

## Supplementary Information

### A New Prenylisoflavone from the Antifungal Extract of Leaves of *Vatairea guianensis* Aubl.

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#### Lupiwighteone (1)

UV  $\lambda$  / nm (acetonitrile-water) 263, 323 (sh); IR (KBr)  $\nu_{\max}$  /  $\text{cm}^{-1}$  3522, 3396, 3165, 1651, 1512, 1431, 1367, 1203, 1064, 827; <sup>1</sup>H NMR (300 MHz, acetone-*d*<sub>6</sub>)  $\delta_{\text{H}}$  1.64 (s, H-4"), 1.79 (s, H-5"), 3.42 (d, *J* 6.6 Hz, H-1"), 5.23 (m, H-2"), 6.36 (s, H-6), 6.89 (d, *J* 8.7 Hz, H-3'/5'), 7.45 (d, *J* 8.7 Hz, H-2'/6'), 8.23 (s, H-2); <sup>13</sup>C NMR (75 MHz, acetone-*d*<sub>6</sub>)  $\delta_{\text{C}}$  17.8 (C-4"), 21.9 (C-1"), 25.8 (C-5"), 99.3 (C-6), 106.0 (C-10), 107.0 (C-8), 115.8 (C-3'/5'), 123.0 (C-2"), 123.0 (C-3), 123.5 (C-1'), 131.1 (C-2'/6'), 131.9 (C-3"), 154.3 (C-2), 156.2 (C-9), 158.3 (C-4), 161.4 (C-5), 162.2 (C-7), 181.9 (C-4); HRESITOF-MS *m/z* 339.1233 [M + H]<sup>+</sup> (calcd. for [M + H]<sup>+</sup>, C<sub>20</sub>H<sub>18</sub>O<sub>5</sub> + H<sup>+</sup>, found: 339.1232).

#### 5,7,4'-Trihydroxy-3'-methoxy-8-prenyl-isoflavone (2)

UV  $\lambda$  / nm (acetonitrile-water) 239, 265; IR (KBr)  $\nu_{\max}$  /  $\text{cm}^{-1}$  3213, 2920, 1652, 1516, 1425, 1369, 1195, 1062, 835; <sup>1</sup>H NMR (300 MHz, CD<sub>3</sub>OD)  $\delta_{\text{H}}$  1.65 (s, H-4"), 1.78 (s, H-5"), 3.37 (d, *J* 6.9 Hz, H-1"), 3.87 (s, OMe-3'), 5.18 (t, *J* 6.9 Hz, H-2"), 6.24 (s, H-6), 6.82 (d, *J* 8.1 Hz, H-5'), 6.94 (brd, *J* 8.1 Hz, H-6'), 7.14 (brs, H-2'), 8.11 (s, H-2); <sup>13</sup>C NMR (75 MHz, CD<sub>3</sub>OD)  $\delta_{\text{C}}$  17.9 (C-5"), 22.3 (C-1"), 25.9 (C-4"), 99.5 (C-6), 106.2 (C-10), 107.8 (C-8), 113.9 (C-2'), 116.2 (C-5'), 122.8 (C-6'), 123.4 (C-2"), 123.9 (C-3), 124.3 (C-1'), 132.4 (C-3"), 148.7 (C-4'), 147.8 (C-3'), 155.0 (C-2), 156.7 (C-9), 161.3 (C-5), 163.2 (C-7), 182.5 (C-4); HRESITOF-MS *m/z* 369.1342 [M + H]<sup>+</sup> (calcd. for [M + H]<sup>+</sup>, C<sub>21</sub>H<sub>20</sub>O<sub>6</sub> + H<sup>+</sup>, 369.1338).

