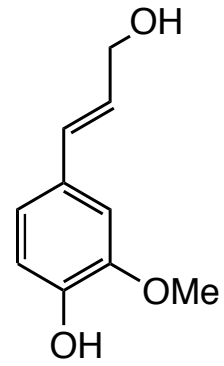
Compound Number 2001



trans

coniferyl alcohol

4-hydroxy-3-methoxy cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ OH	3.78	t	5.65
OMe	3.85	s	
γ	4.18	td	1.5, 5.6
β	6.22	dt	15.9, 5.5
α	6.49	dt	15.9, 1.5
5	6.76	d	8.1
6	6.84	dd	8.1, 1.9
2	7.04	d	1.9
Ar OH	7.63	s	

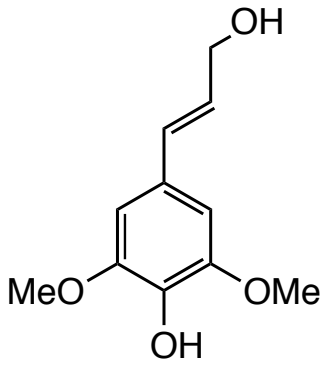
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.78	56.09	55.56	
γ	63.66	63.37	61.73	
2	108.40	109.91	109.72	
5	114.48	115.73	115.47	
6	120.18	120.55	119.43	
β	126.05	127.96	127.49	
1	129.18	130.16	128.52	
α	131.23	130.41	129.00	
4	145.51	147.07	146.17	
3	146.64	148.36	147.72	

Notes:

S. Quideau
Assignments confirmed in all three solvents
JAFC 1992-40(7), 1108-1110

Compound Number 2002



sinapyl alcohol

4-hydroxy-3,5-dimethoxy cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ OH	3.88	t	5.65
OMe	3.82	s	
γ	4.20	td	5.6, 1.5
β	6.24	dt	15.8, 5.5
α	6.48	dt	15.8, 1.5
2,6	6.71	s	
4 OH	7.30	s	

^{13}C

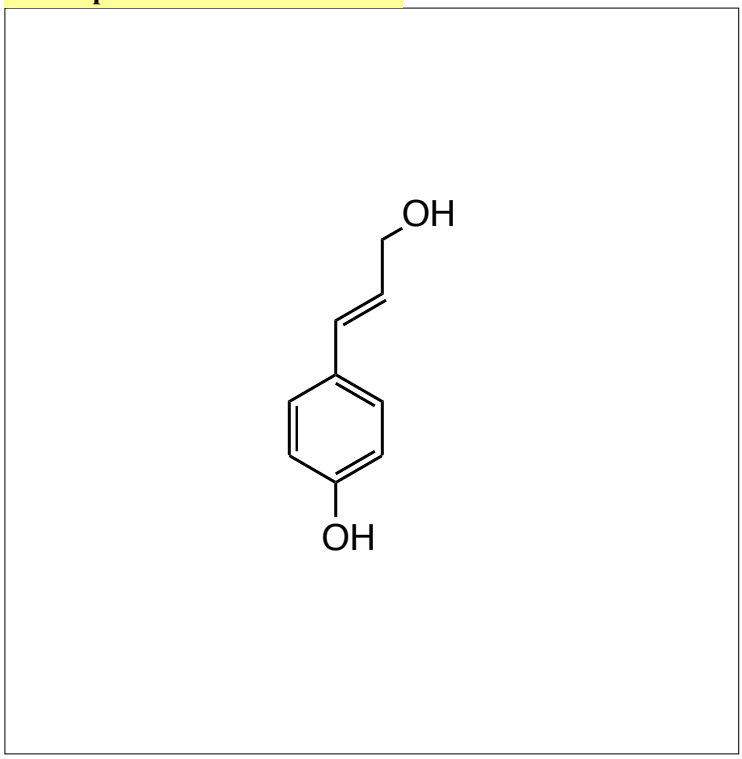
Atom	$CDCl_3$	Acetone	DMSO
OMe	56.27	56.48	55.92
OMe	56.27	56.48	55.92
γ	63.76	63.33	61.62
2	103.35	104.65	103.79
6	103.35	104.65	103.79
β	126.58	128.27	127.89
1	128.22	128.99	127.40
α	131.50	130.62	129.17
4	134.80	136.52	135.17
3	147.13	148.71	148.01
5	147.13	148.71	148.01

Notes:

S. Quideau

Note A1 and β change places in DMSO. Assignments confirmed in CDCl3 and Acetone. JAFC 1992-40(7), 1108-1110

Compound Number 2003



p-coumaryl alcohol

4-hydroxy-cinnamyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ OH	3.85	t	5.65
g's	4.19	td	5.6, 1.6
β	6.19	dt	15.9, 5.6
α	6.50	dt	15.9, 1.6
3,5	6.78	m	
2,6	7.25	m	
4 OH	8.40	s	

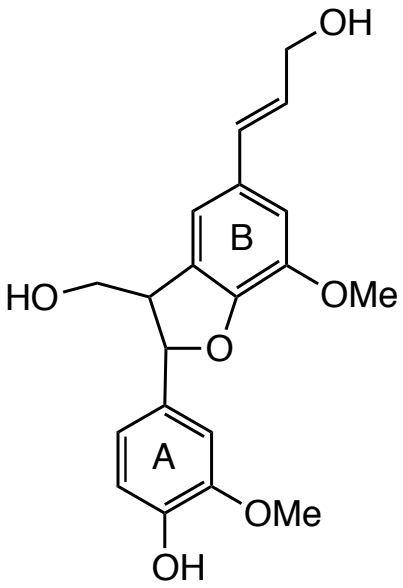
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
γ	63.79	63.41	61.72	
3	115.50	116.15	115.37	
5	115.50	116.15	115.37	
β	125.74	127.71	127.15	
2	127.73	128.33	127.38	
6	127.73	128.33	127.38	
1	128.90	129.68	127.92	
α	131.08	130.13	128.70	
4	156.12	157.76	156.80	

Notes:

S. Quideau
JAFC-1992-40(7), 1108-1110

Compound Number 2004



4-[3-Hydroxymethyl-5-(3-hydroxypropenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-2-methoxyphenol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.53	br q	
γ + γ OH	3.78-3.88	m	
A3 OMe	3.81	s	
B3 OMe	3.85	s	
B γ OH	4.16	t	5.0
B γ	4.19	td	5.2, 1.5
α	5.56	d	6.5
B β	6.23	dt	15.8, 5.5
B α	6.52	dt	15.8, 1.5
A5	6.80	d	8.1
A6	6.87	ddd	8.1, 2.0, 0.5
B2	6.94	br s	
B6	6.97	br s	
A2	7.03	d	2.0
A4 OH	7.73	br s	

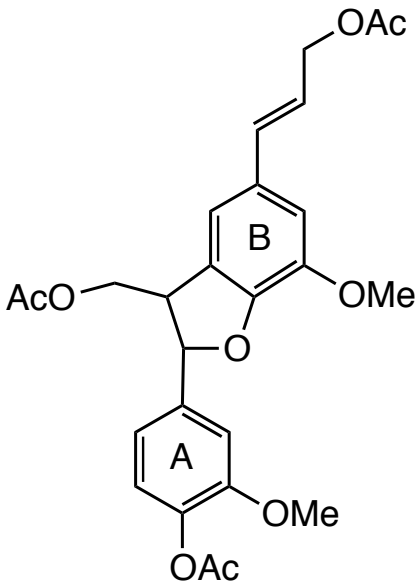
Notes:

S. Quideau-Ag2O oxidation of coniferyl alcohol.
Assignments confirmed in acetone and DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
β	53.53	54.73	53.02
A OMe	55.99	56.26	55.68
B OMe	56.01	56.38	55.73
B γ	63.83	63.39	61.70
γ	64.00	64.60	62.98
α	88.24	88.51	87.26
A2	108.75	110.48	110.37
B2	110.54	111.72	110.37
A5	114.33	115.67	115.37
B6	114.78	116.08	115.00
A6	119.43	119.57	118.58
B β	126.45	128.33	129.52
B5	128.09	130.40	128.02
B α	131.33	130.54	129.04
B1	130.87	131.91	130.56
A1	132.87	134.36	132.39
B3	144.47	145.14	143.72
A4	145.74	147.27	146.42
A3	146.68	148.36	147.60
B4	148.38	148.84	147.13
1H			
β			3.44
γ + γ OH			3.62-3.72
A3 OMe			3.74
B3 OMe			3.79
B γ OH			4.77
B γ			4.08
α			5.47
B β			6.21
B α			6.46
A5			6.75
A6			6.75
B2			6.91
B6			6.94
A2			6.92
A4 OH			9.01

Compound Number 2005



Acetic acid 4-[3-acetoxymethyl-5-(3-acetoxypropenyl)- 7-methoxy-2,3-dihydrobenzofuran-2-yl]-2-methoxyphenyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	2.00	s	
B γ Ac Me	2.01	s	
A4 Ac Me	2.22	s	
β	3.78	m	
A3 OMe	3.79	s	
B3 OMe	3.88	s	
γ1	4.34	dd	11.1, 7.6
γ2	4.46	dd	11.1, 5.4
B γ	4.66	dd	6.5, 1.3
α	5.61	d	6.7
Bβ	6.24	dt	15.8, 6.5
B α	6.63	dt	15.8, 1.3
A6	7.00	br dd	8.1, 1.8
B6	7.03	br s	
B2	7.049	br s	
A5	7.054	d	8.1
A2	7.18	d	1.8

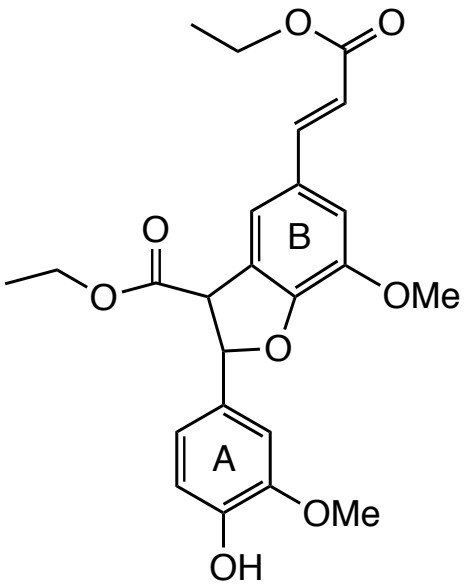
Notes:

S.Quideau-Ag2O oxidation of coniferyl alcohol + acetylation. Assignments confirmed in CDCl3 and acetone
A1 and A4 switch places in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.51	20.43	20.41	
γAc Me	20.68	20.67	20.61	
BγAc Me	20.90	20.78	20.79	
β	50.36	51.33	49.53	
A OMe	55.79	56.24	55.84	
B OMe	55.92	56.41	55.84	
Bγ	65.06	65.47	64.57	
γ	65.22	65.96	64.90	
α	87.91	88.34	87.01	
A2	109.84	111.07	110.59	
B2	110.56	112.20	111.08	
B6	115.23	116.32	115.36	
A6	118.08	118.67	118.00	
B β	121.16	122.30	121.53	
A5	122.79	123.76	123.01	
B5	127.21	128.82	127.84	
B1	130.59	131.65	130.28	
B α	134.13	134.64	133.52	
A4	139.56	140.70	139.14	
A1	139.30	140.99	139.59	
B3	144.30	145.39	143.96	
B4	148.03	149.21	147.55	
A3	151.16	152.38	150.92	
A4 Ac C=O	168.95	168.98	168.60	
γ C=O	170.77	170.97	170.41	
B γ C=O	170.92	170.80	170.27	

Compound Number 2006



5-(2-Ethoxycarbonylvinyl)-2-(4-hydroxy-3-methoxyphenyl)-7-methoxy -2,3-dihydrobenzofuran-3-carboxylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.27	t	7.1
CH3	1.27	t	7.1
A3 OMe	3.82	s	
B3 OMe	3.91	s	
CH2	4.18	q	7.1
CH2	4.25	m	
β	4.43	d	8.0
α	6.03	d	8.0
B β	6.41	d	15.9
A5	6.84	d	8.1
A6	6.91	dd	8.1, 1.9
A2	7.08	d	1.9
B6	7.27	br s	
B2	7.31	br s	
B α	7.62	d	15.9
A4 OH	7.87	s	

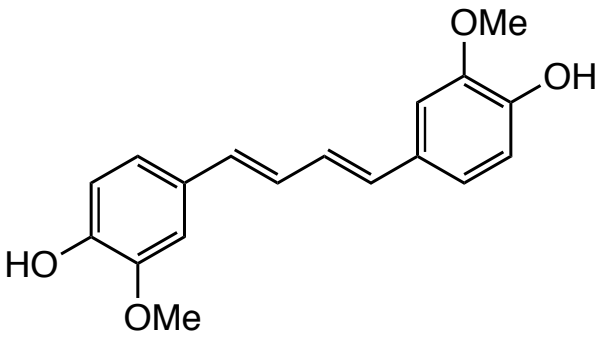
Notes:

S. Quideau-Ag2O oxidation of ethyl ferulate.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A CH3	14.24	14.48	14.12
B CH3	14.31	14.63	14.32
β	55.54	56.06	54.33
A OMe	55.98	56.31	55.78
B OMe	56.08	56.49	56.04
A CH2	61.83	62.20	61.49
B CH2	60.37	60.56	59.99
α	87.46	88.34	87.36
A2	108.74	110.74	110.86
B2	111.93	113.30	112.55
A5	114.49	115.82	115.48
B β	115.93	116.69	115.84
B6	117.86	118.91	118.31
A6	119.44	120.18	119.41
B5	125.85	127.41	126.35
B1	128.61	129.46	128.23
A1	131.44	132.10	129.97
B α	144.50	145.22	144.66
B3	144.69	145.82	147.83
A3	146.69	148.56	144.44
A4	146.03	147.97	149.50
B4	149.90	150.99	147.19
B γ	167.18	167.28	166.65
γ	170.20	171.10	170.42

Compound Number 2007



trans

1,4-bis-(4-hydroxy-3-methoxypheny)l-1,3-butadiene

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.87	s	
α	6.56	m	
A5	6.78	d	8.1
β, A6	6.85-6.92	m	
A2	7.12	d	1.9
Ar OH	7.71	s	

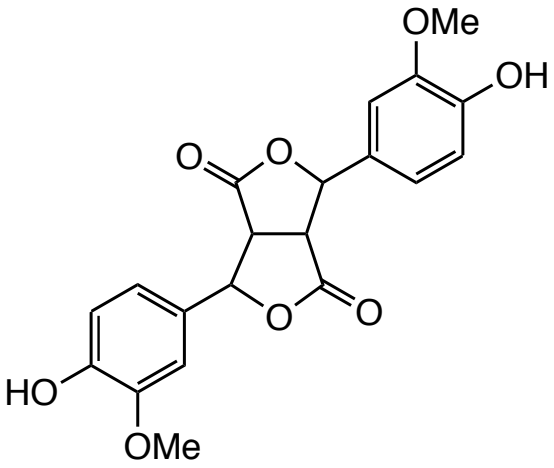
Notes:

S. Quideau
From LiBH4 red. of dilactone
As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe	55.89	56.21	55.55	
2	107.95	109.76	109.38	
5	114.55	115.96	115.55	
6	120.29	120.95	119.81	
β	127.35	128.07	126.90	
1	130.25	130.81	128.96	
α	131.72	132.49	131.37	
4	145.45	147.41	146.43	
3	146.69	148.60	147.80	

Compound Number 2008



dilactone from ferulic acid

3,6-Bis-(4-hydroxy-3-methoxyphenyl) tetrahydrofuro [3,4-c] furan-1,4-dione

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.85	s	
β	4.09	t	1.0
α	5.77	br s	
5	6.86	d	8.2
6	6.92	dd	8.2, 1.8
2	7.05	d	1.8
4 OH	7.90	s	

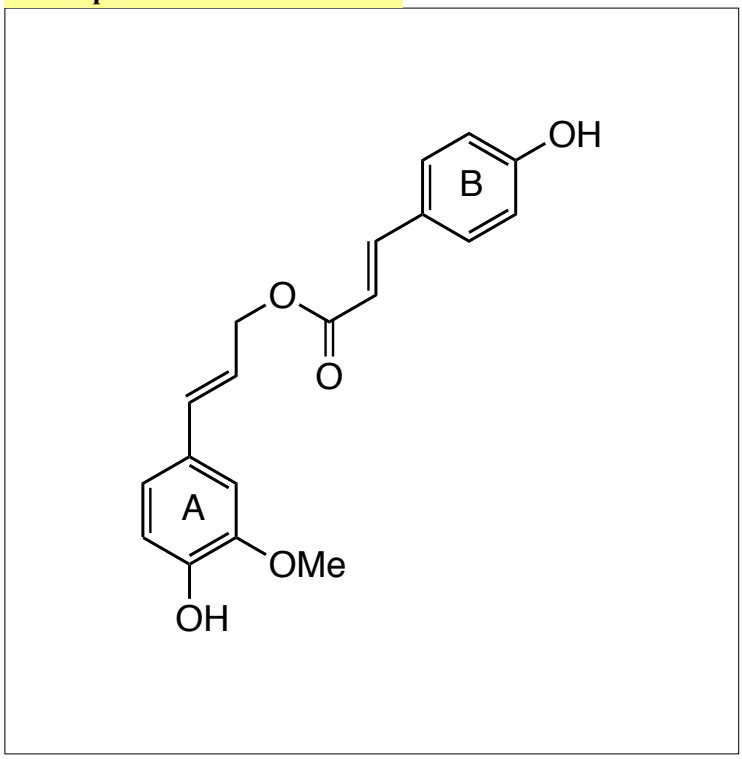
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	48.39	49.11	48.11	
OMe	56.13	56.39	55.81	
α	81.90	83.22	82.06	
2	107.52	110.40	110.64	
5	114.98	116.00	115.46	
6	117.41	119.57	119.22	
1	129.81	130.82	129.00	
4	146.35	148.17	147.36	
3	147.06	148.72	147.88	
γ	174.94	175.99	175.40	

Notes:

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

Compound Number 2009



coniferyl *p*-coumarate

3-(4-Hydroxyphenyl) acrylic acid 3-(4-hydroxy-3-methoxyphenyl) llyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.86	s	
γ	4.78	dd	6.5, 1.3
β	6.25	dt	15.8, 6.5
B β	6.37	d	15.9
α	6.65	dt	15.8, 1.3
A5	6.79	d	8.1
B3,5	6.88	m	
A6	6.91	dd	8.1, 2.0
A2	7.11	d	2.0
B2,6	7.54	m	
B α	7.63	d	15.9
ArOH	7.76	s	
ArOH	9.03	s	

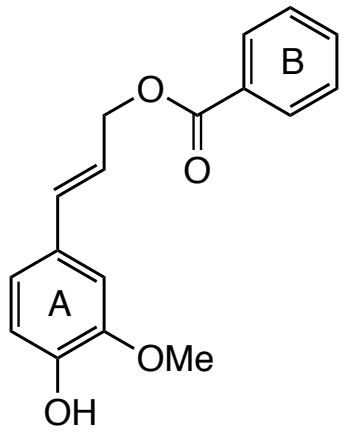
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.87	56.20	55.61
γ	65.35	65.49	64.62
A2	108.44	110.20	109.91
B β	114.45	115.45	114.13
A5	114.98	115.83	115.46
B3	115.93	116.68	115.81
B5	115.93	116.68	115.81
A6	120.62	121.19	120.12
β	120.89	121.72	120.61
B1	126.81	126.90	125.12
A1	128.83	129.39	127.59
B2	130.00	130.91	130.37
B6	130.00	130.91	130.37
α	134.43	134.90	133.9
Bα	145.07	145.49	144.90
A4	145.84	147.80	146.87
A3	146.63	148.53	147.79
B4	158.26	160.65	159.89
B γ	167.57	167.27	166.46

Compound Number 2010



coniferyl benzoate

3-Phenyl-acrylic acid 3-(4-hydroxy-3-methoxyphenyl)allyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.86	s	
γ	4.94	dd	6.5, 1.3
β	6.34	dt	15.8, 6.5
α	6.72	dt	15.8, 1.3
A5	6.80	d	8.1
A6	6.93	dd	8.1, 2.0
A2	7.14	d	2.0
B3,5	7.50	m	
B4	7.62	m	
B2,6	8.03 - 8.06	m	
ArOH	7.76	s	

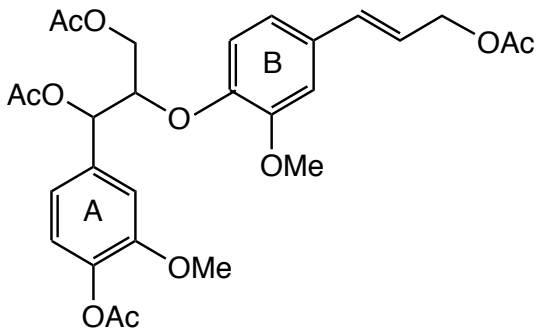
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	55.86	56.21	55.61
γ	65.74	66.35	65.55
A2	108.39	110.25	109.96
A5	114.44	115.84	115.45
A6	120.64	121.29	120.23
β	120.81	121.32	120.23
B3	128.32	129.37	128.82
B5	128.32	129.37	128.82
A1	128.76	129.31	127.52
B2	129.61	130.17	129.20
B6	129.61	130.17	129.20
B1	130.24	131.30	129.78
B4	132.93	133.86	133.39
α	134.50	135.34	134.29
A3	146.63	148.54	147.79
A4	145.91	147.89	146.93
B α C=O	166.46	166.58	165.62

Notes:

S. Quideau
isolated from gum s.am

Compound Number 2011



threo

Guaiacylglycerol-β-coniferyl ether peracetate

^{1}H (acetone)

Atom	H Shifts	Mult	J

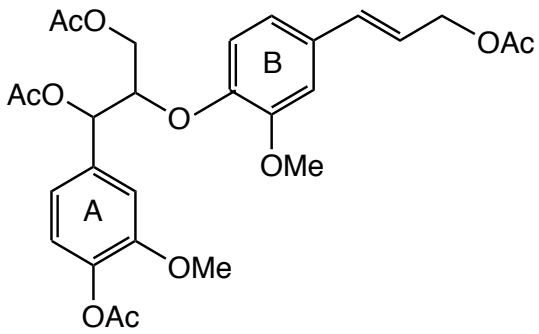
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.63	20.44	20.38	
α Ac Me	20.68	20.58	20.46	
γAc Me	20.99	20.78	20.75	
Bγ Ac Me	21.02	20.91	20.72	
A3 OMe	55.81	56.24	55.67	
B3 OMe	55.93	56.29	55.84	
γ	63.02	63.56	62.49	
B γ	65.08	65.36	64.45	
α	74.40	75.32	74.28	
β	80.19	80.56	78.95	
B2	110.17	111.31	110.22	
A2	111.66	112.64	111.65	
B5	118.31	118.74	116.99	
A6	119.54	120.30	119.46	
B6	119.82	120.54	119.56	
Bβ	122.13	123.26	122.35	
A5	122.83	123.56	122.74	
B1	131.54	132.35	130.64	
B α	133.87	134.16	132.99	
A1	135.18	136.61	135.40	
A4	139.92	140.92	139.23	
B4	148.02	149.09	147.56	
B3	150.71	151.75	150.09	
A3	151.12	152.22	150.73	
A4 Ac C=O	168.76	168.89	168.48	
αAc C=O	169.65	170.00	169.45	
γAc C=O	170.54	170.68	170.05	
BγAc C=O	170.84	170.77	170.21	

