Supplementary Information

Novel Phenylpropanoid Derivative from *Euploca procumbens* (Mill.) Diane & Hilger with Potential Anti-Inflammatory Activity

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Physical and spectral data for compounds **1-5**

Euploic acid (**1**)

^{1}H NMR (500 MHz, CD_3OD) δ 6.85 (d, 1H, *J* 8.5, H-5), 7.11 (d, 1H, *J* 8.5, H-6), 7.33 (d, 1H, *J* 15.9, H-7), 5.98 (d, 1H, *J* 15.9, H-8), 6.84 (d, 1H, *J* 2.0, H-2'), 6.87 (d, 1H, *J* 8.2, H-5'), 6.91 (dd, 1H, *J* 8.2, 2.0, H-6'), 3.08 (dd, 1H, *J* 14.6, 1.8, H-7'), 3.00 (dd, 1H, *J* 14.6, 11.1, H-7'), 5.06 (dd, 1H, *J* 11.1, 1.8, H-8'), 6.83 (d, 1H, *J* 2.0, H-2''), 6.75 (m, 1H, H-5'' and H-6''), 6.10 (d, 1H, *J* 6.3, H-7''), 4.34 (d, 1H, *J* 6.3, H-8''), 5.91 (s, 1H, H-2'''), 5.82 (s, 1H, H-5'''), 3.61 (dd, 1H, *J* 13.9, 2.9, H-7'''), 2.48 (dd, 1H, *J* 13.9, 12.3, H-7'''), 5.69 (dd, 1H, *J* 12.3, 2.9, 1H, H-8'''); ^{13}C NMR (125 MHz, CD_3OD) δ 33.9, 37.7, 59.4, 72.9, 74.6, 88.7,105.7, 113.7, 116.1, 116.5, 117.3, 117.7, 118.6, 119.1, 122.1, 123.1, 123.9, 126.2, 126.9, 131.4, 134.0, 141.1, 142.0, 144.9, 146.0, 146.2, 146.9, 149.0, 149.5, 150.3, 167.1, 172.5, 172.7, 173.1; HRMS (ESI) *m/z*, calcd. for $C_{36}H_{27}O_{16}$ $[M - H]^-$: 715.1305, found: 715.1320.

Lithospermic acid B (**2**)

^{1}H NMR (400 MHz, CD_3OD) δ 6.77 (d, 1H, *J* 2.1, H-2), 6.74 (d, 1H, *J* 8.0, H-5), 6.66 (dd, 1H, *J* 2.0, 8.2, H-6), 5.86 (d, 1H, *J* 4.9, H-7), 4.34 (d, 1H, *J* 4.9, H-8), 6.82 (d, 1H, *J* 8,4, H-5´), 7.13 (d, 1H, *J* 8.4, H-6´), 7.47 (d, 1H, *J* 15.9, H-7´), 6.18 (d, *J* 15.9, H-8), 6.75 (d, 1H, *J* 2.0, H-2´´), 6.70 (d, 1H, *J* 8.0, H-5´´), 6.61 (d, 1H, *J* 2.0, 8.4, H-6´´), 3.06 (dd, 1H, *J* 4.1,14.1, H-7´´), 3.00 (dd, 1H, *J* 8.3, 14.2, H-7´´), 5.18 (d, 1H, *J* 4.4, H-8´´), 6.51 (d, 1H, *J* 2.0, H-2´´´), 6.53 (d, 1H, *J* 8.0, H-5´´´), 6.29 (d, 1H, *J* 2.0, 8.1, H-6´´´), 3.01 (dd, *J* 3.3, 14.1, H-7´´´), 2.81 (dd, *J* 9.7, 14.2, H-7´´´), 5.16 (d, 1H, *J* 3.4, H-8´´´);^{13}C NMR (100 MHz, CD_3OD) δ 37.6, 38.0, 58.0, 75.1, 76.0, 88.3, 113.4, 116.4, 116.5, 117.3, 117.6, 118.3, 118.4, 116.4, 121.7, 122.1, 122.2, 124.7, 126.4, 129.1, 129.5, 133.6, 143.3, 145,0, 145.1, 146.5, 145.9, 146.0, 146.7, 149.0, 168, 174.2, 172.3, 173.2; HRMS (ESI) *m/z*, calcd. for $C_{36}H_{29}O_{16}$ $[M - H]^-$: 717.1461, found: 717.1457.

Lithospermic acid (**3**)

^{1}H NMR (400 MHz, CD_3OD) δ 6.80 (d, 1H, *J* 8.5, H-5), 7.20 (d, 1H, *J* 8.5, H-6), 7.82 (d, 1H, *J* 16.0, H-7), 6.32 (d, 1H, *J* 16.0, H-8), 6.78 (d, 1H, *J* 2.0, H-2´), 6.67 (d, 1H, *J* 8.1, H-5), 6.61 (dd, 1H, *J* 2.1, 8.1, H-6´), 3.06 (dd, 1H, *J* 4.1, 14.1, H-7´), 2.98 (dd, 1H, *J* 8.3, 14.1, H-7´ Hz), 5.12 (dd, 1H, *J* 4.2, 8.2, H-8´), 6.76 (d, 1H, *J* 2.0, H-2''), 6.67 (d, 1H, *J* 8.1, H-5´´), 6.61 (dd, 1H, *J* 2.0, 8.1, H-6´´), 5.89 (d, 1H, *J* 4.7, H-7´´), 4.36 (d, 1H, *J* 4.7, H-8´´); ^{13}C NMR (100 MHz, CD_3OD) δ 36.7 56.9, 74.0, 87.7, 112.0, 115.2, 114.9, 116.4, 116.6, 116.7, 116.8, 120.2, 120.4, 123.3, 126.8, 128.3, 132.6, 142.5, 143.7, 143.8, 145.1, 145.2, 144.6, 147.5, 166.9, 172.8, 174.5; HRMS (ESI) *m/z*, calcd. for $C_{27}H_{21}O_{12}$ $[M - H]^-$: 537.1038, found: 537.1039.

9´´-Methyl lithospermate (**4**)

^{1}H NMR (400 MHz, CD_3OD) δ 6.80 (d, 1H, *J* 8.4, H-5), 7.16 (d, 1H, *J* 8.5, H-6), 7.70 (d, 1H, *J* 16.0, H-7), 6.28 (d, 1H, *J* 16.0, H-8), 6.74 (sl, 1H, H-2´), 6.67 (d, 1H, *J* 8.1, H-5´), 6.71 (dd, 1H, *J* 2.1;8.1, H-6´), 3.08 (dd, 1H, *J* 3.7, 14.1, H-7´), 2.95 (dd, 1H, *J* 9.2, 14.1, H-7´), 5.14 (dd, 1H, *J* 3.7; 9.0, H-8´), 6.77 (d, 1H, *J* 2.0, H-2´´), 6.67 (d, 1H, *J* 8.1, H-5´´), 6.61 (dd, 1H, *J* 1.9, 8.1, H-6´´), 5.86 (d,1H, *J* 4.8, H-7´´), 4.49 (d, 1H, *J* 4.8, H-8´´), 3.86 (s, 3H, OCH3); ^{13}C NMR (100 MHz, CD_3OD) δ 38.3, 53.2, 57.2, 76.2, 88.5, 113.5, 116.3, 116.4, 117.2, 117.5, 118.3, 118.4, 121.7, 121.9, 124.8, 126.9, 130.3, 133.4,143.4, 145.0, 145.1, 146.1, 146.7, 146.8, 148.8, 168.4, 173.7, 175.4; HRMS (ESI) *m/z*, calcd. for $C_{28}H_{23}O_{12}$ $[M - H]^-$: 551.1195, found: 551.1190.

Luteolin-7-*O*-glucoside (**5**)

^{1}H NMR (400 MHz, DMSO) δ 5.07 (d, 1H, *J* 7.3, H-1´´), 6.44 (d, 1H, *J* 2.0, H-6), 6.73 (sl, 1H, H-3), 6.78 (d, 1H, *J* 1.8, H-8), 6.90 (m, 1H, H-5´), 7.45 (m, 1H, H-2´), 7.43 (m, 1H, H-6´); ^{13}C NMR (100 MHz, DMSO) δ 60.6, 69.6, 73.1, 76.4, 77.2, 94.7, 99.5, 99.9, 103.2, 105.3, 113.6, 116.0, 119.2, 121.4, 145.8, 150.0, 156.9, 161.1, 163.0, 164.5, 181.9; HRMS (ESI) *m/z*, calcd. for $C_{21}H_{19}O_{11}$ $[M - H]^-$: 447.0933, found: 447.0932.

Spectral data

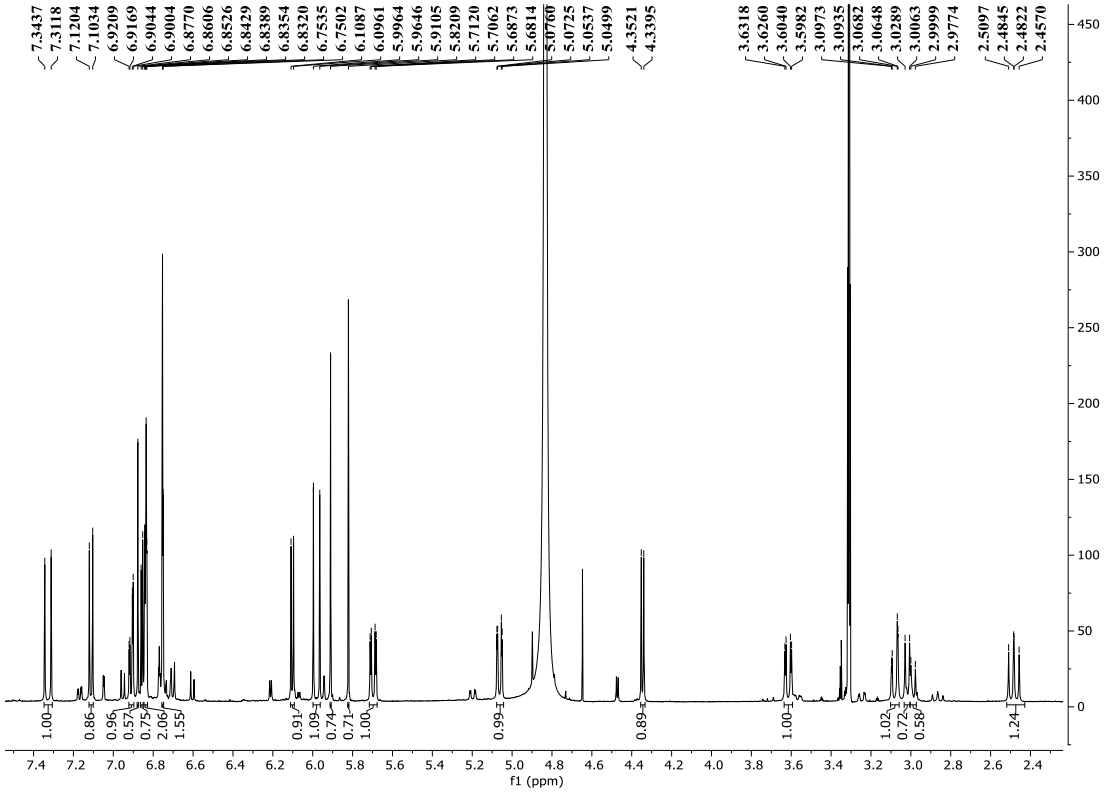

Figure S1. ^{1}H NMR spectrum (500 MHz, methanol-d_4) of compound **1**.

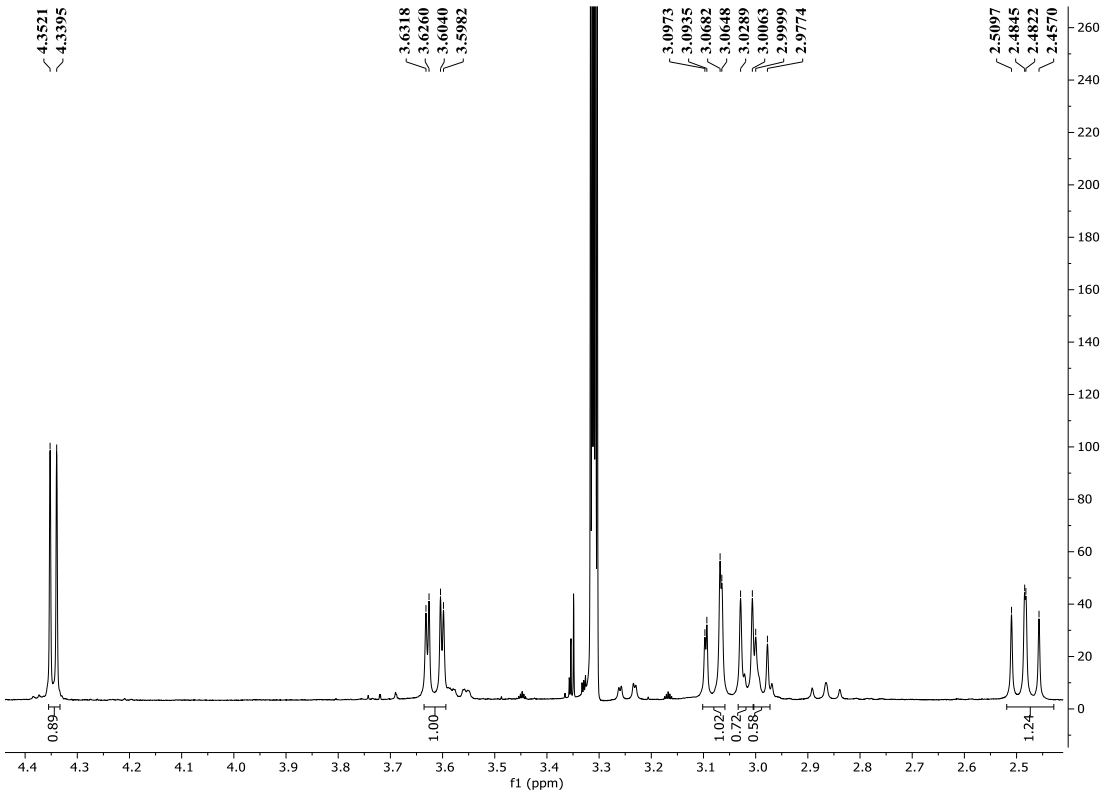

Figure S2. ^{1}H NMR spectrum (500 MHz, methanol-d_4) of compound **1**.

