Supplementary Information

Leaves from the Tree *Poincianella pluviosa* as a Renewable Source of Antiplasmodial Compounds against Chloroquine-Resistant *Plasmodium falciparum*

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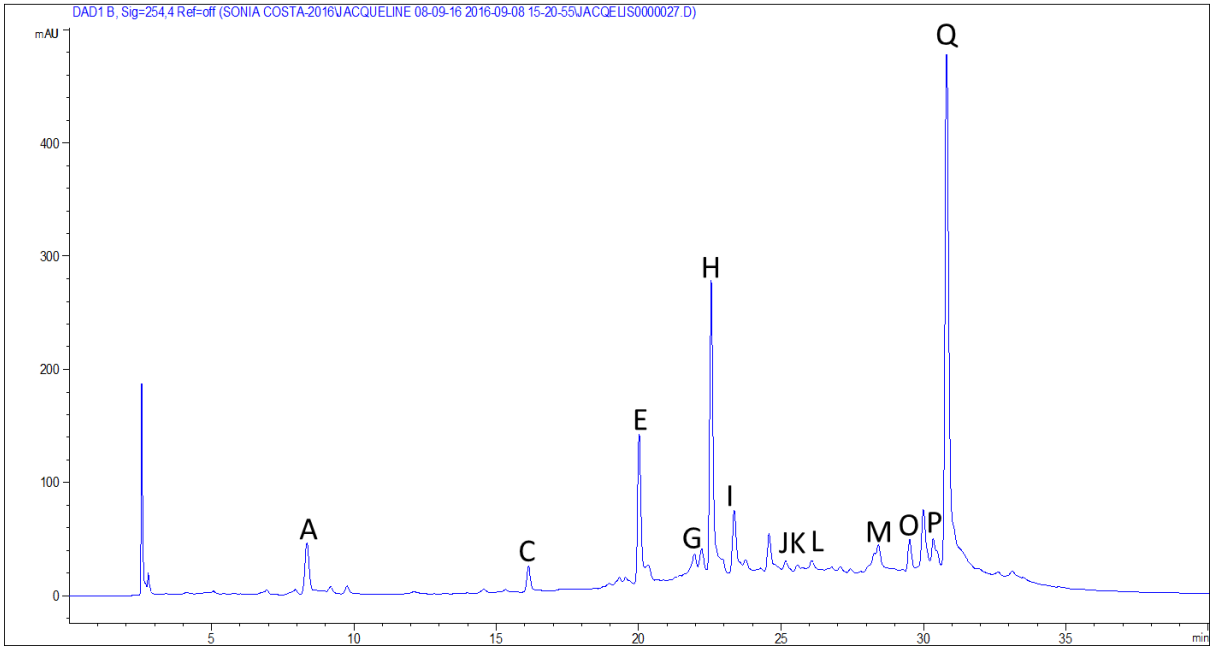

Figure S1. HPLC-DAD chromatograms of flowering-period leaf extract (P2-E, 2.5 mg mL^{-1}, 254 nm, RP-18) from *Poincianella pluviosa*. For conditions, see Experimental section. (A) gallic acid (t_R = 8.35 min); (C) galloyl tannin (t_R = 15.32 min); (E) galloyl tannin (t_R = 20.01 min); (G) brevifolin carboxylic acid (t_R = 21.96 min); (H) corilagin (t_R = 22.54 min); (I) valoneic acid dilactone (t_R = 23.35 min); (J) unidentified galloyl tannin (t_R = 25.18 min); (K) ellagic acid derivate (t_R = 25.57 min); (L) brevifolin derivate (t_R = 26.07 min); (M) quercetin-3-*O*-(6-*O*-galloyl) β-D-glucopyranoside (t_R = 28.79 min); (O) isovitexin (t_R = 29.51 min); (P) isoquercitrin (t_R = 30.34 min); (Q) ellagic acid (t_R = 30.81 min). Labels on x (mAu: milli absorption units) and y (min: minutes).

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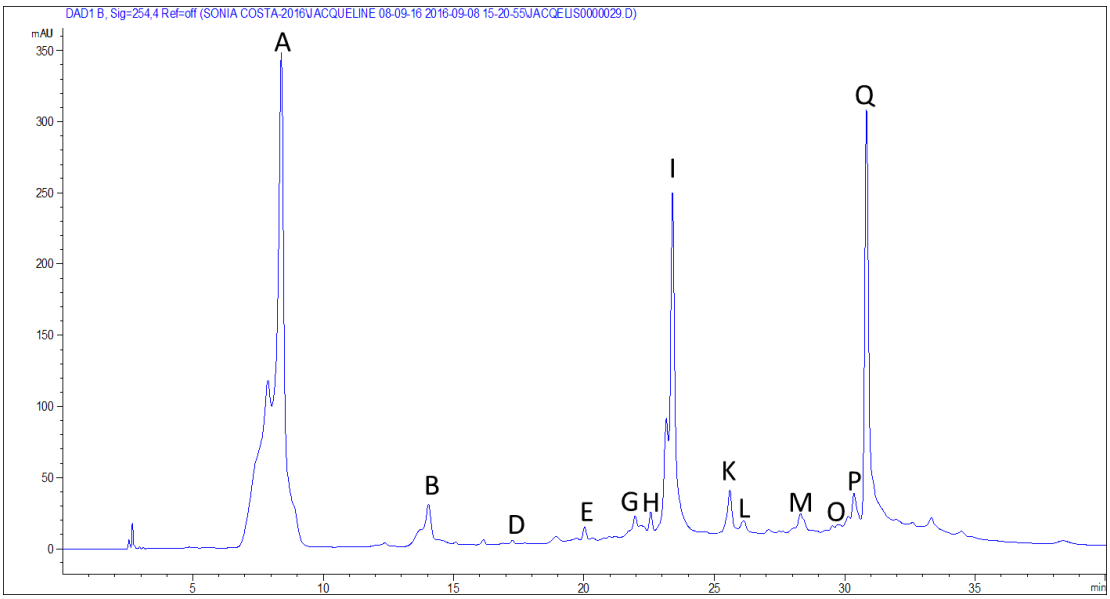

Figure S2. HPLC-DAD chromatogram of acetate fraction (P1-A, 1.25 mg mL^{-1}, 254 nm, RP-18) from *Poincianella pluviosa* leaf extract. For conditions, see Experimental section. (A) gallic acid (t_R = 8.39 min); (B) protocatechuic acid (t_R = 14.03 min); (D) galloyl tannin (t_R = 17.25 min); (E) galloyl tannin (t_R = 20.03 min); (G) brevifolin carboxylic acid (t_R = 21.96 min); (H) corilagin (t_R = 22.56 min); (I) valoneic acid dilactone (t_R = 23.39 min); (K) ellagic acid derivate (t_R = 25.59 min); (L) brevifolin derivate (t_R = 26.12 min); (M) quercetin-3-*O*-(6-*O*-galloyl) β-D-glucopyranoside (t_R = 28.30 min); (O) isovitexin (t_R = 29.53 min); (P) isoquercitrin (t_R = 30.36 min); (Q) ellagic acid (t_R = 30.83 min). Labels on x (mAu: milli absorption units) and y (min: minutes).

Spectral data

Ellagic acid (**1**)

Brown amorphous solid; mp above 300 °C; Rf value: 0.42 (BAW 8: 1:1); t_R = 30.72 min; UV (methanol) λ / nm 256-364; ^{1}H NMR (500 MHz, CD_3OD) δ 7.41 (s, 2H, CH); ^{13}C NMR (125 MHz, CD_3OD) δ 159.7, 148.2, 140.0, 136.6, 112.2, 109.9, 107.9; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 301.

Valoneic acid dilactone (**2**)

Brown amorphous solid; mp 270 °C; Rf value: 0.32 (BAW 8: 1:1); t_R = 23.39 min; UV (methanol) λ / nm 255-364; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.49 (s, 1H, CH), 6.98 (s, 1H, CH), 6.95 (s, 2H, CH); ^{13}C NMR (100 MHz, DMSO-d_6) δ 166.2, 159.7, 159.3, 149.8, 148.9, 143.3, 141.3, 139.9, 139.5, 137.0, 136.0, 135.5, 115.0, 114.2, 112.3, 110.7, 108.7, 108.6, 108.5, 107.0; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 469.

Gallic acid (**3**)

White amorphous solid; mp 210-230 °C; Rf value: 0.63 (BAW 8: 1:1); t_R = 8.43 min; UV (methanol) λ / nm 212-269; ^{1}H NMR (500 MHz, DMSO-d_6) δ 6.9 (s, 2H, CH); ^{13}C NMR (125 MHz, DMSO-d_6) δ 167.8, 145.4, 138.5, 120.5, 109.7; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 169.

Protocatechuic acid (**4**)

White amorphous solid; Rf value: 0.8 (BAW 8: 1:1); t_R = 13.9 min; UV (methanol) λ / nm 280-292; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.31 (d, 1H, *J* 1.6 Hz, CH), 7.26 (dd, 1H, *J* 8.2, 1.6 Hz, CH), 6.74 (d, 1H, *J* 8.2 Hz, CH); ^{13}C NMR (125 MHz, DMSO-d_6, HSQC and HMBC) δ 126.7, 116.9, 145.1, 150.4, 116.7, 168.0; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 154.

Corilagin (**5**)

Brown amorphous solid; mp 218 °C; Rf value: 0.68 (BAW 8: 1:1); t_R = 22.65 min; UV (methanol) λ / nm 210-264; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.01 (s, 2H, CH), 6.55 (s, 1H, CH), 6.47 (s, 1H, CH), glucose : 6.20 (d, 1H, *J* 7.0 Hz, CH), 4.58 (s, 1H, CH), 4.35 (m, 1H, CH), 4.19-4.22 (m, 1H, CH), 3.98 (m, 2H, CH_2), 3.88 (d, 1H, *J* 7.0 Hz, CH); ^{13}C NMR (125 MHz, DMSO-d_6) δ 167.5, 167.1, 145.9, 145.2, 145.3, 144.3, 144.1, 139.3, 135.9, 135.7, 123.4, 124.2, 119.0, 116.1, 116.4, 109.3, 107.3, 106.3, glucose: 92.6, 77.8, 76.6, 71.9, 64.0, 62.4; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 633.0.

