

## SUPPLEMENTARY MATERIAL

### A bioactive cycloartane triterpene from *Garcinia hombroniana*

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### Abstract

The dichloromethane bark extract of *G. hombroniana* yielded one new cycloartane triterpene; (22Z,24E)-3 $\beta$ -hydroxycycloart-14,22,24-trien-26-oic acid (**1**) together with five known compounds; garcihombronane G (**2**), garcihombronane J (**3**), 3 $\beta$  acetoxy-9 $\alpha$ -hydroxy-17,14-friedolanostan-14,24-dien-26-oic acid (**4**), (22Z, 24E)-3 $\beta$ , 9 $\alpha$ -dihydroxy-17,14-friedolanostan-14,22,24-trien-26-oic acid (**5**), 3 $\beta$ , 23 $\alpha$ -dihydroxy-17,14-friedolanostan-8,14,24-trien-26-oic acid (**6**). Their structures were established by the spectral techniques of NMR and ESI-MS. These compounds together with some previously isolated compounds; garcihombronane B (**7**), garcihombronane D (**8**), 2,3',4,5'-tetrahydroxy-6-methoxybenzophenone (**9**), volkensiflavone (**10**), 4''-O-methyl-volkensiflavone (**11**), volkensiflavone-7-O-glucopyranoside (**12**), volkensiflavone-7-O-rhamnopyranoside (**13**), Morelloflavone (**14**), 3''-O-methyl-morelloflavone (**15**) and morelloflavone-7-O-glucopyranoside (**16**) were evaluated for cholinesterase enzymes inhibitory activities using acetylcholinesterase (AChE) and butyrylcholinesterase (BChE). In these activities, compounds **1-9** showed good dual inhibition on both the enzymes while compounds **10-16** did not reasonably contribute to both the cholinesterases inhibitory effects.

**Keywords:** *Garcinia hombroniana*; (22Z, 24E)-3 $\beta$ -hydroxycycloart-14,22,24-trien-26-oic acid, acetylcholinesterase, butyrylcholinesterase

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Table S1.  $^1\text{H}$ ,  $^{13}\text{C}$ , HMBC and ROESY-NMR data of **1** (DMSO- $d_6$ , 500, 125 MHz)

No.	$\delta_{\text{H}}$ in ppm (multiplicity, $J$ in Hz)	$\delta_{\text{C}}$ (ppm) (C-type)*	HMBC	ROESY
1	1.67, <i>m</i>	30.7 (CH <sub>2</sub> )	C-3, C-9, C-19, C-5	H-3
2	Ha; 1.67 Hb; 1.35	22.4 (CH <sub>2</sub> )	C-4, C-10 -	- -
3	3.10, br. <i>d</i> , $J = 10.5$	76.3 (CH)	C-5, C-29	H-1, H-5, H <sub>3</sub> -29
4	-	39.4 (C)	-	-
5	2.44, <i>m</i>	49.3 (CH)	C-3, C-28, C-7	H <sub>3</sub> -29
6	Ha; 1.95, <i>m</i> Hb; 1.50, <i>m</i>	21.2 (CH <sub>2</sub> )	C-7, C-5, C-8 -	H <sub>3</sub> -29 -
7	Ha; 1.73, <i>m</i> Hb; 1.17, <i>m</i>	26.1 (CH <sub>2</sub> )	C-8, C-9, C-6 -	H <sub>3</sub> -18 -
8	1.29, <i>m</i>	40.4 (CH)	C-11, C-6	-
9	-	19.3 (C)	-	-
10	-	25.3 (C)	-	-
11	Ha; 1.60, <i>m</i> Hb; 1.20, <i>m</i>	29.7 (CH <sub>2</sub> )	C-8, C-9, C-13 -	- -
12	1.53, <i>m</i>	31.7 (CH <sub>2</sub> )	C-8, C-9, C-13	-
13	-	44.6 (C)	-	-
14	-	141.8 (C)	-	-
15	4.89, br. <i>s</i>	114.1 (CH)	C-14, C-16, C-8	-
16	Ha; 1.73, <i>m</i> Hb; 1.5, <i>m</i>	37.1 (CH <sub>2</sub> )	C-14, C-17, C-18 -	- -
17	-	48.3 (C)	-	-
18	0.87, <i>s</i>	17.3 (CH <sub>3</sub> )	C-17, C-20	H-7a
19	Ha; 0.68, <i>d</i> , $J = 3.0$ Hb; 0.42, <i>d</i> , $J = 3.0$	26.6 (CH <sub>2</sub> )	C-1, C-5, C-11 -	- -
20	2.92, <i>m</i>	38.5 (CH)	C-17, C-22	-
21	0.95, <i>s</i>	16.1 (CH <sub>3</sub> )	C-13, C-17, C-20	H <sub>3</sub> -30
22	5.95, <i>t</i> , $J = 11.0$	142.6 (CH)	C-17, C-20, C-24	-
23	6.24, <i>t</i> , $J = 11.5$	121.4 (CH)	C-20, C-22, C-24, C-25	-
24	7.40, <i>d</i> , $J = 12.0$	131.5 (CH)	C-22, C-25, C-26, C-27	-
25	-	127.8 (C)	-	-
26	-	169.4 (C)	-	-
27	1.84, <i>s</i>	12.3 (CH <sub>3</sub> )	C-24, C-25, C-26	-
28	0.75, <i>s</i>	12.8 (CH <sub>3</sub> )	C-3, C-4, C-5, C-29	-
29	0.89, <i>s</i>	25.3 (CH <sub>3</sub> )	C-3, C-4, C-5, C-28	H-3
30	0.55, <i>s</i>	13.2 (CH <sub>3</sub> )	C-12, C-14, C-17	H <sub>3</sub> -21