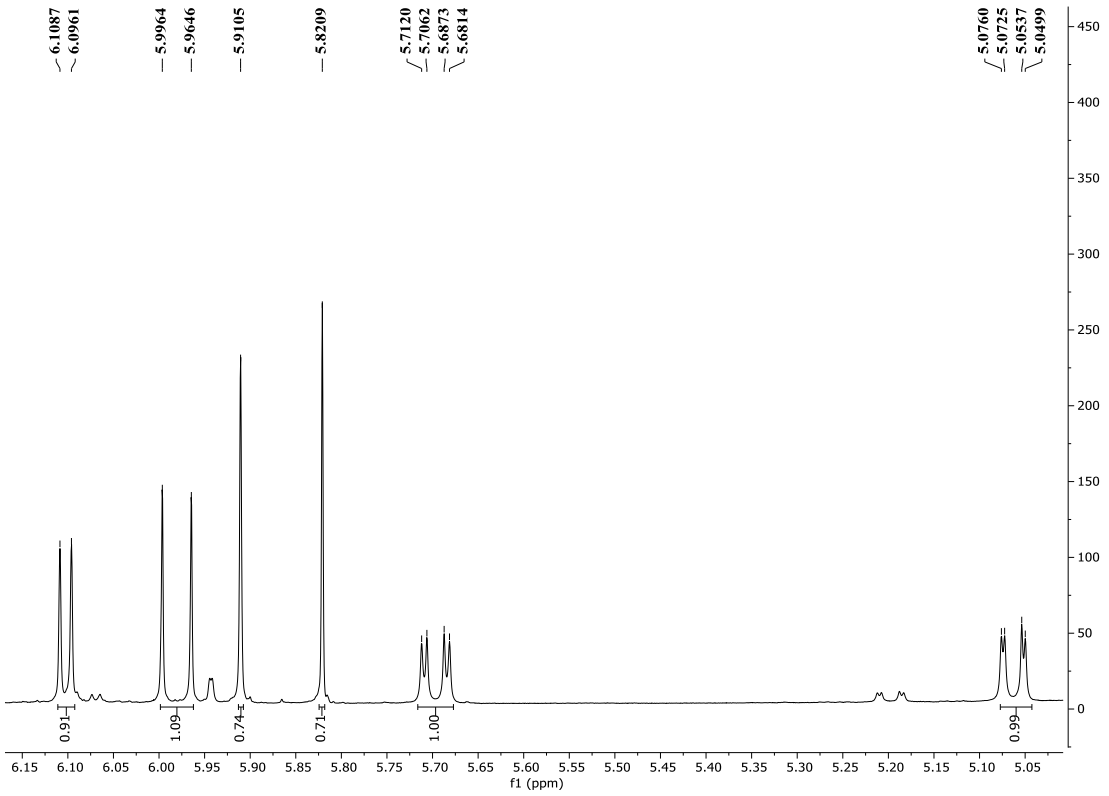

Figure S3. ^{1}H NMR spectrum (500 MHz, methanol-d_4) of compound **1**.

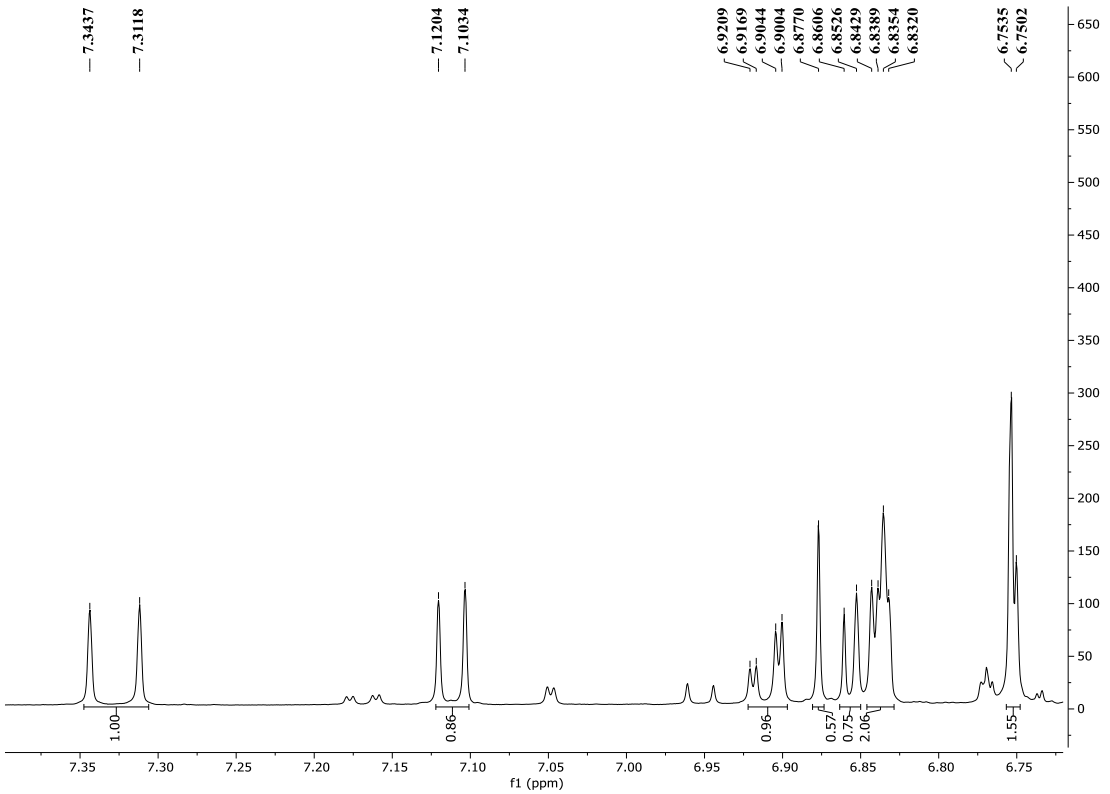

Figure S4. ^{1}H NMR spectrum (500 MHz, methanol-d_4) of compound **1**.

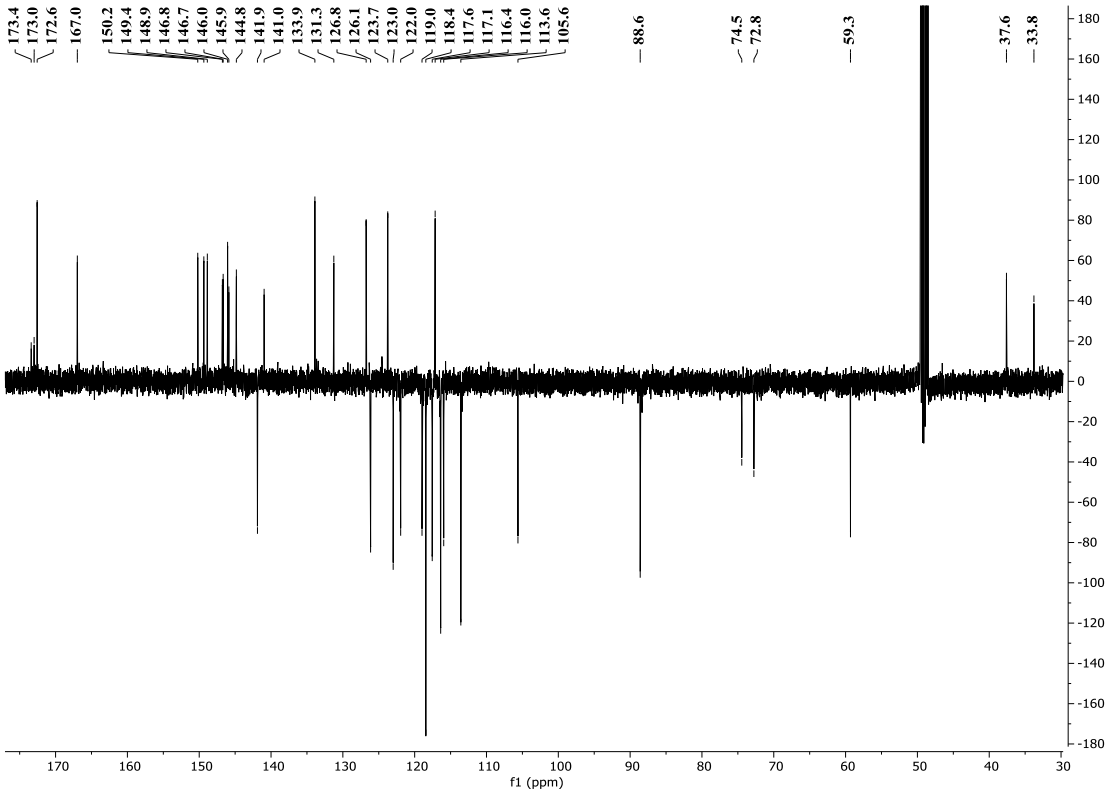

Figure S5. ^{13}C-APT NMR spectrum (125 MHz, methanol-d_4) of compound **1**.

