Supporting Information

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Two new phenolic compounds from *Schizonepeta tenuifolia* (Benth.) Briq

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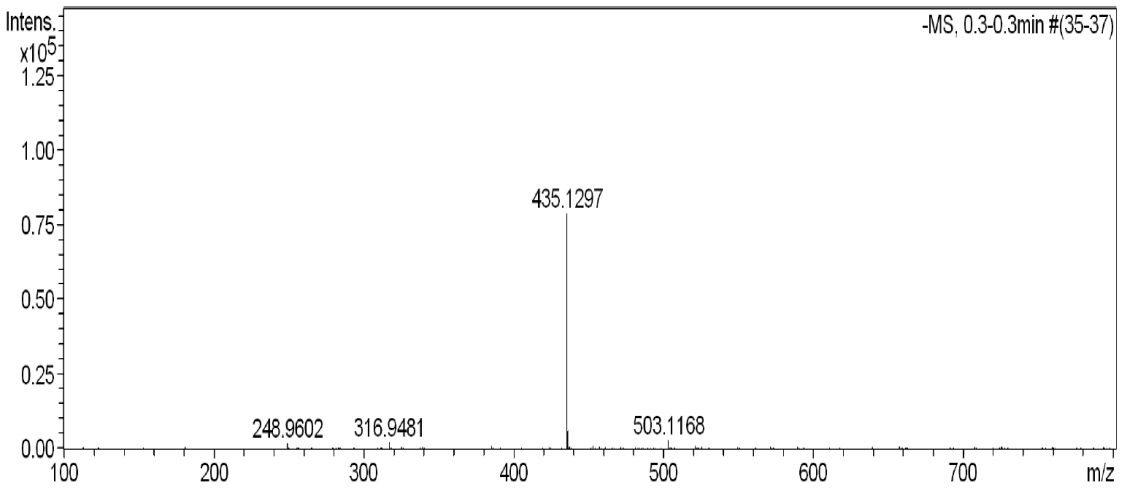
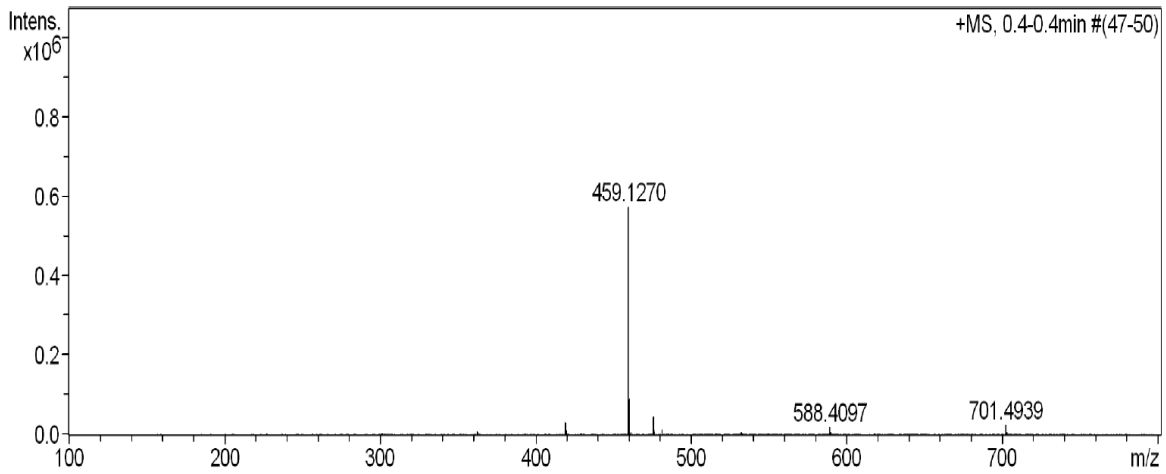


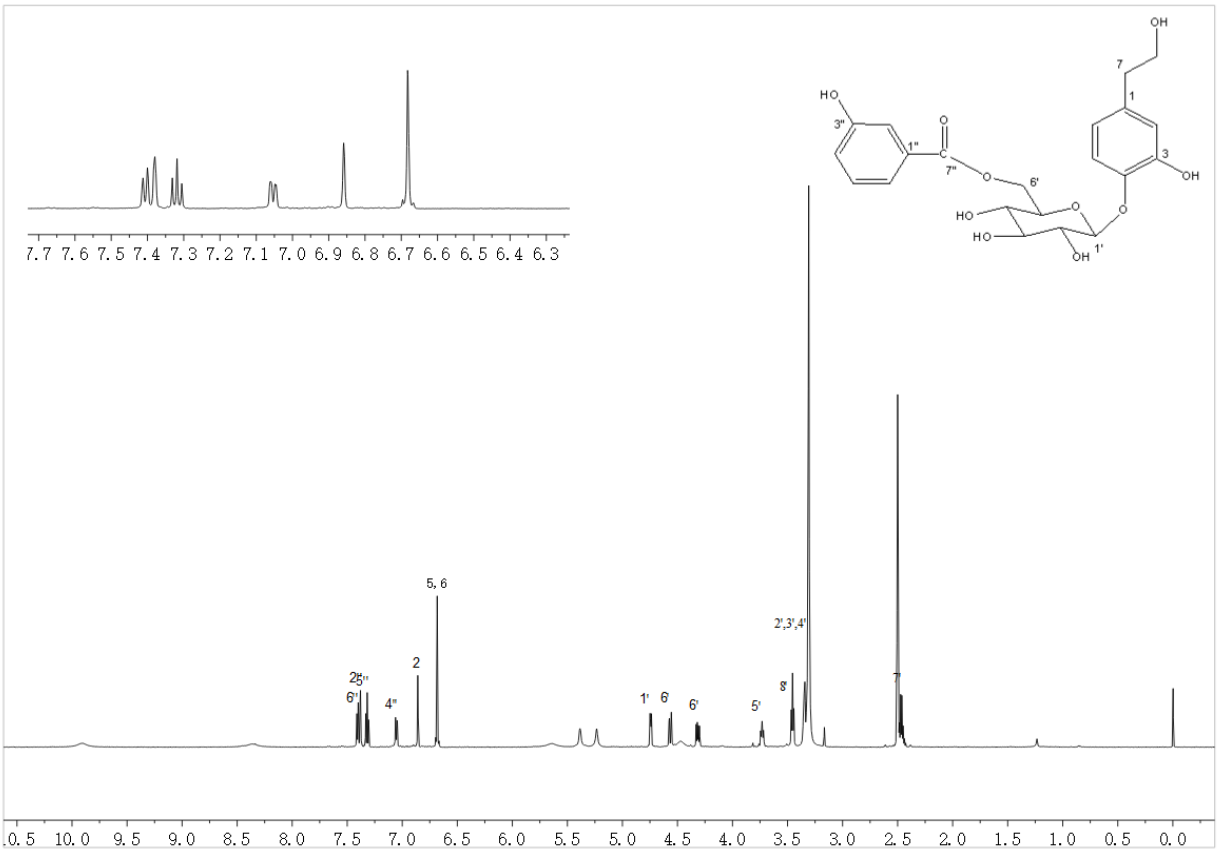
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
435.1297	1	C 21 H 23 O 10	100.00	435.1297	-0.1	-0.2	80.3	10.5	even	ok

