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Supplementary material

SUPPLEMENTARY MATERIAL TO

Studies on the chemical compositions of *Hyptis suaveolens* (L.) Poit.

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NMR AND MASS DATA FOR **1**–**10**

The position of atoms listed in Tables S-I and S-II are related to the chemical structure of each compound, which are presented in Fig. 1.

TABLE S-I. ^{13}C-NMR data of **1**–**10** recorded at 125 MHz; **1**–**7** and **10** in DMSO-d_6; **8** and **9** in CD_3OD

Carbon	Compound									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
	δ / ppm									
1							171.5	172.2	46.1	43.6
2	155.8	164	163.7	148. 2	147.9	165.33	73.5	74.7	45.4	44.0
3	133.2	103.1	102.5	137. 4	136.9	104.16	36.5	37.9	41.9	43.1
4	177.1	182	182.2	177.5	176.8	183.19	127.9	128.8	72.9	67.6
5	161.1	161.7	149.6	162. 7	160.4	163.1	116.1	117.6	107.41	104.8
6	99.2	99.1	129.9	99. 4	99.1	98.67	145.9	146.8	148.8	146.0
7	166.1	164.4	161.1	165. 7	165.4	166.56	144.2	145.3	148.9	146.0
8	93.8	94.2	91.1	94. 6	94.3	93.21	115.1	116.6	110.43	107.5
9	156.5	157.5	146.2	158. 4	162.4	162.08	120.4	121.9	135.5	135.0
10	103.2	103.1	105	104.7	104.4	105.9		52.8	132.5	131.8
11									72.83	69.6
12									177. 2	178. 2
1′	121.5	121.4	121.3	124. 3	123.5	123.1	166.3	168.4	138	138.7
2′	115.2	128.7	128.4	116.4	130.5	129.3	115.7	115.3	109. 6	106. 6
3′	144.9	116.2	115.9	146. 4	116.1	116.9	145.2	148	153. 7	153. 2
4′	148.8	161.4	154.3	148. 9	158.1	158.67	125.7	127.6	138. 1	136. 4
5′	116.0	116.2	115.9	116. 2	116.1	116.9	113.7	114.2	153. 7	153. 2
6′	121	128.7	128.4	121. 8	130.5	129.3	146.1	146.1	109. 6	106. 6

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TABLE S-I. Continued

Carbon	Compound									
	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
	δ / ppm									
7′							148.8	149.8		
8′							117	116.4		
9′							122	123.3		
7–OCH_3			56.3			56.38				
OMe-3′, 5′									56.6	56.2
OMe-4′									61.1	60.3
OCH_2O									102.7	101.0
Sugar										
1″	101.1									
2″	74.1									
3″	77.5									
4″	69.9									
5″	76.5									
6″	61.0									

TABLE S-II. ^{1}H-NMR Data of **1**–**10** recorded at 500 MHz; **1**–**3**, **7** and **10** in DMSO-d_6; **4**–**6**, **8** and **9** in CD_3OD

Position	Compound				
	1	**2**	**3**	**4**	**5**
	δ_H / ppm; J / Hz				
1					
3		6.78 (1H, *s*)	6.80 (1H, *s*)		
4		6.19 (1H, *d*, J = 2.09)			
5					
6	6.12 (1H, *d*, J = 1.90)	6.19 (1H, *d*, J = 2.09)		6.18 (1H, *d*, J = 2.05)	6.19 (1H, *d*, J = 2.10)
7					
8	6.32 (1H, *d*, J = 1.58)	6.48 (1H, *d*, J = 2.11)	6.91 (1H, *s*)	6.39 (1H, *d*, J = 2.01)	6.40 (1H, *d*, J = 2.07)
9		12.95 (1H, *s*)			
10					
2′	7.56-7.58 (2H, *m*)	7.92 (1H, *d*, J = 8.88)	7.95 (1H, *d*, J = 8.8)	7.74 (1H, *d*, J = 2. 2′)	8.09 (1H, *dd*, J = 4.98, 8.95)
3′		6.92 (1H, d, J = 8.88)	6.93 (1H, *d*, J = 8.8)		6.91 (1H, *dd*, J = 4.88, 8.98)
5′	6.82 (1H, *t*)	6.92 (1H, *d*, J = 8.88)	6.93 (1H, *d*, J = 8.8)	6.89 (1H, *d*, J = 8. 50)	6.91 (1H, *dd*, J = 4.88, 8.98)

TABLE S-II. Continued

Position	Compound				
	1	**2**	**3**	**4**	**5**
	δ_H / ppm; *J* / Hz				
6′		7.92 (1H, *d*, *J* = 8.88)	7.95 (1H, *d*, *J* = 8.8)	7.64 (1H, *dd*, *J* = 2.2, 8.46)	8.09 (1H, *dd*, *J* = 4.98, 8.95)
5-OH	12.60 (1H, *s*)	12.95 (1H, *s*)	12.65 (1H, *s*)		
6-OH			8.69 (1H, *d*)		
4′-OH			10.34 (1H, *s*)		
7-OMe			3.91 (3H, *s*)		
1″	5.44 (1H, *d*, *J* = 7.4)				
2″–6″	3.06–3.35 (5H, *m*)				

Position	Compound				
	6	**7**	**8**	**9**	**10**
	δ_H / ppm; *J* / Hz				
1				4.54 (1H, *m*)	3.89 (1H, *d*, *J* = 7.74)
2		5.06 (1H, *m*)	5.20 (1H, *dd*, *J* = 7.51, 5.23)	3.02 (1H, *dd*, *J* = 5.12, 14.26)	2.73 (1H , *m*)
3	6.68 (1H, *s*)	2.97 (2H, *m*)	3.02 (2H, *m*)	2.73 (1H, *m*)	3.21 (1H , *dd*, *J* = 9.6, 5.4)
4				4.73 (1H, *d*, *J* = 9.82)	4.73 (1H, *d*, *J* = 9.82)
5		6.72 (1H, *d*, 1.52)	6.72 (1H, *d*, *J* = 1.96)	7.12 (1H, *s*)	7.05 (1H, *s*)
6	6.33 (1H, *d*, *J* = 2.24)				
8	6.70 (1H, *d*, *J* = 2.26)	6.67 (1H, *d*, *J* = 7.98)	6.71 (1H, *d*, *J* =8.18)	6.42 (1H, *s*)	5.98 (1H, *s*)
9		6.55 (1H, *dd*, *J* = 8.13, 1.69)	6.57 (1H, *dd*, *J* = 8.06, 1.99)		
10			3.68 (2H, *s*)		
11				4.12 (1H, *dd*, *J* = 8.75, 10.46); 4.54 (1H, *m*)	4.40 (1H, *dd*, *J* = 6.54, 9.0); 4.49 (1H, *m*)
2′	7.97 (1H, *d*, *J* = 8.77)	6.27 (1H, *d*, 15.8)	6.26 (1H, *d*, *J* = 15.89)	6.44 (1H, *s*)	6.59 (2H, *s*)
3′	7.04 (1H, *d*, *J* = 8.74)	7.48 (1H, *d*, *J* = 15.8)	7.56 (1H, *d*, *J* = 15.86)		
5′	7.04 (1H, *d*, *J* = 8.74)	7.09 (1H, *s*)	7.05 (1H, *d*, *J* = 1.9)		
6′	7.97 (1H, *d*, *J* = 8.77)			6.44 (1H, *s*)	6. 59 (2H, *s*)
8′		6.8 (1H, *d*, *J* = 8.22)	6.78 (1H, *d*, *J* = 8.18)		

TABLE S-II. Continued

Position	Compound				
	6	**7**	**8**	**9**	**10**
	δ_H / ppm; *J* / Hz				
9′		7.01 (1H, *dd*, *J* = 8.25, 1.6)	6.94 (1H, *dd*, *J* = 8.19, 1.98)		
5-OH	12.99 (1H, *s*)				
7-OMe	3.93 (3H, *s*)				
OMe-3′, 5′				3.72 (6H, *s*)	3.74 (6H, *s*)
OMe-4′				3.71 (3H, *s*)	3.68 (3H, *s*)
OCH_2O				5.93 (2H, *dd*, *J* = 0.94, 7.55)	5.91 (2H, *d*, *J* = 5.83)

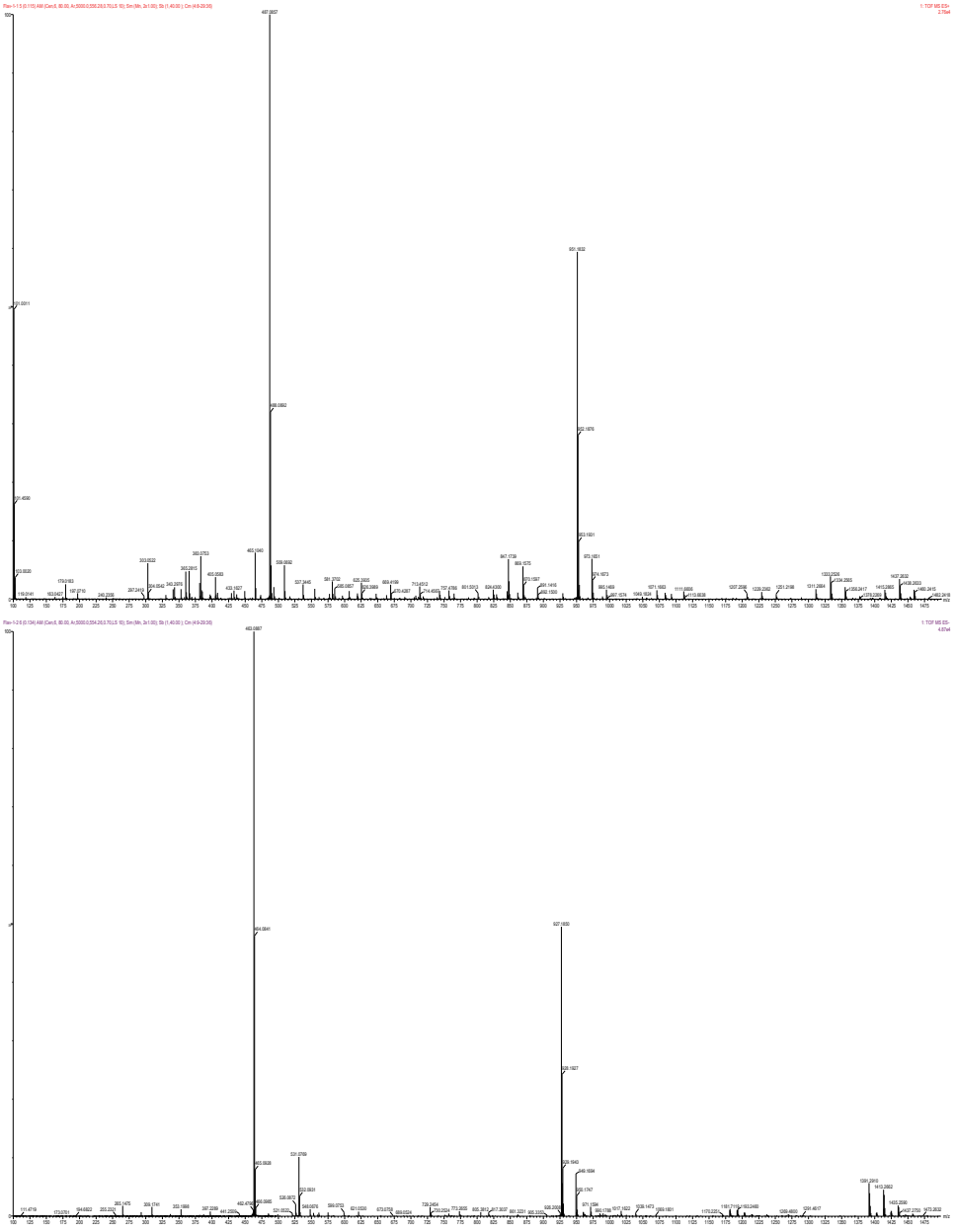

Fig. S-1A. EI-MS spectrum of quercetin-3-*O*-β-D-glucopyranoside (**1**).