Brevifolin carboxylic acid (**6**)

Yellow amorphous solid; mp 200 °C; Rf value: 0.32 (BAW 8: 1:1); t_R = 22.0 min; UV (methanol) λ / nm 277-355; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.11 (s, 1H, CH), 4.35 (d, 1H, *J* 6.0 Hz, CH_2), 2.83 (d, 1H, *J* 18.0 Hz, CH_2), 2.66 (dd, 1H, *J* 18.0, 6.0 Hz, CH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ 195.5, 173.3, 161.7, 148.9, 148.9, 141.9, 142.3, 116.0, 113.1, 108.7, 42.3, 37.7; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 291.

Isoquercitrin (**7**)

Yellow amorphous solid; Rf value: 0.74 (BAW 8: 1:1); t_R = 29.9 min; UV (methanol) λ / nm 255-354; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.57 (dd, 1H, *J* 2.1, 8.0 Hz, CH), 7.56 (d, 1H, *J* 2.1 Hz, CH), 6.82 (d, 1H, *J* 8.0 Hz, CH), 6.39 (d, 1H, *J* 2.0 Hz, CH), 6.18 (d, 1H, *J* 2.0 Hz, CH), 5.47 (d, 1H, *J* 7.3 Hz, CH); ^{13}C NMR (125 MHz, DMSO-d_6) δ 177.8, 156.5, 164.6, 156.7, 148.9, 161.2, 122.2, 121.5, 145.2, 99.1, 133.7, 164.6, glucose: 101.2, 78.5, 78.2, 70.3, 74.5, 61.4; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 463.0.

Isovitexin (**8**)

Yellow amorphous solid; Rf value: 0.69 (BAW 8: 1:1); t_R = 30.97 min; UV (methanol) λ / nm 270-331; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.91 (d, 2H, *J* 8.6 Hz, CH), 6.92 (d, 2H, *J* 8.6 Hz, CH), 6.78 (s, 1H, CH), 6.52 (s, 1H, CH), glucose: 4.56 (d, 1H, *J* 9.8 Hz, CH); ^{13}C NMR (125 MHz, DMSO-d_6) 182.0, 163.9, 163.2, 161.2, 160.5, 156.2, 128.4, 121.1, 116.0, 108.9, 102.8, 93.6, glucose: 81.5, 78.9, 73.0, 70.6, 70.2, 61.5; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 431.

Quercetin-3-*O*-(6-*O*-galloyl) β-D-glucopyranoside (**9**)

Yellow amorphous solid; Rf value: 0.44 (BAW 8: 1:1); t_R = 28.27 min; UV (methanol) λ / nm 263-355; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.58 (dd, 1H, *J* 8.4, 2.1 Hz, CH), 7.44 (d, 1H, *J* 2.1 Hz, CH), 6.73 (d, 1H, *J* 8.4 Hz, CH), 6.89 (s, 2H, galloyl CH), 6.37 (d, 1H, *J* 1.8 Hz, CH), 6.18 (d, 1H, *J* 1.8 Hz, CH), 5.45 (d, 1H, *J* 7.5 Hz, CH), glucose: 4.22-3.37 (m, 5H); ^{13}C NMR (125 MHz, DMSO-d_6, HSQC and HMBC) δ 156.5, 164.6, 156.7, 148.9, 161.2, 122.2, 121.5, 145.2, 99.1, 133.7, 164.6, 108.9, glucose: 101.4, 69.8, 63.5, 63.5, 74.5, 61.4; HRMS (TOF + ESI) *m/z* $[M - H]^-$: 615.

Kaempferol-3-*O*-(6-*O*-galloyl) β-D-glucopyranoside (**10**)

Yellow amorphous solid; Rf value: 0.54 (BAW 8: 1:1); t_R = 31.0 min; UV (methanol) λ / nm 257-365; ^{1}H NMR (500 MHz, DMSO-d_6) δ 7.93 (d, 1H, *J* 8.8 Hz, CH), 6.9 (s, 2H, *J* 2.1 Hz, galloyl, CH), 6.77 (d, 1H, *J* 8.4 Hz, CH), 6.40 (d, 1H, *J* 1.8 Hz, CH), 6.20 (d, 1H, *J* 1.8 Hz, CH); ^{13}C NMR (125 MHz, DMSO-d_6, HSQC) δ 92.07, 94.13, 115.4, 131.1, 108.9, 121.5, 145.2, 99.1, 133.7, 164.6, glucose: 101.4, 69.8, 63.5, 63.5, 74.5, 61.4; HRMS (TOF + ESI) *m/z* [M – H]$^-$: 599.0.

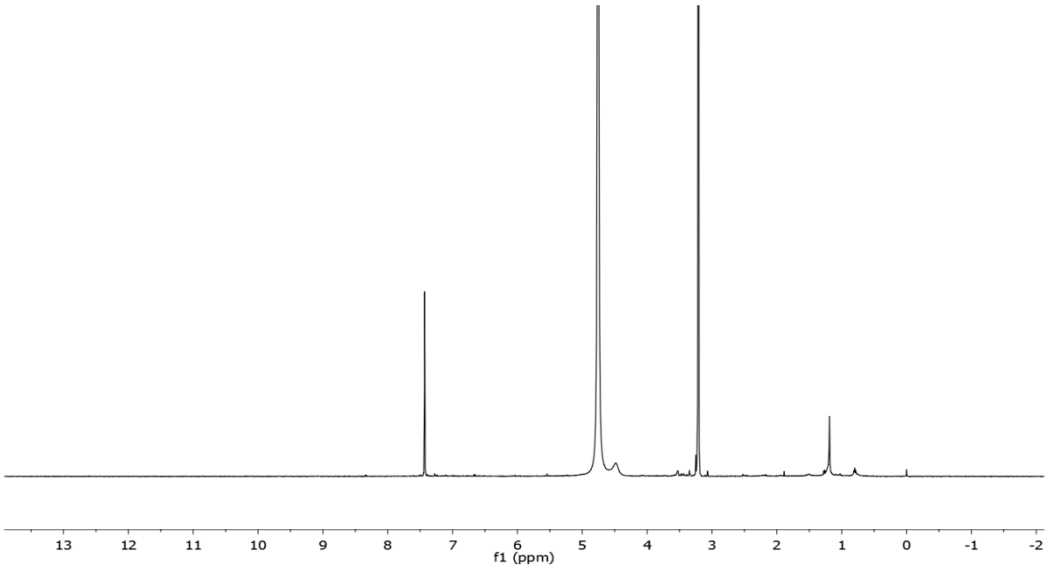

Figure S3. ^{1}H NMR spectrum (500 MHz, CD_3OD) of compound **1**.

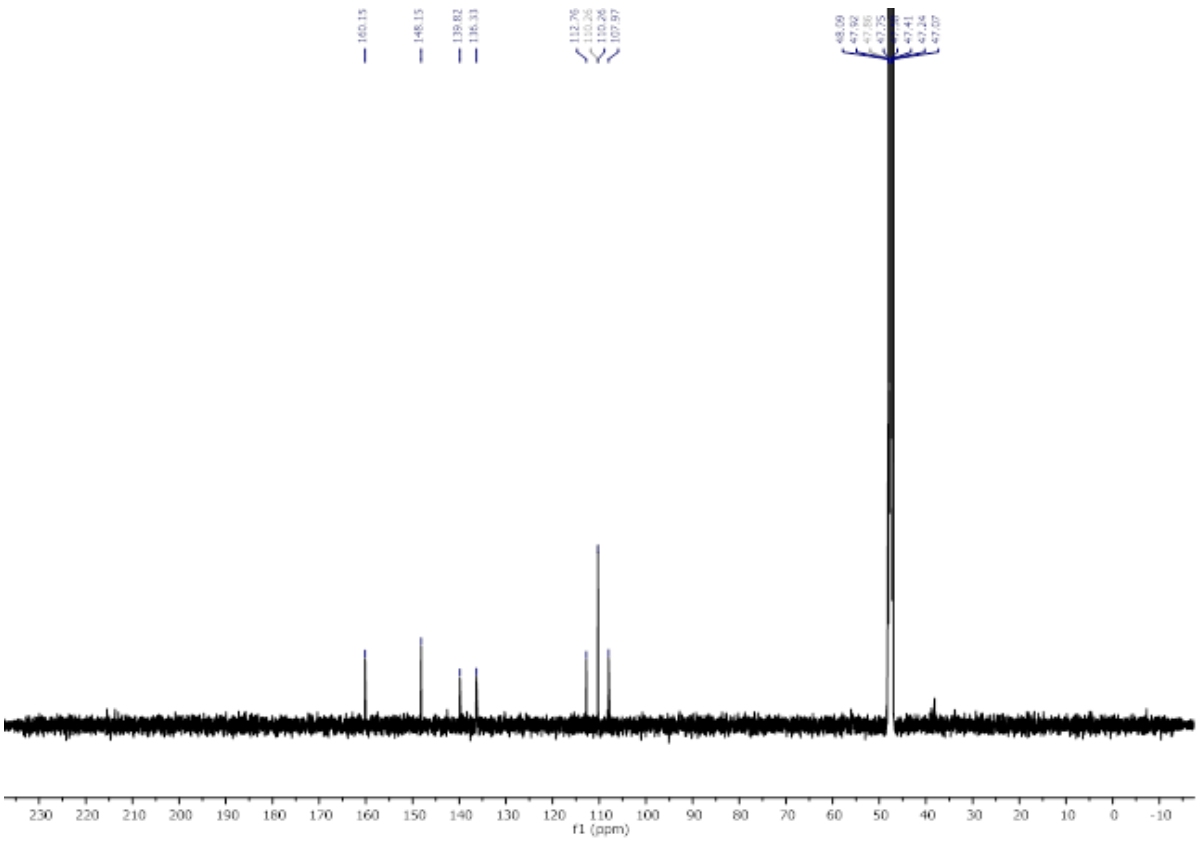

Figure S4. ^{13}C NMR spectrum (125 MHz, CD_3OD) of compound **1**.