S1: HRESI-MS Spectrum of Compound **1** (negative mode)



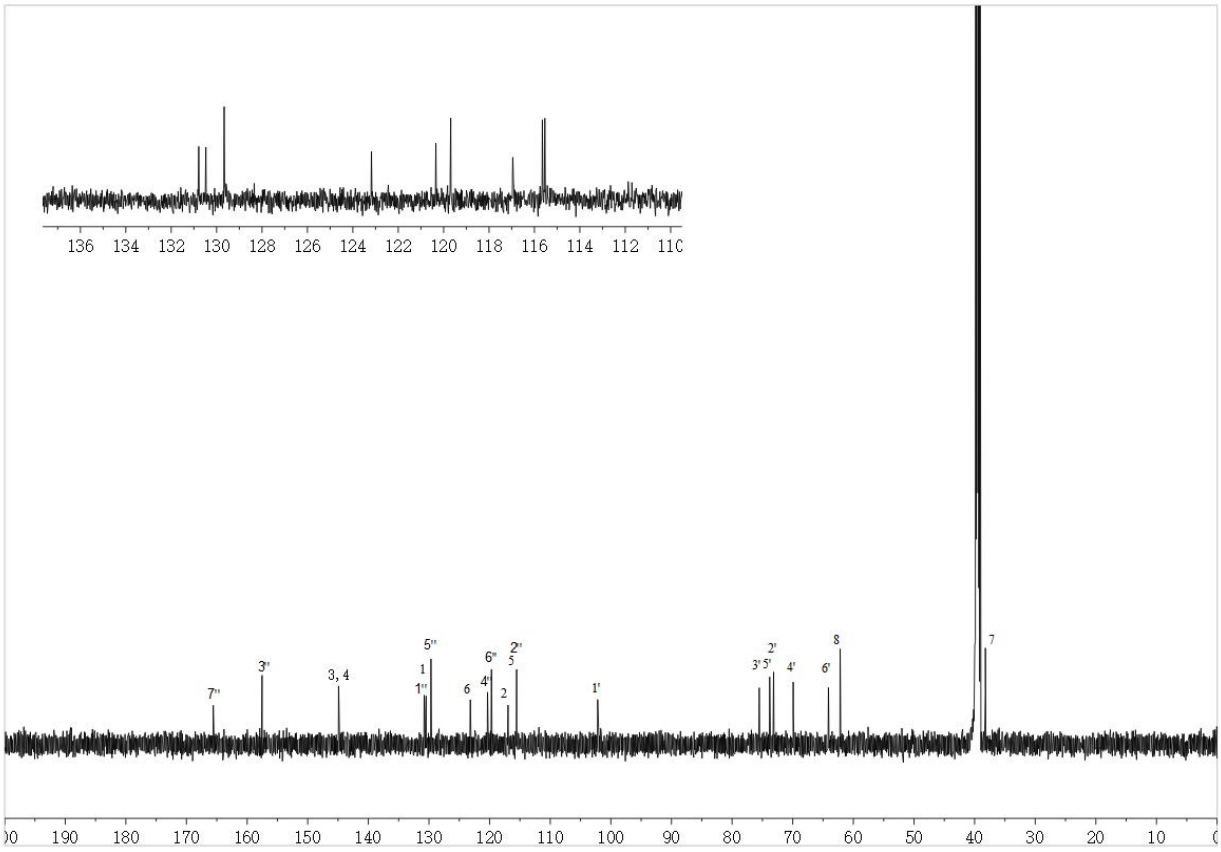
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
459.1270	1	C 21 H 24 Na O 10	100.00	459.1262	-0.9	-1.9	42.6	9.5	even	ok

S2: HRESI-MS Spectrum of Compound **1** (positive mode)

