

## Supporting Information

### Characterization of phytochemicals from the root extract of *Milletia leucantha* and their anti-microbial properties

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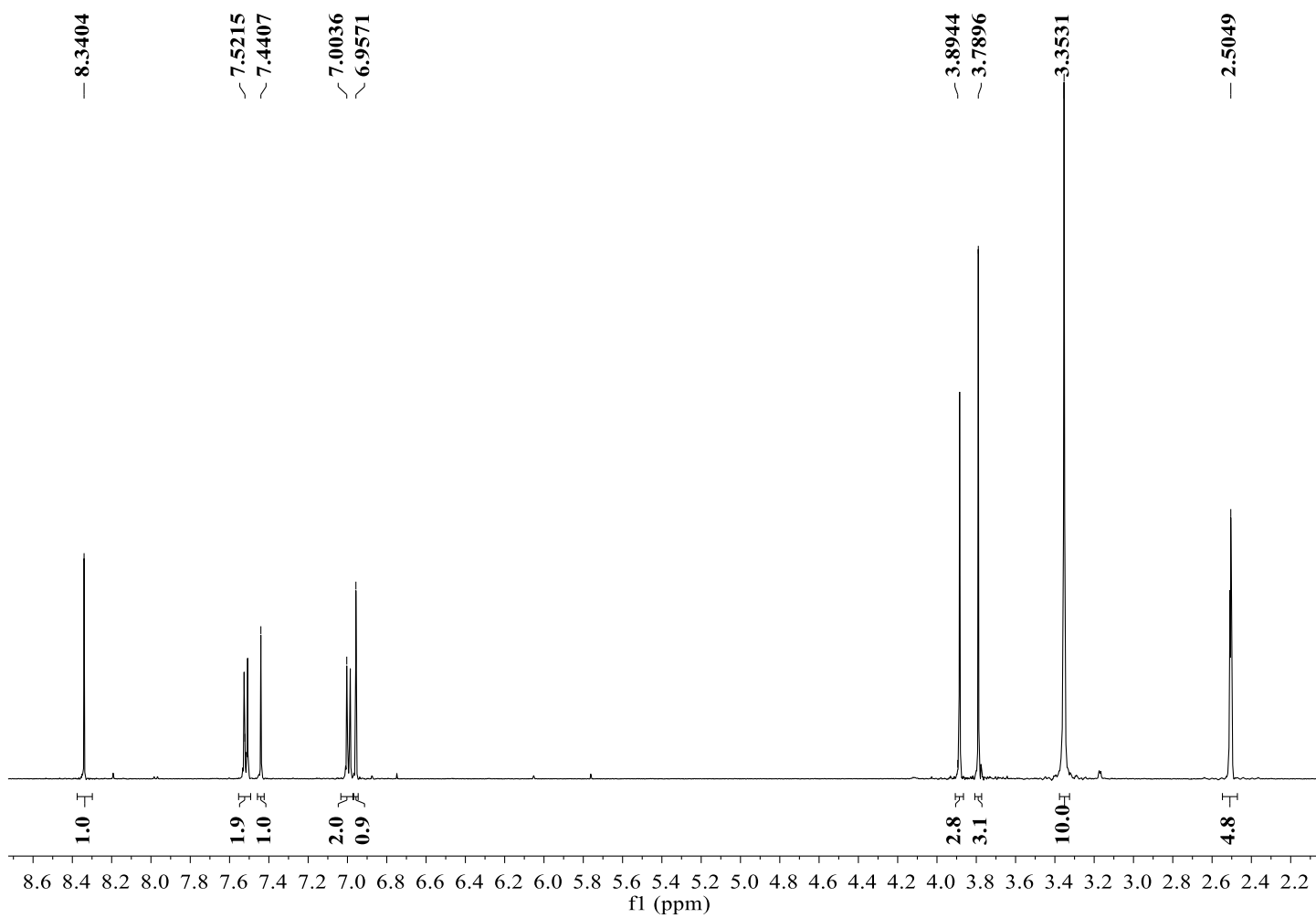


Figure S1:  $^1\text{H}$  NMR spectrum (500 MHz,  $(\text{CD}_3)_2\text{SO}$ ) of compound **1**

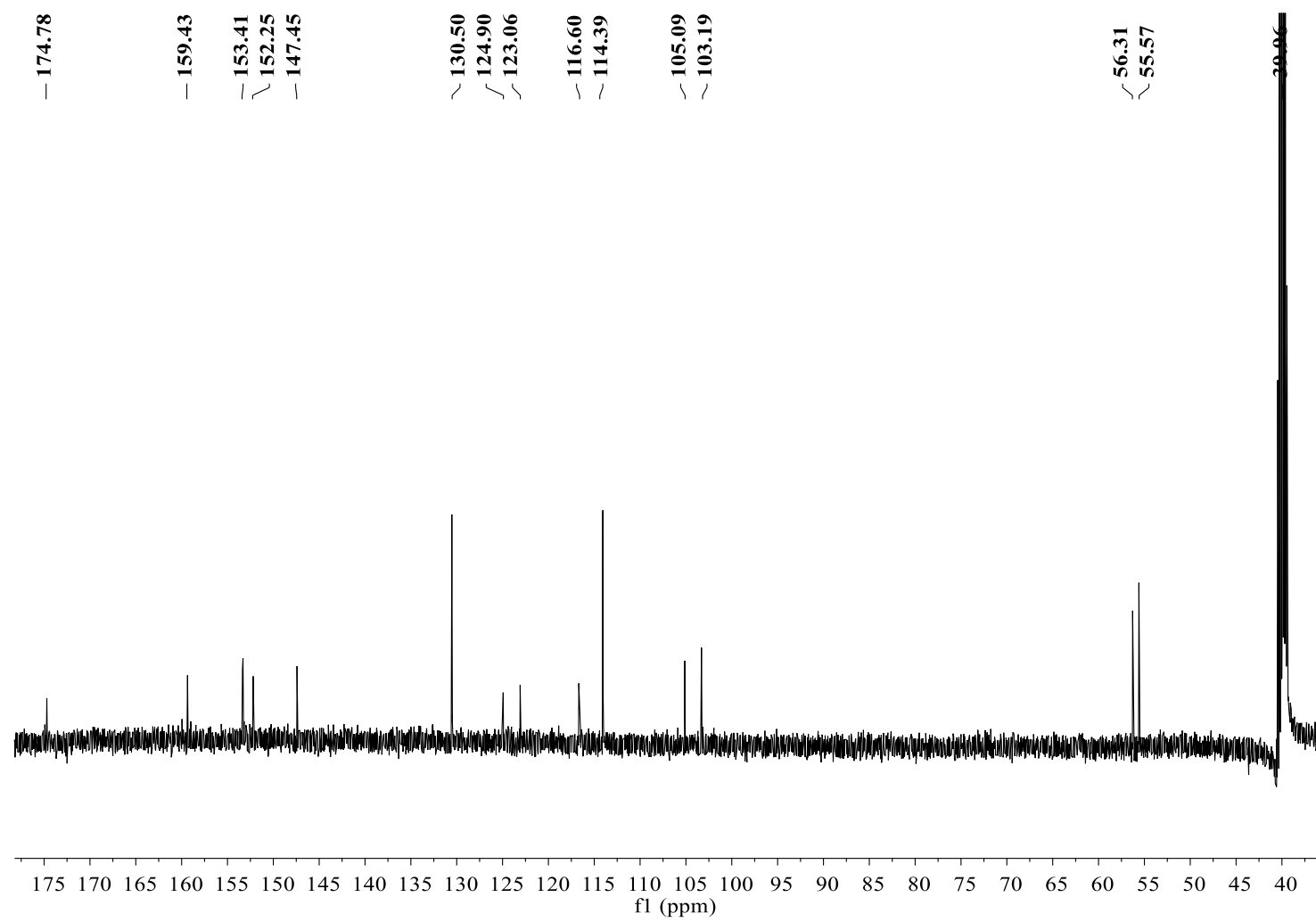


Figure S2:  $^{13}\text{C}$  NMR spectrum (125 MHz,  $(\text{CD}_3)_2\text{SO}$ ) of compound **1**

