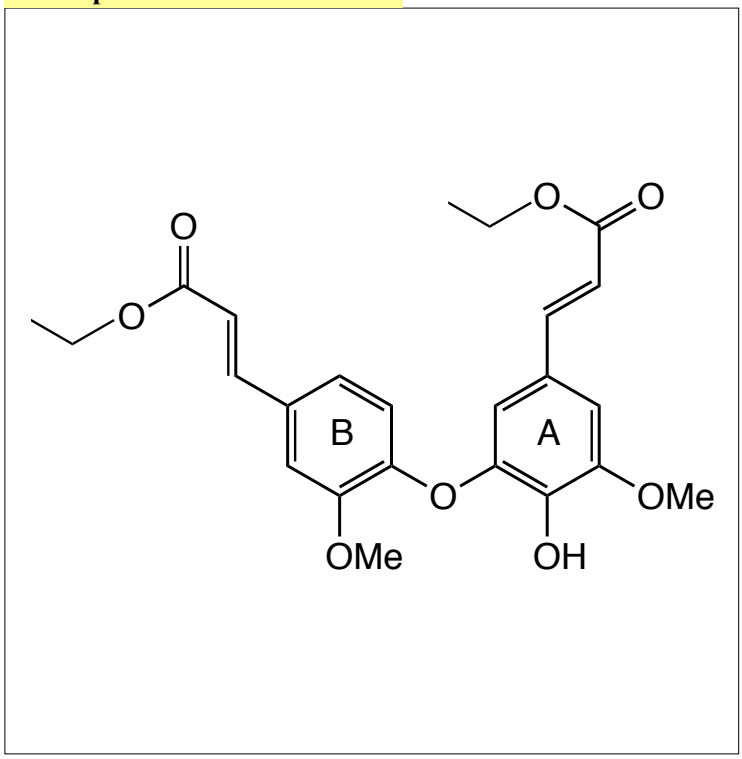
Compound Number 3001



4-O-5 dehydrodiethylferulate

3-{3-[4-(2-ethoxycarbonyl-vinyl)-2-methoxy-phenoxy]-4-hydroxy-5-methoxy-phenyl}acrylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
A CH_3	1.24	t	7.1
B CH_3	1.27	t	7.1
B3 OMe	3.93	s	
A3 OMe	3.96	s	
A CH_2	4.16	q	7.1
B CH_2	4.19	q	7.1
A β	6.36	d	15.9
B β	6.48	d	15.95
B5	6.81	d	8.3
A6	6.89	d	1.9
B6	7.17	dd	8.7, 2.0
A2	7.22	d	1.9
B2	7.46	d	2.0
A α	7.53	d	15.9
B α	7.62	d	15.95

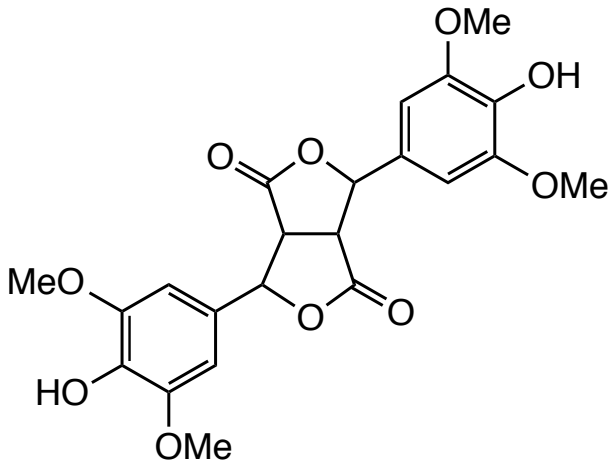
Notes:

jrf107.P1 /1 (H1), /2 (C13), /3 (Dept135)

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A CH_3		14.60		
B CH_3		14.60		
B3 OMe		56.41		
A3 OMe		56.77		
A CH_2		60.53		
B CH_2		60.64		
A2		107.99		
B2		112.66		
A6		114.45		
A β		116.99		
B β		117.93		
B5		118.36		
B6		122.84		
A1		126.67		
B1		131.04		
A4		141.41		
A5		144.45		
B α		144.81		
A α		144.94		
B4		149.35		
A3		150.12		
B3		151.41		
B γ		167.15		
A γ		167.16		

Compound Number 3002



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β		49.06		
OMe		56.77		
OMe		56.77		
α		83.39		
2		104.31		
6		104.31		
4		129.87		
1		137.51		
3		149.04		
5		149.04		
g		176.05		

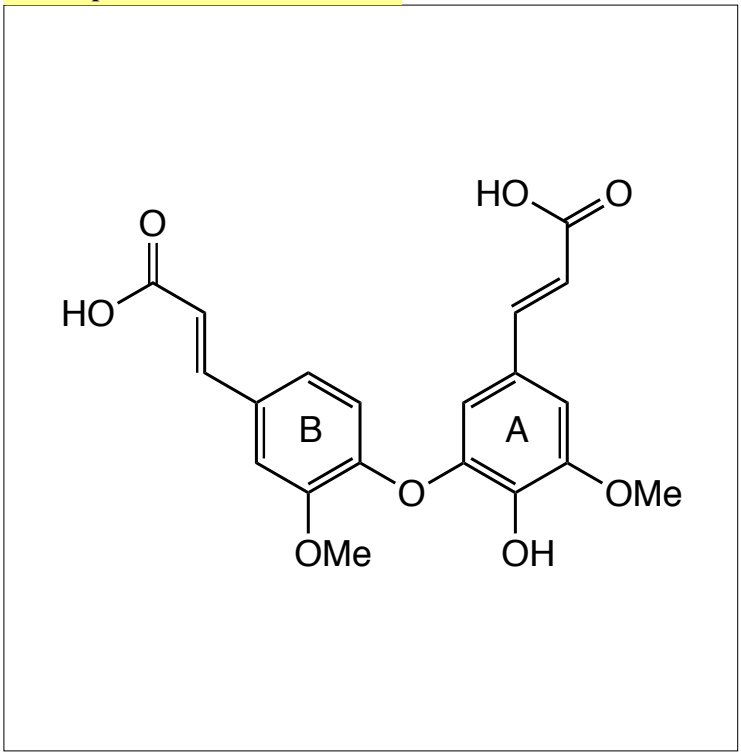
^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.83	s	
β	4.11	s	
α	5.95	s	
2,6	6.73	s	
OH	7.42	s	

Notes:

FLJ144
As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 3003



4-O-5 dehydrodiferulic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
B3 OMe	3.58	s	
A3 OMe	3.88	s	
A β	6.36	d	15.9
B β	6.47	d	15.95
B5	6.82	d	8.3
A6	6.90	d	1.9
B6	7.22	dd	8.3, 2.0
A2	7.22	d	1.9
B2	7.45	d	2.0
A α	7.54	d	15.9
B α	7.63	d	15.95
DMSO			
B3 OMe	3.85		
A3 OMe	3.86		
A β	6.35		
B β	6.47		
B5	6.59		
A6	6.85		
B6	7.12		
A2	7.20		
B2	7.43		
A α	7.42		
B α	7.51		
	7.51		

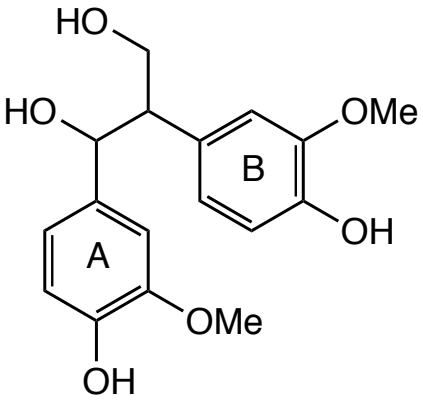
Notes:

Acetone: jrf117 /2 (C13) and /1 (H1) DMSO: jrf127.c7/2 Not soluble in chloroform
1H NMR (DMSO-d6) d: 3.85 (B3-OMe), 3.86 (A3-OMe),6.35 (A8), 6.47 (B8), 6.59 (B5), 6.85 (A6), 7.12 (B6), 7.20 (A2), 7.43 (B2), 7.42 (A7), 7.51 (B7)
JCS Perkin 1, 3485-98 (1994) Cmpd 17

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe		56.40	55.85	
A3 OMe		56.76	56.24	
A2		108.03	107.58	
B2		112.7	111.86	
A6		114.46	114.05	
A β		117.00	116.96	
B β		117.95	118.00	
B5		118.33	116.34	
B6		122.80	121.91	
A1		126.71	125.22	
B1		131.06	129.43	
A4		141.38	140.35	
A5		144.44	142.94	
A α		145.23	143.81	
B α		145.38	143.63	
B4		149.34	148.05	
A3		150.12	149.28	
B3		151.38	149.56	
B γ		168.02	167.82	
A γ		168.05	167.82	

Compound Number 3004



erythro

1,2-diguaiacylpropane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	2.93	m	
γ1	3.72	m	
γ2	3.87	m	
α	5.02	bd	
B6	6.60	bd	
B5	6.66	dd	
A5	6.68	d	8.1
A6	6.68	m	
A2	6.71	m	
B2	6.74	d	1.9

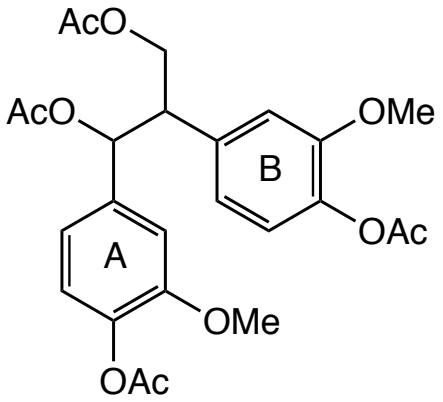
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		55.85		
OMe		55.95		
β		56.31		
γ		64.21		
α		74.66		
A2		111.01		
B2		114.00		
A5		114.81		
B5		115.00		
A6		119.95		
B6		123.05		
B1		132.24		
A1		136.67		
B4		145.96		
A4		146.17		
B3		147.56		
A3		147.63		

Notes:

jrlz 15
Liming Zhang, isolate from mild acidolysis

Compound Number 3005



threo

Acetic acid3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.93	s	
α Ac Me	2.09	s	
Ac Me	2.18	s	
Ac Me	2.19	s	
β	3.56	m	
OMe	3.67	s	
OMe	3.71	s	
γ1	4.38	dd	11.2, 5.2
γ2	4.54	dd	11.2, 7.2
α	6.02	d	8.2
B6	6.77	ddd	8.1, 2.0, 0.3
A2	6.79	bd	1.9
A6	6.82	ddd	8.1, 1.9, 0.5
B2	6.85	bd	1.9
B5	6.90	d	8.1
A5	6.91	d	8.1

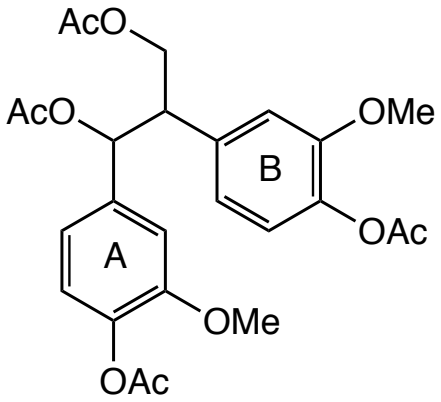
Notes:

jrlz9.1
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.41		
Ac Me		20.44		
Ac Me		20.72		
Ac Me		21.01		
β		50.71		
OMe		56.18		
OMe		56.21		
γ		64.71		
α		76.50		
A2		112.51		
B2		114.33		
A6		119.77		
B6		121.85		
A5		123.14		
B5		123.22		
B1		137.82		
A1		138.39		
B4		139.96		
A4		140.35		
B3		151.76		
A3		151.85		
Ac C=O		168.84		
Ac C=O		168.88		
α Ac C=O		170.01		
γ Ac C=O		170.81		

Compound Number 3006



erythro

Acetic acid3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.92	s	
α Ac Me	1.97	s	
Ac Me	2.20	s	
Ac Me	2.21	s	
β	3.50	m	6.7
OMe	3.69	s	
OMe	3.73	s	
γ1	4.20	dd	11.2, 6.7
γ2	4.37	dd	11.2, 6.8
α	6.16	d	6.6
B6	6.84	ddd	8.1, 1.9, 0.3
A2	6.84	bd	1.8
A6	6.87	ddd	8.1, 1.8, 0.5
B2	6.92	bd	1.9
B5	6.96	d	8.1
A5	6.98	d	8.1

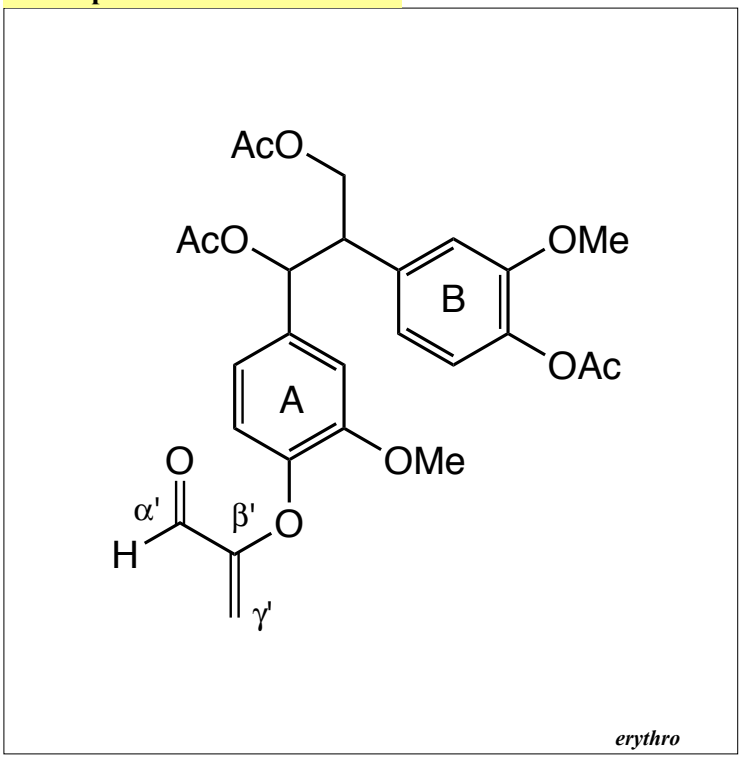
Notes:

jrlz11.1
Liming Zhang, isolate from mild acidolysis
1H data at 600 MHz

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.43		
Ac Me		20.46		
Ac Me		20.65		
Ac Me		20.83		
β		50.98		
OMe		56.20		
OMe		56.22		
γ		64.86		
α		75.56		
A2		112.09		
B2		114.52		
A6		119.73		
B6		121.93		
B5		123.13		
A5		123.30		
B1		137.43		
A1		138.72		
B4		140.05		
A4		140.51		
B3		151.80		
A3		152.00		
Ac C=O		168.89		
Ac C=O		168.95		
α Ac C=O		169.94		
γ Ac C=O		170.74		

Compound Number 3007



erythro

Acetic acid 3-acetoxy-2,3-bis-(4-acetoxy-3-methoxyphenyl)propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.94	s	
α Ac Me	2.00	s	
Ar Ac Me	2.07	s	
β	3.50	m	
OMe	3.69	s	
OMe	3.76	s	
γ1	4.22	dd	11.2, 6.8
γ2	4.38	dd	11.2, 6.8
γ1'	5.00	d	2.8
γ2'	5.38	d	2.8
α	6.19	d	6.4
B6	6.81	dd	8.1, 1.6
A2	6.88	bd	
A6	6.89	dd	7.3, 1.5
B5	6.94	d	8.1
A5	6.97		
A2	6.99		
a'	9.45		

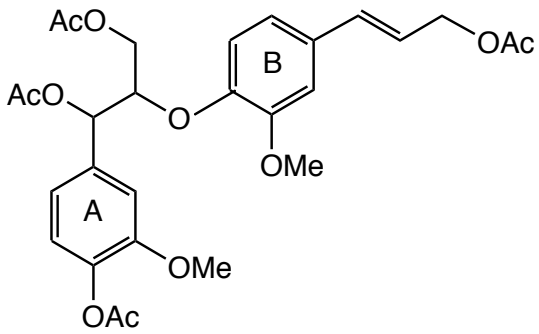
Notes:

jrlz 13
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.60	20.43		
Ac Me	20.79	20.66		
Ac Me	20.96	20.83		
β	50.13	51.07		
OMe	55.85	56.12		
OMe	55.85	56.22		
γ	63.96	64.82		
α	74.76	75.38		
γ'	107.76	108.01		
A2	111.65	122.68		
B2	113.15	114.44		
A6	119.35	120.17		
B6	121.12	122.12		
A5	121.61	122.14		
B5	122.45	123.16		
B1	135.71	137.41		
A1	136.32	138.17		
B4	139.10	140.07		
A4	142.55	143.24		
B3	150.75	151.76		
A3	150.75	151.81		
β'	157.84	159.33		
B4 Ac C=O	168.79	168.91		
α Ac C=O	169.70	169.94		
γAc C=O	170.69	170.71		
α'	186.74	187.55		

Compound Number 3008



threo

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-[4-(3-acetoxypropenyl)-2-methoxyyphenoxy]propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.95	s	
B γ Ac Me	2.01	s	
α Ac Me	2.02	s	
A4 Ac Me	2.21	s	
OMe	3.82	s	
OMe	3.85	s	
γ1	4.02	dd	11.9, 5.7
γ2	4.25	dd	11.9, 4.1
B γ	4.66	dd	6.4, 1.3
β	4.81	m	
α	6.10	d	6.4
B β	6.26	dt	15.9, 6.4
B α	6.63	bdt	15.9
B6	6.95	dd	8.3, 2.0
B5	7.00	d	8.3
A5	7.03	d	8.2
A6	7.09	dd	8.2, 1.7
B2	7.14	d	1.9
A2	7.22	d	1.6

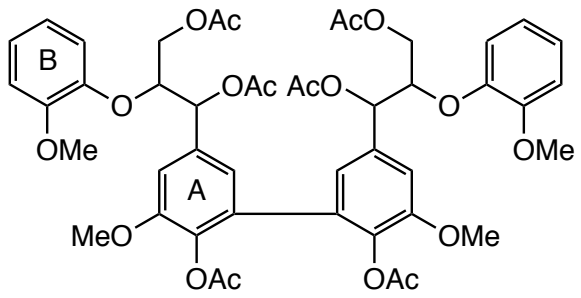
Notes:

jrlz 35
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.41		
Ac Me		20.55		
Ac Me		20.75		
Ac Me		20.89		
OMe		56.23		
OMe		56.27		
γ		63.54		
B γ		65.33		
α		75.29		
β		80.62		
B2		111.30		
A2		112.63		
B5		118.73		
A6		120.28		
B6		120.52		
B β		123.25		
A5		123.54		
B1		132.34		
B α		134.14		
A1		136359		
A4		140.90		
B4		149.08		
B3		151.74		
A3		152.21		
A4 Ac C=O		168.85		
α Ac C=O		169.95		
γ Ac C=O		170.64		
B γ Ac C=O		170.64		

Compound Number 3009



threo

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.77	s	
OMe	3.85	s	
γ1	4.09	m	
γ2	4.29	m	
β	4.78	m	
α	6.08	d	
A6,B6	6.80-6.90	m	
B1	6.96	m	
B2	6.99	m	
B5	7.02	m	
A2	7.26	m	

^{13}C

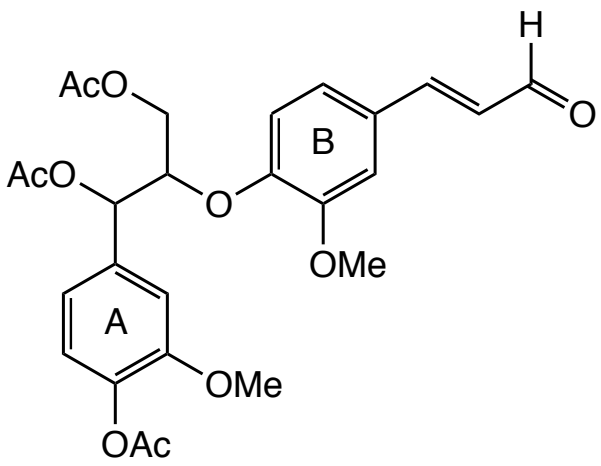
Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.26		
Ac Me		20.61		
Ac Me		20.93		
OMe		56.17		
OMe		56.52		
γ		63.51		
α		75.31		
β		80.70		
A2		111.90		
B2		113.72		
B5		119.41		
A6		121.64		
B6		121.68		
B1		123.87		
A5		131.91		
A1		135.93		
A4		138.48		
B4		148.99		
B3		151.87		
A3		152.58		
4 Ac C=O		168.88		
α Ac C=O		170.09		
γ Ac C=O		170.71		
erythro isomer γ		62.95		
α		74.59		
β		80344		
B5		120.09		
B1		124.19		
A5		131.70		
A4		138.36		
B4		148.19		
B3		152.11		

Notes:

J.Ralph jrf79.5

As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 3010



threo

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-[2-methoxy-4-(3-oxopropenyl)phenoxy]propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.08	s	
Ac Me	2.21	s	
OMe	3.82	s	
OMe	3.91	s	
γ 1	4.07	dd	12.0, 5.8
γ 2	4.28	dd	12.0, 4.1
β	4.96	m	
α	6.11	d	6.4
Bβ	6.70	dd	15.9, 7.7
A5	7.03	d	8.1
A6	7.08	dd	8.5, 1.4
B5	7.15	d	8.4
A2	7.24	bd	
B6	7.25	dd	8.8, 1.7
B2	7.40	d	1.8
B α	7.59	d	16.0
B γ	9.66	d	7.6

