

SUPPORTING INFORMATION

A Meroisoprenoid, Heptenolides and C-Benzylated Flavonoids from *Sphaerocoryne gracilis* ssp. *gracilis*

Gaspar Maeda, Joan J. E. Munissi, Sofia Lindblad, Sandra Duffy, Jerry Pelletier, Vicky M. Avery, Stephen S. Nyandoro and Máté Erdélyi

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The structures of known compounds 6-16

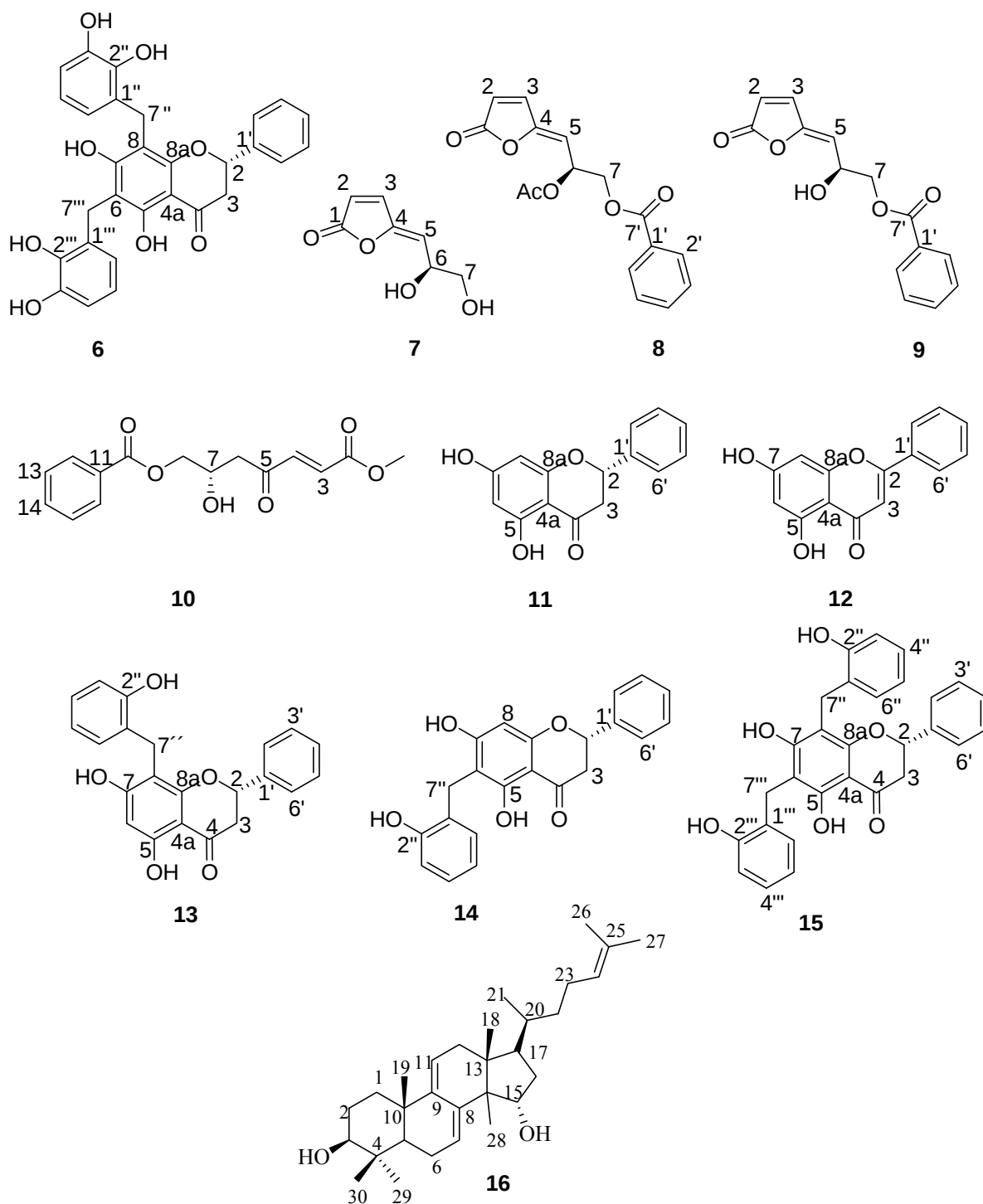


Figure S1. The structures of the known compounds 6-16

¹H and ¹³C NMR data of compound **6**

Table S1. ¹H and ¹³C NMR Spectroscopic Data for 3''-Hydroxygracinol (6**) Acquired in CDCl₃ at 25 °C [(δ_H, Multiplicity (*J* in Hz)]**

6

position	δ _C , type	δ _H	<i>J</i> (Hz)
2	79.7, HC-O	5.40	dd, (13.3, 2.6)
3	43.3, CH ₂	3.09	dd, (17.1, 13.3)
		2.82	dd, (17.1, 2.6)
4	196.5, C=O	--	--
5	159.0, C-O	--	--
5-OH	--	12.79	s
6	108.7, C	--	--
7	160.5, C-O	--	--
8	107.5, C	--	--
8a	158.4, C-O	--	--
4a	103.2, C	--	--
7''	23.0, CH ₂	3.84	s
7'''	22.6, CH ₂	3.91	d, (13.9)
		3.88	d, (13.9)
1'	138.4, C	--	--
2'/6'	126.4, CH	*7.47-7.51	m
3'/5'	129.1, CH	*7.47-7.51	m
4'	129.2, CH	7.44	m
1''	126.8, C	--	--
2''	141.1, C-O	--	--
3''	144.3, C-O	--	--
4''	113.4, CH	*6.74	m
5''	*121.1, CH	*6.74	m
6''	123.3, CH	7.09	dd, (6.7, 2.6)
1'''	127.0, C	--	--
2'''	141.0, C-O	--	--

3'''	143.5, C-O	--	--
4'''	113.6, CH	6.69	dd, (7.9, 1.5)
5'''	*121.1, CH	6.66	dd, (7.9, 7.7)
6'''	123.4, CH	6.84	dd, (7.7, 1.5)

*Overlapping signals

¹H and ¹³C NMR data of compounds **7** and **8**

Table S2. ¹H and ¹³C NMR Spectral Data for (Z)-Sphaerodiol (7**) and (Z)-Acetylmelodorinol (**8**) measured at 800 MHz in CDCl₃**

	7			8		
position	δ _C	δ _H	<i>J</i> (Hz)	δ _C	δ _H	<i>J</i> (Hz)
1	169.1	--	--	168.8	--	--
2	121.0	6.25	d, (5.5)	121.9	6.28	d, (5.5)
3	143.8	7.38	d, (5.5)	143.6	7.37	d, (5.5)
4	150.0	--	--	151.0	--	--
5	113.9	5.38	d, (7.8)	109.2	5.32	d, (8.1)
6	68.0	4.88	ddd, (7.8, 6.7, 3.5)	67.6	6.15	ddd, (8.1, 6.2, 4.1)
7	65.8	3.82	dd, (11.2, 3.5)	64.9	4.56	dd, (11.7, 4.1)
		3.62	dd, (11.2, 6.7)	64.9	4.53	dd, (11.7, 6.2)
1'	--	--	--	129.8	--	--
2'/6'	--	--	--	130.0	8.02	m
3'/5'	--	--	--	128.8	7.45	m
4'	--	--	--	133.6	7.58	m
-CH ₃	--	--	--	21.2	2.10	s
OAc-6	--	--	--	166.3	--	--
7'	--	--	--	170.1	--	--

Table S3. ¹H and ¹³C NMR Spectral Data for (Z)-Melodorinol (9) and 7-Hydroxy-6-hydromelodienone (10) measured at 800 MHz in CDCl₃

9				10			
position	δ _C	δ _H	<i>J</i> (Hz)	Position	δ _C	δ _H	<i>J</i> (Hz)
1	168.9	--	--	2	165.6	--	--
2	121.3	6.26	d, (5.5)	3	131.4	6.72	d, (16.0)
3	143.7	7.39	d, (5.5)	4	139.1	7.09	d, (16.0)
4	150.2	--	--	5	198.5	--	--
5	113.1	5.40	d, (8.0)	6	44.5	2.96	m
6	66.2	5.18	br ddd, (8.0, 6.6, 4.1)			2.96	m
7	67.7	4.48	m	7	66.1	4.54	dddd, (8.3, 5.8, 4.1, 4.1)
		4.48	m	8	67.5	4.40	m
OAc-6	166.8	--	--			4.40	m
1'	129.6	--	--	10	166.5	--	--
2'/6'	129.9	8.05	m	11	129.6	--	--
3'/5'	128.6	7.46	m	12	129.7	8.06	m
4'	133.5	7.58	m	13	128.5	7.46	m
				14	133.3	7.58	m
				-OCH ₃	52.5	3.82	s

¹H and ¹³C NMR data of compounds **11** and **12**

Table S4. ¹H and ¹³C NMR Spectral Data for Pinocembrin (11) and 5, 7-Dihydroxyflavone (12) measured at 800 MHz in CDCl₃ and (CD₃)₂SO, Respectively

	11			12		
position	δ _C	δ _H	<i>J</i> (Hz)	δ _C	δ _H	<i>J</i> (Hz)
2	79.4	5.43	dd, (13.1, 3.1)	163.4	--	--
3	43.5	3.09	dd, (17.1, 13.1)	105.3	6.74	s
		2.83	dd, (17.1, 3.1)	--	--	--
4	195.9	--	--	182.0	--	--
5	164.5	--	--	161.6	--	--
5-OH	--	12.04	s	--	12.61	s
6	95.6	6.00	m	99.2	6.03	d, (2.0)
7	164.5	--	--	164.6	--	--
8	96.9	6.01	m	94.3	6.33	d, (2.0)
8a	163.3	--	--	157.6	--	--
4a	103.4	--	--	104.1	--	--
1'	138.4	--	--	130.8	--	--
2'/6'	126.3	7.45	m	126.6	7.85	m
3'/5'	129.1	7.44	m	129.4	7.38	m
4'	129.0	7.40	m	132.2	7.42	m

¹H and ¹³C NMR data of compounds **13** and **14**

Table S5. ¹H and ¹³C NMR Spectral Data for Chamanetin (13) and Isochamanetin (14) measured at 800 MHz in CDCl₃ and CD₃OD, Respectively

	13			14		
position	δ _C	δ _H	<i>J</i> (Hz)	δ _C	δ _H	<i>J</i> (Hz)
2	80.1	5.52	<i>dd</i> , 12.9, 3.1	80.4	5.45	<i>dd</i> , 12.9, 3.0
3		3.10	<i>dd</i> , 17.1, 12.9	44.3	3.08	<i>dd</i> , 17.0, 13.0
	43.4	2.81	<i>dd</i> , 17.1, 3.1		2.76	<i>dd</i> , 17.0, 3.0
4	197.6	--	--	197.2	--	--
4a	103.6	--	--	103.1	--	--
5	163.3	12.08	<i>s</i>	162.8	--	--
6	97.0	6.03	<i>s</i>	109.0	--	--
7	164.7	--	--	162.8	--	--
8	107.3	--	--	96.3	6.01	<i>s</i>
8a	161.3	--	--	162.8	--	--
7"	22.9	3.78	<i>s</i>	22.7	3.82	AB <i>q</i> , 16.0
1'	139.9	--	--	140.6	--	--
*2'/6'	127.3	7.39 - 7.50	<i>m</i>	127.3	7.50	<i>d</i> , 7.3
*3'/5'	129.6	7.39 - 7.50	<i>m</i>	129.7	7.41	<i>t</i> , 7.7
*4'	129.6	7.39 - 7.50	<i>m</i>	129.6	7.36	<i>m</i>
1"	130.9	--	--	128.4	--	--
2"	154.7	--	--	155.7		
3"	115.9	6.79	<i>dd</i> , 8.0, 0.9	116.0	6.75	<i>dd</i> , 8.0, 1.0
4"	128.2	7.02	<i>m</i>	127.8	6.98	<i>dt</i> , 7.8, 1.6
5"	121.1	6.74	<i>td</i> , 7.5, 1.0	120.7	6.69	<i>dt</i> , 7.6, 1.2
6"	130.9	7.04	<i>dd</i> , 7.5, 1.6	130.8	7.05	<i>dd</i> , 7.6, 1.2

* = Overlapping Signals

¹H and ¹³C NMR data of compound **15**

Table S6. ¹H and ¹³C NMR Spectral Data for Dichamanetin (**15**) measured at 800 MHz in CDCl₃

position	δ _C	δ _H	J (Hz)
2	79.9	5.54	<i>dd</i> , 12.8, 3.0
3	43.0	3.16	<i>dd</i> , 17.2, 12.8
		2.86	<i>dd</i> , 17.2, 3.0
4	197.6	--	--
4a	103.2	--	--
5	160.7	--	--
6	108.1	--	--
7	161.9	--	--
8	107.3	--	--
8a	159.2	--	--
7''	22.3	3.87	<i>d</i> , 6.9
7'''	22.9	3.84	<i>s</i>
1'	139.5	--	--
2'/6'	127.0	7.53	<i>d</i> , 7.5
3'/5'	129.3	7.47	<i>dd</i> 7.5, 7.5
4'	129.3	7.43	<i>m</i>
1''	127.2	--	--
2''	154.0	--	--
3''	115.7	6.85	<i>dd</i> , 8.1, 0.9
4''	128.0	7.08	<i>m</i>
5''	121.1	6.82	<i>m</i>
6''	131.1	7.26	<i>dd</i> , 7.6, 1.3
1'''	127.1	--	--
2'''	153.8	--	--
3'''	115.5	6.83	<i>m</i>
4'''	128.0	7.05	<i>m</i>
5'''	121.1	6.77	<i>m</i>
6'''	130.9	7.09	<i>m</i>
5-OH	--	12.71	<i>s</i>
7-OH	--	8.16	<i>brs</i>
2''-OH	--	8.16	<i>brs</i>
2'''-OH	--	8.16	<i>brs</i>

¹H and ¹³C NMR data of compound 16

Table S7. ¹H and ¹³C NMR Spectral Data for Polycarpol (16) measured at 800 MHz in CDCl₃

position	δ _C	δ _H	<i>J</i> (Hz)
1	35.9	1.98, 1.43	<i>m</i>
2	27.9	1.72, 1.65	<i>m</i>
3	79.0	3.24	<i>dd</i> , 11.6, 3.9
4	38.8	--	--
5	49.1	1.45	<i>dd</i> , 13.3, 3.9
6α	23.1	2.16, 2.07	<i>m</i>
7	121.4	5.85	<i>d</i> , 6.2
8	141.0	--	--
9	146.2	--	--
10	37.6	--	--
11	116.2	5.30	<i>d</i> , 6.2
12α	38.6	2.29, 2.05	<i>d</i> , 17.6, <i>m</i>
13	44.5	--	--
14	51.9	--	--
15	74.9	4.27	<i>m</i>
16	40.3	1.96, 1.72	<i>m</i>
17	49.0	1.31	<i>m</i>
18	16.1	0.61	<i>s</i>
19	23.0	0.93	<i>s</i>
20	36.4	1.86	<i>m</i>
21	18.5	0.88	<i>s</i>
22	35.9	1.35, 1.03	<i>m</i>
23	25.0	1.98	<i>m</i>
24	125.1	5.08	<i>t</i> , 6.9
25	131.3	--	--
26	25.9	1.60	<i>s</i>
27	17.8	1.68	<i>s</i>
28	17.3	0.88	<i>s</i>
29	28.3	0.98	<i>s</i>
30	16.0	1.00	<i>s</i>

Spectroscopic data for gracidiol (1)

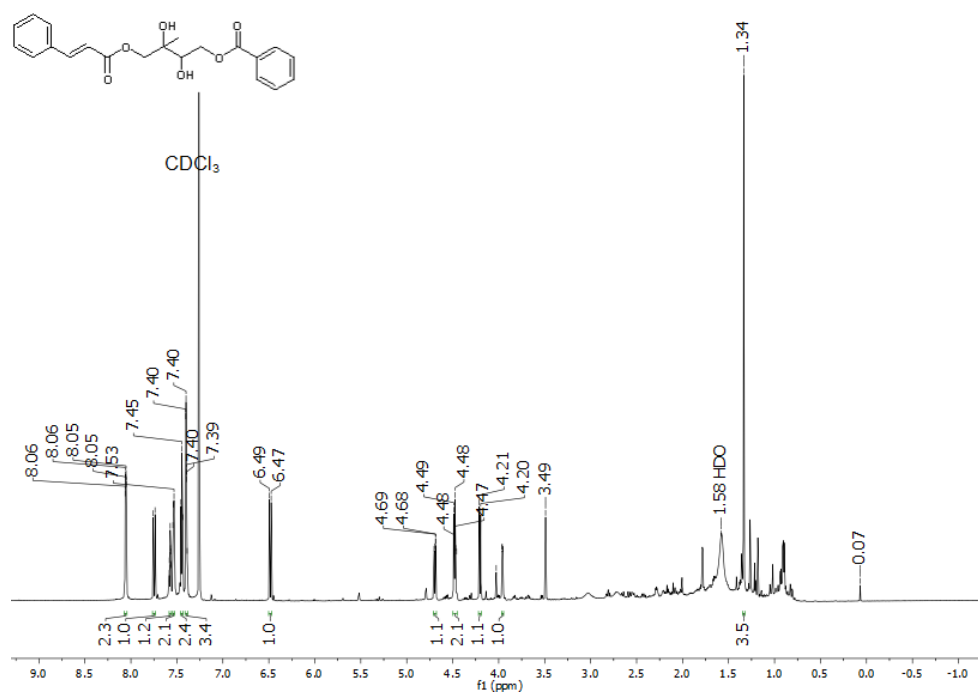


Figure S2. The ¹H NMR Spectrum of Gracidiol (1) measured at 800 MHz in CDCl₃.

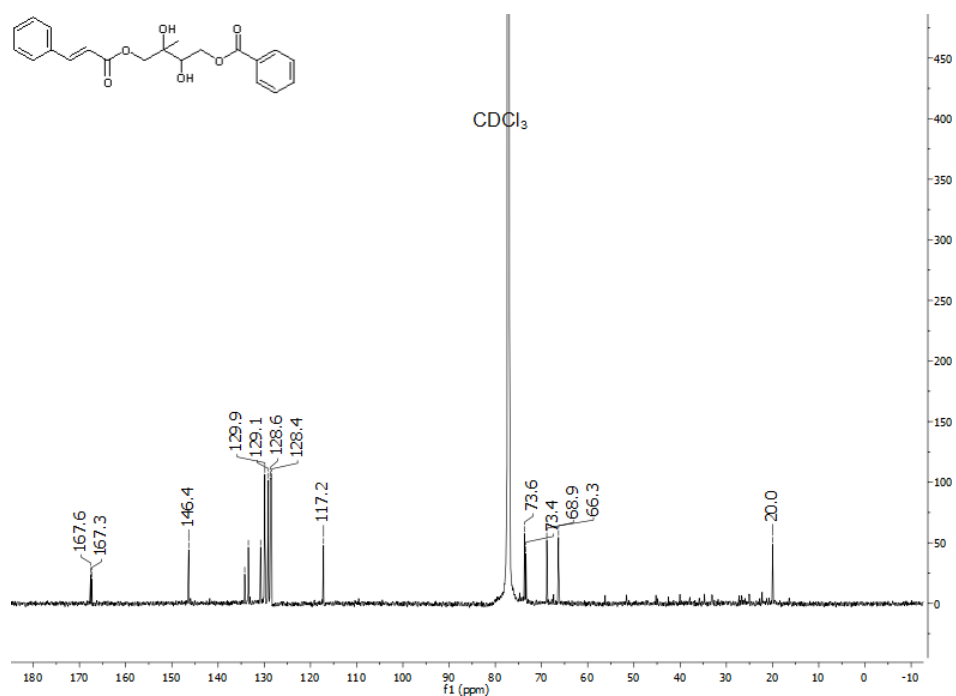


Figure S3. The ¹³C NMR Spectrum of Gracidiol (1) measured at 800 MHz in CDCl₃.

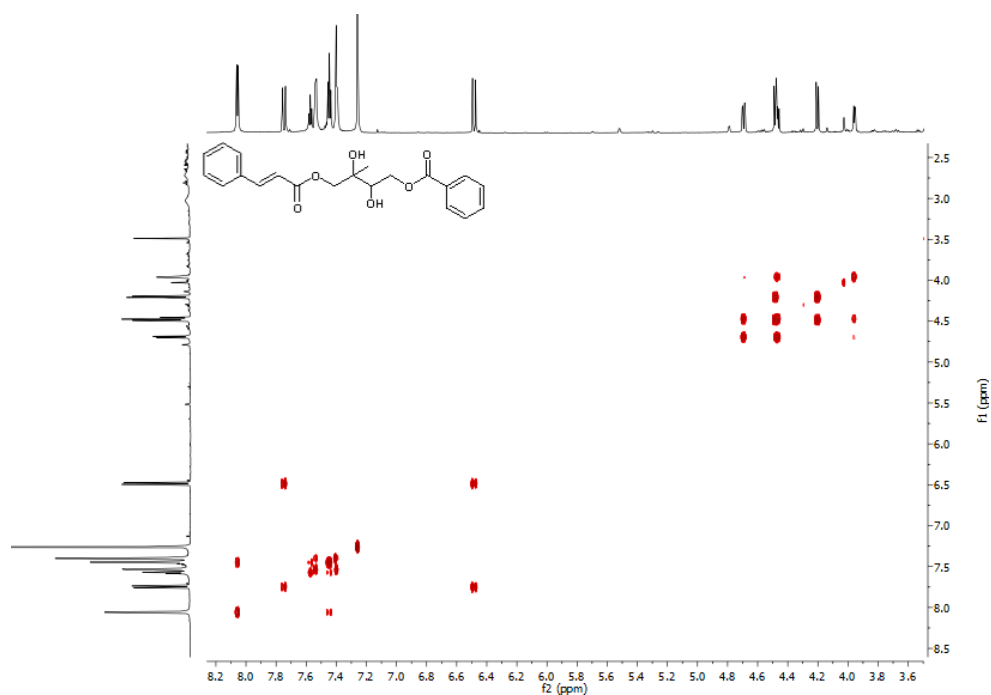


Figure S4. The COSY Spectrum of Gracidiol (**1**) measured at 800 MHz in CDCl₃.

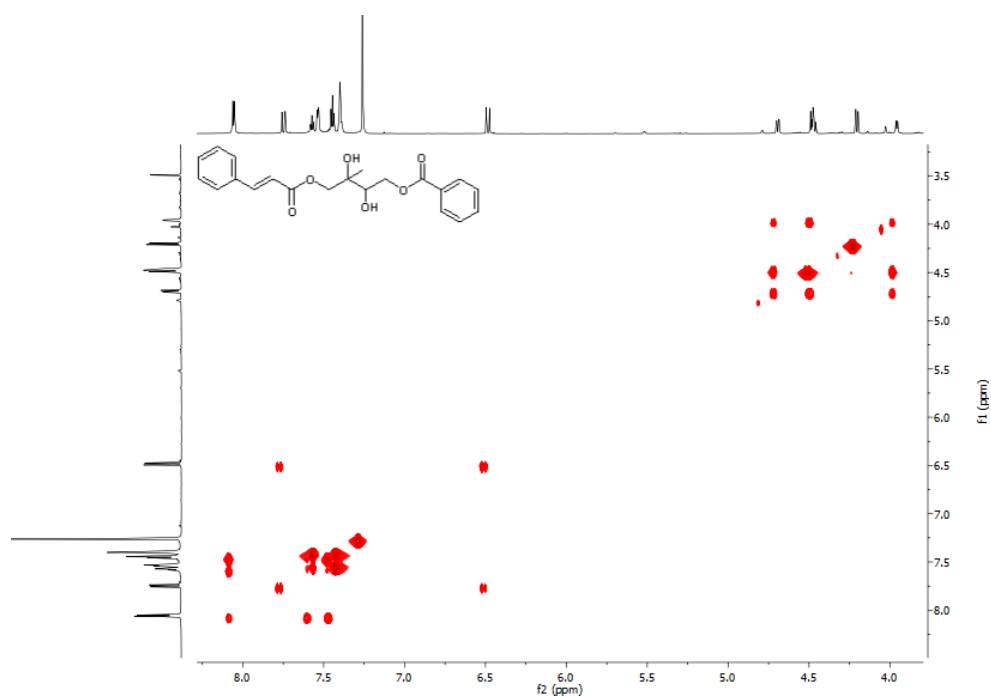


Figure S5. The TOCSY Spectrum of Gracidiol (**1**) measured at 800 MHz in CDCl₃.

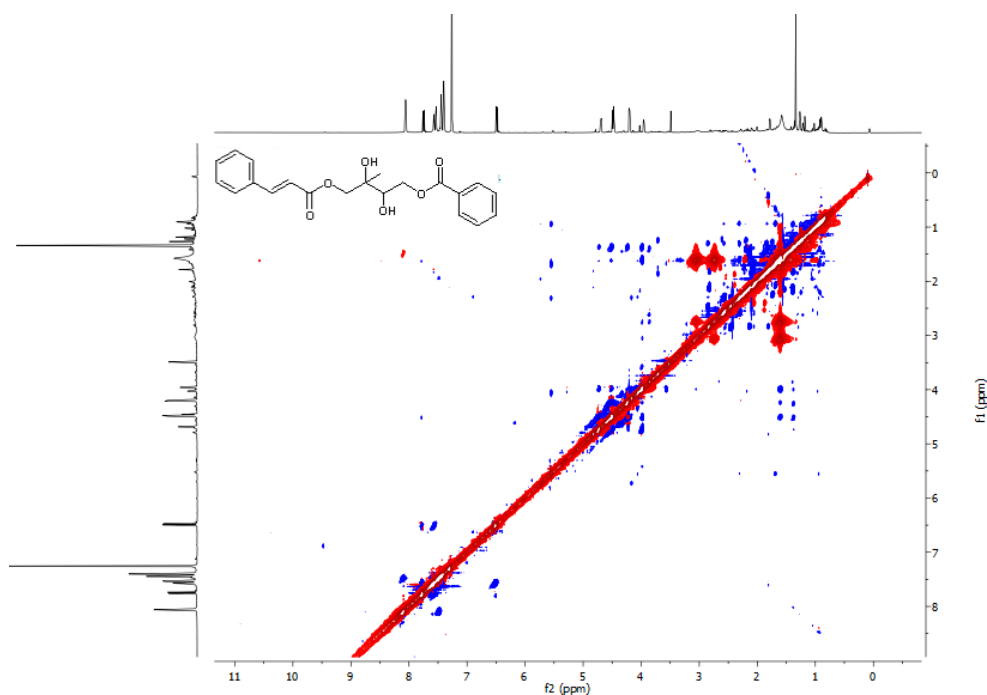


Figure S6. The NOESY Spectrum of Gracidiol (**1**) measured at 800 MHz in CDCl₃.

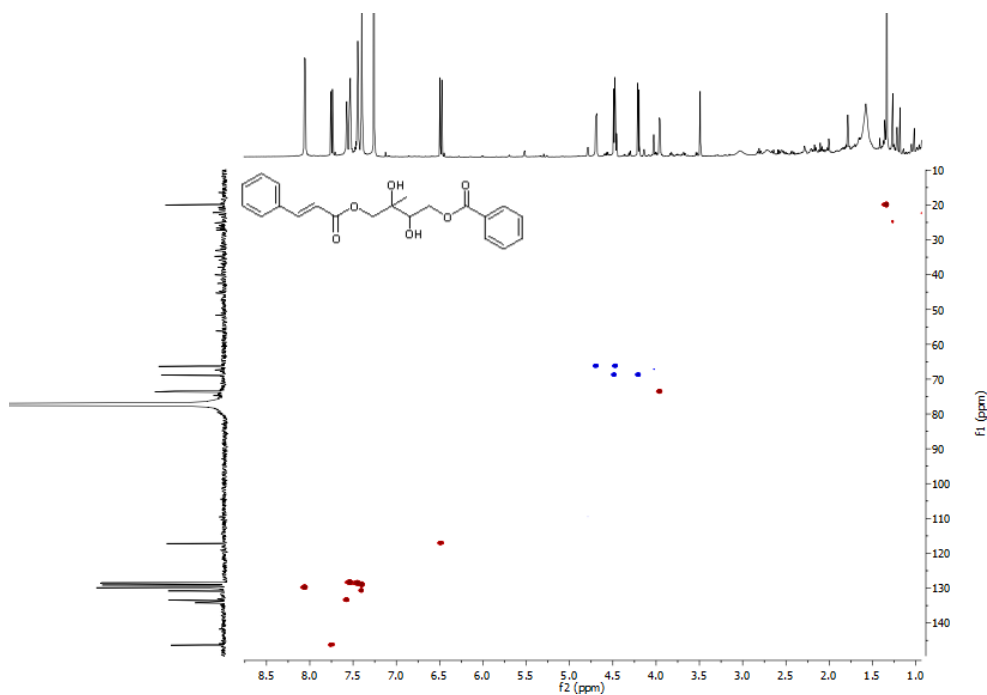


Figure S7. The HSQC Spectrum of Gracidiol (**1**) measured at 800 MHz in CDCl₃.

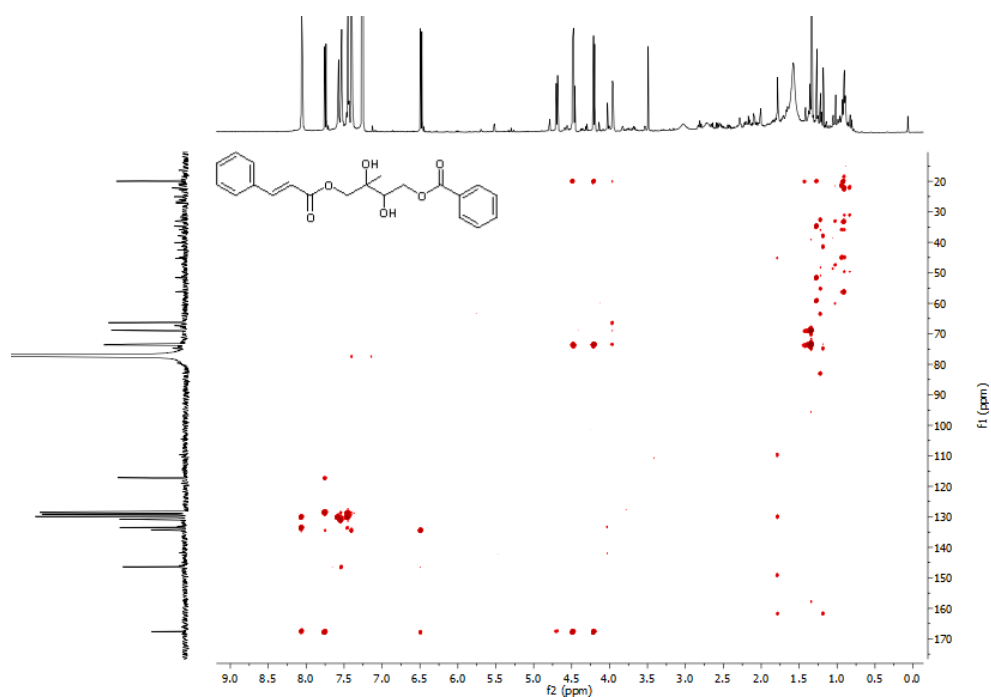


Figure S8. The HMBC Spectrum of Gracidiol (**1**) measured at 800 MHz in CDCl_3 .

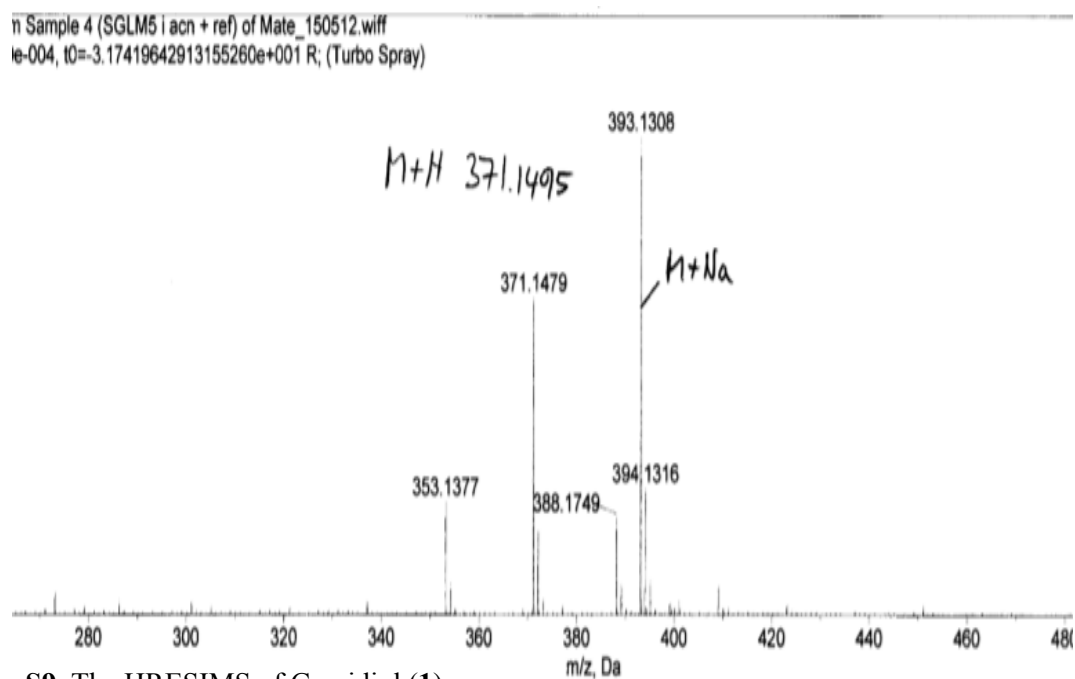


Figure S9. The HRESIMS of Gracidiol (**1**).

Spectroscopic data for (Z)-7-acetylsphaerodol (**2**)

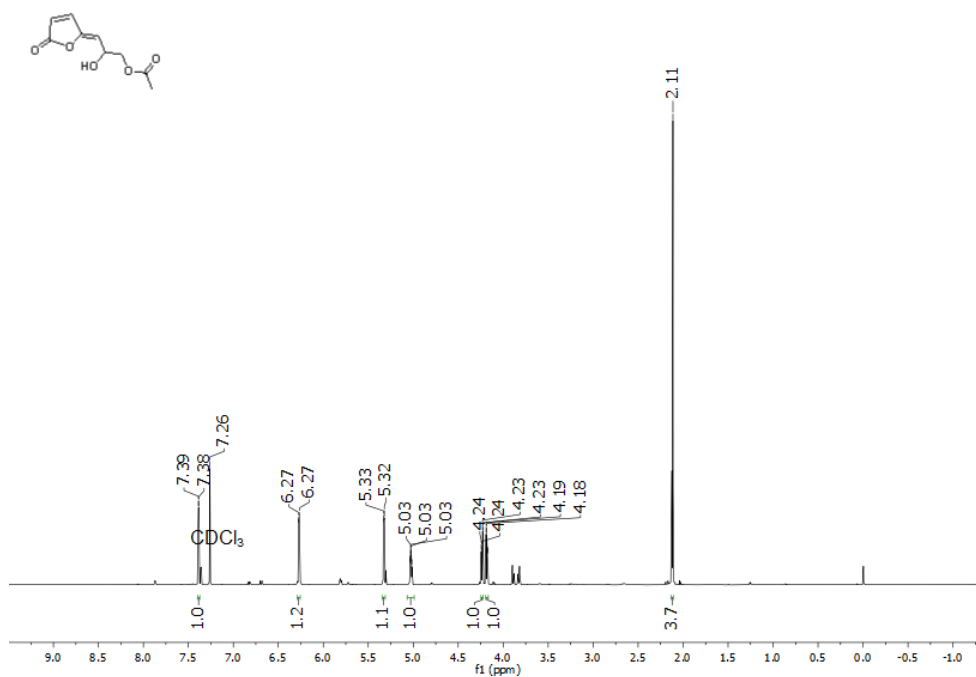


Fig S10. The ¹H NMR Spectrum of (Z)-7-Acetylsphaerodol (**2**) measured at 800 MHz and CDCl₃.

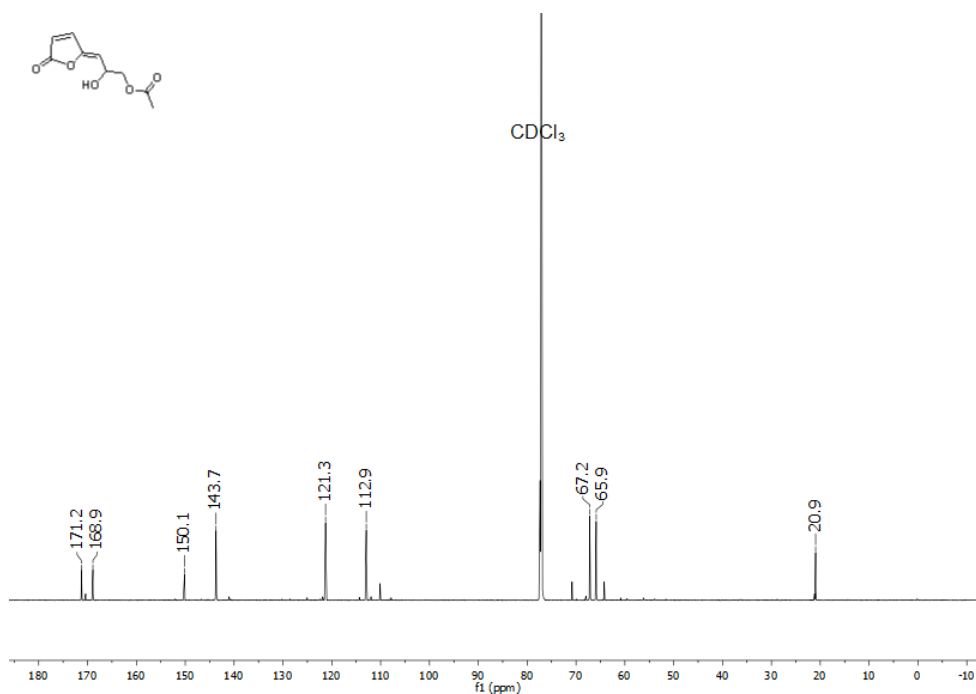


Figure S11. The ¹³C NMR Spectrum of (Z)-7-Acetylsphaerodol (**2**) measured at 800 MHz in CDCl₃.

