

Supporting information for

Antidiabetic Sterols from *Peniocereus greggii* Roots

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Table S1. Spectroscopic data of compounds **2–5** in CDCl₃ (400 MHz for ¹H NMR and 100 MHz for ¹³C NMR).

No.	2		3		4		5	
	¹³ C	¹ H (<i>J</i> in Hz)	¹³ C	¹ H (<i>J</i> in Hz)	¹³ C	¹ H (<i>J</i> in Hz)	¹³ C	¹ H (<i>J</i> in Hz)
1	35.4	1.73 m	36.8	1.33 m; 1.83 m	30.3	1.95 m; 2.15 m	28.9	2.01 m
2	31.0	1.83 m	30.4	1.84 m; 2.20 m	30.7	1.30 m; 1.82 m	30.3	1.88 m
3	71.2	3.58 dd (10.6, 4.8)	70.8	3.61 d (10.8, 4.1)	70.3	3.63 d (11.2, 4.4)	70.2	3.63 d (11.2, 5.6)
4	32.0	2.20 m	30.9	1.41 m	29.7	1.35 m; 2.05 m	30.2	1.39 m; 2.23 m
5	47.8	1.35 m	53.3	2.23 m	44.7	2.82 d (12.3, 3.8)	46.8	3.13 d (12.3, 3.8)
6	67.6	3.71 m	199.7	/	199.2	/	201.5	/
7	37.8	2.45 dd (17.1, 6.6)	123.1	5.73 s	123.9	5.67 s	124.1	5.87 s
8	126.6	/	163.9	/	160.9	/	158.1	/
9	135.2	/	50.1	2.13 m	74.0	/	74.3	/
10	37.7	/	38.2	/	41.9	/	42.5	/
11	22.8	2.07 m	21.9	1.64 m; 1.78 m	28.0	1.40 m; 2.05 m	28.0	1.74 m; 1.99 m
12	36.0	1.32 m	30.3	1.41 m; 1.83 m	28.0	1.70 m; 1.99 m	27.8	2.12 m
13	42.1	/	44.5	/	46.5	/	46.5	/
14	51.6	2.06 m	55.6	2.0 dd (12.0, 4.1)	51.9	2.5 ddd (11.7, 6.8, 2.2)	50.4	1.93 m
15	23.8	1.13 m	22.6	1.48 m; 1.61 m	23.8	1.52 m; 1.64 m	26.3	1.43 m; 2.01 m
16	28.9	1.29 m	38.8	1.30 m; 2.13 m	35.3	1.40 m	31.7	1.58 m; 1.96 m
17	54.9	1.14 m	56.2	1.29 m	56.2	1.40 m	86.8	/
18	11.3	0.59 s	12.2	0.58 s	11.8	0.62 s	16.1	0.71 s
19	18.9	0.96 s	13.2	0.96 s	16.8	0.98 s	16.6	0.95 s
20	36.7	1.38 m	35.9	1.38 m	35.9	1.42 m	35.6	1.44 m
21	18.7	0.90 d (6.5)	18.8	0.94 d (6.5)	18.8	0.94 d (5.6)	18.9	0.95 d (6.0)
22	36.2	0.98 m	35.9	1.01 m; 1.35 m	35.9	1.35 m; 1.50 m	36.2	1.06 m; 1.38 m
23	23.8	1.58 m	23.8	1.32 m	22.8	1.20 m; 1.40 m	23.9	1.06 m; 1.38 m
24	39.6	1.11 m	39.4	1.11 m	39.4	1.16 m	39.4	1.13 m
25	28.1	1.49 m	27.9	1.50 m	28.6	1.54 m	28.0	1.52 m
26	22.7	0.84 d (6.5)	22.5	0.84 d (6.5)	22.5	0.86 d (6.5)	22.5	0.81 d (6.5)
27	23.0	0.85 d (6.5)	22.8	0.86 d (6.5)	22.6	0.88 d (6.5)	22.8	0.88 d (6.5)

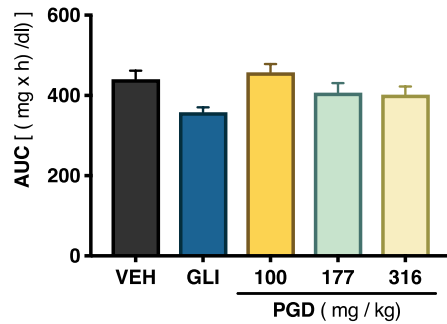
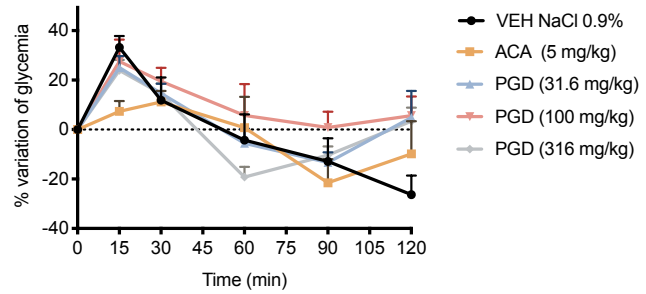
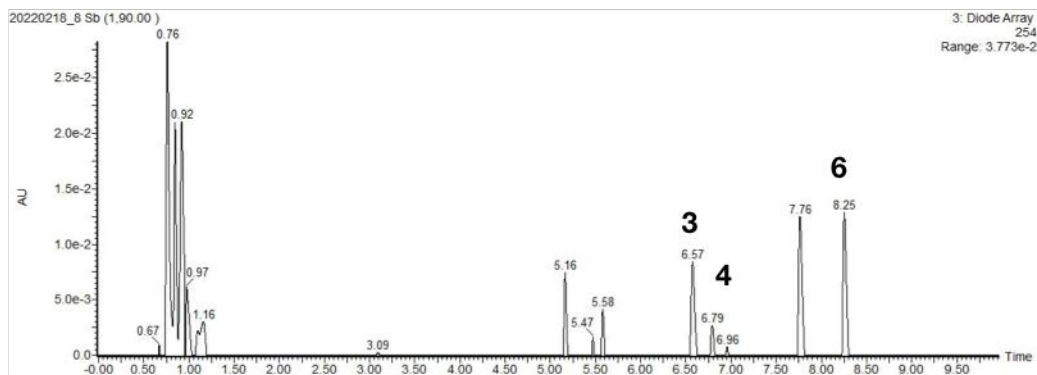
A**B**

Figure S1. Effect of PGD on glucose level on hypoglycemic (A) and OSTT (B) experiments in normoglycemic mice. AUC: area under the curve; VEH: vehicle; GLI: glibenclamide (10 mg/kg); ACA: acarbose (5 mg/kg). Data are expressed as mean \pm SEM ($n = 6$). * $p < 0.05$ and ** $p < 0.01$ significantly different. ANOVA followed by Dunnett *post hoc* test for comparison with respect to vehicle control.

A)



B)

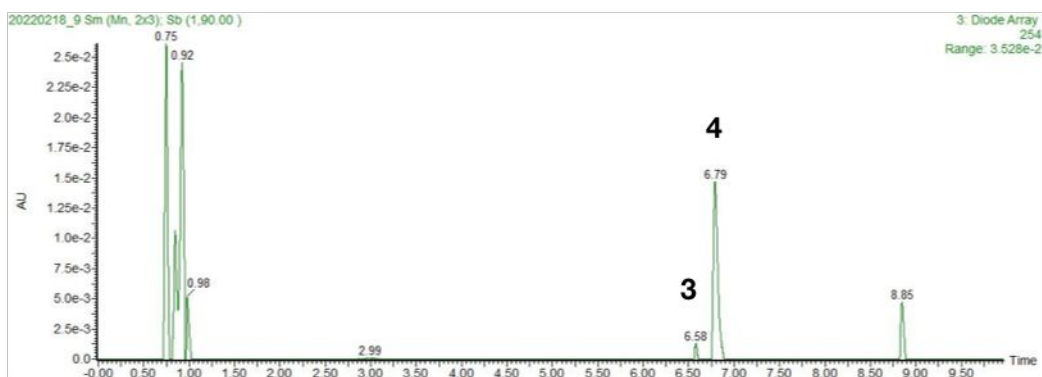


Figure S2. LC chromatograms of the CHCl_3 extracts (CE1; A) and (CE2; B). The elution program was as follows: 0 min, 50% A; 1.0 min 50% A; 3.0 min 85% A; 5.0 min 90% A; 7.0 min 100% A; 9.0 min 100% A; 9.10 min 50% A; 11.0 min 50% A (mobile phase consisting of 50% methanol (A) and water adjusted to pH 2.8 with formic acid (FA; B)). Flow rate: 0.3 mL/min; Injection volume: 3 μL .