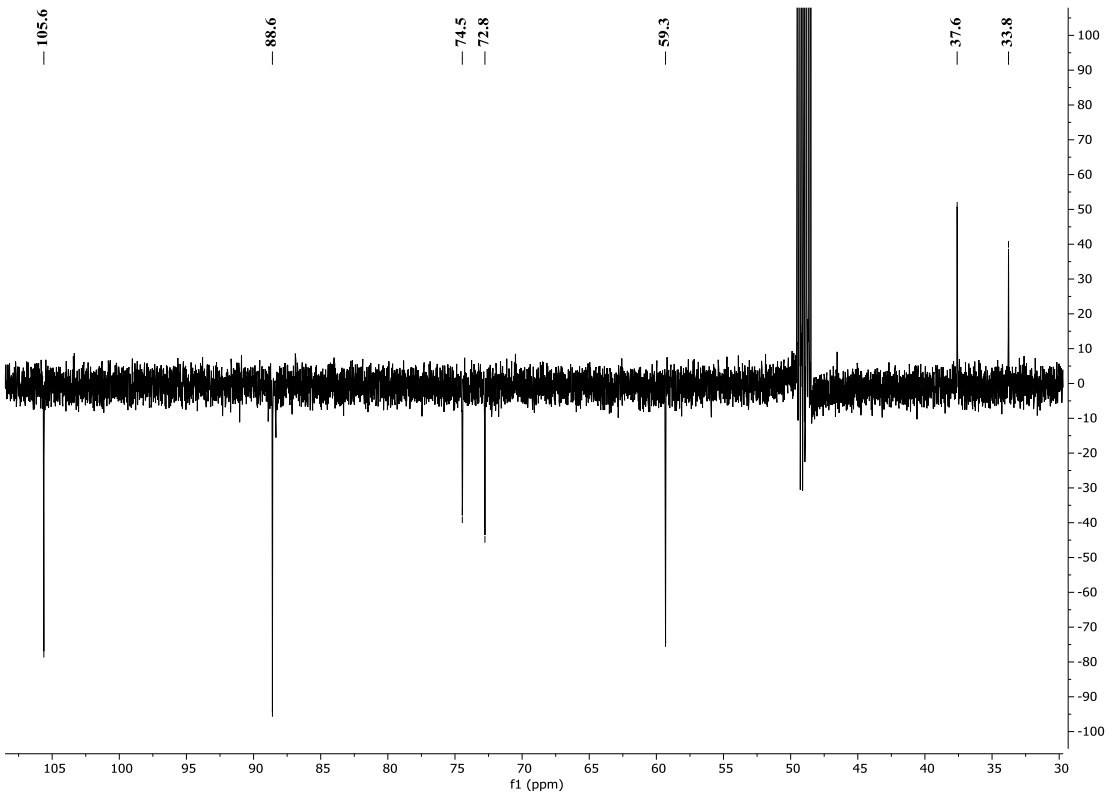

Figure S6. ^{13}C-APT NMR spectrum (125 MHz, methanol-d_4) of compound **1.**

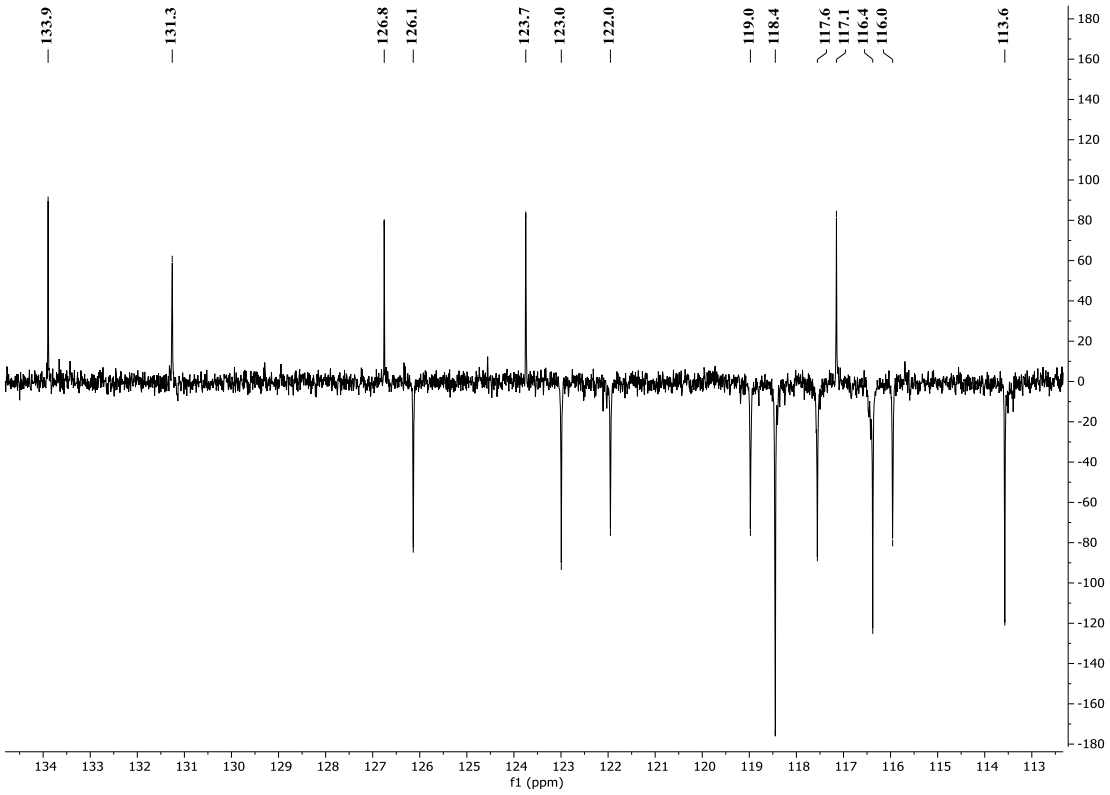

Figure S7. ^{13}C-APT NMR spectrum (125 MHz, methanol-d_4) of compound **1.**

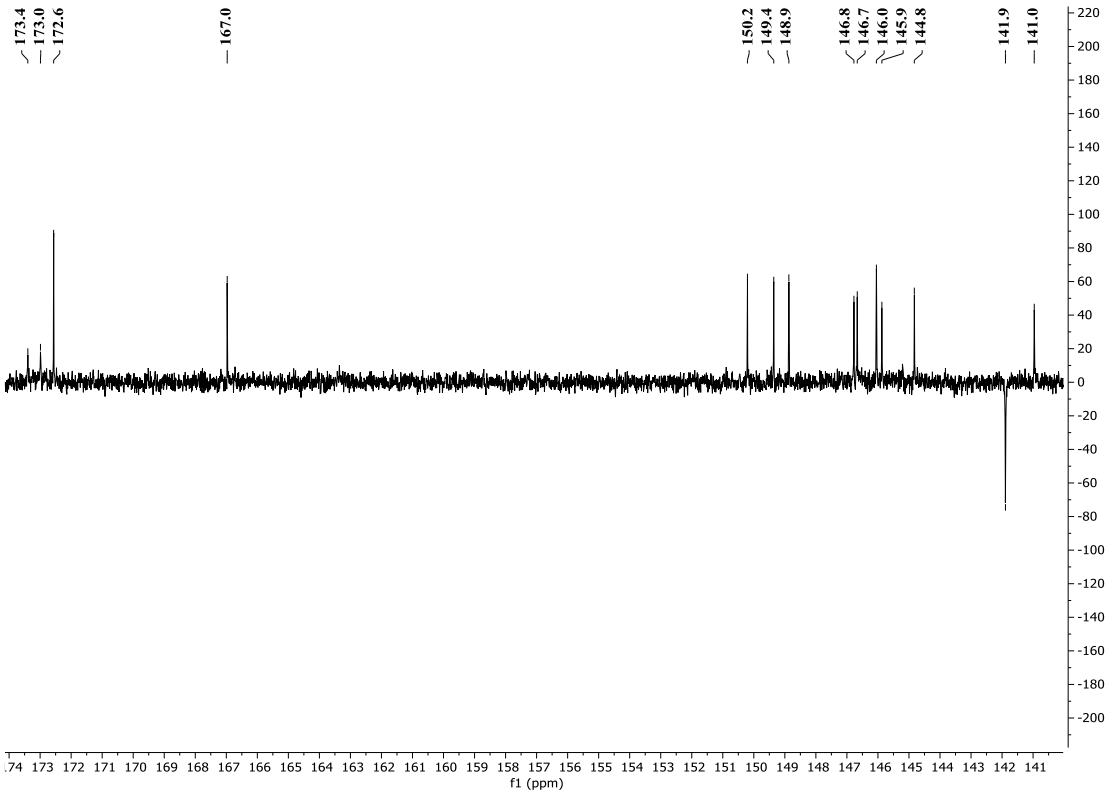

Figure S8. ^{13}C-APT NMR spectrum (125 MHz, methanol-d_4) of compound **1**.

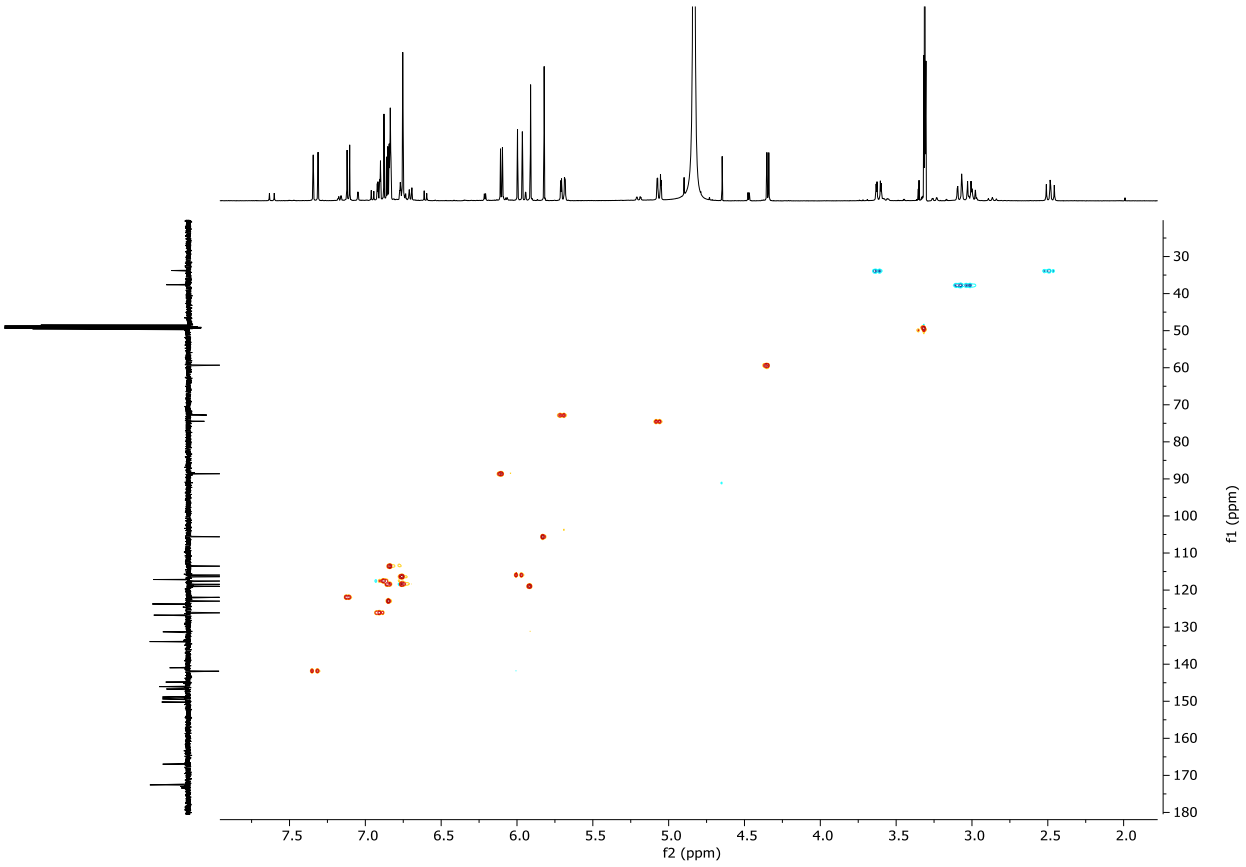

Figure S9. HSQC spectrum (500 MHz, 125 MHz, methanol-d_4) of compound **1**.

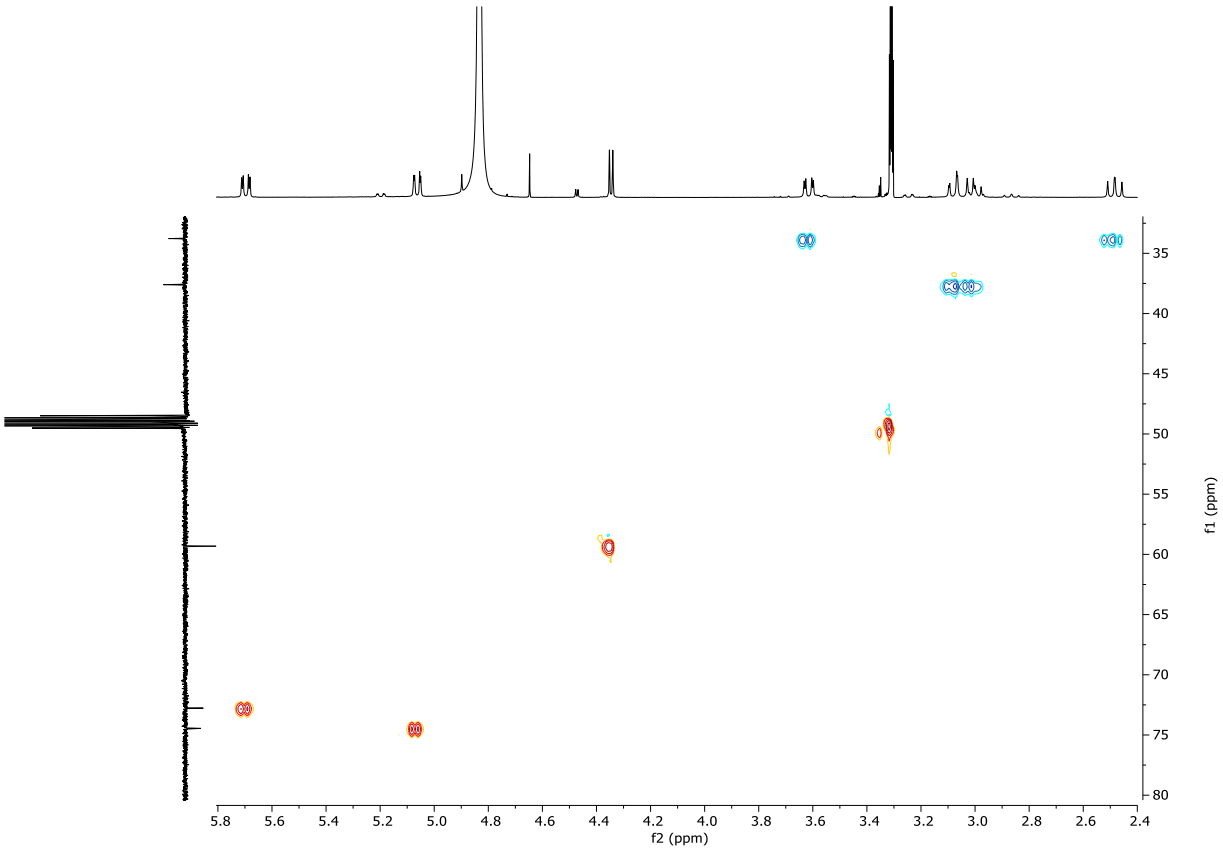

Figure S10. HSQC spectrum (500 MHz, 125 MHz, methanol-d_4) of compound **1**.

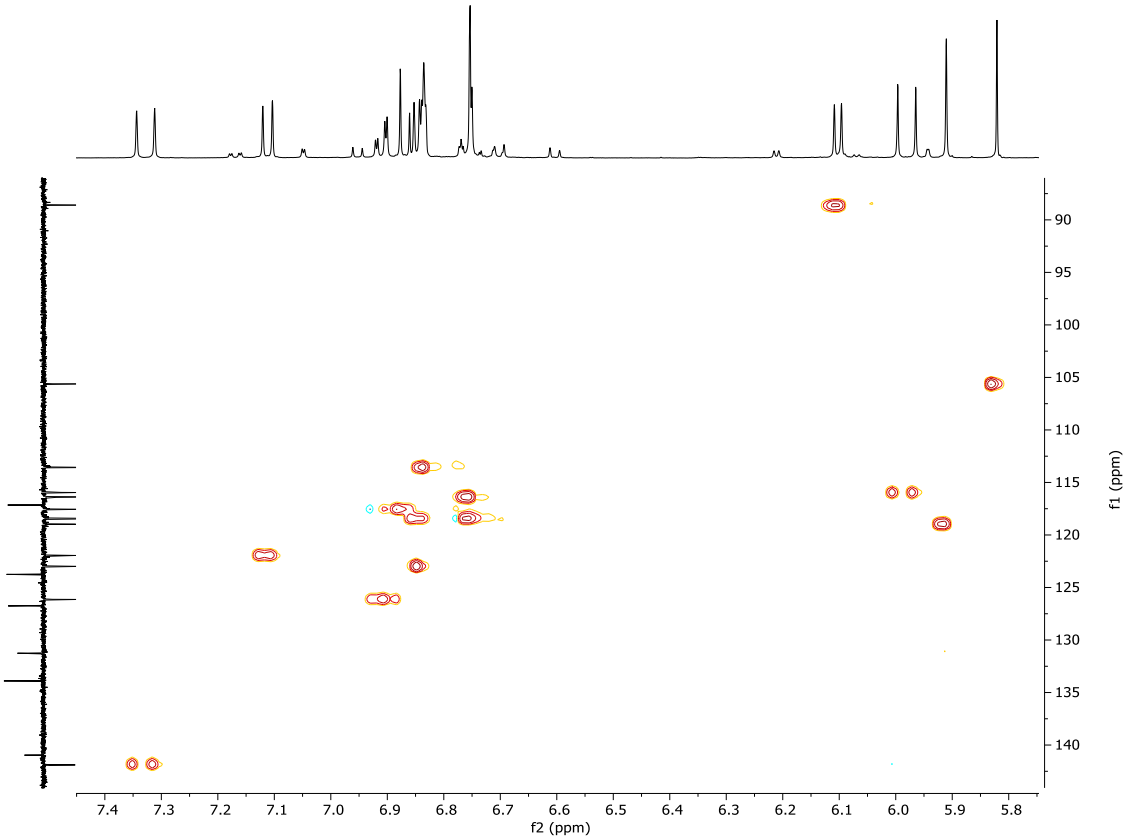

Figure S11. HSQC spectrum (500 MHz, 125 MHz, methanol-d_4) of compound **1**.