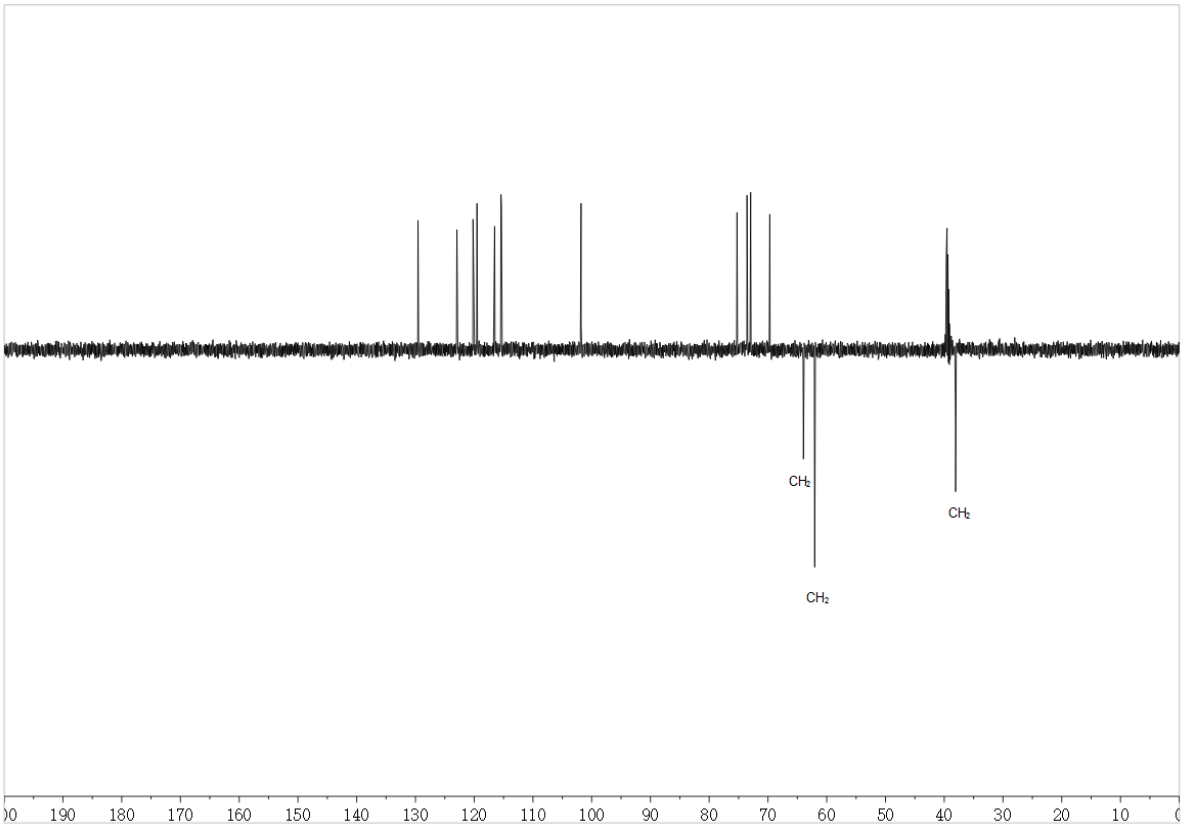


S3: ^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound **1**

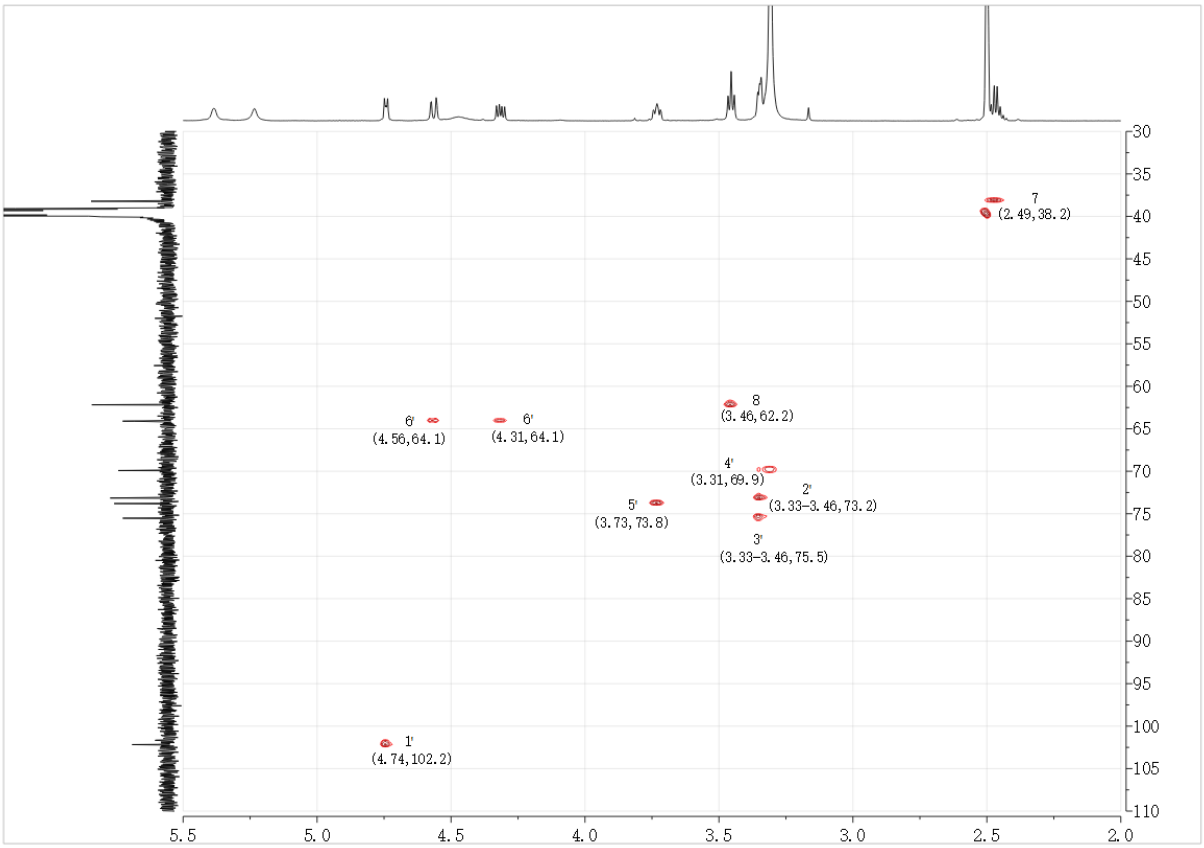
*Schitenoside A (**1**):* yellow amorphous powder. ^{1}H NMR (600 MHz, DMSO-*d6*): δ (ppm) = 7.40 (1H, br.d, *J* = 7.7 Hz, H-6"); 7.38 (1H, br.s, H-2"); 7.32 (1H, br.dd, *J* = 7.7, 8.0 Hz, H-5"); 7.05 (1H, br.d, *J* = 8.0 Hz, H-4"); 6.86 (1H, br.s, H-2); 6.68 (2H, m, H-5, 6); 4.74 (1H, d, *J* = 7.1 Hz, H-1'); 4.56 (1H, br.d, *J* = 10.7 Hz, H-6'); 4.31 (1H, dd, *J* = 6.5, 10.7 Hz, H-6'); 3.73 (1H, m, H-5'); 3.46 (2H, t, *J* = 7.0 Hz, H-8); 3.33-3.46 (2H, m, H-2',3'); 3.31 (1H, m, H-4'); 2.49 (1H, t, J = 7.0 Hz, H-7b); 2.48 (1H, t, J = 7.0 Hz, H-7a). ^{13}C NMR (150 MHz, DMSO-*d6*): δ (ppm) = 165.6 (C-7"); 157.5 (C-3"); 144.9 (C-3,4); 130.8 (C-1"); 130.5 (C-1); 129.7 (C-5"); 123.2 (C-6); 120.3 (C-4"); 119.7 (C-6"); 117.0 (C-2); 115.7 (C-5); 115.6 (C-2"); 102.2 (C-1'); 75.5 (C-3'); 73.8 (C-5'); 73.2 (C-2'); 69.9 (C-4'); 64.1 (C-6'); 62.2 (C-8); 38.2 (C-7). HRMS: positive ion mode: *m/z* 459.1270 $[M+Na]^+$, negative ion mode: m/z 435.1297 $[M-H]^-$.