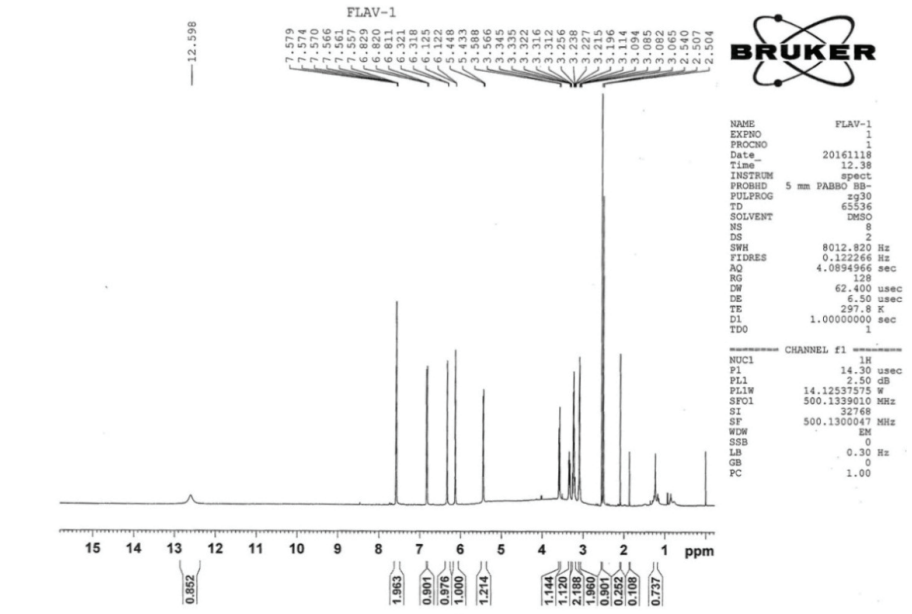

Fig. S-1B. ^{1}H-NMR spectrum of quercetin-3-*O*-β-D-glucopyranoside (**1**).

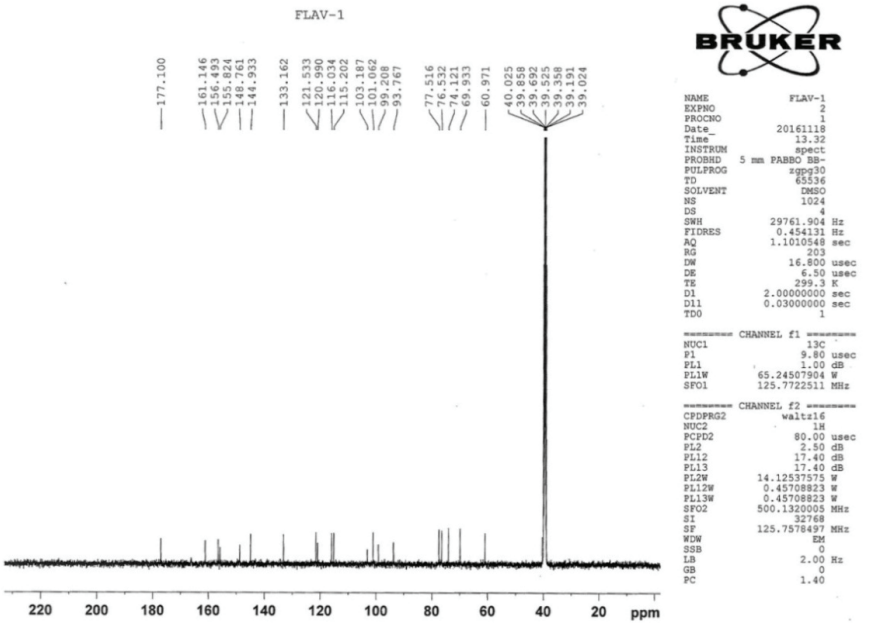

Fig. S1-C. ^{13}C-NMR spectrum of quercetin-3-*O*-β-D-glucopyranoside (**1**).

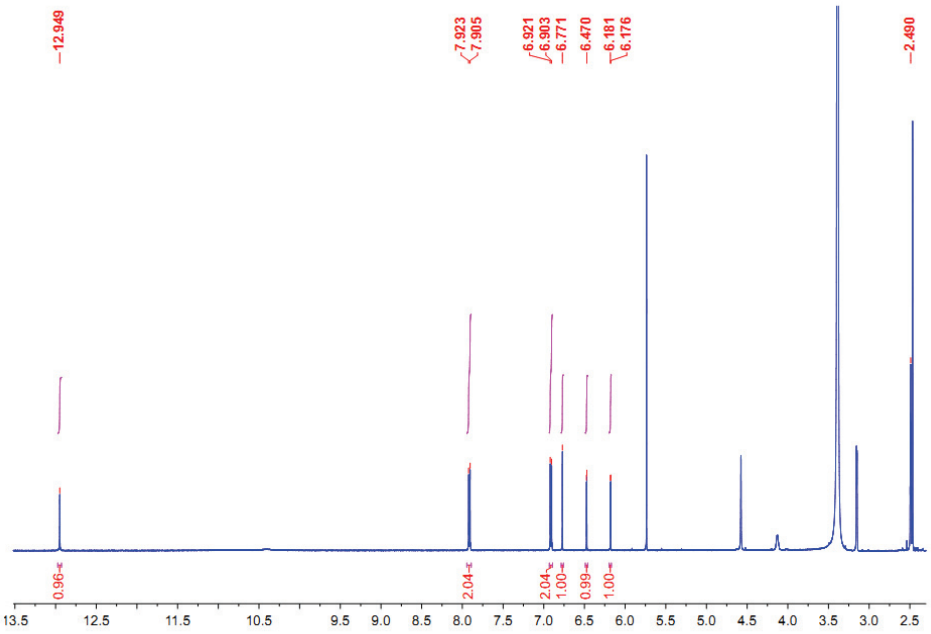

Fig. S-2A. ^{1}H-NMR spectrum of apigenin (**2**).

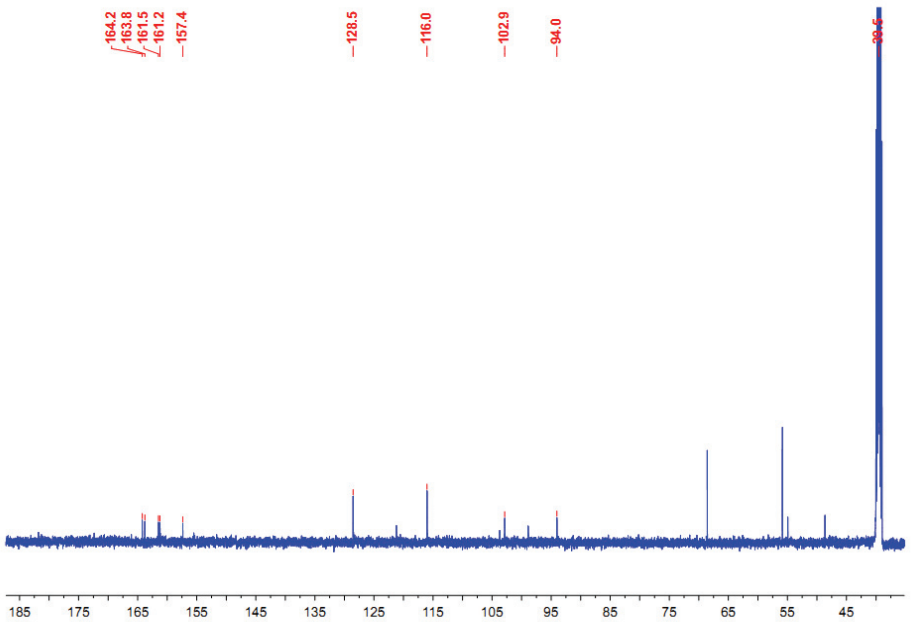

Fig. S-2B. ^{13}C-NMR spectrum of apigenin (**2**).

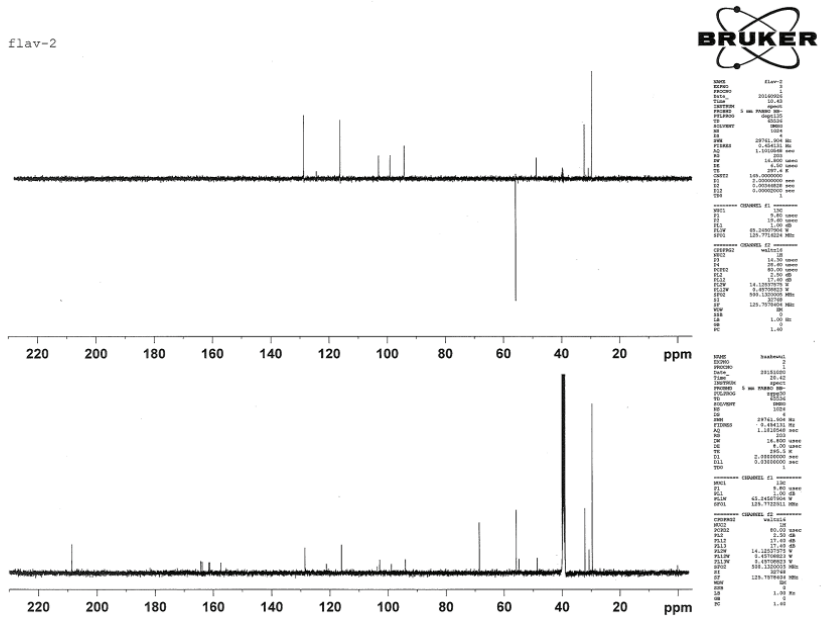

Fig. S-2C. DEPT spectrum of apigenin (**2**).

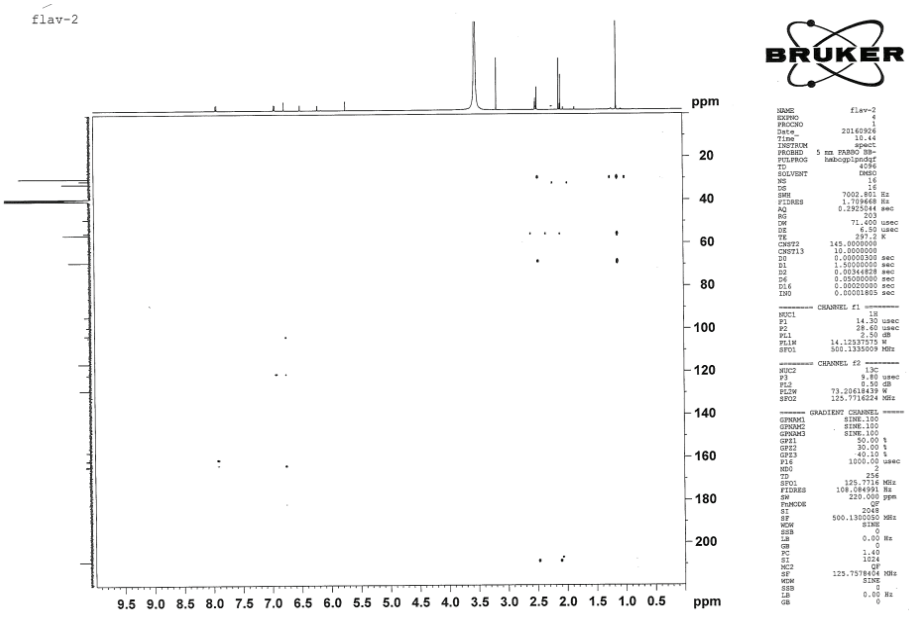

Fig. S-2D. HMBC spectrum of apigenin (**2**).

