Phytochemical profiles and their hypoglycemic effects of tree peony seed coats

Zenggen Liu[a*], Mingzhu Li[a], Dawen Qian[a], Zheng'an Liu[b], Qingyan Shu[b*]

[a] Qinghai Provincial Key Laboratory of Tibetan Medicine Research and Key Laboratory of Tibetan Medicine Research, Northwest Institute of Plateau Biology, CAS, Xining 810001, China

[b] Key Laboratory of Plant Resources/Beijing Botanical Garden, Institute of Botany, CAS, Beijing 100093, China

[*] Corresponding authors. Tel/Fax: +86 971 6143282, E-mail address: lzg@nwipb.ac.cn (ZG Liu), shuqy@ibcas.ac.cn (QY Shu). Addresses for other authors: 695469402@qq.com (MZ Li), dwqian@nwipb.ac.cn (DW Qian), liuzhengan@ibcas.ac.cn (ZA Liu).

Table S1 Phytochemical composition and content (mg/g) in seed coats of three tree peonies (*POSC*, *PDSC* and *PLSC*) located from different production regions.

No.	RD	PF	EG	SA	SB	VF	AD	UN I	UN II
S1	0.31±0.10	0.56±0.11	0.54±0.12	24.37±2.53	209.17±23.60	30.96±3.03	113.24±9.77	47.70±5.50	32.10±2.32
S2	0.30±0.05	0.37±0.04	-	25.86±1.95	227.17±18.77	47.23±2.26	145.75±12.52	12.84±2.21	46.55±3.44
S3	0.15±0.06	0.53±0.12	-	23.09±2.76	197.38±22.18	34.83±3.12	177.12±24.61	16.94±1.99	42.72±2.94
S4	0.08±0.02	0.40±0.07	-	24.05±3.07	209.17±9.80	55.93±3.67	181.24±18.92	8.14±1.24	47.12±3.40
S5	0.12±0.03	0.42±0.05	0.49±0.10	21.52±1.18	187.99±12.86	28.77±2.27	119.37±8.67	28.06±2.34	32.12±1.95
S6	0.01±0.00	0.59±0.14	0.16±0.02	25.92±3.34	232.99±30.67	41.96±2.90	162.76±10.02	11.29±1.29	47.38±3.41
S7	0.32±0.14	0.47±0.10	0.07±0.01	16.15±2.10	132.46±14.29	71.77±5.24	115.97±6.50	19.31±1.05	26.74±1.66
S8	0.12±0.05	0.45±0.08	0.26±0.04	27.44±3.17	240.43±25.40	35.78±1.80	145.57±13.51	23.82±1.81	39.55±2.73
S9	0.16±0.02	0.51±0.12	0.05±0.01	23.57±2.06	199.65±21.69	52.88±4.31	108.41±9.75	34.47±2.94	31.97±2.01
S10	0.64±0.15	0.34±0.03	1.87±0.24	25.83±1.92	216.82±17.92	43.45±2.99	105.58±10.04	28.73±1.12	35.46±1.97
S11	0.58±0.22	0.46±0.05	0.87±0.22	24.07±2.30	197.11±15.33	54.44±3.27	100.95±12.38	13.16±1.50	36.20±2.25
S12	0.26±0.07	0.42±0.05	3.24±0.57	20.51±1.18	190.63±8.96	62.45±5.00	140.31±12.67	26.26±1.33	35.59±1.59
S13	0.18±0.00	0.25±0.07	-	18.11±1.37	156.07±23.07	32.98±1.66	154.67±19.18	38.38±2.94	35.15±2.92
S14	0.25±0.02	0.66±0.12	3.96±0.53	21.76±1.56	190.87±17.94	74.75±4.54	182.08±21.60	12.64±1.17	42.35±3.13
S15	0.16±0.02	0.50±0.04	2.36±0.32	19.41±2.33	180.60±12.89	48.38±3.30	204.34±16.36	14.08±2.11	47.95±2.85
S16	0.21±0.03	0.55±0.10	0.07±0.01	19.76±1.27	189.43±21.37	41.03±3.55	182.36±15.49	18.03±1.53	39.43±2.39
S17	1.05±0.34	0.08±0.03	2.14±0.20	17.76±3.44	118.10±22.96	20.32±4.38	35.60±4.72	3.51±0.92	17.23±1.50
S18	0.55±0.17	0.44±0.02	2.86±0.18	25.76±1.86	242.64±27.90	66.40±2.93	193.60±18.77	26.26±2.33	47.22±2.26
S19	0.14±0.01	0.50±0.07	-	19.96±2.39	169.97±18.72	34.90±3.12	77.75±7.04	60.17±5.28	21.40±1.52
S20	0.21±0.02	0.65±0.06	0.07±0.02	29.16±2.16	278.26±16.40	20.25±3.65	154.37±11.29	7.35±7.04	46.60±3.60
S21	9.26±2.20	0.05±0.01	0.25±0.04	7.04±1.04	35.11±4.29	12.50±1.72	100.50±6.53	4.14±1.02	15.89±1.87
S22	6.86±1.87	0.06±0.01	0.19±0.03	7.50±0.92	42.33±3.95	4.21±0.88	76.00±5.49	4.20±0.88	14.50±1.29
S23	1.96±0.63	0.22±0.04	0.19±0.02	0.69±0.24	2.93±0.77	8.23±1.42	99.87±3.92	3.87±1.30	14.84±0.98
S24	14.91±2.69	0.08±0.02	0.18±0.04	0.31±0.09	0.69±0.16	0.91±0.28	155.01±14.68	5.17±0.94	22.70±1.07
S25	6.29±1.08	0.10±0.00	0.03±0.00	2.96±0.84	9.86±1.30	0.27±0.05	14.49±2.05	1.03±0.37	11.00±0.84
S26	1.85±0.75	0.04±0.01	-	-	-	0.08±0.02	38.63±4.08	1.71±0.45	12.64±1.16

RD: (E)-resveratrol 3,5-*O*-*β*-diglucoside, PF: paeoniflorin, EG: ethyl gallate, SA: suffruticosol A, SB: suffruticosol B, VF: trans-*ε*-viniferin, AD: ampelopsin D, UN I: Unidentified II, UN II: Unidentified II.

The symbol (-) presents that it is below the detection limit.

Table S2 Pearson correlation coefficients among the main phytochemical contents of *Paeonia* seed coats.

Phytochemicals	RD	PF	EG	SA	SB	VF	AD	UN I	UN II
(E)-resveratrol 3,5-*O*-*β*-diglucoside (RD)	1.000								
Paeoniflorin (PF)	-0.673**	1.000							
Ethyl gallate (EG)	-0.199	0.201	1.000						
Suffruticosol A (SA)	-0.716**	0.802**	0.235	1.000					
Suffruticosol B (SB)	-0.723**	0.834**	0.239	0.989**	1.000				
trans-*ε*-Viniferin (VF)	-0.618**	0.711**	0.506**	0.701**	0.706**	1.000			
Ampelopsin D (AD)	-0.245	0.630**	0.252	0.519**	0.591**	0.572**	1.000		
Unidentified I (UN I)	-0.428*	0.461*	0.028	0.473*	0.470*	0.370	0.122	1.000	
Unidentified II (UN II)	-0.551**	0.781**	0.266	0.829**	0.876**	0.694**	0.856**	0.199	1.000

**. $P < 0.01$, correlation is significant at the 0.01 level (2-tailed).

*. $P < 0.05$, correlation is significant at the 0.05 level (2-tailed).

Table S3 Inhibitory effects of acarbose and the main compounds of *Paeonia* seed coats on α-glucosidase

Compound no.	Name/description	IC_{50} (μM)
	Acarbose	0.022 ± 0.0026
1	(E)-resveratrol 3,5-*O*-*β*-diglucoside	>3000
2	Paeoniflorin	>3000
3	Ethyl gallate	>3000
4	Suffruticosol A	12.44 ± 1.10
5	Suffruticosol B	12.55 ± 1.11
6	trans-*ε*-Viniferin	7.75 ± 0.85
7	Ampelopsin D	3.92 ± 0.27
8	Vateriferol	3.01 ± 0.18
9	4-hydroxybenzoic acid	>3000
10	4-hydroxybenzal-dehyde	>3000
11	Unidentified I	>3000
12	Unidentified II	>3000

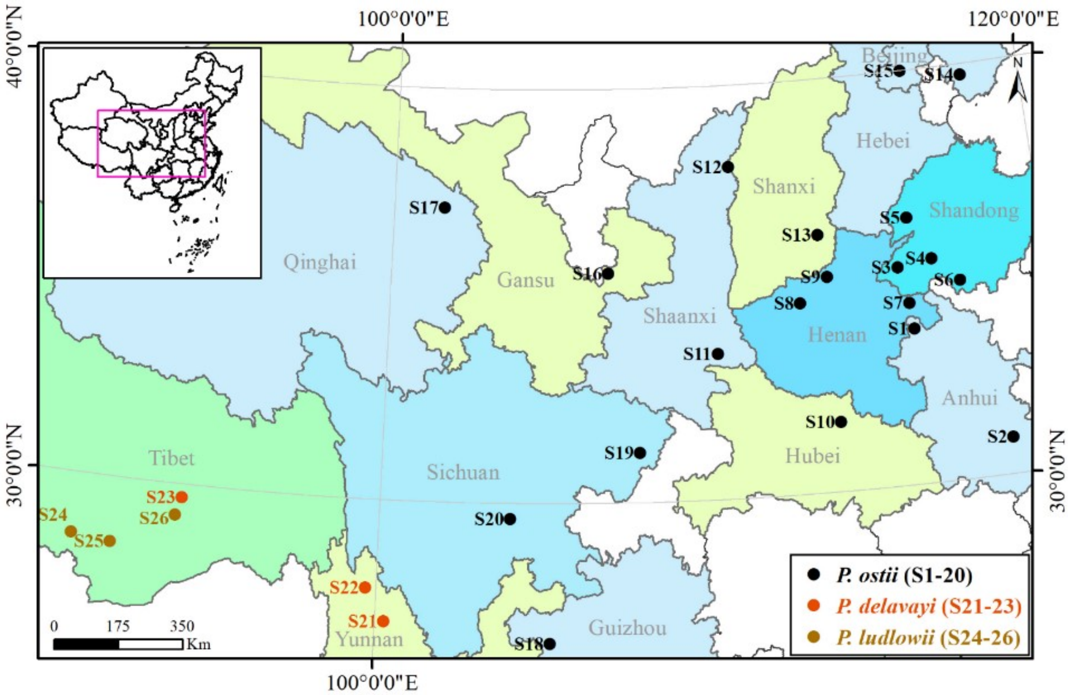


Fig. S1. Geographic distribution of different sampled positions of *Paeonia* plants. Names of the numbered positions were listed in **Table 1**.

