Supplementary material

Triterpenoids, megastigmanes and hydroxycinnamic acid derivatives from *Anisomeles indica*

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Abstract: Six triterpenoids (**1** − **6**), four megastigmanes (**7** − **10**) and five hydroxycinnamic acid derivatives (**11** − **15**) were isolated from the aerial part of *Anisomeles indica* (Lamiaceae). Of these components, compound **1** was identified to be a new triterpenoid with the structure of 2□,3□,19□-trihydroxyurs-12,20(30)-dien-28-oic acid based on extensive analysis of MS, 1D and 2D NMR spectroscopic data, while compounds **2** − **13** were obtained for the first time from Anisomeles species.

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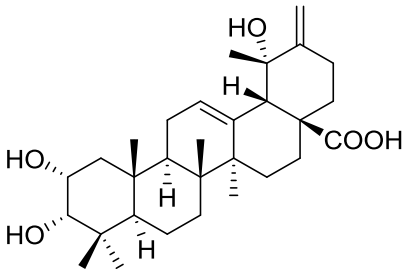

2□,3□,19□-trihydroxyurs-12,20(30)-dien-28-oic acid (**1**)

Table 1S. ^{1}H and ^{13}C NMR spectroscopic data of **1** (400 and 100 MHz, in CD_3OD).

No.	δ_H, mult. (*J* in Hz)	δ_C	mult.	No.	δ_H, mult. (*J* in Hz)	δ_C,	mult.
1	1.58, dd (12.1, 4.0)	42.5	CH_2	16	2.71, td (13.2, 4.0)	27.0	CH_2
	1.29, t (12.0)				1.66, dd (12.9, 4.8)		
2	3.93, ddd (12.0, 4.0, 2.8)	67.2	CH	17	□□□	49.1	C
3	3.32, d (2.8)	80.1	CH	18	2.65, s	55.8	CH
4	□□□	39.5	C	19	□□□	73.6	C
5	1.26, br. d (10.2)	49.3	CH	20	□□□	156.5	C
6	1.46, br. d (13.1)	19.3	CH_2	21	2.78, td-like (13.0, 4.4)	29.2	CH_2
	1.38, qd-like (12.8, 3.1)				2.09 dt (13.2, 4.3)		
7	1.60, br. d (13.1)	34.3	CH_2	22	1.90, dt (12.9, 4.3)	39.7	CH_2
	1.34, td-like (13.1, 3.1)				1.65, td-like (12.9, 4.8)		
8	□□□	41.1	C	23	0.99, s	29.3	CH_3
9	1.86, dd (10.8, 7.1)	48.2	CH	24	0.87, s	22.5	CH_3
10	□□□	39.4	C	25	0.99, s	17.0	CH_3
11	2.04, ddd (18.4, 7.1, 3.3)	24.7	CH_2	26	0.80, s	17.7	CH_3
	1.98, ddd (18.4, 10.8, 3.3)			27	1.36, s	24.2	CH_3
12	5.33, t (3.3)	129.4	CH	28	□□□	182.0	C
13	□□□	139.9	C	29	1.37, s	27.7	CH_3
14	□□□	42.9	C	30	4.88, s	106.1	CH_2
15	1.79, td-like (13.7, 4.3)	29.5	CH_2		4.70, s		
	1.04, dt (13.2, 4.4)						

