

Supporting Information

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Triterpenoids from *Acokanthera schimperi* in Ethiopia

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Lupeol (2): white amorphous powder; $^1\text{H-NMR}$ (600 MHz, CDCl_3) δ_{H} : 4.68 (1H, br.s, H-29), 4.56 (1H, br.s, H-29), 3.18 (1H, dd, $J = 11.5, 4.7$ Hz, H-3), 1.68, 1.02, 0.96, 0.94, 0.82, 0.78, 0.76 (each 3H, s, $7 \times \text{CH}_3$). $^{13}\text{C-NMR}$ (150 MHz, CDCl_3) δ_{C} : 150.9 (C-20), 109.2 (C-29), 78.9 (C-3), 55.2 (C-5), 50.3 (C-9), 48.2 (C-18), 47.9 (C-19), 42.9 (C-17), 42.7 (C-14), 40.7 (C-8), 39.9 (C-22), 38.8 (C-4), 38.6 (C-1), 38.0 (C-13), 37.1 (C-10), 35.5 (C-16), 34.2 (C-7), 29.8 (C-21), 27.9 (C-23), 27.4 (C-2), 27.3 (C-15), 25.1 (C-12), 20.8 (C-11), 19.2 (C-30), 18.2 (C-6), 17.9 (C-28), 16.0 (C-25), 15.9 (C-26), 15.3 (C-24), 14.5 (C-27).

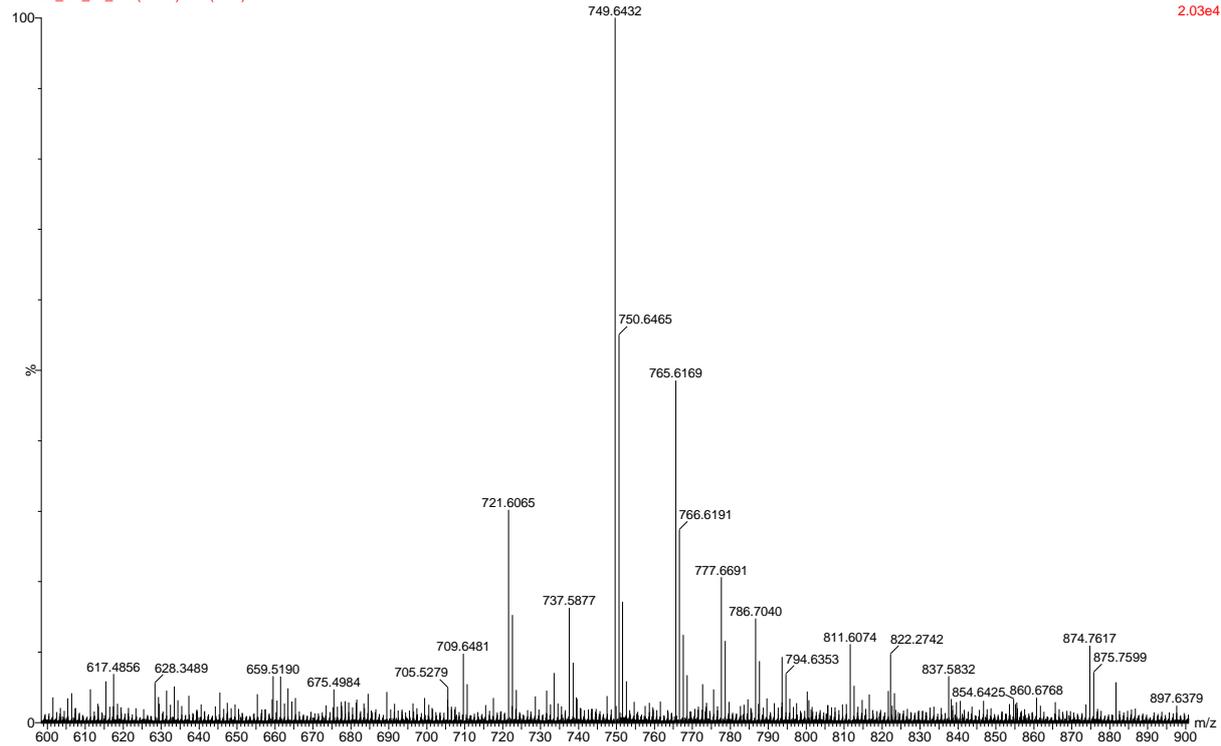
28-Nor-urs-12-ene-3 β ,17 β -diol (3): white amorphous powder; $^1\text{H-NMR}$ (600 MHz, CDCl_3) δ_{H} : 5.30 (1H, br.s, H-12), 3.22 (1H, dd, $J = 11.2, 4.2$ Hz, H-3), 1.08, 1.00, 0.99, 0.95, 0.79 (each 3H, s, $5 \times \text{CH}_3$), 0.93 (3H, d, $J = 6.1$ Hz, CH_3), 0.82 (3H, d, $J = 6.4$ Hz, CH_3). $^{13}\text{C-NMR}$ (150 MHz, CDCl_3) δ_{C} : 137.3 (C-13), 127.7 (C-12), 78.9 (C-3), 72.0 (C-17), 60.5 (C-18), 55.1 (C-5), 47.5 (C-9), 41.8 (C-14), 41.5 (C-19), 40.3 (C-22), 39.7 (C-8), 39.2 (C-20), 38.7 (C-4), 38.6 (C-1), 36.9 (C-10), 32.9 (C-7), 32.2 (C-21), 28.3 (C-16), 28.1 (C-23), 27.1 (C-2), 25.9 (C-15), 23.5 (C-11), 23.0 (C-27), 20.6 (C-30), 18.2 (C-6), 17.2 (C-29), 17.0 (C-26), 15.6 (C-24), 15.4 (C-25).