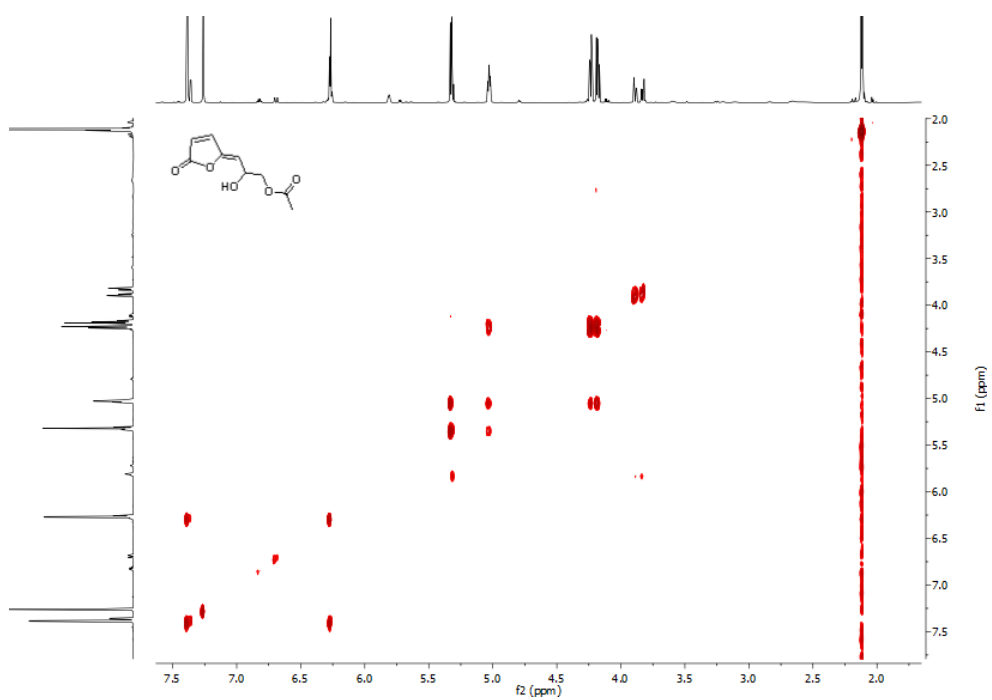


Figure S12. The COSY Spectrum of (Z)-7-Acetylsphaerodol (**2**) measured at 800 MHz in CDCl₃.

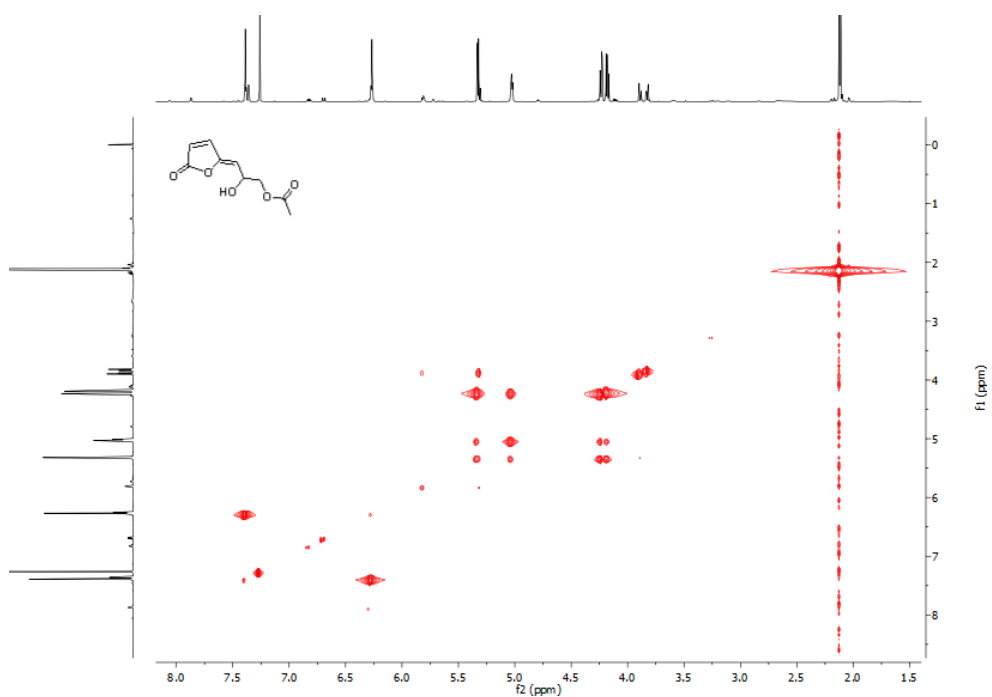


Figure S13. The TOCSY Spectrum of (Z)-7-Acetylsphaerodol (**2**) measured at 800 MHz in CDCl₃.

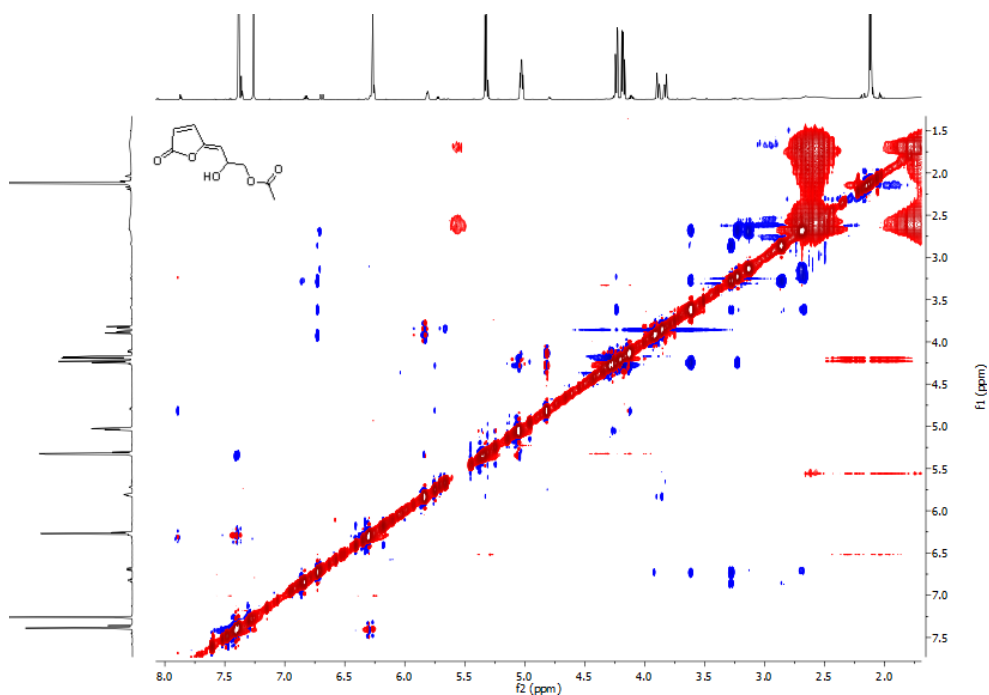


Figure S14. The NOESY Spectrum of (Z)-7-Acetylsphaerodol (**2**) measured at 800 MHz in CDCl₃.

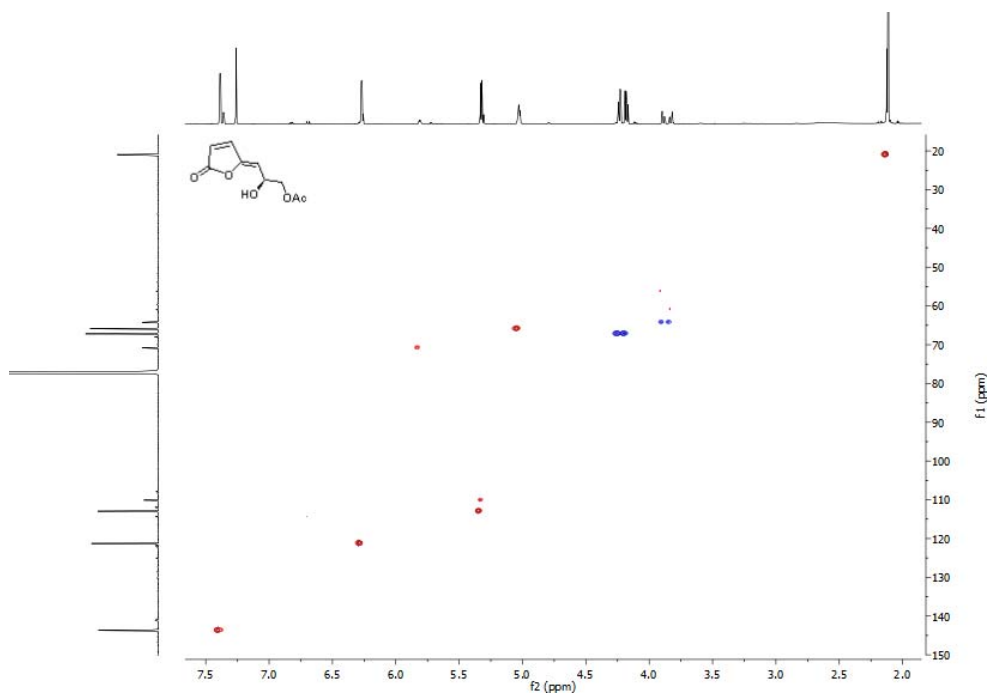


Figure S15. The HSQC Spectrum of (Z)-7-Acetylsphaerodol (**2**) measured at 800 MHz in CDCl₃.

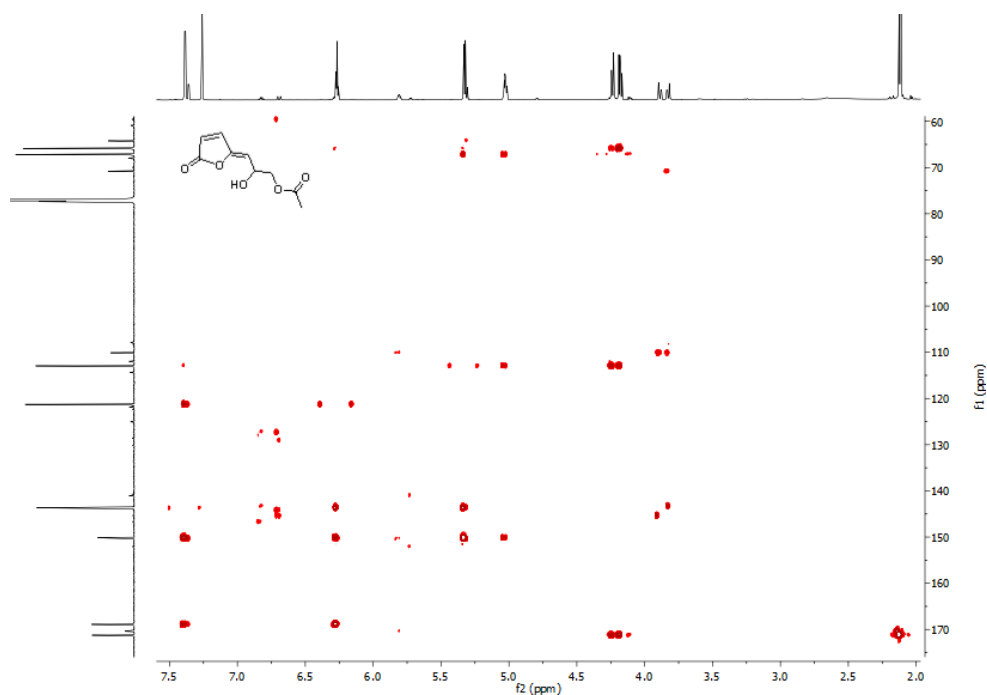


Figure S16. The HMBC Spectrum of (Z)-7-Acetylsphaerodol (**2**) measured at 800 MHz in CDCl₃.

0211462010e-004, t0=-3.08061476785442210e+001 (Turbo Spray)

M+H 199.0606

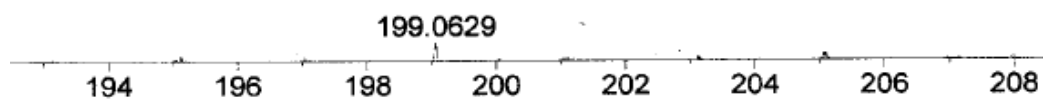


Figure S17. The HRESIMS Spectrum of (Z)-7-Acetylsphaerodiol (**2**).

Spectroscopic data for (Z)-2'-hydroxyacetylmelodorinol (3)

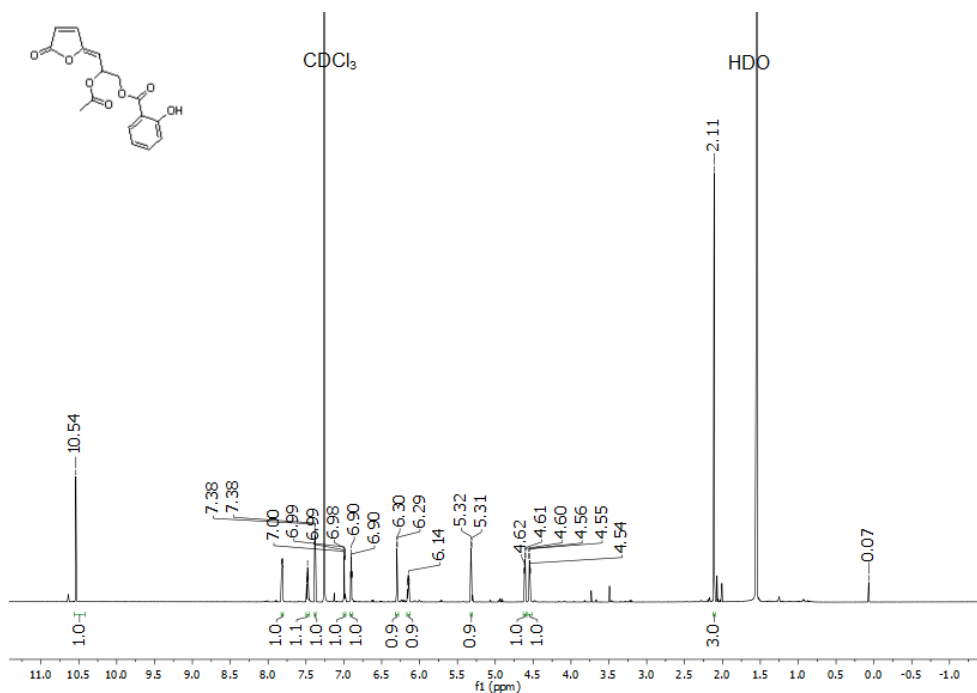


Fig S18. The ¹H NMR Spectrum of (Z)-2'-Hydroxyacetylmelodorinol (**3**) measured at 800 MHz in CDCl₃.

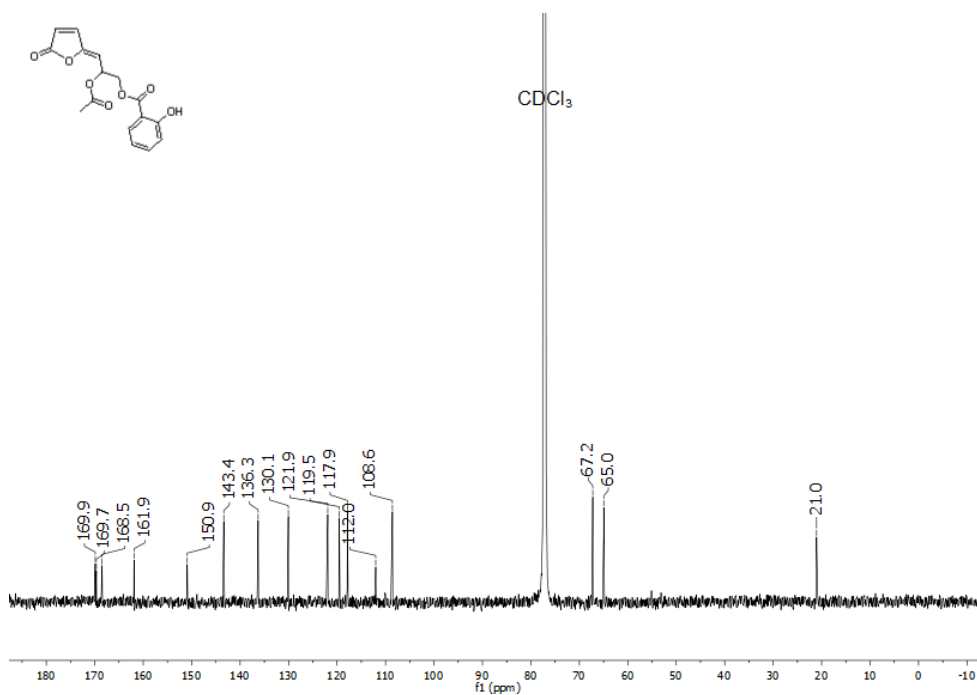


Figure S19. The ¹³C NMR Spectrum of (Z)-2'-Hydroxyacetylmelodorinol (**3**) measured at 800 MHz in CDCl₃.

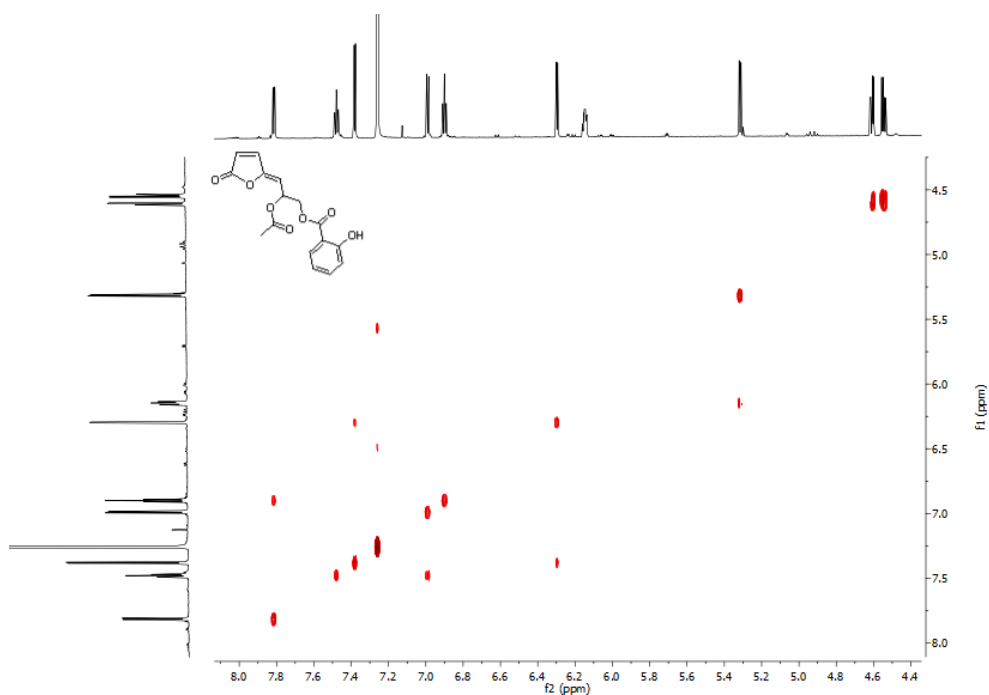


Figure S20. The COSY Spectrum of (Z)-2'-Hydroxyacetylmelodorinol (**3**) measured at 800 MHz in CDCl₃.

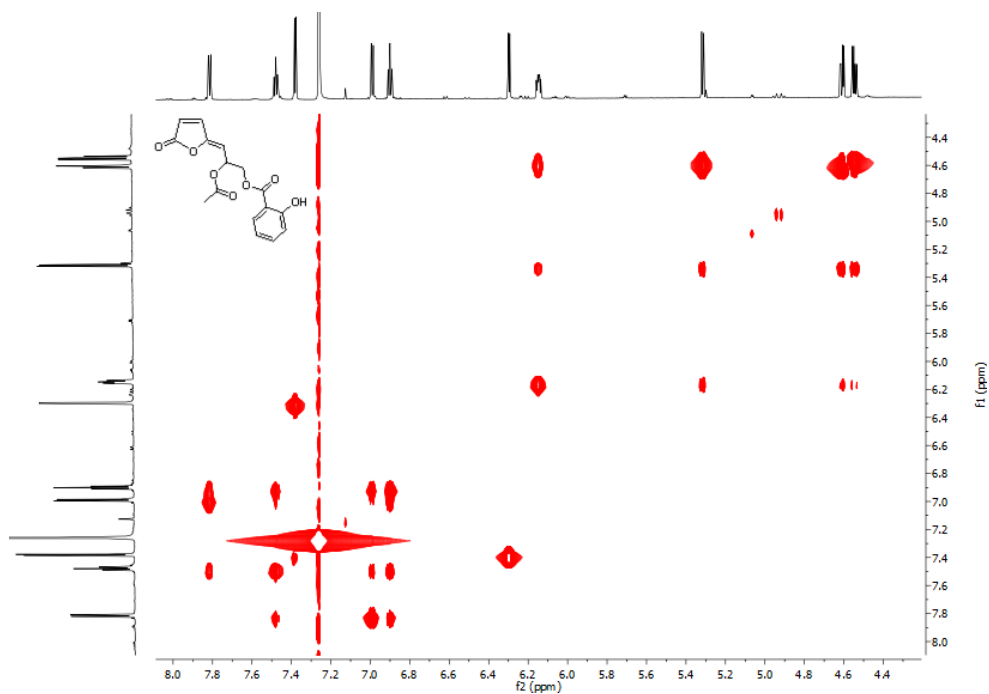


Figure S21. The TOCSY Spectrum of (Z)-2'-Hydroxyacetylmelodorinol (**3**) measured at 800 MHz in CDCl₃.

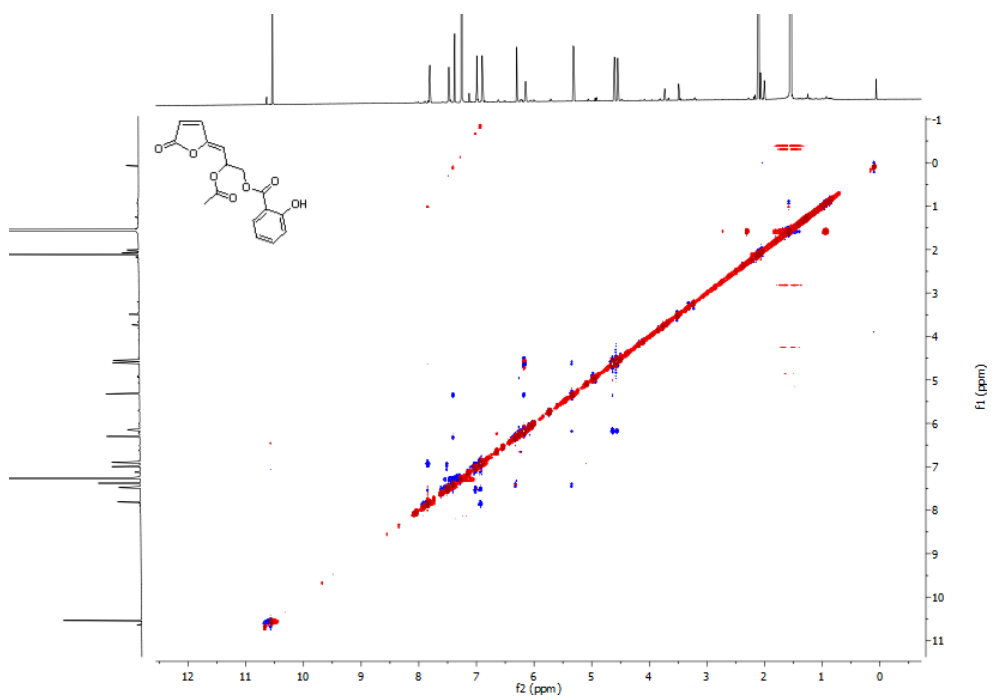


Figure S22. The NOESY Spectrum of (Z)-2'-Hydroxyacetylmelodrinol (**3**) measured at 800 MHz in CDCl₃.

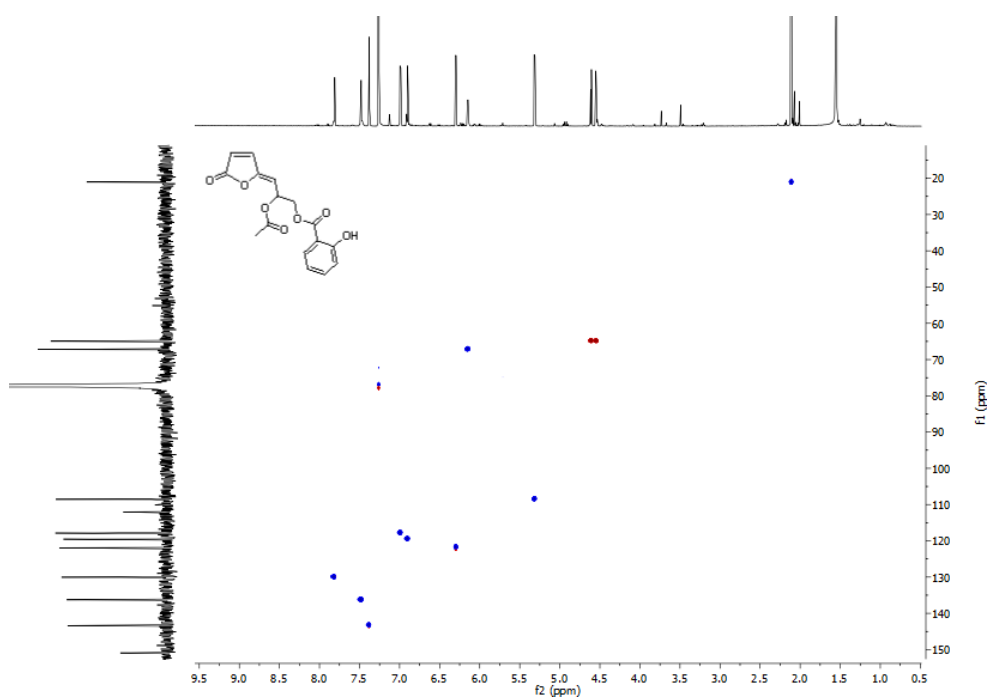


Figure S23. The HSQC Spectrum of (Z)-2'-Hydroxyacetylmelodrinol (**3**) measured at 800 MHz in CDCl₃.

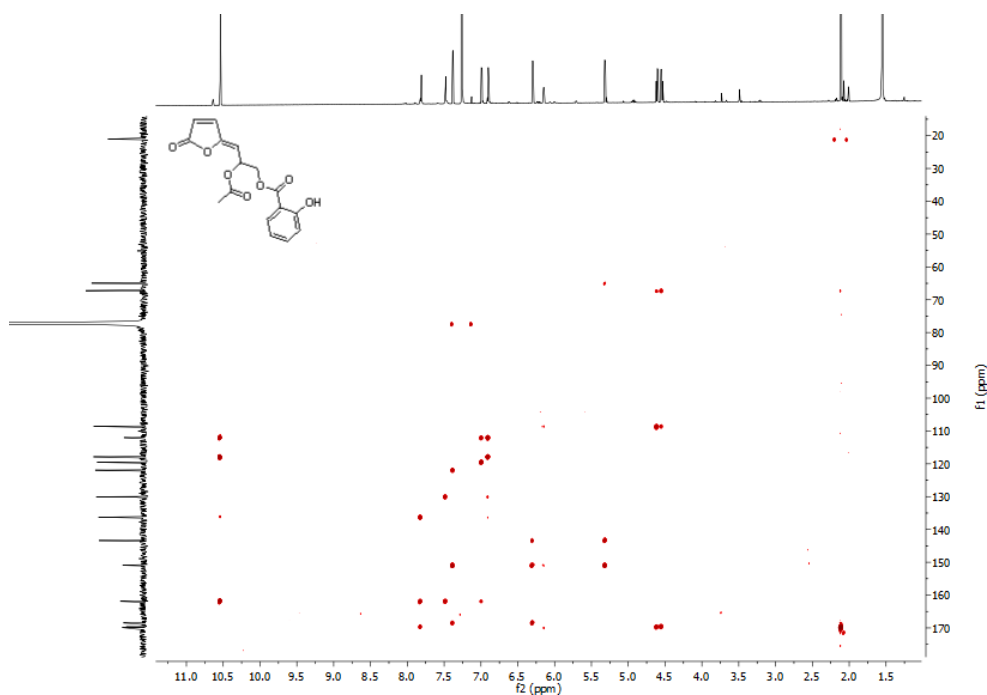


Figure S24. The HMBC Spectrum of (Z)-2'-Hydroxyacetylmelodorinol (**3**) measured at 800 MHz in CDCl_3 .

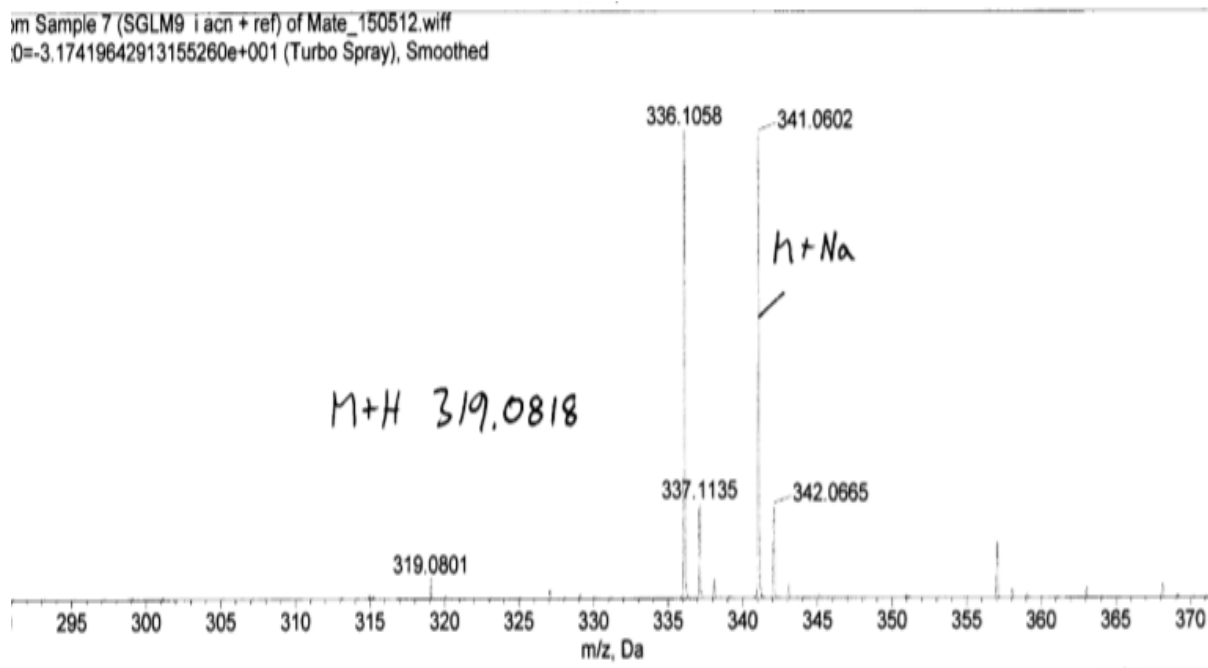


Figure S25. The HRESIMS of (Z)-2'-Hydroxyacetylmelodorinol (**3**).

Spectroscopic data for 3''-hydroxyisochamanetin (4)

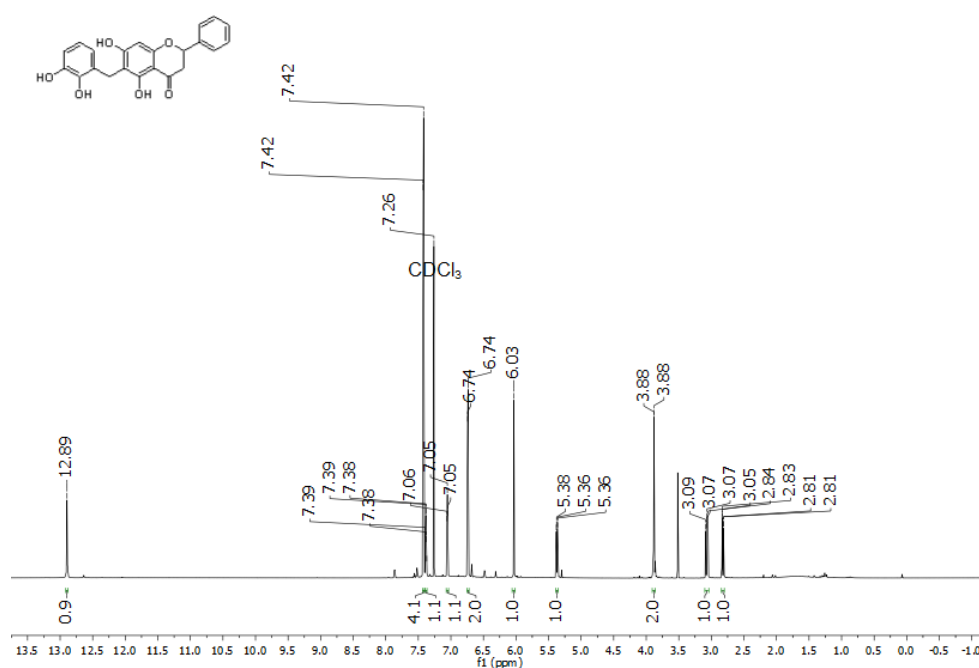


Figure S26. The ¹H NMR Spectrum of 3''-Hydroxyisochamanetin (4) measured at 800 MHz in CDCl₃.

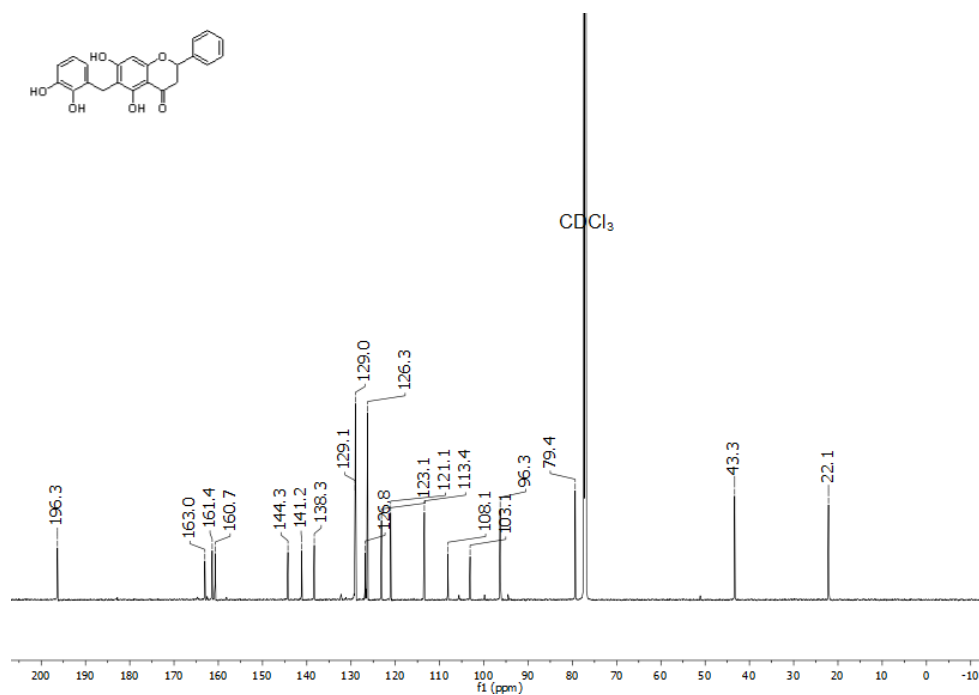


Figure S27. The ¹³C NMR Spectrum of 3''-Hydroxyisochamanetin (4) measured at 800 MHz in CDCl₃.

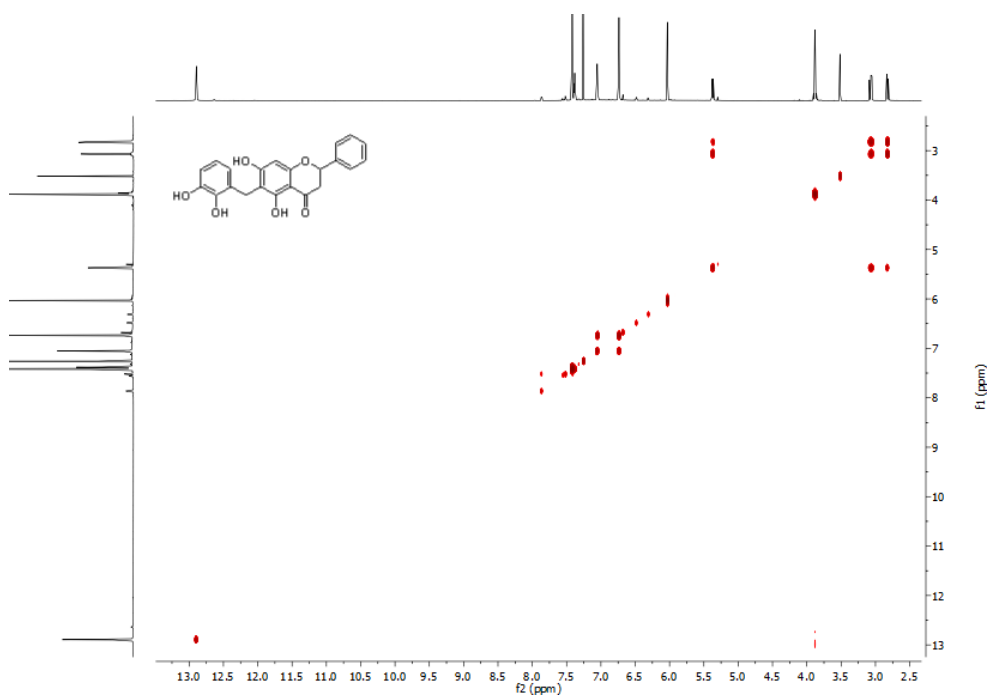


Figure S28. The COSY Spectrum of 3''-Hydroxyisochamanetin (**4**) measured at 800 MHz in CDCl₃.