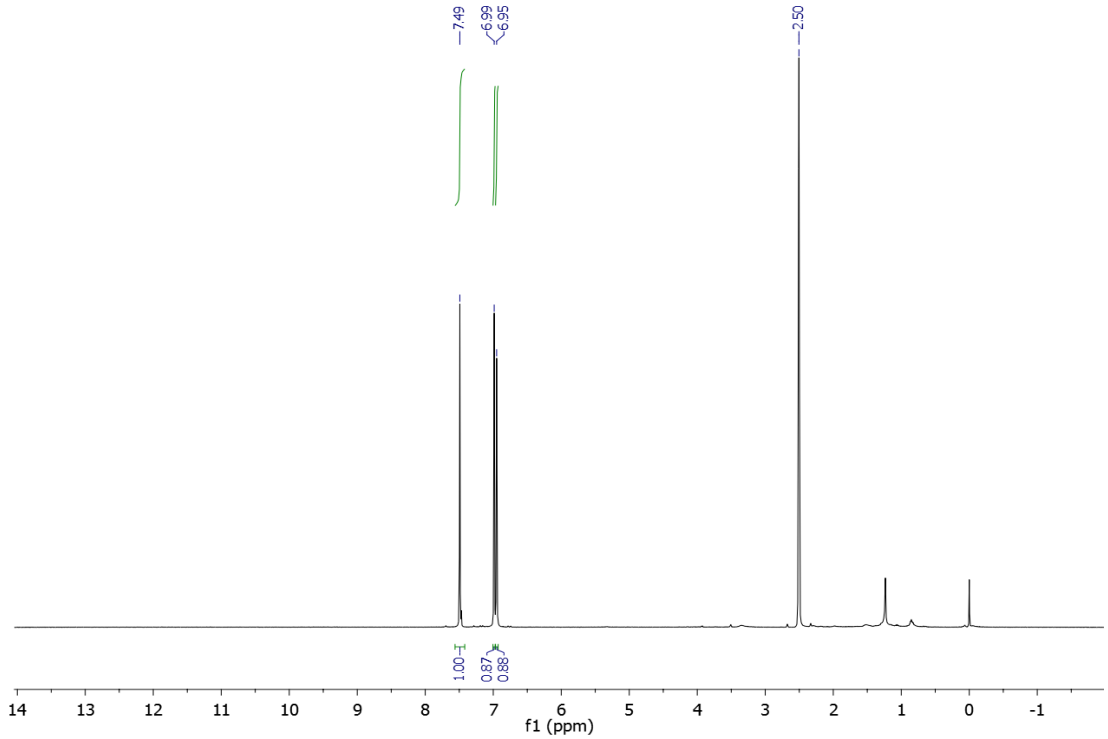

Figure S5. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) of compound **2**.

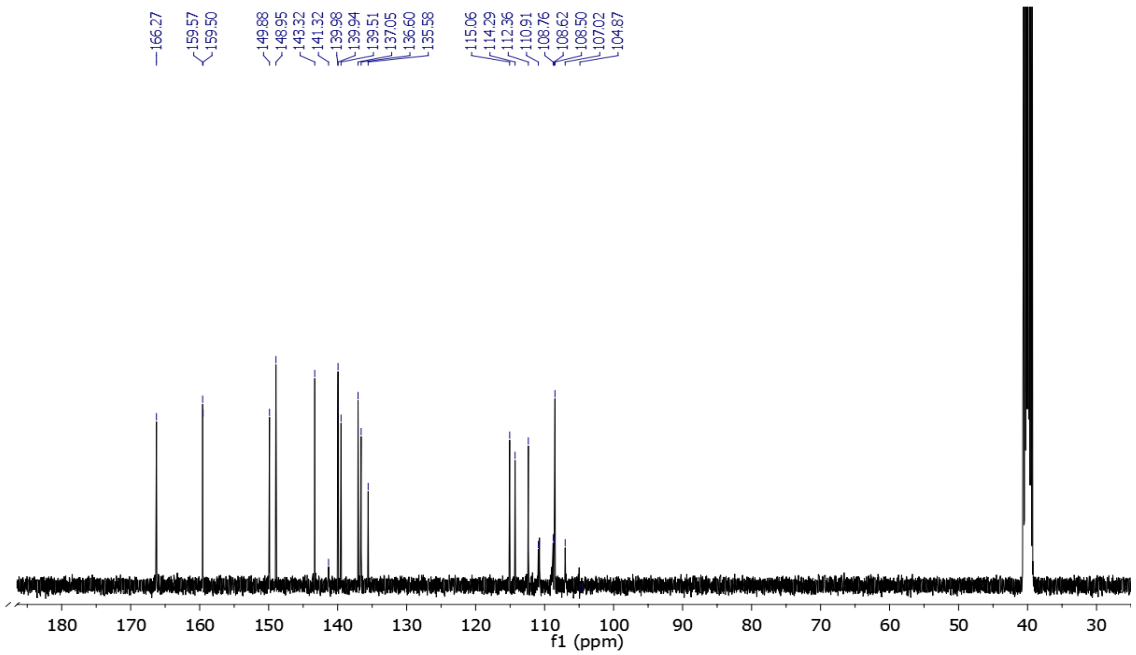

Figure S6. ^{13}C NMR spectrum (100 MHz, DMSO-d_6) of compound **2**.

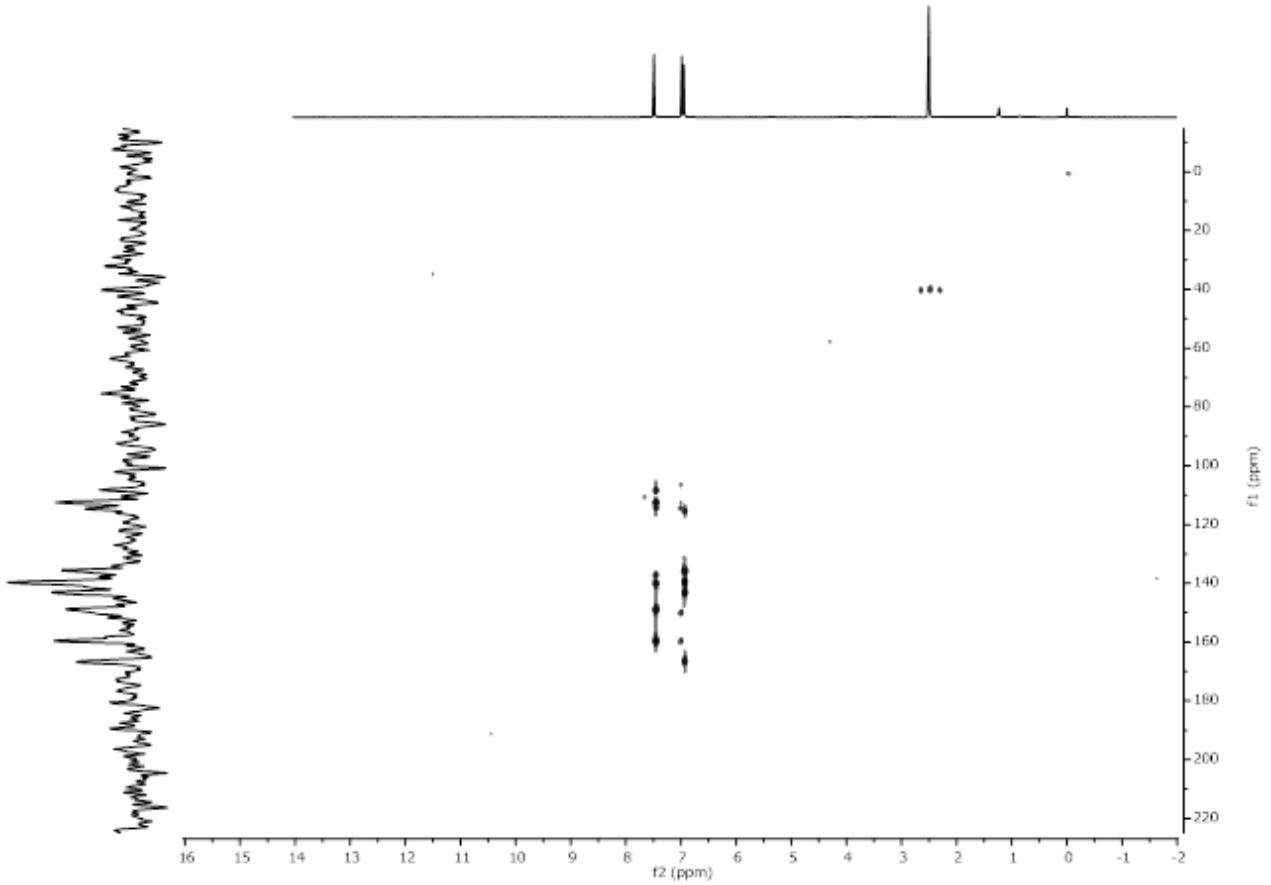

Figure S7. HMBC spectrum (400 MHz, DMSO-d_6) of compound **2**.

