

## Supplementary data

# New Triterpenoids and Anti-inflammatory Constituents from *Glinus oppositifolius*

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Table S1. Inhibitory effect of compounds **1–20** on production of nitric oxide in LPS-stimulated RAW 264.7 cells.

Compounds	N1	N2	N3	NO inhibition IC <sub>50</sub> (μM) <sup>a</sup>
Spergulagenin B ( <b>1</b> )	25.00	23.35	25.93	24.76 ± 1.41 ***
Spergulagenin C ( <b>2</b> )	31.04	25.59	28.15	28.26 ± 2.78 **
Spergulagenin D ( <b>3</b> )	15.79	16.99	18.31	17.03 ± 1.28
Kaempferol ( <b>4</b> )	40.55	39.01	37.33	38.87 ± 1.68 ***
6,8-Dimethyl-5,7,4'-tri- hydroxyflavone ( <b>5</b> )	18.33	19.24	17.06	18.21 ± 1.15
5,7-Dihydroxy-6,8- dimethylflavone ( <b>6</b> )	43.82	46.46	40.65	43.61 ± 2.96 ***
5,4'-Dihydroxy-7-methoxy-6,8- dimethylflavone ( <b>7</b> )	31.95	29.46	34.83	32.08 ± 2.75 **
4-Hydroxybenzoic acid ( <b>8</b> )	69.20	76.00	82.29	75.83 ± 6.63 **
4-Hydroxybenzaldehyde ( <b>9</b> )	95.98	80.63	87.99	88.20 ± 7.78 **
4-Hydroxyacetophenone ( <b>10</b> )	69.90	76.03	82.79	76.24 ± 6.55 **
Methyl 4-Hydroxybenzoate ( <b>11</b> )	78.44	70.56	86.50	78.50 ± 8.00 **
<i>p</i> -Anisic acid ( <b>12</b> )	125.81	105.23	115.70	115.58 ± 10.35 **
Vanillin ( <b>13</b> )	83.96	105.88	95.01	94.95 ± 10.99 **
4-Hydroxy-3-methoxy- acetophenone ( <b>14</b> )	123.20	111.02	98.65	111.29 ± 12.91 **
Acetosyringone ( <b>15</b> )	75.37	68.86	82.06	75.43 ± 6.63 **
4-Hydroxy-3, 5-dimethoxy- benzaldehyde ( <b>16</b> )	86.50	94.36	79.00	86.62 ± 7.74 **
4-Hydroxybenzyl alcohol ( <b>17</b> )	78.72	85.79	71.41	78.64 ± 7.23 **
2-(4-Hydroxyphenyl)ethanol ( <b>18</b> )	30.33	28.55	26.53	28.47 ± 1.94 ***
Cinnamic acid ( <b>19</b> )	15.20	17.71	15.99	16.30 ± 1.41
<i>trans</i> -Ferulic acid ( <b>20</b> )	13.87	12.51	11.63	12.64 ± 1.14 **
Quercetin <sup>b</sup>	17.94	16.80	15.48	16.74 ± 1.26

<sup>a</sup> The IC<sub>50</sub> value was defined as half-maximal inhibitory concentration and was expressed as mean ± SD (n = 3); <sup>b</sup> Quercetin was used as positive control; \* *p* < 0.05, \*\**p* < 0.01, \*\*\**p* < 0.001 compared with the control.

Table S2. Inhibitory effect of compounds **1–20** on the production of pro-inflammatory cytokine, TNF- $\alpha$  in LPS-stimulated RAW 264.7 cells.

Compounds	N1	N2	N3	TNF- $\alpha$ inhibition IC <sub>50</sub> ( $\mu$ M) <sup>a</sup>
Spergulagenin B ( <b>1</b> )	28.54	30.24	32.69	30.49 $\pm$ 2.20 **
Spergulagenin C ( <b>2</b> )	33.95	31.00	29.13	31.36 $\pm$ 2.59 **
Spergulagenin D ( <b>3</b> )	18.24	19.69	17.12	18.35 $\pm$ 1.34 **
Kaempferol ( <b>4</b> )	30.97	40.71	35.45	35.71 $\pm$ 4.74 *
6,8-Dimethyl-5,7,4'-tri- hydroxyflavone ( <b>5</b> )	16.15	19.30	17.23	17.56 $\pm$ 1.41 **
5,7-Dihydroxy-6,8- dimethylflavone ( <b>6</b> )	39.21	42.81	36.42	9.48 $\pm$ 3.06 **
5,4'-Dihydroxy-7-methoxy-6,8- dimethylflavone ( <b>7</b> )	31.68	36.27	34.56	34.17 $\pm$ 2.49 **
4-Hydroxybenzoic acid ( <b>8</b> )	72.97	87.12	79.97	80.02 $\pm$ 7.10 **
4-Hydroxybenzaldehyde ( <b>9</b> )	80.49	92.66	85.99	86.38 $\pm$ 6.28 ***
4-Hydroxyacetophenone ( <b>10</b> )	84.29	78.97	73.83	79.03 $\pm$ 5.26 ***
Methyl 4-Hydroxybenzoate ( <b>11</b> )	75.40	82.01	89.58	82.33 $\pm$ 7.25 **
<i>p</i> -Anisic acid ( <b>12</b> )	137.14	126.01	114.37	125.84 $\pm$ 11.47 **
Vanillin ( <b>13</b> )	111.71	102.22	93.12	102.35 $\pm$ 9.36 **
4-Hydroxy-3-methoxy- acetophenone ( <b>14</b> )	122.90	111.87	134.44	123.07 $\pm$ 11.37 **
Acetosyringone ( <b>15</b> )	73.86	68.17	63.11	68.38 $\pm$ 5.48 **
4-Hydroxy-3, 5-dimethoxy- benzaldehyde ( <b>16</b> )	70.80	77.25	84.12	77.39 $\pm$ 6.73 **
4-Hydroxybenzyl alcohol ( <b>17</b> )	69.50	61.62	77.02	69.38 $\pm$ 7.64 **
2-(4-Hydroxyphenyl)ethanol ( <b>18</b> )	24.14	28.79	26.39	26.44 $\pm$ 2.35 *
Cinnamic acid ( <b>19</b> )	20.54	23.51	21.95	22.00 $\pm$ 1.51 **
<i>trans</i> -Ferulic acid ( <b>20</b> )	14.38	15.45	14.27	14.27 $\pm$ 1.29 **
Quercetin <sup>b</sup>	5.28	5.11	4.85	5.08 $\pm$ 0.23

<sup>a</sup> The IC<sub>50</sub> value was defined as half-maximal inhibitory concentration and was expressed as mean  $\pm$  SD (n = 3); <sup>b</sup> Quercetin was used as positive control; \*  $p$  < 0.05, \*\* $p$  < 0.01, and \*\*\* $p$  < 0.001 compared with the control.

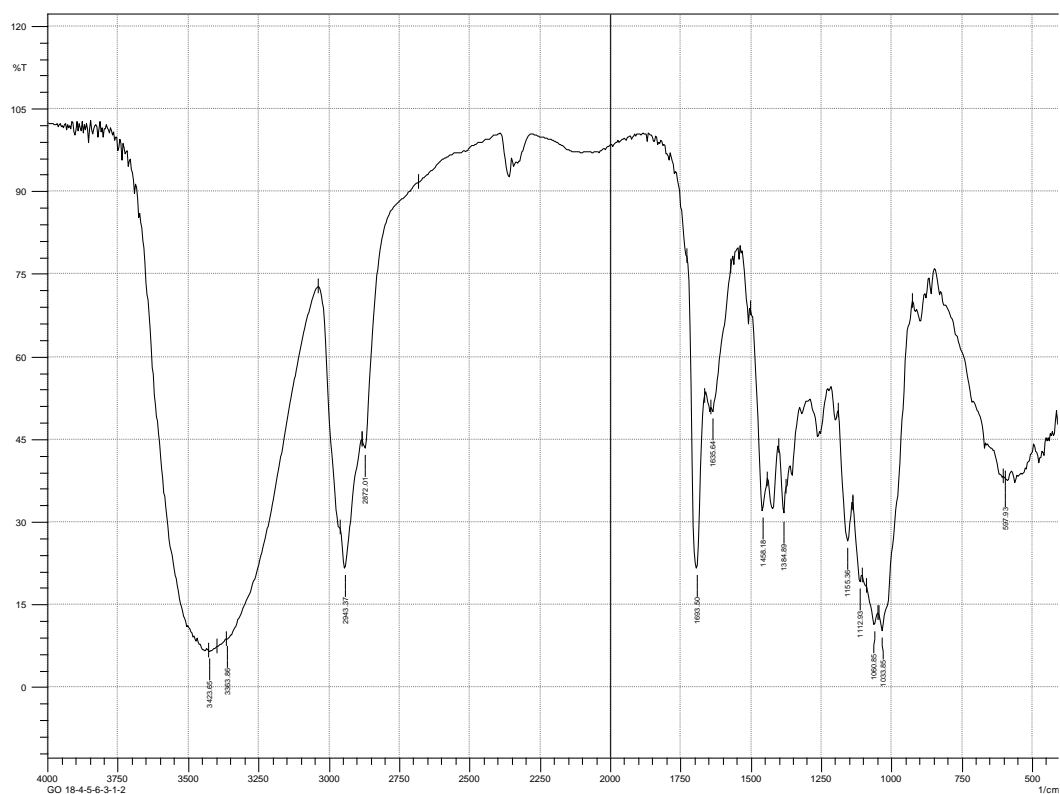


Figure S1. IR spectrum of **1**.

