

Supporting Information

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Polyketides and Alkaloids from the Deep-Sea-Derived Fungus *Aspergillus fumigatus* CBC18132

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SI: Spectral data of the compounds

Compound 1: White powder, ESI-MS m/z : 345.3 [M+H]⁺, 367.3 [M+Na]⁺, molecular formula C₁₈H₁₆O₇, ¹H NMR (CDCl₃ 400 MHz) δ 7.10 (1H, d, J = 1.6 Hz, H-2'), 6.54 (1H, s, H-5), 6.37 (1H, s, H-7), 5.76 (1H, d, J = 1.6 Hz, H-4'), 3.94 (3H, s, 4-OCH₃), 3.68 (3H, s, 6'-OCH₃), 3.65 (3H, s, 5'-OCH₃), 2.43 (3H, s, 8-CH₃). ¹³C NMR (CDCl₃, 100 MHz) δ 190.6 (C-3), 185.8 (C-3'), 174.5 (C-7a), 169.6 (C-5'), 163.6 (C-6'), 158.4 (C-4), 152.3 (C-6), 138.4 (C-1'), 137.2 (C-2'), 108.4 (C-3a), 105.6 (C-7), 105.5 (C-5), 104.0 (C-4'), 84.2 (C-2), 56.8 (5'-OCH₃), 56.2 (4-OCH₃), 52.9 (6'-OCH₃), 23.3 (C-8).

Compound 2: White powder, ESI-MS m/z : 369.3 [M+Na]⁺, 345.4 [M-1]⁺, 691.4 [2M-1]⁺, molecular formula C₁₈H₁₈O₇, ¹H NMR (methanol-*d*₄ 400 MHz) δ 6.96 (1H, d, J = 2.2 Hz, H-2'), 6.68 (1H, d, J = 2.2 Hz, H-4'), 6.39 (1H, s, H-7), 6.21 (1H, s, H-5), 3.69 (3H, s, 5'-OCH₃), 3.66 (3H, s, 6'-OCH₃), 3.38 (3H, s, 4-OCH₃), 2.29 (3H, s, 8-CH₃). ¹³C NMR (methanol-*d*₄ 100 MHz) δ 201.1 (C-3), 168.0 (C-6'), 165.3 (C-7a), 162.6 (C-4), 159.8 (C-5'), 158.5 (C-3'), 149.6 (C-6), 141.9 (C-2), 132.6 (C-1'), 129.9 (C-3a), 111.4 (C-2'), 108.7 (C-7), 104.7 (C-5), 104.1 (C-4'), 56.5 (5'-OCH₃), 56.3 (4-OCH₃), 52.5 (6'-OCH₃), 22.4 (C-8).

Compound 3: Yellow powder, ESI-MS m/z : 283.2 [M-H]⁺, 567.4 [2M-1]⁺, molecular formula C₃₁H₃₇NO₁₀, ¹H NMR (DMSO-*d*₆ 400 MHz) δ 13.24 (1H, s, 5-OH), 7.12 (1H, d, J = 1.2 Hz, H-6), 2.39 (3H, s, 7-CH₃), 7.43 (1H, d, J = 1.7 Hz, H-8), 7.20 (1H, d, J = 2.2 Hz, H-1), 6.84 (1H, d, J = 2.2 Hz, H-3), 3.90 (3H, s, 4-OCH₃). ¹³C NMR (DMSO-*d*₆ 100 MHz) δ 186.33 (C-10), 182.33 (C-9), 164.52 (C-2), 163.46 (C-4), 161.71 (C-5), 146.63 (C-7), 136.82 (C-9a), 132.05 (C-8a), 124.18 (C-6), 119.12 (C-8), 114.39 (C-10a), 112.64 (C-4a), 107.00 (C-1), 105.00 (C-3), 56.34 (4-OCH₃), 21.37 (7-CH₃).

Compound 4: Light yellow powder, ESI-MS m/z : 454.4 [M+Na]⁺, 861.6 [2M-1]⁺, molecular formula C₂₂H₂₅NO₈, ¹H NMR (DMSO-*d*₆ 400 MHz) δ 9.95 (1H, s, 7-NH), 8.25 (2H, d, J = 7.6 Hz, H-19, H-23), 7.68 (1H, t, J = 7.3 Hz, H-21), 7.53 (2H, t, J = 7.7 Hz, H-20, H-22), 6.25 (1H, d, J = 9.2 Hz, H-9), 5.41 (1H, dd, J = 6.42 Hz, 8.7 Hz, H-13), 4.46 (1H, dd, J = 5.8 Hz, 7.7 Hz, H-11), 4.34 (1H, d, J = 5.7 Hz, H-10), 3.24 (3H, s, 8-OCH₃), 2.01 (2H, m, H-14), 1.64 (3H, s, H-16), 0.88 (3H, t, J = 7.5 Hz, H-15).

Compound 5: Light yellow powder, ESI-MS m/z : 440.4 [M+Na]⁺, 416.4 [M-1]⁺, molecular formula C₂₁H₂₃NO₈, ¹H NMR (CDCl₃ 400 MHz) δ 8.32 (2H, d, J = 7.5 Hz, H-19, H-23), 8.11 (1H, s, 7-NH), 7.65 (1H, t, J = 7.5 Hz, H-21), 7.49 (2H, t, J = 7.8 Hz, H-20, H-22), 5.71 (1H, qd, J = 7.1 Hz, 6.9 Hz, H-13), 5.36 (1H, dt, J = 1.9 Hz, 8.9 Hz, H-12), 4.78 (1H, dd, J = 4.8 Hz, 8.7 Hz, H-11), 4.69 (1H, d, J = 8.6 Hz, H-9), 4.62 (1H, d, J = 4.8 Hz, H-10), 3.43 (3H, s, 8-OCH₃), 1.72 (3H, dd, J = 1.82 Hz, 7.08 Hz, H-15), 1.68 (3H s H-16).

Compound 6: Light yellow powder, ESI-MS m/z : 412.4 [M+H]⁺, 434.3 [M+Na]⁺, molecular formula C₂₂H₂₁NO₇, ¹H NMR (CDCl₃ 400 MHz) δ 8.31 (2H, dd, J = 1.2 Hz, 7.3 Hz, H-17, H-21), 7.79 (1H, brs, 12-NH), 7.62 (1H, t, J = 7.8 Hz, 7.3 Hz, H-19), 7.48 (2H, t, J = 7.8 Hz, 7.5 Hz, H-18, H-20), 7.03 (1H, d, J = 3.5 Hz, H-4), 6.22 (1H, d, J = 3.5 Hz, H-3), 4.69 (1H, s, H-14), 3.39 (3H, s, H-25), 2.75 (2H, q, J = 7.6 Hz, H-22), 2.00 (3H, s, H-24), 1.27 (3H, t, J = 7.5 Hz, H-23). ¹³C NMR (CDCl₃ 400 MHz) δ 195.8 (C-8), 194.8 (C-15), 172.7 (C-6), 166.4 (C-11), 163.9 (C-2), 143.5 (C-5), 134.7 (C-19), 132.6 (C-16), 130.7 (C-17, C-21), 128.8 (C-18, C-20), 118.4 (C-4), 108.1 (C-7), 107.9 (C-3), 91.7 (C-9), 89.9 (C-13), 74.3 (C-14), 51.8 (C-25), 21.9 (C-22), 11.9 (C-23), 6.3 (C-24).

Compound 7: Light yellow powder, molecular formula C₂₄H₂₁N₅O₄, ¹H NMR (CDCl₃, 400 MHz) δ 8.34 (1H, dd, J = 7.9 Hz, 1.5 Hz, 2-NH), 7.79 (1H, dd, J = 8.2 Hz, 1.4 Hz, H-7), 7.60 (1H, ddd, J = 8.2 Hz, 7.0 Hz, 1.4 Hz, H-9), 7.44 (1H, d, J = 7.8 Hz, H-24), 7.36 (1H, d, J = 7.6

Hz, H-27), 7.30 (1H, td, $J = 7.7$ Hz, 1.3 Hz, H-25), 7.16 (1H, m, H-26), 5.72 (1H, m, H-14), 5.33 (1H, d, $J = 7.2$ Hz, H-18), 5.29 (1H, s, H-18), 3.71 (1H, m, H-20), 2.97 (1H, dd, $J = 15.1$ Hz, 7.4 Hz, H-15), 2.13 (1H, d, $J = 14.9$ Hz, H-15), 2.05 (3H, s, H-16), 1.13 (1H, d, $J = 6.4$ Hz, H-19), 1.06 (3H, d, $J = 6.8$ Hz, H-29).

Compound 8: Light yellow powder, molecular formula $C_{24}H_{23}N_5O_4$, 1H NMR ($CDCl_3$, 400 MHz) δ 8.24 (1H, m, H-10), 7.76 (1H, m, H-8), 7.54 (1H, d, $J = 7.9$ Hz, H-24), 7.48 (1H, m, H-9), 7.32 (1H, dt, $J = 8.2$ Hz, 6.6 Hz, H-25), 7.17 (1H, t, $J = 7.5$ Hz, H-26), 5.82 (1H, dd, $J = 11.0$ Hz, 4.7 Hz, H-14), 5.46 (1H, s, H-18), 4.77 (1H, dd, $J = 7.3$ Hz, 4.1 Hz, H-3), 4.20 (1H, d, $J = 7.0$ Hz, H-20), 2.62 (1H, dd, $J = 13.6$ Hz, 11.0 Hz, H-15), 2.48 (1H, dd, $J = 13.6$ Hz, 4.8 Hz, H-15), 1.85 (3H, d, $J = 7.1$ Hz, H-16), 1.33 (3H, d, $J = 6.7$ Hz, H-29).

Compound 9: Light yellow powder, molecular formula $C_{24}H_{23}N_5O_4$, 1H NMR ($CDCl_3$, 400 MHz) δ 8.20 (1H, d, $J = 8.0$ Hz, H-10), 7.74 (1H, m, H-8), 7.65 (1H, d, $J = 8.2$ Hz, H-7), 7.58 (1H, d, $J = 7.7$ Hz, H-27), 7.49 (1H, d, $J = 8.3$ Hz, H-24), 7.48 (1H, d, $J = 8.3$ Hz, H-9), 7.29 (1H, d, $J = 7.6$ Hz, H-25), 7.13 (1H, t, $J = 7.5$ Hz, H-26), 5.95 (1H, dd, $J = 11.0$ Hz, 4.7 Hz, H-14), 5.48 (1H, s, H-18), 4.87 (1H, q, $J = 6.6$ Hz, H-3), 4.20 (1H, d, $J = 6.8$ Hz, H-20), 2.51 (1H, dd, $J = 13.7$ Hz, 10.8 Hz, H-15), 2.27 (1H, dd, $J = 13.8$ Hz, 5.8 Hz, H-15), 1.78 (3H, d, $J = 6.6$ Hz, H-16), 1.33 (3H, d, $J = 6.6$ Hz, H-29).