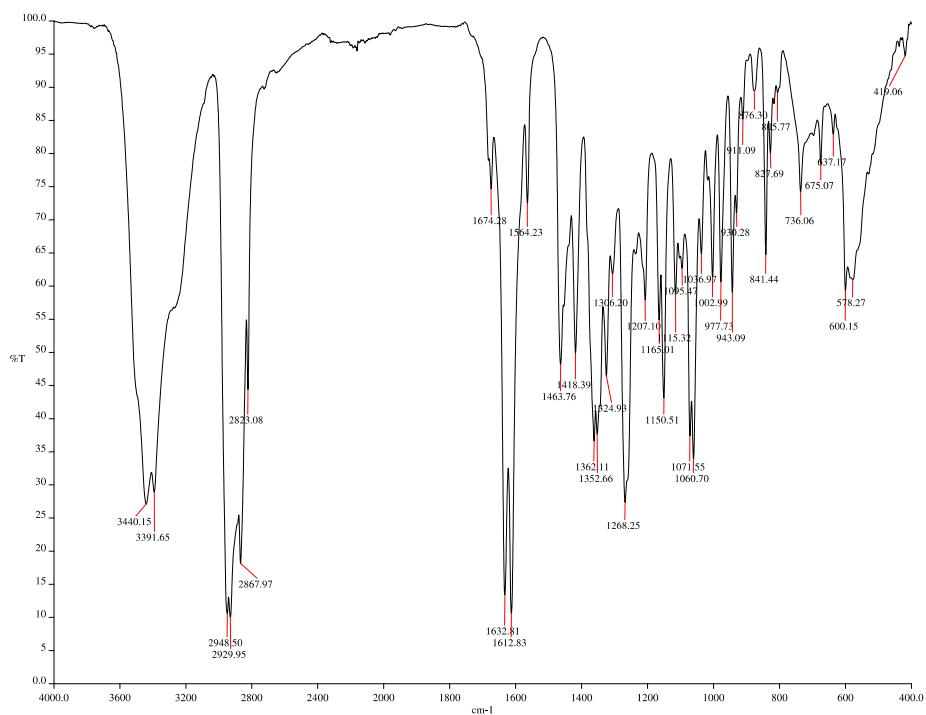


Figure S3. FTIR spectrum by ATR of compound (6)