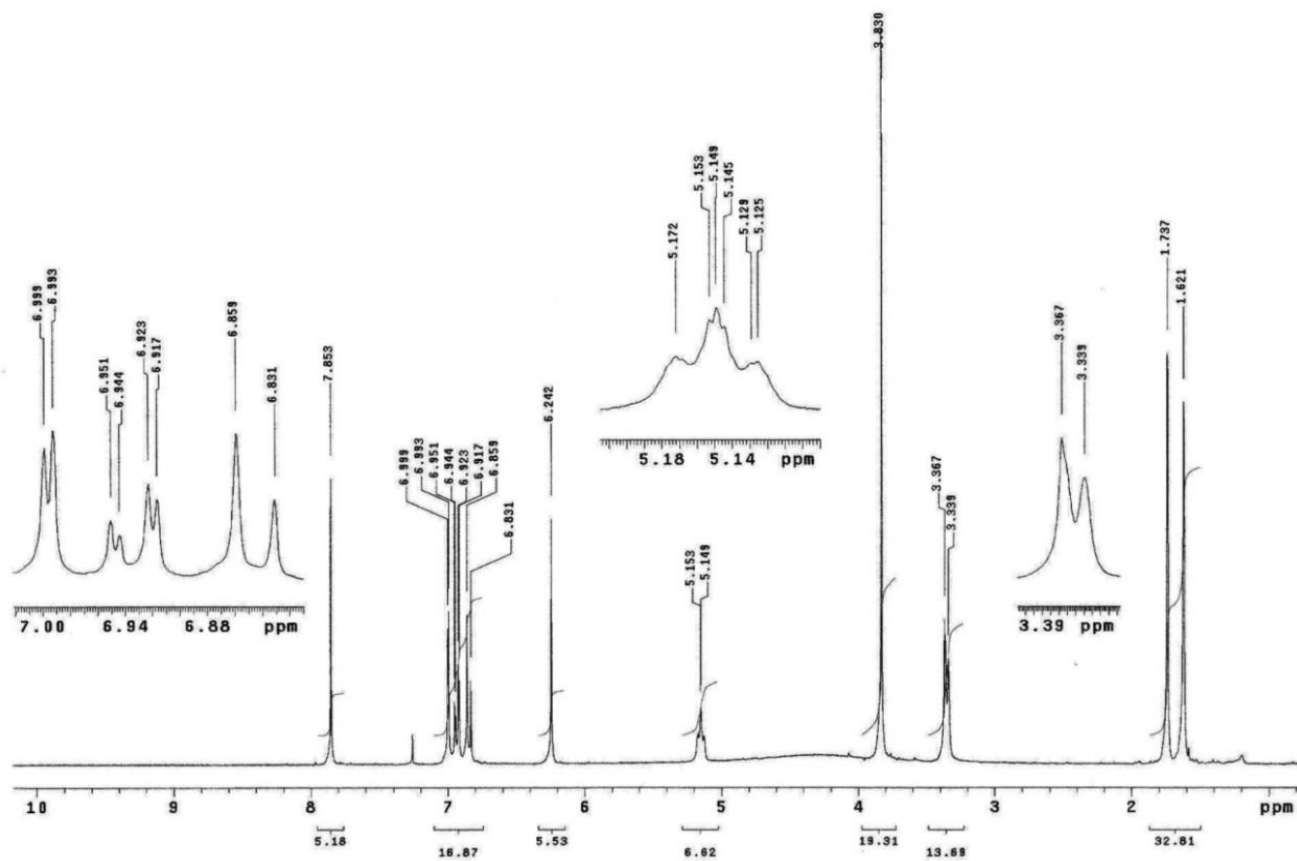


Figure S1.  $^1\text{H}$  NMR spectrum of **3** (300 MHz,  $\text{CDCl}_3$  and a few drops of  $\text{CD}_3\text{OD}$ ).