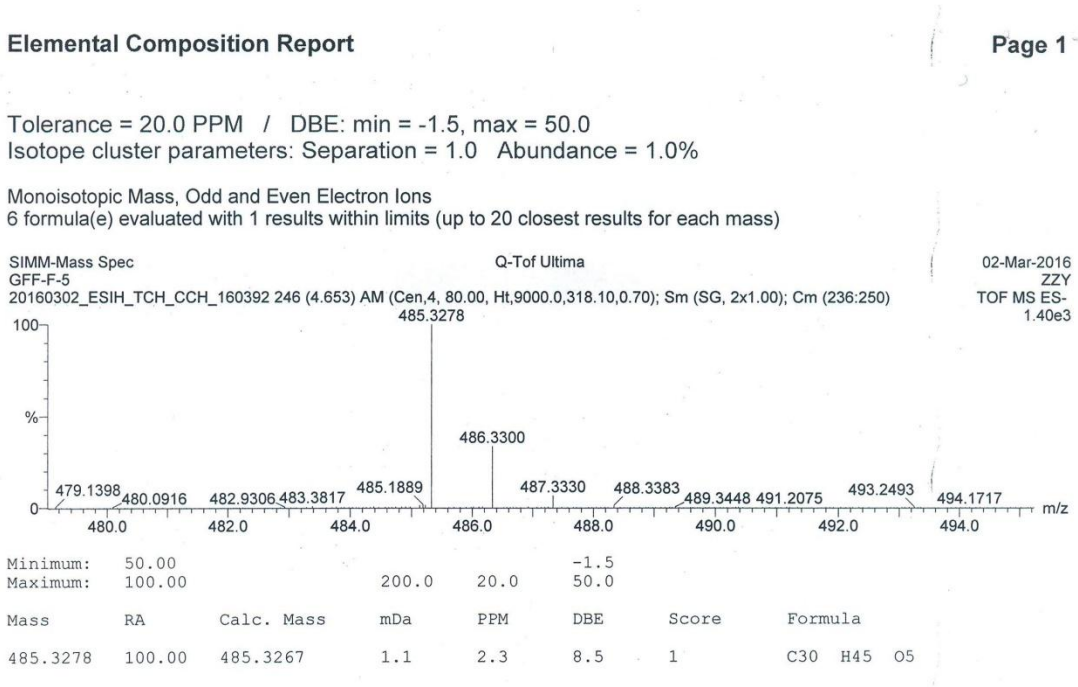

Figure 1S. (-)-HR-ESI-MS spectrum of **1**

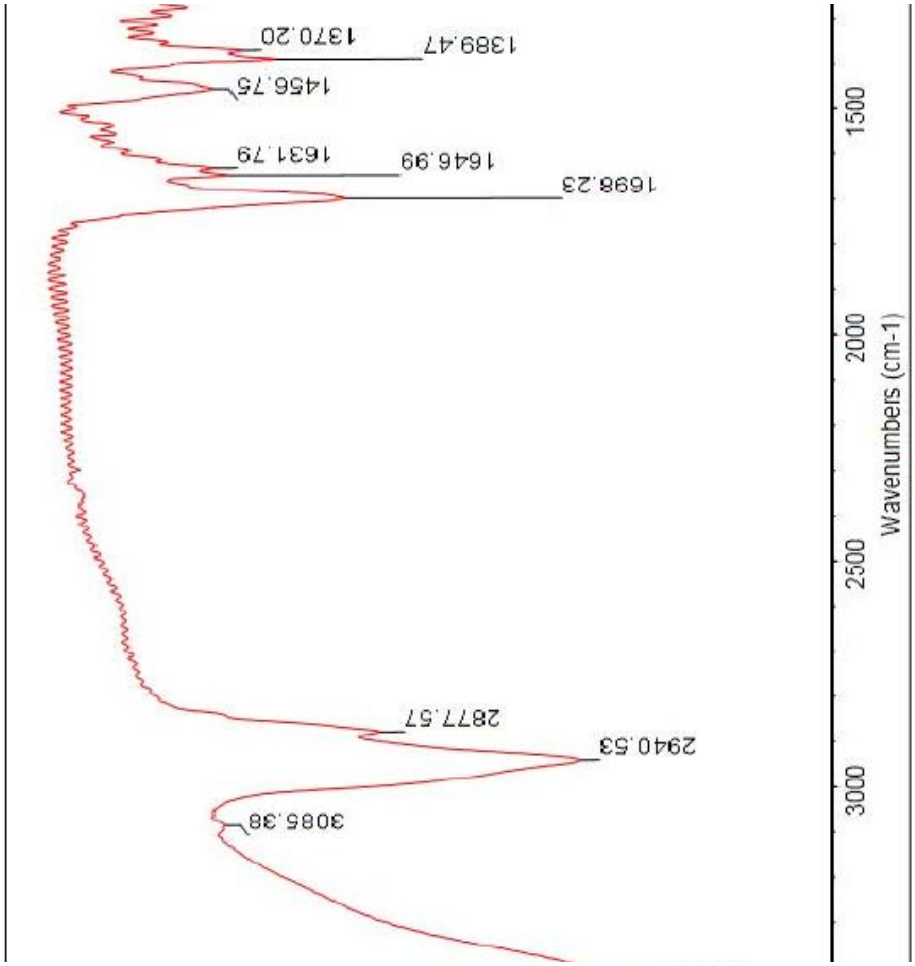