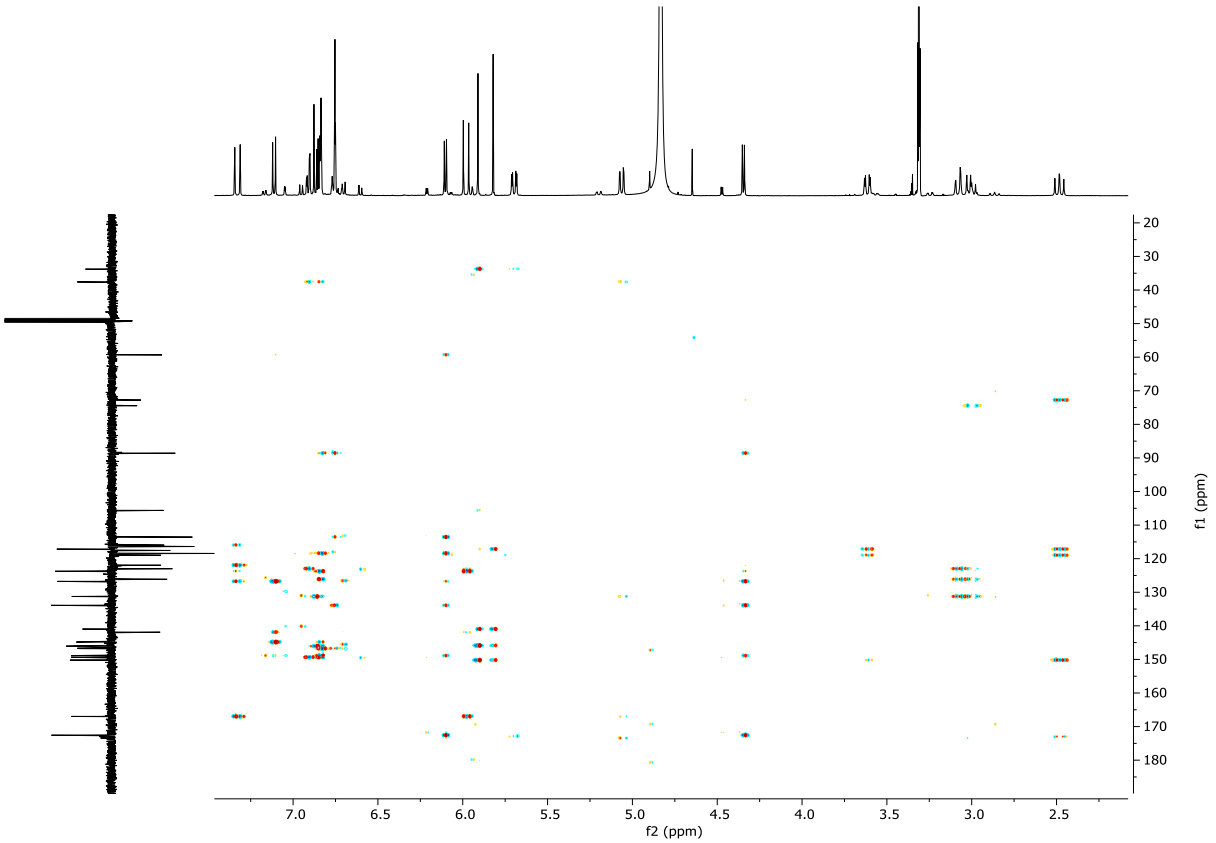

Figure S12. HMBC spectrum (500 MHz, 125 MHz, methanol-d_4) of compound **1**.

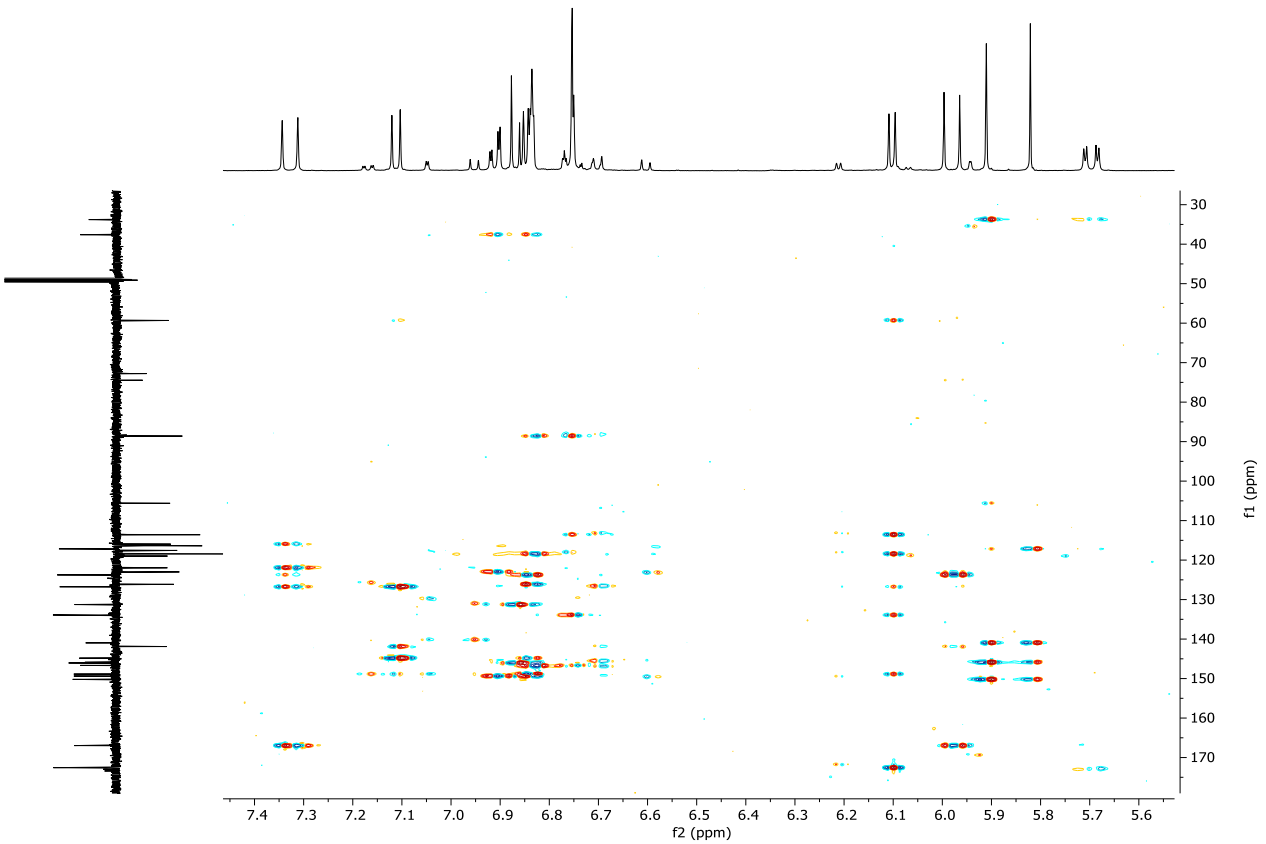

Figure S13. HMBC spectrum (500 MHz, 125 MHz, methanol-d_4) of compound **1**.

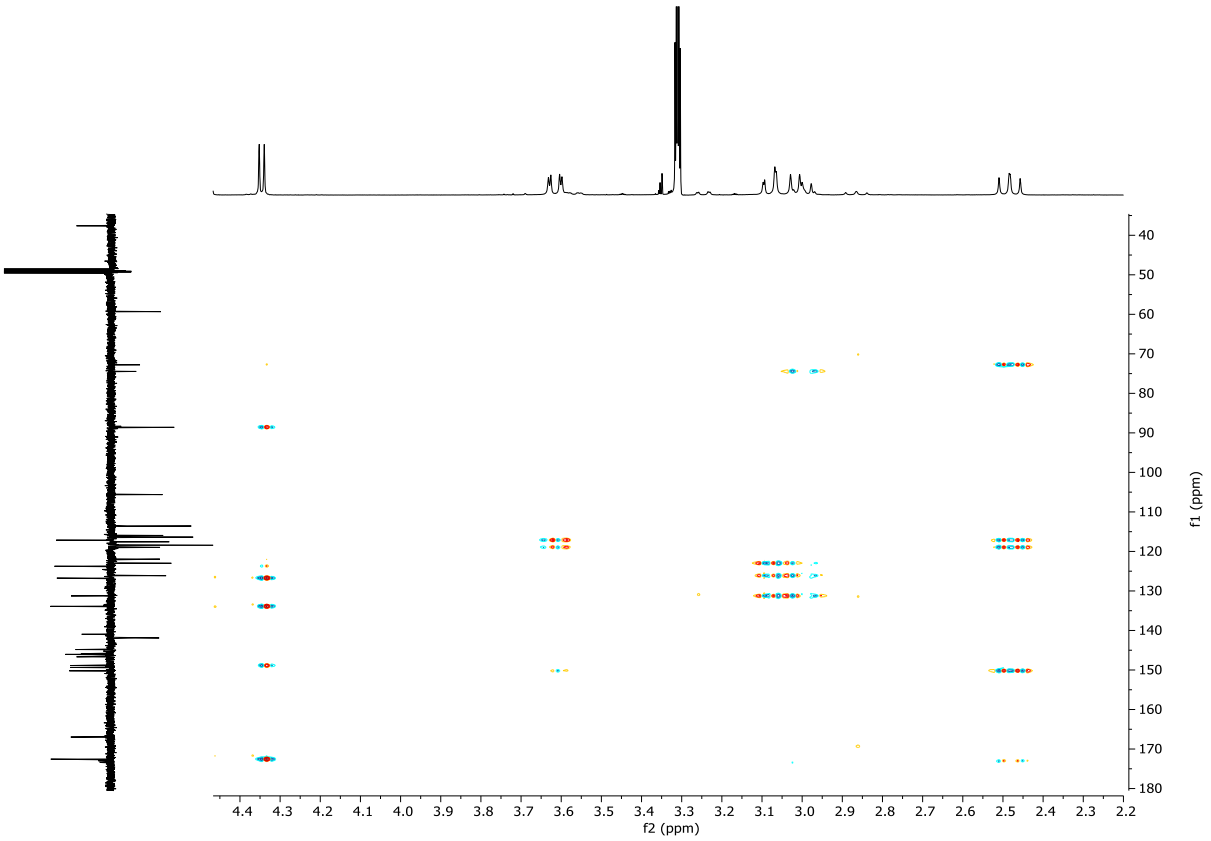

Figure S14. HMBC spectrum (500 MHz, 125 MHz, methanol-d_4) of compound **1**.