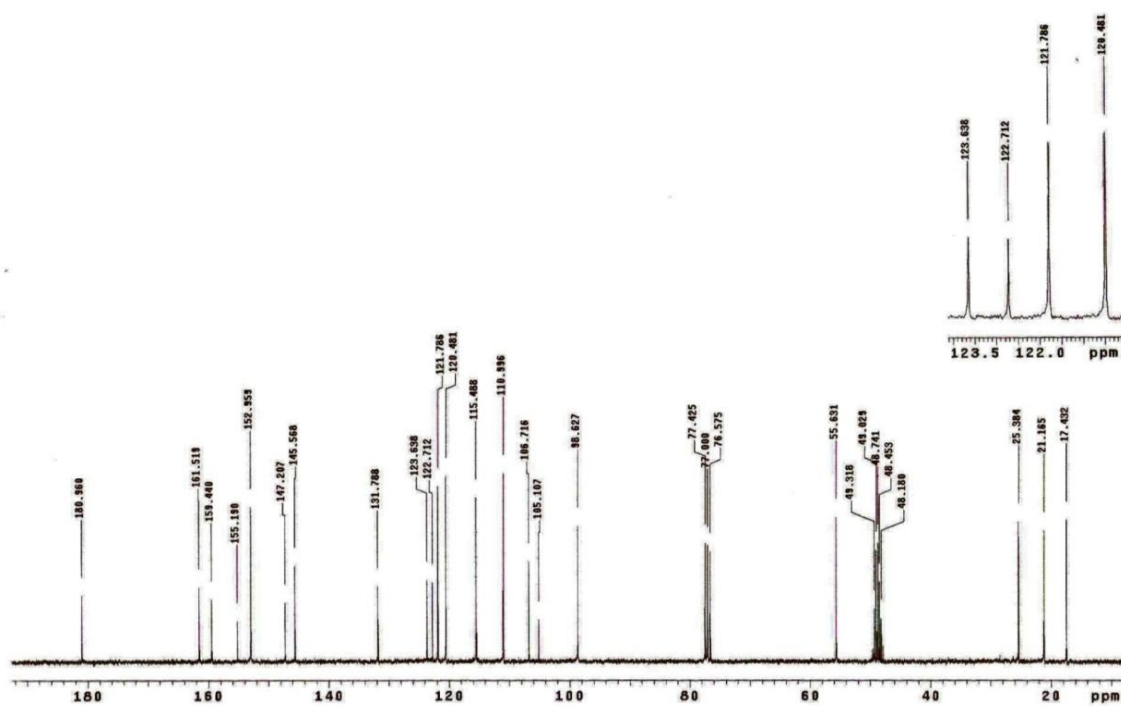
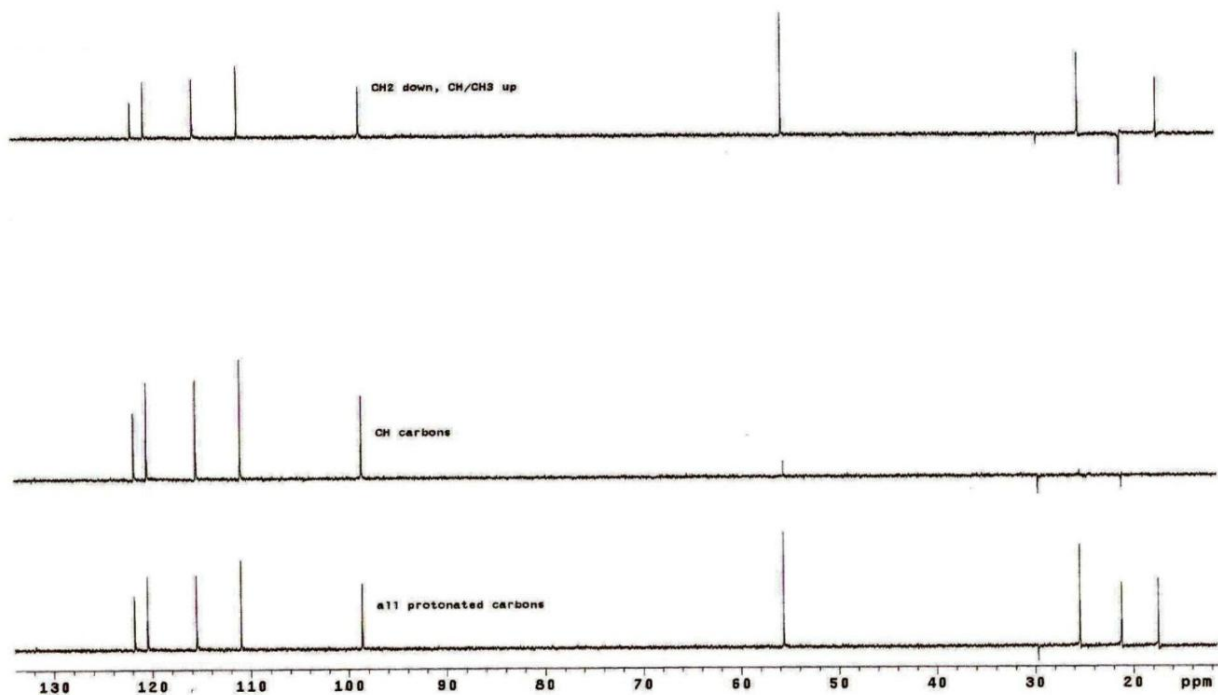