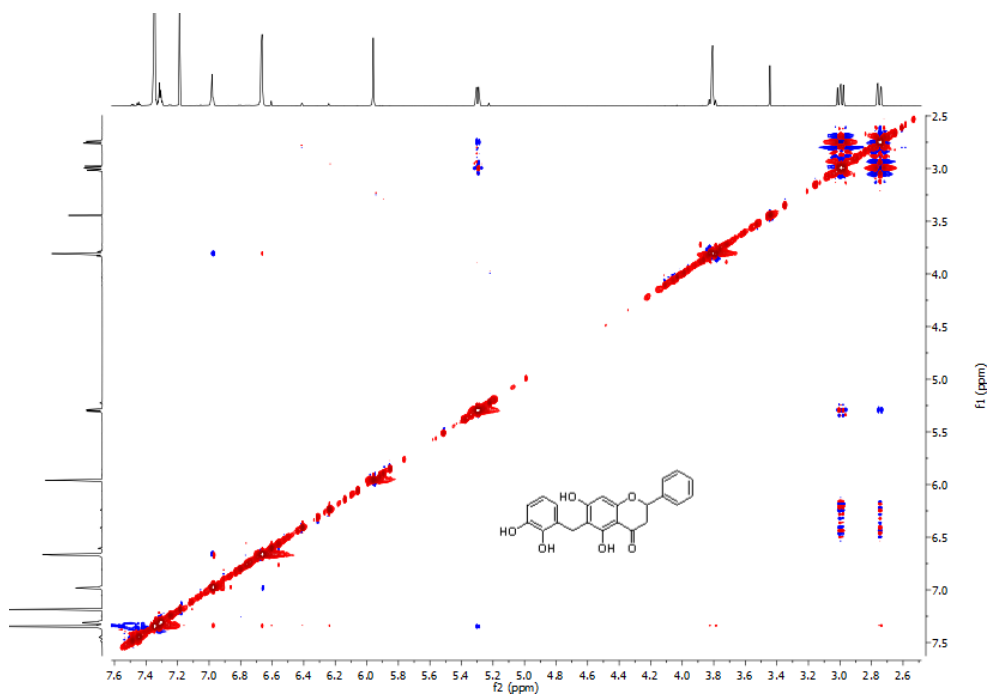


Figure S29. The NOESY Spectrum of 3''-Hydroxyisochamanetin (**4**) measured at 800 MHz in CDCl₃.

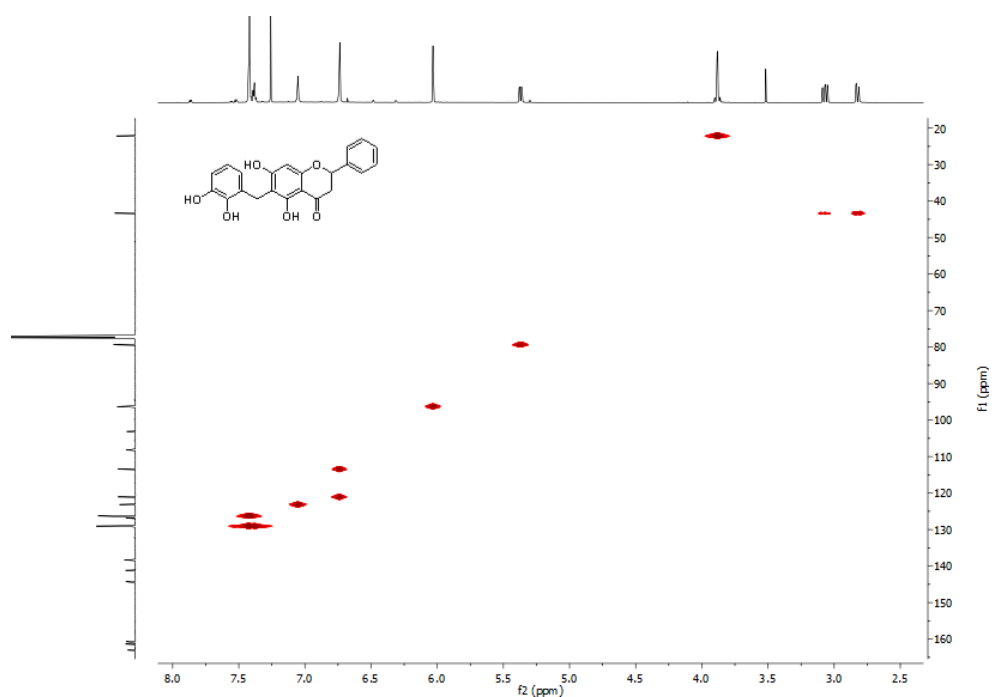


Figure S30. The HSQC Spectrum of 3''-Hydroxyisochamanetin (**4**) measured at 800 MHz in CDCl₃.

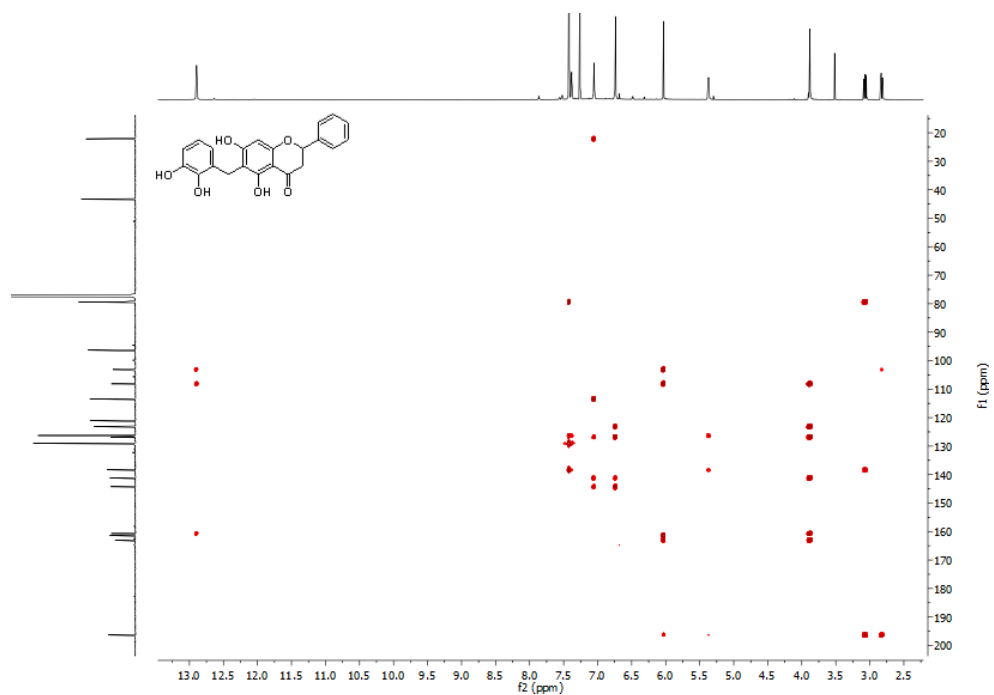


Figure S31. The HMBC Spectrum of 3''-Hydroxyisochamanetin (**4**) measured at 800 MHz in CDCl₃.

ple 2 (SGLM11.acn + ref) of Mate_150512.wiff
t0=-3.18751866987659010e+001 R; (Turbo Spray)

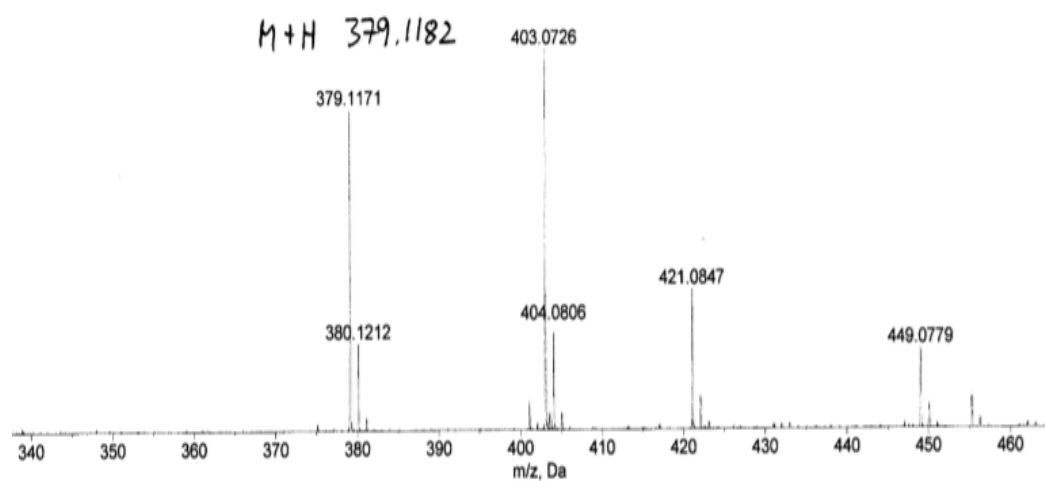


Figure S32. The HRESIMS of 3''-Hydroxyisochamanetin (**4**).

Spectroscopic data for 2,3-dehydro-3''-hydroxychamanetin (5)

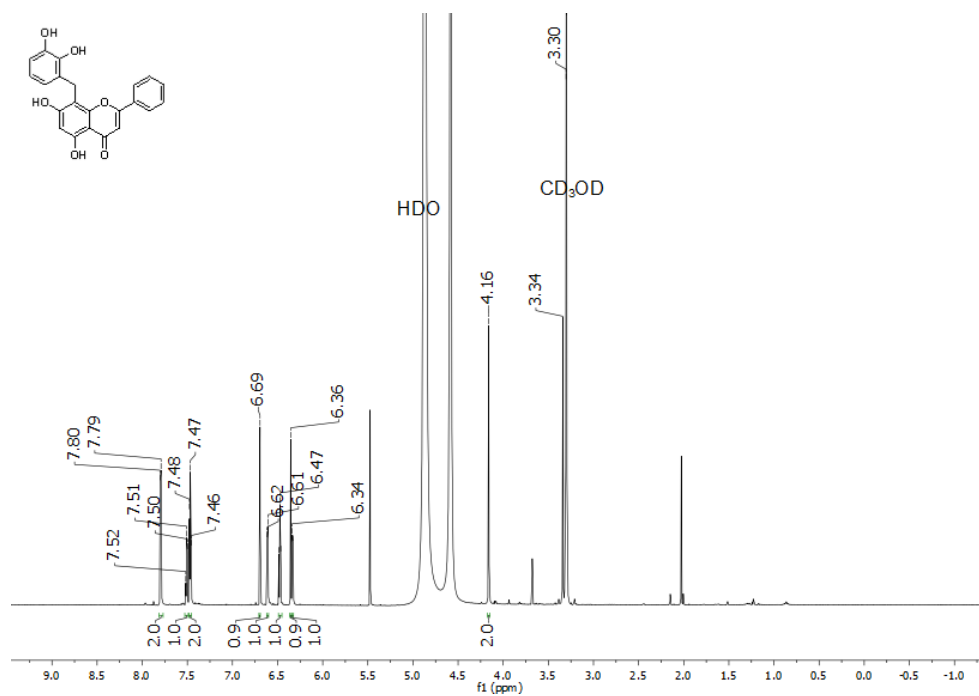


Fig S33. The ¹H NMR Spectrum of 2,3-dehydro-3''-hydroxychamanetin (5) measured at 800 MHz in CD₃OD.

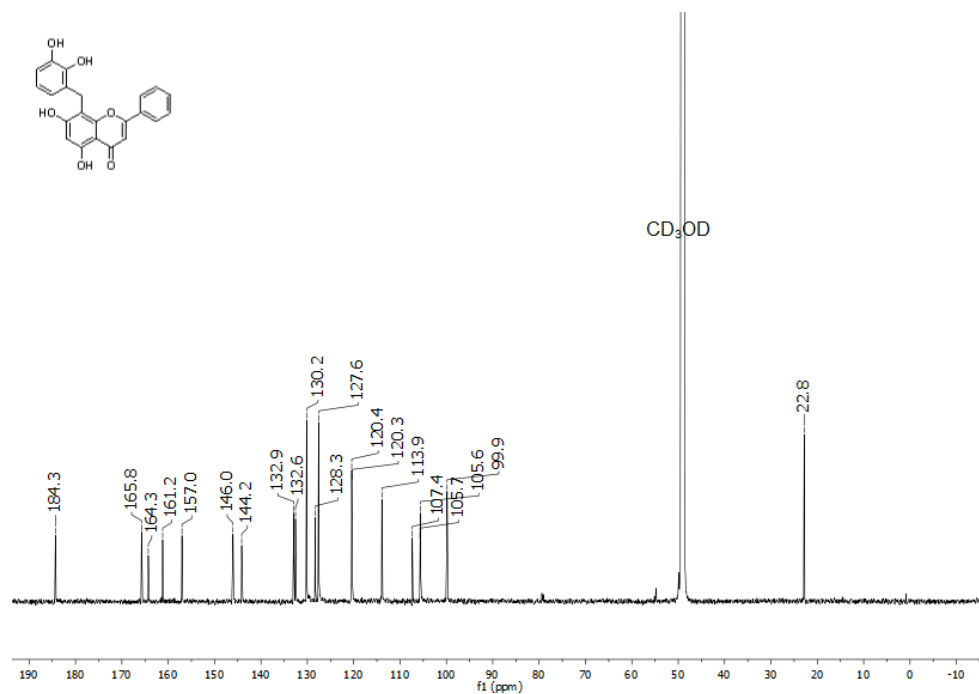


Figure S34. The ¹³C NMR Spectrum of 2,3-dehydro-3''-hydroxychamanetin (5) measured at 800 MHz in CD₃OD.

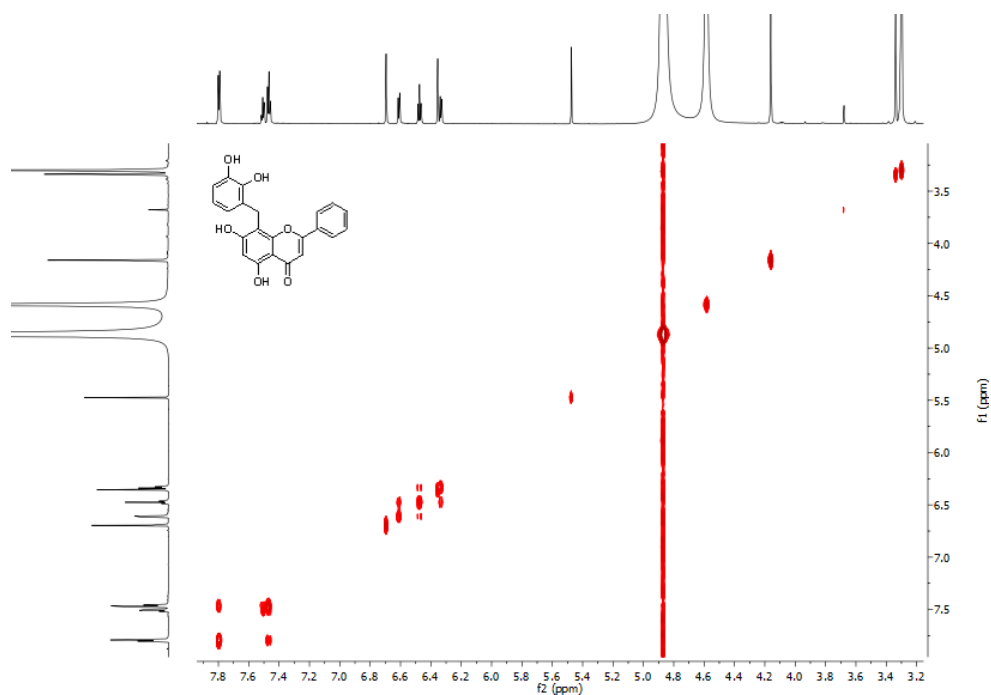


Figure S35. The COSY Spectrum of 2,3-dehydro-3''-hydroxychamanetin (**5**) measured at 800 MHz in CD₃OD.

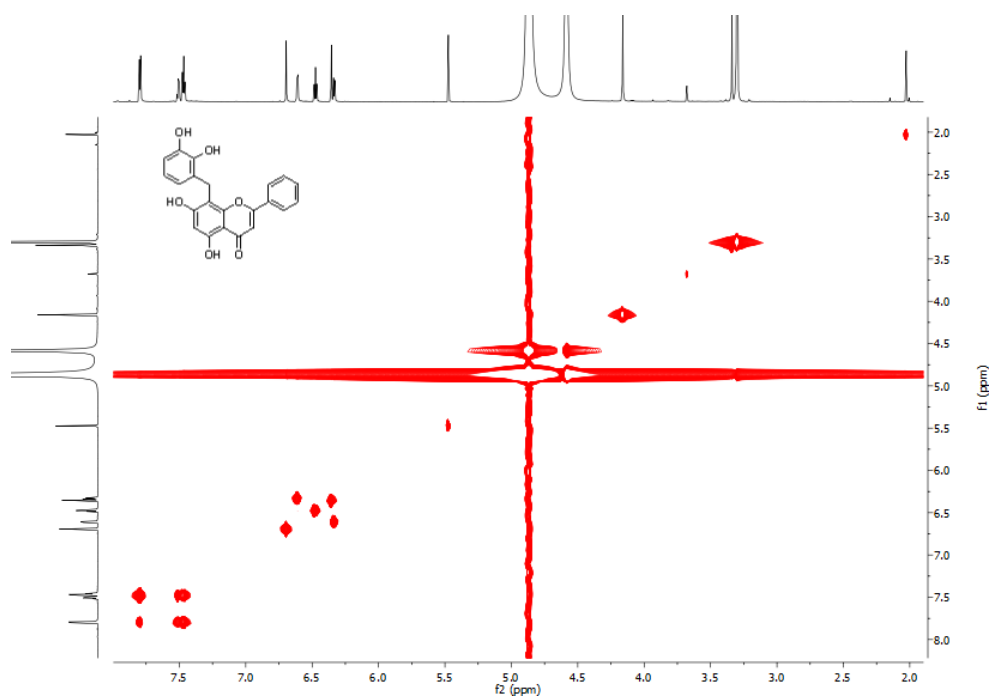


Figure S36. The TOCSY Spectrum of 2,3-dehydro-3''-hydroxychamanetin (**5**) measured at 800 MHz in CD₃OD.

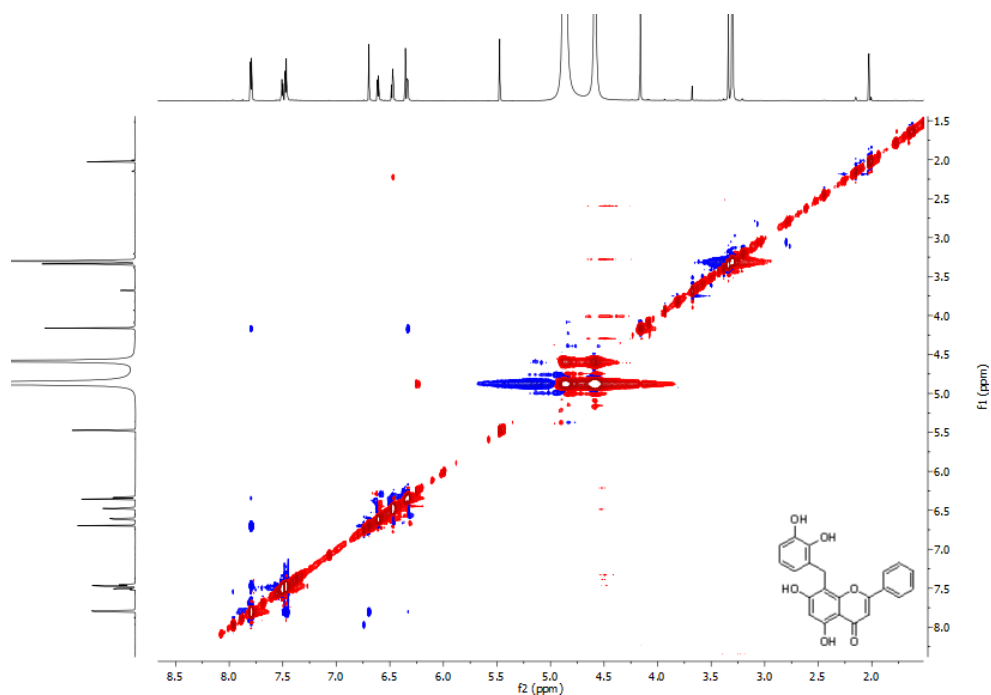


Figure S37. The NOESY Spectrum of 2,3-dehydro-3''-hydroxychamanetin (**5**) measured at 800 MHz in CD₃OD.

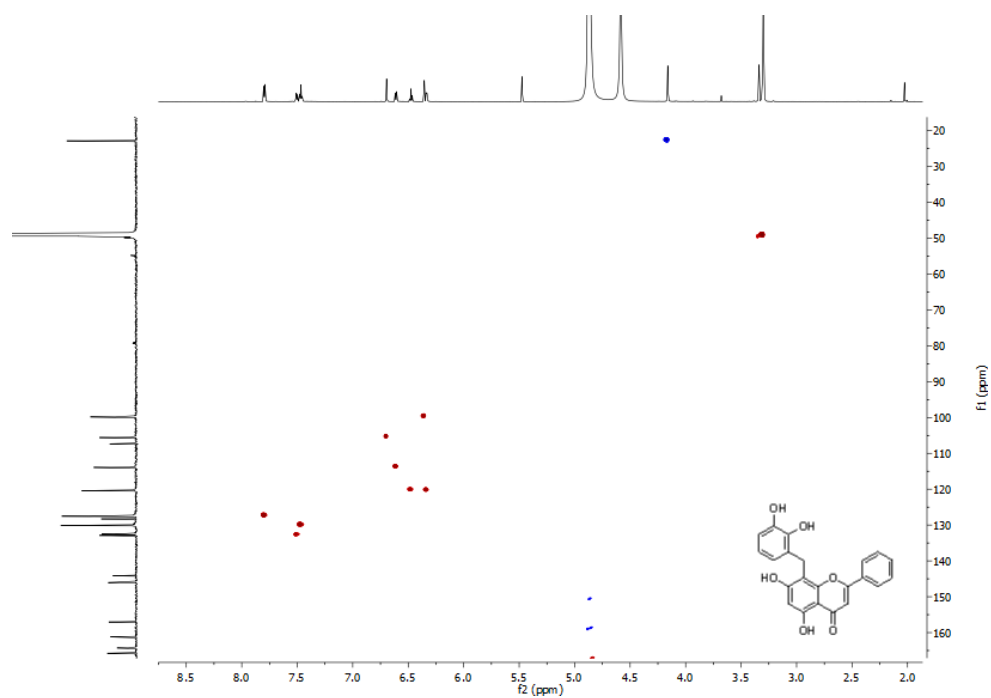


Figure S38. The HSQC Spectrum of 2,3-dehydro-3''-hydroxychamanetin (**5**) measured at 800 MHz in CD₃OD.

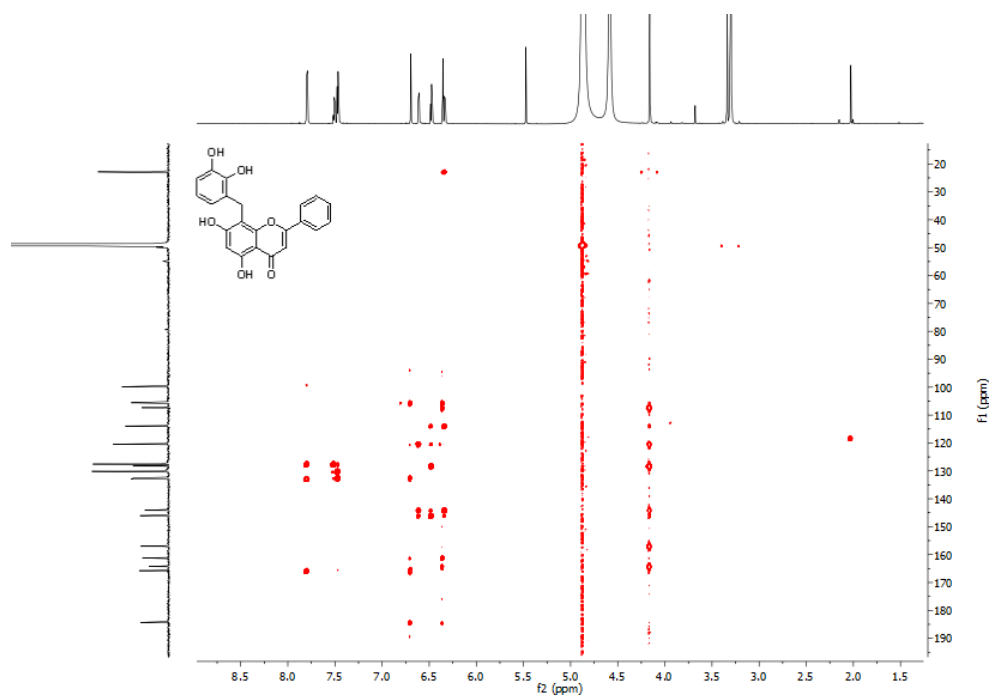


Figure S 39. The HMBC Spectrum of 2,3-dehydro-3''-hydroxychamanetin (**5**) measured at 800 MHz in CD₃OD.

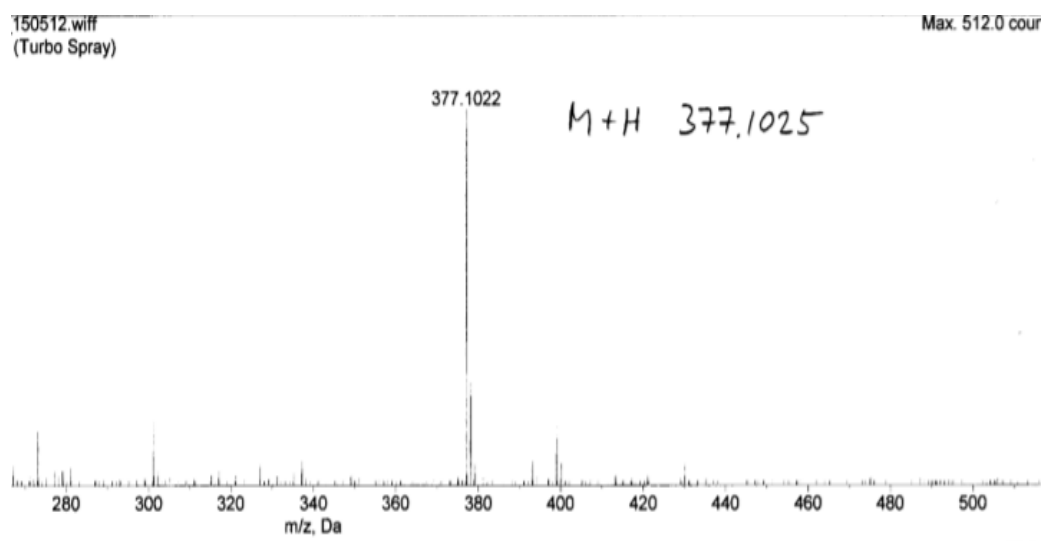
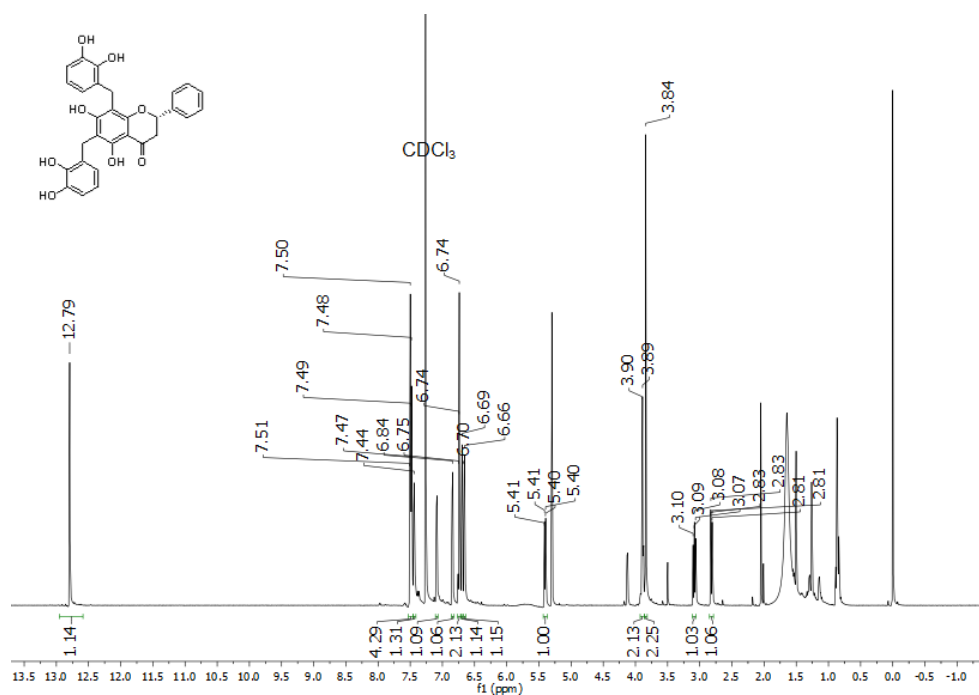


Figure S40. The HRESIMS of 2,3-dehydro-3''-hydroxychamanetin (**5**).

Spectroscopic data for 3''-hydroxygracinol (6)



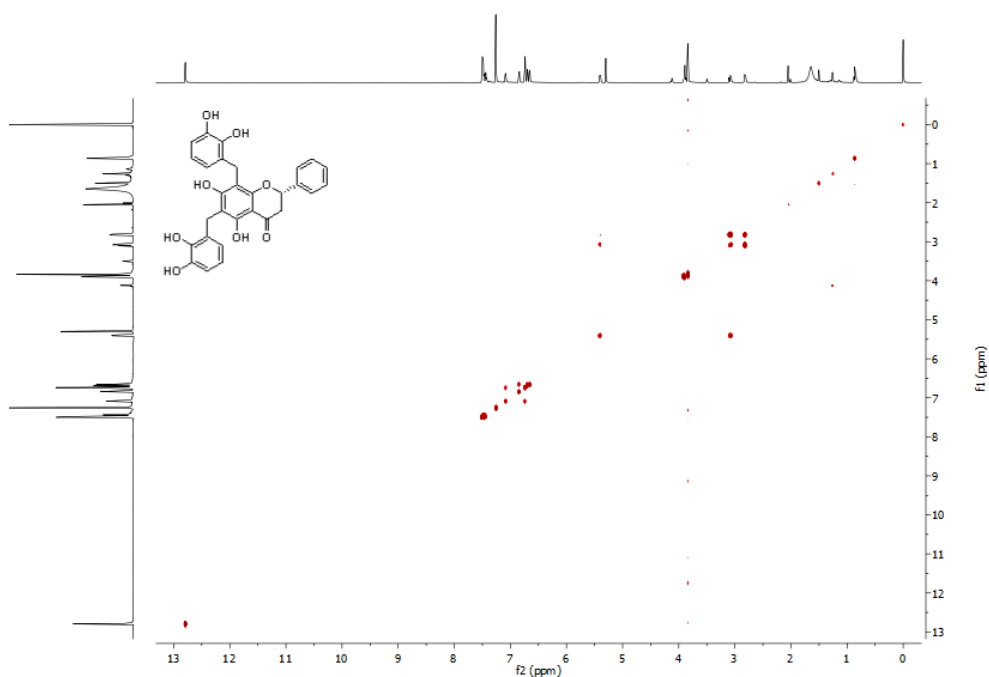


Figure S43. The COSY Spectrum of 3''-Hydroxygracilinol (**6**) measured at 800 MHz in CDCl₃.

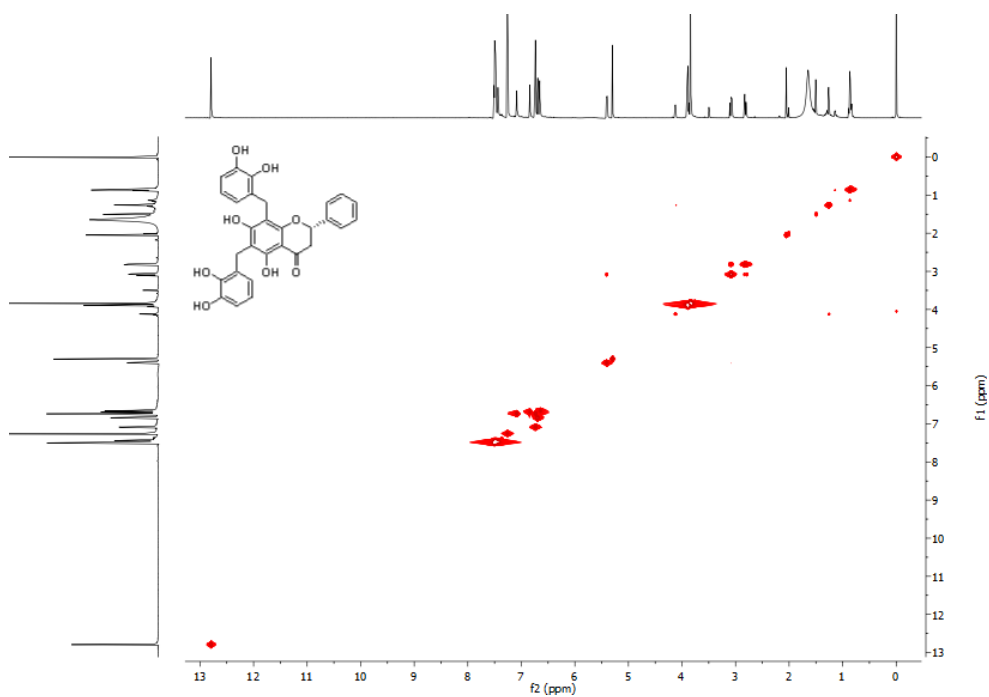


Figure S44. The TOCSY Spectrum of 3''-Hydroxygracilinol (**6**) measured at 800 MHz in CDCl₃.

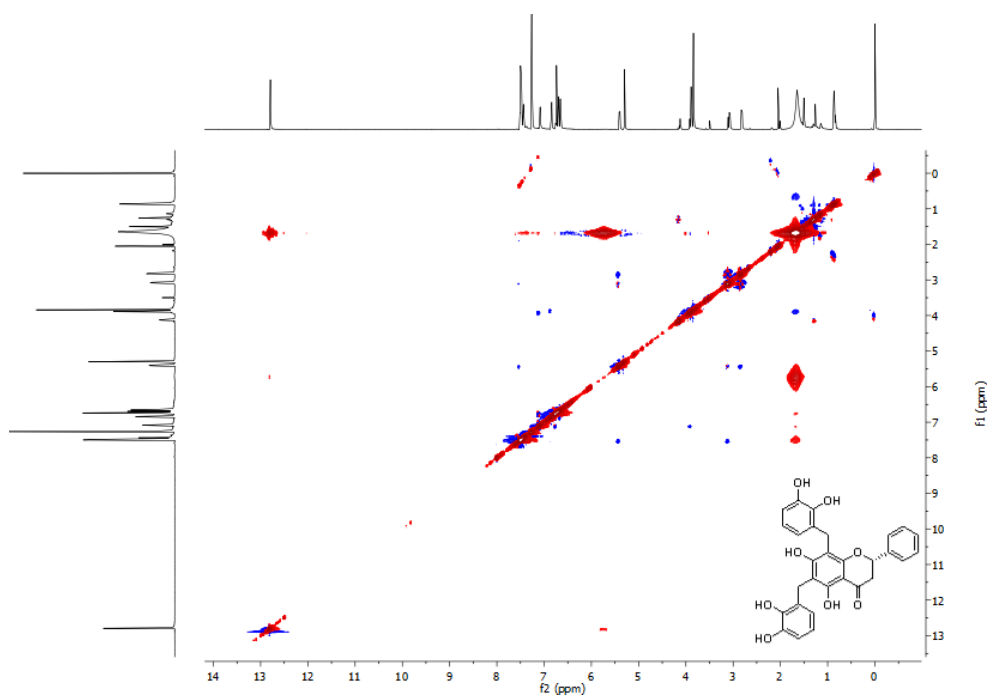


Figure S45. The NOESY Spectrum of 3''-Hydroxygracinol (**6**) measured at 800 MHz in CDCl₃.

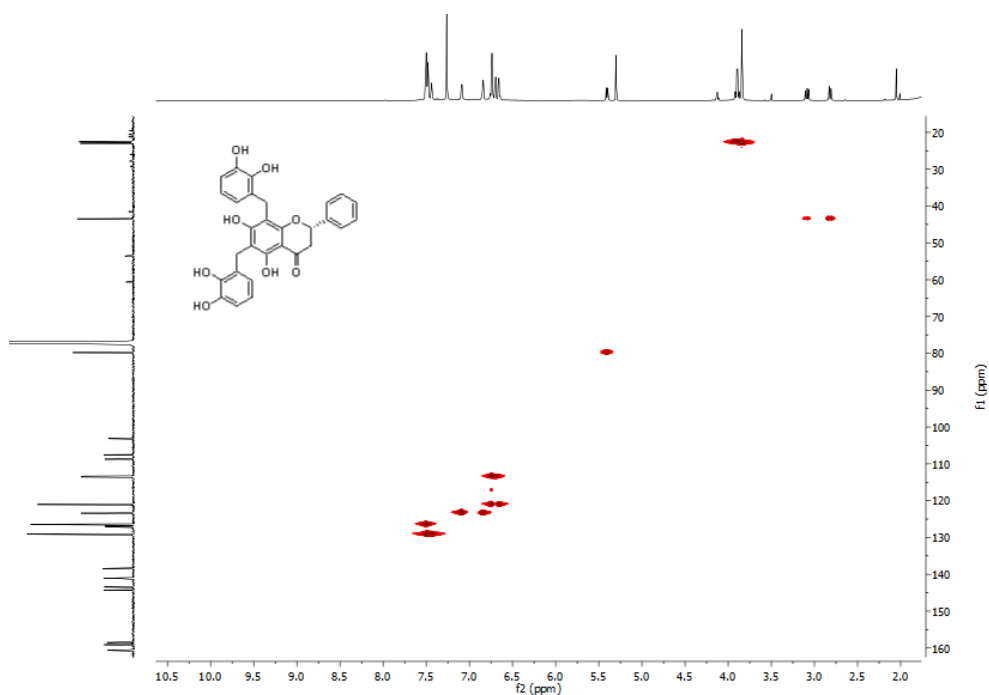


Figure S46. The HSQC Spectrum of 3''-Hydroxygracinol (**6**) measured at 800 MHz in CDCl₃.