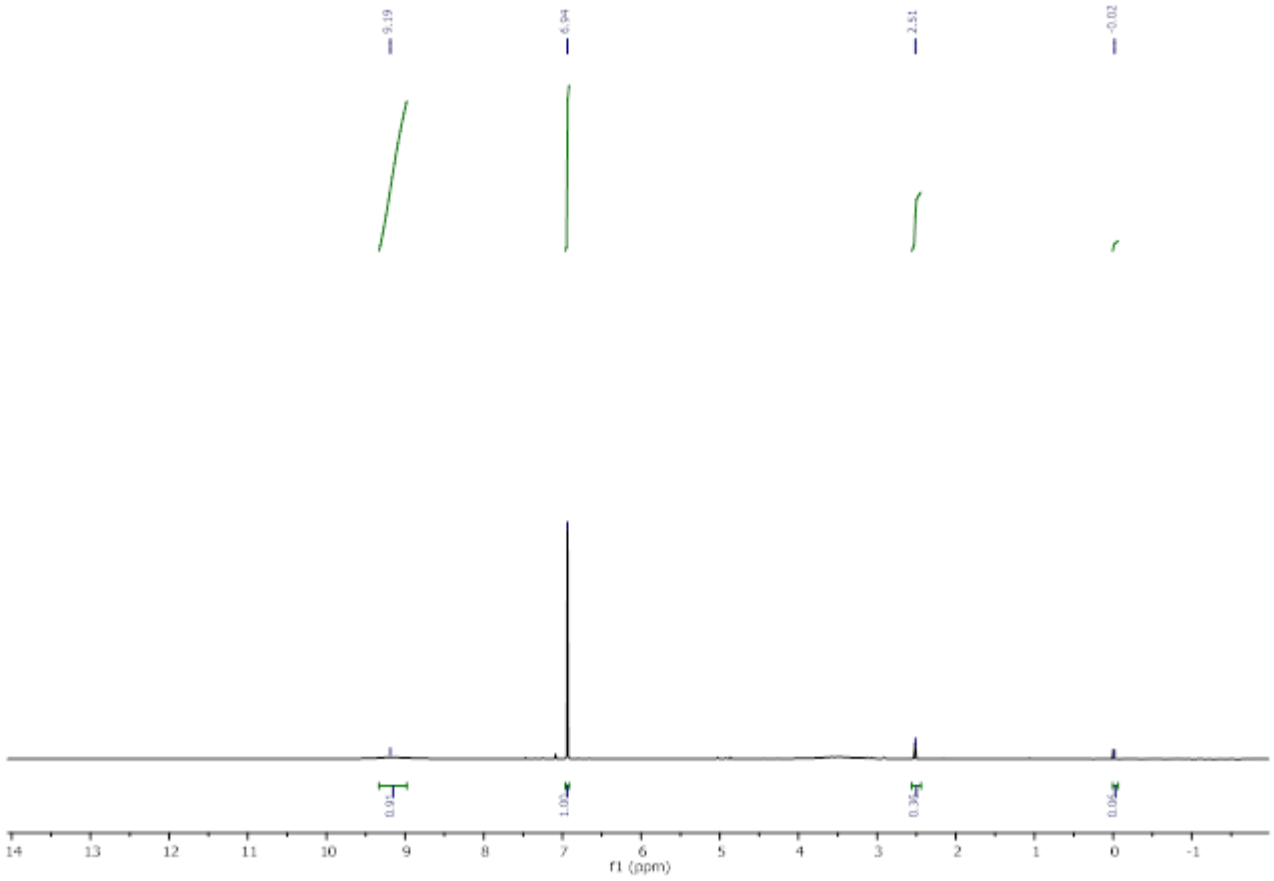

Figure S8. ^{1}H spectrum (500 MHz, DMSO-d_6) of compound **3**.

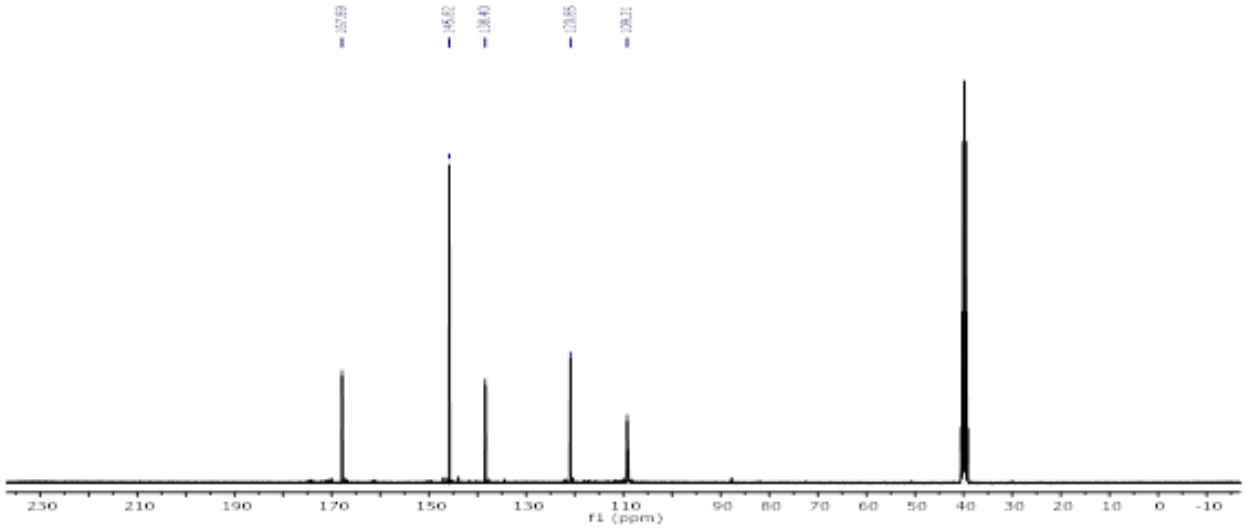

Figure S9. ^{13}C spectrum (125 MHz, DMSO-d_6) of compound **3**.

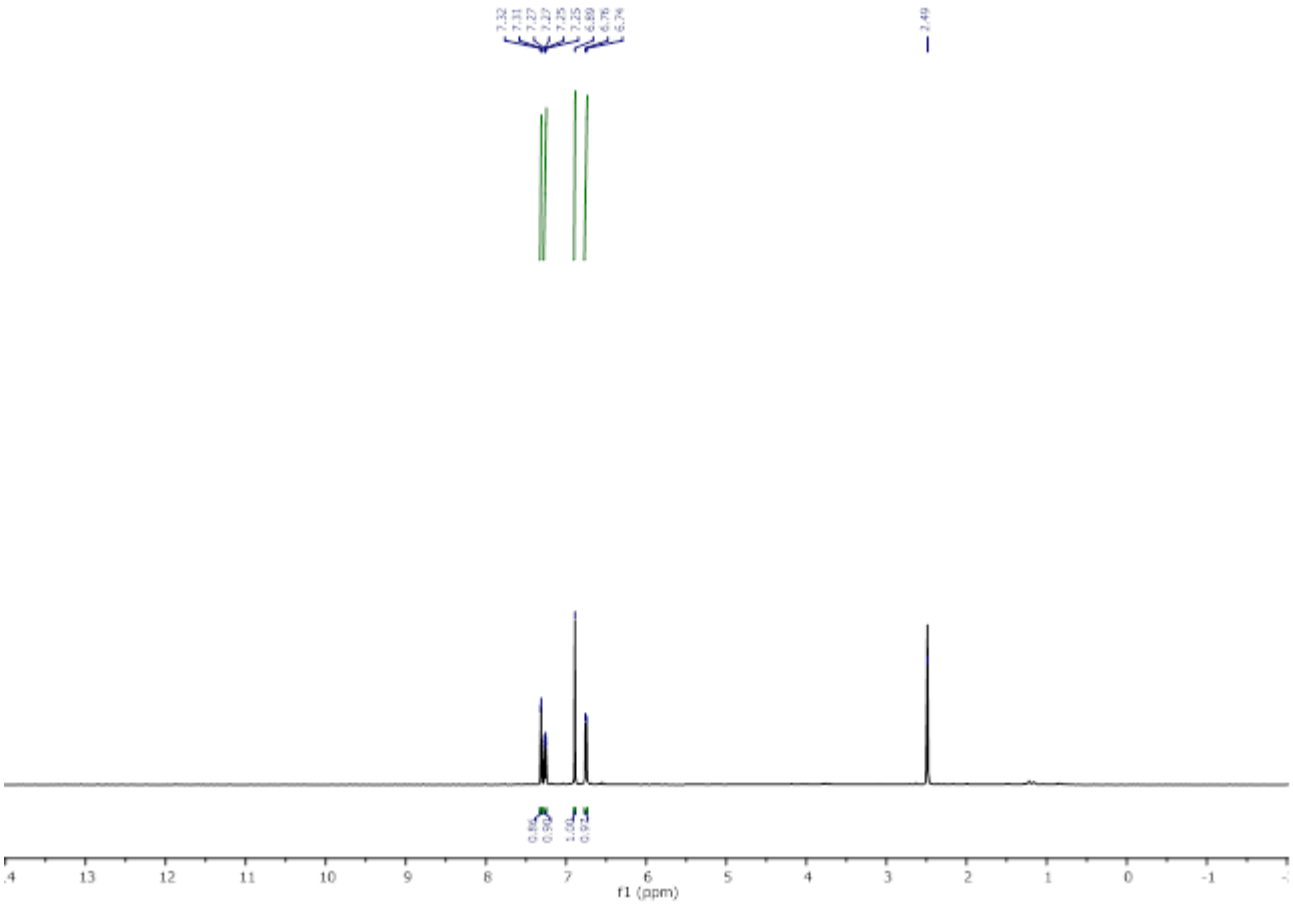

Figure S10. ^{1}H spectrum (500 MHz, DMSO-d_6) of compounds **3** and **4**.