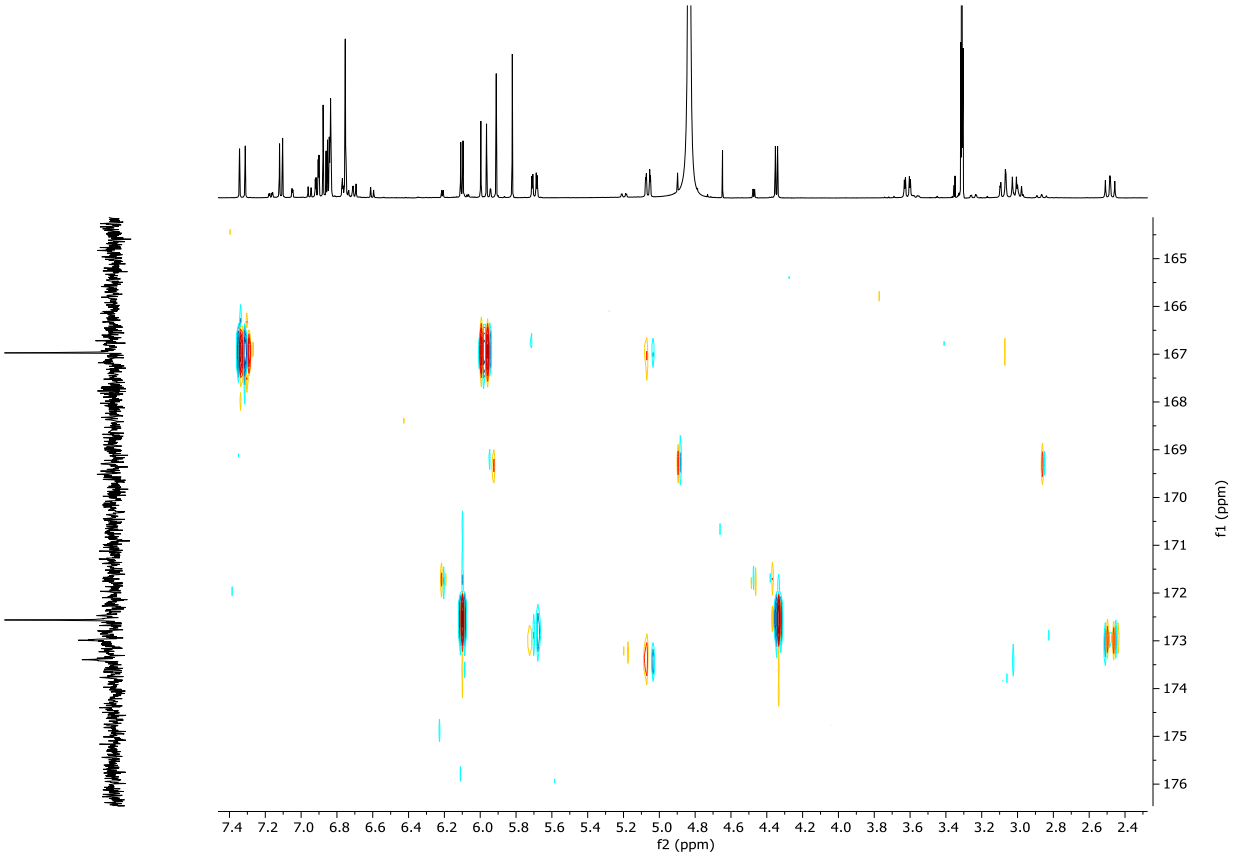

Figure S15. HMBC spectrum (500 MHz, 125 MHz, methanol-d_4) of compound **1**.

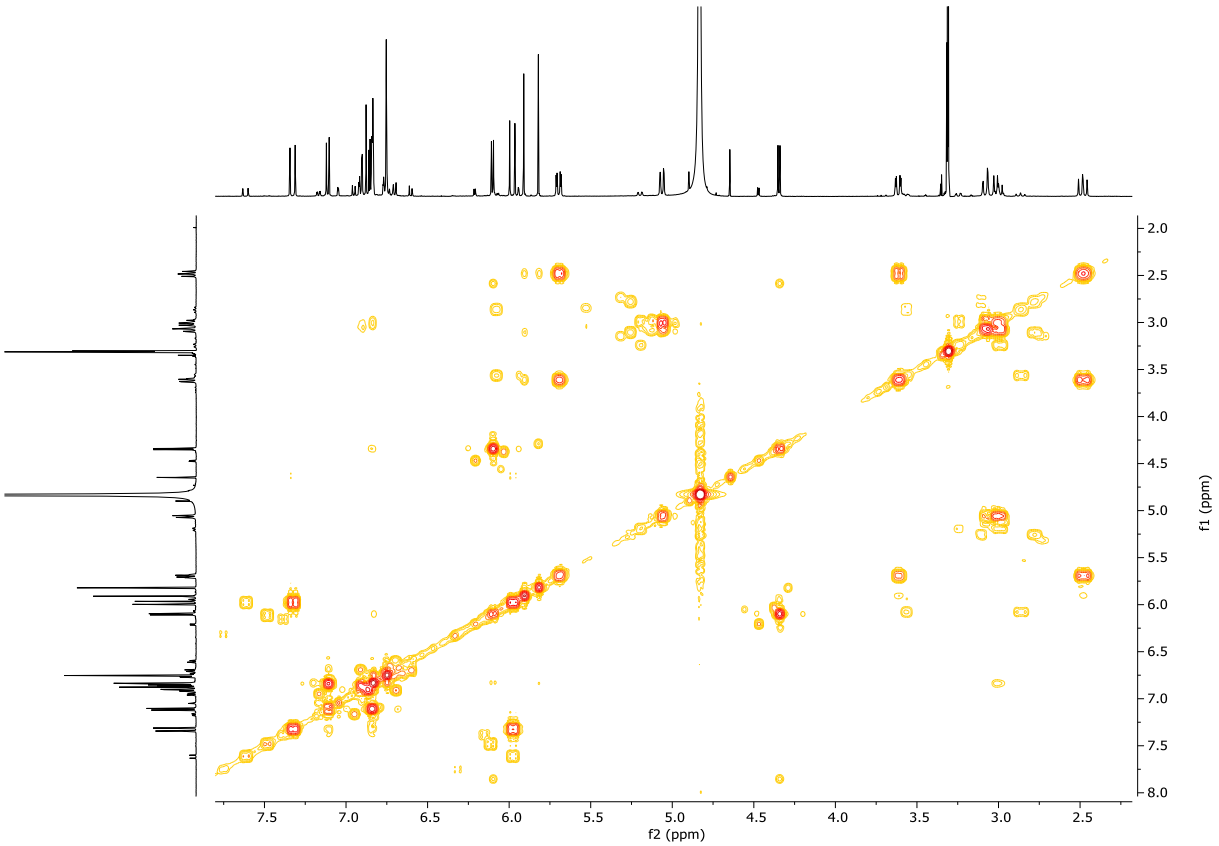

Figure S16. COSY spectrum of compound **1** (500 MHz, methanol-d_4).

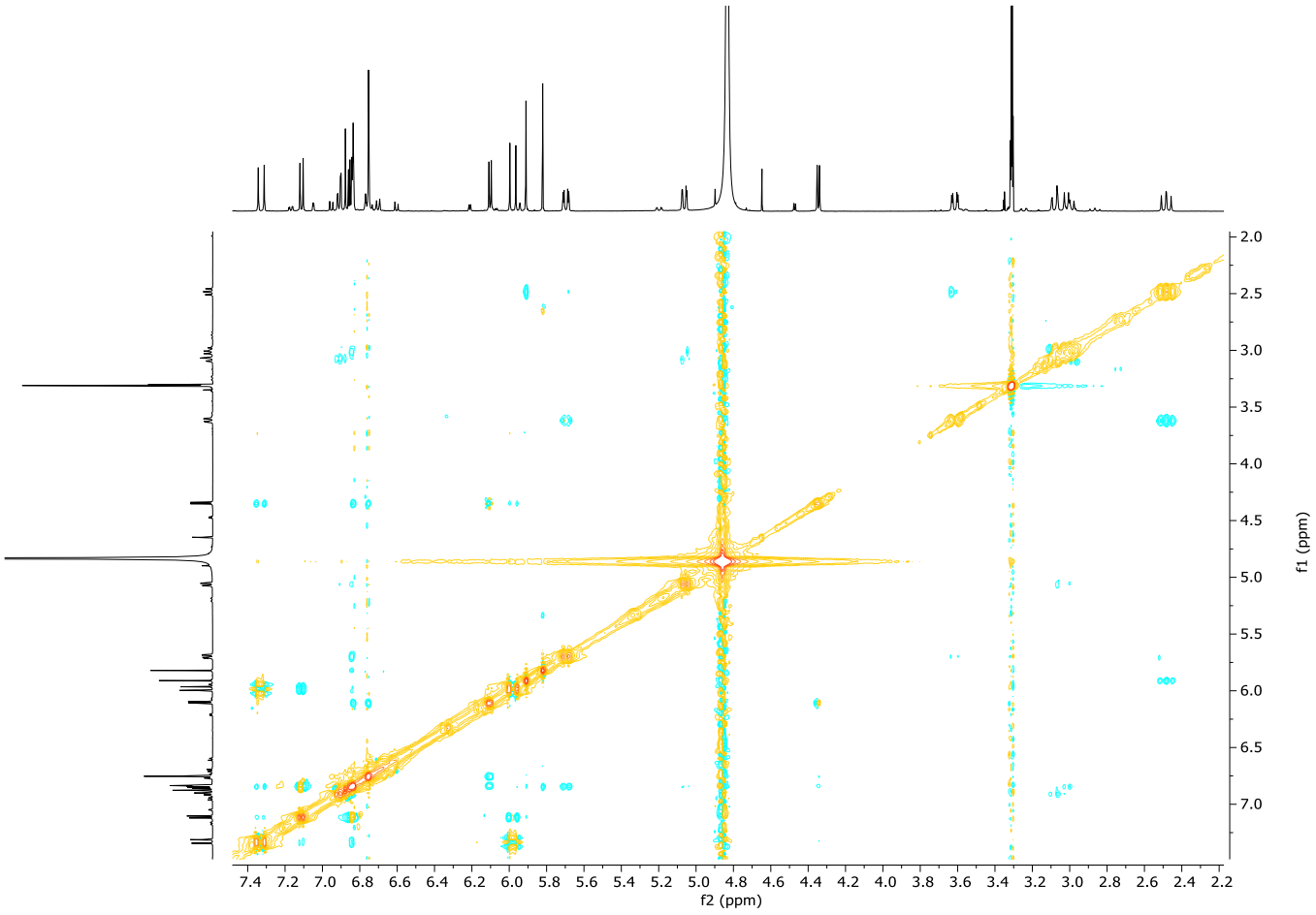

Figure S17. NOESY spectrum (500 MHz, methanol-d_4) of compound **1**.

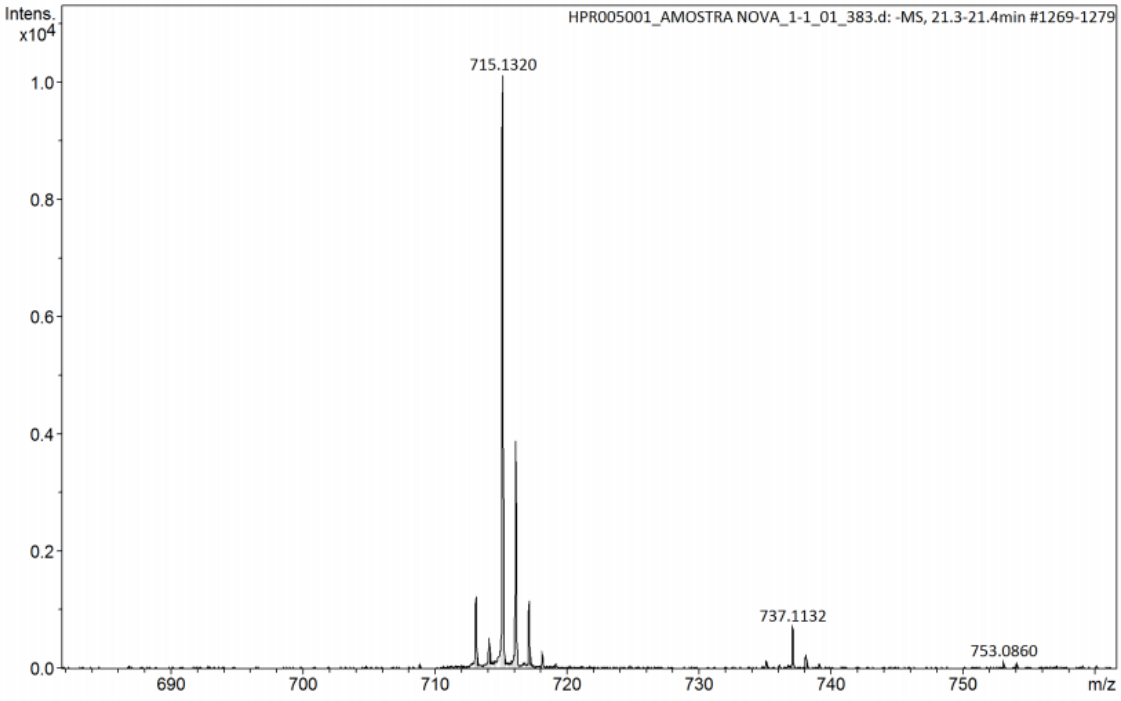

Figure S18. HRESIMS spectrum of compound **1**.

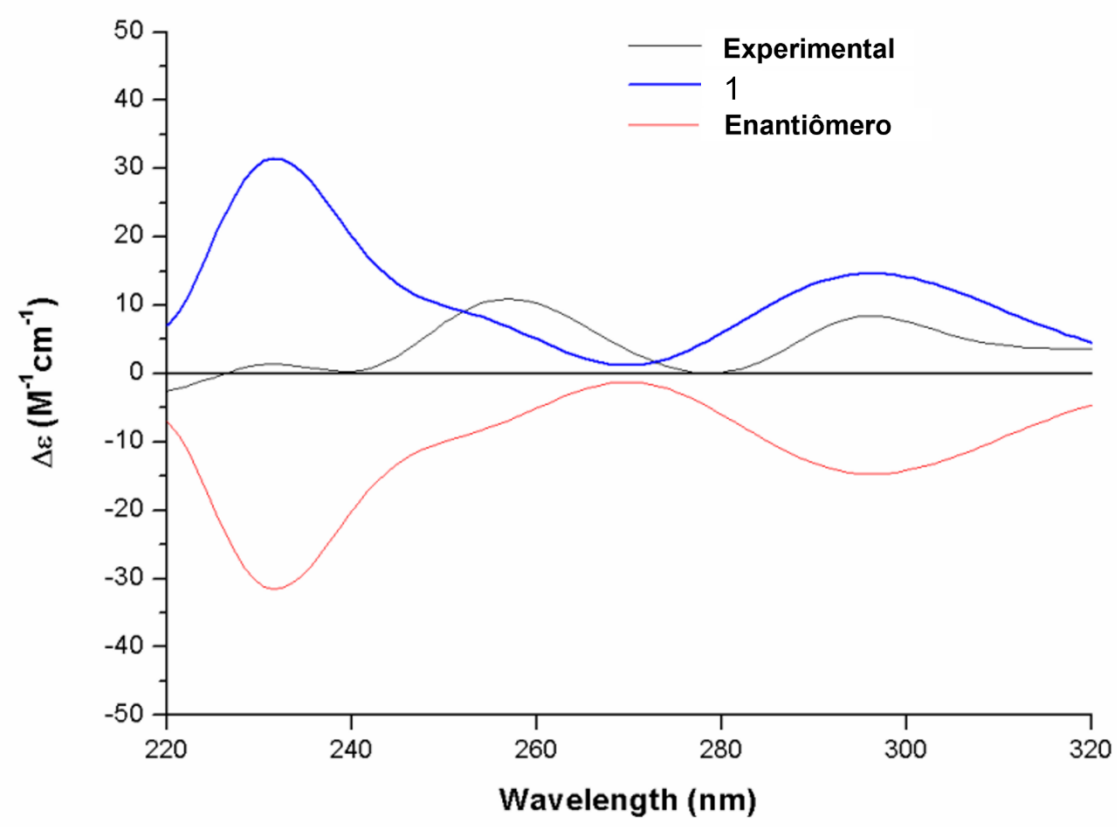

Figure S19. Electronic circular dichroism (ECD) spectrum of compound **1**.