Figure 2S. IR spectrum of **1**

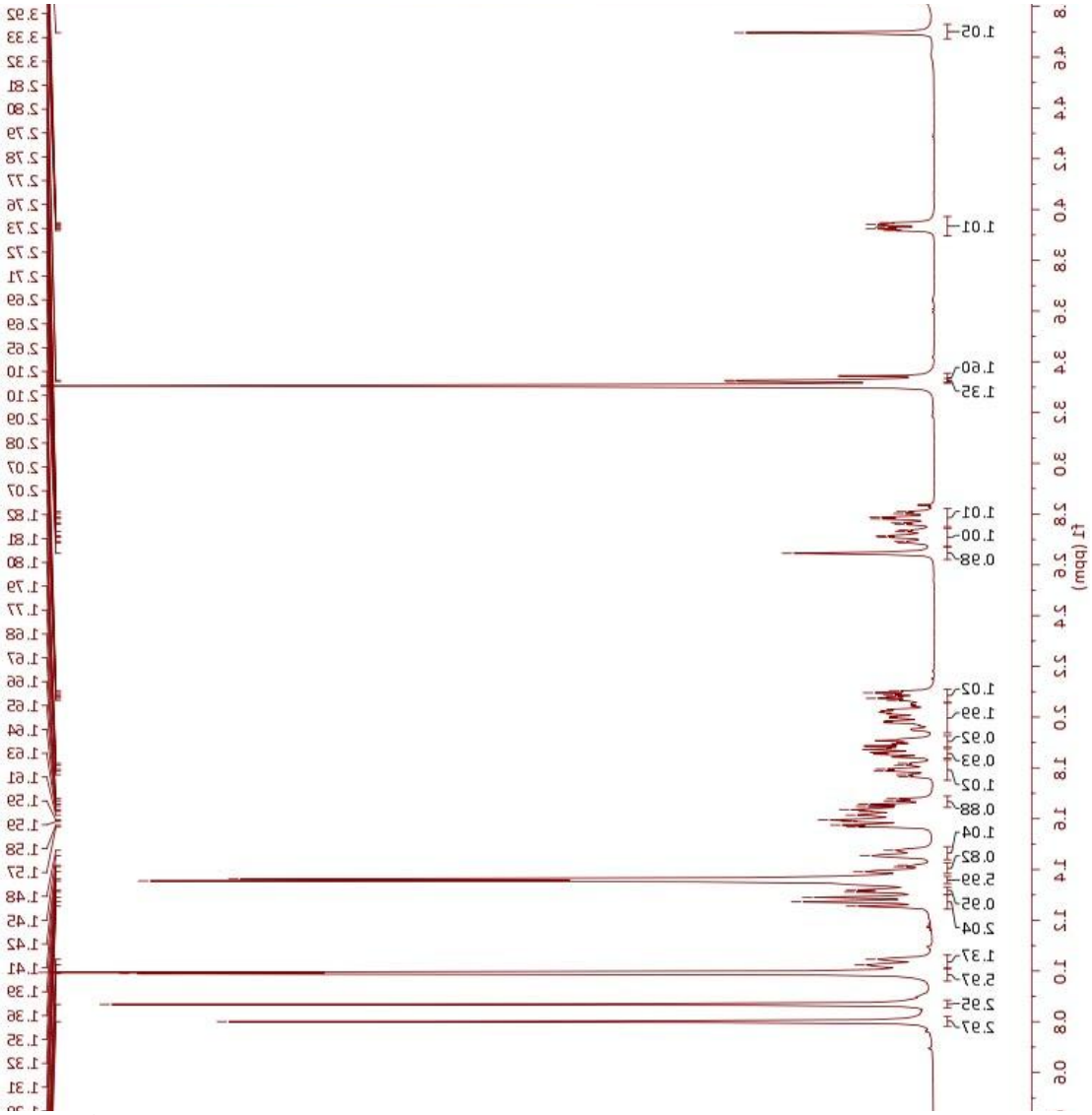

Figure 3S. ^{1}H NMR spectrum of **1** in CD_3OD (400 MHz)