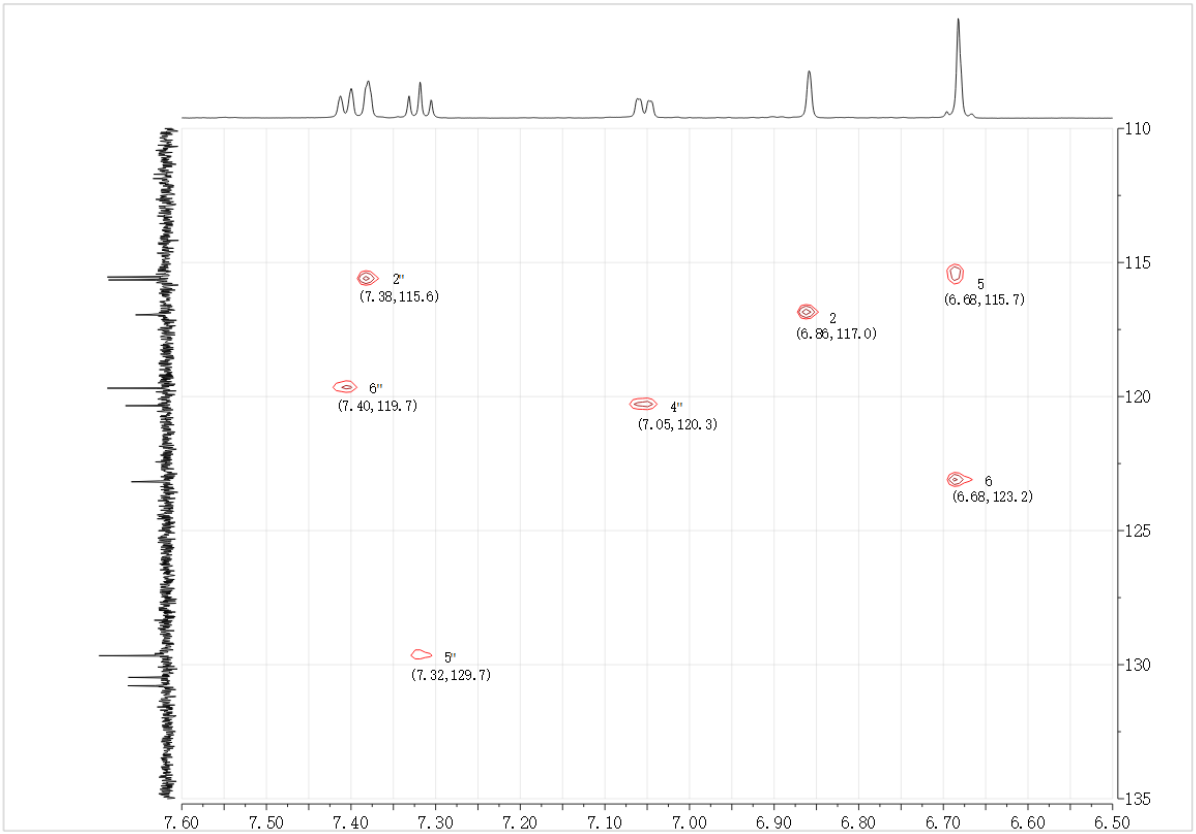
S4: ^{13}C-NMR Spectrum (150 MHz, DMSO-d_6) of Compound **1**



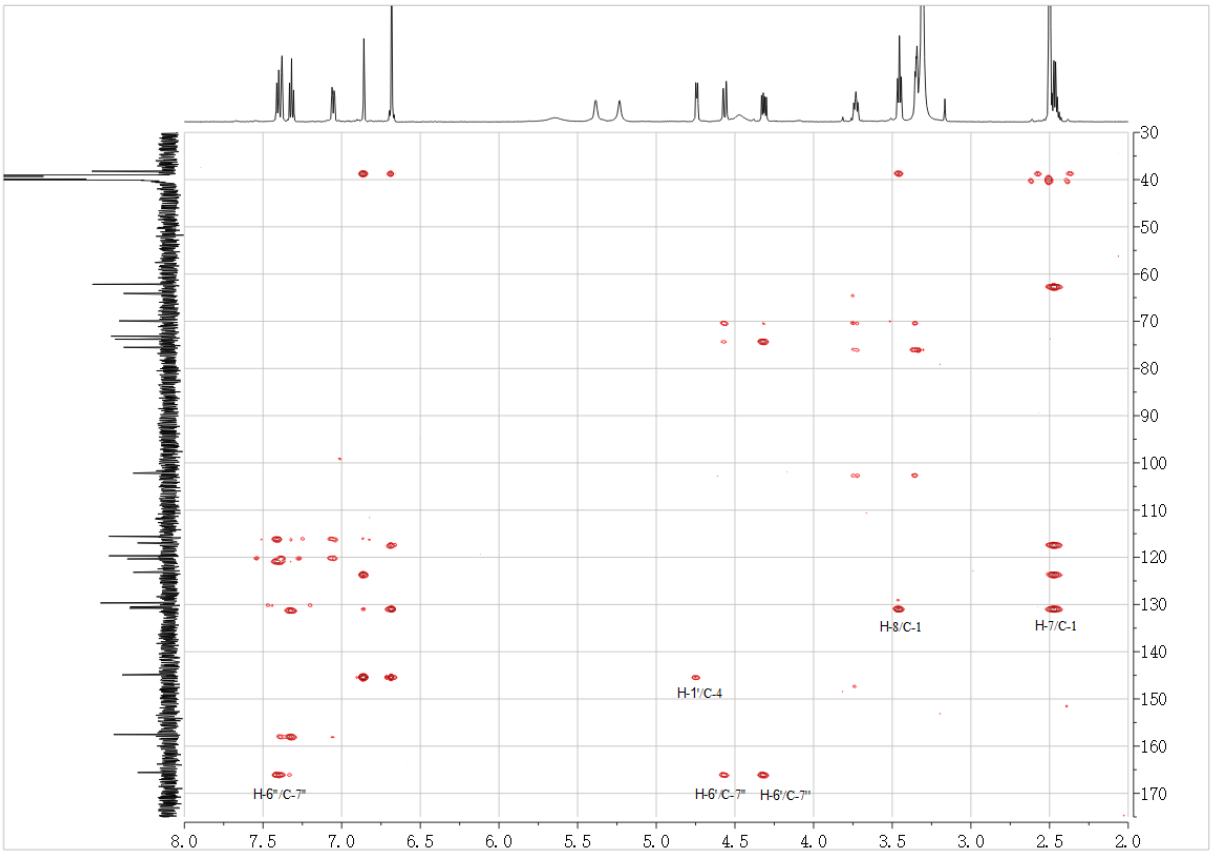
S5: DEPT spectrum of compound **1** (135°)