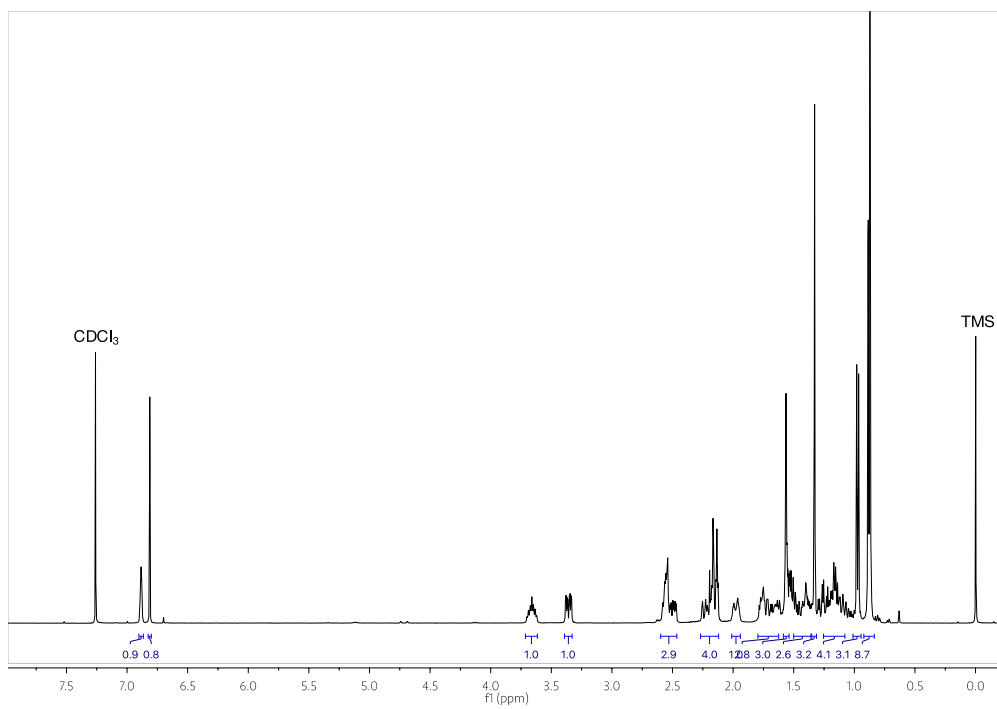


Figure S4. ¹H NMR spectrum of compound 6 in CDCl₃

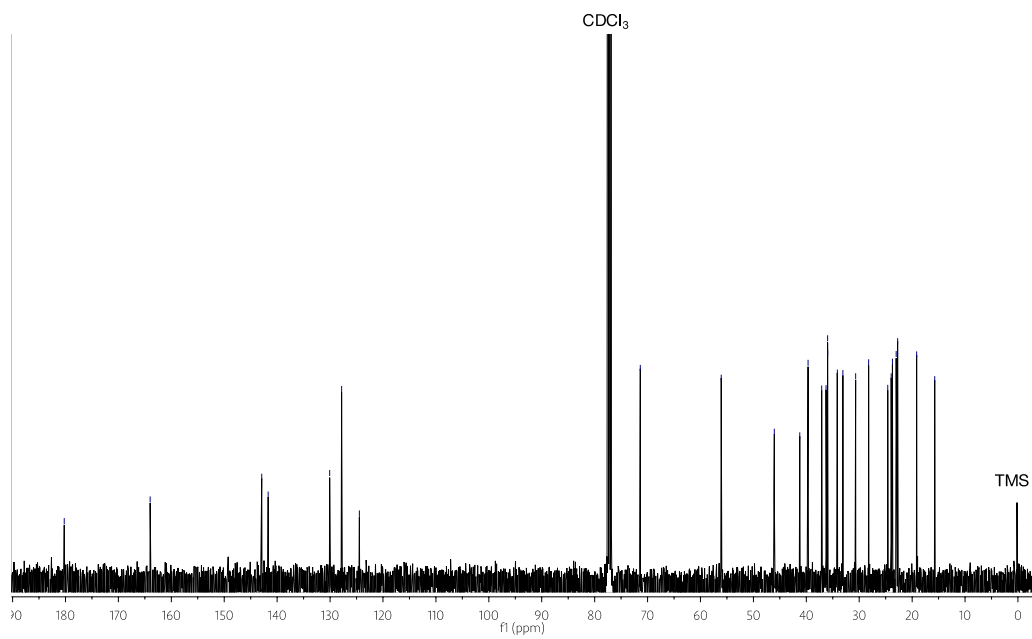


Figure S5. ^{13}C NMR spectrum of compound **6** in CDCl_3

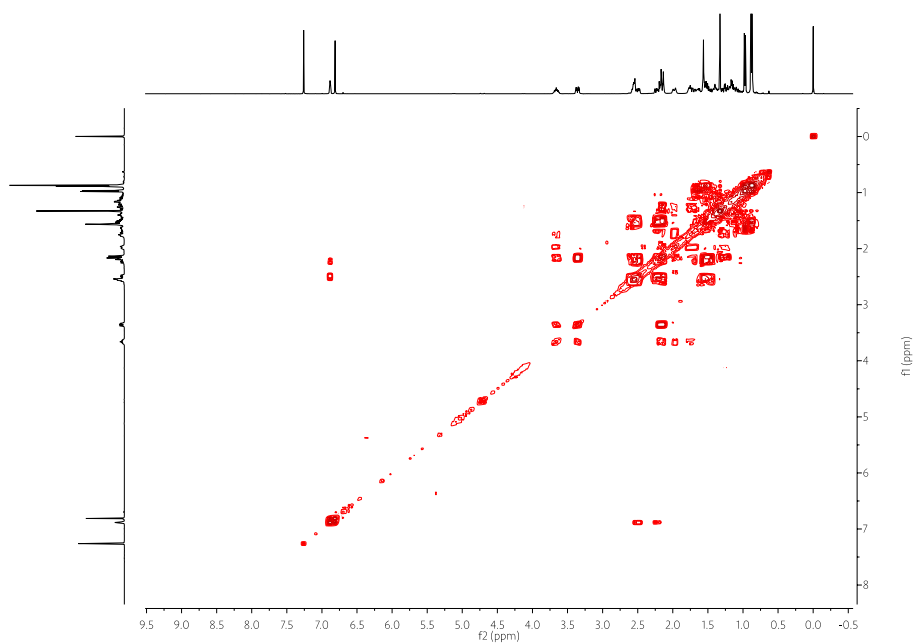


Figure S6. COSY spectrum of compound **6** in CDCl_3

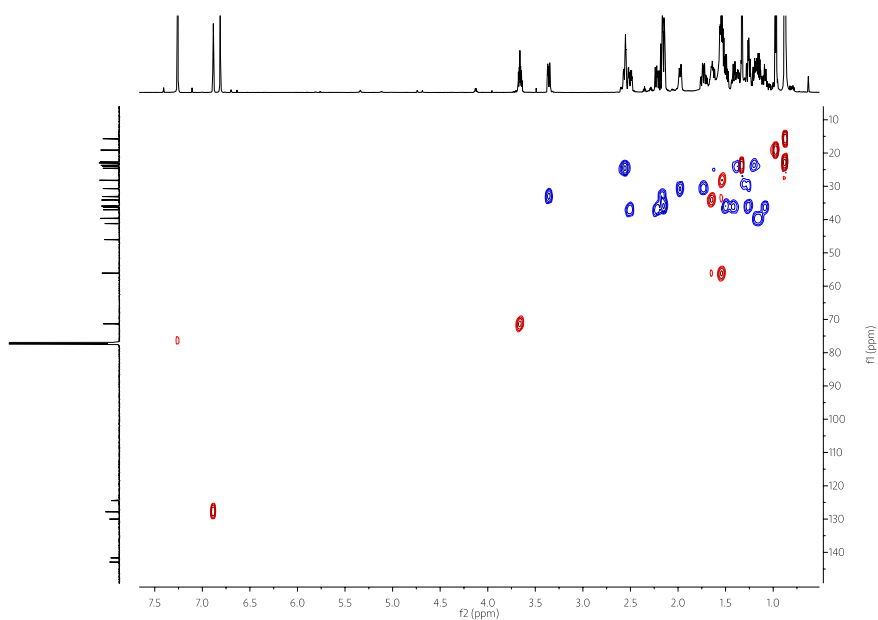


Figure S7. HSQC spectrum of compound **6** in CDCl_3

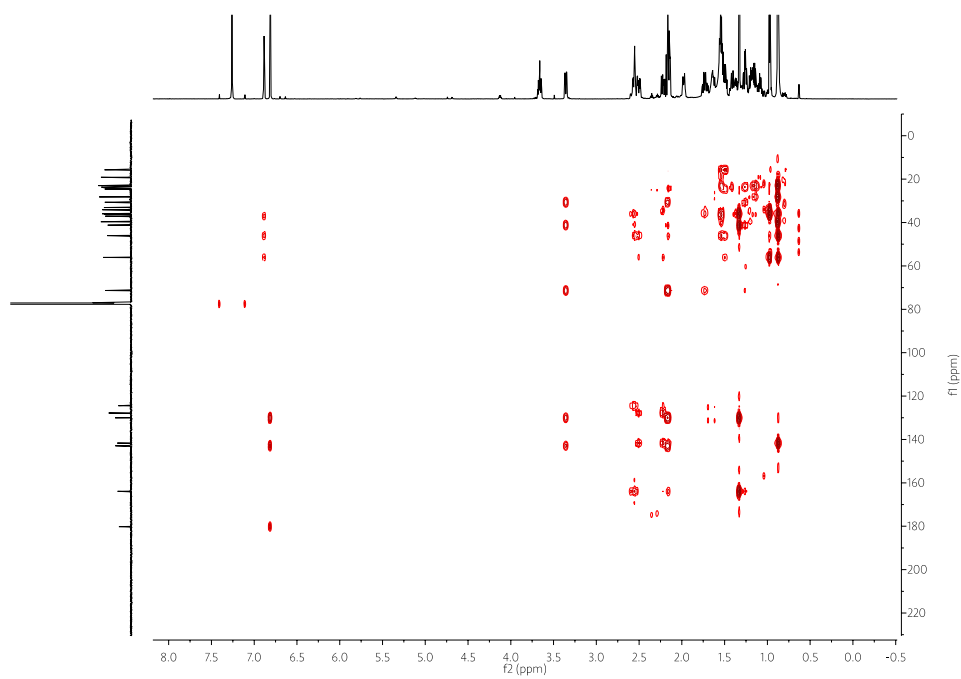


Figure S8. HMBC spectrum of compound **6** in CDCl_3

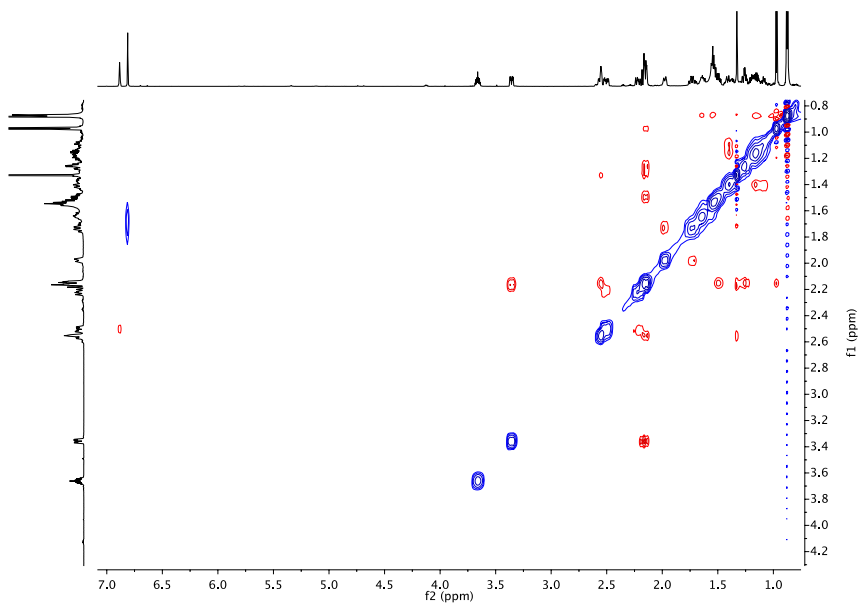


Figure S9. NOESY spectrum of compound **6** in CDCl_3

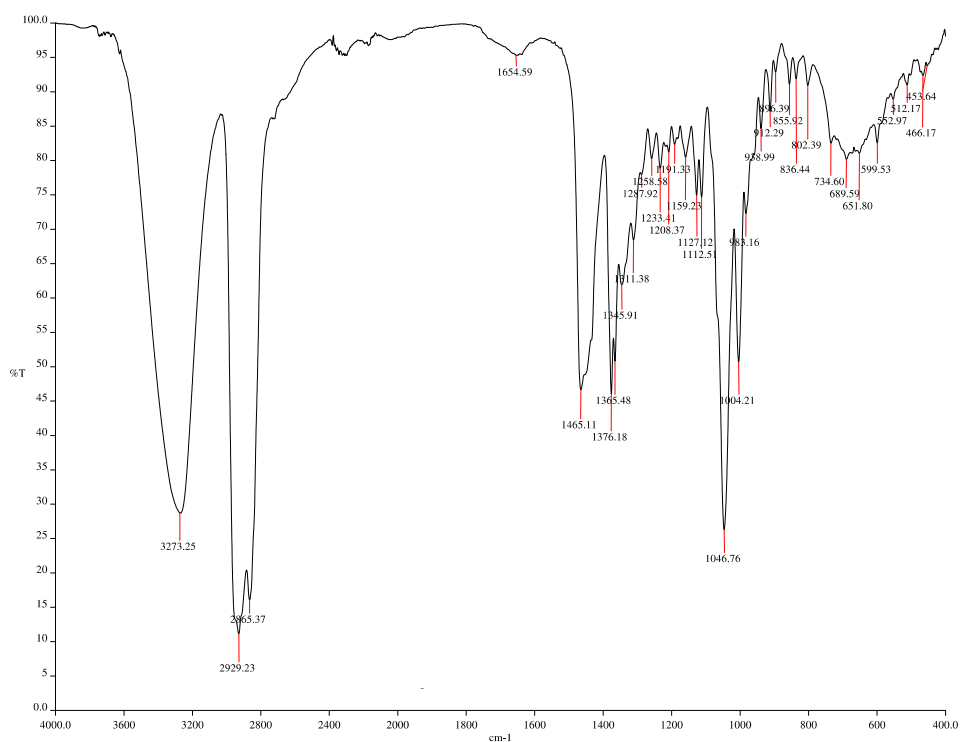


Figure S10. FTIR spectrum by ATR of peniocerol (**2**)