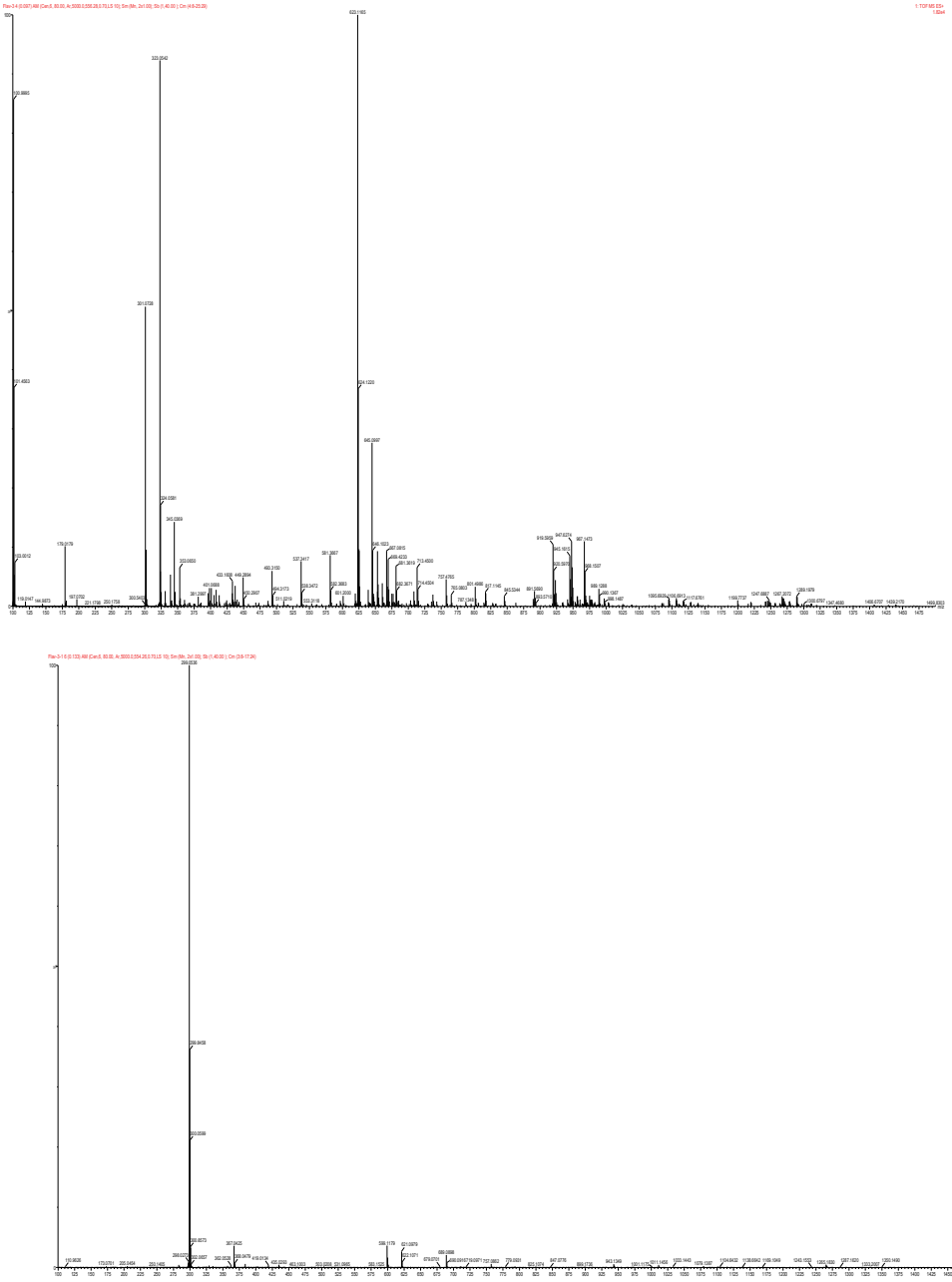

Fig. S-3A. EI-MS spectrum of sorbifolin (**3**).

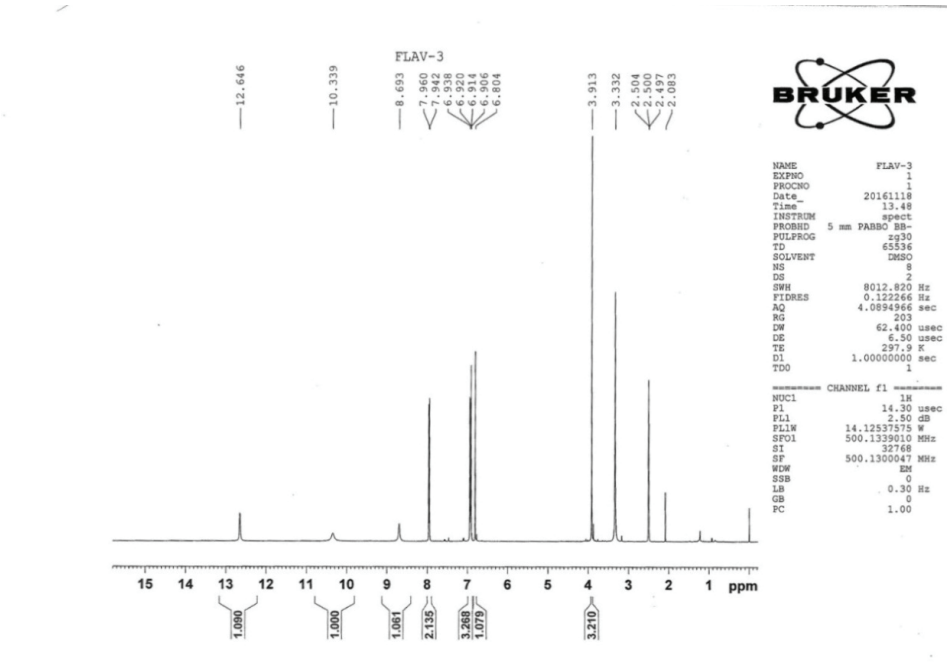

Fig. S-3B. ^{1}H-NMR spectrum of sorbifolin (**3**).

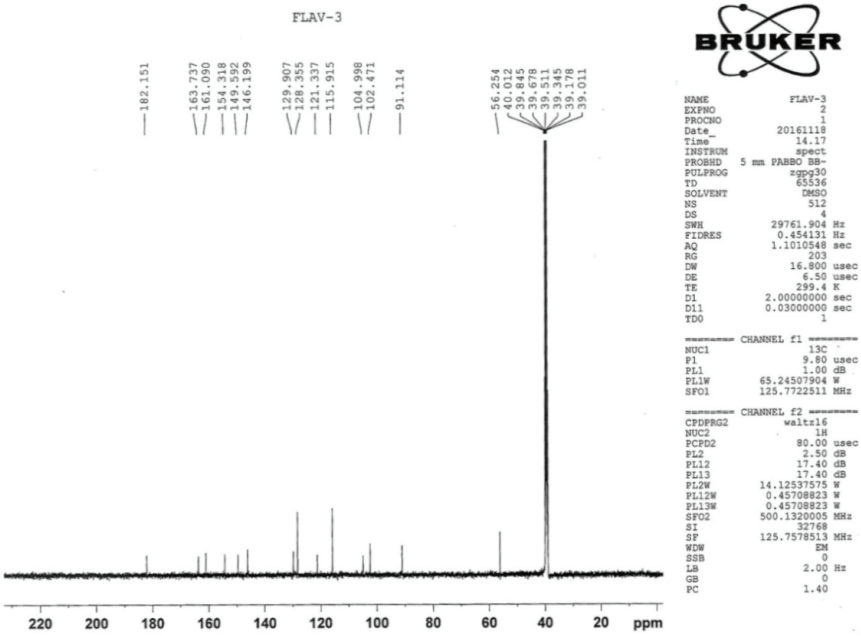

Fig. S-3C. ^{13} C-NMR spectrum of sorbifolin (**3**).

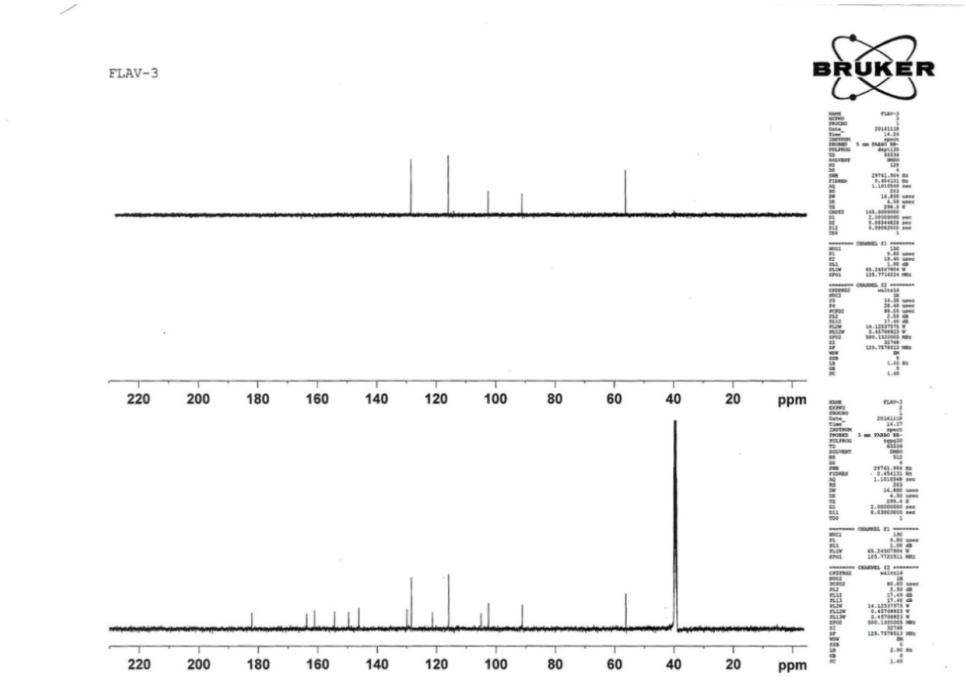

Fig. S-3D. DEPT spectrum of sorbifolin (**3**).

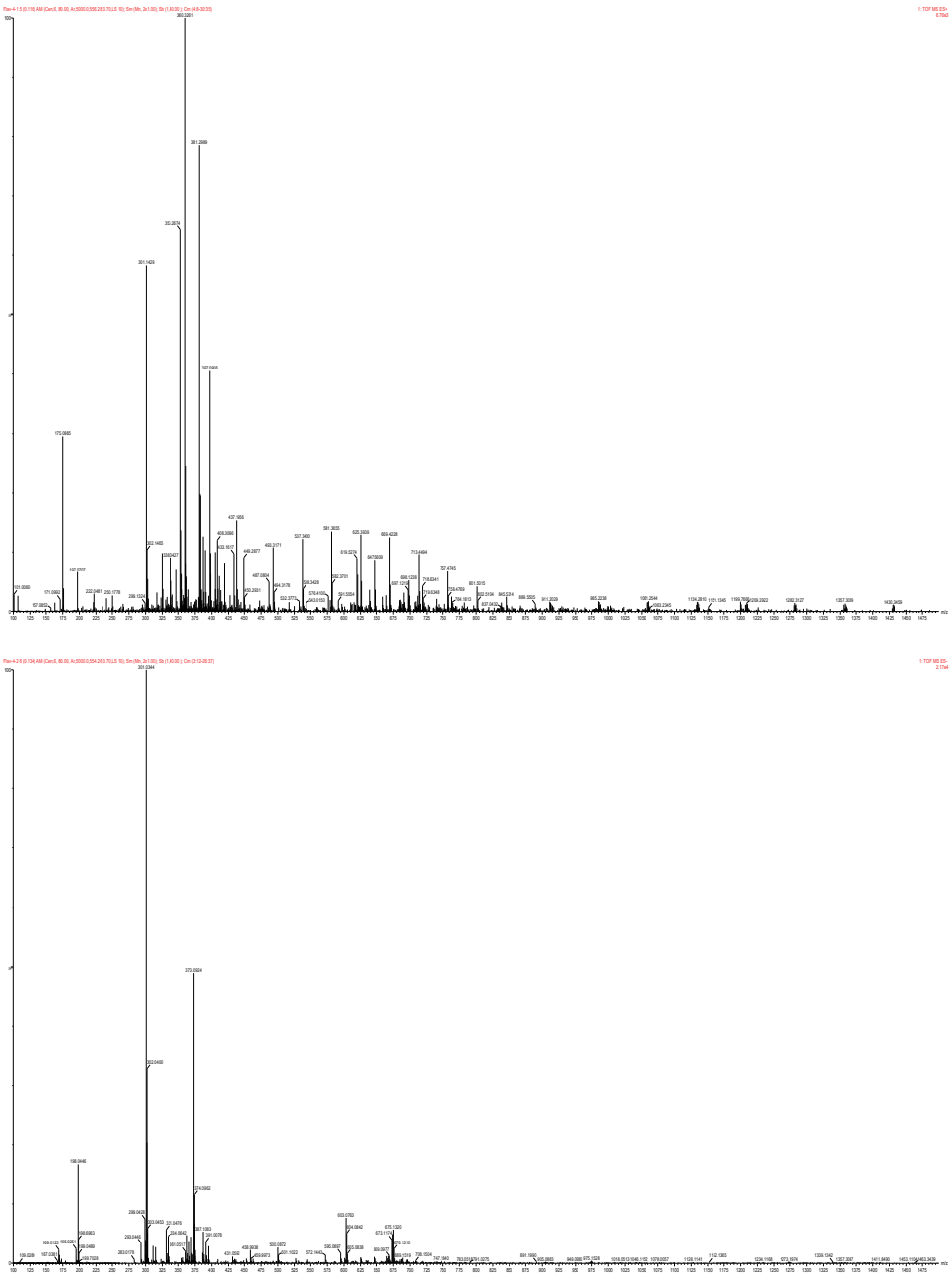

Fig. S-4A. EI-MS spectrum of quercetin (**4**).

