

# Supplementary Materials: New Cyclotetrapeptides and a New Diketopiperazine Derivative from the Marine Sponge-Associated Fungus *Neosartorya glabra* KUFA 0702

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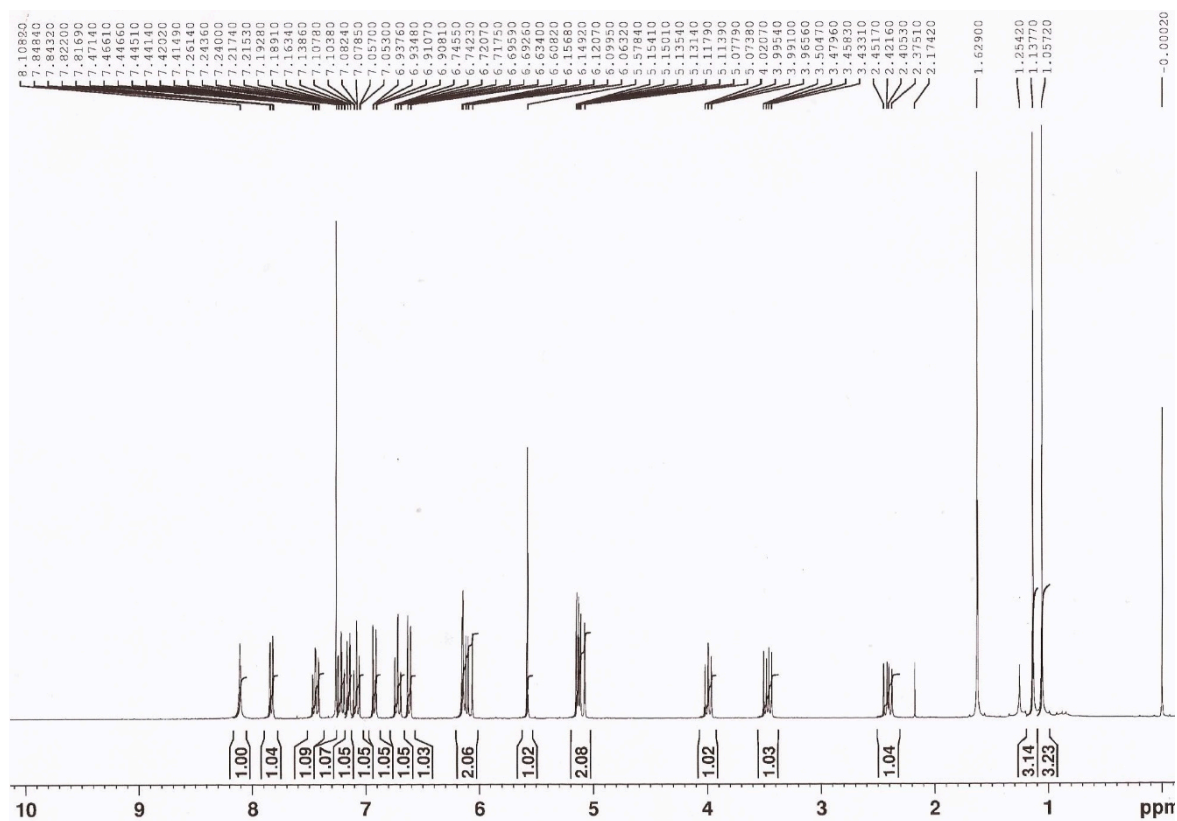


Figure S1. <sup>1</sup>H NMR spectrum of compound 1 (CDCl<sub>3</sub>, 300.13 MHz).

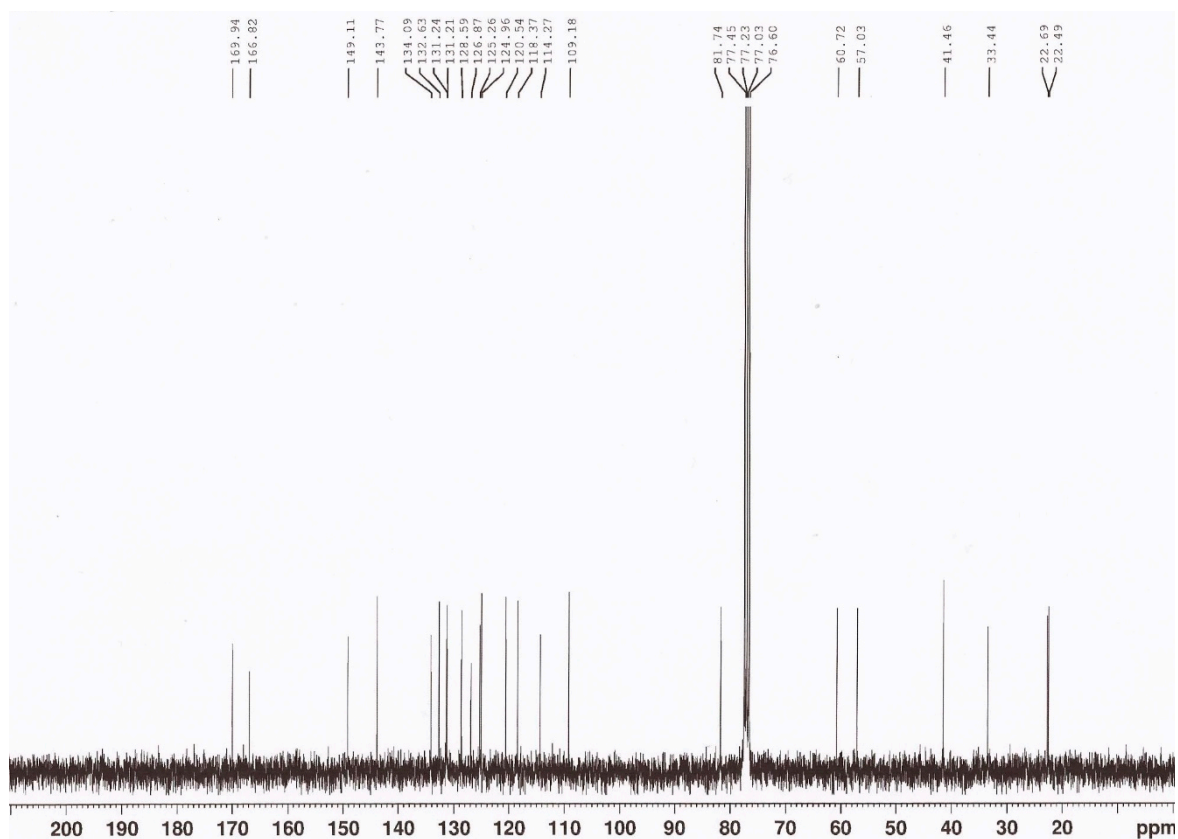


Figure S2.  $^{13}\text{C}$  NMR spectrum of compound 1 ( $\text{CDCl}_3$ , 75.4 MHz).