Compound Number 2012



erythro

Guaiacyl glycerol-β-coniferyl ether peracetate

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

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	1.93	s	
B γ Ac Me	2.02	s	
α Ac Me	2.07	s	
A4 Ac Me	2.21	s	
A3 OMe	3.82	s	
B3 OMe	3.85	s	
γ1	4.22	dd	11.9, 4.1
γ2	4.36	dd	11.9, 5.9
B γ	4.66	dd	6.4, 1.4
β	4.85	m	
α	6.06	d	5.1
B β	6.26	dt	15.9, 6.4
B α	6.62	dt	15.9, 1.4
B6	6.93	dd	8.3, 2.0
B5	6.97	d	8.3
A5	7.02	d	8.1
A6	7.05	dd	8.1, 1.8
B2	7.13	d	2.0
A2	7.25	d	1.8

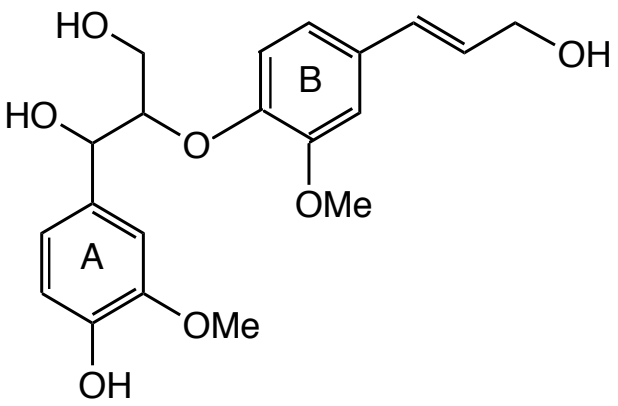
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
A4 Ac Me	20.64	20.45	20.39
α Ac Me	20.74	20.59	20.47
γ Ac Me	20.99	20.77	20.69
B γ Ac Me	20.99	20.85	20.75
A3 OMe	55.80	56.25	55.72
B3 OMe	55.91	56.27	55.78
γ	62.53	62.98	61.92
B γ	65.07	65.34	64.43
α	73.70	74.49	73.07
β	80.17	80.27	78.29
B2	110.24	111.38	110.40
A2	111.94	112.73	111.69
B5	119.11	119.36	117.51
A6	119.65	120.39	119.37
B6	119.80	120.48	119.56
B β	122.23	123.37	122.48
A5	122.60	123.35	122.58
B1	131.86	132.63	130.93
B α	133.85	134.12	132.96
A1	135.28	136.59	135.34
A4	139.78	140.79	139.11
B4	147.23	148.27	146.63
B3	150.98	151.98	150.32
A3	151.02	152.11	150.60
A4 Ac C=O	168.80	168.90	168.51
α Ac C=O	169.49	169.88	169.33
γ Ac C=O	170.76	170.74	170.12
B γ Ac C=O	170.83	170.74	170.21

Compound Number 2013



threo

Guaiacylglycerol-β-coniferyl ether

1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxypropenyl)-2-methoxyphenoxy]propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.48	dd	11.9, 5.7
γ2	3.67	dd	11.9, 3.7
A,B γ OH	3.80-3.90		
A3 OMe	3.80	s	
B3 OMe	3.88	s	
B γ	4.20	br dd	5.3, 1.6
β	4.20	m	
α OH	4.45	d	3.9
α	4.87	br d	5.5
B β	6.28	dt	15.9, 5.4
B α	6.52	dt	15.9, 1.6
A5	6.76	d	8.1
A,B 6	6.88-6.91	m	
A2	7.08	d	1.9
B2	7.09	d	1.9
B5	7.11	d	8.4
A4 OH	7.50	br s	

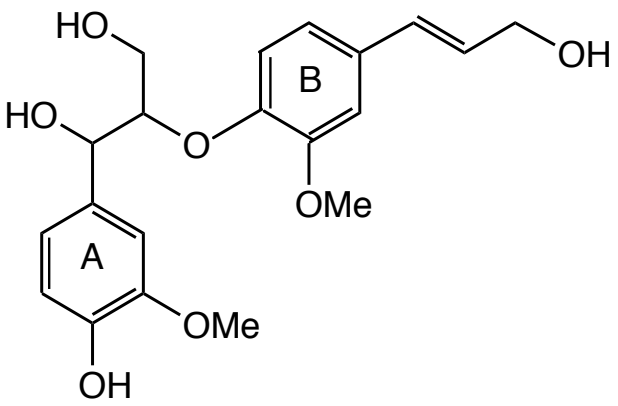
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe	55.97	56.19	55.44	55.40
B3 OMe	56.03	56.31	55.83	55.57
γ	61.21	61.88	60.16	60.28
B γ	63.56	63.25	61.65	61.75
α	74.07	73.83	71.01	71.18
β	89.47	88.37	84.36	84.62
B2	108.94	110.85	109.84	109.84
A2	110.00	111.42	111.05	111.10
A5	114.37	115.21	114.71	114.78
B5	120.15	119.57	115.53	115.68
B6	120.29	120.31	119.05	119.07
A6	120.83	120.54	119.10	119.16
B β	128.24	129.63	128.58	128.59
B α	130.53	129.85	128.60	128.59
B1	131.55	132.96	130.18	130.30
A1	133.15	133.82	132.97	133.04
A4	144.75	146.83	145.46	145.67
A3	145.71	148.03	147.03	147.11
B4	147.47	149.15	147.88	147.99
B3	151.33	151.69	149.70	149.80
1H				
OMe				3.72
OMe				3.78
Aγ				3.73
B γ				4.15
β				4.39
α				4.86
B β				6.28
B α				6.50
B2				7.06
A2				7.08
A5				6.77
B5				7.05
A,B 6				6.88-6.91

Notes:

S. Quideau see erythro isomer 2014
α (e/t) and γ shifts (e/t) interchange from sample to sample, probably due to H-exchange of OH's in d6-acetone. CDCl3 and DMSO shifts not substantiated.
DMSO/pyr data at 700MHz F. Lu w3-F9 HSQC and HMBC

Compound Number 2014



erythro

Guaiacylglycerol-β-coniferyl ether

1-(4-Hydroxy-3-methoxyphenyl)-2-[4-(3-hydroxypropenyl)-2-methoxyphenoxy]propane-1,3-diol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	3.69	dd	11.8, 4.0
γ2	3.81	dd	11.8, 6.2
A,B γ OH	3.80-3.90		
A3 OMe	3.80	s	
B3 OMe	3.84	s	
B γ	4.19	br dd	5.4, 1.6
β	4.29	m	
α OH	4.57	d	4.6
α	4.89	br d	5.2
B β	6.26	dt	15.9, 5.4
B α	6.50	dt	15.9, 1.6
A5	6.75	d	8.1
A,B6	6.86-6.89	m	
B5	6.91	d	1.9
B2	7.05	d	1.9
A2	7.10	d	8.4
A4 OH	7.47	br s	

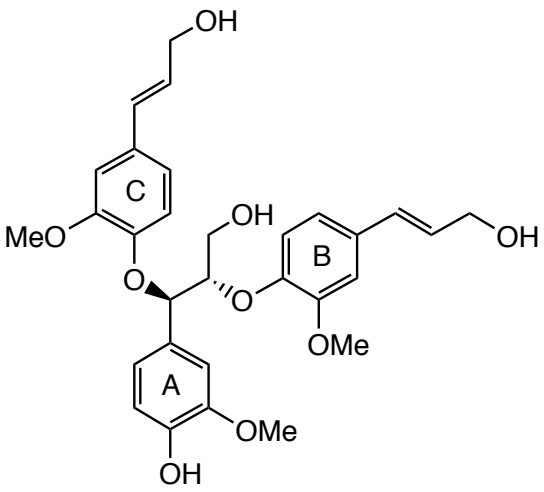
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe	55.97	56.21	55.64	55.40
B3 OMe	56.03	56.29	55.64	55.57
γ	60.87	61.82	60.16	60.28
B γ	63.56	63.25	61.65	61.75
α	72.96	73.81	71.67	71.83
β	87.34	86.63	83.75	83.97
B2	108.82	110.99	109.93	109.94
A2	110.05	111.44	111.47	111.49
A5	114.37	115.13	114.60	114.69
B5	119.14	119.27	115.60	115.76
B6	120.09	120.23	119.05	119.11
A6	120.79	120.46	119.54	119.62
B β	128.19	129.54	128.52	128.59
B α	130.56	129.87	128.60	128.59
B1	131.86	132.84	130.08	130.22
A1	133.11	134.24	133.23	133.33
A4	143.98	146.65	145.46	145.67
A3	145.27	147.96	147.00	147.11
B4	146.75	148.55	147.60	147.68
B3	151.62	151.88	149.75	149.86
1H				
OMe				
OMe				3.72
				3.78
Aγ				
B γ				3.73
				4.15
α				
β				4.86
				4.43
B2				
A2				7.01
A5				7.10
B5				6.77
A,B 6				7.00
B α + β				6.86-6.89
				6.28 + 6.50

Notes:

S. Quideau see threo isomer 2013
α (e/t) and γ shifts (e/t) interchange from sample to sample, probably due to H-exchange of OH's in d6-acetone. CDCl3 and DMSO shifts not substantiated.
DMSO/pyr data at 700MHz F. Lu w3-F9 HSQC and HMBC

Compound Number 2015



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Guaiacylglycerol-α,β-bis-coniferyl ether
4-{3-Hydroxy-1,2-bis-[4-(3-hydroxypropenyl)-2-methoxy phenoxy]propyl}-2-methoxyphenol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.46	d	5.5
A β	4.56	m	
A γ1	3.81	dd	11.7, 7.1
A γ2	3.93	dd	11.7, 4.1

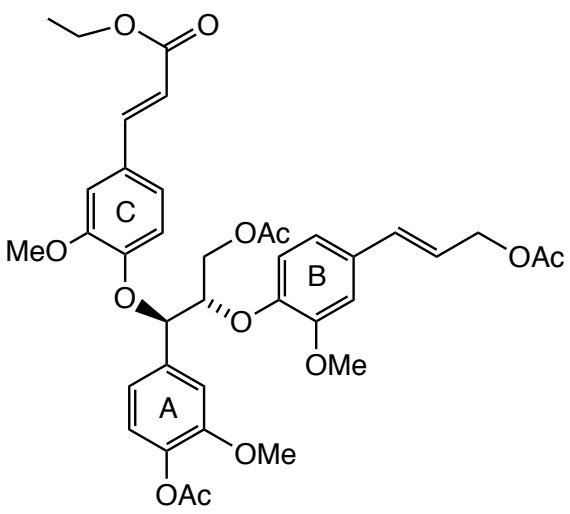
Notes:

S. Quideau Shifts for α and β's and A,B,C 1's change places in CDCl3 and DMSO
S. Quideau, and J. Ralph, A biomimetic route to lignin model compounds via silver (I) oxide oxidation. 2. NMR characterization of non-cyclic benzyl aryl ethers, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe	55.76	56.18	55.41	
B3 OMe	55.85	56.20	55.61	
C3 OMe	55.93	56.32	55.80	
γ	62.17	61.75	59.74	
B γ	63.56	63.25	61.52	
C γ	63.63	63.25	61.58	
α	81.68	81.15	79.01	
β	85.42	85.31	82.53	
C2	109.38	110.74	109.93	
B2	109.54	110.93	109.93	
A2	109.77	112.11	111.91	
A5	114.26	115.23	114.74	
C5	115.94	117.02	115.71	
B5	119.13	119.04	116.15	
C6	119.49	119.90	118.87	
B6	119.74	120.15	119.00	
A6	120.33	121.49	120.34	
C β	127.10	129.22	128.32	
B β	127.60	129.45	128.47	
B α	130.59	129.85	130.49	
C α	130.79	129.85	130.49	
A1	130.43	130.39	128.24	
C1	130.85	132.05	128.71	
B1	132.09	132.74	128.82	
A4	145.49	147.18	146.07	
C4	146.64	147.77	146.27	
A3	146.85	148.10	147.11	
B4	147.08	148.61	147.36	
C3	149.80	151.17	149.73	
B3	150.81	151.71	149.80	

Compound Number 2016



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

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ1	4.45	dd	11.8, 3.8
γ2	4.53	dd	11.9, 6.0
B γ	4.66	dd	6.4, 1.3
β	4.88	m	
α	5.71	d	5.3
B β	6.25	dt	15.8, 6.4
C β	6.39	d	15.9
B α	6.61	dt	15.8, 1.3
C α	7.53	d	15.9

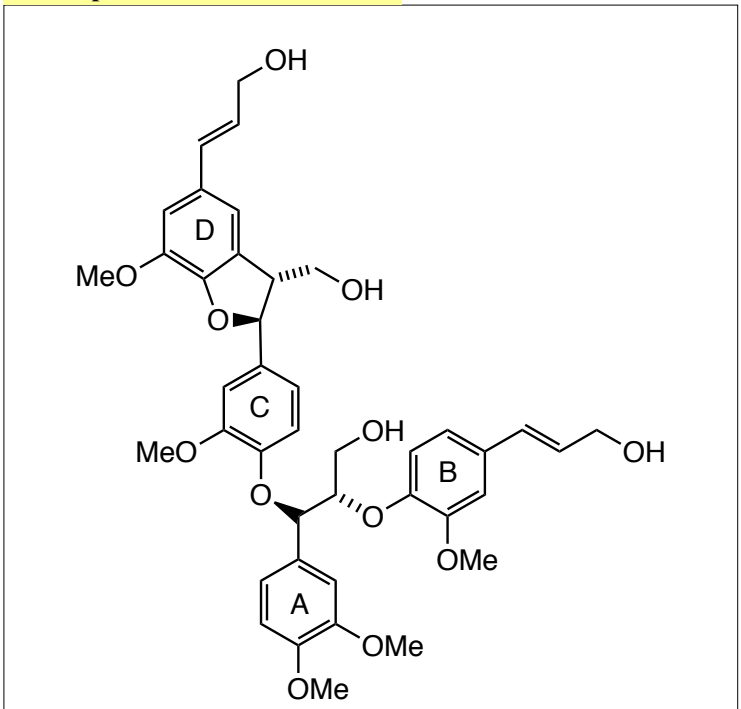
Notes:

S. Quideau Shifts substantiated in d6-acetone but not CDCL3 or DMSO. γ and Bγ Ac C=O shifts may be interchanged S. Quideau, and J. Ralph, A biomimetic route to lignin model compounds via silver (I) oxide oxidation. 2. NMR characterization of non-cyclic benzyl aryl ethers, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Me	14.33	14.57	14.19
A4 Ac Me	20.65	20.43	20.33
γ Ac Me	20.74	20.60	20.43
B γAc Me	21.00	20.77	20.71
A OMe	55.73	56.16	55.67
B OMe	55.96	56.20	55.80
C OMe	55.98	56.44	55.95
CH2	60.39	60.56	59.79
γ	63.22	63.41	62.33
B γ	65.09	65.37	64.41
α	79.99	80.47	78.45
β	81.98	81.70	79.57
B2	110.14	111.19	110.22
C2	110.73	111.92	111.40
A2	111.17	112.80	111.89
C5	115.87	116.69	115.28
C β	116.51	117.15	116.25
B5	119.10	119.28	117.18
A6	119.34	120.33	119.35
B6	119.82	120.47	119.50
C6	122.08	122.57	122.33
B β	122.15	123.17	122.24
A5	122.66	123.36	122.49
C1	128.62	129.41	127.56
B1	131.71	132.37	130.59
B α	133.90	134.18	133.00
A1	136.48	137.19	135.93
A4	139.64	140.63	138.94
C α	144.28	144.96	144.23
B4	147.35	148.51	146.96
C4	149.33	150.06	148.42
C3	150.23	151.36	149.75
B3	150.96	151.86	150.12
A3	151.20	152.12	150.49
C γ C=O	167.13	167.23	166.40
A4 Ac C=O	168.78	168.90	168.36
γAc C=O	170.77	170.81	170.09
B γ Ac C=O	170.86	170.82	170.14

Compound Number 2017



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Veratryglycerol-α-dehydrodiconifyl-β-con.ether

^{1}H Acetone/D2O

Atom	H Shifts	Mult	J
A α	5.48	d	5.8
A β	4.62	m	
A γ1	3.80	dd	11.9, 6.5
A γ2	3.91	dd	11.9, 4.9
C α	5.51	d	5.8
C β	3.43	m	
C γ1	3.69	s	
C γ2	3.80	s	

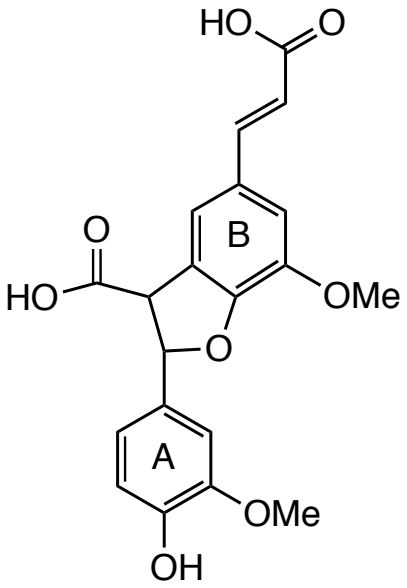
Notes:

S. Quideau Run only in Acetone:D2O (9:1) S. Quideau, and J. Ralph,, Holzforschung, 1994, 48(2), 124-132. Note: Two erythro isomers!! Resolvable pairs are:80.10, 80.05 54.28, 54.21 136.08, 136.05 110.98, 110.89 147.31, 147.30 116.41, 116.42 118.42, 118.40

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
		Note*		
C β		54.28		
A3 OMe		55.83		
A4 OMe		55.80		
B OMe		56.09		
D OMe		56.20		
C OMe		56.33		
γ		61.20		
B γ		62.77		
D γ		62.85		
C γ		64.18		
α		80.10		
β		83.86		
C α		87.80		
B2		110.71		
C2		110.98		
D2		111.35		
A5		111.67		
A2		112.04		
D6		115.96		
C5		116.41		
B5		117.55		
C6		118.42		
B6		119.99		
A6		120.96		
D β		127.73		
B β		128.64		
B α		130.02		
D5		129.64		
D α		130.57		
A1		130.94		
D1		131.83		
B1		132.11		
C1		136.08		
D3		144.75		
C4		147.31		
B4		147.98		
D4		148.27		
A3		149.45		
A4		149.48		
C3		150.58		
B3		150.83		

Compound Number 2018



beta-5-dehydrodiferulic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	6.05	d	7.8
β	4.39	d	7.8
A2	7.08	d	2.0
A5	6.83	d	8.1
A6	6.91	dd	8.1, 2.0
A3 OMe	3.83	s	
B α	7.62	d	15.9
B β	6.39	d	15.9
B2	7.29	br s	
B6	7.33	br s	
B3 OMe	3.91	s	

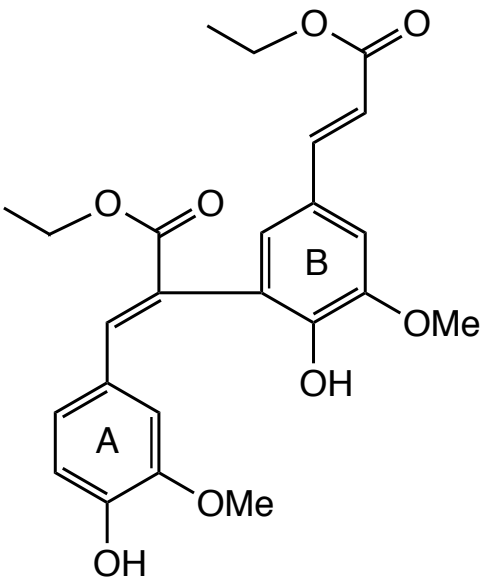
Notes:

S. Quideau
B α changes in CDCl3
JCS Perkin 1, 3485-98 (1994)
Cmpd 13

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe	56.03	56.31	55.61	
B3 OMe	56.15	56.49	55.85	
β	53.76	56.22	55.10	
α	87.53	88.56	87.72	
A2	108.77	110.72	110.61	
B2	112.26	113.34	112.10	
A5	114.53	115.78	115.30	
B β	114.91	116.75	116.43	
B6	118.63	118.95	117.93	
A6	119.49	120.08	119.50	
B5	125.93	128.05	127.82	
B1	128.29	129.38	130.69	
A1	131.44	132.49	137.46	
B α	146.74	145.59	144.09	
B3	144.71	145.73	144.19	
A4	146.06	147.81	146.79	
A3	146.74	148.53	147.60	
B4	150.32	150.96	149.16	
B γ	171.34	168.18	167.79	
γ	173.67	172.55	171.66	

Compound Number 2019



3-(4-Hydroxy-3-methoxyphenyl)-2-[2-hydroxy-3-methoxy-5-(2-propoxycarbonylvinyl)phenyl] acrylic acid ethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.21	t	7.1
CH3	1.24	t	7.1
A3 OMe	3.44	s	
B3 OMe	3.96	s	
CH2	4.16	q	7.1
CH2	4.17	q	7.1
B β	6.38	d	15.9
A2	6.696	d	2.1
A5	6.702	d	8.2
A6	6.83	dd	8.2, 2.1
B6	7.00	d	2.0
B2	7.38	d	2.0
B α	7.56	d	15.9
A α	7.76	s	

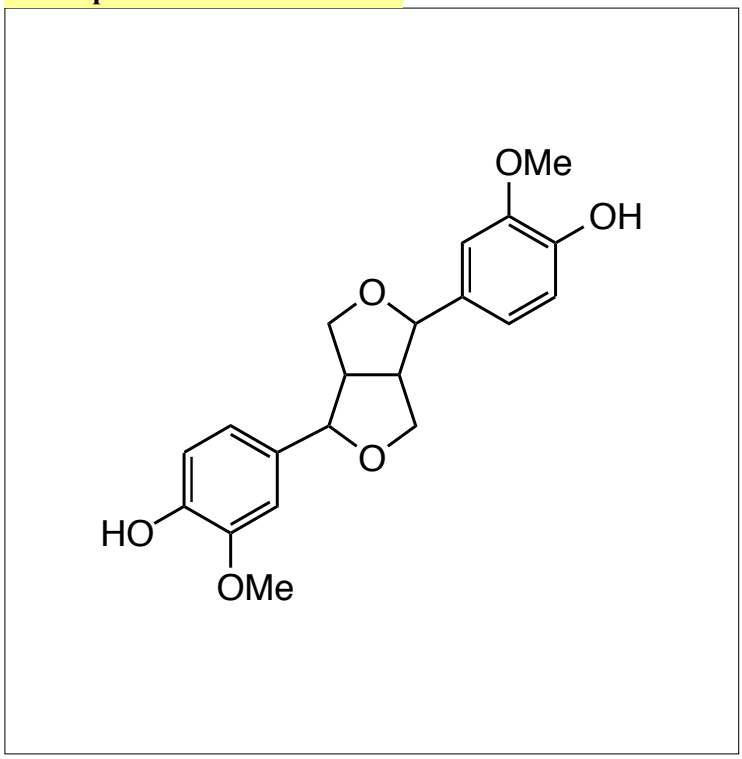
Notes:

S. Quideau
B5,B6 and A6 switch in acetone and DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
CH3	14.28	14.61	14.14
CH3	14.28	14.62	14.16
A3 OMe	55.24	55.51	54.66
B3 OMe	56.12	56.58	56.05
CH2	60.35	60.47	59.62
CH2	61.09	61.05	60.15
B2	108.68	110.25	110.05
A2	111.57	113.28	112.92
A5	114.29	115.63	115.02
B β	116.00	116.31	115.17
β	123.29	124.92	123.97
B5	124.76	126.56	125.09
B6	124.82	125.71	124.61
A6	125.82	126.37	125.16
B1	126.81	127.31	125.56
A1	126.94	127.58	125.66
α	141.45	141.37	140.11
B α	144.30	145.25	144.49
A3	145.86	147.87	147.02
B4	146.05	148.03	147.11
A4	147.11	148.99	148.16
B3	147.31	149.10	148.23
B γ	167.11	167.29	166.44
γ	167.46	167.77	166.83

Compound Number 2020



Pinoresinol

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.08	m	
γ1	3.80	dd	9.1, 3.8
OMe	3.83	s	
γ 2	4.19	dd	9.0, 7.0
α	4.66	d	4.25
A5	6.78	d	8.1
A6	6.83	dd	8.1, 1.8
A2	6.98	d	1..8
Ar OH	7.48	s	

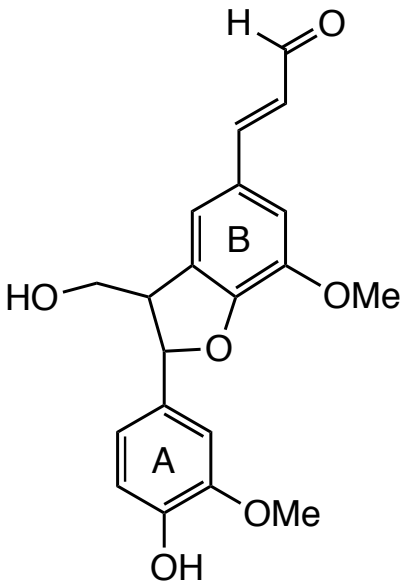
Notes:

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

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	54.15	55.23	53.59	
OMe	55.94	56.24	55.62	
γ	71.66	72.20	70.91	
α	85.86	86.62	85.17	
2	108.60	110.60	110.43	
5	114.27	115.52	115.15	
6	118.95	119.59	118.64	
1	132.91	134.17	132.26	
4	145.24	146.86	145.91	
3	146.70	148.32	147.53	

Compound Number 2021



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3-[2-(4-Hydroxy-3-methoxyphenyl)-3-hydroxymethyl-7-methoxy-2,3-dihydrobenzofuran-5-yl] prop-2-enal

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.61	br q	
A3 OMe	3.82	s	
B3 OMe	3.91	s	
γ	3.87-3.91	m	
α	5.65	d	6.6
B β	6.65	dd	15.8, 7.7
A5	6.81	d	8.1
A6	6.88	dd	8.1, 2.0
A2	7.04	d	2.0
B2	7.29	bro	
B6	7.32	bro	
B α	7.59	d	15.8
B γ	9.63	d	7.7

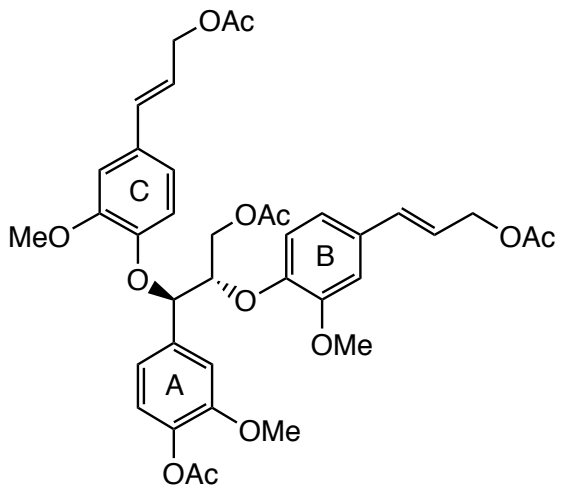
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β		54.25		
A3 OMe		56.29		
B3 OMe		56.46		
γ		64.32		
α		89.39		
A2		110.59		
B2		113.56		
A5		115.76		
B6		119.64		
A6		119.73		
B β		127.14		
B5		129.00		
B1		131.24		
A1		133.75		
B3		145.65		
A4		147.55		
A3		148.46		
B4		152.41		
B α		154.10		
B γ		193.77		

Compound Number 2022



erythro

Guaiacylglycerol-α,β-bis coniferyl ether tetraacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.62		
A β	4.87		
A γ1	4.45		
A γ2	4.53		

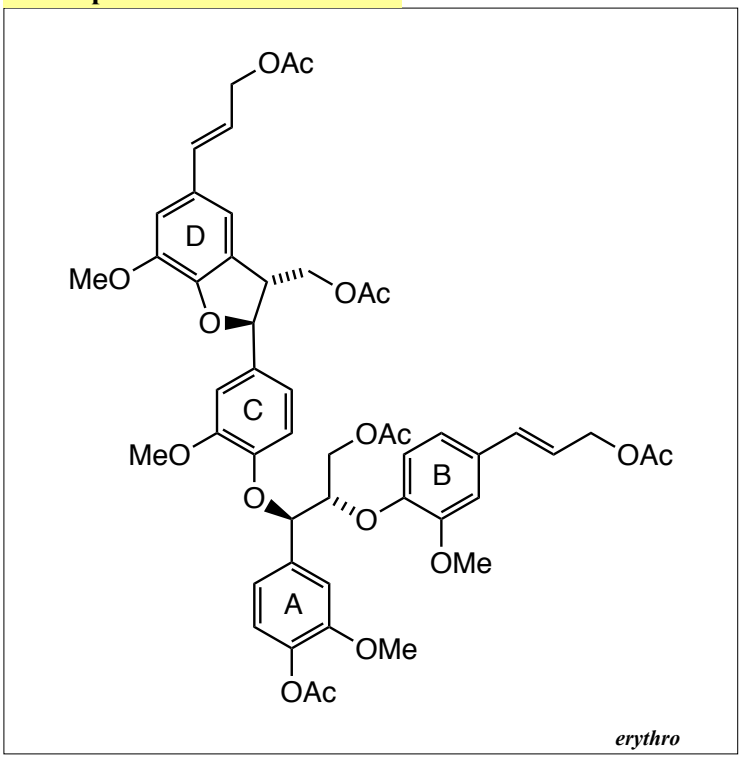
Notes:

S. Quideau
α and β of B and C can interchange in CDCl3
S. Quideau, and J. Ralph, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.63	20.44	20.33	
γ Ac Me	20.73	20.62	20.42	
C γ Ac Me	20.98	20.76	20.70	
B γAc Me	20.98	20.78	20.70	
A3 OMe	55.73	56.23	55.59	
B3 OMe	55.91	56.23	55.64	
C3 OMe	55.94	56.39	55.78	
γ	63.37	63.56	62.39	
C γ	65.08	65.37	64.39	
B γ	65.12	65.37	64.39	
α	80.17	80.85	78.68	
β	81.92	81.74	79.56	
C2	109.94	111.16	110.15	
B2	110.11	111.32	110.21	
A2	111.29	112.74	111.87	
C5	116.41	117.41	115.81	
B5	118.92	119.23	117.06	
C6	119.49	120.45	119.43	
B6	119.77	120.50	119.48	
A6	119.79	120.51	119.50	
C β	121.69	122.99	122.12	
B β	122.03	123.18	122.19	
A5	122.50	123.26	122.38	
C1	130.61	131.73	130.12	
B1	131.55	132.34	130.51	
C α	133.92	134.22	133.00	
B α	134.02	134.22	133.00	
A1	136.80	137.52	136.19	
A4	139.53	140.65	138.88	
C4	147.45	148.20	146.38	
B4	147.47	148.66	146.99	
C3	150.18	151.43	149.75	
B3	150.90	151.91	150.09	
A3	151.09	152.12	150.45	
A4 Ac C=O	168.76	168.85	168.34	
A γ Ac	170.76	170.72	170.07	
C=O	170.83	170.74	170.10	
D γ Ac	170.83	170.77	170.12	
C=O				
C γ Ac C=O				

Compound Number 2023



erythro

Guaiacylglycerol-α-dehydrodiconiferyl-bis-ether peracetate diastereomeric mixture

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.62	d	5.4
A β	4.88	m	
A γ1	4.46	dt	11.9, 3.8
A γ2	4.53	dt	11.9, 5.8
C α	5.49	d	6.9
C β	3.72	s	
C γ1	4.28	dd	11.1, 7.5
C γ2	4.40	dd	11.1, 5.4

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A4 Ac Me	20.52	20.43	20.32	
A γAc Me	20.61	20.61	20.42	
C γ Ac Me	20.74	20.65	20.48	
B γ Ac Me	20.98	20.78	20.70	
D γ Ac Me	20.98	20.78	20.70	
OMe		56.39		
OMe		56.31		
OMe		56.17		
OMe		56.15		
C β	50.25	51.04	49.16	
γ	63.36	63.52	62.38	
B γ	65.06	65.36	64.40	
D γ	65.16	65.48	64.49	
C γ	65.28	65.84	68.42	
α	80.13	80.73	78.62	
β	81.87	81.63	79.49	
C α	88.38	88.61	87.25	
B2	110.09	111.17	110.20	
C2	110.17	111.36	110.74	
D2	110.61	112.02	110.93	
A2	111.33	112.69	111.89	
D6	115.31	116.24	115.24	
C5	116.39	117.29	115.76	
C6	118.64	119.11	118.35	
B5	118.89	119.11	117.00	
A6	119.51	120.45	119.43	
B6	119.77	120.46	119.49	
D β	121.13	122.13	121.31	
B β	122.01	123.10	122.18	
A5	122.47	123.24	122.38	
D5	127.53	128.99	127.93	
D1	130.49	131.41	129.99	
B1	131.52	132.23	130.48	
B α	133.90	134.20	133.00	
D α	134.31	134.69	133.50	
C1	134.49	135.94	134.13	
A1	136.76	137.49	136.18	
A4	139.52	140.56	138.88	
D3	144.36	145.32	143.83	
C4	147.36	147.96	146.31	
B4	147.45	148.56	146.95	
D4	148.22	149.22	147.51	
C3	150.35	151.33	149.63	
B3	150.87	151.82	150.07	
A3	151.06	152.05	150.44	
A4 Ac C=O	168.72	168.84	168.33	
B γ Ac C=O	170.74	170.74	170.12	
D γ Ac C=O	170.74	170.74	170.12	
C γ Ac C=O	170.80	170.76	170.12	
A γ Ac C=O	170.83	170.90	170.23	

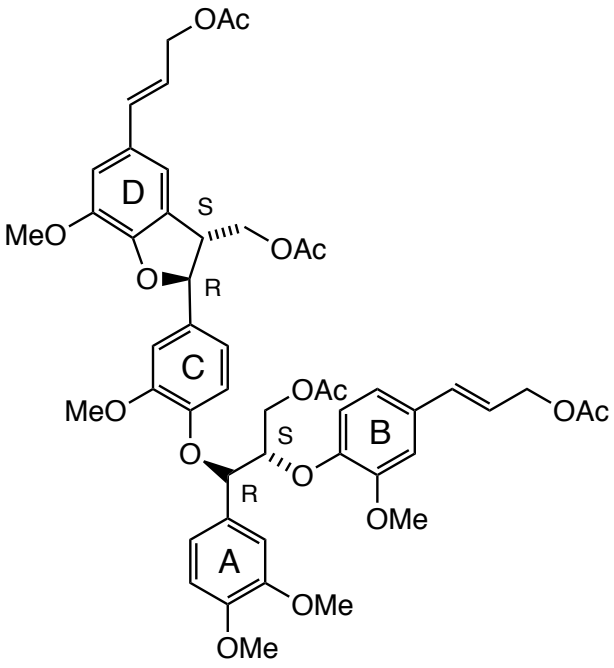
Notes:

S. Quideau

S. Quideau

S. Quideau, and J. Ralph, A biomimetic route to lignin model compounds via silver (I) oxide oxidation. 2. NMR characterization of non-cyclic benzyl aryl ethers, Holzforschung, 1994, 48(2), 124-132.

Compound Number 2024



threo

Veratrylglycerol-α-dehydrodiconiferyl-β-coniferyl-bis-ether peracetate, diastereomeric mixture

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.54	d	5.2
A β	4.87	s	
A γ1	4.44	td	11.8, 3.7
A γ2	4.52	td	11.8, 6.2
C α	5.48	d	6.9
C β	3.70	s	
C γ1	4.28	dt	11.1, 7.5
C γ2	4.39	dt	11.1, 5.5

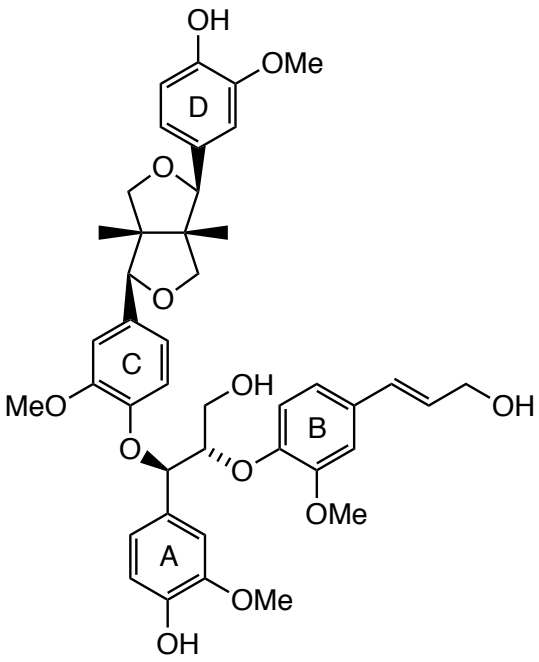
Notes:

S. Quideau
A3 and A4, C and D OMe's, and B and D γ's can be interchanged in all solvents Shifts are confirmed for Acetone
S. Quideau, and J. Ralph, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A γ Ac Me	20.75	20.64	20.45	
C γAc Me	20.75	20.64	20.45	
B γ Ac Me	20.98	20.79	20.70	
D γAc Me	20.98	20.79	20.70	
A4 OMe	55.75	55.97	55.33	
A3 OMe	55.82	56.06	55.59	
B3 OMe	55.86	56.22	55.70	
C3 OMe	56.06	56.38	55.79	
D3 OMe	55.97			
C β	50.18	51.08	49.16	
γ	63.67	63.86	62.64	
B γ	65.09	65.38	64.41	
D γ	65.17	65.49	64.50	
C γ	65.28	65.90	64.71	
α	80.14	80.89	78.77	
β	81.80	81.73	79.57	
C α	88.43	88.65	87.28	
B2	110.02	111.28	110.17	
C2	110.33	111.45	110.63	
D2	110.17	112.16	110.93	
A5	110.56	112.22	111.25	
A2	110.79	112.31	111.12	
D6	115.29	116.31	115.24	
C5	116.53	117.46	115.95	
B5	118.47	118.91	116.79	
C6	118.59	119.11	118.27	
B6	119.73	120.48	119.49	
A6	119.95	120.98	119.81	
D β	121.16	122.19	121.32	
B β	121.91	123.04	122.09	
D5	127.57	129.06	127.93	
A1	130.18	130.90	129.46	
D1	130.49	131.46	129.99	
B1	131.24	132.08	130.30	
B α	133.94	134.26	133.03	
C 1	134.12	135.74	133.92	
D α	134.32	134.71	133.51	
D3	144.37	145.37	143.83	
C4	147.38	148.11	146.38	
B4	147.71	148.83	147.12	
D4	148.21	149.29	147.51	
A3	148.83	150.20	148.37	
A4	148.93	150.23	148.48	
C3	150.39	151.42	149.69	
B3	150.78	151.81	150.02	
D γ Ac C=O	170.70	170.76	170.05	
B γ Ac C=O	170.77	170.76	170.10	
A γ Ac C=O	170.82	170.79	170.13	
C γ Ac C=O	170.85	170.90	170.23	

Compound Number 2025



erythro

Guaiacylglycerol-α-pinoresinol-β-coniferyl-bis-ether diastereomeric mixture

^{1}H (acetone)

Atom	H Shifts	Mult	J
A α	5.45	d	5.6
A β	4.55	m	
A γ1	3.82	dd	11.5, 6.5
A γ2	3.92	dd	11.5, 5.2
C α	4.63		
C β	3.04		
C γ1	3.77		
C γ2	4.17		

Notes:

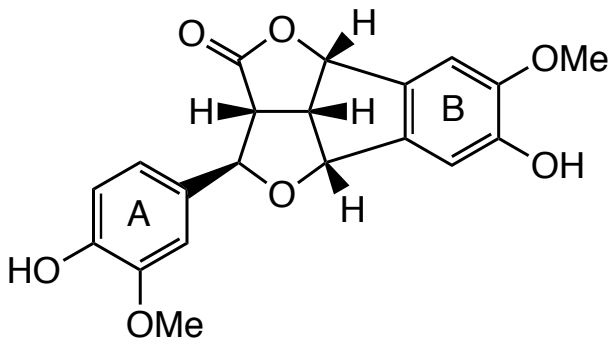
S. Quideau Only run in acetone

S. Quideau, and J. Ralph, A biomimetic route to lignin model compounds via silver (I) oxide oxidation. 2. NMR characterization of non-cyclic benzyl aryl ethers, Holzforschung, 1994, 48(2), 124-132.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
D β		55.15		
C β		55.15		
D3 OMe		56.22		
A3 OMe		56.25		
B3 OMe		56.25		
C3 OMe		56.44		
γ		61.82		
B γ		63.27		
D γ		72.23		
C γ		72.23		
α		81.21		
β		85.38		
C α		86.37		
D α		86.58		
D2		110.59		
B2		111.05		
C2		111.43		
A2		112.21		
A5		115.28		
D5		115.50		
C5		116.83		
C6		118.96		
B5		119.06		
D6		119.61		
B6		120.17		
A6		121.53		
B β		129.50		
B α		129.88		
A1		130.53		
B1		132.78		
D1		134.10		
C1		136.29		
D4		146.85		
A4		147.24		
C4		147.61		
A3		148.15		
D3		148.30		
C3		151.12		
B3		151.75		

Compound Number 2026



11-hydroxy-(4-hydroxy-3methoxyphenyl)-10-methoxy-3a,4,6,6a-tetrahydro 3H-3,4-benzenofuro [3,4-c]f uran-1-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.36	dd	10.7, 6.4
B β	4.24	dddd	10.6, 7.5, 6.9, 0.6
α	4.72	dquin	6.3, 0.6
B α	5.73	br d	
B γ	5.60	dq	

^{13}C

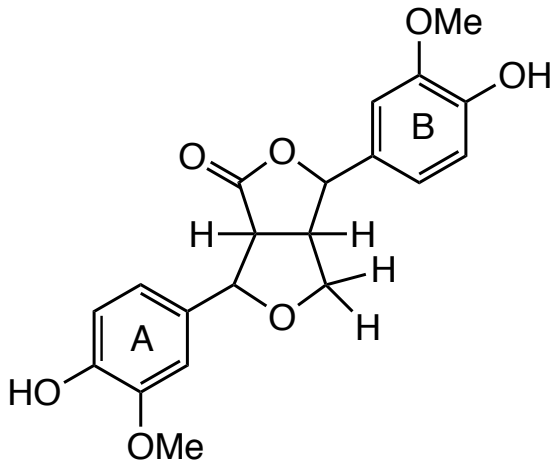
Atom	$CDCl_3$	Acetone	DMSO	
B β	50.40	51.13	49.78	
β	53.87	54.58	53.16	
B3 OMe	56.14	56.38	55.67	
A3 OMe	55.95	56.25	55.58	
α	82.38	84.18	83.14	
B α	83.33	84.22	83.27	
B γ	85.74	86.62	85.15	
B2	106.87	108.57	108.24	
A2	108.61	110.78	110.60	
B5	110.88	112.10	111.46	
A5	114.39	115.56	115.12	
A6	118.82	119.80	118.98	
A1	131.09	132.41	130.35	
B1	132.06	133.24	131.52	
B6	133.95	135.28	133.78	
A4	145.52	147.28	146.38	
A3	146.60	148.30	147.50	
B4	148.42	150.03	149.01	
B3	148.69	150.43	149.63	
γ	176.43	177.32	176.86	

Notes:

S. Quideau

Ref: S. Quideau and John Ralph. J. Chem Soc. Perkin Trans. 1 1993 - issue 6 - 653 -659.

