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# SUPPORTING INFORMATION FOR:

# A novel acid-catalyzed rearrangement of 2-substituted-3-(2-nitrophenyl)oxiranes for the synthesis of di- and mono-oxalamides

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**General Methods**

All NMR experiments were performed with a 600, 500 and 400 MHz (600 MHz for $^{1}$H NMR; 150.9, 125 and 100.6 MHz for $^{13}$C NMR; 60.8 and 50.7 MHz for $^{15}$N NMR) spectrometers equipped with 5 mm diameter gradient inverse broad band probehead and a pulsed gradient unit capable of producing magnetic field pulse gradients in the z-direction of 53.5 G·cm$^{-1}$. NMR experiments were carried out at 303 K. DPFGNOE and TOCSY spectra were obtained using a Hermite-shaped pulse for selective excitation. Chemical shifts ($\delta$ in ppm) are referred to the solvent DMSO-$d_6$ ($\delta$ = 2.49 ppm for $^{1}$H and 39.5 ppm for $^{13}$C NMR), to external $CD_3NO_2$ (380.2 ppm) for $^{15}$N NMR spectra (conversion factor to $NH_3$: -380.2 ppm).

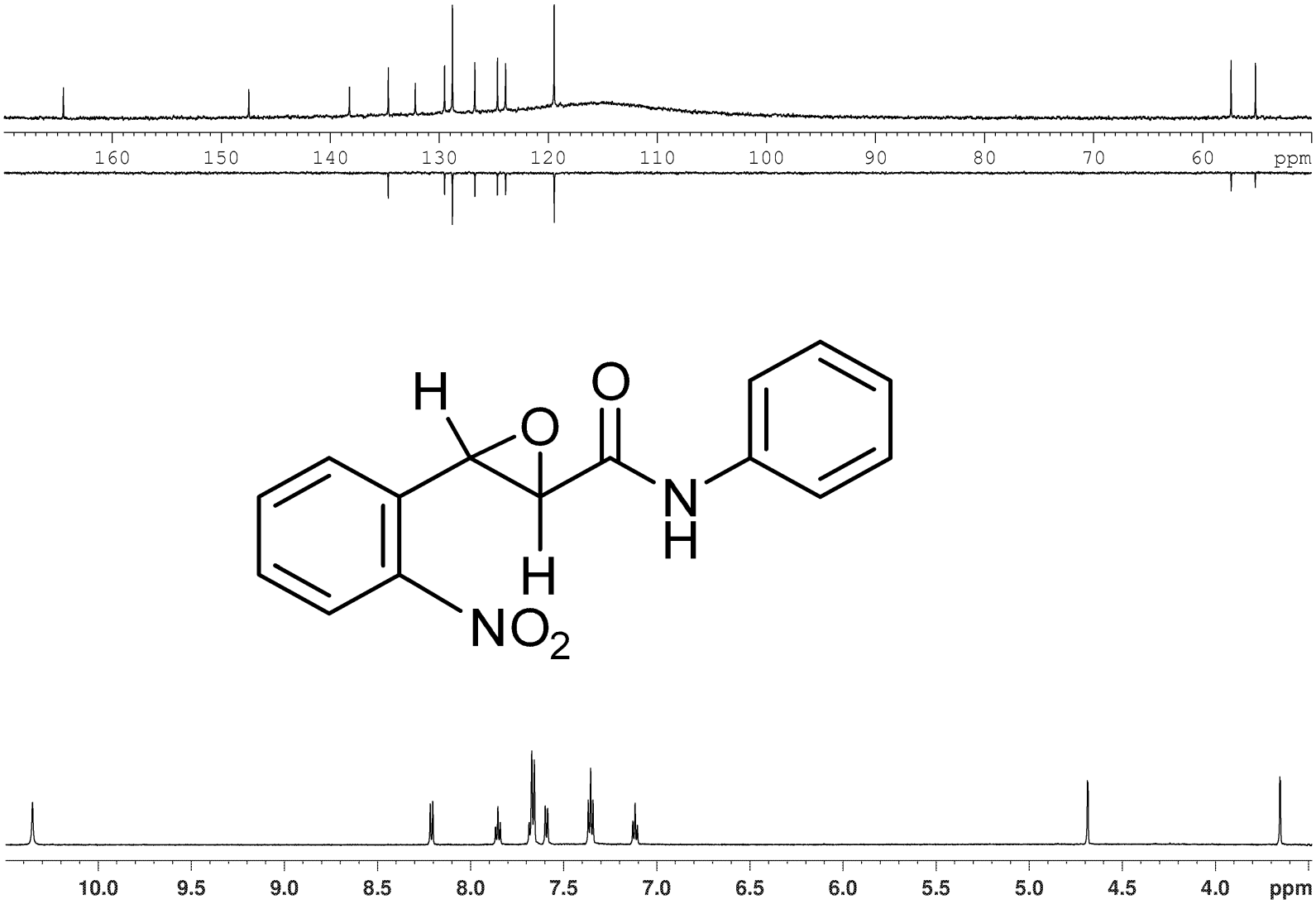



**Figure S1.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **3a** in DMSO at T = 303 K.

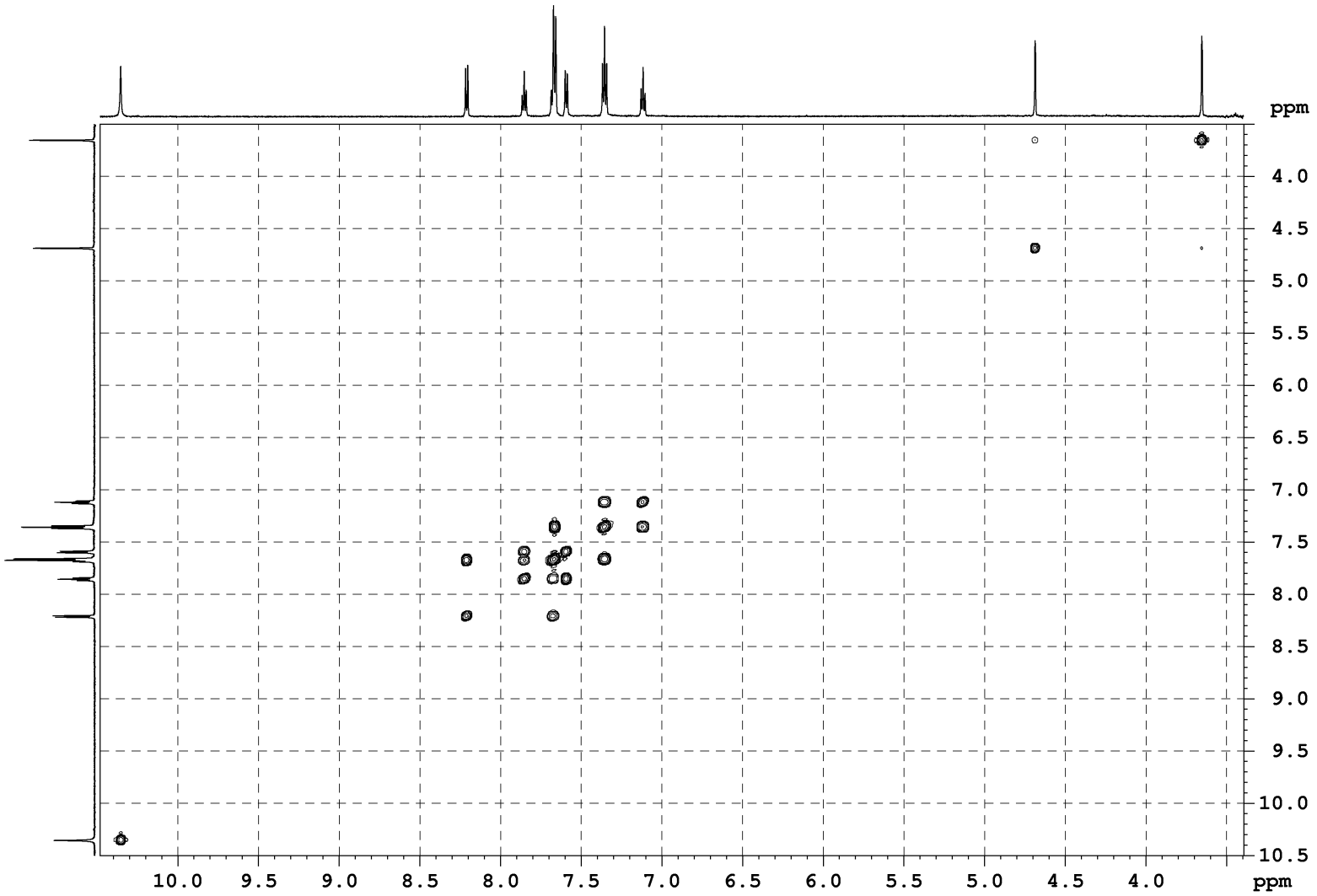



**Figure S2.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **3a** in DMSO at T = 303 K.

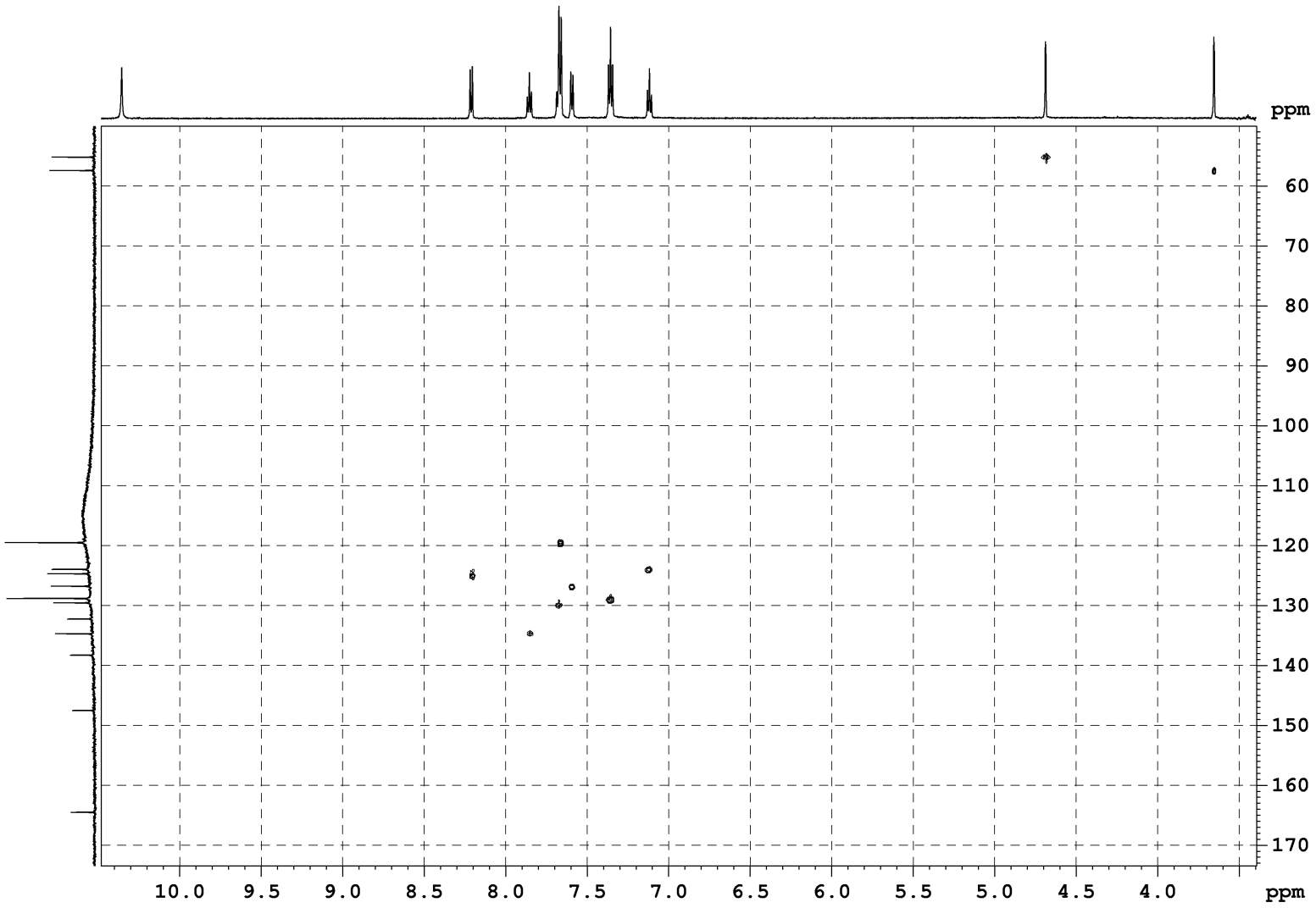



**Figure S3.** 2D $^{1}$H-$^{13}$C HSQC NMR spectra of **3a** in DMSO at T = 303 K.

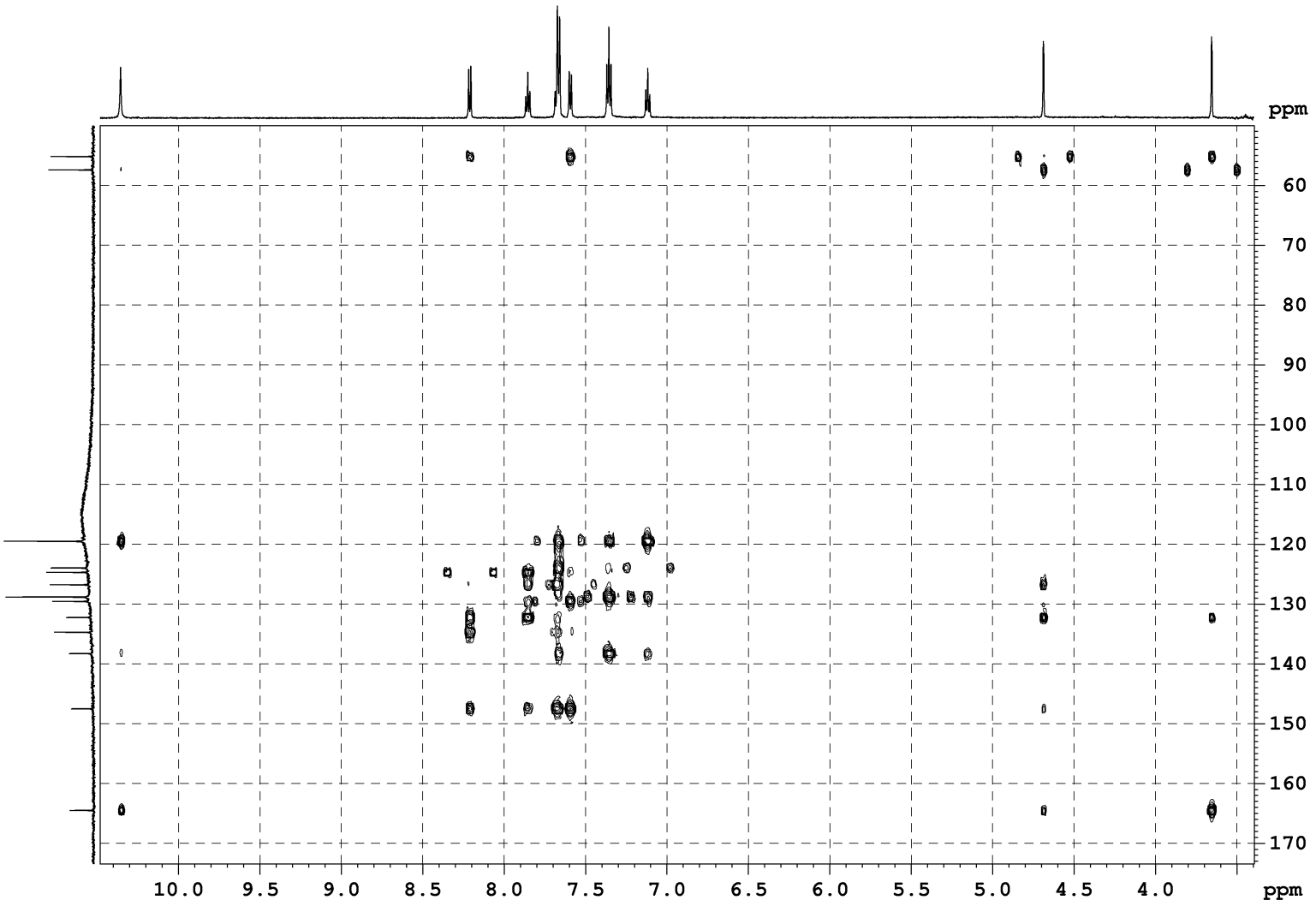



**Figure S4.** 2D $^{1}$H-$^{13}$C HMBC NMR spectra of **3a** in DMSO at T = 303 K.

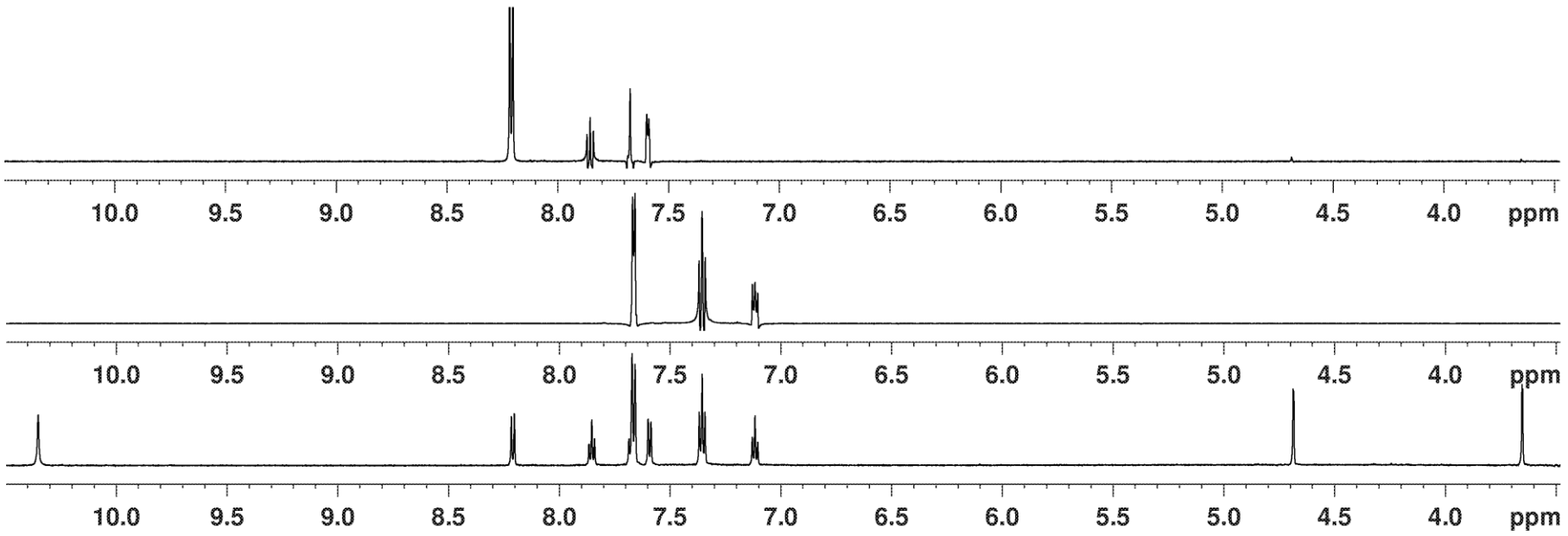



**Figure S5.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **3a** in DMSO at T = 303 K.

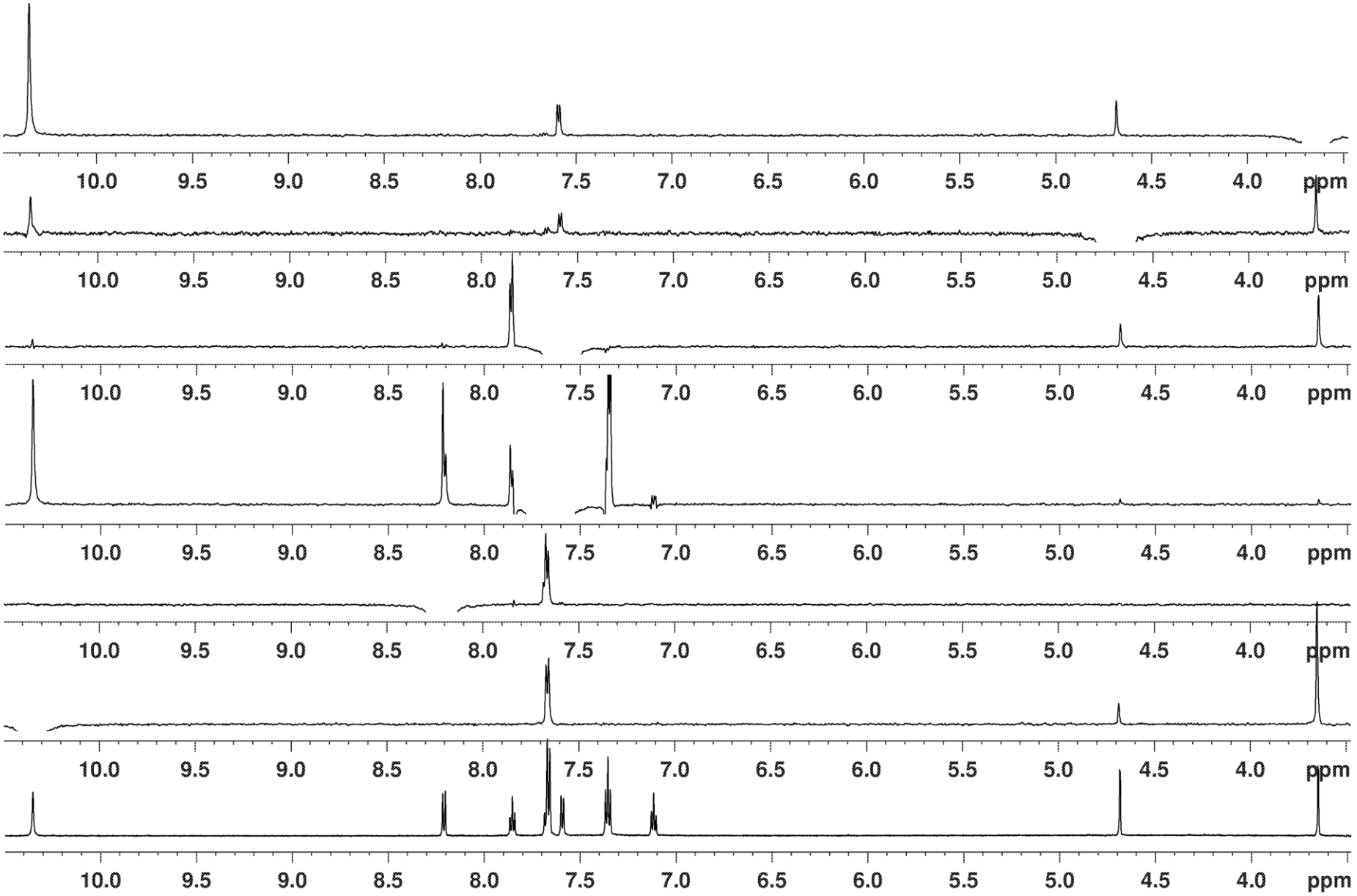



**Figure S6.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **3a** in DMSO at T = 303 K.

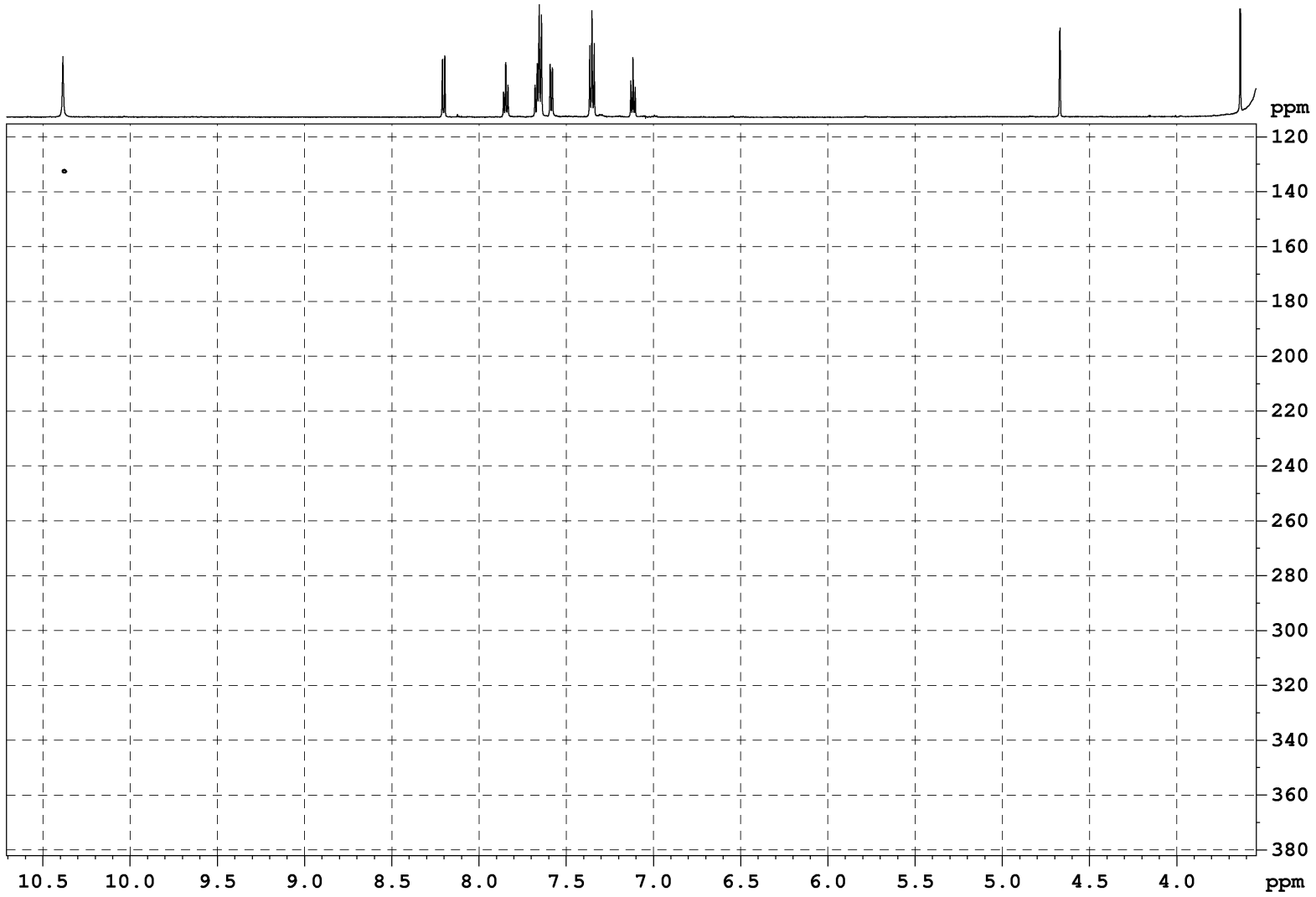



**Figure S7.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **3a** in DMSO at T = 303 K.

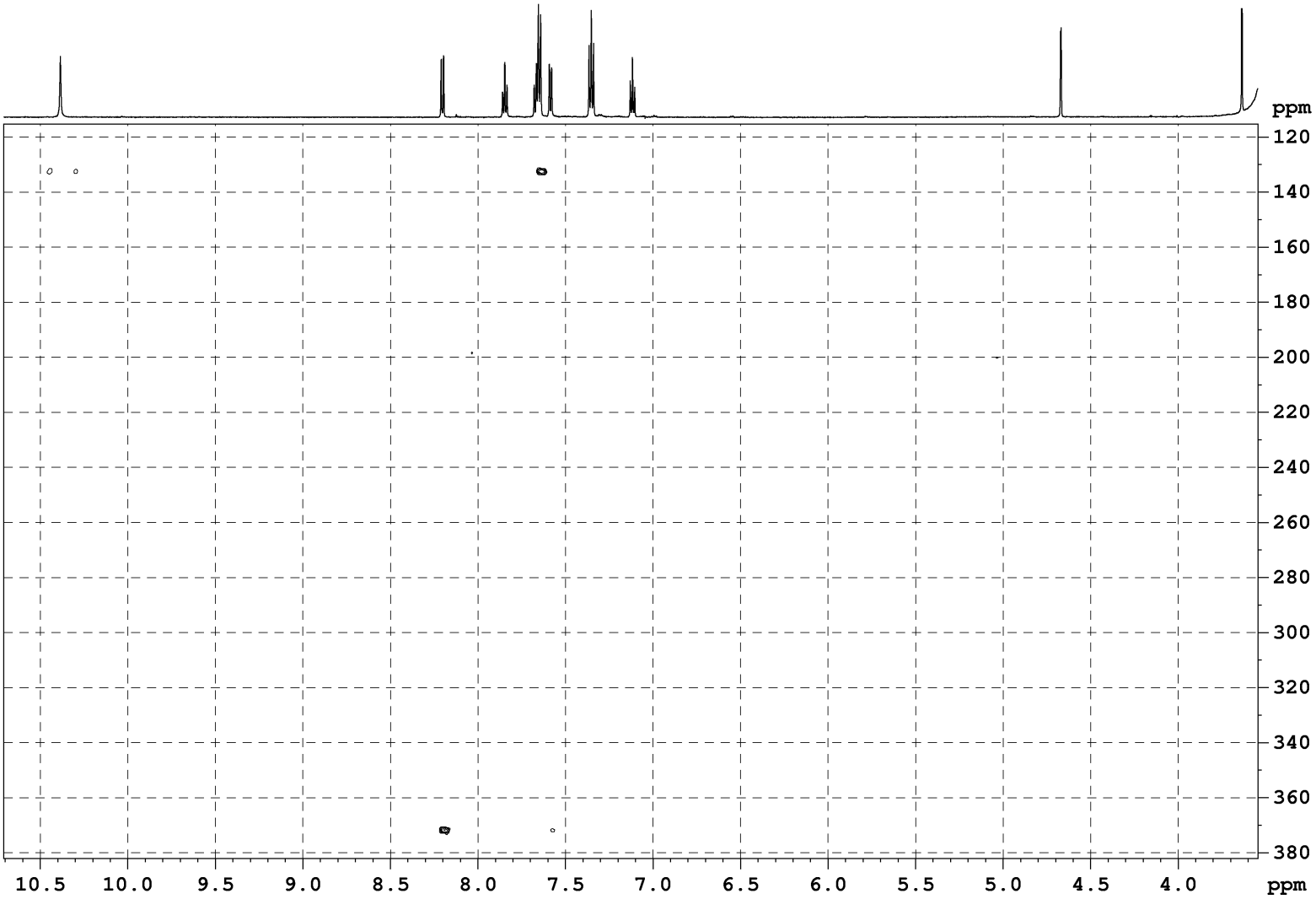



**Figure S8.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **3a** in DMSO at T = 303 K.

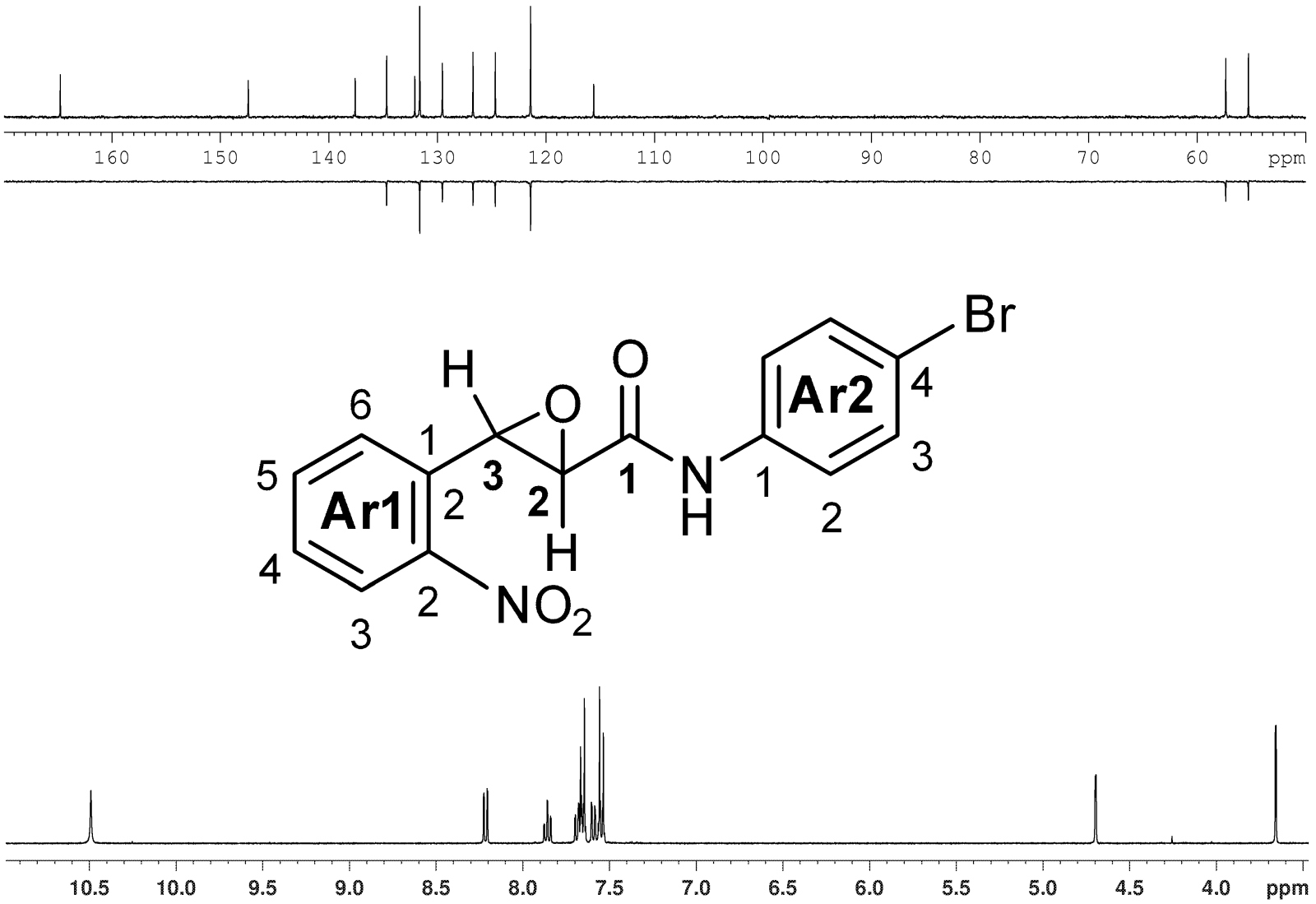



**Figure S9.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **3b** in DMSO at T = 303 K.

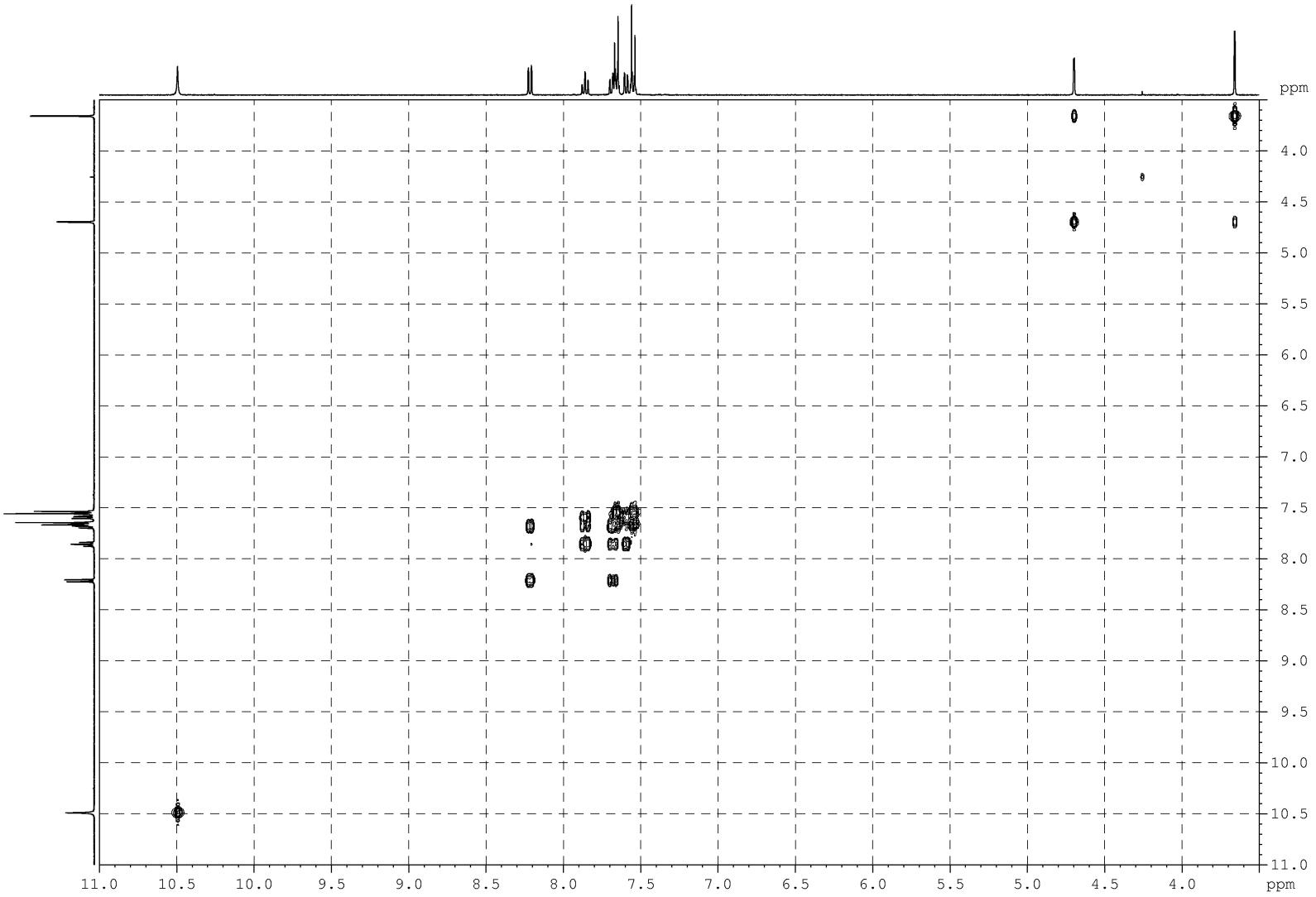



**Figure S10.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **3b** in DMSO at T = 303 K.

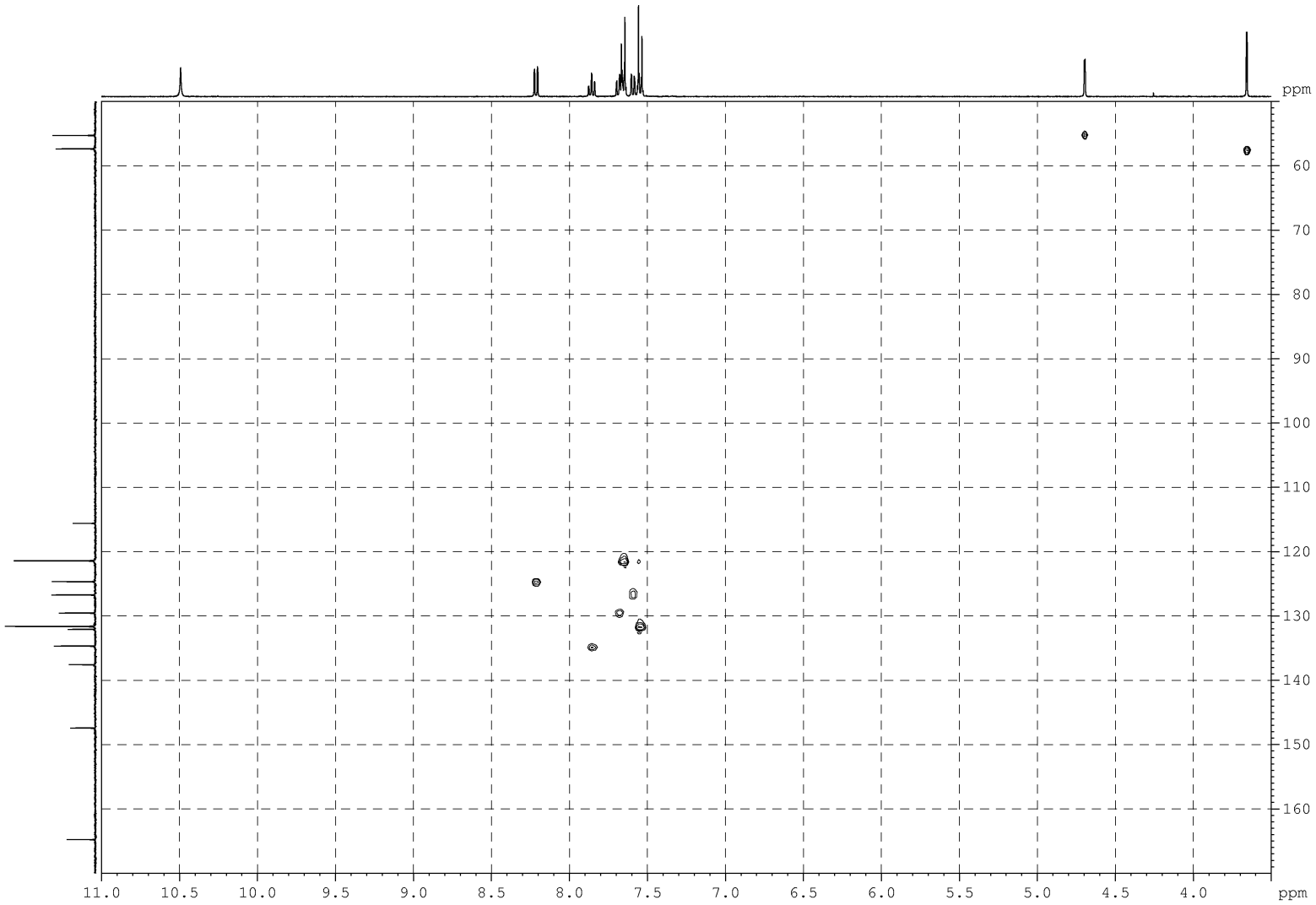



**Figure S11.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **3b** in DMSO at T = 303 K.

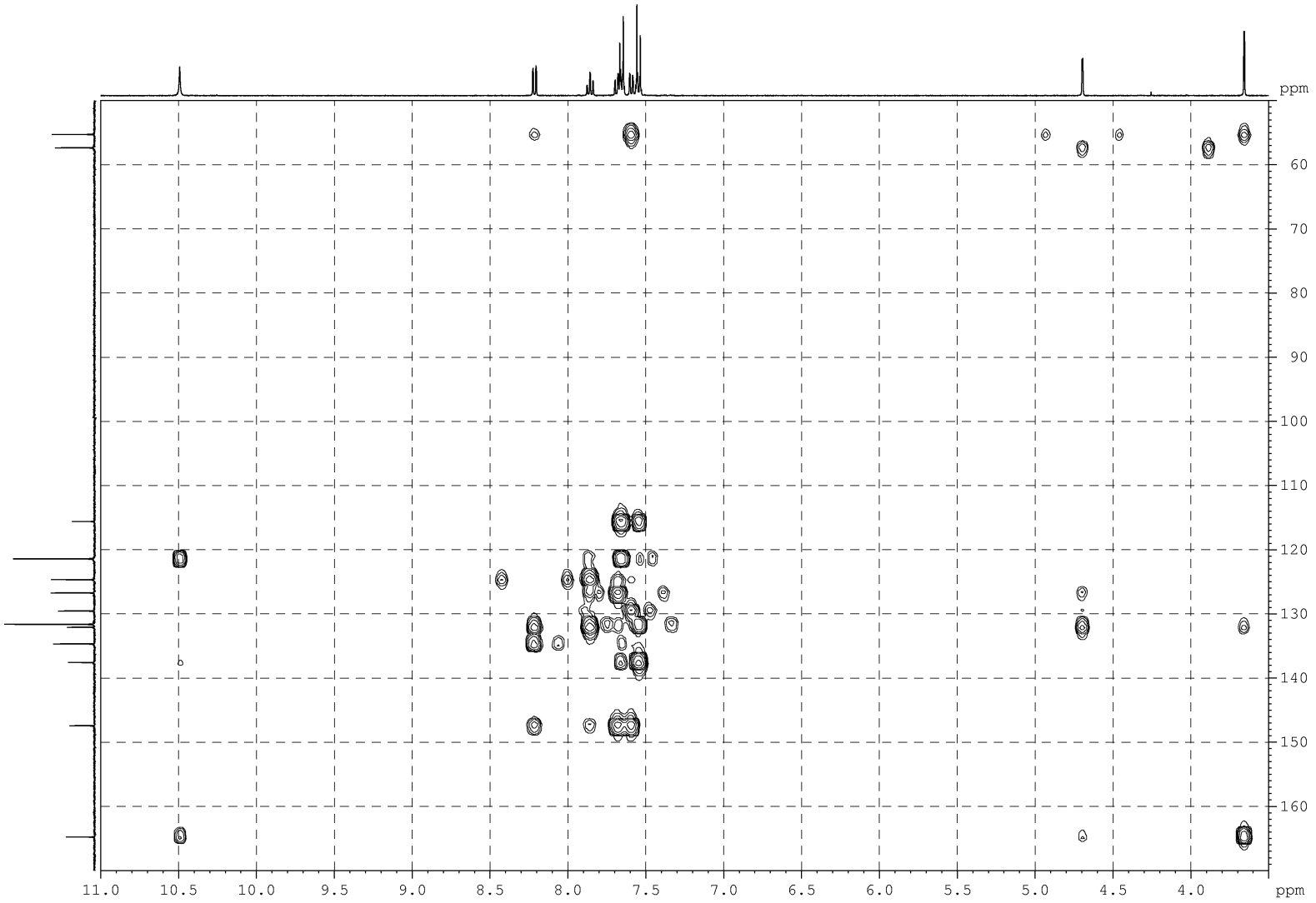



**Figure S12.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **3b** in DMSO at T = 303 K.

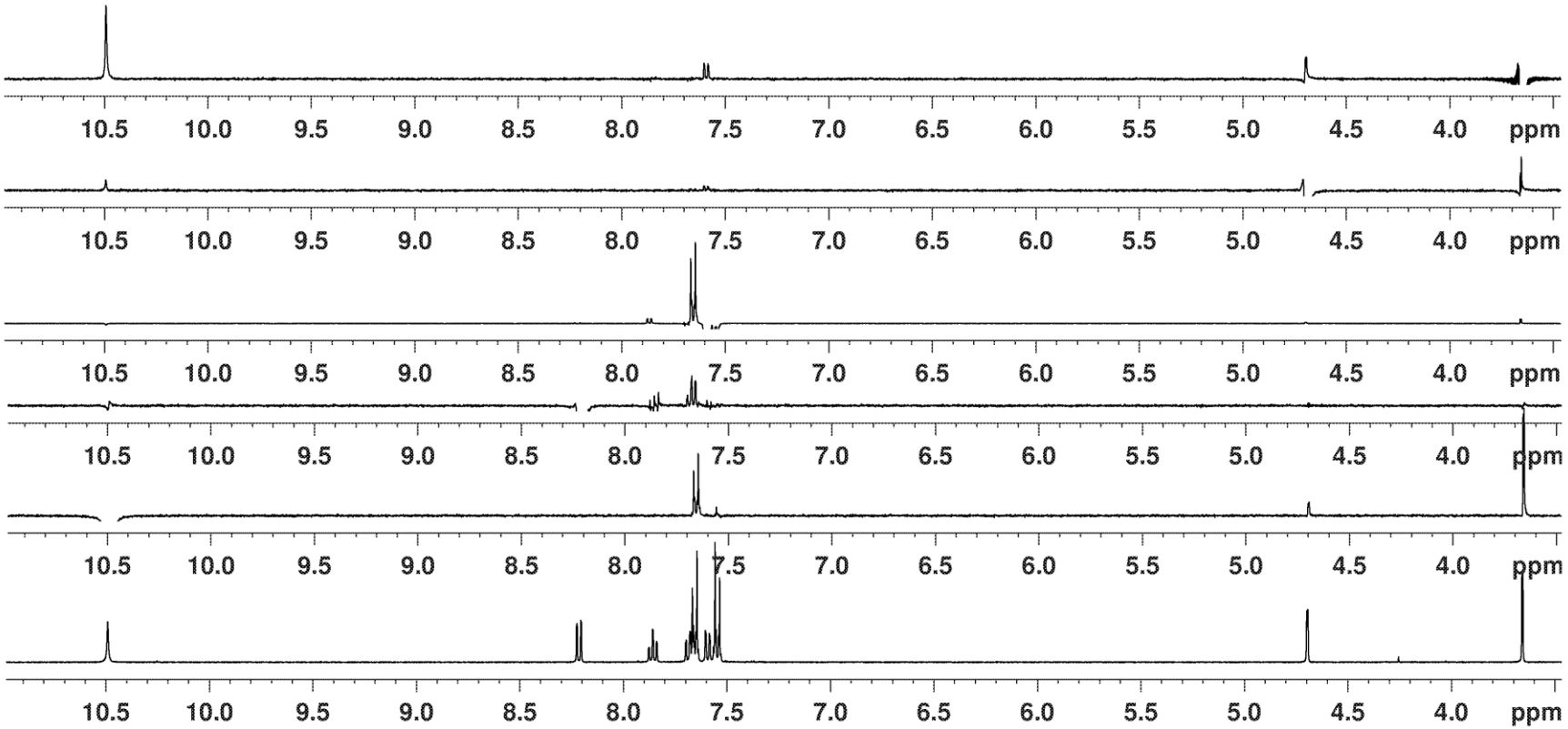



**Figure S13.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **3b** in DMSO at T = 303 K.

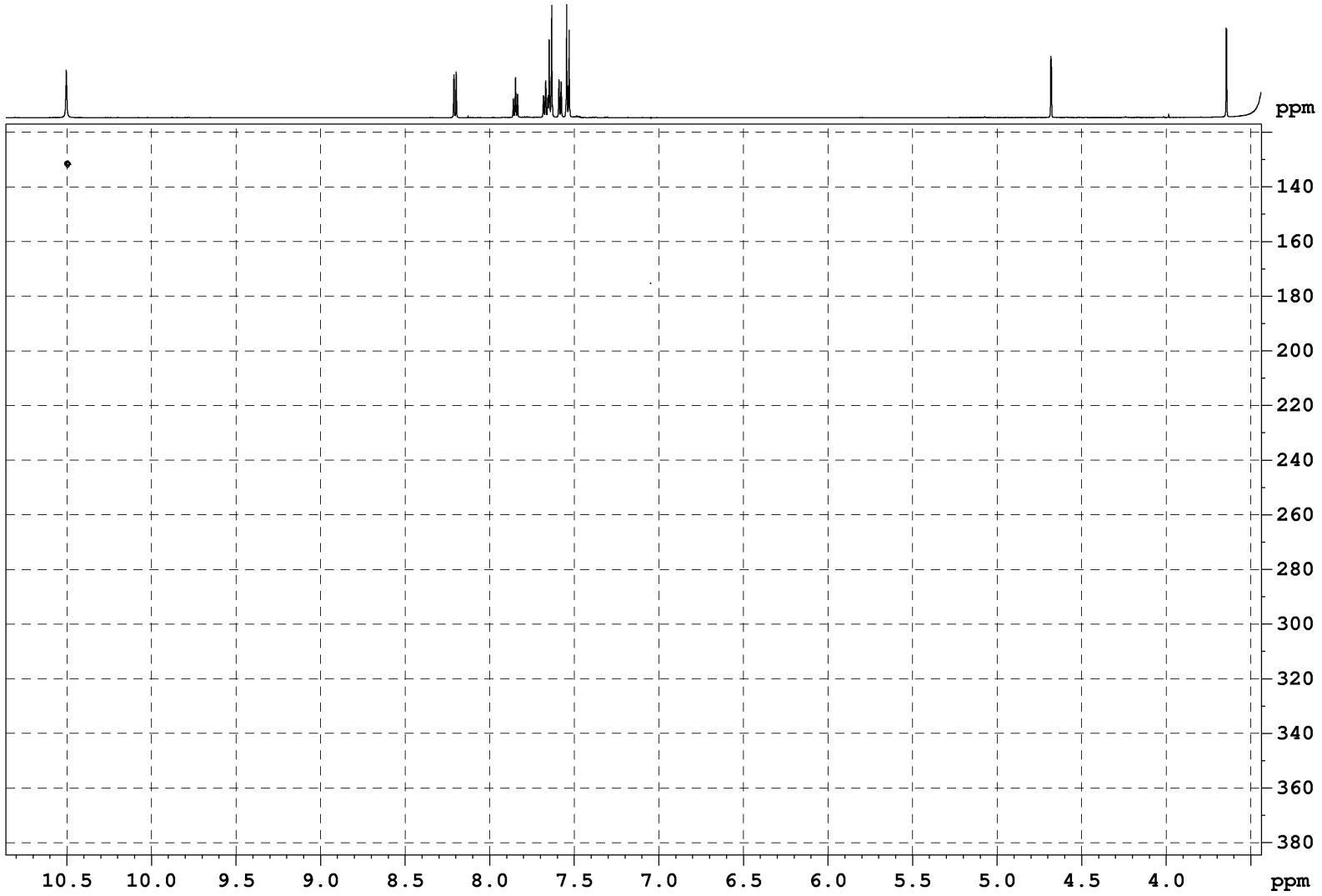



**Figure S14.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **3b** in DMSO at T = 303 K.

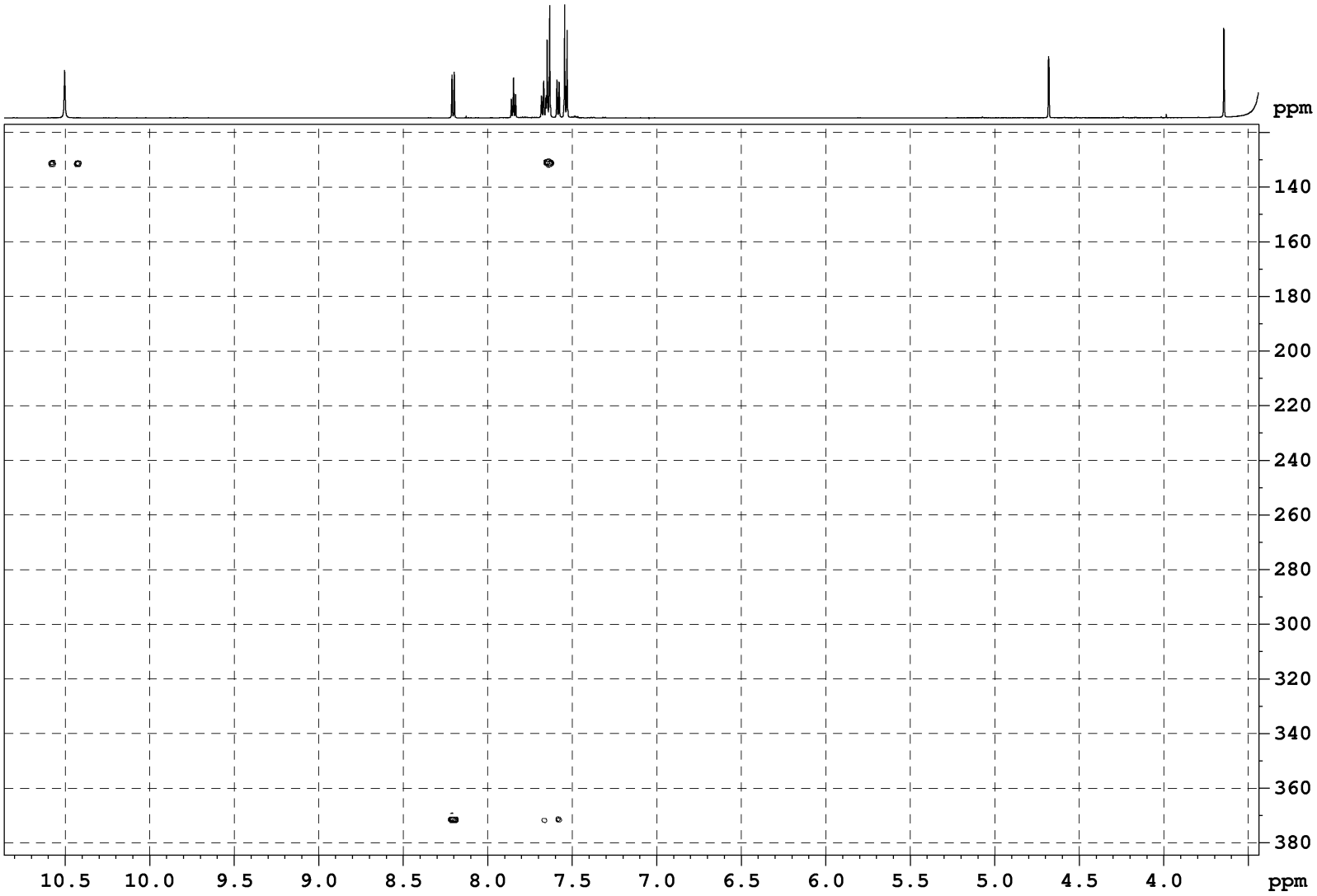



**Figure S15.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **3b** in DMSO at T = 303 K.

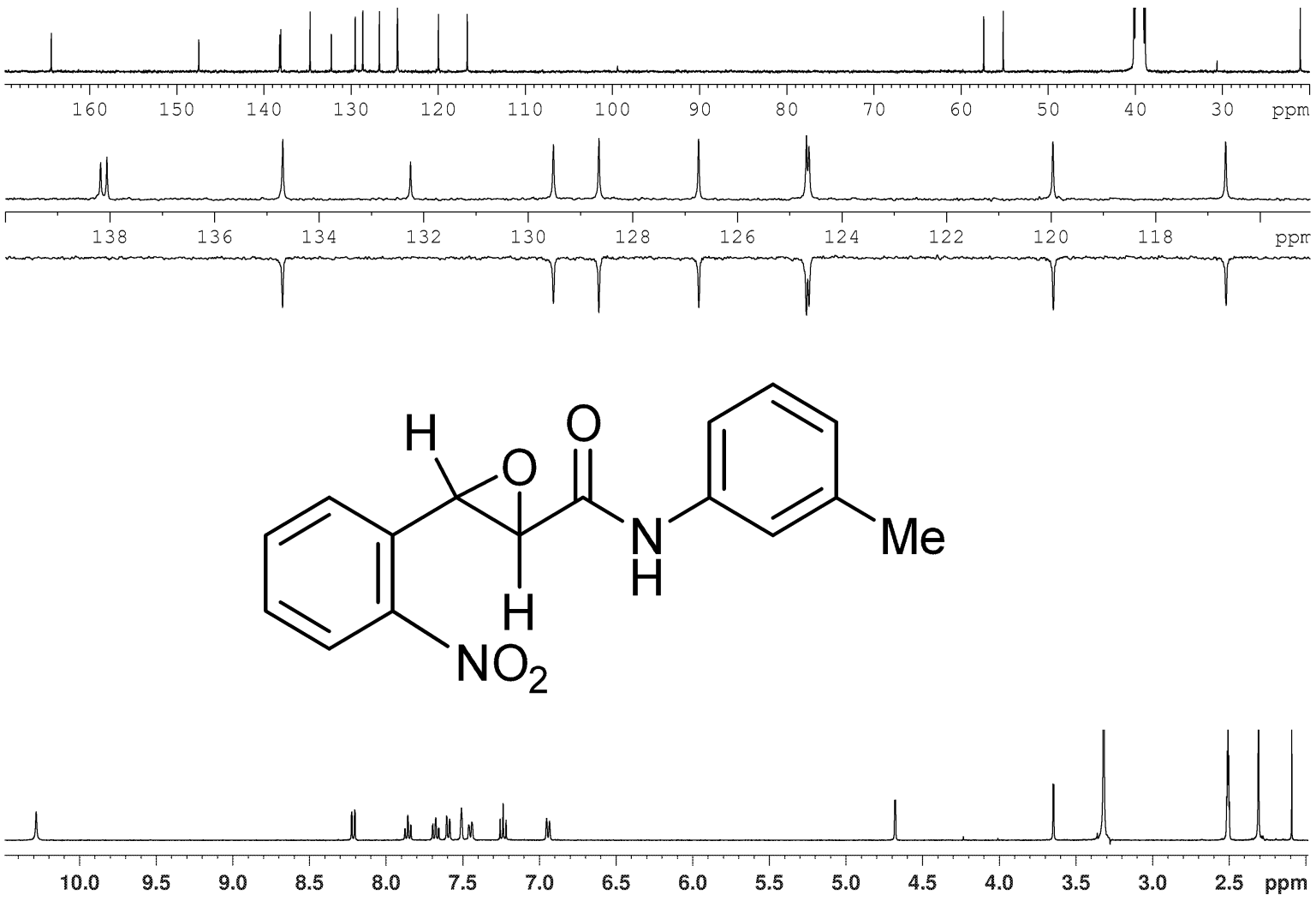



**Figure S16.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **3c** in DMSO at T = 303 K.

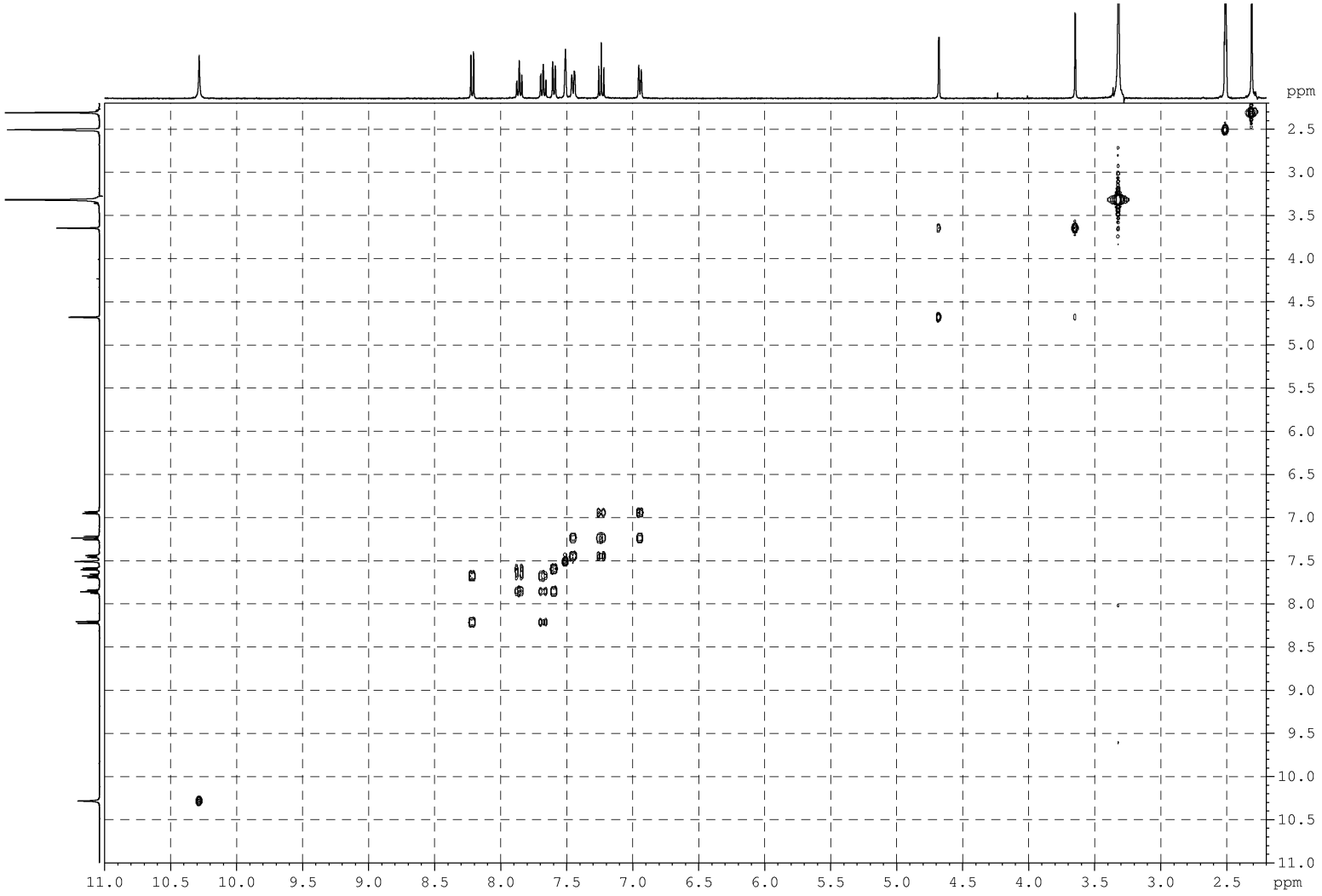



**Figure S17.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **3c** in DMSO at T = 303 K.

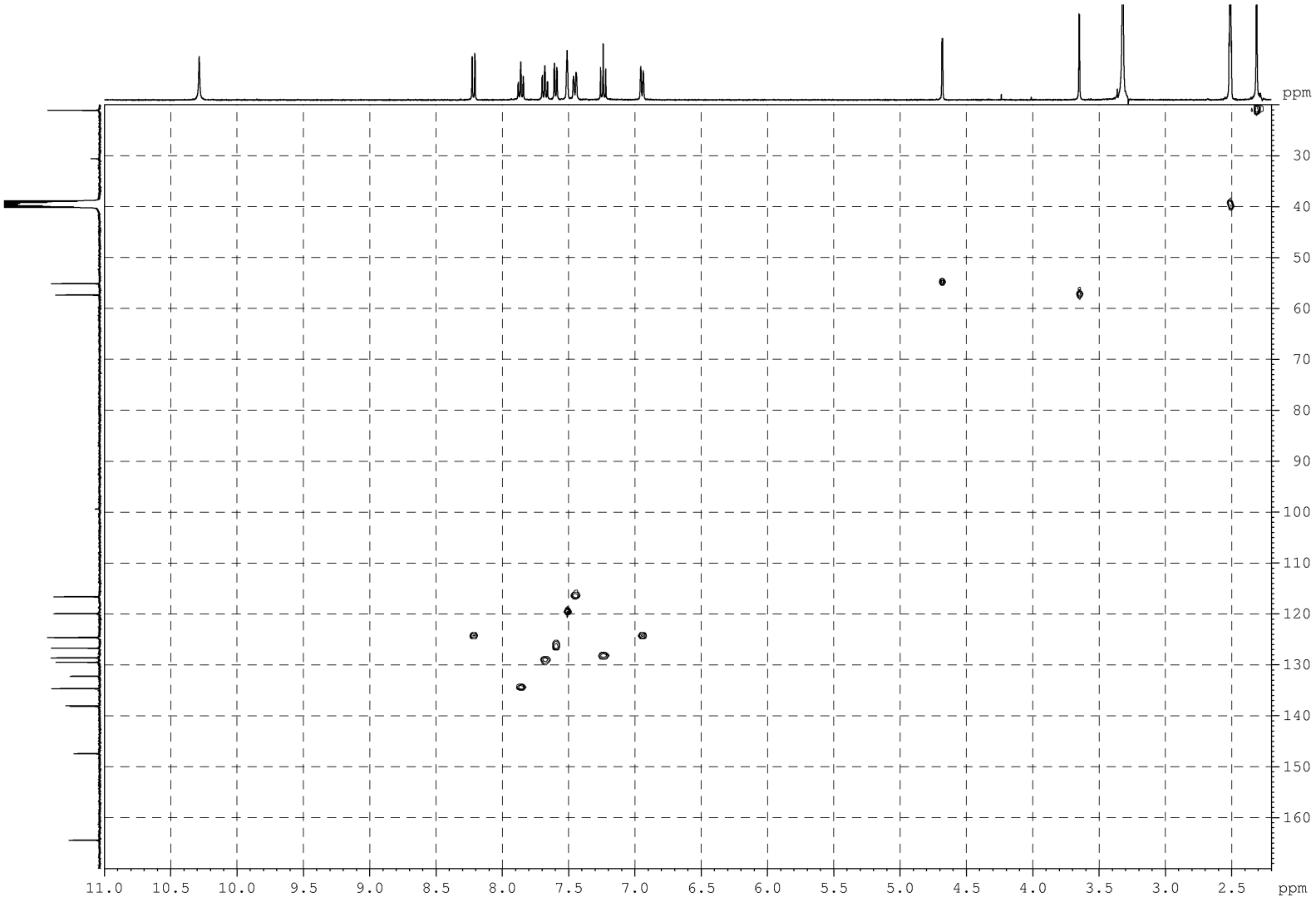



**Figure S18.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **3c** in DMSO at T = 303 K.

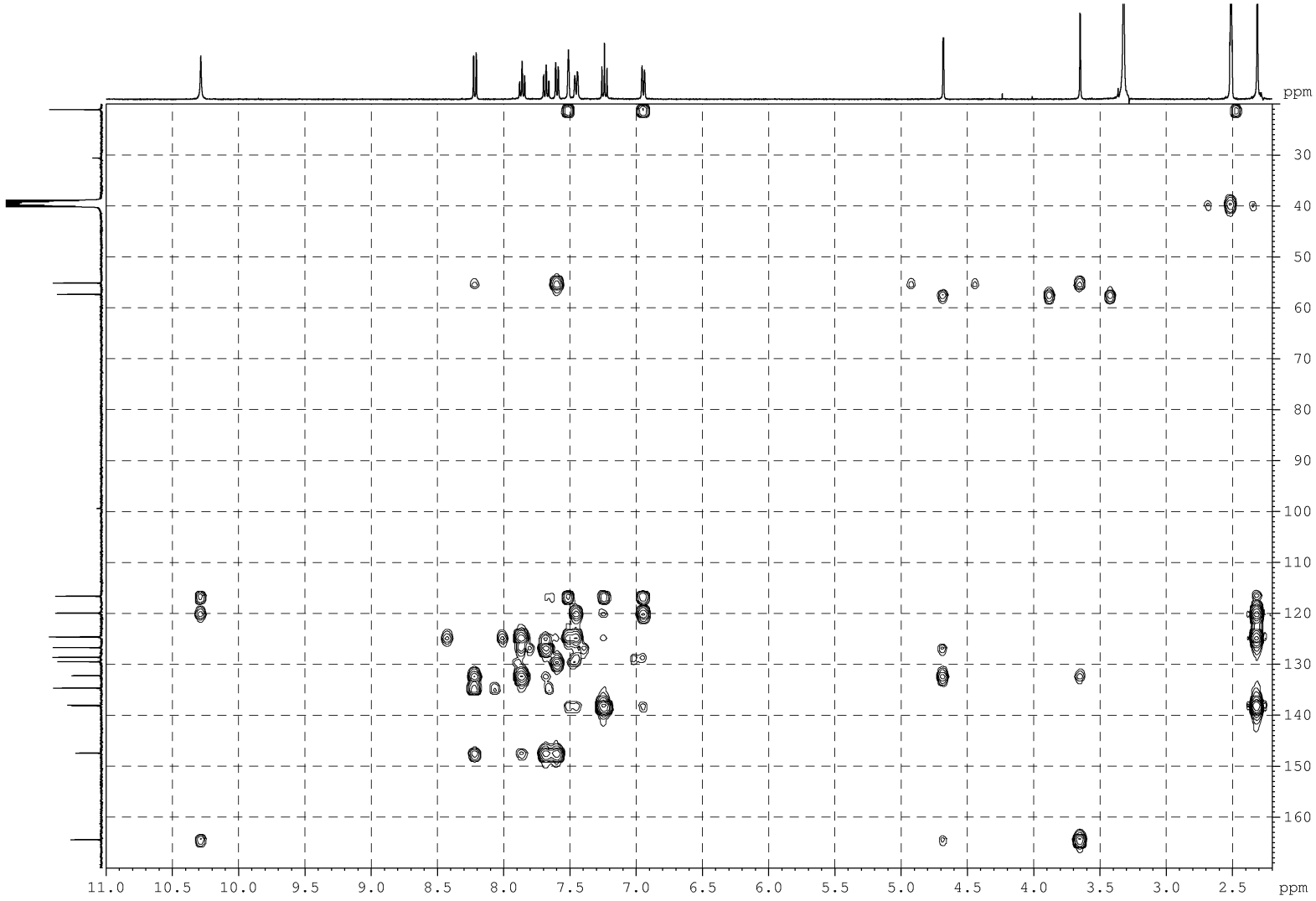



**Figure S19.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **3c** in DMSO at T = 303 K.

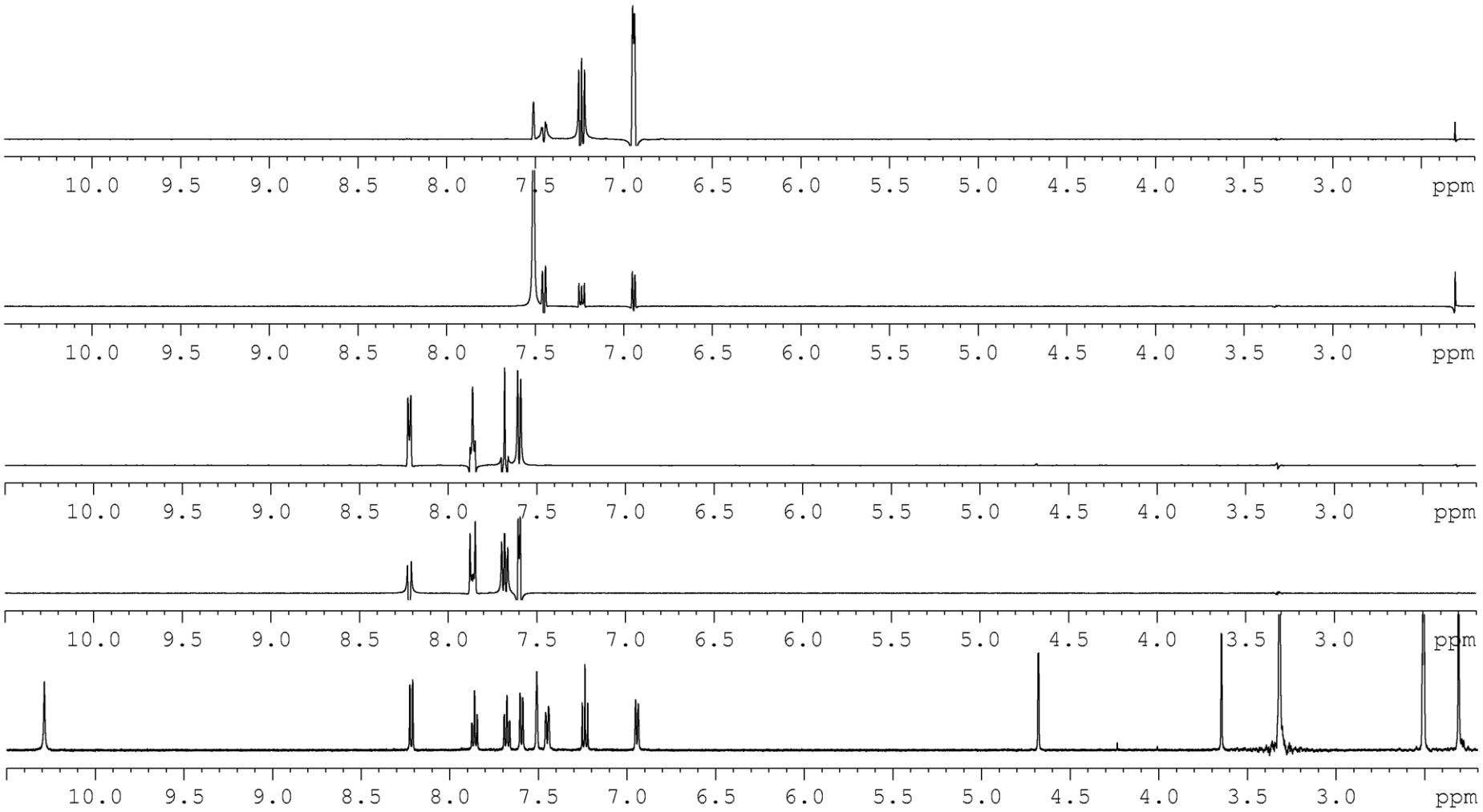