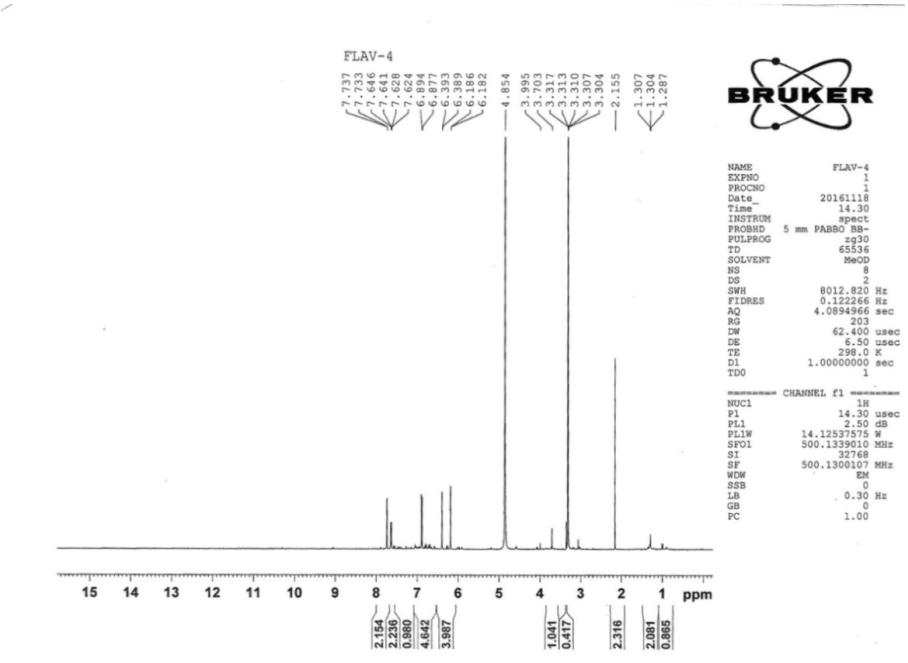

Fig. S-4B. ^{1}H-NMR spectrum of quercetin (**4**).

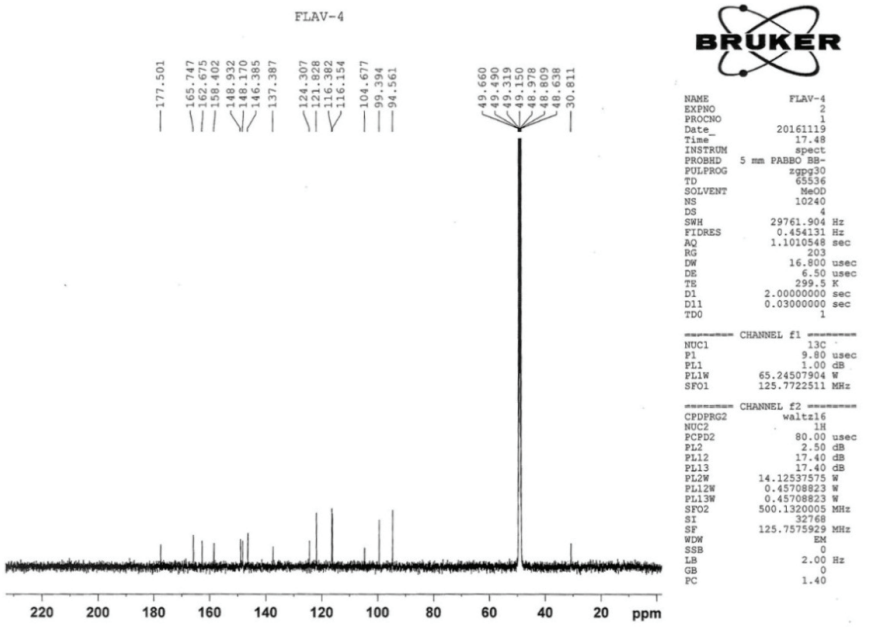

Fig. S-4C. ^{13}C-NMR spectrum of quercetin (**4**).

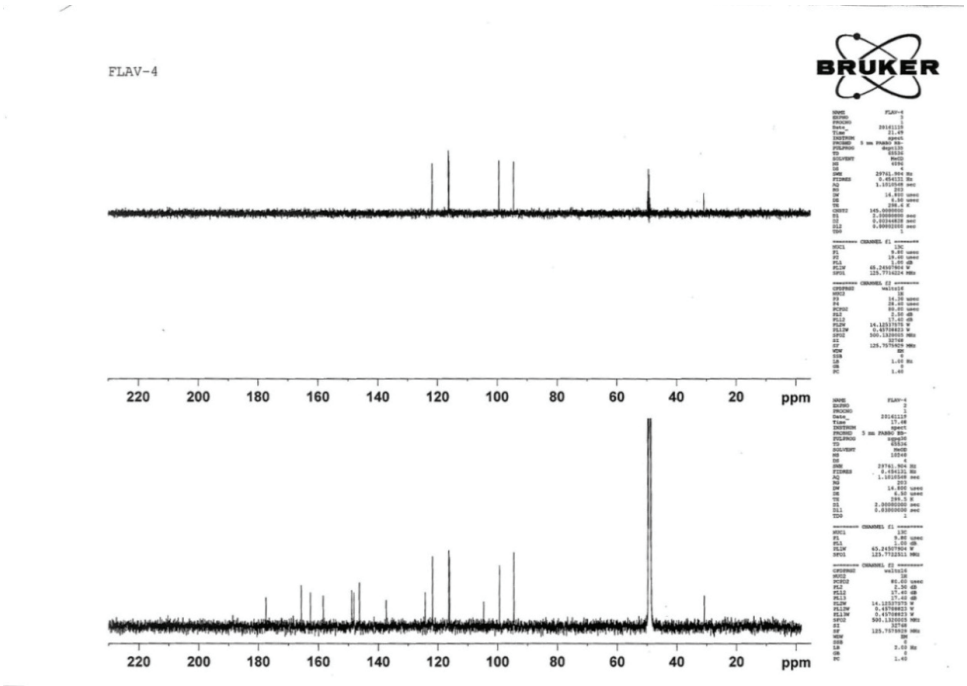

Fig. S-4D. DEPT spectrum of quercetin (**4**).

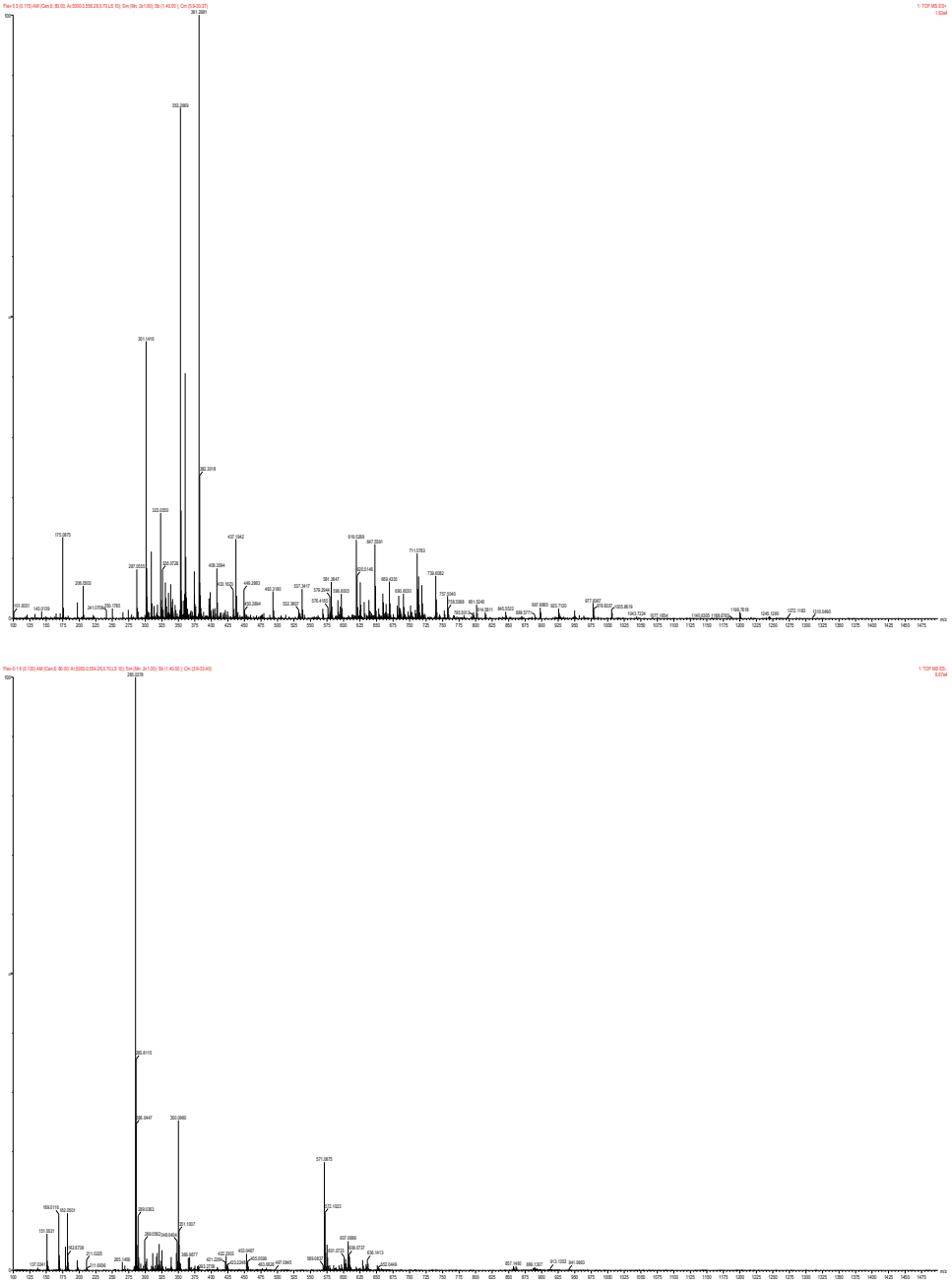

Fig. S-5A. EI-MS spectrum of kaempferol (**5**).