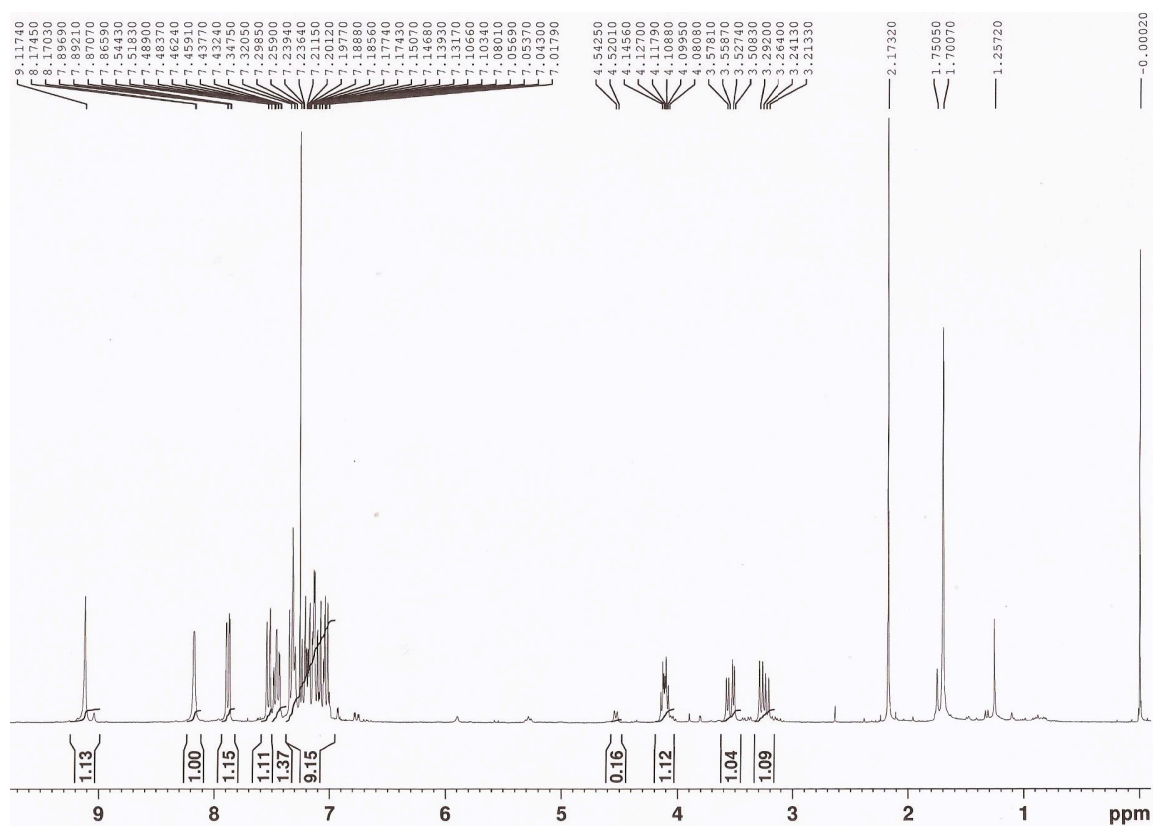
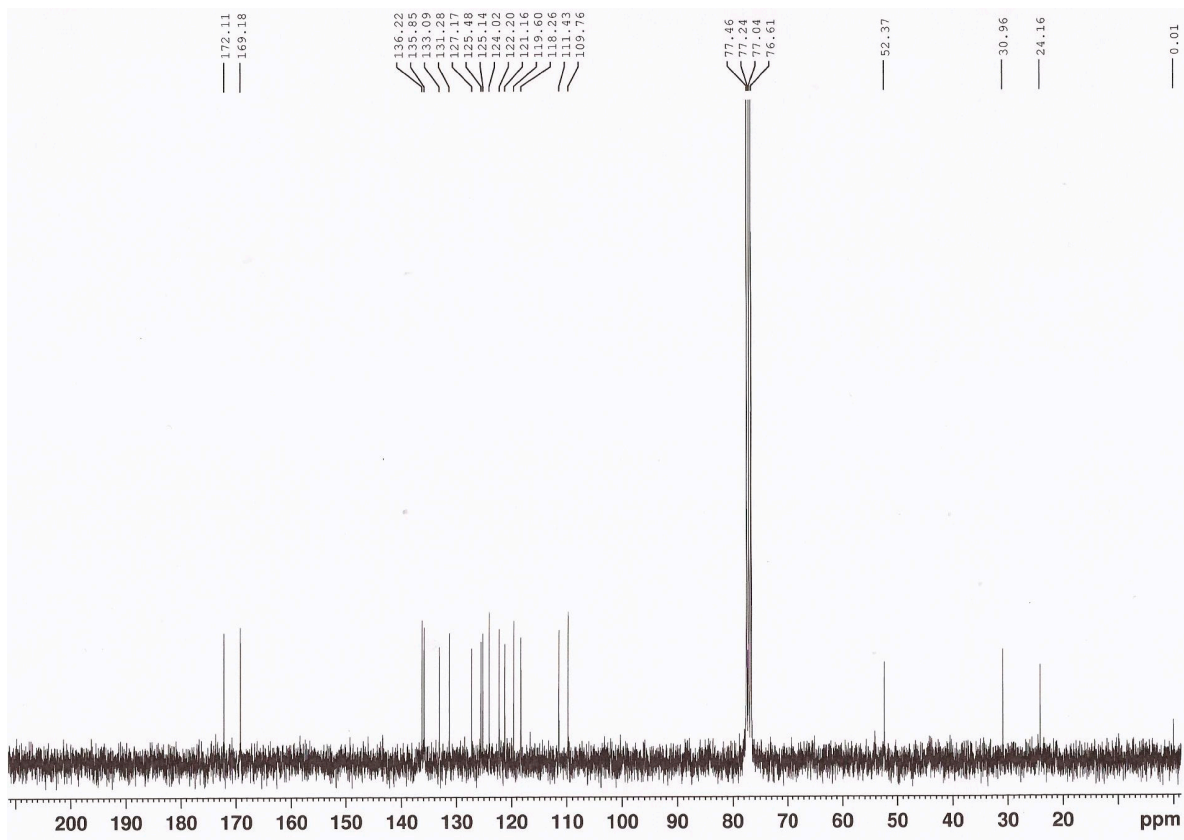
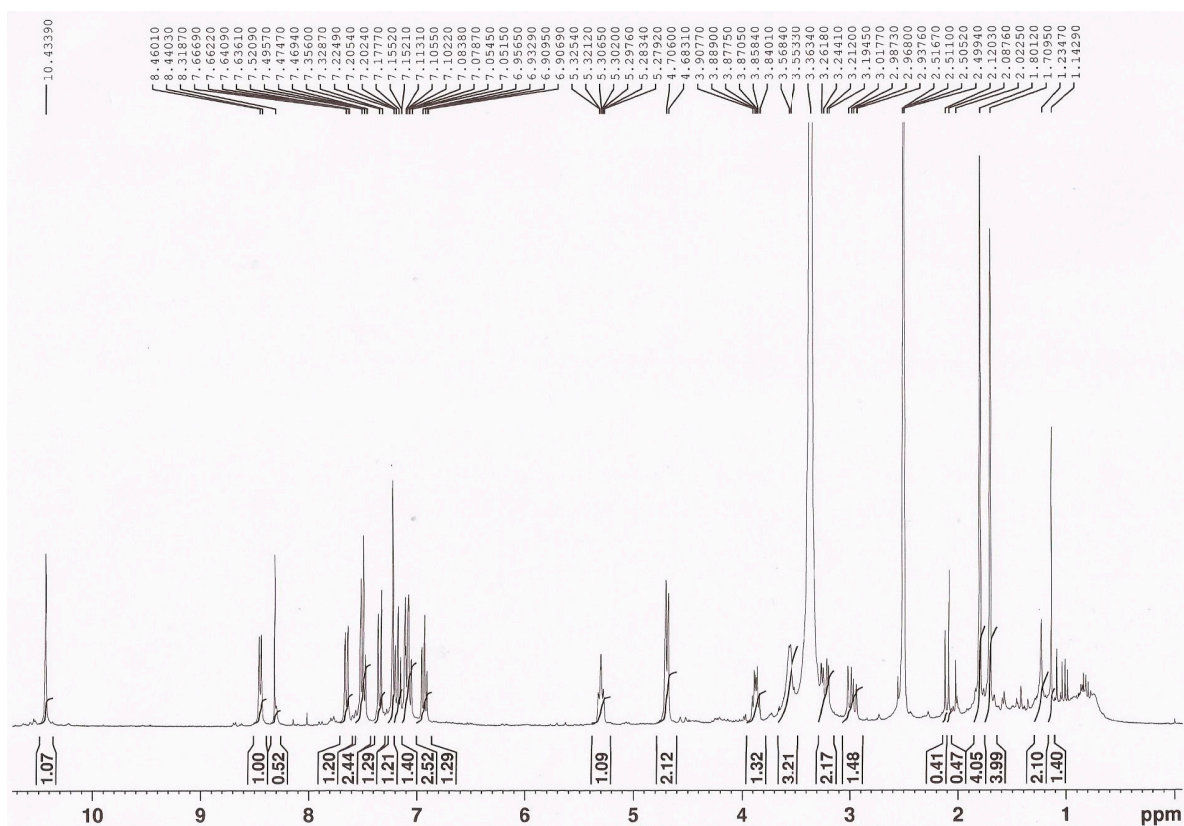


Figure S3.  $^1\text{H}$  NMR spectrum of compound 2 ( $\text{CDCl}_3$ , 300.13 MHz).

Figure S4.  $^{13}\text{C}$  NMR spectrum of compound 2 ( $\text{CDCl}_3$ , 75.4 MHz).Figure S5.  $^1\text{H}$  NMR spectrum of compound 3 ( $\text{CDCl}_3$ , 300.13 MHz).

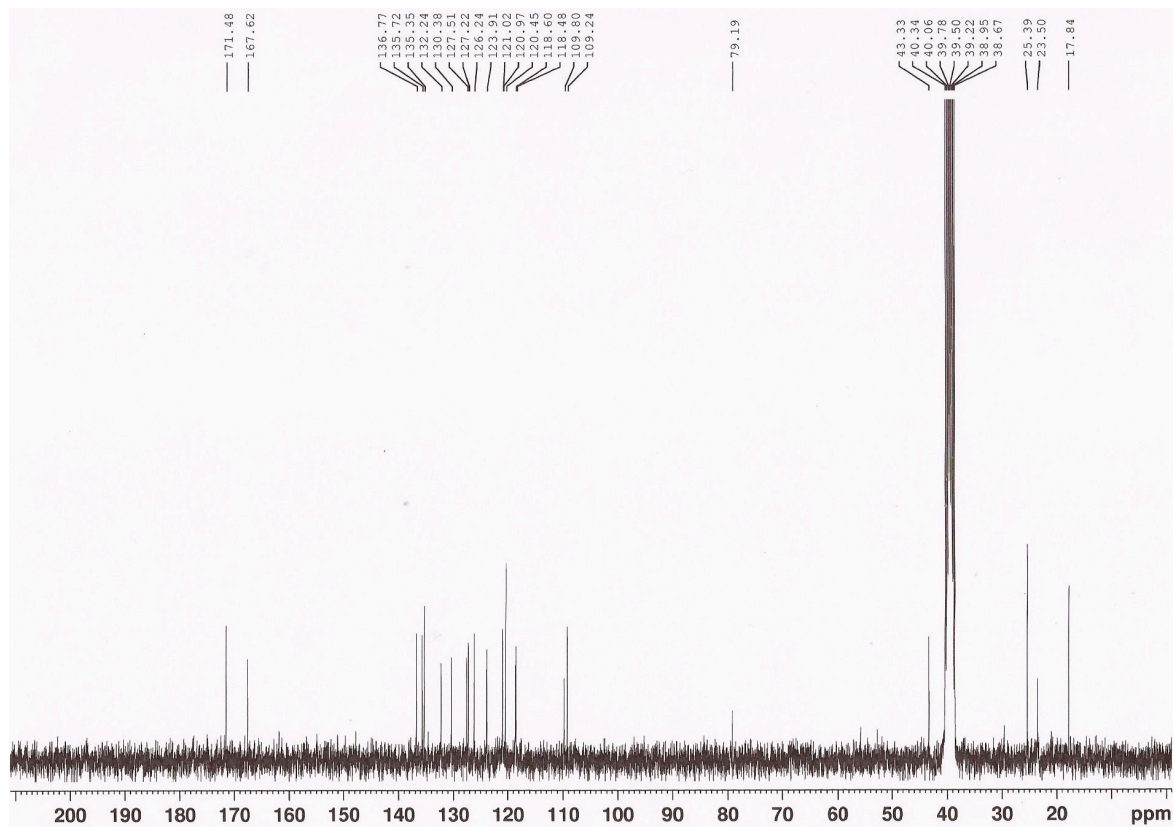


Figure S6.  $^{13}\text{C}$  NMR spectrum of compound 3 ( $\text{CDCl}_3$ , 75.4 MHz).

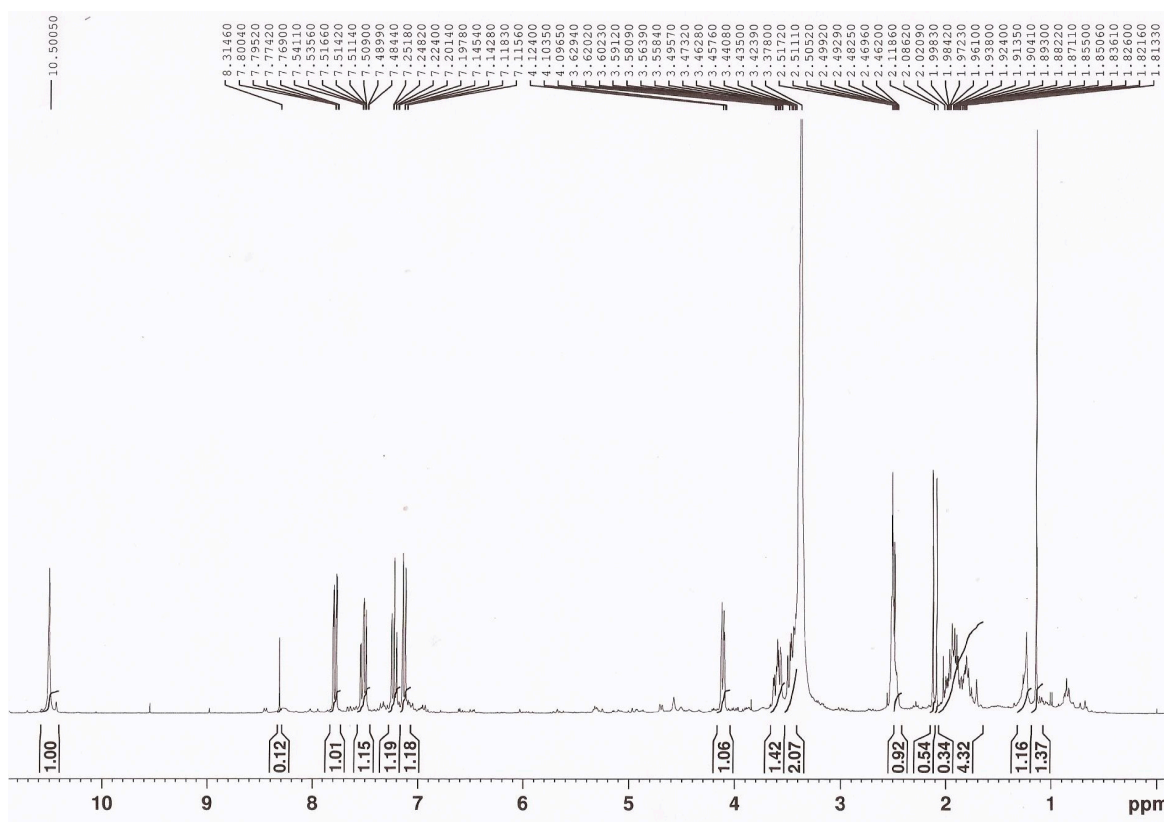


Figure S7.  $^1\text{H}$  NMR spectrum of compound 4 ( $\text{DMSO}$ , 300.13 MHz).