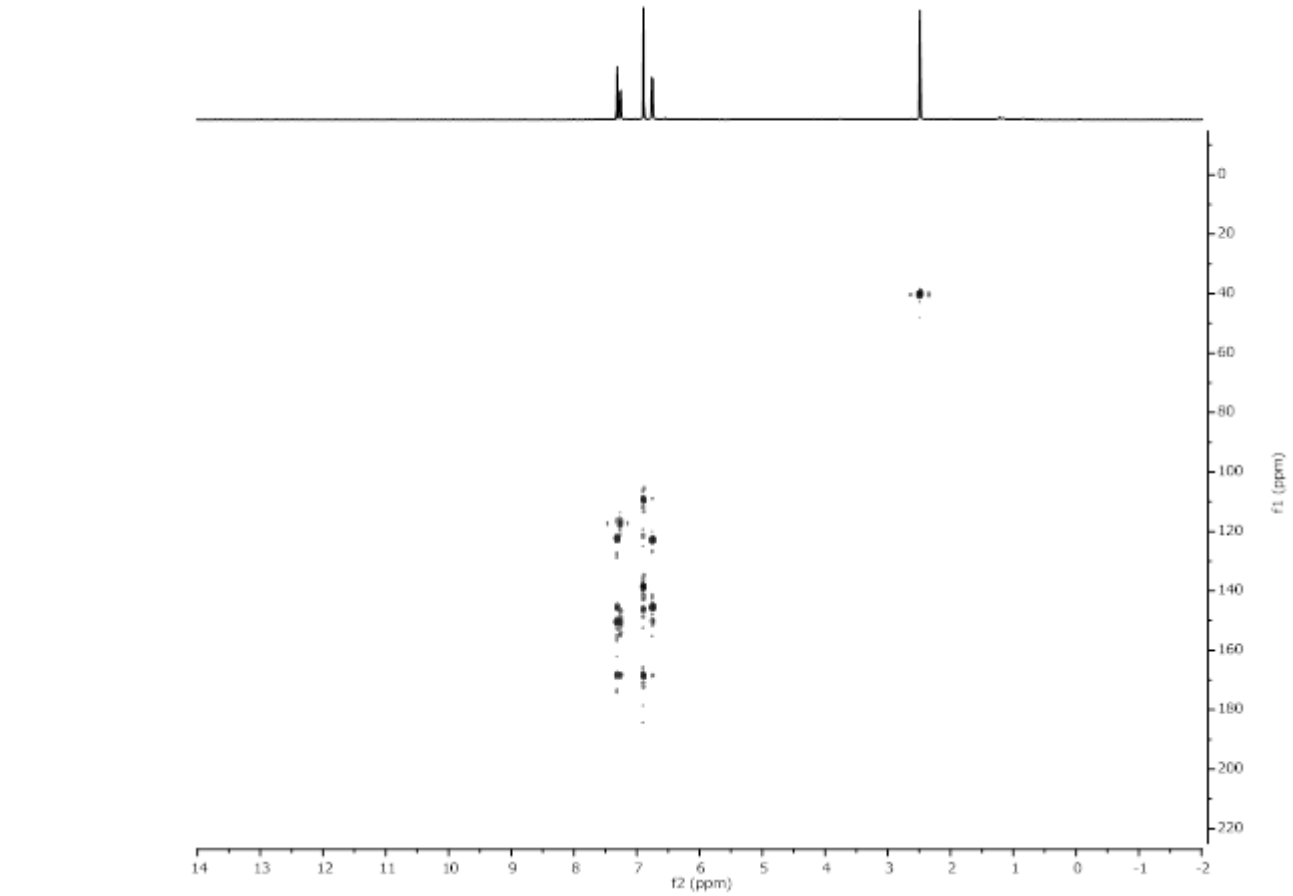

Figure S11. HMBC spectrum (500 MHz, DMSO-d_6) of compounds **3** and **4**.

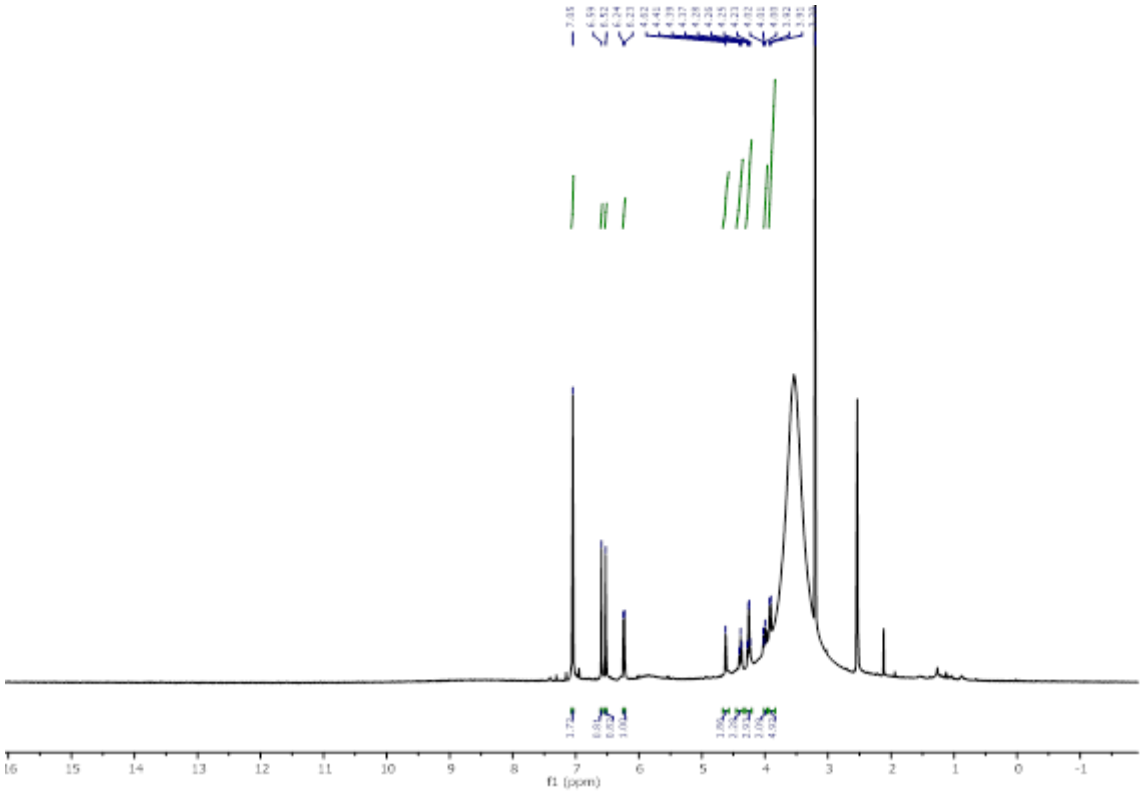

Figure S12. ^{1}H spectrum (500 MHz, DMSO-d_6) of compound **5**.

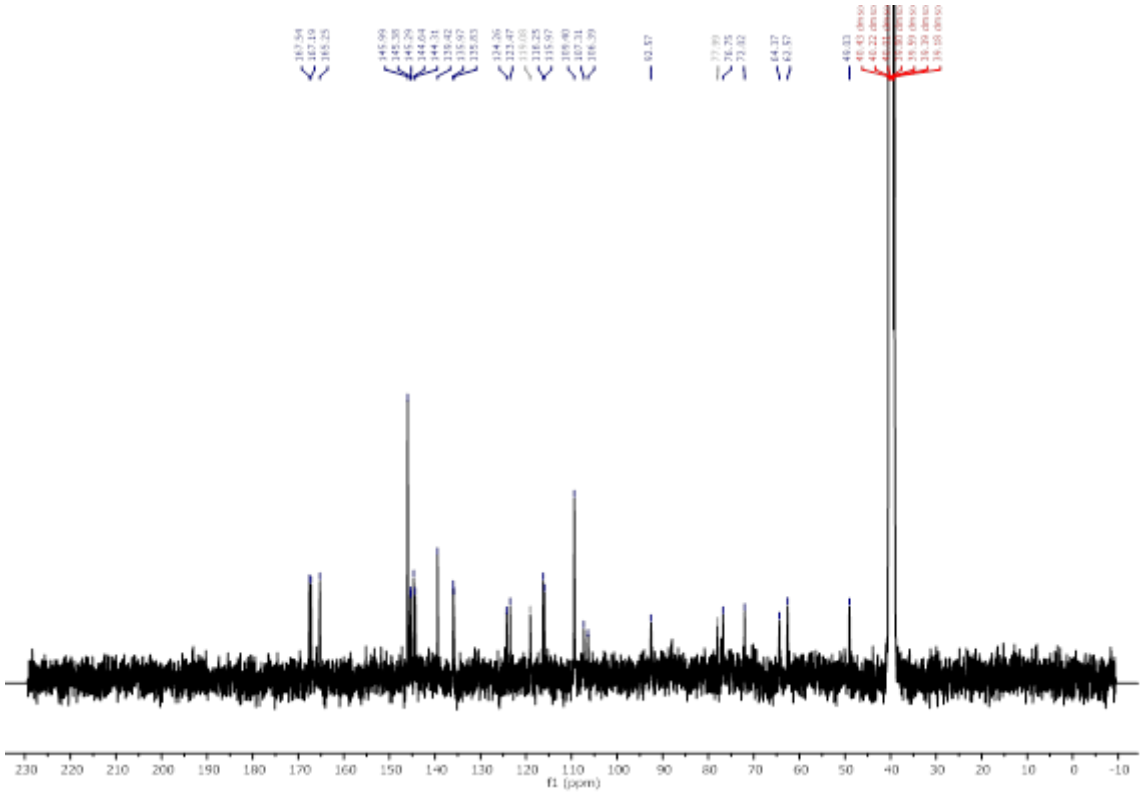

Figure S13. ^{13}C spectrum (125 MHz, DMSO-d_6) of compound **5**.