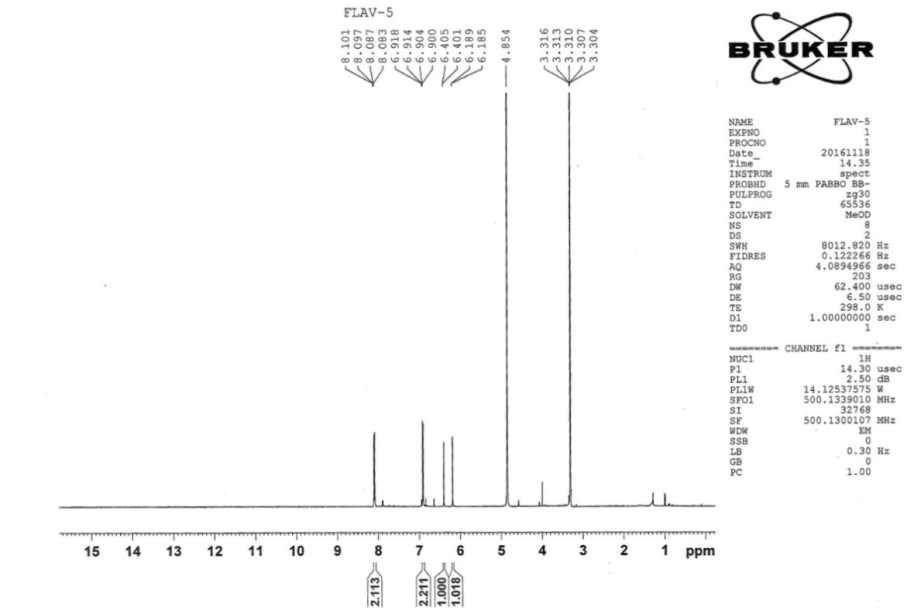

Fig. S-5B. ^{1}H-NMR spectrum of kaempferol (**5**).

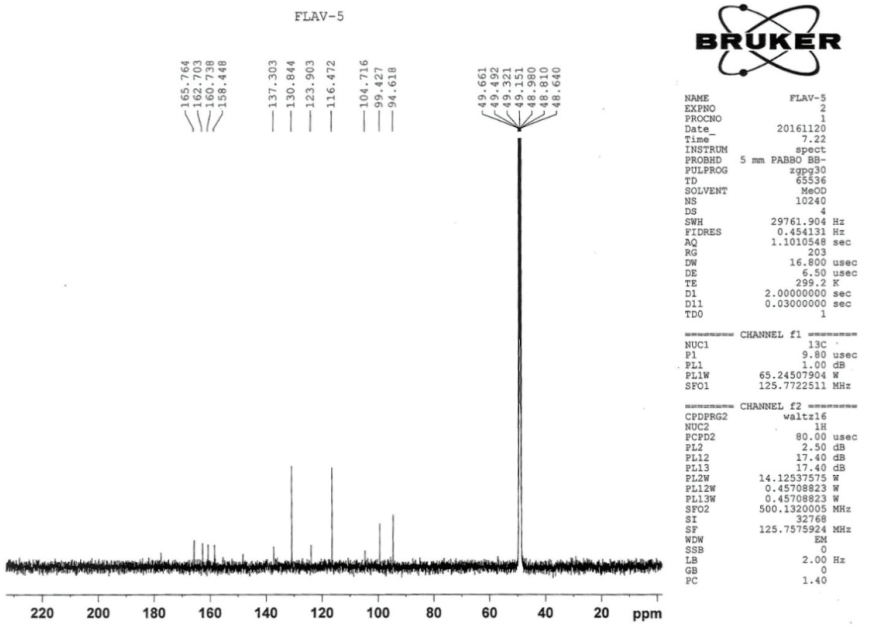

Fig. S-5C. ^{13}C-NMR spectrum of kaempferol (**5**).

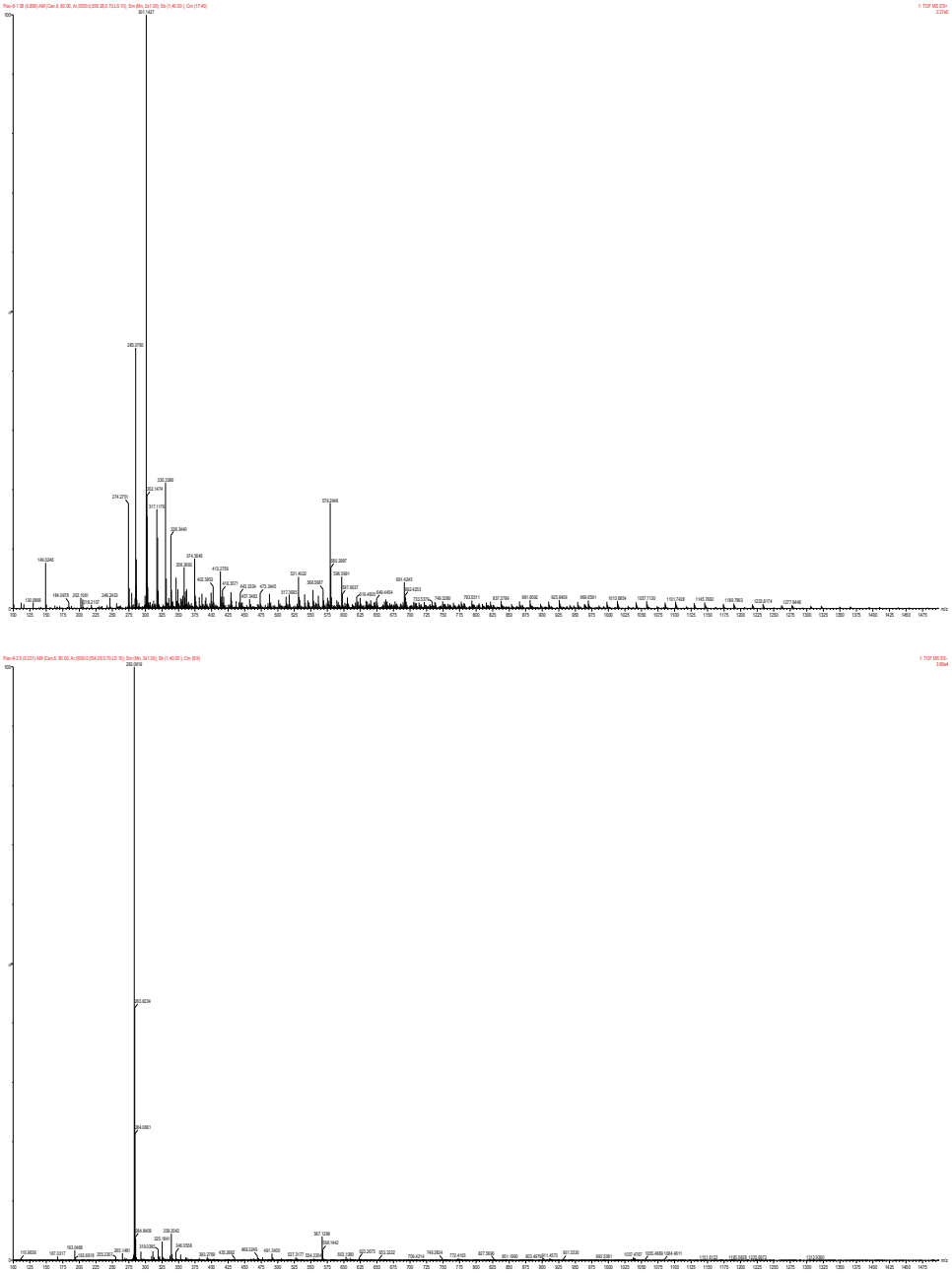

Fig. S-6A. EI-MS spectrum of genkwanin (**6**).

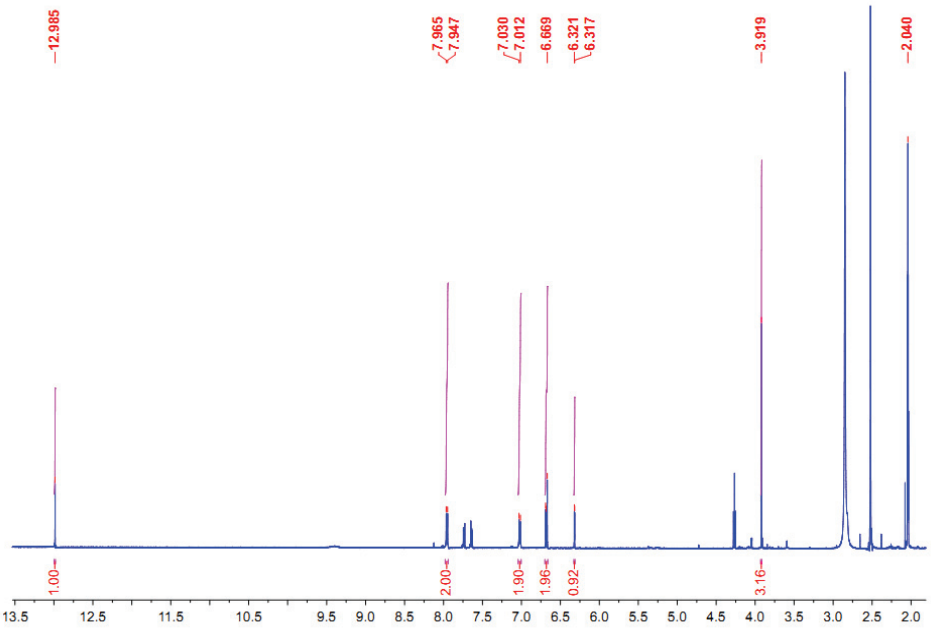

Fig. S-6B. ^{1}H-NMR spectrum of genkwanin (**6**).

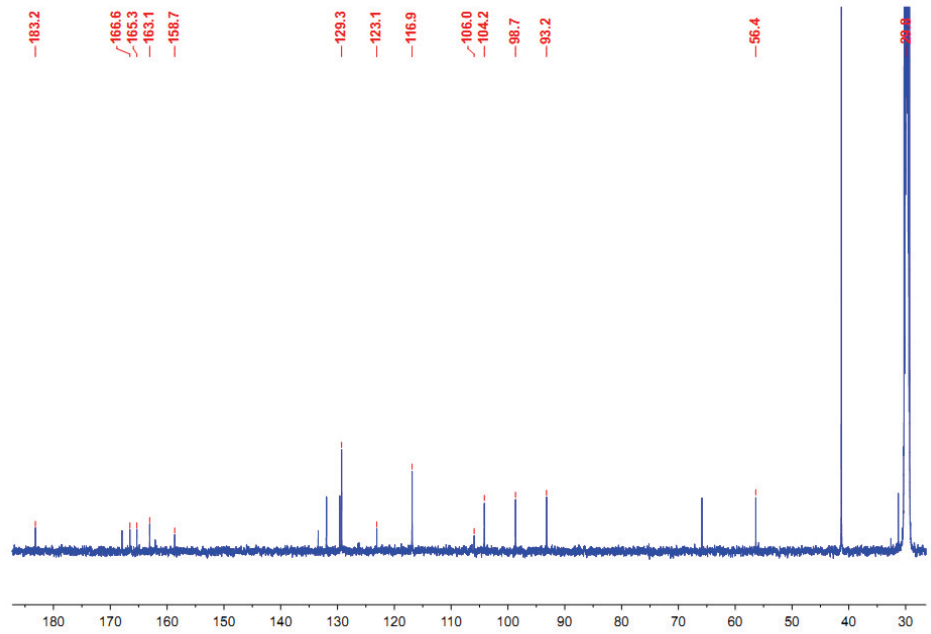

Fig. S-6C. ^{13}C-NMR spectrum of genkwanin (**6**).