**Figure S20.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **3c** in DMSO at T = 303 K.

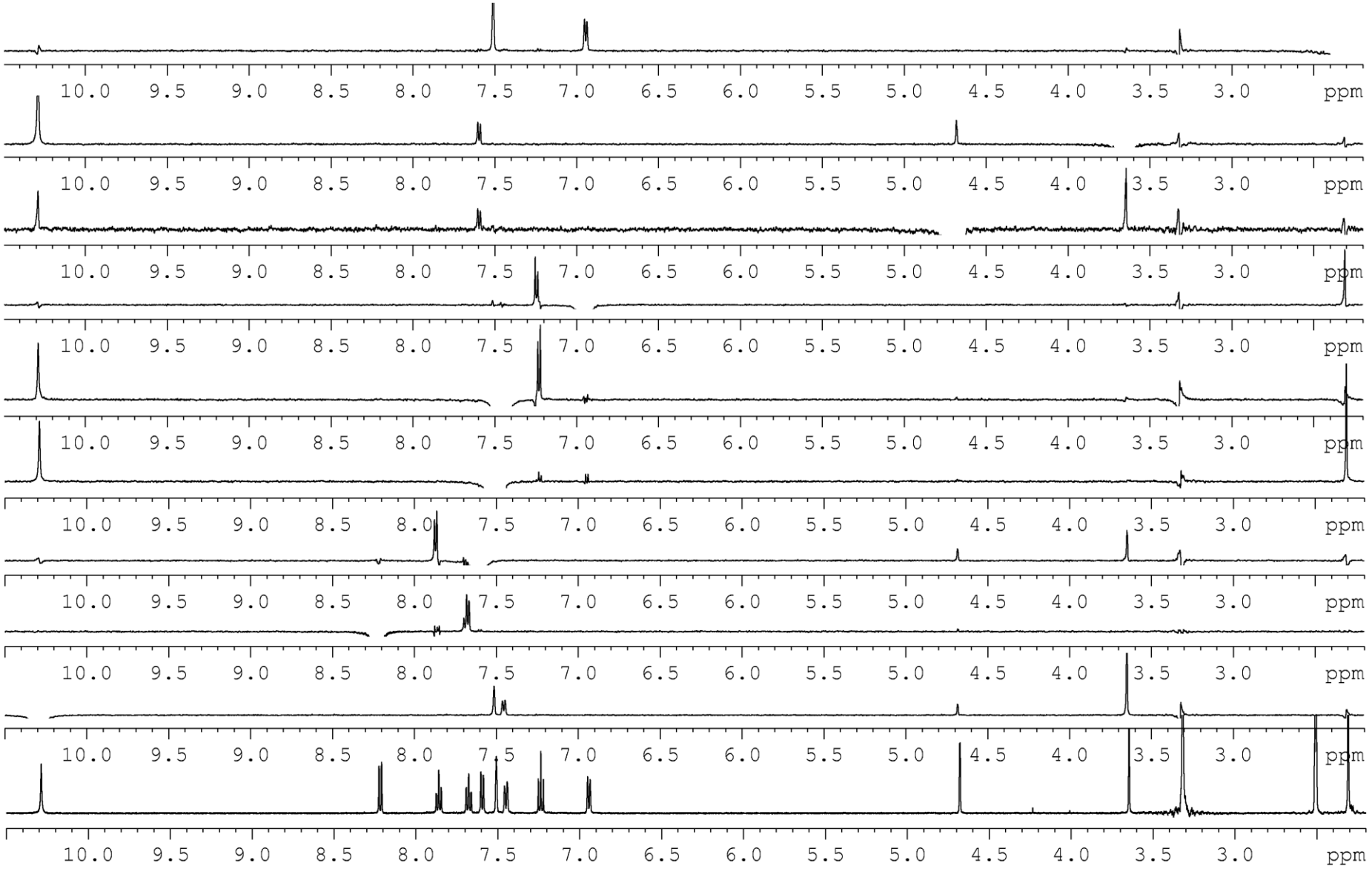



**Figure S21.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **3c** in DMSO at T = 303 K.

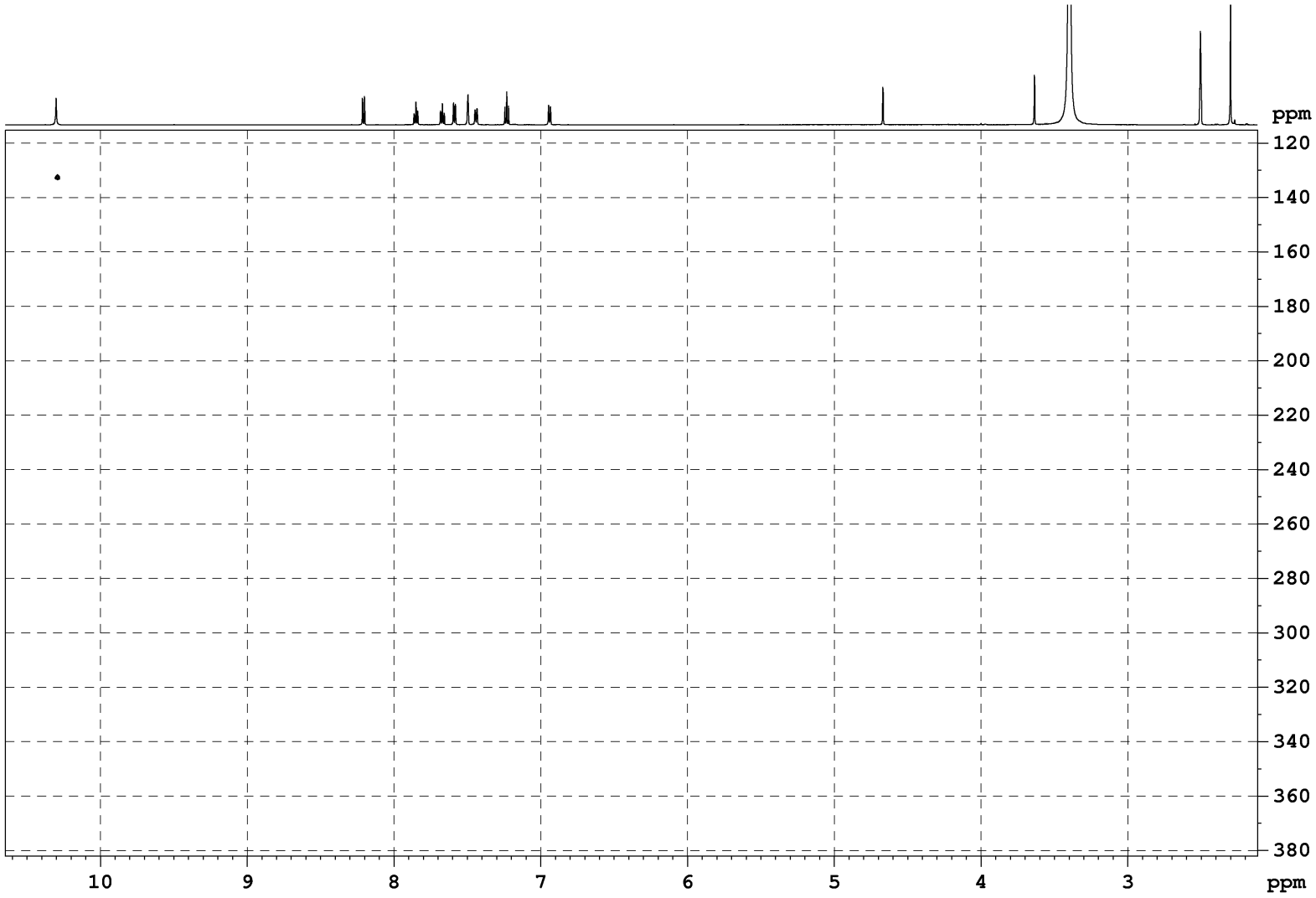



**Figure S22.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **3c** in DMSO at T = 303 K.

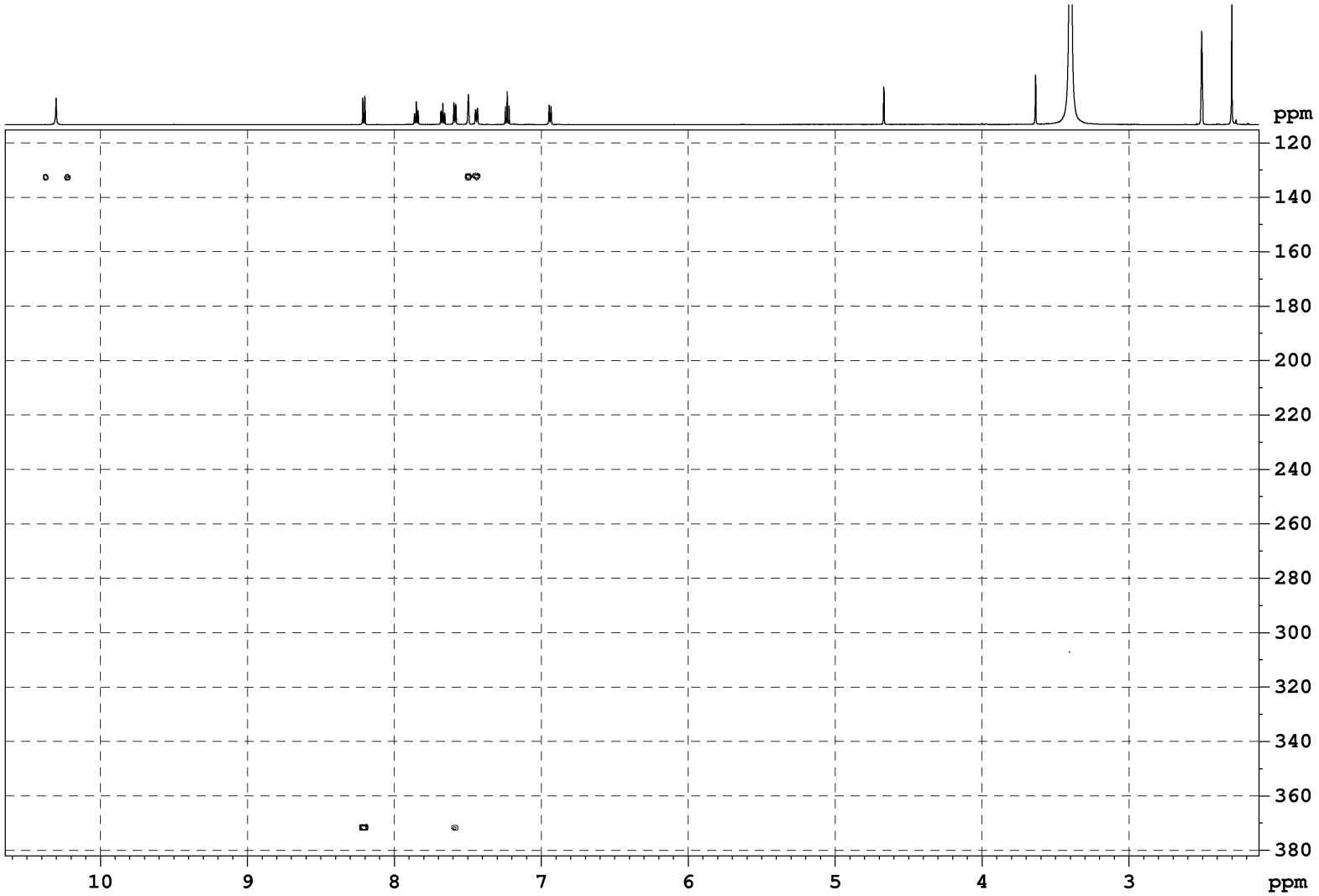



**Figure S23.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **3c** in DMSO at T = 303 K.

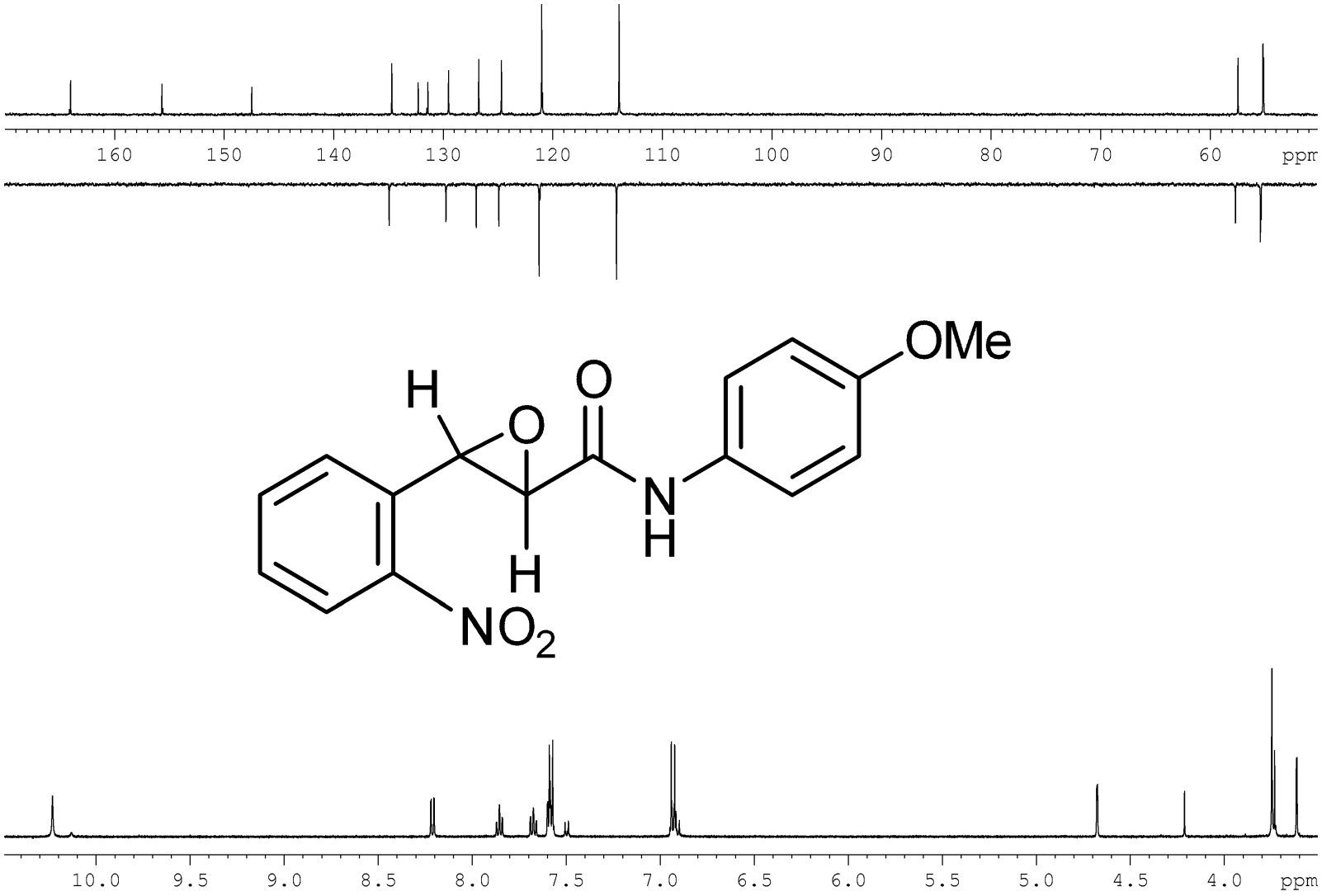



**Figure S24.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **3d** in DMSO at T = 303 K.

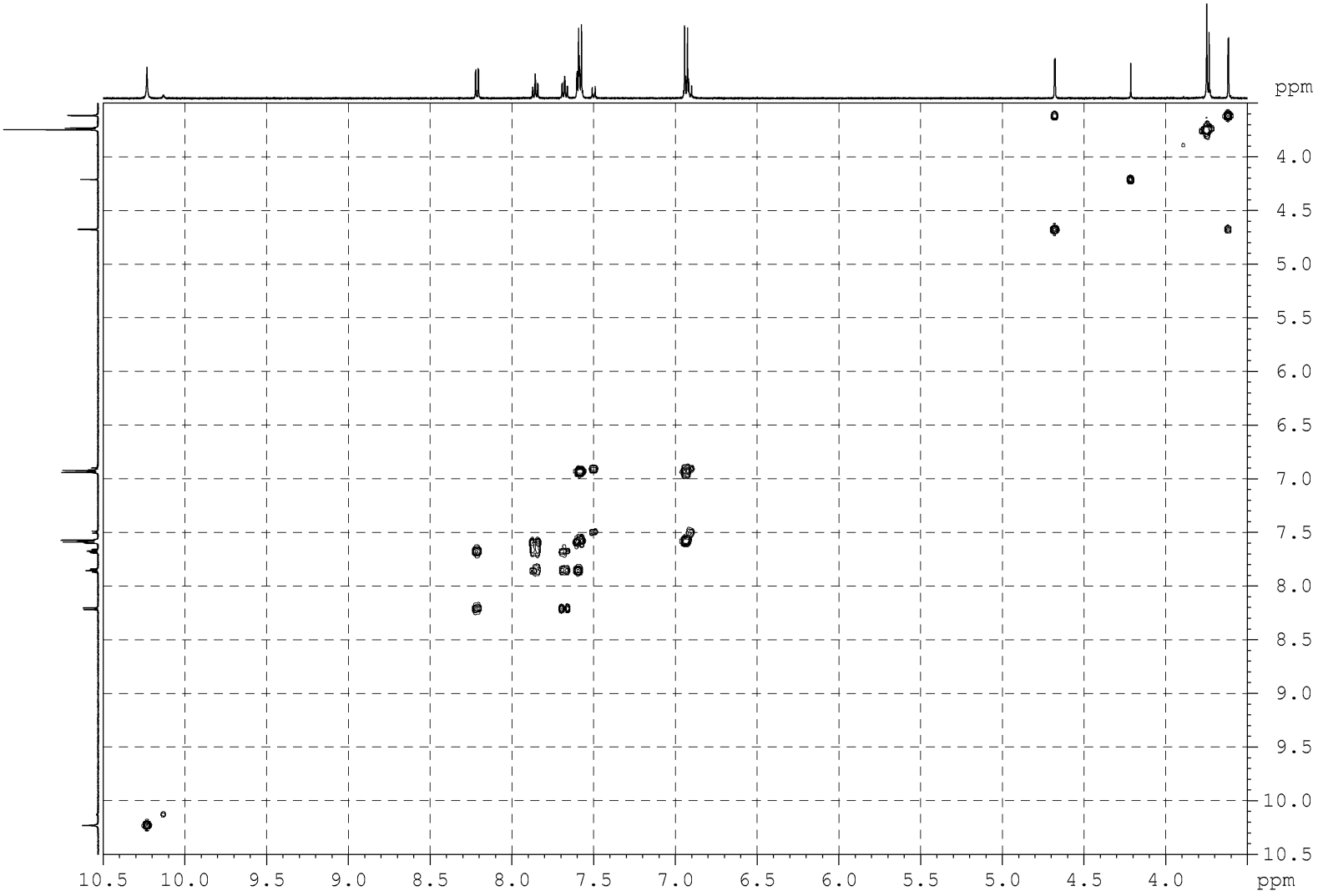



**Figure S25.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **3d** in DMSO at T = 303 K.

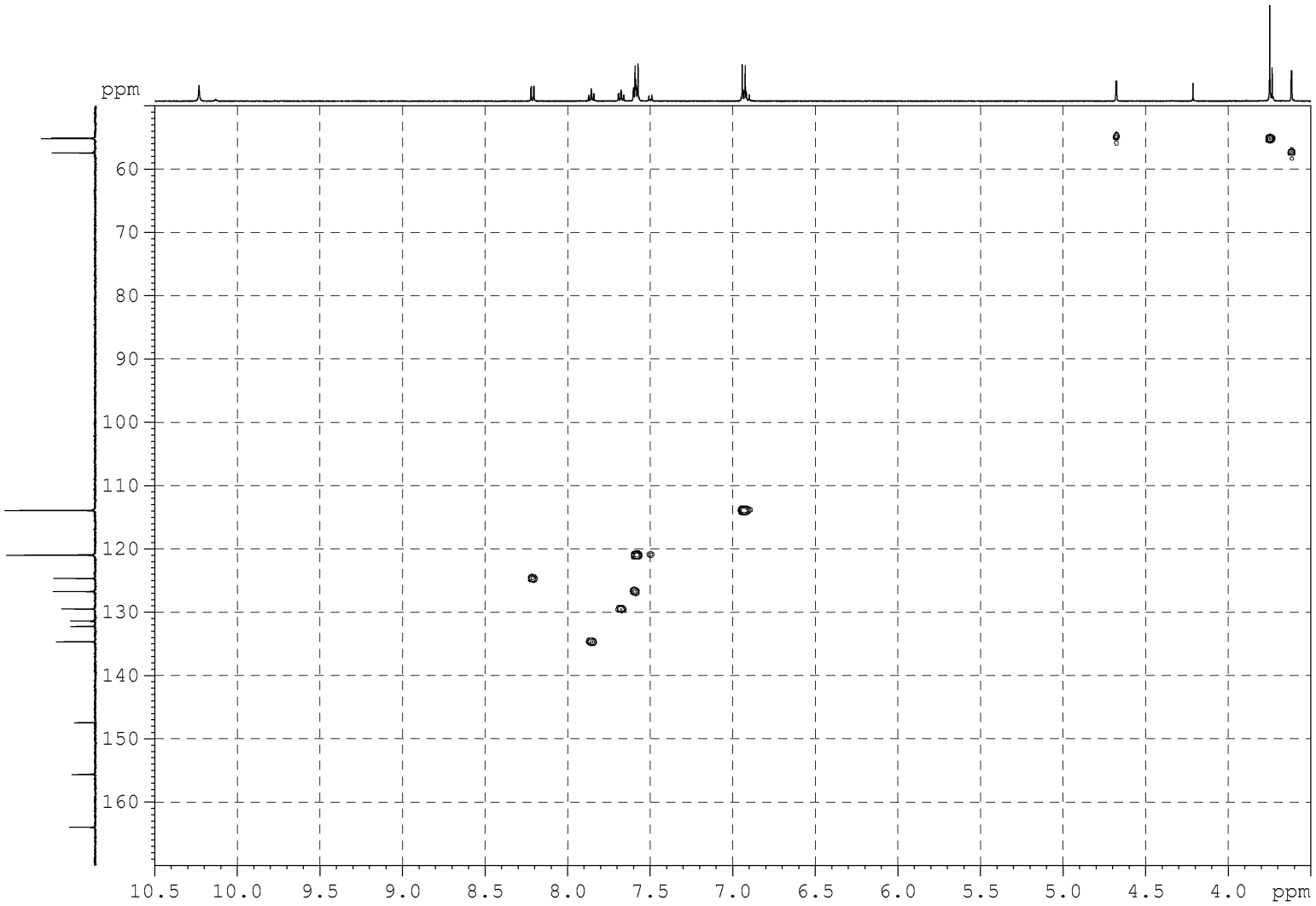



**Figure S26.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **3d** in DMSO at T = 303 K.

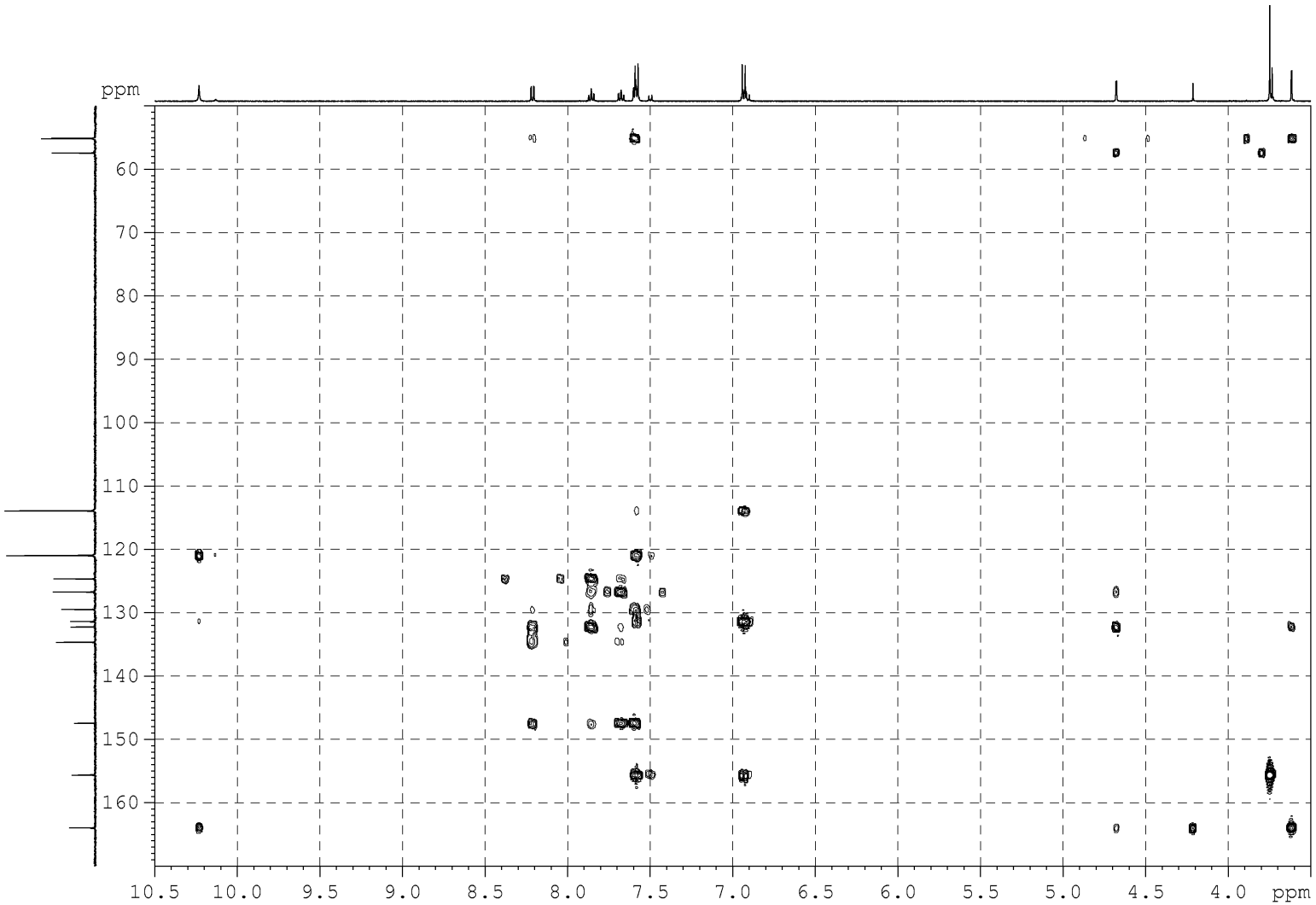



**Figure S27.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **3d** in DMSO at T = 303 K.

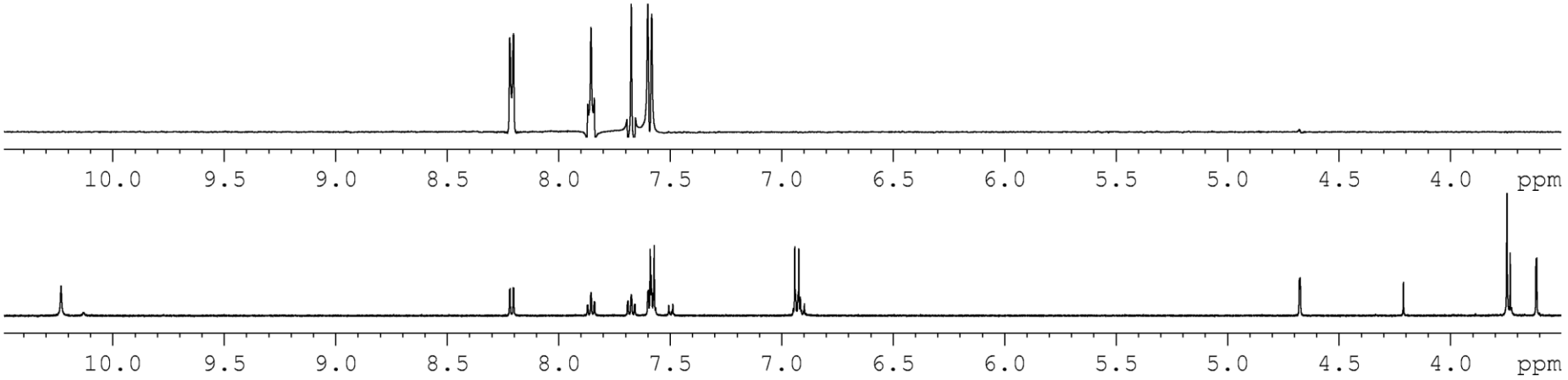



**Figure S28.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **3d** in DMSO at T = 303 K.

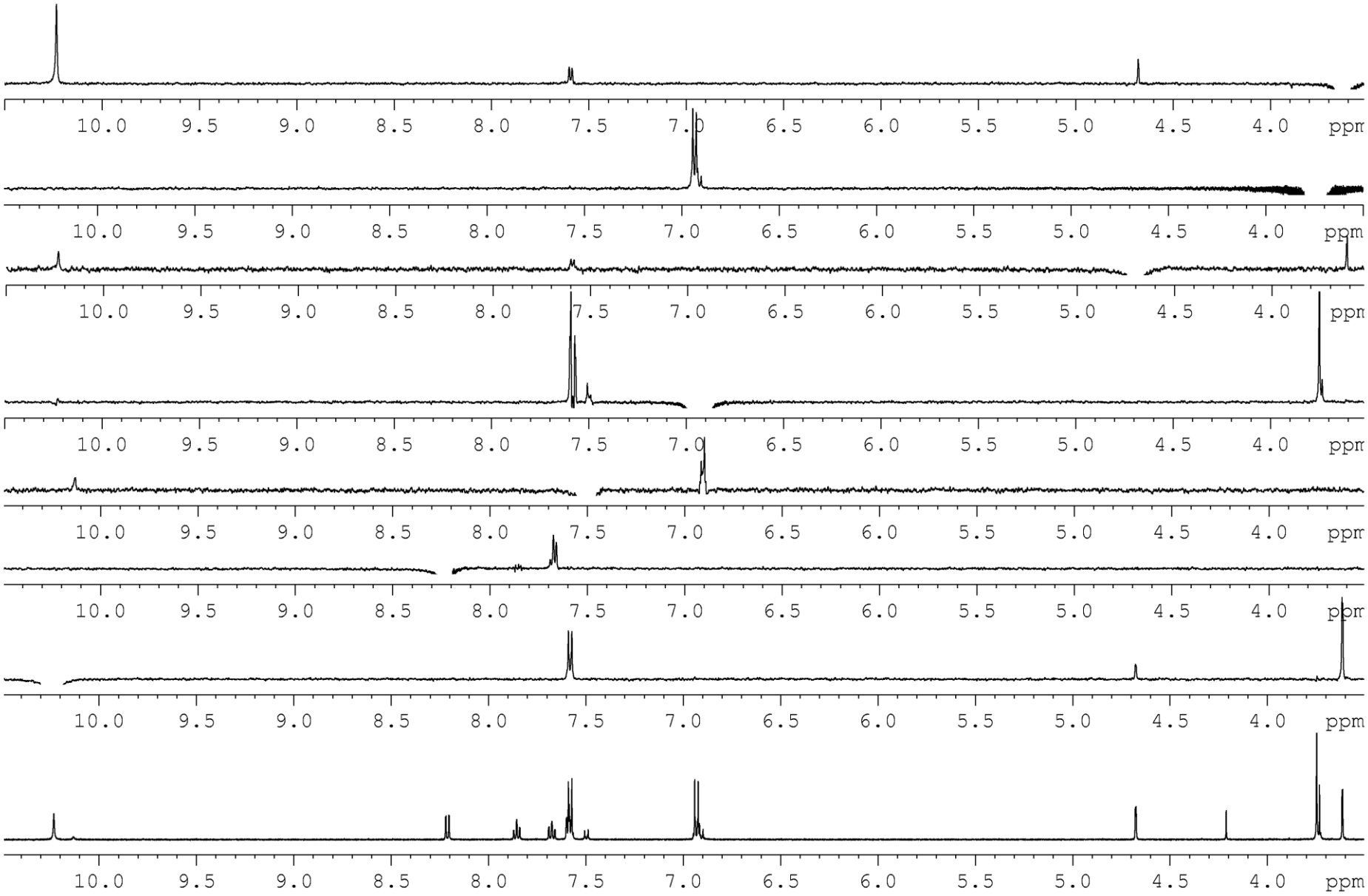



**Figure S29.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **3d** in DMSO at T = 303 K.

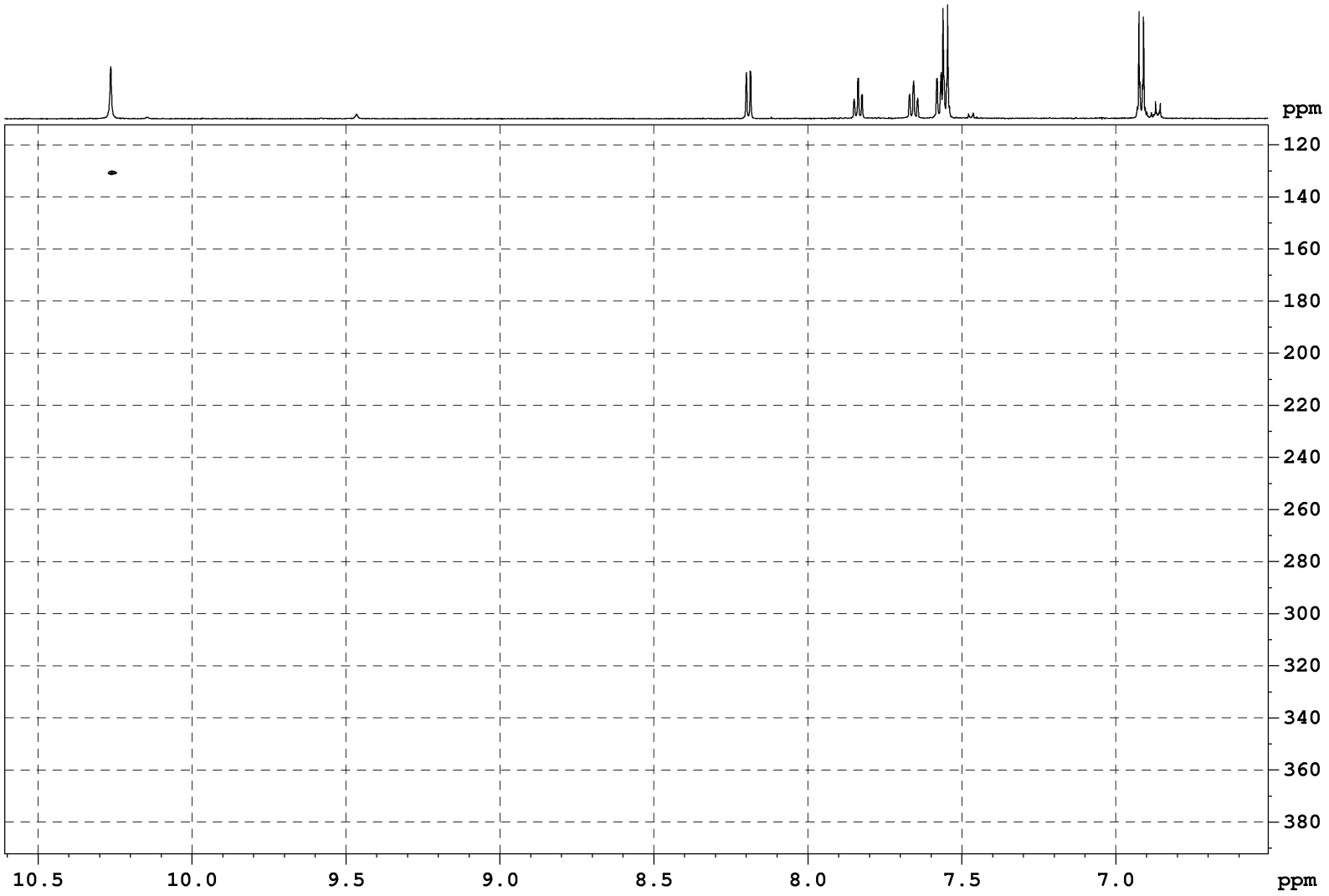



**Figure S30.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **3d** in DMSO at T = 303 K.

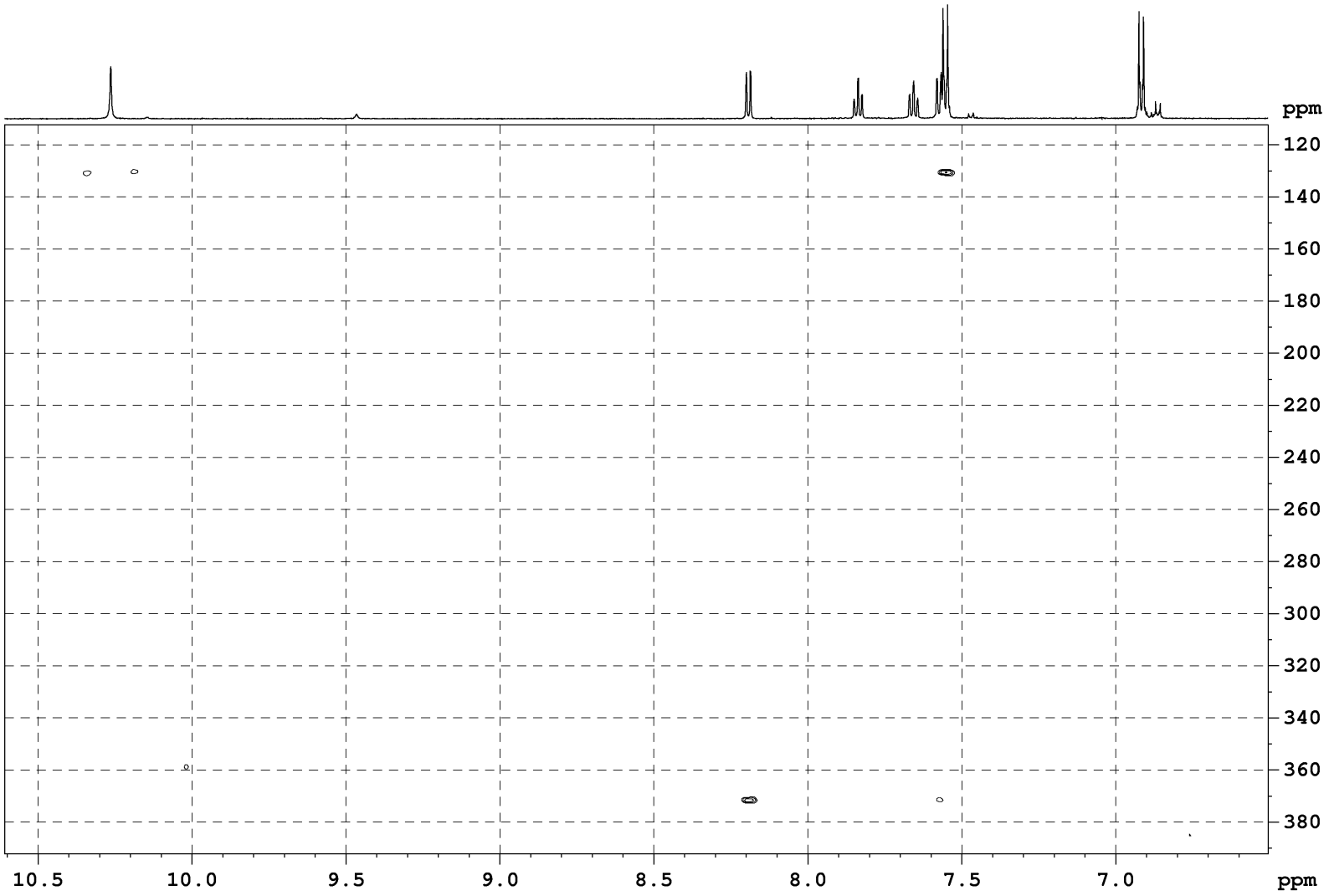



**Figure S31.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **3d** in DMSO at T = 303 K.

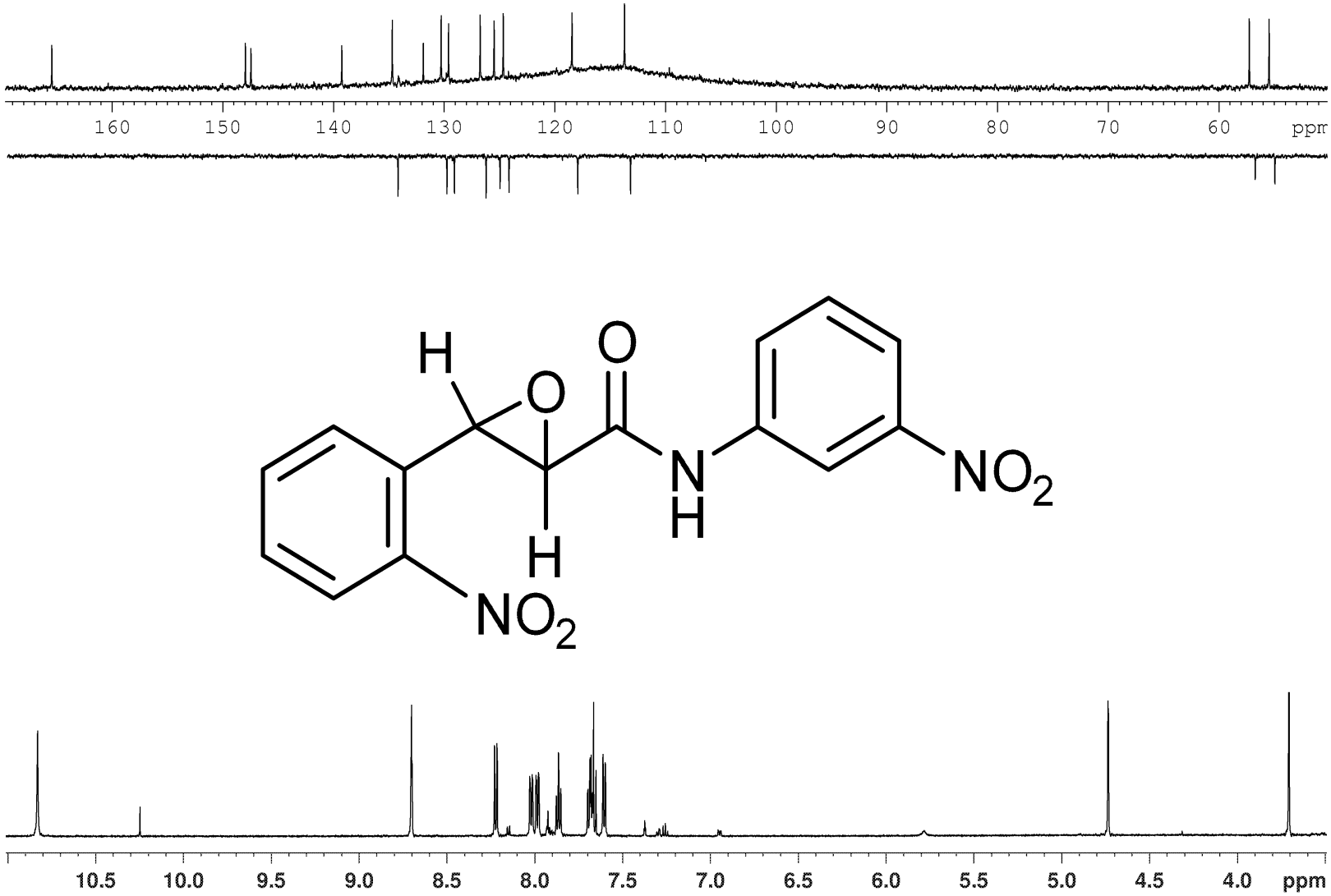



**Figure S32.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **3e** in DMSO at T = 303 K.

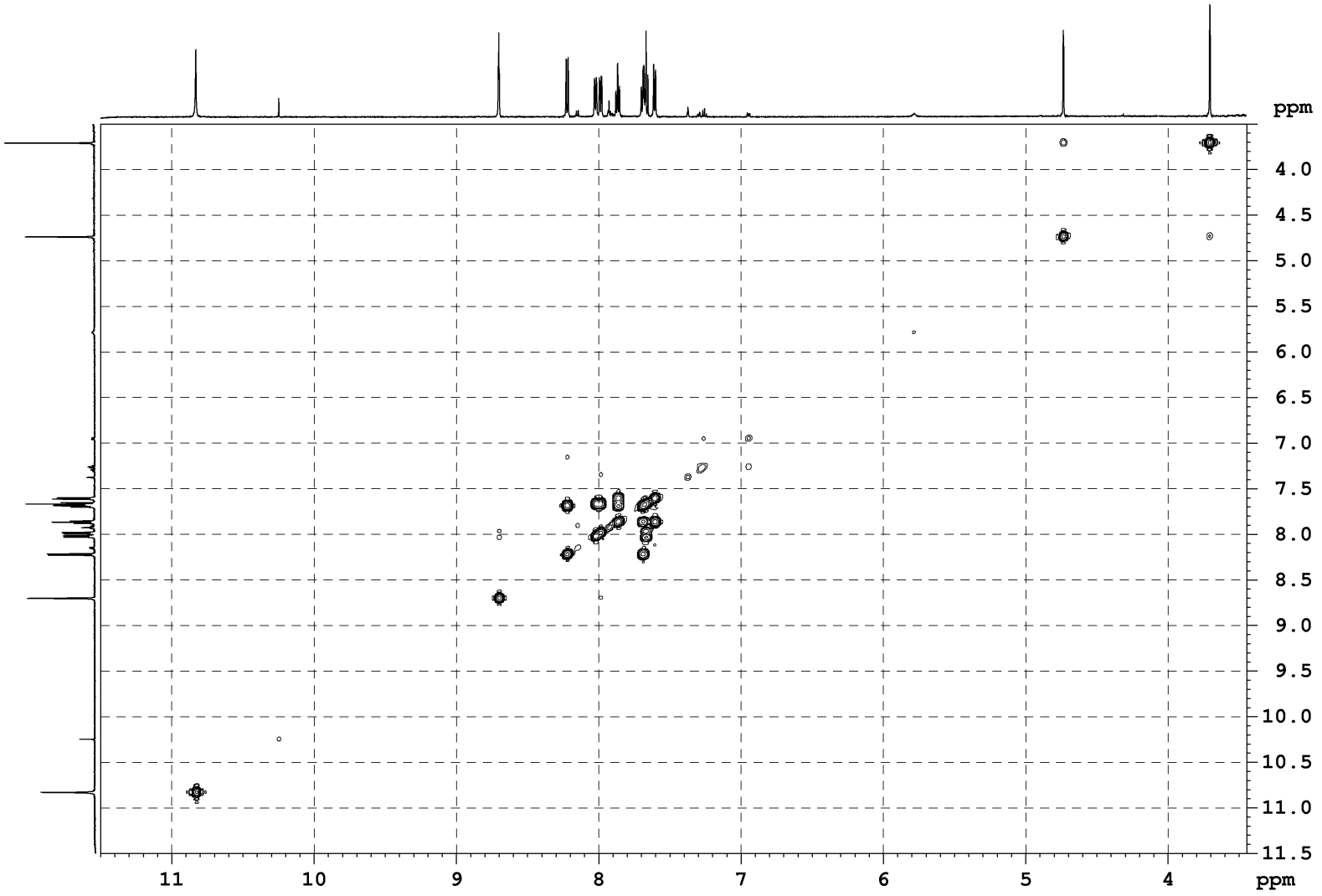



**Figure S33.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **3e** in DMSO at T = 303 K.

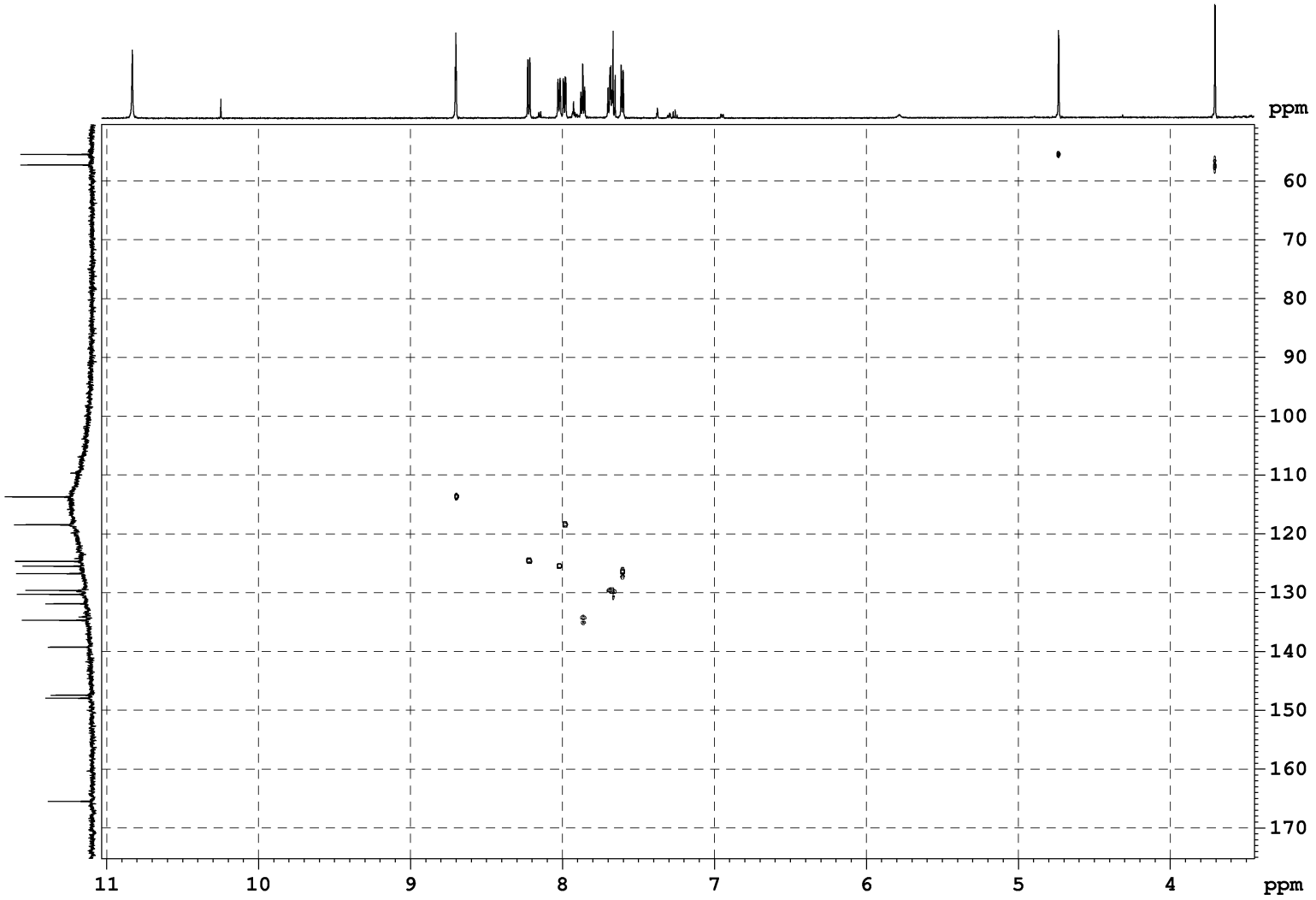



**Figure S34.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **3e** in DMSO at T = 303 K.

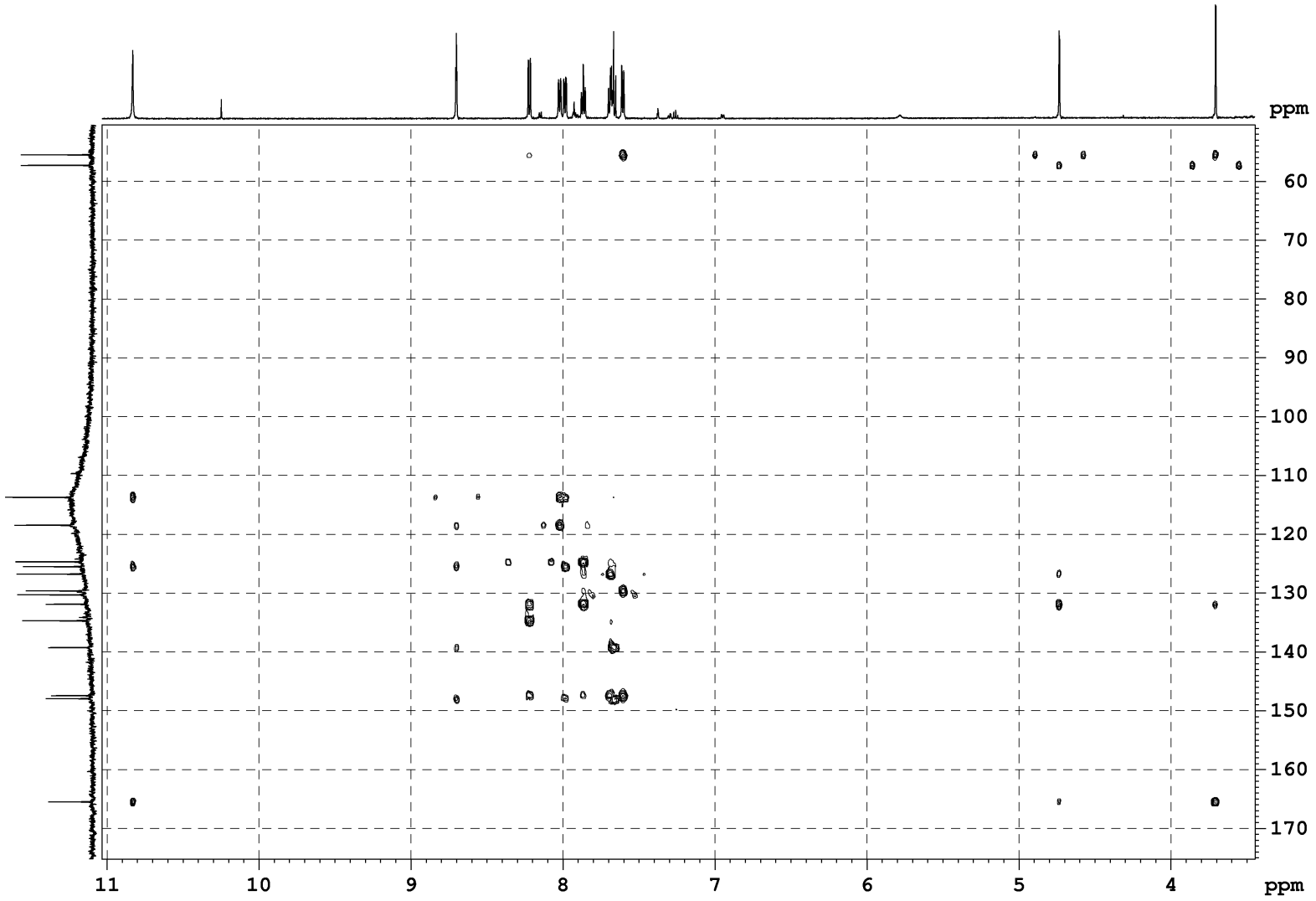



**Figure S35.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **3e** in DMSO at T = 303 K.

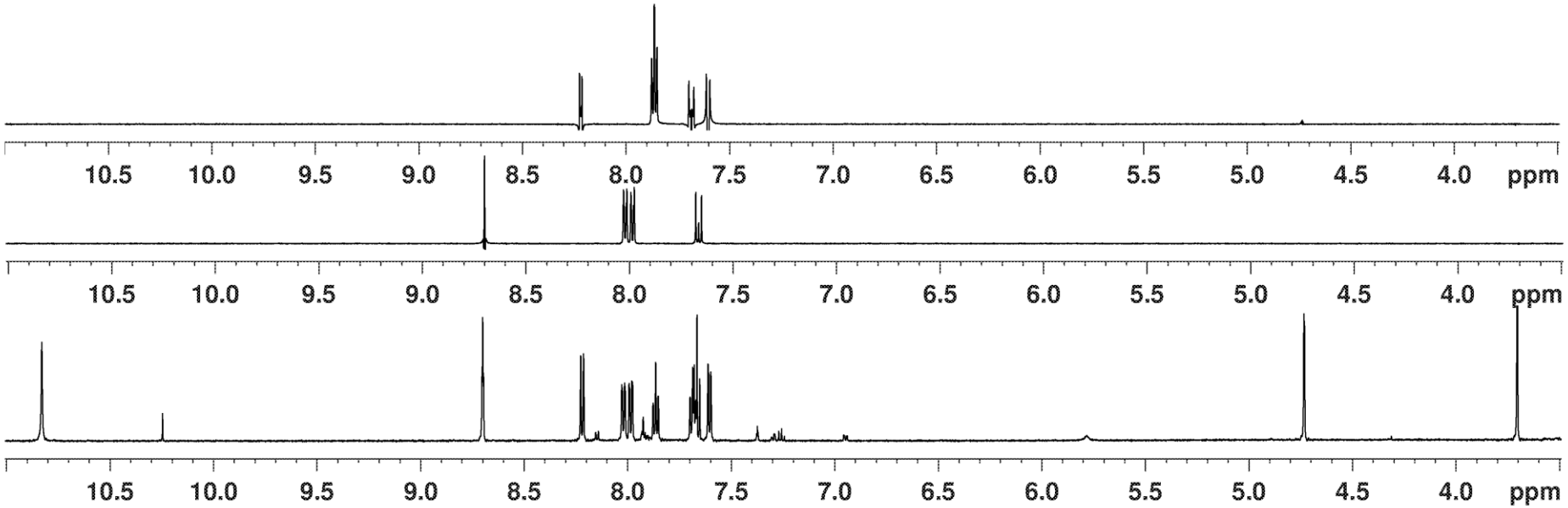



**Figure S36.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **3e** in DMSO at T = 303 K.

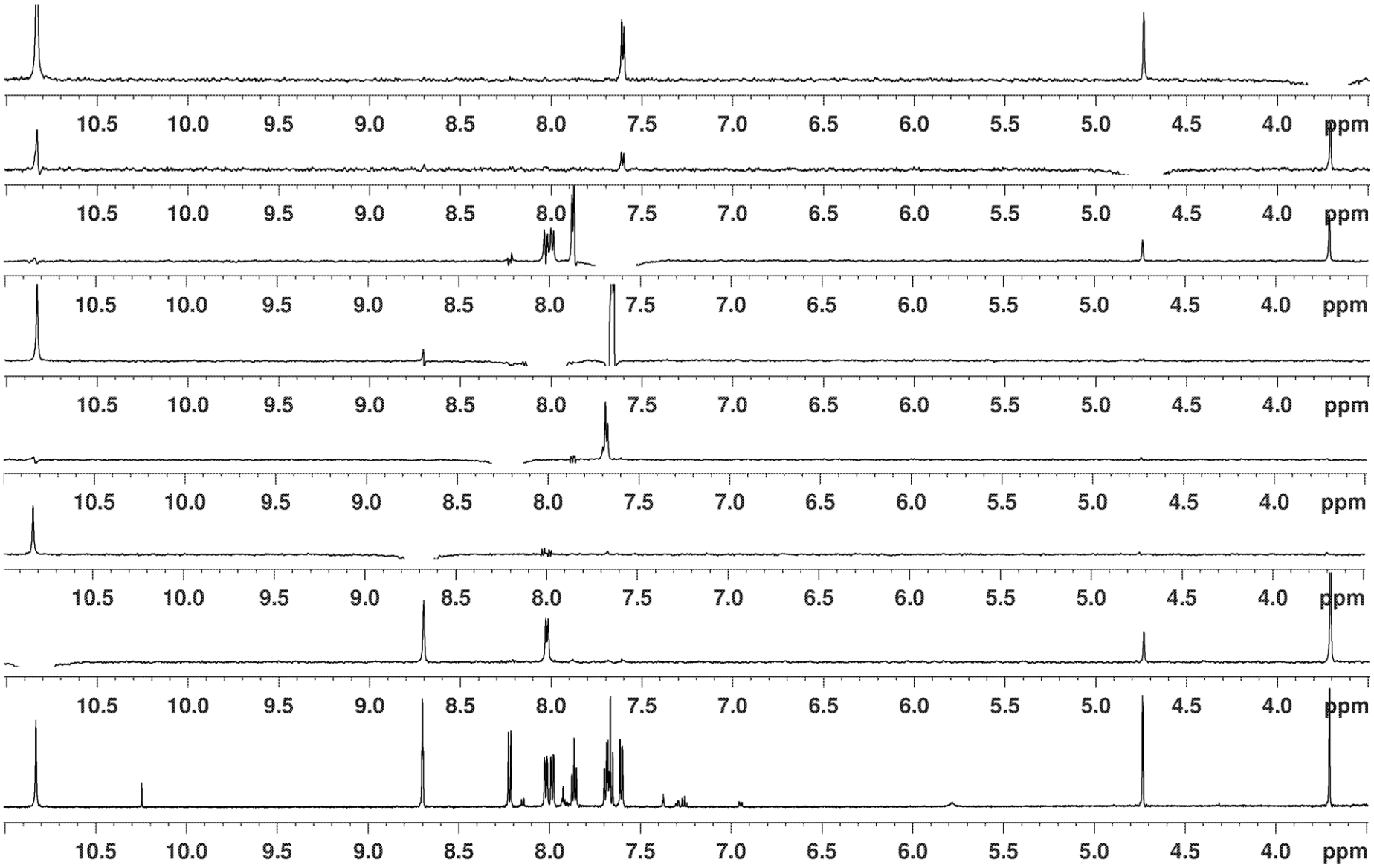



**Figure S37.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **3e** in DMSO at T = 303 K.

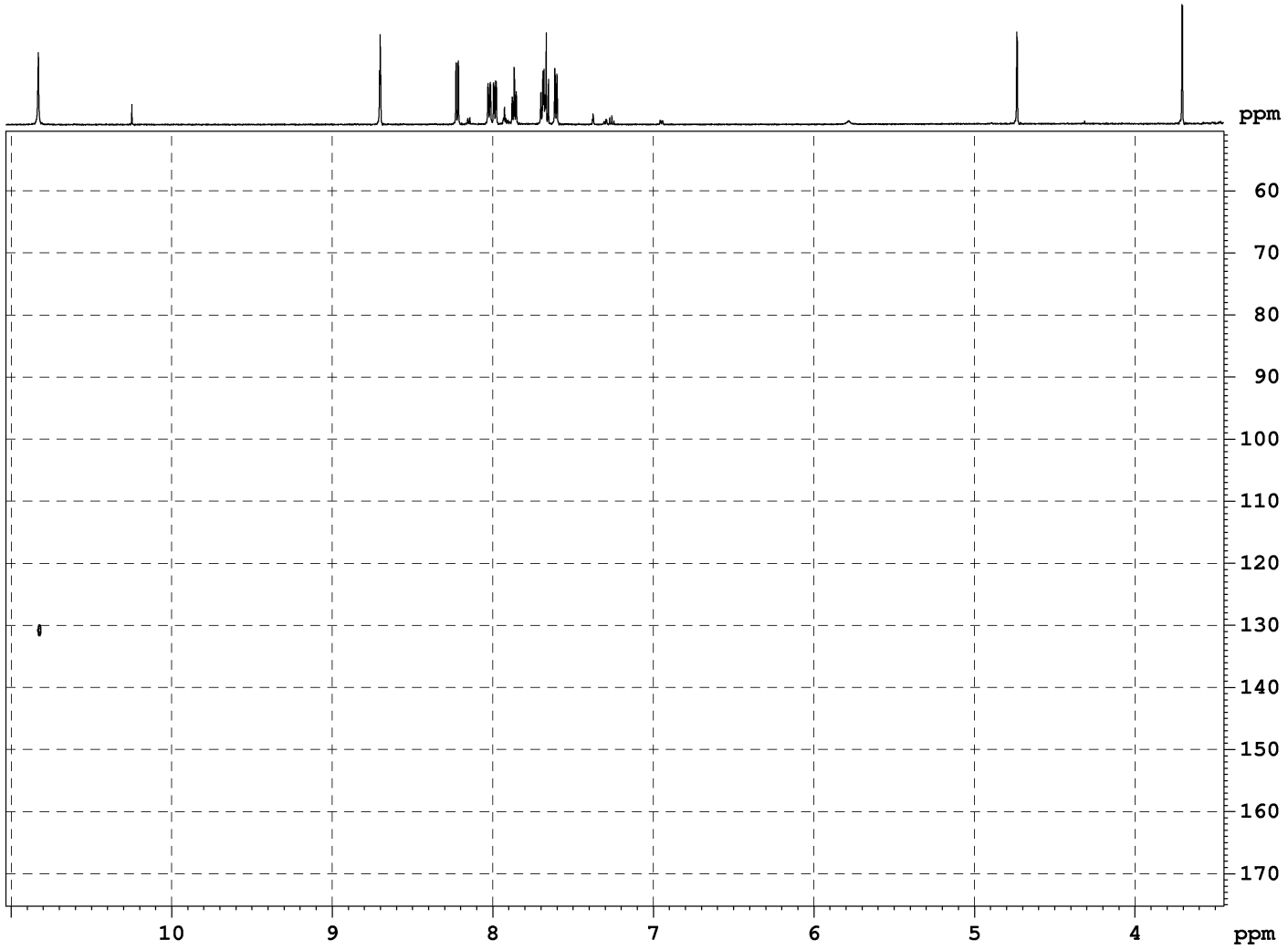



**Figure S38.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **3e** in DMSO at T = 303 K.

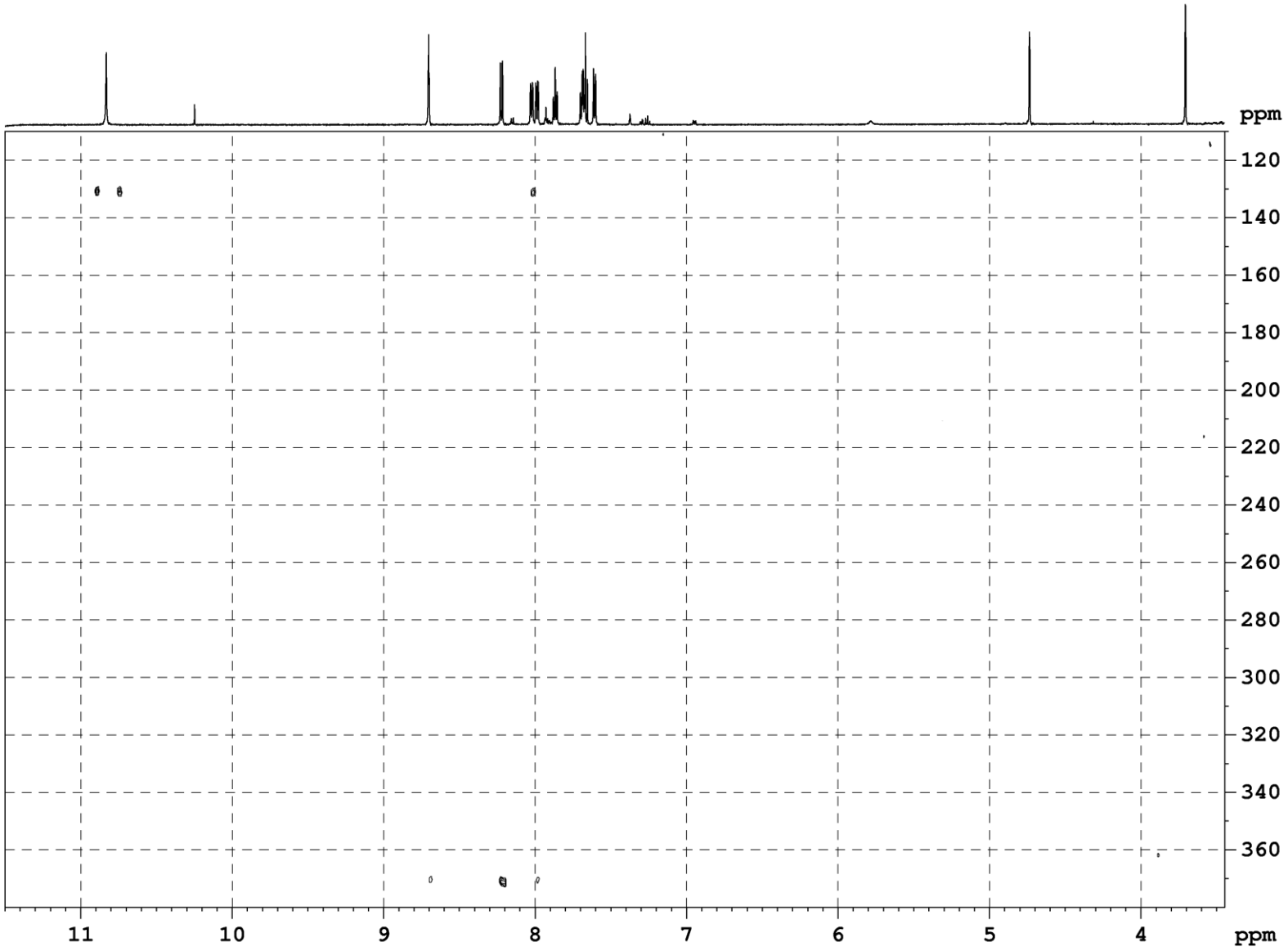



**Figure S39.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **3e** in DMSO at T = 303 K.

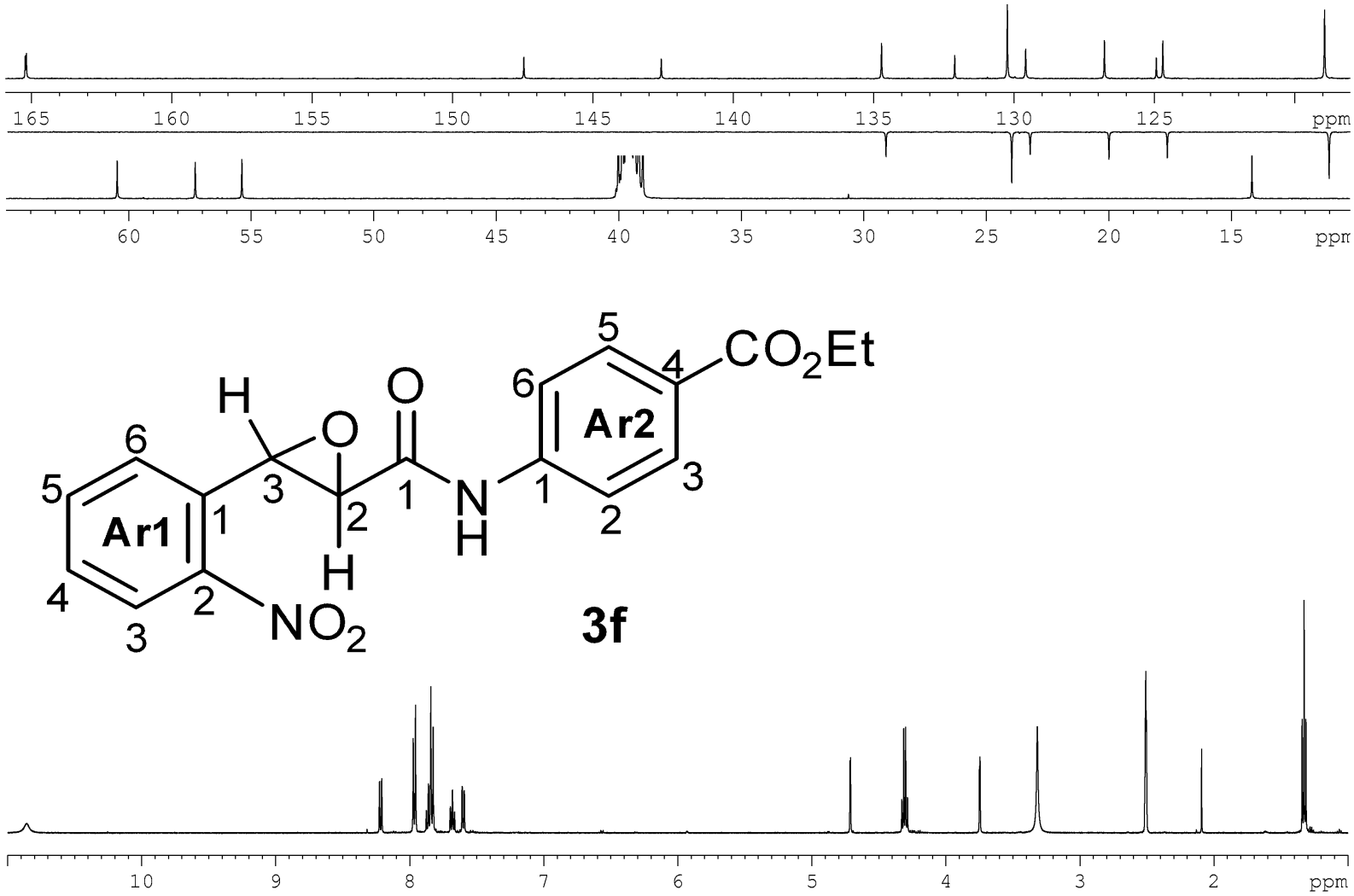



**Figure S40.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **3f** in DMSO at T = 303 K.

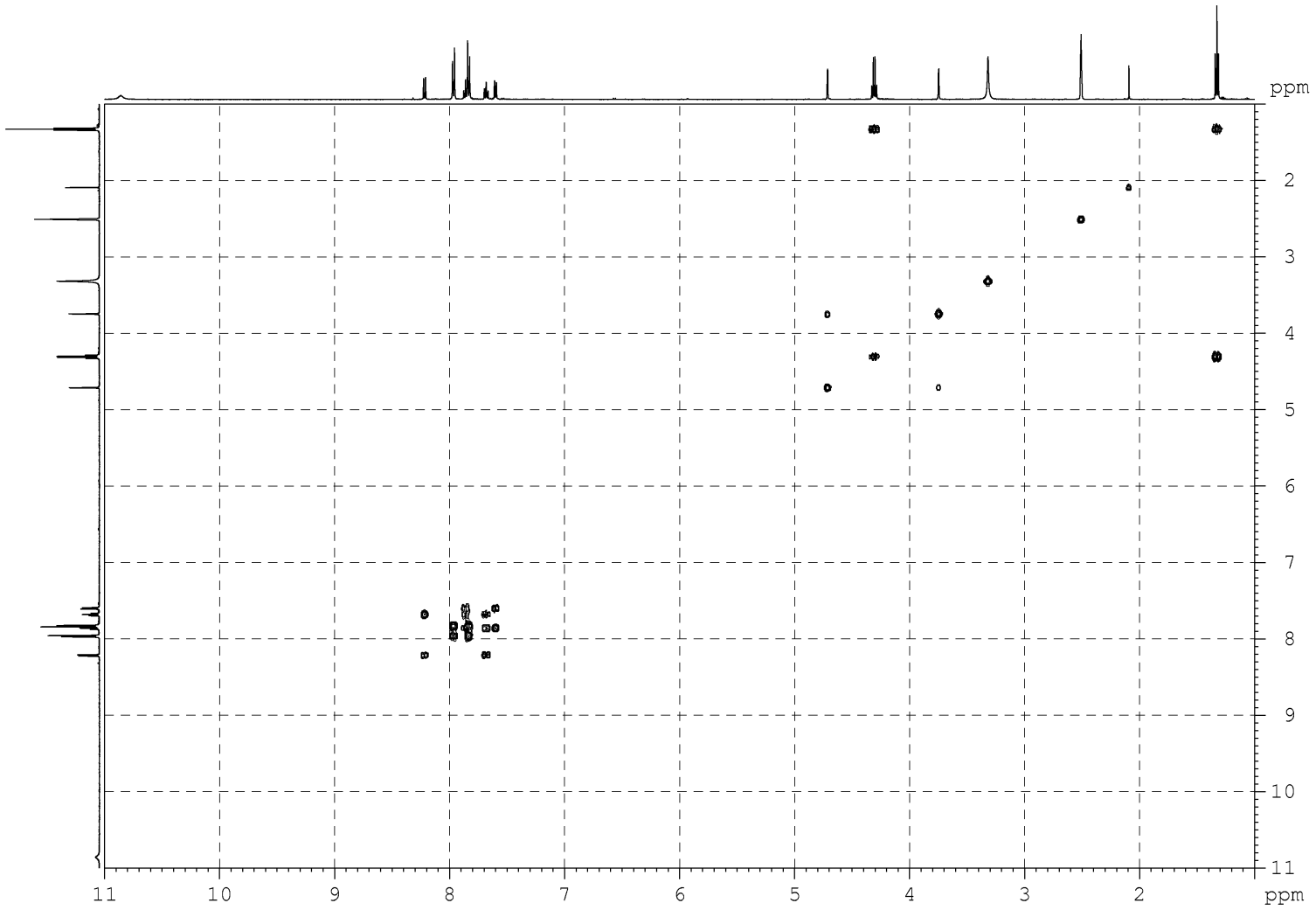



**Figure S41.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **3f** in DMSO at T = 303 K.

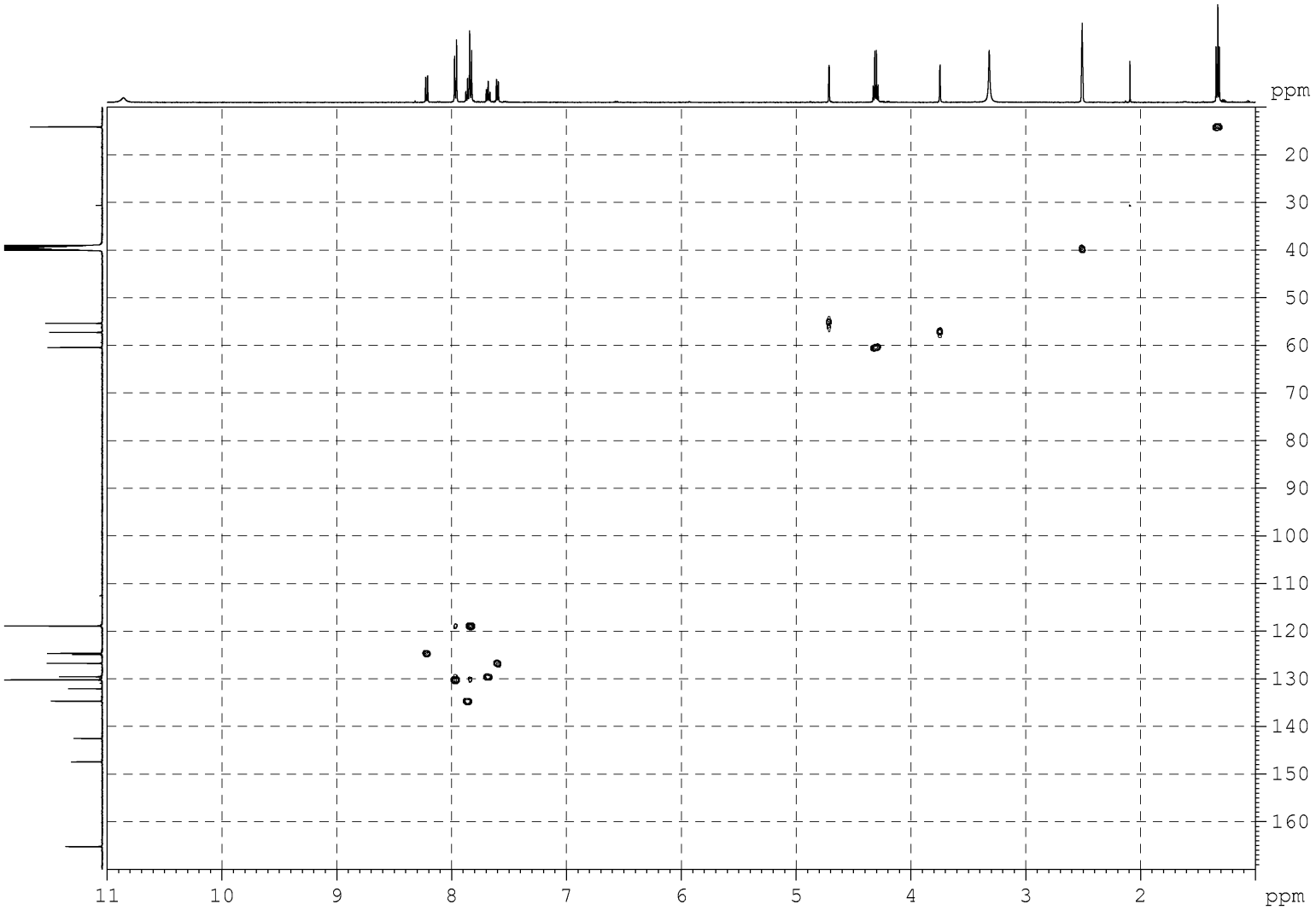



**Figure S42.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **3f** in DMSO at T = 303 K.

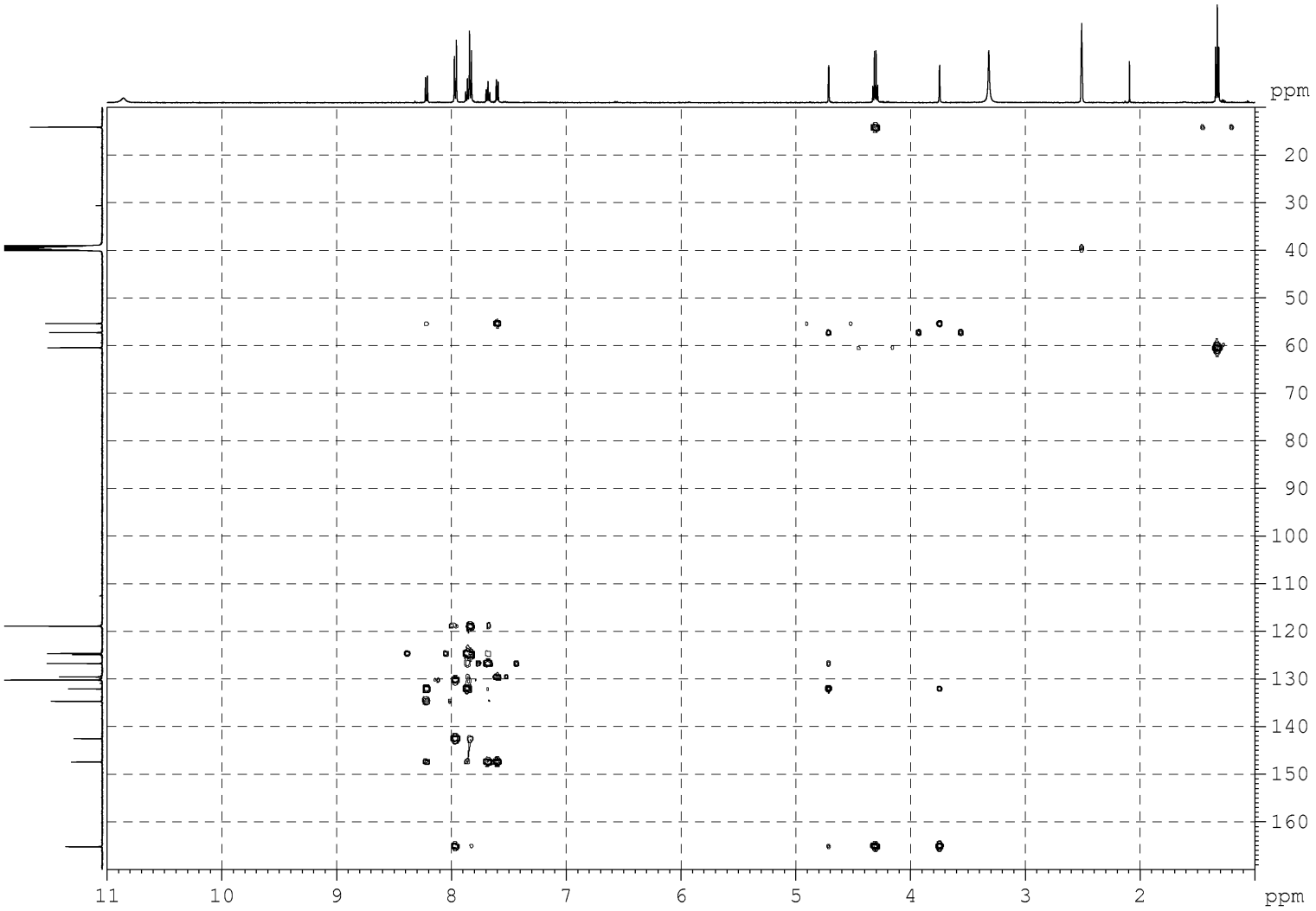



**Figure S43.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **3f** in DMSO at T = 303 K.

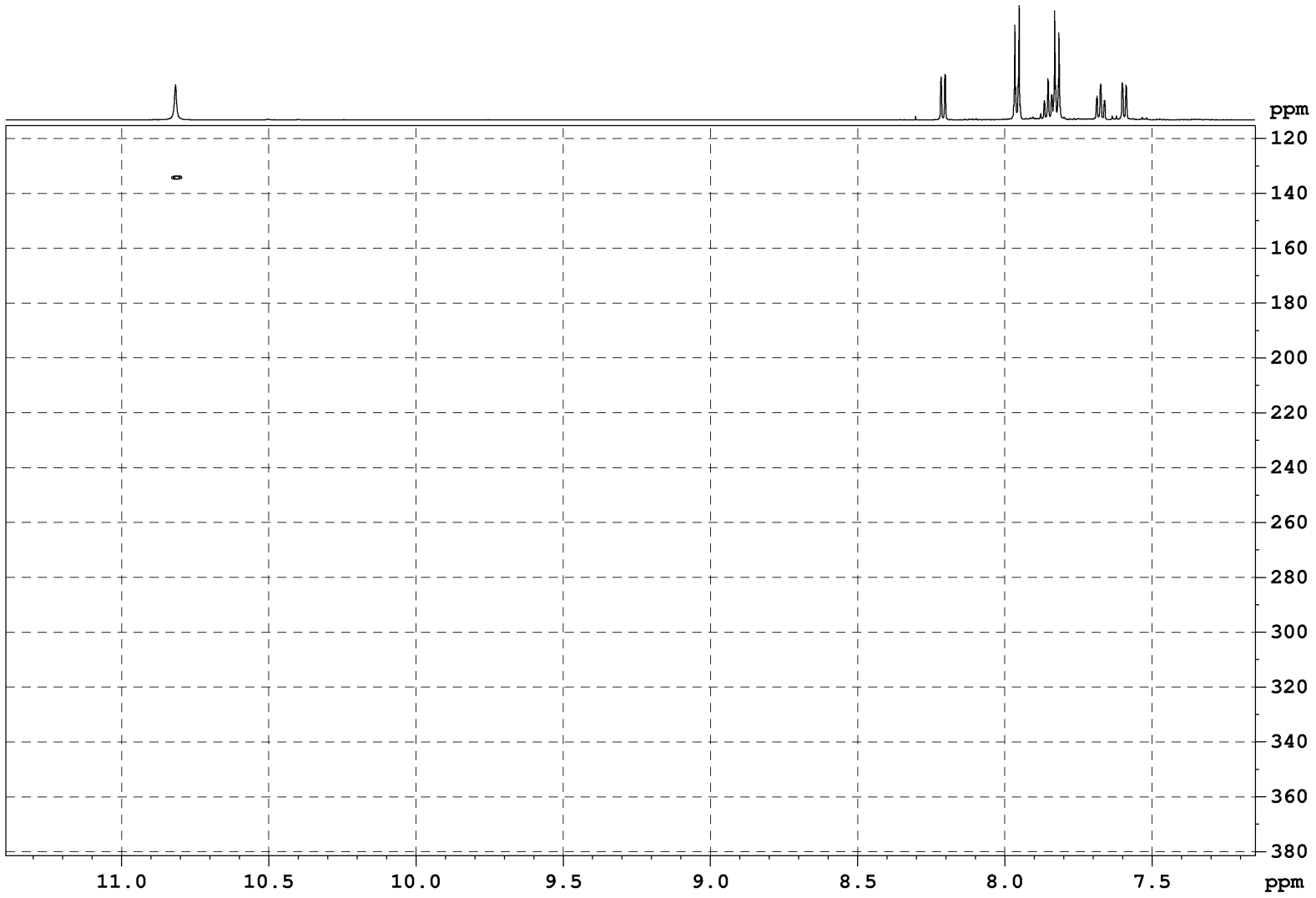



**Figure S44.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **3f** in DMSO at T = 303 K.

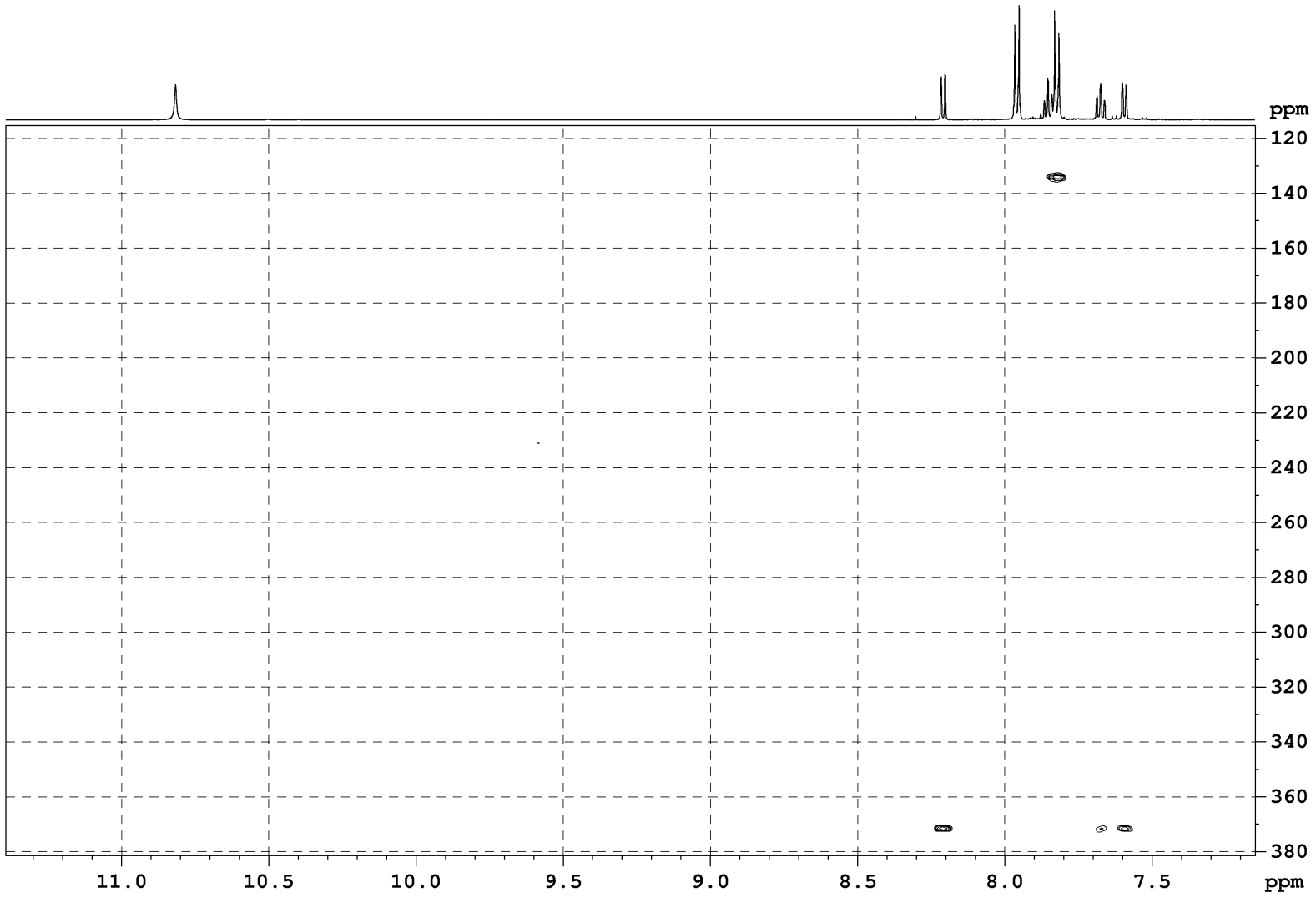



**Figure S45.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **3f** in DMSO at T = 303 K.

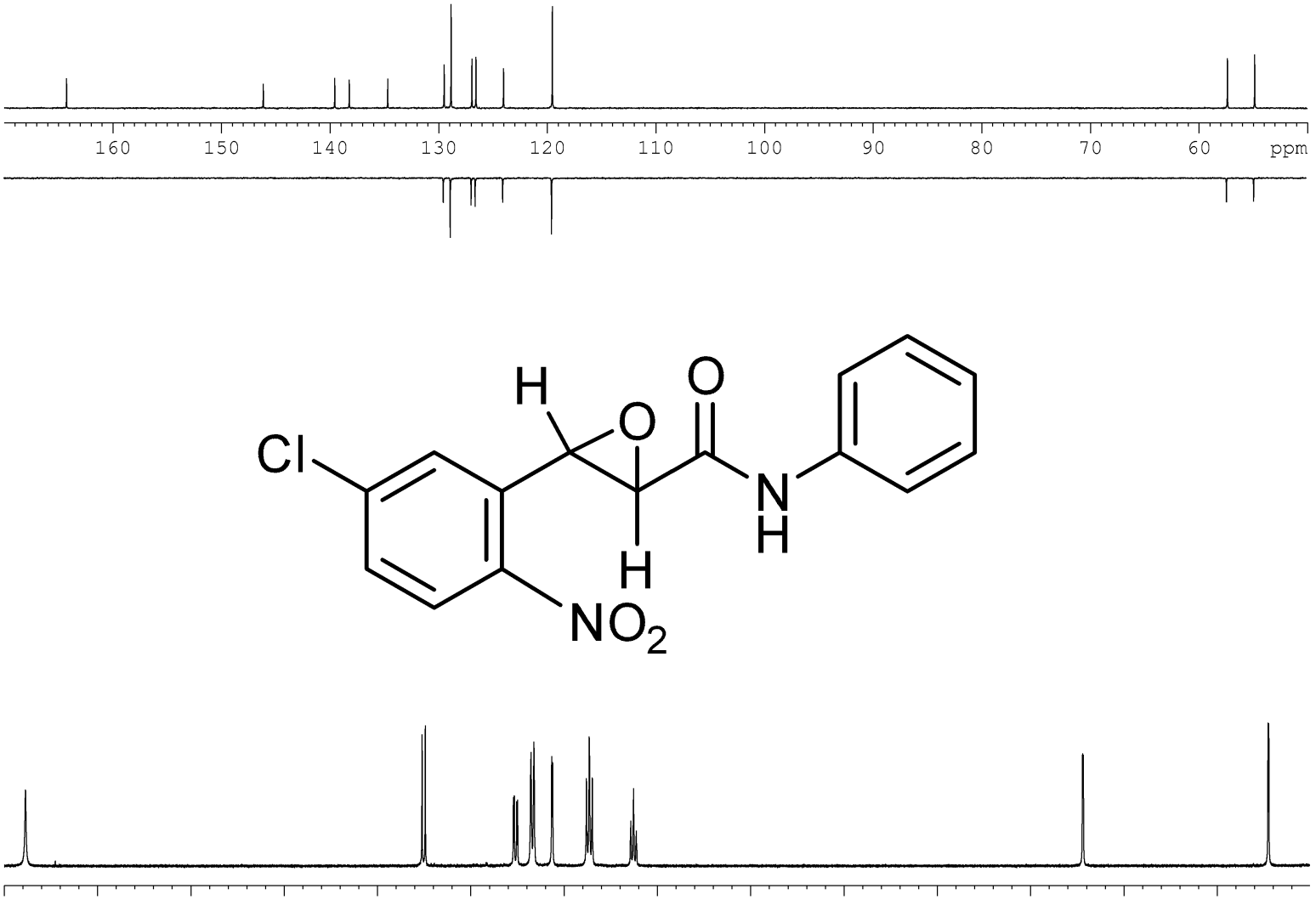