Compound Number 2027



4-cis-8-trans-bis (4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo [3-3-0] octan-2-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.63	t	8.8
B β	3.35	ddd	9.0, 6.6, 4.6
α	5.05	br d	8.6
B α	5.23	br d	6.6
B γ cis	3.88	dd	9.5, 4.8
B γ trans	4.28	br d	9.5

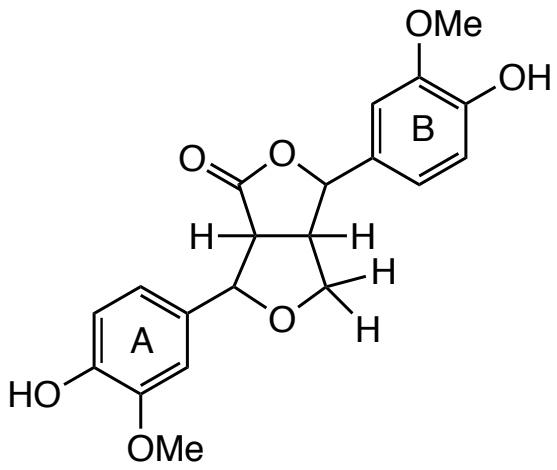
Notes:

S. Quideau
S. Quideau and John Ralph. J. Chem. Soc. Perkin Trans. 1 1993 issue 6 653-659.
Cmpd 14

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	51.31	52.02	50.42	
β	51.67	52.43	51.54	
A3 OMe	55.97	56.28	55.81	
B3 OMe	56.11	56.35	55.91	
B γ	71.63	72.08	71.06	
α	84.00	84.43	83.07	
B α	85.65	86.32	85.45	
B2	107.89	110.68	110.88	
A2	108.78	111.21	110.96	
A5	114.43	115.39	115.28	
B5	114.59	115.80	115.54	
B6	118.83	120.06	119.27	
A6	119.65	120.32	119.48	
A1	127.88	129.78	128.41	
B1	131.26	132.60	130.80	
A4	145.81	147.15	146.24	
B4	146.15	147.82	147.03	
A3	146.60	147.99	147.35	
B3	146.99	148.62	147.96	
γ	174.51	174.93	174.99	

Compound Number 2028



4-trans-8-cis-bis(4-hydroxy-3-methoxyphenyl)-3,7-dioxabicyclo [3-3-0] octan-2-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.65	dd	8.7, 2.6
B β	3.71	m	
γ	5.16	br d	2.6
B α	5.82	br d	5.9
B γ cis	3.80	m	
B γ trans	3.47	dd	9.2, 6.7

Notes:

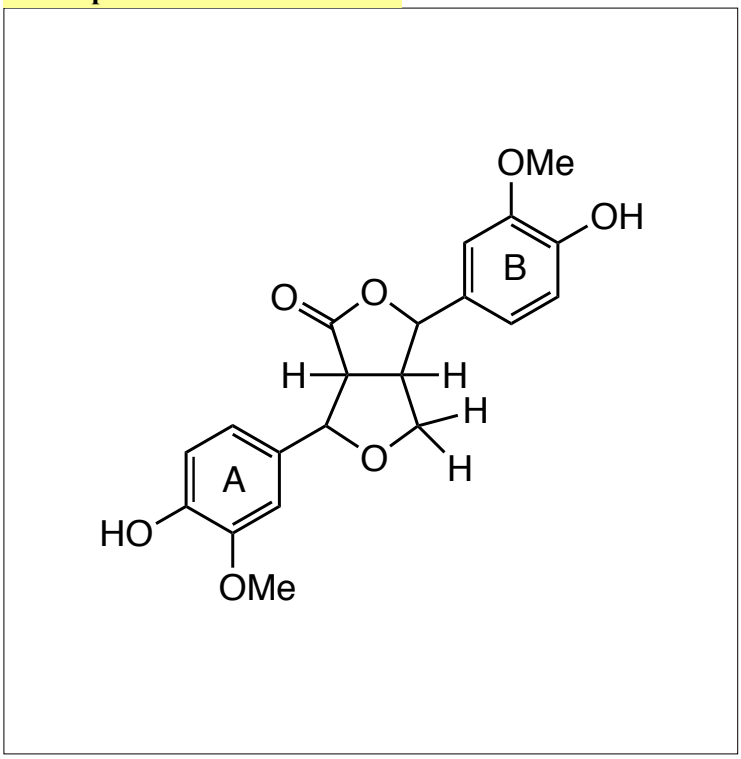
S. Quideau

S. Quideau and J. Ralph. J. Chem Soc . Perkin Trans. 1 1993 (6) 653-659

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β	45.43	46.14		
β	54.80	55.35		
A3 OMe	56.00	56.26		
B3 OMe	56.13	56.34		
B γ	68.66	69.98		
B γ	80.37	81.09		
γ	83.70	84.56		
B2	107.47	109.50		
A2	108.17	110.24		
A5	114.41	115.65		
B5	114.65	115.87		
B6	117.76	118.57		
A6	118.11	119.17		
B1	127.90	129.22		
A1	132.46	133.48		
A4	145.33	147.10		
B4	145.56	147.24		
A3	146.67	148.39		
B3	146.80	148.54		
γ	177.07	177.77		

Compound Number 2029



3,6-bis(4-hydroxy-3-methoxyphenyl)-tetrahydro-furo[3,4-c]furan-1-one

4-cis-8-cis-bis (4-hydroxy-3-methoxyphenyl)-3,7-dioxabicylclo [3-3-0] octan-2-one

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.65	ddd	9.2, 3.7, 0.5
B β	3.39	ddddd	9.2, 7.0, 4.6, 3.6, 0.6
α	5.20	dquin	3.7, 0.6
B α	5.39	br d	3.6
B γ cis	4.30	ddd	9.4, 7.0, 0.5
B γ trans	4.02	ddt	9.4, 4.6, 0.5

Notes:

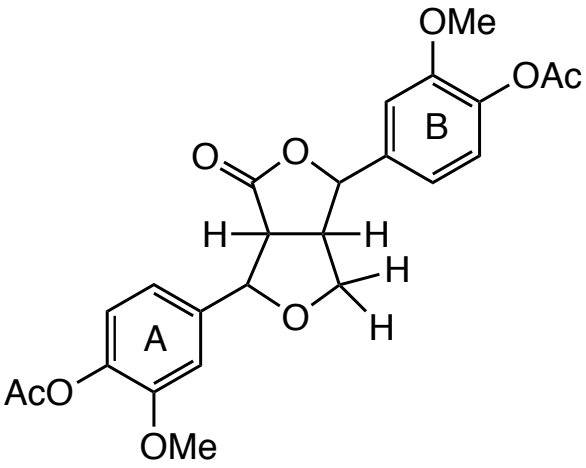
S. Quideau

S.Quideau and J. Ralph. J. Chem. Soc. Perkin Trans. 1 1993 (6) 653-659.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B β	49.99	50.38	48.62
β	53.31	53.71	52.32
A3 OMe	56.02	50.26	55.61
B3 OMe	56.08	50.34	55.71
B γ	72.70	73.44	72.15
α	83.38	84.43	82.91
B α	84.59	85.78	84.83
A2	107.77	110.35	110.30
B2	108.11	110.45	110.54
A5	114.42	115.64	115.16
B5	114.71	115.87	115.34
A6	118.02	119.30	118.50
B6	118.40	119.66	118.88
B1	131.11	132.47	130.58
A1	132.31	133.17	131.08
A4	145.34	147.12	146.19
B4	146.07	147.80	146.85
A3	146.73	148.35	147.55
B3	146.94	148.63	147.73
γ	176.92	177.72	177.14

Compound Number 2030



4-cis-8-cis-bis (4-hydroxy-3-methoxyphenyl)-3,7-dioxabicylclo [3-3-0] octan-2-one diacetate

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.72	ddd	9.25, 3.8, 0.5
B β	3.45	ddddd	9.15, 7.1, 4.8, 3.0, 0.6
B γ trans	4.12	ddt	9.5, 4.8, 0.5
B γ cis	4.39	ddd	9.5, 7.1, 0.5
B α	5.52	br d	3.6
α	5.29	dquin	3.8, 0.6

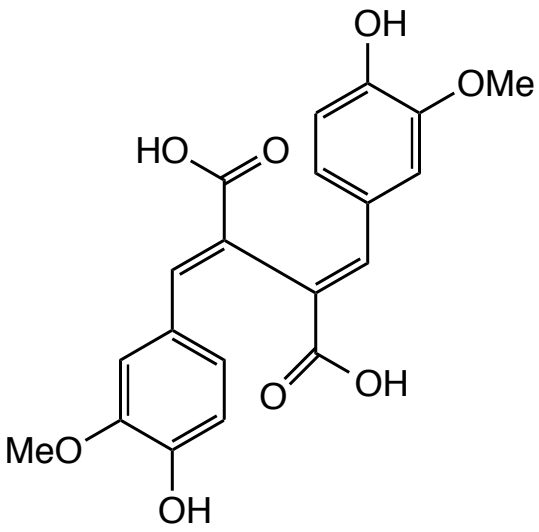
Notes:

S. Quideau
Ralph, Helm, Quideau. J. Chem. Soc. Perkin Trans. 1 1992 2971-2980

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.61	20.45	20.39
Ac Me	20.63	20.45	20.39
B β	49.89	50.33	48.62
β	53.14	53.59	52.19
A3 OMe	55.99	56.24	55.82
B3 OMe	56.06	56.35	55.95
B γ	72.80	73.72	72.51
α	82.99	84.01	82.49
B α	83.89	84.93	83.93
A2	109.13	110.86	110.37
B2	109.35	111.05	110.69
A6	117.14	118.40	117.87
B6	117.22	118.53	118.00
A5	122.98	123.65	122.80
B5	123.38	123.96	123.07
B1	138.04	139.95	138.71
A4	139.26	140.40	138.80
A1	139.32	140.68	139.21
B4	139.96	140.96	139.30
A3	151.35	152.38	150.88
B3	151.66	152.62	151.05
Ac C=O	169.04	168.98	168.57
Ac C=O	168.90	168.94	168.53
γ	176.66	177.49	176.98

Compound Number 2031



4,4′-dihydroxy-3,3′-dimethoxy-β,β′-bicinnamic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.74	s	
5	6.78	d	8.2
6	7.11	dd	8.2, 2.0
2	7.31	d	2.0
α	7.83	s	

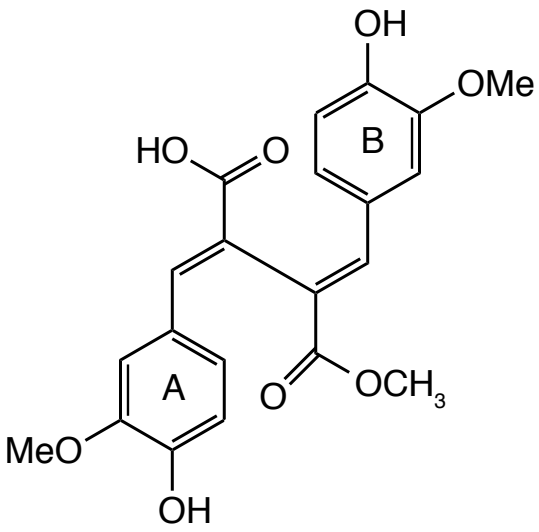
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.05	55.28	
2		113.51	113.23	
5		115.93	115.47	
6		125.60	124.11	
β		126.15	125.12	
1		127.94	126.13	
α		142.26	140.40	
3		148.19	147.29	
4		149.25	148.37	
γ		168.46	168.06	

Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 18
As this compound has a plane of symmetry only one set of shifts are reported.

Compound Number 2032



γ′-methoxy-4,4′-dihydroxy-3,3′-dimethoxy-β,β′-bicinnamic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.66	s	
A3 OMe	3.72	s	
B3 OMe	3.73	s	
A,B 5	6.78	d	8.2
B6	7.11	dd	8.3, 2.0
A6	7.09	dd	8.3, 2.0
A2	7.25	d	2.0
B2	7.30	d	2.0
B α	7.81	s	
α	7.84	s	

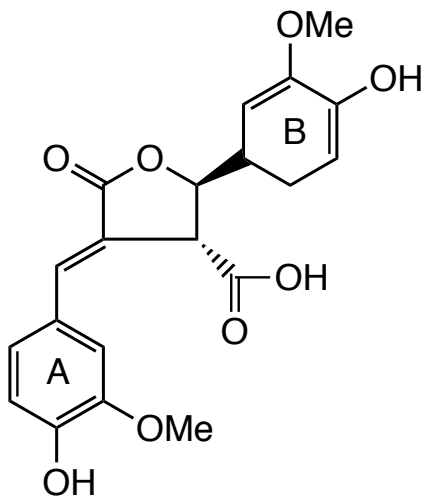
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B γ OMe		52.28		
B3 OMe		56.04		
A3 OMe		56.04		
A2		113.40		
B2		113.54		
A5		115.95		
B5		115.97		
A6		125.60		
β		125.67		
Bβ		125.67		
B6		125.73		
A1		127.78		
B1		127.81		
B α		142.36		
α		142.47		
B3		148.19		
A3		148.20		
A4		149.32		
B4		149.37		
Bγ		168.22		
γ		168.53		

Compound Number 2033



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B β		54.03	52.64	
A3 OMe		56.27	55.54	
B3 OMe		56.27	55.67	
B α		81.24	80.17	
B2		110.17	110.31	
A2		113.95	113.67	
B5		116.04	115.61	
A5		116.20	115.70	
B6		119.17	118.21	
β		120.45	119.08	
A1		126.54	124.72	
A6		126.58	125.56	
B1		132.37	130.42	
α		140.46	139.48	
B4		147.97	147.07	
A3		148.54	147.72	
B3		148.63	147.76	
A4		150.20	149.54	
γ		171.66	171.02	
B γ		172.12	171.72	

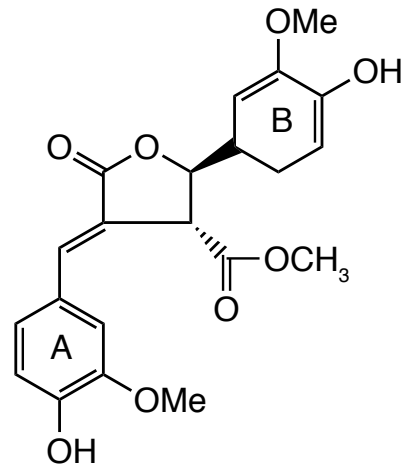
^{1}H (acetone)

Atom	H Shifts	Mult	J
B3 OMe	3.81	s	
A3 OMe	3.87	s	
B β	4.30	t	2.5
B α	5.75	d	2.8
B 5,6	6.82	m	
A5	6.89	d	8.2
B2	6.98	br s	
A6	7.21	dd	8.2, 2.0
A2	7.37	d	2.0
α	7.61	d	2.1

Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 12b (R=H)

Compound Number 2034



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B γOMe	52.98	53.16	51.98	
B β	53.49	53.78	52.75	
B3 OMe	55.97	56.23	55.46	
A3 OMe	55.97	56.26	55.62	
B α	80.22	80.97	79.74	
B2	107.65	110.12	110.26	
A2	112.04	113.78	113.48	
B5	114.78	116.04	115.53	
A5	114.92	116.24	115.68	
B6	118.22	119.23	118.26	
β	118.38	120.03	118.34	
A1	125.66	126.38	124.48	
A6	125.59	126.42	125.44	
B1	131.08	132.08	130.02	
α	141.06	140.75	139.93	
B4	146.12	147.99	147.11	
A3	146.77	148.52	147.69	
B3	146.89	148.61	147.71	
A4	148.39	150.24	149.62	
γ	170.77	171.45	170.53	
B γ	171.23	171.56	170.70	

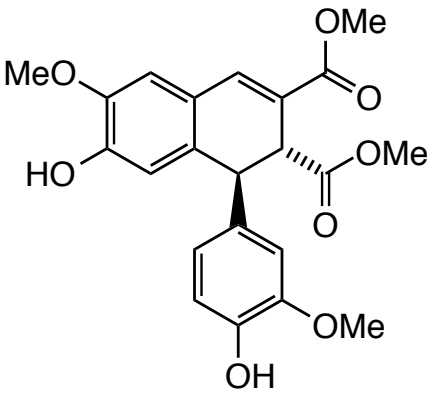
^{1}H (acetone)

Atom	H Shifts	Mult	J
B γ OMe	3.73	s	
B3 OMe	3.81	s	
A3 OMe	3.88	s	
B β	4.39	t	2.6
B α	5.72	d	3.0
B 5,6	6.79 - 6.85	m	
A5	6.9	d	8.2
B2	6.97	br d	1.5
A6	7.17	dd	8.2, 2.0
A2	7.28	d	2.0
α	7.62	d	2.1

Notes:

S. Quideau

Compound Number 2035



Dimethyl 7-hydroxy-6-methoxy-1-(4-hydroxy-3-methoxy phenyl)-trans-1,2-dihydronaphtlalene-2,3-dicarboxylate

^{1}H (acetone)

Atom	H Shifts	Mult	J
A γ OMe	3.56	s	
B γ OMe	3.68	s	
A3 OMe	3.75	s	
B3 OMe	3.88	s	
β	3.94	d	3.0
α	4.53	d	3.0
A6	6.39	dd	8.2, 2.0
A5	6.65	d	8.2
B5	6.66	s	
A2	6.76	d	2.0
B2	7.10	s	
B α	7.65	s	

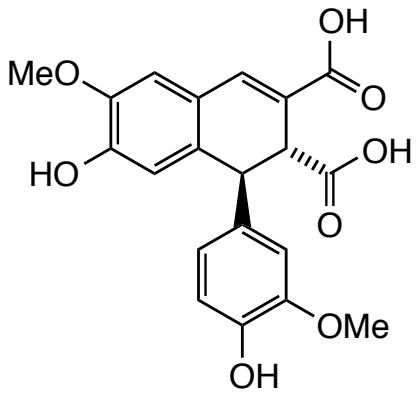
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
α	45.60	46.33	44.69
β	47.20	48.09	46.74
B γ OMe	51.87	51.87	51.67
A γOMe	52.40	52.34	52.11
A3 OMe	55.83	56.21	55.62
B3 OMe	56.03	56.38	55.74
A2	110.12	112.03	111.65
B2	111.21	113.27	113.25
A5	114.17	115.59	115.24
B5	115.58	116.85	116.06
A6	120.35	120.83	119.48
B β	122.37	122.96	120.89
B1	123.85	124.37	122.47
B6	131.19	132.09	130.74
A1	134.28	135.31	133.56
B α	137.74	138.45	137.92
A4	144.42	146.29	145.31
B3	145.78	147.63	146.72
A3	146.40	148.20	147.39
B4	147.69	149.68	148.88
B γ	167.10	167.49	166.52
γ	172.93	173.17	172.31

Notes:

S. Quideau

Compound Number 2036



β-β-coupled dehydrodiferulic acid

7-hydroxy-6-methoxy-1-(4-hydroxy-3-methoxyphenyl)-trans-1,2-dihydronapthlalene-2,3-dicarboxylic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.74	s	
B3 OMe	3.86	s	
β	3.88	d	1.8
α	4.61	br d	1.8
A6	6.42	dd	8.2, 2.0
A5	6.64	d	8.2
B5	6.71	s	
A2	6.79	d	2.0
B2	7.04	s	
B α	7.60	s	

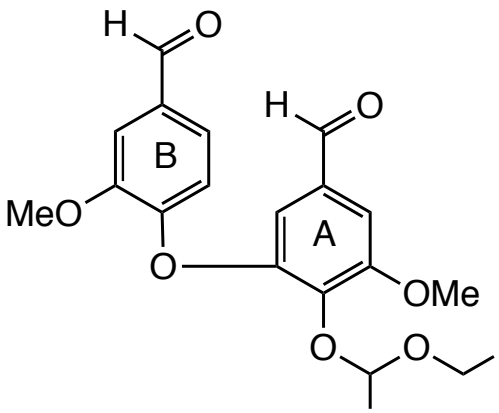
Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 19
Not very soluble in CDCl3

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α		46.00	44.25	
β		48.08	47.80	
A3 OMe		56.19	55.59	
B3 OMe		56.39	55.76	
A2		111.98	111.57	
B2		113.06	112.63	
A5		115.48	115.13	
B5		116.92	116.23	
A6		120.67	119.30	
B β		124.34	123.07	
B1		124.64	124.67	
B6		132.35	130.85	
A1		136.12	134.50	
B α		137.58	135.09	
A4		146.06	145.04	
B3		147.48	146.46	
A3		148.10	147.28	
B4		149.29	147.99	
B γ		169.32	169.23	
γ		173.62	173.27	

Compound Number 2037



^{1}H (acetone)

Atom	H Shifts	Mult	J
'CH3	1.08	t	7.05
CH3	1.38	d	5.1
CH2	3.56 -3.89	m	
OMe	3.95	s	
OMe	3.99	s	
CH	5.53	q	5.1
B5	7.04	d	8.1
A6	7.11	d	1.8
A2	7.42	d	1.8
B6	7.53	dd	8.1
B2	7.62	d	1.9
α	9.85	s	
B α	9.95	s	

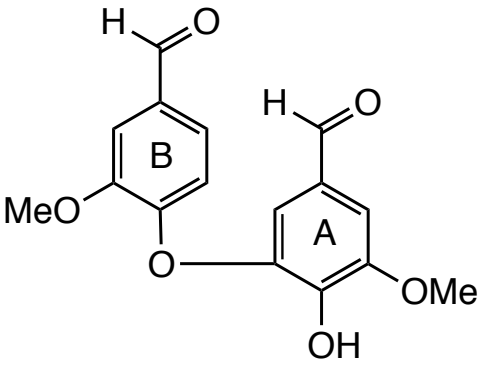
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
'CH3		15.45		
CH3		21.28		
B OMe		56.43		
A OMe		56.66		
CH2		63.26		
CH		104.47		
A2		108.94		
B2		112.46		
A6		114.45		
B5		119.32		
B6		125.46		
B1		133.26		
A1		134.22		
A4		143.42		
A3		150.68		
B3		151.42		
B4		151.95		
A5		155.59		
α		191.23		
B α		191.48		

Notes:

S. Quideau

Compound Number 2038



4-0-5-coupled dehydrodivanillin

3-{3-[4-(2-carboxyvinyl)-2-methoxy-phenoxy]-4-hydroxy-5-methoxy-phenyl} acrylic acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
B OMe	3.95	s	
A OMe	3.98	s	
B5	6.94	d	8.2
A6	7.22	d	1.8
A2	7.40	d	1.8
B6	7.48	dd	8.2, 2.0
B2	7.58	d	2.0
α	9.80	s	
B α	9.92	s	

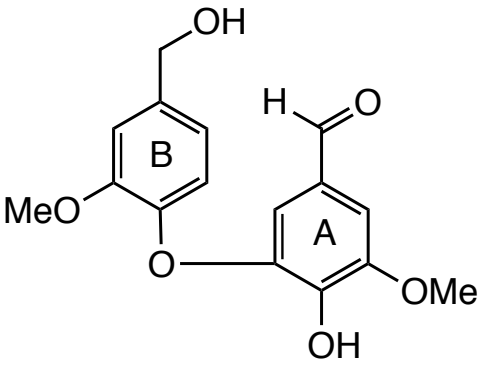
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe	56.07	56.41	55.85	
A3 OMe	56.56	56.80	56.24	
A2	106.80	108.48	108.09	
B2	110.85	112.26	111.60	
A6	116.92	116.99	116.27	
B5	117.31	117.63	116.31	
B6	125.55	125.55	124.80	
A1	128.69	129.54	127.64	
B1	132.76	133.56	131.84	
A5	142.55	143.79	142.52	
A4	143.30	145.22	144.52	
A3	148.60	150.37	149.47	
B3	150.61	151.49	149.82	
B4	151.08	152.48	151.24	
α	190.05	190.75	190.84	
B α	190.84	191.43	191.57	

Compound Number 2039



4-0-5 coupled dehydrovanillin / vanillyl alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
B3 OMe	3.79	s	
A3 OMe	3.95	s	
B α	4.63	s	
A6	6.91	d	1.8
B 5,6	6.94 - 6.97	m	
B2	7.16	br d	
A2	7.27	d	1.8
α	9.71	s	

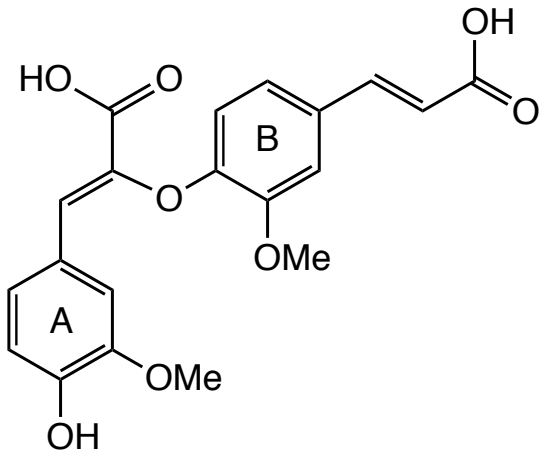
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe	55.94	56.19	55.61	
A3 OMe	56.47	56.73	56.15	
B α	64.91	64.34	62.59	
A2	106.40	107.98	107.74	
B2	111.55	112.52	111.09	
A6	114.09	112.62	111.54	
B6	119.49	119.78	118.81	
B5	120.46	121.17	119.98	
A1	128.30	129.00	127.04	
B1	138.45	140.84	139.77	
A4	142.58	143.92	142.63	
B4	143.95	144.30	143.03	
A5	145.16	146.98	145.90	
A3	148.45	149.86	148.93	
B3	150.87	152.00	150.45	
α	190.44	190.91	190.97	