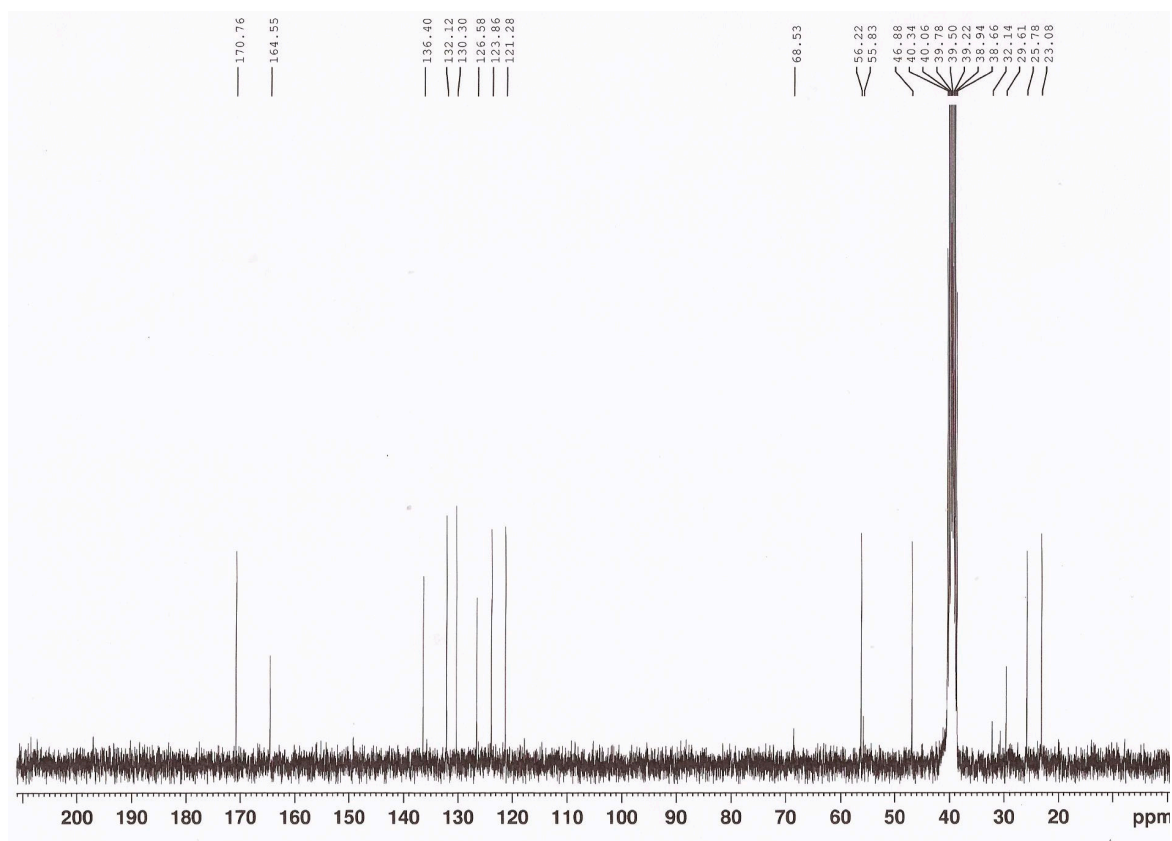


Figure S8.  $^{13}\text{C}$  NMR spectrum of compound 4 (DMSO, 75.4 MHz).

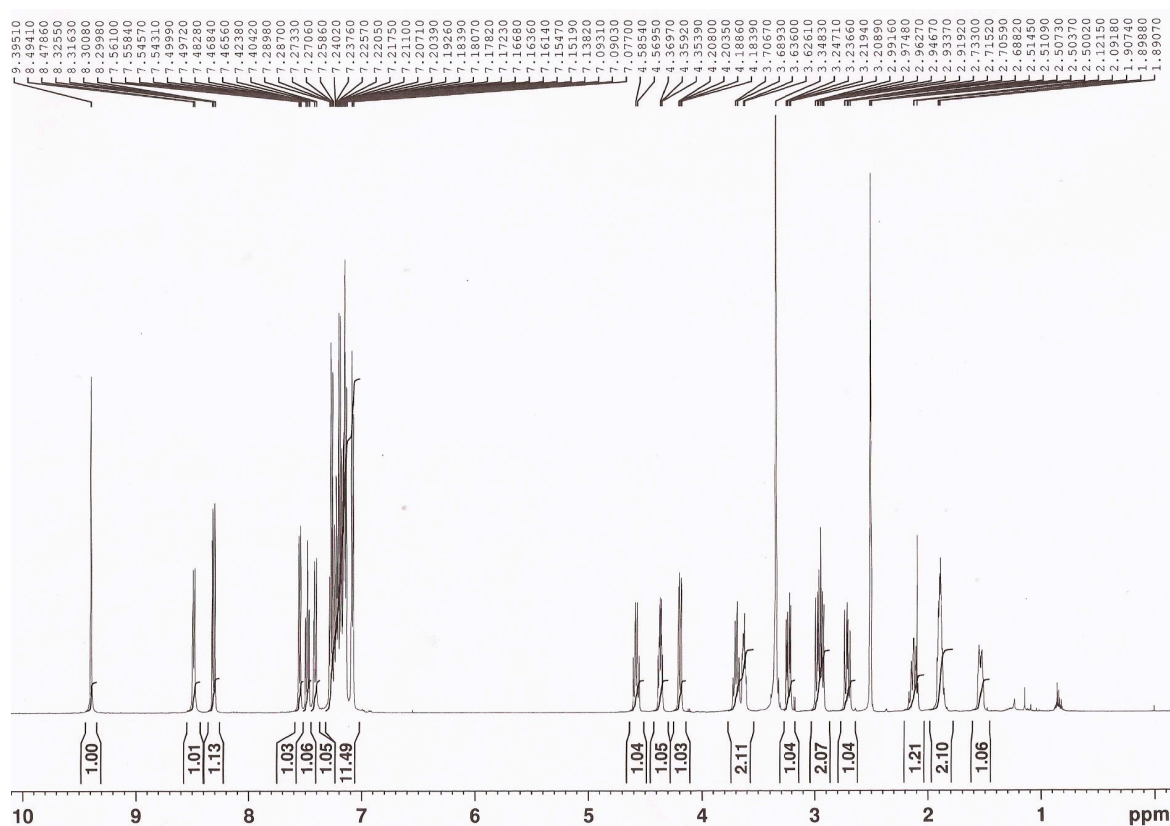


Figure S9.  $^1\text{H}$  NMR spectrum of compound 5 (DMSO, 500.13 MHz).

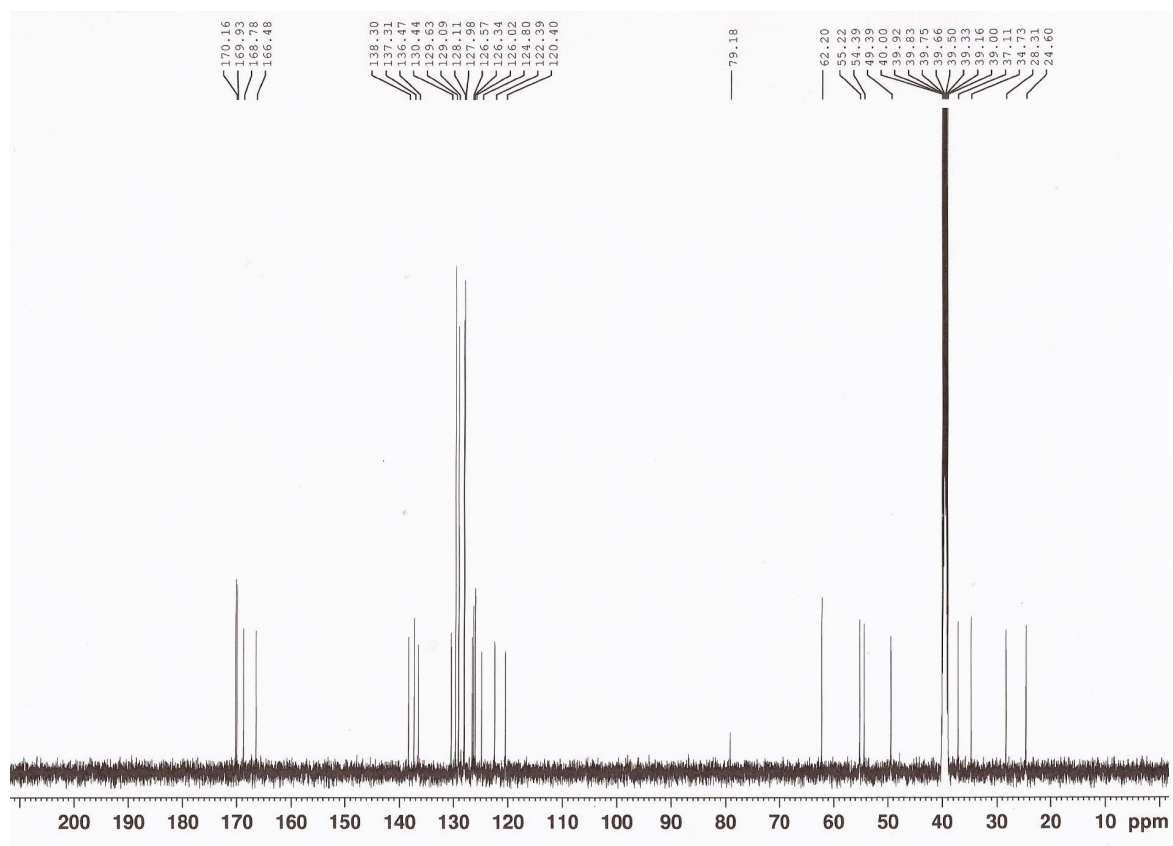


Figure S10.  $^{13}\text{C}$  NMR spectrum of compound 5 (DMSO, 125.8 MHz).

