4-acetoxy-3,5-dimethoxy benzoic acid

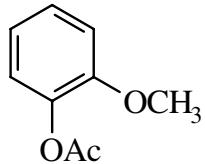
<sup>1</sup>H (acetone)

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

Compound Number 176

<sup>13</sup>C

**Guaiacol acetate**  
**2-methoxyphenyl acetate**

<sup>1</sup>H (acetone)

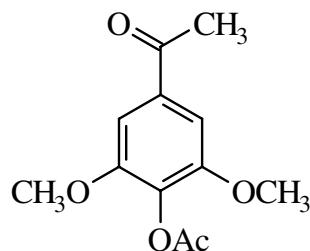
Atom	H Shifts	Mult	J
Ac Me	2.22	s	
OMe	3.79	s	
2	6.93	m	
5	7.20	m	
1	7.05	m	
6	7.05	m	

**Notes:**

Jamie Milhaupt  
 JR-JMA 27.1  
 54 mg

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C

**Acetosyringone acetate**  
**4-acetoxy-3,5-dimethoxy acetophenone**

### <sup>1</sup>H (acetone)

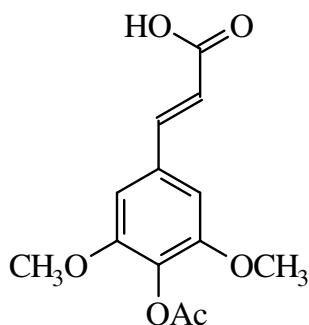
Atom	H Shifts	Mult	J
Ac Me	2.25	s	
β	2.58	s	
OMe	3.87	s	
2,6	7.31	s	

### Notes:

Jamie Milhaupt  
JR-JMA 31.1  
50 mg

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C

**Sinapic acid acetate**  
**4-acetoxy-3,5-dimethoxy cinnamic acid**

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac OMe	2.29	s	
OMe	3.86	s	
2,6	7.13	s	
$\beta$	6.66	d	5.9
$\alpha$	7.79	d	5.9

### Notes:

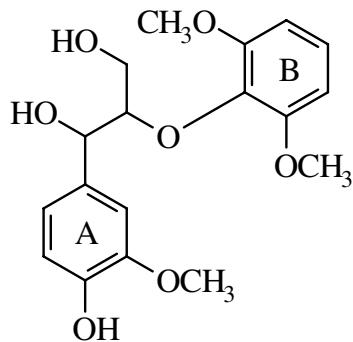
20 mg

sample has a minor impurity

Atom	CDCl <sub>3</sub>		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
$\alpha$	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
$\gamma$	162.19	25	163.11	15	162.61	28
Ac C=O	168.33	25	168.35	20	167.74	32

Compound Number 179

<sup>13</sup>C



*threo*

Guaiacylglycerol- $\beta$ -syringyl ether  
1-(4-hydroxy-3-methoxyphenyl)-2-(2,6-dimethoxyphenoxy)  
propane-1,3-diol

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma 1$	3.29	m	
$\gamma 2$	3.64	m	
$\alpha$	5.00	dd	7.5, 2.6
$\beta$	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	
$\alpha$ OH	4.36	dd	2.6, 1.1

Notes:

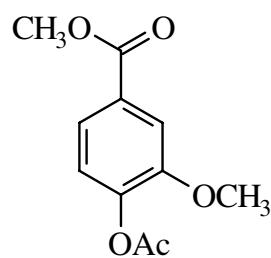
S. Lemke  
SLI 75B  
17.7mg  
erythro isomer shifts

C	A	D
$\gamma$ 60.59	60.94	59.71
$\alpha$ 72.52	73.35	72.04
$\beta$ 87.03	87.83	86.12

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\gamma$	60.49	42	61.31	46	60.08	31
$\alpha$	74.13	45	74.07	44	71.40	39
$\beta$	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

Compound Number 180

<sup>13</sup>C



4-acetoxy-3-methoxy methyl benzoate

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
$\alpha$ 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

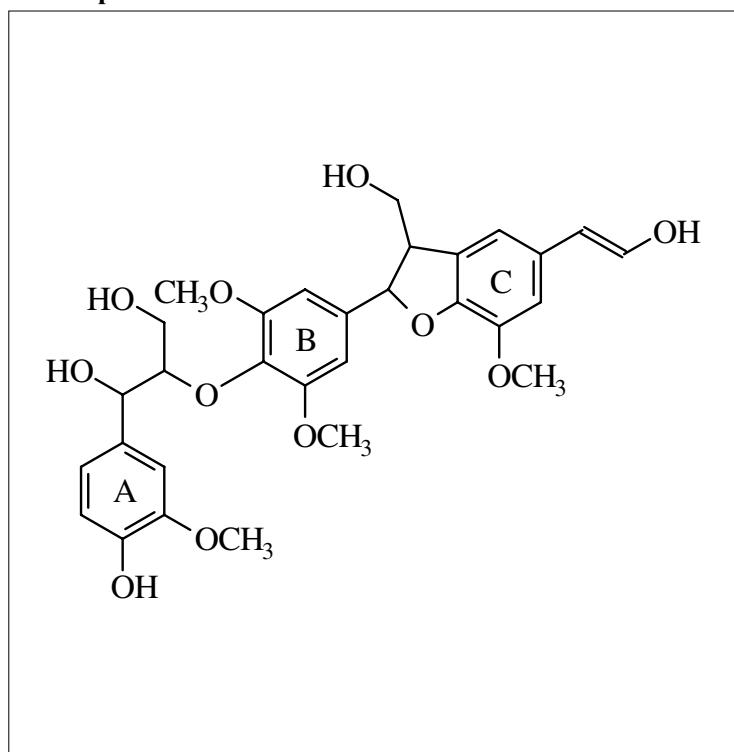
Notes:

Jamie Milhaupt  
JR-JMA 43.1  
50 mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.61	73	20.45	72	20.33	96
$\alpha$ 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
$\alpha$	166.33	33	166.53	20	165.56	46
Ac C=O	168.43	29	168.59	22	168.14	46

**Compound Number 181**

<sup>13</sup>C



G-b-S-c-CA

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$	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
$\gamma$	60.66	33	60.97	38	59.64	24
C $\gamma$	63.81	28	63.36	41	61.52	31
B $\gamma$	64.21	16	64.62	34	62.71	28
$\alpha$	72.64	20	73.37	41	71.98	33
$\beta$	87.19	29	87.87	38	86.14	31
B $\alpha$	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 $\beta$	126.87	23	128.57	35	128.02	22
C5	130.15	13	130.15	15	128.78	24
C $\alpha$	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
B4	134.75	13	136.10	8	134.79	15
B1	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

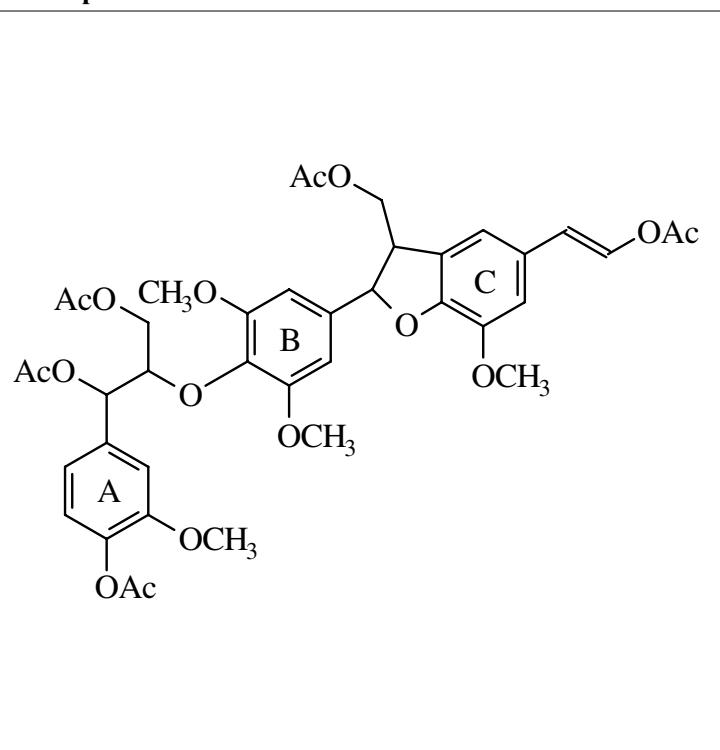
<sup>1</sup>H (acetone)

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

**Notes:**

S. Luque  
SLL 11C  
7mg  
Assignments from 360 MHz exps in acetone  
spectrum in CDCl<sub>3</sub> weak 3's,4's, and 1's  
uncertain

Landucci, Luque and Ralph  
J. Wood Chem. Tech.



Atom	CDCl <sub>3</sub>		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 $\beta$	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
$\gamma$	62.64	24	63.29	26	62.06	15
C $\gamma$	65.19	39	65.51	40	64.51	35
B $\gamma$	65.33	28	65.96	36	64.76	21
$\alpha$	74.00	26	75.03	32	73.68	18
$\beta$	80.95	21	81.37	33	79.94	22
B $\alpha$	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 $\beta$	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 $\alpha$	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

**<sup>1</sup>H** (acetone)

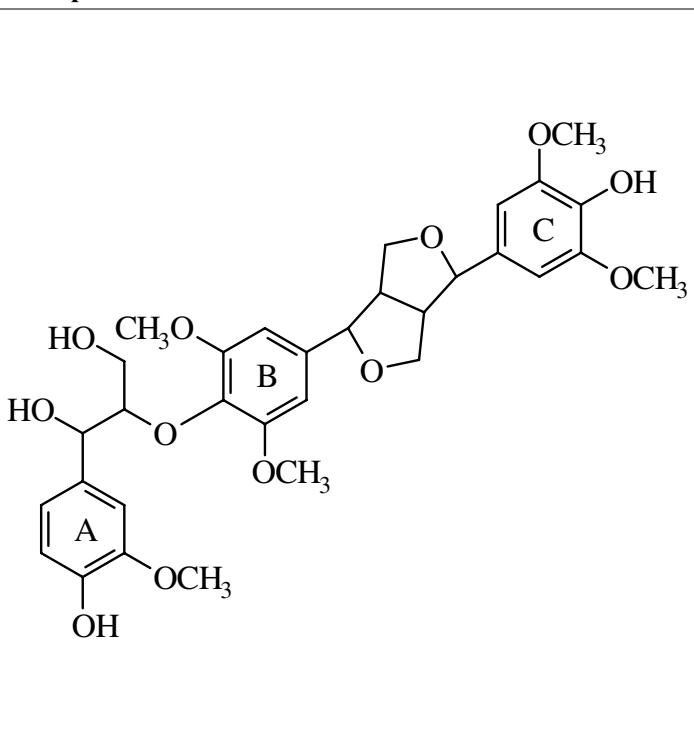
Atom	H Shifts	Mult	J
$\gamma^1$	4.16	dd	11.9, 4.0
C $\gamma$	4.65	dd	6.5, 1.2
$\alpha$	6.06	d	4.5
$\beta$	4.73	m	
B $\alpha$	5.54	d	7.1
B2,6	6.76	s	
C2	7.14	m	
C $\beta$	6.24	dt	15.8, 6.5
C $\alpha$	6.64	d	15.9

**Notes:**

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

**Compound Number 183**

<sup>13</sup>C



G-b-S-r-S

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$	54.32	27	55.23	32	53.61	22
C $\beta$	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
$\gamma$	60.57	36	60.97	34	59.84	22
C $\gamma$	71.76	22	72.38	33	71.13	22
B $\gamma$	72.08	25	72.57	33	71.27	25
$\alpha$	72.56	29	73.38	39	72.12	27
B $\alpha$	85.98	41	86.57	41	85.12	33
C $\alpha$	85.98	41	86.72	30	85.32	23
$\beta$	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

<sup>1</sup>H (acetone)

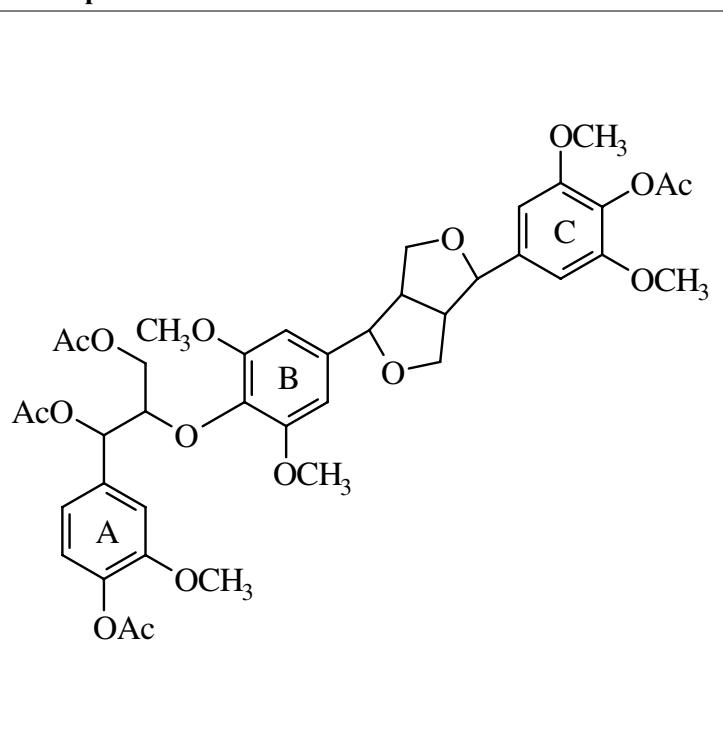
Atom	H Shifts	Mult	J
B $\beta$	3.11	m	
C $\beta$	3.11	m	
$\gamma$ 2	3.44	dd	72.0, 3.4
$\beta$	4.17	m	
C $\gamma$	4.22	m	
B $\gamma$	4.22	m	
C $\alpha$	4.67	d	4.0
B $\alpha$	4.73	d	4.0
$\alpha$	4.98	d	3.4
B2	6.76	s	
C2	6.67	s	
A2	7.03	s	

**Notes:**

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

**Compound Number 184**

<sup>13</sup>C



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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\beta$	54.16	25	55.33	30	53.67	39
C $\beta$	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
$\gamma$	62.50	26	63.29	36	62.10	26
B $\gamma$	71.87	25	72.65	53	71.36	45
C $\gamma$	71.98	25	72.65	53	71.36	45
$\alpha$	73.82	21	75.05	30	73.72	23
$\beta$	80.62	21	81.28	22	79.86	16
B $\alpha$	85.63	33	86.45	31	84.92	32
C $\alpha$	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

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B,C $\gamma$ 1	3.90	dd	
$\gamma$ 1	4.18	ddd	11.9, 4.1, 1.8
B,C $\gamma$ 2	4.27	dd	
$\gamma$ 2	4.39	ddd	11.8, 5.9, 0.8
B $\alpha$	4.72	d	4.4
C $\alpha$	4.76	d	4.4
$\alpha$	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

Assignments in d6-acetone based on the HMBC exp't

H assignments for 360 MHz spectra

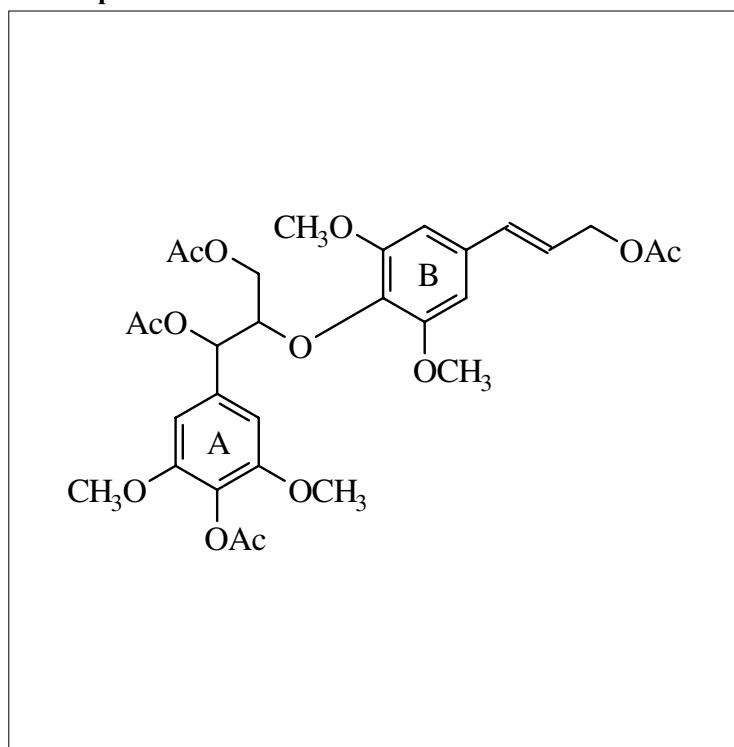
Landucci, Luque and Ralph

J. Wood Chem. Tech.

15(4), 493-513 (1995)

**Compound Number 185**

<sup>13</sup>C



S-b-SA (acetate)

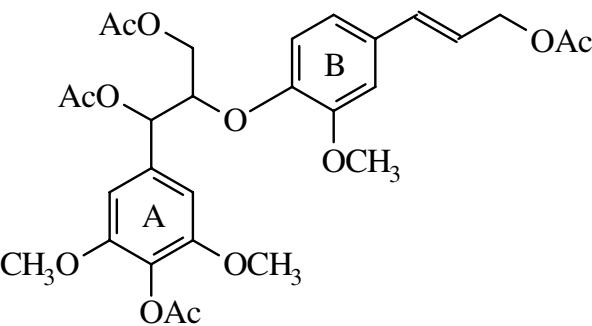
Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.46	43	20.26	49	20.04	47
Ac Me	20.76	43	20.63	47	20.29	52
Ac Me	20.99	43	20.80	44	20.62	75
Ac Me	21.07	47	20.93	47	20.62	75
OMe	56.02	96	56.39	100	55.73	100
OMe	56.02	96	56.39	100	55.73	100
OMe	56.17	100	56.49	96	55.86	91
OMe	56.17	100	56.49	96	55.84	91
$\gamma$	62.76	34	63.28	40	62.07	26
B $\gamma$	64.92	43	65.25	48	64.16	40
$\alpha$	74.25	35	75.29	41	73.84	91
$\beta$	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 $\beta$	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
B $\alpha$	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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac Me	3.81	s	
Ac Me	3.85	s	
$\gamma^2$	4.19	dd	11.8, 4.1
$\gamma^1$	4.43	dd	11.8, 6.1
B $\gamma$	4.68	dd	7.4, 1.2
$\alpha$	6.07	d	4.2
$\beta$	4.74	dt	6.1, 4.2
A6 or B6	3.78	s	
A2 or B2	6.80	s	
B $\beta$	6.33	dt	15.8, 6.3
B $\alpha$	6.63	d	16.0

**Notes:**

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



S-b-CA (acetate)

<sup>1</sup>H (acetone)

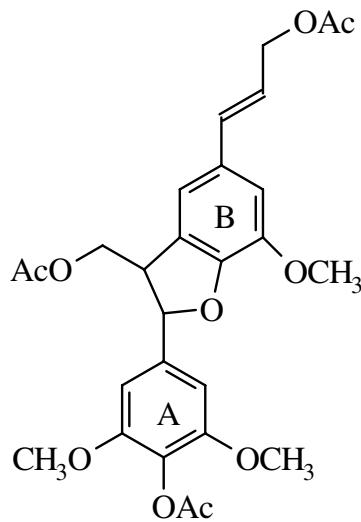
Atom	H Shifts	Mult	J
OMe	3.86	s	
OMe	3.81	s	
$\gamma^1$	4.38	dd	11.9, 5.9
$\gamma^2$	4.26	dd	11.9, 4.1
B $\gamma$	4.68	dd	6.4, 1.2
$\beta$	4.89	m	
$\alpha$	6.05	d	5.1
B $\beta$	6.30	dt	15.8, 6.4
B $\alpha$	6.63	d	15.9
A2,6	6.87	s	
B2	7.15	d	1.6

## Notes:

S. Ralph  
SR VII 16D  
15mg

Landucci, Luque and Ralph  
J. Wood Chem. Tech.  
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Atom	CDCl <sub>3</sub>		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
$\gamma$	62.73	37	63.09	43	61.88	29
B $\gamma$	56.15	43	65.36	52	64.31	45
$\alpha$	74.05	46	74.78	46	73.20	35
$\beta$	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 $\beta$	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 $\alpha$	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



S-c-CA (acetate)

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma_1$	4.48	dd	11.1, 5.5
$\gamma_2$	4.37	dd	11.1, 7.3
B $\gamma$	4.67	d	6.4
$\alpha$	5.59	d	7.1
B $\beta$	6.25	dt	15.9, 6.4
B $\alpha$	6.65	d	15.9
A2	6.84	s	
B2 or B6	7.05	s	
B2 or B6	7.07	s	

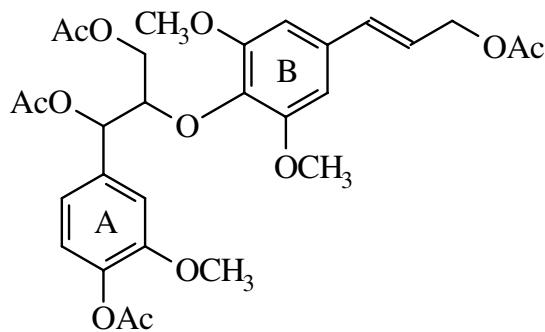
## Notes:

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

Atom	CDCl <sub>3</sub>		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
$\beta$	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 $\gamma$	65.26	53	65.50	35	64.51	48
$\gamma$	65.43	42	65.96	34	64.47	34
$\alpha$	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 $\beta$	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 $\alpha$	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**

**<sup>13</sup>C**



**G-b-SA acetate**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
OMe	3.84	s	
$\gamma^1$	4.42	dd	11.8, 6.0
$\gamma^2$	4.18	dd	11.8, 4.1
B $\gamma$	4.69	dd	6.2, 1.1
$\alpha$	6.08	d	4.3
B2,6	6.80	s	
B $\beta$	6.33	dt	15.9, 6.2
B $\alpha$	6.64	d	16.0

**Notes:**

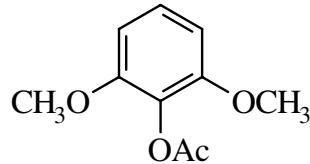
S. Ralph  
SR VII - 17A  
16mg

Landucci, Luque and Ralph  
J. Wood Chem. Tech.  
15(4), 493-513 (1995)

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\gamma$	62.74	32	63.24	43	62.05	27
B $\gamma$	65.00	39	65.26	49	64.24	37
$\alpha$	74.09	35	75.07	38	73.67	29
$\beta$	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 $\beta$	122.97	41	124.14	45	123.43	34
B1	132.46	28	133.39	25	132.02	28
B $\alpha$	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
A5	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**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

**2,6-dimethoxyphenol acetate**

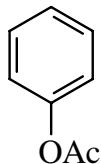
<sup>1</sup>H (acetone)

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

Compound Number 190

<sup>13</sup>C

phenol acetate

<sup>1</sup>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	

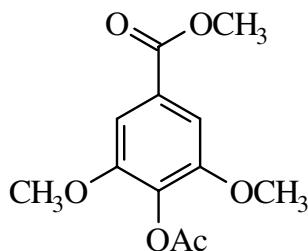
## Notes:

Jamie Milhaupt  
JR-JMA 55  
54mg

Atom	CDCl <sub>3</sub>		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

Compound Number 191

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.40	42	20.22	43	20.06	48
$\alpha$ 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
$\alpha$	166.37	16	166.61	11	165.75	25
Ac C=O	168.14	17	168.17	13	167.67	26

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

<sup>1</sup>H (acetone)

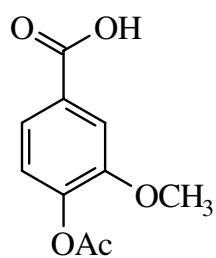
Atom	H Shifts	Mult	J
Ac Me	2.26	s	
$\alpha$ OMe	3.88	s	
OMe	3.87	s	
2,6	7.33	s	

Notes:

Jamie Milhaupt  
JR-JMA 41.1  
40mg

Compound Number 192

<sup>13</sup>C



4-acetoxy-3-methoxy benzoic acid

<sup>1</sup>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

**Notes:**

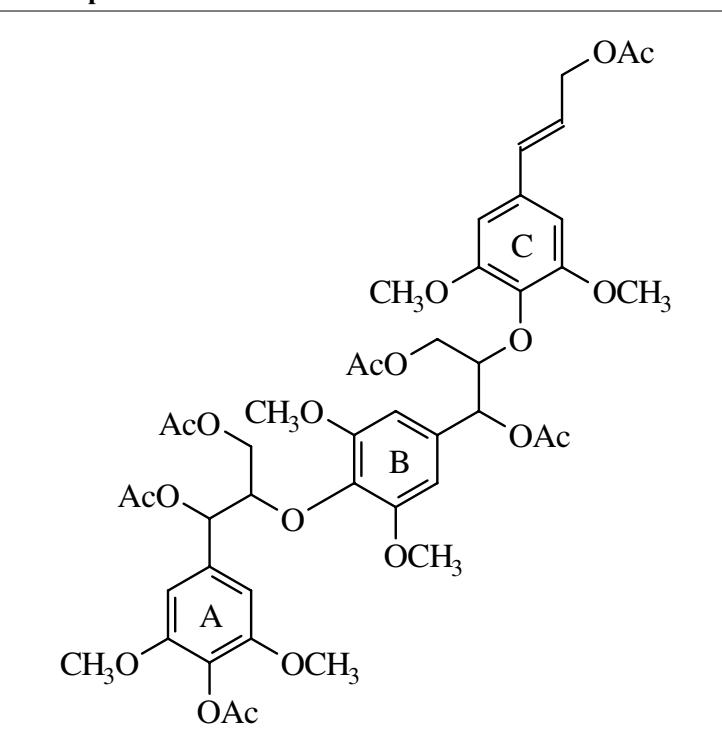
Jamie Milhaupt

JR-JMA 39.1

41mg

2D short range XH corr confirms assignment  
of 5 and 6.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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



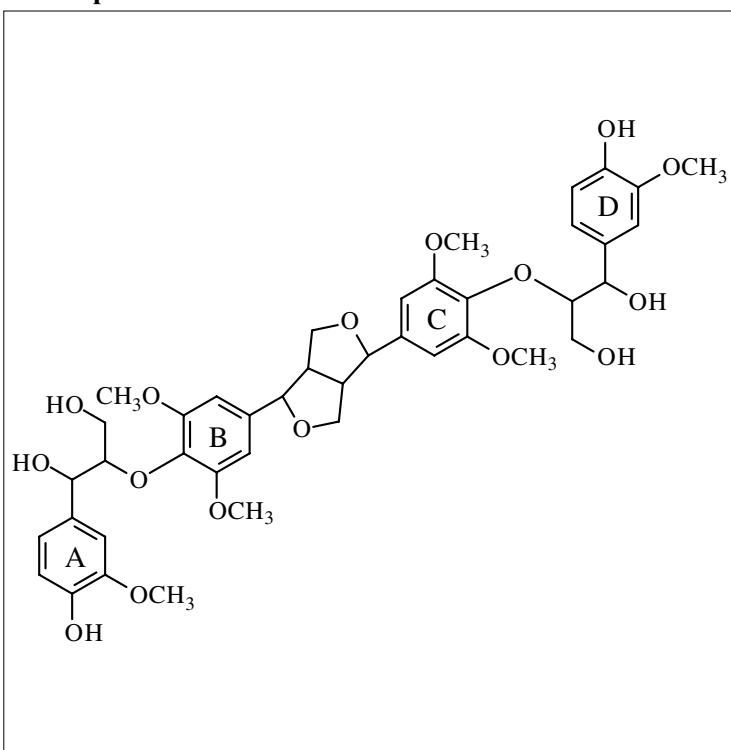
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.53	70	20.26	41	20.04	50
Ac Me	20.53	70	20.26	41	20.04	50
Ac Me	20.85	56	20.67	27	20.21	33
Ac Me	20.85	56	20.80	21	20.30	35
Ac Me	21.15	73	20.95	46	20.61	70
Ac Me	21.15	73	20.95	46	20.61	70
OMe	56.12	100	56.46	100	55.72	100
OMe	56.12	100	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
$\gamma$	62.88	33	63.44	22	62.22	26
B $\gamma$	62.88	33	63.44	22	62.22	26
C $\gamma$	65.00	22	65.26	17	64.16	19
$\alpha$	74.35	23	75.43	32	73.97	20
B $\alpha$	74.50	23	75.43	32	73.97	20
$\beta$	80.89	33	81.42	14	79.89	17
B $\beta$	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 $\beta$	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 $\alpha$	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

**Notes:**

L.Landucci  
LLL XIV 148BA  
10 mg

**Compound Number 194**

**<sup>13</sup>C**



Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
B,C $\beta$	54.48	30	55.37	40	53.56	31
OMe	56.00	80	56.26	70	55.41	69
OMe	56.27	<b>100</b>	56.62	<b>100</b>	55.89	<b>100</b>
OMe	56.27	100	56.62	100	55.89	100
A,D $\gamma$	60.56	43	60.97	34	59.73	25
B,C $\gamma$	72.01	27	72.64	38	71.21	25
A,D $\alpha$	72.55	32	73.38	36	72.00	25
B,C $\alpha$	85.86	25	86.53	40	84.97	25
A,D $\beta$	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

**<sup>1</sup>H (acetone)**

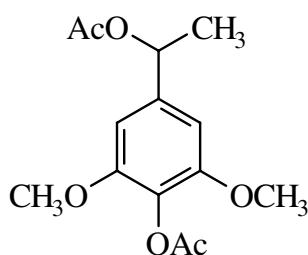
Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.87	s	
A,D $\gamma$ 2	3.71	dd	J=120,34
A,D $\alpha$	4.98	d	J=32
B,C $\alpha$	4.75	d	J=23
B,C 2,6	6.77	s	
A,D 2	7.04	d	J=1.

**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 symmetry  
The shifts for the other half are identical.

Compound Number 195

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

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

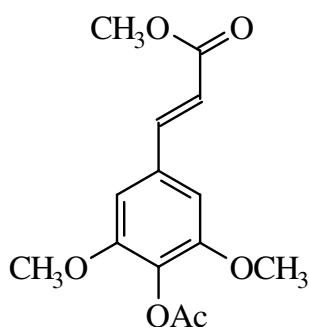
<sup>1</sup>H (acetone)

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

Notes:

J. Milhaupt  
A 51  
41mg

## Compound Number 196

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.36	45	20.23	39	20.00	49
γOMe	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

Acetylated Sinapic acid methyl ester

<sup>1</sup>H (acetone)

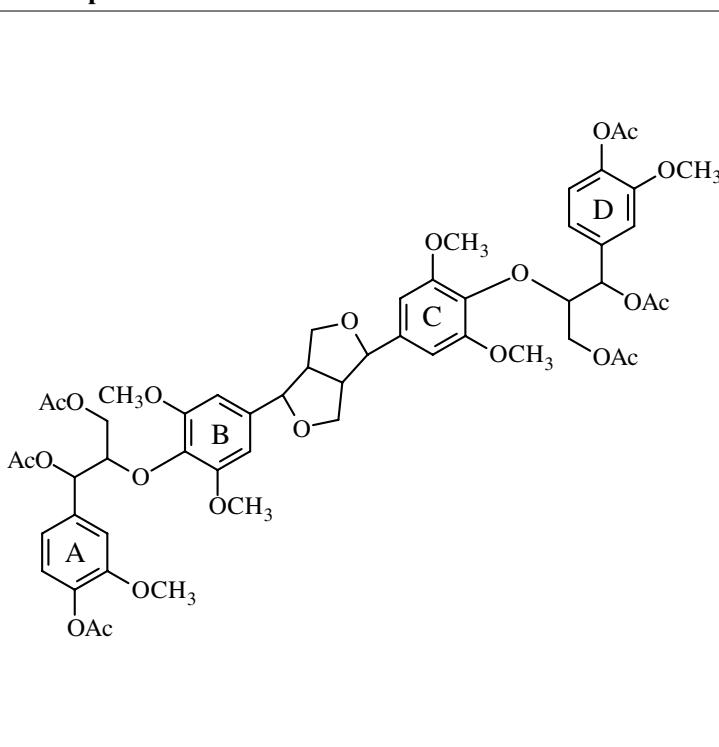
Atom	H Shifts	Mult	J
Ac Me	2.25	s	
γOMe	3.75	s	
OMe	3.87	s	
2,6	7.08	s	
β	6.58	d	J = 16.0
α	7.62	d	J = 16.1

## Notes:

J. Milhaupt  
A 45  
47mg

**Compound Number 197**

**<sup>13</sup>C**



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

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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

**<sup>1</sup>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

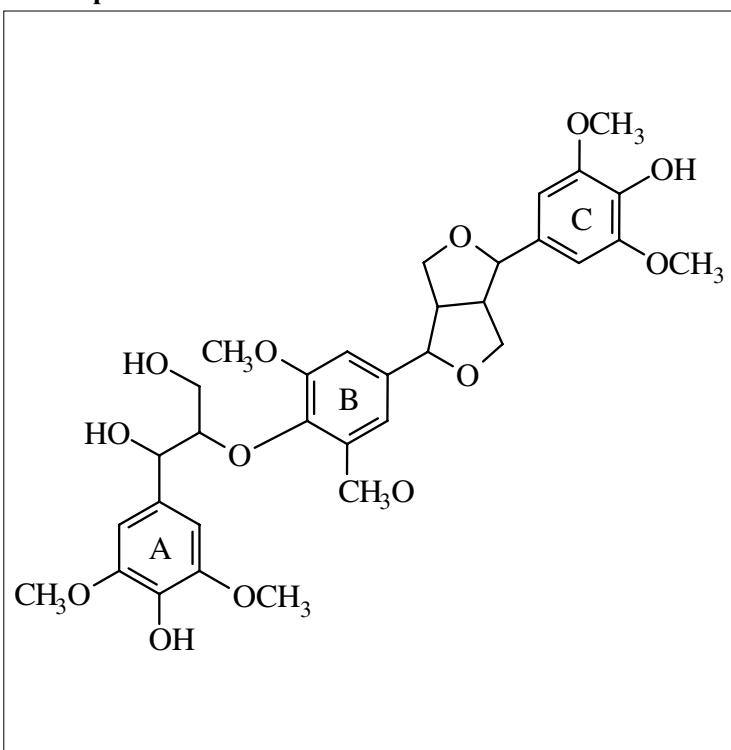
The β-O-4 units are erythro, some splitting of peaks can be seen due to the number of R and S isomers present, especially the resinol beta in CDCl<sub>3</sub>. In acetone a beta isomer at 55.47, in CDCl<sub>3</sub> at 53.93 and fine splitting of many peaks was observed at 360 MHz. Also a peak around 69 is unassigned.

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.

**Compound Number 198**

**<sup>13</sup>C**



**S-b-S-r-S**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B,C $\beta$	3.12	m	
OMe	3.80	s	
OMe	3.82	s	
OMe	3.88	s	
B $\alpha$	4.68	d	
C $\alpha$	4.74	d	J = 4.0
$\alpha$	4.99	m	
B 2,6	6.69	s	
C 2,6	6.71	s	
A 2,6	6.78	s	

**Notes:**

S. Luque  
SLL I 12E

10 mg

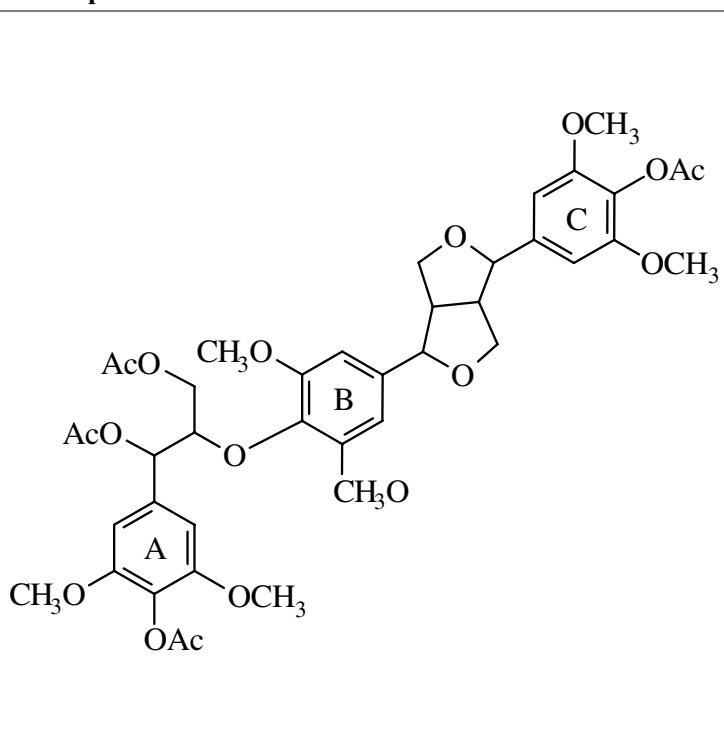
A4 was coincident with other shifts, the assignments were inferred from other models and peak heights.

Landucci, Luque and Ralph  
J. Wood Chem. Tech.  
15(4), 493-513 (1995)

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
B $\beta$	54.43	27	55.27	19	53.59	20
C $\beta$	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
$\gamma$	60.65	27	61.03	17	59.90	14
C $\gamma$	71.80	18	72.40	21	71.10	18
B $\gamma$	72.17	16	72.61	20	71.26	21
$\alpha$	72.77	14	73.63	17	72.38	20
B $\alpha$	86.01	23	86.61	20	85.10	20
C $\alpha$	86.01	23	86.73	21	85.30	22
$\beta$	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

**Compound Number 199**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\beta$	54.39	17	55.33	20	53.61	23
C $\beta$	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
$\gamma$	62.81	18	63.41	19	62.16	13
C $\gamma$	72.07	21	72.66	44	71.31	34
B $\gamma$	72.19	21	72.66	44	71.31	34
$\alpha$	74.25	16	75.33	15	73.92	13
$\beta$	80.78	15	81.29	11	79.76	12
B $\alpha$	85.82	21	86.45	25	84.85	19
C $\alpha$	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
C4	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
C1	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

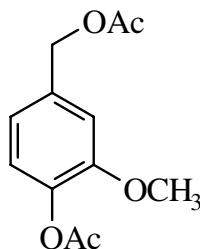
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B,C $\beta$	3.11	m	
B $\alpha$	4.73	d	
C $\alpha$	4.76	d	
$\alpha$	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)

Compound Number 200

<sup>13</sup>C

**Vanillyl alcohol diacetate**  
**4-hydroxy-3-methoxybenzyl alcohol diacetate**

**<sup>1</sup>H** (acetone)

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

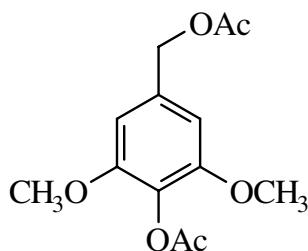
**Notes:**

S. Ralph  
 35mg

Atom	CDCl <sub>3</sub>		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
$\alpha$	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
$\alpha$ Ac C=O	170.66	23	170.79	19	170.15	36

Compound Number 201

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

Syringyl alcohol diacetate

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

<sup>1</sup>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	

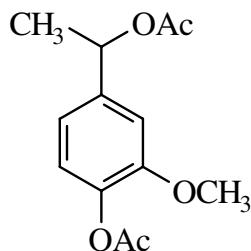
Notes:

J. Milhaupt

A 53

35 mg

Sample has impurity



Atom	CDCl <sub>3</sub>		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	166.95	22	168.44	49
α Ac C=O	170.21	30	170.17	19	169.55	42

**1-(4-acetoxy-3-methoxyphenyl)-1-acetoxyethane****<sup>1</sup>H (acetone)**

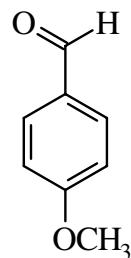
Atom	H Shifts	Mult	J
β	1.49	d	
Ac Me	2.03	s	
Ac Me	2.22	s	
OMe	3.82	s	
α	5.83	q	J = 6.6
6	6.95	dd	J = 8.1,1.8
5	7.02	d	J = 8.1
2	7.11	d	J = 1.8

**Notes:**

J. Milhaupt  
A 49.1  
35mg

**Compound Number 203**

<sup>13</sup>C



Atom	CDCl <sub>3</sub>		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
$\alpha$	190.68	45	191.09	42	191.01	51

**4-methoxy benzaldehyde**

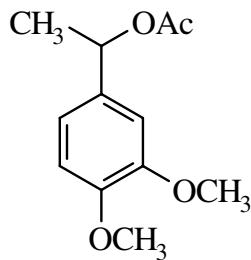
**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
OMe	3.89	s	
3,5	7.08	d	J = 8.8
2,6	7.85	d	J = 8.8
$\alpha$	9.86	s	

**Notes:**

Aldrich  
60mg

Compound Number 204

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

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

<sup>1</sup>H (acetone)

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

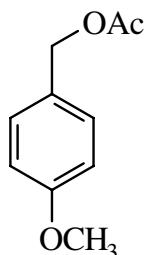
## Notes:

J. Milhaupt  
A 141  
38mg

**Compound Number 205**

**<sup>13</sup>C**

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\alpha$	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



**4-methoxybenzyl alcohol acetate**

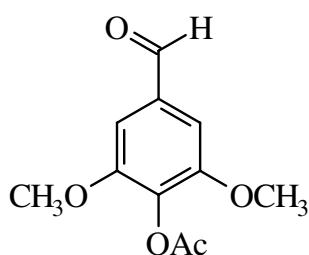
**<sup>1</sup>H (acetone)**

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

**Notes:**

J. Milhaupt  
A 139  
56mg

Compound Number 206

<sup>13</sup>C

**Syringaldehyde acetate**  
**3,5-dimethoxy-4-acetoxy-benzaldehyde**

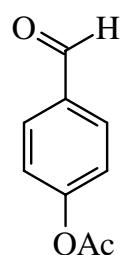
<sup>1</sup>H (acetone)

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

**Notes:**

J. Milhaupt  
 A 147  
 42mg

Atom	CDCl <sub>3</sub>		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
$\alpha$	191.00	45	191.82	31	191.89	48



Atom	CDCl <sub>3</sub>		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
$\alpha$	190.88	38	191.83	34	191.84	42

#### 4-Acetoxy benzaldehyde

#### <sup>1</sup>H (acetone)

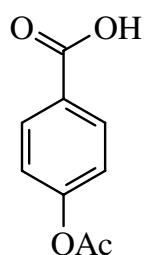
Atom	H Shifts	Mult	J
Ac Me	2.30	s	
3,5	7.35	d	J = 8.6
2,6	7.97	d	J = 8.6
$\alpha$	10.01	s	

#### Notes:

J. milhaupt  
137.5  
42mg

Compound Number 208

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\alpha$	168.89	22	167.00	17	166.55	20
Ac C=O	171.38	13	169.28	15	168.75	25

**4-Acetoxy benzoic acid**

**<sup>1</sup>H (acetone)**

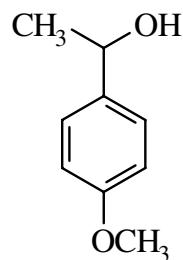
Atom	H Shifts	Mult	J
Ac Me	2.29	s	
3,5	7.26	d	J = 8.8
2,6	8.08	d	J = 8.8

**Notes:**

J. Milhaupt  
27mg

**Compound Number 209**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

4-Methoxy benzyl alcohol

<sup>1</sup>H (acetone)

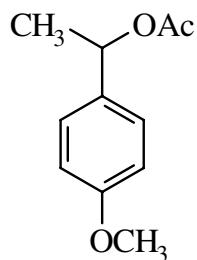
Atom	H Shifts	Mult	J
β	1.37	d	J = 6.5
OMe	3.76	s	
α	4.79	m	
3,5	6.86	d	J = 8.7
2,6	7.29	d	J = 8.6

**Notes:**

J. Milhaupt  
JMA 145  
42mg

Compound Number 210

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

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

<sup>1</sup>H (acetone)

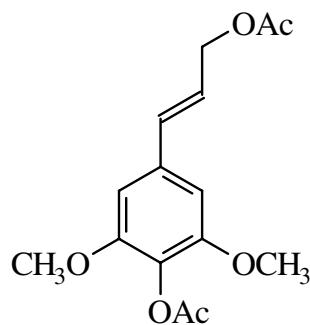
Atom	H Shifts	Mult	J
β	1.46	d	
Ac Me	1.98	s	
OMe	3.78	s	
α	5.79	q	J = 6.6
3,5	6.90	d	J = 8.8
2,6	7.30	d	J = 8.8

Notes:

J. Milhaupt  
JMA 149  
23mg

**Compound Number 211**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

**Sinapyl alcohol diacetate**

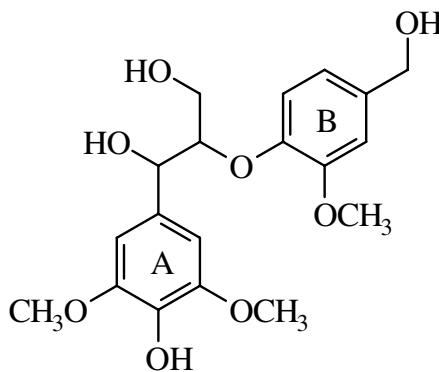
<sup>1</sup>H (acetone)

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

**Notes:**

J.Milhaupt  
JMA 111  
20mg

Compound Number 212

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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
$\gamma$	61.05	44	61.95	41	60.00	51
B $\alpha$	64.87	54	64.54	46	62.74	68
$\alpha$	74.16	47	74.06	51	70.88	57
$\beta$	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
B1	134.61	29	136.17	32	134.31	46
A4	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

**Syringylglycerol- $\beta$ -vanillyl alcohol ether**

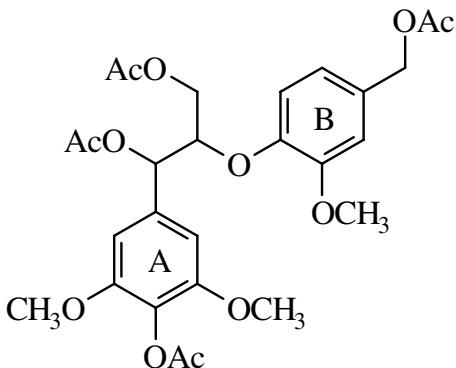
1-(4-Hydroxy-3,5-dimethoxyphenyl)-2-[4-(1-hydroxymethyl)-2-methoxy phenoxy]propane-1,3-diol

