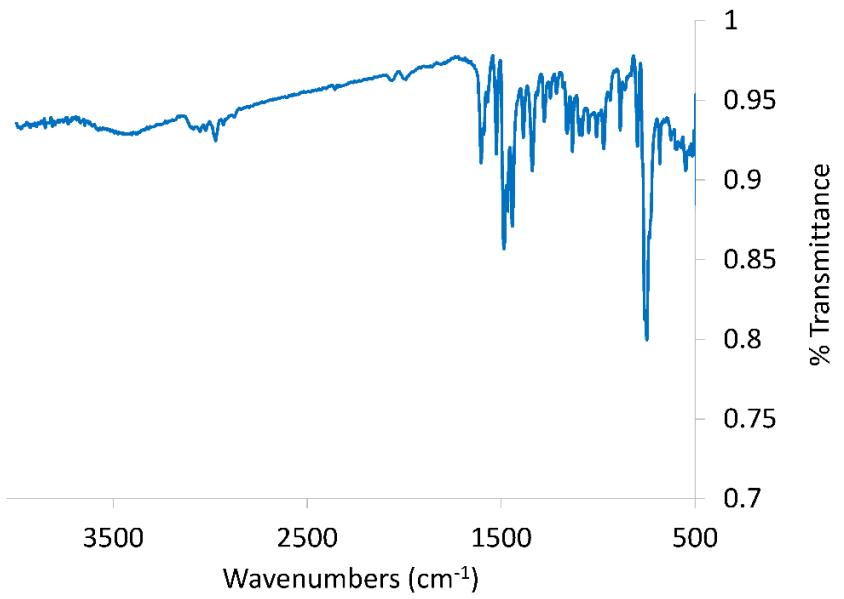
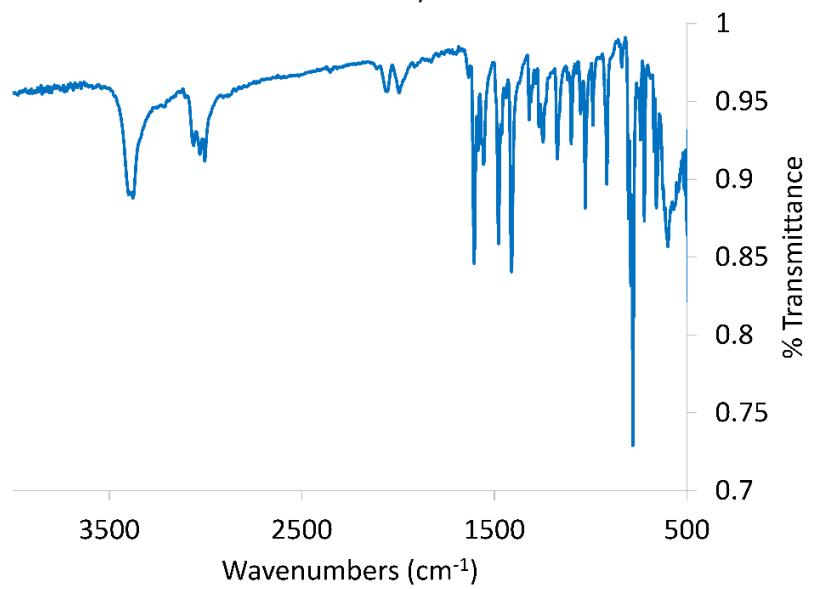


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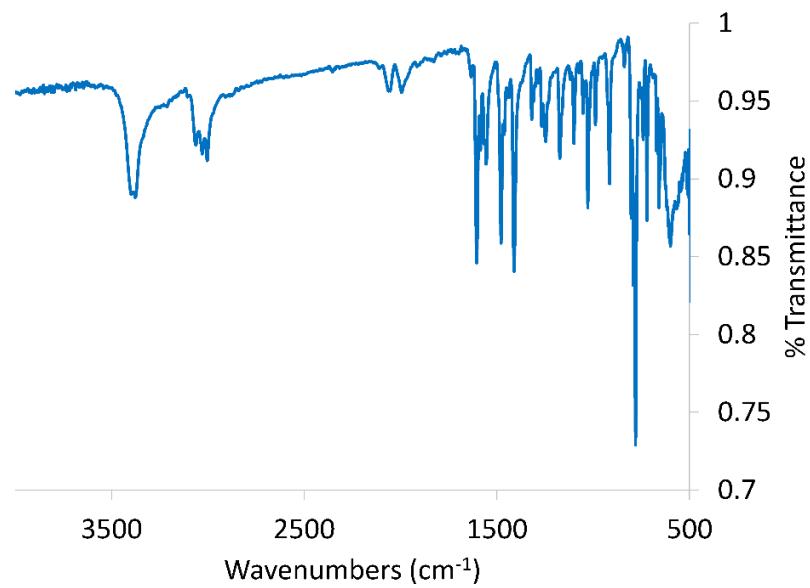


a)

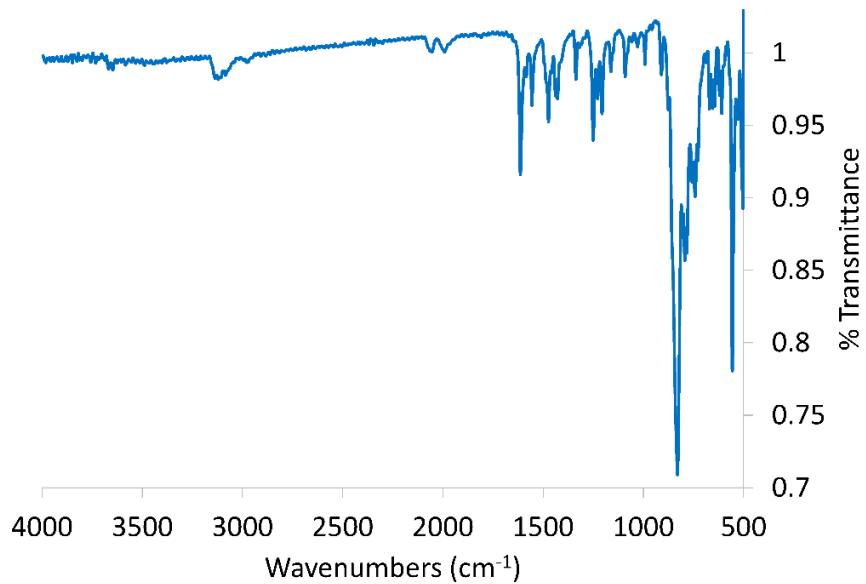


b)

S2

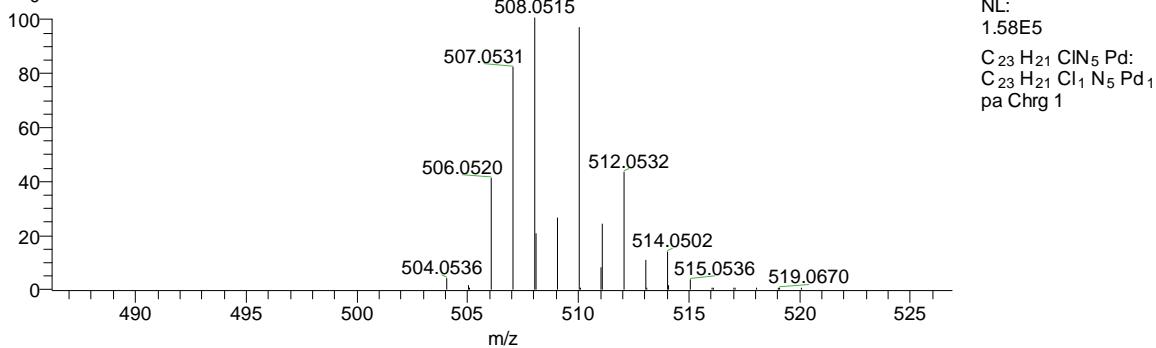
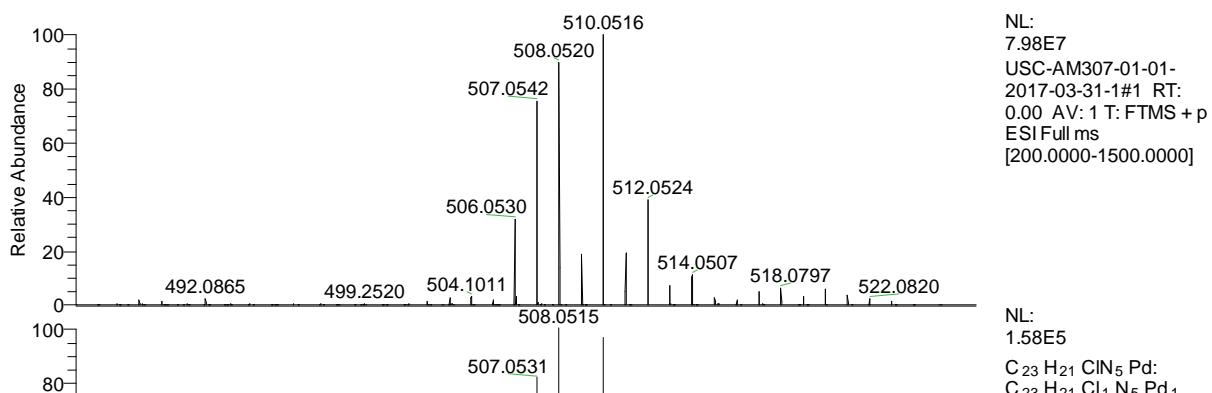


c)