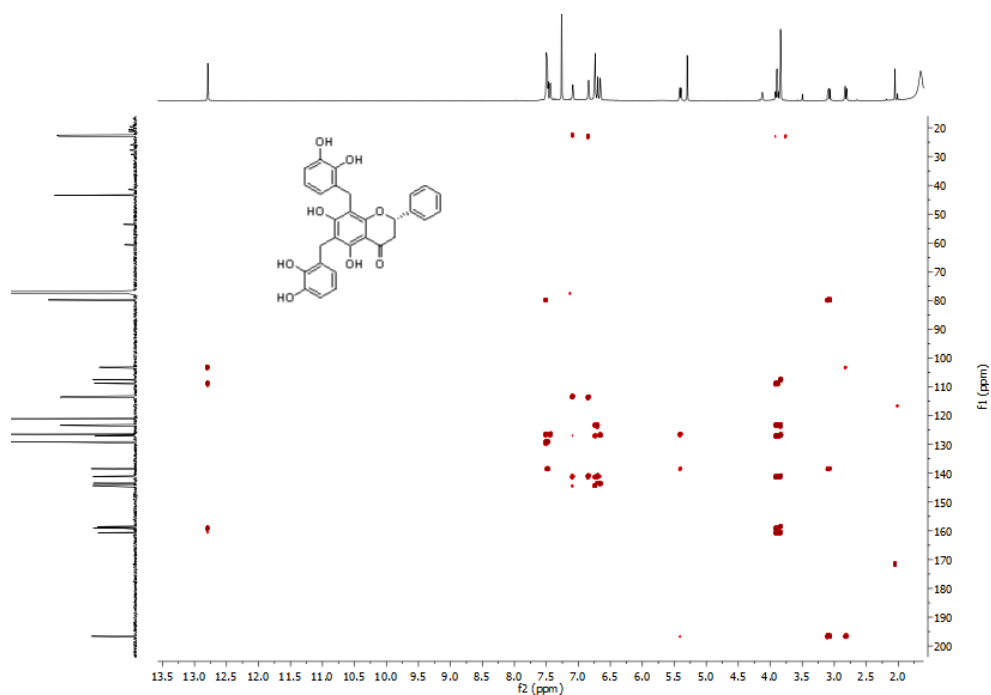


Figure S47. The HMBC Spectrum of 3''-Hydroxygracinol (6) measured at 800 MHz in CDCl_3 .

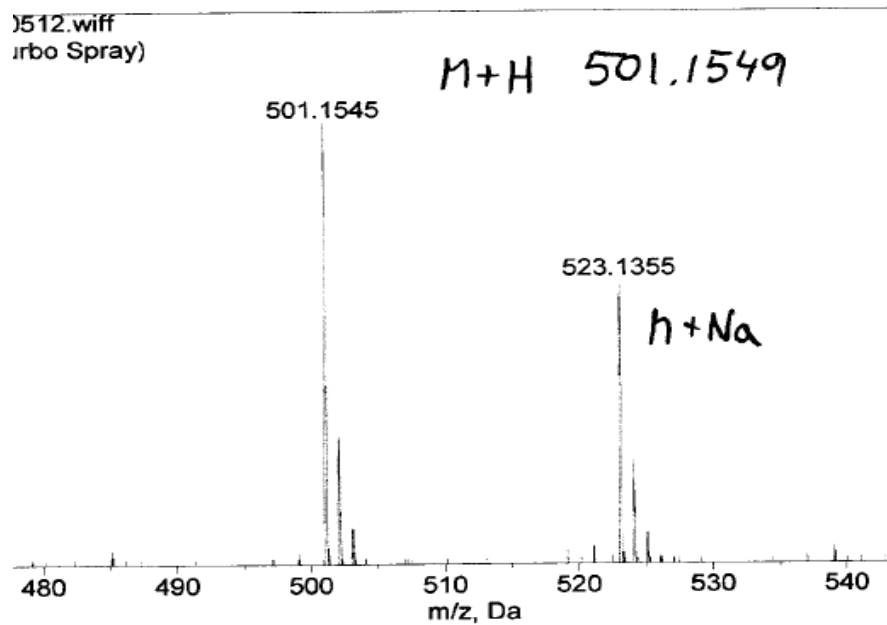


Figure S48. The HRESIMS of 3''-Hydroxygracinol (6).

Spectroscopic data for (Z)-sphaerodiol (7)

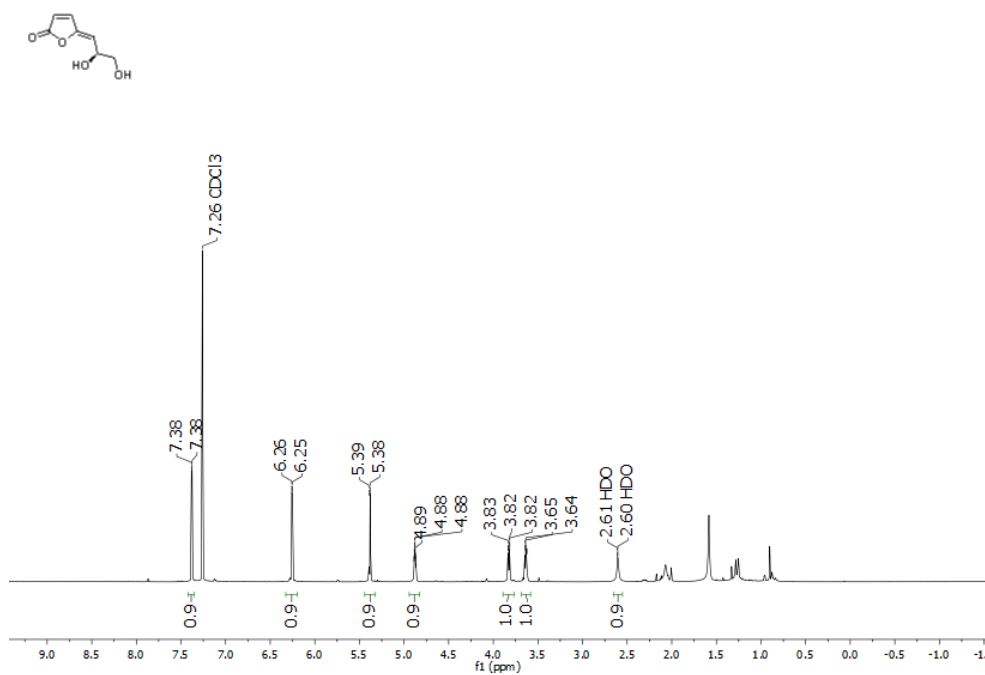


Figure S49. The ¹H NMR Spectrum of (Z)-Sphaerodiol (7) measured at 800 MHz in CDCl₃.

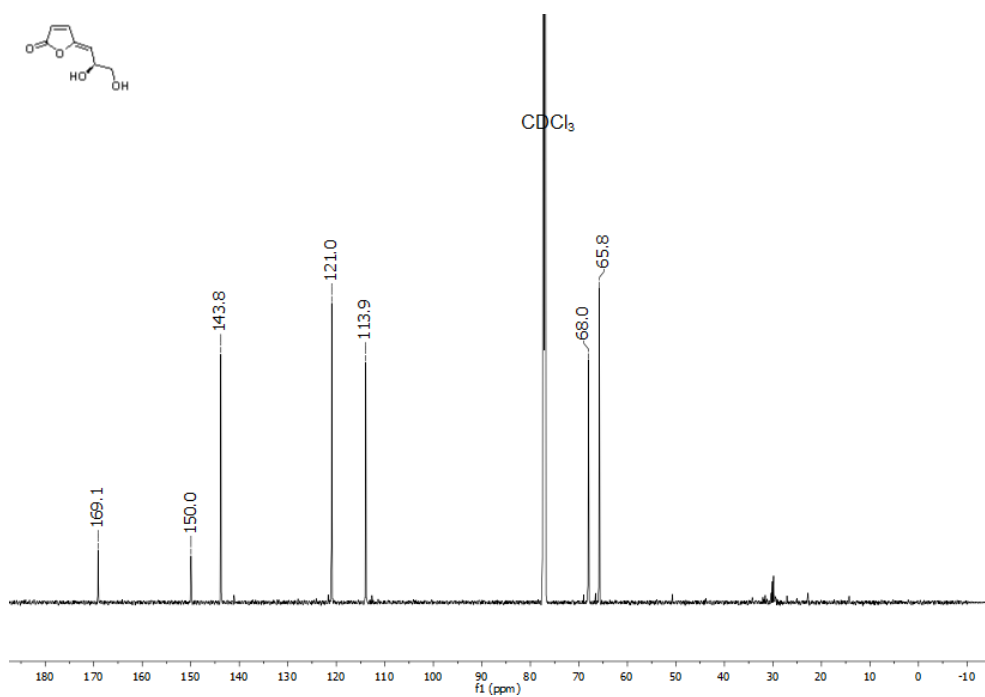


Figure S50. The ¹³C NMR Spectrum of (Z)-Sphaerodiol (7) measured at 800 MHz in CDCl₃.

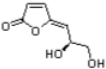


Figure S51. The COSY Spectrum of (Z)-Sphaerodiol (**7**) measured at 800 MHz in CDCl₃.

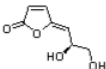


Figure S52. The TOCSY Spectrum of (Z)-Sphaerodiol (**7**) measured at 800 MHz in CDCl₃.

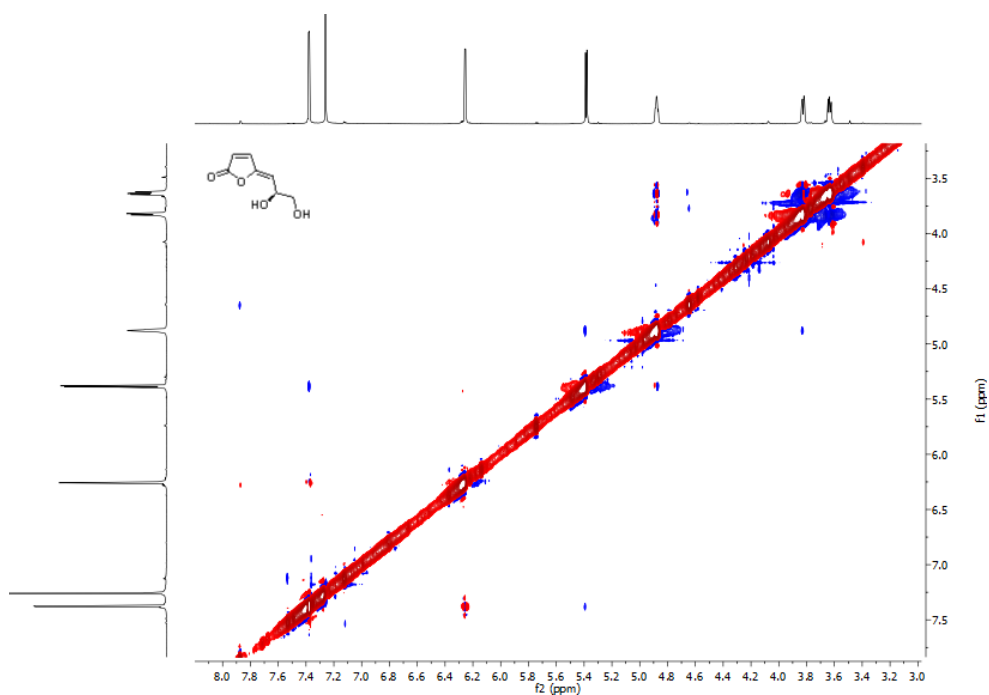


Figure S53. The NOESY Spectrum of (Z)-Sphaerodiol (7) measured at 800 MHz in CDCl₃.

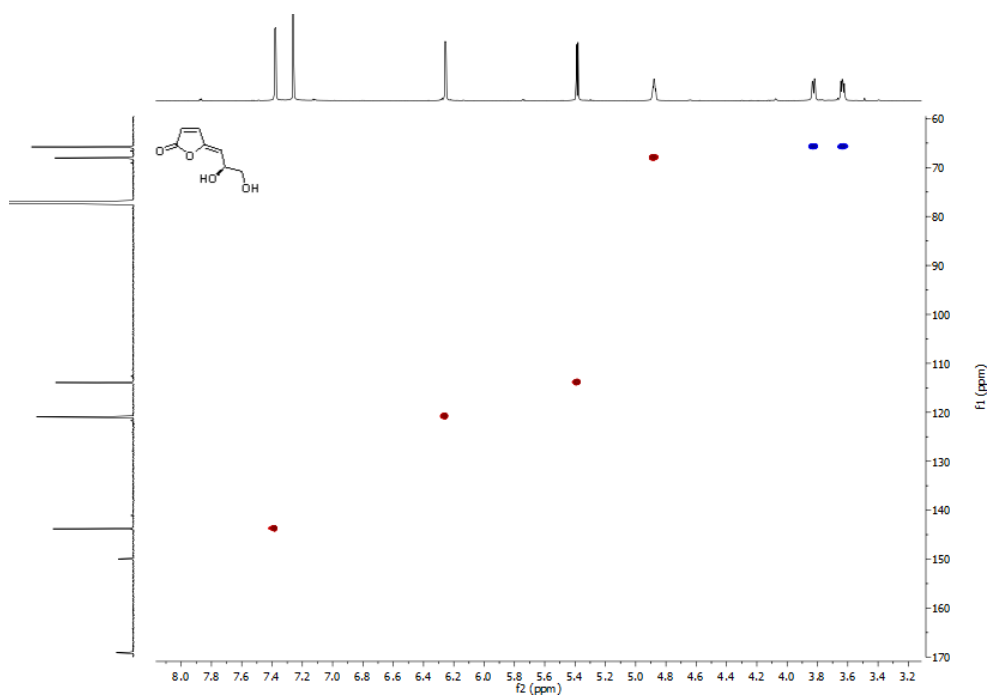


Figure S54. The HSQC Spectrum of (Z)-Sphaerodiol (7) measured at 800 MHz in CDCl₃.

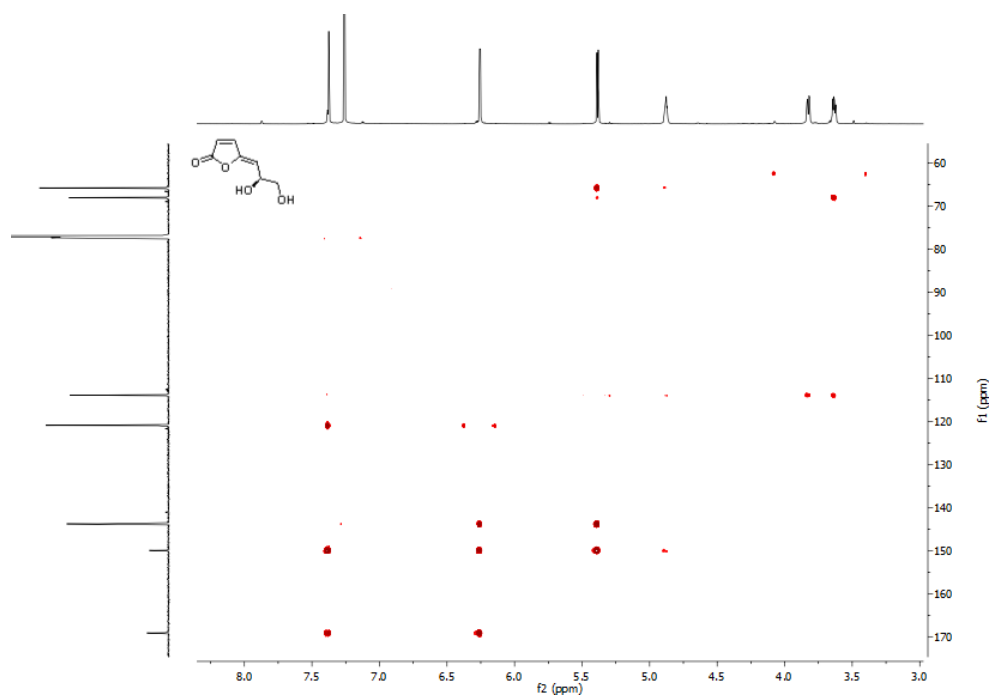


Figure S55. The HMBC Spectrum of (Z)-Sphaerodiol (7) measured at 800 MHz in CDCl_3 .

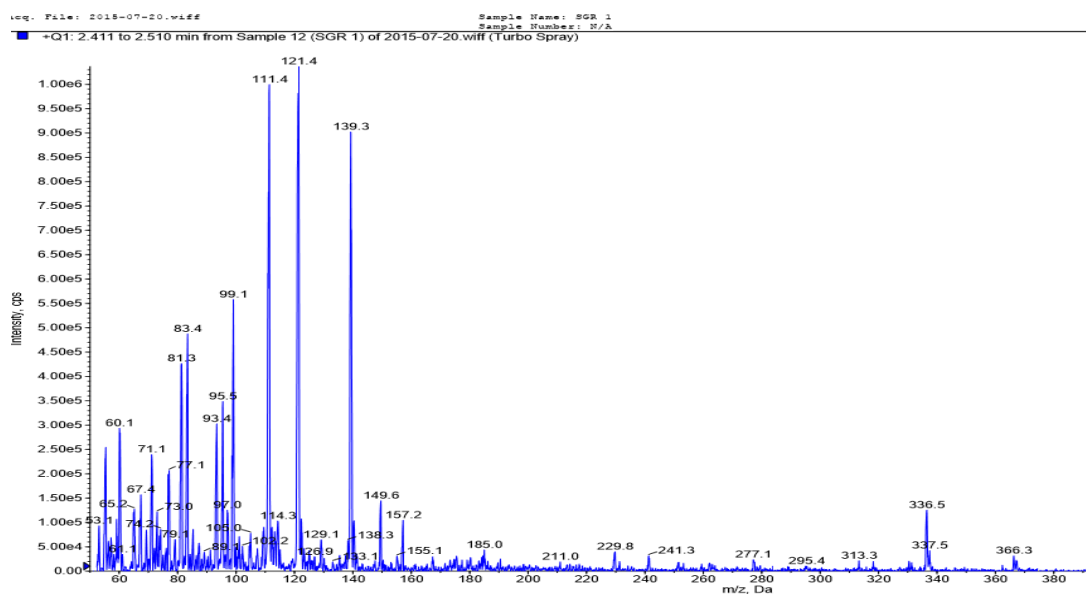


Figure S56. The LC-MS of (Z)-Sphaerodiol (7).

Spectroscopic data for (Z)-acetylmelodorinol (**8**)

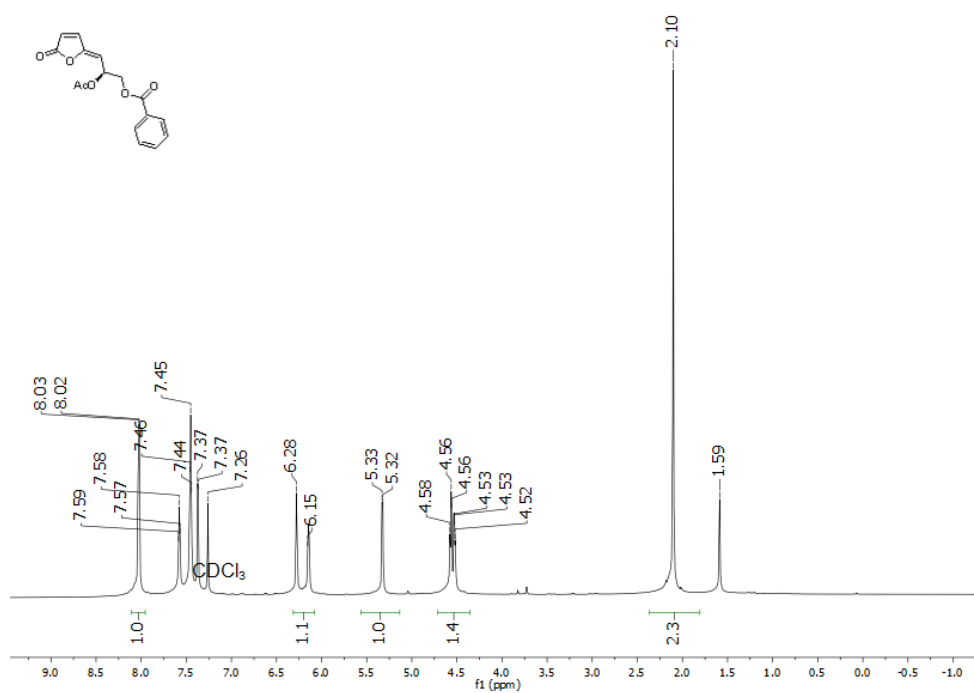


Figure S57. The ¹H NMR Spectrum of (Z)-Acetylmelodorinol (**8**) measured at 800 MHz in CDCl₃.

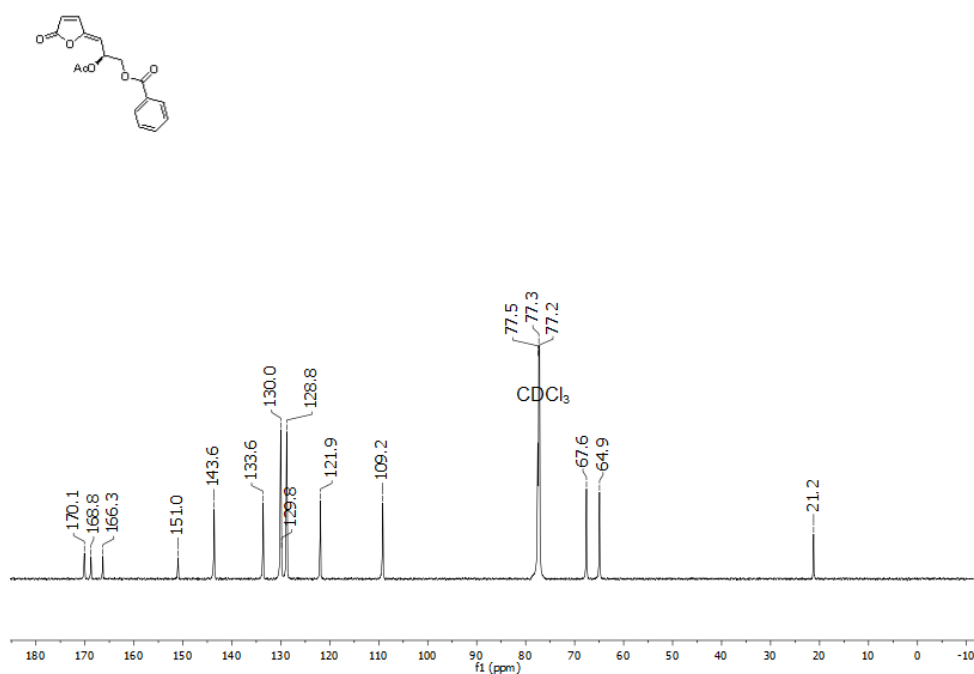


Figure S58. The ¹³C NMR Spectrum of (Z)-Acetylmelodorinol (**8**) measured at 800 MHz in CDCl₃.

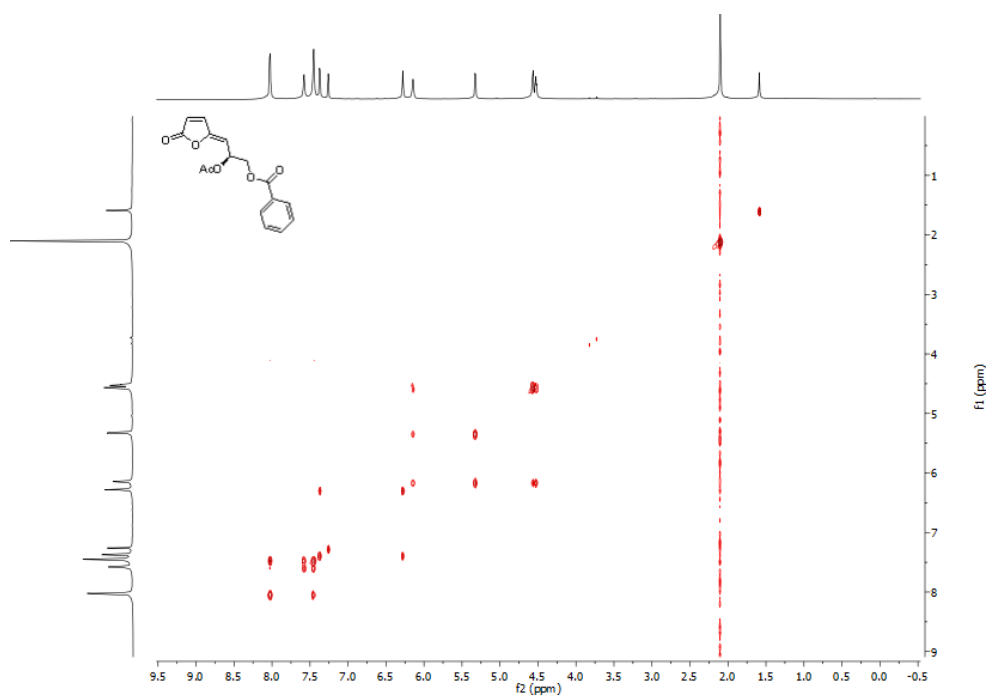


Figure S59. The COSY Spectrum of (Z)-Acetylmelodorinol (**8**) measured at 800 MHz in CDCl₃.

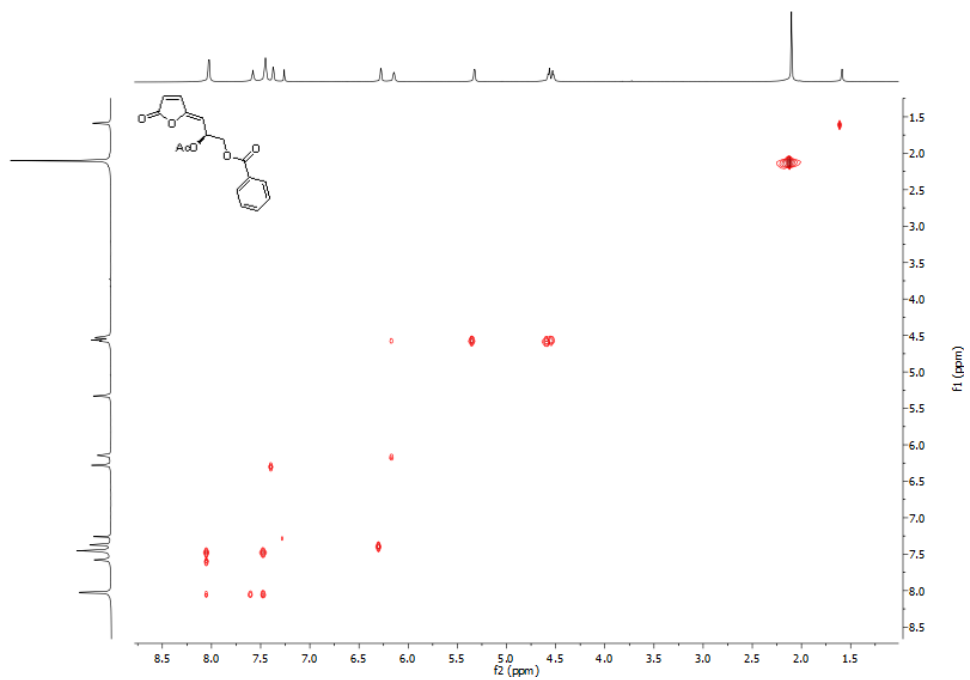


Figure S60. The TOCSY Spectrum of (Z)-Acetylmelodorinol (**8**) measured at 800 MHz in CDCl₃.

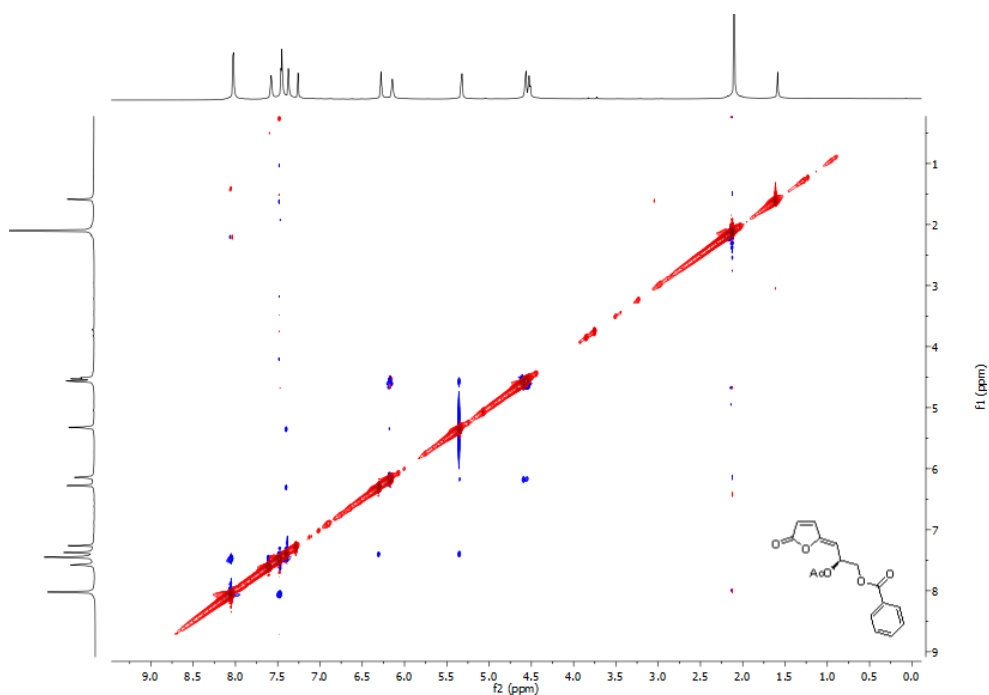


Figure S61. The NOESY Spectrum of (Z)-Acetylmelodorinol (**8**) measured at 800 MHz in CDCl₃.

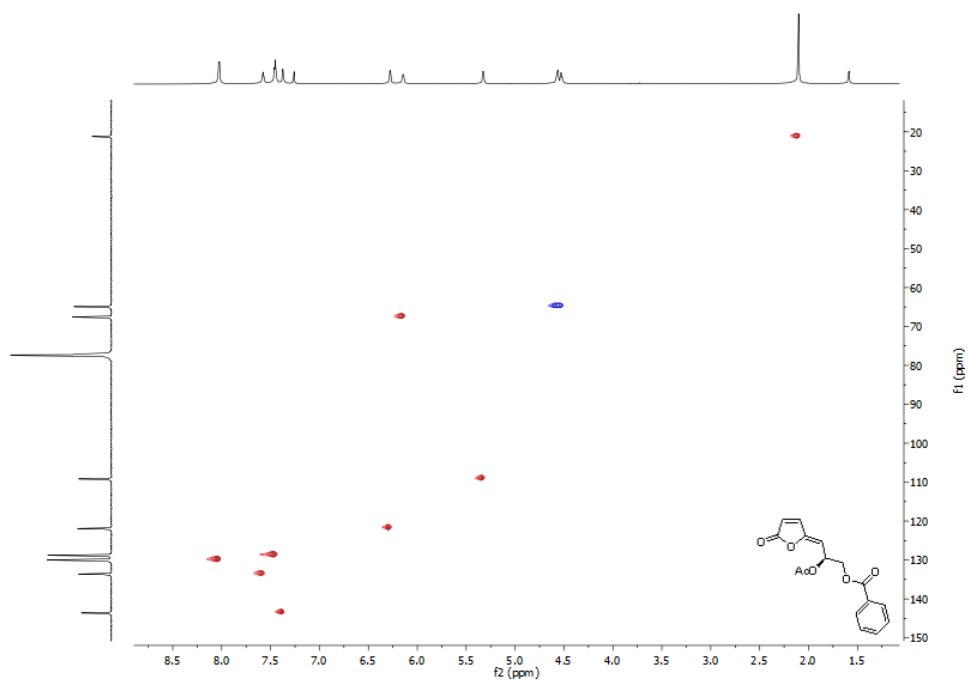


Figure S62. The HSQC Spectrum of (Z)-Acetylmelodorinol (**8**) measured at 800 MHz in CDCl₃.

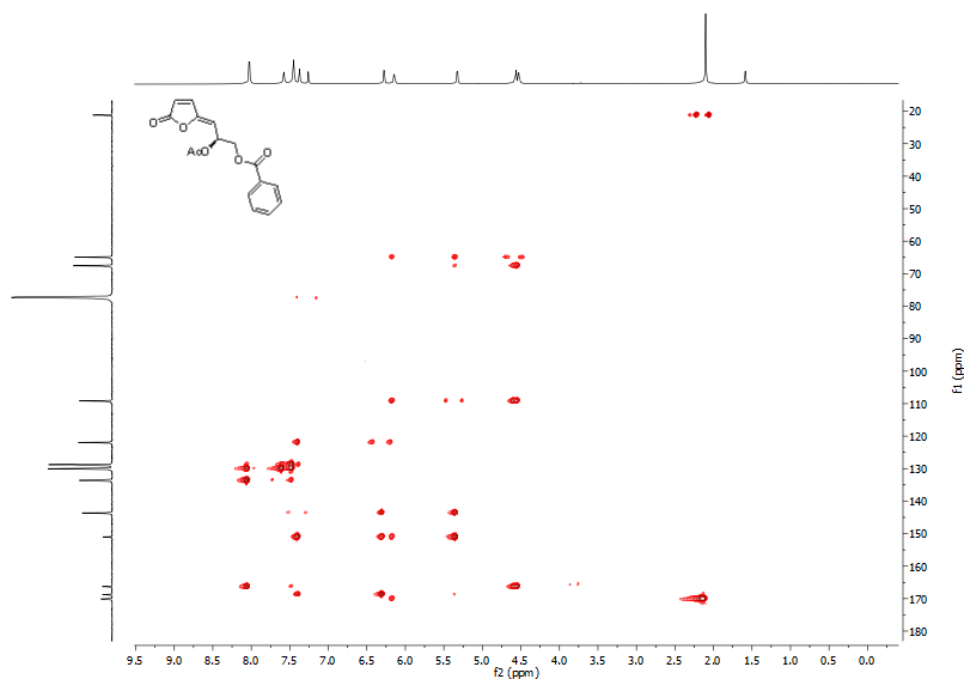


Figure S63. The HMBC Spectrum of (Z)-Acetylmelodorinol (**8**) measured at 800 MHz in CDCl₃.

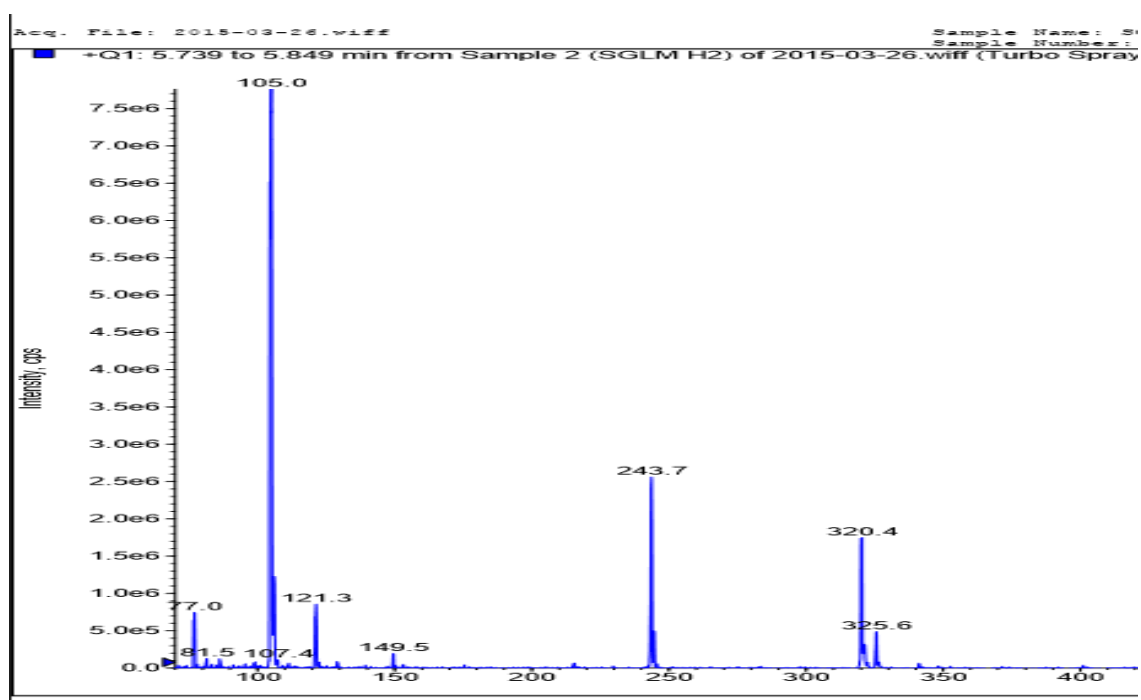


Figure S64. The LC-MS of (Z)-Acetylmelodorinol (**8**).