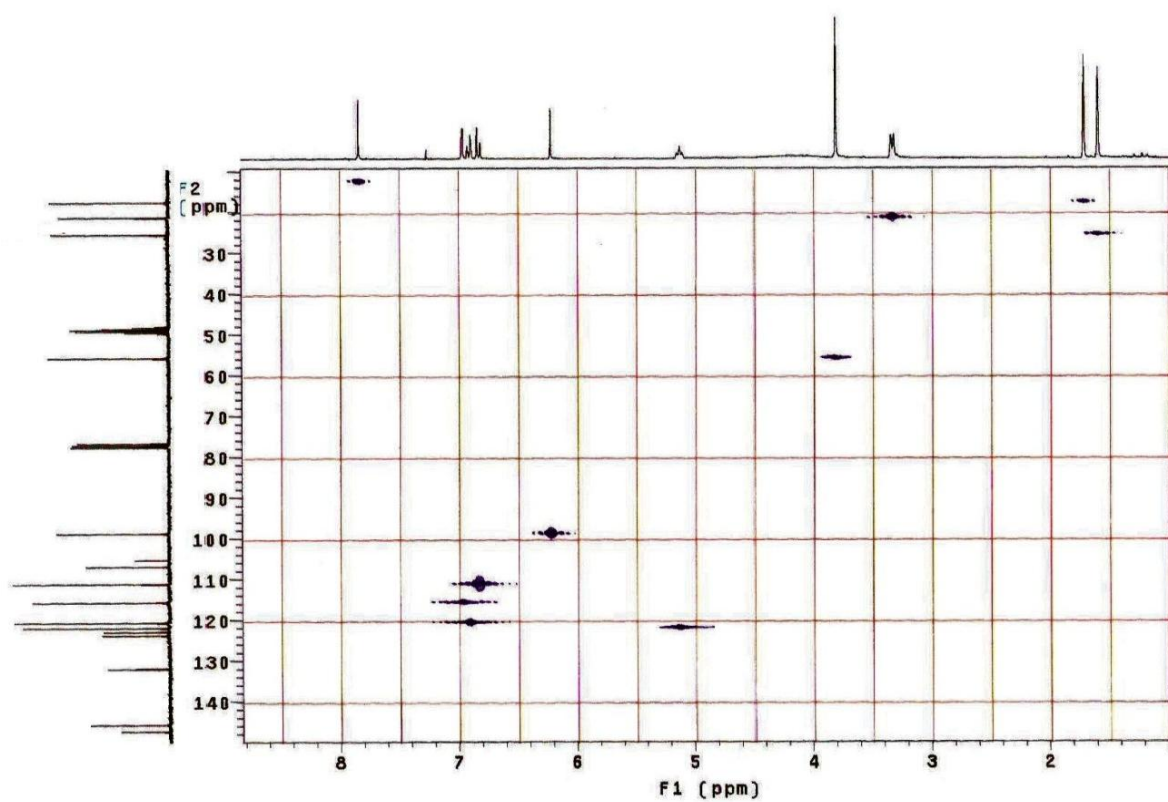