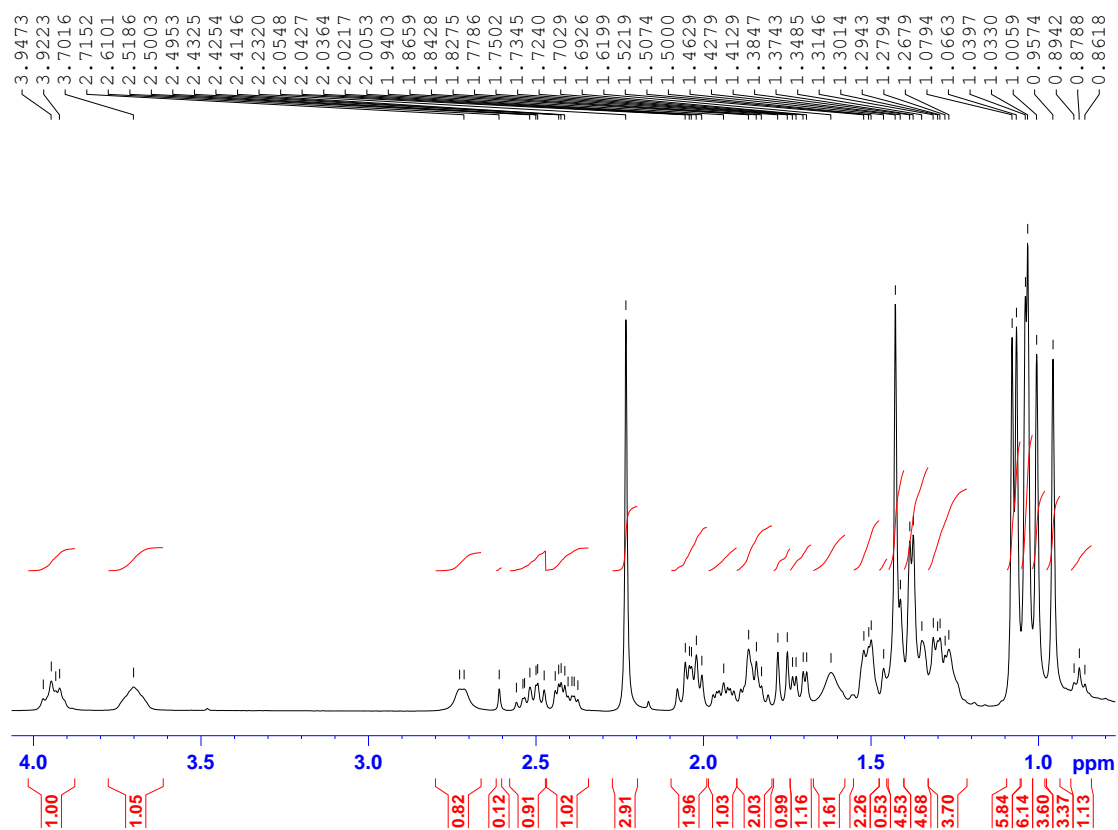


Figure S2.  $^1\text{H}$ -NMR spectrum of **1** ( $\text{CDCl}_3$ , 500 MHz).

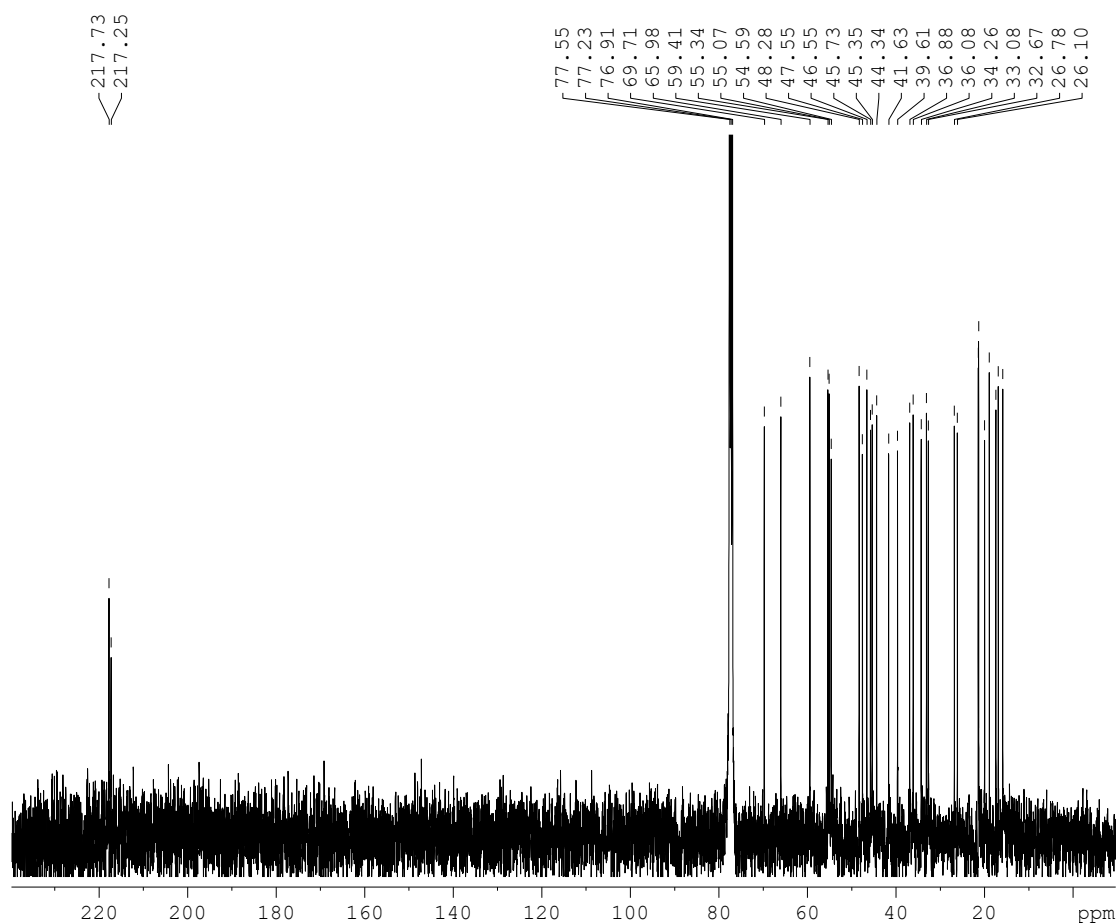


Figure S3.  $^{13}\text{C}$ -NMR spectrum of **1** ( $\text{CDCl}_3$ , 125 MHz).

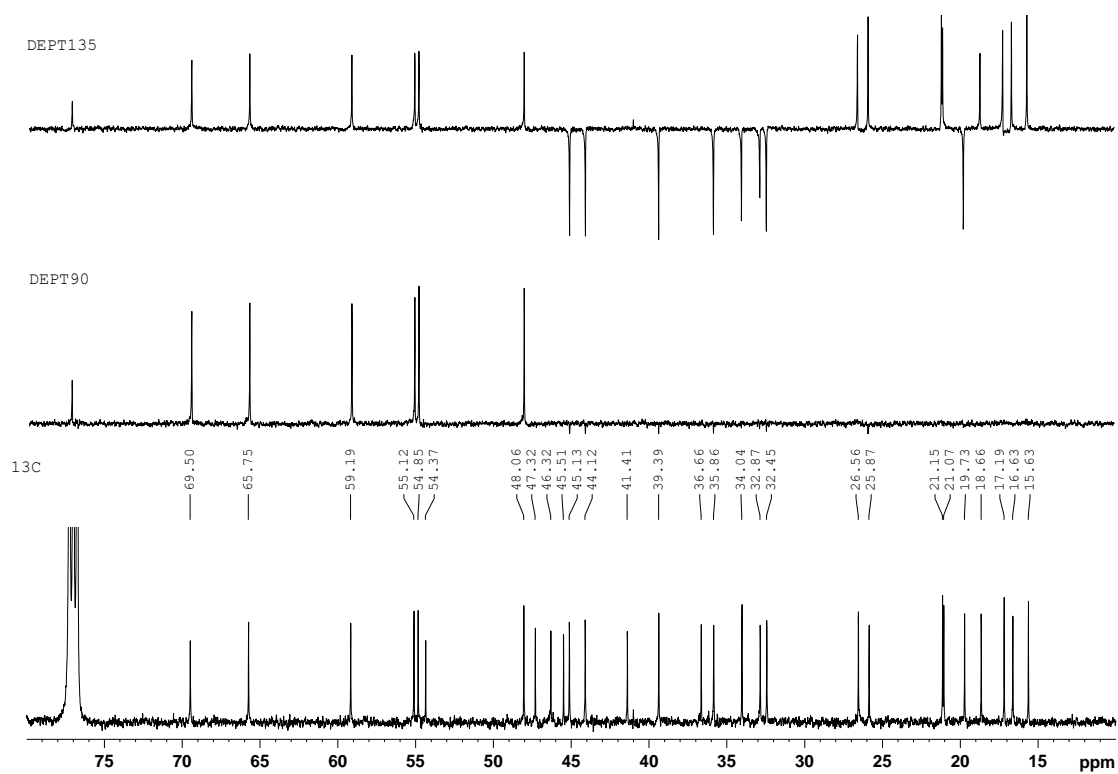


Figure S4.  $^{13}\text{C}$ -DEPT spectrum of **1** ( $\text{CDCl}_3$ , 125 MHz).