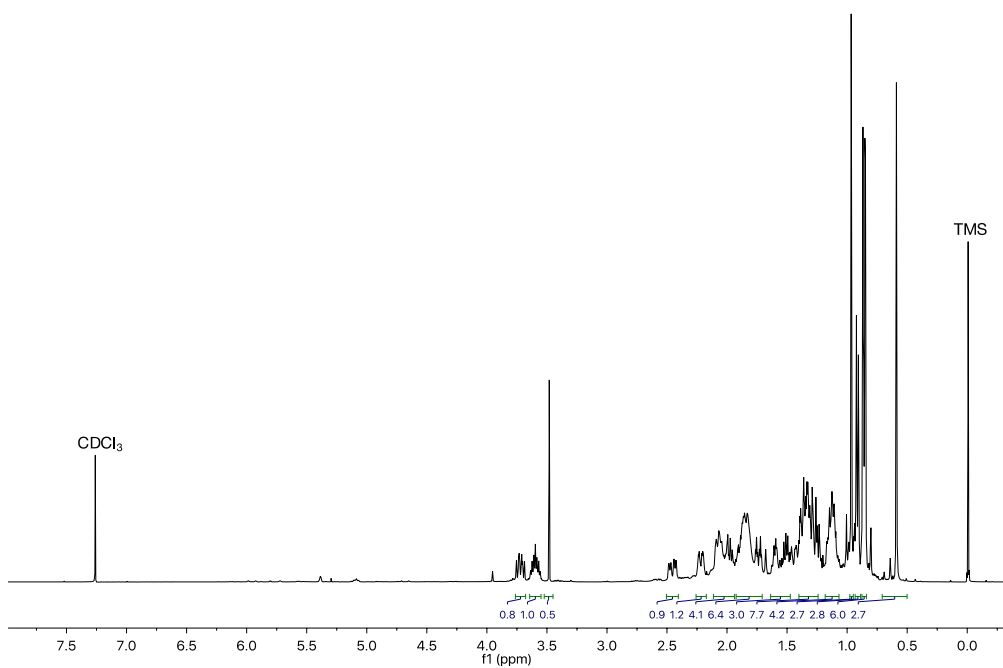


Figure S11. ^1H NMR spectrum of peniocerol (**2**) in CDCl_3

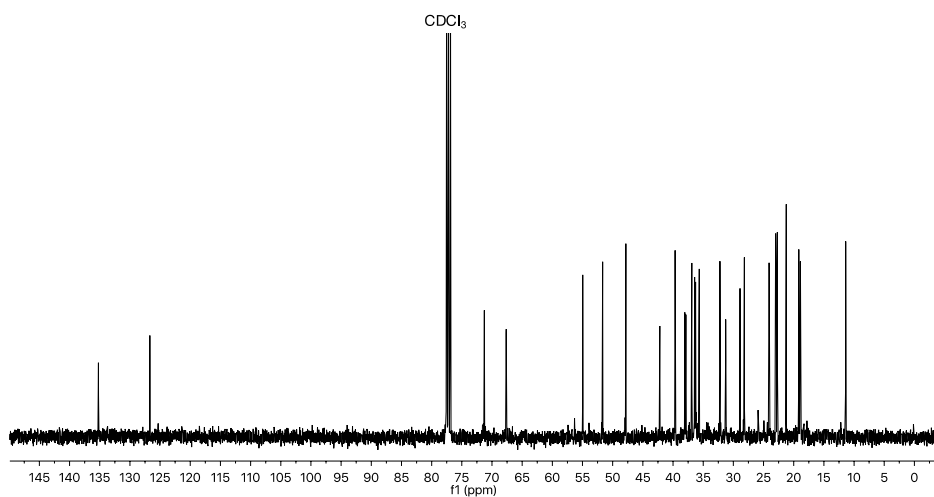


Figure S12. ^{13}C NMR spectrum of peniocerol (**2**) in CDCl_3

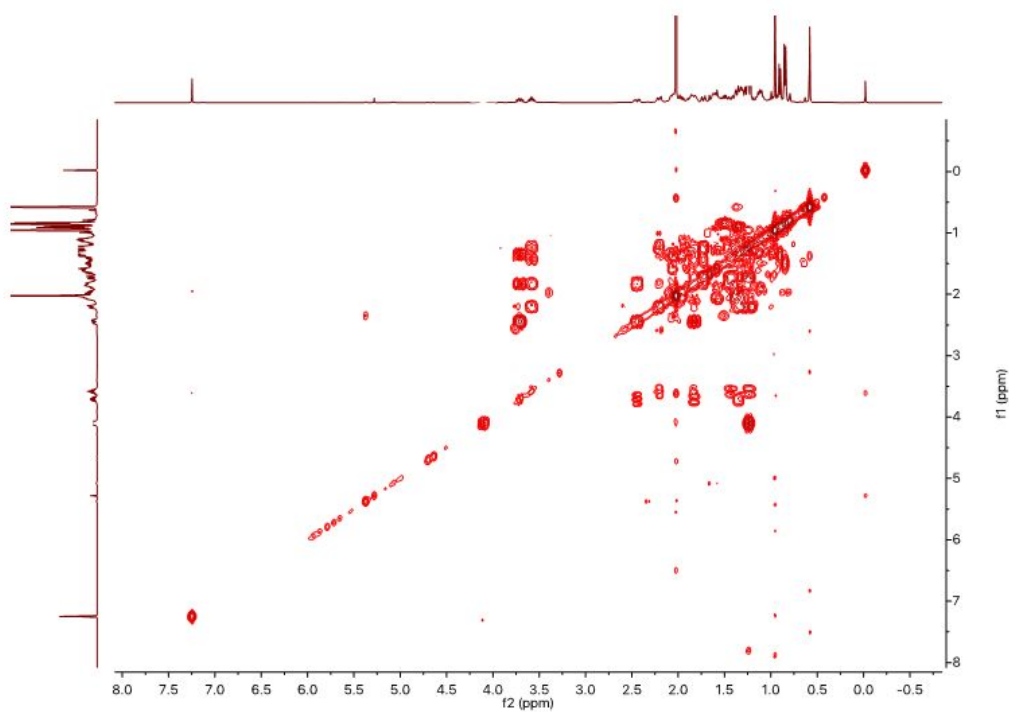


Figure S13. COSY spectrum of peniocerol (**2**) in CDCl_3

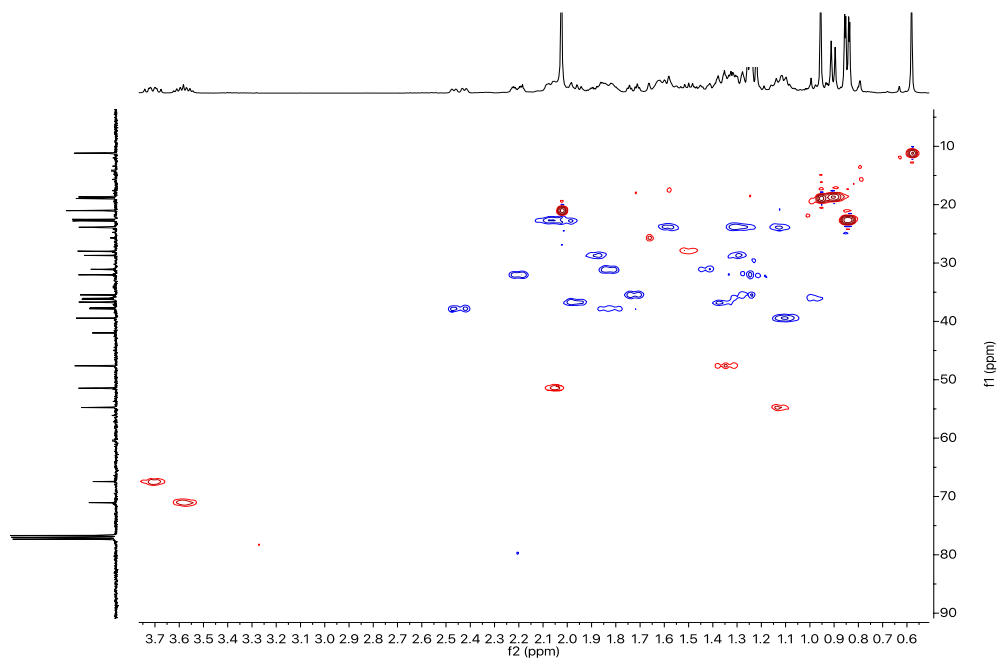