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
A OMe	3.80	s	
B OMe	3.86	s	
$\gamma_1$	3.50	m	
$\gamma_2$	3.69	m	
$\beta$	4.18	m	
B $\alpha$	4.56	d	
$\alpha$	4.87	m	5.6
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



**Syringylglycerol- $\beta$ -vanillyl alcohol ether tetra-acetate**  
**1-(4-acetoxy-3,5-dimethoxyphenyl)-1,3-diacetoxy-2-[4-(1-**  
**acetoxyethyl)-2-methoxyphenoxy]**

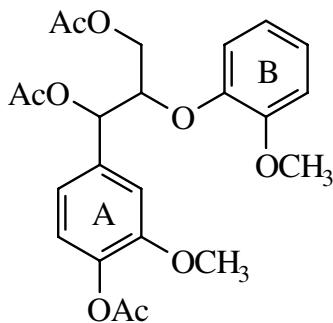
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.98	s	
Ac Me	2.03	s	
Ac Me	2.09	s	
Ac Me	2.21	s	
A OMe	3.80	s	
B OMe	3.83	s	
$\gamma_1$	4.05	s	12.3,5.9
$\gamma_2$	4.27	s	11.9,4.0
$\beta$	4.81	s	
B $\beta$	5.02	s	
$\alpha$	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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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	<b>100</b>
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	<b>100</b>	56.55	<b>100</b>	55.98	100
A OMe	56.14	100	56.55	100	55.98	100
$\gamma$	62.91	27	63.59	46	63.37	48
B $\alpha$	66.08	66	66.35	57	65.28	57
$\alpha$	74.57	50	75.64	50	74.48	53
$\beta$	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
B1	128.79	20	129.70	22	130.30	52
A4	130.88	36	132.09	30	134.92	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
Ac C=O	169.60	32	170.02	34	169.32	57
Ac C=O	170.48	34	170.72	24	167.94	59
Ac C=O	170.79	25	170.88	24	170.15	40

*erythro*

**Guaiacylglycerol- $\beta$ -guaiacyl ether acetate**  
**1-(4-acetoxy-3-methoxyphenyl)-1,3-diacetoxy-2-(2-methoxyphenoxo)propane**

<sup>1</sup>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	
$\gamma^1$	4.22	dd	11.9,4.2
$\gamma^2$	4.39	dd	11.9,5.8
$\beta$	4.83	m	
$\alpha$	6.09	d	5.0

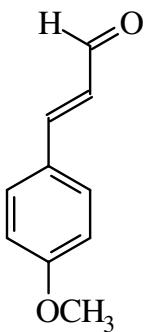
**Notes:**

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

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.57	<b>100</b>	20.46	84	20.22	<b>100</b>
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	<b>100</b>	55.54	81
OMe	55.90	85	56.32	100	55.66	81
$\gamma$	62.55	57	63.03	55	61.84	44
$\alpha$	73.79	60	74.63	55	73.10	49
$\beta$	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

Compound Number 215

<sup>13</sup>C



p-Methoxy cinnamaldehyde

Atom	<sup>13</sup> CDCl <sub>3</sub>		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

<sup>1</sup>H (acetone)

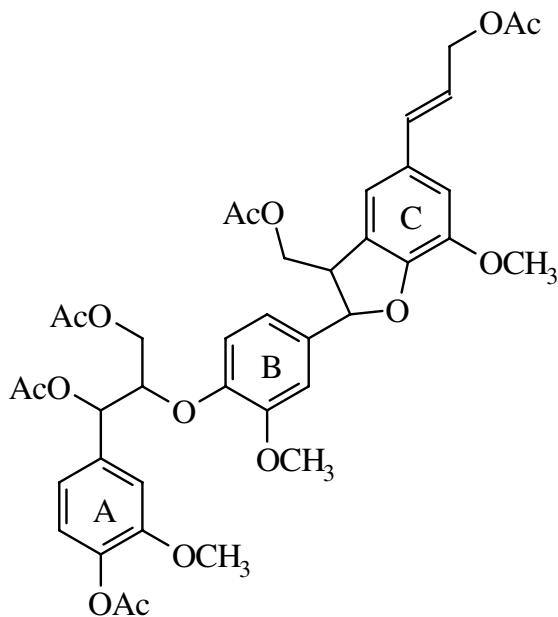
Atom	H Shifts	Mult	J
OMe	3.86	s	
β	6.65	dd	15.9,7.7
2,6	7.02	d	8.9
α	7.60	d	15.9
3,5	7.68	d	8.9
γ	9.66	d	7.7

Notes:

Pew Collection  
50 mg

**Compound Number 216**

**<sup>13</sup>C**



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

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
A4 Ac Me	20.63	111	20.45	104	20.32	97
A $\alpha$ Ac Me	20.74	107	20.60	88	20.40	84
B $\gamma$ Ac Me	20.79	99	20.68	92	20.51	68
C $\gamma$ Ac Me	20.96	141	20.80	86	20.62	73
A $\gamma$ Ac Me	21.00	141	20.86	86	20.70	73
B $\beta$	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
$\gamma$	62.45	46	63.04	65	61.85	33
C $\gamma$	65.18	76	65.49	100	64.49	50
B $\gamma$	65.29	43	65.95	73	64.76	31
$\alpha$	73.66	40	74.48	71	73.01	32
$\beta$	80.25	57	80.30	105	78.30	31
B $\alpha$	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 $\beta$	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 $\alpha$	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 $\alpha$ C=O	169.49	56	169.89	68	169.26	46
C $\gamma$ C=O	170.74	75	170.77	107	170.04	61
B $\gamma$ C=O	170.76	92	170.95	94	170.15	41
A $\gamma$ C=O	170.88	59	170.95	94	170.28	47

**<sup>1</sup>H (acetone)**

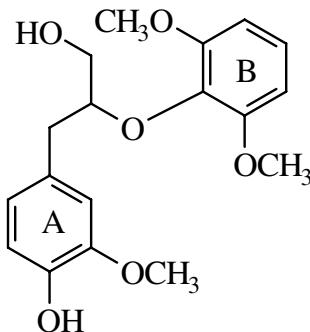
Atom	H Shifts	Mult	J
C $\gamma$ Ac Me	1.93	s	
A,B $\gamma$ Ac Me	2.04	s	
A $\alpha$ Ac Me	2.06	s	
A4 Ac Me	2.21	s	
B $\beta$	3.75	m	
A,B OMe	3.81	s	
C OMe	3.89	s	
A $\gamma$ 1	4.22	dd	4.1,12.0
A $\gamma$ 2	4.36	dd	5.9,12.0
B $\gamma$ 1	4.32	dd	7.6,11.1
B $\gamma$ 2	4.43	dd	5.4,11.1
C $\gamma$	4.65	dd	1.3,6.5
$\beta$	4.86	m	
B $\alpha$	5.55	d	6.8
$\alpha$	6.05	d	5.2
C $\beta$	6.23	dt	6.5,15.8
C $\alpha$	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.



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
$\alpha$	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
$\gamma$	62.21	37	62.78	20	61.69	22
$\beta$	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
A3	135.66	21	137.09	13	135.65	22
A4	144.12	28	145.71	15	144.64	25
B4	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

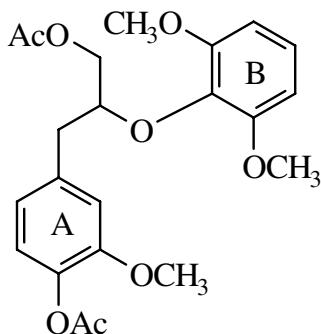
3-(4-hydroxy-3-methoxyphenyl)-2-[2,6-dimethoxyphenoxy]propan-1-ol

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\alpha$	3.03	dd	
$\gamma$	3.50	m	13.6,5.4
A OMe	3.82	s	
B OMe	3.83	s	
$\beta$	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.



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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\alpha$	3.06	t	11.5,6.5
B OMe	3.76	s	
OMe	3.79	s	
$\gamma$	4.11	d	
$\beta$	4.51	m	4.8
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.

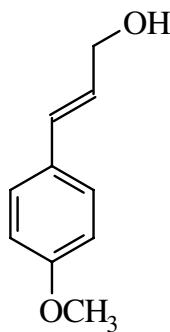
A1,B4, and A4 are too close to positively identify.

Atom	CDCl <sub>3</sub>		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
$\alpha$	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
$\gamma$	65.35	31	65.72	33	64.78	22
$\beta$	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
$\gamma$ Ac C=O	170.92	22	169.08	18	170.16	21

**Compound Number 219**

**<sup>13</sup>C**

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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



*trans*

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

**<sup>1</sup>H (acetone)**

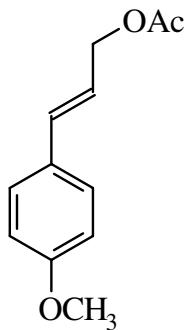
Atom	H Shifts	Mult	J
OMe	3.76	s	
γ	4.20	bs	
β	6.24	dt	J = 15.9, 5.4
α	6.53	d	J = 15.9
3,5	6.86	d	J = 8.7
2,6	7.33	d	J = 8.7

**Notes:**

S.Ralph 55mg  
SRVIII-45

Compound Number 220

<sup>13</sup>C



*trans*

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

<sup>1</sup>H (acetone)

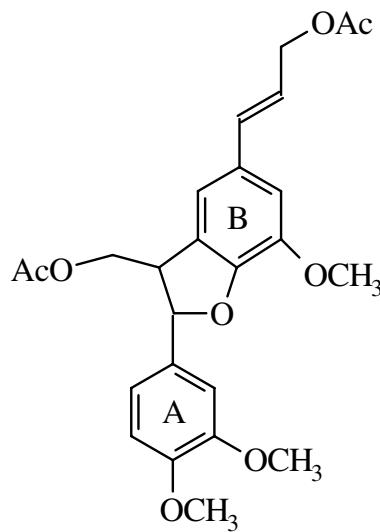
Atom	H Shifts	Mult	J
Ac Me	2.01	s	
OMe	3.78	s	
$\gamma$	4.65	dd	J = 6.4, 1.2
$\beta$	6.19	dt	J = 15.7, 6.4
3,5	6.89	d	J = 8.8
2,6	7.38	d	J = 8.8

**Notes:**

S.Ralph  
30mg

NL220.23 gHSQC  
NL220.24 gHMBC  
Acetone shifts confirmed

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\gamma$	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
$\beta$	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
$\alpha$	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



**V-c-CA**  
4-methoxy phenyl coumaran diacetate

<sup>1</sup>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	
$\gamma_1$	4.38	dd	$J = 11.1, 7.4$
$\gamma_2$	4.43	dd	$J = 11.1, 5.6$
B $\gamma$	4.66	dd	$J = 7.4, 0.9$
A $\alpha$	5.54	d	$J = 7.0$
B $\beta$	6.23	dt	$J = 15.8, 6.4$
B $\alpha$	6.64	d	$J = 15.9$

**Notes:**

S.Ralph 51mg  
SRVII-104

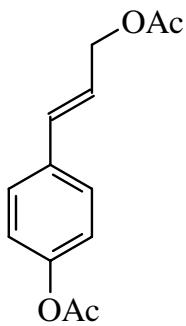
NL221.4 HMBC in acetone  
NL221.5 HMQC in acetone

gamma's and A3 and A4 are very close  
and may be switched

Atom	CDCl <sub>3</sub>		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
$\beta$	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
B $\gamma$	65.19	31	65.52	29	64.51	27
$\gamma$	65.35	29	65.96	29	64.77	19
$\alpha$	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
B $\beta$	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
B $\alpha$	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

<sup>13</sup>C



*trans*

4-hydroxy cinnamyl alcohol diacetate

Coumaryl alcohol acetate

Atom	CDCl <sub>3</sub>		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

### <sup>1</sup>H (acetone)

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

### Notes:

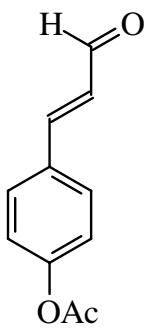
S.Ralph 37mg

NL222.23 gHMQC  
NL222.24 gHMBC

**Compound Number 223**

<sup>13</sup>C

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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



*trans*

**4-acetoxy cinnamaldehyde  
Coumaryl aldehyde acetate**

<sup>1</sup>H (acetone)

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

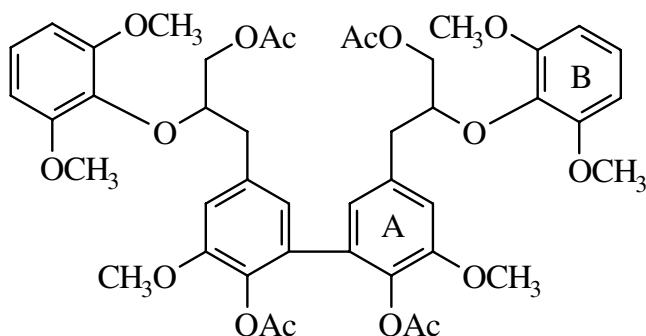
**Notes:**

S.Ralph 27mg

NL223.4 gHMQC in acetone  
NL223.5 gHMBC in acetone

Compound Number 224

<sup>13</sup>C



S-b-G-5,5-G-b-S ( $\alpha = \text{CH}_2$ )

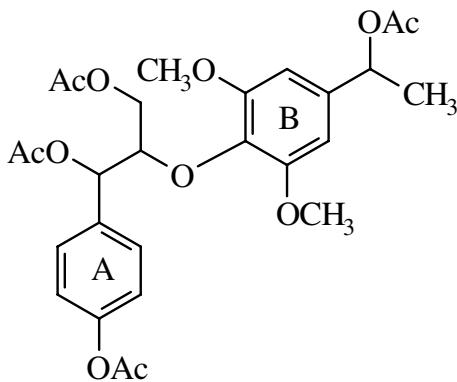
Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.34	30	20.32	18	19.88	34
Ac Me	20.80	37	20.68	20	20.35	59
$\alpha$	38.29	24	38.90	15	37.58	22
OMe	56.00	91	56.33	71	55.71	120
OMe	56.00	91	56.33	71	55.71	120
OMe	56.00	91	56.33	71	55.84	40
$\gamma$	65.26	25	65.69	17	64.70	28
$\beta$	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
$\gamma$ Ac C=O	170.82	19	170.80	10	170.02	35

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.93	s	
Ac Me	1.99	s	
$\alpha$	3.07	m	
OMe	3.74	s	
OMe	3.82	s	
$\gamma$	4.14	d	J = 4.8
$\beta$	4.51	bt	J = 4.9
B2,6	6.62	d	J = 8.4
A6	6.76	s	
A2	7.09	d	J = 1.4

Notes:

S.Ralph  
SRVII 109D 44mg  
2D HMBC in CDCl<sub>3</sub> A4 and A1 identical chemical shift and B4 very close  
NL224.15 gHMBC  
NL224.4 gHMQC  
As compound has a plane of symmetry thru A5 only half the shifts are reported



H-b-S

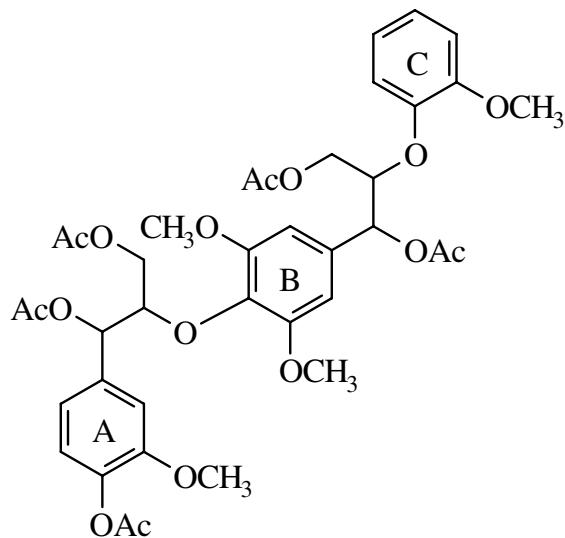
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Bβ	1.47	d	
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	
γ2	4.38	dd	J = 11.9, 4.2
β	4.69	m	J = 11.9, 5.9
Bα	5.78	q	
α	6.07	d	J = 6.6
B2,6	6.68	s	J = 4.6
A3,5	7.11	d	
A2,6	7.45	d	J = 8.5
			J = 8.5

## Notes:

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

Atom	CDCl <sub>3</sub>		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



threo

G-bt-S-bt-G

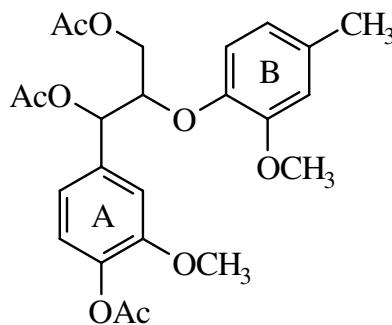
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.84		
$\gamma$ Ac Me	1.98		
$\alpha$ Ac Me	2.00		
$\alpha$ Ac Me	2.10		
A4 Ac Me	2.22		
OMe	3.80		
$\gamma^1$	4.03	m	
$\gamma^2, \gamma^3$	4.22	m	
$\gamma^4$	4.41	dd	J = 11.8, 6.05
A $\beta$	4.71	m	
B $\beta$	4.79	m	
A, B $\alpha$	6.07	bd	J = 6.31
B2,6	6.79	d	J = 2.8

## Notes:

S.Ralph  
SRVII-140C2  
30mg  
gHSQC and gHMBC in acetone  
NL226.4  
NL226.5

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
$\gamma$ Ac Me	20.69	44	20.48	99	20.28	55
$\gamma$ Ac Me	20.75	50	20.58	96	20.28	55
$\alpha$ Ac Me	20.79	43	20.67	96	22.41	41
$\alpha$ Ac 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
A $\gamma$	62.74	27	63.36	63	62.19	22
B $\gamma$	63.16	28	63.72	71	62.56	21
A $\alpha$	73.99	29	75.07	69	73.74	25
B $\alpha$	74.87	28	75.71	54	74.60	19
B $\beta$	80.36	18	80.76	69	79.15	24
A $\beta$	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
$\alpha$ Ac C=O	169.49	18	169.92	49	169.29	26
$\alpha$ Ac C=O	169.76	17	169.99	49	169.29	36
$\gamma$ Ac C=O	170.51	20	170.61	60	169.92	39
$\gamma$ Ac C=O	170.82	19	170.61	60	169.92	39



G-b-G

erythro

Atom	CDCl <sub>3</sub>		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
B $\beta$	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
$\gamma$	62.48	43	62.95	45	61.80	12
$\alpha$	73.70	45	74.58	44	73.10	17
$\beta$	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
$\alpha$ Ac C=O	169.50	24	169.91	17	169.26	14
$\gamma$ Ac C=O	170.78	22	170.76	15	170.03	12

<sup>1</sup>H (acetone)

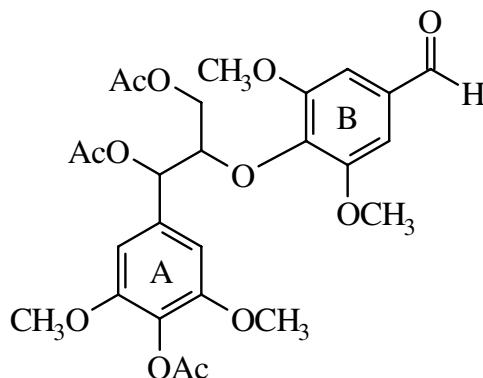
Atom	H Shifts	Mult	J
Ac Me	1.94	s	
Ac Me	2.08	s	
B $\beta$	2.22	s	
Ac Me	2.25	s	
OMe	3.79	s	
OMe	3.83	s	
$\gamma$ 1	4.20	dd	J = 11.9, 4.2
$\gamma$ 2	4.37	dd	J = 11.9, 5.8
$\beta$	4.74	m	
$\alpha$	6.06	d	J = 5.0
B6	6.65	bd	J = 8.1
B2	6.82	bs	
B5	6.85	d	J = 8.2
A5,6	7.04	m	
A2	7.23	s	
$\gamma$ 1 isomer	3.99		
$\gamma$ 2 isomer	4.25		
$\alpha$ isomer	6.10		

## Notes:

S.Ralph  
SRVII-141-1 31mg  
threo isomer shifts  
C A  
 $\gamma$  63.04 63.58  
 $\alpha$  74.54 75.38  
 $\beta$  80.59 80.98  
NL227.4 gHSQC in acetone  
NL227.5 gHMBC in acetone

Compound Number 228

<sup>13</sup>C



S-b-S

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.87	s	
$\alpha$ Ac Me	2.14	s	
A4 Ac Me	2.22	s	
OMe	3.82	s	
OMe	3.95	s	
$\gamma$ 1	4.22	dd	J = 11.9, 3.8
$\gamma$ 2	4.47	dd	J = 11.9, 6.2
$\beta$	4.95	dt	J = 6.6, 4.2
$\alpha$	6.09	d	J = 4.2
A 2,6	6.81	s	
B 2,6	7.25	s	
B $\alpha$	9.90	s	

Notes:

L.Landucci  
LLL XXII-134C  
35mg

NL228.4 gHSQC in acetone  
NL228.5 gHMBC in acetone

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
A4 Ac Me	20.44	21	20.24	147	20.09	45
$\alpha$ AcMe	20.70	15	20.58	108	20.31	34
$\gamma$ 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
$\gamma$	62.90	11	63.40	96	62.26	18
$\alpha$	74.17	12	75.17	93	73.81	22
$\beta$	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
$\alpha$ Ac C=O	169.46	9	169.94	50	169.35	25
$\gamma$ Ac C=O	170.76	6	170.66	46	169.96	23
B $\alpha$	191.01	12	191.69	98	191.82	22

**Compound Number 229**

<sup>13</sup>C

		<sup>13</sup> C					
Atom	CDCl <sub>3</sub>		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	
γ Ac C=O	170.84	27	170.81	12	169.97	27	
Bα Ac C=O	170.92	34	170.97	6	170.20	16	

S-b-S

*erythro*

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.86	s	
Bα Ac 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	
γ2	4.43	dd	J = 11.9, 6.0
β	4.74	dt	J = 6.2, 4.2
Bα	5.02	s	
α	6.08	d	J = 4.3
B 2,6	6.71	s	
A 2,6	6.78	s	

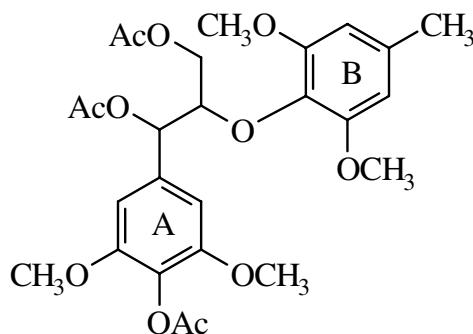
**Notes:**

S.Ralph  
SRIX-17D  
18mg

NL229.4 gHSQC in acetone  
NL229.5 gHMBC in acetone

Compound Number 230

<sup>13</sup>C



S-b-S

*erythro*

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
A4 Ac Me	20.43	29	20.24	41	20.04	79
γAc 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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
γAc 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	J = 11.9, 4.4
γ2	4.40	dd	J = 11.9, 6.2
β	4.66	dt	J = 5.8, 4.4
α	6.06	d	J = 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

C	A
γ 63.53	64.13
α 75.60	76.58
β 80.87	81.65

NL230.4 gHSQC in acetone  
NL230.5 gHMBC in acetone

**Compound Number    231**

**<sup>13</sup>C**

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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

*cis*

**cis-coniferyl alcohol**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
OMe	3.83	s	
γ	4.41	d	J = 5.8
β	5.73	dt	J = 11.9, 6.2
α	6.39	d	J = 11.7
6	6.72	dd	J = 8.2, 2.0
5	6.82	d	J = 8.2
2	6.87	d	J = 2.0
CDCl <sub>3</sub>	CDCl <sub>3</sub>		
OMe	3.89	s	
γ	4.44	dd	J = 6.4, 1.4
β	5.79	dt	J = 11.5, 6.6
α	6.49	d	J = 11.9
6	6.74	dd	J = 8.2, 1.8
5	6.78	d	J = 1.8
2	6.89	d	J = 8.2

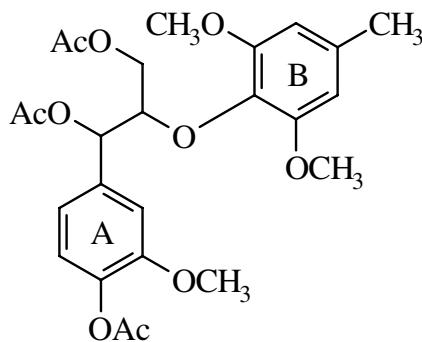
**Notes:**

J.Ralph 10mg

NL231.4 gHSQC in acetone

NL231.5 gHMBC in acetone

NL231.24 gHSQC in DMSO



G-b-S

<sup>1</sup>H (acetone)

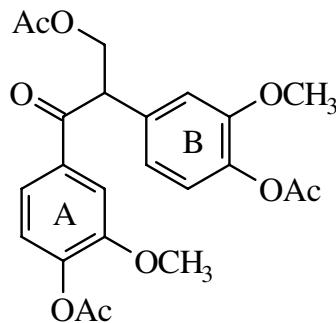
Atom	H Shifts	Mult	J
Ac Me	1.85	s	
Ac Me	2.12	s	
Ac Me	2.22	s	
B $\alpha$	2.27	s	
B OMe	3.76	s	
A OMe	3.82	s	
$\gamma_1$	4.16	dd	J = 11.8,4.4
$\gamma_2$	4.43	dd	J = 11.7,5.8
$\beta$	4.67	dt	J = 5.8,4.2
$\alpha$	6.10	d	J = 4.2
B 2,6	6.51	s	
A6	6.99	dd	J = 8.3,1.8
A5	7.06	d	J = 8.2
A2	7.18	d	J = 1.8

## Notes:

S.Ralph  
SRIX-43G  
55 mg

HSQC and HMBC in d6-DMSO

Atom	CDCl <sub>3</sub>		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
B $\alpha$	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
$\gamma$	62.64	157	63.10	122	61.98	59
$\alpha$	74.02	160	75.04	125	73.72	66
$\beta$	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
$\alpha$ Ac C=O	169.56	85	169.93	56	169.39	57
$\gamma$ Ac C=O	170.92	79	170.67	50	170.03	64



G-b1-G

Atom	CDCl <sub>3</sub>		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

<sup>1</sup>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	J = 10.5,5.8
γ2	4.76	dd	J = 10.5,8.5
β	5.19	dd	J = 8.5,5.7
B6	6.98	dd	J = 8.0,2.0
B5	7.03	d	J = 8.0
A5	7.16	d	J = 8.2
B2	7.22	d	J = 1.8
A6	7.73	d	J = 6.2,1.8
A2	7.77	d	J = 1.8

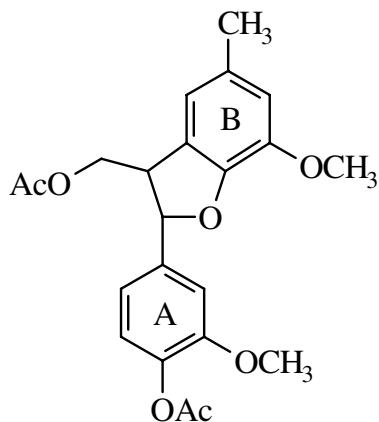
## Notes:

S.Lempke  
I-31

HSQC and HMBC in d6-acetone

Compound Number 234

<sup>13</sup>C



G-e-G

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
B $\alpha$	22.13	31	21.18	32	20.80	111
$\beta$	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
$\gamma$	66.49	38	66.19	44	65.03	75
$\alpha$	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
$\gamma$ Ac C=O	171.66	15	170.96	14	170.29	66

### <sup>1</sup>H (acetone)

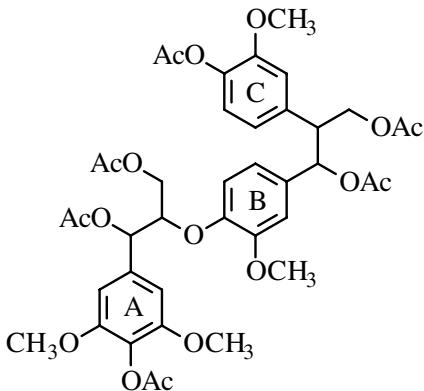
Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.22	s	
B $\alpha$	2.26	s	
$\beta$	3.74	m	
A OMe	3.80	s	
B OMe	3.83	s	
$\gamma$ 1	4.29	dd	J = 11.1,8.0
$\gamma$ 2	4.42	dd	J = 10.9,5.6
$\alpha$	5.55	d	J = 6.6
B6	6.70	s	
B2	6.73	s	
A6	6.99	dd	J = 8.2,1.8
A5	7.05	d	J = 8.2
A2	7.18	d	J = 1.8

### Notes:

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

**Compound Number 235**

<sup>13</sup>C



S-b-G-b1-G

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>1</sup>H (acetone)

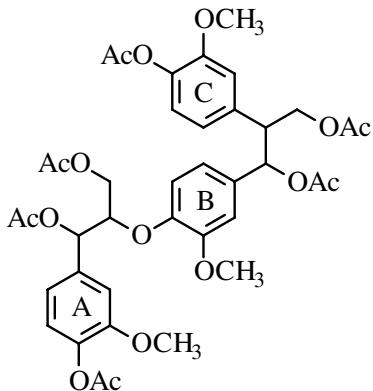
Atom	H Shifts	Mult	J
Ac Me	1.89	s	
Ac Me	1.90	s	
Ac Me	2.04	s	
Ac Me	2.17	s	
Ac Me	2.18	s	
Bβ	3.46	m	
OMe	3.69	s	
OMe	3.72	s	
OMe	3.75	s	
OMe	3.76	s	
Byl	4.22	m	
Aγ1	4.31	m	
By2	4.36	m	
Aγ2	4.38	m	
Aβ	4.82	m	
Aα	5.99	d	J = 5.8
Bα	6.08	d	J = 7.2
A2,6	6.80	s	
C2	6.97	s	

**Notes:**

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

**Compound Number 236**

<sup>13</sup>C



**G-b-G-b1-G**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.95	s	
$\alpha$ Ac Me	2.07	s	
4 Ac Me	2.15	s	
B $\beta$	3.50	m	
OMe	3.74	s	
OMe	3.78	s	
OMe	3.83	s	
B $\gamma$ 1	4.21	m	
A $\gamma$ 1	4.27	m	
B $\gamma$ 2	4.33	m	
A $\gamma$ 2	4.37	m	
A $\beta$	4.85	m	
A $\alpha$	6.06	d	J = 5.0
B $\alpha$	6.13	d	J = 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	

**Notes:**

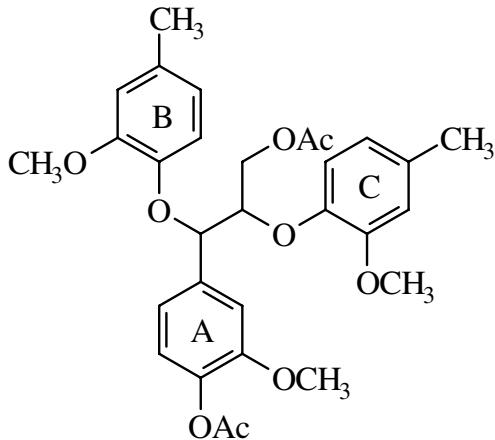
SRIX-47C2

21 mg

B $\beta$ ,A $\beta$ ,A2,B5,B1,B4 appear as two very close signals, the shift reported is the average.

HSQC and HMBC in d6-acetone

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
$\gamma$ Ac Me	20.69	44	20.49	90	20.35	99
$\gamma$ Ac Me	20.69	44	20.49	90	20.35	99
$\alpha$ Ac Me	20.78	24	20.62	53	20.35	99
$\alpha$ 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
B $\beta$	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
A $\gamma$	62.52	12	63.04	29	61.94	20
B $\gamma$	64.29	14	65.05	32	64.17	20
A $\alpha$	73.72	15	74.55	30	73.14	22
B $\alpha$	75.07	12	75.70	26	74.68	21
A $\beta$	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
$\alpha$ Ac C=O	169.55	10	169.93	29	169.23	33
$\alpha$ Ac C=O	169.78	10	169.93	29	169.28	32
$\gamma$ Ac C=O	170.74	11	170.75	31	170.06	55
$\gamma$ Ac C=O	170.80	11	170.75	31	170.06	55



G-a-G-b-G

Atom	CDCl <sub>3</sub>		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
C $\alpha$	21.05	23	20.96	28	20.56	136
B $\alpha$	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
$\gamma$	63.56	21	65.62	30	62.46	86
$\alpha$	80.41	21	81.09	24	79.08	93
$\beta$	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

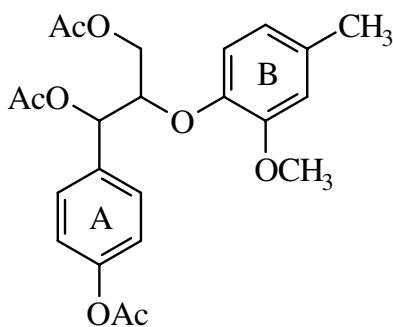
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.90	s	
Ac Me	2.20	s	
B or C $\alpha$	2.20	s	
B or C $\alpha$	2.24	s	
OMe	3.75	s	
OMe	3.79	s	
OMe	3.83	s	
$\gamma$ 1	4.43	dd	
$\gamma$ 2	4.54	dd	J = 11.7, 5.8
$\beta$	4.74	m	
$\alpha$	5.55	d	J = 5.4
C6	6.53	dd	
B6	6.61	dd	J = 8.0, 1.4
C5	6.76	d	
B,C 2	6.78	s	
B5	6.83	d	J = 8.0
A5	6.98	d	J = 8.0
A6	7.05	dd	J = 8.0, 1.8
A2	7.33	d	J = 1.8

## Notes:

SRIX-46DB  
33mg

HSQC and HMBC in d6-acetone  
Shifts for B and C  $\alpha$ 's, 2's and 6's were too close to assign with complete confidence

*erythro***H-b-G**

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
γAc Me	20.82	21	20.59	46	20.34	66
αAc 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

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
γAc Me	1.92	s	
αAc Me	2.07	s	
A4 Ac Me	2.24	s	
Bα	2.25	s	
OMe	3.77	s	
γ1	4.17	dd	
γ2	4.37	dd	J = 11.9,4.4 J = 11.9,5.6
β	4.69	m	
α	6.06	d	J = 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

minor isomer shifts

C A D      <sup>1</sup>H in acetone

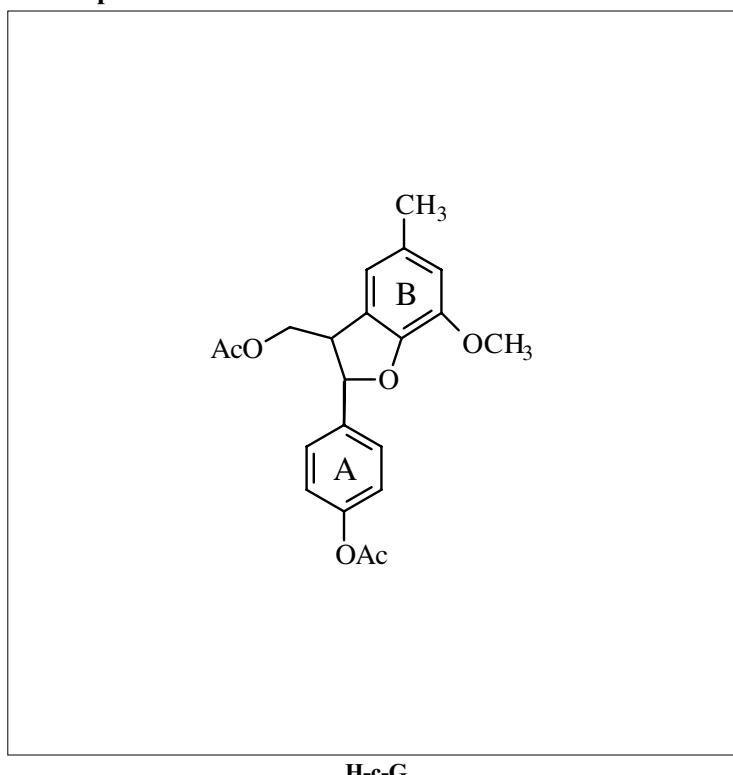
γ 63.10 63.56 62.38      γ1 3.96, dd J = 11.8,5.6

α 74.53 75.24 74.03      γ2 4.24, dd J = 11.8,4.2

β 80.73 81.06 79.39      α 6.12,d J = 6.8

**Compound Number 239**

**<sup>13</sup>C**



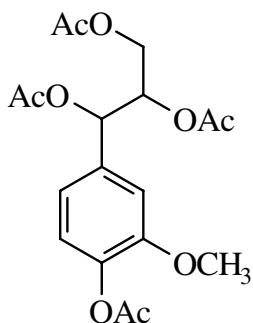
Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
γAc Me	20.89	25	20.68	53	20.48	26
A4 Ac Me	21.21	36	20.95	77	20.73	56
Bα	21.35	33	21.18	49	20.73	56
β	50.94	21	51.78	54	49.85	19
OMe	56.11	30	56.38	43	55.56	19
γ	65.83	22	66.29	57	65.02	20
α	87.46	21	87.57	53	85.95	20
B2	113.35	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
γAc C=O	170.88	9	170.94	18	170.21	12

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
γAc 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	
γ2	4.41	dd	
α	5.58	d	J = 10.9, 5.6 J = 6.4
B2	6.70	bs	
B6	6.73	bs	
A3,5	7.11	d	J = 8.5
A2,6	7.44	d	J = 8.5

**Notes:**

SRIX-53E 2mg  
HSQC and HMBC in acetone



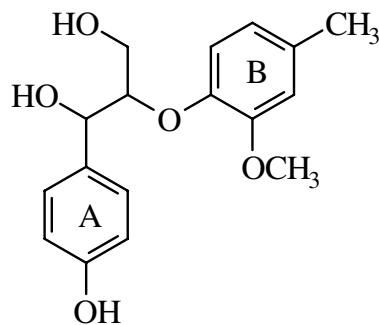
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.67	167	20.44	216	20.36	57
Ac Me	20.67	167	20.52	182	20.41	54
Ac Me	20.80	126	20.66	173	20.46	47
Ac Me	20.96	111	20.79	172	20.66	41
OMe	56.02	134	56.34	192	55.84	41
$\gamma$	62.11	93	62.81	156	61.93	24
$\beta$	72.22	95	72.92	167	71.68	27
$\alpha$	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
$\alpha$ Ac C=O	169.65	39	170.08	70	169.44	39
$\beta$ Ac C=O	170.04	44	170.30	63	169.44	39
$\gamma$ Ac C=O	170.43	40	170.73	66	169.97	22

<sup>1</sup>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	
$\gamma$ 1	3.90	dd	J = 11.9, 6.2
$\gamma$ 2	4.24	dd	J = 11.9, 4.0
$\beta$	5.42	m	
$\alpha$	5.97	d	J = 6.6
6	7.00	dd	J = 8.2, 1.6
5	7.06	d	J = 8.2
2	7.17	d	J = 1.6

## Notes:

SRIX-69E  
 7mg  
 gHSQC d6-acetone  
 gHMBC d6-acetone  
 minor isomer shifts in acetone  
 $\gamma$  62.31  
 $\beta$  72.92  
 $\alpha$  73.53



H-b-G

*threo*

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\alpha$	21.16	16	21.08	21	20.51	31
OMe	55.81	19	56.24	28	55.55	37
$\gamma$	60.79	11	61.73	22	60.00	17
$\alpha$	73.72	13	73.84	21	70.94	19
$\beta$	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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\alpha$	2.27	s	
$\gamma$ 2	3.43	m	
$\gamma$ 1	3.64	m	
OMe	3.85	s	
$\beta$	4.03	m	
$\alpha$	4.83	dd	J = 6.9, 3.2
B6	6.66	m	
A3,5	6.79	d	J = 8.7
B2	6.85	d	J = 2.0
B5	7.07	d	J = 8.0
A2,6	7.28	d	J = 8.7
A4 OH	8.26	s	

## Notes:

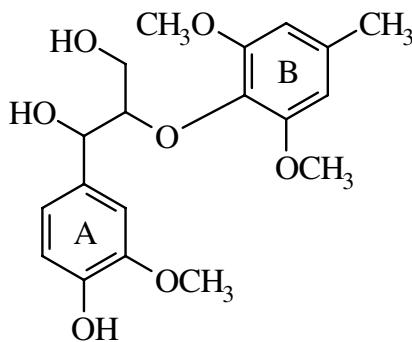
SRIX-84

35mg

erythro isomer shifts

C	A	D
$\gamma$	60.79	61.64
$\alpha$	72.72	73.55
$\beta$	87.06	87.53

59.89  
71.41  
84.57

*threo*

G-b-S

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\alpha$	2.29	s	
$\gamma$ 1	3.28	dd	
$\gamma$ 2	3.64	dd	J = 12.5, 3.2
OMe	3.80	s	J = 12.6, 3.6
$\beta$	3.88	m	
OMe	3.85	s	
$\alpha$	5.00	d	J = 7.6
B2,6	6.55	s	
A5	6.79	d	J = 8.34
A6	6.92	dd	J = 8.3, 1.8
A2	7.07	d	J = 1.8

## Notes:

SRIX-86B,C

40 mg

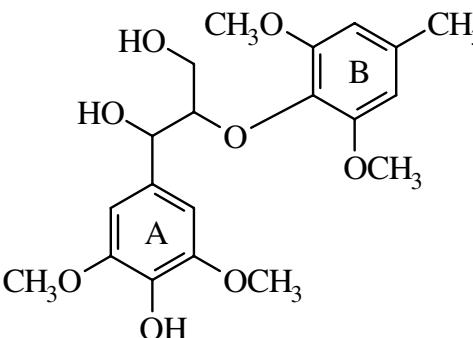
erythro isomer shifts

C	A	D
$\gamma$ 60.63	60.86	59.57
$\alpha$ 72.49	73.26	71.93
$\beta$ 87.13	87.90	86.11

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\alpha$	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
$\gamma$	60.51	30	61.19	35	60.11	29
$\alpha$	74.20	32	74.08	38	71.53	37
$\beta$	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

**Compound Number 243**

<sup>13</sup>C

		<i>threo</i>					
		S-b-S					

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\alpha$	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
$\gamma$	60.37	33	61.31	47	60.18	49
$\alpha$	74.33	39	74.29	52	71.59	62
$\beta$	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

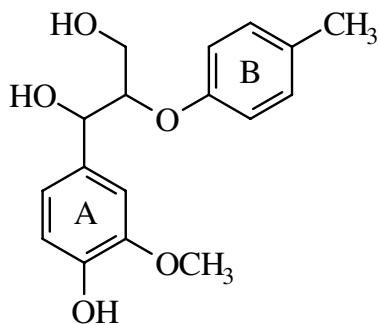
<sup>1</sup>H (acetone)

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

**Notes:**

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

C	A
$\gamma$ 60.50	61.23
a 72.50	73.43
$\beta$ 87.03	86.32



G-b-H

*threo*

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\alpha$	20.53	27	20.46	42	20.05	125
OMe	55.98	34	56.20	49	55.49	119
$\gamma$	61.11	18	61.67	36	60.04	63
$\alpha$	73.81	20	73.36	36	70.92	75
$\beta$	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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\alpha$	2.22	s	
OMe	3.79	s	
$\gamma$ 1	3.54	m	
$\gamma$ 2	3.78	m	
$\beta$	4.39	m	
$\alpha$	4.94	m	
A5	6.77	d	
A2	7.08	bs	
A4 OH	7.44	s	J = 8.2

## Notes:

SRIX-88GHB

36mg A1 and B1 may be interchanged

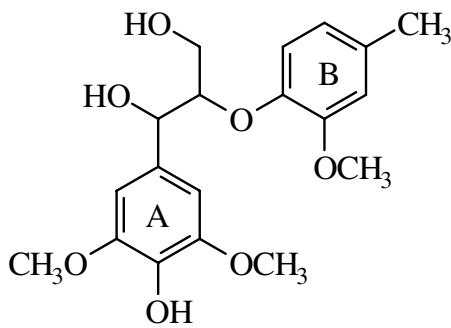
gHSQC, gHMBC in acetone and CDCl<sub>3</sub>

erythro isomer shifts

C	A	D	
$\gamma$	61.44	62.03	60.17
$\alpha$	73.94	74.03	71.55
b	81.22	83.98	83.37

**Compound Number 245**

<sup>13</sup>C



*threo*

**S-b-G**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\alpha$	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
$\gamma$	60.99	15	61.89	40	60.05	27
$\alpha$	74.18	19	74.05	42	70.90	28
$\beta$	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

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B $\alpha$	2.25	s	
$\gamma$ 1	3.48	m	
A OMe	3.78	s	
B OMe	3.84	s	
$\gamma$ 2	4.10	m	
$\beta$	4.48	d	
$\alpha$	4.85	dd	J = 3.8
B6	6.65	m	J = 3.6, 6.4
A2,6	6.76	s	
B2	6.83	d	J = 1.8
B5	7.04	d	J = 8.2

**Notes:**

SRIX-95BR

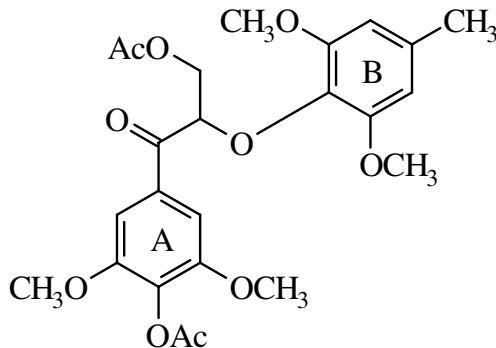
erythro shifts

C	A	D
$\alpha$ 72.87	73.98	71.90

$\beta$ 87.70	87.09	83.97
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$\gamma$ 60.76	61.75	59.94
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HSQC and HMBC in <sup>CDCl<sub>3</sub></sup>



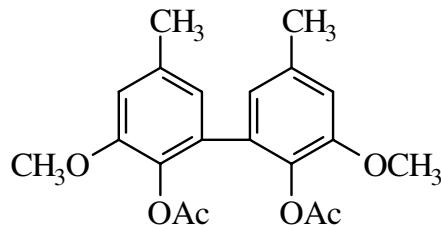
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.43	25	20.22	129	20.08	149
γ Ac Me	20.75	21	20.60	113	20.42	139
Bα	21.82	20	21.73	109	21.32	130
B OMe	55.86	49	56.19	268	55.65	293
B OMe	55.86	49	56.19	268	55.65	293
A OMe	56.29	48	56.60	249	56.12	272
A OMe	56.29	48	56.60	249	56.12	272
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

<sup>1</sup>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	
β	4.49 5.50	m t	J = 5.4
B2,6 A2,6	6.47 7.49	s s	

## Notes:

SRTSII-131-Ac 12mg  
 A2,6 and B2,6 ; A1 and B1 switch in DMSO  
 HSQC and HMBC in Acetone, CDCl<sub>3</sub> and DMSO



Atom	CDCl <sub>3</sub>		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

<sup>1</sup>H (acetone)

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

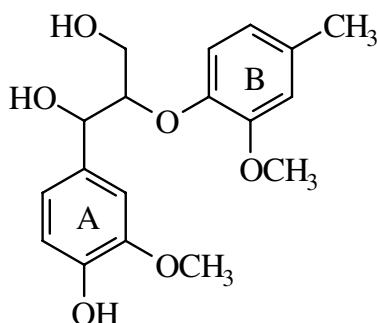
**Notes:**

LLL-XXIII-76DA 37mg

As this dimer contains a plane of symmetry the CSs are reported for one unit.