Compound Number 2040



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe		55.92	55.09	
B3 OMe		56.47	55.86	
B2		112.39	111.55	
A2		113.77	112.98	
B5		114.39	113.30	
A5		115.96	115.53	
B β		117.50	117.52	
B6		122.92	122.02	
A1		125.31	123.44	
A6		126.06	124.62	
α		128.49	127.09	
B1		130.10	128.74	
β		138.28	137.01	
B α		145.25	143.71	
A3		148.30	147.24	
B4		148.90	147.42	
A4		149.46	148.59	
B3		150.23	148.59	
γ		164.51	164.11	
B γ		167.91	167.70	

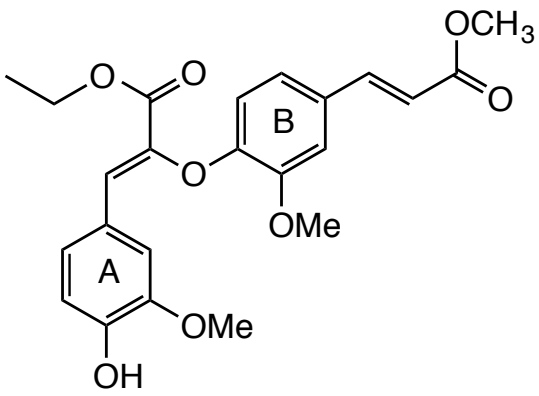
^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.73	s	
B3 OMe	4.00	s	
B β	6.43	d	15.9
A5	6.82	d	8.2
B5	6.83	d	8.3
B6	7.13	dd	8.3, 2.0
A6	7.23	dd	8.2, 2.0
α	7.42	s	
B2	7.44	d	2.0
A2	7.52	d	2.0
B α	7.59	d	15.9

Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 15

Compound Number 2041



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	14.14	14.47	14.05	
B γ OMe	51.65	51.58	51.32	
A3 OMe	55.59	55.92	55.11	
B3 OMe	56.21	56.49	55.93	
CH2	61.42	61.72	60.96	
B2	111.24	112.45	111.79	
A2	112.03	113.78	113.17	
B5	114.14	114.53	113.46	
A5	114.47	115.99	115.57	
B β	116.32	117.10	116.29	
B6	122.12	122.92	122.27	
A1	124.74	125.19	123.18	
A6	125.54	126.03	124.79	
α	127.80	128.05	127.43	
B1	129.31	130.09	128.78	
β	137.73	138.39	136.44	
B α	144.42	145.02	144.23	
A3	146.43	148.29	147.27	
B4	147.44	148.89	147.43	
A4	147.80	149.48	148.67	
B3	149.16	150.24	148.67	
γ	163.41	163.75	162.67	
B γ	167.50	167.63	166.80	

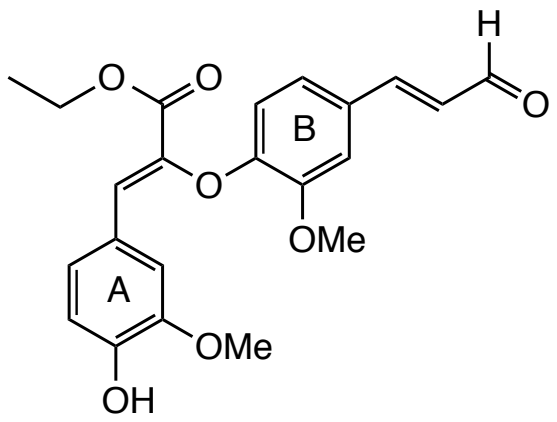
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.21	t	7.1
B γ OMe	3.71	s	
A3 OMe	3.73	s	
B3 OMe	3.99	s	
CH2	4.17	q	7.1
B β	6.45	d	16.0
B5	6.79	d	8.3
A5	6.81	d	8.3,
B6	7.12	dd	8.3, 2.0
A6	7.22	dd	8.3, 2.0
α	7.37	s	
B2	7.44	d	2.0
A2	7.49	d	2.0
B α	7.59	d	16.0
Ar OH	8.12	br s	

Notes:

S. Quideau
Toward β-O-4 dehydro diferulic acid
(steryl ether, Z isomer)

Compound Number 2042



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	14.06	14.48	14.05	
B3 OMe	56.15	56.55	55.97	
A3 OMe	55.47	55.94	55.11	
CH2	61.37	61.76	60.99	
B2	111.31	112.58	111.82	
A2	112.06	113.81	113.35	
B5	114.11	114.66	113.44	
A5	114.57	116.03	115.59	
B6	122.87	123.76	123.13	
A1	124.41	125.16	123.13	
A6	125.42	126.08	124.85	
B β	127.19	128.29	128.89	
α	127.90	128.16	127.35	
B1	128.83	130.13	127.53	
β	137.35	138.31	136.34	
A3	146.51	148.31	147.45	
A4	147.59	149.53	147.90	
B4	148.54	149.58	148.78	
B3	149.21	150.38	148.86	
B α	152.33	153.18	152.98	
γ	163.19	163.70	162.62	
B γ	193.42	193.89	194.19	

^{1}H (acetone)

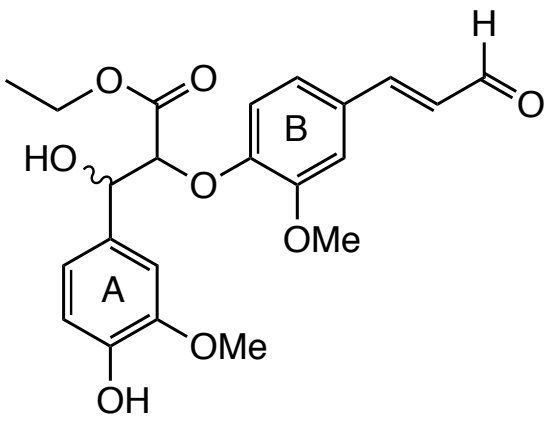
Atom	H Shifts	Mult	J
CH3	1.21	t	7.1
A3 OMe	3.73	s	
B3 OMe	4.00	s	
CH2	4.21	q	7.1
B β	6.70	dd	15.9, 7.7
A5	6.81	d	8.3
B5	6.83	d	8.3
B6	7.18	dd	8.3, 2.0
A6	7.23	ddd	8.3, 2.0, 0.4
α	7.38	s	
A2	7.49	d	2.0
B2	7.50	d	2.0
B α	7.58	d	15.9
B γ	9.65	d	7.7
Ar OH	8.14	s	

Notes:

S. Quideau

Toward β-O-4 dehydro diferulic acid(steryl ether, Z isomer)

Compound Number 2043



erythro

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	13.86			
OMe	55.72			
OMe	55.78			
CH2	61.33			
α	73.70			
β	82.29			
A2	109.63			
B2	111.09			
A5	113.93			
B5	115.99			
A6	119.80			
B6	122.72			
B β	127.15			
B1	128.79			
A1	130.89			
A3	145.48			
A4	146.36			
B3	149.72			
B4	150.11			
B α	152.38			
γ	168.80			
B γ	193.53			

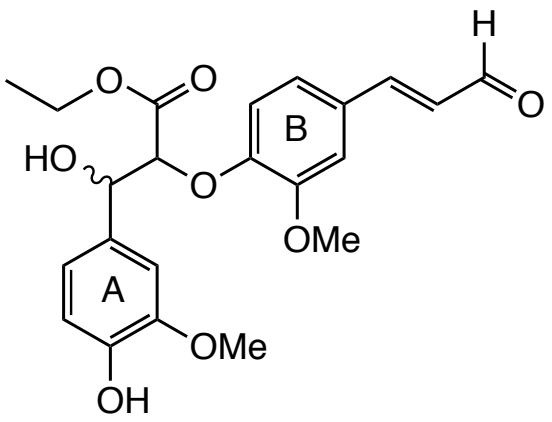
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.16	t	7.2
OMe	3.85	s	
OMe	3.86	s	
CH2	4.15	q	7.1
β	4.81	d	5.4
a	5.16	d	5.4
B β	6.58	dd	15.8, 7.7
B α	7.37	d	15.8
B γ	9.61	d	7.7
Ar OH	6.07		

Notes:

S. Quideau Compds 2043 and 2044 were run as a mixture and the different isomers were assigned. Relative intensities reflect the spectrum of the mixture.e isomer for synthesis of β-O-4 dehydro diferulic acid

Compound Number 2044



threo

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	13.73			
OMe	55.67			
OMe	55.82			
CH3	61.28			
α	74.49			
β	83.43			
A2	109.51			
B2	110.98			
A5	114.02			
B5	115.56			
A6	119.91			
B6	122.72			
B β	127.19			
B1	128.79			
A1	129.94			
A3	145.73			
A4	146.55			
B3	149.74			
B4	149.92			
B α	152.32			
γ	168.73			
B γ	193.53			

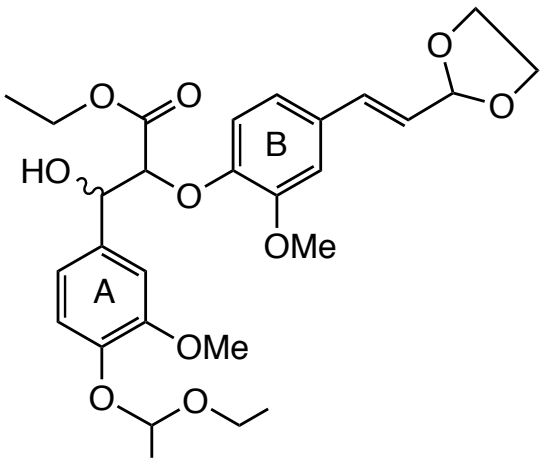
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.08	t	7.2
OMe	3.85	s	
OMe	3.87	s	
CH2	4.04-4.11	m	
β	4.67	d	6.2
α	5.10	d	6.2
B β	6.59	dd	15.8, 7.7
B α	7.38	d	15.8
B γ	9.62	d	7.7
Ar OH	6.10		

Notes:

S.Quideau Compounds 2043 and 2044 were run as a mixture and the different isomers were assigned. Relative intensities reflect the spectrum of the mixture. threo isomer for synthesis of β-O-4 dehydro diferulic acid

Compound Number 2045



erythro

^{1}H (chloroform)

Atom	H Shifts	Mult	J
CH3	1.47	d	5.1
β *t*	4.56	d	6.6
β *e*	4.72	d	5.4
α *t*	5.06	br d	6.3
α *e*	5.13	br s	
A 4 CH	5.32	q	5.2
B γ	5.36	d	6.0
B β	6.03	dd	15.9, 6.0
B α	6.66	d	16.0

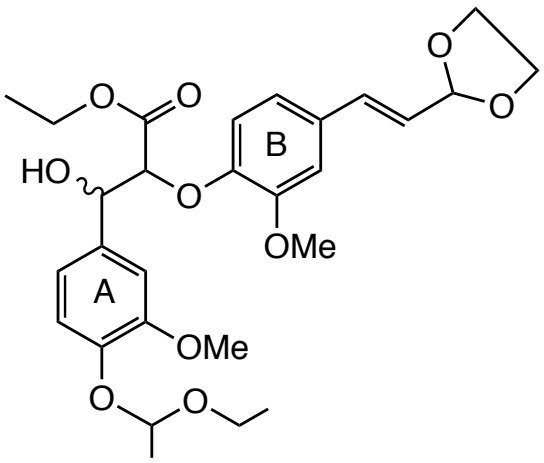
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A γ CH3	13.82			
CH3	14.93			
CH3	20.10			
OMe	55.54			
OMe	55.63			
4 CH2	61.01			
A CH2	61.84			
B CH2	64.82			
B CH2	64.82			
α	73.57			
β	83.09			
	100.92			
	103.59			
	110.04			
	110.76			
	117.40			
	118.63			
	119.09			
	120.07			
	124.08			
	131.25			
	133.82			
	133.84			
	134.08			
	145.39			
	147.22			
	150.12			
	150.40			
γ	169.03			

Notes:

S. Quideau
intermediate toward β--O-4 dehydro
diferulic acid

Compound Number 2046



threo

^{1}H (chloroform)

Atom	H Shifts	Mult	J
β	4.56	d	6.6
α	5.06	br d	6.3

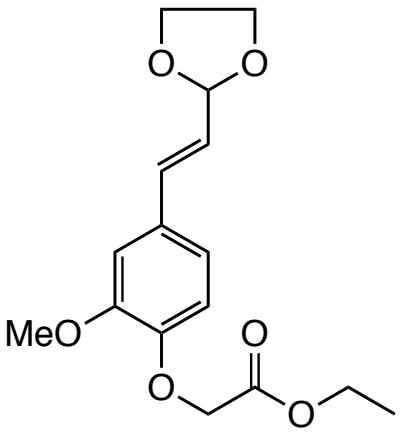
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	-			
CH3	-			
CH3	-			
OMe	55.59			
OMe	55.59			
CH2	61.86			
CH2				
CH2	74.51			
α	84.39			
β	100.94			
	109.98			
	110.69			
	116.92			
	118.70			
	124.14			
	132.73			
	134.06			
	145.67			
	147.26			
	149.92			
	150.00			

Notes:

S. Quideau
intermediate toward b--O-4 dehydro diferulic acid

Compound Number 2047



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	14.09			
OMe	55.84			
CH2	61.27			
CH2	65.01			
CH2	65.01			
CH2	66.42			
γ	103.90			
2	109.88			
5	113.88			
6	120.14			
β	123.75			
α	130.39			
1	134.47			
3	147.58			
4	149.56			
C=O	168.78			

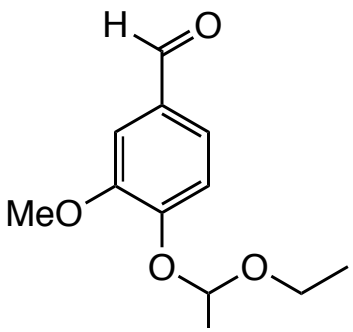
^{1}H (chloroform)

Atom	H Shifts	Mult	J
CH3	1.26	t	7.1
OMe	3.87	s	
CH2	3.90-4.05	m	
CH2	4.24	q	7.1
CH2	4.67	s	
γ	5.39	d	6.1
β	6.05	dd	15.9, 6.1
α	6.69	d	15.9
5	6.76	d	8.3
6	6.90	dd	8.3, 2.0
2	6.99	d	2.0

Notes:

S. Quideau
For synthesis of b--O-4 dehydro diferulic acid

Compound Number 2048



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
'CH3	15.03			
CH3	19.95			
OMe	55.90			
CH2	61.72			
CH	100.61			
2	109.81			
5	116.59			
6	126.06			
1	130.97			
3	150.78			
4	151.64			
α	190.89			

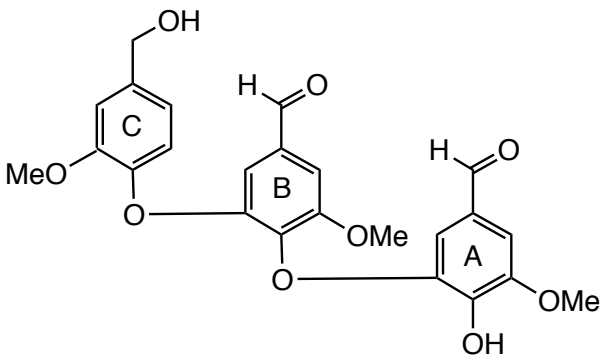
^{1}H (chloroform)

Atom	H Shifts	Mult	J
'CH3	1.21	t	7.1
CH3	1.58	d	5.3
CH2	3.50-3.85	m	
OMe	3.92	s	
CH	5.54	q	5.3
Aromatics	7.21-7.43		
α	9.87	s	

Notes:

S. Quideau
Intermediate for synthesis of β--O-4 dehydro diferulic acid

Compound Number 2049



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
C3 OMe		56.07		
A3 OMe		56.75		
B3 OMe		56.89		
C α		64.25		
B2		108.03		
A2		108.40		
B6		109.92		
A6		110.17		
C2		112.36		
C6		119.76		
C5		122.66		
A1		128.73		
B1		134.75		
B4		138.25		
C1		142.09		
C4		142.49		
A4		143.04		
A5		147.16		
A3		149.70		
C3		152.34		
B5		153.71		
B3		155.04		
α		191.02		
B α		191.69		

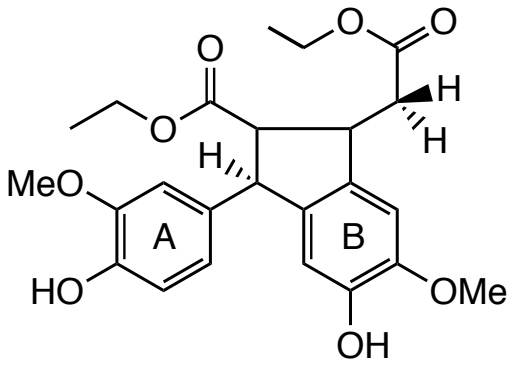
^{1}H (acetone)

Atom	H Shifts	Mult	J
C3 OMe	3.72	s	
B3 OMe	3.90	s	
A3 OMe	3.94	s	
C α	4.62	s	
B6	6.88	d	1.7
C6	6.94	dd	8.1, 1.7
C5	7.00	d	8.1
A6	7.01	d	1.7
C2	7.14	d	1.7
A2	7.26	d	1.7
B2	7.40	d	1.7
α	9.74	s	
B α	9.86	s	

Notes:

S. Quideau
5-O-4 trimer

Compound Number 2050



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A CH3	14.19	14.52	13.97	
B CH3	14.22	14.47	14.07	
B β	36.90	37.50	36.41	
B α	42.15	43.06	41.74	
α	51.31	52.35	50.93	
A3 OMe	55.93	56.23	55.56	
B3 OMe	56.10	56.39	55.64	
β	58.66	59.09	56.96	
B CH2	60.47	60.79	59.94	
A CH2	60.63	60.95	60.07	
B2	106.61	108.23	107.86	
B5	110.87	112..04	111.25	
A2	110.99	112.60	112.08	
A5	114.29	115.76	115.32	
A6	121.39	121.75	120.35	
A1	134.34	135.02	133.25	
B1	135.12	135.58	133.61	
B6	137.10	137.90	136.47	
A4	144.54	146.45	145.36	
B4	145.61	147.43	146.34	
B3	146.04	147.92	147.08	
A3	146.50	148.37	147.51	
B γ	172.30	172.45	171.45	
γ	172.43	173.00	172.10	

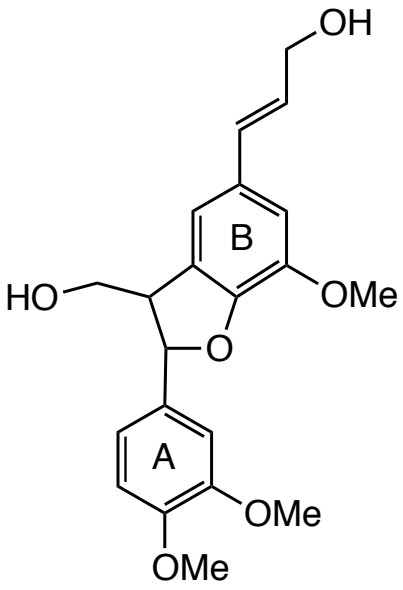
^{1}H (acetone)

Atom	H Shifts	Mult	J
B β1	2.43	dd	16.0, 8.0
B β2	2.61	dd	16.0, 7.0
β	3.43	dd	9.85, 8.20
B α	3.90	brq	8.0
α	4.56	d	10.1

Notes:

S. Quideau
Sterochemistry determined from NOESY experiments
αβ-/α6 model

Compound Number 2051



4-[3-Hydroxymethyl-5-(3-hydroxypropenyl)-7-methoxy-2,3-dihydrobenzofuran-2-yl]-1,2-dimethoxyphenyl

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	3.52	br q	
A3 OMe	3.77	s	
A4 OMe	3.78	s	
B3 OMe	3.86	s	
γ 's	3.80-3.92	m	
B γ OH	4.14	t	5.50
B γ	4.19	td	5.7, 1.7
α	5.58	d	6.4
B β	6.23	dt	15.8, 5.5
B α	6.52	dt	15.8, 1.7
A5	6.91	d	8.1
A,B6 + B2	6.94-9.67	m	
A2	7.03	d	1.8

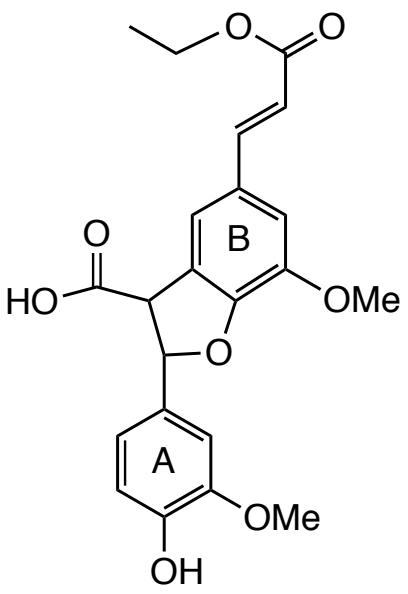
Notes:

S. Quideau
veratryl phenylcoumaran
Additional data FLw-79 700MHz

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	53.49	54.81	53.12	53.29
A3 OMe	55.92	56.12	55.47	55.38
A4 OMe	55.92	56.12	55.53	55.46
B3 OMe	55.99	56.39	55.68	55.63
B γ	63.81	63.38	61.63	61.75
γ	63.97	64.65	62.90	63.01
α	88.13	88.34	86.99	81.12
A2	109.29	110.84	109.72	109.79
B2	110.50	111.74	110.32	110.41
A5	111.01	112.67	111.68	111.67
B6	114.77	116.08	114.92	114.97
A6	118.70	119.02	118.08	118.13
B β	126.44	128.42	128.05	128.12
B5	128.04	130.30	129.32	129.40
B α	131.32	130.49	128.91	128.94
B1	130.87	132.00	130.60	130.73
A1	133.44	135.59	133.91	134.04
B3	144.48	145.18	143.69	143.79
B4	148.38	148.93	147.03	147.21
A4	149.08	150.15	148.53	148.62
A3	149.19	150.45	148.74	148.84
1H				
β	3.62		3.43	3.53
A3 OMe	3.83		3.72	3.70
A4 OMe	3.85		3.73	3.72
B3 OMe	3.89		3.79	3.80
γ 's B γ OH	3.91, 3.97		3.62, 3.71	3.72, 3.84
B γ	4.29		4.07	4.16
α	5.58		5.49	5.61
B β	6.22		6.20	6.28
B α	6.54		6.45	6.53
A5	6.81		6.92	6.91
B2	6.87		6.82	6.97
B6	6.88		6.93	7.01
A2	6.91		6.93	7.00
A6	6.93		6.87	6.94

Compound Number 2052



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3		14.63		
β		55.43		
A3 OMe		56.30		
B3 OMe		56.47		
CH2		60.51		
α		88.70		
A2		110.70		
B2		113.20		
A5		115.72		
B β		116.46		
B6		119.08		
A6		120.05		
B5		128.35		
B1		129.20		
A1		132.64		
B α		145.36		
B3		145.70		
A4		147.70		
A3		148.47		
B4		151.03		
B γ		167.31		
γ		172.24		