Compound 10: Light yellow powder, molecular formula $C_{22}H_{18}N_4O_4$, 1H NMR ($CDCl_3$, 400 MHz) δ 8.19 (1H, d, $J = 8.0$ Hz, H-19), 7.89 (s, 1H), 7.72 (1H, d, $J = 8.1$ Hz, H-22), 7.66 (1H, d, $J = 8.1$ Hz, H-22), 7.60 (1H, d, $J = 8.1$ Hz, H-20), 7.47 (1H, t, $J = 7.6$ Hz, H-8), 7.42 (1H, t, $J = 7.6$ Hz, H-5), 7.39 (1H, d, $J = 7.5$ Hz, H-7), 7.20 (1H, t, $J = 7.5$ Hz, H-6), 5.48 (1H, d, $J = 16.9$ Hz, H-14), 4.42 (1H, q, $J = 6.9$ Hz, H-11), 2.63 (1H, d, $J = 12.2$ Hz, H-13), 1.73 (3H, d, $J = 6.9$ Hz, H-12). ^{13}C NMR ($CDCl_3$, 400 MHz) δ 171.7 (C-10), 161.2 (C-15), 146.7 (C-24), 139.3 (C-9), 134.9 (C-4), 134.7 (C-21), 131.2 (C-7), 127.8 (C-22), 127.1 (C-20), 126.2 (C-19), 124.4 (C-6), 115.8 (C-8), 77.7 (C-3), 60.4 (C-11), 14.6 (C-12).

Compound 11: Light yellow powder, ESI-MS m/z : 402.4 $[M+Na]^+$, molecular formula $C_{22}H_{25}N_3O_3$, 1H NMR ($CDCl_3$, 400 MHz) δ 7.84 (1H, brs, 1-NH), 7.43 (1H, d, $J = 8.6$ Hz, H-16), 6.85 (1H, d, $J = 2.2$ Hz, H-19), 6.81 (1H, dd, $J = 2.2$ Hz, 8.5 Hz, H-17), 5.98 (1H, brd, $J = 9.6$ Hz, H-2), 4.90 (1H, d, $J = 9.6$ Hz, H-21), 4.17 (1H, dd, $J = 11.6$ Hz, 5.0 Hz, H-12), 4.09 (1H, d, $J = 8.2$ Hz, H-6), 3.83 (3H, s, 18-OCH₃), 3.64 (2H, m, H-9), 3.51 (1H, dd, $J = 5.0$ Hz, 16.0 Hz, H-13), 3.09 (1H, ddd, $J = 10.5$ Hz, 16.0 Hz, 1.0 Hz, H-13), 2.41 (1H, m, H-7), 2.23 (1H, m, H-7), 2.05 (1H, m, H-8), 1.99 (3H, s, H-24), 1.94 (1H, m, H-8), 1.64 (3H, s, H-23). ^{13}C NMR ($CDCl_3$, 400 MHz) δ 169.7 (C-5), 165.9 (C-11), 156.6 (C-18), 137.1 (C-20), 134.1 (C-22), 132.2 (C-2), 124.3 (C-21), 120.8 (C-15), 119.0 (C-16), 109.6 (C-17), 106.4 (C-14), 95.4 (C-19), 59.4 (C-6), 56.9 (C-12), 55.9 (18-OCH₃), 51.1 (C-3), 45.5 (C-9), 28.7 (C-7), 25.8 (C-23), 23.2 (C-8), 22.1 (C-13), 18.2 (C-24).

Compound 12: Colorless solid, ESI-MS m/z : 306.3 $[M+Na]^+$, molecular formula $C_{16}H_{17}N_3O_2$, 1H NMR ($DMSO-d_6$, 400 MHz) δ 10.85 (1H, s, 1-NH), 7.73 (1H, s, 14-NH), 7.56 (1H, d, $J = 7.83$ Hz, H-4), 7.32 (1H, d, $J = 8.08$ Hz, H-7), 7.18 (1H, d, $J = 2.41$ Hz, H-2), 7.05 (1H, dd, $J = 6.9$ Hz, 8.1 Hz, H-6), 6.96 (1H, dd, $J = 7.0$ Hz, 8.0 Hz, H-5), 4.30 (1H, t, $J = 5.3$ Hz, H-9), 4.06 (1H, dd, $J = 8.6$ Hz, 7.9 Hz, H-12), 3.39 (1H, m, H-16), 3.26 (1H, m, H-15), 3.22 (1H, d, $J = 4.61$ Hz, H-8), 3.07 (1H, dd, $J = 14.9$ Hz, 5.7 Hz, H-8), 1.97 (1H, dt, $J = 2.9$ Hz, 7.0 Hz, H-16), 1.67 (1H, m, H-16), 1.64 (1H, m, H-17), 1.38 (1H, m, H-17).

Compound 13: Colorless solid, ESI-MS m/z : 584.5 $[M+H]^+$, 606.5 $[M+Na]^+$, molecular formula $C_{31}H_{37}NO_{10}$, 1H NMR (methanol- d_4 , 300 MHz) δ 4.80 (1H, dd, $J = 5.6$ Hz, 10.7 Hz, H-1), 1.88 (1H, m, H-2), 1.86 (1H, m, H-2), 1.43 (1H, m, H-5), 4.99 (1H, m, H-7), 4.97 (1H, m, H-13), 1.82 (1H, m, H-8), 1.68 (1H, s, H-8), 1.62 (1H, m, H-9), 3.77 (1H, d, $J = 11.9$ Hz, H-11)

3.74 (1H, d, $J = 11.9$ Hz, H-11) 6.81 (1H, s, H-5), 9.03 (1H, s, H-2), 8.28 (1H, ddd, $J = 8.2$ Hz, 1.8 Hz, H-4), 8.63 (1H, d, $J = 4.2$ Hz, H-6), 1.49 (3H, s, 12-CH₃), 1.75 (3H, s, 14-CH₃), 0.92 (3H, s, 15-CH₃), 2.13 (3H, s, 7-OCOCH₃), 2.03 (3H, s, 1-OCOCH₃), 2.07 (3H, s, 11-OCOCH₃). ¹³C NMR (methanol-*d*₄ 75 MHz) δ 172.6 (11-OCOCH₃), 172.5 (7-OCOCH₃), 172.0 (1-OCOCH₃), 165.1 (C-2), 164.1 (C-4), 158.2 (C-6), 151.9 (C-6), 147.4 (C-2), 134.9 (C-4), 129.2 (C-3), 125.4 (C-5), 104.5 (C-3), 101.0 (C-5), 84.5 (C-6), 79.8 (C-7), 75.3 (C-5), 66.0 (C-11), 60.3 (C-13), 55.5 (C-5), 46.6 (C-9), 41.7 (C-10), 39.1 (C-4), 37.1 (C-3), 26.1 (C-8), 23.8 (C-2), 21.1 (7-OCOCH₃), 21.0 (1-OCOCH₃), 20.7 (11-OCOCH₃), 17.9 (C-12), 16.8 (C-14), 13.5 (C-15).

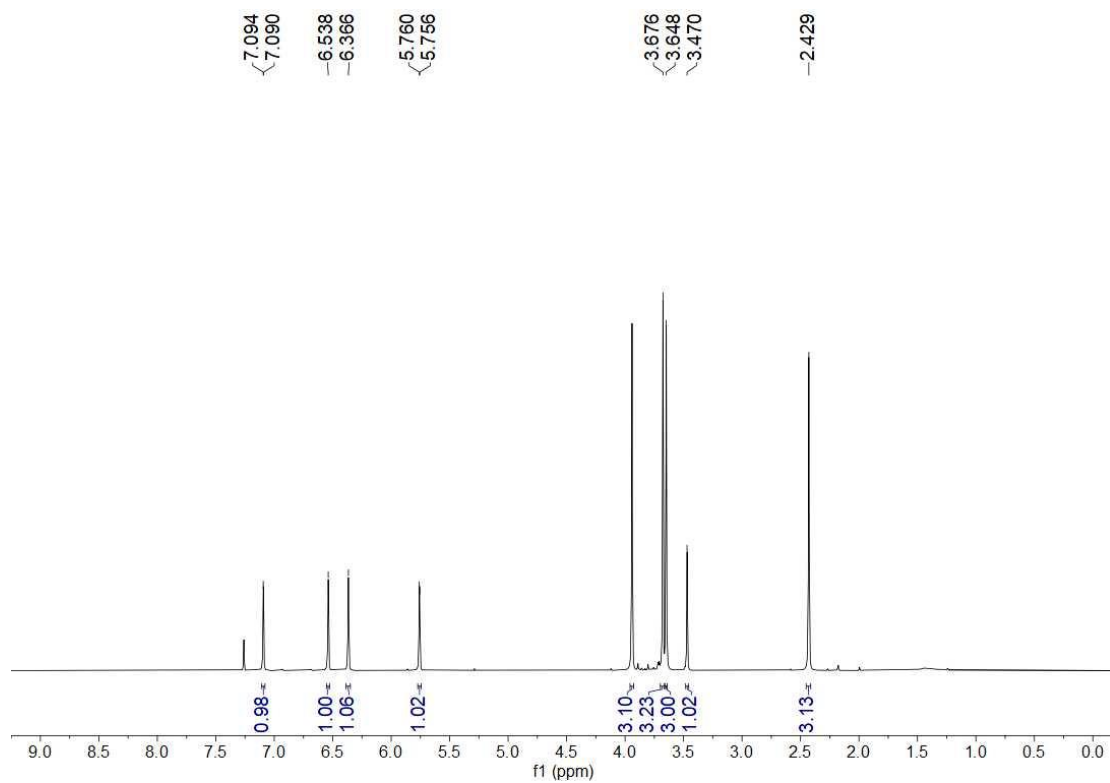


Figure S1: ^1H NMR spectrum of **1** in CDCl_3 (400 MHz)

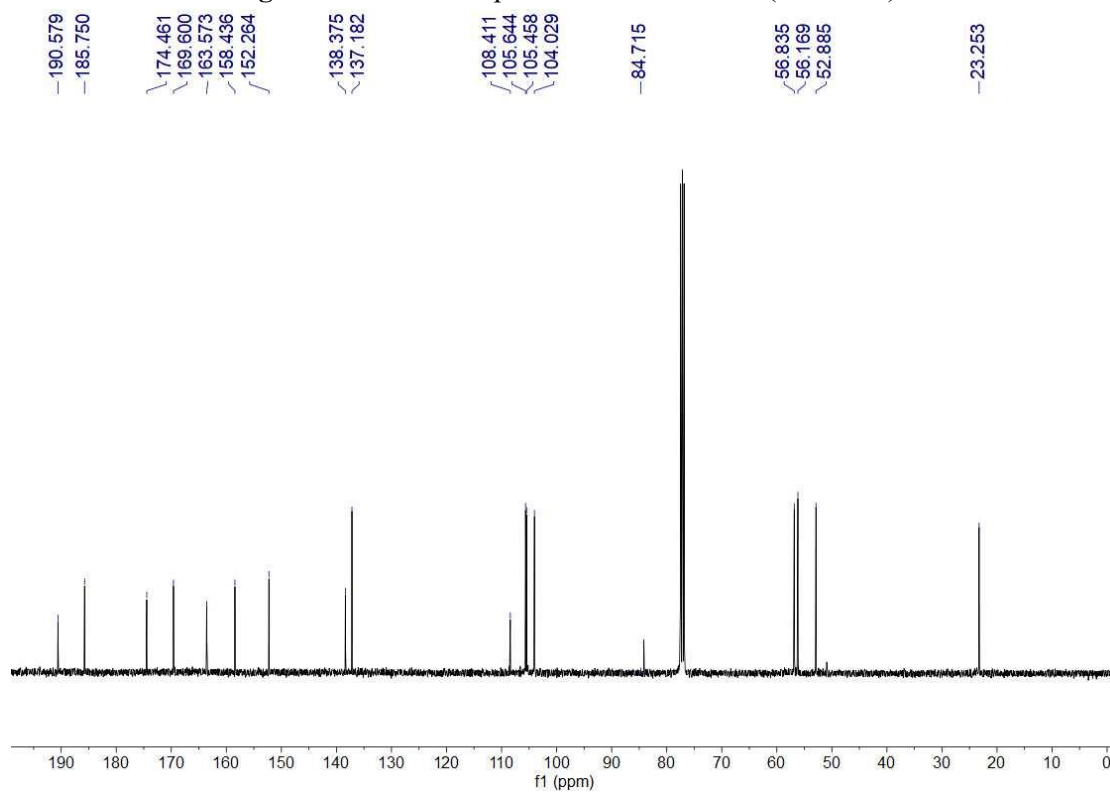


Figure S2: ^{13}C NMR spectrum of **1** in CDCl_3 (100 MHz)