Compound Number 248

<sup>13</sup>C



*threo*

G-b-G

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\alpha$	2.27	s	
$\gamma$ 1	3.51	m	
$\gamma$ 2	3.68	m	
OMe	3.81	s	
OMe	3.85	s	
$\beta$	4.07	m	
$\alpha$	4.88	d	
B6	6.66	bd	J = 6.0
B5	6.87	bd	J = 7.3
A4 OH	7.37	s	J = 8.0

Notes:

SRIX-98 27mg

B5 and A6 may be switched

HSQC and HMBC in CDCl<sub>3</sub>

C      A      D      erythro shifts

$\gamma$  60.69 61.69 59.97

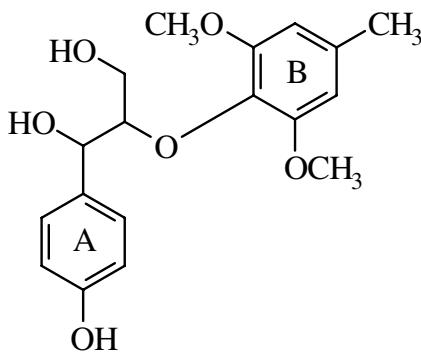
$\alpha$  72.71 73.78 71.72

$\beta$  87.33 87.08 84.21

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\alpha$	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
$\gamma$	60.96	17	61.82	26	60.10	47
$\alpha$	73.96	24	73.95	28	70.96	52
$\beta$	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

**Compound Number 249**

<sup>13</sup>C



**H-b-S**

*threo*

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\alpha$	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
$\gamma$	60.50	18	61.06	21	60.08	23
$\alpha$	74.10	23	73.95	22	71.53	27
$\beta$	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

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B $\alpha$	2.28	s	
$\gamma$ 1	3.21	dd	
$\gamma$ 2	3.60	dd	J = 12.3, 3.2
$\beta$	3.82	m	
OMe	3.85	s	
$\alpha$	4.98	d	J = 7.8
B2,6	6.55	s	
A3,5	6.78	d	J = 8.5
A2,6	7.27	d	J = 8.5
<u>CDCl<sub>3</sub></u>	<u>CDCl<sub>3</sub></u>		
B $\alpha$	2.36		
$\gamma$ 1	3.32		
$\gamma$ 2	3.57		
$\beta$	3.87		
OMe	3.90		
$\alpha$	5.03		
B2,6	6.47		
A3,5	6.72		
A2,6	7.26		

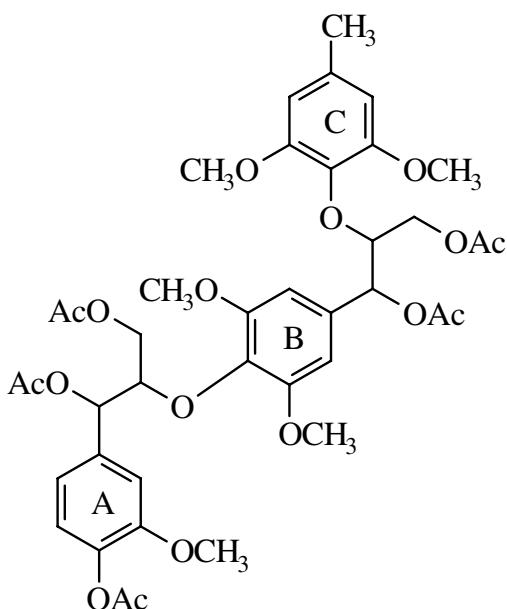
**Notes:**

SRIX-101B 21mg  
HSQC acetone  
HSQC & HMBC CDCl<sub>3</sub>  
erythro shifts  

C	A
$\gamma$ 60.6	60.8
$\alpha$ 72.4	73.1
$\beta$ 87.0	87.8

**Compound Number 250**

**$^{13}\text{C}$**



**G-b-S-b-S**

**$^1\text{H}$  (acetone)**

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.84	d	
$\alpha$ Ac Me	1.93	d	$J = 1.4$
$\gamma$ Ac Me	2.00	d	$J = 3.0$
$\alpha$ Ac Me	2.11	d	$J = 1.0$
A4 Ac Me	2.21	s	
C $\alpha$	2.28	s	
OMe	3.77	s	
OMe	3.79	s	
OMe	3.81	s	
B $\gamma$ 1	3.83	m	
A $\gamma$ 1	4.16	dd	$J = 11.7, 4.2$
B $\gamma$ 2	4.22	ddd	$J = 11.7, 3.8, 1.8$
A $\gamma$ 2	4.40	dd	$J = 11.7, 6.0$
B $\beta$	4.52	m	
A $\beta$	4.70	m	
A $\alpha$	6.06	d	
B $\alpha$	6.06	d	overlapping
C2,6	6.49	s	
B2,6	6.74	d	
A5,6	7.00	m	$J = 1.6$
A2	7.16	d	$J = 1.4$

**Notes:**

SRIX-105 30mg

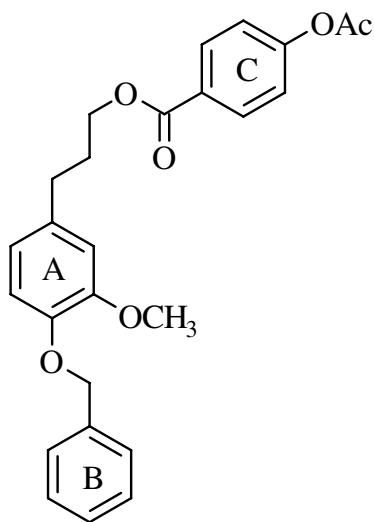
Order of Ac Me changes in  $\text{CDCl}_3$

HSQC and HMBC in  $\text{CDCl}_3$  and d6-acetone

B $\alpha$ , A $\beta$ , B $\beta$ , A2 and A6 show two signals c.a. 0.1ppm apart due to isomer effects and the CS reported is an average value

The first  $\beta$ -O-4 linkage appears to be erythro and the second linkage appears to be threo.

Atom	$\text{CDCl}_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.85	47	20.48	55	20.27	35
$\gamma$ Ac Me	20.67	46	20.59	48	20.35	47
$\gamma$ Ac Me	20.73	41	20.74	41	20.48	36
$\alpha$ Ac Me	21.08	75	20.93	53	20.67	41
$\alpha$ Ac Me	21.08	75	21.02	48	20.73	40
C $\alpha$	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
A $\gamma$	62.76	21	63.39	39	62.25	19
B $\gamma$	63.74	25	64.30	36	63.20	15
A $\alpha$	74.06	23	75.15	44	73.83	22
B $\alpha$	75.99	29	76.75	28	75.77	13
A $\beta$	80.89	57	81.45	34	80.00	17
B $\beta$	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
$\alpha$ Ac C=O	169.55	23	169.90	29	169.29	28
$\alpha$ Ac C=O	169.85	21	169.95	34	169.38	29
$\gamma$ Ac C=O	170.54	21	170.69	45	169.99	34
$\gamma$ Ac C=O	170.88	21	170.69	45	169.99	34



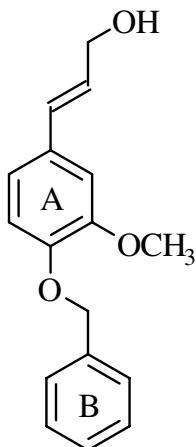
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			21.00	21		
β			31.15	12		
α			32.42	15		
OMe			56.13	18		
γ			64.98	14		
Bα			71.56	11		
A2			113.72	12		
A5			115.39	11		
A6			121.14	12		
C3			122.79	36		
C5			122.79	36		
B2			128.40	33		
B6			128.40	33		
B4			128.40	33		
C1			128.72	6		
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		

<sup>1</sup>H (acetone)

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

## Notes:

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



Atom	CDCl <sub>3</sub>		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		

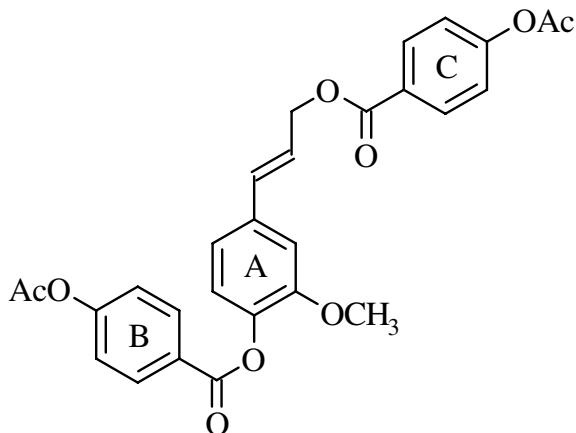
<sup>1</sup>H (acetone)

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

**Notes:**

L.Landucci XXIII-127G 48 mg  
 HSQC and HMBC in acetone d-6  
 gamma singal is split and CS value is avg. - 0.06

Atom	CDCl <sub>3</sub>		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		

<sup>1</sup>H (acetone)

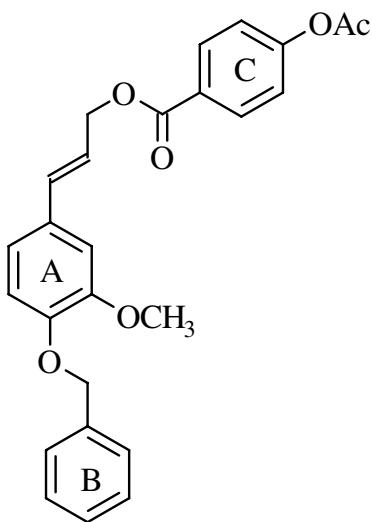
Atom	H Shifts	Mult	J
Ac Me	2.29	s	
Ac Me	2.31	s	
OMe	3.84	s	
γ	5.00	bd	
β	6.55	dt	J = 6.0, 6.0
α	6.85	bd	J = 16.0
A6	7.13	dd	J = 8.3, 1.8
A5	7.20	d	J = 8.3
C3,5	7.28	d	J = 8.7
A2	7.33	bs	
B3,5	7.35	d	J = 8.7
C2,6	8.11	d	J = 8.7
B2,6	8.21	d	J = 8.7

## Notes:

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

**Compound Number 254**

**<sup>13</sup>C**



Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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		

**<sup>1</sup>H (acetone)**

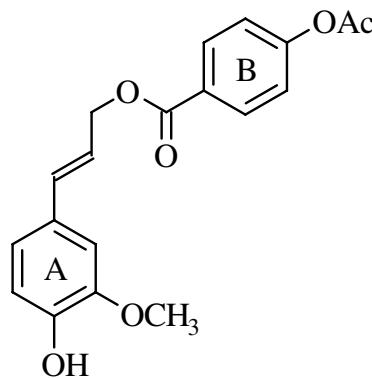
Atom	H Shifts	Mult	J
Ac Me	2.28	s	
OMe	3.85	s	
γ	4.95	dd	
Bα	5.10	s	
β	6.38	dt	J = 6.4, 1.3
α	6.74	d	J = 15.9
A5,6	6.97	m	
A2	7.16	bs	
C3,5	7.26	d	J = 8.7
B3,4,5	7.31-7.41	m	
B2,6	7.47	bd	J = 7.4
C2,6	8.09	d	J = 8.7

**Notes:**

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

**Compound Number 255**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		

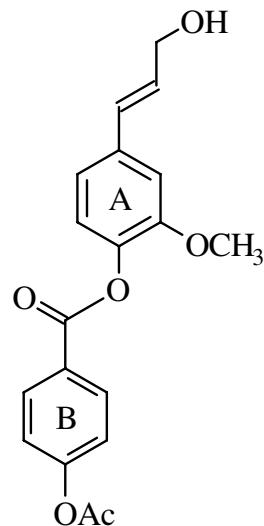
<sup>1</sup>H (acetone)

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

**Notes:**

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

Compound Number 256

<sup>13</sup>C

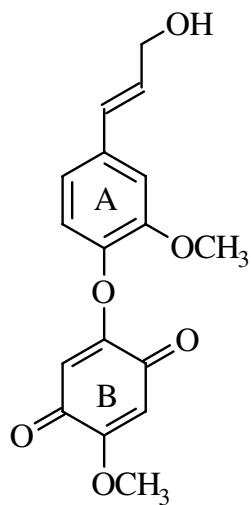
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.99	35		
OMe			56.22	39		
γ			63.10	29		
A2			111.04	37		
A6			119.58	36		
B3			123.15	76		
B5			123.15	76		
A5			123.81	38		
B1			127.80	16		
α			129.30	36		
β			131.61	37		
B2			132.32	73		
B6			132.32	73		
A1			137.50	17		
A4			140.16	11		
A3			152.44	16		
B4			156.10	13		
Bα			164.29	8		
Ac C=O			169.30	13		

<sup>1</sup>H (acetone)

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

## Notes:

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



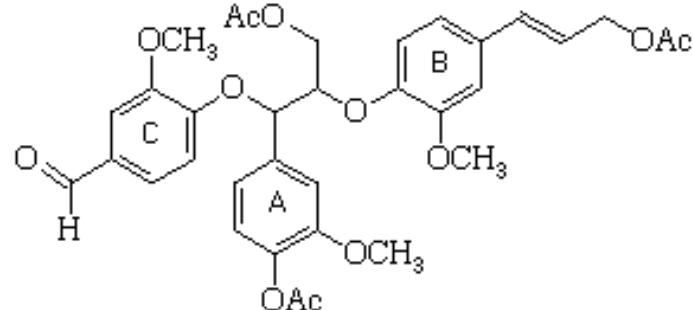
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
A OMe			56.27	26		
B OMe			57.07	27		
γ			62.98	26		
B2			106.32	28		
B5			108.77	26		
A2			111.75	24		
A6			120.19	27		
A5			122.94	27		
α			128.91	24		
β			132.31	26		
A1			138.15	13		
A4			140.96	6		
A3			151.65	9		
B6			159.23	6		
B3			160.39	9		
B4			181.63	9		
B1			182.05	7		

<sup>1</sup>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	
α	6.63	dt	J = 15.9, 5.0 J = 16.1, 1.7
A5,6	7.09	m	
A2	7.27	bs	

**Notes:**

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



Vanillin-a-G-b-CA

<sup>1</sup>H (acetone)

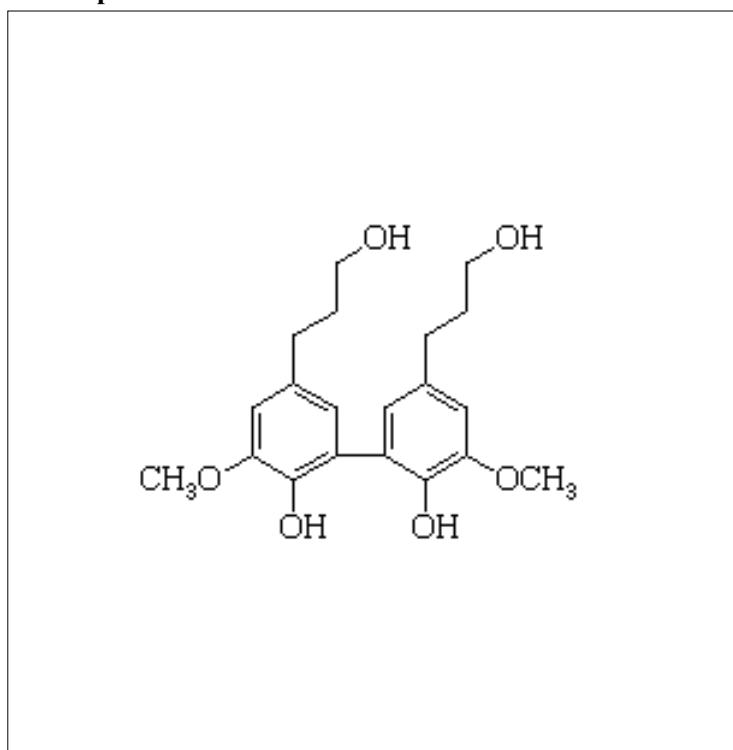
Atom	H Shifts	Mult	J
Ac Me s	1.91, 2.03, 2.07	s s	
OMe	3.81	s	
OMe	3.83	s	
OMe	3.97	s	
$\gamma_1$	4.45	dd	J = 11.9, 4.0
$\gamma_2$	4.56	dd	J = 11.9, 5.8
B $\gamma$	4.67	dd	J = 6.4, 1.2
$\beta$	4.91	m	
$\alpha$	5.84	d	J = 5.2
B $\beta$	6.27	dt	J = 15.9, 6.4
B $\alpha$	6.63	d	J = 15.9
B6	6.93	dd	J = 8.2, 1.6
B5	7.01	d	J = 8.3
A5	7.03	d	J = 8.2
A6	7.14	dd	J = 8.2, 1.8
B2	7.15	d	J = 2.0
C5	7.15	d	J = 8.3
A2	7.36	d	J = 2.4
C6	7.39	dd	J = 8.2, 1.8
C2	7.46	d	J = 1.8
C $\alpha$	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)

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.74	32	20.46	29		
$\gamma$ Ac Me	20.82	31	20.62	27		
B $\gamma$ Ac 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		
$\gamma$	63.12	23	63.32	26		
B $\gamma$	65.17	25	65.38	29		
$\alpha$	79.98	23	80.55	26		
$\beta$	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		
B $\beta$	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		
B $\alpha$	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		
$\gamma$ Ac C=O	170.82	12	170.77	18		
$\gamma$ Ac C=O	170.95	10	170.77	18		
C $\alpha$	190.96	25	191.26	30		

## Compound Number 259

<sup>13</sup>C

dihydrodiconiferyl alcohol

Atom	CDCl <sub>3</sub>		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
1	124.52	13	126.47	11	125.89	18
5	133.76	16	134.15	19	132.26	30
3	140.83	17	142.49	13	141.36	24
4	147.33	18	148.64	14	147.61	20

<sup>1</sup>H (acetone)

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

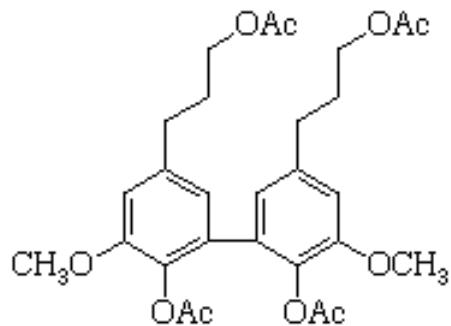
## Notes:

L.Landucci  
XXIII-52H 25 mg

As this dimer contains a plane of symmetry the CSs are reported for one unit.

Compound Number 260

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
β	30.30	19	30.99	28	29.58	8
α	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

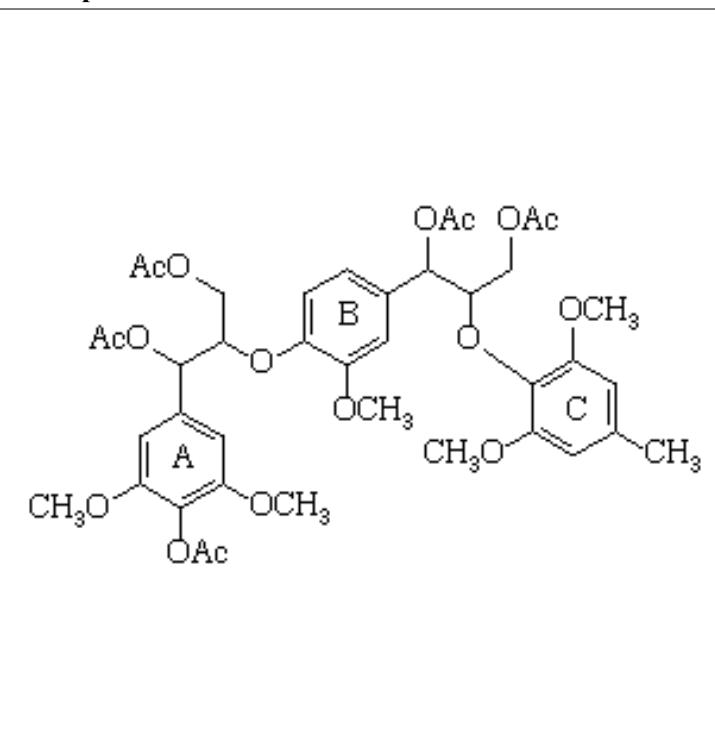
### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
β	1.97	m	
Ac Me	1.98	s	
Ac Me	2.01	s	
α	2.70	bt	J = 8.0
OMe	3.83	s	
γ	4.07	t	J = 6.4
6	6.66	d	J = 1.8
2	6.99	d	J = 1.8

### Notes:

L.Landucci  
XXIII-146ACH

As this dimer contains a plane of symmetry the CS's are reported for one unit.



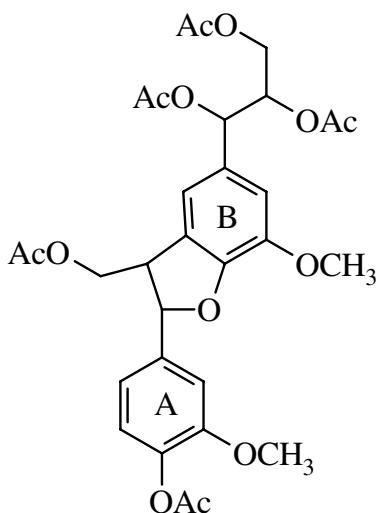
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.48	32	20.24	46	20.05	27
$\gamma$ Ac Me	20.75	26	20.64	81	20.35	38
$\gamma$ Ac Me	20.84	35	20.64	81	20.35	38
$\alpha$ Ac Me	21.08	26	20.96	68	20.62	37
$\alpha$ Ac Me	21.14	29	20.96	68	20.62	37
C $\alpha$	21.90	31	21.77	51	21.35	24
OMe	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
B $\gamma$	62.82	15	63.35	26	62.12	15
A $\gamma$	63.09	15	63.63	19	62.46	12
B $\alpha$	74.33	19	75.22	27	73.76	14
A $\alpha$	74.48	18	75.68	27	74.59	10
A $\beta$	80.20	18	80.65	15	78.96	10
B $\beta$	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
$\alpha$ Ac C=O	169.75	16	169.96	27	169.26	17
$\alpha$ Ac C=O	169.79	12	170.01	27	169.33	17
$\gamma$ Ac C=O	170.62	14	170.70	32	169.94	25
$\gamma$ Ac C=O	170.91	14	170.70	32	169.94	25

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.88	s	
$\gamma$ Ac Me	1.97	s	
$\alpha$ Ac Me	2.01	d	
$\alpha$ Ac Me	2.12	d	
A4 Ac Me	2.21	s	
C $\alpha$	2.27	s	
OMe s	3.77, 3.80, 3.84	s s	
A $\gamma$ 1	4.05	dd	
B $\gamma$ 1	4.13	dd	J = 11.5, 3.2
A $\gamma$ 2	4.26	m	
B $\gamma$ 2	4.39	m	
B $\beta$	4.65	m	
A $\beta$	4.81	m	
B $\alpha$	6.01	d	
A $\alpha$	6.08	d	J = 4.2 J = 6.6
C 2,6	6.48	s	
A 2,6	6.85	s	
B 6	6.90	m	
B 5	7.02	d	
B 2	7.06	m	J = 8.3

**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  
 B1 +/- (0.05 ppm)  
 B2 +/- (0.08 ppm)  
 B3 +/- (0.02 ppm)  
 B4 +/- (0.02 ppm)  
 in acetone



Atom	CDCl <sub>3</sub>		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		
A $\beta$	50.64	23	51.45	43		
A OMe	56.02	42	56.29	62		
B OMe	56.26	38	56.59	52		
B $\gamma$	62.36	23	63.00	38		
A $\gamma$	64.98	13	65.79	19		
B $\beta$	72.47	22	73.27	36		
B $\alpha$	73.95	17	74.55	17		
A $\alpha$	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		
B $\alpha$ Ac C=O	169.87	14	170.01	17		
B $\beta$ Ac C=O	170.10	15	170.26	17		
B $\gamma$ Ac C=O	170.45	15	170.63	20		
A $\gamma$ Ac C=O	170.75	18	170.95	23		

<sup>1</sup>H (acetone)

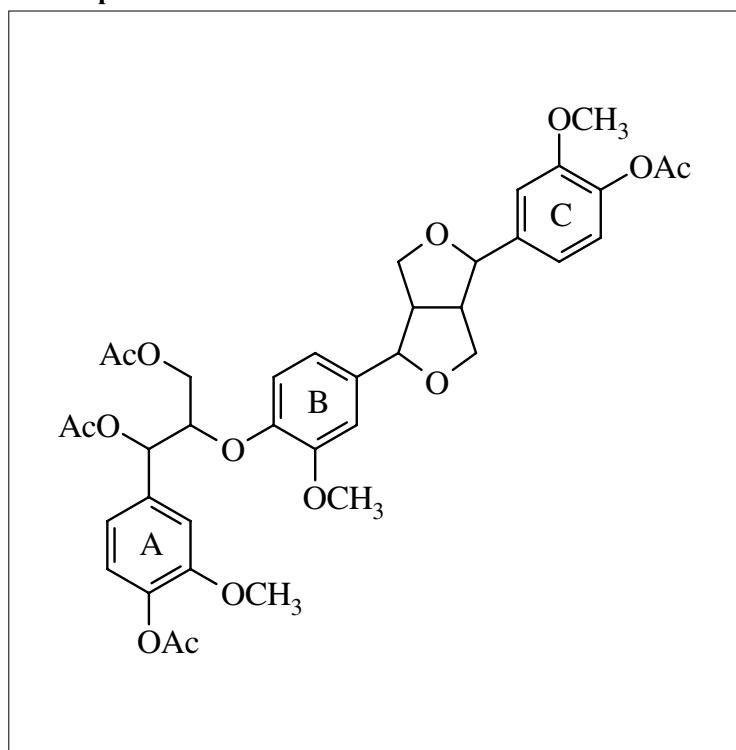
Atom	H Shifts	Mult	J
Ac Me	1.98	m	
Ac Me	2.00	m	
Ac Me	2.03	s	
Ac Me	2.04	s	
A4 Ac Me	2.21	s	
A $\beta$	3.78	m	
A OMe	3.79	s	
B $\gamma$ l	3.82	m	
B OMe	3.87	s	
B $\gamma$ 2	4.17	m	
A $\gamma$	4.38	m	
B $\beta$	5.38	m	
A $\alpha$	5.61	d	
B $\alpha$	5.92	dd	J = 6.8 J = 7.2, 2.8
B2,6,A6	6.99	m	
A5	7.04	d	J = 8.2
A2	7.18	bs	

## Notes:

SRVII-91D 8mg HSQC and HMBC in acetone and CDCl<sub>3</sub>  
A1 and A4 tentative assignments, some signals split due to isomers  
CDCl<sub>3</sub>: A $\gamma$  +/- (0.13), B2 +/- (0.14), B6 +/- (0.10)  
Acetone: A $\gamma$  +/- (0.15), B $\alpha$  +/- (0.04), A2 +/- (0.03), B2 +/- (0.22), B6 +/- (0.17), A6 +/- (0.02), B5 +/- (0.02), A4 +/- (0.03) ppm.

**Compound Number 263**

**$^{13}\text{C}$**



Atom	$\text{CDCl}_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
C4 Ac Me			20.48	71		
A4 Ac Me			20.48	71		
A $\alpha$ Ac Me			20.63	29		
A $\gamma$ Ac Me			20.89	17		
B $\beta$			55.27	23		
C $\beta$			55.41	23		
OMe			56.21	41		
OMe			56.26	38		
OMe			56.28	19		
A $\gamma$			63.03	14		
B $\gamma$			72.50	40		
C $\gamma$			72.62	40		
A $\alpha$			74.54	13		
A $\beta$			80.31	15		
B $\alpha$			86.17	42		
C $\alpha$			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		
A $\alpha$ Ac C=O			169.91	7		
A $\gamma$ Ac C=O			170.77	7		

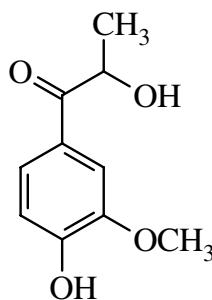
**$^1\text{H}$  (acetone)**

Atom	H Shifts	Mult	J

**Notes:**

SRVII-143D 13 mg  
*Erythro* isomer shirts reported  
 $^{13}\text{C}$  CS in Acetone for *threo* isomer  
A $\gamma$  63.58  
A $\alpha$  75.33  
A $\beta$  80.74  
sample contains small amt of 5,5 resinol tetramer.

## Compound Number 264

<sup>13</sup>C

alpha,4-dihydroxy-3-methoxypropiophenone

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
$\gamma$	22.91	48	22.69	58	21.17	37
OMe	56.19	50	56.33	68	55.57	36
$\beta$	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
$\alpha$	200.75	16	201.10	18	199.72	20

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$	1.35	d	
OMe	3.91	s	
$\beta$ -OH	4.10	d	J = 6.4
b	5.13	m	
5	6.94	d	J = 8.2
2	7.57	d	J = 2.0
6	7.60	dd	J = 8.2, 2.0
4-OH	8.61	bs	
<u>CDCl<sub>3</sub></u>			
$\gamma$	1.46	d	J = 6.6
OMe	3.96	s	
$\beta$	5.13	m	
4-OH	6.61	bs	
5	6.98	d	J = 8.2
6	7.48	dd	J = 8.2, 2.0
2	7.54	d	J = 2.0

## Notes:

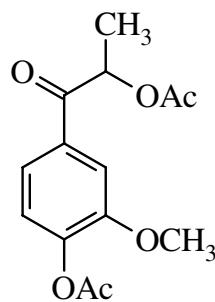
Pearl collection

25 mg

HSQC and HMBC in acetone

**Compound Number 265**

<sup>13</sup>C



alpha,4-diacetoxy-3-methoxypropiophenone

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
$\gamma$	17.16	63	17.41	76	16.90	26
$\beta$ 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
$\beta$	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
$\beta$ Ac C=O	170.32	23	170.54	22	169.74	13
$\alpha$	195.65	23	196.21	24	195.52	13

<sup>1</sup>H (acetone)

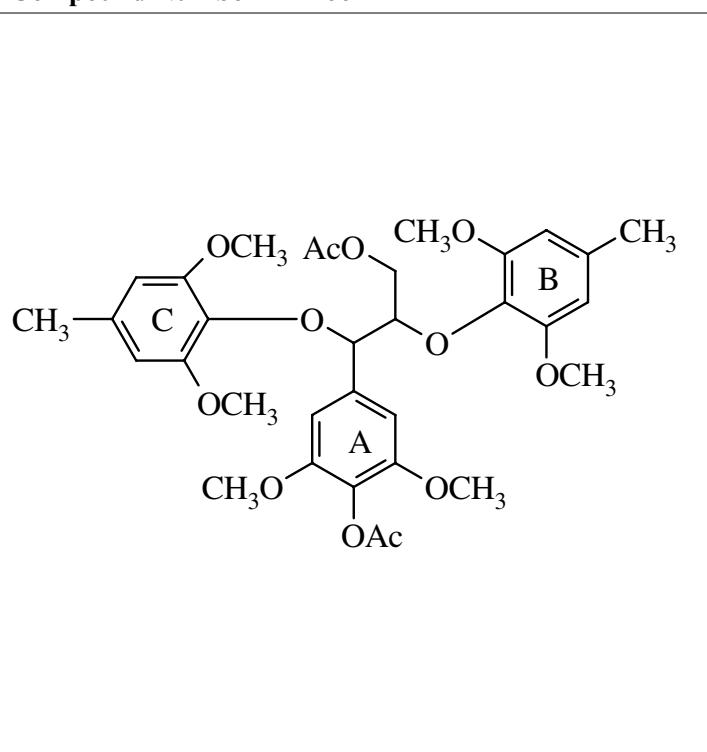
Atom	H Shifts	Mult	J
$\gamma$	1.48	d	
$\beta$ Ac Me	2.06	s	
4 Ac Me	2.27	s	
OMe	3.90	s	
$\beta$	6.00	q	
5	7.23	d	J = 7.0
2	7.64	O/L	J = 8.0
6	7.66	O/L	
<u>CDCl<sub>3</sub></u>			
$\gamma$	1.53	d	J = 7.0
$\beta$ Ac Me	2.14	s	
4 Ac Me	2.33	s	
OMe	3.89	s	
$\beta$	3.93	q	
5	7.14	d	J = 7.0
6	7.55	dd	J = 8.1, 2.0
2	7.59	d	J = 2.0

**Notes:**

Pearl Collection

25 mg

HSQC and HMBC in acetone



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.56	34	20.27	37	20.05	13
γAc 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

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
γAc Me	1.83	s	
A4 Ac Me	2.17	s	
C α	2.18	s	
B α	2.22	s	
B OMe	3.69	s	
A/C OMe	3.73	s	
C/A OMe	3.74	s	
γ1	4.53	dd	J = 11.7, 2.8
γ2	4.63	m	
β	4.73	m	
α	5.72	d	J = 6.2
C 2,6	6.37	s	
B 2,6	6.40	s	
A 2,6	6.81	s	

**Notes:**

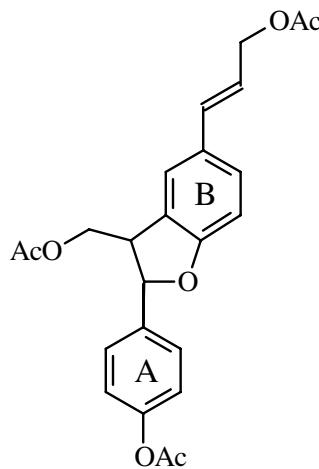
SRIX-138A2

3mg

HSQC and HMBC in acetone

A and C OMe shifts may be switched

B and C CH3's may be switched



Atom	CDCl <sub>3</sub>		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		
Aγ C=O	170.84	20	170.94	13		

<sup>1</sup>H (acetone)

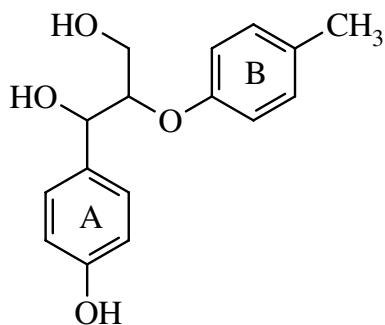
Atom	H Shifts	Mult	J
Ac Me	2.00	s	
Ac Me	2.01	s	
Ac Me	2.24	s	
β	3.74	m	
γ1	4.34	dd	J = 11.1, 7.8
γ2	4.46	dd	J = 11.1, 5.4
Bγ	4.66	dd	J = 6.4, 1.4
α	5.64	d	J = 6.4
Bβ	6.23	dt	J = 15.9, 6.4
Bα	6.66	d	J = 15.9
B3	6.85	d	J = 8.3
A 3,5	7.13	d	J = 8.5
B2	7.33	dd	J = 8.3, 2.0
A 2,6	7.45	d	J = 8.5
B6	7.45		

## Notes:

LLL XXV-17A-E 11mg

Note: B5 and Bγ C=O move in CDCl<sub>3</sub> to lower ppm relative to acetone shifts  
HSQC and HMBC run in AcetoneProton  
shifts in  
CDCl<sub>3</sub>

Ac Me	2.07
Ac Me	2.10
Ac Me	2.30
β	3.70
γ1	4.29
γ2	4.46
Bγ	4.71
α	5.54
Bβ	6.14
Bα	6.61
B3	6.85
A 3,5	7.09
B2	7.27
B6	7.27
A 2,6	7.37



*erythro*  
H-b-H5e

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\alpha$	2.19	s	
$\gamma$ 1	3.77	dd	J = 11.7, 4.4
$\gamma$ 2	3.85	dd	J = 11.7, 5.2
$\beta$	4.34	m	
$\alpha$	4.89	d	J = 5.6
A,B 3,5	6.78		
B 2,6	6.99		J = 8.5
A 2,6	7.28		J = 8.5
CDCl <sub>3</sub>			
B $\alpha$	2.25	s	
$\gamma$ 1	3.80	dd	J = 11.9, 4.0
$\gamma$ 2	3.90	dd	J = 11.9, 4.4
$\beta$	4.28	m	
$\alpha$	4.98	d	J = 5.2
A,B 3,5	6.74		
A 2,6	7.02	d	J = 8.3
B 2,6	7.20	d	J = 8.3

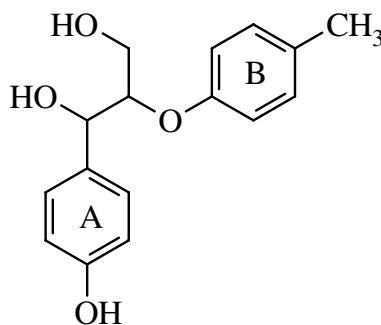
### Notes:

S. Ralph SRIX-62 24mg  
 70% erythro  
 A4 and B4 switch in CDCl<sub>3</sub>  
 B1 falls between A and B 2,6 in DMSO  
 HSQC and HMBC in all solvents

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\alpha$	20.58	58	20.45	28	20.07	43
$\gamma$	61.32	34	61.90	22	60.07	26
$\alpha$	73.89	35	73.81	20	71.36	26
$\beta$	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

**Compound Number 269**

**<sup>13</sup>C**



**H-b-H5t**

*threo*

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\alpha$	20.53	44	20.46	28	20.05	45
$\gamma$	60.95	27	61.54	24	59.99	18
$\alpha$	73.64	26	73.15	19	70.79	25
$\beta$	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

**<sup>1</sup>H (acetone)**

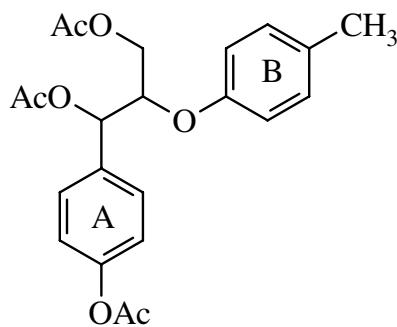
Atom	H Shifts	Mult	J
B $\alpha$	2.21	s	
$\gamma$ 1	3.48	dd	
$\gamma$ 2	3.78	dd	J = 11.5, 4.2
$\beta$	4.35	m	
$\alpha$	4.94	d	J = 5.2
A 3,5	6.78		
B 3,5	6.87		
B 2,6	7.02		
A 2,6	7.27		
CDCl <sub>3</sub>			
B $\alpha$	2.25	s	
$\gamma$ 1	3.46	dd	J = 12.1, 3.8
$\gamma$ 2	3.73	dd	J = 12.1, 4.0
$\beta$	4.28	m	
$\alpha$	4.91	d	J = 6.8
A 3,5	6.72		
B 3,5	6.84		
A 2,6	7.01		
B 2,6	7.18		

**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 CDCl<sub>3</sub>



*erythro*  
**H-b-H5e**

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\alpha$	20.31	64	20.49	46	20.04	42
A $\gamma$ Ac Me	20.50	52	20.58	41	20.40	42
A $\alpha$ Ac Me	20.77	67	20.86	41	20.63	42
A4 Ac Me	20.88	74	20.94	52	20.77	48
$\gamma$	62.15	49	62.86	36	61.77	21
$\alpha$	73.33	50	74.12	34	72.74	24
$\beta$	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
$\alpha$ Ac C=O	169.31	22	169.86	11	169.21	19
$\gamma$ Ac C=O	170.48	20	170.76	11	170.04	18

### <sup>1</sup>H (acetone)

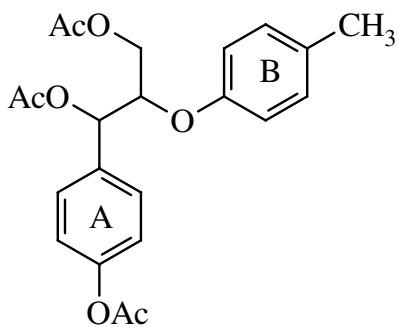
Atom	H Shifts	Mult	J
A $\gamma$ Ac Me	1.94	s	
A $\alpha$ Ac Me	2.06	s	
B $\alpha$	2.23	s	
A4 Ac Me	2.23	s	
$\gamma$ 1	4.23	dd	
$\gamma$ 2	4.34	dd	J = 11.9, 6.0
$\beta$	4.83	m	
$\alpha$	6.04	d	J = 5.4
B 3,5	6.85	m	
B 2,6	7.08	m	
A 3,5	7.08	m	
A 2,6	7.51	d	J = 8.7

Proton shifts in CDCl<sub>3</sub>

A $\gamma$ Ac Me	2.02	s
A $\alpha$ Ac Me	2.09	s
B $\alpha$	2.28	s
A4 Ac Me	2.28	s
$\gamma$ 1	4.20	dd
$\gamma$ 2	4.37	dd
$\beta$	4.66	m
$\alpha$	6.04	d
B 3,5	6.77	d
B 2,6	7.07	m
A 3,5	7.07	m
A 2,6	7.42	d

### Notes:

SRIX-62 25mg  
70% erythro  
HSQC and HMBC in acetone

**H-b-H5t***threo*

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\alpha$	20.49	65	20.49	59	20.03	
A $\gamma$ Ac Me	20.64	54	20.55	54	20.39	
A $\alpha$ Ac Me	20.97	65	20.88	57	20.64	
A4 Ac Me	21.08	75	20.94	72	20.77	
$\gamma$	62.68	56	63.27	53	62.23	
$\alpha$	73.94	55	74.88	55	73.77	
$\beta$	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	
$\alpha$ Ac C=O	169.73	24	170.04	19	169.41	
$\gamma$ Ac C=O	170.57	24	170.68	17	169.98	

**<sup>1</sup>H** (acetone)

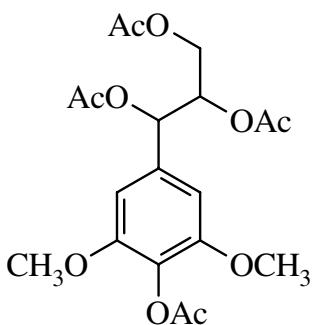
Atom	H Shifts	Mult	J
A $\gamma$ Ac Me	1.94	s	
A $\alpha$ Ac Me	2.01	s	
B $\alpha$	2.24	s	
A4 Ac Me	2.24	s	
$\gamma$ 1	4.01	dd	
$\gamma$ 2	4.23	dd	J = 11.9, 4.2
$\beta$	4.83	m	
$\alpha$	6.10	d	J = 6.4
B 3,5	6.90		
B 2,6	7.10		
A 3,5	7.10		
A 2,6	7.51	d	J = 8.5

**Notes:**

SRIX-62 25mg  
75% threo

Proton  
shifts in  
CDCl<sub>3</sub>

A $\gamma$ Ac Me	1.98	s	
A $\alpha$ Ac Me	2.05	s	
B $\alpha$	2.28	s	
A4 Ac Me	2.28	s	
$\gamma$ 1	4.00	dd	11.7, 6.0
$\gamma$ 2	4.26	dd	11.7, 4.4
$\beta$	4.64	m	
$\alpha$	6.09	d	J = 6.4
B 3,5	6.85	d	J = 8.5
B 2,6	7.07	m	
A 3,5	7.07	m	
A 2,6	7.42	d	J = 8.5



Atom	CDCl <sub>3</sub>		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

Proton  
shifts in  
CDCl<sub>3</sub>

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	J = 7.6
2,6	6.61	s	

<sup>1</sup>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	J = 12.1, 6.2
γ2	4.23	dd	J = 12.1, 3.8
β	5.41	m	
α	5.95	d	
2,6	6.80	s	J = 6.8

**Notes:**

L. Landucci XXV-138D7 19mg

2:1 mix of isomers

minor isomer shifts in acetone and CDCl<sub>3</sub>

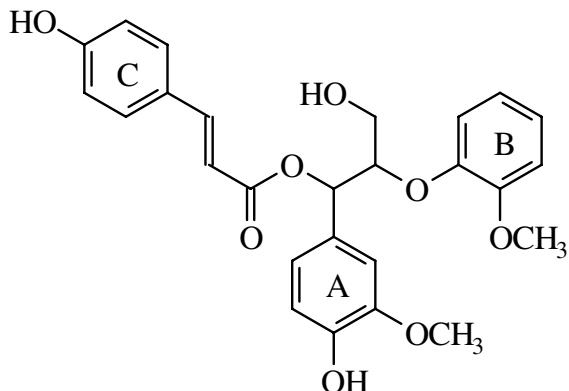
62.34, 72.99, 73.76, 104.67, 135.63, 153.19

61.42, 72.48, 73.03, 103.75, 134.19, 152.27

Compound Number 1001

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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			
Cβ			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			157.87			
C4			160.48			
C γ			166.51			



3-(4-Hydroxyphenyl)acrylic acid 3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