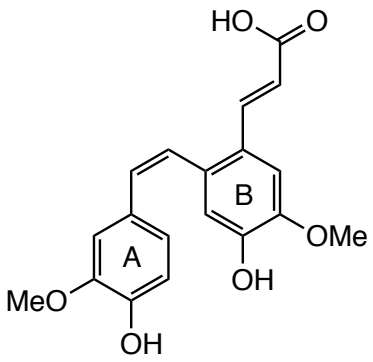
^{1}H (acetone)

Atom	H Shifts	Mult	J
β	4.37	br d	7.8
α	6.06	d	7.9
B β	6.38	d	15.9
B α	7.60	d	15.9

Notes:

S. Quideau

Compound Number 2053



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe		56.25		
B3 OMe		56.56		
B2		109.15		
A2		110.16		
A5		115.99		
B β		116.50		
β		120.61		
B6		120.84		
A6		121.14		
B5		125.47		
B1		126.98		
α		130.68		
A1		130.90		
B α		146.00		
B4		146.96		
A4		147.61		
A3		148.61		
B3		148.83		
B γ		168.22		

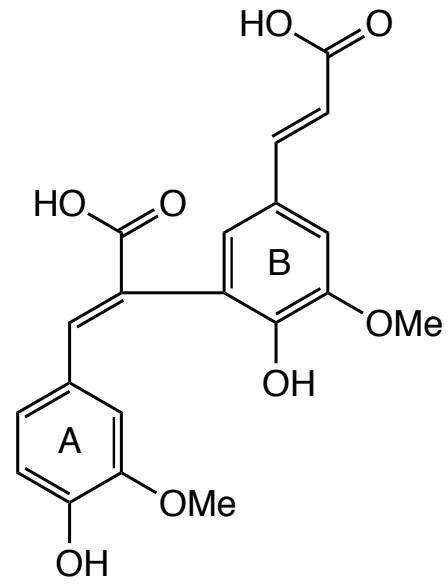
^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.91	s	
B3 OMe	3.95	s	
B β	6.44	d	15.9
A5	6.83	d	8.1
A6	7.05	dd	8.1, 2.0
A2	7.22	d	2.0
B2	7.23	d	1.9
α	7.31	dd	16.5, 7.38
β	7.33	dd	16.5, 7.38
B6	7.54	d	1.9
B α	7.63	d	15.9

Notes:

S. Quideau

Compound Number 2054



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 OMe		55.48	54.62	
B3 OMe		56.55	56.06	
B2		110.27	109.76	
A2		113.26	112.79	
A5		115.63	115.63	
B β		116.23	115.92	
B5		125.14	124.57	
B6		125.60	124.38	
β		126.34	125.90	
A6		126.36	124.95	
B1		127.26	125.66	
A1		127.58	125.88	
α		141.81	139.75	
B α		145.80	144.28	
A3		147.86	145.82	
B4		148.01	147.00	
A4		148.98	148.05	
B3		149.10	148.12	
B γ		168.56	167.86	
γ		169.15	168.38	

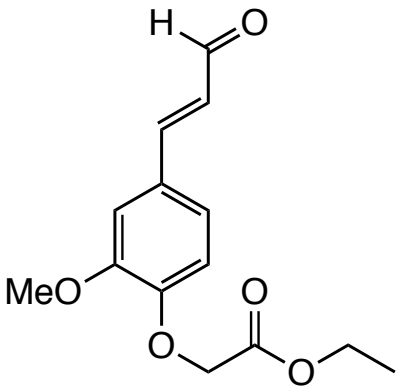
^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.45	s	
B3 OMe	3.95	s	
B β	6.38	d	15.4
A5	6.71	d	8.2
A2	6.73	d	1.9
A6	6.85	dd	8.2, 2.0
B6	7.03	d	1.9
B2	7.37	d	1.9
B α	7.60	d	15.9
α	7.81	s	

Notes:

S. Quideau
JCS Perkin 1, 3485-98 (1994)
Cmpd 14
Not soluble in CDCl3

Compound Number 2055



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
CH3	14.06			
OMe	55.95			
CH2	61.44			
CH2	65.99			
2	110.77			
5	113.40			
6	122.75			
α	127.17			
1	128.31			
3	149.74			
4	149.96			
β	152.36			
C=O	168.25			
γ	193.41			

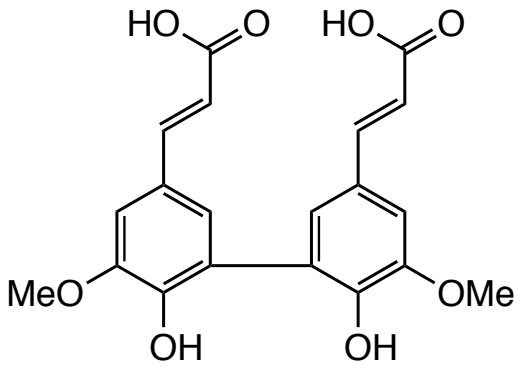
^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.25	t	7.1
OMe	3.89	s	
CH2	4.23	q	7.1
CH2	4.69	s	
β	6.57	dd	15.8, 7.7
5	6.78	d	7.9
2,6	7.06-7.08	m	
α	7.36	d	15.8
γ	9.62	d	7.7

Notes:

S. Quideau
intermediate for systhesis of β-O-4 dehydro diferulic acid

Compound Number 2056



5-5, Dehydrodiferulic Acid

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.97	s	
β	6.42	d	15.4
6	7.21	d	2.0
2	7.35	d	2.0
α	7.64	d	15.9

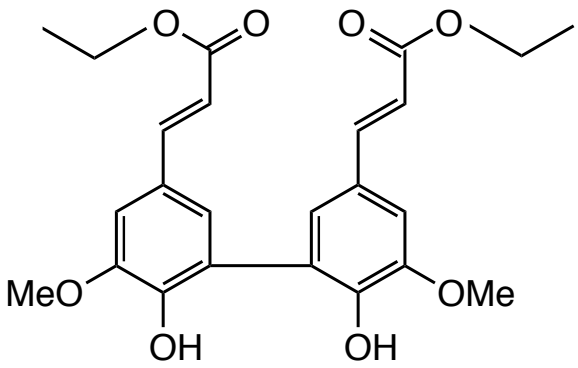
Notes:

S. Quideau JCS Perkin 1, 3485-98 (1994) Cmpd 16
Note chemical shift differences of 5,6,1 between solvents. Shifts were verified in both solvents As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.52	56.04	
2		109.97	109.44	
β		116.28	115.82	
5		125.62	125.20	
6		126.07	125.05	
1		126.60	124.83	
α		145.89	144.56	
4		147.38	146.43	
3		148.92	147.90	
γ		168.36	167.94	

Compound Number 2057



5-5 Dehydrodiferulate diethyl ester

^{1}H (acetone)

Atom	H Shifts	Mult	J
CH3	1.26	t	7.1
CH2	4.18	q	7.1
OMe	3.97	s	
β	6.43	d	15.9
6	7.20	d	2.0
2	7.36	d	2.0
α	7.62	d	15.9

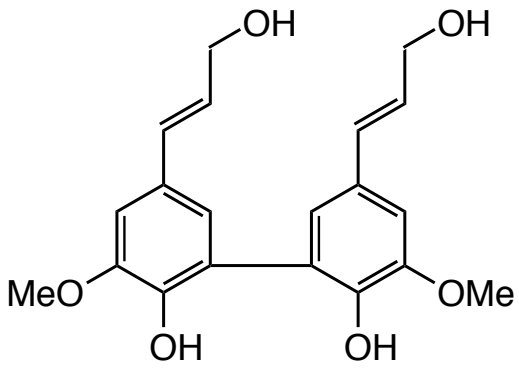
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
CH3	14.31	14.64	14.22
OMe	56.17	56.56	56.03
CH2	60.34	60.46	59.63
2	108.78	109.95	109.47
β	116.21	116.23	114.70
5	123.59	125.59	125.20
6	124.81	126.22	125.35
1	126.73	126.64	124.58
α	144.46	145.58	144.98
4	145.10	147.47	146.84
3	147.27	148.93	147.94
γ	167.14	167.39	166.59

Notes:

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

Compound Number 2058



5,5 Dehydrodiconiferyl Alcohol

^{1}H (acetone)

Atom	H Shifts	Mult	J
A3 OMe	3.89	s	
γ	4.21	br d	5.4
β	6.26	dt	15.8, 5..5
α	6.54	dt	15.8, 1.6
A6	6.92	d	2.0
A2	7.06	d	2.0
ArOH	7.42	s	

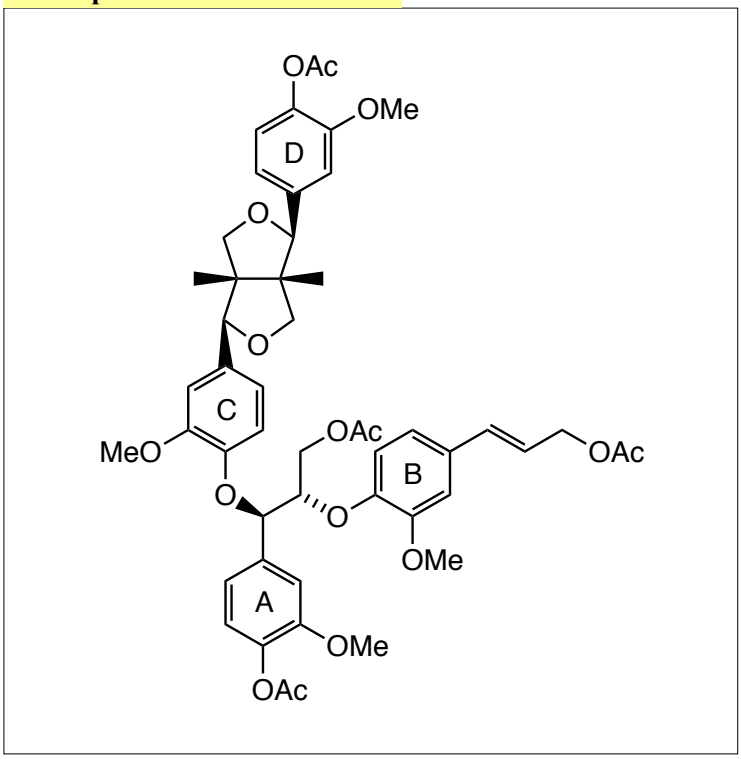
Notes:

S. Quideau Run only in acetone, no HMBC run. Assignment of quatenary carbons based on shift assignments of diacid/diester parents. Poor solubility on CDCl3... sample degraded, no DMSO data.As this compound has a plane of symmetry the shifts for the other half are identical.

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
OMe		56.52		
γ		63.49		
2		108.97		
6		123.16		
5		126.15		
β		128.53		
1		129.69		
α		130.57		
4		144.53		
3		148.87		

Compound Number 2059



Guaiacylglycerol-α-pinoresinol-β-coniferyl-bis-ether (Ac′d)

^{1}H (acetone)

Atom	H Shifts	Mult	J
α	5.60	d	5.6
β	4.86	m	
γ1	4.45	dd	11.9, 3.8
γ2	4.53	dd	11.9, 5.9
C α	4.66	s	
C α	3.06	m	
C γ1	3.83	m	
C γ2	4.17	m	
D α	4.74	d	4.5
D γ	4.23	m	

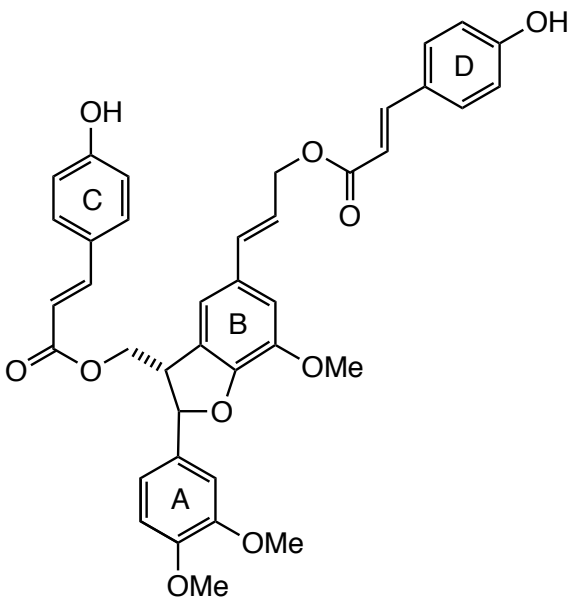
Notes:

S.Quideau
not substantiated in CDCl3 & d6 DMSO
Peracetate/diastereomeric mixture

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.59	20.45	20.35
Ac Me	20.59	20.45	20.35
Ac Me	20.70	20.62	20.43
Ac Me	20.93	20.78	20.70
C β	53.91	55.11	53.49
B β	54.39	55.36	53.74
A3 OMe	55.82	56.19	55.59
B3 OMe	55.95	56.23	55.65
D3 OMe	55.95	56.23	55.71
C3 OMe	56.11	56.40	55.79
A γ	63.45	63.62	62.44
B γ	65.05	65.38	64.40
C γ	71.88	72.37	71.07
D γ	71.88	72.48	71.18
A α	80.34	80.88	78.69
A β	81.87	81.73	79.56
D α	85.53	86.20	84.67
C α	85.64	86.27	84.75
D2	110.01	111.07	110.38
B2	110.35	111.31	110.20
C2	110.39	111.47	110.71
A2	111.55	112.77	111.89
C5	116.58	117.29	115.64
D6	117.93	118.62	116.96
C6	118.19	118.90	118.18
B5	118.87	119.11	117.83
A6	119.65	120.51	119.43
B6	119.65	120.51	119.43
B β	122.08	123.14	122.17
A5	122.45	123.25	122.37
D5	122.73	123.43	122.55
B1	131.55	132.27	130.46
B α	133.93	134.23	133.01
C1	135.13	136.85	135.21
A1	136.93	137.72	136.37
D4	139.19	140.08	138.42
A4	139.62	140.62	138.86
D1	140.23	141.84	140.50
C4	146.94	147.42	145.70
B4	147.63	148.67	147.00
C3	150.46	151.27	149.61
B3	150.93	151.86	150.06
A3	151.12	152.10	150.43
D3	151.27	152.24	150.72
A4 AcC=O	168.71	168.90	168.36
D4 AcC=O	168.98	169.05	168.54
B γ AcC=O	170.68	170.78	170.08
A γ AcC=O	170.76	170.81	170.12

Compound Number 2060



^{1}H (acetone)

Atom	H Shifts	Mult	J
A3,4 OMe	3.77	s	
β	3.85	m	
B3 OMe	3.88	s	
γ1	4.45	dd	11.1, 7.6
γ2	4.58	dd	11.1, 5.4
B γ	4.78	dd	6.5, 1.2
a	5.61	d	7.1
B β	6.31	dt	15.8, 6.5
D β	6.33	d	15.9
C β	6.37	d	15.9
B α	6.70	dt	15.8, 1.2
C,D 3,5	6.88	m	
A5	6.93	d	8.3
A6	7.00	d	8.3, 2.0
A,B 2	7.07	br d	2.0
B6	7.11	br s	
D 2,6	7.51	m	
C 2,6	7.54	m	
C α	7.63	d	15.9
D α	7.53	d	15.9

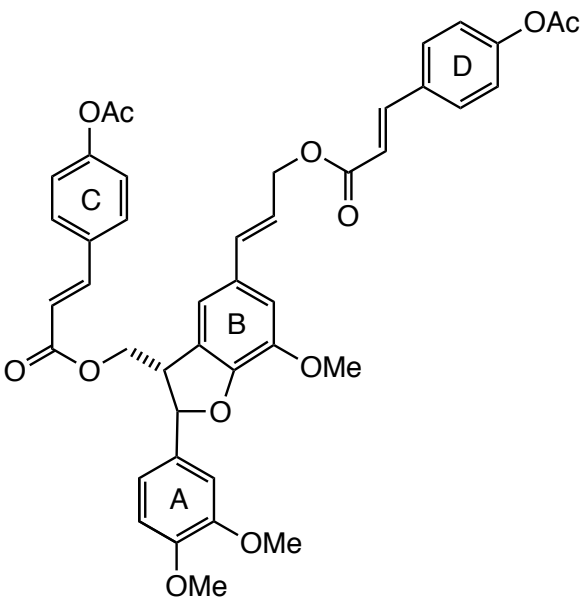
Notes:

S. Quideau
C3,4,5 and D3,4,5 Can be interchanged
not substantiated in CDCl3 & DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
β	50.40	51.33	49.47	
A3 OMe	55.90	56.09	55.48	
A4 OMe	55.90	56.13	55.76	
B3 OMe	56.03	56.41	55.82	
B γ	65.19	65.42	64.46	
γ	65.38	65.92	64.80	
α	88.86	89.15	87.87	
A2	109.31	110.93	110.01	
B2	110.67	112.25	111.03	
A5	111.06	112.65	111.67	
D β	114.53	115.08	113.68	
C β	115.14	115.49	114.05	
B6	115.39	116.36	115.31	
D3	115.93	116.68	115.77	
D5	115.83	116.68	115.77	
C3	115.96	116.70	115.77	
C5	115.96	116.70	115.77	
A6	118.91	119.44	118.66	
B β	121.37	122.40	121.56	
D1	126.75	126.85	124.94	
C1	126.98	126.97	125.08	
B5	127.79	129.21	128.08	
C2	130.00	130.94	130.34	
C6	130.00	130.94	130.34	
D2	130.06	131.02	130.34	
D6	130.06	131.02	130.34	
B1	130.62	131.51	130.06	
A1	132.86	134.52	133.61	
B α	134.27	134.78	132.79	
B3	144.40	145.42	143.91	
C α	144.94	145.50	144.89	
D α	145.40	145.91	145.13	
B4	148.27	149.42	147.65	
A3	149.14	150.43	148.72	
A4	149.17	150.51	148.81	
D4	158.05	160.61	159.87	
C4	158.23	160.71	159.94	
C γ	167.20	167.23	166.38	
D γ	167.37	167.23	166.38	

Compound Number 2061



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.26	s	
A3,4 OMe	3.76	s	
B3 OMe	3.88	s	
β	~3.88	m	
γ1	4.48	dd	11.1, 7.5
γ2	4.61	dd	11.1, 5.4
B γ	4.81	dd	6.5, 1.3
α	5.61	d	7.2
B β	6.32	dt	15.8, 6.5
A5	6.43	d	8.3
D β	6.50	d	16.0
Cβ	6.54	d	16.0
B α	6.71	dt	15.8, 1.2
A6	7.00	dd	8.2, 2.0
A2	7.08	d	2.0
B2	7.08	br s	
B6	7.11	br s	
C,D 3,5	7.16-7.21	m	
D 2,6	7.68	m	
C α	7.70	d	16.0
C 2,6	7.72	m	

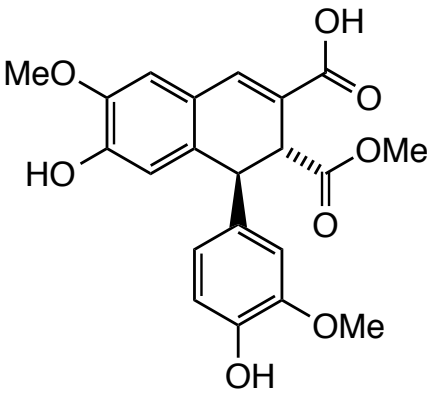
Notes:

S. Quideau
C4,D4 and Cg,Dg Can be interchanged
Not substantiated in CDCl3 & DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
C4 AcMe	21.08	20.94	20.76	
D4 AcMe	21.08	20.94	20.76	
β	50.45	51.21	49.36	
A3 OMe	55.97	56.08	55.50	
A4 OMe	56.00	56.14	55.50	
B3 OMe	56.13	56.41	55.76	
B γ	65.31	65.71	64.66	
γ	65.56	66.15	64.98	
α	88.94	89.17	87.72	
A2	109.53	110.97	110.11	
B2	110.96	112.28	111.18	
A5	111.26	112.63	111.77	
B6	115.41	116.35	115.30	
D β	117.59	118.61	117.65	
C β	118.21	119.01	118.01	
A6	118.94	119.53	118.65	
B β	121.34	122.17	121.32	
D3	122.14	123.23	122.24	
D5	122.14	123.23	122.24	
C3	122.19	123.23	122.28	
C5	122.19	123.23	122.28	
B5	127.79	129.17	128.02	
C2	129.21	130.16	129.49	
C6	129.21	130.16	129.49	
D2	129.42	130.21	129.53	
D6	129.42	130.21	129.53	
B1	130.66	131.47	130.01	
D1	131.92	132.77	131.47	
C1	132.16	132.91	131.62	
A1	132.96	134.41	132.74	
B α	134.47	134.99	133.72	
C α	143.91	144.43	143.59	
D α	144.39	144.79	143.81	
B3	144.53	145.42	143.87	
B4	148.45	149.44	147.67	
A3	149.36	150.45	148.81	
C4	152.21	153.46	151.99	
D4	152.36	153.53	152.03	
C γ	166.47	166.80	165.84	
D γ	166.61	166.80	165.87	
C4 C=O	168.97	169.45	168.87	
D4 C=O	169.01	169.45	168.87	

Compound Number 2062



Methyl 7-hydroxy-5-methoxy-1-(4-hydroxy-3-methoxyphenyl)- trans -1,1-dihydronapthalene-3-carboxylic Acid 2-carboxylate

^{1}H (acetone)

Atom	H Shifts	Mult	J
A γ OMe	3.55	s	
A3 OMe	3.74	s	
B3 OMe	3.87	s	
β	3.96	d	3.1
α	4.51	d	3.1
A6	6.43	dd	8.3, 1.9
A5	6.657	d	8.3
B5	6.661	s	
A2	6.77	d	2.0
B2	7.06	s	
B α	7.66	s	

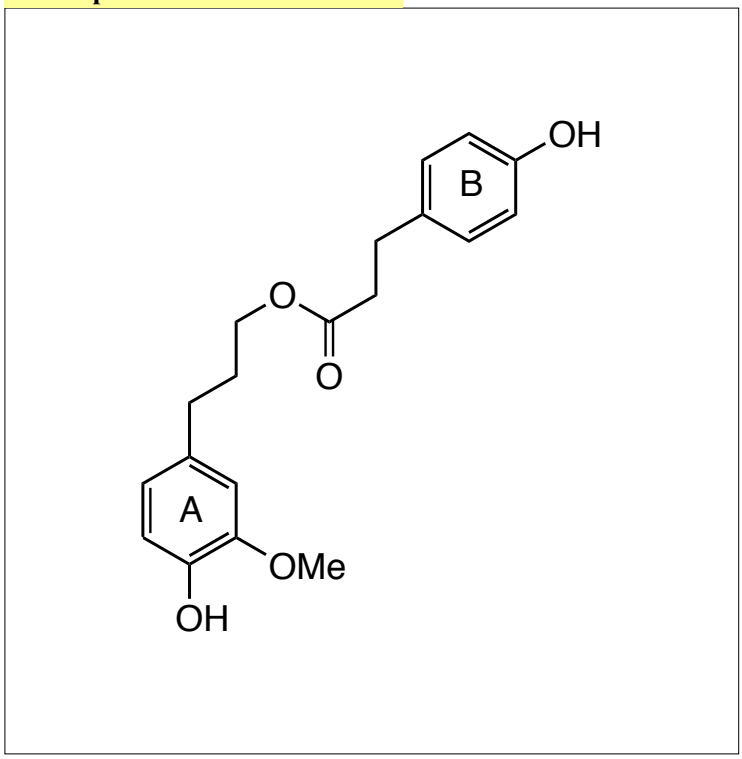
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
α		46.46		
β		48.06		
A g OMe		52.25		
A3 OMe		56.18		
B3 OMe		56.36		
A2		112.01		
B2		113.11		
A5		115.52		
B5		116.75		
A6		120.82		
B β		123.97		
B1		124.58		
B6		132.08		
A1		135.45		
B α		138.07		
A4		146.14		
B3		147.51		
A3		148.11		
B4		149.34		
B γ		168.80		
A γ		173.44		