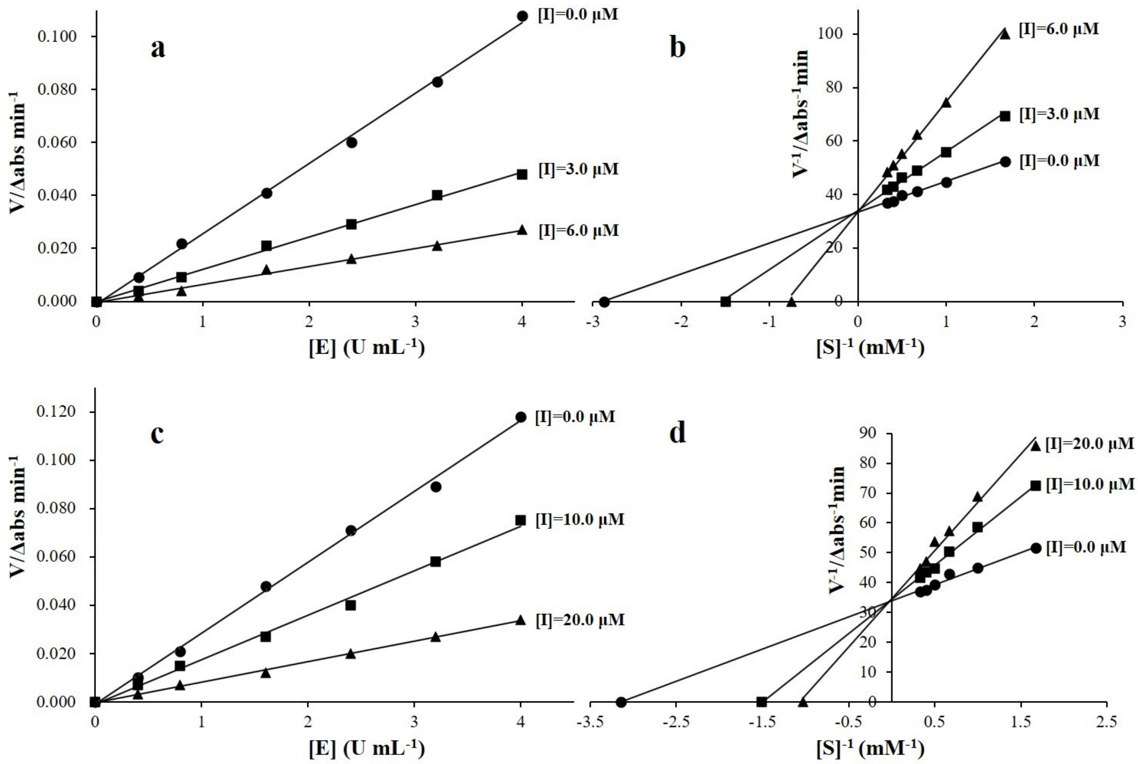


Fig. S2. Inhibition mechanism of ampelopsin D (a) and suffruticosol B (c) on α-glucosidase and Lineweaver-Burk plots for the inhibition of α-glucosidase by ampelopsin D (b) and suffruticosol B (d).

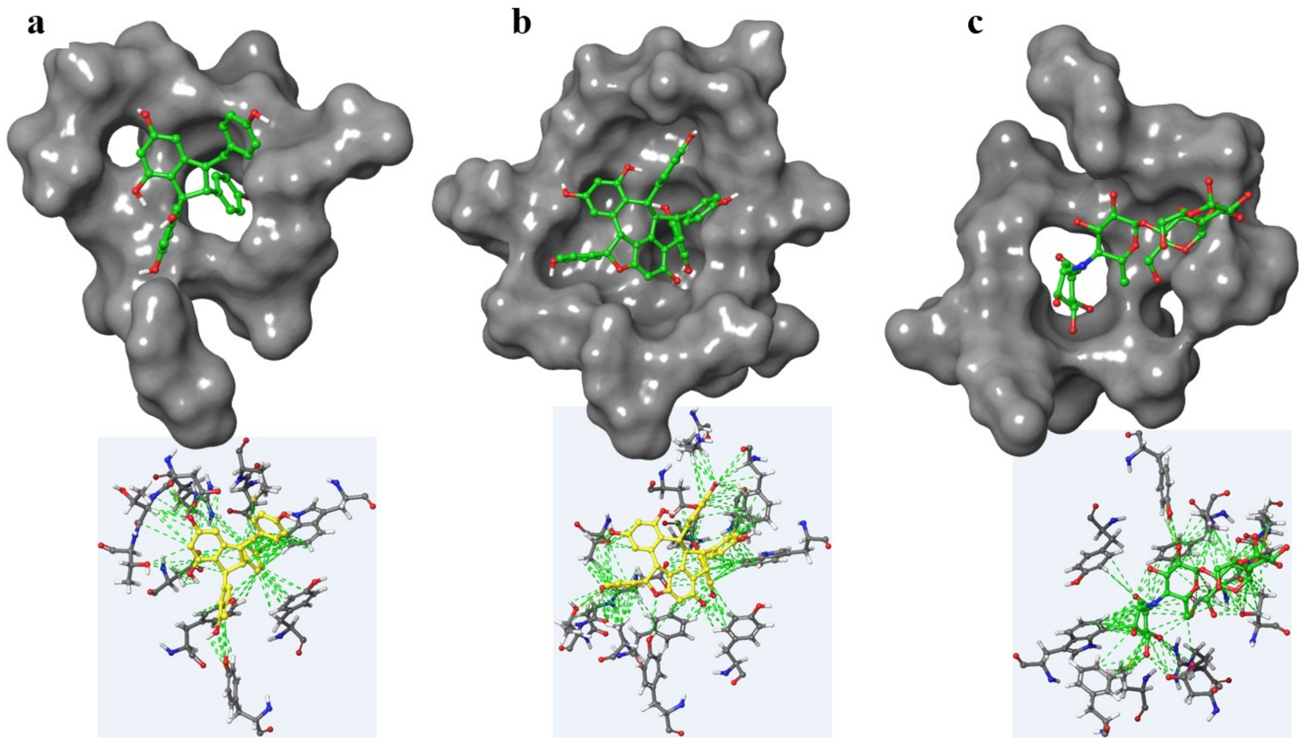


Fig. S3. Molecular docking of ampelopsin D (a), suffruticosol B (b) and acarbose (c) in the region of the active site of the protein (PDB: 2QMJ).

Supplementary data

The NMR and MS data of the phytochemicals (**1-10**) isolated from *POSC* are as follows.

(**1**) (E)-Resveratrol 3,5-*O*-*β*-diglucoside

ESI-MS m/z 553 $[M+H]^+$ ($C_{26}H_{32}O_{13}$). ^1H NMR (600 MHz, MeOD) δ_H: 7.42 (2H, d, J = 8.5 Hz, H-2′, 6′), 7.11 (1H, d, J = 16.0 Hz, H-8), 6.98 (2H, brs, H-2, 6), 6.93 (1H, d, J = 16.0 Hz, H-7), 6.80 (2H, d, J = 8.5 Hz, H-3′, 5′), 6.49 (1H, overlapped, H-4), 4.97 (2H, d, J = 7.5 Hz, H-1″, 1‴), 3.97 (2H, d, J = 11.0 Hz, H-6a″, 6a‴), 3.30~3.78 (10H, Glu); ^{13}C NMR (151 MHz, MeOD) δ_C: 160.2 (C-4′), 158.6 (C-3, 5), 141.4 (C-1), 130.7 (C-), 130.6 (C-8), 130.2 (C-2′, 6′), 129.0 (C-1′), 126.3 (C-7), 116.5 (C-3′, 5′), 109.7 (C-2, 6), 104.8 (C-4), 102.3 (C-1″, 1‴), 78.3 (C-3″, 3‴), 78.0 (C-5″, 5‴), 74.9 (C-2″, 2‴), 71.7 (C-4″, 4‴), 62.7 (C-6″, 6‴).

(**2**) Paeoniflorin

ESI-MS m/z 481 $[M+H]^+$ ($C_{23}H_{28}O_{11}$). ^1H NMR (600 MHz, MeOD) δ_H: 8.05 (2H, d, J = 7.5 Hz, H-2″, 6″), 7.61 (1H, t, J = 7.5 Hz, H-4″), 7.48 (2H, t, J = 7.5 Hz, H-3″, 5″), 5.44 (1H, s, H-9), 4.74 (1H, overlapped, H-8), 4.54 (1H, d, J = 7.5 Hz, H-1′), 3.86 (1H, d, J = 11.5 Hz, Hb-6′), 3.62 (1H, d, J = 8.5 Hz, Ha-6′), 3.20~3.40 (4H, overlapped, H-3′, 5′, 2′, 4′), 2.59 (1H, d, J = 6.0 Hz, H-5), 2.49 (1H, m, Hb-6), 2.20 (1H, d, J = 12.5 Hz, Hb-1), 1.96 (1H, d, J = 12.0 Hz, Ha-6), 1.82 (1H, d, J = 12.5 Hz, Ha-1), 1.37 (3H, s, H-10); ^{13}C NMR (151 MHz, MeOD) δ_C: 168.0 (C-7″), 134.4 (C-4″), 131.1 (C-1″), 130.6 (C-2″, 6″), 129.6 (C-3″, 5″), 106.4 (C-4), 102.2 (C-9), 100.1 (C-1′), 89.3 (C-1), 87.2 (C-2), 78.0 (C-5′), 77.9 (C-3′), 74.9 (C-2′), 72.1 (C-7), 71.7 (C-4′), 62.8 (C-6′), 61.7 (C-8), 44.5 (C-3), 43.9 (C-5), 23.4 (C-6), 19.6 (C-10).

(**3**) Ethyl gallate

ESI-MS m/z 199 $[M+H]^+$ ($C_9H_{10}O_5$). ^1H NMR (600 MHz, MeOD) δ_H: 7.08 (2H, s, H-2, 6), 4.30 (2H, d, J = 7.0 Hz, H-8), 1.37 (3H, t, J = 7.0 Hz, H-9); ^{13}C NMR (151 MHz, MeOD) δ_C: 168.6 (C-7), 146.5 (C-3, 4), 139.7 (C-4), 121.8 (C-1), 110.0 (C-2, 6), 61.7 (C-8), 14.6 (C-9).

(**4**) Suffruticosol A

ESI-MS m/z 681 $[M+H]^+$ ($C_{42}H_{32}O_9$). ^1H NMR (600 MHz, MeOD) δ_H: 7.14 (2H, d, J = 8.5 Hz, H-2″, 6″), 6.99 (2H, d, J= 8.5 Hz, H-2, 6), 6.72 (2H, d, J = 8.5 Hz, H-3″, 5″), 6.52 (2H, d, J = 8.5 Hz, H-2′, 6′), 6.41 (2H, d, J = 8.5 Hz, H-3, 5), 6.29 (1H, brs, H-12″), 6.23 (1H, s, H-12′), 6.15 (2H, d, J = 8.5 Hz, H-3′, 5′), 6.10 (1H, brs, H-12), 6.02 (2H, brs, H-10, 14), 5.96 (1H, brs, H-14″), 5.72 (1H, d, J = 12.0 Hz, H-7″), 5.46 (1H, d, J = 3.0 Hz, H-7′), 4.78 (1H, s, H-8), 4.39 (1H, d, J = 11.5 Hz, H-8″), 3.97 (1H, m, H-8′), 3.72 (1H, d, J = 7.5 Hz, H-7); ^{13}C NMR (151 MHz, MeOD) δ_C: 160.2 (C-11′), 159.3 (C-11, 13), 159.0 (C-4″), 156.7 (C-13″), 156.5 (C-4), 155.1 (C-13′), 155.0 (C-11″), 154.5 (C-4′), 148.4 (C-9), 144.7 (C-9′), 141.8 (C-9″), 135.5 (C-1), 133.9 (C-1′), 130.9 (C-1″), 130.8 (C-2′, 6′), 130.7 (C-2, 6), 130.5 (C-2″, 6″), 126.9 (C-10″), 123.0 (C-14′), 117.3 (C-10′), 116.2 (C-3″, 5″), 115.4 (C-3, 5), 114.2 (C-3′, 5′), 106.8 (C-10, 14), 105.9 (C-14″), 101.9 (C-12″), 101.4 (C-12), 96.2 (C-12′), 91.5 (C-7″), 61.1 (C-7), 54.6 (C-8), 49.6 (C-8″), 48.8 (C-8′), 39.7 (C-7′).