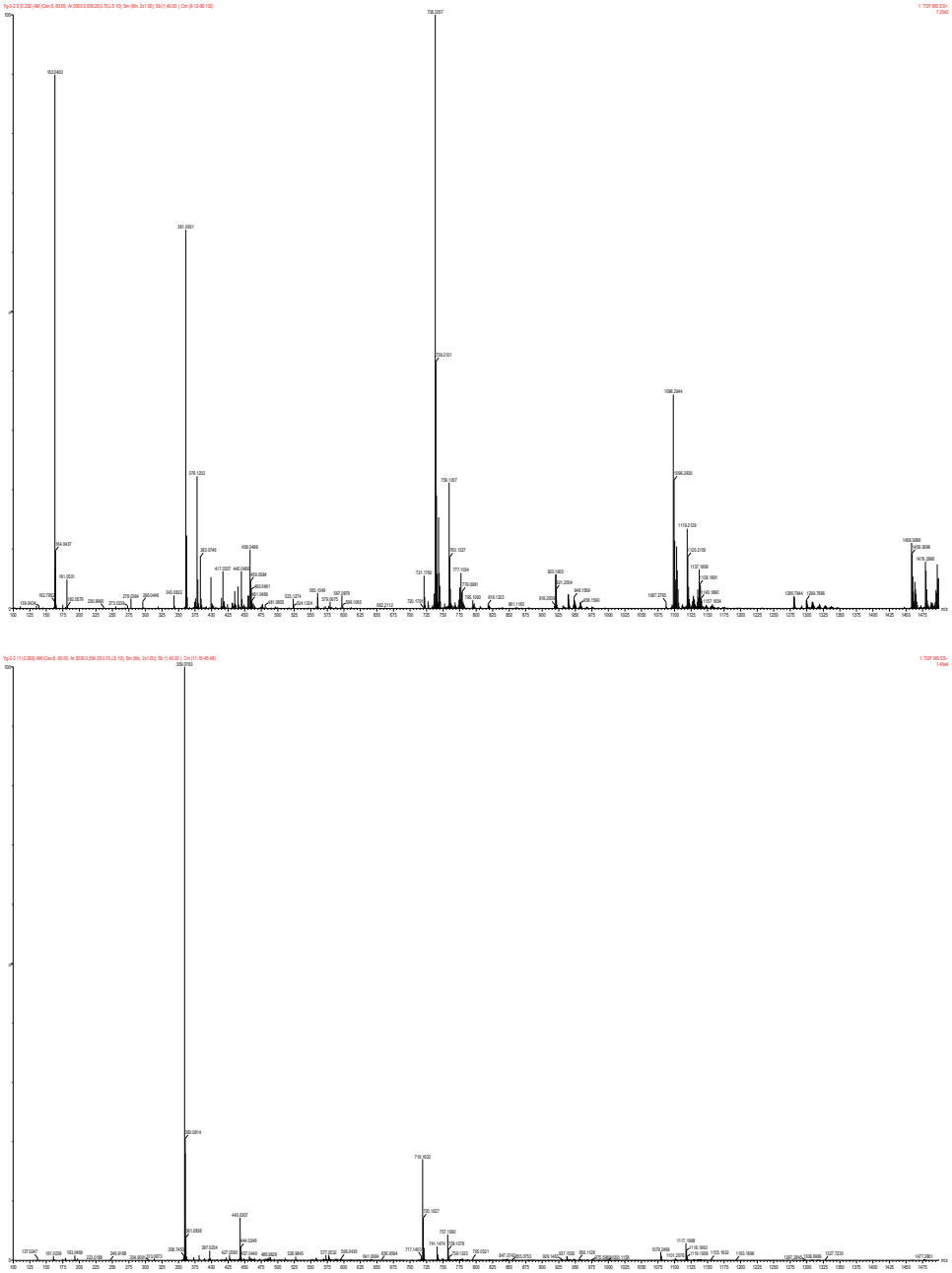

Fig. S-7A. EI-MS spectrum of rosmarinic acid (**7**).

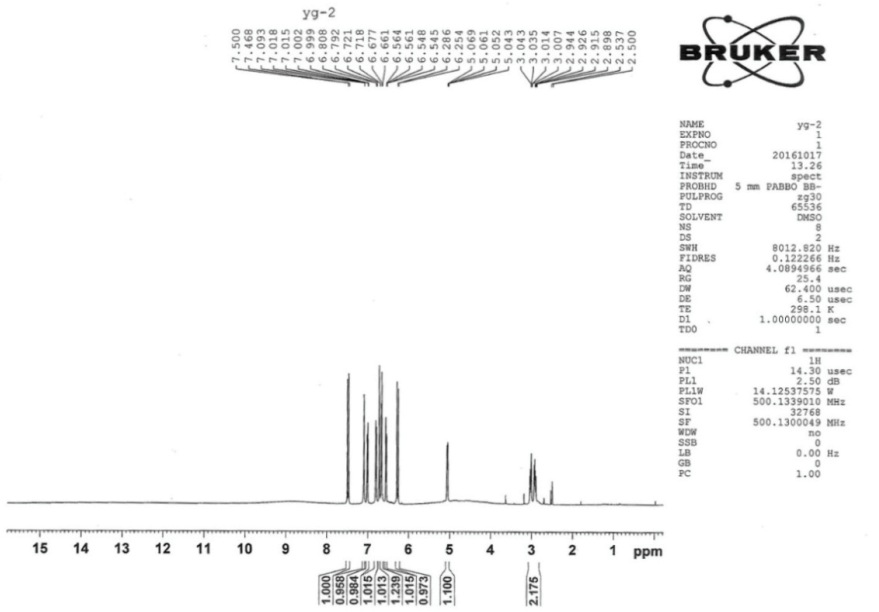

Fig. S-7B. ^{1}H-NMR spectrum of rosmarinic acid (**7**).

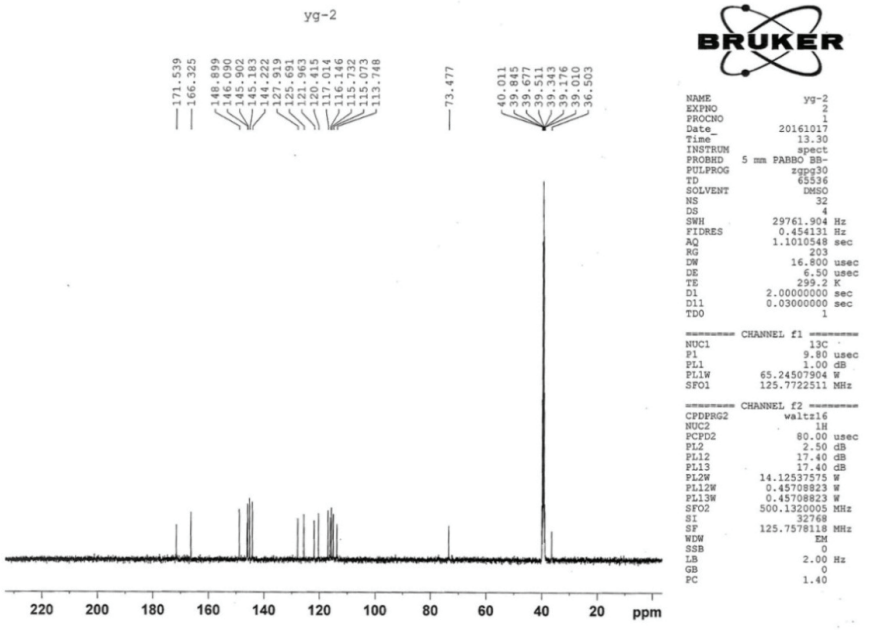

Fig. S-7C. ^{13}C-NMR spectrum of rosmarinic acid (**7**).

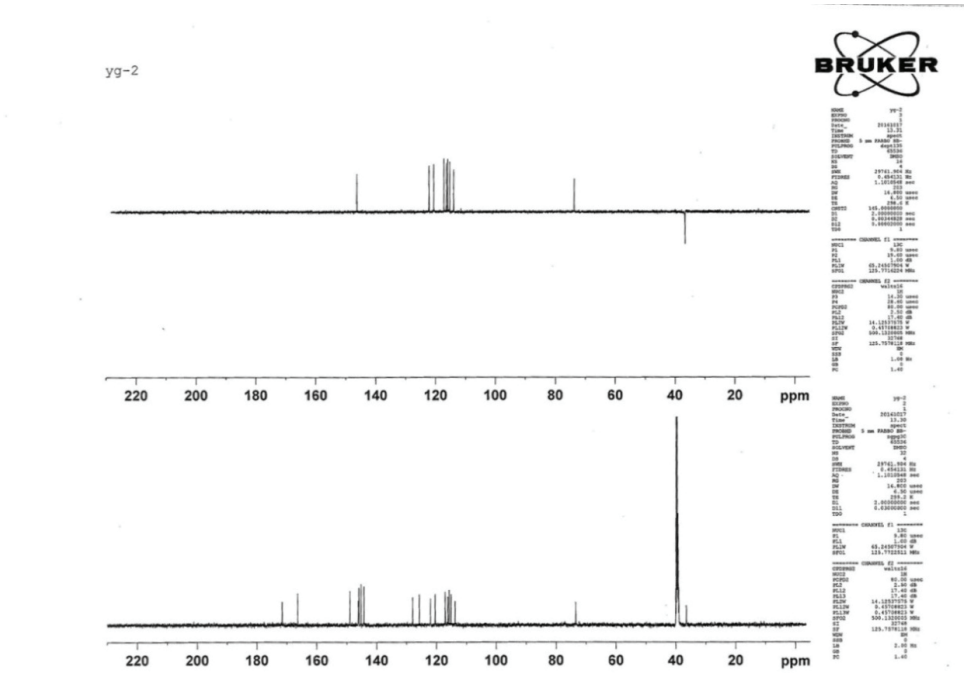

Fig. S-7D. DEPT spectrum of rosmarinic acid (**7**).

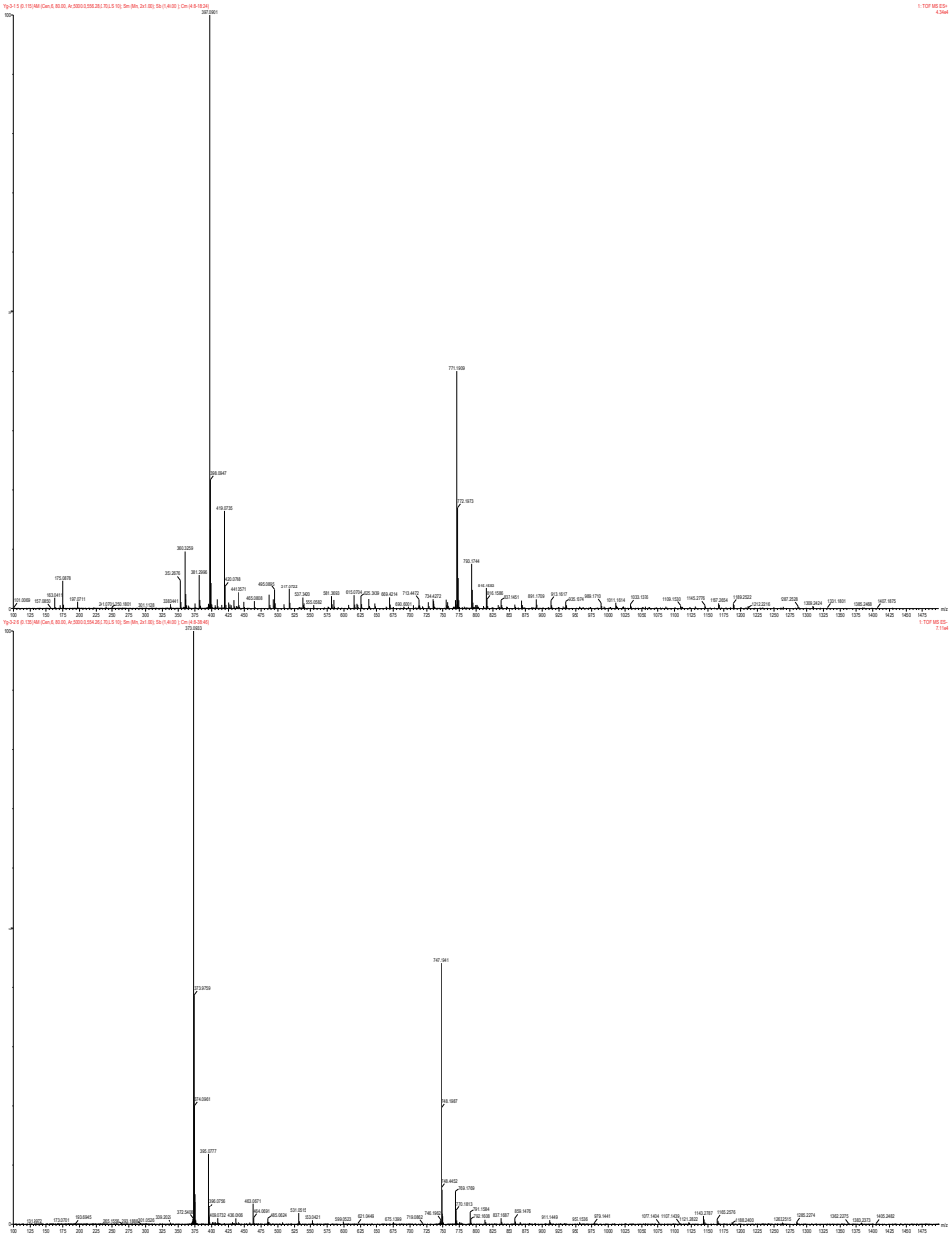

Fig. S-8A. EI-MS spectrum of methylrosmarinate (**8**).