Notes:

S. Quideau

Compound Number 2063



Dihydroconiferyl 4-hydroxydihydrocinnamate

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.86	m	
α	2.55	t	7.4
B β	2.56	t	7.6
B α	2.82	t	7.6
OMe	3.80	s	
γ	4.03	t	6.5
A6	6.61	dd	8.0, 2.0
A5	6.73	d	7.9
B 3,5	6.75	m	
A2	6.79	d	2.0
B 2,6	7.06	m	
ArOH	7.86	s	
ArOH	8.10	s	

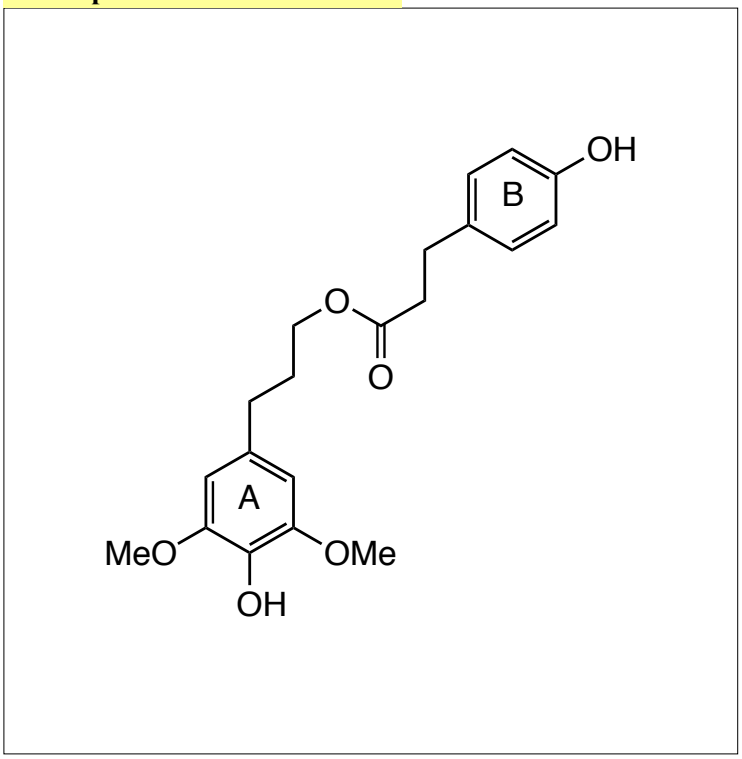
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B α	30.11	30.75	29.49	
β	30.40	31.33	29.95	
α	31.75	32.24	30.91	
B β	36.17	36.69	35.47	
OMe	55.87	56.16	55.48	
γ	63.85	64.03	63.13	
A2	110.96	112.73	112.43	
A5	114.28	115.62	115.28	
B3	115.31	116.00	115.03	
B5	115.31	116.00	115.03	
A6	120.93	121.55	120.30	
B2	129.37	130.05	129.04	
B6	129.37	130.05	129.04	
B1	132.46	132.38	130.50	
A1	133.09	133.55	131.83	
A4	143.76	146.58	144.53	
A3	146.40	148.16	147.38	
B4	154.13	156.57	155.55	
B γ	173.26	173.09	172.32	

Compound Number 2064



Dihydrosinapyl dihydro-*p*-coumarate

^{1}H (acetone)

Atom	H Shifts	Mult	J
β	1.87	m	
α	2.55	t	7.6
B β	2.56	t	7.5
B α	2.82	t	7.6
OMe	3.79	s	
γ	4.03	t	6.5
A 2,6	6.48	s	
B 3,5	6.74	m	
A4 OH	6.89	s	
B 2,6	7.06	m	
B4 OH	8.08	s	

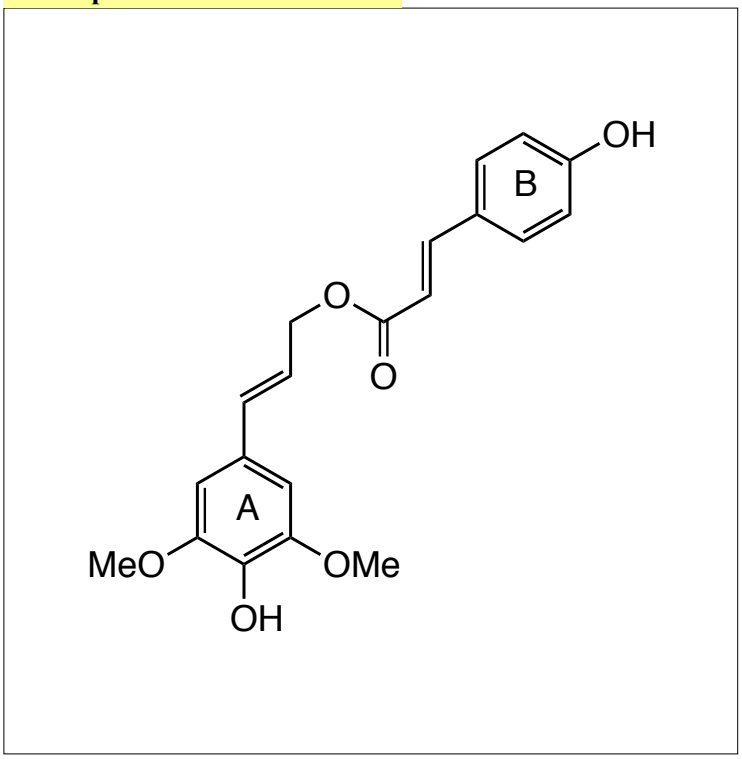
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B α	30.11	30.77	29.49	
β	30.41	31.31	29.90	
α	32.26	32.71	31.41	
B β	36.17	36.71	35.46	
OMe	56.27	56.57	55.87	
OMe	56.27	56.57	55.87	
γ	63.82	64.04	63.15	
A2	105.03	106.69	105.63	
A6	105.03	106.69	105.63	
B3	115.32	116.01	115.02	
B5	115.32	116.01	115.02	
B2	129.34	130.07	129.03	
B6	129.34	130.07	129.03	
B1	132.28	132.40	130.50	
A1	132.36	132.59	131.04	
A4	132.93	135.07	133.55	
A3	146.93	148.62	147.85	
A5	146.93	148.62	147.85	
B4	154.19	156.61	155.55	
B γ	173.21	173.08	172.32	

Compound Number 2065



Sinapyl p-coumarate

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.84	s	
γ	4.78	dd	6.5, 1.3
β	6.28	dt	15.8, 6.5
B β	6.38	d	15.9
α	6.64	dt	15.8, 1.3
A 2,6	6.79	s	
B 3,5	6.89	m	
B 2,6	7.55	m	
B α	7.63	d	15.9

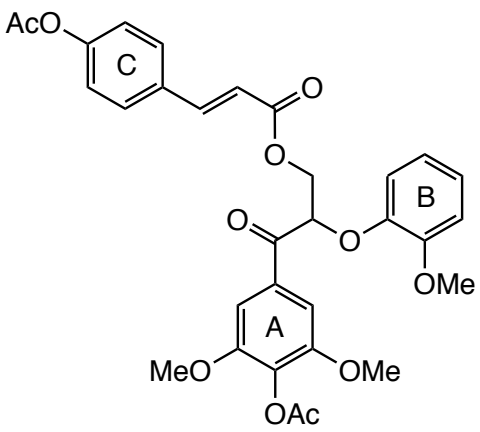
^{13}C

Atom	$CDCl_3$	Acetone	DMSO
OMe	56.28	56.61	55.97
OMe	56.28	56.61	55.97
γ	65.15	65.42	64.50
A2	103.55	105.16	104.20
A6	103.55	105.16	104.20
B β	115.15	115.52	114.08
B3	115.92	116.70	115.78
B5	115.92	116.70	115.78
β	121.44	122.07	121.06
B1	126.98	126.99	125.08
A1	127.84	128.22	126.47
B2	129.98	130.95	130.34
B6	129.98	130.95	130.34
α	134.53	135.14	134.03
A4	135.03	137.27	135.80
B α	144.91	145.45	144.88
A3	147.10	148.84	148.04
A5	147.10	148.84	148.04
B4	158.06	160.62	159.87
B γ	167.32	167.22	166.40

Notes:

S. Quideau

Compound Number 2066



2-(4-Acetoxy-3,5-dimethoxybenzoyl)-2-(2-methoxyphenoxy) ethyl 4-acetoxycinnamate

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.26	s	
Ac Me	2.26	s	
B3 OMe	3.75	s	
OMe	3.86	s	
γ1	4.60	dd	12.0, 6.8
γ2	4.86	dd	12.0, 3.6
β	5.96	dd	6.8, 3.6
C α	6.50	d	16.0
B6	6.83	ddd	7.9, 8.8, 2.5
B 1,2,5	6.98	m	
C 3,5	7.18	m	
A 2,6	7.56	s	
C β	7.62	d	16.0
C 2,6	7.69	m	

^{13}C

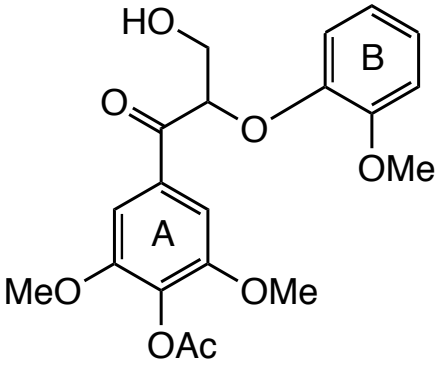
Atom	$CDCl_3$	Acetone	DMSO	
Ac	20.41	20.21	20.08	
Ac	21.10	20.94	20.83	
B3 OMe	55.71	56.12	55.55	
OMe	56.34	56.68	56.21	
OMe	56.34	56.68	56.21	
γ	64.70	65.07	63.82	
β	80.76	80.41	78.23	
A2	105.93	106.52	105.47	
A6	105.93	106.52	105.47	
B2	112.59	113.82	112.95	
B5	117.42	118.33	116.01	
C β	118.35	118.38	117.39	
B6	121.03	121.64	120.63	
C3	122.18	123.24	122.38	
C5	122.18	123.24	122.38	
B1	123.60	12334	122.55	
C2	129.32	130.27	129.69	
C6	129.32	130.27	129.69	
C1	131.84	132.66	131.49	
A1	132.66	133.94	132.49	
A4	133.39	134.24	132.55	
C α	144.59	145.13	144.28	
B4	146.72	147.84	146.32	
B3	150.37	151.34	149.51	
A3	152.28	153.40	151.95	
A5	152.28	153.40	151.95	
C4	152.36	153.59	152.13	
C γ	166.62	166.84	165.85	
Ac C=O	168.05	168.13	167.63	
Ac C=O	169.08	169.41	168.94	
α	194.44	194.92	194.02	

Notes:

S. Quideau

B5 and C β can be interchanged

Compound Number 2067



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

^{1}H (acetone)

Atom	H Shifts	Mult	J
B3 OMe	3.77	s	
OMe	3.85	s	
γ	4.10	dd	6.2, 5.0
γ OH	4.28	t	6.2
β	5.56	t	5.0
A 2,6	7.49	s	
B6	6.80	m	
B 1,5	6.41	m	
B2	6.96	m	

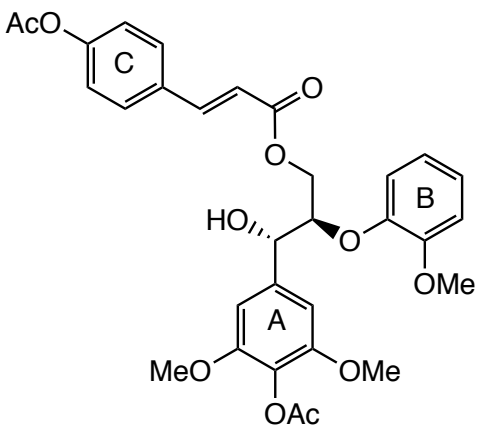
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.20		
B3 OMe		56.11		
OMe		56.62		
OMe		56.62		
γ		63.90		
β		84.04		
A2		106.56		
A6		106.56		
B2		113.67		
B5		117.03		
B6		121.61		
B1		123.24		
A4		133.99		
A1		134.39		
B4		148.26		
B3		151.03		
A3		153.25		
A5		153.25		
Ac C=O		168.15		
α		196.77		

Compound Number 2068



erythro

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac	2.20	s	
Ac	2.26	s	
OMe	3.78	s	
B3 OMe	3.81	s	
γ1	4.47	dd	11.9, 3.9
γ2	4.52	dd	11.9, 6.1
β	4.73	m	
α OH	4.78	d	4.5
α	5.07	br t	4.8
C β	6.41	d	16.0
B6	6.84	ddd	7.9, 6.4, 2.7
A 2,6	6.88	s	
B 1,2	6.95	m	
B5	7.04	br dd	1.4
C 3,5	7.17	m	
C α	7.51	d	16.0
C 2,6	7.66	m	

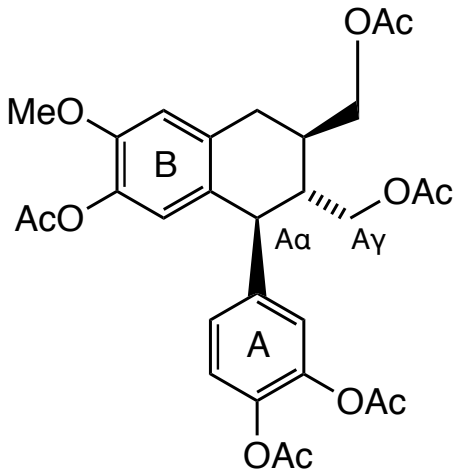
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac		20.25		
Ac		20.94		
B3 OMe		56.21		
OMe		56.39		
OMe		56.39		
γ		64.01		
α		73.49		
β		83.04		
A2		104.37		
A6		104.37		
B2		113.66		
C β		118.84		
B5		119.77		
B6		121.73		
C3		123.18		
C5		123.18		
B1		123.67		
A4		128.89		
C2		130.15		
C6		130.15		
C1		132.86		
A1		140.77		
C α		144.38		
B4		148.69		
B3		152.04		
A3		152.89		
A5		152.89		
C4		153.43		
C γ		166.80		
Ac C=O		168.58		
Ac C=O		169.43		

Compound Number 2069



Isotaxiresinol

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.00	s	
Ac Me	2.01	s	
Ac Me	2.10	s	
β	2.14	m	
Ac Me	2.22	s	
Ac Me	2.24	s	
B β	2.26	m	
B α	2.90	m	
A3 OMe	3.78	s	
γ1	3.90	dd	11.7, 3.5
α	4.06	br d	10.2
Bγ1	4.11	dd	11.2, 6.0
γ2	4.12	dd	11.7, 3.5
B γ2	4.22	dd	11.2, 4.4
B5	6.34	d	0.9
B2	6.88	br s	
A2	7.04	d	2.1
A6	7.10	dd	8.3, 4.1
A5	7.14	d	8.3

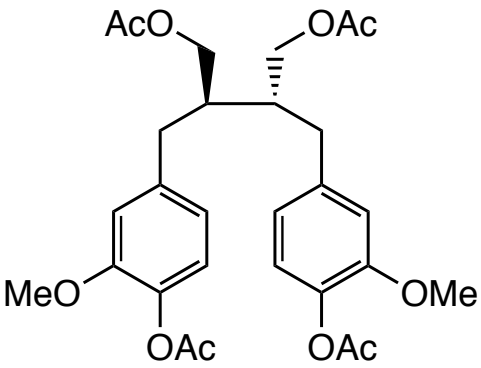
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
A3 Ac Me		20.36		
A4 Ac Me		20.45		
B4 Ac Me		20.50		
Ac Me		20.60		
Ac Me		20.72		
B α		33.50		
B β		36.27		
β		44.34		
α		47.51		
OMe		56.18		
γ		63.57		
B γ		66.69		
B2		112.97		
B5		124.12		
A5		124.36		
A2		124.92		
A6		127.98		
B6		131.84		
B1		135.41		
B4		139.26		
A4		142.08		
A3		143.41		
A1		144.19		
B3		150.55		
A4 Ac C=O		168.52		
B4 Ac C=O		168.63		
A3 Ac C=O		168.92		
Ac C=O		171.04		
Ac C=O		171.05		

Notes:

S. Quideau
Diaxial configuration on 6-membered ring --Trans 7,8
Natural occuring isomer is (+), i.e. 7S.8R, 8R'

Compound Number 2070



Seco-isolariciresinol

^{1}H (acetone)

Atom	H Shifts	Mult	J
γ Ac Me	2.00	s	
4 Ac Me	2.21	s	
β	2.22	m	
α1	2.70	dd	13.9, 7.9
α2	2.83	dd	13.8, 6.7
A3 OMe	3.74	s	
γ1	4.03	dd	11.4, 5.5
γ2	4.25	dd	11.4, 6.1
A6	6.70	dd	8.0, 1.95
A2	6.87	d	1.92
A5	6.92	d	8.0

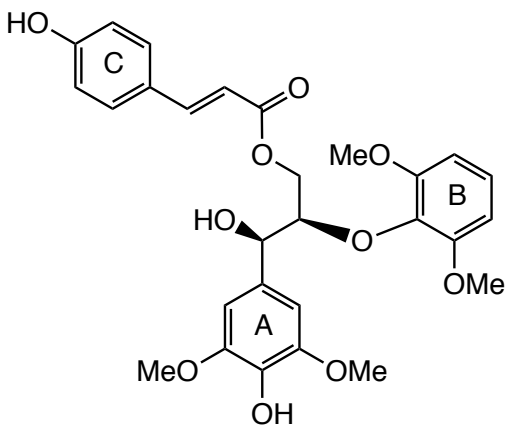
^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
4 Ac Me		20.47		
γ AcMe		20.83		
α		35.51		
β		40.81		
γ		64.67		
2		114.00		
6		121.67		
5		123.32		
4		139.14		
1		140.00		
3		152.01		
4 Ac C=O		169.04		
γAc C=O		171.04		

Notes:

S. Quideau
natural occuring isomer (-), i.e. 8R, 8R'
As this compound has a plane of symmetry the shifts for the other half are identical.

Compound Number 2071



threo

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B OMe	56.01	56.44	55.78	
B OMe	56.01	56.44	55.78	
A OMe	56.25	56.59	55.93	
A OMe	56.25	56.59	55.93	
γ	63.92	64.78	64.09	
α	74.66	74.81	72.17	
β	87.07	86.87	83.84	
A2	103.75	105.39	104.32	
A6	103.75	105.39	104.32	
B2	105.16	106.35	105.58	
B6	105.16	106.35	105.58	
C β	114.87	115.52	114.12	
C3	115.97	116.68	115.82	
C5	115.97	116.68	115.82	
B1	124.30	124.72	123.62	
C1	126.83	126.97	125.07	
C2	129.98	130.92	130.21	
C6	129.98	130.92	130.21	
A1	130.58	132.00	131.16	
A4	134.50	136.27	134.63	
B4	136.62	137.85	136.12	
C α	144.86	145.28	144.38	
A3	146.99	148.38	147.49	
A5	146.99	148.38	147.49	
B3	152.93	154.03	152.97	
B5	152.93	154.03	152.97	
C4	158.23	160.58	159.80	
C γ	167.12	167.12	166.25	

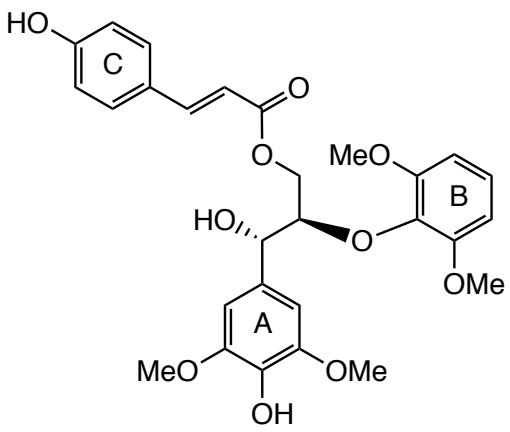
^{1}H (acetone)

Atom	H Shifts	Mult	J
A 3,5 OMe	3.76	s	
B 3,5 OMe	3.83	s	
γ1	4.06	dd	11.9, 4.2
β	4.27	ddd	7.3, 4.2, 3.1
γ2	4.45	dd	12.0, 3.2
α	5.00	br d	7.1
α OH	4.60	d	3.2
C β	6.33	d	16.0
B 2,6	6.68	d	8.4
A 2,1	6.67	d	0.3
C 3,5	6.89	m	
B1	7.01	dd	8.7, 8.1
C α	7.48	d	16.0
C 2,6	7.53	m	

Notes:

S. Quideau

Compound Number 2072



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^{1}H (acetone)

Atom	H Shifts	Mult	J
A 3,5 OMe	3.79	s	
B 3,5 OMe	3.82	s	
γ1	4.23	dd	11.8, 3.4
γ2	4.45	dd	11.8, 7.3
β	4.58	m	
α OH	4.697	d	3.9
α	4.96	br m	
C β	6.15	d	16.0
B 2,6	6.68	d	8.4
A 2,6	6.71	d	0.7
C 3,5	6.84	m	
B1	7.01	dd	8.6, 8.2
C α	7.33	d	16.0
C 2,6	7.46	m	

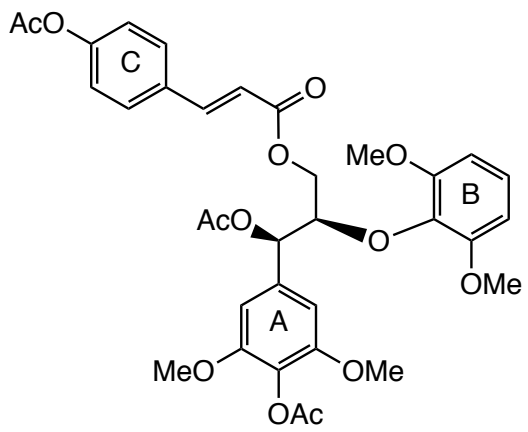
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
B OMe	56.20	56.48	55.77
B OMe	56.20	56.48	55.77
A OMe	56.33	56.60	55.92
A OMe	56.33	56.60	55.92
γ	62.59	63.57	63.38
α	71.90	73.19	72.62
β	83.18	84.40	83.51
A2	102.78	104.59	103.77
A6	102.78	104.59	103.77
B2	105.36	106.34	105.32
B6	105.36	106.34	105.32
C β	115.19	115.73	114.12
C3	115.91	116.65	115.81
C5	115.91	116.65	115.81
B1	124.44	124.75	123.40
C1	126.85	127.03	125.03
C2	129.88	130.82	130.11
C6	129.88	130.82	130.11
A1	129.75	131.66	132.10
A4	133.91	135.91	134.45
B4	134.69	136.59	135.92
C α	144.58	144.99	144.16
A3	147.00	148.49	147.63
A5	147.00	148.49	147.63
B3	153.69	154.53	152.89
B5	153.69	154.53	152.89
C4	158.15	160.43	159.74
C γ	167.29	167.16	166.27