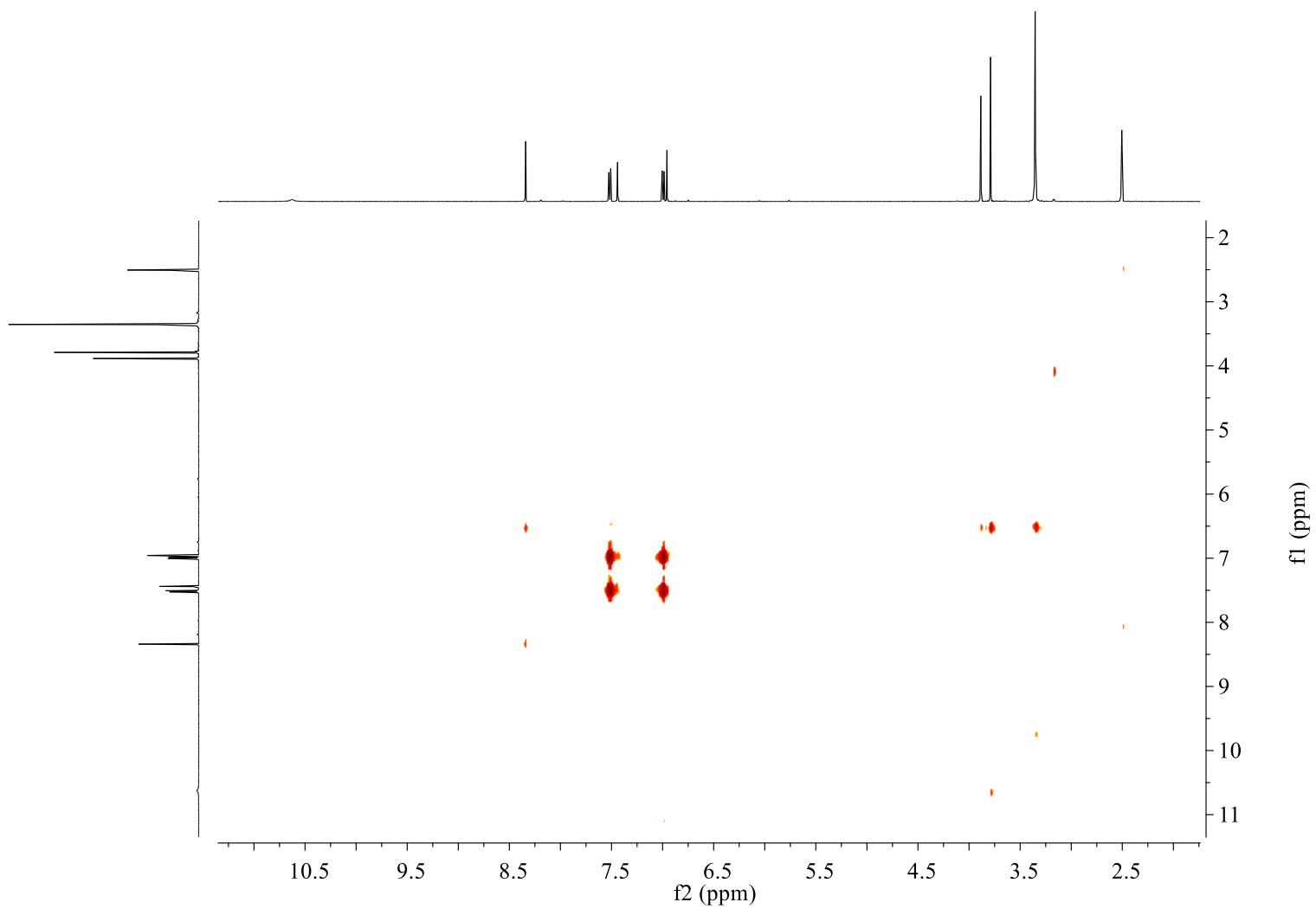


Figure S3:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum  $(\text{CD}_3)_2\text{SO}$  of compound **1**