(**5**) Suffruticosol B

ESI-MS m/z 681 $[M+H]^+$ ($C_{42}H_{32}O_9$). ^1H NMR (600 MHz, MeOD) δ_H: 7.57 (2H, d, J = 8.5 Hz, H-2″, 6″), 6.96 (2H, brd, H-2′, 6′), 6.91 (2H, d, J = 8.5 Hz, H-3″, 5″), 6.50 (2H, d, J = 8.5 Hz, H-3′, 5′), 6.27 (4H, overlapped, H-3, 5, 2, 6), 6.22 (2H, brd, H-10, 14), 6.19 (1H, s, H-12′), 6.17 (1H, s, H-12″), 6.14 (1H, s, H-12), 5.95 (1H, d, J = 2.0 Hz, H-14″), 5.86 (1H, d, J = 11.5Hz, H-7″), 5.08 (1H, d, J = 11.5 Hz, H-8′), 4.22 (1H, d, J = 11.5 Hz, H-7′), 4.09 (2H, overlapped, H-8, 8′), 3.81 (1H, d, J = 6.0 Hz, H-7); ^{13}C NMR (151 MHz, MeOD) δ_C: 160.2 (C-11′), 159.4 (C-11, 13), 159.1 (C-4″), 158.4 (C-13″), 157.2 (C-11″), 156.1 (C-4′), 156.1 (C-4), 155.7 (C-13′), 147.5 (C-9′), 147.5 (C-9), 142.4 (C-9″), 135.5 (C-1), 133.8 (C-1′), 133.1 (C-2′, 6′), 130.9 (C-1″), 130.5 (C-2″, 6″), 129.5 (C-2, 6), 123.6 (C-14′), 122.9 (C-10″), 118.5 (C-10′), 116.5 (C-3″, 5″), 115.2 (C-3, 5), 114.7 (C-3′, 5′), 107.3 (C-10, 14), 104.9 (C-12″), 103.7 (C-14″), 101.4 (C-12), 96.2 (C-12′), 91.1 (C-7″), 63.1 (C-7), 56.9 (C-8), 47.8 (C-8″), 46.5 (C-8′), 39.7 (C-7′).

(**6**) Trans-*ε*-viniferin

ESI-MS m/z 455 $[M+H]^+$ ($C_{28}H_{22}O_6$). ^1H NMR (600 MHz, MeOD) δ_H: 7.16 (2H, d, J = 8.6 Hz, H-2,6), 7.11 (2H, d, J = 8.3 Hz, H-2',6'), 6.77 (2H, d, J = 9.2 Hz, H-3,5), 6.67 (2H, d, J = 8.8 Hz, H-3',5'), 6.64(1H, d, J = 2.0 Hz, H-10'), 6.25 (1H, d, J = 2.0 Hz, H-12'), 6.81 (1H, d, J = 16.0 Hz, H-7'), 6.55 (1H, d, J = 16.0 Hz, H-8'), 6.18 (1H, d, J = 2.0 Hz, H-12), 6.15 (2H, d, J = 2.0 Hz, H-10,14), 5.34 (1H, d, J = 6.5 Hz, H-7), 4.35 (1H, d, J = 6.5 Hz, H-8); ^{13}C NMR (151 MHz, MeOD) δ_C: 133.8 (C-1), 128.5 (C-2,6), 116.0 (C-3, 5), 157.9 (C-4), 94.8 (C-7), 57.5 (C-8), 147.4 (C-9), 107.3 (C-10), 159.6 (C-11,13), 101.9 (C-12), 107.4 (C-14), 130.2 (C-1'), 131.0 (C-2',6'), 115.7 (C-3', 5'), 158.4 (C-4'), 131.7 (C-7'), 126.5 (C-8'), 137.7 (C-9'), 108.9 (C-10'), 159.1 (C-11'), 96.7 (C-12'), 162.8 (C-13'), 120.5 (C-14').

(**7**) Ampelopsin D

ESI-MS m/z 455 $[M+H]^+$ ($C_{28}H_{22}O_6$). ^1H NMR (600 MHz, MeOD) δ_H: 7.01 (2H, d, J = 8.8 Hz, H-2,6), 6.67 (2H, d, J = 8.8 Hz, H-3,5), 4.18 (1H, brs, H-7), 4.05 (1H, brs, H-8), 6.05 (2H, d, J = 2.2 Hz, H-10,14), 6.04 (1H, t, J = 2.2 Hz, H-12), 7.09 (2H, d, J = 8.8 Hz, H-2',6'), 6.57 (2H, d, J = 8.8 Hz, H-3',5'), 6.95 (1H, d, J = 2.2 Hz, H-7'), 6.18 (1H, d, J = 2.2 Hz, H-12'), 6.70 (1H, d, J = 2.2 Hz, H-14'); ^{13}C NMR (151 MHz, MeOD) δ_C: 137.9 (C-1), 129.0 (C-2,6), 116.5 (C-3, 5), 156.7 (C-4), 59.9 (C-7), 59.0 (C-8), 150.0 (C-9), 106.5 (C-10,14), 159.2 (C-11,13), 101.4 (C-12), 130.2 (C-1'), 131.2 (C-2',6'), 115.9 (C-3', 5'), 157.4 (C-4'), 122.7 (C-7'), 143.8 (C-8'), 148.0 (C-9'), 124.7 (C-10'), 156.4 (C-11'), 103.7 (C-12'), 159.8 (C-13'), 98.5 (C-14').

(**8**) Vateriferol

ESI-MS m/z 679 $[M+H]^+$ ($C_{42}H_{30}O_9$). ^1H NMR (600 MHz, MeOD) δ_H: 6.74 (2H, d, J = 8.4 Hz, H-2",6"), 3.19 (1H, t, J = 10.0 Hz, H-7"), 6.49 (2H, d, J = 8.6 Hz, H-3",5"), 4.18 (1H, d, J = 9.6 Hz, H-8"), 5.76 (2H, d, J = 2.0 Hz, H-10",14"), 6.02 (1H, d, J = 2.1 Hz, H-12"), 6.95 (2H, d, J = 8.6 Hz, H-2,6), 6.86 (2H, d, J = 8.6 Hz, H-3,5), 5.23 (1H, d, J = 3.9 Hz, H-7), 3.92 (1H, dd, J = 10.4 Hz, J = 3.9 HZ, H-8), 6.69 (1H, s, H-12), 7.58 (2H, d, J = 8.6 Hz, H-2',6'), 7.05 (2H, d, J = 8.4 Hz, H-3',5'), 6.17 (1H, d, J = 2.5 Hz, H-12'), 6.69 (1H, d, J = 2.5 Hz, H-14'); ^{13}C NMR (151 MHz, MeOD) δ_C: 134.5 (C-1), 131.1 (C-2,6), 116.1 (C-3, 5), 159.2 (C-4), 42.7 (C-7), 55.2 (C-8), 140.2 (C-9), 119.4 (C-10), 155.4 (C-11), 96.8 (C-12), 152.7 (C-13), 125.8 (C-14), 135.4 (C-1"), 132.4 (C-2",6"), 115.5 (C-3",5"), 156.9 (C-4"), 63.4 (C-7"), 59.6 (C-8"), 147.5 (C-9"), 107.7 (C-10",14"), 158.8 (C-11",13"), 101.5 (C-12"), 123.9 (C-1'), 130.7 (C-2',6'), 116.5 (C-3', 5'), 157.8 (C-4'), 152.6 (C-7'), 116.7 (C-8'), 134.3 (C-9'), 124.9 (C-10'), 156.2 (C-11'), 102.6 (C-12'), 155.6 (C-13'), 110.2 (C-14').

(**9**) 4-Hydroxybenzoic acid

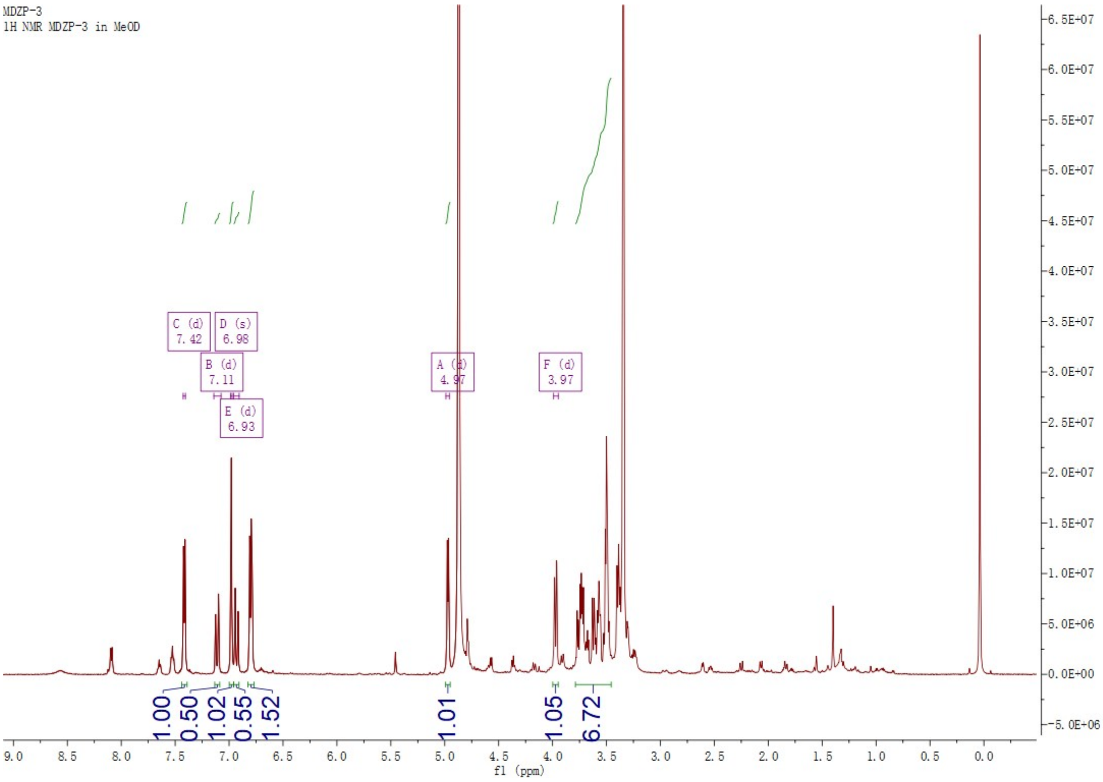
ESI-MS m/z 139 $[M+H]^+$ ($C_7H_6O_3$). ^1H NMR (600 MHz, MeOD) δ_H: 7.85 (2H, d, J = 8.5 Hz, H-2, 6), 6.79 (2H, d, J = 8.5 Hz, H-3, 5). ^{13}C NMR (151 MHz, MeOD) δ_C: 170.2 (C-7), 163.3 (C-4), 133.0 (C-2, 6), 122.9 (C-1), 116.0 (C-3, 5).

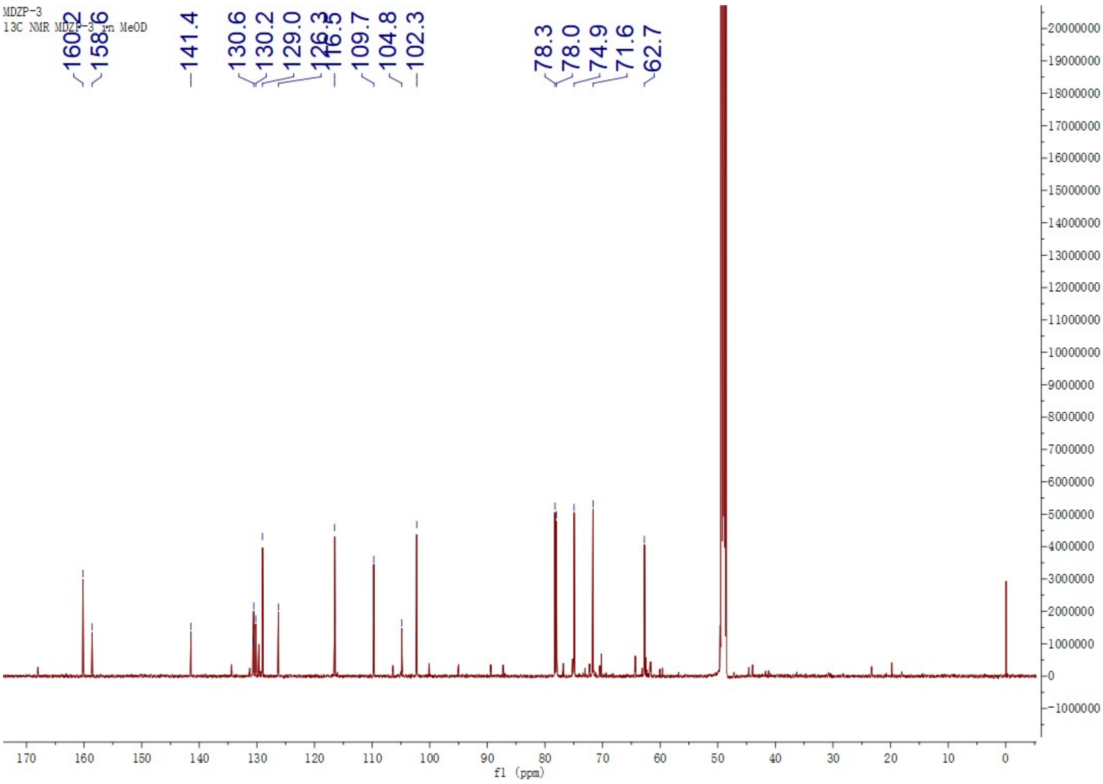
(**10**) 4-Hydroxybenzal-dehyde

ESI-MS m/z 123 $[M+H]^+$ ($C_7H_6O_2$). ^1H NMR (600 MHz, MeOD) δ_H: 9.73 (1H, s, H-7), 7.74 (2H, d, J = 8.5 Hz, H-2, 6), 6.88 (2H, d, J = 8.5 Hz, H-3, 5); ^{13}C NMR (151 MHz, MeOD) δ_C: 192.8 (C-7), 165.4 (C-4), 130.2 (C-1), 133.5 (C-2, 6), 116.9 (C-3, 5).