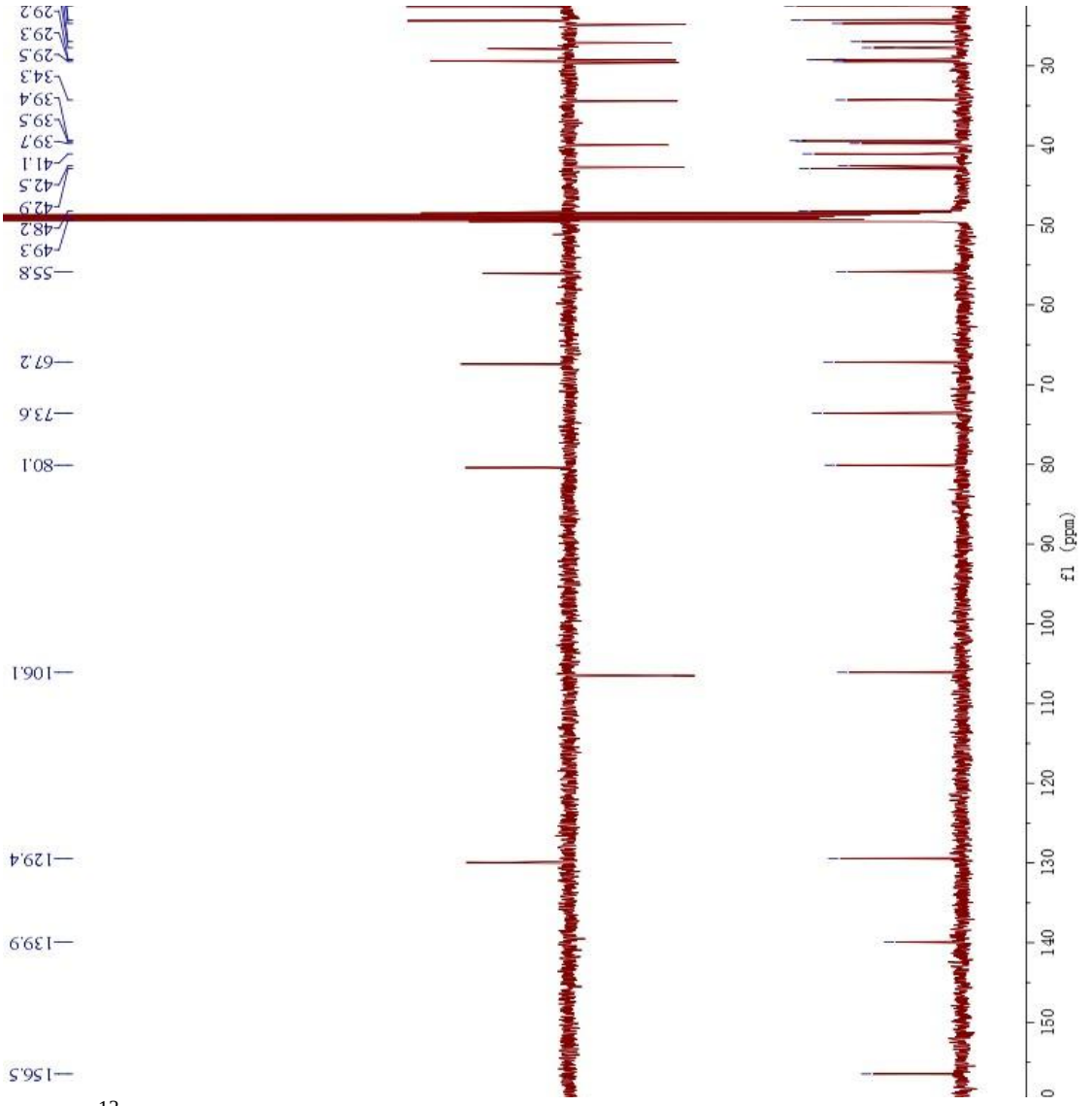

Figure 4S. ^{13}C NMR spectrum of **1** in CD_3OD (100 MHz)