Figure S2.  $^{13}\text{C}$  NMR spectrum of **3** (75 MHz,  $\text{CDCl}_3$  and a few drops of  $\text{CD}_3\text{OD}$ ).



**Figure S3.** DEPT NMR spectrum of **3** (300 × 75 MHz, CDCl<sub>3</sub> and a few drops of CD<sub>3</sub>OD).



**Figure S4.** HETCOR NMR spectrum of **3** (300 × 75 MHz, CDCl<sub>3</sub> and a few drops of CD<sub>3</sub>OD).

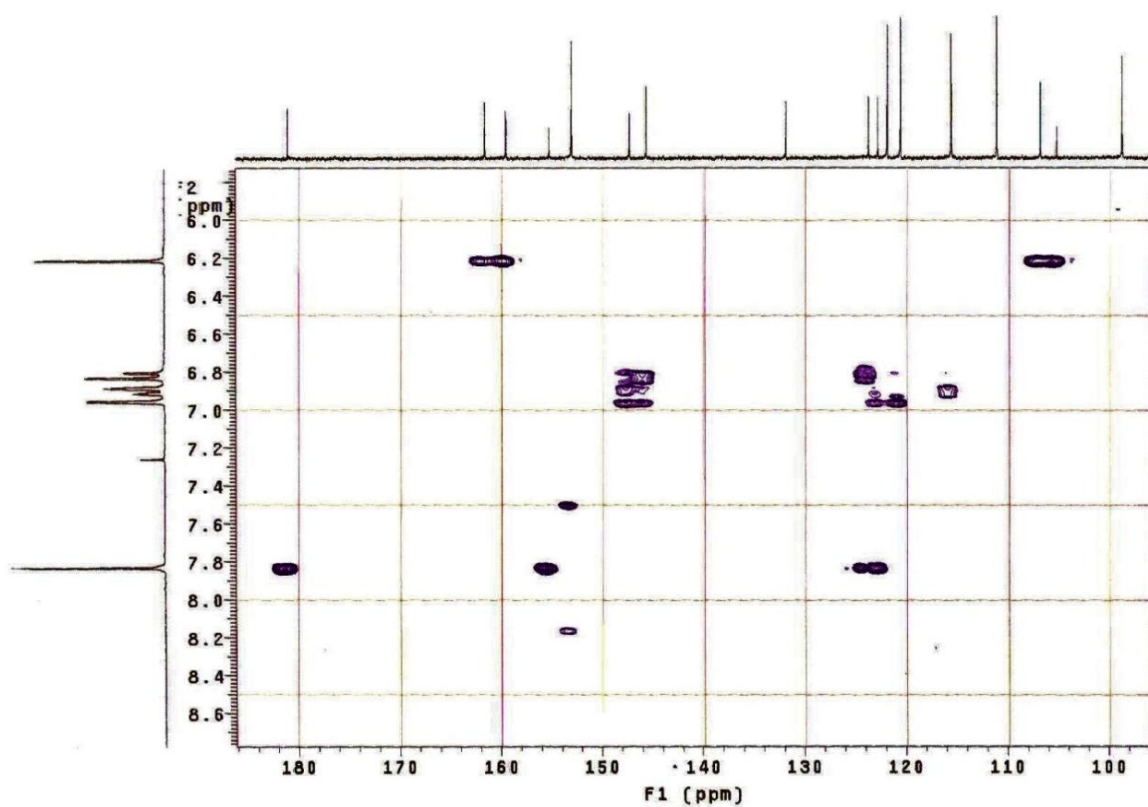


Figure S5. HMBC NMR spectrum of **3** ( $300 \times 75$  MHz,  $\text{CDCl}_3$  and a few drops of  $\text{CD}_3\text{OD}$ ) (expansion 1).