Compound **2**

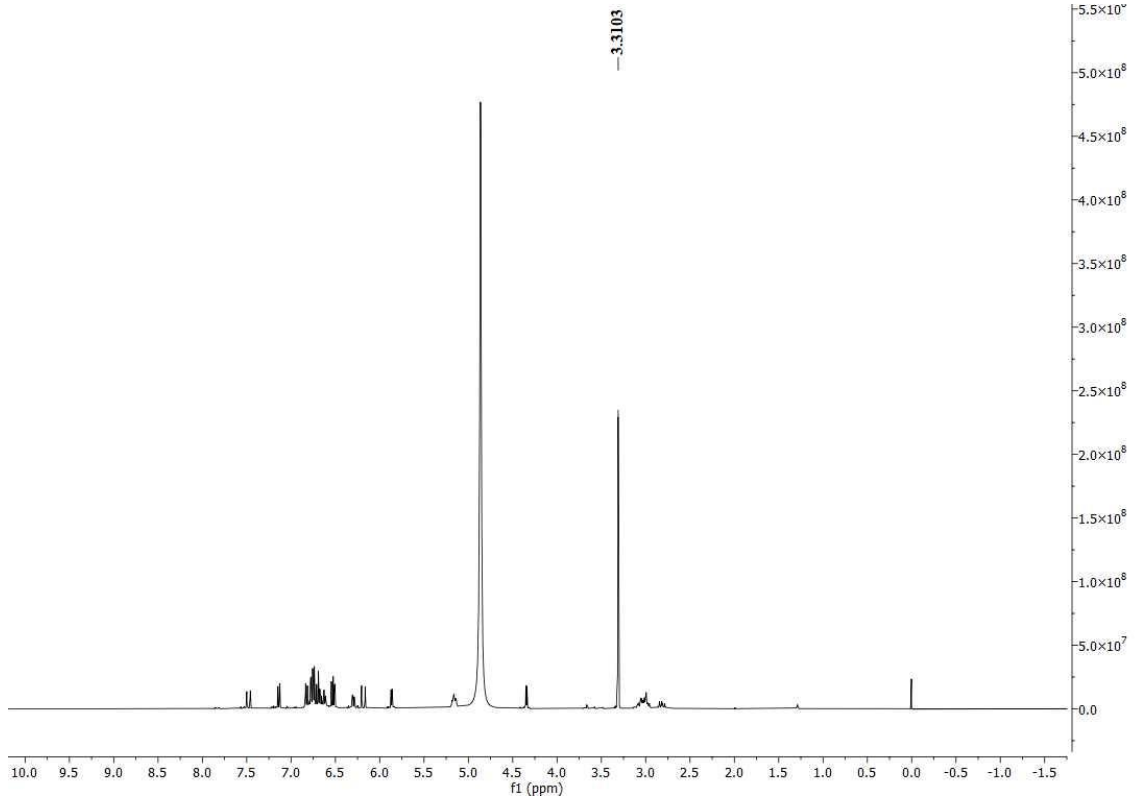

Figure S20. ^{1}H NMR spectrum (500 MHz, methanol-d_4) of compound **2**.

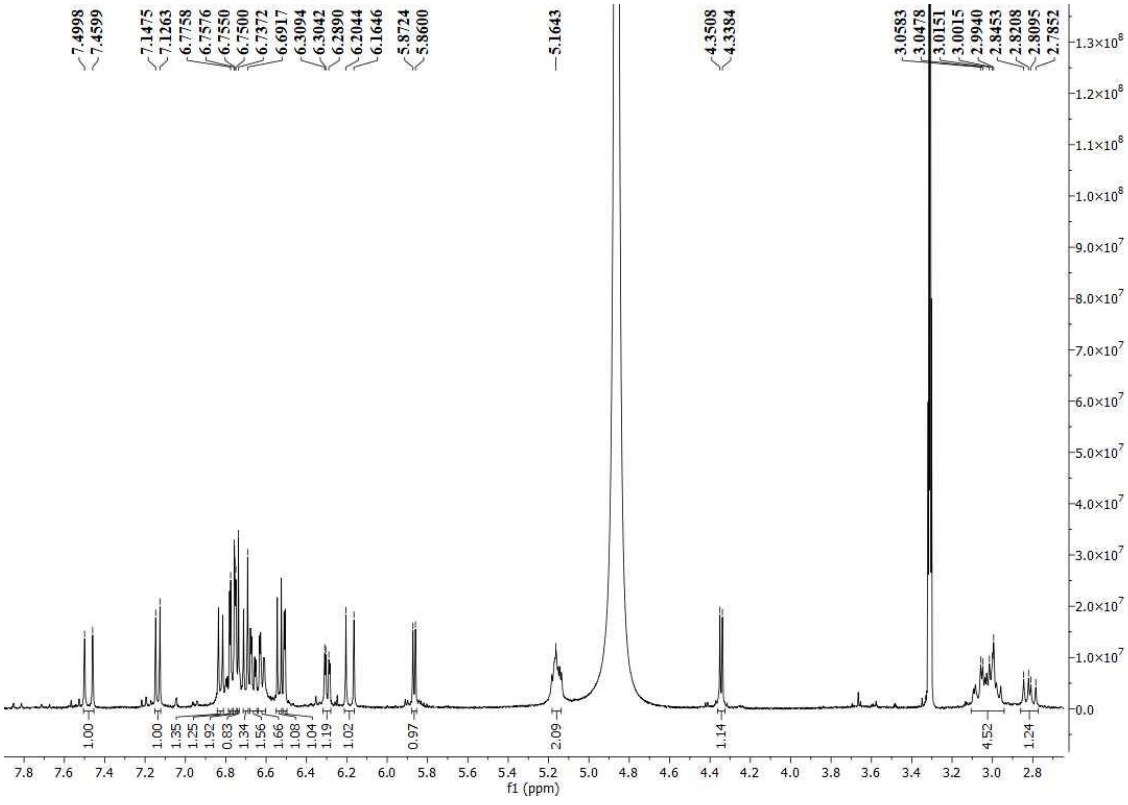

Figure S21. Expansion of ^{1}H NMR spectrum (500 MHz, methanol-d_4) of compound **2**.

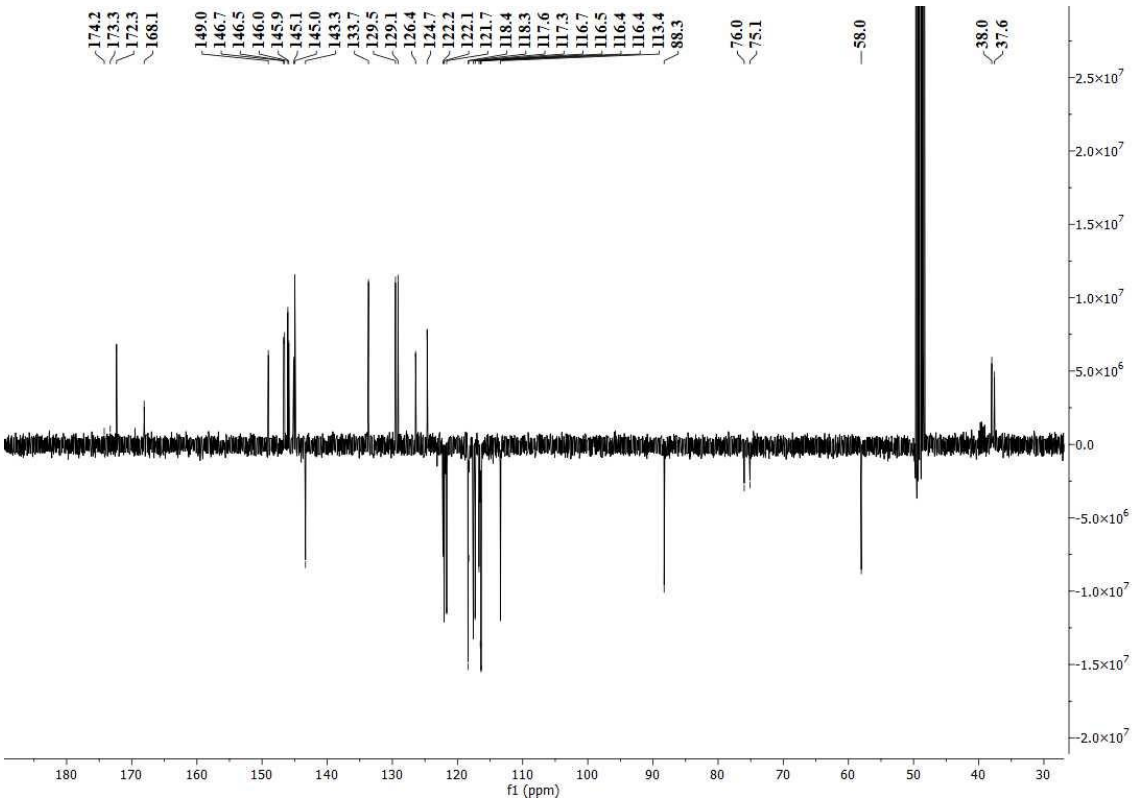

Figure S22. ^{13}C NMR spectrum (125 MHz, methanol-d_4) of compound **2**.

Table S1. NMR data obtained for compound **2** and comparison with literature

Pos.	Compound **2**		Lithospermic acid B (literature)[1]	
	δ_H[a,b] (*J* / Hz) / ppm	δ_C[a,c] / ppm	δ_H (*J* / Hz) / ppm	δ_C / ppm
1	–	133.6	–	133.6
2	6.77 (d, 1H, *J* 2.1)	113.4	6.79 (d, 1H, *J* 2.1)	113.4
3	–	146.5	–	146.6
4	–	146.7	–	146.8
5	6.74 (d, 1H, *J* 8.0)	117.3	6.74 (d, 1H, *J* 8.1)	116.4
6	6.66 (dd, 1H, *J* 2.0, 8.2)	118.4	6.65 (ddd, 1H, *J* 0.6, 2.2, 8.2)	118.4
7	5.86 (d, 1H, *J* 4.9)	88.3	5.86 (d, 1H, *J* 4.8)	88.3
8	4.34 (d, 1H, *J* 4.9)	58.0	4.35 (d, 1H, *J* 4.8)	57.9
9	–	172.3	–	172.3
1´	–	124.7	–	124.6
2´	–	126.4	–	126.4
3´	–	149.0	–	149.1
4´	–	145.1	–	145.1
5´	6.82 (d, 1H, *J* 8,4)	118.3	6.83 (d, 1H, *J* 8,4)	118.3
6´	7.13 (d, 1H, *J*8.4)	122.1	7.15 (d, 1H, *J* 8.4)	122.3
7´	7.47 (d, 1H, *J* 15.9)	143.3	7.52 (d, 1H, *J* 15.9)	143.6
8´	6.18 (d, *J* 15.9)	116.5	6.20 (d, *J* 15.9)	116.6
9´	–	168.1	–	168.0
1´´	–	129.5	–	129.2
2´´	6.75 (d, 1H, *J* 2.0)	117.6	6.75 (d, 1H, *J* 2.0)	117.5

Table S1. NMR data obtained for compound **2** and comparison with literature (cont.)

Pos.	Compound **2**		Lithospermic acid B (literature)[1]	
	δ_H[a,b] (*J* / Hz) / ppm	δ_C[a,c] / ppm	δ_H (*J* / Hz)/ ppm	δ_C / ppm
3´´	–	146.0	–	146.1
4´´	–	145.1	–	145.2
5´´	6.70 (d, 1H, *J* 8.0)	116.4	6.70 (d, 1H, *J* 8.0)	116.4
6´´	6.61 (d, 1H, *J* 2.0, 8.4)	122.2	6.62 (d, 1H, *J* 2.1, 8.1)	122.1
7´´	3.06 (dd, 1H, *J* 4.1,14.1)	38.0	3.07 (dd, 1H, *J* 4.4, 14.3)	37.9
	3.00 (dd, 1H, *J* 8.3, 14.2)	–	3.00 (dd, 1H, *J* 7.9, 14.2)	–
8´´	5.18 (d, 1H, *J* 4.4)	75.1	5.18 (dd, 1H, *J* 5.0, 7.3)	74.6
9´´	–	174.2	–	173.6
1´´´	–	129.1	–	128.9
2´´´	6.51 (d, 1H, *J* 2.0)	117.3	6.52 (d, 1H, *J* 2.1)	117.3
3´´´	–	145.9	–	145.9
4´´´	–	145.0	–	145.1
5´´´	6.53 (d, 1H, *J* 8.0)	116.4	6.54 (d, 1H, *J* 8.0)	116.5
6´´´	6.29 (d, 1H, *J* 2.0, 8.1)	121.7	6.31 (dd, 1H, *J* 2.1, 8.1)	121.7
7´´´	3.01 (dd, *J* 3.3, 14.1)	37.6	3.01 (dd, *J* 3.3, 14.3)	37.5
	2.81 (dd, *J* 9.7, 14.2)	–	2.83 (dd, *J* 9.6, 14.3)	–
8´´´	5.16 (d, 1H, *J* 3.4)	76.0	5.17 (dd, 1H, *J* 3.3, 9.6)	75.5
9´´´	–	173.2	–	172.5

[a]Measured in CD_3OD, [b]125 MHz, [c]500 MHz.

