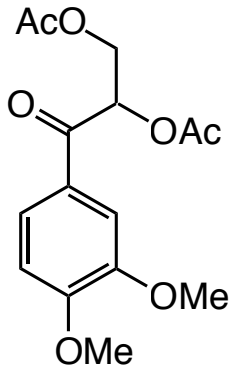
Compound Number 1



2,3-Diacetoxypropioveratrone
2,3-diacetoxy-3',4'-dimethoxypropiophenone
Hibbert's Ketone

^{1}H (chloroform)

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

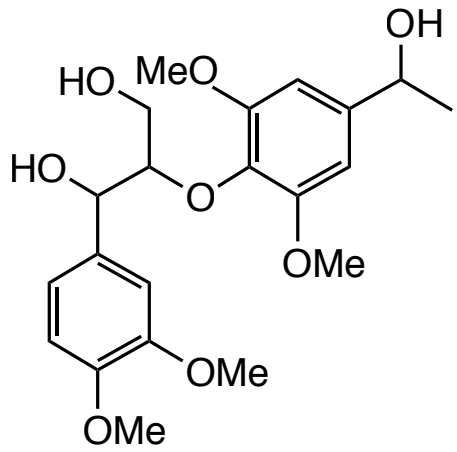
Notes:

M. Mozuch #36/46/Ac
21 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.67	20.49	20.30	
Ac Me	20.72	20.58	20.42	
OMe	56.05	56.11	55.51	
OMe	56.15	56.25	55.77	
γ	63.22	63.64	62.60	
β	72.99	74.14	73.28	
2	110.32	111.60	110.35	
5	110.64	111.66	111.03	
6	123.33	123.85	123.02	
1	127.41	128.35	126.67	
3	149.31	150.31	148.72	
4	154.16	155.21	153.72	
Ac C=O	170.21	170.35	169.61	
Ac C=O	170.75	170.88	170.03	
α	191.52	192.03	191.18	

Compound Number 2



threo

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

^{1}H (chloroform)

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

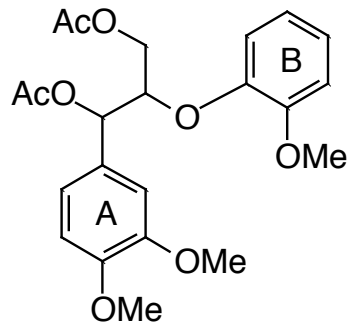
Notes:

S. Ralph III-12
60mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	25.45	26.23	25.86
OMe	55.87	55.97	55.31
OMe	55.87	56.03	55.43
B OMe	56.08	56.44	55.80
B OMe	56.08	56.44	55.80
γ	60.48	61.26	60.13
B α	70.11	69.93	68.17
α	73.98	73.89	71.36
β	88.94	89.58	87.10
B2	102.25	103.30	102.50
B6	102.25	103.30	102.50
A2	110.28	111.78	110.60
A5	111.02	112.18	111.08
A6	119.80	120.22	118.84
A1	132.56	134.74	134.53
B1	134.08	135.39	134.53
B4	143.04	144.54	143.01
A4	148.73	149.58	147.64
A3	148.90	149.86	148.03
B3	152.84	153.52	152.20
B5	152.84	153.52	152.20
1H			
B β			1.30
γ1			3.19
γ2			3.62
β			3.97
OMe			3.71
OMe			3.71
OMe			3.73
OMe			3.73
B α			4.64
α			4.89
B2,6			6.64
A2			7.03
A5			6.87
A6			6.93

Compound Number 3



erythro

Veratrylglycerol-β-guaiacyl ether diacetate

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

^{1}H (chloroform)

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

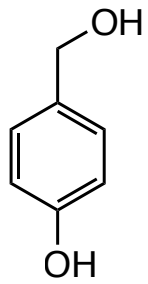
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.78	20.61	20.41
Ac Me	21.05	20.89	20.65
OMe	55.78	56.02	55.38
OMe	55.88	56.08	55.38
OMe	55.88	56.15	55.54
γ	62.82	63.23	62.10
α	74.12	74.77	73.35
β	80.10	80.28	78.39
A2	110.86	112.24	110.87
A5	110.89	112.24	111.27
B2	112.55	113.68	112.80
B5	119.18	119.51	117.70
A6	120.08	120.79	119.63
B6	120.93	121.56	120.62
B1	123.41	123.82	122.70
A1	128.98	130.15	128.71
B4	147.32	148.36	146.74
A4	148.84	150.10	148.43
A3	149.09	150.29	148.65
B3	151.04	151.93	150.27
Ac C=O	169.67	169.85	169.18
Ac C=O	170.75	170.71	170.00

Notes:

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

Compound Number 4



p-Hydroxybenzyl alcohol
4-hydroxybenzyl alcohol

^{1}H (chloroform)

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

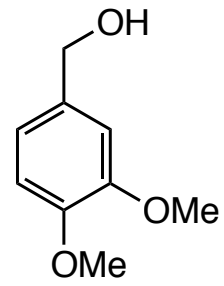
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α		64.54	62.68	
3		115.69	114.66	
5		115.69	114.66	
2		129.05	127.92	
6		129.05	127.92	
1		133.96	132.61	
4		157.23	156.03	

Compound Number 5



3,4-Dimethoxybenzyl alcohol

3,4-dimethoxybenzyl alcohol

^{1}H (chloroform)

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

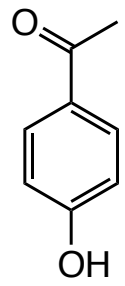
Notes:

J. Ralph: JR A91.14
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.78	55.93	55.27	
OMe	55.90	56.11	55.47	
α	65.04	64.58	62.79	
2	110.45	111.69	110.51	
5	111.04	112.54	111.48	
6	119.33	119.62	118.50	
1	133.66	135.95	135.03	
4	148.43	149.32	147.60	
3	149.00	150.19	148.54	

Compound Number 6



p-Hydroxyacetophenone
4-hydroxyacetophenone

^{1}H (chloroform)

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

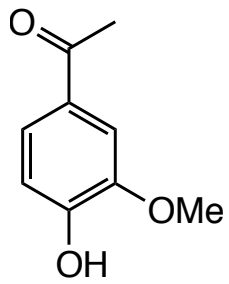
Notes:

J.Ralph: JR A95.11
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	26.28	26.25	26.16	
3	115.66	115.89	115.11	
5	115.66	115.89	115.11	
1	129.16	130.38	128.56	
2	131.35	131.48	130.64	
6	131.35	131.48	130.64	
4	161.90	162.54	161.98	
α	199.32	196.40	195.89	

Compound Number 7



Acetovanillone

4-hydroxy-3-methoxyacetophenone

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	2.49	s	
OMe	3.90	s	
2	6.90	d	2.0
5	7.52	d	8.2
6	7.56	dd	2.0, 8.2

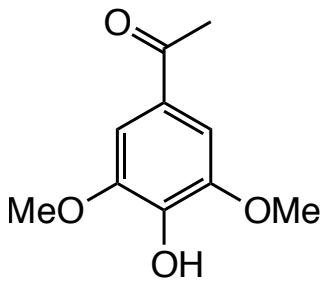
Notes:

J. Ralph: JR A95.12
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	26.16	26.22	26.14	
OMe	56.01	56.17	55.52	
2	109.89	111.40	111.04	
5	113.97	115.26	114.85	
6	124.06	124.22	123.34	
1	130.02	130.65	128.84	
3	146.77	148.16	147.45	
4	150.66	152.12	151.65	
α	197.14	196.30	195.98	
1H				
β	2.56		2.48	
OMe	3.91		3.81	
5	6.95		6.85	
2	7.53		7.42	
6	7.53		7.49	

Compound Number 8



Acetosyringone

3,5-dimethoxy-4-hydroxyacetophenone

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	2.57	s	
3,5 OMe	3.94	s	
2,6	7.24	s	
Acetone			
β	2.51	s	
3,5 OMe	3.88	s	
2,6	7.30	s	
DMSO			
β	2.51	s	
3,5 OMe	3.82	s	
2,6	7.22	s	

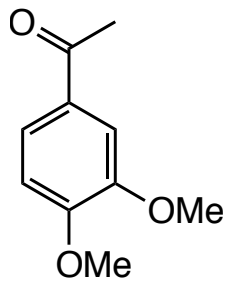
Notes:

Aldrich
CAS# 2478-38-8

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	26.21	26.30	26.22	
OMe OMe	56.45 56.45	56.63 56.63	56.02 56.02	
2 6	105.81 105.81	106.97 106.97	106.13 106.13	
1	128.21	129.13	127.33	
4	139.89	141.75	140.86	
3 5	146.79 146.79	148.29 148.29	147.44 147.44	
α	196.64	196.31	196.06	

Compound Number 9



Acetoveratrone

3,4-dimethoxyacetophenone

^{1}H (chloroform)

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

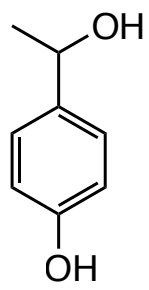
Notes:

J. Ralph: JR A95.14
55mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
β	26.17	26.25	26.23
OMe	55.95	55.96	55.43
OMe	56.04	56.10	55.68
2	109.99	111.17	110.17
5	110.09	111.30	110.74
6	123.27	123.73	123.04
1	130.48	131.24	129.88
3	148.99	150.00	148.55
4	153.30	154.38	153.06
α	196.70	196.34	196.22
1H			
β		2.51	2.51
OMe		3.85	3.80
OMe		3.88	3.83
5		2.03	7.05
2		7.50	7.42
6		7.62	7.61

Compound Number 10



1-(4-Hydroxyphenyl)ethanol

1-(4-hydroxyphenyl)ethanol

^{1}H (chloroform)

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

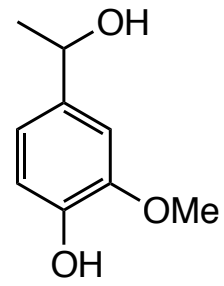
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β		26.10	25.83	
α		69.61	67.70	
3	115.28	115.55	114.54	
5	115.28	115.55	114.54	
2	126.91	127.31	126.31	
6	126.91	127.31	126.31	
1		138.90	137.56	
4		156.98	155.86	

Compound Number 11



Apocynol

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

^{1}H (chloroform)

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

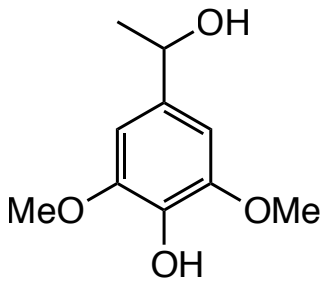
Notes:

J. Ralph: JR A97.12

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	25.07	26.22	25.88	
OMe	55.88	56.09	55.42	
α	70.30	69.81	67.89	
2	108.05	109.76	109.54	
5	114.20	115.21	114.80	
6	118.31	118.65	117.47	
1	137.91	139.67	138.35	
4	144.96	146.13	144.98	
3	146.62	147.97	147.11	

Compound Number 12



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

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

^{1}H (chloroform)

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

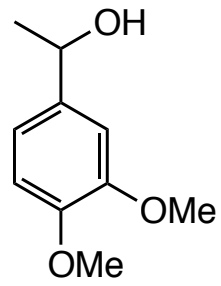
Notes:

J. Ralph: JR A97.13

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	25.22	26.28	25.94	
OMe	56.25	56.49	55.79	
OMe	56.25	56.49	55.79	
α	70.50	70.07	68.16	
2	102.15	103.61	102.65	
6	102.15	103.61	102.65	
1	133.90	135.46	133.93	
4	137.22	138.70	137.53	
3	147.01	148.36	147.56	
5	147.01	148.36	147.56	

Compound Number 13



1-(3,4-Dimethoxyphenyl)ethanol

1-(3,4-dimethoxyphenyl)ethanol

^{1}H (chloroform)

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

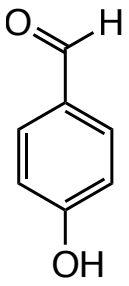
Notes:

J. Ralph: JR A97.14

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	25.12	26.25	25.92	
OMe	55.80	55.99	55.29	
OMe	55.91	56.15	55.48	
α	70.08	69.72	67.82	
2	108.68	110.38	109.24	
5	110.98	112.56	111.43	
6	117.50	118.18	117.10	
1	138.65	140.97	139.99	
4	148.26	149.17	147.40	
3	148.99	150.14	148.43	

Compound Number 14



p-Hydroxybenzaldehyde
4-hydroxybenzaldehyde

^{1}H (chloroform)

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

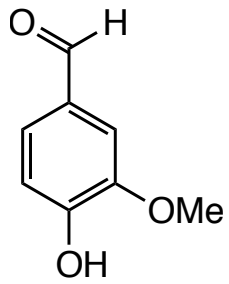
Notes:

J. Ralph: JR A87.11
52mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3	116.01	116.62	115.80	
5	116.01	116.62	115.80	
1	129.81	130.34	128.40	
2	132.54	132.77	132.04	
6	132.54	132.77	132.04	
4	161.65	163.80	163.28	
α	191.28	191.02	190.80	

Compound Number 15



Vanillin

4-hydroxy-3-methoxybenzaldehyde

^{1}H (chloroform)

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

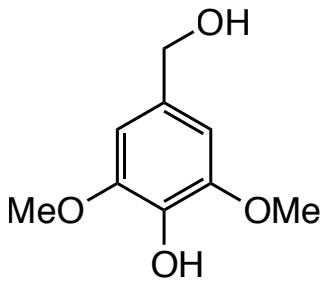
Notes:

J. Ralph: JR A87.12
66mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.07	56.24	55.52	
2	109.02	110.82	110.63	
5	114.59	115.87	115.36	
6	127.57	126.98	126.04	
1	129.70	130.62	128.70	
3	147.34	148.86	148.12	
4	151.99	153.45	153.00	
α	191.16	191.07	190.89	
1H				
OMe			3.83	
2			7.37	
5			6.95	
6			7.40	
α			9.76	

Compound Number 16



Syringyl alcohol

4-hydroxy-3,5-dimethoxybenzyl alcohol

^{1}H (chloroform)

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

Notes:

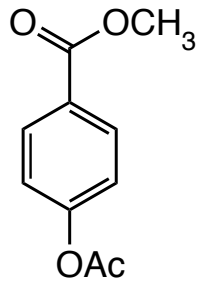
J. Ralph: JR A91.13

20mg Almost insoluble in acetone.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.29	56.54	55.77	
OMe	56.29	56.54	55.77	
α	65.68	64.98	63.09	
2	103.88	105.08	103.91	
6	103.88	105.08	103.91	
1	132.06	133.80	132.48	
4	134.19	135.75	134.03	
3	147.10	148.54	147.67	
5	147.10	148.54	147.67	

Compound Number 17



Methyl 4-acetoxybenzoate

4-acetoxybenzoic acid methyl ester

^{1}H (chloroform)

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

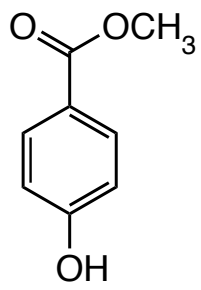
Notes:

L. Landucci
53mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.12	20.97	20.82	
OMe	52.16	52.37	52.13	
3	121.60	122.82	122.21	
5	121.60	122.82	122.21	
1	127.70	128.46	127.08	
2	131.14	131.60	130.70	
6	131.14	131.60	130.70	
4	154.30	155.56	154.20	
α	166.25	166.47	165.49	
Ac C=0	168.79	169.23	168.72	

Compound Number 18



Methyl 4-hydroxybenzoate

4-hydroxybenzoic acid methyl ester

^{1}H (chloroform)

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

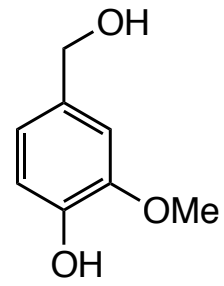
Notes:

Aldrich
62mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	52.12	51.86	51.55	
3	115.31	116.00	115.31	
5	115.31	116.00	115.31	
1	122.22	122.33	120.29	
2	131.97	132.37	131.40	
6	131.97	132.37	131.40	
4	160.36	162.58	161.97	
α	167.53	167.07	166.05	

Compound Number 19



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

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.87	s	
α	4.57	s	
α OH	5.65	s	
6	6.81	dd	1.6, 8.0
5	6.85	d	8.0
2	6.89	d	1.6

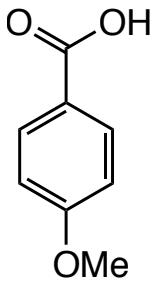
Notes:

Aldrich

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.90	56.11	55.38	
α	65.44	64.76	62.93	
2	109.94	111.37	110.91	
5	114.27	115.37	114.93	
6	120.22	120.29	119.00	
1	132.93	134.62	133.37	
4	145.26	146.37	145.17	
3	146.65	148.10	147.24	
1H				
OMe		3.82	3.74	
α		4.50	4.35	
α OH		3.95	4.96	
5		6.75	6.68	
6		6.77	6.68	
2		6.95	6.86	
PhOH		7.83	8.74	

Compound Number 20



p-Anisic acid
4-methoxybenzoic acid

^{1}H (chloroform)

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

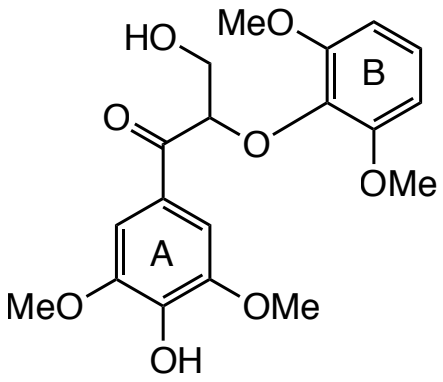
Notes:

Aldrich
52mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.48	55.86	55.36	
3	113.75	114.50	113.74	
5	113.75	114.50	113.74	
1	121.67	123.67	122.97	
2	132.35	132.48	131.32	
6	132.35	132.48	131.32	
4	164.04	164.39	162.80	
α	171.45	167.54	167.00	

Compound Number 21



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

^{1}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

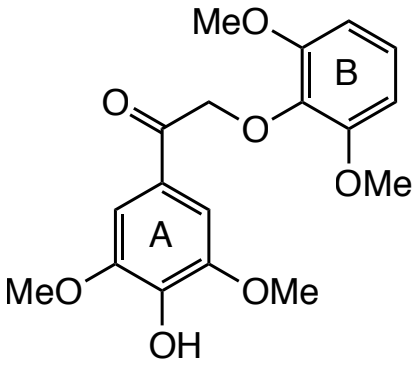
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.97	56.35	55.73
OMe	55.97	56.35	55.73
OMe	56.49	56.71	55.97
OMe	56.49	56.71	55.97
γ	63.48	63.66	61.95
β	87.16	86.21	82.80
B2	105.27	106.32	105.46
B6	105.27	106.32	105.46
A2	106.35	107.69	106.56
A6	106.35	107.69	106.56
B1	124.34	124.78	123.51
A1	126.98	127.86	126.22
B4	136.46	137.37	135.80
A4	140.05	141.99	140.92
A3	146.79	148.31	147.30
A5	146.79	148.31	147.30
B3	152.73	153.86	152.43
B5	152.73	153.86	152.43
α	194.84	195.15	194.71

Compound Number 22



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

^{1}H (chloroform)

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

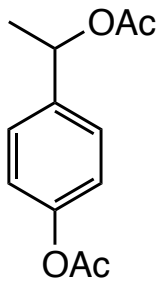
Notes:

J. Ralph JRA127.P2
23mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B OMe	56.09	56.42	55.82
B OMe	56.09	56.42	55.82
A OMe	56.48	56.72	56.03
A OMe	56.48	56.72	56.03
β	75.45	75.90	74.39
B2	105.33	106.47	105.52
B6	105.33	106.47	105.52
A2	106.07	107.45	105.97
A6	106.07	107.45	105.97
B1	124.20	124.87	123.84
A1	126.68	127.09	124.92
B4	136.48	137.55	135.85
A4	139.89	142.15	141.14
A3	146.74	148.39	147.50
A5	146.74	148.39	147.50
B3	153.30	154.43	152.85
B5	153.30	154.43	152.85
α	193.61	193.69	192.75

Compound Number 23



Hydroxyphenylethanol diacetate

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

^{1}H (acetone)

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

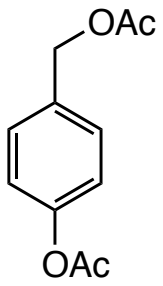
Notes:

J. Ralph JRA93.5
22mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.10	20.91	20.74	
Ac Me	21.30	21.08	20.89	
β	22.14	22.48	21.95	
α	71.68	72.03	71.01	
3	121.57	122.53	121.70	
5	121.57	122.53	121.70	
2	127.31	127.84	126.99	
6	127.31	127.84	126.99	
1	139.18	140.39	139.13	
4	150.16	151.29	149.79	
A4 Ac C=O	169.41	169.58	169.11	
α Ac C=O	170.21	170.16	169.54	

Compound Number 24



p-Hydroxybenzyl alcohol diacetate

4-acetoxybenzyl acetate

^{1}H (chloroform)

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

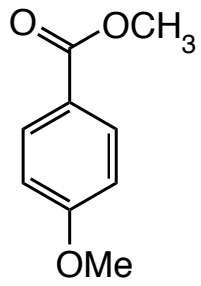
Notes:

S. Ralph SRIII-20
52mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.95	20.76	20.62	
Ac Me	21.08	20.92	20.75	
α	65.58	65.80	64.83	
3	121.70	122.59	121.78	
5	121.70	122.59	121.78	
2	129.50	130.02	129.25	
6	129.50	130.02	129.25	
1	133.56	134.84	133.67	
4	150.53	151.60	150.15	
A4 Ac C=O	169.31	169.53	169.08	
α Ac C=O	170.72	170.77	170.14	

Compound Number 25



Methyl-p-anisate
methyl 4-methoxybenzoate

^{1}H (chloroform)

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

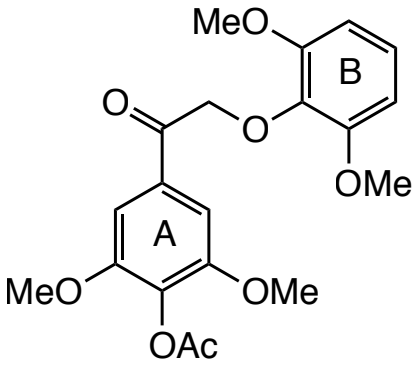
Notes:

S. Ralph SRIII-21
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
4 OMe	51.82	51.94	51.73	
α OMe	55.39	55.83	55.45	
3	113.59	114.51	113.95	
5	113.59	114.51	113.95	
1	122.60	123.36	121.88	
2	131.57	132.12	131.20	
6	131.57	132.12	131.20	
4	163.33	164.35	163.12	
α	166.82	166.84	165.88	

Compound Number 26



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

^{1}H (chloroform)

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

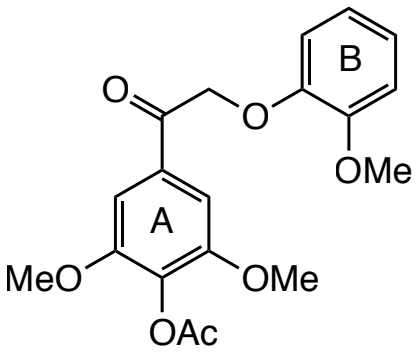
Notes:

J. Ralph GV 49.1
25mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.42	20.23	20.02
B OMe	56.08	56.44	55.82
B OMe	56.08	56.44	55.82
A OMe	56.37	56.71	56.18
A OMe	56.37	56.71	56.18
β	75.54	75.99	74.59
B2	105.35	106.34	104.87
B6	105.35	106.34	104.87
A2	105.54	106.50	105.53
A6	105.54	106.50	105.53
B1	124.26	124.95	123.88
A1	133.12	133.94	132.10
A4	133.12	134.21	132.64
B4	136.45	137.50	135.81
A3	152.26	153.30	151.80
A5	152.26	153.30	151.80
B3	153.27	154.36	152.74
B5	153.27	154.36	152.74
Ac C=0	168.11	168.15	167.60
α	194.03	194.58	193.75

Compound Number 27



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

^{1}H (chloroform)

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

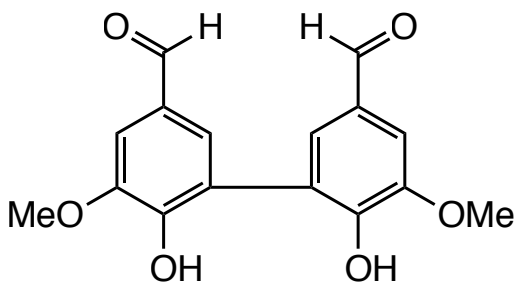
Notes:

J. Ralph GV 35.1
25mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.41	20.23	20.03	
B OMe	55.85	56.25	55.51	
A OMe	56.34	56.73	56.24	
A OMe	56.34	56.73	56.24	
β	72.53	72.65	70.85	
A2	105.25	105.90	104.78	
A6	105.25	105.90	104.78	
B2	112.26	113.68	112.48	
B5	114.95	115.73	113.80	
B6	120.89	121.56	120.45	
B1	122.64	122.80	121.37	
A1	133.41	134.14	132.32	
A4	132.58	133.81	132.38	
B3	147.37	148.96	147.33	
B4	149.79	150.90	148.96	
A3	152.41	153.45	151.90	
A5	152.41	153.45	151.90	
Ac C=0	168.06	168.14	167.59	
α	193.77	194.35	193.70	

Compound Number 28



Dehydrodivanillin

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

^{1}H (DMSO)

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

Notes:

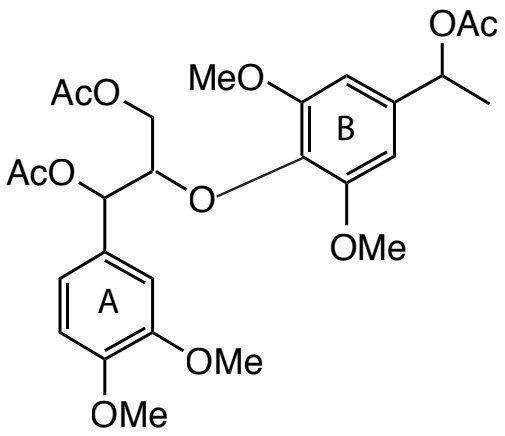
J. Ralph KM 77.1

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe			55.94	
2			109.08	
6			124.54	
5			127.61	
1			128.05	
4			148.12	
3			152.93	
α			190.97	

Compound Number 29



threo

Veratrylglycerol-β-syringol ether triacetate
1,3-diacetoxy-1-(3,4-dimethoxyphenyl)-2-(4-(1-acetoxyethyl)-2,6-dimethoxyphenoxy)propane

^{1}H (chloroform)

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

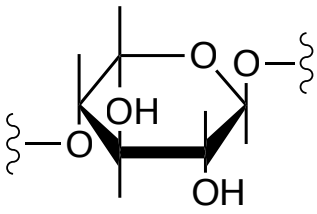
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.75	20.62	20.36
Ac Me	21.01	20.96	20.62
Ac Me	21.34	21.14	20.96
B β	22.22	22.58	22.03
A OMe	55.88	56.02	55.43
A OMe	55.97	56.02	55.50
B OMe	56.08	56.33	55.80
B OMe	56.08	56.33	55.80
γ	63.84	64.43	63.36
B α	72.38	72.70	71.70
α	76.01	76.69	75.65
β	80.76	81.52	80.30
B2	103.29	103.91	102.90
B6	103.29	103.91	102.90
A2	110.70	112.03	110.80
A5	111.02	112.31	111.51
A6	119.92	120.59	119.58
A1	129.64	130.68	129.28
B1	136.22	137.06	135.43
B4	137.37	138.53	137.28
A3	148.89	150.05	148.53
A4	149.10	150.25	148.74
B3	152.88	153.68	152.27
B5	152.88	153.68	152.27
Ac C=0	169.76	169.78	169.11
Ac C=O	170.15	170.14	169.52
Ac C=O	170.57	170.59	169.89

Compound Number 30



Xylan

Xylan,Birch

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
			58.94	
			63.09	
			72.56	
			73.83	
			75.40	
			101.14	
			101.65	

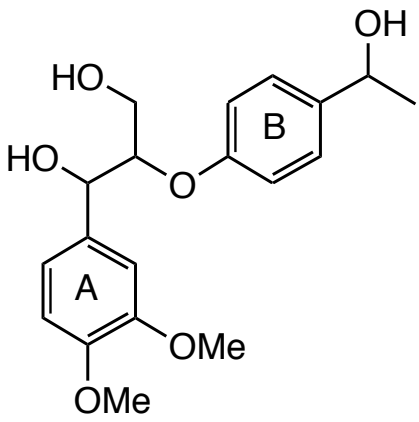
^{1}H (DMSO)

Atom	H Shifts	Mult	J

Notes:

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

Compound Number 31



threo

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

^{1}H (DMSO)

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

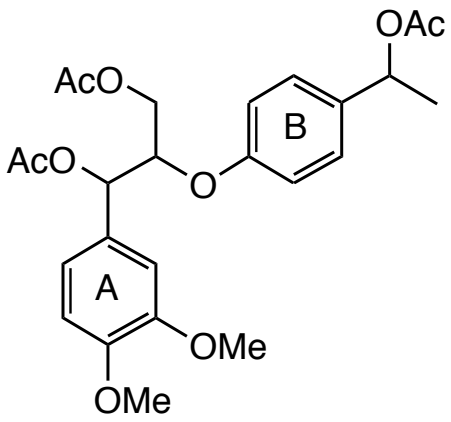
Notes:

S. Ralph SR111-7 28mg

^{13}C

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

Compound Number 32



threo

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

^{1}H (chloroform)

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

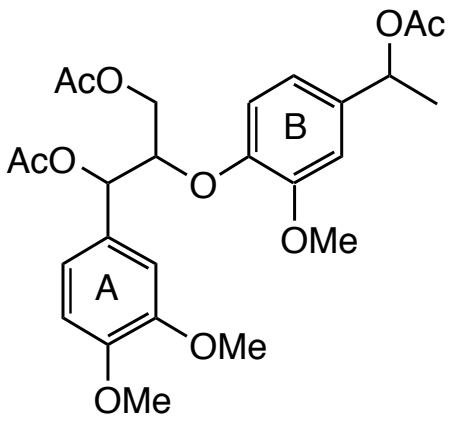
Notes:

S. Ralph SR III-17AC
28mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.69	20.56	20.38
Ac Me	21.04	20.89	20.64
Ac Me	21.35	21.13	20.93
B β	22.01	22.35	21.78
OMe	55.91	56.06	55.41
OMe	55.99	56.17	55.51
γ	62.91	63.46	62.32
B α	71.86	72.17	71.14
α	74.34	75.35	74.25
β	78.43	79.30	77.67
A2	110.51	112.16	110.85
A5	111.20	112.54	111.52
B3	116.40	117.10	115.98
B5	116.40	117.10	115.98
A6	119.92	120.84	119.82
B2	127.62	128.22	127.29
B6	127.62	128.22	127.29
A1	128.58	130.00	128.62
B1	135.13	136.10	134.59
A3	149.10	150.34	148.60
A4	149.41	150.61	148.87
B4	158.17	159.27	157.76
Ac C=0	169.81	169.90	169.28
Ac C=O	170.27	170.11	169.51
Ac C=O	170.55	170.58	169.92
erythro isomer:			
γ	62.59	63.11	61.88
α	73.95	74.41	72.92
β	78.43	78.93	76.96

Compound Number 33



threo

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

^{1}H (chloroform)

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

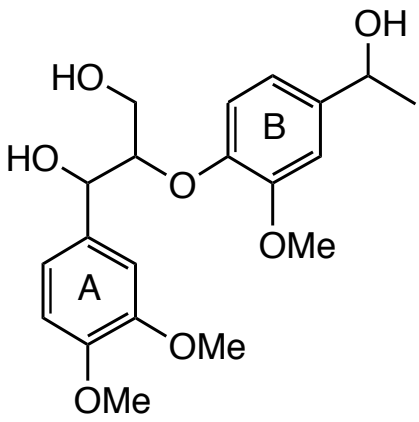
Notes:

S. Ralph SR III-15AC
35mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.71	20.59	20.36	
Ac Me	21.05	20.95	20.64	
Ac Me	21.35	21.14	20.94	
B β	22.09	22.45	21.87	
OMe	55.91	56.06	55.41	
OMe	55.95	56.14	55.46	
OMe	55.95	56.32	55.66	
γ	63.26	63.80	62.61	
B α	72.06	72.39	71.36	
α	74.87	75.67	74.54	
β	80.44	80.88	79.23	
B2	110.58	111.79	110.64	
A2	110.75	112.17	110.84	
A5	111.12	112.49	111.48	
B5	118.23	118.74	117.02	
B6	118.66	119.19	118.08	
A6	119.88	120.73	119.74	
A1	128.93	130.22	128.75	
B1	136.59	137.61	135.92	
B4	147.72	148.68	147.12	
A3	149.04	150.28	148.57	
A4	149.30	150.51	148.83	
B3	150.65	151.56	149.86	
Ac C=O	169.76	169.88	169.22	
Ac C=O	170.23	170.14	169.52	
Ac C=O	170.54	170.59	169.91	
erythro isomer:				
γ	62.74	63.25	62.04	
α	74.08	74.76	73.25	
β	79.98	80.23	78.29	

Compound Number 34



threo

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

^{1}H (chloroform)

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

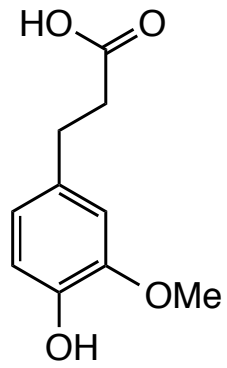
Notes:

S. Ralph SR III-15
28mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	25.22	26.10	25.83	
OMe	55.92	55.93	55.20	
OMe	55.92	56.01	55.41	
OMe	55.92	56.17	55.52	
γ	61.08	61.68	59.96	
B α	69.98	69.66	67.79	
α	73.84	73.62	70.72	
β	89.01	88.12	84.56	
B2	109.33	110.46	109.79	
A2	110.03	111.67	110.65	
A5	111.10	112.14	111.08	
B5	118.40	118.58	115.57	
B6	119.56	119.22	117.24	
A6	120.22	119.99	118.59	
A1	132.23	134.87	134.50	
B1	141.94	142.61	140.50	
B4	146.76	148.03	146.78	
A3	148.90	149.54	147.68	
A4	149.08	149.87	148.07	
B3	151.00	151.20	149.33	
erythro isomer:				
γ	60.82	61.68	59.96	
α	72.78	73.62	71.51	
β	87.01	86.50	83.82	

Compound Number 35



Dihydroferulic Acid

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

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	2.56	t	8.0
β	2.81	t	8.0
OMe	3.82	s	
6	6.67	dd	1.9, 8.0
5	6.72	d	8.0
2	6.86	2	1.9

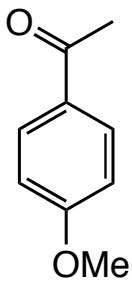
Notes:

J. Obst
35mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	30.38	31.24	30.00	
β	36.01	36.38	35.68	
OMe	55.92	56.22	55.52	
2	111.10	112.81	112.52	
5	114.52	115.64	115.25	
6	120.89	121.47	120.21	
1	132.15	133.23	131.62	
4	144.16	145.76	144.68	
3	146.55	148.17	147.34	
γ	178.88	174.26	173.77	
1H				
α	2.64		2.46	
β	2.88		2.70	
OMe	3.84		3.72	
6	6.69		6.57	
5	6.82		6.64	
2	6.71		6.77	

Compound Number 36



4-Methoxyacetophenone

4-methoxyacetophenone

^{1}H (chloroform)

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

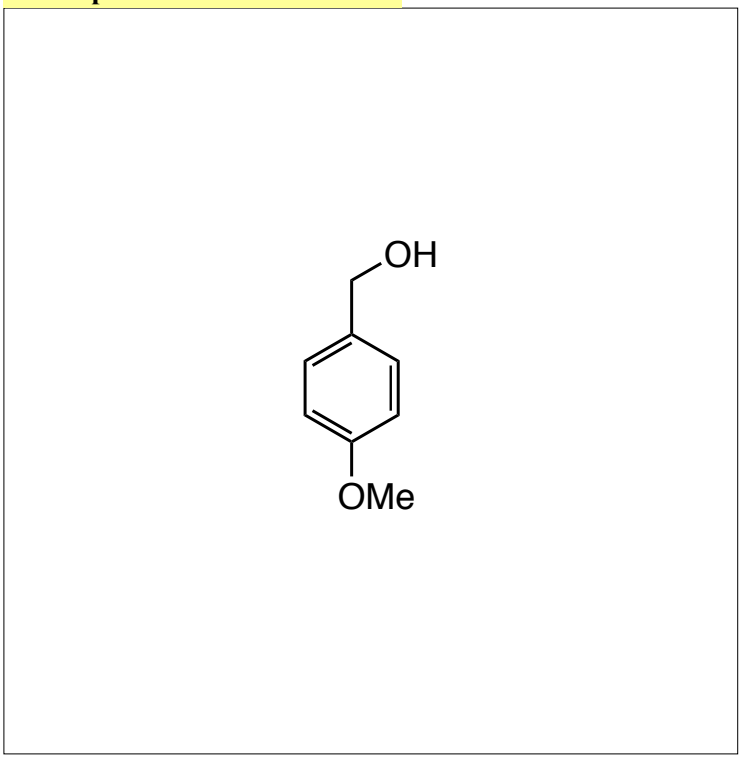
Notes:

Aldrich
57mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	26.28	26.33	26.29	
OMe	55.43	55.85	55.44	
3	113.68	114.45	113.75	
5	113.68	114.45	113.75	
1	130.35	131.28	129.89	
2	130.55	131.18	130.40	
6	130.55	131.18	130.40	
4	163.48	164.31	163.06	
α	196.62	196.23	196.14	

Compound Number 37



p-Methoxybenzyl alcohol

4-methoxybenzyl alcohol

^{1}H (chloroform)

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

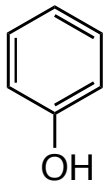
Notes:

Aldrich
65mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.23	55.39	54.94	
α	64.68	64.34	62.59	
3	113.87	114.27	113.40	
5	113.87	114.27	113.40	
2	128.56	128.82	127.86	
6	128.56	128.82	127.86	
1	133.21	135.23	134.49	
4	159.05	159.64	158.14	

Compound Number 38



Phenol

phenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
3,5	6.84	m	
1	6.93	m	
2,6	7.22	m	
acetone			
3,5	6.86	d	
1	6.82	t	
2,6	7.19	d	
DMSO			
3,5	6.73		
1	6.74		
2,6	7.13		
Ph-OH	9.30		

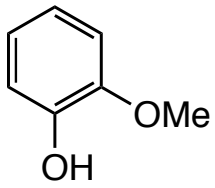
Notes:

Aldrich JR 85-11
54mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3	115.41	116.03	115.18	
5	115.41	116.03	115.18	
1	120.89	120.13	118.70	
2	129.71	130.16	129.26	
6	129.71	130.16	129.26	
4	155.25	158.16	157.29	

Compound Number 39



Guaiacol

2-methoxyphenol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.87	s	
OH	5.68	s	
2	6.85		
1	6.85		
6	6.86		
5	6.93		

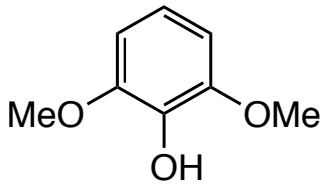
Notes:

Aldrich JR A85.12
54mg
500MHz 1H shifts change, assignments made from hsqc and hmbc
all solvents

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.82	56.15	55.60	
2	110.69	112.48	112.40	
5	114.50	115.88	115.68	
1	120.10	120.42	119.32	
6	121.41	121.96	121.02	
4	145.62	147.52	146.66	
3	146.54	148.37	147.76	
1H				
OMe		3.81	3.74	
6		6.79	6.73	
1		6.77	6.74	
5		6.83	6.78	
2		6.92	6.88	
OH		7.47	8.89	

Compound Number 40



Syringol

2,6-dimethoxyphenol

^{1}H (chloroform)

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

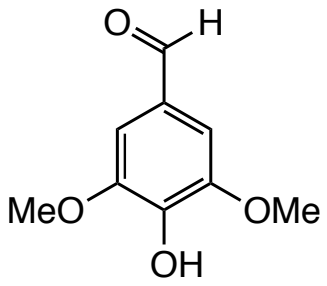
Notes:

Aldrich JR A 85.13
56mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.27	56.55	55.89	
OMe	56.27	56.55	55.89	
2	105.03	106.57	105.70	
6	105.03	106.57	105.70	
1	119.06	119.16	118.06	
4	134.97	137.08	135.70	
3	147.31	148.86	148.16	
5	147.31	148.86	148.16	

Compound Number 41



Syringaldehyde

3,5-dimethoxy-4-hydroxybenzaldehyde

^{1}H (chloroform)

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

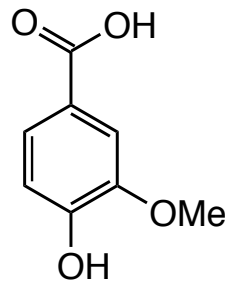
Notes:

J. Ralph JRA87.13
62mg
Poor solubility

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.48	56.64	56.02	
OMe	56.48	56.64	56.02	
2	106.81	107.74	107.05	
6	106.81	107.74	107.05	
1	128.34	129.02	127.14	
4	141.03	142.92	142.11	
3	147.44	148.94	148.09	
5	147.44	148.94	148.09	
α	190.79	191.05	190.99	

Compound Number 42



Vanillic acid

4-hydroxy-3-methoxy benzoic acid

^{1}H (chloroform)

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

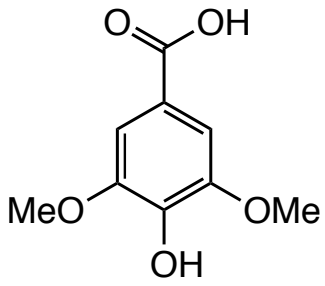
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.28	55.50	
2		113.46	112.73	
5		115.43	115.00	
1		122.70	121.62	
6		124.90	123.46	
3		147.96	147.17	
4		152.03	151.05	
α		167.84	167.16	

Compound Number 43



Syringic acid

3,5-dimethoxy-4-hydroxybenzoic acid

^{1}H (chloroform)

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

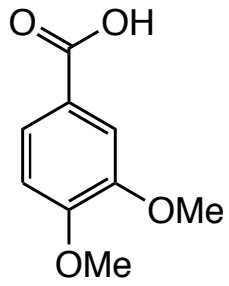
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.45	56.66	55.92	
OMe	56.45	56.66	55.92	
2	107.24	108.20	106.85	
6	107.24	108.20	106.85	
1	119.93	121.40	120.32	
4	139.98	141.61	140.17	
3	146.67	148.30	147.37	
5	146.67	148.30	147.37	
α	170.56	167.68	167.14	

Compound Number 44



Veratric acid

3,4-dimethoxybenzoic acid

^{1}H (chloroform)

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

^{13}C

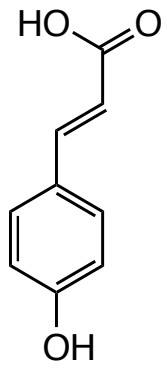
Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.02	56.08	55.41	
OMe	56.06	56.12	55.58	
2	110.36	111.64	110.93	
5	112.38	113.34	111.93	
1	121.77	123.64	122.98	
6	124.61	124.42	123.16	
3	148.72	149.89	148.30	
4	153.78	154.37	152.60	
α	172.08	167.53	167.08	

Notes:

J. Ralph JRA 89-14

55mg

Compound Number 45



trans

***p*-Coumaric acid**

4-hydroxycinnamic acid

^{1}H (DMSO)

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

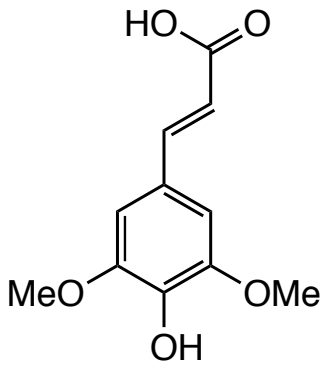
Notes:

Fluka
60mg
*not soluble in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β		115.51	115.30	
3		116.66	115.72	
5		116.66	115.72	
1		126.95	125.24	
2		130.90	129.98	
6		130.90	129.98	
α		145.95	144.11	
4		160.49	159.54	
γ		169.03	167.90	

Compound Number 46



trans

Sinapinic acid

3,5-dimethoxy-4-hydroxycinnamic acid

^{1}H (DMSO)

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

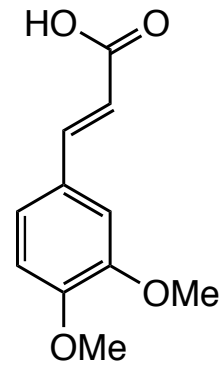
Notes:

Lancaster Synthesis
60mg *not very soluble in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.68	56.04	
OMe		56.68	56.04	
2		106.84	106.04	
6		106.84	106.04	
β		116.20	116.03	
1		126.19	124.59	
4		139.43	138.05	
α		146.23	144.74	
3		148.90	148.00	
5		148.90	148.00	
γ		168.26	167.90	

Compound Number 47



trans

3,4-Dimethoxycinnamic acid

3,4-dimethoxycinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.92	s	
OMe	3.92	s	
β	6.30	d	15.9
5	6.86	d	8.3
2	7.06	d	2.0
6	7.12	dd	8.3, 2.0
α	7.73	d	15.9

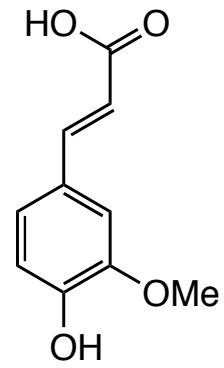
Notes:

K & K Labs
60mg
500MHz all solvents HSQC and HMBC
note H2 switches order with H6 in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.88	56.07	55.60
OMe	55.96	56.11	55.64
2	109.74	111.10	110.32
5	111.00	112.36	111.58
β	114.86	116.81	116.75
6	123.00	123.47	122.70
1	127.08	128.34	127.08
α	146.96	145.64	144.20
3	149.23	150.60	149.00
4	151.50	152.45	150.81
γ	172.52	168.23	167.96
1H			
OMe		3.84	3.77
OMe		3.88	3.78
β		6.39	6.42
5		6.98	6.96
6		7.19	7.19
2		7.31	7.29
α		7.59	7.51

Compound Number 48



trans

Ferulic acid

4-hydroxy-3-methoxycinnamic acid

^{1}H (DMSO)

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

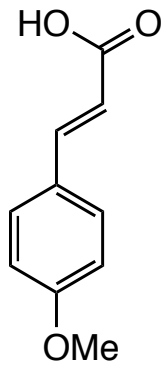
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	d4-MeOH
OMe		56.28	55.64	56.44
2		111.30	111.14	111.71
β		115.77	115.52	115.89
5		116.00	115.60	116.46
6		123.80	122.72	123.94
1		127.38	125.76	127.77
α		146.16	144.44	146.89
3		148.64	147.87	149.30
4		149.97	149.04	150.43
γ		168.88	167.93	170.93

Compound Number 49



trans

4-Methoxycinnamic acid

4-methoxycinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.82	s	
β	6.29	m	8.8
3,5	6.89	d	15.9
2,6	7.48	m	8.8
α	7.71	d	15.9

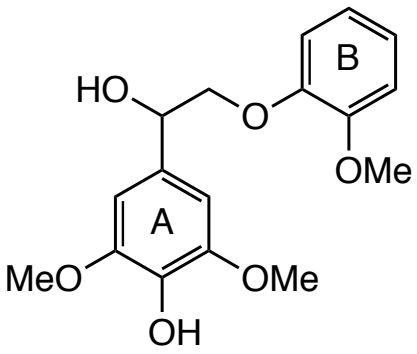
Notes:

Aldrich
1H run at 500MHz
13C in CDCl3 500MHz

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.37	55.68	55.22	
3	114.37	115.14	114.30	
5	114.37	115.14	114.30	
β	114.66	116.52	116.51	
1	126.80	128.02	126.82	
2	130.06	130.58	129.84	
6	130.06	130.58	129.84	
α	146.55	145.19	143.65	
4	161.70	162.41	160.90	
γ	172.00	168.11	167.78	
1H				
OMe		3.84	3.78	
β		6.37	6.36	
3,5		6.98	6.96	
α		7.62	7.53	
2,6		7.62	7.62	

Compound Number 50



Syringylglycol-β-guaiacyl ether

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

^{1}H (chloroform)

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

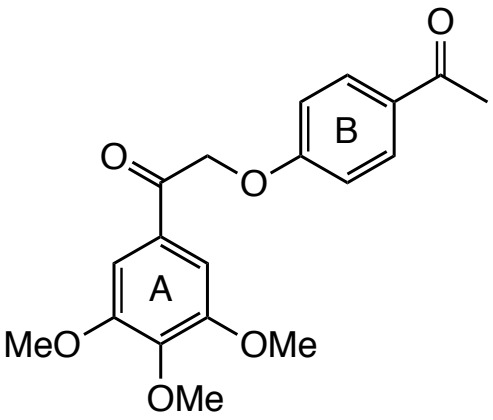
Notes:

S. Ralph SG 100mg
33mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B OMe	55.84	56.24	55.41	
A OMe	56.32	56.58	55.81	
A OMe	56.32	56.58	55.81	
α	72.47	72.85	70.97	
β	76.39	76.15	73.98	
A2	103.11	104.79	103.73	
A6	103.11	104.79	103.73	
B2	112.06	113.44	112.25	
B5	115.96	115.52	113.40	
B6	121.12	121.76	120.66	
B1	122.50	122.29	120.79	
A1	130.84	133.07	132.54	
A4	134.46	136.13	134.51	
A3	147.12	148.46	147.57	
A5	147.12	148.46	147.57	
B3	148.06	149.62	148.11	
B4	150.11	150.84	148.94	

Compound Number 51



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

^{1}H (chloroform)

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

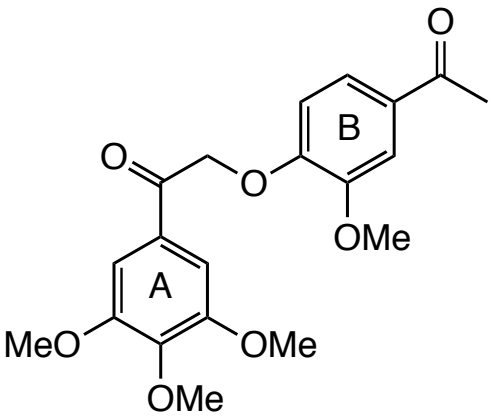
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	26.34	26.37	26.34	
A3 OMe A5 OMe	56.42 56.42	56.68 56.68	56.12 56.12	
A4 OMe	61.00	60.72	60.12	
β	70.62	71.10	70.11	
A2 A6	105.84 105.84	106.60 106.60	105.47 105.47	
B3 B5	114.44 114.44	115.27 115.27	114.45 114.45	
A1	129.36	130.72	129.38	
B2 B6	130.62 130.62	131.11 131.11	130.26 130.26	
B1	131.16	131.70	130.11	
A4	143.65	144.27	142.41	
A3 A5	153.32 153.32	154.41 154.41	152.88 152.88	
B4	161.77	163.09	161.79	
α B α	192.49 196.55	193.05 196.23	192.70 196.12	

Compound Number 52



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

^{1}H (chloroform)

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

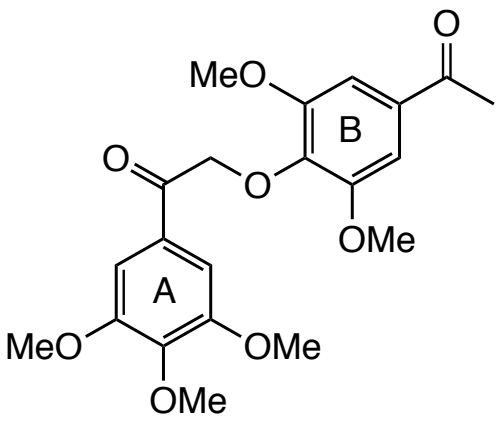
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	26.23	26.30	26.25
B OMe	56.01	56.28	55.58
A3 OMe	56.32	56.64	56.12
A5 OMe	56.32	56.64	56.12
A4 OMe	60.96	60.70	60.13
β	71.57	71.84	70.48
A2	105.79	106.70	105.57
A6	105.79	106.70	105.57
B2	110.85	112.10	110.84
B5	112.27	113.40	112.24
B6	122.87	123.39	122.56
A1	129.33	130.74	129.40
B1	131.48	131.98	130.24
A4	143.44	144.21	142.45
B3	149.31	150.23	148.52
B4	151.49	152.98	151.61
A3	153.23	154.34	152.85
A5	153.23	154.34	152.85
α	192.68	193.34	192.76
Bα	196.64	196.32	196.19

Notes:

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

Compound Number 53



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

^{1}H (chloroform)

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

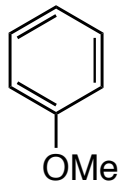
Notes:

L. Landucci LLL XVII 9d
37mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	26.43	26.55	26.52	
A3 OMe A5 OMe	56.33 56.33	56.61 56.61	56.04 56.04	
B3 OMe B5 OMe	56.33 56.33	56.66 56.66	56.09 56.09	
A4 OMe	60.94	60.67	60.08	
β	74.82	75.43	74.15	
A2 A6	105.87 105.87	106.81 106.81	105.52 105.52	
B2 B6	105.87 105.87	106.95 106.95	105.84 105.84	
A1 B1	129.99 132.67	131.21 133.62	129.69 132.05	
B4 A4	140.75 142.94	141.68 143.88	140.24 142.15	
B3 B5	152.53 152.53	153.61 153.61	152.04 152.04	
A3 A5	153.12 153.12	154.23 154.23	152.80 152.80	
α B α	193.28 196.71	193.81 196.70	193.11 196.61	

Compound Number 54



Anisole

Methoxybenzene

^{1}H (chloroform)

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

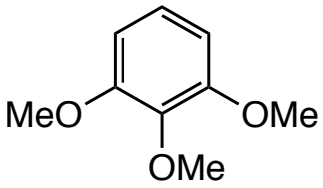
Notes:

Aldrich
40mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.08	55.28	54.86	
3	113.92	114.62	113.84	
5	113.92	114.62	113.84	
1	120.64	121.19	120.39	
2	129.52	130.14	129.39	
6	129.52	130.14	129.39	
4	159.60	160.63	159.24	

Compound Number 55



1,2,3-trimethoxybenzene

^{1}H (chloroform)

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

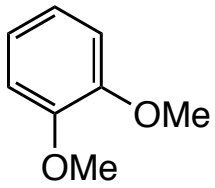
Notes:

Aldrich
40mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3 OMe	56.09	56.35	55.77	
5 OMe	56.09	56.35	55.77	
4 OMe	60.80	60.43	59.90	
2	105.34	106.54	105.56	
6	105.34	106.54	105.56	
1	123.61	124.30	123.57	
4	138.27	139.52	137.69	
3	153.56	154.67	153.16	
5	153.56	154.67	153.16	

Compound Number 56



Veratrole

1,2-dimethoxybenzene

^{1}H (chloroform)

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

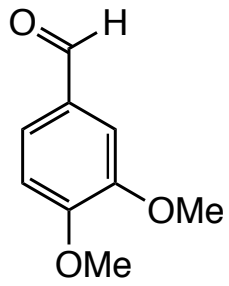
Notes:

Aldrich
40mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.80	56.01	55.38	
OMe	55.80	56.01	55.38	
2	111.44	113.02	111.98	
5	111.44	113.02	111.98	
1	120.85	121.60	120.67	
6	120.85	121.60	120.67	
3	149.08	150.50	148.88	
4	149.08	150.50	148.88	

Compound Number 57



Veratraldehyde

3,4-dimethoxybenzaldehyde

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.94	s	
OMe	3.97	s	
5	6.98	d	8.2
2	7.41	d	1.8
6	7.46	dd	8.2, 1.8
α	9.85	s	
DMSO			
OMe	3.81	s	
OMe	3.85	s	
5	7.14	d	8.07
2	7.36	d	1.71
6	7.53	d	
α	9.82	s	

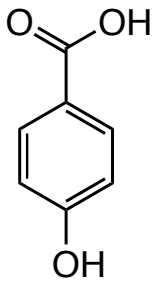
Notes:

Aldrich
CAS# 120-14-9
40mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3 OMe	56.00	56.07	55.47	
4 OMe	56.17	56.29	55.82	
2	109.05	110.31	109.46	
5	110.46	111.85	111.22	
6	126.77	126.72	126.00	
1	130.19	131.21	129.65	
3	149.66	150.77	149.17	
4	154.51	155.63	154.18	
α	190.78	191.16	191.21	
1H				
OMe		3.88		
OMe		3.92		
5		7.14		
2		7.41		
6		7.52		
α		9.85		

Compound Number 58



4-hydroxybenzoic acid

^{1}H (DMSO)

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

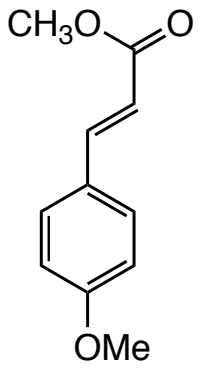
Notes:

Aldrich
40mg *CDCl3 insoluble

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3		115.99	115.06	
5		115.99	115.06	
1		122.43	121.35	
2		132.78	131.47	
6		132.78	131.47	
4		162.65	161.55	
α		168.24	167.11	

Compound Number 59



methyl (4-methoxy)cinnamate

^{1}H (chloroform)

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

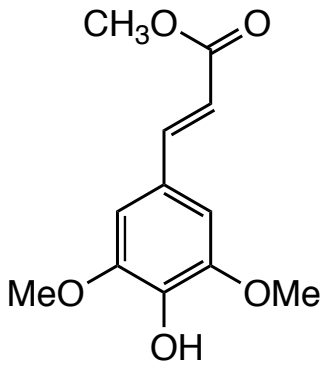
Notes:

J. Ralph PS 137x1
95mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ OMe	51.50	51.58	51.23	
4 OMe	55.32	55.70	55.28	
3	114.34	115.14	114.36	
5	114.34	115.14	114.36	
β	115.30	115.96	115.09	
1	127.14	127.84	126.65	
2	129.71	130.63	130.08	
6	129.71	130.63	130.08	
α	144.49	145.04	144.28	
4	161.42	162.42	161.17	
γ	167.68	167.81	166.90	

Compound Number 60



trans

Methyl Sinapate

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

^{1}H (chloroform)

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

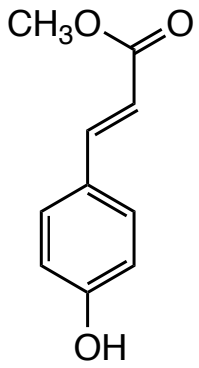
Notes:

J. Ralph JRPS 135x1
52mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ OMe	51.60	51.46	51.13	
3 OMe 5 OMe	56.34 56.34	56.68 56.68	56.06 56.06	
2 6	105.17 105.17	106.83 106.83	106.26 106.26	
β	115.50	115.73	114.58	
1	125.85	126.08	124.34	
4	137.30	139.46	138.36	
α	145.15	145.99	145.32	
3 5	147.29 147.29	148.88 148.88	148.00 148.00	
γ	167.58	167.78	166.98	

Compound Number 61



trans

Methyl *p*-Coumarate

methyl 4-hydroxycinnamate

^{1}H (chloroform)

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

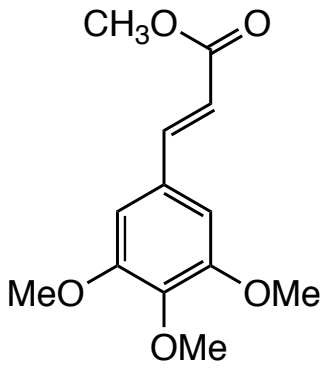
Notes:

J. Ralph JRPS 133.2x1
68mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ OMe	51.71	51.49	51.13	
β	114.98	115.22	113.90	
3	115.95	116.64	115.78	
5	115.95	116.64	115.78	
1	126.98	126.90	125.07	
2	130.00	130.82	130.21	
6	130.00	130.82	130.21	
α	144.89	145.33	144.69	
4	158.12	160.45	159.87	
γ	168.18	167.87	166.99	

Compound Number 62



trans

methyl (3,4,5-trimethoxy)cinnamate

^{1}H (chloroform)

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

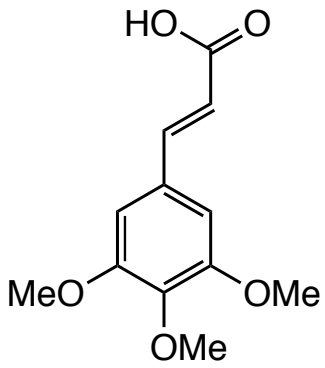
Notes:

J. Ralph JRPS 139x1
92mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ OMe	51.61	51.57	51.31	
3 OMe	56.15	56.45	56.02	
5 OMe	56.15	56.45	56.02	
4 OMe	60.89	60.58	60.06	
2	105.36	106.58	105.99	
6	105.36	106.58	105.99	
β	117.04	117.70	117.06	
1	129.90	130.70	129.61	
4	140.24	141.27	139.61	
α	144.81	145.45	144.75	
3	153.46	154.51	153.11	
5	153.46	154.51	153.11	
γ	167.29	167.51	166.78	

Compound Number 63



trans

3,4,5-trimethoxy cinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
3,5 OMe	3.88	s	
4 OMe	3.87	s	
2,6	6.76	s	
α	7.69	d	15.9
β	6.34	d	15.9
Acetone			
3,5 OMe	3.88	s	
4 OMe	3.76	s	
2,6	7.01	s	
α	7.59	d	15.9
β	6.47	d	15.9
DMSO			
3,5 OMe	3.80		
4 OMe	3.67		
2,6	7.01		
α	7.59		
β	6.47		

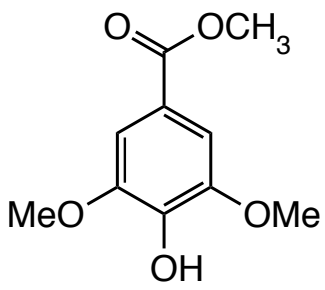
Notes:

Aldrich
Bruker 500 MHz
30mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
3 OMe	56.15	56.50	56.03
5 OMe	56.15	56.50	56.03
4 OMe	60.97	60.61	60.11
2	105.52	106.59	105.78
6	105.52	106.59	105.78
β	116.43	118.28	118.53
1	129.46	130.93	129.88
4	140.51	141.18	139.29
α	147.03	145.74	144.21
3	153.44	154.62	153.11
5	153.44	154.62	153.11
γ	172.28	167.90	167.77

Compound Number 64



Syringic acid methyl ester

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

^{1}H (chloroform)

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

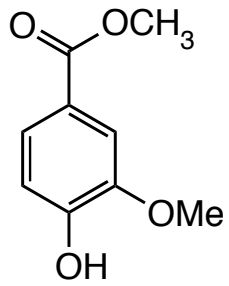
Notes:

J. Ralph JRPS 7x1
93.3mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α OMe	52.07	52.11	51.78	
3 OMe	56.41	56.67	56.04	
5 OMe	56.41	56.67	56.04	
2	106.80	107.87	106.82	
6	106.80	107.87	106.82	
1	120.96	121.07	119.28	
4	139.49	141.65	140.72	
3	146.78	148.33	147.58	
5	146.78	148.33	147.58	
α	166.92	167.16	166.10	

Compound Number 65



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

^{1}H (chloroform)

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

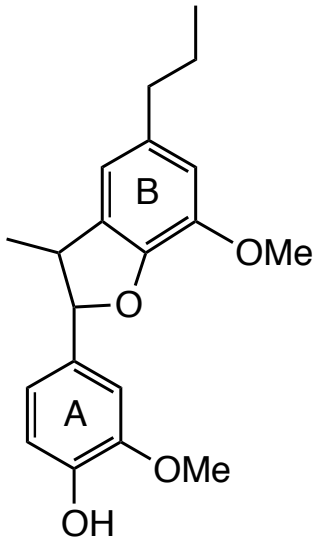
Notes:

J. Ralph JRPS 3.1
101mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α OMe	52.02	52.00	51.64	
4 OMe	56.07	56.29	55.60	
2	111.98	113.20	112.54	
5	114.33	115.58	115.19	
1	122.13	122.43	120.52	
6	124.23	124.53	123.44	
3	146.41	148.08	147.36	
4	150.29	152.14	151.53	
α	167.12	167.15	166.06	

Compound Number 66



Dihydrodehydrodiisoeugenol

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

^{1}H (chloroform)

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

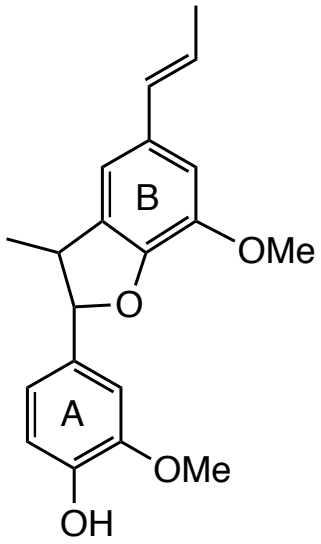
Notes:

J. Ralph JRL 109x2
44mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B γ	13.90	14.08	13.65	
γ	17.44	17.83	17.17	
B β	25.07	25.74	24.52	
B α	38.09	38.54	37.27	
β	45.81	46.43	44.71	
OMe	55.99	56.28	55.59	
OMe	55.99	56.41	55.64	
α	93.61	93.80	92.37	
A2	109.04	110.69	110.56	
B2	111.91	113.63	112.24	
A5	114.11	115.55	115.20	
B6	115.46	116.39	115.35	
A6	119.94	120.22	119.25	
A1	132.28	133.03	130.82	
B5	132.98	134.12	132.91	
B1	136.29	136.62	135.32	
B4	143.86	144.78	143.30	
A4	145.41	146.59	144.93	
B3	145.77	147.52	146.67	
A3	146.71	148.39	147.59	

Compound Number 67



Dehydrodiisoeugenol

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

^{1}H (chloroform)

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

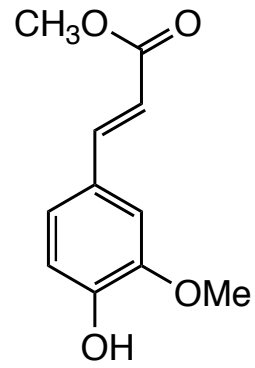
Notes:

J. Ralph JRKM 67-1
150mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	17.60	17.86	17.25	
B γ	18.34	18.42	18.06	
β	45.62	46.21	44.51	
OMe	55.97	56.25	55.59	
OMe	55.97	56.33	55.61	
α	93.76	93.96	92.55	
A2	108.97	110.66	109.74	
B2	109.40	111.06	110.58	
A5	113.36	114.30	113.29	
B6	114.14	115.55	115.23	
A6	119.91	120.21	119.25	
B β	123.41	123.22	122.60	
B α	130.98	132.05	130.68	
A1	132.11	132.81	130.93	
B5	132.22	132.83	131.39	
B1	133.30	134.43	133.30	
B4	144.15	145.03	143.61	
A4	145.82	147.53	146.07	
B3	146.62	147.72	146.71	
A3	146.71	148.36	147.59	

Compound Number 68



trans

Methyl ferulate

methyl 4-hydroxy-3-methoxycinnamate

^{1}H (chloroform)

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

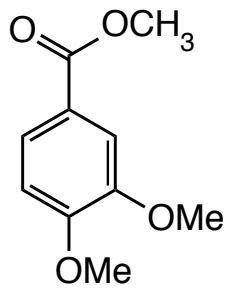
Notes:

J. Ralph JRKM 85.1
54mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ OMe	51.60	51.47	51.12	
3 OMe	55.93	56.32	55.68	
2	109.56	111.34	111.32	
β	114.86	115.51	114.19	
5	115.09	116.03	115.54	
6	123.00	123.78	122.99	
1	126.92	127.38	125.56	
α	145.03	145.65	145.02	
3	146.89	148.66	147.92	
4	148.11	149.99	149.38	
γ	167.80	167.82	167.02	

Compound Number 69



Methylveratrate

methyl 3,4-dimethoxybenzoate

^{1}H (chloroform)

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

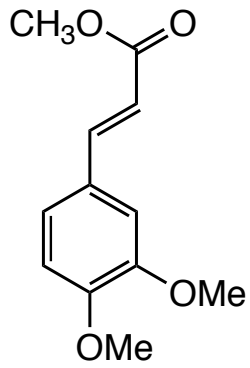
Notes:

J. Ralph JRPS 5.1
55mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α OMe	51.93	52.00	51.79	
OMe	55.99	56.10	55.50	
OMe	55.99	56.10	55.66	
2	110.32	111.65	111.07	
5	112.05	112.99	111.70	
1	122.71	123.37	121.84	
6	123.58	124.08	123.13	
3	148.65	149.90	148.46	
4	153.00	154.38	152.98	
α	166.82	166.92	165.96	
1H				
3 OMe		3.83	3.79	
α OMe		3.85	3.81	
4 OMe		3.88	3.82	
5		7.03	7.06	
2		7.50	7.43	
6		7.62	7.58	

Compound Number 70



trans

methyl 3,4-dimethoxycinnamate

^{1}H (chloroform)

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

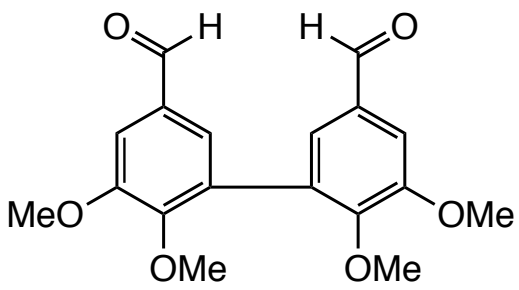
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ OMe	51.55	51.50	51.20	
3 OMe	55.89	56.07	55.52	
4 OMe	55.96	56.12	55.59	
2	109.77	111.23	110.49	
5	111.12	112.38	111.51	
β	115.53	116.15	115.26	
6	122.56	123.46	122.81	
1	127.41	128.19	126.85	
α	144.74	145.41	144.67	
3	149.27	150.59	149.00	
4	151.18	152.54	151.02	
γ	167.58	167.71	166.92	

Notes:

J. Ralph JRPS 21x1
52mg

Compound Number 71



Dehydrodiveratraldehyde

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

^{1}H (chloroform)

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

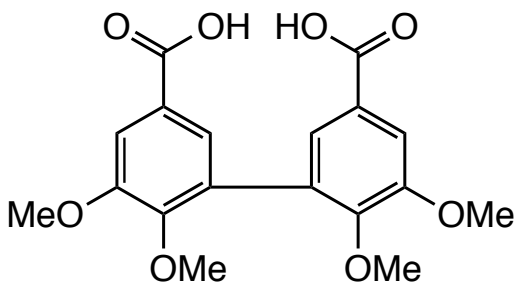
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3 OMe	56.05	56.40	55.94	
4 OMe	60.95	60.98	60.36	
2	110.43	111.92	111.39	
6	127.51	127.15	125.97	
5	131.76	133.01	131.52	
1	132.06	133.21	131.76	
4	152.36	153.02	151.50	
3	153.37	154.27	152.82	
α	190.87	191.51	191.60	

Compound Number 72



Dehydrodiveratric acid

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

^{1}H (DMSO)

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

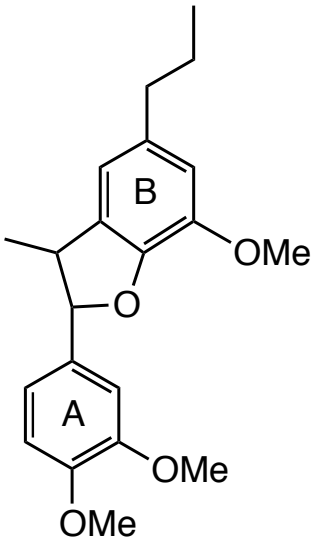
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3 OMe			55.81	
4 OMe			60.19	
2			112.91	
6			124.10	
1			125.84	
5			131.27	
4			150.04	
3			152.11	
α			166.72	