Ursolic aldehyde (4): white amorphous powder; $^1\text{H-NMR}$ (600 MHz, CDCl_3) δ_{H} : 9.34 (1H, s, H-28), 5.32 (1H, m, H-12), 3.22 (1H, dd, $J = 11.5, 4.8$ Hz, H-3), 1.10, 1.00, 0.93, 0.79, 0.78 (each 3H, s, $5 \times \text{CH}_3$), 0.98 (3H, d, $J = 6.4$ Hz, CH_3), 0.89 (3H, d, $J = 6.4$ Hz, CH_3). $^{13}\text{C-NMR}$ (150 MHz, CDCl_3) δ_{C} : 207.4 (C-28), 137.7 (C-13), 126.1 (C-12), 78.9 (C-3), 55.1 (C-5), 52.5 (C-18), 50.1 (C-17), 47.5 (C-9), 42.1 (C-14), 39.7 (C-8), 38.9 (C-19), 38.7 (C-20), 38.7 (C-4), 38.6 (C-1), 36.9 (C-10), 33.0 (C-22), 31.8 (C-7), 30.1 (C-21), 28.1 (C-15), 27.1 (C-2), 26.8 (C-23), 23.2 (C-11), 23.2 (C-16), 23.2 (C-27), 21.0 (C-30), 18.2 (C-6), 17.1 (C-26), 16.6 (C-29), 15.6 (C-24), 15.5 (C-25).

3 β -Hydroxy-oleana-11,13(18)-dien-28-oic acid (5): white amorphous powder; $^1\text{H-NMR}$ (600 MHz, CDCl_3) δ_{H} : 6.42 (1H, dd, $J = 10.5, 2.5$ Hz, H-11), 5.64 (1H, d, $J = 10.3$ Hz, H-12), 3.24 (1H, dd, $J = 11.5, 4.7$ Hz, H-3), 0.93, 0.97, 0.94, 0.90, 0.79, 0.78, 0.78 (each 3H, s, $7 \times \text{CH}_3$). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ_{C} : 181.3 (C-28), 137.0 (C-13), 131.1 (C-18), 127.1 (C-12), 125.2 (C-11), 79.0 (C-3), 54.8 (C-5), 54.3 (C-9), 48.0 (C-17), 42.0 (C-14), 40.7 (C-8), 40.4 (C-19), 38.8 (C-4), 37.9 (C-1), 36.8 (C-21), 36.6 (C-10), 35.5 (C-22), 32.5 (C-15), 32.4 (C-7), 32.1 (C-20), 31.9 (C-29), 27.8 (C-23), 27.1 (C-2), 24.9 (C-16), 24.0 (C-30), 19.7 (C-27), 18.2 (C-6), 18.0 (C-25), 16.4 (C-26), 15.0 (C-24).