\*C-type was deduced from DEPT experiments

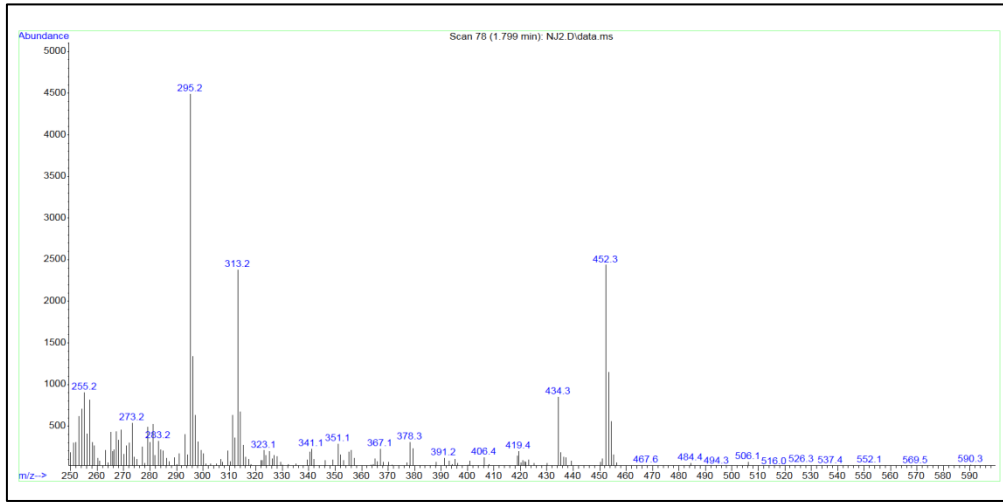


Figure S1: EI-MS of **1**

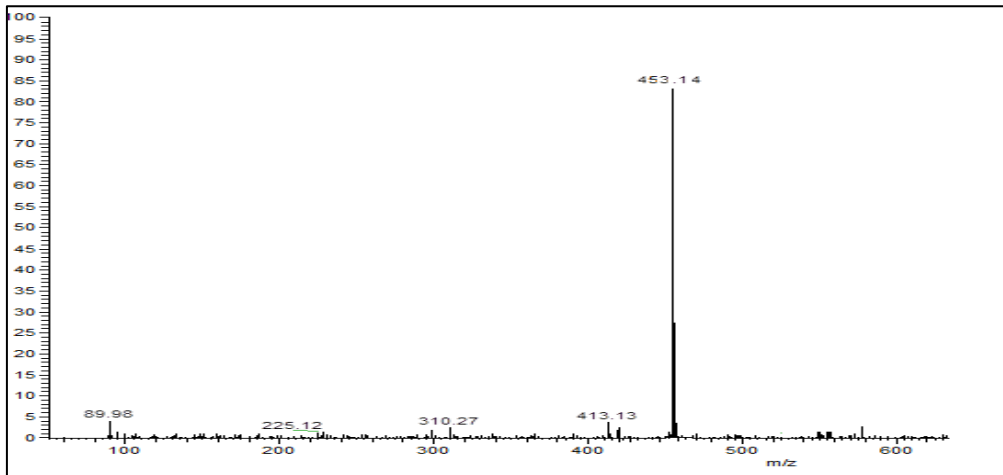


Figure S2: +ESI-MS of **1**

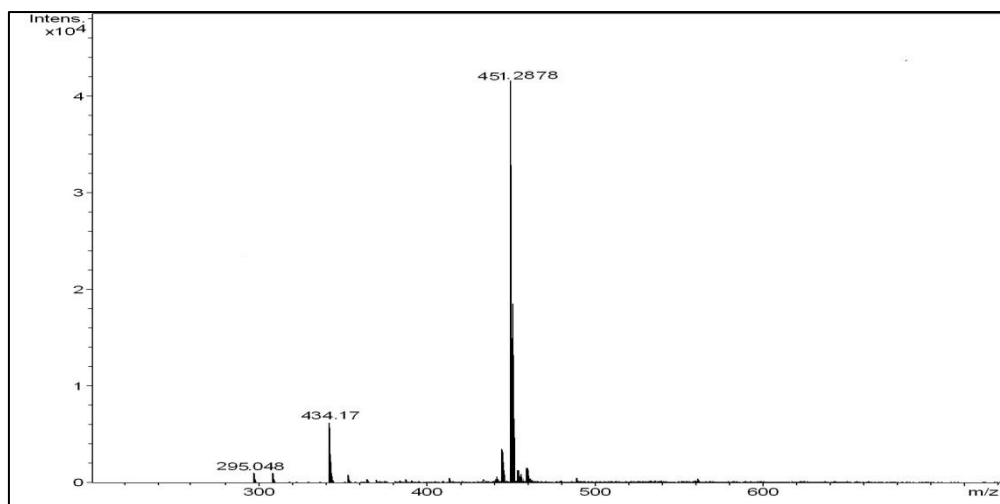


Figure S3: –HRESI-MS of **1**

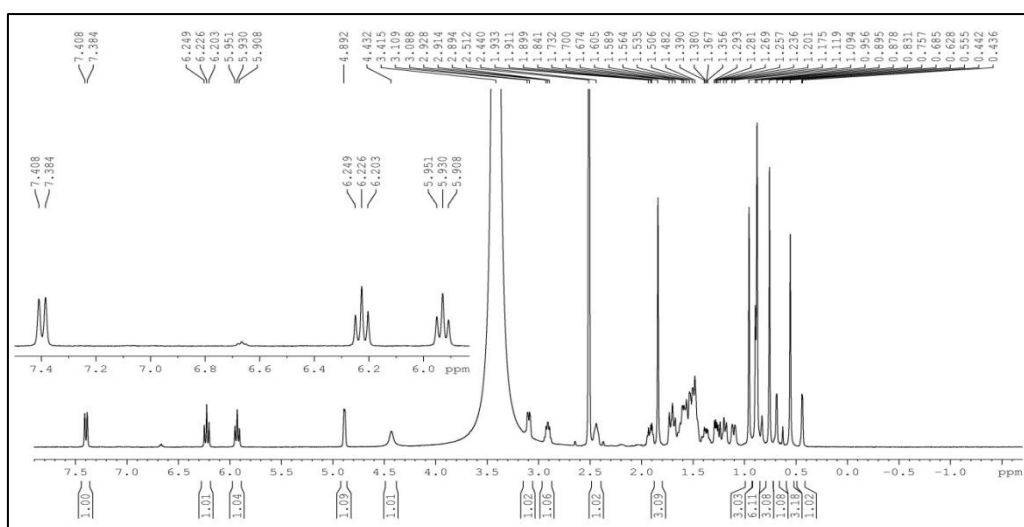


Figure S4: <sup>1</sup>H NMR spectrum of **1** (DMSO-d<sub>6</sub>, 500 MHz)