Compound Number 73



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

^{1}H (chloroform)

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

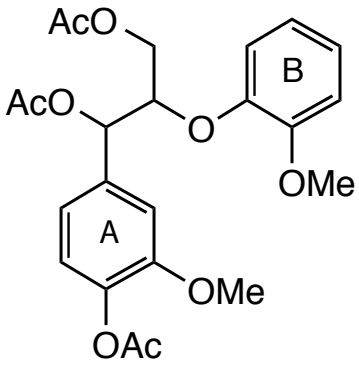
Notes:

Obst
45mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B γ	13.90	14.08	13.66	
γ	17.47	17.90	17.18	
B β	25.06	25.74	24.53	
B α	38.09	38.53	37.28	
β	45.77	46.47	44.87	
OMe	55.92	56.12	55.47	
OMe	55.92	56.12	55.47	
OMe	56.00	56.41	55.66	
α	93.48	93.58	92.11	
A2	109.62	111.03	110.01	
A5	110.88	112.57	111.58	
B2	111.90	113.62	112.28	
B6	115.44	116.40	115.37	
A6	119.22	119.68	118.85	
B5	132.90	134.07	132.49	
A1	132.95	134.25	132.86	
B1	136.30	136.69	135.46	
B4	143.87	144.80	143.34	
B3	145.42	146.57	144.92	
A3	149.10	150.40	148.83	
A4	149.16	150.49	148.83	

Compound Number 74



threo

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

^{1}H (DMSO)

Atom	H Shifts	Mult	J
Ac Me	1.93	s	
Ac Me	1.98	s	
Ac Me	2.22	s	
OMe	3.72	s	
OMe	3.75	s	
γ1	3.96	dd	5.7, 12.0
γ2	4.12	dd	3.9, 12.0
β	4.78	m	
α	5.98	d	6.5
A2	7.15	d	1.8
B2	6.96		
B5	6.98		
A6	6.99		
B6	6.84	dt	7.5
A5	7.05	d	8.1
B1	6.95		

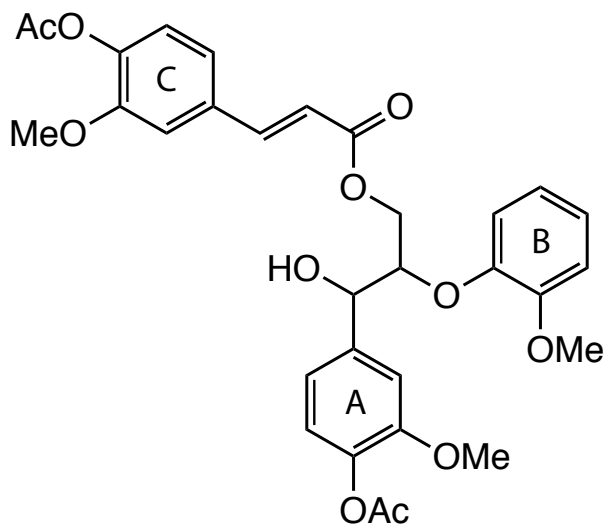
Notes:

R. Helm RFH5C
50mg
1H data for acetone and DMSO 500MHz
some 1H CS taken from HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.63	20.45	20.28	
Ac Me	20.68	20.58	20.35	
Ac Me	21.02	20.91	20.63	
OMe	55.81	56.21	55.54	
OMe	55.96	56.30	55.76	
γ	63.09	63.58	62.47	
α	74.52	75.37	74.28	
β	80.26	80.68	79.05	
A2	111.75	112.66	111.62	
B2	112.58	113.76	112.75	
B5	118.79	119.22	117.47	
A6	119.58	120.27	119.36	
B6	121.00	121.66	120.64	
A5	122.79	123.52	122.57	
B1	123.31	123.75	122.62	
A1	135.35	136.66	135.40	
A4	139.93	140.88	139.19	
B4	147.96	149.05	147.54	
B3	150.84	151.81	150.13	
A3	151.12	152.18	150.67	
A4 Ac C=O	168.71	168.83	168.31	
α Ac C=O	169.65	169.94	169.30	
γ Ac C=O	170.52	170.62	169.89	
1H				
Ac Me	1.99	1.95		
Ac Me	2.05	2.01		
Ac Me	2.29	2.22		
OMe	3.80	3.80		
OMe	3.81	3.81		
γ1	4.06	4.01		
γ2	4.32	4.25		
β	4.63	4.78		
α	6.12	6.10		
A2		7.23		
B2		6.99		
B5		7.03		
A6		7.05		
B6		6.86		
A5		7.04		
B1		6.97		

Compound Number 75



threo

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

^{1}H (chloroform)

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

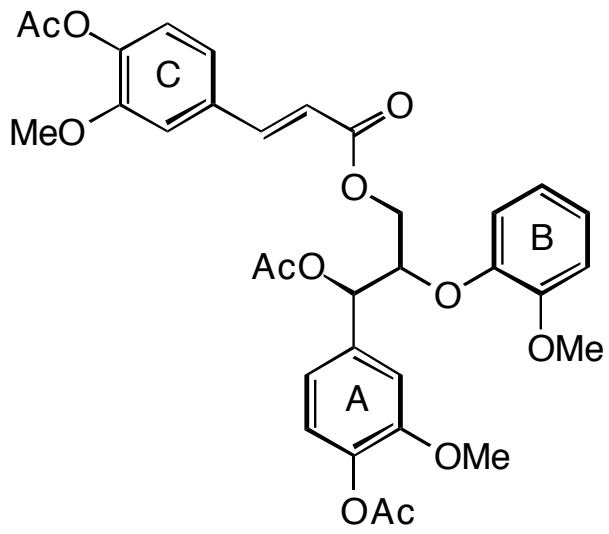
^{13}C

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

Notes:

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

Compound Number 76



erythro

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

^{1}H (chloroform)

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

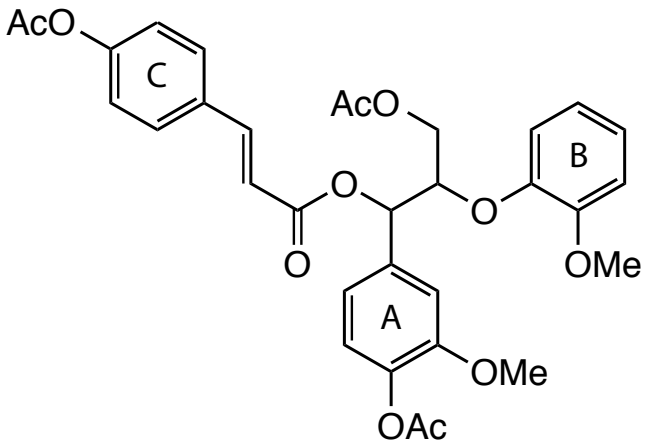
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.64	20.46	20.32
Ac Me	20.64	20.46	20.32
Ac Me	21.05	20.90	20.66
OMe	55.81	56.22	55.60
OMe	55.96	56.30	55.73
OMe	55.96	56.41	55.97
γ	62.88	63.34	62.26
α	73.96	74.72	73.28
β	80.46	80.52	78.58
C2	111.31	112.47	111.72
A2	112.05	112.77	111.86
B2	112.63	113.80	112.91
C β	117.70	118.62	117.70
B5	119.74	119.97	118.08
A6	119.74	120.44	119.41
B6	121.00	121.65	120.67
C6	121.44	122.22	121.60
A5	122.60	123.37	122.50
B1	123.23	124.09	122.90
C5	123.66	124.09	123.16
C1	133.22	134.09	132.80
A1	135.53	136.71	135.37
A4	139.80	140.79	139.11
C4	141.58	142.74	141.11
C α	144.61	145.13	144.28
B4	147.23	148.30	146.70
B3	151.00	152.11	150.38
A3	151.20	152.11	150.58
C3	151.42	152.65	151.16
C γ	166.40	166.64	165.77
Ac C=O	168.68	168.75	168.20
Ac C=O	168.75	168.86	168.31
Ac C=O	169.50	169.89	169.20

Compound Number 77



erythro

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

^{1}H (chloroform)

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

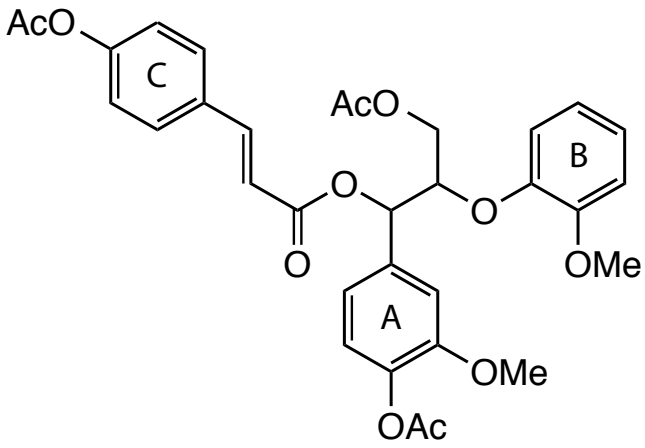
Notes:

R. Helm RFH119D1
47mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.64	20.46	20.30
Ac Me	20.75	20.62	20.39
Ac Me	21.09	20.95	20.79
OMe	55.82	56.24	55.61
OMe	55.94	56.31	55.74
γ	62.73	63.16	62.06
α	74.12	74.97	73.50
β	80.25	80.43	78.57
A2	111.88	112.82	111.73
B2	112.68	113.82	112.91
C β	117.66	118.65	117.55
B5	119.58	119.87	118.04
A6	119.66	120.45	119.31
B6	121.02	121.67	120.68
C3	122.15	123.20	122.31
C5	122.15	123.20	122.31
A5	122.60	123.38	122.52
B1	123.63	124.06	122.89
C2	129.31	130.25	129.65
C6	129.31	130.25	129.65
C1	131.91	132.79	131.49
A1	135.38	136.60	135.32
A4	139.78	140.82	139.12
C α	144.58	145.09	144.32
B4	147.18	148.38	146.76
B3	151.01	152.04	150.34
A3	151.15	152.11	150.57
C4	152.28	153.54	152.10
C γ	165.33	165.76	164.86
Ac C=O	168.74	168.85	168.32
Ac C=O	168.99	169.36	168.82
Ac C=O	170.72	170.71	169.95

Compound Number 78



threo

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

^{1}H (chloroform)

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

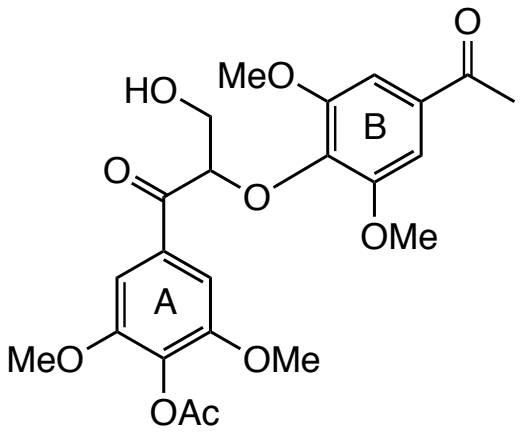
Notes:

R. Helm RFH119D2
44mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.64	20.44	20.29
Ac Me	20.72	20.60	20.38
Ac Me	21.10	20.95	20.78
OMe	55.77	56.17	55.53
OMe	55.97	56.31	55.80
γ	63.26	63.69	62.58
α	74.96	75.78	74.61
β	80.52	80.86	79.18
A2	111.71	112.73	111.71
B2	112.47	113.68	112.71
C β	117.78	118.73	117.56
B5	118.91	119.33	117.63
A6	119.49	120.27	119.36
B6	120.96	121.62	120.62
C3	122.14	123.16	122.28
C5	122.14	123.16	122.28
A5	122.84	123.56	122.57
B1	123.30	123.75	122.69
C2	129.26	130.15	129.56
C6	129.26	132.78	129.56
C1	131.96	132.78	131.50
A1	135.41	136.68	135.44
A4	139.94	140.94	139.25
C α	144.34	144.86	144.10
B4	148.08	149.10	147.56
B3	150.89	151.87	150.17
A3	151.14	152.21	150.69
C4	152.23	153.47	152.04
C γ	165.46	165.84	165.03
Ac C=O	168.70	168.77	168.27
Ac C=O	169.02	169.32	168.81
Ac C=O	170.56	170.62	169.90

Compound Number 79



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

^{1}H (chloroform)

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

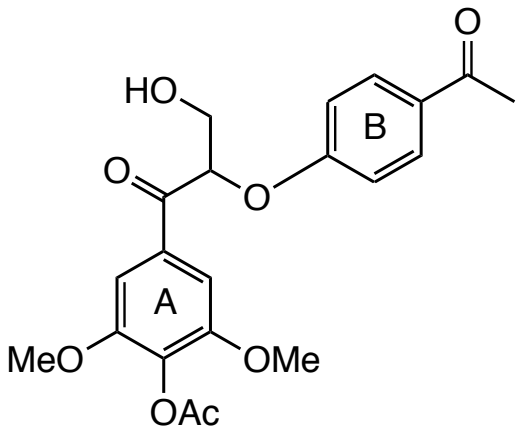
Notes:

SR III - 39
45mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.41	20.22	20.06
B β	26.41	26.54	26.48
OMe	56.24	56.56	56.01
OMe	56.24	56.56	56.01
OMe	56.39	56.70	56.18
OMe	56.39	56.70	56.18
γ	63.36	63.67	62.39
β	87.06	86.08	83.67
A2	105.72	106.52	105.44
A6	105.72	106.52	105.44
B2	105.75	106.62	105.85
B6	105.75	106.62	105.85
A1	133.17	133.66	131.79
A4	133.27	133.80	132.05
B1	133.27	134.87	133.69
B4	140.52	141.29	140.22
A3	152.33	153.21	151.62
A5	152.33	153.21	151.62
B3	152.36	153.21	151.71
B5	152.36	153.21	151.71
Ac C=O	168.05	168.15	167.60
B α	194.74	195.71	195.27
α	196.50	196.65	196.51

Compound Number 80



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

^{1}H (chloroform)

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

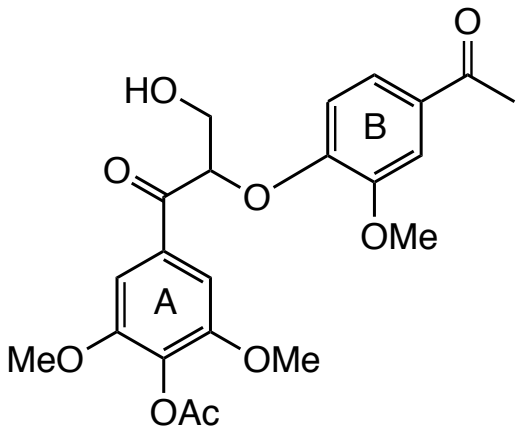
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.40	20.21	20.05
B β	26.33	26.34	26.28
OMe	56.36	56.76	56.31
OMe	56.36	56.76	56.31
γ	63.32	63.94	62.41
β	81.33	82.26	80.64
A2	105.67	106.40	105.42
A6	105.67	106.40	105.42
B3	114.83	115.68	114.78
B5	114.83	115.68	114.78
B2	130.78	131.20	130.36
B6	130.78	131.20	130.36
A1	131.38	131.80	130.19
B1	132.25	133.97	132.74
A4	133.87	134.34	132.55
A3	152.55	153.47	151.98
A5	152.55	153.47	151.98
B4	161.00	162.44	161.22
Ac C=O	168.06	168.11	167.62
B α	194.60	195.47	194.76
α	196.64	196.21	196.08

Compound Number 81



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

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.34	s	
B β	2.53	s	
B3 OMe A3,5 OMe	3.89 3.85	s s	
γ β	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

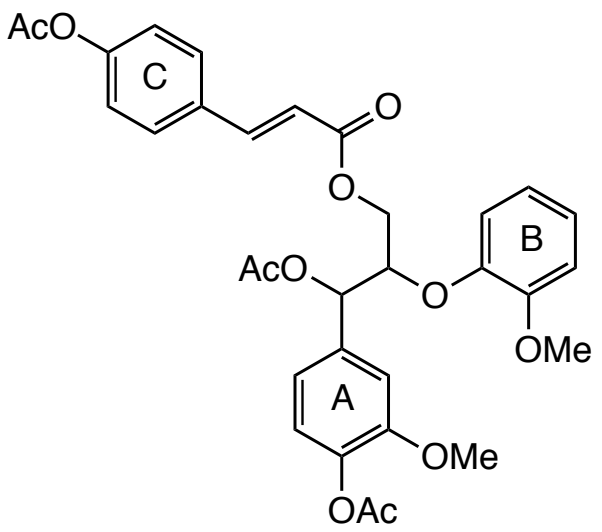
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.39	20.21	20.05
B β	26.23	26.30	26.23
B OMe A OMe A OMe	55.91 56.32 56.32	56.28 56.69 56.69	55.55 56.22 56.22
γ β	63.47 83.63	63.91 83.76	62.32 81.51
A2 A6	105.80 105.80	106.56 106.56	105.45 105.45
B2 B5	111.17 114.89	112.34 114.72	111.05 113.02
B6	123.01	123.46	122.65
A1 B1 A4	132.23 132.38 133.75	132.37 134.04 134.22	130.46 132.75 132.46
B3 B4 A3 A5	149.76 150.76 152.47 152.47	150.40 152.27 153.35 153.35	148.67 150.96 151.87 151.87
Ac C=O	168.00	168.08	167.57
B α α	194.85 196.57	195.94 196.27	195.02 196.14

Notes:

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

Compound Number 82



threo

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

^{1}H (chloroform)

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

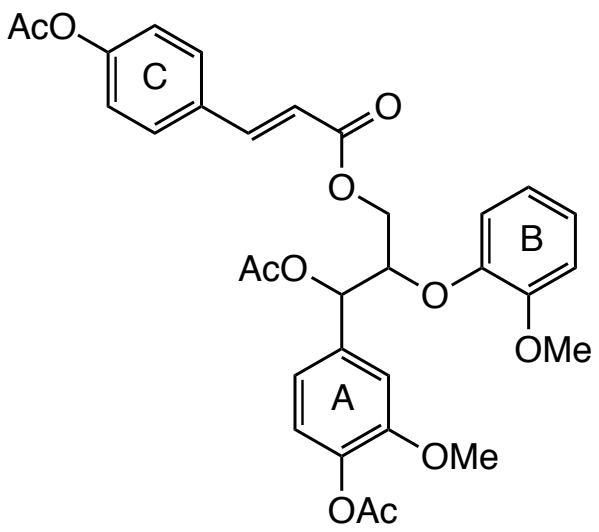
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.63	20.46	20.29
Ac Me	21.07	20.95	20.67
Ac Me	21.10	20.95	20.78
OMe	55.81	56.21	55.55
OMe	55.95	56.28	55.75
γ	63.39	63.93	62.86
α	74.62	75.53	74.43
β	80.50	80.88	79.25
A2	111.78	112.71	111.70
B2	112.55	113.75	112.76
C β	117.58	118.56	117.51
B5	118.98	119.36	117.59
A6	119.56	120.30	119.38
B6	121.01	121.68	120.66
C3	122.13	123.17	122.29
C5	122.13	123.17	122.29
A5	122.84	123.56	122.59
B1	123.35	123.78	129.85
C2	129.30	130.20	129.57
C6	129.30	130.20	129.57
C1	131.95	132.78	131.49
A1	135.36	136.67	135.43
A4	139.94	140.90	139.21
C α	144.22	144.71	143.87
B4	148.00	149.10	147.59
B3	150.92	151.88	150.18
A3	151.14	152.20	150.67
C4	152.23	153.48	152.04
C γ	166.28	166.56	165.66
Ac C=O	168.70	168.81	168.28
Ac C=O	169.02	169.35	168.83
Ac C=O	169.68	169.96	169.32

Compound Number 83



erythro

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

^{1}H (chloroform)

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

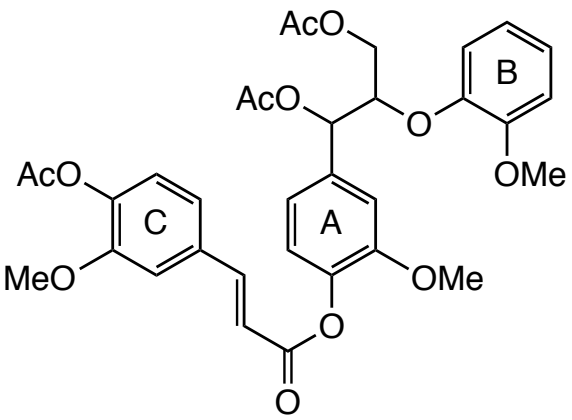
Notes:

Rich Helm RFH87D2
38.6mg
see 1020

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.65	20.47	20.29
Ac Me	21.03	20.90	20.63
Ac Me	21.10	20.95	20.78
OMe	55.80	56.21	55.58
OMe	55.94	56.28	55.70
γ	62.93	63.34	62.26
α	74.01	74.73	73.28
β	80.43	80.54	78.58
A2	112.04	112.78	111.71
B2	112.64	113.79	112.89
C β	117.67	118.54	117.46
B5	119.73	120.01	118.09
A6	119.73	120.44	119.39
B6	121.01	121.64	120.65
C3	122.11	123.17	122.29
C5	122.11	123.17	122.29
A5	122.59	123.35	122.48
B1	123.66	124.09	122.89
C2	129.30	130.18	129.54
C6	129.30	130.18	129.54
C1	132.00	132.77	131.46
A1	135.53	136.71	135.36
A4	139.80	140.78	139.08
C α	144.19	144.68	143.85
B4	147.25	148.31	146.69
B3	151.00	152.10	150.35
A3	151.19	152.10	150.55
C4	152.21	153.48	152.02
C γ	166.42	166.57	165.67
Ac C=O	168.74	168.84	168.32
Ac C=O	169.02	169.35	168.84
Ac C=O	169.50	169.87	169.21

Compound Number 84



erythro

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

^{1}H (chloroform)

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

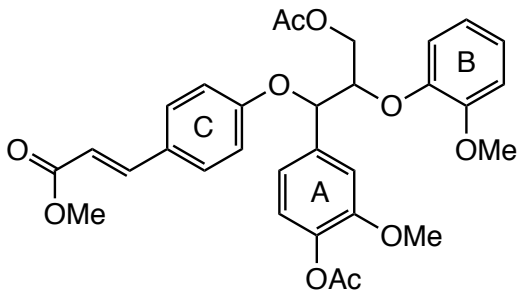
Notes:

R. Helm RFH9D
39.4mg
see 1026

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.62	20.47	20.31
Ac Me	20.76	20.61	20.37
Ac Me	21.01	20.87	20.60
OMe	55.81	56.21	55.58
OMe	55.94	56.28	55.72
OMe	56.00	56.44	55.98
γ	62.59	63.00	61.89
α	73.84	74.61	73.17
β	80.22	80.32	78.40
C2	111.41	112.60	111.69
A2	112.04	112.79	112.13
B2	112.68	113.81	112.90
C β	117.16	118.04	117.09
B5	119.55	119.82	117.96
A6	119.75	120.45	119.36
B6	121.01	121.63	120.64
C6	121.54	122.47	121.90
A5	122.67	123.42	122.54
B1	123.33	124.04	122.87
C5	123.63	124.16	123.18
C1	133.17	134.02	132.77
A1	135.48	136.73	135.40
A4	139.77	140.70	139.03
C4	141.78	142.96	141.30
C α	145.85	146.39	145.79
B4	147.18	148.26	146.63
B3	151.10	152.04	150.32
A3	151.14	152.17	150.63
C3	151.49	152.73	151.17
C γ	164.57	164.96	164.22
Ac C=O	168.64	168.74	168.21
Ac C=O	169.50	169.86	169.20
Ac C=O	170.74	170.70	169.96

Compound Number 85



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

^{1}H (chloroform)

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

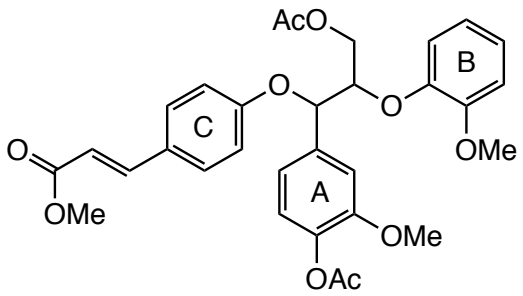
Notes:

R. Helm RFH111D1
39.0 mg
Isomer of 86

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.62	20.45	20.29
Ac Me	20.72	20.60	20.39
C γ OMe	51.54	51.52	51.19
OMe	55.72	56.17	55.53
OMe	55.96	56.27	55.70
γ	62.79	63.18	62.20
α	78.84	79.69	77.75
β	82.13	81.73	79.67
A2	110.95	112.62	111.97
B2	112.61	113.79	112.85
C β	115.75	116.52	115.50
C3	116.22	117.18	116.08
C5	116.22	117.18	116.08
B5	119.05	119.93	117.78
A6	119.92	120.27	119.39
B6	121.05	121.63	120.62
A5	122.86	123.50	122.52
B1	123.75	123.99	122.69
C1	127.82	128.60	127.21
C2	129.63	130.56	129.96
C6	129.63	130.56	129.96
A1	136.23	137.03	135.78
A4	139.65	140.73	139.00
C α	144.26	144.77	143.99
B4	147.06	148.41	146.95
B3	151.23	152.04	150.26
A3	151.32	152.26	150.58
C4	159.48	160.44	158.88
C γ C=O	167.59	167.59	166.74
A4 C=O	168.70	168.78	168.24
A γ	170.74	170.69	169.98

Compound Number 86



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

^{1}H (chloroform)

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

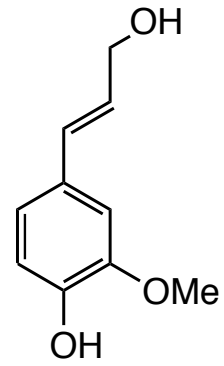
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.62	20.45	20.28	
Ac Me	20.72	20.59	20.36	
C γ OMe	51.53	51.52	51.17	
OMe	55.69	56.14	55.45	
OMe	55.96	56.30	55.74	
γ	63.32	63.70	62.55	
α	79.79	80.57	78.99	
β	81.51	81.71	79.91	
A2	111.00	112.61	111.77	
B2	112.43	113.68	112.70	
C β	115.68	116.43	115.36	
C3	116.25	117.12	116.02	
C5	116.25	117.12	116.02	
B5	119.13	119.33	117.27	
A6	119.23	120.27	119.42	
B6	120.95	121.61	120.58	
A5	122.93	123.67	122.35	
B1	123.40	123.67	122.70	
C1	127.72	128.47	127.02	
C2	129.58	130.52	129.90	
C6	128.58	130.52	129.90	
A1	135.56	136.80	135.66	
A4	139.86	140.88	139.12	
C α	144.28	144.80	144.02	
B4	148.03	149.21	147.68	
B3	150.94	151.85	150.07	
A3	151.42	152.37	150.75	
C4	159.50	160.59	159.19	
C γ C=O	167.60	167.60	166.74	
A4 C=O	168.64	168.76	168.21	
A γ	170.50	170.62	169.91	

Notes:

Rich Helm RFH111D2
35mg
Isomer of 85

Compound Number 87



trans

Coniferyl alcohol

4-hydroxy-3-methoxy cinnamyl alcohol

^{1}H (acetone)

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

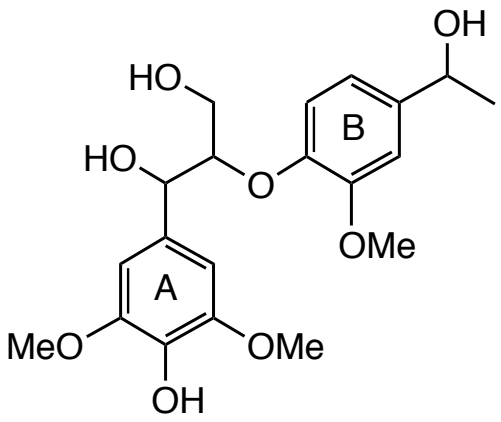
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.88	56.20	55.47
γ	63.71	63.42	61.63
2	108.52	110.06	109.66
5	114.57	115.76	115.36
6	120.25	120.60	119.30
β	126.22	128.07	127.38
1	129.30	130.26	128.41
α	131.24	130.45	128.87
4	145.63	147.14	146.06
3	146.75	148.41	147.60
1H			
OMe	3.89		3.76
γ's	4.28		4.06
β	6.20		6.16
α	6.52		6.40
5	6.90		6.69
6	6.88		6.78
2	6.84		6.97

Compound Number 88



threo

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

^{1}H (acetone)

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

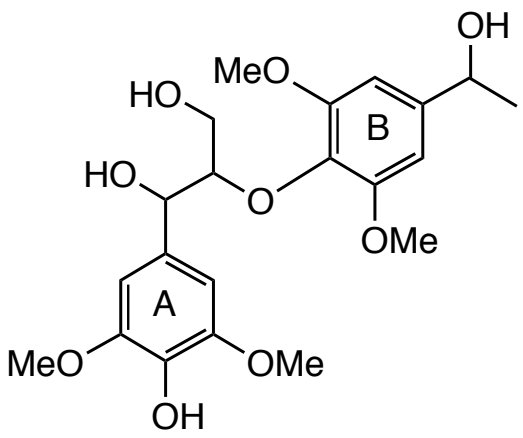
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	25.24	26.23	25.84	
B OMe	55.87	56.27	55.44	
A OMe	56.33	56.59	55.73	
A OMe	56.33	56.59	55.73	
γ	61.04	61.94	59.99	
B α	69.95	69.73	67.80	
α	74.12	74.05	70.87	
β	89.03	88.50	84.39	
A2	103.79	105.36	104.06	
A6	103.79	105.36	104.06	
B2	109.30	110.58	109.65	
B5	118.40	118.65	115.29	
B6	120.27	119.45	117.20	
A1	130.71	132.80	131.93	
A4	134.56	136.12	134.24	
B1	142.02	142.85	140.36	
B4	146.66	148.27	146.73	
A3	147.09	148.38	147.30	
A5	147.09	148.38	147.30	
B3	150.99	151.38	149.23	

Compound Number 89



threo

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

^{1}H (acetone)

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

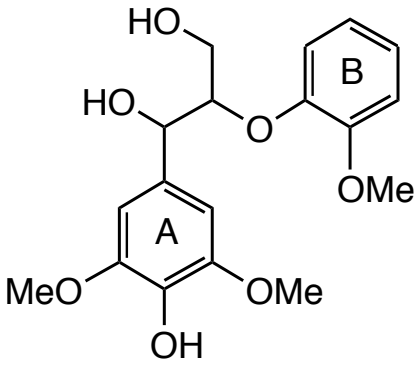
Notes:

S Ralph SRIII-44
30mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	25.43	26.27	25.84
OMe	56.12	56.50	55.80
OMe	56.12	56.50	55.80
OMe	56.31	56.57	55.80
OMe	56.31	56.57	55.80
γ	60.48	61.41	60.15
B α	70.21	69.98	68.09
α	74.34	74.22	71.54
β	88.97	89.69	87.11
B2	102.27	103.41	102.49
B6	102.27	103.41	102.49
A2	104.04	105.46	104.14
A6	104.04	105.46	104.14
A1	130.99	132.60	131.97
B1	134.10	135.54	134.22
A4	134.46	136.11	134.50
B4	142.94	144.61	142.91
A3	147.02	148.30	147.25
A5	147.02	148.30	147.25
B3	152.88	153.58	152.14
B5	152.88	153.58	152.14

Compound Number 90



threo

Syringylglycerol-β-guaiacyl ether

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

^{1}H (acetone)

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

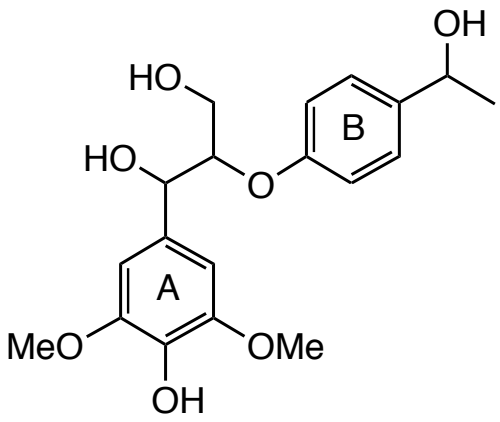
Notes:

S. Ralph SRIII-45
30mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B OMe	55.88	56.24	55.45
A OMe	56.32	56.54	55.72
A OMe	56.32	56.54	55.72
γ	61.02	61.89	60.01
α	74.16	73.97	70.88
β	89.22	88.19	84.03
A2	103.81	105.28	104.07
A6	103.81	105.28	104.07
B2	112.16	113.27	112.38
B5	120.86	119.66	115.52
B6	121.67	121.91	120.58
B1	124.17	123.30	120.90
A1	130.71	132.72	131.89
A4	134.57	136.07	134.26
A3	147.10	148.34	147.31
A5	147.10	148.34	147.31
B4	147.58	149.60	148.18
B3	151.22	151.65	149.55

Compound Number 91



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

^{1}H (acetone)

Atom	H Shifts	Mult	J
B β	1.35	d	6.4
3,5 OMe	3.79	s	
A2,6	6.77	s	
B2,6	7.23	m	8.6

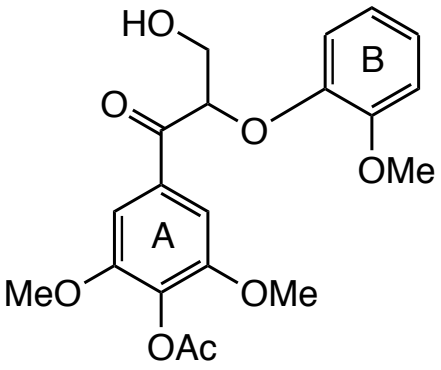
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	25.07	26.17	25.81	
OMe	56.34	56.58	55.82	
OMe	56.34	56.58	55.82	
γ	61.14	61.73	60.01	
B α	69.75	69.50	67.57	
α	73.85	73.54	71.09	
β	82.97	84.14	83.01	
A2	103.70	105.27	104.12	
A6	103.70	105.27	104.12	
B3	116.34	116.64	115.34	
B5	116.34	116.64	115.34	
B2	126.84	127.15	126.13	
B6	126.84	127.15	126.13	
A1	130.90	133.23	132.31	
A4	134.56	136.00	134.31	
B1	139.33	140.47	139.21	
A3	147.07	148.32	147.36	
A5	147.07	148.32	147.36	
B4	157.42	158.98	157.69	

Compound Number 92



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

^{1}H (chloroform)

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

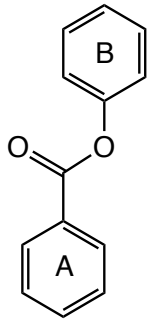
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.41	20.21	20.04
B OMe	55.73	56.07	55.39
A OMe	56.29	56.60	56.12
A OMe	56.29	56.60	56.12
γ	63.39	63.88	62.35
β	84.41	84.02	81.59
A2	105.84	106.50	105.38
A6	105.84	106.50	105.38
B2	112.33	113.57	112.64
B5	117.86	116.84	114.73
B6	121.23	121.57	120.49
B1	123.61	123.15	121.67
A4	133.42	133.93	132.25
A1	132.81	134.31	132.99
B4	146.71	148.17	146.73
B3	150.24	150.90	149.13
A3	152.32	153.19	151.75
A5	152.32	153.19	151.75
Ac C=O	168.06	168.10	167.58
α	195.72	196.70	195.86

Compound Number 93



Phenyl benzoate

Benzoic acid phenyl ester

^{1}H (chloroform)

Atom	H Shifts	Mult	J
A2,6	8.21	m	8.3

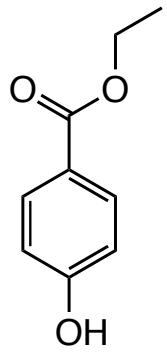
Notes:

Aldrich
60mg
Al changes position in DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3	121.70	122.61	121.85	
B5	121.70	122.61	121.85	
B1	125.84	126.51	125.92	
A2	128.54	129.47	128.88	
A6	128.54	129.47	128.88	
B2	129.45	130.15	129.50	
B6	129.45	130.15	129.50	
A1	129.57	130.42	128.94	
A3	130.13	130.60	129.72	
A5	130.13	130.60	129.72	
A4	133.53	134.39	133.93	
B4	150.96	151.99	150.62	
α	165.11	165.32	164.51	

Compound Number 94



Ethyl 4-hydroxybenzoate

ethyl 4-hydroxybenzoate

^{1}H (chloroform)

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

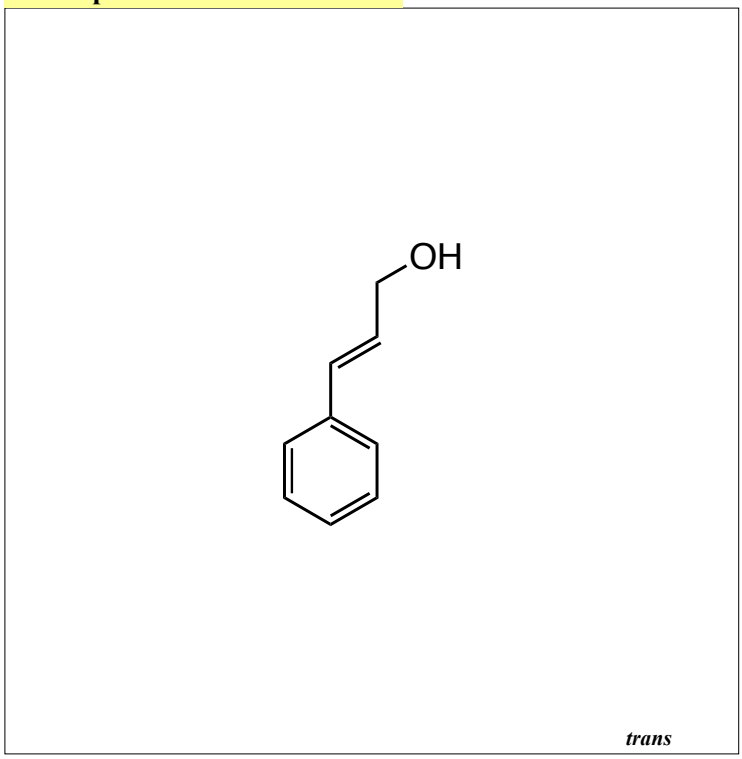
Notes:

Aldrich
60mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	14.30	14.63	14.24	
CH2	61.13	60.84	60.04	
3	115.34	115.92	115.27	
5	115.34	115.92	115.27	
1	122.13	122.69	120.61	
2	131.94	132.30	131.35	
6	131.94	132.30	131.35	
4	160.74	162.44	161.93	
α	167.45	166.49	165.56	

Compound Number 95



trans

Cinnamyl alcohol

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

^{1}H (chloroform)

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

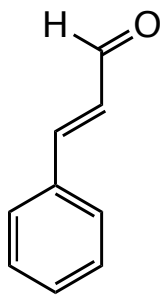
Notes:

Fluka
60mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	63.39	63.12	61.50	
2	126.40	126.98	126.05	
6	126.40	126.98	126.05	
β	127.57	127.93	127.08	
3	128.52	129.25	128.49	
5	128.52	129.25	128.49	
4	128.52	129.90	128.37	
α	130.86	130.90	130.72	
1	136.66	138.08	136.87	

Compound Number 96



trans

Cinnamaldehyde

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

^{1}H (chloroform)

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

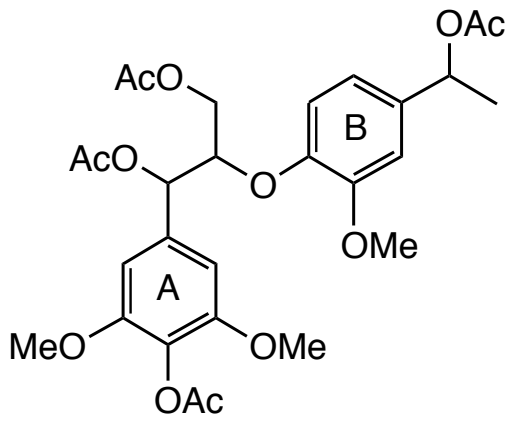
Notes:

Fluka
60mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
2	128.45	129.30	128.69	
6	128.45	129.30	128.69	
4	128.45	129.40	128.50	
3	129.04	129.81	129.02	
5	129.04	129.81	129.02	
β	131.20	131.78	131.13	
1	133.96	135.19	134.07	
α	152.66	153.19	153.00	
γ	193.54	193.96	194.19	

Compound Number 97



threo

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

^{1}H (chloroform)

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

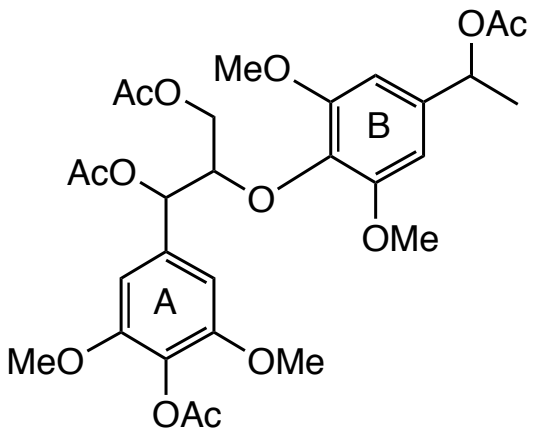
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.42	20.23	20.04	
Ac Me	20.70	20.62	20.37	
Ac Me	21.04	20.93	20.63	
Ac Me	21.35	21.15	20.93	
B β	22.08	22.46	21.87	
B OMe	55.88	56.29	55.61	
A OMe	56.21	56.52	55.96	
A OMe	56.21	56.52	55.96	
γ	62.98	63.58	62.42	
B α	72.06	72.40	71.35	
α	74.65	75.64	74.54	
β	80.12	80.68	79.08	
A2	104.09	104.93	103.91	
A6	104.09	104.93	103.91	
B2	110.64	111.71	110.55	
B5	118.22	118.71	117.03	
B6	118.65	119.18	118.05	
A4	128.83	129.65	127.78	
A1	134.71	136.12	134.92	
B1	136.72	137.72	136.00	
B4	147.53	148.51	146.99	
B3	150.58	151.52	149.82	
A3	152.17	153.14	151.52	
A5	152.17	153.14	151.52	
A4 Ac C=O	168.47	168.40	167.88	
α Ac C=O	169.66	169.96	169.32	
B αAc C=O	170.27	170.17	169.52	
γAc C=O	170.55	170.65	169.92	

Compound Number 98



threo

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

^{1}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	

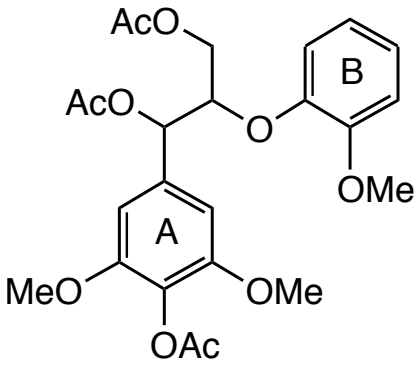
Notes:

S. Ralph SRIII-44
131mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.42	20.23	20.06	
Ac Me	20.72	20.63	20.37	
Ac Me	21.02	20.92	20.62	
Ac Me	21.33	21.14	20.95	
Bβ	22.25	22.56	22.02	
OMe	56.02	56.36	55.78	
OMe	56.02	56.36	55.78	
OMe	56.21	56.45	55.98	
OMe	56.21	56.45	55.98	
γ	63.53	64.18	63.22	
B α	72.35	72.68	71.72	
α	75.61	76.62	75.73	
β	80.64	81.44	80.27	
B2	103.14	103.92	102.85	
B6	103.14	103.92	102.85	
A2	104.18	104.78	103.76	
A6	104.18	104.78	103.76	
A4	128.64	129.42	127.75	
A1	135.46	136.61	135.39	
B1	135.95	136.96	135.48	
B4	137.57	138.68	137.40	
A3	151.98	152.94	151.52	
A5	151.98	152.94	151.52	
B3	152.87	153.69	152.27	
B5	152.87	153.69	152.27	
A4 Ac C=O	168.49	168.37	167.93	
α Ac C=O	169.70	169.80	169.27	
B αAc C=O	170.16	170.11	169.56	
γ Ac C=O	170.50	170.56	169.95	

Compound Number 99



threo

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

^{1}H (acetone)

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

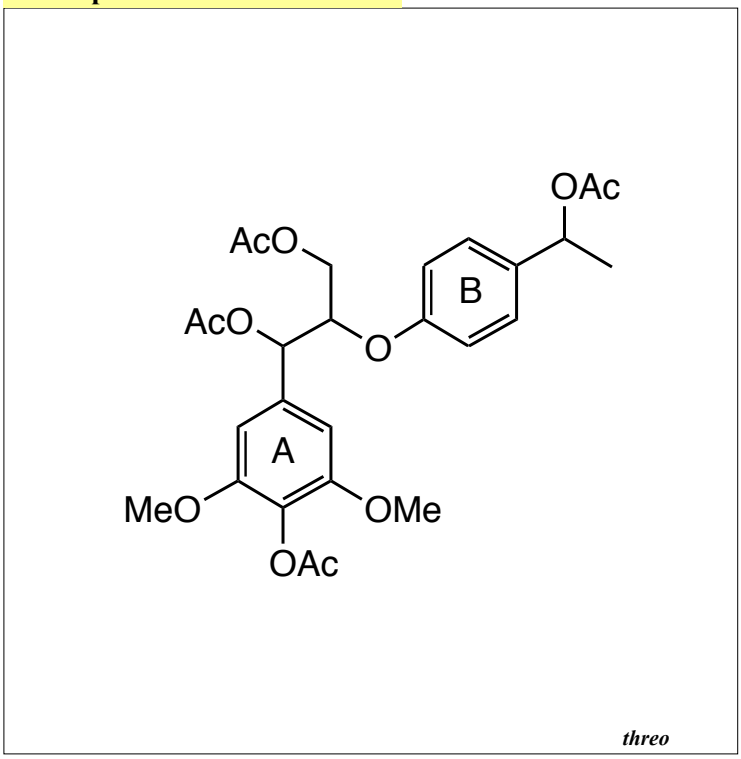
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.42	20.24	20.05	
Ac Me	20.71	20.62	20.39	
Ac Me	21.05	20.94	20.65	
B OMe	55.77	56.20	55.52	
OMe	56.20	56.52	55.97	
OMe	56.20	56.52	55.97	
γ	63.08	63.60	62.48	
α	74.77	75.67	74.58	
b	80.23	80.64	79.00	
A2	104.08	104.93	103.92	
A6	104.08	104.93	103.92	
B2	112.48	113.71	112.69	
B5	118.61	119.04	117.31	
B6	120.98	121.66	120.63	
B1	123.28	123.68	122.49	
A4	128.79	129.65	127.81	
A1	134.80	136.18	134.99	
B4	147.92	149.06	147.54	
B3	150.76	151.75	150.06	
A3	152.16	153.14	151.56	
A5	152.16	153.14	151.56	
A4 Ac C=O	168.47	168.41	167.89	
α Ac C=O	169.68	169.97	169.34	
γ Ac C=O	170.55	170.66	169.94	

Compound Number 100



threo

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

^{1}H (chloroform)

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

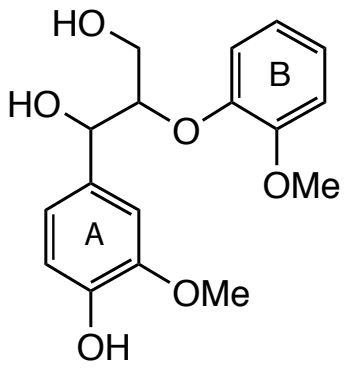
Notes:

S. Ralph SRIII-46
24mg
CDCl3 spectrum poor

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.43	20.23	20.04	
Ac Me	20.68	20.60	20.38	
Ac Me	21.03	20.89	20.62	
Ac Me	21.36	21.15	20.92	
B β	22.01	22.36	21.76	
OMe	56.25	56.58	56.01	
OMe	56.25	56.58	56.01	
γ	62.67	63.31	62.15	
B α	71.85	72.19	71.12	
α	74.24	75.45	74.32	
β	78.17	79.23	77.60	
A2	104.09	105.05	104.00	
A6	104.09	105.05	104.00	
B3	116.32	117.12	116.00	
B5	116.32	117.12	116.00	
B2	127.67	128.29	127.28	
B6	127.67	128.29	127.28	
A4	128.95	129.80	127.83	
B1	134.35	135.98	134.66	
A1	135.26	136.24	134.81	
A3	152.28	153.25	151.57	
A5	152.28	153.25	151.57	
B4	158.02	159.20	157.68	
A4 Ac C=O	168.44	168.39	167.86	
α Ac C=O	169.69	170.02	169.37	
Bα Ac C=O	170.30	170.19	169.52	
γ Ac C=O	170.56	170.68	169.94	

Compound Number 101



erythro

Guaiacylglycerol-β-guaiacyl ether

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

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.83	s	
OMe	3.84	s	
γ1	3.64	dd	3.35, 12.2
γ2	3.89	dd	obscured
β	4.16	m	
α	4.95	d	4.8
B5	6.81	dd	
A5	6.87		
B6	6.90		
B2	6.92		
A2	6.95		
A6	6.96		
B1	7.05		

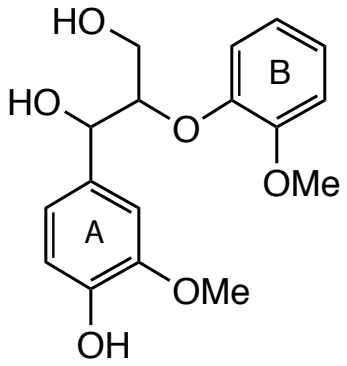
Notes:

J. Ralph JRB 178.3
30mg
J. Ralph Holzforschung 42(1988) p273-5
13C CDCl3 data S.Ralph, 1H from HSQC 500MHz

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.88	56.20	55.93
OMe	55.97	56.27	56.08
γ	60.71	61.81	60.65
α	72.73	73.82	72.17
β	87.51	86.72	83.89
A2	108.57	111.38	111.78
B2	112.16	113.50	113.09
A5	114.24	115.12	115.09
A6	118.99	119.70	116.23
B5	121.12	120.45	120.06
B6	121.65	121.85	121.29
B1	124.30	123.32	121.75
A1	131.72	134.23	133.63
A4	145.09	146.61	145.80
A3	146.60	147.93	147.48
B4	146.84	149.04	148.31
B3	151.64	151.96	150.11
1H			
OMe		3.80	3.66
OMe		3.80	3.68
γ1		3.68	3.58
γ2		3.80	
β		4.28	4.29
α		4.88	4.68
B5		6.88	6.91
A5		6.76	6.65
B6		6.81	6.77
B2		6.95	6.86
A2		7.10	6.95
A6		6.96	6.74
B1		6.92	6.81

Compound Number 102



threo

Guaiacylglycerol-β-guaiacyl ether

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

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.71	s	
OMe	3.75	s	
γ1	3.23	dd	6.4, 11.6
γ2	3.57	dd	4.0, 11.6
β	4.24	dt	4.4, 6.4
α	4.71	d	4.8
B5	7.01	dd	1.6, 7.9
A5	6.67	d	8.0
B6	6.82	dt	1.6, 7.7
B2	6.94	dd	1.7, 8.0
A2	6.96	d	2.0
A6	6.75	dd	2.0, 8.0
B1	6.85	dt	1.6, 7.7

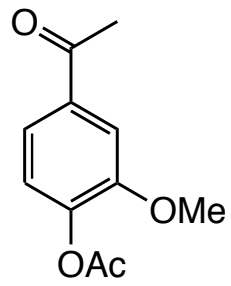
Notes:

J. Ralph JRGV 135.X1
21mg
J. Ralph Holzforschung 42(1988) p.273-5
CDCl3 data S.Ralph, 500MHz, 1H from HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.88	56.21	55.38
OMe	55.97	56.31	55.58
γ	61.04	61.90	60.07
α	74.02	73.93	70.92
β	89.64	88.58	84.36
A2	109.36	111.41	110.98
B2	112.16	113.40	112.54
A5	114.30	115.21	114.65
B5	120.28	120.06	115.75
A6	121.12	120.57	118.99
B6	121.70	121.95	120.69
B1	124.30	123.44	121.03
A1	131.45	133.81	132.97
A4	145.58	146.82	145.40
A3	146.64	148.00	146.97
B4	147.58	149.70	148.39
B3	151.33	151.80	149.69
1H			
OMe	3.89	3.81	
OMe	3.90	3.86	
γ1	3.47	3.48	
γ2	3.61	3.66	
β	4.00	4.16	
α	4.95	4.86	
B5	6.91	7.18	
A5	6.88	6.76	
B6	6.92	6.85	
B2	6.94	6.99	
A2	6.96	7.08	
A6	6.96	6.89	
B1	7.06	6.95	

Compound Number 103



Acetylated acetovanillone
4-acetoxy-3-methoxyacetophenone

^{1}H (chloroform)

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

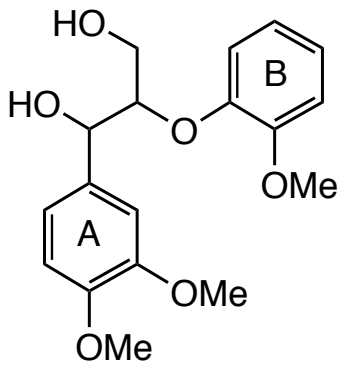
Notes:

IPC
45mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.61	20.46	20.29	
β	26.49	26.63	26.62	
OMe	56.05	56.37	55.88	
2	111.51	112.44	111.62	
6	121.94	122.38	121.56	
5	122.80	123.77	123.02	
1	135.96	136.93	135.62	
4	143.87	144.80	143.21	
3	151.41	152.40	150.92	
Ac C=O	168.46	168.64	168.12	
α	196.91	196.89	196.88	

Compound Number 104



threo

Veratrylglycerol-β-guaiacyl ether
1-(3,4-Dimethoxyphenyl)-2-(2-methoxyphenoxy)propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.76		
OMe	3.81		
B OMe	3.85		
γ1	3.47	m	
γ2	3.62	m	
β	4.01	m	
α	4.98	m	
α OH			
B6	6.92		
A5	6.84		
B1	7.06		
B5	7.12		
B2	6.94		
A6	6.97		
A2	6.98		

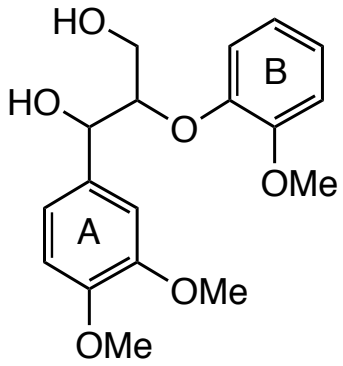
Notes:

LL Landucci
Shifts are for threo isomer from a mixture
see 105

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.87	55.97	55.22	
OMe	55.91	56.05	55.42	
OMe	55.91	56.25	55.52	
γ	61.02	61.79	60.02	
α	73.93	73.74	70.77	
β	89.63	88.37	84.26	
A5	110.98	112.19	111.13	
A2	109.84	111.76	110.67	
B2	112.15	113.33	112.52	
B5	121.15	119.91	115.84	
A6	118.34	120.07	118.62	
B6	121.71	121.93	120.56	
B1	124.34	123.42	120.95	
A1	132.02	134.98	134.47	
A4	147.55	149.62	147.72	
B4	148.90	149.71	147.98	
A3	149.08	150.03	148.25	
B3	151.34	151.76	149.67	
OMe		3.77	3.70	
OMe		3.77	3.70	
B OMe		3.85	3.75	
γ1		3.48	3.22	
γ2		3.68	3.59	
β		4.19	4.26	
α		4.91	4.75	
α OH		4.49	4.64	
γ OH			5.33	
B6		6.85	6.82	
A5		6.87	6.84	
B1		6.95	6.85	
B5		7.17	7.01	
B2		6.99	6.94	
A6		6.96	6.89	
A2		7.10	7.01	

Compound Number 105



erythro

Veratrylglycerol-β-guaiacyl ether
1-(3,4-Dimethoxyphenyl)-2-(2-methoxyphenoxy)-propane-1,3-diol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
OMe	3.85	s	
OMe	3.85	s	
OMe	3.85	s	
α	4.99	d	4.8
β	4.17	m	
γ1	3.69	m	
γ2	3.92	m	
A2	6.90	m	
A6	6.99	m	

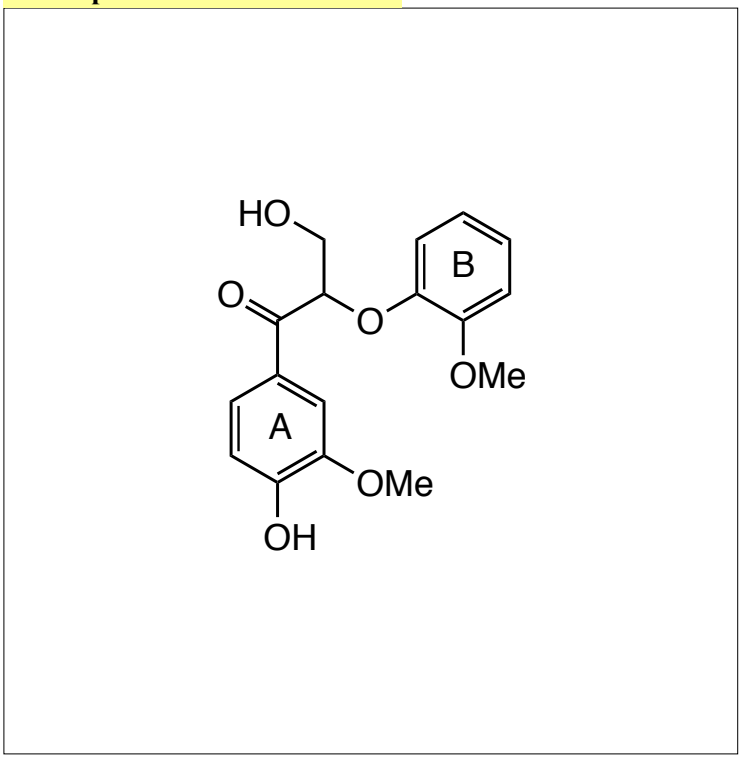
Notes:

LL Landucci, S.Ralph
30mg
Aromatic protons from HSQC
Many assignments are very close and may be switched
HMBC for acetone, DMSO, DMSO/pyridine 500MHz

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.87	56.07	55.23	55.23
OMe	55.91	56.15	55.44	55.44
OMe	55.91	56.30	55.54	55.51
γ	60.81	61.79	60.03	60.25
α	72.75	73.75	71.54	71.81
β	87.10	86.58	83.62	83.87
A2	109.41	111.97	111.03	111.26
A5	111.08	112.35	111.14	111.10
B2	112.21	113.55	112.61	112.62
A6	118.49	120.06	115.95	119.35
B5	120.68	119.64	119.18	116.09
B6	121.58	121.86	120.56	120.69
B1	124.02	123.32	120.95	121.40
A1	132.70	135.50	134.79	135.02
B4	146.96	149.03	147.76	148.16
A4	148.48	149.63	147.99	147.96
A3	149.02	150.04	148.10	148.34
B3	151.47	151.96	149.72	149.92
1H				
OMe		3.76	3.68	3.67
OMe		3.77	3.69	3.69
OMe		3.81	3.70	3.70
γ1		3.67	3.58	3.74
γ2		3.81	3.58	3.80
β		4.29	4.30	4.49
α		4.91	4.73	4.95
α OH		4.55	5.38	5.74
B6		6.81	6.79	6.80
A5		6.87	6.84	6.84
B1		6.92	6.82	6.82
B5		6.95	6.96	7.08
B2		6.96	6.89	6.87
A6		6.96	6.88	7.00
A2		7.11	7.01	7.15

Compound Number 106



Erone

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

^{1}H (chloroform)

Atom	H Shifts	Mult	J
A OMe	3.84	s	
B OMe	3.92	s	
γ	4.04	d	5.1
β	5.38	t	5.1
OH	6.13	s	
B6	6.80	t	7.8
B5	6.88		
B2	6.89		
A5	6.93		
B1	6.98	t	7.8
A2	7.61	bs	
A6	7.68	bd	8.4

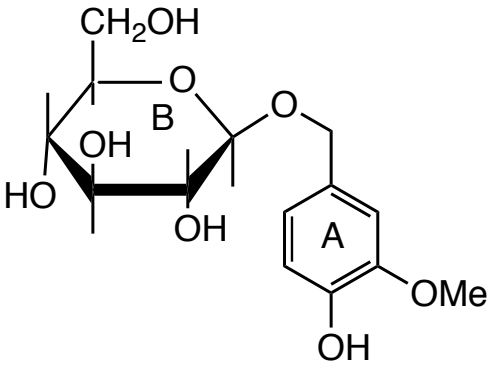
Notes:

S. Ralph
CS for B5, B2, A5 are taken from HSQC
HSQC and HMBC in all solvents
B4, A3 change order in CDCl3 and A5, B5 change order in DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B OMe	55.79	56.19	55.51
A OMe	56.09	56.23	55.55
γ	63.73	64.14	62.56
β	84.48	83.78	81.25
A2	110.71	112.47	111.67
B2	112.31	113.69	112.68
A5	114.01	115.48	115.02
B5	118.61	116.89	114.37
B6	121.16	121.58	120.55
B1	123.69	123.00	121.51
A6	124.25	124.70	123.57
A1	127.80	128.74	126.83
B4	146.93	148.29	146.98
A3	146.77	148.49	147.56
B3	150.51	151.03	149.15
A4	151.08	152.71	152.27
α	194.80	195.63	194.78
1H			
A OMe		3.79	3.73
B OMe		3.88	3.79
γ		4.03	3.86
β		5.52	5.58
B6		6.77	6.74
B5		6.85	6.71
B2		6.96	6.95
A5		6.91	6.86
B1		6.89	6.85
A2		7.67	7.53
A6		7.75	7.66

Compound Number 107



Vanillyl-β-D-Glucoside

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

^{1}H Not run

Atom	H Shifts	Mult	J

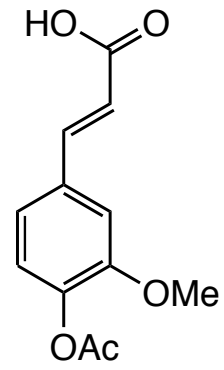
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.30	55.46	
B6		63.00	61.09	
B4		70.98	69.40	
B2		71.74	70.09	
B5		74.90	73.40	
α		77.48	76.66	
B3		78.02	76.82	
B1		102.70	101.52	
A2		112.81	112.29	
A5		115.41	114.90	
A6		121.77	120.50	
A1		130.28	128.57	
A3		147.00	145.80	
A4		148.21	147.25	

Compound Number 108



threo

Acetylated ferulic acid

4-acetoxy-3-methoxycinnamic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.33	s	
OMe	3.88	s	
β	6.38	d	15.9
5	7.05	d	8.0
6	7.13	dd	1.7, 8.0
2	7.11	d	1.7
α	7.72	d	15.9

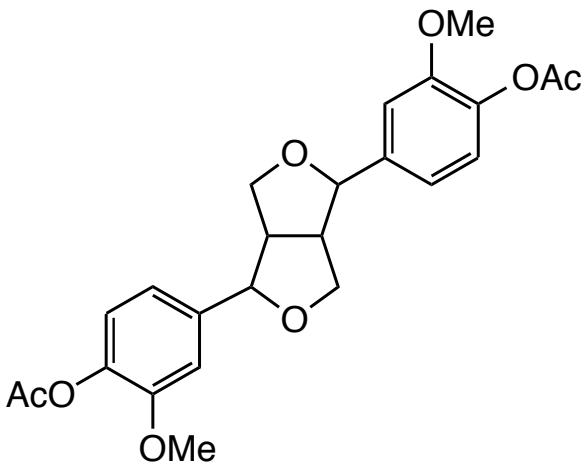
Notes:

R. Helm RFH 83F1
FPL Collection all data
500MHz
HSQC and HMBC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.64	20.47	20.43	
OMe	55.93	56.39	56.01	
2	111.40	112.42	111.86	
β	117.14	119.42	119.60	
6	121.57	122.07	121.36	
5	123.34	124.12	123.24	
1	132.97	134.37	133.30	
4	141.80	142.60	140.82	
α	146.26	144.84	143.34	
3	151.46	152.70	151.18	
Ac C=O	168.73	167.67	167.65	
γ	170.45	168.84	168.47	
1H				
Ac Me		2.24	2.25	
OMe		3.90	3.81	
β		6.53	6.57	
5		7.10	7.10	
6		7.25	7.25	
2		7.45	7.46	
α		7.64	7.56	

Compound Number 109



Pinoresinol diacetate

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

^{1}H (chloroform)

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

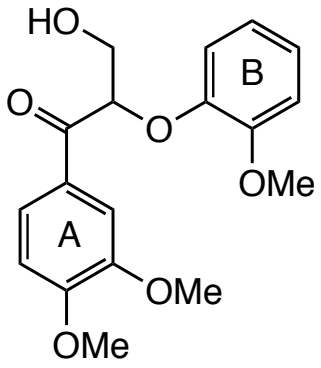
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.62	20.48	20.28	
β	54.36	55.42	53.75	
OMe	55.92	56.23	55.67	
γ	71.95	72.58	71.24	
α	85.50	86.22	84.64	
2	109.91	111.12	110.33	
6	117.92	118.63	117.78	
5	122.74	123.46	122.50	
4	139.13	140.15	138.42	
1	140.11	141.80	140.41	
3	151.23	152.28	150.70	
Ac C=O	168.99	168.98	168.44	

Notes:

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

Compound Number 110



Veratrone

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

^{1}H (chloroform)

Atom	H Shifts	Mult	J
B3 OMe	3.84	s	
A3 OMe	3.90	s	
A4 OMe	3.93	s	
γ	4.05	d	5.2
β	5.38	t	5.2
B6	6.80	dt	1.4, 7.9
B5	6.86	dd	1.5, 7.9
A5	6.86	d	8.5
B2	6.89	dd	1.2, 8.2
B1	6.97	dt	1.5, 8.1
A2	7.60	d	2.0
A6	7.73	dd	8.4, 2.0

Notes:

LL Landucci
S.Ralph, J. Ralph 700MHz
HSQC and HMBC all solvents

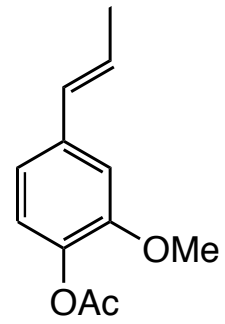
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe	55.82	56.02	55.45	55.35
A3 OMe	55.97	56.20	55.51	55.43
A4 OMe	56.10	56.20	55.79	55.67
γ	63.73	64.13	62.52	62.68
β	84.31	83.86	81.33	81.61
A5	110.08	111.50	110.72	110.84
A2	110.93	112.17	110.93	110.87
B2	112.26	113.72	112.69	112.65
B5	118.27	116.97	114.52	114.63
B6	121.16	121.59	120.53	120.52
B1	123.55	123.06	121.57	121.58
A6	123.61	124.30	123.31	123.35
A1	128.02	129.45	127.91	128.04
B4	146.91	148.47	146.93	147.07
A3	149.19	150.09	148.56	148.64
B3	150.38	151.06	149.16	149.26
A4	153.93	154.91	153.46	153.52
α	195.96	195.96	195.21	195.30

1H

B3 OMe		3.78	3.73	3.72
A3 OMe		3.84	3.79	3.77
A4 OMe		3.89	3.84	3.82
γ		4.05	3.88	4.01
β		5.53	5.62	5.71
B6		6.77	6.75	6.75
B5		6.86	6.73	6.83
A5		7.04	7.07	7.05
B2		6.96	6.95	6.94
B1		6.89	6.86	6.86
A2		7.64	7.52	7.61
A6		7.83	7.80	7.87

Compound Number 111



acetylated isoeugenol

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

^{1}H (chloroform)

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

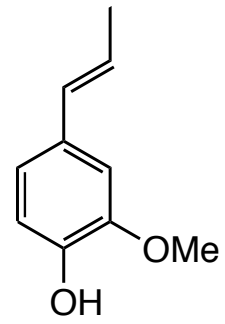
Notes:

J. Ralph JRPS115.1
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	18.37	18.45	18.11	
Ac Me	20.62	20.45	20.32	
OMe	55.77	56.10	55.64	
2	109.69	110.54	109.73	
6	118.36	118.90	117.99	
5	122.65	123.53	122.68	
β	126.01	126.34	125.80	
α	130.48	131.36	130.24	
1	137.06	137.70	136.44	
4	138.65	139.88	138.24	
3	151.02	152.26	150.86	
Ac C=O	169.04	168.95	168.46	

Compound Number 112



Isoeugenol

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

^{1}H (chloroform)

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

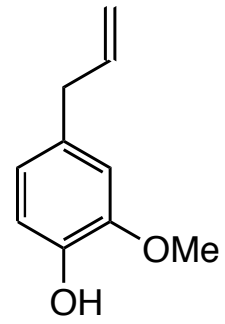
Notes:

Aldrich
50mg contains an impurity

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	18.30	18.38	18.05	
OMe	55.82	56.13	55.50	
2	108.01	109.64	109.41	
5	114.43	115.66	115.41	
6	119.30	119.89	118.78	
β	123.34	122.97	121.98	
1	130.66	130.93	129.11	
α	130.78	131.86	130.87	
4	144.79	146.61	145.80	
3	146.61	148.28	147.64	

Compound Number 113



Eugenol
4-Allyl-2-methoxyphenol

^{1}H (chloroform)

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

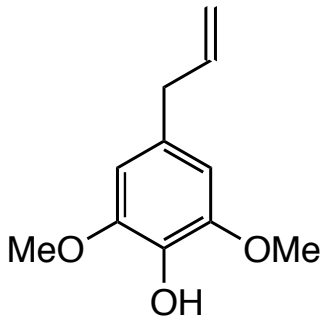
Notes:

Aldrich
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	39.88	40.32	39.08	
OMe	55.86	56.16	55.49	
2	111.17	112.83	112.58	
γ	114.31	115.31	115.11	
5	115.46	115.61	115.35	
6	121.19	121.66	120.48	
1	131.90	132.07	130.39	
β	137.83	139.05	138.13	
4	143.93	145.68	144.72	
3	146.47	148.13	147.43	

Compound Number 114



4-Allyl-2,6-dimethoxyphenol

^{1}H (chloroform)

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

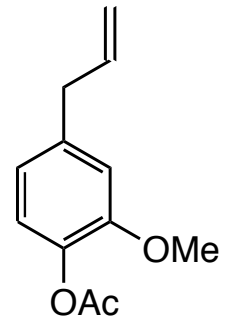
Notes:

Aldrich 50mg Extraneous peaks
around 106 and 119

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	40.31	40.73	39.53	
OMe	56.26	56.58	55.89	
OMe	56.26	56.58	55.89	
2	105.26	106.83	105.83	
6	105.26	106.83	105.83	
γ	115.65	115.42	115.26	
1	131.06	131.13	129.63	
4	133.10	135.19	133.81	
β	137.60	138.95	137.98	
3	147.03	148.60	147.93	
5	147.03	148.60	147.93	

Compound Number 115



acetylated eugenol

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

^{1}H (chloroform)

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

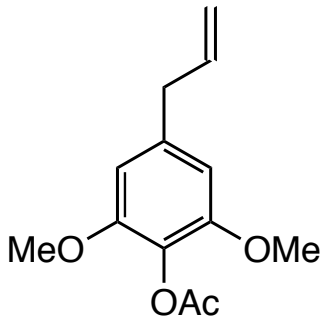
Notes:

J. Ralph JRC91.1
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.64	20.45	20.30	
α	40.08	40.51	39.26	
OMe	55.81	56.08	55.57	
2	112.76	113.66	112.82	
γ	116.12	116.03	115.87	
5	120.66	121.10	120.15	
6	122.51	123.37	122.48	
β	137.03	138.32	137.34	
4	138.05	139.24	137.53	
1	138.98	139.72	138.66	
3	150.89	152.10	150.61	
Ac C=O	169.12	168.95	168.47	

Compound Number 116



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

^{1}H (chloroform)