Oleanolic acid (7): white amorphous powder; $^1\text{H-NMR}$ (400 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) δ_{H} : 5.25 (1H, br.s, H-12), 3.16 (1H, m, H-3), 1.12, 0.95, 0.91, 0.89, 0.88, 0.76, 0.75 (each 3H, s, $7 \times \text{CH}_3$). $^{13}\text{C-NMR}$ (100 MHz, $\text{CDCl}_3 + \text{CD}_3\text{OD}$) δ_{C} : 181.0 (C-28), 144.1 (C-13), 122.5 (C-12), 79.0 (C-3), 55.5 (C-5), 47.9 (C-9), 46.6 (C-17), 46.2 (C-19), 41.9 (C-14), 41.5 (C-18), 39.5 (C-8), 38.9 (C-1), 38.7 (C-4), 37.2 (C-10), 34.1 (C-21), 33.2 (C-29), 33.0 (C-7), 32.8 (C-22), 30.8 (C-20), 28.1 (C-23), 27.9 (C-15), 26.9 (C-2), 26.0 (C-27), 23.6 (C-30), 23.6 (C-16), 23.2 (C-11), 18.5 (C-6), 17.0 (C-26), 15.7 (C-24), 15.4 (C-25).

Ursolic acid lactone (8): white amorphous powder; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ_{H} : 5.96 (1H, d, $J = 10.3$ Hz, H-12), 5.53 (1H, dd, $J = 10.3, 3.1$ Hz, H-11), 3.22 (1H, dd, $J = 11.2, 5.0$ Hz, H-3), 1.16, 1.05, 0.98, 0.98, 0.78 (each 3H, s, $5 \times \text{CH}_3$), 0.99 (3H, d, $J = 6.0$ Hz, CH_3), 0.92 (3H, d, $J = 7.5$ Hz, CH_3). $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ_{C} : 179.9 (C-28), 133.4 (C-12), 128.8 (C-11), 89.6 (C-13), 78.8 (C-3), 60.5 (C-18), 54.7 (C-5), 53.0 (C-9), 45.0 (C-17), 41.9 (C-8), 41.7 (C-14), 40.2 (C-19), 38.9 (C-4), 38.2 (C-1), 38.1 (C-20), 36.3 (C-10), 31.3 (C-22), 31.2 (C-7), 30.8 (C-21), 27.7 (C-23), 27.0 (C-2), 25.5 (C-15), 22.8 (C-16), 19.1 (C-25), 18.8 (C-26), 17.9 (C-30), 17.8 (C-29), 17.6 (C-6), 16.1 (C-27), 14.9 (C-24).



Elemental Composition Report

Single Mass Analysis

Tolerance = 100.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Even Electron Ions

112 formula(e) evaluated with 20 results within limits (up to 5 closest results for each mass)

Elements Used:

C: 0-200 H: 0-200 O: 0-5 Na: 0-1

Minimum: -1.5

Maximum: 5.0 100.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
749.6432	749.6424	0.8	1.1	5.5	13.6	C48 H86 O4 Na
	749.6448	-1.6	-2.1	8.5	7.4	C50 H85 O4
	749.6576	-14.4	-19.2	9.5	57.6	C52 H86 O Na
	749.6600	-16.8	-22.4	12.5	98.6	C54 H85 O
	749.6237	9.5	26.0	13.5	95.2	C53 H81 O2