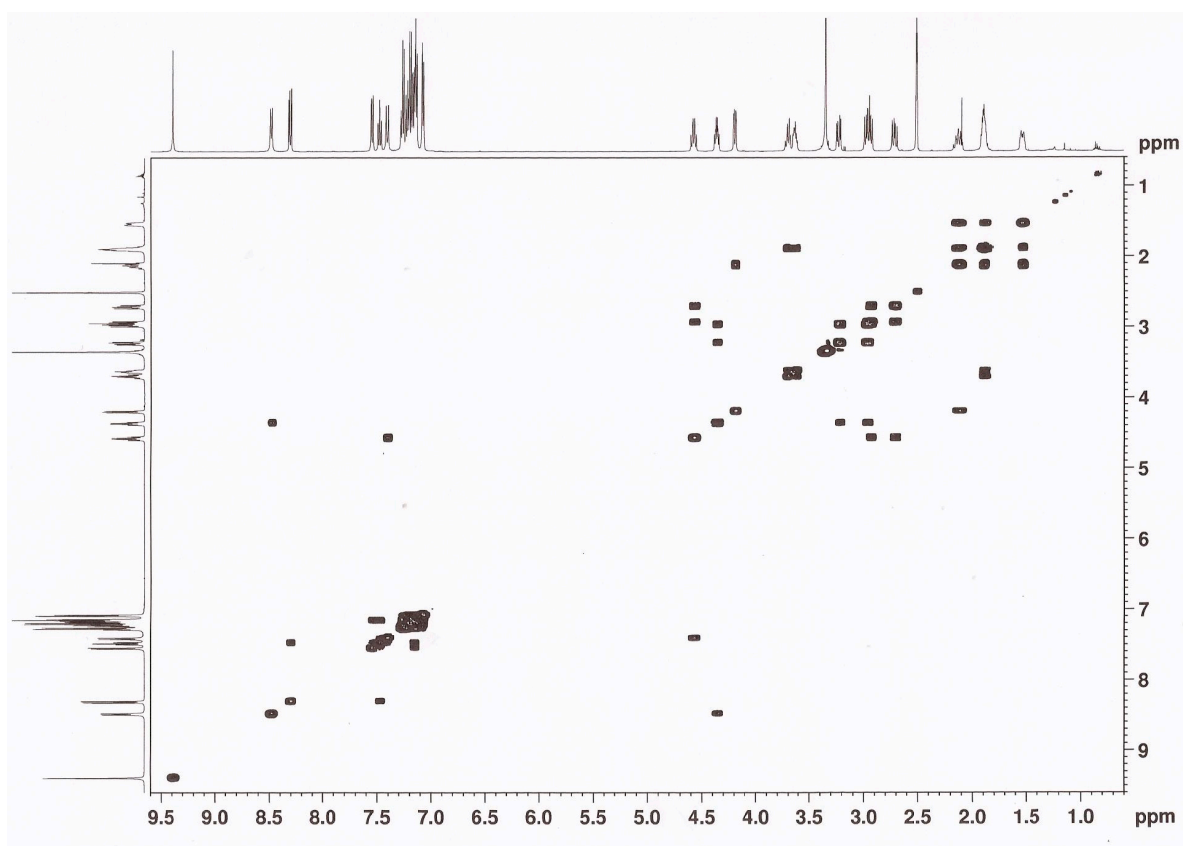


Figure S11. COSY spectrum of compound 5 (DMSO, 500.13 MHz).

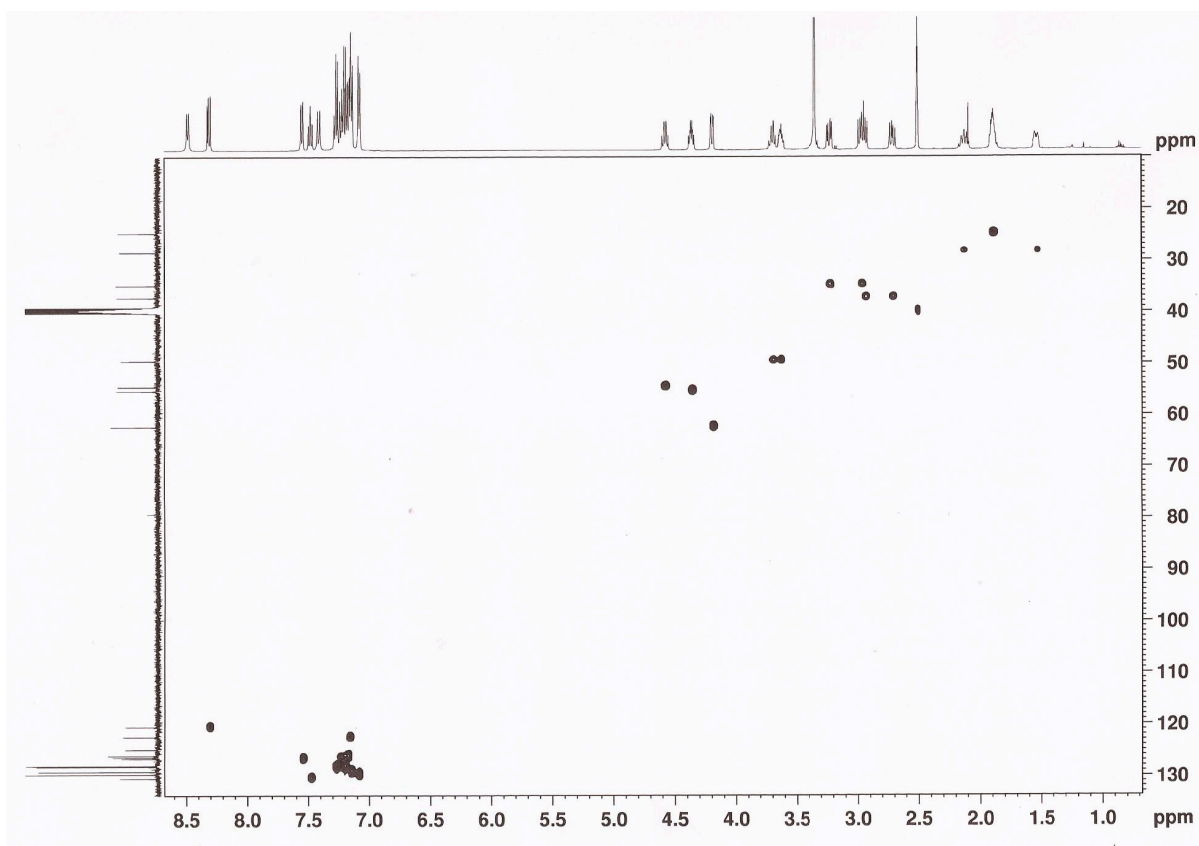


Figure S12. HSQC spectrum of compound 5 (DMSO, 500.13 MHz).

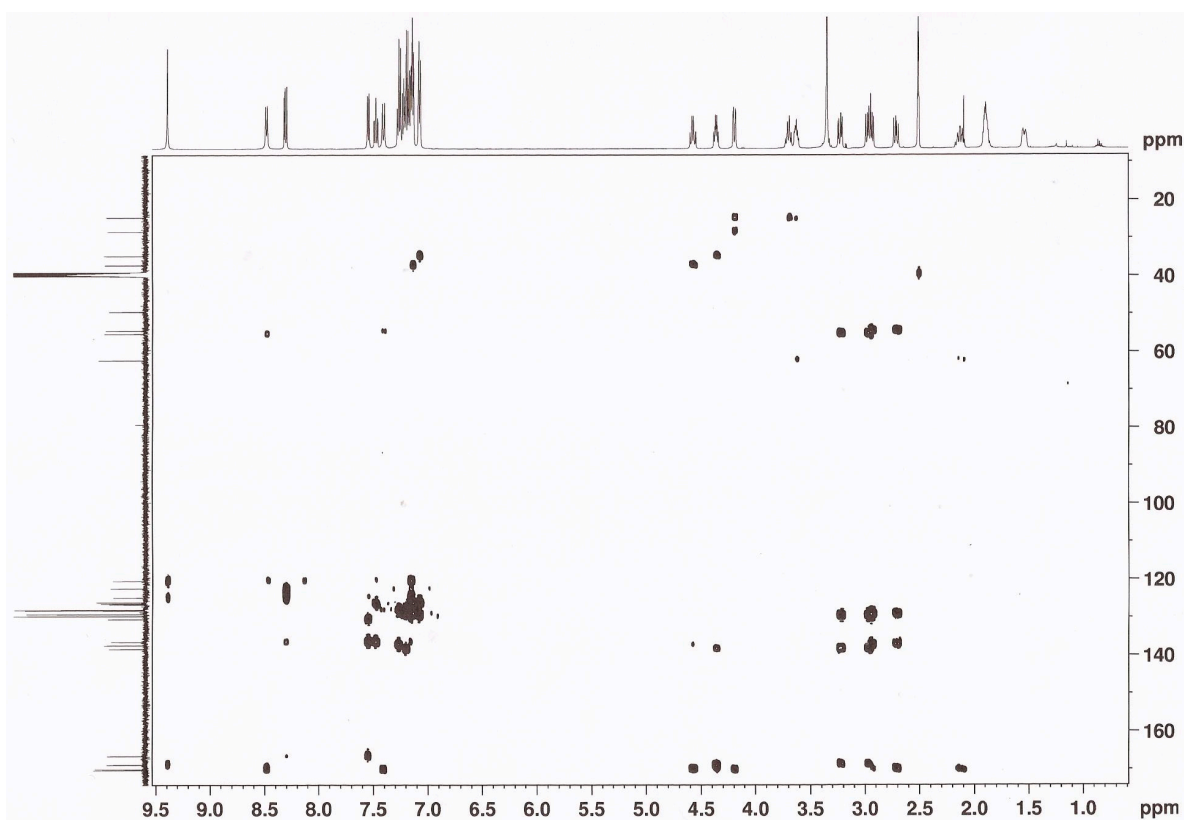
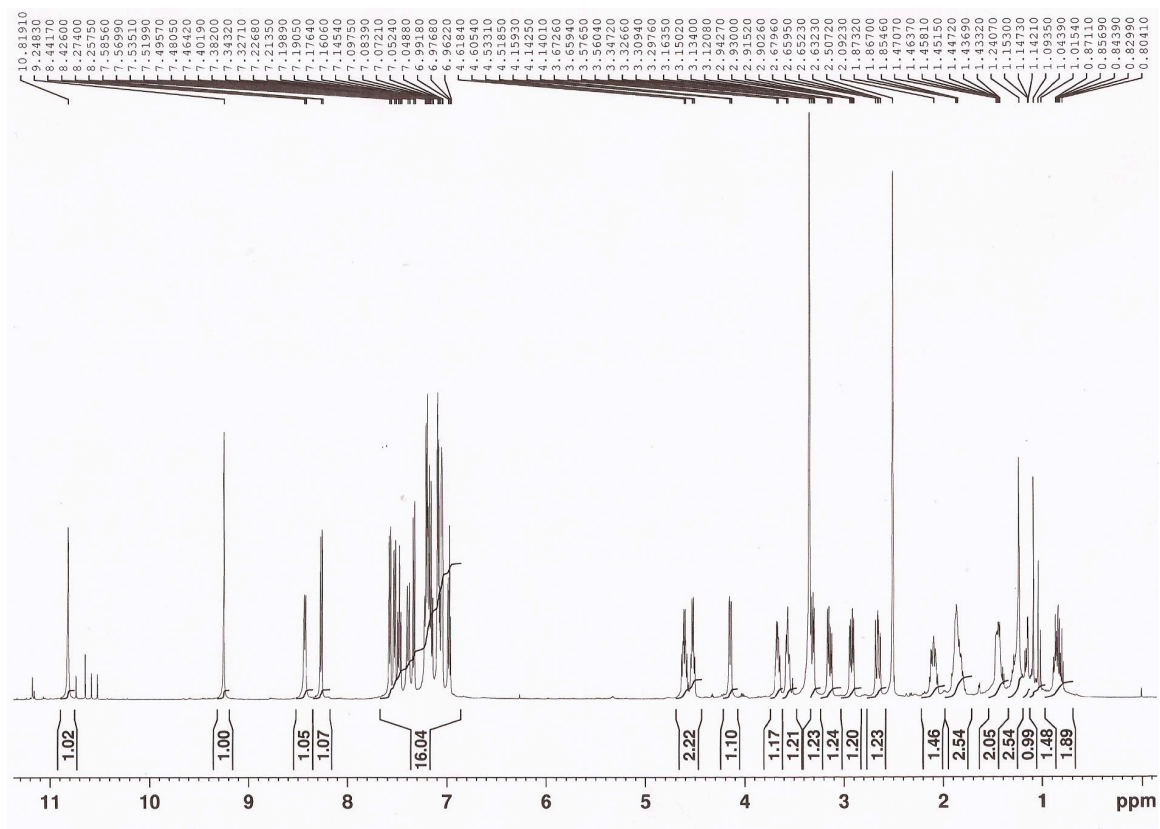
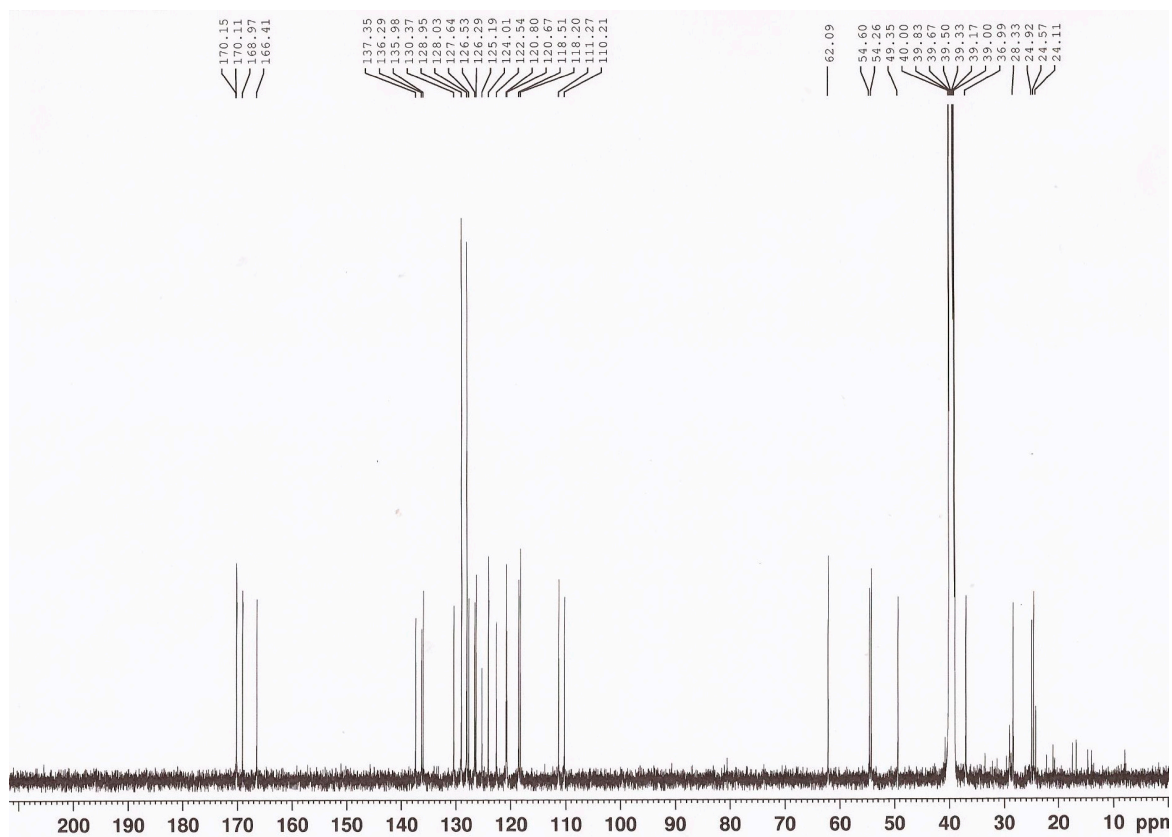


