

Article

# New terpendole congeners, inhibitors of sterol O-acyltransferase, produced by *Volutella citrinella* BF-0440

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**Table S1:** <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts of terpendole O (**2**) in CDCl<sub>3</sub>.

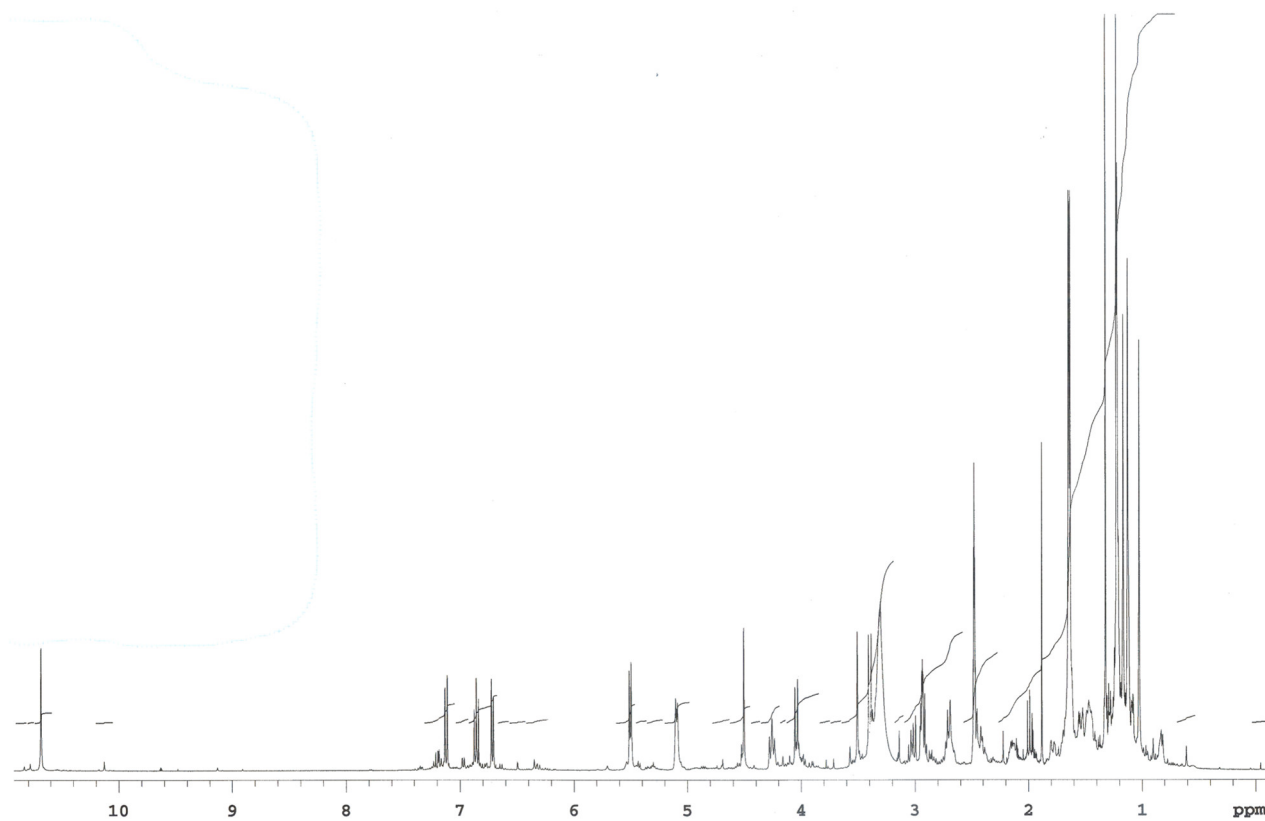


Figure S1. <sup>1</sup>H-NMR spectrum of terpendole O (2) in DMSO-*d*<sub>6</sub>.

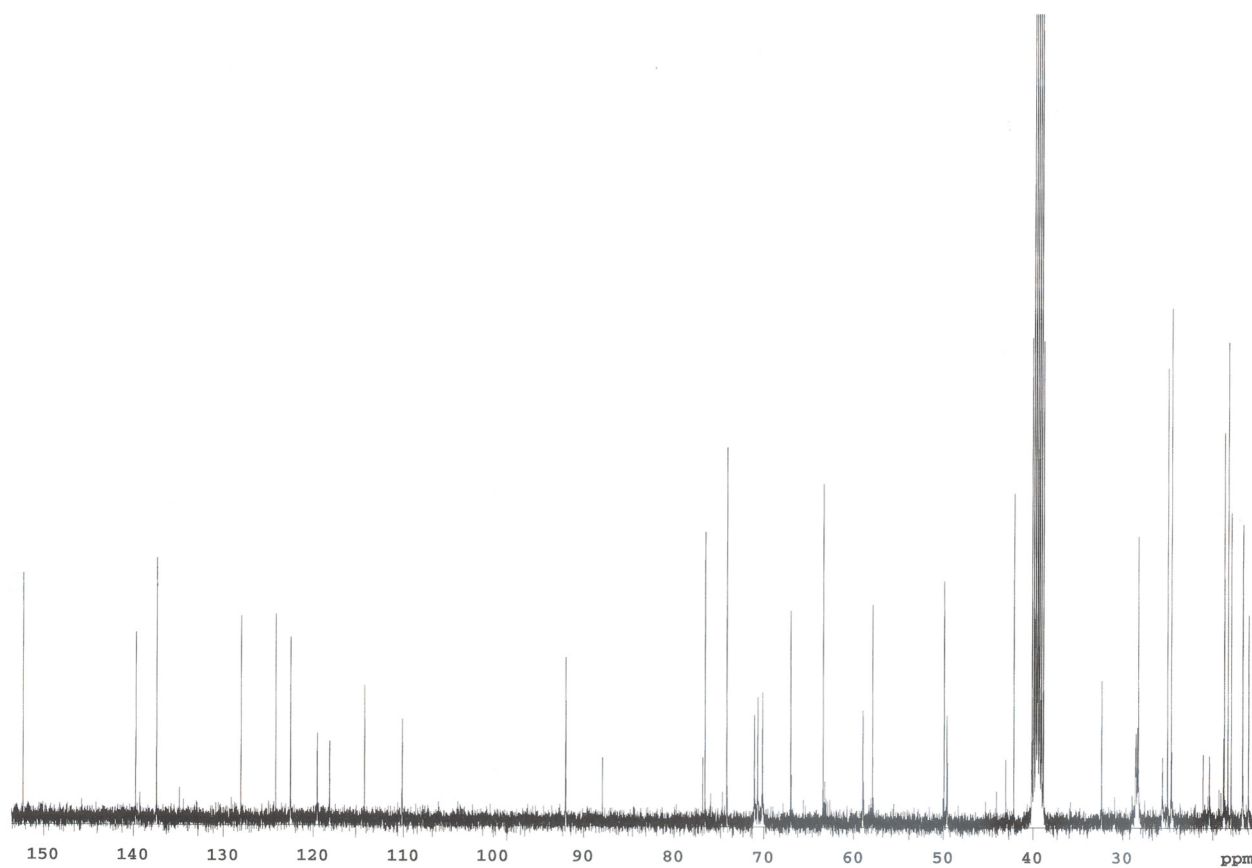


Figure S2. <sup>13</sup>C-NMR spectrum of terpendole O (2) in DMSO-*d*<sub>6</sub>.

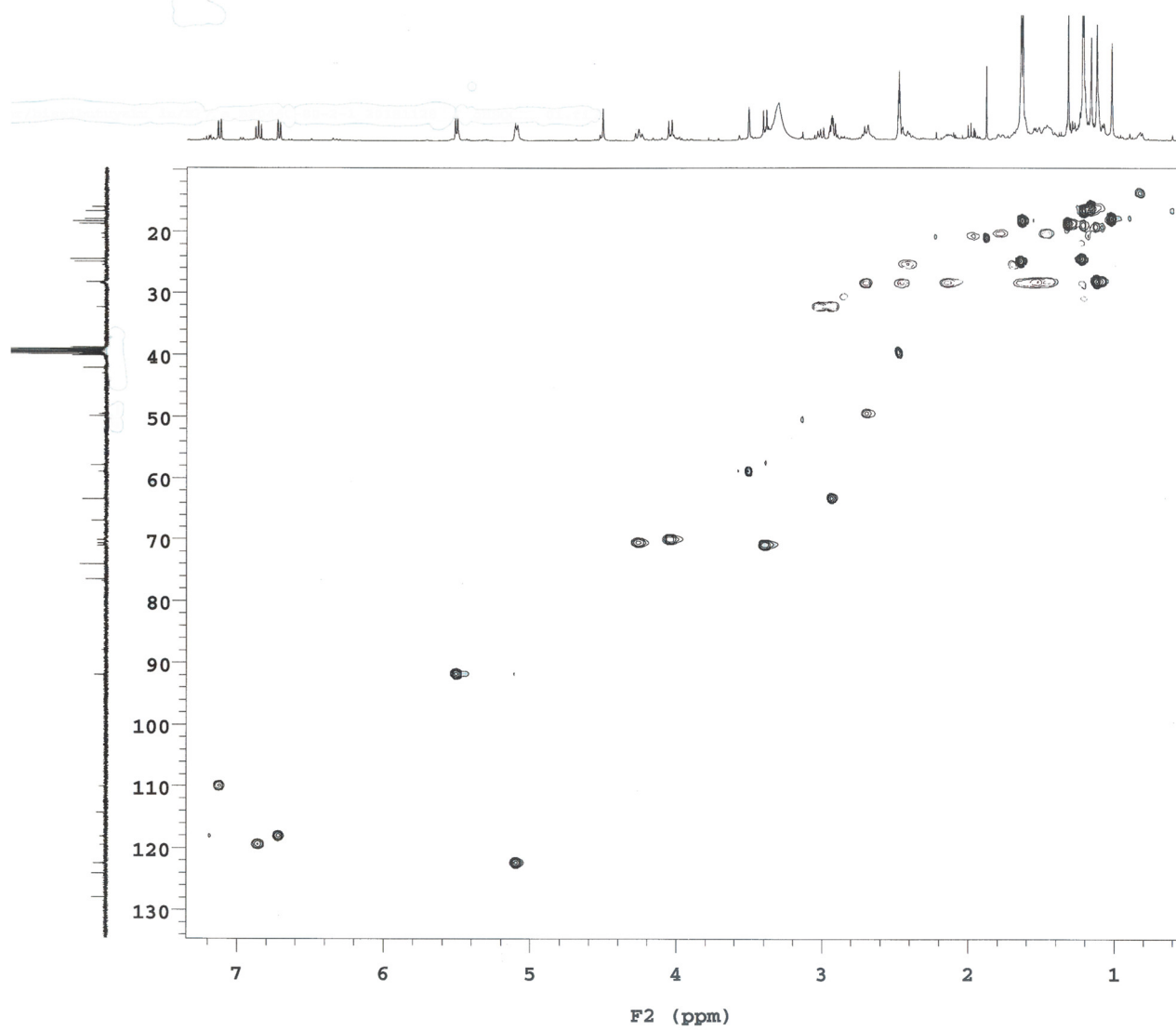


Figure S3. HSQC spectrum of terpendole O (2) in DMSO-*d*<sub>6</sub>.