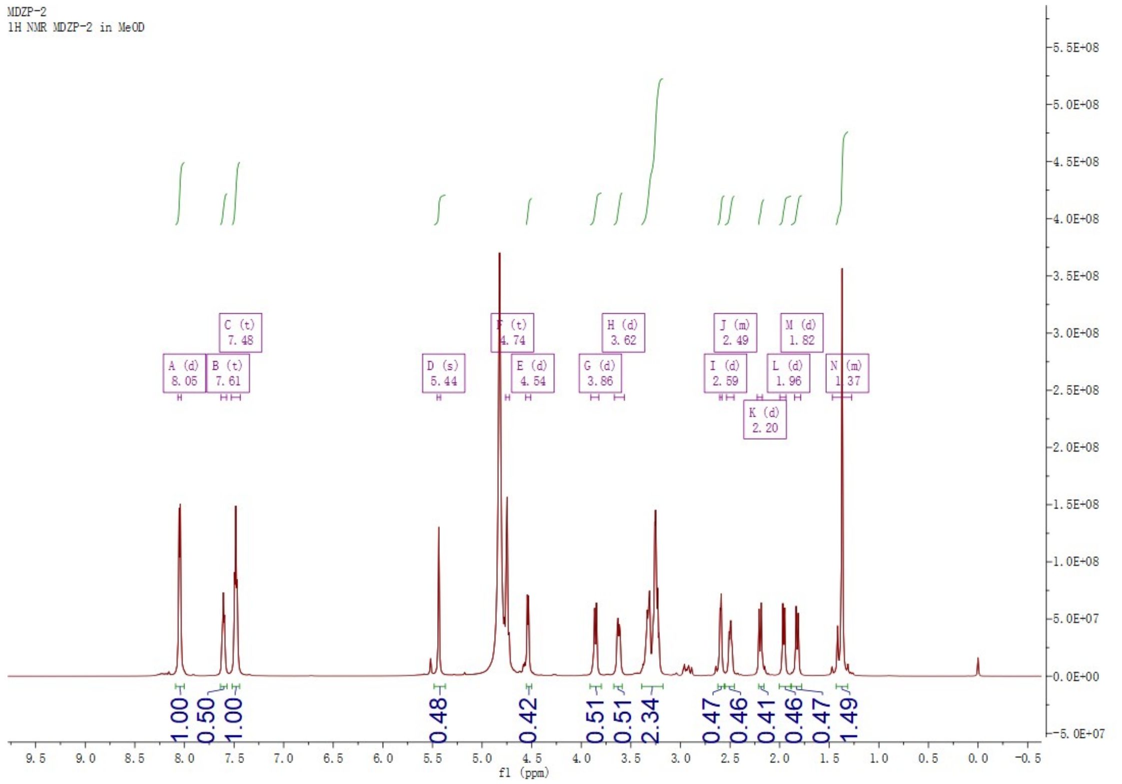
The NMR spectra (^1H NMR and ^{13}C NMR) of these compounds were as follows.

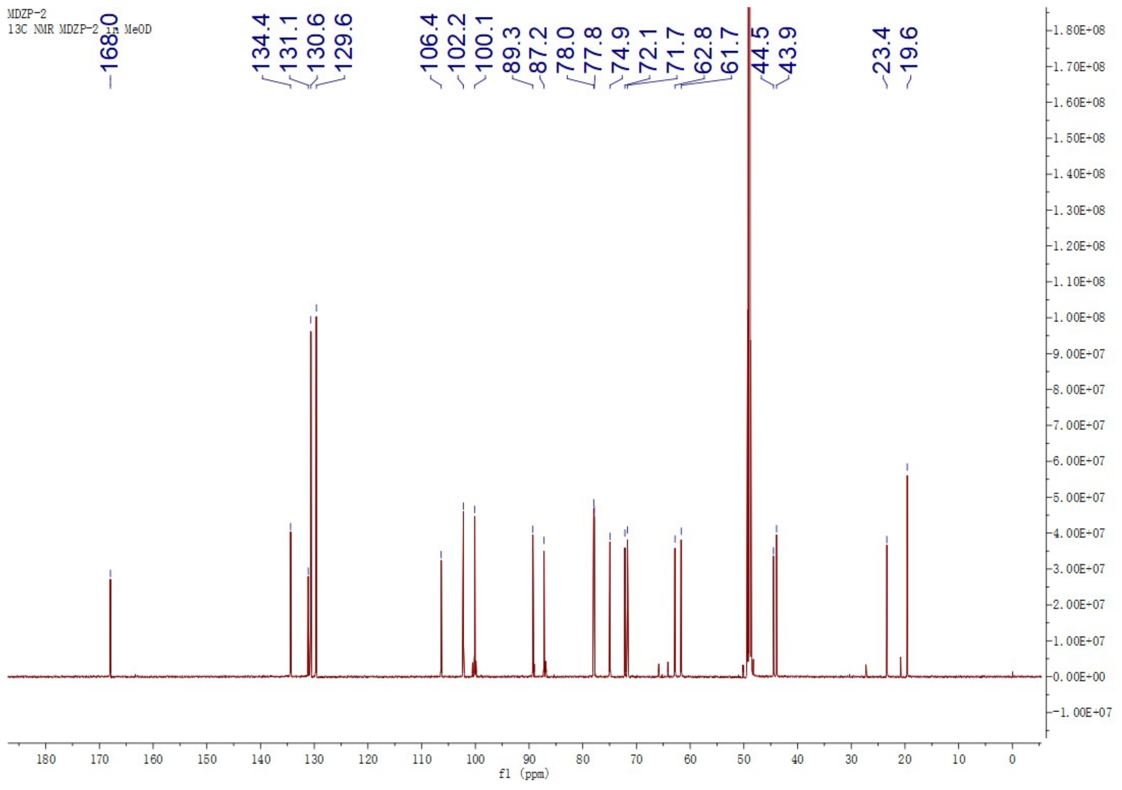
1

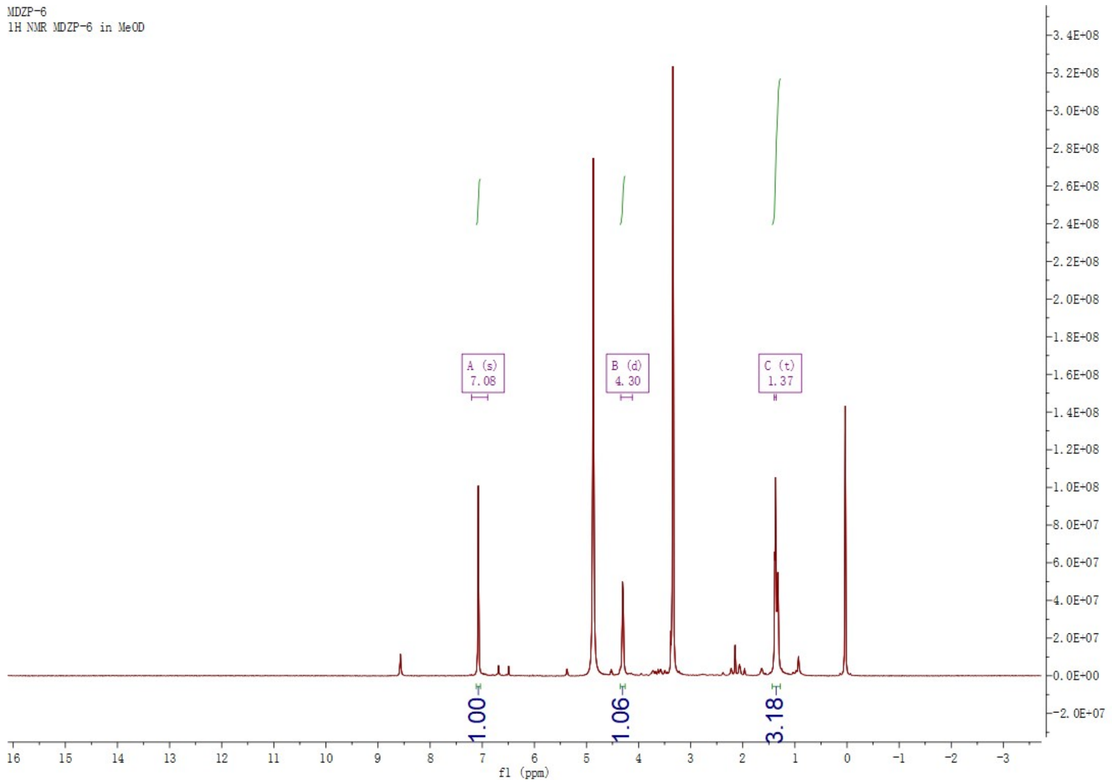

MDZP-3
1H NMR MDZP-3 in MeOD
C (d) 7.42
D (s) 6.98
B (d) 7.11
E (d) 6.93
A (d) 4.97
F (d) 3.97
1.00
0.50
1.02
0.55
1.52
1.01
1.05
6.72
f1 (ppm)

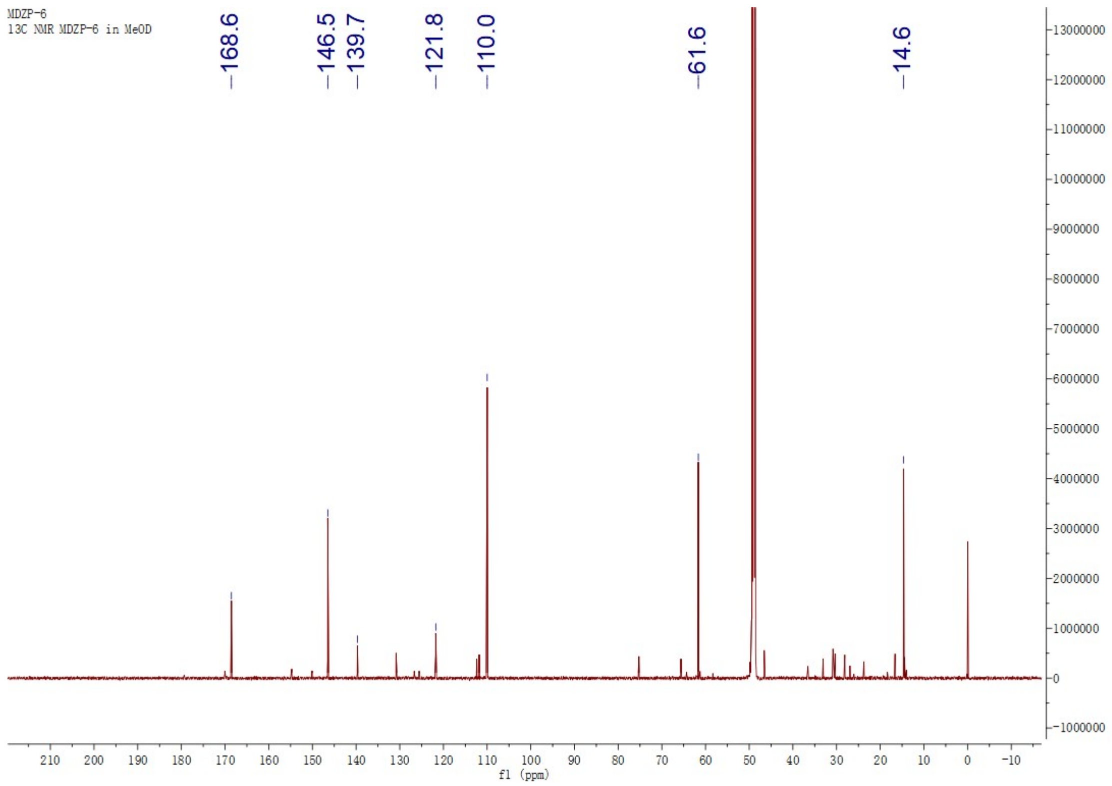

MDZP-3
13C NMR MDZP-3 in MeOD
160.2
158.6
141.4
130.6
130.2
129.0
126.3
116.5
109.7
104.8
102.3
78.3
78.0
74.9
71.6
62.7
f1 (ppm)