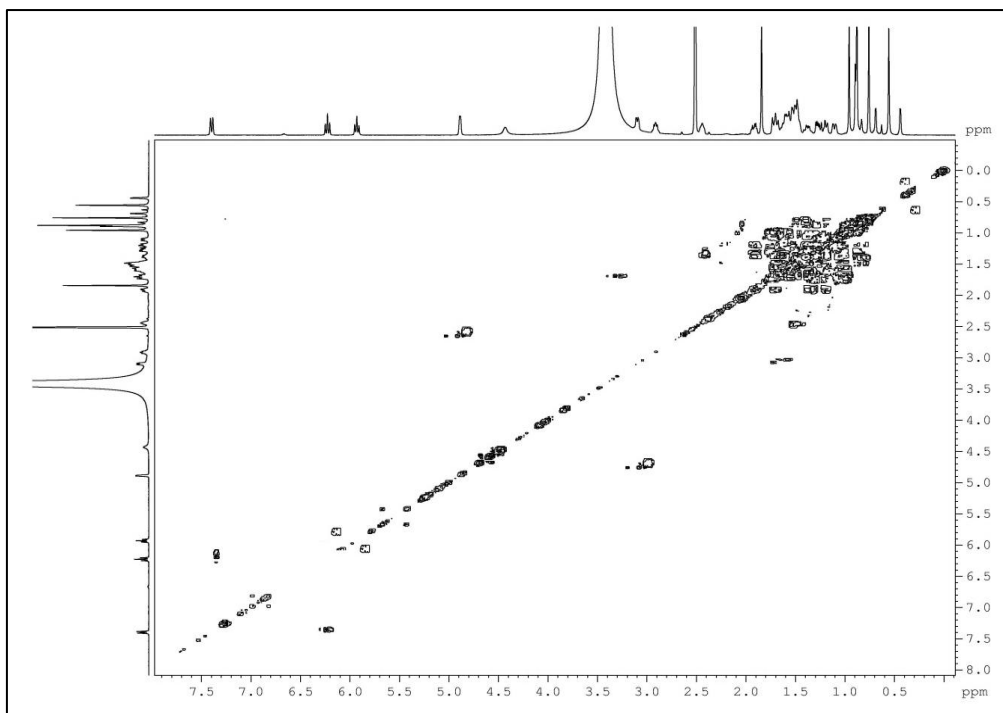


Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**

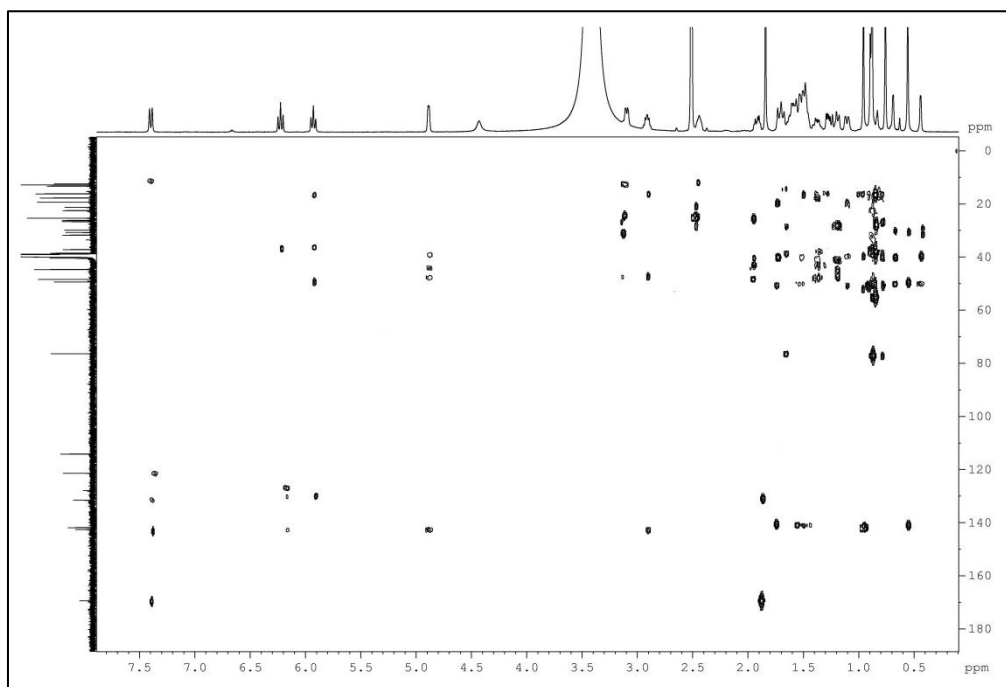


Figure S6: HMBC spectrum of **1**