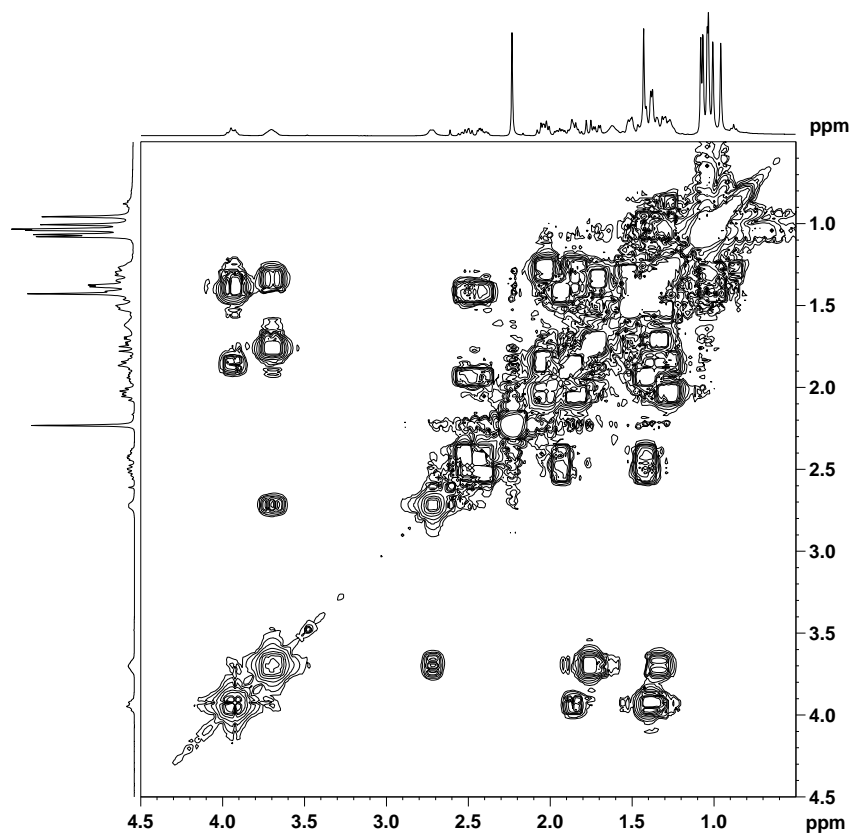


Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1**.

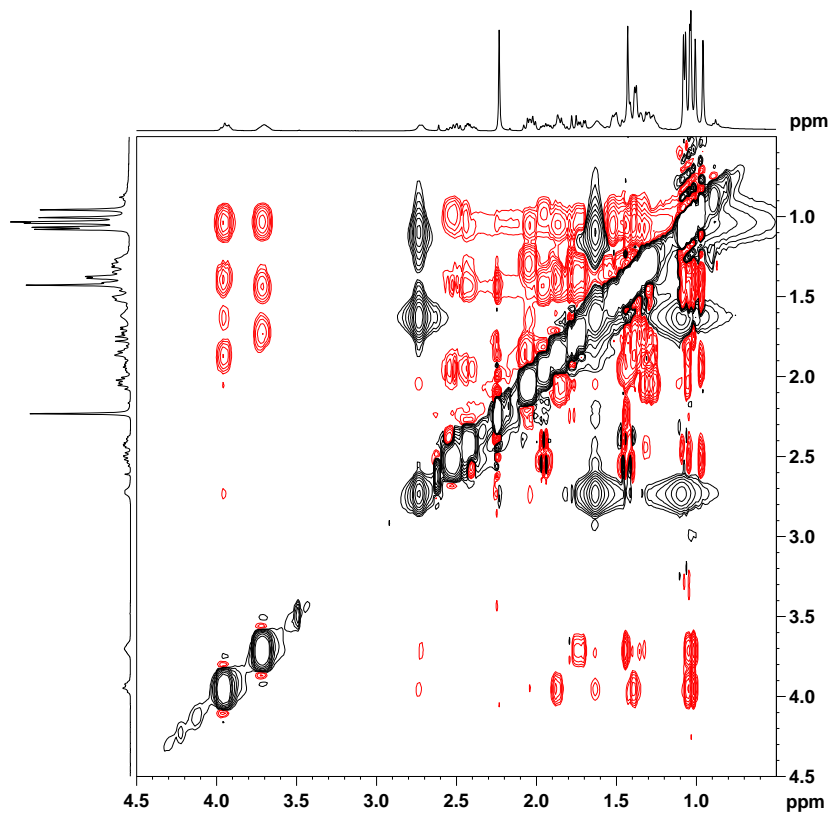


Figure S6. NOESY spectrum of **1**.



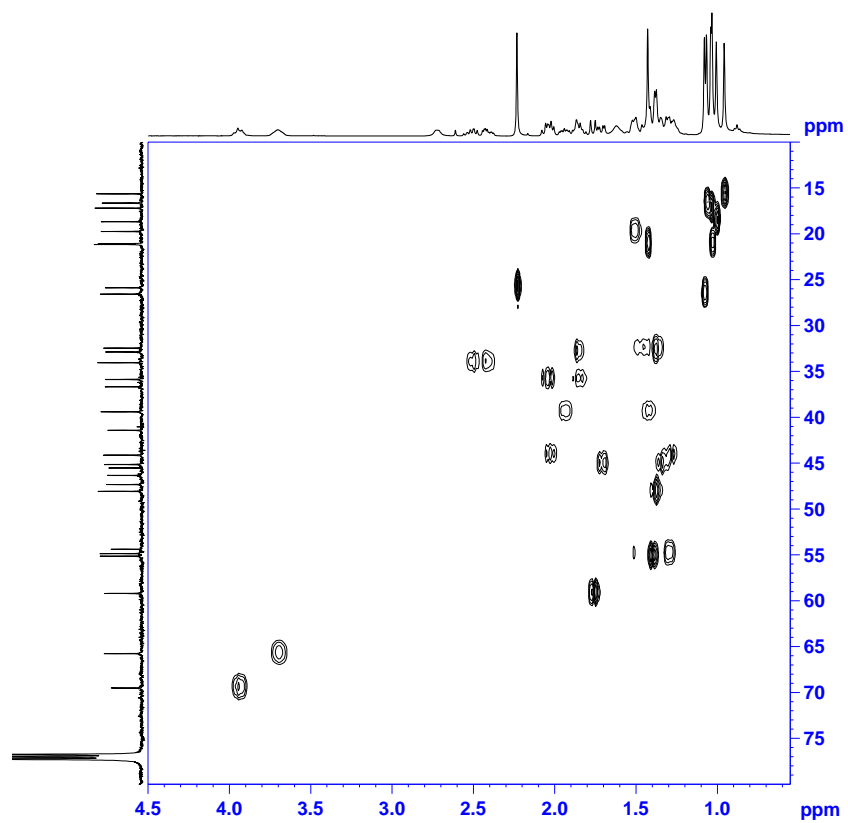


Figure S7. HSQC spectrum of **1**.

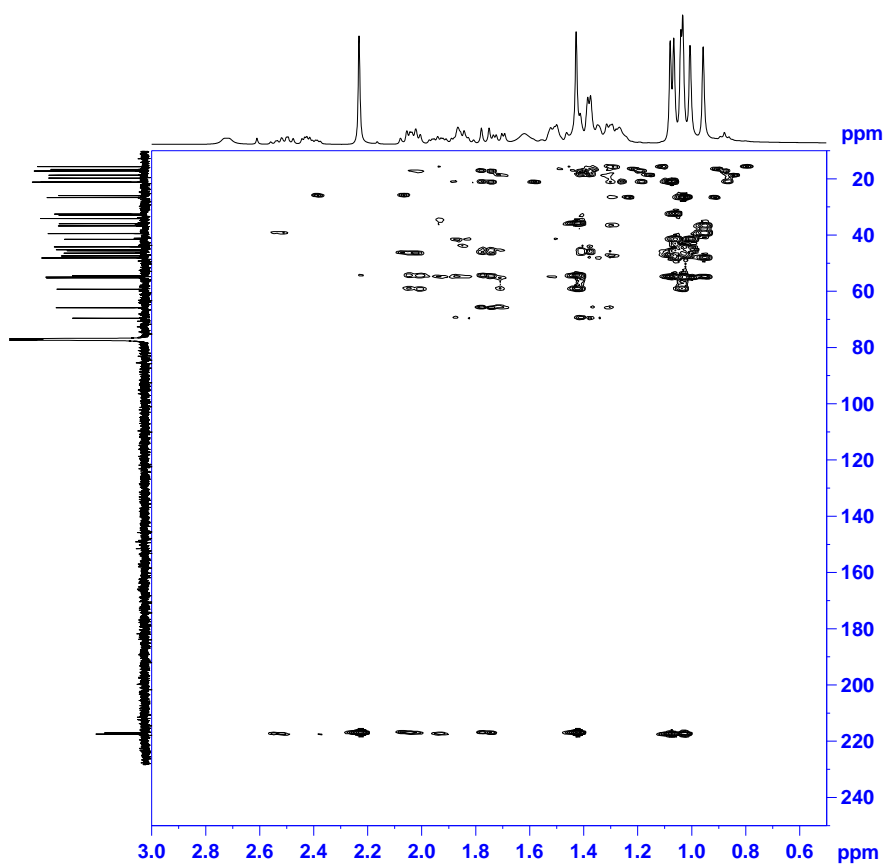


Figure S8. HMBC spectrum of **1**.