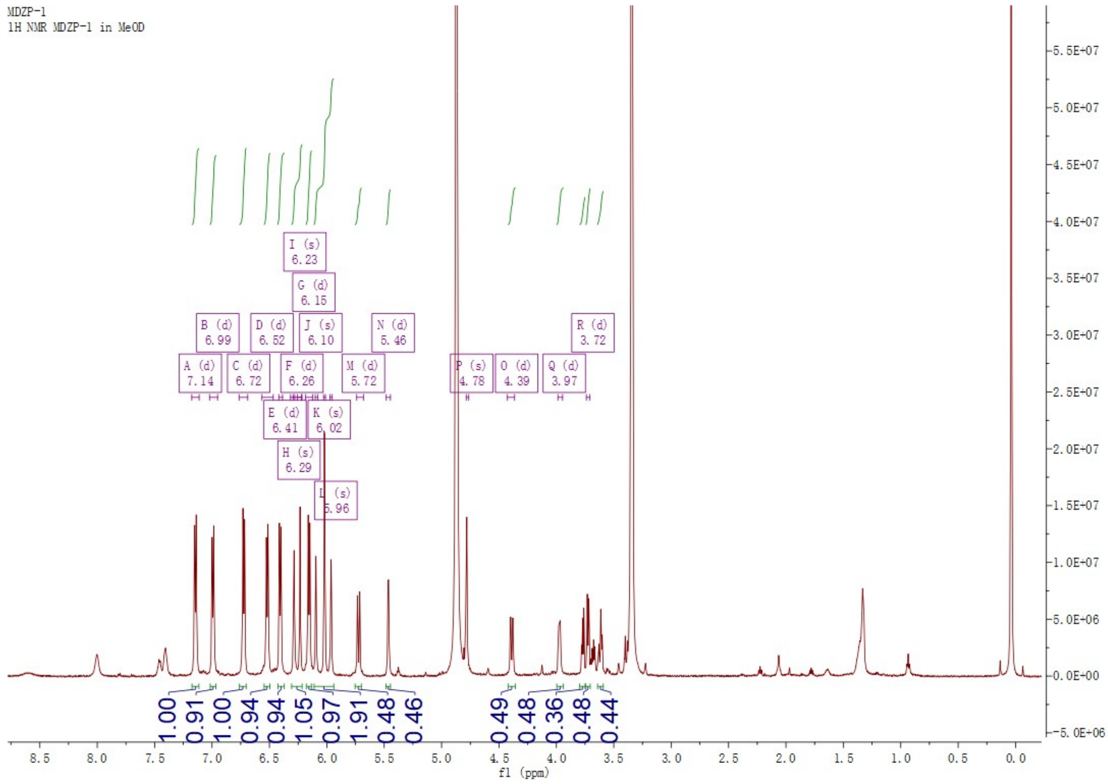
2

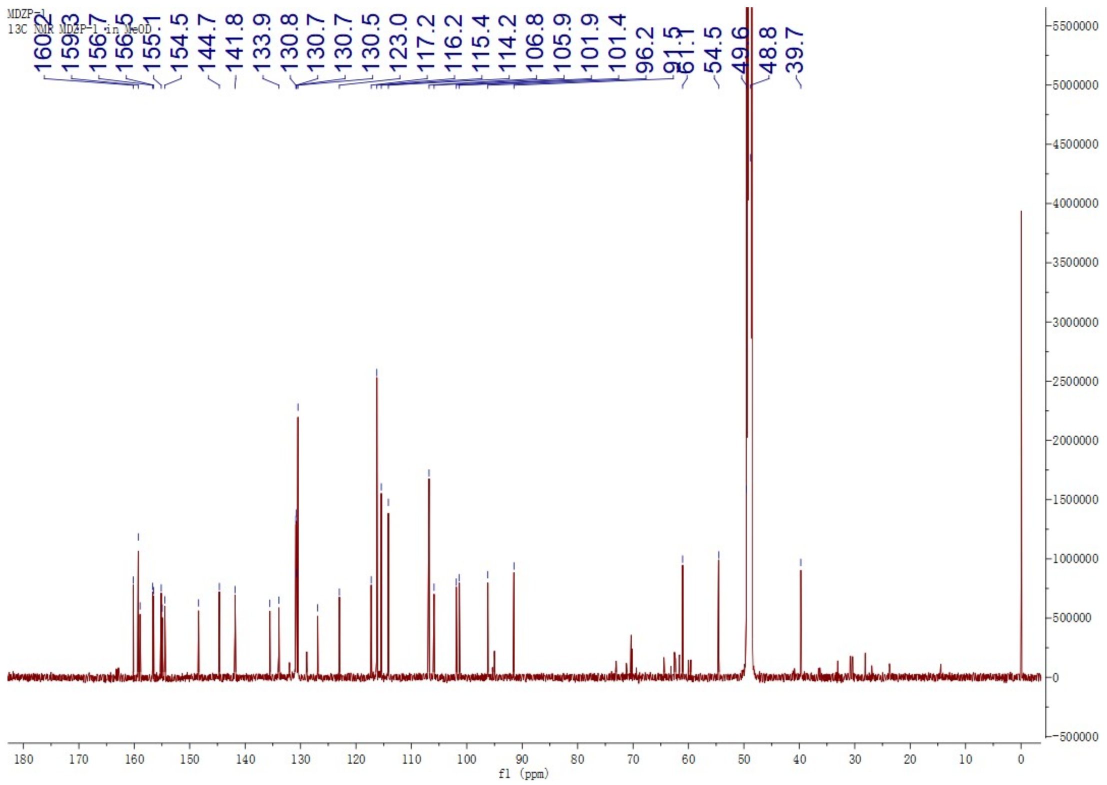

MDZP-2
1H NMR MDZP-2 in MeOD
A (d) 8.05
B (t) 7.61
C (t) 7.48
D (s) 5.44
F (t) 4.74
E (d) 4.54
G (d) 3.86
H (d) 3.62
I (d) 2.59
J (m) 2.49
K (d) 2.20
L (d) 1.96
M (d) 1.82
N (m) 1.37
1.00
0.50
1.00
0.48
0.42
0.51
0.51
2.34
0.47
0.46
0.41
0.46
0.47
1.49
f1 (ppm)

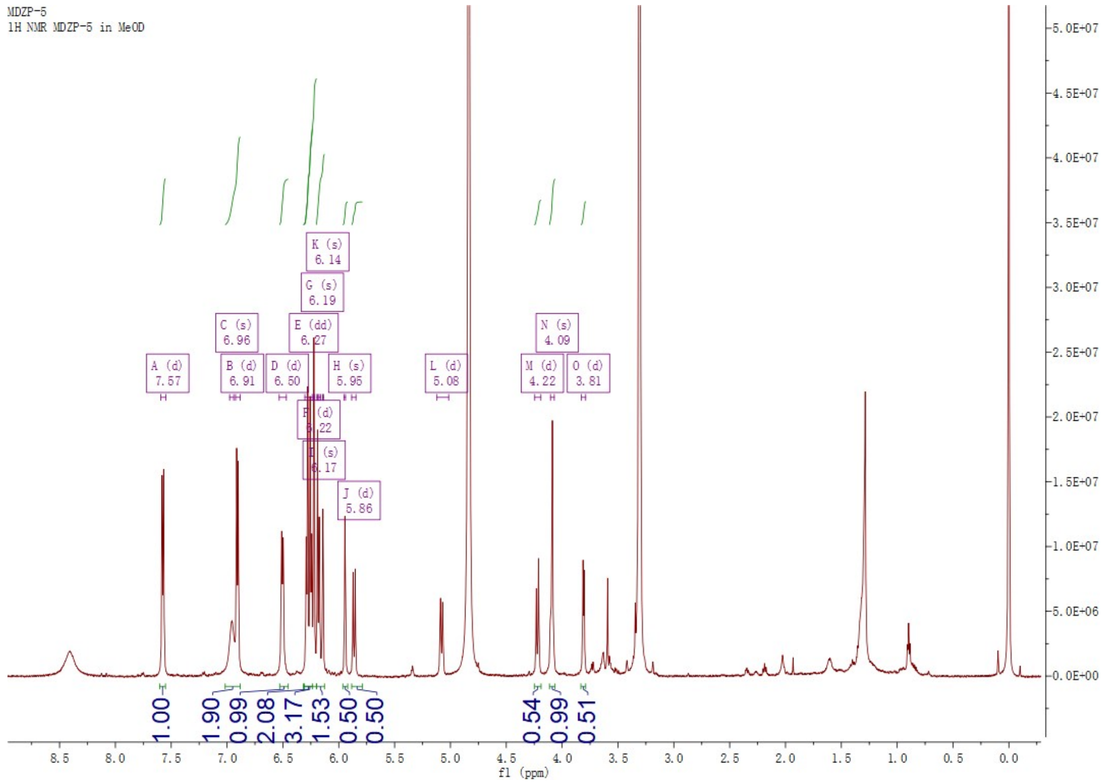

MDZP-2
13C NMR MDZP-2 in MeOD
168.0
134.4
131.1
130.6
129.6
106.4
102.2
100.1
89.3
87.2
78.0
77.8
74.9
72.1
71.7
62.8
61.7
44.5
43.9
23.4
19.6
f1 (ppm)