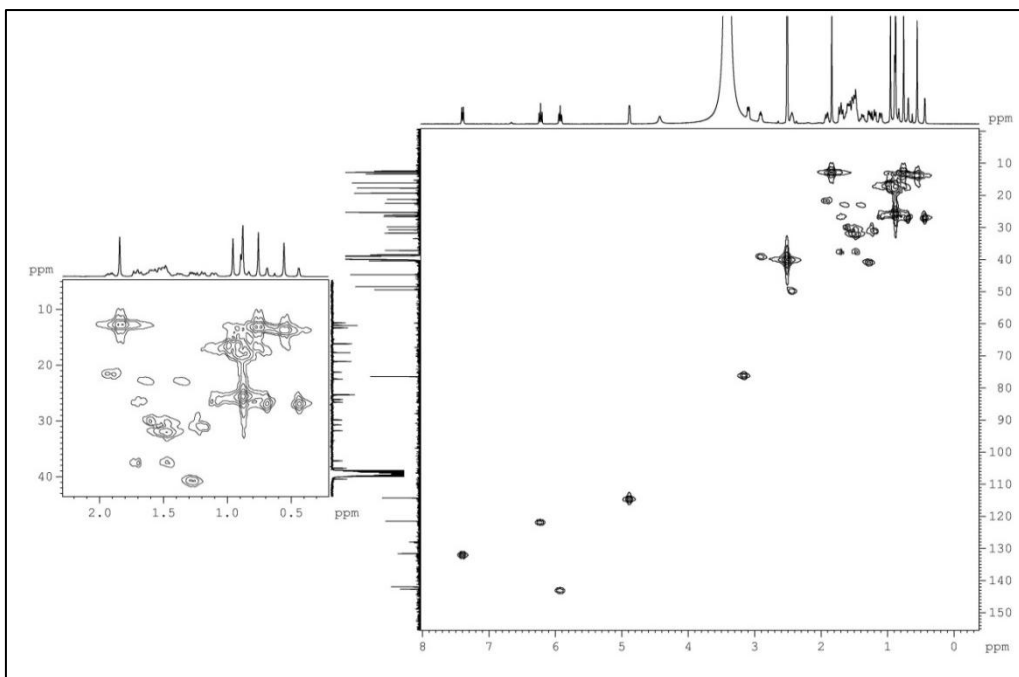


Figure S7: HMQC spectrum of **1**

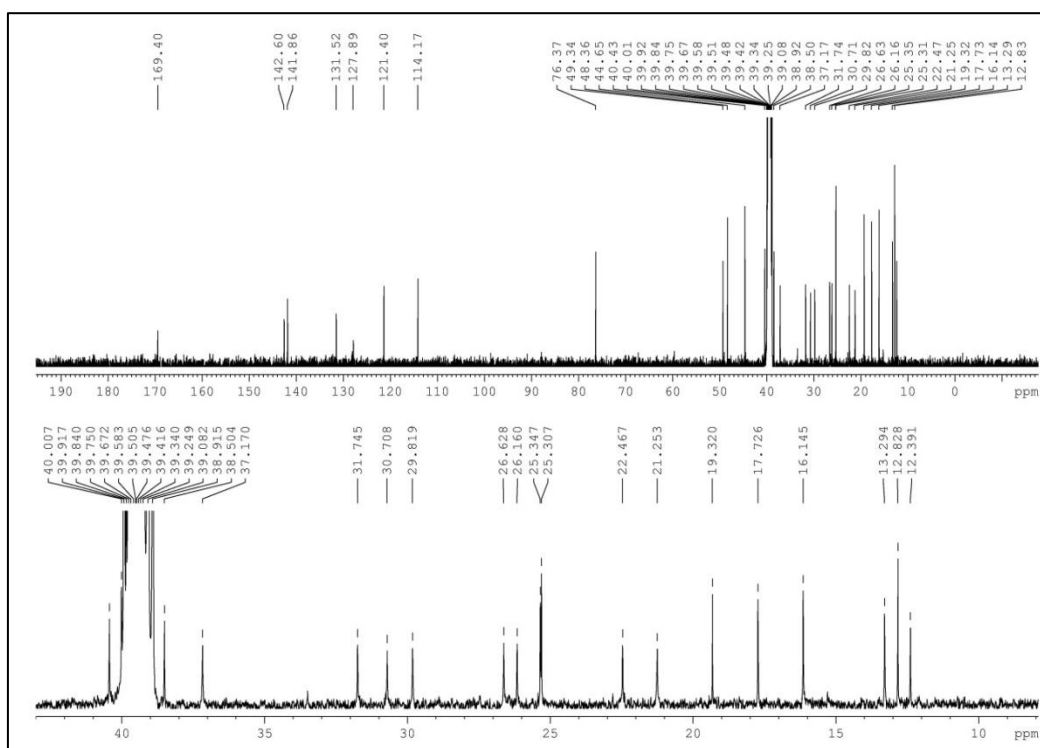


Figure S8:  $^{13}\text{C}$  NMR spectrum of **1** (DMSO- $d_6$ , 125 MHz)