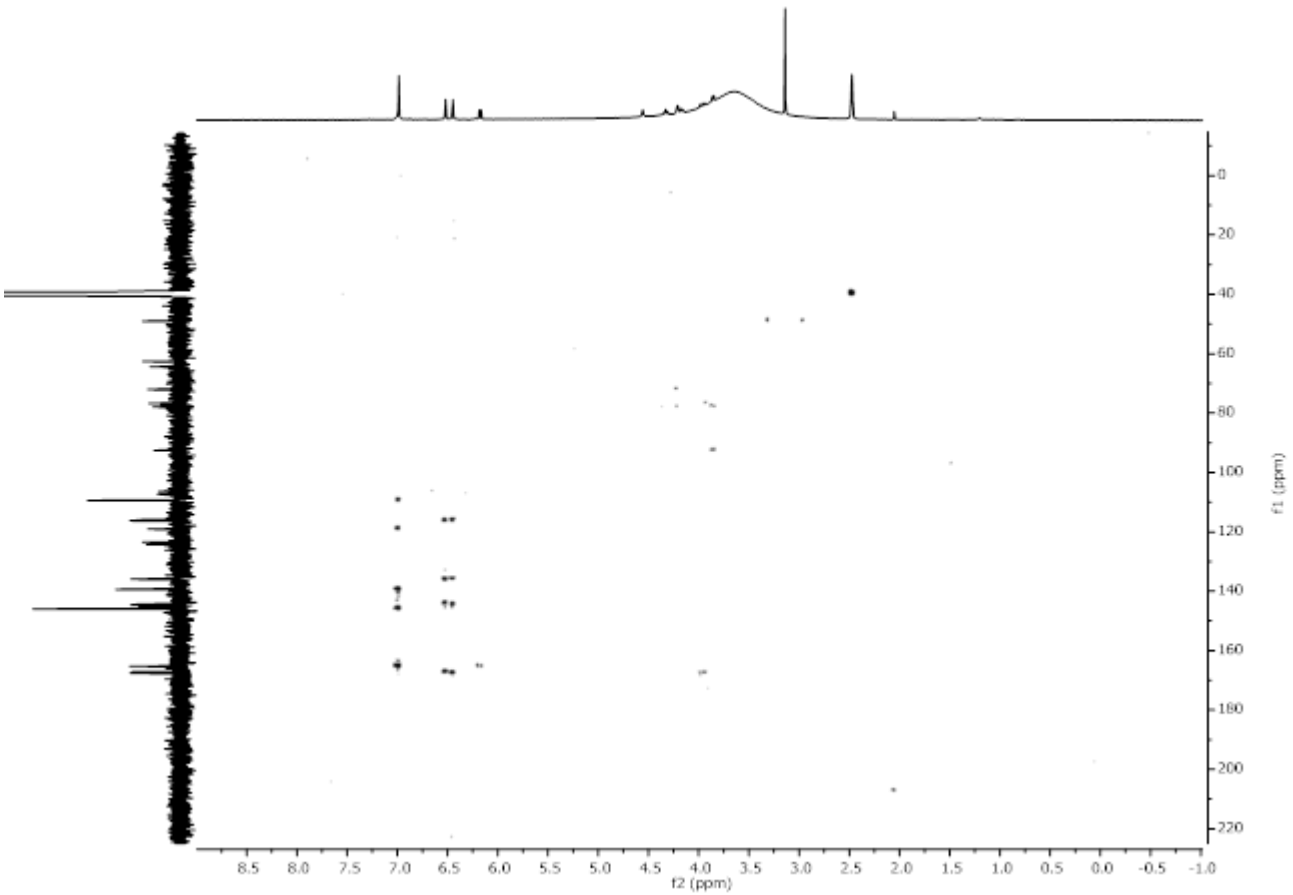

Figure S14. HMBC spectrum (500 MHz, DMSO-d_6) of compound **5**.

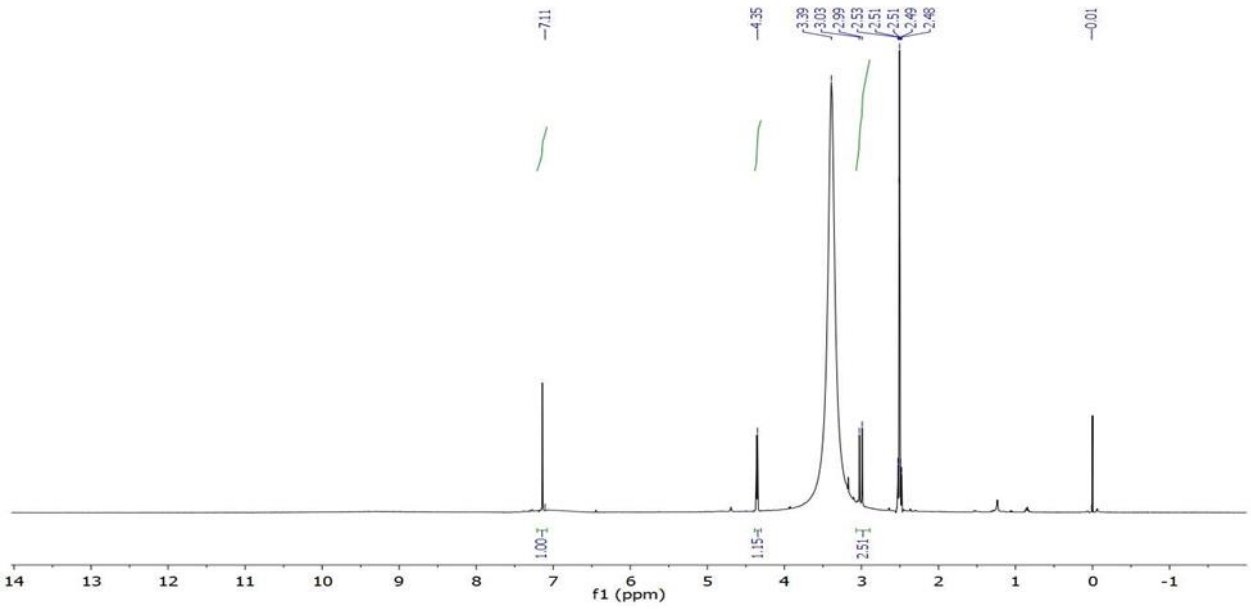

Figure S15. ^{1}H spectrum (400 MHz, DMSO-d_6) of compound **6**.

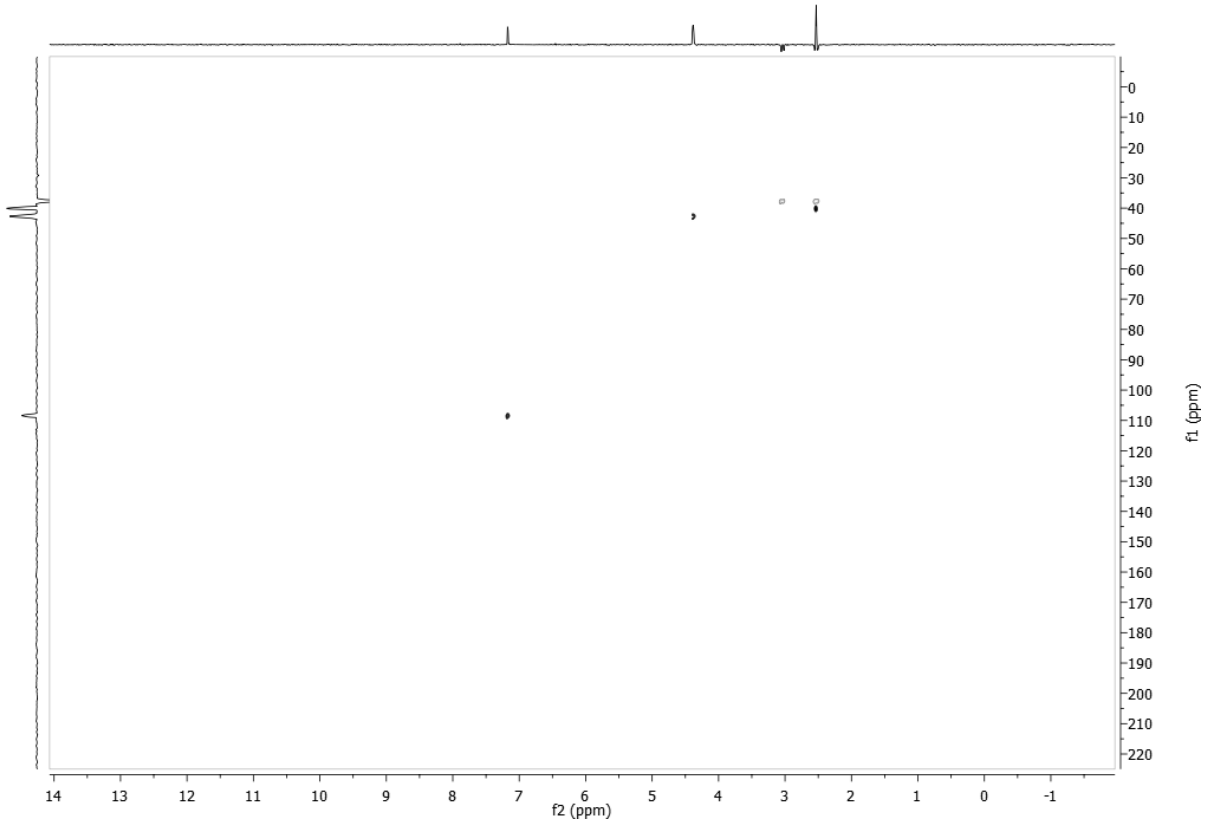

Figure S16. HSQC spectrum (400 MHz, DMSO-d_6) of compound **6**.