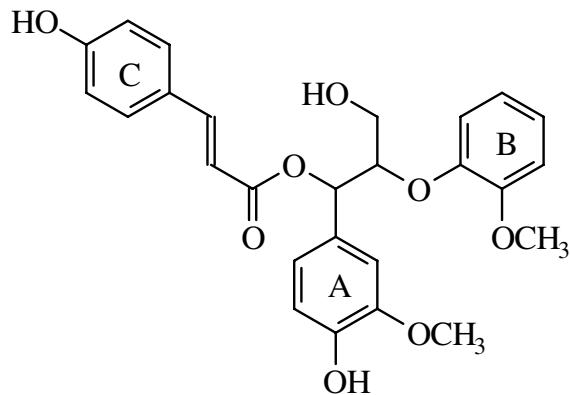
<sup>1</sup>H (acetone)

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

## Compound Number 1002

<sup>13</sup>C*erythro*

**3-(4-Hydroxyphenyl)acrylic acid 3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma^1$	3.68	dd	11.7,4.8
$\gamma^2$	3.79	dd	11.8,5.7
$\beta$	4.66	m	
$\alpha$	6.12	d	4.8
C $\beta$	6.35	d	16.0
C $\alpha$	7.56	d	16.0

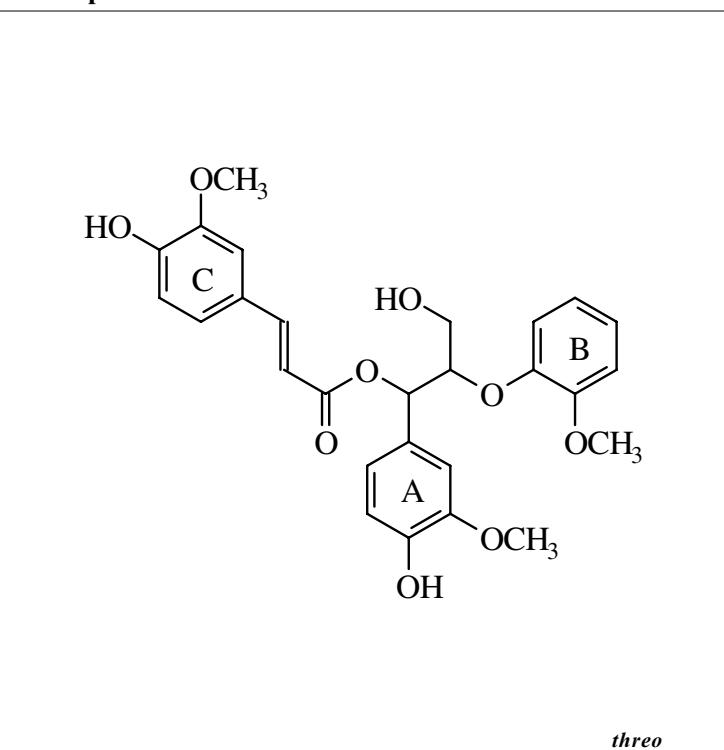
Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
OMe			56.29			
OMe			56.29			
$\gamma$			61.49			
$\alpha$			75.08			
$\beta$			84.09			
A2			112.57			
B2			113.67			
A5			115.21			
C $\beta$			115.62			
C3			116.67			
C5			116.67			
B5			119.18			
B6			121.75			
A6			121.79			
B1			123.31			
C1			126.97			
A1			129.64			
C2			130.96			
C6			130.96			
C $\alpha$			145.65			
A4			147.35			
A3			147.99			
B4			149.22			
B3			157.86			
C4			160.59			
C $\gamma$			166.32			

**Notes:**

R. Helm

**Compound Number 1003**

<sup>13</sup>C



3-(4-Hydroxy-3-methoxyphenyl)acrylic acid 3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
γ1	3.52	dd	119.53
γ2	3.69	dd	119.38
β	4.58	m	
α	6.16	d	23
C β	6.34	d	159
C α	7.49	d	159

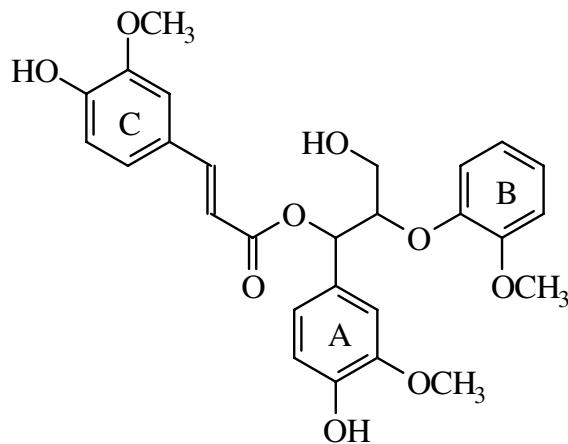
**Notes:**

R. Helm

Atom	CDCl <sub>3</sub>		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			157.82			
C γ			166.55			

**Compound Number 1004**

**<sup>13</sup>C**



3-(4-Hydroxy-3-methoxyphenyl)acrylic acid3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)propyl ester

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
γ1	3.60	dd	11.7,4.8
γ2	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

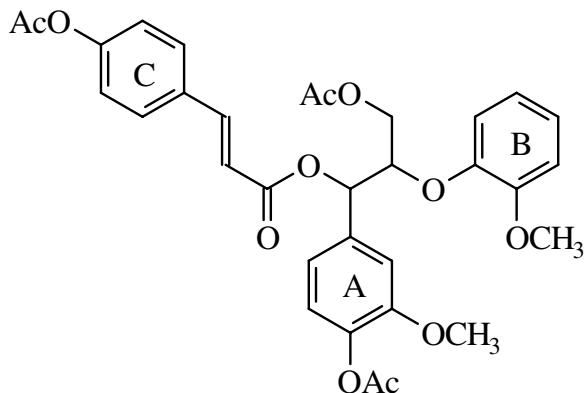
**Notes:**

R. Helm  
CDCl<sub>3</sub> column is D<sub>2</sub>O/Acetone-d<sub>6</sub>

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Acet /D <sub>2</sub> O						
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	157.85		157.84			
C γ	166.35		166.34			

**Compound Number 1005**

<sup>13</sup>C



*threo*

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

<sup>1</sup>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

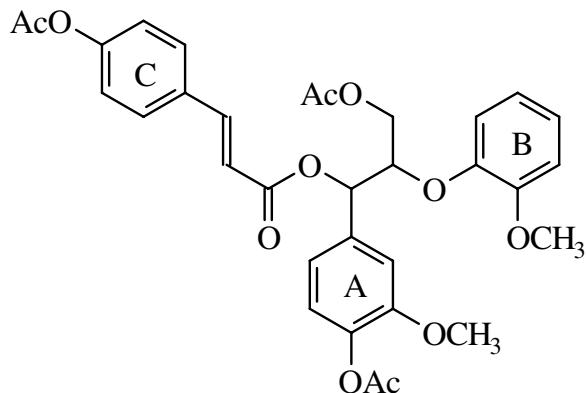
**Notes:**

R. Helm

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			157.89			
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

<sup>13</sup>C



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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
γ1	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
Cβ	6.61	d	16.1
Cα	7.71	d	16.1

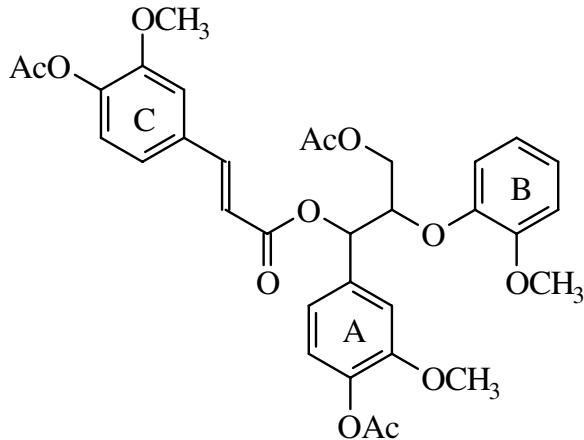
Notes:

R. Helm

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			
Cβ			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			
Cα			145.12			
B4			148.39			
B3			152.06			
A3			152.14			
C4			153.58			
Cγ			165.79			
Ac C=O			168.89			
Ac C=O			169.42			
Ac C=O			170.75			

**Compound Number 1007**

<sup>13</sup>C



*threo*

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

<sup>1</sup>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

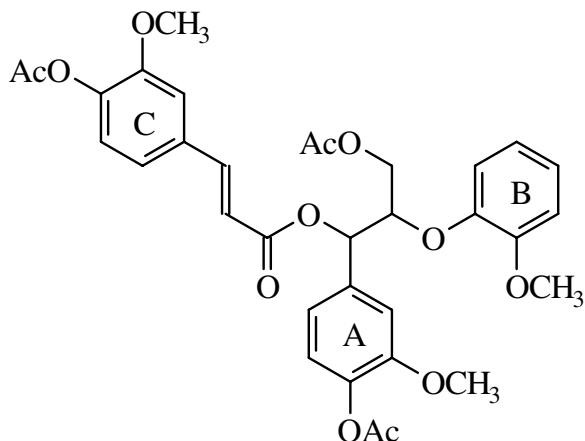
**Notes:**

R. Helm  
16mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			157.88			
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**

**<sup>13</sup>C**



*erythro*

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

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
$\gamma^1$	4.28	dd	11.8,4.4
$\gamma^2$	4.40	dd	11.8,6.1
$\beta$	4.96	m	
$\alpha$	6.22	d	4.7
C $\alpha$	6.65	d	16.0
C $\beta$	7.68	d	16.0

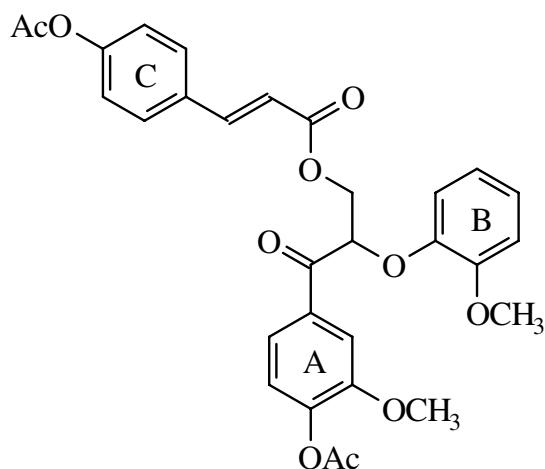
Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
Ac Me			20.44			
Ac Me			20.44			
Ac Me			20.61			
OMe			56.22			
OMe			56.30			
OMe			56.41			
$\gamma$			63.16			
$\alpha$			74.97			
$\beta$			80.39			
C2			112.46			
A2			112.79			
B2			113.79			
C $\beta$			118.75			
B5			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 $\alpha$			145.57			
B4			148.37			
B3			152.05			
A3			152.14			
C3			152.69			
C $\gamma$			165.89			
Ac C=O			168.79			
Ac C=O			168.90			
Ac C=O			170.76			

**Notes:**

R. Helm  
19mg  
Acetone run at 300 K

**Compound Number 1009**

<sup>13</sup>C



**3-(4-Acetoxyphenyl) acrylic acid 3-(4-acetoxy-3-methoxyphenyl)-2-(2-methoxyphenoxy)-3-oxopropyl ester**

<sup>1</sup>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

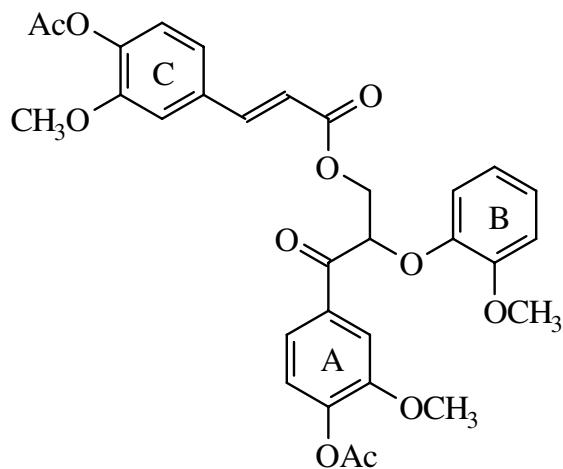
**Notes:**

R. Helm  
25.5mg  
acetone-d6 at 300 K

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			157.42			
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

<sup>13</sup>C



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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma^1$	4.61	dd	12.0,6.5
$\gamma^2$	4.81	dd	12.0,3.8
$\beta$	5.91	dd	6.5,3.8
$C\beta$	6.52	d	16.0
$C\alpha$	7.58	d	16.0

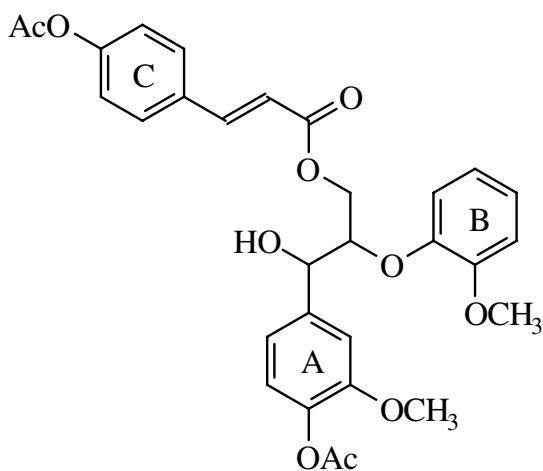
Notes:

R. Helm  
25mg  
300k, acetone-d6

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me			20.44			
Ac Me			20.44			
OMe			56.10			
OMe			56.40			
OMe			56.43			
$\gamma$			64.93			
$\beta$			80.54			
C2			112.41			
A2			113.48			
B2			113.83			
$C\beta$			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			
$C\alpha$			145.50			
B4			147.82			
B3			157.40			
A3			152.50			
C3			152.69			
$C\gamma$			166.81			
Ac C=O			168.58			
Ac C=O			168.80			
$\alpha$			195.11			

Compound Number 1011

<sup>13</sup>C



*threo*

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

<sup>1</sup>H (acetone)

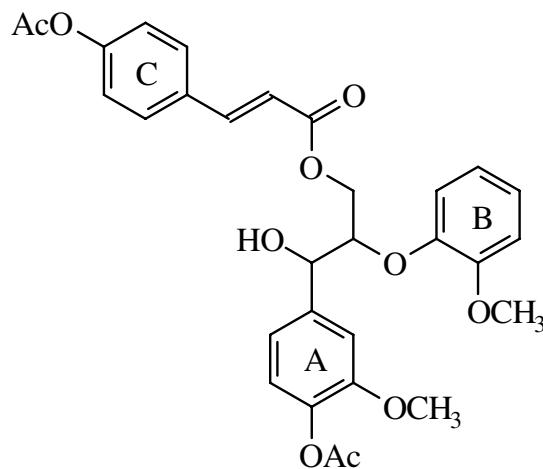
Atom	H Shifts	Mult	J
α	5.08	d	4.3
α OH	4.75		
β	4.64	m	
γ1	4.17	dd	11.9,6.3
γ2	4.44	dd	11.9,3.7
C β	6.46	d	16.1
C α	7.54	d	16.0

Notes:

R. Helm

Compound Number 1012

<sup>13</sup>C



*erythro*

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

<sup>1</sup>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

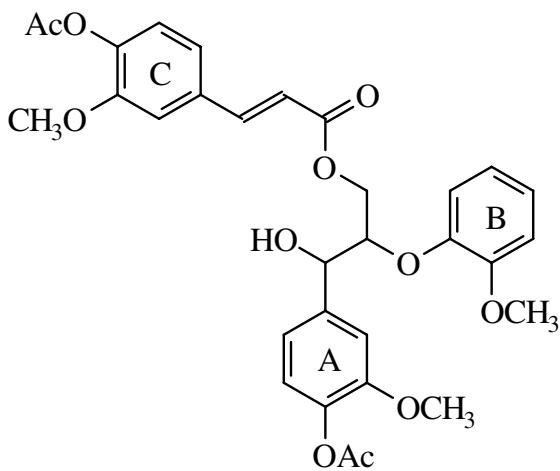
Notes:

R. Helm

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C



*threo*

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

<sup>1</sup>H (acetone)

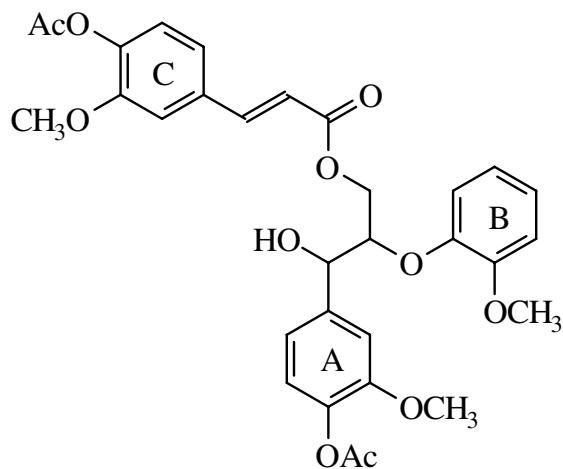
Atom	H Shifts	Mult	J
α	5.08	d	4.2
α OH	4.75		
β	4.64	m	
γ1	4.17	dd	11.9,6.2
γ2	4.44	dd	11.9,3.7
Cβ	6.49	d	16.0
C α	7.51	d	16.0

Notes:

R. Helm

Compound Number 1014

<sup>13</sup>C



*erythro*

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

<sup>1</sup>H (acetone)

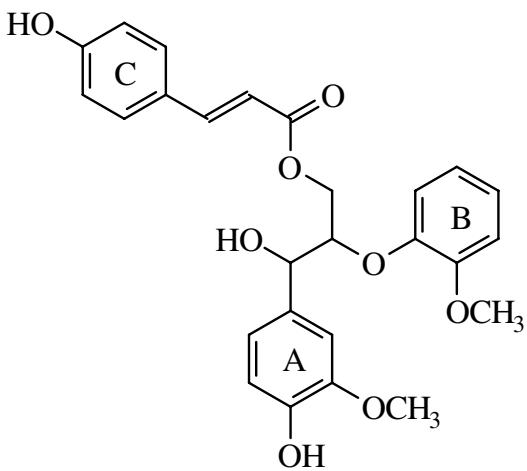
Atom	H Shifts	Mult	J
α	5.08	d	4.4
α OH	4.79		
β	4.70	m	
γ1	4.45	dd	11.8,3.7
γ2	4.58	dd	11.8,6.2
C β	6.44	d	16.0
C α	7.47	d	16.0

Notes:

R. Helm

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			

## Compound Number 1015

<sup>13</sup>C

**3-(4-Hydroxyphenyl) acrylic acid 3-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester**

<sup>1</sup>H (acetone)

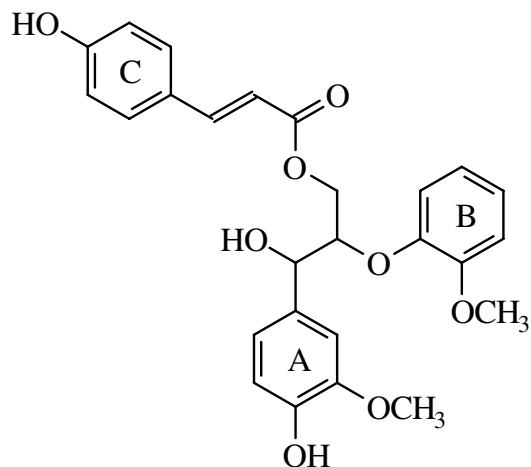
Atom	H Shifts	Mult	J
γ1	4.10	dd	12.0,6.2
γ2	4.36	dd	12.0,3.5
β	4.56	m	
α OH	4.59	d	3.9
α	4.97	dd	6.2,3.9
C β	6.29	d	16.0
C α	7.47	d	16.0

**Notes:**

R. Helm

Atom	CDCl <sub>3</sub>		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			157.79			
C4			160.63			
C γ			167.15			

## Compound Number 1016

<sup>13</sup>C*erythro*

**3-(4-Hydroxyphenyl) acrylic acid 3-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester**

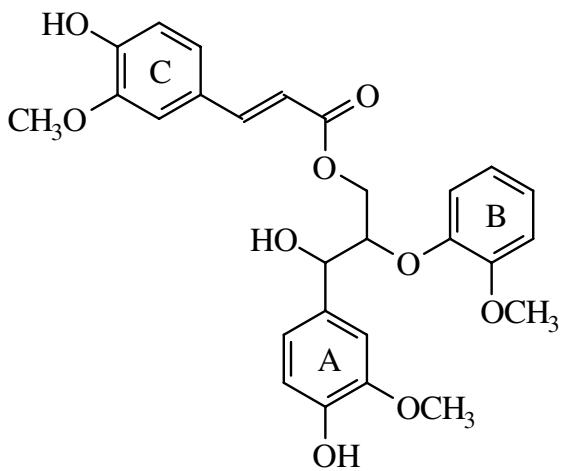
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma 1$	4.39	dd	11.8,3.6
$\gamma 2$	4.46	dd	11.8,6.6
$\beta$	4.66	m	
$\alpha$	4.91	d	4.9
C $\beta$	6.24	d	16.0
C $\alpha$	7.42	d	16.0

**Notes:**

R. Helm

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
OMe			56.20			
OMe			56.22			
$\gamma$			63.98			
$\alpha$			73.28			
$\beta$			83.54			
A2			111.20			
B2			113.64			
C $\beta$			115.24			
			115.34			
A5			116.64			
C3			116.64			
C5			119.67			
B5			120.32			
A6			121.71			
B6			123.51			
B1			126.91			
C1			130.88			
C2			130.88			
C6			133.59			
A1			145.39			
C $\alpha$			146.72			
A4			148.02			
A3			148.86			
B4			152.02			
B3			160.52			
C4			167.28			
C $\gamma$						

*threo*

3-(4-Hydroxy-3-methoxyphenyl) acrylic acid 3-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester

<sup>1</sup>H (acetone)

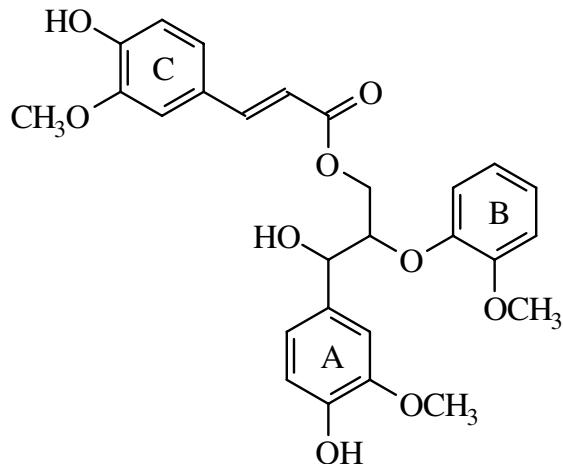
Atom	H Shifts	Mult	J
$\alpha$	4.96	d	6.3
$\beta$	4.56	m	
$\gamma^2$	4.36	dd	12.0,3.5
$\gamma^1$	4.10	dd	12.0,6.2
C $\beta$	6.33	d	16.0
C $\alpha$	7.45	d	16.0

Notes:

R. Helm

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.20			
OMe			56.26			
OMe			56.32			
$\gamma$			64.16			
$\alpha$			73.94			
$\beta$			84.48			
C2			111.37			
A2			111.46			
B2			113.60			
A5			115.33			
C $\beta$			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 $\alpha$			145.91			
A4			147.01			
A3			148.08			
C3			148.71			
B4			149.36			
C4			150.09			
B3			151.80			
C $\gamma$			167.14			

## Compound Number 1018

<sup>13</sup>C

**3-(4-Hydroxy-3-methoxyphenyl) acrylic acid 3-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxyphenoxy) propyl ester**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma 1$	4.40	dd	3.7,
$\gamma 2$	4.46	dd	6.7,
$\beta$	4.66	m	
$\alpha$	4.97	d	4.9
C $\alpha$	6.28	d	15.9
C $\beta$	7.40	d	15.9

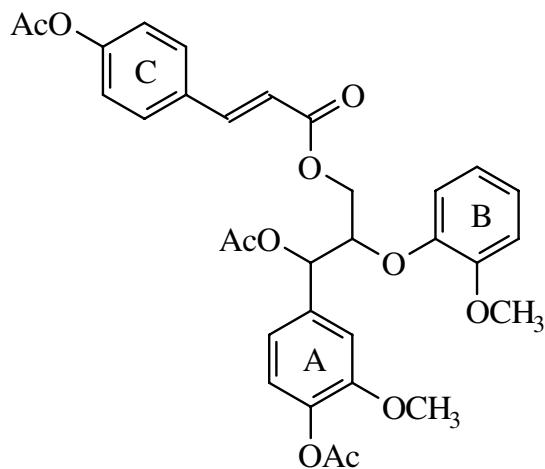
**Notes:**

R. Helm  
27mg  
300K, acetone-d6

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
OMe			56.23			
OMe			56.23			
OMe			56.31			
$\gamma$			63.94			
$\alpha$			73.26			
$\beta$			83.57			
A2			111.21			
C2			111.29			
B2			113.66			
A5			115.25			
C $\beta$			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 $\alpha$			145.74			
A4			146.74			
A3			148.05			
C3			148.70			
B4			148.86			
C4			150.04			
B3			152.04			
C $\gamma$			167.28			

**Compound Number 1019**

<sup>13</sup>C



*threo*

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

<sup>1</sup>H (acetone)

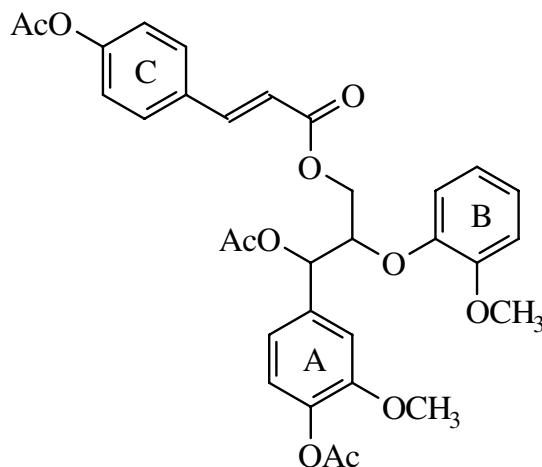
Atom	H Shifts	Mult	J
γ1	4.17	dd	5.6,
γ2	4.40	dd	4.0,
β	4.88	m	
α	6.18	d	6.5
C β	6.51	d	16.0
C α	7.57	d	16.1

**Notes:**

R. Helm  
18mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			157.90			
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

<sup>13</sup>C*erythro*

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

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma^1$	4.40	dd	11.9,4.2
$\gamma^2$	4.48	dd	11.9,5.9
$\beta$	4.92	m	
$\alpha$	6.13	d	5.1
C $\beta$	6.45	d	16.0
C $\alpha$	7.56	d	16.1

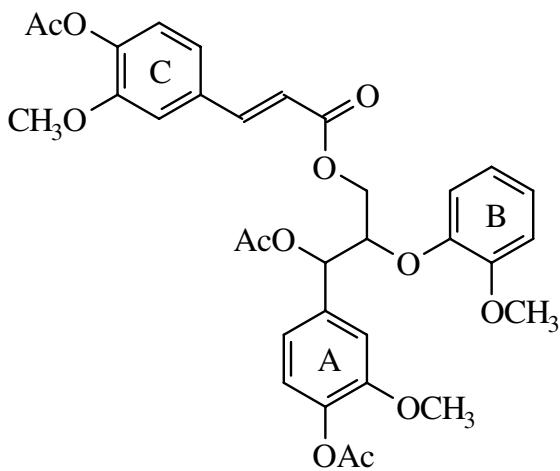
### Notes:

R. Helm

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me			20.46			
Ac Me			20.89			
Ac Me			20.94			
OMe			56.19			
OMe			56.26			
$\gamma$			63.33			
$\alpha$			74.71			
$\beta$			80.52			
A2			112.74			
B2			113.76			
C $\beta$			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 $\alpha$			144.71			
B4			148.30			
B3			152.09			
A3			152.11			
C4			153.49			
C $\gamma$			166.60			
Ac C=O			168.89			
Ac C=O			169.41			
Ac C=O			169.92			

**Compound Number 1021**

<sup>13</sup>C



*threo*

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

<sup>1</sup>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

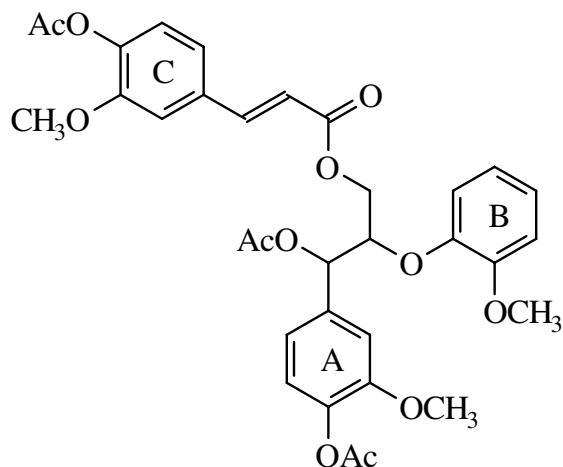
**Notes:**

R. Helm  
18.5mg  
300K

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

<sup>13</sup>C



*erythro*

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

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma^1$	4.40	dd	11.9,4.2
$\gamma^2$	4.49	dd	11.9,5.9
$\beta$	4.92	m	
$\alpha$	6.13	d	5.1
$C\beta$	6.48	d	16.0
$C\alpha$	7.53	d	16.0

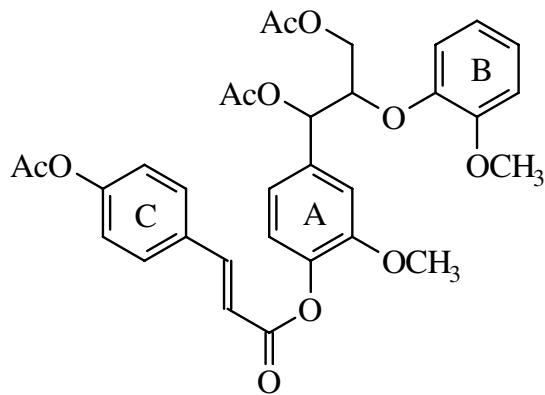
Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me			20.45			
Ac Me			20.45			
Ac Me			20.89			
OMe			56.19			
OMe			56.28			
OMe			56.40			
$\gamma$			63.33			
$\alpha$			74.70			
$\beta$			80.50			
C2			112.44			
A2			112.74			
B2			113.77			
$C\beta$			118.63			
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			
$C\alpha$			145.16			
B4			148.30			
B3			152.10			
A3			152.12			
C3			152.67			
$C\gamma$			166.67			
Ac C=O			168.80			
Ac C=O			168.90			
Ac C=O			169.94			

### Notes:

R. Helm  
18.5mg  
300K

Compound Number 1023

<sup>13</sup>C



3-(4-acetoxyphenyl) acrylic acid 4-[1,3-diacetoxymethyl] phenyl ester

<sup>1</sup>H (acetone)

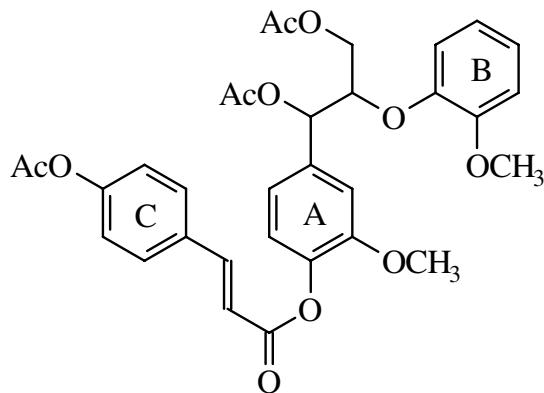
Atom	H Shifts	Mult	J
C $\alpha$	7.84	d	16.1
C $\beta$	6.74	d	16.1
$\alpha$	6.14	d	6.5
$\beta$	4.81	m	
$\gamma^1$	4.28	dd	11.9,4.2
$\gamma^2$	4.04	dd	11.9,5.6

Notes:

R. Helm  
20.6mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me			20.59			
Ac Me			20.92			
Ac Me			20.96			
OMe			56.30			
OMe			56.20			
$\gamma$			63.60			
$\alpha$			75.40			
$\beta$			80.70			
A2			112.70			
B2			113.74			
C $\beta$			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 $\alpha$			146.05			
B4			149.08			
B3			151.84			
A3			152.30			
C4			153.74			
C $\gamma$			164.91			
Ac C=O			169.42			
Ac C=O			170.01			
Ac C=O			170.68			

## Compound Number 1024

<sup>13</sup>C

**3-(4-acetoxyphenyl) acrylic acid 4-[1,3-diacetoxymethyl] phenyl ester**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
C $\alpha$	7.84	d	15.7
C $\beta$	6.74	d	16.1
$\alpha$	6.10	d	5.1
$\beta$	4.85	m	
$\gamma$ 1	4.39	dd	11.9,5.9
$\gamma$ 2	4.24	dd	11.9,4.2

**Notes:**

R. Helm  
25mg

Atom	CDCl <sub>3</sub>		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			
$\gamma$			63.00			
$\alpha$			74.60			
$\beta$			80.32			
A2			112.77			
B2			113.79			
C $\beta$			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 $\alpha$			146.02			
B4			148.27			
B3			152.06			
A3			152.19			
C4			153.74			
C $\gamma$			164.95			
Ac C=O			169.42			
Ac C=O			169.92			
Ac C=O			170.76			

Compound Number 1025

<sup>13</sup>C

|--|--|

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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
C $\alpha$	7.81	d	15.9
C $\beta$	6.77	d	16.0
$\alpha$	6.14	d	6.5
$\beta$	4.81	m	
$\gamma^1$	4.28	dd	11.9,4.2
$\gamma^2$	4.04	dd	11.9,5.6

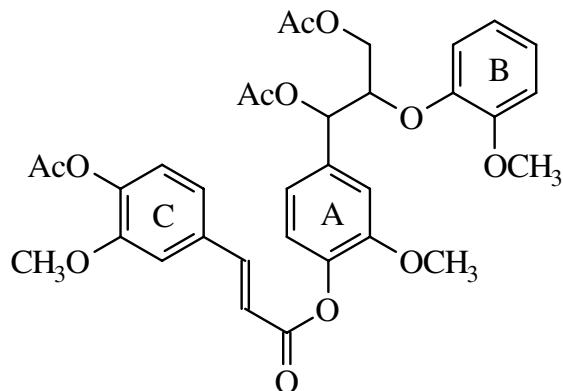
Notes:

R. Helm  
20.6mg  
std conditions

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			
$\gamma$			63.61			
$\alpha$			75.40			
$\beta$			80.70			
C2			112.61			
A2			112.70			
B2			113.75			
C $\beta$			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 $\alpha$			146.46			
B4			149.08			
B3			151.84			
A3			152.30			
C3			152.76			
C $\gamma$			164.97			
Ac C=O			168.79			
Ac C=O			170.01			
Ac C=O			170.69			

Compound Number 1026

<sup>13</sup>C



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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
C $\alpha$	7.81	d	15.8
C $\beta$	6.78	d	16.0
$\alpha$	6.10	d	5.1
$\beta$	4.85	m	
$\gamma$ 1	4.39	dd	11.9,5.6
$\gamma$ 2	4.24	dd	11.9,4.2

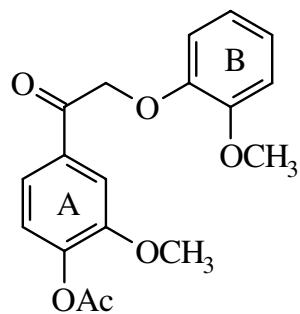
Notes:

R. Helm  
20.9mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			
$\gamma$			63.00			
$\alpha$			74.60			
$\beta$			80.32			
C2			112.60			
A2			112.77			
B2			113.79			
C $\beta$			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 $\alpha$			146.44			
B4			148.27			
B3			152.06			
A3			152.19			
C3			152.76			
C $\gamma$			165.00			
Ac C=O			168.80			
Ac C=O			169.92			
Ac C=O			170.76			

Compound Number 1027

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			

Acetic acid 2-methoxy-4-[2-(2-methoxyphenoxy) acetyl] phenyl ester

### <sup>1</sup>H (acetone)

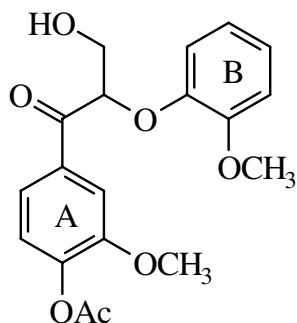
Atom	H Shifts	Mult	J
β	5.43		

### Notes:

R. Helm  
crystalline

Compound Number 1028

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			

Acetic acid 4-[3-hydroxy-2-(2-methoxyphenoxy) propionyl]-2-methoxy phenyl ester

<sup>1</sup>H (acetone)

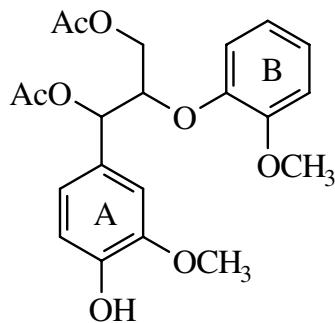
Atom	H Shifts	Mult	J
β	5.55		
γ's	4.09		

Notes:

R. Helm  
20mg  
300K acetone-d6

**Compound Number 1029**

<sup>13</sup>C



*threo*

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			

**Acetic acid 3-acetoxy-3-(4-hydroxy-3-methoxyphenyl)  
-2-(2-methoxyphenoxy) propyl ester**

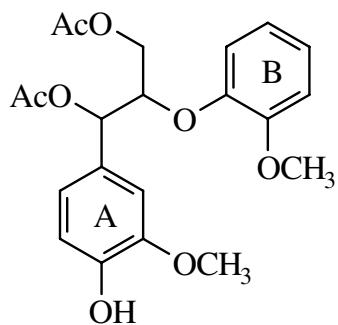
<sup>1</sup>H (acetone)

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

Compound Number 1030

<sup>13</sup>C*erythro*

**Acetic acid 3-acetoxy-3-(4-hydroxy-3-methoxyphenyl)  
-2-(2-methoxyphenoxy) propyl ester**

### <sup>1</sup>H (acetone)

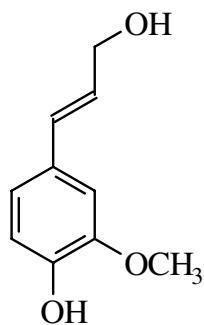
Atom	H Shifts	Mult	J
$\alpha$	5.99	d	4.99
$\beta$	4.81	m	
$\gamma 1$	4.34	dd	11.9,6.2
$\gamma 2$	3.98	dd	11.9,4.0

### Notes:

R. Helm  
15mg  
std conditions

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me			20.60			
Ac Me			20.90			
OMe			56.20			
OMe			56.29			
$\gamma$			63.30			
$\alpha$			74.89			
$\beta$			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

<sup>13</sup>C*trans*

coniferyl alcohol

4-hydroxy-3-methoxy cinnamyl alcohol

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$ OH	3.78	t	5.65
OMe	3.85	s	
$\gamma$	4.18	td	1.5, 5.6
$\beta$	6.22	dt	15.9,5.5
$\alpha$	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	

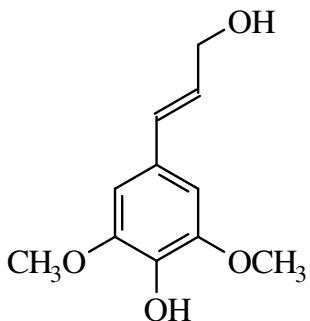
## Notes:

S. Quideau

Assignments confirmed in all three solvents

JAFC 1992-40(7)

1108-1110

**Compound Number    2002**
<sup>13</sup>C


**sinapyl alcohol**  
**4-hydroxy-3,5-dimethoxy cinnamyl alcohol**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
γOH	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	

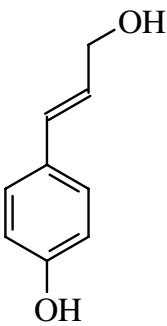
**Notes:**

S. Quideau  
 Note A1 and β change places in DMSO  
 Assignments confirmed in CDCl<sub>3</sub> and Acetone  
 JAFC 1992-40(7)  
 1108-1110

Atom	CDCl <sub>3</sub>		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

Compound Number 2003

<sup>13</sup>C



**p-coumaryl alcohol**  
**4-hydroxy-cinnamyl alcohol**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
γOH g's	3.85 4.19	t td	5.65 5.6,1.6
β	6.19	dt	15.9, 5.6
α	6.50	dt	15.9,1.6
3,5 2,6	6.78 7.25	m m	
4 OH	8.40	s	

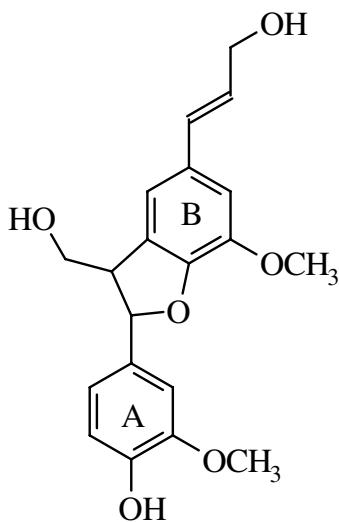
**Notes:**

S. Quideau  
JAFC-1992-40(7)  
1108-1110

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

Compound Number 2004

<sup>13</sup>C



4-[3-Hydroxymethyl-5-(3-hydroxypropenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-2-methoxyphenol

<sup>1</sup>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	
BγOH	4.16	t	5.0
Bγ	4.19	td	5.2, 1.5
α	5.56	d	6.5
Bβ	6.23	dt	15.8, 5.5
Bα	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:

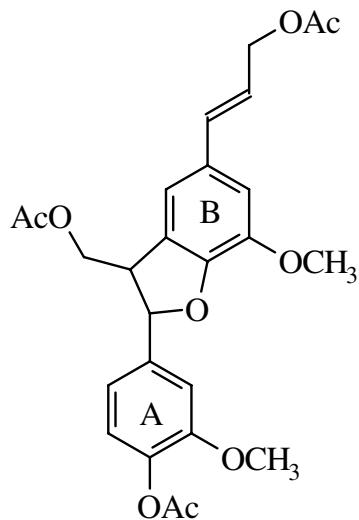
S. Quideau-Ag<sub>2</sub>O oxidation of coniferyl alcohol.