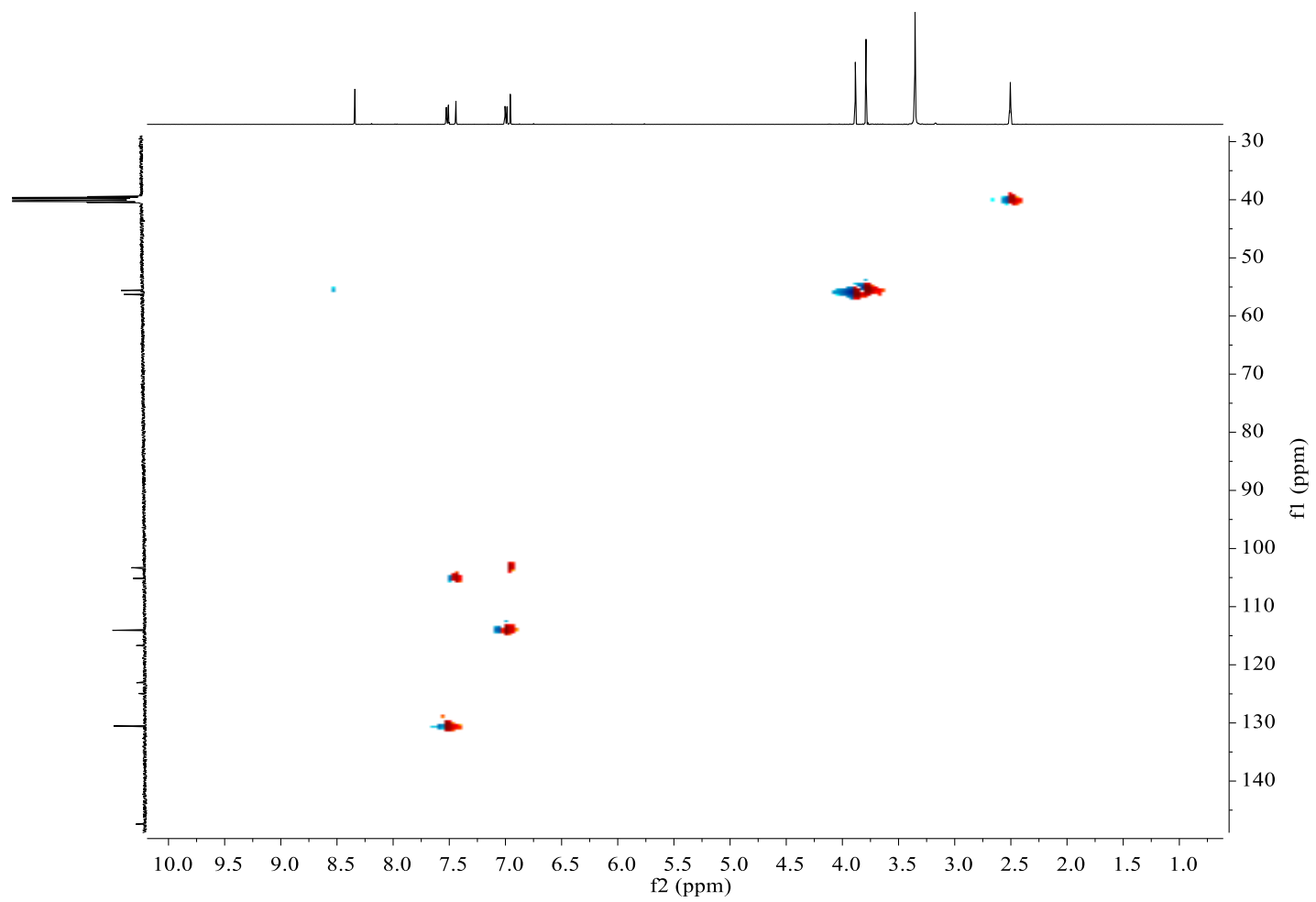


Figure S4: HSQC spectrum  $(\text{CD}_3)_2\text{SO}$  of compound **1**

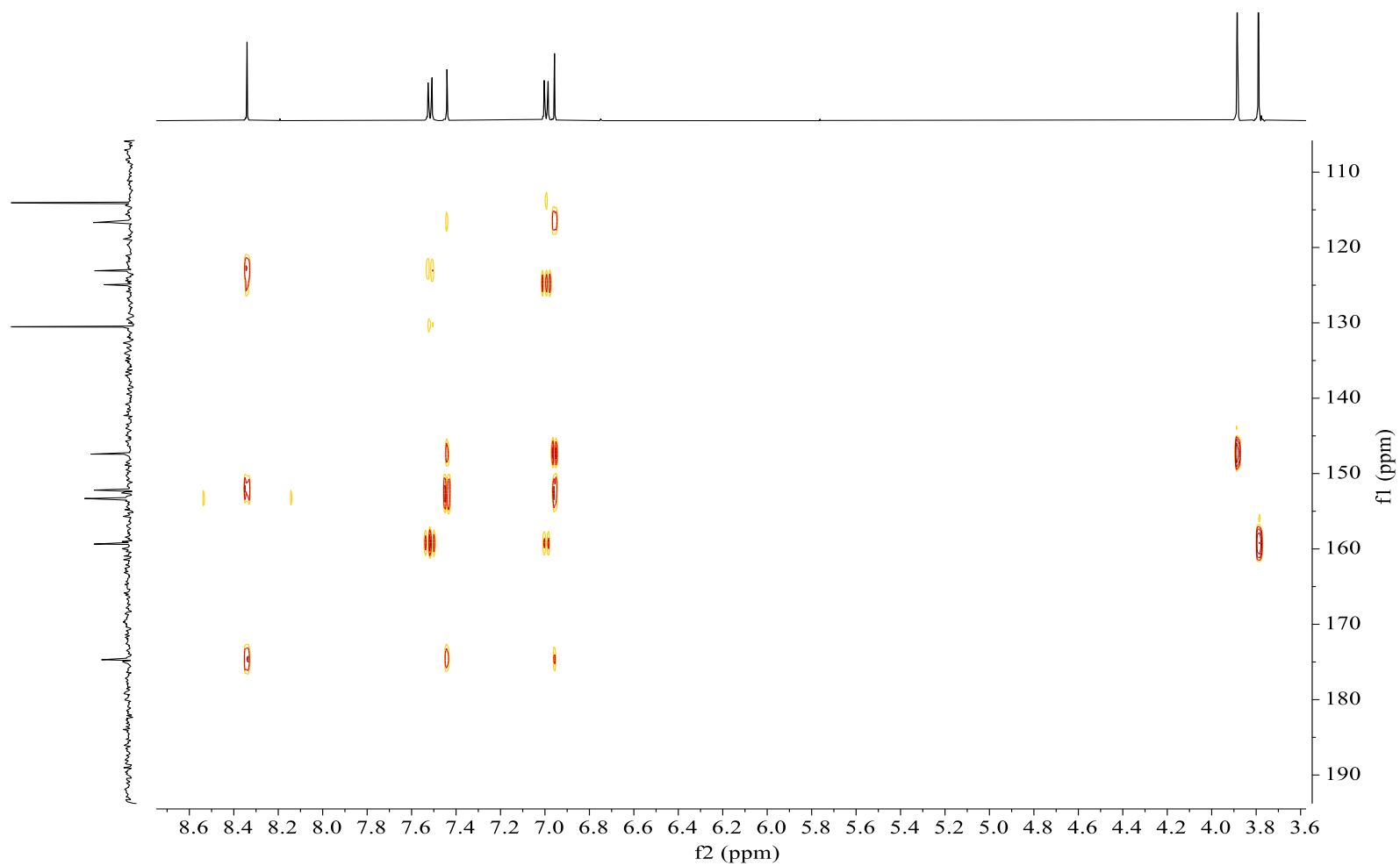


Figure S5: HMBC spectrum  $(\text{CD}_3)_2\text{SO}$  of compound **1**

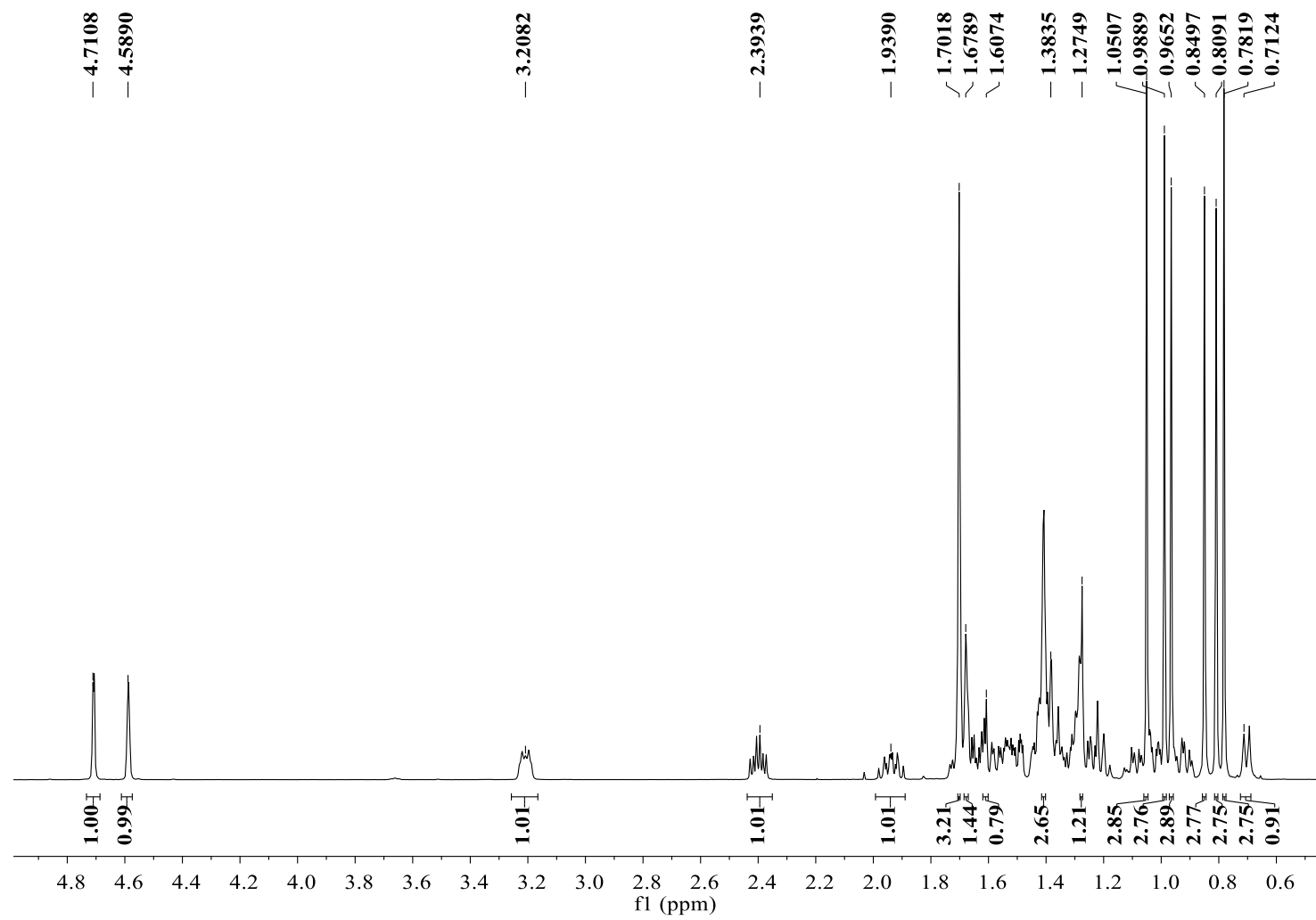


Figure S16: <sup>1</sup>H NMR spectrum (500 MHz, CD<sub>2</sub>Cl<sub>2</sub>) of compound **2**