Figure S13. HMBC spectrum of compound 5 (DMSO, 500.13 MHz).

Figure S14.  $^1\text{H}$  NMR spectrum of compound 6 (DMSO, 500 MHz).Figure S15.  $^{13}\text{C}$  NMR spectrum of compound 6 (DMSO, 125.8 MHz).



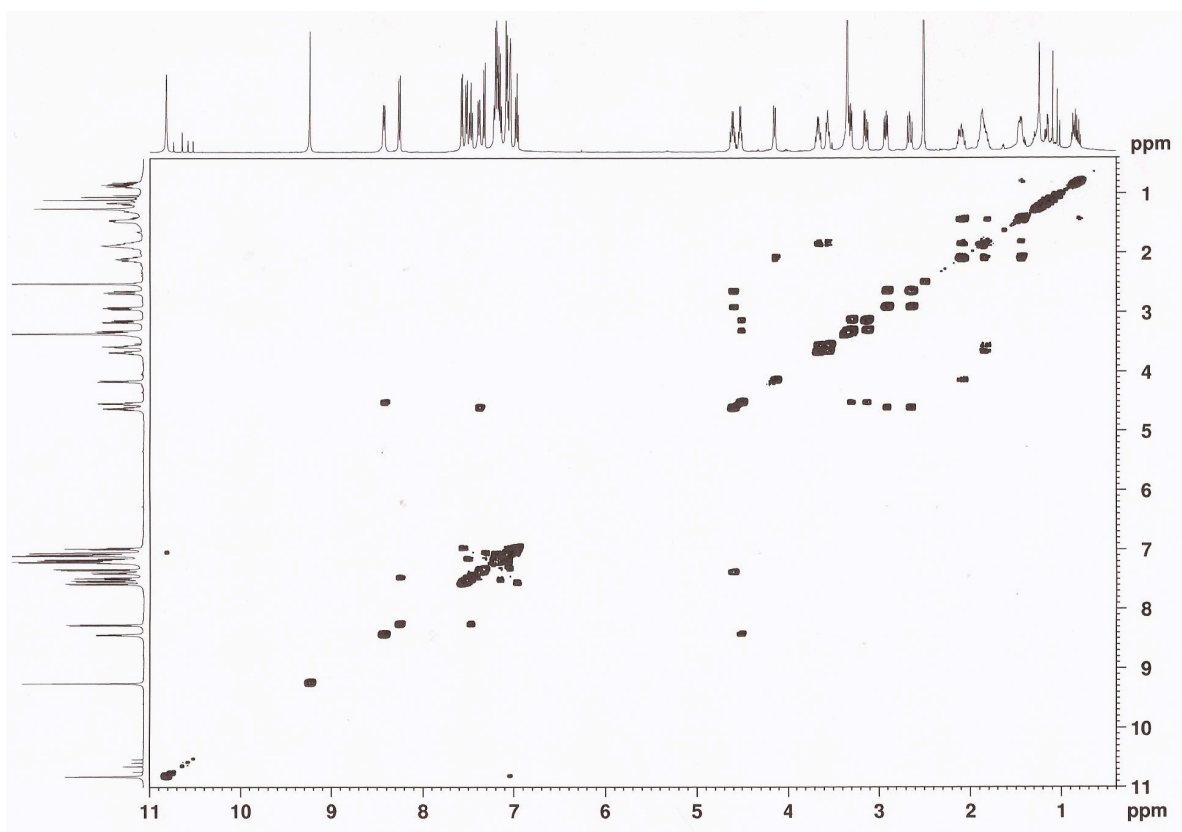


Figure S16. COSY spectrum of compound 6 (DMSO, 500.13 MHz).

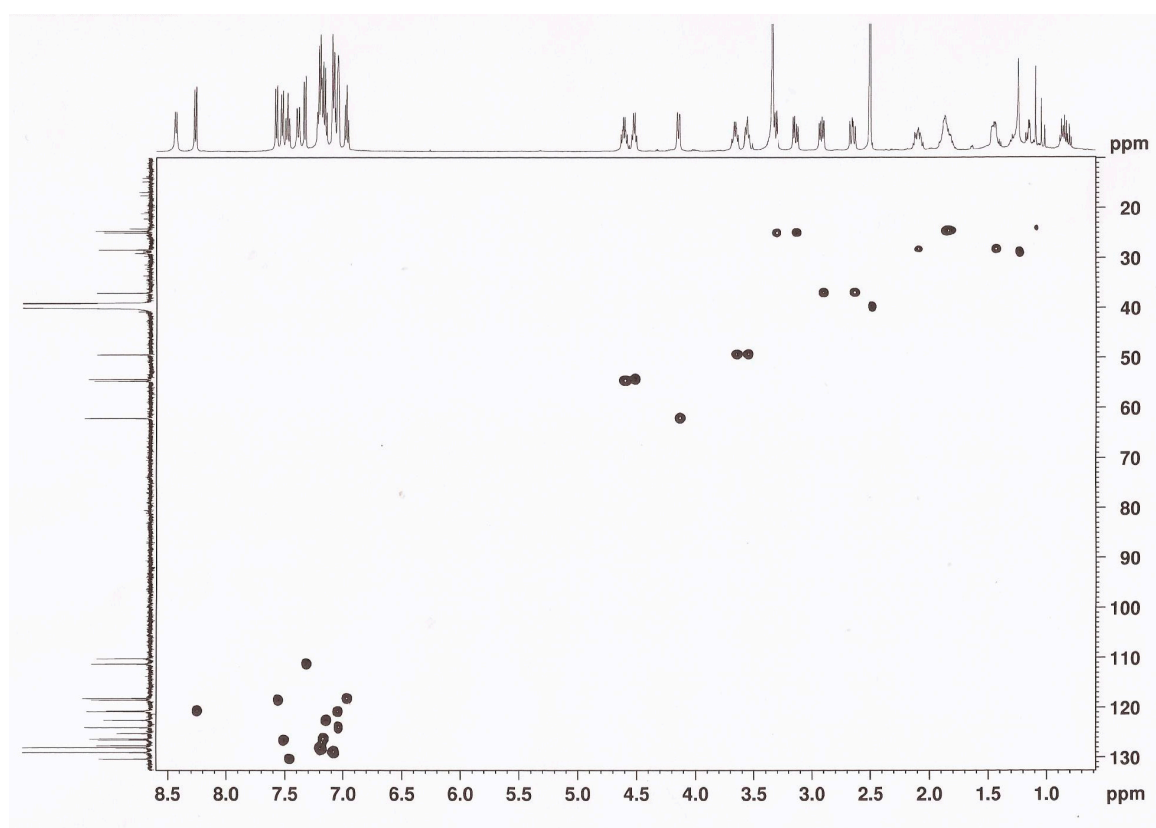


Figure S17. HSQC spectrum of compound 6 (DMSO, 500.13 MHz).