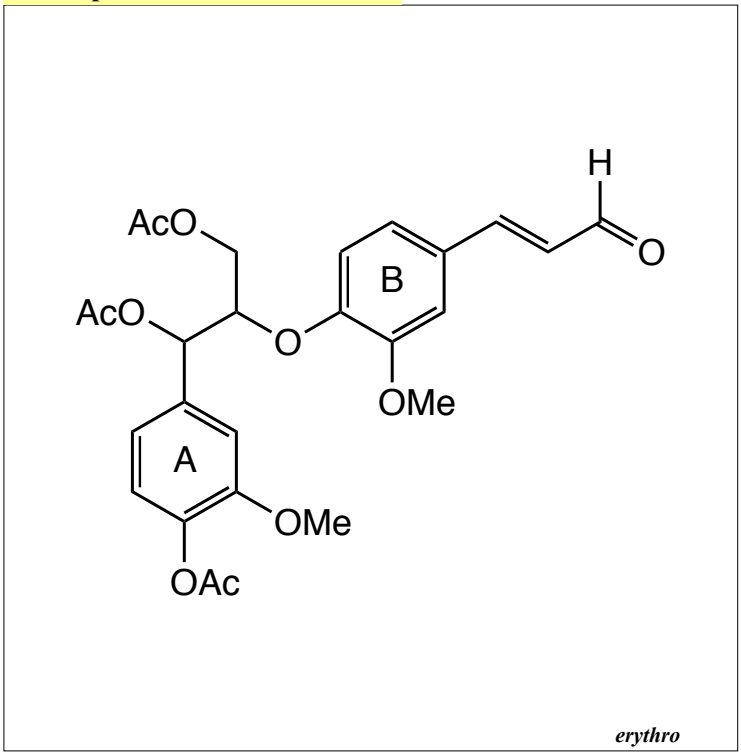
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
g Ac Me	20.60	20.43		
a Ac Me	20.68	20.57		
A4 Ac Me	20.94	20.88		
OMe	55.90	56.30		
OMe	55.98	56.41		
γ	62.81	63.45		
α	74.14	75.19		
β	79.67	80.26		
B2	111.28	112.56		
A2	111.58	112.66		
B5	117.36	117.85		
A6	119.48	120.34		
A5	122.71	123.61		
B6	122.89	123.76		
B β	127.40	128.23		
B1	128.88	129.89		
A1	134.87	136.40		
A4	140.01	140.99		
B4	150.72	151.73		
B3	150.68	151.73		
A3	151.16	152.26		
B α	152.26	153.29		
A4 Ac C=O	168.72	168.87		
α Ac C=O	169.41	169.85		
γ Ac C=O	170.48	170.66		
B γ	193.43	193.61		

Notes:

jrlz 29 1mg
Liming Zhang, isolate from mild acidolysis
see 3011 some shifts taken from isomer mix

Compound Number 3011



erythro

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-[2-methoxy-4-(3-oxopropenyl)phenoxy]propyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me			
Ac Me			
Ac Me			
OMe	3.82	s	
OMe	3.90	s	
γ 1	4.27	m	
γ 2	4.37	m	
β	4.99	m	
α	6.07	d	5.2
B β	6.79	dd	15.9, 7.7
A5	7.02	d	8.1
A6	7.07	m	
B5	7.11	d	8.3
A2	7.23	m	
B6	7.27	d	1.8
B2	7.38	d	2.0
B α	7.58	d	15.9
B γ	9.65	d	7.7

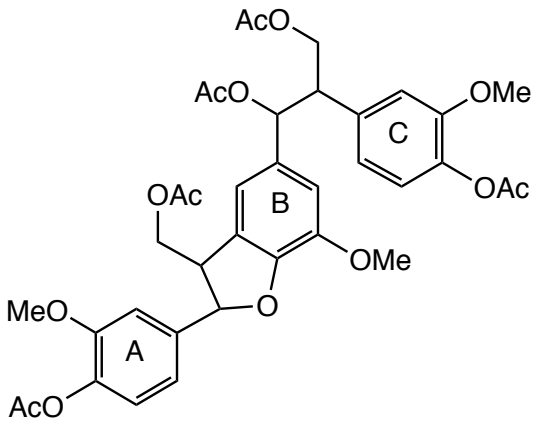
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me	20.60	20.65		
α Ac Me	20.68	20.79		
A4 Ac Me	20.94	21.10		
OMe	55.87	56.51		
OMe	55.90	56.65		
γ	62.44	63.19		
α	73.55	74.57		
β	79.56	80.02		
B2	111.38	112.85		
A2	112.00	113.08		
B5	117.93	118.49		
A6	119.76	120.75		
A5	122.61	123.50		
B6	122.81	123.91		
B β	127.47	128.53		
B1	129.10	130.22		
A1	134.80	136.48		
A4	139.90	141.11		
B4	150.02	151.22		
B3	150.95	152.12		
A3	151.00	152.35		
B α	152.26	153.45		
A4 Ac C=O	168.74	169.09		
α Ac C=O	169.57	170.07		
γ Ac C=O	170.65	170.88		
B γ	193.43	194.10		

Notes:

jrlz41
Liming Zhang, isolate from mild acidolysis
CS's taken from isomer mix spectrum

Compound Number 3012



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β *t*		50.64		
B β *t*		50.67		
B β *e*		50.90		
B β *e*		50.95		
A β		50.95		
A β		51.23		
A β		51.26		
B γ *t*		64.74		
B γ *e*		64.85		
B γ *e*		64.89		
A γ		65.55		
A γ		65.63		
A γ		65.85		
B α *e*		75.75		
B α *e*		75.76		
B α *t*		76.56		
B α *t*		76.62		
α		87.91		
α		88.03		
α		88.04		

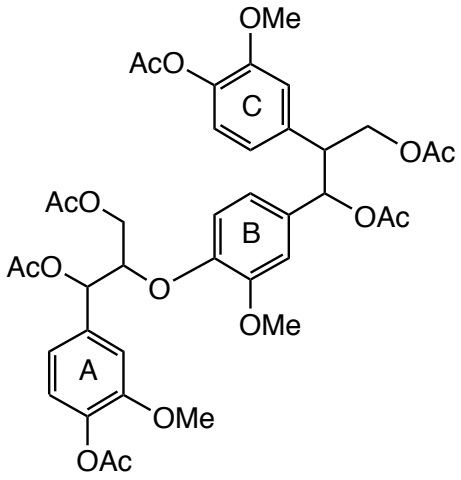
^{1}H (acetone)

Atom	H Shifts	Mult	J

Notes:

jrlz 19 15mg Liming Zhang, isolate from mild acidolysis. Due to the complexity of the model and the number of isomers present only the side chains chemical shifts have been assigned. The A side chain is a single isomer and the B chain is both erythro and threo giving 4 isomers.

Compound Number 3013



threo

Acetic acid 3-acetoxy-3-(4-acetoxy-3-methoxyphenyl)-2-{4-[1,3 -diacetoxy-2-(4-acetoxy-3-methoxyphenyl)propyl]-2-methoxyphenoxy}

^{1}**H** (acetone)

Atom	H Shifts	Mult	J

Notes:

jrlz 7 and jrlz 17 Liming Zhang - isolate from mild acidolysis.

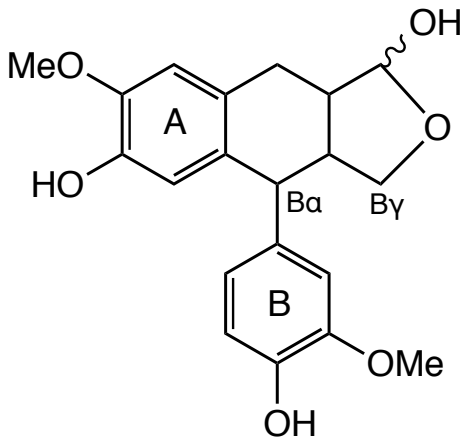
threo β-O-4/threo+erythro β-1

Due to the complexity of the model and the number of isomers present only the side chains chemical shifts have been assigned.

^{13}**C**

Atom	$CDCl_3$	Acetone	DMSO	
B β *t*		50.37		
B β *t*		50.46		
B β *e*		50.71		
B β *e*		50.75		
γ		63.37		
B γ *t*		64.74		
B γ *t*		64.75		
B γ *e*		64.84		
B γ *e*		64.86		
α		75.13		
α		75.35		
α		75.19		
B α *e*		75.47		
B α *e*		75.53		
B α *t*		76.30		
B α *t*		76.35		
β		80.34		
β		80.36		
β		80.42		

Compound Number 3014



4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-1,3,3a,4,9,9a-hexahydronaphtho[2,3-c]furan-1,6-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A β	1.98	m	
B β	2.54	m	
A α1	2.84	m	
A α2	3.00	m	
B γ1	3.47	dd	10.0, 8.0
B α	3.64	d	12.2
B γ2	3.77	m	
OMe	3.77	s	
OMe	3.80	s	
A γ OH	4.99	d	4.3
A γ	5.40	d	4.3
A5	6.22	d	0.9
B6	6.63	dd	8.0, 2.0
A2	6.72	s	
B2	6.74	d	2.0
B5	6.77	d	8.0
A4 OH	7.17	s	
B4 OH	7.39	s	

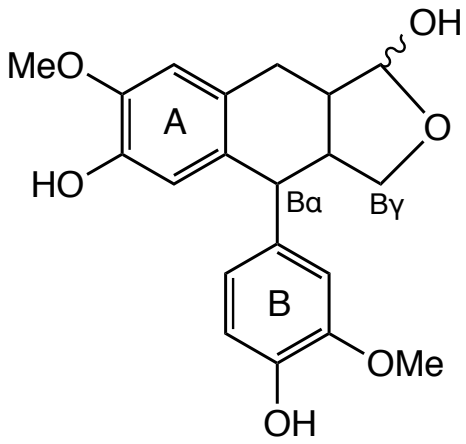
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α		29.84		
B β		46.24		
β		47.00		
B α		51.09		
OMe		55.96		
OMe		56.05		
B γ		72.06		
γ		98.75		
B2		112.38		
A2		112.84		
B5		115.51		
A5		116.17		
B6		121.75		
A1		128.34		
A6		133.42		
B1		137.28		
A4		145.11		
B4		145.93		
A3		146.61		
B3		148.24		

Notes:

jrlz5, mixture of 2 isomers in ca. 2:1 ratio.
Data for major isomer
Liming Zhang, isolate from mild acidolysis

Compound Number 3015



4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-1,3,3a,4,9,9a-hexahydronaphtho[2,3-c]furan-1,6-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A β	1.98	m	
B β	2.28	m	
A α1	2.80	m	
A α2	3.00	m	
B γ 1,2	3.64	m	
B α	3.72	bd	11.4
OMe	3.77	s	
OMe	3.80	s	
A γ	5.18	d	6.2
A γOH	5.28	d	
A5	6.55	d	
B6	6.62	dd	10.1, 2.0
A2	6.72	s	
B2	6.74	d	2.0
B5	6.77	d	8.0
A4 OH	7.17	s	
B4 OH	7.39	s	

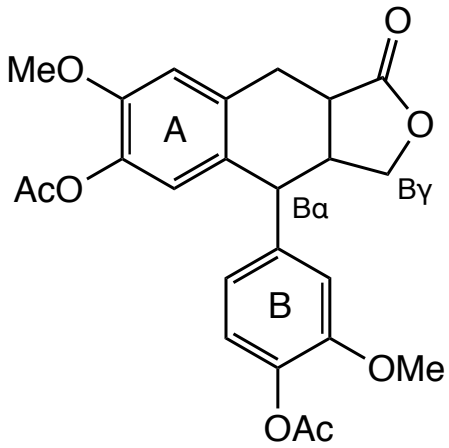
Notes:

jrlz5, mixture of 2 isomers in ca. 2:1 ratio.
Data for minor isomer
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α		31.98		
Bβ		49.88		
β		49.88		
B α		50.12		
OMe		55.96		
OMe		56.05		
Bγ		70.96		
γ		104.08		
B2		112.28		
A2		112.79		
B5		115.51		
A5		116.28		
B6		121.75		
A1		127.93		
A6		133.38		
B1		136.75		
A4		145.31		
B4		145.95		
A3		146.63		
B3		148.20		

Compound Number 3016



Acetic acid 4-(4-acetoxy-3-methoxyphenyl)-7-methoxy-1-oxo-1,3,3a,4,9,9a-hexahydroanphtho[2,3-c]furan-6-yl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.13	s	
Ac Me	2.23	s	
B β	2.75	m	
A β	2.78	m	
A α1	2.98	m	
A α2	3.18	dd	16.0, 5.0
OMe	3.75	s	
OMe	3.81	s	
B α	4.16	m	
B γ	4.16	m	
A5	6.44	s	
B6	6.83	dd	8.1, 1.9
B2	6.96	d	1.9
A2	6.98	s	
B5	7.03	d	8.1

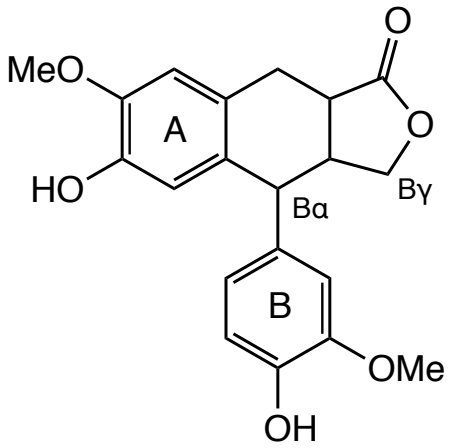
Notes:

jrlz25
Liming Zhang, isolate from mild acidolysis
FPL Collection analog alpha-Conidendrin
The B2 and B6 carbon signals are broad and 1/4 height of B5

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.53	20.36	20.64
Ac Me	20.63	20.48	20.76
α	29.57	30.12	29.23
β	41.66	41.87	40.93
B β	47.44	47.65	45.93
Bα	49.93	50.09	48.52
OMe	55.87	56.20	56.13
OMe	55.93	56.20	56.16
B γ	71.60	71.85	71.46
B2	111.77	113.40	112.90
A2	112.98	114.00	113.88
B6	120.61	121.45	120.94
B5	123.20	123.86	123.03
A5	123.70	124.12	123.41
A6	130.39	132.09	131.54
A1	133.59	134.97	134.47
A4	138.36	139.27	137.88
B4	139.08	140.00	138.51
B1	140.74	142.52	141.90
A3	149.92	150.80	149.50
B3	151.59	152.59	151.29
Ac C=O	168.90	168.75	169.22
Ac C=O	169.03	168.75	169.25
γ	176.43	176.77	177.46
1H			
AcMe	2.21		2.11
AcMe	2.29		2.21
B β	2.50		2.69
β	2.59		2.82
A α1	3.00		2.95
A α2	3.25		3.12
OMe	3.73		3.65
OMe	3.81		3.72
B α	3.95		4.09
B γ1	4.02		4.05
B γ2	4.22		4.11
A5	6.51		6.28
B6	6.71		6.75
B2	6.63		6.87
A2	6.77		6.98
B5	6.98		7.02

Compound Number 3017



6-Hydroxy-4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-3a,4,9,9a-tetrahydro-3H-naphtho[2,3-c]furan-1-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
B β	2.67	m	
A β	2.67	m	
A α	3.07	dd	16.2, 4.5
OMe	3.78	s	
OMe	3.82	s	
B α	3.95	bd	9.5
B γ	4.10	m	
A5	6.26	d	0.9
B6	6.69	dd	8.0, 2.0
A2	6.79	s	
B2	6.80	d	2.0
B5	6.80	d	8.0

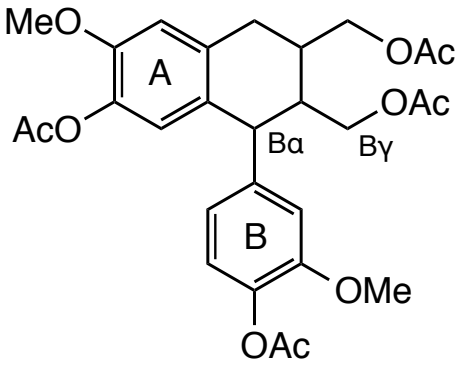
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α		29.73		
β		41.98		
B β		47.61		
B α		49.95		
OMe		55.99		
OMe		56.03		
B γ		71.78		
B2		112.25		
A2		112.93		
B5		115.61		
A5		116.23		
B6		121.92		
A1		126.77		
A6		132.87		
B1		135.09		
A4		145.61		
B4		146.29		
A3		146.89		
B3		148.42		
γ		177.15		

Notes:

jrlz33
Liming Zhang, isolate from mild acidolysis

Compound Number 3018



Acetic acid 8-(4-acetoxy-3-methoxyphenyl)-6,7-bis-acetoxy methyl-3-methoxy-5,6,7,8-tetrahydronaphthalen-2-yl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.02	s	
Ac Me	2.11	s	
Ac Me	2.22	s	
Bβ	2.16	m	
β	2.29	m	
α	2.92	m	
OMe	3.74	s	
OMe	3.78	s	
B γ1	3.92	dd	11.7, 3.6
B α	4.02	d	10.5
B γ2	4.09	m	
A γ1	4.11	m	
A γ2	4.23	dd	11.1, 5.3
A5	6.34	bs	
B6	6.74	dd	8.1, 2.0
A2	6.87	s	
B2	6.92	d	2.0
B5	6.99	d	8.1

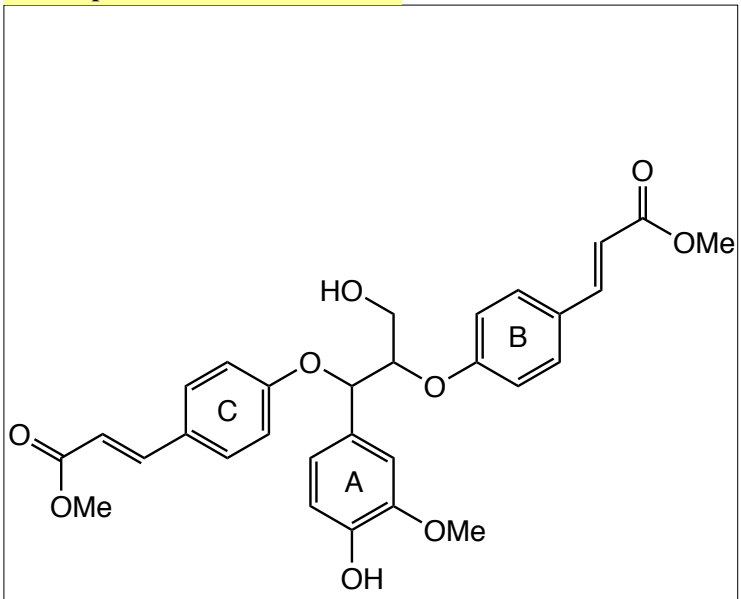
Notes:

jrlz27
Liming Zhang, isolate from mild acidolysis

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.56	20.36		
Ac Me	20.65	20.47		
Ac Me	20.77	20.69		
Ac Me	20.82	20.72		
α	33.02	33.53		
β	35.13	36.29		
B β	43.44	44.25		
B α	47.22	47.98		
OMe	55.83	56.17		
OMe	55.91	56.19		
B γ	63.04	63.57		
γ	66.20	66.74		
A2	111.81	112.90		
B2	113.17	114.53		
B6	121.52	121.11		
B5	122.81	123.64		
A5	123.71	124.16		
A6	131.13	132.26		
A1	134.05	135.25		
A4	138.03	139.17		
B4	138.03	139.63		
B1	142.77	144.24		
A3	149.35	150.46		
B3	151.16	152.28		
Ac C=O	168.91	168.93		
Ac C=O	169.11	168.96		
Ac C=O	170.80	171.06		
Ac C=O	170.97	171.06		

Compound Number 3019



erythro

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

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.70	s	
C γ OMe	3.71	s	
A3 OMe	3.78	s	
γ 's	3.95	m	5.8
γ OH	4.16	t	5.8
β	4.88	m	
α	5.60	d	5.5
C β	6.34	d	16.0
B β	6.37	d	16.0
A5	6.79	d	8.1
A6	7.00	m	
C2,6	6.97	m	8.8
B2,6	7.02	m	8.8
A2	7.12	d	1.9
C3,5	7.50	m	8.6
B3,5	7.54	m	8.6
C α	7.55	d	16.0
B α	7.59	d	16.0

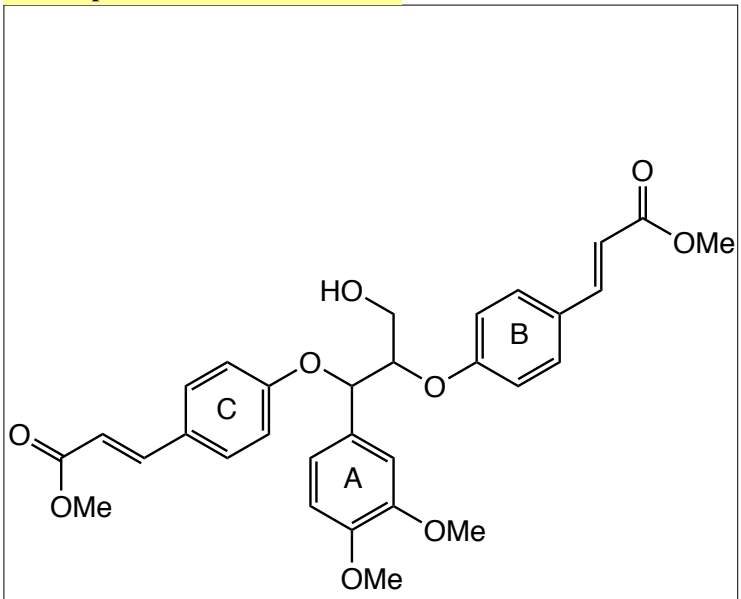
Notes:

jrf101.C9-12
Authenticated assignments in acetone.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
C γ OMe	51.55	51.52	51.27	
B γ OMe	51.59	51.53	55.63	
A3 OMe	55.92	56.26	55.80	
γ	61.43	61.42	59.79	
α	78.70	79.32	77.75	
β	81.89	82.67	81.24	
A2	109.26	112.00	111.78	
A5	114.48	115.55	115.29	
B β	115.68	116.15	115.13	
C β	115.86	116.25	115.13	
C2	116.24	117.23	116.20	
C6	116.24	117.23	116.20	
B2	116.54	117.34	116.24	
B6	116.54	117.34	116.24	
A6	120.21	121.43	120.28	
C1	127.73	128.19	126.74	
B1	128.00	128.22	126.86	
A1	128.67	129.37	127.73	
B3	129.57	130.46	129.93	
B5	129.57	130.46	129.93	
C3	129.61	130.48	129.93	
C5	129.61	130.48	129.93	
C α	144.12	144.87	144.16	
B α	144.23	144.94	144.26	
A4	145.72	147.35	146.29	
A3	146.78	148.23	147.31	
C4	159.14	160.49	159.17	
B4	159.81	161.67	160.5	
C γ	167.62	167.67	166.86	
B γ	167.63	167.72	166.92	