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

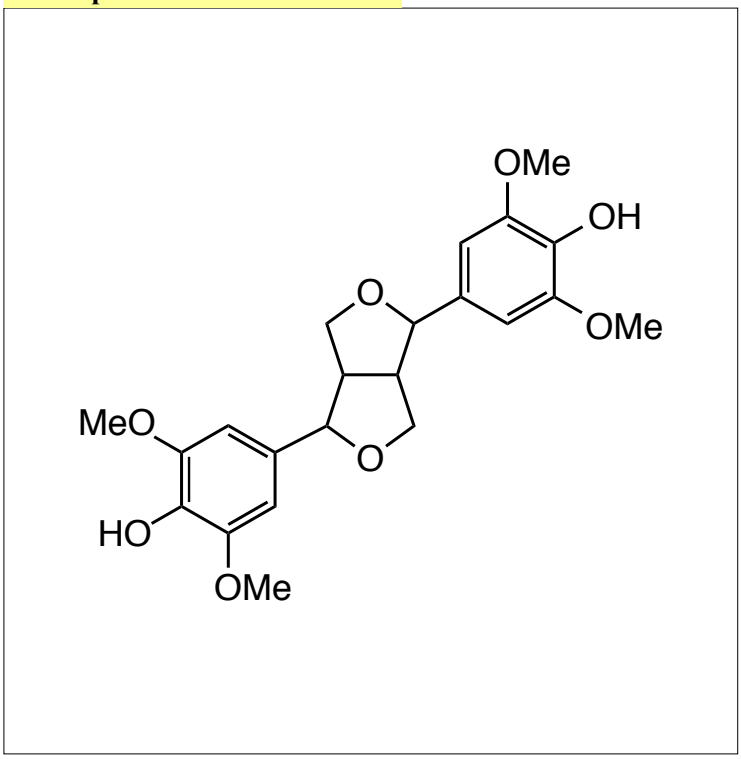
Notes:

J. Ralph JRPS143.1
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.43	20.24	20.09
α	40.64	41.06	39.89
OMe	56.07	56.32	55.80
OMe	56.07	56.32	55.80
2	105.16	105.93	105.01
6	105.16	105.93	105.01
γ	116.22	116.11	115.97
4	126.99	128.10	126.33
β	136.90	138.24	137.27
1	138.52	139.32	138.31
3	151.97	153.06	151.58
5	151.97	153.06	151.58
Ac C=O	168.81	168.56	168.06

Compound Number 117



Syringylresinol

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

^{1}H (chloroform)

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

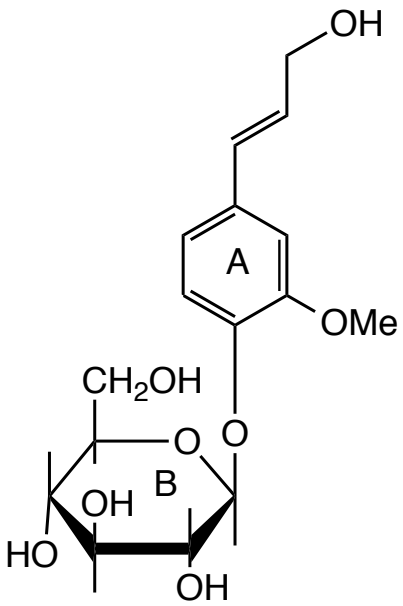
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	54.38	55.33	53.59	
OMe	56.41	56.69	55.95	
OMe	56.41	56.69	55.95	
γ	71.83	72.37	70.99	
α	86.08	86.81	85.26	
2	102.78	104.52	103.59	
6	102.78	104.52	103.59	
1	132.13	133.24	131.36	
4	134.38	136.23	134.81	
3	147.19	148.69	147.82	
5	147.19	148.69	147.82	

Compound Number 118



Coniferin

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

^{1}H (DMSO)

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

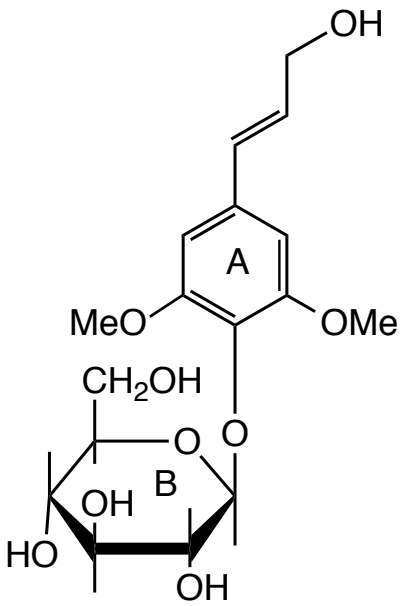
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe			55.57
B6			60.60
γ			61.51
B4			69.60
B2			73.12
B5			76.76
B3			76.91
B1			100.00
A2			109.84
A5			115.25
A6			118.89
β			128.31
α			128.87
A1			130.95
A4			145.89
A3			148.94

Notes:

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

Compound Number 119



Syringin

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

^{1}H (DMSO)

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

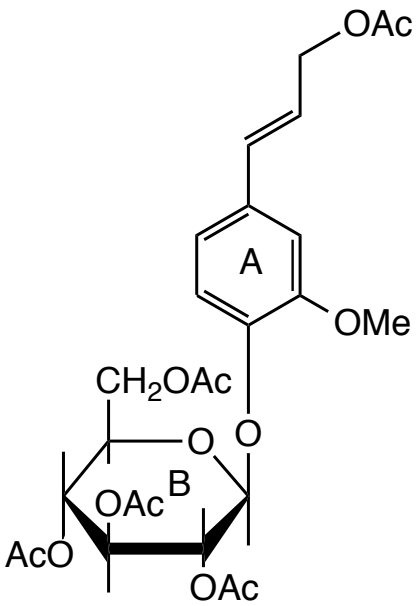
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe			56.27	
OMe			56.27	
B6			60.82	
γ			61.37	
B4			69.86	
B2			74.09	
B5			76.45	
B3			77.08	
B1			102.51	
A2			104.39	
A6			104.39	
β			128.35	
α			130.05	
A1			132.52	
A4			133.80	
A3			152.60	
A5			152.60	

Notes:

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

Compound Number 120



Coniferin acetate

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

^{1}H (chloroform)

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

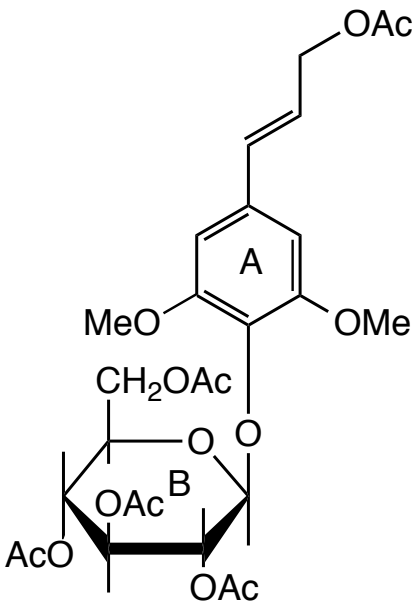
Notes:

S. Ralph III-58
50mg
Assignments determined from HSQC and HMBC in DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B2 Ac Me	20.60	20.51	20.26	
B4 Ac Me	20.60	20.59	20.30	
B3 Ac Me	20.60	20.59	20.34	
B6Ac Me	20.66	20.59	20.45	
γ Ac Me	20.95	20.78	20.68	
OMe	56.07	56.47	55.88	
B6	61.97	62.69	61.63	
γ	64.93	65.23	64.33	
B4	68.46	69.33	68.09	
B2	71.24	71.96	70.71	
B5	72.02	72.56	70.80	
B3	72.61	73.23	71.84	
B1	100.67	100.79	98.65	
A2	110.58	111.55	110.63	
A5	119.57	119.77	117.95	
A6	119.93	120.26	119.35	
β	122.83	123.86	123.04	
A1	133.02	133.63	132.10	
α	133.58	133.82	132.66	
A4	146.09	147.19	145.61	
A3	150.69	151.44	149.87	
B3 Ac C=O	169.26	169.58	168.97	
B4 Ac C=O	169.36	169.96	169.30	
B2 Ac C=O	170.15	170.22	169.55	
B6 Ac C=O	170.47	170.58	169.96	
γ Ac C=O	170.71	170.69	170.14	
1H				
B2 Ac Me			1.96	
B4 Ac Me			2.00	
B3 Ac Me			2.01	
B6 Ac Me			2.01	
γ Ac Me			2.05	
OMe			3.77	
B6			4.06, 4.21	
B5			4.17	
γ			4.67	
B4			4.99	
B3			5.04	
B1			5.36	
B2			5.39	
β			6.62	
α			6.61	
A6			6.98	
A5			7.05	
A2			7.14	

Compound Number 121



Syringin acetate

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

^{1}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	
γ	4.71	d	6.4
β	6.22	dt	16.8, 6.4
α	6.57	d	16.8
A2,6	6.61	s	

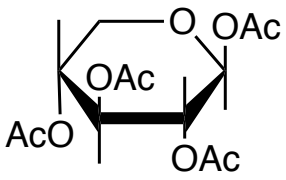
Notes:

S. Ralph III - 58
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.60	20.56	20.25
Ac Me	20.68	20.56	20.36
Ac Me	20.68	20.56	20.36
Ac Me	20.68	20.67	20.36
Ac Me	20.95	20.77	20.64
OMe	56.32	56.69	56.13
OMe	56.32	56.69	56.13
B6	62.35	62.91	61.82
γ	64.84	65.14	64.19
B4	68.56	69.47	68.26
B2	71.99	72.51	70.73
B5	72.08	72.81	71.54
B3	73.11	73.61	72.14
B1	101.21	101.69	100.48
A2	104.09	105.10	104.09
A6	104.09	105.10	104.09
β	123.30	124.38	123.74
A1	133.11	134.02	132.79
α	133.86	134.11	132.79
A4	134.56	135.38	133.87
A3	153.07	154.06	152.68
A5	153.07	154.06	152.68
Ac C=O	169.25	169.59	168.94
Ac C=O	169.41	169.94	169.24
Ac C=O	170.31	170.24	169.48
Ac C=O	170.51	170.48	169.81
Ac C=O	170.75	170.64	170.04

Compound Number 122



α + β Xylose Acetate

^{1}H (chloroform)

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

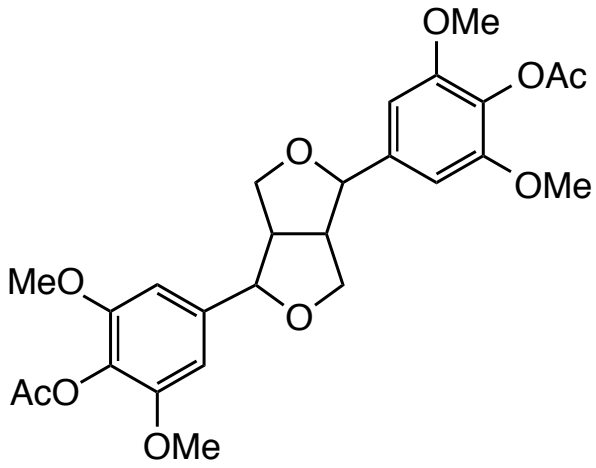
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.42	20.35	20.21	
Ac Me	20.54	20.46	20.25	
Ac Me	20.60	20.51	20.34	
Ac Me	20.60	20.55	20.34	
Ac Me	20.66	20.55	20.34	
Ac Me	20.66	20.55	20.34	
Ac Me	20.74	20.65	20.44	
Ac Me	20.79	20.65	20.52	
5	60.65	61.12	60.05	
5	62.76	63.14	62.01	
4	68.35	69.09	67.99	
4	68.67	69.22	68.10	
3	69.39	69.87	68.83	
3	69.39	70.24	68.93	
2	69.53	70.30	69.36	
2	70.97	71.54	70.52	
1	89.26	89.76	88.60	
1	92.05	92.67	91.49	
Ac C=O	168.92	169.35	168.78	
Ac C=O	168.92	169.53	169.02	
Ac C=O	169.22	169.66	169.02	
Ac C=O	169.65	170.01	169.36	
Ac C=O	169.68	170.10	169.41	
Ac C=O	169.68	170.19	169.49	
Ac C=O	169.75	170.22	169.54	
Ac C=O	170.02	170.22	169.58	

Compound Number 123



Syringylresinol diacetate

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

^{1}H (chloroform)

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

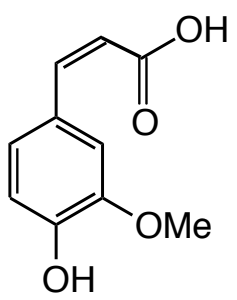
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.46	20.26	20.07
β	54.42	55.41	53.72
OMe OMe	56.23 56.23	56.46 56.46	55.90 55.90
γ	72.11	72.71	71.38
α	85.85	86.51	84.93
2 6	102.29 102.29	103.30 103.30	102.44 102.44
1	128.06	128.91	127.04
4	139.63	141.41	140.03
3 5	152.30 152.30	153.23 153.23	151.60 151.60
Ac C=O	168.76	168.59	168.01

Compound Number 124



cis

cis - Ferulic Acid

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

^{1}H (methanol)

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

^{13}C

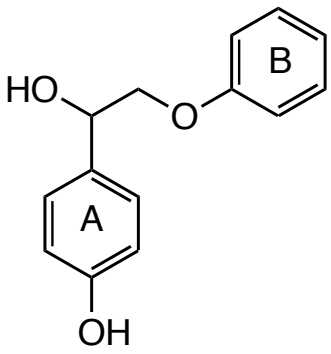
Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.93	56.16	55.38	
2	113.15	114.99	114.30	
5	113.98	115.23	114.78	
6	115.50	116.82	116.77	
β	126.17	126.51	124.78	
1	126.79	127.80	126.09	
α	145.97	144.40	141.90	
3	146.36	147.60	146.72	
4	147.50	149.04	147.90	
γ	171.34	167.85	167.54	

Notes:

J. Obst

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

Compound Number 125



1-(4-hydroxyphenyl)-2-phenoxyethanol

^{1}H (chloroform)

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

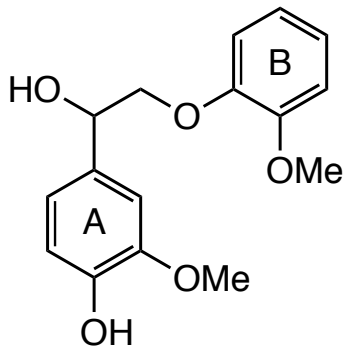
Notes:

JR C37.1
52mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	72.31	72.42	70.55	
β	73.25	74.32	73.07	
B3	114.73	115.43	114.49	
B5	114.73	115.43	114.49	
A3	115.51	115.76	114.74	
A5	115.51	115.76	114.74	
B1	121.33	121.37	120.38	
A2	127.80	128.39	127.42	
A6	127.80	128.39	127.42	
B2	129.55	130.12	129.32	
B6	129.55	130.12	129.32	
A1	131.68	133.53	132.63	
A4	155.77	157.61	156.54	
B4	158.41	159.84	158.52	

Compound Number 126



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

^{1}H (chloroform)

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

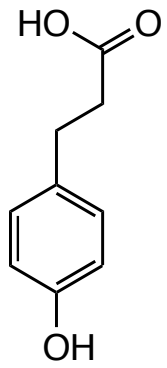
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.90	56.28	55.52
OMe	55.97	56.35	55.52
α	72.20	72.71	70.81
β	76.50	76.32	74.15
A2	108.87	111.01	110.75
B2	112.16	113.67	112.51
A5	114.26	115.37	113.75
B5	116.21	115.93	114.92
A6	119.37	119.89	118.67
B6	121.13	121.83	120.74
B1	122.58	122.45	120.92
A1	131.61	134.17	133.46
A4	145.46	146.84	145.66
A3	146.68	148.12	147.21
B3	148.10	149.74	148.23
B4	150.26	151.06	149.10

Compound Number 127



Dihydrocoumaric acid

3-(4-hydroxyphenyl)propionic acid

^{1}H (chloroform)

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

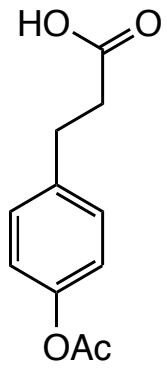
Notes:

IPC Pearl Coll.
60mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	29.94	30.68	29.58	
β	35.75	36.33	35.70	
3	115.46	115.99	115.04	
5	115.46	115.99	115.04	
2	129.36	130.00	129.00	
6	129.36	130.00	129.00	
1	132.10	132.54	130.92	
4	154.55	156.42	155.46	
γ	176.90	174.68	173.81	

Compound Number 128



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

^{1}H (chloroform)

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

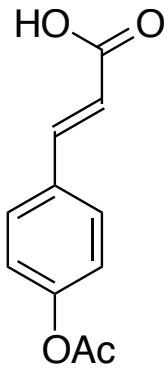
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.06	20.91	20.73	
α	29.96	30.80	29.68	
β	35.48	35.80	35.14	
3	121.56	122.37	121.47	
5	121.56	122.37	121.47	
2	129.24	129.94	129.09	
6	129.24	129.94	129.09	
1	137.78	139.24	138.29	
4	149.17	150.24	148.70	
Ac C=O	169.78	169.65	169.14	
γ	178.63	174.18	173.60	

Notes:

IPC Pearl Coll.
60mg Contains unacetylated cmpd also

Compound Number 129



trans

acetylated coumaric acid

(E)-4-acetoxycinnamic acid

^{1}H (chloroform)

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

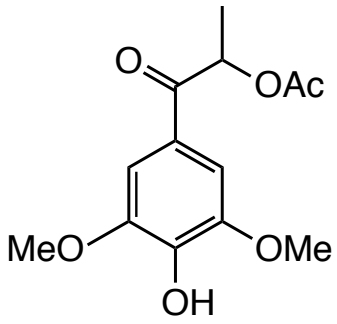
Notes:

IPC Pearl coll.
60mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.12	20.96	20.76	
β	117.38	119.32	119.29	
3	122.22	123.19	122.28	
5	122.22	123.19	122.28	
2	129.48	130.07	129.32	
6	129.48	130.07	129.32	
1	131.82	133.04	131.89	
α	145.80	144.44	142.88	
4	152.50	153.41	151.80	
γ	168.98	167.68	167.48	
Ac C=O	171.14	169.39	168.92	

Compound Number 130



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

^{1}H (chloroform)

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

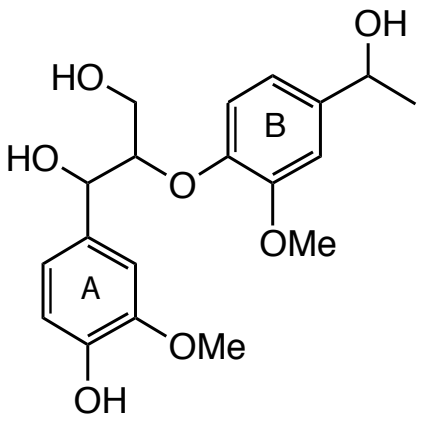
Notes:

IPC Pearl coll.
60mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	17.44	17.77	17.43	
Ac Me	20.78	20.63	20.40	
OMe	56.57	56.85	56.22	
OMe	56.57	56.85	56.22	
β	70.94	71.98	71.15	
2	106.12	107.38	106.43	
6	106.12	107.38	106.43	
1	125.83	126.17	124.02	
4	140.42	142.41	141.67	
3	147.02	148.59	147.75	
5	147.02	148.59	147.75	
Ac C=O	170.45	170.42	169.70	
α	195.11	195.30	194.63	

Compound Number 131



threo

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

^{1}H (chloroform)

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

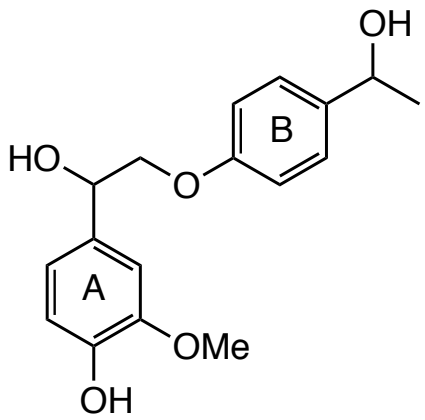
Notes:

S. Ralph SRIII-62-1
35mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	25.20	26.21	25.80
OMe	55.90	56.24	55.35
OMe	55.98	56.31	55.52
γ	61.09	61.89	60.02
B α	70.01	69.74	67.78
α	73.93	73.95	70.91
β	89.03	88.72	84.74
B2	109.35	110.67	109.79
A2	109.54	111.45	110.98
A5	114.42	115.24	114.57
B5	118.41	118.70	115.62
B6	120.17	119.68	117.24
A6	120.23	120.59	118.93
A1	131.56	133.85	132.89
B1	141.90	142.92	140.44
A4	145.57	146.83	145.31
A3	146.72	148.04	146.87
B4	146.78	148.31	146.87
B3	150.99	151.45	149.31
erythro isomer:			
γ	60.8	61.9	60.0
α	72.8	73.8	71.6
β	86.9	86.9	83.9
A1	132.0	134.3	133.2

Compound Number 132



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

^{1}H (chloroform)

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

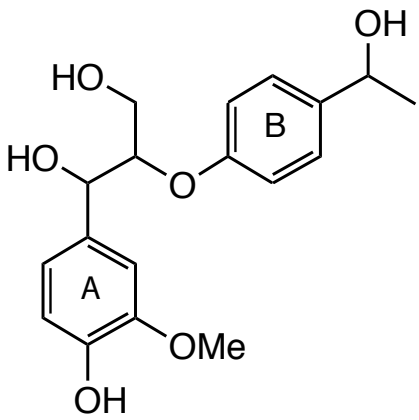
Notes:

S. Ralph SRIII-63-1
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	25.05	26.20	25.83	
OMe	55.98	56.27	55.50	
B α	69.91	69.50	67.52	
α	72.43	72.65	70.68	
β	73.58	74.65	73.22	
A2	108.82	110.89	110.55	
B3	114.64	115.07	113.95	
B5	114.64	115.07	113.95	
A5	114.37	115.42	114.88	
A6	119.33	119.88	118.63	
B2	126.73	127.27	126.28	
B6	126.73	127.27	126.28	
A1	131.66	134.30	133.30	
B1	138.66	140.41	139.30	
A4	145.57	146.86	145.60	
A3	146.70	148.16	147.17	
B4	157.81	158.80	157.19	

Compound Number 133



major

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

^{1}H (chloroform)

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

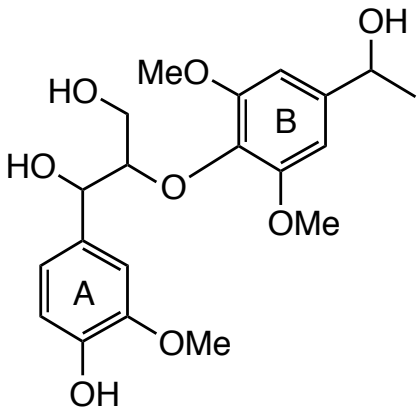
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	25.08	26.07	25.78
OMe	56.00	56.22	55.45
γ	61.24	61.69	60.00
B α	69.86	69.52	67.60
α	73.94	73.38	70.95
β	83.28	84.16	83.14
A2	109.42	111.37	110.90
A5	114.38	115.19	114.68
B3	116.47	116.69	115.39
B5	116.47	116.69	115.39
A6	119.99	120.34	118.96
B2	126.88	127.14	126.14
B6	126.88	127.14	126.14
A1	131.60	134.18	133.19
B1	139.39	140.38	139.20
A4	145.68	146.63	145.33
A3	146.72	147.92	146.93
B4	157.50	158.92	157.71
minor isomer shifts			
γ	61.54	62.04	60.11
α	74.04	73.99	71.50
β	82.09	83.75	83.14
B3,5	116.54	116.81	115.54
A6	119.33	120.47	119.37
B2,6	126.78	127.10	126.07
A1	132.35	134.44	133.32
B4	157.06	158.55	157.41

Compound Number 134



threo

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

^{1}H (chloroform)

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

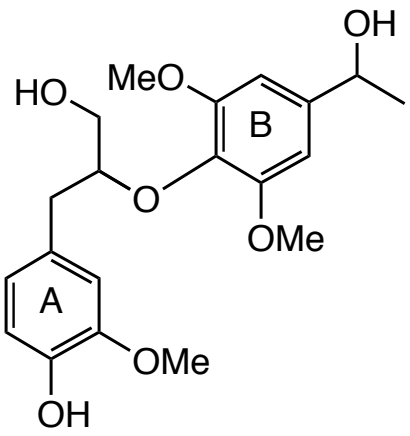
Notes:

S. Ralph SRIII-64-1
35mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	25.39	26.27	25.81
A OMe	55.96	56.23	55.46
B OMe	56.14	56.54	55.80
B OMe	56.14	56.54	55.80
γ	60.55	61.35	60.09
B α	70.29	70.01	68.07
α	74.10	74.10	71.48
β	89.00	89.82	87.20
B2	102.32	103.48	102.53
B6	102.32	103.48	102.53
A2	109.90	111.51	110.97
A5	114.36	115.24	114.56
A6	120.34	120.75	119.14
A1	131.89	133.67	132.82
B1	134.26	135.57	134.56
B4	142.80	144.64	142.88
A4	145.44	146.79	145.23
A3	146.56	147.95	146.77
B3	152.91	153.64	152.13
B5	152.91	153.64	152.13

Compound Number 135



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

^{1}H (chloroform)

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

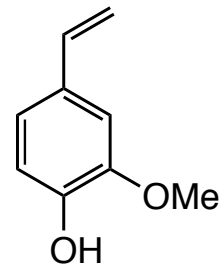
Notes:

S. Ralph SRIII-64-2
30mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	25.30	26.26	25.81
α	37.32	38.03	36.77
A OMe	55.94	56.23	55.46
B OMe	56.11	56.44	55.74
B OMe	56.11	56.44	55.74
γ	62.31	62.84	61.58
B α	70.42	70.04	68.13
β	84.52	85.30	83.40
B2	102.45	103.53	102.50
B6	102.45	103.53	102.50
A2	112.31	113.93	113.55
A5	114.27	115.51	115.01
A6	122.10	122.80	121.57
A1	130.13	130.80	129.24
B1	134.64	135.57	133.95
B4	142.09	144.15	142.83
A4	144.07	145.80	144.55
A3	146.38	148.04	147.03
B3	153.29	154.08	152.61
B5	153.29	154.08	152.61

Compound Number 136



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

^{1}H (acetone)

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

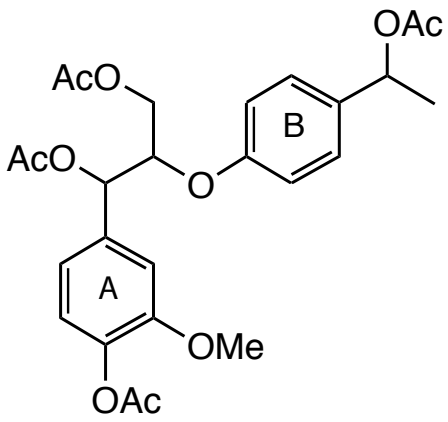
Notes:

J. Ralph
30mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.86	56.17	55.52	
2	108.14	109.85	109.61	
β	111.38	111.09	110.81	
5	114.40	115.69	115.34	
6	120.03	120.58	119.46	
1	130.26	130.59	128.77	
α	136.62	137.70	136.63	
A4	145.64	147.55	146.68	
A3	146.63	148.38	147.64	

Compound Number 137



threo

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

^{1}H (chloroform)

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

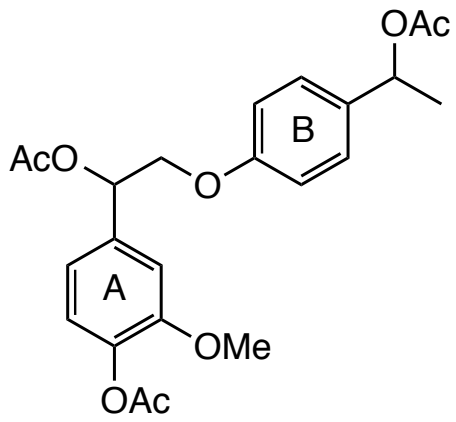
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.62	20.45	20.28
Ac Me	20.62	20.56	20.36
Ac Me	20.98	20.86	20.61
Ac Me	21.34	21.14	20.92
B β	22.00	22.34	21.78
OMe	55.98	56.31	55.82
γ	62.64	63.24	62.16
B α	71.85	72.17	71.14
α	74.00	75.07	74.00
β	78.08	79.10	77.57
A2	111.64	112.61	111.65
B5	116.31	117.08	116.01
B3	116.31	117.08	116.01
A6	119.60	120.37	119.45
A5	122.96	123.63	122.71
B2	127.66	128.27	127.30
B6	127.66	128.27	127.30
B1	134.86	136.20	134.71
A1	135.22	136.39	135.25
A4	140.05	140.97	139.25
A3	151.20	152.25	150.73
B4	157.97	159.12	157.69
A4 Ac C=O	168.71	168.81	168.30
Ac C=O	169.69	169.99	169.35
Ac C=O	170.29	170.18	169.51
Ac C=O	170.55	170.65	169.82
erythro isomer:			
γ	62.32	62.88	61.73
B α	71.85	72.17	71.14
α	73.62	74.21	72.81
β	78.40	78.86	76.99
B4	157.58	158.59	157.03

Notes:

S. Ralph SRIII-65-A 52mg

Compound Number 138



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

^{1}H (chloroform)

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

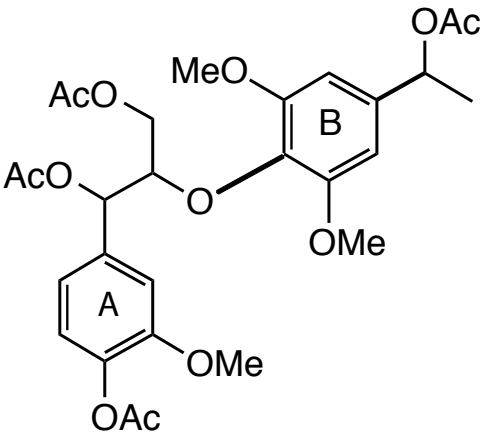
Notes:

S. Ralph SRIII-65-B
14mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.65	20.45	20.28	
Ac Me	21.12	20.94	20.73	
Ac Me	21.37	21.13	20.92	
B β	21.98	22.35	21.78	
OMe	55.98	56.30	55.79	
β	70.49	71.18	69.76	
B α	71.92	72.20	71.13	
α	73.52	74.21	73.01	
A2	111.26	112.20	111.34	
B3	114.72	115.45	114.55	
B5	114.72	115.45	114.55	
A6	119.09	119.70	118.71	
A5	122.95	123.61	122.66	
B2	127.62	128.27	127.29	
B6	127.62	128.27	127.29	
B1	134.50	135.58	134.09	
A1	135.85	137.17	135.84	
A4	139.90	140.87	139.09	
A3	151.20	152.28	150.69	
B4	158.09	159.08	157.55	
A4 Ac C=O	168.88	168.84	168.38	
Ac C=O	169.98	170.13	169.49	
Ac C=O	170.30	170.13	169.58	

Compound Number 139



threo

G-β-S5

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

^{1}H (chloroform)

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

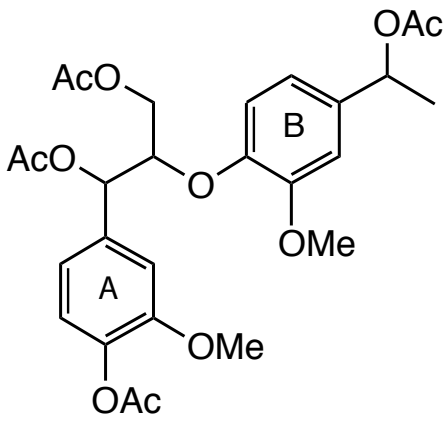
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.64	20.45	20.30
Ac Me	20.70	20.58	20.60
Ac Me	21.00	20.92	20.95
Ac Me	21.34	21.14	22.01
B β	22.23	22.57	22.06
A OMe	55.99	56.28	55.78
B OMe	56.02	56.39	55.78
B OMe	56.02	56.39	55.78
γ	63.48	64.17	63.14
B α	72.38	72.71	71.70
α	75.25	76.25	75.28
β	80.59	81.38	80.11
B2	103.21	104.01	102.88
B6	103.21	104.01	102.88
A2	111.92	112.64	111.53
A6	119.65	120.24	119.25
A5	122.51	123.34	122.53
A1	135.96	136.92	135.25
B1	135.96	137.14	135.84
B4	137.54	138.78	137.44
A4	139.72	140.71	139.08
A3	150.91	152.02	150.58
B3	152.91	153.79	152.30
B5	152.91	153.79	152.30
A4 Ac C=O	168.80	168.86	168.37
Ac C=O	169.71	169.85	169.25
Ac C=O	170.19	170.16	169.56
Ac C=O	170.54	170.57	169.89
erythro isomer			
γ		63.28	
Bα		72.68	
α		75.06	
β		81.26	
B2,6		103.91	
2		112.17	
6		119.99	
5		123.36	

Compound Number 140



threo

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

^{1}H (chloroform)

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

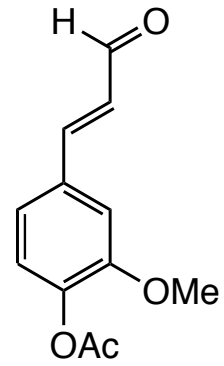
Notes:

S. Ralph SRIII-65-D
44mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.64	20.45	20.28
Ac Me	20.68	20.58	20.35
Ac Me	21.01	20.91	20.62
Ac Me	21.35	21.15	20.94
B β	22.09	22.45	21.89
OMe	55.92	56.29	55.66
OMe	55.97	56.29	55.78
γ	62.99	63.55	62.43
B α	72.06	72.39	71.37
α	74.41	75.34	74.26
β	80.14	80.68	79.10
B2	110.74	111.76	110.64
A2	111.74	112.64	111.62
B5	118.35	118.85	117.18
B6	118.67	119.19	118.09
A6	119.57	120.28	119.38
A5	122.80	123.51	122.63
A1	135.24	136.60	135.36
B1	136.76	137.78	136.11
A4	139.94	140.88	139.21
B4	147.53	148.48	147.00
B3	150.65	151.57	149.92
A3	151.12	152.18	150.68
A4 Ac C=O	168.74	168.82	168.32
Ac C=O	169.66	169.94	169.31
Ac C=O	170.25	170.16	169.53
Ac C=O	170.53	170.62	169.91
erythro isomer			
γ	63.0	62.5	61.8
α	73.7	74.5	73.1
β	80.1	80.2	78.3
B4	146.7	147.7	146.1

Compound Number 141



acetylated coniferylaldehyde
4-acetoxy-3-methoxycinnamaldehyde

^{1}H (acetone)

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

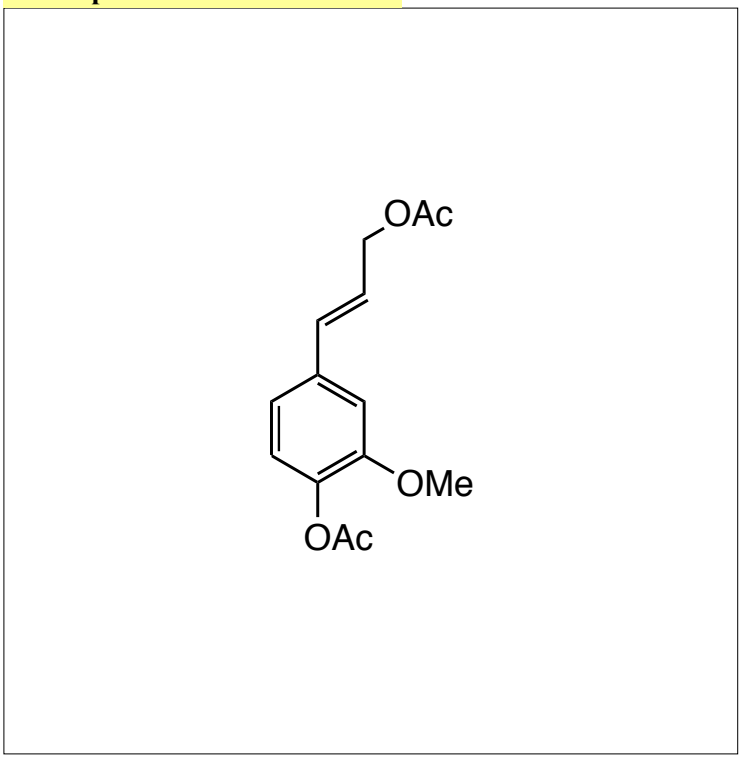
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.57	20.43	20.28	
OMe	55.98	56.44	55.99	
2	111.55	112.65	112.08	
6	121.82	122.68	122.04	
5	123.49	124.25	123.32	
β	128.74	129.68	128.72	
1	132.97	134.17	133.00	
4	142.30	143.22	141.55	
3	151.66	152.77	151.22	
α	151.74	152.55	152.29	
Ac C=O	168.52	168.72	168.19	
γ	193.27	193.89	194.17	

Compound Number 142



acetylated coniferyl alcohol

4-acetoxy-3-methoxycinnamylacetate

^{1}H (acetone)

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

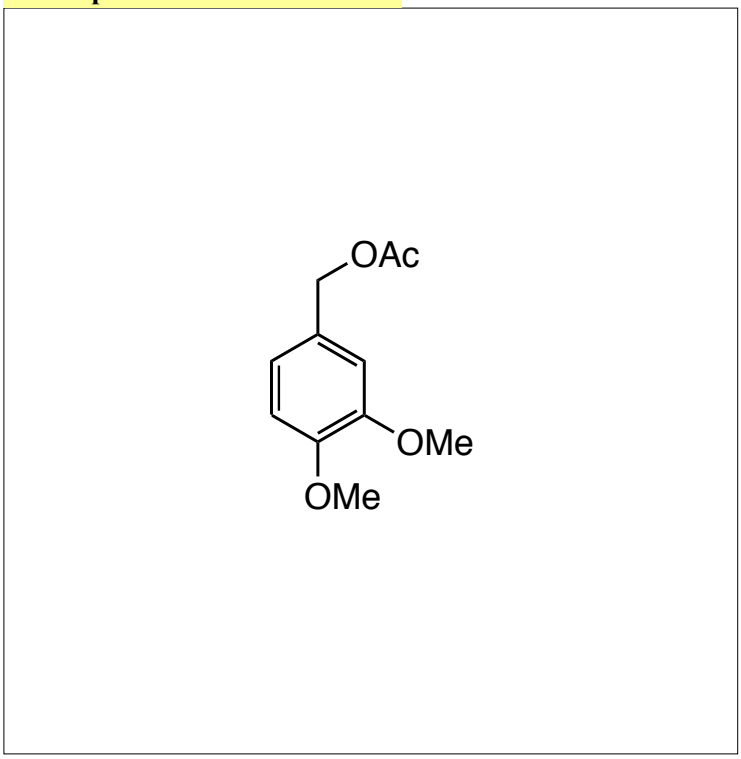
Notes:

M.Mozuch 177/95 47mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me Ac Me	20.59 20.92	20.45 20.76	20.27 20.60	
OMe	55.88	56.24	55.75	
γ	64.84	65.13	64.12	
2	110.34	111.23	110.41	
6	119.37	119.92	118.99	
5	122.88	123.74	122.83	
β	123.61	124.90	124.16	
α	133.52	133.62	132.29	
1	135.30	136.26	134.97	
4	139.76	140.82	139.08	
3	151.21	152.43	150.94	
A4 Ac C=O γ Ac C=O	168.83 170.68	168.89 170.69	168.37 170.02	

Compound Number 143



Acetylated veratryl alcohol
3,4-dimethoxybenzylacetate

^{1}H (acetone)

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

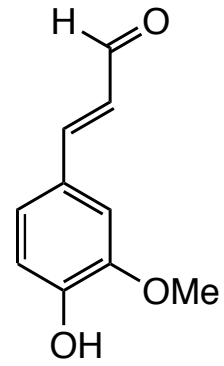
Notes:

M.Mozuch 177/95 48mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.03	20.83	20.66	
OMe	55.96	56.18	55.50	
OMe	55.96	56.18	55.50	
α	66.38	66.53	65.47	
2	111.27	112.76	111.70	
5	112.06	113.50	112.34	
6	121.33	121.90	120.88	
1	128.60	129.99	128.45	
3	149.14	150.38	148.66	
4	149.26	150.45	148.75	
Ac C=O	170.82	170.85	170.15	

Compound Number 144



coniferaldehyde

4-hydroxy-3-methoxycinnamaldehyde

^{1}H (acetone)

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

Notes:

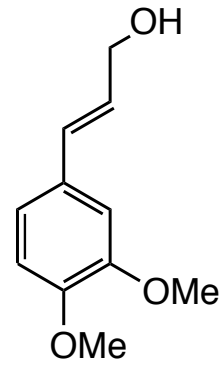
Aldrich 40mg

Note: In DMSO β and 1 are coincident

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.05	56.41	55.74	
2	109.75	111.66	111.59	
5	115.06	116.21	115.68	
6	124.03	124.68	123.86	
β	126.35	127.03	125.69	
1	126.66	127.46	125.69	
4	147.11	148.83	148.02	
3	149.12	150.78	150.15	
α	153.16	153.89	153.83	
γ	193.62	193.78	193.84	

Compound Number 145



3,4-dimethoxycinnamyl alcohol

^{1}H (acetone)

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

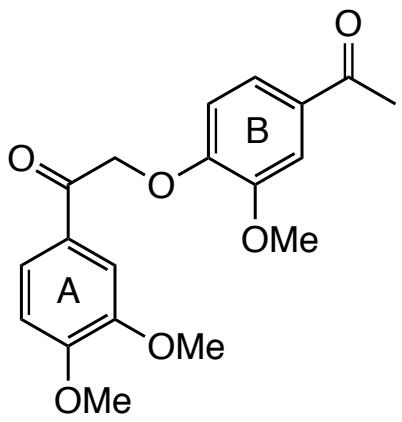
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.87	56.12	55.50	
OMe	55.95	56.18	55.55	
γ	63.76	63.34	61.63	
2	109.14	110.59	109.33	
5	111.34	112.92	111.91	
6	119.69	120.24	119.16	
β	126.65	128.90	128.53	
α	131.09	130.14	128.60	
1	129.87	131.40	129.94	
3	149.01	150.10	148.36	
4	149.14	150.55	148.91	

Notes:

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

Compound Number 146



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

^{1}H (acetone)

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

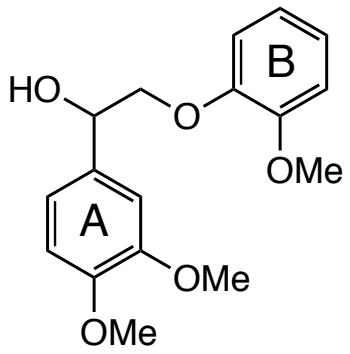
Notes:

LLL XVII -19A

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	26.16	26.29	26.22	
OMe	56.03	56.21	55.59	
OMe	56.10	56.30	55.63	
OMe	56.10	56.36	55.78	
β	71.39	71.71	70.30	
A2	110.30	111.63	110.32	
B2	110.54	111.77	110.92	
A5	111.10	112.29	111.03	
B5	112.57	113.55	112.28	
A6	122.74	123.45	122.58	
B6	122.85	123.54	122.58	
A1	127.58	128.67	127.08	
B1	131.52	132.02	130.24	
A3	149.40	150.32	148.54	
B3	149.40	150.32	148.69	
B4	151.79	153.19	151.73	
A4	154.14	155.19	153.61	
α	192.22	192.90	192.24	
B α	196.56	196.36	196.17	
1H				
B β			2.46	
OMe			3.58	
OMe			3.79	
OMe			3.80	
β			5.54	
B5			6.83	
A5			7.04	
A6			7.64	
B6			7.48	
A2, B2			7.40	

Compound Number 147



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

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.72	s	
OMe	3.73	s	
OMe	3.74	s	
β1	3.91	dd	9.9, 4.6
β2	3.96	dd	9.9, 7.2
α	4.84	dt	4.6
A2	7.04		
A5	6.89	d	8.4
B2	6.94		
B5	6.93		
A6	6.93		
B6	6.84		
B1	6.87		

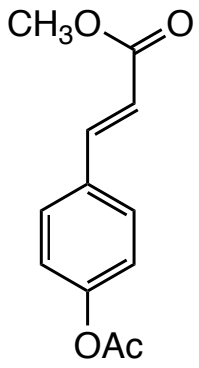
Notes:

LLL V-59B
A4 and B4 change order in DMSO
HSQC and HMBC 500MHz run in all solvents
obscured 1H shifts taken from HSQCs

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.83	56.01	55.39
OMe	55.87	56.13	55.56
OMe	55.93	56.24	55.58
α	72.11	72.59	70.74
β	76.45	76.15	74.01
A2	109.36	111.37	110.36
A5	111.01	112.49	111.46
B2	111.98	113.50	112.42
B5	116.18	115.71	113.59
A6	118.60	119.35	118.37
B6	121.07	121.76	120.81
B1	122.61	122.40	121.00
A1	132.10	135.45	135.12
B4	147.98	149.67	148.19
A4	148.76	149.76	148.01
A3	149.08	150.19	148.46
B3	150.20	151.00	149.01
<u>1H</u>			
OMe	3.86	3.78	
OMe	3.87	3.81	
OMe	3.88	3.81	
β1	3.95	4.00	
β2	4.15	4.06	
α	5.03	4.98	
A2	6.99	7.13	
A5	6.84	6.90	
B2	6.91	6.96	
B5	6.93	6.97	
A6	6.92	6.99	
B6	6.88	6.85	
B1	6.98	6.90	
α OH		4.44 d J=3.4	

Compound Number 148



acetylated methyl coumarate
methyl 4-acetoxycinnamate

^{1}H (acetone)

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

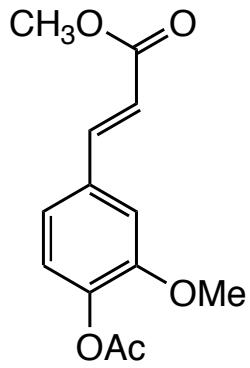
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.02	20.93	20.79	
OMe	51.66	51.70	51.70	
β	118.04	118.75	118.75	
3	122.23	123.10	122.30	
5	122.23	123.10	122.30	
2	129.24	130.02	129.50	
6	129.24	130.02	129.50	
1	132.13	132.81	131.70	
α	143.80	144.21	143.49	
4	152.31	153.34	152.06	
γ	167.31	167.36	166.56	
Ac C=O	169.05	169.36	168.84	

Compound Number 149



acetylated methyl ferulate
methyl 4-acetoxy-3-methoxycinnamate

^{1}H (acetone)

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

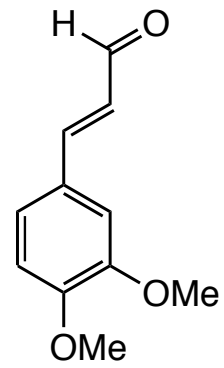
Notes:

J. Ralph P.S. 171.1

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.54	20.46	20.28	
γ OMe	51.62	51.69	51.34	
OMe	55.94	56.44	55.95	
2	111.52	112.59	112.01	
β	118.13	118.95	118.05	
6	120.20	122.04	121.37	
5	123.30	124.12	123.11	
1	133.41	134.25	132.92	
4	141.66	142.73	140.98	
α	144.12	144.68	143.81	
3	151.57	152.72	151.10	
γ	167.15	167.41	166.52	
Ac C=O	168.59	168.76	168.19	

Compound Number 150



3,4-dimethoxy cinnamaldehyde

^{1}H (acetone)

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

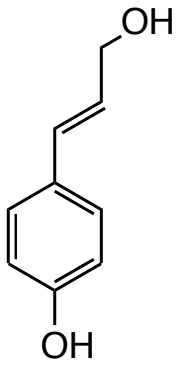
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	56.01	56.26	55.51
OMe	56.06	56.32	55.51
2	110.20	111.66	110.58
5	111.32	112.61	111.55
6	123.41	124.30	123.50
β	126.78	127.57	126.42
1	127.17	128.28	126.80
3	149.52	150.73	148.93
4	152.11	153.24	151.53
α	152.71	153.64	153.27
γ	193.39	193.83	193.81

Compound Number 151



***p*-Coumaryl alcohol**

4-hydroxycinnamyl alcohol

^{1}H (acetone)

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

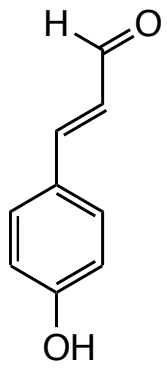
Notes:

S. Ralph
36mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ		63.47	61.66	
3		116.19	115.28	
5		116.19	115.28	
β		127.67	127.06	
2		128.33	127.27	
6		128.33	127.27	
1		129.73	127.86	
α		130.29	128.64	
4		157.78	156.70	

Compound Number 152



***p*-Coumaraldehyde**

4-hydroxy cinnamaldehyde

^{1}H (acetone)

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

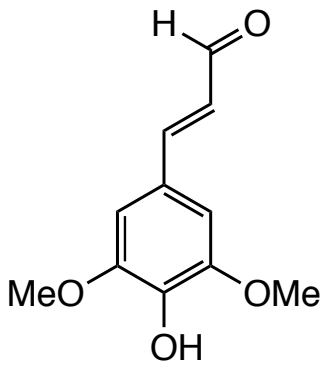
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
3	116.14	116.84	116.10
5	116.14	116.84	116.10
1	126.53	126.73	125.51
β	126.97	126.96	125.32
2	130.63	131.48	131.11
6	130.63	131.48	131.11
α	152.84	153.64	153.93
4	158.51	161.24	160.70
γ	193.88	193.81	194.29
1H			
β	6.59		6.63
3,5	6.87		6.83
α	7.40		7.60
2,6	7.47		7.58
γ	9.63		9.56

Compound Number 153



Sinapaldehyde

3,4-dimethoxy-4-hydroxycinnamaldehyde

^{1}H (acetone)

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

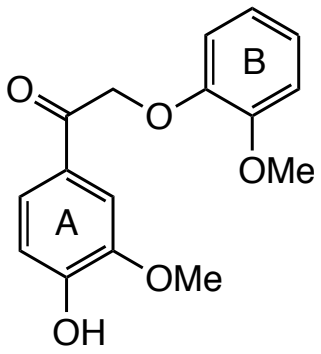
Notes:

S. Ralph
25mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.45	56.76	56.08	
OMe	56.45	56.76	56.08	
2	105.73	107.39	106.71	
6	105.73	107.39	106.71	
1	125.62	126.15	124.40	
β	126.81	127.28	126.03	
4	138.24	140.26	139.13	
3	147.44	149.02	148.02	
5	147.44	149.02	148.02	
α	153.09	154.22	154.12	
γ	193.32	193.70	193.75	

Compound Number 154



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

^{1}H (acetone)

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

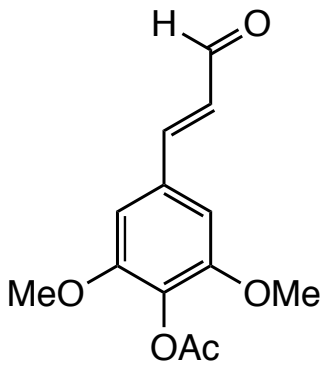
Notes:

S. Ralph

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.95	56.26	55.54	
OMe	56.12	56.26	55.62	
β	72.08	72.42	70.46	
A2	110.31	111.84	111.21	
B2	112.31	113.68	112.50	
A5	114.06	115.42	113.70	
B5	114.88	115.71	115.00	
B6	120.86	121.48	120.46	
B1	122.38	122.55	121.19	
A6	123.41	123.94	122.79	
A1	127.62	128.24	126.18	
A3	146.86	148.30	147.56	
B3	147.69	149.14	147.56	
B4	149.82	150.86	148.96	
A4	151.02	152.69	152.18	
α	193.17	193.27	192.60	

Compound Number 155



Acetylated sinapaldehyde

4-acetoxy-3,5-dimethoxycinnamaldehyde

^{1}H (acetone)

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

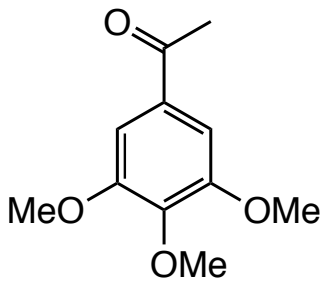
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.39	20.23	20.05	
OMe	56.25	56.68	56.20	
OMe	56.25	56.68	56.20	
2	105.13	106.26	105.63	
6	105.13	106.26	105.63	
β	128.79	129.80	128.93	
1	131.23	132.01	130.20	
4	132.30	133.55	132.39	
α	152.20	153.08	15277	
3	152.63	153.64	152.05	
5	152.63	153.64	152.05	
Ac C=O	168.30	168.37	167.76	
γ	193.25	193.94	194.18	

Compound Number 156



3,4,5-Trimethoxyacetophenone

^{1}H (acetone)

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

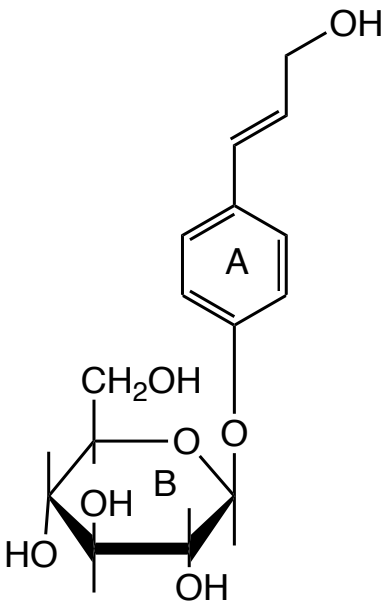
Notes:

Aldrich
48mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	26.39	26.52	26.50	
OMe	56.34	56.57	56.01	
OMe	56.34	56.57	56.01	
4 OMe	60.91	60.64	60.07	
2	106.00	106.85	105.80	
6	106.00	106.85	105.80	
1	132.49	133.51	132.18	
4	142.77	143.62	141.91	
3	153.08	154.16	152.68	
5	153.08	154.16	152.68	
α	196.79	196.76	196.70	

Compound Number 157



***p*-Gluco-cinnamyl alcohol**

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

^{1}H (DMSO)

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

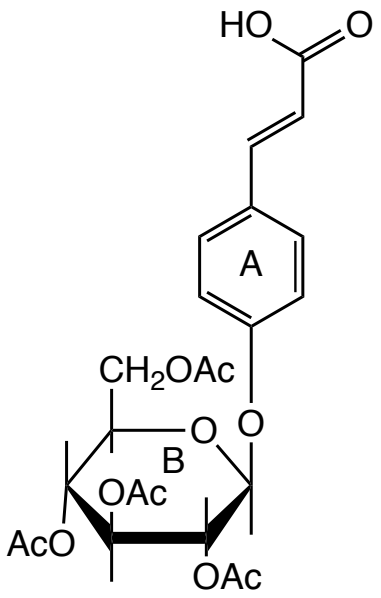
^{13}C

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

Notes:

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

Compound Number 158



acetylated *p*-gluco-cinnamic acid

^{1}H (acetone)

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

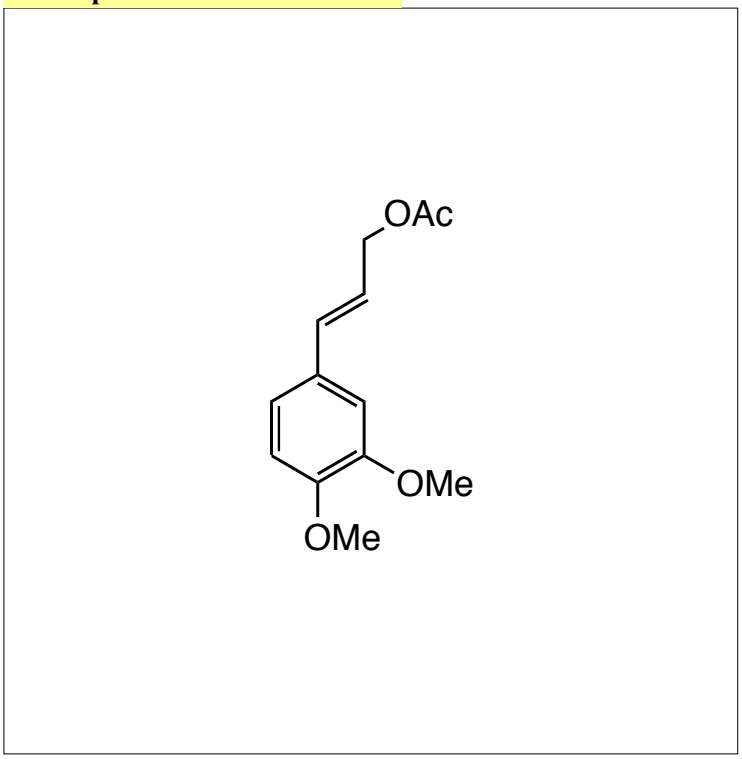
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.58	18.86	20.22	
Ac Me	20.58	18.86	20.22	
Ac Me	20.58	20.52	20.28	
Ac Me	20.58	20.58	20.37	
B6	61.97	62.73	61.52	
B4	68.29	69.29	67.96	
B2	71.17	71.96	70.60	
B5	72.23	72.75	70.84	
B3	72.68	73.33	71.86	
B1	98.55	98.86	96.67	
A3	117.18	117.81	116.48	
A5	117.18	117.81	116.48	
β	116.31	117.96	117.80	
A1	129.38	130.39	128.98	
A2	129.90	130.60	129.76	
A6	129.90	130.60	129.76	
α	145.76	144.67	143.05	
4	158.52	159.39	157.60	
γ	169.25	167.83	167.50	
Ac C=O	169.39	169.71	168.95	
Ac C=O	170.20	170.02	169.17	
Ac C=O	170.51	170.29	169.44	
Ac C=O	171.26	170.62	169.82	

Compound Number 159



3,4-dimethoxycinnamyl acetate

^{1}H (acetone)

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

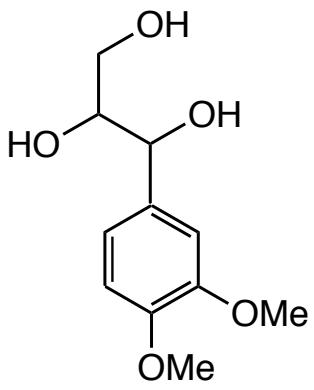
Notes:

S. Ralph 15mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.01	20.79	20.64	
OMe	55.88	56.08	55.41	
OMe	55.94	56.08	55.41	
γ	65.25	65.48	64.43	
2	109.07	110.48	109.28	
5	111.20	112.67	111.63	
6	120.03	120.78	119.73	
β	121.19	122.28	121.37	
1	129.34	130.37	128.81	
α	134.28	134.54	133.25	
3	149.14	150.54	148.83	
4	149.31	150.62	148.83	
Ac C=O	170.84	170.72	170.05	

Compound Number 160



Veratryl glycerol

1-(3,4-dimethoxyphenyl)glycerol

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.70	s	
OMe	3.71	s	
γ1	3.14	dd	
γ2	3.32	dd	
β	3.45	m	
α	4.43	d	
5	6.85	m	
6	6.81	m	
2	6.91	bs	

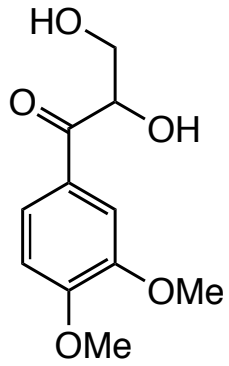
Notes:

M. Mozuch 2mg
2nd sample FPL Collection
500MHz CDCl3 and DMSO
beta shift for DMSO from HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.98	56.10	55.47	
OMe	55.98	56.20	55.63	
γ	63.41	63.98	62.69	
β	74.87	74.70	72.78	
α	75.81	77.21	75.93	
2	109.71	111.82	110.65	
5	111.25	112.54	111.35	
6	119.04	119.91	118.82	
1	133.04	136.24	136.05	
4	149.08	149.70	147.69	
3	149.28	150.16	148.28	
1H				
OMe	3.85	3.77		
OMe	3.86	3.78		
γ1	3.49	3.36		
γ2	3.60	3.48		
β	3.75	3.62		
α	4.64	4.58		
5	6.82	6.86		
6	6.88	6.86		
2	6.90	7.00		

Compound Number 161



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

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe OMe	3.89 3.92	s 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

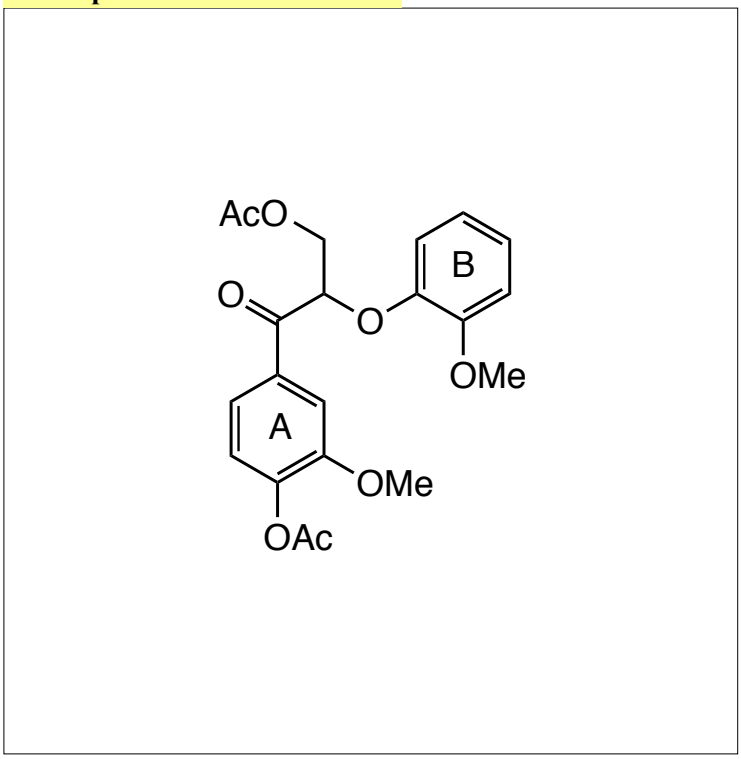
Notes:

M. Mozuch 17 mg Hibbert's Ketone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe OMe	56.11 56.21	56.20 56.28		
γ	65.95	66.30		
β	74.17	75.28		
2	110.34	111.64		
5	110.77	112.03		
6	123.46	124.23		
1	126.55	128.45		
3	149.52	150.28		
4	154.42	155.09		
α	197.65	199.22		

Compound Number 162



Erone diacetate

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

^{1}H (acetone)

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

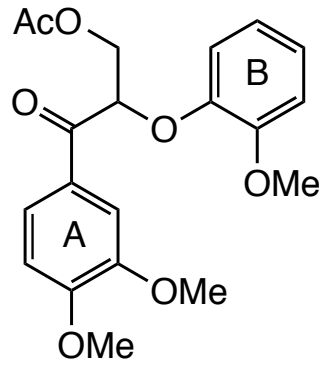
Notes:

L.Landucci 30 mg
K. Hirth
Assignments in CDCl3 and DMSO
500MHz HSQC and HMBC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ Ac Me	20.58	20.48	20.40
A4 Ac Me	20.75	20.64	20.52
B3 OMe	55.65	56.16	55.58
A4 OMe	56.00	56.46	56.00
γ	64.29	64.66	63.47
β	80.40	80.50	78.19
A2	112.51	113.45	112.35
B2	112.55	113.93	112.97
B5	118.34	118.58	115.97
B6	120.94	121.67	120.68
A6	122.25	122.81	121.81
B1	122.92	124.04	122.62
A5	123.58	124.04	123.41
A1	133.53	134.87	133.35
A4	144.27	145.35	143.84
B4	146.66	147.86	146.30
B3	150.28	151.40	149.52
A3	151.38	152.50	151.13
A4 Ac C=O	168.33	168.58	168.19
γ Ac C=O	170.86	170.90	170.17
α	194.53	195.10	194.19
1H			
γ Ac Me	2.02		1.96
A4 Ac Me	2.30		2.28
B3 OMe	3.73		3.70
A3 OMe	3.86		3.82
γ1	4.48		4.43
γ2	4.64		4.56
β	5.60		5.99
B6	6.81		6.81
B2	6.86		6.98
B5	6.92		6.87
B1	6.96		6.94
A5	7.11		7.29
A2	7.75		7.71
A6	7.77		7.74

Compound Number 163



Veratrone acetate

^{1}H (acetone)

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

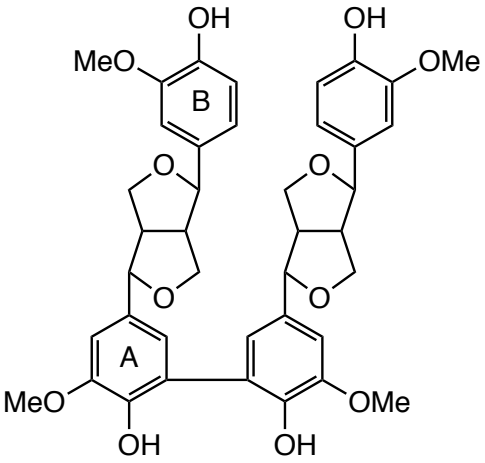
Notes:

L.Landucci
35 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.78	20.64	20.44	
OMe	55.79	56.05	55.40	
OMe	55.96	56.17	55.53	
OMe	56.07	56.22	55.74	
γ	64.62	64.85	63.60	
β	80.28	80.00	79.08	
A2	110.22	111.59	110.70	
A5	111.10	112.06	110.98	
B2	112.67	113.85	112.88	
B5	118.05	117.99	115.61	
B6	120.96	121.57	120.53	
A6	123.33	123.69	122.28	
B1	123.76	124.27	123.23	
A1	128.04	128.96	127.29	
B4	146.92	147.95	146.33	
A3	149.04	150.13	148.58	
B3	150.32	151.25	149.37	
A4	153.88	155.11	153.67	
Ac C=O	170.84	170.89	170.00	
α	194.05	194.24	193.22	

Compound Number 164



Pinoresinol biphenyl

^{1}H (acetone)

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

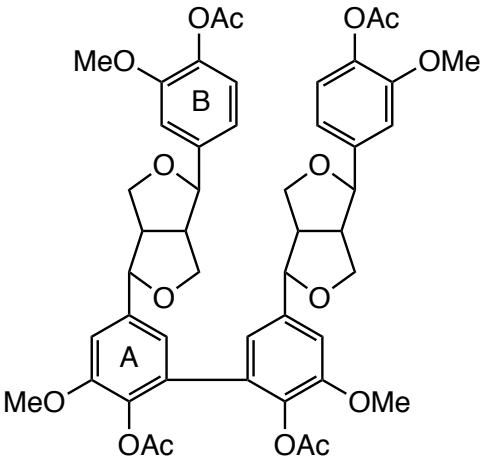
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A β	54.13	55.26	53.60
B β	54.18	55.26	53.60
OMe	55.97	56.25	55.57
OMe	56.22	56.48	55.90
A γ	71.66	72.19	70.86
B γ	71.82	72.33	70.98
A α	85.82	86.67	85.14
B α	85.93	86.67	85.21
A2	108.17	109.38	108.61
B2	108.64	110.58	110.39
B5	114.28	115.51	115.08
B6	118.98	119.62	118.60
A6	120.93	121.96	120.90
A5	124.06	125.96	125.44
A1	132.82	133.50	131.28
B1	132.82	134.17	132.16
A4	142.31	144.01	142.96
B4	145.26	146.82	145.85
B3	146.73	148.28	147.46
A3	147.40	148.68	147.63

Compound Number 165



Pinoresinol biphenyl acetate

^{1}H (acetone)

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

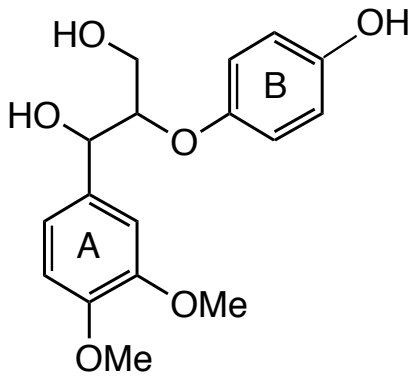
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.47	20.42	20.19	
Ac Me	20.67	20.49	21.16	
A β	54.28	55.40	54.57	
B β	54.37	55.40	54.57	
OMe	55.96	56.22	56.52	
OMe	56.17	56.47	56.82	
A γ	71.95	72.62	72.09	
B γ	72.05	72.62	72.09	
A α	85.49	86.17	85.32	
B α	85.49	86.17	85.42	
A2	109.40	110.55	110.80	
B2	109.89	111.09	111.18	
B6	117.96	118.62	118.63	
A6	119.79	120.26	119.80	
B5	122.76	123.47	123.36	
A5	131.38	132.09	131.16	
A4	136.93	137.76	136.84	
B4	139.13	140.12	139.23	
A1	139.40	141.07	140.59	
B1	140.02	141.80	141.24	
A3	151.24	152.27	151.52	
B3	151.51	152.59	151.86	
A Ac C=O	168.71	168.83	168.93	
B Ac C=O	169.08	169.02	169.32	

Compound Number 166



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

^{1}H (acetone)

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

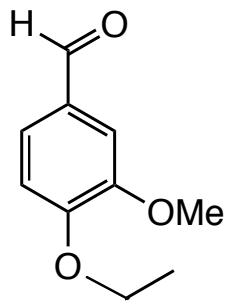
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.03		
OMe		56.09		
γ		61.58		
α		73.29		
β		85.37		
A2		111.84		
A5		112.30		
B2		116.42		
B6		116.42		
B3		118.70		
B5		118.70		
A6		119.90		
A1		135.53		
A3		149.56		
A4		149.97		
B1		152.52		
B4		153.12		
minor isomer				
γ		61.96		
α		73.94		
β		85.17		

Compound Number 167



Ethyl vanillin

^{1}H (acetone)

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

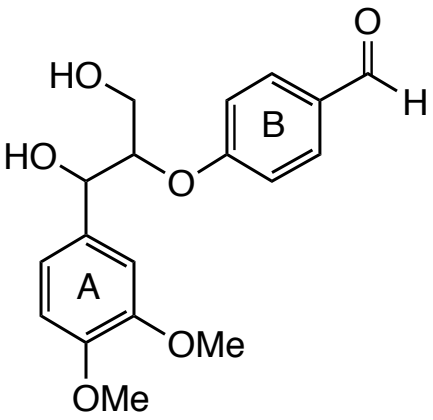
Notes:

M. Mozuch
40 mg
Not run in DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Me	14.38	14.92		
OMe	55.77	56.00		
CH2	64.39	65.02		
2	108.97	110.36		
5	111.07	112.52		
6	126.53	126.65		
1	129.69	130.98		
3	149.51	150.72		
4	153.71	154.88		
α	190.60	191.06		

Compound Number 168



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

^{1}H (chloroform)

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

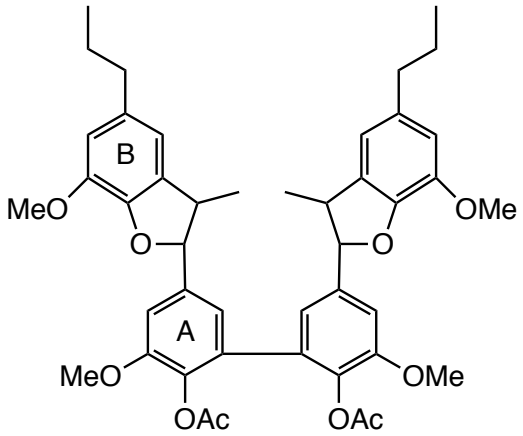
Notes:

S. Kawai
50 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.87	56.03		
γ	61.71	62.00		
α	74.04	73.55		
β	81.49	83.70		
A2	109.66	111.84		
A5	111.06	112.22		
B3	116.00	116.94		
B5	116.00	116.94		
A6	119.16	120.09		
A1	130.24	130.89		
B2	131.94	132.18		
B6	131.94	132.18		
B1	132.82	135.16		
A3	148.82	149.63		
A4	149.00	149.93		
B4	162.93	164.83		
B α	190.78	191.01		
Minor isomer				
γ	61.37			
α	73.62			
β	82.58			