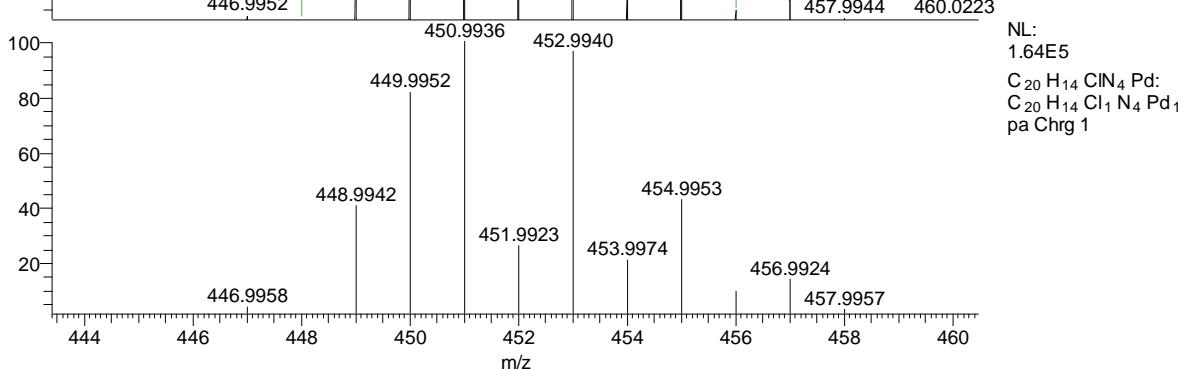
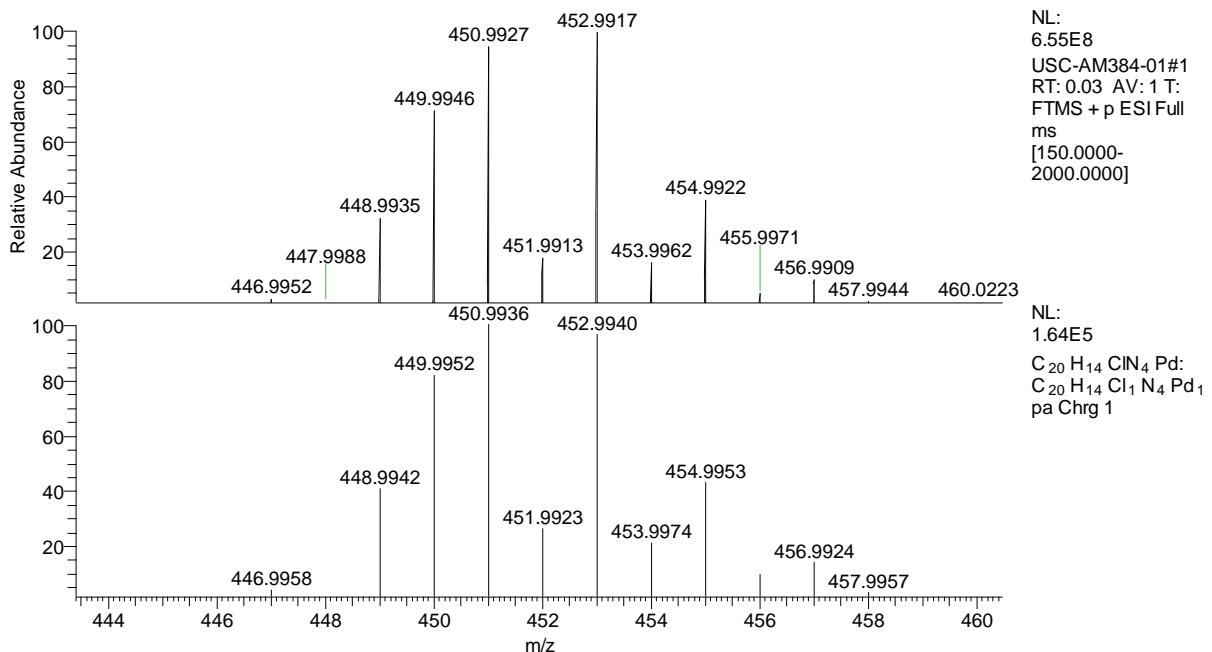


d)

Fig. S1 ATR IR spectra of a) **1**, b) **2**, c) **3** and d) **4**.

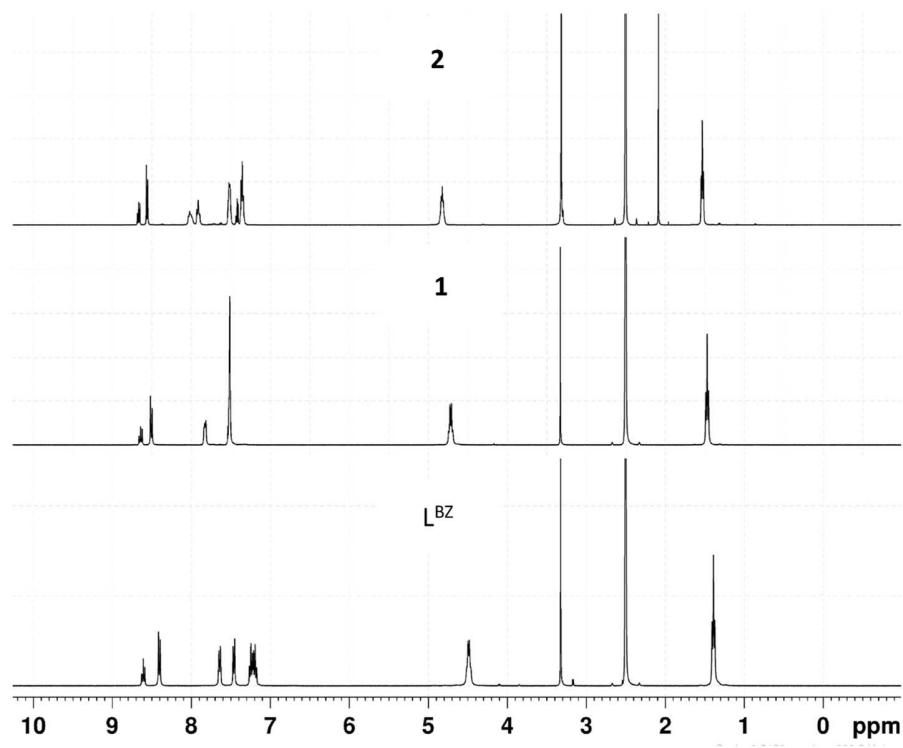


a)

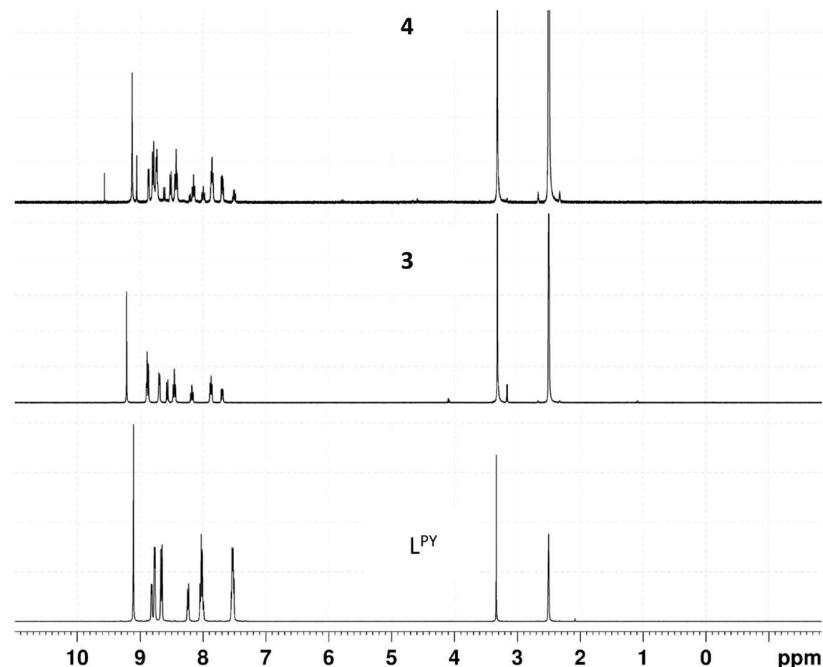


b)

Fig. S2 Electrospray ionization mass spectra: Experimental (Up) and theoretical (down) ISOTOPIC pattern for {PdCL}⁺ (L = L^{BZ} and L^{PY}) ion of a) compounds **1** and b) **3**.



a)



b)

Fig. S3 Comparative ¹H NMR spectra of the free ligands and their complexes a) L^{BZ} and b) L^{PY}.