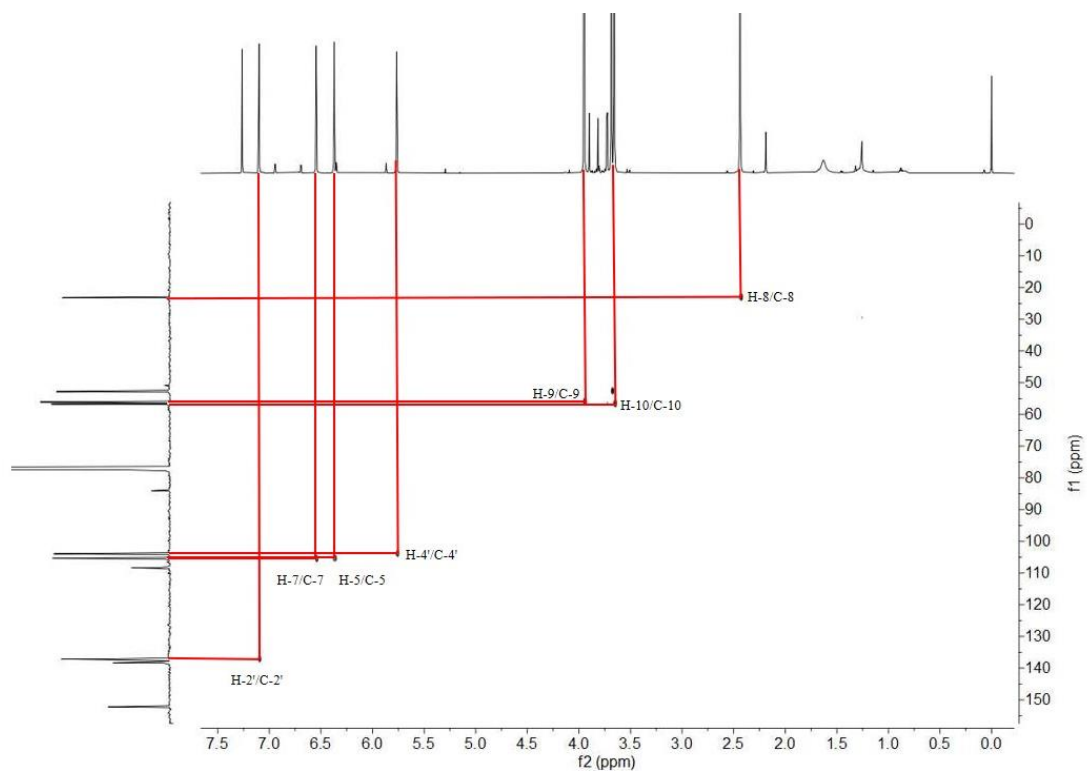


Figure S3: HSQC spectrum of **1** in CDCl_3

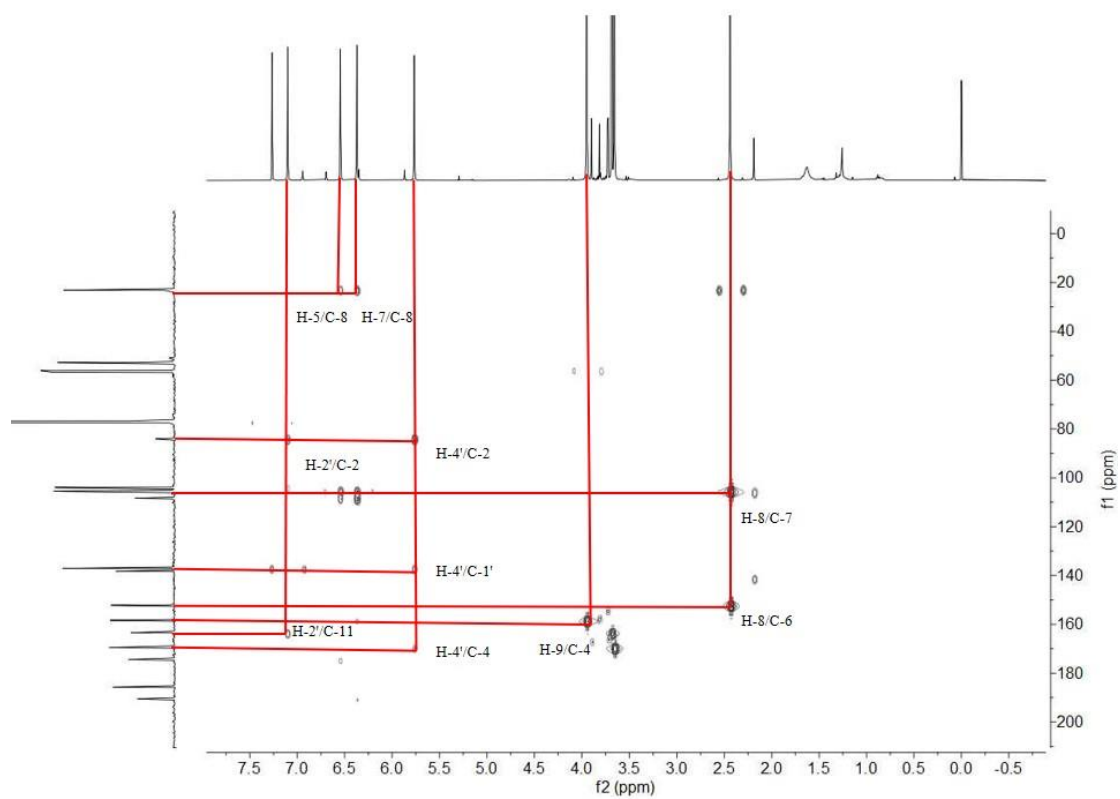


Figure S4: HMBC spectrum of **1** in CDCl_3

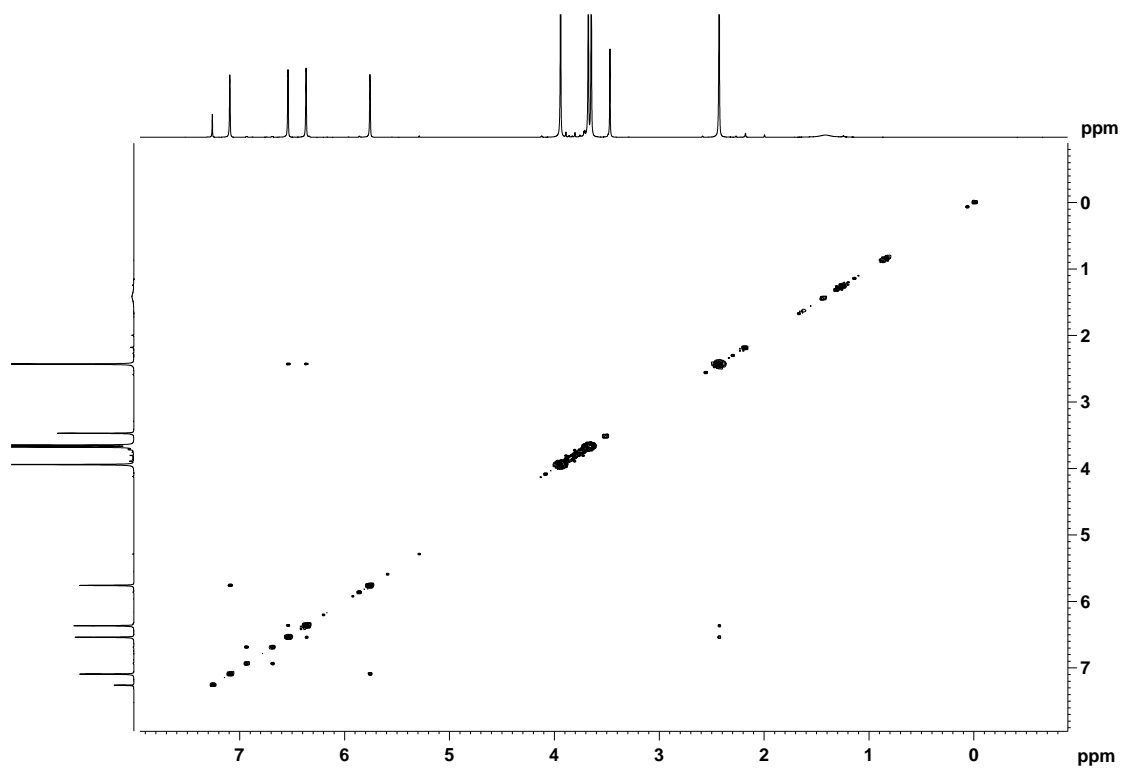


Figure S5: ^1H - ^1H COSY spectrum of compound **1** in CDCl_3

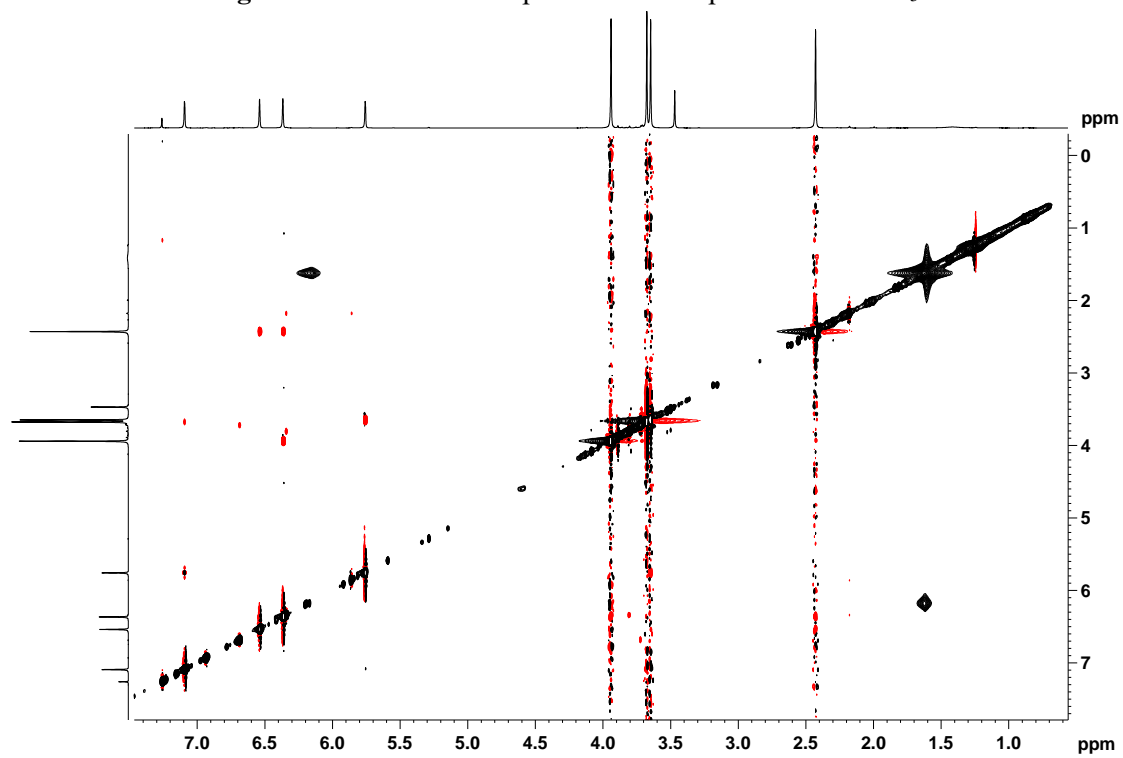


Figure S6: NOESY spectrum of compound **1** in CDCl_3

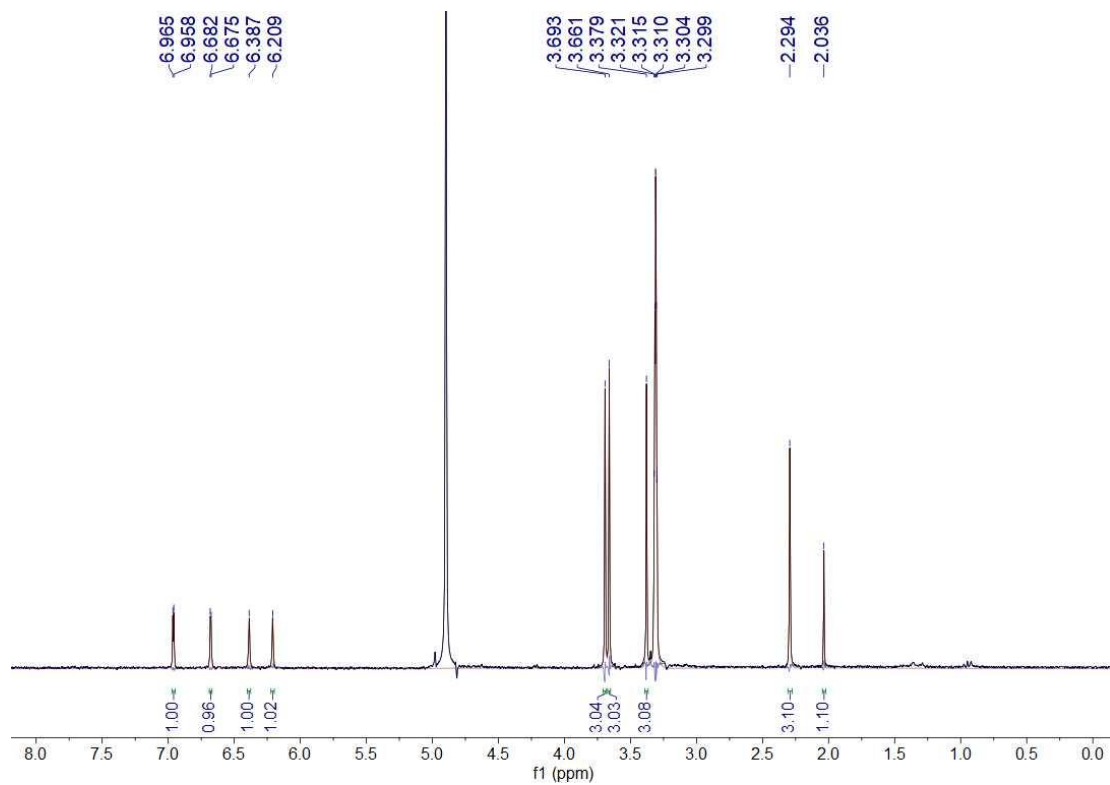