Assignments confirmed in acetone.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
Bγ	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
Bβ	126.45	70	128.33	85	128.02	46
B5	128.09	50	130.40	59	129.52	48
Bα	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**

**<sup>13</sup>C**



Atom	<i>CDCl</i> <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.51	91	20.43	94	20.41	68
$\gamma$ Ac Me	20.68	81	20.67	92	20.61	78
B $\gamma$ Ac Me	20.90	84	20.78	77	20.79	84
$\beta$	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
$B\gamma$	65.06	83	65.47	100	64.57	60
$\gamma$	65.22	61	65.96	75	64.90	37
$\alpha$	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 $\beta$	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 $\alpha$	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
$\gamma$ C=O	170.63	53	170.97	43	170.41	51
B $\gamma$ C=O	170.76	43	170.80	32	170.27	44

Acetic acid 4-[3-acetoxymethyl-5-(3-acetoxypropenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-2-methoxyphenyl ester

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	2.0	s	
B $\gamma$ Ac Me	2.01	s	
A4 Ac Me	2.22	s	
$\beta$	3.78	m	
A3 OMe	3.79	s	
B3 OMe	3.88	s	
$\gamma$ 1	4.34	dd	11.1, 7.6
$\gamma$ 2	4.46	dd	11.1, 5.4
B $\gamma$	4.66	dd	6.5, 1.3
$\alpha$	5.61	d	6.7
B $\beta$	6.24	dt	15.8, 6.5
B $\alpha$	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

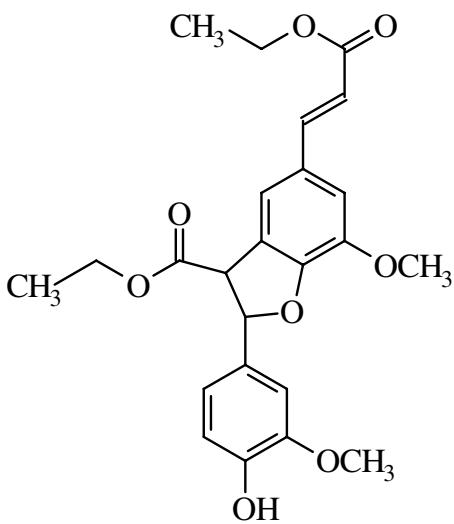
**Notes:**

S.Quideau-Ag<sub>2</sub>O oxidation of coniferyl alcohol + acetylation. Assignments confirmed in *CDCl*<sub>3</sub> and acetone

A1 and A4 switch places in *CDCl*<sub>3</sub>

**Compound Number 2006**

**<sup>13</sup>C**



**5-(2-Ethoxycarbonylvinyl)-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy-2,3-dihydrobenzofuran-3-carboxylic acid ethyl ester**

**<sup>1</sup>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	
$\beta$	4.43	d	8.0
$\alpha$	6.03	d	8.0
B $\beta$	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 $\alpha$	7.62	d	15.9
A4 OH	7.87	s	

**Notes:**

S. Quideau-Ag<sub>2</sub>O oxidation of ethyl ferulate.

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\beta$	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
$\alpha$	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 $\beta$	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 $\alpha$	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 $\gamma$	167.18	58	167.28	53	166.65	57
$\gamma$	170.20	64	171.10	53	170.42	65

**Compound Number 2007**

**<sup>13</sup>C**

 <i>trans</i>						
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**1,4-bis-(4-hydroxy-3-methoxyphenyl)-1,3-butadiene**

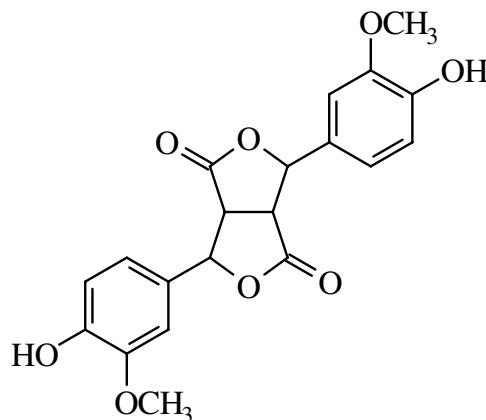
**<sup>1</sup>H (acetone)**

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	

**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

<sup>13</sup>C**dilactone from ferulic acid**

**3,6-Bis-(4-hydroxy-3-methoxyphenyl) tetrahydrofuro [3,4-c] furan-1,4-dione**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
OMe	3.85	s	
β	4.09	t	
α	5.77	br s	
5	6.86	d	1.0
6	6.92	dd	
2	7.05	d	8.2, 1.8
4 OH	7.90	s	1.8

**Notes:**

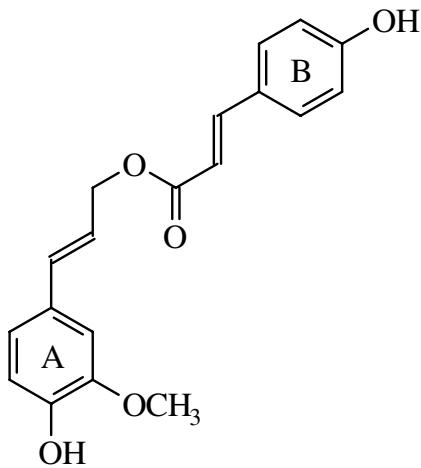
S. Quideau

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

Atom	CDCl <sub>3</sub>		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

**Compound Number 2009**

**<sup>13</sup>C**



**coniferyl p-coumarate**  
**3-(4-Hydroxyphenyl) acrylic acid 3-(4-hydroxy-3-methoxyphenyl) llyl ester**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
OMe	3.86	s	
$\gamma$	4.78	dd	6.5, 1.3
$\beta$	6.25	dt	15.8, 6.5
B $\beta$	6.37	d	15.9
$\alpha$	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 $\alpha$	7.63	d	15.9
ArOH	7.76	s	
ArOH	9.03	s	

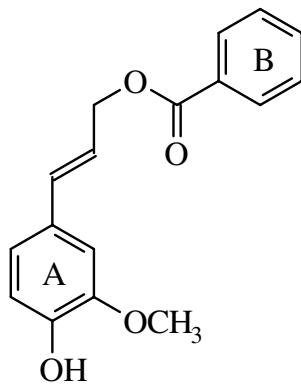
**Notes:**

S. Quideau

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
OMe	55.87	55	56.20	47	55.61	77
$\gamma$	65.35	43	65.49	55	64.62	34
A2	108.44	51	110.20	47	109.91	52
B $\beta$	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
$\beta$	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
$\alpha$	134.43	50	134.90	45	133.9	49
B $\alpha$	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 $\gamma$	167.57	28	167.27	23	166.46	40

Compound Number 2010

<sup>13</sup>C



coniferyl benzoate

3-Phenyl-acrylic acid 3-(4-hydroxy-3-methoxyphenyl)allyl ester

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
OMe	3.86	s	
$\gamma$	4.94	dd	6.5, 1.3
$\beta$	6.34	dt	15.8, 6.5
$\alpha$	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	

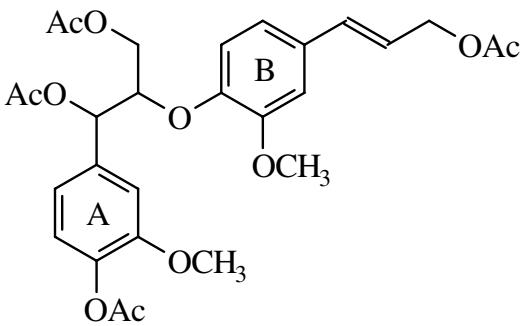
Notes:

S. Quideau  
isolated from gum s.am

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
OMe	55.86	43	56.21	59	55.61	58
$\gamma$	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
$\beta$	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
$\alpha$	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 $\alpha$ C=O	166.46	16	166.58	16	165.62	25

Compound Number 2011

<sup>13</sup>C



*threo*  
**Guaiacylglycerol- $\beta$ -coniferyl ether peracetate**

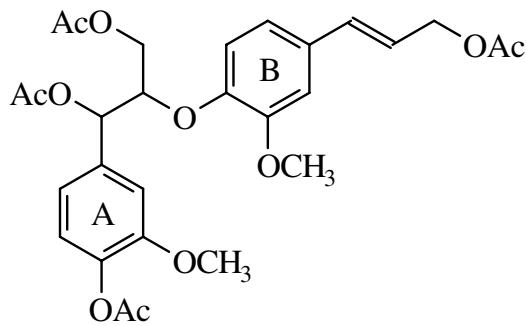
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J

**Notes:**

S. Quideau

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
A4 Ac Me	20.63		20.44		20.38	
$\alpha$ Ac Me	20.68		20.58		20.46	
$\gamma$ Ac Me	20.99		20.78		20.75	
B $\gamma$ Ac Me	21.02		20.91		20.72	
A3 OMe	55.81		56.24		55.67	
B3 OMe	55.93		56.29		55.84	
$\gamma$	63.02		63.56		62.49	
B $\gamma$	65.08		65.36		64.45	
$\alpha$	74.40		75.32		74.28	
$\beta$	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	
B $\beta$	122.13		123.26		122.35	
A5	122.83		123.56		122.74	
B1	131.54		132.35		130.64	
B $\alpha$	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	
$\alpha$ Ac C=O	169.65		170.00		169.45	
$\gamma$ Ac C=O	170.54		170.68		170.05	
B $\gamma$ Ac C=O	170.84		170.77		170.21	

*erythro*

**Guaiacyl glycerol- $\beta$ -coniferyl ether peracetate**  
**Acetic acid 4-{1,3-diacetoxy-2-[4-(3-acetoxypropenyl)-2-methoxyphenoxy] propyl}-2-methoxyphenyl ester**

**<sup>1</sup>H** (acetone)

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.93	s	
B $\gamma$ Ac Me	2.02	s	
$\alpha$ Ac Me	2.07	s	
A4 Ac Me	2.21	s	
A3 OMe	3.82	s	
B3 OMe	3.85	s	
$\gamma$ 1	4.22	dd	11.9, 4.1
$\gamma$ 2	4.36	dd	11.9, 5.9
B $\gamma$	4.66	dd	6.4, 1.4
$\beta$	4.85	m	
$\alpha$	6.06	d	5.1
B $\beta$	6.26	dt	15.9, 6.4
B $\alpha$	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

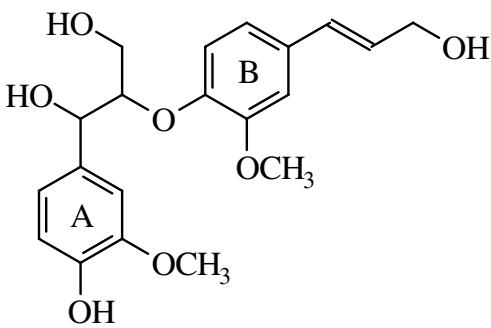
**Notes:**

S. Quideau

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
A4 Ac Me	20.64		20.45	87	20.39	
$\alpha$ Ac Me	20.74		20.59	92	20.47	
$\gamma$ Ac Me	20.99		20.77	86	20.69	
B $\gamma$ 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	
$\gamma$	62.53		62.98	71	61.92	
B $\gamma$	65.07		65.34	93	64.43	
$\alpha$	73.70		74.49	83	73.07	
$\beta$	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 $\beta$	122.23		123.37	97	122.48	
A5	122.60		123.35	97	122.58	
B1	131.86		132.63	49	130.93	
B $\alpha$	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	
$\alpha$ Ac C=O	169.49		169.88	45	169.33	
$\gamma$ Ac C=O	170.76		170.74	77	170.12	
B $\gamma$ Ac C=O	170.83		170.74	77	170.21	

**Compound Number 2013**

**<sup>13</sup>C**



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
$\gamma$	61.21	22	61.88	60	60.16	50
B $\gamma$	63.56	57	63.25	100	61.65	100
$\beta$	74.07	21	73.83	50	71.01	35
$\alpha$	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 $\beta$	128.24	67	129.63	70	128.58	83
B $\alpha$	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

*threo*

**Guaiacylglycerol- $\beta$ -coniferyl ether**

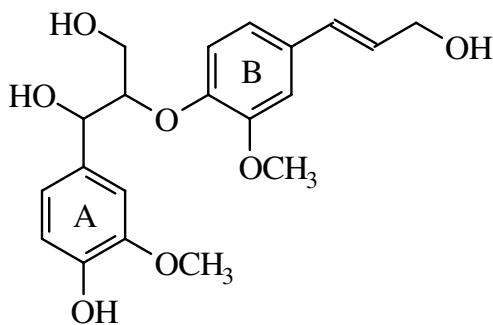
**1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxypropenyl)-2-methoxyphenoxy]propane-1,3-diol**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
$\gamma_1$	3.48	dd	11.9, 5.7
$\gamma_2$	3.67	dd	11.9, 3.7
A,B $\gamma$ OH	3.80-3.90		
A3 OMe	3.80	s	
B3 OMe	3.88	s	
B $\gamma$	4.20	br dd	5.3, 1.6
$\beta$	4.20	m	
$\alpha$ OH	4.45	d	3.9
$\alpha$	4.87	br d	5.5
B $\beta$	6.28	dt	15.9, 5.4
B $\alpha$	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	

**Notes:**

S. Quideau  
 $\alpha$  (e/t) and  $\gamma$  shifts (e/t) interchange from sample to sample, probably due to H-exchange of OH's in d6-acetone.  
 CDCl<sub>3</sub> and DMSO shifts not substantiated.

*erythro***Guaiacylglycerol- $\beta$ -coniferyl ether**

**1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxypropenyl)-2-methoxyphenoxy]propane-1,3-diol**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
$\gamma_1$	3.69	dd	11.8, 4.0
$\gamma_2$	3.81	dd	11.8, 6.2
A,B $\gamma$ OH	3.80-3.90		
A3 OMe	3.80	s	
B3 OMe	3.84	s	
$\beta$	4.19	br dd	5.4, 1.6
$\alpha$	4.29	m	
$\alpha$ OH	4.57	d	4.6
$\alpha$	4.89	br d	5.2
B $\beta$	6.26	dt	15.9, 5.4
B $\alpha$	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	

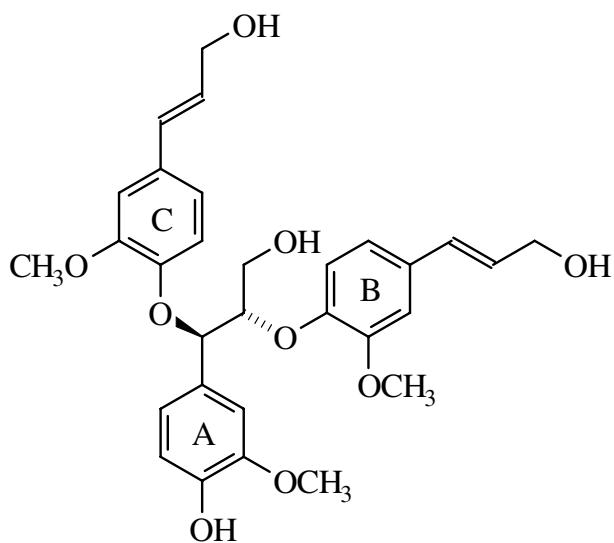
**Notes:**

S. Quideau  
 $\alpha$  (e/t) and  $\gamma$  shifts (e/t) interchange from sample to sample, probably due to H-exchange of OH's in d6-acetone.  
 CDCl<sub>3</sub> and DMSO shifts not substantiated.

Atom	CDCl <sub>3</sub>		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
$\gamma$	60.87	16	61.82	60	60.16	92
B $\gamma$	63.56	58	63.25	99	61.65	92
$\alpha$	72.96	11	73.81	70	71.67	24
$\beta$	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 $\beta$	128.19	63	129.54	55	128.52	34
B $\alpha$	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

**Compound Number 2015**

**<sup>13</sup>C**



**Guaiacylglycerol- $\alpha,\beta$ -bis-coniferyl ether**  
**4-{3-Hydroxy-1,2-bis-[4-(3-hydroxypropenyl)-2-methoxy phenoxyl]propyl}-2-methoxyphenol**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
A $\alpha$	5.46	d	5.5
A $\beta$	4.56	m	
A $\gamma 1$	3.81	dd	11.7, 7.1
A $\gamma 2$	3.93	dd	11.7, 4.1

**Notes:**

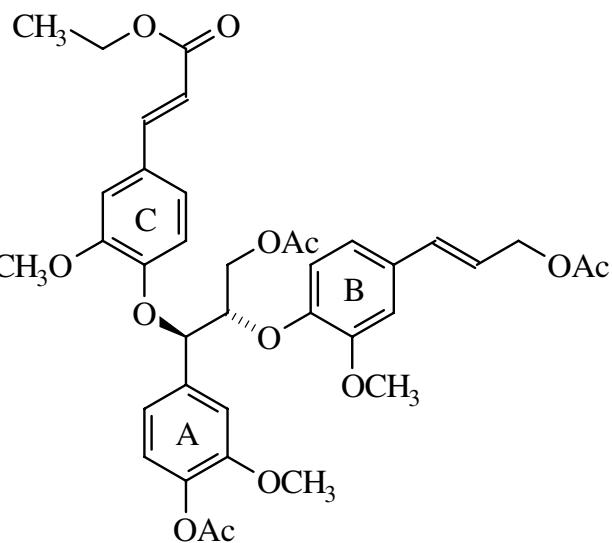
S. Quideau  
Shifts for  $\alpha$  and  $\beta$ 's and A,B,C 1's change  
places in CDCl<sub>3</sub> and DMSO

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.

Atom	CDCl <sub>3</sub>		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
$\gamma$	62.17	40	61.75	46	59.74	31
B $\gamma$	63.56	61	63.25	100	61.52	71
C $\gamma$	63.63	64	63.25	100	61.58	72
$\alpha$	81.68	52	81.15	49	79.01	39
$\beta$	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 $\beta$	127.10	68	129.22	56	128.32	72
B $\beta$	127.60	70	129.45	61	128.47	58
B $\alpha$	130.59	62	129.85	100	130.49	79
C $\alpha$	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**

**<sup>13</sup>C**



3-(4-{3-Acetoxy-1-(4-acetoxy-3-methoxyphenyl)-2-[4-(3-acetoxypropenyl)-2-methoxyphenoxy]propanoyl}-3-methoxyphenyl) acrylic acid ethyl ester

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
$\gamma_1$	4.45	dd	11.8, 3.8
$\gamma_2$	4.53	dd	11.9, 6.0
B $\gamma$	4.66	dd	6.4, 1.3
$\beta$	4.88	m	
$\alpha$	5.71	d	5.3
B $\beta$	6.25	dt	15.8, 6.4
C $\beta$	6.39	d	15.9
B $\alpha$	6.61	dt	15.8, 1.3
C $\alpha$	7.53	d	15.9

**Notes:**

S. Quideau

Shifts substantiated in d6-acetone but not CDCl<sub>3</sub> or DMSO.

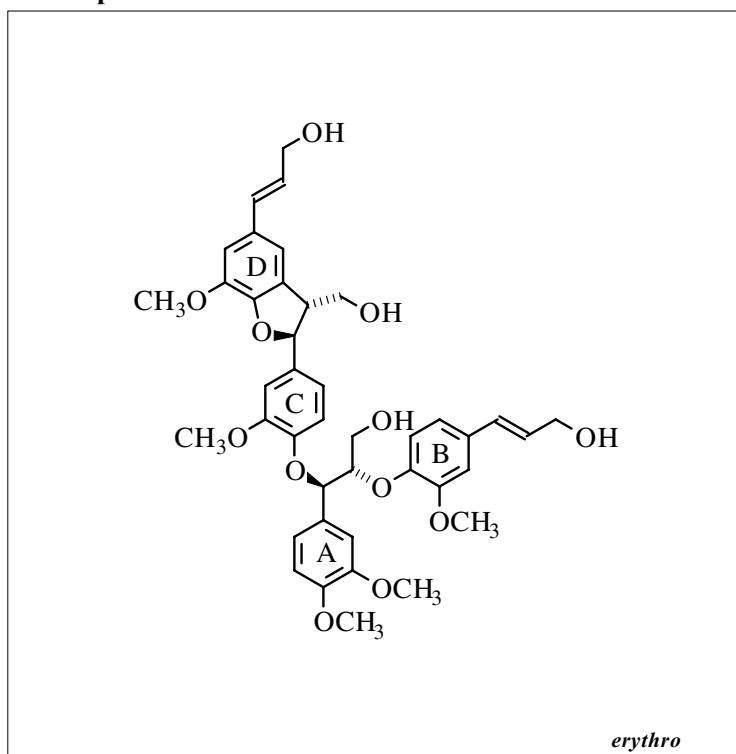
$\gamma$  and B $\gamma$  Ac C=O shifts may be interchanged

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.

Atom	CDCl <sub>3</sub>		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
$\gamma$ Ac Me	20.74	84	20.60	62	20.43	81
B $\gamma$ Ac 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
CH <sub>2</sub>	60.39	75	60.56	62	59.79	53
$\gamma$	63.22	44	63.41	38	62.33	24
B $\gamma$	65.09	87	65.37	54	64.41	59
$\alpha$	79.99	42	80.47	38	78.45	27
$\beta$	81.98	50	81.70	46	79.57	33
B2	110.14	72	111.19	38	110.22	37
C3	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 $\beta$	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 $\beta$	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 $\alpha$	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 $\alpha$	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 $\gamma$ C=O	167.13	52	167.23	69	166.40	53
A4 Ac C=O	168.78	48	168.90	54	168.36	44
$\gamma$ Ac C=O	170.77	27	170.81	31	170.09	48
B $\gamma$ Ac C=O	170.86	55	170.82	69	170.14	54

**Compound Number 2017**

**<sup>13</sup>C**



**<sup>1</sup>H Acetone/D<sub>2</sub>O**

Atom	H Shifts	Mult	J
A $\alpha$	5.48	d	5.8
A $\beta$	4.62	m	
A $\gamma 1$	3.80	dd	11.9, 6.5
A $\gamma 2$	3.91	dd	11.9, 4.9
C $\alpha$	5.51	d	5.8
C $\beta$	3.43	m	
C $\gamma 1$	3.69	s	
C $\gamma 2$	3.80	s	

**Notes:**

S. Quideau

Run only in Acetone:D<sub>2</sub>O (9:1)

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.

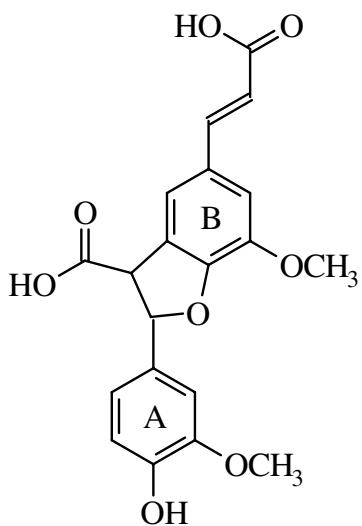
Note: Two erythro isomers!! Resolvable pairs are:

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

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
C $\beta$			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		
$\gamma$			61.20	46		
B $\gamma$			62.77	94		
D $\gamma$			62.85	50		
C $\gamma$			64.18	52		
$\alpha$			80.10	29		
$\beta$			83.86	46		
C $\alpha$			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 $\beta$			127.73	65		
B $\beta$			128.64	64		
B $\alpha$			130.02	85		
D5			129.64	33		
D $\alpha$			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

<sup>13</sup>C



beta-5-dehydroniferulic acid

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

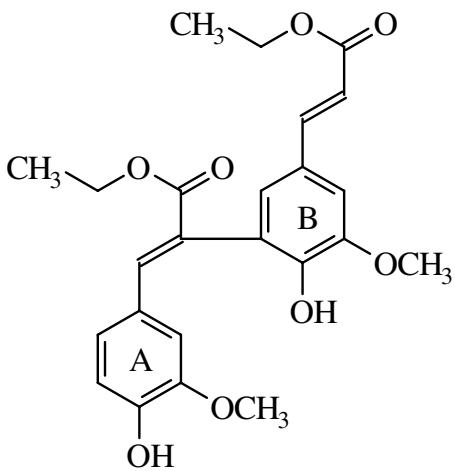
### <sup>1</sup>H (acetone)

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 CDCl<sub>3</sub>

JCS Perkin 1, 3485-98 (1994)  
Cmpd 13



3-(4-Hydroxy-3-methoxyphenyl)-2-[2-hydroxy-3-methoxy-5-(2-propoxycarbonylvinyl)phenyl] acrylic acid ethyl ester

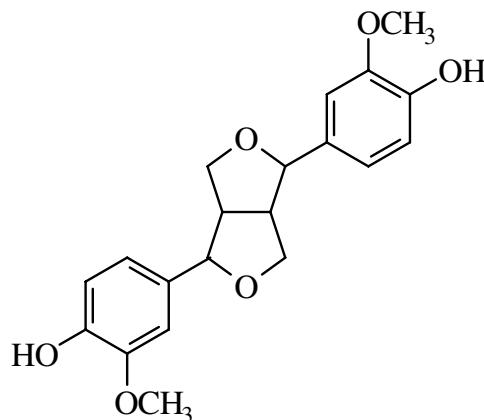
<sup>1</sup>H (acetone)

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

Atom	CDCl <sub>3</sub>		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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
β	3.08	m	
γ1	3.80	dd	9.1, 3.8
OMe	3.83	s	
γ2	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	

**Notes:**

S. Quideau

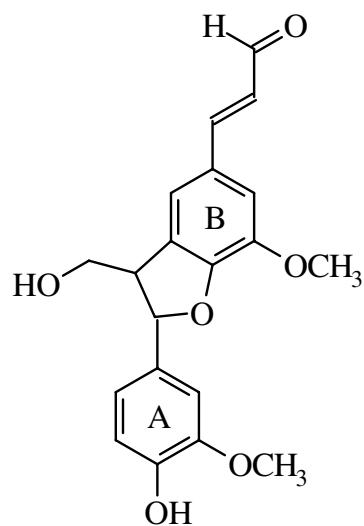
As this compound has a plane of symmetry  
the shifts for the other half are identical.

Atom	CDCl <sub>3</sub>		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

**Compound Number 2021**

**<sup>13</sup>C**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		



*erythro*

3-[2-(4-Hydroxy-3-methoxyphenyl)-3-hydroxymethyl-7-methoxy-2,3-dihydrobenzofuran-5-yl] prop-2-enal

**<sup>1</sup>H (acetone)**

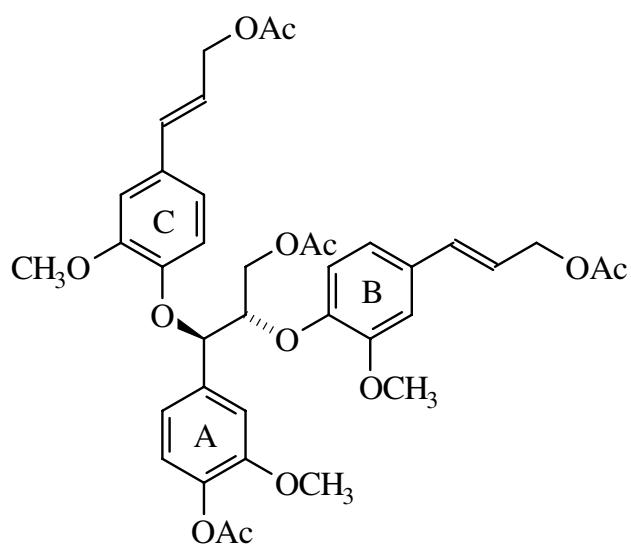
Atom	H Shifts	Mult	J
β	3.61	br q	
A3 OMe	3.82	s	
B3 OMe	3.91	s	
γ	3.87-3.91	m	
α	5.65	d	
B β	6.65	dd	6.60 15.8, 7.7
A5	6.81	d	8.10
A6	6.88	dd	8.1, 2.0
A2	7.04	d	2.0
B2	7.29	bro	
B6	7.32	bro	
B α	7.59	d	15.8
B γ	9.63	d	7.7

**Notes:**

S. Quideau

**Compound Number 2022**

<sup>13</sup>C



*erythro*

**Guaiacylglycerol- $\alpha,\beta$ -bis coniferyl ether acetate**

Atom	$\text{CDCl}_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A4 Ac Me	20.63	45	20.44	57	20.33	87
$\gamma$ Ac Me	20.73	40	20.62	57	20.42	87
C $\gamma$ Ac Me	20.98	100	20.76	58	20.70	92
B $\gamma$ Ac 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
$\gamma$	63.37	20	63.56	28	62.39	31
C $\gamma$	65.08	35	65.37	55	64.39	100
B $\gamma$	65.12	41	65.37	55	64.39	100
$\alpha$	80.17	25	80.85	31	78.68	38
$\beta$	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 $\beta$	121.69	31	122.99	44	122.12	58
B $\beta$	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 $\alpha$	133.92	32	134.22	91	133.00	76
B $\alpha$	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 $\gamma$ Ac C=O	170.76	29	170.72	32	170.07	73
D $\gamma$ Ac C=O	170.83	29	170.74	32	170.10	73
C $\gamma$ Ac C=O	170.83	29	170.77	40	170.12	73

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
A $\alpha$	5.62		
A $\beta$	4.87		
A $\gamma$ 1	4.45		
A $\gamma$ 2	4.53		

**Notes:**

S. Quideau

$\alpha$  and  $\beta$  of B and C can interchange in  $\text{CDCl}_3$

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.

<p style="text-align: center;"><i>erythro</i></p>	
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**Guaiacylglycerol- $\alpha$ -dehydrodiconiferyl-bis-ether peracetate  
diastereomeric mixture**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
A a	5.62	d	5.4
A b	4.88	m	
A $\gamma$ 1	4.46	dt	11.9, 3.8
A $\gamma$ 2	4.53	dt	11.9, 5.8
C a	5.49	d	6.9
C b	3.72	s	
C $\gamma$ 1	4.28	dd	11.1, 7.5
C $\gamma$ 2	4.40	dd	11.1, 5.4

**Notes:**

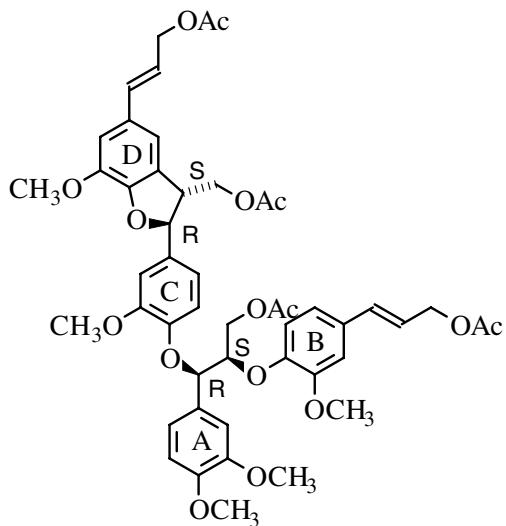
S. Quideau  
S. Quideau

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.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
A4 Ac Me	20.52	88	20.43	97	20.32	
A $\gamma$ Ac Me	20.61	88	20.61	89	20.42	
C $\gamma$ Ac Me	20.74	100	20.65	89	20.48	
B $\gamma$ Ac Me	20.98	89	20.78	95	20.70	
D $\gamma$ 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 b	50.25	35	51.04	49	49.16	
$\gamma$	63.36	35	63.52	50	62.38	
B $\gamma$	65.06	84	65.36	85	64.40	
D $\gamma$	65.16	84	65.48	35	64.49	
C $\gamma$	65.28	43	65.84	55	68.42	
$\alpha$	80.13	34	80.73	42	78.62	
$\beta$	81.87	47	81.63	48	79.49	
C a	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 b	121.13	60	122.13	66	121.31	
B b	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 a	133.90	69	134.20	74	133.00	
D a	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 $\gamma$ Ac C=O	170.74		170.74		170.12	
D $\gamma$ Ac C=O	170.74		170.74		170.12	
A $\gamma$ Ac C=O	170.80		170.76		170.12	
C $\gamma$ Ac C=O	170.83		170.90		170.23	

**Compound Number 2024**

**$^{13}\text{C}$**



**Veratrylglycerol- $\alpha$ -dehydrodiconiferyl- $\beta$ -coniferyl-bis-ether peracetate, diastereomeric mixture**

**$^1\text{H}$  (acetone)**

Atom	H Shifts	Mult	J
A $\alpha$	5.54	d	5.2
A $\beta$	4.87	s	
A $\gamma 1$	4.44	td	11.8, 3.7
A $\gamma 2$	4.52	td	11.8, 6.2
C $\alpha$	5.48	d	6.9
C $\beta$	3.70	s	
C $\gamma 1$	4.28	dt	11.1, 7.5
C $\gamma 2$	4.39	dt	11.1, 5.5

**Notes:**

S. Quideau

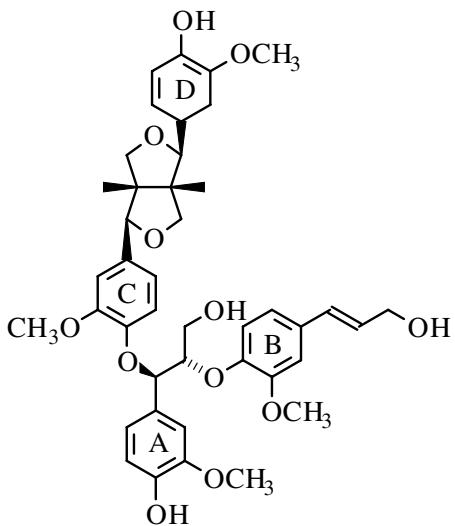
A3 and A4, C and D OMe's, and B and D  $\gamma$ 's can be interchanged in all solvents Shifts are confirmed for Acetone

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.

Atom	$\text{CDCl}_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
A $\gamma$ Ac Me	20.75	72	20.64	98	20.45	97
C $\gamma$ Ac Me	20.75	72	20.64	98	20.45	97
B $\gamma$ Ac Me	20.98	100	20.79	98	20.70	97
D $\gamma$ Ac 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 $\beta$	50.18	28	51.08	39	49.16	54
$\gamma$	63.67	28	63.86	52	62.64	40
B $\gamma$	65.09	79	65.38	98	64.41	100
D $\gamma$	65.17	87	65.49	98	64.50	100
C $\gamma$	65.28	50	65.90	59	64.71	49
$\alpha$	80.14	33	80.89	46	78.77	29
$\beta$	81.80	31	81.73	53	79.57	38
C $\alpha$	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 $\beta$	121.16	48	122.19	76	121.32	61
B $\beta$	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 $\alpha$	133.94	58	134.26	75	133.03	76
C 1	134.12	38	135.74	28	133.92	39
D $\alpha$	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 $\gamma$ Ac C=O	170.70		170.76		170.05	
B $\gamma$ Ac C=O	170.77		170.76		170.10	
A $\gamma$ Ac C=O	170.82		170.79		170.13	
C $\gamma$ Ac C=O	170.85		170.90		170.23	

**Compound Number 2025**

**<sup>13</sup>C**



**Guaiacylglycerol- $\alpha$ -pinoresinol- $\beta$ -coniferyl-bis-ether  
diastereomeric mixture**

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
A $\alpha$	5.45	d	5.6
A $\beta$	4.55	m	
A $\gamma$ 1	3.82	dd	11.5, 6.5
A $\gamma$ 2	3.92	dd	11.5, 5.2
C $\alpha$	4.63		
C $\beta$	3.04		
C $\gamma$ 1	3.77		
C $\gamma$ 2	4.17		

**Notes:**

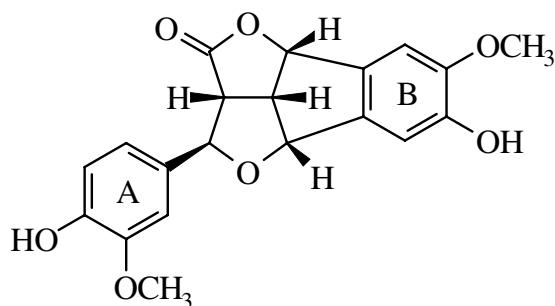
S. Quideau  
Only run in acetone

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.

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
D $\beta$			55.15	100		
C $\beta$			55.15	100		
D3 OMe			56.22	75		
A3 OMe			56.25	75		
B3 OMe			56.25	74		
C3 OMe			56.44	52		
$\gamma$			61.82	28		
B $\gamma$			63.27	44		
D $\gamma$			72.23	71		
C $\gamma$			72.23	71		
$\alpha$			81.21	28		
$\beta$			85.38	36		
C $\alpha$			86.37	51		
D $\alpha$			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 $\beta$			129.50	37		
B $\alpha$			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**

**<sup>13</sup>C**



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B <sub>β</sub>	50.40 53.87	100 88	51.13 54.58	86 81	49.78 53.16	54 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

**11-hydroxy-(4-hydroxy-3methoxyphenyl)-10-methoxy-3a,4,6,6a-tetrahydro 3H-3,4-c]furan-1-one**

**<sup>1</sup>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	

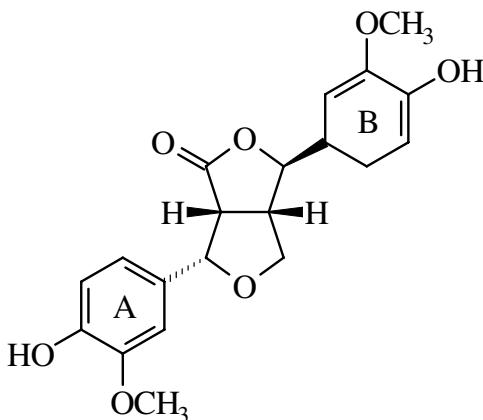
**Notes:**

S. Quideau

Ref: S. Quideau and John Ralph. J. Chem Soc. Perkin Trans. 1 1993 - issue 6 - 653 -659.

**Compound Number 2027**

**<sup>13</sup>C**



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B <sub>β</sub>	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 <sub>γ</sub>	71.63	91	72.08	87	71.06	58
α	84.00	93	84.43	95	83.07	54
B <sub>α</sub>	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

**4-cis-8-trans-bis (4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo [3.3.0] octan-2-one**

**<sup>1</sup>H (acetone)**

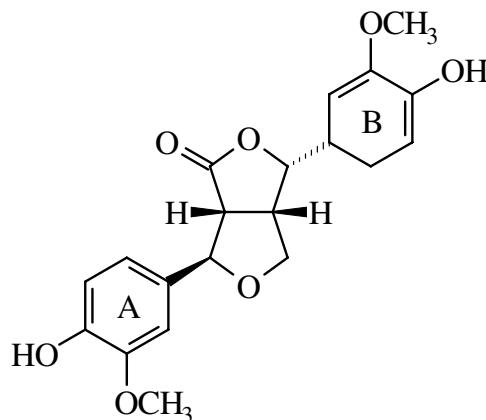
Atom	H Shifts	Mult	J
β	3.63	t	8.8
B <sub>β</sub>	3.35	ddd	9.0, 6.6, 4.6
α	5.05	br d	8.6
B <sub>α</sub>	5.23	br d	6.6
B <sub>γ</sub> cis	3.88	dd	9.5, 4.8
B <sub>γ</sub> trans	4.28	br d	9.5

**Notes:**

S. Quideau

S. Quideau and John Ralph. J. Chem. Soc. Perkin Trans. 1 1993 issue 6  
653-659.

Cmpd 14



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$	45.43	90	46.14	77		
$\beta$	54.80	99	55.35	78		
A3 OMe	56.00	82	56.26	100		
B3 OMe	56.13	93	56.34	82		
B $\gamma$	68.66	86	69.98	78		
B $\gamma$	80.37	89	81.09	78		
$\gamma$	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		
$\gamma$	177.07	54	177.77	38		

4-trans-8-cis-bis(4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo [3.3.0]octan-2-one

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\beta$	3.65	dd	8.7, 2.6
B $\beta$	3.71	m	
$\gamma$	5.16	br d	2.6
B $\alpha$	5.82	br d	5.9
B $\gamma$ cis	3.80	m	
B $\gamma$ 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

**Compound Number 2029**

**<sup>13</sup>C**

		<sup>13</sup> C					
Atom	CDCl <sub>3</sub>		Acetone		DMSO		
	CS	i	CS	i	CS	i	
B $\beta$	49.99	84	50.38	93	48.62	69	
$\beta$	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 $\gamma$	72.70	90	73.44	96	72.15	66	
$\alpha$	83.38	75	84.43	90	82.91	77	
B $\alpha$	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	
$\gamma$	176.92	54	177.72	39	177.14	67	

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-dioxabicyclo  
[3.3.0] octan-2-one**

**<sup>1</sup>H (acetone)**

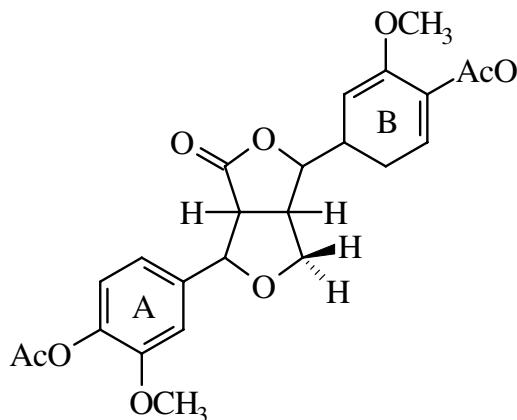
Atom	H Shifts	Mult	J
$\beta$	3.65	ddd	9.2, 3.7, 0.5
B $\beta$	3.39	ddddd	9.2, 7.0, 4.6, 3.6, 0.6
$\alpha$	5.20	dquin	3.7, 0.6
B $\alpha$	5.39	br d	3.6
B $\gamma$ cis	4.30	ddd	9.4, 7.0, 0.5
B $\gamma$ trans	4.02	ddt	9.4, 4.6, 0.5

**Notes:**

S. Quideau  
S. Quideau and J. Ralph. J. Chem. Soc. Perkin Trans. 1 1993 (6) 653-659.

Compound Number 2030

<sup>13</sup>C



4-cis-8-cis-bis (4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo [3.3.0] octan-2-one diacetate

<sup>1</sup>H (acetone)

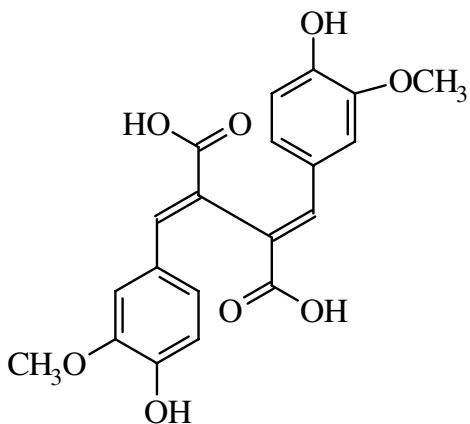
Atom	H Shifts	Mult	J
$\beta$	3.72	ddd	9.25, 3.8, 0.5
B $\beta$	3.45	ddddd	9.15, 7.1, 4.8, 3.0, 0.6
B $\gamma$ trans	4.12	ddt	9.5, 4.8, 0.5
B $\gamma$ cis	4.39	ddd	9.5, 7.1, 0.5
B $\alpha$	5.52	br d	3.6
$\alpha$	5.29	dquin	3.8, 0.6

Notes:

S. Quideau  
Ralph, Helm, Quideau. J. Chem. Soc. Perkin Trans. 1 1992 2971-2980

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\beta$	49.89	84	50.33	76	48.62	
$\beta$	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 $\gamma$	72.80	90	73.72	81	72.51	
$\alpha$	82.99	80	84.01	82	82.49	
B $\alpha$	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	
$\gamma$	176.66	54	177.49	36	176.98	

Compound Number 2031

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

4,4'-dihydroxy-3,3'-dimethoxy-β,β'-bicinnamic acid

<sup>1</sup>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	

**Notes:**

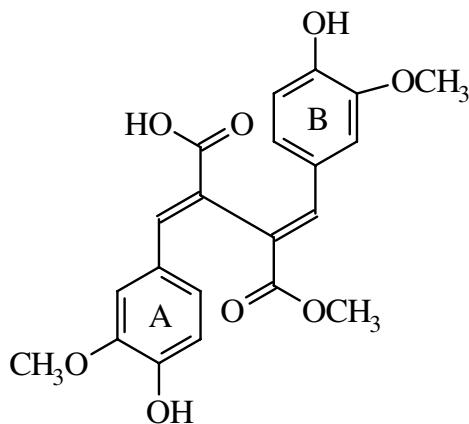
S. Quideau

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

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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		

*γ*-methoxy-4,4'-dihydroxy-3,3'-dimethoxy-β,β'-bicinnamic acid<sup>1</sup>H (acetone)

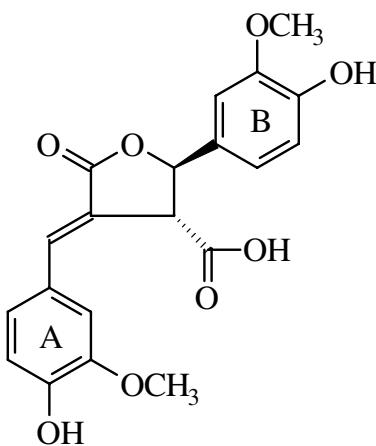
Atom	H Shifts	Mult	J
B γOMe	3.66	s	
A3 OMe	3.72	s	
B3 OMe	3.73	s	
A,B 5	6.78	d	8.2
B6	7.11	dd	
A6	7.09	dd	8.3, 2.0
A2	7.25	d	2.0
B2	7.30	d	2.0
B α	7.81	s	
α	7.84	s	

## Notes:

S. Quideau

**Compound Number 2033**

**<sup>13</sup>C**



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\beta$			54.03	56	52.64	49
A3 OMe			56.27	100	55.54	90
B3 OMe			56.27	100	55.67	100
B $\alpha$			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
$\beta$			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
$\alpha$			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
$\gamma$			171.66	23	171.02	55
B $\gamma$			172.12	34	171.72	76

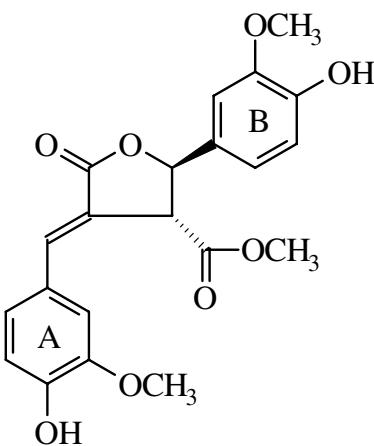
**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B3 OMe	3.81	s	
A3 OMe	3.87	s	
B $\beta$	4.30	t	2.5
B $\alpha$	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
$\alpha$	7.61	d	2.1

**Notes:**

S. Quideau  
JCS Perkin 1, 3485-98 (1994)  
Cmpd 12b (R=H)

## Compound Number 2034

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\gamma$ OMe	52.98	51	53.16	82	51.98	56
B $\beta$	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 $\alpha$	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
$\beta$	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
$\alpha$	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
$\gamma$	170.77	38	171.45	33	170.53	68
B $\gamma$	171.23	26	171.56	52	170.70	48

<sup>1</sup>H (acetone)

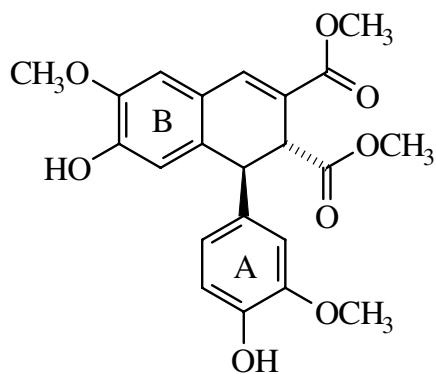
Atom	H Shifts	Mult	J
B $\gamma$ OMe	3.73	s	
B3 OMe	3.81	s	
A3 OMe	3.88	s	
B $\beta$	4.39	t	2.6
B $\alpha$	5.72	d	3.0
B 5,6	6.79 - 6.85	m	
A5	6.9	d	8.2
B2	6.97	br d	1.5
A6	7.17	dd	8.2, 2.0
A2	7.28	d	2.0
$\alpha$	7.62	d	2.1

## Notes:

S. Quideau

Compound Number 2035

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 γ OMe	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

Dimethyl 7-hydroxy-6-methoxy-1-(4-hydroxy-3-methoxyphenyl)-trans-1,2-dihydronaphthalene-2,3-dicarboxylate

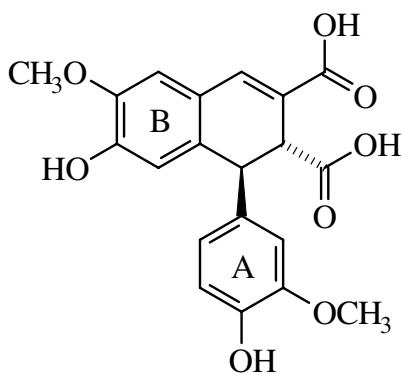
<sup>1</sup>H (acetone)

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

Compound Number 2036

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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

**β-β-coupled dehydodiferulic acid**

**7-hydroxy-6-methoxy-1-(4-hydroxy-3-methoxyphenyl)-trans-1,2-dihydr  
onaphthalene-2,3-dicarboxylic acid**

**<sup>1</sup>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:**

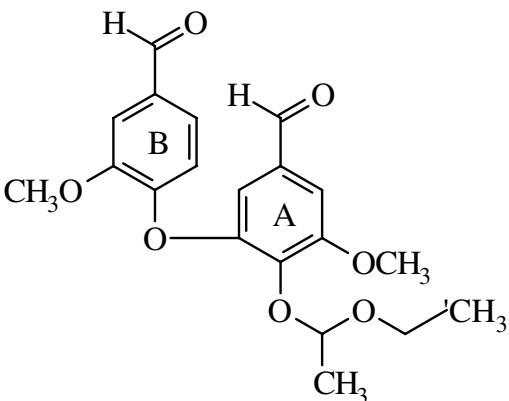
S. Quideau  
JCS Perkin 1, 3485-98 (1994)  
Cmpd 19

Not very soluble in CDCl<sub>3</sub>

**Compound Number 2037**

**<sup>13</sup>C**

		<sup>13</sup> C				
Atom	CDCl <sub>3</sub>		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		
$\alpha$			191.23	94		
B $\alpha$			191.48	96		