Compound Number 3020



erythro

3-(4-{1-(3,4-dimethoxyphenyl)-3-hydroxy-2[4-(2-methoxy-carbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.693	s	
C γ OMe	3.711	s	
A4 OMe	3.732	s	
A3 OMe	3.752	s	
γ 's	3.954	m	5.9, *
γ OH	4.157	t	5.9
β	4.881	m	5.5, 4.9
α	5.603	d	5.5
C β	6.335	d	16.0
B β	6.363	d	16.0
A5	6.876	d	8.2
C2,6	6.973	m	8.8
B2,6	7.015	m	8.7
A6	7.047	dd	8.2, 1.9
A2	7.126	d	1.9
C3,5	7.515	m	8.8
B3,5	7.550	m	8.7
C α	7.543	d	16.0
B α	7.582	d	16.0

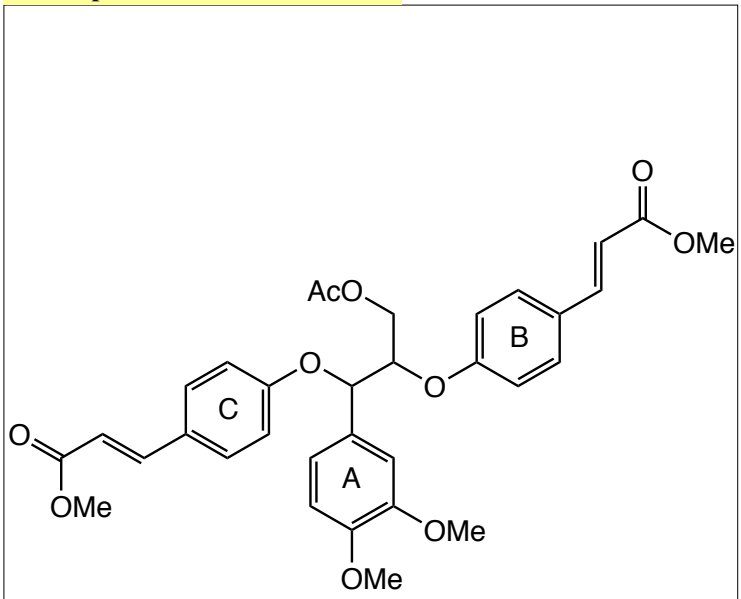
Notes:

jrf119.C2
assignments not authenticated - from #3019

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
C γ OMe		51.52		
B γ OMe		51.52		
A4 OMe		55.97		
A3 OMe		56.12		
γ		61.38		
α		79.21		
β		82.64		
A2		112.38		
A5		112.47		
B β		116.21		
C β		116.33		
C2		117.26		
C6		117.26		
B2		117.38		
B6		117.38		
A6		121.02		
C1		128.26		
B1		128.32		
B3		130.51		
B5		130.51		
C3		130.52		
C5		130.52		
A1		130.56		
C α		144.87		
B α		144.96		
A4		150.25		
A3		150.26		
C4		160.50		
B4		161.69		
C γ		167.66		
B γ		167.72		

Compound Number 3021



erythro

3-(4-{3-carboxyoxy-1-(3,4-dimethoxyphenyl)-2-[4-(2-methoxy carbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.920	s	
B γ OMe	3.694	s	
C γ OMe	3.712	s	
A4 OMe	3.736	s	
A3 OMe	3.759	s	
γ 1	4.460	dd	11.9, 6.2
γ 2	4.507	dd	11.9, 3.8
β	5.084	m	6.2, 5.8, 3.8
α	5.629	d	5.8
C β	6.343	d	16.0
B β	6.378	d	16.0
A5	6.888	d	8.3
C2,6	6.992	m	8.7
B2,6	7.018	m	8.7
A6	7.073	dd	8.3, 2.0
A2	7.161	d	2.0
C3,5	7.527	m	8.7
B3,5	7.570	m	8.7
Cα	7.548	d	16.0
Bα	7.584	d	16.0

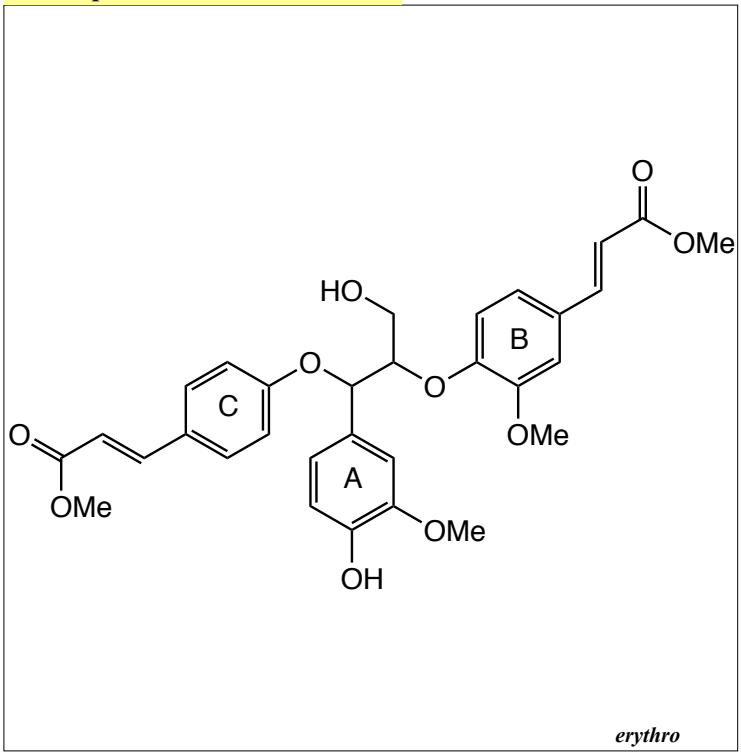
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me		20.58		
C γ OMe		51.54		
B γ OMe		51.57		
A4 OMe		55.97		
A3 OMe		56.14		
γ		63.49		
α		79.32		
β		79.81		
A2		112.17		
A5		112.47		
B β		116.49		
C β		116.55		
C2		117.27		
C6		117.27		
B2		117.41		
B6		117.41		
A6		120.88		
C1		128.55		
B1		128.74		
A1		130.09		
B3		130.53		
B5		130.53		
C3		130.61		
C5		130.61		
C α		144.81		
B α		144.81		
A4		150.38		
A3		150.43		
C4		160.24		
B4		161.18		
C γ		167.66		
B γ		167.69		
γ Ac C=O		170.79		

Notes:

jrf137
assignments not authenticated - from #3019/3020
A4 vs A3 OMe may be switched

Compound Number 3022



erythro

3-(4-{3-hydroxy-1-(4-hydroxy-3-methoxyphenyl)-2-[2-methoxy-4-(2-methoxycarbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.696	s	
C γ OMe	3.720	s	
A3 OMe	3.804	s	
B3 OMe	3.853	s	
γ 's	3.95	m	
β	4.791	m	-
α	5.621	d	5.3
C β	6.330	d	16.0
B β	6.417	d	16.0
A5	6.798	d	8.2
C2,6	6.978	m	8.8
A6	7.013	dd	8.2, 1.9
B5	7.065	d	8.3
B6	7.123	dd	8.3, 1.9
A2	7.205	d	1.9
B2	7.283	d	1.9
C3,5	7.493	d	8.8
C α	7.554	d	16.0
B α	7.584	d	16.0

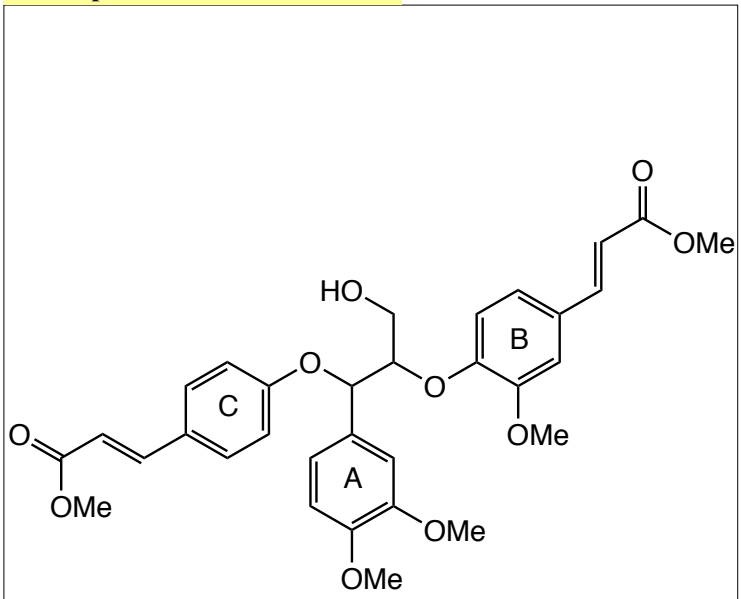
Notes:

jrf103.C12-25
fully authenticated in acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B γ OMe	51.55	51.52	51.27
C γ OMe	51.66	51.56	51.28
A3 OMe	55.83	56.22	55.48
B3 OMe	55.96	56.32	55.79
γ	61.29	61.31	59.66
α	78.46	79.44	77.95
β	86.25	84.21	81.84
B2	110.87	112.14	111.43
A2	109.37	112.21	112.01
A5	114.49	115.38	114.89
C β	115.62	116.16	115.16
B β	116.77	116.59	115.24
C2	116.28	117.23	116.22
C6	116.28	117.23	116.22
B5	120.21	117.54	115.45
A6	119.50	121.53	120.44
B6	122.14	123.04	122.48
C1	127.67	128.13	126.79
B1	129.92	129.21	127.27
A1	129.32	129.39	127.54
C3	129.57	130.42	129.91
C5	129.57	130.42	129.91
C α	144.21	144.89	144.18
B α	144.28	145.23	144.61
A4	145.68	147.29	146.27
A3	146.78	148.17	147.24
B4	149.40	151.24	149.76
B3	151.14	151.54	150.11
C4	159.30	160.57	159.25
C γ	167.39	167.68	166.86
B γ	167.64	167.71	166.95

Compound Number 3023



erythro

3-(4-{1-(3,4-dimethoxyphenyl)-3-hydroxy-2-[2-methoxy-4-(2-methoxycarbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.693	s	
C γ OMe	3.715	s	
A3 OMe	3.741	s	
A4 OMe	3.773	s	
B3 OMe	3.865	s	
γ *	*	*	-
β	4.787	m	-
α	5.640	d	5.3
C β	6.337	d	16.0
B β	6.416	d	16.0
A5	6.871	d	8.3
C2,6	6.981	m	8.8
A6	7.067	dd	8.3, 1.9
B5	7.068	d	8.3
B6	7.134	dd	8.3, 1.9
A2	7.200	d	1.9
B2	7.302	d	1.9
C3,5	7.517	d	8.8
C α	7.537	d	16.0
B α	7.573	d	16.0

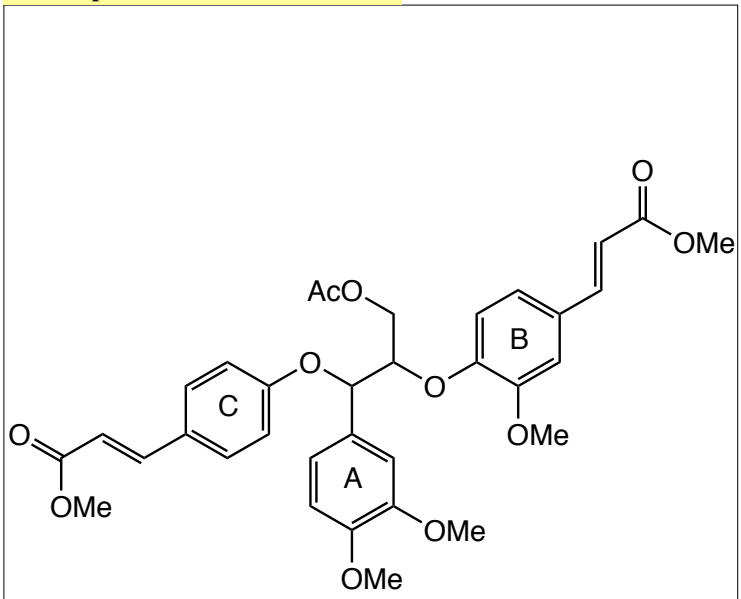
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B γ OMe		51.52		
C γ OMe		51.55		
A4 OMe		55.98		
A3 OMe		56.07		
B3 OMe		56.37		
γ		61.29		
α		79.37		
β		84.19		
B2		112.19		
B5		112.24		
A2		112.70		
C β		116.27		
B β		116.67		
C2		117.29		
C6		117.29		
B5		117.60		
A6		121.14		
B6		123.10		
C1		128.25		
B1		129.30		
C3		130.49		
C5		130.49		
A1		130.59		
C α		144.91		
B α		145.25		
A4		150.20		
A3		150.23		
B4		151.31		
B3		151.65		
C4		160.63		
C γ		167.68		
B γ		167.71		

Notes:

jrf121.C5-7
assignments not authenticated - from #3022 and 3020
A4 vs A3 OMe may be switched
*γ and γ-OH protons buried, C-H correlations not run.

Compound Number 3024



erythro

3-(4-{3-carboxyoxy-1-(3,4-dimethoxyphenyl)-2-[2-methoxy-4-(2-methoxycarbonylvinyl)phenoxy]propoxy}phenyl)acrylic acid methyl

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.920	s	
B γ OMe	3.695	s	
C γ OMe	3.716	s	
A3 OMe	3.745	s	
A4 OMe	3.775	s	
B3 OMe	3.877	s	
γ1	4.428	dd	11.9, 3.8
γ2	4.487	dd	11.9, 6.2
β	4.988	m	6.2, 5.3, 3.8
α	5.659	d	5.3
C β	6.345	d	16.0
B β	6.431	d	16.0
A5	6.888	d	8.3
C2,6	6.995	m	8.8
B5	7.051	m	8.3
A6	7.066	dd	8.3, 2.0, 0.4
B6	7.143	dd	8.3, 2.0, 0.4
A2	7.190	d	2.0
B2	7.323	d	2.0
C3,5	7.527	m	8.8
C α	7.553	d	16.0
B α	7.576	d	16.0

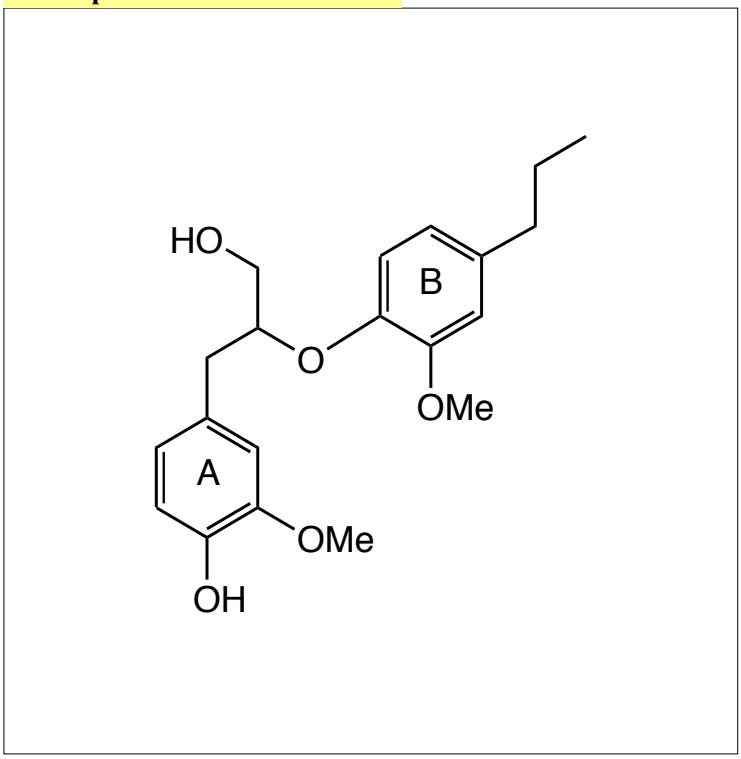
Notes:

jrf139
assignments not authenticated - from #3023 and 3021
A4 vs A3 OMe may be switched
Note γ's, J's switch from #3021!!

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
g Ac Me		20.61		
B γ OMe		51.54		
C γOMe		51.58		
A4 OMe		55.99		
A3 OMe		56.09		
B3 OMe		56.35		
γ		63.49		
α		79.62		
β		81.21		
A2		112.24		
B5		112.38		
B2		112.38		
C β		116.42		
B β		116.98		
C2		117.28		
C6		117.28		
B5		118.21		
A6		120.82		
B6		122.93		
C1		128.46		
B1		129.89		
A1		130.14		
C3		130.52		
C5		130.52		
C α		144.85		
B α		145.14		
A4		150.33		
A3		150.37		
B4		150.72		
B3		151.80		
C4		160.44		
C γ		167.67		
B γ		167.67		
γ OAc C=O		170.79		

Compound Number 3025



3-(4-hydroxy-3-methoxyphenyl)-2-(2-methoxy-4-propylphenoxy)propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.895	t	7.3
B β	1.585	m	
B α	2.492	m	
α1	2.91	m	
α2	2.94	m	
γ	3.59	m	
γ OH	3.731	t	6.1
OMe	3.786	s	
OMe	3.802	s	
β	4.308	m	
B6	6.646	ddt	8.1, 2.1, 0.6
A5	6.72	m	
A6	6.72	m	
B2	6.816	d	2.1
B5	6.827	d	8.1
A2	6.918	m	
Ar OH	7.333	s	

Notes:

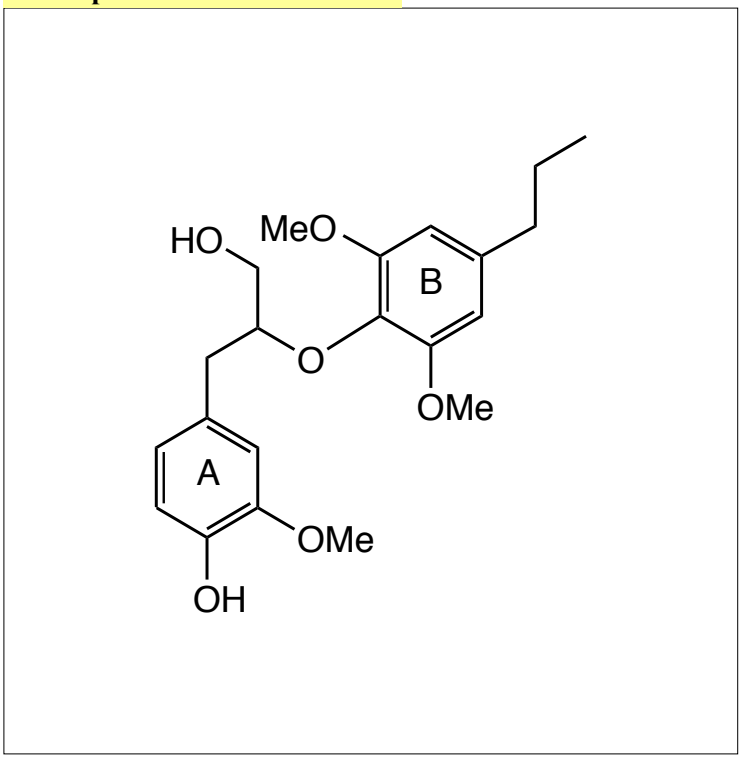
jrbha69

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B γ	13.77	14.01	13.75
B β	24.58	25.39	24.29
α	37.37	37.74	36.52
B α	37.76	38.22	36.97
OMe	55.76	56.15	55.49
OMe	55.89	56.20	55.58
γ	63.41	63.38	61.82
β	85.32	83.67	80.83
B2	112.16	113.85	112.89
A2	112.32	113.99	113.64
A5	114.34	115.49	115.19
B5	119.95	118.72	115.70
B6	121.00	121.37	120.21
A6	122.08	122.83	121.63
A1	129.75	130.58	129.16
B1	138.23	137.46	135.30
A4	144.20	145.88	144.79
B4	145.33	146.82	145.45
A3	146.44	148.05	147.26
B3	150.88	151.63	149.69

1H	CDCl3	DMSO
B γ	0.915	0.856
B β	1.594	1.531
B α	2.504	2.46
α1	2.866	2.733
α2	3.040	2.831
γ1	3.574	
γ2	3.656	
γ OH		4.761
OMe	3.823	3.680
OMe	3.841	3.703
β	4.160	4.265
Ar-OH	5.611	8.70

Compound Number 3026



2-(2,6-dimethoxy-4-propylphenoxy)-3-(4-hydroxy-3-methoxyphenyl)propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.917	t	7.3
B β	1.619	m	
B α	2.523	dd	
α1	2.941	dd	13.6, 8.2
α2	3.077	dd	13.6, 5.4
γ1	3.392	m	12.0, 4.1
γ2	3.483	m	12.0, 3.4
γ OH	3.5	m	
A OMe	3.809	s	
B OMe	3.817	s	
β	4.128	m	
B2,6	6.540	s	
A6	6.711	dd	8.0, 1.8
A5	6.740	dd	8.0, 0.4
A2	6.892	d	1.8
Ar OH	7.349	s	

Notes:

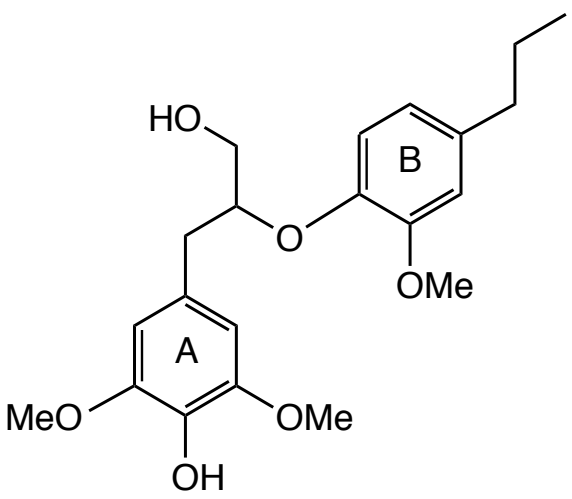
jrbha61
Hγ's are perfect dd's after adding D2O to acetone - otherwise complex multiplets; J's are from D2O exchanged spectra. All spectra ref'd to solvent, Acetone 2.04, 29.8
CDCl3 7.24, 77.0, DMSO 2.49, 39.5

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B γ	13.76	14.06	13.73
B β	24.51	25.30	24.10
α	37.28	38.00	36.86
B α	38.39	38.91	37.64
A OMe	55.81	56.17	55.51
B OMe	55.97	56.41	55.81
γ	62.17	62.77	61.65
β	84.36	85.24	83.39
B2	105.42	106.55	105.58
B6	105.42	106.55	105.58
A2	112.20	113.87	113.58
A5	114.15	115.50	115.06
A6	122.03	122.78	121.64
A1	130.19	130.81	129.36
B4	133.40	134.92	133.46
B1	138.77	139.25	137.62
A4	143.99	145.78	144.60
A3	146.31	148.03	147.11
B3	152.99	154.09	152.76
B5	152.99	154.09	152.76

1H	CDCl3		DMSO
B γ	0.928		0.886
B β	1.614		1.573
B α	2.513		2.753
α1	2.966		2.871
α2	3.192		~3.35?
γ1	3.418		~3.35?
γ2	3.54		~3.35?
γ OH	3.56		~3.35?
A OMe	3.805		3.697
B OMe	3.831		3.708
β	4.150		4.068
B2,6	6.392		6.465
A6	6.745		6.583
A5	6.809		6.641
A2	6.796		6.763
Ar OH	5.698		8.634

Compound Number 3027



3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2-methoxy-4-propylphenoxy)propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.894	t	7.4
B β	1.585	m	
B α	2.491	m	
α1	2.85	dd	13.9, 6.2
α2	2.922	dd	13.9, 6.1
γ	3.602	m	
γ OH	3.734	t	
A OMe	3.770	s	
B OMe	3.806	s	
β	4.335	m	
A2,6	6.596	s	
B6	6.646	ddt	8.2, 2.1, 0.6
B2	6.817	d	2.1
B5	6.833	d	8.2
Ar OH	6.940		

Notes:

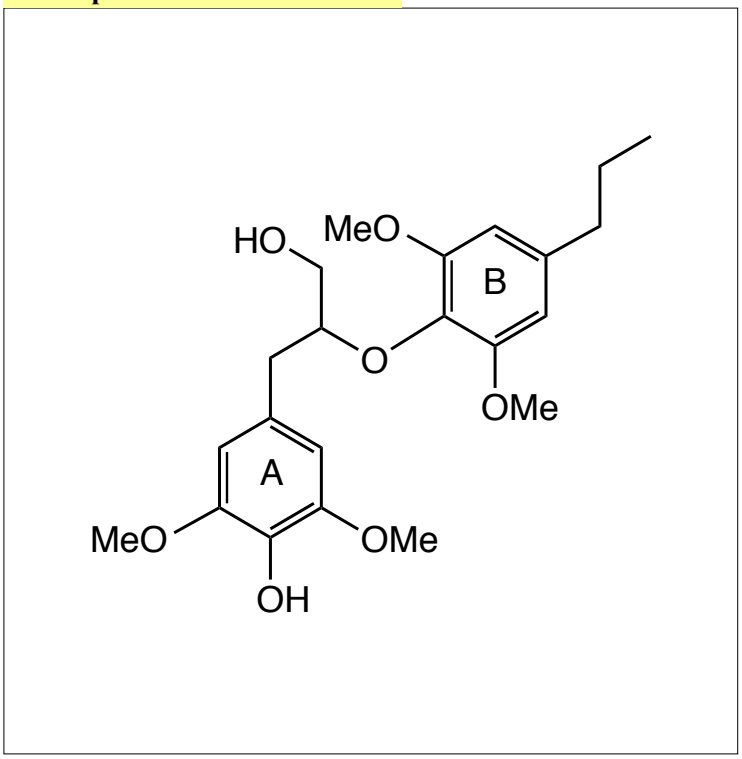
jrbha67

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B γ	13.77	14.01	13.67
B β	24.57	25.40	24.22
A α	37.76	38.21	36.90
B α	37.94	38.23	36.90
B OMe	55.77	56.19	55.47
A OMe	56.28	56.56	55.82
γ	63.47	63.46	61.84
β	85.35	83.47	80.56
A2	106.13	107.93	106.83
A6	106.13	107.93	106.83
B2	112.30	113.81	112.74
B5	120.04	118.54	115.44
B6	121.03	121.36	120.11
A1	128.98	129.59	128.24
A4	133.32	135.34	133.78
B1	138.31	137.38	135.09
B4	145.32	146.85	145.41
A3	146.97	148.48	147.64
A5	146.97	148.48	147.64
B3	150.89	151.57	149.53

1H	CDCl3		DMSO
B γ	0.910		0.86
B β	1.589		1.54
B α	2.499		2.45
α1	2.856		2.74
α2	3.032		2.84
γ1	3.578		
γ2	3.655		
γ OH			4.75
A OMe	3.831		3.68
B OMe	3.841		3.71
β	4.160		4.30
A2,6	6.478		6.49
B6	6.628		6.62
B2	6.697		6.76
B5	6.651		6.83
Ar OH	8.03		8.03

Compound Number 3028



3-(4-hydroxy-3,5-dimethoxyphenyl)-2-(2,5-dimethoxy-4-propylphenoxy)propan-1-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ	0.917	t	7.4
B β	1.620	m	
B α	2.525	m	
α1	2.925	dd	13.6, 8.1
α2	3.074	dd	13.6, 5.3
γ1	3.402	m	12.0, 4.1
γ2	3.486	m	12.0, 3.6
γ OH	3.47	m	
A OMe	3.793	s	
B OMe	3.825	s	
β	4.142	m	
B2,6	6.544	s	
A2,6	6.573	s	
Ar OH	6.949	s	

Notes:

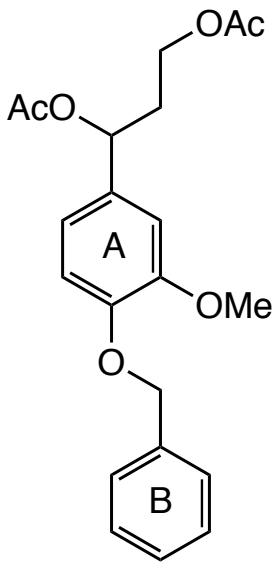
jrbha63 Hγ's are dd's after adding D2O to acetone - otherwise complex multiplets; J's are from D2O exchanged spectra. In acetone: Many peaks were split with a 2:1 ratio. Aα 38.38 & 38.50, Bα 38.80 & 38.93, A1 129.69 & 129.86, B4 134.94 & 134.97, A4 135.24 & 135.28, B1 139.10 & 139.26 , A3/5 148.44 & 148.49, B3/5 154.07 & 154.12

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B γ	13.70	14.06	13.82
B β	24.47	25.30	24.18
α	37.65	38.38	37.35
B α	38.24	38.80	37.60
A OMe	55.96	56.43	55.91
B OMe	56.19	56.58	55.97
γ	62.19	62.93	61.88
β	84.19	85.20	83.32
B2	105.42	106.57	105.67
B6	105.42	106.57	105.67
A2	106.12	107.83	106.89
A6	106.12	107.83	106.89
A1	129.21	129.69	128.54
B4	133.07	134.94	133.46
A4	133.28	135.24	133.70
B1	138.64	139.10	137.61
A3	146.75	148.44	147.65
A5	146.75	148.44	147.65
B3	152.92	154.07	152.79
B5	152.92	154.07	152.79

1H	CDCl3		DMSO
B γ	0.917		0.879
B β	1.592		1.562
B α	2.489		2.45
α1	2.950		2.756
α2	3.175		2.868
γ1	3.408		
γ2	3.542		
γ OH	3.47		4.334?
A OMe	3.798		3.692
B OMe	3.829		3.696
β	4.152		4.103
B2,6	6.386		6.449
A2,6	6.498		6.462
Ar OH	5.493		8.044

Compound Number 3029



1-(4-benzyloxy-3-methoxyphenyl)-propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.99	s	
α Ac Me	2.03	s	
β	2.18	m	
OMe	3.83	s	
γ	4.08	m	
B α	5.09	s	
α	5.85	dd	8.2, 5.7
A6	6.91	dd	8.3, 2.0
A5	6.99	d	8.3
A2	7.04	d	2.0
Bz H's	7.28-7.51	m	

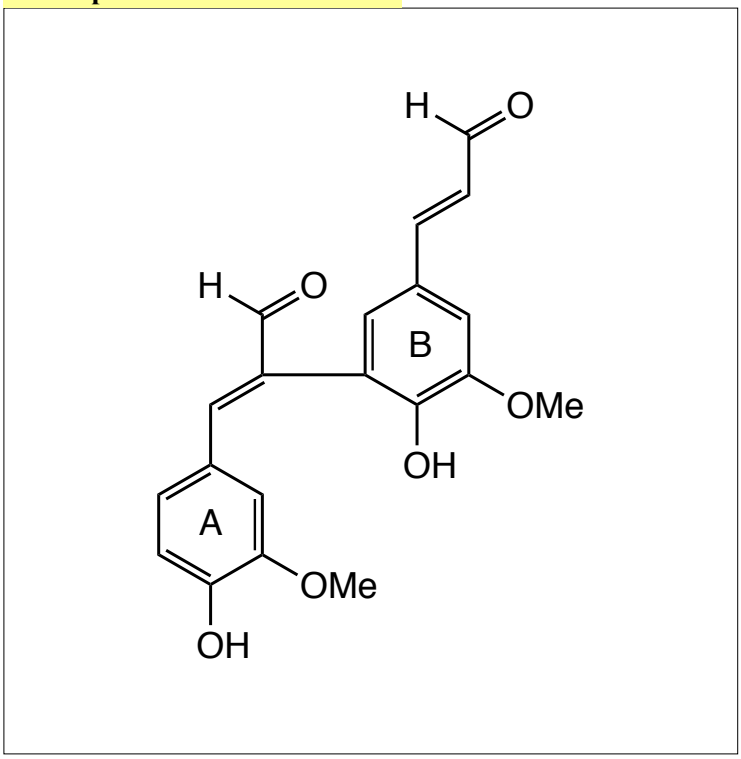
Notes:

JRHKC25

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me		20.70		
α Ac Me		21.01		
β		35.78		
OMe		56.16		
γ		61.20		
B α		71.26		
α		73.17		
A2		111.49		
A5		114.64		
A6		119.58		
B3		128.28		
B5		128.28		
B2		129.09		
B6		129.09		
B4		128.45		
A1		134.19		
B1		138.33		
A4		149.02		
A3		150.68		
α Ac C=O		170.17		
γ Ac C=O		170.80		

Compound Number 3030



beta-[5-(2-formylvinyl)-2-hydroxy-3-methoxyphenyl] coniferyl aldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.47	s	
B3 OMe	3.96	s	
B β	6.66	dd	15.8, 7.8
A5	6.77	d	8.3
A2	6.87	d	2.0
A6	6.98	dd	8.3, 2.0
B6	7.01	d	2.0
B2	7.44	d	2.0
A α	7.57	s	
B α	7.57	d	15.8
OH	8.43	s	
B γ	9.61	d	7.8
A γ	9.69	s	

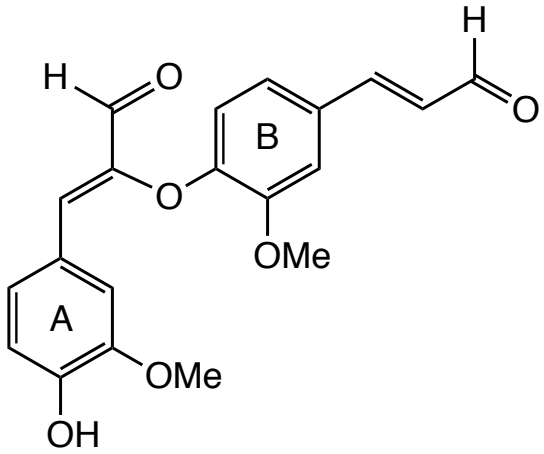
Notes:

JRHKB117 (Higuchi)
13mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe		55.55		
B3 OMe		56.63		
B2		110.61		
A2		113.56		
A5		115.95		
A β		123.15		
B6		126.36		
A6		126.92		
B β		127.29		
A1		127.38		
B1		127.44		
B5		136.33		
A3		148.13		
B4		148.59		
A3		149.30		
B4		150.16		
A α		151.36		
B α		153.79		
A γ		193.43		
B γ		193.96		

Compound Number 3031



beta-[4-(2-formylvinyl)-2-methoxyphenoxy] coniferyl aldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J

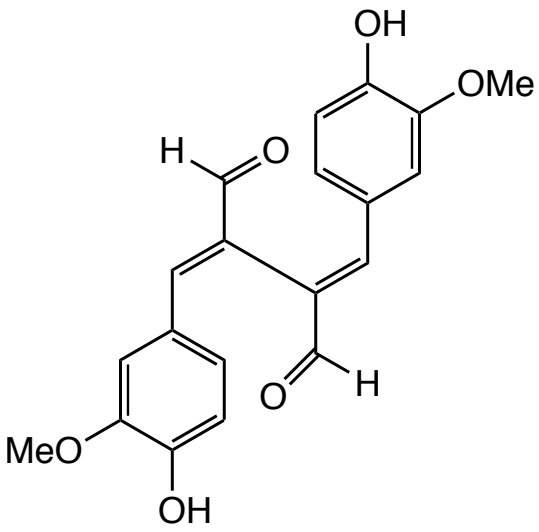
Notes:

JRHKB119 (Higuchi)
4 mg

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe		56.01		
A3 OMe		56.52		
B2		112.55		
A2		113.98		
B5		115.25		
A5		116.25		
B6		123.63		
A1		125.31		
A6		126.80		
B β		128.32		
B1		130.20		
A α		138.21		
A β		147.70		
B3		148.48		
B4		148.90		
A3		150.37		
A4		150.56		
B α		153.15		
A γ		197.48		
B γ		193.85		

Compound Number 3032



2,3-diformyl-1,4-bis(4-hydroxy-3-methoxyphenyl) buta-1,3-diene

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.70	s	
5	6.82	d	8.31
6	7.21	dd	8.31, 2.15
2	7.28	d	2.15
α	7.78	s	
OH	8.29	s	
γ	9.66	s	

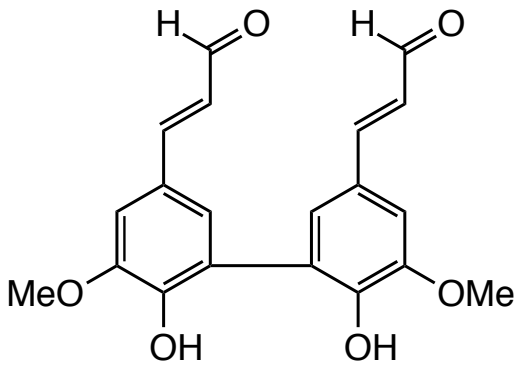
Notes:

JRHKb121 11mg
Higuchi
As this dimer contains a plane of symmetry the CSs are reported for one unit.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.11		
2		113.71		
5		116.24		
6		126.25		
1		127.47		
β		134.42		
3		148.41		
4		150.51		
α		152.83		
γ		192.74		

Compound Number 3033



5,5'-bis-coniferyl aldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.95	s	
β	6.68	dd	15.84, 7.84
6	7.27	s	2.0
2	7.36	s	2.0
α	7.59	s	15.84
γ	9.65	s	7.84

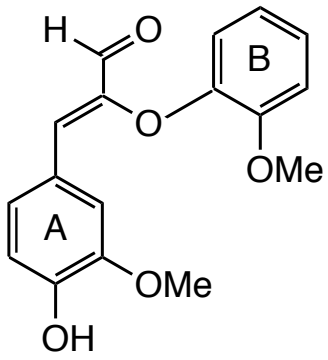
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.52		
2		110.00		
1		126.05		
5		126.13		
β		126.81		
6		127.10		
3		149.42		
4		149.63		
α		154.40		
γ		193.92		

Notes:

JRHKb123 37mg
Higuchi
As this dimer contains a plane of symmetry the CSs are reported for one unit.

Compound Number 3034



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe		55.84		
B3 OMe		56.17		
B2		113.51		
A2		113.82		
B5		114.85		
A5		116.07		
B6		121.34		
B1		123.35		
A1		125.49		
A6		126.57		
α		137.82		
B4		146.22		
β		148.09		
A3		148.30		
B3		149.89		
A4		150.20		
γ		187.90		

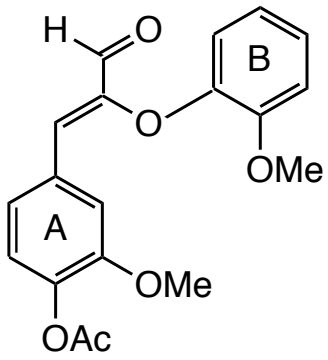
^{1}H (acetone)

Atom	H Shifts	Mult	J
A4 OMe	3.73	s	
B3 OMe	3.88	s	
B5	6.72	dd	8.0, 2.0
B6	6.76	ddd	8.2, 7.1, 2.0
A5	6.87	d	8.3
B1	6.95	ddd	8.2, 7.1, 2.0
B2	7.05	dd	8.2, 2.0
α	7.26	s	
A6	7.33	dd	8.3, 2.0
A2	7.59	d	2.0
γ	9.50	s	

Notes:

HKc63.4

Compound Number 3035



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.41		
A3 OMe		55.97		
B3 OMe		56.20		
B2		113.62		
A2		114.66		
B5		115.56		
B6		121.39		
B1		123.83		
A5		124.06		
A6		124.53		
A1		132.33		
α		135.40		
A4		142.47		
B4		146.01		
β		149.94		
B3		150.01		
A3		152.27		
Ac C=O		168.73		
γ		188.21		

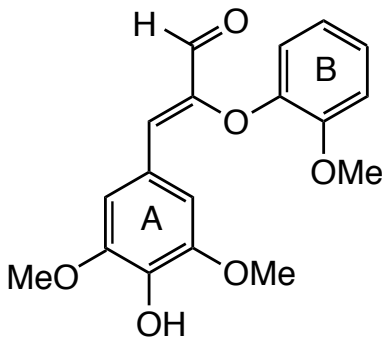
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.23	s	
A3 OMe	3.73	s	
B3 OMe	3.87	s	
B5	6.79	m	
B6	6.79	m	
B1	6.97	m	
B2	7.06	bd	7.8
A5	7.11	d	8.3
α	7.30	s	
A6	7.45	dd	8.3, 2.0
A2	7.68	d	2.0
γ	9.55	s	

Notes:

HKc 63.4Ac

Compound Number 3036



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe		56.11		
A3 OMe		56.31		
A5 OMe		56.31		
A2		109.27		
A6		109.27		
B2		113.39		
B5		114.53		
B6		121.32		
B1		123.27		
A1		124.05		
α		138.23		
A4		139.74		
B4		146.16		
β		148.15		
A3		148.57		
A5		148.57		
B3		149.76		
γ		187.91		

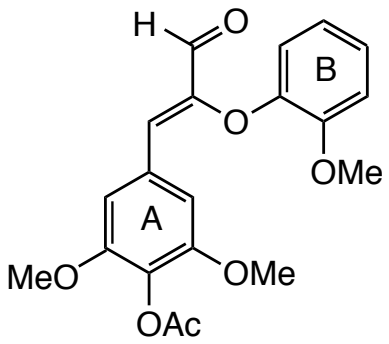
^{1}H (acetone)

Atom	H Shifts	Mult	J
A3,5 OMe	3.74	s	
B3 OMe	3.88	s	
B5	6.70	dd	8.2, 1.7
B6	6.76	ddd	8.2, 7.2, 1.5
B1	6.94	ddd	8.2, 7.2, 1.7
B2	7.05	dd	8.2, 1.5
A2,6	7.24	s	
α	7.26	s	
γ	9.51	s	

Notes:

HKd 59.1

Compound Number 3037



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.17		
B3 OMe		56.14		
A3 OMe		56.29		
A5 OMe		56.29		
A2		108.10		
A6		108.10		
B2		113.48		
B5		115.07		
B6		121.37		
B1		123.68		
A1		131.35		
A4		131.53		
α		136.12		
B4		145.97		
b		149.81		
B3		149.84		
A3		153.20		
A5		153.20		
Ac C=O		168.30		
γ		188.26		

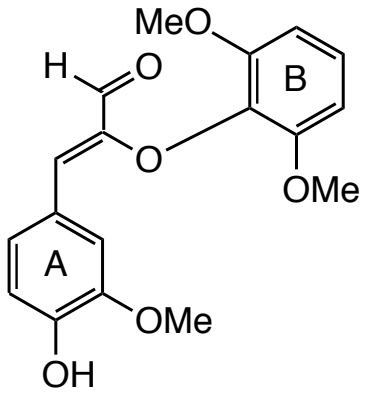
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.21	s	
A3,5 OMe	3.73	s	
B3 OMe	3.88	s	
B5	6.76	dd	8.2, 2.4
B6	6.77	ddd	8.2, 6.5, 1.4
B1	6.97	ddd	8.2, 6.5, 2.4
B2	7.06	dd	8.2, 1.4
A2,6	7.29	s	
α	7.31	s	
γ	9.57	s	