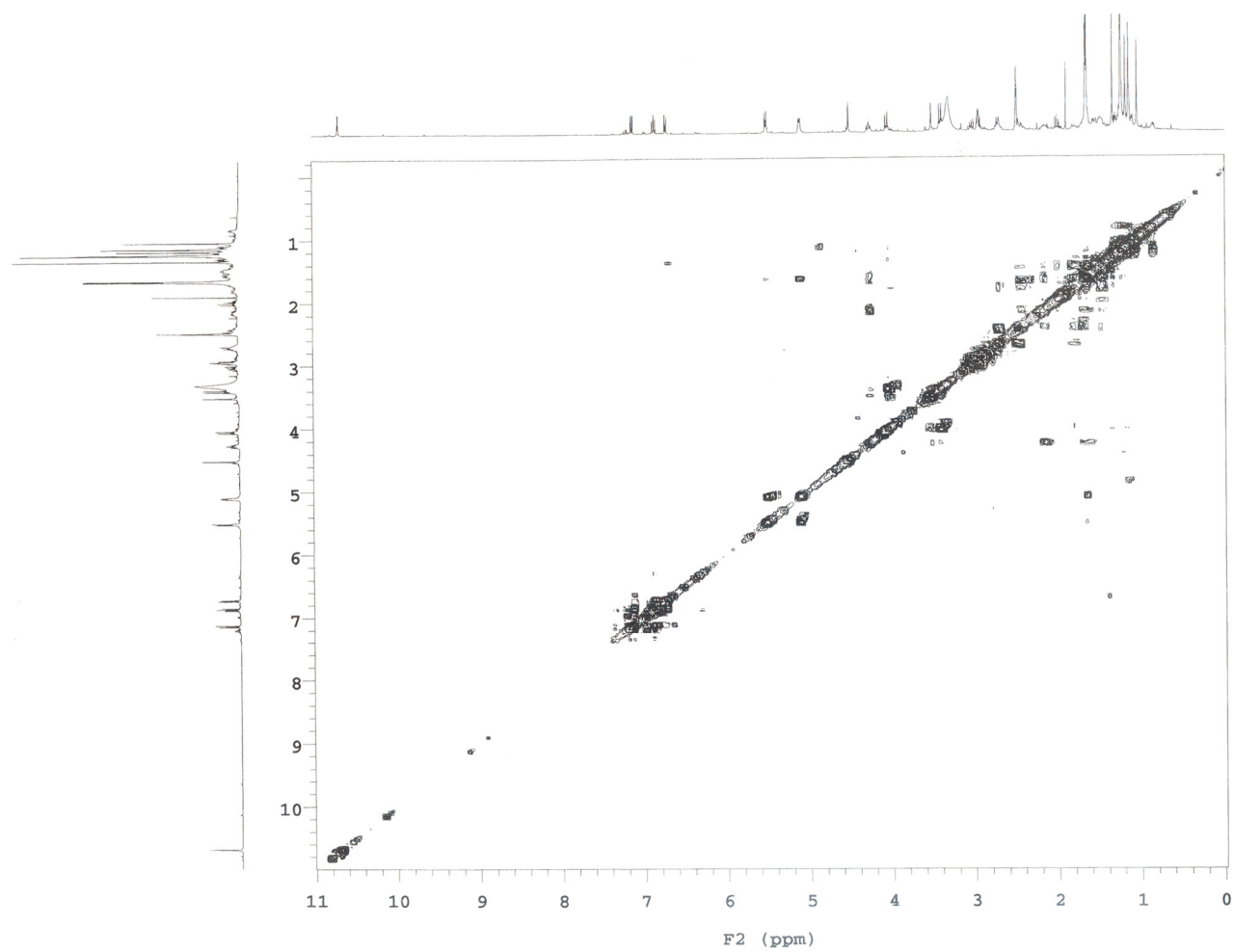


Figure S4.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of terpendole O (**2**) in  $\text{DMSO-}d_6$ .

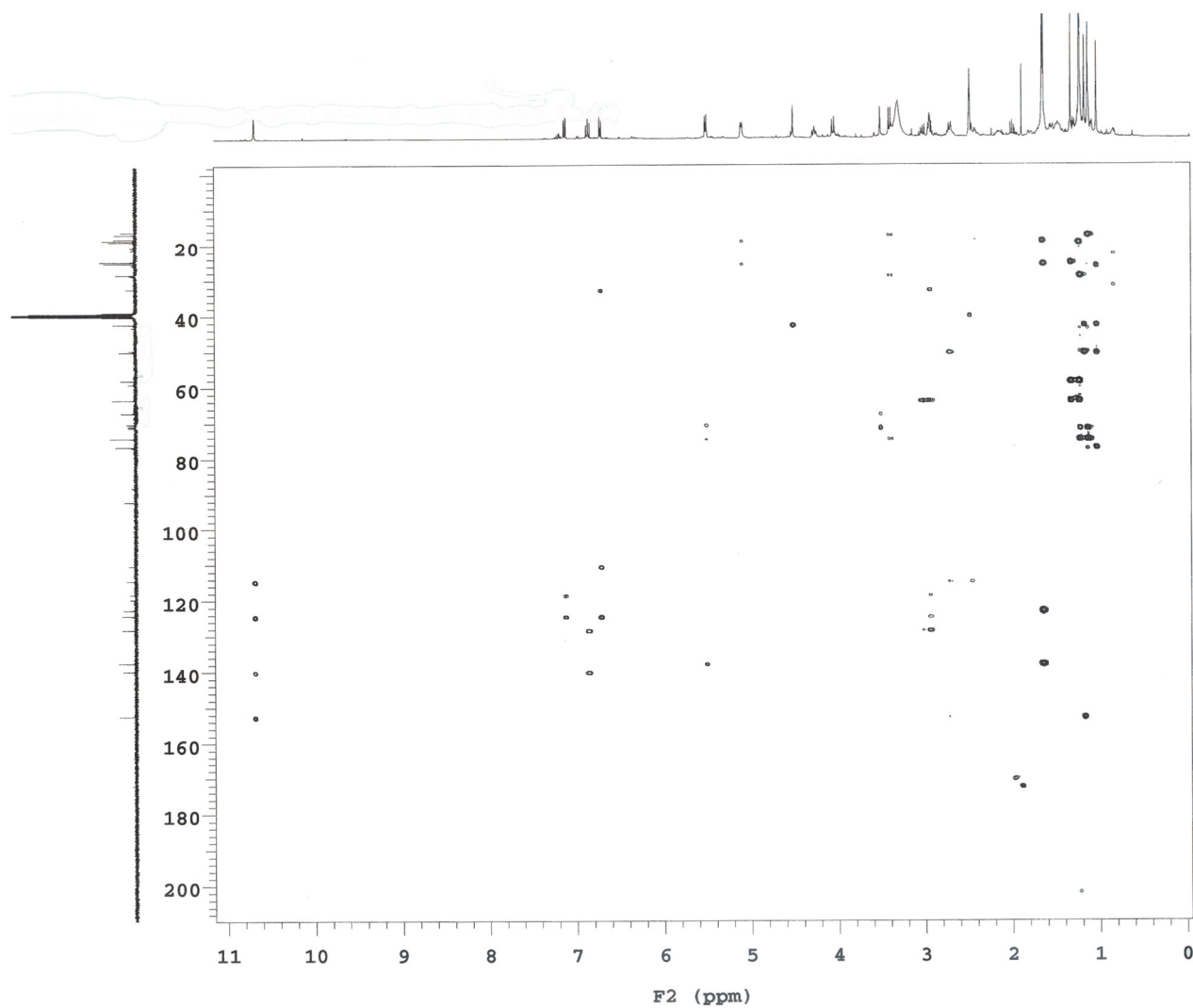


Figure S5. HMBC spectrum of terpendole O (2) in DMSO-*d*<sub>6</sub>.

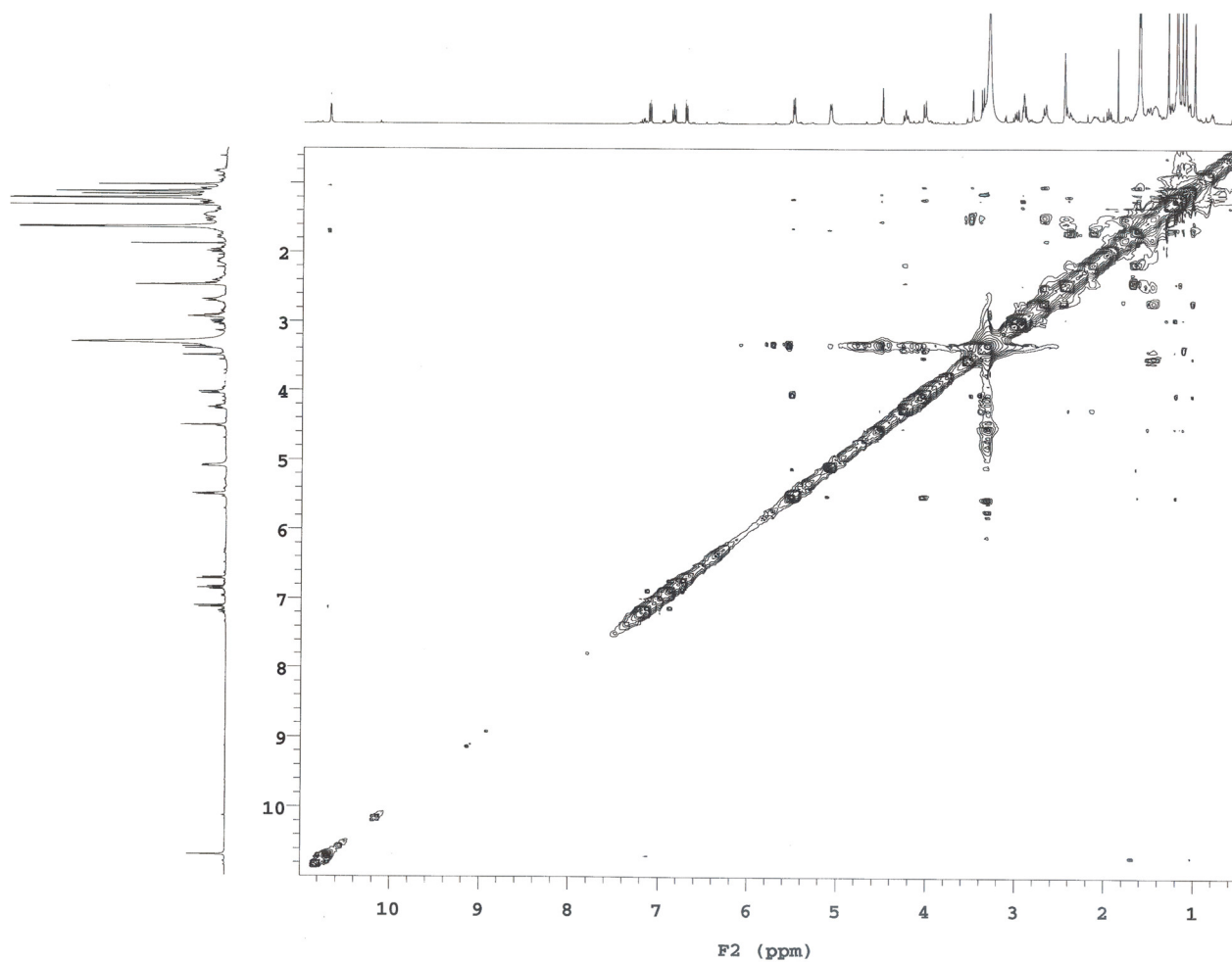


Figure S6. NOESY spectrum of terpendole O (**2**) in DMSO-*d*<sub>6</sub>.