Figure S7: ^1H NMR spectrum of **2** in methanol- d_4 (300 MHz)

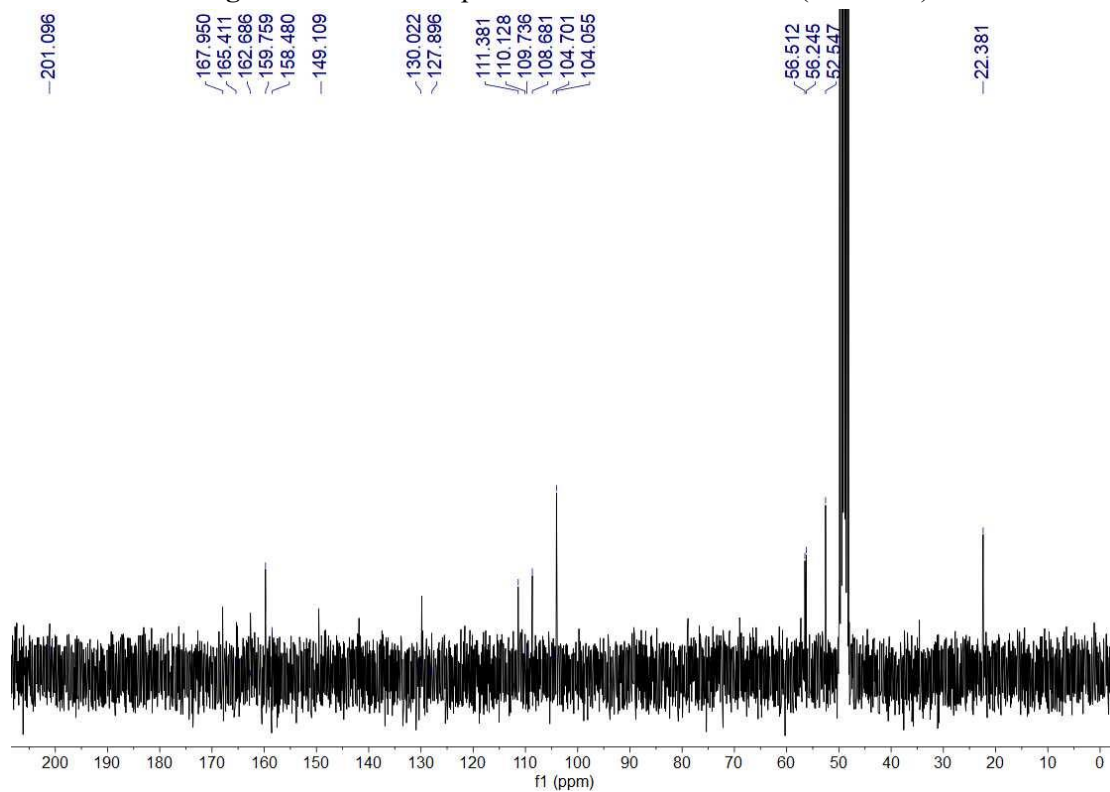


Figure S8: ^{13}C NMR spectrum of **2** in methanol- d_4 (75 MHz)

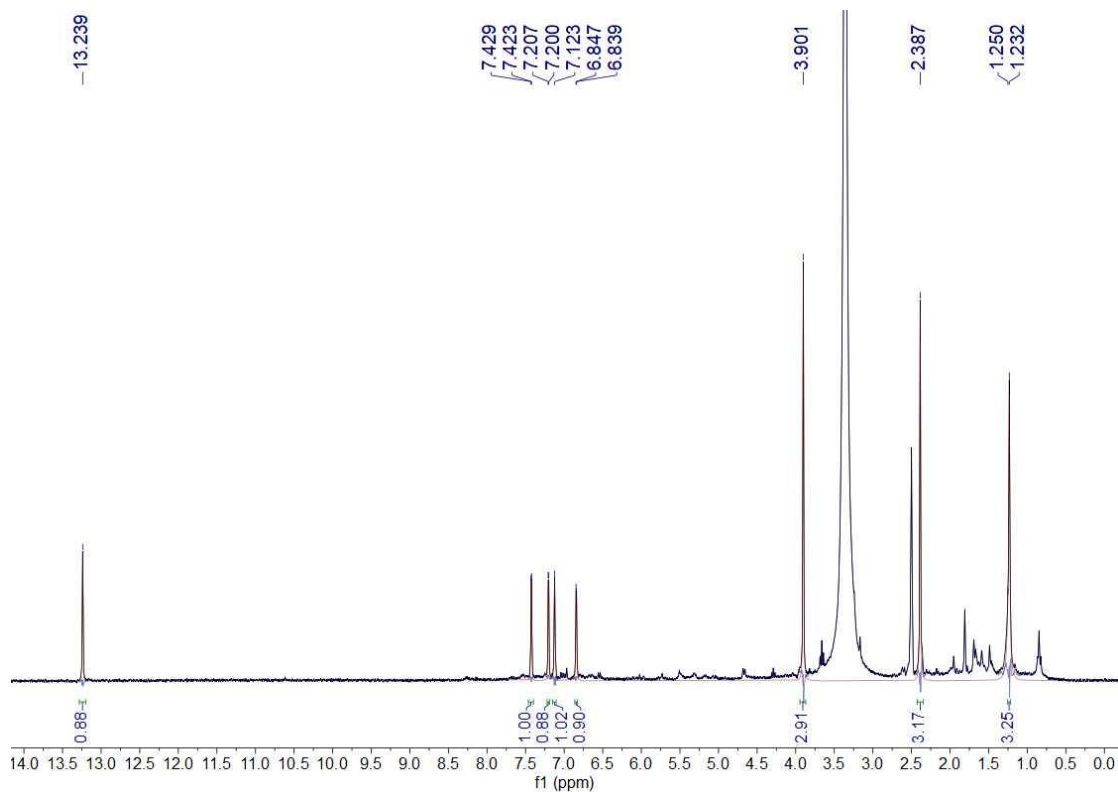


Figure S9: ^1H NMR spectrum of **3** in $\text{DMSO-}d_6$ (300 MHz)

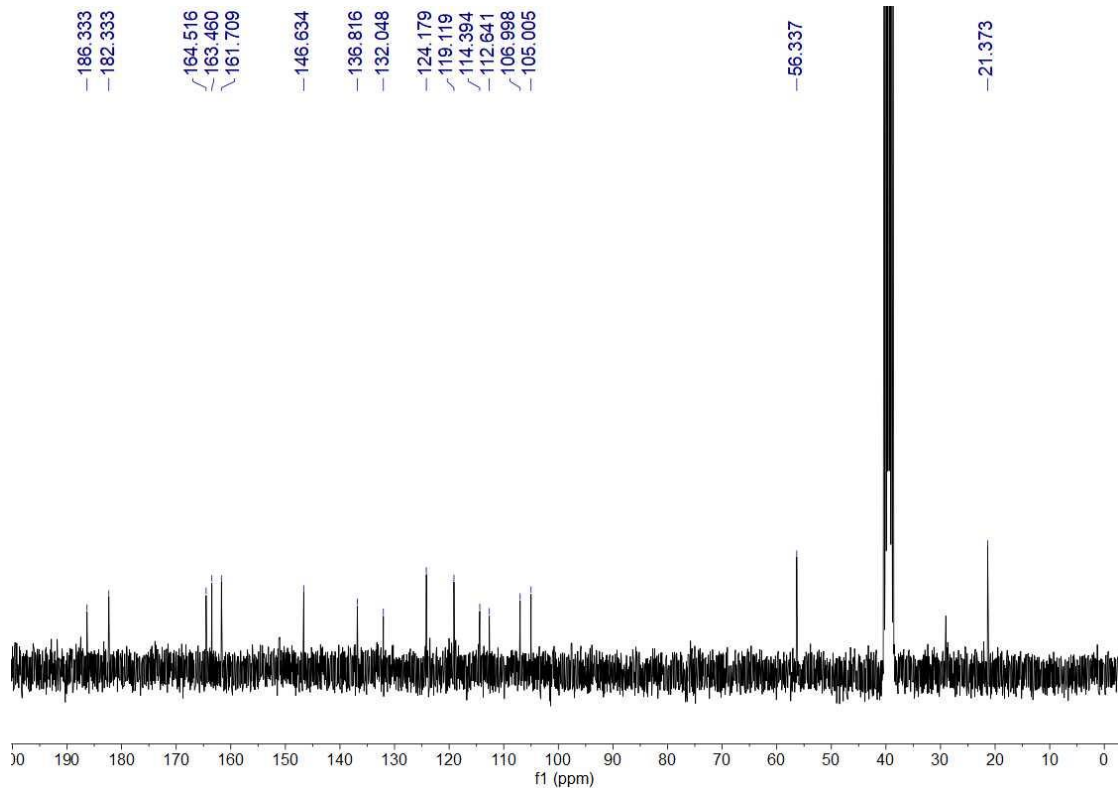


Figure S10: ^{13}C NMR spectrum of **3** in $\text{DMSO-}d_6$ (75 MHz)