Notes:

HKd 59.1 Ac

Compound Number 3038



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe		56.07		
B3 OMe		56.53		
B5 OMe		56.53		
B2		106.40		
B6		106.40		
A2		114.55		
A5		115.95		
B1		124.17		
A6		125.77		
A1		126.72		
α		129.06		
B4		135.22		
A3		148.04		
A4		149.05		
β		150.82		
B3		152.47		
B5		152.47		
γ		186.64		

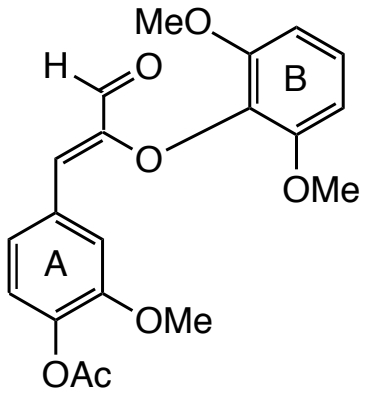
^{1}H (acetone)

Atom	H Shifts	Mult	J
B3,5 OMe	3.74	s	
A3 OMe	3.81	s	
α	6.64	s	
B2,6	6.65	d	8.2
A5	6.88	d	8.3
B1	6.99	dd	8.2, 7.6
A6	7.45	dd	8.3, 2.0
A2	7.60	d	2.0
γ	9.25	s	

Notes:

HKd 23.3

Compound Number 3039



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.24	s	
B3,5 OMe	3.75	s	
A3 OMe	3.80	s	
B2,6	6.67	d	8.3
α	6.71	s	
B1	7.01	dd	8.3, 7.9
A5	7.11	d	8.2
A6	7.54	dd	8.2, 1.9
A2	7.68	d	1.9
γ	9.32	s	

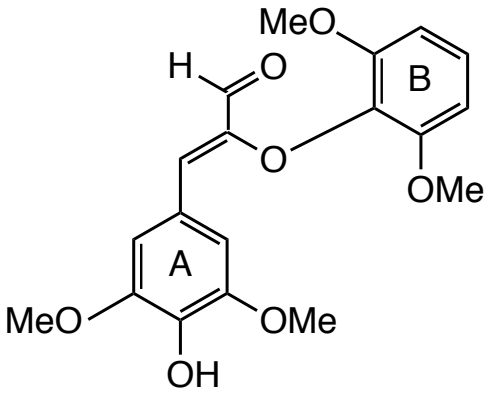
Notes:

HKd 23.3 Ac

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.45		
A3 OMe		56.09		
B3 OMe		56.52		
B5 OMe		56.52		
B2		106.29		
B6		106.29		
A2		115.15		
A5		123.78		
A6		124.04		
B1		124.53		
α		126.73		
A1		133.43		
B4		134.81		
A4		141.52		
A3		152.04		
β		152.11		
B3		152.41		
B5		152.41		
Ac C=O		168.85		
γ		187.00		

Compound Number 3040



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe		56.51		
A5 OMe		56.51		
B3 OMe		56.59		
B5 OMe		56.59		
B2		106.50		
B6		106.50		
A2		109.41		
A6		109.41		
B1		124.18		
A1		125.37		
α		129.08		
B4		135.21		
A4		138.72		
A3		148.44		
A5		148.44		
β		150.91		
B3		152.46		
B5		152.46		
γ		186.60		

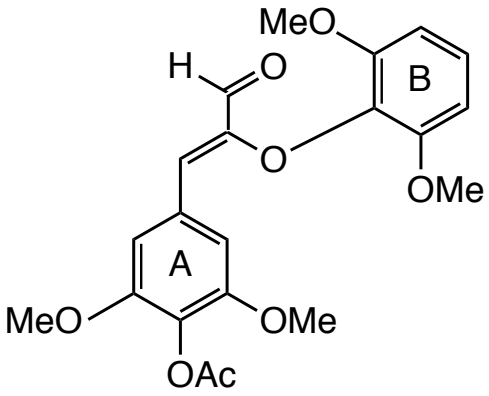
^{1}H (acetone)

Atom	H Shifts	Mult	J
B3,5 OMe	3.75	s	
A3,5 OMe	3.80	s	
α	6.63	s	
	6.66	d	8.3
B2,6	6.99	t	8.3
B1	7.31	s	
A2,6	9.25	s	
γ			

Notes:

HKd 63.1

Compound Number 3041



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.23	s	
A3,5 OMe	3.77	s	
B3,5 OMe	3.78	s	
B2,6	6.67	d	8.3
α	6.69	s	
B1	7.01	dd	8.6, 8.2
A2,6	7.34	s	
γ	9.32	s	

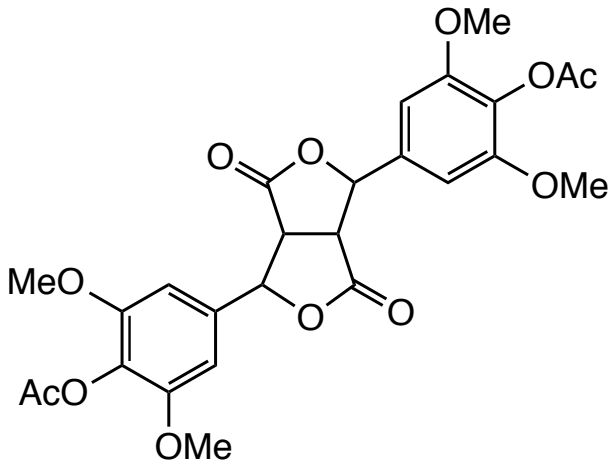
Notes:

HKd 63.1 Ac

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.22		
B3 OMe		56.35		
B5 OMe		56.35		
A3 OMe		56.56		
A5 OMe		56.56		
B2		106.37		
B6		106.37		
A2		108.07		
A6		108.07		
B1		124.51		
α		126.81		
A4		130.47		
A1		132.69		
B4		134.76		
β		152.09		
B3		152.35		
B5		152.35		
A3		153.01		
A5		153.01		
Ac C=O		168.43		
γ		186.95		

Compound Number 3042



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.18		
β		48.76		
3 OMe		55.56		
5 OMe		55.56		
α		82.61		
2		103.05		
6		103.05		
4		129.76		
1		137.84		
3		153.54		
5		153.54		
Ac C=O		168.50		
γ		175.77		

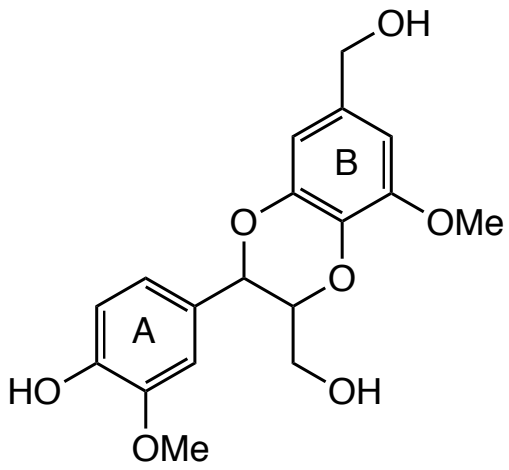
^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.23	s	
OMe	3.81	s	
β	4.20	s	
α	5.86	s	
2,6	6.81	s	

Notes:

FLj 144
As this dimer contains a plane of symmetry the CS's are reported for one unit.

Compound Number 3043



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe		56.26		
A3 OMe		56.32		
γ		61.83		
Bα		64.61		
α		76.97		
β		79.30		
B2		104.10		
B6		108.55		
A2		111.90		
A5		115.70		
A6		121.49		
A1		129.50		
B4		133.24		
B1		135.46		
B5		145.19		
A4		147.92		
A3		148.44		
B3		149.84		

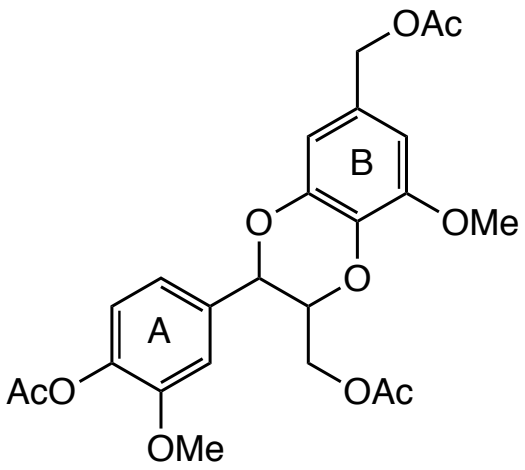
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.47	m	
γ2	3.76	m	
B3 OMe	3.81	s	
A3 OMe	3.85	s	
β	3.99	ddd	7.9, 3.9, 2.5
Bα	4.49	m	
α	4.95	d	7.9
B6	6.53	ddd	1.8, 0.75, 0.75
B2	6.60	d	1.8
A5	6.86	d	8.1
A6	6.94	ddd	8.1, 1.9, 0.5
A2	7.09	d	1.9
A4 OH	7.80	s	

Notes:

F. Lu
flm11

Compound Number 3044



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me		20.45		
γ Ac Me		20.49		
Bα Ac Me		20.81		
A3 OMe		56.36		
B3 OMe		56.44		
γ		63.36		
Bα		66.36		
β		75.97		
α		77.01		
B2		106.08		
B6		110.41		
A2		112.77		
A6		120.75		
A5		123.88		
B1		129.92		
B4		133.65		
A1		136.00		
A4		141.45		
B5		144.92		
B3		149.98		
A3		152.57		
A4 Ac C=O		168.86		
γ Ac C=O		170.62		
Bα Ac C=O		170.83		

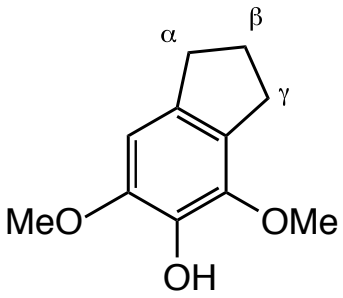
^{1}H (acetone)

Atom	H Shifts	Mult	J
Bα Ac Me	1.99	s	
γ Ac Me	2.03	s	
A4 Ac Me	2.24	s	
B3 OMe	3.83	s	
A3 OMe	3.84	s	
γ1	4.02	dd	12.4, 4.3
γ2	4.28	dd	12.4, 3.4
β	4.40	ddd	7.7, 4.3, 3.4
Bα	4.98	s	
α	5.04	d	7.7
B6	6.61	d	1.9
B2	6.66	d	1.9
A6	7.08	dd	8.1, 1.7
A5	7.11	d	8.1
A2	7.26	d	1.7

Notes:

F. Lu
flm11Ac

Compound Number 3045



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β		26.11		
γ		30.33		
α		33.51		
5 OMe		56.73		
3 OMe		59.83		
6		104.24		
2		128.60		
1		134.89		
4		138.17		
3		144.71		
5		148.47		

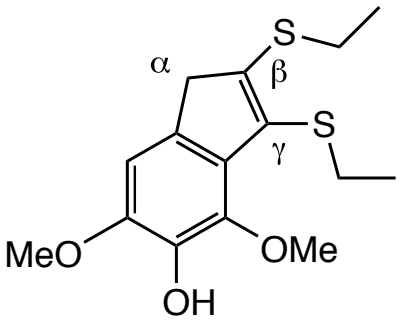
^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.98	quint	7.2
α	2.78	br t	7.2
γ	2.83	br t	7.2
5 OMe	3.77	s	
3 OMe	3.79	s	
6	6.58	s	
Benzene			
β	1.86	quin	7.37
α	2.71	td	7.37, 0.66
γ	2.86	t	7.37
5 OMe	3.28	s	
3 OMe	3.75	s	
6	6.32	s	

Notes:

HKE-11
Raney nickel reaction of hke5.5

Compound Number 3046



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ S-CH3		15.11		
β S-CH3		15.41		
β S-CH2		26.33		
γ S-CH2		29.12		
α		41.68		
5 OMe		56.91		
3 OMe		62.30		
6		105.00		
γ		126.93		
2		131.50		
1		133.78		
3		104.04		
4		141.58		
5		147.06		
β		148.43		

^{1}H (acetone)

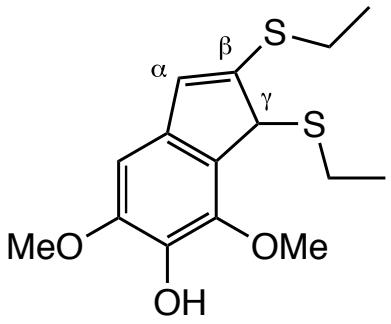
Atom	H Shifts	Mult	J
γ S-CH3	1.15	t	7.37
β S-CH3	1.30	t	7.37
γ S-CH2	2.89	q	7.37
β S-CH2	2.95	q	7.37
α	3.58	d	0.92
5 OMe	3.82	s	
3 OMe	3.85	s	
6	6.87	br t	0.92

Notes:

hke 5.4.1

Thioacidolysis product of β-O-4 (S-G) aldehyde dimer

Compound Number 3047



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ S-CH3		14.39		
β S-CH3		14.45		
γ S-CH2		22.23		
β S-CH2		26.80		
γ		52.56		
5 OMe		56.71		
3 OMe		60.09		
6		100.11		
α		124.89		
2		128.89		
1		135.82		
4		137.70		
β		145.14		
3		145.23		
5		149.46		

^{1}H (acetone)

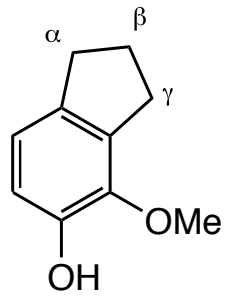
Atom	H Shifts	Mult	J
γ S-CH3	1.00	t	7.5
β S-CH3	1.33	t	7.37
γ S-CH2	2.22,2.04	dq, dq	12.1, 7.5
β S-CH2	2.94	q	7.37
5 OMe	3.82	s	
3 OMe	3.96	s	
γ	4.39	d	1.18
α	6.38	d	1.18
6	6.63	s	

Notes:

hke 5.5

Thioacidolysis product of γ-O-4 (S-G) aldehyde dimer

Compound Number 3048



6-methoxy-indan-5-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.99	quint	7.63
α	2.74	t	7.63
γ	2.76	t	7.63
OMe	3.79	s	
3	6.66	s	
6	6.78	s	

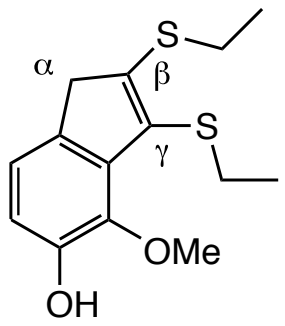
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β		26.45		
α		33.13		
γ		33.25		
OMe		56.48		
6		108.74		
3		111.56		
1		135.00		
2		136.73		
4		146.11		
5		147.01		

Notes:

hke87
Desulfurized (Raney-nickle Rxn)
thioacidolysis product of β-O-4 (G-S) aldehyde model compound

Compound Number 3049



2,3-bis-ethylsulfanyl-6-methoxy-1H-inden-5-ol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ S CH3	1.67	t	7.37
β S CH3	1.31	t	7.37
γ S CH2	2.81	q	7.37
β S CH2	2.99	q	7.37
α	3.58	d	0.79
OMe	3.83	s	
3	6.87	s	
6	7.06	br t	0.79

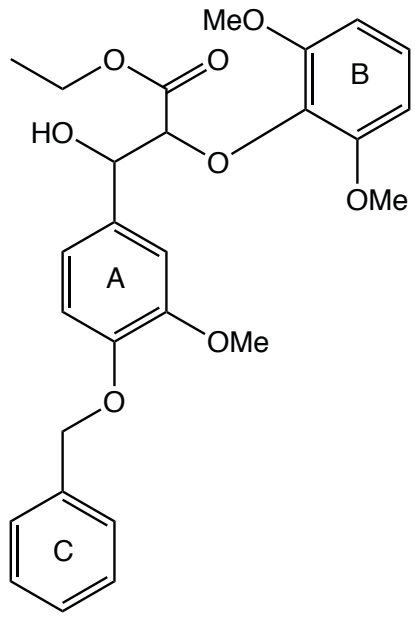
Notes:

hke83.3
Thioacidolysis product of β-O-4 (G-S) aldehyde dimer model.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β S CH3		15.47		
γ S CH3		15.74		
β S CH2		23.65		
γ S CH2		27.70		
α		41.57		
OMe		56.83		
4		106.37		
6		109.01		
γ		128.64		
1		133.31		
2		140.13		
5		146.09		
4		146.91		
β		148.16		

Compound Number 3050



erythro?

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.09	t	7.10
B OMe	3.75	s	
A OMe	3.82	s	
CH2	4.04	m	
β	4.68	d	5.39
α	4.96	d	5.39
C α	5.09	s	
B 2,6	6.64	d	8.16
A6	6.92	dd	8.29, 1.71
A5	6.96	d	8.29
B1	6.99	t	8.16
A2	7.17	d	1.71
C 3,4,5	7.27-7.40	m	
C 2,6	7.37	br d	7.37

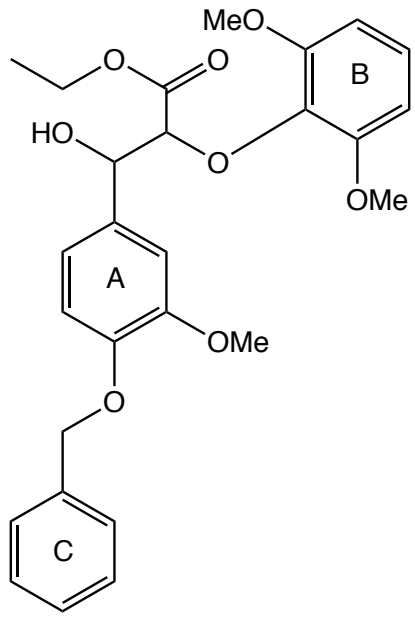
Notes:

hkd79.2C
possibly erythro

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3		14.41		
A OMe		56.13		
B OMe		56.44		
B OMe		56.44		
CH2		60.69		
C α		71.37		
α		74.31		
β		86.14		
B2		106.37		
B6		106.37		
A2		112.31		
A5		114.41		
A6		120.34		
B1		124.73		
C2		128.31		
C6		128.31		
C4		128.41		
C3		129.09		
C5		129.09		
A1		134.57		
B4		137.19		
C1		138.62		
A4		148.71		
A3		150.33		
B3		153.64		
B5		153.64		
γ		169.44		

Compound Number 3051



threo?

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	0.99	t	7.23
A OMe	3.79	s	
B OMe	3.82	s	
CH2	3.95	m	
β	4.02	d	8.42
α	4.84	d	8.42
C α	5.09	s	
B 2,6	6.71	d	8.5
A6	6.81	dd	8.29, 1.97
A5	6.94	d	8.29
A2	6.99	d	1.97
B1	7.05	t	8.55
C 3,4,5	7.29-7.39	m	
C 2,6	7.46	br d	7.37

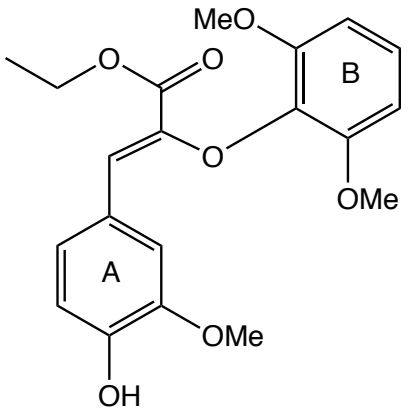
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3		14.30		
A OMe		56.15		
B OMe		56.42		
B OMe		56.42		
CH2		60.68		
C α		71.38		
α		76.04		
β		90.35		
B2		106.26		
B6		106.26		
A2		112.09		
A5		114.61		
A6		120.46		
B1		125.18		
C2		128.33		
C6		128.33		
C4		128.44		
C3		129.11		
C5		129.11		
A1		132.51		
B4		138.07		
C1		138.56		
A4		149.17		
A3		150.62		
B3		153.39		
B5		153.39		
γ		169.49		

Notes:

hkd79.2Ex
possibly threo

Compound Number 3052



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3		14.35		
A OMe		56.09		
B OMe		56.79		
B OMe		56.79		
CH2		61.05		
B2		107.08		
B6		107.08		
A2		114.38		
A5		115.74		
α		119.07		
B1		123.37		
A6		125.09		
A1		126.76		
B4		136.27		
β		143.08		
A3		148.01		
A4		148.10		
B3		152.01		
B5		152.01		
γ		163.74		

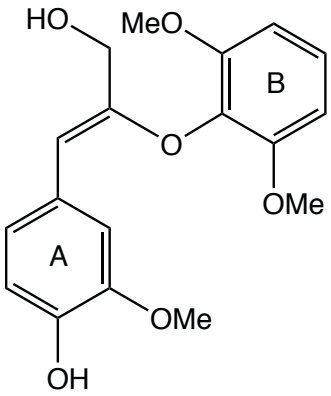
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.11	t	7.10
B OMe	3.74	s	
A OMe	3.76	s	
CH2	4.06	q	7.10
B 2,6	6.67	d	8.68
α	6.79	s	
A5	6.82	d	8.29
B1	6.94	t	8.68
A6	7.29	dd	8.29, 1.84
A2	7.52	d	1.84

Notes:

hkd 17.2.1.3

Compound Number 3053



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
1H data only				

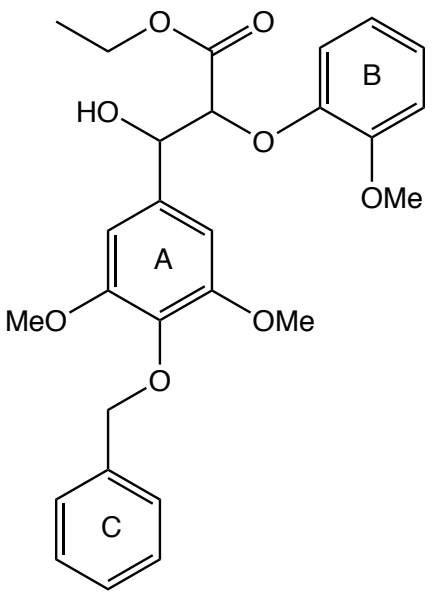
^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.76	s	
B OMe	3.77	s	
γ	3.97	br s	
α	5.75	br s	
B 2,6	6.68	d	8.42
A5	6.79	d	8.29
B1	7.07	t	8.42
A6	7.18	dd	8.29, 1.84
A2	7.46	d	1.84

Notes:

hkd87

Compound Number 3054



erythro?