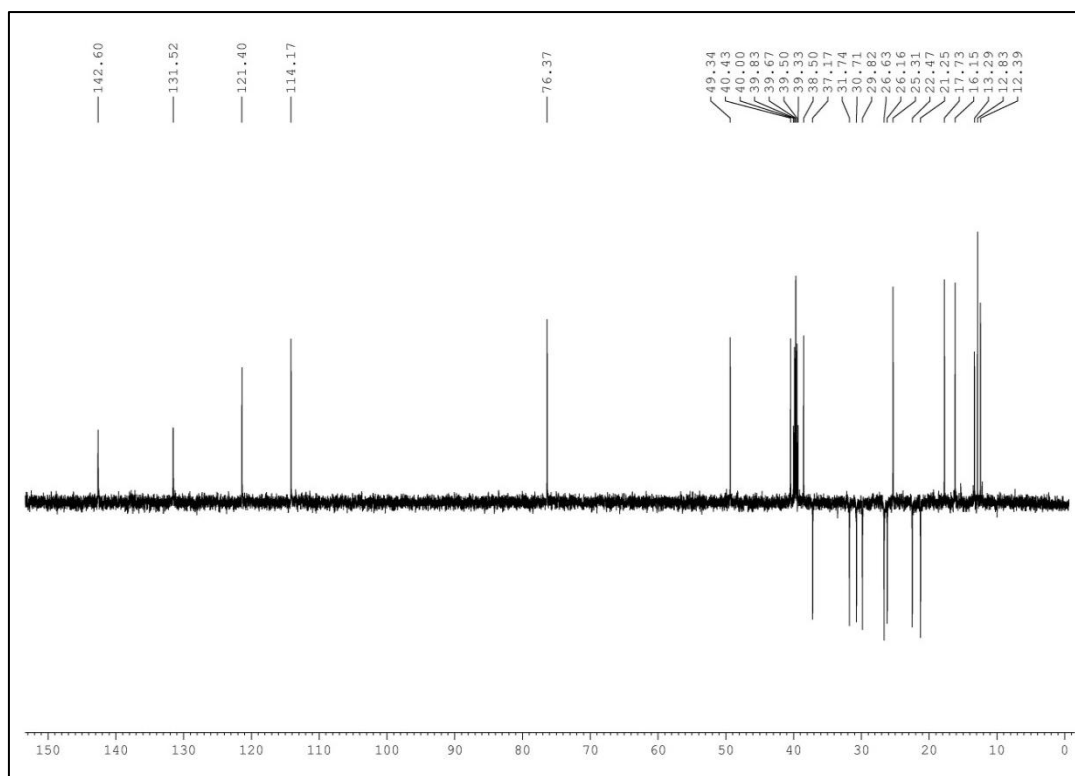


Figure S9. DEPT 135 spectrum of **1** (DMSO-*d*<sub>6</sub>, 125 MHz)

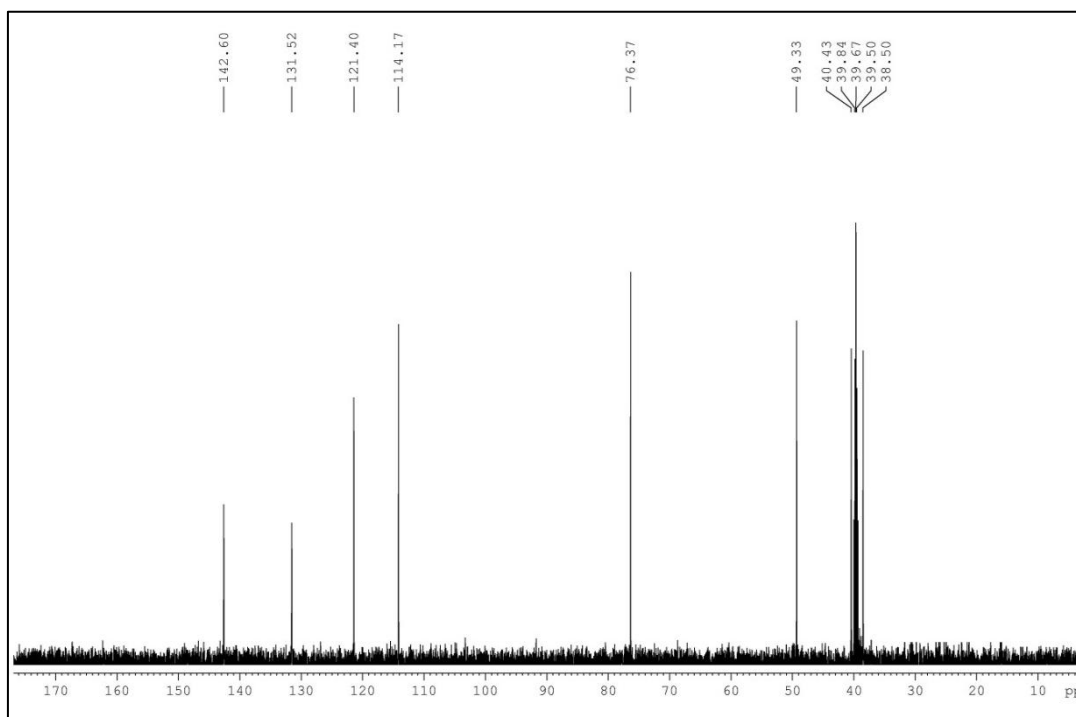


Figure S10. DEPT 90 spectrum of **1** (DMSO-*d*<sub>6</sub>, 125 MHz)