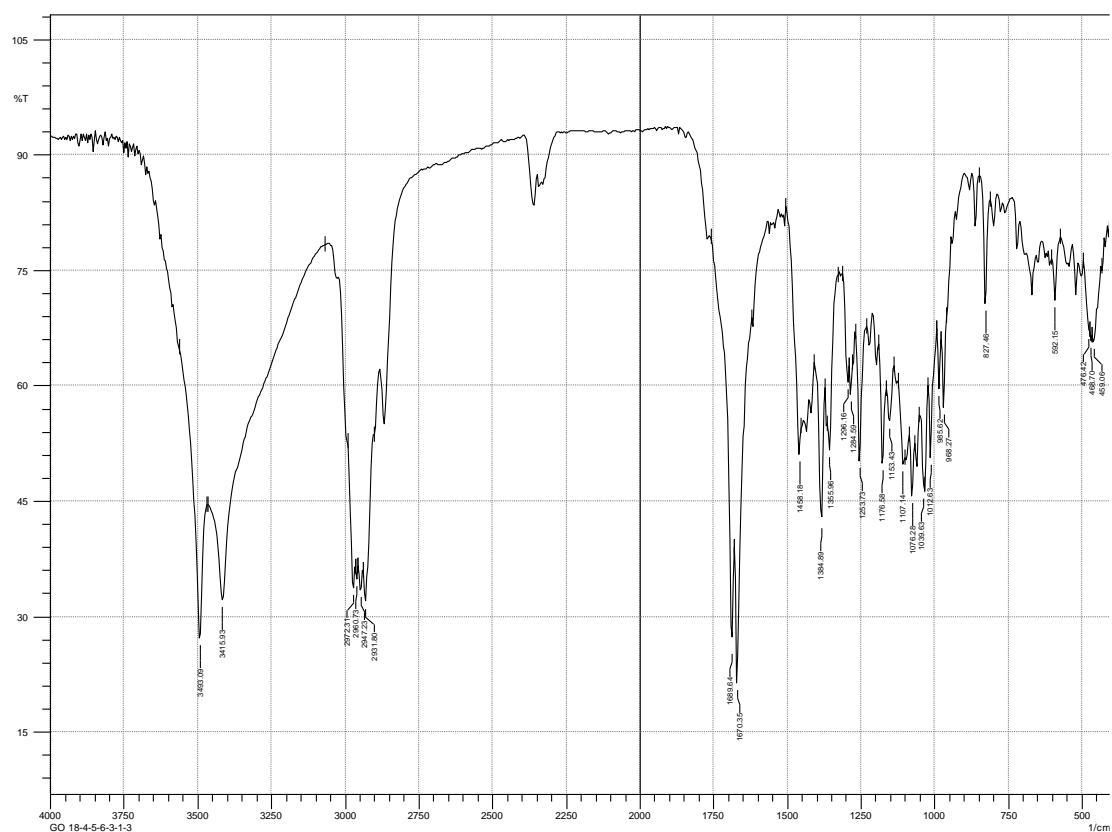


Figure S9. IR spectrum of **2**.

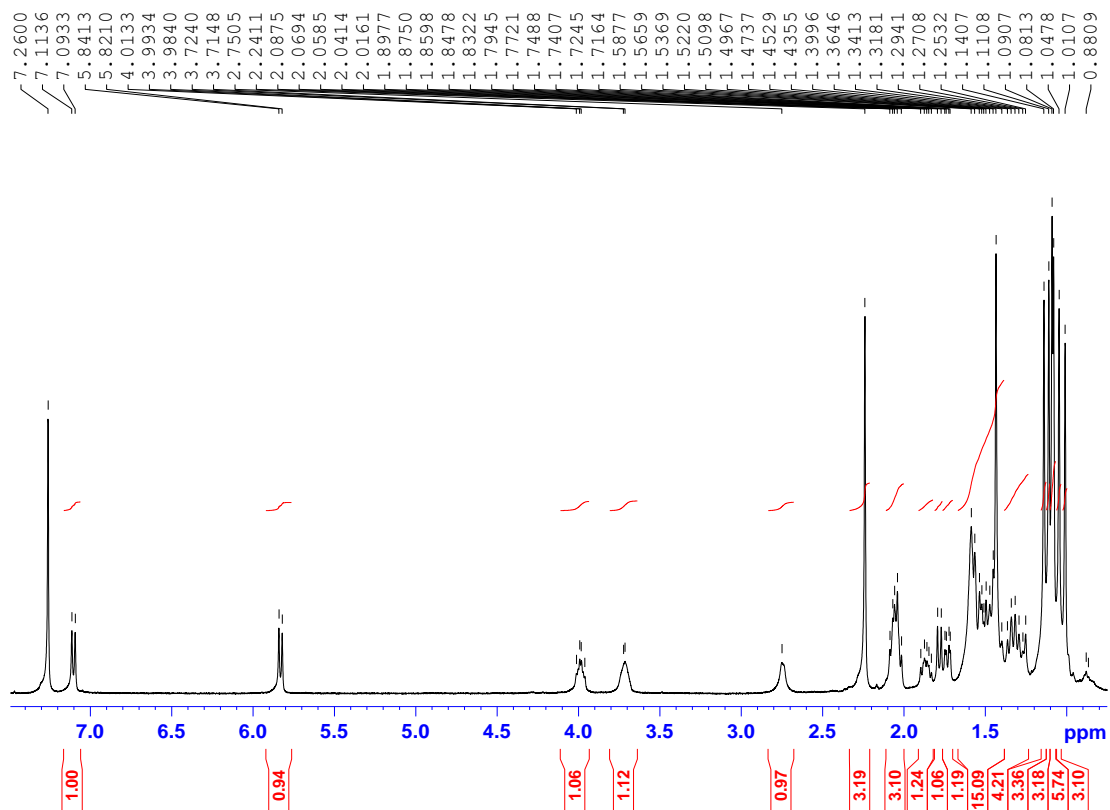


Figure S10. <sup>1</sup>H-NMR spectrum of **2** (CDCl<sub>3</sub>, 500 MHz).