Spectroscopic data for (Z)-melodorinol (9)

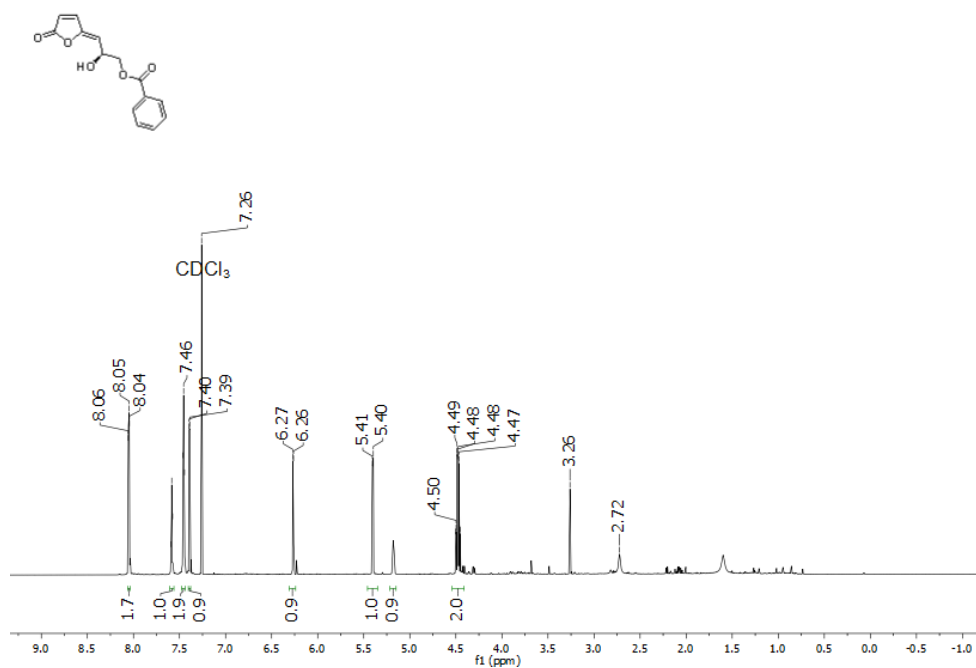


Fig S65. The ¹H NMR Spectrum of (Z)-Melodorinol (9) measured at 800 MHz in CDCl₃.

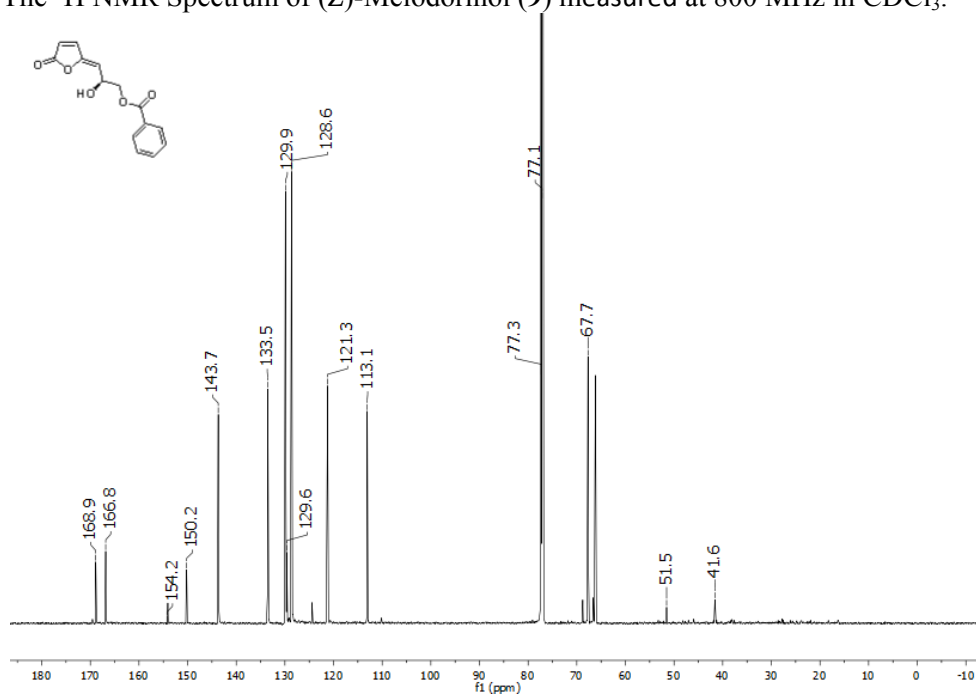


Figure S66. The ¹³C NMR Spectrum of (Z)-Melodorinol (9) measured at 800 MHz in CDCl₃.

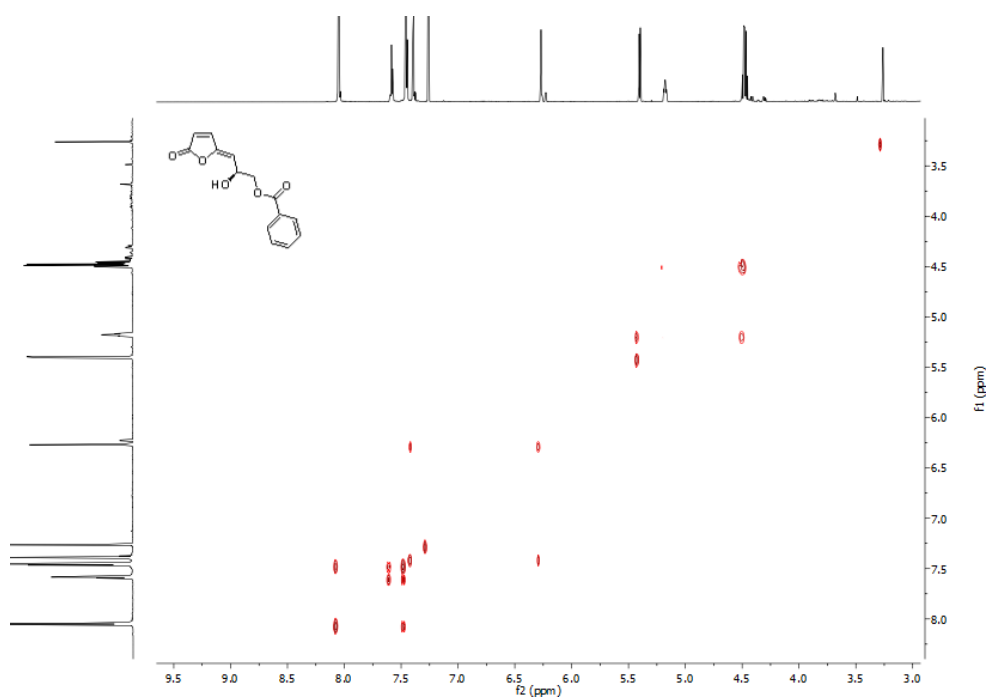


Figure S67. The COSY Spectrum of (Z)-Melodorinol (**9**) measured at 800 MHz in CDCl₃.

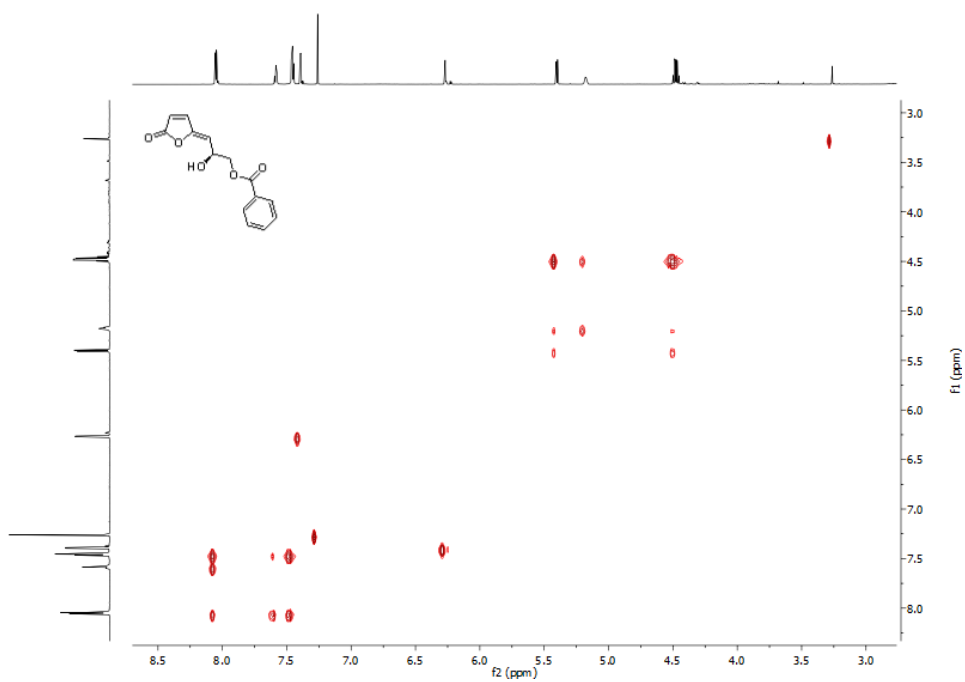


Figure S68. The TOCSY Spectrum of (Z)-Melodorinol (**9**) measured at 800 MHz in CDCl₃.

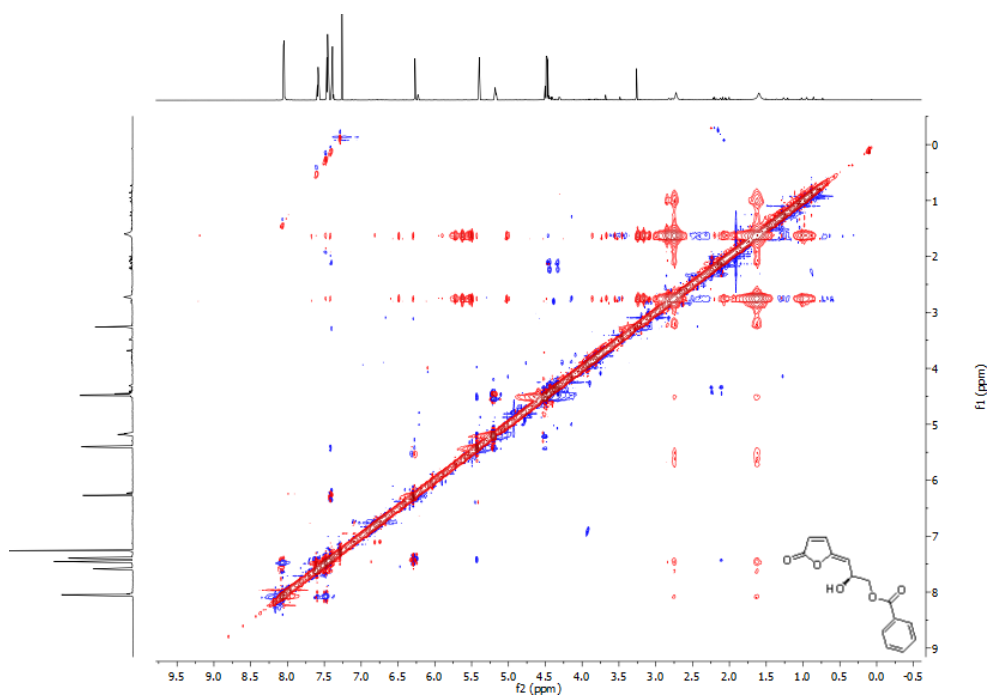


Figure S69. The NOESY Spectrum of (Z)-Melodorinol (**9**) measured at 800 MHz in CDCl₃.

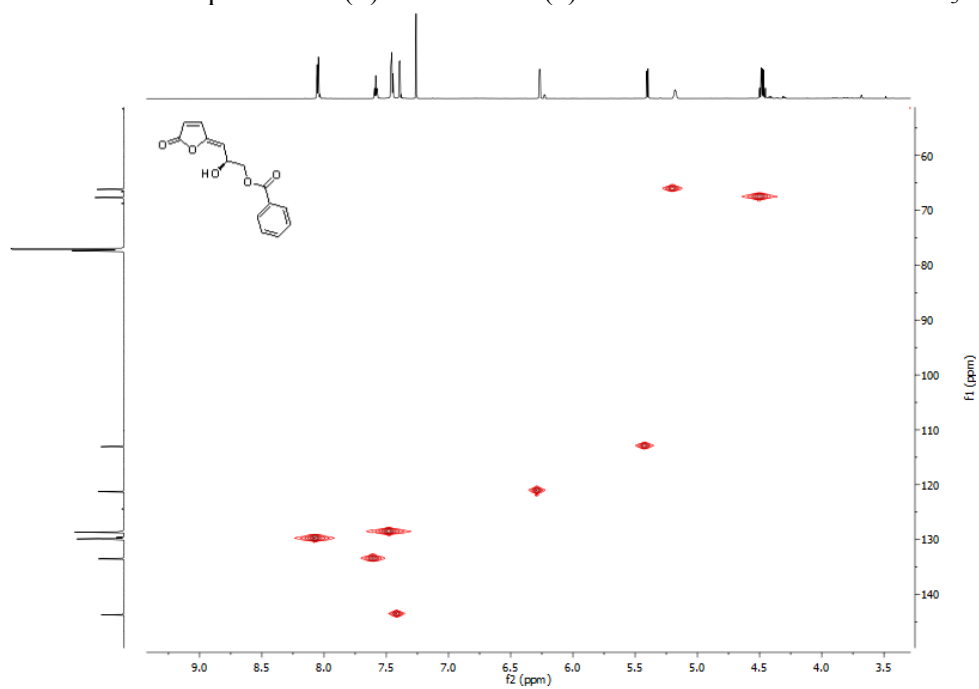


Figure S70. The HSQC Spectrum of (Z)-Melodorinol (**9**) measured at 800 MHz in CDCl₃.

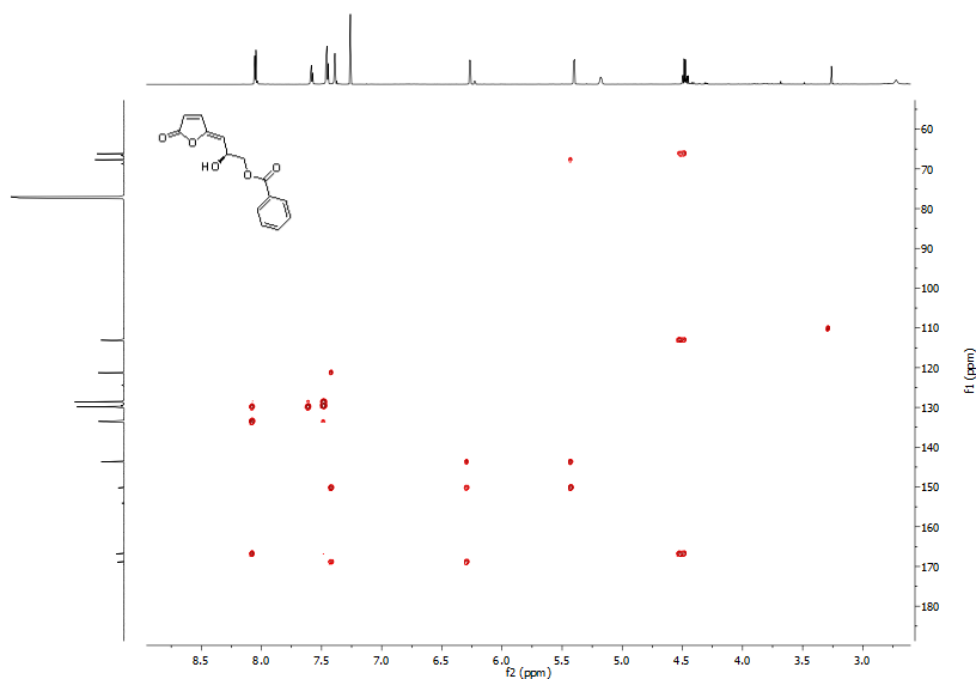


Figure S71. The HMBC Spectrum (Z)-Melodorinol (**9**) measured at 800 MHz in CDCl₃.

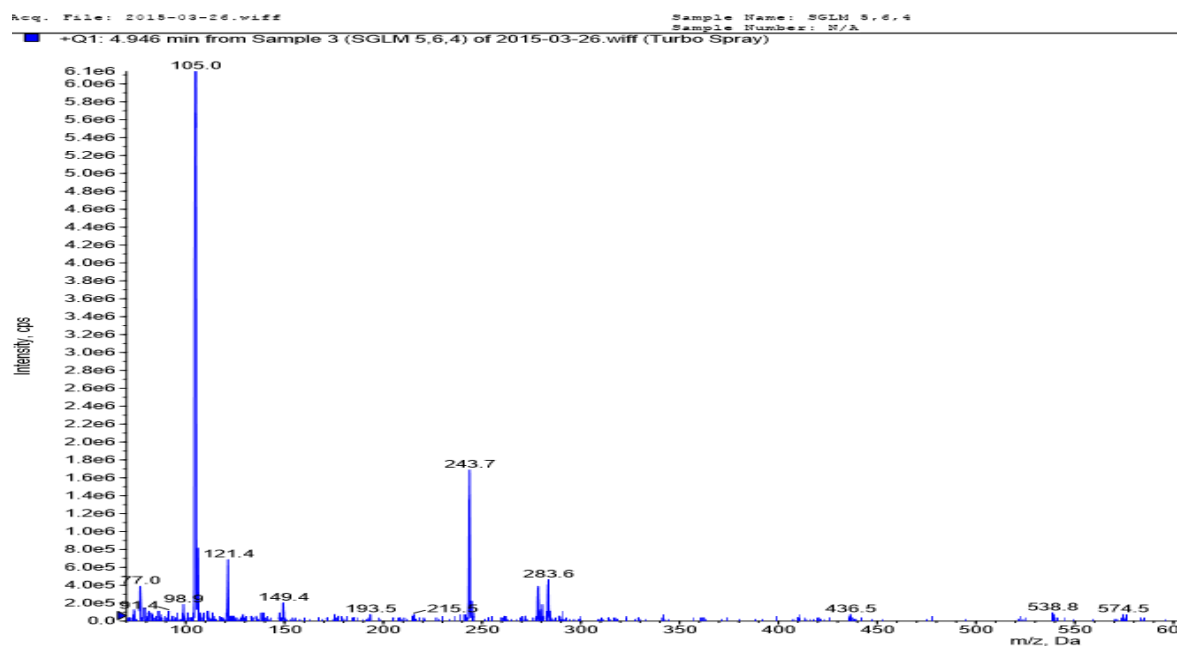


Figure S72. The LC-MS of (Z)-Melodorinol (**9**).

Spectroscopic data for 7-hydroxy-6-hydromelodienone (10)

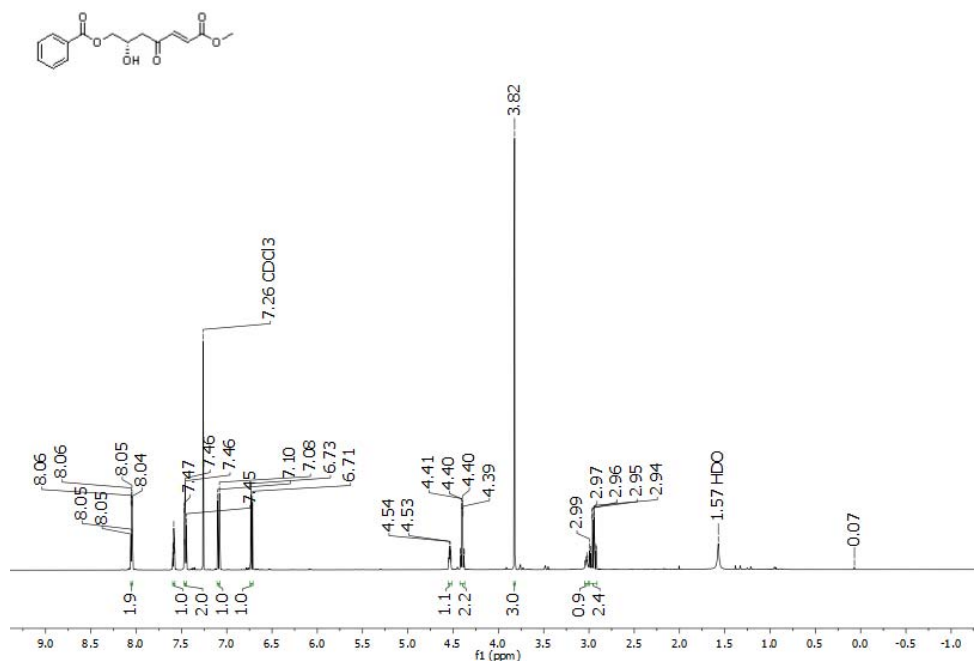


Figure S73. The ¹H NMR Spectrum of 7-Hydroxy-6-hydromelodienone (10) measured at 800 MHz in CDCl₃.

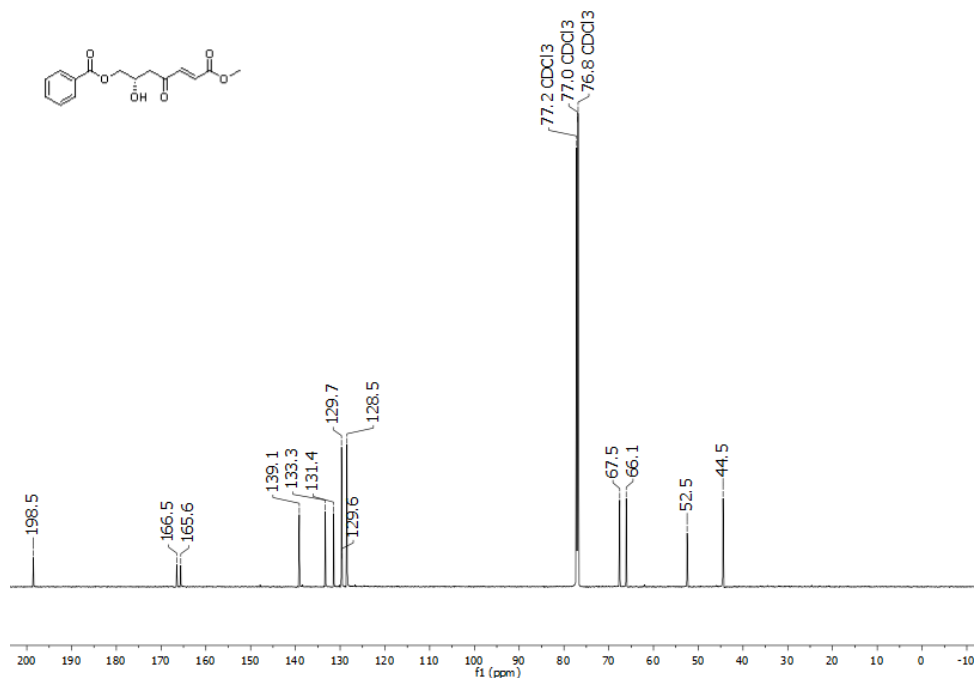


Figure S74. The ¹³C NMR Spectrum of 7-Hydroxy-6-hydromelodienone (10) measured at 800 MHz in CDCl₃.

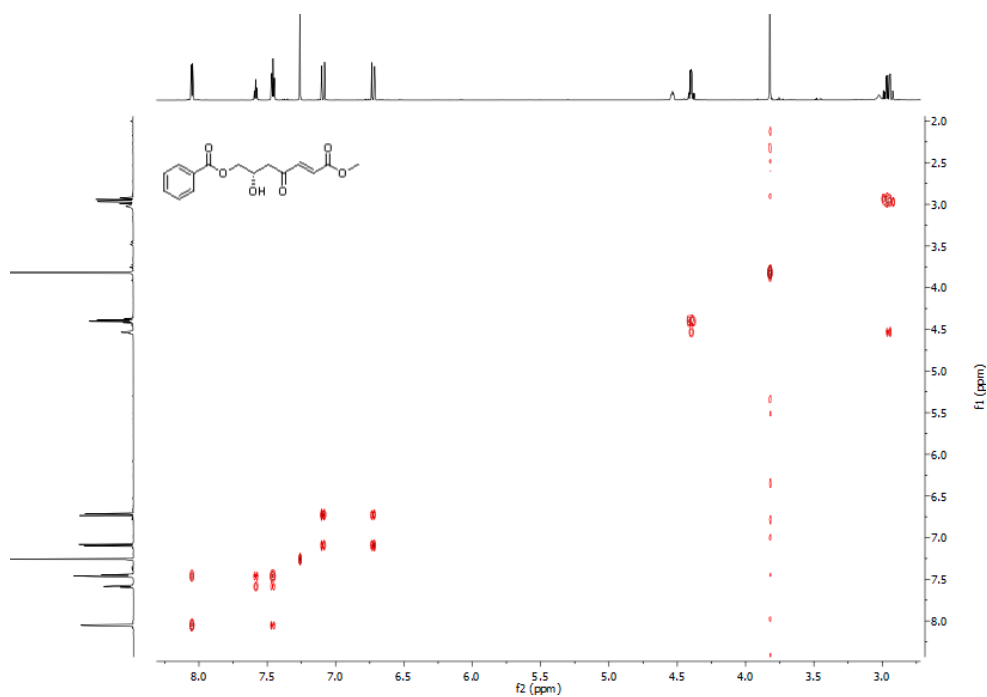


Figure S75. The COSY Spectrum of 7-Hydroxy-6-hydromelodienone (**10**) measured at 800 MHz in CDCl_3 .

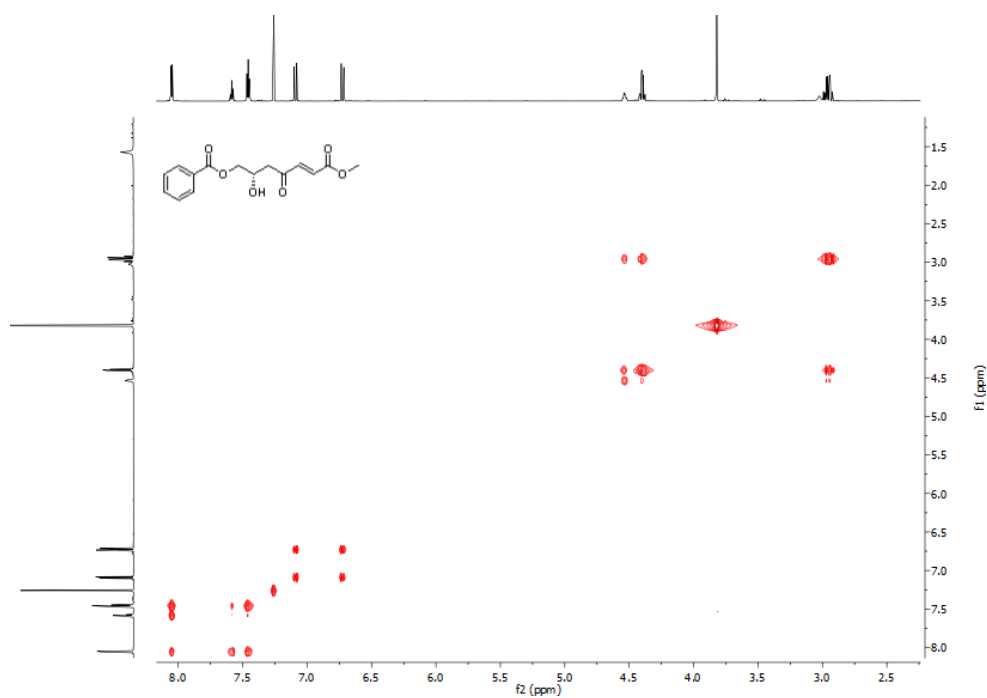


Figure S76. The TOCSY Spectrum of 7-Hydroxy-6-hydromelodienone (**10**) measured at 800 MHz in CDCl_3 .

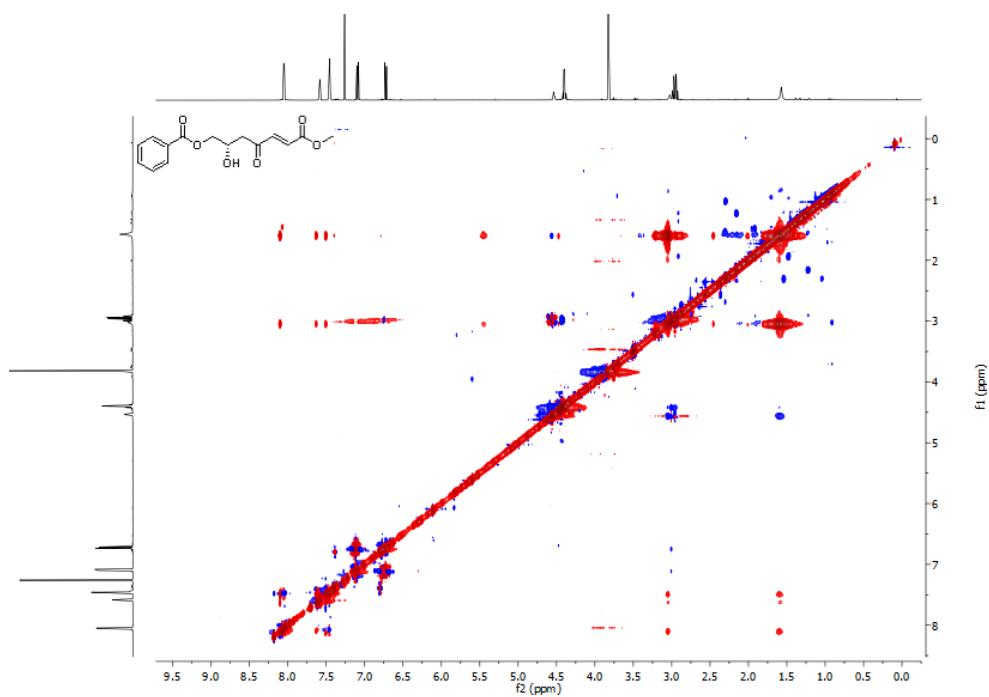


Figure S77. The NOESY Spectrum of 7-Hydroxy-6-hydromelodienone (**10**) measured at 800 MHz in CDCl₃.

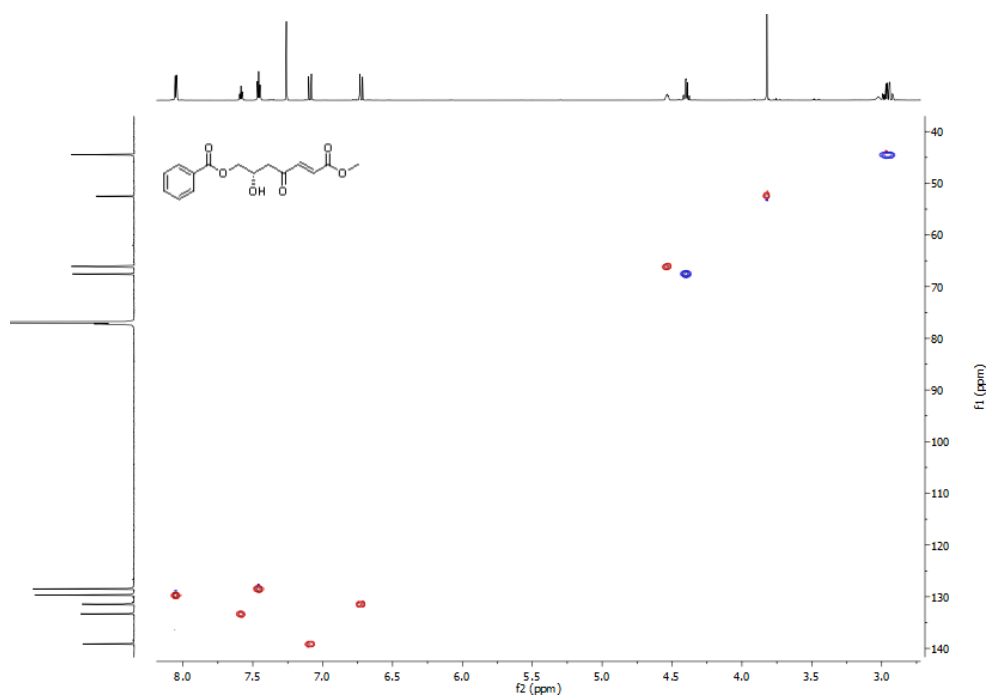


Figure S78. The HSQC Spectrum of 7-Hydroxy-6-hydromelodienone (**10**) measured at 800 MHz in CDCl₃.

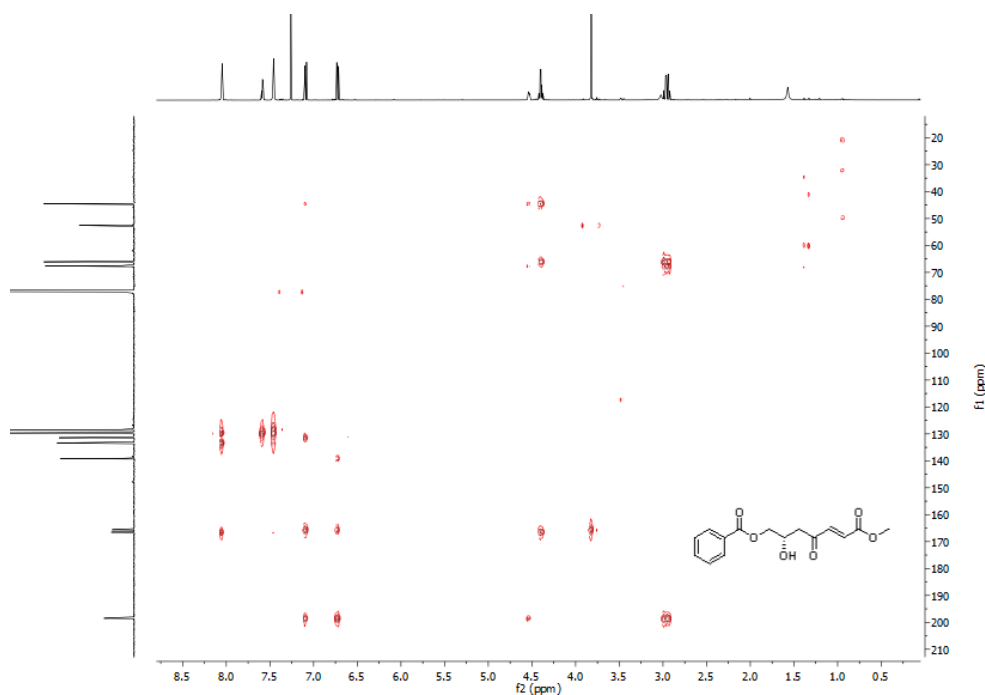


Figure S79. The HMBC Spectrum of 7-Hydroxy-6-hydromelodienone (**10**) measured at 800 MHz in CDCl₃.

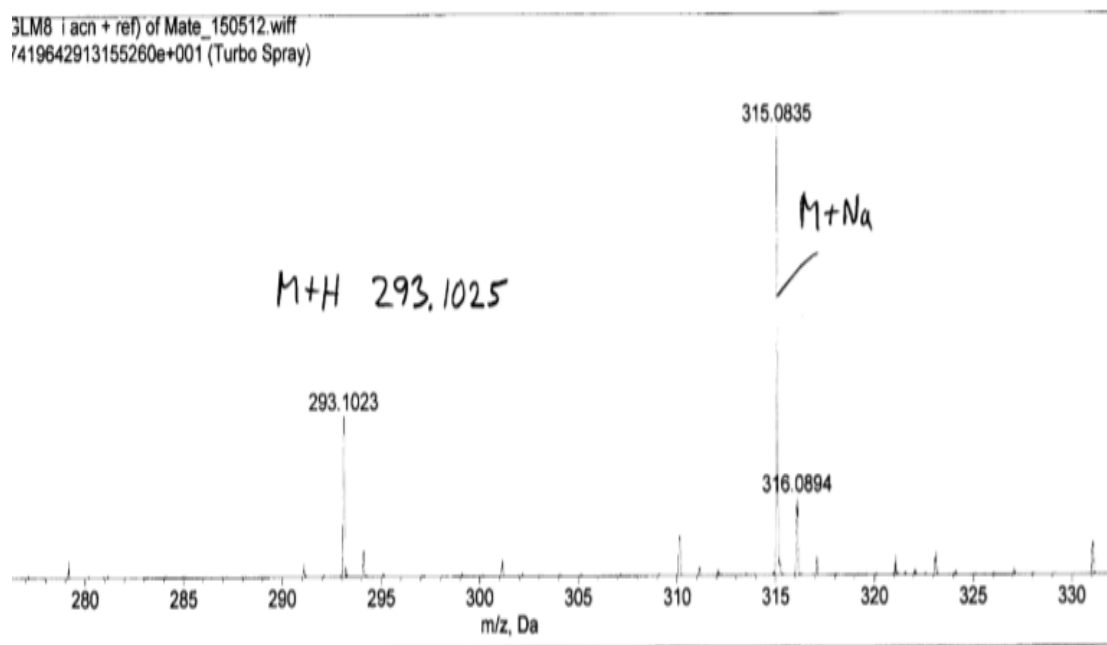


Figure S80. The HRESIMS of 7-Hydroxy-6-hydromelodienone (**10**).

Spectroscopic data for pinocembrin (11)

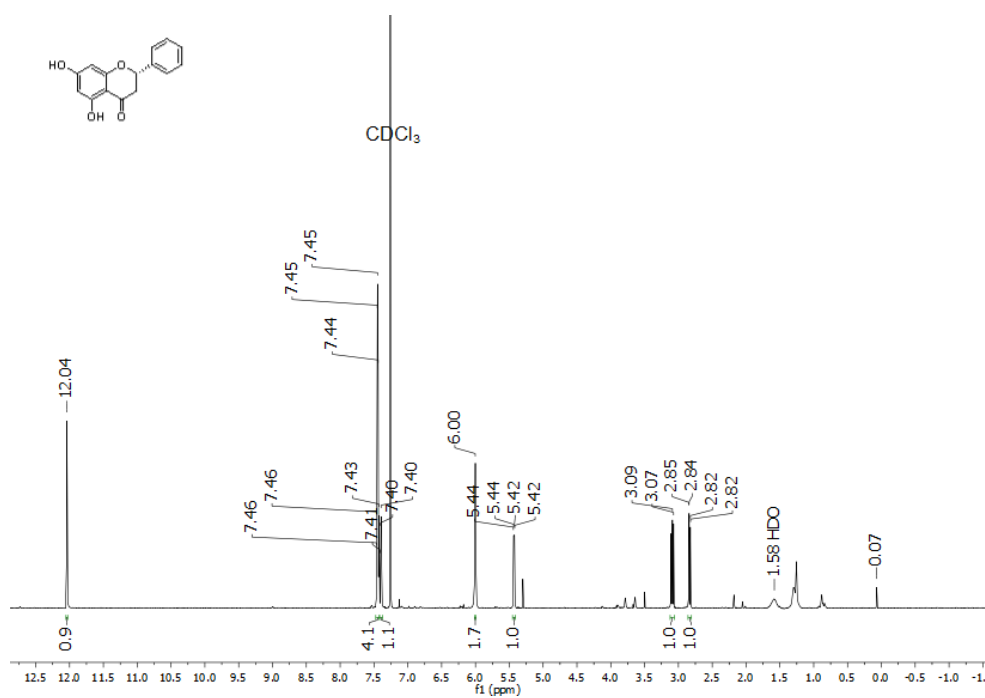


Fig S81. The ¹H NMR Spectrum of Pinocembrin (11) measured at 800 MHz in CDCl₃.