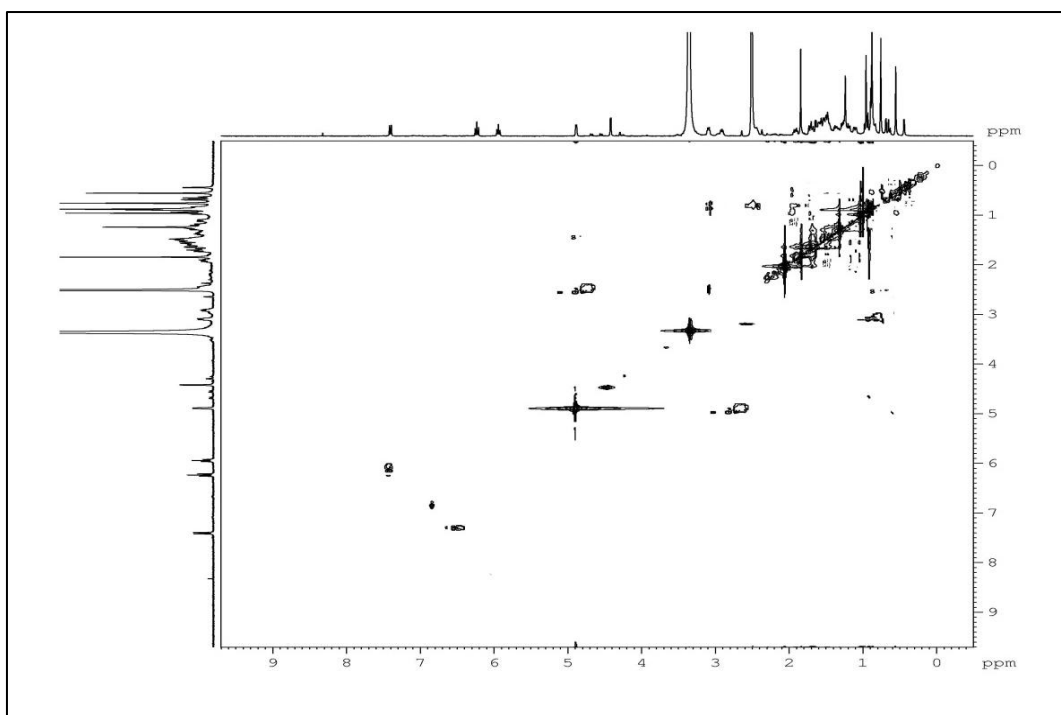


Figure S11. ROESY spectrum of **1**

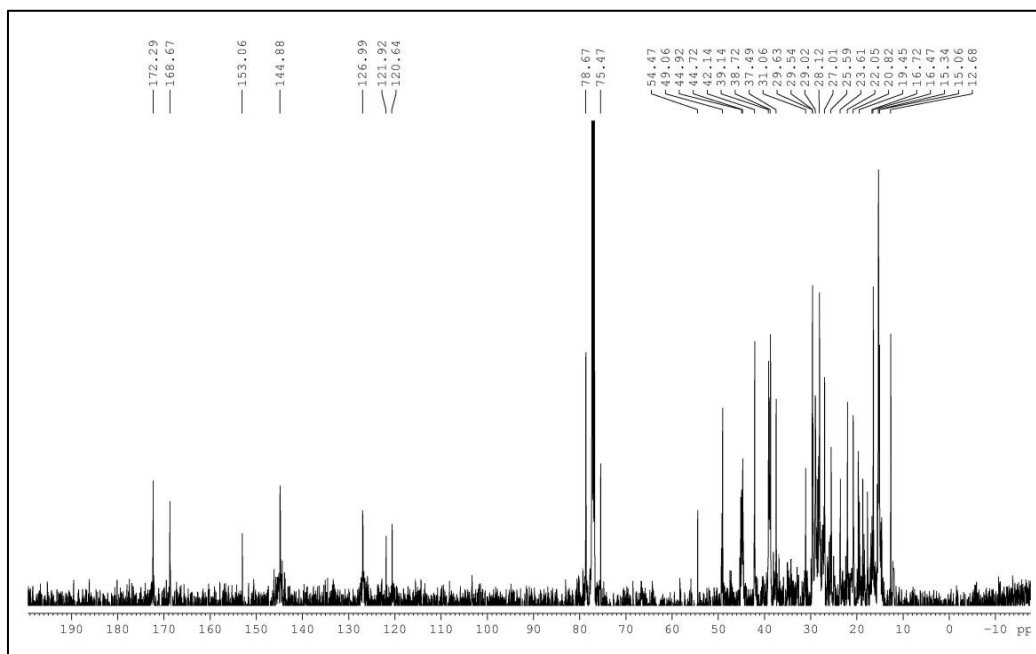


Figure S12.  $^{13}\text{C}$  NMR spectrum of **4** ( $\text{CDCl}_3$ , 125 MHz)