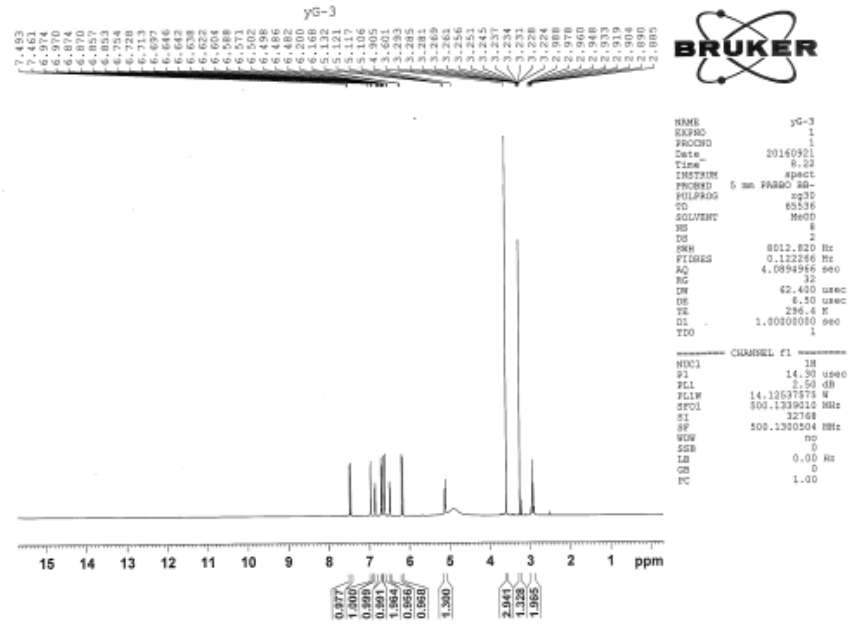

Fig. S-8B. ^{1}H-NMR spectrum of methylrosmarinate (**8**).

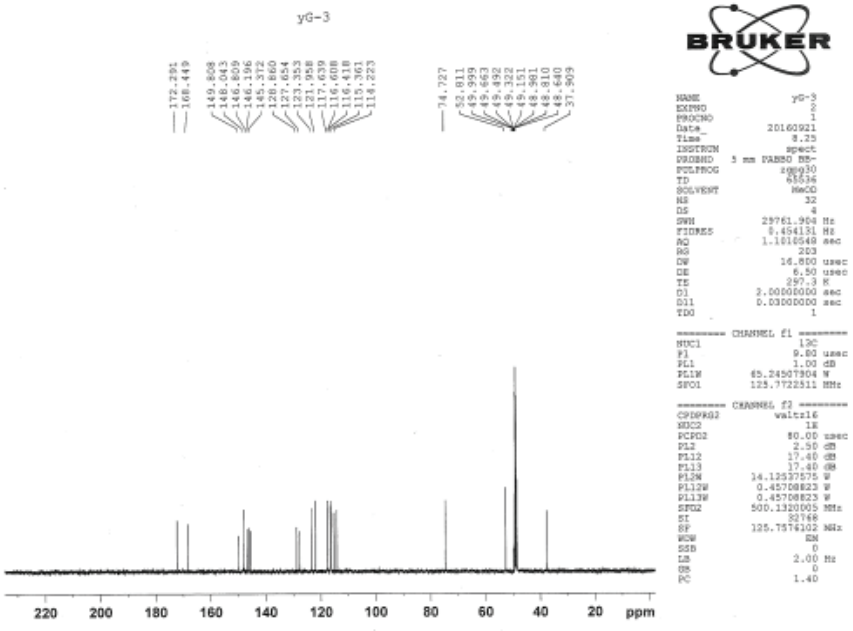

Fig. S-8C. ^{13}C-NMR spectrum of methylrosmarinate (**8**).

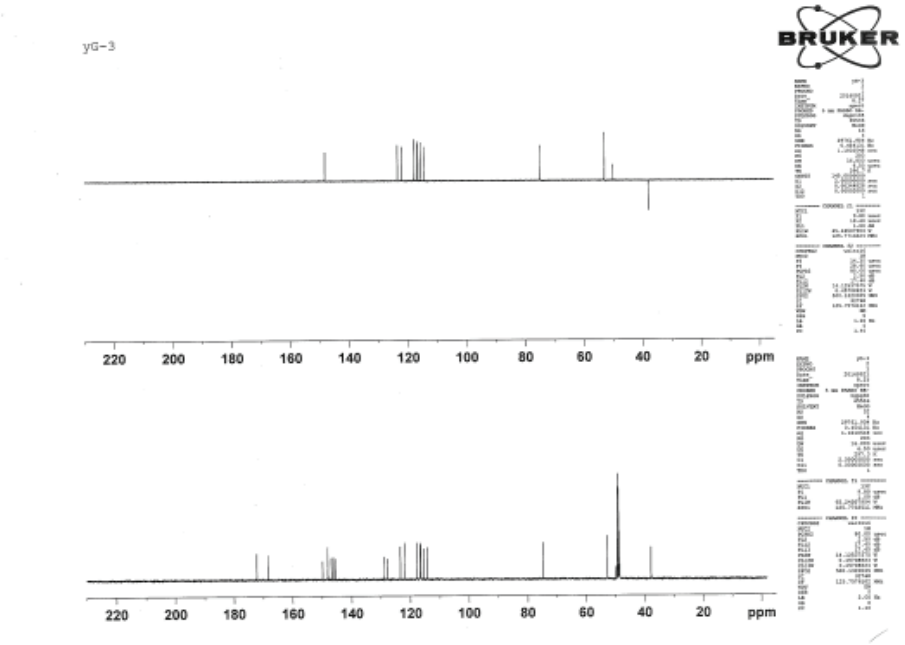

Fig. S-8D. DEPT spectrum of methylrosmarinate (**8**).

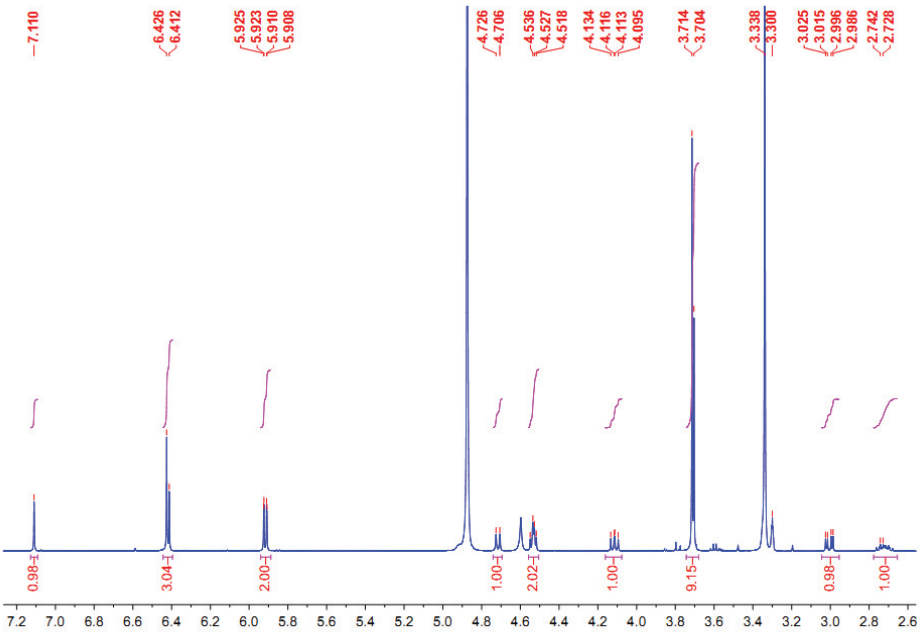

Fig. S-9A. ^{1}H-NMR spectrum of podophyllotoxin (**9**).

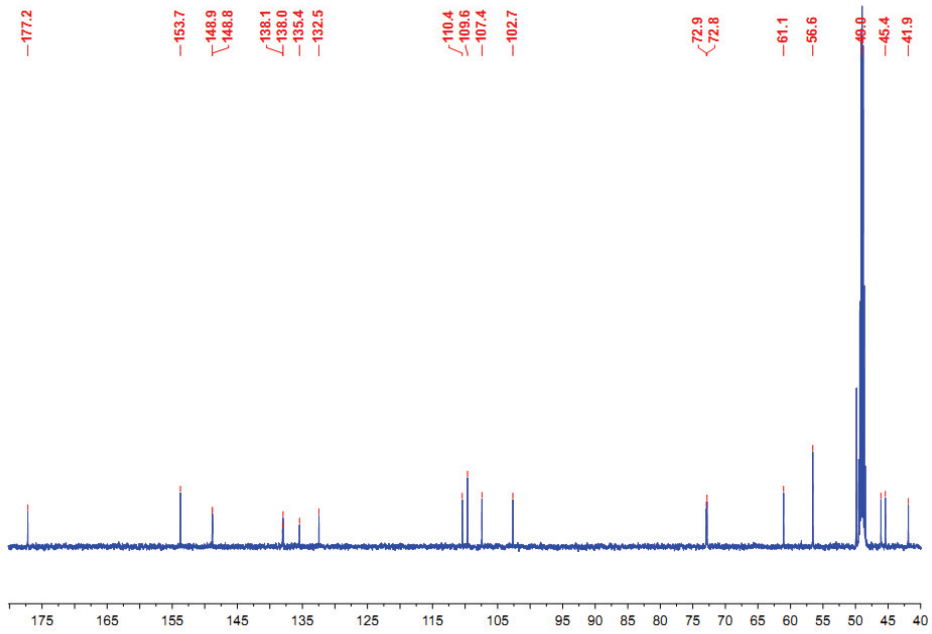

Fig. S-9B. ^{13}C-NMR spectrum of podophyllotoxin (**9**).

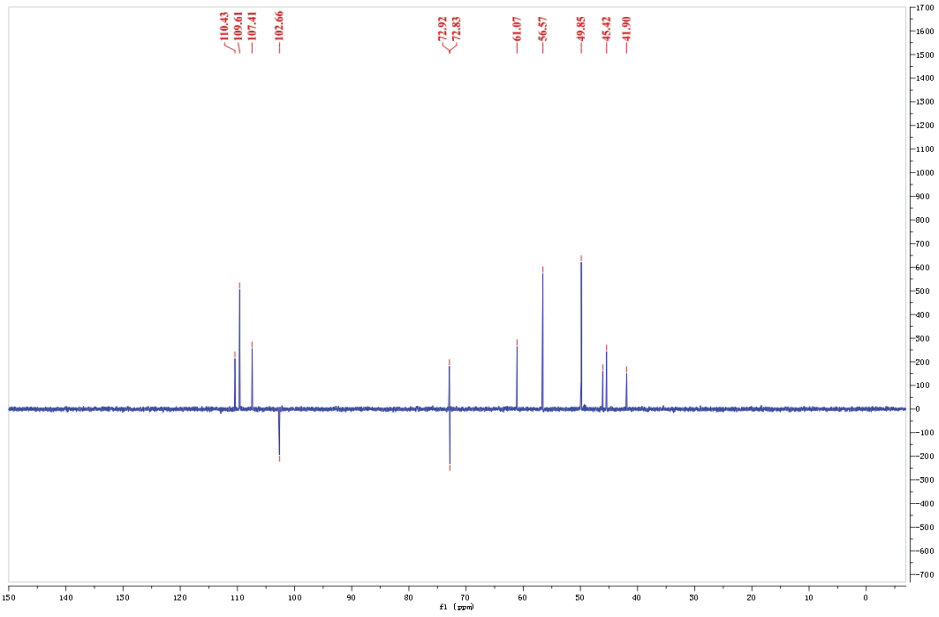

Fig. S-9C. DEPT spectrum of podophyllotoxin (**9**).