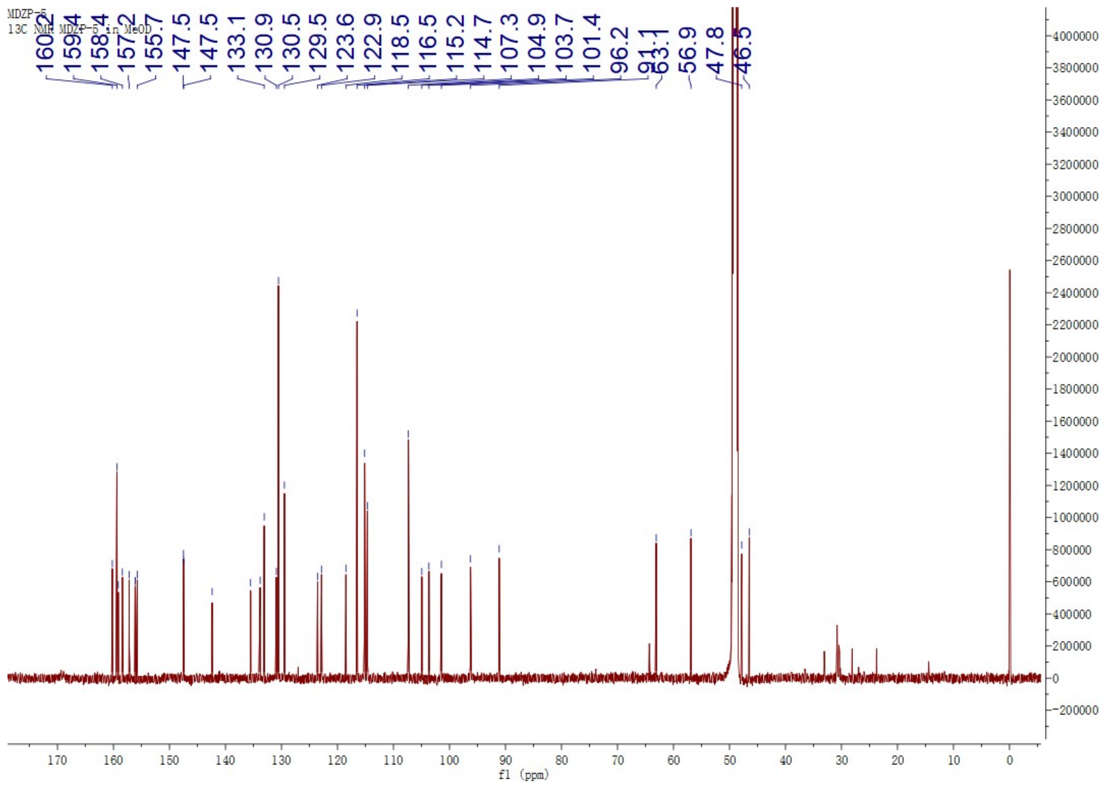

MDZP-6
1H NMR MDZP-6 in MeOD
A (s)
7.08
B (d)
4.30
C (t)
1.37
1.00
1.06
3.18
f1 (ppm)

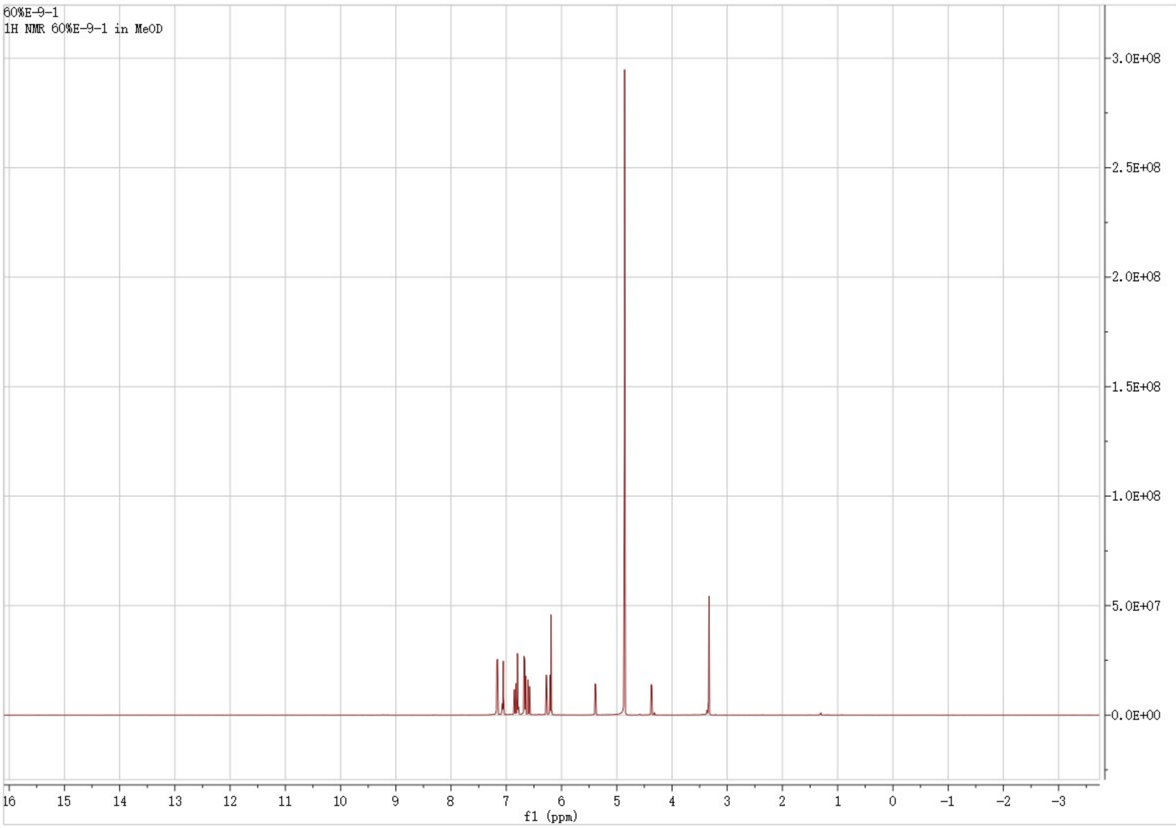

MDZP-6
13C NMR MDZP-6 in MeOD
168.6
146.5
139.7
121.8
110.0
61.6
14.6
f1 (ppm)

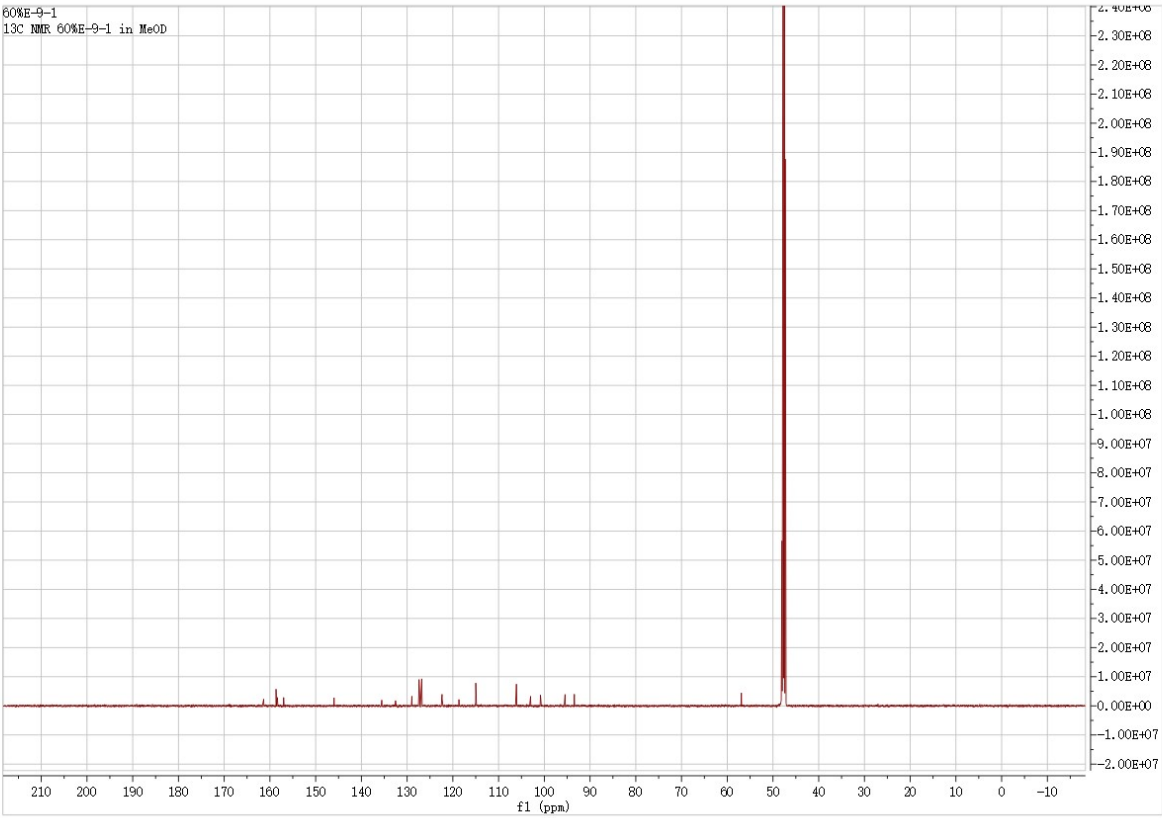

MDZP-1
1H NMR MDZP-1 in MeOD
A (d) 7.14
B (d) 6.99
C (d) 6.72
D (d) 6.52
E (d) 6.41
F (d) 6.26
H (s) 6.29
I (s) 6.23
G (d) 6.15
J (s) 6.10
K (s) 6.02
L (s) 5.96
M (d) 5.72
N (d) 5.46
P (s) 4.78
O (d) 4.39
Q (d) 3.97
R (d) 3.72
1.00 0.91 1.00 0.94 0.94 1.05 0.97 1.91 0.48 0.46 0.49 0.48 0.36 0.48 0.44
f1 (ppm)

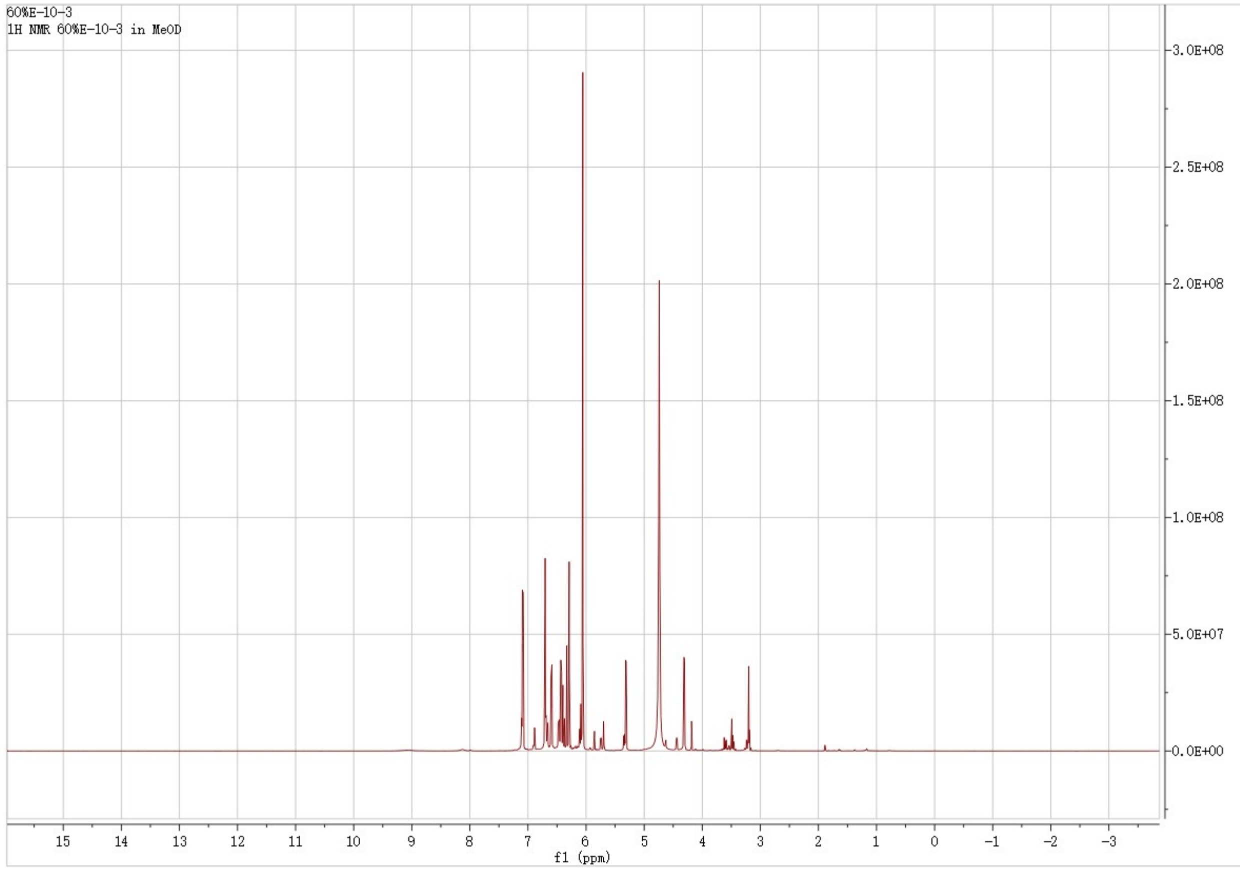

MDZP-1
13C NMR MDZP-1 in MeOD
160.2 159.3 156.7 156.5 155.1 154.5 144.7 141.8 133.9 130.8 130.7 130.7 130.5 123.0 117.2 116.2 115.4 114.2 106.8 105.9 101.9 101.4 96.2 91.5 61.1 54.5 49.6 48.8 39.7
f1 (ppm)