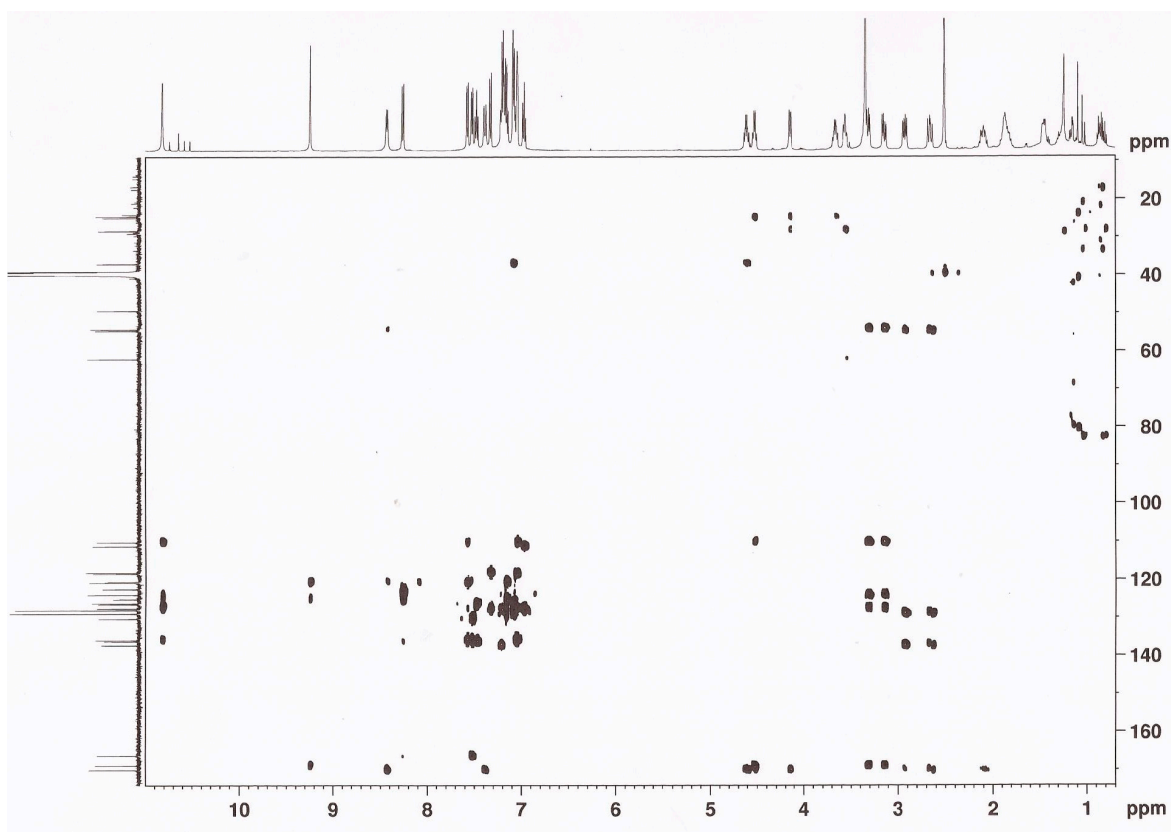


Figure S18. HMBC spectrum of compound 6 (DMSO, 500.13 MHz).

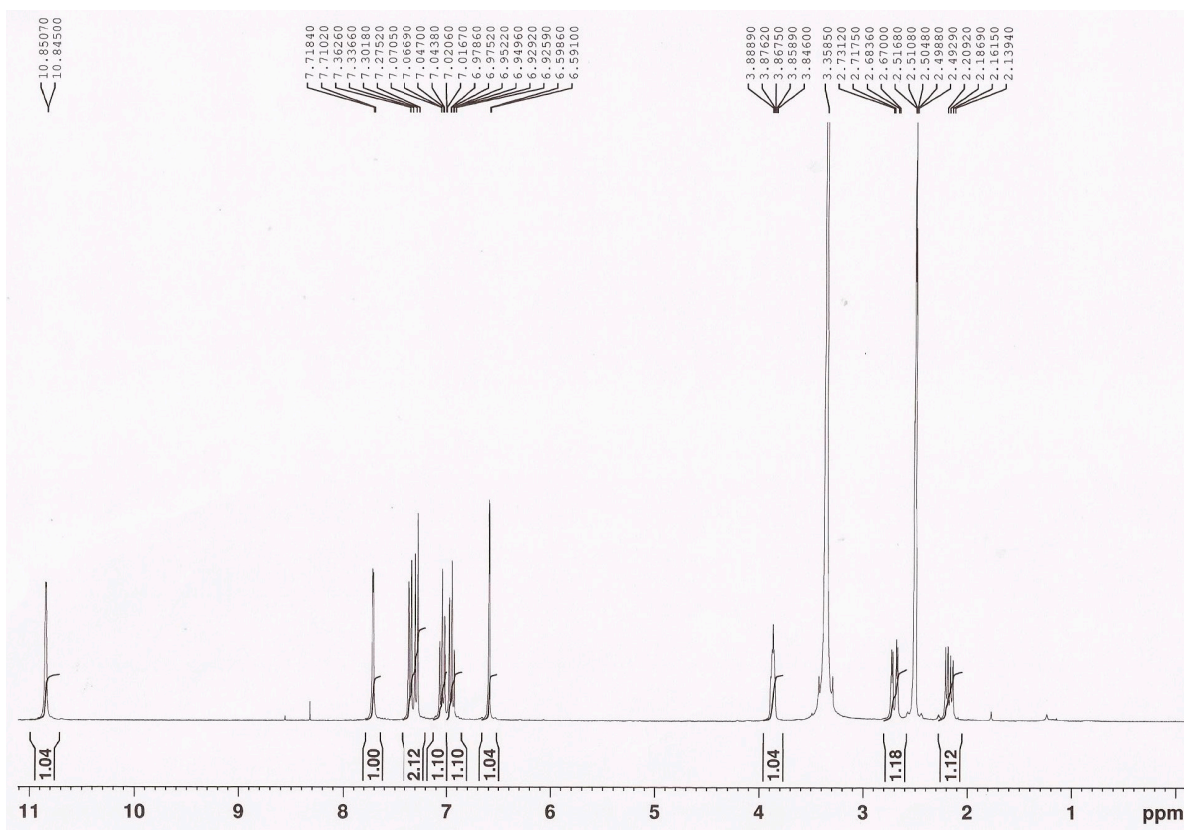


Figure S19.  $^1\text{H}$  NMR spectrum of compound 7 (DMSO, 300.13 MHz).

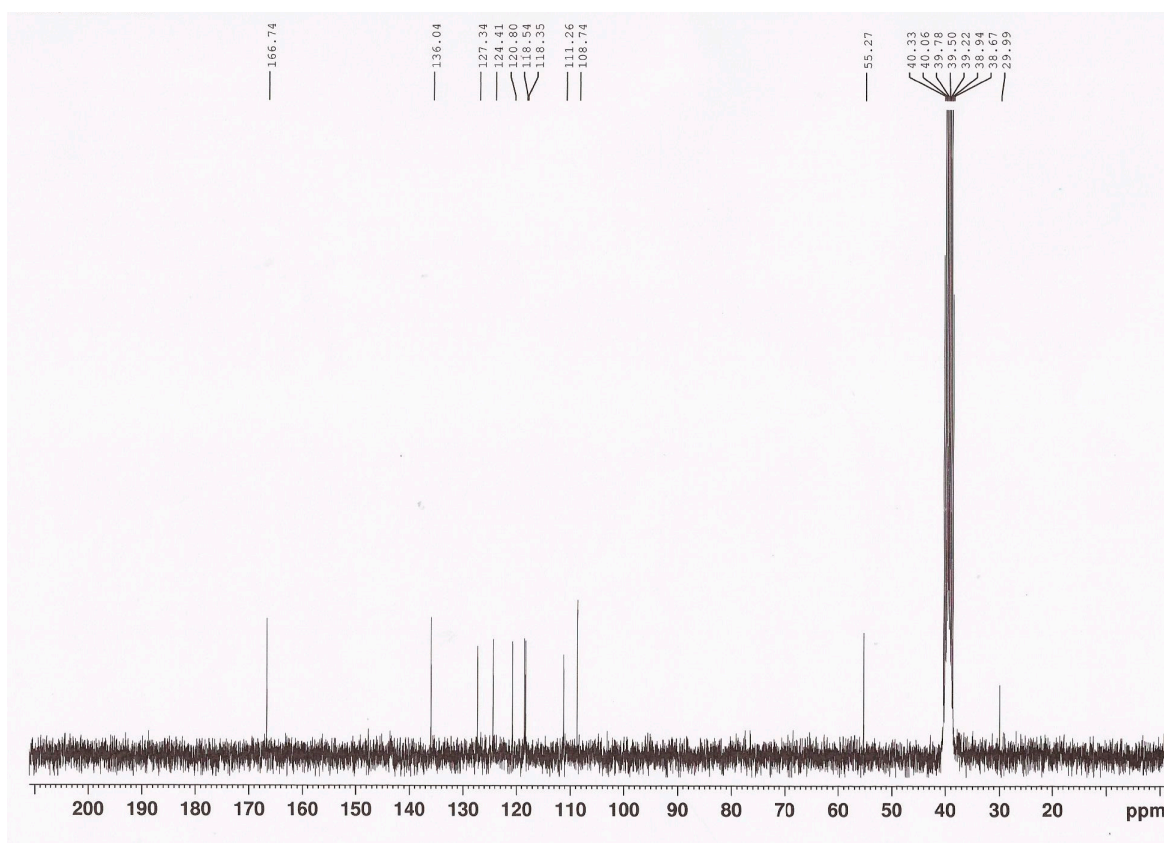


Figure S20.  $^{13}\text{C}$  NMR spectrum of compound 7 (DMSO, 75.4 MHz).

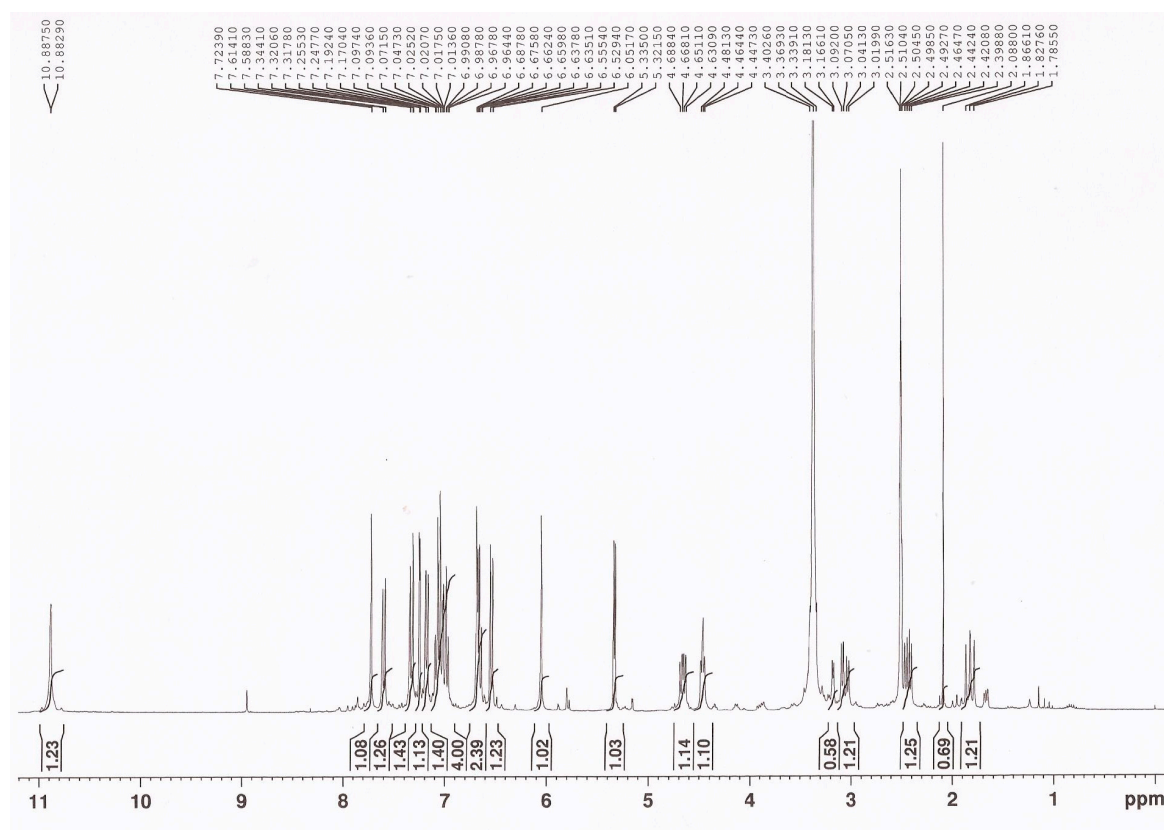


Figure S21.  $^1\text{H}$  NMR spectrum of compound 8 (DMSO, 300.13 MHz).