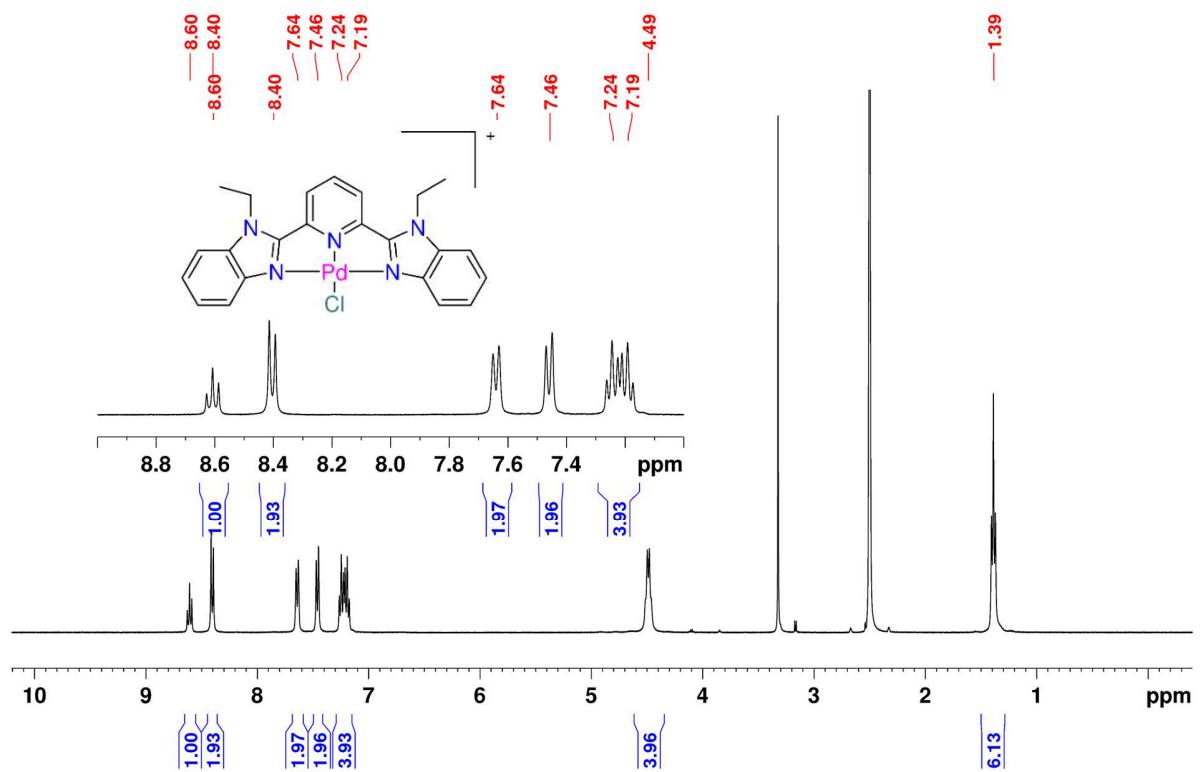


Fig. S4 ^1H NMR spectrum of **1** in DMSO-d_6 .

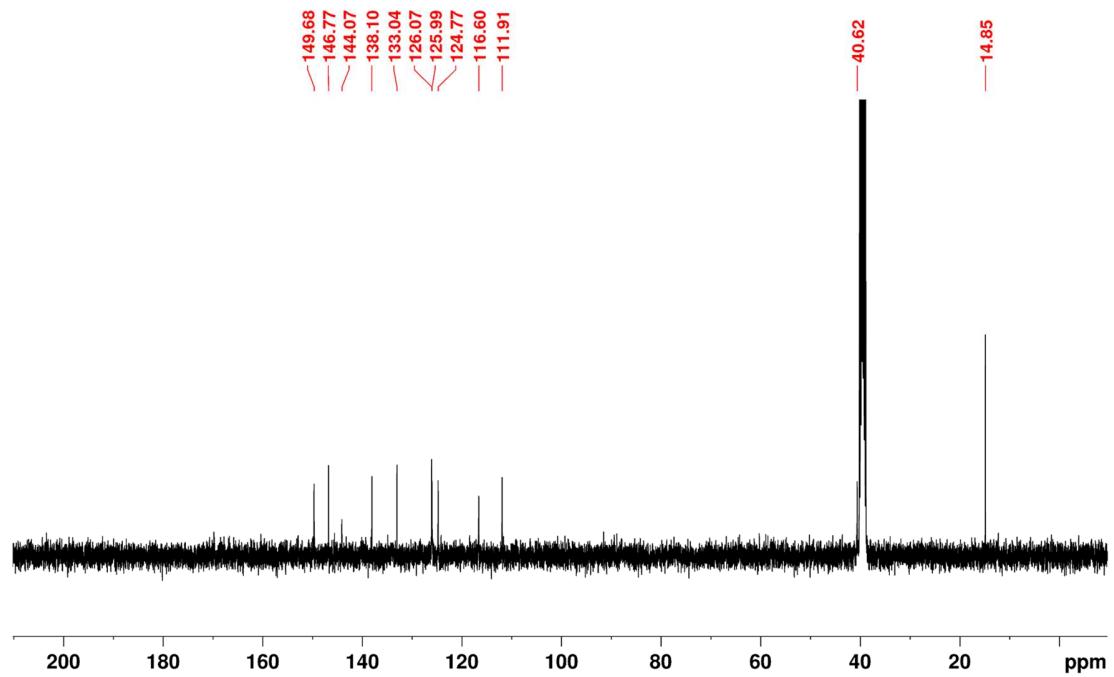


Fig. S5 ¹³C NMR spectrum of **1** in DMSO-d₆.

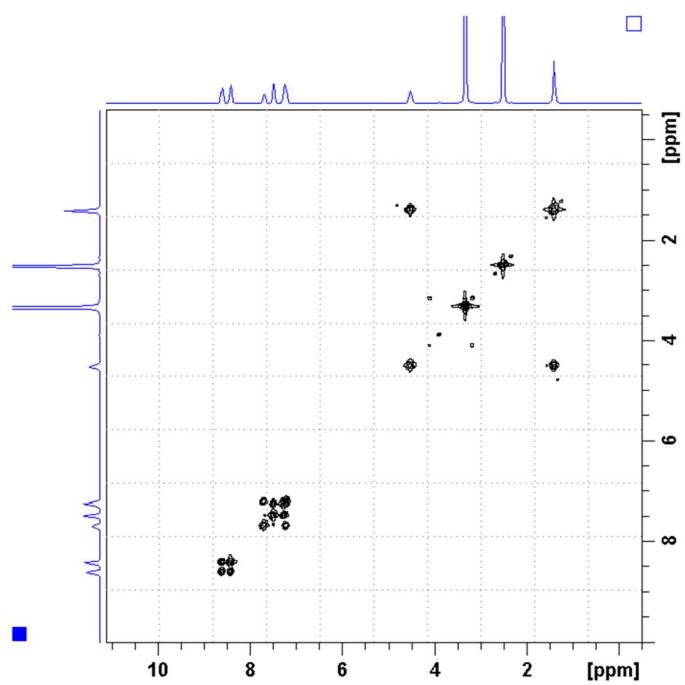


Fig. S6 $\{^1\text{H}, ^1\text{H}\}$ COS90 NMR spectrum of **1** in DMSO-d_6 .

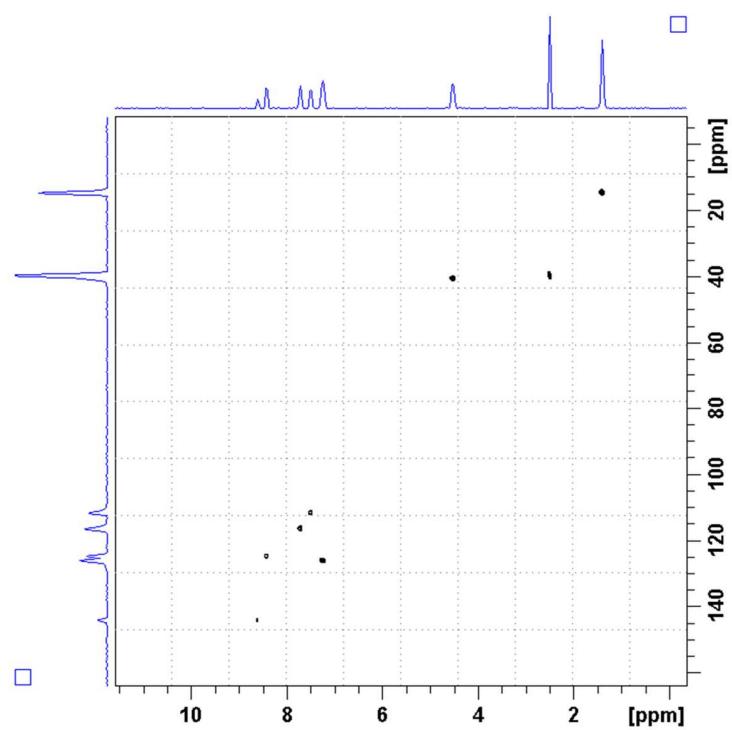


Fig. S7 $\{{}^{13}\text{C}, {}^1\text{H}\}$ HSQC NMR spectrum of **1** in DMSO-d_6 .