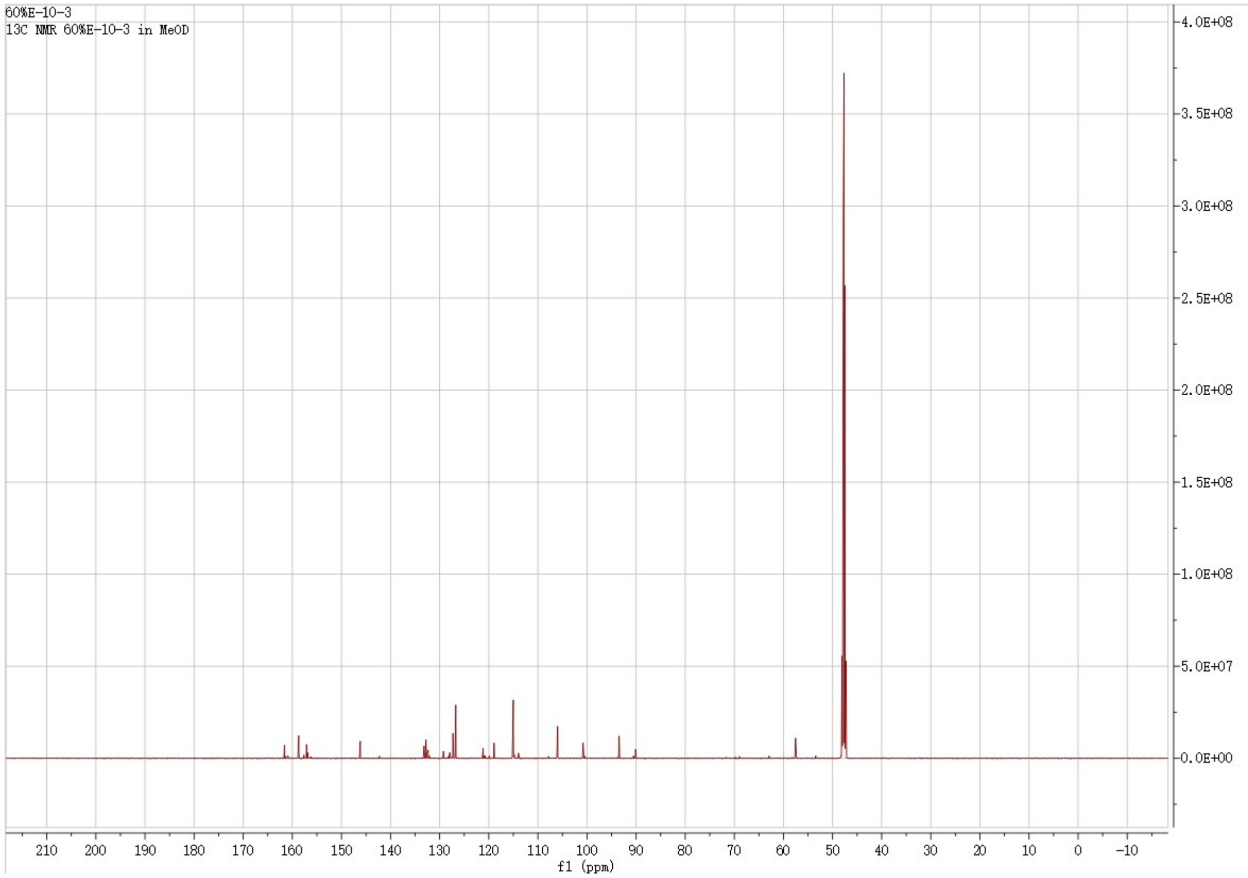

MDZP-5
1H NMR MDZP-5 in MeOD
f1 (ppm)


MDZP-5
13C NMR MDZP-5 in MeOD
f1 (ppm)

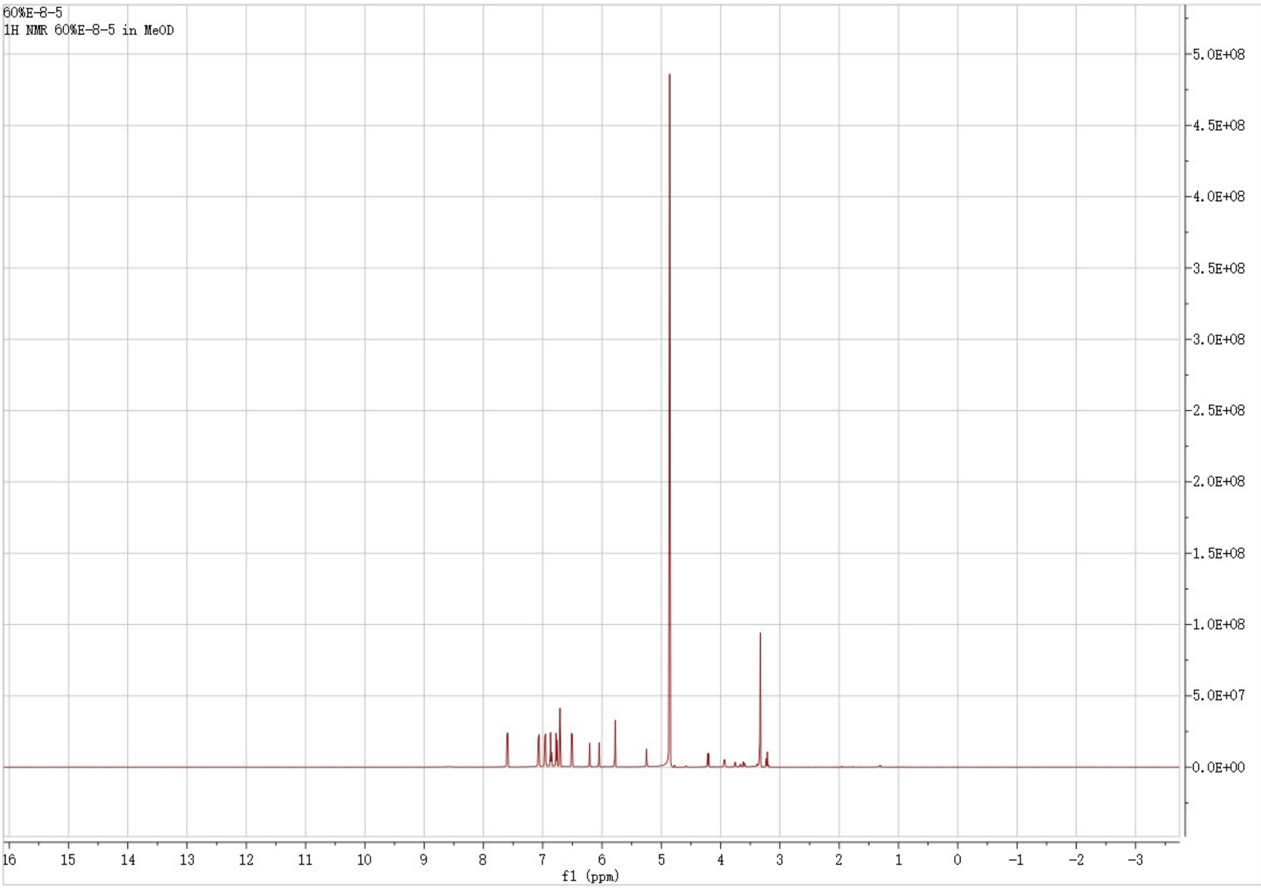

60%E-9-1
1H NMR 60%E-9-1 in MeOD
f1 (ppm)

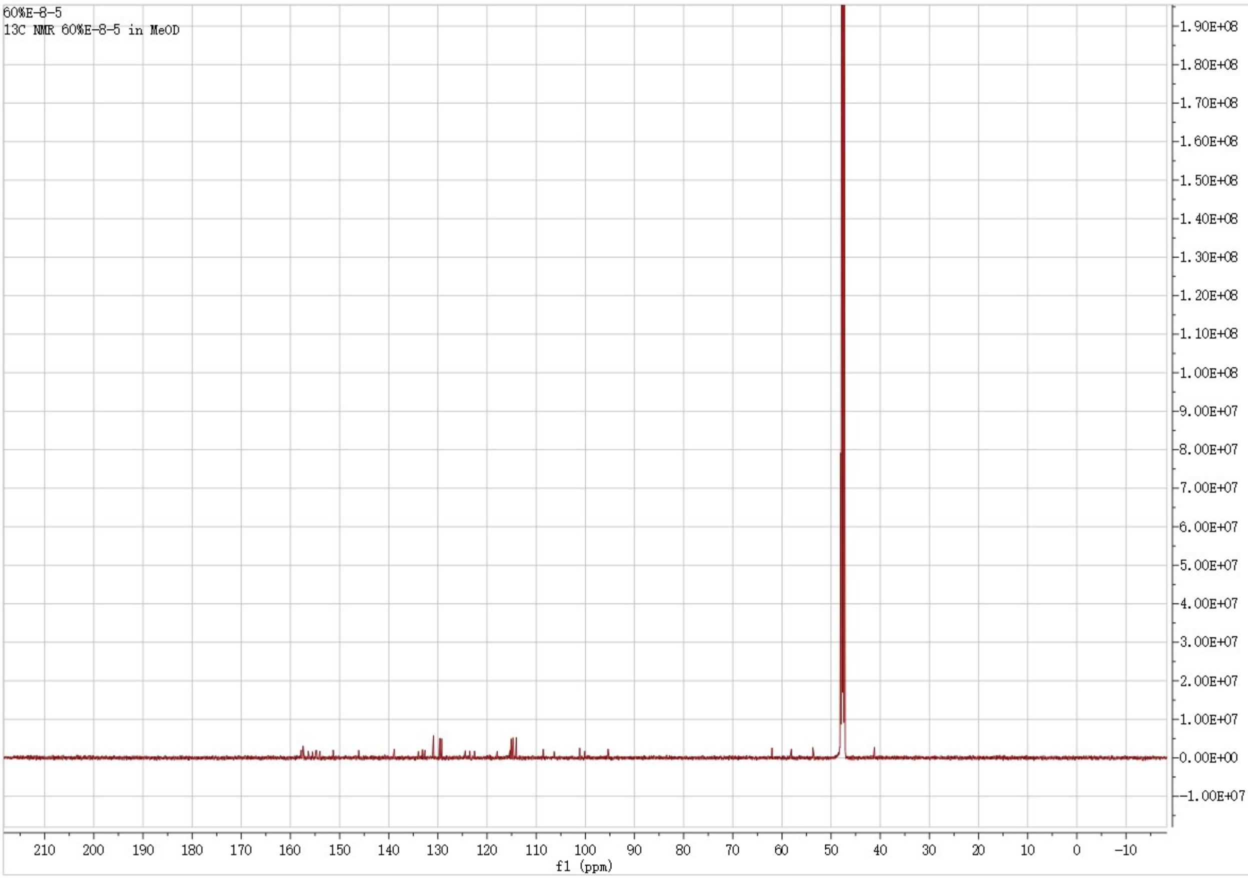

60%E-9-1
13C NMR 60%E-9-1 in MeOD
f1 (ppm)


60%E-10-3
1H NMR 60%E-10-3 in MeOD
f1 (ppm)