Figure S1: HRESIMS Spectrum of Compound 1

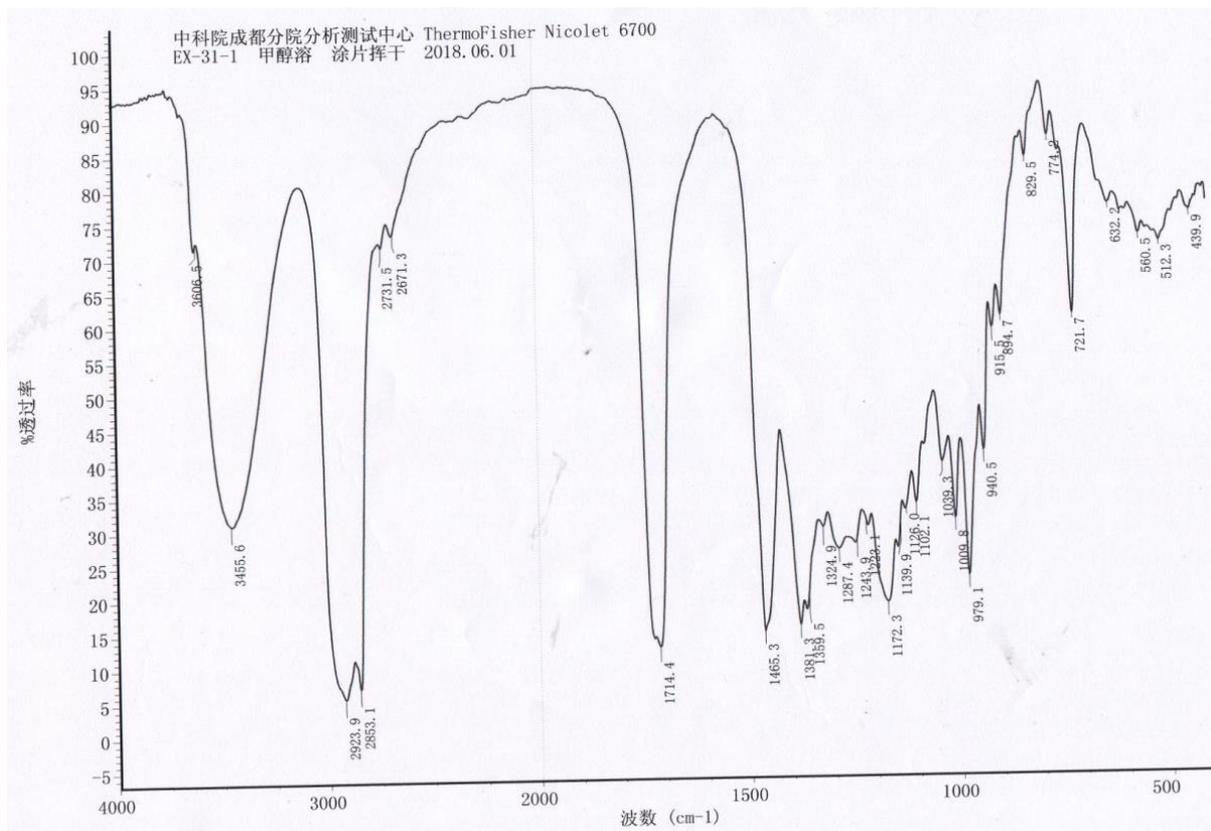


Figure S2: IR Spectrum of Compound 1