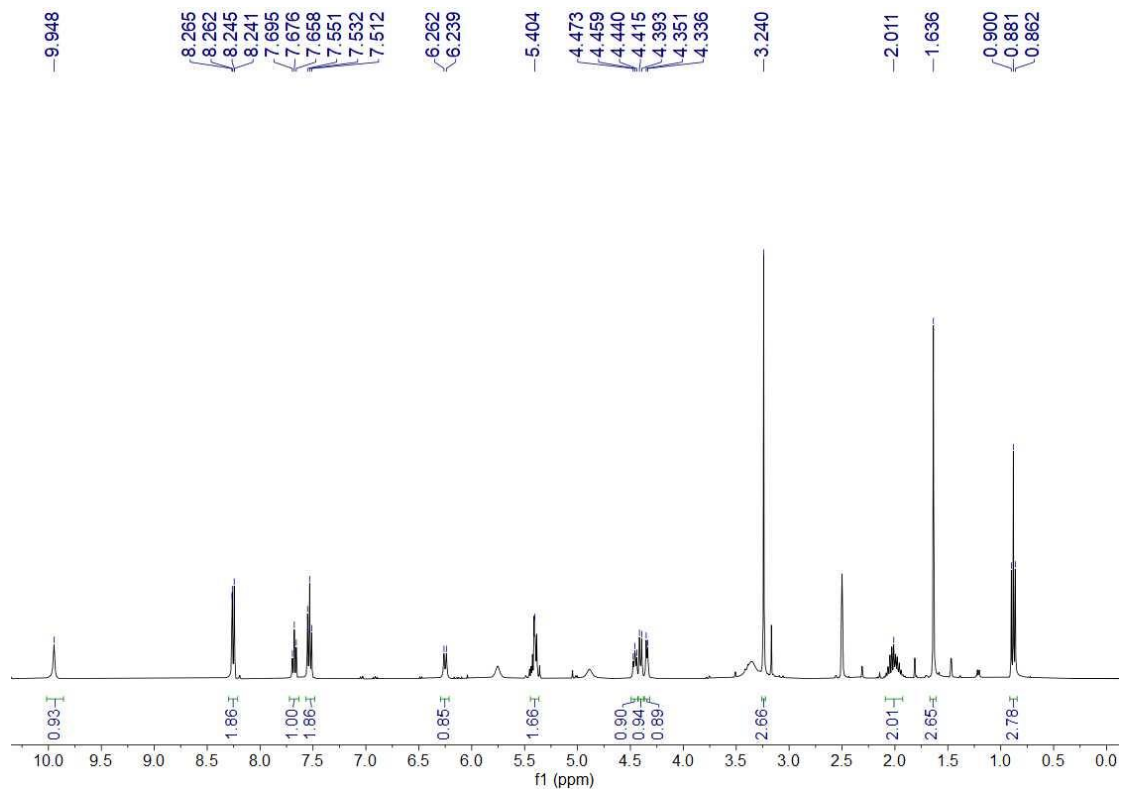


Figure S11: ^1H NMR spectrum of **4** in $\text{DMSO-}d_6$ (400 MHz)

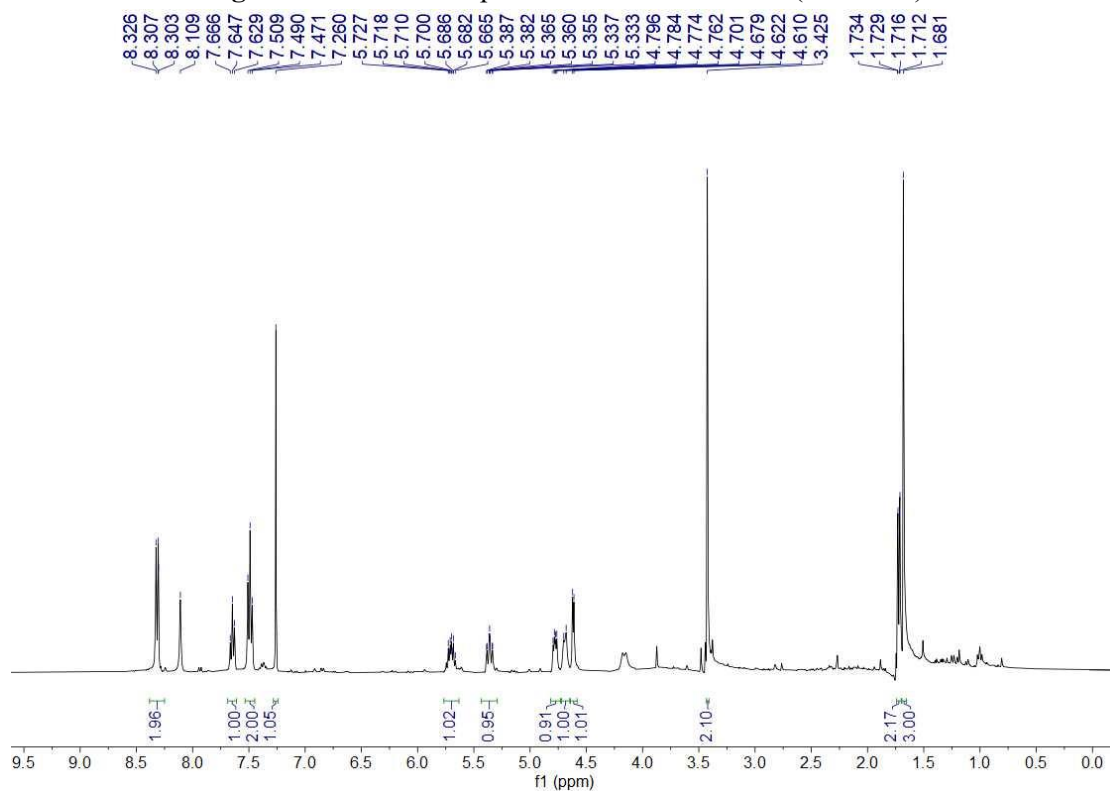


Figure S12: ^1H NMR spectrum of **5** in CDCl_3 (400 MHz)

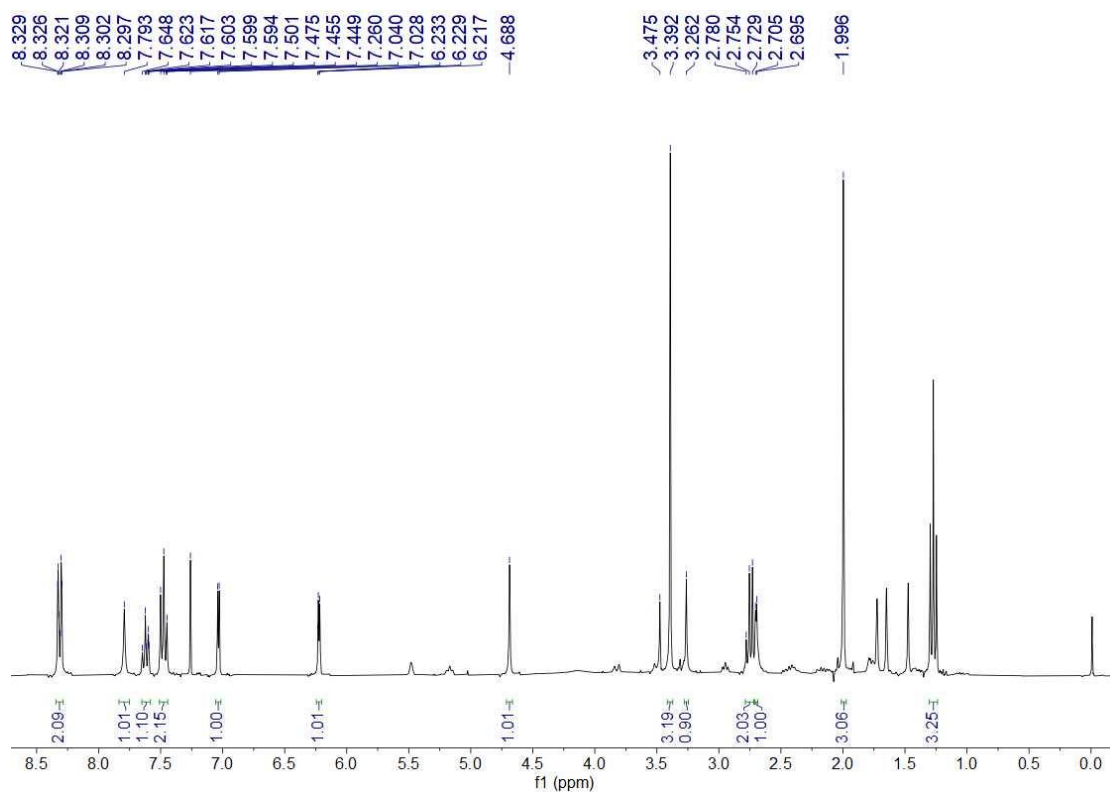


Figure S13: ^1H NMR spectrum of **6** in CDCl_3 (300 MHz)

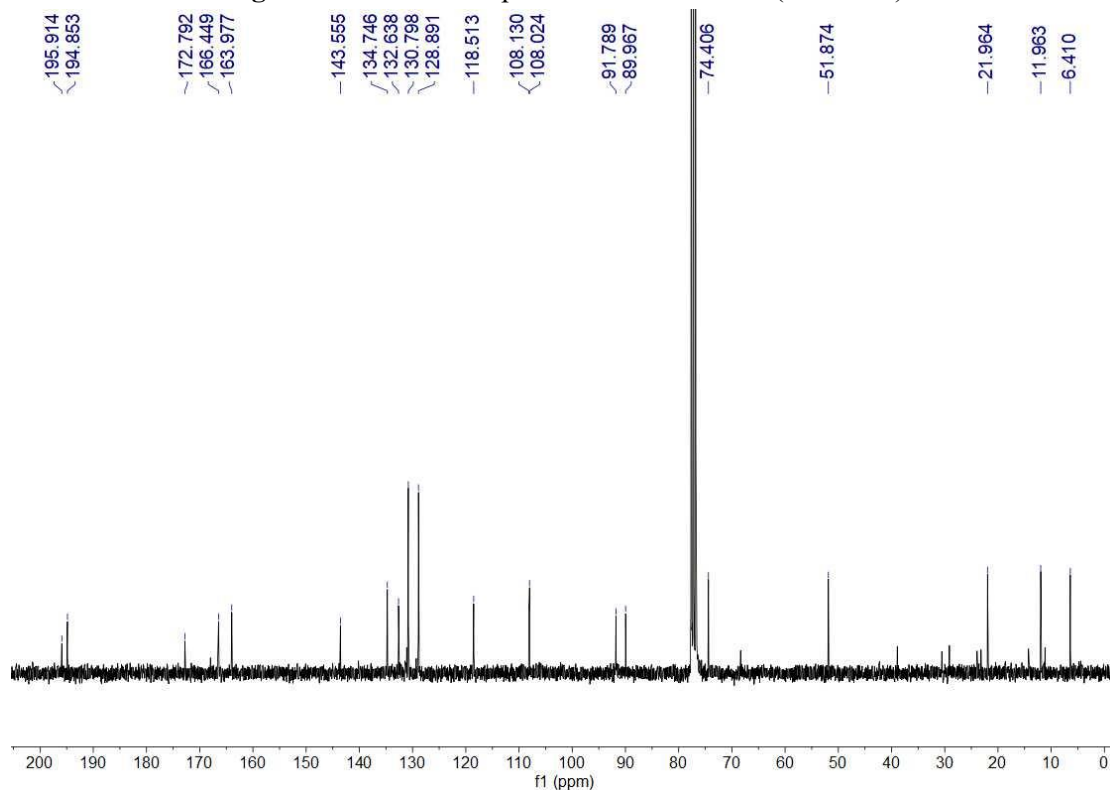


Figure S14: ^{13}C NMR spectrum of **6** in CDCl_3 (75 MHz)