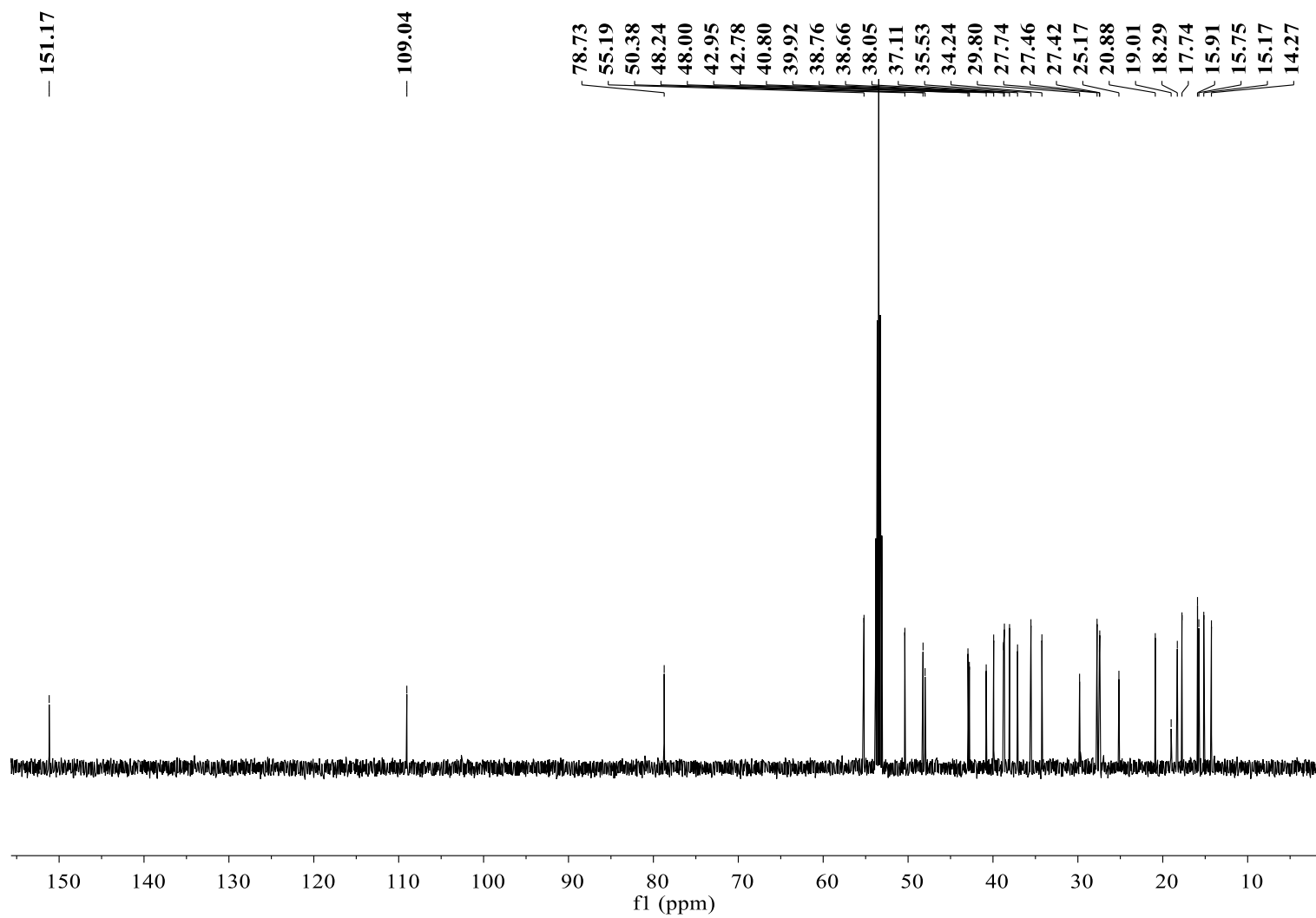


Figure S17:  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_2\text{Cl}_2$ ) of compound 2

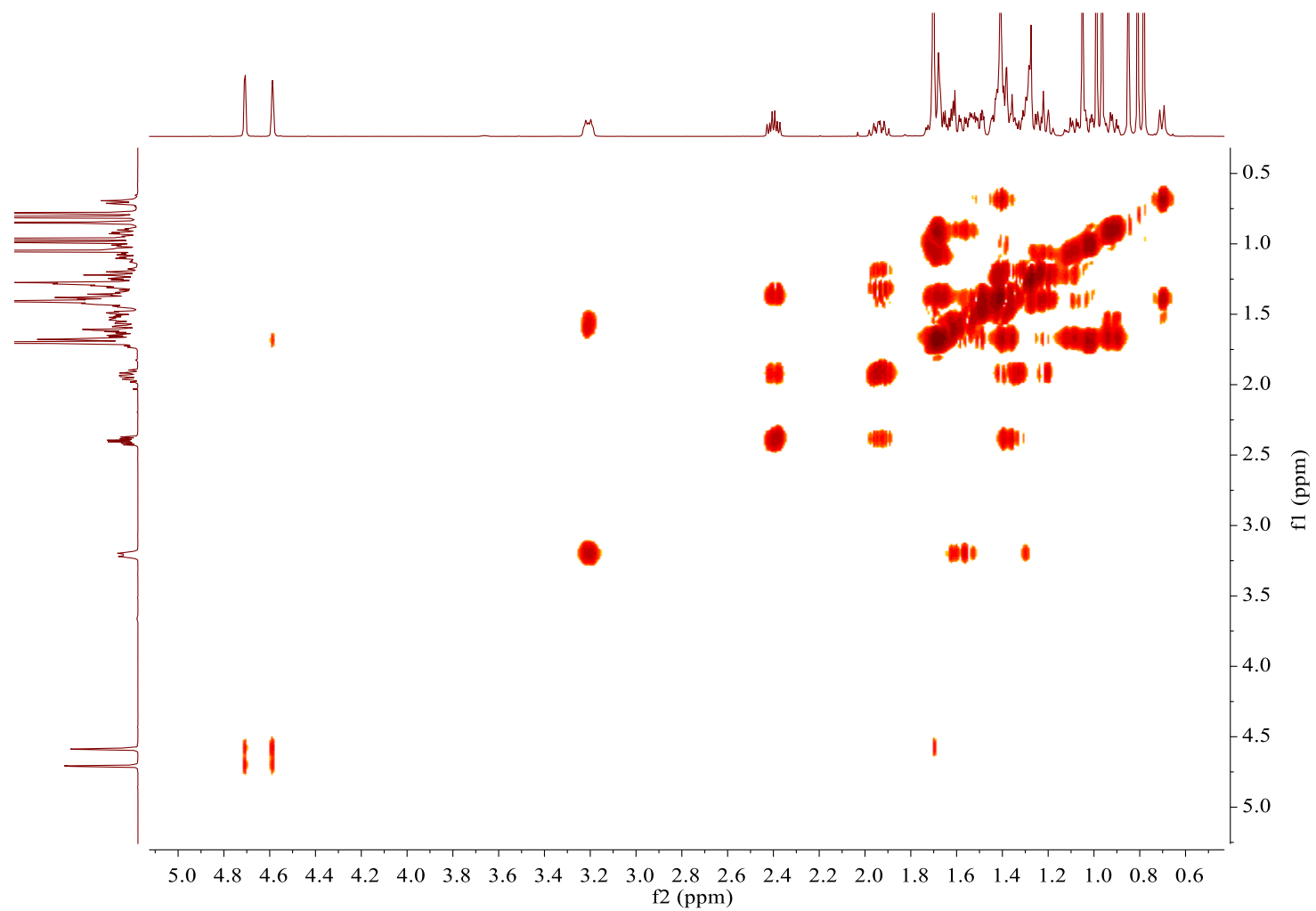


Figure S18:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum ( $\text{CD}_2\text{Cl}_2$ ) of compound **2**