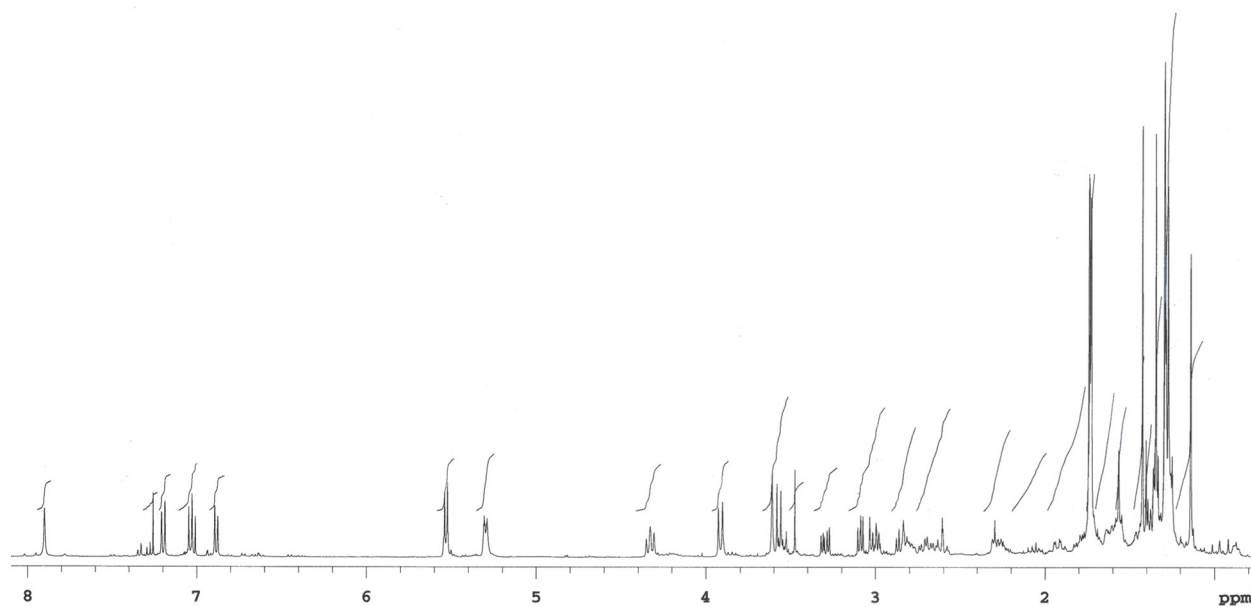


Figure S7. <sup>1</sup>H-NMR spectrum of terpendole O (2) in CDCl<sub>3</sub>.

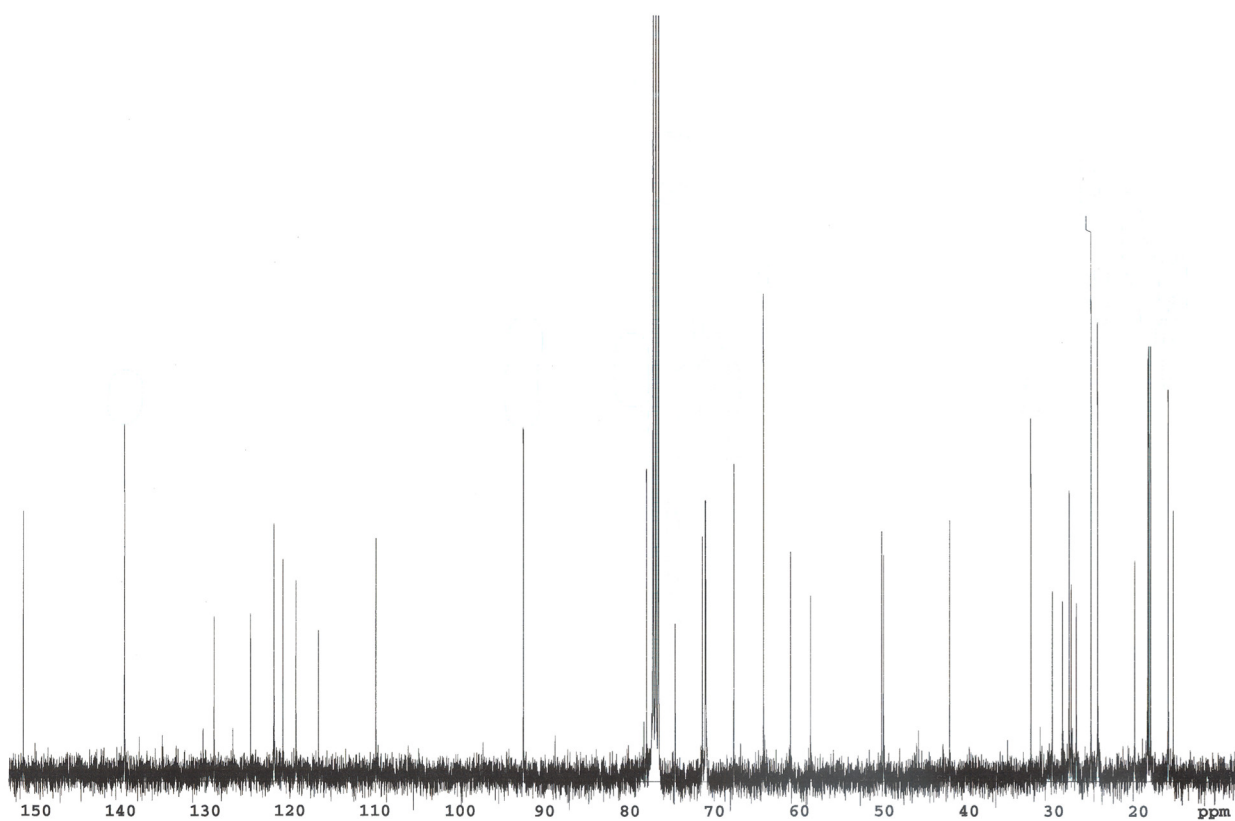


Figure S8. <sup>13</sup>C-NMR spectrum of terpendole O (2) in CDCl<sub>3</sub>.

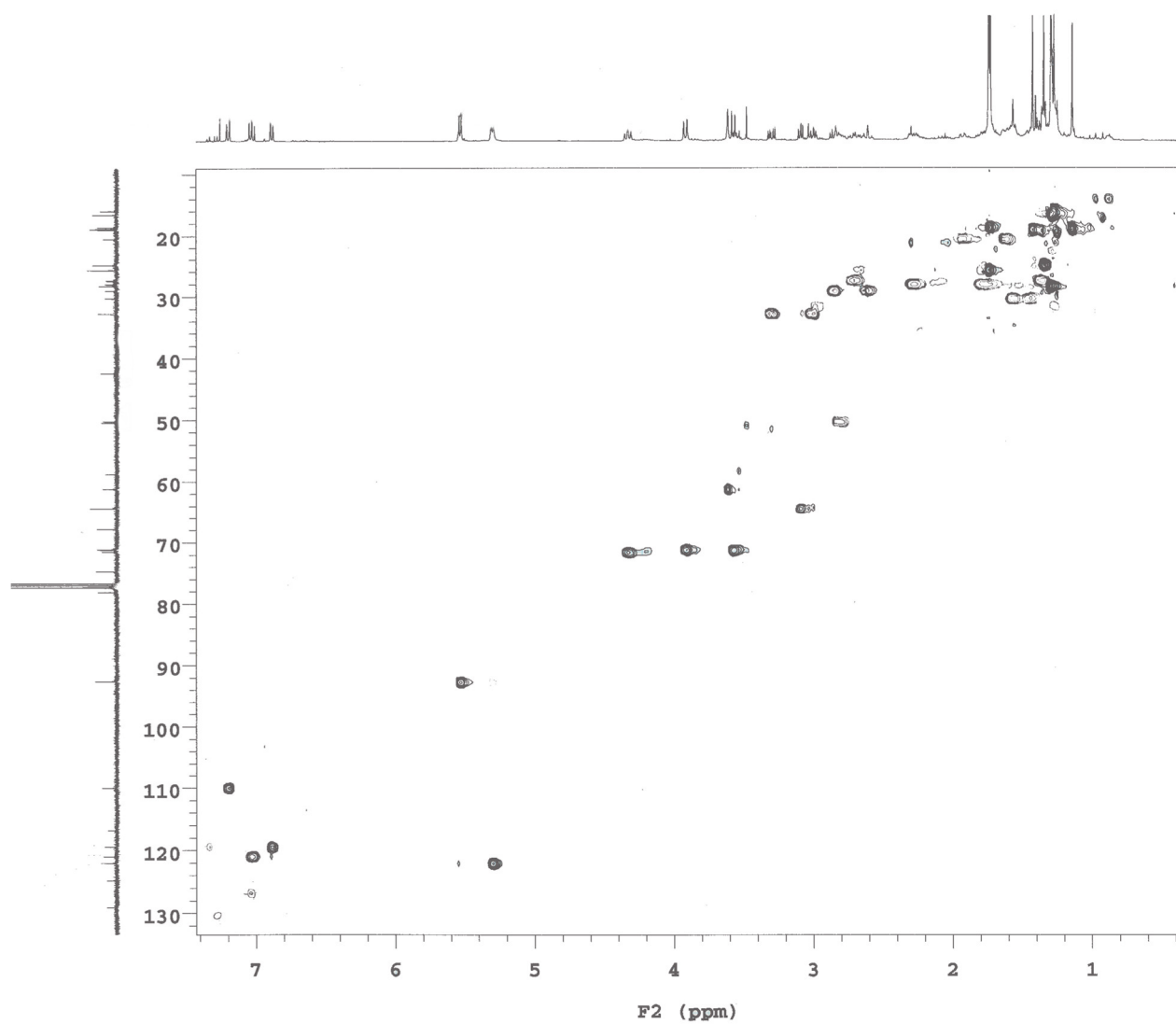


Figure S9. HSQC spectrum of terpendole O (2) in CDCl<sub>3</sub>.