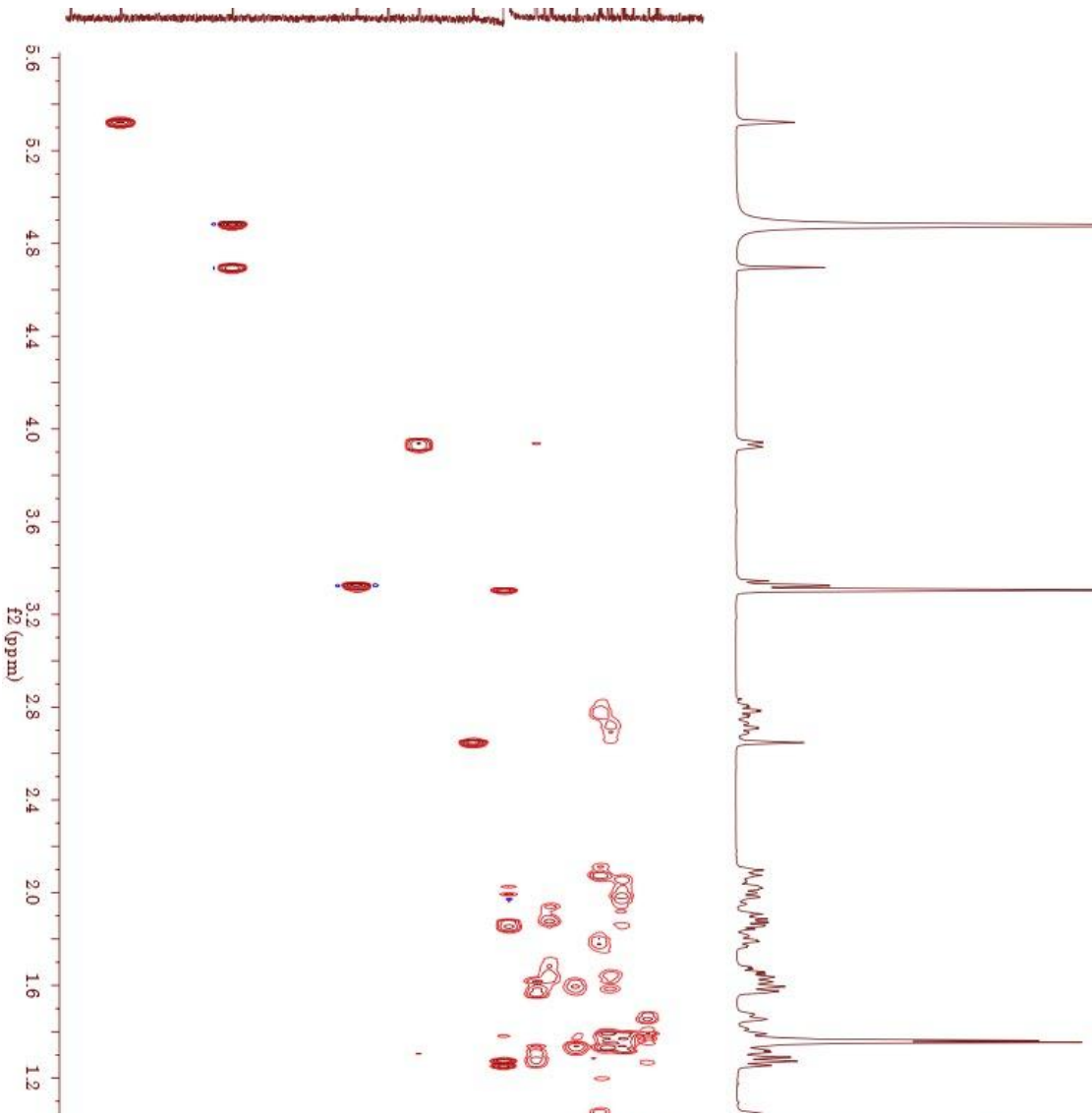

Figure 5S. HSQC spectrum of **1** in CD_3OD