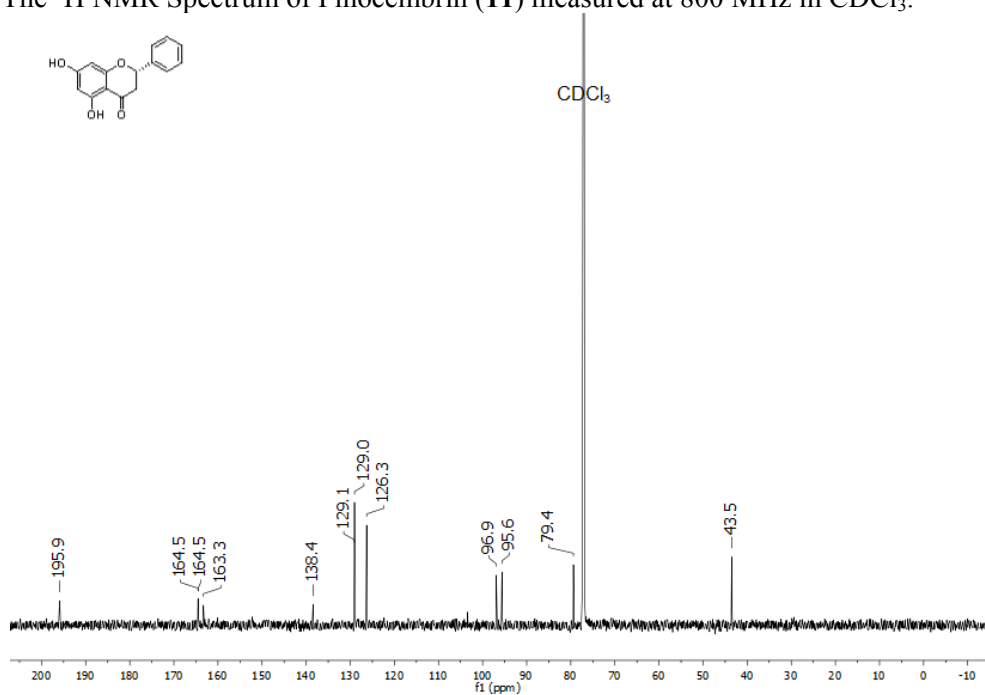


Figure S82. The ¹³C NMR Spectrum of Pinocembrin (11) measured at 200 MHz in CDCl₃.

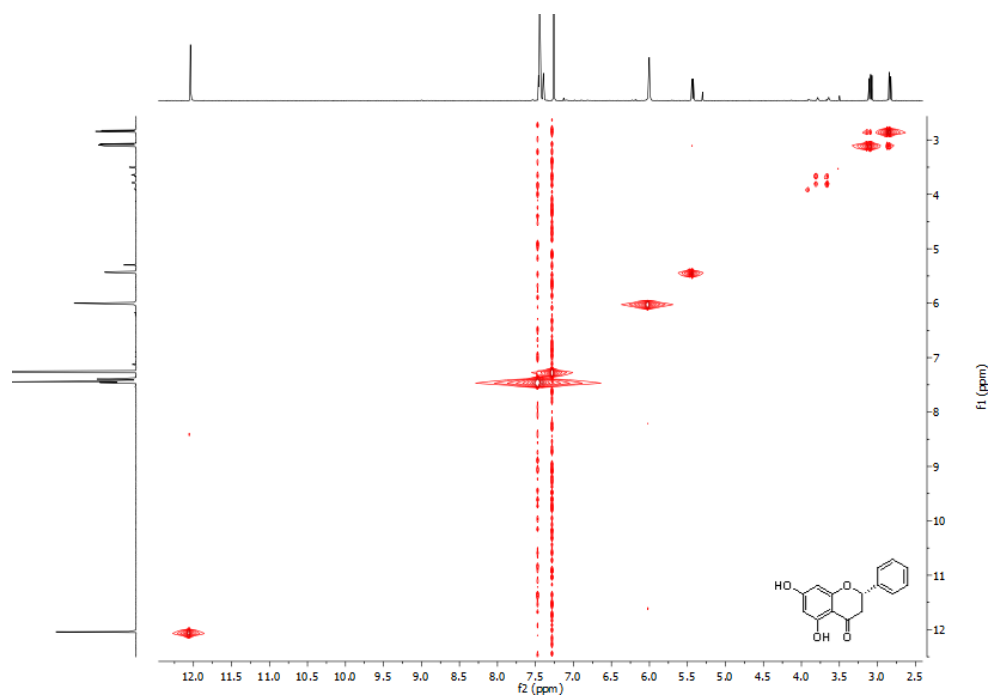


Figure S83. The TOCSY Spectrum of Pinocembrin (**11**) measured at 800 MHz in CDCl₃.

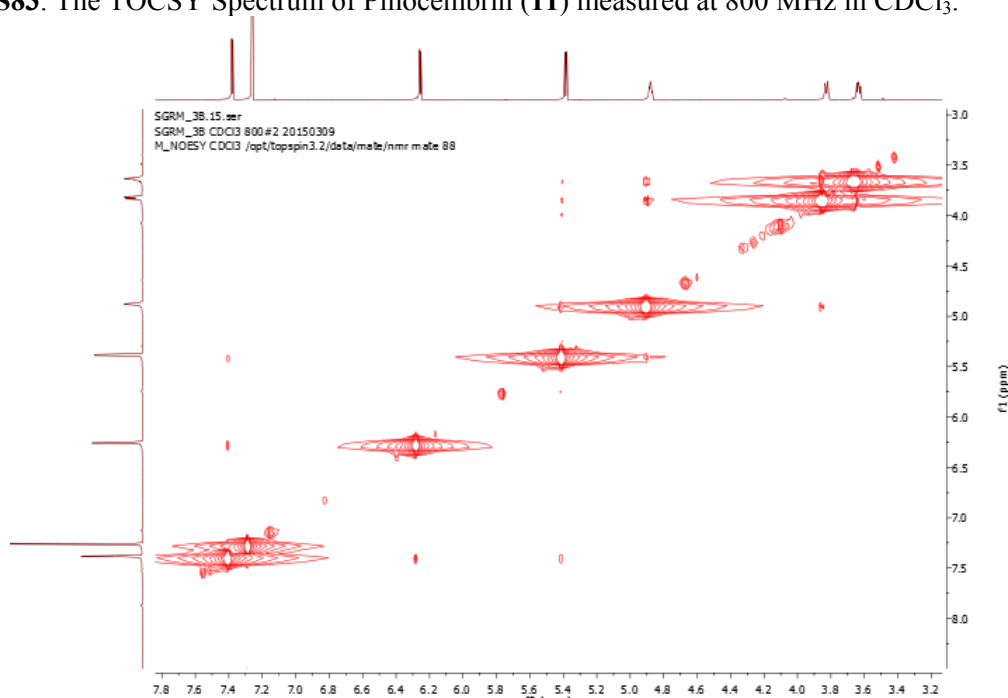


Figure S84. The NOESY Spectrum of Pinocembrin (**11**) measured at 800 MHz in CDCl₃.

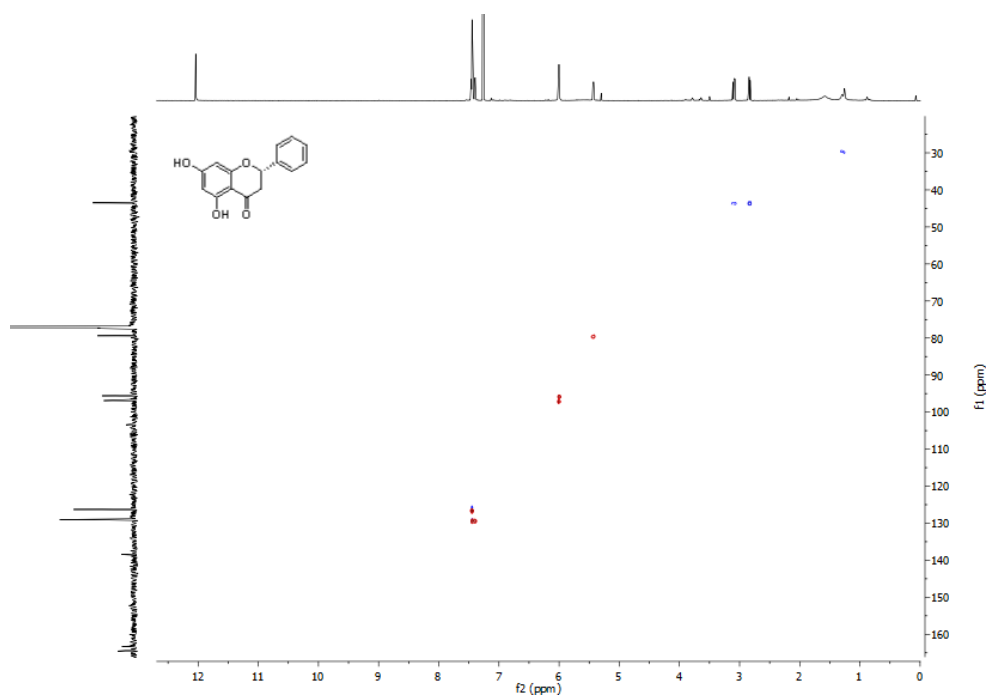


Figure S85. The HSQC Spectrum of Pinocembrin (**11**) measured at 800 MHz in CDCl₃.

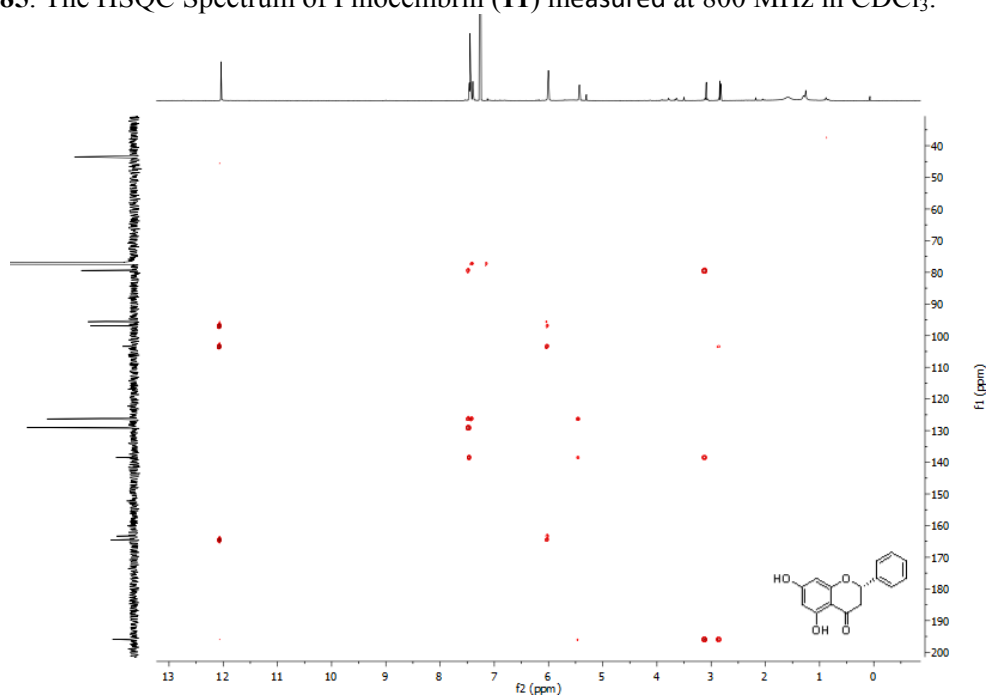


Figure S86. The HMBC Spectrum of Pinocembrin (**11**) measured at 800 MHz in CDCl₃.

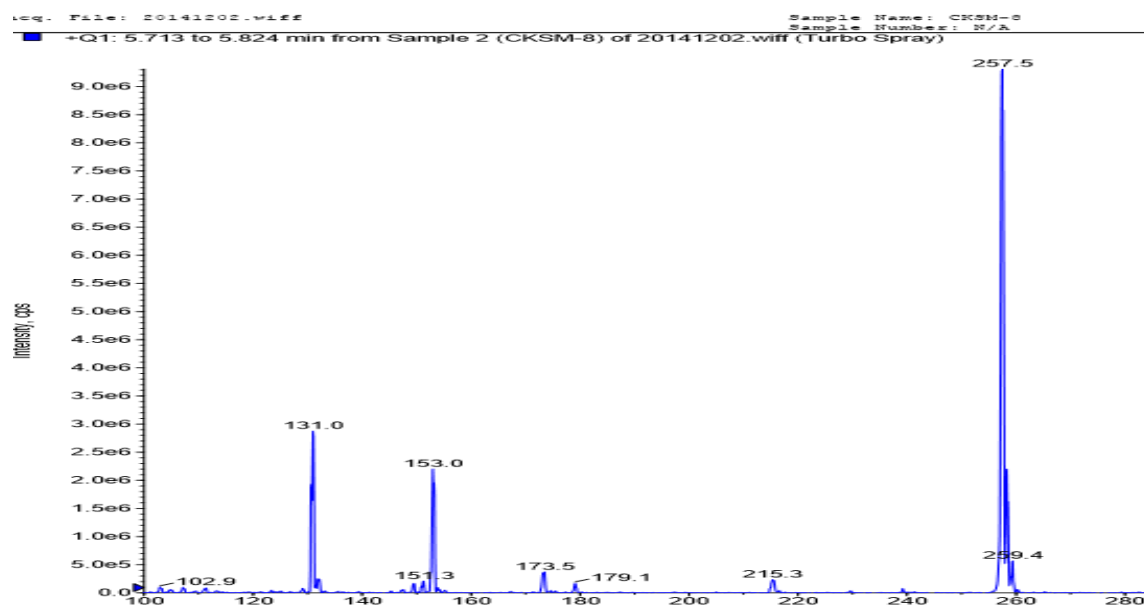


Figure S87. The LC-MS of Pinocembrin (**11**).

Spectroscopic data for 5,7-dihydroxyflavone (12)

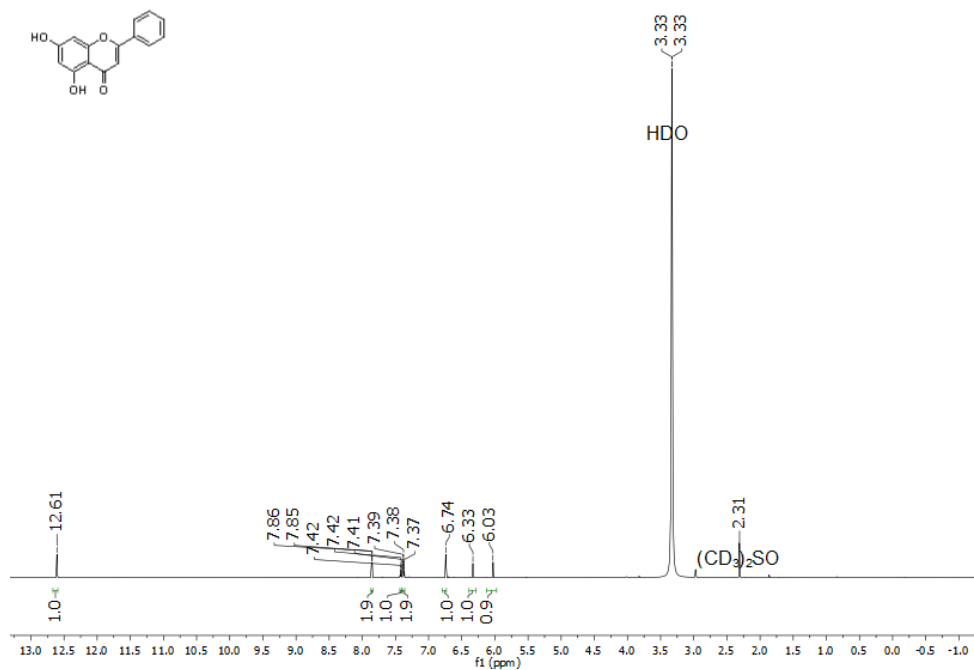


Figure S88. The ^1H NMR Spectrum of 5,7-Dihydroxyflavone (**12**) measured at 800 MHz in $(\text{CD}_3)_2\text{SO}$.

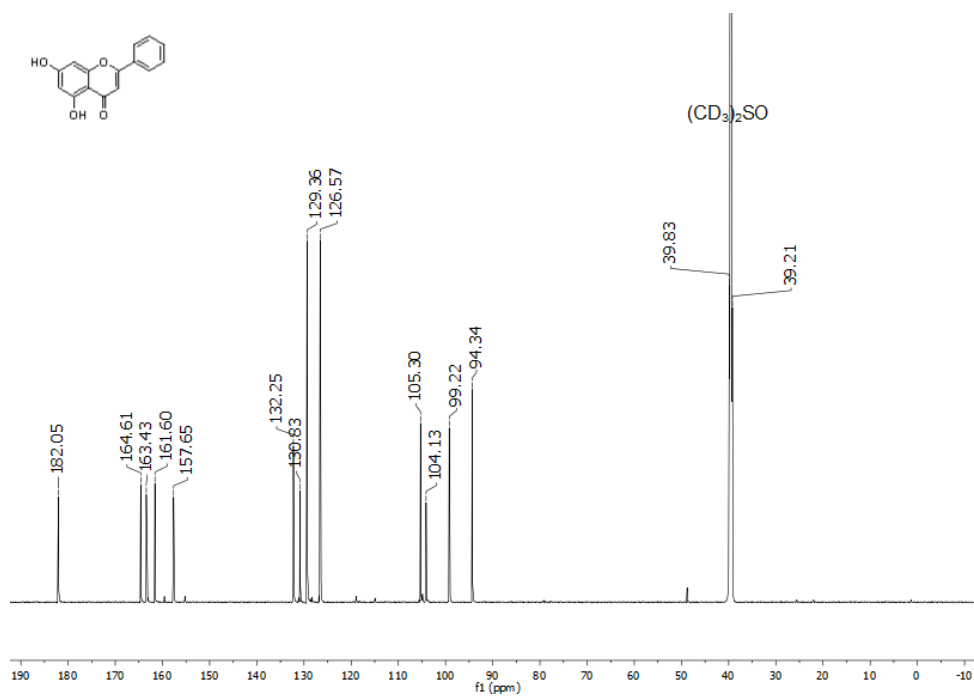


Figure S89. The ^{13}C NMR Spectrum of 5,7-Dihydroxyflavone (**12**) measured at 800 MHz in $(\text{CD}_3)_2\text{SO}$.

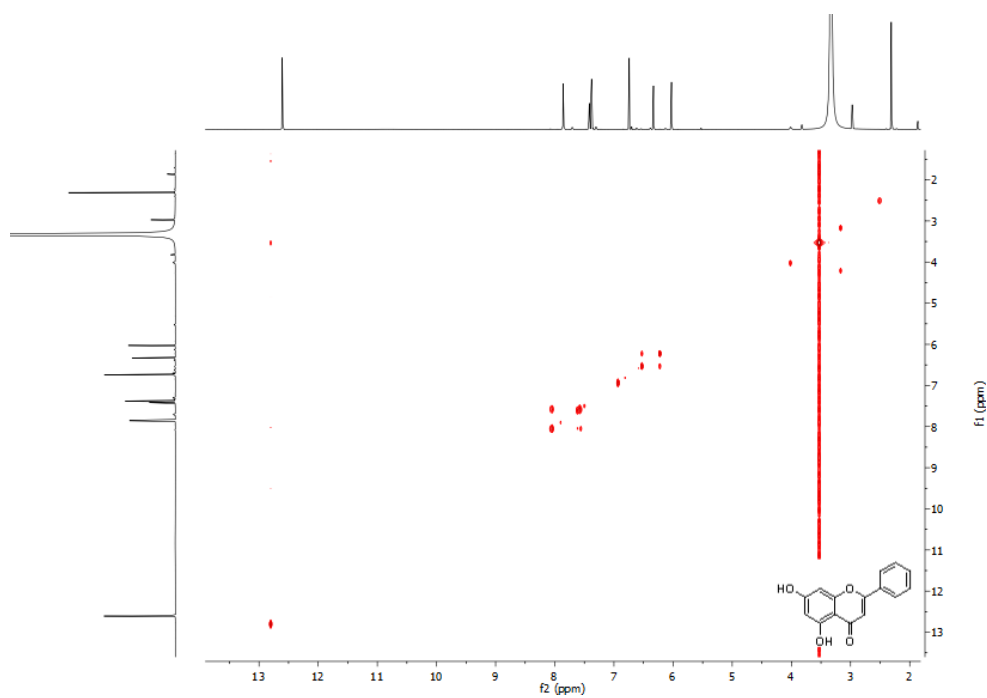


Figure S90. The COSY Spectrum of 5,7-Dihydroxyflavone (**12**) measured at 800 MHz in (CD₃)₂SO.

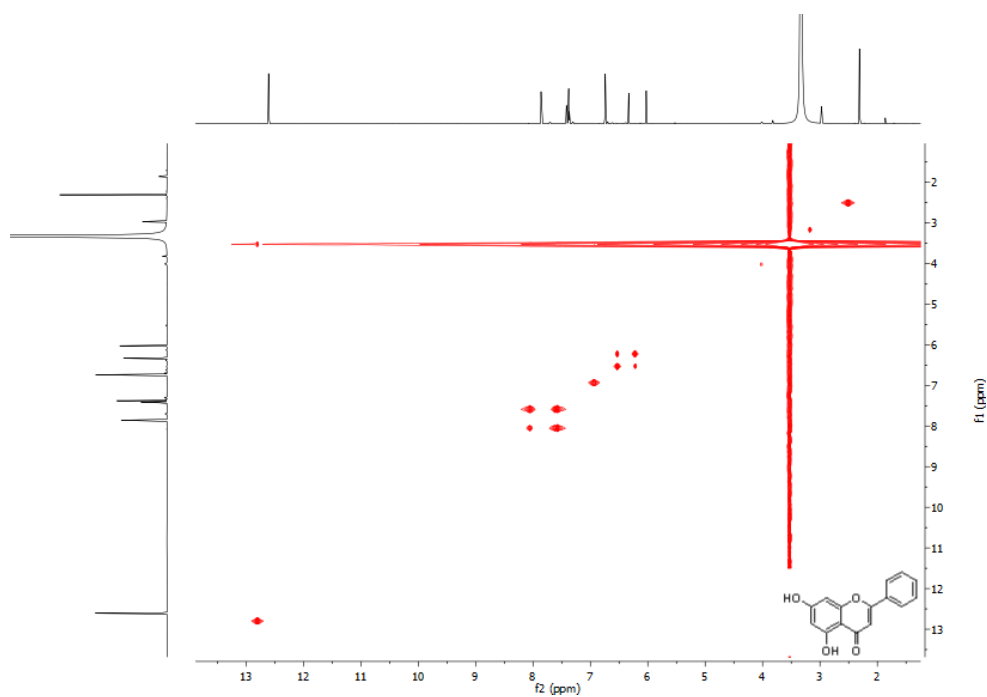


Figure S91. The TOCSY Spectrum of 5,7-Dihydroxyflavone (**12**) measured at 800 MHz in (CD₃)₂SO.

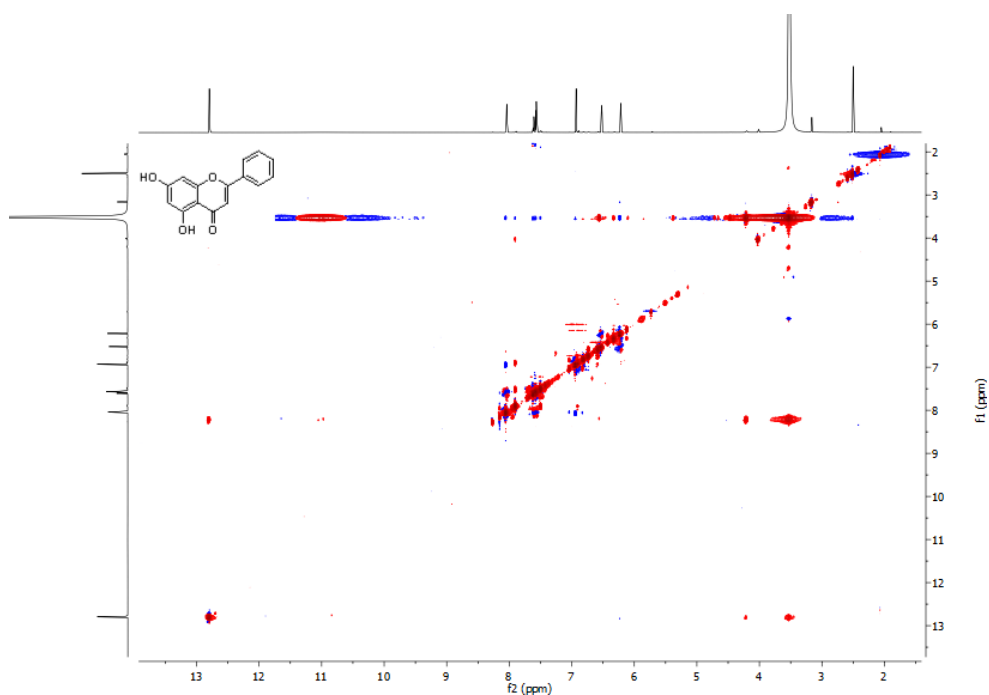


Figure S92. The NOESY Spectrum of 5,7-Dihydroxyflavone (**12**) measured at 800 MHz in (CD₃)₂SO.

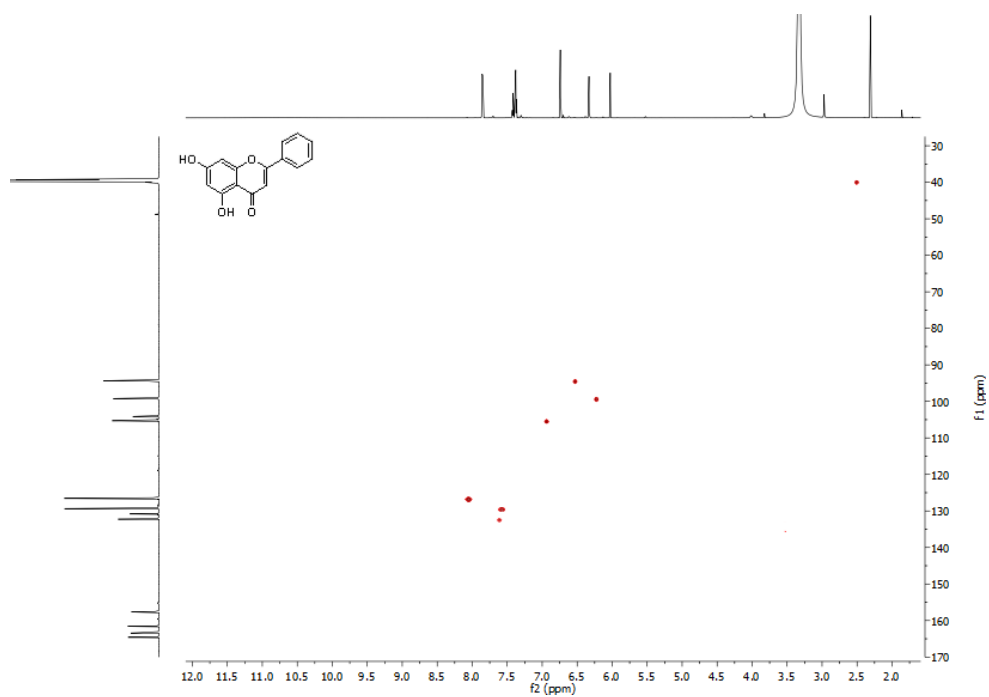


Figure S93. The HSQC Spectrum of 5,7-Dihydroxyflavone (**12**) measured at 800 MHz in (CD₃)₂SO.

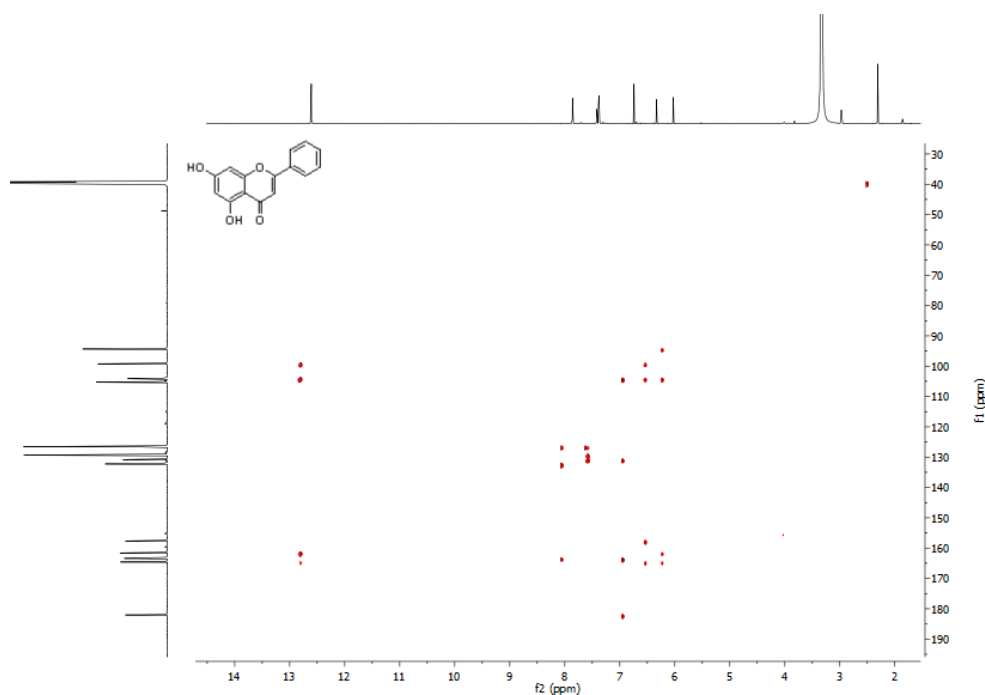


Figure S94. The HMBC Spectrum of 5,7-Dihydroxyflavone (**12**) measured at 800 MHz in (CD₃)₂SO.

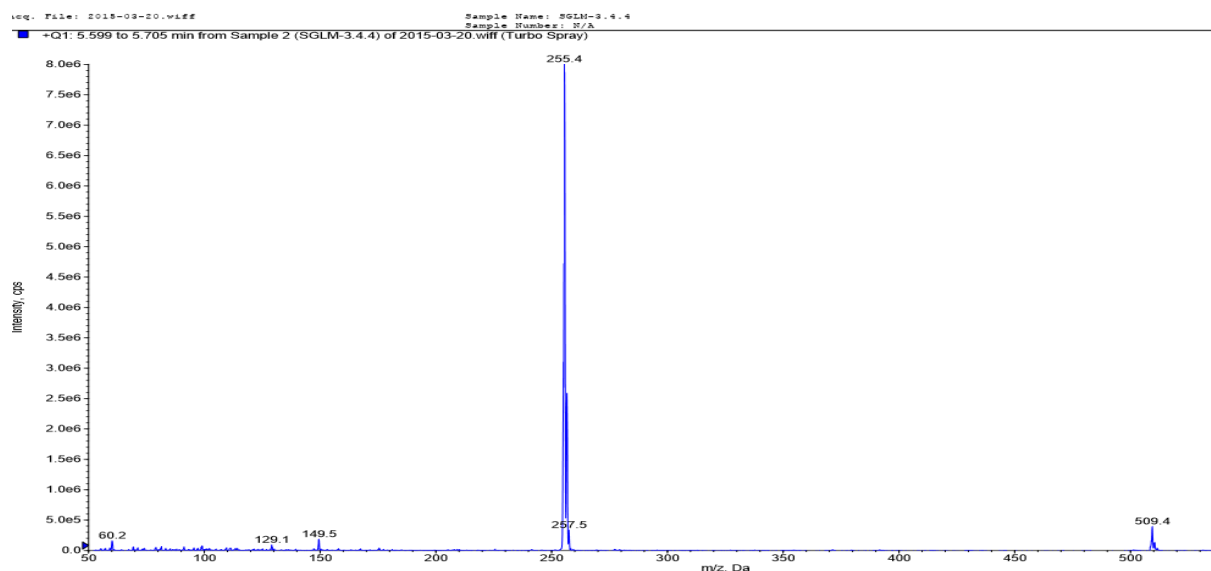


Figure S95. The LC-MS of 5,7-dihydroxyflavone (**12**).

Chemical structure of compound 10: Oc1cc(O)c2c(c1)oc(c3ccccc3)c(=O)c2Cc4ccccc4O

¹H NMR spectrum (CDCl₃) of compound 10. The spectrum shows peaks in the aromatic region (6.5–7.5 ppm), a methine proton (5.53 ppm), and a methoxy group (3.78 ppm). Integration values are provided for several peak groups.

Oc1ccc(cc1)Cc2c(O)c(O)c(=O)c3ccccc3o2

13C NMR spectrum (CDCl₃) of 2-(2-hydroxy-3-phenyl-2,4-dihydro-1H-benzopyran-6-yl)phenol. The spectrum shows peaks at the following chemical shifts (ppm): 197.6, 164.7, 163.3, 161.3, 154.7, 139.9, 130.9, 129.6, 129.6, 129.6, 128.2, 127.4, 127.3, 121.1, 115.9, 107.3, 97.0, 80.1, 43.4, 22.9.

S60

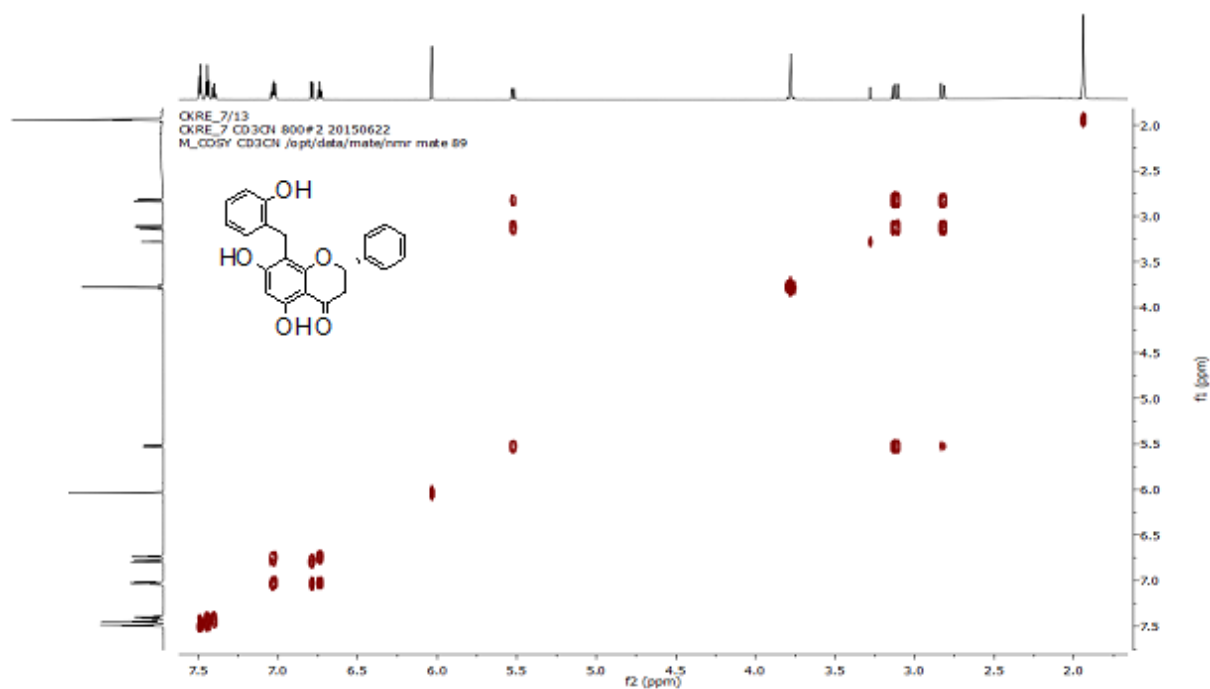


Figure S98. The COSY Spectrum of Chamanetin (**13**) measured at 800 MHz in CDCl_3 .