**Figure S46.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **3g** in DMSO at T = 303 K.

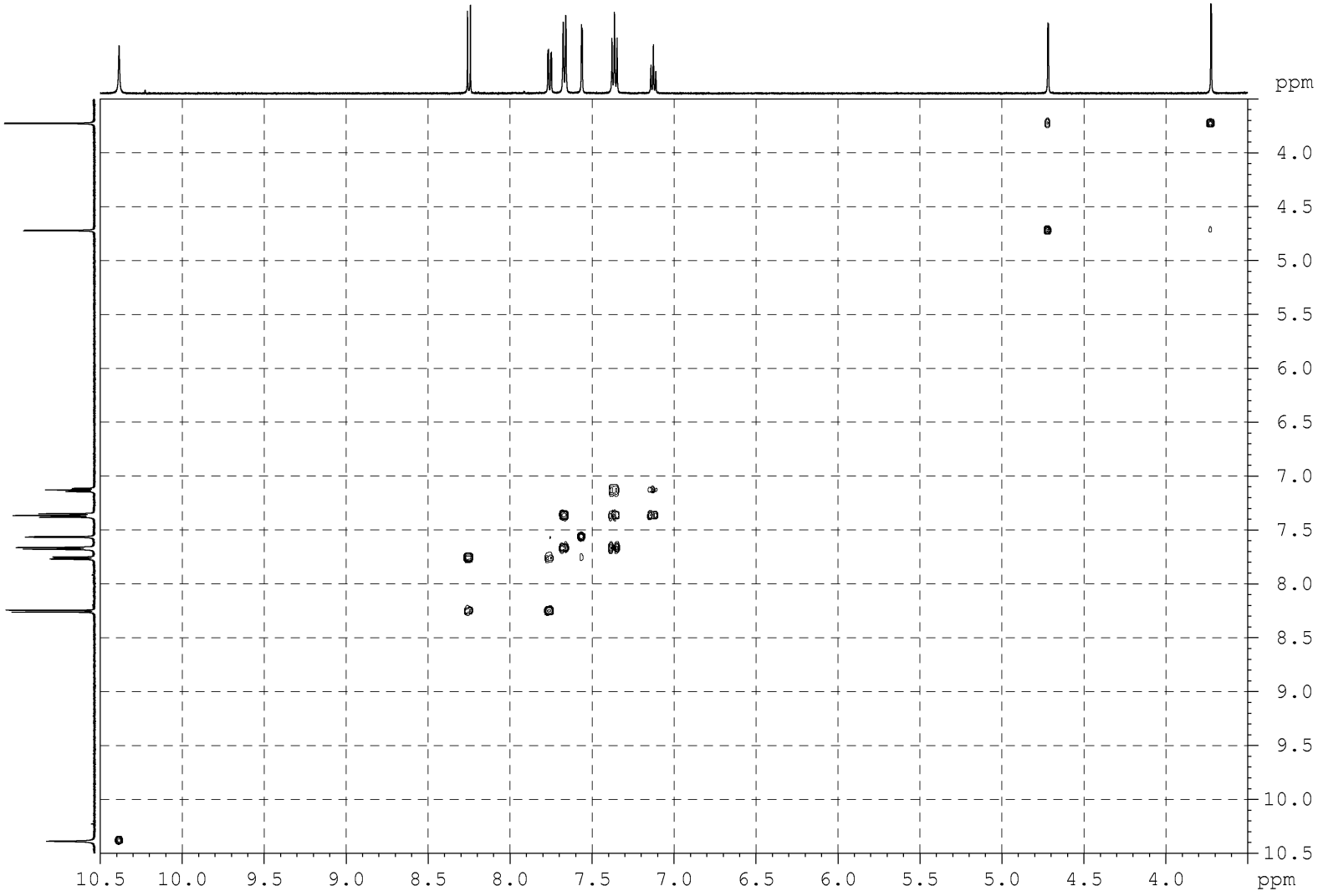



**Figure S47.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **3g** in DMSO at T = 303 K.

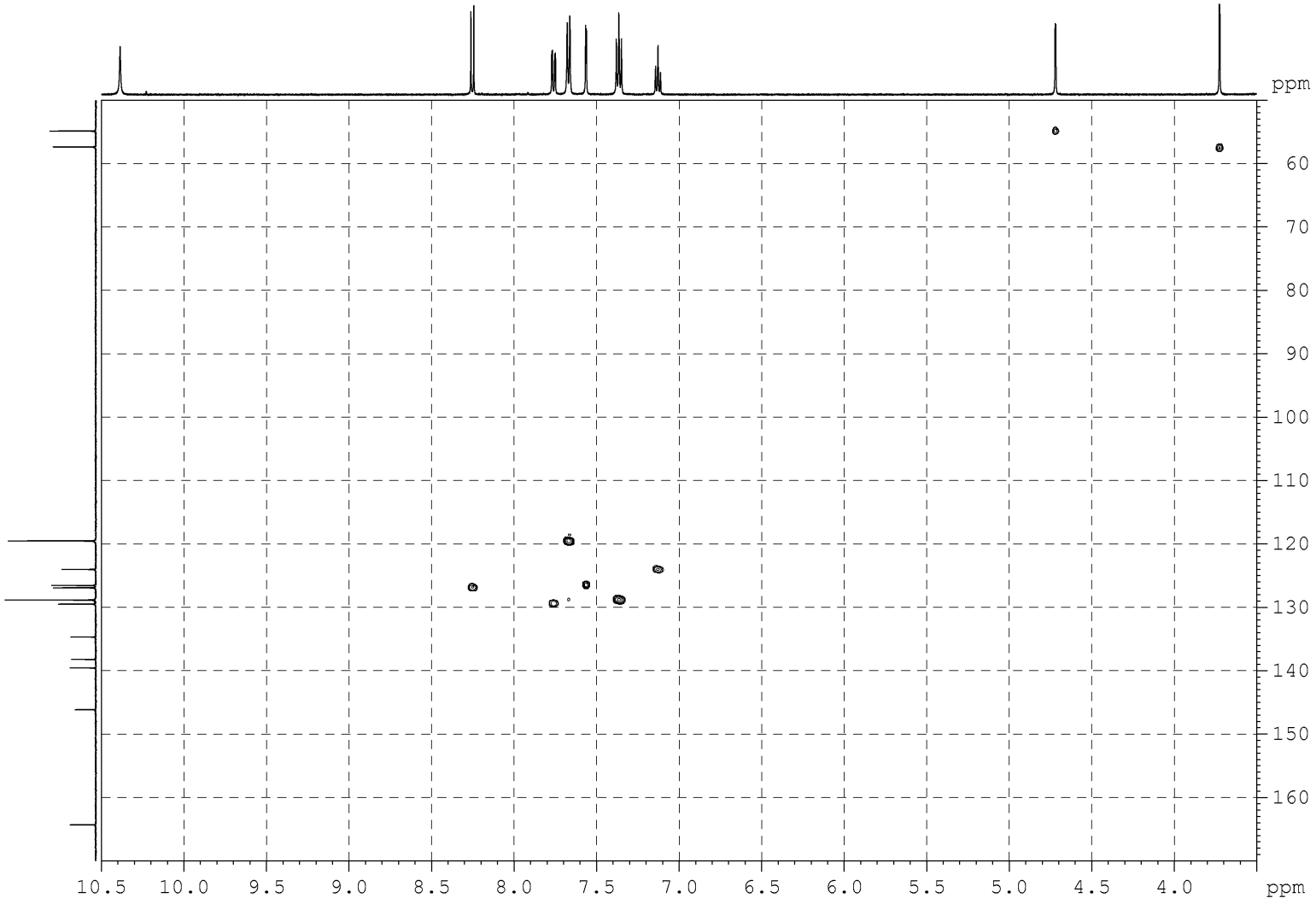



**Figure S48.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **3g** in DMSO at T = 303 K.

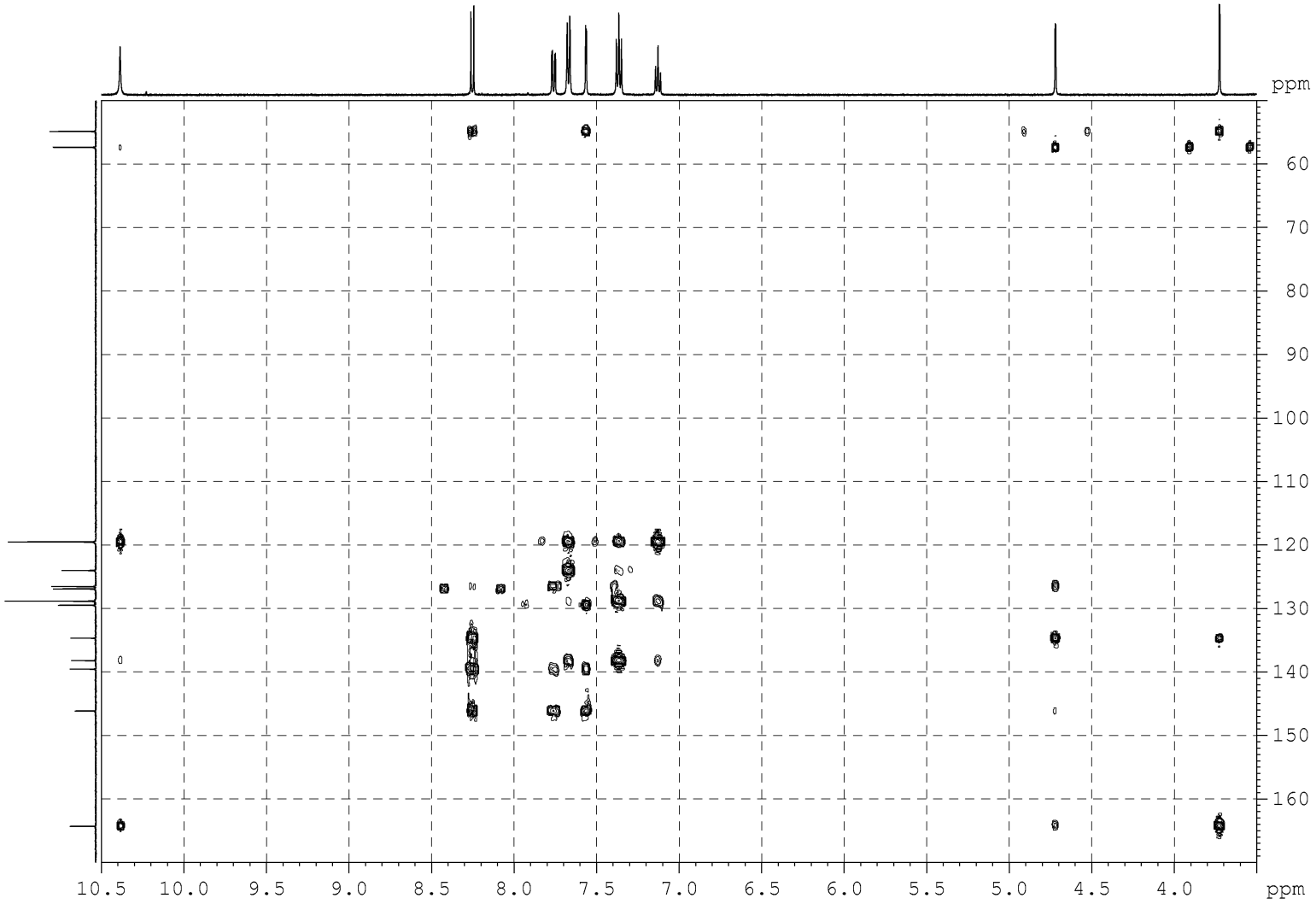



**Figure S49.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **3g** in DMSO at T = 303 K.

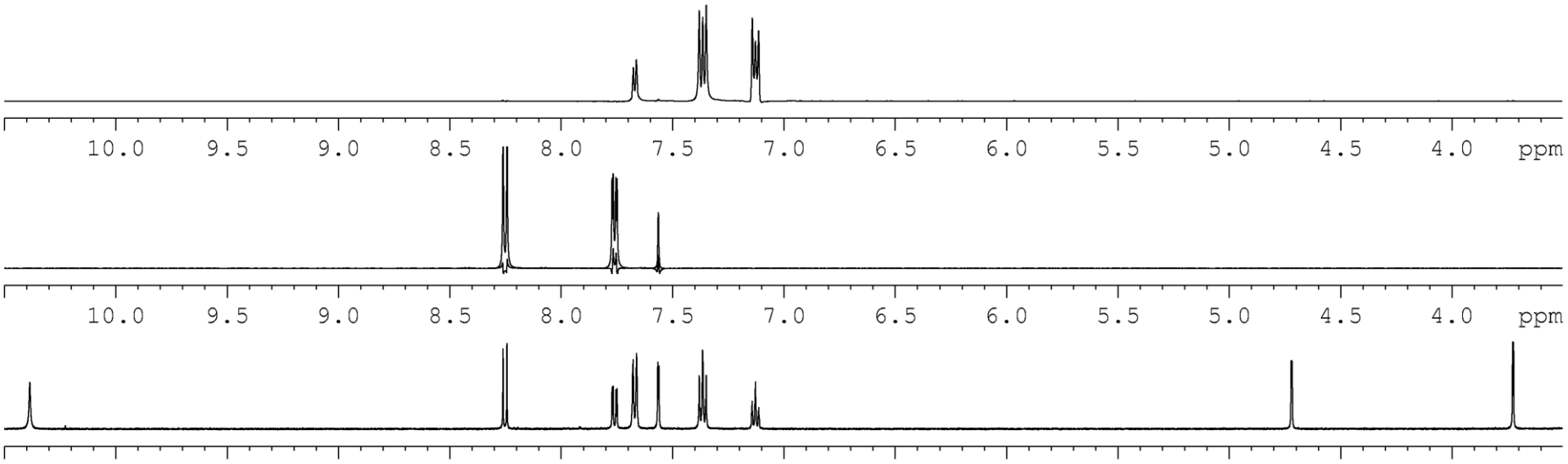



**Figure S50.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **3g** in DMSO at T = 303 K.

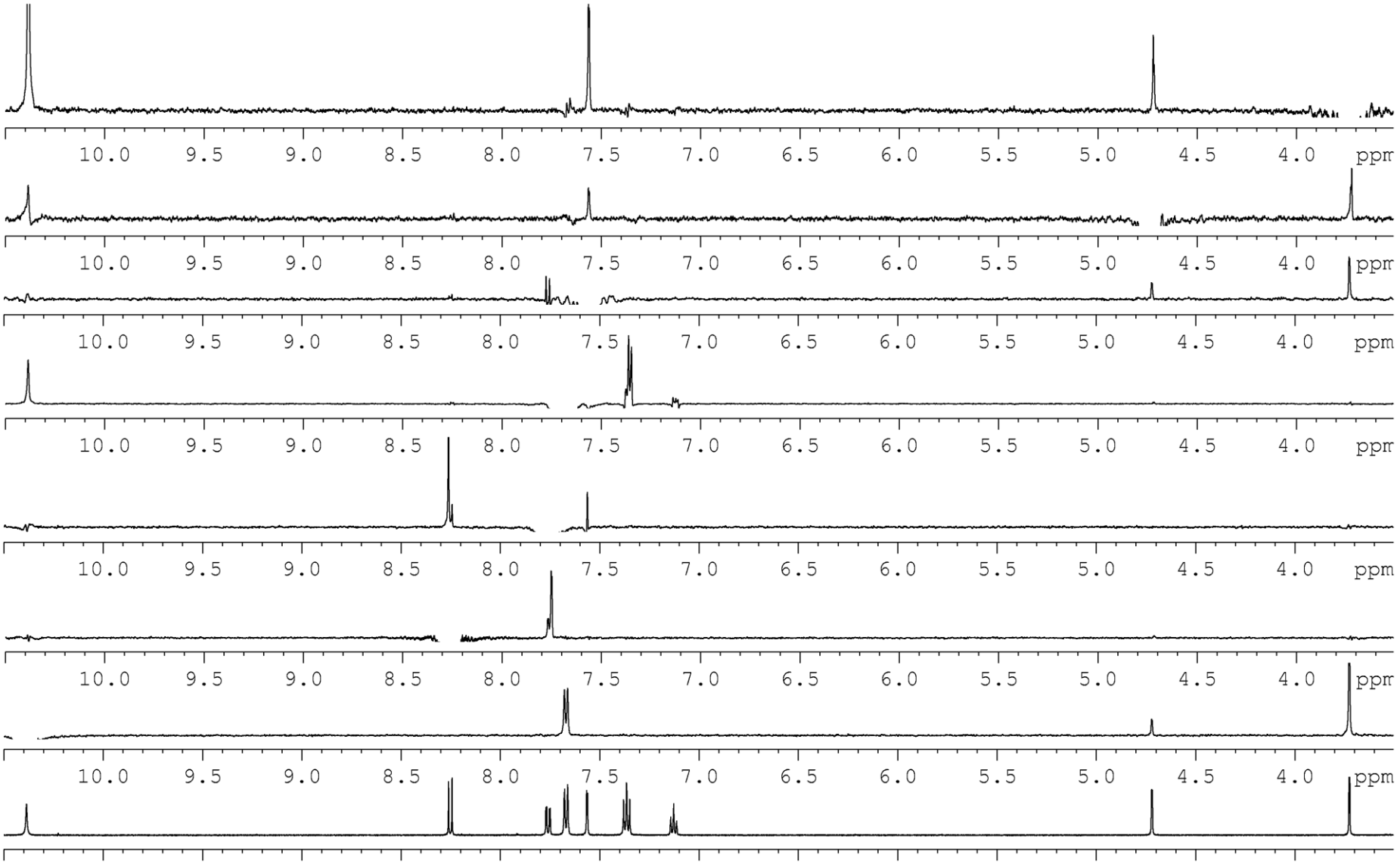



**Figure S51.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **3g** in DMSO at T = 303 K.

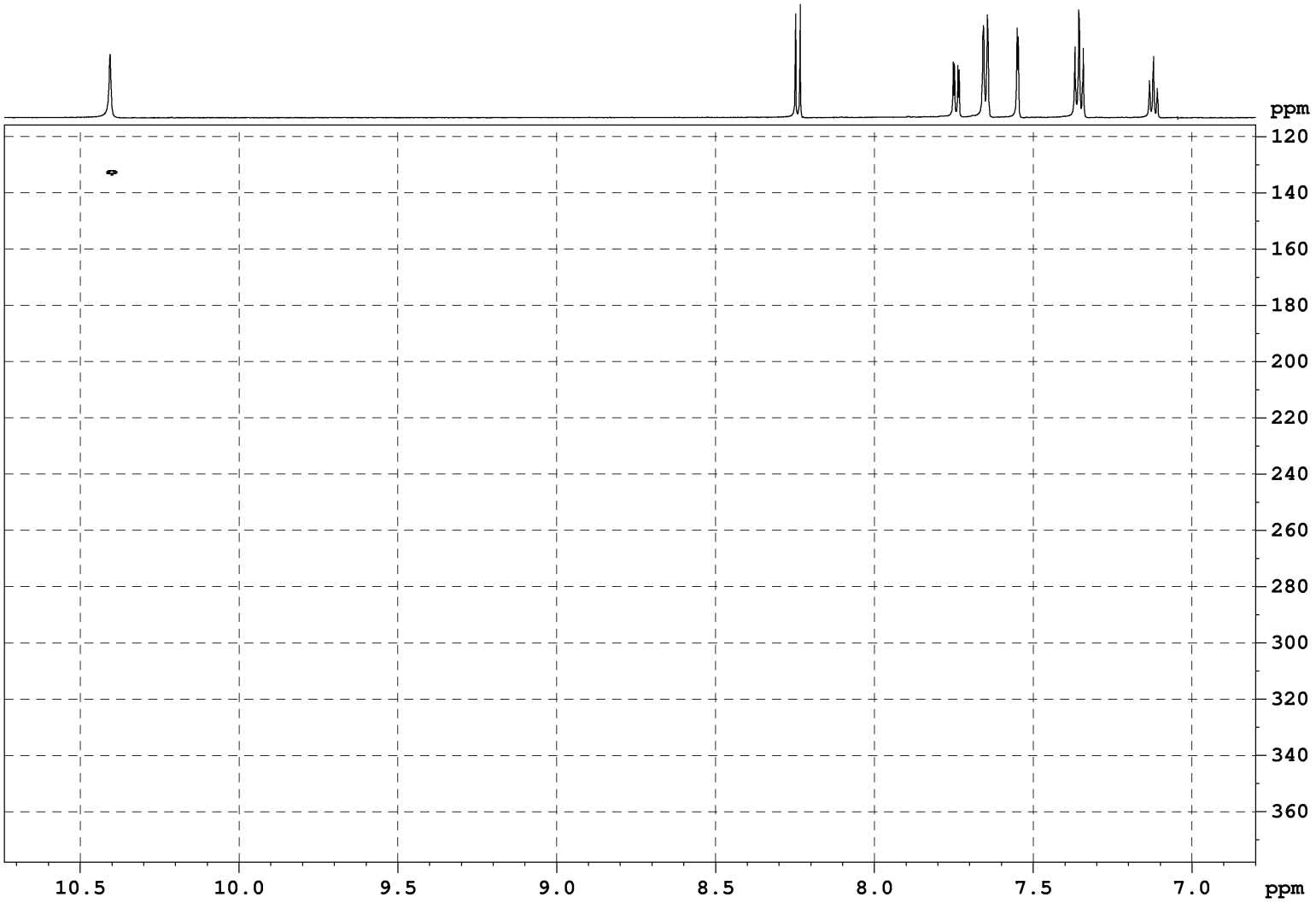



**Figure S52.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **3g** in DMSO at T = 303 K.

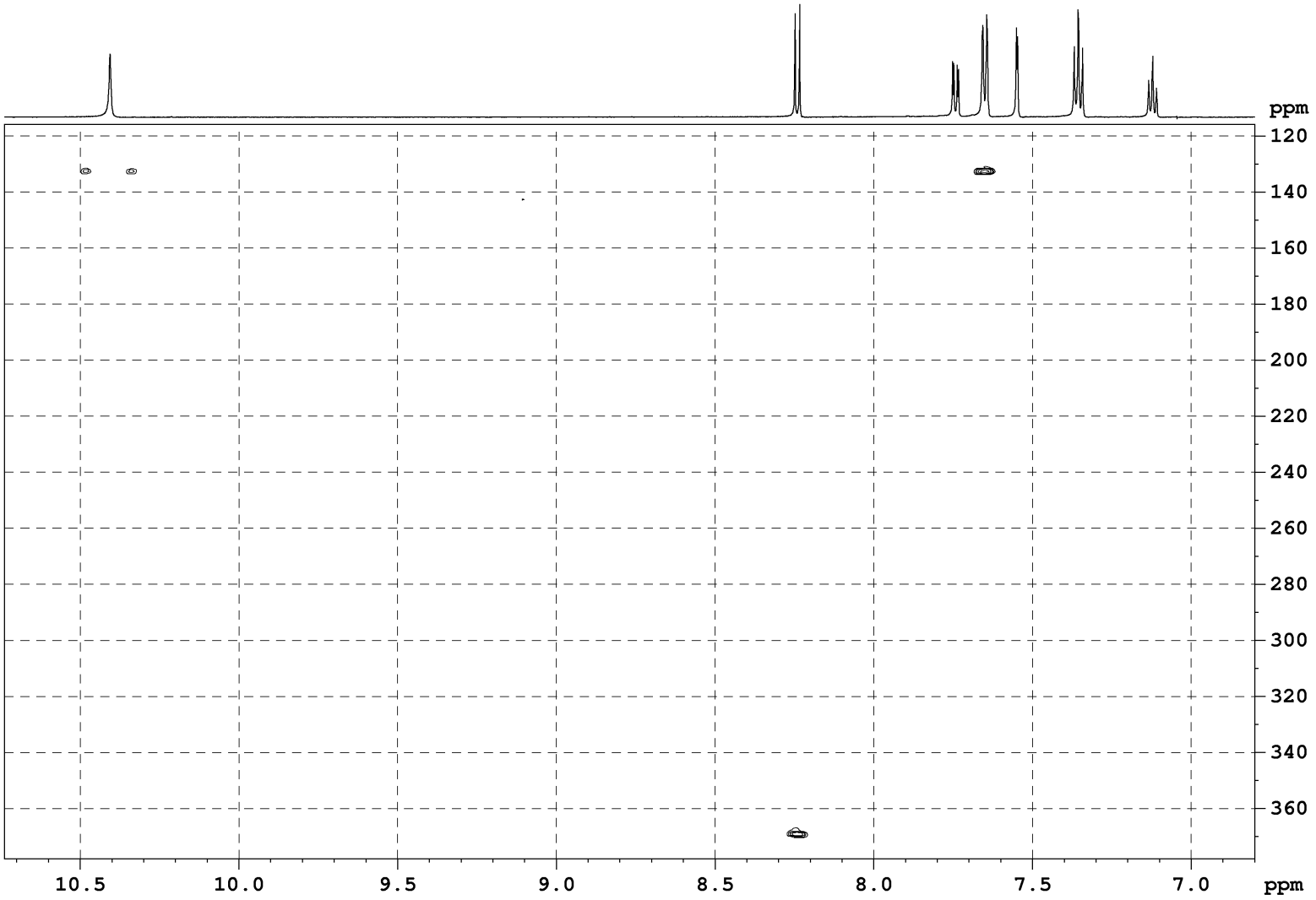



**Figure S53.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **3g** in DMSO at T = 303 K.

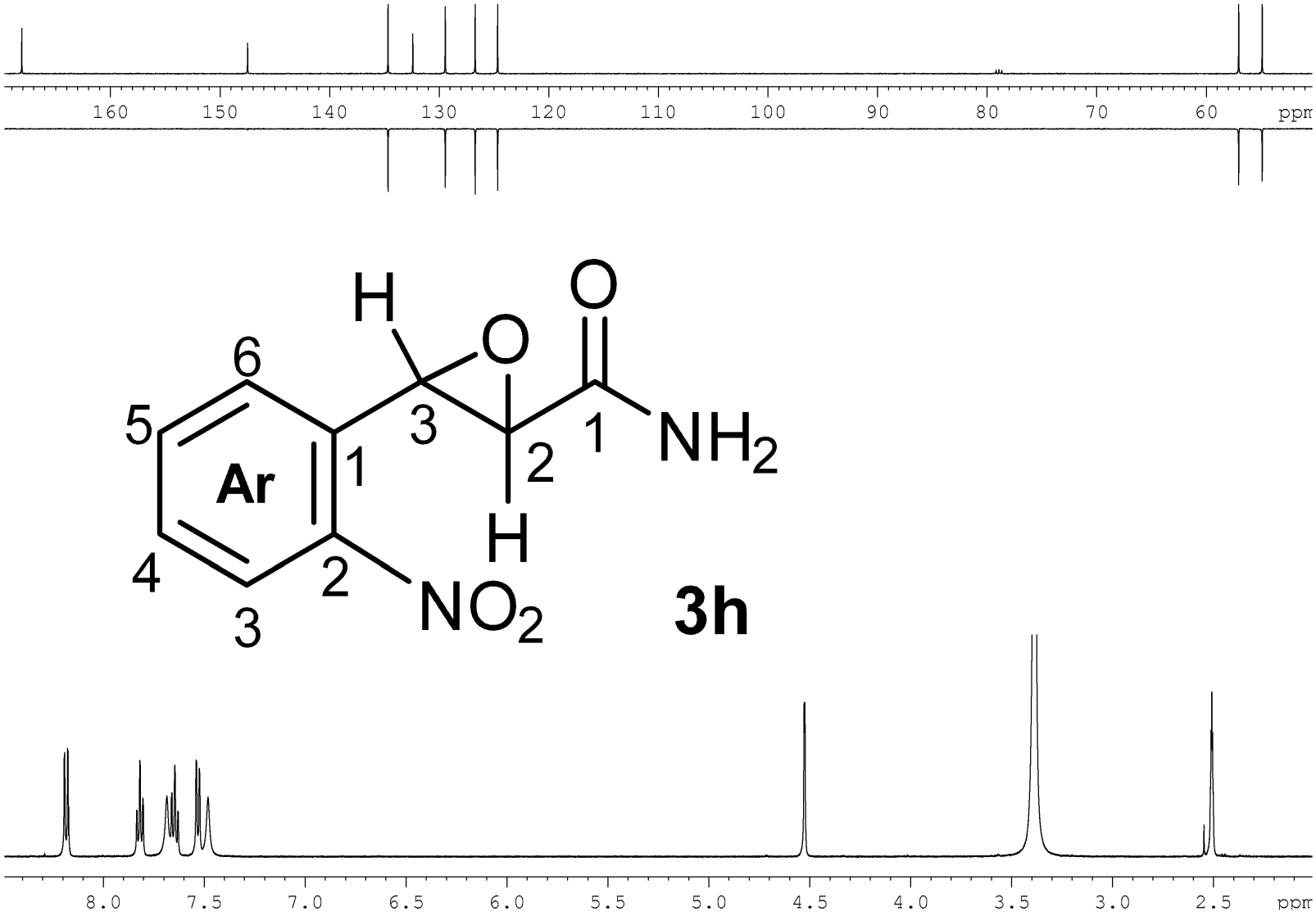



**Figure S54.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **3h** in DMSO at T = 303 K.

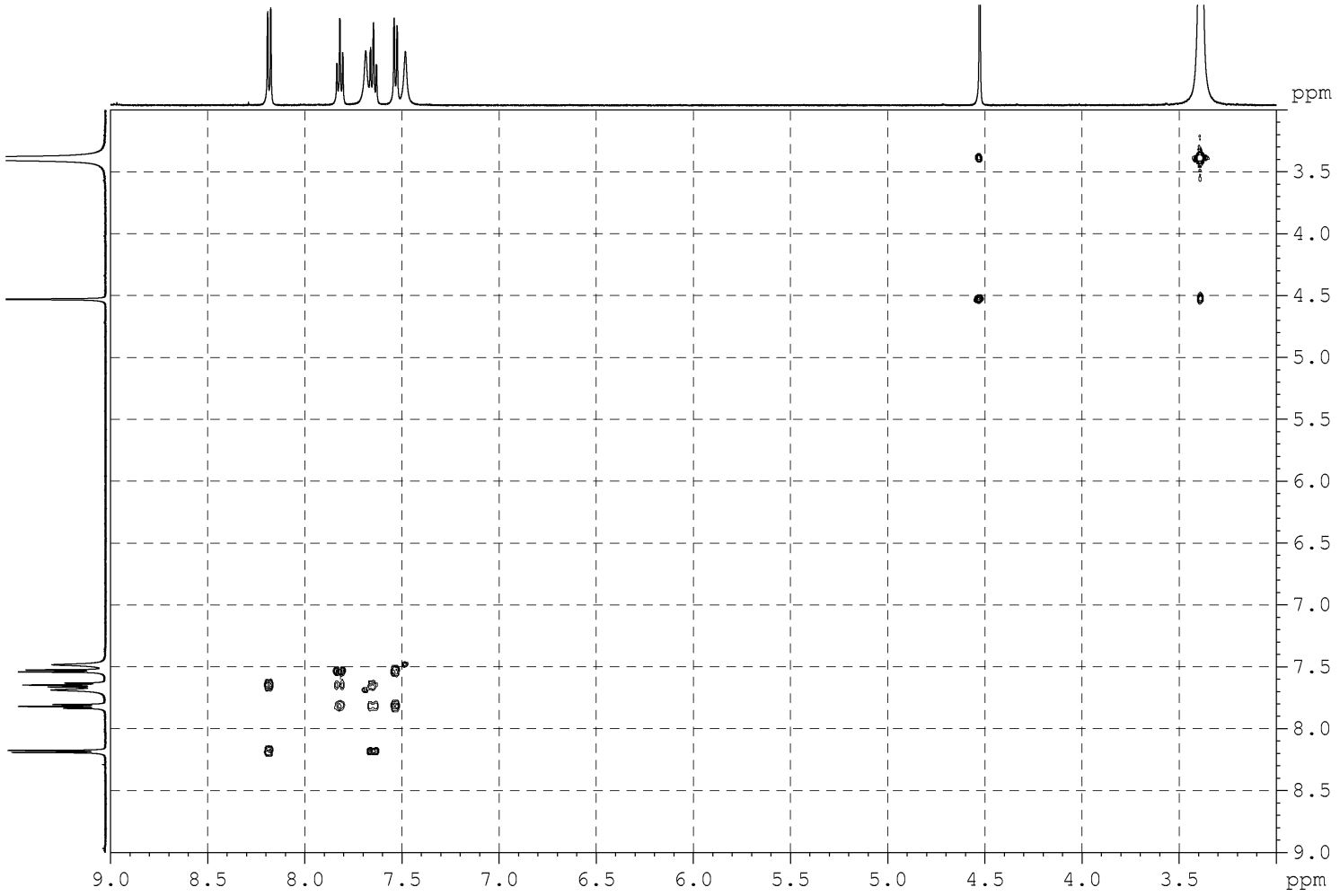



**Figure S55.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **3h** in DMSO at T = 303 K.

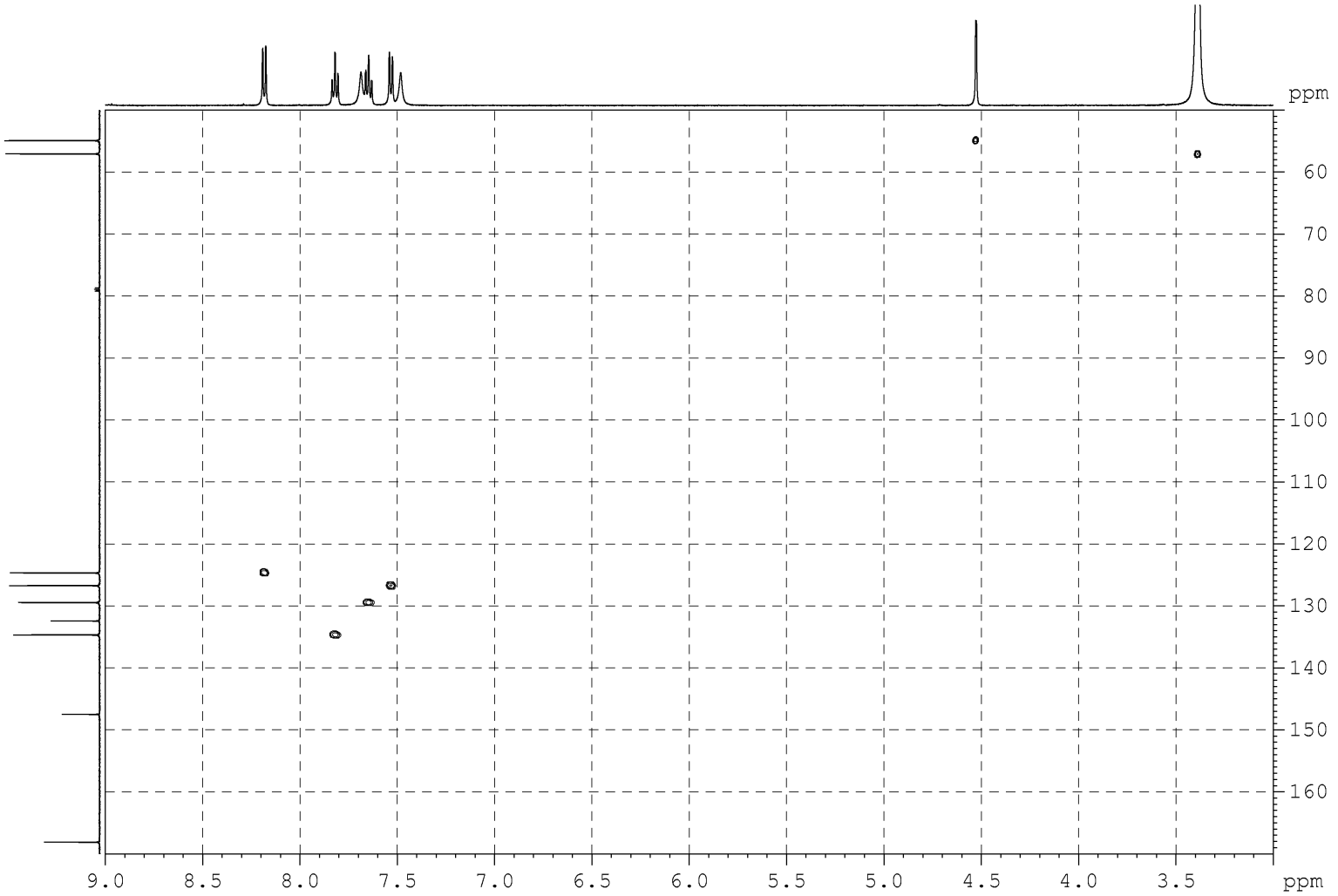



**Figure S56.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **3h** in DMSO at T = 303 K.

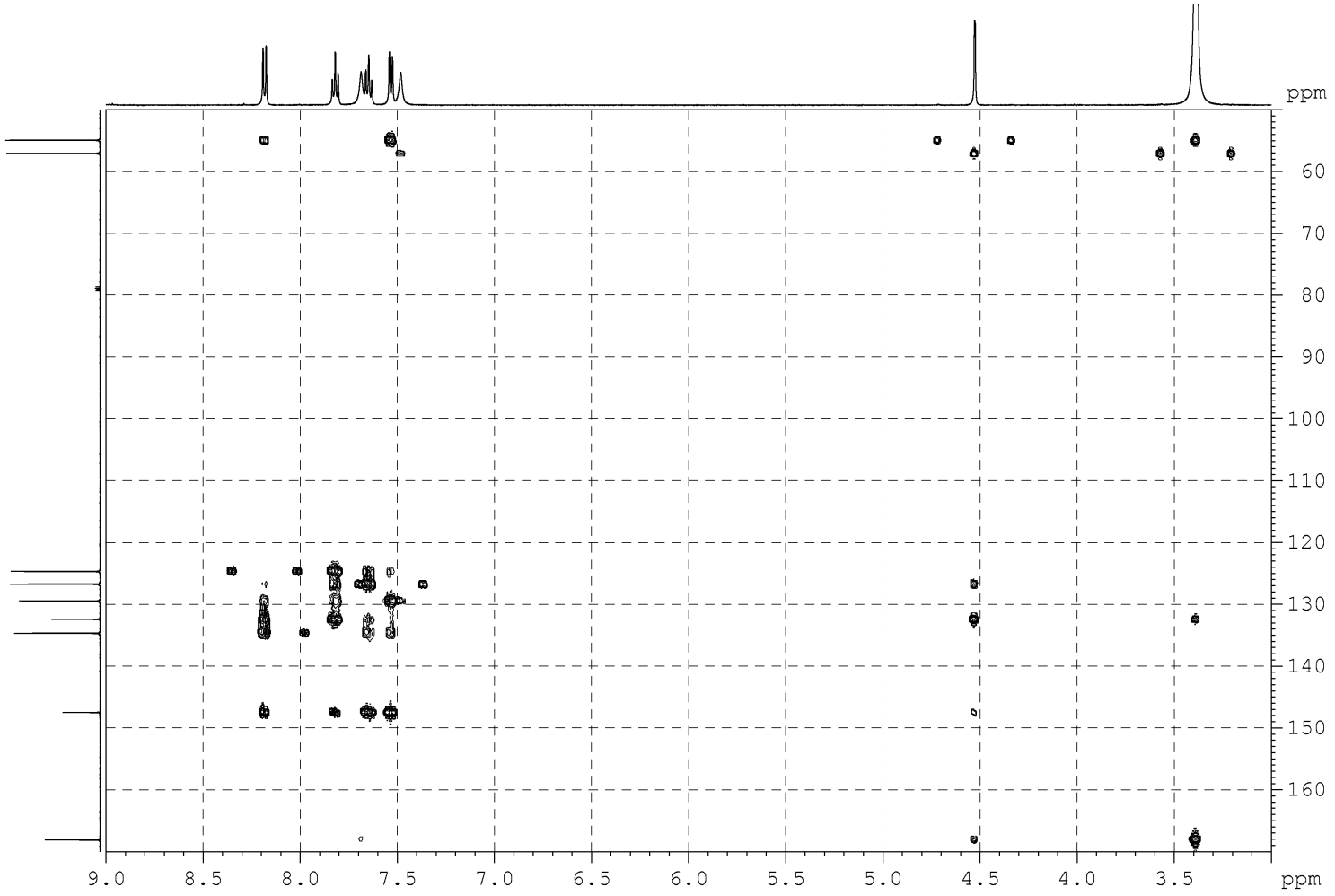



**Figure S57.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **3h** in DMSO at T = 303 K.

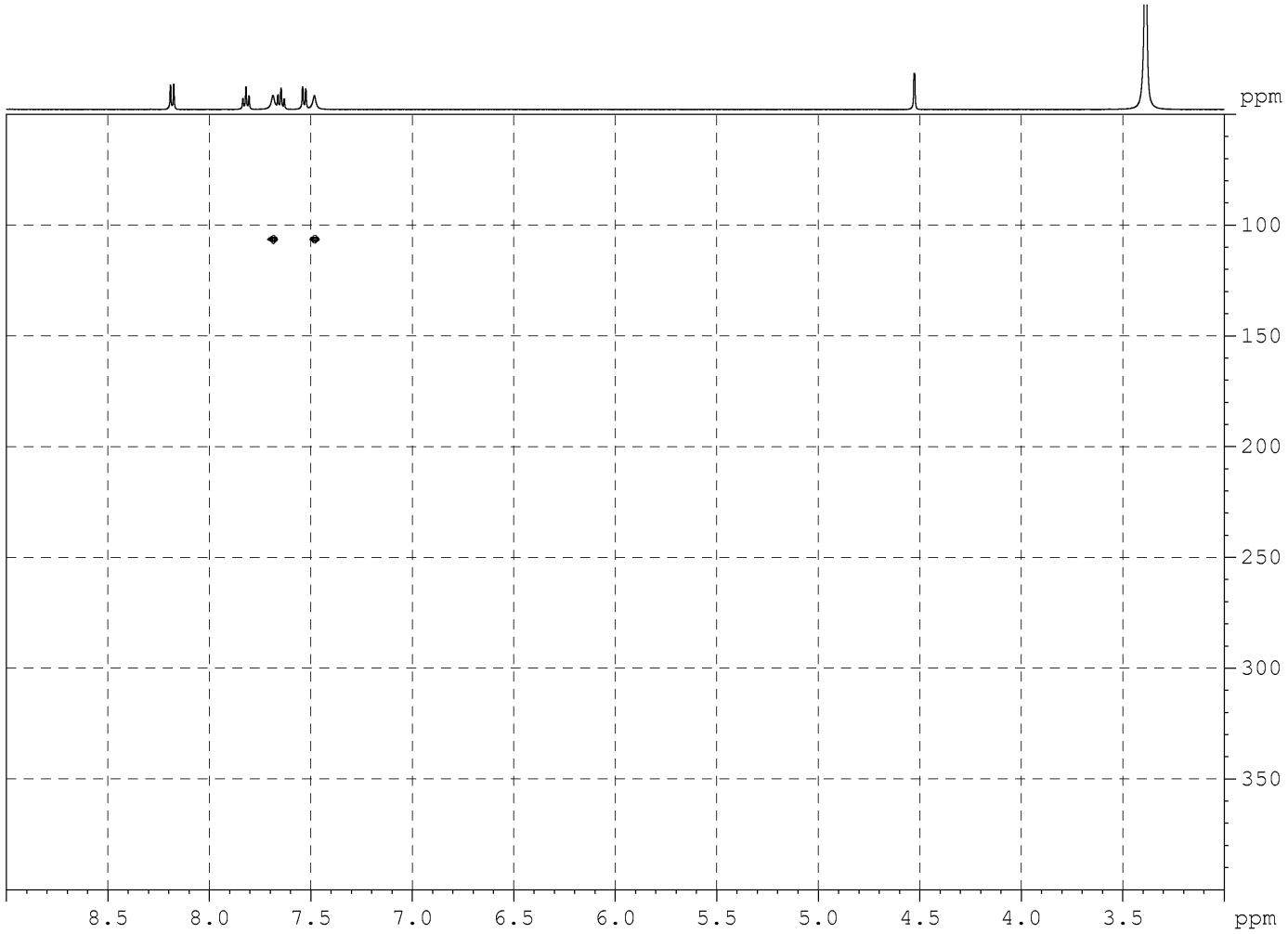



**Figure S58.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **3h** in DMSO at T = 303 K.

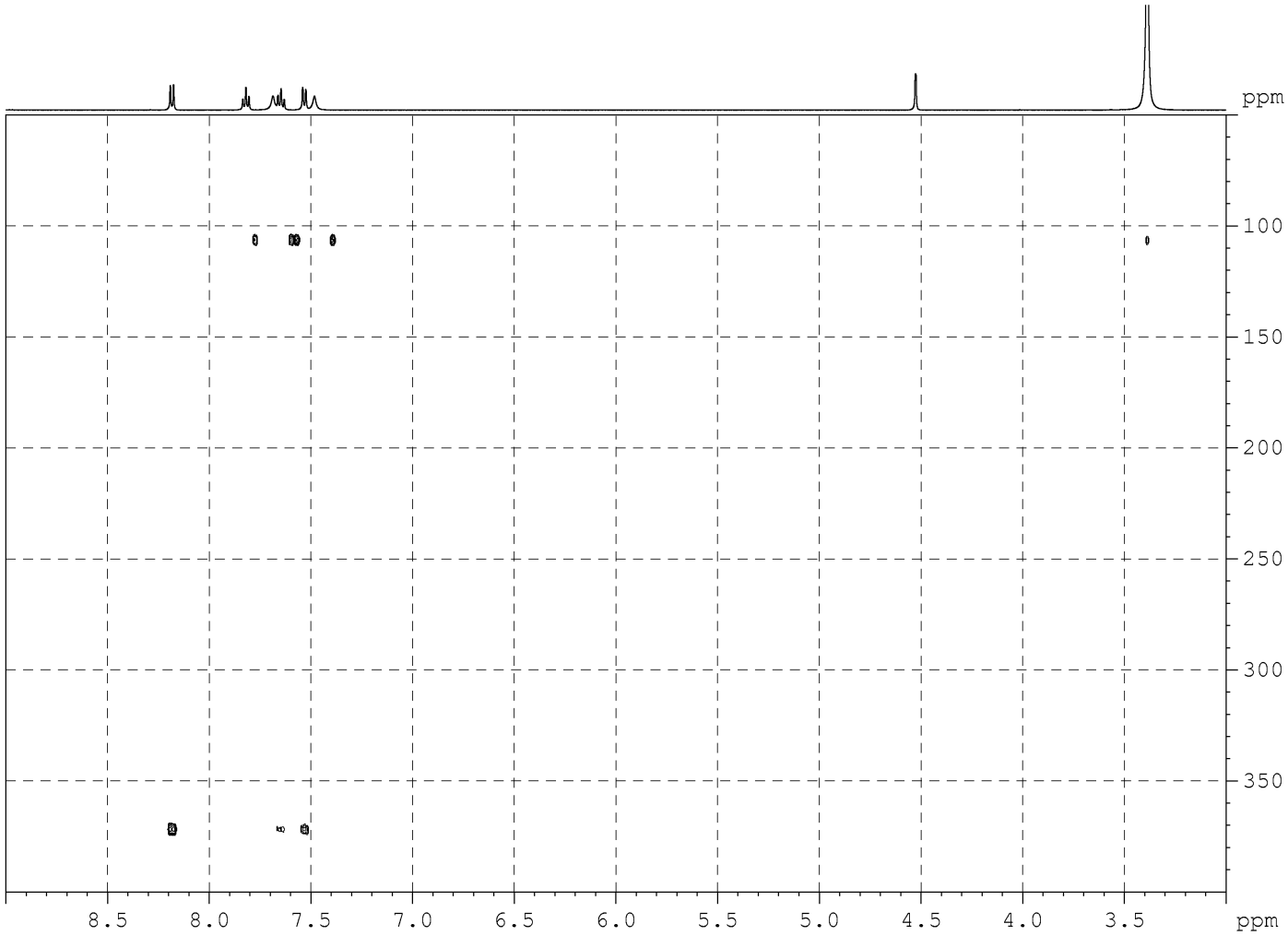



**Figure S59.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **3h** in DMSO at T = 303 K.

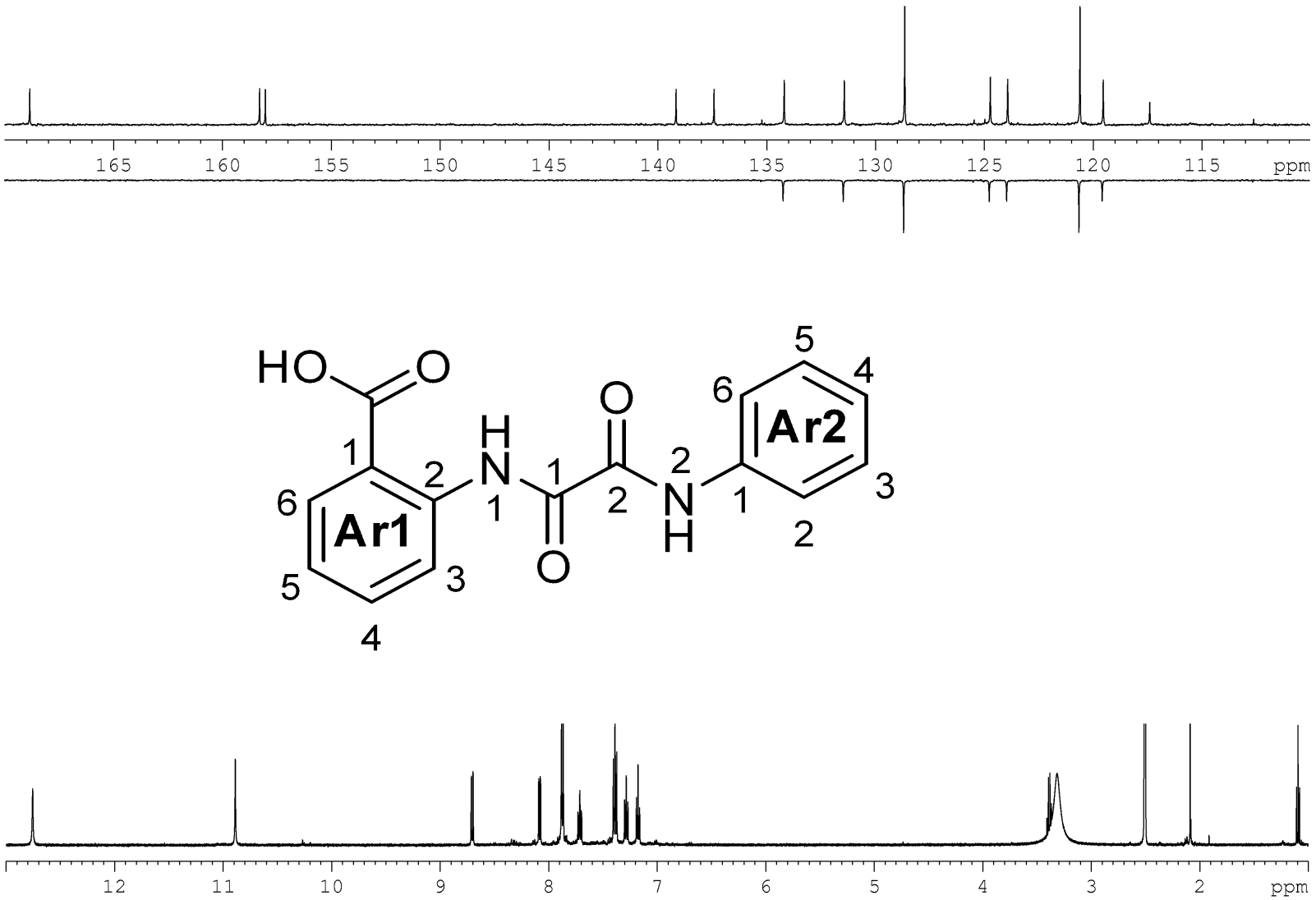



**Figure S60.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **4a** in DMSO at T = 303 K.

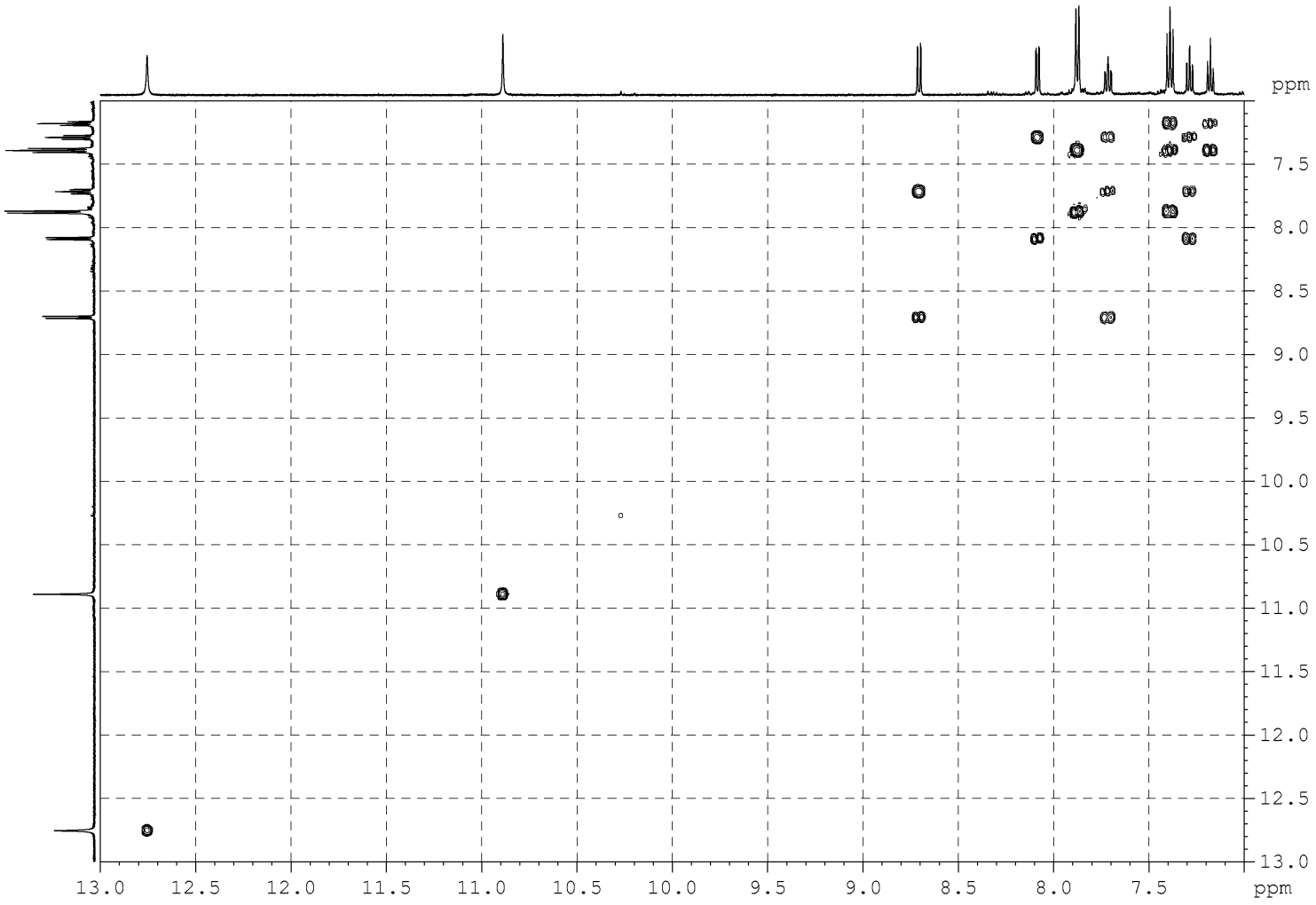



**Figure S61.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **4a** in DMSO at T = 303 K.

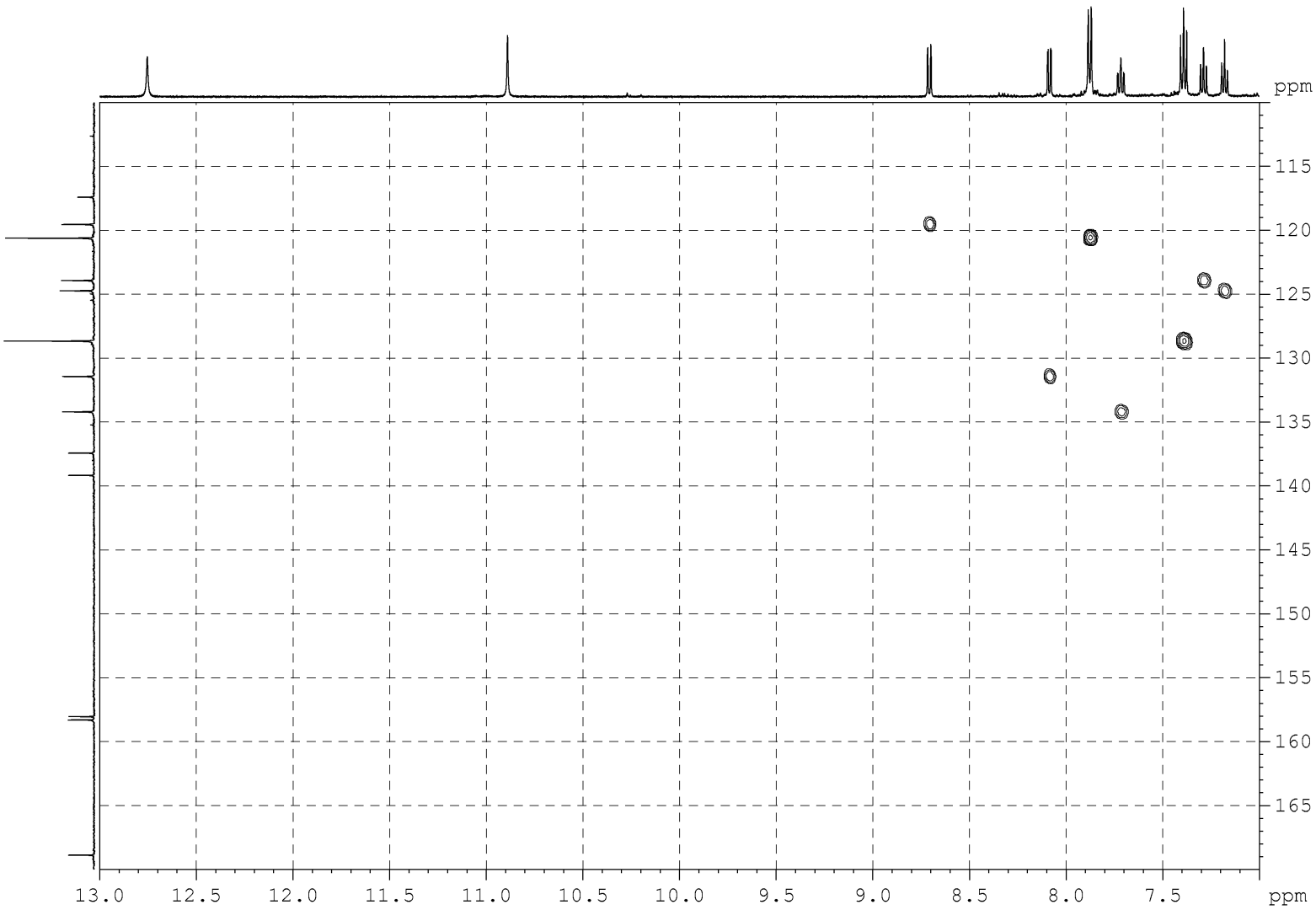



**Figure S62.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **4a** in DMSO at T = 303 K.

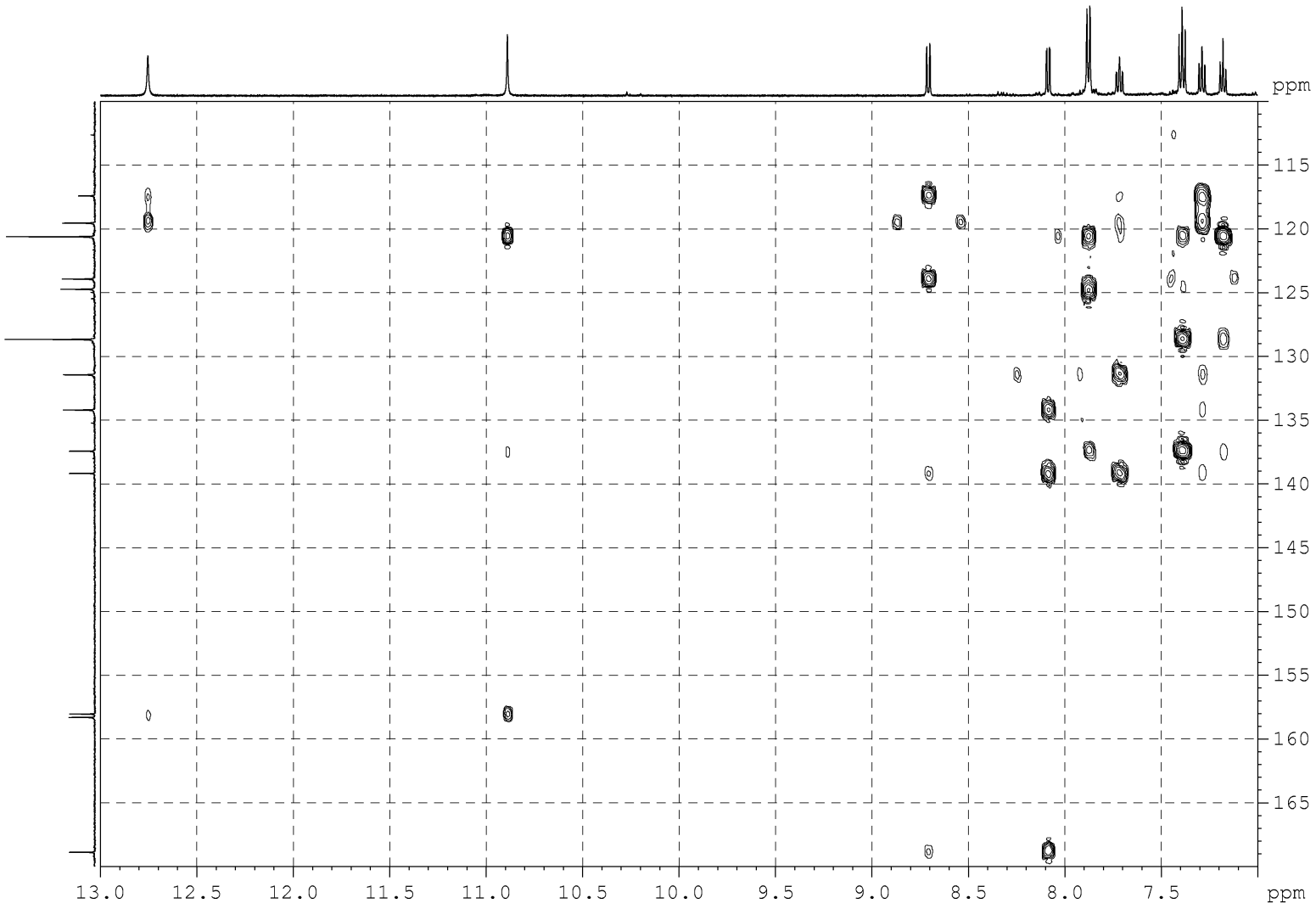



**Figure S63.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **4a** in DMSO at T = 303 K.

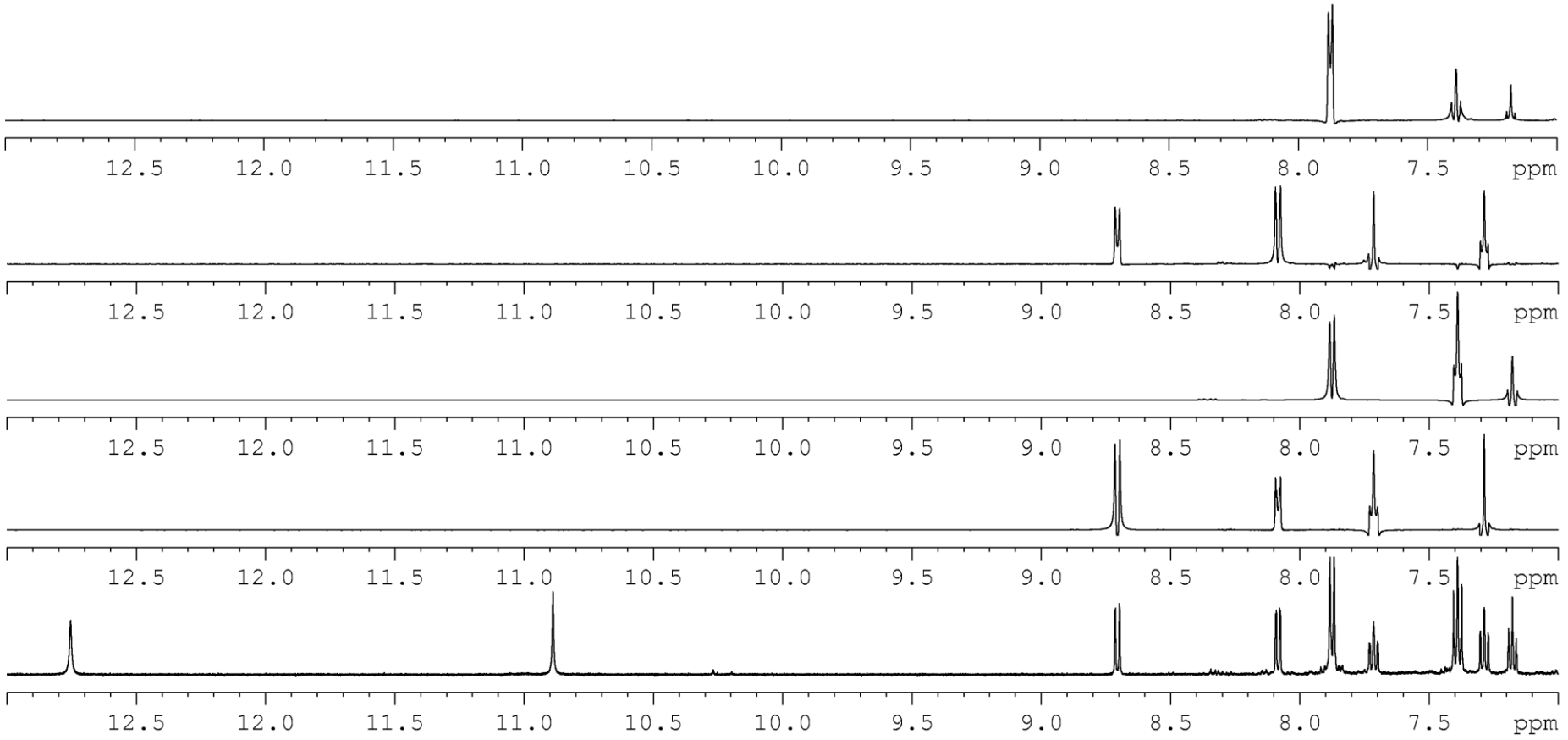



**Figure S64.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **4a** in DMSO at T = 303 K.

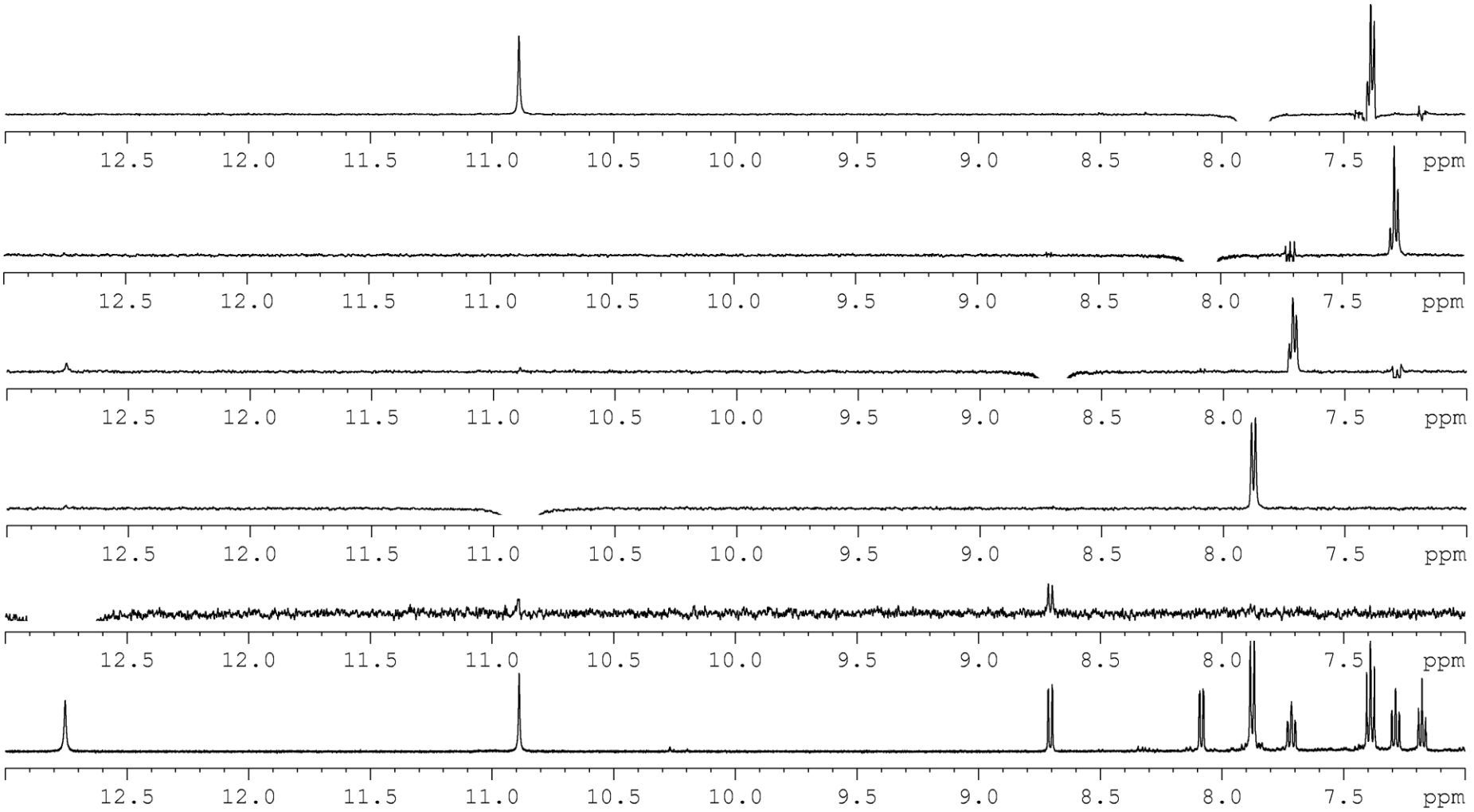



**Figure S65.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **4a** in DMSO at T = 303 K.

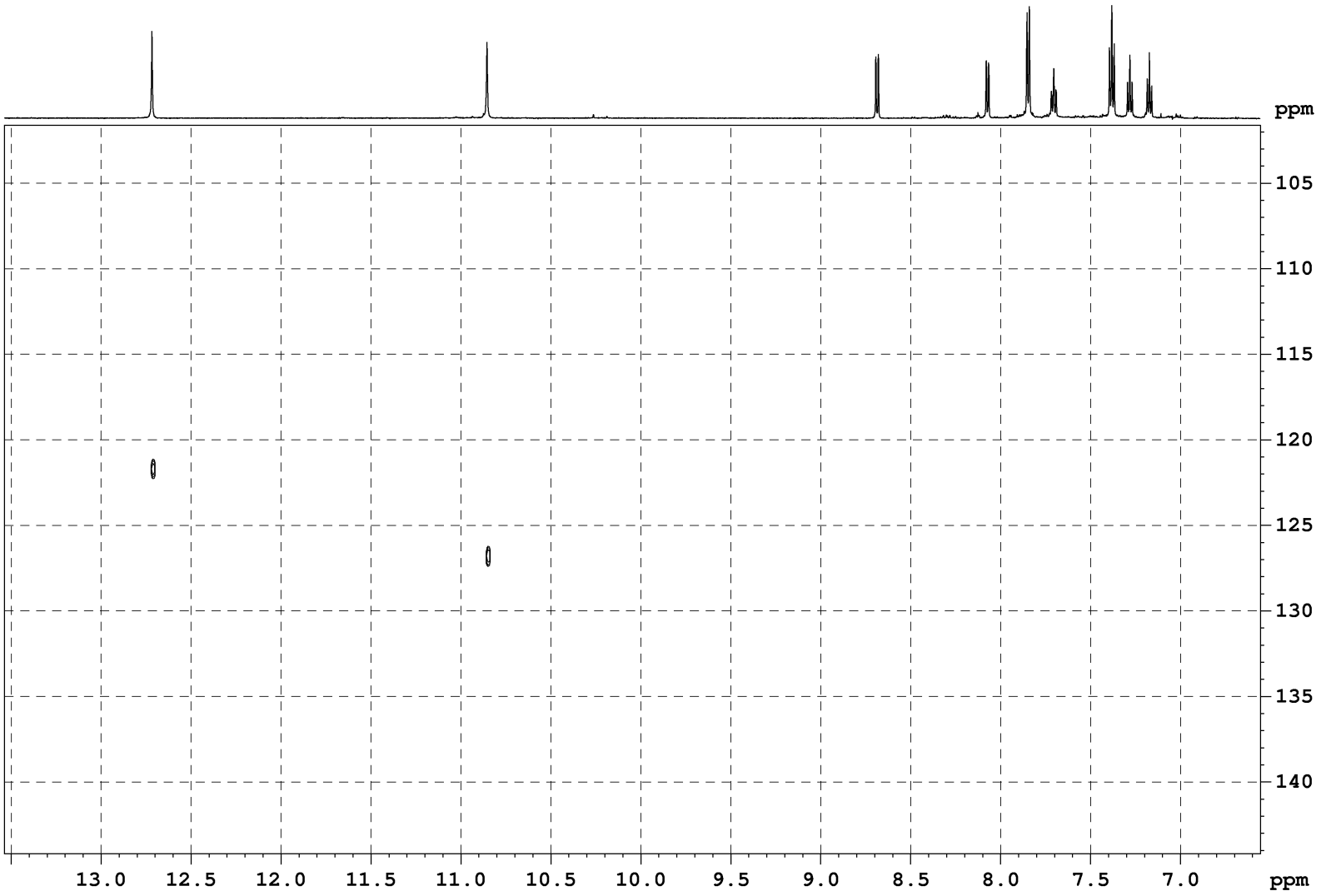



**Figure S66.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **4a** in DMSO at T = 303 K.

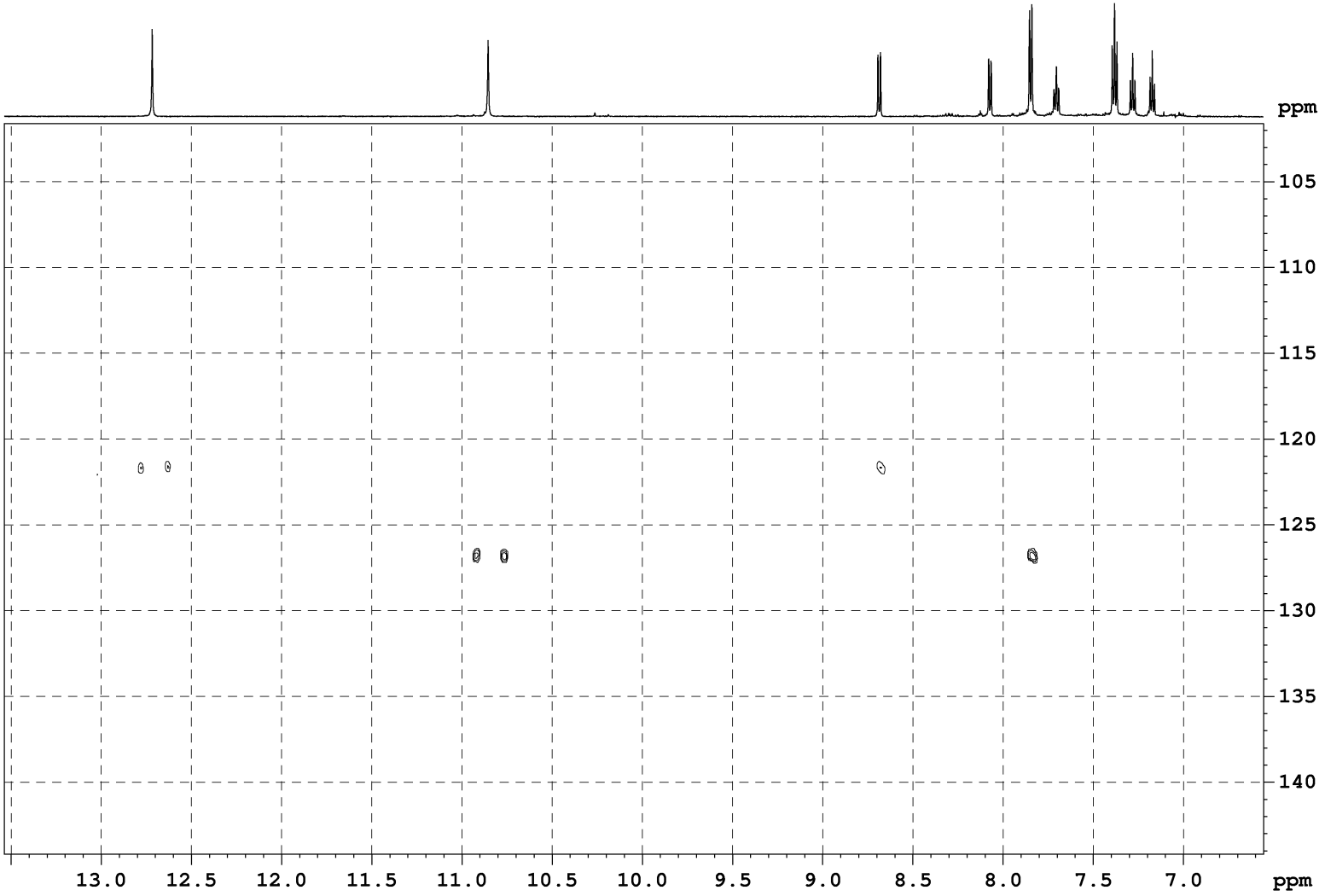



**Figure S67.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **4a** in DMSO at T = 303 K.

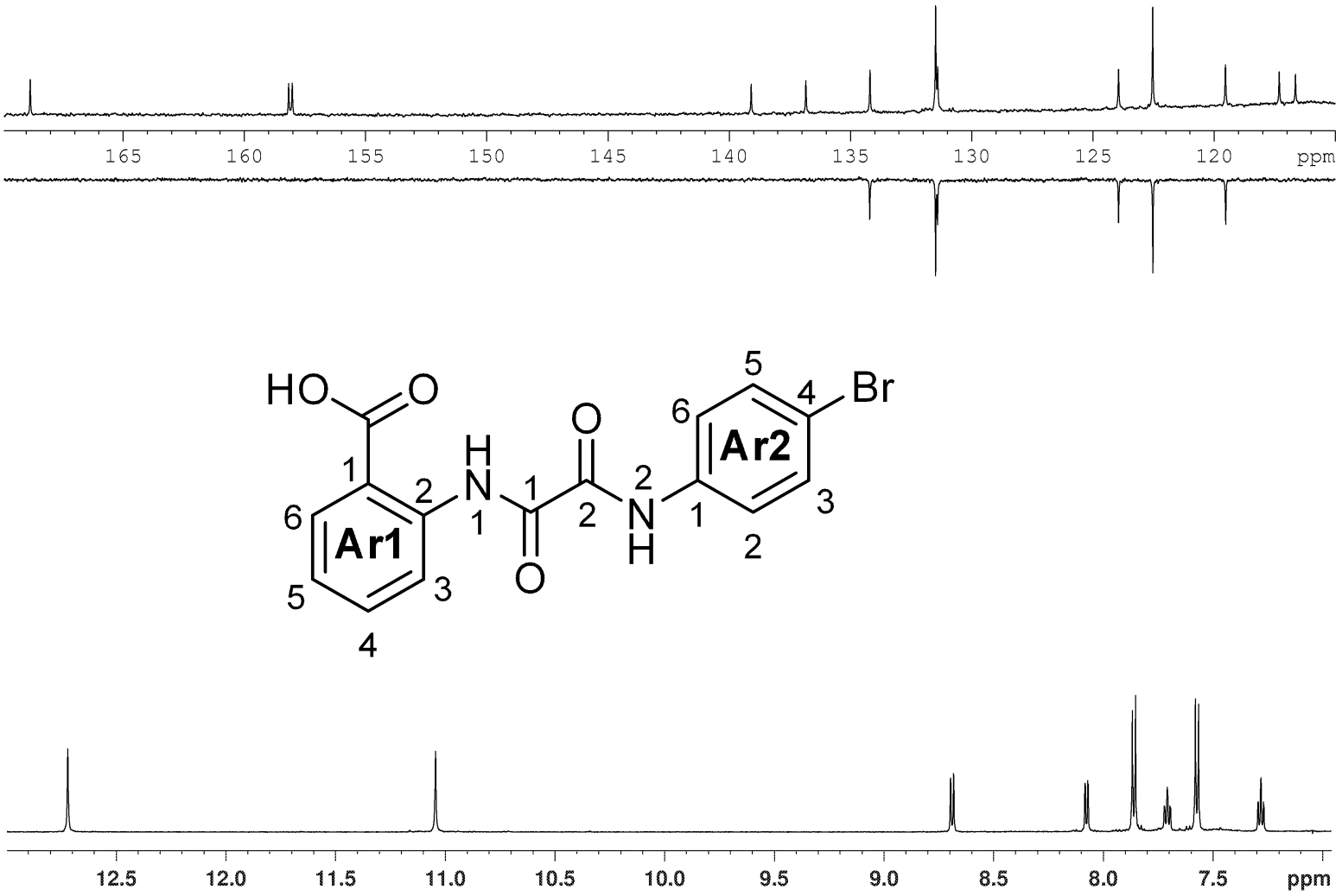



**Figure S68.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **4b** in DMSO at T = 303 K.

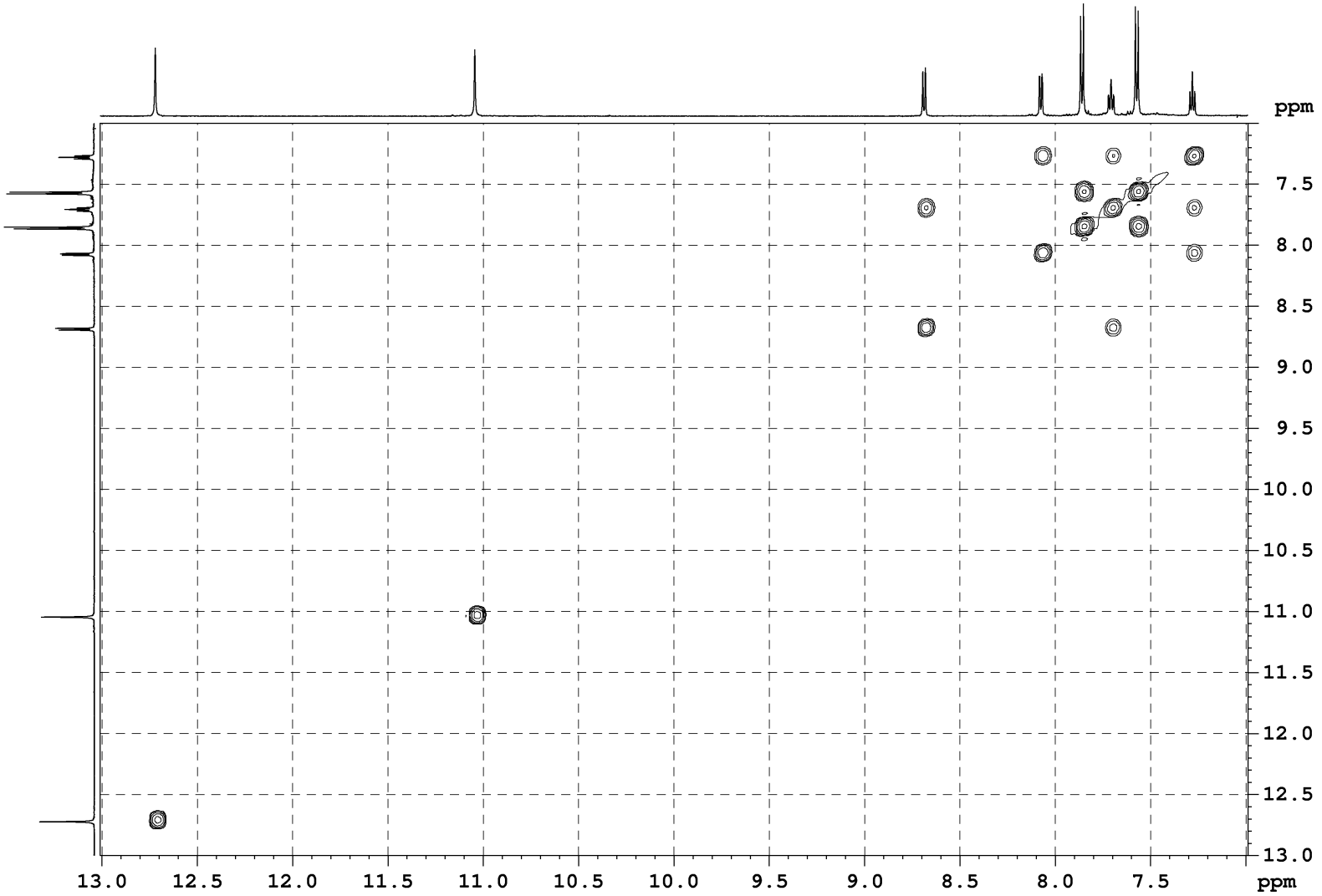



**Figure S69.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **4b** in DMSO at T = 303 K.

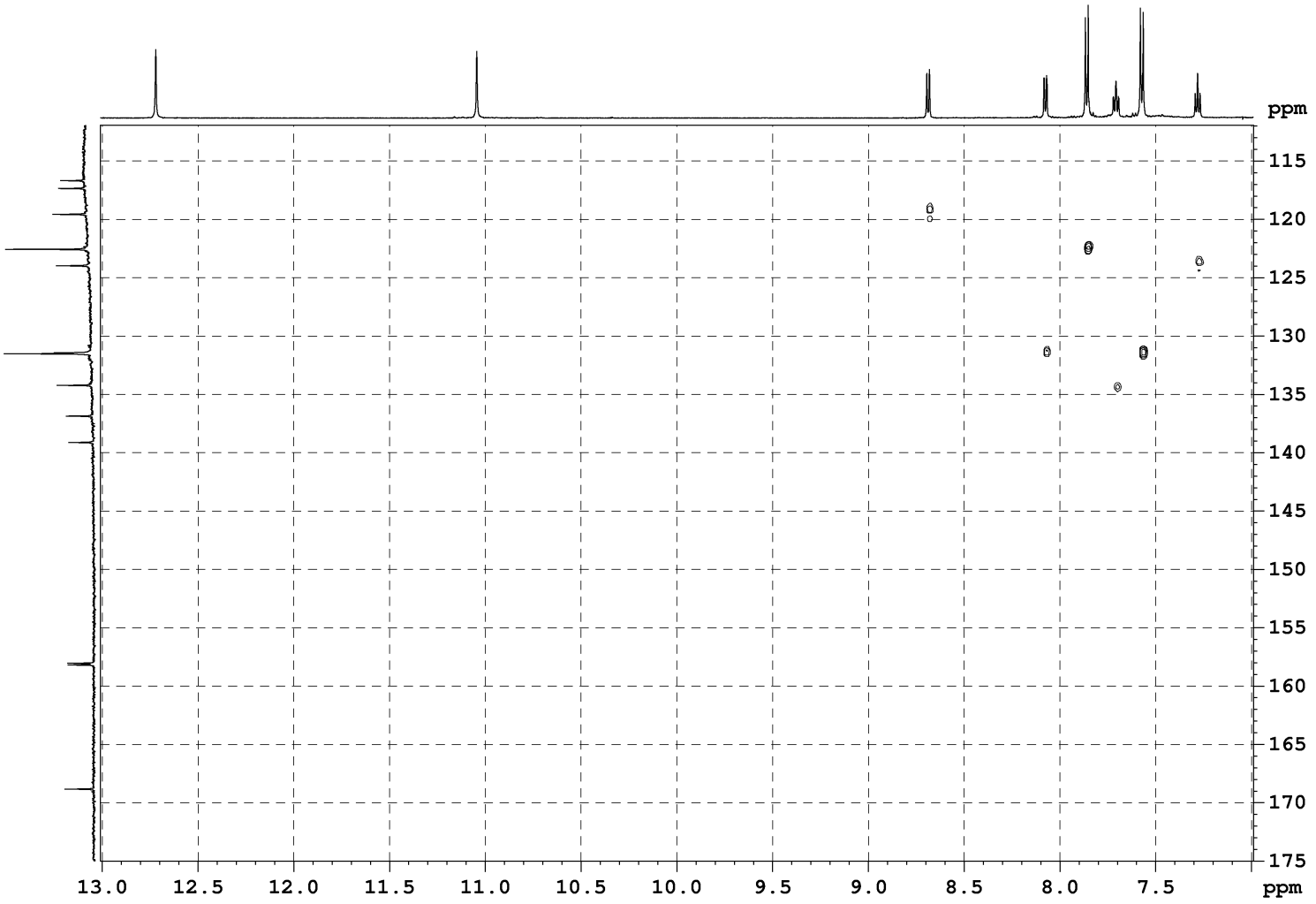



**Figure S70.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **4b** in DMSO at T = 303 K.

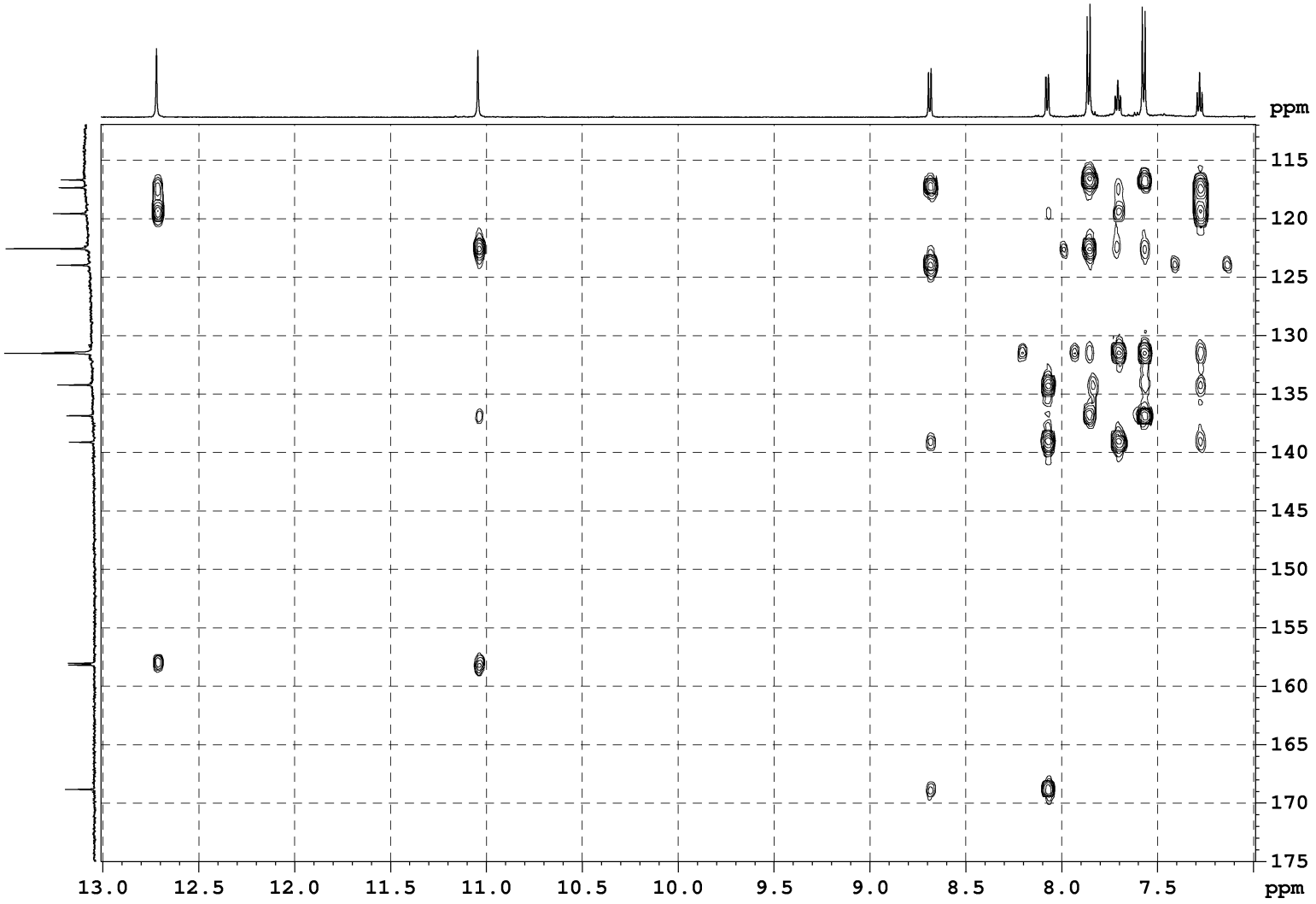



**Figure S71.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **4b** in DMSO at T = 303 K.

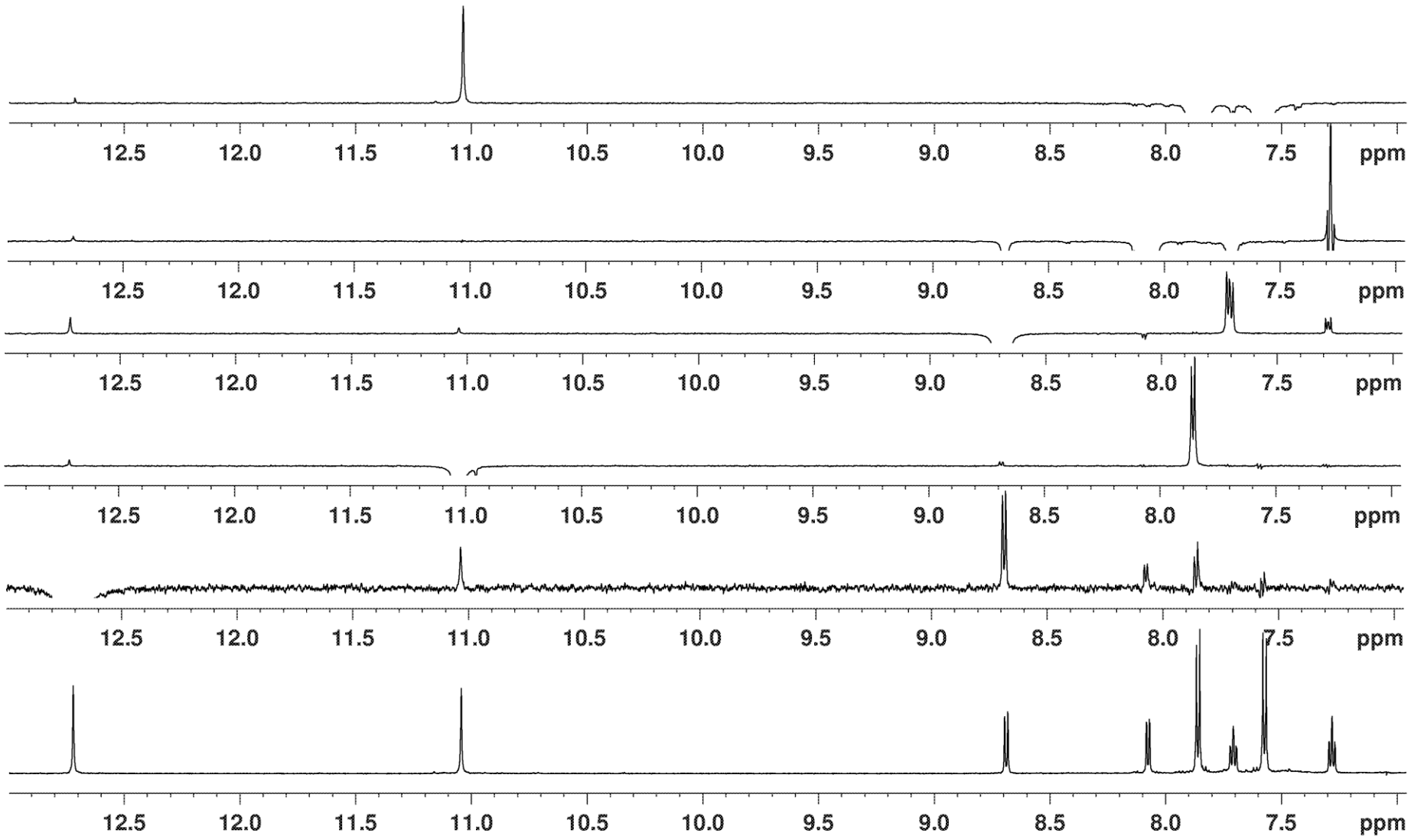