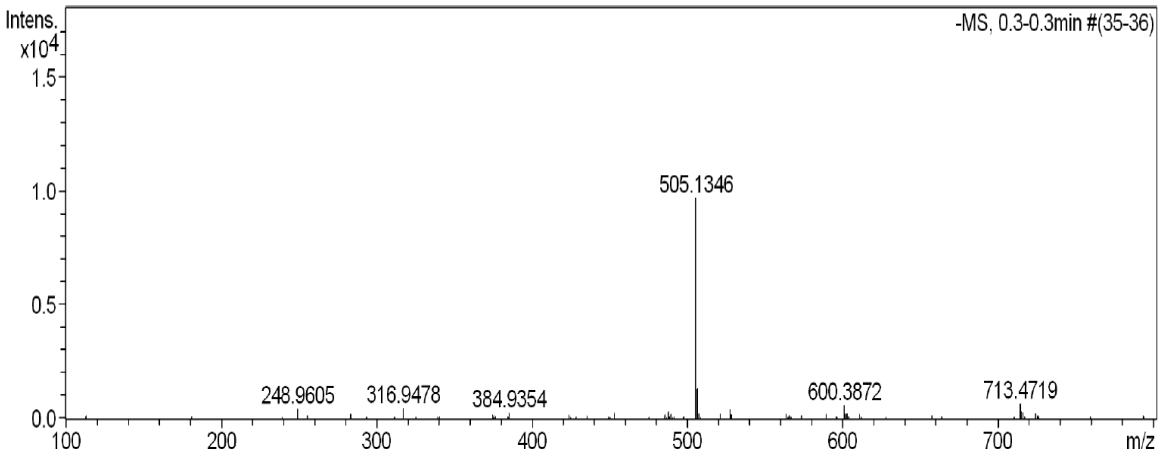
S6: HSQC (600 MHz) Spectrum of Compound **1** (From 30 to 110 ppm)



S7: HSQC (600 MHz) Spectrum of Compound **1** (From 110 to 135 ppm)

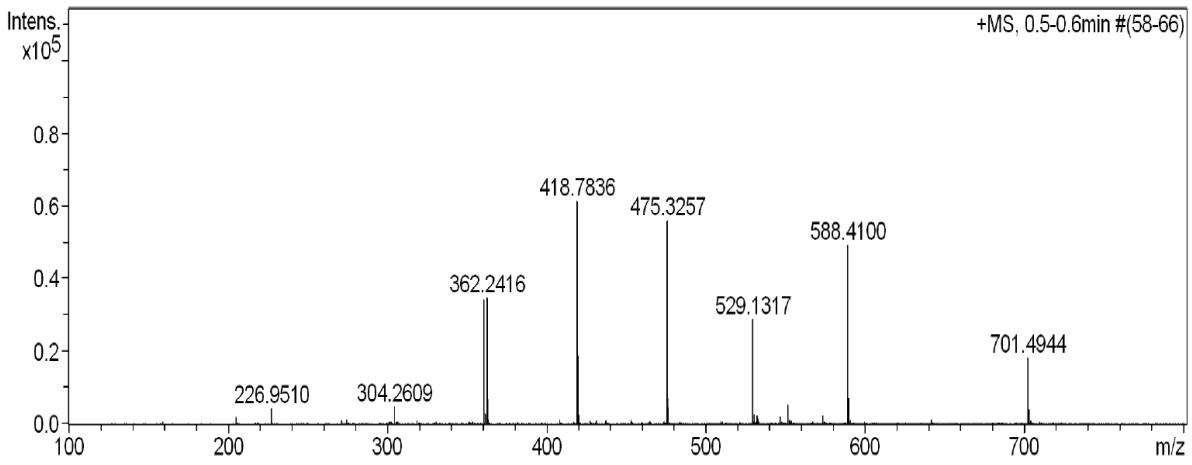


S8: HMBC (600 MHz) Spectrum of Compound **4** (From 30 to 175 ppm)