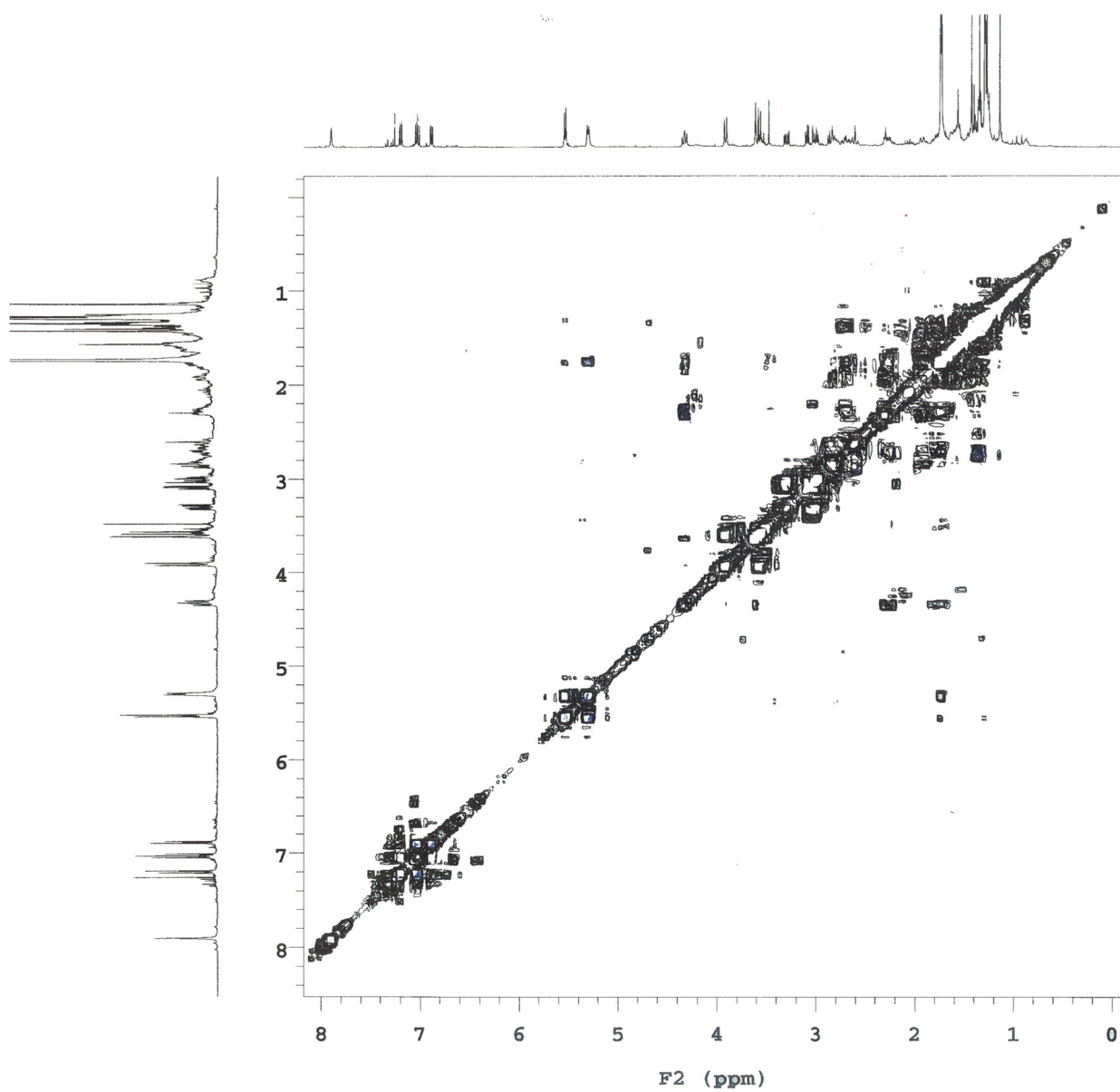


Figure S10.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of terpendole O (**2**) in  $\text{CDCl}_3$ .

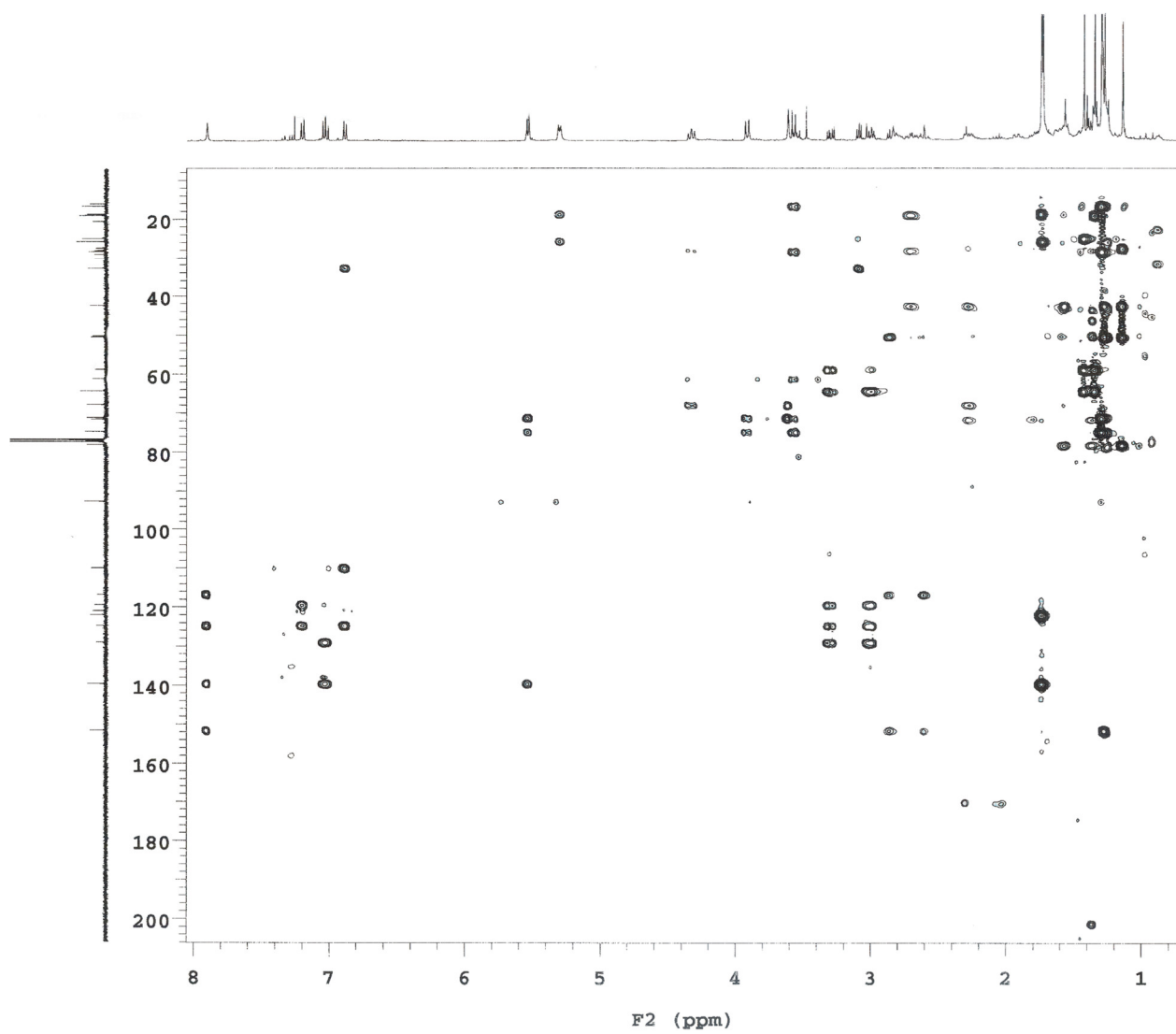


Figure S11. HMBC spectrum of terpendole O (2) in CDCl<sub>3</sub>.

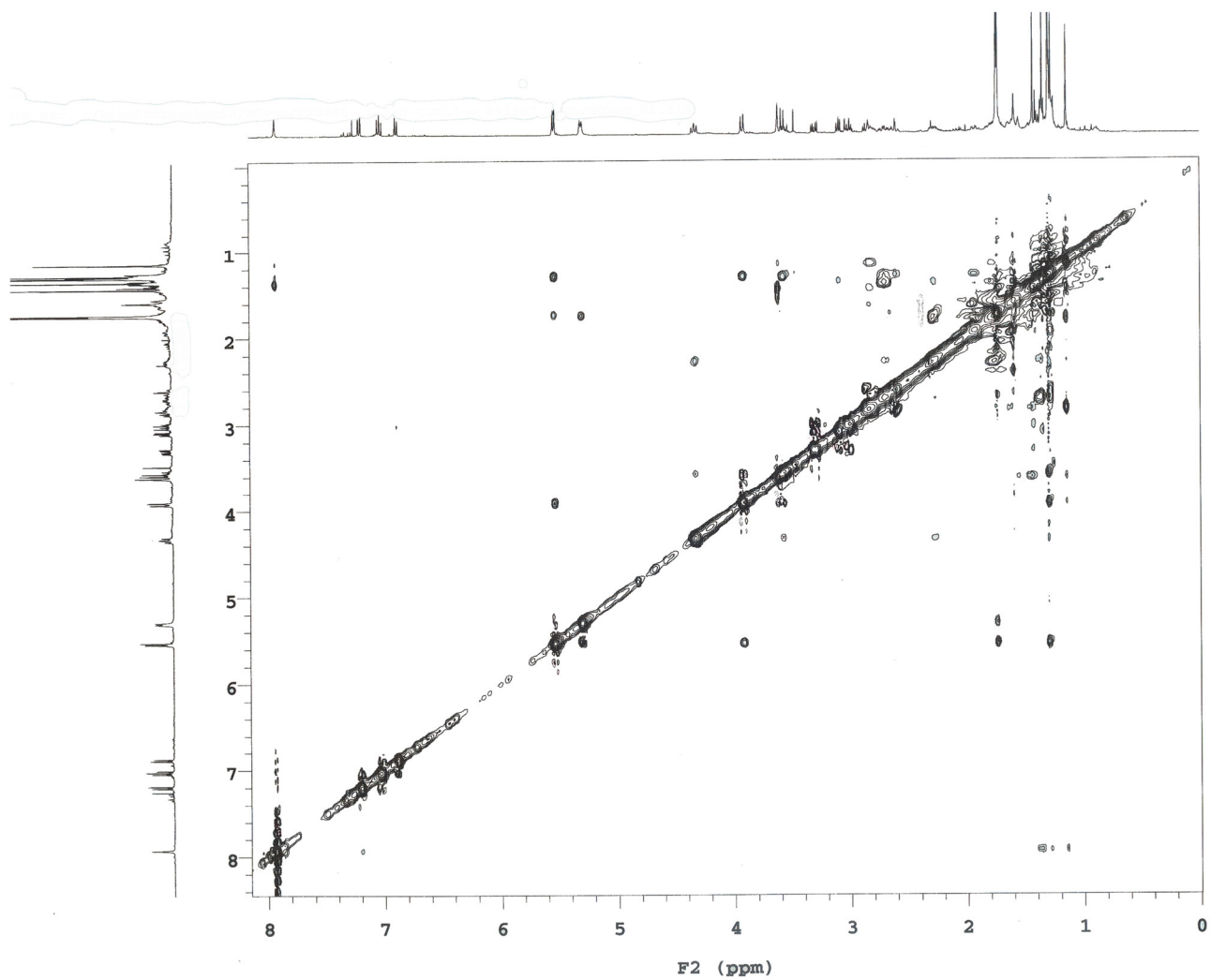


Figure S12. NOESY spectrum of terpendole O (**2**) in  $\text{CDCl}_3$ .