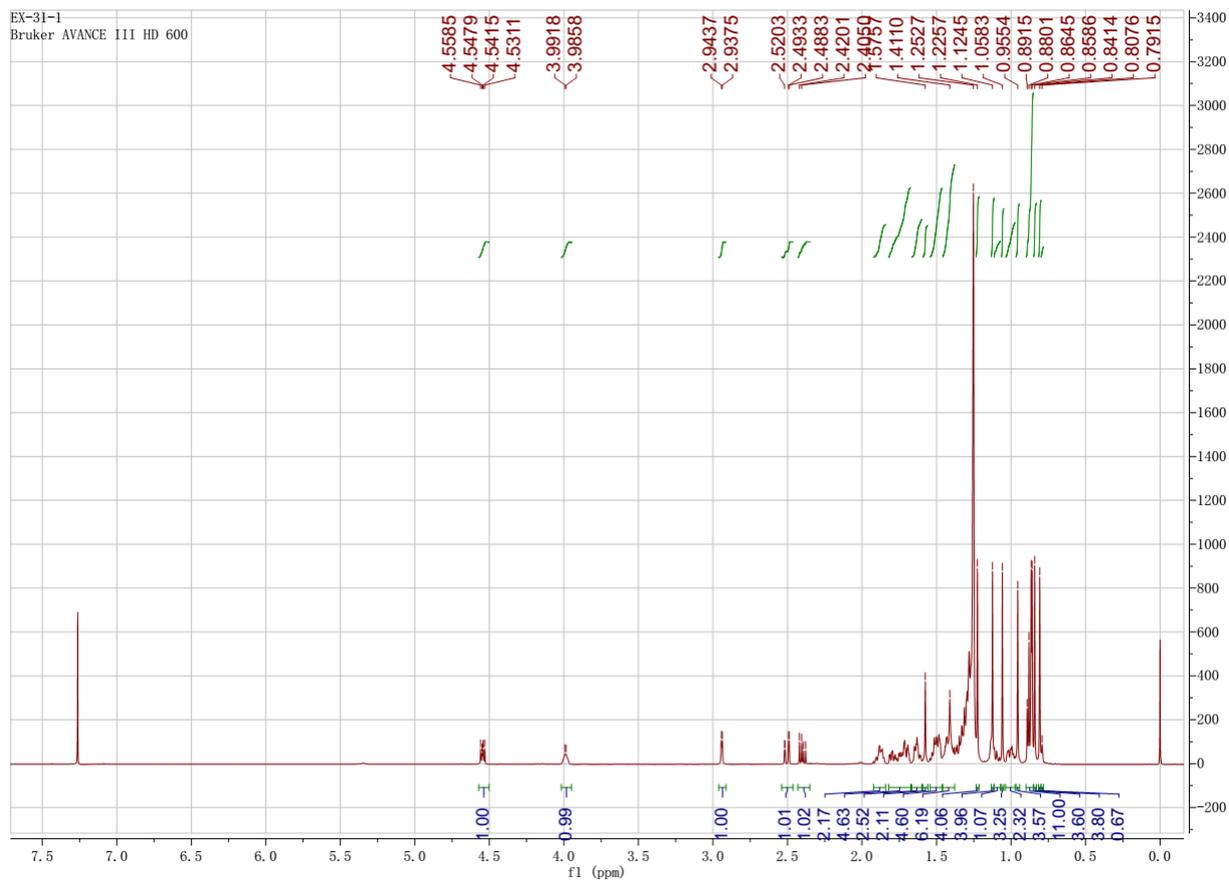


Figure S3: ^1H -NMR Spectrum of Compound 1

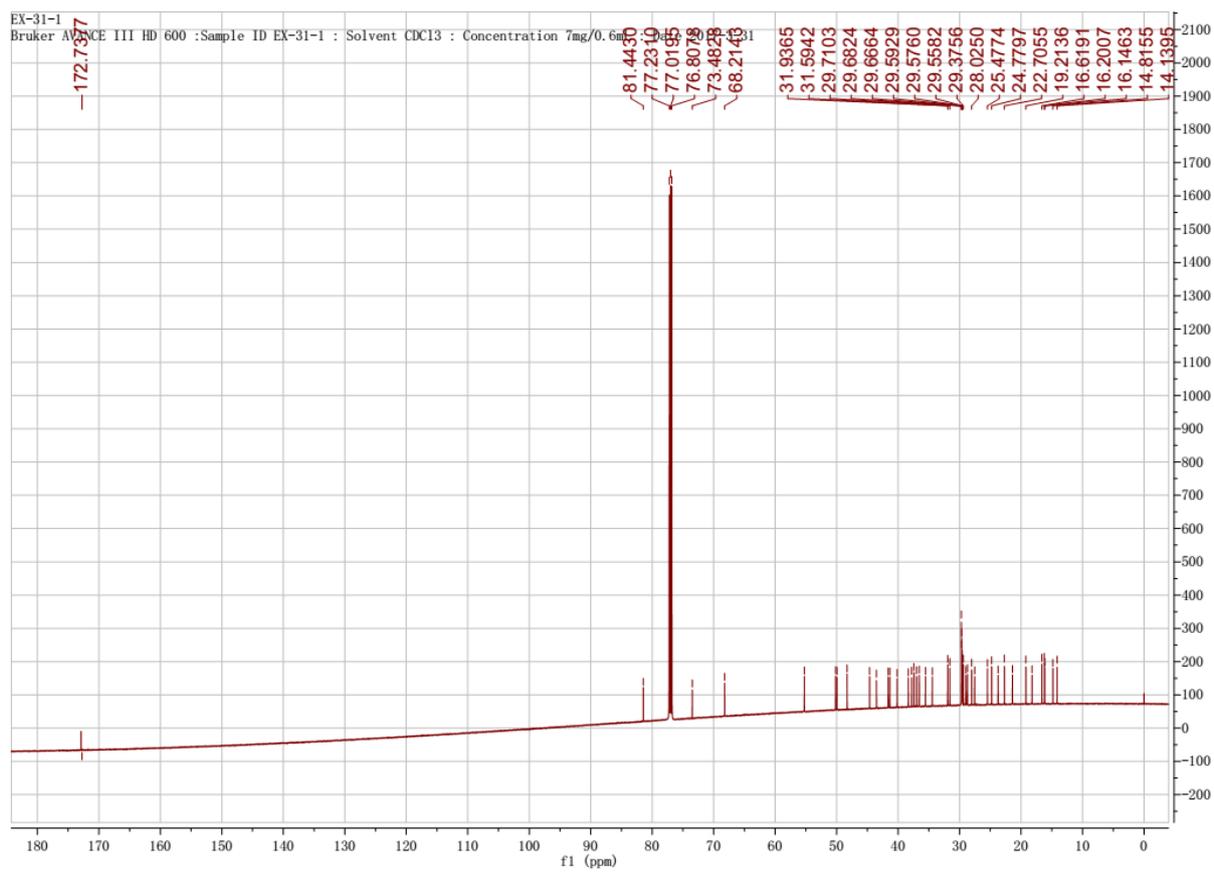