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.08	t	7.1
B OMe	3.80	s	
A OMe	3.82	s	
CH2	4.04	m	7.1
β	4.72	d	5.52
Cα	4.93	s	
α	5.08	d	5.52
A 2,6	6.83	s	
B 5,6	6.77-6.85	m	
B 1,2	6.90-7.00	m	
C 3,4,5	7.24-7.38	m	
C 2,6	7.50	br d	7.37

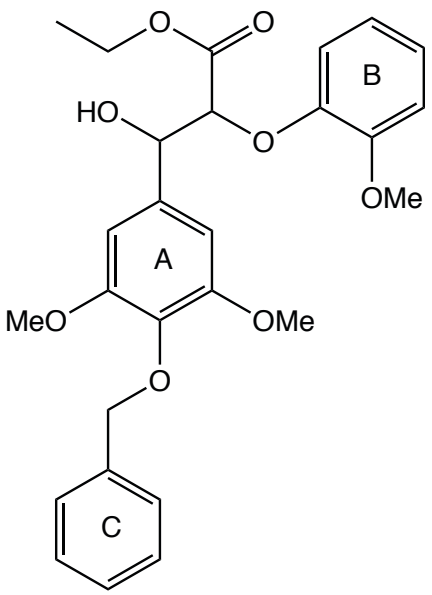
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3		14.35		
B OMe		56.36		
A OMe		56.44		
A OMe		56.44		
CH2		61.29		
C α		75.06		
α		75.59		
β		84.38		
A2		105.44		
A6		105.44		
B2		113.87		
B5		117.25		
B6		121.61		
B1		123.44		
C4		128.31		
C3		128.76		
C5		128.76		
C2		128.82		
C6		128.82		
A1		136.70		
A4		137.61		
C1		139.47		
B4		148.70		
B3		151.03		
A3		154.17		
A5		154.17		
γ		169.85		

Notes:

hkd35.2.1.2
possibly erythro (see 3055)
separated by cyclohexane:EtOAc:Acetic Acid (100:50:1)

Compound Number 3055



threo?

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.19	t	7.10
B OMe	3.77	s	
A OMe	3.83	s	
CH2	4.16	q	7.10
β	4.70	d	6.71
C α	4.94	s	
α	5.07	d	6.71
B 5,6	6.79	m	
A 2,6	6.90	s	
B 1,2	6.90-6.97	m	
C 3,4,5	7.24-7.37	m	
C 2,6	7.5	br d	7.37

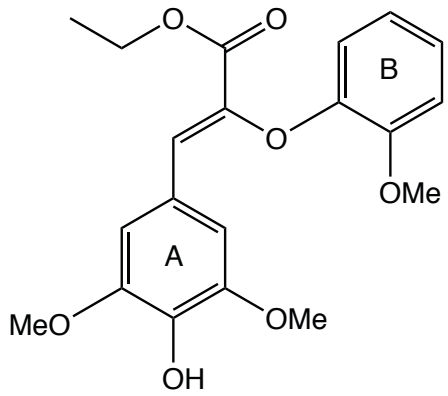
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3		14.16		
B OMe		56.28		
A OMe		56.40		
A OMe		56.40		
CH2		61.28		
α		74.84		
C α		75.04		
β		83.40		
A2		105.51		
A6		105.51		
B2		113.77		
B5		116.96		
B6		121.52		
B1		123.43		
C4		128.28		
C3		128.73		
C5		128.73		
C2		128.80		
C6		128.80		
A4		137.51		
A1		137.79		
C1		139.50		
B4		148.35		
B3		151.08		
A3		154.04		
A5		154.04		
γ		170.25		

Notes:

hkd35.2.1.1
Possible threo (see 3054)
separated by cyclohexane:EtOAc:Acetic Acid (100:50:1)

Compound Number 3056



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3		14.19		
B OMe		56.30		
A OMe		56.37		
A OMe		56.37		
CH2		61.58		
A2		109.09		
A6		109.09		
B2		113.72		
B5		114.15		
B6		121.49		
B1		123.24		
A1		124.12		
α		127.99		
β		138.78		
A4		138.94		
B4		146.94		
A3		148.50		
A5		148.50		
B3		149.87		
γ		164.06		

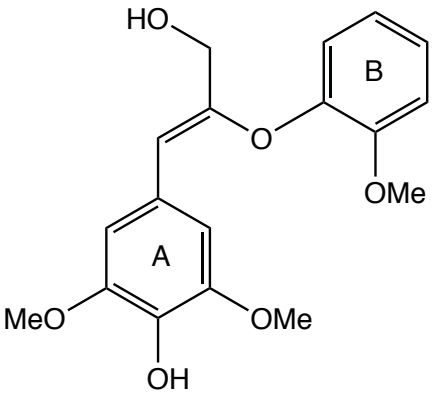
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.21	t	7.10
A OMe	3.73	s	
B OMe	3.90	s	
CH2	4.20	q	7.10
B5	6.72	dd	8.02, 1.58
B6	6.79	ddd	8.02, 7.37, 1.58
B1	6.94	ddd	8.02, 7.37, 1.58
B2	7.06	dd	8.02, 1.58
A 2,6	7.16	s	
α	7.33	s	

Notes:

hkd91.1.2

Compound Number 3057



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
1H data only				

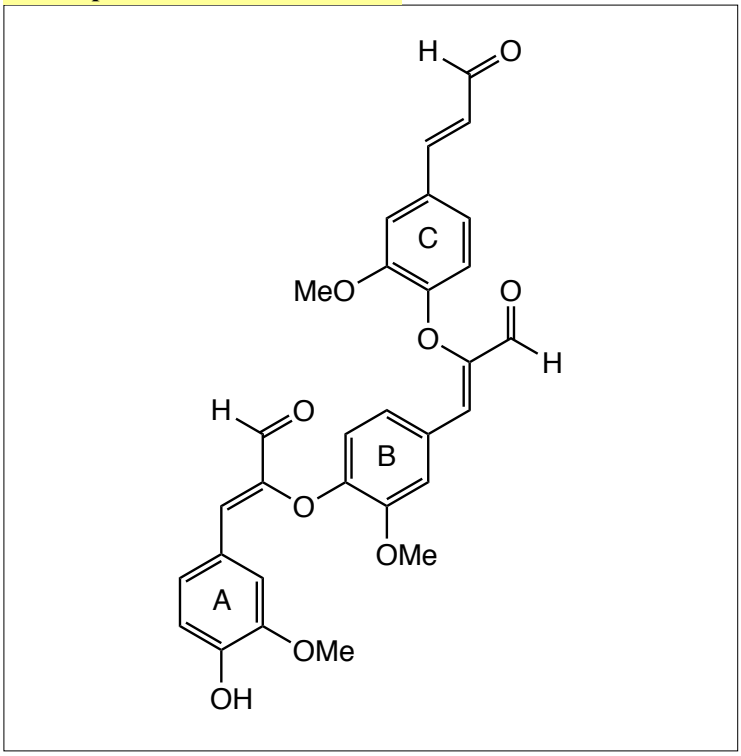
^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.67	s	
B OMe	3.90	s	
γ	4.15	br s	
α	6.21	br s	
A 2,6	6.90	s	
B 1,2,5,6	6.75-7.05	m	
A4 OH	8.00	s	

Notes:

hkd57.4
1H Data only

Compound Number 3058



CAld-b-CAld-b-CAld

^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.69	s	
B OMe	3.83	s	
C OMe	3.98	s	
C β	6.70	dd	15.92, 7.65
B5	6.79	d	8.29
C5	6.82	d	8.29
A5	6.85	d	8.29
C6	7.15	dd	8.29, 1.97
B6	7.28	dd	8.29, 1.97
A6	7.30	dd	8.29, 1.97
A α	7.30	s	
B α	7.33	s	
C2	7.48	d	1.97
A2	7.52	d	1.97
C α	7.58	d	15.92
B2	7.67	d	1.97
A OH	8.37	bs	
Aγ	9.48	s	
Bγ	9.53	s	
Cγ	9.65	d	7.65

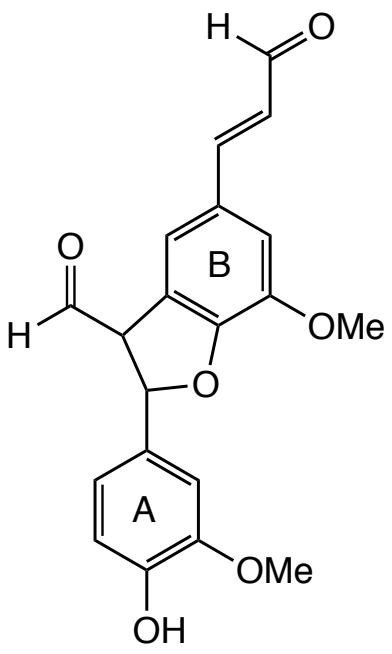
Notes:

hkc43.4.1

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A OMe		55.93		
B OMe		56.14		
C OMe		56.50		
C2		112.55		
A2		113.95		
B2		114.87		
B5		115.18		
C5		115.42		
A5		116.26		
C6		123.59		
A1		125.21		
B6		125.59		
A6		126.78		
B1		128.03		
Cβ		128.38		
C1		130.35		
Bα		137.15		
Aα		138.31		
Aβ		147.52		
A3		148.46		
B4		148.47		
Bβ		148.51		
C4		148.72		
B3		149.91		
C3		150.35		
A4		150.58		
Cα		153.13		
Aγ		187.43		
Bγ		187.65		
Cγ		193.91		

Compound Number 3059



CAld-c-CAld

^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.82	s	
B OMe	3.92	s	
β	4.50	d	6.5
α	6.20	d	6.5
B β	6.70	dd	15.78, 7.76
A5	6.84	d	8.16
A6	6.90	dd	8.16, 1.84
A2	7.06	d	1.84
B2	7.38	s	
B6	7.43	s	
B α	7.61	d	15.78
A OH	8.29	s	
B γ	9.64	d	7.76
A γ	9.94	s	

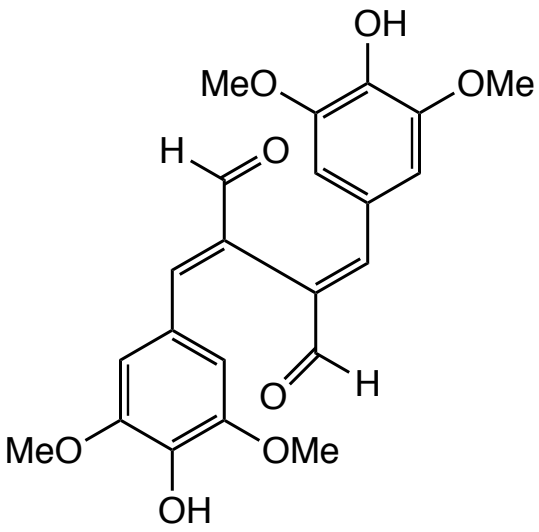
Notes:

hkf69.2.2
Fll73.12

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A OMe		56.31		
B OMe		56.54		
β		62.91		
α		85.24		
A2		110.66		
B2		114.27		
A5		115.93		
B6		119.49		
A6		119.81		
B5		125.79		
Bβ		127.69		
B1		129.66		
A1		132.18		
B3		146.01		
A3		147.91		
A4		148.57		
B4		151.77		
Bα		153.45		
Bγ		193.83		
γ		197.57		

Compound Number 3060



^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.72	s	
2,6	7.02	s	
α	7.79	s	
OH	7.94	bs	
γ	9.67	s	

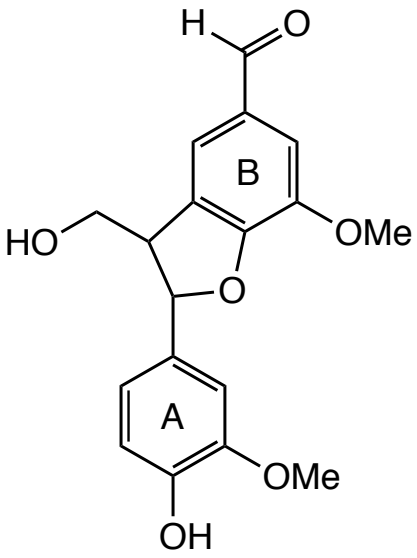
Notes:

hkf7-1
This compound has a plane of symmetry and so the signals are reported for only one half.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.54		
2		109.07		
6		109.07		
1		126.05		
β		134.78		
4		140.10		
3		148.71		
5		148.71		
α		152.98		
γ		192.70		

Compound Number 3061



G-c-Van

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.67	bq	
A OMe	3.82	s	
B OMe	3.92	s	
γ	3.92	m	
α	5.69	d	6.84
A5	6.81	d	8.16
A6	6.88	dd	8.16, 1.97
A2	7.05	d	1.97
B2	7.42	d	1.45
B6	7.53	dd	1.45. 0.92
A OH	7.65	bs	
B α	9.82	s	

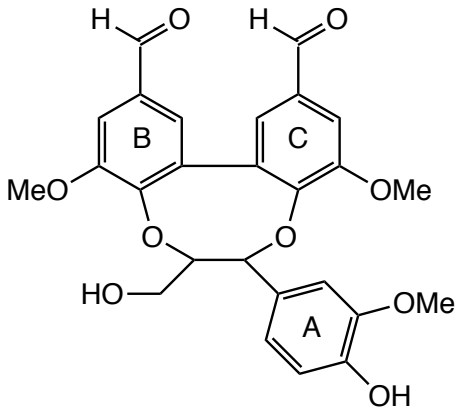
Notes:

hkf75.322

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β		53.84		
A OMe		56.30		
B OMe		56.37		
γ		64.22		
α		89.87		
A2		110.65		
B2		113.44		
A5		115.79		
A6		119.82		
B6		121.43		
B5		131.19		
B1		132.40		
A1		133.42		
B3		145.81		
A4		147.67		
A3		148.49		
B4		154.87		
B α		190.90		

Compound Number 3062



Dibenzodioxicin

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.48	m	
γ2	3.95	m	
A OMe	3.82	s	
C OMe	3.91	s	
B OMe	4.03	s	
β	4.18	m	
α	5.05	d	10.14
A5	6.84	d	8.16
A6	6.93	dd	8.16, 1.97
A2	7.05	d	1.97
C2	7.56	d	1.84
B2	7.65	d	1.84
C6	7.70	d	1.84
B6	7.74	d	1.84
C α	10.02	s	
B α	10.06	s	

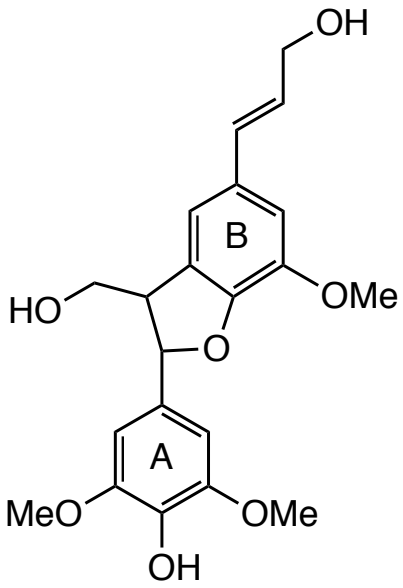
Notes:

hkf83.2.1 (6 mg)

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
C OMe		56.32		
A OMe		56.37		
B OMe		56.62		
γ		62.29		
α		85.11		
β		87.48		
B2		111.71		
C2		111.88		
A2		112.08		
A5		115.64		
A6		121.57		
C6		125.15		
B6		125.32		
A1		130.25		
B5		133.27		
C5		133.72		
B1		134.42		
C1		134.56		
A4		147.73		
A3		148.23		
B4		152.46		
C4		152.81		
B3		154.23		
C3		154.39		
Cα		191.66		
Bα		191.71		

Compound Number 3063



Simulanol, S-(8-5)-G

4-[3-hydroxy-5-(3-hydroxy-propenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-2,6-dimethoxy-phenol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.79	s	
B OMe	3.86	s	
Aβ	3.54	m	
Bγ	4.19	td	J = 5.52, 1.58
Aα	5.54	d	J = 6.71
Bβ	6.23	dt	J = 15.92, 5.52
Bα	6.52	dt	J = 15.92, 1.58
A 2,6	6.74	s	
B2	6.84	s	
B6	6.97	s	
A4-OH	7.19	s	

^{13}C

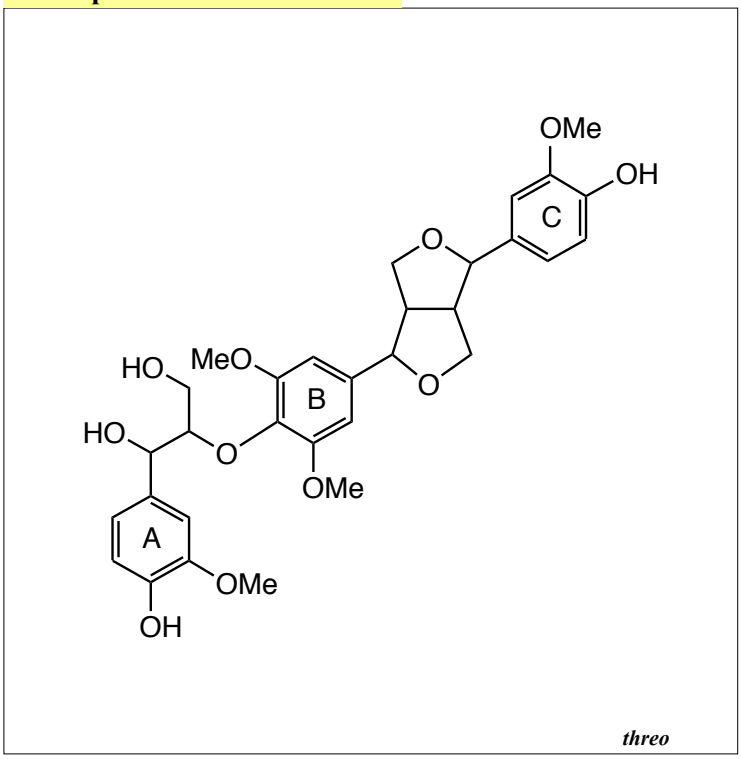
Atom	$CDCl_3$	Acetone	DMSO	
Aβ		54.78		
B OMe		56.44		
B OMe		56.44		
A OMe		56.67		
Bγ		63.39		
Aγ		64.52		
Aα		88.74		
A2		104.55		
A6		104.55		
B2		111.80		
B6		116.07		
Bβ		128.38		
B5		130.47		
Bα		130.52		
B1		131.95		
A1		133.30		
A4		136.68		
B3		145.16		
A3		148.74		
A5		148.74		
B4		148.95		

Notes:

hkh 99.14 Morreel #6

Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W.Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

Compound Number 3064



threo

buddlenol E, G-(8-O-4)-S-(8-8)-G

1-(4-hydroxy-3-methoxy-phenyl)-2-{4-[4-(4-hydroxy-3-methoxy-phenyl)-tetrahydro-furo[3,4c]furan-1-yl]-2,6-dimethoxy-phenoxy}-

^{1}H (acetone)

Atom	H Shifts	Mult	J
Cβ +Bβ	3.10	m	
Aγ1	3.43	m	
Aγ2	3.84	m	
Cγ2 + Bγ2	3.86	m	
Aβ	4.15	m	
Cγ1 + Bγ1	4.24	m	
Cα	4.68	d	J = 4.34
Bα	4.73	d	J = 4.34
Aα	4.97	m	
B 2,6	6.76	s	
C2	6.98	d	J = 1.84
A2	7.03	d	J = 1.84
A4-OH	7.37	s	
C4-OH	7.49	s	

^{13}C

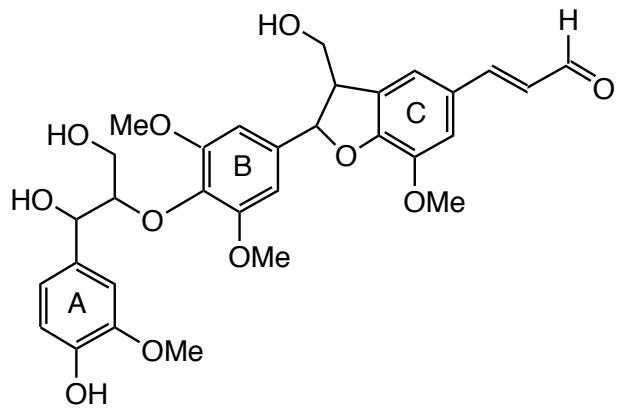
Atom	$CDCl_3$	Acetone	DMSO	
Cβ		55.15		
Bβ		55.46		
OMe		56.24		
B OMe		56.59		
B OMe		56.59		
OMe		56.70		
Aγ		60.98		
Cγ		72.30		
Bγ		72.54		
Aα		73.38		
Bα		86.57		
Cα		86.60		
Aβ		87.86		
B2		104.12		
B6		104.12		
C2		110.62		
A2		110.92		
A5		115.20		
C5		115.54		
C6		119.60		
A6		120.04		
C1		133.77		
B1		133.80		
A1		134.10		
C4		135.72		
B4		139.10		
A3		146.47		
C3		146.90		
A4		147.98		
B3		154.20		
B5		154.20		

Notes:

hkh 99.6 Morreel #22

Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W. Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

Compound Number 3065



threo

buddlenol A, G-(t8-O-4)-S-(8-5)-G'

3-(2-{4-[2-hydroxy-3-methoxy-phenyl)1-hydroxymethyl-ethoxy]-3.5-dimethoxy-phenyl}-3-hydroxymethyl-7-methoxy-2,3-