Compound Number 2073



threo

^{1}H (acetone)

Atom	H Shifts	Mult	J
α Ac Me	1.97	s	
Ac Me	2.02	s	
Ac Me	2.27	s	
OMe	3.78	s	
OMe	3.79	s	
γ1	4.07	dd	11.9, 4.7
γ2	4.41	dd	11.9, 3.8
β	4.68	ddd	6.8, 4.7, 3.8
α	6.18	d	6.8
C β	6.56	d	16.0
B 2,6	6.66	d	8.4
A 2,6	6.86	br s	
B1	6.99	t	8.4
C 3,5	7.19	m	
C α	7.55	d	16.0
C 2,6	7.72	m	

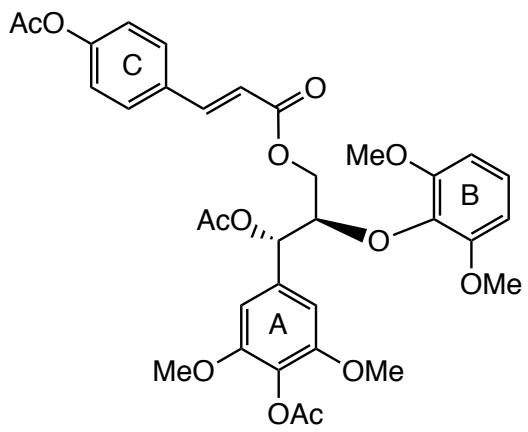
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.36	20.23	20.15	
Ac Me	21.02	20.95	20.75	
α Ac Me	21.02	20.95	20.88	
OMe	55.89	56.35	55.80	
OMe	55.89	56.35	55.80	
OMe	56.13	56.49	56.01	
OMe	56.13	56.49	56.01	
γ	64.01	64.66	63.72	
α	75.63	76.79	75.97	
β	80.86	81.83	80.62	
A2	104.10	104.92	103.89	
A6	104.10	104.92	103.89	
B2	105.09	106.22	105.29	
B6	105.09	106.22	105.29	
C β	117.75	118.88	117.82	
C3	122.09	123.20	122.43	
C5	122.09	123.20	122.43	
B1	123.74	124.47	123.68	
A4	128.57	129.54	127.74	
C2	129.19	130.22	129.68	
C6	129.19	130.22	129.68	
C1	131.92	132.90	131.66	
B4	135.42	136.76	135.61	
A1	136.56	137.85	136.15	
C α	143.86	144.48	143.76	
A3	151.94	153.07	151.55	
A5	151.94	153.07	151.55	
C4	152.10	153.46	152.09	
B3	153.14	154.19	152.69	
B5	153.14	154.19	152.69	
C γ	166.24	166.62	165.86	
Ac C=O	168.45	168.46	168.06	
Ac C=O	169.05	169.45	169.06	
Ac C=O	169.68	169.93	169.44	

Compound Number 2074



erythro

^{1}H (acetone)

Atom	H Shifts	Mult	J
α Ac Me	2.15	s	
Ac Me	2.21	s	
Ac Me	2.26	s	
B 3,5 OMe	3.79	s	
A 3,5 OMe	3.81	s	
γ1	4.36	dd	11.9, 4.0
γ2	4.53	dd	11.9, 6.2
β	4.80	dt	6.2, 4.0
α	6.14	d	4.2
C β	6.35	d	16.0
B 2,6	6.65	d	8.4
A 2,6	6.83	br s	
B1	6.99	t(dd)	8.4
C 3,5	7.18	m	
C α	7.44	d	16.0
C 2,6	7.66	m	

Notes:

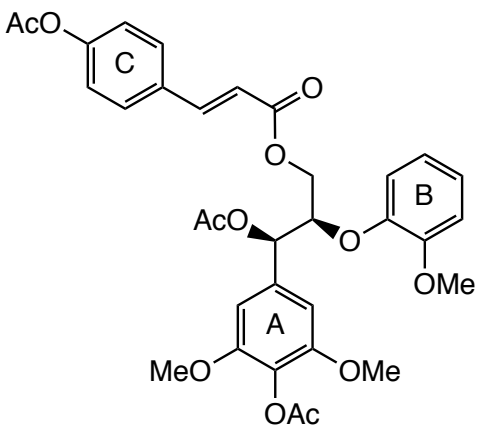
S. Quideau

B3,5 OMe and A3,5 OMe can be interchanged

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.36	20.24	20.15
α Ac Me	21.02	20.95	20.76
Ac Me	21.02	20.95	20.87
B OMe	55.87	56.32	55.78
B OMe	55.87	56.32	55.78
A OMe	56.07	56.47	55.97
A OMe	56.07	56.47	55.97
γ	63.13	63.73	62.64
α	74.50	75.58	74.23
β	80.92	81.67	80.19
A2	103.93	104.60	103.45
A6	103.93	104.60	103.45
B2	105.05	106.12	105.27
B6	105.05	106.12	105.27
C β	117.84	118.80	117.70
C3	122.03	123.19	122.43
C5	122.03	123.19	122.43
B1	124.00	124.72	124.00
A4	128.37	129.35	127.59
C2	129.19	130.15	129.57
C6	129.19	130.15	129.57
C1	131.98	132.85	131.56
B4	135.39	136.69	134.77
A1	135.73	136.77	135.43
C α	143.73	144.29	143.54
A3	151.84	153.06	151.58
A5	151.84	153.06	151.58
C4	152.04	153.44	152.06
B3	153.32	154.34	152.85
B5	153.32	154.34	152.85
C γ	166.42	166.52	165.70
Ac C=O	168.49	168.51	168.10
Ac C=O	169.04	169.44	169.05
Ac C=O	169.43	170.00	169.49

Compound Number 2075



threo

γ-p-coumaroylated syringylglycerol-β04-guaiacol ether (Ac′d)

^{1}H (acetone)

Atom	H Shifts	Mult	J
α Ac Me	2.04	s	
Ac Me	2.20	s	
Ac Me	2.27	s	
B OMe	3.79	s	
A 3,5 OMe	3.81	s	
γ1	4.19	dd	12.0, 5.5
γ2	4.39	dd	11.9, 3.9
β	4.88	ddd	6.6, 5.5
α	6.15	d	6.6
C β	6.54	d	16.0
B6	6.87	m	
A 2,6	6.88	br s	
B 1,2	6.93 - 7.00	m	
B5	7.08 - 7.10	m	
C 3,5	7.19	m	
C α	7.58	d	16.0
C 2,6	7.71	m	

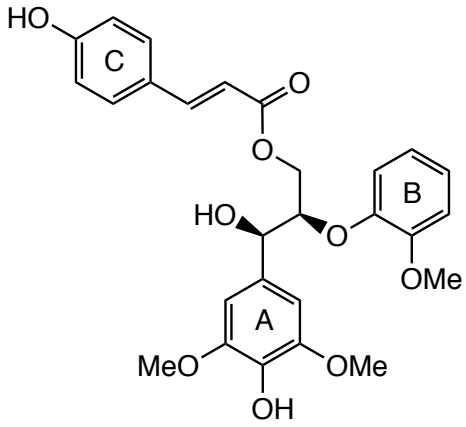
Notes:

S. Quideau
Not run in DMSO

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.42	20.23		
Ac Me	21.10	20.94		
αAc Me	21.10	20.94		
B3 OMe	35.77	56.21		
OMe	56.20	56.51		
OMe	56.20	56.51		
γ	63.39	63.97		
α	74.88	75.92		
β	80.50	80.89		
A2	104.09	105.00		
A6	104.09	105.00		
B2	112.45	113.74		
C β	117.52	118.62		
B5	118.85	119.25		
B6	121.00	121.70		
C3	122.14	123.22		
C5	122.14	123.22		
B1	123.34	123.75		
A4	128.81	129.70		
C2	129.31	130.26		
C6	129.31	130.26		
C1	131.91	132.83		
A1	134.81	136.23		
C α	144.25	144.78		
B4	147.99	149.16		
B3	150.86	151.87		
A3	152.01	153.21		
A5	152.01	153.21		
C4	152.20	153.53		
C γ	166.32	166.64		
Ac C=O	168.47	168.43		
Ac C=O	169.09	169.43		
Ac C=O	169.71	170.03		

Compound Number 2076



threo

γ-p-coumaroylated syringylglycerol-β04-guaiacyl ether

^{1}H (acetone)

Atom	H Shifts	Mult	J
A OMe	3.79	s	
B3 OMe	3.84	s	
γ1	4.11	dd	12.0, 6.2
γ2	4.36	dd	12.0, 3.4
β	4.57	td	6.1, 3.4
α	4.96	(br)d	5.9
C β	6.31	d	16.0
A 2,6	6.82	d	0.4
B6	6.85-6.90	m	
C 3,5	6.88	m	
B 1,2	6.94-7.01	m	
B5	7.15	dd	7.9, 1.5
C α	7.48	d	16.0
C 2,6	7.51	m	

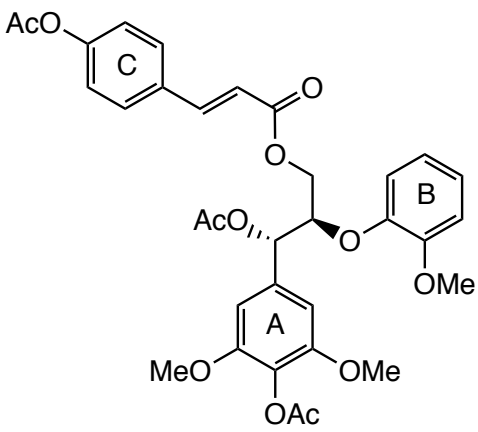
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe	55.82	56.27	55.60	
OMe	56.31	56.59	55.88	
OMe	56.31	56.59	55.88	
γ	63.19	64.23	63.47	
α	74.70	74.11	71.53	
β	86.09	84.42	81.02	
A2	103.82	105.41	104.24	
A6	103.82	105.41	104.24	
B2	112.19	113.60	112.70	
C β	114.66	115.30	113.86	
C3	115.95	116.68	115.78	
C5	115.95	116.68	116.25	
B5	120.53	119.33	116.25	
B6	121.45	121.82	120.71	
B1	124.12	123.52	121.71	
C1	126.89	126.96	125.00	
C2	130.04	130.97	130.30	
C6	130.04	130.97	131.30	
A1	130.29	132.11	131.22	
A4	134.73	136.36	134.67	
C α	145.18	145.57	144.84	
A3	147.11	148.47	147.58	
A5	147.11	148.47	147.58	
B4	147.91	149.37	147.86	
B3	150.91	151.80	149.91	
C4	158.08	160.60	159.87	
C γ	166.86	167.15	166.38	

Compound Number 2077



erythro

γ-p-coumaroylated syringylglycerol-β04-guiacol ether (Ac′d)

^{1}H (acetone)

Atom	H Shifts	Mult	J
α Ac Me	2.09	s	
Ac Me	2.21	s	
Ac Me	2.26	s	
B3 OMe	3.81	s	
A OMe	3.81	s	
γ1	4.43	dd	11.9, 4.3
γ2	4.49	dd	11.9, 5.8
β	4.94	m	
α	6.12	d	5.1
C β	6.45	d	16.0
B6	6.85	m	
A 2,6	6.89	d	0.4
B 1,2	6.95-7.00	m	
B5	7.03-7.06	m	
C 3,5	7.19	m	
C α	7.57	d	16.0
C 2,6	7.69	m	

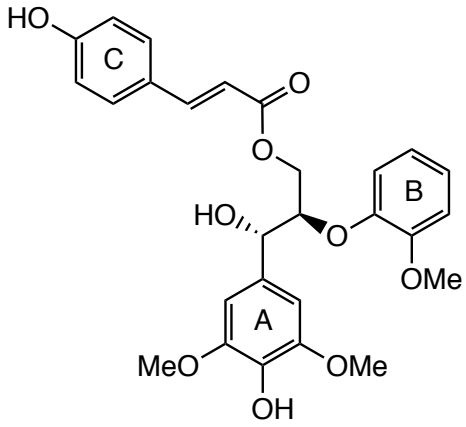
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me	20.40	20.24	20.12	
α Ac Me	21.01	20.90	20.70	
Ac Me	21.06	20.94	20.84	
B3 OMe	55.73	56.20	55.61	
A OMe	56.14	56.50	55.97	
A OMe	56.14	56.50	55.97	
γ	62.98	63.41	62.35	
α	74.17	74.99	73.53	
β	80.31	80.38	78.34	
A2	104.43	105.14	104.10	
A6	104.43	105.14	104.10	
B2	112.51	113.75	112.88	
C β	117.59	118.57	117.53	
B5	119.50	119.79	117.81	
B6	120.95	121.65	120.69	
C3	122.09	123.21	122.38	
C5	122.09	123.21	122.38	
B1	123.58	124.02	122.81	
A4	128.67	129.57	127.73	
C2	129.28	130.22	129.63	
C6	129.28	130.22	129.63	
C1	131.93	132.79	131.51	
A1	134.92	136.25	134.99	
C α	144.23	144.74	143.94	
B4	147.24	148.36	146.75	
B3	151.07	152.03	150.27	
A3	151.98	153.07	151.48	
A5	151.98	153.07	151.48	
C4	152.16	153.51	152.08	
C γ	166.44	166.63	165.76	
Ac C=O	168.49	168.48	168.01	
Ac C=O	169.06	169.43	168.97	
α Ac C=O	169.48	169.95	169.34	

Compound Number 2078



erythro

γ-p-coumaroylated syringylglycerol-β04-guaiacyl ether

^{1}H (acetone)

Atom	H Shifts	Mult	J
OMe	3.80	s	
B3 OMe	3.81	s	
γ1	4.41	dd	11.8, 3.8
γ2	4.47	dd	11.8, 6.4
β	4.68	ddd	6.4, 5.0, 3.8
α	4.98	br d	4.9
C β	6.25	d	16.0
A 2,6	6.81	brs	
B6	6.83	m	
C 3,5	6.87	m	
B 1,2	6.91-6.96	m	
B5	7.05	br dd	7.8, 1.5
C α	7.44	d	16.0
C 2,6	7.48	m	

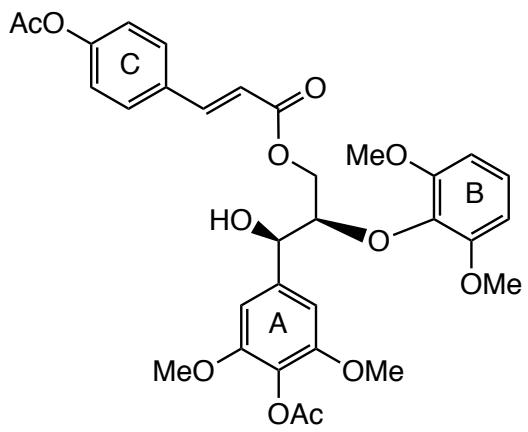
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
B3 OMe	55.83	56.23	55.54	
OMe	56.29	56.60	55.90	
OMe	56.29	56.60	55.90	
γ	62.70	64.04	63.29	
α	72.39	73.51	71.77	
β	84.23	83.41	80.92	
A2	103.13	105.23	104.38	
A6	103.13	105.23	104.38	
B2	112.22	113.63	112.74	
C β	114.40	115.37	113.93	
C3	115.95	116.67	115.75	
C5	115.95	116.67	115.75	
B5	120.53	119.55	116.89	
B6	121.46	121.72	120.62	
B1	124.03	123.46	121.83	
C1	126.44	126.92	124.99	
C2	129.98	130.90	130.24	
C6	129.98	130.90	130.24	
A1	130.16	132.59	132.05	
A4	134.15	136.12	134.61	
C α	145.25	145.42	144.71	
A3	147.00	148.42	147.52	
A5	147.00	148.42	147.52	
B4	147.02	148.91	147.52	
B3	151.42	152.00	150.03	
C4	158.68	160.58	159.82	
C γ	167.39	167.28	166.41	

Compound Number 2079



threo

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.19	s	
Ac Me	2.27	s	
A OMe	3.75	s	
B OMe	3.82	s	
γ1	4.16	dd	11.9, 4.6
β	4.38	ddd	6.3, 4.5, 3.6
γ2	4.50	dd	11.9, 3.6
α	5.07	br d	6.4
C β	6.47	d	16.0
B 2,6	6.68	d	8.4
A 2,6	6.87	br s	
B1	7.01	t	8.4
C 3,5	7.19	m	
C α	7.63	d	16.0
C 2,6	7.70	m	

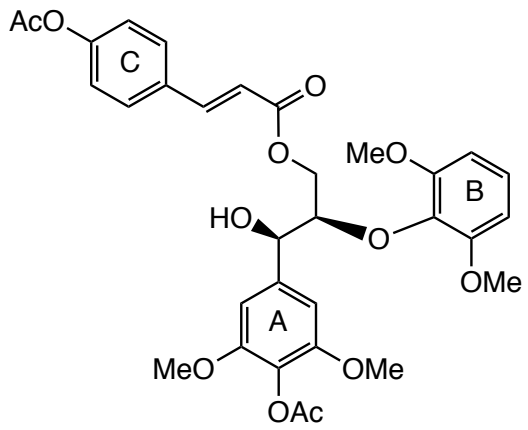
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.25		
Ac Me		21.06		
A OMe		56.36		
A OMe		56.36		
B OMe		56.45		
B OMe		56.45		
γ		64.93		
α		74.56		
β		85.88		
A2		104.48		
A6		104.48		
B2		106.35		
B6		106.35		
C β		118.98		
C3		123.19		
C5		123.19		
B1		124.80		
A4		128.98		
C2		130.17		
C6		130.17		
C1		132.93		
B4		137.65		
A1		140.28		
C α		144.26		
A3		152.82		
A5		152.82		
C4		153.43		
B3		154.07		
B5		154.07		
C γ		166.65		
Ac C=O		168.54		
Ac C=O		169.45		

Compound Number 2080



erythro

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.19	s	
Ac Me	2.26	s	
A OMe	3.78	s	
B OMe	3.83	s	
γ1	4.30	dd	11.7, 3.8
γ2	4.51	dd	11.7, 6.9
β	4.62	m	
α	5.05	br t	3.7
C β	6.34	d	16.0
B 2,6	6.09	d	8.4
A 2,6	6.82	br s	
B1	7.03	t	8.4
C 3,5	7.17	m	
C α	7.44	d	16.0
C 2,6	7.66	m	

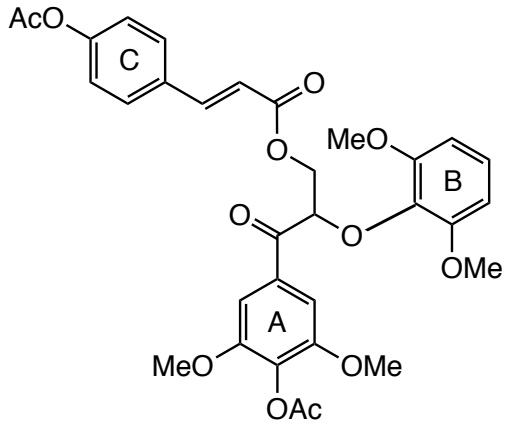
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.26		
Ac Me		20.94		
A OMe		56.38		
A OMe		56.38		
B OMe		56.48		
B OMe		56.48		
γ		63.67		
α		73.30		
β		84.07		
A2		103.76		
A6		103.76		
B2		106.31		
B6		106.31		
C β		119.10		
C3		123.16		
C5		123.16		
B1		124.83		
A4		128.69		
C2		130.11		
C6		130.11		
C1		132.93		
B4		136.57		
A1		140.05		
C α		144.00		
A3		152.94		
A5		152.94		
C4		153.36		
B3		154.51		
B5		154.51		
C γ		166.71		
Ac C=O		168.59		
Ac C=O		169.45		

Compound Number 2081



^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.26	s	
Ac Me	2.28	s	
B OMe	3.72	s	
A OMe	3.85	s	
γ1	4.63	dd	11.7, 6.2
γ2	4.74	dd	11.7, 4.6
β	5.69	dd	6.2, 4.6
C β	6.39	d	16.0
B 2,6	6.64	d	8.4
B1	6.49	t	8.4
C 3,5	7.17	m	
C α	7.50	d	16.0
A 2,6	7.58	br s	
C 2,6	7.64	m	

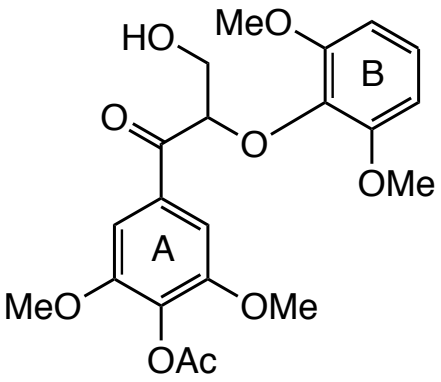
Notes:

S. Quideau

^{13}C

Atom	$CDCl_3$	Acetone	DMSO
Ac Me	20.40	20.23	20.12
Ac Me	21.08	20.95	20.85
B OMe	55.88	56.31	55.80
B OMe	55.88	56.31	55.80
A OMe	56.28	56.67	56.20
A OMe	56.28	56.67	56.20
γ	64.49	64.90	63.77
β	81.85	81.50	79.82
B2	105.11	106.18	105.39
B6	105.11	106.18	105.39
A2	106.37	106.93	105.86
A6	106.37	106.93	105.86
C β	117.67	118.55	117.57
C3	122.15	123.25	122.45
C5	122.15	123.25	122.45
B1	124.23	124.99	124.07
C2	129.21	130.19	129.61
C6	129.21	130.19	129.61
C1	131.90	132.72	131.48
A4	133.05	133.96	132.28
A1	133.49	134.72	133.31
B4	135.68	136.63	135.12
C α	144.02	144.62	143.83
A3	152.08	153.20	151.80
A5	152.08	153.20	151.80
C4	152.16	153.52	152.11
B3	153.03	154.07	152.53
B5	153.03	154.07	152.53
C γ	166.34	166.55	165.73
Ac C=O	168.06	168.19	167.72
Ac C=O	169.08	169.43	169.02
α	194.81	195.26	184.38

Compound Number 2082



^{13}C

Atom	$CDCl_3$	Acetone	DMSO	
Ac Me		20.21		
B OMe		56.28		
B OMe		56.28		
A OMe		56.61		
A OMe		56.61		
γ		63.35		
β		86.41		
B2		106.22		
B6		106.22		
A2		106.51		
A6		106.51		
B1		124.92		
A4		133.59		
A1		135.01		
B4		137.01		
A3		153.06		
A5		153.06		
B3		153.77		
B5		153.77		
Ac C=O		168.18		
α		196.25		

^{1}H (acetone)

Atom	H Shifts	Mult	J
Ac Me	2.27	s	
B OMe	3.73	s	
A OMe	3.86	s	
γ + γ OH	3.90-3.98	m	
β	5.22	dd	5.7, 4.5
B 2,6	6.67	d	8.4
B1	7.02	dd t	8.6, 8.2, 8.4
A 2,6	7.48	s	

Notes:

S.Quideau