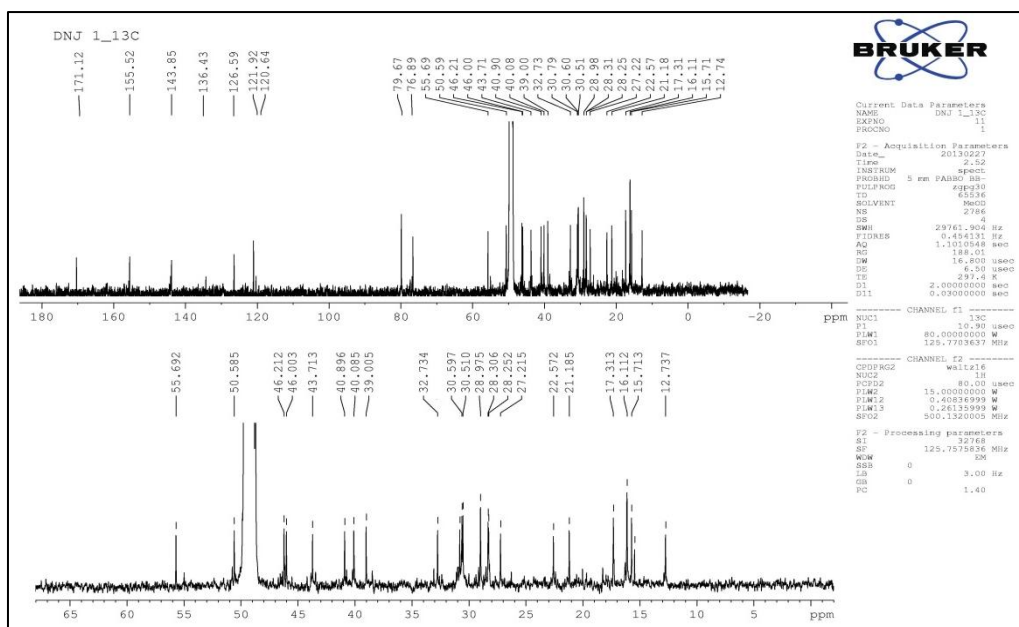


Figure S13.  $^{13}\text{C}$  NMR spectrum of **5** (MeOD, 125 MHz)

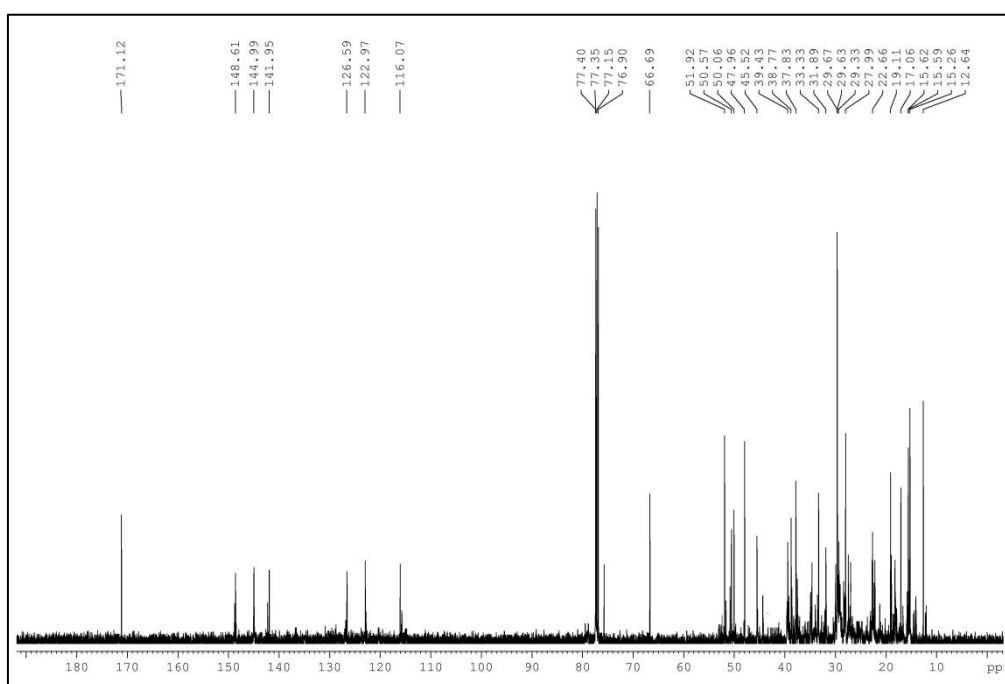


Figure S14.  $^{13}\text{C}$  NMR spectrum of **6** ( $\text{CDCl}_3$ , 125 MHz)