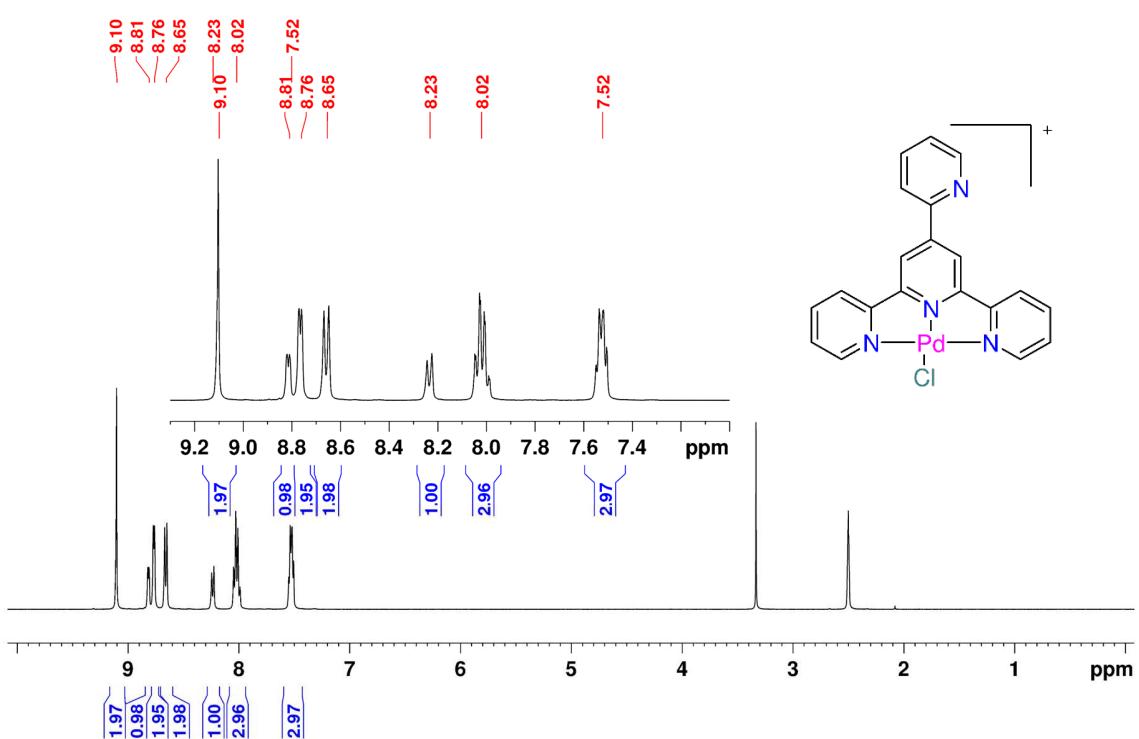


Fig. S8 ^1H NMR spectrum of **3** in DMSO-d_6 .

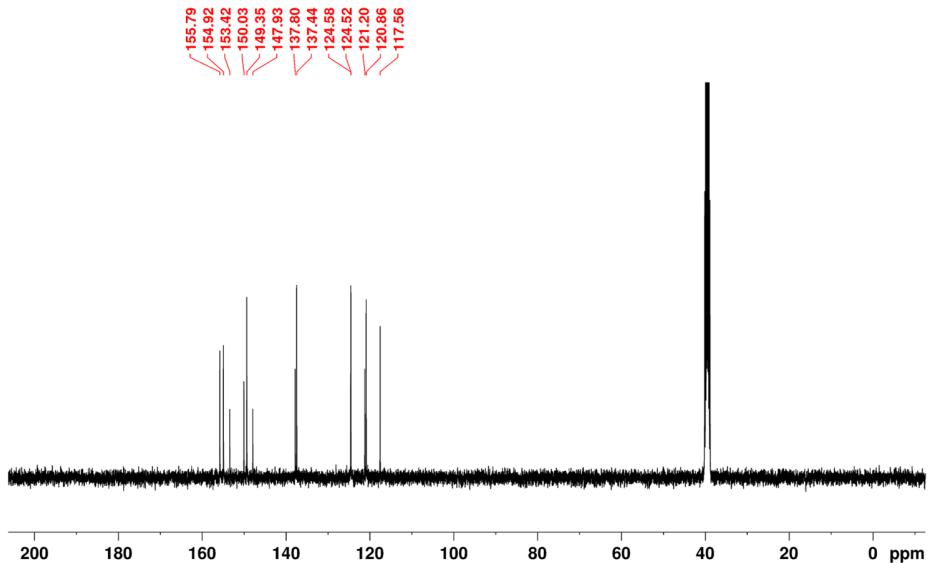


Fig. S9 ^{13}C NMR spectrum of **3** in DMSO-d_6 .

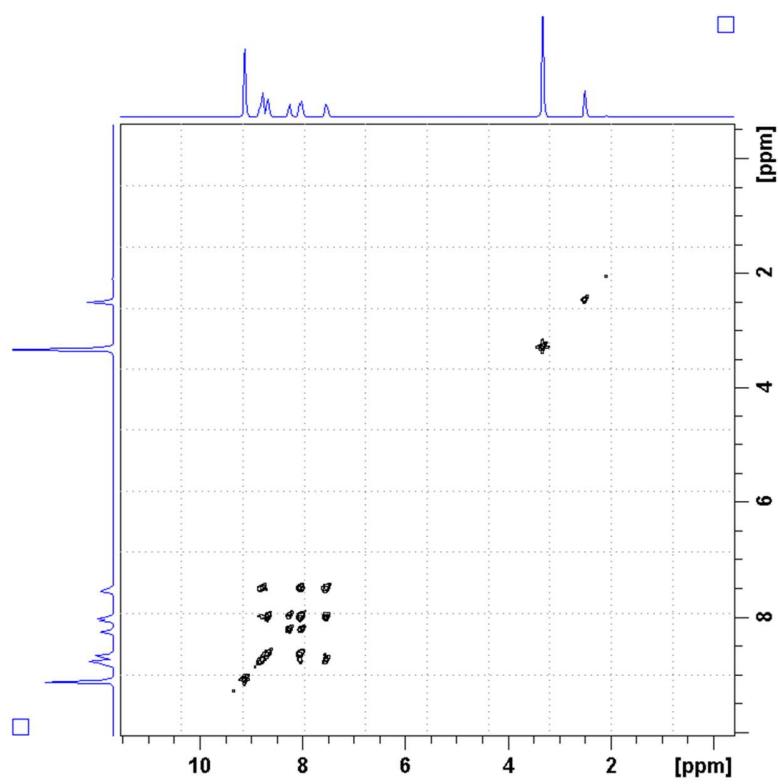


Fig. S10 $\{{}^1\text{H}, {}^1\text{H}\}$ COSY NMR spectrum of **3** in DMSO-d_6 .