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.82	s	
B OMe	3.84	s	
OMe	3.94	s	
Aα	4.97	t	J = 4.47
Bα	5.70	d	J = 6.45
Cβ	6.66	dd	J = 15.78, 7.63
A5	6.76	d	J = 8.02
A6	6.83	dd	J = 8.02, 1.84
B 2,6	6.83	s	
A2	7.03	d	J =1.84
Cα	7.59	d	J = 15.78
Cγ	9.64	d	J = 7.63

Notes:

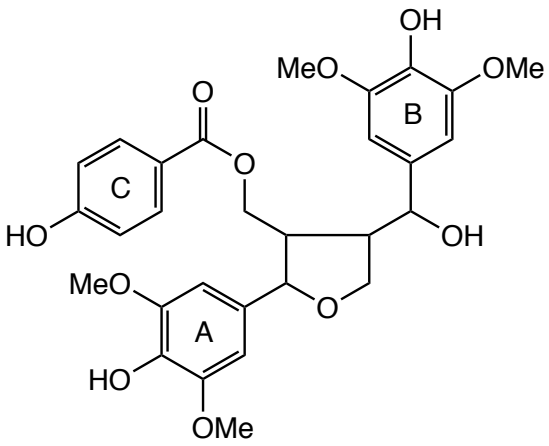
hkh 19.1t Morreel #23

Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W.Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
PROTON data only				

Compound Number 3066



SP-(8,8)-S

tetrahydro-α4,2-bis-(4-hydroxy-3,5-dimethoxyphenyl) α-3O-(4-hydroxybenzoyl)-3,4-furandimethanol

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aβ	2.55	m	
OMe	3.74	s	
OMe	3.78	s	
Bβ	3.99	m	
Bγ	4.14	m	
Aγ1	4.41	m	
Aγ2	4.68	m	
Aα	4.90	d	J = 6.3
Bα	4.96	d	J = 5.0
A2,6	6.66	s	
B2,6	6.72	s	
C3,5	6.87	m	
C2,6	7.77	m	

^{13}C

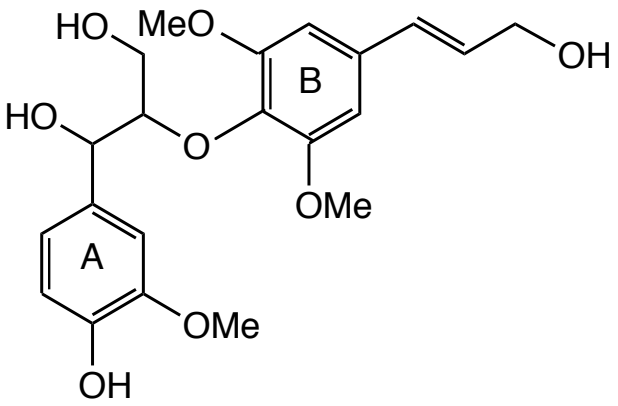
Atom	$CDCl_3$	Acetone	DMSO	
Bβ		48.37		
Aβ		49.80		
OMe		56.50		
OMe		56.50		
OMe		56.50		
OMe		56.50		
Aγ		63.99		
Bγ		69.95		
Bα		72.59		
Aα		85.34		
A2		104.45		
A6		104.45		
B2		104.53		
B6		104.53		
C3		115.98		
C5		115.98		
C1		122.40		
C2		132.45		
C6		132.45		
A1		134.49		
B1		134.91		
A4		136.01		
B4		136.01		
A3		148.54		
A5		148.54		
B3		148.54		
B5		148.54		
C4		162.56		
Cα		166.43		

Notes:

Fln 117 Morreel #19

Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

Compound Number 3067



threo

G-(8-O-4)-S

***threo*-1-(4-hydroxy-3-methoxy-phenyl)-2-[2,6 dimethoxy-phenoxy-4-(3-**

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ	3.39	m	-
A3 OMe	3.83	s	
B3 OMe	3.87	s	
Bγ	4.21	m	-
Aα–OH	4.33	d	J = 3.8
Aα	4.96	dd	J = 6.8, 8.4
Bβ	6.37	dt	J = 15.8, 5.1
Bα	6.54	d	J = 15.8
A5	6.76	d	J = 8.2
B2/6	6.79	s	
A6	6.82	dd	J = 8.2, 1.3
A2	7.03	d	J = 1.3
A4-OH	7.33	br s	

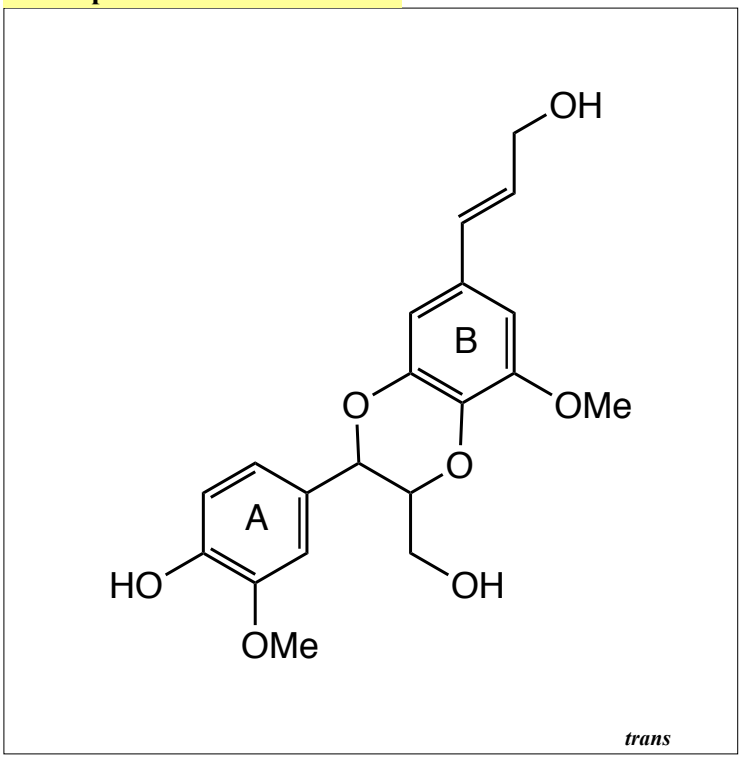
Notes:

HKh83.5, FL1112 Compound #8, Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W. Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549 See compound #118 for peracetate

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
PROTON data only				

Compound Number 3068



trans

G-(8-O-4)-5H [nocomtol]

4-[3-hydroxymethyl-7-(E)-(3-hydroxypropenyl)-5-methoxy-2,3-dihydro-benzo[1,4]dioxin-2-yl]-2-methoxyphenol

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ1	3.50	m	-
Aγ2	3.76	m	-
B3 OMe	3.85	s	
A3 OMe	3.85	s	
Aβ	4.05	m	-
Bγ	4.20	dd	J = 5.4, 1.6
Aα	4.96	d	J = 7.9
Bα	6.26	dt	J = 15.9, 5.4
Bβ	6.47	dt	J = 15.9, 1.6
B6	6.68	d	J = 1.8
A5	6.87	d	J = 8.1
A6	6.95	dd	J = 8.1, 1.8
A2	7.10	d	J = 1.8

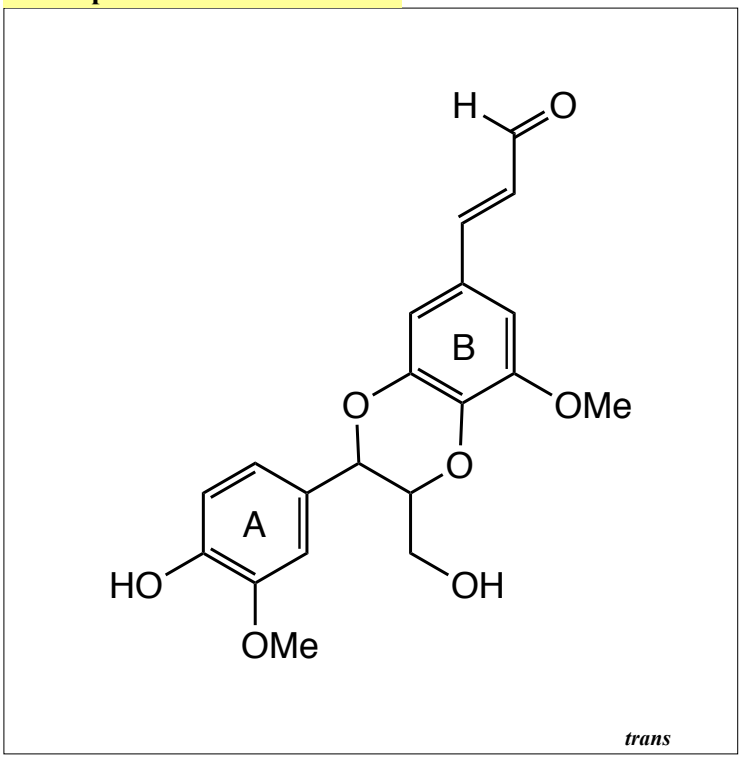
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3-OMe		56.2		
A3-OMe		56.2		
Aγ		61.9		
Bγ		63.6		
Aα		76.7		
Aβ		79.3		
B2		103.2		
B6		108.5		
A2		111.7		
A5		115.7		
A6		121.4		
Bβ		129.0		
A1		129.1		
Bα		130.1		
B1		130.3		
B4		133.7		
B5		145.2		
A4		147.8		
A3		148.3		
B3		149.8		

Notes:

FLm08 Cmpd 1a:Phenolic profiling of caffeic acid O-methyltransferase-deficient poplar reveals novel benzodioxane oligolignols. K. Morreel, J. Ralph, F. Lu, G. Goeminne, R. Busson, P. Herdewijn, J.L. Goeman, J. Van der Eycken, W. Boerjan and E. Messens. Plant Physiology, 136(4), 4023-4036 (2004).

Compound Number 3069



trans

G-(8-O-4)-5H′ [nocomtal]

(2E)-3-[3-(4-hydroxy-3-methoxy-phenyl)-2(hydroxymethyl)-8-methoxy-2,3-dihydro-1,4-benzodioxin-6-yl]acrylaldehyde

^{1}H (acetone)

Atom	H Shifts	Mult	J
Aγ1	3.53	m	-
Aγ2	3.82	m	-
A3 OMe	3.86	s	
B3 OMe	3.91	s	
Aβ	4.14	ddd	J = 8.0, 3.8, 2.6
Aα	5.01	d	J = 8.0
Bβ	6.67	dd	J = 15.8, 7.6
A5	6.88	d	J = 8.0
B6	6.92	dd	J = 2.0, 0.4
A6	6.97	ddd	J = 8.0, 2.0, 0.4
B2	7.02	d	J = 2.0
A2	7.12	d	J = 2.0
Bα	7.53	d	J = 15.8
A4-OH	7.59	bs	-
Bγ	9.64	d	7.6

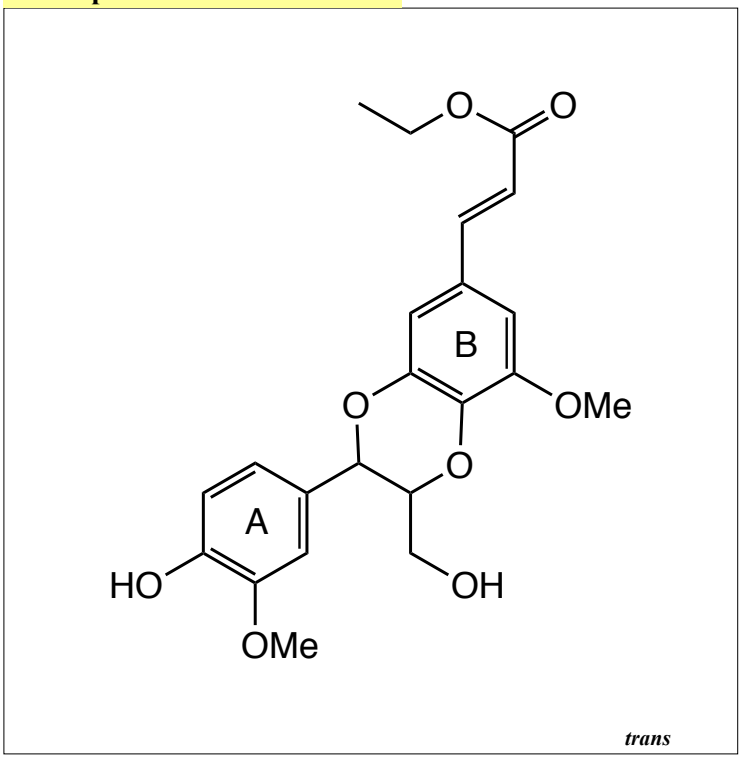
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3-OMe		56.4		
B3-OMe		56.5		
Aγ		61.6		
Aα		77.0		
Aβ		79.8		
B2		105.5		
B6		111.9		
A2		112.0		
A5		115.8		
A6		121.6		
B1		127.5		
Bβ		128.0		
A1		128.9		
Bα		137.4		
B5		145.6		
A3		148.1		
A4		148.5		
B3		150.4		
B4		153.7		
Bγ		193.8		

Notes:

FLn55 Cmpd 3:Phenolic profiling of caffeic acid O-methyltransferase-deficient poplar reveals novel benzodioxane oligolignols. K. Morreel, J. Ralph, F. Lu, G. Goeminne, R. Busson, P. Herdewijn, J.L. Goeman, J. Van der Eycken, W. Boerjan and E. Messens. Plant Physiology, 136(4), 4023-4036 (2004).

Compound Number 3070



trans

G-(8-O-4)-5H″

3-[3-(4-hydroxy-4-methoxyphenyl)-2-hydroxymethyl-8-methoxy-2,3-dihydrobenzo[1,4] dioxin-6-yl]-acrylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
Me	1.25	t	J = 7.1
Aγ1	3.50	m	-
Aγ2	3.83	m	-
B3 OMe	3.85	s	
A3 OMe	3.92	s	
Aβ	4.09	m	-
CH2	4.17	q	J = 7.1
Aα	4.98	d	J = 8.0
Bβ	6.40	d	J = 15.9
B6	6.85	d	J = 1.5
A5	6.88	d	J = 8.1
B2	6.95	d	J = 1.5
A6	6.96	dd	J = 8.1, 1.8
A2	7.10	d	J = 1.8
Bα	7.54	d	J = 15.9

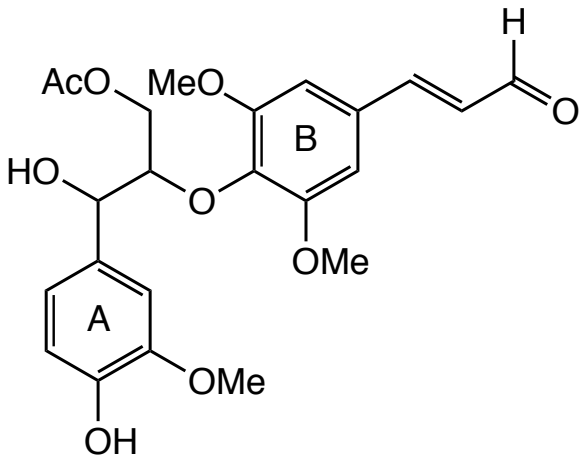
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Me		14.6		
B3-OMe		56.2		
A3-OMe		56.3		
Aγ		61.6		
CH2		61.6		
Aα		76.9		
Aβ		79.5		
B2		104.7		
B6		111.1		
A2		111.7		
A5		115.7		
Bβ		117.0		
A6		121.4		
B1		127.4		
A1		128.8		
B4		136.4		
Bα		145.2		
B5		145.3		
A4		147.8		
B3		148.3		
A3		150.1		
Bγ		167.2		

Notes:

FLl111 Cmpd c:Phenolic profiling of caffeic acid O-methyltransferase-deficient poplar reveals novel benzodioxane oligolignols. K. Morreel, J. Ralph, F. Lu, G. Goeminne, R. Busson, P. Herdewijn, J.L. Goeman, J. Van der Eycken, W. Boerjan and E. Messens. Plant Physiology, 136(4), 4023-4036 (2004).

Compound Number 3071



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me		20.66		
A3 OMe		56.62		
B3 OMe		56.73		
γ		63.59		
α		73.31		
β		84.56		
A2/6		104.65		
B2/6		106.94		
Bβ		129.11		
B1		131.09		
A1		131.65		
A4		136.04		
B4		139.26		
A3/5		148.51		
Bα		153.45		
B3/5		154.57		
γ Ac C=O		167.76		
Bγ		193.90		

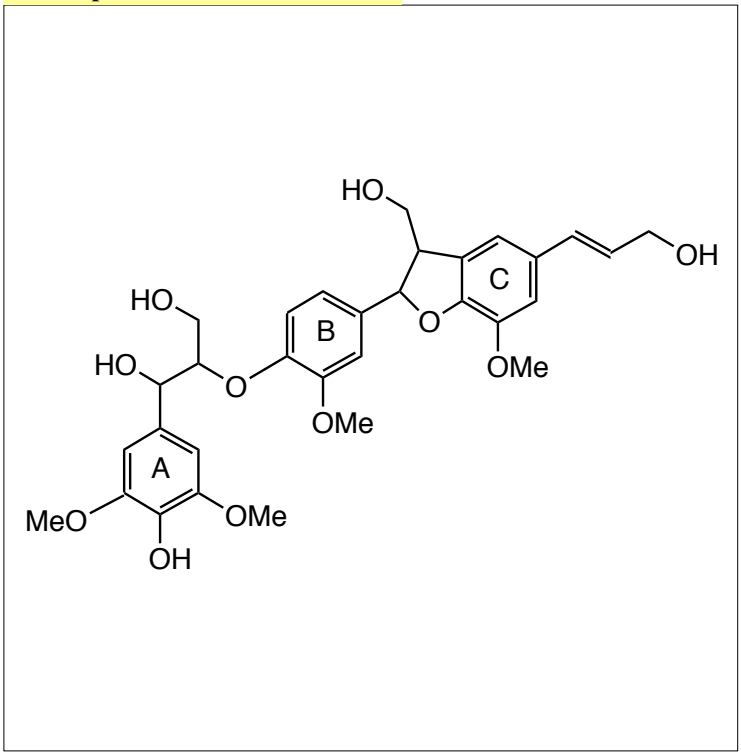
^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.84	s	-
A3/5 OMe	3.80	s	-
B3/5 OMe	3.94	s	-
γ1	4.12	dd	J = 11.9, 3.2
γ2	4.39	dd	J - 11.9, 7.4
β	4.62	m	-
α	4.94	dd	J = 6.7, 4.0
A2/6	6.70	s	-
Bβ	6.77	dd	J = 15.8, 7.6
B2/6	7.12	s	-
Bα	7.61	d	J = 15.8
Bγ	9.67	d	J = 7.6

Notes:

HKj51T6.7 Cmpd #9, Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W. Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549 Note the single γ-acetate!