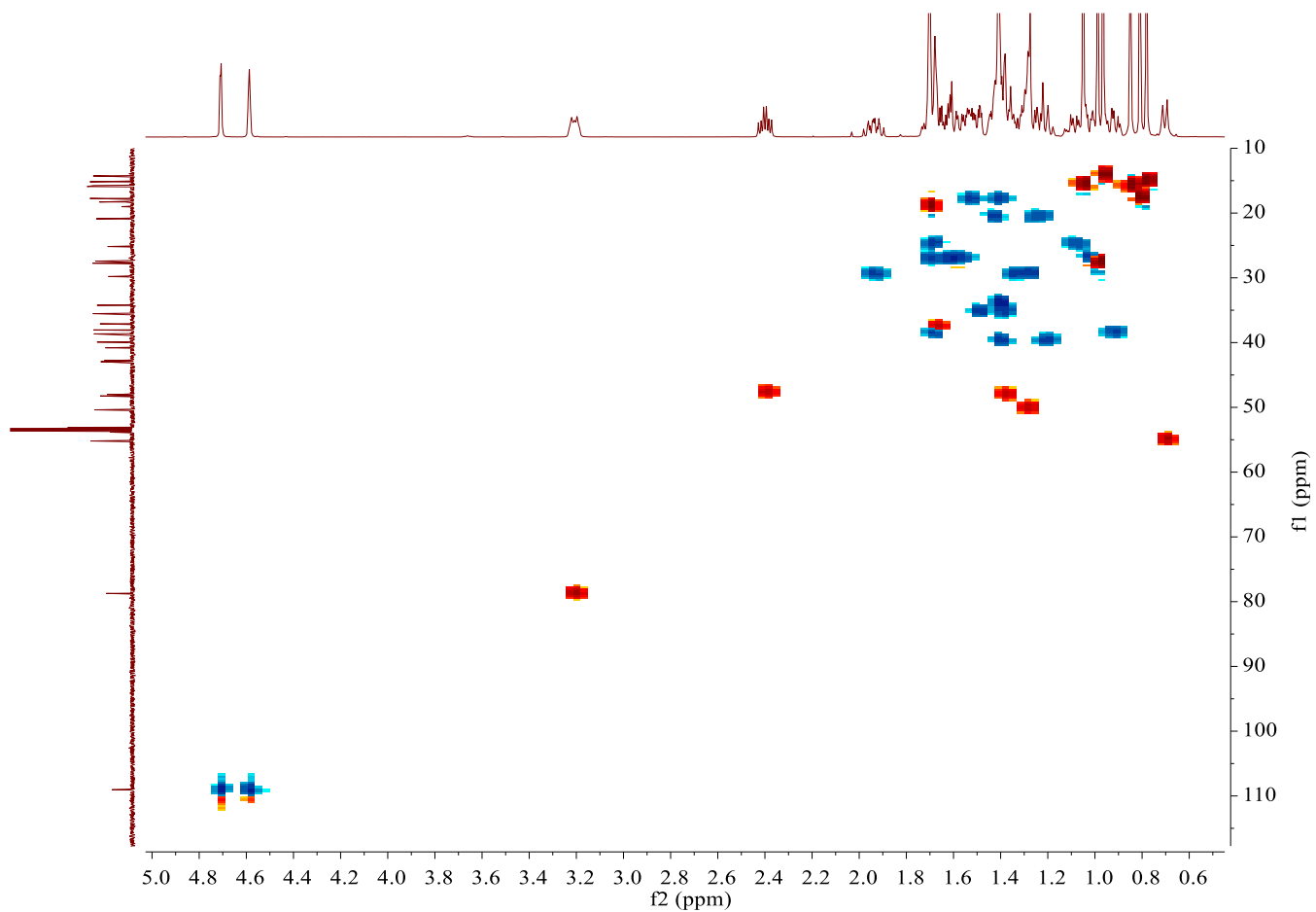


Figure S19: HSQC spectrum ( $\text{CD}_2\text{Cl}_2$ ) of compound **2**

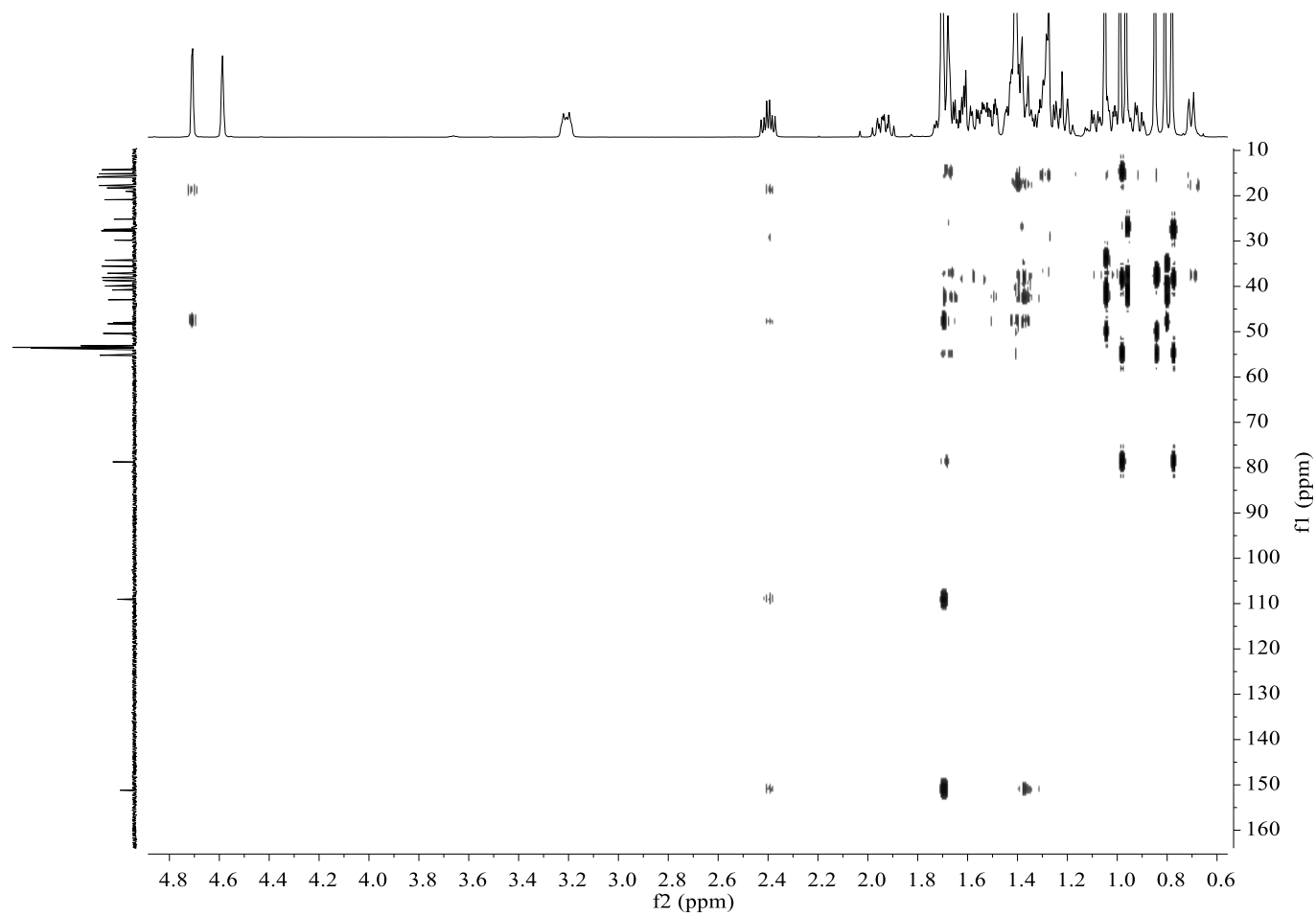


Figure S20: HMBC spectrum (CD<sub>2</sub>Cl<sub>2</sub>) of compound **2**

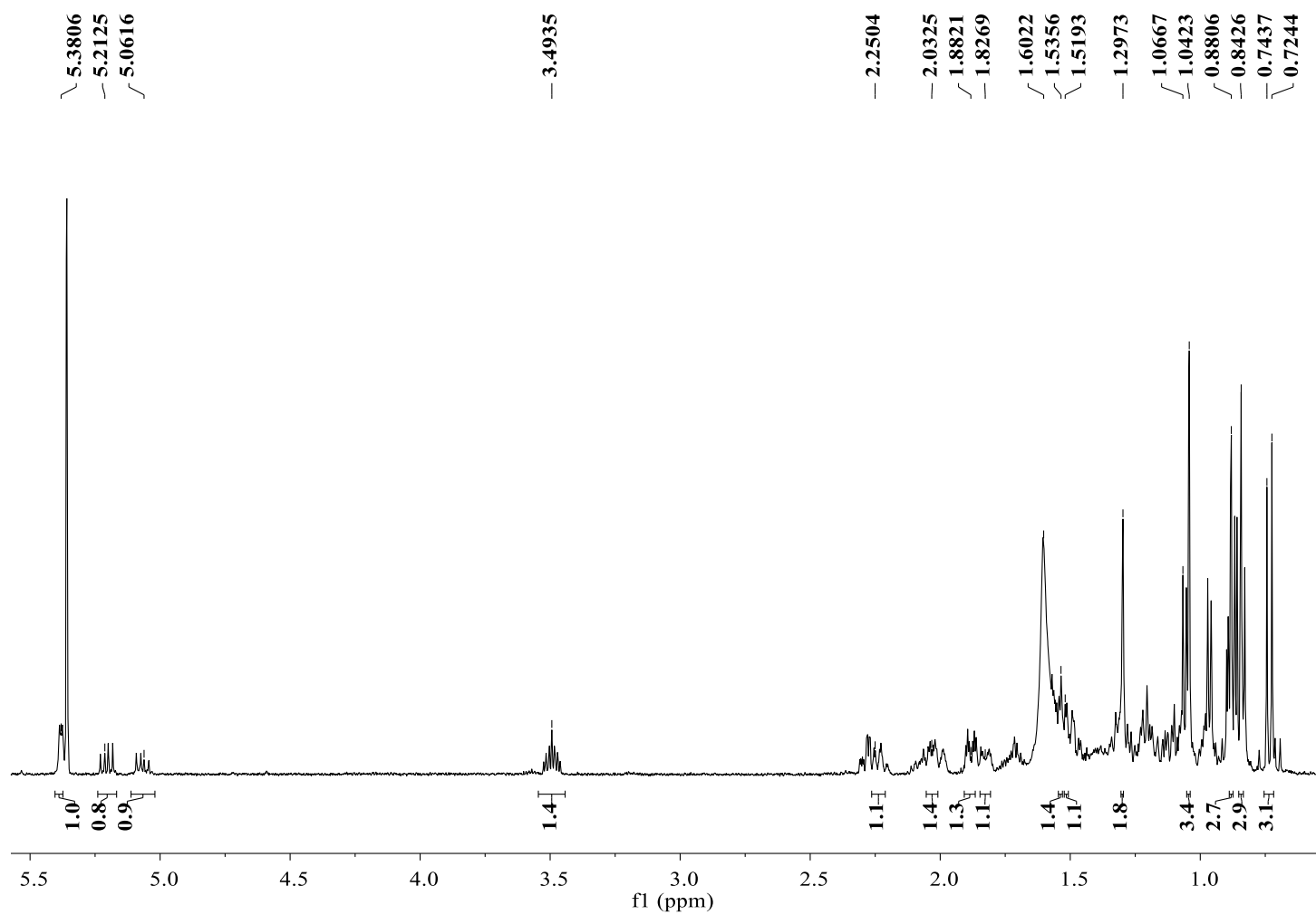