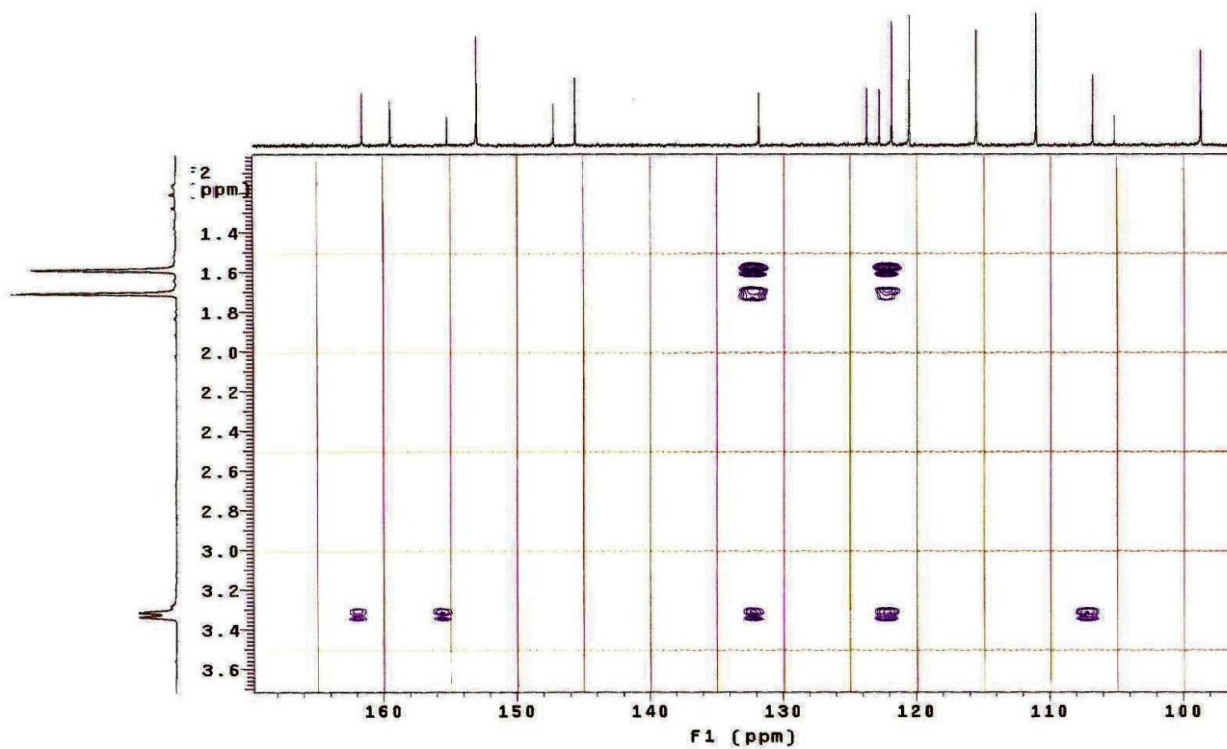
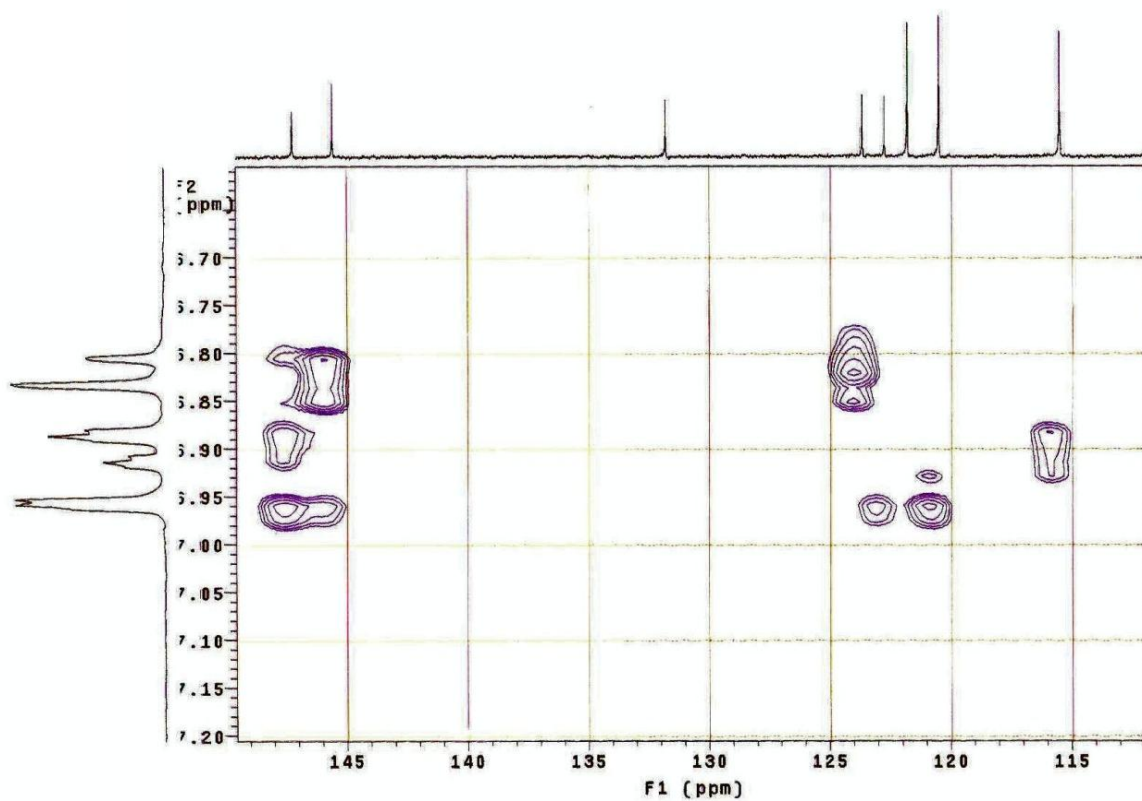