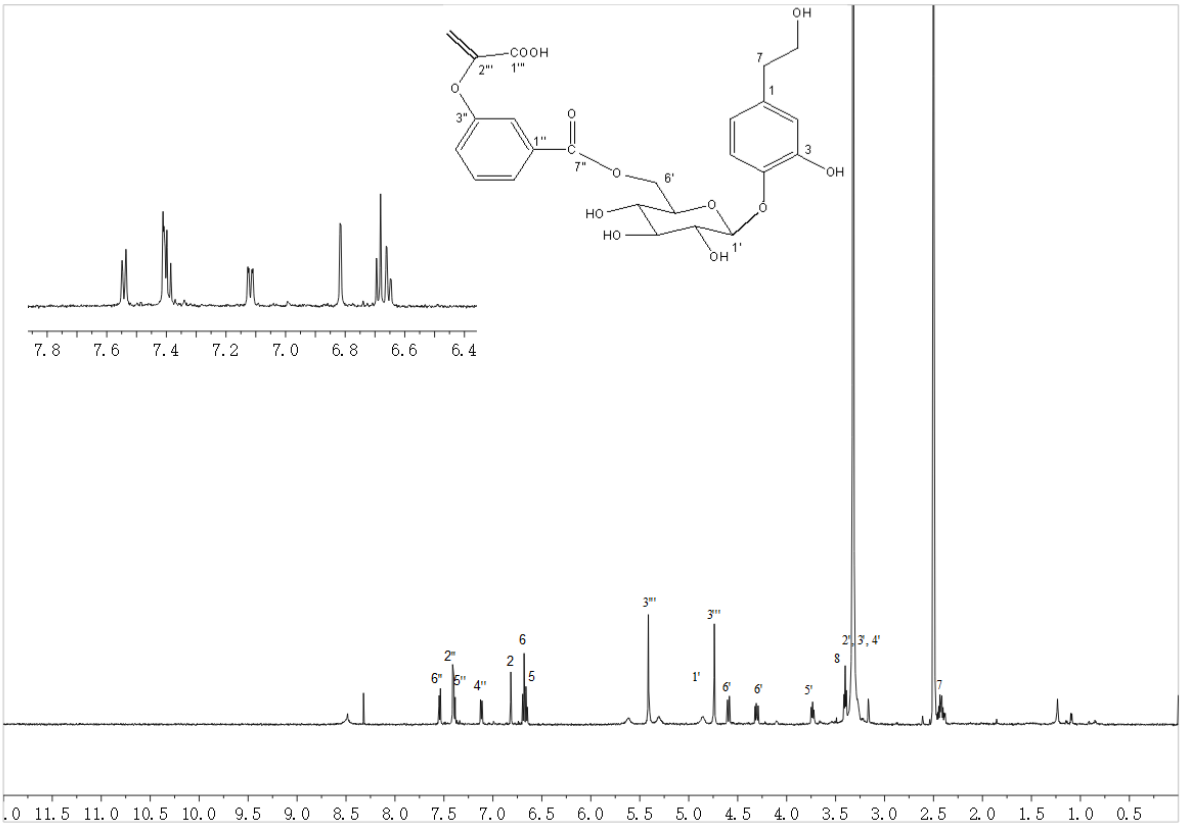
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
505.1346	1	C 24 H 25 O 12	100.00	505.1351	0.6	1.1	68.7	12.5	even	ok

S9: HRESI-MS Spectrum of Compound **2** (negative mode)



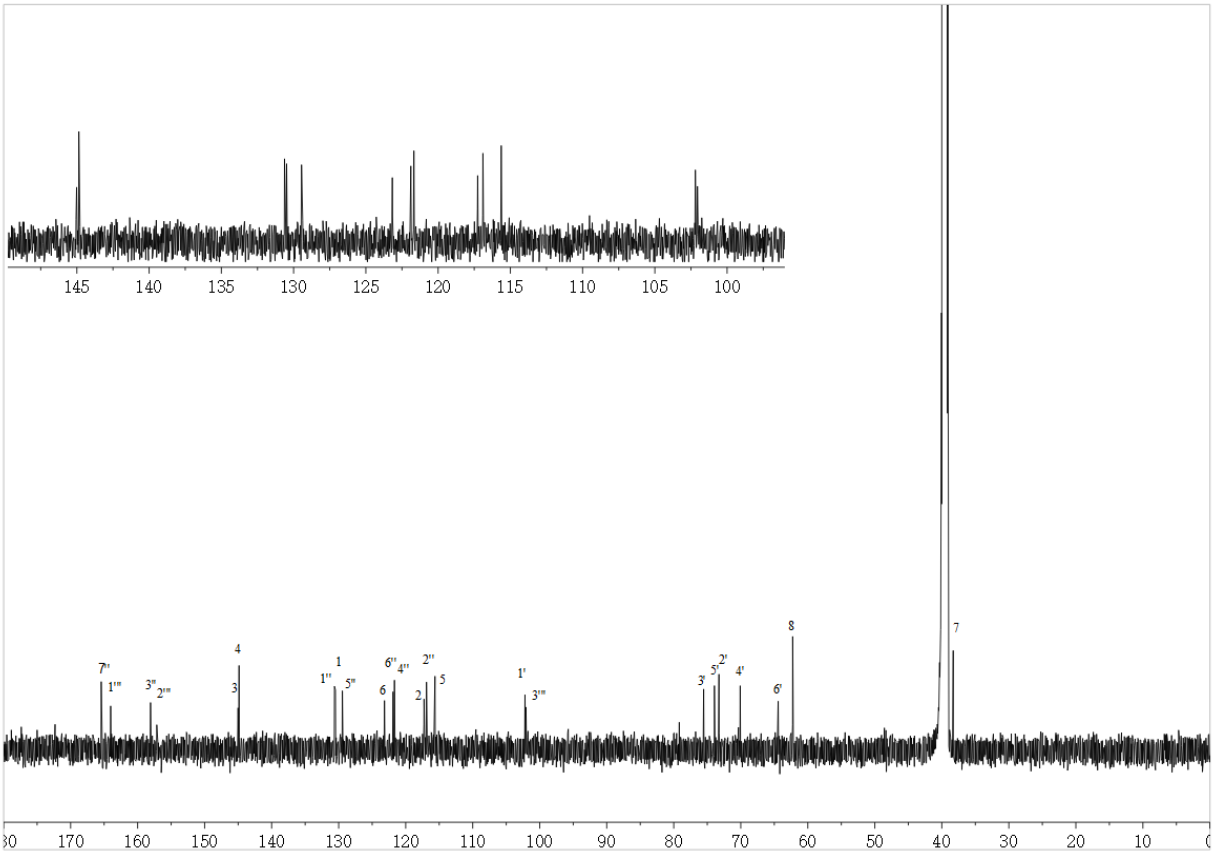
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
529.1317	1	C 24 H 26 Na O 12	100.00	529.1316	-0.0	-0.0	92.6	11.5	even	ok