Figure S14. HSQC spectrum of peniocerol (**2**) in CDCl_3

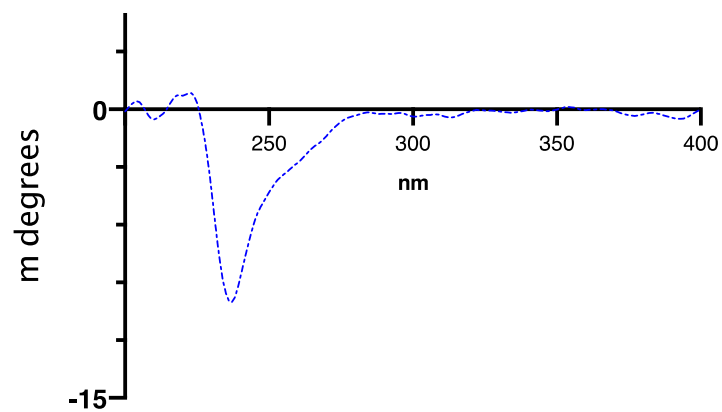


Figure S15. ECD spectrum of peniocerol (**2**) in CDCl_3

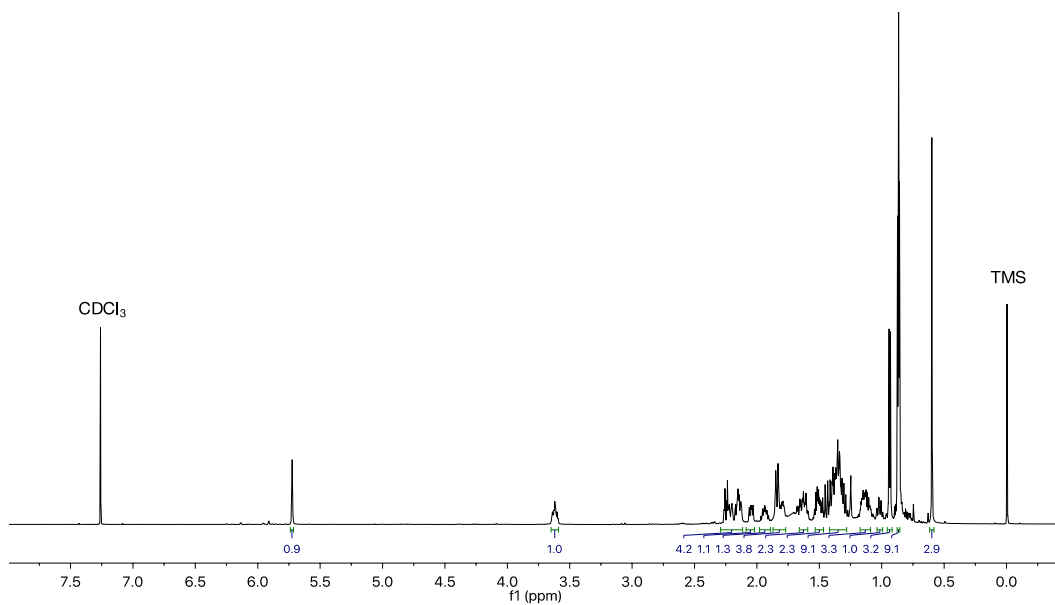


Figure S16. ^1H NMR spectrum of desoxyviperidone (**3**) in CDCl_3

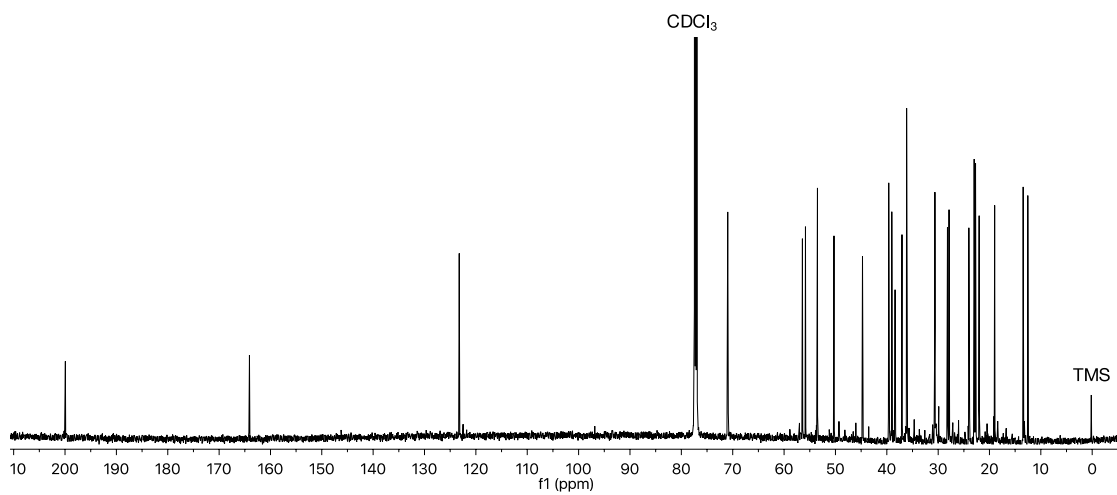


Figure S17. ^{13}C NMR spectrum of desoxyviperidone (**3**) in CDCl_3

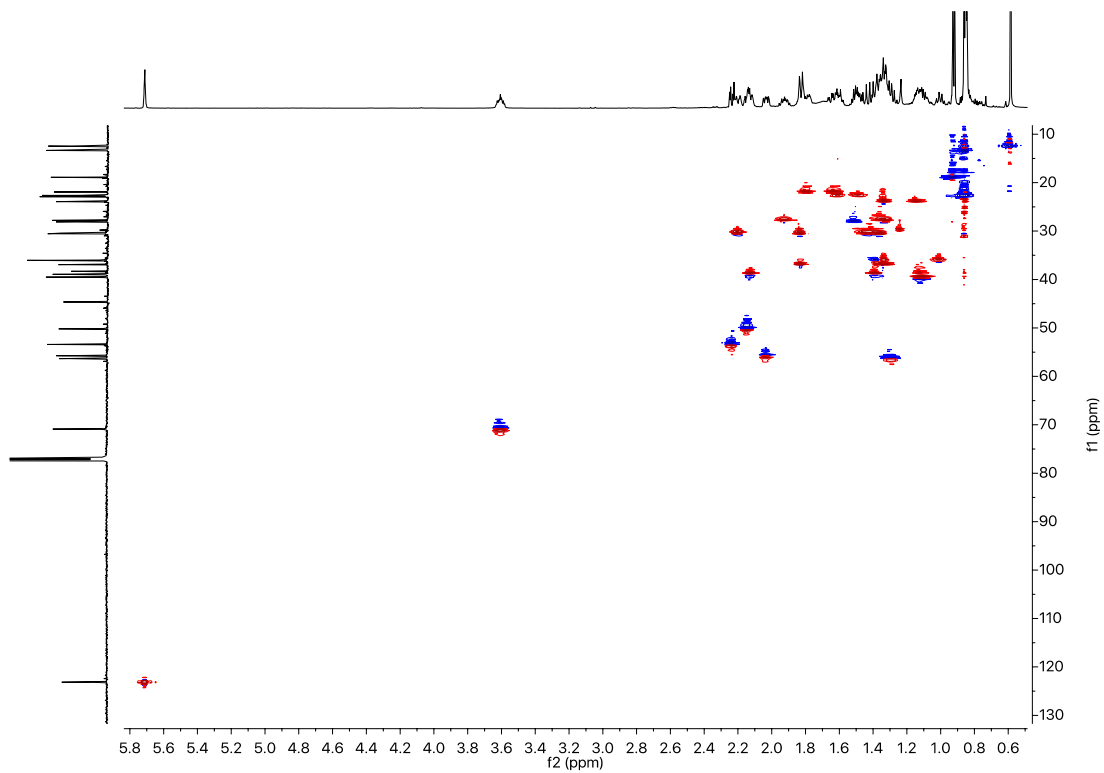