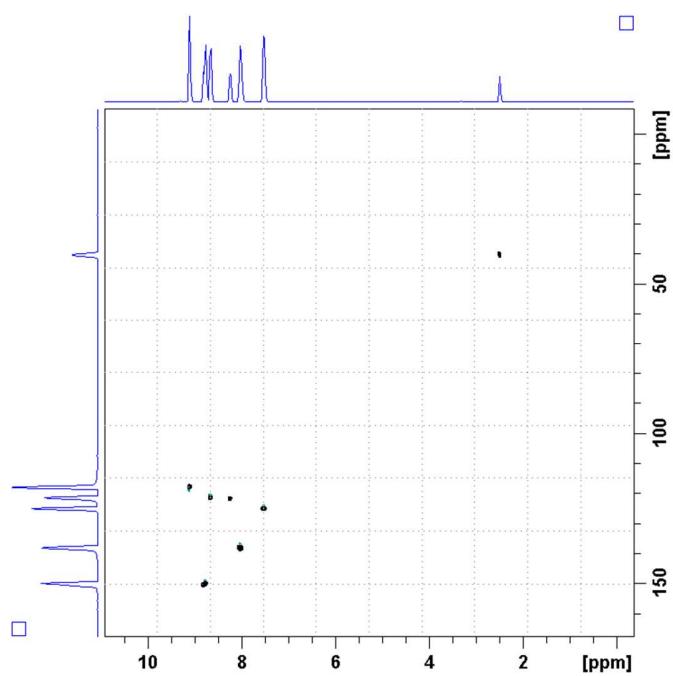
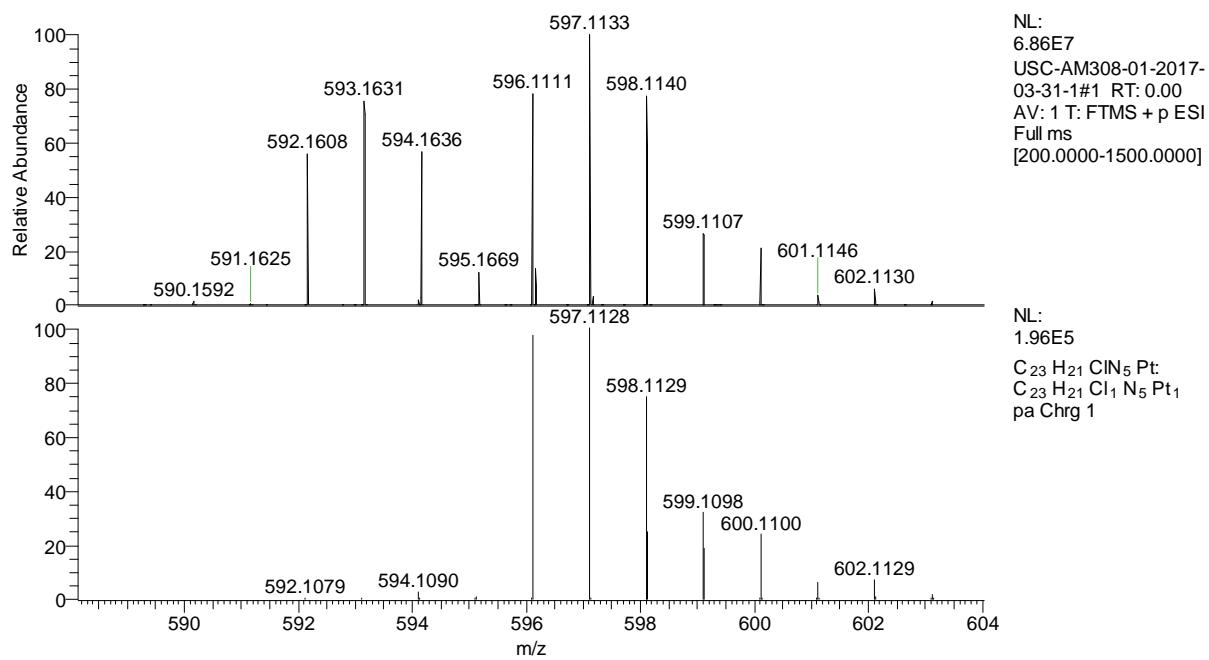
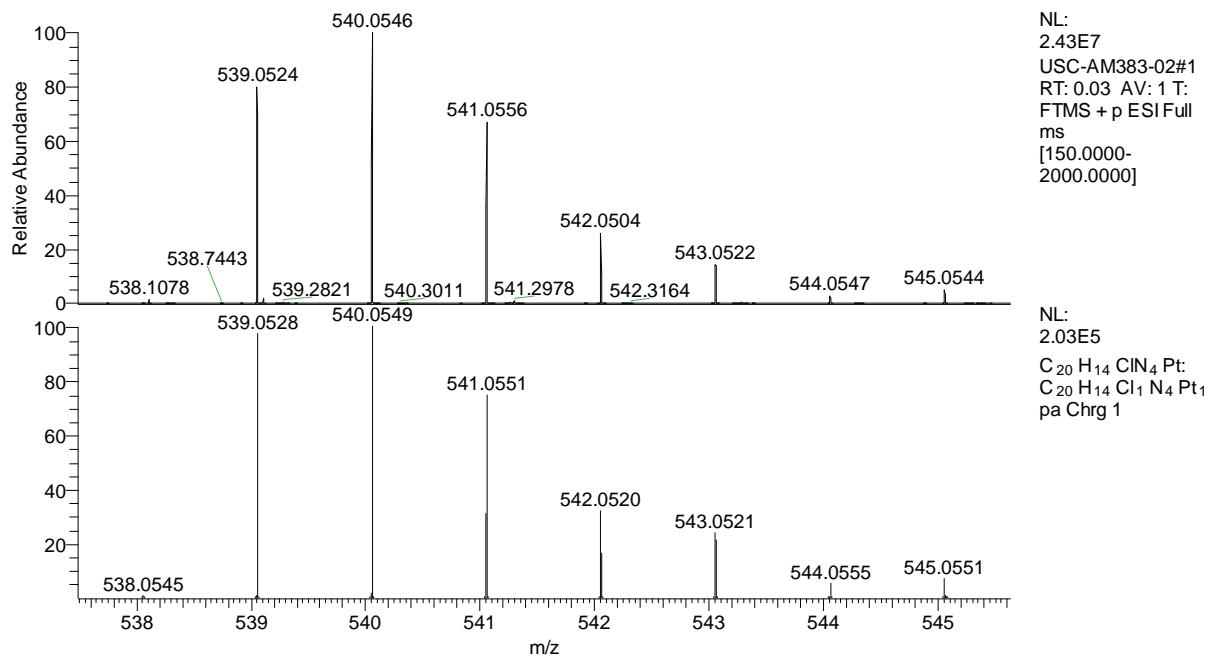


Fig. S11 $\{{}^{13}\text{C}, {}^1\text{H}\}$ HSQC NMR spectrum of **3** in DMSO-d_6 .



a)



b)

Fig. S12 Electrospray ionization mass spectra: Experimental (Up) and theoretical (down) ISOTOPIC pattern for $\{PtClL\}^+$ ($L = L^{BZ}$ and L^{PY}) ion of a) compounds **2** and b) **4**.

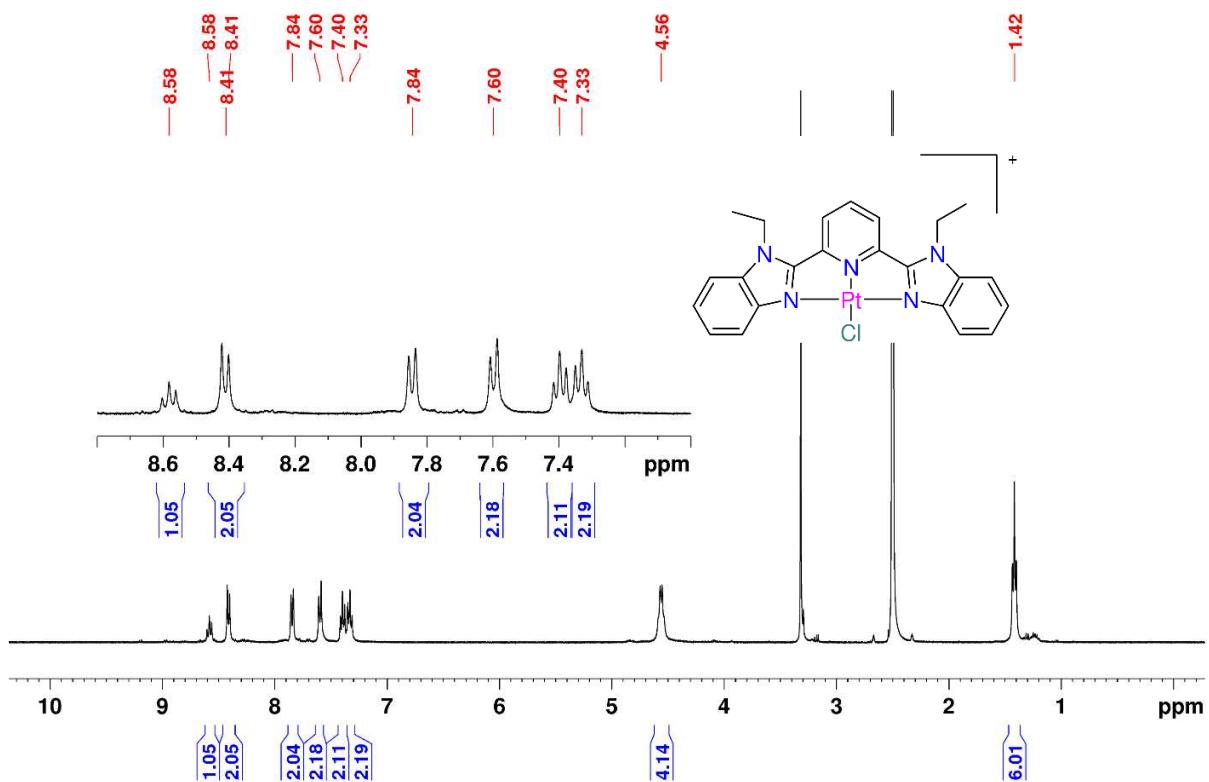


Fig. S13 ^1H NMR spectrum of **2** in DMSO-d_6 .

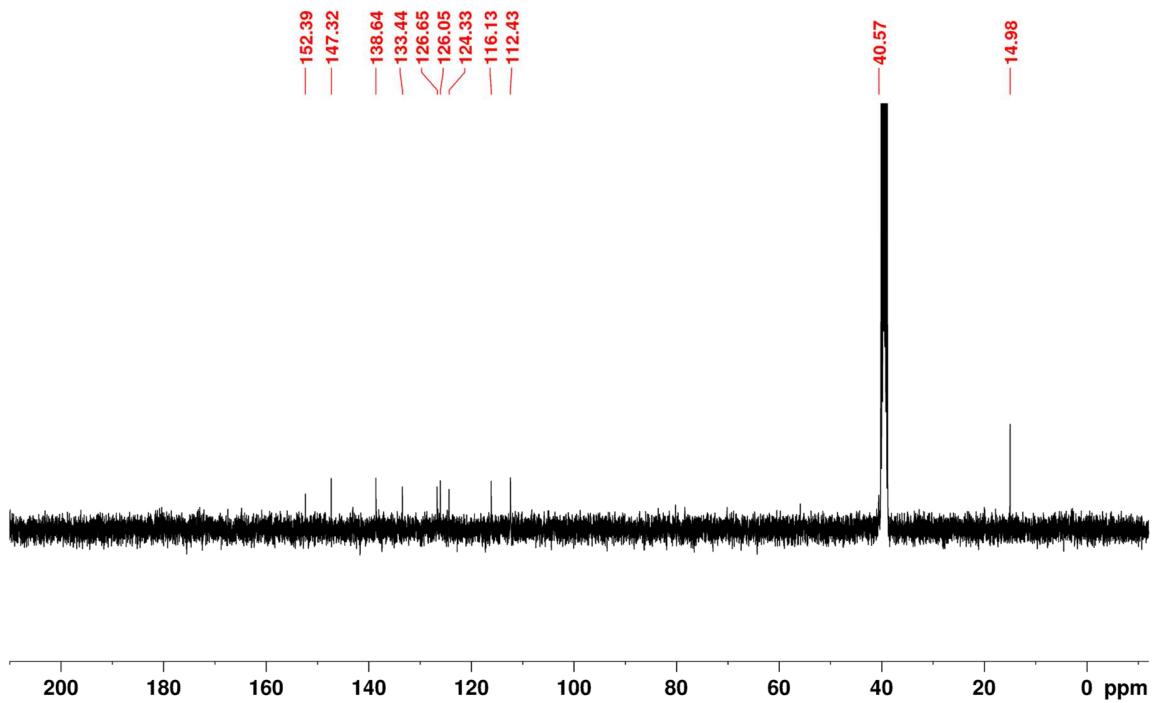


Fig. S14 ^{13}C NMR spectrum of **2** in DMSO-d_6 .