S10: HRESI-MS Spectrum of Compound **2** (positive mode)

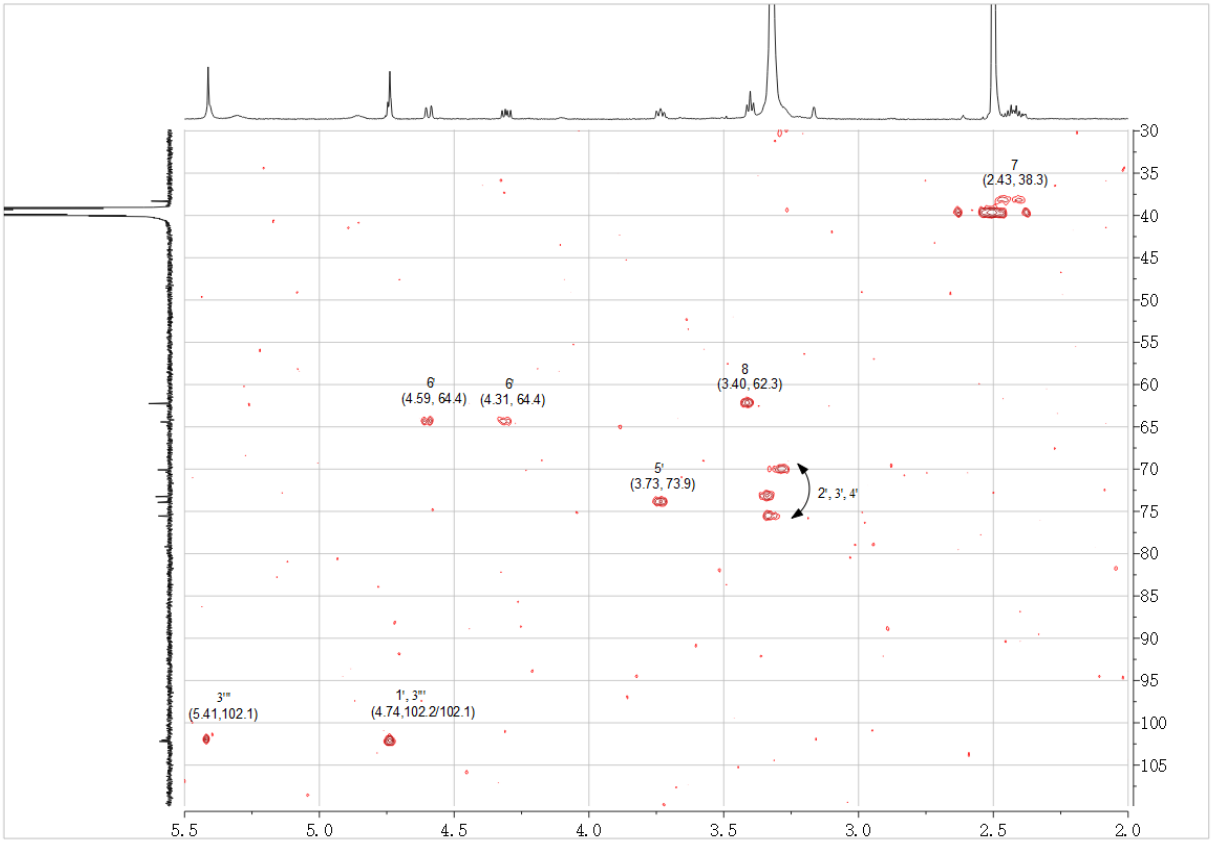


S11: ^{1}H-NMR Spectrum (600 MHz, DMSO-d_6) of Compound **2**

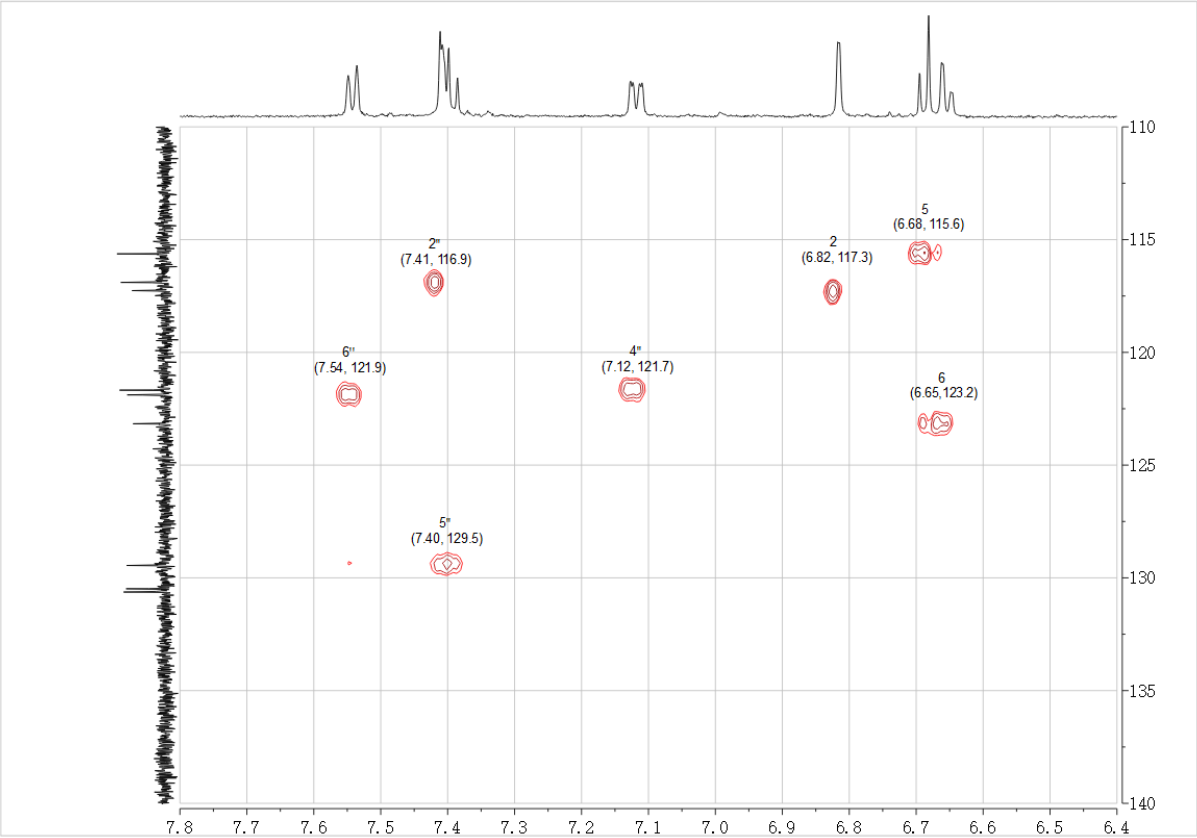
*Schitenoside B (**2**):* yellow amorphous powder. δ (ppm) = 7.54 (1H, br.d, J = 7.7, H-6"); 7.41 (1H, d, J = 2.1, H-2"); 7.40 (1H, br.dd, J = 7.7, 8.2, H-5"); 7.12 (1H, dd, J = 2.1, 8.2, H-4"); 6.82 (1H, d, J = 1.1, H-2); 6.68 (1H, d, J = 8.1, H-5); 6.65 (1H, dd, J = 1.1, 8.1, H-6); 5.41 (1H, br.s, H-3'"); 4.74 (1H, d, J = 7.1, H-1'); 4.74 (1H, br.s, H-3'"); 4.59 (1H, br.d, J = 11.2, H-6'); 4.31 (1H, dd, J = 7.0, 11.2, H-6'); 3.73 (1H, m, H-5'); 3.40 (2H, t, J = 6.8, H-8); 3.34-3.46 (2H, m, H-2', 3'); 3.28 (1H, m, H-4'); 2.43 (2H, t, J = 6.8, H-7). ^{13}C NMR (150 MHz, DMSO-*d6*): δ (ppm) = 165.4 (C-7"); 164.0 (C-1'"); 158.1 (C-3"); 157.2 (C-2'"); 145.0 (C-3); 144.9 (C-4); 130.6 (C-1"); 130.5 (C-1); 129.5 (C-5"); 123.2 (C-6); 121.9 (C-6"); 121.7 (C-4"); 117.3 (C-2); 116.9 (C-2"); 115.6 (C-5); 102.2 (C-1'); 102.1 (C-3'"); 75.5 (C-3'); 73.9 (C-5'); 73.3 (C-2'); 70.1 (C-4'); 64.4 (C-6'); 62.3 (C-8); 38.3 (C-7). HRMS: positive ion mode: *m*/*z* 529.1317 $[M+Na]^+$, negative ion mode: m/z 505.1346 $[M-H]^-$.