Compound **3**

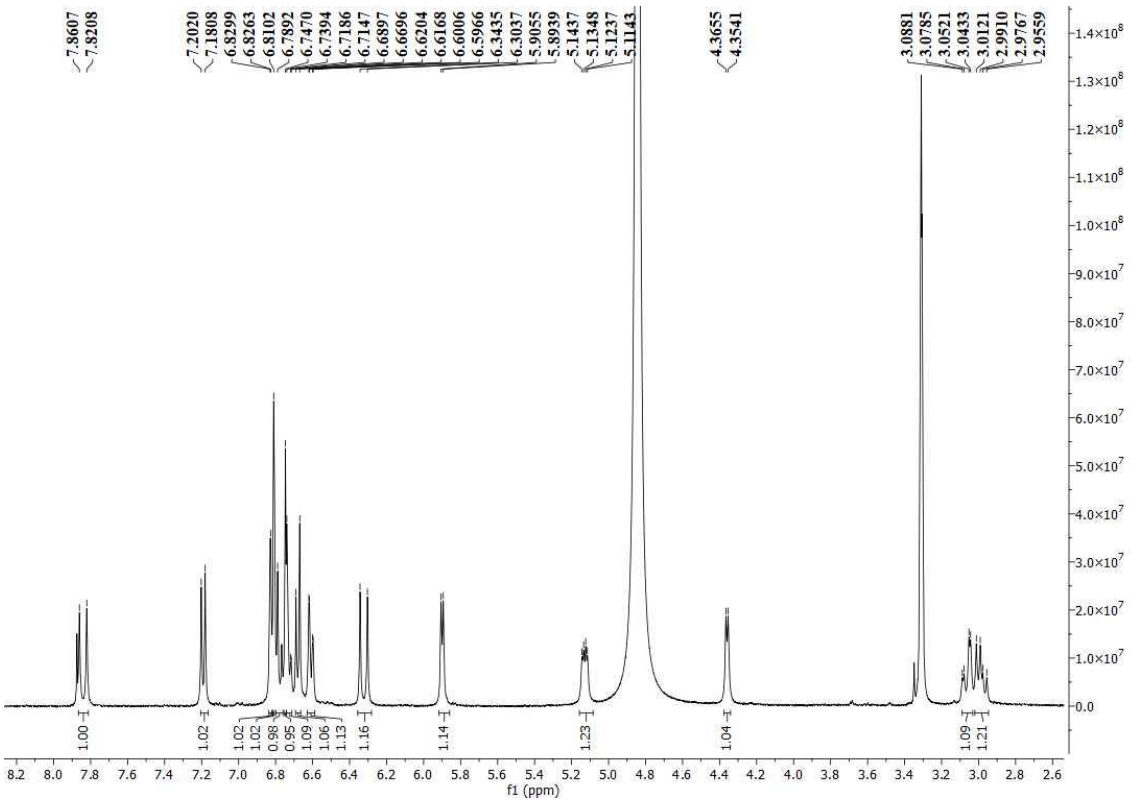

Figure S23. ^{1}H NMR spectrum (500 MHz, methanol-d_4) of compound **3**.

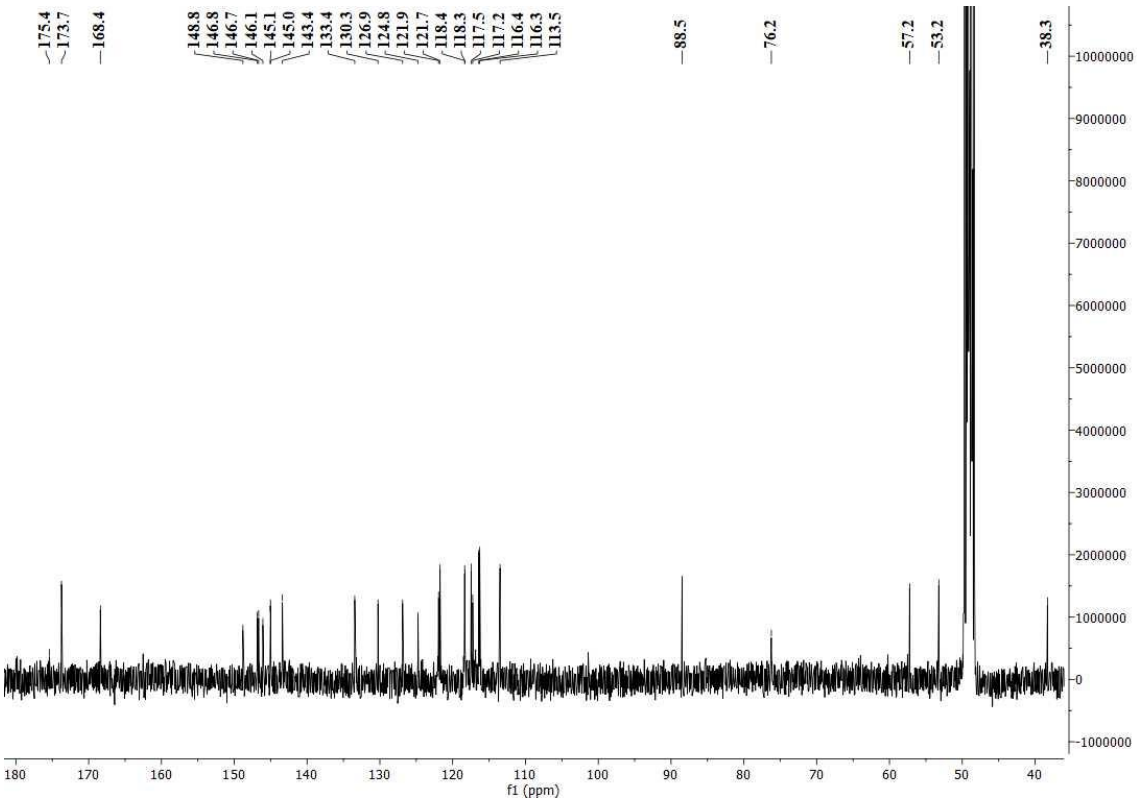

Figure S24. ^{13}C NMR spectrum (125 MHz, methanol-d_4) of compound **3**.

Table S2. NMR data obtained for compound **3** and comparison with literature

Pos.	Compound **3**		Lithospermic acid (literature)[2]	
	δ_H[a,b] (*J* / Hz) / ppm	δ_C[a,c] / ppm	δ_H (*J* / Hz) / ppm	δ_C / ppm
1	–	123.6	–	124.8
2	–	126.8	–	128.4
3	–	147.5	–	149.0
4	–	145.2	–	145.2
5	6.80 (d, 1H, *J* 8.5)	116.6	6.82 (d, 1H, *J* 8.4)	118.2
6	7.20 (d, 1H, *J* 8.5)	120.2	7.20 (d, 1H, *J* 8.4)	121.7
7	7.82 (d, 1H, *J* 16.0)	142.5	7.84 (d, 1H, *J* 16.2)	144.0
8	6.32 (d, 1H, *J* 16.0)	115.2	6.32 (d, 1H, *J* 16.2)	116.4
9	–	166.9	–	168.4
1´	–	128.3	–	129.8
2´	6.78 (d, 1H, *J* 2.0)	112.0	6.80 (sl, 1H)	113.6
3´	–	145.1	–	145.3
4´	–	144.6	–	146.2
5´	6.67 (d, 1H, *J* 8,1)	116.4	6.68 (d, 1H, *J* 8,1)	116.5
6´	6.61 (dd, 1H, *J* 2.1, 8.1)	116.8	6.61 (dd, 1H, *J* 2.1, 8.1)	118.5
7´	3.06 (dd, 1H, *J* 4.1, 14.1)	36.7	3.05 (dd, 1H, *J* 3.6, 14.1)	38.3
	2.98 (dd, 1H, *J* 8.3, 14.1)	–	2.99 (dd, 1H, *J* 8.4, 14.1)	–

Table S2. NMR data obtained for compound **3** and comparison with literature (cont.)

Pos.	Compound **3**		Lithospermic acid (literature)[2]	
	δ_H[a,b] (*J* / Hz) / ppm	δ_C[a,c] / ppm	δ_H (*J* / Hz) / ppm	δ_C / ppm
8´	5.12 (dd, *J* 4.2, 8.2)	74.0	5.12 (dd, *J* 3.6, 8.0)	75.1
9´	–	172.8	–	174.2
1´´	–	132.6	–	134.2
2´´	6.76 (d, 1H, *J* 2.0)	116.7	6.80 (sl, 1H)	118.0
3´´	–	143.7	–	146.7
4´´	–	143.8	–	146.8
5´´	6.67 (d, 1H, *J* 8.1)	114.9	6.77 (d, 1H, *J* 8.1)	116.4
6´´	6.61 (dd, 1H, *J* 2.0, 8.1)	120.4	6.72 (dd, 1H, *J* 2.0, 8.1)	121.9
7´´	5.89 (d, 1H, *J* 4.7)	87.7	5.90 (d, 1H, *J* 4.8)	89.3
8´´	4.36 (d, 1H, *J* 4.7)	56.9	4.36 (d, 1H, *J* 4.5)	58.5
9´´	–	174.5	–	176.2

[a]Measured in CD_3OD, [b]125 MHz, [c]500 MHz.

Compound **4**

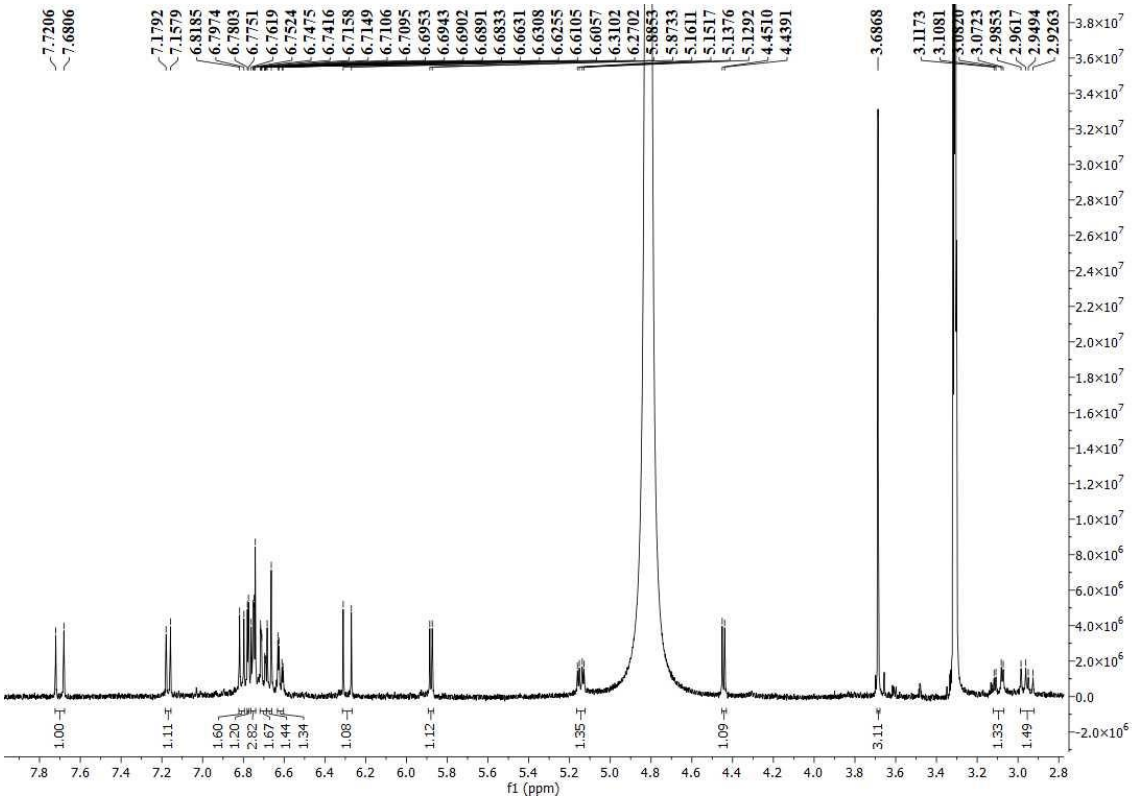

Figure S25. ^{1}H NMR spectrum (500 MHz, methanol-d_4) of compound **4**.