Figure S18. HSQC NMR spectrum of desoxyviperidone (**3**) in CDCl_3

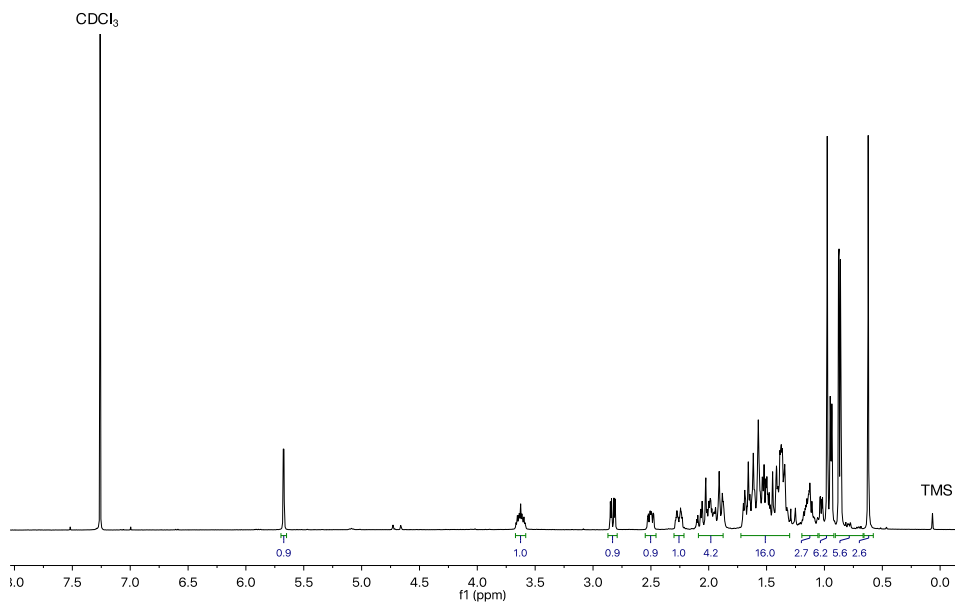


Figure S19. ^1H NMR spectrum of viperidone (**4**) in CDCl_3

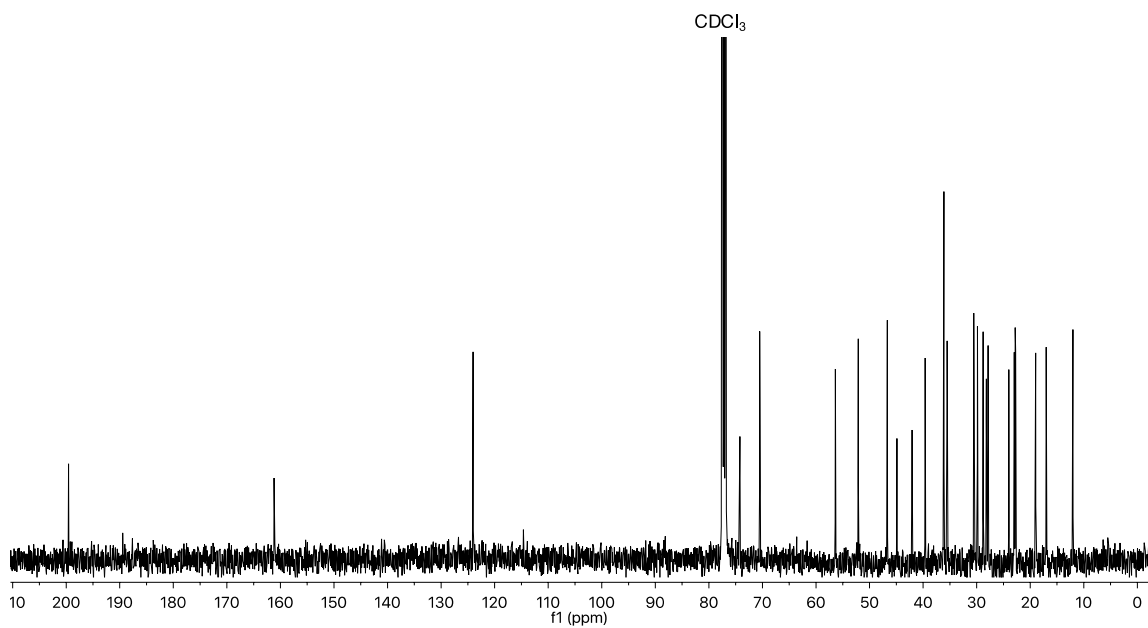


Figure S20. ^{13}C NMR spectrum of viperidone (4) in CDCl_3

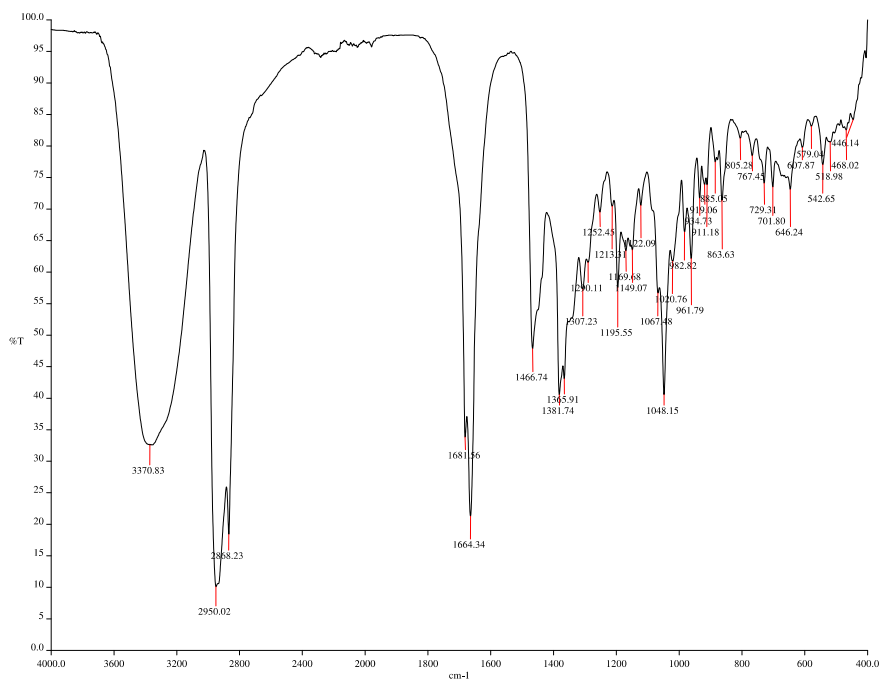


Figure S21. FTIR spectrum by ATR of viperidinone (5)