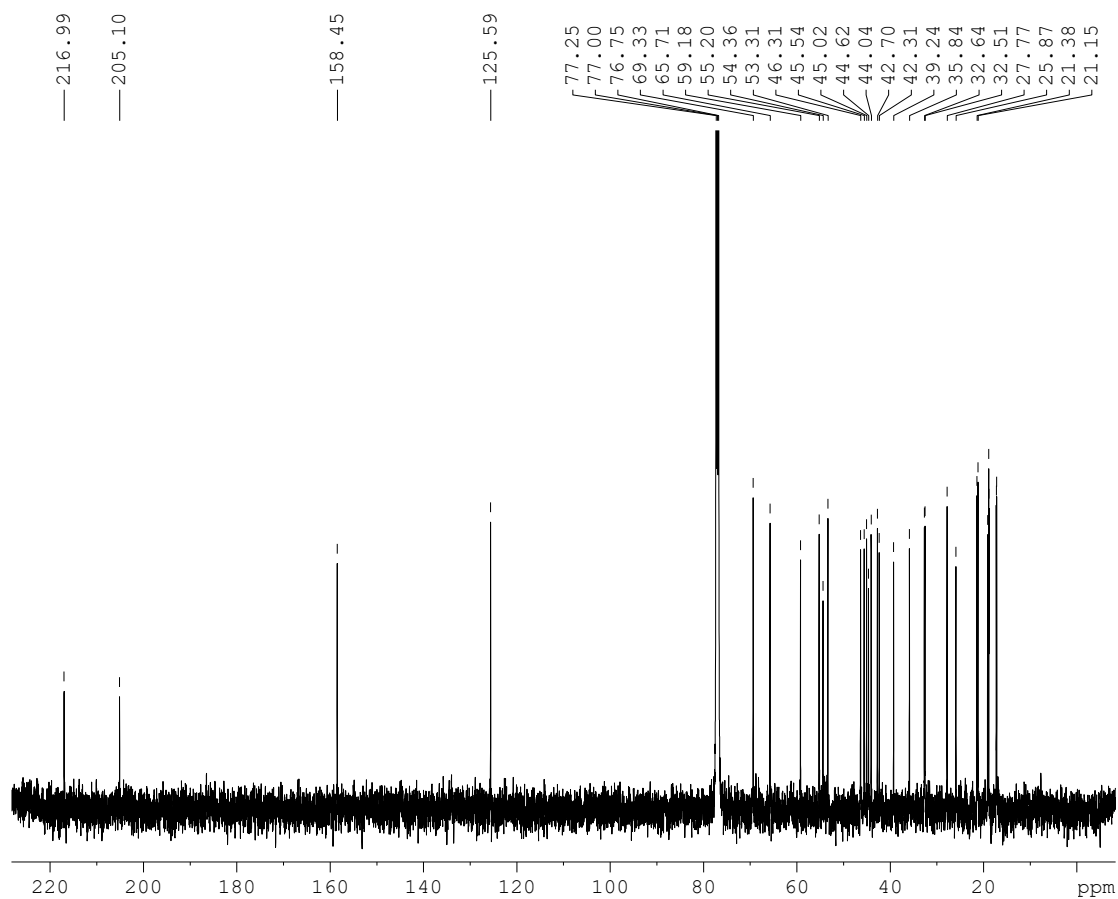


Figure S11.  $^{13}\text{C}$ -NMR spectrum of **2** ( $\text{CDCl}_3$ , 125 MHz).

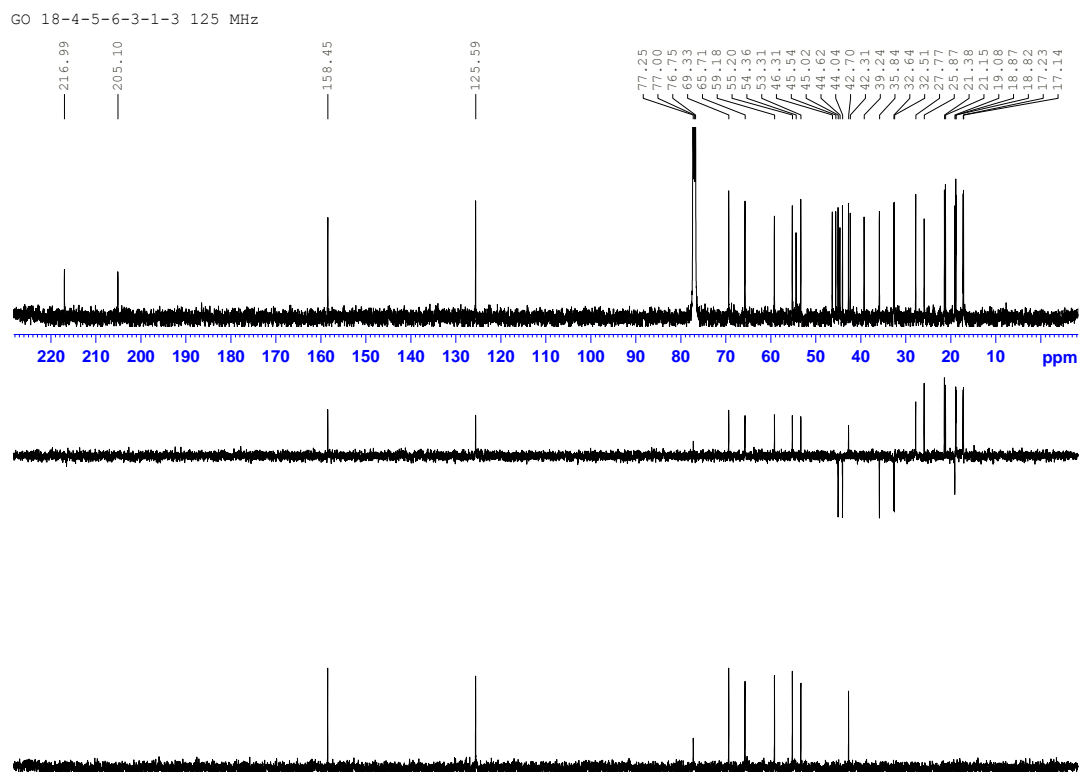


Figure S12.  $^{13}\text{C}$ -DEPT spectrum of **2** ( $\text{CDCl}_3$ , 125 MHz).

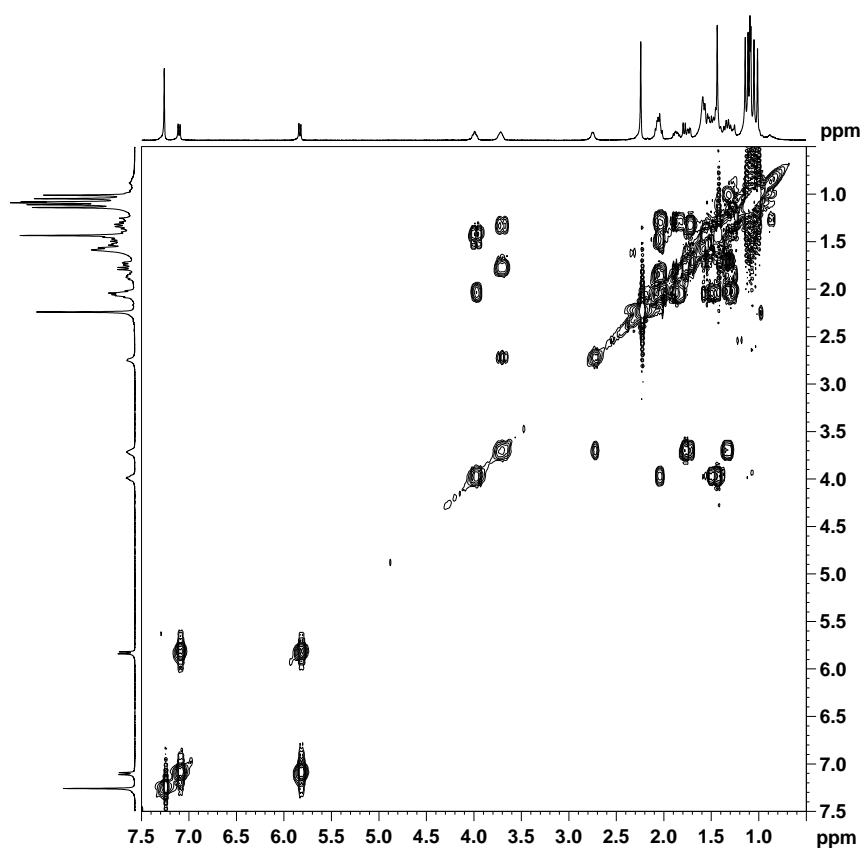


Figure S13.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2**.

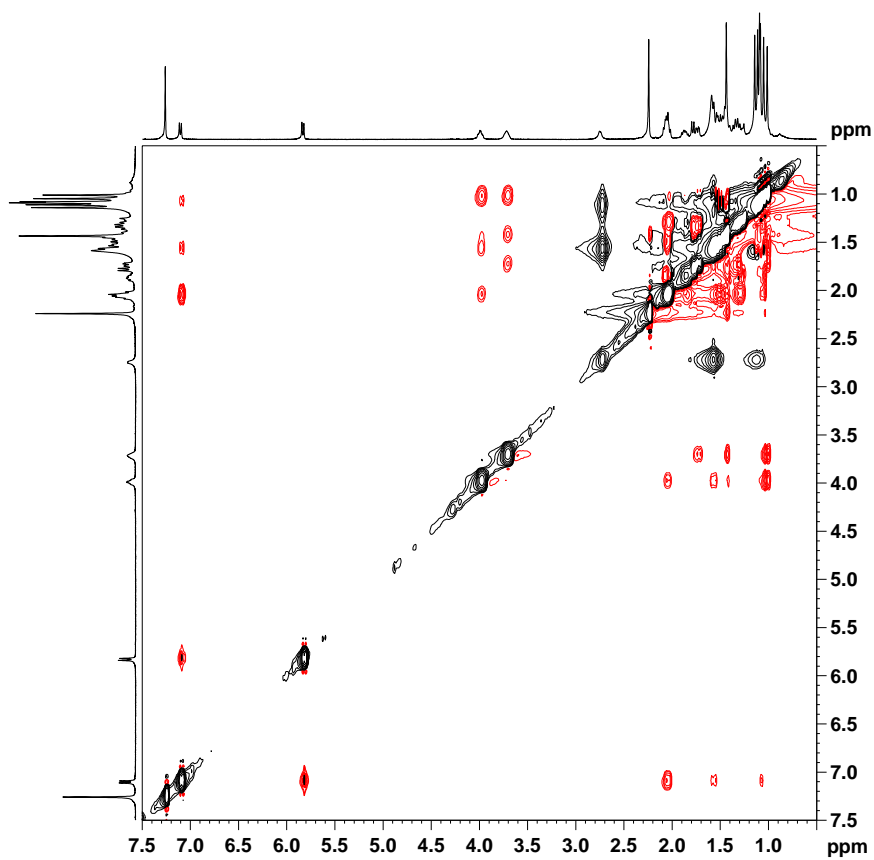


Figure S14. NOESY spectrum of **2**.