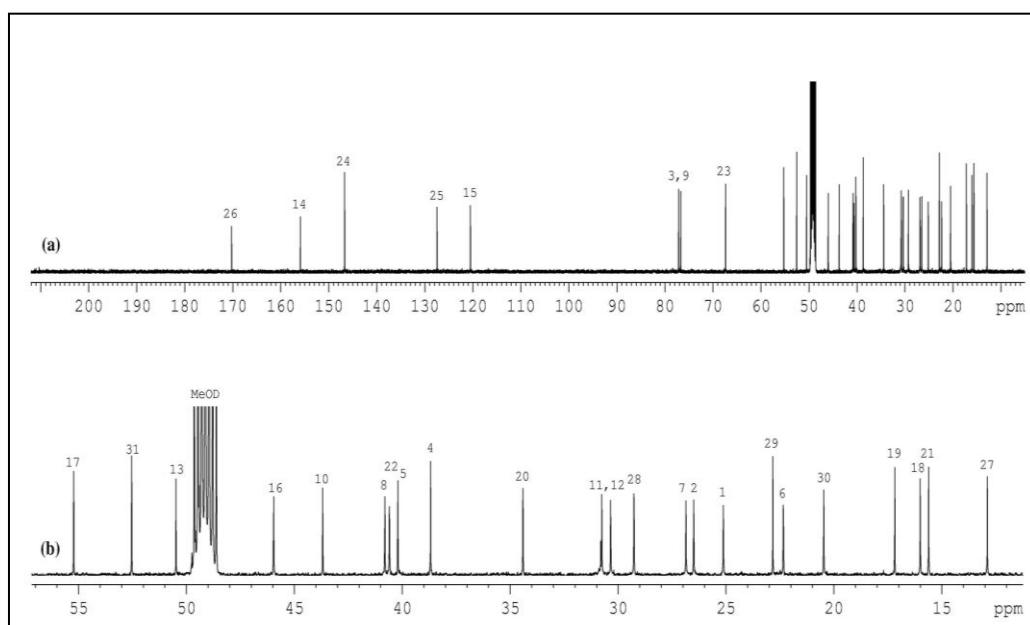


Figure S15.  $^{13}\text{C}$  NMR (a) full and (b) expanded ( $\delta_{\text{C}}$  12-56 ppm) spectra of **7**

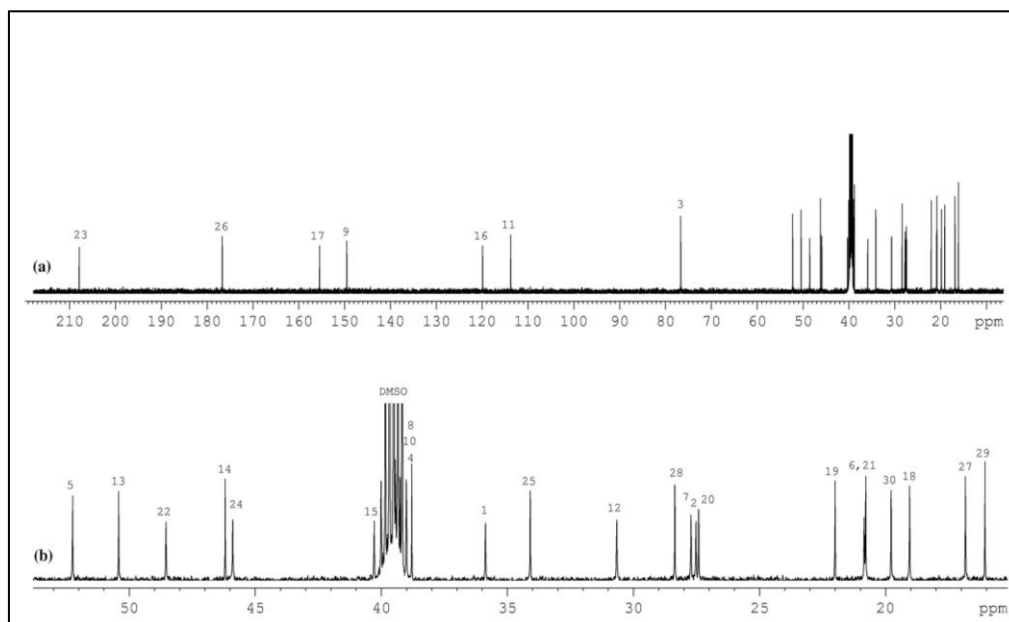
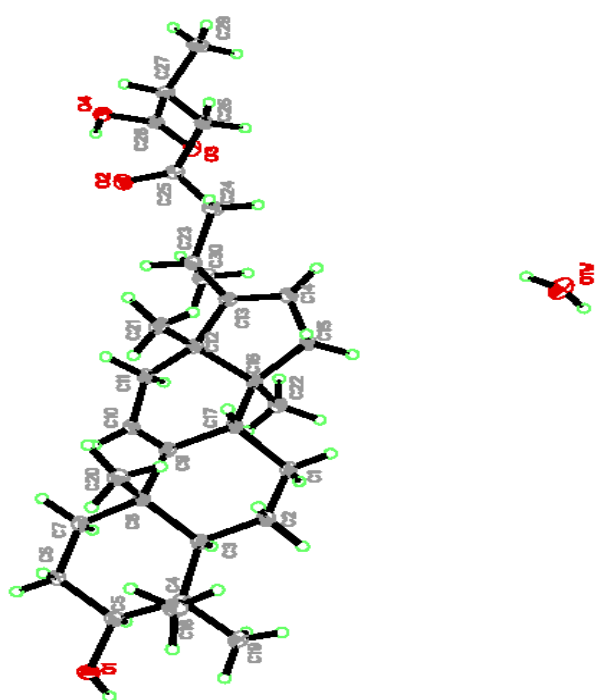
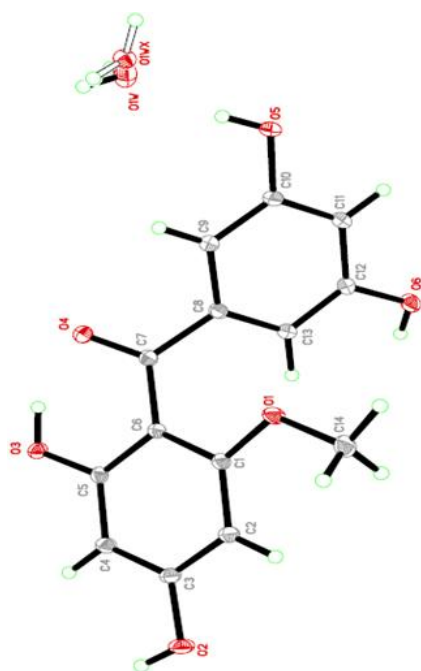


Figure S16.  $^{13}\text{C}$  NMR (a) full and (b) expanded ( $\delta_{\text{C}}$  12-56 ppm) spectra of **8**



ORTEP view of 8



ORTEP view of 9