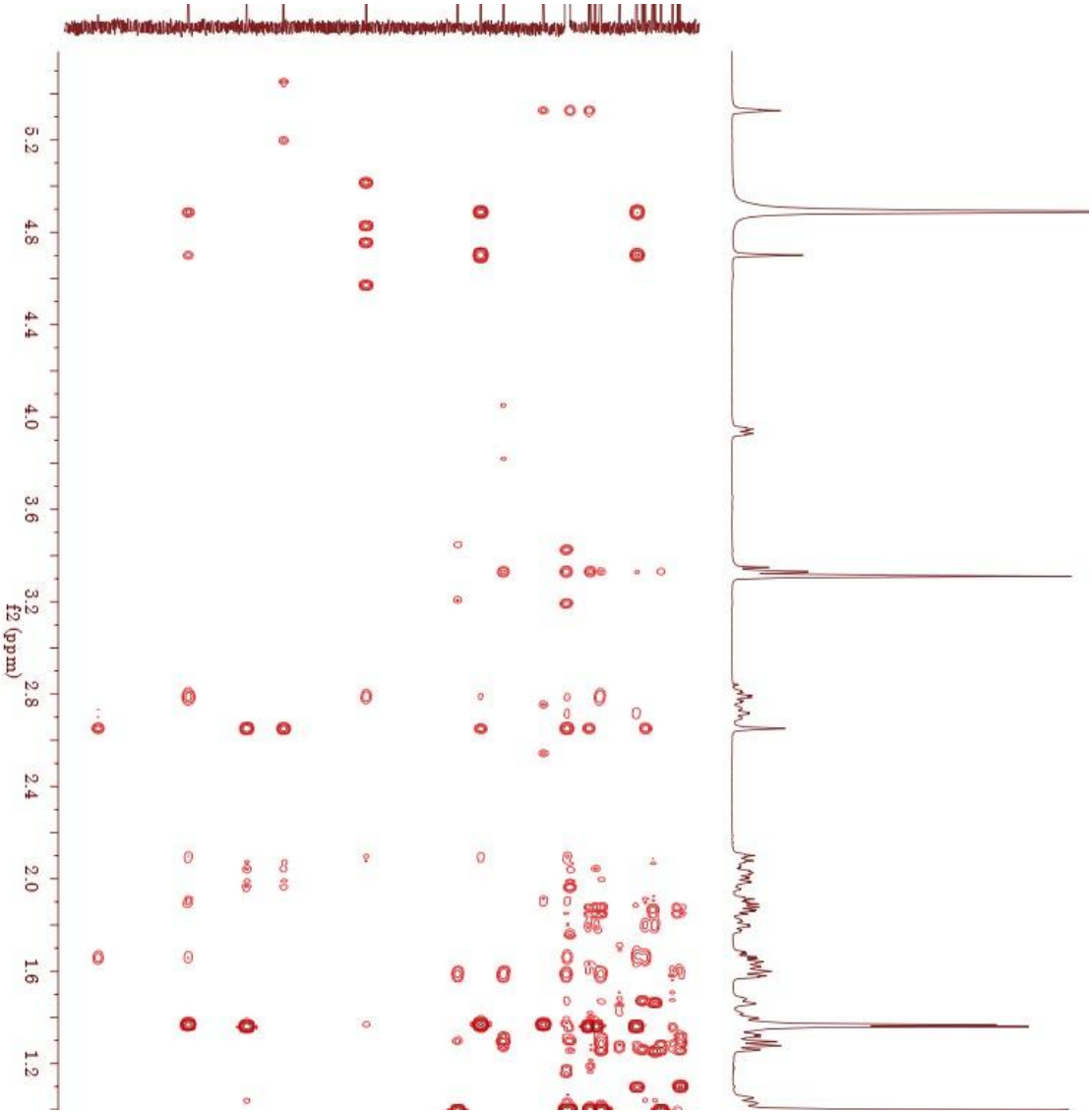

Figure 6S. HMBC spectrum of **1** in CD_3OD

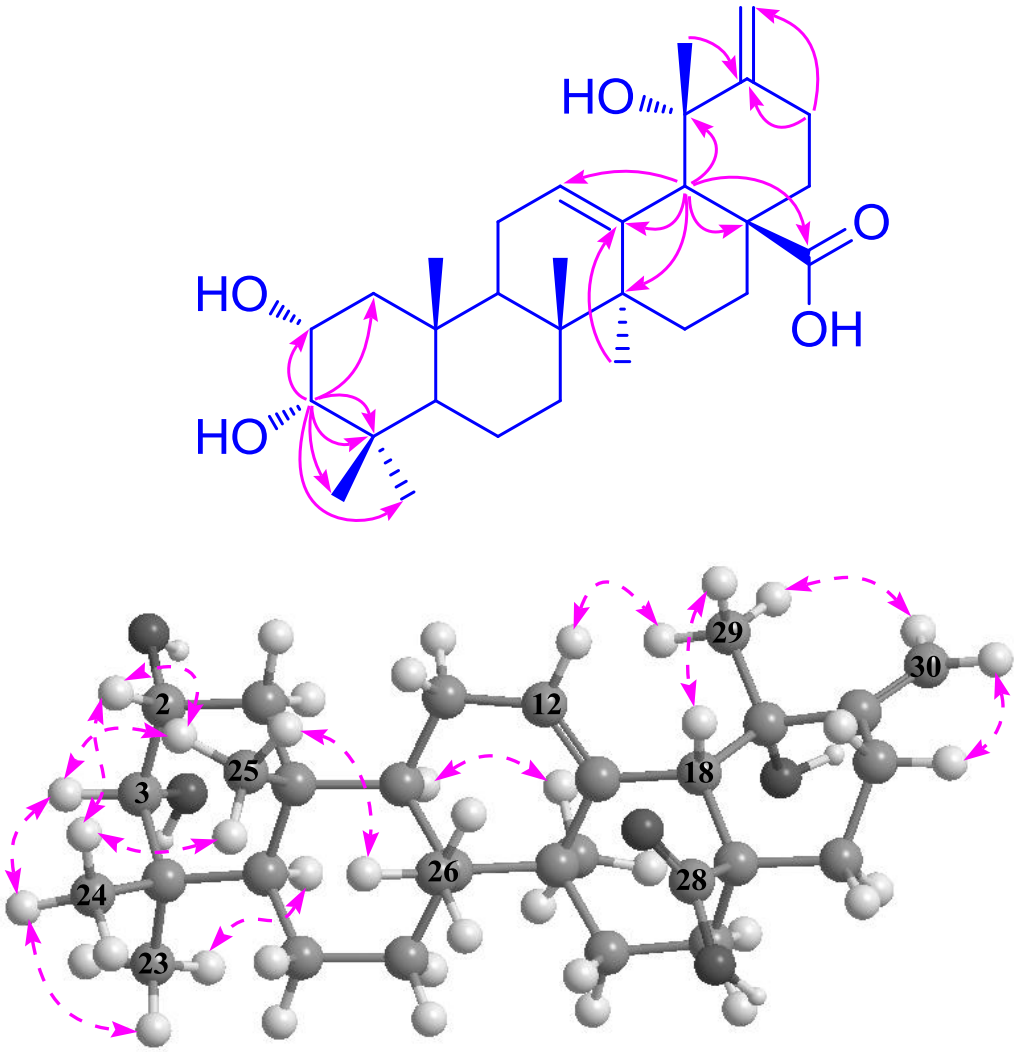

Figure 7S. Selected HMBC (H to C, upper) and NOESY (under) correlations of **1**.