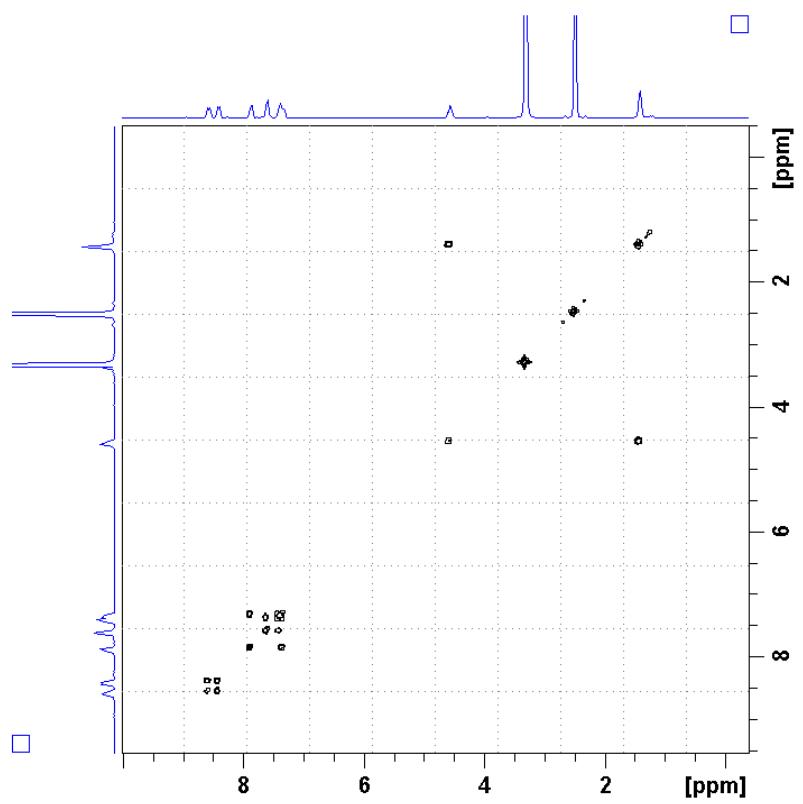


Fig. S15 $\{^1\text{H}, ^1\text{H}\}$ COSY NMR spectrum of **2** in DMSO-d_6 .

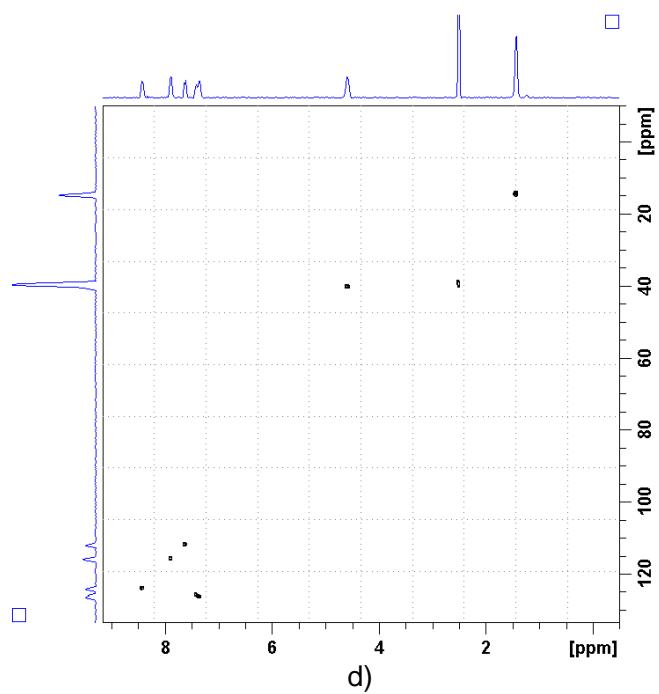


Fig. S16 $\{{}^{13}\text{C}, {}^1\text{H}\}$ HSQC NMR spectrum of **2** in DMSO-d_6 .

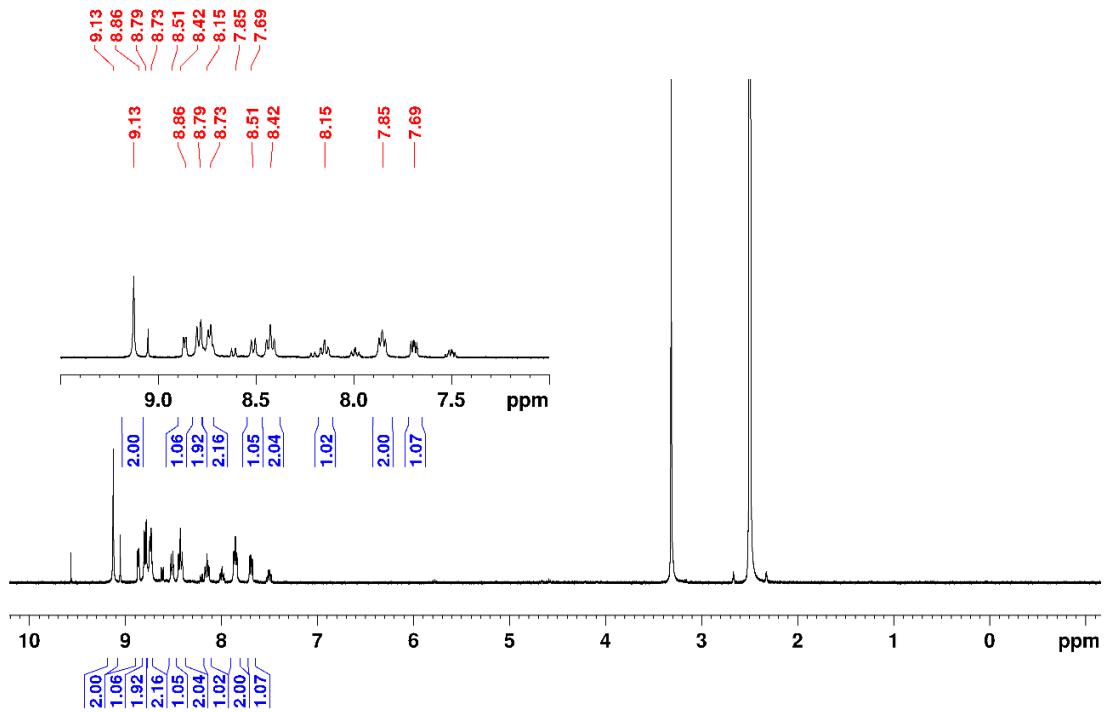


Fig. S17 ^1H NMR spectrum of **4** in DMSO-d_6 .

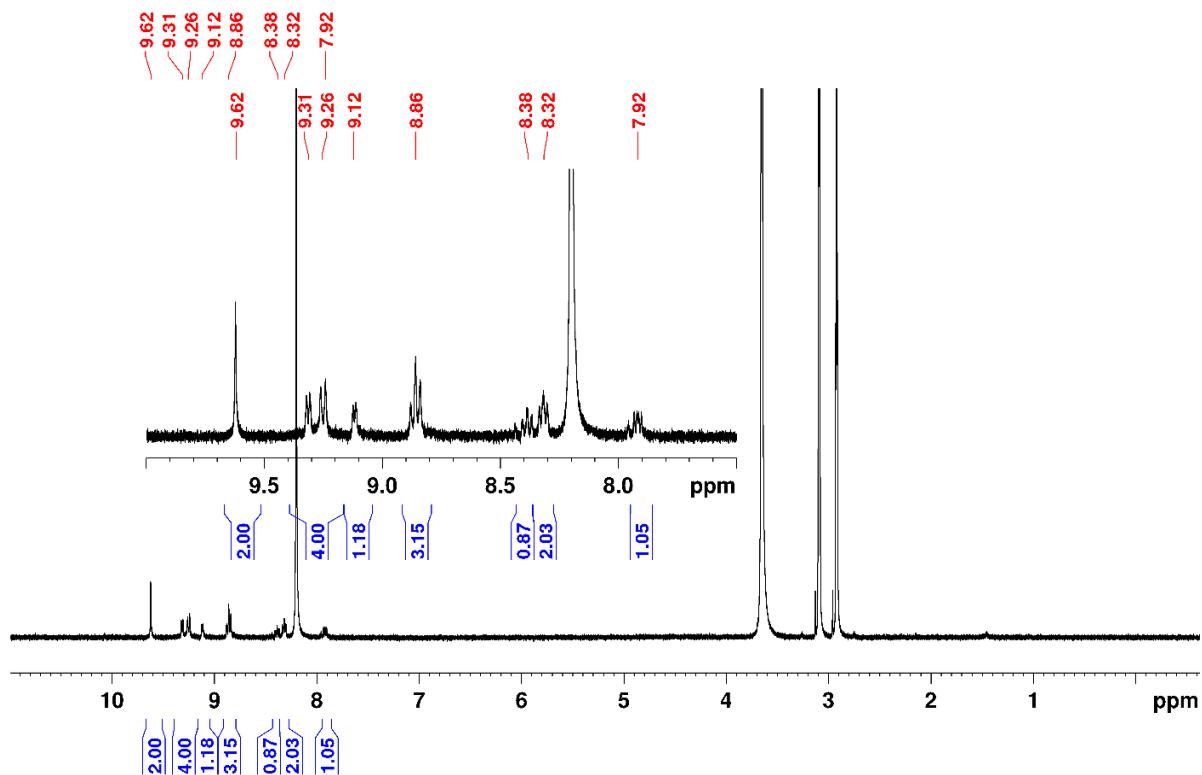


Fig. S18 ^1H NMR spectrum of **4** in DMF-d_7 .