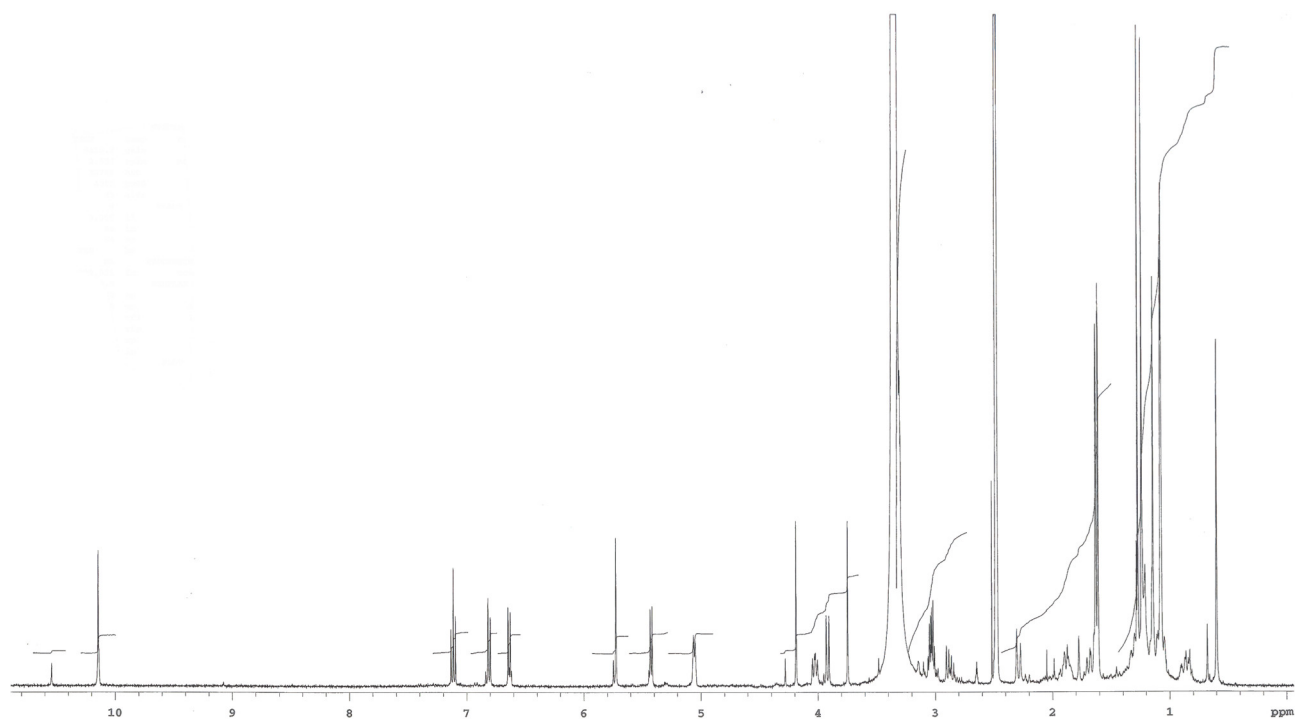


Figure S13.  $^1\text{H-NMR}$  spectrum of terpendole N (**1**) in  $\text{DMSO-}d_6$ .

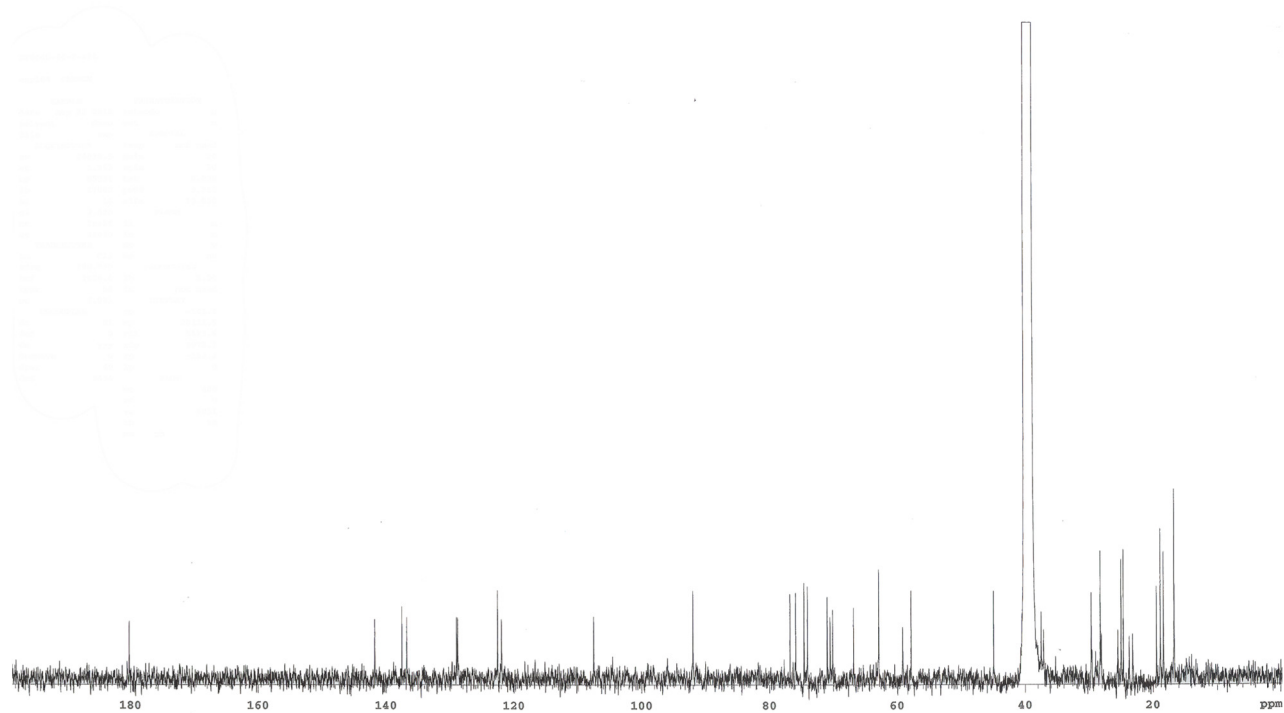


Figure S14.  $^{13}\text{C-NMR}$  spectrum of terpendole N (**1**) in  $\text{DMSO-}d_6$ .

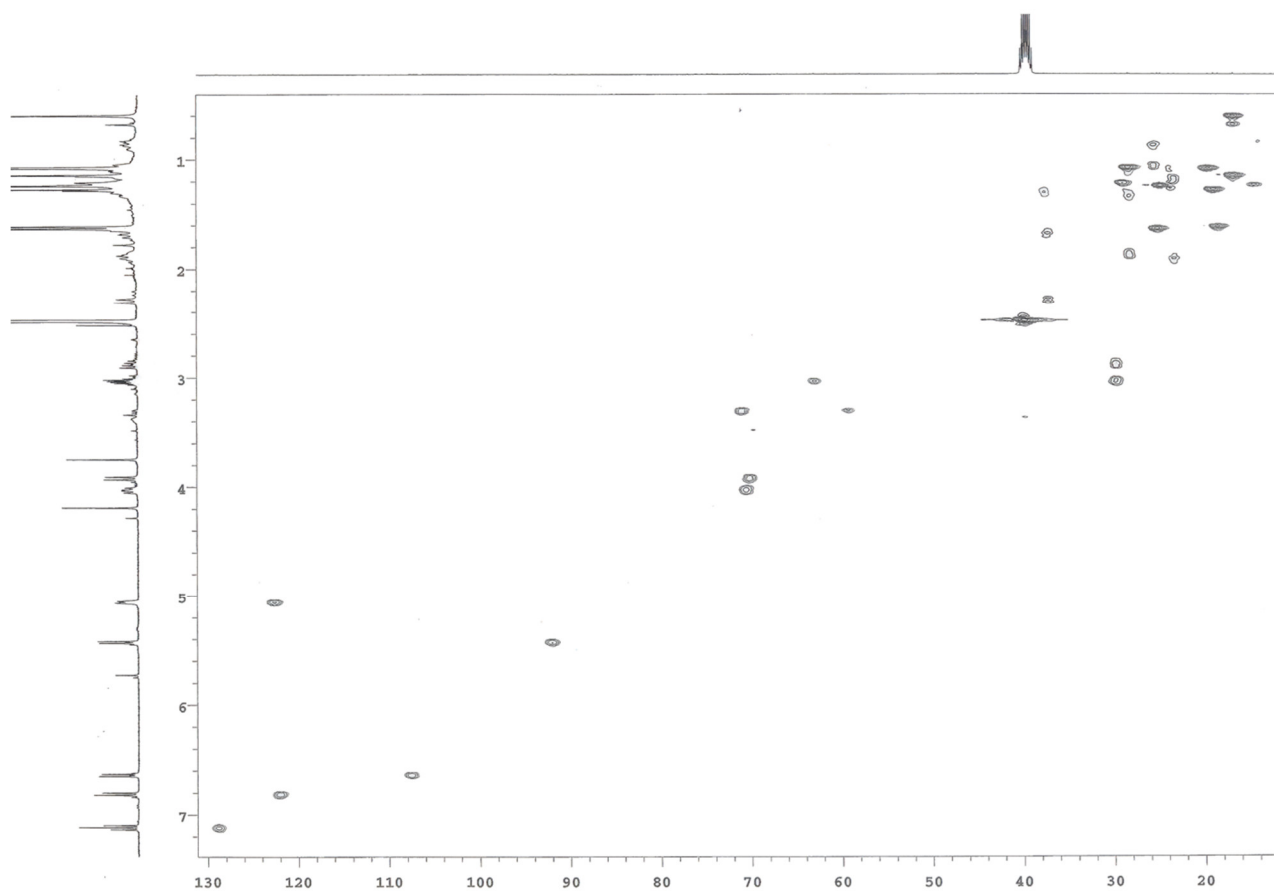


Figure S15. HSQC spectrum of terpendole N (**1**) in  $\text{DMSO-}d_6$ .