Compound Number 3072



S-(8-O-4)-G-(8-5)-G

^{1}H (acetone)

Atom	H Shifts	Mult	J
Bβ	3.51	m	
Aγ1	3.51	m	
Aγ2	3.71	m	
Bγ	3.85	m	
OMε	3.77	s	
OMε	3.86	s	
OMε	3.94	s	
Cγ	4.19	dd	J = 5.5, 1.3
Aβt	4.24	m	
Aβe	4.32	m	
Aα	4.86	d	J = 5.9
Bα	5.59	d	J = 6.5
Cβ	6.23	dt	J = 15.9, 5.5
Cα	6.51	d	J = 15.9
A 2,6	6.76	s	

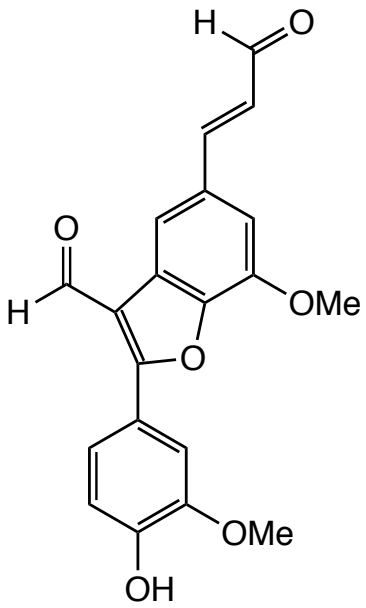
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Bβ		54.8		
OMe		56.35		
OMe		56.39		
OMe		56.58		
Aγ		61.86		
Cγ		63.26		
Bγ		64.58		
Aα		73.84		
Aβe		86.32		
Aβt		88.03		
Bα		88.24		
A2/6		105.36		
C2/6		111.14		
B2/5/6		119.33		
Cβ		128.42		
Cα		130.48		

Notes:

HKf145, mixture of isomers Morreel #39 Morreel, K., Ralph, J., Kim, H., Lu, F., Goeminne, G., Ralph, S.A., Messens, E., Boerjan, W. Profiling of oligolignols reveals monolignol coupling conditions in lignifying poplar xylem. Plant Physiol. November 2004, Vol.136, pp.3537-3549

Compound Number 3073



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A OMe	56.20	56.52	55.90	55.84
B OMe	56.31	56.74	56.28	56.18
B2	106.58	107.79	107.04	107.08
A2	110.94	112.97	112.43	112.40
B5	115.19	116.71	115.37	115.44
B6	116.54	116.97	116.07	116.05
A5	116.73	116.99	116.14	116.20
A1	120.10	120.52	118.44	118.50
A6	123.80	124.24	123.12	123.18
A β	127.96	128.85	127.37	127.43
B β	128.43	129.44	128.46	128.42
B1	132.13	133.54	132.35	132.33
B4	144.65	145.29	143.70	143.77
B3	145.39	146.56	145.11	145.12
A3	147.04	149.08	148.13	148.20
A4	149.06	151.05	150.36	150.52
B α	153.00	153.89	153.74	153.64
A α	166.60	167.07	165.77	165.80
A γ	186.37	186.93	186.72	186.62
B γ	193.54	194.07	194.38	194.21

^{1}H (DMSO)

Atom	H Shifts	Mult	J
A OMe	3.89	s	
B OMe	4.04	s	
B β	6.97	dd	7.6, 15.8
A5	7.00	d	8.2
A6	7.46	dd	2.1, 8.2
A2	7.51	d	2.0
B2	7.52	d	1.4
B α	7.90	d	15.8
B6	7.99	d	1.4
B γ	9.69	d	7.7
A γ	10.24	s	

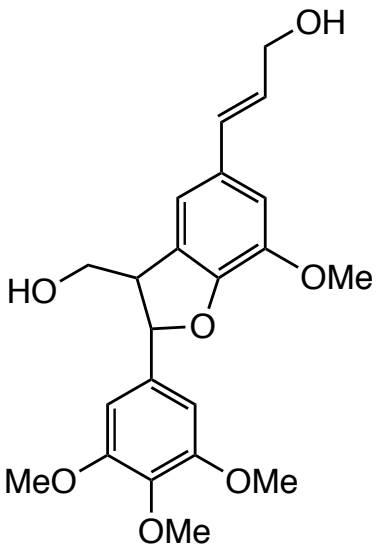
^{1}H

A OMe	4.01	3.97		3.86
B OMe	4.07	4.09		4.03
B β	6.75	6.82		6.95
A5	7.08	7.06		7.06
A6	7.42	7.50		7.46
A2	7.37	7.56		7.47
B2	7.09	7.45		7.49
B α	7.58	7.79		7.85
B6	8.05	8.01		8.02
B γ	9.72	9.71		9.71
A γ	10.30	10.31		10.26

Notes:

KY CAld dimer (KY-98f1)
Not very soluble in CDCl3 or d6-acetone
some shifts taken from HMBC

Compound Number 3074



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	53.59	54.90	53.15	53.35
A3 OMe	56.16	56.37	55.87	55.74
A5 OMe	56.16	56.37	55.87	55.74
B3 OMe	56.01	56.40	55.78	55.72
A4 OMe	60.81	60.46	59.98	59.90
B γ	63.75	63.35	61.62	61.74
γ	63.95	64.53	62.79	62.93
α	88.16	88.40	87.10	87.22
A2	103.12	103.99	103.13	103.16
A6	103.12	103.99	103.13	103.16
B2	110.54	111.68	110.45	110.53
B6	114.74	116.02	114.90	114.96
B β	126.54	128.47	128.14	128.21
B5	127.90	130.16	129.31	129.36
B α	131.19	130.39	128.87	128.89
B1	131.00	132.09	130.74	130.88
A1	136.63	138.63	137.14	137.26
A4	137.86	138.69	137.06	137.18
B3	144.45	145.18	143.73	143.82
B4	148.27	148.81	146.99	147.17
A3	153.40	154.42	152.92	153.00
A5	153.40	154.42	152.92	153.00
1H				
β	3.61		3.46	3.56
A4 OMe	3.80		3.64	3.65
A3 A5 OMe	3.81		3.74	3.71
B3 OMe	3.89		3.81	3.82
γ 's	3.91		3.65	3.75
	3.96		3.74	3.85
B γ	4.28		4.07	4.16
α	5.57		5.49	5.62
B β	6.22		6.21	6.28
B α	6.53		6.45	6.53
A2, A6	6.61		6.66	6.74
B2	6.87		6.93	6.98
B6	6.87		6.93	7.01
γ OH	3.69		5.05	

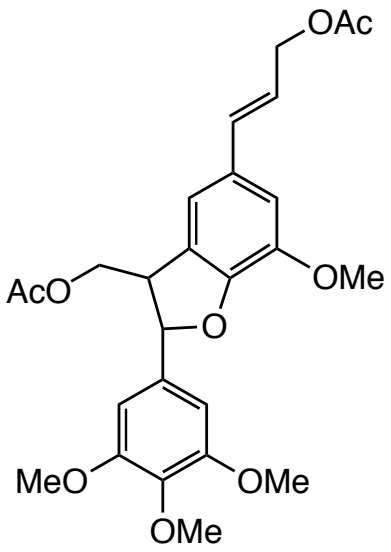
^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.54	q	
A4 OMe	3.70	s	
A3 A5 OMe	3.78	s	
B3 OMe	3.87	s	
γ 's	3.83	dd	7.04, 10.9
	3.90	dd	5.4, 10.9
B γ	4.19	dd	1.6, 5.6
α	5.59	d	6.5
B β	6.24	dt	5.6, 15.8
B α	6.52	dt	1.6, 15.8
A2, A6	6.75	s	
B2	6.95		
B6	6.96		

Notes:

F. Lu MS-b5-G (FLw80)

Compound Number 3075



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.01	s	
Ac Me	2.01	s	
β	3.78	m	
A4 OMe	3.71	s	
A3 A5 OMe	3.80	s	
B3 OMe	3.89	s	
γ 's	4.34, 4.44	dd	7.3, 11.1
		dd	5.5, 11.1
B γ	4.66	dd	1.2, 6.5
α	5.53	d	7.1
B β	6.24	dt	6.5, 15.9
B α	6.64	bd	15.9
A2, A6	6.76	s	
B6	7.03	bs	
B2	7.05	bs	

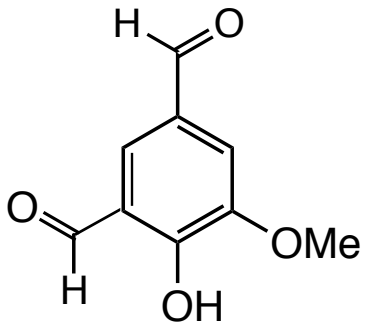
Notes:

F. Lu MS-b5-G (FLw80Ac)
Ac C=O switch order in solvents checked by HMBC

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me	20.78	20.74	20.58	20.45
B γ Ac Me	20.99	20.82	20.73	20.60
β	50.37	51.29	49.36	49.51
A3 OMe	56.13	56.47	55.79	55.74
A5 OMe	56.13	56.47	55.88	55.78
B3 OMe	55.98	56.47	55.88	55.78
A4 OMe	60.79	60.51	59.98	59.92
B γ	65.16	65.51	64.53	64.53
γ	65.29	65.94	64.72	64.80
α	88.62	88.89	87.54	87.62
A2	103.10	104.29	103.42	103.41
A6	103.10	104.29	103.42	103.41
B2	110.59	112.24	111.01	111.08
B6	115.26	116.34	115.26	115.29
B β	121.23	122.29	121.39	121.37
B5	127.49	129.12	128.03	128.03
B1	130.60	131.57	130.11	130.20
B α	134.26	134.72	133.51	133.55
A1	135.94	137.61	136.07	136.17
A4	138.02	139.11	137.32	137.44
B3	144.40	145.42	143.89	143.97
B4	148.17	149.33	147.55	147.70
A3	153.41	154.55	152.96	153.05
A5	153.41	154.55	152.96	153.05
B γ Ac C=O	170.86	170.78	170.16	170.09
γ Ac C=O	170.71	170.96	170.30	170.25
1H				
γ Ac Me	2.02		1.98	1.97
B γ Ac Me	2.07		2.04	2.03
β	3.76		3.77	3.82
A4 OMe	3.80		3.65	3.66
A3 A5 OMe	3.81		3.75	3.73
B3 OMe	3.89		3.82	3.83
γ 's	4.30		4.30	4.35
	4.42		4.40	4.45
B γ	4.68		4.65	4.67
α	5.44		5.49	5.56
B β	6.13		6.24	6.27
B α	6.57		6.60	6.64
A2, A6	6.57		6.69	6.74
B6	6.86		7.01	7.06
B2	6.86		7.04	7.07

Compound Number 3076



5-formyl vanillin

^{1}H (DMSO)

Atom	H Shifts	Mult	J
OMe	3.93		
2	7.58		
6	7.85		
α	9.86		
formyl H	10.33		
4-OH	11.28		
CDCl3			
OMe	3.96		
2	7.58		
6	7.71		
α	9.87		
formyl H	9.99		
4-OH	11.66		
Acetone			
OMe	3.99		
2	7.66		
6	7.96		
α	9.92		
formyl H	10.25		
4-OH	11.13		

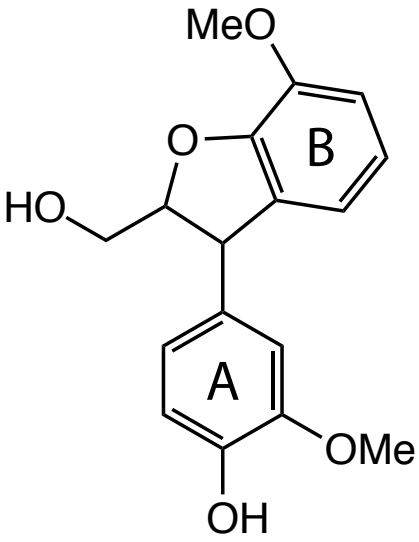
Notes:

FPL Collection
C1 and C6 change order in CDCl3
Aldehyde C=Os change order in DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	56.42	56.72	56.30	
2	114.17	114.87	113.33	
5	119.95	122.06	122.40	
6	129.40	128.45	124.87	
1	129.06	130.15	128.07	
3	14936	150.13	149.22	
4	157.01	157.26	156.06	
α	189.44	190.70	191.16	
5 C=O	195.84	195.35	190.22	

Compound Number 3077



phenyl dihydrobenzofuran

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.77	m	
OMe	3.77	s	
OMe	3.84	s	
γ2	3.86	m	
γ-OH	4.16	t	
α	4.50	d	8.1
β	4.58-4.61	m	
B6	6.54	dt	7.6
A6	6.67	dd	8.1, 2.0
B1	6.76	dd	8.0, 7.6
A5	6.78	d	8.1
B2	6.81	d	8.0
A2	6.83	d	2.0
Ar OH	7.52	s	

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α		50.74		
OMe		56.14		
OMe		56.20		
γ		63.40		
β		93.49		
A2		112.34		
B2		112.73		
A5		115.93		
B6		118.07		
A6		121.48		
B1		121.83		
B5		133.03		
A1		134.88		
B3		145.44		
A4		146.49		
A3		148.49		
B4		149.26		

Notes:

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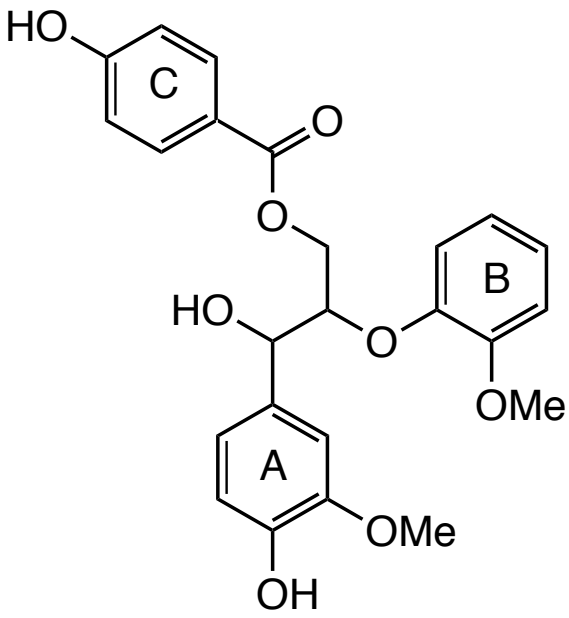
Compound Number 3078



erythro

^{1}H (chloroform)

Atom	H Shifts	Mult	J
A OMe	3.81	s	
B OMe	3.83	s	
γ1	4.37	dd	3.4, 11.1
γ2	4.55	dd	7.0, 11.1
β	4.56	m	
α	4.97	bd	2.4
C 3,5	6.76	d	8.7
C 2,6	7.75	d	8.7
A2	7.01	bd	1.4
A5	6.84	d	8.1
A6	6.82	dd	1.4, 8.1
B1	7.03	dt	1.3, 7.9
B2	7.03	d	7.9
B5	7.06	dd	1.3, 7.9
B6	6.89	dd	1.2, 7.7

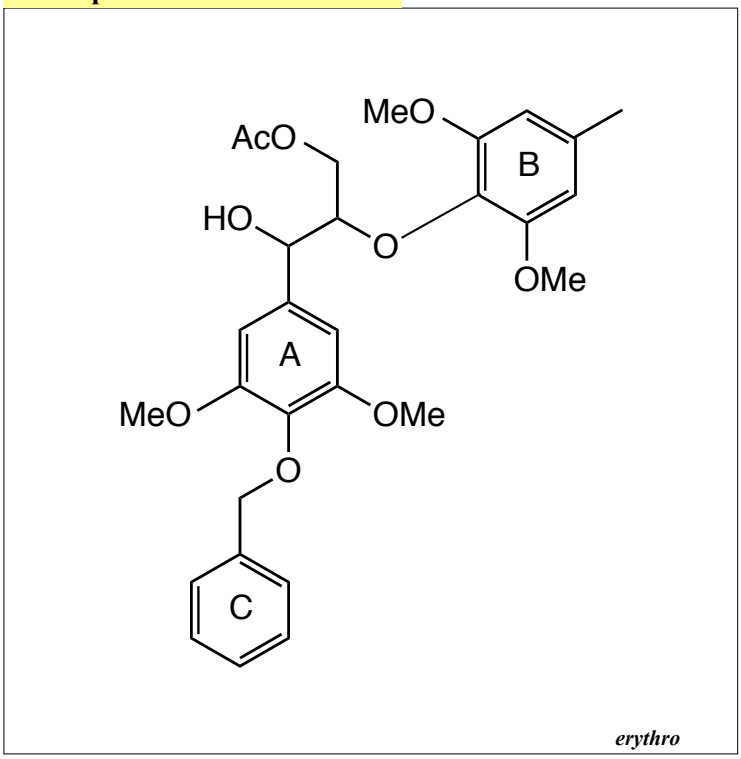
Notes:

J. Ralph
26
A6 and B5 switch order in DMSO and DMSO/pyr from CDCl3 and acetone

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A OMe	55.89	56.18	55.49	55.40
B OMe	55.83	56.23	55.50	55.44
γ	62.83	64.52	63.61	63.63
α	72.39	73.40	71.68	71.82
β	84.19	83.72	81.39	81.64
A2	108.82	111.47	111.00	111.05
B2	112.28	113.63	112.81	112.76
A5	114.19	115.28	114.81	114.92
C3	115.14	115.86	115.11	115.13
C5	115.14	115.86	115.11	115.13
A6	119.25	119.91	119.30	119.37
B5	120.56	120.36	117.40	117.56
B6	121.51	121.73	120.61	120.61
B1	124.09	123.61	121.99	122.00
C1	122.03	122.43	120.17	120.28
C2	131.95	132.58	131.41	131.45
C6	131.95	132.58	131.41	131.45
A1	130.84	133.72	132.97	133.04
A4	145.11	146.80	145.63	145.84
A3	146.64	148.10	147.15	147.27
B4	146.91	149.40	147.57	147.66
B3	151.39	152.15	150.18	150.30
C4	160.20	162.51	161.87	161.99
C α	166.30	166.43	165.39	165.49
1 H				
A OMe		3.81	3.72	3.73
B OMe		3.76	3.63	3.62
γ1		4.49	4.39	4.56
γ2		4.54	4.45	4.53
β		4.72	4.63	4.74
α		5.01	4.81	4.96
C 3,5		6.84	7.57	6.82
C 2,6		7.71	6.75	7.66
A2		7.16	7.02	7.13
A5		6.78	6.70	6.80
A6		6.94	6.82	6.92
B1		6.93	6.87	6.87
B2		6.94	6.89	6.87
B5		7.04	6.96	7.03
B6		6.82	6.78	6.79

Compound Number 3079



BzS-b-S

^{1}H (DMSO)

Atom	H Shifts	Mult	J
γ Ac Me	1.77 (1.87)	s	
B Me	2.24	s	
A OMe	3.70	s	
B OMe	3.76	s	
γ1	4.04 (3,83)	m	
γ2	4.27 (4.06)	m	
β	4.30 (4.27)	m	
α	4.91 (4.82)	t	4.6
Bz CH_2	4.85	s	
C 4	7.29	dt	7.4
C 3,5	7.35	dt	7.4
C 2,6	7.44	d	7.4
B 2,6	6.45 (6.48)	s	
A 2,6	6.66 (6.81)	s	

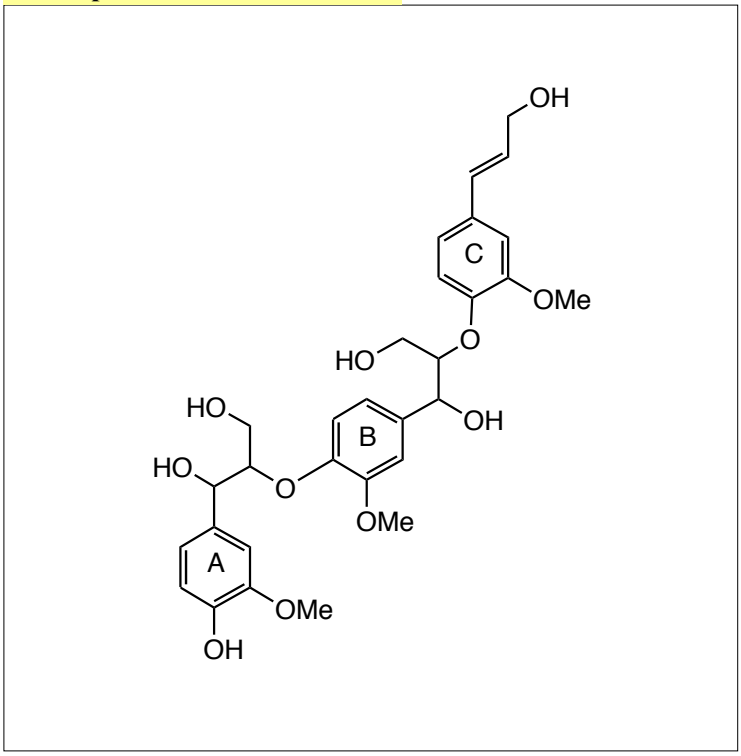
Notes:

FL w
S.Ralph
shifts can change order among the solvents
significant *threo* isomer 1H shifts in ( )
alpha 13C shifts are split in acetone shift is average

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ Ac Me	20.88	20.72	20.42	20.34
B Me	21.94	21.80	21.37	21.27
A OMe	56.15	56.41	55.64	55.59
B OMe	56.15	56.47	55.80	5.70
γ	62.46	63.24	62.79	62.88
α	71.47	72.82	72.33	72.44
β	82.73	83.87	82.94	83.08
Bz CH_2	74.92	75.06	73.93	73.97
A 2,6	102.88	104.28	103.47	103.54
B 2,6	106.17	107.12	105.89	105.90
C4	127.73	128.32	127.62	127.55
C 3,5	128.06	128.79	127.84	127.81
C 2,6	128.48	128.84	128.05	127.99
B4	132.03	133.92	132.83	132.89
B1	134.54	134.71	133.28	133.37
A4	135.90	136.99	135.15	135.29
A1	134.43	137.05	137.94	138.01
C1	137.83	139.51	137.97	138.04
A 3,5	153.47	154.30	152.33	152.42
B 3,5	153.21	154.06	152.58	152.68
γ Ac C=O	170.88	170.82	170.08	170.08
1 H				
γ Ac Me	1.97 (2.03)	1.86 (1.96)	1.77	1.78 (1.87)
B Me	2.33	2.29	2.24	2.21
A OMe	3.78	3.80	3.70	3.71
B OMe	3.84	3.84	3.76	3.75
γ1	4.13 (3.90)	4.09 (3.95)	4.04	4.17 (3.95)
γ2	4.36 (4.51)	4.33 (4.35)	4.27	4.41 (4.20)
β	4.45 (3.96)	4.48 (4.20)	4.30	4.42 (4.39)
α	4.82 (4.96)	4.91 (4.91)	4.91	5.05 (4.97)
Bz CH_2	4.95	4.93	4.85	4.89
C 4	7.26	7.27	7.29	7.27
C 3,5	7.30	7.33	7.35	7.33
C 2,6	7.44	7.49	7.44	7.47
B 2,6	6.43 (6.38)	6.54 (6.51)	6.45	6.45 (6.47)
A 2,6	6.53 (6.54)	6.71 (6.75)	6.66	6.74 (6.90)
13C *threo*				
γ	63.92	64.58	63.57	63.68
α	74.61	74.44	71.68	71.93
β	86.59	86.11	83.27	83.44
A 2,6	104.06	105.05	103.91	104.02
B 2,6	105.85	107.02	106.11	106.07
B4			133.08	133.12
B1			133.50	133.63
A 3,5	152.26	153.45	152.40	152.45
B 3,5	153.43	154.18	152.43	152.45
γ Ac C=O	170.65	170.76	170.06	170.03

Compound Number 3080



G-b-G-b-CA

^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.80	s	
B OMe	3.80	s	
C OMe	3.83	s	
A,B γ1	3.66-3.71	m	
A,B γ2	3.78-3.81	m	
C γ1	3.82	dt	1.6, 5.6
C γ2	4.18		
A β	4.24	m	
B β	4.29	m	
A α	4.86	t	5.4
B α	4.89	t	5.3
C β	6.26	dt	5.3, 15.9
C α	6.49	bd	15.9
A5	6.75	d	8.1
C6	6.84	dd	1.8, 8.3
B,C 5-A,B 6	6.85--6.89		
C2	7.04	d	1.7
A2	7.09	d	1.7
B2	7.12	d	1.5
Ph OH	7.46	s	

Notes:

Ruili Gao (rg316-30)
Shifts for A, B 6, and
B, C 5 are too close to assign with confidence

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.16		
OMe		56.21		
OMe		56.23		
A γ		61.73		
B γ		61.83		
C γ		63.25		
B α		73.63		
A α		73.72		
B β		86.48		
A β		86.86		
C2		110.81		
A2		111.30		
B2		112.27		
A5		115.16		
5		118.97		
5		119.21		
C6		120.17		
6		120.37		
6		120.41		
C1		132.81		
A1		134.41		
B1		137.34		
C β		129.54		
C α		129.83		
A4		146.60		
A3		147.95		
B4		148.08		
C4		148.46		
B3		151.48		
C3		151.81		