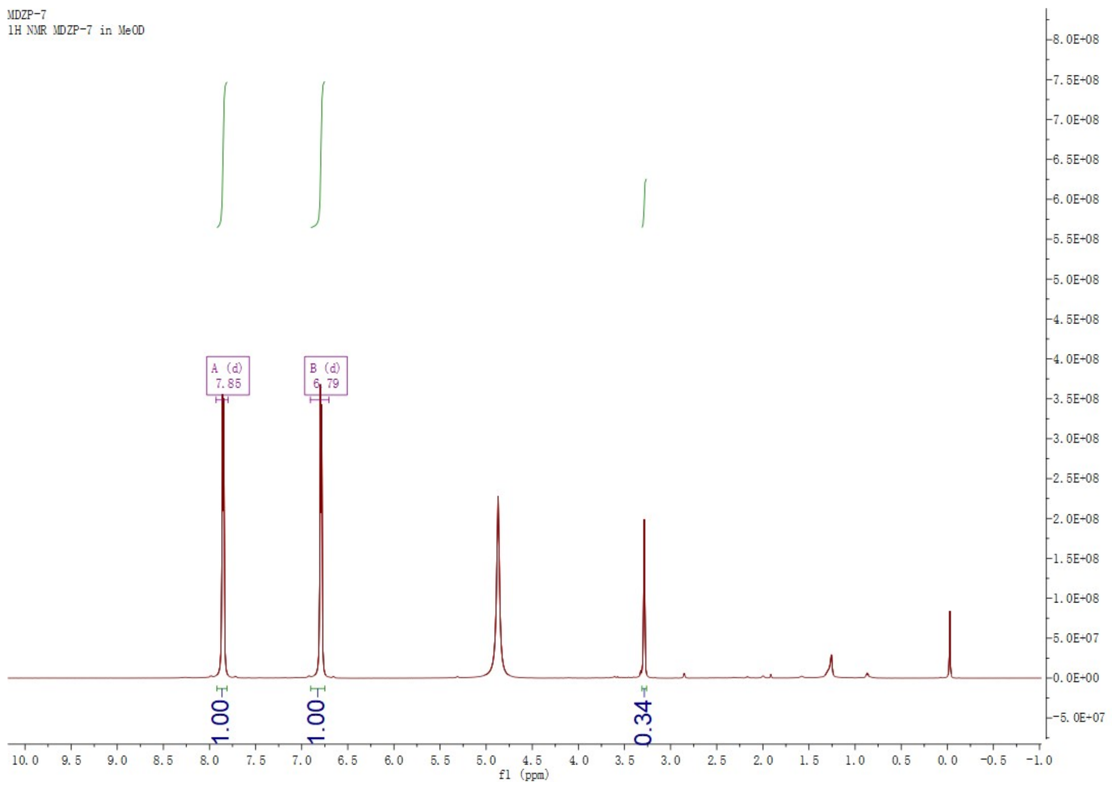

60%E-10-3
13C NMR 60%E-10-3 in MeOD
f1 (ppm)

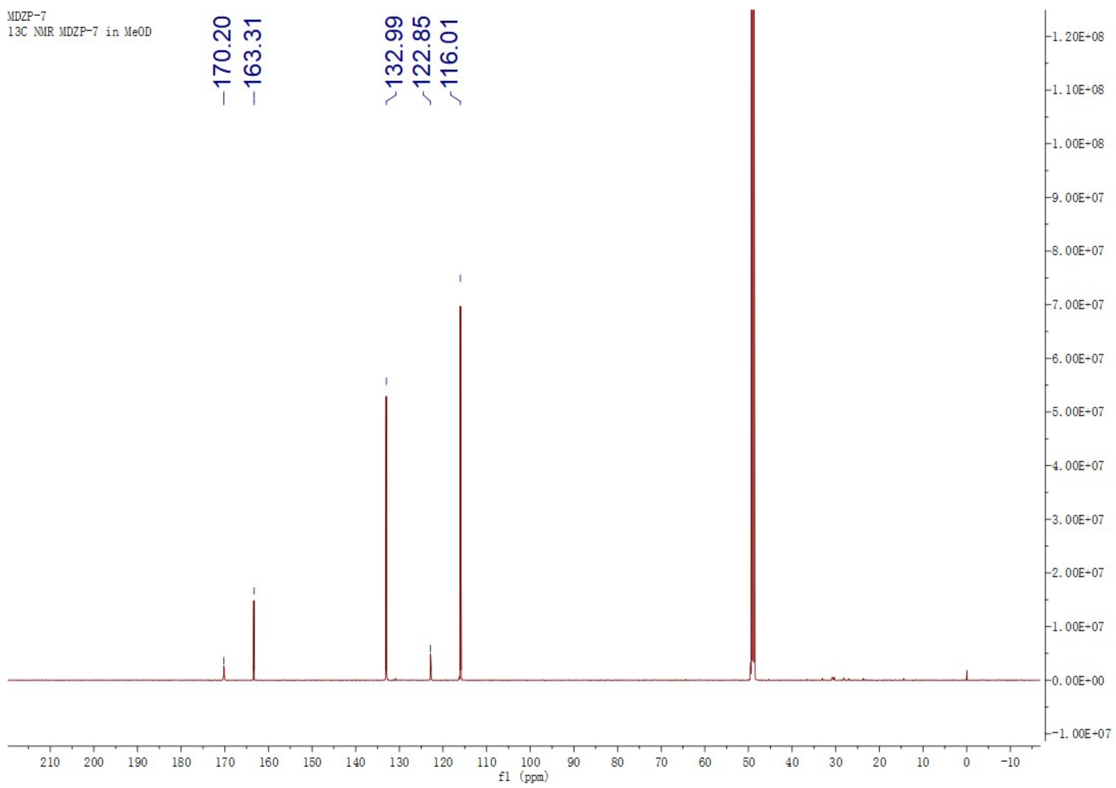
8


60%E-8-5
1H NMR 60%E-8-5 in MeOD
f1 (ppm)

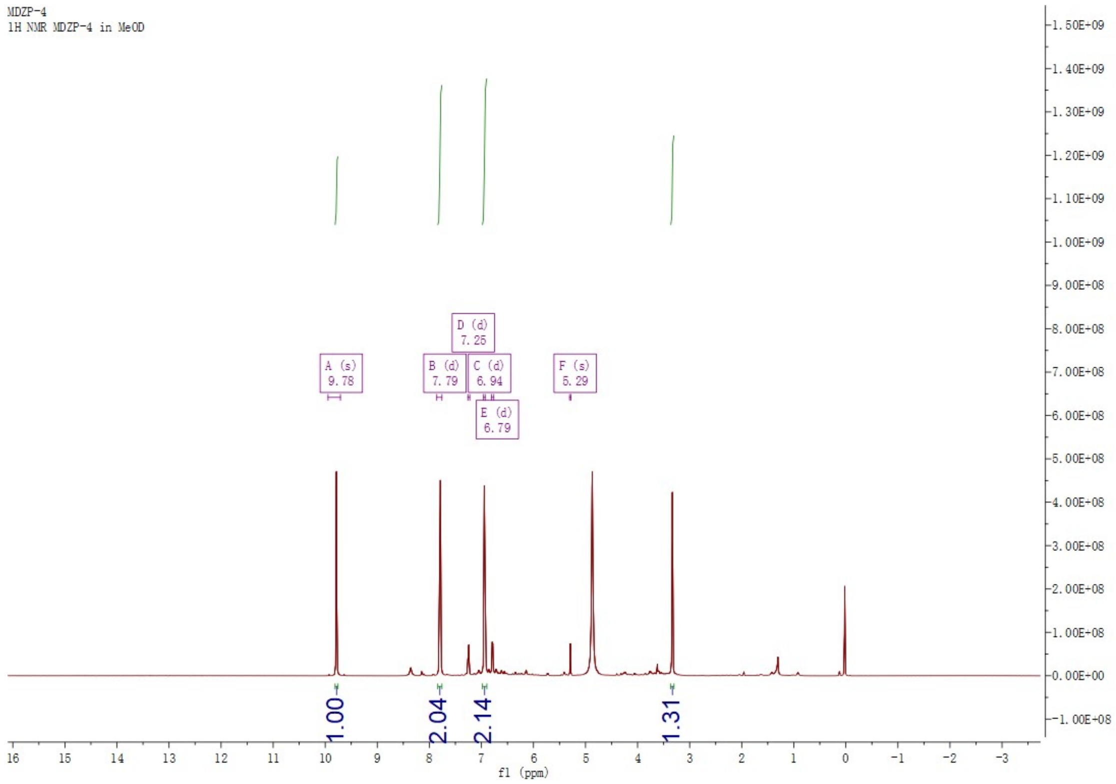

60%E-8-5
13C NMR 60%E-8-5 in MeOD
f1 (ppm)

9

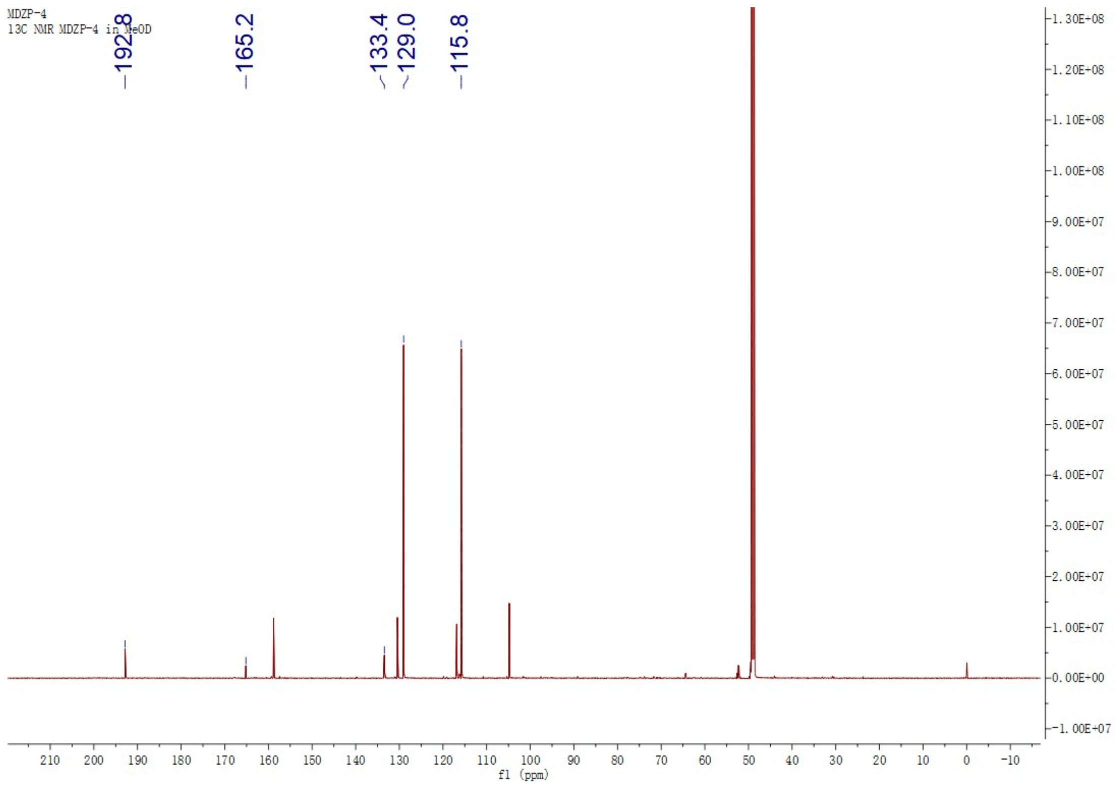

MDZP-7
1H NMR MDZP-7 in MeOD
A (d)
7.85
B (d)
6.79
1.00
1.00
0.34
f1 (ppm)


MDZP-7
13C NMR MDZP-7 in MeOD
170.20
163.31
132.99
122.85
116.01
f1 (ppm)

10



MDZP-4
1H NMR MDZP-4 in MeOD
A (s)
9.78
B (d)
7.79
D (d)
7.25
C (d)
6.94
E (d)
6.79
F (s)
5.29
1.00
2.04
2.14
1.31
f1 (ppm)



MDZP-4
13C NMR MDZP-4 in MeOD
192.8
165.2
133.4
129.0
115.8
f1 (ppm)