Figure S11:  $^1\text{H}$  NMR spectrum (500 MHz,  $\text{CD}_2\text{Cl}_2$ ) of compound **3** and **4**

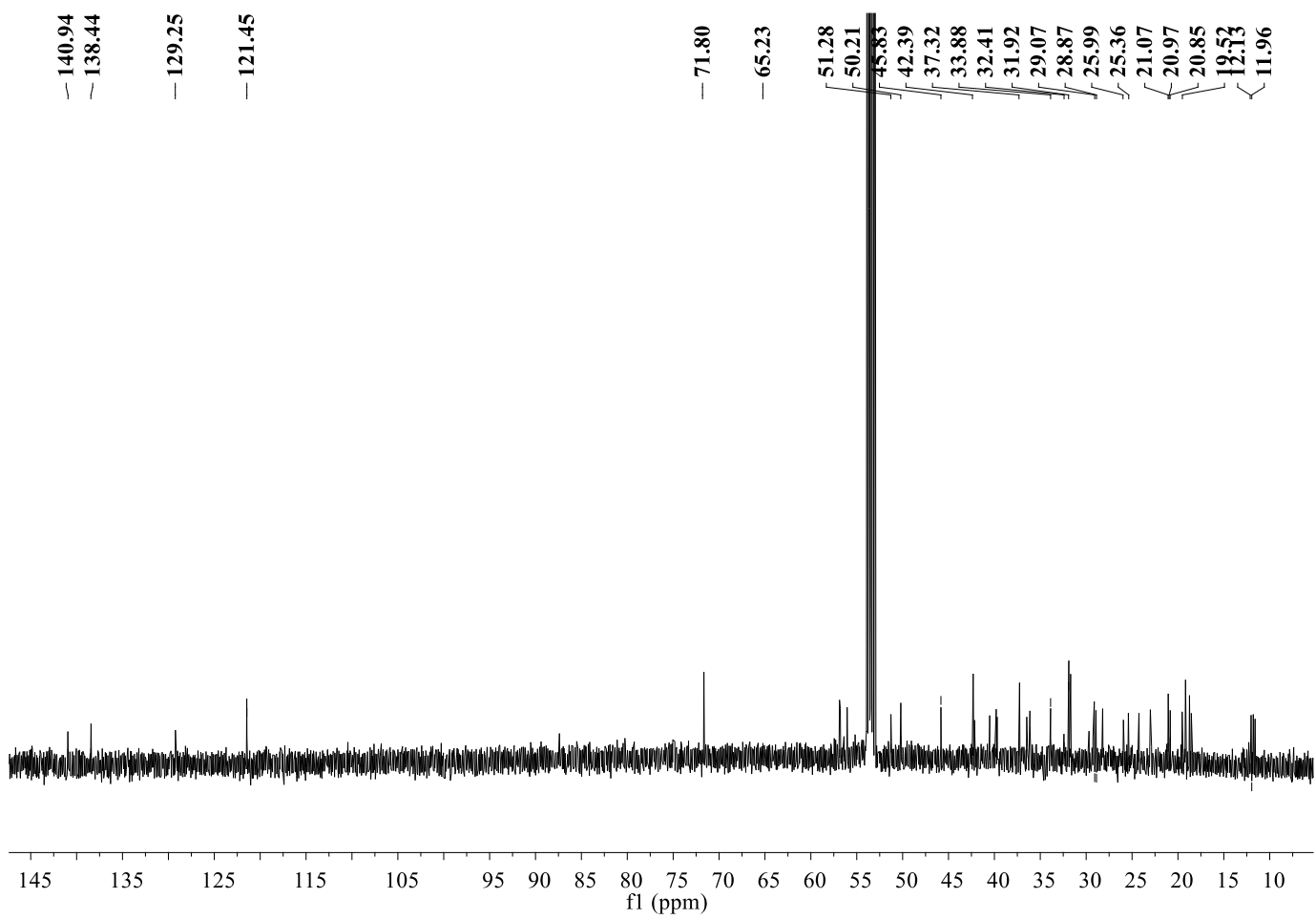


Figure S12:  $^{13}\text{C}$  NMR spectrum (125 MHz,  $\text{CD}_2\text{Cl}_2$ ) of compound **3** and **4**