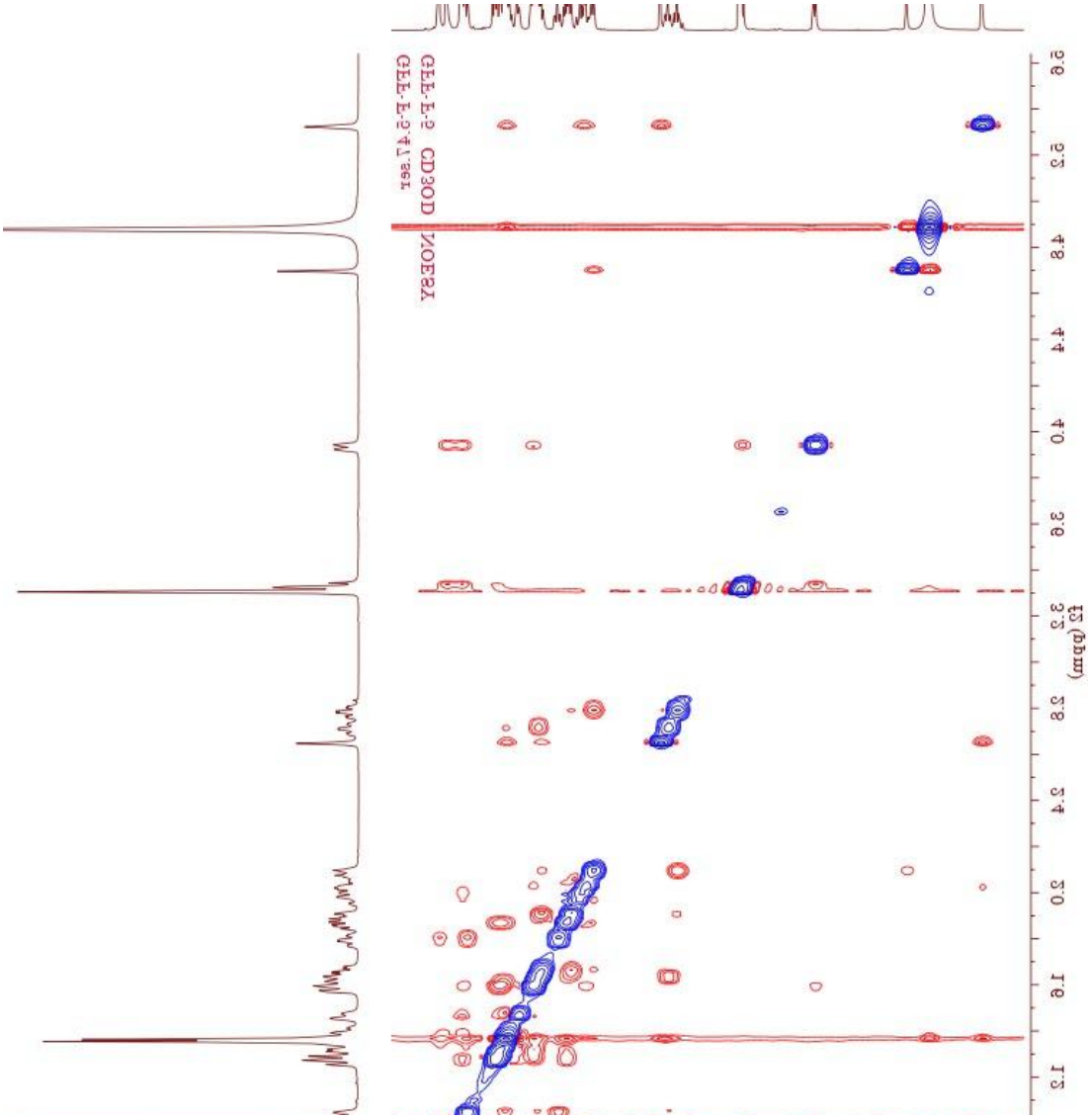

Figure 8S. NOESY spectrum of **1** in CD_3OD