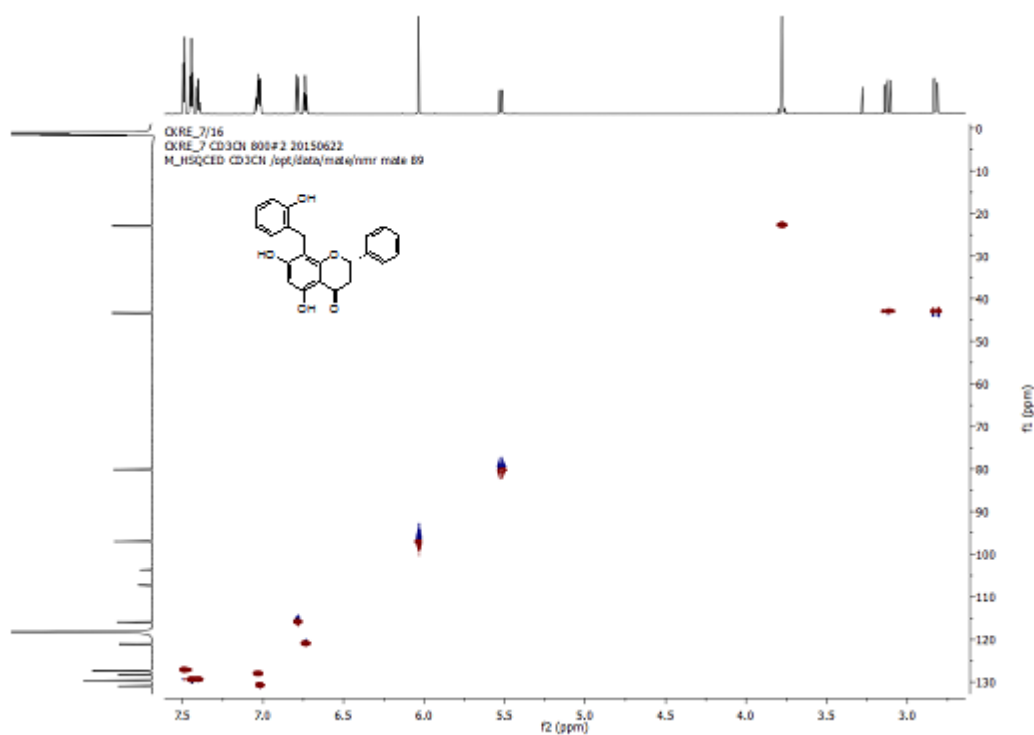


Figure S99. The HSQC Spectrum of Chamanetin (**13**) measured at 800 MHz in CDCl_3 .

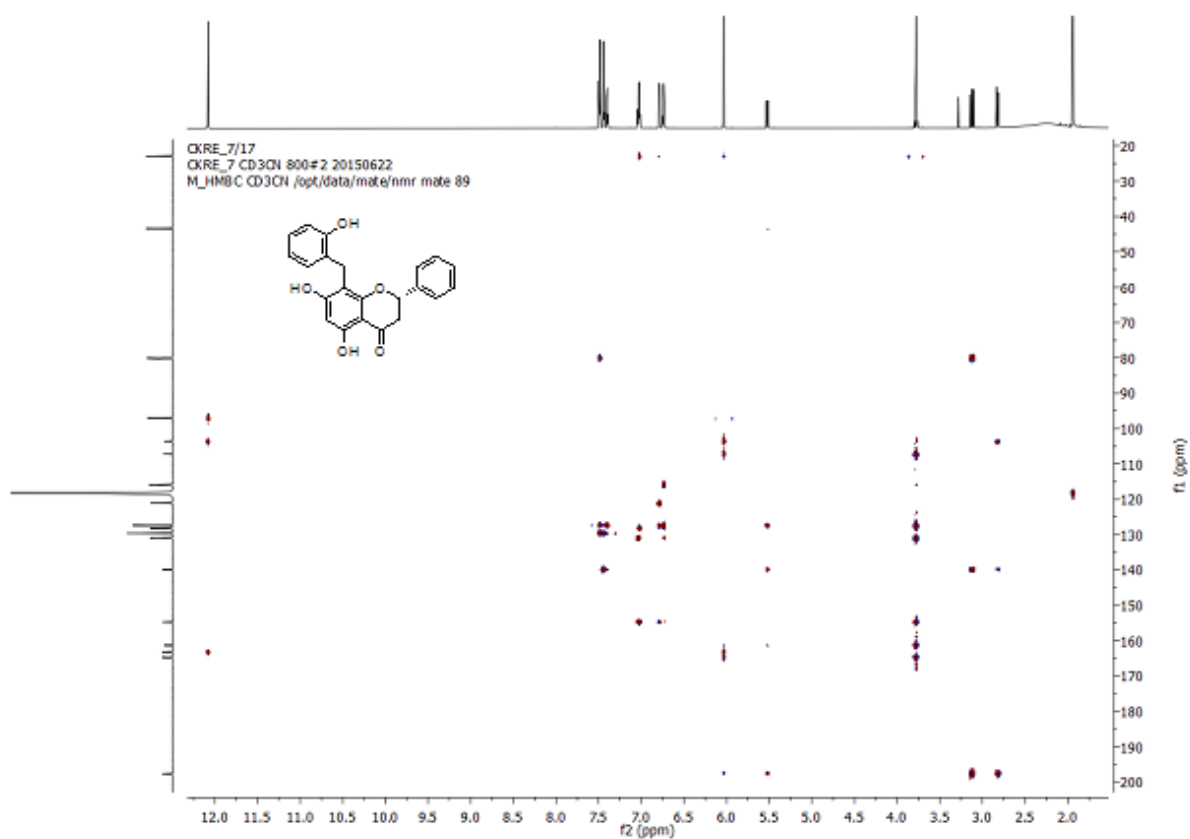


Figure S100. The HMBC Spectrum of Chamanetin (**13**) measured at 800 MHz in CDCl₃

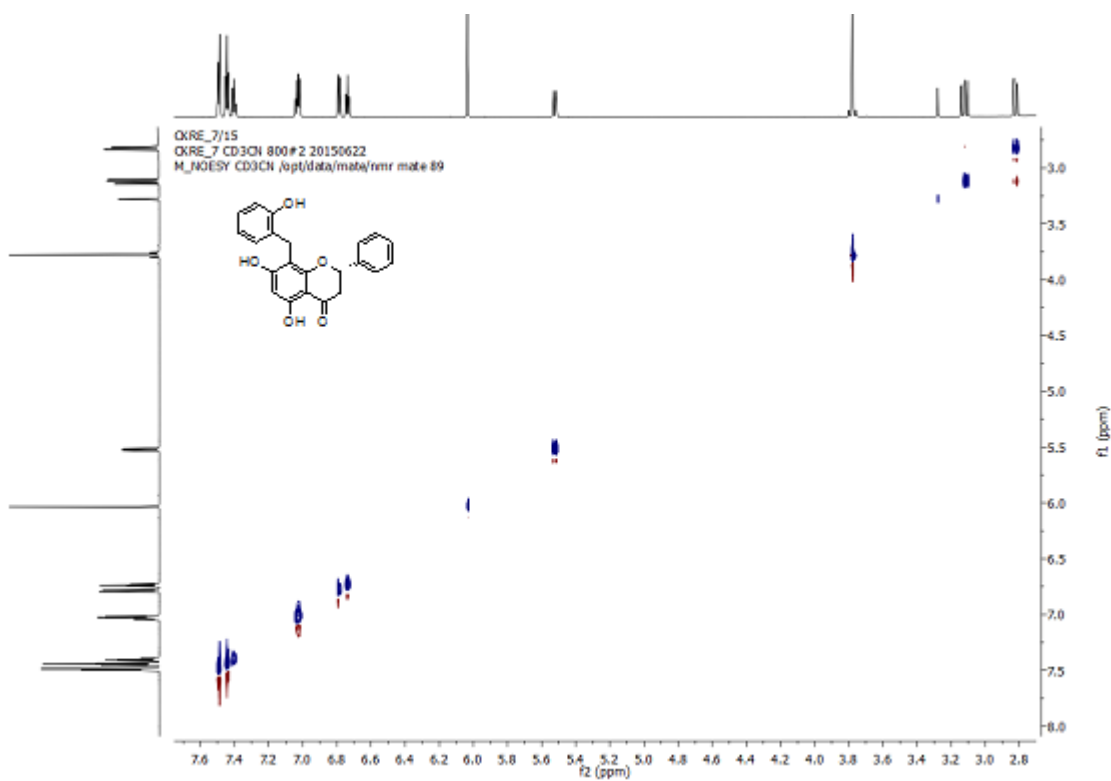
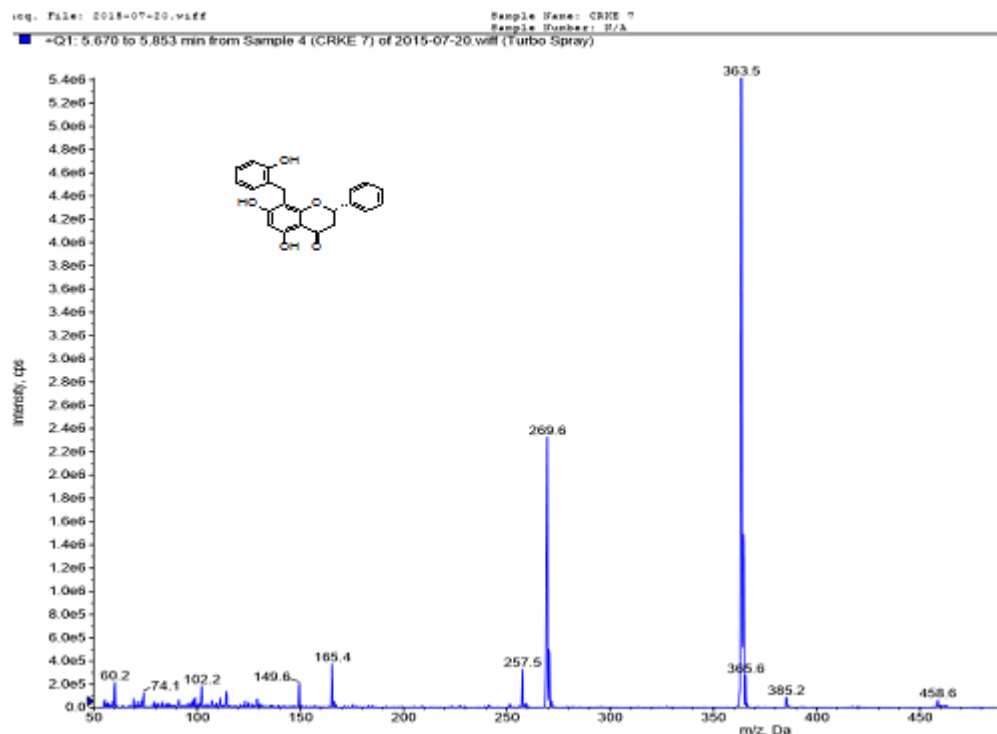
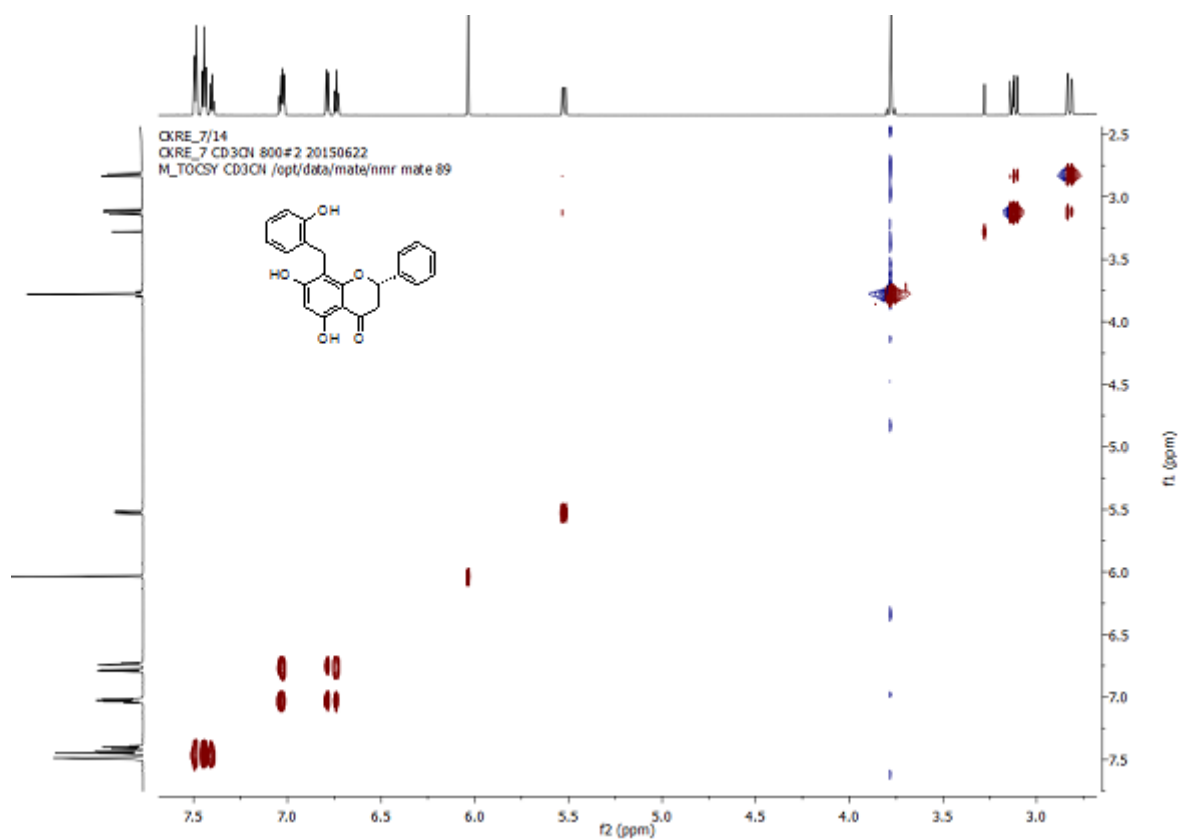


Figure S101. The NOESY Spectrum of Chamanetin (**13**) measured at 800 MHz in CDCl₃



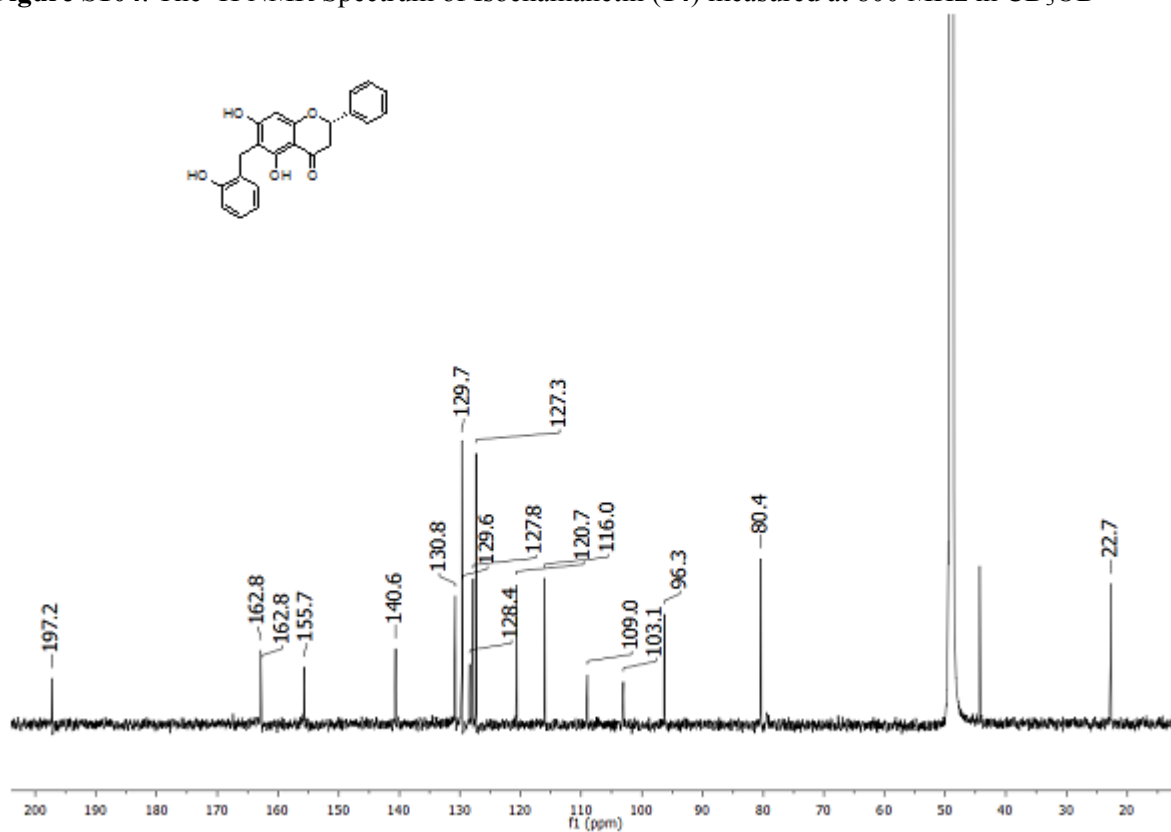
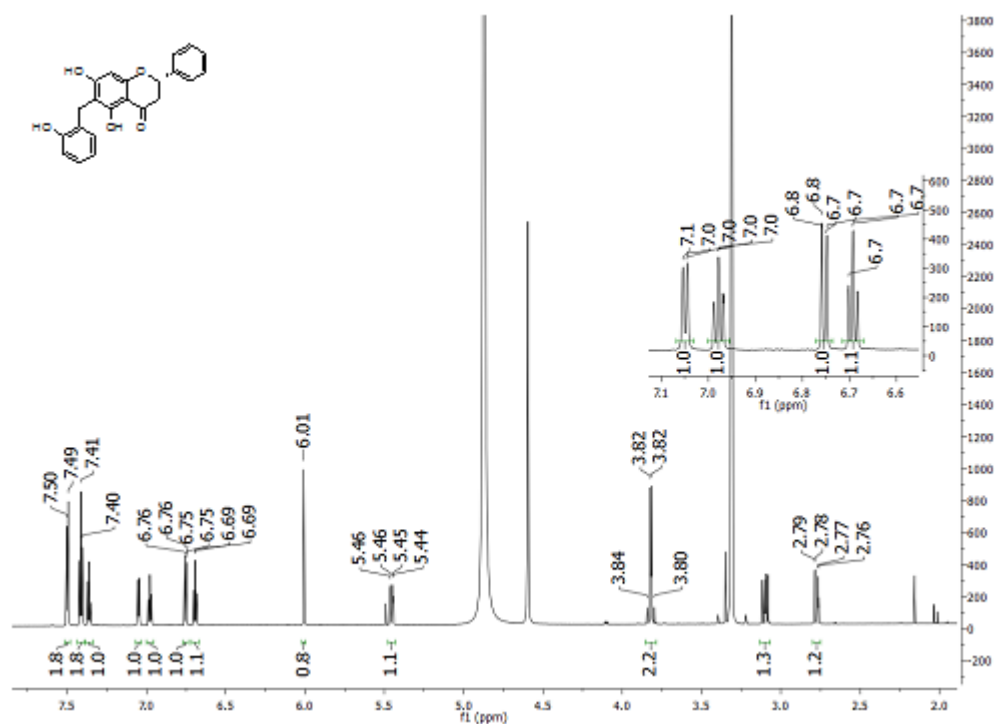


Figure S105. The ^{13}C NMR Spectrum of Isochamanetin (**14**) measured at 800 MHz in CD_3OD .

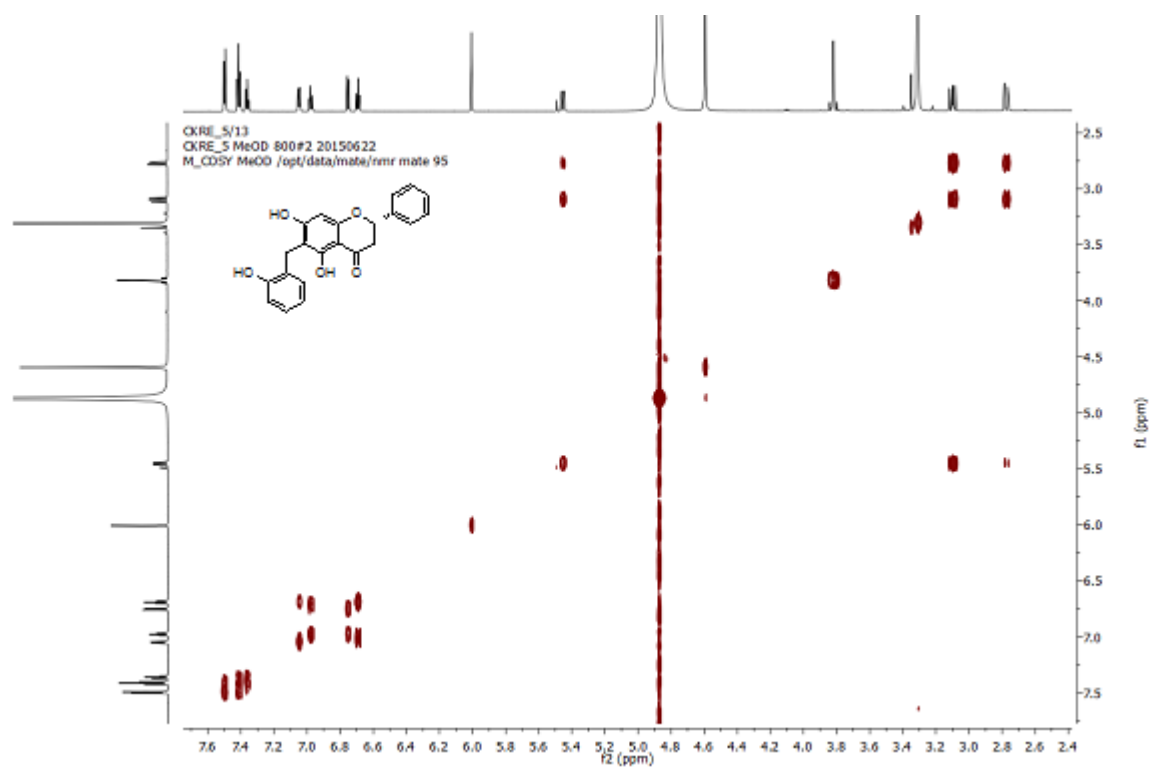


Figure S106. The COSY Spectrum of Isochamanetin (**14**) measured at 800 MHz in CD₃OD.

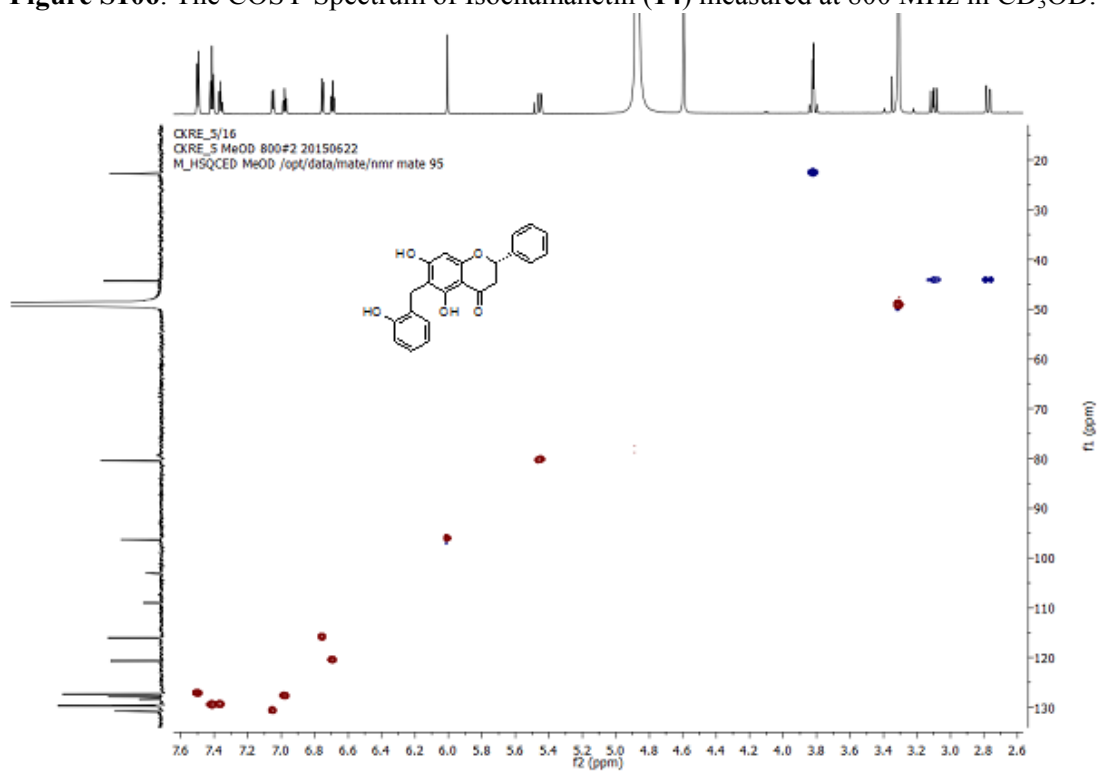


Figure S107. The HSQC Spectrum of Isochamanetin (**14**) measured at 800 MHz in CD₃OD

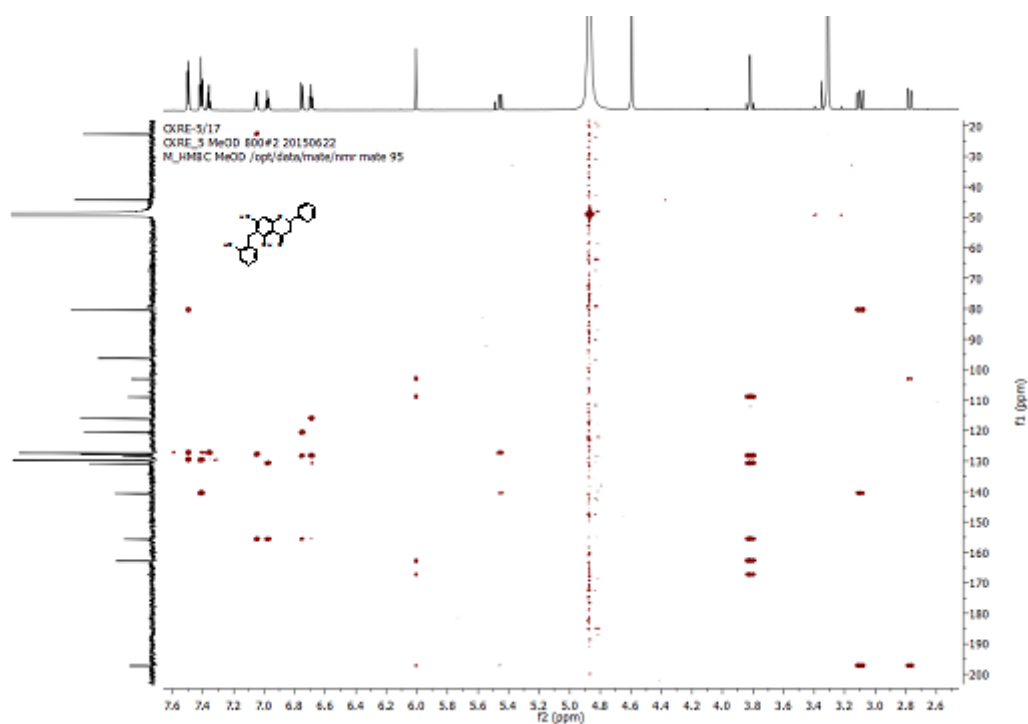


Figure S108. The HMBC Spectrum of Isochamanetin (14) measured at 800 MHz in CD₃OD.

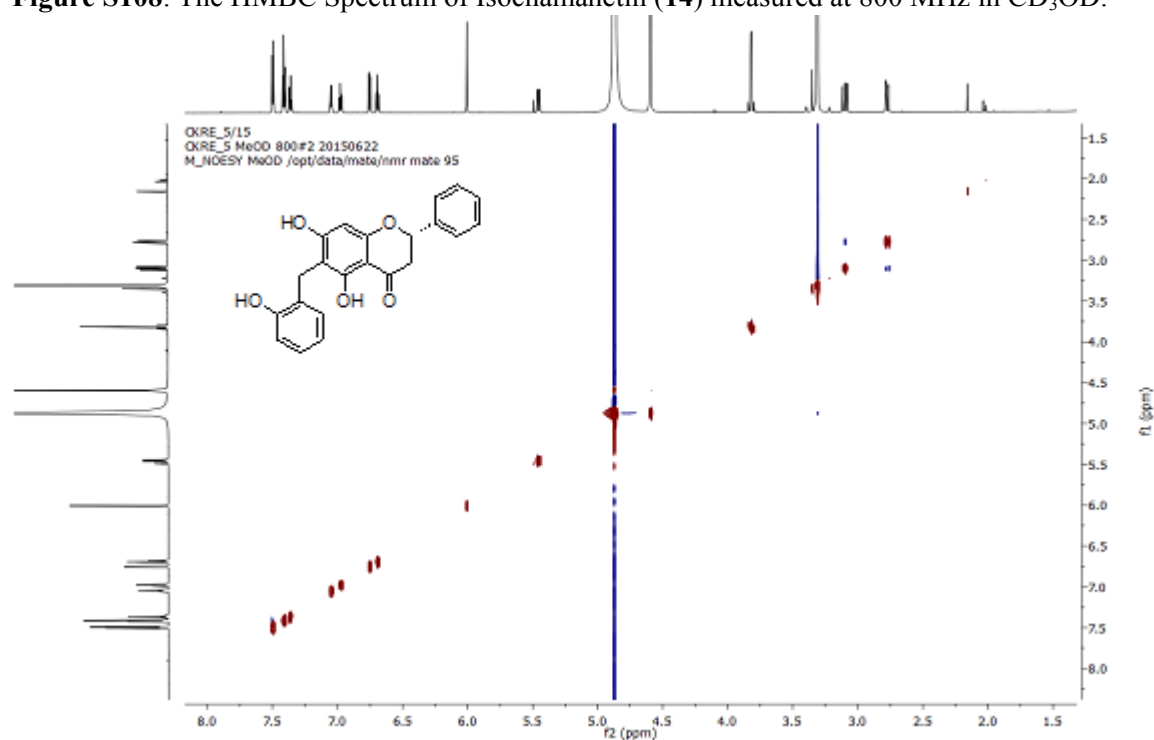


Figure S109. The NOESY Spectrum of Isochamanetin (14) measured at 800 MHz in CD₃OD

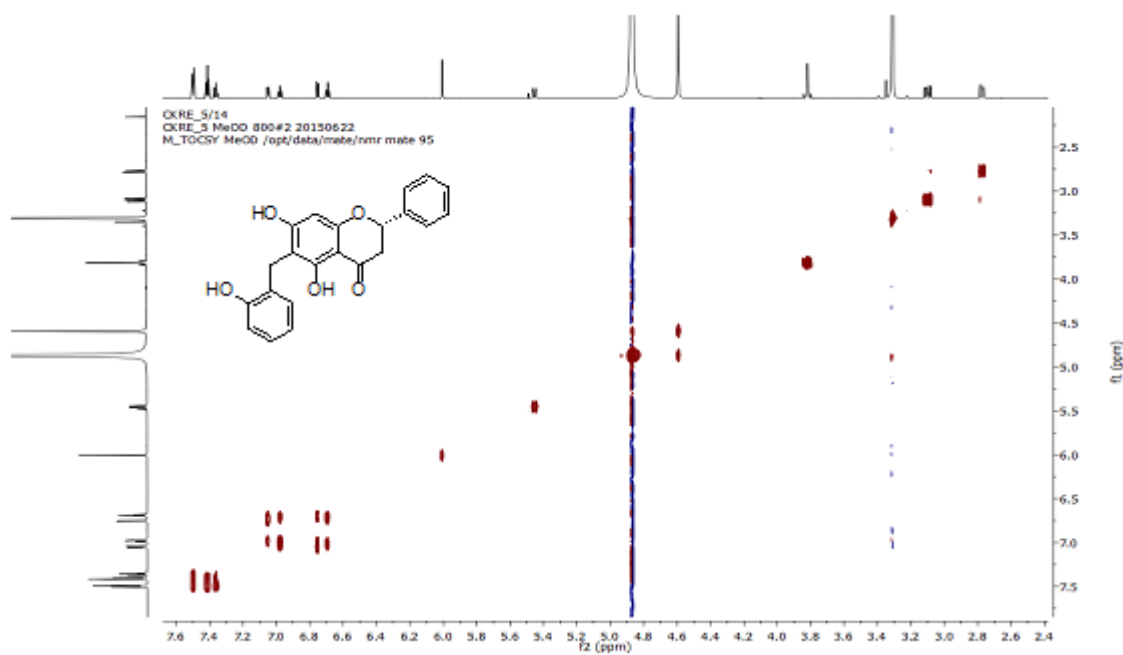


Figure S110. The TOCSY Spectrum of Isochamanetin (**14**) measured at 800 MHz in CD₃OD

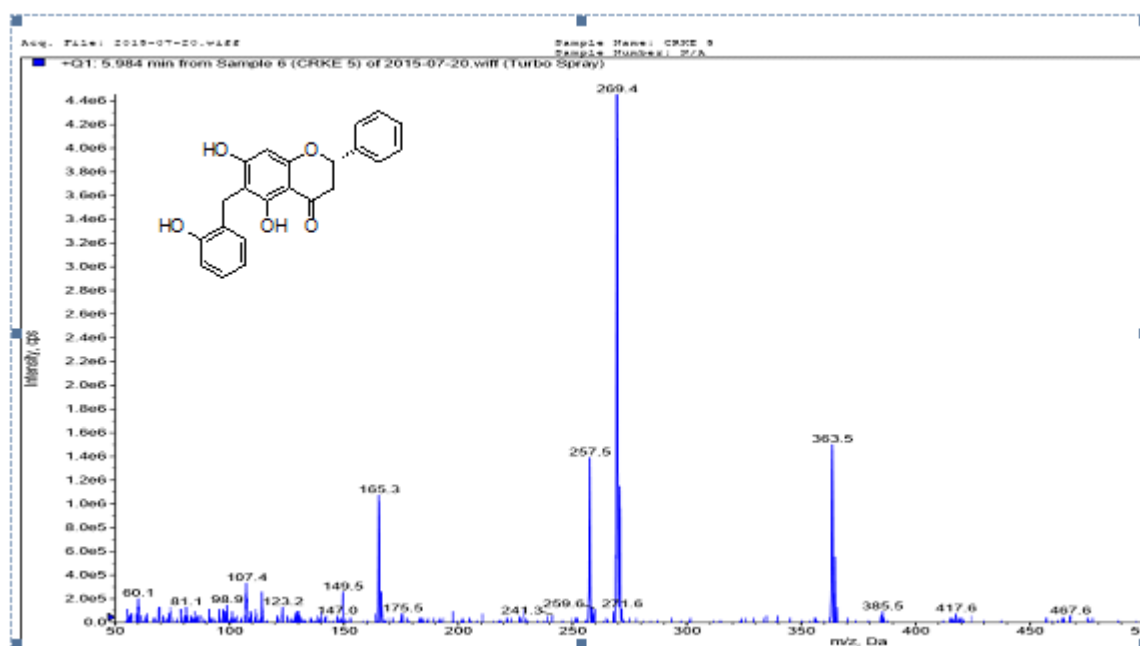


Figure S111. The LC-MS of Isochamanetin (**14**)

Spectroscopic data for dichamanetin (15)

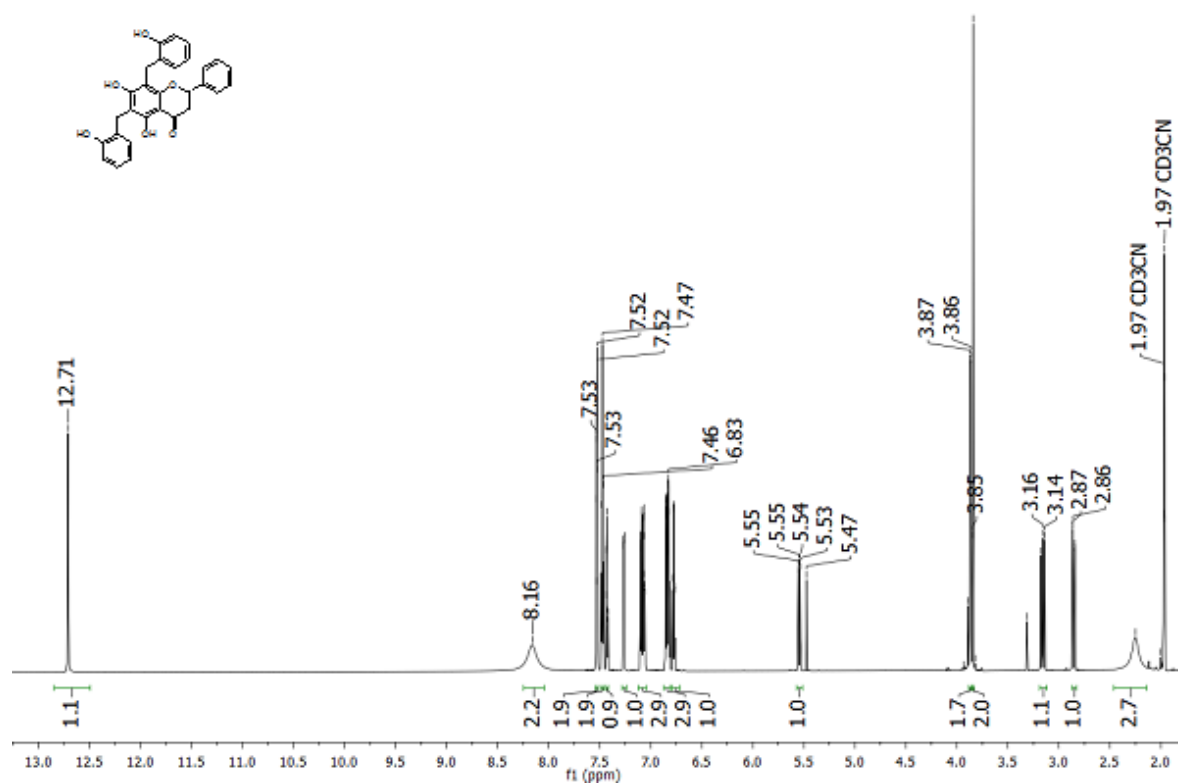


Figure S112. The ¹H NMR Spectrum of Dichamanetin (15) measured at 800 MHz in CDCl₃.