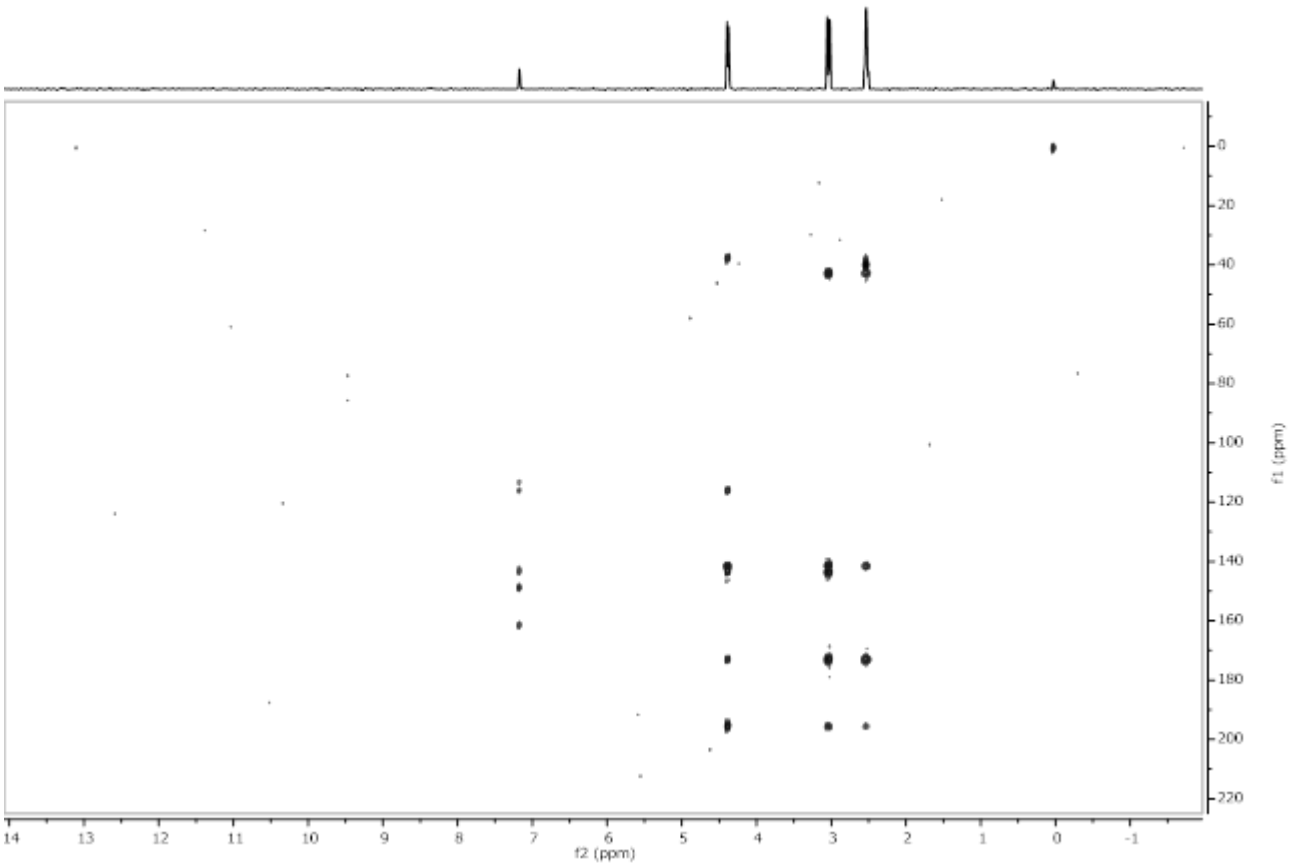

Figure S17. HMBC spectrum (400 MHz, DMSO-d_6) of compound **6**.

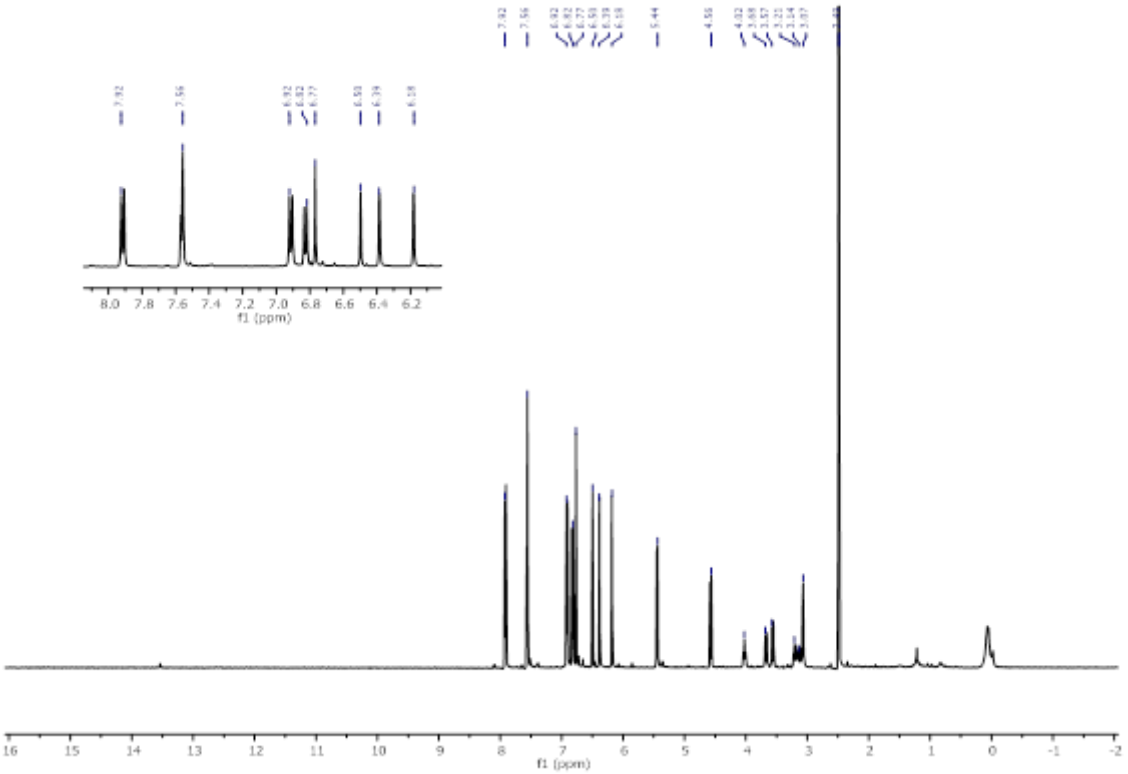

Figure S18. ^{1}H spectrum (500 MHz, DMSO-d_6) of compounds **7** and **8**.

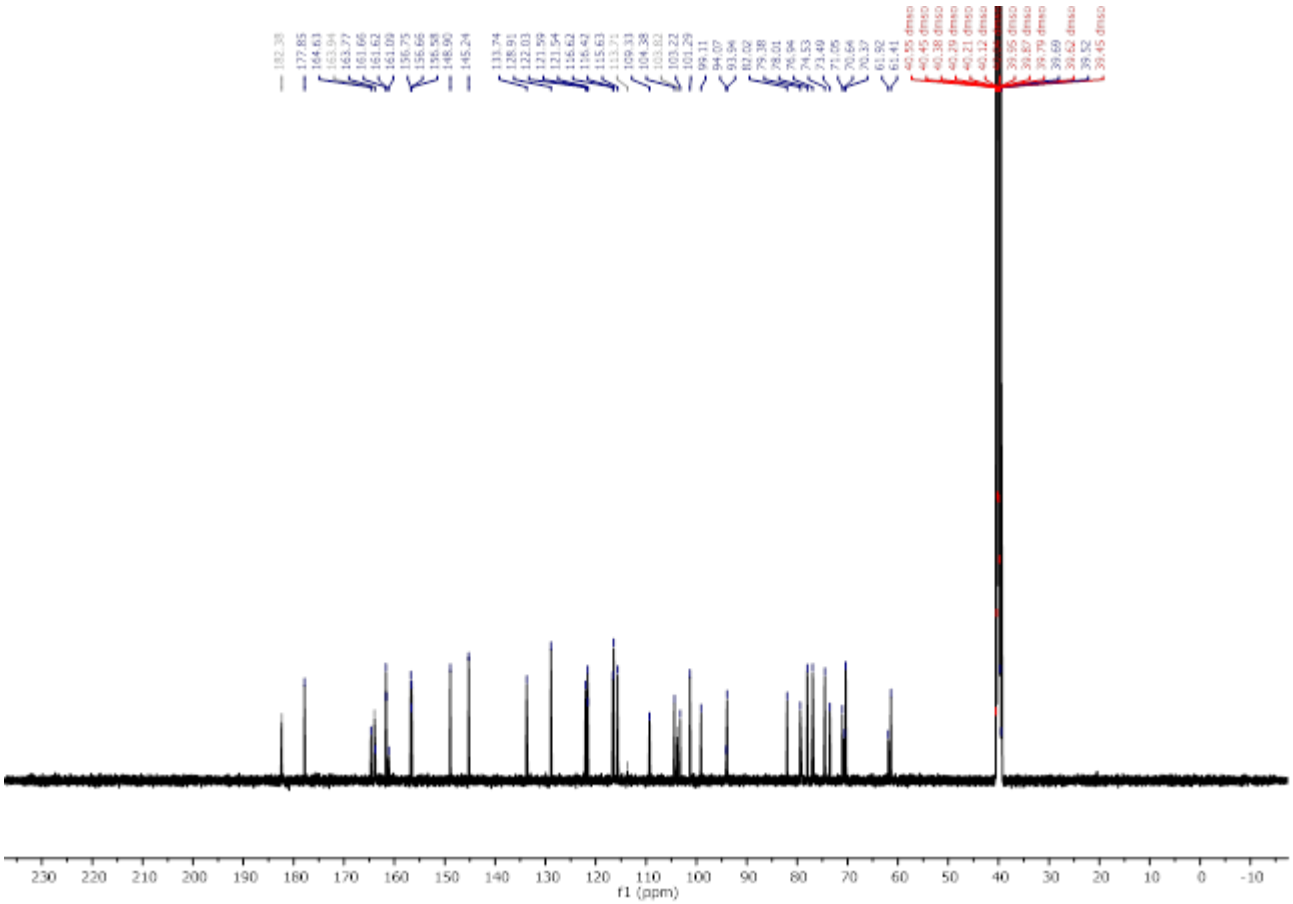

Figure S19. ^{13}C spectrum (125 MHz, DMSO-d_6) of compounds **7** and **8**.