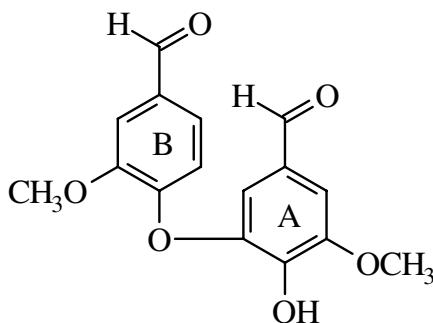
**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
'CH3	1.08	t	
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
$\alpha$	9.85	s	
B $\alpha$	9.95	s	

**Notes:**

S. Quideau

Compound Number 2038

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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
$\alpha$	190.05	96	190.75	9	190.84	39
B $\alpha$	190.84	100	191.43	97	191.57	27

## 4-0-5-coupled dehydrodivanillin

3-{3-[4-(2-carboxyvinyl)-2-methoxy-phenoxy]-4-hydroxy-5-methoxy-phenyl} acrylic acid

<sup>1</sup>H (acetone)

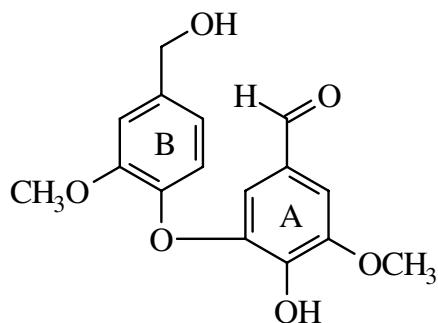
Atom	H Shifts	Mult	J
B OMe	3.95	s	
A OMe	3.98	s	
B5	6.94	d	8.2
A6	7.22	d	1.8
A2	7.40	d	1.8
B6	7.48	dd	8.2, 2.0
B2	7.58	d	2.0
$\alpha$	9.80	s	
B $\alpha$	9.92	s	

## Notes:

S. Quideau

**Compound Number 2039**

**<sup>13</sup>C**



**4-O-5 coupled dehydrovanillin / vanillyl alcohol**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\alpha$	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
$\alpha$	190.44	83	190.91	92	190.97	67

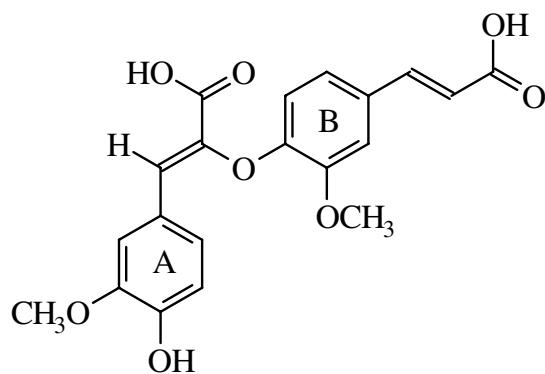
**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B3 OMe	3.79	s	
A3 OMe	3.95	s	
B $\alpha$	4.63	s	
A6	6.91	d	
B 5,6	6.94 - 6.97	m	
B2	7.16	br d	
A2	7.27	d	1.8
$\alpha$	9.71	s	

**Notes:**

S. Quideau

Compound Number 2040

<sup>13</sup>C

Atom	$\text{CDCl}_3$		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 $\beta$			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
$\alpha$			128.49	63	127.09	34
B1			130.10	56	128.74	52
$\beta$			138.28	27	137.01	44
B $\alpha$			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
$\gamma$			164.51	13	164.11	56
B $\gamma$			167.91	22	167.70	72

<sup>1</sup>H (acetone)

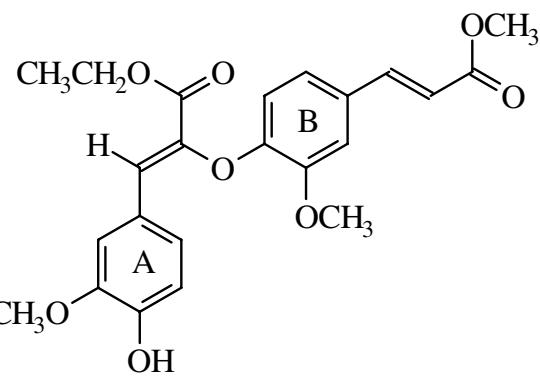
Atom	H Shifts	Mult	J
A3 OMe	3.73	s	
B3 OMe	4.00	s	
B $\beta$	6.43	d	15.9
A5	6.82	d	8.2
B5	6.83	d	8.3
B6	7.13	dd	8.3, 2.0
A6	7.23	dd	8.2, 2.0
$\alpha$	7.42	s	
B2	7.44	d	2.0
A2	7.52	d	2.0
B $\alpha$	7.59	d	15.9

## Notes:

S. Quideau  
JCS Perkin 1, 3485-98 (1994)  
Cmpd 15

Compound Number 2041

<sup>13</sup>C



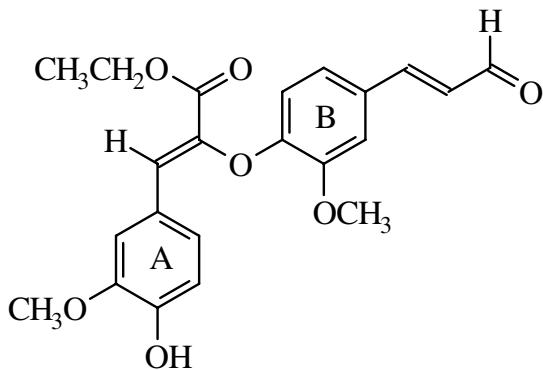
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	14.14	95	14.47	100	14.05	100
B <sub>γ</sub> OMe	51.65	83	51.58	78	51.32	62
A3 OMe	55.59	100	55.92	93	55.11	75
B3 OMe	56.21	97	56.49	90	55.93	59
CH2	61.42	92	61.72	74	60.96	61
B2	111.24	83	112.45	70	111.79	41
A2	112.03	97	113.78	70	113.17	34
B5	114.14	89	114.53	71	113.46	35
A5	114.47	87	115.99	70	115.57	26
B <sub>β</sub>	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

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
CH3	1.21	t	
B <sub>γ</sub> OMe	3.71	s	
A3 OMe	3.73	s	
B3 OMe	3.99	s	
CH2	4.17	q	7.1
B <sub>β</sub>	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
ArOH	8.12	br s	

### Notes:

S. Quideau  
Toward β-O-4 dehydro diferulic acid  
(steryl ether, Z isomer)



Atom	CDCl <sub>3</sub>		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
Bβ	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

<sup>1</sup>H (acetone)

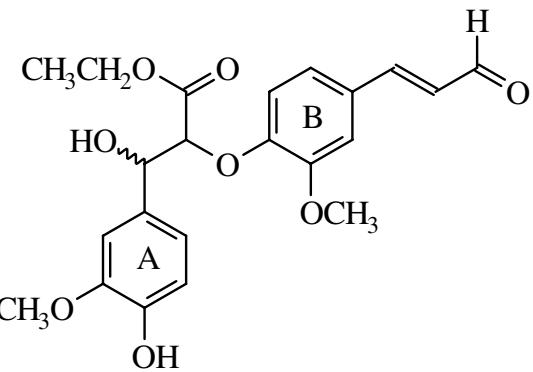
Atom	H Shifts	Mult	J
CH3	1.21	t	
A3 OMe	3.73	s	
B3 OMe	4.00	s	
CH2	4.21	q	7.1
Bβ	6.70	dd	15.9, 7.7
A5	6.81	d	8.3
B5	6.83	d	8.3
B6	7.18	dd	8.3, 2.0
A6	7.23	ddd	8.3, 2.0, 0.4
α	7.38	s	
A2	7.49	d	2.0
B2	7.50	d	2.0
B α	7.58	d	15.9
B γ	9.65	d	7.7
Ar OH	8.14	s	

## Notes:

S. Quideau  
Toward β-O-4 dehydro diferulic acid(steryl ether, Z isomer)

Compound Number 2043

<sup>13</sup>C



*erythro*

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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				

### <sup>1</sup>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:

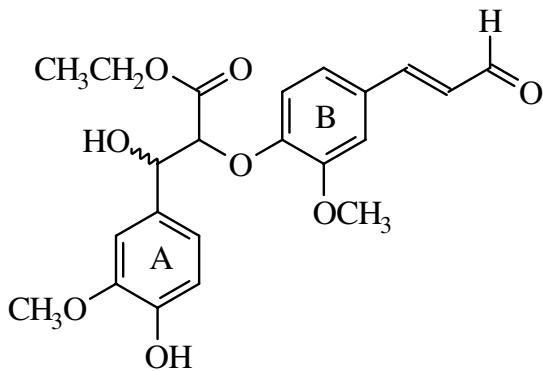
S. Quideau

Compounds 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

<sup>13</sup>C*threo*

Atom	CDCl <sub>3</sub>		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				

<sup>1</sup>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

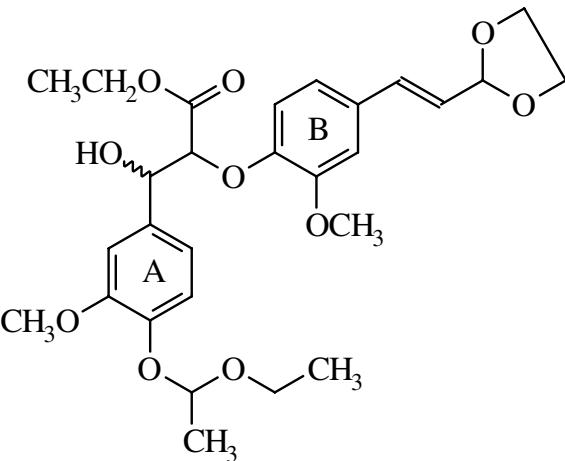
Compounds 2043 and 2044 were run as a mixture and the different isomers were assigned. Relative intensities reflect the spectrum of the mixture.

t isomer

for synthesis of β-O-4 dehydro diferulic acid

**Compound Number 2045**

<sup>13</sup>C



*erythro*

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
A γCH <sub>3</sub>	13.82	47				
CH <sub>3</sub>	14.93	57				
CH <sub>3</sub>	20.10	36				
OMe	55.54	54				
OMe	55.63	37				
4 CH <sub>2</sub>	61.01	50				
A CH <sub>2</sub>	61.84	32				
B CH <sub>2</sub>	64.82	100				
B CH <sub>2</sub>	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				

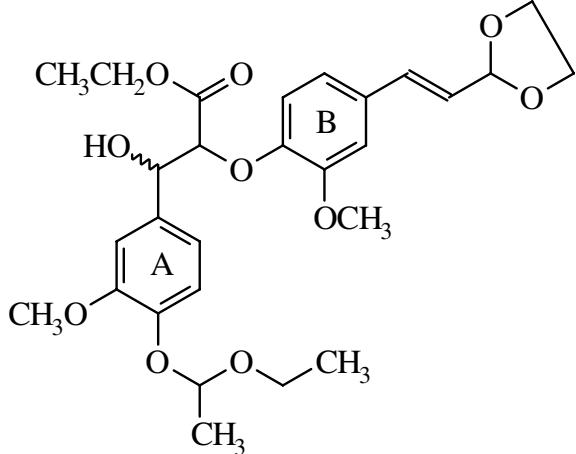
<sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
CH <sub>3</sub>	1.47	d	5.1
β <i>t</i>	4.56	d	6.6
β <i>e</i>	4.72	d	5.4
α <i>t</i>	5.06	br d	6.3
α <i>e</i>	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

## Compound Number 2046

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
CH3	-					
CH3	-					
CH3	-					
OMe	55.59	100				
OMe	55.59	100				
CH2	61.86	55				
CH2	74.51	22				
CH2	84.39	21				
α	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				

<sup>1</sup>H (chloroform)

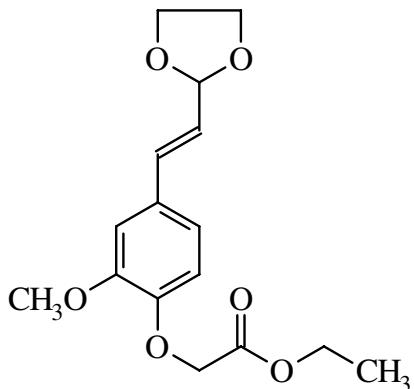
Atom	H Shifts	Mult	J
β	4.56	d	6.6
α	5.06	br d	6.3

## Notes:

S. Quideau  
intermediate toward β-O-4 dehydro diferulic acid

Compound Number 2047

<sup>13</sup>C



Atom	<sup>13</sup> CDCl <sub>3</sub>		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				

<sup>1</sup>H (chloroform)

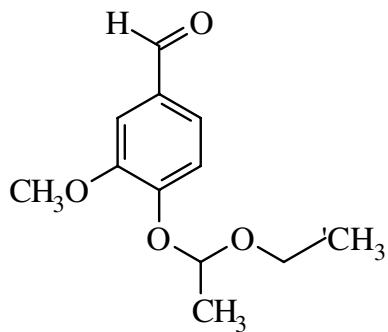
Atom	H Shifts	Mult	J
CH3	1.26	t	
OMe	3.87	s	
CH2	3.90-4.05	m	
CH2	4.24	q	
CH2	4.67	s	
γ	5.39	d	6.1
β	6.05	dd	15.9, 6.1
α	6.69	d	15.9
5	6.76	d	8.3
6	6.90	dd	8.3, 2.0
2	6.99	d	2.0

Notes:

S. Quideau  
For synthesis of b-O-4 dehydro diferulic acid

Compound Number 2048

<sup>13</sup>C



Atom	CDCl <sub>3</sub>		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				

### <sup>1</sup>H (chloroform)

Atom	H Shifts	Mult	J
'CH3	1.21	t	
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	

### Notes:

S. Quideau

Intermediate for synthesis of β--O-4 dehydro diferulic acid

**Compound Number 2049**

<sup>13</sup>C

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
C3 OMe			56.07	100		
A3 OMe			56.75	97		
B3 OMe			56.89	90		
C $\alpha$			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		
$\alpha$					191.02	55
B $\alpha$					191.69	55

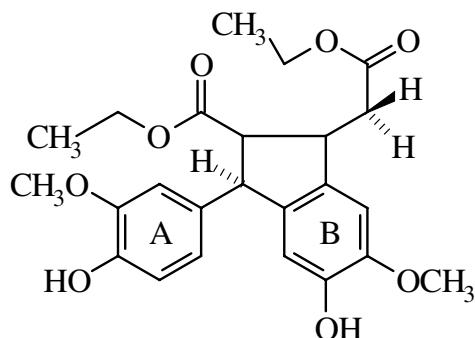
  

<sup>1</sup> H (acetone)			
Atom	H Shifts	Mult	J
C3 OMe	3.72	s	
B3 OMe	3.90	s	
A3 OMe	3.94	s	
C $\alpha$	4.62	s	
B6	6.88	d	1.7
C6	6.94	dd	8.1, 1.7
C5	7.00	d	8.1
A6	7.01	d	1.7
C2	7.14	d	1.7
A2	7.26	d	1.7
B2	7.40	d	1.7
$\alpha$			
B $\alpha$	9.74	s	
	9.86	s	

**Notes:**

S. Quideau  
5-O-4 trimer

## Compound Number 2050

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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 $\beta$	36.90	57	37.50	80	36.41	44
B $\alpha$	42.15	75	43.06	85	41.74	54
$\alpha$	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
$\beta$	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	135.5	50	133.61	46
B6	137.10	49	8	47	136.47	49
A4	144.54	63	137.90	56	145.36	53
B4	145.61	60	146.45	57	146.34	58
B3	146.04	52	147.43	46	147.08	52
A3	146.50	59	147.92	48	147.51	55
			148.37			
B $\gamma$	172.30	54		58	171.45	77
$\gamma$	172.43	55	172.45	61	172.10	61
			173.00			

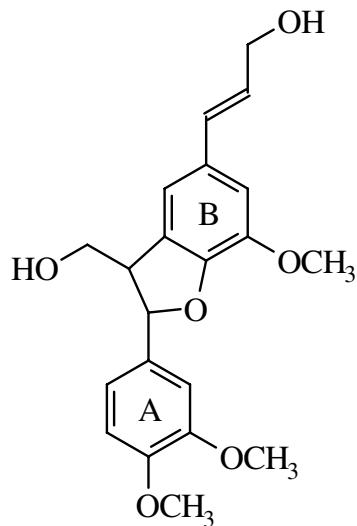
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\beta$ 1	2.43	dd	16.0,8.0
B $\beta$ 2	2.61	dd	16.0,7.0
$\beta$	3.43	dd	9.85, 8.20
B $\alpha$	3.90	brq	8.0
$\alpha$	4.56	d	10.1

## Notes:

S. Quideau  
Stereochemistry determined from NOESY experiments  
 $\alpha\beta$ -/ $\alpha\delta$  model

## Compound Number 2051

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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		

4-[3-Hydroxymethyl-5-(3-hydroxypropenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-1,2-dimethoxyphenyl

<sup>1</sup>H (acetone)

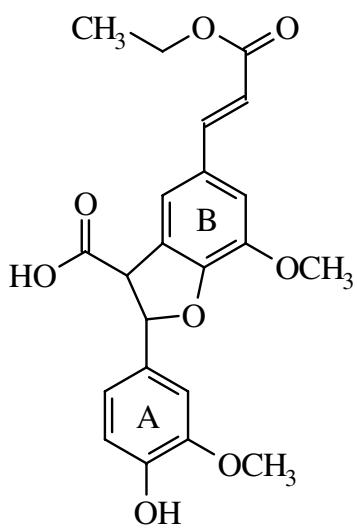
Atom	H Shifts	Mult	J
β	3.52	br q	
A3 OMe	3.77	s	
A4 OMe	3.78	s	
B3 OMe	3.86	s	
γ's	3.80-3.92	m	
B γ OH	4.14	t	
B γ	4.19	td	5.50
α	5.58	d	5.7, 1.7
B β	6.23	dt	6.4
B α	6.52	dt	15.8, 5.5
A5	6.91	d	15.8, 1.7
A,B6 + B2	6.94-9.67	m	8.1
A2	7.03	d	1.8

## Notes:

S. Quideau  
veratryl phenylcoumaran

Compound Number 2052

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		

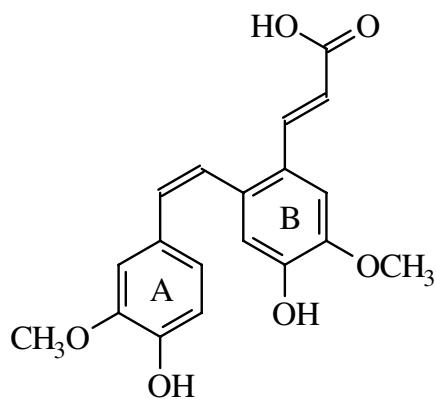
<sup>1</sup>H (acetone)

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

## Compound Number 2053

<sup>13</sup>C

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\beta$			116.50	76		
$\beta$			120.61	78		
B6			120.84	74		
A6			121.14	88		
B5			125.47	48		
B1			126.98	56		
$\alpha$			130.68	81		
A1			130.90	58		
B $\alpha$			146.00	69		
B4			146.96	50		
A4			147.61	55		
A3			148.61	46		
B3			148.83	54		
B $\gamma$			168.22	47		

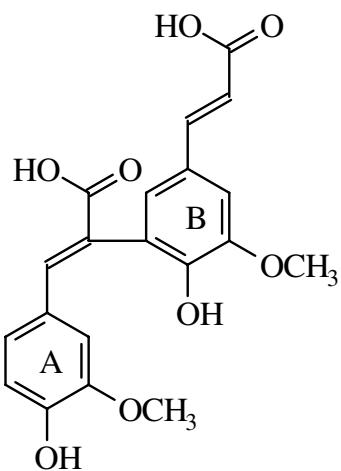
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.91	s	
B3 OMe	3.95	s	
B $\beta$	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
$\alpha$	7.31	dd	16.5, 7.38
$\beta$	7.33	dd	16.5, 7.38
B6	7.54	d	1.9
B $\alpha$	7.63	d	15.9

## Notes:

S. Quideau

## Compound Number 2054

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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 $\beta$			116.23	67	115.92	48
B5			125.14	40	124.57	42
B6			125.60	71	124.38	42
$\beta$			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
$\alpha$			141.81	62	139.75	34
B $\alpha$			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 $\gamma$			168.56	41	167.86	80
$\gamma$			169.15	36	168.38	68

<sup>1</sup>H (acetone)

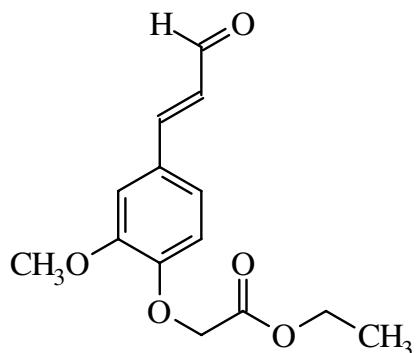
Atom	H Shifts	Mult	J
A3 OMe	3.45	s	
B3 OMe	3.95	s	
B $\beta$	6.38	d	15.4
A5	6.71	d	8.2
A2	6.73	d	1.9
A6	6.85	dd	8.2, 2.0
B6	7.03	d	1.9
B2	7.37	d	1.9
B $\alpha$	7.60	d	15.9
$\alpha$	7.81	s	

## Notes:

S. Quideau  
 JCS Perkin 1, 3485-98 (1994)  
 Cmpd 14  
 Not soluble in CDCl<sub>3</sub>

**Compound Number 2055**

**<sup>13</sup>C**



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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				
$\alpha$	127.17	99				
1	128.31	54				
3	149.74	46				
4	149.96	40				
$\beta$	152.36	84				
C=O	168.25	44				
$\gamma$	193.41	100				

**<sup>1</sup>H (acetone)**

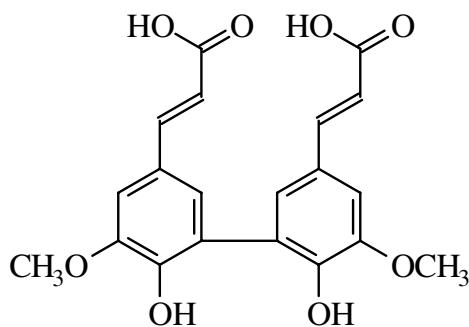
Atom	H Shifts	Mult	J
CH3	1.25	t	7.1
OMe	3.89	s	
CH2	4.23	q	7.1
CH2	4.69	s	
$\beta$	6.57	dd	15.8, 7.7
5	6.78	d	7.9
2,6	7.06-7.08	m	
$\alpha$	7.36	d	15.8
$\gamma$	9.62	d	7.7

**Notes:**

S. Quideau

intermediate for synthesis of  $\beta$ -O-4 dehydro diferulic acid

## Compound Number 2056

<sup>13</sup>C

5-5, Dehydoriferulic Acid

Atom	CDCl <sub>3</sub>		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

<sup>1</sup>H (acetone)

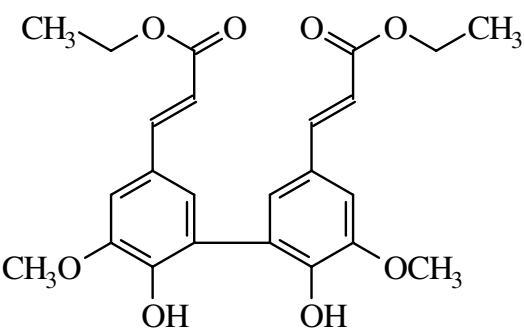
Atom	H Shifts	Mult	J
OMe	3.97	s	
β	6.42	d	15.4
6	7.21	d	2.0
2	7.35	d	2.0
α	7.64	d	15.9

## 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**

<sup>13</sup>C



**5,5-Dehydodiferulate diethyl ester**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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	

<sup>1</sup>H (acetone)

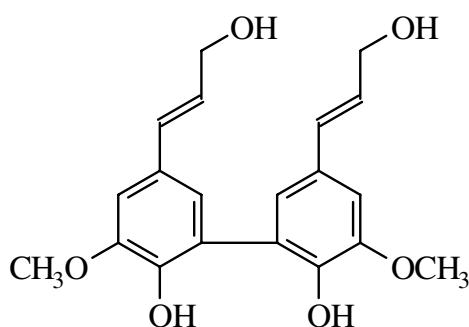
Atom	H Shifts	Mult	J
CH3	1.26	t	7.1
CH2	4.18	q	7.1
OMe	3.97	s	
β	6.43	d	15.9
6	7.20	d	2.0
2	7.36	d	2.0
α	7.62	d	15.9

**Notes:**

S. Quideau

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

## Compound Number 2058

<sup>13</sup>C

5,5 Dehydrodiconiferyl Alcohol

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
OMe			56.52	100		
β			63.49	68		
2			108.97	69		
6			123.16	79		
5			126.15	21		
b			128.53	71		
1			129.69	45		
α			130.57	80		
4			144.53	26		
3			148.87	27		

<sup>1</sup>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	

## Notes:

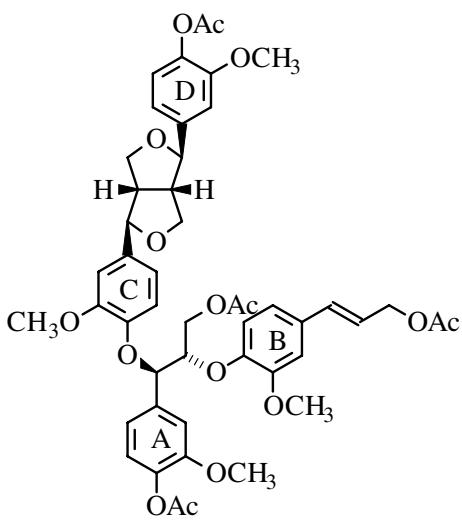
S. Quideau

Run only in acetone, no HMBC run.

Assignment of quaternary carbons based  
on shift assignments of diacid/diester parents.Poor solubility on CDCl<sub>3</sub>...sample degraded,  
no DMSO data. As this compound has a plane of symmetry  
the shifts for the other half are identical.

**Compound Number 2059**

<sup>13</sup>C



**Guaiacylglycerol- $\alpha$ -pinoresinol- $\beta$ -coniferyl-bis-ether (Ac'd)**

<sup>1</sup>H (acetone)

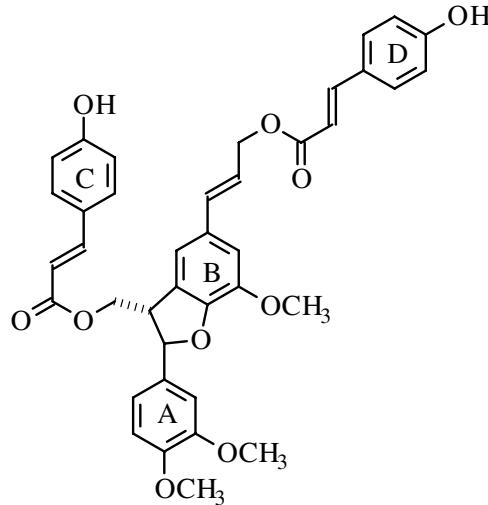
Atom	H Shifts	Mult	J
$\alpha$	5.60	d	5.6
$\beta$	4.86	m	
$\gamma 1$	4.45	dd	11.9, 3.8
$\gamma 2$	4.53	dd	11.9, 5.9
C $\alpha$	4.66	s	
C $\alpha$	3.06	m	
C $\gamma 1$	3.83	m	
C $\gamma 2$	4.17	m	
D $\alpha$	4.74	d	4.5
D $\gamma$	4.23	m	

**Notes:**

S.Quideau  
not substantiated in CDCl<sub>3</sub> & d6 DMSO  
Peracetate/diastereomeric mixture

Atom	CDCl <sub>3</sub>		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 $\beta$	53.91	66	55.11	64	53.49	61
B $\beta$	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 $\gamma$	63.45	36	63.62	40	62.44	36
B $\gamma$	65.05	69	65.38	59	64.40	61
C $\gamma$	71.88	70	72.37	48	71.07	52
D $\gamma$	71.88	70	72.48	48	71.18	52
A $\alpha$	80.34	43	80.88	30	78.69	33
A $\beta$	81.87	43	81.73	43	79.56	32
D $\alpha$	85.53	51	86.20	51	84.67	47
C $\alpha$	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 $\beta$	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 $\alpha$	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 $\gamma$ AcC=O	170.68	36	170.78	40	170.08	25
A $\gamma$ AcC=O	170.76	36	170.81	40	170.12	25

**Compound Number 2060**



**<sup>13</sup>C**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
Dβ	114.53	39	115.08	51	113.68	21
Cβ	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

**<sup>1</sup>H (acetone)**

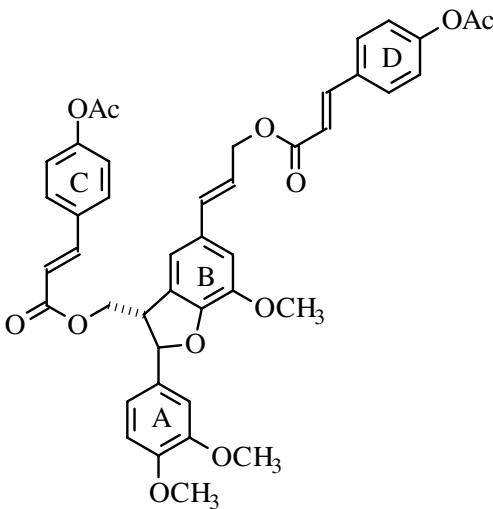
Atom	H Shifts	Mult	J
A3,4 OMe	3.77	s	
β	3.85	m	
B3 OMe	3.88	s	
γ <sup>1</sup>	4.45	dd	11.1, 7.6
γ <sup>2</sup>	4.58	dd	11.1, 5.4
B γ	4.78	dd	6.5, 1.2
a	5.61	d	7.1
B β	6.31	dt	15.8, 6.5
D β	6.33	d	15.9
C β	6.37	d	15.9
B α	6.70	dt	15.8, 1.2
C,D 3,5	6.88	m	
A5	6.93	d	8.3
A6	7.00	d	8.3, 2.0
A,B 2	7.07	br 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 CDCl<sub>3</sub> & DMSO

**Compound Number 2061**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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

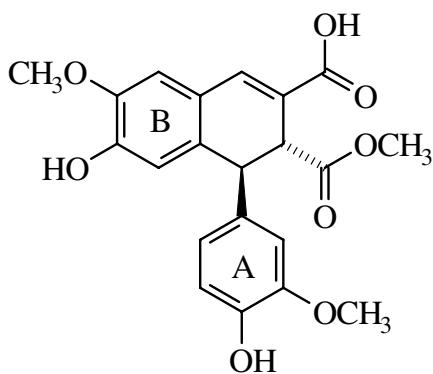
<sup>1</sup>H (acetone)

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
C β	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 CDCl<sub>3</sub> & DMSO

## Compound Number 2062

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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		

Methyl 7-hydroxy-5-methoxy-1-(4-hydroxy-3-methoxyphenyl)-trans-1,1-dihydronaphthalene-3-carboxylic Acid 2-carboxylate

<sup>1</sup>H (acetone)

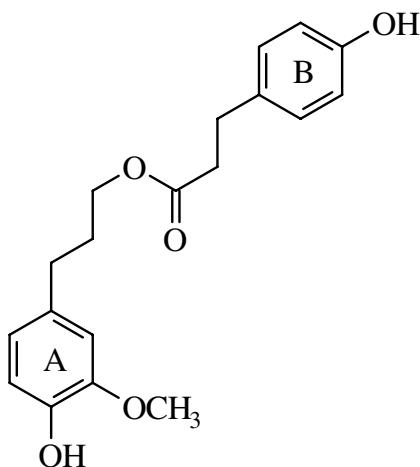
Atom	H Shifts	Mult	J
A γ OMe	3.55	s	
A3 OMe	3.74	s	
B3 OMe	3.87	s	
β	3.96	d	3.1
α	4.51	d	3.1
A6	6.43	dd	
A5	6.657	d	8.3
B5	6.661	s	
A2	6.77	d	2.0
B2	7.06	s	
B α	7.66	s	

## Notes:

S. Quideau

**Compound Number 2063**

**<sup>13</sup>C**



**Dihydroconiferyl 4-hydroxydihydrocinnamate**

**<sup>1</sup>H (acetone)**

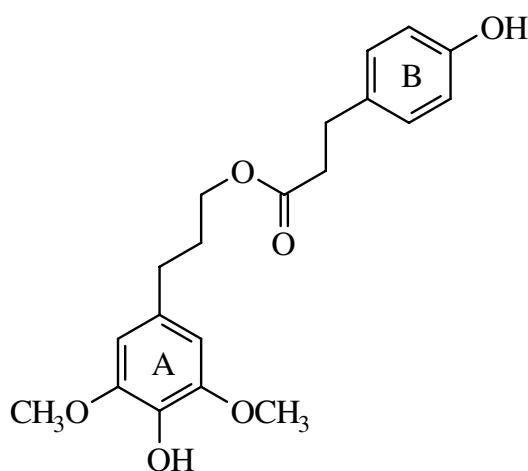
Atom	H Shifts	Mult	J
$\beta$	1.86	m	
$\alpha$	2.55	t	
B $\beta$	2.56	t	7.6
B $\alpha$	2.82	t	7.6
OMe	3.80	s	
$\gamma$	4.03	t	
A6	6.61	dd	6.5
A5	6.73	d	8.0, 2.0
B 3,5	6.75	m	7.9
A2	6.79	d	
B 2,6	7.06	m	2.0
ArOH	7.86	s	
ArOH	8.10	s	

**Notes:**

S. Quideau

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
B $\alpha$	30.11	46	30.75	47	29.49	37
$\beta$	30.40	42	31.33	47	29.95	38
$\alpha$	31.75	44	32.24	47	30.91	36
B $\beta$	36.17	45	36.69	49	35.47	39
OMe	55.87	47	56.16	45	55.48	47
$\gamma$	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 $\gamma$	173.26	24	173.09	21	172.32	34

Compound Number 2064

<sup>13</sup>C

Dihydrosinapyl dihydro-p-coumarate

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\alpha$	30.11	48	30.77	49	29.49	36
$\beta$	30.41	44	31.31	48	29.90	37
$\alpha$	32.26	46	32.71	47	31.41	32
B $\beta$	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
$\gamma$	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 $\gamma$	173.21	29	173.08	26	172.32	30

<sup>1</sup>H (acetone)

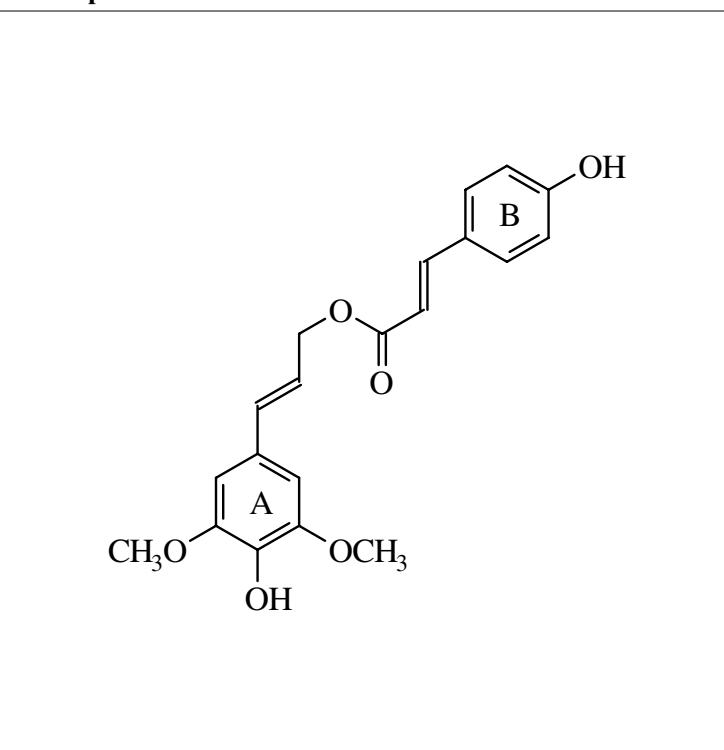
Atom	H Shifts	Mult	J
$\beta$	1.87	m	
$\alpha$	2.55	t	
B $\beta$	2.56	t	7.5
B $\alpha$	2.82	t	7.6
OMe	3.79	s	
$\gamma$	4.03	t	6.5
A 2,6	6.48	s	
B 3,5	6.74	m	
A4 OH	6.89	s	
B 2,6	7.06	m	
B4 OH	8.08	s	

## Notes:

S. Quideau

**Compound Number 2065**

<sup>13</sup>C



**Sinapyl p-coumarate**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
Bβ	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
Bα	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
Bγ	167.32	26	167.22	23	166.40	24

**<sup>1</sup>H (acetone)**

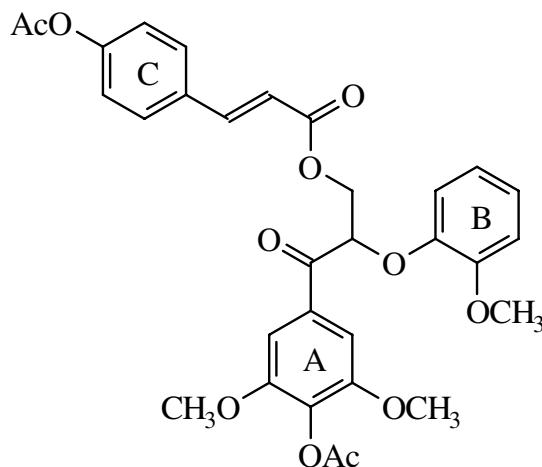
Atom	H Shifts	Mult	J
OMe	3.84	s	
γ	4.78	dd	6.5, 1.3
β	6.28	dt	15.8, 6.5
Bβ	6.38	d	15.9
α	6.64	dt	15.8, 1.3
A 2,6	6.79	s	
B 3,5	6.89	m	
B 2,6	7.55	m	
Bα	7.63	d	15.9

**Notes:**

S. Quideau

**Compound Number 2066**

**<sup>13</sup>C**



**2-(4-Acetoxy-3,5-dimethoxybenzoyl)-2-(2-methoxyphenoxy)  
ethyl 4-acetoxycinnamate**

**<sup>1</sup>H (acetone)**

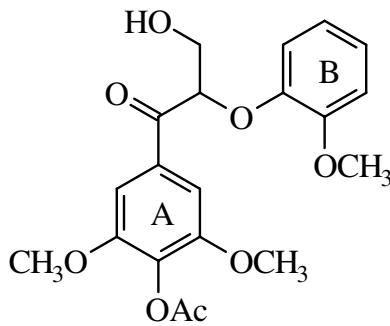
Atom	H Shifts	Mult	J
Ac Me	2.26	s	
Ac Me	2.26	s	
B3 OMe	3.75	s	
OMe	3.86	s	
$\gamma_1$	4.60	dd	120, 68
$\gamma_2$	4.86	dd	120, 36
$\beta$	5.96	dd	68, 36
C $\alpha$	6.50	d	160
B6	6.83	ddd	79, 88, 25
B 1,2,5	6.98	m	
C 3,5	7.18	m	
A 2,6	7.56	s	
C $\beta$	7.62	d	160
C 2,6	7.69	m	

**Notes:**

S. Quideau

B5 and C  $\beta$  can be interchanged

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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
$\gamma$	64.70	31	65.07	36	63.82	20
$\beta$	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 $\beta$	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	123.34	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 $\alpha$	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 $\gamma$	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
$\alpha$	194.44	33	194.92	24	194.02	35



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		

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

<sup>1</sup>H (acetone)

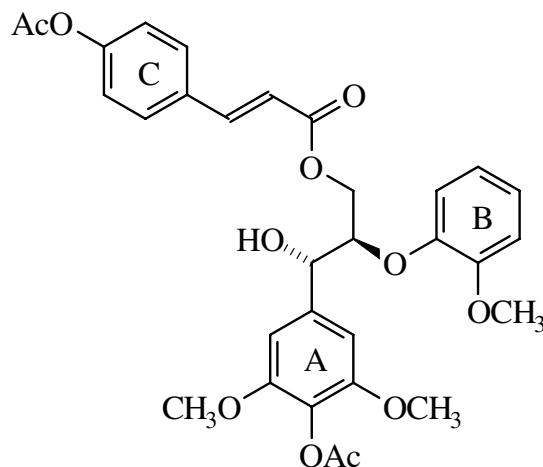
Atom	H Shifts	Mult	J
B3 OMe	3.77	s	
OMe	3.85	s	
γ	4.10	dd	
γOH	4.28	t	6.2
β	5.56	t	5.0
A 2,6	7.49	s	
B6	6.80	m	
B 1,5	6.41	m	
B2	6.96	m	

Notes:

S. Quideau

**Compound Number 2068**

**<sup>13</sup>C**



Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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		

**<sup>1</sup>H (acetone)**

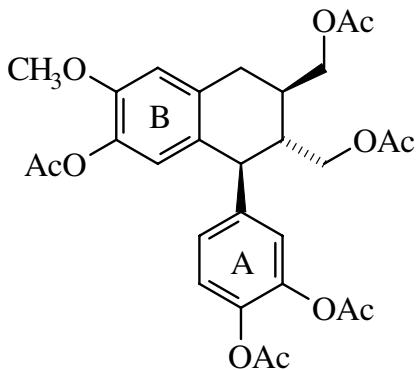
Atom	H Shifts	Mult	J
Ac	2.20	s	
Ac	2.26	s	
OMe	3.78	s	
B3 OMe	3.81	s	
γ1	4.47	dd	11.9, 3.9
γ2	4.52	dd	11.9, 6.1
β	4.73	m	
α OH	4.78	d	4.5
α	5.07	br t	4.8
C β	6.41	d	16.0
B6	6.84	ddd	7.9, 6.4, 2.7
A 2,6	6.88	s	
B 1,2	6.95	m	
B5	7.04	br dd	1.4
C 3,5	7.17	m	
C α	7.51	d	16.0
C 2,6	7.66	m	

**Notes:**

S. Quideau

**Compound Number 2069**

<sup>13</sup>C



**Isotaxiresinol**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\alpha$			33.50	67		
B $\beta$			36.27	82		
$\beta$			44.34	80		
$\alpha$			47.51	80		
OMe			56.18	96		
$\gamma$			63.57	65		
B $\gamma$			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		

**<sup>1</sup>H (acetone)**

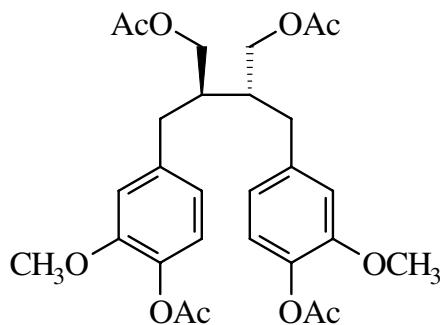
Atom	H Shifts	Mult	J
Ac Me	2.00	s	
Ac Me	2.01	s	
Ac Me	2.10	s	
$\beta$	2.14	m	
Ac Me	2.22	s	
Ac Me	2.24	s	
B $\beta$	2.26	m	
B $\alpha$	2.90	m	
A3 OMe	3.78	s	
$\gamma$ 1	3.90	dd	11.7, 3.5
$\alpha$	4.06	br d	10.2
B $\gamma$ 1	4.11	dd	11.2, 6.0
$\gamma$ 2	4.12	dd	11.7, 3.5
B $\gamma$ 2	4.22	dd	11.2, 4.4
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

**Notes:**

S. Quideau

Diaxial configuration on 6-membered ring --Trans 7,8

Natural occurring isomer is (+), i.e. 7S.8R, 8R'



Seco-isolariciresinol

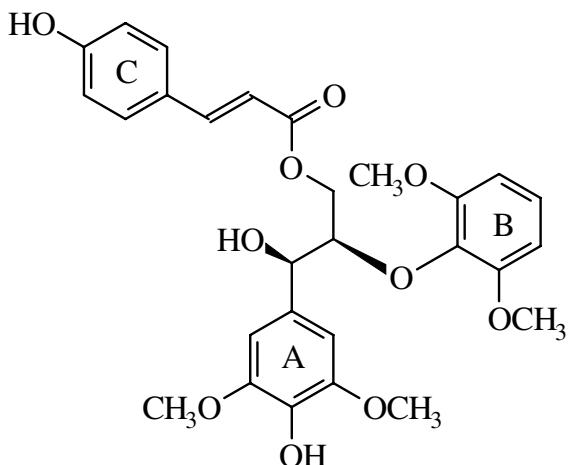
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	2.00	s	
4 Ac Me	2.21	s	
$\beta$	2.22	m	
$\alpha_1$	2.70	dd	13.9, 7.9
$\alpha_2$	2.83	dd	13.8, 6.7
A3 OMe	3.74	s	
$\gamma_1$	4.03	dd	11.4, 5.5
$\gamma_2$	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

## Notes:

S. Quideau  
natural occurring isomer (-), i.e. 8R, 8R'  
As this compound has a plane of symmetry  
the shifts for the other half are identical.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
4 Ac Me			20.47	100		
$\gamma$ AcMe			20.83	84		
$\alpha$			35.51	64		
$\beta$			40.81	77		
$\gamma$			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		
$\gamma$ Ac C=O			171.04	52		



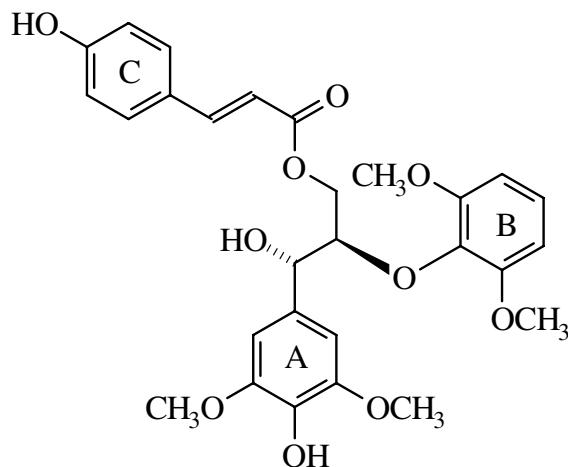
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B OMe	56.01	54	56.44	81	55.78	26
B OMe	56.01	54	56.44	81	55.78	26
A OMe	56.25	56	56.59	49	55.93	100
A OMe	56.25	56	56.59	49	55.93	100
γ	63.92	23	64.78	28	64.09	8
α	74.66	35	74.81	35	72.17	17
β	87.07	29	86.87	38	83.84	17
A2	103.75	78	105.39	72	104.32	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
Cβ	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
Cα	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
Cγ	167.12	23	167.12	27	166.25	32