Compound Number 169



Phenylcoumaran biphenyl acetate

^{1}H (acetone)

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

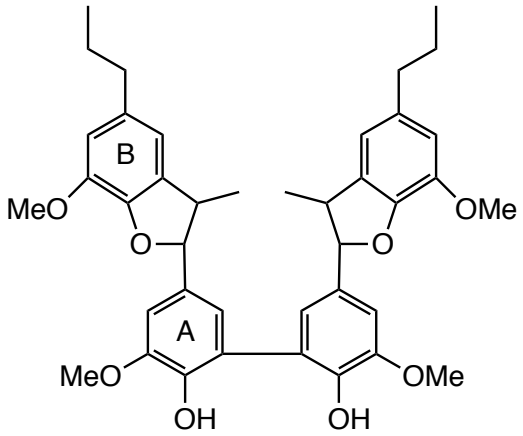
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B γ	13.75	14.10	13.71
γ	17.71	18.49	17.81
Ac Me	20.26	20.30	19.96
B β	24.92	25.73	24.56
B α	37.91	38.53	37.29
β	45.76	46.82	45.26
OMe	55.85	56.43	55.66
OMe	56.00	56.48	56.04
α	92.66	92.74	91.15
B2	109.60	110.63	110.13
A2	111.74	113.65	112.29
B6	115.33	116.42	115.42
A6	120.42	120.46	119.24
A1	130.96	132.00	130.33
B1	132.48	133.69	132.47
A5	136.36	137.00	135.76
A4	137.28	138.28	136.61
B5	138.51	140.22	138.84
B3	143.69	144.86	143.40
A3	145.07	146.36	144.73
B4	151.39	152.72	151.24
Ac C=O	168.36	168.66	168.02

Notes:

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

Compound Number 170



Phenyl coumaran biphenyl

^{1}H (acetone)

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

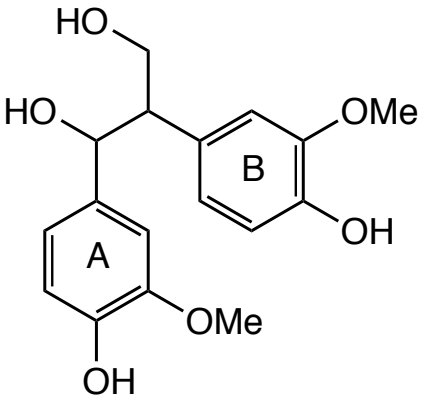
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B γ	13.91	14.10	13.77
γ	17.48	17.87	17.28
B β	25.08	25.79	24.62
B α	38.07	38.54	37.32
β	45.68	46.48	44.80
OMe	56.00	56.40	55.66
OMe	56.20	56.50	55.94
α	93.52	93.84	92.39
B2	108.42	109.38	108.67
A2	111.83	113.57	112.19
B6	115.44	116.40	115.42
A6	122.01	122.57	121.57
A5	123.90	125.82	125.33
B1	132.15	132.38	129.98
A1	132.96	134.15	132.94
B5	136.28	136.65	135.41
B3	142.71	144.74	143.32
A4	143.82	144.79	143.78
A3	145.34	146.58	144.91
B4	147.41	148.76	147.74

Notes:

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

Compound Number 171



1,2-diguaiacylpropane-1,3-diol

^{1}H (acetone)

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

Notes:

S. Ralph

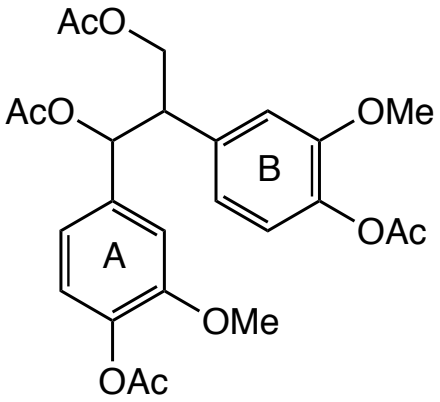
15 mg

β higher ppm than OMe's in acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	55.60	56.46	54.69	
OMe	55.90	56.05	54.87	
OMe	55.90	56.15	55.06	
γ	64.25	64.42	62.20	
α	75.78	74.86	71.96	
A2	109.06	111.18	110.27	
B2	111.80	114.18	113.46	
A5	113.98	114.82	113.98	
B5	114.58	115.01	114.03	
A6	119.70	119.92	118.13	
B6	121.54	123.00	121.32	
B1	130.29	132.17	130.96	
A1	133.99	136.59	135.49	
B4	144.97	145.91	144.13	
A4	145.32	146.12	144.36	
B3	146.53	147.54	146.05	
A3	146.63	147.60	146.24	

Compound Number 172



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

^{1}H (acetone)

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

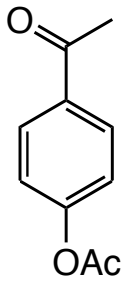
Notes:

S. Ralph
15 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.63	20.45	20.28
Ac Me	20.63	20.45	20.28
Ac Me	20.79	20.67	20.44
Ac Me	20.96	20.84	20.53
β	50.09	50.97	49.08
OMe	55.88	56.20	55.60
OMe	55.88	56.20	55.60
γ	64.02	64.86	63.94
α	74.87	75.56	74.49
A2	111.24	112.07	111.00
B2	113.32	114.49	113.38
A6	119.13	119.71	118.69
B6	120.98	121.91	120.71
B5	122.46	123.12	122.15
A5	122.58	123.29	122.38
B1	135.77	137.41	136.55
A1	136.91	138.70	137.52
B4	139.04	140.02	138.15
A4	139.58	140.48	138.71
B3	150.71	151.78	150.14
A3	150.86	151.97	150.40
Ac C=O	168.76	168.88	168.32
Ac C=O	168.84	168.94	168.32
α Ac C=O	169.63	169.64	169.19
γAc C=O	170.74	170.74	169.98
Minor isomer			
β		50.70	
γ		64.71	
α		76.50	

Compound Number 173



4-acetoxy-acetophenone

^{1}H (acetone)

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

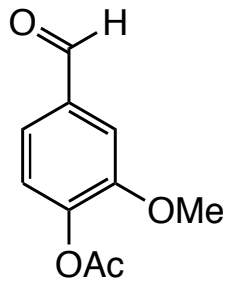
Notes:

Jamie Milhaupt
JR-JMA 29.1
50 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.11	20.98	20.51	
β	26.55	20.64	26.62	
3	121.75	122.75	122.02	
5	121.75	122.75	122.02	
2	129.91	130.53	129.78	
6	129.91	130.53	129.78	
1	134.72	135.65	134.39	
4	154.35	155.43	154.08	
Ac C=O	168.78	169.27	168.73	
α	196.75	196.80	196.75	

Compound Number 174



Vanillin acetate

4-formyl-2-methoxy phenyl acetate

^{1}H (acetone)

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

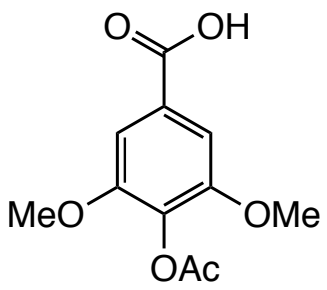
Notes:

Jamie Milhaupt
JR-JMA 23.1
50mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.58	20.45	20.29	
OMe	56.06	56.46	55.96	
2	110.92	112.31	111.84	
6	123.40	124.39	123.46	
5	124.59	124.44	123.63	
1	135.23	136.43	135.00	
4	144.93	145.83	144.19	
3	151.96	153.03	151.50	
Ac C=O	168.26	168.57	168.01	
α	190.97	191.76	191.87	
1H				
Ac Me	2.32		2.29	
OMe	3.88		3.86	
2	7.48		7.60	
5	7.20		7.34	
6	7.45		7.57	
α	9.92		9.96	

Compound Number 175



Syringic Acid Acetate

4-acetoxy-3,5-dimethoxy benzoic acid

^{1}H (acetone)

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

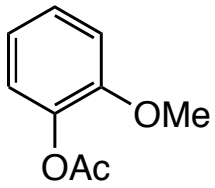
Notes:

Jamie Milhaupt
JR-JMA 25.1 25 mg
NOTE: In CDCl3 only alpha moves to 171.25 ppm as confirmed by HMBC
see also NL-175 and NL-208

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.43	20.23	19.93	
OMe	56.34	56.65	55.92	
OMe	56.34	56.65	55.92	
2	106.90	107.12	105.72	
6	106.90	107.12	105.72	
1	127.15	129.34	128.72	
4	133.37	133.63	131.44	
3	152.19	153.21	151.48	
5	152.19	153.21	151.48	
α	171.25	166.97	166.44	
Ac C=O	168.17	168.18	167.52	

Compound Number 176



Guaiacol acetate
2-methoxyphenyl acetate

^{1}H (acetone)

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

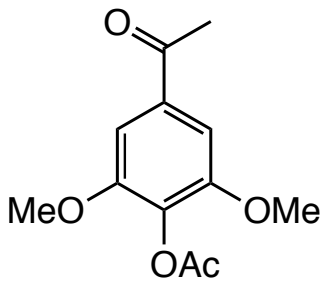
Notes:

Jamie Milhaupt
JR-JMA 27.1
54 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.64	20.48	20.21	
OMe	55.78	56.12	55.62	
2	112.39	113.41	112.74	
5	120.72	121.30	120.47	
1	122.78	123.66	122.76	
6	126.86	127.50	126.79	
4	139.75	141.01	139.33	
3	151.10	152.36	150.87	
Ac C=O	168.99	168.93	168.43	

Compound Number 177



Acetosyringone acetate

4-acetoxy-3,5-dimethoxy acetophenone

^{1}H (acetone)

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

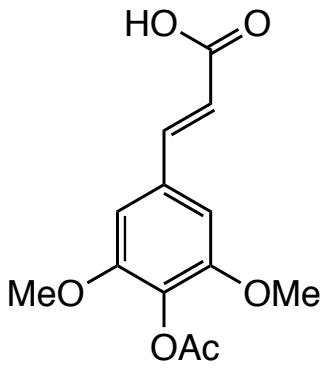
Notes:

Jamie Milhaupt
JR-JMA 31.1
50 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.41	20.23	20.86	
β	26.50	26.68	27.47	
OMe OMe	52.28 56.28	56.66 56.66	56.94 56.94	
2 6	105.10 105.10	105.89 105.89	105.79 105.79	
4	132.81	133.70	132.75	
1	135.11	136.19	135.69	
3 5	152.20 152.20	153.28 153.28	152.56 156.56	
Ac C=O	168.14	168.21	168.43	
α	196.75	196.92	197.64	

Compound Number 178



Sinapic acid acetate

4-acetoxy-3,5-dimethoxy cinnamic acid

^{1}H (acetone)

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

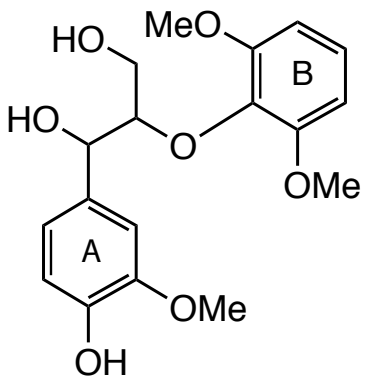
Notes:

FPL Collection
20 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.41	20.23	20.03	
OMe	56.27	56.66	56.20	
OMe	56.27	56.66	56.20	
2	105.19	106.42	105.93	
6	105.19	106.42	105.93	
β	116.92	117.90	117.16	
4	131.30	132.15	130.30	
1	131.93	132.95	131.78	
α	148.34	149.06	148.37	
3	152.60	153.60	151.97	
5	152.60	153.60	151.97	
γ	162.19	163.11	162.61	
Ac C=O	168.33	168.35	167.74	

Compound Number 179



threo

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

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.29	m	
γ2	3.64	m	
α	5.00	dd	7.5, 2.6
β	3.51	m	
B2,6	6.73	d	8.4
A2	7.07	d	1.8
A5	6.78	d	8.0
A6	6.92	dd	8.0, 1.8
B1	7.04	t	8.4
A4	7.46	s	
α OH	4.36	dd	2.6, 1.1

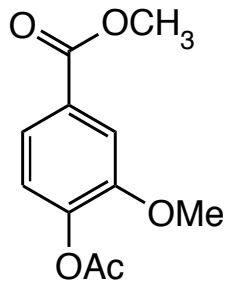
Notes:

S. Lemke SLI 75B
17.7mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A OMe	55.97	56.23	55.45
B OMe	56.16	56.58	55.85
B OMe	56.16	56.58	55.85
γ	60.49	61.31	60.08
α	74.13	74.07	71.40
β	89.06	89.76	86.96
B2	105.36	106.53	105.64
B6	105.36	106.53	105.64
A2	109.91	111.51	110.93
A5	114.33	115.23	114.55
A6	120.40	120.76	119.10
B1	124.50	124.90	123.26
A1	132.00	133.71	132.86
B4	135.38	137.16	136.18
A4	145.46	146.81	145.20
A3	146.58	147.95	146.76
B3	153.26	154.19	152.69
B5	153.26	154.19	152.69
erythro isomer			
γ	60.59	60.94	59.71
α	72.52	73.35	72.04
β	87.03	87.83	86.12

Compound Number 180



4-acetoxy-3-methoxy methyl benzoate

^{1}H (acetone)

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

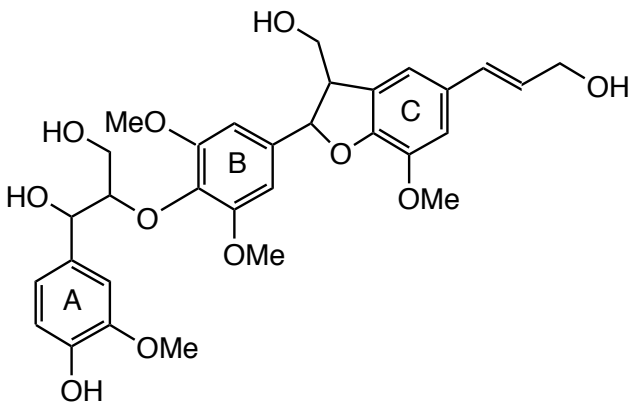
Notes:

Jamie Milhaupt
JR-JMA 43.1
50 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.61	20.45	20.33	
α OMe	52.26	52.45	52.60	
OMe	56.07	56.40	55.95	
2	113.44	113.96	112.96	
6	122.60	123.05	122.06	
5	122.78	123.85	123.24	
1	128.82	129.67	128.32	
4	143.64	144.81	143.28	
3	151.07	152.30	150.93	
α	166.33	166.53	165.56	
Ac C=O	168.43	168.59	168.14	

Compound Number 181



G-b-S-c-CA

^{1}H (acetone)

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

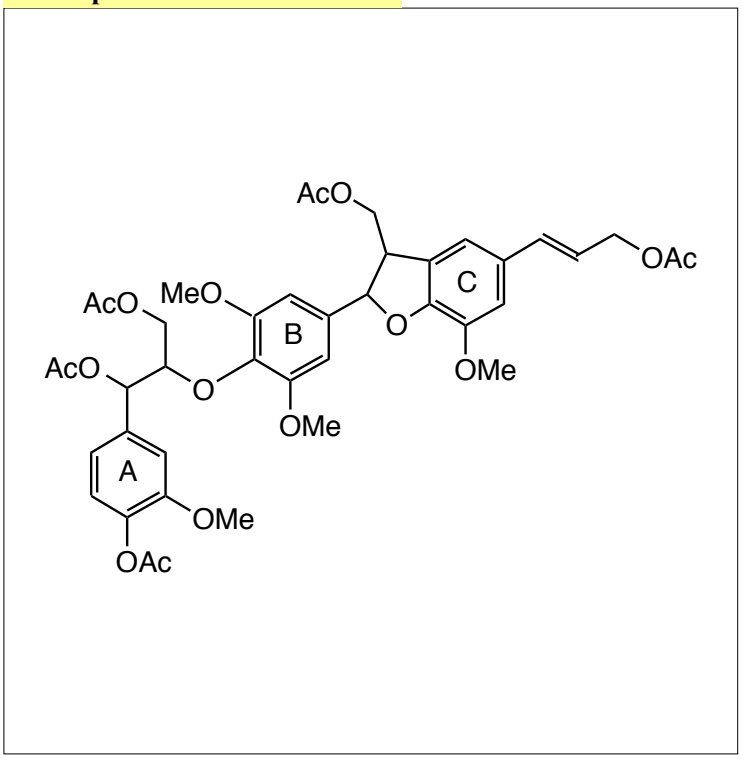
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	53.94	54.91	52.93	
OMe	56.10	56.24	55.42	
OMe	56.10	56.50	55.90	
OMe	56.34	56.61	55.71	
OMe	56.34	56.61	55.71	
γ	60.66	60.97	59.64	
C γ	63.81	63.36	61.52	
B γ	64.21	64.62	62.71	
α	72.64	73.37	71.98	
β	87.19	87.87	86.14	
B α	88.18	88.36	86.93	
B2	103.26	104.10	103.24	
B6	103.26	104.10	103.24	
A2	108.53	110.89	110.81	
C2	110.67	111.89	110.88	
A5	114.29	115.20	114.56	
C6	114.89	116.06	114.82	
A6	118.84	120.01	119.19	
C β	126.87	128.57	128.02	
C5	130.15	130.15	128.78	
C α	131.51	130.40	129.22	
C1	131.34	132.20	130.63	
A1	131.34	133.73	133.15	
B1	134.75	136.10	134.79	
B4	137.86	139.09	136.59	
C3	144.57	145.22	143.59	
A4	144.94	146.44	145.18	
A3	146.71	147.97	146.86	
C4	148.76	148.82	146.86	
B3	153.53	154.26	152.60	
B5	153.53	154.26	152.60	

Compound Number 182



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

^{1}H (acetone)

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

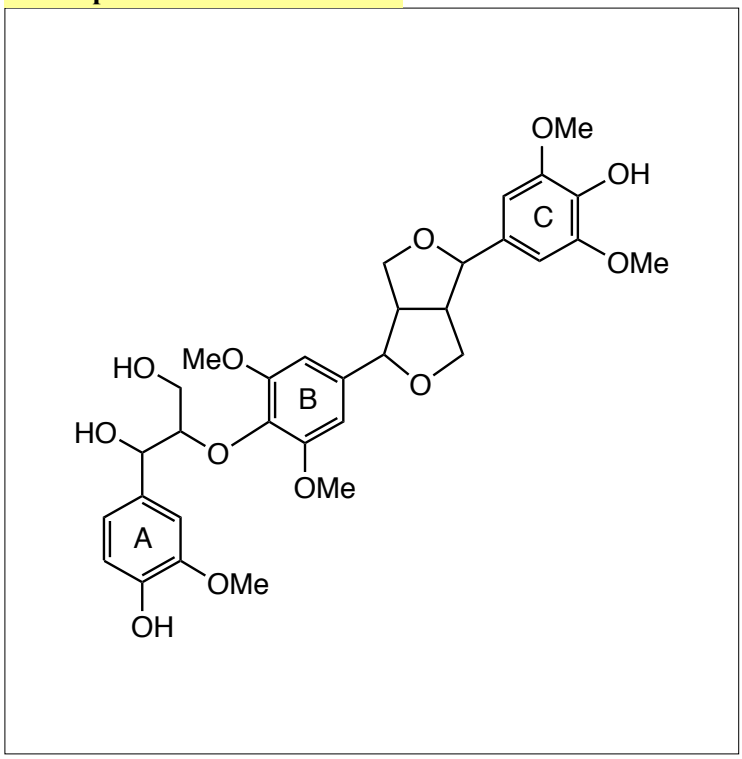
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.68	20.49	20.33
Ac Me	20.78	20.61	20.31
Ac Me	20.85	20.77	20.55
Ac Me	21.07	20.82	20.67
Ac Me	21.07	20.93	20.71
B β	50.51	51.32	49.37
OMe	55.96	56.28	55.73
OMe	56.10	56.45	55.82
OMe	56.10	56.45	55.82
OMe	56.10	56.51	55.82
γ	62.64	63.29	62.06
C γ	65.19	65.51	64.51
B γ	65.33	65.96	64.76
α	74.00	75.03	73.68
β	80.95	81.37	79.94
B α	88.55	88.86	87.60
B2	103.08	103.94	103.13
B6	103.08	103.94	103.13
C2	110.72	112.19	111.07
A2	111.50	112.30	111.07
C6	115.33	116.33	115.24
A6	119.18	120.01	118.79
C β	121.37	122.30	121.41
A5	122.44	123.29	122.54
C5	127.52	129.08	127.99
C1	130.74	131.60	130.13
C α	134.28	134.70	133.48
B4	135.16	136.15	134.30
A1	136.12	137.09	135.63
B1	136.62	138.02	136.41
A4	139.51	140.56	138.89
C3	144.46	145.41	143.89
C4	148.19	149.31	147.55
A3	150.86	152.03	150.57
B3	153.38	154.19	152.65
B5	153.38	154.19	152.65
Ac C=O	168.88	168.97	168.44
Ac C=O	169.50	169.95	169.32
Ac C=O	170.71	170.70	169.94
Ac C=O	170.85	170.79	170.12
Ac C=O	170.85	170.98	170.25

Compound Number 183



G-b-S-r-S

^{1}H (acetone)

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

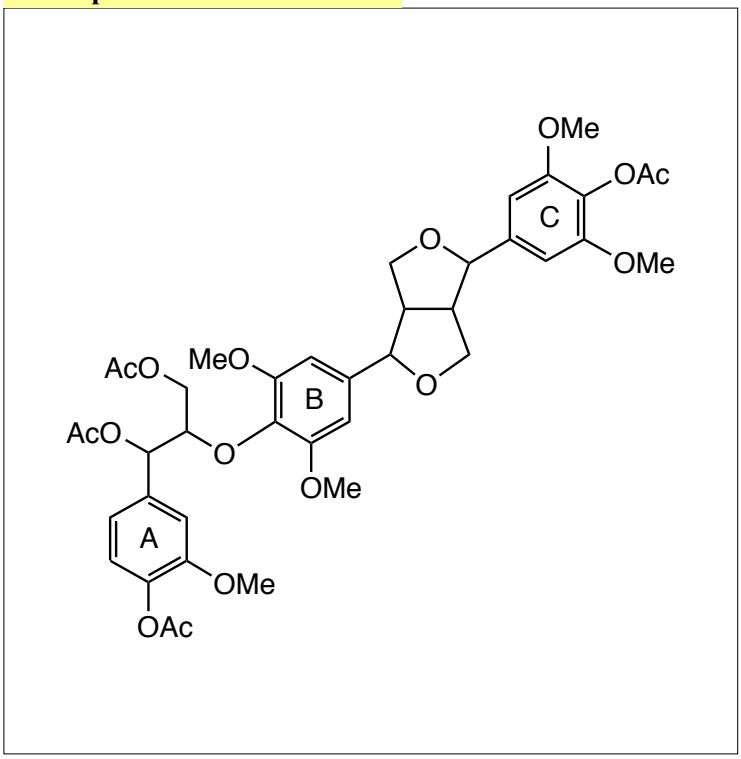
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	54.32	55.23	53.61
C β	54.48	55.39	53.76
OMe	56.00	56.28	55.53
OMe	56.27	56.60	55.99
OMe	56.27	56.60	55.99
OMe	56.44	56.67	55.99
OMe	56.44	56.67	55.99
γ	60.57	60.97	59.84
C γ	71.76	72.38	71.13
B γ	72.08	72.57	71.27
α	72.56	73.38	72.12
B α	85.98	86.57	85.12
C α	85.98	86.72	85.32
β	87.03	87.78	86.14
B2	102.88	104.09	103.29
B6	102.88	104.09	103.29
C2	102.88	104.50	103.68
C6	102.88	104.50	103.67
A2	108.61	110.93	110.96
A5	114.28	115.21	114.65
A6	118.80	120.04	119.36
C1	131.37	133.10	131.38
A1	131.91	133.74	133.26
B1	134.36	135.67	134.77
C4	134.52	136.20	134.89
B4	137.80	139.05	136.89
A3	144.94	146.43	145.32
A4	146.71	147.96	146.96
C3	147.29	148.67	147.90
C5	147.29	148.67	147.90
B3	153.45	154.15	152.61
B5	153.45	154.15	152.61

Notes:

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

Compound Number 184



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

^{1}H (acetone)

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

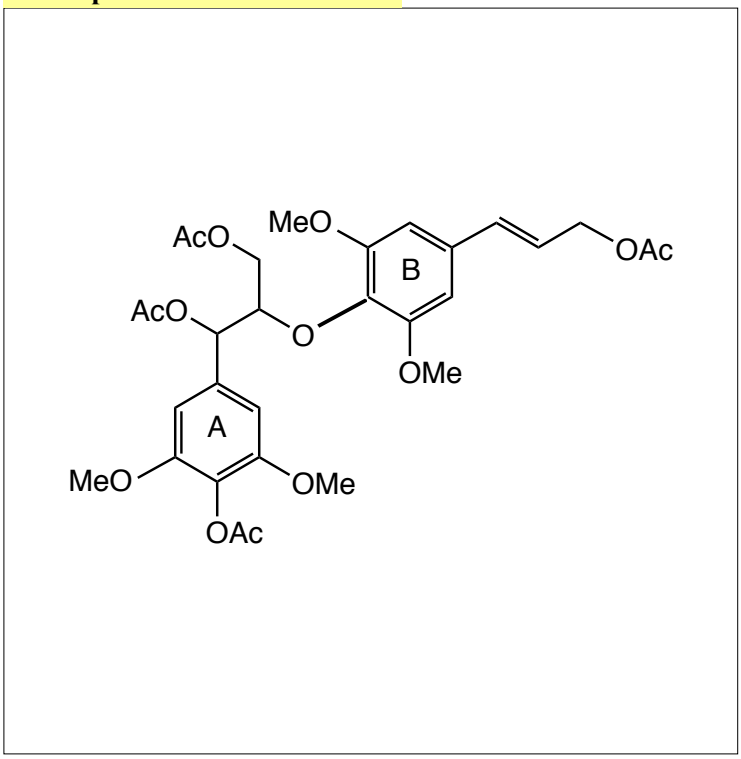
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.32	20.24	20.11	
Ac Me	20.51	20.48	20.31	
Ac Me	20.63	20.61	20.31	
Ac Me	20.93	20.94	20.66	
B β	54.16	55.33	53.67	
C β	54.33	55.43	53.81	
OMe	55.79	56.26	55.69	
OMe	55.96	56.38	55.78	
OMe	55.96	56.38	55.78	
OMe	56.09	56.46	55.94	
OMe	56.09	56.46	55.94	
γ	62.50	63.29	62.10	
B γ	71.87	72.65	71.36	
C γ	71.98	72.65	71.36	
α	73.82	75.05	73.72	
β	80.62	81.28	79.86	
B α	85.63	86.45	84.92	
C α	85.77	86.54	85.06	
C2	102.12	103.23	102.44	
C6	102.12	103.23	102.44	
B2	102.64	103.73	102.80	
B6	102.64	103.73	102.80	
A2	111.37	112.21	110.95	
A6	119.09	120.04	118.80	
A5	122.26	123.26	122.49	
C4	127.87	128.85	127.06	
B4	134.41	135.48	133.63	
A1	135.97	137.12	135.71	
B1	137.13	138.89	137.53	
A4	139.35	140.54	138.86	
C1	139.58	141.44	140.14	
A3	150.68	152.00	150.53	
C3	152.16	153.21	151.64	
C5	152.16	153.21	151.64	
B3	153.19	154.04	152.54	
B5	153.19	154.04	152.54	
Ac C=O	168.64	168.61	168.08	
Ac C=O	168.72	168.94	168.41	
Ac C=O	169.36	169.92	169.31	
Ac C=O	170.70	170.67	169.94	

Compound Number 185



S-b-SA (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ AcMe	1.82	s	
B γ AcMe	2.00	s	
α AcMe	2.10	s	
A4 AcMe	2.18	s	
OMe	3.81	s	
OMe	3.85	s	
γ2	4.19	dd	11.8, 4.1
γ1	4.43	dd	11.8, 6.1
B γ	4.68	dd	7.4, 1.2
α	6.07	d	4.2
β	4.74	dt	6.1, 4.2
2,6	6.78	s	
2,6	6.80	s	
B β	6.33	dt	15.8, 6.3
B α	6.63	d	16.0

Notes:

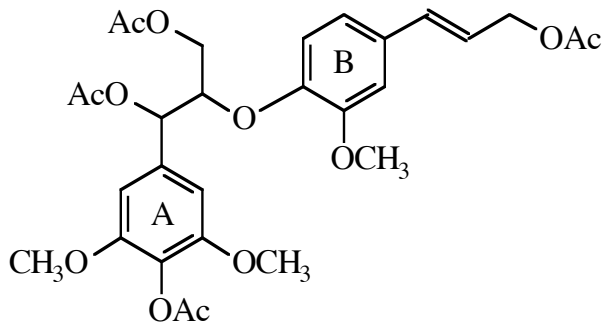
S. Ralph SRVII 15A

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.46	20.26	20.04
γ Ac Me	20.77	20.63	20.29
β Ac Me	21.00	20.80	20.62
α Ac Me	21.07	20.93	20.62
OMe	55.89	56.39	55.73
OMe	55.89	56.39	55.73
OMe	56.15	56.49	55.86
OMe	56.15	56.49	55.84
γ	62.74	63.28	62.07
B γ	64.95	65.25	64.16
α	74.25	75.29	73.84
β	80.93	81.56	79.98
A2	103.87	104.52	103.20
A6	103.87	104.52	103.20
B2	103.63	104.60	103.53
B6	103.63	104.60	103.53
B β	122.89	124.09	123.32
A4	128.49	129.32	127.47
B1	132.41	133.30	131.88
B α	134.07	134.36	132.96
A1	135.37	136.46	134.40
B4	135.53	136.62	135.19
A3	151.93	153.02	151.44
A5	151.93	153.02	151.44
B3	153.22	154.14	152.58
B5	153.22	154.14	152.58
A4 Ac C=O	168.64	168.51	167.91
α Ac C=O	169.51	169.95	169.24
B γ Ac C=O	170.90	170.68	169.86
γ Ac C=O	170.90	170.74	170.00
1H			
γ AcMe	1.97		
B γ AcMe	2.09		
α AcMe	2.13		
A4 AcMe	2.30		
OMe	3.74		
OMe	3.78		
γ2	4.26		
γ1	4.47		
B γ	4.70		
α	6.05		
β	4.62		
B 2,6	6.56		
A 2,6	6.62		
B β	6.18		
B α	6.54		

Compound Number 186



S-b-CA (acetate)

^{1}H (acetone)

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

Notes:

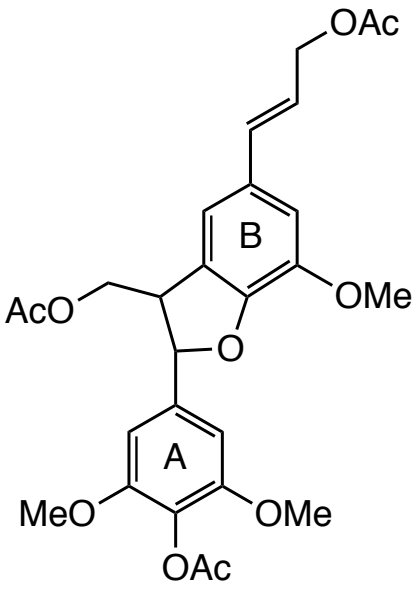
S. Ralph SR VII 16D

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.54	20.25	20.04	
Ac Me	20.86	20.64	20.38	
Ac Me	21.12	20.80	20.63	
Ac Me	21.12	20.89	20.63	
OMe	55.91	56.29	55.61	
A OMe	56.29	56.54	55.90	
A OMe	56.29	56.54	55.90	
γ	62.73	63.09	61.88	
B γ	56.15	65.36	64.31	
α	74.05	74.78	73.20	
β	80.21	80.17	78.01	
A2	104.52	105.14	103.94	
A6	104.52	105.14	103.94	
B2	110.41	111.40	110.26	
B5	119.04	119.16	117.14	
B6	119.89	120.49	119.43	
B β	122.36	123.52	122.30	
A4	128.85	129.61	127.66	
B1	131.93	132.56	130.71	
B α	133.90	134.13	132.84	
A1	134.82	136.11	134.78	
B4	147.37	148.33	146.56	
B3	151.06	151.92	150.11	
A3	152.13	153.06	151.38	
A5	152.13	153.06	151.38	
Ac C=O	168.59	168.46	167.90	
Ac C=O	169.55	169.89	169.18	
Ac C=O	170.84	170.75	169.96	
Ac C=O	170.90	170.75	170.03	

Compound Number 187



S-c-CA (acetate)

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.80	s	
A OMe	3.90	s	
β obscured	3.8-3.9		
γ1	4.48	dd	11.1, 5.5
γ2	4.37	dd	11.1, 7.3
B γ	4.67	d	6.4
α	5.59	d	7.1
B β	6.25	dt	15.9, 6.4
B α	6.65	d	15.9
A2	6.84	s	
B2 or B6	7.05	s	
B2 or B6	7.07	s	

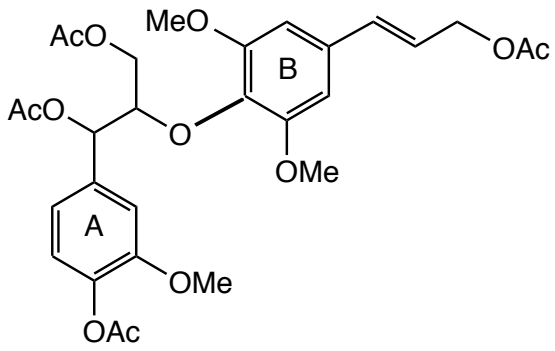
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.53	20.25	20.13
Ac Me	20.92	20.74	20.57
Ac Me	21.11	20.82	20.73
β	50.62	51.37	49.37
OMe	56.18	56.54	55.84
OMe	56.31	56.54	56.00
OMe	56.31	56.54	56.00
B γ	65.26	65.50	64.51
γ	65.43	65.96	64.47
α	88.44	88.76	87.46
A2	102.65	103.51	102.86
A6	102.65	103.51	102.86
B2	110.87	112.38	111.11
B6	115.42	116.34	115.24
B β	121.44	122.36	121.46
B5	127.51	129.03	127.98
A4	128.68	129.52	127.74
B1	130.85	131.70	130.22
B α	134.33	134.67	133.46
A1	135.97	140.50	138.92
B3	144.53	145.55	143.90
B4	148.26	149.28	147.49
A3	152.43	153.40	151.77
A5	152.43	153.40	151.77
Ac C=O	168.69	168.57	168.02
Ac C=O	170.79	170.75	170.13
Ac C=O	170.93	170.94	170.28

Compound Number 188



G-b-SA acetate

^{1}H (acetone)

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

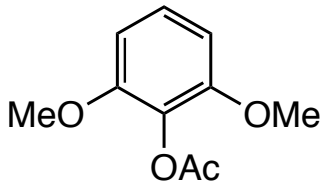
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.72	20.49	20.35
Ac Me	20.81	20.61	20.35
Ac Me	21.06	20.81	20.70
Ac Me	21.02	20.94	20.70
OMe	55.99	56.31	55.73
OMe	56.07	56.44	55.82
OMe	56.07	56.44	55.82
γ	62.74	63.24	62.05
B γ	65.00	65.26	64.24
α	74.09	75.07	73.67
β	81.03	81.57	80.04
B2	103.76	104.71	103.62
B6	103.76	104.71	103.62
A2	111.56	111.46	110.92
A6	119.24	119.94	118.72
A5	122.51	123.34	122.58
B β	122.97	124.14	123.43
B1	132.46	133.39	132.02
B α	134.16	134.40	133.02
A1	135.38	136.46	134.36
B4	136.11	137.14	135.66
A4	139.56	140.60	138.88
A3	150.91	152.10	150.59
B3	153.29	154.23	152.69
B5	153.29	154.23	152.69
Ac C=O	168.92	168.94	168.45
Ac C=O	169.55	169.92	169.33
Ac C=O	170.88	170.66	169.95
Ac C=O	170.88	170.66	170.10

Compound Number 189



2,6-dimethoxyphenol acetate

^{1}H (acetone)

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

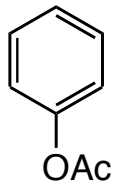
Notes:

Jamie Milhaupt
JR-JMA 35.1
40mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.45	20.27	20.12	
OMe	56.12	56.40	55.89	
OMe	56.12	56.40	55.89	
2	104.91	105.77	105.00	
6	104.91	105.77	105.00	
1	126.23	126.92	126.23	
4	128.85	129.94	128.11	
3	152.34	153.43	151.90	
5	152.34	153.43	151.90	
Ac C=O	168.71	168.56	168.04	

Compound Number 190



phenol acetate

^{1}H (acetone)

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

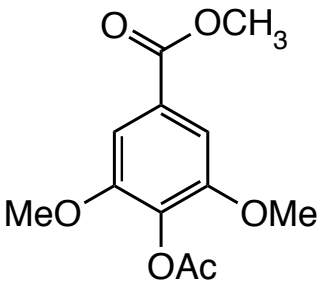
Notes:

Jamie Milhaupt
JR-JMA 55
54mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.12	20.94	20.75	
3	121.58	122.57	121.70	
5	121.58	122.57	121.70	
1	125.82	126.36	125.63	
2	129.42	130.09	129.35	
6	129.42	130.09	129.35	
4	150.74	151.96	150.44	
Ac C=O	169.48	169.61	169.05	

Compound Number 191



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

^{1}H (acetone)

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

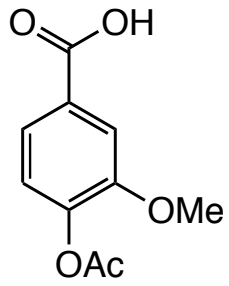
Notes:

Jamie Milhaupt
JR-JMA 41.1
40mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.40	20.22	20.06	
α OMe	52.34	52.57	52.36	
OMe	56.32	56.68	56.17	
OMe	56.32	56.68	56.17	
2	106.34	106.87	105.79	
6	106.34	106.87	105.79	
1	128.10	129.04	127.70	
4	132.63	133.69	131.96	
3	152.10	153.27	151.81	
5	152.10	153.27	151.81	
α	166.37	166.61	165.75	
Ac C=O	168.14	168.17	167.67	

Compound Number 192



4-acetoxy-3-methoxy benzoic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.28	s	
OMe	3.90	s	
2	7.70	s	
6	7.67	dd	7.6, 1.8
5	7.19	dd	7.7, 1.0
CDCl3			
Ac Me	2.32		
OMe	3.89		
2	7.69		
6	7.74		
5	7.12		

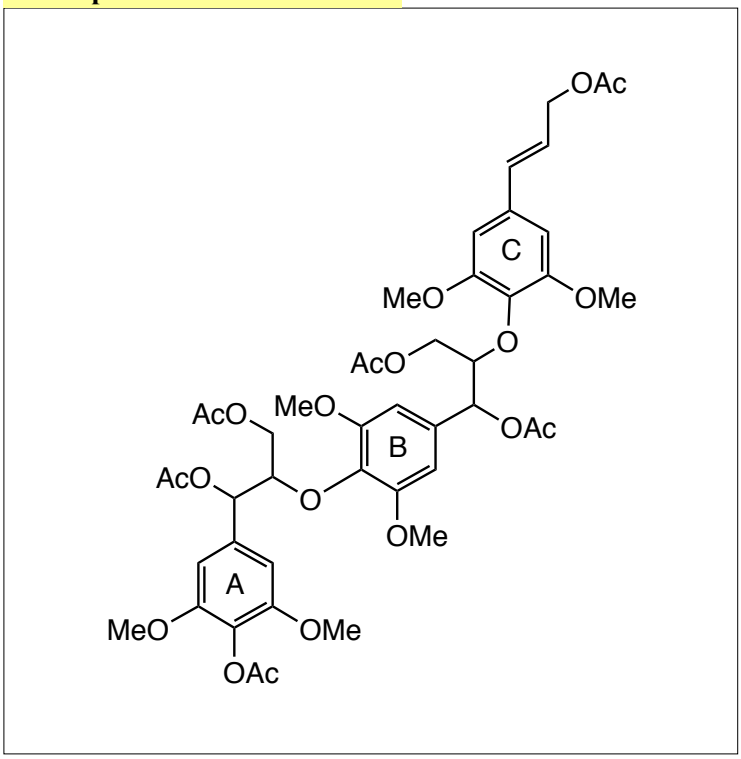
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.64	20.46	20.37	
OMe	56.07	56.40	55.90	
2	113.80	114.25	113.18	
6	123.43	123.31	122.16	
5	122.95	123.80	123.05	
1	127.84	129.96	129.58	
4	144.36	144.79	142.98	
3	151.14	152.26	150.82	
α	171.12	167.04	166.66	
Ac C=O	168.45	168.65	168.21	

Notes:

Jamie Milhaupt JR-JMA 39.1
41mg 2D short range XH corr confirms assignment of 5 and 6.
NOTE: In CDCl3 only alpha moves to 171.37 ppm as confirmed by HMBC
see also NL-175 and NL-208

Compound Number 193



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

^{1}H (acetone)

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

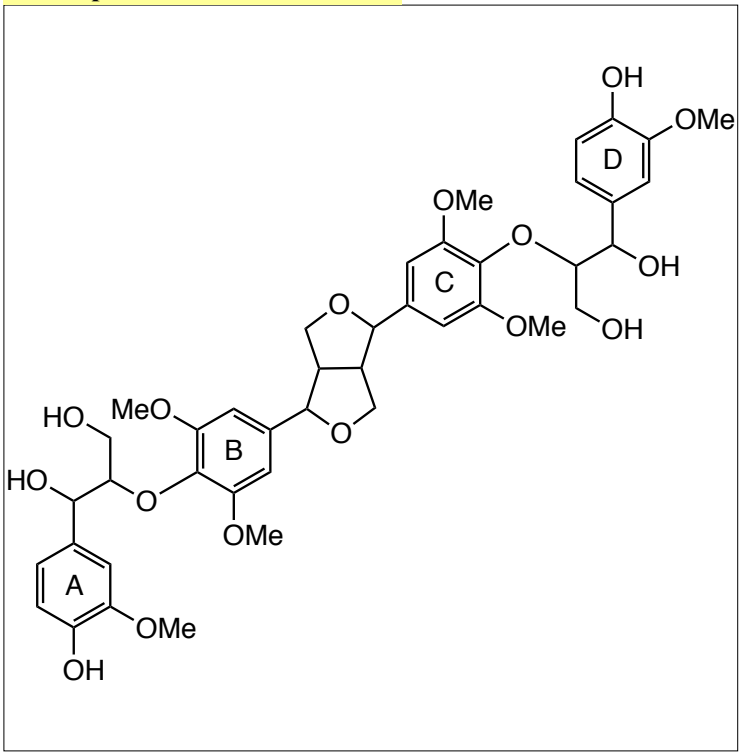
Notes:

L.Landucci
LLL XIV 148BA
10 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.53	20.26	20.04
Ac Me	20.53	20.26	20.04
Ac Me	20.85	20.67	20.21
Ac Me	20.85	20.80	20.30
Ac Me	21.15	20.95	20.61
Ac Me	21.15	20.95	20.61
OMe	56.12	56.46	55.72
OMe	56.12	56.46	55.72
OMe	56.26	56.46	55.72
OMe	56.26	56.46	55.72
OMe	56.26	56.46	55.85
OMe	56.26	56.46	55.85
γ	62.88	63.44	62.22
B γ	62.88	63.44	62.22
C γ	65.00	65.26	64.16
α	74.35	75.43	73.97
B α	74.50	75.43	73.97
β	80.89	81.42	79.89
B β	80.89	81.56	79.89
A2	103.81	104.67	103.35
A6	103.81	104.67	103.35
B2	104.10	104.67	103.35
B6	104.10	104.67	103.35
C2	104.33	104.96	103.53
C6	104.33	104.96	103.53
C β	123.04	124.09	123.29
A4	128.54	129.36	127.48
C1	132.45	133.25	131.80
B1	133.24	134.06	132.46
C α	134.12	134.38	132.95
C4	135.40	136.54	134.25
A1	135.63	136.60	134.45
B4	135.81	136.64	135.16
A3	151.96	153.01	151.40
A5	151.96	153.01	151.40
B3	153.08	153.88	152.29
B5	153.08	153.88	152.29
C3	153.29	154.16	152.54
C5	153.29	154.16	152.54
A4 Ac C=O	168.68	168.50	167.89
Ac C=O	169.52	169.95	169.23
Ac C=O	169.66	169.95	169.23
Ac C=O	170.79	170.67	169.83
Ac C=O	170.94	170.67	169.83
Ac C=O	170.94	170.67	169.98

Compound Number 194



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

^{1}H (acetone)

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

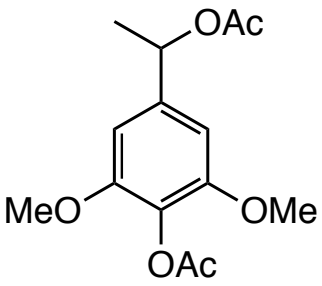
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B,C β	54.48	55.37	53.56
OMe	56.00	56.26	55.41
OMe	56.27	56.62	55.89
OMe	56.27	56.62	55.89
A,D γ	60.56	60.97	59.73
B,C γ	72.01	72.64	71.21
A,D α	72.55	73.38	72.00
B,C α	85.86	86.53	84.97
A,D β	87.08	87.84	86.05
B,C 2	102.82	104.12	103.22
B,C 6	102.82	104.12	103.22
A,D 2	108.45	110.93	110.85
A,D 5	114.19	115.19	114.54
A,D 6	118.75	120.05	119.24
A,D 1	131.31	133.77	133.18
B,C 1	134.41	135.74	134.69
B,C 4	137.63	139.00	136.68
A,D 4	144.89	146.45	145.20
A,D 3	146.64	147.96	146.85
B,C 3	153.49	154.20	152.50
B,C 5	153.49	154.20	152.50

Compound Number 195



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

^{1}H (acetone)

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

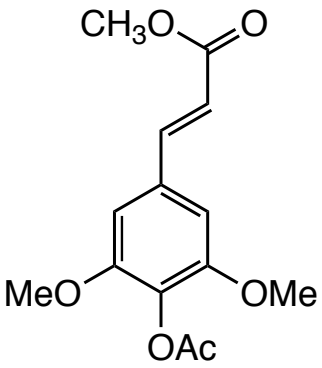
Notes:

J. Milhaupt
A 51
41mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me Ac Me	20.47 21.36	20.24 21.12	20.03 20.90	
β	22.24	22.62	22.02	
OMe OMe	56.17 56.17	56.44 56.44	56.89 56.89	
α	72.28	72.64	71.58	
2 6	102.94 102.94	103.51 103.51	102.54 102.54	
4	128.24	129.11	127.25	
1	140.03	141.50	140.23	
3 5	152.12 152.12	153.16 153.16	151.57 151.57	
Ac C=O α Ac C=O	168.69 170.15	168.52 170.16	168.00 169.54	

Compound Number 196



Acetylated Sinapic acid methyl ester

^{1}H (acetone)

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

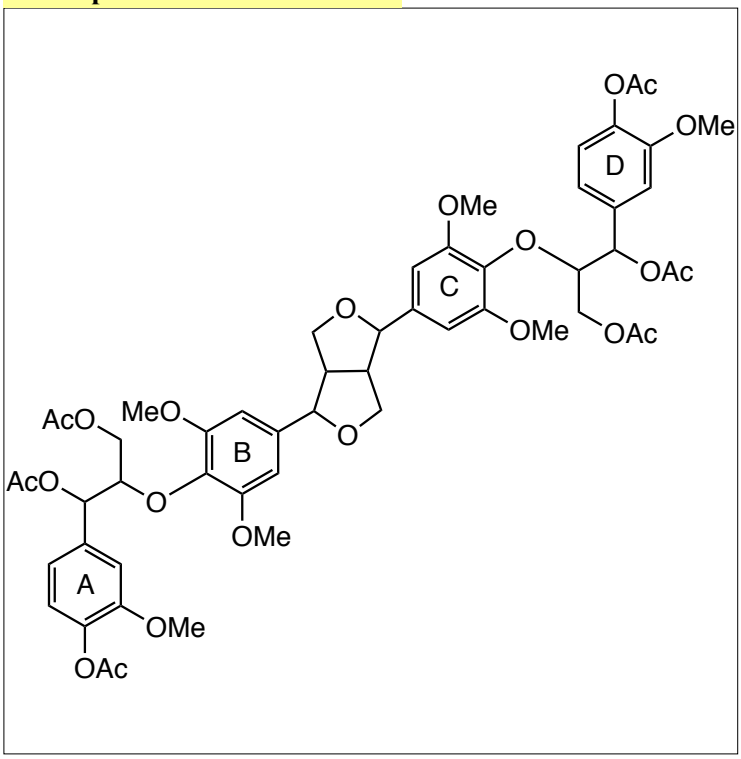
Notes:

J. Milhaupt
A 45
47mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.36	20.23	20.00	
γ OMe	51.68	51.70	51.34	
OMe OMe	56.12 56.12	56.61 56.61	56.08 56.08	
2 6	104.65 104.65	105.83 105.83	105.24 105.24	
β	118.05	118.97	118.18	
4	130.40	131.45	129.60	
1	132.64	133.56	132.30	
α	144.51	145.15	144.26	
3 5	152.38 152.38	153.53 153.53	151.90 151.90	
γ	167.11	167.44	166.57	
Ac C=O	168.39	168.38	167.83	

Compound Number 197



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

^{1}H (acetone)

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

Notes:

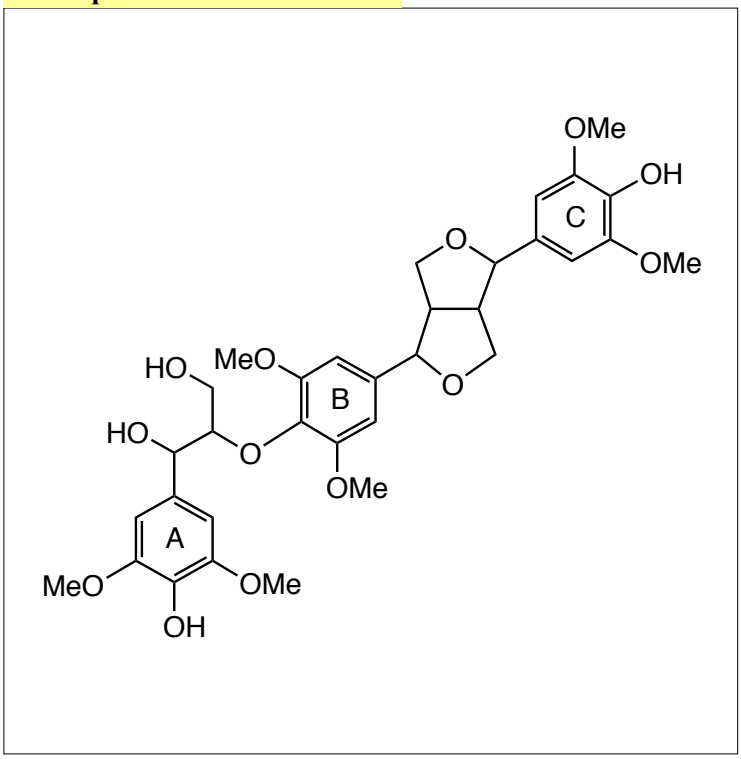
S. Luque SLL 13F, 11 mg

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.74	20.48	20.27	
Ac Me	20.83	20.61	20.27	
Ac Me	21.14	20.94	20.61	
B,C β	54.45	55.38	53.65	
A,D OMe	56.00	56.26	55.63	
B,C OMe	56.18	56.39	55.73	
B,C OMe	56.18	56.39	55.73	
A,D γ	62.78	63.27	62.02	
B,C γ	72.06	72.60	71.24	
A,D α	74.01	75.04	73.64	
A,D β	80.87	81.30	79.83	
B,C α	85.94	86.52	84.93	
B,C 2	102.86	103.71	102.69	
B,C 6	102.86	103.71	102.69	
A,D 2	111.58	112.20	110.85	
A,D 6	119.27	120.03	118.72	
A,D 5	122.48	123.25	122.43	
B,C 4	134.60	135.47	133.51	
A,D 1	136.19	137.15	135.61	
B,C 1	137.35	138.96	137.50	
A,D 4	139.56	140.54	138.79	
A,D 3	150.90	152.01	150.46	
B,C 3	153.42	154.05	152.46	
B,C 5	153.42	154.05	152.46	
4 Ac C=O	168.92	168.92	168.35	
αAc C=O	169.56	169.90	169.24	
γAc C=O	170.91	170.65	169.87	

Compound Number 198



S-b-S-r-S

^{1}H (acetone)

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

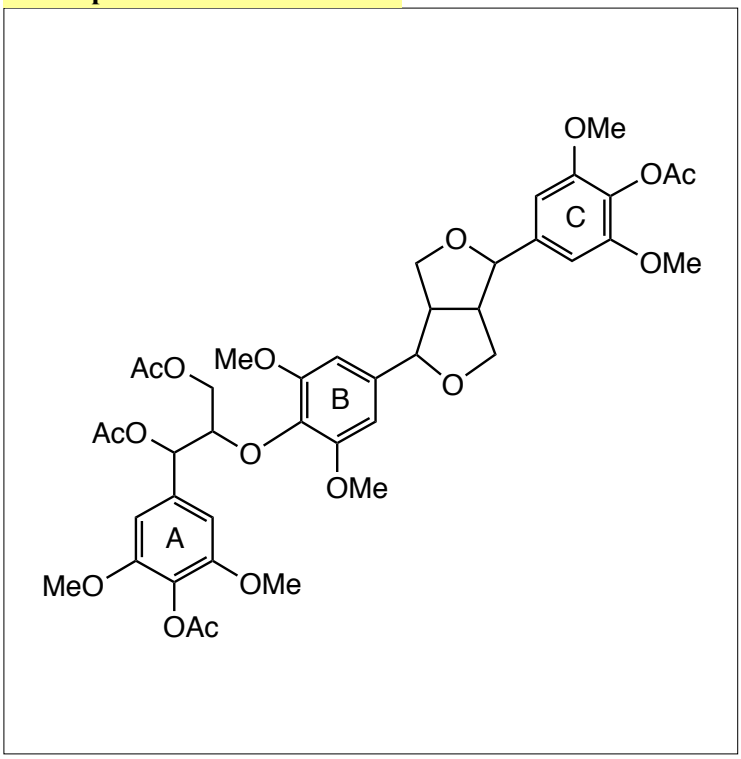
Notes:

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)

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	54.43	55.27	53.59	
C β	54.57	55.42	53.73	
OMe	56.34	56.63	55.88	
OMe	56.34	56.63	55.88	
OMe	56.45	56.63	56.01	
OMe	56.45	56.63	56.01	
OMe	56.49	56.63	56.01	
OMe	56.49	56.63	56.01	
γ	60.65	61.03	59.90	
C γ	71.80	72.40	71.10	
B γ	72.17	72.61	71.26	
α	72.77	73.63	72.38	
B α	86.01	86.61	85.10	
C α	86.01	86.73	85.30	
β	87.24	87.87	86.20	
B2	102.69	104.10	103.28	
B6	102.69	104.10	103.28	
C2	102.84	104.51	103.65	
C6	102.84	104.51	103.65	
A2	102.94	104.91	104.29	
A6	102.94	104.91	104.29	
A1	130.46	132.73	131.36	
C1	132.00	133.13	132.42	
B1	134.05	135.86	134.42	
A4	134.51	135.86	134.86	
C4	134.51	136.23	134.86	
B4	137.91	139.07	136.79	
A3	147.15	148.38	147.40	
A5	147.15	148.38	147.40	
C3	147.29	148.68	147.88	
C5	147.29	148.68	147.88	
B3	153.55	154.16	152.55	
B5	153.55	154.16	152.55	

Compound Number 199



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

^{1}H (acetone)

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

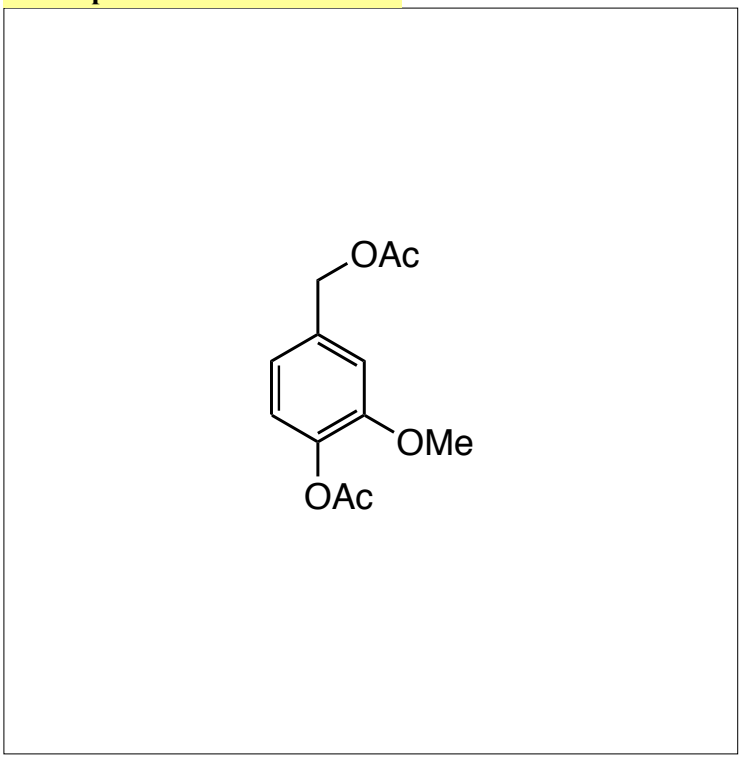
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.53	20.26	20.06	
Ac Me	20.53	20.26	20.06	
Ac Me	20.86	20.63	20.29	
Ac Me	21.16	20.94	20.63	
B β	54.39	55.33	53.61	
Cβ	54.52	55.44	53.85	
OMe	56.17	56.38	55.72	
OMe	56.17	56.38	55.72	
OMe	56.23	56.46	55.87	
OMe	56.23	56.46	55.87	
OMe	56.29	56.46	55.87	
OMe	56.29	56.46	55.87	
γ	62.81	63.41	62.16	
C γ	72.07	72.66	71.31	
B γ	72.19	72.66	71.31	
α	74.25	75.33	73.92	
β	80.78	81.29	79.76	
B α	85.82	86.45	84.85	
C α	85.98	86.56	85.00	
C2	102.30	103.23	102.36	
C6	102.30	103.23	102.36	
B2	102.84	103.71	102.70	
B6	102.84	103.71	102.70	
A2	104.07	104.68	103.30	
A6	104.07	104.68	103.30	
C1	128.05	128.85	126.98	
A4	128.51	129.34	127.45	
B4	134.67	135.61	133.69	
A1	135.66	136.65	135.21	
B1	137.27	138.83	137.38	
C4	139.74	141.45	140.08	
A3	151.92	152.95	151.38	
A5	151.92	152.95	151.38	
C3	152.34	153.22	151.58	
C5	152.34	153.22	151.58	
B3	153.35	153.98	152.41	
B5	153.35	153.98	152.41	
Ac C=O	168.63	168.48	167.91	
Ac C=O	168.85	168.58	168.02	
Ac C=O	169.53	169.91	169.26	
Ac C=O	170.94	170.76	169.89	

Compound Number 200



Vanillyl alcohol diacetate

4-hydroxy-3-methoxybenzyl alcohol diacetate

^{1}H (acetone)

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

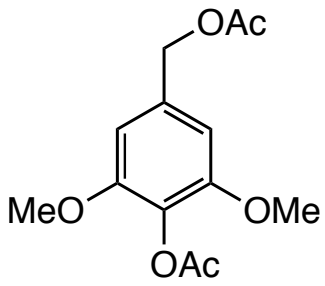
Notes:

S. Ralph
35mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me Ac Me	20.57 20.93	20.45 20.78	20.25 20.59	
OMe	55.84	56.20	55.68	
α	65.86	66.10	65.10	
2	112.50	113.32	112.58	
6	120.67	121.04	120.16	
5	122.77	123.57	122.67	
1	134.80	136.23	134.99	
4	139.62	140.64	138.97	
3	151.07	152.19	150.69	
4 Ac C=O	168.84	168.93	168.42	
α Ac C=O	170.66	170.79	170.15	

Compound Number 201



Syringyl alcohol diacetate

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

^{1}H (acetone)

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

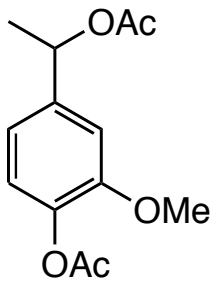
Notes:

J. Milhaupt A 53
35 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.47	20.23	20.05	
Ac Me	21.05	20.79	20.63	
OMe	56.21	56.46	55.91	
OMe	56.21	56.46	55.91	
α	66.37	66.46	65.45	
2	105.13	105.67	104.84	
6	105.13	105.67	401.84	
4	128.58	129.43	127.57	
1	134.42	135.77	134.49	
3	152.21	153.19	151.59	
5	152.21	153.19	151.59	
4 Ac C=O	168.67	168.50	167.97	
α Ac C=O	170.77	170.80	170.14	

Compound Number 202



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

^{1}H (acetone)

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

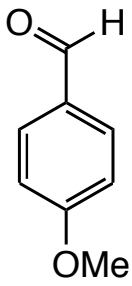
Notes:

J. Milhaupt
A 49.1
35mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.69	20.47	20.28	
Ac Me	21.37	21.12	20.90	
β	22.21	22.57	22.00	
OMe	55.93	56.21	55.70	
α	71.96	72.31	71.26	
2	110.60	111.30	110.46	
6	118.44	118.73	117.74	
5	122.75	123.51	122.60	
1	139.33	140.32	138.62	
4	140.52	141.88	140.60	
3	151.05	152.18	150.66	
4 Ac C=O	169.01	168.95	168.44	
α Ac C=O	170.21	170.17	169.55	

Compound Number 203



4-methoxy benzaldehyde

^{1}H (acetone)

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

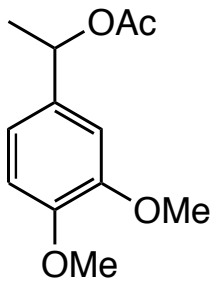
Notes:

Aldrich
60mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.51	56.03	55.51	
3	114.26	115.16	114.35	
5	114.26	115.16	114.35	
1	129.90	131.11	129.57	
2	131.88	132.43	131.65	
6	131.88	132.43	131.65	
4	164.55	165.44	164.10	
α	190.68	191.09	191.01	

Compound Number 204



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

^{1}H (acetone)

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

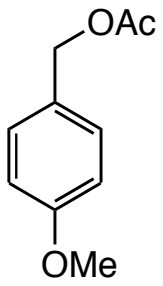
Notes:

J. Milhaupt
A 141
38mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.39	21.18	20.93	
β	21.99	22.41	21.82	
OMe	55.91	56.13	55.43	
OMe	55.91	56.13	55.43	
α	72.20	72.51	71.42	
2	109.69	111.16	109.93	
5	111.06	112.63	111.57	
6	118.64	119.25	118.12	
1	134.19	135.54	134.02	
4	148.76	150.01	148.32	
3	148.96	150.29	148.58	
Ac C=O	170.29	170.21	169.51	

Compound Number 205



4-methoxybenzyl alcohol acetate

^{1}H (acetone)

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

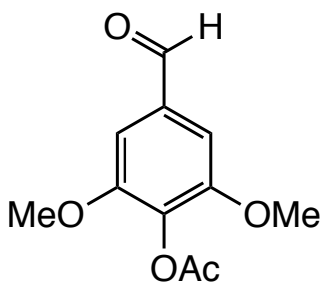
Notes:

J. Milhaupt
A 139
56mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.01	20.85	20.61	
OMe	55.23	55.53	54.98	
α	66.07	66.25	65.18	
3	113.94	114.60	113.70	
5	113.94	114.60	113.70	
1	128.10	129.43	128.03	
2	130.08	130.78	129.85	
6	130.08	130.78	129.85	
4	159.65	160.57	159.07	
Ac C=O	170.85	170.85	170.13	

Compound Number 206



Syringaldehyde acetate

3,5-dimethoxy-4-acetoxy-benzaldehyde

^{1}H (acetone)

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

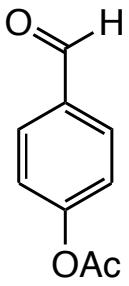
Notes:

J. Milhaupt
A 147
42mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.41	20.21	20.01	
OMe	56.35	56.72	56.20	
OMe	56.35	56.72	56.20	
2	106.09	106.72	106.00	
6	106.09	106.72	106.00	
4	133.82	134.60	132.83	
1	134.36	135.62	134.20	
3	152.88	153.91	152.35	
5	152.88	153.91	152.35	
Ac C=O	168.01	168.15	167.58	
α	191.00	191.82	191.89	

Compound Number 207



4-Acetoxy benzaldehyde

^{1}H (acetone)

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

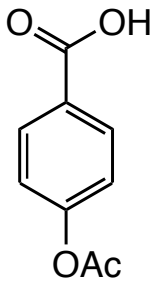
Notes:

J. milhaupt
137.5
42mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.06	20.98	20.78	
3	122.32	123.43	122.63	
5	122.32	123.43	122.63	
2	131.12	131.68	130.85	
6	131.12	131.68	130.95	
1	133.93	135.13	133.75	
4	155.30	156.42	154.99	
Ac C=O	168.62	169.27	168.64	
α	190.88	191.83	191.84	

Compound Number 208



4-Acetoxy benzoic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.29	s	
3,5	7.26	d	8.8
2,6	8.08	d	8.8
CDCl3			
Ac Me	2.30	s	
3,5	7.20	d	8.7
2,6	8.13	d	8.7

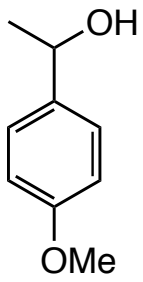
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.14	20.98	20.80	
3	121.75	122.76	121.96	
5	121.75	122.76	121.96	
1	126.79	128.81	128.31	
2	131.86	131.91	130.78	
6	131.86	131.91	130.78	
4	154.99	155.55	153.86	
α	171.33	167.00	166.55	
Ac C=O	168.80	169.28	168.75	

Notes:

J. Milhaupt
27mg
NOTE: In CDCl3 only, alpha moves to 171.38 ppm as confirmed by HMBC
see also NL-175 and NL-208

Compound Number 209



4-Methoxy benzyl alcohol

^{1}H (acetone)

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

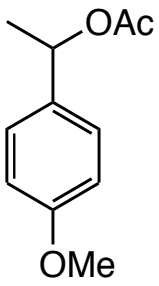
Notes:

J. Milhaupt
JMA 145
42mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	25.04	26.20	25.89	
OMe	55.27	55.43	54.92	
α	69.84	69.50	67.60	
3	113.82	114.20	113.25	
5	113.82	114.20	113.25	
2	126.67	127.27	126.34	
6	126.67	127.27	126.34	
1	138.12	140.18	139.34	
4	158.90	159.49	157.90	

Compound Number 210



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

^{1}H (acetone)

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

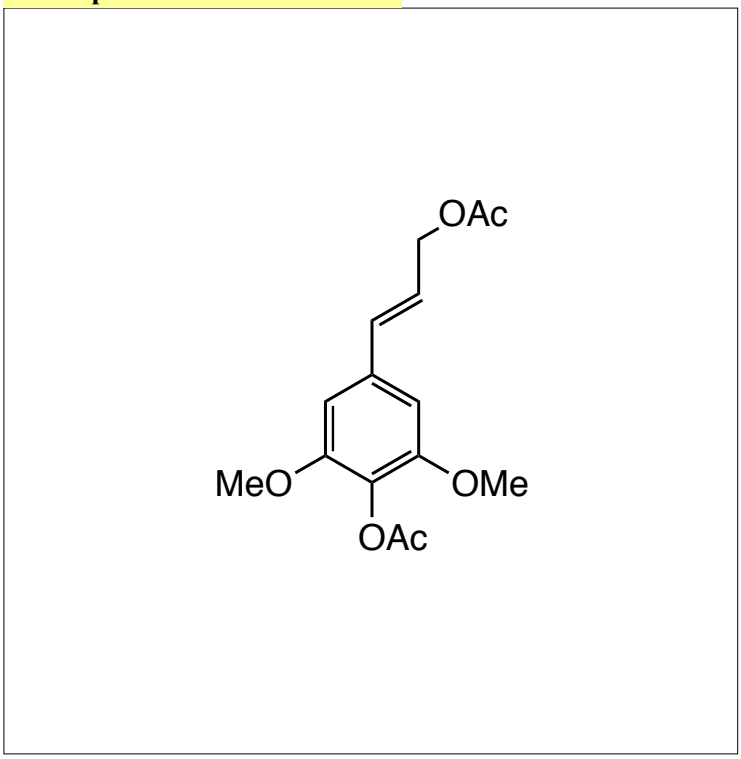
Notes:

J. Milhaupt
JMA 149
23mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.44	21.16	20.92	
β	22.01	22.35	21.76	
OMe	55.32	55.51	54.98	
α	72.06	72.28	71.18	
3	113.90	114.52	113.63	
5	113.90	114.52	113.63	
2	127.64	128.26	127.28	
6	127.64	128.26	127.28	
1	133.82	134.94	133.52	
4	159.34	160.22	158.69	
Ac C=O	170.38	170.20	169.49	

Compound Number 211



Sinapyl alcohol diacetate

^{1}H (acetone)

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

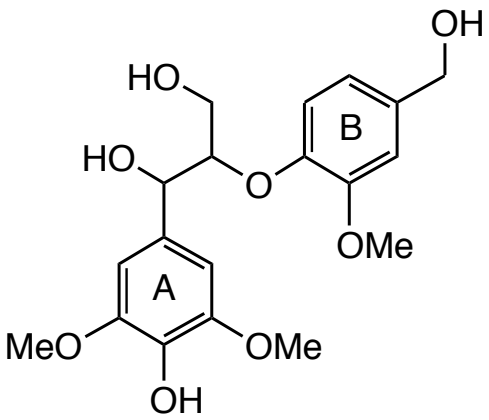
Notes:

J.Milhaupt
JMA 111
20mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.51	20.26	20.05	
Ac Me	21.05	20.79	20.62	
OMe	56.21	56.47	55.90	
OMe	56.21	56.47	55.90	
γ	64.90	65.13	64.06	
2	103.38	104.18	103.22	
6	103.38	104.18	103.22	
β	123.71	124.99	124.32	
4	128.75	129.68	127.69	
α	134.01	134.04	132.55	
1	134.71	135.67	134.33	
3	152.28	153.36	151.73	
5	152.28	153.36	151.73	
4 Ac C=O	168.71	168.51	167395	
γ Ac C=O	170.85	170.72	170.01	

Compound Number 212



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

^{1}H (acetone)

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

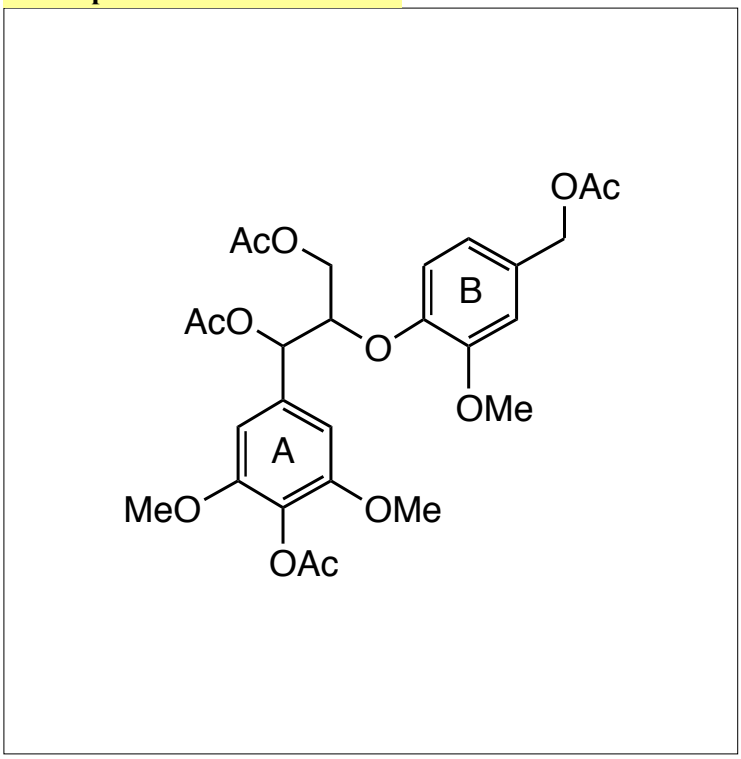
Notes:

T. Duch
I-57
25mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B OMe	55.90	56.28	55.44	
A OMe	56.34	56.60	55.74	
A OMe	56.34	56.60	55.74	
γ	61.05	61.95	60.00	
Bα	64.87	64.54	62.74	
α	74.16	74.06	70.88	
β	89.20	88.56	84.44	
A2	103.82	105.41	104.13	
A6	103.82	105.41	104.13	
B2	110.98	111.95	110.97	
B5	119.98	119.60	115.43	
B6	120.50	120.02	118.58	
A1	130.66	132.82	131.93	
A4	134.61	136.17	134.31	
B1	137.06	137.97	135.45	
B4	146.93	148.42	146.93	
A3	147.10	148.50	147.34	
A5	147.10	148.50	147.34	
B3	151.16	151.54	149.39	

Compound Number 213



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

^{1}H (acetone)

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

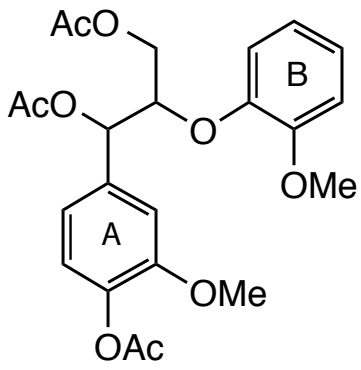
Notes:

T.Duch
I-55
40 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.36	20.24	20.03	
Ac Me	20.64	20.63	20.38	
Ac Me	20.97	20.83	20.65	
Ac Me	20.97	20.95	20.65	
B OMe	55.80	56.31	55.60	
A OMe	56.14	56.55	55.98	
A OMe	56.14	56.55	55.98	
γ	62.91	63.59	63.37	
B α	66.08	66.35	65.28	
α	74.57	75.64	74.48	
β	80.14	80.72	79.02	
A2	104.02	105.13	103.94	
A6	104.02	105.13	103.94	
B2	112.70	113.94	112.86	
B5	118.12	118.67	116.91	
B6	121.15	121.77	120.69	
A4	128.79	129.70	127.92	
B1	130.88	132.09	130.30	
A1	134.63	136.18	134.92	
B4	147.90	148.97	147.38	
B3	150.60	151.57	149.79	
A3	152.14	153.21	151.55	
A5	152.14	153.21	151.55	
A4 Ac C=O	168.42	168.46	167.88	
α Ac C=O	169.60	170.02	169.32	
γ Ac C=O	170.48	170.72	167.94	
Bα Ac C=O	170.79	170.88	170.15	
1H				
Ac Me	2.0			
Ac Me	2.25			
Ac Me	2.6			
A4 Ac Me	2.8			
A OMe	3.80			
B OMe	3.83			
γ1	4.08			
γ2	4.31			
β	4.61			
B α	5.03			
α	6.08			
A 2,6	6.66			

Compound Number 214



erythro

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

^{1}H (acetone)

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

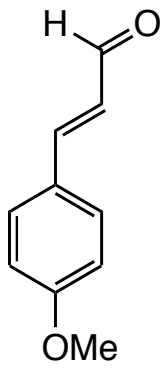
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.57	20.46	20.22	
Ac Me	20.66	20.59	20.29	
Ac Me	20.93	20.86	20.53	
OMe	55.78	56.26	55.54	
OMe	55.90	56.32	55.66	
γ	62.55	63.03	61.84	
α	73.79	74.63	73.10	
β	80.15	80.37	78.36	
A2	112.02	112.83	111.61	
B2	112.70	113.90	112.89	
B5	119.51	119.88	117.93	
A6	119.71	120.46	119.28	
B6	120.98	121.68	120.61	
A5	122.52	123.36	122.43	
B1	123.58	124.08	122.83	
A1	135.41	136.71	135.30	
A4	139.80	140.85	139.05	
B4	147.18	148.33	146.61	
B3	150.97	152.11	150.30	
A3	151.11	152.11	150.52	
Ac C=O	168.69	168.89	168.31	
Ac C=O	169.44	169.89	169.16	
Ac C=O	170.68	170.74	169.94	
1H CDCl3				
Ac Me	1.94			
Ac Me	2.03			
Ac Me	2.25			
OMe	3.75			
OMe	3.78			
γ1	4.25			
γ2	4.41			
β	4.63			
α	6.06			

Compound Number 215



***p*-Methoxycinnamaldehyde**

^{1}H (acetone)

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

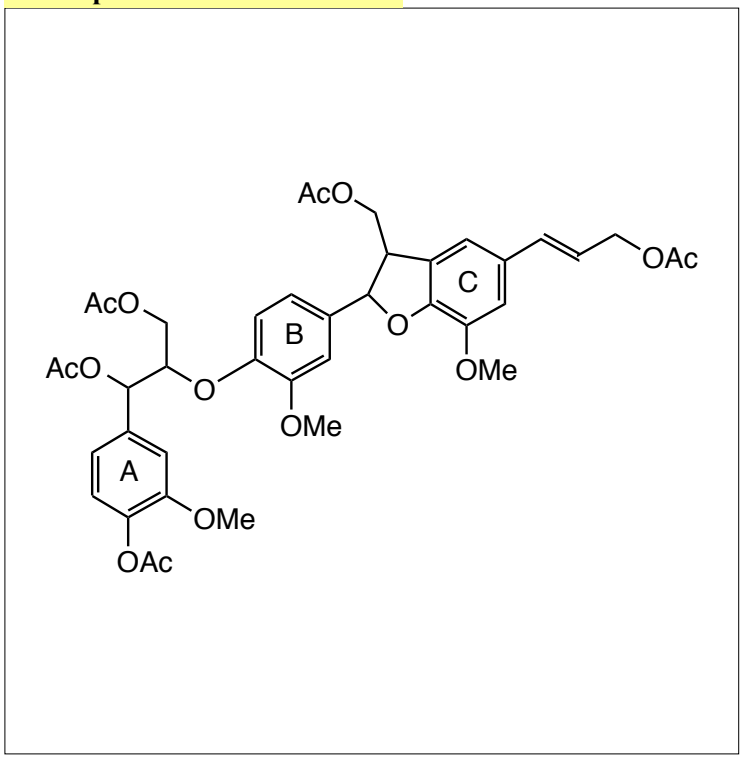
Notes:

Pew Collection
50 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.34	55.81	55.35
3	114.48	115.35	114.51
5	114.48	115.35	114.51
β	126.33	127.37	126.31
1	126.67	127.91	126.69
2	130.28	131.26	130.65
6	130.28	131.26	130.65
α	152.72	153.22	153.10
4	162.13	163.08	161.75
γ	193.66	193.81	194.00

Compound Number 216



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

^{1}H (acetone)

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

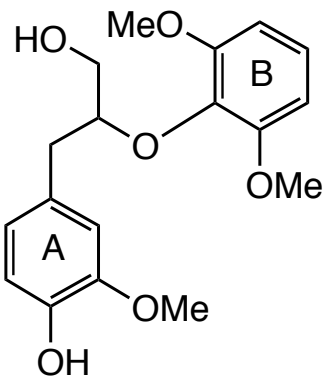
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.63	20.45	20.32	
A αAc Me	20.74	20.60	20.40	
B γAC Me	20.79	20.68	20.51	
C γAc Me	20.96	20.80	20.62	
A γAc Me	21.00	20.86	20.70	
B β	50.37	51.24	49.34	
OMe	55.88	56.28	55.71	
OMe	55.91	56.28	55.71	
OMe	56.00	56.28	55.71	
γ	62.45	63.04	61.85	
C γ	65.18	65.49	64.49	
B γ	65.29	65.95	64.76	
α	73.66	74.48	73.01	
β	80.25	80.30	78.30	
B α	88.23	88.54	87.17	
B2	110.28	111.50	110.74	
C2	110.60	112.17	110.93	
A2	111.88	112.71	111.62	
C6	115.31	116.33	115.26	
B6	118.69	119.14	117.49	
B5	119.18	119.41	118.30	
A6	119.60	120.45	119.33	
C β	121.24	122.23	121.34	
A5	122.59	123.33	122.50	
C5	127.49	129.01	127.89	
C1	130.60	131.53	130.04	
C α	134.30	134.71	133.49	
A1	135.30	136.60	135.05	
B1	135.80	137.06	135.26	
A4	139.75	140.78	139.06	
C3	144.41	145.39	143.84	
B4	147.19	148.14	146.54	
C4	148.20	149.31	147.53	
B3	150.96	151.95	150.16	
A3	151.19	152.08	150.54	
A4 C=O	168.80	168.92	168.43	
A αC=O	169.49	169.89	169.26	
C γC=O	170.74	170.77	170.04	
B γC=O	170.76	170.95	170.15	
A γC=O	170.88	170.95	170.28	

Compound Number 217



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

^{1}H (acetone)

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

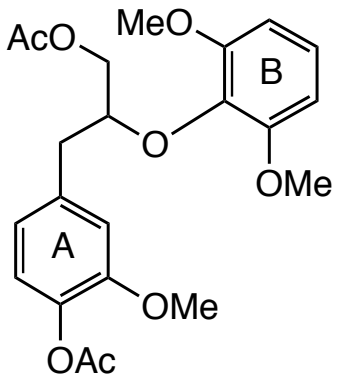
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
α	37.30	37.97	36.86
A OMe	55.90	56.19	55.52
B OMe	56.09	56.45	55.86
B OMe	56.09	56.45	55.86
γ	62.21	62.78	61.69
β	84.48	85.29	83.46
B2	105.42	106.49	105.65
B6	105.42	106.49	105.65
A2	112.31	113.89	113.58
A5	114.28	115.52	115.11
A6	122.09	122.81	121.68
B1	123.95	124.51	123.41
A1	130.13	130.76	129.32
B4	135.66	137.09	135.65
A4	144.12	145.71	144.64
A3	146.44	148.05	147.15
B3	153.60	154.61	153.29
B5	153.60	154.61	153.29

Compound Number 218



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

^{1}H (acetone)

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

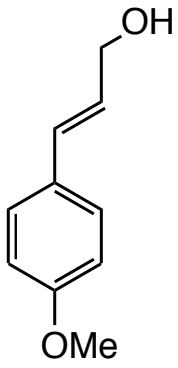
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.70	20.49	20.37
Ac Me	20.85	20.65	20.46
α	38.26	38.82	37.51
OMe	55.97	56.12	55.60
OMe	55.97	56.30	55.74
OMe	55.97	56.30	55.74
γ	65.35	65.72	64.78
β	80.49	80.86	79.44
B2	105.20	106.29	105.39
B6	105.20	106.29	105.39
A2	113.95	114.77	113.76
A6	121.64	122.34	121.30
A5	122.30	123.12	122.27
B1	123.92	124.53	123.74
B4	135.89	137.12	137.28
A1	137.13	137.89	136.71
A4	138.26	139.37	137.69
A3	150.69	151.85	150.35
B3	153.66	154.65	153.16
B5	153.66	154.65	153.16
Ac C=O	169.17	169.08	168.60
γ Ac C=O	170.92	170.79	170.16

Compound Number 219



trans

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

^{1}H (acetone)

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

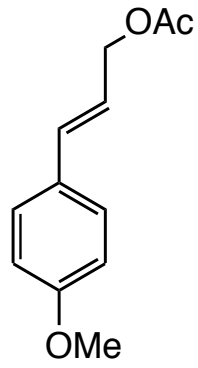
Notes:

S.Ralph 55mg
SRVIII-45

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.30	55.48	55.00	
γ	63.76	63.36	61.62	
3	113.99	114.73	113.96	
5	113.99	114.73	113.96	
2	127.69	128.24	127.27	
6	127.69	128.24	127.27	
β	126.43	128.61	128.20	
α	130.82	129.76	128.27	
1	129.57	130.78	129.51	
4	159.32	160.05	158.57	
1H				
OMe	3.78			
γ	4.25			
β	6.19			
α	6.52			
3,5	6.83			
2,6	7.28			

Compound Number 220



trans

Coumaryl alcohol acetate
4-methoxycinnamyl alcohol acetate

^{1}H (acetone)

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

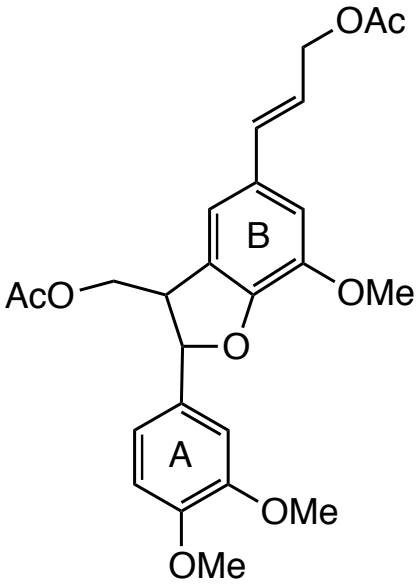
Notes:

S.Ralph
30mg
gHSQC, gHMBC Acetone shifts confirmed

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	21.07	20.82	20.64
OMe	55.35	55.59	55.05
γ	65.39	65.52	64.48
3	114.13	114.91	114.02
5	114.13	114.91	114.02
β	121.00	122.21	121.17
2	127.94	128.69	127.74
6	127.94	128.69	127.74
1	130.17	130.80	129.86
α	134.10	134.32	133.00
4	159.73	160.71	159.13
Ac C=O	170.90	170.77	170.07
1H			
Ac Me	2.08		2.04
OMe	3.80		3.76
γ	4.70		4.65
β	6.14		6.19
3,5	6.85		6.90
2,6	7.32		7.40

Compound Number 221



V-c-CA

4-methoxy phenylcoumaran diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Bγ Ac Me	2.02	s	
β	3.76		
OMe	3.79	s	
OMe	3.80	s	
OMe	3.87	s	
γ1	4.33	dd	11.1, 7.4
γ2	4.42	dd	11.1, 5.6
Bγ	4.66	dd	7.4, 0.9
α	5.53	d	7.0
Bβ	6.23	dt	15.8, 6.4
Bα	6.64	d	15.9
A5	6.93	d	8.25
A5	6.96	dd	2.0, 8.25
A6	7.04	m	
B2	7.04	m	
B6	7.04	m	

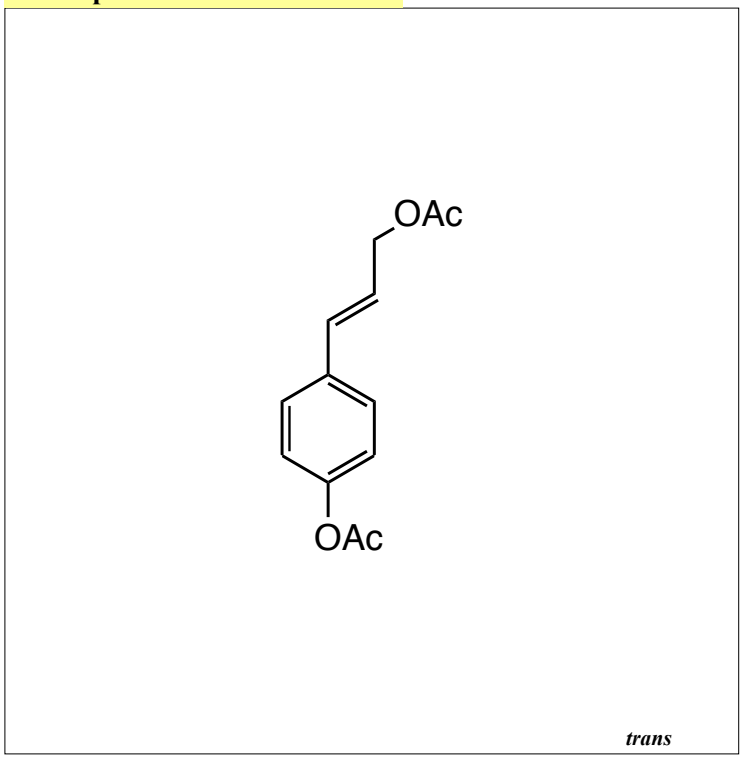
Notes:

F. Lu, FLw79
S.Ralph, SRVII-104
A3 and A4 are very close and may be switched
gamma acetate C=O switches order in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.78	20.71	20.57	20.45
Bγ Ac Me	20.99	20.82	20.73	20.62
β	50.24	51.16	49.32	49.44
OMe	55.87	56.12	55.48	55.41
OMe	55.90	56.13	55.52	55.47
OMe	55.97	56.39	55.71	55.68
Bγ	65.19	65.53	64.54	64.56
γ	65.26	65.94	64.73	64.71
α	88.61	88.84	87.44	87.53
A2	109.16	110.82	109.85	109.89
B2	110.53	112.14	110.91	110.99
A5	110.97	112.63	111.64	111.65
B6	115.26	116.34	115.28	115.30
A6	118.74	119.33	118.47	118.49
Bβ	121.11	122.18	121.31	121.30
B5	127.64	129.17	128.03	128.05
B1	130.46	131.44	129.99	130.09
A1	132.78	134.50	132.80	132.90
Bα	134.34	134.77	133.56	133.60
B3	144.38	145.41	143.87	143.95
B4	148.24	149.38	147.60	147.74
A3	149.17	150.44	148.78	148.88
A4	149.17	150.51	148.80	148.89
Bγ Ac C=O	170.87	170.78	170.16	170.11
Ac C=O	170.75	170.94	170.30	170.26
1H				
Ac Me	2.01		1.97	1.96
Bγ Ac Me	2.07		2.04	2.03
β	3.75		3.73	3.78
OMe	3.83		3.73	3.72
OMe	3.84		3.74	3.73
OMe	3.88		3.81	3.82
γ1	4.29		4.27	4.32
γ2	4.41		4.37	4.42
Bγ	4.69		4.65	4.67
α	5.47		5.49	5.55
Bβ	6.13		6.24	6.27
Bα	6.57		6.60	6.64
A2	6.88		6.96	6.93
A5	6.81		6.94	6.93
A6	6.90		6.89	7.06
B2	6.86		7.01	7.01
B6	6.86		7.03	7.05

Compound Number 222



trans

4-hydroxycinnamyl alcohol diacetate

Coumaryl alcohol acetate

^{1}H (acetone)

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

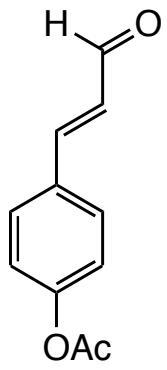
Notes:

S.Ralph 37mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me	20.98	20.78	20.63	
4 Ac Me	21.12	20.96	20.86	
γ	64.95	65.17	64.18	
3	121.79	122.85	121.97	
5	121.79	122.85	121.97	
β	123.58	124.89	123.97	
2	127.62	128.29	127.43	
6	127.62	128.29	127.43	
α	133.19	133.28	132.05	
1	134.08	134.99	133.64	
4	150.52	151.70	150.13	
4 Ac C=O	169.32	169.55	169.03	
γ Ac C=O	170.78	170.74	170.07	
1H				
γ Ac Me	2.09		2.04	
4 Ac Me	2.28		2.26	
γ	4.71		4.69	
β	6.23		6.34	
α	6.63		6.69	
3,5	7.05		7.10	
2,6	7.38		7.50	

Compound Number 223



trans

4-acetoxy cinnamaldehyde
Coumaryl aldehyde acetate

^{1}H (acetone)

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

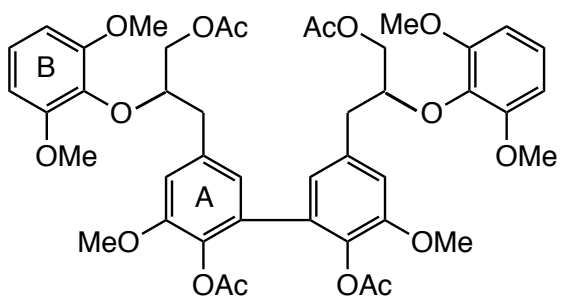
Notes:

S.Ralph
27mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	21.11	20.98	20.65
3	122.43	123.40	122.33
5	122.43	123.40	122.33
β	128.73	129.60	128.41
2	129.70	130.60	129.81
6	129.70	130.60	129.81
1	131.75	132.91	131.59
α	151.44	152.21	151.73
4	152.90	154.01	152.41
Ac C=O	168.97	169.40	168.70
γ	193.44	193.95	193.97
1H CDCl3			
Ac Me	2.31		
β	6.67		
3,5	7.17		
α	7.45		
2,6	7.58		
γ	9.69		

Compound Number 224



S-b-G-5,5-G-b-S (α = CH2)

^{1}H (acetone)

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

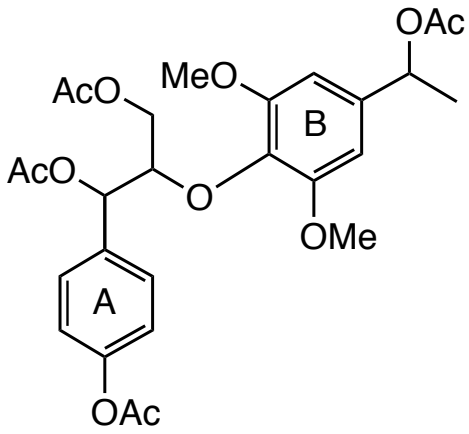
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
4 Ac Me	20.34	20.32	19.88	
γ Ac Me	20.80	20.68	20.35	
α	38.29	38.90	37.58	
OMe	56.00	56.33	55.71	
OMe	56.00	56.33	55.71	
OMe	56.00	56.33	55.84	
γ	65.26	65.69	64.70	
β	80.43	80.91	79.49	
B2	105.31	106.27	105.42	
B6	105.31	106.27	105.42	
A2	113.43	114.11	113.29	
A6	128.48	124.07	122.66	
B1	123.92	124.57	123.70	
A5	131.10	131.92	130.30	
B4	136.00	137.04	135.36	
A1	136.19	137.04	135.42	
A4	136.19	137.04	135.84	
A3	151.02	152.12	150.67	
B3	153.17	154.64	153.17	
B5	153.17	154.64	153.17	
4 Ac C=O	168.68	168.80	167.98	
γ Ac C=O	170.82	170.80	170.02	
1H CDCl3				
γ Ac Me	2.04			
A4 Ac Me	2.05, 2.20			
α	3.12			
OMe	3.76			
OMe	3.85			
γ	4.20			
β	4.51			
B2,6	6.46			
A6	6.74			
A2, B1	6.98			

Compound Number 225



erythro

H-b-S

^{1}H (acetone)

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

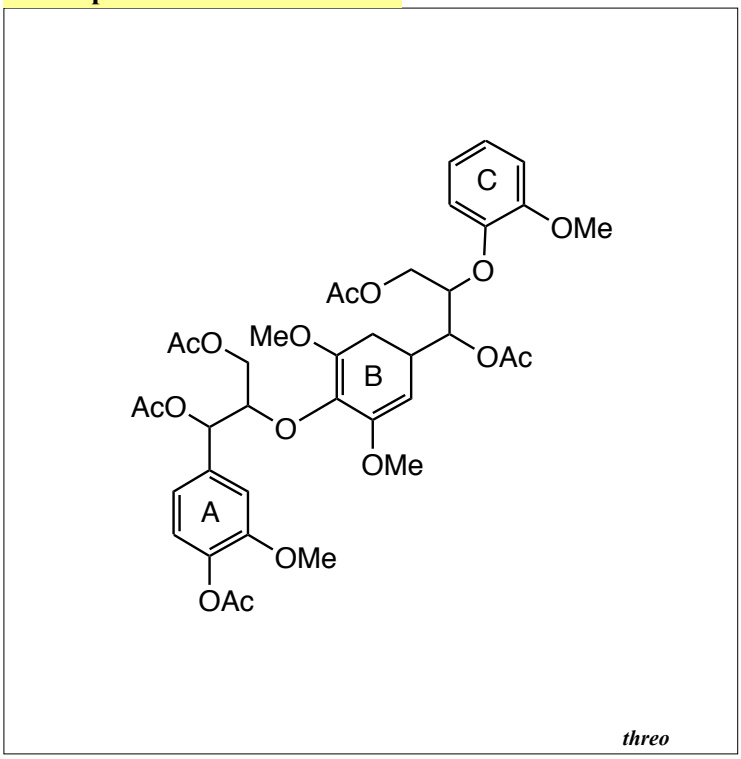
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.78	20.55	20.22
Aα Ac Me	20.12	20.95	20.60
Bα Ac Me	21.19	20.95	20.74
Aγ Ac Me	21.44	21.16	20.95
Bβ	22.26	22.60	21.99
OMe	56.08	56.38	55.75
OMe	56.08	56.38	55.75
γ	62.66	63.19	61.94
Bα	72.38	72.68	71.59
α	73.94	74.90	73.49
β	80.88	81.26	79.79
B2	103.29	103.98	102.85
B6	103.29	103.98	102.85
A3	121.36	122.33	121.56
A5	121.36	122.33	121.56
A2	128.06	128.89	128.72
A6	128.06	128.89	128.72
A1	134.69	135.64	134.26
B4	134.96	135.84	135.05
B1	137.91	139.17	137.40
A4	150.37	151.53	149.96
B3	153.22	154.08	152.52
B5	153.22	154.08	152.52
A4 Ac C=O	169.36	169.61	169.08
Aα Ac C=O	169.62	169.93	169.08
Bα Ac C=O	170.29	170.21	169.55
Aγ Ac C=O	170.29	170.66	169.90
1H CDCl3			
Bβ	1.52		
γ Ac Me	1.98		
Bα Ac Me	2.09		
α Ac Me	2.16		
A4 Ac Me	2.30		
OMe	3.76		
γ1	4.25		
γ2	4.45		
β	4.61		
Bα	5.81		
α	6.12		
B2,6	6.53		
A3,5	7.05		
A2,6	7.37		

Compound Number 226



threo

G-bt-S-bt-G

^{1}H (acetone)

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

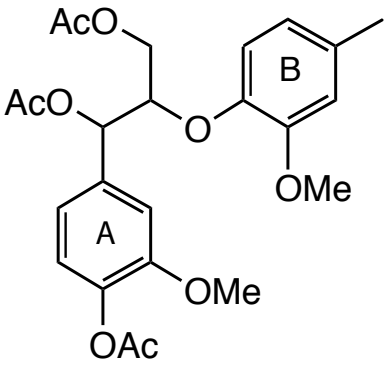
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ Ac Me	20.69	20.48	20.28
γAc Me	20.75	20.58	20.28
α Ac Me	20.79	20.67	22.41
αAc Me	21.09	20.92	22.41
4 Ac Me	21.09	20.96	20.65
OMe	55.80	56.19	55.48
OMe	55.90	56.24	55.62
OMe	56.04	56.43	55.78
OMe	56.04	56.43	55.78
Aγ	62.74	63.36	62.19
Bγ	63.16	63.72	62.56
Aα	73.99	75.07	73.74
Bα	74.87	75.71	74.60
Bβ	80.36	80.76	79.15
Aβ	80.78	81.38	79.94
B2	104.30	105.27	104.13
B6	104.30	105.27	104.13
A2	111.60	112.26	110.95
C2	112.49	113.68	112.61
C5	118.50	118.95	117.23
A6	119.24	120.01	118.78
C6	120.98	121.66	120.60
A5	122.37	123.26	122.46
C1	123.24	123.61	122.46
B1	132.59	133.70	132.42
B4	135.35	136.40	134.48
A1	136.03	137.04	135.59
A4	139.49	140.53	138.85
C4	148.00	149.14	147.58
C3	150.77	151.74	150.03
A3	150.77	152.01	150.53
B3	153.14	153.96	152.43
B5	153.14	153.96	152.43
A4 Ac C=O	168.84	168.95	168.40
α Ac C=O	169.49	169.92	169.29
α Ac C=O	169.76	169.99	169.29
γ Ac C=O	170.51	170.61	169.92
γAc C=O	170.82	170.61	169.92

Compound Number 227



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G-b-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.94	s	
α Ac Me	2.08	s	
Bα	2.22	s	
A4 Ac Me	2.25	s	
OMe	3.79	s	
OMe	3.83	s	
γ1	4.20	dd	11.9, 4.2
γ2	4.37	dd	11.9, 5.8
β	4.74	m	
α	6.06	d	5.0
B6	6.65	bd	8.1
B2	6.82	bs	
B5	6.85	d	8.2
A5,6	7.04	m	
A2	7.23	s	
γ1 isomer	3.99		
γ2 isomer	4.25		
α isomer	6.10		

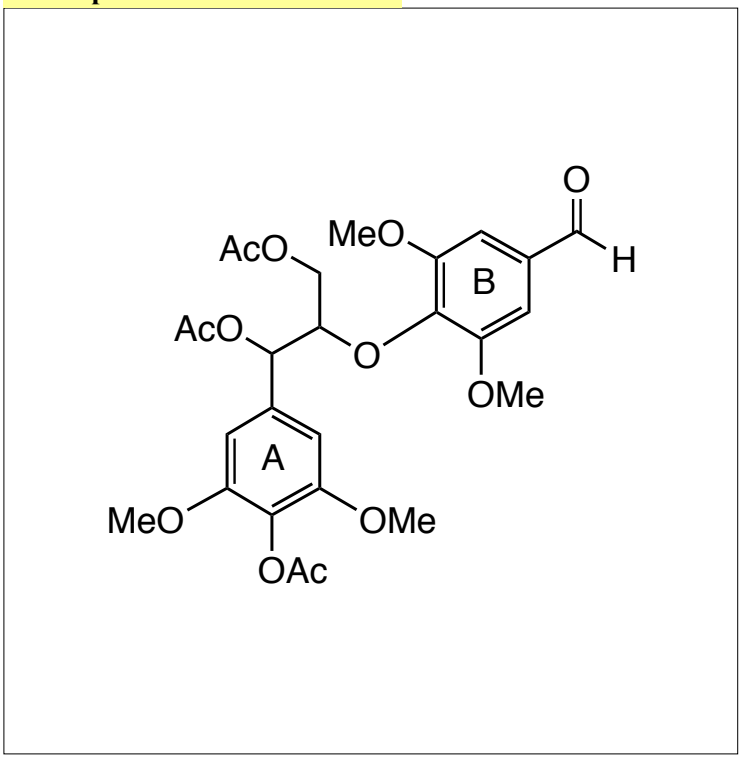
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.61	20.47	20.31
α Ac Me	20.74	20.62	20.40
γ Ac Me	20.99	20.89	20.62
Bα	21.09	21.07	20.68
OMe	55.70	56.14	55.47
OMe	55.89	56.27	55.69
γ	62.48	62.95	61.80
α	73.70	74.58	73.10
β	80.57	80.63	78.71
A2	111.84	112.63	111.50
B2	113.49	114.61	113.60
B5	119.54	120.07	118.21
A6	119.69	120.30	119.17
B6	121.21	121.85	120.77
A5	122.55	123.36	122.50
B1	133.53	133.79	132.26
A1	135.62	136.82	135.45
A4	139.69	140.73	138.98
B4	144.76	145.94	144.24
B3	150.86	151.83	150.12
A3	150.95	152.11	150.53
A4 Ac C=O	168.79	168.92	168.41
α Ac C=O	169.50	169.91	169.26
γ Ac C=O	170.78	170.76	170.03
threo isomer			
γ	63.04	63.58	
α	74.54	75.38	
β	80.59	80.98	
1H CDCl3			
γ Ac Me	2.02		
α Ac Me	2.10		
Bα	2.28		
A4 Ac Me	2.29		
OMe	3.76		
OMe	3.81		
γ1	4.25		
γ2	4.45		
β	4.58		
α	6.07		

Compound Number 228



S-b-S

^{1}H (acetone)

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

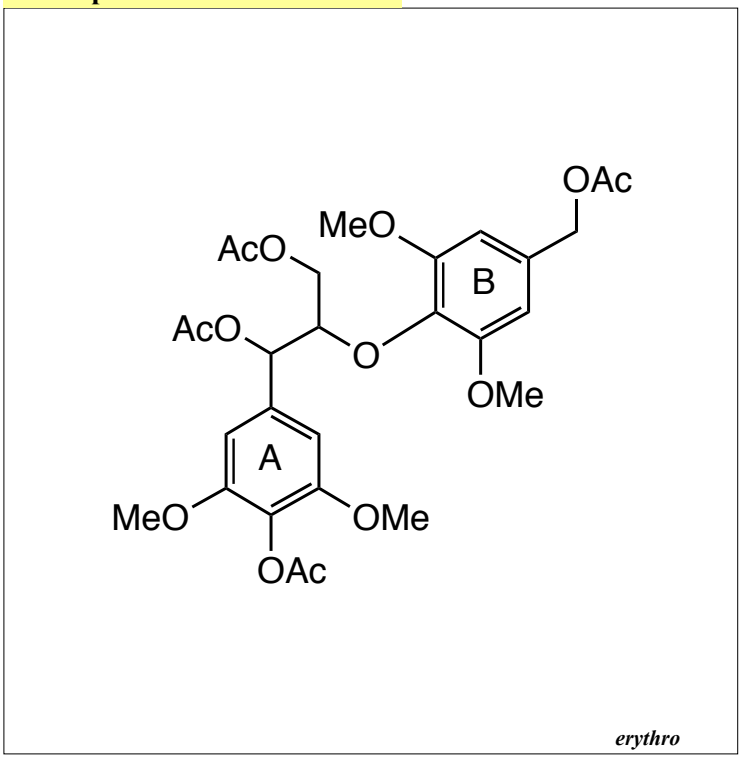
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.44	20.24	20.09
α Ac Me	20.70	20.58	20.31
γ Ac Me	21.04	20.89	20.63
A OMe	56.18	56.50	55.93
A OMe	56.18	56.50	55.93
B OMe	56.18	56.58	55.99
B OMe	56.18	56.58	55.99
γ	62.90	63.40	62.26
α	74.17	75.17	73.81
β	80.87	81.67	80.21
A2	104.07	104.61	103.39
A6	104.07	104.61	103.39
B2	106.50	107.18	106.37
B6	106.50	107.18	106.37
A4	128.61	129.41	127.60
B1	132.08	133.26	131.82
A1	135.04	136.27	134.94
B4	140.89	141.81	140.06
A3	151.95	153.06	151.54
A5	151.95	153.06	151.54
B3	153.46	154.43	152.95
B5	153.46	154.43	152.95
A4 Ac C=O	168.60	168.52	168.03
α Ac C=O	169.46	169.94	169.35
γ Ac C=O	170.76	170.66	169.96
Bα	191.01	191.69	191.82

Compound Number 229



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S-b-S

^{1}H (acetone)

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

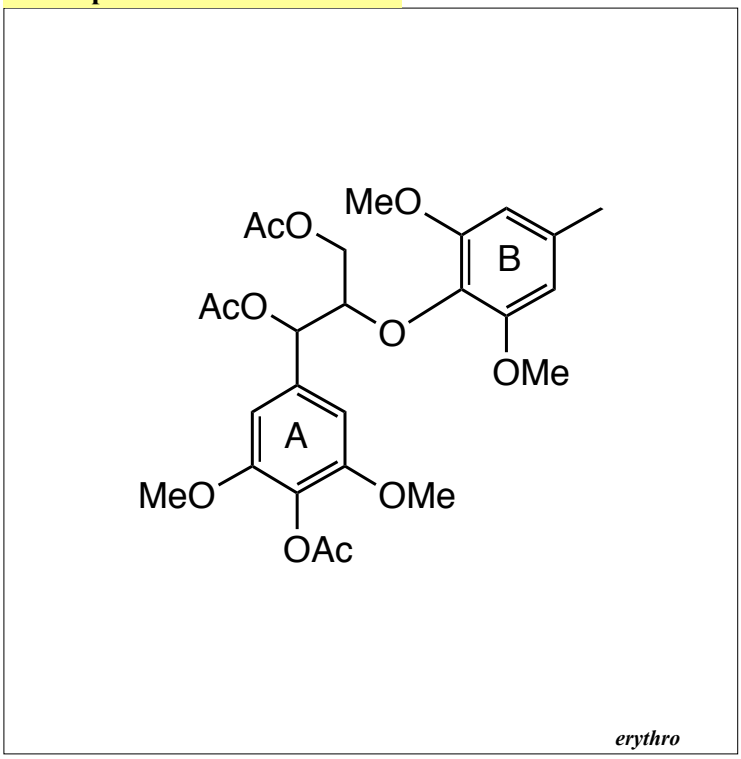
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.48	20.35	20.06
γ Ac Me	20.77	20.71	20.29
α Ac Me	21.06	20.93	20.64
Bα Ac Me	21.10	21.04	20.66
OMe	56.05	56.50	55.74
OMe	56.05	56.50	55.74
OMe	56.17	56.58	55.88
OMe	56.17	56.58	55.88
γ	62.73	63.42	62.09
Bα	66.45	66.71	65.58
α	74.19	75.41	73.88
β	80.79	81.55	79.96
A2	103.92	104.61	103.18
A6	103.92	104.61	103.18
B2	105.47	106.29	105.20
B6	105.47	106.29	105.20
A4	128.44	129.41	127.45
B1	132.02	133.40	131.90
B4	135.09	136.29	134.12
A1	135.59	136.76	135.26
A3	151.90	153.12	151.47
A5	151.90	153.12	151.47
B3	153.19	154.13	152.47
B5	153.19	154.13	152.47
A4 Ac C=O	168.64	168.64	168.10
α Ac C=O	169.54	170.09	169.35
γ Ac C=O	170.84	170.81	169.97
Bα Ac C=O	170.92	170.97	170.20

Compound Number 230



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S-b-S

^{1}H (acetone)

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

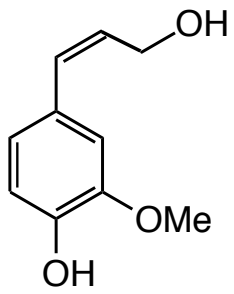
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.43	20.24	20.04
γ Ac Me	20.76	20.62	20.30
α Ac Me	21.06	20.93	20.61
Bα	21.82	21.76	21.32
OMe	55.91	56.25	55.57
OMe	55.91	56.25	55.57
OMe	56.12	56.46	55.84
OMe	56.12	56.46	55.84
γ	62.69	63.22	62.00
α	74.20	75.33	73.88
β	80.80	81.45	79.94
A2	103.81	104.43	103.08
A6	103.81	104.43	103.08
B2	105.95	106.85	105.77
B6	105.95	106.85	105.77
A4	128.33	129.25	127.39
B4	132.79	134.15	132.12
B1	134.13	134.52	133.35
A1	135.77	136.80	135.39
A3	151.86	153.01	151.45
A5	151.86	153.01	151.45
B3	152.87	153.84	152.27
B5	152.87	153.84	152.27
A4 Ac C=O	168.62	168.54	167.99
α Ac C=O	169.54	169.98	169.33
γ Ac C=O	170.94	170.72	169.95
threo isomer			
γ	63.53	64.13	
α	75.60	76.58	
β	80.87	81.65	

Compound Number 231



cis

cis-coniferyl alcohol

^{1}H (acetone)

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

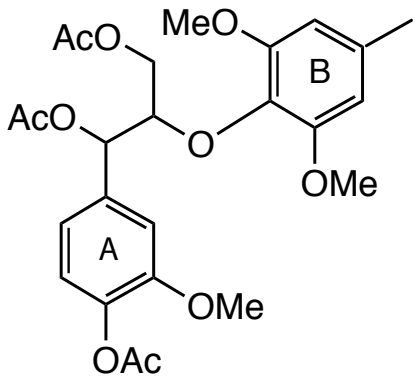
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.97	56.13	55.47
γ	59.75	59.73	58.16
2	111.53	113.19	112.84
5	114.33	115.55	115.15
6	122.25	122.78	121.56
1	129.04	129.73	128.06
α	129.51	130.19	128.62
β	131.10	131.44	130.95
4	145.17	146.69	145.74
3	146.38	147.93	147.13

Notes:

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

Compound Number 232



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G-b-S

^{1}H (acetone)

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

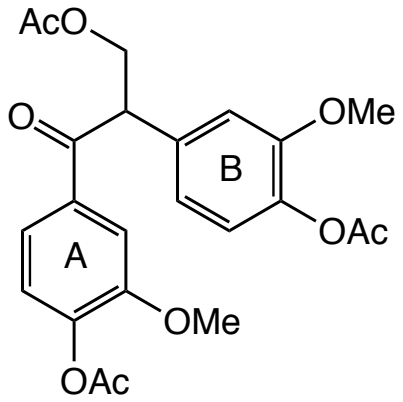
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.67	20.47	20.34
α Ac Me	20.78	20.59	20.34
γ Ac Me	21.09	20.93	20.67
Bα	21.87	21.77	21.40
OMe	55.94	56.25	55.66
OMe	55.94	56.25	55.66
OMe	55.94	56.25	55.70
γ	62.64	63.10	61.98
α	74.02	75.04	73.72
β	80.92	81.40	80.03
B2	106.02	106.87	105.90
B6	106.02	106.87	105.90
A2	111.46	112.07	110.83
A6	119.10	119.81	118.66
A5	122.43	123.29	122.61
B4	132.81	134.03	132.13
B1	134.16	134.56	133.51
A1	136.35	137.26	135.87
A4	139.44	140.56	138.86
A3	150.84	152.02	150.63
B3	152.96	153.86	152.42
B5	152.96	153.86	152.42
A4 Ac C=O	168.91	168.94	168.51
α Ac C=O	169.56	169.93	169.39
γ Ac C=O	170.92	170.67	170.03

Compound Number 233



G-b1-G

^{1}H (acetone)

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

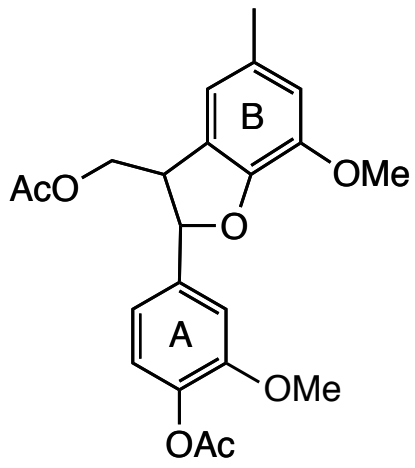
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.67	20.43	20.32	
Ac Me	20.67	20.43	20.32	
γ Ac Me	20.92	20.66	20.55	
β	52.08	52.37	50.52	
OMe	56.03	56.29	55.80	
OMe	56.03	56.40	55.95	
γ	65.58	65.94	64.74	
A2	111.99	113.14	112.35	
B2	112.32	113.66	112.95	
A6	120.95	121.30	120.26	
B6	122.22	122.88	122.14	
A5	122.94	123.95	123.28	
B5	123.54	124.21	123.28	
B1	133.94	135.54	134.26	
A1	135.02	135.77	134.42	
B4	139.64	140.53	138.79	
A4	144.13	145.10	143.59	
B3	151.54	152.52	151.11	
A3	151.72	152.70	151.11	
A4 Ac C=O	168.46	168.58	138.10	
B4 Ac C=O	168.83	168.87	168.41	
γ Ac C=O	170.89	170.75	170.10	
α	195.95	196.63	195.91	

Compound Number 234



G-c-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	2.01	s	
A4 Ac Me	2.22	s	
Bα	2.26	s	
β	3.74	m	
A OMe	3.80	s	
B OMe	3.83	s	
γ1	4.29	dd	11.1, 8.0
γ2	4.42	dd	10.9, 5.6
α	5.55	d	6.6
B6	6.70	s	
B2	6.73	s	
A6	6.99	dd	8.2, 1.8
A5	7.05	d	8.2
A2	7.18	d	1.8

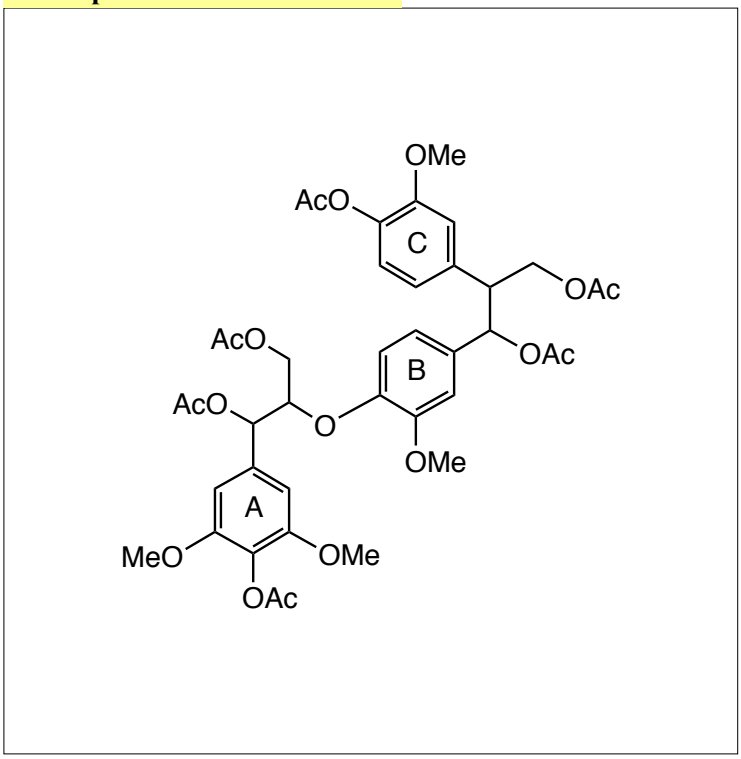
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	21.51	20.47	20.33
γ Ac Me	21.67	20.70	20.54
Bα	22.13	21.18	20.80
β	51.63	51.65	49.82
OMe	56.77	56.23	55.66
OMe	56.77	56.41	55.73
γ	66.49	66.19	65.03
α	88.49	87.85	86.41
A2	110.89	111.02	110.39
B2	114.11	114.79	113.50
B6	117.76	117.92	116.90
A6	119.09	118.61	117.81
A5	123.68	123.72	122.87
B5	127.71	128.29	127.22
B1	132.29	131.92	130.68
A4	140.42	140.61	138.98
A1	140.73	141.40	139.88
B3	144.89	145.00	143.48
B4	146.62	146.96	145.26
A3	152.09	152.36	150.83
A4 Ac C=O	169.81	168.97	168.47
γ Ac C=O	171.66	170.96	170.29

Compound Number 235



S-b-G-b1-G

^{1}H (acetone)

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

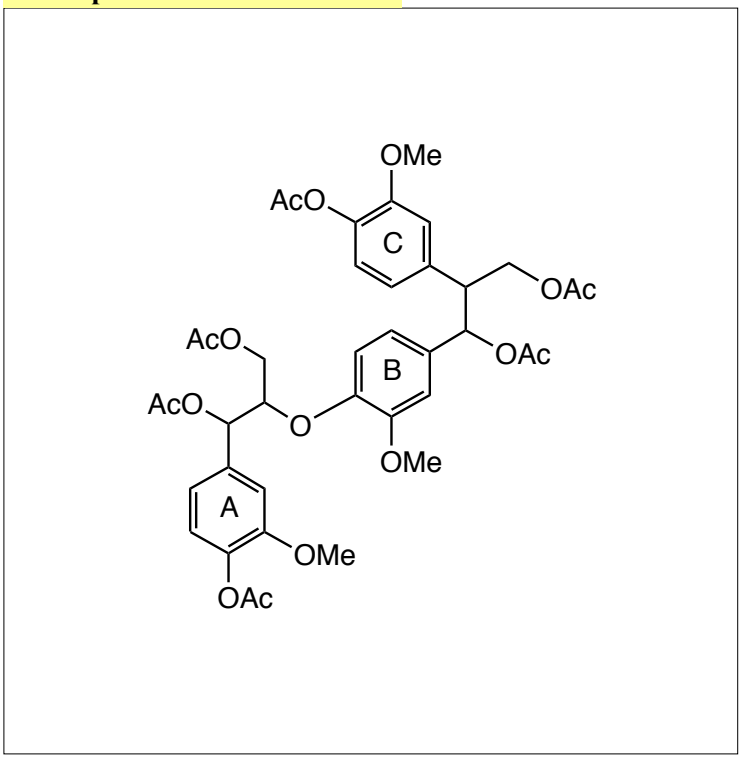
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me	20.19	20.25	19.99	
γ Ac Me	20.39	20.49	20.24	
α Ac Me	20.52	20.63	20.30	
α Ac Me	20.56	20.68	20.38	
4 Ac Me	20.73	20.87	20.50	
4 Ac Me	20.76	20.87	20.50	
Bβ	49.86	50.93	49.21	
OMe	55.59	56.22	55.54	
OMe	55.67	56.22	55.59	
OMe	55.97	56.51	55.87	
OMe	55.97	56.51	55.87	
Aγ	62.37	63.07	61.95	
Bγ	64.04	65.02	64.07	
Aα	73.74	74.77	73.39	
Bα	74.82	75.66	74.62	
Aβ	79.64	79.97	78.10	
A2	104.20	105.11	104.04	
A6	104.20	105.11	104.04	
B2	111.11	112.37	111.22	
C2	112.95	114.30	113.27	
B5	118.27	118.61	116.86	
B6	119.26	120.13	119.06	
C6	120.99	122.06	120.84	
C5	122.25	123.12	122.10	
A4	128.50	129.52	127.83	
B1	133.19	134.59	133.00	
A1	134.81	136.05	134.76	
C1	136.11	137.79	136.85	
C4	138.85	139.98	138.27	
B4	146.81	147.93	146.40	
B3	150.44	151.43	149.76	
C3	150.59	151.80	150.26	
A3	151.84	153.01	151.47	
A5	151.84	153.01	151.47	
A4 Ac C=O	168.23	168.49	167.81	
C4 Ac C=O	168.61	168.98	168.27	
α Ac C=O	169.27	169.93	169.07	
α Ac C=O	169.50	169.93	169.12	
γ Ac C=O	170.42	170.74	169.89	
γ Ac C=O	170.50	170.77	169.89	

Compound Number 236



G-b-G-b1-G

^{1}H (acetone)

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

Notes:

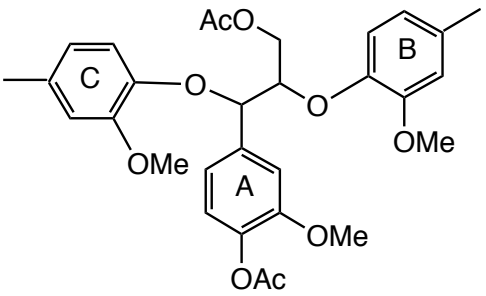
SRIX-47C2 21 mg

Bβ,Aβ,A2,B5,B1,B4 appear as split 13C signals, the shift reported is the average.
HSQC and HMBC in d6-acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me	20.69	20.49	20.35	
γ Ac Me	20.69	20.49	20.35	
α Ac Me	20.78	20.62	20.35	
α Ac Me	20.85	20.69	20.50	
4 Ac Me	21.03	20.87	20.61	
4 Ac Me	21.03	20.87	20.61	
Bβ	50.07	50.96	49.13	
OMe	55.83	56.25	55.63	
OMe	55.94	56.25	55.68	
OMe	55.97	56.30	55.72	
Aγ	62.52	63.04	61.94	
Bγ	64.29	65.05	64.17	
Aα	73.72	74.55	73.14	
Bα	75.07	75.70	74.68	
Aβ	80.01	80.16	78.15	
B2	111.36	112.43	111.27	
A2	111.98	112.78	111.68	
C2	113.12	114.34	113.32	
B5	118.74	118.93	116.97	
B6	119.48	120.14	119.12	
A6	119.73	120.46	119.40	
C6	121.22	122.10	120.89	
C5	122.50	123.13	122.19	
A5	122.62	123.36	122.51	
B1	133.41	134.76	133.13	
A1	135.34	136.60	135.26	
C1	136.29	137.84	137.02	
C4	139.06	140.02	138.21	
A4	139.82	140.80	139.10	
B4	147.00	147.92	146.35	
B3	150.75	151.55	149.81	
C3	150.80	151.83	150.26	
A3	151.02	152.11	150.57	
4 Ac C=O	168.84	168.92	168.46	
4 Ac C=O	168.90	168.98	168.46	
α Ac C=O	169.55	169.93	169.23	
α Ac C=O	169.78	169.93	169.28	
γ Ac C=O	170.74	170.75	170.06	
γ Ac C=O	170.80	170.75	170.06	
1H				
Bβ			3.42	
OMe			3.61	
OMe			3.65	
OMe			3.71	
Bγ 1			4.04	
Aγ 1			4.13	
Bγ 2			4.13	
Aγ 2			4.19	
Aβ			4.80	
Aα			5.86	
Bα			5.94	
B2			6.73	
B6			6.74	
C6			6.77	
B5			6.90	
C5			6.94	
C2			6.92	
A6			6.95	
A5			7.02	
A2			7.10	

Compound Number 237



G-a-G-b-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.90	s	
A4 Ac Me	2.20	s	
B or C α	2.20	s	
B or C α	2.24	s	
OMe	3.75	s	
OMe	3.79	s	
OMe	3.83	s	
γ1	4.43	dd	11.7, 3.8
γ2	4.54	dd	11.7, 5.8
β	4.74	m	
α	5.55	d	5.4
C6	6.53	dd	8.2, 1.6
B6	6.61	dd	8.0, 1.4
C5	6.76	d	
B,C 2	6.78	s	
B5	6.83	d	8.0
A5	6.98	d	8.0
A6	7.05	dd	8.0, 1.8
A2	7.33	d	1.8

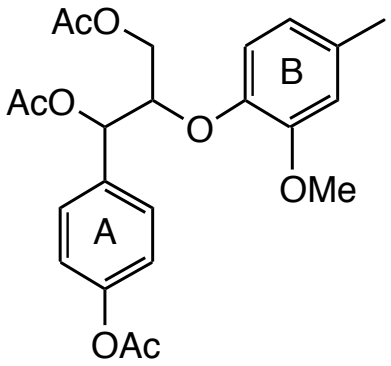
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.69	20.46	20.34
γ Ac Me	20.82	20.65	20.44
Cα	21.05	20.96	20.56
Bα	21.12	21.05	20.61
OMe	55.71	56.11	55.48
OMe	55.96	56.19	55.63
OMe	55.96	56.28	55.63
γ	63.56	65.62	62.46
α	80.41	81.09	79.08
β	82.44	82.14	80.19
A2	111.53	112.70	111.79
B2	113.37	114.51	113.58
C2	113.41	114.54	113.58
C5	116.77	117.73	116.22
B5	119.45	119.80	117.84
A6	119.72	120.54	119.51
B6	121.01	121.64	120.67
C6	121.21	121.80	120.77
A5	122.36	123.13	122.30
C1	131.97	132.54	131.23
B1	133.11	133.32	131.83
A1	138.62	138.11	136.70
A4	139.42	140.48	138.81
C4	145.22	146.01	144.25
B4	145.32	146.37	144.77
C3	149.95	151.12	149.52
B3	150.79	151.69	150.00
A3	151.02	152.03	150.45
A4 Ac C=O	168.85	168.89	168.39
γ Ac C=O	170.91	170.81	170.13

Compound Number 238



erythro

H-b-G

^{1}H (acetone)

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

Notes:

SRIX-51D-C

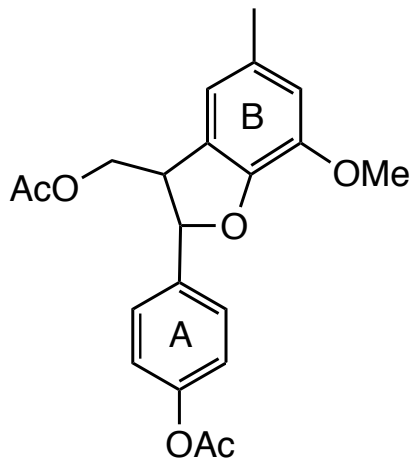
13mg HMBC,HSQC,selective INEPT in acetone

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ Ac Me	20.82	20.59	20.34
α Ac Me	21.06	20.88	20.58
A4 Ac Me	21.18	20.95	20.58
Bα	21.18	21.07	20.73
OMe	55.79	56.13	55.46
γ	62.48	62.84	61.67
α	73.67	74.43	72.93
β	80.80	80.84	78.98
B2	113.60	114.65	113.64
B5	120.09	120.44	118.60
B6	121.27	121.85	120.77
A3	121.53	122.41	121.56
A5	121.53	122.41	121.56
A2	128.41	129.25	128.13
A6	128.41	129.25	128.13
B1	133.72	133.96	132.43
A1	134.44	135.53	134.05
B4	144.75	145.86	144.14
A4	150.59	151.71	150.11
B3	151.03	151.95	150.23
A4 Ac C=O	169.29	169.57	169.05
α Ac C=O	169.60	169.90	169.21
γ Ac C=O	170.87	170.73	169.97
minor isomer			
γ	63.10	63.56	62.38
α	74.53	75.24	74.03
β	80.73	81.06	79.39

Compound Number 239



H-c-G

^{1}H (acetone)

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

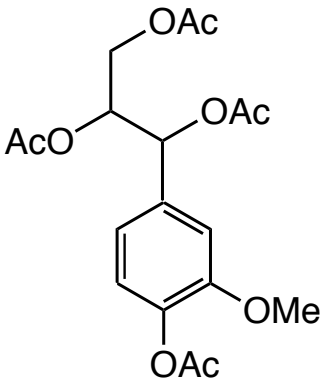
Notes:

SRIX-53E 2mg
HSQC and HMBC in acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ AcMe	20.89	20.68	20.48
A4 AcMe	21.21	20.95	20.73
Bα	21.35	21.18	20.73
β	50.94	51.78	49.85
OMe	56.11	56.38	55.56
γ	65.83	66.29	65.02
α	87.46	87.57	85.95
B2	113.35	114.79	113.40
B6	117.04	118.02	116.88
A3	121.81	122.82	121.90
A5	121.81	122.82	121.90
A2	127.10	127.64	126.83
A6	127.10	127.64	126.83
B5	128.30	128.12	127.67
B1	131.59	131.95	130.59
A1	138.76	140.15	138.55
B3	144.09	145.03	143.38
B4	145.86	146.96	145.14
A4	150.54	151.66	150.07
A4 Ac C=O	169.44	169.62	169.08
γ Ac C=O	170.88	170.94	170.21

Compound Number 240



^{1}H (acetone)

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

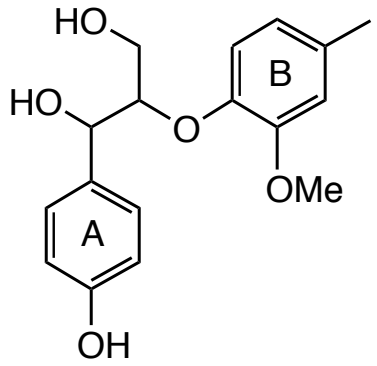
Notes:

SRIX-69E
7mg
gHSQCand gHMBC d6-acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.67	20.44	20.36	
γ Ac Me	20.67	20.52	20.41	
β Ac Me	20.80	20.66	20.46	
α Ac Me	20.96	20.79	20.66	
OMe	56.02	56.34	55.84	
γ	62.11	62.81	61.93	
β	72.22	72.92	71.68	
α	73.43	74.15	72.90	
2	111.30	112.29	111.25	
6	119.75	120.15	119.00	
5	123.10	123.72	122.81	
1	134.70	136.28	135.20	
4	140.20	140.98	139.19	
3	151.37	152.30	150.72	
4 Ac C=O	168.77	168.95	168.40	
α Ac C=O	169.65	170.08	169.44	
β Ac C=O	170.04	170.30	169.44	
γ Ac C=O	170.43	170.73	169.97	
minor isomer				
γ		62.31		
β		72.92		
α		73.53		

Compound Number 241



threo

H-b-G

^{1}H (acetone)

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

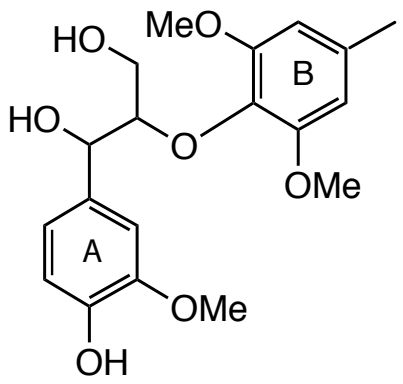
Notes:

SRIX-84
35mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B α	21.16	21.08	20.51	
OMe	55.81	56.24	55.55	
γ	60.79	61.73	60.00	
α	73.72	73.84	70.94	
β	89.12	89.41	85.34	
B2	113.07	114.18	113.46	
A3	115.53	115.62	114.35	
A5	115.53	115.62	114.35	
B5	120.78	120.73	116.69	
B6	121.96	122.21	120.75	
A2	128.42	129.10	127.75	
A6	128.42	129.10	127.75	
A1	131.29	133.16	130.38	
B1	133.99	133.35	132.21	
B4	145.21	147.33	146.17	
B3	150.97	151.67	149.60	
A4	156.37	157.63	156.19	
erythro isomer				
γ	60.79	61.64	59.89	
α	72.72	73.55	71.41	
β	87.06	87.53	84.57	
1H CDCL3				
B α	2.2			
γ1	3.44			
γ2	3.62			
OMe	3.91			
β	3.98			
α	4.98			
A3,5,B2,6	6.77			
B5	7.05			
A2,6	7.30			

Compound Number 242



threo

G-b-S

^{1}H (acetone)

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

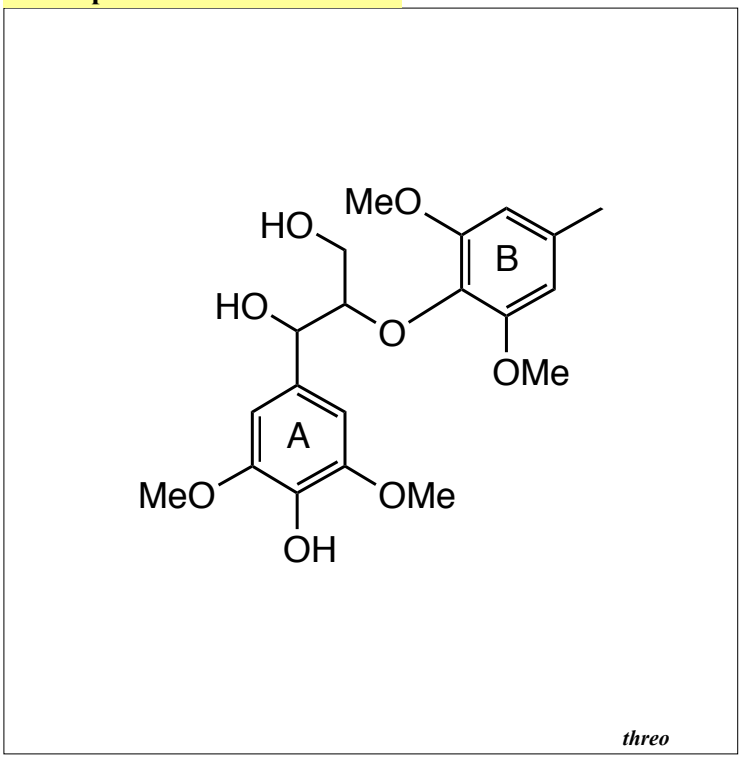
Notes:

SRIX-86B,C
40 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B α	21.99	21.77	21.31
OMe	56.01	56.16	55.48
OMe	56.14	56.46	55.82
OMe	56.14	56.46	55.82
γ	60.51	61.19	60.11
α	74.20	74.08	71.53
β	89.20	89.83	87.29
B2	106.10	107.09	106.28
B6	106.10	107.09	106.28
A2	109.92	111.45	111.01
A5	114.36	115.22	114.62
A6	120.47	120.73	119.22
A1	132.06	133.60	132.79
B4	133.04	134.65	132.90
B1	134.67	134.82	133.80
A4	145.46	146.75	145.29
A3	146.58	147.90	146.83
B3	152.75	153.60	152.27
B5	152.75	153.60	152.27
erythro isomer			
γ	60.63	60.86	59.57
α	72.49	73.26	71.93
β	87.13	87.90	86.11
1H CDCL3			
B α	2.36		
γ1	3.32		
γ2	3.59		
OMe	3.89		
β			
OMe	3.90		
α	5.04		
B2,6	6.46		
A5	6.89		
A6	6.97		
A2	6.99		

Compound Number 243



threo

S-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
B α	2.29	s	
γ1	3.40		
γ2	3.60		
β	obsc'd		
OMe	3.80	s	
OMe	3.86	s	
α	4.99	d	6.8
A2,6	6.54	s	
B2,6	6.77	s	
A4 OH	7.08	s	

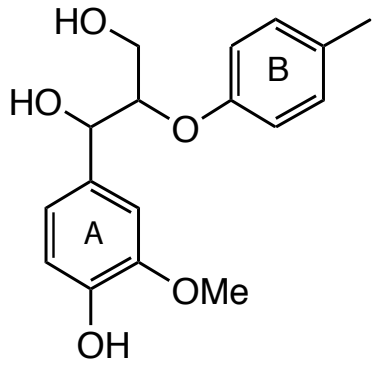
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B α	21.85	21.78	21.31
OMe	56.02	56.48	55.88
OMe	56.02	56.48	55.88
OMe	56.25	56.56	55.90
OMe	56.25	56.56	55.90
γ	60.37	61.31	60.18
α	74.33	74.29	71.59
β	89.04	89.56	87.18
A2	104.04	105.39	104.30
A6	104.04	105.39	104.30
B2	105.99	107.05	106.34
B6	105.99	107.05	106.34
A1	131.04	132.54	132.13
B1	132.90	134.55	132.88
B4	134.43	134.78	133.92
A4	134.58	136.00	134.32
A3	146.99	148.23	147.37
A5	146.99	148.23	147.37
B3	152.63	153.52	152.34
B5	152.63	153.52	152.34
erythro isomer			
γ	60.50	61.23	
α	72.50	73.43	
β	87.03	86.32	
1H CDCl3			
B α	2.35		
γ1	3.34		
γ2	3.65		
β	3.90		
OMe	3.80		
OMe	3.86		
α	4.98		
A2,6	6.70		
B2,6	6.44		

Compound Number 244



threo

G-b-H

^{1}H (acetone)

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

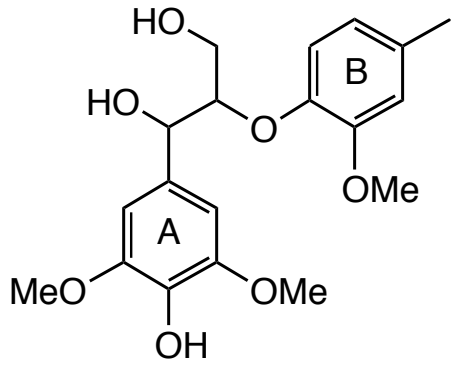
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Bα	20.53	20.46	20.05	
OMe	55.98	56.20	55.49	
γ	61.11	61.67	60.04	
α	73.81	73.36	70.92	
β	83.38	84.30	83.25	
A2	109.56	111.36	110.95	
A5	114.43	115.17	114.73	
B3	116.57	117.08	115.88	
B5	116.57	117.08	115.88	
A6	120.00	120.36	119.01	
B2	130.18	130.47	129.55	
B6	130.18	130.47	129.55	
B1	131.43	130.55	128.97	
A1	131.76	134.24	133.25	
A4	145.59	146.66	145.41	
A3	146.75	147.93	146.99	
B4	155.98	157.98	156.93	
erythro isomer				
γ	61.44	62.03	60.17	
α	73.94	74.03	71.55	
β	81.22	83.98	83.37	
1H CDCl3				
Bα	2.31			
OMe	3.83			
γ1	3.57			
γ2	3.74			
β	4.33			
α	4.96			
A5,6,B3,6	6.68-6.92			
	6.95			
A2	7.09			
B2,6				

Compound Number 245



threo

S-b-G

^{1}H (acetone)

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

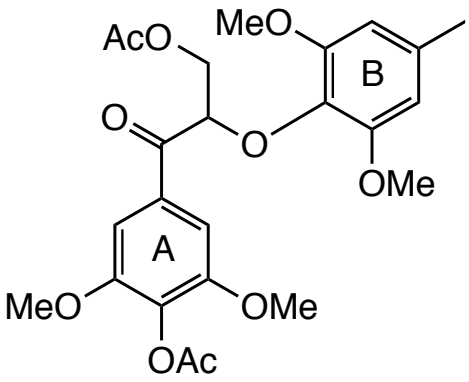
Notes:

SRIX-95BR
HSQC and HMBC in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Bα	21.73	21.06	20.57	
B OMe	55.85	56.26	55.50	
A OMe	56.34	56.60	55.80	
A OMe	56.34	56.60	55.80	
γ	60.99	61.89	60.05	
α	74.18	74.05	70.90	
β	89.51	88.73	84.58	
A2	103.86	105.41	104.15	
A6	103.86	105.41	104.15	
B2	113.06	114.20	113.34	
B5	120.90	120.10	115.95	
B6	121.96	122.19	120.76	
A1	130.82	132.84	130.21	
B1	134.17	133.10	132.00	
A4	134.58	136.15	134.33	
B4	145.25	147.36	145.98	
A3	147.12	148.40	147.39	
A5	147.12	148.40	147.39	
B3	150.93	151.50	149.46	
erythro shifts				
γ	60.76	61.75	59.94	
α	72.87	73.98	71.90	
β	87.70	87.09	83.97	

Compound Number 246



^{1}H (acetone)

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

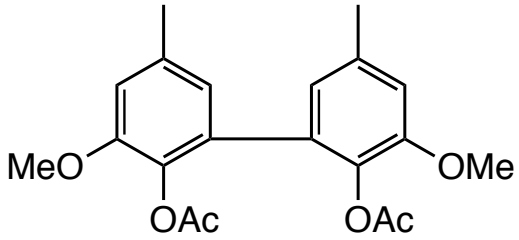
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.43	20.22	20.07
γ Ac Me	20.75	20.60	20.42
Bα	21.82	21.73	21.32
B OMe	55.86	56.19	55.65
B OMe	55.86	56.19	55.65
A OMe	56.29	56.60	56.12
A OMe	56.29	56.60	56.12
γ	64.15	64.34	63.26
β	81.65	81.24	79.70
B2	105.93	106.75	105.93
B6	105.93	106.75	105.93
A2	106.25	106.80	105.58
A6	106.25	106.80	105.58
A4	133.03	133.82	132.20
B4	133.50	134.25	132.74
A1	133.57	134.72	133.61
B1	134.31	134.88	133.33
A3	152.09	153.11	151.75
A5	152.09	153.11	151.75
B3	152.49	153.51	152.05
B5	152.49	153.51	152.05
A4 Ac C=O	168.14	168.20	167.79
γ Ac C=O	170.75	170.73	170.03
α	194.84	195.23	194.40
1H			
A4 Ac Me	2.35		2.29
Bα	2.30		2.26
γ Ac Me	1.98		1.92
B OMe	3.71		3.69
A OMe	3.85		3.81
γ	4.56		4.40
β	5.40		5.55
B2,6	6.36		6.49
A2,6	7.50		7.39

Compound Number 247



^{1}H (acetone)

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

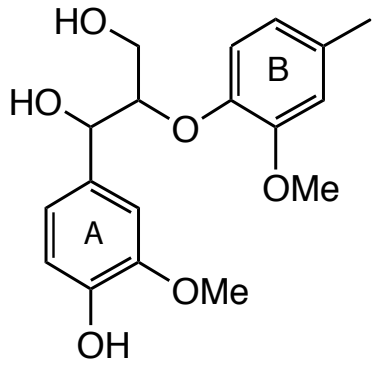
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.54	20.36	20.10	
α	21.51	21.32	20.87	
OMe	56.08	56.28	55.83	
2	112.75	113.52	112.90	
6	123.17	123.44	122.22	
5	131.30	132.13	130.49	
4	135.39	136.48	134.74	
1	136.02	136.48	135.52	
3	150.95	152.17	150.64	
Ac C=O	168.96	168.67	168.00	

Notes:

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

Compound Number 248



erythro

G-b-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.24 (2.25)	s	
γ1	3.65 (3.46)	m	
γ2	3.79 ((3.65)	m	
OMe	3.80-3.84	s	
OMe	3.80-3.84	s	
β	4.19 (4.08)	m	
α	4.87 (4.86)	d	6.0
B6	6.66 (6.62)	bd	7.3
A5	6.78 (6.76)	bd	8.0
B2	6.79 (6.83)	s	
B5	6.82 (7.05)		
A6	6.89 (6.87)		
A2	7.08 (7.07)		
α OH	4.52 (4.43)		
A4 OH	7.44 (7.47)		

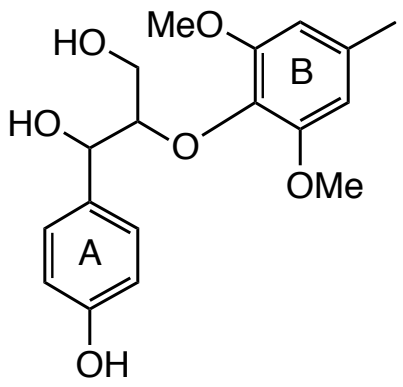
Notes:

SRIX-98 27mg
500MHz HSQC (some 1H shifts) and HMBC
A6 and B5 change order in CDCl3 and poss. A4 and B4
1H shifts for threo in ( )

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Bα	21.68	21.05	20.60	
OMe	55.76	56.19	55.44	
OMe	55.86	56.22	55.57	
γ	60.59	61.72	60.04	
α	72.57	73.74	71.66	
β	87.36	87.25	84.15	
A2	108.66	111.31	111.37	
B2	112.96	114.29	113.51	
A5	114.24	115.15	114.59	
B5	120.68	120.12	116.33	
A6	118.92	120.38	119.48	
B6	121.83	122.11	120.77	
B1	131.83	133.11	130.22	
A1	133.99	134.28	133.34	
A4	145.16	146.59	145.41	
B4	144.43	146.71	145.77	
A3	146.58	147.95	146.97	
B3	151.08	151.78	149.62	
threo				
Bα	21.68	21.07	20.62	
OMe	55.76	56.17	55.41	
OMe	55.86	56.23	55.57	
γ	60.83	61.83	60.07	
α	73.87	73.95	70.90	
β	89.48	89.11	84.89	
A2	109.44	111.36	111.00	
B2	112.96	114.16	113.40	
A5	114.31	115.22	114.66	
B5	120.79	120.38	116.18	
A6	120.16	120.58	119.00	
B6	121.88	122.19	120.81	
B1	131.46	133.20	130.31	
A1	134.07	133.82	132.99	
A4	145.16	146.80	145.39	
B4	147.97	147.37	146.10	
A3	146.64	148.01	146.97	
B3	150.80	151.53	149.53	
1H				
Bα	2.24 (2.25)		2.20 (2.21)	
γ1	2.62 (3.42)		3.54 (3.21)	
γ2	3.87 (3.59)		3.58 (3.57)	
OMe	3.82		3.76 (3.71)	
OMe	3.82		3.68 (3.74)	
β	4.06 (3.93)		4.19 (4.15)	
α	4.92 (4.92)		4.69 (4.70)	
B6	6.68 (6.68)		6.59 (6.62)	
A5	6.71 (6.72)		6.68 (6.67)	
B2	6.80 (6.97)		6.72 (6.77)	
B5	6.83 (6.84)		6.82 (6.88)	
A6	6.78 (6.88)		6.75 (6.76)	
A2	6.92 (6.94)		6.97 (6.96)	
α OH			4.53 (4.59)	
A4 OH			8.74 (8.75)	

Compound Number 249



threo

H-b-S

^{1}H (acetone)

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

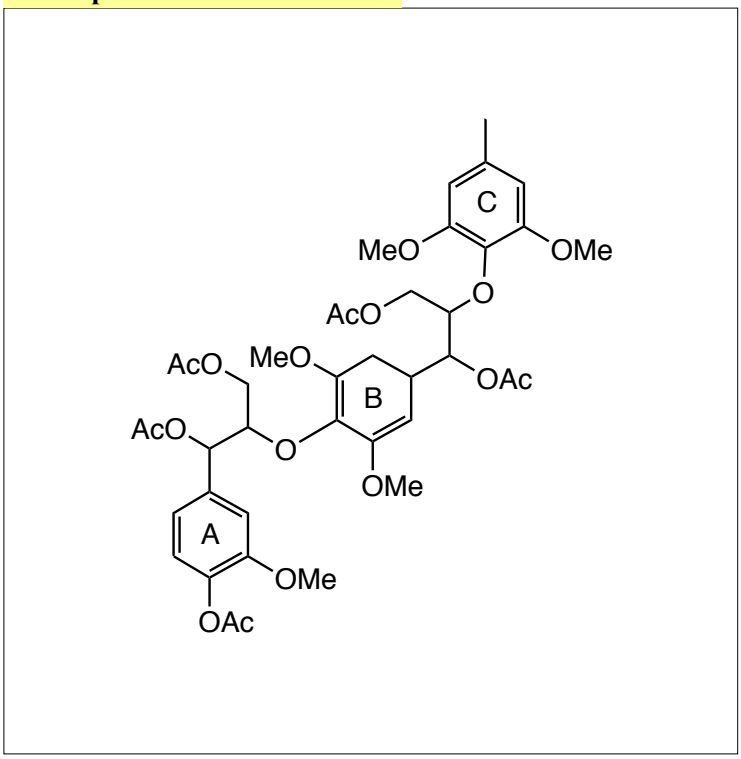
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Bα	22.01	21.78	21.34	
OMe	56.19	56.48	55.86	
OMe	56.19	56.48	55.86	
γ	60.50	61.06	60.08	
α	74.10	73.95	71.53	
β	89.14	89.98	87.36	
B2	106.16	107.12	106.33	
B6	106.16	107.12	106.33	
A3	115.56	115.58	114.37	
A5	115.56	115.58	114.37	
A2	128.75	129.22	127.88	
A6	128.75	129.22	127.88	
A1	131.26	133.06	132.21	
B4	133.02	134.67	132.86	
B1	134.77	134.84	133.93	
B3	152.69	153.67	152.32	
B5	152.69	153.67	152.32	
A4	156.28	157.68	156.23	
erythro isomer				
γ	60.6	60.8		
α	72.4	73.1		
β	87.0	87.8		

Compound Number 250



G-b-S-b-S

^{1}H (acetone)

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

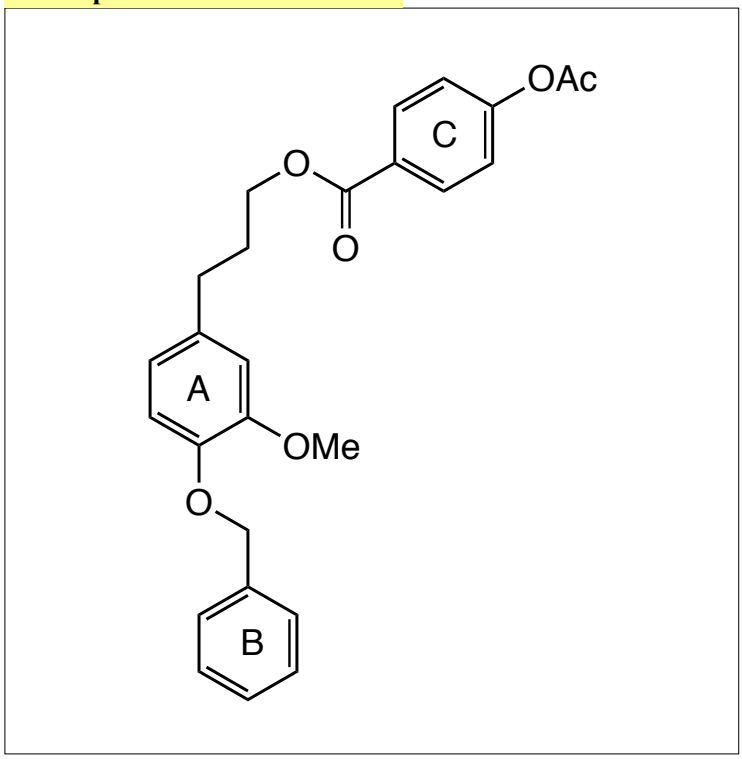
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.85	20.48	20.27	
γ Ac Me	20.67	20.59	20.35	
γ Ac Me	20.73	20.74	20.48	
α Ac Me	21.08	20.93	20.67	
α Ac Me	21.08	21.02	20.73	
Cα	21.85	21.74	21.37	
B OMe	55.99	56.32	55.71	
B OMe	55.99	56.32	55.71	
C OMe	55.99	56.45	55.71	
C OMe	55.99	56.45	55.71	
A OMe	56.07	56.86	55.85	
Aγ	62.76	63.39	62.25	
Bγ	63.74	64.30	63.20	
Aα	74.06	75.15	73.83	
Bα	75.99	76.75	75.77	
Aβ	80.89	81.45	80.00	
Bβ	80.89	81.76	80.50	
B2	104.44	105.27	104.01	
B6	104.44	105.27	104.01	
C2	106.05	106.99	105.89	
C6	106.05	106.99	105.89	
A2	111.60	112.30	111.04	
A6	119.23	120.02	118.85	
A5	122.42	123.30	122.57	
C1	133.37	134.17	133.02	
B1	133.74	134.36	133.02	
C4	134.40	135.56	133.79	
B4	135.22	136.33	134.35	
A1	136.15	137.10	135.67	
A4	139.50	140.57	138.92	
A3	150.85	152.05	150.59	
C3	152.65	153.67	152.13	
C5	152.65	153.67	152.13	
B3	153.06	153.91	152.43	
B5	153.06	153.91	152.43	
A4 Ac C=O	168.89	168.96	168.49	
α Ac C=O	169.55	169.90	169.29	
α Ac C=O	169.85	169.95	169.38	
γ Ac C=O	170.54	170.69	169.99	
γAc C=O	170.88	170.69	169.99	

Compound Number 251



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.21	21.00		
β	30.41	31.15		
α	32.01	32.42		
OMe	56.01	56.13		
γ	64.42	64.98		
Bα	71.22	71.56		
A2	112.31	113.72		
A5	114.27	115.39		
A6	120.28	121.14		
C3	121.61	122.79		
C5	121.61	122.79		
B2	127.27	128.40		
B6	127.27	128.40		
B4	127.73	128.40		
C1	127.88	128.72		
B3	128.48	129.11		
B5	128.48	129.11		
C2	131.08	131.62		
C6	131.08	131.62		
A1	134.38	135.56		
B1	137.32	138.76		
A4	146.45	147.68		
A3	149.57	150.88		
C4	154.25	155.53		
Cα	165.80	166.03		
Ac C=O	168.86	169.26		
1H CDCl3				
β	2.04			
Ac Me	2.29			
α	2.69			
OMe	3.84			
γ	4.31			
Bα	5.09			
A6	6.65			
A2	6.73			
A5	6.78			
C3,5	7.15			
B4	7.27			
B3,5	7.33			
B2,6	7.41			
C2,6	8.03			

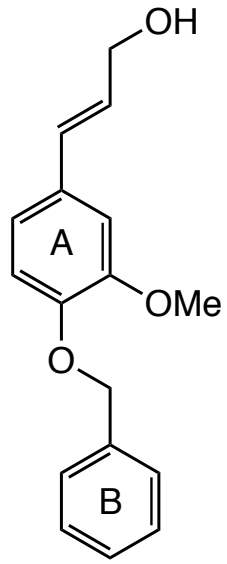
^{1}H (acetone)

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

Notes:

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

Compound Number 252



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.16		
γ		63.26		
Bα		71.47		
A2		110.73		
A5		115.12		
A6		120.11		
B2		128.46		
B6		128.46		
B4		128.54		
B3		129.19		
B5		129.19		
β		129.19		
α		130.01		
A1		131.94		
B1		138.60		
A4		148.98		
A3		151.02		

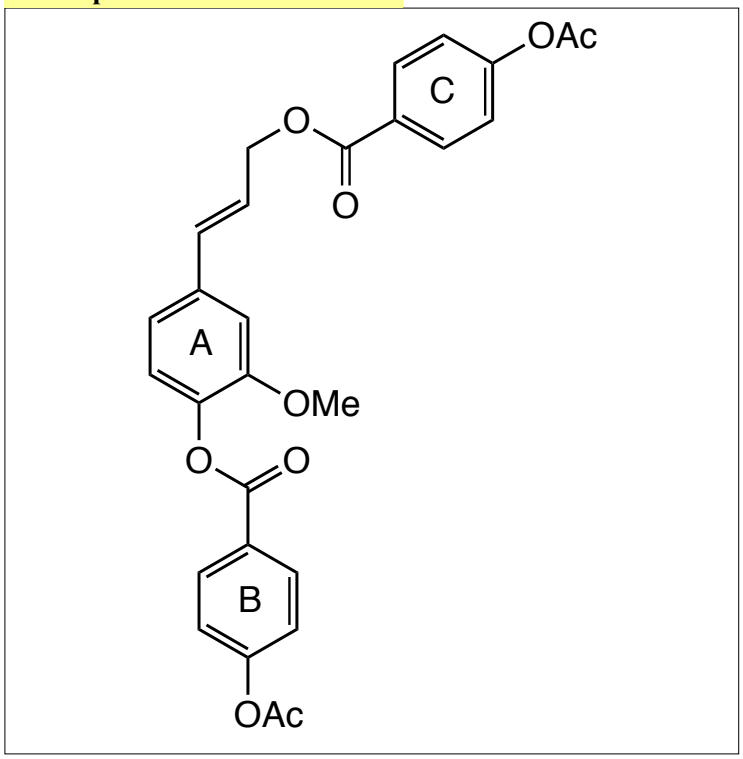
^{1}H (acetone)

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

Notes:

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

Compound Number 253



^{1}H (acetone)

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

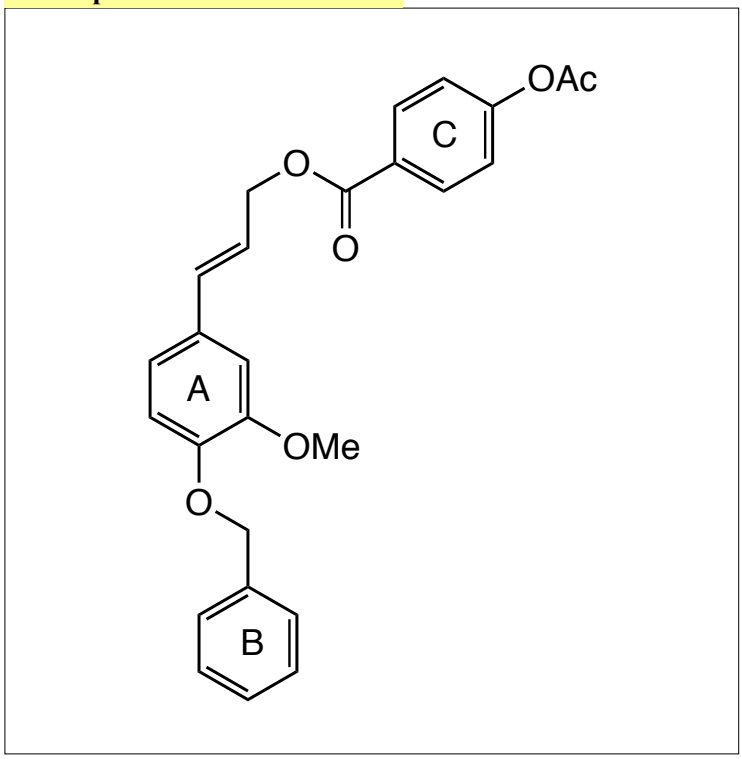
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.98		
Ac Me		20.98		
OMe		56.30		
γ		66.01		
A2		111.31		
A6		120.16		
C3		122.93		
C5		122.93		
B3		123.16		
B5		123.16		
A5		123.95		
β		124.89		
B1		127.72		
C1		128.57		
C2		131.77		
C6		131.77		
B2		132.34		
B6		132.34		
α		134.01		
A1		136.55		
A4		140.81		
A3		152.54		
C4		155.72		
B4		156.13		
Bα		164.23		
Cα		165.84		
Ac C=O		169.29		
Ac C=O		169.29		

Compound Number 254



^{1}H (acetone)

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

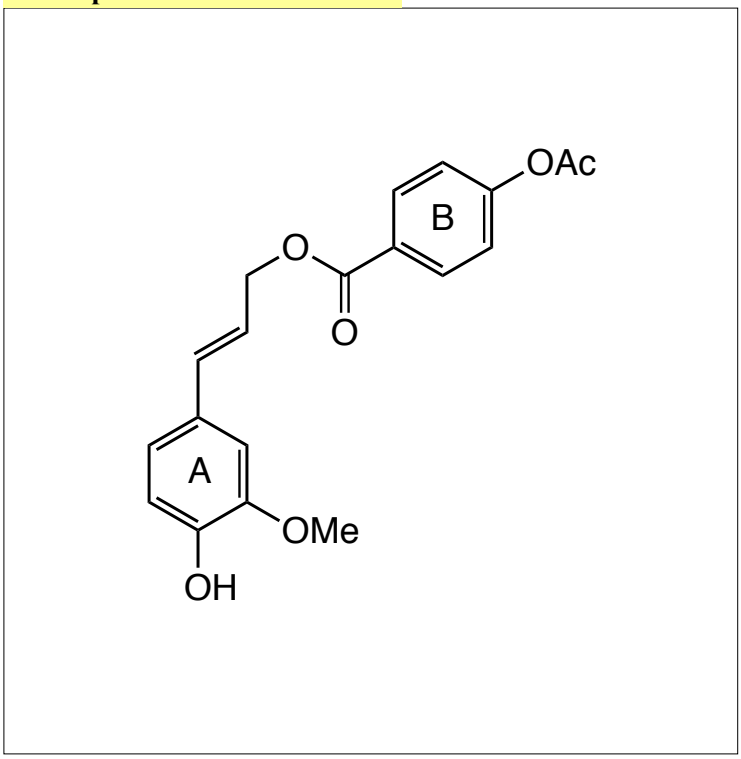
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.14	21.00		
OMe	55.96	56.31		
γ	65.82	66.34		
Bα	70.96	71.53		
A2	109.51	111.16		
A5	113.82	115.17		
A6	119.92	120.82		
β	121.21	122.39		
C3	121.61	122.83		
C5	121.61	122.83		
B2	127.24	128.45		
B6	127.24	128.45		
B4	127.86	128.57		
C1	127.86	128.69		
B3	128.53	129.20		
B5	128.53	129.20		
A1	129.70	131.00		
C2	131.24	131.74		
C6	131.24	131.74		
α	134.38	134.95		
B1	136.92	138.49		
A4	148.34	149.70		
A3	149.68	151.13		
C4	154.33	155.68		
Cα	165.68	165.93		
Ac C=O	168.90	169.25		
1H CDCl3				
Ac Me	2.30			
OMe	3.88			
γ	4.91			
Bα	5.14			
β	6.23			
α	6.63			
A5	6.81			
A6	6.84			
A2	6.96			
C3,5	7.16			
B4	7.28			
B3,5	7.33			
B2,6	7.40			
C2,6	8.09			

Compound Number 255



^{1}H (acetone)

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

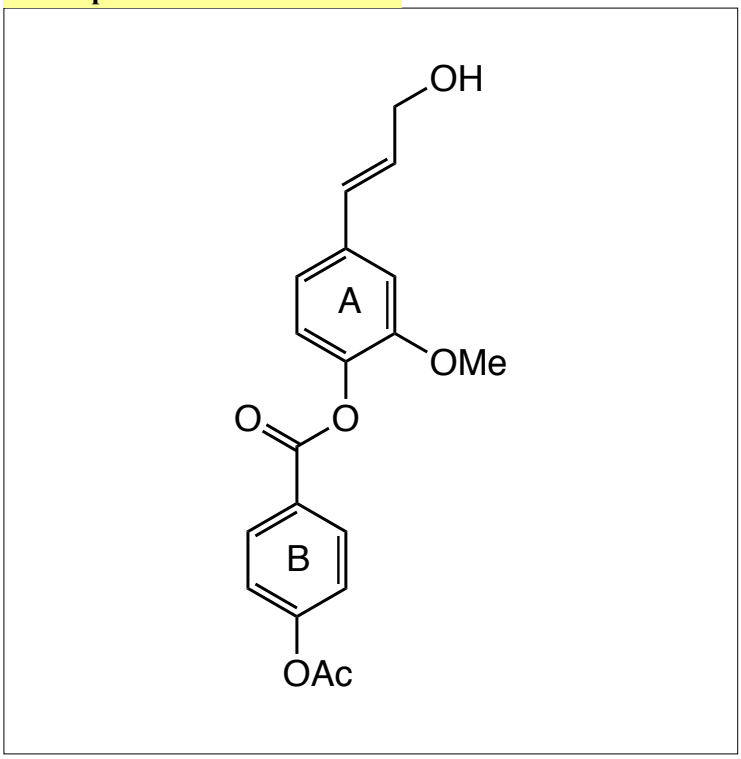
Notes:

L.Landucci XXIII-114D2 8mg
HSQC and HMBC in acetone d-6
sample since degraded unsure of some shifts
HSQC and HMBC in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.15	20.98		
OMe	55.89	56.24		
γ	65.77	66.47		
A2		110.24		
A5		115.83		
A6		121.33		
β	121.16	121.33		
B3	121.63	122.90		
B5	121.63	122.90		
B1	127.78	128.70		
A1	130.54	129.35		
B2	131.24	131.73		
B6	131.24	131.73		
α	134.44	135.40		
A4		147.91		
A3		148.55		
B4		155.68		
Bα	165.46	165.90		
Ac C=O	168.85	169.29		

Compound Number 256



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	21.09	20.99		
OMe	55.93	56.22		
γ		63.10		
A2		111.04		
A6		119.58		
B3		123.15		
B5		123.15		
A5		123.81		
B1		127.80		
α	127.23	129.30		
β	128.44	131.61		
B2		132.32		
B6		132.32		
A1		137.50		
A4		140.16		
A3		152.44		
B4		156.10		
Bα		164.29		
Ac C=O	168.86	169.30		
1H CDCl3				
Ac Me	2.29			

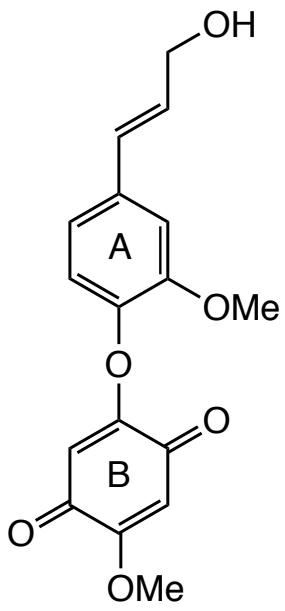
^{1}H (acetone)

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

Notes:

L.Landucci XXIII-114D1 4mg
HSQC and HMBC in acetone d-6
some CDCl3 from HSQC and HMBC

Compound Number 257



^{13}C

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

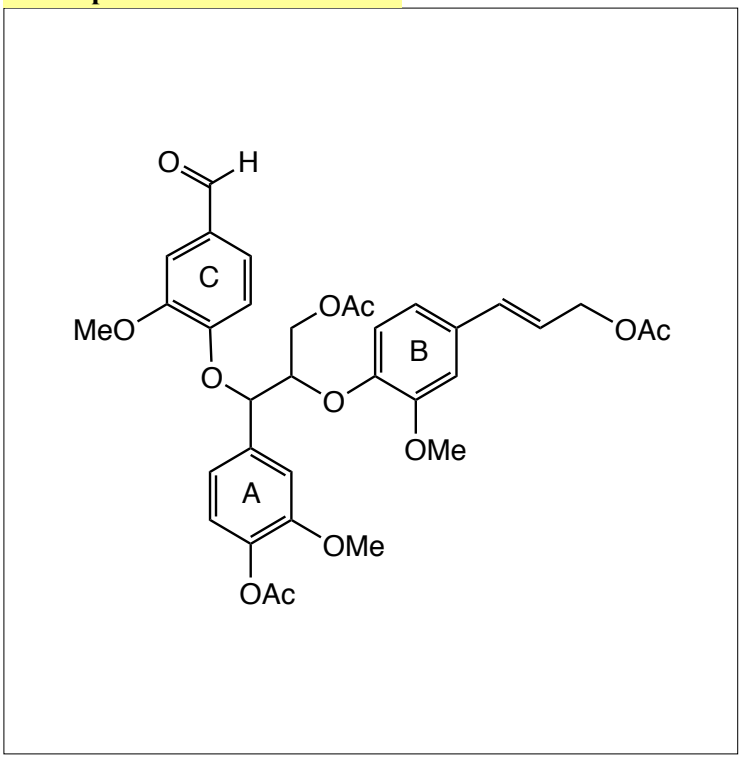
^{1}H (acetone)

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

Notes:

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

Compound Number 258



Vanillin-a-G-b-CA

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me's	1.91, 2.03, 2.21	s's	
OMe	3.81	s	
OMe	3.83	s	
OMe	3.97	s	
γ1	4.45	dd	11.9, 4.0
γ2	4.56	dd	11.9, 5.8
Bγ	4.67	dd	6.4, 1.2
β	4.91	m	
α	5.84	d	5.2
Bβ	6.27	dt	15.9, 6.4
Bα	6.63	d	15.9
B6	6.93	dd	8.2, 1.6
B5	7.01	d	8.3
A5	7.03	d	8.2
A6	7.14	dd	8.2, 1.8
B2	7.15	d	2.0
C5	7.15	d	8.3
A2	7.36	d	2.4
C6	7.39	dd	8.2, 1.8
C2	7.46	d	1.8
Cα	9.81	s	

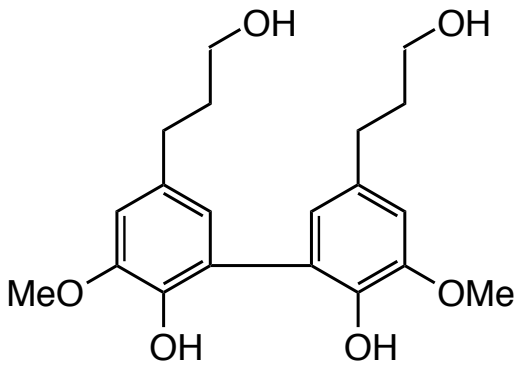
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.74	20.46		
γ Ac Me	20.82	20.62		
Bγ Ac Me	21.10	20.80		
OMe	55.84	56.24		
OMe	56.09	56.29		
OMe	56.13	56.51		
γ	63.12	63.32		
Bγ	65.17	65.38		
α	79.98	80.55		
β	82.11	81.82		
B2	109.93	111.36		
C2	110.29	111.36		
A2	111.14	112.68		
C5	114.77	115.94		
B5	119.31	119.62		
A6	119.46	120.33		
B6	119.93	120.53		
Bβ	122.39	123.35		
A5	122.94	123.53		
C6	126.32	126.04		
C1	130.99	132.08		
B1	132.03	132.61		
Bα	133.93	134.20		
A1	136.05	136.78		
A4	139.89	140.85		
B4	147.31	148.54		
C3	150.68	151.58		
A3	151.13	152.02		
B3	151.43	152.28		
C4	152.81	153.36		
A4 Ac C=O	168.86	168.87		
Aγ Ac C=O	170.82	170.77		
Bγ Ac C=O	170.95	170.77		
Cα	190.96	191.26		

Compound Number 259



dihydrodiconiferyl alcohol

^{1}H (acetone)

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

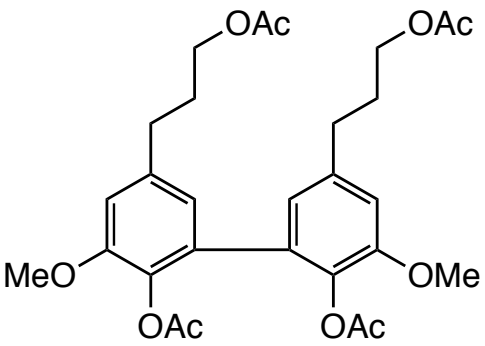
Notes:

L.Landucci
XXIII-152H 25 mg
As this dimer contains a plane of symmetry the CSs are reported for one unit.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	31.94	32.53	31.34	
β	34.45	35.75	34.59	
OMe	56.20	56.42	55.85	
γ	62.38	61.85	60.24	
2	110.71	111.75	110.77	
6	123.04	123.94	122.73	
5	124.52	126.47	125.89	
1	133.76	134.15	132.26	
4	140.83	142.49	141.36	
3	147.33	148.64	147.61	

Compound Number 260



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
4 Ac Me	20.39	20.46	19.99	
γ Ac Me	20.91	20.78	20.56	
α	30.30	30.99	29.58	
β	32.15	32.61	31.32	
OMe	56.02	56.34	55.79	
γ	63.72	64.04	63.10	
2	111.95	112.93	112.16	
6	122.27	122.80	121.46	
5	131.36	132.20	130.51	
4	135.76	136.81	135.09	
1	139.28	140.33	139.20	
3	151.13	152.37	150.82	
4 Ac C=O	168.76	168.76	167.98	
γ Ac C=O	171.08	171.00	170.25	

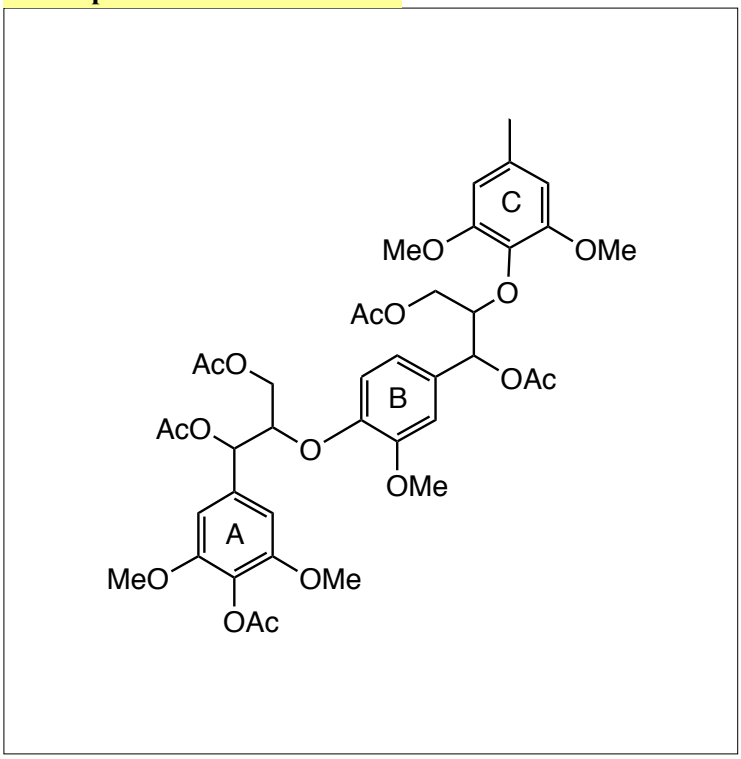
^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.97	m	
Ac Me	1.98	s	
Ac Me	2.01	s	
α	2.70	bt	8.0
OMe	3.83	s	
γ	4.07	t	6.4
6	6.66	d	1.8
2	6.99	d	1.8

Notes:

L.Landucci
XXIII-146ACH
As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 261



S-b(t)-G-b(e)-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.88	s	
γ Ac Me	1.97	s	
α Ac Me	2.01	d	
α Ac Me	2.12	d	
A4 Ac Me	2.21	s	
Cα	2.27	s	
OMe's	3.77, 3.80, 3.84	s's	
Aγ 1	4.05	dd	11.9, 5.4
Bγ 1	4.13	dd	11.5, 3.2
Aγ 2	4.26	m	
Bγ 2	4.39	m	
Bβ	4.65	m	
Aβ	4.81	m	
Bα	6.01	d	4.2
Aα	6.08	d	6.6
C 2,6	6.48	s	
A 2,6	6.85	s	
B6	6.90	m	
B5	7.02	d	8.3
B2	7.06	m	

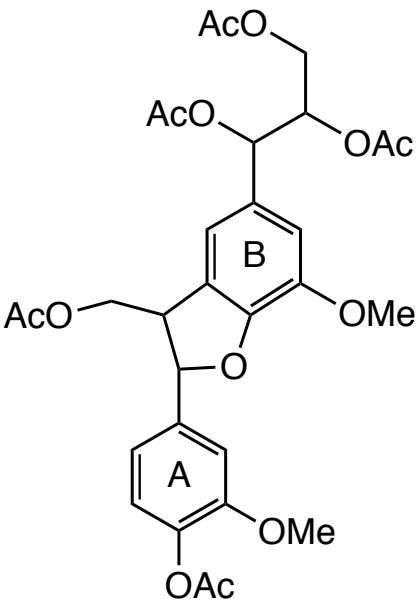
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.48	20.24	20.05
γ Ac Me	20.75	20.64	20.35
γ Ac Me	20.84	20.64	20.35
α Ac Me	21.08	20.96	20.62
α Ac Me	21.14	20.96	20.62
Cα	21.90	21.77	21.35
OMe	55.97	56.28	55.61
OMe	55.97	56.28	55.61
OMe	55.97	56.28	55.61
OMe	56.28	56.28	55.98
OMe	56.28	56.55	55.98
Bγ	62.82	63.35	62.12
Aγ	63.09	63.63	62.46
Bα	74.33	75.22	73.76
Aα	74.48	75.68	74.59
Aβ	80.20	80.65	78.96
Bβ	80.84	81.16	79.94
A2	104.16	104.97	103.97
A6	104.16	104.97	103.97
C2	106.09	106.92	105.87
C6	106.09	106.92	105.87
B2	111.59	112.49	110.87
B5	118.00	118.39	116.75
B6	119.52	120.29	118.89
A4	128.90	129.69	127.84
B1	132.33	132.98	131.07
C4	132.90	134.16	132.16
C1	134.14	134.48	133.32
A1	134.78	136.15	134.92
B4	147.69	148.70	147.19
B3	150.46	151.38	149.68
A3	152.26	153.20	151.58
A5	152.26	153.20	151.58
C3	152.98	153.88	152.34
C5	152.98	153.88	152.34
A4 Ac C=O	168.52	168.45	167.91
α AcC=O	169.75	169.96	169.26
α AcC=O	169.79	170.01	169.33
A γ AcC=O	170.62	170.70	169.94
B γ AcC=O	170.91	170.70	169.94

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
1H data from HSQC in CDCL3

Compound Number 262



G-b5-glycerol

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.98	m	
Ac Me	2.00	m	
Ac Me	2.03	s	
Ac Me	2.04	s	
A4 Ac Me	2.21	s	
Aβ	3.78	m	
A OMe	3.79	s	
B γ1	3.82	m	
B OMe	3.87	s	
B γ2	4.17	m	
Aγ	4.38	m	
Bβ	5.38	m	
Aα	5.61	d	6.8
Bα	5.92	dd	7.2, 2.8
B2,6,A6	6.99	m	
A5	7.04	d	8.2
A2	7.18	bs	

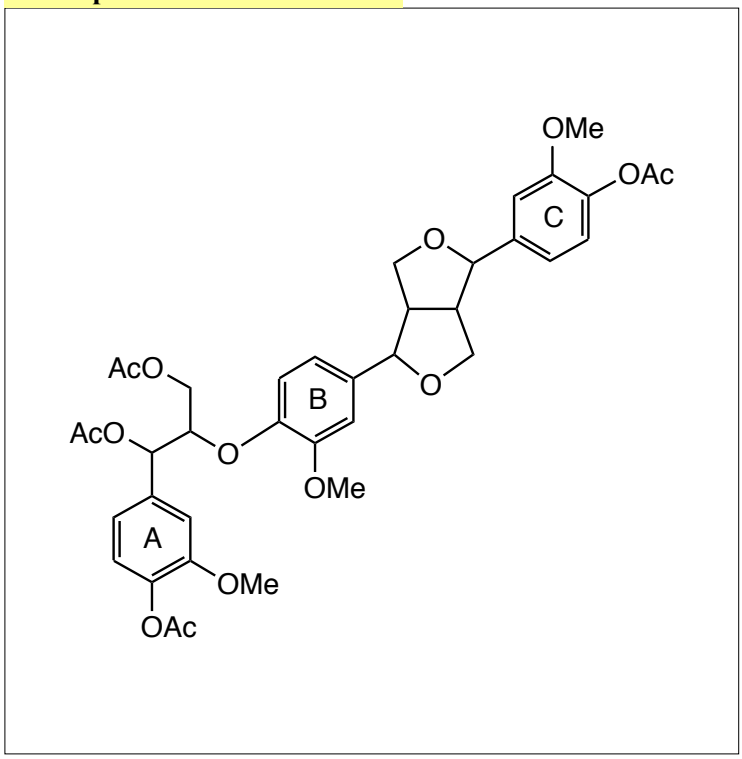
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.76	20.47		
Aγ Ac Me	20.76	20.56		
Bγ Ac Me	20.76	20.73		
Bβ Ac Me	20.85	20.73		
Bα Ac Me	21.07	20.89		
Aβ	50.64	51.45		
A OMe	56.02	56.29		
B OMe	56.26	56.59		
Bγ	62.36	63.00		
Aγ	64.98	65.79		
Bβ	72.47	73.27		
Bα	73.95	74.55		
Aα	88.20	88.40		
A2	110.13	111.11		
B2	111.74	113.19		
B6	115.87	116.84		
A6	118.40	118.78		
A5	122.97	123.80		
B5	127.58	128.83		
B1	129.80	131.06		
A1	139.29	140.82		
A4	139.84	140.92		
B3	144.61	145.31		
B4	148.54	149.38		
A3	151.39	152.46		
A4 Ac C=O	168.96	168.96		
Bα Ac C=O	169.87	170.01		
Bβ Ac C=O	170.10	170.26		
Bγ Ac C=O	170.45	170.63		
Aγ Ac C=O	170.75	170.95		

Notes:

SRVII-91D 8mg HSQC and HMBC in acetone and CDCl3
A1 and A4 tentative assignments, some signals split due to isomers
CDCl3: Aγ +/- (0.13), B2 +/- (0.14), B6 +/- (0.10)
Acetone: Aγ +/- (0.15), Bα +/-(0.04), A2 +/-(0.03), B2 +/- (0.22), B6 +/- (0.17), A6 +/- (0.02), B5 +/- (0.02), A4 +/- (0.03) ppm.

Compound Number 263



G-b-G-r-G

^{1}H (acetone)

Atom	H Shifts	Mult	J

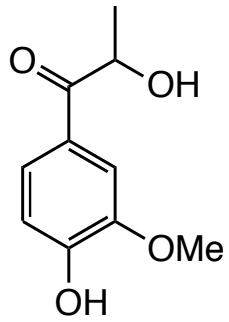
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
C4 Ac Me		20.48		
A4 Ac Me		20.48		
Aα Ac Me		20.63		
Aγ Ac Me		20.89		
Bβ		55.27		
Cβ		55.41		
OMe		56.21		
OMe		56.26		
OMe		56.28		
Aγ		63.03		
Bγ		72.50		
Cγ		72.62		
Aα		74.54		
Aβ		80.31		
Bα		86.17		
Cα		86.17		
C2		111.08		
B2		111.58		
A2		112.74		
C6		118.61		
B5		119.03		
B6		119.42		
A6		120.48		
A5		123.33		
C5		123.47		
A1		136.69		
B1		136.69		
C4		140.12		
A4		141.08		
C1		141.88		
B4		147.48		
B3		151.88		
C3		152.27		
A3		152.27		
A4 Ac C=O		168.92		
C4 Ac C=O		169.05		
AαAc C=O		169.91		
Aγ Ac C=O		170.77		
threo isomer				
Aγ		63.58		
Aα		75.33		
Aβ		80.74		

Notes:

SRVII-143D 13 mg
Erythro isomer shifts reported
sample contains small amt of 5,5 resinol tetramer.

Compound Number 264



alpha,4-dihydroxy-3-methoxypropiophenone
Hibbert's Ketone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.35	d	6.8
OMe	3.91	s	
β-OH	4.10	d	6.4
β	5.13	m	
5	6.94	d	8.2
2	7.57	d	2.0
6	7.60	dd	8.2, 2.0
4-OH	8.61	bs	
CDCl3			
γ	1.46	d	6.6
OMe	3.96	s	
β	5.13	m	
4-OH	6.61	bs	
5	6.98	d	8.2
6	7.48	dd	8.2, 2.0
2	7.54	d	2.0

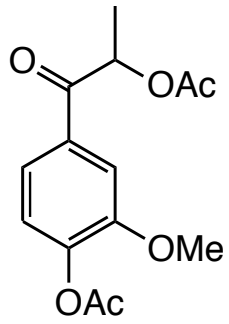
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	22.91	22.69	21.17
OMe	56.19	56.33	55.57
β	68.89	69.42	68.10
2	110.64	112.20	111.74
5	114.30	115.60	114.89
6	124.08	124.65	123.51
1	125.91	127.08	126.15
3	147.10	148.48	147.48
4	151.41	152.84	151.73
α	200.75	201.10	199.72

Notes:

FPL - Pearl collection
25 mg
HSQC and HMBC in acetone

Compound Number 265



alpha,4-diacetoxy-3-methoxypropiophenone

Hibbert's Ketone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.48	d	7.0
β Ac Me	2.06	s	
4 Ac Me	2.27	s	
OMe	3.90	s	
β	6.00	q	7.0
5	7.23	d	8.0
2	7.64	O/Lap	
6	7.66	O/Lap	
CDCl3			
γ	1.53	d	7.0
βAc Me	2.14	s	
4 Ac Me	2.33	s	
OMe	3.89	s	
β	3.93	q	7.0
5	7.14	d	8.1
6	7.55	dd	8.1, 2.0
2	7.59	d	2.0

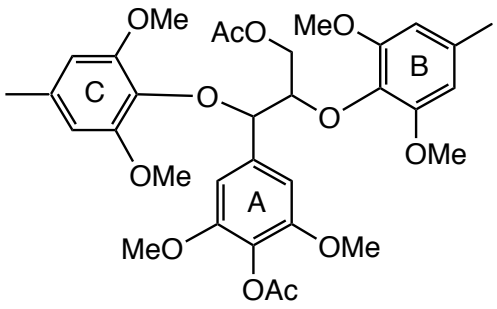
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	17.16	17.41	16.90
β Ac Me	20.56	20.47	20.26
4 Ac Me	20.66	20.54	20.26
OMe	56.02	56.46	55.94
β	71.23	72.21	71.26
2	112.09	112.79	111.85
6	121.55	122.34	121.56
5	122.97	124.10	123.32
1	133.03	134.07	132.46
4	144.22	145.25	143.69
3	151.66	152.72	151.23
4 Ac C=O	168.31	168.62	168.02
β Ac C=O	170.32	170.54	169.74
α	195.65	196.21	195.52

Notes:

FPL - Pearl Collection
25 mg
HSQC and HMBC in acetone

Compound Number 266



S-a-S-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac 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	11.7, 2.8
γ2	4.63	m	
β	4.73	m	
α	5.72	d	6.2
C 2,6	6.37	s	
B 2,6	6.40	s	
A 2,6	6.81	s	

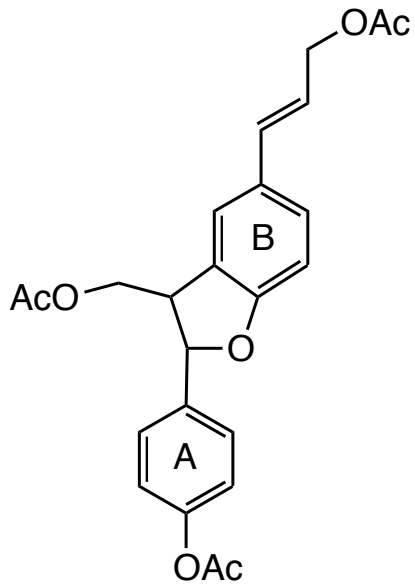
Notes:

SRIX-138A2
3mg
HSQC and HMBC in acetone. A and C OMe shifts may be switched, B and C CH3's may be switched

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.56	20.27	20.05	
γ Ac Me	20.87	20.69	20.30	
B α	21.76	21.61	21.18	
C α	21.82	21.68	21.25	
B OMe	55.87	56.27	55.46	
B OMe	55.87	56.27	55.46	
A OMe	55.96	56.35	55.62	
A OMe	55.96	56.35	55.62	
C OMe	56.12	56.39	55.67	
C OMe	56.12	56.39	55.67	
γ	64.44	64.64	62.98	
β	81.52	82.68	80.92	
α	81.89	83.16	81.36	
A2	105.52	105.94	104.49	
A6	105.52	105.94	104.49	
B2	105.81	107.01	105.74	
B6	105.81	107.01	105.74	
C2	106.22	107.26	106.08	
C6	106.22	107.26	106.08	
A4	128.10	129.11	127.23	
C1	133.01	133.61	132.21	
B1	133.48	133.87	132.47	
C4	133.48	134.38	132.72	
B4	133.62	135.03	132.75	
A1	138.02	138.47	136.90	
A3	150.94	152.21	150.59	
A5	150.94	152.21	150.59	
C3	152.47	153.62	151.95	
C5	152.47	153.62	151.95	
B3	152.87	153.87	152.22	
B5	152.87	153.87	152.22	
A4 Ac C=O	168.75	168.52	167.91	
γ Ac C=O	171.15	170.78	169.99	
1H CDCl3				
γ Ac Me	1.95			
A4 Ac Me	2.30			
C α	2.24			
B α	2.23			
B OMe	3.58			
A/C OMe	3.67			
C/A OMe	3.71			
γ1	4.64			
γ2	4.72			
β	4.72			
α	5.60			
C 2,6	6.26			
B 2,6	6.25			
A 2,6	6.76			

Compound Number 267



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.89	20.67		
γAc Me	21.11	20.81		
BγAc Me	21.19	20.94		
β	50.26	51.06		
Bγ	65.35	65.51		
Aγ	65.68	66.10		
α	87.22	87.85		
B3	109.86	110.20		
Bβ	121.03	122.13		
A3	121.98	122.88		
A5	121.98	122.88		
B6	122.89	123.88		
A2	126.89	127.70		
A6	126.89	127.70		
B5	126.49	127.98		
B2	128.55	129.19		
B1	129.87	130.82		
Bα	134.16	134.43		
A1	138.63	139.84		
A4	150.64	151.77		
B4	159.85	160.77		
A4 C=O	169.44	169.62		
Bγ C=O	170.96	170.77		
AγC=O	170.84	170.94		
1H CDCl3				
γ Ac Me	2.07			
B γ Ac Me	2.10			
A4 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			
A 2,6	7.27			
B6	7.45			

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	2.00	s	
B γ Ac Me	2.01	s	
A4 Ac Me	2.24	s	
β	3.74	m	
γ1	4.34	dd	11.1, 7.8
γ2	4.46	dd	11.1, 5.4
Bγ	4.66	dd	6.4, 1.4
α	5.64	d	6.4
Bβ	6.23	dt	15.9, 6.4
Bα	6.66	d	15.9
B3	6.85	d	8.3
A 3,5	7.13	d	8.5
B2	7.33	dd	8.3, 2.0
A 2,6	7.45	d	8.5
B6	7.45		

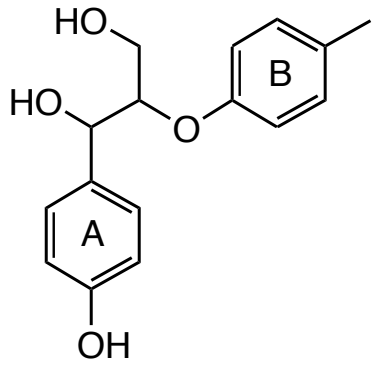
Notes:

LLL XXV-17A-E 11mg

Note: B5 and Bγ C=O move in CDCl3 to lower ppm relative to acetone shifts

HSQC and HMBC run in Acetone

Compound Number 268



erythro

H-b-H

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Bα	20.58	20.45	20.07	
γ	61.32	61.90	60.07	
α	73.89	73.81	71.36	
β	82.25	84.15	83.58	
A3	115.52	115.50	114.46	
A5	115.52	115.50	114.46	
B3	116.79	117.33	116.22	
B5	116.79	117.33	116.22	
A2	127.71	128.89	128.01	
A6	127.71	128.89	128.01	
B2	130.18	130.44	129.52	
B6	130.18	130.44	129.52	
B1	131.41	130.61	129.03	
A1	132.13	133.98	132.76	
A4	155.78	157.43	156.25	
B4	155.53	157.65	156.67	

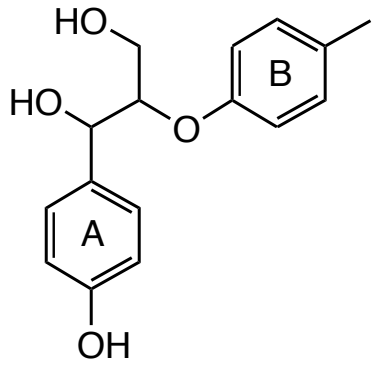
^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.19	s	
γ1	3.77	dd	11.7, 4.4
γ2	3.85	dd	11.7, 5.2
β	4.34	m	
α	4.89	d	5.6
A,B 3,5	6.78		
B 2,6	6.99		8.5
A 2,6	7.28		8.5
<u>CDCl3</u>			
Bα	2.25	s	
γ1	3.80	dd	11.9, 4.0
γ2	3.90	dd	11.9, 4.4
β	4.28	m	
α	4.98	d	5.2
A,B 3,5	6.74		
A 2,6	7.02	d	8.3
B 2,6	7.20	d	8.3

Notes:

S. Ralph SRIX-62
24mg, 70% erythro
A4 and B4 switch in CDCl3, B1 falls between A and B 2,6 in DMSO
HSQC and HMBC in all solvents

Compound Number 269



threo

H-b-H

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα	2.21	s	
γ1	3.48	dd	11.5, 5.4
γ2	3.78	dd	11.5, 4.2
β	4.35	m	
α	4.94	d	5.2
A 3,5	6.78		
B 3,5	6.87		
B 2,6	7.02		
A 2,6	7.27		
CDCl3			
Bα	2.25	s	
γ1	3.46	dd	12.1, 3.8
γ2	3.73	dd	12.1, 4.0
β	4.28	m	
α	4.91	d	6.8
A 3,5	6.72		
B 3,5	6.84		
A 2,6	7.01		
B 2,6	7.18		

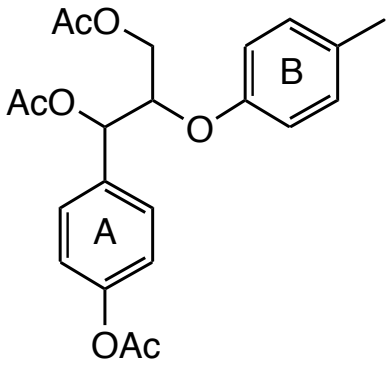
Notes:

SRIX-62 20mg
75% threo, HSQC and HMBC in DMSO
B1 falls between A and B 2,6 in DMSO
A4 and B4 may be switched in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Bα	20.53	20.46	20.05
γ	60.95	61.54	59.99
α	73.64	73.15	70.79
β	83.32	84.43	83.41
A3	115.61	115.52	114.45
A5	115.61	115.52	114.45
B3	116.64	117.15	115.96
B5	116.64	117.15	115.96
A2	128.38	128.87	127.68
A6	128.38	128.87	127.68
B2	130.19	130.47	129.55
B6	130.19	130.47	129.55
B1	131.17	130.56	128.99
A1	131.42	133.58	132.50
A4	155.95	157.51	156.22
B4	156.21	159.00	156.95

Compound Number 270



erythro

H-b-H

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ Ac Me	1.94	s	
Aα Ac Me	2.06	s	
Bα	2.23	s	
A4 Ac Me	2.23	s	
γ1	4.23	dd	11.9, 4.2
γ2	4.34	dd	11.9, 6.0
β	4.83	m	
α	6.04	d	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	8.7

Notes:

SRX-62 25mg
70% erythro
HSQC and HMBC in acetone

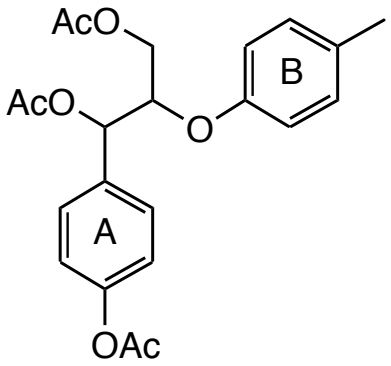
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Bα	20.49	20.49	20.04	
Aγ Ac Me	20.64	20.58	20.40	
Aα Ac Me	20.97	20.86	20.63	
A4 Ac Me	21.08	20.94	20.77	
γ	62.31	62.86	61.77	
α	73.48	74.12	72.74	
β	78.85	79.27	77.41	
B3	116.91	117.56	116.37	
B5	116.91	117.56	116.37	
A3	121.59	122.49	121.66	
A5	121.59	122.49	121.66	
A2	128.47	129.31	128.31	
A6	128.47	129.31	128.31	
B2	130.04	130.74	130.33	
B6	130.04	130.74	130.33	
B1	131.59	131.85	130.51	
A1	133.94	135.33	134.09	
A4	150.66	151.79	150.23	
B4	155.89	157.04	155.46	
A4 Ac C=O	169.15	169.53	169.05	
α Ac C=O	169.51	169.86	169.21	
γ Ac C=O	170.70	170.76	170.04	

1H CDCl3

Aγ Ac Me	2.02
Aα Ac Me	2.09
Bα	2.28
A4 Ac Me	2.28
γ1	4.20
γ2	4.37
β	4.66
α	6.04
B 3,5	6.77
B 2,6	7.07
A 3,5	7.07
A 2,6	7.51

Compound Number 271



threo

H-b-H

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Bα	20.49	20.49	20.03	
Aγ Ac Me	20.64	20.55	20.39	
Aα Ac Me	20.97	20.88	20.64	
A4 Ac Me	21.08	20.94	20.77	
γ	62.68	63.27	62.23	
α	73.94	74.88	73.77	
β	78.49	79.27	77.74	
B3	116.48	117.24	116.09	
B5	116.48	117.24	116.09	
A3	121.78	122.67	121.81	
A5	121.78	122.67	121.81	
A2	128.47	129.33	128.37	
A6	128.47	129.33	128.37	
B2	130.04	130.74	129.81	
B6	130.04	130.74	129.81	
B1	131.37	131.66	130.33	
A1	133.81	135.22	134.04	
A4	150.84	151.94	150.36	
B4	156.33	157.59	156.12	
A4 Ac C=O	169.15	169.52	169.04	
α Ac C=O	169.73	170.04	169.41	
γ Ac C=O	170.57	170.68	169.98	

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ Ac Me	1.94	s	
Aα Ac Me	2.01	s	
Bα	2.24	s	
A4 Ac Me	2.24	s	
γ1	4.01	dd	11.9, 5.8
γ2	4.23	dd	11.9, 4.2
β	4.83	m	
α	6.10	d	6.4
B 3,5	6.90		
B 2,6	7.10		
A 3,5	7.10		
A 2,6	7.51	d	8.5

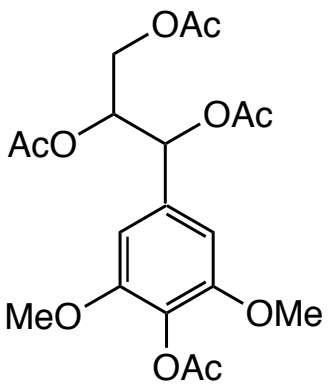
1H CDCl3

Aγ Ac Me	1.98
Aα Ac Me	2.05
Bα	2.28
A4 Ac Me	2.28
γ1	4.00
γ2	4.26
β	4.64
α	6.09
B 3,5	6.85
B 2,6	7.07
A 3,5	7.07
A 2,6	7.42

Notes:

SRX-62 25mg
75% threo

Compound Number 272



S-glycerol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γAc Me	1.99	s	
β Ac Me	2.01	s	
αAc Me	2.08	s	
A4 Ac Me	2.21	s	
OMe	3.81	s	
γ1	3.91	dd	12.1, 6.2
γ2	4.23	dd	12.1, 3.8
β	5.41	m	
α	5.95	d	6.8
2,6	6.80	s	
CDCl3			
γ Ac Me	2.06	s	
β Ac Me	2.08	s	
α Ac Me	2.10	s	
A4 Ac Me	2.33	s	
OMe	3.83	s	
γ1	3.83		hidden
γ2	4.26	dd	12.1, 3.6
β	5.42	m	
α	5.92	d	7.6
2,6	6.61	s	

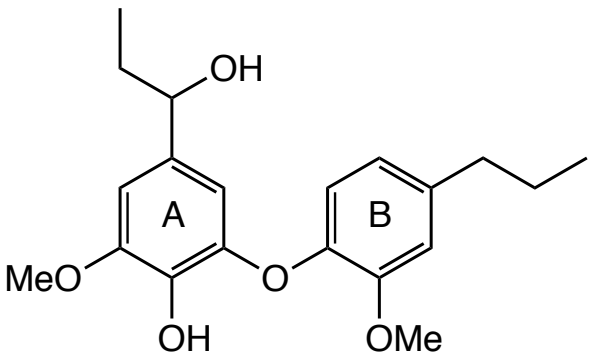
Notes:

L. Landucci XXII-138D7 19mg
2:1 mix of isomers

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.48	20.23	20.08	
γAc Me	20.72	20.55	20.39	
β Ac Me	20.85	20.71	20.46	
α Ac Me	21.01	20.83	20.65	
OMe	56.31	56.58	56.03	
OMe	56.31	56.58	56.03	
γ	62.17	62.85	61.92	
β	72.24	72.99	71.73	
α	73.78	74.45	73.17	
2	104.05	104.76	103.59	
6	104.05	104.76	103.59	
4	129.13	129.79	127.83	
1	134.19	135.85	134.79	
3	152.45	153.30	151.64	
5	152.45	153.30	151.64	
A4 Ac C=O	168.51	168.42	167.93	
α Ac C=O	169.67	170.00	169.43	
β Ac C=O	170.09	170.21	169.43	
γ Ac C=O	170.43	170.65	169.95	
minor isomer				
γ	61.42	62.34		
β	72.48	72.99		
α	73.03	73.76		
2, 6	103.75	104.67		
1	134.19	135.63		
3, 5	152.27	153.19		

Compound Number 273



G-5-O-4-G

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Aγ	10.16	10.48	10.06	
Bγ	13.85	14.05	13.68	
Bβ	24.61	25.41	24.15	
Aβ	31.83	33.20	32.05	
Bα	37.87	38.33	38.50	
B OMe	55.95	56.27	55.57	
A OMe	56.29	56.56	55.91	
Aα	75.94	75.40	73.36	
A2	104.43	105.66	104.81	
A6	109.38	109.81	108.57	
B2	112.88	114.27	113.19	
B5	119.57	119.64	118.00	
B6	120.77	121.35	120.25	
A4	136.18	137.28	135.77	
A1	135.83	137.69	136.52	
B1	139.42	139.25	137.60	
B4	143.63	145.23	143.69	
A5	144.59	145.44	144.24	
A3	148.01	149.29	148.46	
B3	150.27	151.45	149.79	

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	0.83	t	J = 7.3
Bγ	0.93	t	J = 7.3
Aβ,Bβ	1.62	m	
Bα	2.56	bt	J = 7.6
OMe	3.81	s	
OMe	3.86	s	
Aα	4.39	bt	J = 6.1
A6	6.45	d	J = 1.5
B6	6.70	dd	J = 8.1, 1.5
B5	6.75	d	J = 8.1
A2	6.76	d	J = 1.5
B2	6.94	d	J = 1.5
A4-OH	7.39	s	

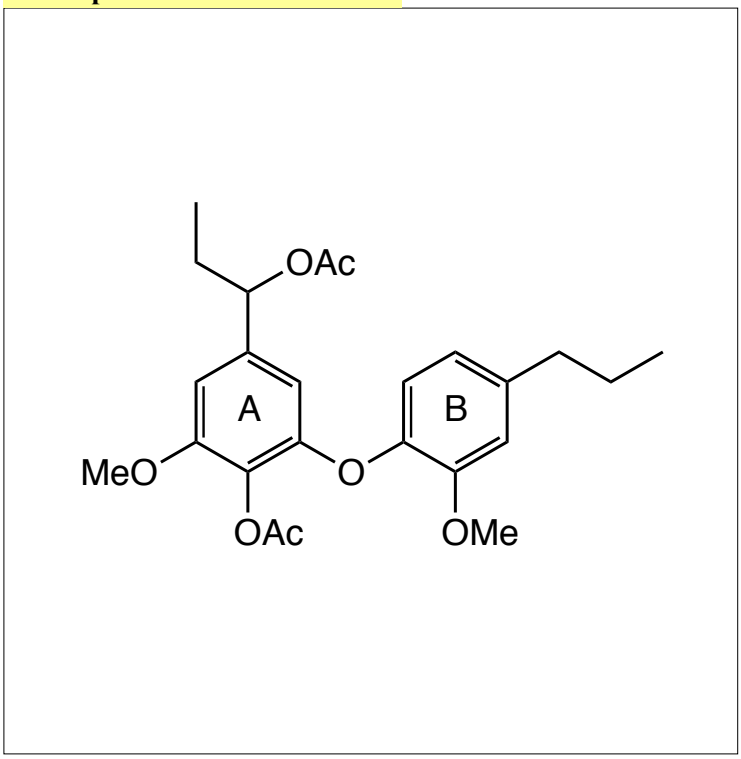
1H CDCl3

		t	
Aγ	0.86	t	7.6
Bγ	0.95	m	7.6
Aβ,Bβ	1.67	bt	
Bα	2.56	s	7.6
OMe	3.85	s	
OMe	3.91	bt	
Aα	4.43	d	6.6
A6	6.53	m	1.8
A2,B6	6.69	d	
B2	6.79	d	2.0
B5	6.88		8.1

Notes:

FPL Collection 11mg
Both A5 and A1 change order in CDCl3 compared to acetone-d6
B4 and A4 assignments taken from 2D in CDCl3
gHSQC and gHMBC in all solvents

Compound Number 274



G-5-O-4-G diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	0.82	t	J = 7.3
Bγ	0.93	t	J = 7.3
Bβ	1.64	m	
Aβ	1.73	m	
Aα Ac Me	1.96	s	
A4 Ac Me	2.18	s	
Bα	2.58	bt	J = 7.3
B OMe	3.76	s	
A OMe	3.84	s	
Aα	5.48	m	
A6	6.32	m	overlapped
B6	6.75	m	overlapped
A2	6.77	m	overlapped
B5	6.84	d	J = 8.1
B2	6.96	d	J = 1.7

Notes:

FPL Collection 6 mg
gHSQC and gHMBC in CDCl3 and acetone-d6
A4 upon acetylation appears as cluster of signals
in acetone-d6 B5 and B6 too close to assign definitively

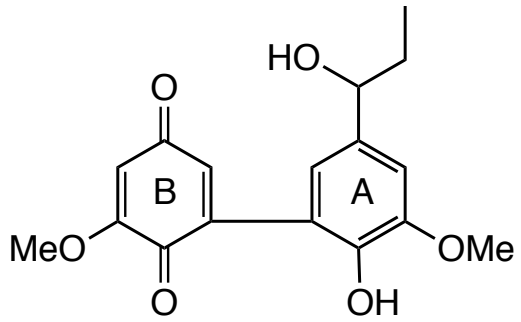
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Aγ	9.90	10.12	9.75
Bγ	13.81	14.00	13.63
A4 Ac Me	20.42	20.22	20.09
Aα Ac Me	21.19	20.94	20.78
Bβ	24.62	25.36	24.14
Aβ	29.31	30.11	28.91
Bα	37.87	38.36	37.05
B OMe	55.98	56.18	55.64
A OMe	56.22	56.56	56.17
Aα	76.92	77.23	76.07
A2	104.58	104.97	104.20
A6	108.53	107.93	106.52
B2	113.11	114.36	113.48
B6	120.49	121.58	120.55
B5	120.86	121.73	120.68
A4	129.59	129.57	128.30
A1	138.79	140.24	139.23
B1	139.73	141.00	139.90
B4	142.84	143.37	141.62
A5	150.39	151.63	150.02
B3	150.72	152.15	150.66
A3	152.46	153.60	152.18
A4 AcC=O	168.48	168.46	168.05
Aα AcC=O	170.26	170.25	169.76

1H CDCl3

Aγ	0.84	t	J = 7.6
Bγ	0.95	t	J = 7.6
Bβ	1.65	m	
Aβ	1.76	m	
Aα Ac Me	2.03	s	
A4 Ac Me	2.24	s	
Bα	2.57	bt	J = 7.6
B OMe	3.80	s	
A OMe	3.85	s	
Aα	5.52	bt	J = 6.8
A6	6.38	d	J = 1.7
A2	6.63	d	J = 2.0
B6	6.69	dd	2.0, 8.1
B2	6.78	d	J = 1.7
B5	6.84	d	J = 8.1

Compound Number 275



G-5-5-*p*-quinone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.91	t	J = 7.4
β	1.70	m	
A OMe	3.88	s	
B OMe	3.89	s	
α	4.50	bt	J = 6.4
B2	6.07	d	J = 2.2
B6	6.69	d	J = 2.2
A6	6.77	d	J = 1.7
A2	7.07	d	J = 1.7
A4-OH	7.76	s	
CDCl3			
γ	0.93	t	J = 7.6
β	1.76	m	
B OMe	3.86	s	
A OMe	3.93	s	
α	4.54	bt	J = 6.9
α OH	5.93		
B2	5.98	d	J = 2.2
A6	6.74	bd	J = 1.2
B6	6.83	d	J = 2.2
A2	6.98	bd	J = 1.2

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	10.21	10.64	10.30
β	31.90	33.21	32.03
B OMe	56.19	56.46	55.87
A OMe	56.39	56.84	56.57
α	75.72	75.40	73.45
B2	107.16	107.77	107.06
A2	109.43	110.91	110.48
A5	118.56	120.61	120.06
A6	120.19	120.61	119.35
B6	135.42	135.34	134.11
A1	136.30	138.14	136.85
A4	143.07	144.12	144.04
B5	142.53	144.79	142.84
A3	146.78	148.08	147.29
B3	159.02	160.27	159.09
B4	180.27	180.63	179.87
B1	187.51	188.03	187.39

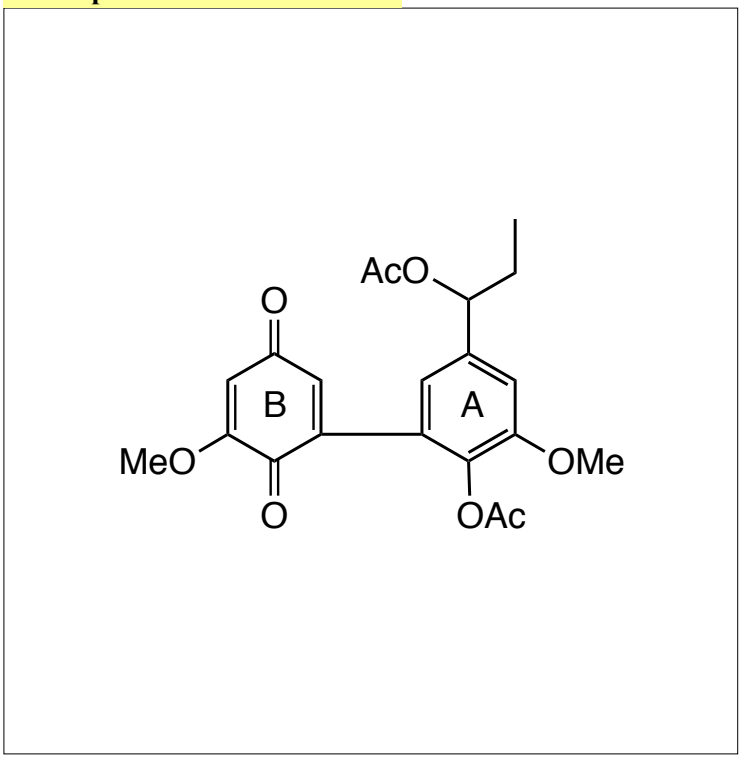
1H DMSO

γ	0.82	t	J = 7.1
β	1.58	m	
OMe	3.80	s	
α	4.33	m	
α OH	5.06	d	J = 3.9
B2	6.14	d	J = 1.7
B6	6.61	d	J = 1.7
A6	6.64	s	
A2	6.96	s	
A4-OH	8.81	s	

Notes:

FPL Collection SRX-84 5 mg
gHSQC and gHMBC in all solvents, A5 is coincident with A6 in acetone-d6
B5 and A4 change order in CDCl3, A6 and A5 change order in DMSO
A and B OMe not definitively assigned in 13C DMSO-d6

Compound Number 276



G-5-5-*p*-quinone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.91	t	J = 7.3
β	1.88	m	
Aα Ac Me	2.06	s	
A4 Ac Me	2.11	s	
A OMe	3.87	s	
B OMe	3.89	s	
α	5.68	t	J = 6.9
B2	6.10	d	J = 2.2
B6	6.59	d	J = 2.2
A6	6.94	d	J = 1.7
A2	7.19	d	J = 1.7
CDCl3			
γ	0.93		
β	1.86		
Aα Ac Me	2.10		
A4 Ac Me	2.18		
A OMe	3.86		
α	5.66	t	J = 6.9
B2	5.99	d	J = 2.5
B6	6.70	d	J = 2.5
A6	6.81	d	J = 2.2
A2	7.00	d	J = 2.0

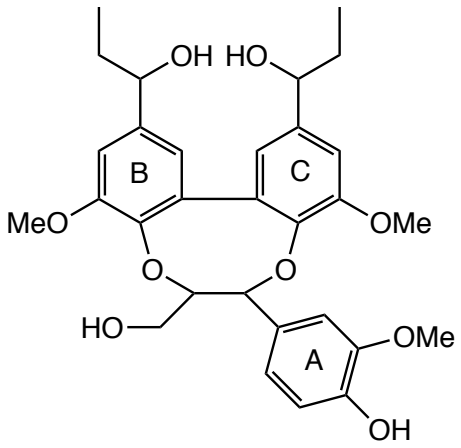
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	10.06	10.22	9.84
A4 Ac Me	20.56	20.31	20.13
Aα Ac Me	21.28	21.02	20.88
β	29.33	30.13	28.85
A OMe	56.26	56.55	56.15
B OMe	56.53	56.91	56.60
α	77.29	77.01	75.82
B2	107.40	108.00	107.33
A2	112.23	112.42	111.63
A6	120.36	120.65	119.58
A5	126.86	128.45	127.00
B6	135.67	135.94	134.85
A4	137.30	138.05	136.35
A1	139.15	140.40	139.08
B5	141.95	142.79	141.15
A3	151.44	152.38	150.83
B3	158.88	159.98	158.74
A4 Ac C=O	168.19	168.42	167.88
Aα Ac C=O	170.44	170.38	169.95
B4	179.90	180.40	179.51
B1	186.98	187.46	186.80

Notes:

FPL Collection SRX-84 5 mg
beta carbon shift taken from DEPT-135, obscured by solvent in 13C acetone-d6
Compound began to degrade after being taken up in CDCl3, shifts taken from mixture with unknown for CDCl3 and DMSO-d6

Compound Number 277



dibenzodioxicin

^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C γ	0.96	m	
B,C β	1.75	m	
A γ1	3.48	m	
A γ2	3.70	m	
OMe	3.77	s	
OMe	3.83	s	
OMe	3.92	s	
A β	4.03	m	
B,C α	4.60	m	
A α	4.77	d	J = 10.0
A5	6.84	d	J = 8.1
A6	6.89	dd	J = 8.1, 1.7
C6	6.96	m	
A2	7.01	d	J = 1.7
B6	7.05	m	
C2	7.06, 7.08	d's	J = 2.0
B2	7.14, 7.16	d's	J = 2.0

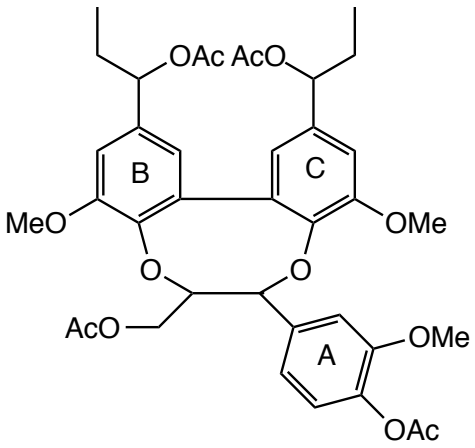
Notes:

SRVII-81 16mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B or C γ	10.34	10.71	10.39	
B or C γ	10.38	10.77	10.49	
B or C β	31.88	33.23	32.11	
B or C β	32.08	33.30	32.11	
OMe	55.78	56.06	55.54	
A OMe	55.85	56.29	55.69	
OMe	56.00	56.33	55.80	
A γ	62.97	62.97	60.66	
B or C α	75.84	75.52	73.63	
B or C α	75.84	75.52	73.63	
A α	84.82	85.18	83.34	
A β	86.93	87.71	85.57	
B2	108.86	110.17	109.45	
C2	109.47	110.55	109.57	
A2	109.47	111.94	111.82	
A5	114.41	115.56	115.14	
C6	118.92	119.26	117.93	
B6	119.35	119.57	117.93	
A6	120.90	121.33	120.11	
A1	130.01	131.38	129.59	
C5	133.19	133.24	131.87	
B5	132.12	133.91	132.08	
C1	141.36	143.38	142.41	
B1	141.74	143.72	142.41	
B4	144.75	145.95	144.87	
C4	145.98	146.73	145.04	
A4	145.98	147.43	146.31	
A3	146.80	148.16	147.18	
B3	151.72	152.75	151.68	
C3	152.24	153.15	151.68	
1H				
B,C γ	0.97		0.90	
B,C β	1.81		1.66	
A γ	3.55		3.22	
OMe	3.76		3.86	
OMe	3.84		3.84	
OMe	3.92		4.47	
A β	4.14		4.81	
A,B,C α	4.59			

Compound Number 278



dibenzodioxicin

^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C γ	0.93	m	
B,C β	1.91	m	
γAc Me	1.91	s	
B,C α AcMe	2.07	s	
A4 Ac Me	2.24	s	
OMe	3.79	s	
OMe	3.94	s	
γ1	4.05	dd	J = 12.0, 3.4
β	4.30	m	
γ2	4.43	dd	J = 12.0, 3.4
α	4.93	d	J = 10.0
B,C α	5.71	m	
A5,A,B,C6	7.00-7.06	m	from HSQC
B or C 2	7.09	m	from HSQC
B or C 2	7.13	m	from HSQC
A2	7.17	m	from HSQC

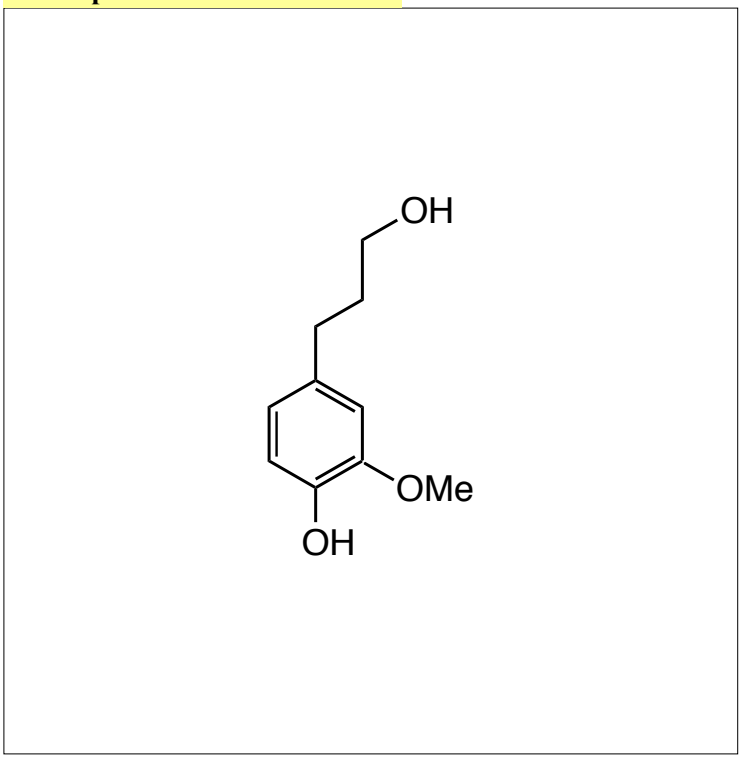
Notes:

SRVII-81Ac
gHSQC and gHMBC in d6-acetone and CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Bγ	10.19	10.43	10.02
Cγ	10.19	10.43	10.02
A4 Ac Me	20.74	20.50	20.36
AαAc Me	20.84	20.58	20.42
B Ac Me	21.40	21.10	20.90
C Ac Me	21.40	21.10	20.90
B or C β	29.28	30.08	28.75
B or C β	29.38	30.43	29.22
OMe	56.10	56.19	55.74
OMe	56.17	56.32	55.94
OMe	56.22	56.38	56.02
Aγ	63.93	64.33	63.14
B or Cα	77.26	77.49	76.34
B or Cα	77.51	77.62	76.39
A β	82.76	83.41	81.80
A α	84.45	85.33	84.06
B or C2	110.27	110.79	109.96
B or C2	111.03	111.19	110.43
A2	111.51	112.78	112.08
B or C6	119.26	119.35	118.00
B or C6	119.74	120.00	118.71
A6	119.91	120.74	119.98
A5	122.76	123.46	122.61
B or C5	132.63	133.22	131.58
B or C5	132.63	133.42	131.77
A1	137.13	138.06	136.45
B or C1	137.28	138.57	137.33
B or C1	137.28	138.75	137.60
A4	139.95	140.80	139.23
B4	146.17	146.86	145.13
C4	146.57	147.24	145.55
A3	151.32	152.14	150.63
B or C3	152.32	153.35	151.98
B or C3	152.52	153.53	152.16
A4 Ac C=O	168.84	168.94	168.47
B,CAcC=O	170.48	170.45	169.89
B,CAcC=O	170.58	170.45	169.92
Aγ Ac C=O	170.76	170.74	170.07
CDCl3			
B,C γ	0.94		
B,C β	1.88		
Ac Me	1.97		
Ac Me	2.08		
Ac Me	2.12		
Ac Me	2.30		
OMe	3.74		
OMe	3.82		
OMe	3.90		
γ1	4.08		
β	4.14		
γ2	4.49		
α	4.85		
B,C α	5.70		
aromatic H	6.87-7.05		

Compound Number 279



dihydro-coniferyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.78	m	
α	2.60	bt	J = 8.0
γ	3.55	bt	J = 5.4
OMe	3.82	s	
6	6.64	dd	J = 8.1, 1.7
5	6.73	d	J = 8.1
2	6.81	d	J = 1.7
DMSO			
β	1.66		
α	2.48		
γ	3.40		
OMe	3.73		
γ OH	4.40		
6	6.55		
5	6.65		
2	6.72		
phenolic OH	8.60		
CDCl3			
β	1.86		
α	2.63		
γ	3.67		
OMe	3.86		
6	6.68		
5	6.70		
2	6.83		

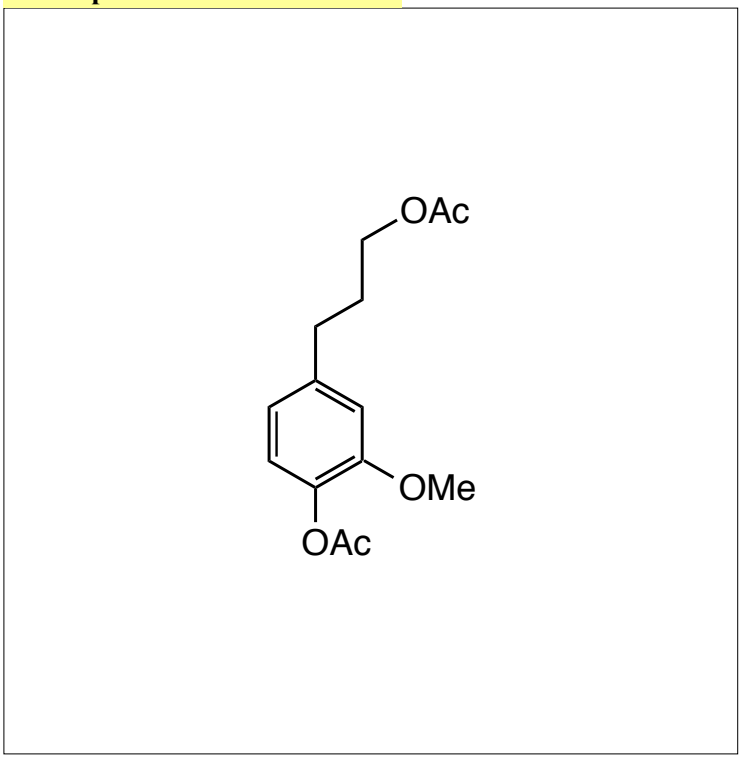
Notes:

J. Ralph 16 mg
gHSQC, gHMBC in d6-acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	31.72	32.44	32.62	
β	34.43	35.85	35.99	
OMe	55.84	56.21	56.95	
γ	62.22	61.83	61.58	
2	111.03	112.87	113.96	
5	114.27	115.59	116.67	
6	120.90	121.55	121.71	
1	133.70	134.61	134.38	
4	143.72	145.47	145.77	
3	146.43	148.17	148.77	

Compound Number 280



dihydro-coniferyl alcohol diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.94	m	
γ Ac Me	1.99	s	
A4 Ac Me	2.21	s	
α	2.68	bt	J = 7.8
OMe	3.79	s	
γ	4.05	t	J = 6.6
6	6.78	dd	J = 8.1, 1.7
5	6.94	d	J = 8.1
2	6.97	d	J = 1.7
CDCl3			
β	1.95	m	
γ Ac Me	2.05	s	
A4 Ac Me	2.29	s	
α	2.67	bt	J = 7.8
OMe	3.81	s	
γ	4.10	t	J = 6.6
6	6.75	bdd	8.1, 1.5
2	6.78	bs	
5	6.93	d	J = 8.1

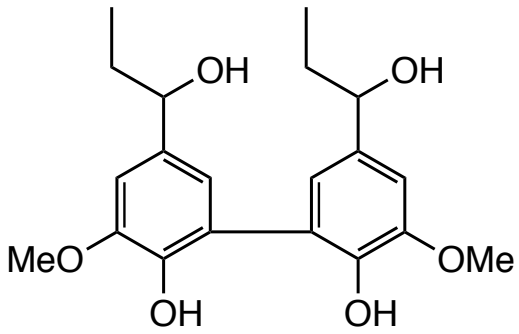
Notes:

JRalph 25mg
gHSQC, gHMBC in d6-acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 AcMe	20.49	20.79	20.31
γ AcMe	20.78	20.50	20.61
β	30.02	31.08	29.67
α	32.03	32.63	31.34
OMe	55.68	56.14	55.59
γ	63.63	64.10	63.21
2	112.45	113.63	112.76
6	120.30	121.05	120.06
5	122.43	123.39	122.41
4	137.84	139.17	137.45
1	140.06	141.27	140.14
3	150.77	152.14	150.60
A4 Ac C=O	169.01	169.07	168.56
γ Ac C=O	170.94	171.00	170.38

Compound Number 281



G-5-5-G

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	10.40	10.70	10.33	
β	31.89	33.21	32.06	
OMe	56.22	56.43	55.81	
α	76.08	75.70	73.71	
2	108.03	109.18	108.28	
6	121.13	121.81	120.58	
5	124.15	126.11	125.54	
1	136.76	138.09	136.43	
4	142.08	143.38	142.10	
3	147.47	148.56	147.36	

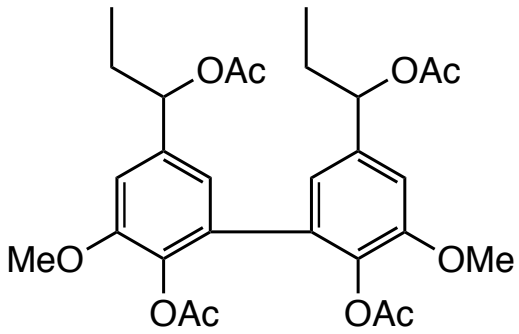
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.91	t	J = 7.3
β	1.71	m	
OMe	3.88	s	
α	4.50	t	J = 6.36
6	6.85	d	J = 2.0
2	6.99	d	J = 2.0
CDCl3			
γ	0.93	t	J = 7.3
β	1.79	m	
OMe	3.92	s	
α	4.54	t	J = 6.36
6	6.87	d	J = 2.0
2	6.93	d	J = 2.0
DMSO			
γ	0.84	t	J = 7.34
β	1.60	m	
OMe	3.81	s	
α	4.34	bs	
α OH	4.98	s	
6	6.66	d	J = 1.71
2	6.87	d	J = 1.71
4-OH	8.20	s	

Notes:

FPL Collection 10 mg
Compound has plane of symmetry

Compound Number 282



G-5-5-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.91	t	J = 7.34
β	1.87	m	
4 Ac Me	2.03	s	
α Ac Me	2.07	s	
OMe	3.87	s	
α	5.63	t	J = 6.6
6	6.79	bs	
2	7.11	bs	
CDCl3			
γ	0.90	t	J = 7.34
β	1.85	m	
4 Ac Me	2.08	s	
α Ac Me	2.09	s	
OMe	3.86	s	
α	5.63	t	J = 6.7
6	6.81	d	J = 1.7
2	6.90	d	J = 1.7

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	10.01	10.27	9.81
4 Ac Me	20.37	20.33	19.99
α Ac Me	21.23	21.04	20.82
β	29.46	30.20	28.90
OMe	56.10	56.46	56.04
α	76.86	77.29	76.03
2	110.14	110.87	110.20
6	120.24	120.41	118.88
5	131.15	131.87	130.12
4	137.00	137.91	136.15
1	138.66	140.04	138.82
3	151.37	152.64	151.14
Ac C=O	168.76	168.99	168.33
α Ac C=O	170.36	170.46	169.84

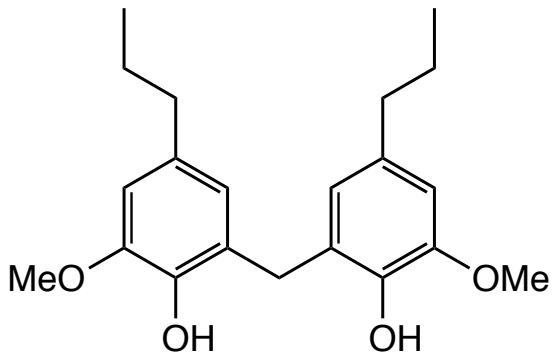
1H DMSO

γ	0.86
β	1.81
4 Ac Me	2.02
α Ac Me	2.07
OMe	3.81
α	5.58
6	6.67
2	7.11

Notes:

FPL Collection 8mg
Compound has plane of symmetry
beta shifts in acetone taken from DEPT 135 spectrum
g-HSQC, g-HMBC all solvents

Compound Number 283



diphenyl methane

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.87	t	J = 7.34
β	1.53	m	J = 7.34
α	2.41	dd	J = 7.34
OMe	3.79	s	
5 CH2	3.94	bs	
6	6.57	bd	J = 1.71
2	6.63	bd	J = 1.71
OH	7.23	bs	
DMSO			
γ	0.82	t	J = 7.34
β	1.47	m	J = 7.34
α	2.35	bt	
OMe	3.75	s	
5 CH2	3.74	s	
6	6.37	bd	J = 1.71
2	6.59	bd	J = 1.71
OH	8.22	s	

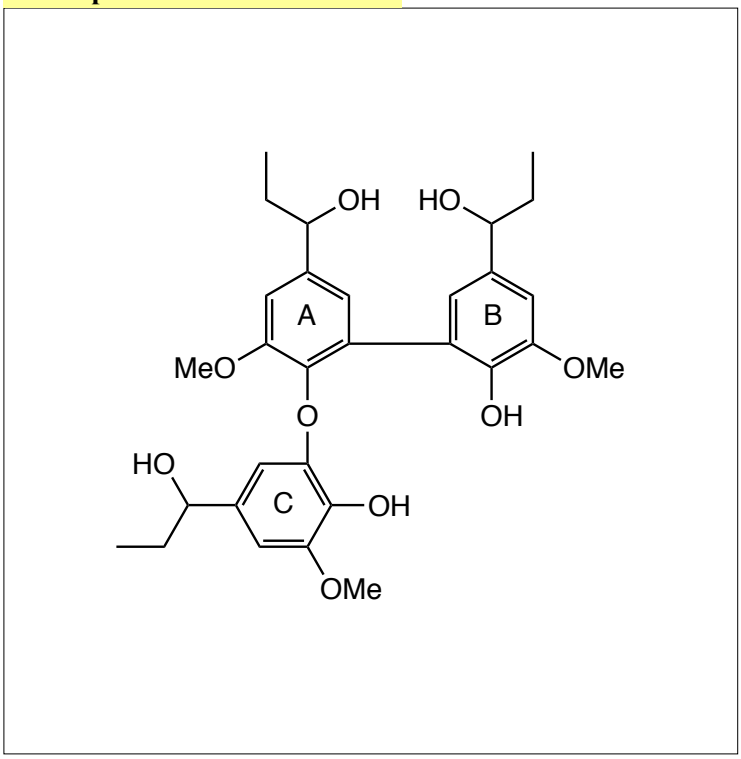
Notes:

FPL Collection 20 mg
Plane of symmetry runs through molecule
CH2 shift obscured by solvent in acetone, taken from Dept 135
2 and 6 switch places in 1H in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	13.78	14.04	13.59
β	24.79	25.57	24.34
5 CH2	29.39	29.56	28.74
α	27.80	38.42	37.10
OMe	55.93	56.27	55.73
2	109.14	110.18	109.62
6	122.36	123.13	121.77
5	126.13	127.59	127.08
1	134.02	133.74	132.02
4	141.01	142.84	141.72
3	146.41	147.75	147.05
1H CDCl3			
γ	0.91		
β	1.57		
α	2.46		
OMe	3.85		
5 CH2	3.93		
6	6.55		
2	6.61		
OH	6.00		

Compound Number 284



G-5-O-4-G-5-5-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
B,C γ	0.76	m	
A γ	0.96	t	
B,C β	1.53	m	
A β	1.74	m	
OMe	3.75	s	
OMe	3.81	s	
C α	4.23 (4.25)	t	J = 6.36
B α	4.35 (4.40)	t	J = 6.36
A α	4.60 (4.63)	t	J = 6.36
C6	6.18 (6.14)	d	J = 1.7
C2	6.52 (6.41)	bd	J = 1.7
B6	6.75 (6.76)	d	J = 1.7
B2	6.86 (6.78)	d	J = 1.7
A6	6.98 (6.97)	d	J = 1.7
A2	7.11 (7.04)	d	J = 1.7

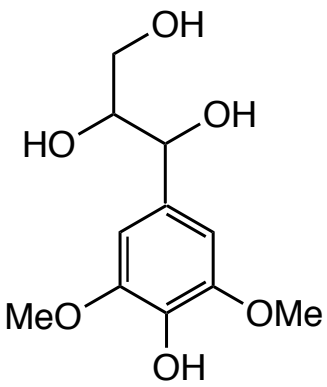
Notes:

FPL Collection 5 mg
g-HSQC and g-HMBC all solvents
Obscured 1H shifts taken from g-HSQC in CDCl3
A1 and B4 may switch order in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	10.15	10.51	9.95	
γ	10.25	10.59	10.06	
γ	10.30	10.59	10.26	
B β	31.42	32.97	32.06	
C β	31.48	33.11	32.06	
A β	32.00	33.27	32.06	
OMe	56.15	55.34	55.68	
OMe	56.15	55.34	55.74	
OMe	56.30	56.52	55.83	
A α	75.80	75.42	73.51	
B α	75.80	75.57	73.60	
C α	76.02	75.66	73.66	
C2	103.82	104.50	103.06	
C6	106.66	106.31	104.51	
B2	108.03	109.13	108.35	
A2	109.45	110.37	109.50	
B6	120.98	121.58	120.18	
A6	121.20	122.17	121.16	
B5	123.38	124.87	124.13	
A5	132.06	133.71	132.72	
C4	134.74	135.37	133.50	
C1	135.22	136.74	135.41	
B1	136.04	137.33	135.91	
A4	141.12	141.12	139.14	
B4	142.24	143.44	142.18	
A1	142.01	143.71	142.47	
C5	145.59	147.29	146.54	
B3	146.79	148.14	147.28	
C3	147.44	148.53	147.59	
A3	152.39	153.21	151.70	
1H				
B,C γ	0.80		0.66	
A γ	0.98		0.88	
B,C β	1.62		1.40	
A β	1.82		1.65	
OMe	3.79			
OMe	3.84			
C α	4.25		4.13	
B α	4.40		4.13	
A α	4.63		4.45	
C6	6.14		6.02	
C2	6.41		6.45	
B6	6.76		6.59	
B2	6.78		6.82	
A6	6.97		6.88	
A2	7.04		7.04	
C4 OH			7.93	
B4 OH			8.14	

Compound Number 285



α-(4-hydroxy-3,5-dimethoxyphenyl)-glycerol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	3.63	d	J = 6.11
β	3.72	m	
OMe	3.81	s	
α	4.60	d	J = 6.11
2,6	6.71	s	
4 OH	7.09	bs	
CDCl3			
γ	3.77		
β	3.81		
OMe	3.91		
α	4.77		
2,6	6.64		
DMSO			
γ	3.42		
β	3.49		
OMe	3.72		
α	4.34		
2,6	6.58		

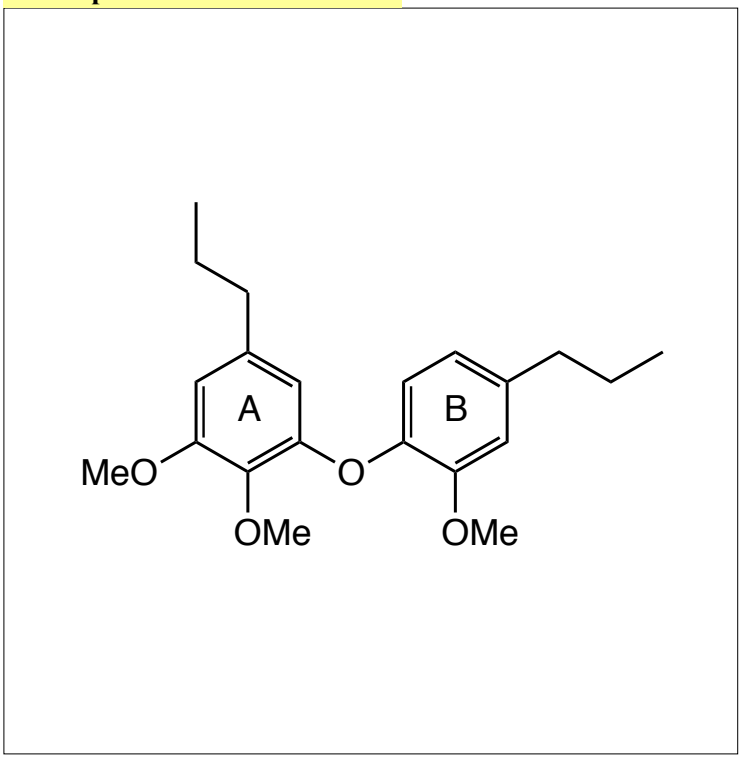
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	56.40	56.60	55.99
OMe	56.40	56.60	55.99
γ	63.24	64.24	63.10
β	74.69	76.26	75.49
α	75.99	76.26	74.24
2	103.03	105.32	104.72
6	103.03	105.32	104.72
1	131.60	133.98	133.58
4	134.57	135.90	134.31
3	147.28	148.32	147.42
5	147.28	148.32	147.42

Notes:

FPL Collection 20 mg
Marginally soluble in CDCl3 and acetone-d6, g-HSQC and g-HMBC in all solvents
1H shifts for β and γ taken from HSQC in DMSO
β and α 13C shifts change order in DMSO (HSQC data)

Compound Number 286



G-5-O-4-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	0.85	t	7.3
Bγ	0.93	t	7.3
Aβ	1.52	m	7.3
Bβ	1.64	m	7.3
Aα	2.41	bt	7.3
Bα	2.57	bt	7.3
A4 OMe	3.74	s	
B3 OMe	3.78	s	
A3 OMe	3.83	s	
A6	6.17	d	2.0
A2	6.58	d	2.0
B6	6.72	dd	1.7, 8.1
B5	6.78	d	8.1
B2	6.95	d	1.7

Notes:

SRX-110

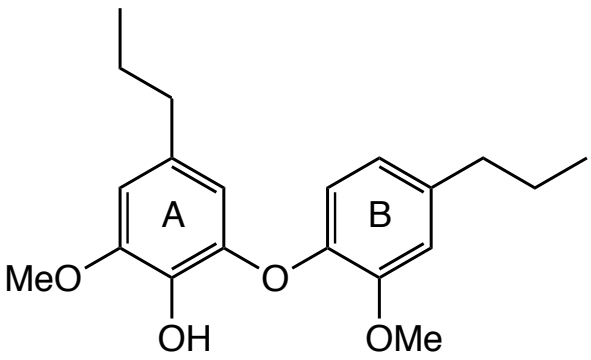
12 mg

α,β,γ and B3, A5 are too close to assign with certainty
HSCQ and HMBC all solvents

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Aγ	13.67	13.93	13.54	
Bγ	13.78	14.04	13.70	
Aβ	24.42	25.26	24.08	
Bβ	24.57	25.39	24.18	
Bα	37.80	38.36	37.08	
Aα	37.99	38.58	37.28	
OMe	55.95	56.24	55.70	
OMe	56.04	56.38	55.88	
A4 OMe	60.94	60.67	60.21	
A2	107.18	108.19	107.36	
A6	111.16	111.12	109.83	
B2	113.01	114.37	113.43	
B5	119.20	120.54	119.39	
B6	120.55	121.41	120.50	
A4	137.70	138.59	136.89	
A1	138.19	138.86	137.90	
B1	138.63	139.80	138.71	
B4	143.82	144.64	142.89	
B3	150.37	151.82	150.31	
A5	150.48	151.94	150.31	
A3	153.27	154.67	153.26	
1H-CDCl3				
γ	0.88			
γ	0.95			
Aβ	1.55			
Bβ	1.65			
Aα	2.43			
Bα	2.56			
B3 OMe	3.83			
A 3,4 OMe	3.87			
A6	6.26			
A2	6.47			
B6	6.68			
B 2,5	6.79			
1H-DMSO				
γ	0.82			
γ	0.90			
β	1.47			
β	1.60			
Aα	2.37			
Bα	2.53			
A4 OMe	3.67			
B3 OMe	3.73			
A3 OMe	3.79			
A6	6.09			
A2	6.58			
B6	6.70			
B5	6.75			
B2	6.94			

Compound Number 287



G-5-O-4-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.85	t	7.3
γ	0.98	t	7.3
A β	1.52	m	7.3
B β	1.62	m	7.3
A α	2.41	bt	7.3
B α	2.55	bt	7.3
B OMe	3.80	s	
A OMe	3.83	s	
A6	6.25	d	2.0
A2	6.58	d	2.0
B6	6.69	dd	1.7, 8.3
B5	6.74	d	8.3
B2	6.92	d	1.7

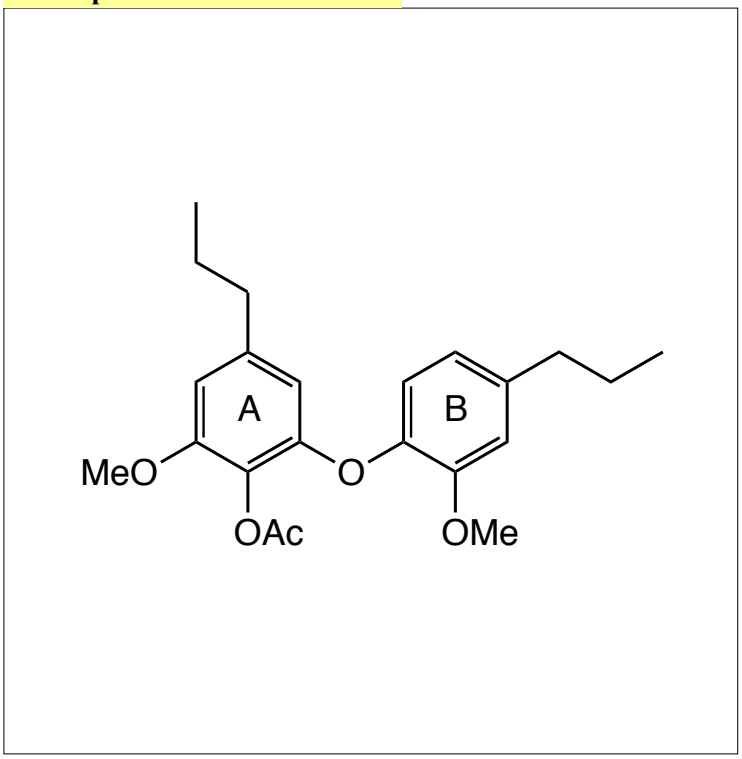
Notes:

FPL Collection
12 mg
A5 and B4 may be switched in acetone but confirmed in CDCl3 by 4-OH correlation to A5

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	13.49	13.91	13.48
γ	13.63	14.04	13.67
β	24.44	25.42	24.17
β	24.47	25.42	24.17
α	37.67	38.34	36.96
α	37.67	38.34	36.98
OMe	55.81	56.28	55.57
OMe	56.04	56.57	55.90
A2	107.05	108.23	107.39
A6	111.46	112.07	110.95
B2	112.75	114.27	113.17
B5	119.17	119.60	117.84
B6	120.53	121.37	120.27
A1	133.56	133.80	132.29
A4	134.79	136.58	135.22
B1	138.87	139.23	137.53
B4	143.84	145.27	143.77
A5	144.28	145.58	144.34
A3	147.59	149.43	148.71
B3	150.10	151.43	149.71
^{1}H CDCl3			
γ	0.80		
γ	0.86		
A β	1.47		
B β	1.56		
A α	2.35		
B α	2.47		
B OMe	3.78		
A OMe	3.80		
4 OH	5.94		
A6	6.30		
A2	6.41		
B6	6.60		
B5	6.71		
B2	6.78		
^{1}H DMSO			
γ	0.80		
γ	0.87		
A β	1.45		
B β	1.57		
A α	2.34		
B α	2.49		
B OMe	3.74		
A OMe	3.76		
A6	6.11		
A2	6.53		
B6	6.57		
B5	6.64		
B2	6.89		
4 OH	8.39		

Compound Number 288



G-5-O-4-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.86	t	7.3
Bγ	0.93	t	7.3
A β	1.53	m	7.3
B β	1.64	m	7.3
Ac Me	2.20	s	
A α	2.45	bt	7.3
B α	2.57	bt	7.3
B OMe	3.77	s	
A OMe	3.81	s	
A6	6.18	d	1.7
A2	6.63	d	1.7
B6	6.73	dd	2.0, 8.3
B5	6.82	d	8.3
B2	6.96	d	2.0

Notes:

SRX-110BAc

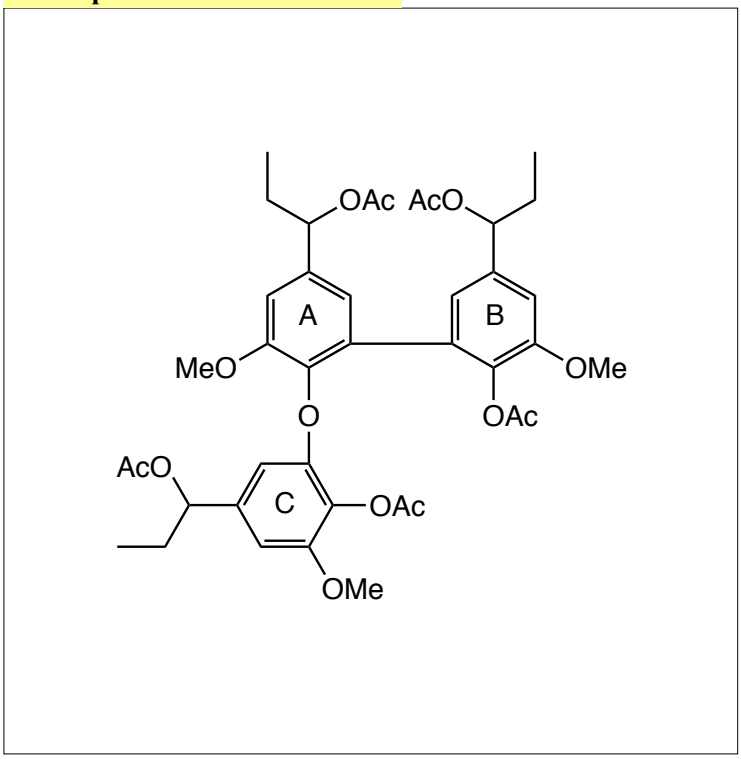
12 mg

α, β, γ shifts are too close to assign with absolute certainty
B2 and B5 change order in CDCl3 1H

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A γ	13.73	13.94	13.52	
B γ	13.78	14.02	13.61	
Ac Me	20.39	20.25	20.05	
A β	24.33	25.22	24.00	
B β	24.57	25.37	24.09	
B α	37.83	38.37	37.03	
A α	38.23	38.73	37.36	
B OMe	56.08	56.24	55.63	
A OMe	56.08	56.44	55.96	
A2	106.59	107.26	106.58	
A6	110.36	110.24	108.99	
B2	113.16	114.39	113.39	
B5	120.40	121.55	120.23	
B6	120.82	121.55	120.53	
A4	128.18	129.04	127.29	
B1	139.36	140.62	139.39	
A1	141.02	141.66	140.63	
B4	143.25	143.86	142.07	
A5	150.12	151.45	149.76	
B3	150.73	152.14	150.53	
A3	152.11	153.44	151.94	
A4 Ac C=O	168.70	168.57	168.04	
1H				
γ	0.89		0.81	
γ	0.95		0.88	
A β	1.55		1.47	
B β	1.65		1.58	
Ac Me	2.24		2.15	
A α	2.45		2.39	
B α	2.56		2.51	
B OMe	3.82		3.70	
A OMe	3.82		3.74	
A6	6.25		6.09	
A2	6.49		6.62	
B6	6.68		6.69	
B2	6.78		6.74	
B5	6.85		6.92	

Compound Number 289



G-5-O-4-G-5-5-G Acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.78		
γ	0.82		
B γ	0.91		
A,C β	1.73		
B β	1.88		
AcMe Cα	1.95		
AcMe Aα	2.04		
AcMe Bα	2.05		
AcMe B4	2.10		
AcMe C4	2.16		
OMe	3.73		
OMe	3.76		
OMe	3.81		
Cα	5.46		
Aα	5.55		
Bα	5.65		
C6	6.20		
C2	6.64		
B6	6.81		
A6	6.83		
A2	6.99		
B2	7.13		

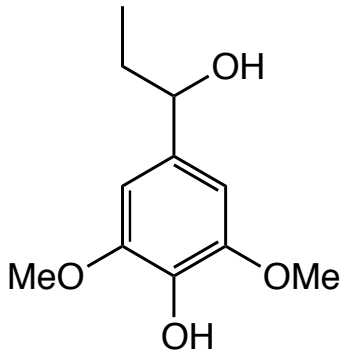
Notes:

FPL Collection 2 mg
COSY, HSQC and HMBC in acetone at 600MHz
1H in CDCl3 some shifts taken from HSQC and HMBC
Aromatic carbon shifts in DMSO are weak, no 2D spectra in DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	9.79	10.19	9.57	
γ	9.85	10.19	9.57	
γ	9.90	10.19	9.57	
C4AcMe	20.21	20.18	19.77	
B4AcMe	20.32	20.18	19.88	
AαAcMe	21.12	20.46	20.59	
CαAcMe	21.16	21.25	20.68	
BαAcMe	21.22	21.36	20.80	
β	28.94	29.77	28.50	
β	29.21	29.97	28.68	
B β	29.46	30.18	28.84	
OMe	56.00	56.38	55.89	
OMe	56.00	56.38	55.89	
OMe	56.07	56.65	55.89	
α	76.83	77.28	75.94	
α	76.88	77.28	75.94	
α	76.88	77.28	75.94	
C2	103.60	104.30	103.38	
C6	105.82	106.11	106.53	
A2	110.40	110.99	110.12	
B2	110.70	111.63	110.88	
B6	120.30	119.42	119.39	
A6	120.78	120.81	119.64	
C4	128.02	128.90	127.11	
A5	130.86	131.83	130.23	
B5	131.77	133.47	130.83	
A4	136.95	137.91	136.20	
B1	137.84	139.40	138.03	
A1	138.16	139.65	138.31	
C1	138.16	139.65	138.50	
B4	140.05	140.78	138.96	
C5	150.42	151.59	149.99	
A3	151.11	152.36	150.84	
B3	152.20	153.33	151.80	
C3	152.20	153.33	151.80	
C4AcC=O	167.92	167.62	167.29	
B4AcC=O	168.77	169.09	168.23	
AαAcC=O	170.30	169.09	169.71	
CαAcC=O	170.40	170.37	169.71	
BαAcC=O	170.40	170.50	169.71	
1H CDCl3	1H		1H	
γ	0.72		0.71	
γ	0.79		0.78	
B γ	0.89		0.86	
β	1.72		1.67	
β	1.72		1.67	
B β	1.86		1.84	
AcMe Cα	1.99		1.92	
AcMe Aα	2.07		|	
AcMe Bα	2.10		|	
AcMe B4	2.16		|	
AcMe C4	2.21		2.15	
OMe	3.71		3.67	
OMe	3.74		3.72	
OMe	3.79		3.76	
Cα	5.45		5.42	
Aα	5.54		5.49	
Bα	5.63		5.61	
C6	6.13		6.03	
C2	6.46		6.62	
B6	6.82		6.70	
A6	6.76		6.70	
A2	6.81		6.99	
B2	6.87		7.13	

Compound Number 290



1-(4-hydroxy-3,5-dimethoxy)-1-propanol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.87	t	7.3
β	1.66	m	
OMe	3.79	s	
α	4.44	bt	6.4
2,6	6.63	s	
4 OH	6.99	s	
CDCl3			
γ	0.91		
β	1.75		
OMe	3.88		
α	4.50		
2,6	6.57		
DMSO			
γ	0.79		
β	1.56		
OMe	3.72		
α	4.30		
2,6	6.54		
4 OH	8.08		

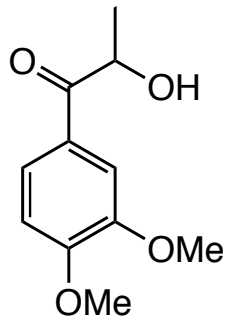
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	10.19	10.61	10.32
β	31.87	33.24	32.16
OMe	56.23	56.59	55.95
OMe	56.23	56.59	55.95
α	76.20	75.81	73.92
2	102.60	104.32	103.33
6	102.60	104.32	103.33
4	133.91	135.66	134.10
1	135.87	137.56	136.44
3	146.91	148.41	147.65
5	146.91	148.41	147.65

Notes:

FPL Collection
22 mg
HSQC and HMBC in acetone

Compound Number 291



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	22.77	22.59	21.09	
OMe	55.97	56.14	55.54	
OMe	56.06	56.24	55.75	
β	68.78	69.53	68.31	
5	110.13	111.62	110.89	
2	110.68	111.95	110.89	
6	123.32	124.22	123.31	
1	126.16	127.80	127.38	
3	149.25	150.30	148.61	
4	153.96	155.01	153.11	
α	200.73	201.30	200.09	

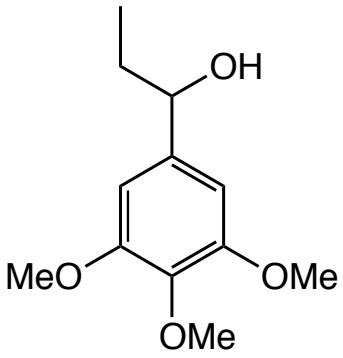
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.35	d	6.85
OMe	3.87	s	
OMe	3.90	s	
β	5.14	q	6.85
5	7.06	d	8.6
2	7.54	d	2.0
6	7.68	dd	8.6, 2.0
CDCl3			
γ	1.43		
OMe	3.92		
OMe	3.93		
β	5.10		
5	6.89		
2	7.49		
6	7.49		
1H DMSO			
γ	1.27		
OMe	3.81		
OMe	3.84		
β	5.05		
β OH	5.21		
5	7.06		
2	7.48		
6	7.69		

Notes:

SRX-115G 26 mg Hibbert's Ketone
HSQC in acetone and CDCl3, HMBC in acetone
HSQC shows that C2 is downfield of C5 for acetone and CDCl3
C2 = C5 in DMSO

Compound Number 292



1-(3,4,5-trimethoxyphenyl)-1-propanol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.89	t	7.3
β	1.67	m	
4 OMe	3.68	s	
OMe	3.79	s	
α	4.12	d	4.0
α OH	4.48	bt	6.4
2,6	6.65	s	
CDCl3			
γ	0.93		
β	1.76		
4 OMe	3.82		
OMe	3.86		
α	4.52		
2,6	6.58		
DMSO			
γ	0.81		
β	1.56		
4 OMe	3.60		
OMe	3.73		
α	4.35		
αOH	5.08		
2,6	6.59		

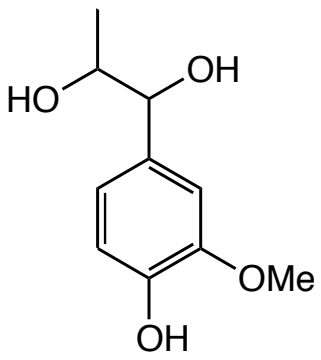
Notes:

SRX-115S
39 mg
HSQC and HMBC in acetone
CAS# 835922-48-0

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	10.06	10.58	10.29
β	31.84	33.20	32.08
OMe	55.86	56.32	55.78
OMe	55.86	56.32	55.78
4 OMe	60.57	60.44	59.98
α	75.80	75.69	73.81
2	102.68	104.06	103.00
6	102.68	104.06	103.00
4	136.84	137.95	136.05
1	140.60	142.75	142.09
3	152.96	154.08	152.55
5	152.96	154.08	152.55

Compound Number 293



^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.02 (0.92)	d	6.4
β	3.81 (3.69)	m	
OMe	3.80 (3.80)	s	
α	4.45 (4.20)	d	5.1 (7.3)
5	6.73 (6.73)	d	8.1
6	6.77 (6.77)	dd	8.1, 1.7
2	6.98 (6.95)	d	1.7
CDCl3			
γ	1.03 (0.96)		
β	3.87 (3.74)		
OMe	3.81 (3.81)		
α	4.49 (4.20)		
DMSO			
γ	0.93 (0.77)		
β	3.56 (3.56)		
OMe	3.69 (3.69)		
α	4.20 (4.09)		
5,6	6.64 (6.64)		
2	6.83 (6.81)		

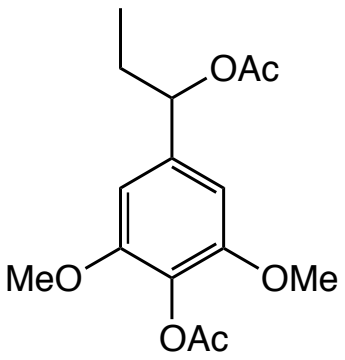
Notes:

FPL Collection 20 mg
g-HSQC and g-HMBC in d6-acetone
2 isomers ^{1}H minor shifts and j's in ( )

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
major				
γ	18.34	18.08	18.42	
OMe	56.83	56.20	55.56	
β	72.25	72.03	70.67	
α	78.37	78.15	76.83	
2	110.18	111.20	111.04	
5	115.09	115.09	114.65	
6	120.61	120.32	119.26	
1	133.49	134.95	134.56	
4	146.17	146.39	145.16	
3	147.55	147.81	146.97	
minor isomer				
γ	19.67	19.30	19.00	
OMe	56.83	56.20	55.56	
β	73.15	72.68	70.89	
α	80.27	79.80	77.79	
2	110.12	111.27	111.12	
5	115.16	115.21	114.76	
6	120.90	120.66	119.50	
1	134.08	134.90	133.98	
4	146.40	146.77	145.46	
3	147.61	148.02	147.04	

Compound Number 294



1-(4-hydroxy-3,5-dimethoxy)-1-propanol diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.88	t	7.3
β	1.83	m	
α Ac Me	2.05	s	
4 Ac Me	2.21	s	
OMe	3.80	s	
α	5.61	dd	7.3
2,6	6.71	s	
CDCl3			
γ	0.91		
β	1.85		
α Ac Me	2.09		
4 Ac Me	2.33		
OMe	3.82		
α	5.62		
2,6	6.58		
DMSO			
γ	0.85		
β	1.80		
α Ac Me	2.07		
4 Ac Me	2.22		
OMe	3.74		
α	5.56		
2,6	6.68		

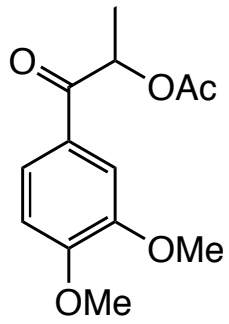
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	10.01	10.29	9.93
4 AcMe	20.41	20.26	20.14
α AcMe	21.20	21.04	20.90
β	29.30	30.13	28.96
OMe	56.10	56.45	55.98
OMe	56.10	56.45	55.98
α	77.26	77.61	76.49
2	103.29	103.86	102.85
6	103.29	103.86	102.85
4	128.18	129.21	127.27
1	138.92	140.45	139.33
3	152.01	153.13	151.60
5	152.01	153.13	151.60
4 Ac C=O	168.65	168.55	168.14
α Ac C=O	170.25	170.39	169.89

Notes:

SRX-115SSMAc
19 mg
C4 has very long T1, D1 set to 6 sec.

Compound Number 295



Hibbert's Ketone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.46	d	6.85
AcMe	2.05	s	
3 OMe	3.86	s	
4 OMe	3.90	s	
β	5.97	q	6.85
5	7.06	d	8.6
2	7.50	d	2.0
6	7.67	dd	8.6, 2.0
CDCl3			
γ	1.53		
AcMe	2.15		
OMe	3.93, 3.96		
β	5.96		
5	6.91		
2	7.52		
6	7.59		
DMSO			
γ	1.40		
AcMe	2.06		
OMe	3.81, 3.85		
β	5.99		
5	7.08		
2	7.43		
6	7.68		

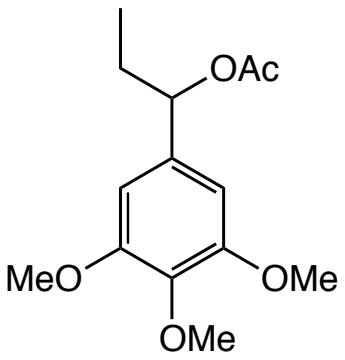
Notes:

SRX-115GAc
12 mg
g-HSQC and g-HMBC in d6-acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	17.40	17.70	17.32
AcMe	20.69	20.60	20.42
OMe	55.92	56.12	55.55
OMe	56.03	56.25	55.80
β	70.95	71.98	71.13
5	110.10	111.66	110.45
2	110.66	111.69	111.05
6	122.92	123.75	123.08
1	127.29	128.23	126.48
3	149.23	150.39	148.83
4	153.70	154.98	153.57
Ac C=O	170.35	170.47	169.78
α	195.21	195.54	194.95

Compound Number 296



1-(3,4,5-trimethoxyphenyl)-1-propanol acetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	0.86	t	7.3
β	1.82	m	
α Ac Me	2.03	s	
4 OMe	3.69	s	
3,5 OMe	3.81	s	
α	5.56	bt	6.6
2,6	6.64	s	
CDCl3			
γ	0.90		
β	1.85		
α Ac Me	2.09		
4 OMe	3.83		
3,5 OMe	3.87		
α	5.59		
2,6	6.55		
DMSO			
γ	0.82		
β	1.77		
α Ac Me	2.05		
4 OMe	3.63		
3,5 OMe	3.76		
α	5.52		
2,6	6.60		

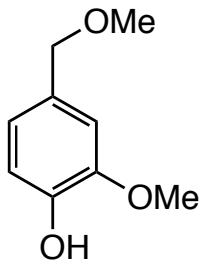
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	9.92	10.30	9.90
α AcMe	21.13	21.05	20.89
β	29.20	30.13	28.90
3 OMe	55.98	56.43	55.86
5 OMe	55.98	56.43	55.86
4 OMe	60.63	60.45	59.91
α	77.41	77.75	76.60
2	103.58	104.71	103.49
6	103.58	104.71	103.49
1	136.12	137.56	136.39
4	137.45	138.71	136.85
3	153.08	154.32	152.80
5	153.08	154.32	152.80
α Ac C=O	170.26	170.37	169.83

Notes:

SRX-115SAc
29mg
g-HMBC in d6-acetone

Compound Number 297



Veratryl alcohol methyl ether

^{1}H (acetone)

Atom	H Shifts	Mult	J
α OMe	3.27	s	
OMe	3.78	s	
OMe	3.79	s	
α	4.33	s	
6	6.83	dd	8.1, 2.0
5	6.89	d	8.1
2	6.91	d	2.0
CDCl3			
α	4.37		
5	6.81		
6	6.85		
2	6.87		
DMSO			
α	4.31		
6	6.83		
2	6.89		
5	6.90		

Notes:

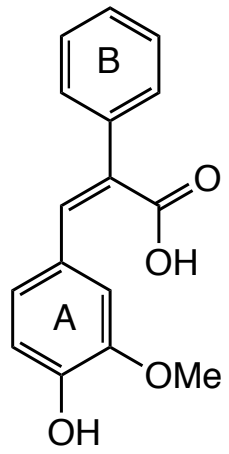
S. Ralph

Carbon pairs 2 & 5 and 3 & 4 are too close for definitive assignment

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.80	56.03	55.37	
OMe	55.89	56.12	55.46	
α OMe	57.86	57.74	57.15	
α	74.61	74.86	73.55	
2 or 5	110.84	112.49	111.45	
5 or 2	110.99	112.60	111.50	
6	120.29	120.95	120.03	
1	130.73	132.16	130.65	
3 or 4	148.58	149.89	148.23	
4 or 3	149.02	150.34	148.64	

Compound Number 298



3-Methoxy-4-hydroxy stilbene carboxylic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.38	s	
A2	6.50	d	2.0
A5	6.71	d	8.1
A6	6.80	dd	8.1, 2.0
B 2,6	7.27	m	
B4	7.36	m	
B 3,5	7.43	m	
α	7.80	s	
CDCl3			
A2	6.41		
A5	6.77		
A6	6.83		
B 2,6	7.29		
B4, B 3,5	7.37, 7.41		
α	7.87		
DMSO			
A2	6.41		
A5	6.64		
A6	6.66		
B 2,6	7.19		
B4, B 3,5	7.35, 7.41		
α	7.66		

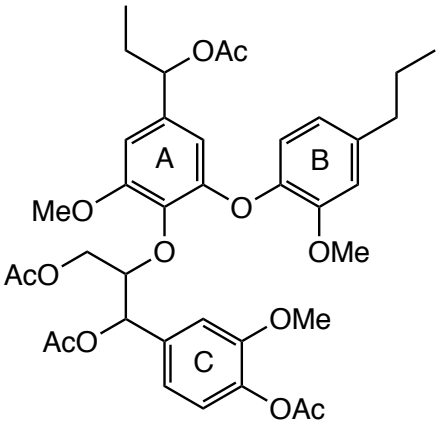
Notes:

FPL - Pearl Collection
30 mg, beta under B3,5 shift from APT experiment, HSQC and HMBC all solvents
Some 1H shifts taken from HSBC expt.s

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.25	55.42	54.61
A2	112.07	113.60	113.05
A5	114.19	115.58	115.11
A6	126.78	126.69	125.35
A1	126.73	127.30	125.35
B4	127.90	128.25	127.28
B3	128.91	129.48	128.59
B5	128.91	129.48	128.59
β	128.91	130.55	129.64
B2	130.03	130.81	129.66
B6	130.03	130.81	129.66
B1	136.18	138.15	137.15
α	142.49	141.18	139.52
A3	145.76	147.68	146.88
A4	147.37	148.91	148.05
γ	172.08	169.12	168.58

Compound Number 299



beta-O-4, 5-O-4 trimer

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	**0.79 (0.79)	t	7.3
Bγ	0.94 (0.97)	t	7.3
Bβ--Aβ	1.6-1.75 (1.66-1.76)	m	
Cγ Ac Me	1.78 (1.86)	d	1.0
Aα Ac Me	1.93 (2.01)	s	
Cα Ac Me	2.08 (2.10)	s	
C4 Ac Me	2.20 (2.28)	s	
Bα	2.60 (2.59)	m	
C OMe	3.70 (3.69)	d	2.2
B OMe	3.74 (3.72)	s	
A OMe	3.82 (3.76)	s	
Cγ1	4.21 (4.26)	dd	4.2, 11.7
Cγ2	4.41 (4.47)	dd	5.9, 11.7
Cβ	4.98 (4.90)	m	
Aα	5.44 (5.44)	t	7.3
Cα	6.13 (6.14)	d	4.4
A6	6.24 (6.27)	bs	
A2	6.69 (6.52)	bs	
B6	6.80 (6.70)	dd	2.0, 8.1
B5	6.90 (6.80)	d	8.1
C6	6.97 (6.92)		
C5	6.98 (6.91)		
B2	6.99 (6.77)		
C2	7.15 (7.02)	bs	

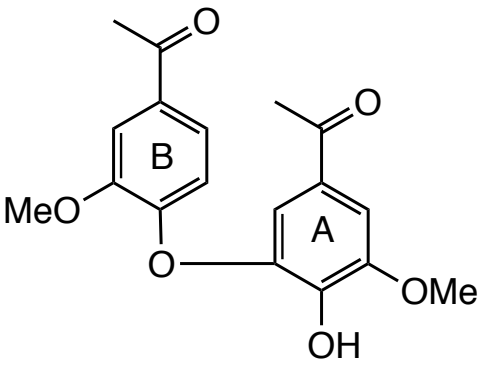
Notes:

SR X 125D1-2
B5 and B6 change order in CDCl3
***1H shifts in CDCl3 in ( )s after acetone shift*
C6, C5 and B2 shifts from HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Aγ	9.83	10.08		
Bγ	13.85	14.04		
C4 Ac Me	20.68	20.46		
Cγ Ac Me	20.68	20.53		
α Ac Me	21.03	20.89		
α Ac Me	21.19	20.95		
Bβ	24.63	25.38		
Aβ	29.27	30.02		
Bα	37.89	38.39		
OMe	55.63	56.11		
OMe	55.75	56.11		
A OMe	56.01	56.42		
Cγ	62.77	63.39		
Cα	74.22	75.20		
Aα	77.03	77.30		
Cβ	80.66	81.27		
A2	104.53	105.23		
A6	108.03	107.60		
C2	111.51	112.18		
B2	112.97	114.27		
C6	119.46	120.06		
B6	120.75	121.57		
B5	120.43	121.75		
C5	122.30	123.25		
A4	135.88	136.38		
C1	136.35	136.94		
A1	136.35	137.60		
C4	139.38	140.66		
B1	139.64	140.90		
B4	142.32	143.02		
B3	150.58	152.04		
C3	150.78	152.04		
A5	150.98	152.12		
A3	153.40	154.40		
C4 Ac C=O	168.98	168.91		
Cα Ac C=O	169.67	169.96		
Aα Ac C=O	170.28	170.17		
Cγ Ac C=O	170.93	170.66		

Compound Number 300



5-O-4 diacetovanillone

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aβ	2.49	s	
Bβ	2.53	s	
OMe	3.93	s	
OMe	3.95	s	
B5	6.78	d	8.3
A6	7.30	d	2.0
A2	7.47	d	2.0
B6	7.56	dd	8.3, 2.0
B2	7.64	d	2.0

Notes:

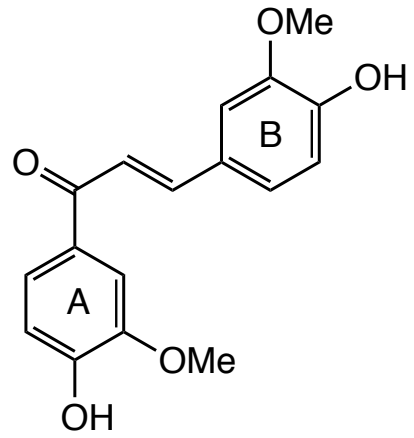
SRX-146C

A4-OH has strong HMBC correlations in DMSO to A3,4 ,5

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Aβ	25.92	26.33	26.32	
Bβ	26.09	26.47	26.51	
B OMe	56.17	56.36	55.79	
A OMe	56.50	56.76	56.23	
A2	107.30	108.56	108.09	
B2	112.30	112.68	111.65	
A6	114.80	115.45	114.62	
B5	116.82	116.80	115.44	
B6	122.48	123.22	122.51	
A1	129.24	129.73	127.91	
B1	133.33	133.65	132.01	
A5	142.21	143.16	141.97	
A4	142.41	144.09	143.37	
A3	148.16	149.67	148.83	
B3	150.08	150.73	149.09	
B4	150.43	151.69	150.44	
Aα	195.70	195.93	195.87	
Bα	196.37	196.55	196.50	
1H CDCl3				
Aβ	2.48			
Bβ	2.56			
OMe	3.95			
OMe	3.99			
B5	6.85			
A6	7.28			
A2	7.41			
B6	7.49			
B2	7.63			
DMSO				
Aβ	2.49			
Bβ	2.55			
OMe	3.90			
OMe	3.92			
B5	6.67			
A6	7.25			
A2	7.42			
B6	7.54			
B2	7.59			
A4-OH	10.00			

Compound Number 301



guaiacyl chalcone

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.93	bs	
B5	6.83	d	8.3
A5	6.93	d	8.3
B6	7.29	dd	1.7, 8.3
B2	7.49	d	1.7
A2	7.61	d	1.7
γ	7.63	d	15.4
β	7.76	d	15.4
A6	7.80	dd	1.7, 8.3
CDCl3			
OMe	3.93	s	
OMe	3.95	s	
5	6.93	d	8.3
5	6.97	d	8.3
B2	7.10	d	1.96
B6	7.20	dd	1.96, 8.3
β	7.37	d	15.4
A2	7.61	d	obscured
A6	7.62	dd	obscured
γ	7.73	d	15.4

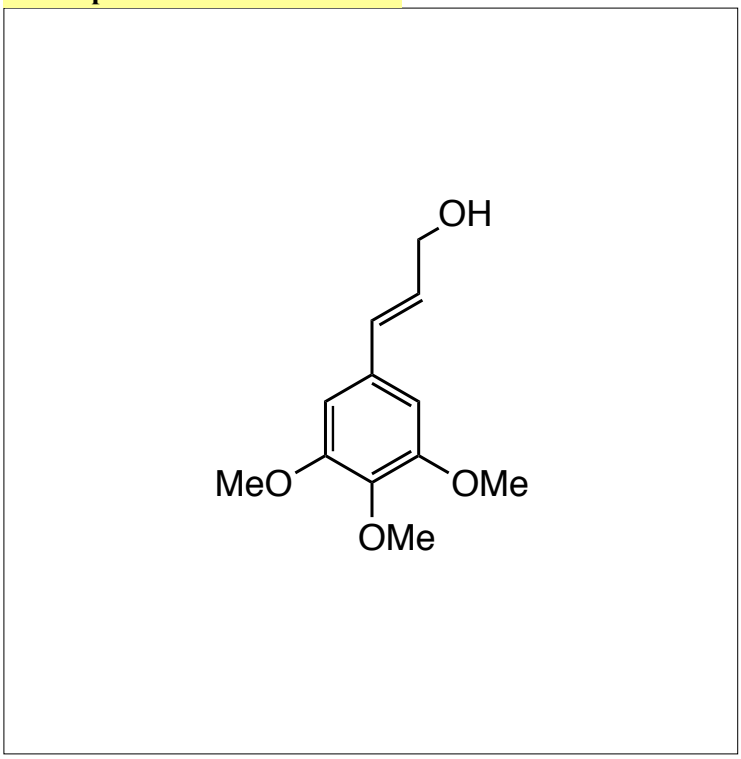
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.99	56.34	55.70
OMe	56.09	56.40	55.84
B2	110.07	111.95	111.79
A2	110.50	112.05	111.57
A5	113.71	115.36	114.92
B5	114.85	116.14	115.60
β	119.25	119.87	118.71
6	123.13	124.15	123.55
6	123.49	124.21	123.70
B1	127.62	128.33	126.51
A1	131.22	131.84	129.85
γ	144.33	144.36	143.60
A3	146.79	148.54	147.78
B3	146.85	148.74	147.96
B4	148.12	150.10	149.41
A4	150.21	152.17	151.66
α	188.62	187.90	187.02
1H DMSO			
OMe	3.87		
B5	6.83		
A5	6.97		
B2	7.49		
B6	7.28		
β	7.76		
A2	7.61		
A6	7.80		
γ	7.63		

Notes:

FPL collection
A2 and B2 change order in DMSO
1H DMSO chemical shifts in ( )'s
13C C6 shift assignments not confirmed, also C5s in CDCl3

Compound Number 302



3,4,5-trimethoxy cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
4 OMe	3.69	s	
3,5 OMe	3.82	s	
OH	3.89	t	5.4
γ	4.21	dt	1.5, 5.4
β	6.32	dt	15.9, 5.2
α	6.53	bt	15.9, 1.5
2,6	6.72	s	
DMSO			
4 OMe	3.64		
3,5 OMe	3.78		
γ	4.10		
β	6.33		
α	6.47		
2,6	6.72		
CDCl3			
4 OMe	3.81		
3,5 OMe	3.83		
γ	4.28		
β	6.24		
α	6.50		
2,6	6.72		

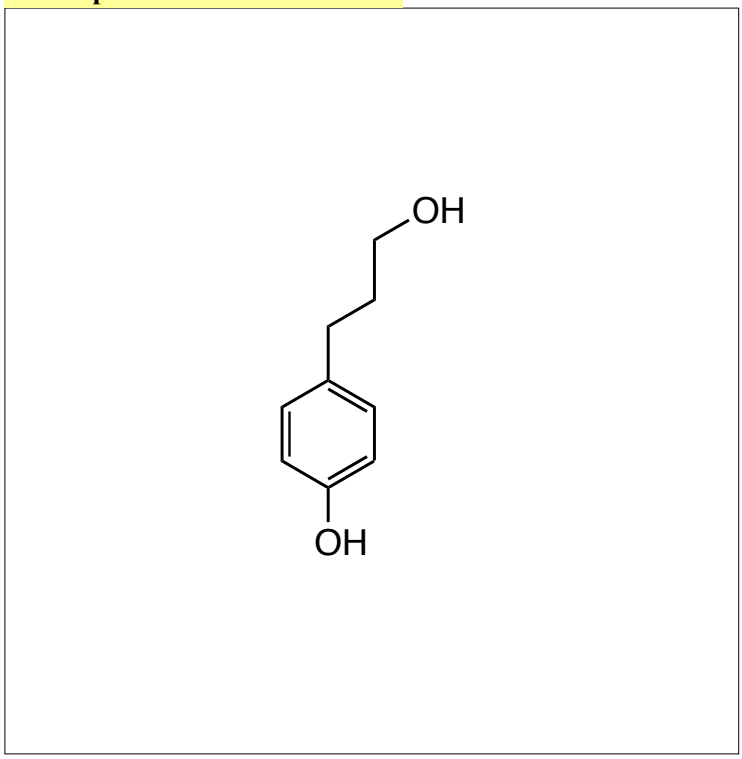
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
3 OMe	55.99	56.33	55.78
5 OMe	55.99	56.33	55.78
4 OMe	60.85	60.53	59.99
γ	63.47	63.17	61.43
2	103.47	104.55	103.43
6	103.47	104.55	103.43
α	128.04	130.11	128.55
β	130.92	130.32	130.16
1	132.40	133.87	132.65
4	137.78	138.76	136.83
3	153.22	154.41	152.94
5	153.22	154.41	152.94

Notes:

S. Ralph
FPL collection

Compound Number 303



dihydro-coumaryl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.75	m	6.3
α	2.57	bdd	7.5
γ	3.53	m (+OH?)	
3,5	6.73	d	8.4
2,6	7.01	d	8.4
Ph-OH	8.05	s	
CDCl3			
β	1.84	m	
α	2.61	dd	7.6
γ	3.65	t	6.5
3,5	6.72	d	8.4
2,6	7.03	d	8.4
Ph-OH			
DMSO	1.63		
β	2.48	m	
α	3.36	m(+DMSO)	
γ	4.39	m	
γ-OH	6.63	t	5.1
3,5	6.94	d	8.3
2,6	9.06	d	8.3
Ph-OH		s	

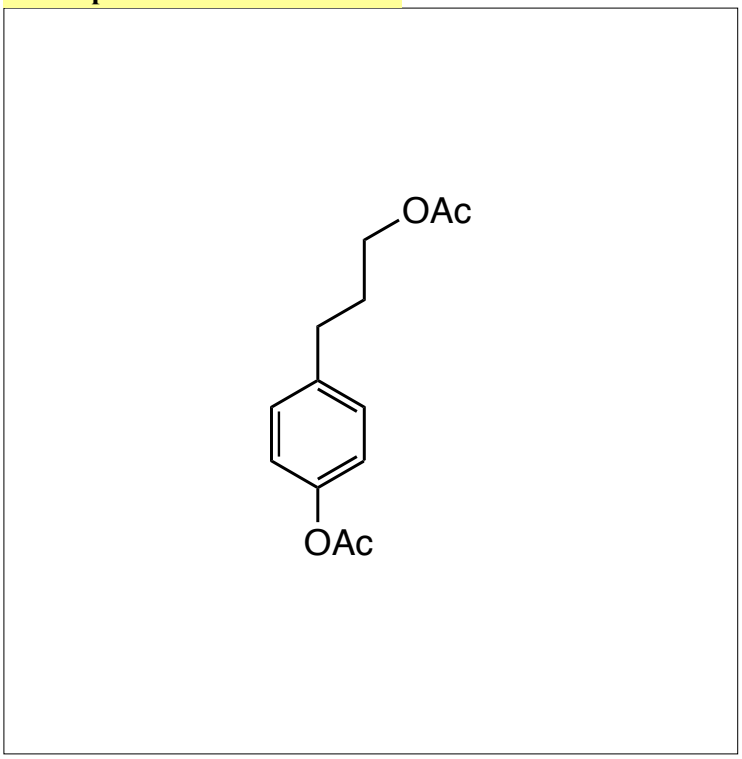
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
α	31.11	31.90	30.76
β	34.35	35.85	34.65
γ	62.30	61.76	60.12
3,5	115.22	115.88	114.98
3,5	115.22	115.88	114.98
2,6	129.47	130.08	129.06
2,6	129.47	130.08	129.06
1	133.82	133.89	132.16
4	153.72	156.23	155.18

Notes:

S.Ralph 35mg
Pearl Collection

Compound Number 304



Dihydrocoumaryl alcohol diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ AcMe	1.98	s	
4 AcMe	2.22	s	
β	1.92	m	
α	2.69	dd	7.8
γ	4.04	t	6.6
3,5	7.02	d	8.4
2,6	7.24	d	8.4
CDCl3			
γ AcMe	2.03	s	
4 AcMe	2.26	s	
β	1.92	m	
α	2.66	dd	7.8
γ	4.07	t	6.6
3,5	6.98	d	8.4
2,6	7.16	d	8.4
DMSO			
γ AcMe	1.99	s	
4 AcMe	2.24	s	
β	1.86	m	
α	2.62	dd	7.6
γ	3.99	t	6.6
3,5	7.02	d	8.4
2,6	7.22	d	8.4

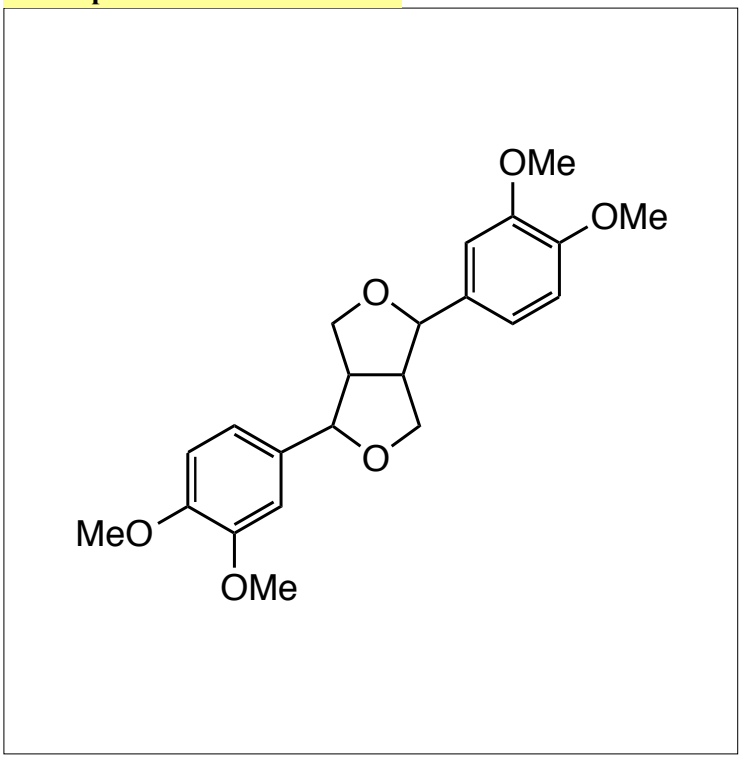
Notes:

S.Ralph 35mg
Acetylated cmpd from
Pearl Collection

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ AcMe	20.89	20.77	20.65
4 AcMe	21.05	20.95	20.79
β	30.09	31.10	29.68
α	31.54	32.06	30.77
γ	63.66	64.03	63.14
3,5	121.40	122.46	121.57
3,5	121.40	122.46	121.57
2,6	129.23	130.01	129.17
2,6	129.23	130.01	129.17
1	138.71	139.76	138.63
4	148.84	150.15	148.61
4 AcC=O	169.55	169.70	169.24
γ AcC=O	171.05	170.98	170.38

Compound Number 305



Veratrylresinol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.08	m	
OMe	3.78	s	
OMe	3.80	s	
γ1	3.82	dd	3.5, 9.0
γ2	4.20	dd	6.9, 8.9
α	4.69	d	4.2
5	6.90	bs	
6	6.90	bs	
2	6.98	bs	
CDCl3			
β	3.10		
OMe	3.86		
OMe	3.88		
γ1	3.87		
γ2	4.24		
α	4.74	d	4.5
5	6.82	d	8.2
6	6.86	dd	1.8, 8.2
2	6.89	d	1.8

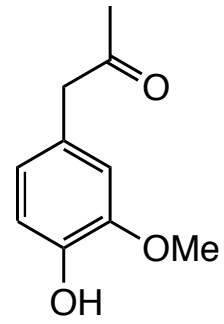
Notes:

FPL Rowe Collection 9mg
As this compound has a plane of symmetry the chemical shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
β	54.14	55.25	53.64
OMe	55.90	56.07	55.44
OMe	55.93	56.13	55.52
γ	71.70	72.28	70.96
α	85.77	86.47	84.92
2	109.19	110.97	109.87
5	111.00	112.61	111.56
6	118.22	119.06	118.14
1	133.51	135.38	133.82
4	148.60	149.79	148.17
3	149.17	150.43	148.73
DMSO			
β			3.03
OMe			3.72
OMe			3.74
γ1			3.76
γ2			4.13
α			4.65
6			6.87
5			6.90
2			6.92

Compound Number 306



4-hydroxy-3-methoxyphenylacetone
Hibbert's Ketone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	2.07	s	
α	3.60	s	
OMe	3.81	s	
6	6.66	dd	2.0, 8.1
5	6.76	d	8.0
2	6.81	d	2.0
CDCl3			
γ	2.12	s	
α	3.59	s	
OMe	3.84	s	
6	6.66	m	
2	6.67	m	
5	6.85	d	7.7
DMSO			
γ	2.05	s	
α	3.57	s	
OMe	3.84	s	
6	6.55	dd	1.8, 8.0
5	6.69	d	8.0
2	6.72	d	1.8

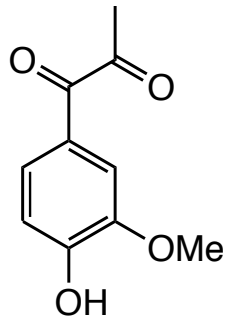
Notes:

Sigma-Aldrich CAS# 2503-46-0
24mg
1H CS of 2,5 and 6 change order in CDCl3, checked by HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	28.98	28.93	29.18	
α	50.61	50.57	49.48	
OMe	55.85	56.20	55.65	
2	111.62	113.78	113.69	
5	114.54	115.79	115.47	
6	122.23	122.86	121.93	
1	125.95	127.19	125.73	
4	144.72	146.37	145.32	
3	146.64	148.31	147.54	
β	207.08	206.27	206.82	

Compound Number 307



G-1,2-diketo-propane
Hibbert's Ketone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	2.45	s	
OMe	3.90	s	
5	6.95	d	8.1
6	7.52	dd	1.7, 8.2
2	7.53	d	1.7
CDCl3			
γ	2.48		
OMe	3.93		
5	6.95	d	8.3
2	7.55	d	1.8
6	7.58	dd	1.8, 8.4
DMSO			
γ	2.44		
OMe	3.82		
5	6.91	d	8.7
2	7.42	m	obs.
6	7.43	m	obs.