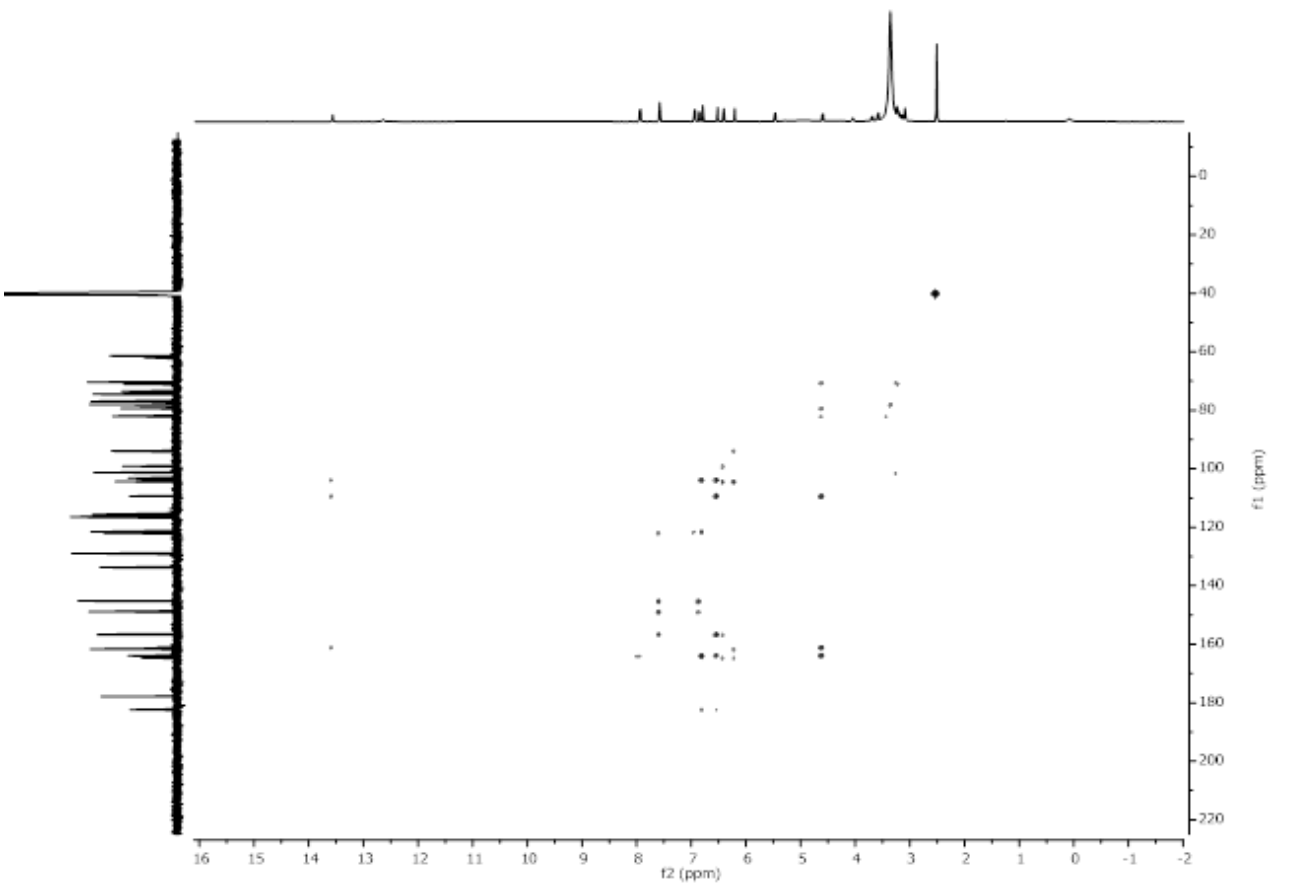

Figure S20. HMBC spectrum (500 MHz, DMSO-d_6) of compounds **7** and **8**.

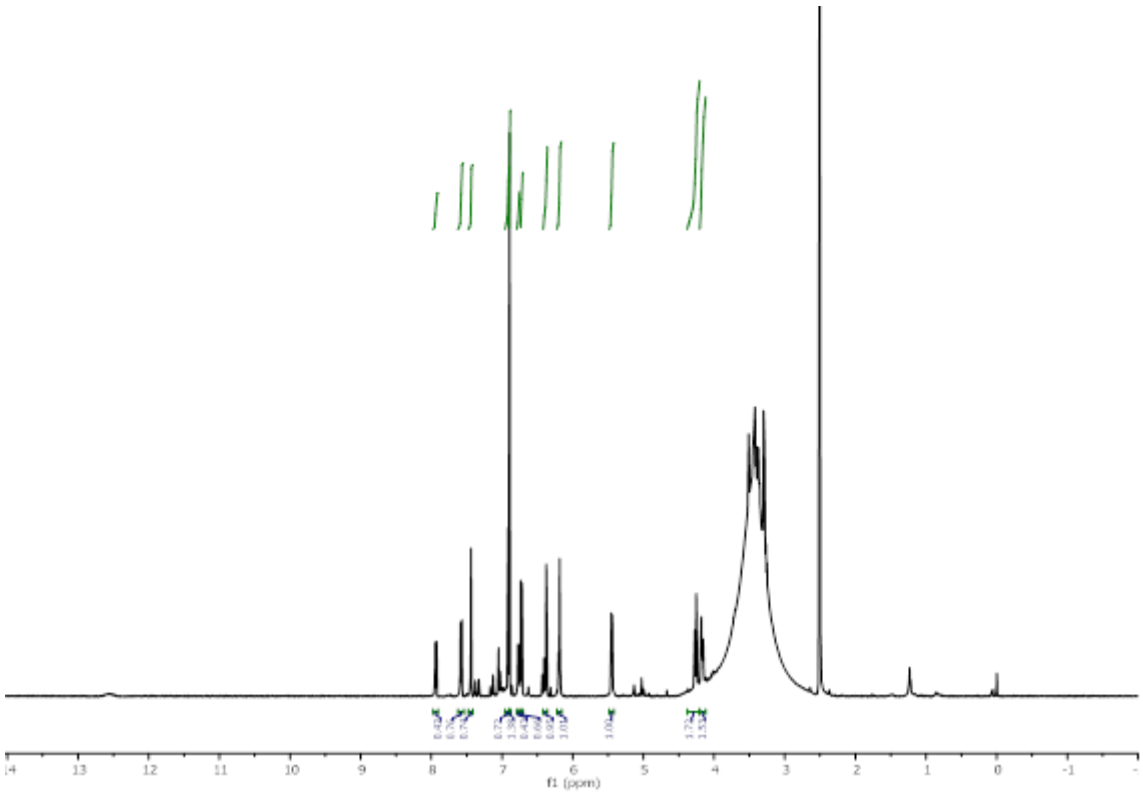

Figure S21. ^{1}H spectrum (500 MHz, DMSO-d_6) of compounds **9** and **10**.

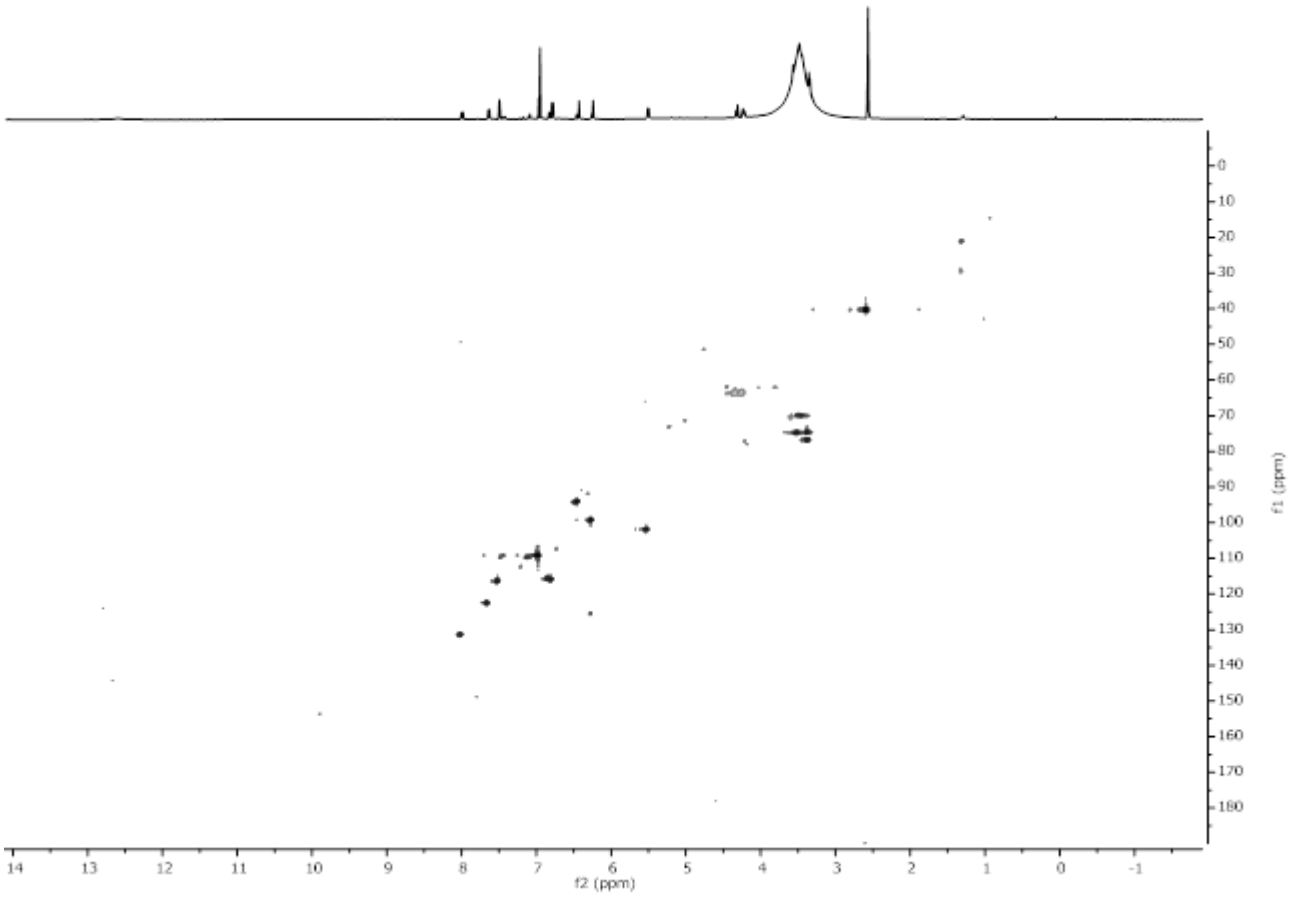

Figure S22. HSQC spectrum (500 MHz, DMSO-d_6) of compounds **9** and **10**.