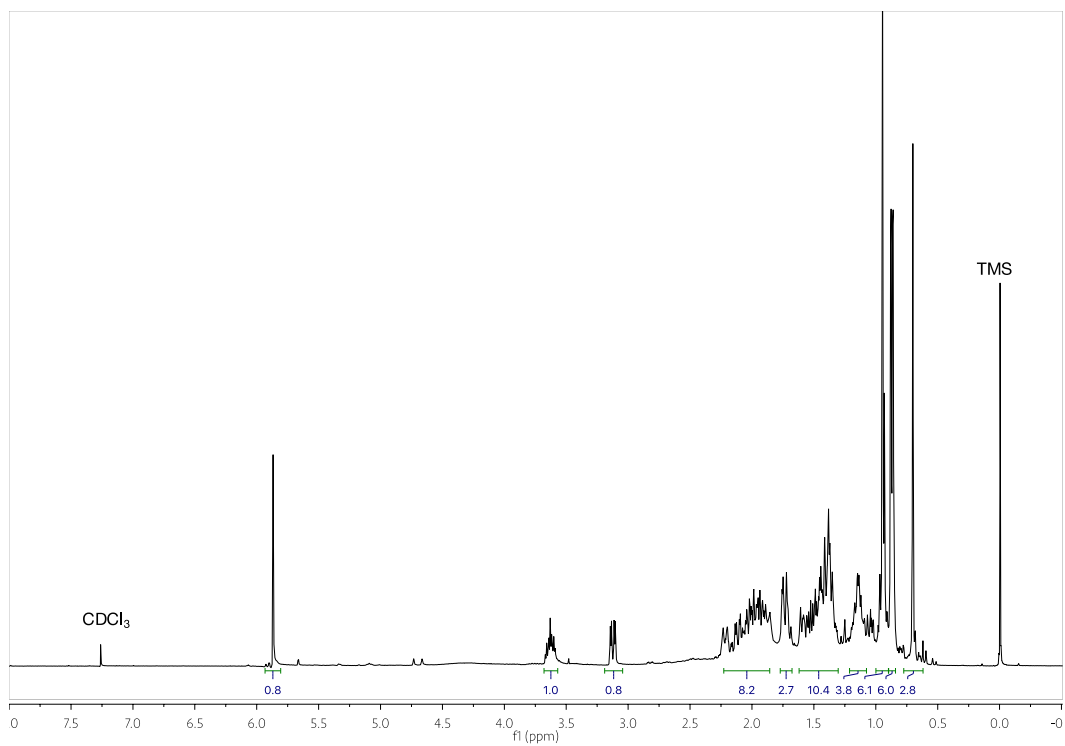


Figure S22. ¹H NMR spectrum of viperidinone (**5**) in CDCl₃

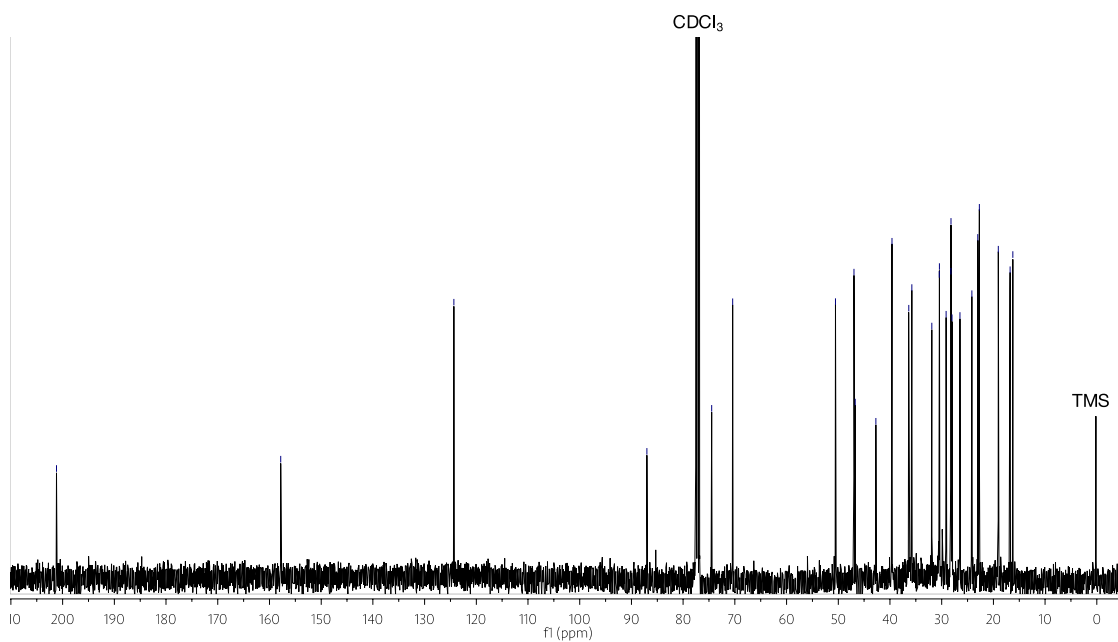


Figure S23. ¹³C NMR spectrum of viperidinone (**5**) in CDCl₃

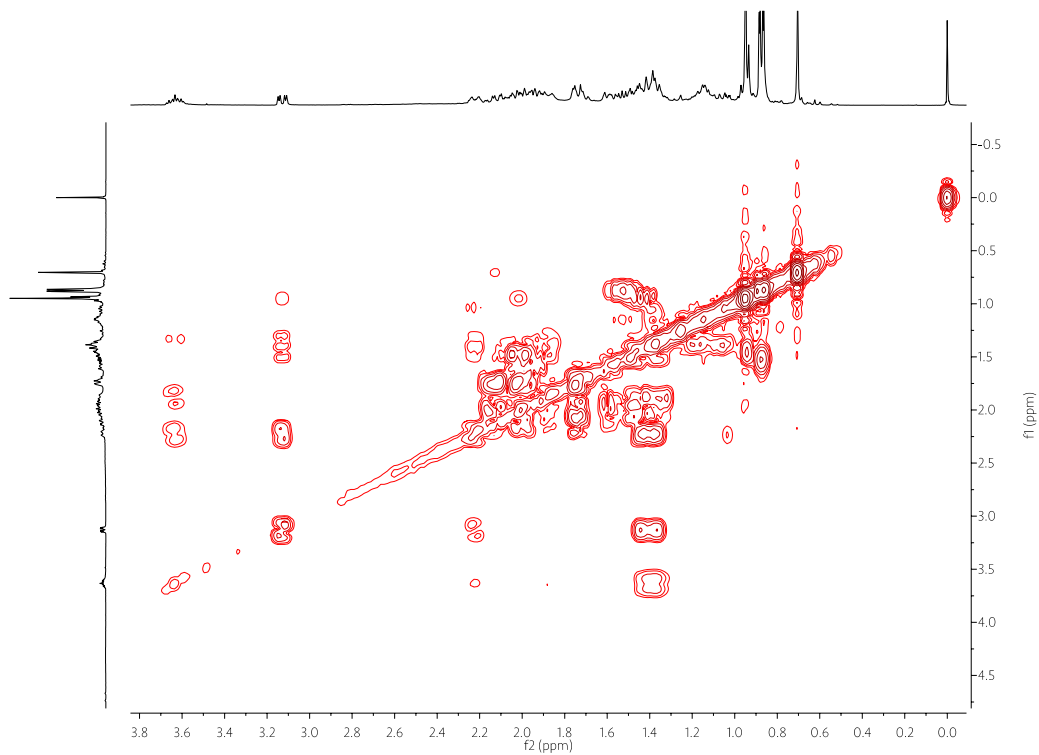


Figure S24. COSY NMR spectrum of viperidinone (**5**) in CDCl_3

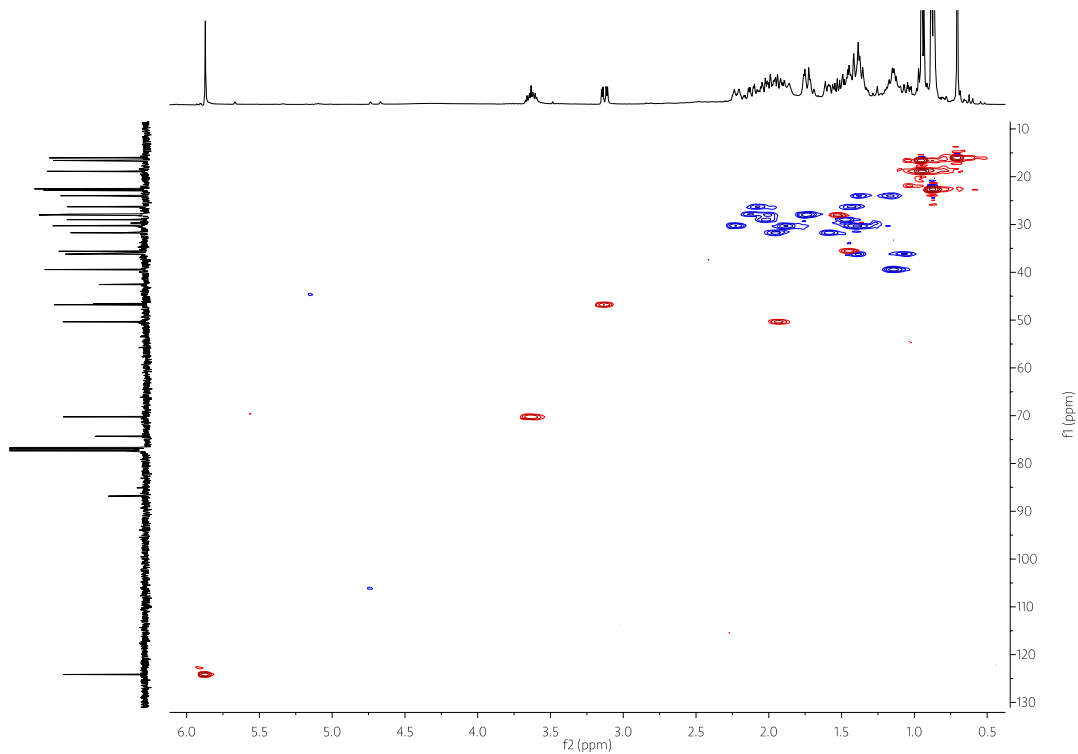


Figure S25. HSQC NMR spectrum of viperidinone (**5**) in CDCl_3

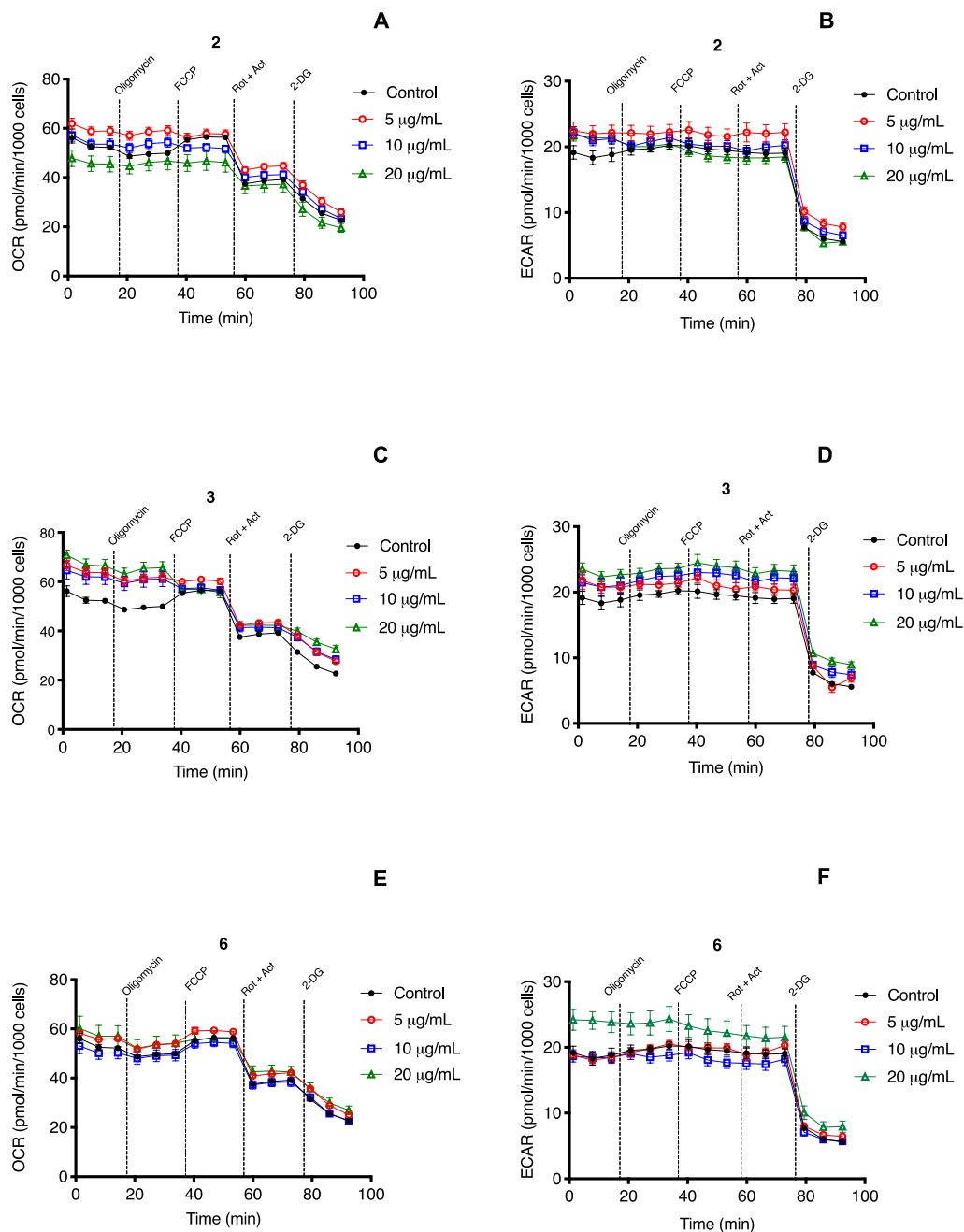


Figure S26. Oxygen consumption rate (A, C and E) and extracellular acidification rate (B, D and F) in mouse myoblast cells C2C12 for compounds **2**, **3** and **6**. Each point represents the mean \pm SEM of three independent experiments. *** $p < 0.01$ and **** $p < 0.0001$ significantly different. ANOVA followed by Tukey *post hoc* test for comparison with respect to control.

Table S2. Linearity, Sensitivity, Precision and Accuracy for **3** and **4**

	3	4
Calibration curve equation		