**Figure S72.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **4b** in DMSO at T = 303 K.

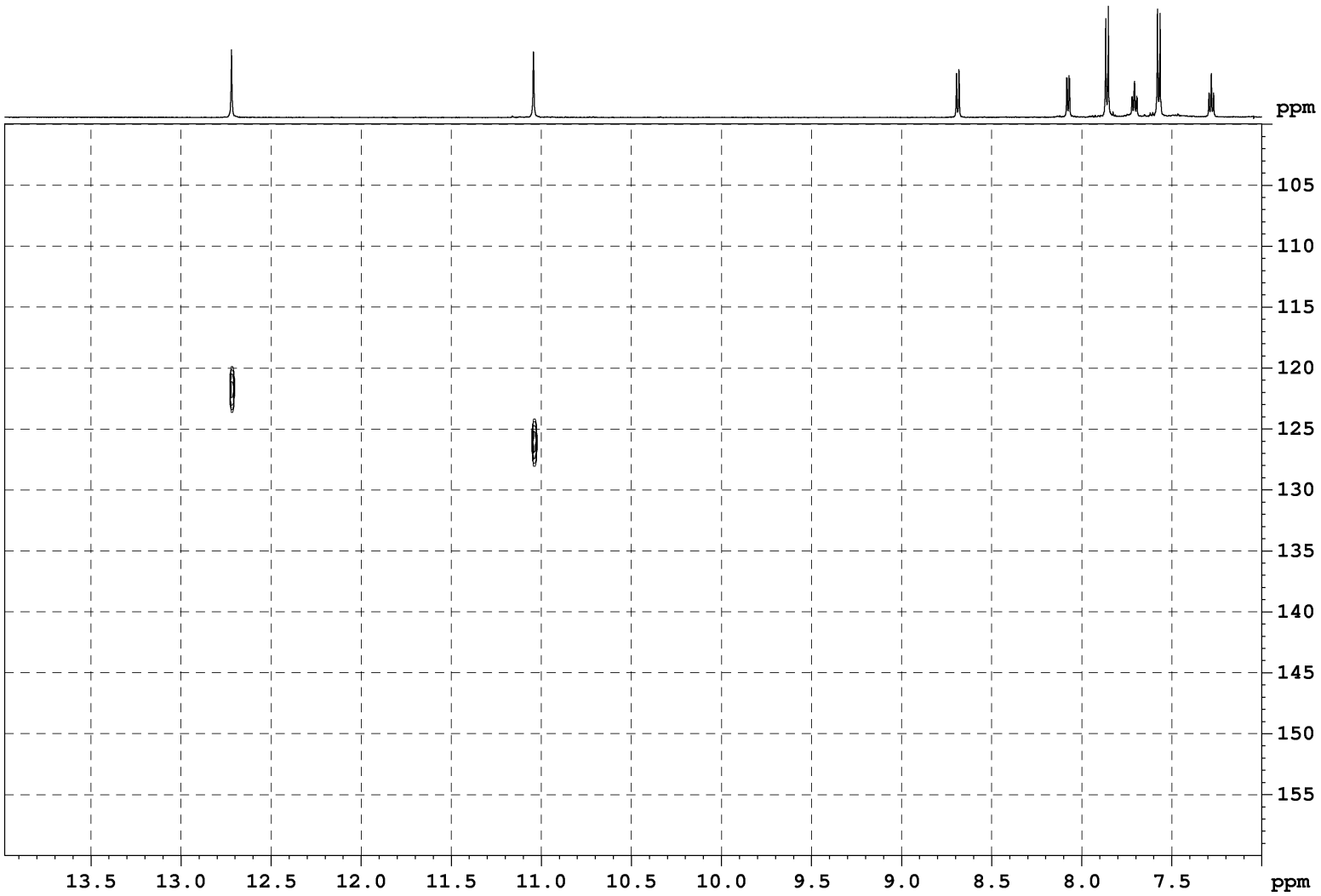



**Figure S73.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **4b** in DMSO at T = 303 K.

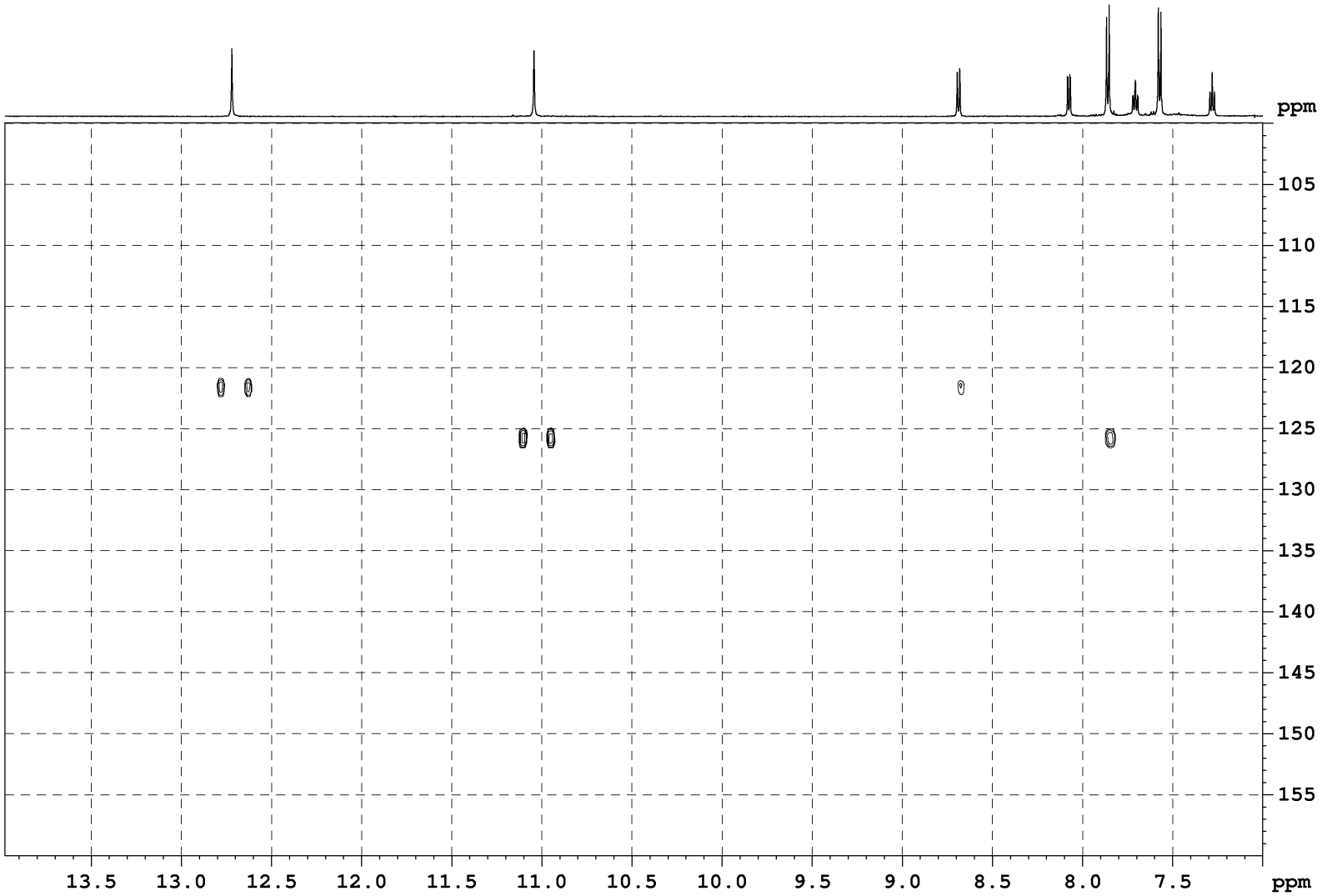



**Figure S74.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **4b** in DMSO at T = 303 K.

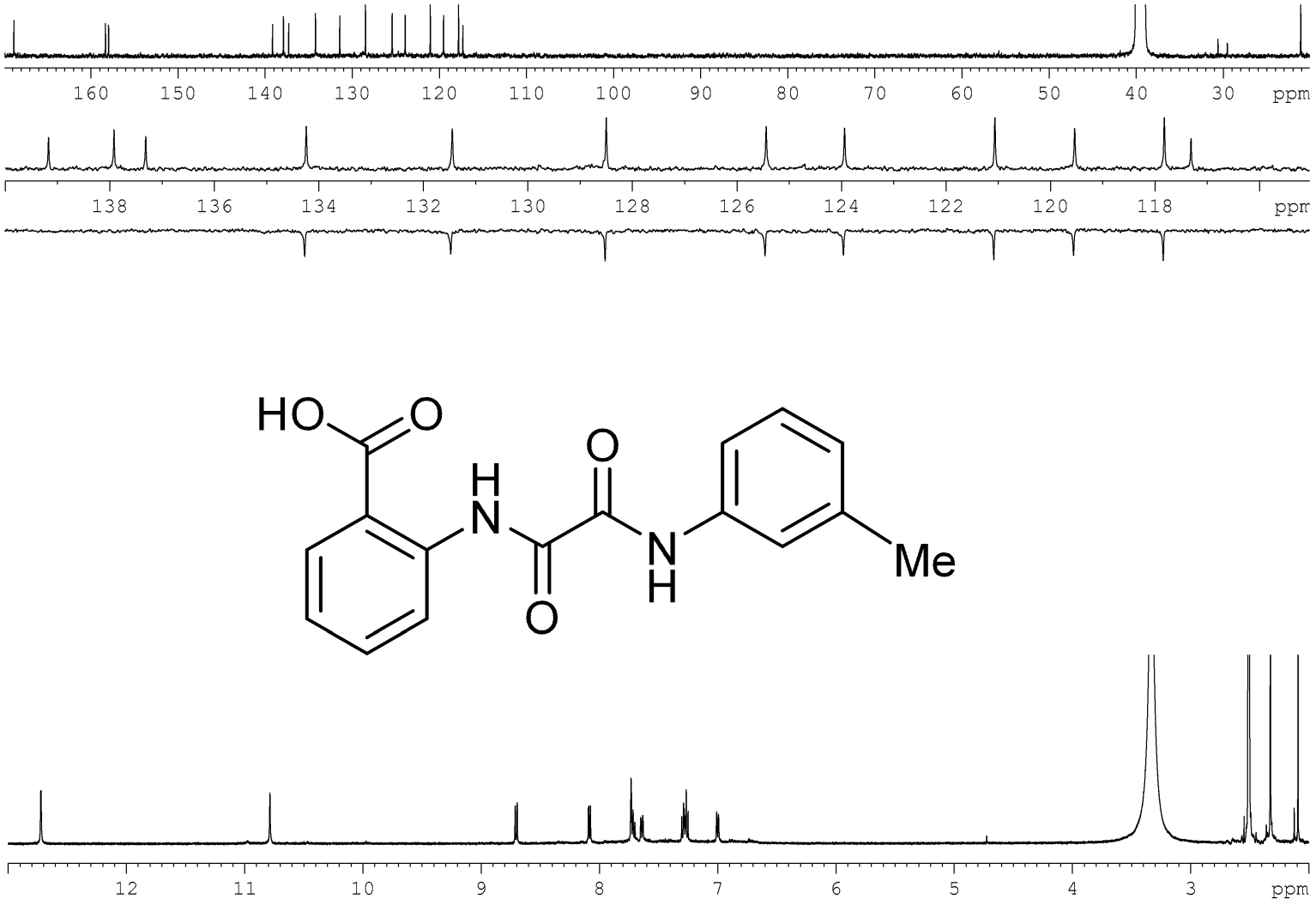



**Figure S75.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **4c** in DMSO at T = 303 K.

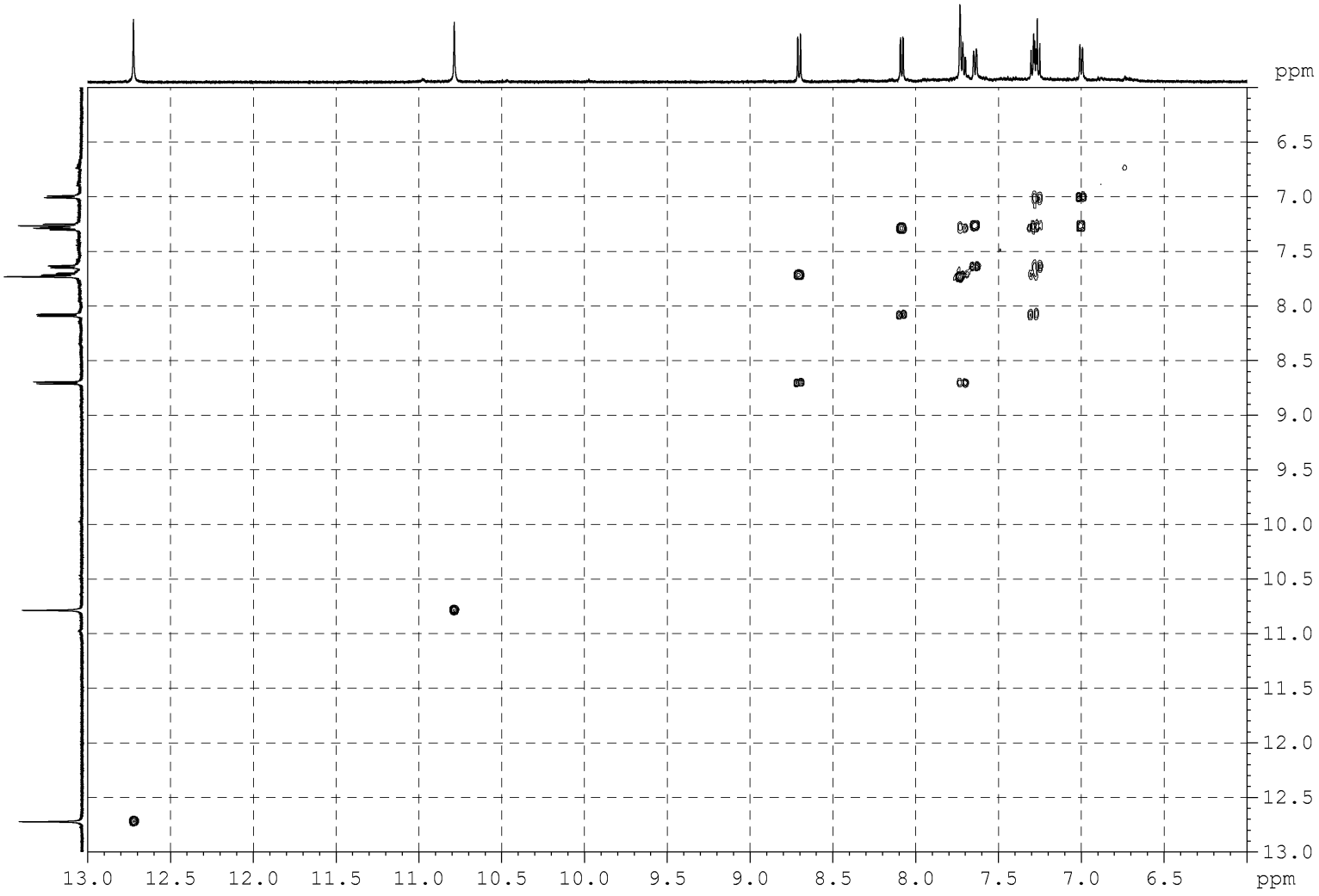



**Figure S76.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **4c** in DMSO at T = 303 K.

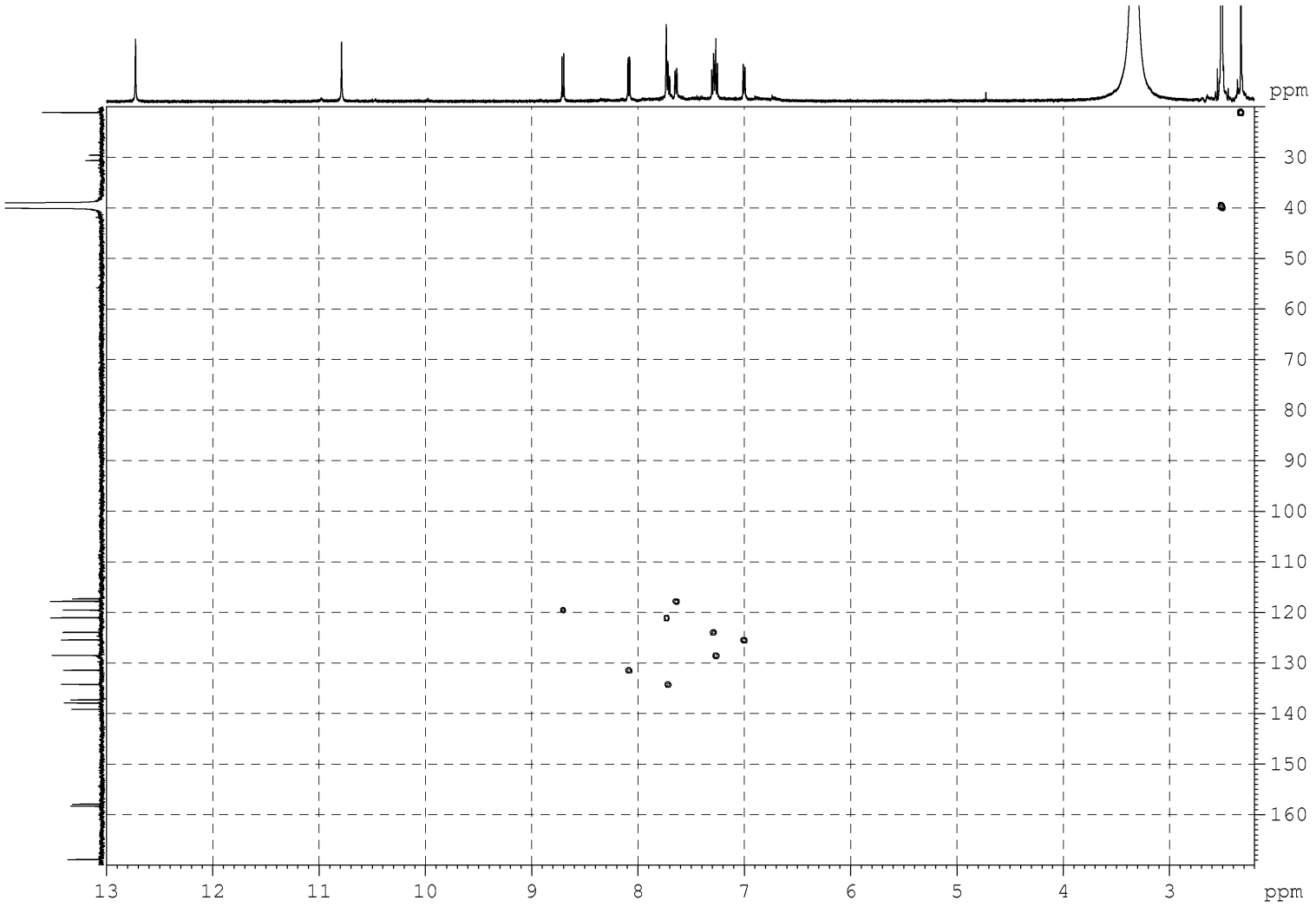



**Figure S77.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **4c** in DMSO at T = 303 K.

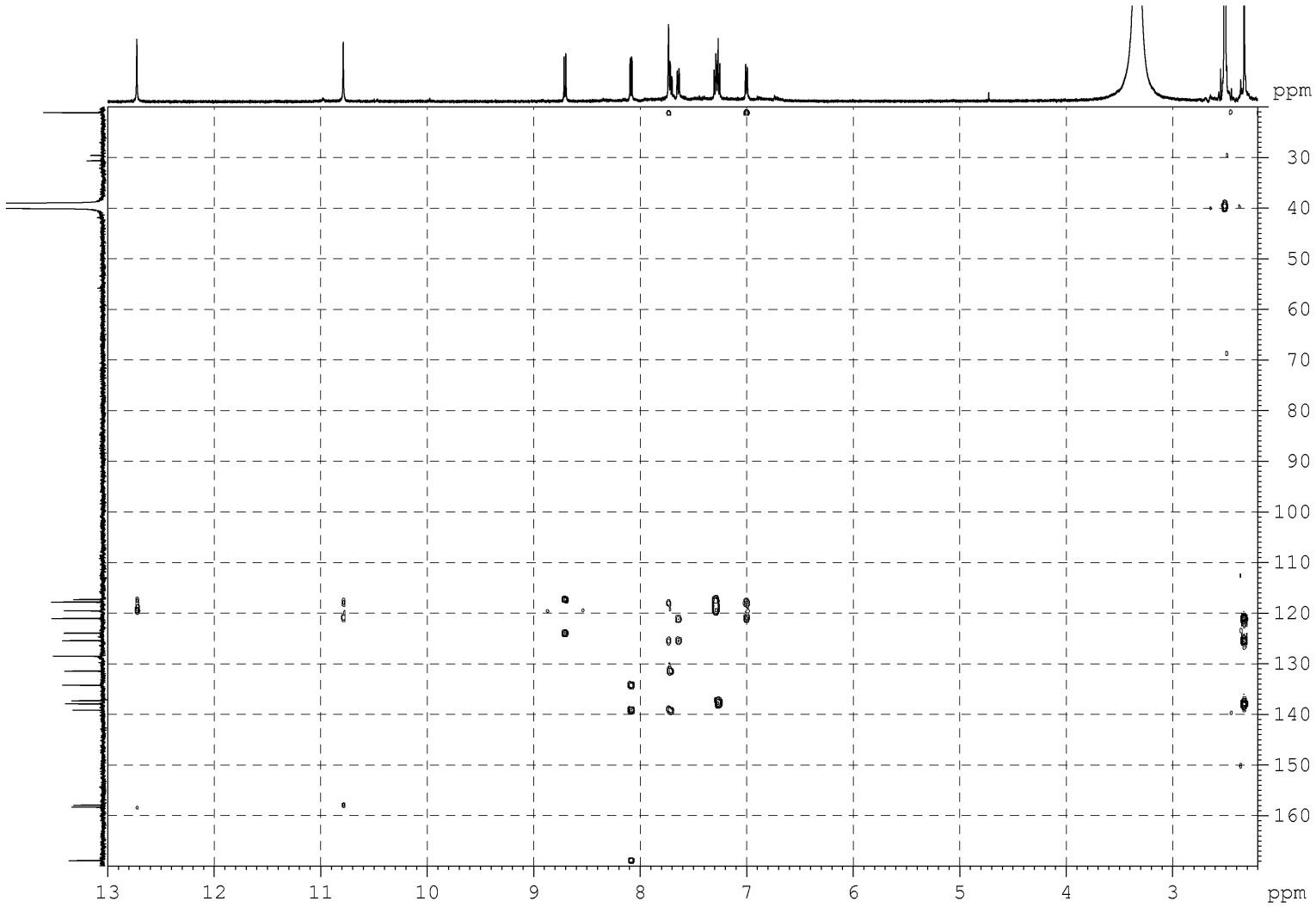



**Figure S78.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **4c** in DMSO at T = 303 K.

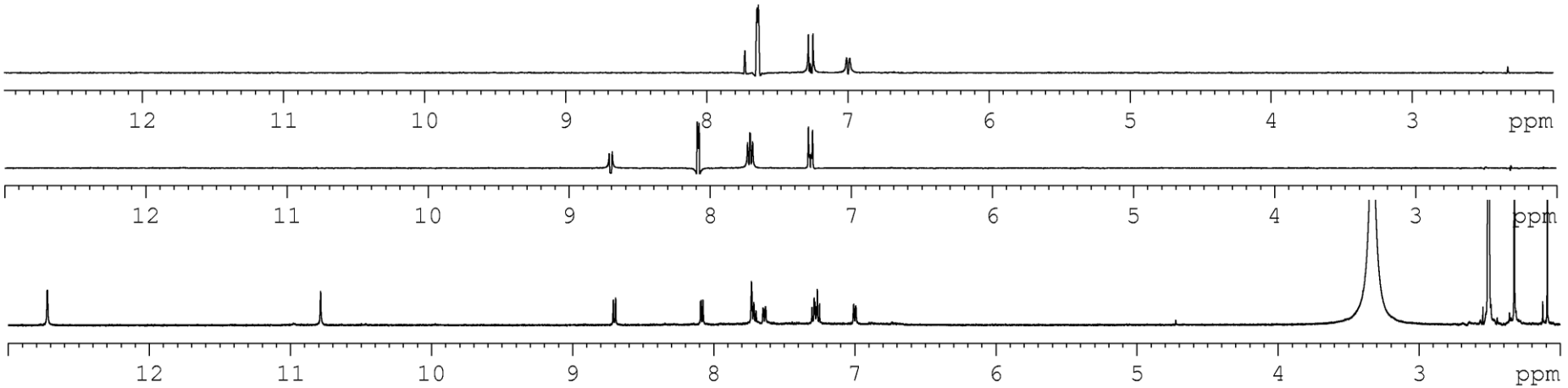



**Figure S79.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **4c** in DMSO at T = 303 K.

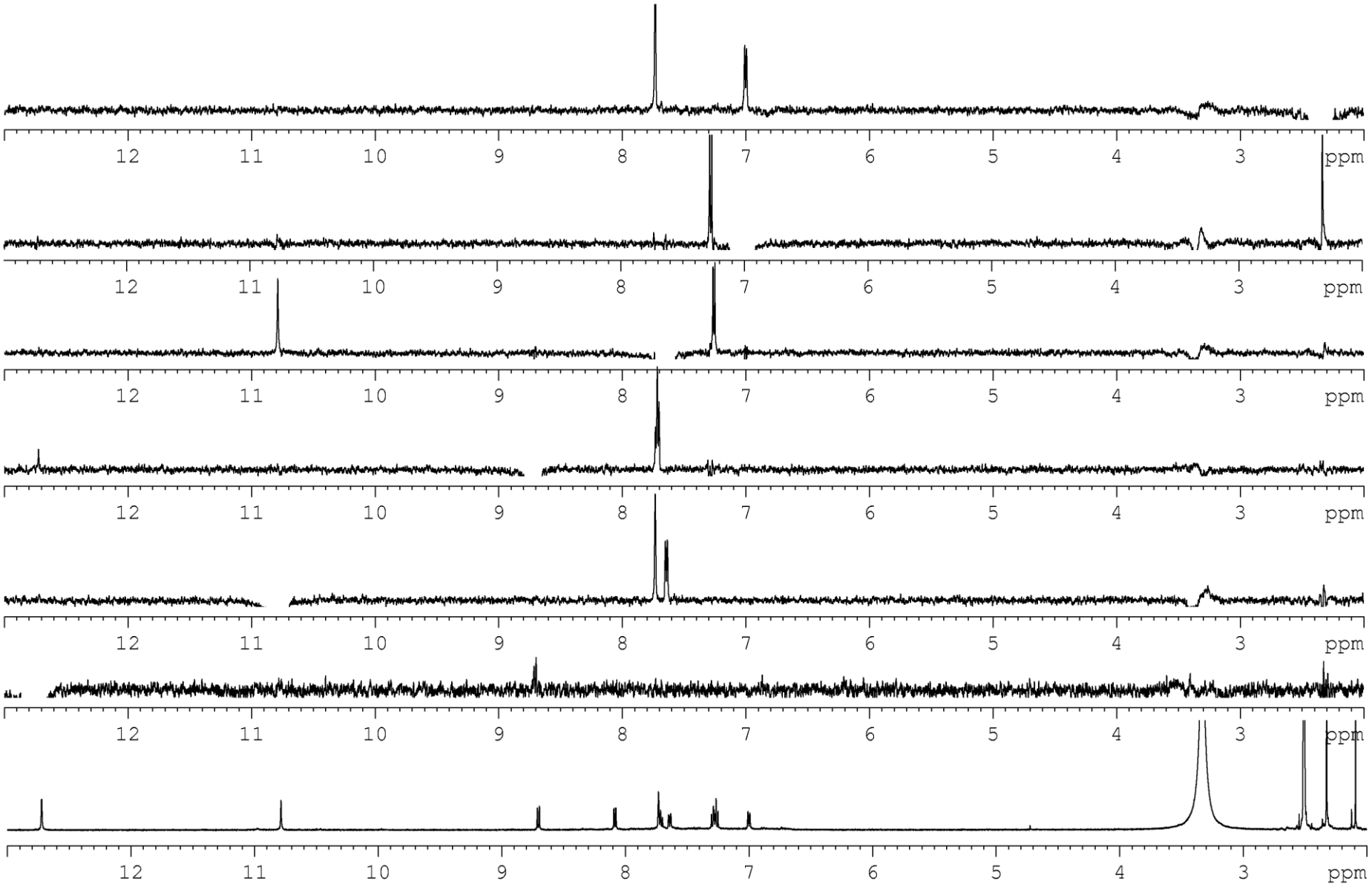



**Figure S80.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **4c** in DMSO at T = 303 K.

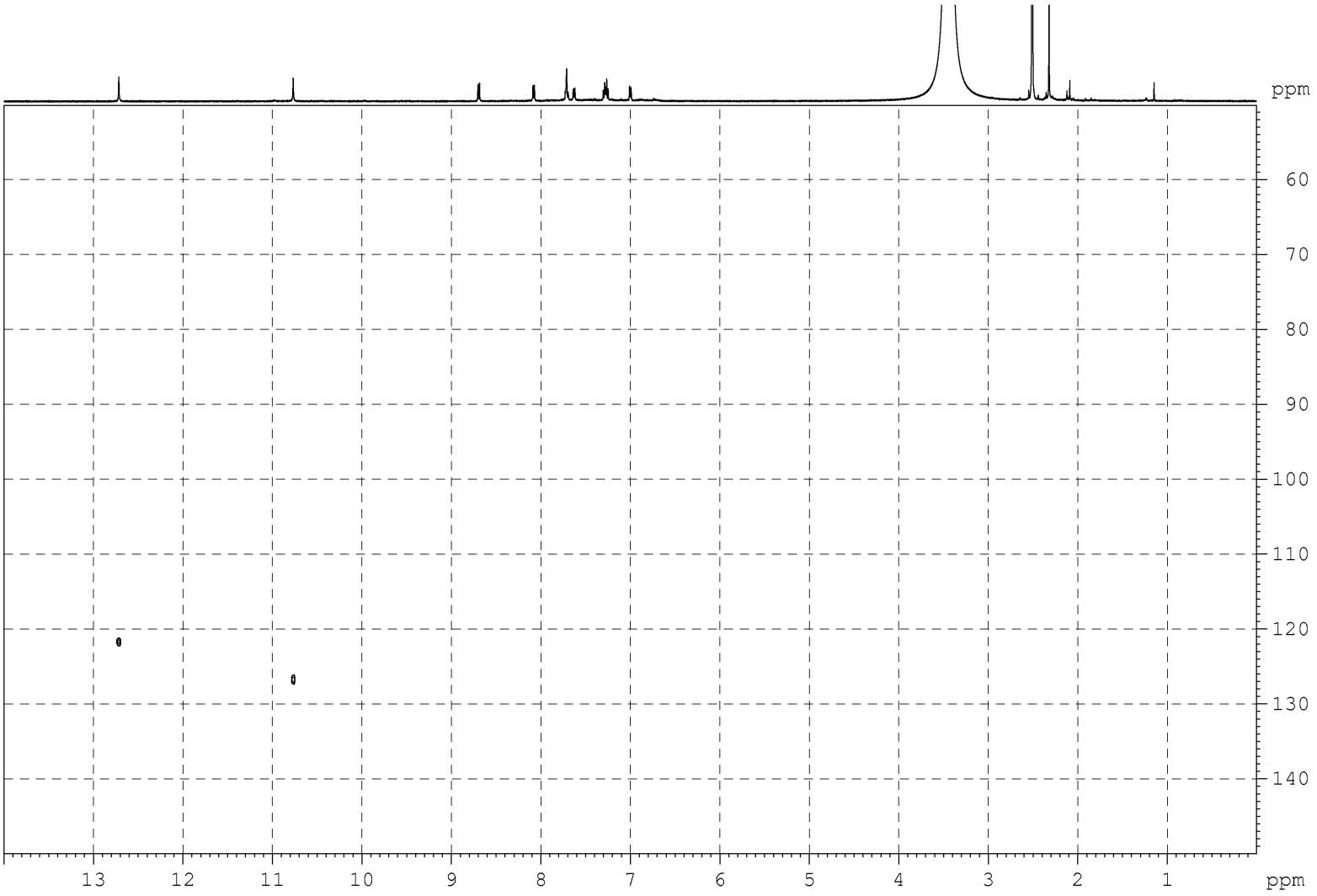



**Figure S81.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **4c** in DMSO at T = 303 K.

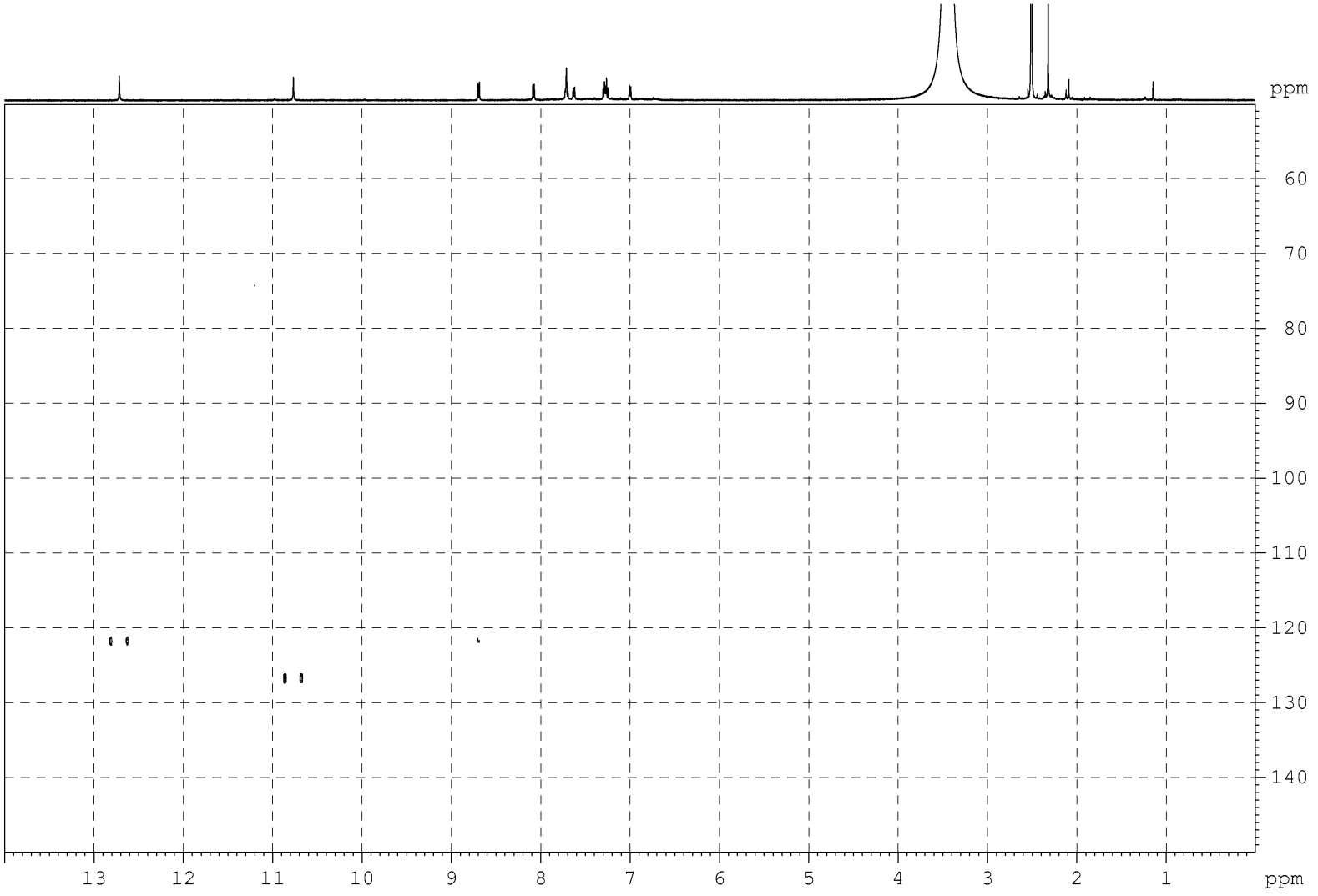



**Figure S82.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **4c** in DMSO at T = 303 K.

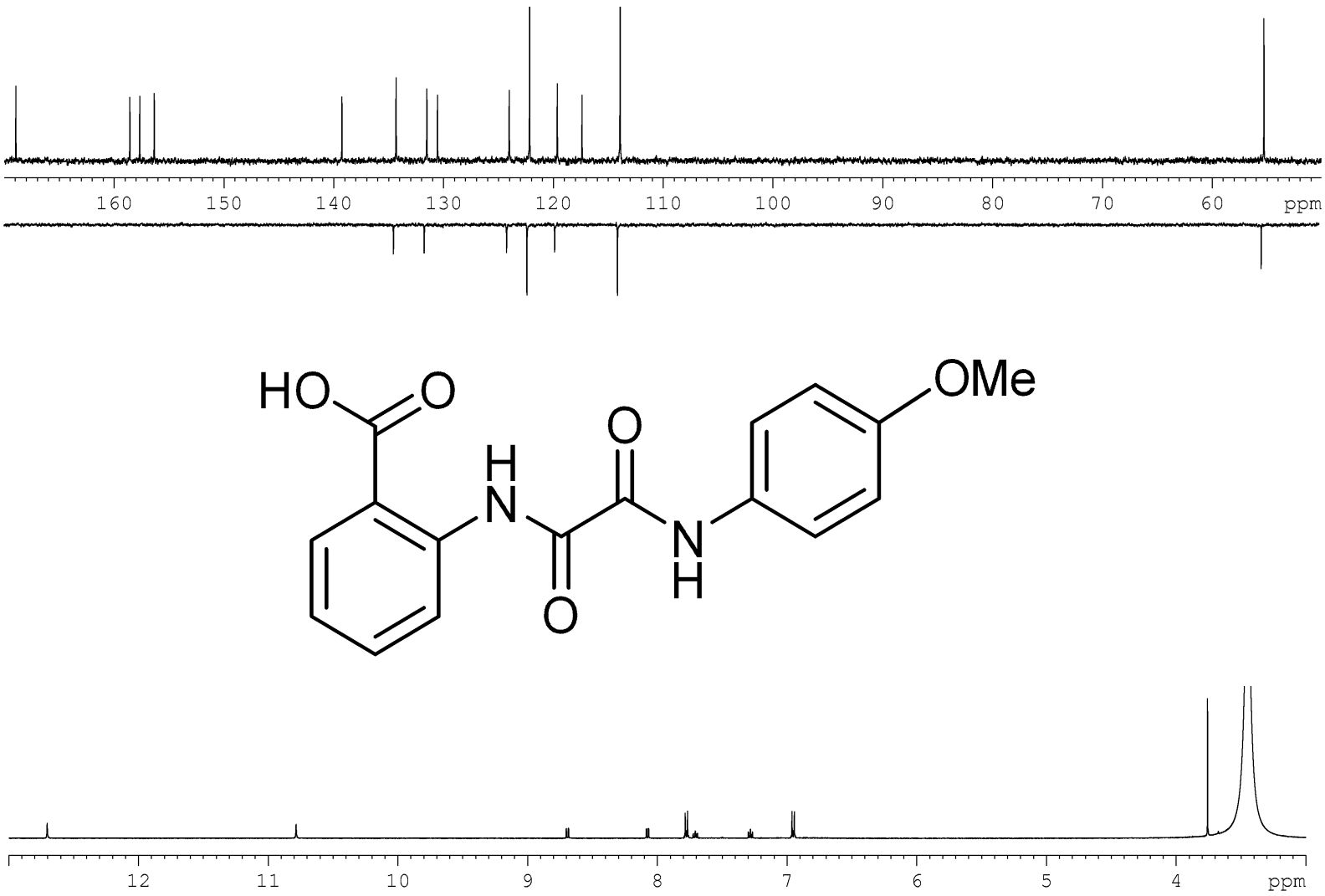



**Figure S83.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **4d** in DMSO at T = 303 K.

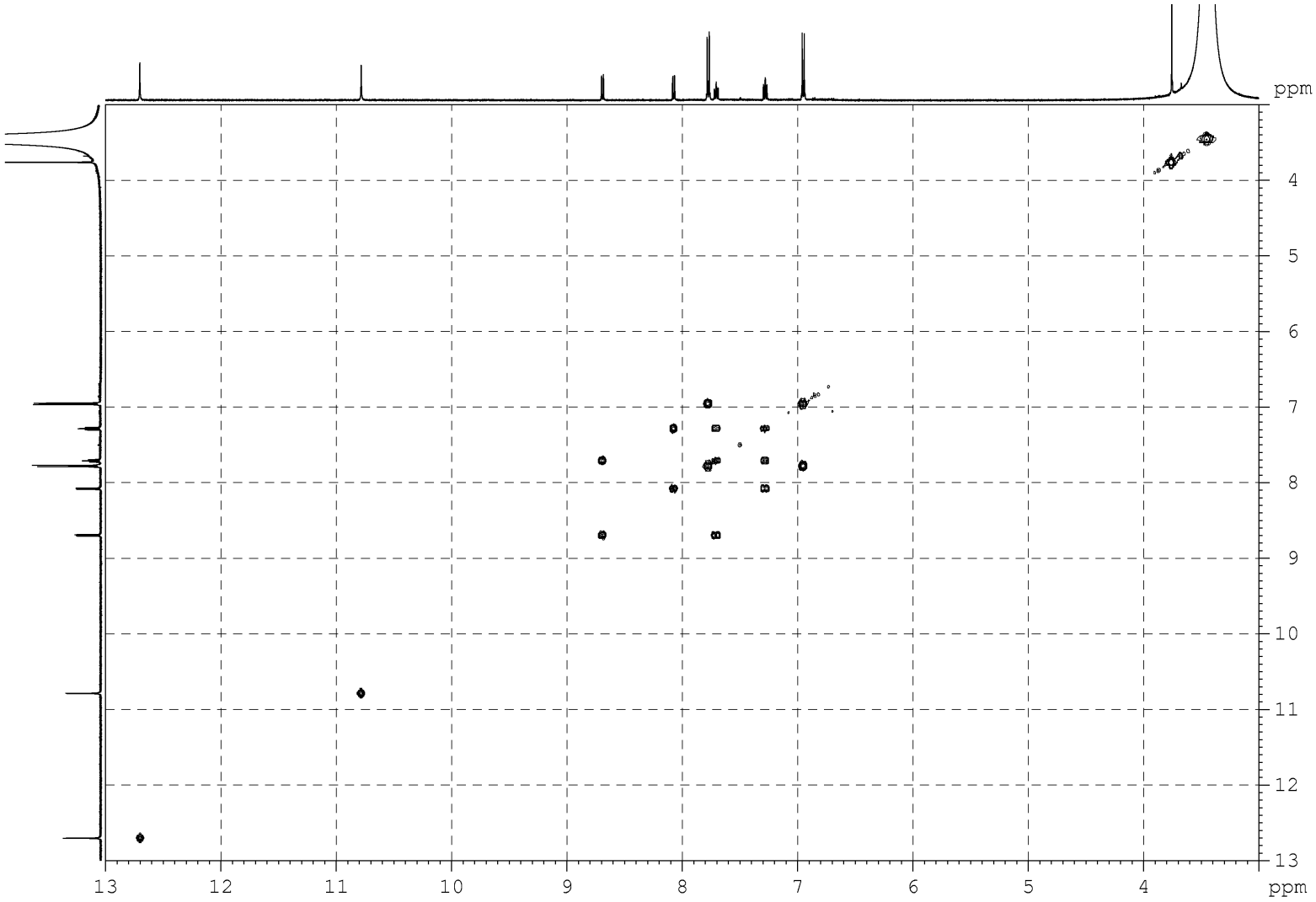



**Figure S84.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **4d** in DMSO at T = 303 K.

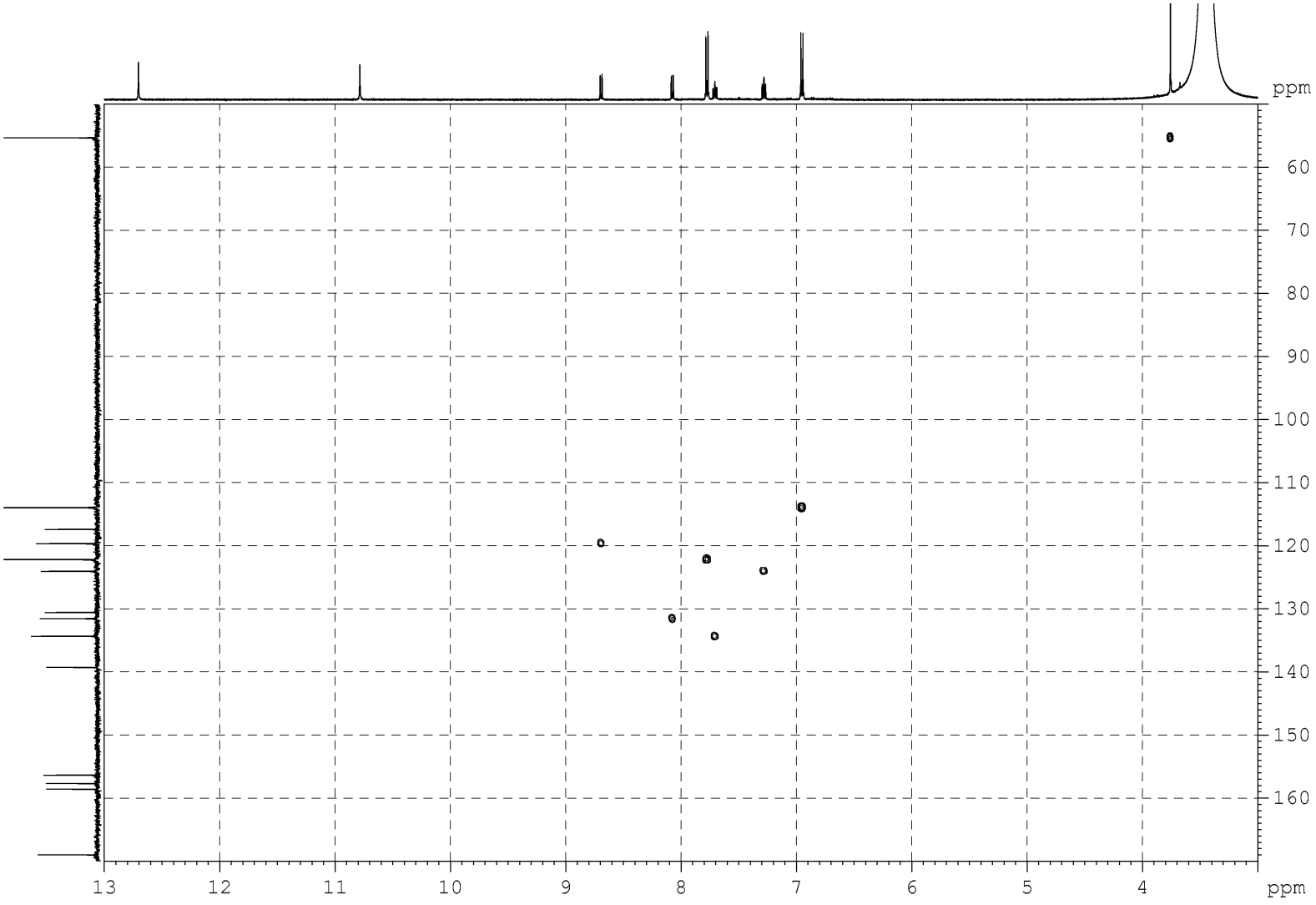



**Figure S85.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **4d** in DMSO at T = 303 K.

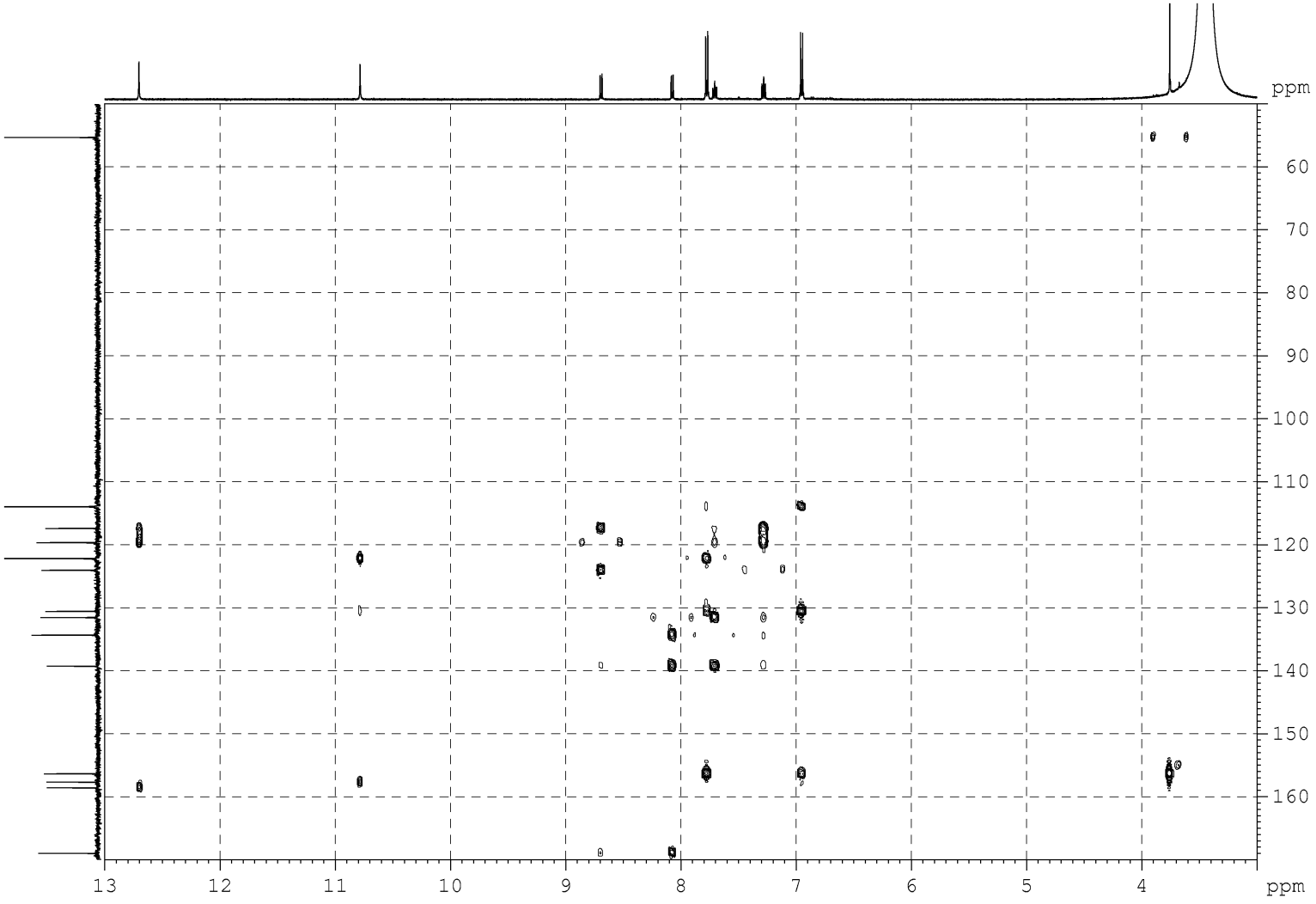



**Figure S86.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **4d** in DMSO at T = 303 K.

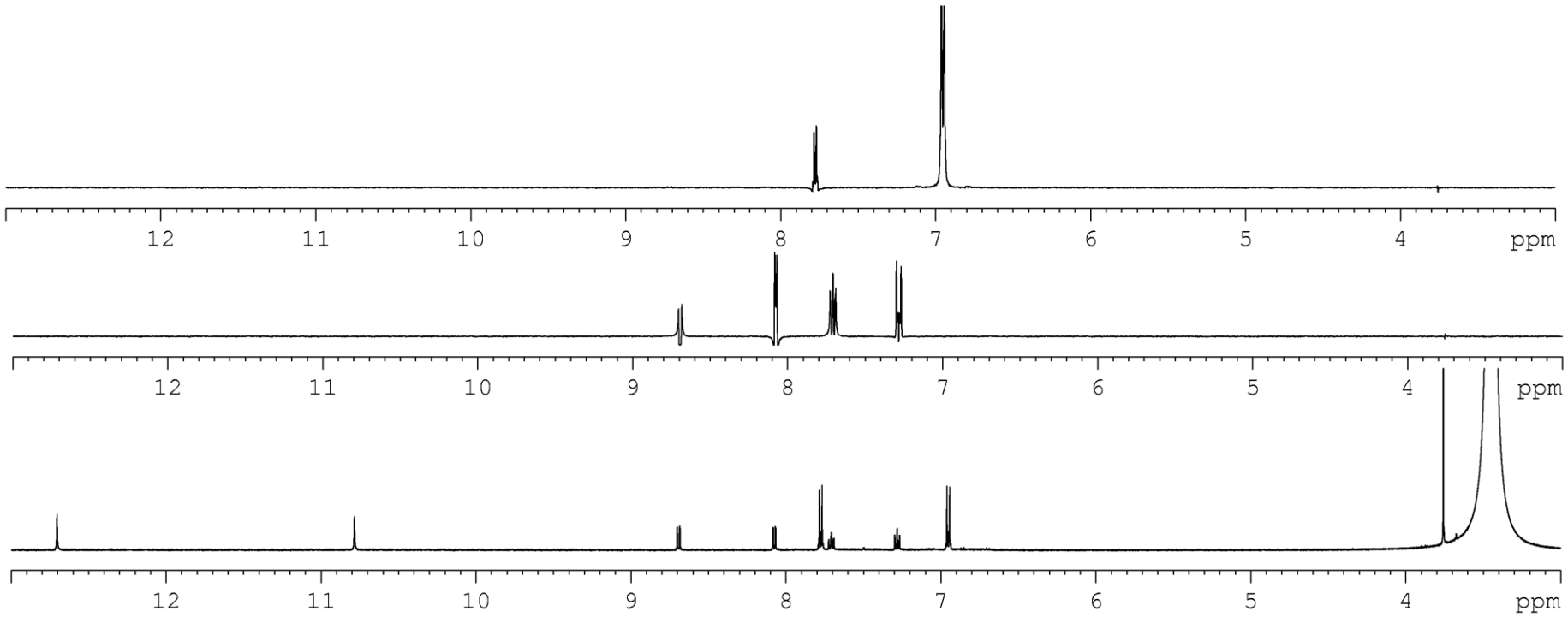



**Figure S87.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **4d** in DMSO at T = 303 K.

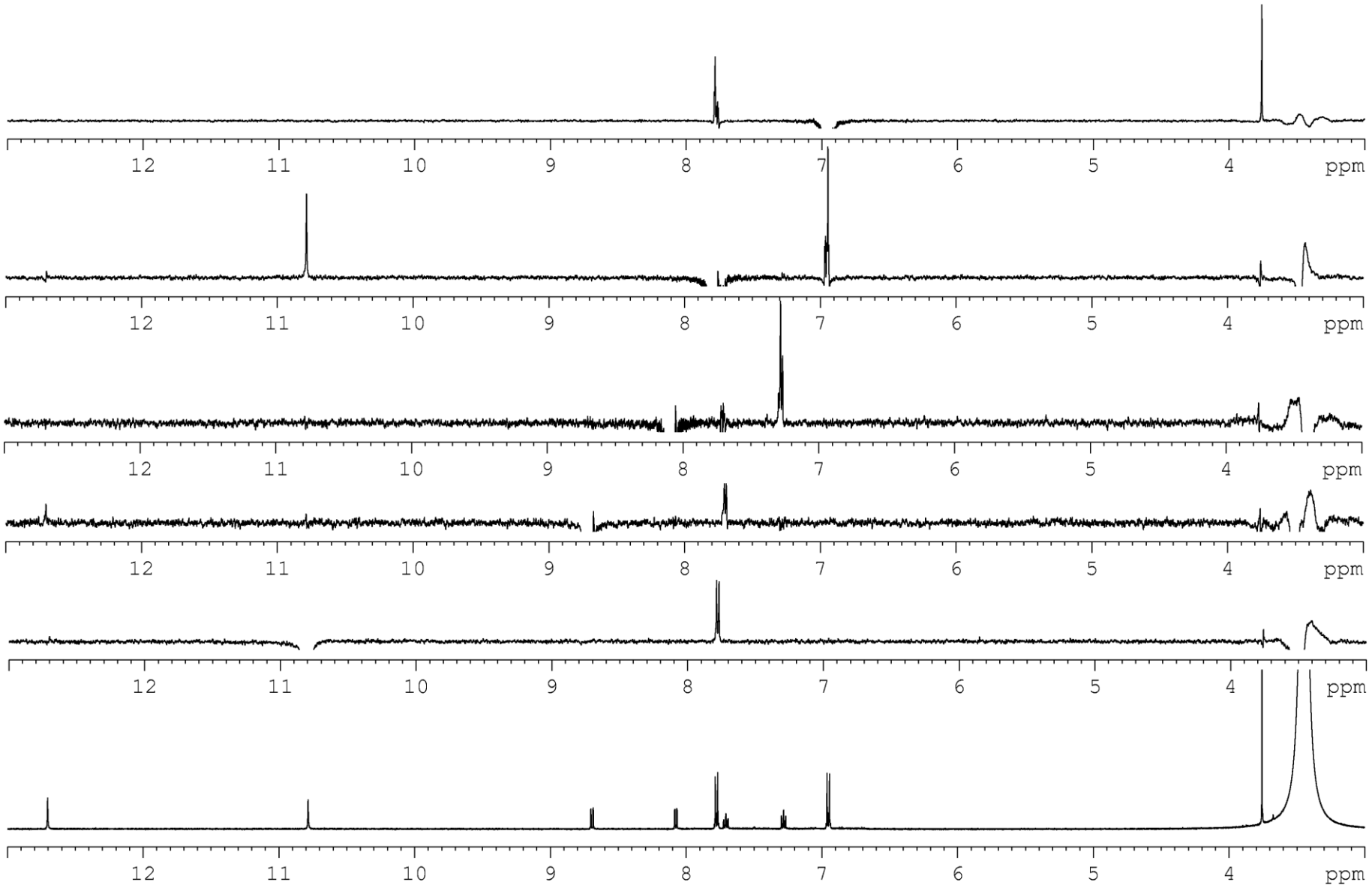



**Figure S88.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **4d** in DMSO at T = 303 K.

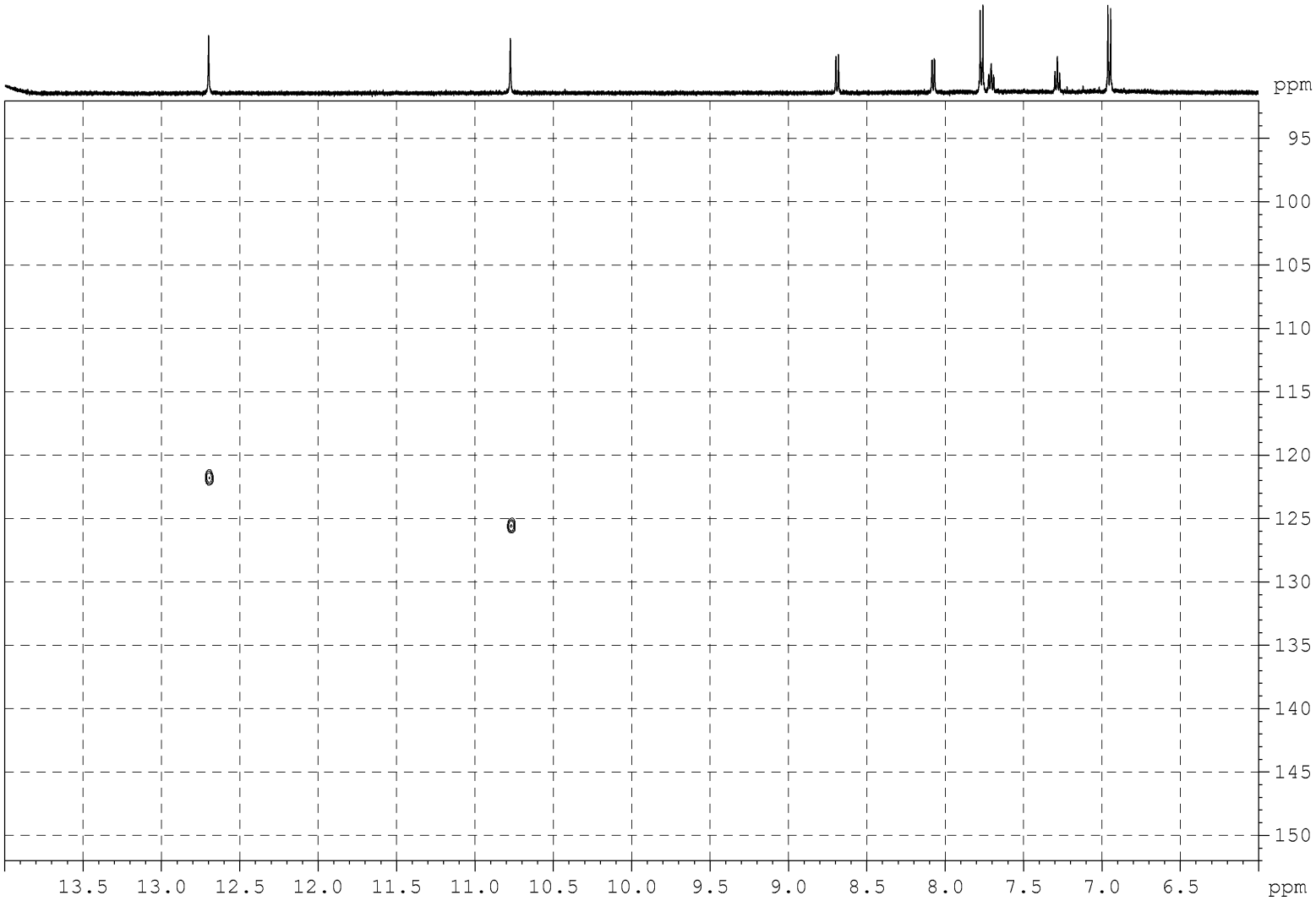



**Figure S89.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **4d** in DMSO at T = 303 K.

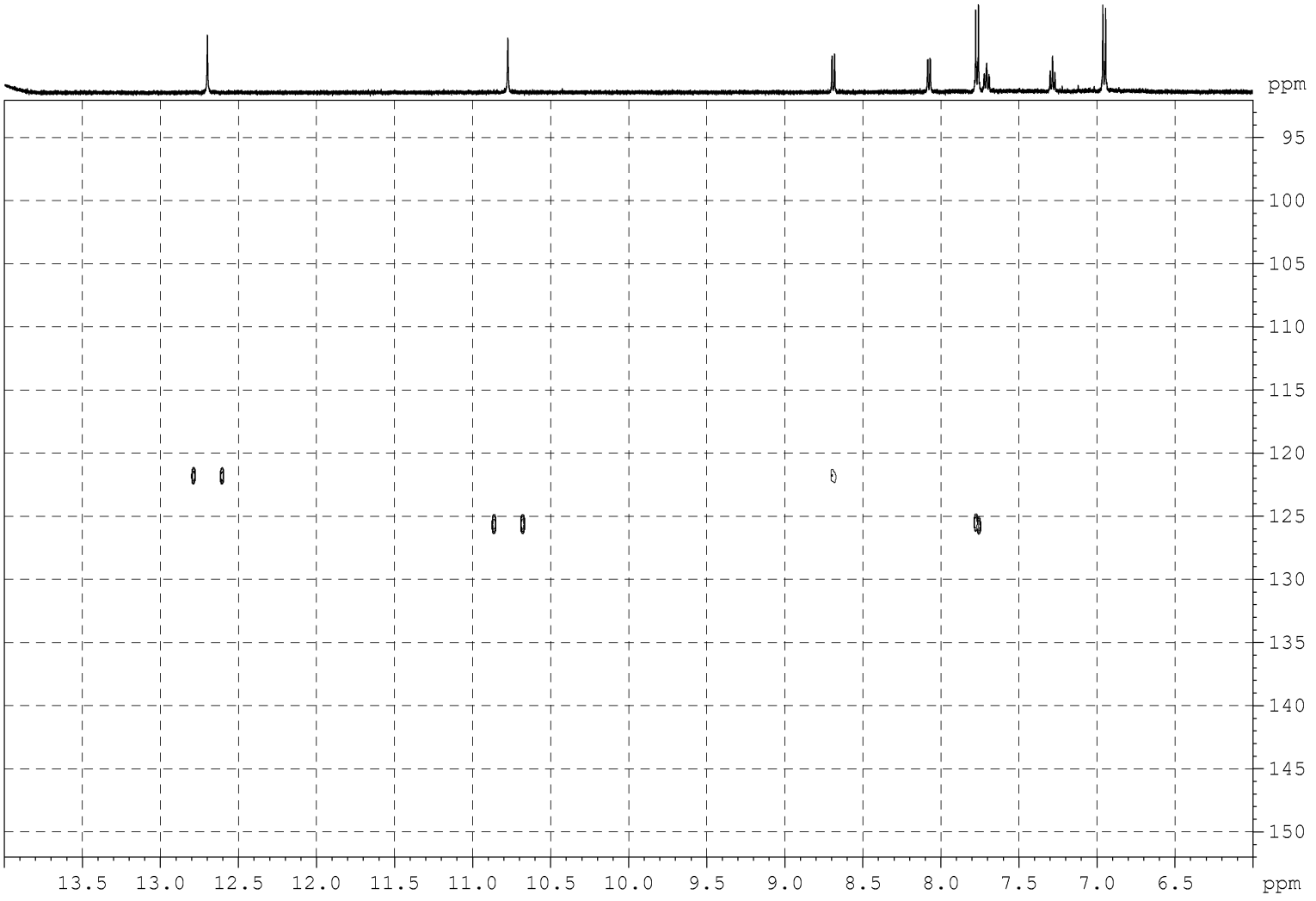



**Figure S90.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **4d** in DMSO at T = 303 K.

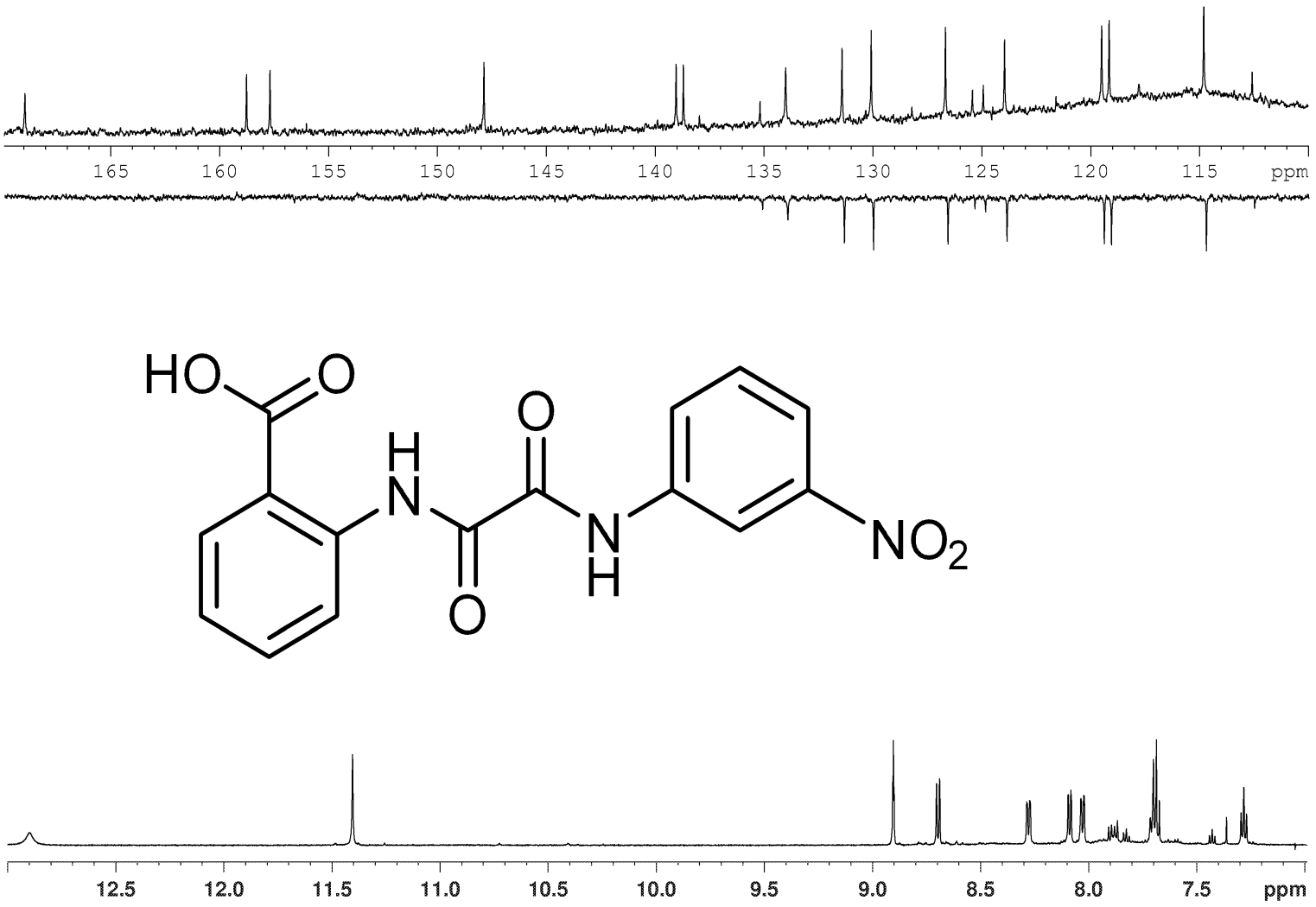



**Figure S91.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **4e** in DMSO at T = 303 K.

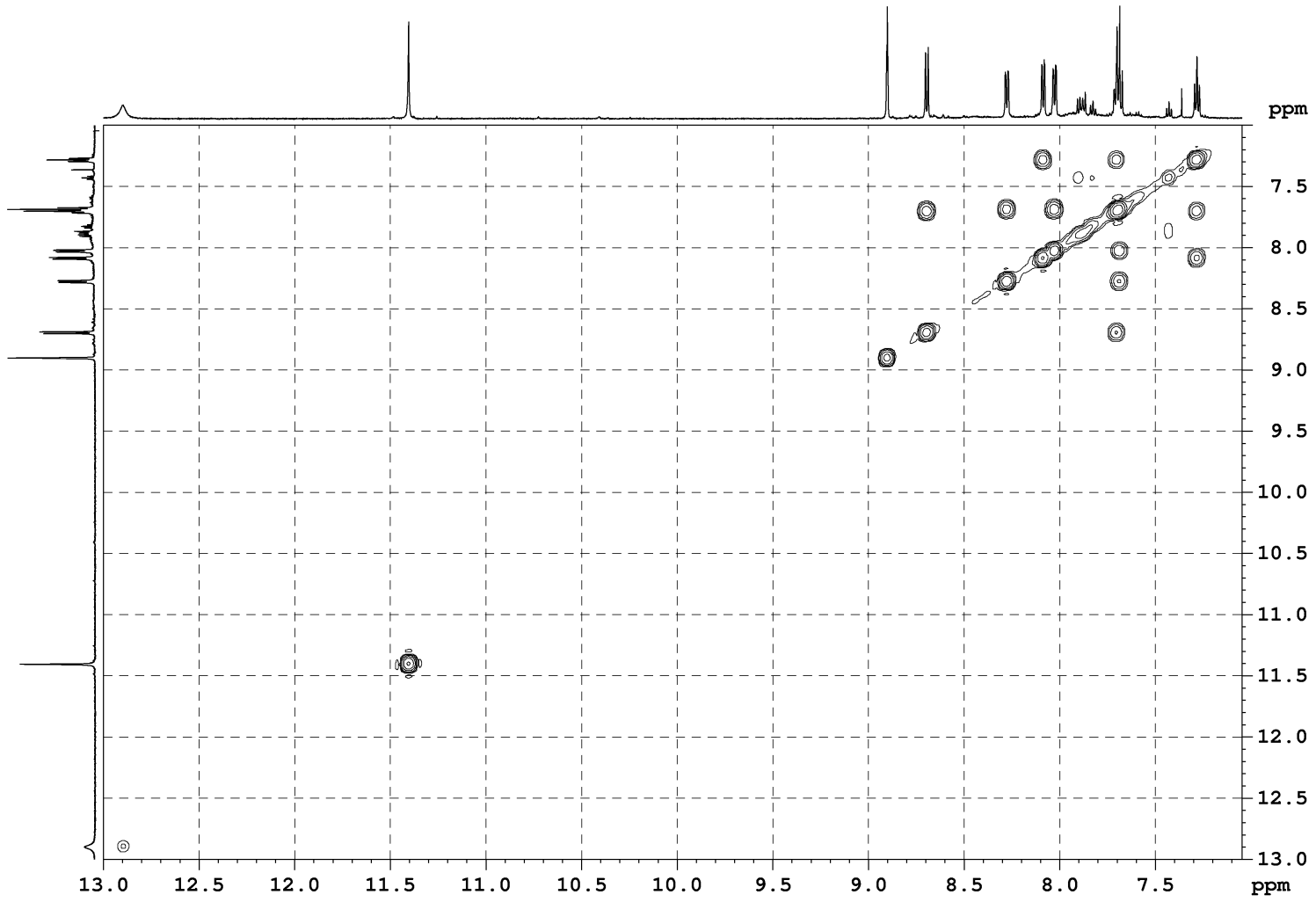



**Figure S92.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **4e** in DMSO at T = 303 K.

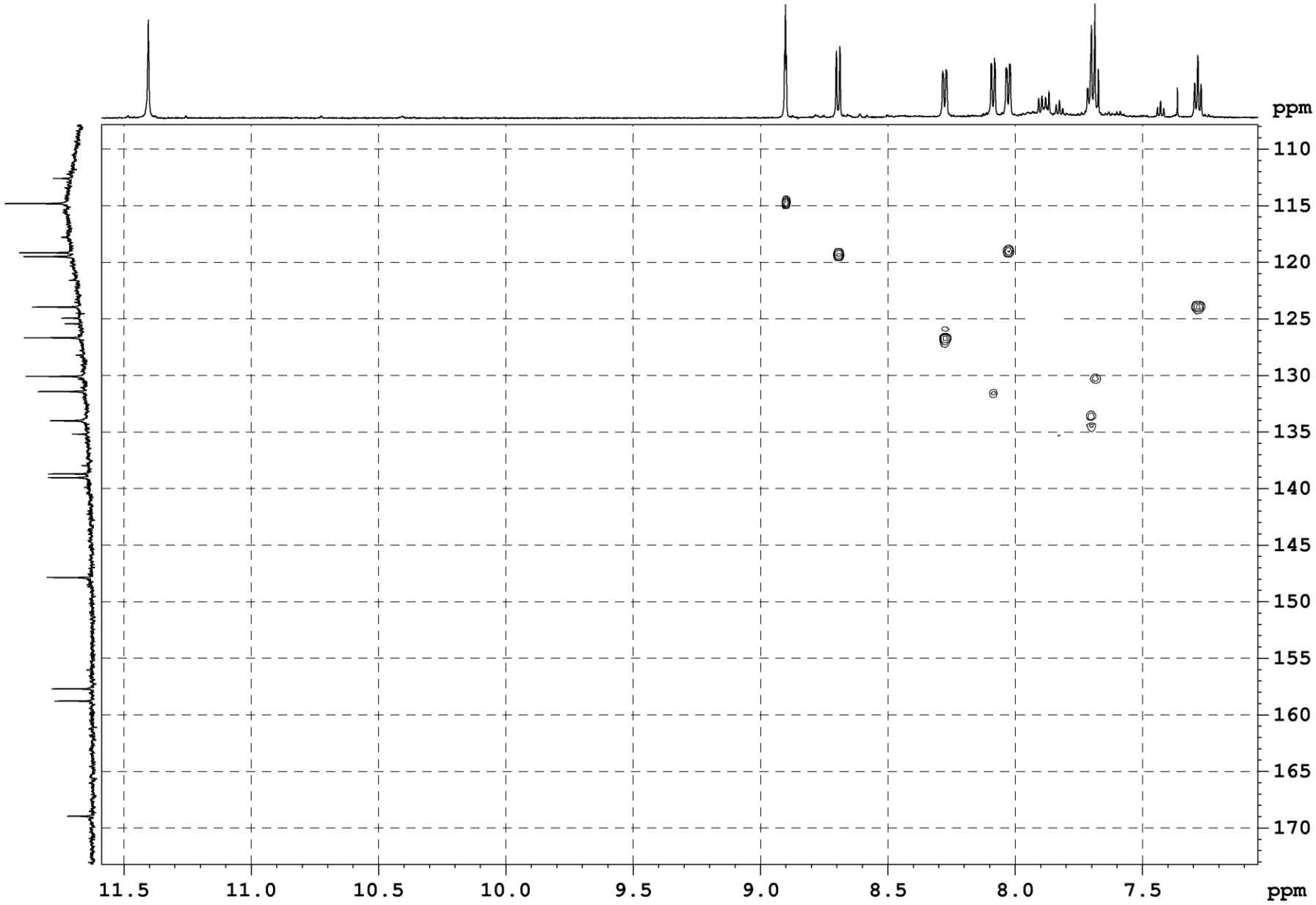



**Figure S93.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **4e** in DMSO at T = 303 K.

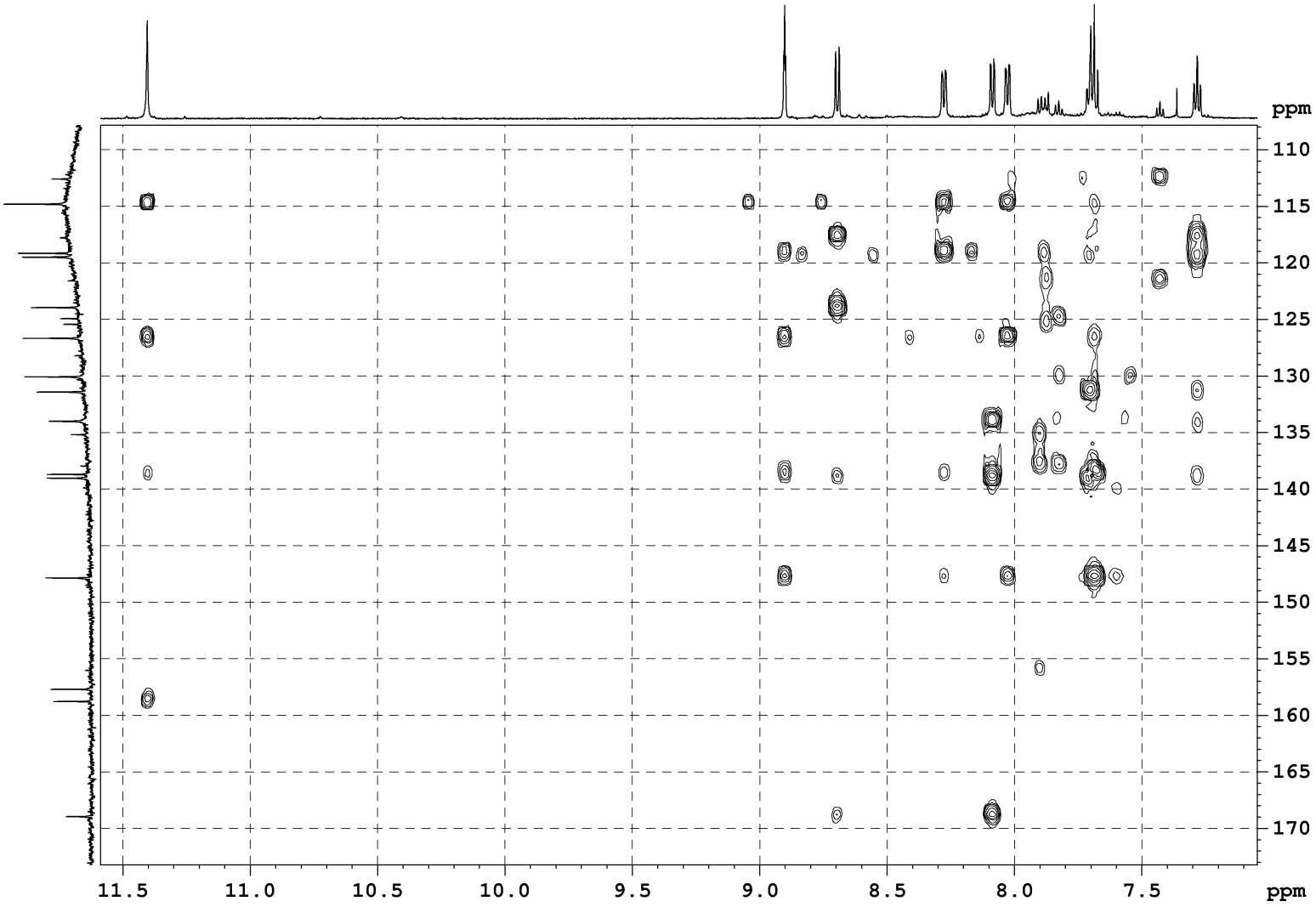



**Figure S94.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **4e** in DMSO at T = 303 K.

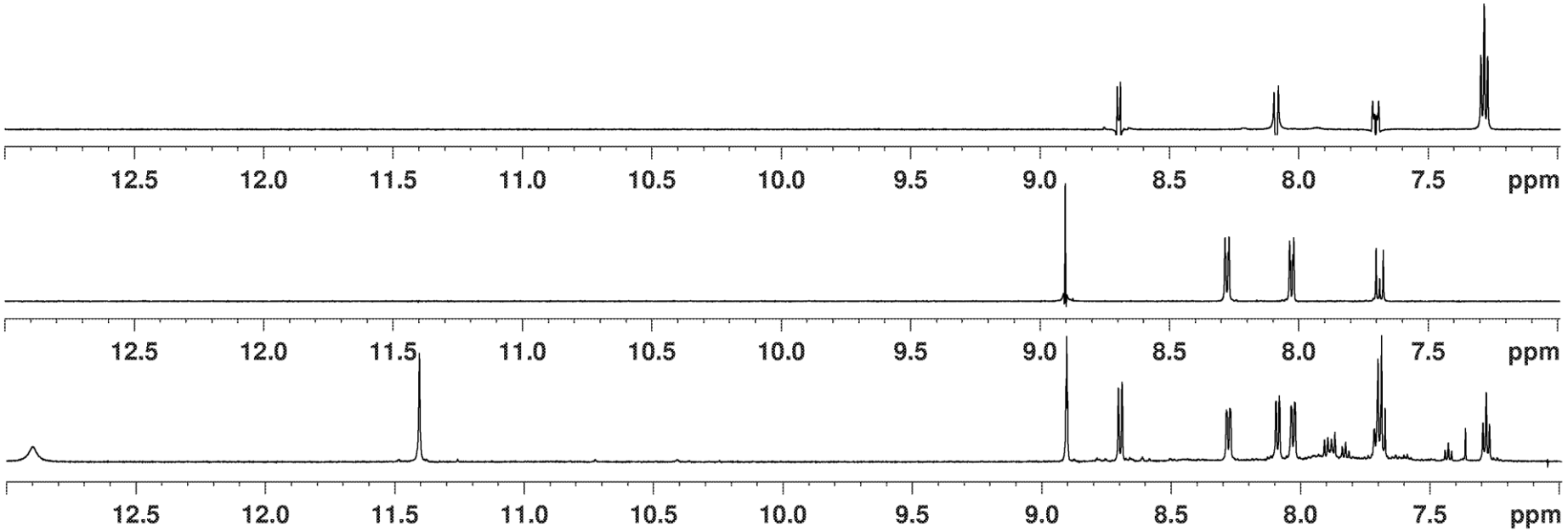



**Figure S95.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **4e** in DMSO at T = 303 K.

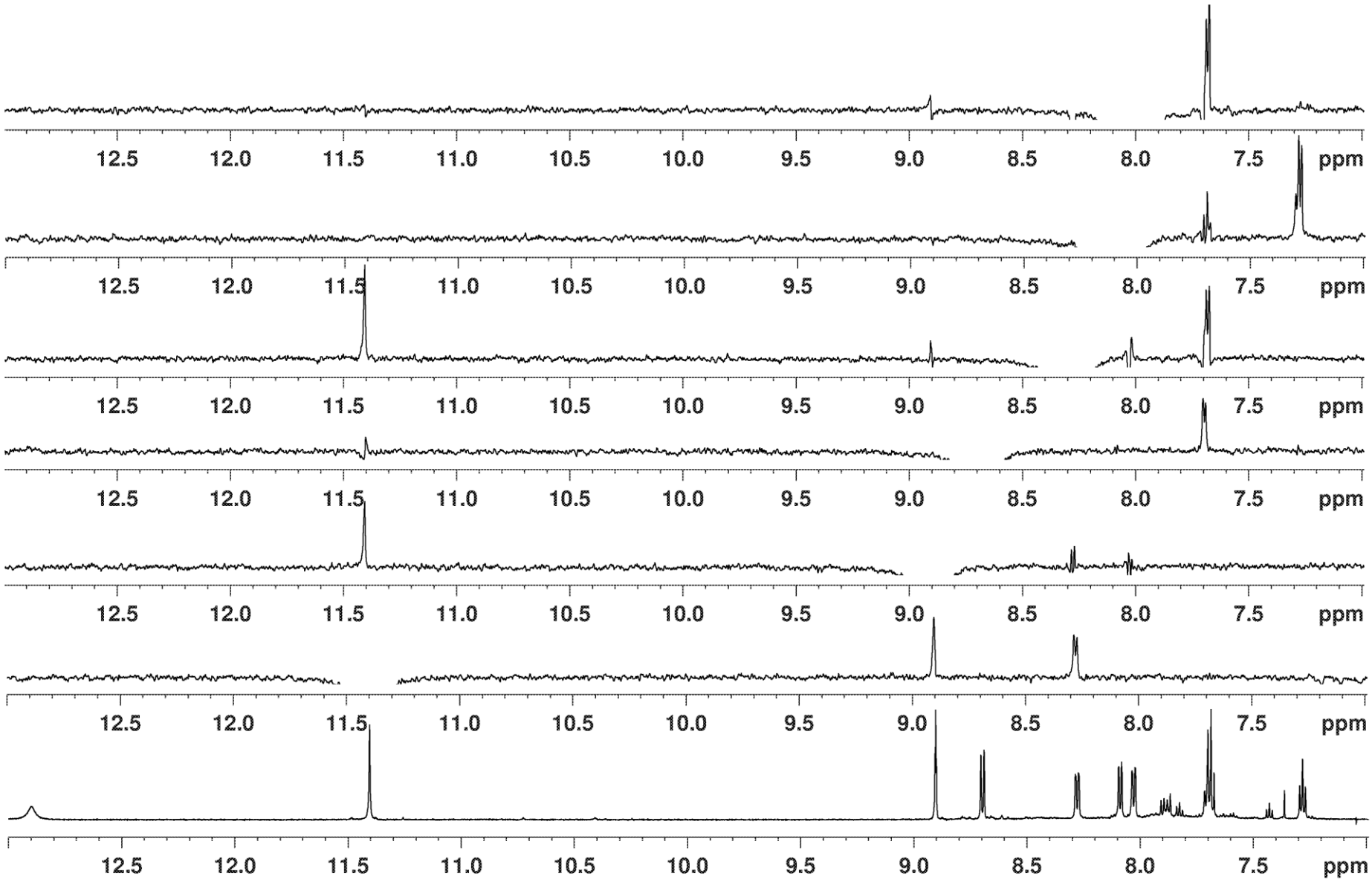



**Figure S96.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **4e** in DMSO at T = 303 K.

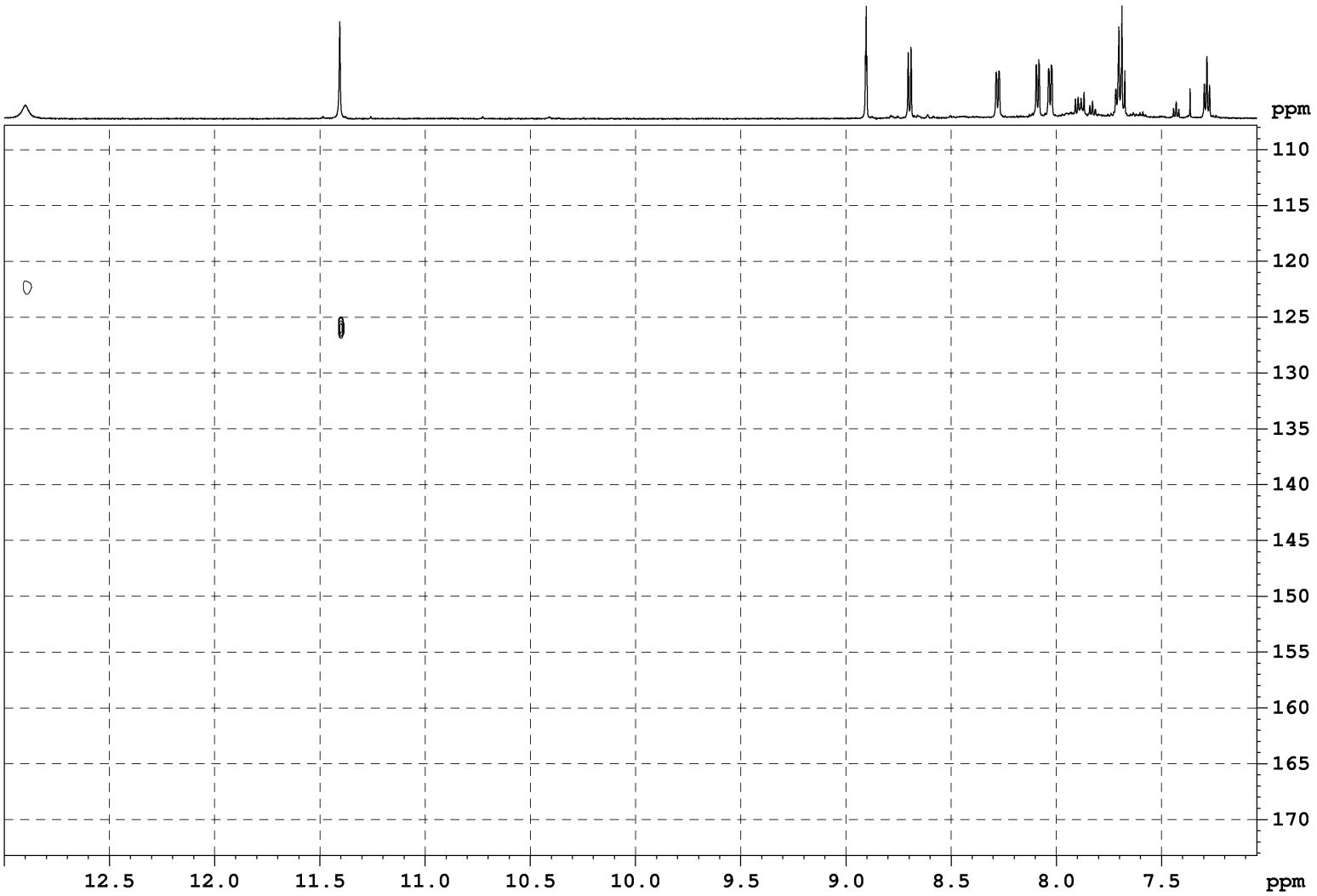



**Figure S97.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **4e** in DMSO at T = 303 K.

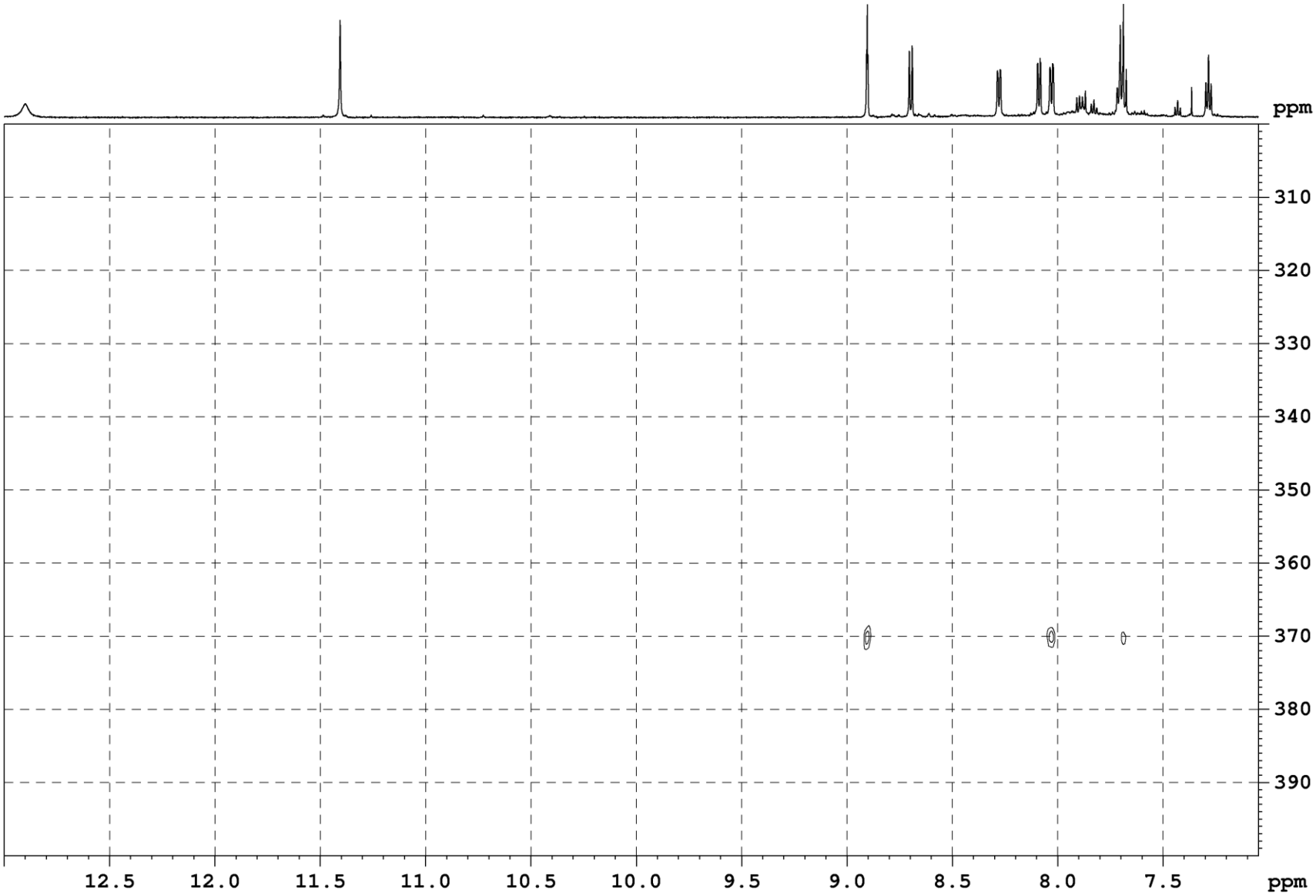