Figure S4: ^{13}C -NMR Spectrum of Compound 1

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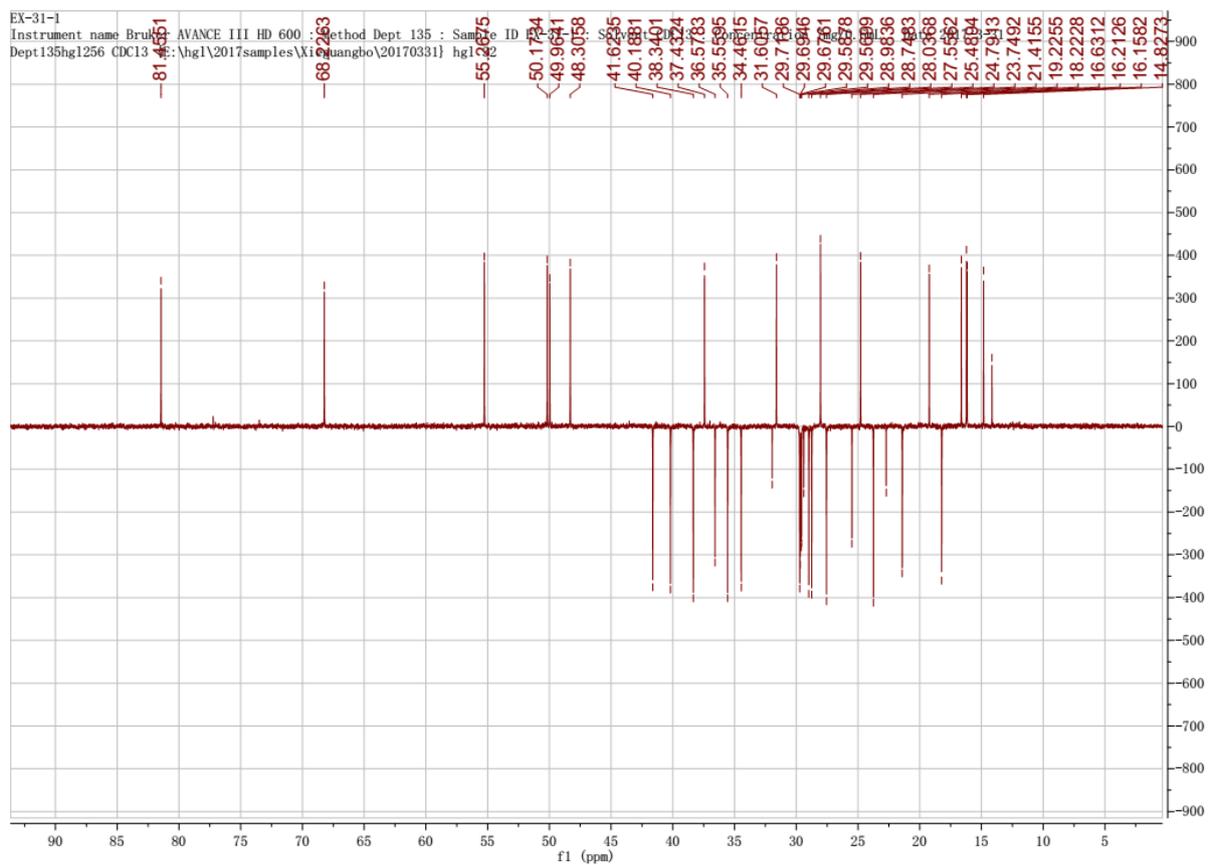