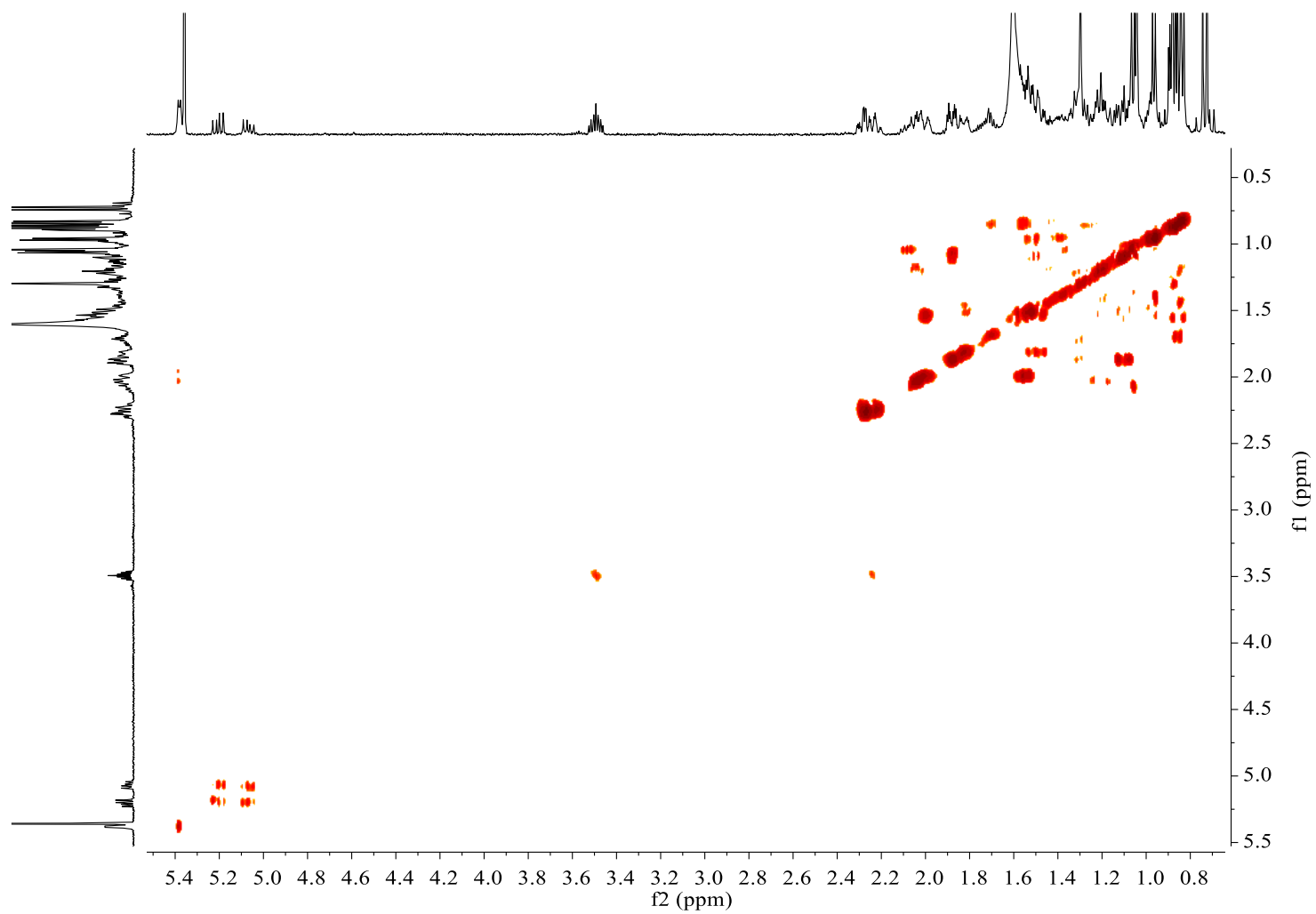


Figure S13:  $^1\text{H}$ - $^1\text{H}$  COSY spectrum ( $\text{CD}_2\text{Cl}_2$ ) of compound **3** and **4**

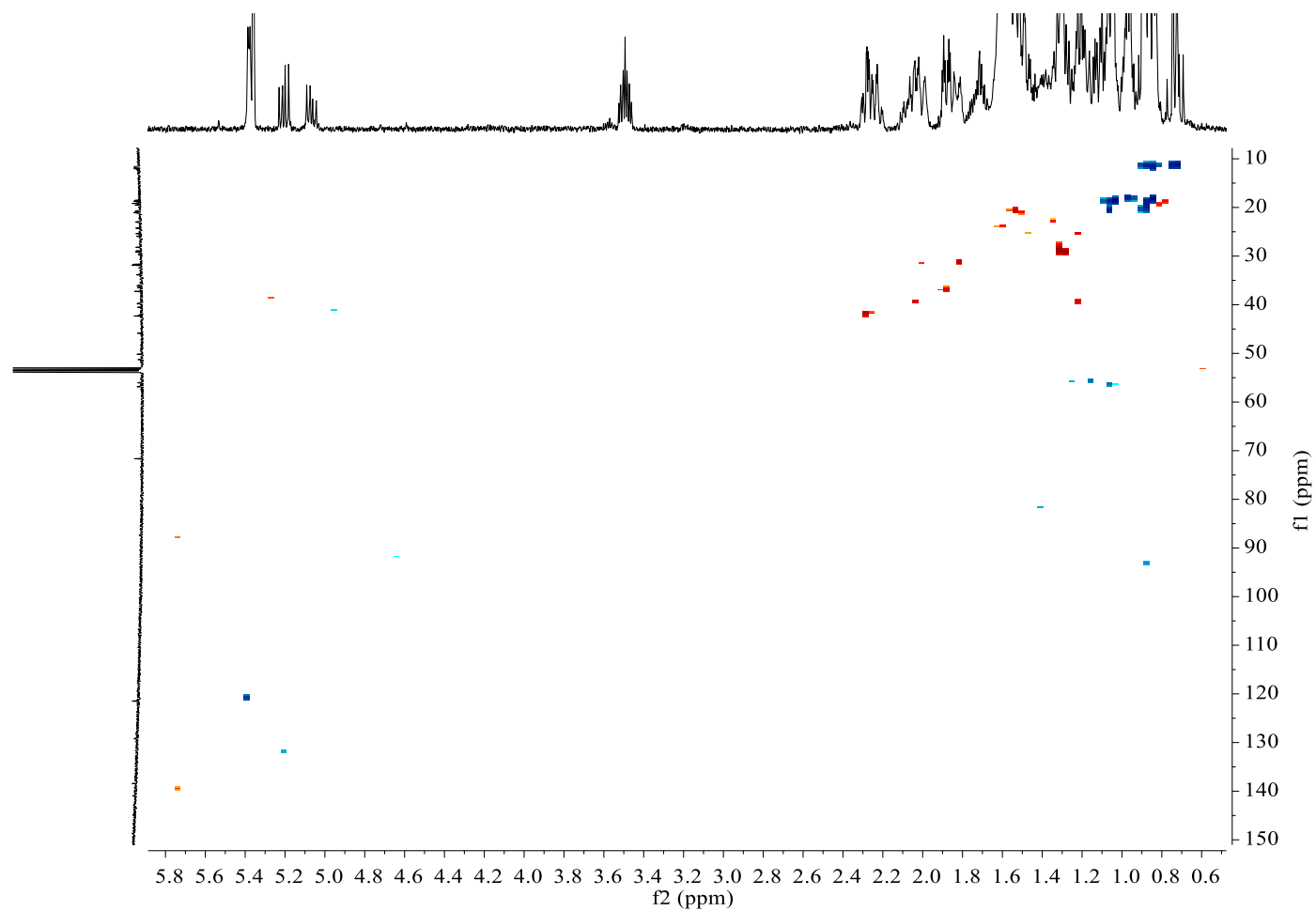


Figure S14: HSQC spectrum ( $\text{CD}_2\text{Cl}_2$ ) of compound **3** and **4**