**Figure S98.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **4e** in DMSO at T = 303 K.

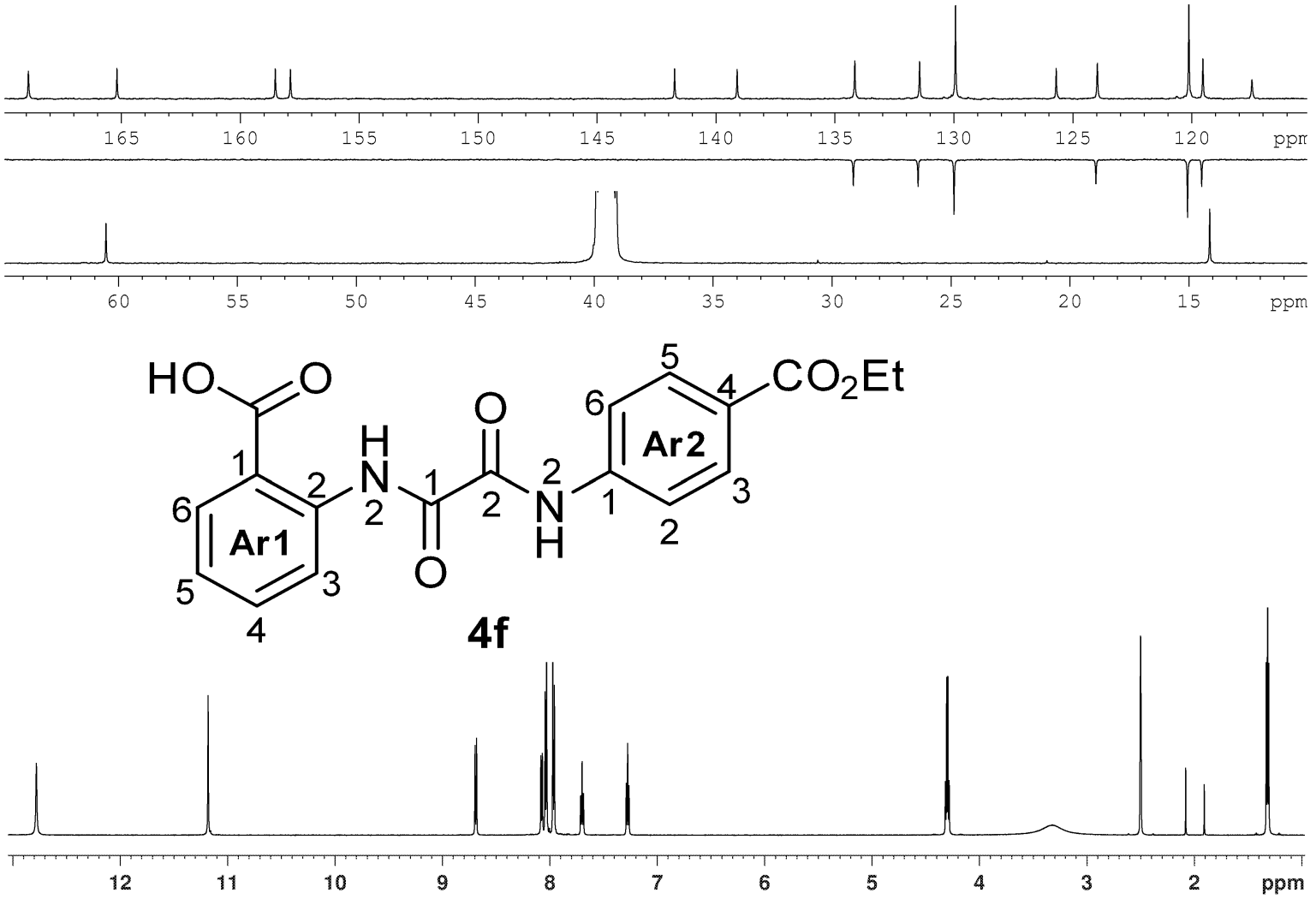



**Figure S99.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **4f** in DMSO at T = 303 K.

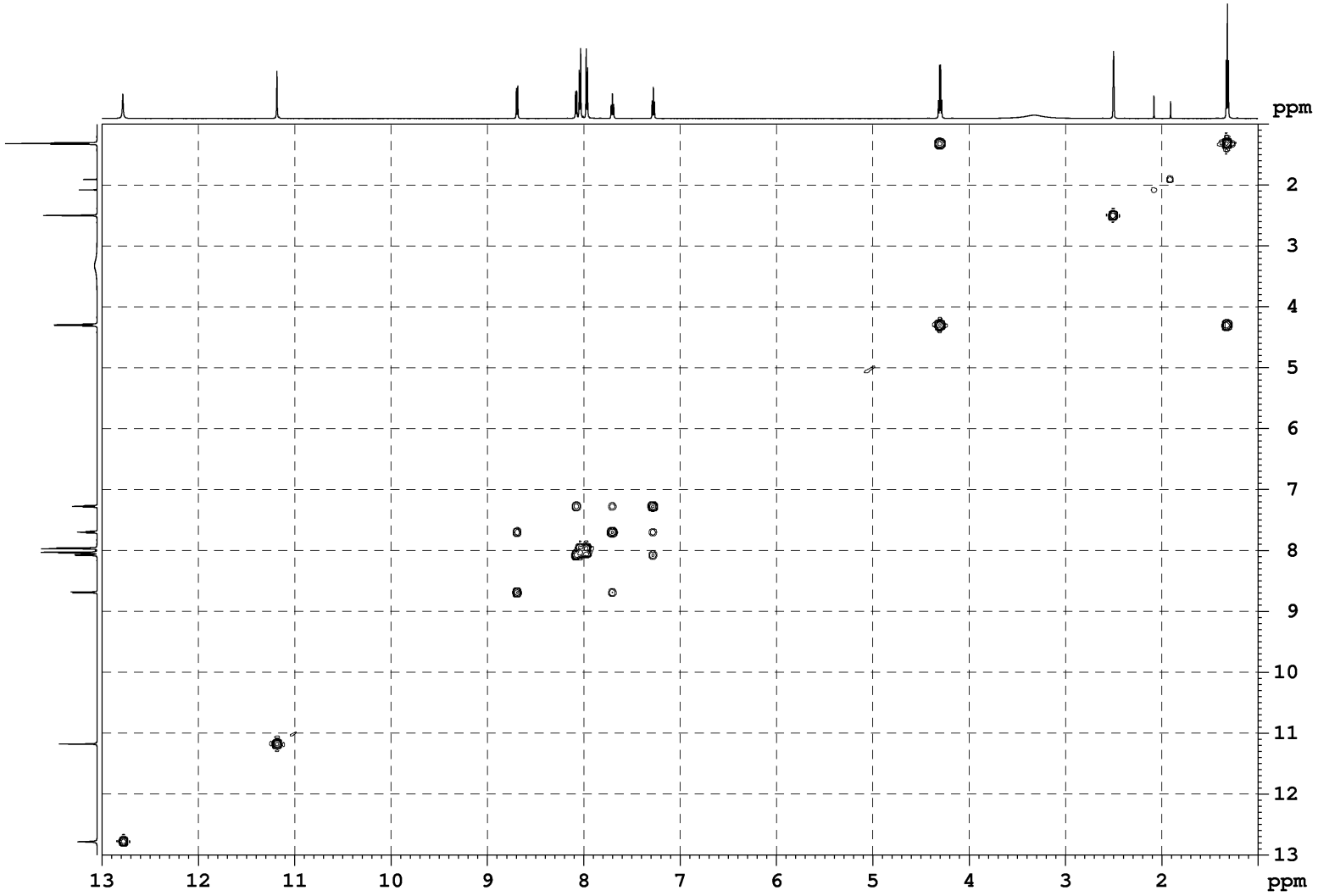



**Figure S100.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **4f** in DMSO at T = 303 K.

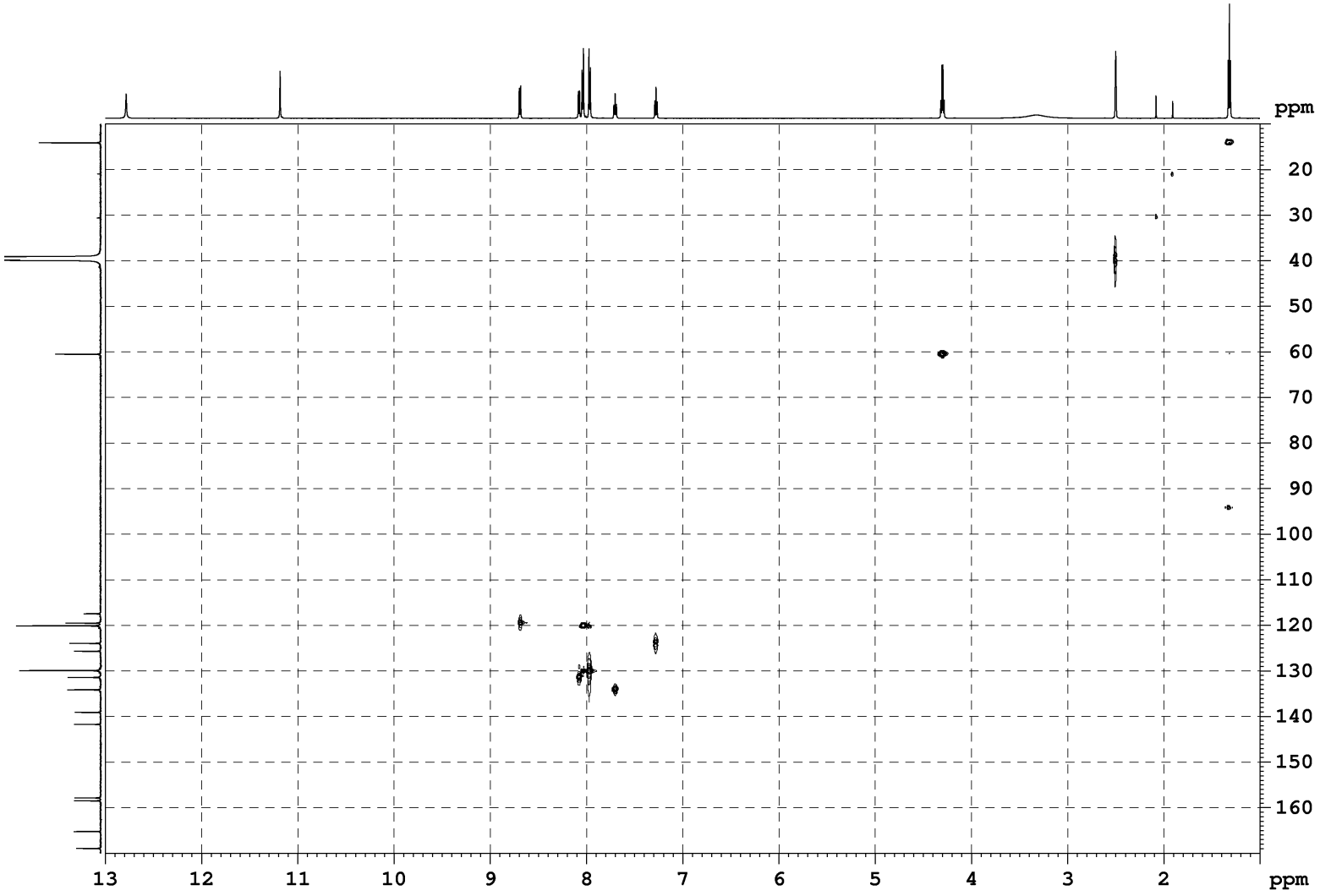



**Figure S101.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **4f** in DMSO at T = 303 K.

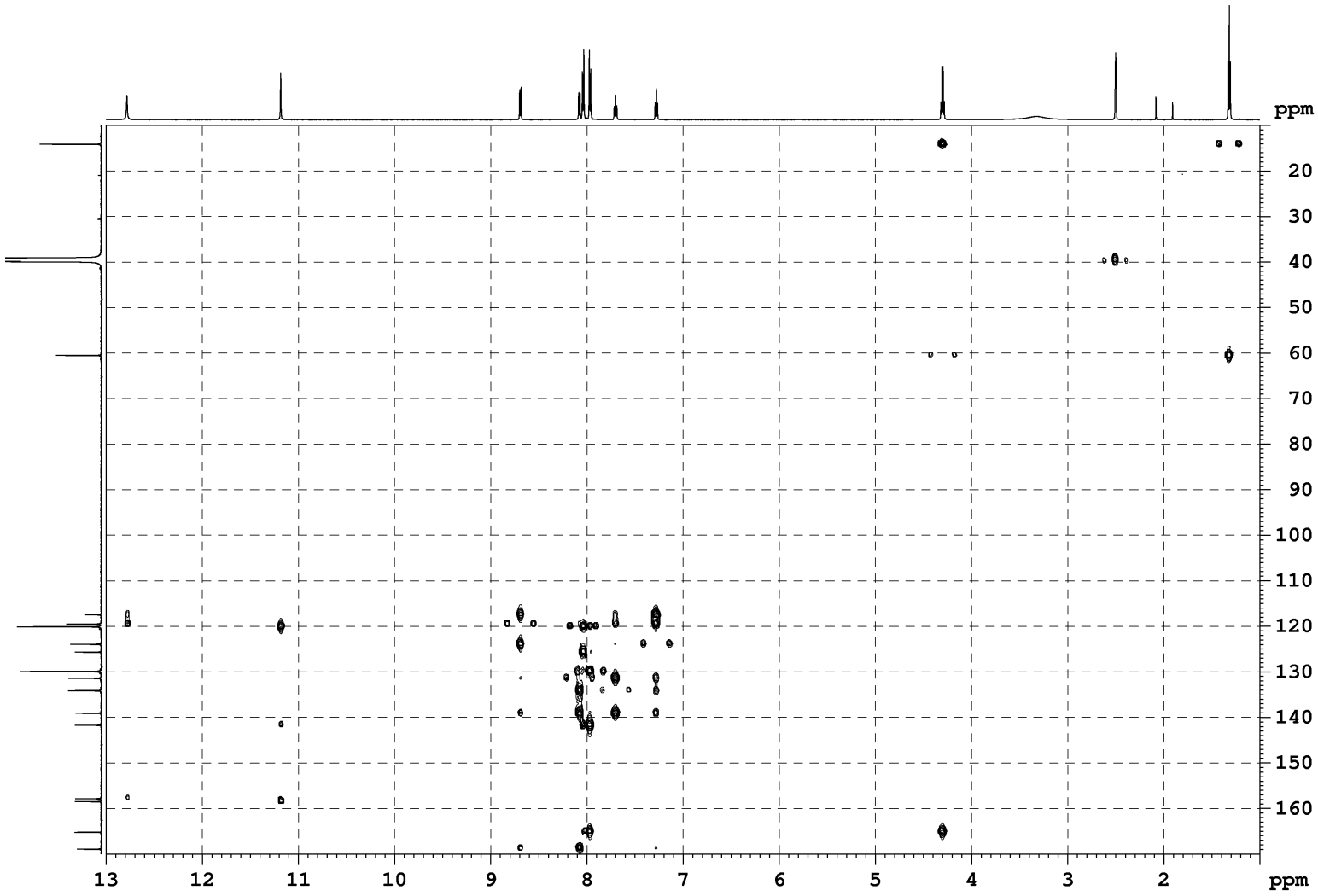



**Figure S102.** 2D $^{1}$H-$^{13}$C HMBC NMR spectra of **4f** in DMSO at T = 303 K.

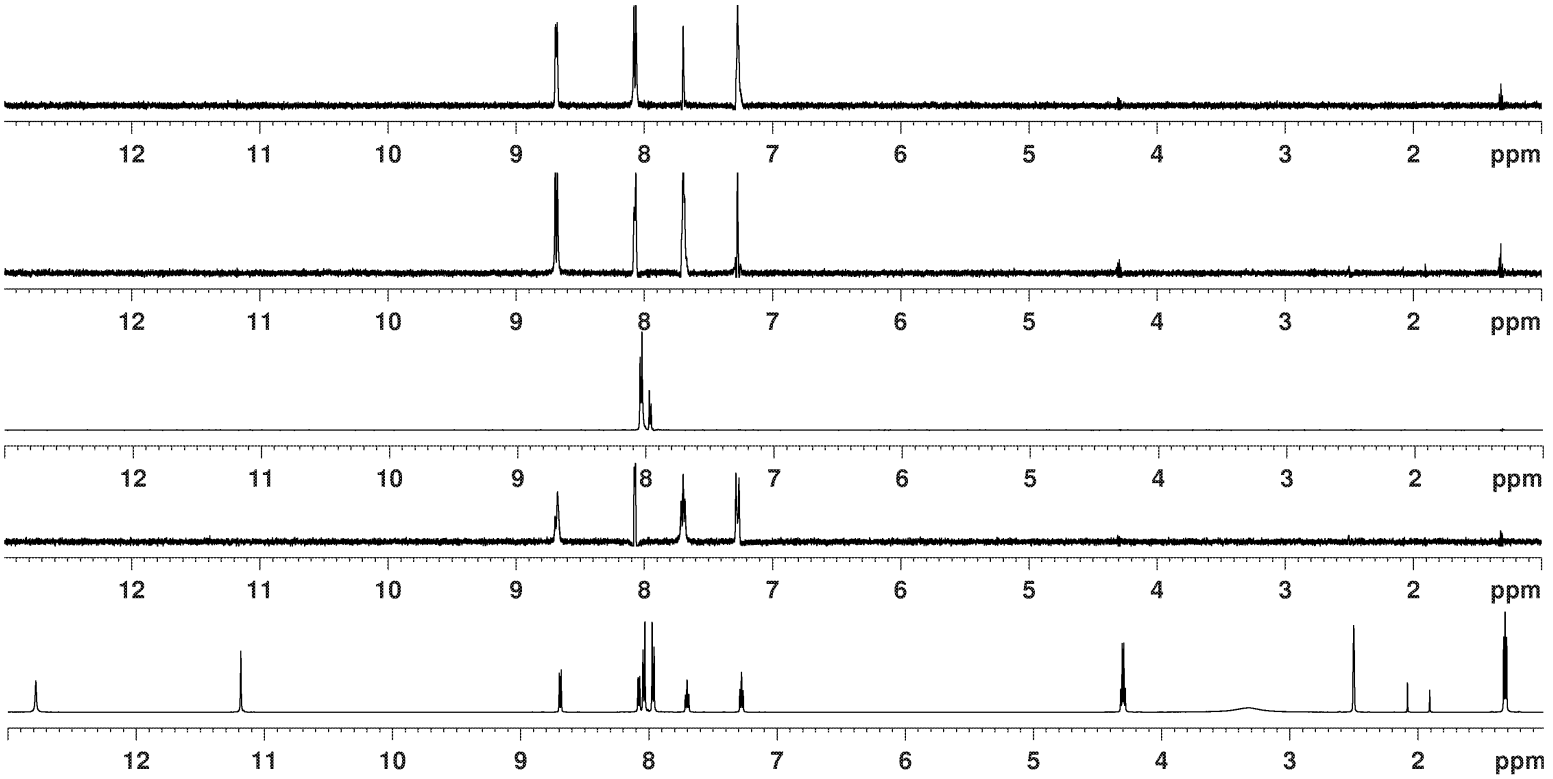



**Figure S103.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **4f** in DMSO at T = 303 K.

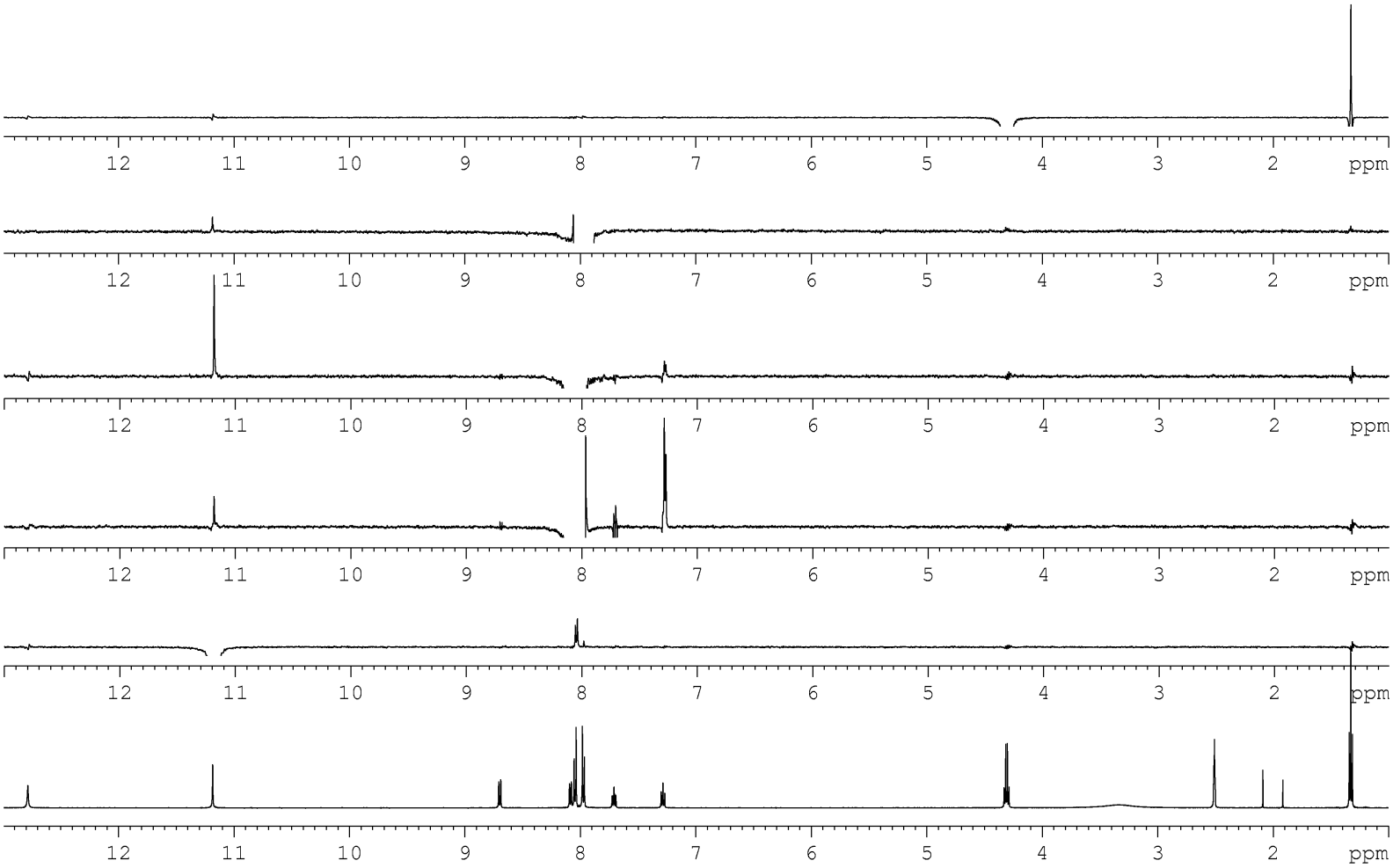



**Figure S104.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **4f** in DMSO at T = 303 K.

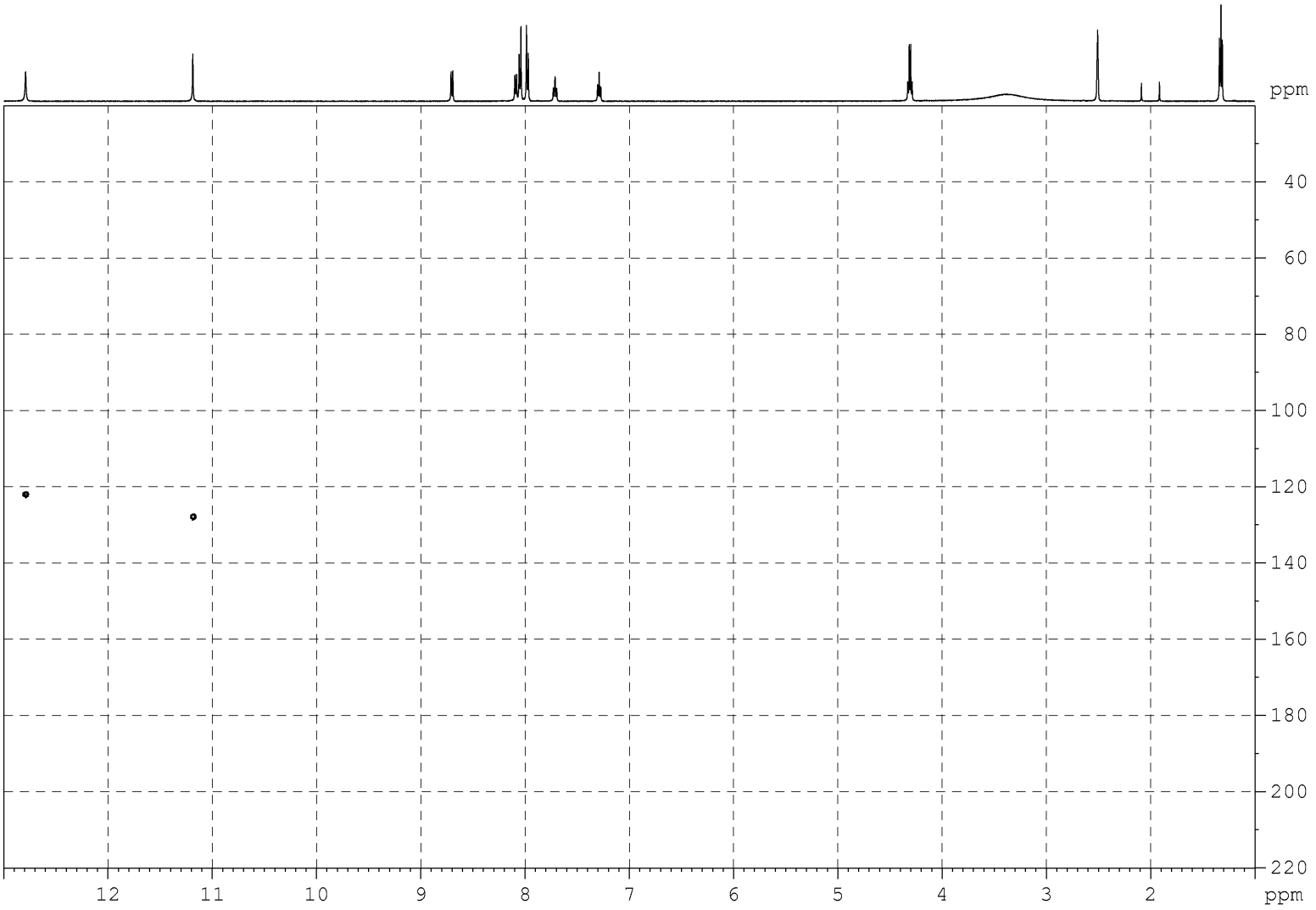



**Figure S105.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **4f** in DMSO at T = 303 K.

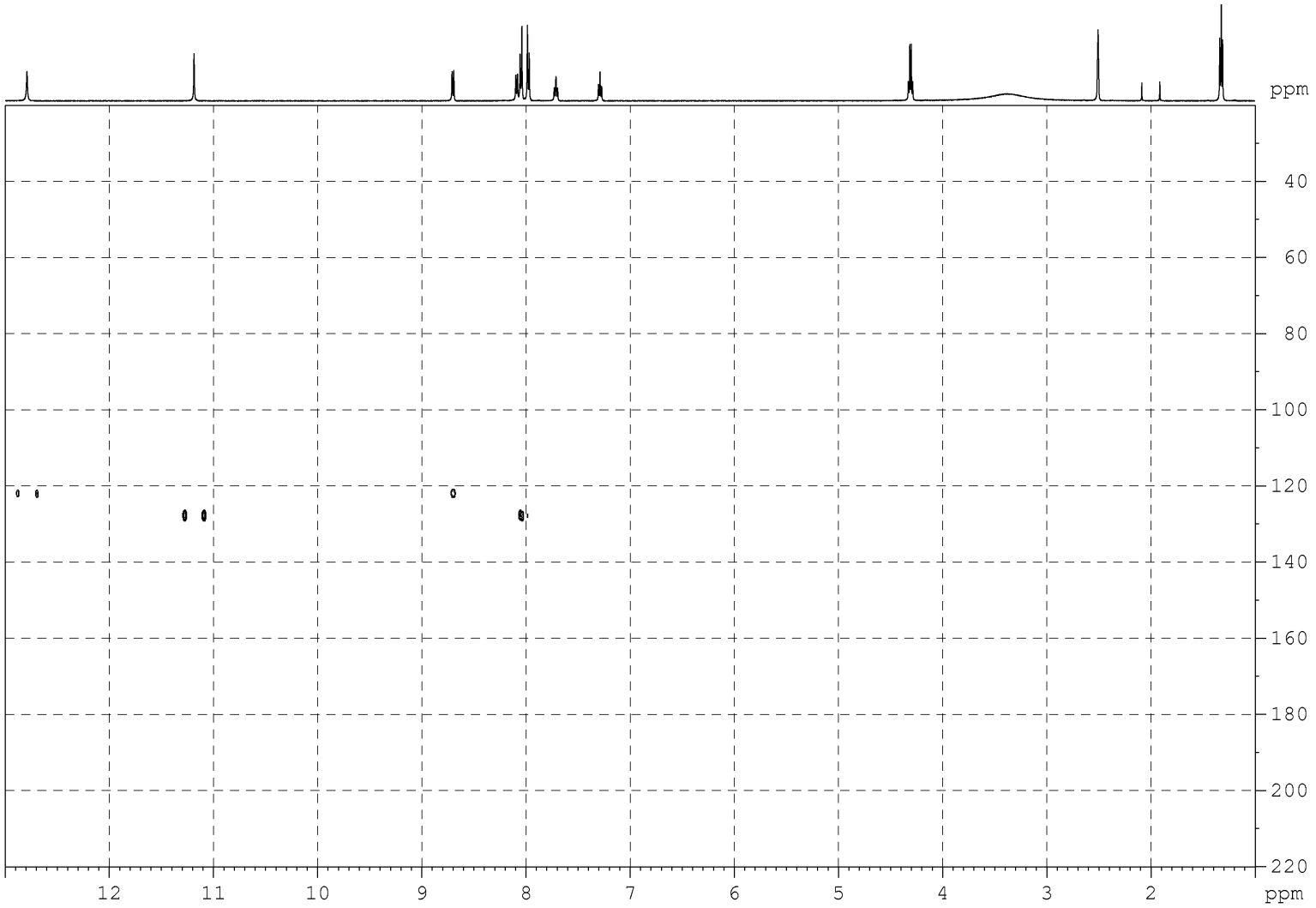



**Figure S106.** 2D $^{1}$H-$^{15}$N HMBC NMR spectra of **4f** in DMSO at T = 303 K.

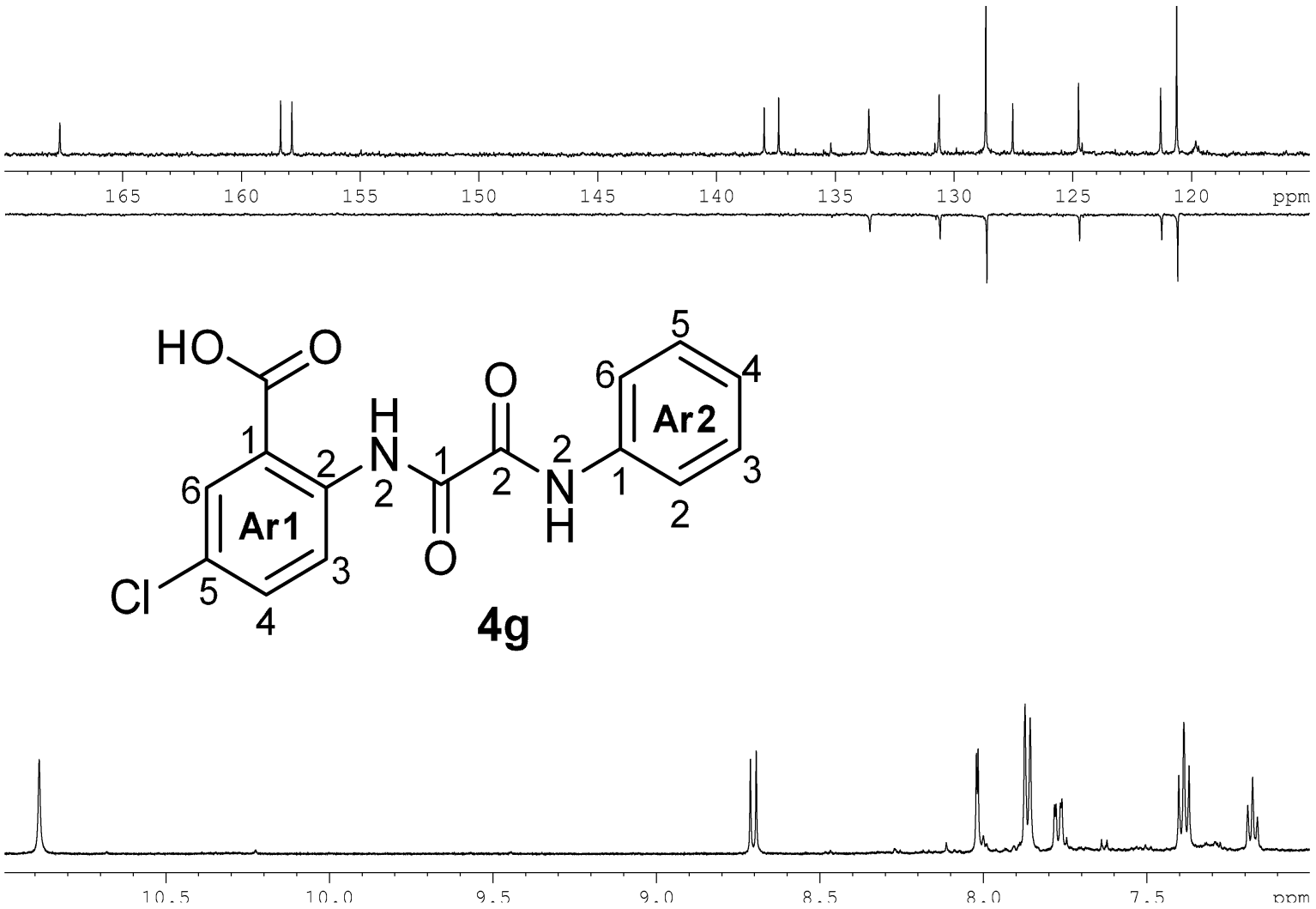



**Figure S107.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **4g** in DMSO at T = 303 K.

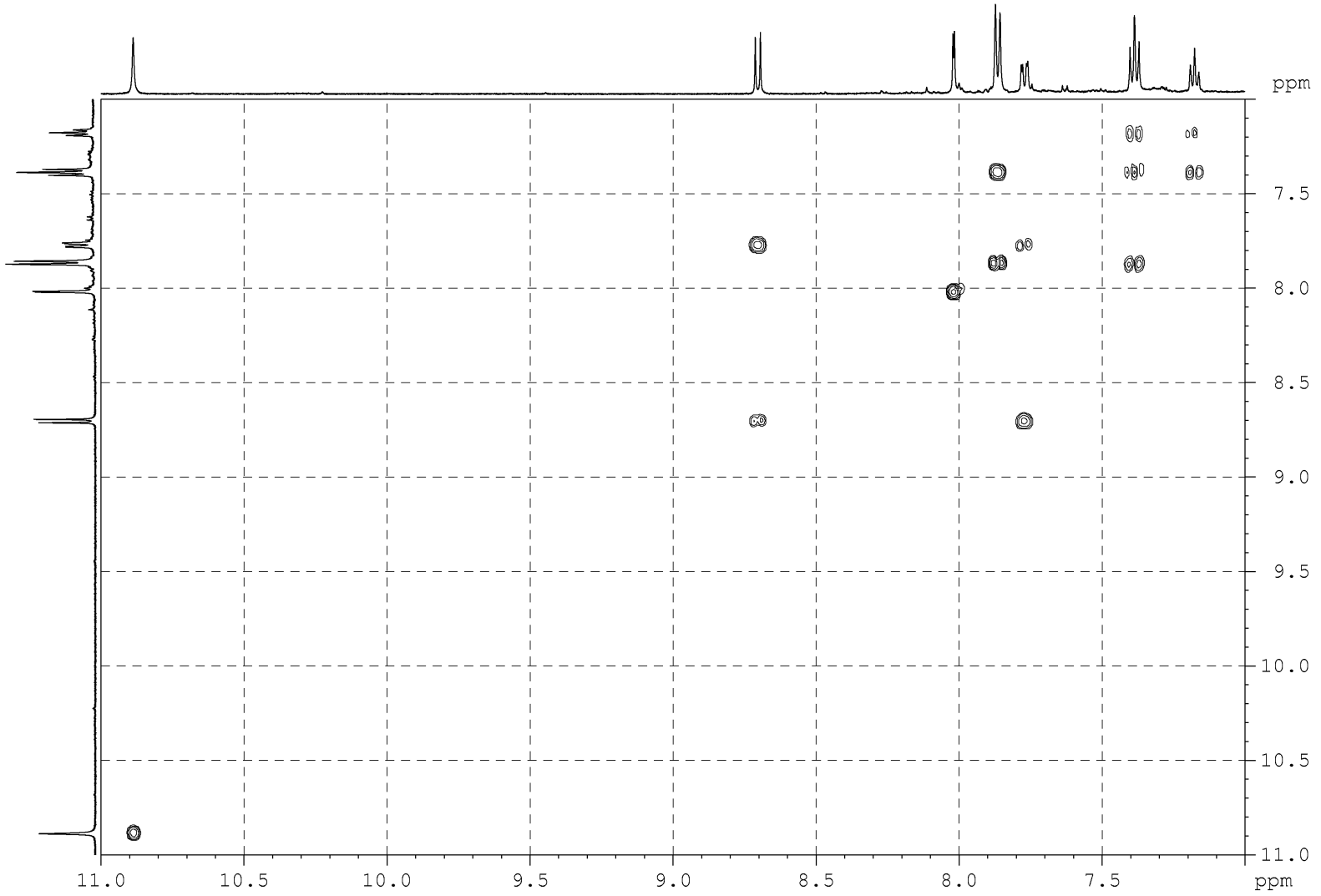



**Figure S108.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **4g** in DMSO at T = 303 K.

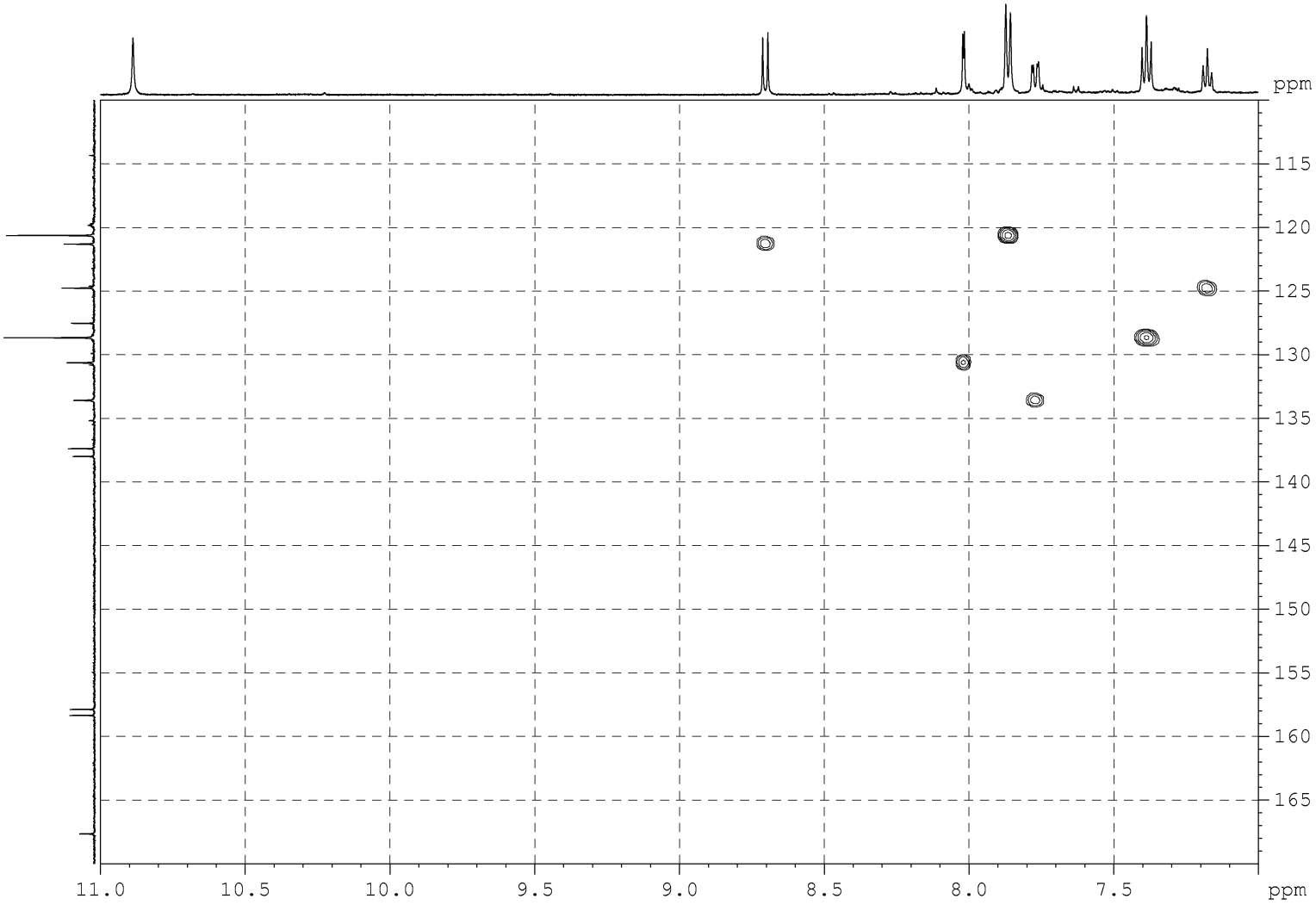



**Figure S109.** 2D $^{1}$H-$^{13}$C HSQC NMR spectra of **4g** in DMSO at T = 303 K.

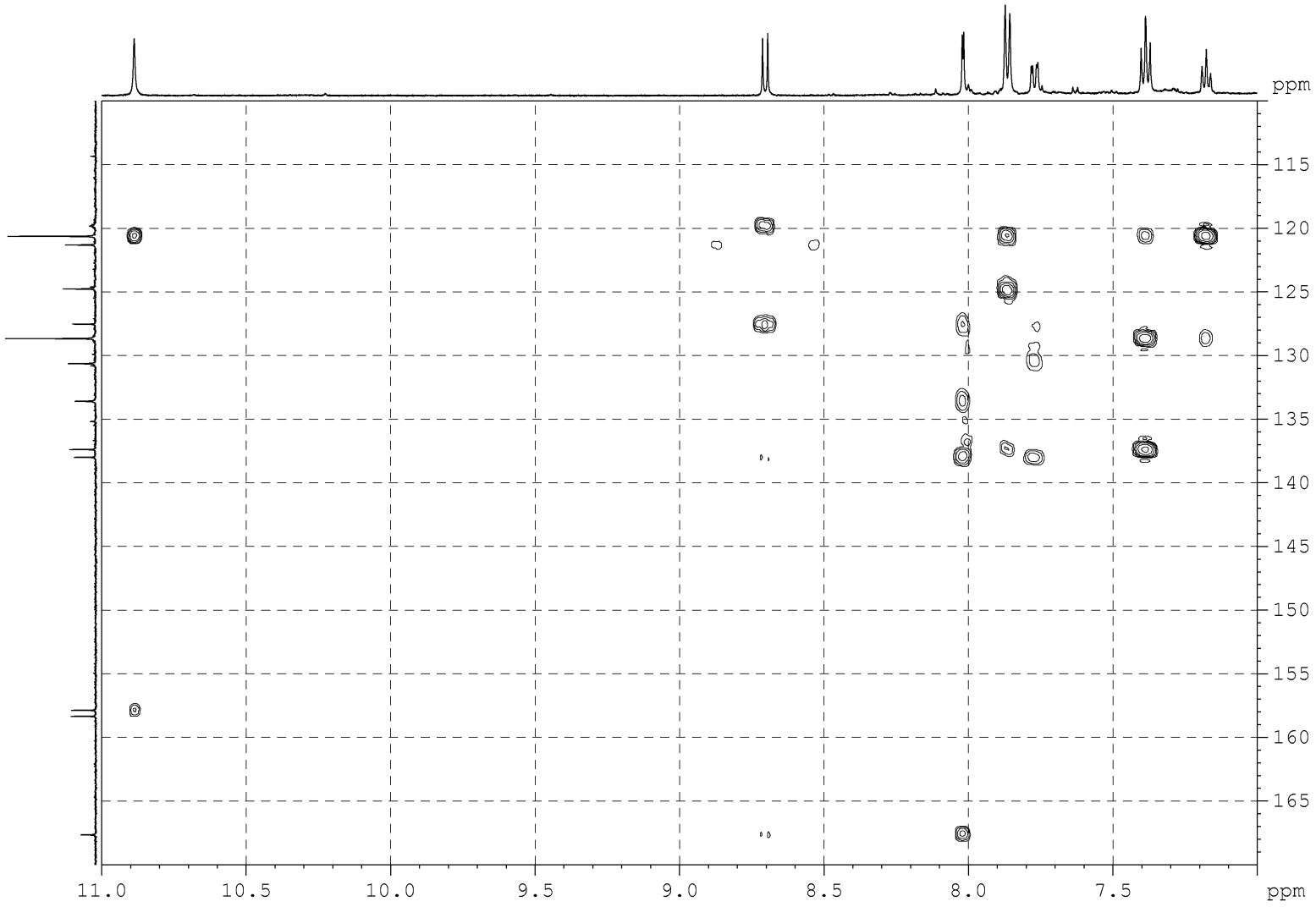



**Figure S110.** 2D $^{1}$H-$^{13}$C HMBC NMR spectra of **4g** in DMSO at T = 303 K.

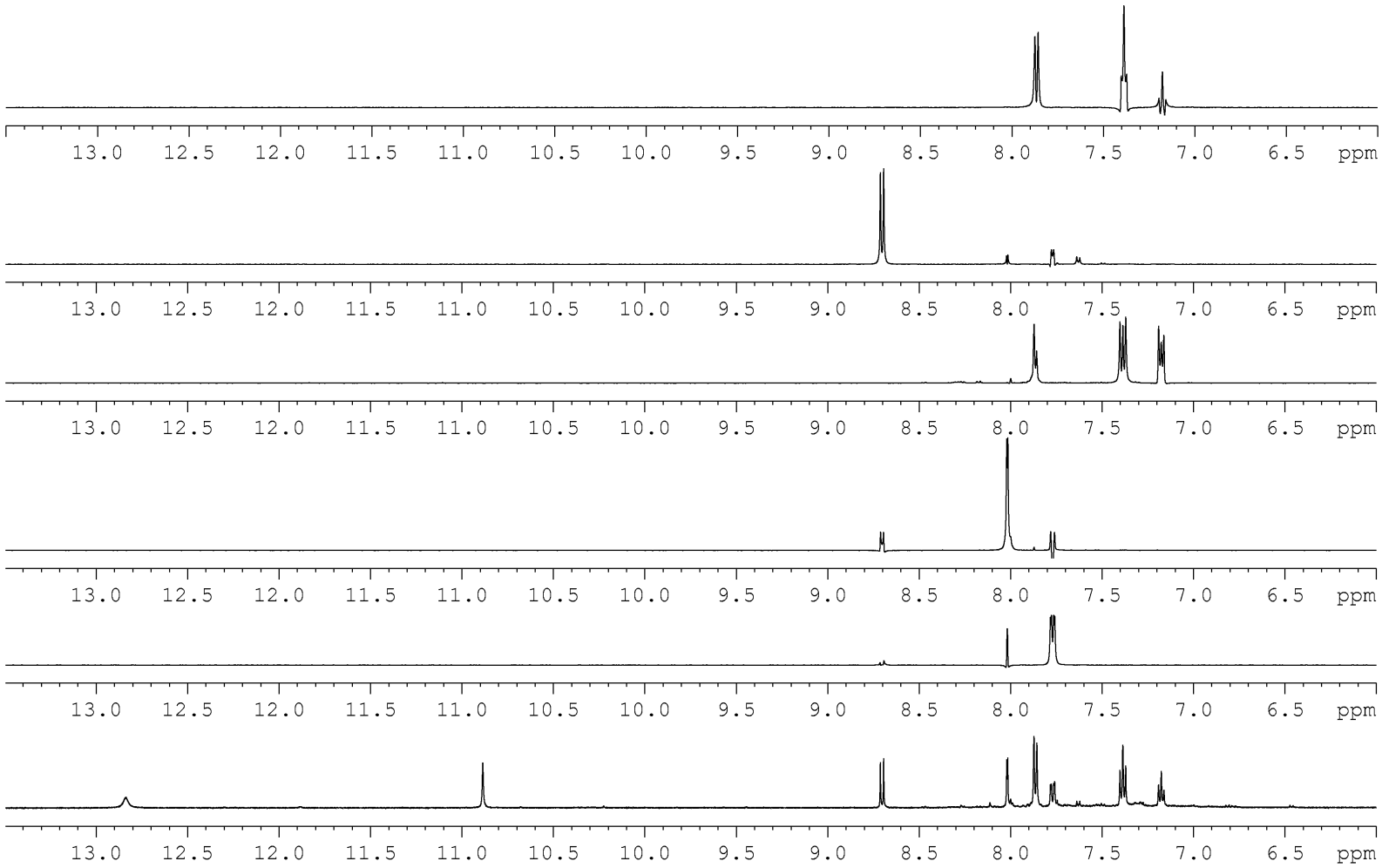



**Figure S111.** 1D $^{1}$H and $^{1}$H TOCSY NMR spectra of **4g** in DMSO at T = 303 K.

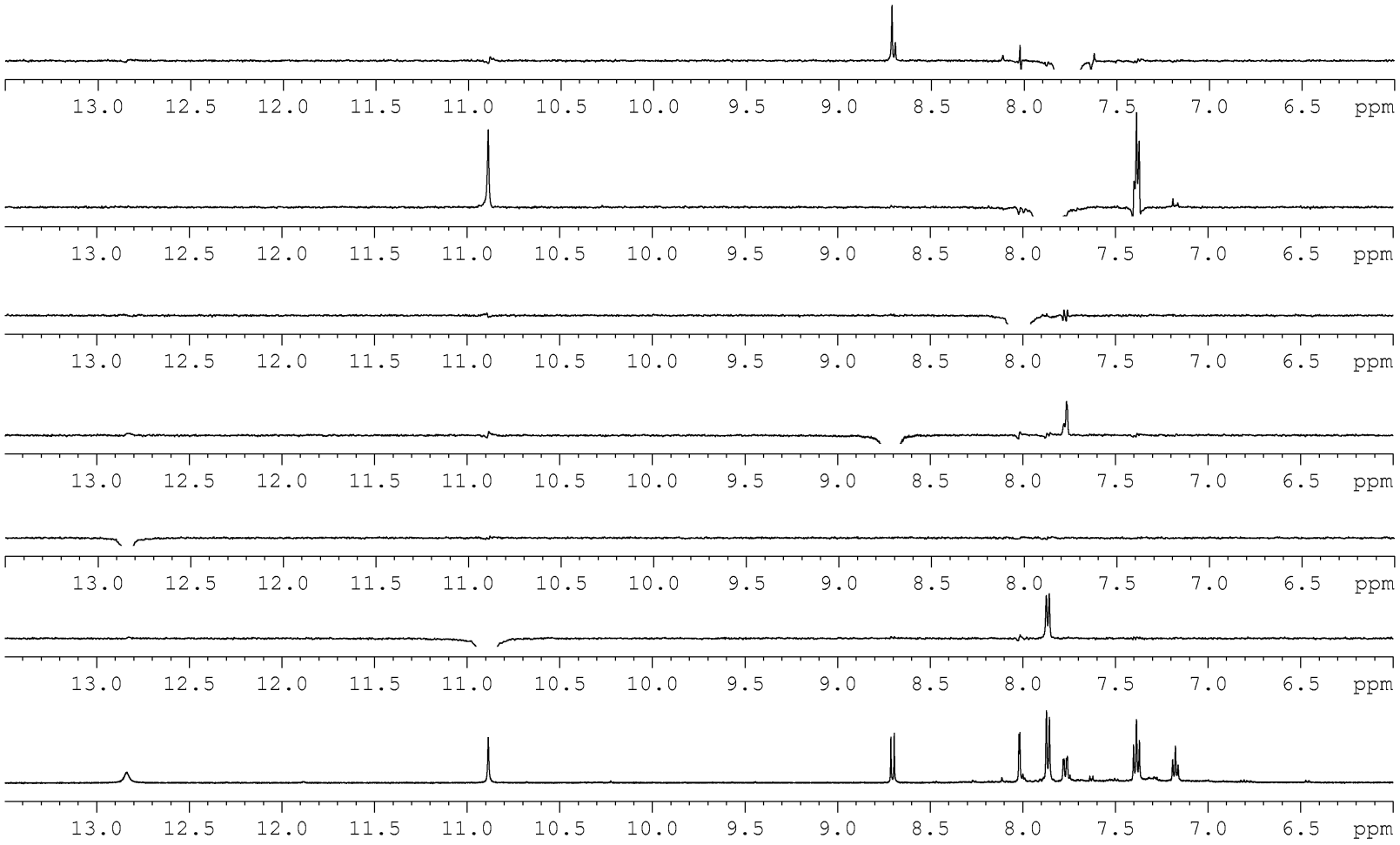



**Figure S112.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **4g** in DMSO at T = 303 K.

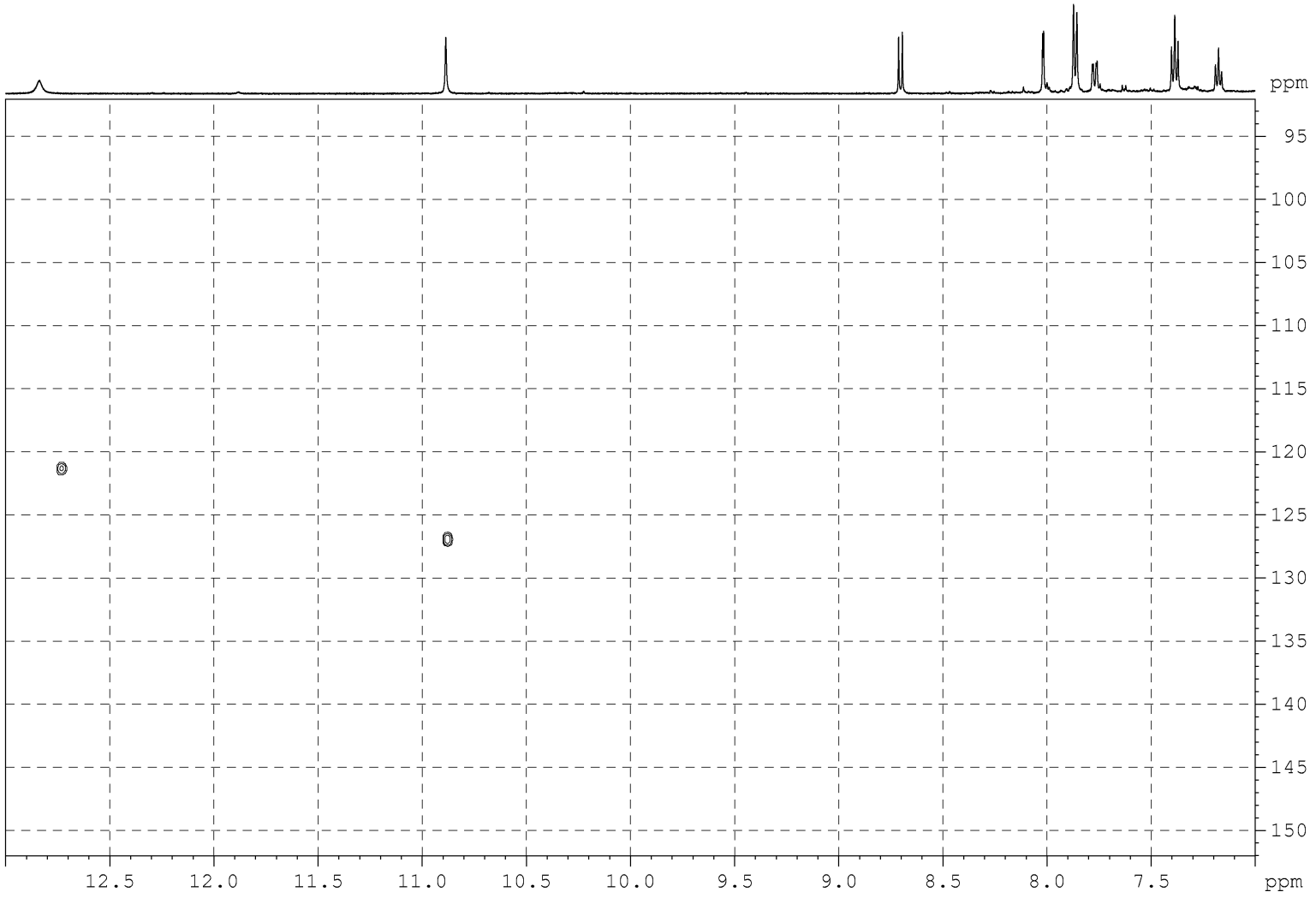



**Figure S113.** 2D $^{1}$H-$^{15}$N HSQC NMR spectra of **4g** in DMSO at T = 303 K.

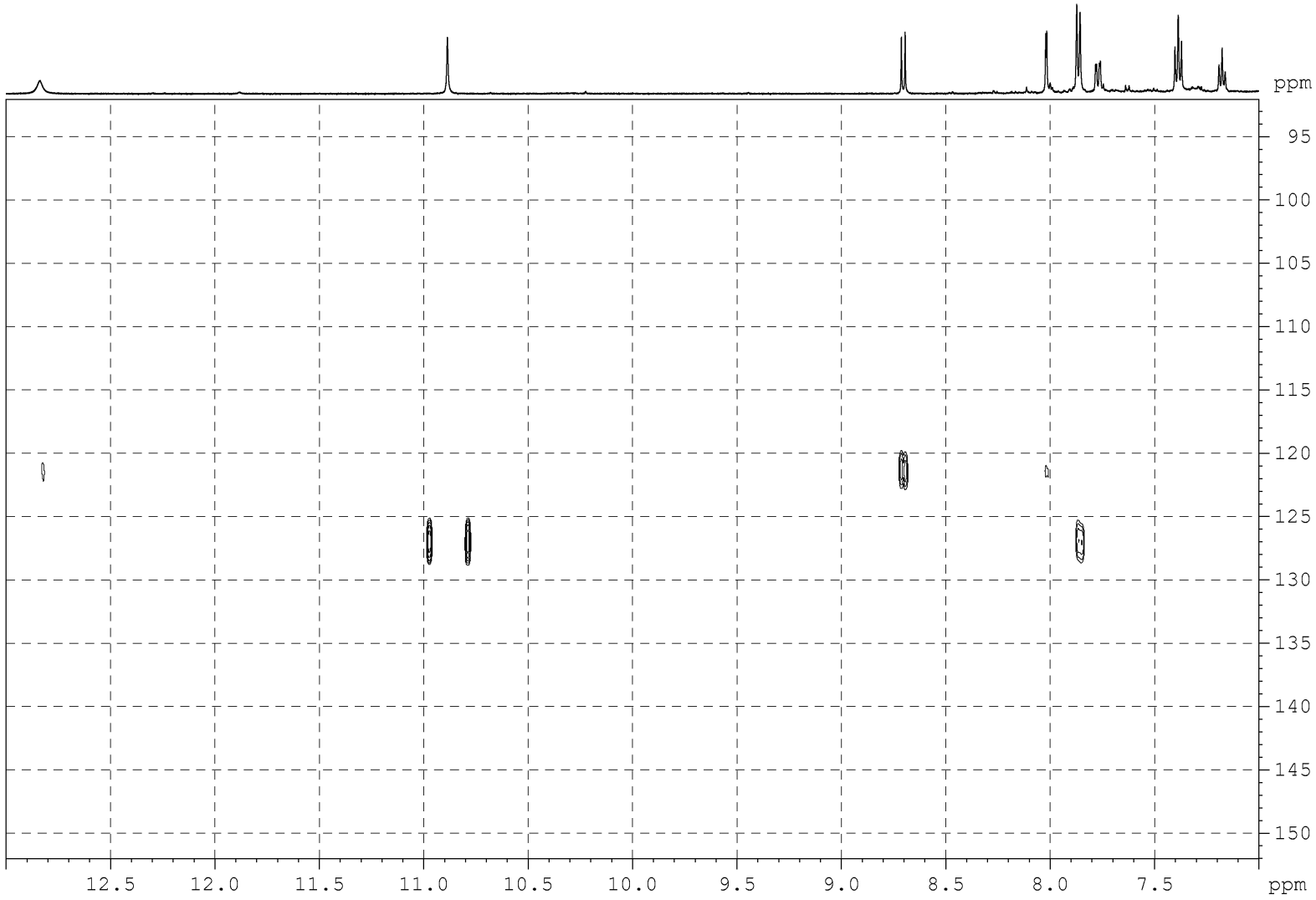



**Figure S114.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **4g** in DMSO at T = 303 K.

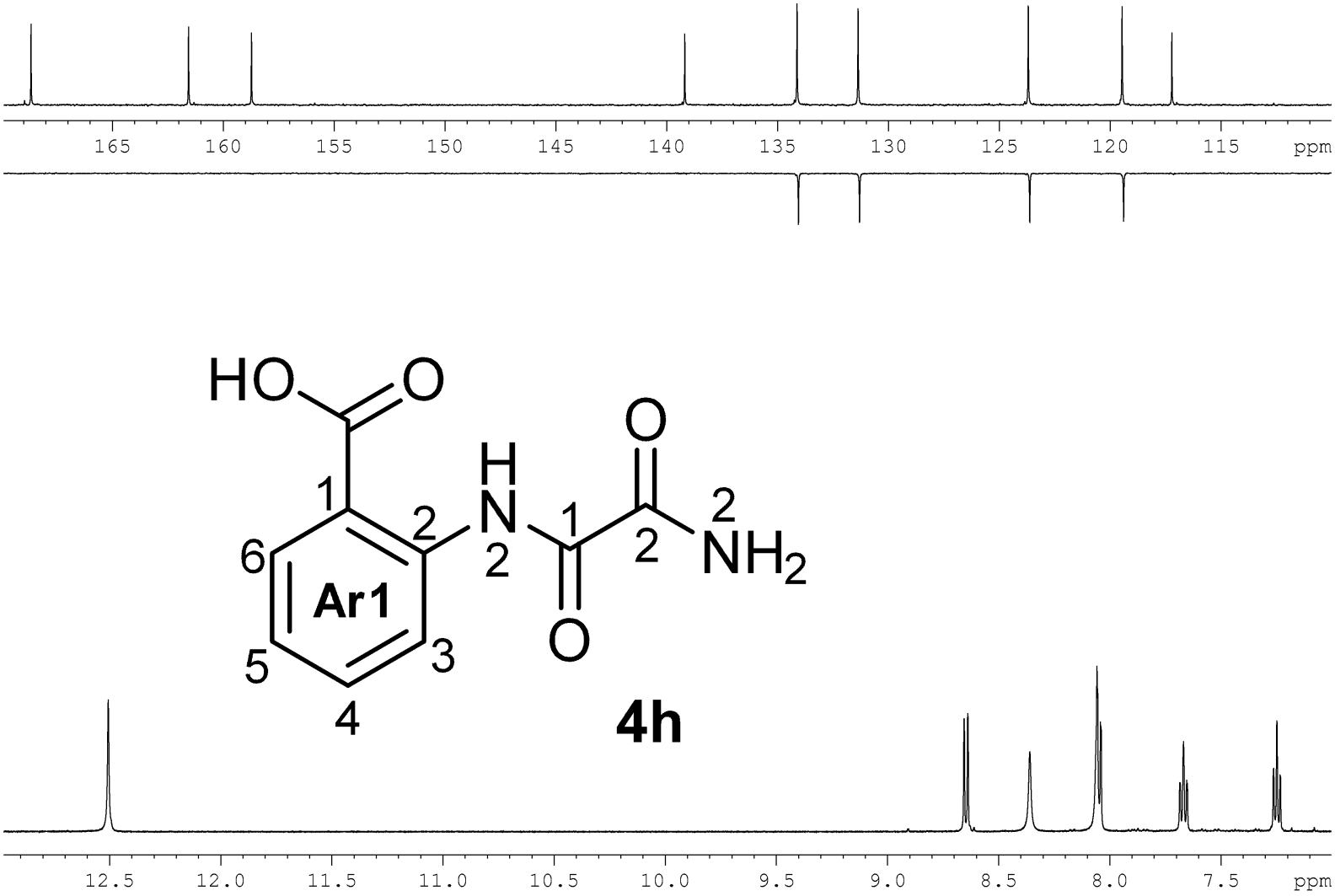



**Figure S115.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **4h** in DMSO at T = 303 K.

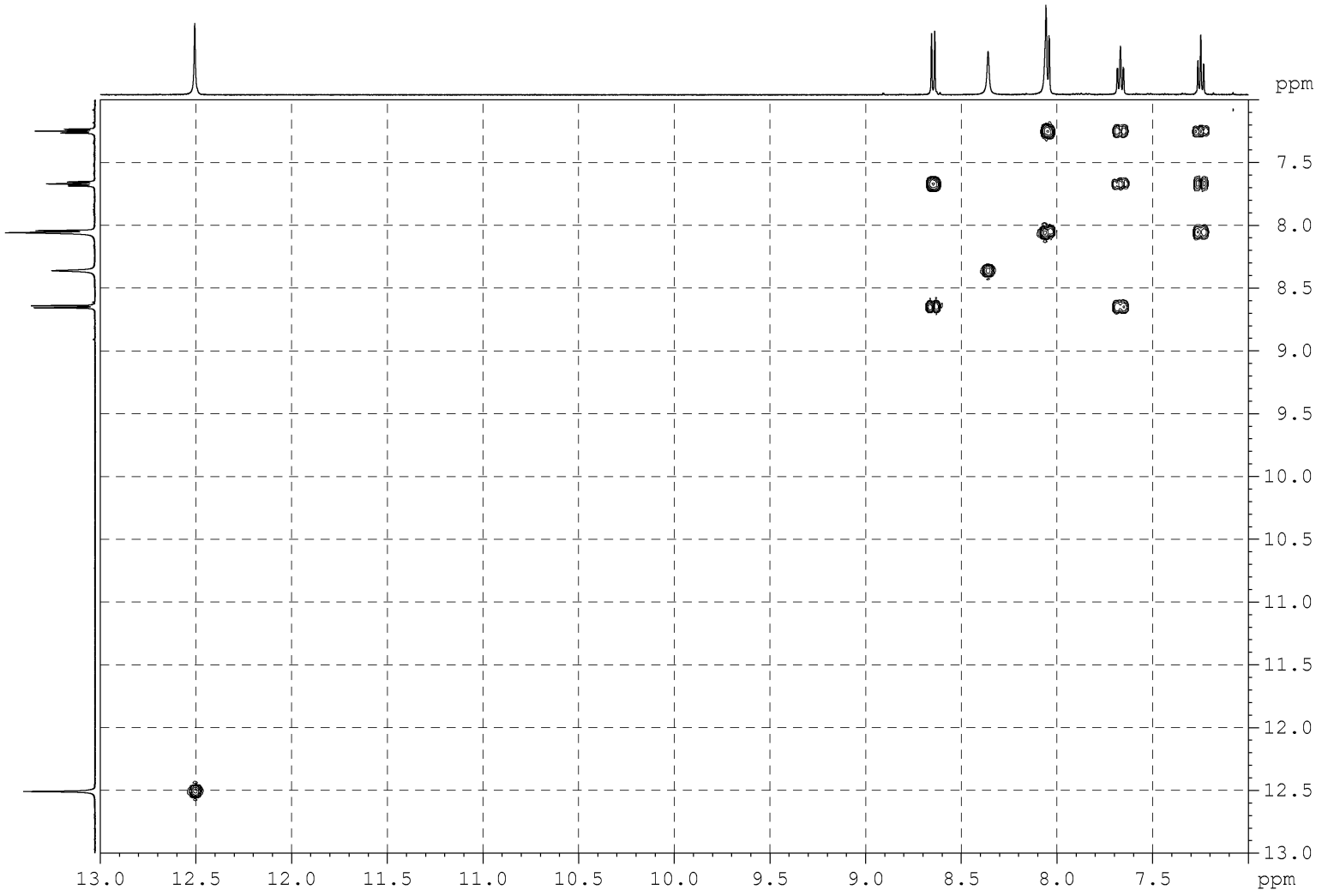



**Figure S116.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **4h** in DMSO at T = 303 K.

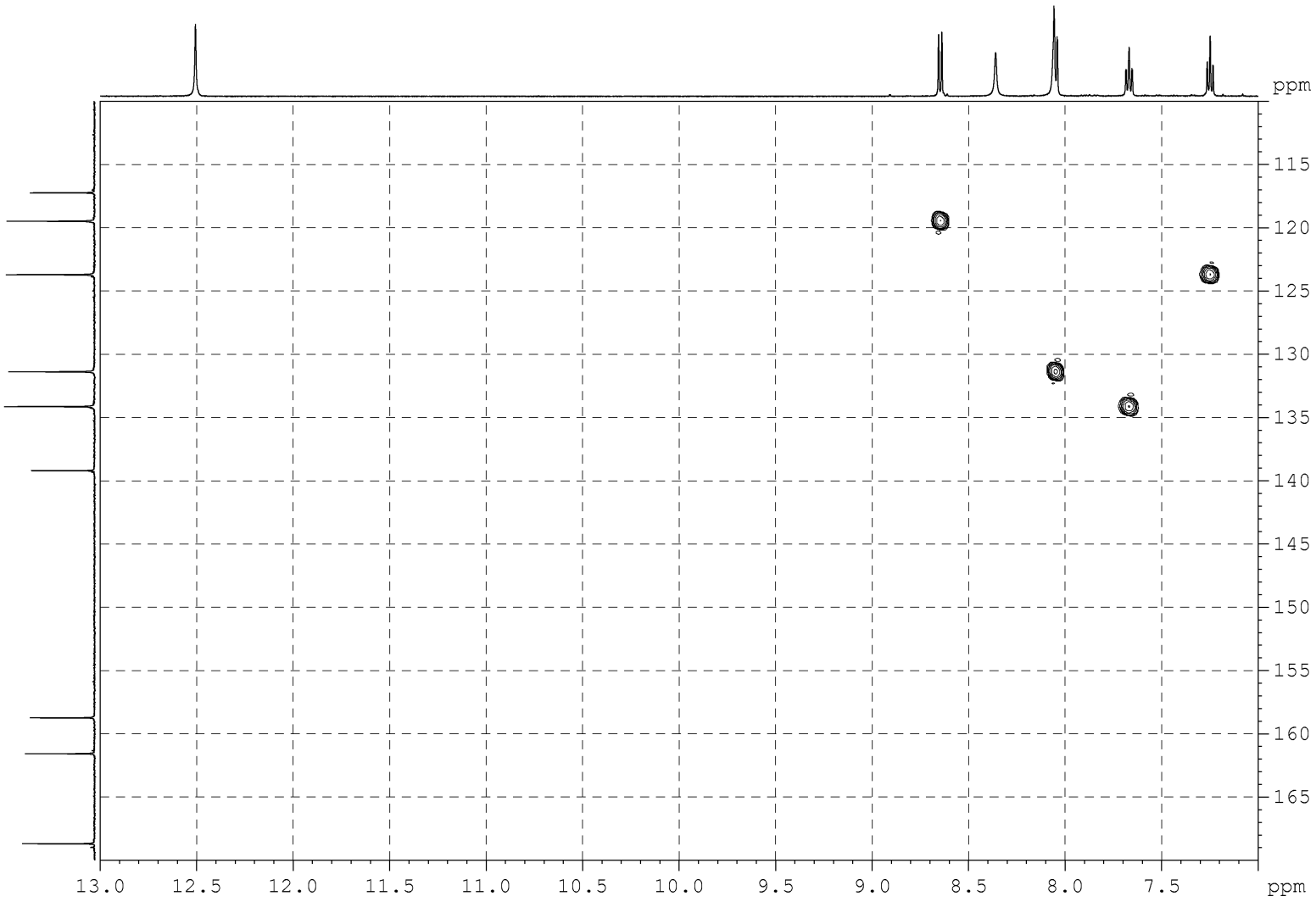



**Figure S117.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **4h** in DMSO at T = 303 K.

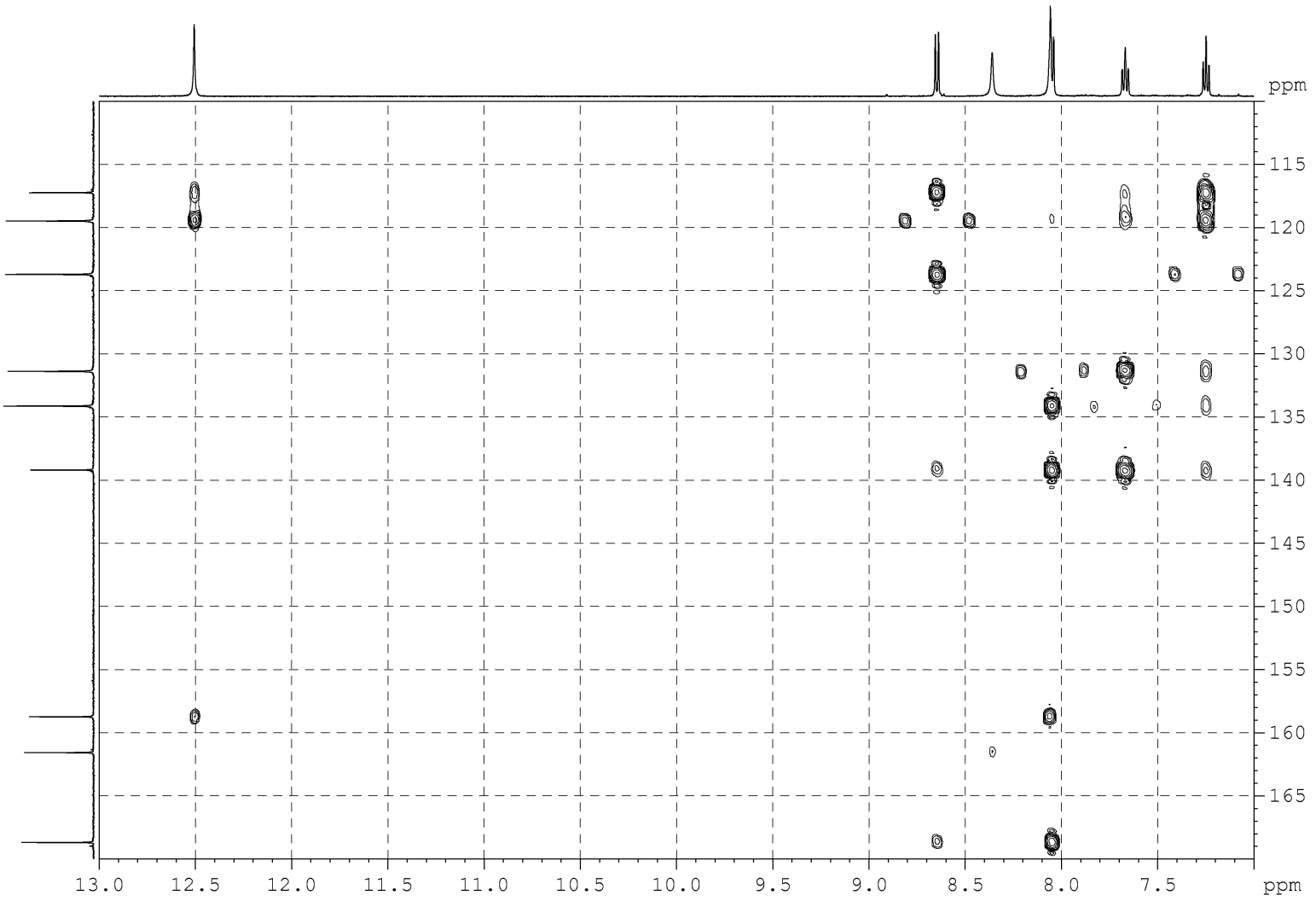



**Figure S118.** 2D $^{1}$H-$^{13}$C HMBC NMR spectra of **4h** in DMSO at T = 303 K.

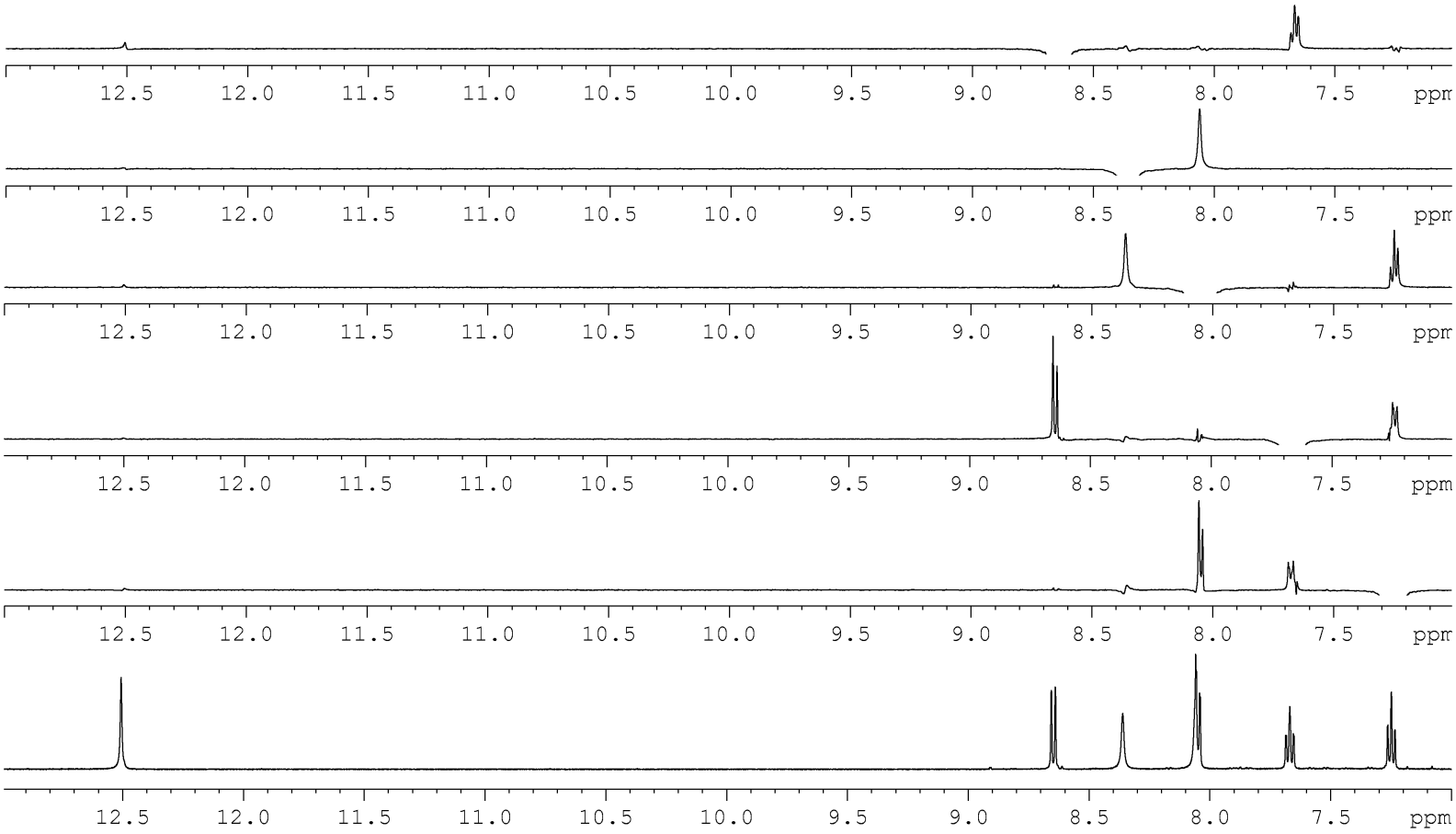



**Figure S119.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **4h** in DMSO at T = 303 K.

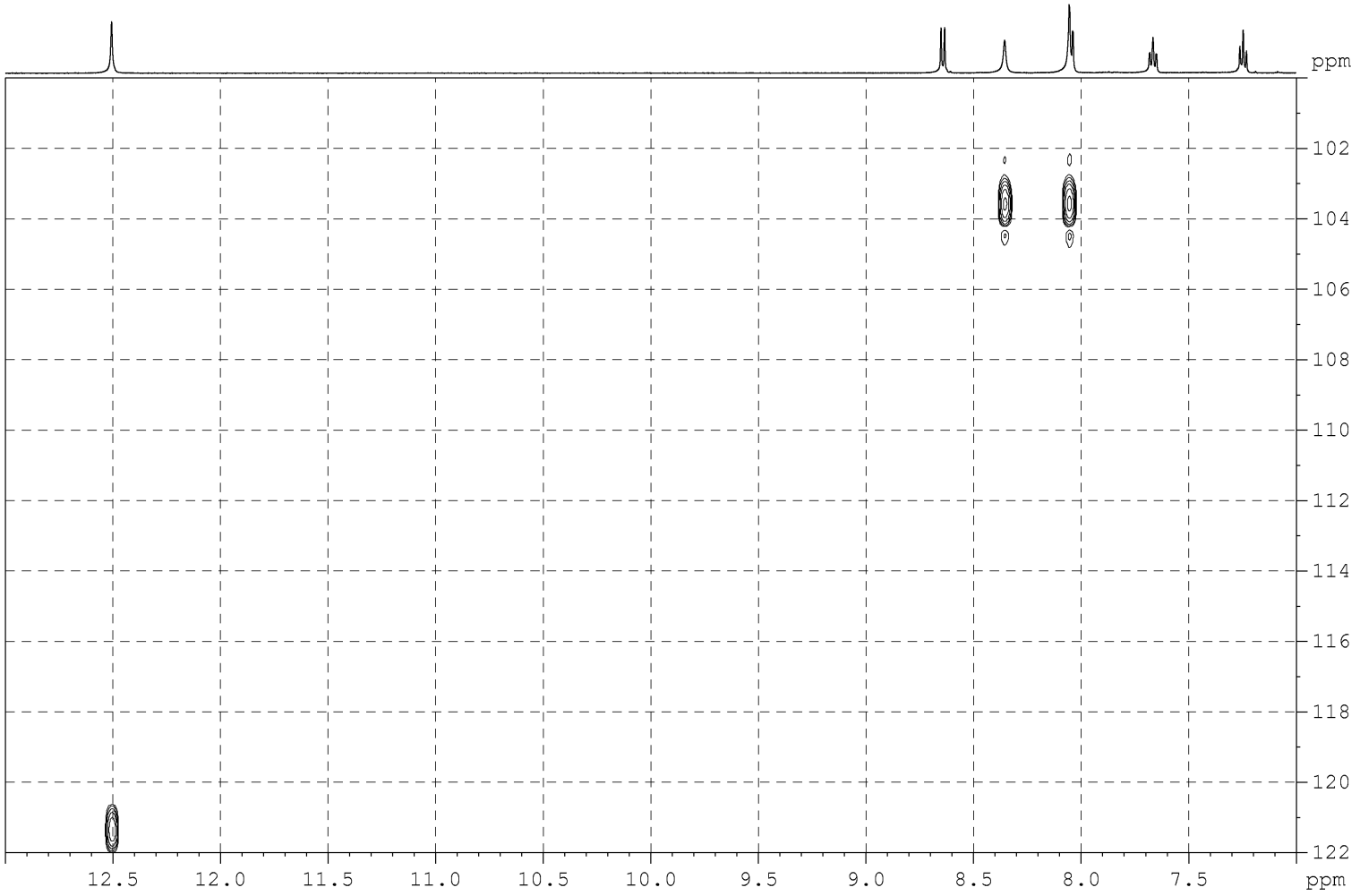



**Figure S120.** 2D $^{1}H$-$^{15}N$ HSQC NMR spectra of **4h** in DMSO at T = 303 K.

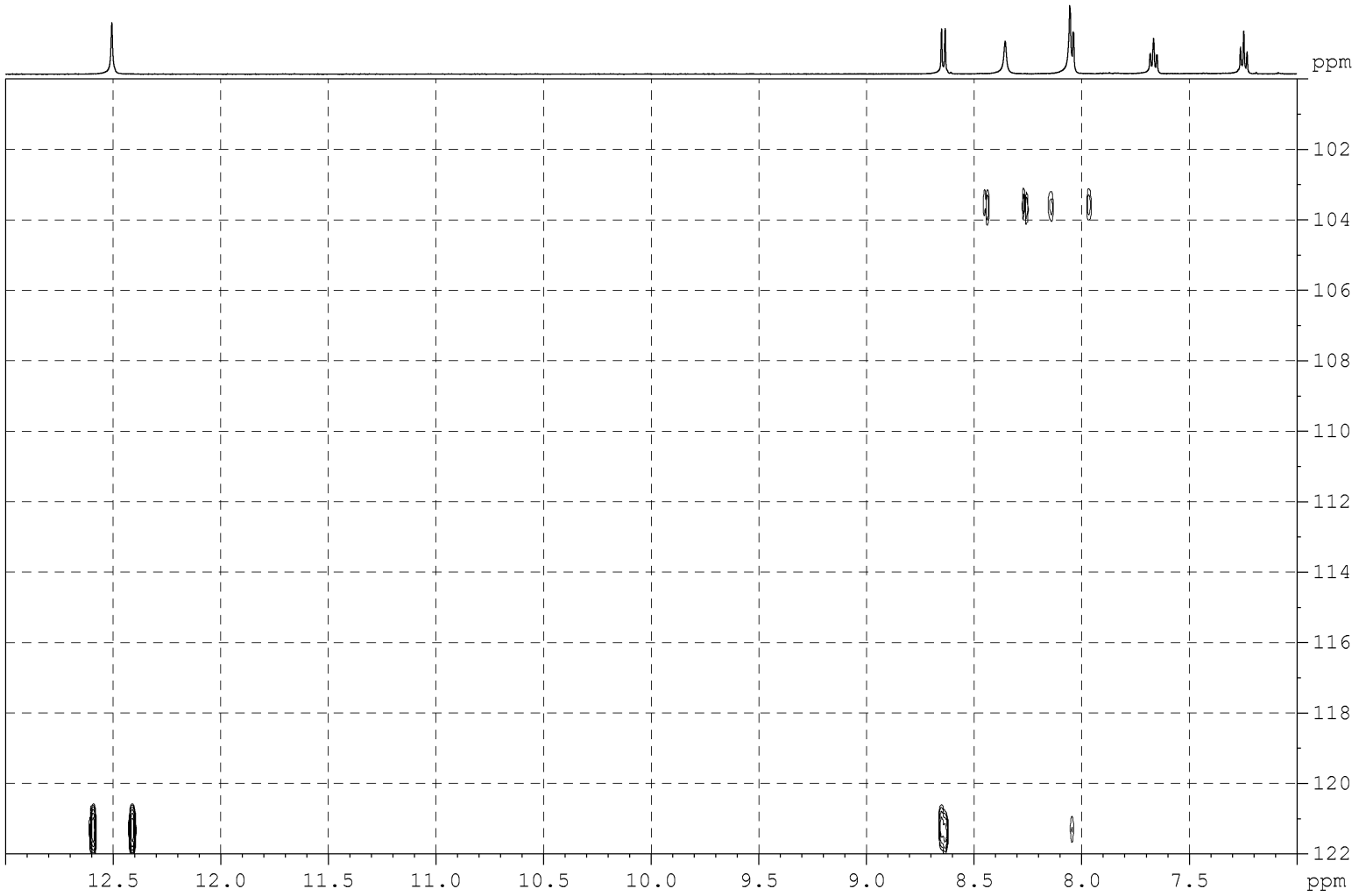



**Figure S121.** 2D $^{1}H$-$^{15}N$ HMBC NMR spectra of **4h** in DMSO at T = 303 K.

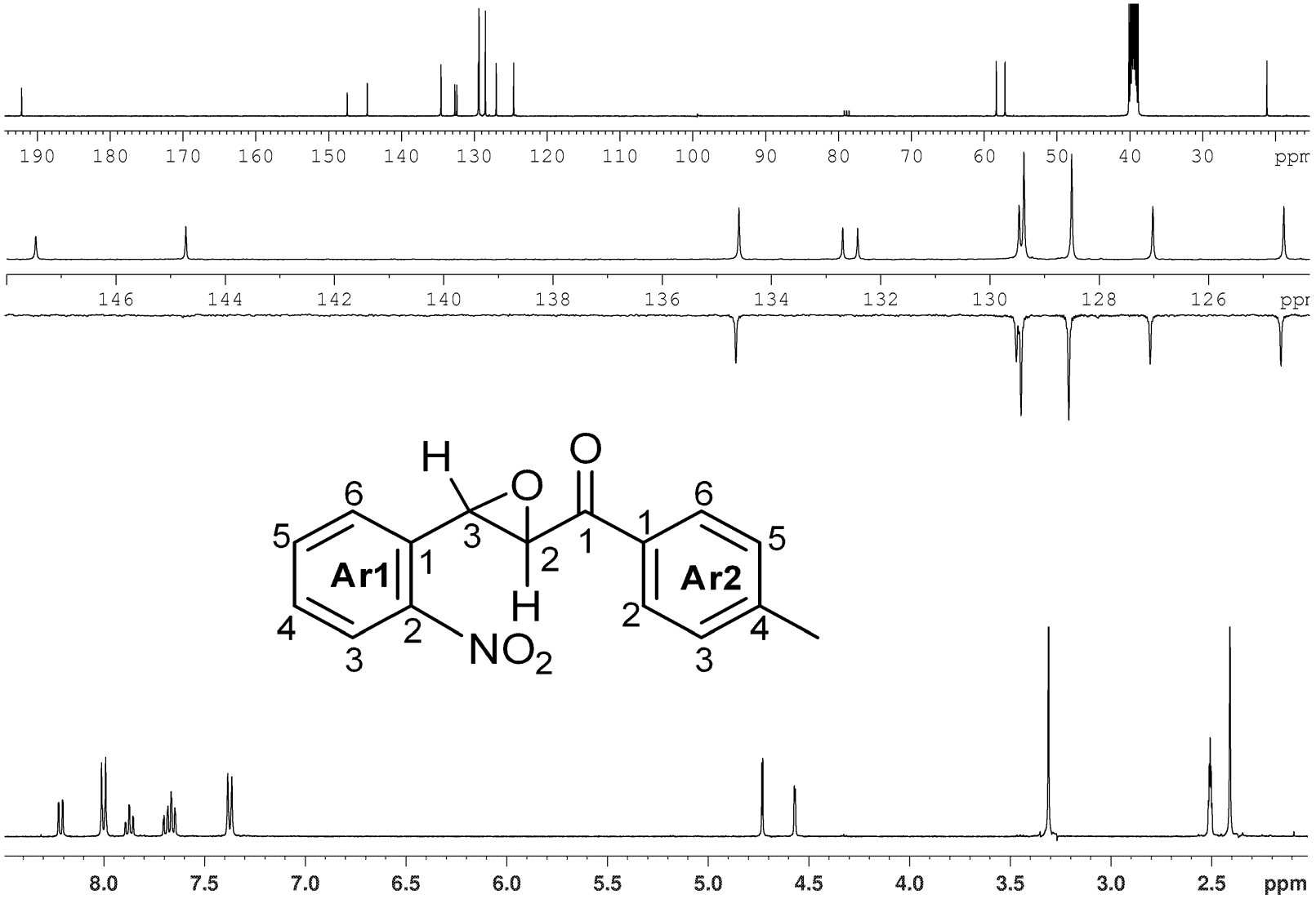



**Figure S122.** 1D $^{1}$H, $^{13}$C DEPT and $^{13}$C{$^{1}$H} NMR spectra of **6a** in DMSO at T = 303 K.

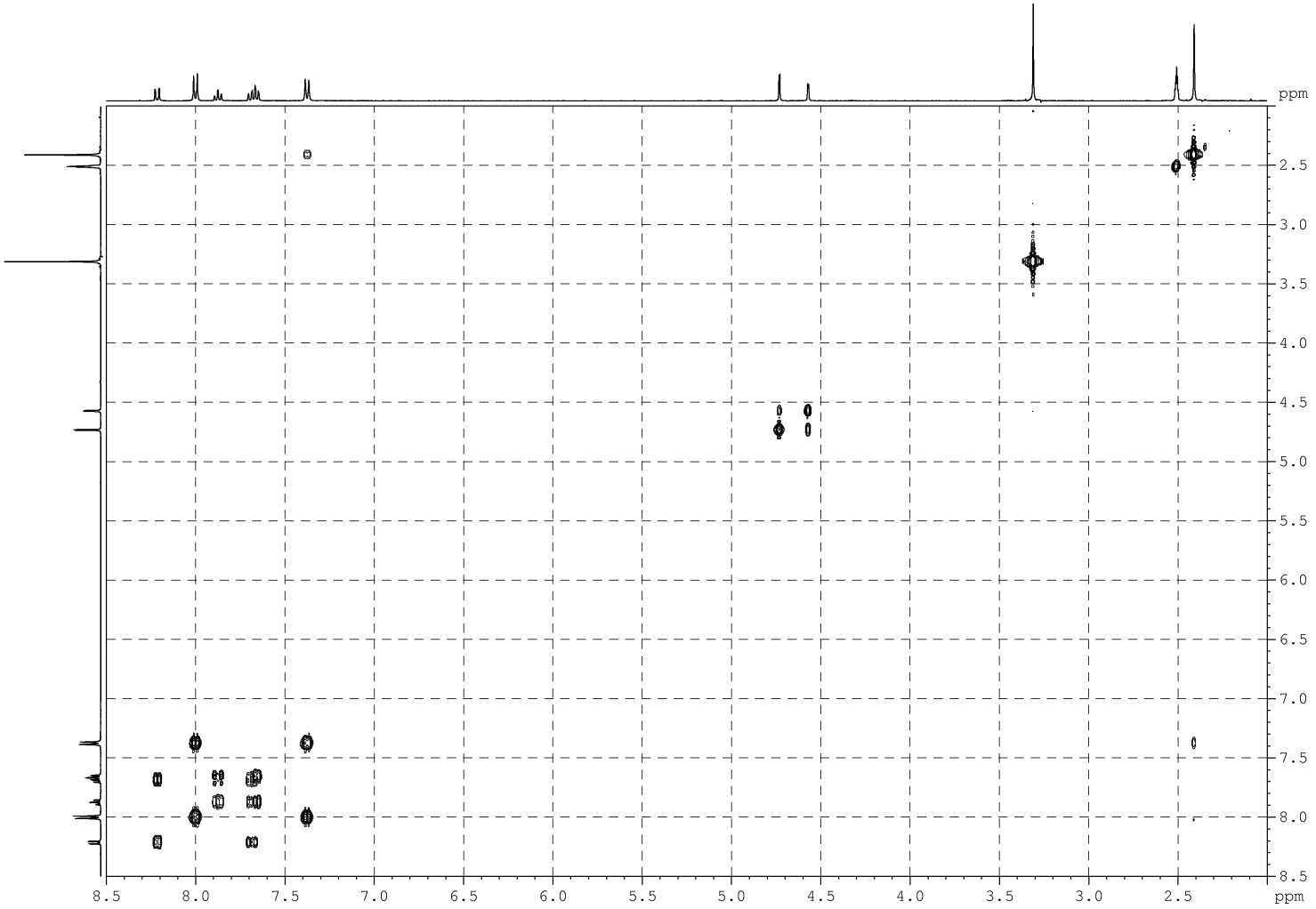



**Figure S123.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **6a** in DMSO at T = 303 K.

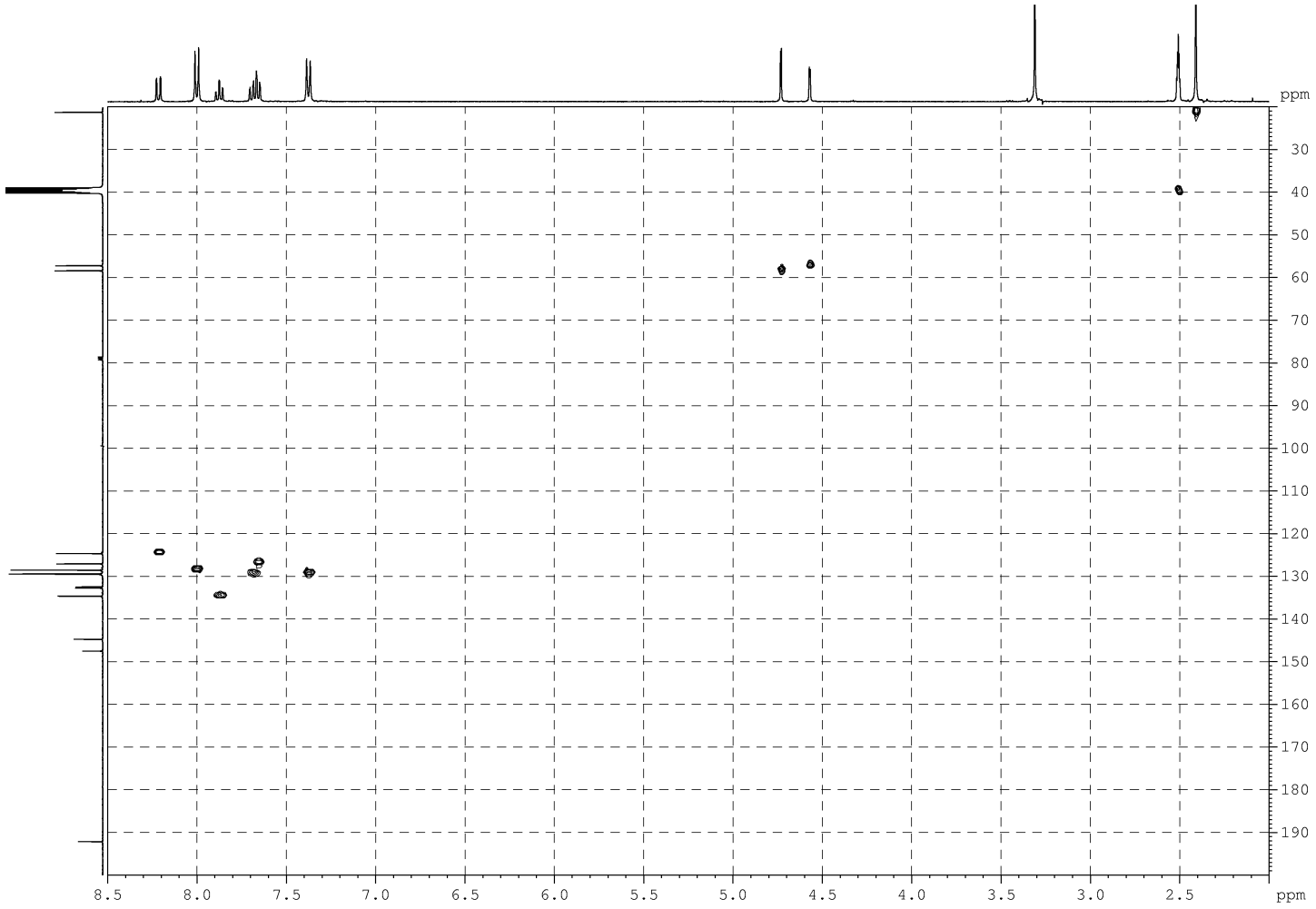



**Figure S124.** 2D $^{1}$H-$^{13}$C HSQC NMR spectra of **6a** in DMSO at T = 303 K.

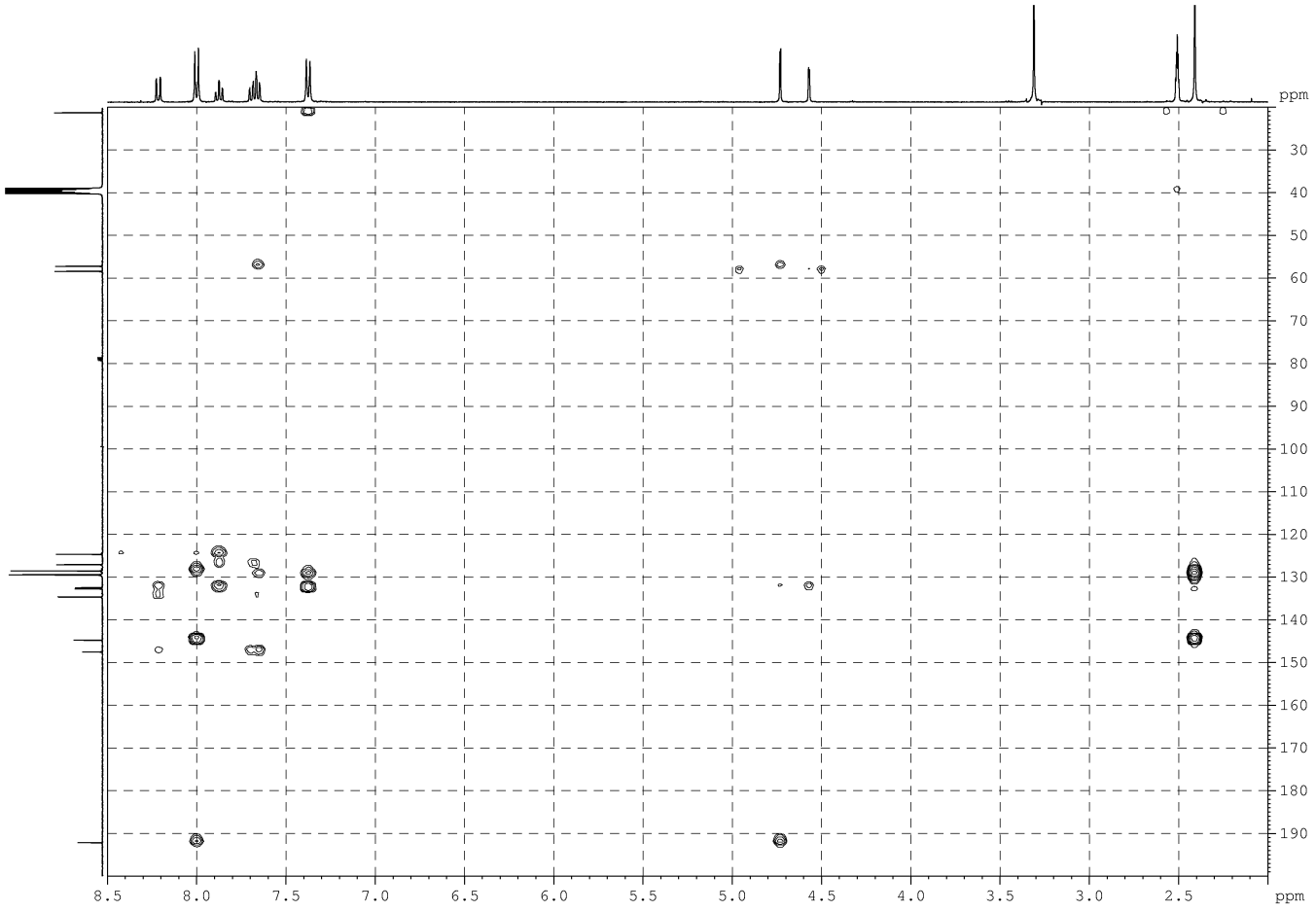