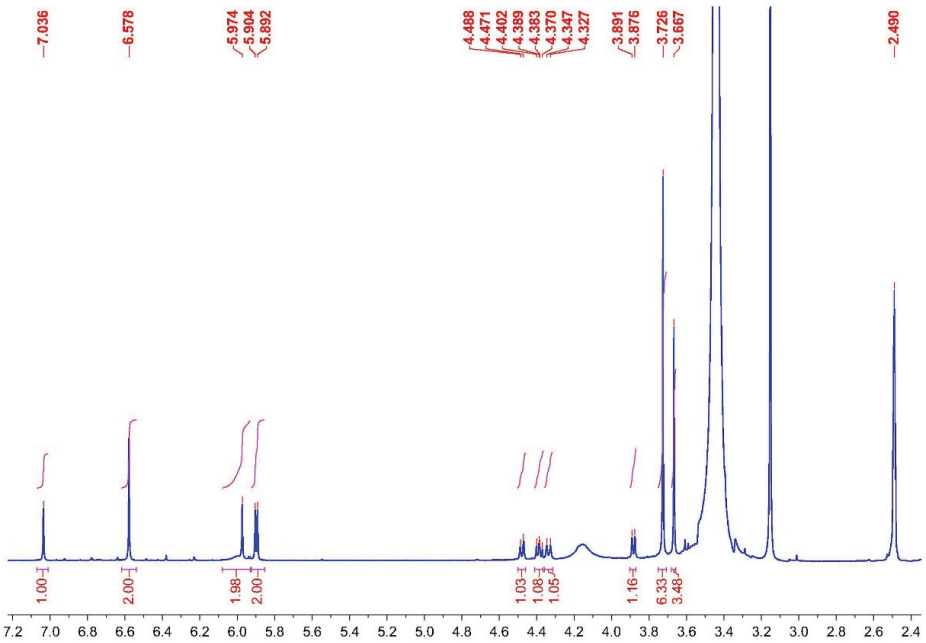

Fig. S-10A. ^{1}H-NMR spectrum of picropodophyllotoxin (**10**).

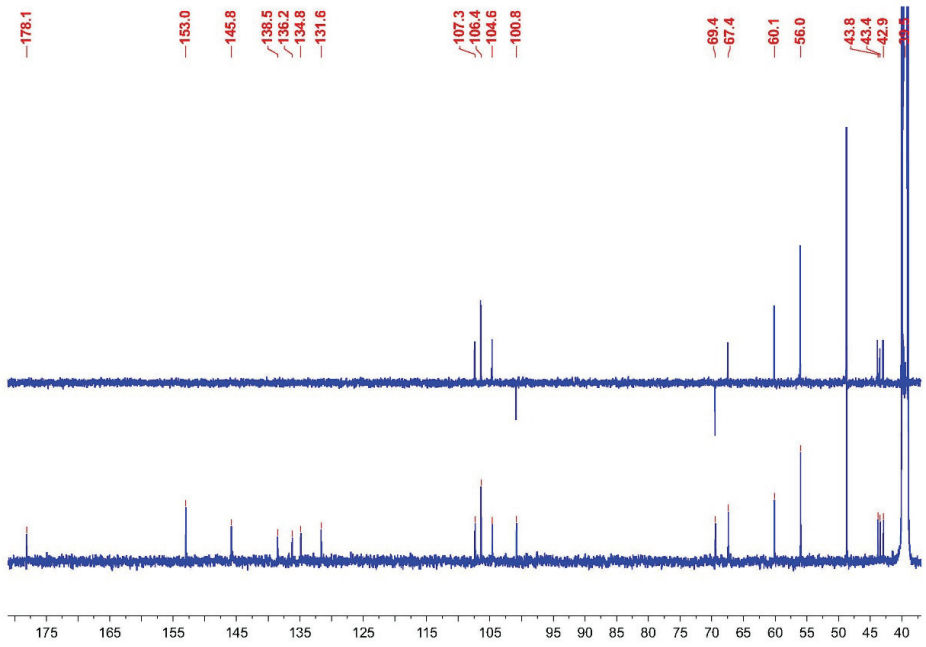

Fig. S-10B. ^{3}C-NMR and DEPT spectra of picropodophyllotoxin (**10**).

LC CHROMATOGRAMS OF **1, 3, 4** AND **7–10**

(LC chromatograms of **2, 5** and **6** were not performed)

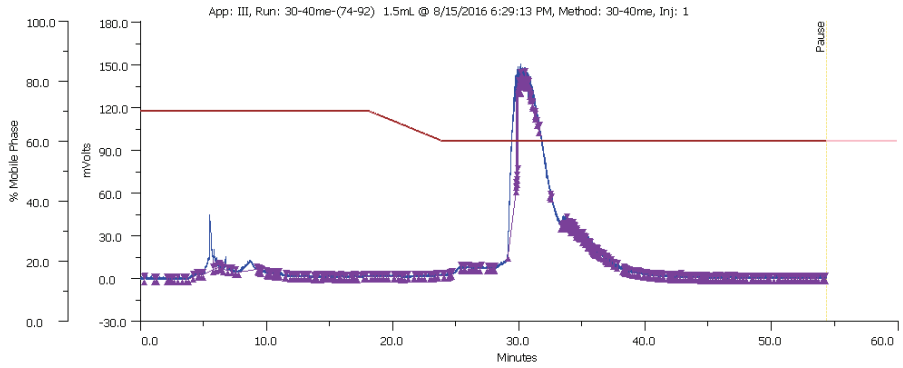

Fig. S-11. Preparation liquid chromatogram of quercetin-3-*O*-β-D-glucopyranoside (**1**).

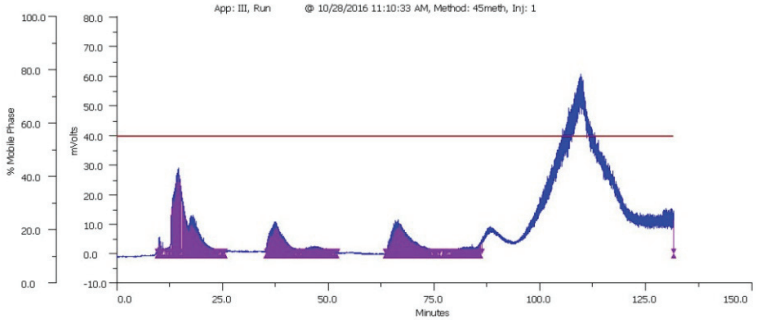

Fig. S12. Preparation liquid chromatogram of sorbifolin (**3**).

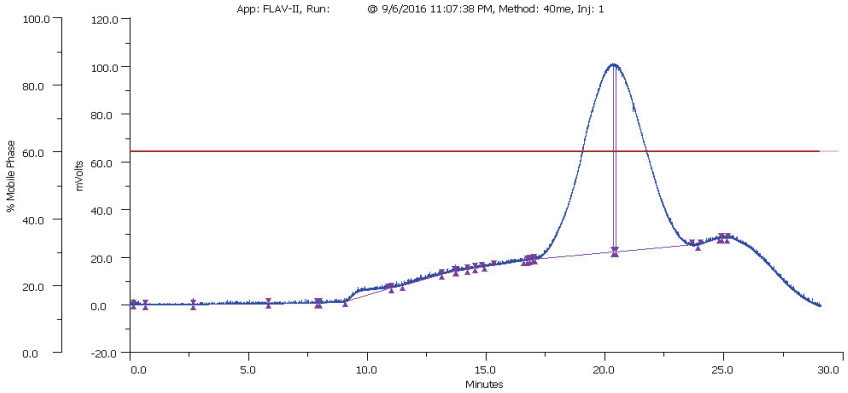

Fig. S-13. Preparation liquid chromatogram of quercetin (**4**).

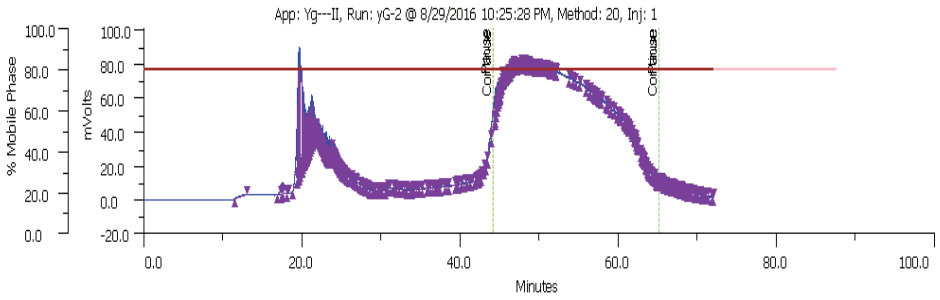

Fig. S-14. Preparation liquid chromatogram of rosmarinic acid (**7**).

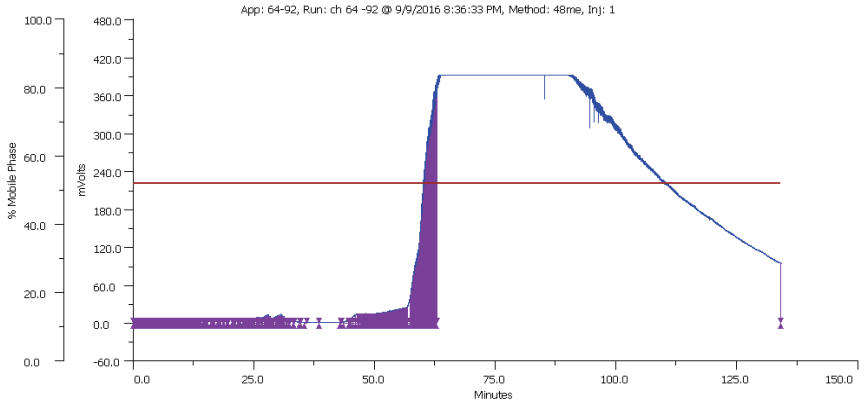

Fig. S-15. Preparation liquid chromatogram of methylrosmarinate (**8**).

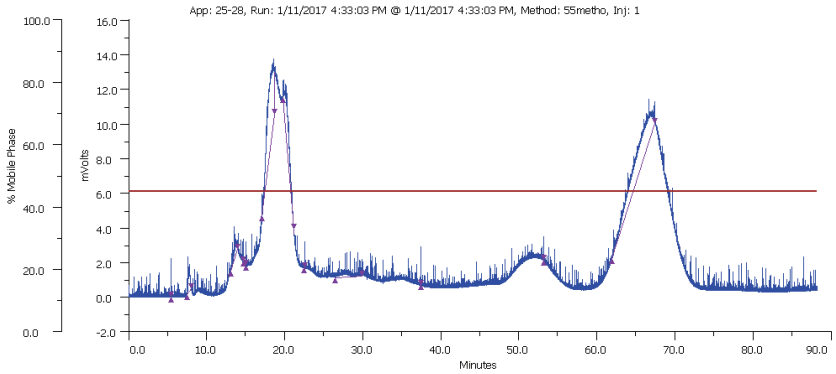

Fig. S-16. Preparation liquid chromatogram of podophyllotoxin (**9**).

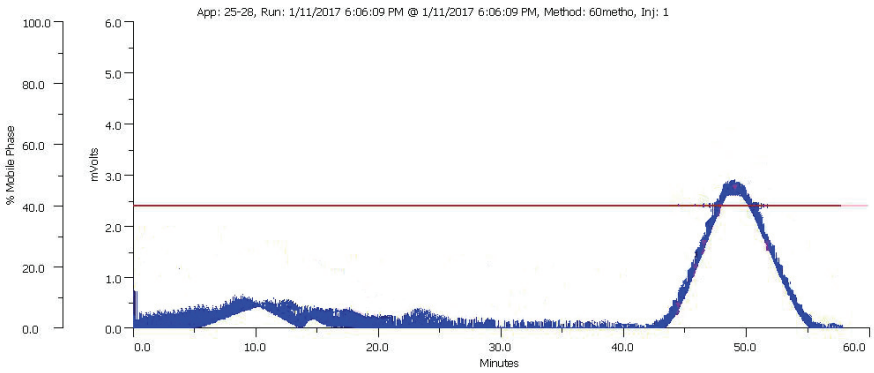

Fig. S-17. Preparation liquid chromatogram of picropodophyllotoxin (**10**).