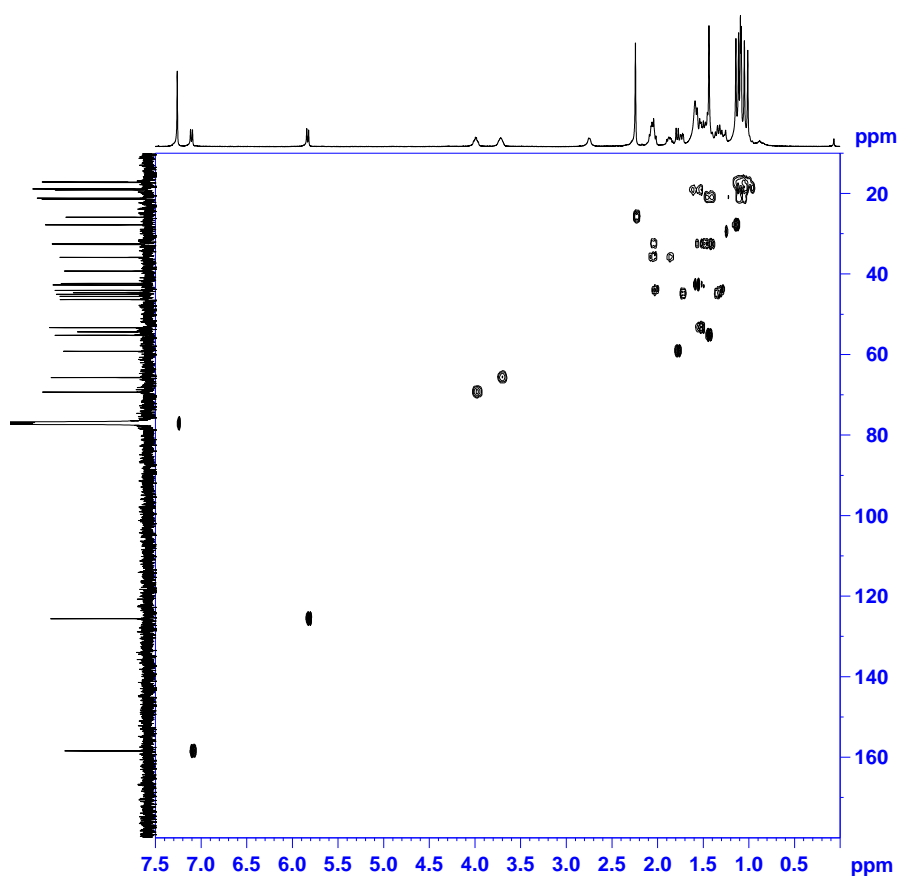


Figure S15. HSQC spectrum of 2.

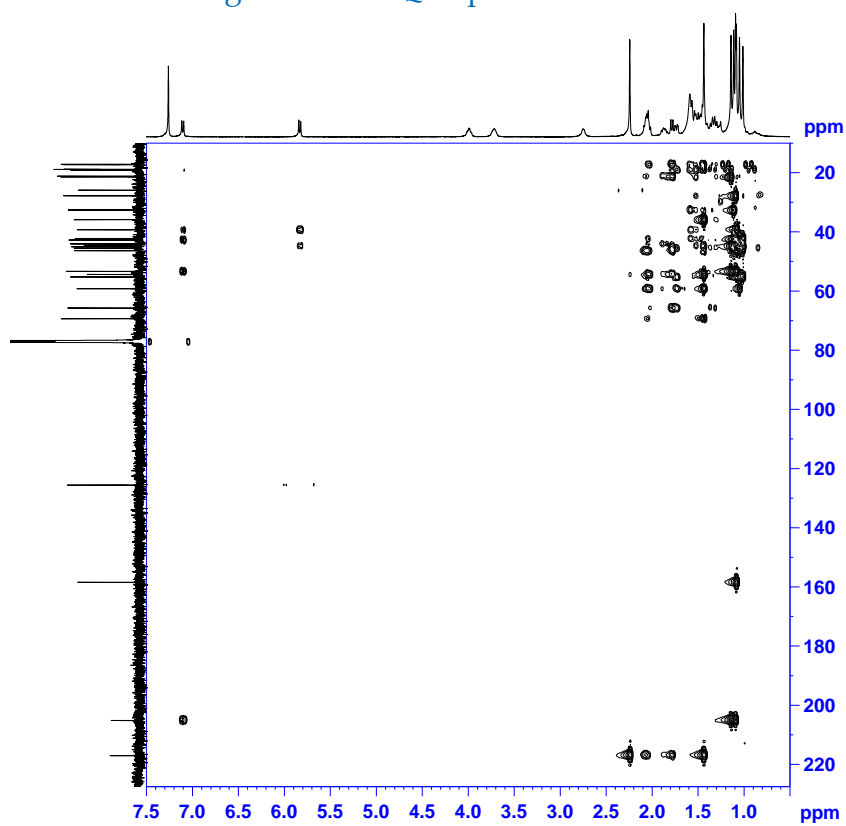


Figure S16. HMBC spectrum of 2.

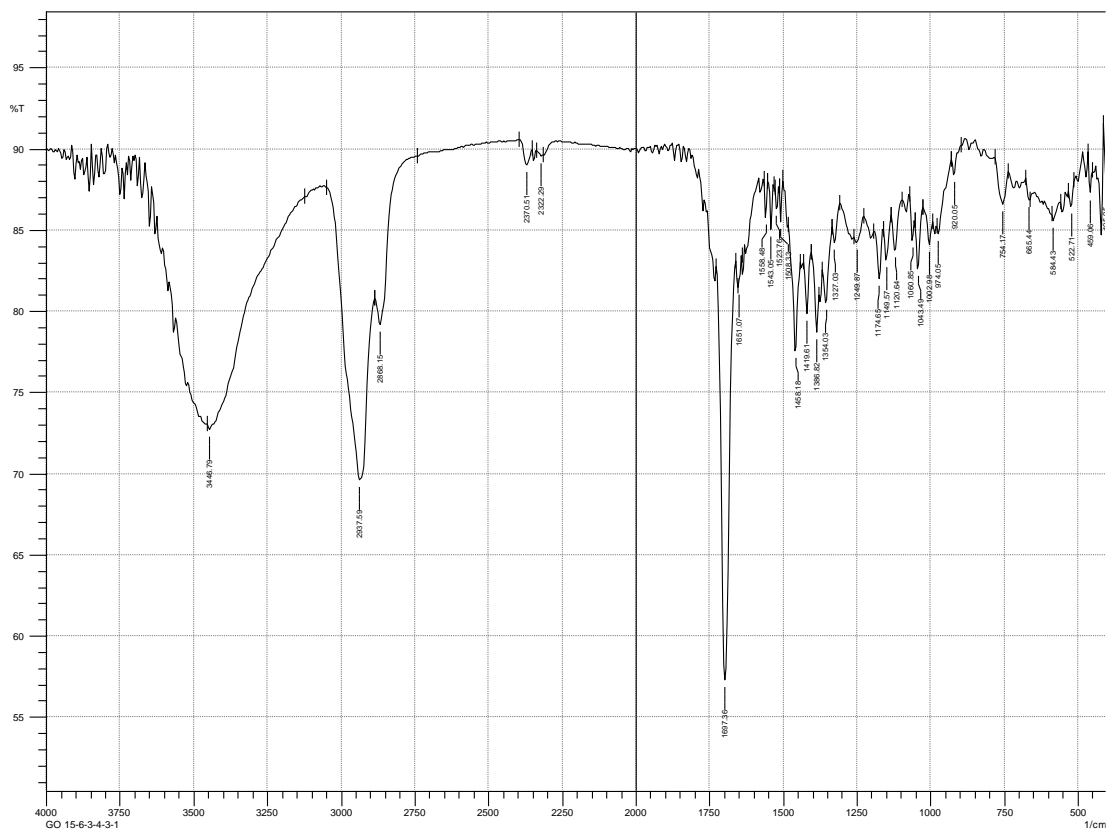


Figure S17. IR spectrum of 3.