**Figure S125.** 2D $^{1}$H-$^{13}$C HMBC NMR spectra of **6a** in DMSO at T = 303 K.

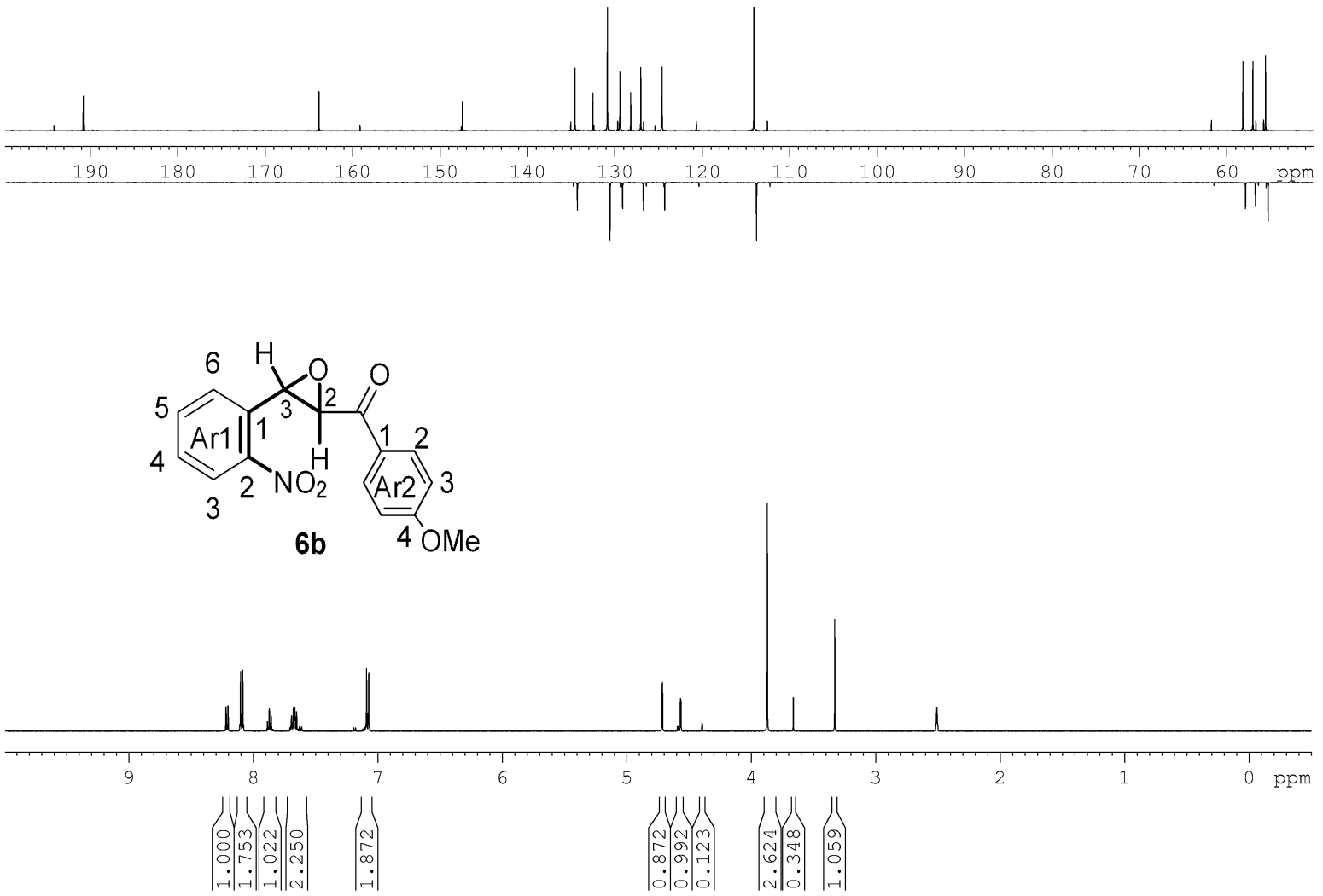



**Figure S126.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **6b** in DMSO at T = 303 K.

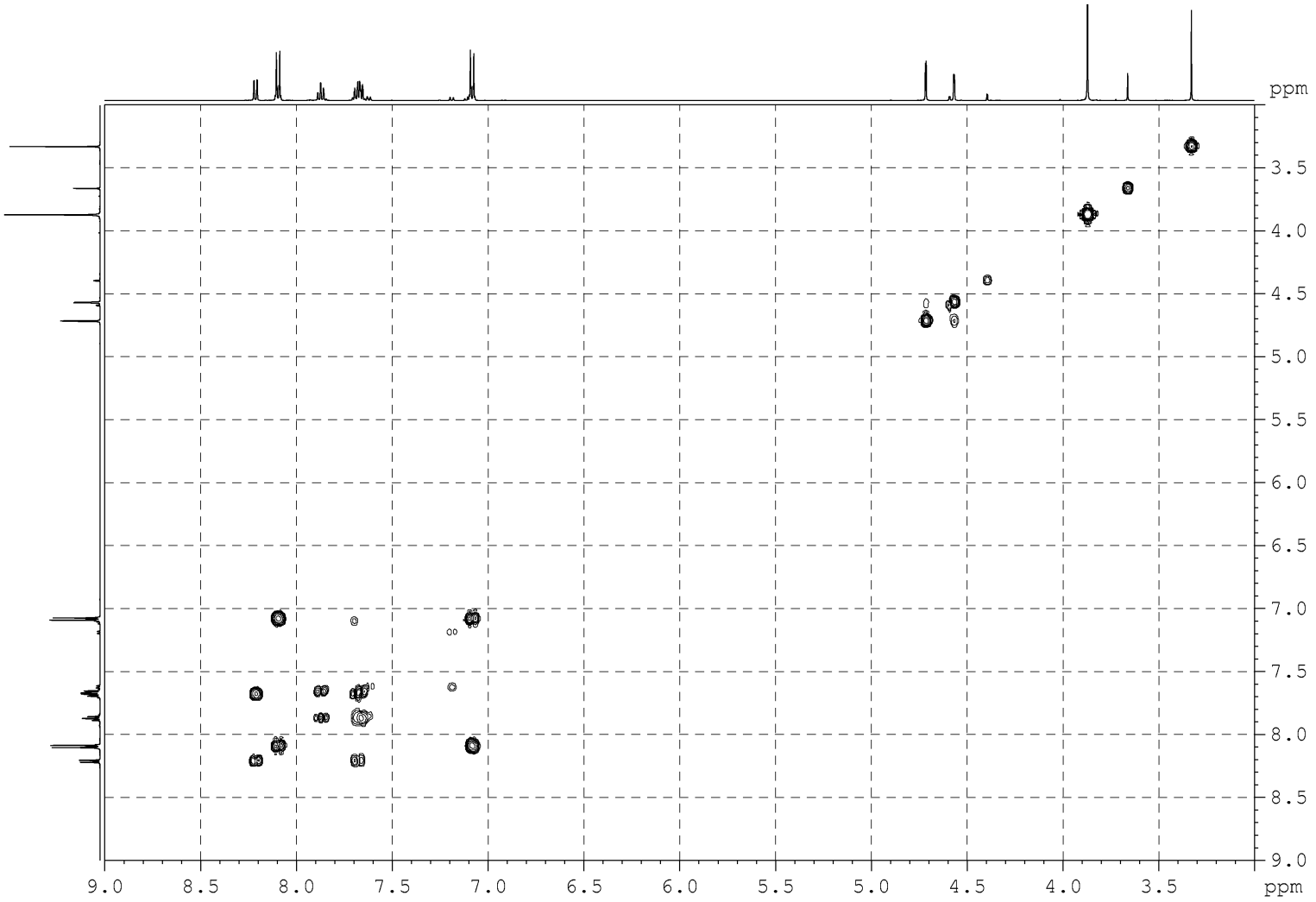



**Figure S127.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **6b** in DMSO at T = 303 K.

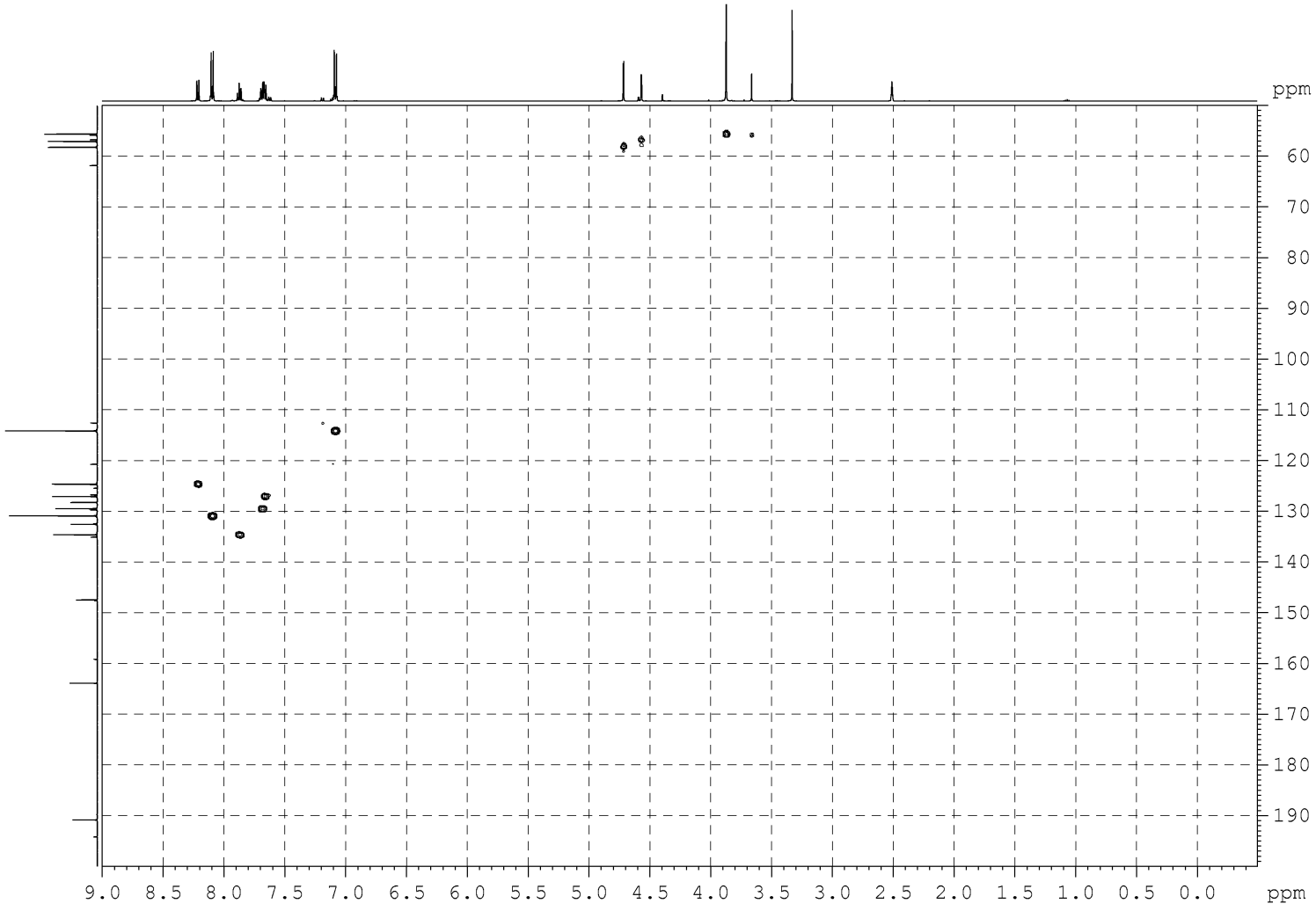



**Figure S128.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **6b** in DMSO at T = 303 K.

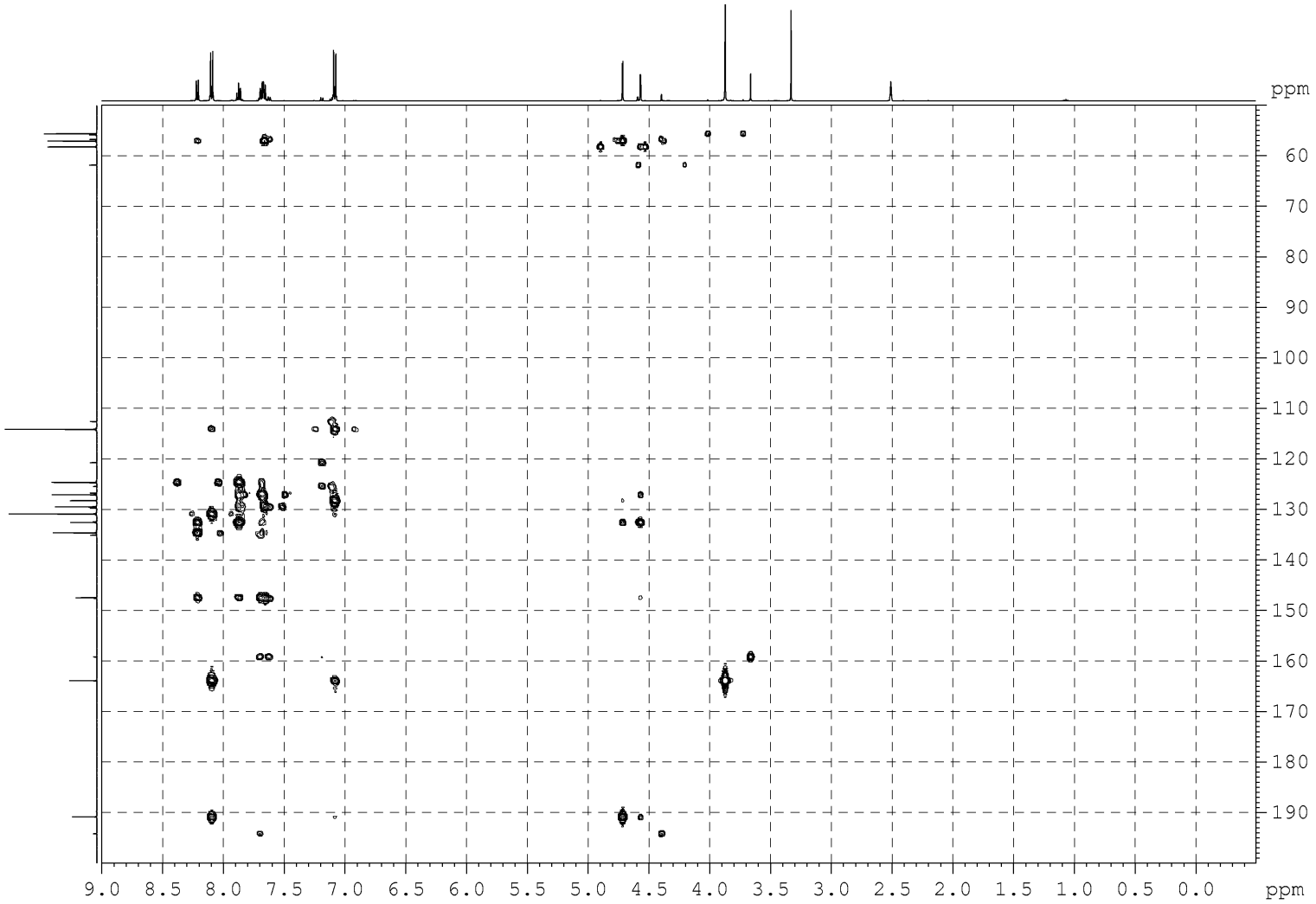



**Figure S129.** 2D $^{1}$H-$^{13}$C HMBC NMR spectra of **6b** in DMSO at T = 303 K.

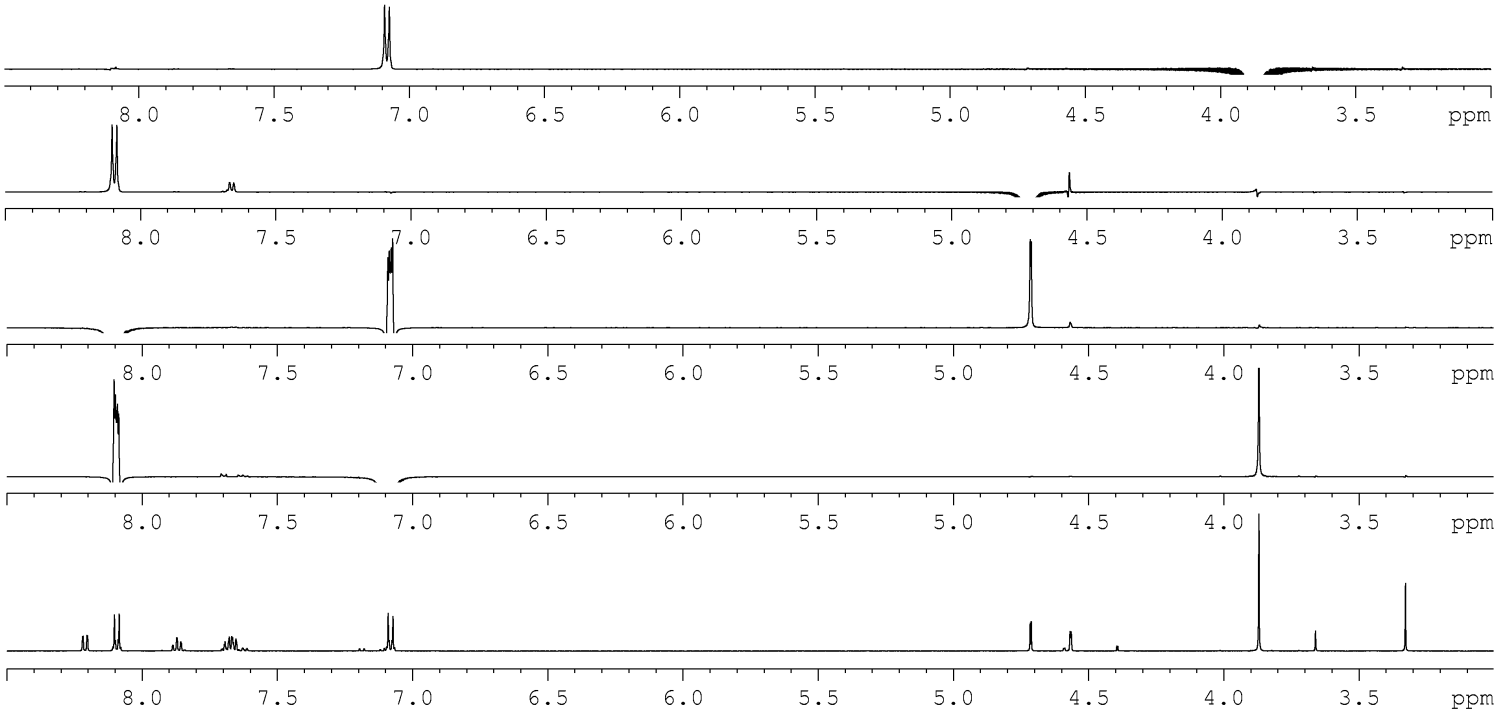



**Figure S130.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **6b** in DMSO at T = 303 K.

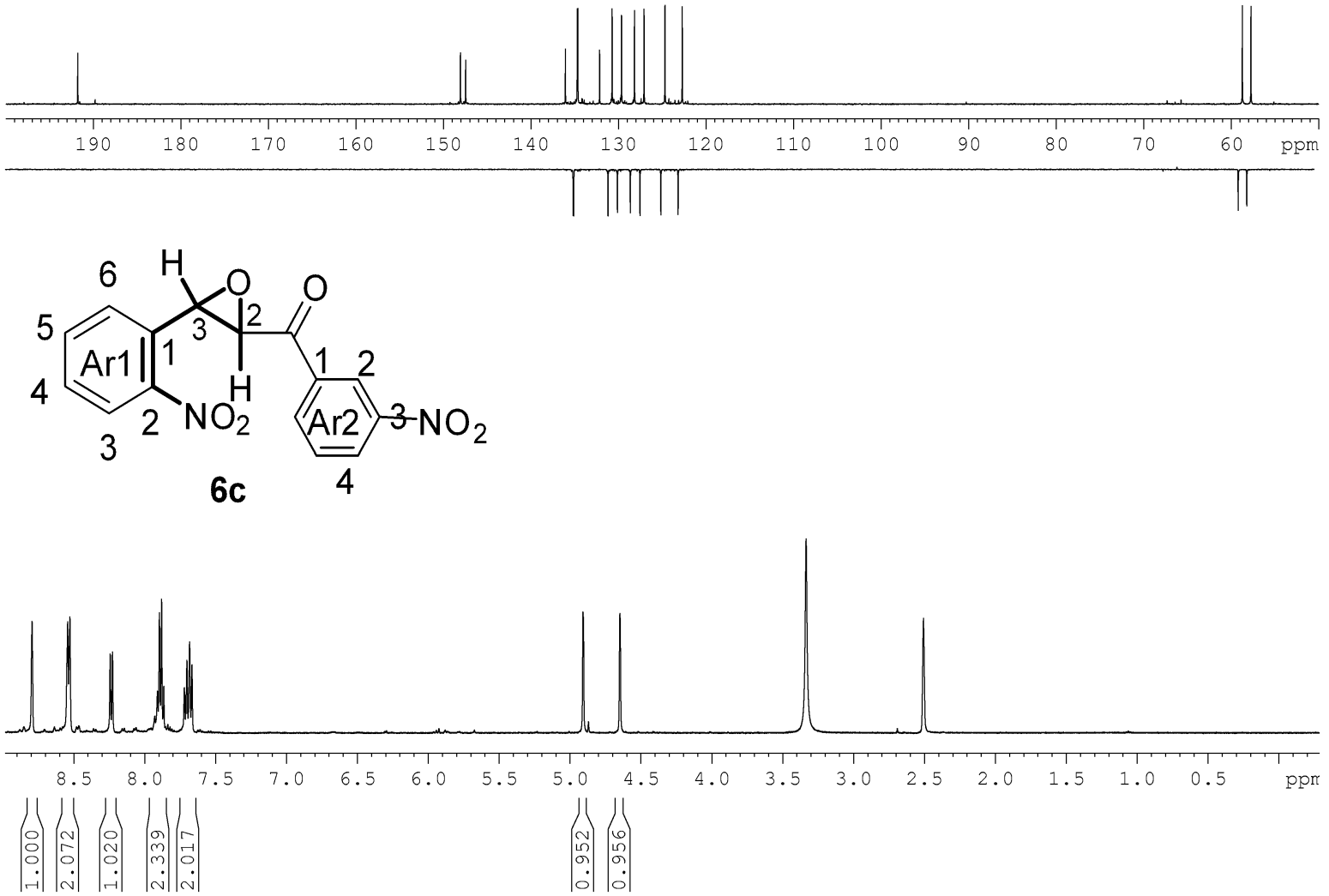



**Figure S131.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **6c** in DMSO at T = 303 K.

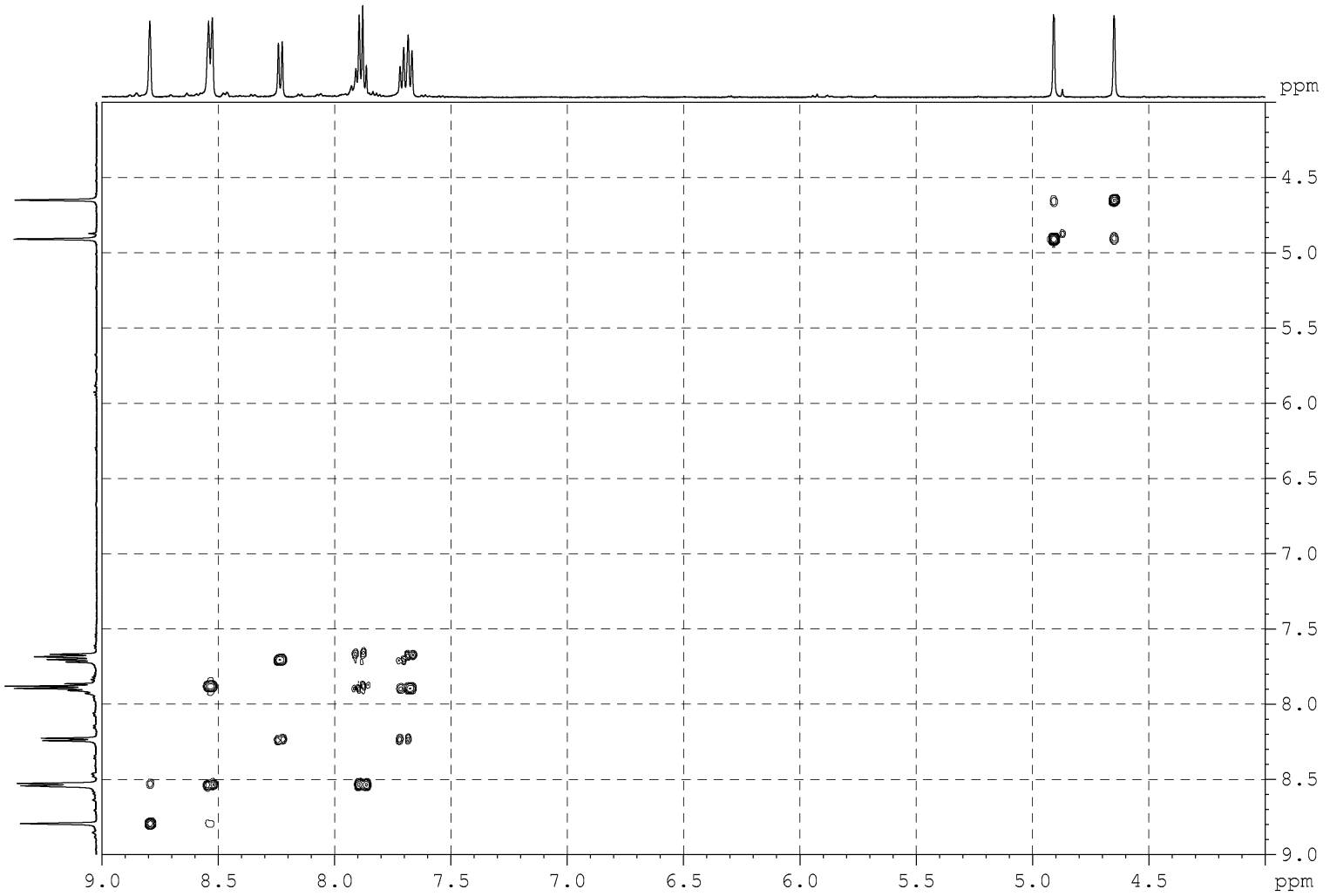



**Figure S132.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **6c** in DMSO at T = 303 K.

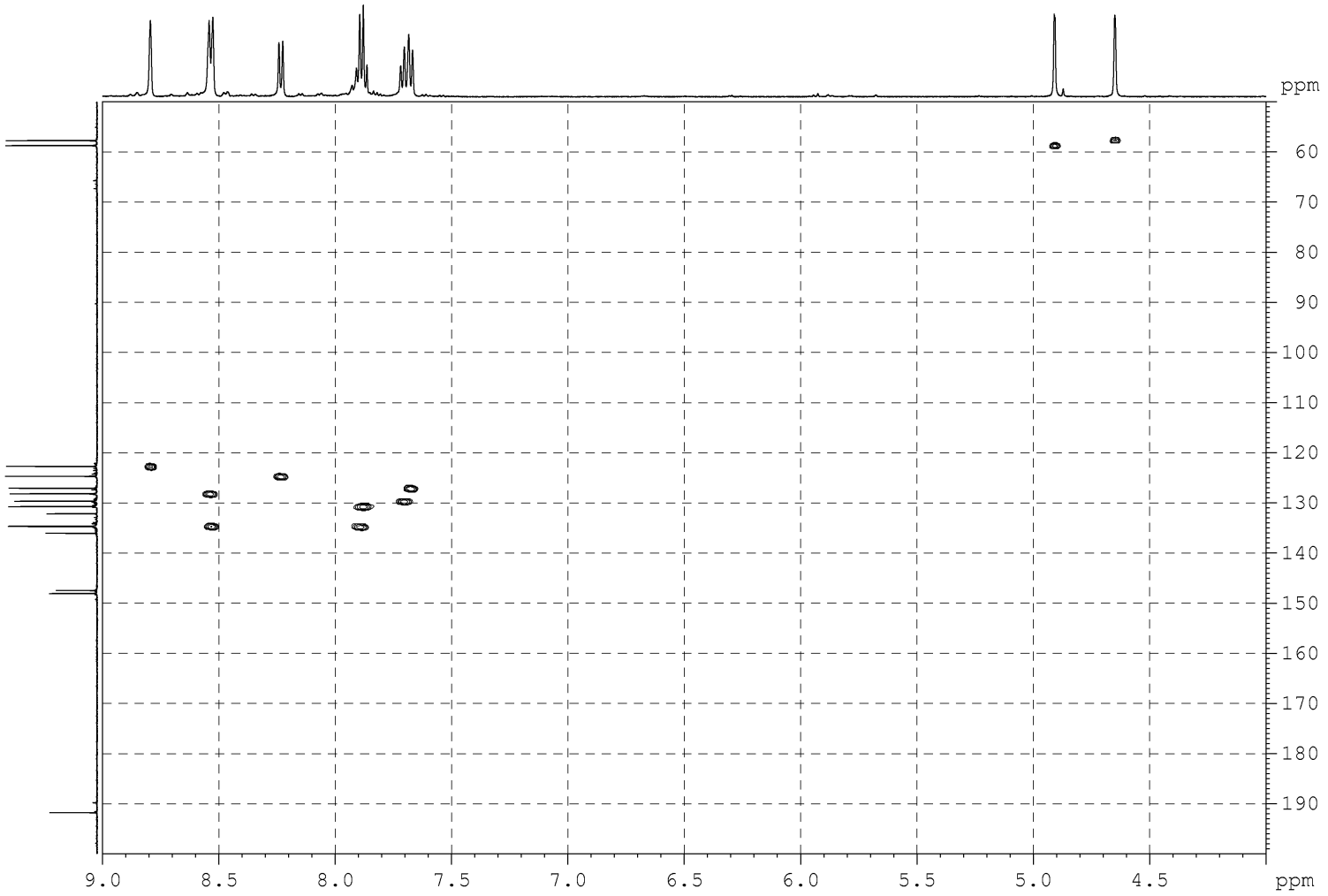



**Figure S133.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **6c** in DMSO at T = 303 K.

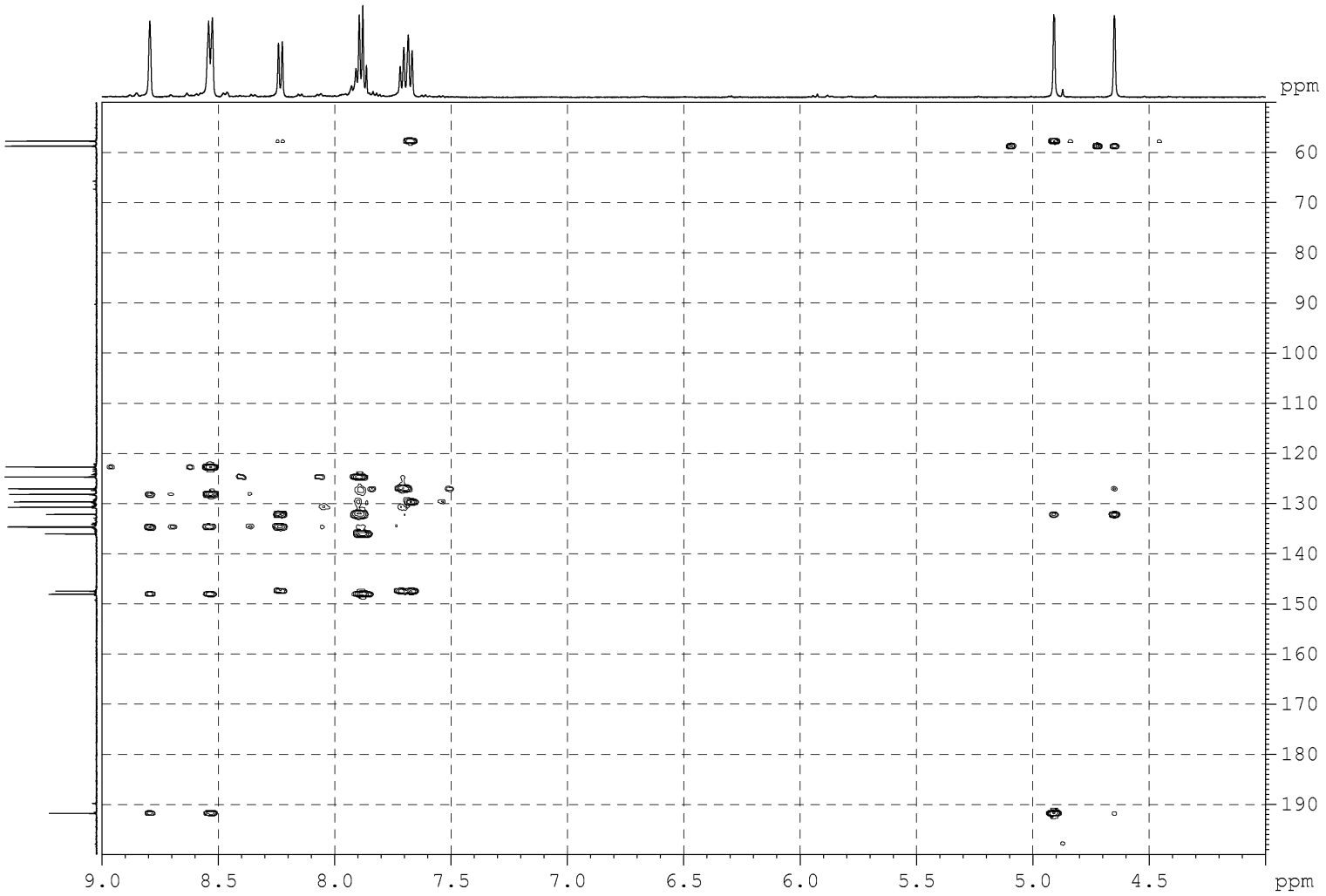



**Figure S134.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **6c** in DMSO at T = 303 K.

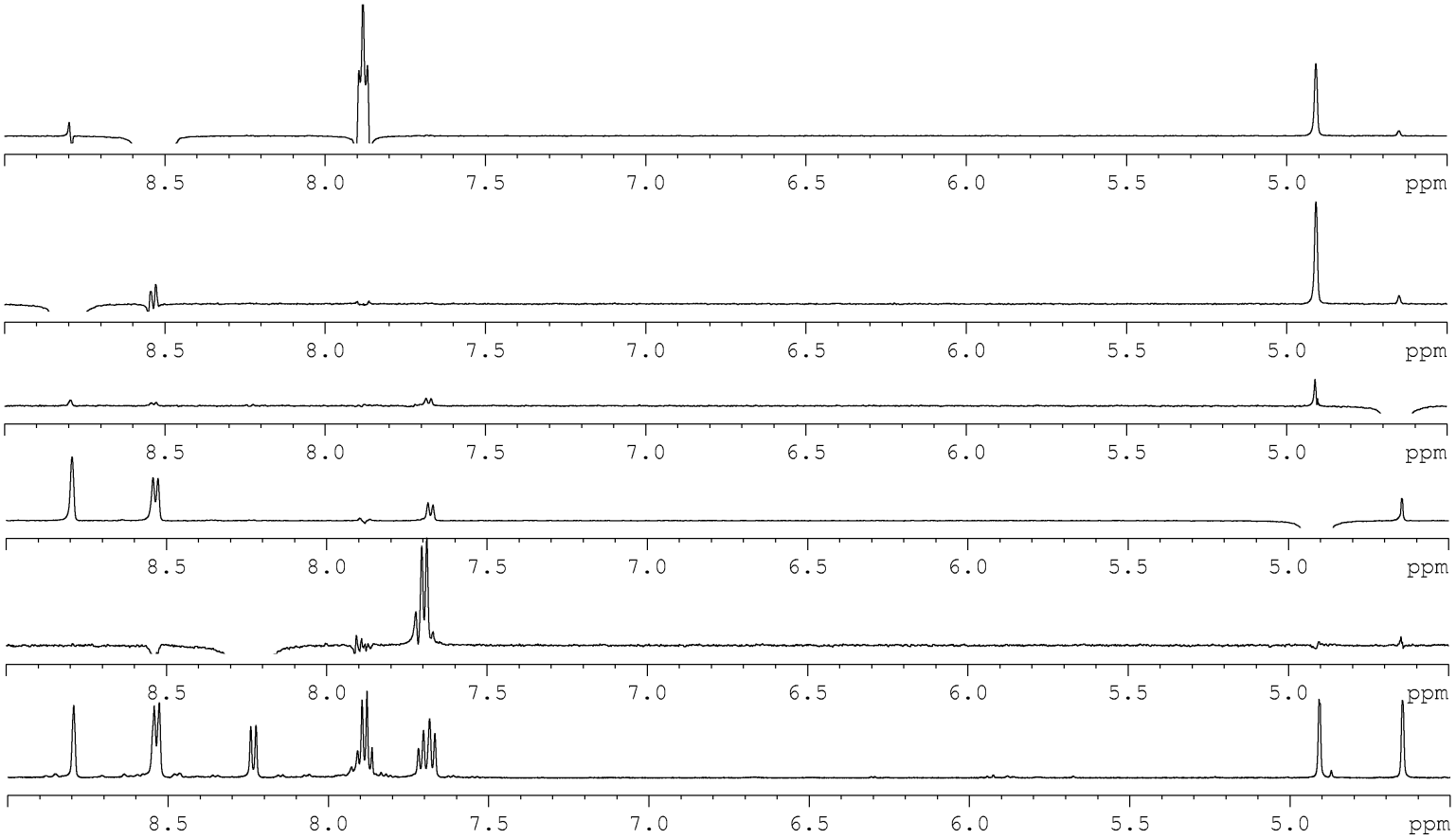



**Figure S135.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **6c** in DMSO at T = 303 K.

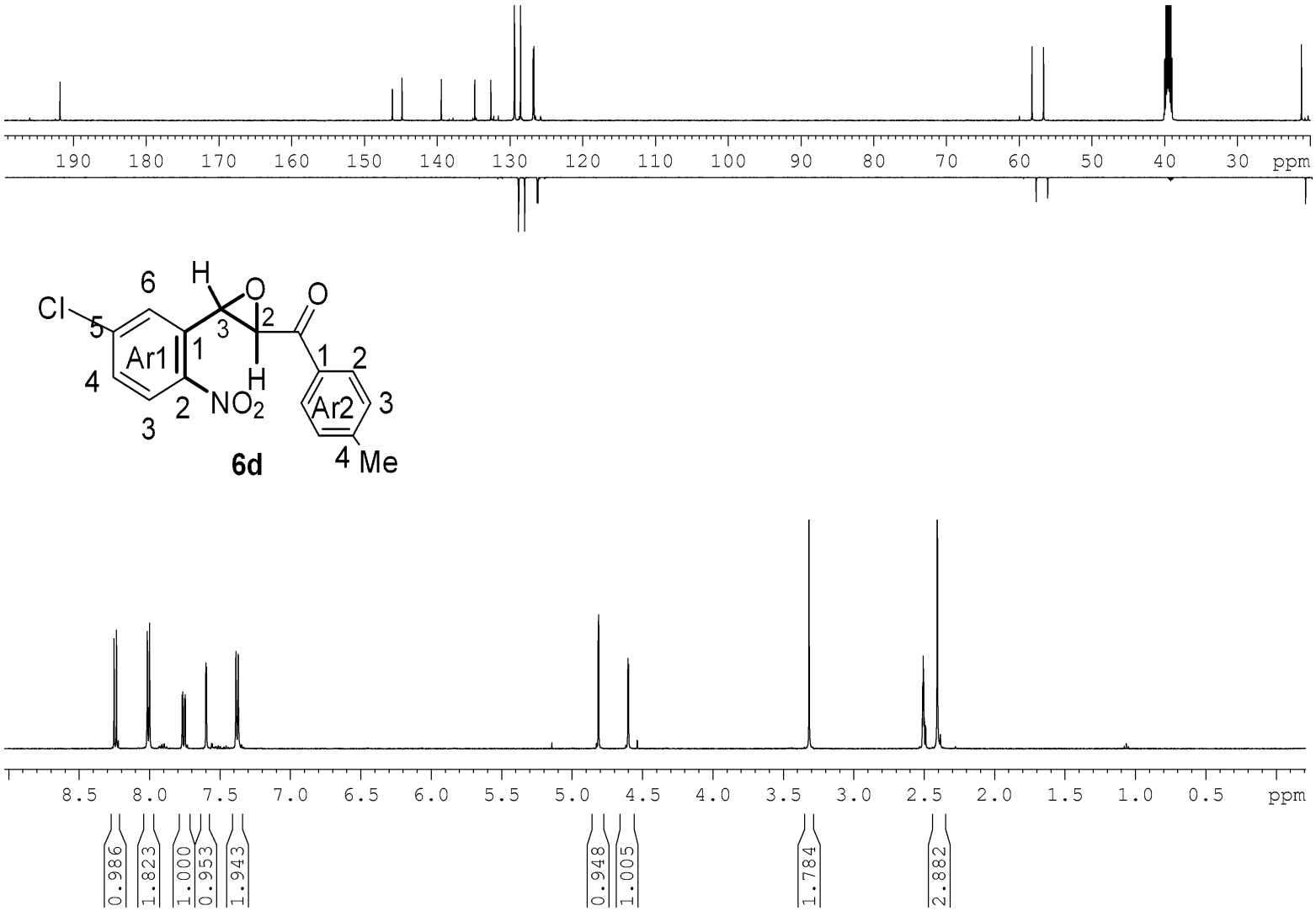



**Figure S136.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **6d** in DMSO at T = 303 K.

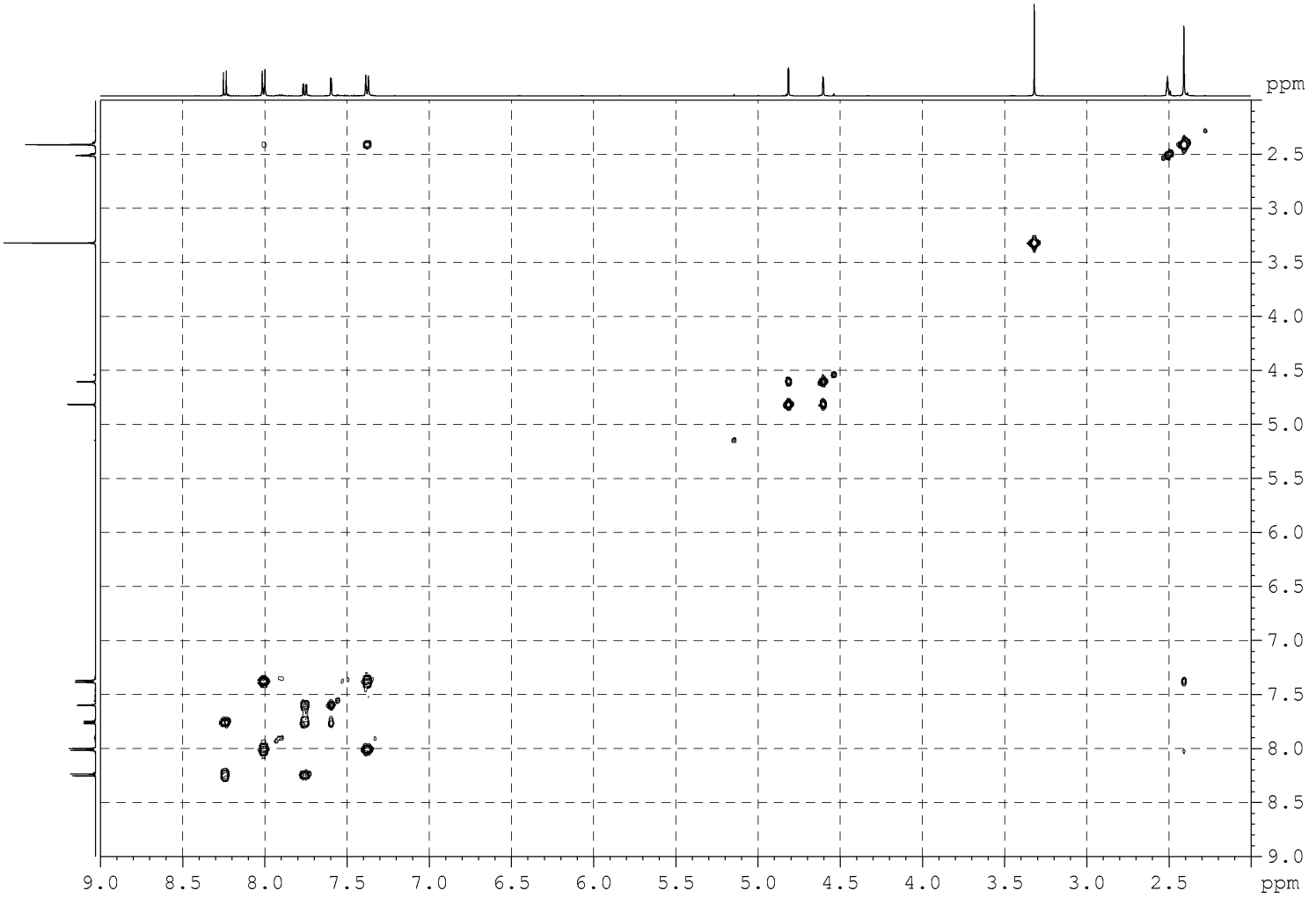



**Figure S137.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **6d** in DMSO at T = 303 K.

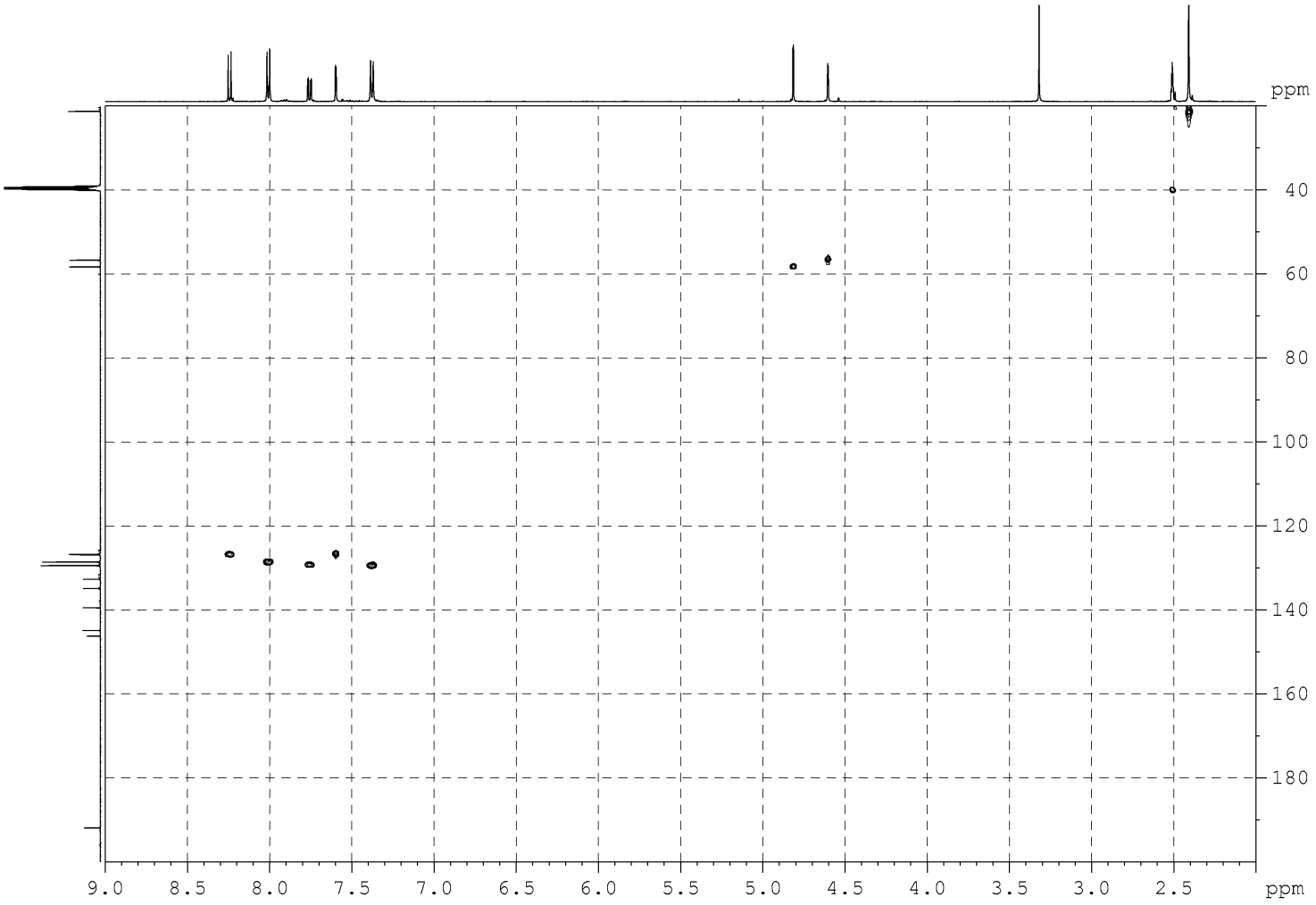



**Figure S138.** 2D $^{1}$H-$^{13}$C HSQC NMR spectra of **6d** in DMSO at T = 303 K.

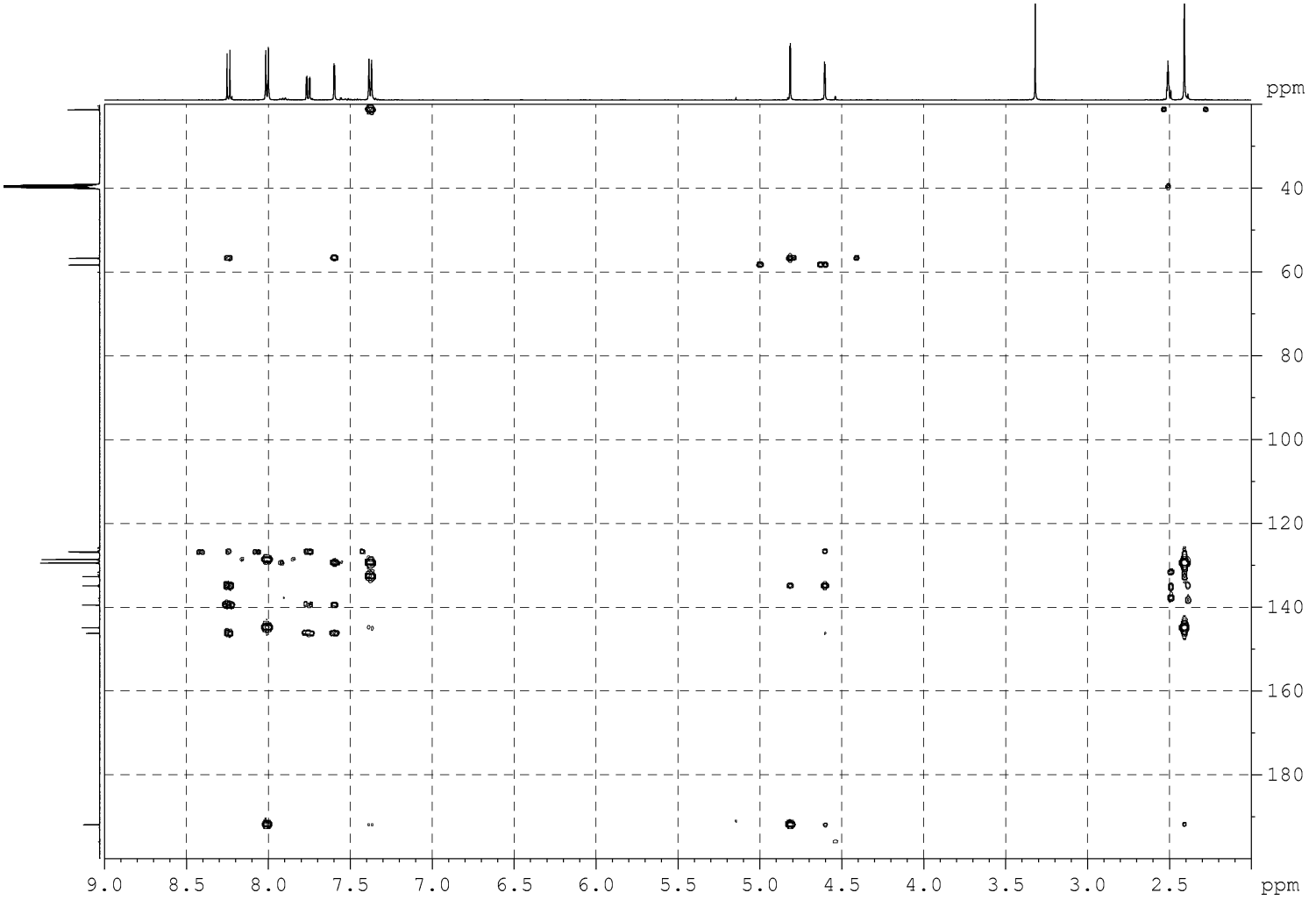



**Figure S139.** 2D $^{1}$H-$^{13}$C HMBC NMR spectra of **6d** in DMSO at T = 303 K.

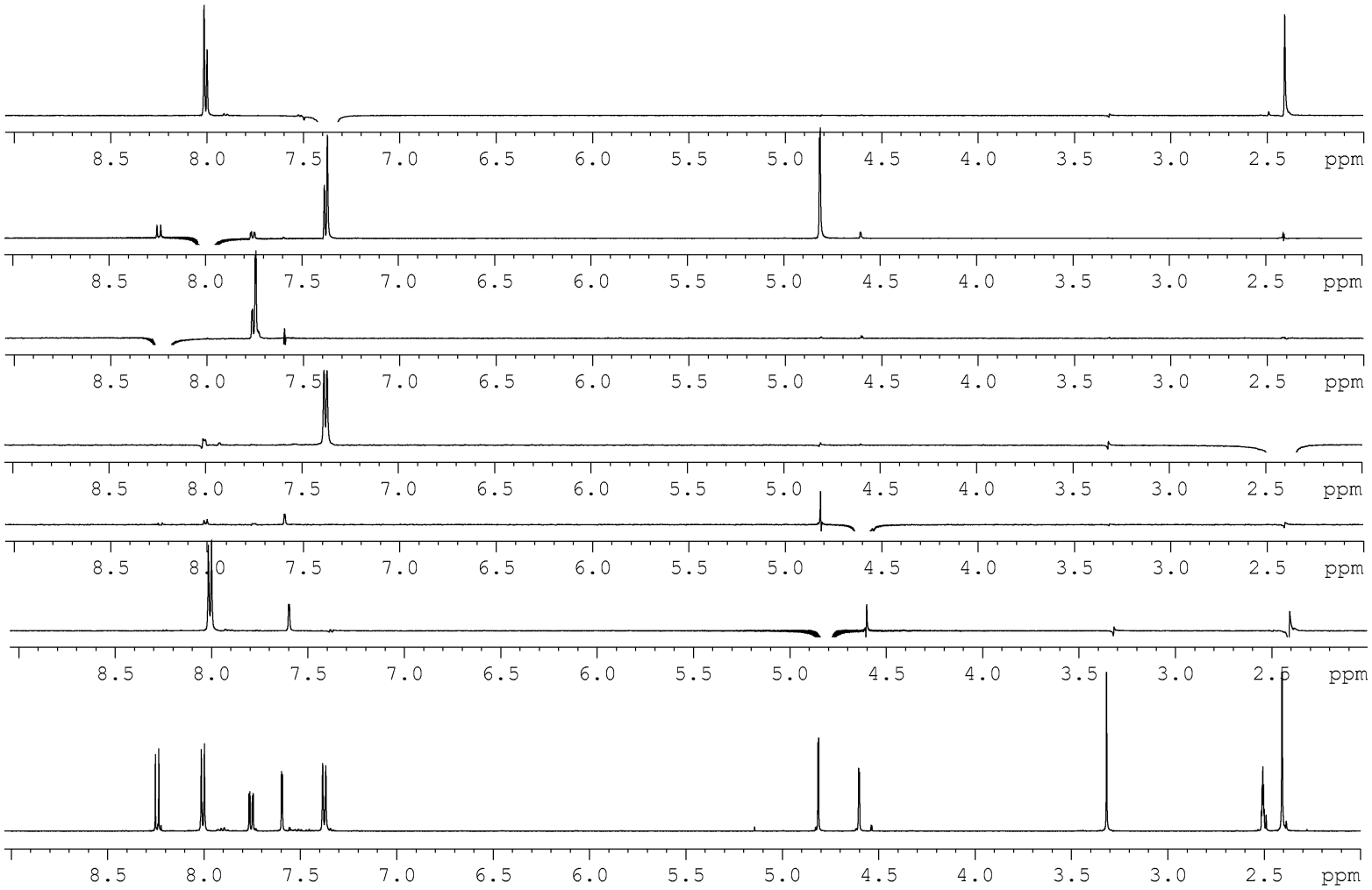



**Figure S140.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **6d** in DMSO at T = 303 K.

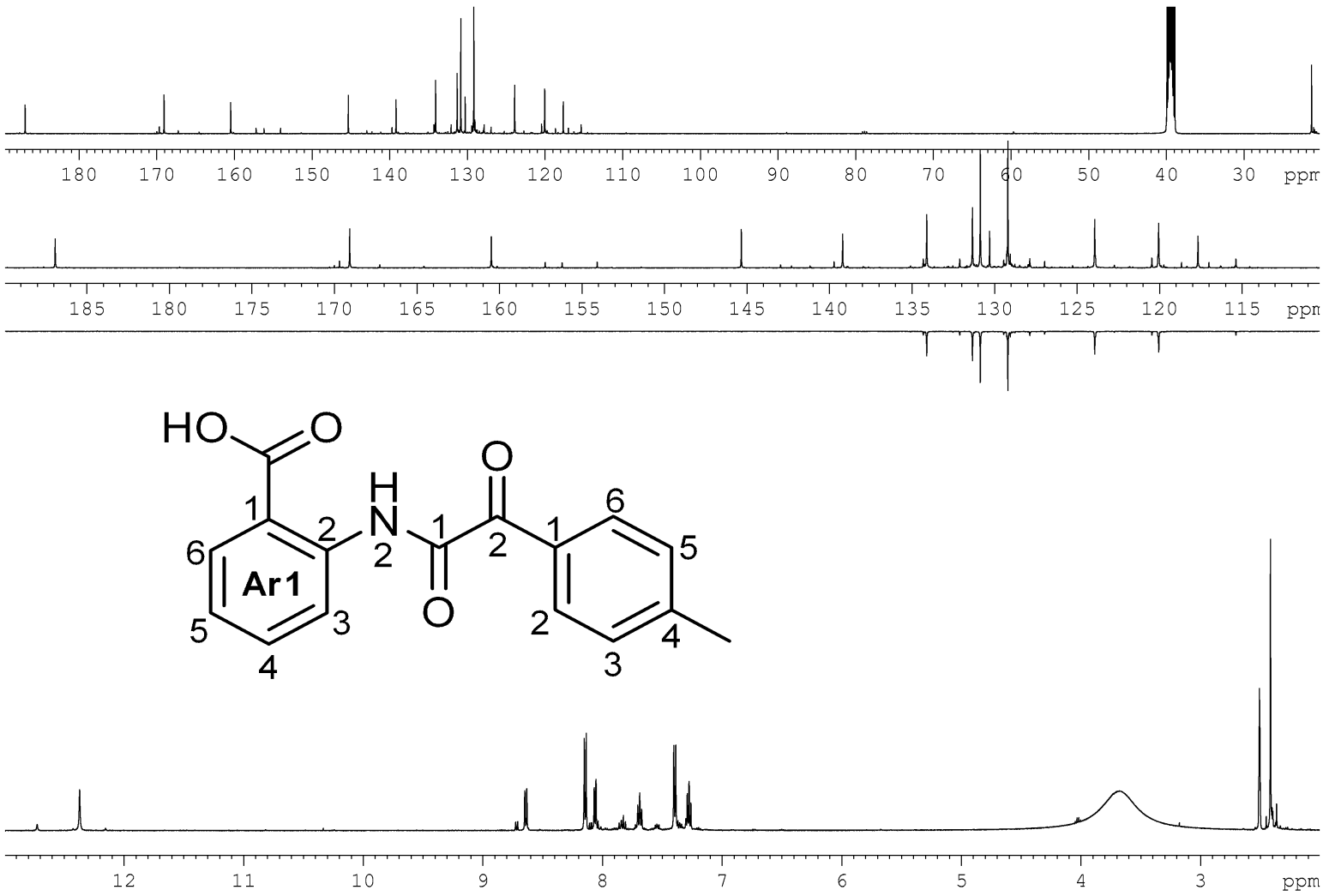



**Figure S1141.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **7a** in DMSO at T = 303 K.

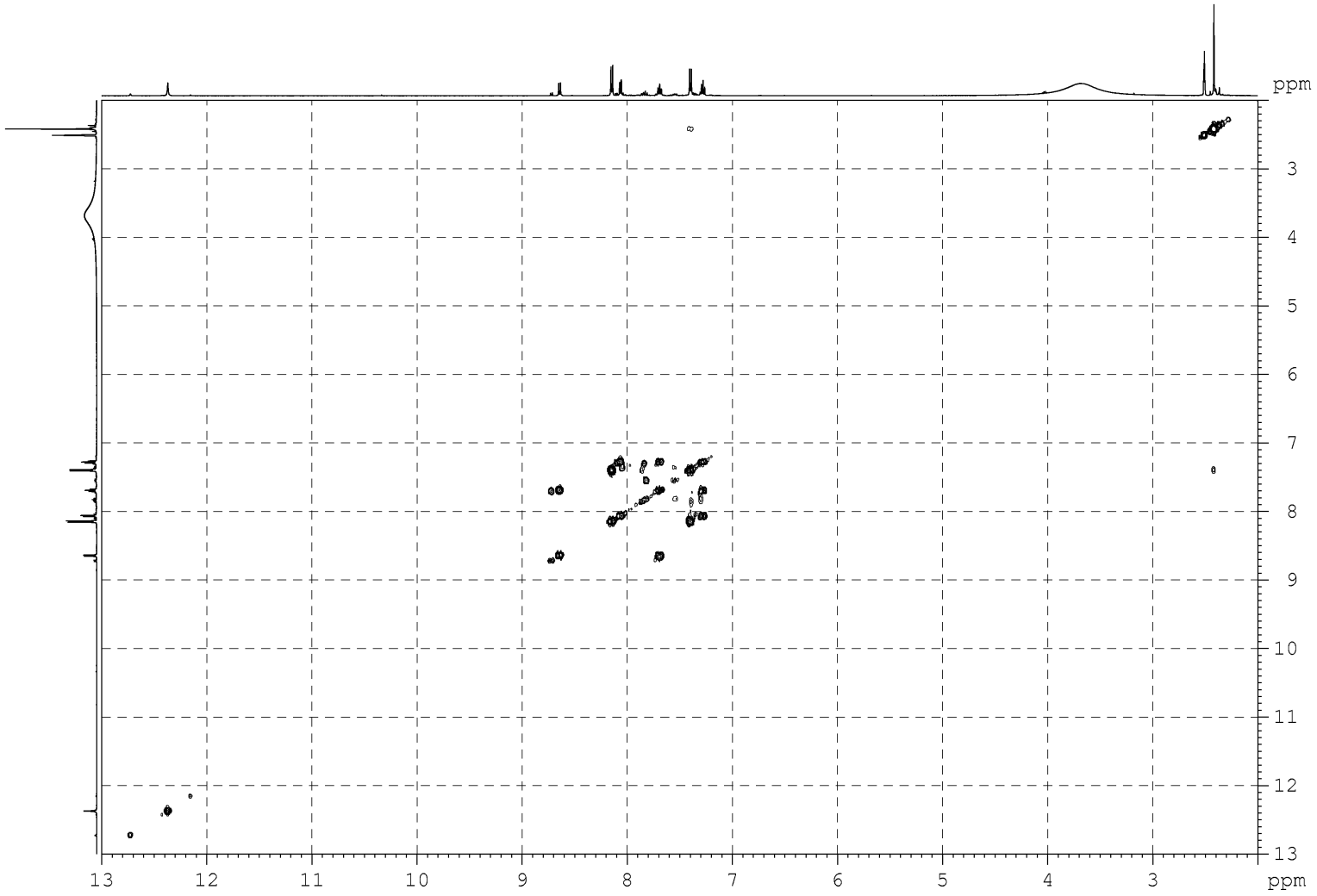



**Figure S142.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **7a** in DMSO at T = 303 K.

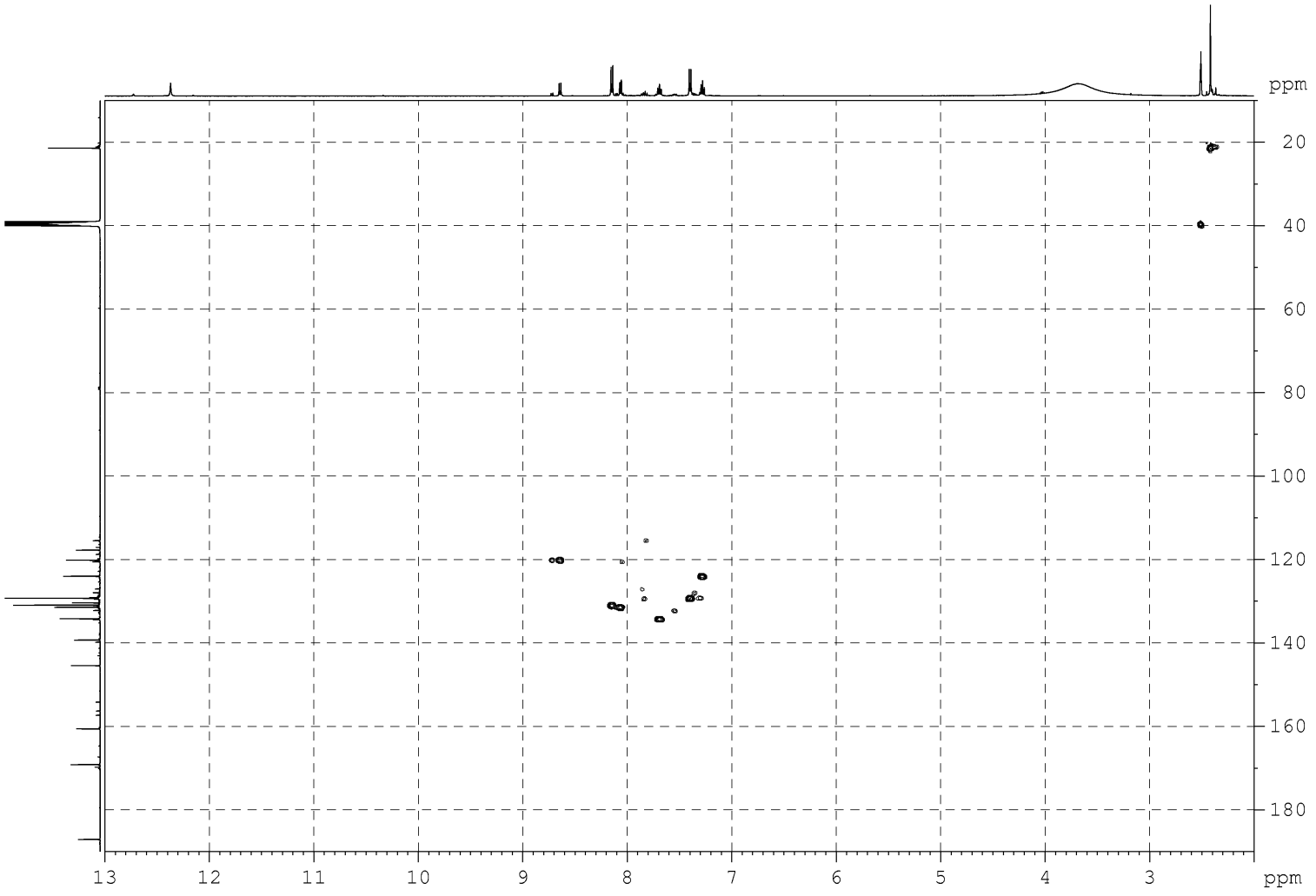



**Figure S143.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **7a** in DMSO at T = 303 K.

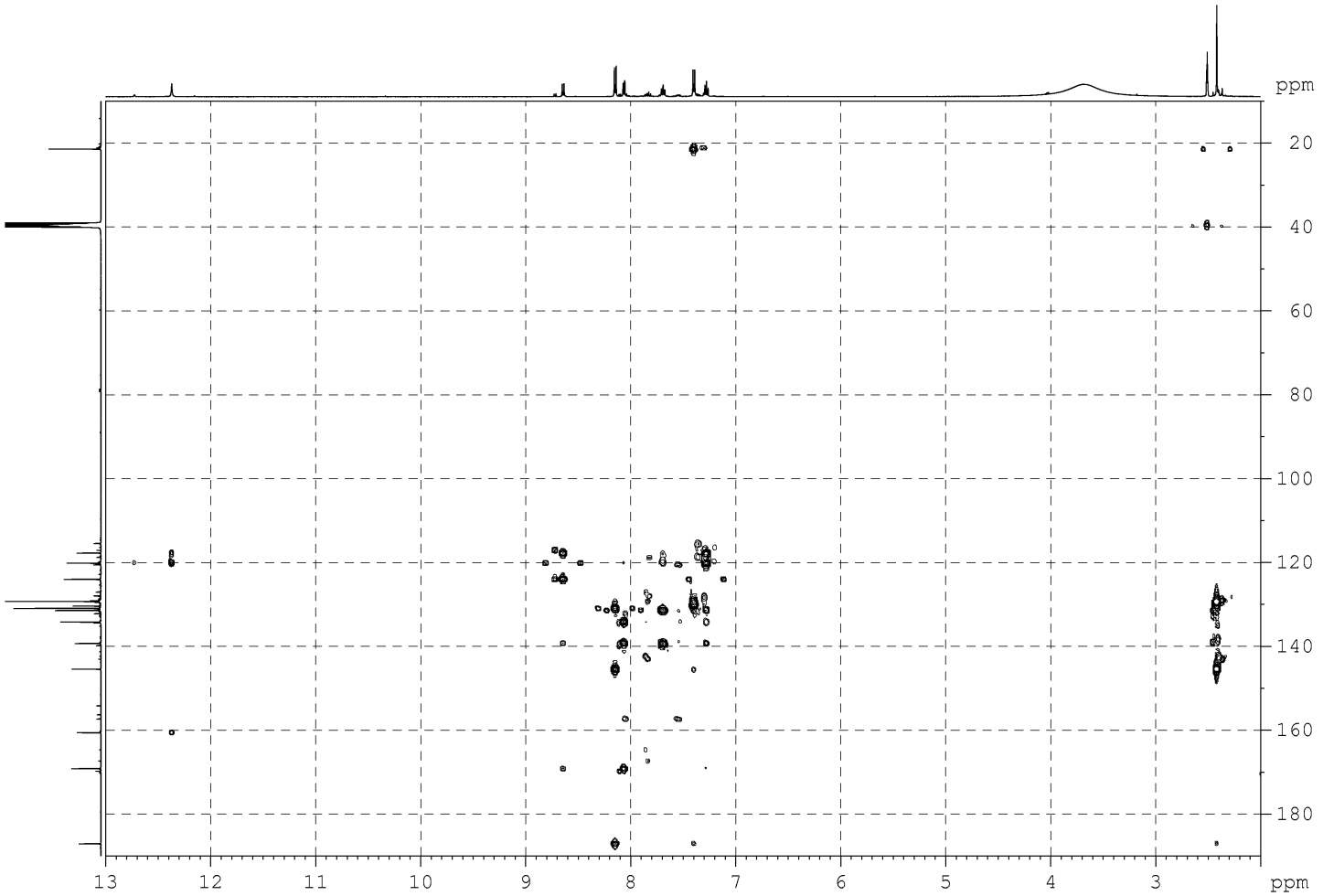



**Figure S144.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **7a** in DMSO at T = 303 K.

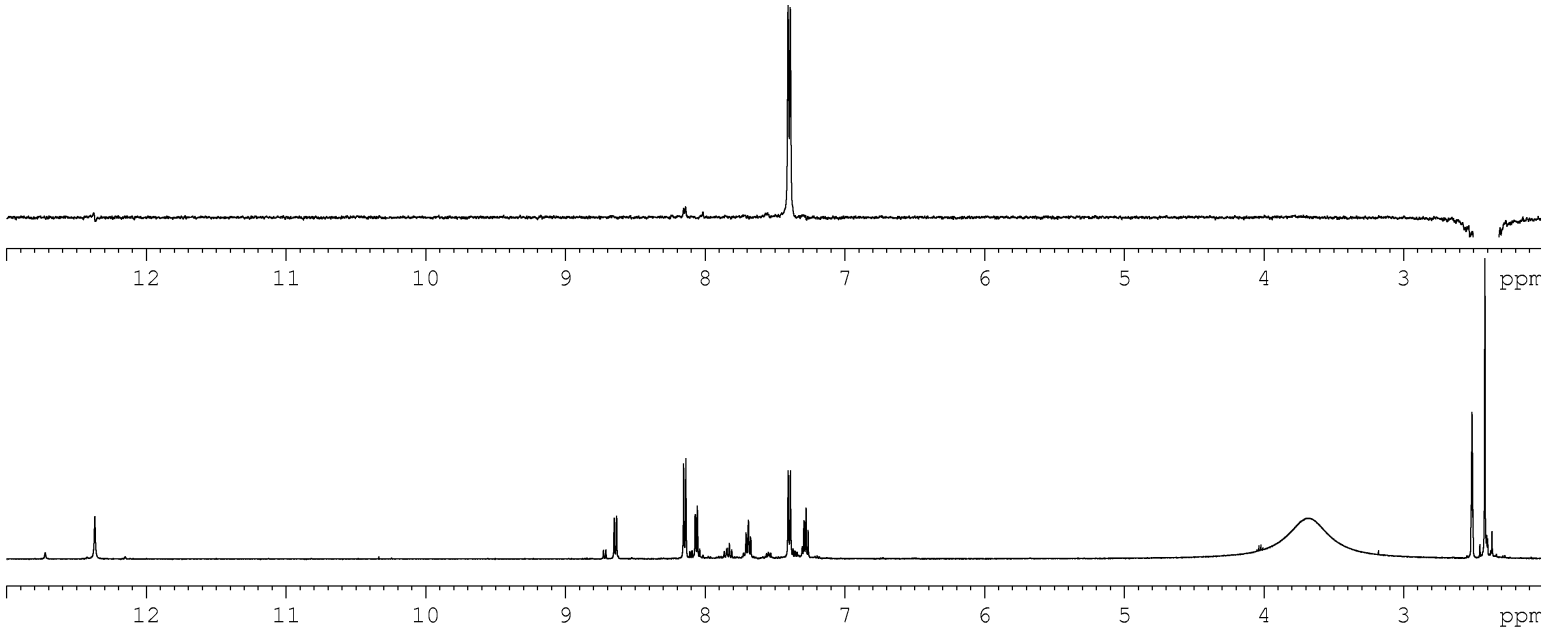



**Figure S145.** 1D $^{1}$H and $^{1}$H DPFGROE NMR spectra of **7a** in DMSO at T = 303 K.

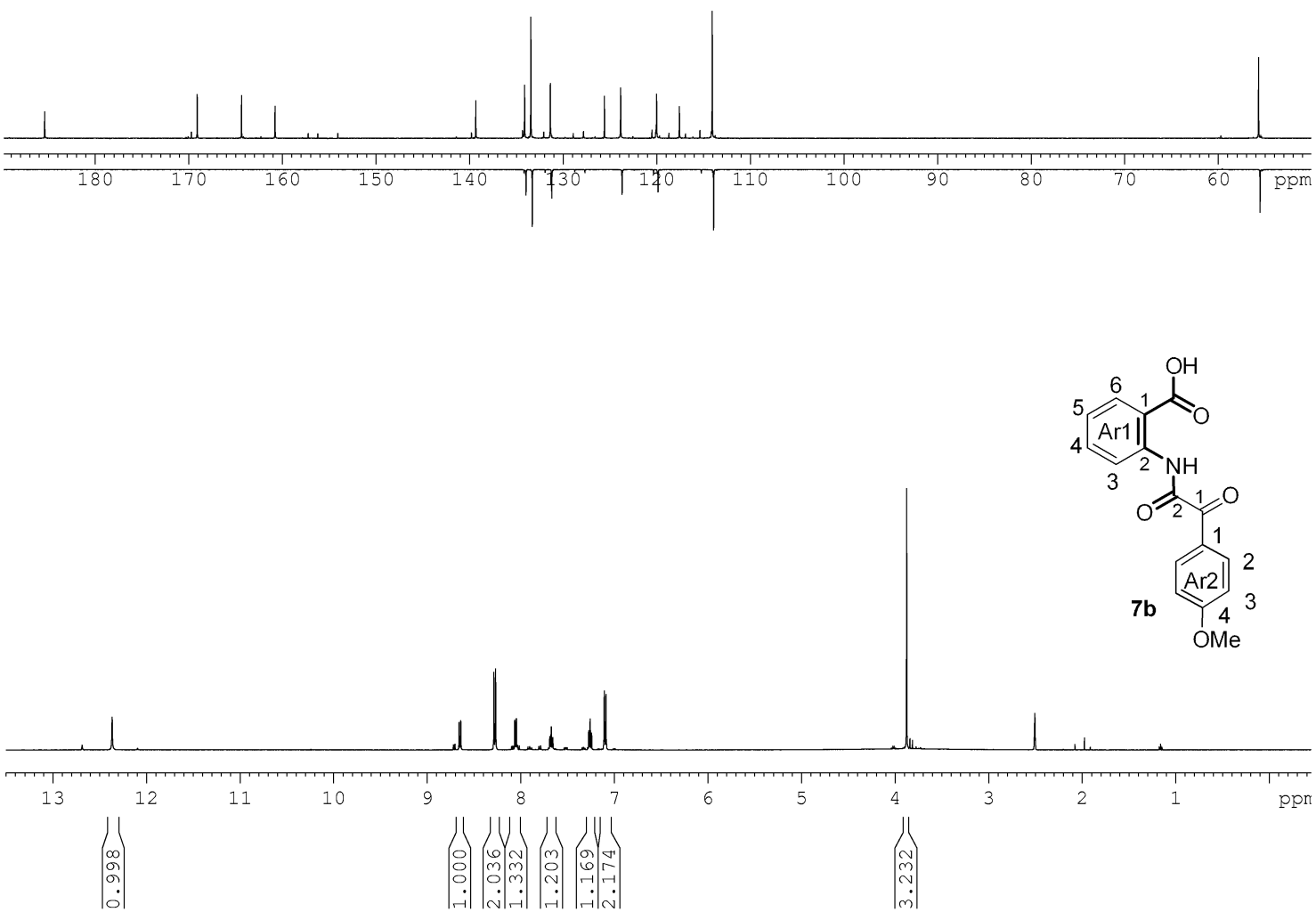



**Figure S146.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **7b** in DMSO at T = 303 K.

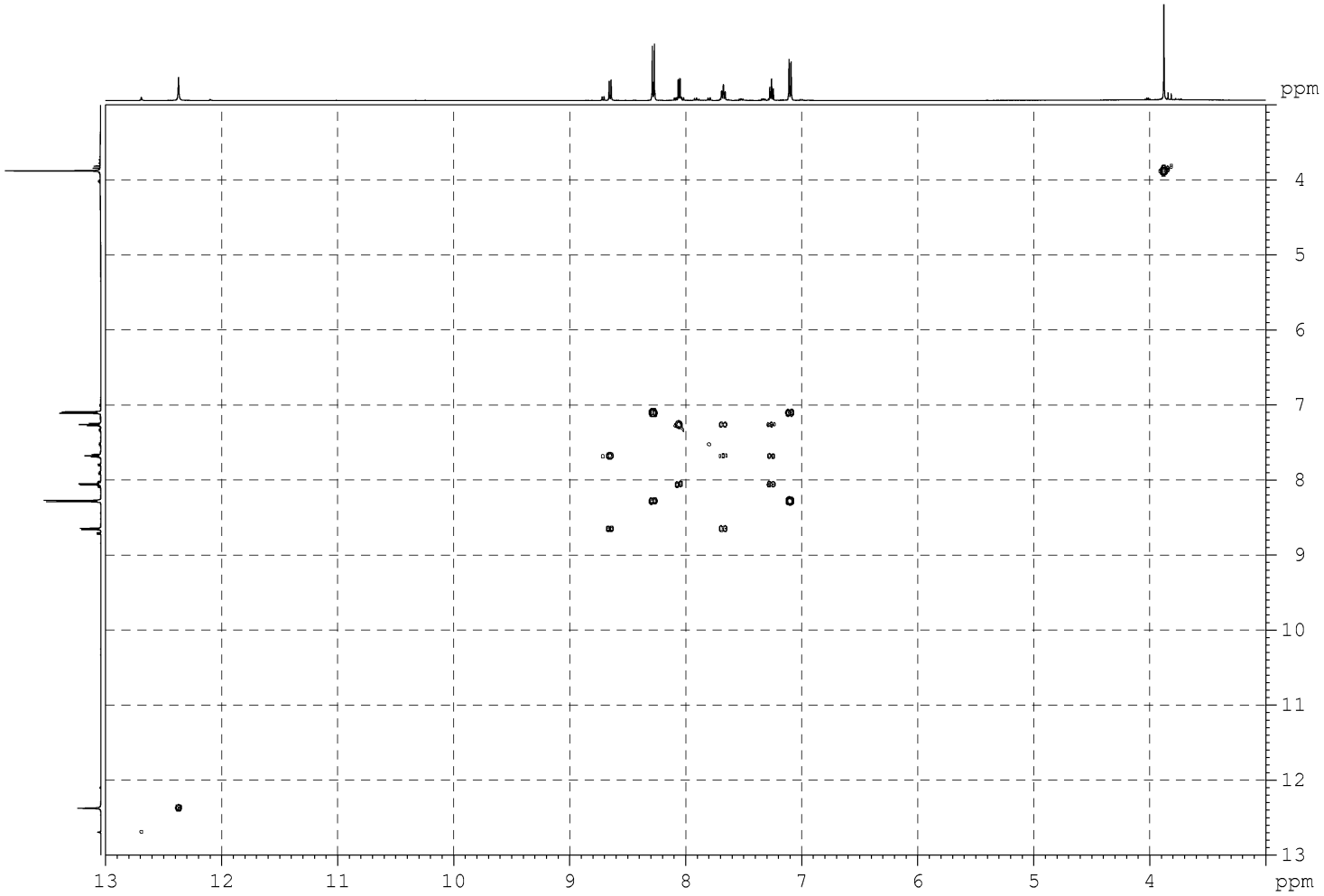



**Figure S147.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **7b** in DMSO at T = 303 K.

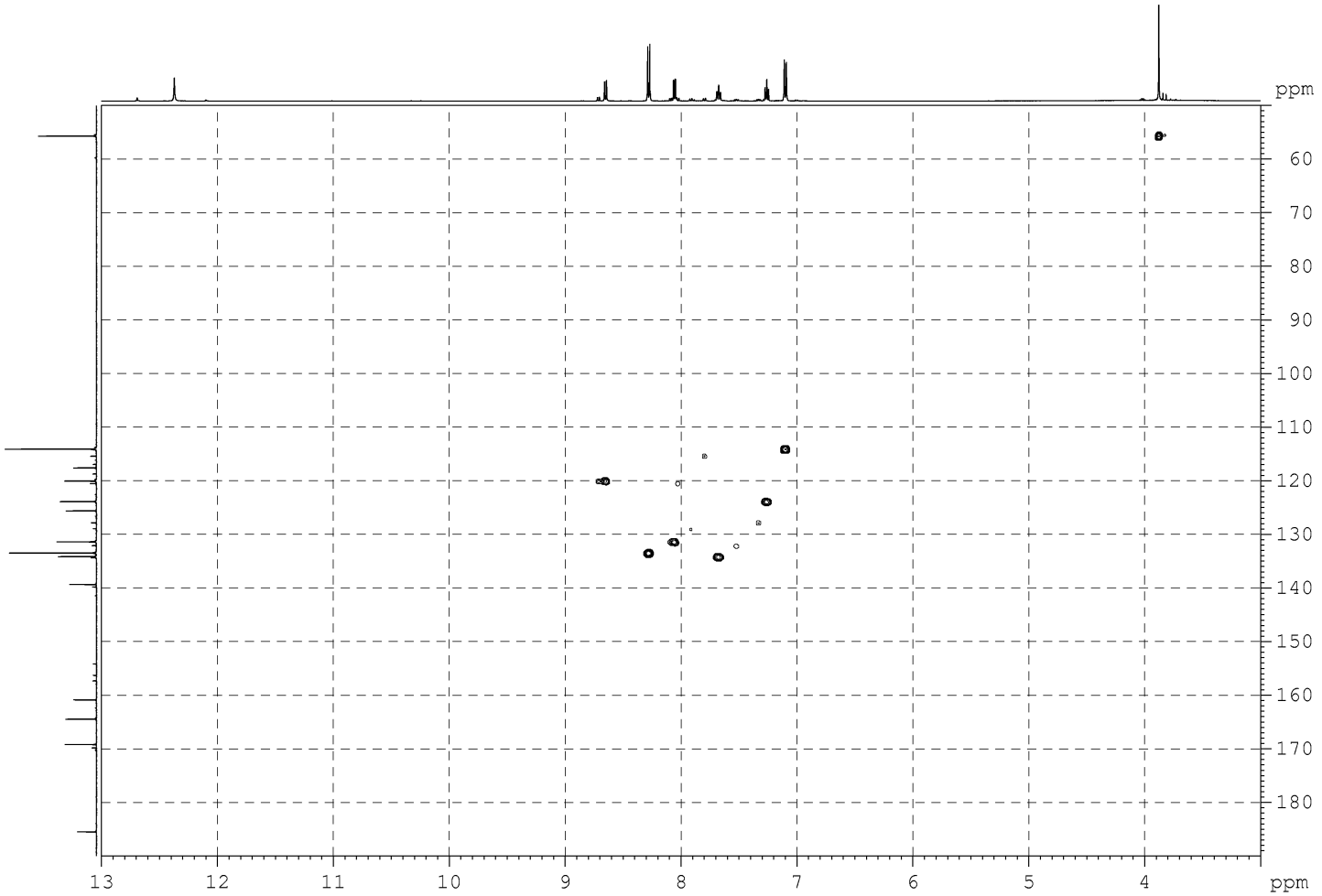



**Figure S148.** 2D $^{1}$H-$^{13}$C HSQC NMR spectra of **7b** in DMSO at T = 303 K.

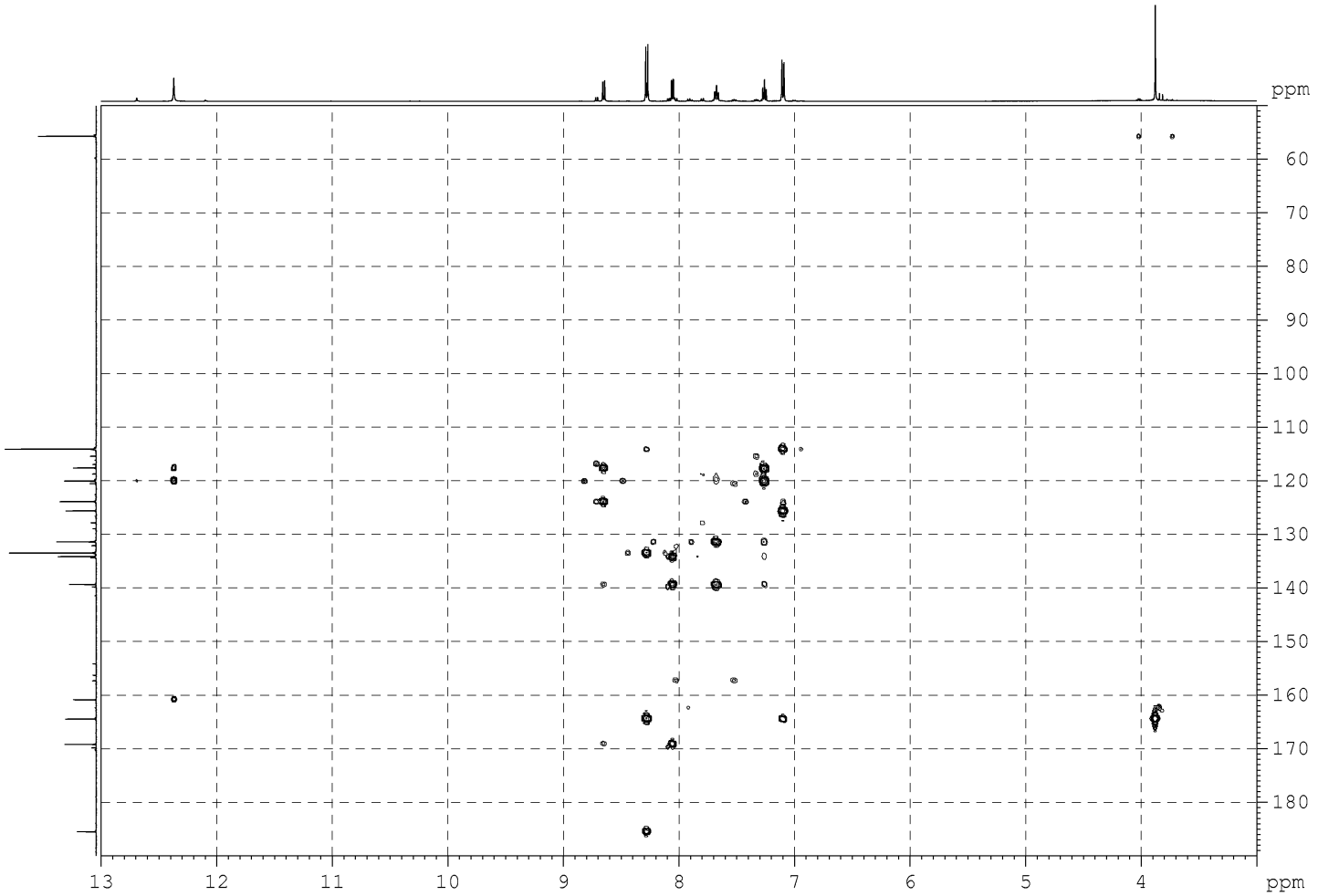



**Figure S149.** 2D $^{1}$H-$^{13}$C HMBC NMR spectra of **7b** in DMSO at T = 303 K.

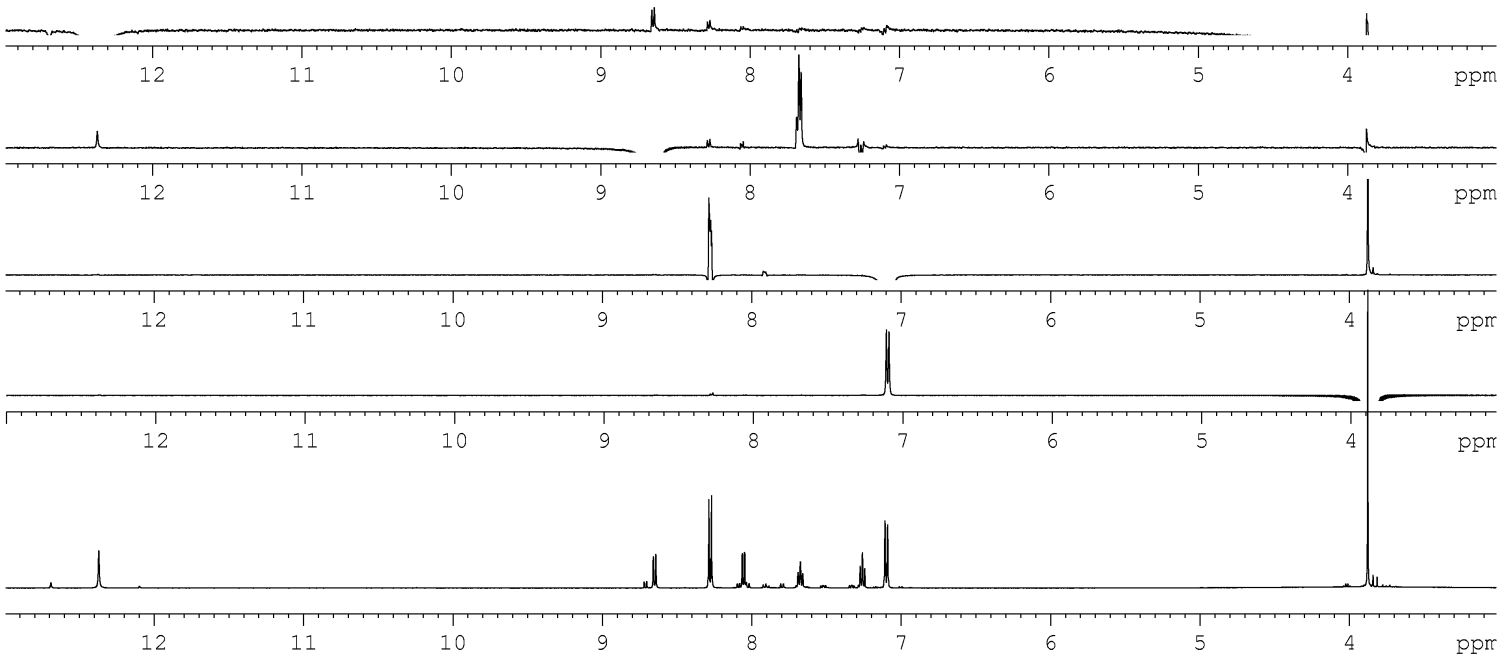



**Figure S150.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **7b** in DMSO at T = 303 K.

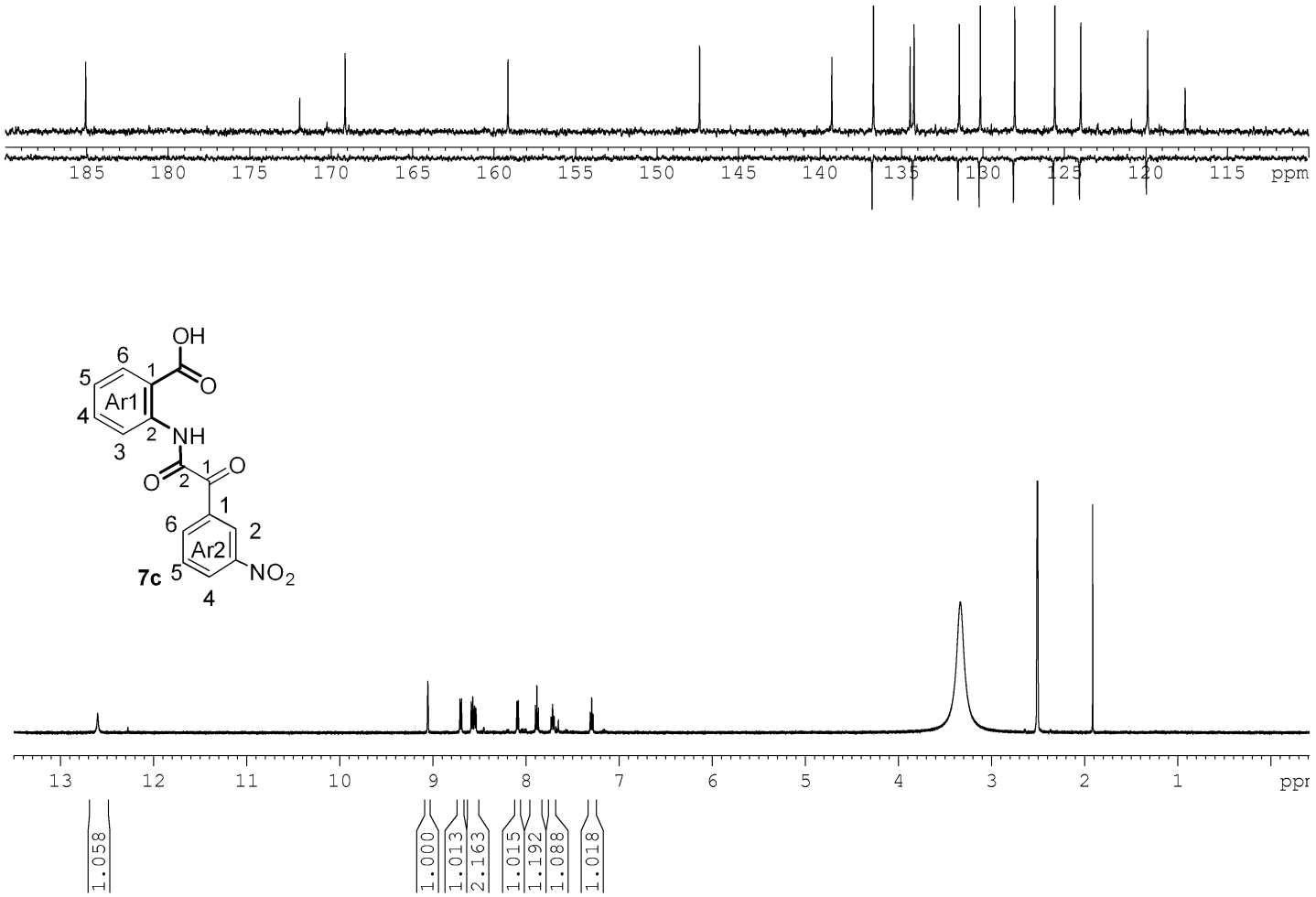