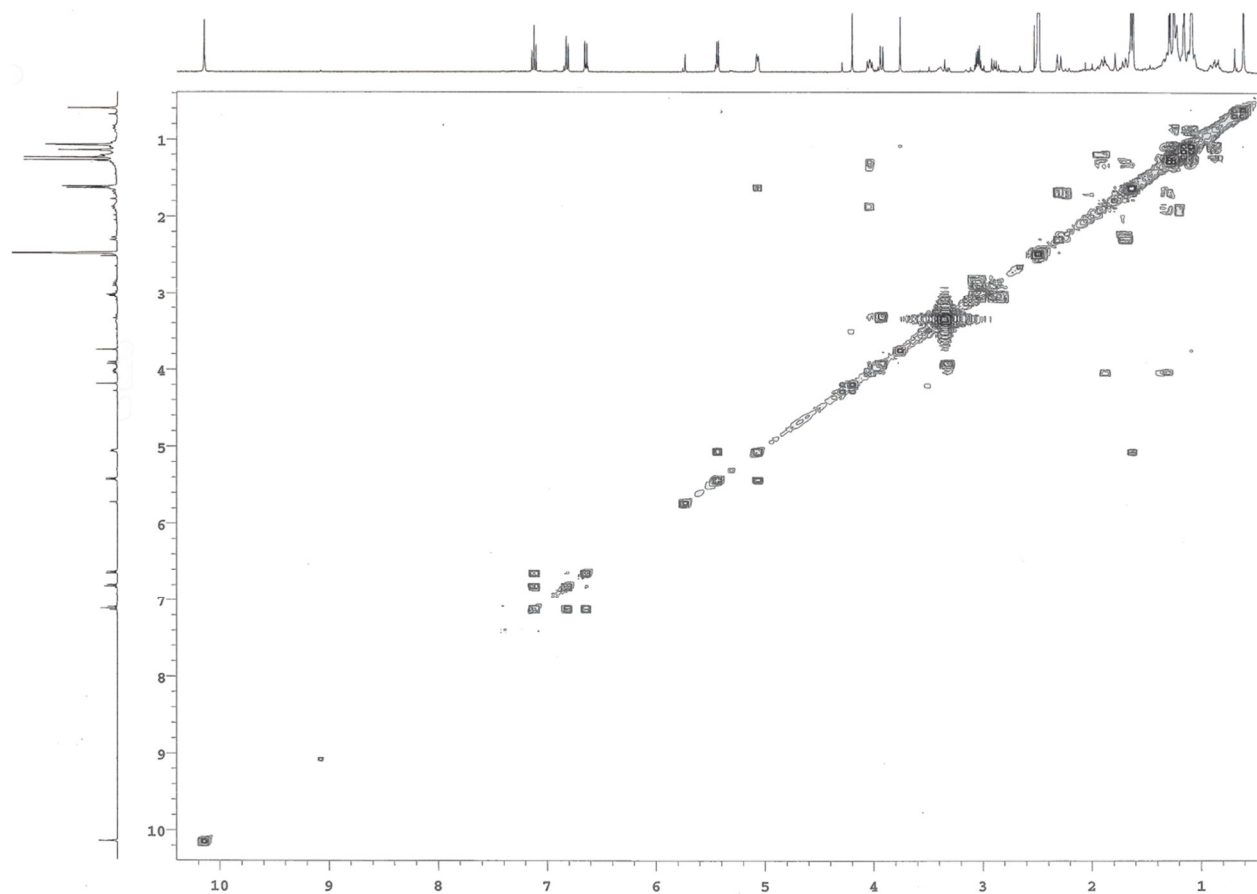


Figure S16.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of terpendole N (**1**) in  $\text{DMSO-}d_6$ .

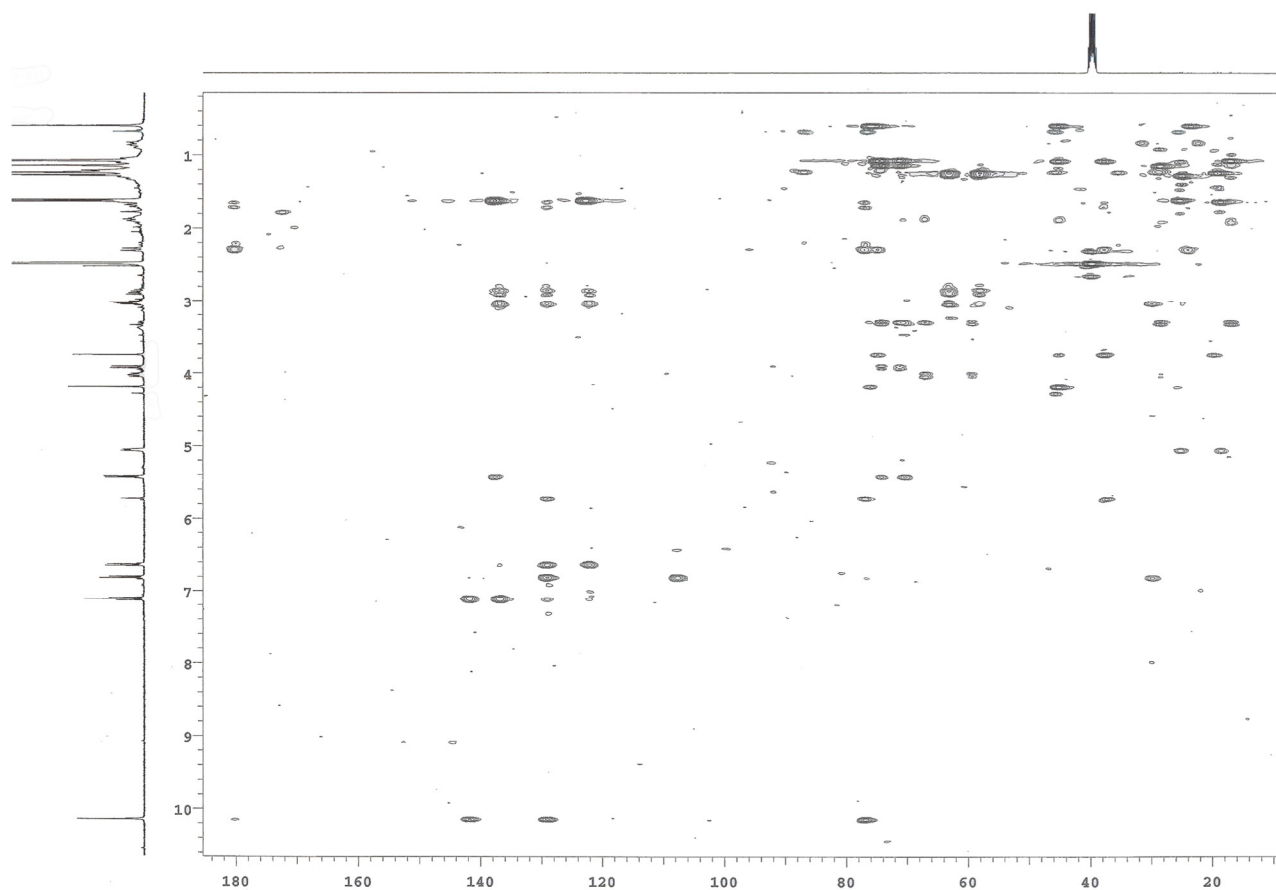


Figure S17. HMBC spectrum of terpendole N (**1**) in DMSO-*d*<sub>6</sub>.

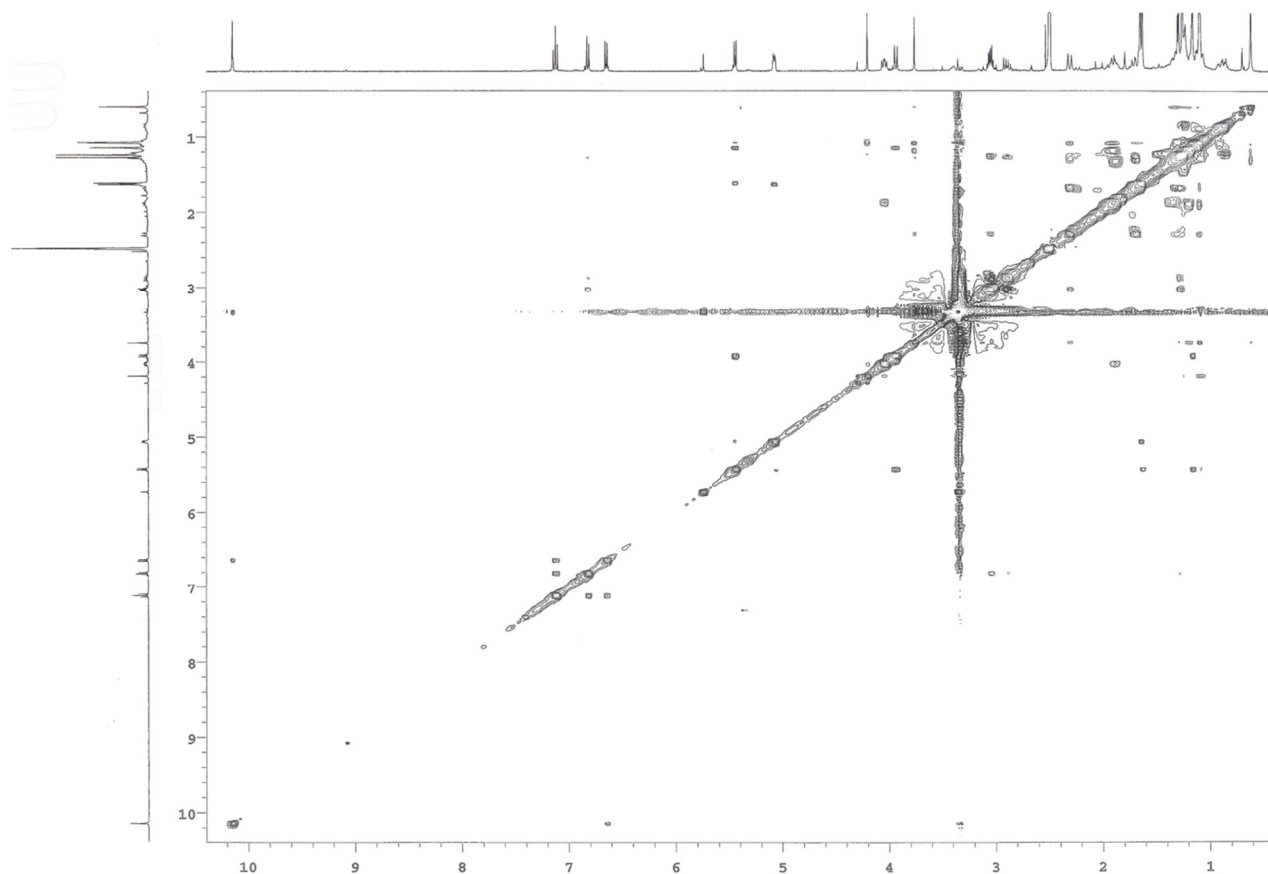


Figure S18. ROESY spectrum of terpendole N (1) in DMSO-*d*<sub>6</sub>.