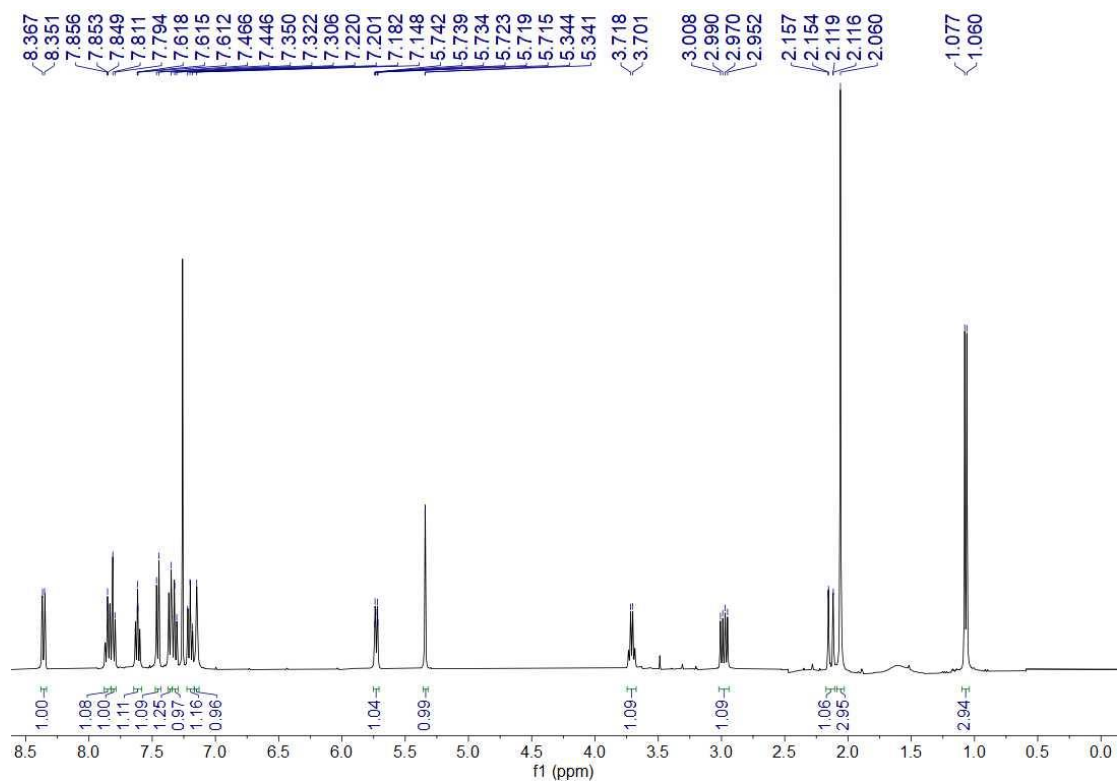


Figure S15: ^1H NMR spectrum of 7 in CDCl_3 (400 MHz)

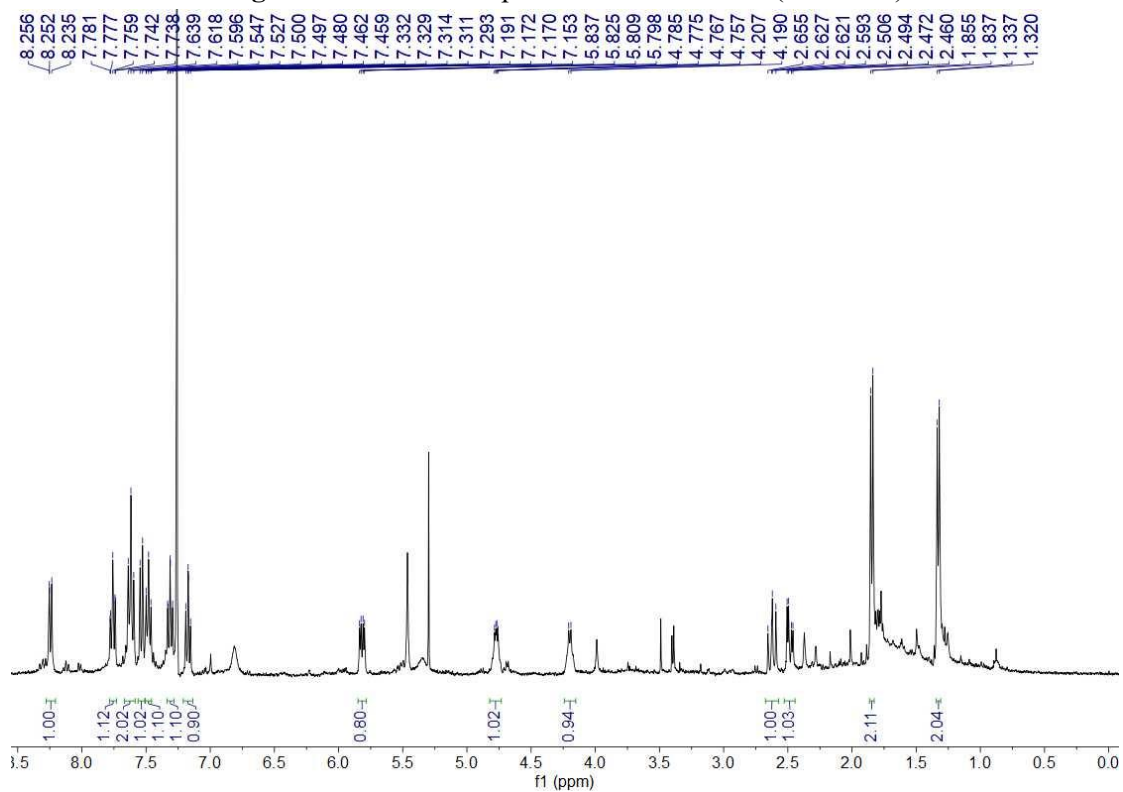


Figure S16: ^1H NMR spectrum of 8 in CDCl_3 (400 MHz)

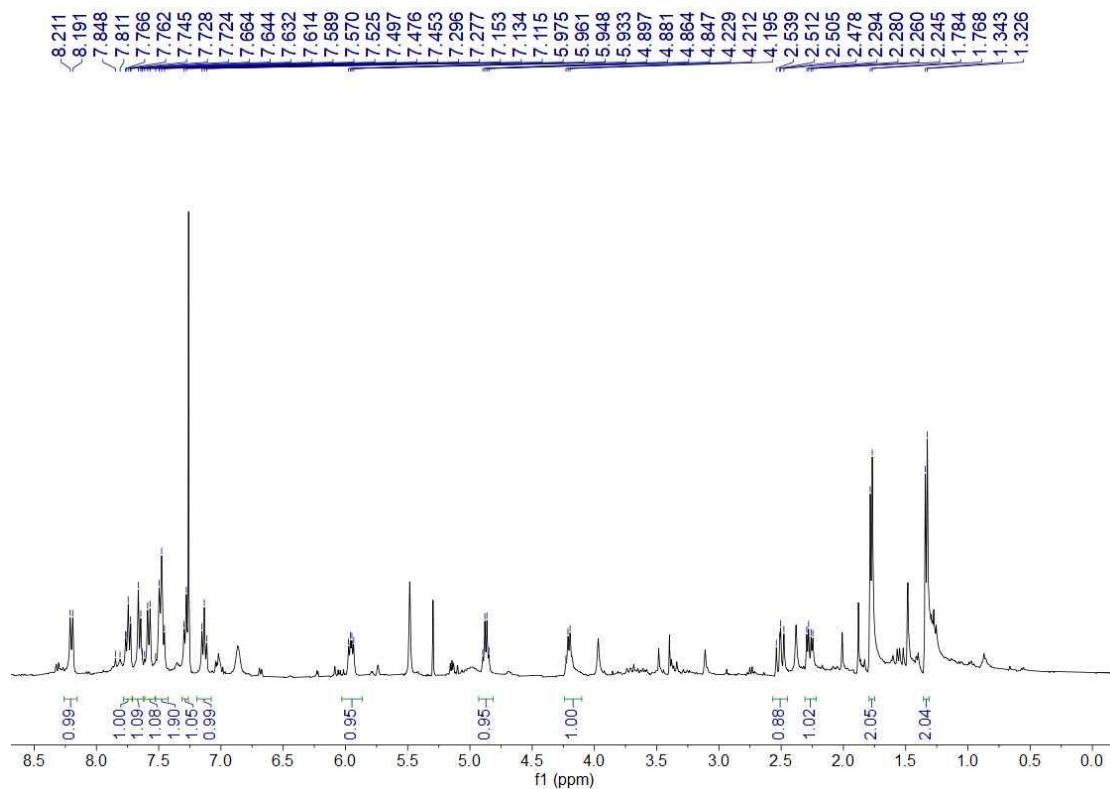


Figure S17: ^1H NMR spectrum of **9** in CDCl_3 (400 MHz)

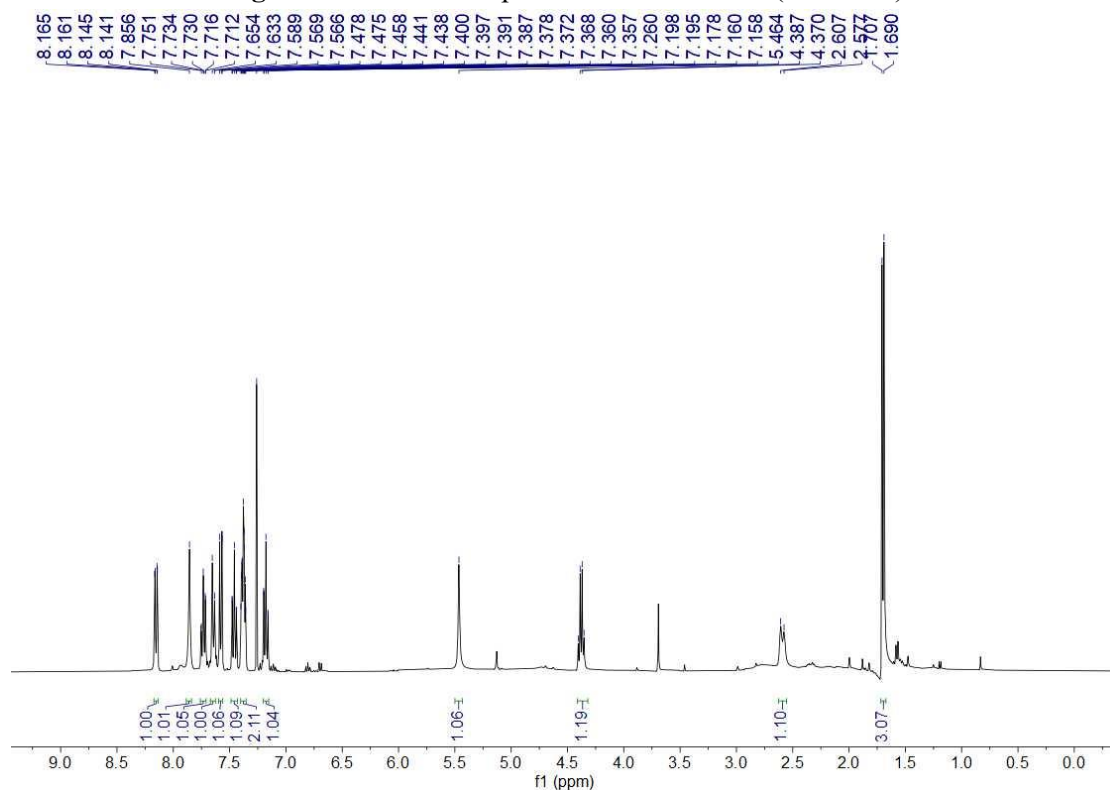


Figure S18: ^1H NMR spectrum of **10** in CDCl_3 (400 MHz)