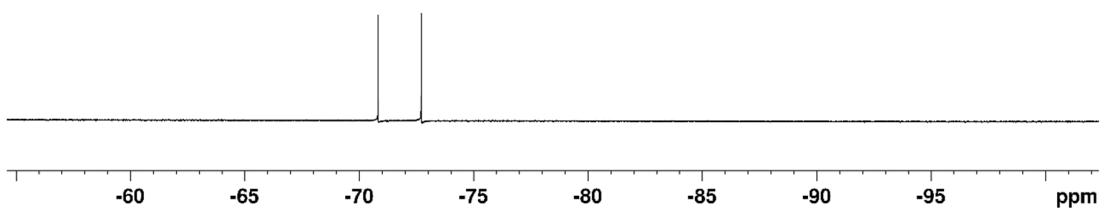
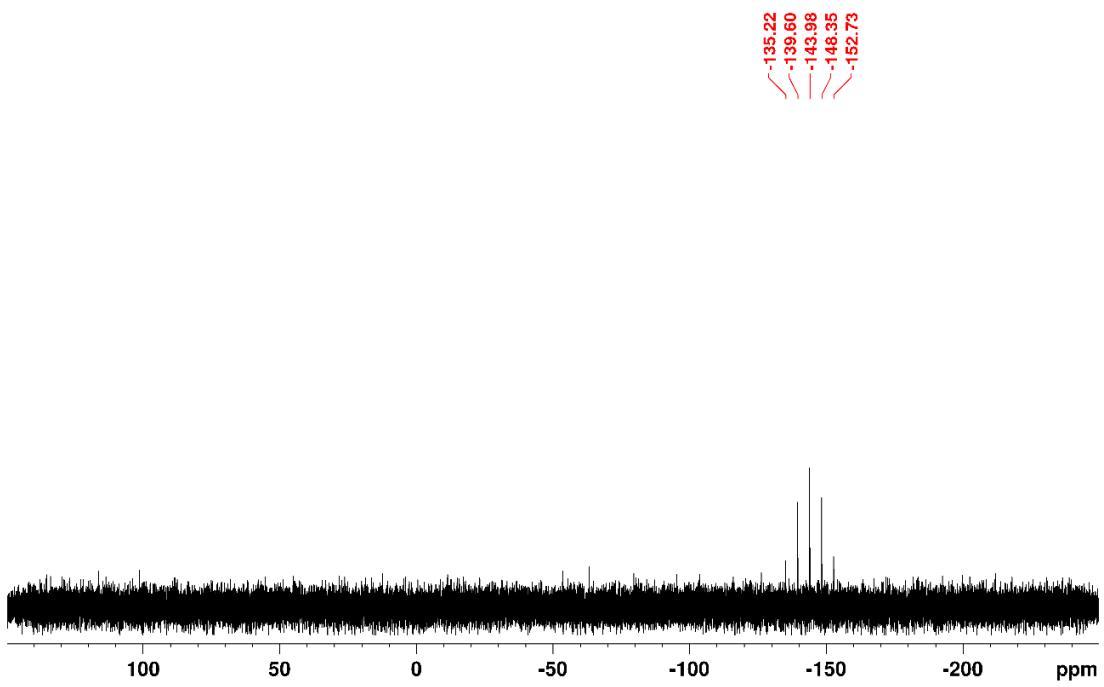


Fig. S19 ^{19}F NMR spectrum of **4** in DMF-d_7 .



c)

Fig. S20 ^{31}P NMR spectrum of **4** in DMF-d_7 .

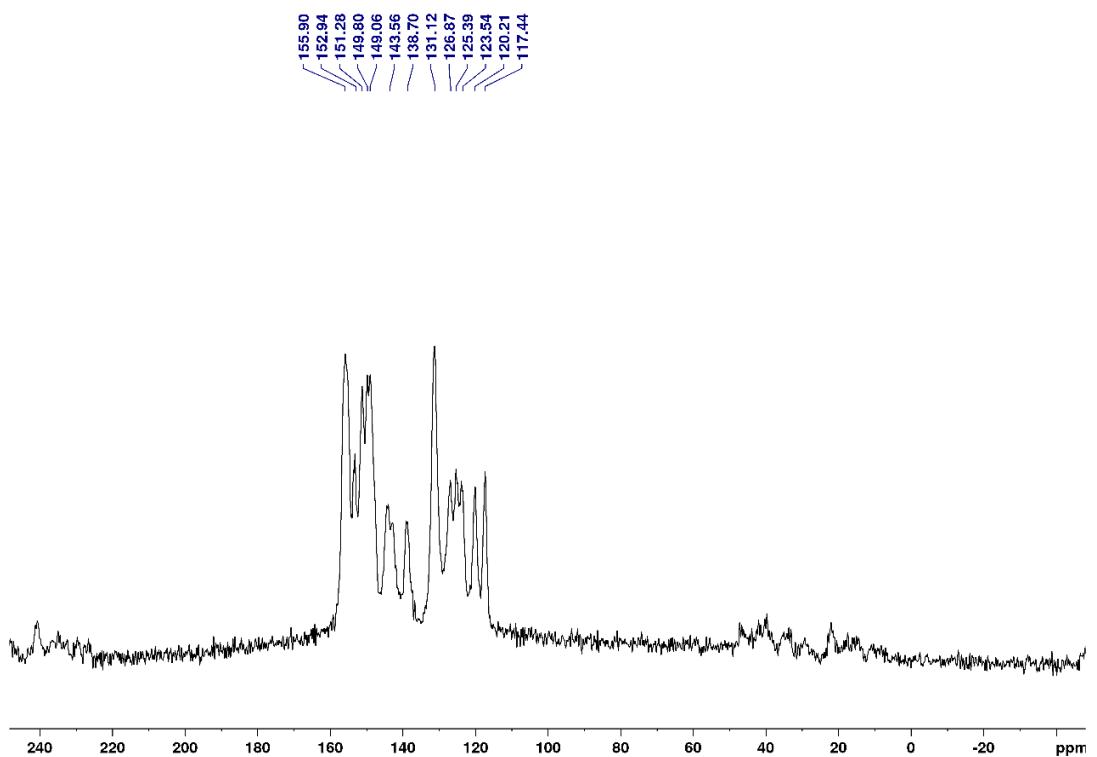


Fig. S21 Solid-state ^{13}C NMR spectrum of **4**.

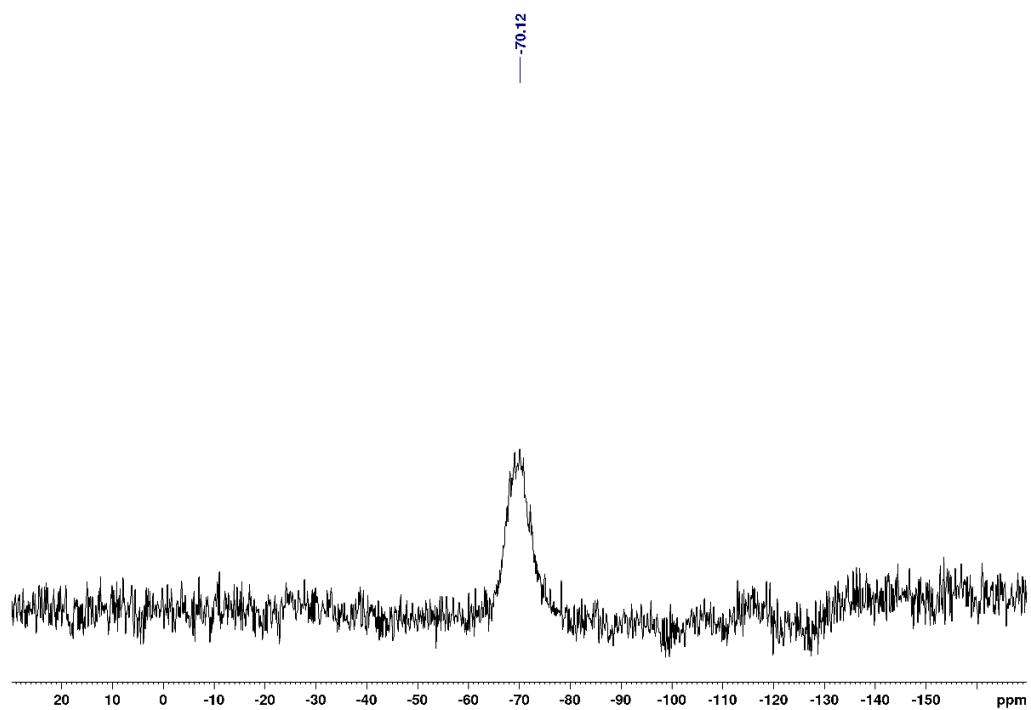


Fig. S22 Solid-state ^{19}F NMR spectrum of **4**.