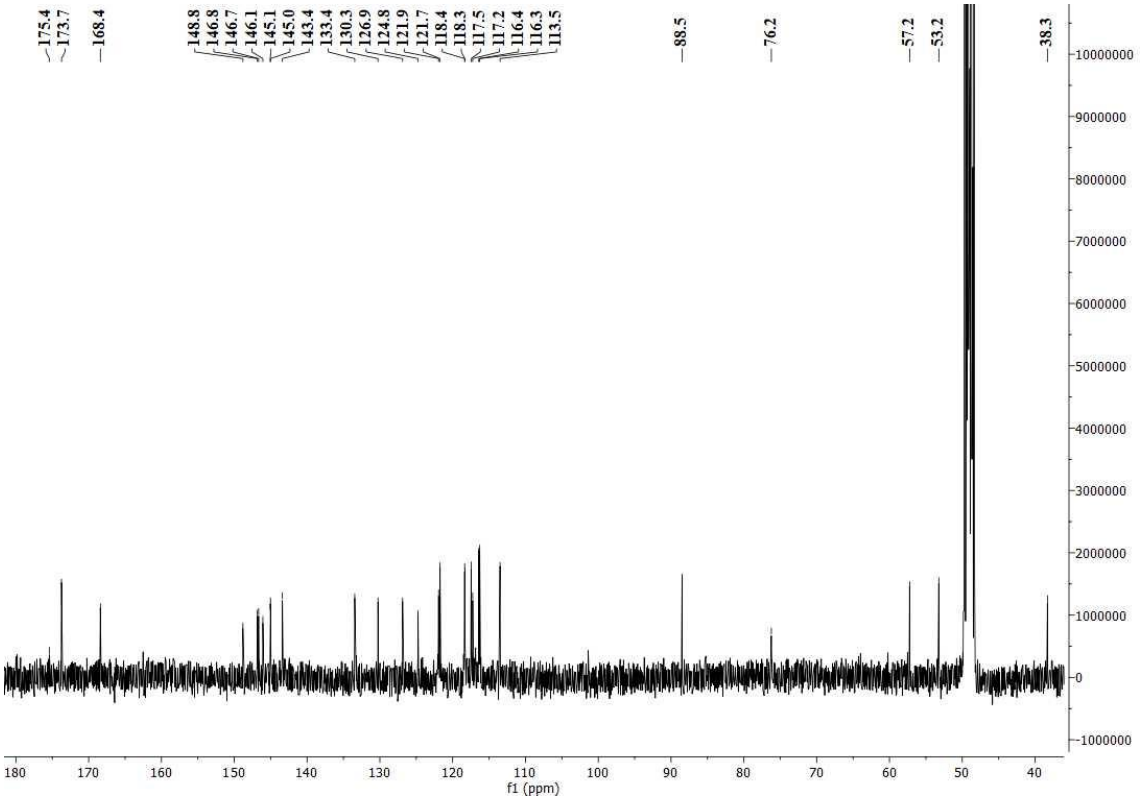

Figure S24. ^{13}C NMR spectrum (125 MHz, methanol-d_4) of compound **4**.

Table S3. NMR data obtained for compound **4** and comparison with literature

Pos.	Compound **4**		9´´-Methyl lithospermate (literature)[3]	
	δ_H[a,b] (*J* / Hz) / ppm	δ_C[a,c] / ppm	δ_H (*J* / Hz) / ppm	δ_C / ppm
1	–	124.8	–	124.7
2	–	126.9	–	127.1
3	–	148.8	–	149.0
4	–	145.2	–	145.4
5	6.80 (d, 1H, *J* 8.4)	118.3	6.81 (d, 1H, *J* 8.4)	118.5
6	7.16 (d, 1H, *J* 8.5)	121.9	7.19 (d, 1H, *J* 8.4)	122.1
7	7.70 (d, 1H, *J* 16.0)	143.4	7.72 (d, 1H, *J* 15.9)	144.0
8	6.28 (d, 1H, *J* 16.0)	117.2	6.30 (d, 1H, *J* 15.9)	116.8
9	–	168.4	–	168.3
1´	–	130.3	–	129.4
2´	6.74 (sl, 1H)	113.5	6.74 (sl, 1H)	113.6
3´	–	145.0	–	145.4
4´	–	146.1	–	146.3
5´	6.67 (d, 1H, *J* 8,1)	116.4	6.68 (d, 1H, *J* 8,1)	116.5
6´	6.71 (dd, 1H, *J* 2.1, 8.2)	118.4	6.68 (dd, 1H, *J* 2.1, 8.1)	118.5
7´	3.08 (dd, 1H, *J* 3.7, 14.1)	38.3	3.09 (dd, 1H, *J* 3.9, 14.4)	38.0
	2.95 (dd, 1H, *J* 9.2, 14.4)		2.99 (dd, 1H, *J* 8.7, 14.4)	
8´	5.14 (dd, *J* 3.7, 9.0)	76.2	5.19 (dd, *J* 3.9, 8.7)	75.0
9´	–	175.4	–	173.8

Table S3. NMR data obtained for compound **4** and comparison with literature (cont.)

Pos.	Compound **4**		9´´-Methyl lithospermate (literature)[3]	
	δ_H[a,b] (*J* / Hz) / ppm	δ_C[a,c] / ppm	δ_H (*J* / Hz) / ppm	δ_C / ppm
1´´	–	133.4	–	133.5
2´´	6.77 (d, 1H, *J* 2.1)	117.5	6.78 (d, 1H, *J* 1.8)	117,6
3´´	–	146.7	–	146.8
4´´	–	146.8	–	147.0
5´´	6.67 (d, 1H, *J* 8.1)	116.3	6.77 (d, 1H, *J* 8.1)	116.5
6´´	6.61 (dd, 1H, *J* 1.9, 8.1)	121.7	6.61 (dd, 1H, *J* 1.8, 8.1)	121.9
7´´	5.86 (d, 1H, *J* 4.8)	88.5	5.89 (d, 1H, *J* 4.8)	88.5
8´´	4.49 (d, 1H, *J* 4.8)	57.2	4.43 (d, 1H, *J* 4.8)	57.4
9´´	–	173.7	–	173.6
OCH_3	3.68 (s, 1H)	53.4	3.70 (s, 1H)	53.4

[a]Measured in CD_3OD, [b]125 MHz, [c]500 MHz.

Compound **5**

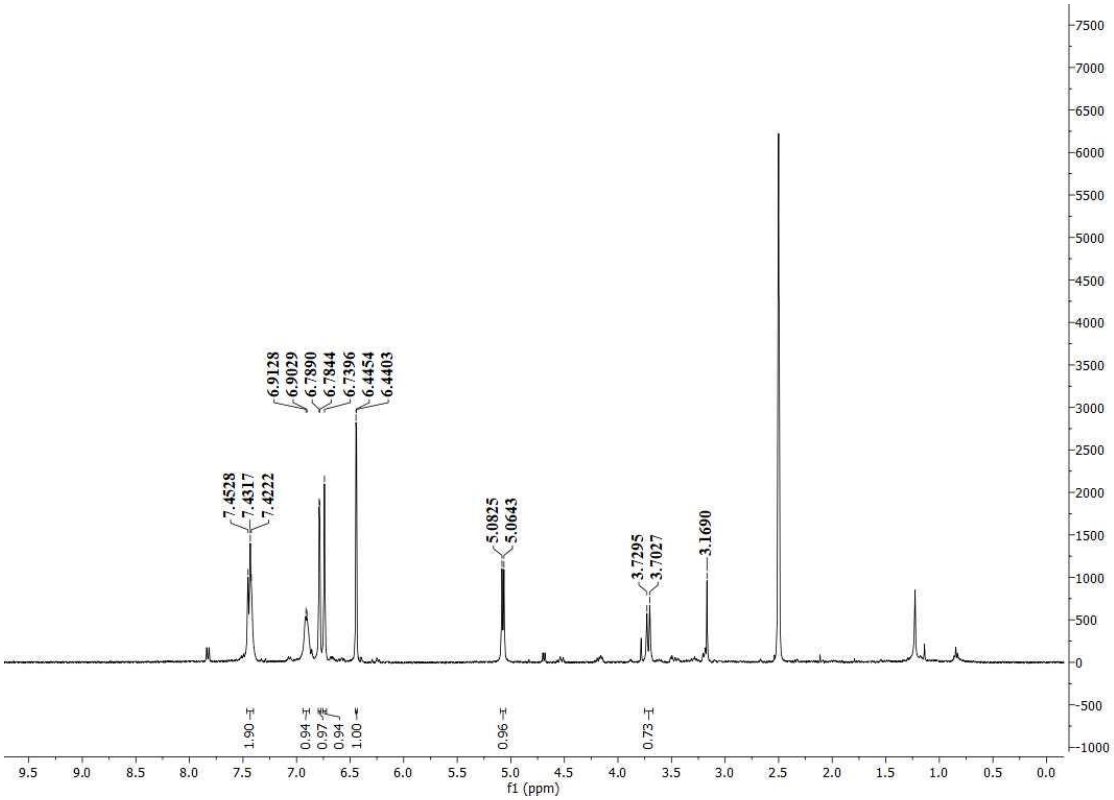

Figure S25. ^{1}H NMR spectrum (500 MHz, DMSO-d_6) of compound **5**.

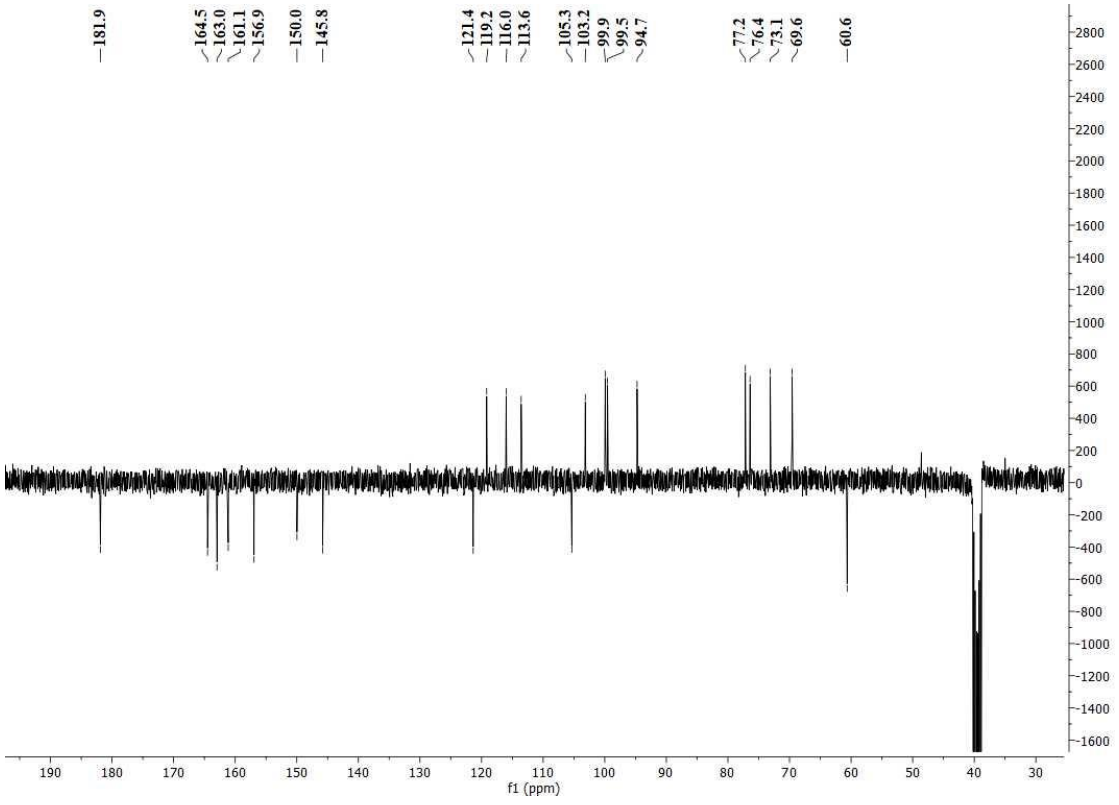

Figure S26. ^{13}C NMR spectrum (125 MHz, DMSO-d_6) of compound **5**.

Table S4. NMR data obtained for compound **5** and comparison with literature

Pos.	Compound **5**		Luteolin-7-*O*-glucoside (literature)[4]	
	δ_H[a,b] (*J* / Hz) / ppm	δ_C[a,c] / ppm	δ_H (*J* / Hz) / ppm	δ_C / ppm
2	–	164.5	–	164.6
3	6.73 (sl, 1H)	103.2	6.73 (s, 1H)	103.3
4	–	181.9	–	182.1
5	–	161.1	–	161.2
6	6.44 (d, 1H, *J* 2.0)	99.5	6.43 (d, 1H, *J* 2.0)	99.7
7	–	163.0	–	163.1
8	6.78 (d, 1H, *J* 1.8)	94.7	6.78 (d, 1H, *J* 2.0)	94.9
9	–	156.9	–	157.1
10	–	105.3	–	105.5
1´	–	121.4	–	121.5
2´	7.45 (m)	113.6	7.40 (d, 1H, *J* 2.0)	113.6
3´	–	145.8	–	145.9
4´	–	150.0	–	150.1
5´	6.90 (m)	116.0	6.89 (d, 1H, *J* 2.0)	116.1
6´	7.43 (m)	119.2	7.43 (dd, 1H, *J* 8.5, 2.0)	119.4
1´´	5.07 (d, 1H, *J* 7.3)	99.9	5.05 (d, 1H, *J* 7.5)	100.1
2´´	–	73.1	–	73.2
3´´	–	76.4	–	76.5
4´´	–	69.6	–	69.7

Table S4. NMR data obtained for compound **5** and comparison with literature (cont.)

Pos.	Compound **5**		Luteolin-7-*O*-glucoside (literature)[4]	
	δ_H[a,b] (*J* / Hz) / ppm	δ_C[a,c] / ppm	δ_H (*J* / Hz) / ppm	δ_C / ppm
5´´	–	77.2	–	77.3
6´´	–	60.6	–	60.8

[a]Measured in DMSO-d_6, [b]125 MHz, [c]500 MHz.

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