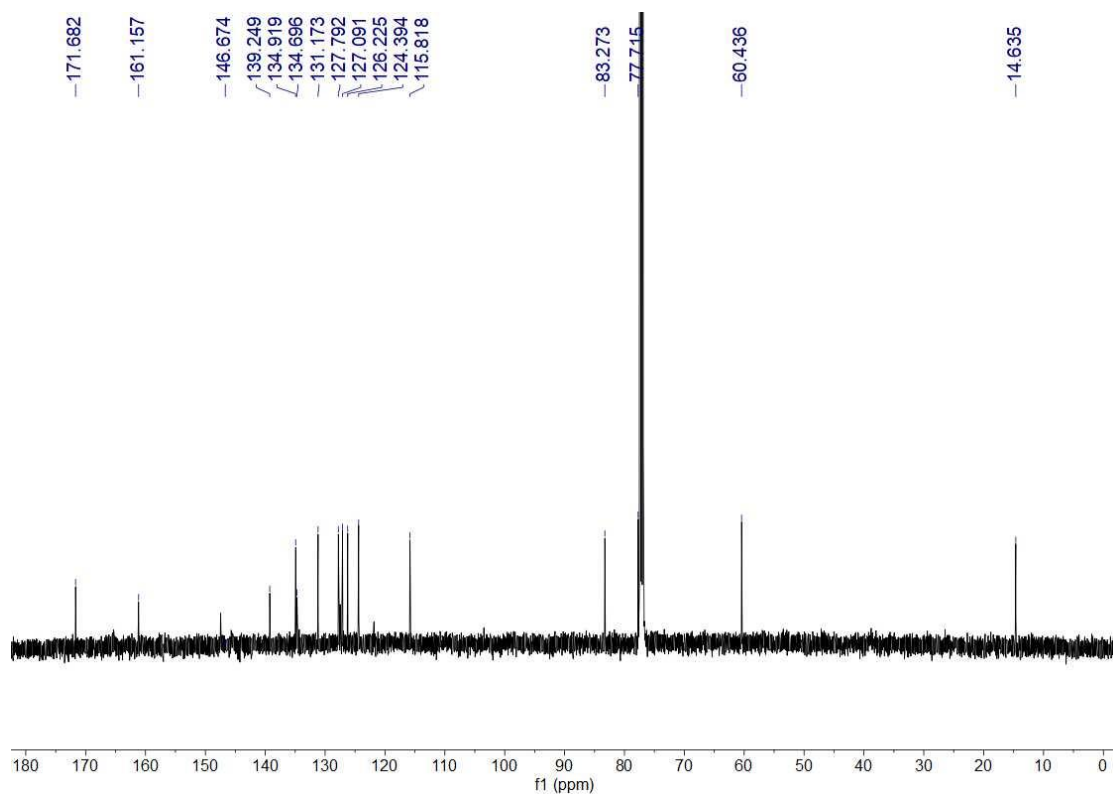


Figure S19: ^{13}C NMR spectrum of **10** in CDCl_3 (100 MHz)

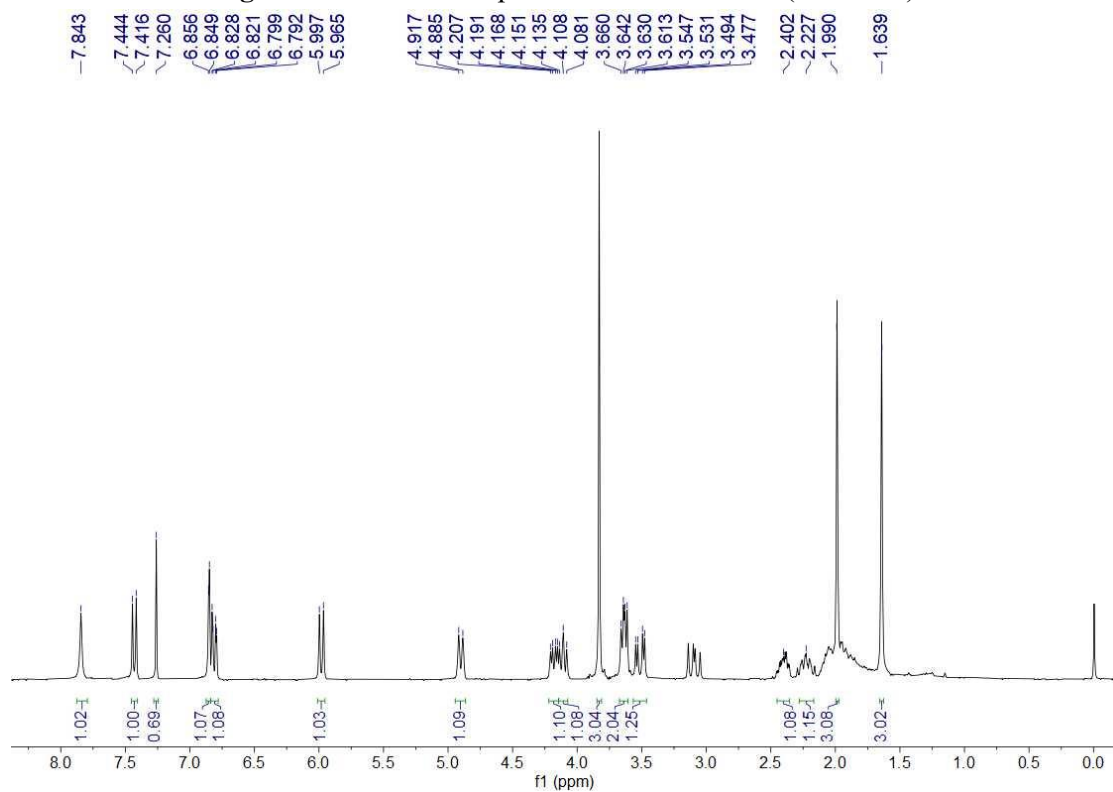


Figure S20: ^1H NMR spectrum of **11** in CDCl_3 (400 MHz)

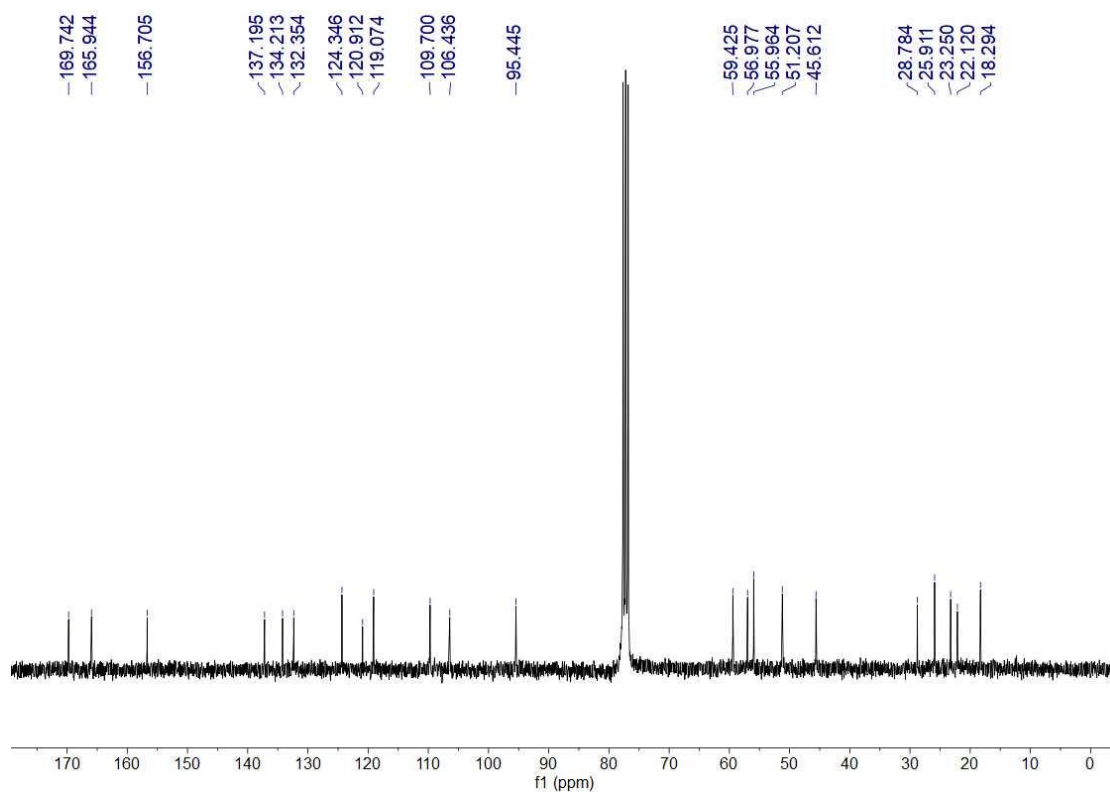


Figure S21: ^{13}C NMR spectrum of **11** in methanol- d_4 (100 MHz)