**Figure S151.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **7c** in DMSO at T = 303 K.

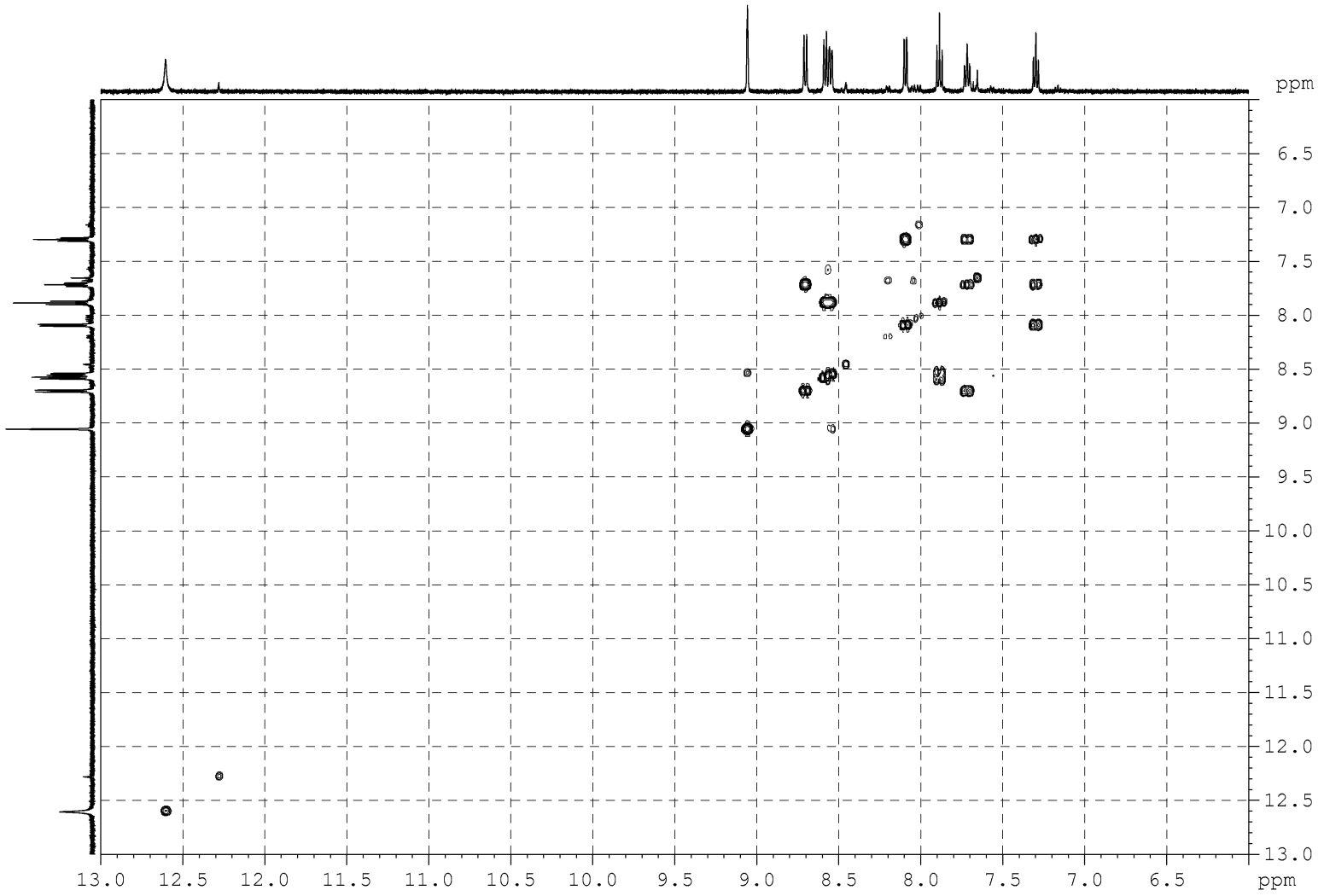



**Figure S152.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **7c** in DMSO at T = 303 K.

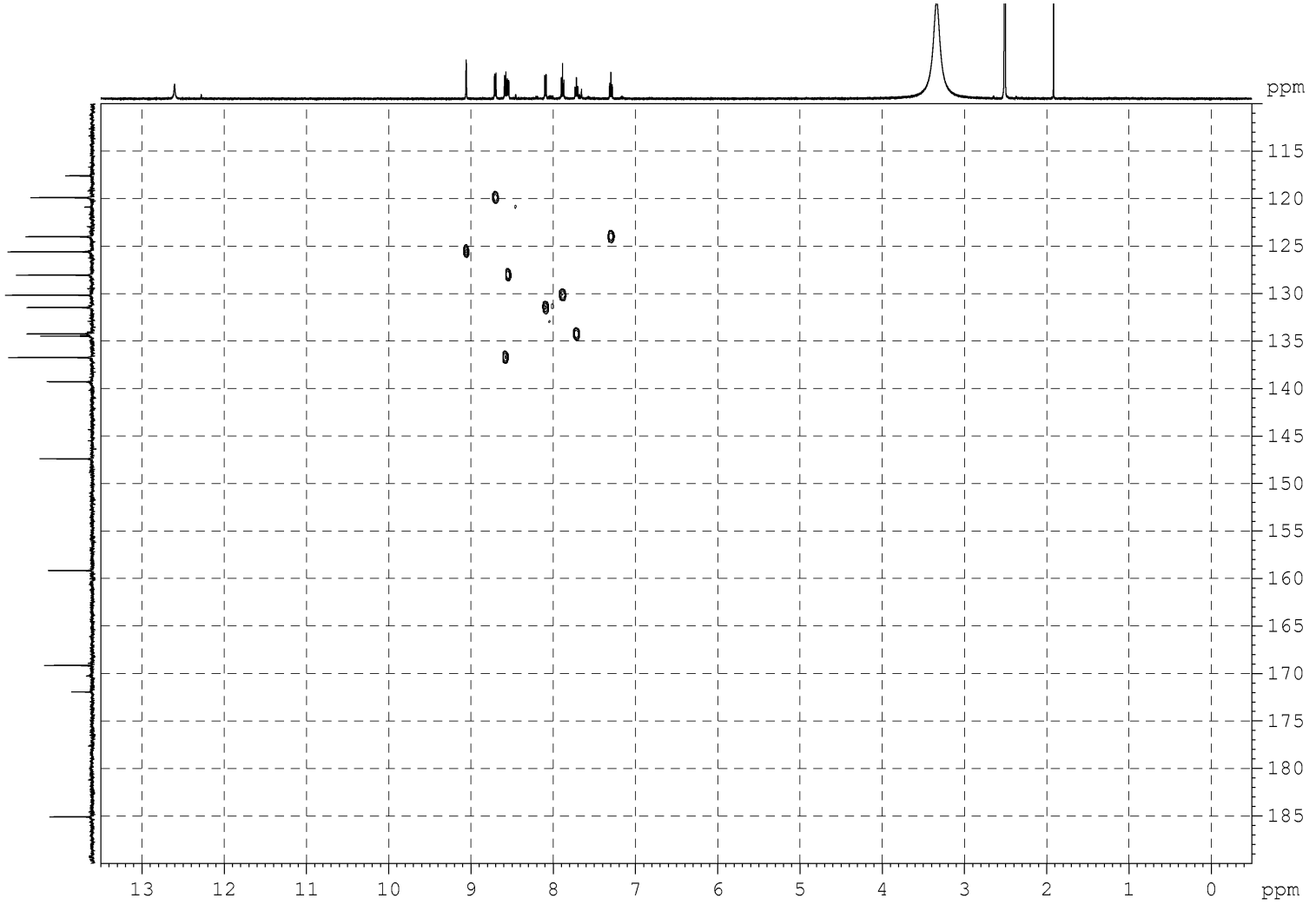



**Figure S153.** 2D $^{1}$H-$^{13}$C HSQC NMR spectra of **7c** in DMSO at T = 303 K.

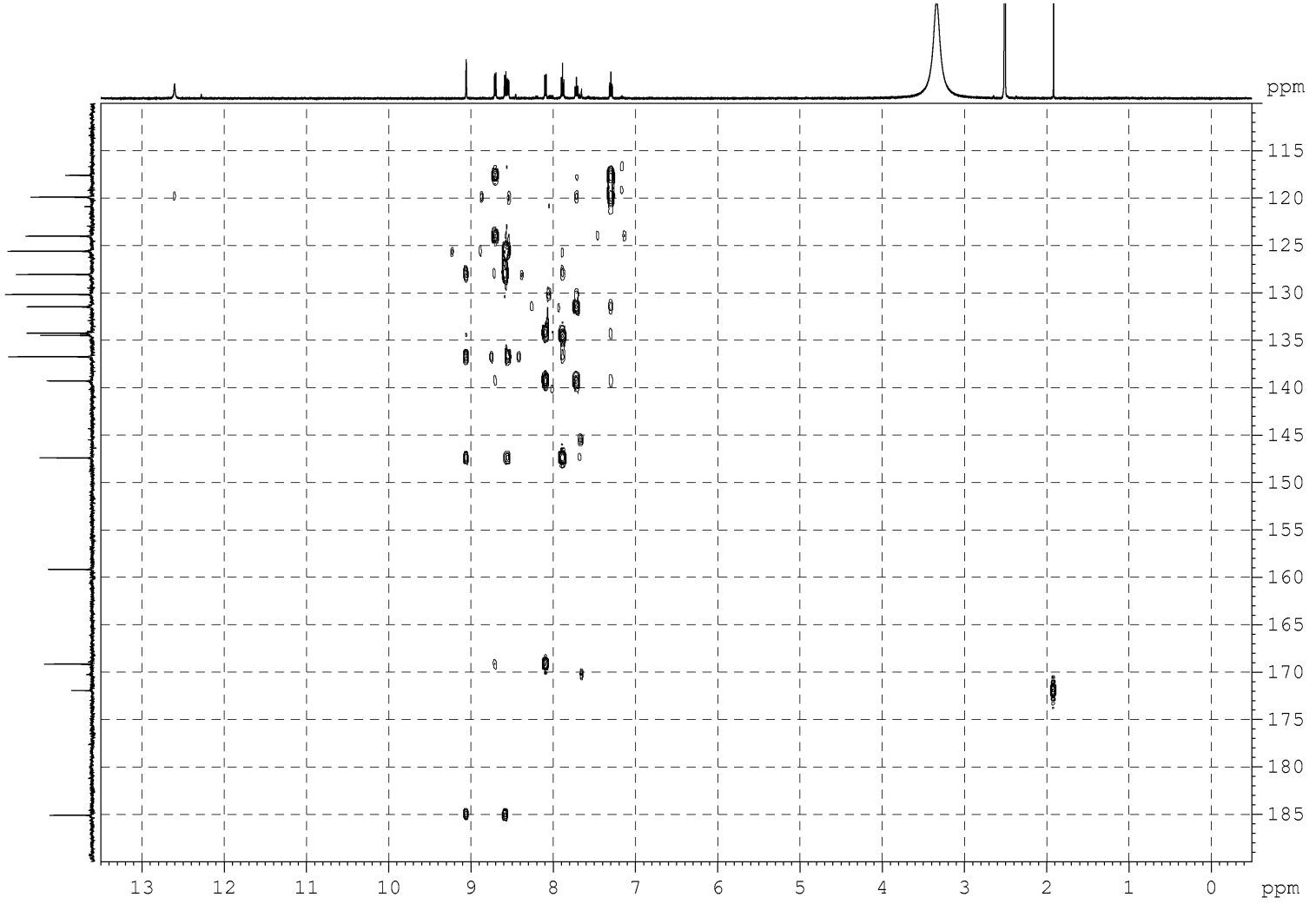



**Figure S154.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **7c** in DMSO at T = 303 K.

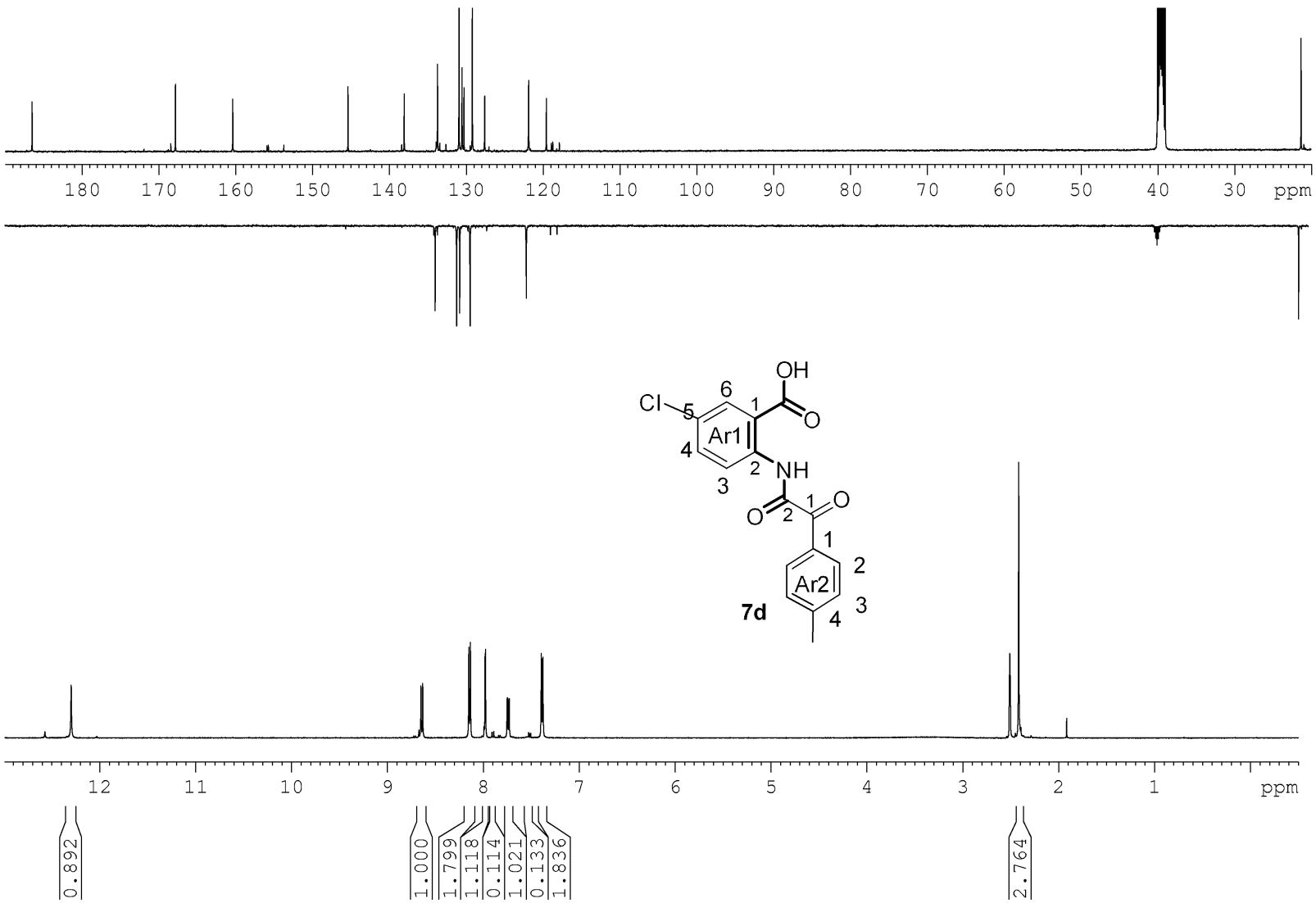



**Figure S155.** 1D $^{1}H$, $^{13}C$ DEPT and $^{13}C\{^{1}H\}$ NMR spectra of **7d** in DMSO at T = 303 K.

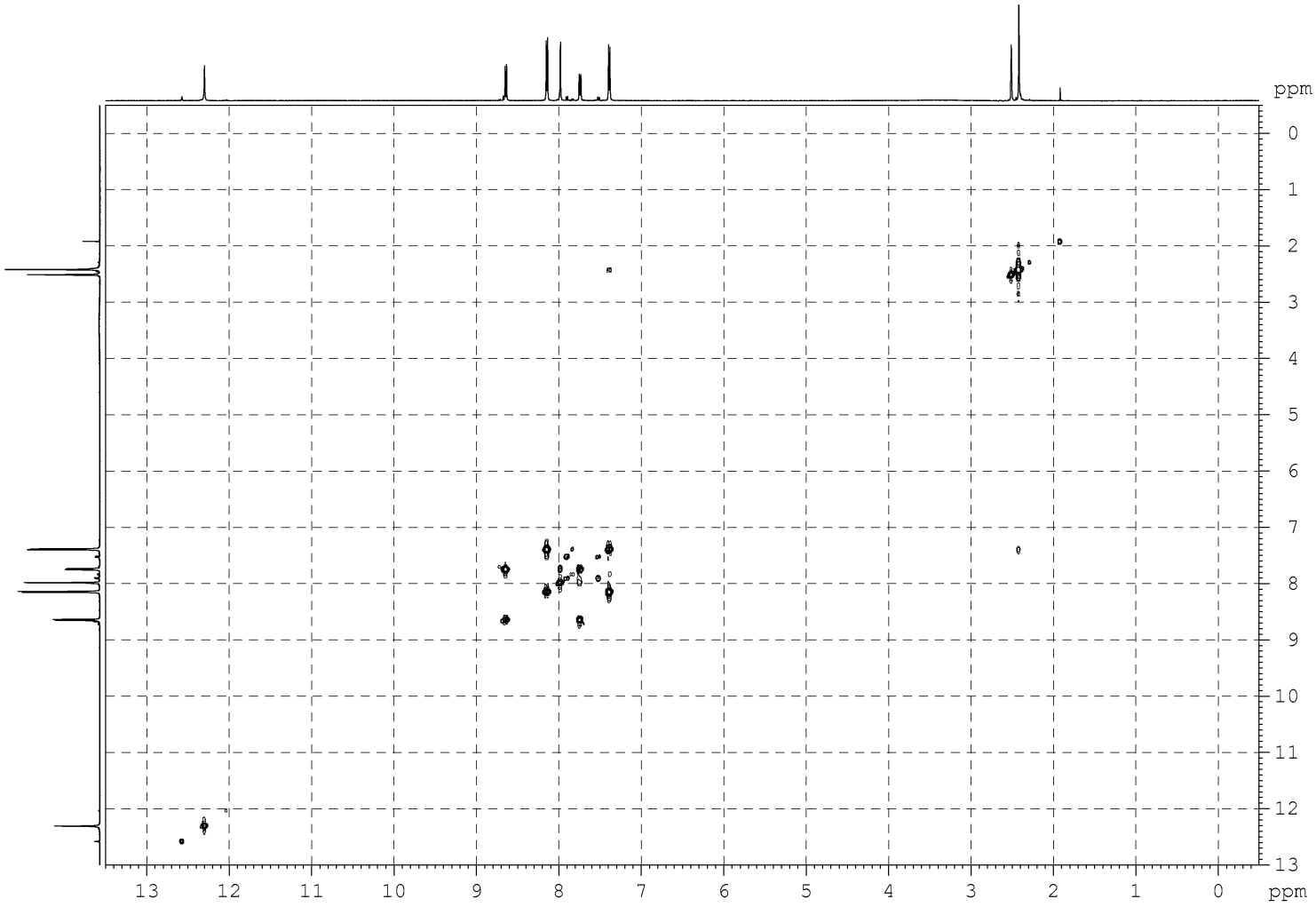



**Figure S156.** 2D $^{1}$H-$^{1}$H COSY NMR spectra of **7d** in DMSO at T = 303 K.

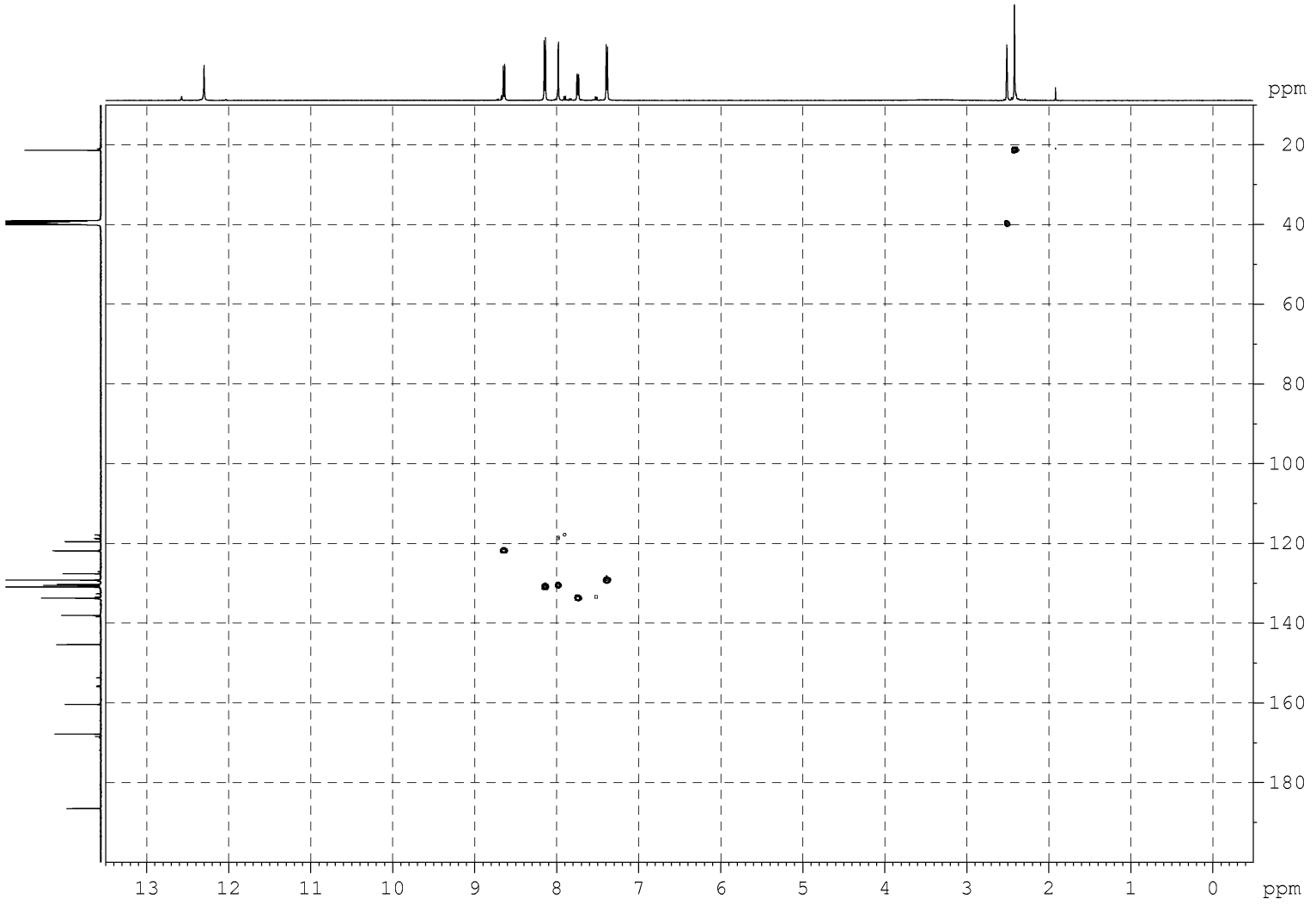



**Figure S157.** 2D $^{1}H$-$^{13}C$ HSQC NMR spectra of **7d** in DMSO at T = 303 K.

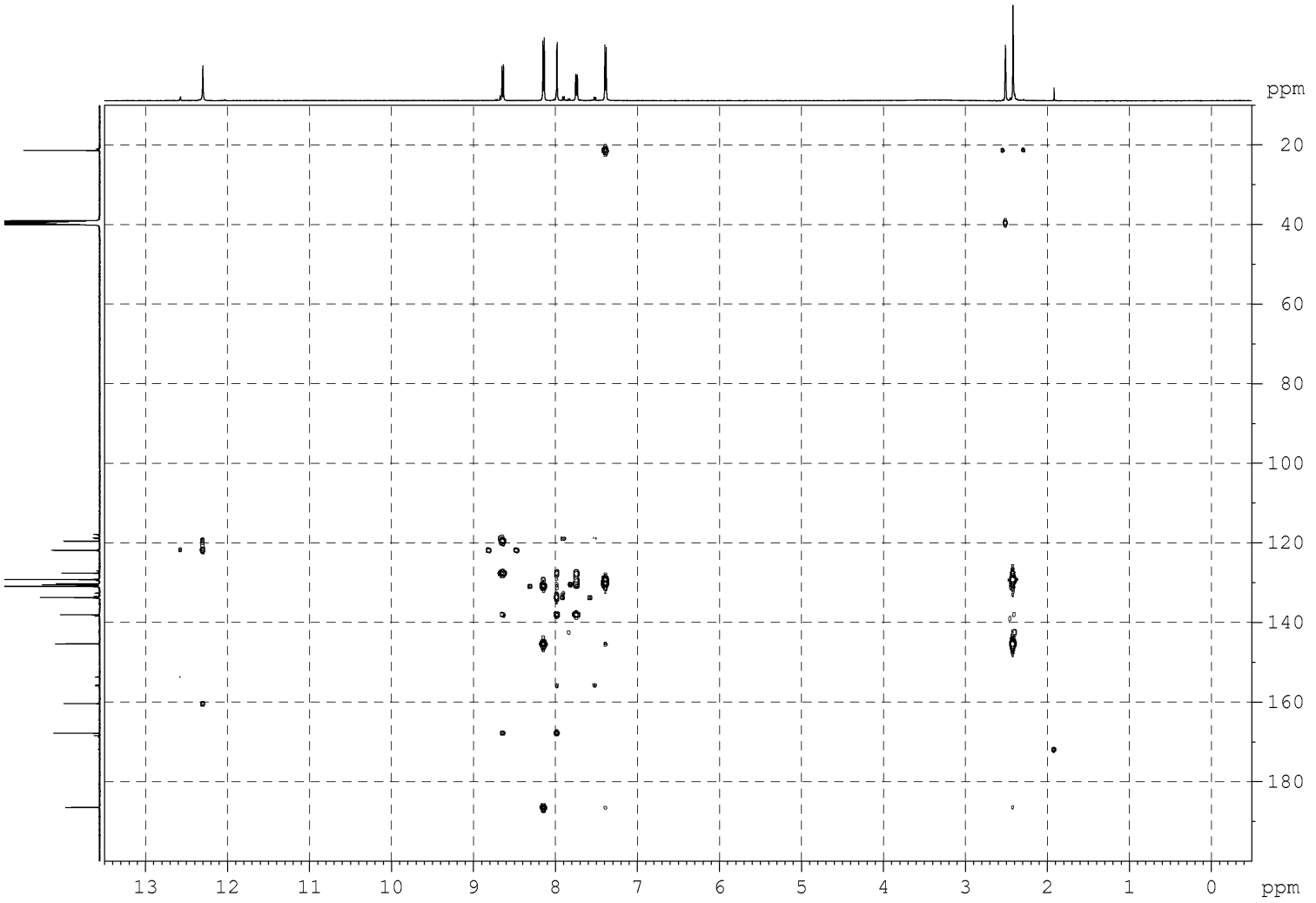



**Figure S158.** 2D $^{1}H$-$^{13}C$ HMBC NMR spectra of **7d** in DMSO at T = 303 K.

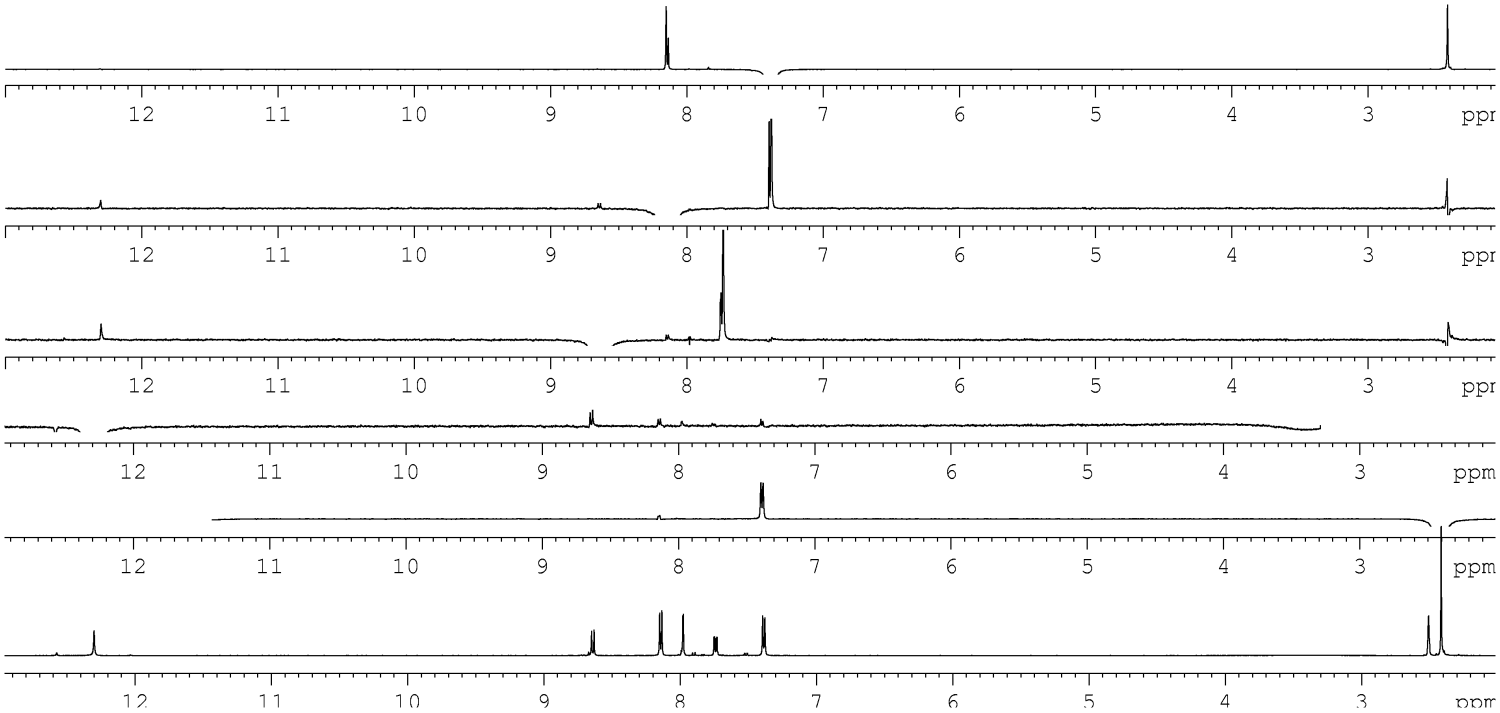



**Figure S159.** 1D $^{1}$H and $^{1}$H DPFGNOE NMR spectra of **7d** in DMSO at T = 303 K.

**The establishment of structure of 3a by variety of 1D/2D NMR correlation methods.**[1]

First, the proton spin systems of $Ar_1$ and $Ar_2$ were established from 2D homo- and heterocorrelations. After that these structural fragments were "bonded" according to $^{1}H$-$^{13}C$ HMBC connectivities in a single whole. The conclusion on the *trans*-configuration of compounds **3** is based upon NOE and $^{3}J_{HH}$ data. Namely, there is only a small NOE between the vicinal protons of epoxy fragments due to its mutual *trans*-orientation and small values of $^{3}J_{HH}$ (1.8 Hz) is also attributed to such geometry (calculations of $^{3}J_{HH}$ for **3a** predict 4.3 and 1.8 Hz for *cis*- and *trans*-isomers, respectively; Figure 1).

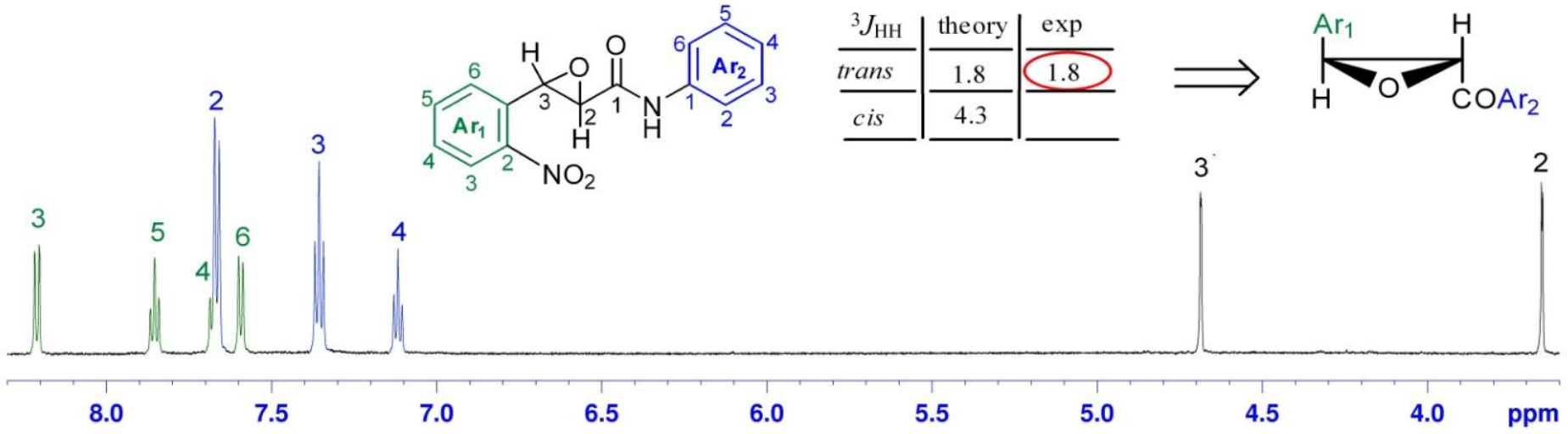


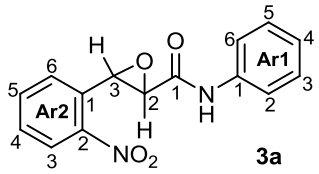

**Figure 1**. Fragment of $^{1}H$ NMR spectra (DMSO-$d_6$, T = 303 K) of **3a**. Comparison of the calculated $^{3}J_{HH}$ for *trans*- and *cis*-isomers of **3a** *versus* their experimental value.

(1) (a) Derome, A. E. *Modern NMR Techniques for Chemistry Research*; Pergamon: Cambridge, U.K, **1988**. (b) Atta-ur-Rahman, T. I. *One and Two Dimensional NMR Spectroscopy*; Elsevier: Amsterdam, **1989**, pp. 578.

# HRMS spectra

HRMS spectra were obtained using the MALDI method (analyzer type: TOF-TOF reflectron). Measurements were made in the range *m*/*z* 200-1000. The *m*/*z* values of monoisotopic ions are given in the descriptions. Samples were dissolved in DMF at concentration 10-3 mg/mL. A solution of the matrix (*p*-nitroaniline) in acetonitrile at concentration 10 mg/mL was prepared. A calibration mixture of PEG-400, (acetonitrile solution at concentration 1 mg/mL) was used to obtain high-resolution mass spectra. Samples were deposited by the dried-droplet method. Matrix solution (0.5 mkL), analyte solution (0.5 mkL) and calibration-mixture solutions (0.5 mkL) was deposited on an maldi target plate.

*trans-3-(2-Nitrophenyl)-N-pheniloxiran-2-carboxamides (**3a**).*




**3a**

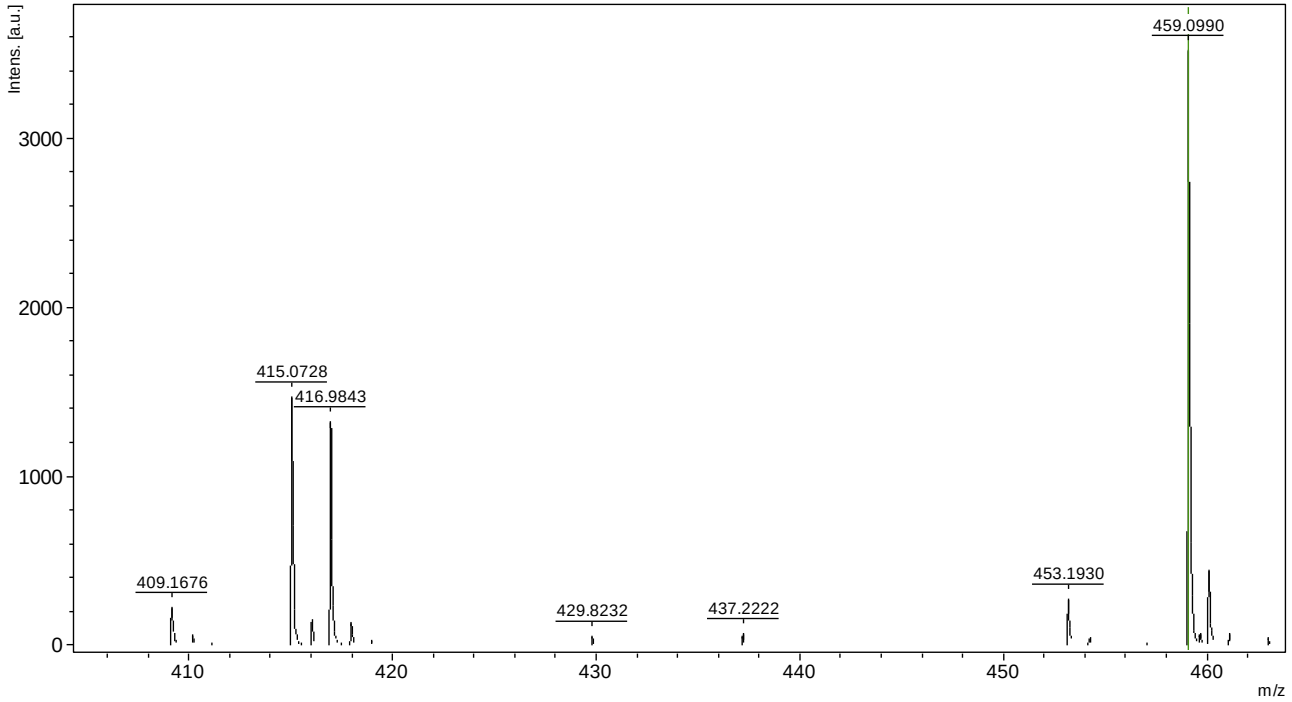
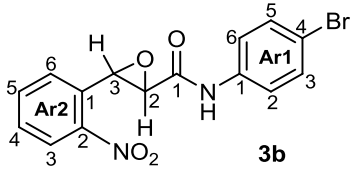


**Figure S1.** HRMS of **3a.** m/z calcd. for $C_{15}H_{12}N_2O_4$ $[M+Cs]^+$ 416.9846, found 416.9843 (MALDI).

*trans-N-(4-Bromophenyl)- 3-(2-nitrophenyl)oxiran-2-carboxamide (**3b**).*



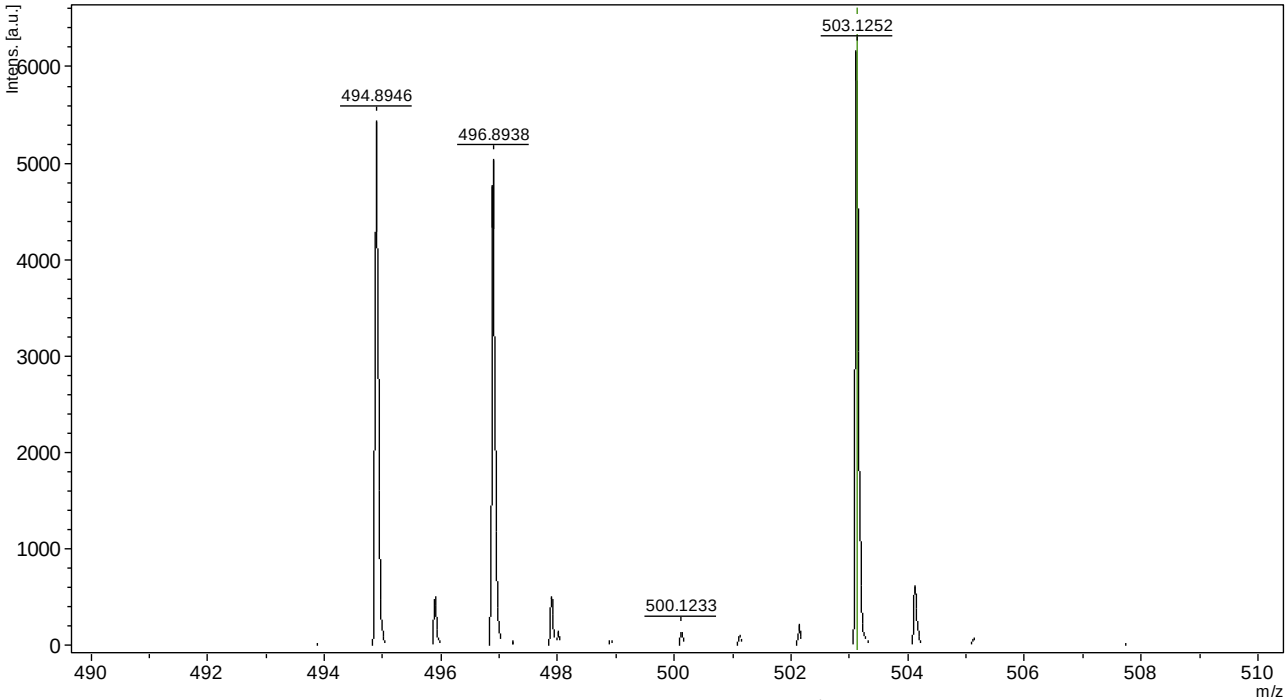
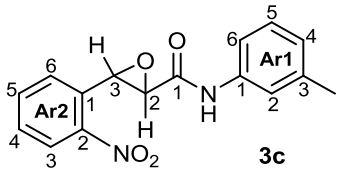




**Figure S2.** HRMS of **3b.** m/z calcd. for $C_{15}H_{11}BrN_2O_4$ $[M+Cs]^+$ 494.8951;496.8932, found 494.8946; 496.8938 (MALDI).