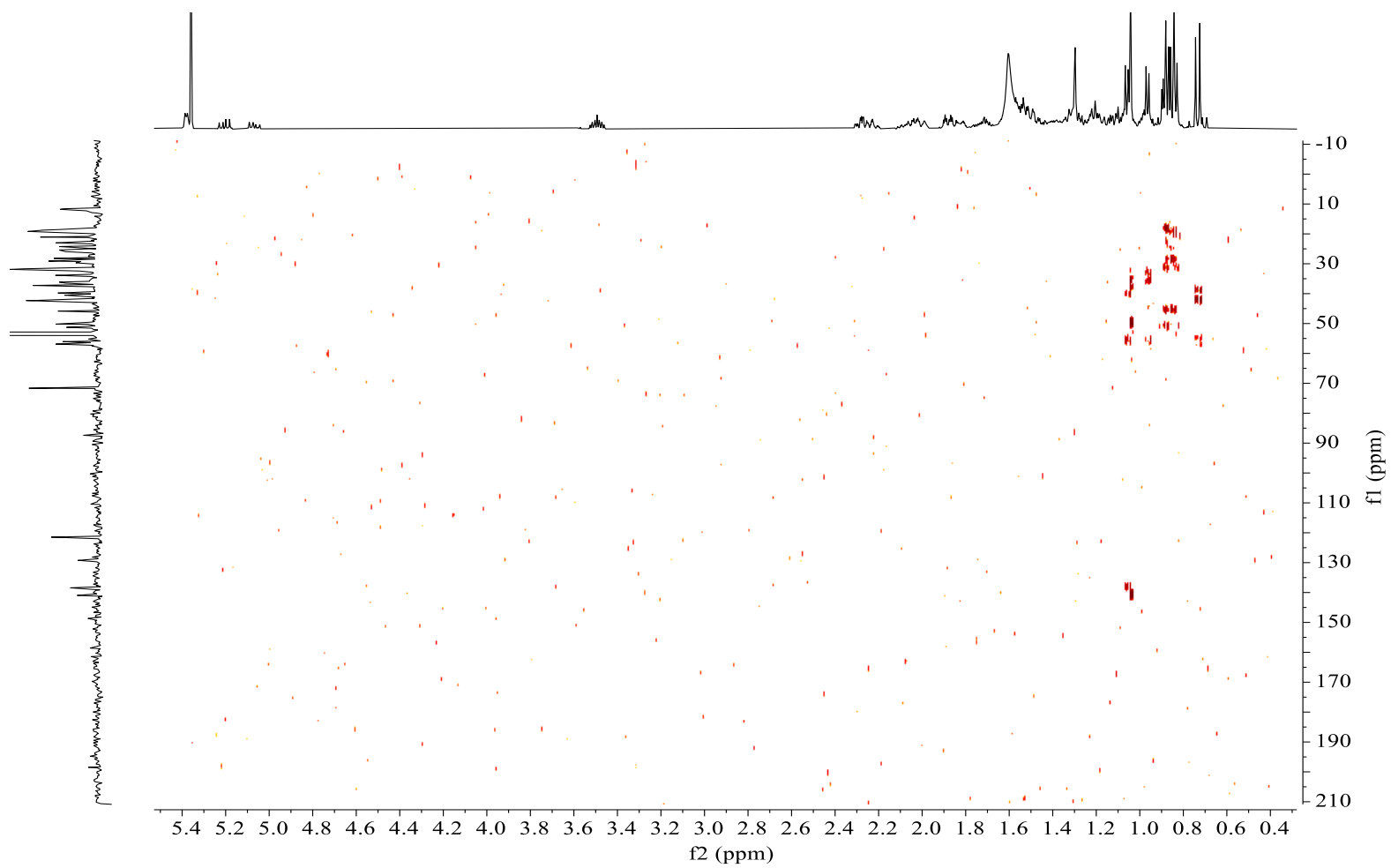


Figure S15: HMBC spectrum ( $\text{CD}_2\text{Cl}_2$ ) of compound **3** and **4**

## Spectral data for compounds 1-4

### *Afromosin (1)*

White crystals,  $^1\text{H}$  NMR (500 MHz,  $(\text{CD}_3)_2\text{SO}$ )  $\delta_{\text{H}}$  3.79 (OCH<sub>3</sub>, *s*, C-4'), 3.89 (OCH<sub>3</sub>, *s*, C-6), 7.44 (1H, *s*, H-8), 8.34 (1H, *s*, H-7), 6.96 (1H, *s*, H-5), 7.52 (2H, *d*,  $J = 10$  Hz, H-2', 6'), 7.00 (2H, *d*,  $J = 10$  Hz, H-3', 5');  $^{13}\text{C}$  NMR (125 MHz,  $(\text{CD}_3)_2\text{SO}$ )  $\delta_{\text{C}}$  55.6 (OCH<sub>3</sub>), 56.3 (OCH<sub>3</sub>), 153.4 (C-2), 124.9 (C-3), 174.8 (C-4), 116.6 (C-4a), 103.2 (C-5), 147.5 (C-6), 153.3 (C-7), 105.1 (C-8), 152.2 (C-8a), 123.1 (C-1'), 130.5 (C-2', 6'), 114.4 (C-3', 5'), 159.4 (C-4')

### *Lupeol (2)*

White crystals,  $^1\text{H}$ -NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta_{\text{H}}$  1.61 (1H, *m*,  $J = 10$ , H-2), 3.21 (1H, *d*,  $J = 10$ , H-3), 0.70 (1H, *d*,  $J = 10$ , H-5), 1.27 (1H, *s*, H-9), 1.70 (1H, *s*, H-13), 1.94 (1H, *m*,  $J = 20$  H-21), 1.38 (1H, *s*, H-22), 0.99 (3H, *s*, H-23), 0.78 (3H, *s*, H-24), 0.85 (3H, *s*, H-25), 1.05 (3H, *s*, H-26), 0.97 (3H, *s*, H-27), 0.81 (3H, *s*, H-28), 4.71 (1H, *s*, H-29), 4.59 (1H, *s*, H-29), 1.70 (3H, *s*, H-30);  $^{13}\text{C}$ -NMR (125 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta_{\text{C}}$  38.0 (C-1), 27.4 (C-2), 78.7 (C-3), 38.8 (C-4), 55.2 (C-5), 18.3 (C-6), 34.2 (C-7), 40.8 (C-8), 50.4 (C-9), 37.1 (C-10), 20.9 (C-11), 25.2 (C-12), 38.7 (C-13), 42.8 (C-14), 27.7 (C-15), 35.5 (C-16), 42.9 (C-17), 48.2 (C-18), 48.0 (C-19), 151.2 (C-20), 29.8 (C-21), 39.9 (C-22), 27.5 (C-23), 15.2 (C-24), 15.9 (C-25), 15.8 (C-26), 14.3 (C-27), 17.7 (C-28), 109.0 (C-29), 19.0 (C-30)

### *Stigmasterol (3)*

White crystals,  $^1\text{H}$ -NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta_{\text{H}}$  1.88 (1H, *m*,  $J = 20$ , H-1), 1.83 (1H, *m*,  $J = 15$ , H-2), 3.49 (1H, *m*,  $J = 30$ , H-3), 2.25 (1H, *m*,  $J = 10$ , H-4), 5.38 (1H, *m*,  $J = 10$ , H-6), 1.52 (1H, *m*,  $J = 10$ , H-11), 2.03 (1H, *m*,  $J = 10$ , H-12), 1.60 (1H, *m*,  $J = 10$ , H-15) 1.07 (1H, *m*,  $J = 10$ , H-15), 1.30 (1H, *m*,  $J = 10$ , H-16), 0.74 (3H, *s*, H-18), 1.04 (3H, *d*,  $J = 5$ , H-21), 5.21 (1H, *dd*,  $J = 10, 10$ , H-22),

5.06 (1H, *dd*,  $J = 10,10$ , H-23), 0.88 (3H, *d*, H-26), 0.84 (3H, *d*, H-27);  $^{13}\text{C}$ -NMR (125 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta_{\text{C}}$  37.4 (C-1), 31.9 (C-2), 71.8 (C-3), 42.4 (C-4), 140.9 (C-5), 121.5 (C-6), 31.7 (C-7), 31.9 (C-8), 50.2 (C-9), 36.6 (C-10), 20.9 (C-11), 39.8 (C-12), 42.3 (C-13), 56.9 (C-14), 24.3 (C-15), 28.9 (C-16), 56.4 (C-17), 12.0 (C-18), 19.5 (C-19), 40.5 (C-20), 20.9 (C-21), 138.5 (C-22), 129.3 (C-23), 51.3 (C-24), 32.4 (C-25), 21.1 (C-26), 19.2 (C-27), 25.4 (C-28), 12.3 (C-29).

*$\beta$ -sitosterol (4)*

White crystals,  $^1\text{H}$ -NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta_{\text{H}}$  1.88 (1H, *m*,  $J = 20$ , H-1), 1.83 (1H, *m*,  $J = 15$ , H-2), 3.49 (1H, *m*,  $J = 30$ , H-3), 2.25 (1H, *m*,  $J = 10$ , H-4), 5.38 (1H, *m*,  $J = 10$ , H-6), 1.52 (1H, *m*,  $J = 10$ , H-11), 2.03 (1H, *m*,  $J = 10$ , H-12), 1.60 (1H, *m*,  $J = 10$ , H-15) 1.07 (1H, *m*,  $J = 10$ , H-15), 1.30 (1H, *m*,  $J = 10$ , H-16), 0.72 (3H, *s*, H-18), 1.04 (3H, *d*,  $J = 5$ , H-21), 5.21 (1H, *dd*,  $J = 10,10$ , H-22), 5.06 (1H, *dd*,  $J = 10,10$ , H-23), 0.88 (3H, *d*, H-26), 0.84 (3H, *d*, H-27);  $^{13}\text{C}$ -NMR (125 MHz,  $\text{CD}_2\text{Cl}_2$ )  $\delta_{\text{C}}$  37.4 (C-1), 31.9 (C-2), 71.8 (C-3), 42.4 (C-4), 140.9 (C-5), 121.5 (C-6), 31.7 (C-7), 31.9 (C-8), 50.2 (C-9), 36.6 (C-10), 20.9 (C-11), 39.8 (C-12), 42.3 (C-13), 56.9 (C-14), 24.3 (C-15), 28.9 (C-16), 56.4 (C-17), 12.0 (C-18), 19.5 (C-19), 40.5 (C-20), 20.9 (C-21), 33.9 (C-22), 26.0 (C-23), 45.8 (C-24), 32.4 (C-25), 21.1 (C-26), 19.2 (C-27), 25.4 (C-28), 12.3 (C-29).