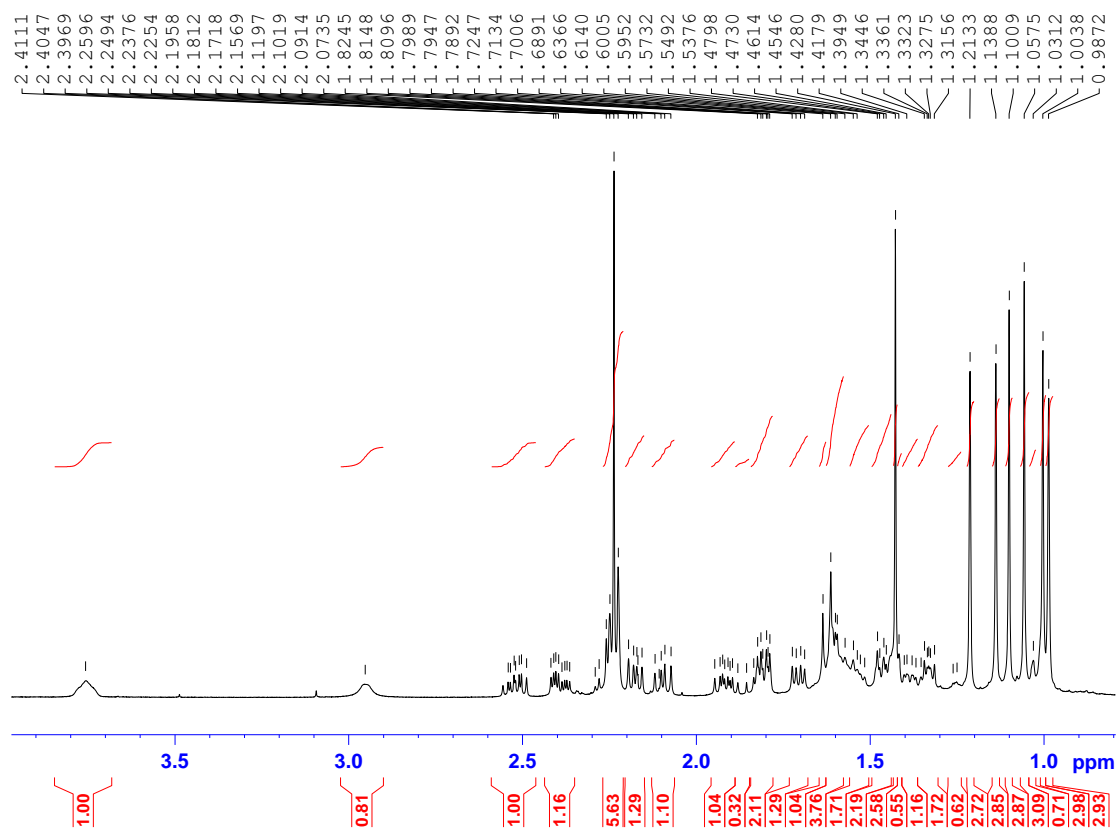


Figure S18.  $^1\text{H}$ -NMR spectrum of 3 ( $\text{CDCl}_3$ , 500 MHz).

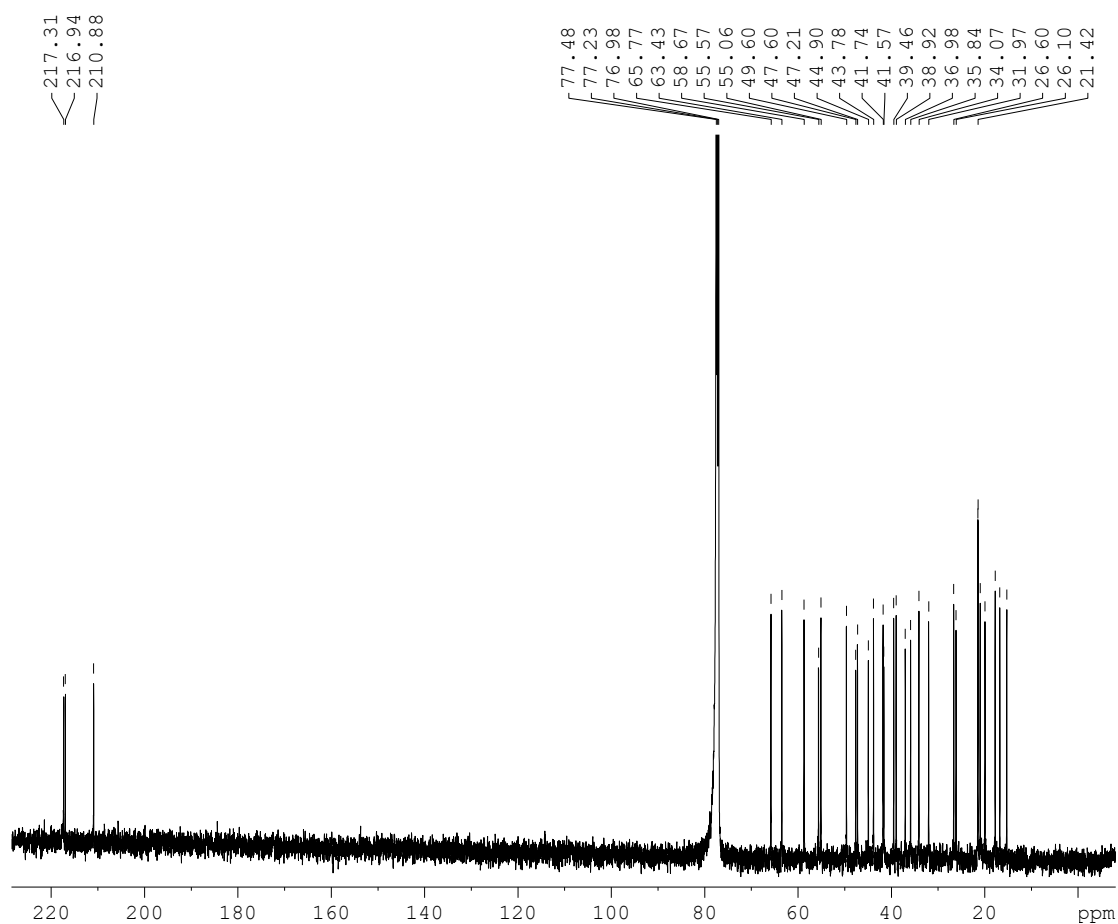


Figure S19.  $^{13}\text{C}$ -NMR spectrum of **3** ( $\text{CDCl}_3$ , 125 MHz).

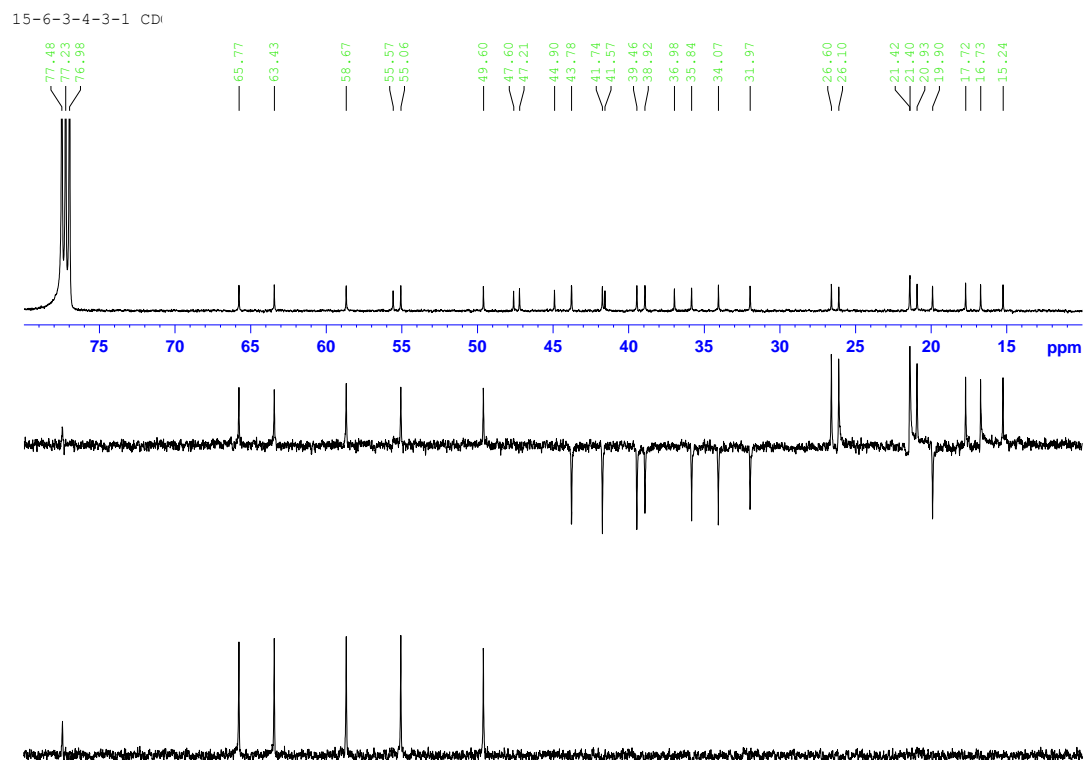


Figure S20.  $^{13}\text{C}$ -DEPT spectrum of **3** ( $\text{CDCl}_3$ , 125 MHz).