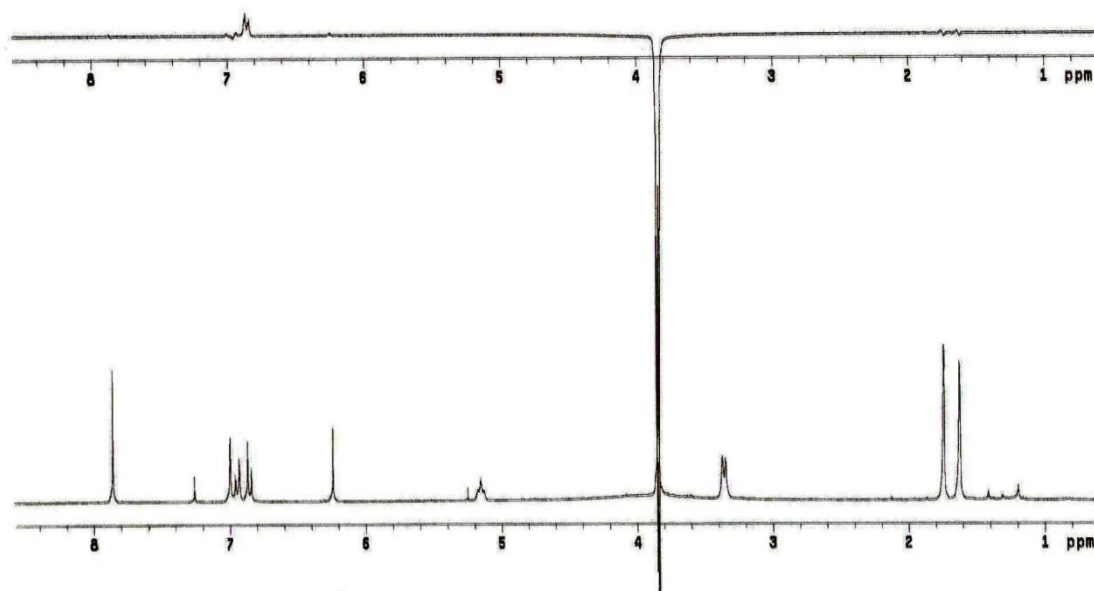