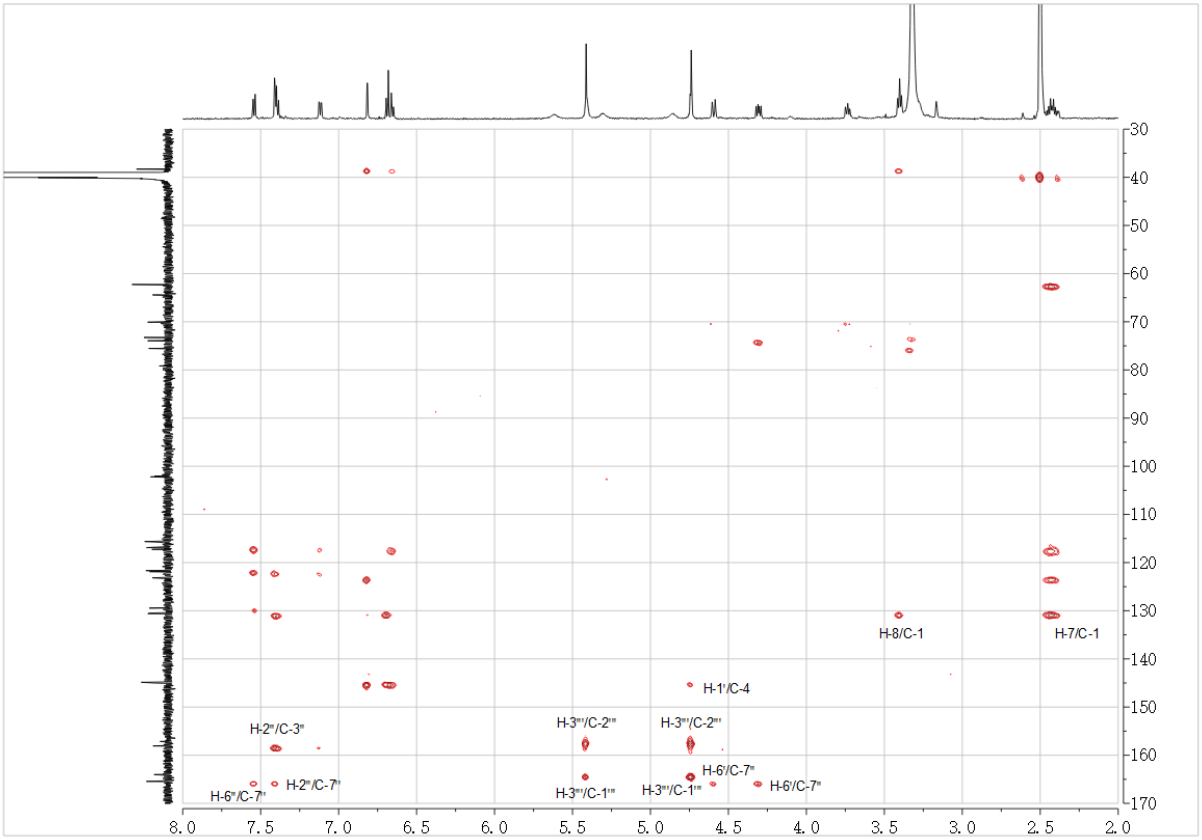
S12: ^{13}C-NMR Spectrum (150 MHz, DMSO-d_6) of Compound **2**



S13: HSQC (600 MHz) Spectrum of Compound **2** (From 30 to 110 ppm)



S14: HSQC (600 MHz) Spectrum of Compound **2** (From 110 to 140 ppm)



S15: HMBC (600 MHz) Spectrum of Compound **2** (From 30 to 170 ppm)