<sup>1</sup>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
αOH	4.60	d	3.2
Cβ	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
Cα	7.48	d	16.0
C 2,6	7.53	m	

## Notes:

S. Quideau



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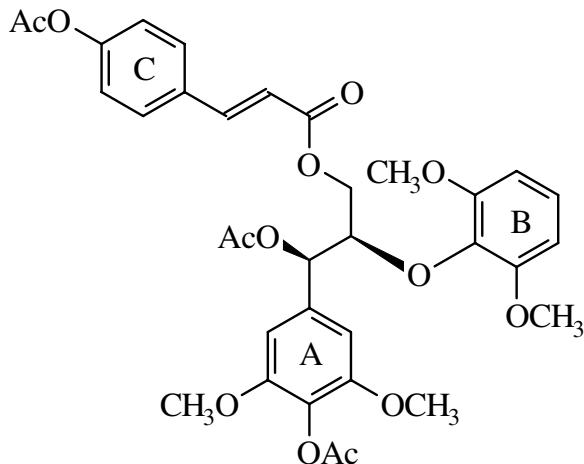
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B OMe	56.20	92	56.48	78	55.77	76
B OMe	56.20	92	56.48	78	55.77	76
A OMe	56.33	89	56.60	76	55.92	100
A OMe	56.33	89	56.60	76	55.92	100
γ	62.59	30	63.57	31	63.38	19
α	71.90	36	73.19	40	72.62	27
β	83.18	41	84.40	42	83.51	28
A2	102.78	85	104.59	88	103.77	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
Cβ	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
Cα	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
Cγ	167.29	37	167.16	32	166.27	38

<sup>1</sup>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	
Cβ	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



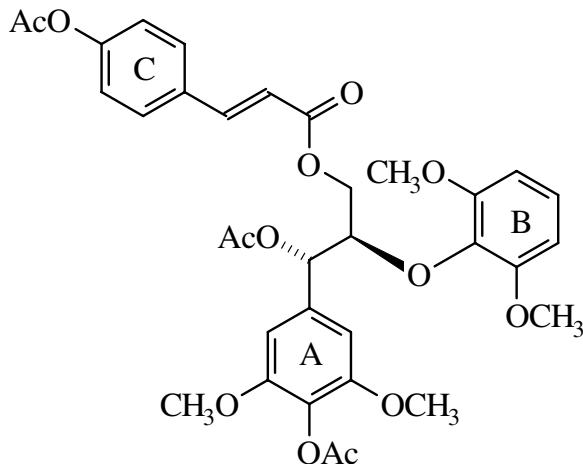
Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.36	49	20.23	47	20.15	54
Ac Me	21.02	83	20.95	73	20.75	47
α Ac Me	21.02	83	20.95	73	20.88	52
OMe	55.89	<b>100</b>	56.35	72	55.80	77
OMe	55.89	100	56.35	72	55.80	77
OMe	56.13	78	56.49	73	56.01	56
OMe	56.13	78	56.49	73	56.01	56
γ	64.01	22	64.66	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
Cβ	117.75	34	118.88	38	117.82	27
C3	122.09	79	123.20	<b>100</b>	122.43	<b>100</b>
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

<sup>1</sup>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	119,47
γ2	4.41	dd	119,38
β	4.68	ddd	68,47,38
α	6.18	d	68
C β	6.56	d	160
B 2,6	6.66	d	84
A 2,6	6.86	br s	
B1	6.99	t	84
C 3,5	7.19	m	
C α	7.55	d	160
C 2,6	7.72	m	

## Notes:

S. Quideau



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
Ac Me	20.36	57	20.24	42	20.15	61
$\alpha$ 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
$\gamma$	63.13	25	63.73	28	62.64	15
$\alpha$	74.50	34	75.58	37	74.23	26
$\beta$	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 $\beta$	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 $\alpha$	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 $\gamma$	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

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\alpha$ 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	
$\gamma$ 1	4.36	dd	11.9, 4.0
$\gamma$ 2	4.53	dd	11.9, 6.2
$\beta$	4.80	dt	6.2, 4.0
$\alpha$	6.14	d	4.2
C $\beta$	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 $\alpha$	7.44	d	16.0
C 2,6	7.66	m	

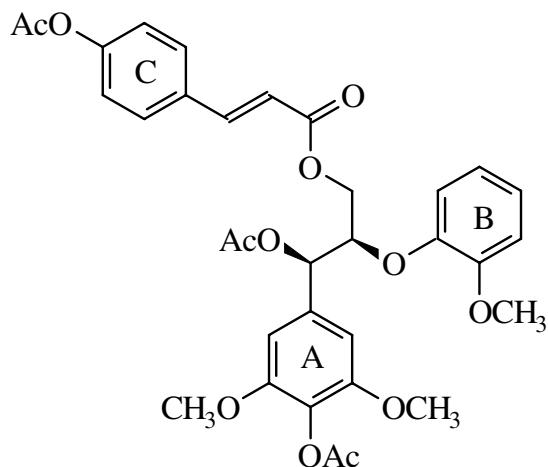
## Notes:

S. Quideau

B3,5 OMe and A3,5 OMe can be interchanged

Compound Number 2075

<sup>13</sup>C



*threo*

**γ-p-coumaroylated syringylglycerol-β-O-4-guaiacol ether (Ac'd)**

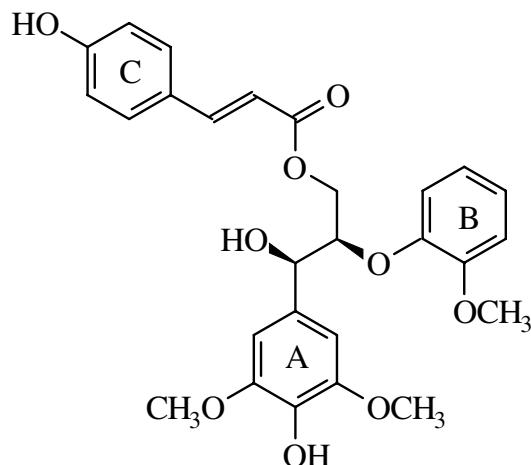
Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
Ac Me	20.42		20.23	25		
Ac Me	21.10		20.94	40		
αAc Me	21.10		20.94	40		
B3 OMe	35.77		56.21	30		
OMe	56.20		56.51	51		
OMe	56.20		56.51	51		
γ	63.39		63.97	14		
α	74.88		75.92	20		
β	80.50		80.89	19		
A2	104.09		105.00	41		
A6	104.09		105.00	41		
B2	112.45		113.74	31		
Cβ	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		
Cα	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		
Cγ	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		

<sup>1</sup>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
Cβ	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	
Cα	7.58	d	16.0
C 2,6	7.71	m	

**Notes:**

S. Quideau  
Not run in DMSO

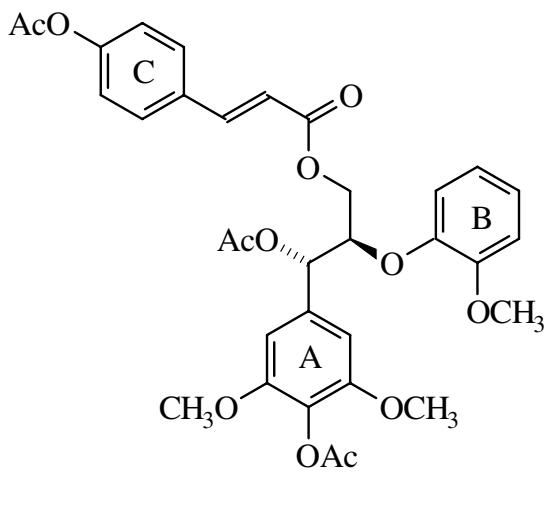
*threo* **$\gamma$ -p-coumaroylated syringylglycerol- $\beta$ O4-guaiacyl ether****<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
A OMe	3.79	s	
B3 OMe	3.84	s	
$\gamma$ 1	4.11	dd	12.0, 6.2
$\gamma$ 2	4.36	dd	12.0, 3.4
$\beta$	4.57	td	6.1, 3.4
$\alpha$	4.96	(br)d	5.9
C $\beta$	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 $\alpha$	7.48	d	16.0
C 2,6	7.51	m	

**Notes:**

S. Quideau

Atom	CDCl <sub>3</sub>		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
$\gamma$	63.19	29	64.23	31	63.47	15
$\alpha$	74.70	39	74.11	32	71.53	31
$\beta$	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 $\beta$	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 $\alpha$	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 $\gamma$	166.86	36	167.15	29	166.38	52

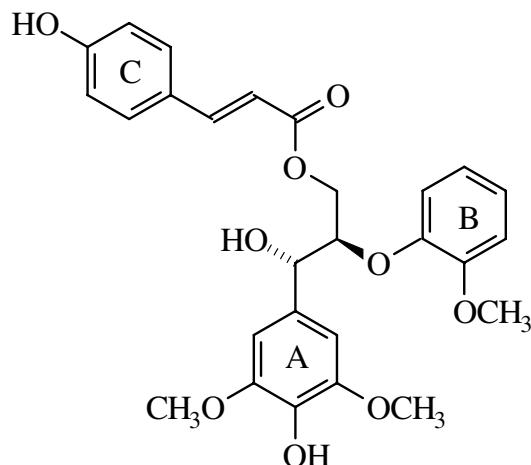
***erythro***  
 **$\gamma$ -p-coumaroylated syringylglycerol- $\beta$ 4-guaiacol ether (Ac'd)****<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
$\alpha$ 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	
$\gamma$ 1	4.43	dd	11.9, 4.3
$\gamma$ 2	4.49	dd	11.9, 5.8
$\beta$	4.94	m	
$\alpha$	6.12	d	5.1
C $\beta$	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 $\alpha$	7.57	d	16.0
C 2,6	7.69	m	

**Notes:**

S. Quideau

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
Ac Me	20.40	51	20.24	43	20.12	50
$\alpha$ 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
$\gamma$	62.98	27	63.41	27	62.35	18
$\alpha$	74.17	35	74.99	35	73.53	29
$\beta$	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 $\beta$	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 $\alpha$	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 $\gamma$	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
$\alpha$ Ac C=O	169.48	27	169.95	21	169.34	30

***erythro***  
**γ-p-coumaroylated syringylglycerol-β-O-4-guaiaacyl ether****<sup>1</sup>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
Cβ	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	

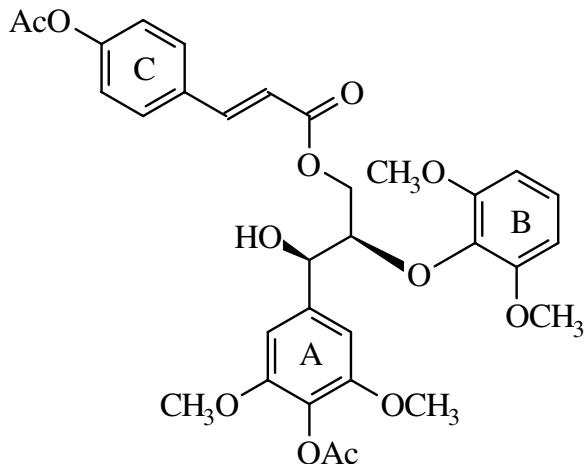
**Notes:**

S. Quideau

Atom	CDCl <sub>3</sub>		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	
Cβ	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	
Cα	145.25	44	145.42	43	144.71	
C3	147.00	60	148.42	51	147.52	
C5	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	
Cγ	167.39	39	167.28	28	166.41	

Compound Number 2079

<sup>13</sup>C



*threo*

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		

<sup>1</sup>H (acetone)

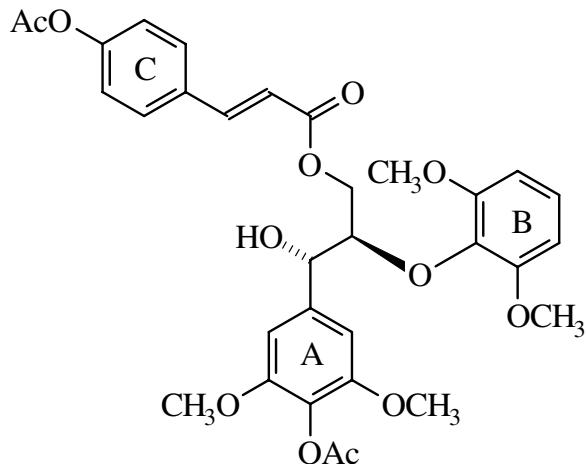
Atom	H Shifts	Mult	J
Ac Me	2.19	s	
Ac Me	2.27	s	
A OMe	3.75	s	
B OMe	3.82	s	
γ1	4.16	dd	11.9, 4.6
β	4.38	ddd	6.3, 4.5, 3.6
γ2	4.50	dd	11.9, 3.6
α	5.07	br d	6.4
C β	6.47	d	16.0
B 2,6	6.68	d	8.4
A 2,6	6.87	br s	
B1	7.01	t	8.4
C 3,5	7.19	m	
C α	7.63	d	16.0
C 2,6	7.70	m	

Notes:

S. Quideau

**Compound Number 2080**

**<sup>13</sup>C**



*erythro*

**<sup>1</sup>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	
$\gamma_1$	4.30	dd	11.7, 3.8
$\gamma_2$	4.51	dd	11.7, 6.9
$\beta$	4.62	m	
$\alpha$	5.05	br t	3.7
C $\beta$	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 $\alpha$	7.44	d	16.0
C 2,6	7.66	m	

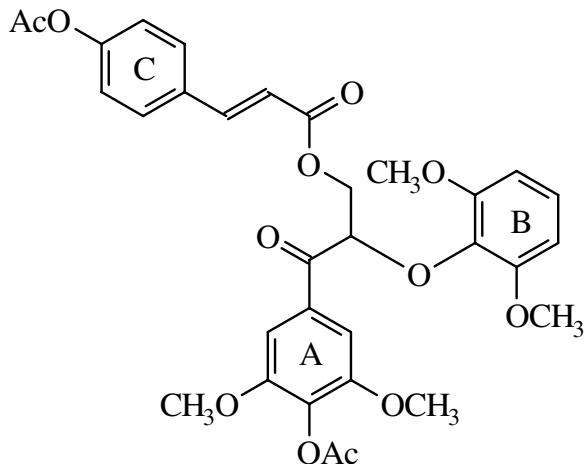
**Notes:**

S. Quideau

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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		
$\gamma$			63.67	31		
$\alpha$			73.30	37		
$\beta$			84.07	39		
A2			103.76	82		
A6			103.76	82		
B2			106.31	88		
B6			106.31	88		
C $\beta$			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 $\alpha$			144.00	42		
A3			152.94	48		
A5			152.94	48		
C4			153.36	21		
B3			154.51	52		
B5			154.51	52		
C $\gamma$			166.71	28		
Ac C=O			168.59	23		
Ac C=O			169.45	27		

**Compound Number 2081**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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
Cβ	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
Cα	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
Cγ	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

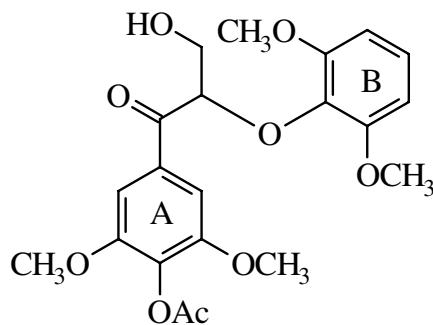
<sup>1</sup>H (acetone)

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
Cβ	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	
Cα	7.50	d	16.0
A 2,6	7.58	br s	
C 2,6	7.64	m	

**Notes:**

S. Quideau

## Compound Number 2082

<sup>13</sup>C

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		
gamma			63.35	42		
beta			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		
alpha			196.25	27		

<sup>1</sup>H (acetone)

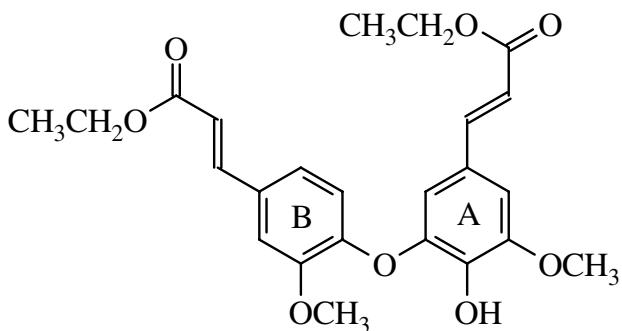
Atom	H Shifts	Mult	J
Ac Me	2.27	s	
B OMe	3.73	s	
A OMe	3.86	s	
gamma + gamma OH beta	3.90-3.98 5.22	m dd	5.7, 4.5
B 2,6 B1 A 2,6	6.67 7.02 7.48	d dd t s	8.4 8.6, 8.2, 8.4

## Notes:

S.Quideau

Compound Number 3001

<sup>13</sup>C



**4-O-5 dehydrodiethylf erulate**  
**3-[3-{4-(2-ethoxycarbonyl-vinyl)-2-methoxy-phenoxy]-4-hydroxy-5-methoxy-phenylacrylic acid ethyl ester}**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
A CH3	1.24	t	J = 7.1
B CH3	1.27	t	J = 7.1
B3 OMe	3.93	s	
A3 OMe	3.96	s	
A CH2	4.16	q	J = 7.1
B CH2	4.19	q	J = 7.1
A $\beta$	6.36	d	J = 15.9
B $\beta$	6.48	d	J = 15.95
B5	6.81	d	J = 8.3
A6	6.89	d	J = 1.9
B6	7.17	dd	J = 8.7, 2.0
A2	7.22	d	J = 1.9
B2	7.46	d	J = 2.0
A $\alpha$	7.53	d	J = 15.9
B $\alpha$	7.62	d	J = 15.95

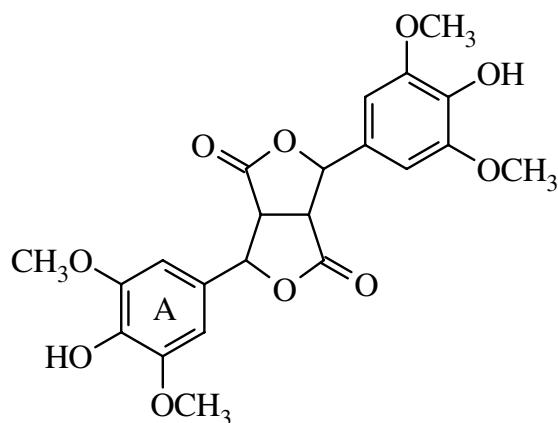
**Notes:**

jrf107.P1 /1 (H1), /2 (C13), /3 (Dept135)

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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 $\beta$			116.99	76		
B $\beta$			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 $\alpha$			144.81	75		
A $\alpha$			144.94	73		
B4			149.35	39		
A3			150.12	34		
B3			151.41	43		
B $\gamma$			167.15	53		
A $\gamma$			167.16	56		

Compound Number 3002

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			

### <sup>1</sup>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**

**<sup>13</sup>C**

		<sup>13</sup> C					
Atom	CDCl <sub>3</sub>		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 $\beta$			117.00	75	116.96	25	
B $\beta$			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 $\alpha$			145.23	76	143.81	36	
B $\alpha$			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 $\gamma$			168.02	62	167.82	61	
A $\gamma$			168.05	66	167.82	61	

4-O-5 dehydodiferulic acid

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B3 OMe	3.58	s	
A3 OMe	3.88	s	
A $\beta$	6.36	d	J = 15.9
B $\beta$	6.47	d	J = 15.95
B5	6.82	d	J = 8.3
A6	6.90	d	J = 1.9
B6	7.22	dd	J = 8.3, 2.0
A2	7.22	d	J = 1.9
B2	7.45	d	J = 2.0
A $\alpha$	7.54	d	J = 15.9
B $\alpha$	7.63	d	J = 15.95

**Notes:**

Acetone: jrf117 /2 (C13) and /1 (H1)

DMSO: jrf127.c7/2

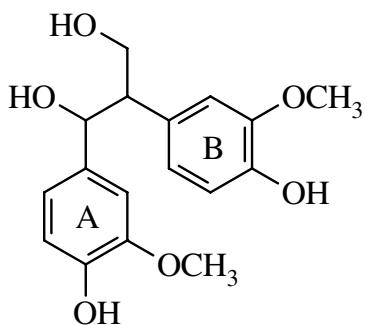
1H NMR (DMSO-d6) d: 3.85 (B3-OMe), 3.86 (A3-OMe), 6.35 (A8), 6.47 (B8), 6.59 (B5), 6.85 (A6), 7.12 (B6), 7.20 (A2), 7.43 (B2), 7.42 (A7), 7.51 (B7) - J's same as in acetone.

Not soluble in chloroform

JCS Perkin 1, 3485-98 (1994)

Cmpd 17

Compound Number 3004

<sup>13</sup>C

## 1,2-diguaiaacylpropane-1,3-diol

<sup>1</sup>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	J = 8.1
A6	6.68	m	
A2	6.71	m	
B2	6.74	d	J = 1.9

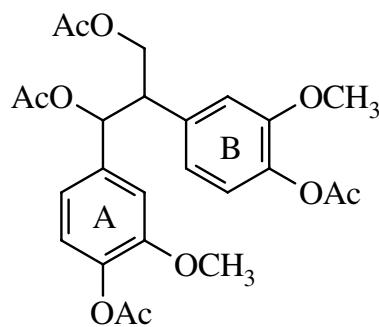
## Notes:

jrlz 15

Liming Zhang, isolate from mild acidolysis

Atom	CDCl <sub>3</sub>		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

<sup>13</sup>C*threo*

Acetic acid3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

Atom	CDCl <sub>3</sub>		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		

<sup>1</sup>H (acetone)

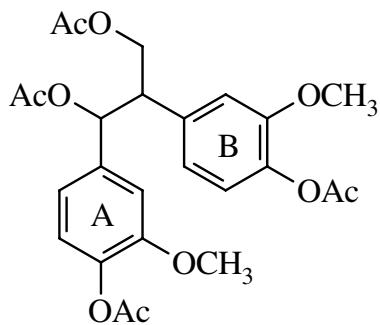
Atom	H Shifts	Mult	J
γ Ac Me	1.93	s	
α Ac Me	2.09	s	
Ac Me	2.18	s	
Ac Me	2.19	s	
β	3.56	m	
OMe	3.67	s	
OMe	3.71	s	
γ1	4.38	dd	J = 11.2, 5.2
γ2	4.54	dd	J = 11.2, 7.2
α	6.02	d	J = 8.2
B6	6.77	ddd	J = 8.1, 2.0, 0.3
A2	6.79	bd	J = 1.9
A6	6.82	ddd	J = 8.1, 1.9, 0.5
B2	6.85	bd	J = 1.9
B5	6.90	d	J = 8.1
A5	6.91	d	J = 8.1

## Notes:

jrlz9.1  
Liming Zhang, isolate from mild acidolysis

**Compound Number 3006**

**<sup>13</sup>C**



*erythro*

Acetic acid3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.92	s	
$\alpha$ Ac Me	1.97	s	
Ac Me	2.20	s	
Ac Me	2.21	s	
$\beta$	3.50	m	J = 6.7
OMe	3.69	s	
OMe	3.73	s	
$\gamma$ 1	4.20	dd	J = 11.2, 6.7
$\gamma$ 2	4.37	dd	J = 11.2, 6.8
$\alpha$	6.16	d	J = 6.6
B6	6.84	ddd	J = 8.1, 1.9, 0.3
A2	6.84	bd	J = 1.8
A6	6.87	ddd	J = 8.1, 1.8, 0.5
B2	6.92	bd	J = 1.9
B5	6.96	d	J = 8.1
A5	6.98	d	J = 8.1

**Notes:**

jrlz11.1

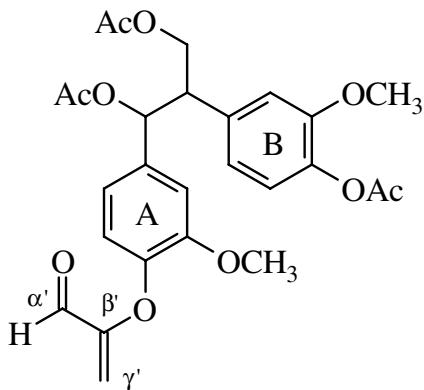
Liming Zhang, isolate from mild acidolysis

1H data at 600 MHz

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	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		
$\beta$			50.98	76		
OMe			56.20	97		
OMe			56.22	92		
$\gamma$			64.86	65		
$\alpha$			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		
$\alpha$ Ac C=O			169.94	46		
$\gamma$ Ac C=O			170.74	46		

**Compound Number 3007**

<sup>13</sup>C



Acetic acid 3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.94	s	
$\alpha$ Ac Me	2.00	s	
Ar Ac Me	2.07	s	
$\beta$	3.50	m	
OMe	3.69	s	
OMe	3.76	s	
$\gamma^1$	4.22	dd	$J = 11.2, 6.8$
$\gamma^2$	4.38	dd	$J = 11.2, 6.8$
$\gamma^1'$	5.00	d	$J = 2.8$
$\gamma^2'$	5.38	d	$J = 2.8$
$\alpha'$	6.19	d	$J = 6.4$
B6	6.81	dd	$J = 8.1, 1.6$
A2	6.88	bd	
A6	6.89	dd	$J = 7.3, 1.5$
B5	6.94	d	$J = 8.1$
A5	6.97		
A2	6.99		

**Notes:**

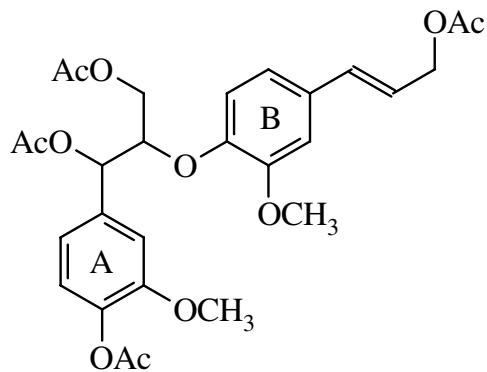
jrlz 13

Liming Zhang, isolate from mild acidolysis

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		
$\beta$	50.13	61	51.07	41		
OMe	55.85	120	56.12	66		
OMe	55.85	120	56.22	66		
$\gamma$	63.96	49	64.82	42		
$\alpha$	74.76	68	75.38	40		
$\gamma'$	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		
$\beta'$	157.84	60	159.33	25		
B4 Ac C=O	168.79	29	168.91	21		
$\alpha$ Ac C=O	169.70	52	169.94	23		
$\gamma$ Ac C=O	170.69	65	170.71	24		
$\alpha'$	186.74	93	187.55	45		

Compound Number 3008

<sup>13</sup>C



*threo*

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-  
2-[4-(3-acetoxypropenyl)-2-methoxyphenoxy]propyl ester

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.95	s	
B $\gamma$ Ac Me	2.01	s	
$\alpha$ Ac Me	2.02	s	
A4 Ac Me	2.21	s	
OMe	3.82	s	
OMe	3.85	s	
$\gamma$ 1	4.02	dd	J = 11.9, 5.7
$\gamma$ 2	4.25	dd	J = 11.9, 4.1
B $\gamma$	4.66	dd	J = 6.4, 1.3
$\beta$	4.81	m	
$\alpha$	6.10	d	J = 6.4
B $\beta$	6.26	dt	J = 15.9, 6.4
B $\alpha$	6.63	bdt	J = 15.9
B6	6.95	dd	J = 8.3, 2.0
B5	7.00	d	J = 8.3
A5	7.03	d	J = 8.2
A6	7.09	dd	J = 8.2, 1.7
B2	7.14	d	J = 1.9
A2	7.22	d	J = 1.6

### Notes:

jrlz 35

Liming Zhang, isolate from mild acidolysis

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		
$\gamma$			63.54	44		
B $\gamma$			65.33	57		
$\alpha$			75.29	56		
$\beta$			80.62	57		
B2			111.30	58		
A2			112.63	47		
B5			118.73	57		
A6			120.28	44		
B6			120.52	44		
B $\beta$			123.25	57		
A5			123.54	51		
B1			132.34	32		
B $\alpha$			134.14	54		
A1			136.359	31		
A4			140.90	22		
B4			149.08	26		
B3			151.74	23		
A3			152.21	22		
A4 Ac C=O			168.85	26		
$\alpha$ Ac C=O			169.95	30		
$\gamma$ Ac C=O			170.64	23		
B $\gamma$ Ac C=O			170.64	23		

**Compound Number 3009**

**<sup>13</sup>C**

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		

**<sup>1</sup>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	

**Notes:**

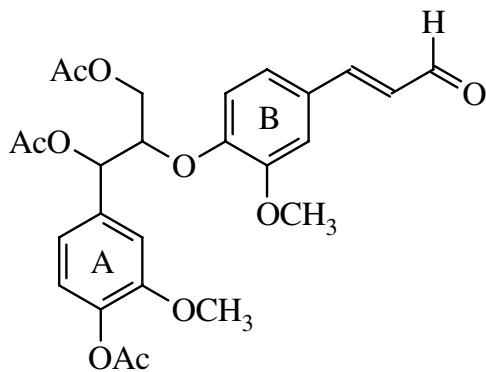
J.Ralph jrf79.5

As this dimer contains a plane of symmetry the CS's are reported for one unit.  
erythro shifts in acetone:

γ (62.95)α (74.59), β (80.44), B5 (120.09), B1 (124.19), A5 (131.70),  
A4 (138.36), B4 (148.19), B3 (152.11).

Compound Number 3010

<sup>13</sup>C



*threo*

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-  
2-[2-methoxy-4-(3-oxopropenyl)phenoxy]propyl ester

<sup>1</sup>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	
$\gamma$ 1	4.07	dd	J = 12.0, 5.8
$\gamma$ 2	4.28	dd	J = 12.0, 4.1
$\beta$	4.96	m	
$\alpha$	6.11	d	J = 6.4
B $\beta$	6.70	dd	J = 15.9, 7.7
A5	7.03	d	J = 8.1
A6	7.08	dd	J = 8.5, 1.4
B5	7.15	d	J = 8.4
A2	7.24	bd	
B6	7.25	dd	J = 8.8, 1.7
B2	7.40	d	J = 1.8
B $\alpha$	7.59	d	J = 16.0
B $\gamma$	9.66	d	J = 7.6

Notes:

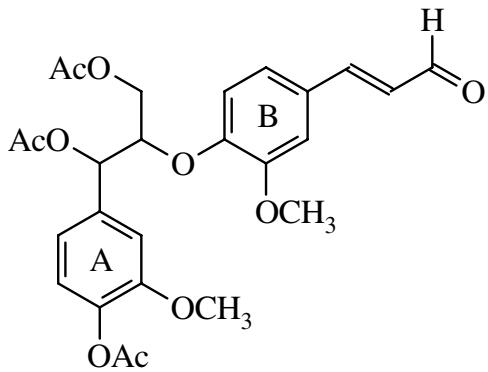
jrlz 29 1mg

Liming Zhang, isolate from mild acidolysis  
see 3011 some shifts taken from isomer mix

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		
$\gamma$	62.81	25	63.45	25		
$\alpha$	74.14	28	75.19	25		
$\beta$	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 $\beta$	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 $\alpha$	152.26	45	153.29	26		
A4 Ac C=O	168.72	23	168.87	17		
$\alpha$ Ac C=O	169.41	24	169.85	15		
$\gamma$ Ac C=O	170.48	24	170.66	15		
B $\gamma$	193.43	58	193.61	32		

Compound Number 3011

<sup>13</sup>C



*erythro*

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-  
2-[2-methoxy-4-(3-oxopropenyl)phenoxy]propyl ester

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac Me			
Ac Me			
Ac Me			
OMe	3.82	s	
OMe	3.90	s	
γ1	4.27	m	
γ2	4.37	m	
β	4.99	m	
α	6.07	d	J = 5.2
B β	6.79	dd	J = 15.9, 7.7
A5	7.02	d	J = 8.1
A6	7.07	m	
B5	7.11	d	J = 8.3
A2	7.23	m	
B6	7.27	d	J = 1.8
B2	7.38	d	J = 2.0
B α	7.58	d	J = 15.9
B γ	9.65	d	J = 7.7

Notes:

jrlz41

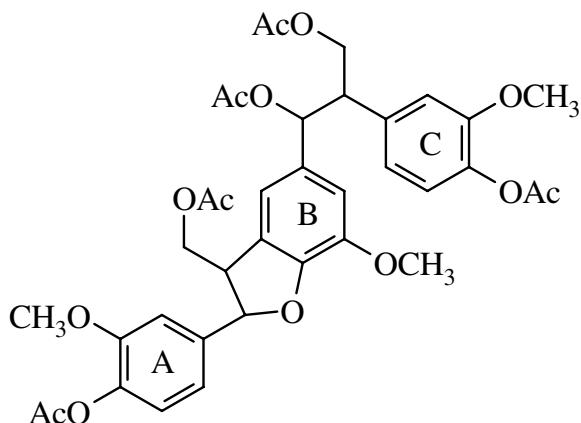
Liming Zhang, isolate from mild acidolysis  
CS's taken from isomer mix spectrum

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		

## Compound Number 3012

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\beta$ <i>t</i>			50.64			
B $\beta$ <i>t</i>			50.67			
B $\beta$ <i>e</i>			50.90			
B $\beta$ <i>e</i>			50.95			
A $\beta$			50.95			
A $\beta$			51.23			
A $\beta$			51.26			
B $\gamma$ <i>t</i>			64.74			
B $\gamma$ <i>e</i>			64.85			
B $\gamma$ <i>e</i>			64.89			
A $\gamma$			65.55			
A $\gamma$			65.63			
A $\gamma$			65.85			
B $\alpha$ <i>e</i>			75.75			
B $\alpha$ <i>e</i>			75.76			
B $\alpha$ <i>t</i>			76.56			
B $\alpha$ <i>t</i>			76.62			
$\alpha$			87.91			
$\alpha$			88.03			
$\alpha$			88.04			

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J

## Notes:

jrlz 19 15mg

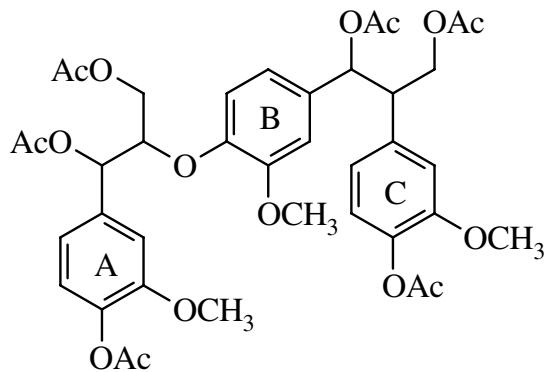
Liming Zhang, isolate from mild acidolysis

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

<sup>13</sup>C



Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-{4-[1,3-diacetoxy-2-(4-acetoxy-3-methoxyphenyl)propyl]-2-methoxyphenoxy}propyl ester

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J

**Notes:**

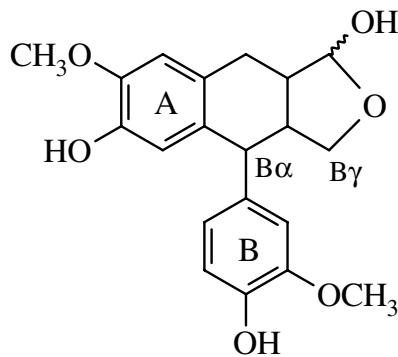
jrlz 7 and jrlz 17

threo β-O-4/threo+erythro β-1  
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.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B β <i>t</i>			50.37			
B β <i>t</i>			50.46			
B β <i>e</i>			50.71			
B β <i>e</i>			50.75			
γ			63.37			
B γ <i>t</i>			64.74			
B γ <i>t</i>			64.75			
B γ <i>e</i>			64.84			
B γ <i>e</i>			64.86			
α			75.13			
α			75.35			
α			75.19			
B α <i>e</i>			75.47			
B α <i>e</i>			75.53			
B α <i>t</i>			76.30			
B α <i>t</i>			76.35			
β			80.34			
β			80.36			
β			80.42			

## Compound Number 3014

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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		

4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-1,3,3a,4,9,9a-hexahydronaphtho[2,3-c]furan-1,6-diol

<sup>1</sup>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	J = 10.0, 8.0
B α	3.64	d	J = 12.2
B γ2	3.77	m	
OMe	3.77	s	
OMe	3.80	s	
A γ OH	4.99	d	J = 4.3
A γ	5.40	d	J = 4.3
A5	6.22	d	J = 0.9
B6	6.63	dd	J = 8.0, 2.0
A2	6.72	s	
B2	6.74	d	J = 2.0
B5	6.77	d	J = 8.0
A4 OH	7.17	s	
B4 OH	7.39	s	

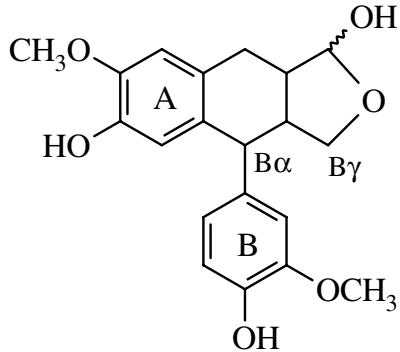
## Notes:

jrlz5, mixture of 2 isomers in ca. 2:1 ratio.

Data for major isomer

Liming Zhang, isolate from mild acidolysis

Compound Number 3015

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
$\alpha$			31.98	22		
B $\beta$			49.88	48		
$\beta$			49.88	48		
B $\alpha$			50.12	18		
OMe			55.96	79		
OMe			56.05	86		
B $\gamma$			70.96	23		
$\gamma$			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		

4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-1,3,3a,4,9,9a-hexahydronaphtho[2,3-c]furan-1,6-diol

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
A $\beta$	1.98	m	
B $\beta$	2.28	m	
A $\alpha$ 1	2.80	m	
A $\alpha$ 2	3.00	m	
B $\gamma$ 1,2	3.64	m	
B $\alpha$	3.72	bd	J = 11.4
OMe	3.77	s	
OMe	3.80	s	
A $\gamma$	5.18	d	
A $\gamma$ OH	5.28	d	
A5	6.55	d	
B6	6.62	dd	J = 10.1, 2.0
A2	6.72	s	
B2	6.74	d	J = 2.0
B5	6.77	d	J = 8.0
A4 OH	7.17	s	
B4 OH	7.39	s	

### Notes:

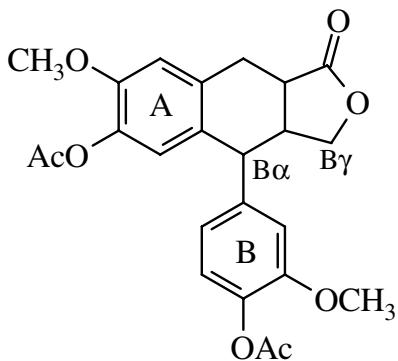
jrlz5, mixture of 2 isomers in ca. 2:1 ratio.

Data for minor isomer

Liming Zhang, isolate from mild acidolysis

Compound Number 3016

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		
Bβ	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		
Bγ	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		

Acetic acid 4-(4-acetoxy-3-methoxyphenyl)-7-methoxy-1-oxo-1,3,3a,4,9,9a-hexahydroanaphtho[2,3-c]furan-6-yl ester

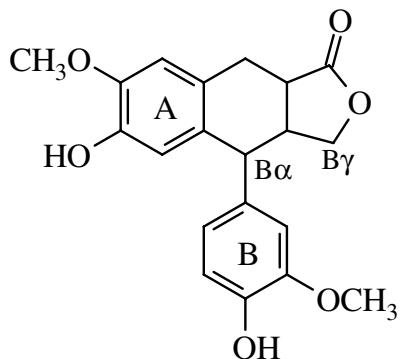
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.13	s	
Ac Me	2.23	s	
Bβ	2.75	m	
Aβ	2.78	m	
Aα1	2.98	m	
Aα2	3.18	dd	J = 16.0, 5.0
OMe	3.75	s	
OMe	3.81	s	
Bα	4.16	m	
Bγ	4.16	m	
A5	6.44	s	
B6	6.83	dd	
B2	6.96	d	J = 1.9
A2	6.98	s	
B5	7.03	d	J = 8.1

Notes:

jrlz25  
Liming Zhang, isolate from mild acidolysis

Compound Number 3017

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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		

6-Hydroxy-4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-3a,4,9,9a-tetrahydro-3H-naphtho[2,3-c]furan-1-one

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B β	2.67	m	
A β	2.67	m	
A α	3.07	dd	J = 16.2, 4.5
OMe	3.78	s	
OMe	3.82	s	
B α	3.95	bd	
B γ	4.10	m	
A5	6.26	d	
B6	6.69	dd	J = 0.9
A2	6.79	s	J = 8.0, 2.0
B2	6.80	d	J = 2.0
B5	6.80	d	J = 8.0

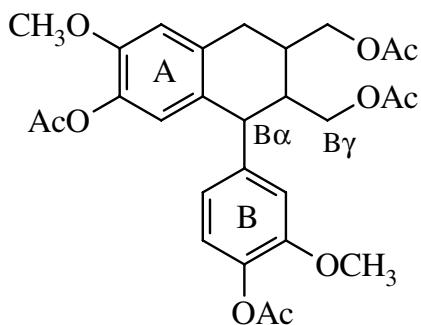
Notes:

jrlz33

Liming Zhang, isolate from mild acidolysis

Compound Number 3018

<sup>13</sup>C



Acetic acid 8-(4-acetoxy-3-methoxyphenyl)-6,7-bis-acetoxy methyl-3-methoxy-5,6,7,8-tetrahydronaphthalen-2-yl ester

<sup>1</sup>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	J = 11.7, 3.6
B α	4.02	d	J = 10.5
B γ2	4.09	m	
A γ1	4.11	m	
A γ2	4.23	dd	J = 11.1, 5.3
A5	6.34	bs	
B6	6.74	dd	J = 8.1, 2.0
A2	6.87	s	
B2	6.92	d	J = 2.0
B5	6.99	d	J = 8.1

Notes:

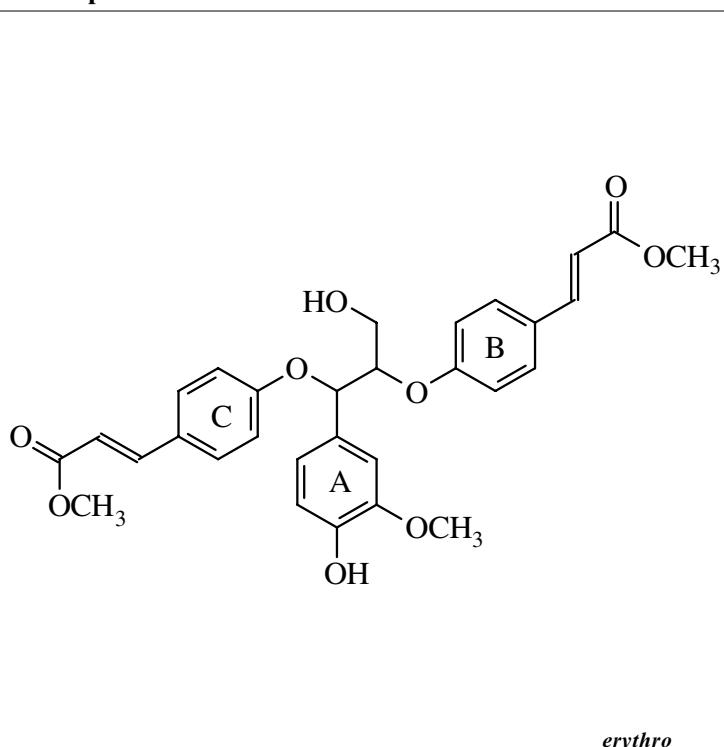
jrlz27

Liming Zhang, isolate from mild acidolysis

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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**

<sup>13</sup>C



**3-(4-{3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2[4-(2-methoxycarbonylvinyl)phenoxy]prooxy}phenyl)acrylic acid methyl ester**

**<sup>1</sup>H (acetone)**

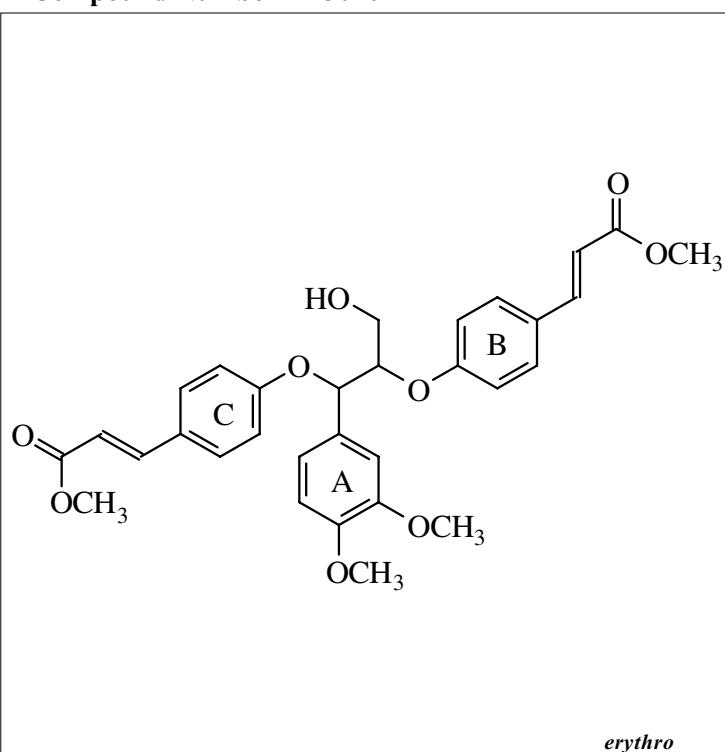
Atom	H Shifts	Mult	J
B $\gamma$ OMe	3.70	s	
C $\gamma$ OMe	3.71	s	
A3 OMe	3.78	s	
$\gamma$ 's	3.95	m	J = 5.8
$\gamma$ OH	4.16	t	J = 5.8
$\beta$	4.88	m	
$\alpha$	5.60	d	J = 5.5
C $\beta$	6.34	d	J = 16.0
B $\beta$	6.37	d	J = 16.0
A5	6.79	d	J = 8.1
A6	7.00	m	
C2,6	6.97	m	J = 8.8
B2,6	7.02	m	J = 8.8
A2	7.12	d	J = 1.9
C3,5	7.50	m	J = 8.6
B3,5	7.54	m	J = 8.6
C $\alpha$	7.55	d	J = 16.0
B $\alpha$	7.59	d	J = 16.0

**Notes:**

jrf101.C9-12

Authenticated assignments in acetone.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
C $\gamma$ OMe	51.55	54	51.52	51	51.27	59
B $\gamma$ OMe	51.59	50	51.53	51	55.63	66
A3 OMe	55.92	65	56.26	58	55.80	22
$\gamma$	61.43	27	61.42	24	59.79	15
$\alpha$	78.70	35	79.32	34	77.75	18
$\beta$	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 $\beta$	115.68	41	116.15	45	115.13	37
C $\beta$	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 $\alpha$	144.12	43	144.87	39	144.16	24
B $\alpha$	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 $\gamma$	167.62	44	167.67	40	166.86	55
B $\gamma$	167.63	48	167.72	39	166.92	56



**3-(4-{1-(3,4-dimethoxyphenyl)-3-hydroxy-2[4-(2-methoxy-carbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B <sub>γ</sub> OMe	3.693	s	
C <sub>γ</sub> OMe	3.711	s	
A4 OMe	3.732	s	
A3 OMe	3.752	s	
γ 's	3.954	m	J = 5.9, *
γ OH	4.157	t	J = 5.9
β	4.881	m	J = 5.5, 4.9
α	5.603	d	J = 5.5
C <sub>β</sub>	6.335	d	J = 16.0
B <sub>β</sub>	6.363	d	J = 16.0
A5	6.876	d	J = 8.2
C2,6	6.973	m	J = 8.8
B2,6	7.015	m	J = 8.7
A6	7.047	dd	J = 8.2, 1.9
A2	7.126	d	J = 1.9
C3,5	7.515	m	J = 8.8
B3,5	7.550	m	J = 8.7
C <sub>α</sub>	7.543	d	J = 16.0
B <sub>α</sub>	7.582	d	J = 16.0

**Notes:**

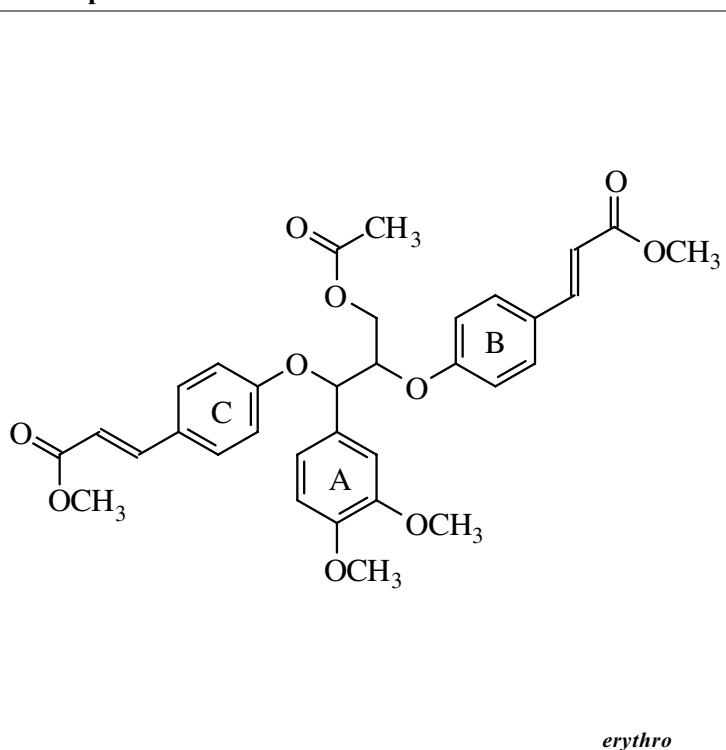
jrf119.C2

assignments not authenticated - from #3019

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
C <sub>γ</sub> OMe			51.52	38		
B <sub>γ</sub> 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 <sub>β</sub>			116.21	40		
C <sub>β</sub>			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 <sub>α</sub>			144.87	38		
B <sub>α</sub>			144.96	40		
A4			150.25	32		
A3			150.26	28		
C4			160.50	30		
B4			161.69	32		
C <sub>γ</sub>			167.66	30		
B <sub>γ</sub>			167.72	28		

**Compound Number 3021**

<sup>13</sup>C



**3-(4-{3-carboxyoxy-1-(3,4-dimethoxyphenyl)-2-[4-(2-methoxy carbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester**

<sup>1</sup>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	J = 11.9, 6.2
γ 2	4.507	dd	J = 11.9, 3.8
β	5.084	m	J = 6.2, 5.8, 3.8
α	5.629	d	J = 5.8
C β	6.343	d	J = 16.0
B β	6.378	d	J = 16.0
A5	6.888	d	J = 8.3
C2,6	6.992	m	J = 8.7
B2,6	7.018	m	J = 8.7
A6	7.073	dd	J = 8.3, 2.0
A2	7.161	d	J = 2.0
C3,5	7.527	m	J = 8.7
B3,5	7.570	m	J = 8.7
Cα	7.548	d	J = 16.0
Bα	7.584	d	J = 16.0

**Notes:**

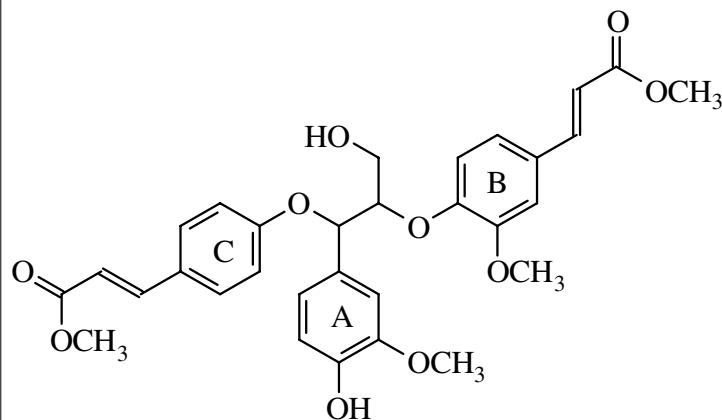
jrf137  
assignments not authenticated - from #3019/3020

check A4 vs A3 OMe!