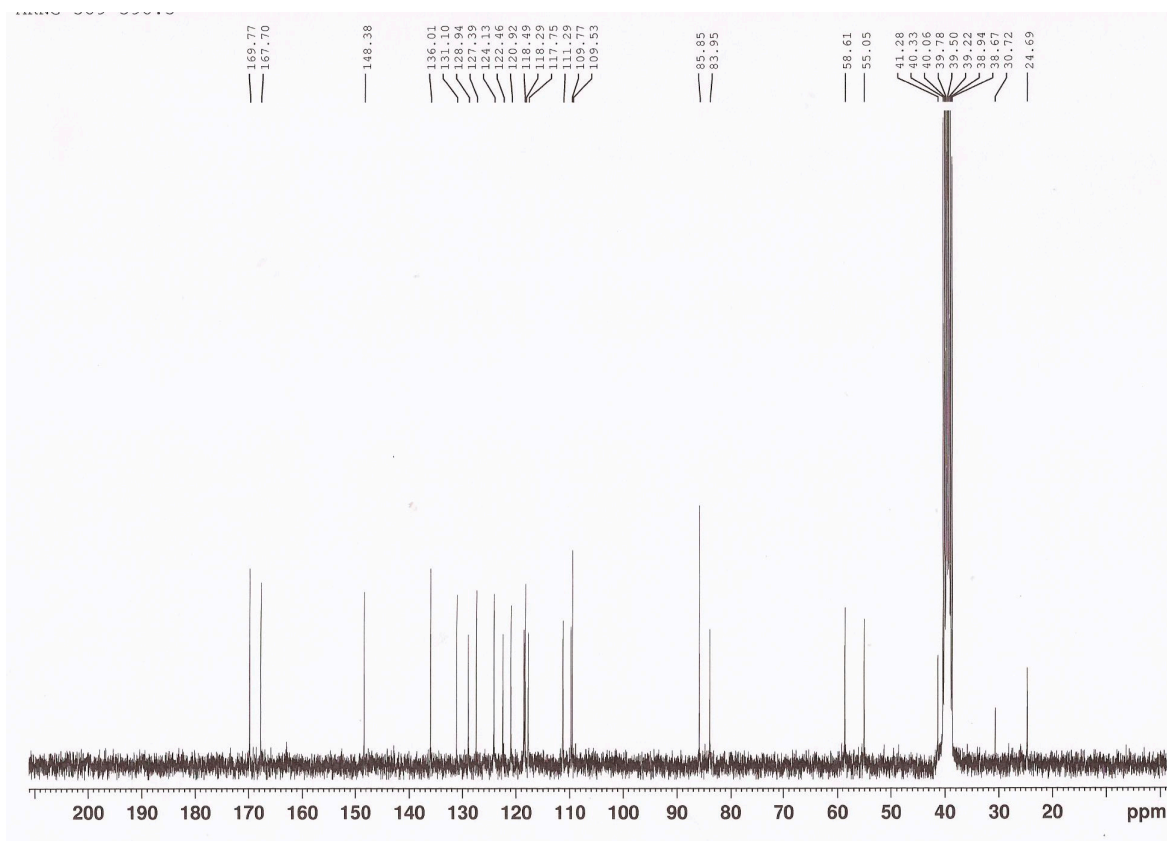


Figure S22.  $^{13}\text{C}$  NMR spectrum of compound 8 (DMSO, 75.4 MHz).

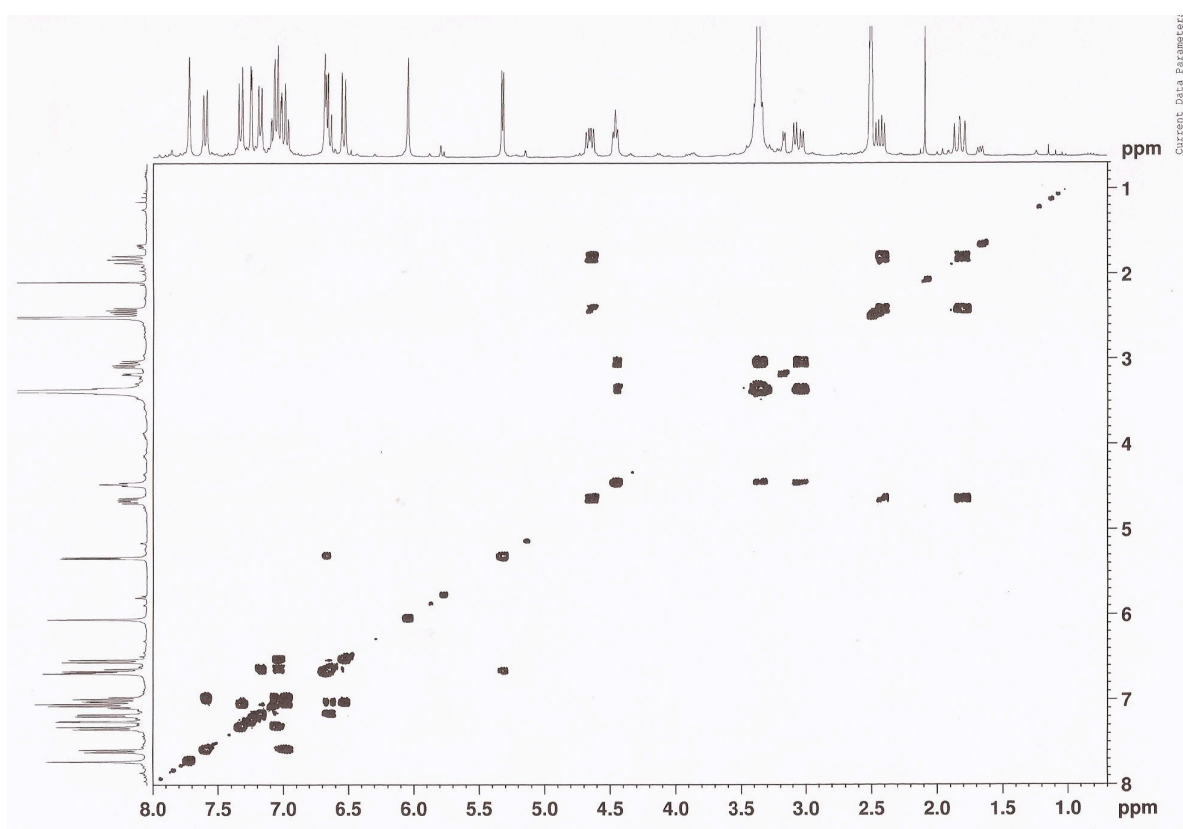


Figure S23. COSY spectrum of compound 8 (DMSO, 300.13 MHz).

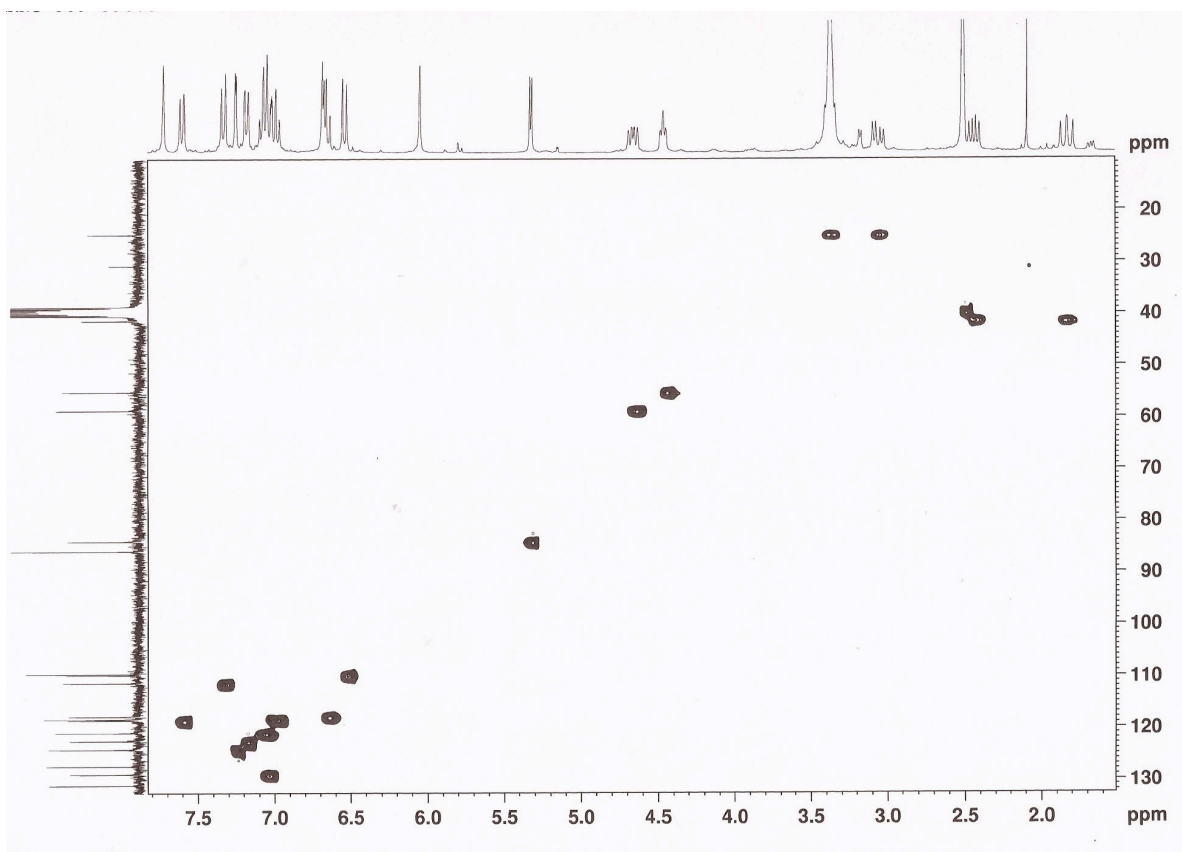


Figure S24. HSQC spectrum of compound 8 (DMSO, 300.13 MHz).