UV detection	$y = 11339.72x - 15272.90$	$y = 151541.56x - 17617.53$
MS detection	$y = 2811132.97x - 440840.39$	$y = 3229290.07x - 743236.71$
Correlation coefficient (R^2)		
UV detection	0.9935	0.9963
MS detection	0.9915	0.9950
LOD ($\mu\text{g/mL}$)		
UV detection	0.6	1.81
MS detection	1.18	3.60
LOQ ($\mu\text{g/mL}$)		
UV detection	1.03	3.13
MS detection	1.17	3.53
Precision (RSD %)		
Intra-day		
UV detection	1.9	0.4
MS detection	1.1	0.3
Inter-day		
UV detection	0.5	0.9
MS detection	1.1	0.7
Recovery (%)		
UV detection	98.8–101.1	100.3–100.4
MS detection	99.5–100.4	100.4–100.6

Table S3. Quantification of **3** and **4** (Batches I-IV) from *P. greggii* using the method validated.

Sample (Batch)	Mean content (mg/g)			
	3		4	
	UV detection	APCI ⁺ detection	UV detection	APCI ⁺ detection
I	68.0 ± 1.5	52.0 ± 0.4	225.3 ± 1.2	248.0 ± 0.7
II	21.3 ± 1.4	12.0 ± 0.2	128.0 ± 1.1	116.0 ± 0.3
III	33.3 ± 1.6	21.3 ± 0.2	168.0 ± 1.2	153.3 ± 0.4
IV	36.0 ± 1.4	22.7 ± 0.3	177.3 ± 1.2	170.1 ± 0.3