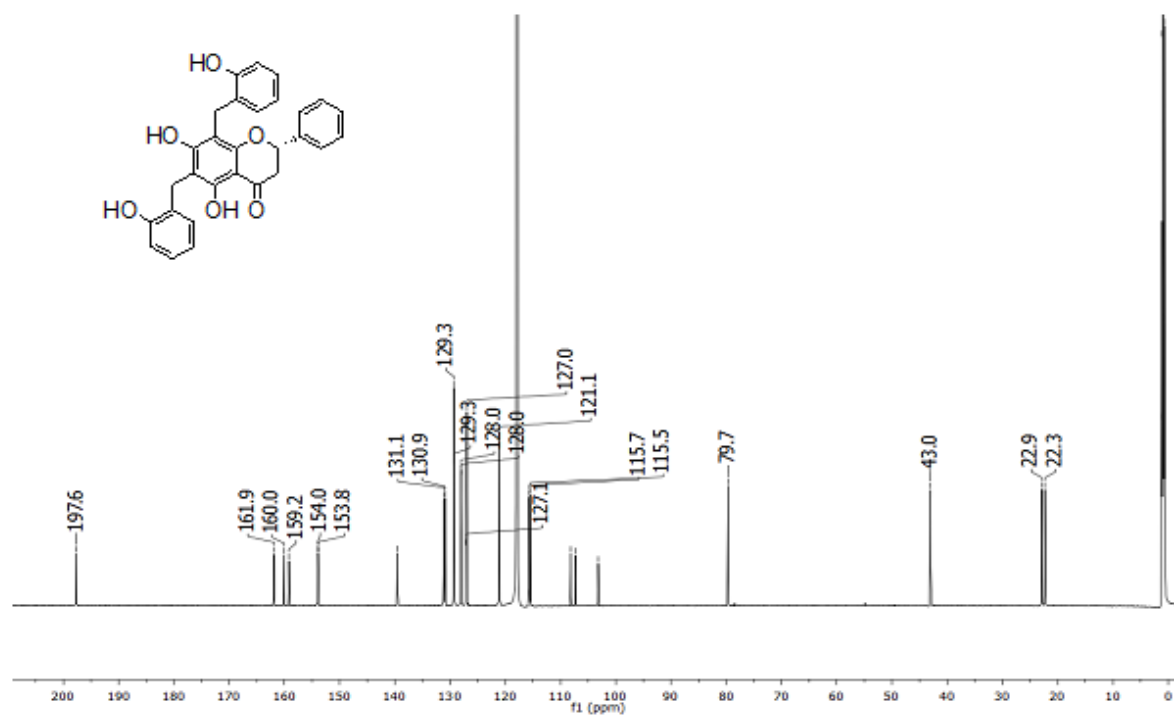


Figure S113. The ¹³C NMR Spectrum of Dichamanetin (15) Acquired at 800 MHz in CDCl₃.

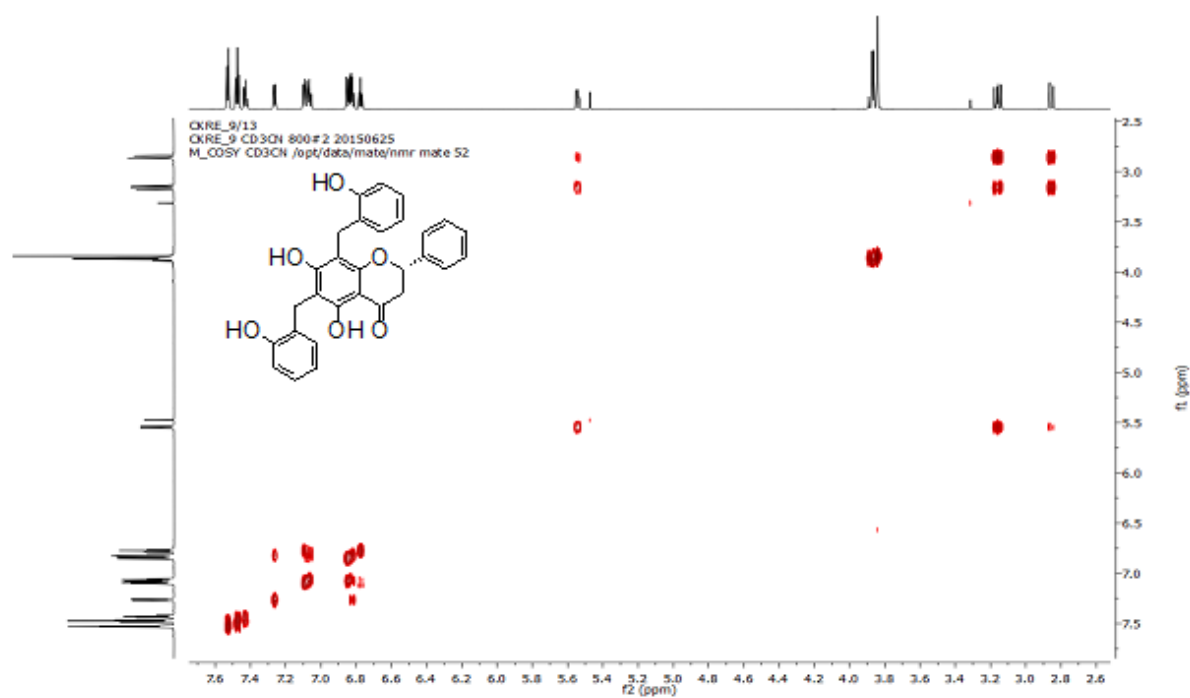


Figure S114. The COSY Spectrum of Dichamanetin (**15**) measured at 800 MHz in CDCl₃

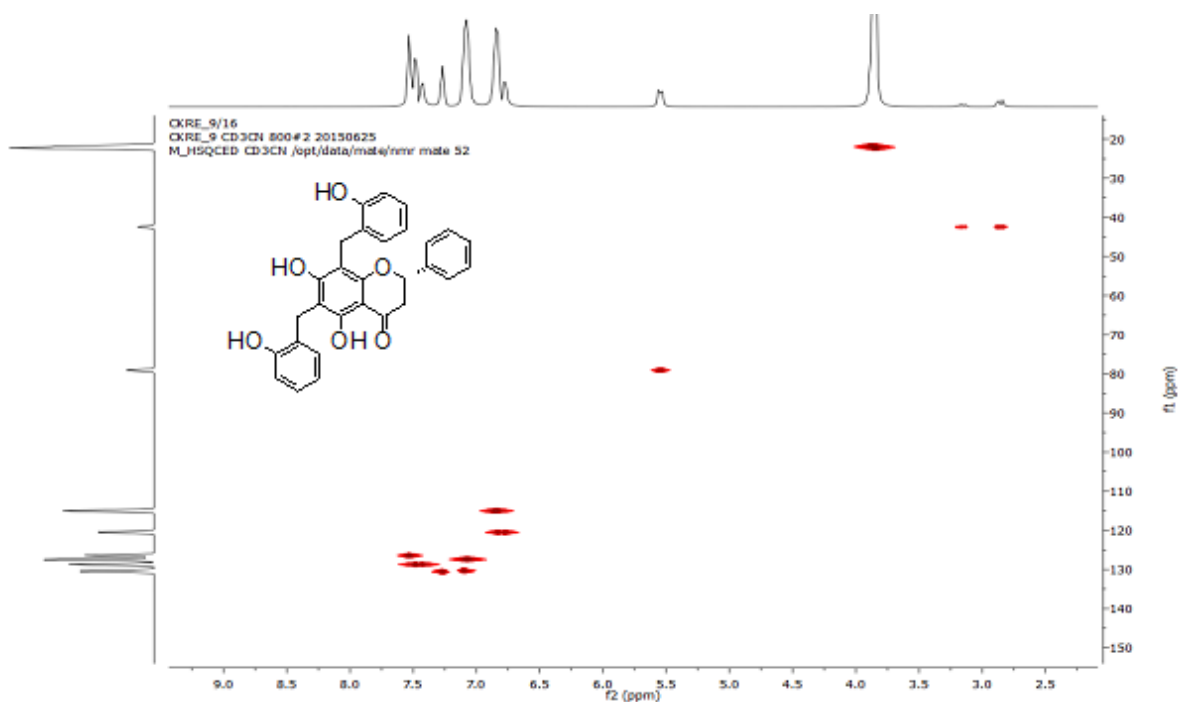


Figure S115. The HSQC Spectrum of Dichamanetin (**15**) measured at 800 MHz in CDCl₃

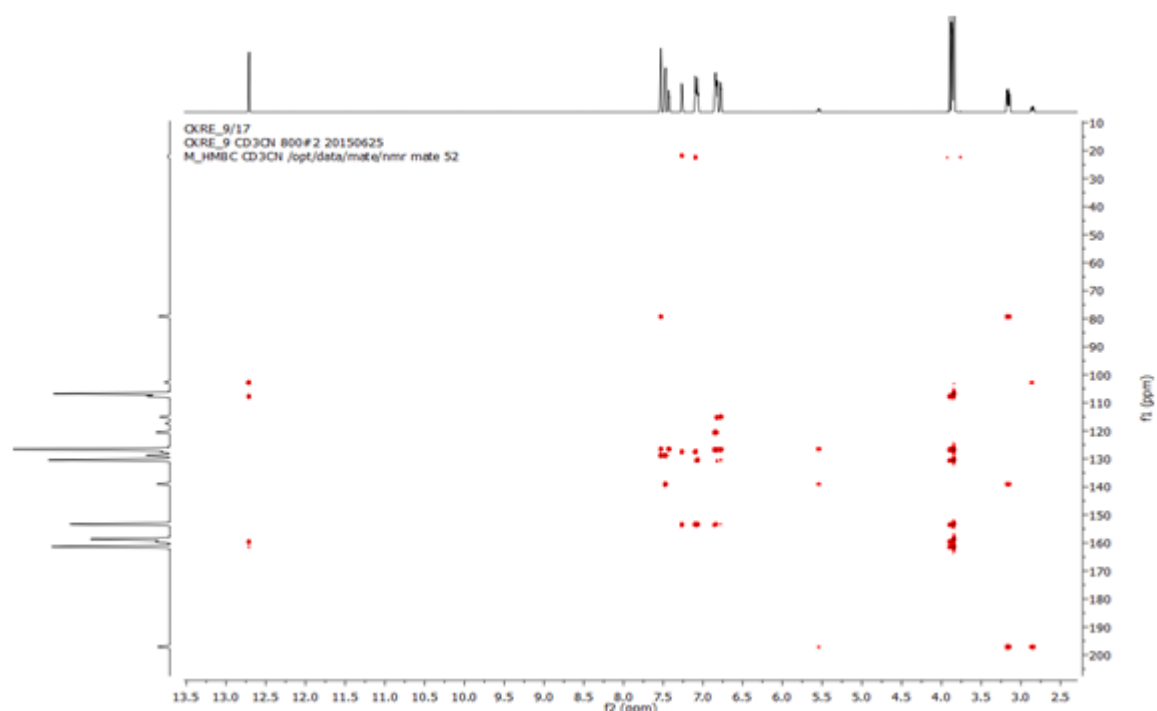


Figure S116. The HMBC Spectrum of Dichamanetin (**15**) measured at 800 MHz in CDCl₃

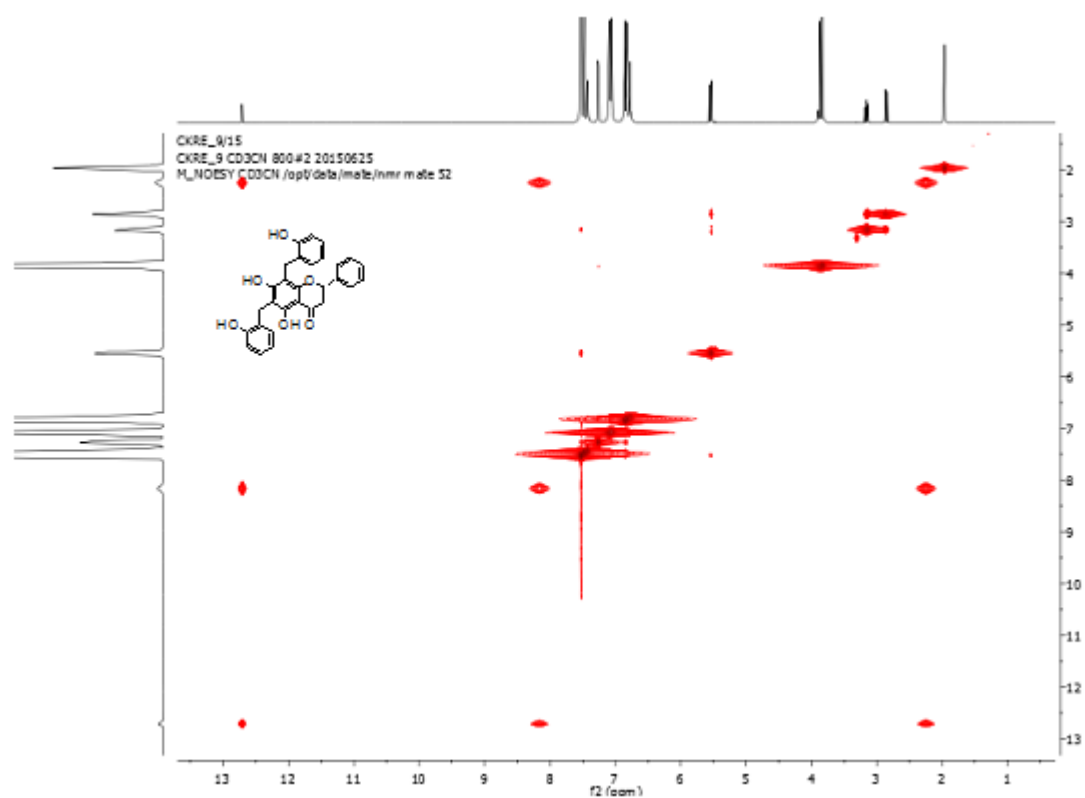


Figure S117. The NOESY Spectrum of Dichamanetin (**15**) measured at 800 MHz in CDCl₃

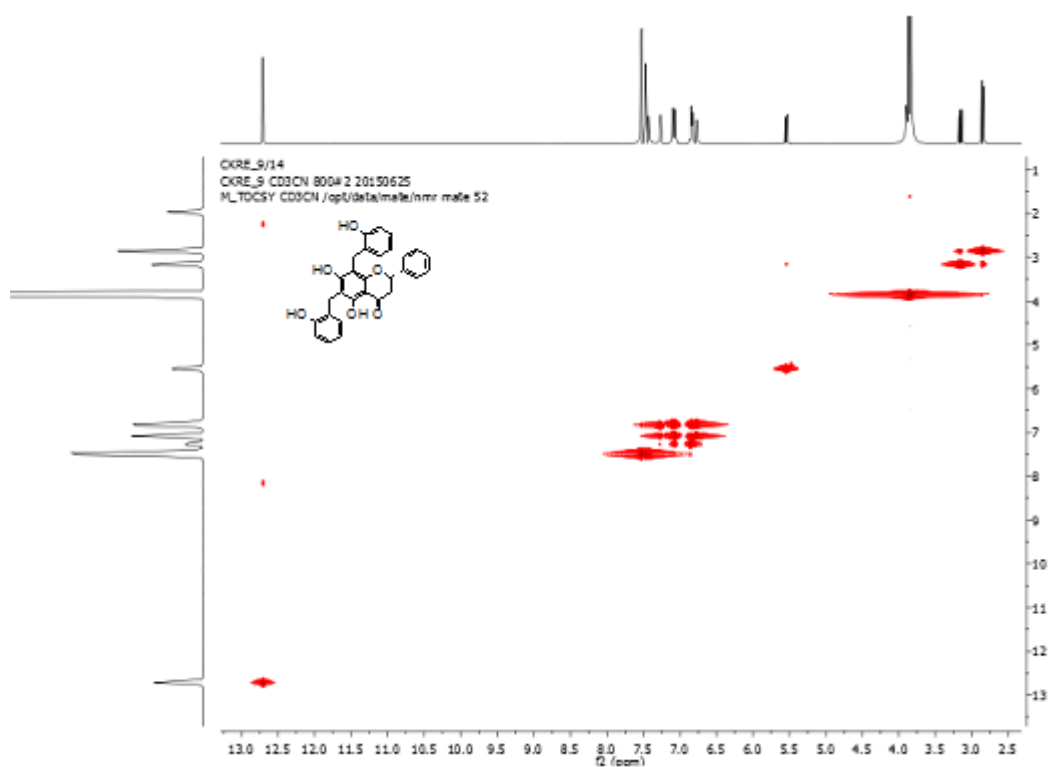


Figure S118. The TOCSY Spectrum of Dichamanetin (**15**) measured at 800 MHz in CDCl_3

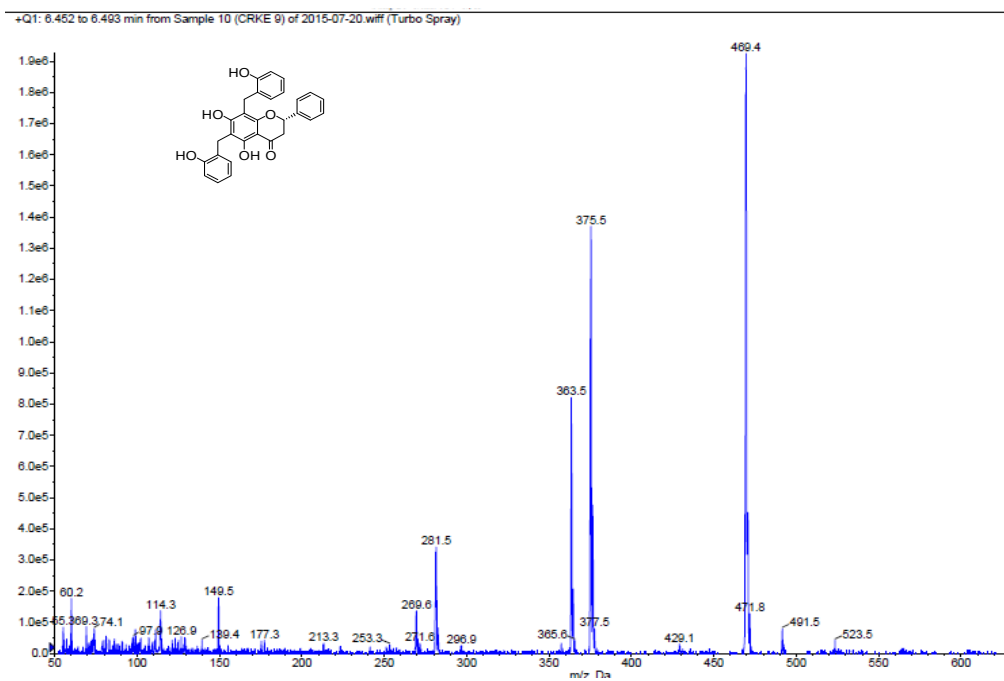


Figure S119. The LC-MS of Dichamanetin (**15**)

Spectroscopic data for polycarpol (16)

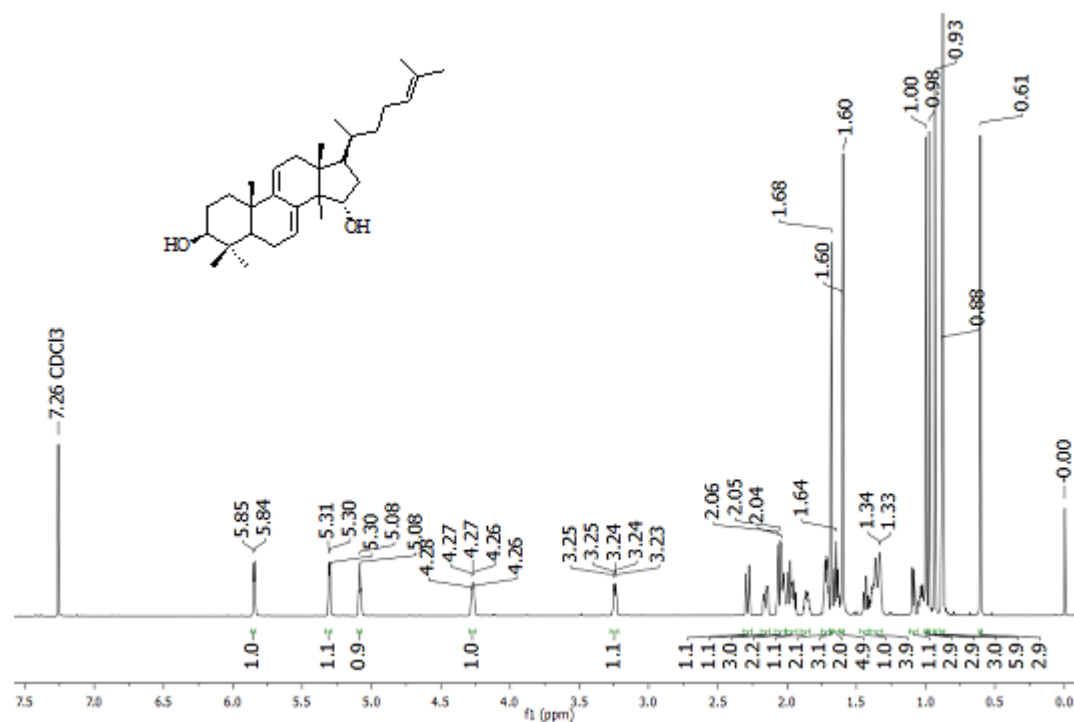


Figure S120. The ¹H NMR Spectrum of Polycarpol (16) measured at 800 MHz in CDCl₃.

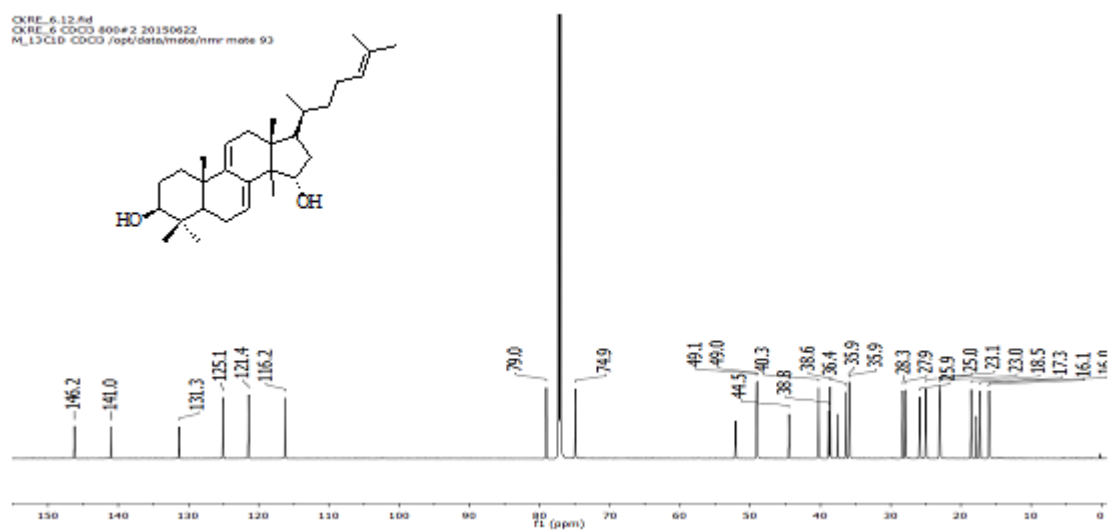


Figure S121. The ¹³C NMR Spectrum of Polycarpol (16) measured at 800 MHz in CDCl₃.

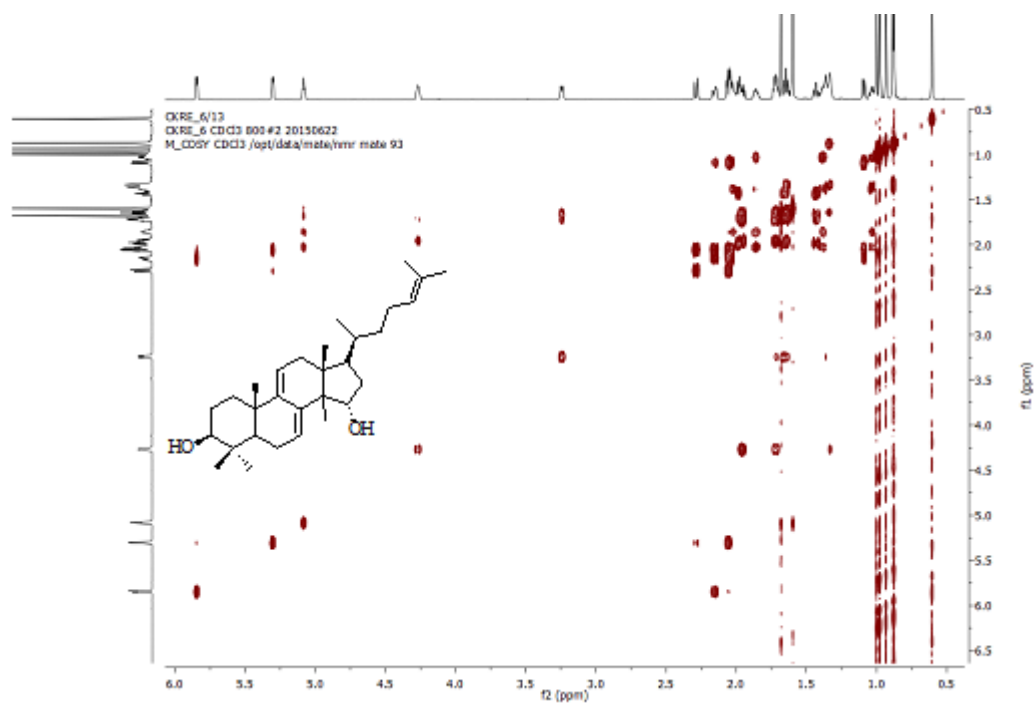


Figure S122. The COSY Spectrum of Polycarpol (**16**) measured at 800 MHz in CDCl₃.

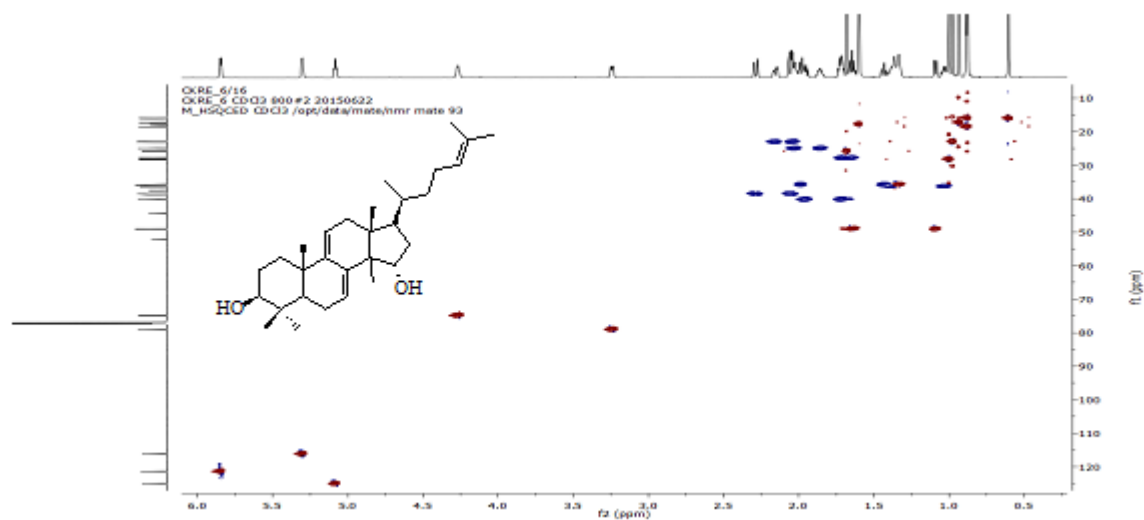


Figure S123. The HSQC Spectrum of Polycarpol (**16**) measured at 800 MHz in CDCl₃.

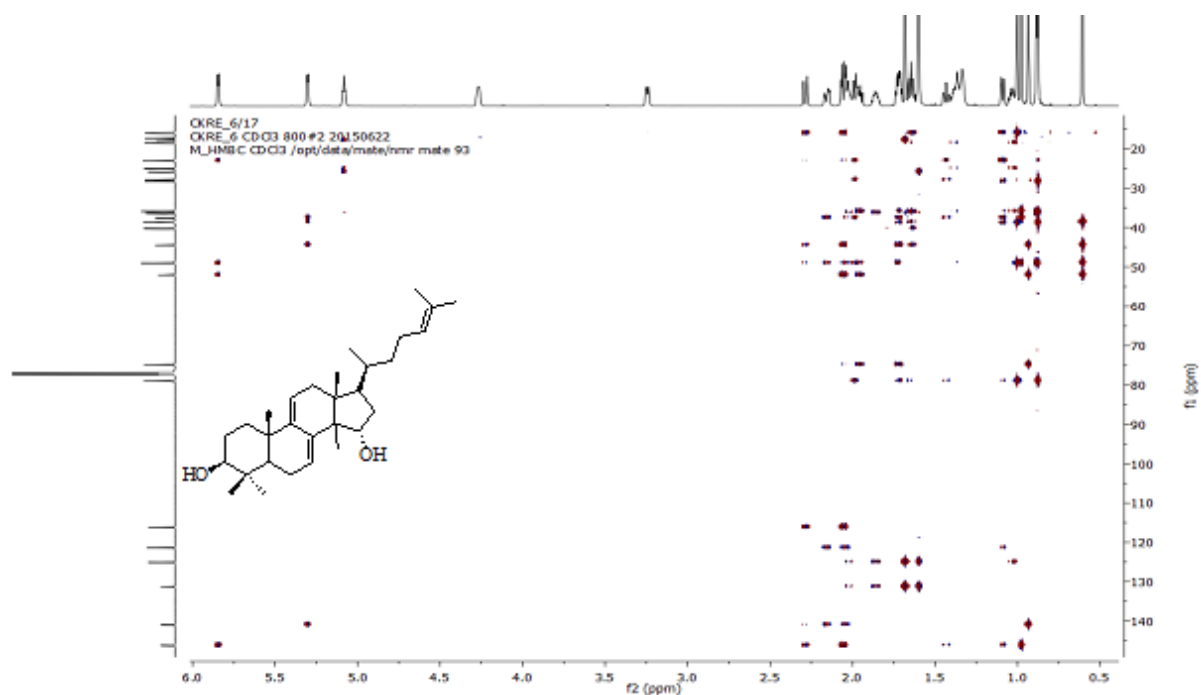


Figure S124. The HMBC Spectrum of Polycarpol (16) measured at 800 MHz in CDCl_3 .

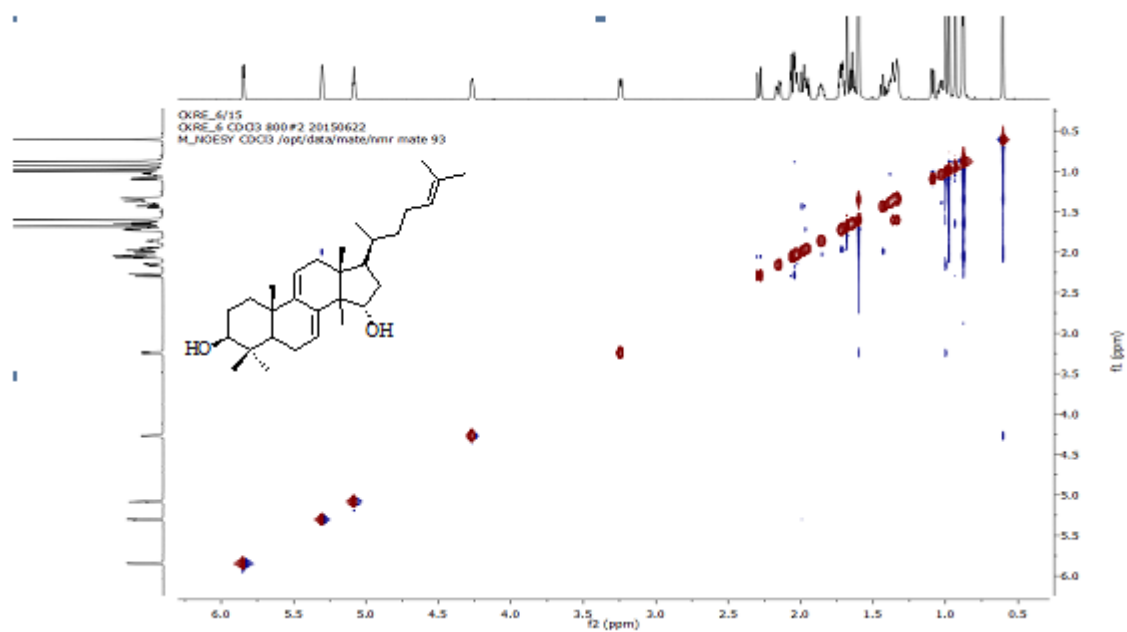


Figure S125. The NOESY Spectrum of Polycarpol (16) measured at 800 MHz in CDCl_3 .

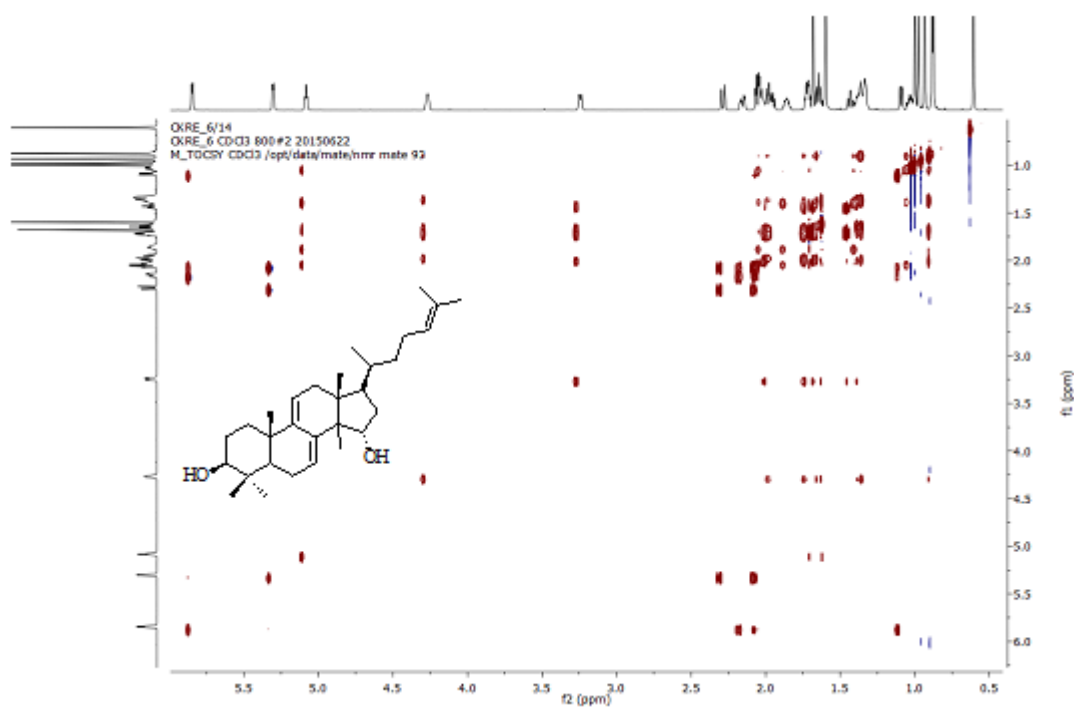


Figure S126. The TOCSY Spectrum of Polycarpol (**16**) measured at 800 MHz in CDCl_3 .

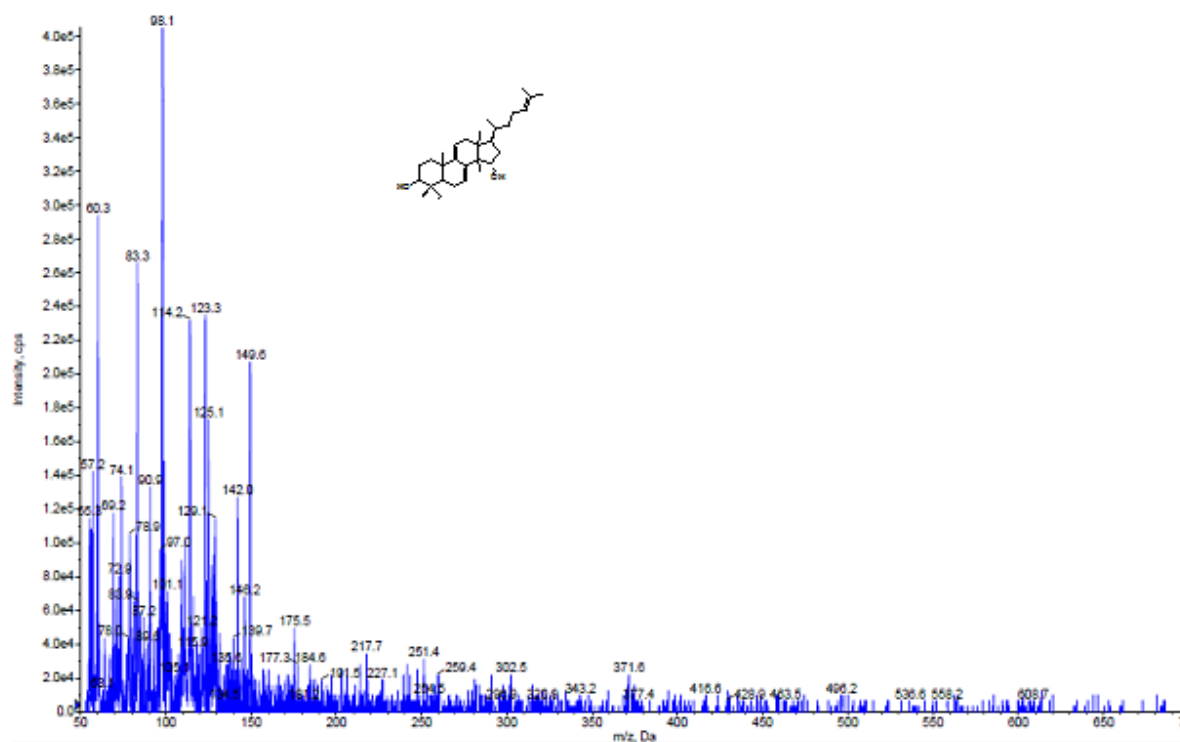


Figure S127. The LC-MS of Polycarpol (**16**)