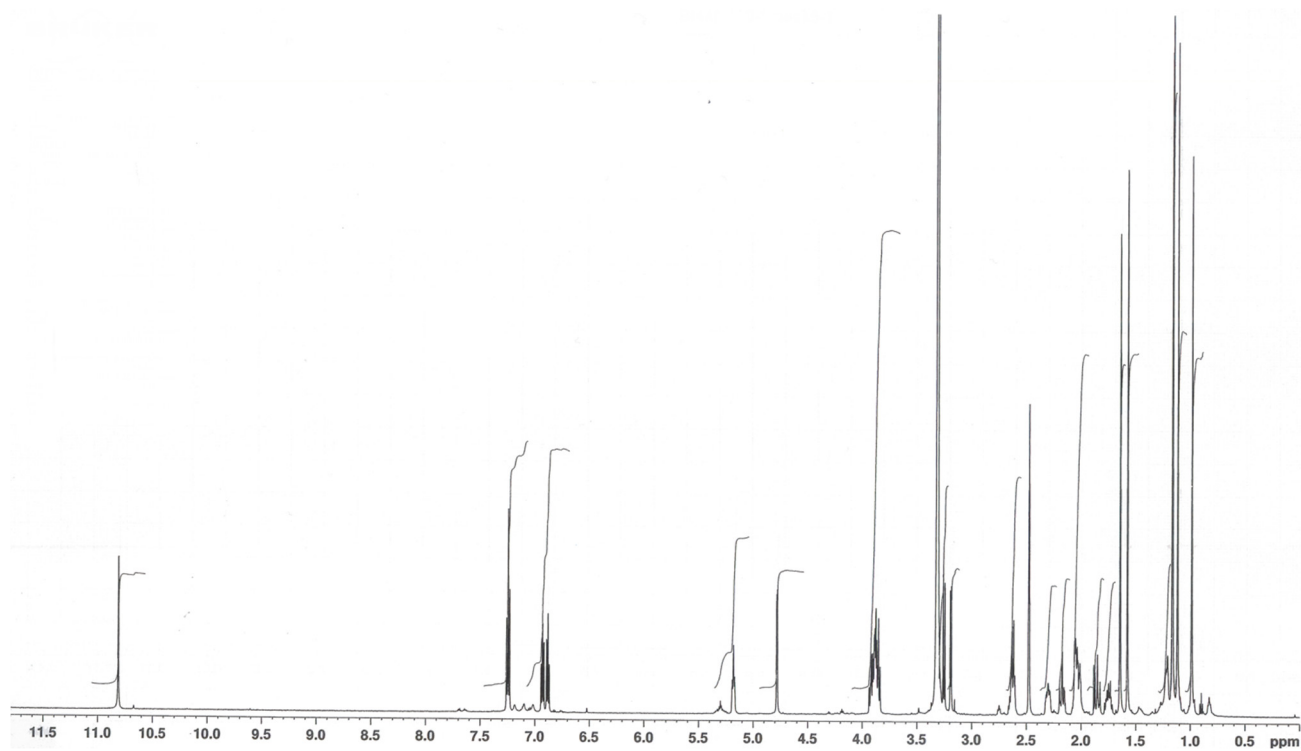


Figure S19. <sup>1</sup>H-NMR spectrum of terpendole P (3) in DMSO-*d*<sub>6</sub>.

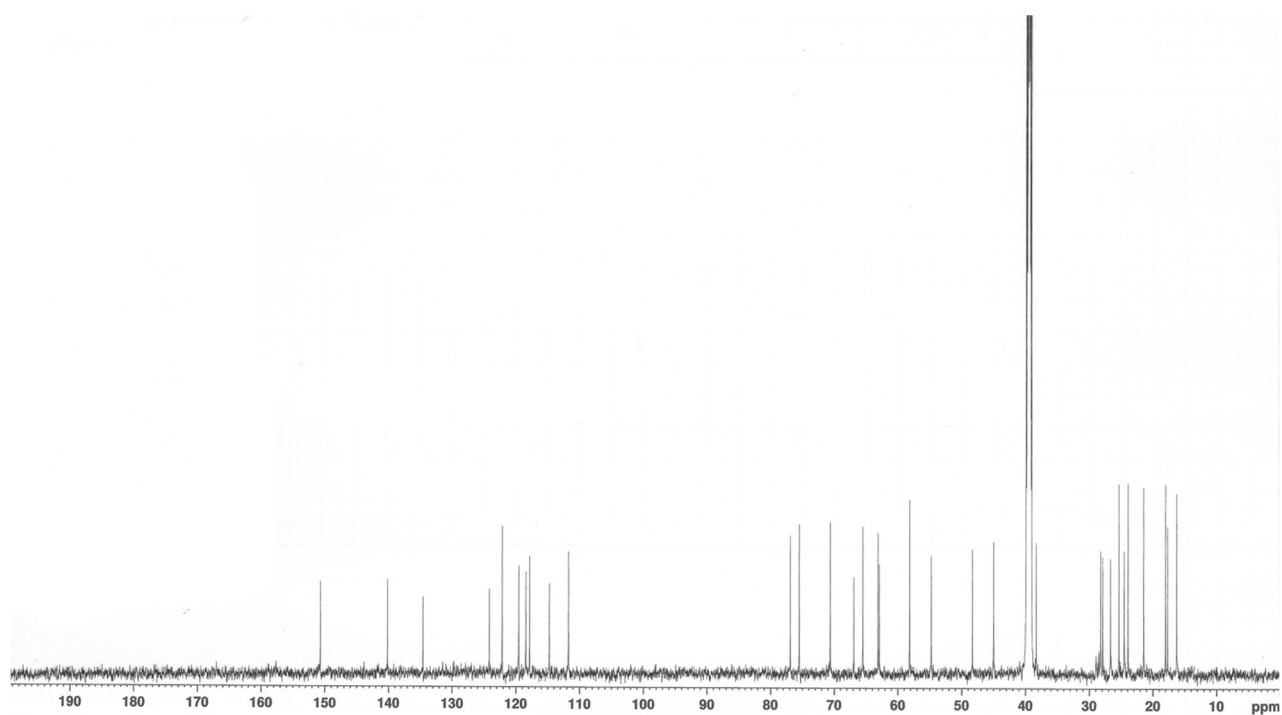
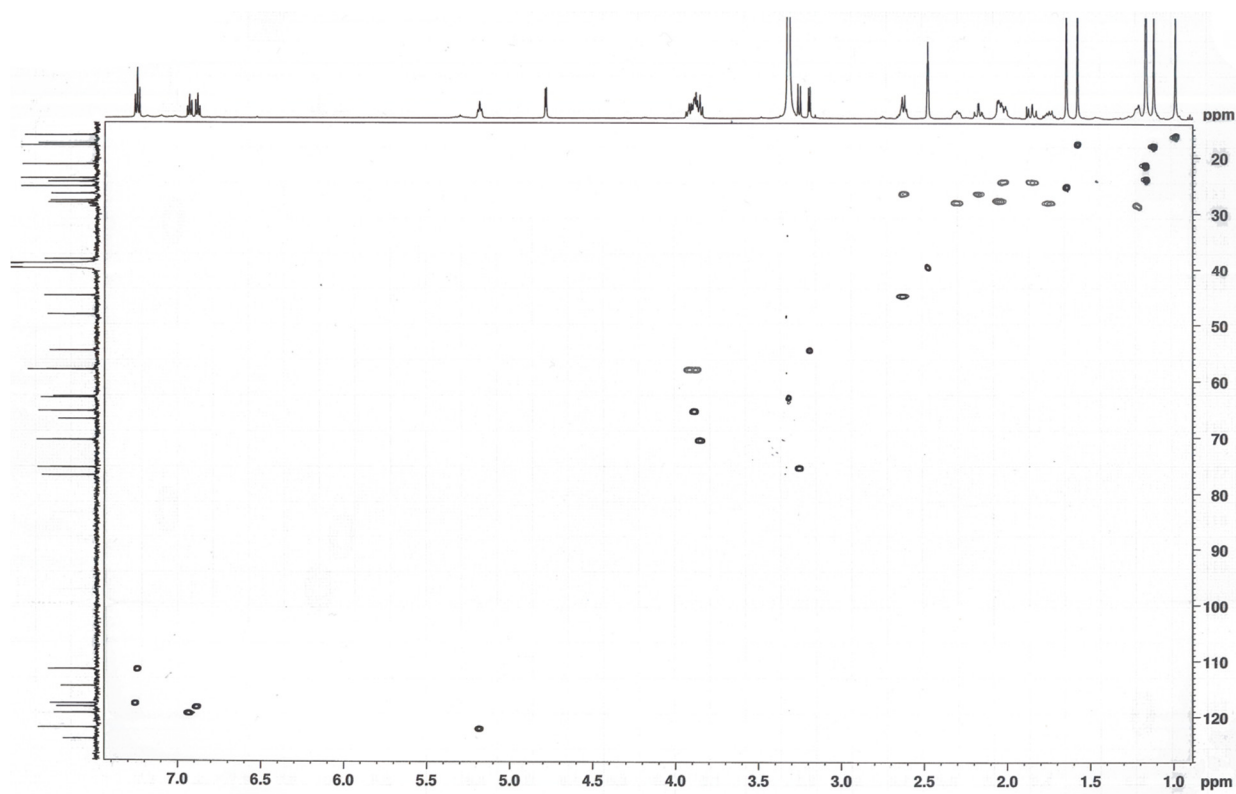
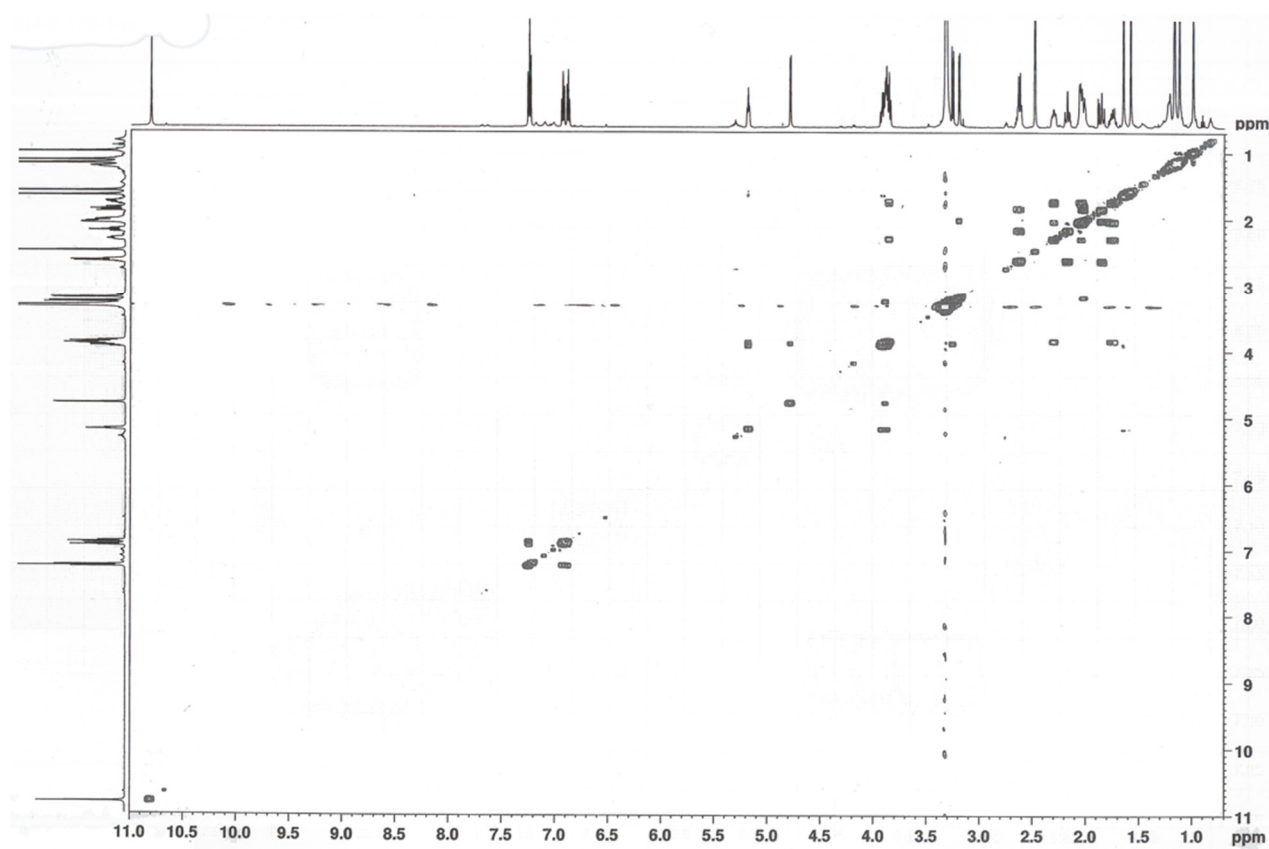
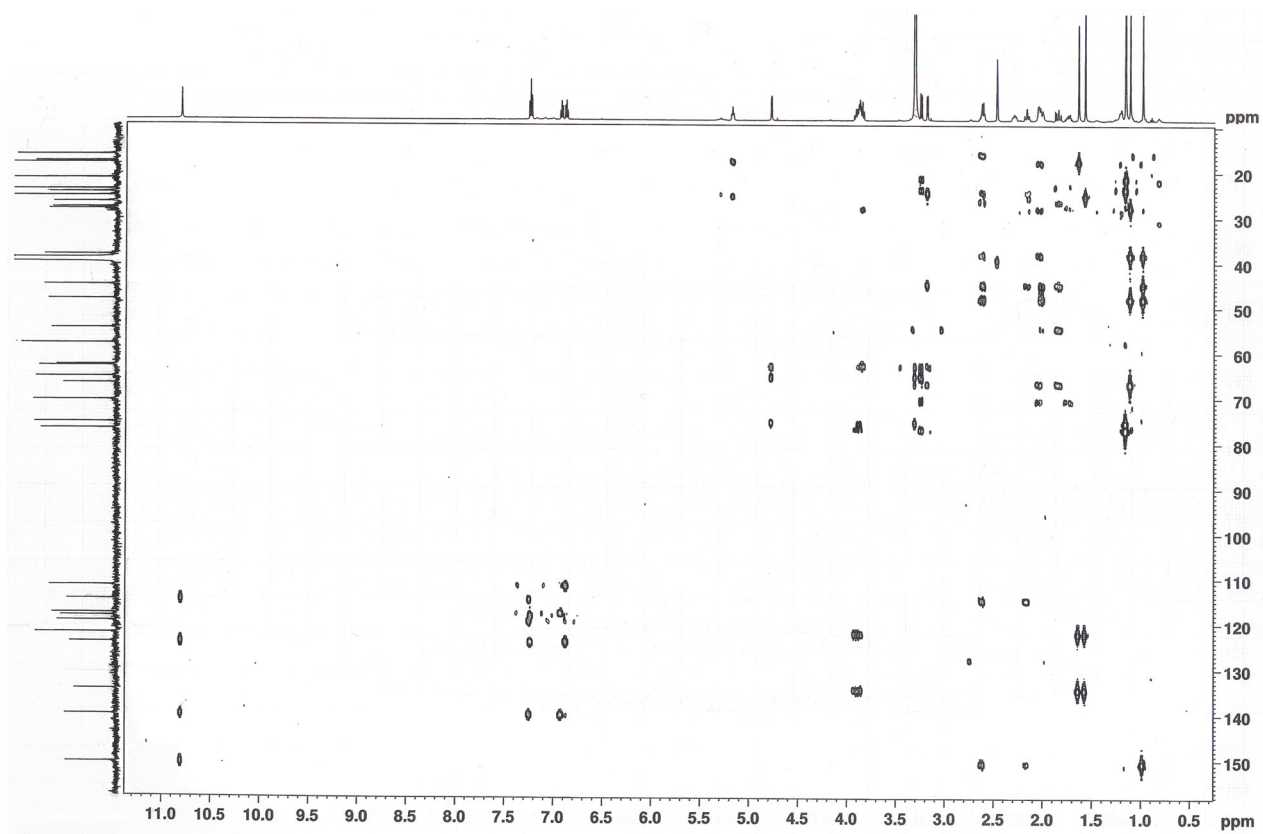
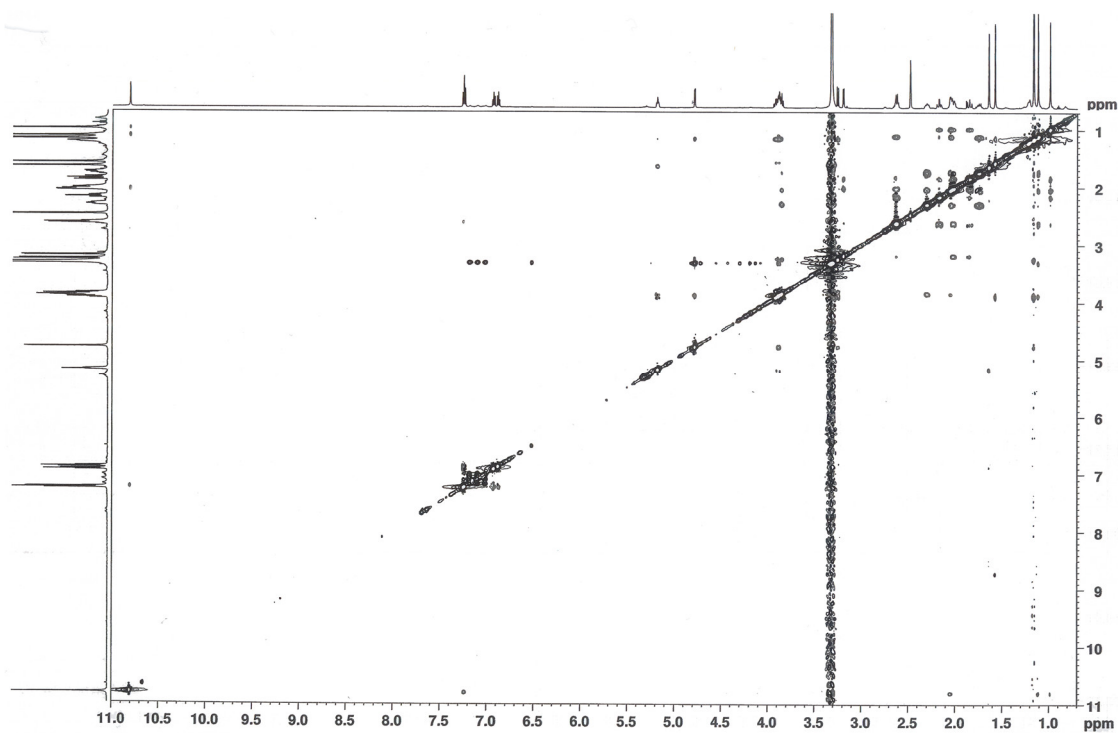