Figure S5: DEPT Spectrum of Compound 1

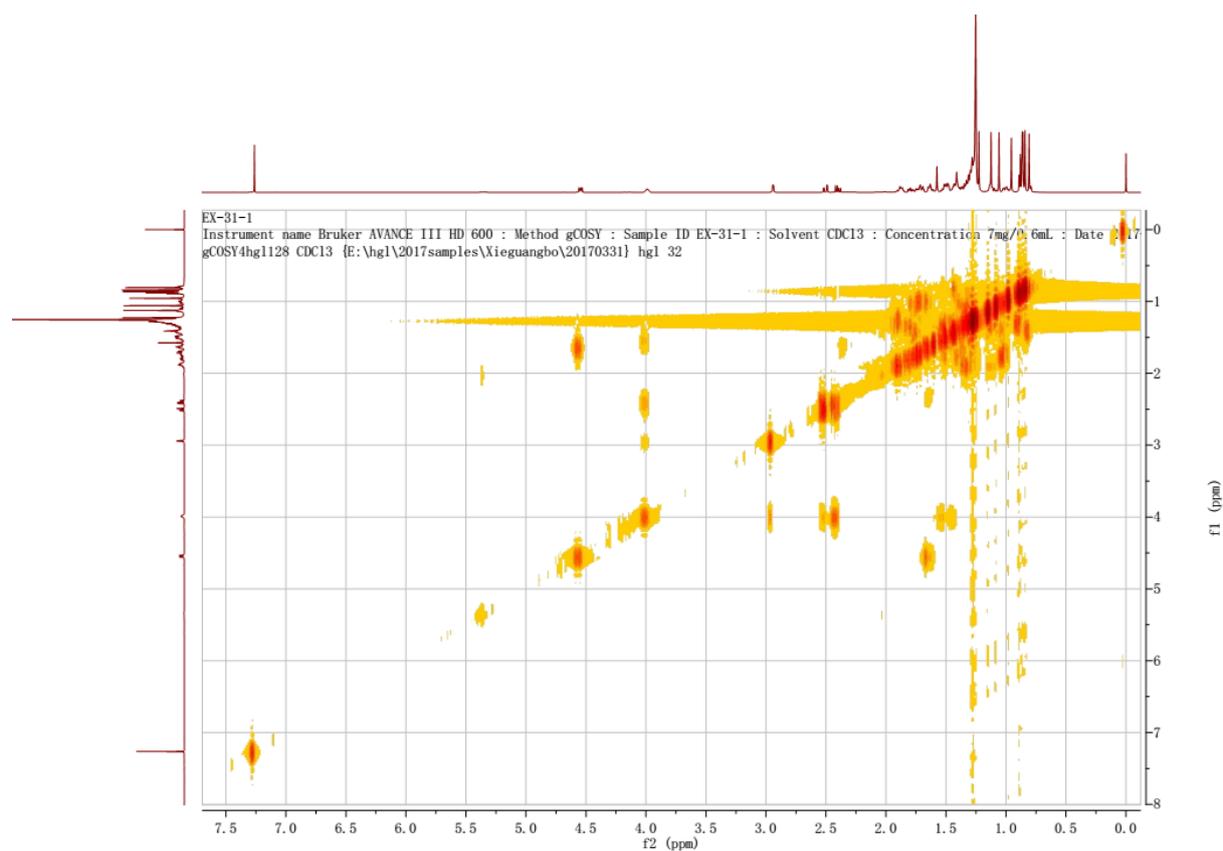


Figure S6: ^1H - ^1H COSY Spectrum of Compound **1**