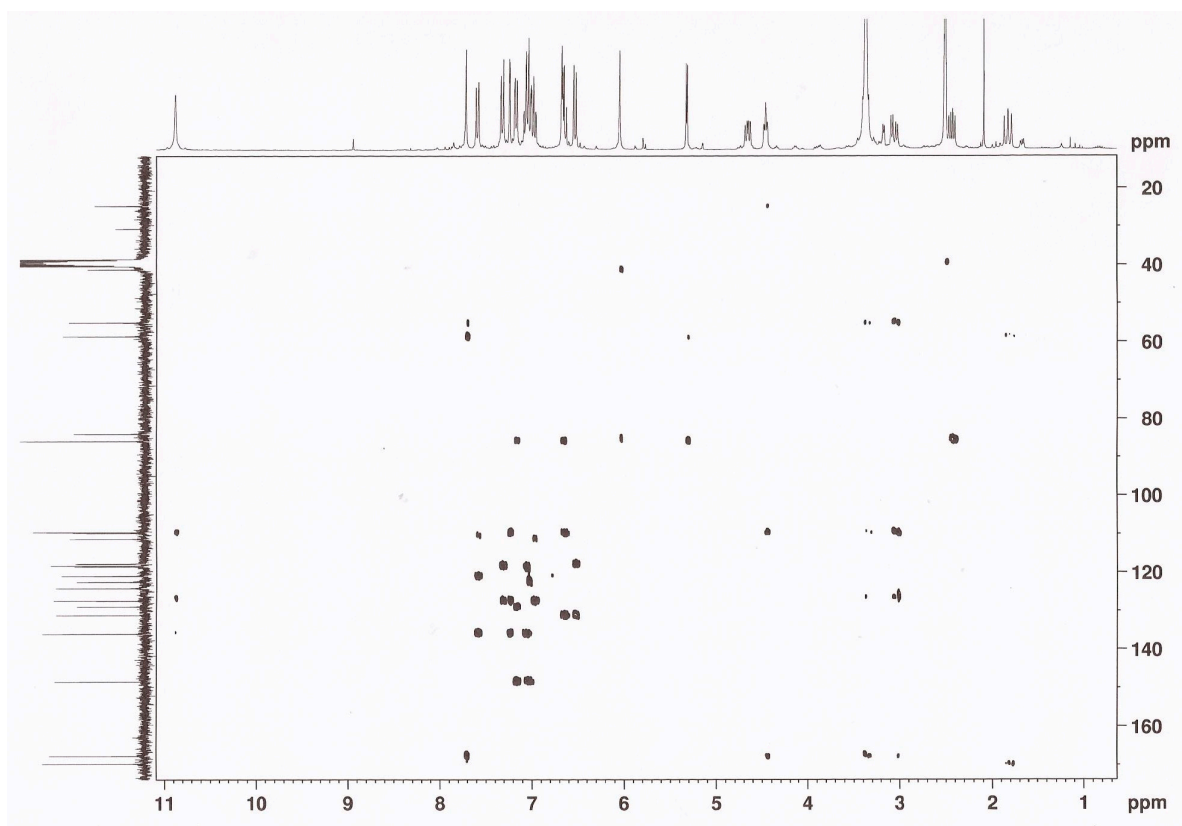


Figure S25. HMBC spectrum of compound 8 (DMSO, 300.13 MHz).

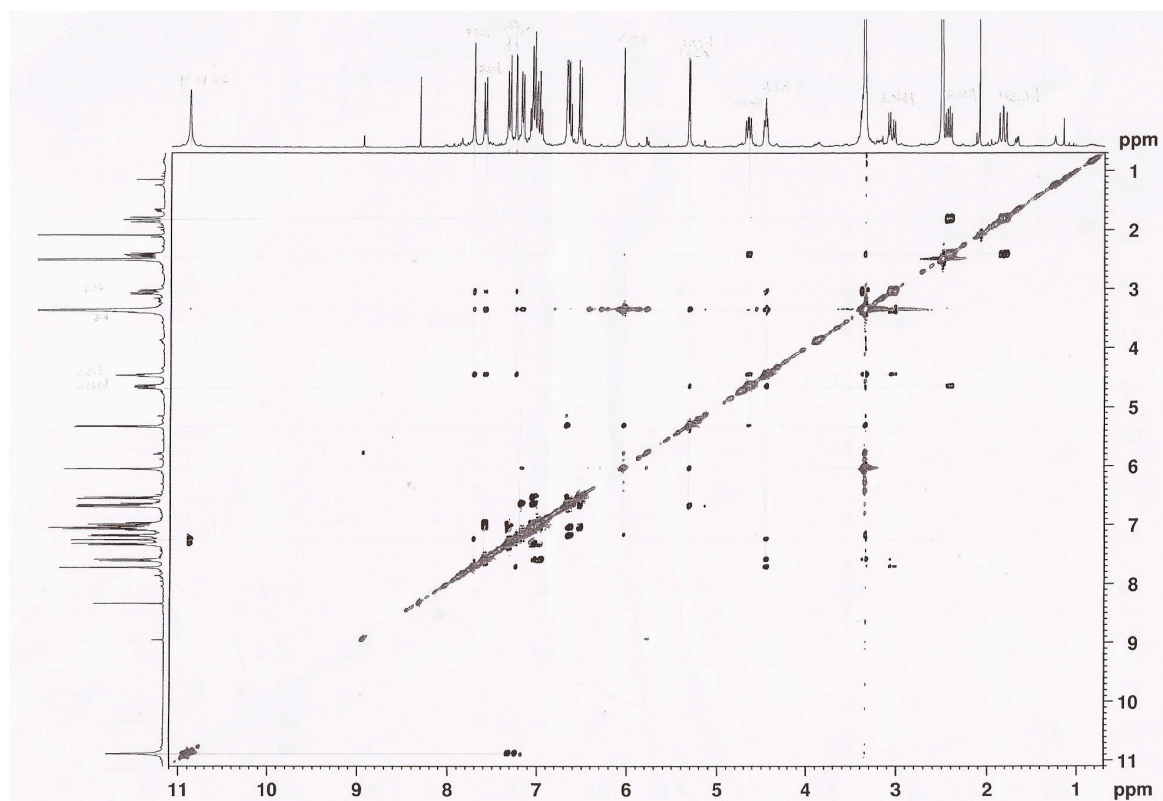


Figure S26. NOESY spectrum of compound 8 (DMSO, 300.13 MHz).

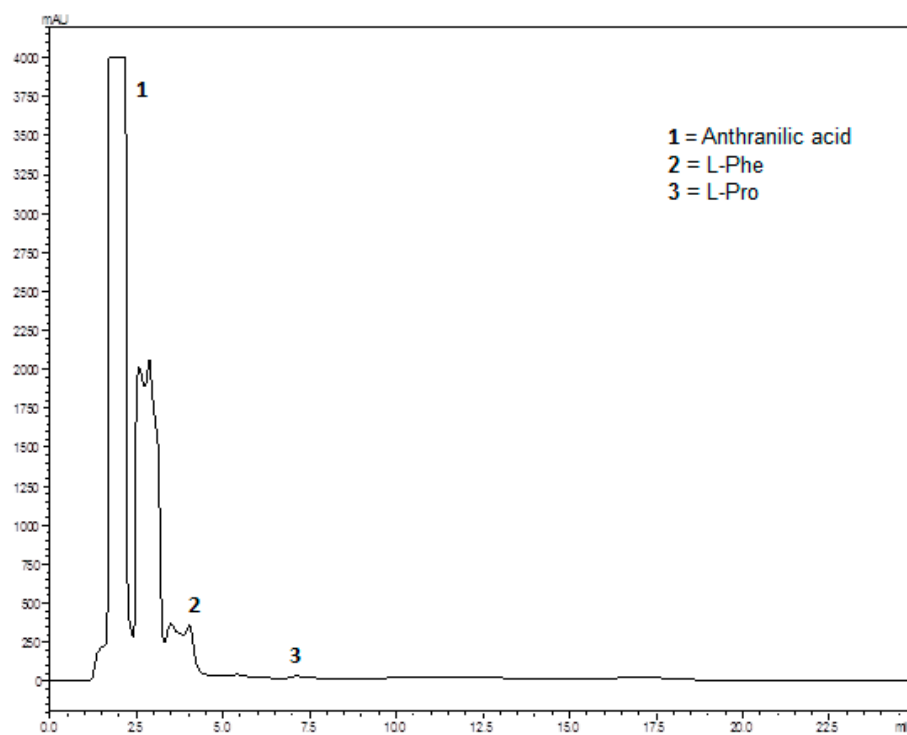
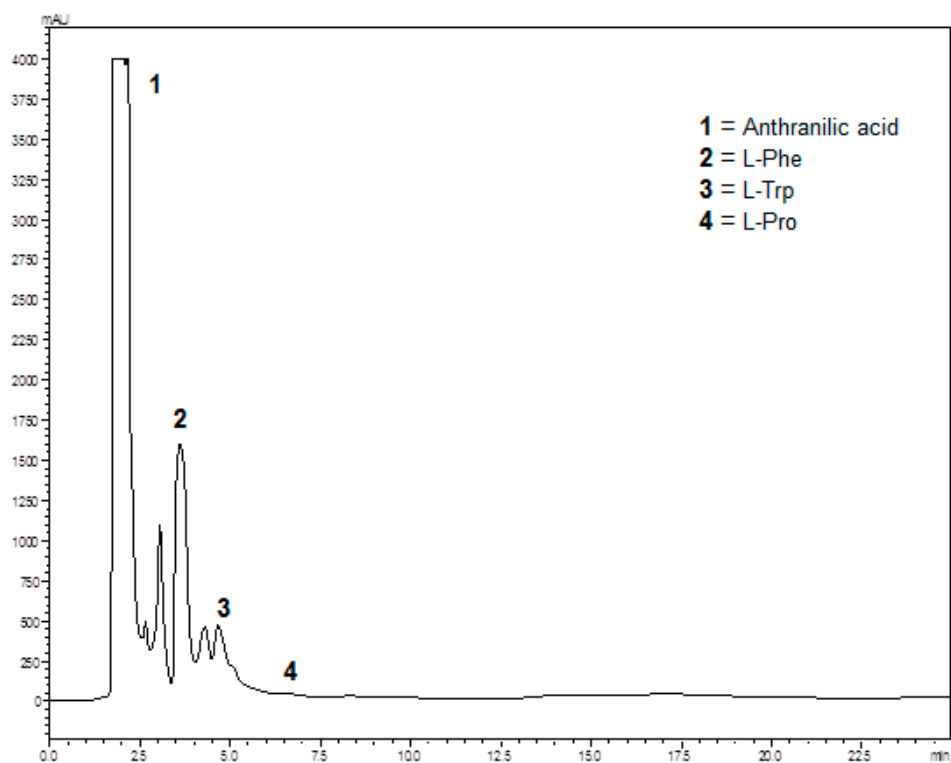


Figure S27. Chromatogram of the acidic hydrolysate of compound 5. Chromatographic conditions: column, Chirobiotic T; mobile phase, MeOH: H<sub>2</sub>O (80:20 *v/v*); flow rate, 1.0 mL/min; detection, 210 nm.



**Figure S28.** Chromatogram of the acidic hydrolysate of compound **6**. Chromatographic conditions: column, Chirobiotic T; mobile phase, MeOH: H<sub>2</sub>O (80:20 *v/v*); flow rate, 1.0 mL/min; detection, 210 nm.

**Table S1.** Chiral HPLC analysis of the acidic hydrolysate of compound **5** and **6**.

	Retain Time (min)
L-Phe	3.81
D-Phe	5.00
l-Pro	6.72
D-Pro	20.10
L-Trp	4.51
D-Trp	5.20
Anthranilic acid	1.92
Acidic hydrolysate of <b>5</b>	1.91, 2.55, 2.86, 3.49, 3.89, 6.79
Acidic hydrolysate of <b>5</b> + DL-Phe (coinjection)	1.87, 2.50, 2.89, 3.68, 5.01, 6.82
Acidic hydrolysate of <b>5</b> + DL-Pro (coinjection)	1.96, 2.60, 2.96, 3.52, 3.92, 6.70, 21.09
Acidic hydrolysate of <b>6</b>	1.93, 3.07, 3.80, 4.29, 4.60, 6.62
Acidic hydrolysate of <b>6</b> + DL-Phe (coinjection)	1.90, 3.10, 3.78, 4.39, 5.04, 6.70
Acidic hydrolysate of <b>6</b> + DL-Pro (coinjection)	2.04, 3.02, 3.72, 4.30, 4.60, 6.66, 19.40
Acidic hydrolysate of <b>6</b> + DL-Trp (coinjection)	1.93, 2.99, 3.70, 4.29, 4.60, 5.07, 6.33

Chromatographic conditions: column, Chirobiotic T; mobile phase, MeOH: H<sub>2</sub>O (80:20 *v/v*); flow rate, 1.0 mL/min; detection, 210 nm.