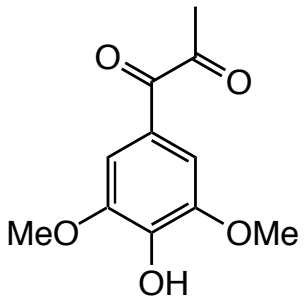
Notes:

FPL Collection
10mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
γ	29.90	26.62	26.54
OMe	56.32	56.14	55.67
2	112.54	111.03	111.91
5	115.78	114.33	115.30
1	124.88	124.43	122.83
6	127.12	126.88	126.31
3	148.76	146.88	148.05
4	154.03	152.00	153.65
α	191.60	190.20	190.92
β	202.30	201.18	202.28

Compound Number 308



S-diketo-propane
Hibbert's Ketone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	2.46	s	
OMe	3.87	s	
2,6	7.29	s	
CDCl3			
γ	2.49	s	
OMe	3.92	s	
4-OH	6.15		
2,6	7.31	s	
DMSO			
γ	2.46	s	
OMe	3.81	s	
2,6	7.18	s	

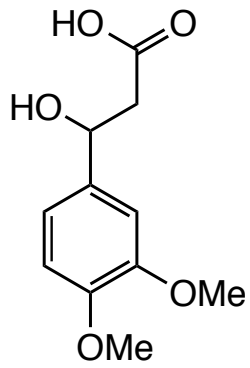
Notes:

FPL Collection
11 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	26.68	26.58	26.58	
OMe	56.40	56.73	56.16	
2,6	107.56	108.75	107.81	
1	122.99	123.24	121.30	
4	141.33	143.74	142.94	
3,5	147.00	148.70	147.82	
α	189.78	191.54	190.84	
β	201.07	202.26	202.11	

Compound Number 309



^{1}H (acetone)

Atom	H Shifts	Mult	J
β	2.	m	
OMe	3.77	s	
OMe	3.80	s	
α	5.05	dd	5.0, 8.6
5	6.87	d	8.2
6	6.92	dd	1.8, 8.2
2	7.04	d	1.8
CDCl3			
β	2.72, 2.82	dq	3.6, 16.4, 9.4, 16.4
OMe	3.84	s	
OMe	3.86	s	
α	5.08	dd	3.5, 9.5
5	6.81	d	8.2
6	6.87	dd	1.7, 8.3
2	6.91	d	1.7
DMSO			
β	2.50	d	7.0
OMe	3.71	s	
OMe	3.73	s	
α	4.87	t	6.9
6	6.83	dd	1.7, 8.2
5	6.86	d	8.2
2	6.97	d	1.7

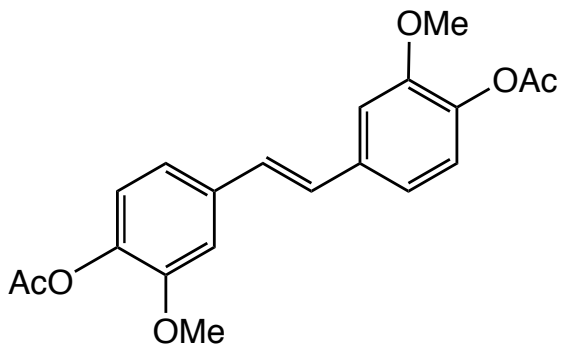
Notes:

FPL Collection
14 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
β	43.11	44.71	44.74
4 OMe	55.85	56.00	55.43
3 OMe	55.90	56.11	55.59
α	70.08	70.77	69.39
2	108.82	110.69	109.68
5	111.06	112.50	111.50
6	117.91	118.72	117.77
1	134.72	138.07	137.63
4	148.72	149.58	147.84
3	149.11	150.24	148.55
γ	177.12	172.91	172.43

Compound Number 310



3,3'-Dimethoxy-4,4'-diacetoxyphenyl-stilbene

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.23	s	
OMe	3.87	s	
2	7.33	d	1.8
6	7.15	dd	1.8, 8.2
5	7.03	d	8.2
α	7.24	s	
CDCl3			
Ac Me	2.30	s	
OMe	3.87	s	
2	7.07	bs	
6	7.06	dd	1.8, - 8.0
5	7.00	d	
α	6.99	s	
DMSO			
Ac Me	2.25	s	
OMe	3.83	s	
2	7.25	d	1.6
6	7.16	dd	1.6, 8.2
5	7.07	d	8.2
α	7.26	s	

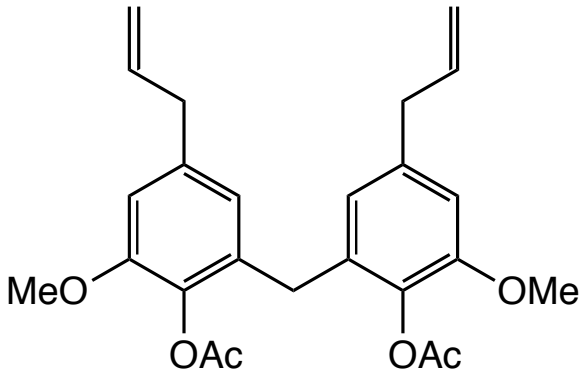
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.66	20.49	20.46	
OMe	55.86	56.29	55.83	
2	110.06	111.02	110.25	
6	119.22	119.92	119.15	
5	122.94	123.85	123.07	
α	128.32	129.09	128.16	
1	136.17	137.23	136.07	
4	139.35	140.59	138.91	
3	151.18	152.50	151.07	
Ac C=O	169.06	169.00	168.66	

Notes:

FPL Collection 13mg
As this compound has a plane of symmetry the chemical shifts for the other half are identical.
1H CDCl3 aryl proton CS from HSQC

Compound Number 311



4,4'-diacetoxy-1,1'-diallyl-3,3'-dimethoxy-5,5'diphenyl methane

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.20	s	
α	3.30	d	6.8
CH2	3.68	s	
OMe	3.76	s	
γ1	5.01	dd	1.7, 10.0
γ2	5.07	dd	1.7, 17.0
β1	5.91	dt	6.8
β2	5.97	dt	6.8
6	6.58	d	1.7
2	6.78	d	1.7
DMSO			
Ac Me	2.18	s	
α	3.27	d	6.7
5 CH2	3.58	s	
OMe	3.70	s	
γ1	5.02	d	10.4
γ2	5.06	d	17.1
β1	5.88	dt	6.8
β2	5.94	dt	7.0
6	6.54	s	
2	6.78	s	

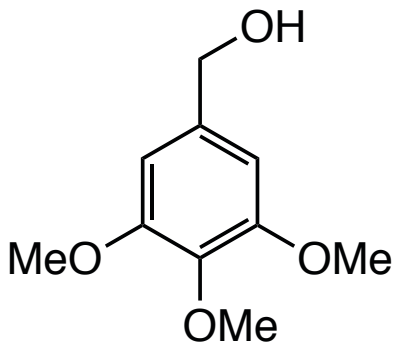
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.34	20.41	20.24
5 CH2	30.15	30.87	30.04
α	40.01	40.60	39.40
OMe	55.78	56.17	55.78
2	110.25	111.56	110.91
γ	115.92	116.06	116.06
6	122.16	122.82	121.78
5	132.54	133.75	32.47
4	136.39	137.67	136.08
β	137.02	138.34	137.38
1	138.14	138.88	137.83
3	150.85	152.20	150.79
Ac C=O	168.74	168.73	168.22
CDCl3			
Ac Me	2.23		
α	3.28		
CH2	3.69		
OMe	3.77		
γ1	5.04		
γ2	5.05		
β1	5.90		
β2	5.90		
6	6.51		
2	6.64		

Notes:

FPL Pew Collection 20mg
As this compound has a plane of symmetry the chemical shifts for the other half are identical.
alpha, beta, 1, 3, 4 confirmed by HSQC and HMBC

Compound Number 312



3,4,5-Trimethoxybenzyl alcohol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
4-OMe	3.789	s	
3,5-OMe	3.809	s	
α	4.57	s	
2,6	6.55	s	
<u>acetone</u>			
4-OMe	3.69	s	
3,5-OMe	3.79	s	
α	4.55	s	
2,6	6.65	s	
<u>DMSO</u>			
4-OMe	3.62	s	
3,5-OMe	3.75	s	
α	4.42	d	J = 5.9
2,6	6.61	s	
α OH	5.15	t	J = 5.9

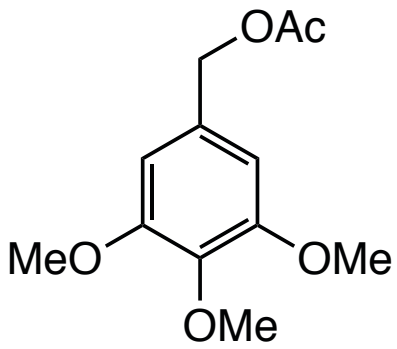
Notes:

Aldrich
CAS# 3840-31-1
24mg
C1 and C4 change order in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3 OMe	55.96	56.27	55.73	
5 OMe	55.96	56.27	55.73	
4 OMe	60.75	60.45	59.98	
α	65.30	64.75	63.01	
2	103.66	104.54	103.44	
6	103.66	104.54	103.44	
4	137.09	137.97	136.08	
1	136.67	139.00	138.30	
3	153.21	154.23	152.72	
5	153.21	154.23	152.72	

Compound Number 313



3,4,5-Trimethoxybenzyl alcohol Acetate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.06	s	
4-OMe	3.79	s	
3,5-OMe	3.81	s	
α	4.98	s	
2,6	6.54	s	
<u>acetone</u>			
Ac Me	2.04	s	
4-OMe	3.71	s	
3,5-OMe	3.18	s	
α	5.00	s	
2,6	6.69	s	
<u>DMSO</u>			
Ac Me	2.05	s	
4-OMe	3.64	s	
3,5-OMe	3.76	s	
α	4.98	s	
2,6	6.68	s	

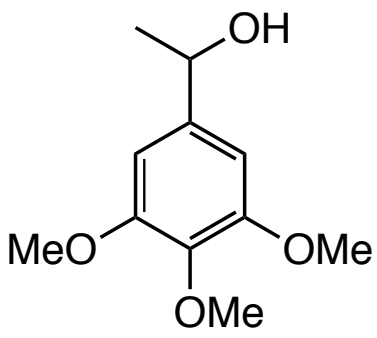
Notes:

S. Ralph
12mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.88	20.82	20.71	
3 OMe	55.95	56.40	55.85	
5 OMe	55.95	56.40	55.85	
4 OMe	60.63	60.48	59.98	
α	66.43	66.67	65.72	
2	105.42	106.56	105.62	
6	105.42	106.56	105.62	
1	131.30	132.89	131.69	
4	137.80	139.03	137.28	
3	153.15	154.36	152.89	
5	153.15	154.36	152.89	
Ac C=O	170.70	170.86	170.30	

Compound Number 314



3,4,5-Trimethoxyphenyl ethanol

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	1.45	d	J = 6.5
4-OMe	3.79	s	
3,5-OMe	3.83	s	
α	4.79	q	J = 6.5
2,6	6.56	s	
<u>acetone</u>			
β	1.37	d	J = 6.4
4-OMe	3.68	s	
3,5-OMe	3.80	s	
α	4.76	m	
2,6	6.68	s	
α OH	4.10	d	J = 4.2
<u>DMSO</u>			
β	1.29	d	J = 6.5
4-OMe	3.61	s	
3,5-OMe	3.75	s	
α	4.63	m	
2,6	6.62	s	
α OH	5.11	d	J = 4.2

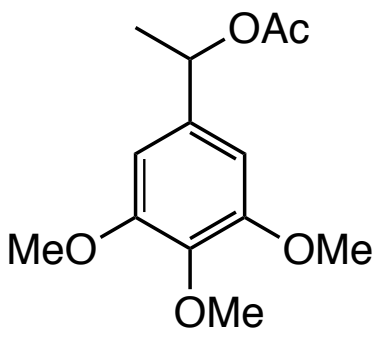
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
β	25.16	26.31	25.98
3 OMe	56.01	56.29	55.74
5 OMe	56.01	56.29	55.74
4 OMe	60.75	60.41	59.95
α	70.48	70.08	68.23
2	102.16	103.47	102.41
6	102.16	103.47	102.41
4	136.99	137.88	135.96
1	141.68	144.01	143.25
3	153.18	154.15	102.41
5	153.18	154.15	102.41

Notes:

Aldrich
CAS# 37785-48-1,
20mg
Assignments of C1 and C4 confirmed by HMBC in CDCl3

Compound Number 315



3,4,5-Trimethoxyphenyl ethanol Acetate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	1.48	d	J = 6.7
Ac Me	2.04	s	
4-OMe	3.79	s	
3,5-OMe	3.80	s	
α	5.77	q	J = 6.7
2,6	6.57	s	
acetone			
β	1.47	d	J = 6.6
Ac Me	2.02	s	
4-OMe	3.70	s	
3,5-OMe	3.82	s	
α	3.82	q	J = 6.6
2,6	6.68	s	
DMSO			
β	1.45	d	J = 6.5
Ac Me	2.03	s	
4-OMe	3.63	s	
3,5-OMe	3.77	s	
α	5.71	q	J = 6.5
2,6	6.64	s	

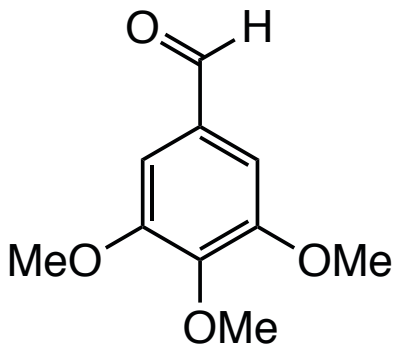
Notes:

S Ralph
45mg
C1 and C4 are coincident in d6-acetone
C and C4 switch order in $CDCl_3$ and DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	21.27	21.15	21.01
β	22.09	22.59	22.09
3 OMe	56.00	56.40	55.86
5 OMe	56.00	56.40	55.86
4 OMe	60.67	60.44	59.92
α	72.35	72.74	71.76
2	103.14	104.28	103.20
6	103.14	104.28	103.20
4	137.48	138.67	136.89
1	137.20	138.67	137.48
3	153.15	154.34	152.86
5	153.15	154.34	152.86
Ac C=O	170.18	170.21	169.66

Compound Number 316



3,4,5-Trimethoxybenzaldehyde

^{1}H (chloroform)

Atom	H Shifts	Mult	J
4-OMe	3.90	s	
3,5-OMe	3.896	s	
2,6	7.09	s	
α	9.83	s	
acetone			
4-OMe	3.82	s	
3,5-OMe	3.91	s	
2,6	7.23	s	
α	9.88	s	
DMSO			
4-OMe	3.76	s	
3,5-OMe	3.85	s	
2,6	7.24	s	
α	9.87	s	

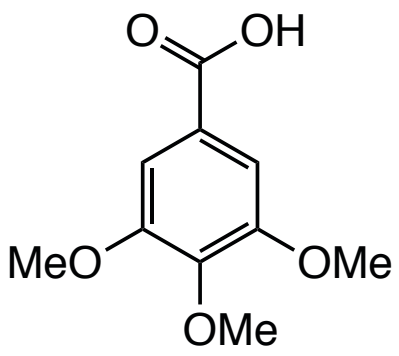
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3 OMe	56.51	56.58	56.51	
5 OMe	56.51	56.58	56.51	
4 OMe	60.67	60.70	60.67	
2	107.19	107.51	107.19	
6	107.19	107.51	107.19	
1	132.12	133.08	132.12	
4	143.29	144.50	143.29	
3	153.80	154.83	153.80	
5	153.80	154.83	153.80	
α	192.35	191.71	192.35	

Notes:

Aldrich
3,4,5-Trimethoxybenzaldehyde
CAS# 86-81-7
19mg,

Compound Number 317



3,4,5-Trimethoxybenzoic acid

^{1}H (chloroform)

Atom	H Shifts	Mult	J
3,5 OMe	3.90	s	
4 OMe	3.94	s	
2,6	7.36	s	
OH	11.12	bs	
<u>acetone</u>			
4-OMe	3.79	s	
3,5-OMe	3.88	s	
2,6	7.31	s	
<u>DMSO</u>			
4-OMe	3.71	s	
3,5-OMe	3.81	s	
2,6	7.22	s	

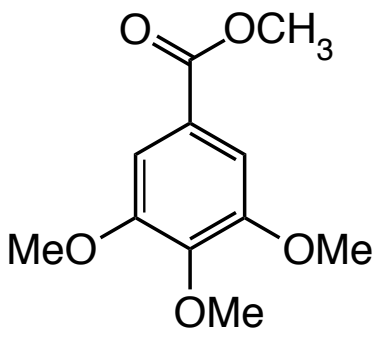
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3 OMe	56.21	56.48	55.94	
5 OMe	56.21	56.48	55.94	
4 OMe	60.92	60.62	60.13	
2	107.38	107.89	106.57	
6	107.38	107.89	106.57	
1	124.08	126.34	125.94	
4	142.95	143.35	141.39	
3	152.93	154.12	152.68	
5	152.93	154.12	152.68	
α	171.81	167.29	166.96	

Notes:

Aldrich
CAS# 118-41-2
16mg,
C1 and C4 assignments confirmed by HMBC in $CDCl_3$

Compound Number 318



Methyl 3,4,5-Trimethoxybenzoate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Me	2.55	s	
4 OMe	3.88	s	
3,5 OMe	3.89	s	
2,6	7.18	s	
acetone			
Me	2.55	s	
4 OMe	3.79	s	
3,5 OMe	3.88	s	
2,6	7.28	s	
DMSO			
Me	2.56	s	
4 OMe	3.73	s	
3,5 OMe	3.84	s	
2,6	7.23	s	

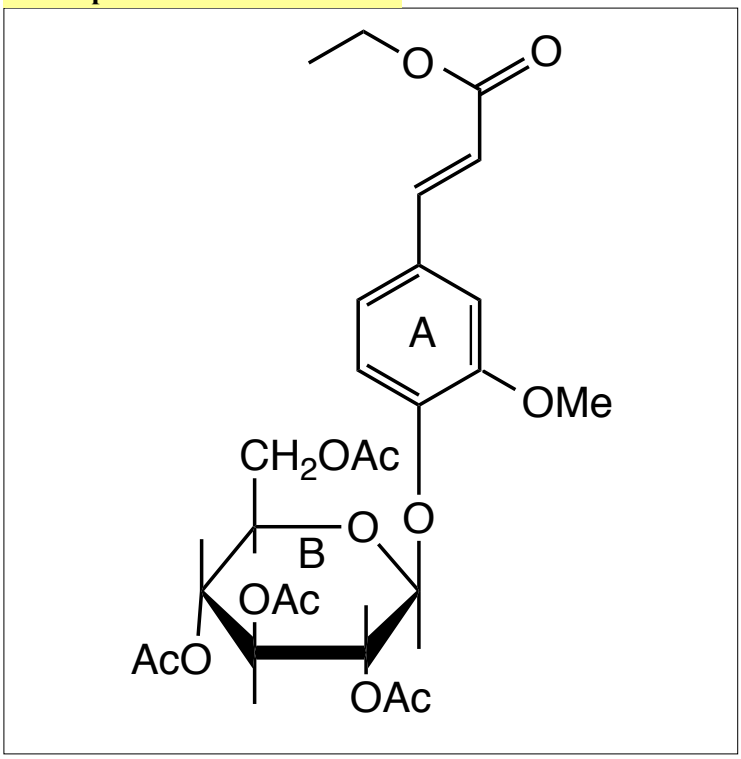
Notes:

S Ralph
CAS# 1916-07-0
18mg,

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
ester Me	26.38	26.56	26.61	
3 OMe	56.24	56.53	56.03	
5 OMe	56.24	56.53	56.03	
4 OMe	60.88	60.63	60.14	
2	105.78	106.74	105.76	
6	105.78	106.74	105.76	
1	132.39	133.51	132.22	
4	142.57	143.52	141.85	
3	152.98	154.17	152.73	
5	152.98	154.17	152.73	
α	196.83	196.81	196.87	

Compound Number 319



acetylated *p*-gluco-ethylferulate

^{1}H (DMSO)

Atom	H Shifts	Mult	J
CH3	1.25	t	7.2
B2 Ac Me	1.96	s	
B4 Ac Me	1.99	s	
B3 Ac Me	2.00	s	
B6 AcMe	2.01	s	
OMe	3.79	s	
B6 H1	4.07		
CH2	4.17		
B6 H2	4.20		
B5	4.20		
B4	4.99	dd	9.5
B2	5.06	dd	9.5, 8.0
B3	5.38	dd	9.5
B1	5.45	d	8.0
β	6.62	d	16
A5	7.10	d	8.5
A6	7.27	dd	1.7, 8.5
A2	7.42	d	1.7
α	7.59	d	16

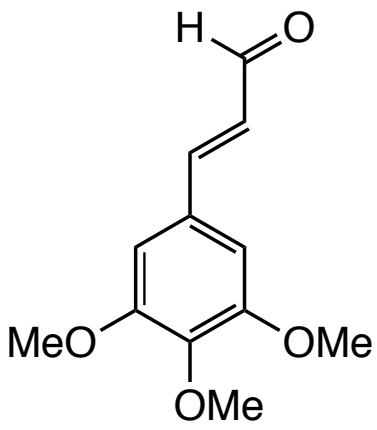
Notes:

SRV-67
!H in DMSO, almost first order. B6 and CH2 CS from HSQC
B1 is the anomeric carbon.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
CH3	14.30	14.61	14.18
B3 Ac Me	20.57	20.53	20.26
B4 Ac Me	20.60	20.59	20.29
B2 Ac Me	20.60	20.59	20.35
B6 Ac Me	20.67	20.63	20.46
OMe	56.02	56.57	56.03
CH2	60.50	60.68	59.89
B6	61.87	62.72	61.59
B4	68.30	69.32	68.02
B3	71.08	71.93	70.61
B5	72.07	72.70	70.87
B2	72.47	73.22	71.82
B1	100.27	100.39	98.14
A2	111.34	112.55	111.93
β	117.59	118.22	117.18
A5	119.48	119.24	117.30
A6	121.59	122.71	122.04
A1	130.98	131.48	129.88
α	143.89	144.72	144.01
A4	147.72	149.09	147.48
A3	150.70	151.55	149.80
γ	166.90	167.12	166.32
B2 Ac C=O	169.28	169.63	168.95
B4 Ac C=O	169.37	170.04	169.29
B3 Ac C=O	170.23	170.29	169.56
B6 Ac C=O	170.53	170.65	169.95
1H			
CH3	1.31	1.27	
B2 Ac Me	2.01	1.97	
B4 Ac Me	2.01	2.01	
B3 Ac Me	2.04	2.02	
B6 AcMe	2.05	2.02	
OMe	3.82	3.89	
B6 H1	4.15	4.16	
CH2	4.23	4.18	
B6 H2	4.25	4.28	
B5	3.77	4.15	
B4	5.14	5.12	
B2	5.26	5.21	
B3	5.26	5.36	
B1	4.98	5.34	
β	6.31	6.47	
A5	7.05	7.22	
A6	7.05	7.22	
A2	7.05	7.39	
α	7.59	7.60	

Compound Number 320



3,4,5-Trimethoxy-cinnamaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
4 OMe	3.78	s	
3,5 OMe	3.89	s	
β	6.74	dd	7.75, 16.0
2,6	7.07	s	
α	7.58	d	16.0
γ	9.66	d	7.75
1CDCl3			
4 OMe	3.88		
3,5 OMe	3.88		
β	6.61		
2,6	6.77		
α	7.37		
γ	9.66		
1DMSO			
4 OMe	3.70		
3,5 OMe	3.82		
β	6.88		
2,6	7.08		
α	7.63		
γ	9.63		

Notes:

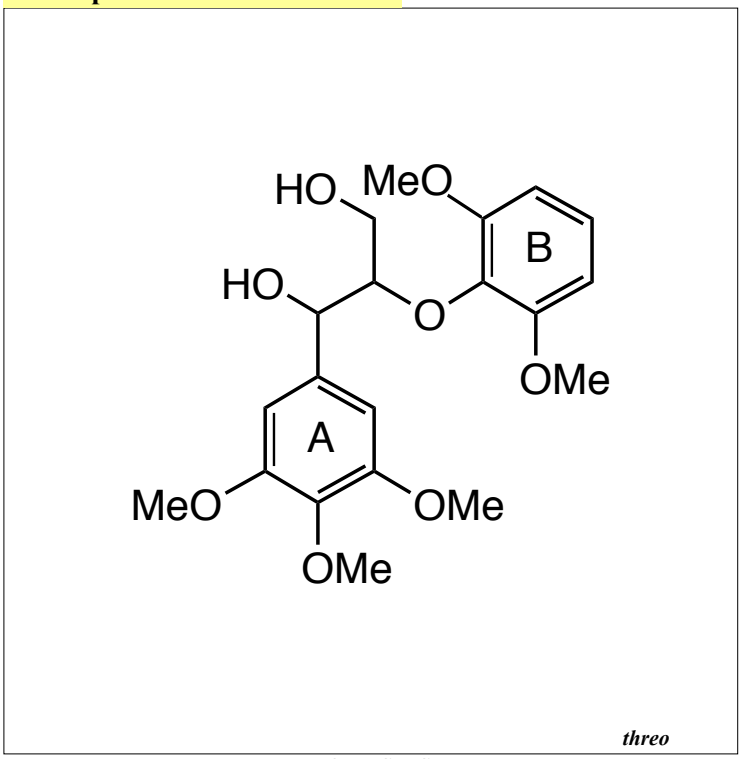
SRXIV-35B 8mg

Note: in DMSO and DMSO/Pyr C3,5 and α change order

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
3 OMe	56.19	56.55	56.12	56.00
5 OMe	56.19	56.55	56.12	56.00
4 OMe	61.00	60.66	60.20	60.11
2	105.68	107.05	106.38	106.33
6	105.68	107.05	106.38	106.33
β	127.94	128.92	128.11	128.08
1	129.42	130.78	129.72	140.27
4	140.94	141.86	140.15	129.73
α	152.70	153.67	153.57	153.38
3	153.53	154.69	153.21	153.26
5	153.53	154.69	153.21	153.26
γ	193.41	193.94	194.37	194.12
1H				
4 OMe				3.72
3,5 OMe				3.82
β				6.94
2,6				7.10
α				7.62
γ				9.69

Compound Number 321



threo

4-OMe-S-b-S

^{1}H (chloroform)

Atom	H Shifts	Mult	J
4 OMe	3.80 3.79	s	
A 3,5 OMe	3.82-3.88	s	
B 3,5 OMe	3.82-3.88	s	
γ	3.33, 3.59 3.46, 3.89	dd ddd	2.0, 12.7+2.6, 12.7 4.0 2.4, 11.9+m
α	5.02 4.99	d d	8.6 3.6
β	3.88 4.11	m obsd	
A 2,6	6.68 6.55	s	
B 2,6	6.61 6.63	d	8.5 8.5
B1	7.04 7.06	t t	8.5 8.5

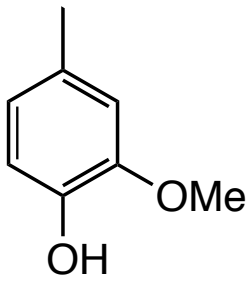
Notes:

J. Obst FPL Collection
Threo is major isomer ~70/30
IH data as threo-erythro pair
some shifts taken from HSQC
500MHz HSQC and HMBC all solvents

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A 3,5 OMe	56.10	56.32	55.74	55.64
B 3,5 OMe	56.10	56.34	55.93	55.84
A4 OMe	60.76	60.43	59.96	59.90
γ	60.45	61.49	60.16	60.27
α	74.31	74.03	71.37	71.56
β	88.75	89.12	86.41	86.61
A 2,6	104.19	105.20	103.80	103.89
B 2,6	105.26	106.45	105.67	105.62
B1	124.51	124.90	123.49	123.45
B4	135.18	137.07	136.06	136.15
A1	135.64	137.99	138.07	136.27
A4	137.54	138.36	136.15	138.07
A 3,5	153.13	153.95	152.21	152.28
B 3,5	153.17	154.11	152.85	152.88
erythro isomer				
A 3,5 OMe	56.08	56.35	55.74	55.64
B 3,5 OMe	56.08	56.54	55.95	55.86
A4 OMe	60.79	60.47	59.96	59.90
γ	60.54	60.90	59.83	59.90
α	72.62	73.58	72.42	72.44
β	86.98	87.74	85.97	86.05
A 2,6	102.69	104.75	104.11	104.16
B 2,6	105.22	106.57	105.72	105.68
B1	124.51	124.90	123.37	123.45
B4	134.86	136.70	135.71	135.72
A1	134.96	138.07	138.30	138.35
A4	137.06	138.15	136.28	136.37
A 3,5	153.50	154.03	152.33	152.39
B 3,5	153.20	154.43	152.91	152.97
1H				
4 OMe	3.80 3.79	3.68 3.69	3.62	3.64
A 3,5 OMe	3.82-3.88	3.79 3.80	3.73 3.74	3.71
B 3,5 OMe	3.82-3.88	3.87 3.84	3.70 3.73	3.70
γ	3.33, 3.59 3.46, 3.89	3.35, 3.68 3.44, 3.85	3.26, 3.65 3.43, 3.72	3.38, 3.77 3.55, 3.85
α	5.02 4.99	5.01 5.01	4.87 4.84	5.01 4.97
β	3.88 4.11	4.01 4.18	4.10 4.15	4.20 4.26
A 2,6	6.68 6.55	6.78 6.73	6.72 6.65	6.80 6.73
B 2,6	6.61 6.63	6.70 6.70	6.63-6.65 6.63-6.65	6.63 6.63
B1	7.04 7.06	7.02	6.92-6.97	6.94

Compound Number 322



4-methyl-guaiacol

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	2.22	s	
OMe	3.79	s	
2	6.59	dd	1.7, 8.0
5	6.69	d	8.0
6	6.75	d	1.7
OH	7.22	s	

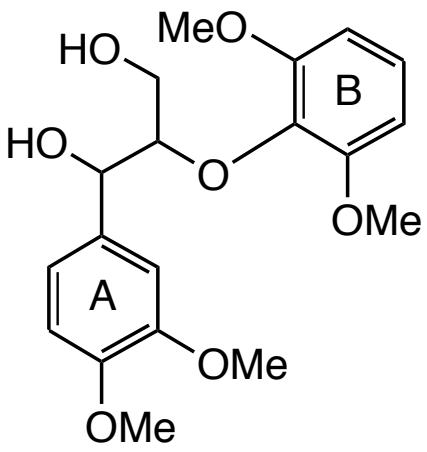
Notes:

FPL Collection
re-distilled
HSQC and HMBC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	20.96	20.96	20.63	20.52
OMe	55.75	56.13	55.55	55.48
2	111.65	113.35	113.19	113.15
5	114.10	115.56	115.40	115.48
6	121.43	122.08	121.08	121.12
1	129.55	129.52	128.04	128.04
4	143.24	145.20	144.29	144.48
3	146.23	148.07	147.47	147.53
1H				
α	2.29		2.19	2.18
OMe	3.81		3.73	3.73
2	6.61		6.54	6.57
5	6.72		6.67	6.73
6	6.77		6.71	6.77
OH			8.62	8.99

Compound Number 323



threo

V-b-S

^{1}H (acetone)

Atom	H Shifts	Mult	J
threo			
A3,4 OMe	3.77		
B2,6 OMe	3.87	s	
α	5.03		
β	3.94		
γ1	3.29		
γ2	3.65		
B2,6	6.71	d	8.4
A5	6.87	d	8.2
A6	6.99	dd	1.8, 8.3
A2	7.08	d	1.8
B1	7.03	dt	8.4

Notes:

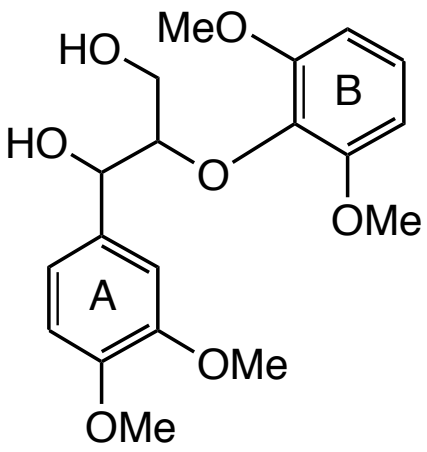
FPL Collection
S. Ralph

see 324 for erythro shifts

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
threo				
OMe	55.68	56.00	56.36	
OMe	55.68	56.06	55.51	
B 2 OMe	55.93	56.52	55.92	
B 6 OMe	55.93	56.52	55.92	
γ	60.23	61.26	60.13	
α	73.79	73.91	71.32	
β	88.76	89.60	86.92	
B2	105.11	106.41	105.69	
B6	105.11	106.41	105.69	
A2	110.06	111.83	110.61	
A5	110.80	112.23	111.14	
A6	119.63	120.28	118.87	
B1	124.32	124.90	123.43	
A1	132.45	134.82	134.65	
B4	135.09	137.01	136.20	
A4	148.51	149.66	147.65	
A3	148.70	149.93	148.06	
B3	153.01	154.11	152.83	
B5	153.01	154.11	152.83	
1 H				
threo				
A3,4 OMe	3.79-3.84		3.70-3.71	
B2,6 OMe	3.79-3.84		3.73	
α	5.02		4.89	
β	3.84		4.01	
γ1	3.25		3.19	
γ2	3.53		3.62	
B2,6	6.57		6.64	
A5	6.78		6.86	
A6	6.96		6.92	
A2	6.96		7.02	
B1	7.00		6.96	

Compound Number 324



erythro

V-b-S*e*

^{1}H (acetone)

Atom	H Shifts	Mult	J
erythro			
A3,4 OMe	3.77		
B2,6 OMe	3.83	s	
α	5.01		
β	4.18		
γ1	3.44		
γ2	3.86		
B2,6	6.70	d	8.4
A5	6.87	d	8.3
A6	6.91	dd	1.7, 8.3
A2	7.06	d	1.7
B1	7.03	dt	8.4

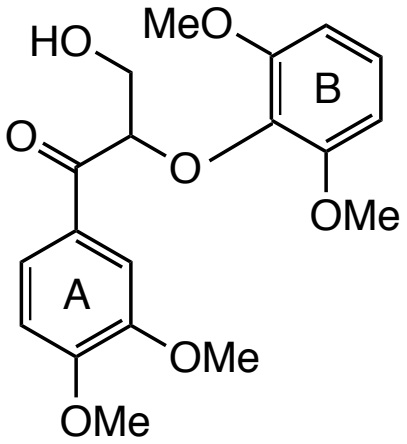
Notes:

FPL Collection
S. Ralph
see 323 for threo shifts

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
erythro				
OMe	55.70	56.04	56.36	
OMe	55.70	56.10	55.53	
B 2 OMe	55.93	56.50	55.92	
B 6 OMe	55.93	56.50	55.92	
γ	60.36	60.85	59.69	
α	72.23	73.20	71.94	
β	86.76	87.71	86.01	
B2	105.11	106.48	105.72	
B6	105.11	106.48	105.72	
A2	108.86	111.29	110.61	
A5	110.80	112.31	111.19	
A6	117.97	119.60	119.12	
B1	124.28	124.80	123.37	
A1	131.94	134.97	134.98	
B4	134.76	136.57	135.60	
A4	147.99	149.36	147.69	
A3	148.75	149.98	148.19	
B3	153.31	154.40	152.94	
B5	153.31	154.40	152.94	
1 H				
threo				
A3,4 OMe	3.79-3.84		3.70-3.71	
B2,6 OMe	3.79-3.84		3.73	
α	4.97		4.83	
β	4.11		4.12	
γ1	3.45		3.38	
γ2	3.86		3.70	
B2,6	6.58		6.64	
A5	6.78		6.86	
A6	6.79		6.86	
A2	6.91		6.96	
B1	7.00		6.96	

Compound Number 325



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe	56.02	56.10	55.45	55.38
A4 OMe	56.05	56.17	55.71	55.63
B 3,5 OMe	55.93	56.34	55.79	55.71
γ	63.66	63.79	62.11	62.31
β	87.57	86.97	83.45	83.77
B 2,6	105.23	106.36	105.55	105.53
A5	109.96	111.39	110.73	110.67
A2	110.91	112.24	110.80	110.95
A6	123.43	124.32	123.42	123.46
B1	124.25	124.85	123.63	123.60
A1	128.65	130.05	128.80	128.94
B4	136.71	137.51	135.97	136.14
A3	149.07	150.05	148.40	148.49
B 3,5	152.70	153.87	152.44	152.52
A4	153.43	154.56	153.01	153.09
α	194.94	195.48	195.24	195.36
1H				
B 2,6 OMe		3.71	3.63	3.63
A4 OMe		3.86	3.79	3.77
A3 OMe		3.89	3.84	3.82
γ1		3.82	3.75	3.89
γ2		3.87	3.82	3.96
β		5.14	5.19	5.31
B 2,6		6.67	6.64	6.63
A5		7.04	7.06	7.05
B1		7.01	6.97	6.97
A2		7.65	7.50	7.60
A6		7.80	7.71	7.79

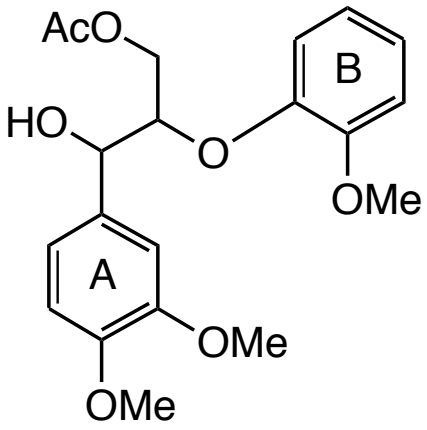
^{1}H (chloroform)

Atom	H Shifts	Mult	J
B 2,6 OMe	3.71	s	
A3 OMe	3.92	s	
A4 OMe	3.93		
γ1	3.81	dd	3.1, 12.2
γ2	3.98	dd	7.8, 12.1
β	5.07	dd	3.0, 7.8
B 2,6	6.55	d	8.4
A5	6.86	d	8.4
B1	7.00	t	8.4
A2	7.64	d	2.0
A6	7.71	dd	2.0, 8.4

Notes:

S. Ralph, J. Ralph
FPL Collection

Compound Number 326



erythro

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	1.89	s	
A4 OMe	3.76		
A3 OMe	3.78		
B3 OMe	3.81		
α	4.94	d	4.5
β	4.58	m	
γ1	4.23	dd	3.2, 11.8
γ2	4.35	dd	6.8, 11.8
B6	6.83	dt	8.0
A5	6.88	d	8.2
B1	6.94	dt	8.0
B2	6.97		
A6	6.97		
B5	7.00	dd	1.4, 8.0
A2	7.10	d	1.8

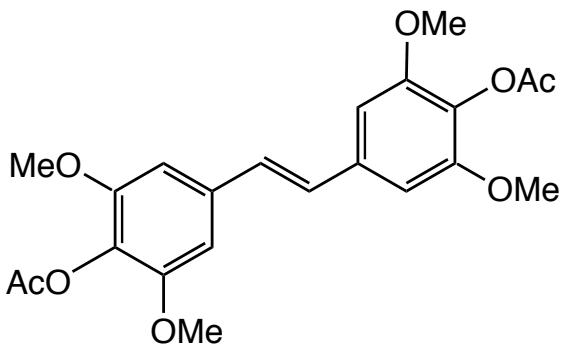
Notes:

F. Lu FLW-52p3
Methoxy 1H and 13C are very close and may be switched

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.81	20.67	20.54	20.42
A4 OMe	55.84	56.03	55.32	55.26
A3 OMe	55.86	56.10	55.46	55.40
B3 OMe	55.88	56.24	55.55	55.47
γ	62.79	63.87	62.95	63.01
α	71.97	72.97	71.25	71.40
β	84.39	83.28	80.77	80.96
A2	109.31	111.60	110.59	110.67
A5	110.96	112.35	111.22	111.25
B2	112.21	113.69	112.77	112.73
B5	118.49	119.65	117.00	117.12
A6	120.73	119.83	118.90	118.94
B6	121.45	121.75	120.61	120.60
B1	124.15	123.59	121.96	121.97
A1	131.48	134.77	134.46	134.55
B4	146.95	148.76	147.31	147.40
A4	148.45	149.70	147.90	148.01
A3	148.98	150.11	148.26	148.39
B3	151.56	152.05	150.08	150.18
γ Ac C=O	170.92	170.91	170.22	170.19
1 H				
Ac Me	1.98		1.88	1.86
A4 OMe	3.84		3.70	3.69
A3 OMe	3.86		3.70	3.70
B3 OMe	3.86		3.71	3.71
α	4.42		4.77	4.91
β	4.87		4.52	4.62
γ1	4.10		4.22	4.31
γ2	4.36		4.26	4.37
B6	6.91		6.79	6.80
A5	6.81		6.86	6.87
B1	7.04		6.88	6.88
B2	6.92		6.92	6.91
A6	7.03		6.90	6.98
B5	6.85		6.90	6.98
A2	6.97		7.00	7.09

Compound Number 327



syringyl Stilbene Acetate

^{1}H (chloroform)

Atom	H Shifts	Mult	J
Ac Me	2.33	s	
OMe	3.86	s	
2,6	6.96	s	
α	7.24	s	
<u>Acetone</u>			
Ac Me	2.22	s	
OMe	3.84	s	
2,6	6.95	s	
α	7.24	s	
<u>DMSO</u>			
Ac Me	2.24	s	
OMe	3.81	s	
2,6	6.98	s	
α	7.28	s	

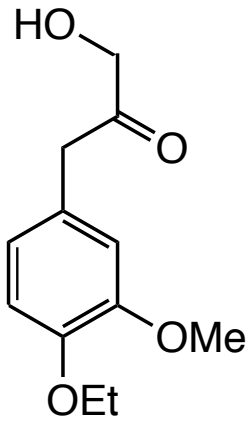
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.47	20.27	20.19	
OMe	56.15	56.46	55.98	
2,6	103.18	104.08	103.17	
α	128.82	129.60	128.61	
1	135.47	136.59	135.35	
3,5	152.28	153.44	151.89	
Ac C=O	168.79	168.59	168.17	

Notes:

S. Ralph
As this compound has a plane of symmetry the chemical shifts for the other half are identical.

Compound Number 328



Hibbert's Ketone

^{1}H (DMSO)

Atom	H Shifts	Mult	J
Me	1.29	t	7.0
α	3.63	s	
OMe	3.71	s	
CH2	3.95	q	7.0
γ	4.13	d	5.9
6	6.67	dd	1.7, 8.2
2	6.78	d	1.7
5	6.85	d	8.2
γ-OH	5.10	t	5.9

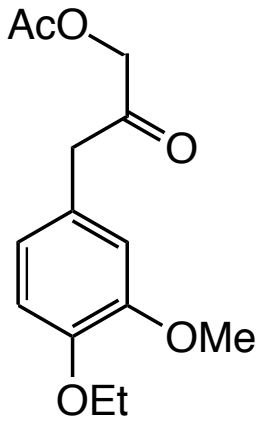
Notes:

S. Ralph
SRXIV-39
Hibbert's Ketone
C2 and C5 switch order in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	14.74	15.24	14.80	
α	45.40	45.31	44.14	
OMe	55.93	56.08	55.38	
CH2	64.35	64.92	63.68	
γ	67.47	68.13	67.13	
5	112.88	114.29	112.94	
2	112.51	114.58	113.46	
6	121.48	122.55	121.59	
1	125.02	127.67	126.86	
4	147.74	148.64	146.71	
3	149.49	150.59	148.72	
β	207.64	208.53	208.52	
1H				
Me	1.42	1.34		
α	3.63	3.69		
OMe	3.83	3.78		
CH2	4.05	4.00		
γ	4.25	4.24		
6	6.70	6.74		
2	6.69	6.86		
5	6.79	6.85		

Compound Number 329



^{1}H (DMSO)

Atom	H Shifts	Mult	J
CH3	1.29	t	6.8
Ac Me	2.07	s	
α	3.68	s	
OMe	3.71	s	
CH2	3.96	q	6.8
γ	4.81	s	
6	6.69	bdd	8.1
2	6.79	bs	
5	6.86	d	8.1

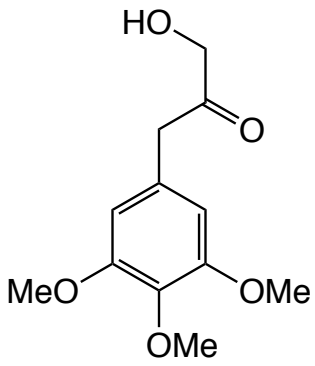
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	14.79	15.23	15.26	
Ac Me	20.48	20.33	20.77	
α	46.09	45.73	44.87	
OMe	55.95	56.06	55.85	
CH2	64.35	64.89	64.13	
γ	67.39	68.16	68.01	
5	112.86	114.25	113.39	
2	112.55	114.52	113.93	
6	121.56	122.60	122.15	
1	125.05	127.18	126.49	
4	147.70	148.70	147.36	
3	149.51	150.59	149.21	
Ac C=O	170.21	170.32	170.18	
β	201.59	201.86	202.35	
1H				
CH3	1.44	1.34		
Ac Me	2.13	2.06		
α	3.65	3.70		
OMe	3.84	3.78		
CH2	4.06	4.01		
γ	4.67	4.77		
2	6.70	6.85		
6	6.71	6.74		
5	6.80	6.86		

Notes:

S. Ralph
SRXIV-39-Ac
Hibbert's Ketone
C2 and C5 switch order in CDCl3

Compound Number 330



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	45.93	45.95	44.85	
3 OMe	56.08	56.38	55.87	
5 OMe	56.08	56.38	55.87	
4 OMe	60.79	60.47	60.04	
γ	67.49	68.20	67.27	
2	106.25	107.92	106.97	
6	106.25	107.92	106.97	
1	128.20	130.70	130.23	
4	137.30	138.22	136.21	
3	153.43	154.36	152.76	
5	153.43	154.36	152.76	
β	207.23	208.27	208.36	

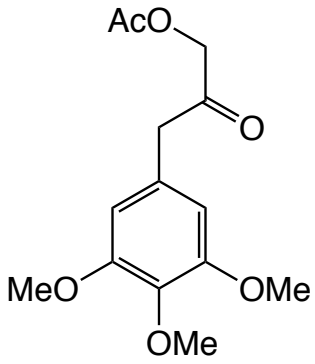
^{1}H (DMSO)

Atom	H Shifts	Mult	J
4 OMe	3.61	s	
α	3.64	s	
3,5 OMe	3.72	s	
γ	4.15	s	
2,6 OMe	6.49	s	
γ OH	5.15	t	
<u>CDCl3</u>			
4 OMe	3.80	s	
α	3.62	s	
3,5 OMe	3.81	s	
γ	4.27	s	
2,6 OMe	6.39	s	
<u>Acetone</u>			
4 OMe	3.69	s	
α	3.71	s	
3,5 OMe	3.79	s	
γ	4.30	s	
2,6 OMe	6.57	s	

Notes:

FPL Collectiom
1H order changes in CDCl3 for 4 OMe and alpha
SRXIV-40-B

Compound Number 331



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.45	20.33	20.35	
α	46.59	46.33	45.03	
3 OMe 5 OMe	56.13 56.13	56.38 56.38	55.88 55.88	
4 OMe	60.84	60.47	60.05	
γ	67.42	68.23	67.70	
2 6	106.34 106.34	107.91 107.91	107.01 107.01	
1	128.25	130.24	129.43	
4	137.31	138.26	136.34	
3 5	153.49 153.49	154.39 154.39	152.80 152.80	
Ac C=O	170.21	170.36	169.84	
β	201.16	201.63	201.71	

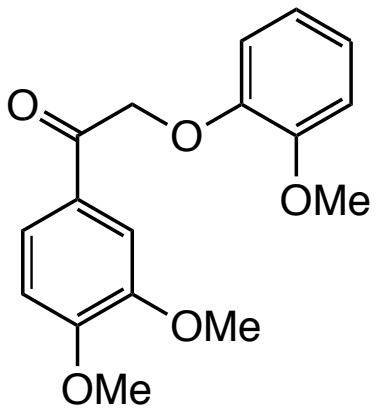
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.06		
4 OMe	3.70		
α	3.72		
3,5 OMe	3.79		
γ	4.80		
2,6 OMe	6.57		
<u>CDCl3</u>			
Ac Me	2.14		
4 OMe	3.81		
α	3.65		
3,5 OMe	3.82		
γ	4.70		
2,6 OMe	6.40		
<u>DMSO</u>			
Ac Me	2.07		
4 OMe	3.61		
α	3.69		
3,5 OMe	3.73		
γ	4.83		
2,6 OMe	6.50		

Notes:

FPL Collectiom
1H order changes in CDCl3 for 4 OMe and alpha
SRXIV-40-B

Compound Number 332



^{1}H (DMSO)

Atom	H Shifts	Mult	J
B3 OMe	3.77	s	
A3 OMe	3.82	s	
A4 OMe	3.85	s	
β	5.45	s	
B6	6.81	m	
B5	6.84	m	
B1	6.89	d	7.3
B2	6.98	d	7.8
A5	7.09	d	8.4
A2	7.49	bs	
A6	7.70	d	8.3

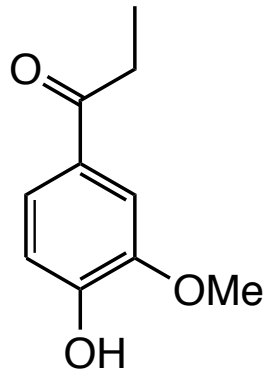
Notes:

J. Obst
FPL Collection
A2 and A5 switch order in 13C CDCl3
Aromatic 1H shifts assigned from HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B3 OMe	55.90	56.22	55.56
A3 OMe	56.01	56.10	55.56
A4 OMe	56.11	56.22	55.82
β	72.04	72.28	70.52
A2	110.45	111.49	110.20
A5	110.11	111.60	111.01
B2	112.14	113.59	112.46
B5	114.68	115.51	113.65
B6	120.81	121.53	120.54
B1	122.35	122.62	121.31
A6	122.78	123.58	122.63
A1	127.85	128.87	127.28
B4	147.58	149.12	147.50
A3	149.21	150.26	148.70
B3	149.72	150.85	148.98
A4	153.81	154.98	153.52
α	193.30	193.73	193.13
1H			
B3 OMe	3.87	3.82	
A3 OMe	3.92	3.87	
A4 OMe	3.94	3.90	
β	5.27	5.36	
B6	6.83	6.82	
B5	6.83	6.90	
B1	6.94	6.91	
B2	6.90	6.97	
A5	6.89	7.07	
A2	7.59	7.59	
A6	7.66	7.75	

Compound Number 333



Propioguaiacone

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ	1.11	t	7.3
OMe	2.95	q	7.3
β	3.89	s	
5	6.89	d	8.2
6	7.54	m	
2	7.56	m	

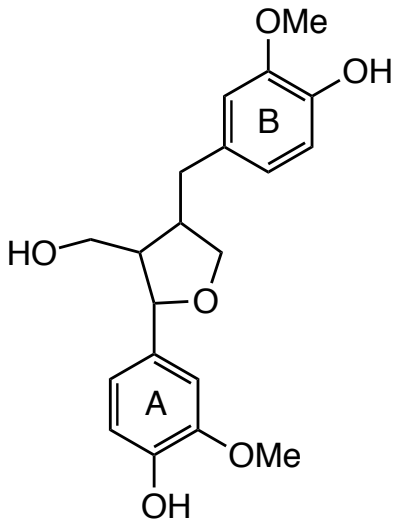
Notes:

FPL Collection

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	8.53	8.75	8.50	
β	31.19	31.54	30.60	
OMe	55.97	56.25	55.58	
2	109.81	111.48	111.02	
5	113.82	115.35	114.91	
6	123.13	123.63	122.73	
1	129.76	130.45	128.50	
3	146.69	148.28	147.49	
4	150.25	152.03	151.49	
α	199.48	198.95	198.69	
1H				
γ	1.17		1.05	
OMe	2.91		2.93	
β	3.90		3.81	
5	6.89		6.84	
6	7.50		7.44	
2	7.50		7.50	

Compound Number 334



Lariciresinol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A β	2.30	p	6.7
B α1	2.52	dd	11.3, 13.5
B β	2.68	m	
B α2	2.94	dd	5.0, 13.5
A γ1	3.65	m	
B γ1	3.67	m	
γ OH	3.74	t	3.8
OMe	3.80, 3.80	s	
B γ2	3.84	m	
A γ2	3.94	dd	6.7, 8.4
A α	4.77	d	6.1
B6	6.65	dd	1.3, 8.0
B5	6.72	d	8.0
A5	6.76	d	8.0
A6	6.77	dd	1.1, 8.0
B2	6.82	bs	
A2	6.93	bs	
B4 OH	7.29	s	
A4 OH	7.38	s	

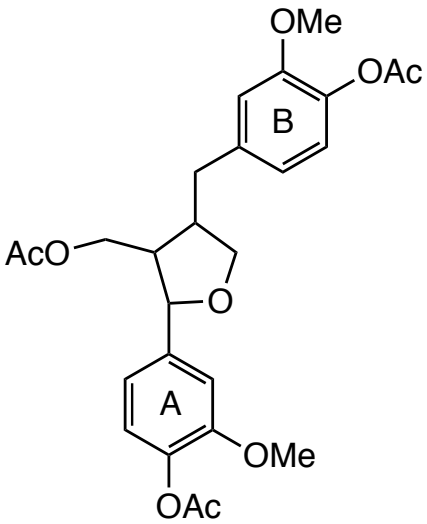
Notes:

FPL Collection
Some proton shifts taken from HSQC
and aromatic protons shift order between solvents
1H shifts for phenolic OHs vary widely between solvents
HSQC and HMBC in all solvents

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B α	33.37	33.50	32.20	
B β	42.41	43.45	41.98	
A β	52.61	53.90	52.47	
OMe	55.91	56.19	55.54	
OMe	55.93	56.19	55.59	
B γ	60.97	60.31	58.60	
A γ	72.90	73.10	71.83	
A α	82.82	83.24	81.77	
A2	108.26	110.15	109.91	
B2	111.16	112.97	112.69	
A5	114.15	115.28	115.04	
B5	114.38	115.62	115.37	
A6	118.76	119.21	118.19	
B6	121.19	121.80	120.60	
B1	132.27	133.36	131.75	
A1	134.78	136.58	134.71	
B4	143.98	145.57	144.55	
A4	144.99	146.38	145.51	
A3	146.50	148.08	147.37	
B3	146.61	148.19	147.45	
1H				
A β	2.39		2.17	
B α1	2.53		2.40	
B β	2.72		2.56	
B α2	2.90		2.80	
A γ1	3.73		3.53	
B γ1	3.77		3.44	
OMe	3.86		3.72	
OMe	3.87		3.73	
B γ2	3.90		3.63	
A γ2	4.04		3.85	
A α	4.77		4.63	
γ OH			4.67	
B6	6.68		6.56	
B5	6.82		6.65	
A5	6.85		6.68	
A6	6.79		6.67	
B2	6.67		6.73	
A2	6.85		6.81	
B4 OH	5.46		8.68	
A4 OH	5.54		8.81	

Compound Number 335



Laricresinol-Acetate

^{1}H (DMSO)

Atom	H Shifts	Mult	J
Aγ AcMe	1.92	s	
4 AcMe	2.22	s	
4 AcMe	2.23	s	
A β	2.50	obs. dd	7.1
B α1	2.58	dd	10.6, 13.5
B β	2.75	m	
B α2	2.86	dd	5.0, 13.5
B γ1	3.65	dd	6.7, 8.5
OMe	3.75	s	
OMe	3.75	s	
B γ2	3.98	dd	6.5, 8.5
A γ1	4.14	dd	7.6, 11.3
A γ2	4.31	dd	6.8, 11.3
A α	4.77	d	6.5
B6	6.79	dd	1.9, 8.1
A6	6.89	dd	1.9, 8.2
B5	6.96	d	8.1
B2	6.99	d	1.9
A5	7.02	d	8.1
A2	7.04	d	1.8

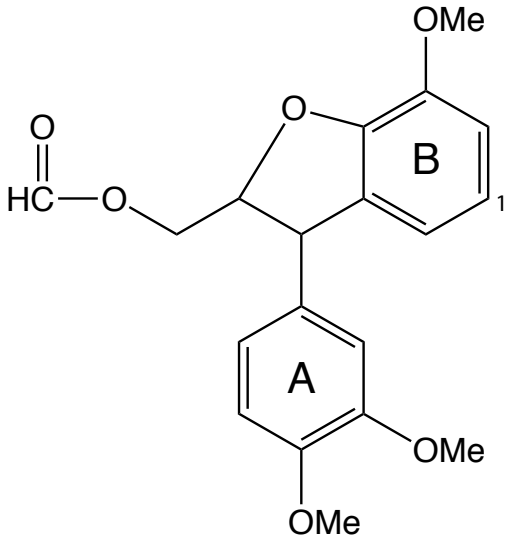
Notes:

FPL Collection
Some proton shifts taken from HSQC
and aromatic 1H and 13C can shift order between solvents
HSQC and HMBC in all solvents

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
4 AcMe	20.68	20.48	20.41	
4 AcMe	20.68	20.48	20.41	
γ AcMe	20.86	20.78	20.60	
B α	33.46	33.86	32.64	
B β	42.08	43.20	41.76	
A β	49.05	50.33	48.76	
OMe	55.88	56.16	55.69	
OMe	55.91	56.16	55.72	
A γ	62.64	63.17	62.26	
B γ	72.79	73.23	72.10	
A α	82.79	83.56	82.17	
A2	109.62	110.91	110.26	
B2	112.73	111.88	113.12	
A6	117.73	118.59	117.95	
B6	120.53	121.28	120.39	
5	122.62	123.34	122.54	
5	122.80	123.48	122.58	
B4	138.20	139.26	137.53	
A4	138.94	140.02	138.43	
B1	138.85	140.44	139.46	
A1	141.54	143.22	141.86	
B3	151.01	152.14	150.64	
A3	151.07	152.18	150.67	
4 Ac C=O	169.10	169.03	168.64	
4 Ac C=O	169.15	169.03	168.64	
γ Ac C=O	170.93	170.99	170.39	
1H				
Aγ AcMe	2.01	1.97		
4 AcMe	2.29	2.21		
4 AcMe	2.29	2.21		
A β	2.56	2.55		
B α1	2.57	2.66		
B β	2.71	2.82		
B α2	2.85	2.96		
B γ1	3.74	3.74		
OMe	3.80	3.79		
OMe	3.82	3.80		
B γ2	4.08	4.05		
A γ1	4.18	4.21		
A γ2	4.36	4.38		
A α	4.84	4.85		
B6	6.72	6.82		
B2	6.74	7.01		
A6	6.85	6.92		
B5	6.93	6.94		
A2	6.93	7.09		
A5	6.97	6.99		

Compound Number 336



^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe OMe OMe	3.75 3.78 3.85		
α	4.49		
γ1 γ2	4.44 4.80		
β	4.42-4.47		
B6	6.56	ddd	1.0, 1.7, 7.0
A6	6.76		
B1	6.81		
A2, B2, A5	6.83-6.93		
formyl H	8.20		

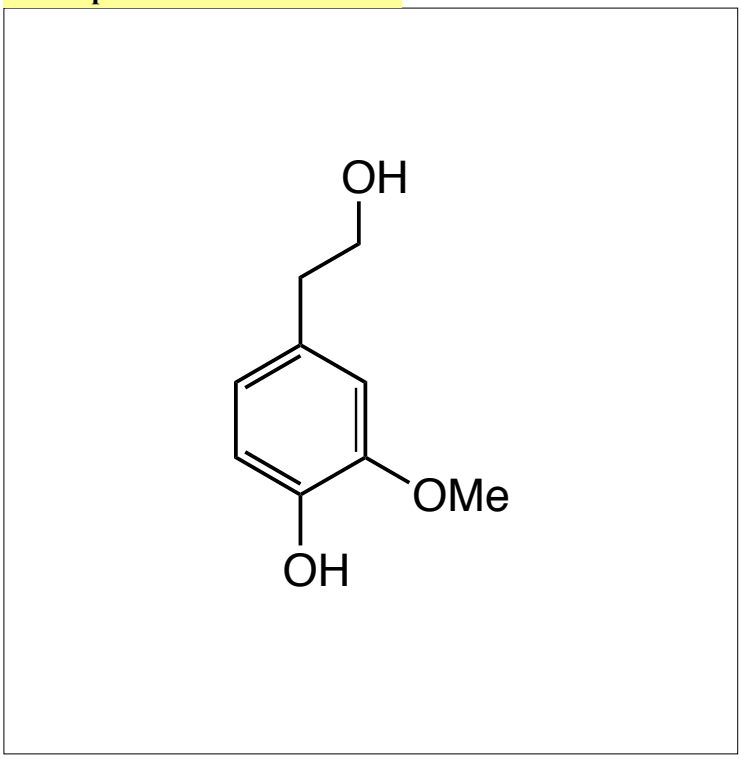
Notes:

S. Ralph, SRXI-14A
some proton shifts from HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	50.99	51.38		
OMe OMe OMe	55.92 55.92 55.92	56.15 56.15 56.26		
γ	63.71	64.48		
β	88.89	89.63		
A2	110.92	112.82		
B2	111.43	113.09		
B6	117.21	117.98		
A6	120.41	121.09		
B1	121.96	122.44		
B5	130.78	132.88		
A1	133.63	135.20		
B3	144.56	145.65		
B4	147.61	148.84		
A3	148.48	149.74		
A4	149.41	150.68		
formyl C=O	160.72	161.82		
1H				
OMe OMe OMe	3.79 3.85 3.90			
α	4.42			
γ	4.48			
β	4.83			
B6 A2 A6 A5 B2 B1	6.58 6.66 6.76 6.84 6.80 6.82			
formyl H	8.10			

Compound Number 337



Homo Vanillyl Alcohol

^{1}H (DMSO)

Atom	H Shifts	Mult	J
α	2.59	t	7.3
β	3.53	m	
OMe	3.72	s	
6	6.56	dd	1.8, 8.0
5	6.64	d	8.0
2	6.74	d	1.8
4-OH	8.63	s	
β-OH	4.54	t	

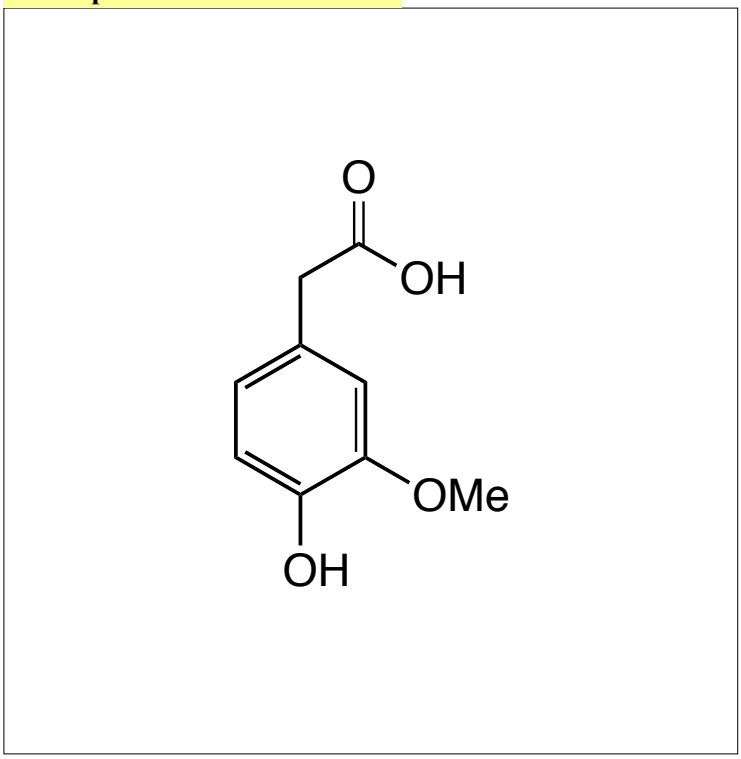
Notes:

Aldrich
1H for 5 and 2 change order in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	38.81	39.96	38.67	
OMe	55.87	56.15	55.49	
β	63.81	64.22	62.54	
2	111.49	113.35	113.04	
5	114.44	115.54	115.17	
6	121.60	132.16	120.92	
1	130.20	131.66	130.15	
4	144.25	145.73	144.59	
3	146.54	148.07	147.25	
1 H				
α	2.78	2.70		
β	3.81	3.68		
OMe	3.87	3.81		
6	6.70	6.65		
5	6.84	6.82		
2	6.71	6.71		

Compound Number 338



Homo Vanillic Acid

^{1}H (DMSO)

Atom	H Shifts	Mult	J
α	3.43	s	
OMe	3.73	s	
6	6.63	dd	1.8, 8.0
5	6.70	d	8.0
2	6.80	d	1.8
β-OH	12.18	bs	

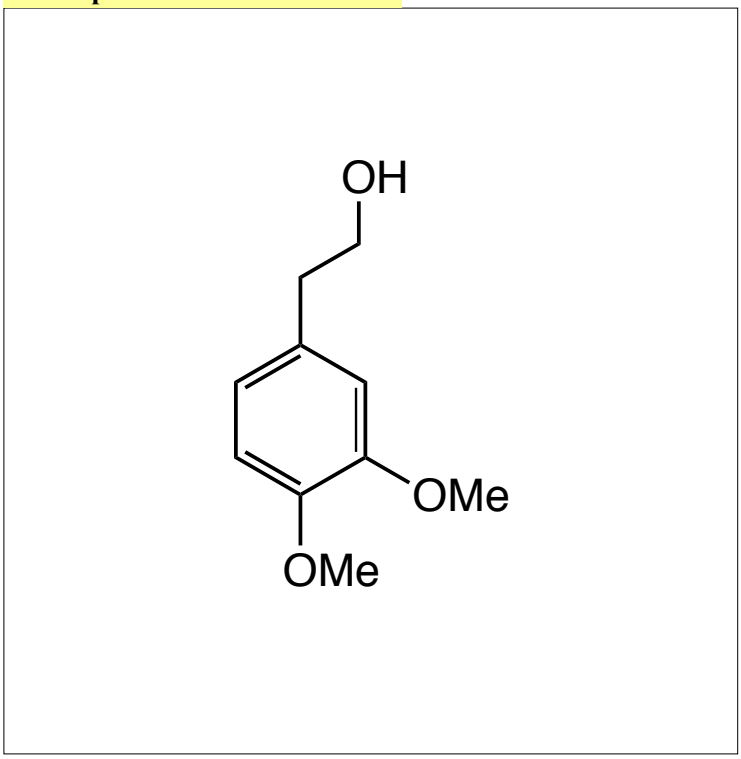
Notes:

FPL Collection
Proton Shifts for Acetone 5 and 6 from HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	40.51	40.84	40.35	
OMe	55.90	56.21	55.62	
2	111.74	113.75	113.58	
5	114.44	115.59	115.32	
6	122.27	122.75	121.71	
1	124.96	126.99	125.79	
4	144.96	146.39	145.32	
3	146.51	148.13	147.38	
β	177.04	173.14	173.16	
1H				
α	3.56	3.50		
OMe	3.87	3.82		
6	6.76	6.74		
5	6.85	6.75		
2	6.77	6.90		

Compound Number 339



4-Methoxy homovanillyl alcohol

^{1}H (DMSO)

Atom	H Shifts	Mult	J
α	2.63	t	7.4
β	3.55	bq	5.3
4 OMe	3.68	s	
3 OMe	3.71	s	
5	6.82	d	8.1
2	6.79	d	1.4
6	6.69	dd	8.1, 1.4
OH	4.62	t	5.3

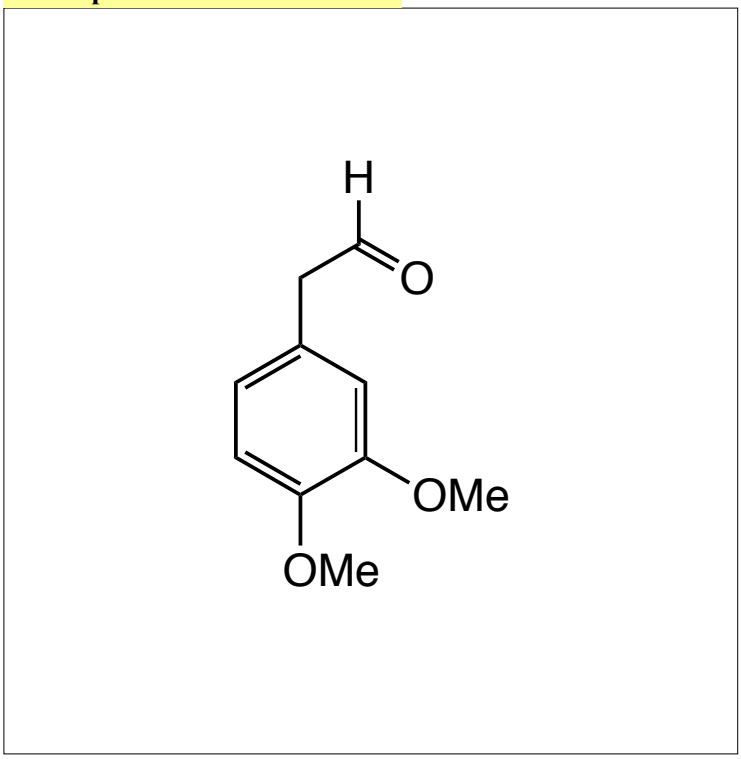
Notes:

SRXIV-47B

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	38.71	39.90	38.68	
3 OMe	55.81	56.01	55.47	
4 OMe	55.90	56.16	55.63	
β	63.70	64.10	62.51	
5	111.35	112.95	111.92	
2	112.19	114.01	112.88	
6	120.90	121.76	120.76	
1	130.97	133.09	132.03	
4	147.68	148.79	147.15	
3	148.99	150.23	148.59	
1H				
α	2.79	2.73		
β	3.82	3.70		
4 OMe	3.84	3.77		
3 OMe	3.85	3.75		
5	6.80	6.82		
2	6.73	6.84		
6	6.74	6.73		

Compound Number 340



4-Methoxy-Homovanillin

^{1}H (chloroform)

Atom	H Shifts	Mult	J
α	3.60	d	2.5
OMe	3.86	s	
OMe	3.86	s	
5	6.85	d	8.1
2	6.68	d	2.0
6	6.75	m	
β	9.71	t	2.5

Notes:

SRXIV-47-C
Some proton shifts from HSQC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α	50.14	50.37	49.20	
OMe	55.89	56.09	5632	
OMe	55.89	56.09	56.32	
5	111.60	113.14	112.16	
2	112.58	114.43	113.51	
6	121.84	122.68	121.87	
1	124.09	126.10	125.04	
4	148.41	149.60	147.96	
3	149.32	150.62	148.94	
β	199.53	200.02	200.88	
1H				
α		3.61	3.64	
OMe		3.78	3.71	
OMe		3.78	3.72	
5		6.92	6.90	
2		6.87	6.83	
6		6.78	6.73	
β		9.68	9.63	