*trans-3-(2-Nitrophenyl)-N-3-tolyloxiran-2-carboxamide (**3c**).*



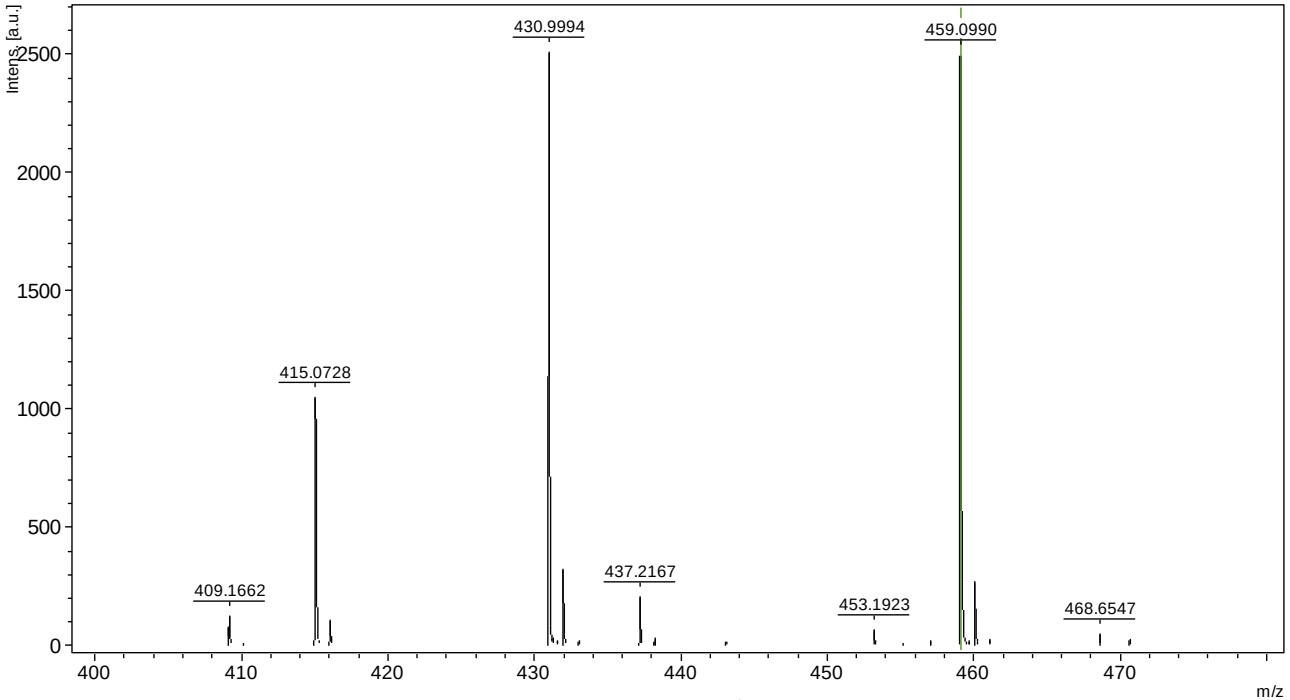
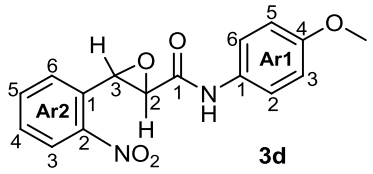




**Figure S3.** HRMS of **3c.** m/z calcd. for $C_{16}H_{14}N_2O_4$ $[M+Cs]^+$ 431.0003, found 430.9994 (MALDI).

*trans-N-(4-Methoxyphenyl)-3-(2-nitrophenyl)oxirane-2-carboxamide (**3d**).*



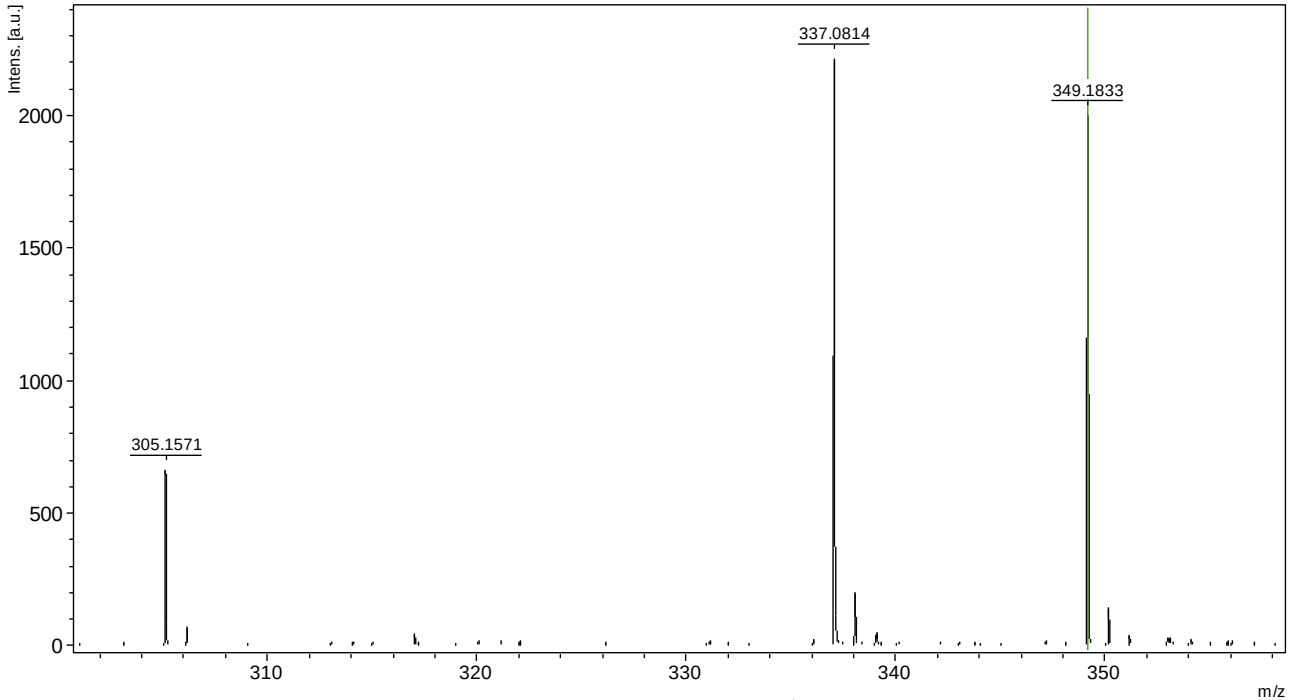
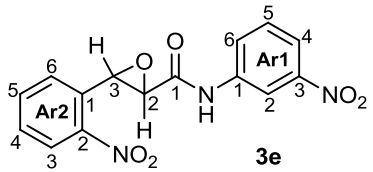




**Figure S4.** HRMS of **3d.** m/z calcd. for $C_{16}H_{14}N_2O_5$ $[M+Na]^+$ 337.0795, found 337.0814 (MALDI).

*trans-N-(3-Nitrophenyl)-3-(2-nitrophenyl)oxirane-2-carboxamide (**3e**).*



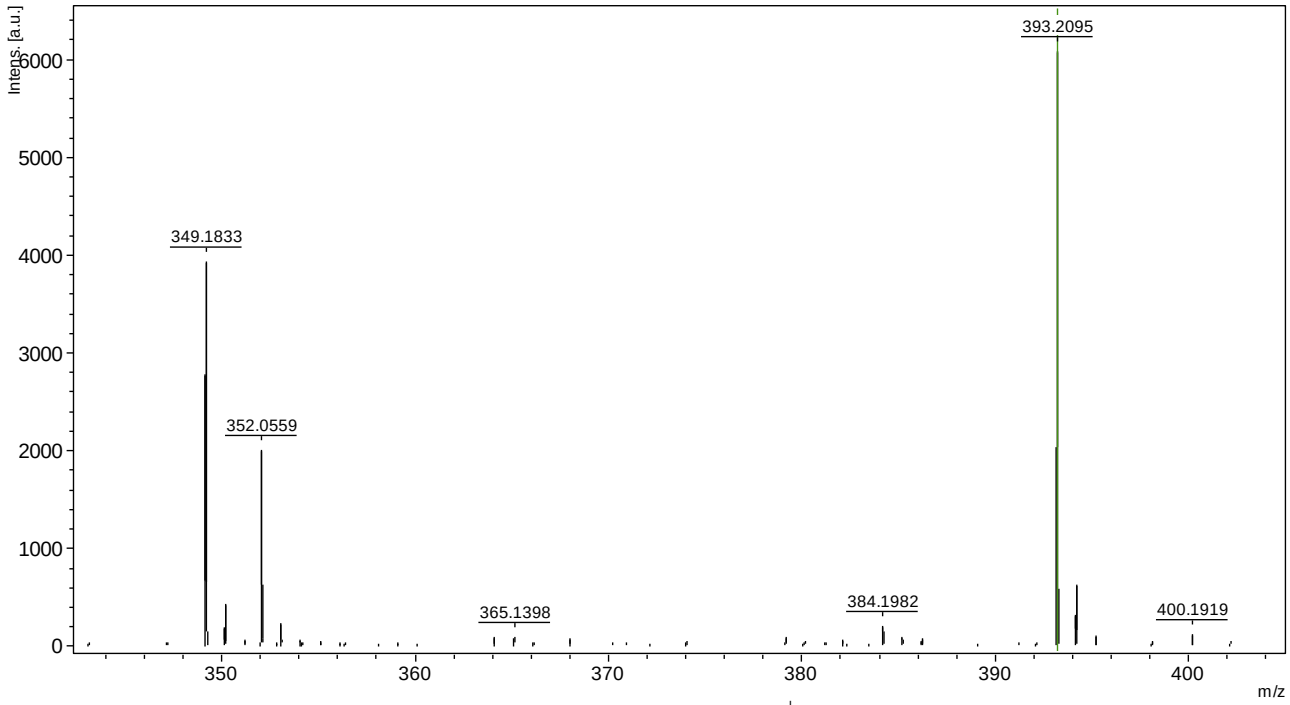
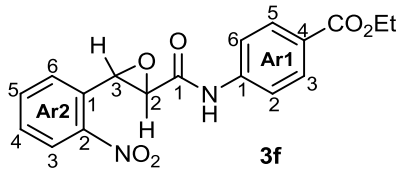




**Figure S5.** HRMS of **3e.** m/z calcd. for $C_{15}H_{11}N_3O_6$ $[M+Na]^+$ 352.0540, found 352.0559 (MALDI).

*trans-3-(2-Nitrophenyl)-N-(4-ethylcarboxyphenyl)oxiran-2-carboxamide (**3f**).*




**3f**

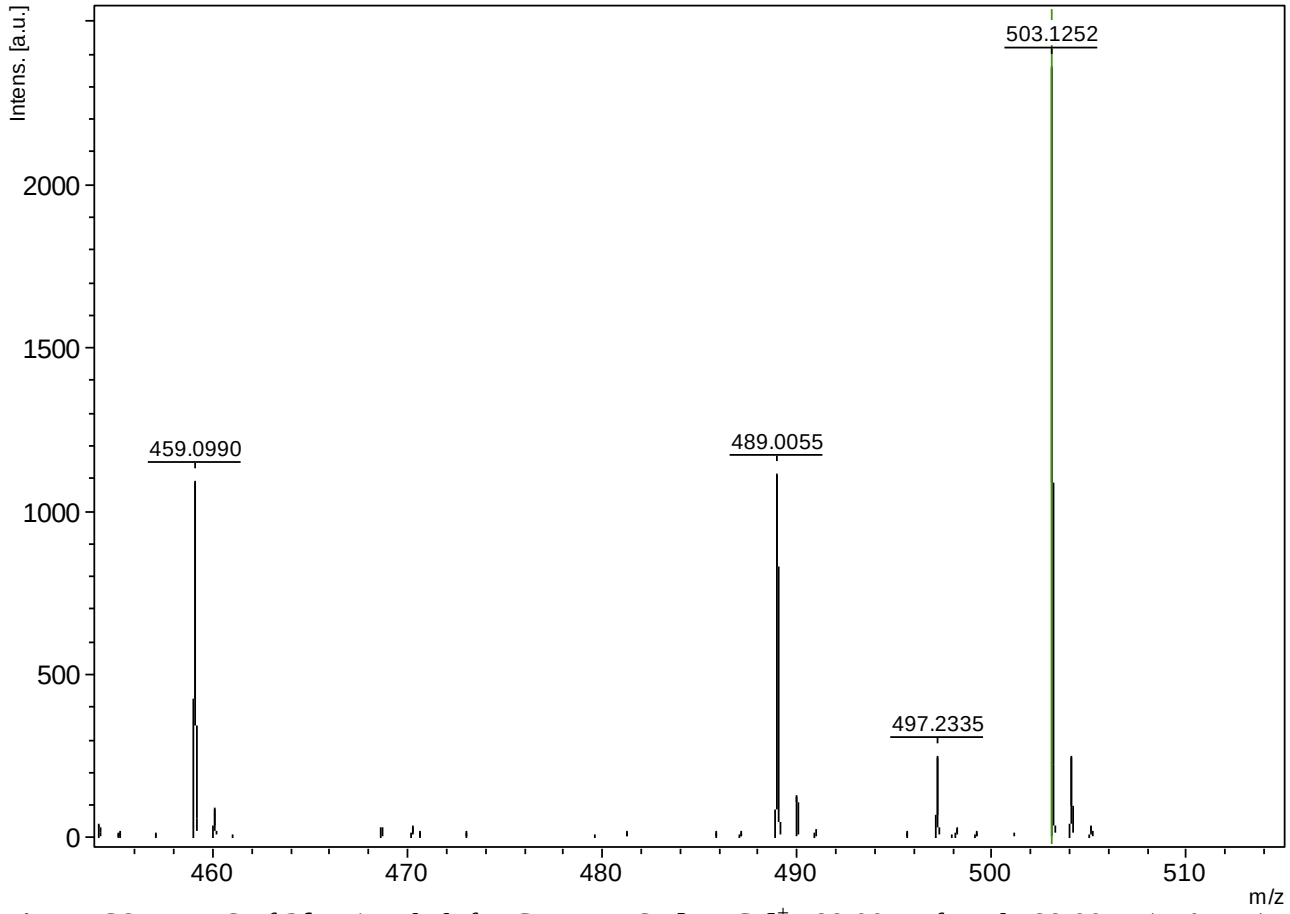
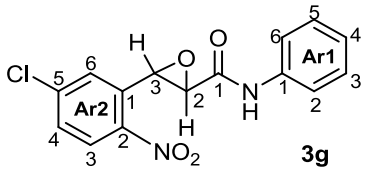



**Figure S6.** HRMS of **3f.** m/z calcd. for $C_{18}H_{16}N_2O_6$ $[M+Cs]^+$ 489.0057, found 489.0055 (MALDI).

*trans-3-(2-Nitro-5-chlorophenyl)-N-phenyloxiran-2-carboxamide (**3g**).*




**3g**

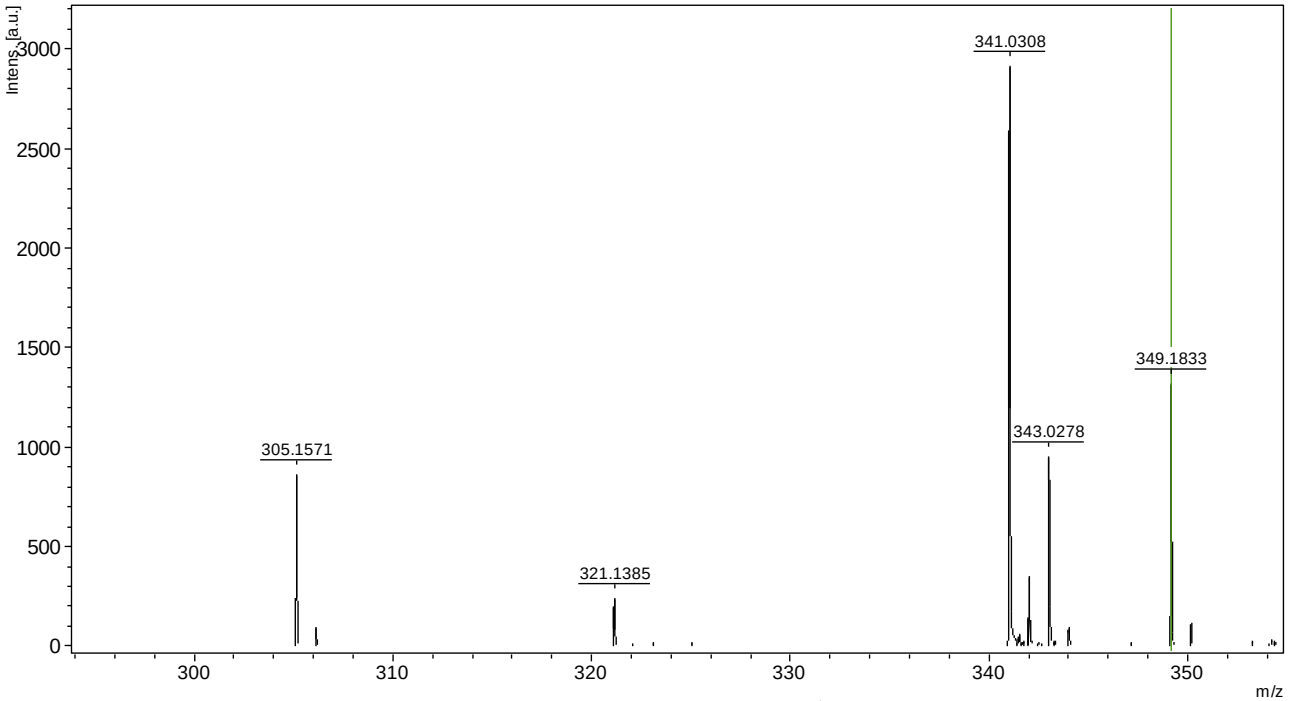
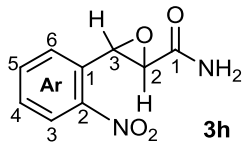



**Figure S7.** HRMS of **3g.** m/z calcd. for $C_{15}H_{11}ClN_2O_4$ $[M+Na]^+$ 341.0299, found 341.0308 (MALDI).

*trans-3-(2-Nitrophenyl)oxiran-2-carboxamide (**3h**).*




**3h**

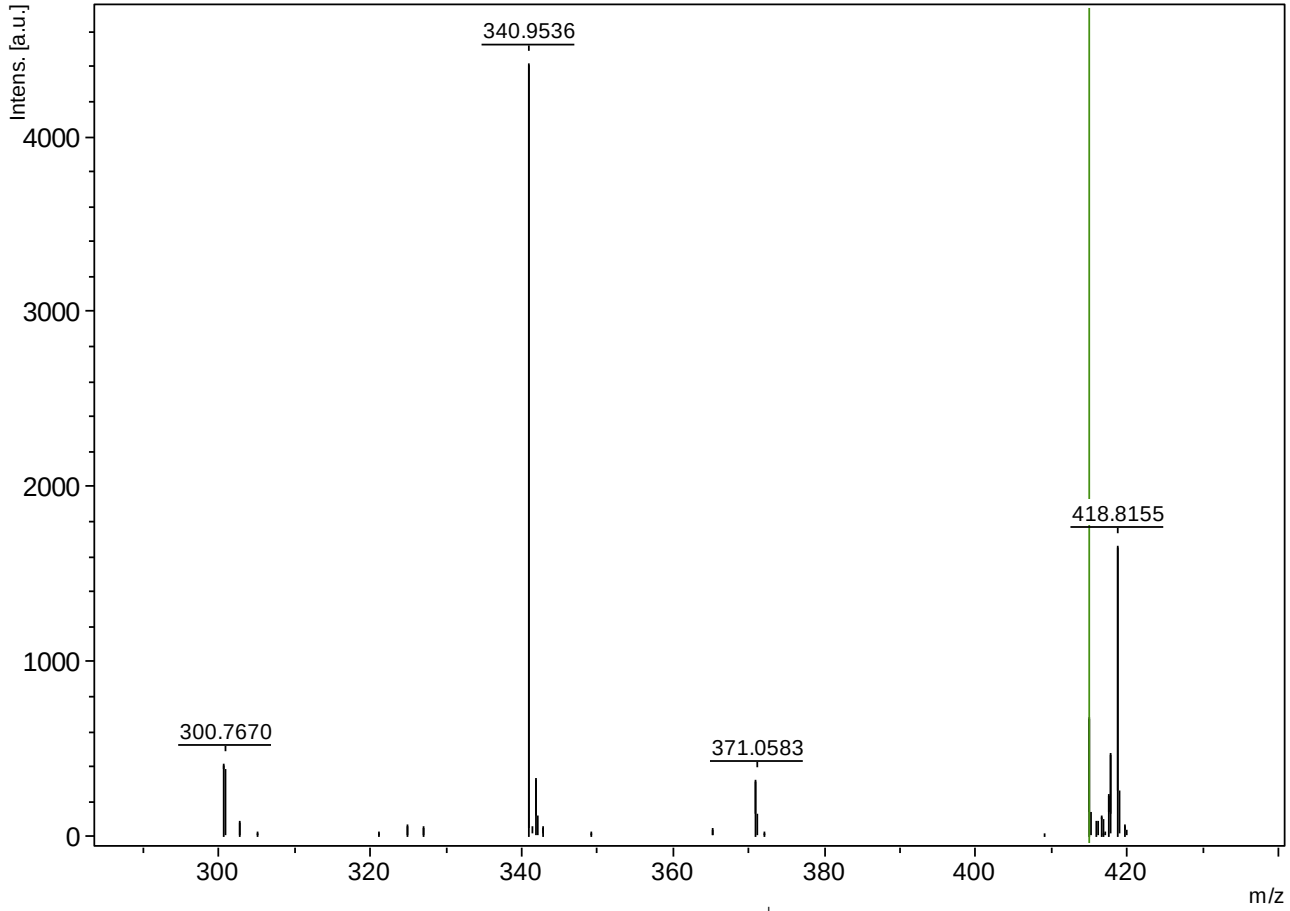



**Figure S8.** HRMS of **3h.** m/z calcd. for $C_9H_8N_2O_4$ $[M+Cs]^+$ 340.9533, found 340.9536 (MALDI).

*$N^1$-(2-carboxyphenyl)-$N^2$-phenyloxalamide (**4a**).*

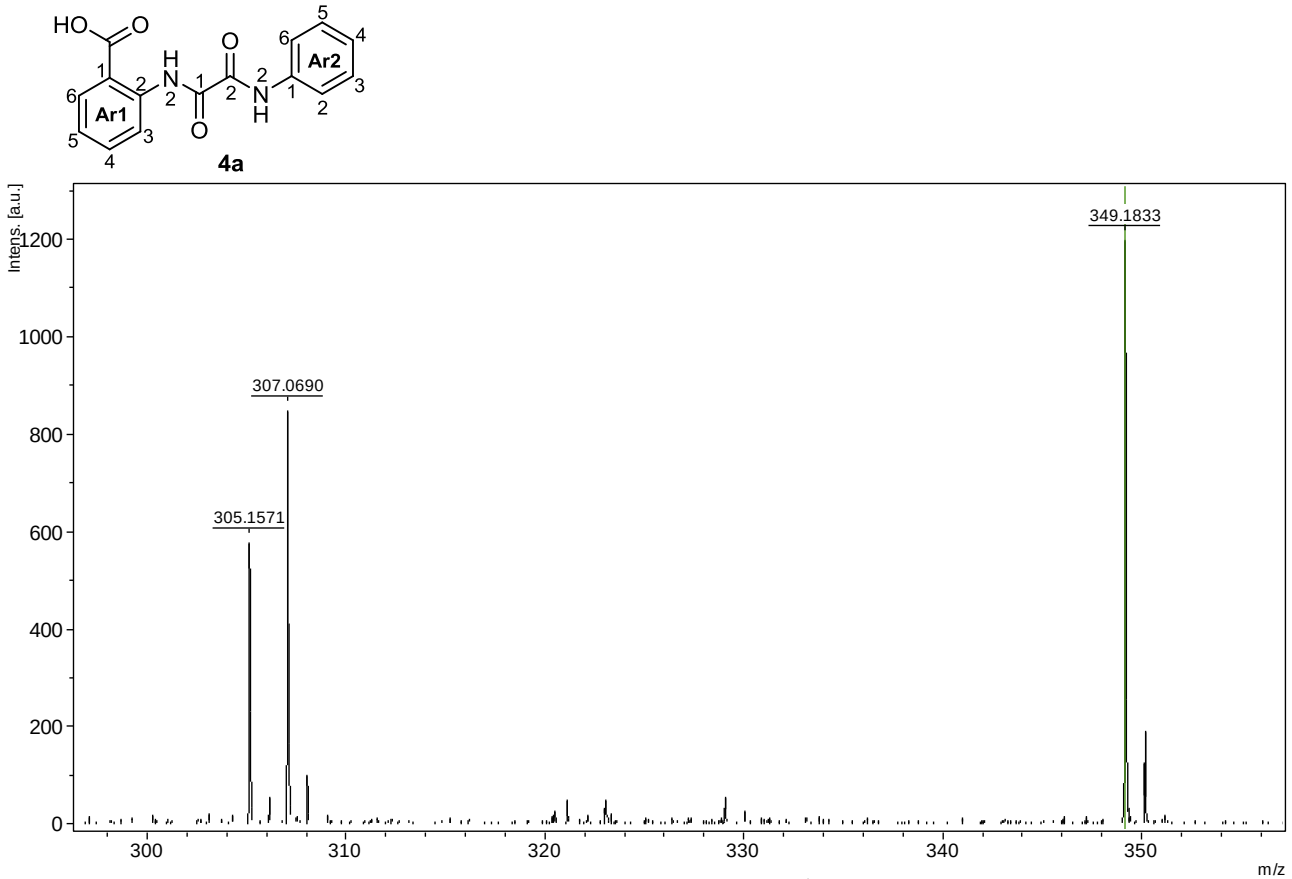
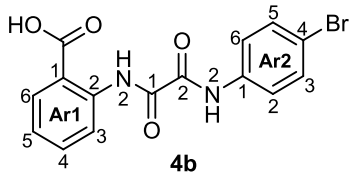



**Figure S11.** HRMS of **4a.** m/z calcd. for $C_{15}H_{12}N_2O_4$ $[M+Na]^+$ 307.0689, found 307.0690 (MALDI).

*$N^1$-(2-carboxyphenyl)-$N^2$-(4-bromophenyl)oxalamide (**4b**).*




**4b**

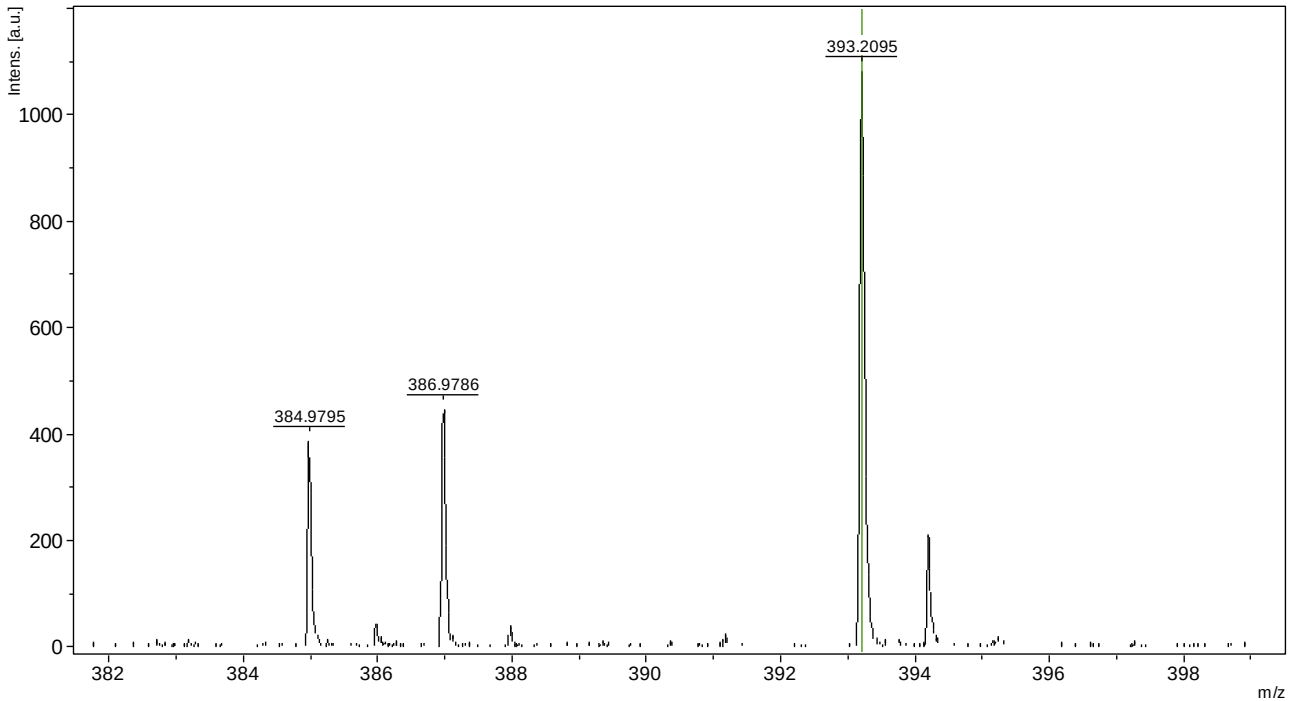



**Figure S12.** HRMS of **4b.** m/z calcd. for $C_{15}H_{11}BrN_2O_4$ $[M+Na]^+$ 384.9794;386.9776, found 384.9795;386.9786 (MALDI).

*$N^1$-(2-carboxyphenyl)-$N^2$-(3-methylphenyl)oxalamide (**4c**).*

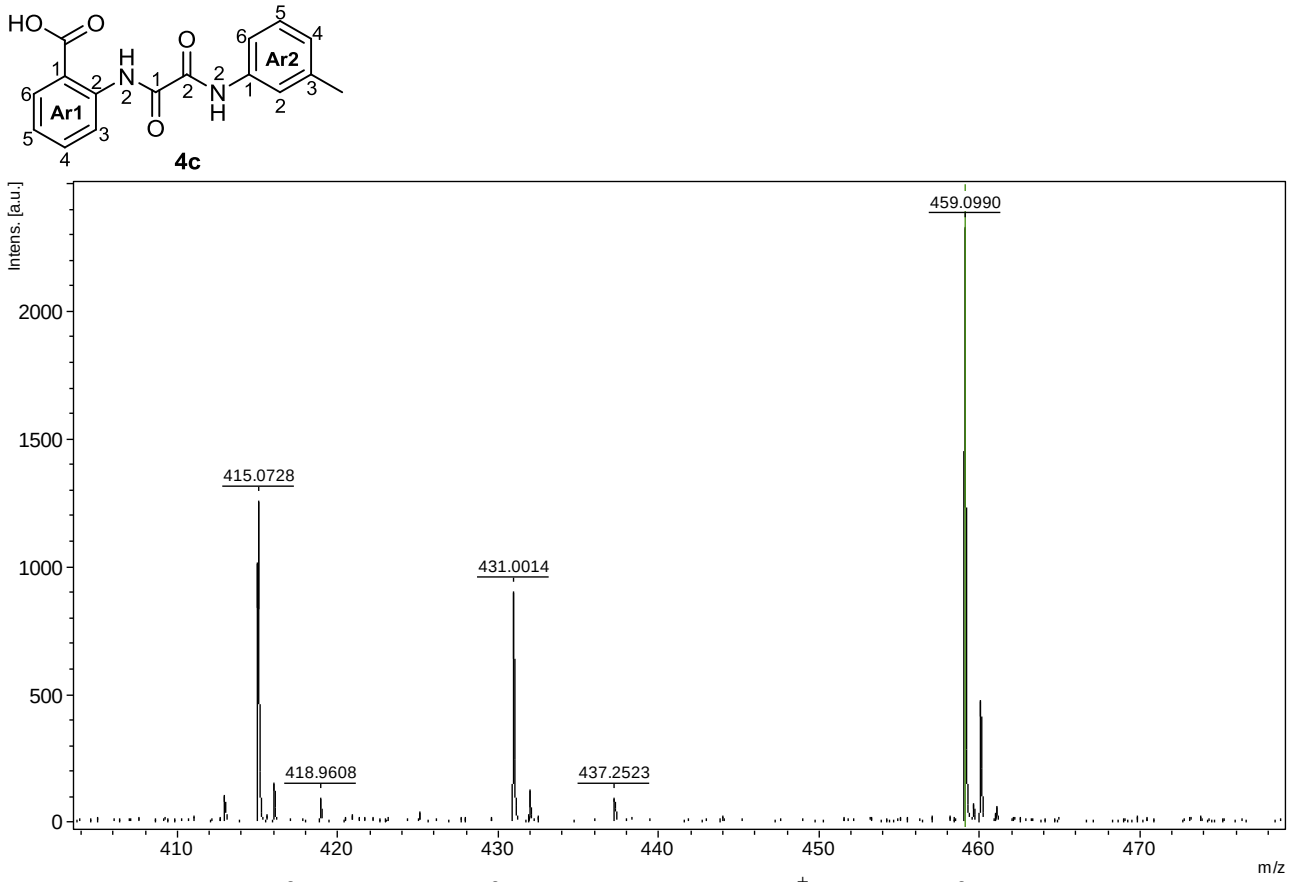
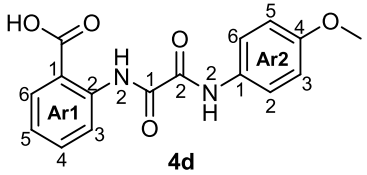



**Figure S13.** HRMS of **4c.** m/z calcd. for $C_{16}H_{14}N_2O_4$ $[M+Cs]^+$ 431.0003, found 431.0014 (MALDI).

*$N^1$-(2-carboxyphenyl)-$N^2$-(4-methoxyphenyl)oxalamide (**4d**).*




**4d**

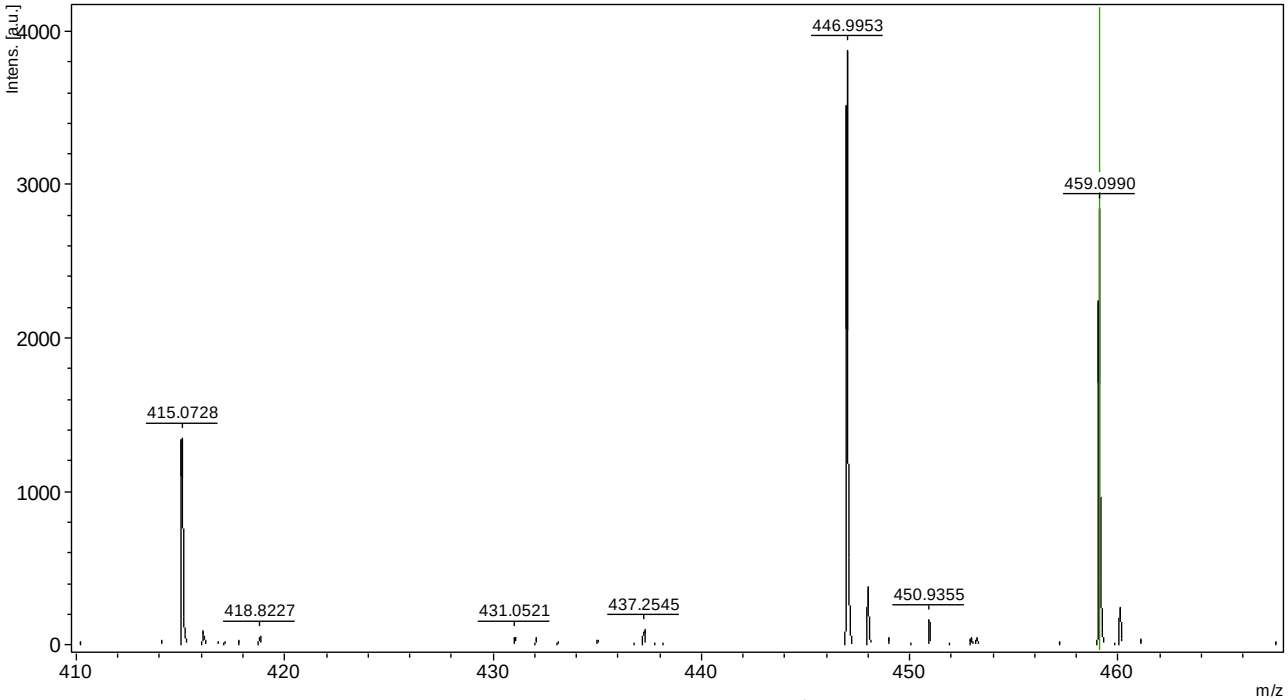
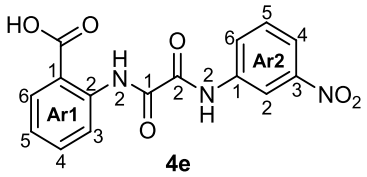



**Figure S14.** HRMS of **4d.** m/z calcd. for $C_{16}H_{14}N_2O_5$ $[M+Cs]^+$ 446.9952, found 446.9953 (MALDI).

*$N^1$-(2-carboxyphenyl)-$N^2$-(3-nitrophenyl)oxalamide (**4e**).*



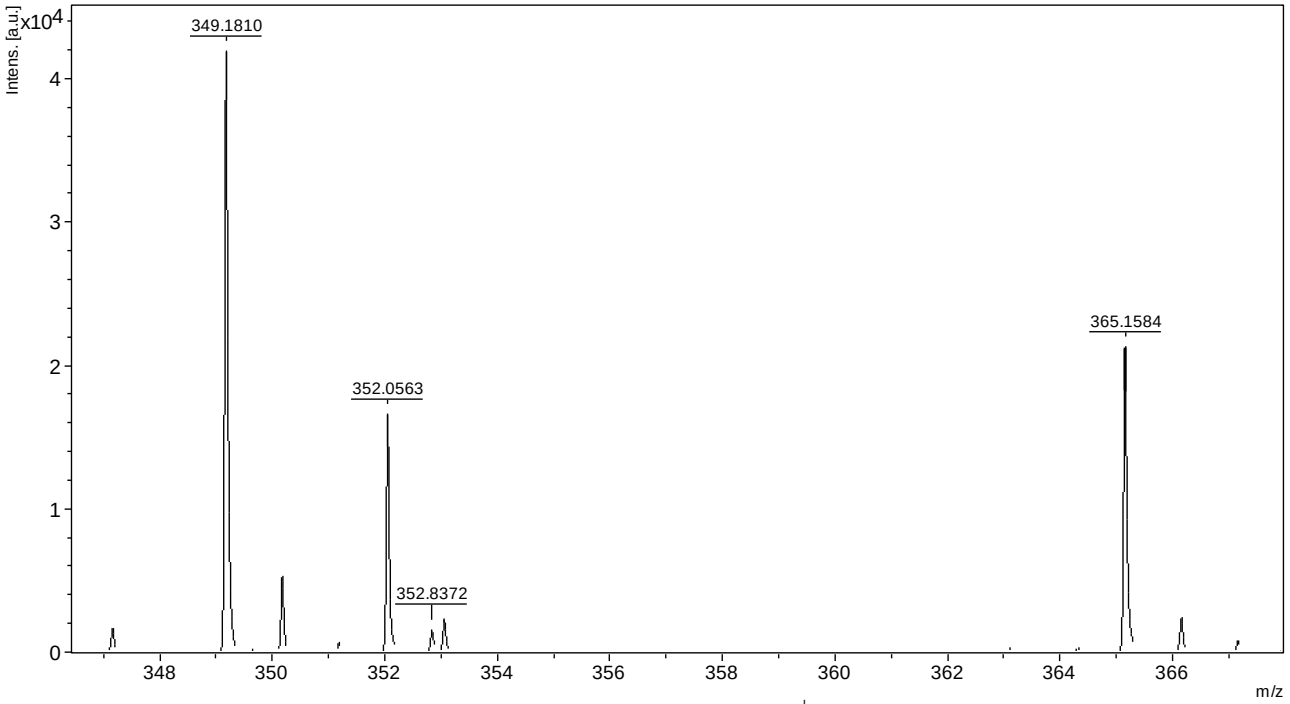
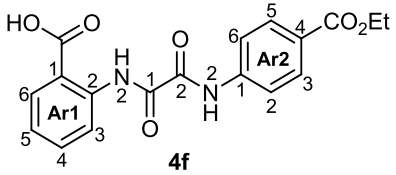




**Figure S15.** HRMS of **4e.** m/z calcd. for $C_{15}H_{11}N_3O_6$ $[M+Na]^+$ 352.0540, found 352.0563 (MALDI).

*$N^1$-(2-carboxyphenyl)-$N^2$-(4-ethylcarboxypheny)oxalamide (**4f**).*




**4f**

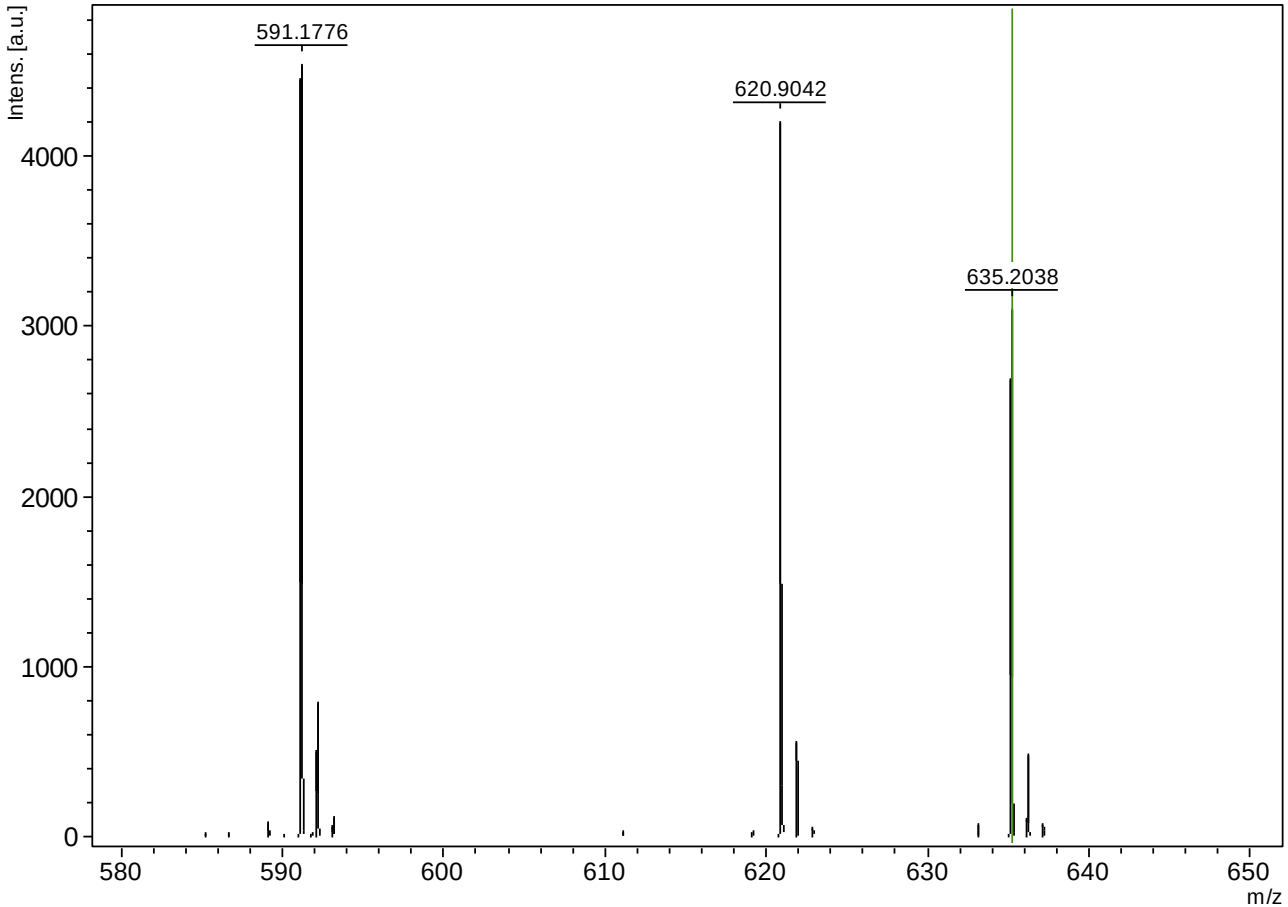
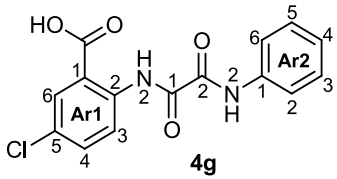



**Figure S16.** HRMS of **4f.** m/z calcd. for $C_{18}H_{16}N_2O_6$ $[M+2Cs-H]^+$ 620.9034, found 620.9042 (MALDI).

*$N^1$-(4-chloro-2-carboxyphenyl)-$N^2$-phenyloxalamide (**4g**).*



**4g**

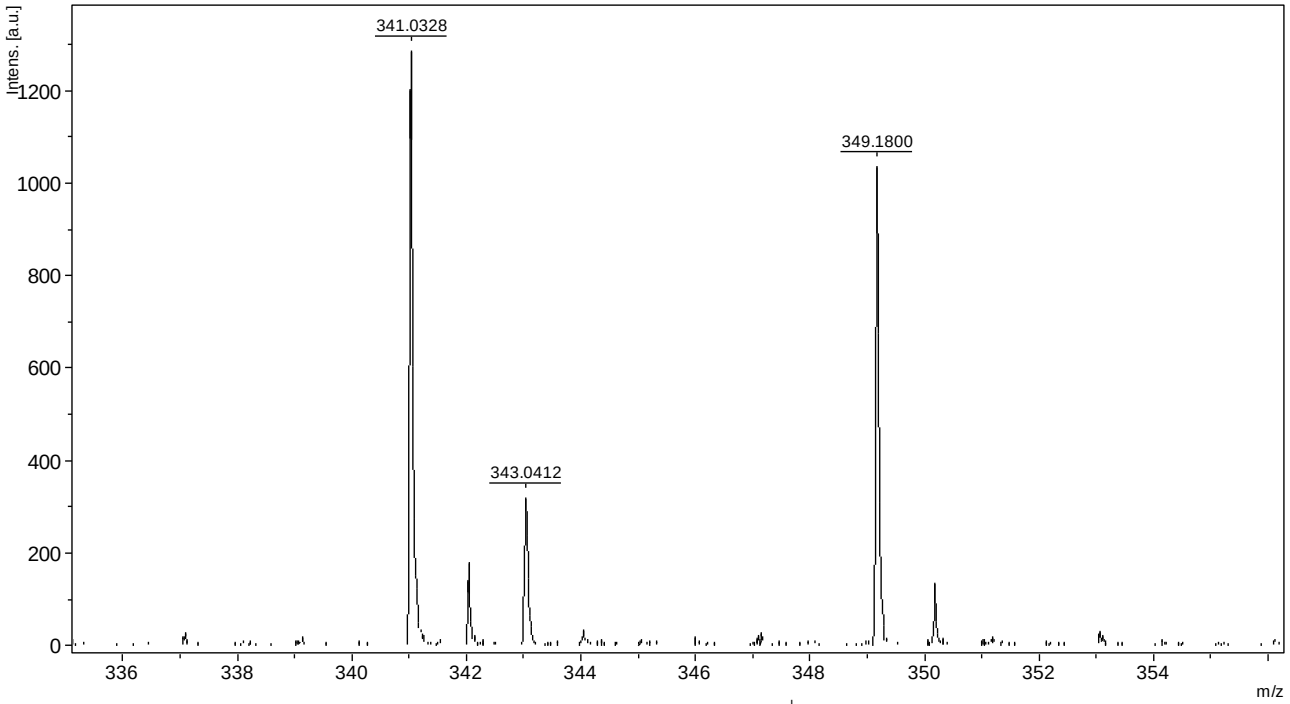
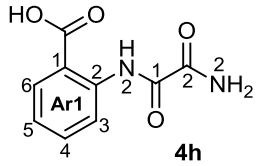


**Figure S17.** HRMS of **4g.** m/z calcd. for $C_{15}H_{11}ClN_2O_4$ $[M+Na]^+$ 341.0300, found 341.0328 (MALDI).

*N-(2-carboxyphenyl)oxalamide (**4h**).*




**4h**

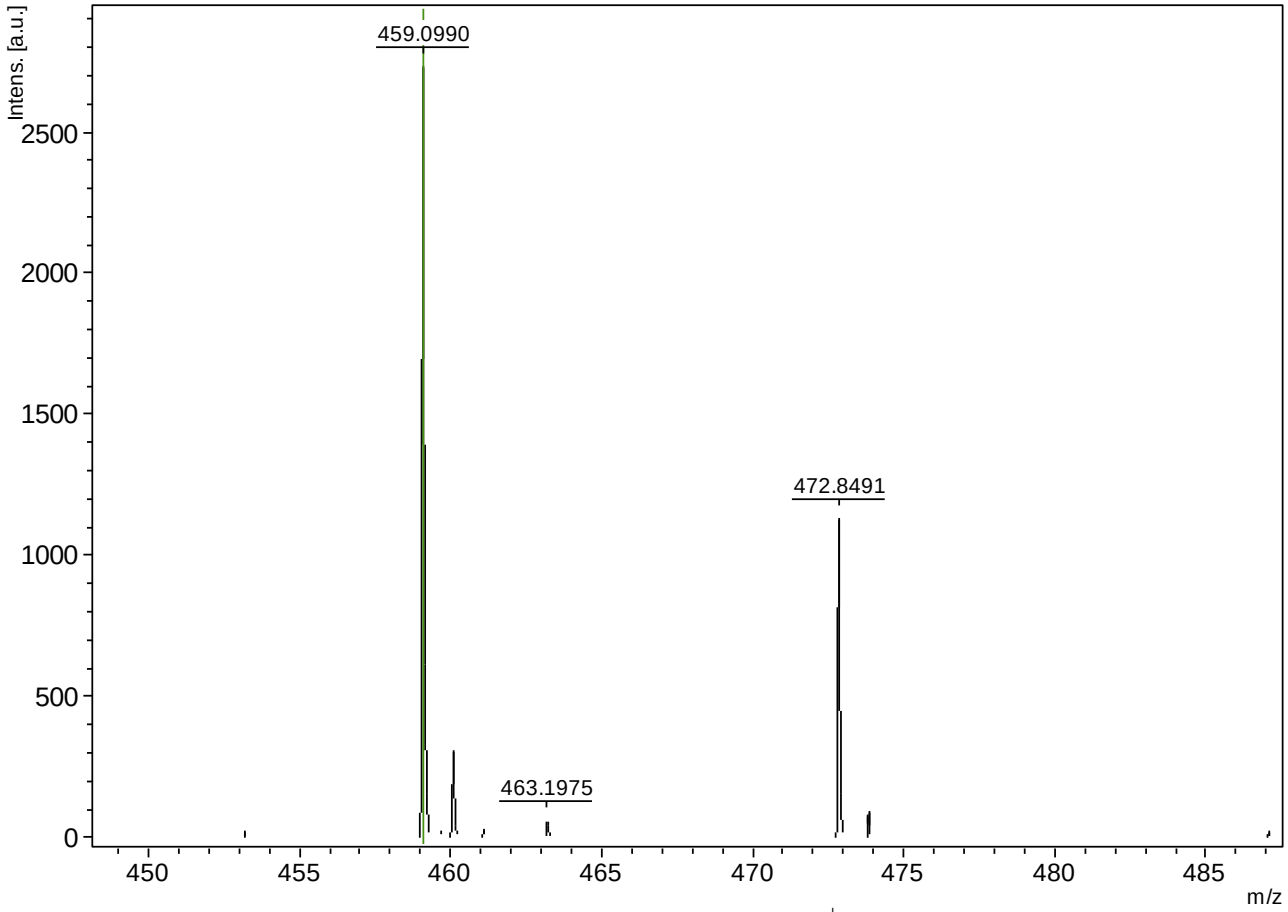
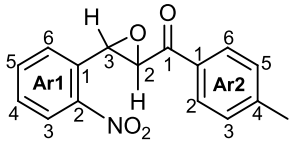



**Figure S18.** HRMS of **4h.** m/z calcd. for $C_9H_8N_2O_4$ $[M+2Cs-H]^+$ 472.8509, found 472.8491 (MALDI).

*trans-3-(2-Nitrophenyl)oxiran-2-carboxtolyl (**6a***




**6a**

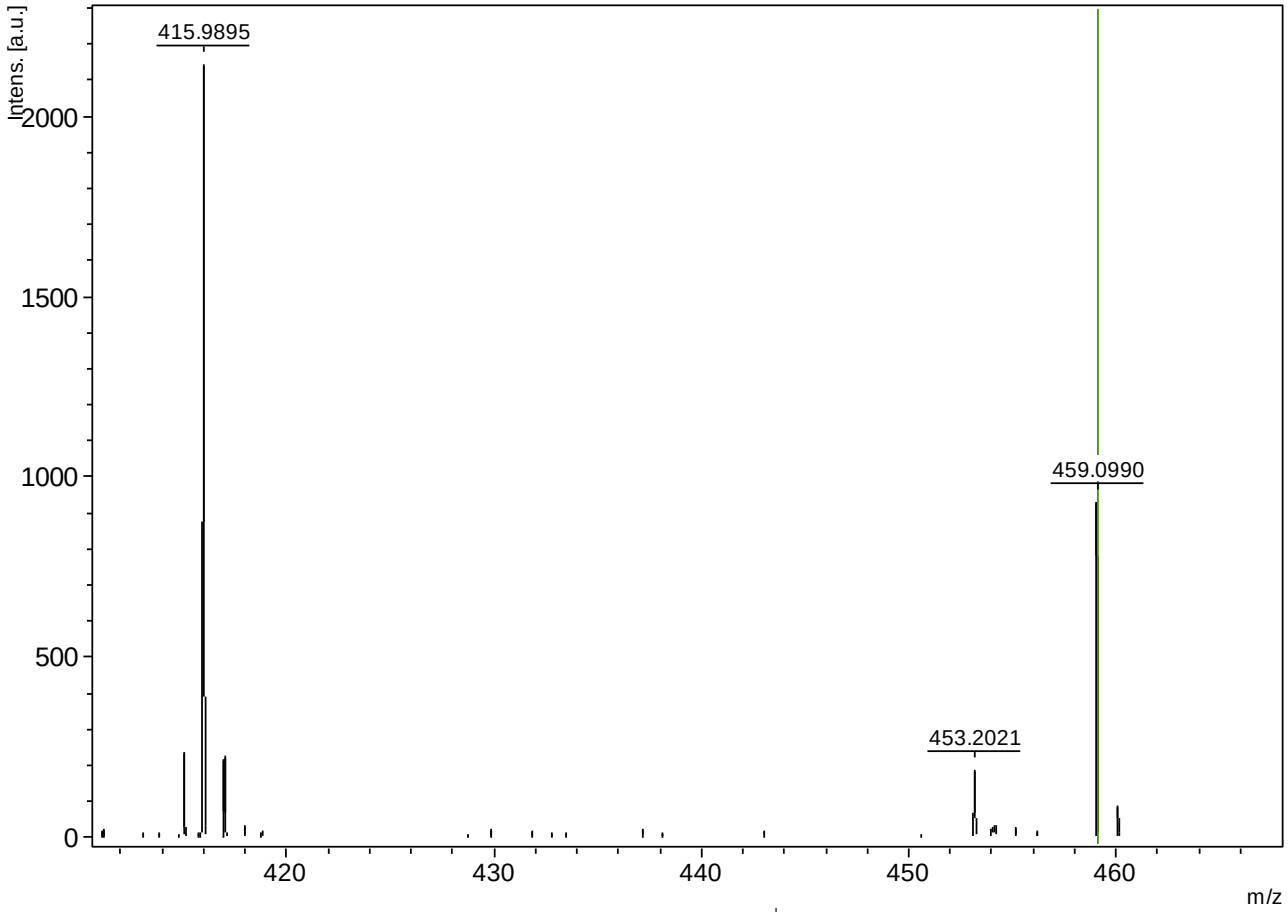
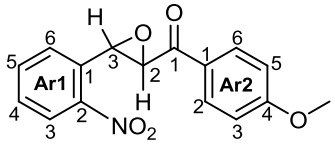



**Figure S10.** HRMS of **6a**m/z calcd. for $C_{16}H_{13}NO_4$ $[M+Cs]^+$ 415.9894, found 415.9895 (MALDI).

*(4-Methoxyphenyl)(3-(2-nitrophenyl)oxiran-2-yl)methanone (**6b**)*




**6b**

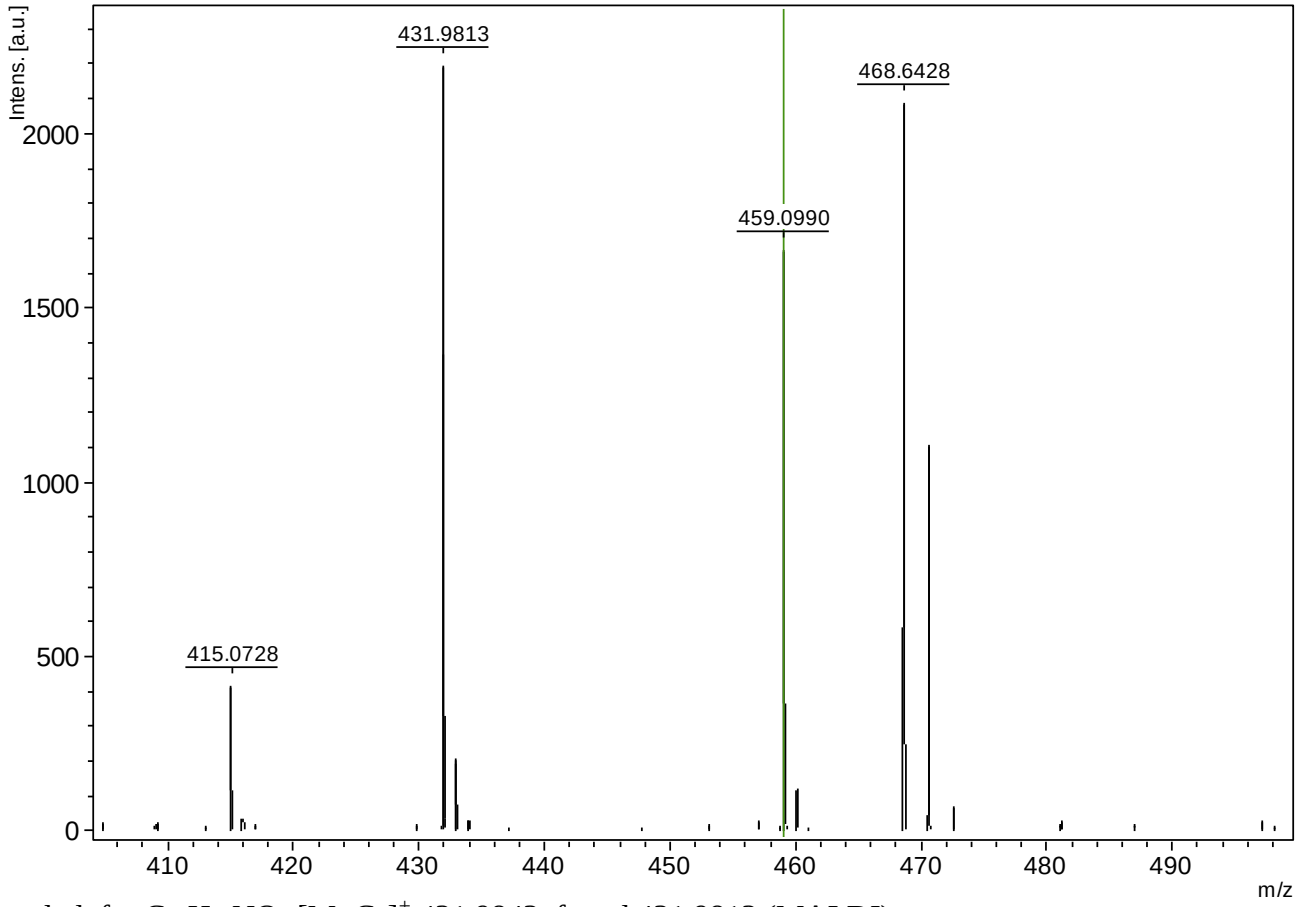
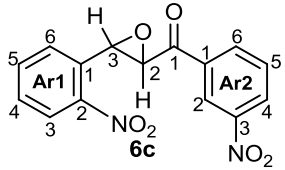



**Figure** HRMS of **6b.** m/z calcd. for $C_{16}H_{13}NO_5$ $[M+Cs]^+$ 431.9843, found 431.9813 (MALDI).

*(3-Nitrophenyl)(3-(2-nitrophenyl)oxiran-2-yl)methanone (**6c**).*



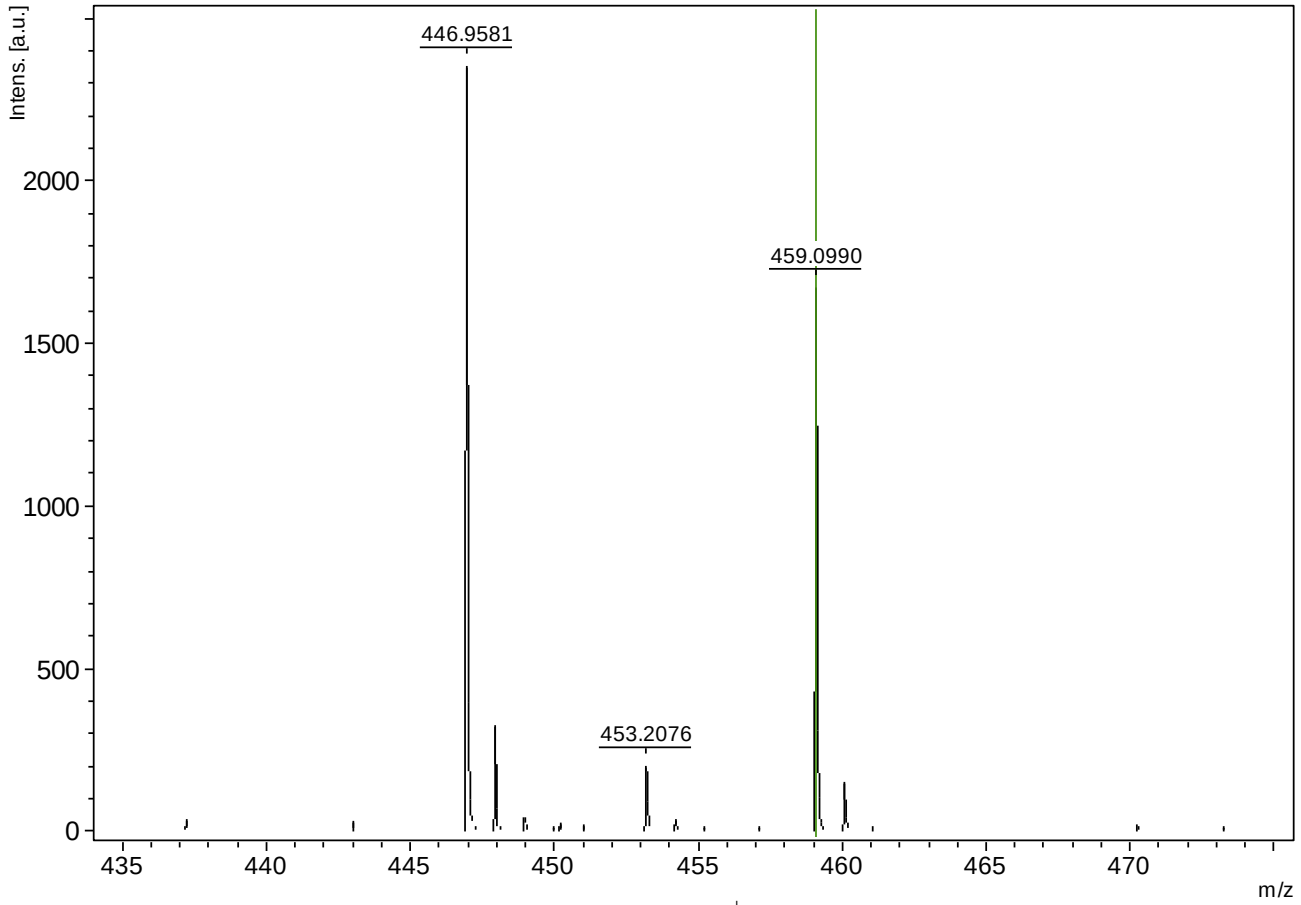




**Figure** HRMS of **6c.** m/z calcd. for $C_{15}H_{10}N_2O_6$ $[M+Cs]^+$ 446.9588, found 446.9581 (MALDI).

*(3-(5-Chloro-2-nitrophenyl)oxiran-2-yl)(4-tolyl)methanone (**6d**).*

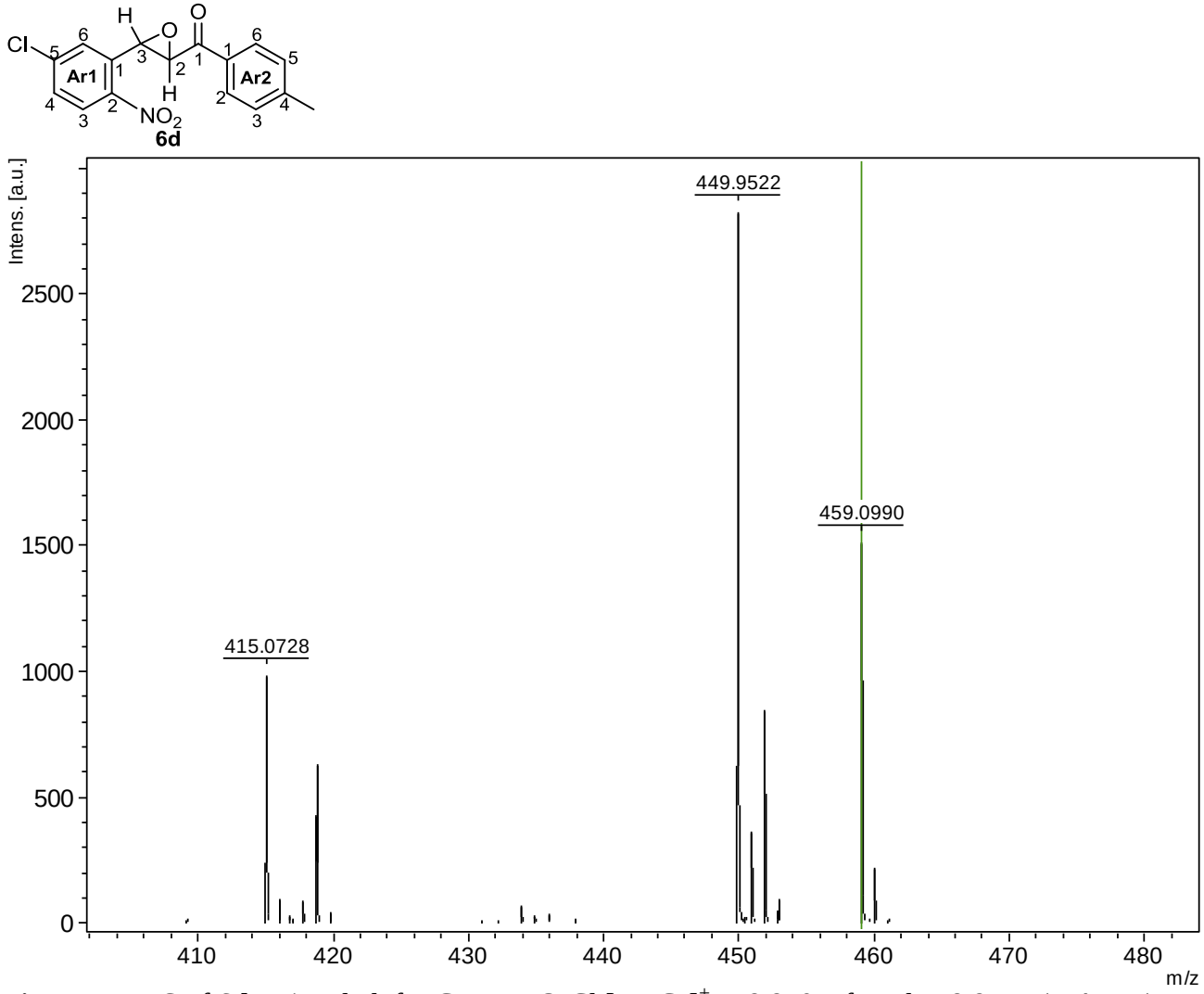
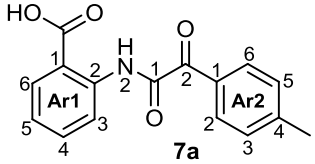



**Figure** HRMS of **6d.** m/z calcd. for $C_{16}H_{12}NO_4Cl$ $[M+Cs]^+$ 449.9504, found 449.9522 (MALDI).

*N-(2-carboxyphenyl)tolyloxalmonoamid (**7a**).*



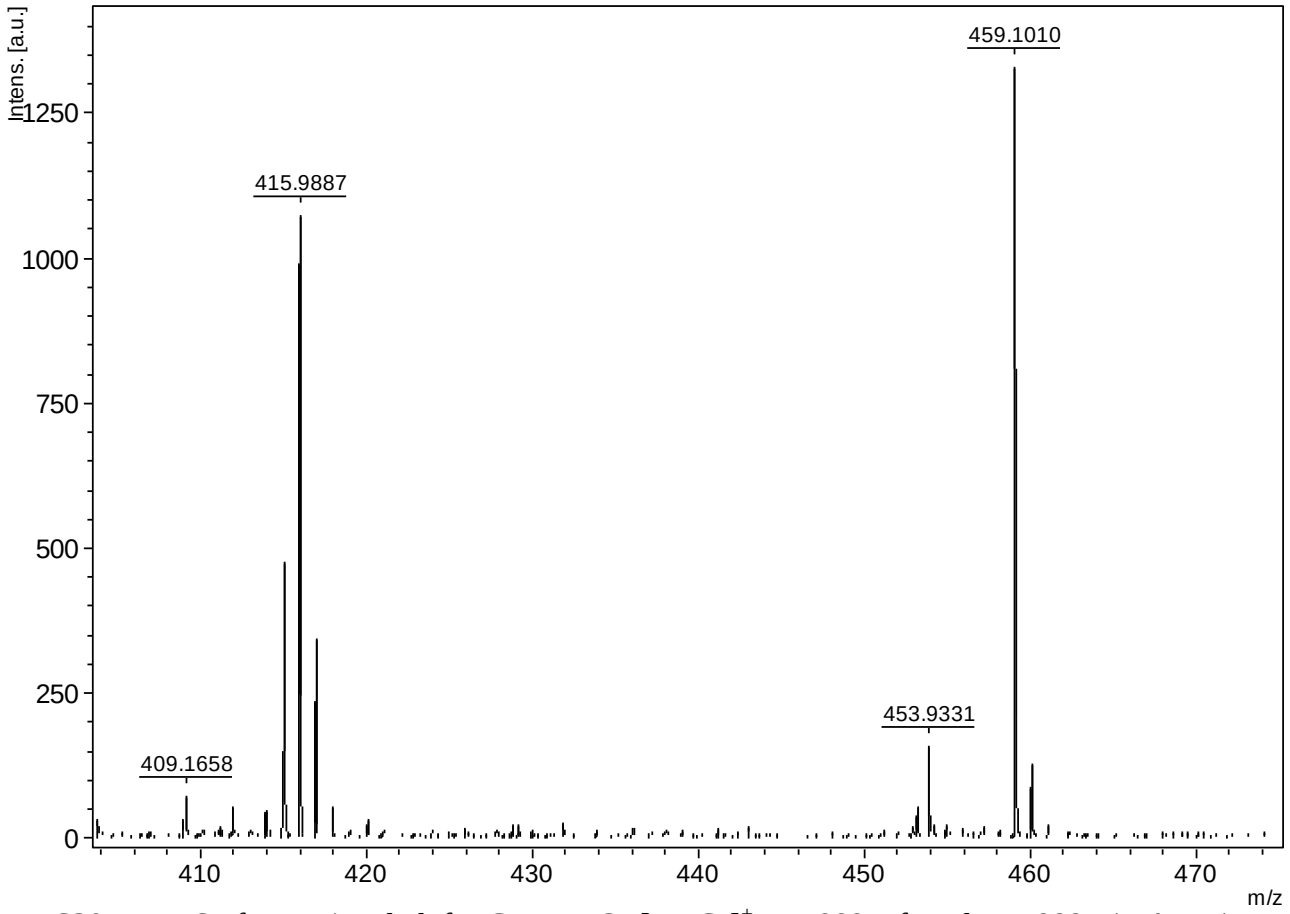
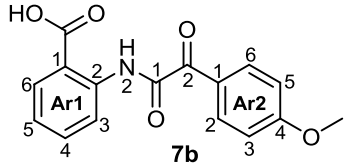




**Figure S20.** HRMS of **7a.** m/z calcd. for $C_{16}H_{13}NO_4$ $[M+Cs]^+$ 415.9894, found 415.9887 (MALDI).

*2-[2-(4-Methoxyphenyl)-2-oxoacetamido]benzoic acid (**7b**).*




**7b**

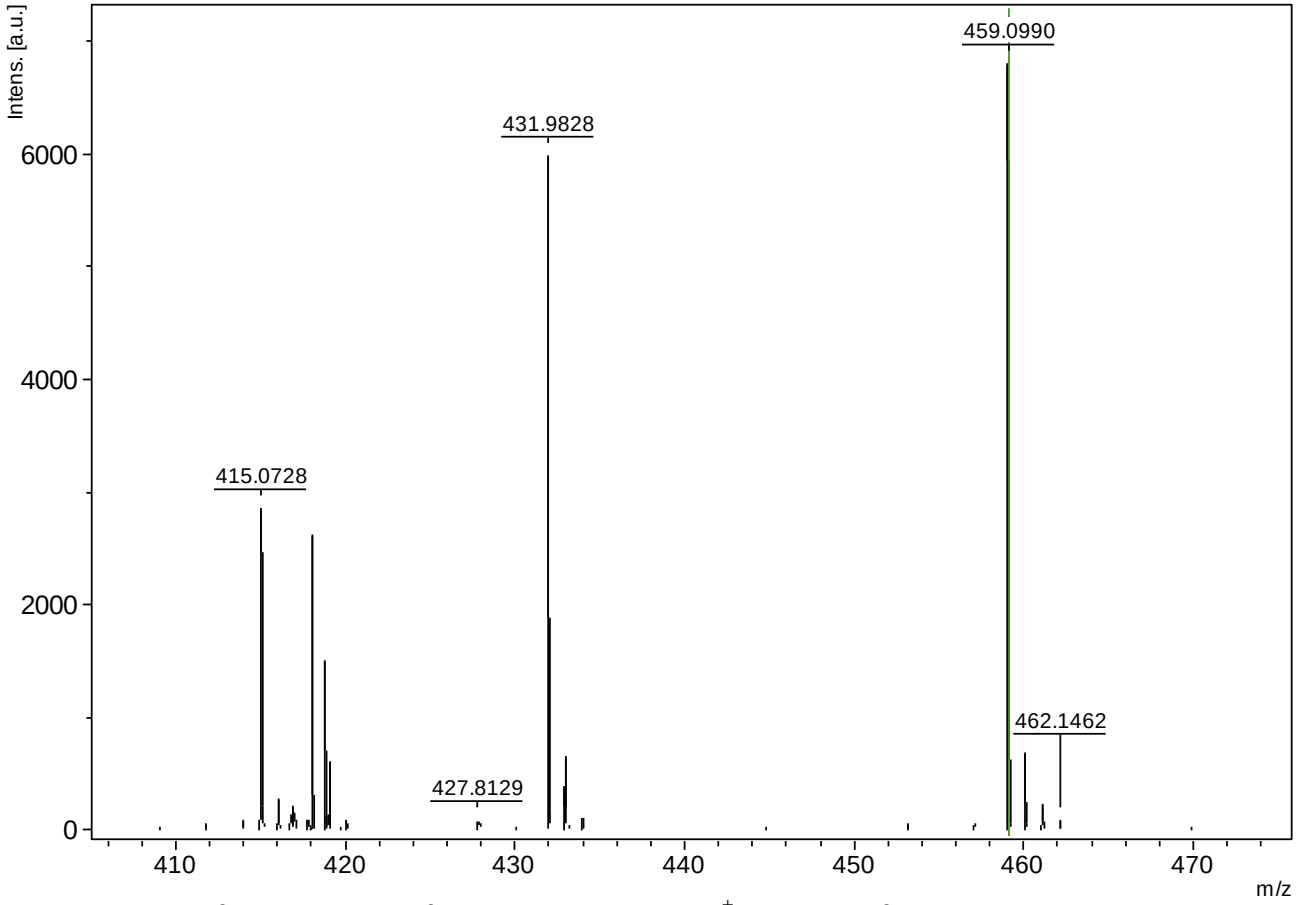
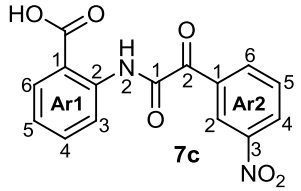



**Figure** HRMS of **7b.** m/z calcd. for $C_{16}H_{13}NO_5$ $[M+Cs]^+$ 431.9843, found 431.9828 (MALDI).

*2-[2-(3-Nitrophenyl)-2-oxoacetamido]benzoic acid (**7c**).*



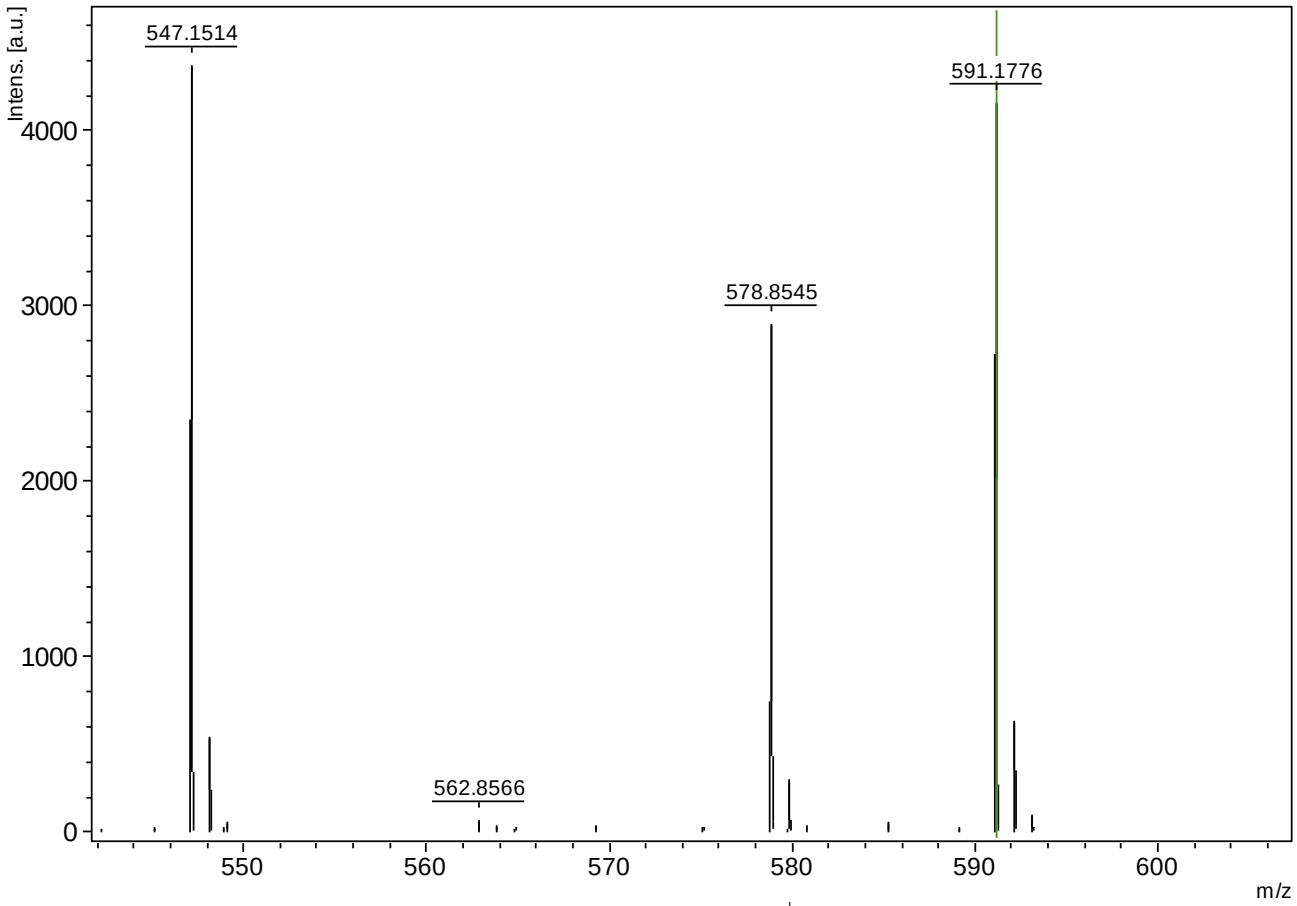
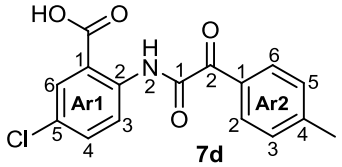




**Figure** HRMS of **7c.** m/z calcd. for $C_{15}H_{10}N_2O_6$ $[M+2Cs–H]^+$ 578.8564, found 578.8545 (MALDI).

*5-Chloro-2-[2-oxo-2-(4-tolyl)acetamido]benzoic acid (**7d**).*



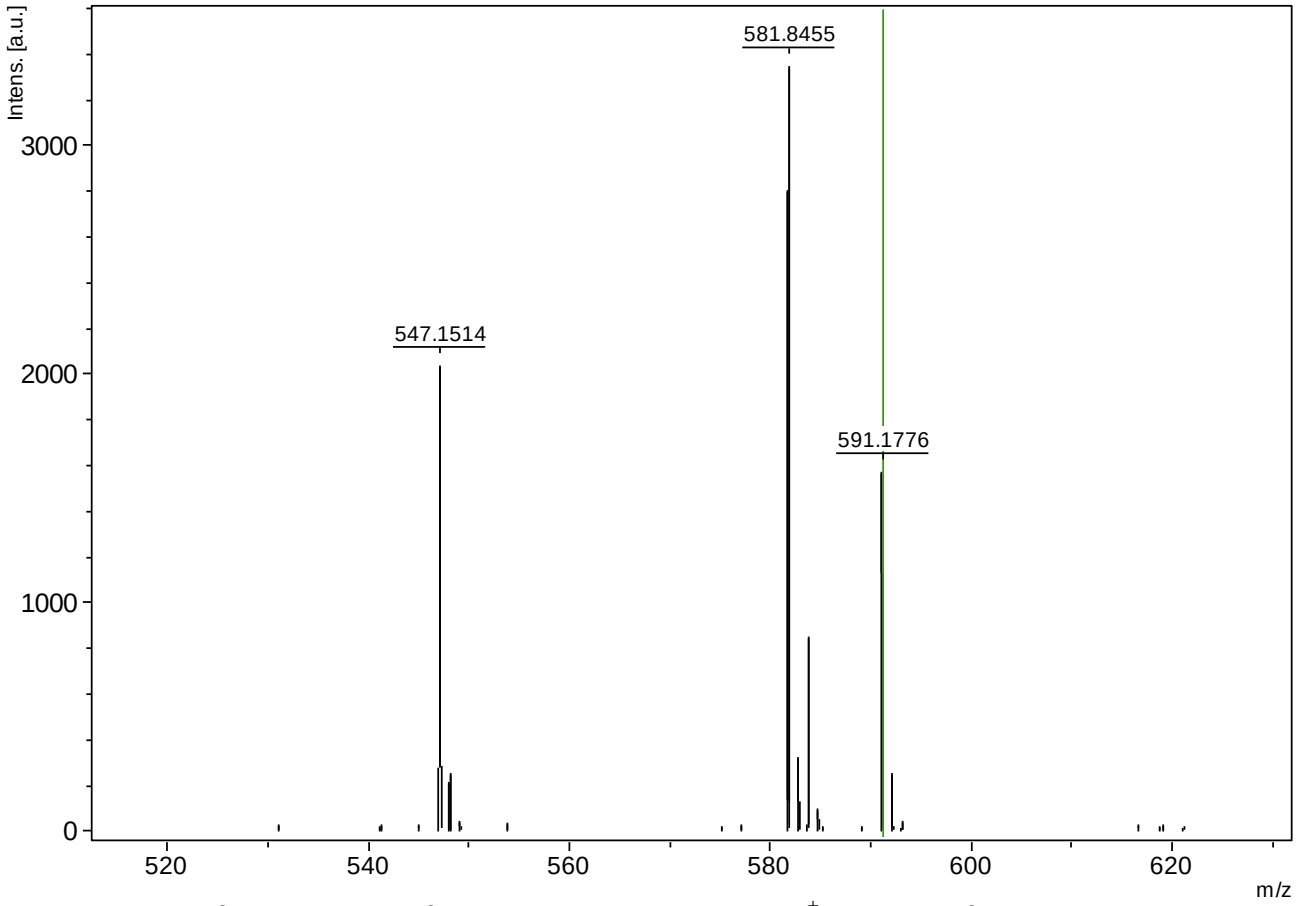




**Figure** HRMS of **7d.** m/z calcd. for $C_{16}H_{12}NO_4Cl$ $[M+2Cs–H]^+$ 581.8480, found 581.8455 (MALDI).

## X-ray crystallographic data

Crystal structure was determined by X-ray diffraction of suitable monocrystal. Crystal data were collected on a Bruker Smart Apex II CCD diffractometer using graphite monochromated $MoK_\alpha$ (0.71073 Å) radiation and ω-scan. Data collection images were indexed, integrated, and scaled using the APEX2 data reduction package [1]. Multi-scan empirical absorption corrections were applied to all data sets, where appropriate, using the program SADABS [2]. The structure was solved and refined using SHELX [3] program. All pictures of crystal structures were created using *Mercury CSD 3.3* [4].

The X-ray diffraction data for crystals of **4a** were collected on a Bruker AXS Smart APEX II CCD diffractometer at 150 K. ***Crystallographic data for 4a***. $C_{15}H_{12}N_2O_4 \cdot C_2H_4O_2$, colorless prism, formula weight 344.32, monoclinic, *P2₁/c*, $a$ = 15.40(2) Å, $b$ = 4.991(5) Å, $c$ = 20.26(2) Å, $\beta$ = 97.67(1)º, $V$ = 1543(3) Å$^3$, $Z$ = 4, $\rho_{calc}$ = 1.48 g cm$^{-3}$, μ(λMo$K_\alpha$) = 1.14 cm$^{-1}$, F(000) = 720, reflections collected = 13178, unique = 3735, $R_{(int)}$ = 0.0541, full matrix least squares on F$^2$, parameters = 243, restrains = 0. Final indices $R_1$ = 0.0508, $wR_2$ = 0.1286 for 2444 reflections with I > 2σ(*I*); $R_1$ = 0.0812, $wR_2$ = 0.1485 for all data, goodness-of-fit on F$^2$ = 1.045, largest difference in peak and hole (0.217 and –0.288 *e*Å$^{-3}$).

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1417946. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk).

The X-ray diffraction data for crystals of **4b** were collected on a Bruker AXS Smart APEX II CCD diffractometer at 296 K. ***Crystallographic data for 4b***. $C_{15}H_{11}BrN_2O_4$, colorless prism, formula weight 726.34, triclinic, *P-1*, $a$ = 9.555(3) Å, $b$ = 11.210(3) Å, $c$ = 15.335(4) Å, $\alpha$ = 108.324(3)º, $\beta$ = 97.068(4)º, $\gamma$ = 105.848(4)º, $V$ = 1460.3(7) Å$^3$, $Z$ = 2, $\rho_{calc}$ = 1.65 g cm$^{-3}$, μ(λMo$K_\alpha$) = 28.4 cm$^{-1}$, F(000) = 728, reflections collected = 23079, unique = 5742, $R_{(int)}$ = 0.0272, full matrix least squares on F$^2$, parameters = 421, restrains = 0. Final indices $R_1$ = 0.0381, $wR_2$ = 0.1162 for 4286 reflections with I > 2σ(*I*); $R_1$ = 0.0560, $wR_2$ = 0.1332 for all data, goodness-of-fit on F$^2$ = 0.880, largest difference in peak and hole (0.615 and – 0.556 *e*Å$^{-3}$).

Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1015263. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (Fax: +44-1223/336-033; E-mail: deposit@ccdc.cam.ac.uk).

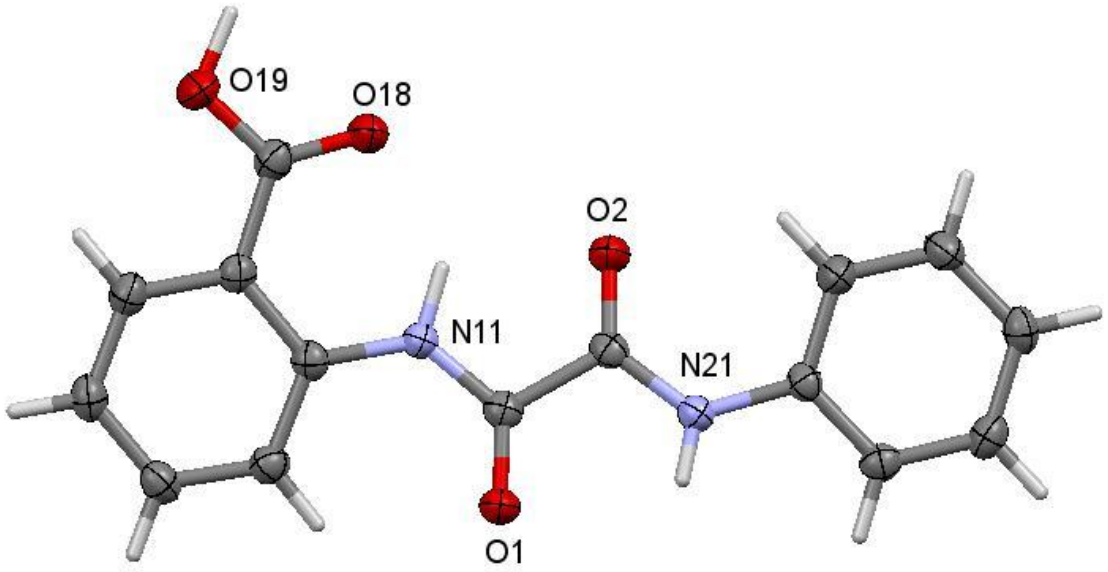



**Figure 1**. ORTEP plot of compound **4a** and partial numbering scheme. Displacement ellipsoids are drawn at the 50 % probability level. H-atoms are represented in stick mode for clarity. The solvent molecule is omitted for clarity.

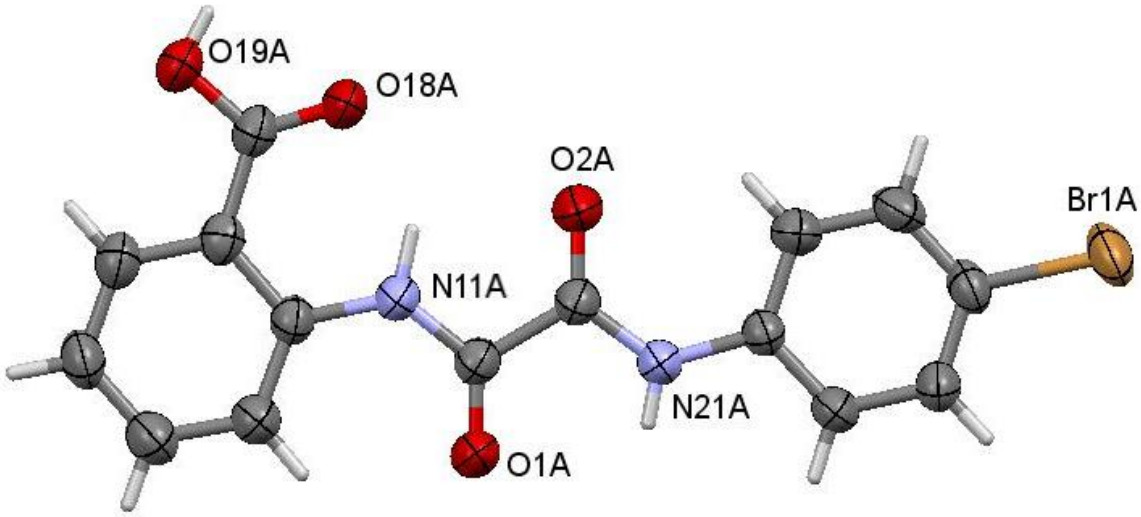



**Figure 2**. ORTEP plot of compound **4b** and partial numbering scheme. Displacement ellipsoids are drawn at the 50 % probability level. H-atoms are represented in stick mode for clarity. Only one independent molecule from two is presented for clarity.

The asymmetric part of the unit cell of **4a** includes two independent molecules, and **4b** contents one independent molecule and one solvent acetic acid molecule (see Fig. 1 and 2, on both figures only one molecule of the corresponding compound is presented for clarity).

In Cambrige Structural Database [5] we have found only about 20 closest literature analogues of the corresponding structures **4a** and **4b**. All of them can be presented by the common formula R'NHC(O)C(O)NHR", where R' = R", that is symmetrical amides. Thus, the crystal and molecular structure of asymmetric amides of ethanedioic acid, where R' ≠ R" (the same as **4a** and **4b**), has not been widely discussed in literature, and even the surveys regarding the symmetric amides of ethanedioic acid are rather poor [6-9]. The two independent molecules of **4b** have practically the same geometrical parameters. The main difference between them is the values of the dihedral angle between the 6-atom amide plane and the aromatic substituents. For the molecule **4a**: the dihedral angle between the amide plane and 2-carboxyphenyl substituent is 3.5(1)º, and the one between the

amide plane and the 4-brominephenyl substituent is 7.4(1)º. For the molecule **4b** those angles are 14.2(1) and 47.8(1)º respectively. Thus it can be assumed, that the molecule **4a** has actually a planar arrangement, while the molecule **4b** has an asymmetrical distortion of the geometry and is not planar, as well as the molecule **4a**, in which the corresponding angles are 14.27(8) and 13.59(8)º respectively.

## References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[5] Cambrige Structural Database System. Version 5.34. Cambrige Crystallographic Data Centre, 2013.

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