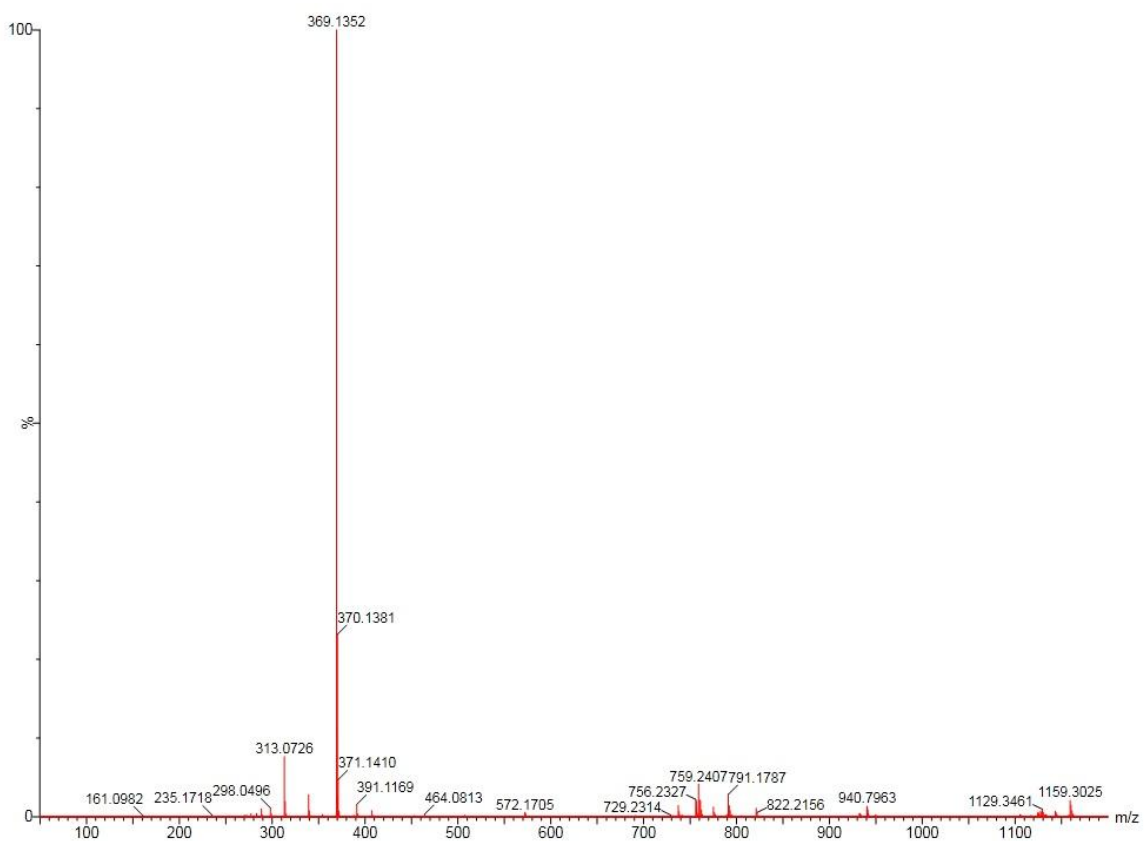
Figure S6. HMBC NMR spectrum of **3** ( $300 \times 75$  MHz,  $\text{CDCl}_3$  and a few drops of  $\text{CD}_3\text{OD}$ ) (expansion 2).



**Figure S7.** HMBC NMR spectrum of **3** (300 × 75 MHz, CDCl<sub>3</sub> and a few drops of CD<sub>3</sub>OD) (expansion 3).



**Figure S8.** NOEdiff NMR spectrum of **3** (300 MHz, CDCl<sub>3</sub> and a few drops of CD<sub>3</sub>OD).



**Figure S9.** HRESITOF-MS spectrum of **3**.