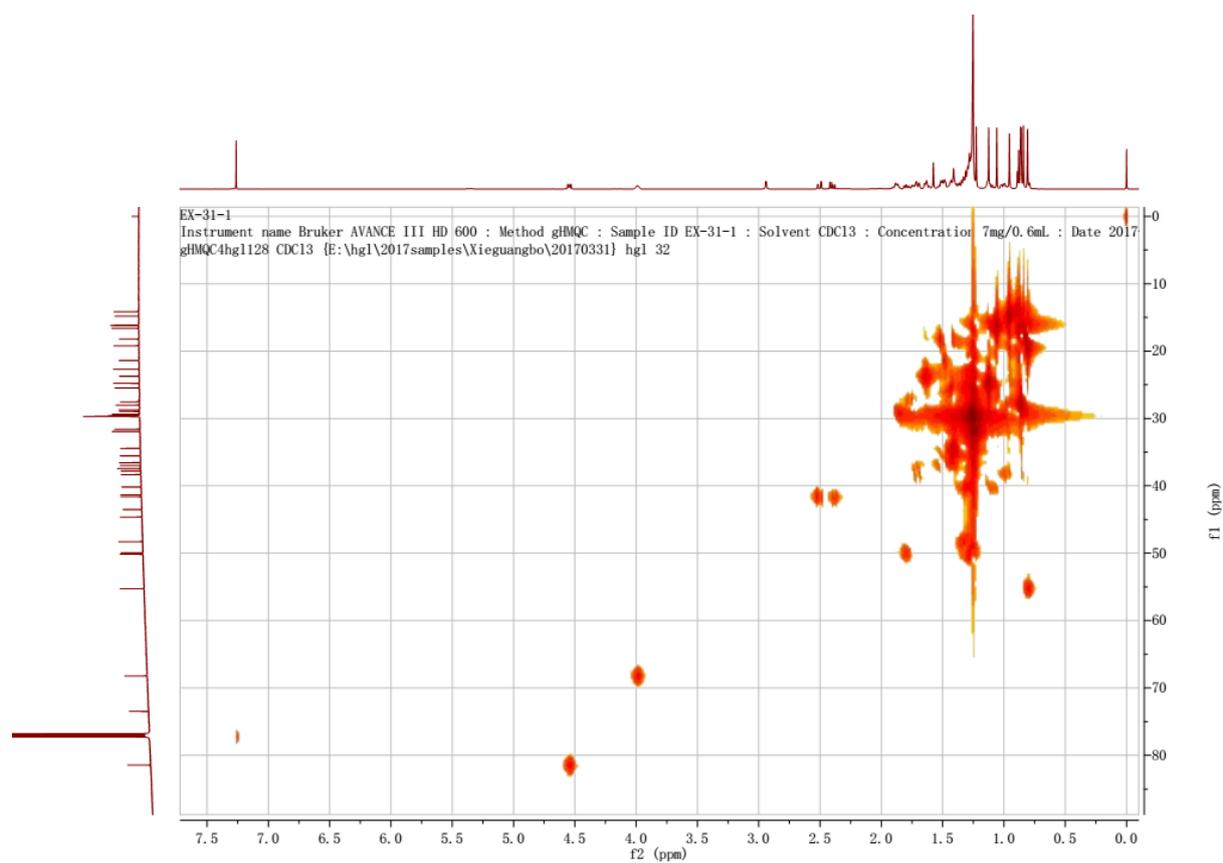


Figure S7: HMQC Spectrum of Compound 1

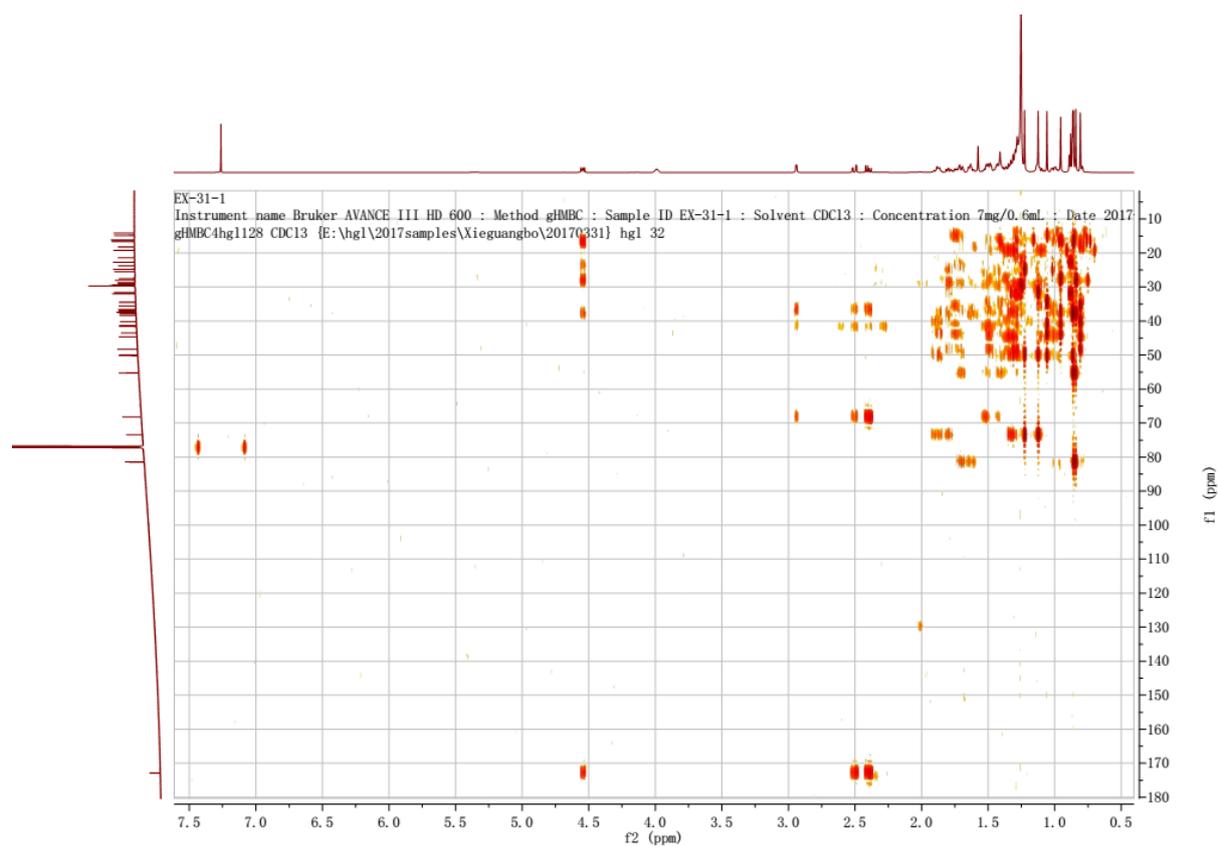


Figure S8: HMBC Spectrum of Compound 1