Figure S20. <sup>13</sup>C-NMR spectrum of terpendole P (3) in DMSO-*d*<sub>6</sub>.

Figure S21. HSQC spectrum of terpendole P (**3**) in DMSO-  $d_6$ .Figure S22.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of terpendole P (**3**) in DMSO-  $d_6$ .

Figure S23. HMBC spectrum of terpendole P (3) in DMSO- *d*<sub>6</sub>.Figure S24. ROESY spectrum of terpendole P (3) in DMSO- *d*<sub>6</sub>.

**Supplementary Table 1.** <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts of 2 in CDCl<sub>3</sub>

Position	Terpendole O (2)		
	$\delta_c^a$ , type	$\delta_H^b$ (multi, J Hz)	HMBC
1-NH	-	7.90 (s)	2, 18, 19, 24
2	151.5, C	-	-
3	50.3, C	-	-
4	42.3, C	-	-
5	27.4, CH <sub>2</sub>	1.34 (t, 6.4) 2.70 (br td, 13,4 6.4)	13, 26
6	28, CH <sub>2</sub>	2.28 (m) 1.78 (m)	4
7	71.5, CH	4.38 (t, 10.0)	9, 11, 12
9	71.18, CH	3.57 (d, 10.0)	7, 27, 28, 29
10	71.12, CH	3.91 (d, 9.6)	27
11	61.1, CH	3.61 (s)	7
12	67.8, C	-	-
13	78, C	-	-
13-OH	-	-	-
14	30.2, CH <sub>2</sub>	1.43 (br m) 1.56 (br s)	-
15	20.5, CH <sub>2</sub>	1.60 (br m) 1.90 (br m)	-
16	50.2, CH	2.80 (br m)	-
17	29, CH <sub>2</sub>	2.60 (br t, 11.2) 2.83 (t, 6.0)	2, 18
18	116.7, C	-	-
19	124.7, C	-	-
20	129, C	-	-
21	119.3, CH	6.86 (d, 6.8)	19, 23
22	120.9, CH	7.02 (t, 7.6)	20, 24
23	109.9, CH	7.19 (d, 7.6)	19, 21
24	139.6, C	-	-
25	15.9, CH <sub>3</sub>	1.27 (s)	2, 4, 16
26	18.8, CH <sub>3</sub>	1.14 (s)	3, 4, 5, 14, 16
27	74.7, C	-	-
28	16.6, CH <sub>3</sub>	1.29 (d, 2.8)	9, 27, 29
29	28.2, CH <sub>3</sub>	1.29 (d, 2.8)	9, 27, 28
31	92.6, CH	5.53 (d, 6.8)	10, 27, 34
33	121.9, CH	5.30 (d, 6.8)	35, 36
34	139.6, C	-	-
35	18.6, CH <sub>3</sub>	1.74 (d, 0.8)	33, 34, 36
36	25.6, CH <sub>3</sub>	1.73 (d, 1.2)	33, 34, 35
37	32.7, CH <sub>2</sub>	2.98 (m) 3.29 (m)	21, 39
38	64.3, CH	3.09 (dd, 5.2)	19, 20
39	58.7, C	-	-
40	18.9, CH <sub>3</sub>	1.42 (s)	38, 39, 41
41	24.9, CH <sub>3</sub>	1.34 (s)	38, 39, 40

<sup>13</sup>C (100 MHz) and <sup>1</sup>H (400 MHz) spectra were taken on the NMR system 400 MHz spectrometer (Agilent). Chemical shifts are shown with reference to <sup>a</sup>CDCl<sub>3</sub> as  $\delta$  77.0, <sup>b</sup>CDCl<sub>3</sub> as  $\delta$  7.26. Multiplicity of signals as follows: s = singlet, d = doublets, dd = double doublets, t = triplet, m = multi. Coupling constants (Hz) were determined by the <sup>1</sup>H-<sup>1</sup>H decoupling experiments.