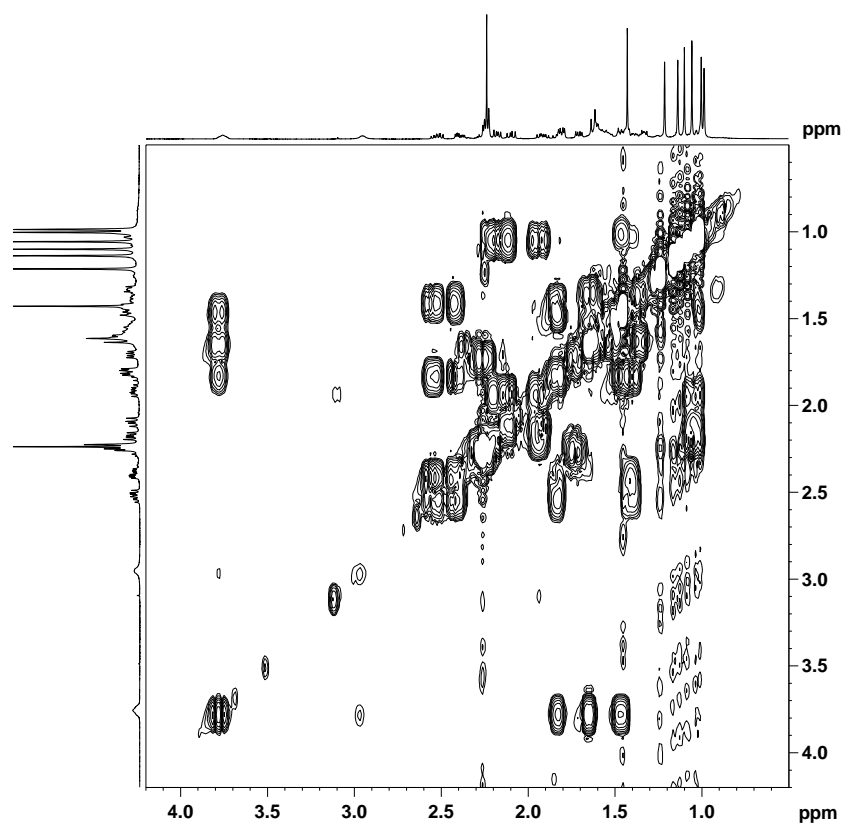


Figure S21.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3**.

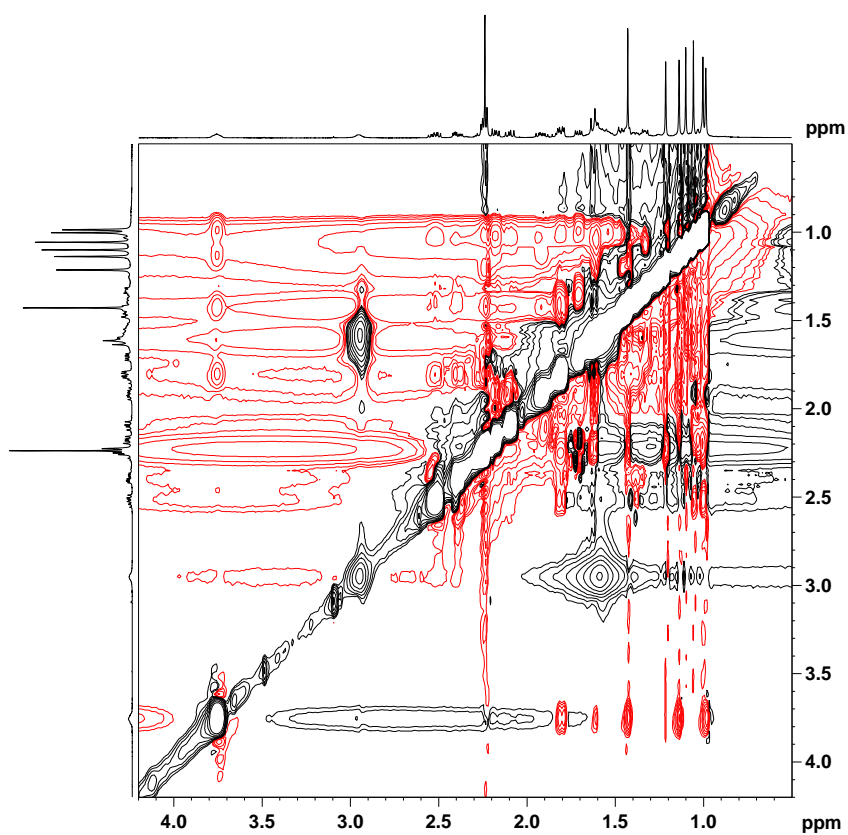


Figure S22. NOESY spectrum of **3**.



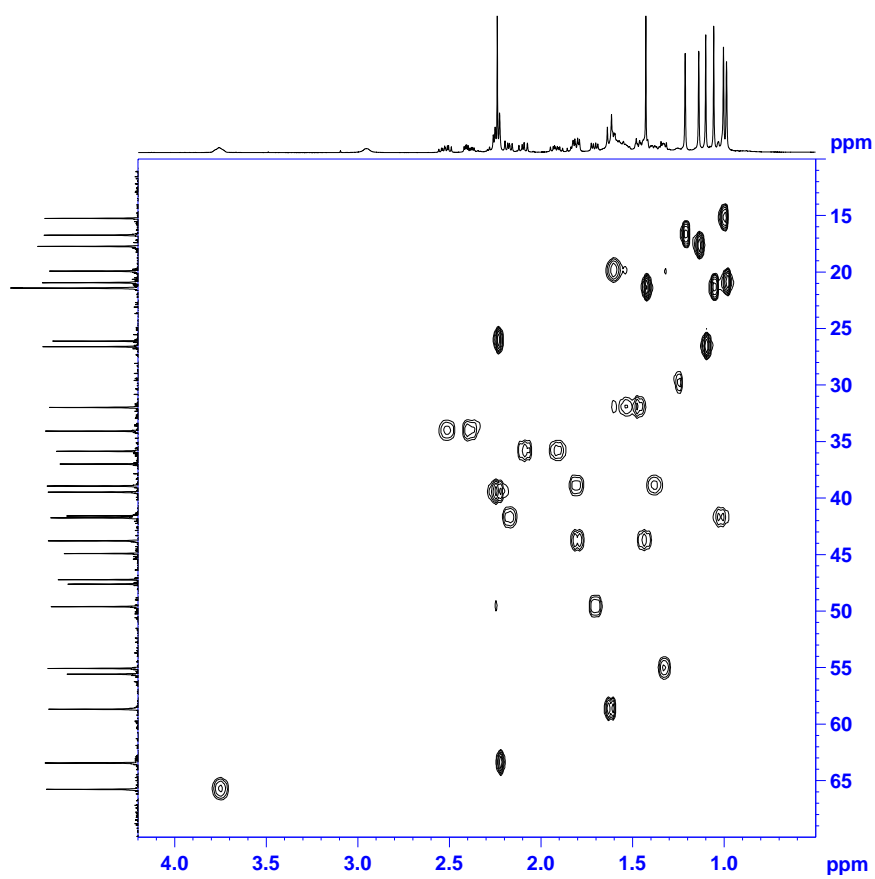


Figure S23. HSQC spectrum of **3**.

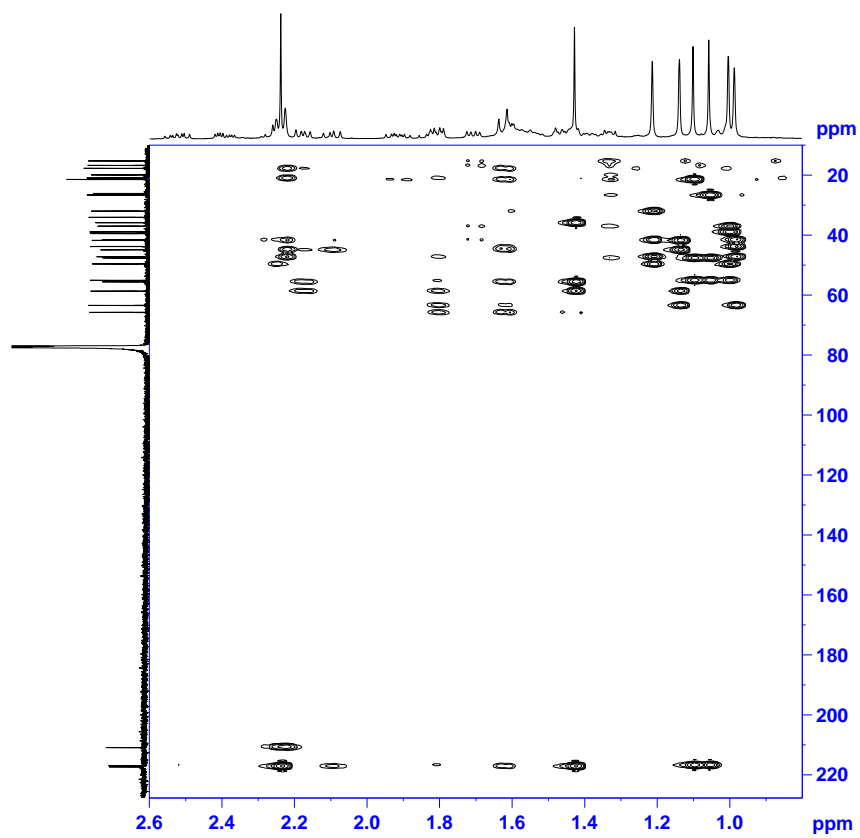


Figure S24. HMBC spectrum of **3**.