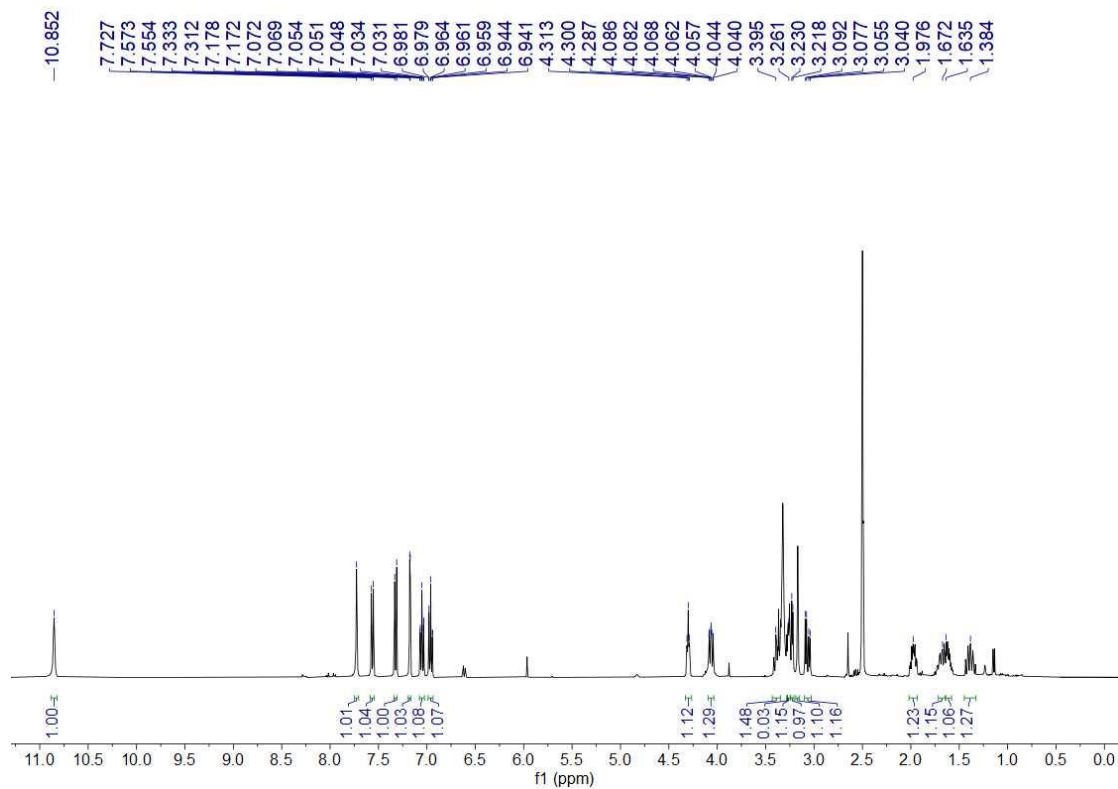


Figure S22: ^1H NMR spectrum of **12** in DMSO- d_6 (400 MHz)

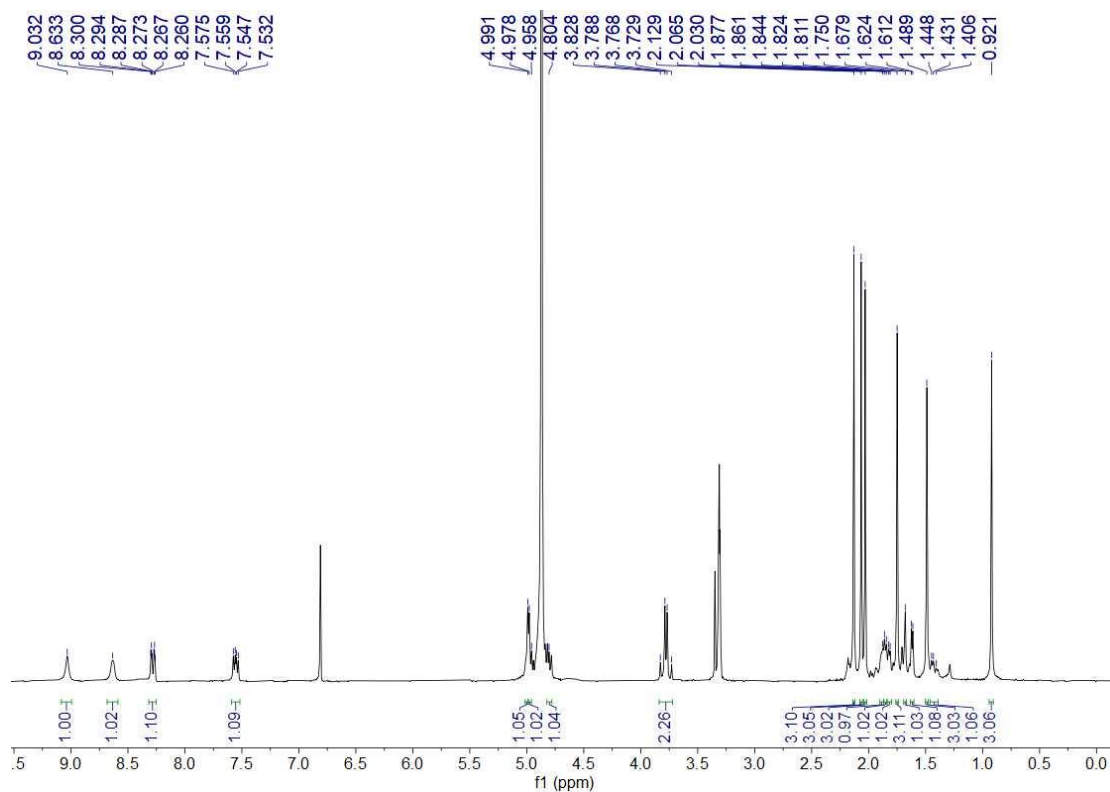


Figure S23: ^1H NMR spectrum of **13** in methanol- d_4 (300 MHz)

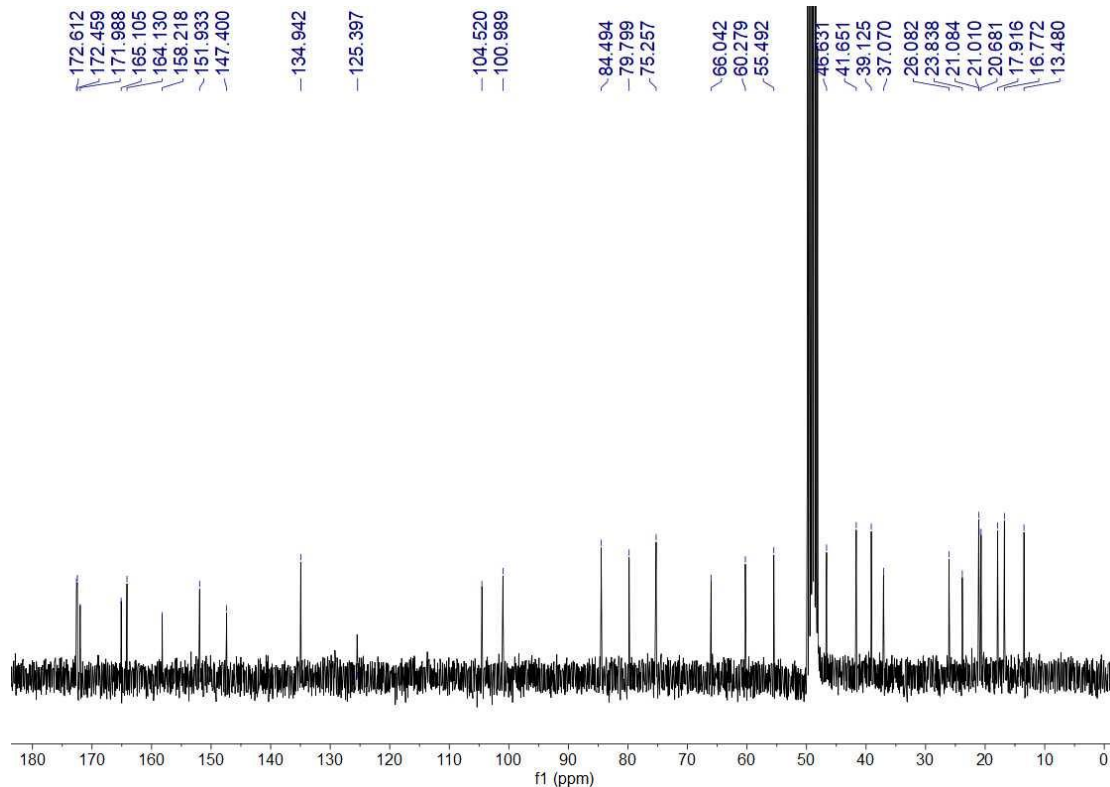


Figure S24: ^{13}C NMR spectrum of **13** in methanol- d_4 (75 MHz)

ly#175 RT: 0.77684 AV: 1 NL: 2.65E8
T: FTMS + p ESI Full ms [100.0000-1050.0000]

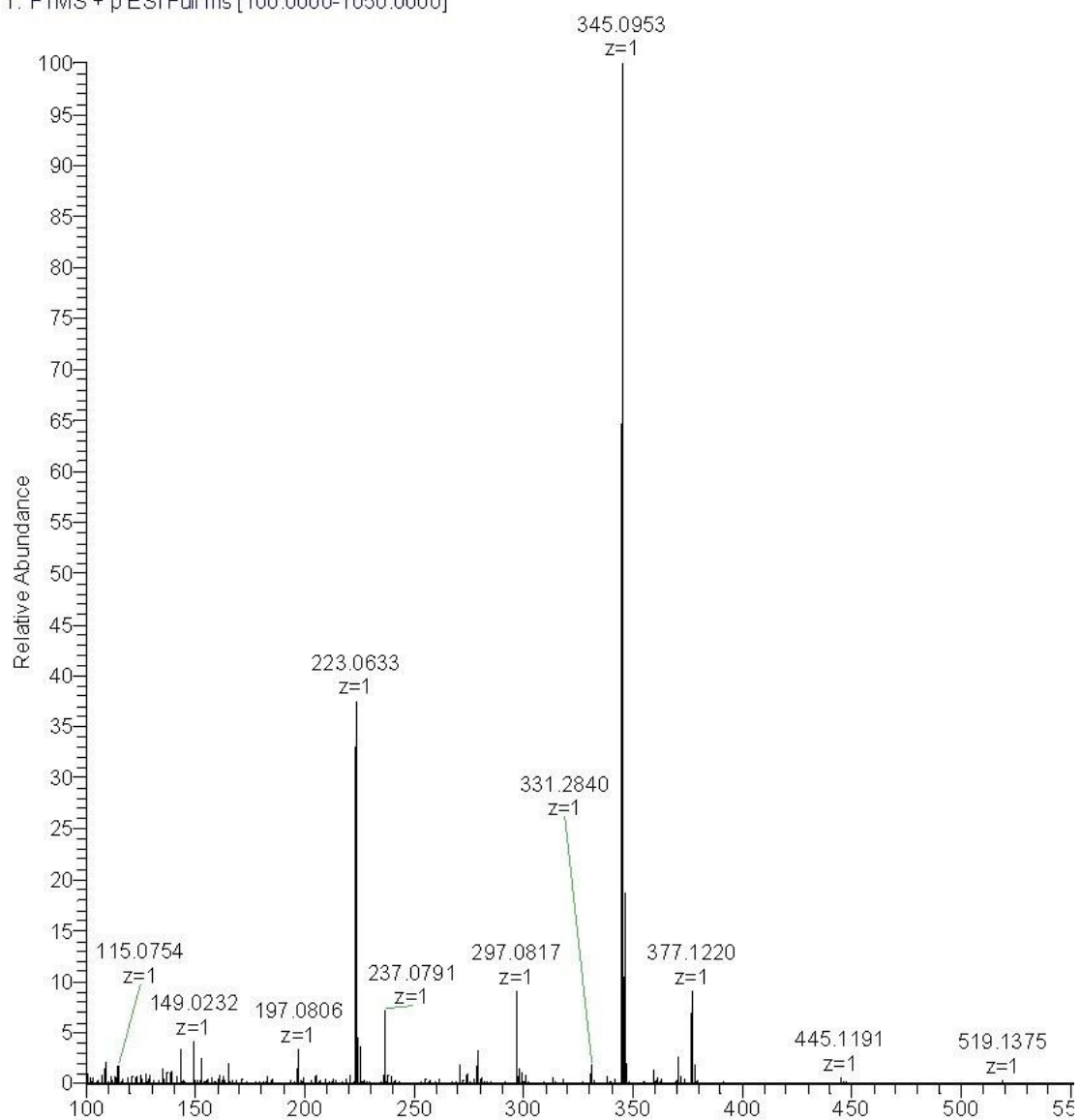


Figure S25: HRESIMS spectrum of **1**