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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**

**<sup>13</sup>C**



*erythro*

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

**<sup>1</sup>H (acetone)**

Atom	H Shifts	Mult	J
B <sub>γ</sub> OMe	3.696	s	
C <sub>γ</sub> 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	J = 5.3
Cβ	6.330	d	J = 16.0
Bβ	6.417	d	J = 16.0
A5	6.798	d	J = 8.2
C2,6	6.978	m	J = 8.8
A6	7.013	dd	J = 8.2, 1.9
B5	7.065	d	J = 8.3
B6	7.123	dd	J = 8.3, 1.9
A2	7.205	d	J = 1.9
B2	7.283	d	J = 1.9
C3,5	7.493	d	J = 8.8
C α	7.554	d	J = 16.0
B α	7.584	d	J = 16.0

**Notes:**

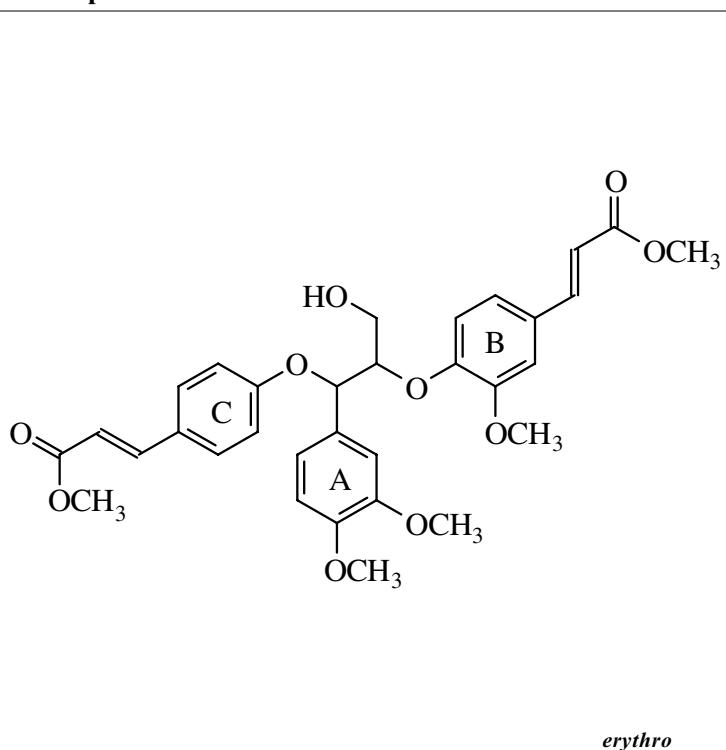
jrf103.C12-25

fully authenticated in acetone

Atom	<b>CDCl<sub>3</sub></b>		<b>Acetone</b>		<b>DMSO</b>	
	CS	i	CS	i	CS	i
B <sub>γ</sub> OMe	51.55	57	51.52	59	51.27	89
C <sub>γ</sub> 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
Cβ	115.62	47	116.16	52	115.16	44
Bβ	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**

<sup>13</sup>C



**3-(4-{1-(3,4-dimethoxyphenyl)-3-hydroxy-2-[2-methoxy-4-(2-methoxycarbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\gamma$ OMe	3.693	s	
C $\gamma$ OMe	3.715	s	
A3 OMe	3.741	s	
A4 OMe	3.773	s	
B3 OMe	3.865	s	
$\gamma^*$	*	*	-
$\beta$	4.787	m	-
$\alpha$	5.640	d	J = 5.3
C $\beta$	6.337	d	J = 16.0
B $\beta$	6.416	d	J = 16.0
A5	6.871	d	J = 8.3
C2,6	6.981	m	J = 8.8
A6	7.067	dd	J = 8.3, 1.9
B5	7.068	d	J = 8.3
B6	7.134	dd	J = 8.3, 1.9
A2	7.200	d	J = 1.9
B2	7.302	d	J = 1.9
C3,5	7.517	d	J = 8.8
C $\alpha$	7.537	d	J = 16.0
B $\alpha$	7.573	d	J = 16.0

**Notes:**

jrf121.C5-7

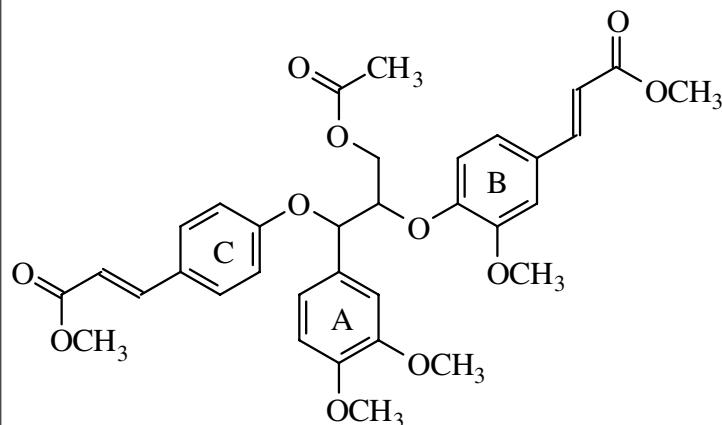
assignments not authenticated - from #3022 and 3020  
check A4 vs A3 OMe!

\* $\gamma$  and  $\gamma$ -OH protons buried, C-H correlations not run.

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\gamma$ OMe			51.52	53		
C $\gamma$ OMe			51.55	45		
A4 OMe			55.98	50		
A3 OMe			56.07	50		
B3 OMe			56.37	50		
$\gamma$			61.29	23		
$\alpha$			79.37	37		
$\beta$			84.19	32		
B2			112.19	42		
B5			112.24	40		
A2			112.70	37		
C $\beta$			116.27	42		
B $\beta$			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 $\alpha$			144.91	42		
B $\alpha$			145.25	40		
A4			150.20	26		
A3			150.23	27		
B4			151.31	24		
B3			151.65	27		
C4			160.63	27		
C $\gamma$			167.68	27		
B $\gamma$			167.71	26		

Compound Number 3024

<sup>13</sup>C



3-(4-{3-carboxyoxy-1-(3,4-dimethoxyphenyl)-2-[2-methoxy-4-(2-methoxycarbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
γAc Me	1.920	s	
B γOMe	3.695	s	
C γOMe	3.716	s	
A3 OMe	3.745	s	
A4 OMe	3.775	s	
B3 OMe	3.877	s	
γ1	4.428	dd	J = 11.9, 3.8
γ2	4.487	dd	J = 11.9, 6.2
β	4.988	m	J = 6.2, 5.3, 3.8
α	5.659	d	J = 5.3
C β	6.345	d	J = 16.0
B β	6.431	d	J = 16.0
A5	6.888	d	J = 8.3
C2,6	6.995	m	J = 8.8
B5	7.051	m	J = 8.3
A6	7.066	dd	J = 8.3, 2.0, 0.4
B6	7.143	dd	J = 8.3, 2.0, 0.4
A2	7.190	d	J = 2.0
B2	7.323	d	J = 2.0
C3,5	7.527	m	J = 8.8
C α	7.553	d	J = 16.0

Notes:

jrf139

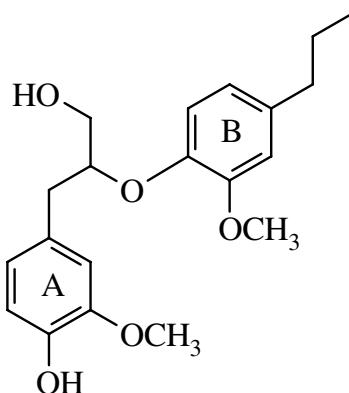
assignments not authenticated - from #3023 and 3021  
check A4 vs A3 OMe!

Note γ's, J's switch from #3021!!

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
g Ac Me			20.61	46		
B γOMe			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		
γOAc C=O			170.79	30		

Compound Number 3025

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\gamma$	13.77	80	14.01	79	13.75	86
B $\beta$	24.58	100	25.39	89	24.29	96
$\alpha$	37.37	61	37.74	66	36.52	61
B $\alpha$	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
$\gamma$	63.41	67	63.38	44	61.82	57
$\beta$	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

3-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxy-4-propylphenoxy)propan-1-ol

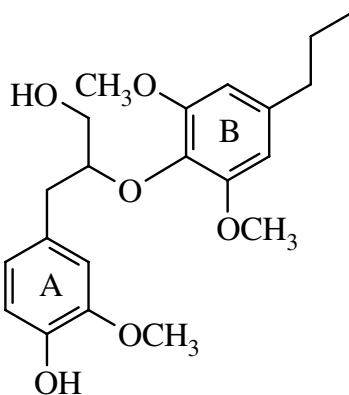
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\gamma$	0.895	t	
B $\beta$	1.585	m	
B $\alpha$	2.492	m	
$\alpha$ 1	2.91	m	
$\alpha$ 2	2.94	m	
$\gamma$	3.59	m	
$\gamma$ OH	3.731	t	J = 6.1
OMe	3.786	s	
OMe	3.802	s	
$\beta$	4.308	m	
B6	6.646	ddt	J = 8.1, 2.1, 0.6
A5	6.72	m	
A6	6.72	m	
B2	6.816	d	J = 2.1
B5	6.827	d	J = 8.1
A2	6.918	m	
Ar OH	7.333	s	

Notes:

jrba69

1H	<sup>CDCl<sub>3</sub></sup>	DMSO
B $\gamma$	0.915	0.856
B $\beta$	1.594	1.531
B $\alpha$	2.504	2.46
$\alpha$ 1	2.866	2.733
$\alpha$ 2	3.040	2.831
$\gamma$ 1	3.574	
$\gamma$ 2	3.656	
$\gamma$ OH		4.761
OMe	3.823	3.680
OMe	3.841	3.703
$\beta$	4.160	4.265
Ar-OH	5.611	8.70



Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
B $\gamma$	13.76	64	14.06	44	13.73	55
B $\beta$	24.51	86	25.30	47	24.10	57
$\alpha$	37.28	48	38.00	38	36.86	27
B $\alpha$	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
$\gamma$	62.17	45	62.77	28	61.65	29
$\beta$	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

2-(2,6-dimethoxy-4-propylphenoxy)-3-(4-hydroxy-3-methoxyphenyl)propan-1-ol

### <sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\gamma$	0.917	t	
B $\beta$	1.619	m	
B $\alpha$	2.523	dd	
$\alpha$ 1	2.941	dd	J = 13.6, 8.2
$\alpha$ 2	3.077	dd	J = 13.6, 5.4
$\gamma$ 1	3.392	m	J = 12.0, 4.1
$\gamma$ 2	3.483	m	J = 12.0, 3.4
$\gamma$ OH	3.5	m	
A OMe	3.809	s	
B OMe	3.817	s	
$\beta$	4.128	m	
B2,6	6.540	s	
A6	6.711	dd	J = 8.0, 1.8
A5	6.740	dd	J = 8.0, 0.4
A2	6.892	d	J = 1.8
Ar OH	7.349	s	

### Notes:

jrbha61

Proton Note: H<sub>y</sub>'s are perfect dd's after adding D<sub>2</sub>O to acetone - otherwise complex multiplets; J's are from D<sub>2</sub>O exchanged spectra.

All spectra ref'd to solvent

Acetone 2.04, 29.8

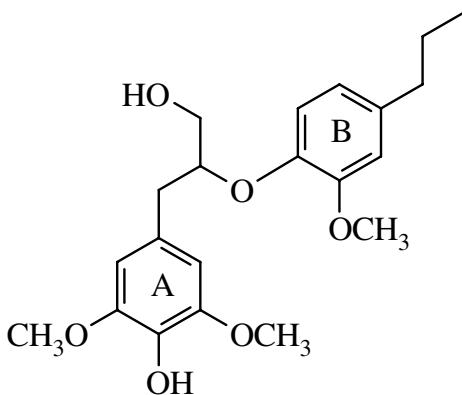
CDCl<sub>3</sub> 7.24, 77.0

DMSO 2.49, 39.5

<u>1</u> H	CDCl <sub>3</sub>	DMSO
B $\gamma$	0.928	0.886
B $\beta$	1.614	1.573
B $\alpha$	2.513	2.753
$\alpha$ 1	2.966	2.871
$\alpha$ 2	3.192	~3.35?
$\gamma$ 1	3.418	~3.35?
$\gamma$ 2	3.54	~3.35?
$\gamma$ OH	3.56	~3.35?
A OMe	3.805	3.697
B OMe	3.831	3.708
$\beta$	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

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\gamma$	13.77	63	14.01	45	13.67	66
B $\beta$	24.57	84	25.40	49	24.22	75
A $\alpha$	37.76	53	38.21	41	36.90	59
B $\alpha$	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
$\gamma$	63.47	53	63.46	22	61.84	28
$\beta$	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

3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxy-4-propylphenoxy)propan-1-ol

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\gamma$	0.894	t	
B $\beta$	1.585	m	
B $\alpha$	2.491	m	
$\alpha$ 1	2.85	dd	J = 13.9, 6.2
$\alpha$ 2	2.922	dd	J = 13.9, 6.1
$\gamma$	3.602	m	
$\gamma$ OH	3.734	t	
A OMe	3.770	s	
B OMe	3.806	s	
$\beta$	4.335	m	
A2,6	6.596	s	
B6	6.646	ddt	J = 8.2, 2.1, 0.6
B2	6.817	d	J = 2.1
B5	6.833	d	J = 8.2
Ar OH	6.940		

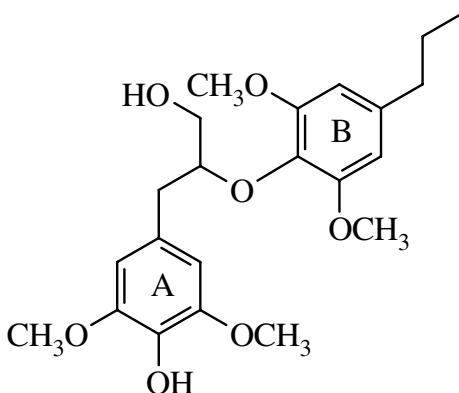
Notes:

jrbha67

<u>1H</u>	<u>CDCl<sub>3</sub></u>	<u>DMSO</u>
B $\gamma$	0.910	0.86
B $\beta$	1.589	1.54
B $\alpha$	2.499	2.45
$\alpha$ 1	2.856	2.74
$\alpha$ 2	3.032	2.84
$\gamma$ 1	3.578	
$\gamma$ 2	3.655	
$\gamma$ OH		4.75
A OMe	3.831	3.68
B OMe	3.841	3.71
$\beta$	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

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
B $\gamma$	13.70	37	14.06	100	13.82	49
B $\beta$	24.47	100	25.30	82	24.18	48
$\alpha$	37.65	39	38.38	45	37.35	25
B $\alpha$	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
$\gamma$	62.19	51	62.93	49	61.88	27
$\beta$	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

3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2,5-dimethoxy-4-propylphenoxy)propan-1-ol

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
B $\gamma$	0.917	t	
B $\beta$	1.620	m	
B $\alpha$	2.525	m	
$\alpha$ 1	2.925	dd	J = 13.6, 8.1
$\alpha$ 2	3.074	dd	J = 13.6, 5.3
$\gamma$ 1	3.402	m	J = 12.0, 4.1
$\gamma$ 2	3.486	m	J = 12.0, 3.6
$\gamma$ OH	3.47	m	
A OMe	3.793	s	
B OMe	3.825	s	
$\beta$	4.142	m	
B2,6	6.544	s	
A2,6	6.573	s	
Ar OH	6.949	s	

Notes:

jrbha63

Proton Note: H's are perfect dd's after adding D<sub>2</sub>O to acetone - otherwise complex multiplets; J's are from D<sub>2</sub>O exchanged spectra.

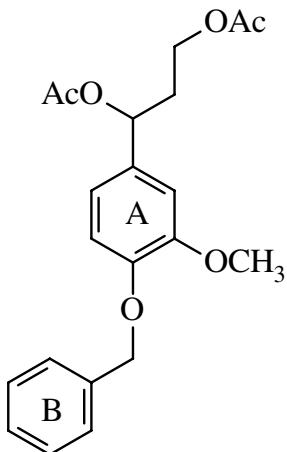
Carbon in acetone: Many peaks were split with a 2:1 ratio. The first thought that it was due to partial deuteration (acetone-d<sub>6</sub> contains some D<sub>2</sub>O) was disproved by fully D-exchanging: the splitting remained. It must be due to rotational isomers freezing out on the C<sub>13</sub> timescale but not on the 1H NMR timescale. The relevant peaks are:

A $\alpha$  38.38 45, A $\alpha$  38.50 21, B $\alpha$  38.80 45, B $\alpha$  38.93 20, A1 129.69 38

<u>1H</u>	<u>CDCl<sub>3</sub></u>	<u>DMSO</u>
B $\gamma$	0.917	0.879
B $\beta$	1.592	1.562
B $\alpha$	2.489	2.45
$\alpha$ 1	2.950	2.756
$\alpha$ 2	3.175	2.868
$\gamma$ 1	3.408	
$\gamma$ 2	3.542	
$\gamma$ OH	3.47	4.334?
A OMe	3.798	3.692
B OMe	3.829	3.696
$\beta$	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

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
$\gamma$ Ac Me			20.70			
$\alpha$ Ac Me			21.01			
$\beta$			35.78			
OMe			56.16			
$\gamma$			61.20			
B $\alpha$			71.26			
$\alpha$			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			
$\alpha$ Ac C=O			170.17			
$\gamma$ Ac C=O			170.80			

1-(4-benzyloxy-3-methoxyphenyl)-propane-1,3-diol

<sup>1</sup>H (acetone)

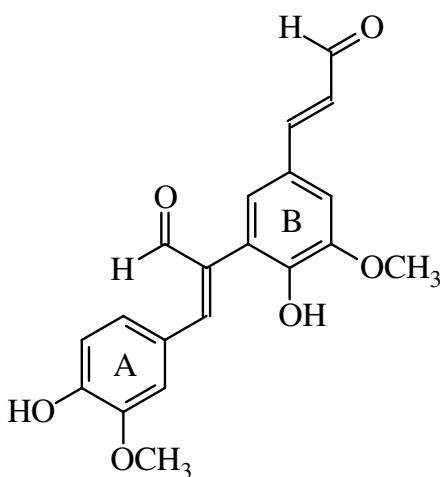
Atom	H Shifts	Mult	J
$\gamma$ Ac Me	1.99	s	
$\alpha$ Ac Me	2.03	s	
$\beta$	2.18	m	
OMe	3.83	s	
$\gamma$	4.08	m	
B $\alpha$	5.09	s	
$\alpha$	5.85	dd	
A6	6.91	dd	J = 8.2, 5.7
A5	6.99	d	J = 8.3
A2	7.04	d	J = 2.0
Bz H's	7.28-7.51	m	

Notes:

JRHKC25

Compound Number 3030

<sup>13</sup>C



beta-[5-(2-formylvinyl)-2-hydroxy-3-methoxyphenyl]  
coniferyl aldehyde

<sup>1</sup>H (acetone)

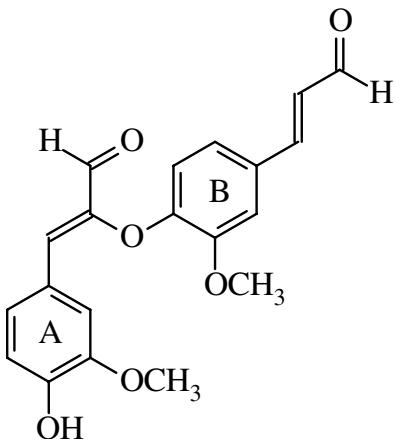
Atom	H Shifts	Mult	J
A3 OMe	3.47	s	
B3 OMe	3.96	s	
B $\beta$	6.66	dd	J = 15.8, 7.8
A5	6.77	d	J = 8.3
A2	6.87	d	J = 2.0
A6	6.98	dd	J = 8.3, 2.0
B6	7.01	d	J = 2.0
B2	7.44	d	J = 2.0
A $\alpha$	7.57	s	
B $\alpha$	7.57	d	J = 15.8
OH	8.43	s	
B $\gamma$	9.61	d	J = 7.8
A $\gamma$	9.69	s	

Notes:

JRHKB117 (Higuchi)  
13mg

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
A3 OMe			55.55			
B3 OMe			56.63			
B2			110.61			
A2			113.56			
A5			115.95			
A $\beta$			123.15			
B6			126.36			
A6			126.92			
B $\beta$			127.29			
A1			127.38			
B1			127.44			
B5			136.33			
A3			148.13			
B4			148.59			
A3			149.30			
B4			150.16			
A $\alpha$			151.36			
B $\alpha$			153.79			
A $\gamma$			193.43			
B $\gamma$			193.96			

Compound Number 3031

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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 $\beta$			128.32			
B1			130.20			
A $\alpha$			138.21			
A $\beta$			147.70			
B3			148.48			
B4			148.90			
A3			150.37			
A4			150.56			
B $\alpha$			153.15			
A $\gamma$			197.48			
B $\gamma$			193.85			

beta-[4-(2-formylvinyl)-2-methoxyphenoxy] coniferyl aldehyde

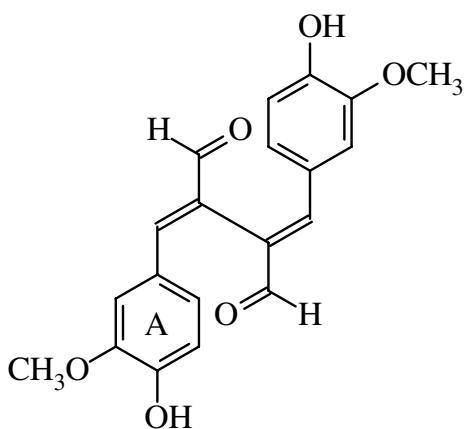
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J

## Notes:

JRHKB119 (Higuchi)  
4 mg

Compound Number 3032

<sup>13</sup>C

**2,3-diformyl-1,4-bis(4-hydroxy-3-methoxyphenyl)  
buta-1,3-diene**

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
OMe	3.70	s	
5	6.82	d	J = 8.31
6	7.21	dd	J = 8.31, 2.15
2	7.28	d	J = 2.15
$\alpha$	7.78	s	
OH	8.29	s	
$\gamma$	9.66	s	

**Notes:**

JRHKb121 11mg

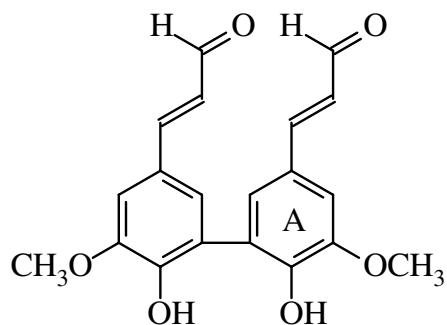
Higuchi

As this dimer contains a plane of symmetry the CSs are reported for one unit.

Atom	CDCl <sub>3</sub>		Acetone		DMSO	
	CS	i	CS	i	CS	i
OMe			56.11			
2			113.71			
5			116.24			
6			126.25			
1			127.47			
$\beta$			134.42			
3			148.41			
4			150.51			
$\alpha$			152.83			
$\gamma$			192.74			

Compound Number 3033

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
OMe			56.52			
2			110.00			
1			126.05			
4			126.13			
β			126.81			
6			127.10			
3			149.42			
5			149.63			
α			154.40			
γ			193.92			

5,5'-bis-coniferyl aldehyde

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
OMe	3.95	s	
β	6.68	dd	J = 15.84, 7.84
6	7.27	s	J = 2.0
2	7.36	s	J = 2.0
α	7.59	s	J = 15.84
γ	9.65	s	J = 7.84

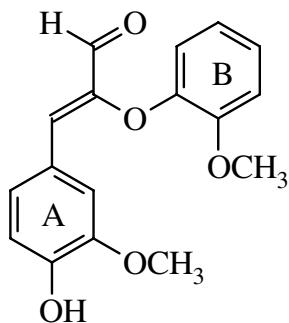
Notes:

JRHKb123 37mg

Higuchi

As this dimer contains a plane of symmetry the CSs are reported for one unit.

## Compound Number 3034

<sup>13</sup>C

Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			
$\alpha$			137.82			
B4			146.22			
$\beta$			148.09			
A3			148.30			
B3			149.89			
A4			150.20			
$\gamma$			187.90			

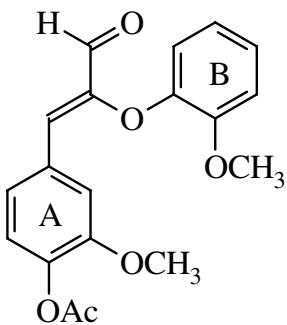
<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
A4 OMe	3.73	s	
B3 OMe	3.88	s	
B5	6.72	dd	
B6	6.76	ddd	J = 8.0, 2.0
A5	6.87	d	J = 8.2, 7.1, 2.0
B1	6.95	ddd	J = 8.3
B2	7.05	dd	J = 8.2, 7.1, 2.0
$\alpha$	7.26	s	
A6	7.33	dd	J = 8.2, 2.0
A2	7.59	d	J = 2.0
$\gamma$	9.50	s	

## Notes:

HKc63.4

## Compound Number 3035

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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			
$\alpha$			135.40			
A4			142.47			
B4			146.01			
$\beta$			149.94			
B3			150.01			
A3			152.27			
Ac C=O			168.73			
$\gamma$			188.21			

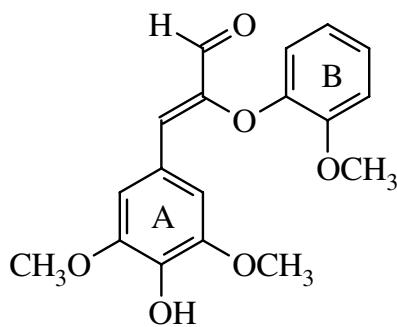
<sup>1</sup>H (acetone)

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	
A5	7.11	d	J = 7.8 J = 8.3
$\alpha$	7.30	s	
A6	7.45	dd	
A2	7.68	d	J = 8.3, 2.0 J = 2.0
$\gamma$	9.55	s	

## Notes:

HKc 63.4Ac

Compound Number 3036

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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			
$\alpha$			138.23			
A4			139.74			
B4			146.16			
$\beta$			148.15			
A3			148.57			
A5			148.57			
B3			149.76			
$\gamma$			187.91			

<sup>1</sup>H (acetone)

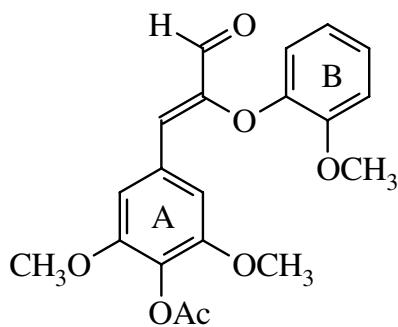
Atom	H Shifts	Mult	J
A3,5 OMe	3.74	s	
B3 OMe	3.88	s	
B5	6.70	dd	J = 8.2, 1.7
B6	6.76	ddd	
B1	6.94	ddd	J = 8.2, 7.2, 1.5
B2	7.05	dd	J = 8.2, 7.2, 1.7
A2,6	7.24	s	J = 8.2, 1.5
$\alpha$	7.26	s	
$\gamma$	9.51	s	

## Notes:

HKd 59.1

Compound Number 3037

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			

<sup>1</sup>H (acetone)

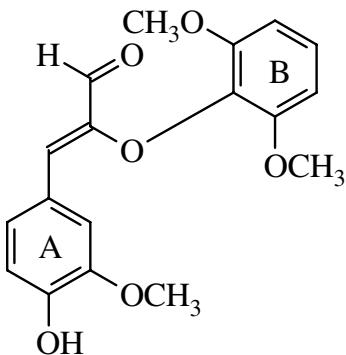
Atom	H Shifts	Mult	J
Ac Me	2.21	s	
A3,5 OMe	3.73	s	
B3 OMe	3.88	s	
B5	6.76	dd	
B6	6.77	ddd	
B1	6.97	ddd	J = 8.2, 6.5, 1.4
B2	7.06	dd	J = 8.2, 6.5, 2.4
A2,6	7.29	s	J = 8.2, 1.4
α	7.31	s	
γ	9.57	s	

Notes:

HKd 59.1 Ac

Compound Number 3038

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			
$\alpha$			129.06			
B4			135.22			
A3			148.04			
A4			149.05			
$\beta$			150.82			
B3			152.47			
B5			152.47			
$\gamma$			186.64			

<sup>1</sup>H (acetone)

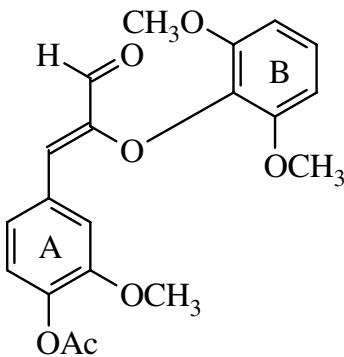
Atom	H Shifts	Mult	J
B3,5 OMe	3.74	s	
A3 OMe	3.81	s	
$\alpha$	6.64	s	
B2,6	6.65	d	J = 8.2
A5	6.88	d	J = 8.3
B1	6.99	dd	J = 8.2, 7.6
A6	7.45	dd	J = 8.3, 2.0
A2	7.60	d	J = 2.0
$\gamma$	9.25	s	

Notes:

HKd 23.3

**Compound Number 3039**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			
$\alpha$			126.73			
A1			133.43			
B4			134.81			
A4			141.52			
A3			152.04			
$\beta$			152.11			
B3			152.41			
B5			152.41			
Ac C=O			168.85			
$\gamma$			187.00			

<sup>1</sup>H (acetone)

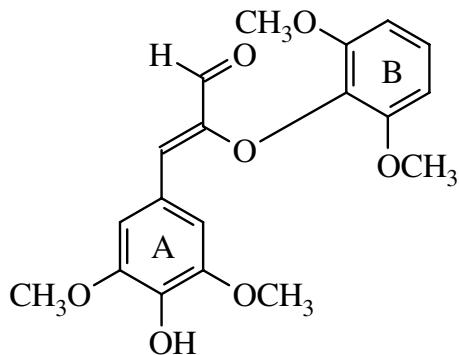
Atom	H Shifts	Mult	J
Ac Me	2.24	s	
B3,5 OMe	3.75	s	
A3 OMe	3.80	s	
B2,6	6.67	d	J = 8.3
$\alpha$	6.71	s	
B1	7.01	dd	J = 8.3, 7.9
A5	7.11	d	J = 8.2
A6	7.54	dd	J = 8.2, 1.9
A2	7.68	d	J = 1.9
$\gamma$	9.32	s	

**Notes:**

HKd 23.3 Ac

Compound Number 3040

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			
$\alpha$			129.08			
B4			135.21			
A4			138.72			
A3			148.44			
A5			148.44			
$\beta$			150.91			
B3			152.46			
B5			152.46			
$\gamma$			186.60			

<sup>1</sup>H (acetone)

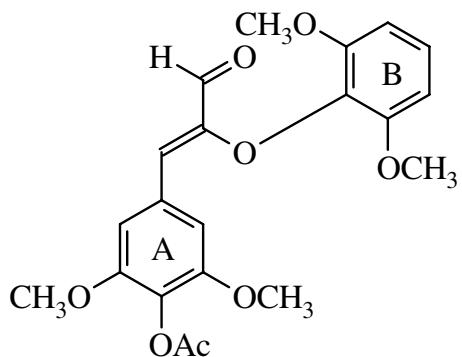
Atom	H Shifts	Mult	J
B3,5 OMe	3.75	s	
A3,5 OMe	3.80	s	
$\alpha$	6.63	s	J = 8.3
B2,6	6.66	d	
B1	6.99	t	
A2,6	7.31	s	
$\gamma$	9.25	s	

Notes:

HKd 63.1

**Compound Number 3041**

**<sup>13</sup>C**



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			

**<sup>1</sup>H (acetone)**

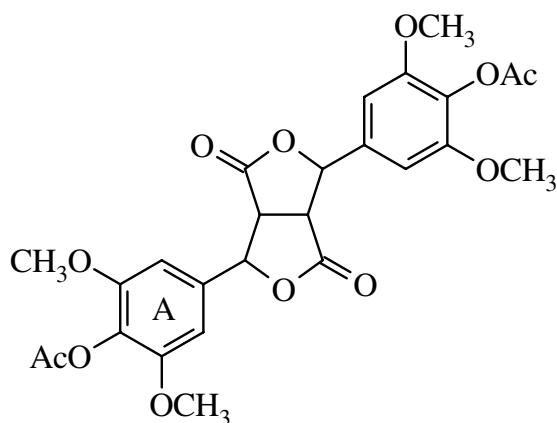
Atom	H Shifts	Mult	J
Ac Me	2.23	s	
A3,5 OMe	3.77	s	
B3,5 OMe	3.78	s	
B2,6	6.67	d	J = 8.3
α	6.69	s	
B1	7.01	dd	J = 8.6, 8.2
A2,6	7.34	s	
γ	9.32	s	

**Notes:**

HKd 63.1 Ac

Compound Number 3042

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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			

<sup>1</sup>H (acetone)

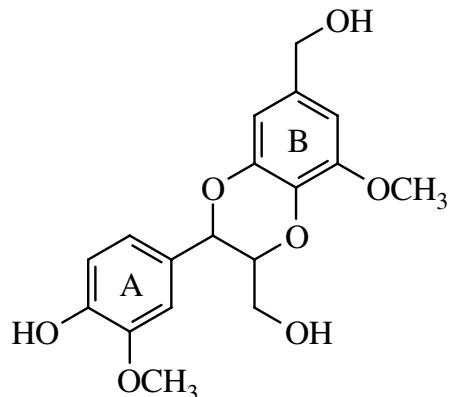
Atom	H Shifts	Mult	J
Ac Me	2.23	s	
OMe	3.81	s	
β	4.20	s	
α	5.86	s	
2,6	6.81	s	

Notes:

FLj 144

As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 3043

<sup>13</sup>C

Atom	CDCl <sub>3</sub>		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		

<sup>1</sup>H (acetone)

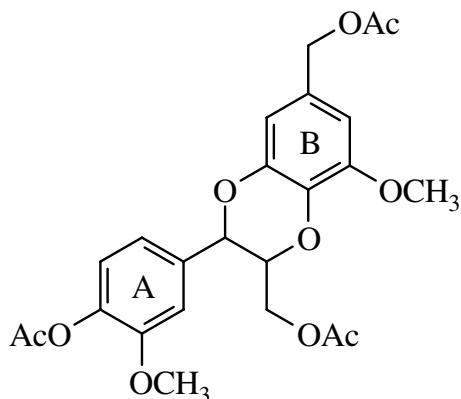
Atom	H Shifts	Mult	J
γ1	3.47	m	
γ2	3.76	m	
B3 OMe	3.81	s	
A3 OMe	3.85	s	
β	3.99	ddd	
Bα	4.49	m	J = 7.9, 3.9, 2.5
α	4.95	d	J = 7.9
B6	6.53	ddd	
B2	6.60	d	J = 1.8
A5	6.86	d	J = 8.1
A6	6.94	ddd	J = 8.1, 1.9, 0.5
A2	7.09	d	J = 1.9
A4 OH	7.80	s	

## Notes:

F. Lu  
flm11

Compound Number 3044

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	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		

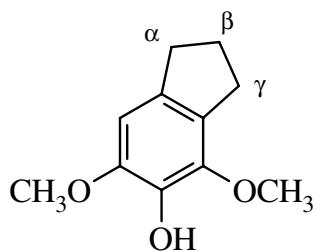
<sup>1</sup>H (acetone)

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	J = 12.4, 4.3
γ2	4.28	dd	J = 12.4, 3.4
β	4.40	ddd	J = 7.7, 4.3, 3.4
Bα	4.98	s	
α	5.04	d	J = 7.7
B6	6.61	d	J = 1.9
B2	6.66	d	J = 1.9
A6	7.08	dd	J = 8.1, 1.7
A5	7.11	d	J = 8.1
A2	7.26	d	J = 1.7

Notes:

F. Lu  
flm11Ac

## Compound Number 3045

<sup>13</sup>C

Atom	<sup>13</sup> CDCl <sub>3</sub>		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			

<sup>1</sup>H (acetone)

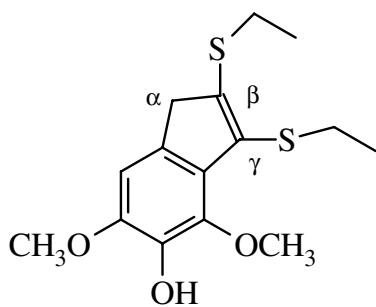
Atom	H Shifts	Mult	J
β	1.98	quint	J = 7.2
α	2.78	br t	J = 7.2
γ	2.83	br t	J = 7.2
5 OMe	3.77	s	
3 OMe	3.79	s	
6	6.58	s	
<u>Benzene</u>			
β	1.86	quin	J = 7.37
α	2.71	td	J = 7.37, 0.66
γ	2.86	t	J = 7.37
5 OMe	3.28	s	
3 OMe	3.75	s	
6	6.32	s	

## Notes:

HKE-11  
Raney nickel reaction of hke5.5

**Compound Number 3046**

**$^{13}\text{C}$**



Atom	$\text{CDCl}_3$		Acetone		DMSO	
	CS	i	CS	i	CS	i
$\gamma$ S-CH <sub>3</sub>			15.11			
$\beta$ S-CH <sub>3</sub>			15.41			
$\beta$ S-CH <sub>2</sub>			26.33			
$\gamma$ S-CH <sub>2</sub>			29.12			
$\alpha$			41.68			
5 OMe			56.91			
3 OMe			62.30			
6			105.00			
$\gamma$			126.93			
2			131.50			
1			133.78			
3			104.04			
4			141.58			
5			147.06			
$\beta$			148.43			

**$^1\text{H}$  (acetone)**

Atom	H Shifts	Mult	J
$\gamma$ S-CH <sub>3</sub>	1.15	t	
$\beta$ S-CH <sub>3</sub>	1.30	t	J = 7.37
$\gamma$ S-CH <sub>2</sub>	2.89	q	J = 7.37
$\beta$ S-CH <sub>2</sub>	2.95	q	J = 7.37
$\alpha$	3.58	d	J = 0.92
5 OMe	3.82	s	
3 OMe	3.85	s	
6	6.87	br t	J = 0.92

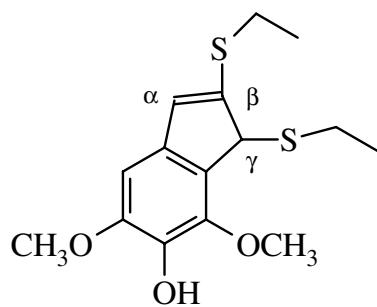
**Notes:**

hke 5.4.1

Thioacidolysis product of  $\beta$ -O-4 (S-G) aldehyde dimer

**Compound Number 3047**

<sup>13</sup>C



Atom	<sup>CDCl<sub>3</sub></sup>		<sup>Acetone</sup>		<sup>DMSO</sup>	
	CS	i	CS	i	CS	i
γ S-CH <sub>3</sub>			14.39			
β S-CH <sub>3</sub>			14.45			
γ S-CH <sub>2</sub>			22.23			
β S-CH <sub>2</sub>			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			

<sup>1</sup>H (acetone)

Atom	H Shifts	Mult	J
γ S-CH <sub>3</sub>	1.00	t	J = 7.5
β S-CH <sub>3</sub>	1.33	t	J = 7.37
γ S-CH <sub>2</sub>	2.22,2.04	dq, dq	J = 12.1, 7.5
β S-CH <sub>2</sub>	2.94	q	J = 7.37
5 OMe	3.82	s	
3 OMe	3.96	s	
γ	4.39	d	J = 1.18
α	6.38	d	J = 1.18
6	6.63	s	

**Notes:**

hke 5.5

Thioacidolysis product of γ-O-4 (S-G) aldehyde dimer