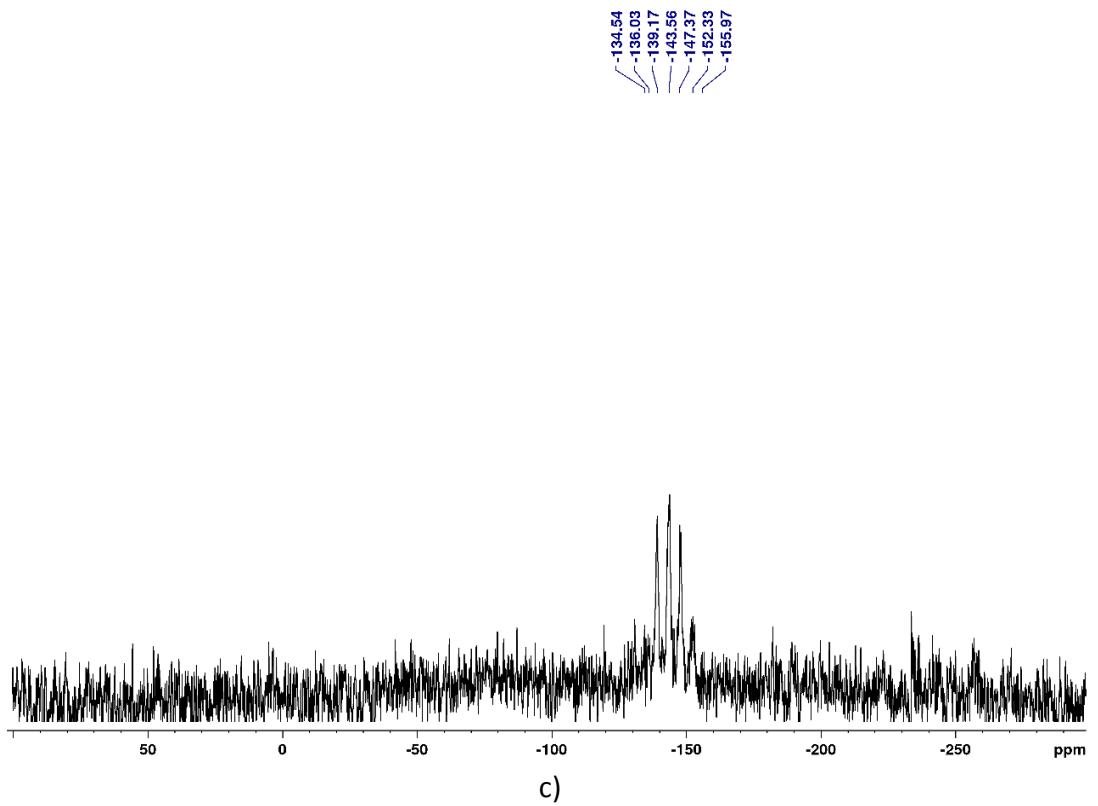


Fig. S23 Solid-state ^{31}P NMR spectrum of **4**.

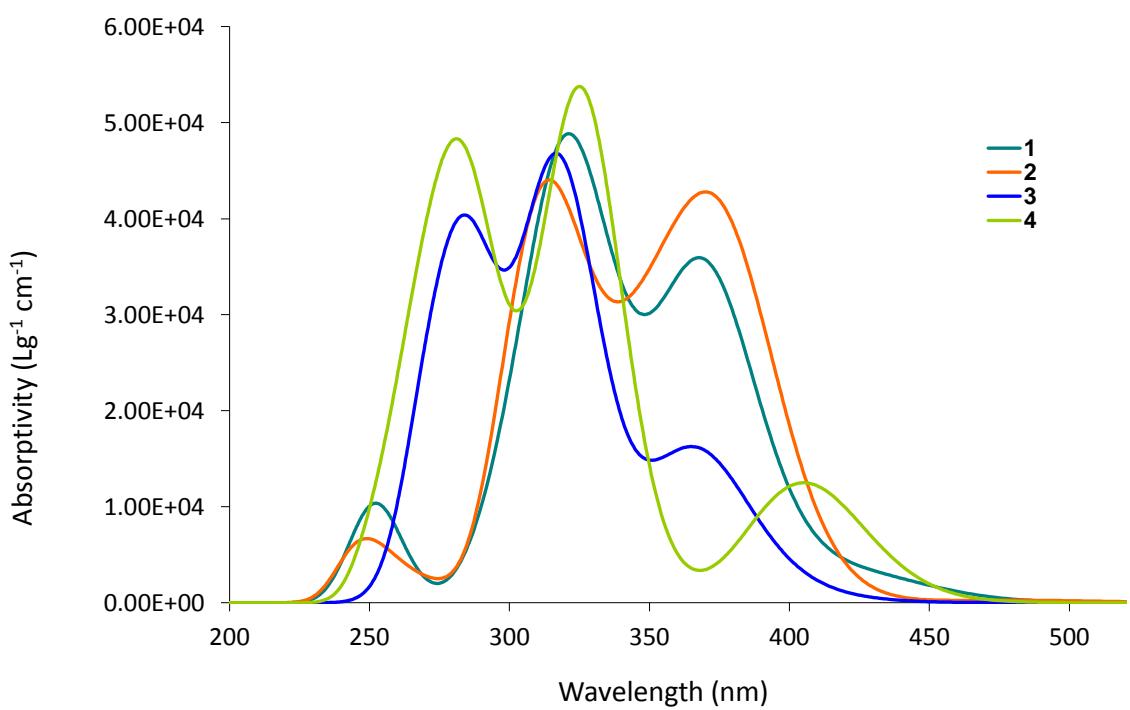


Fig. S24 Theoretical electronic spectra of **1–4** obtained at CAM-B3LYP/LANL2DZ level of theory.

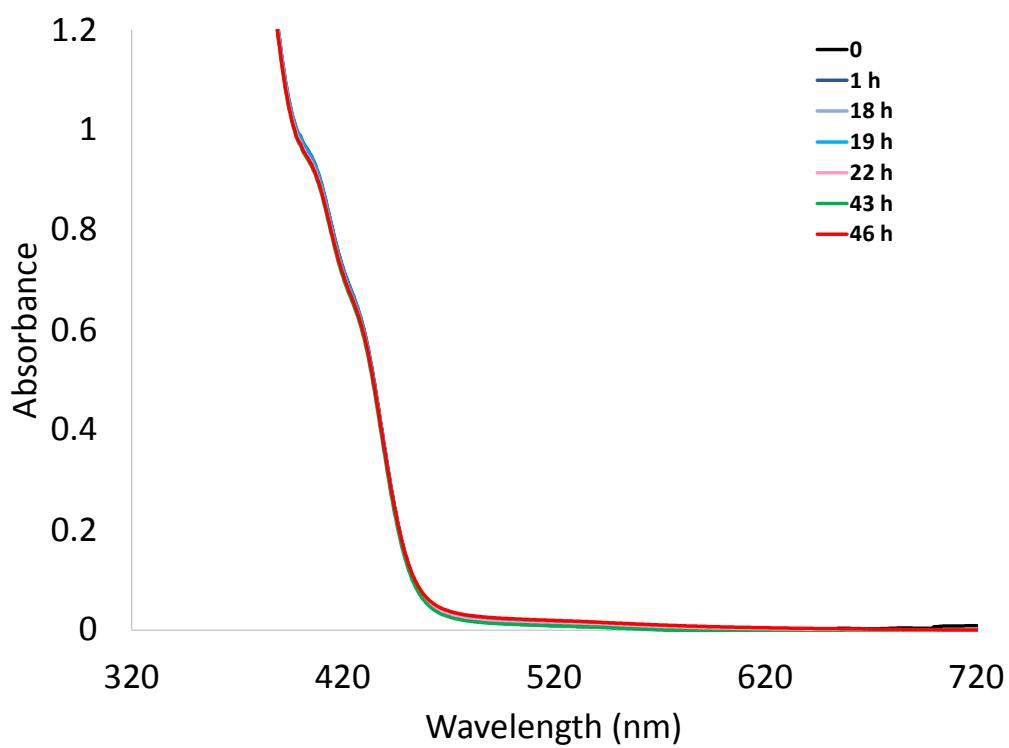


Fig. S25 UV-Vis spectra of **1** (0.17 mM) in DMSO recorded as a function of time during the incubation for 46 h. (Note: the absolute scale on the left Y-axis)

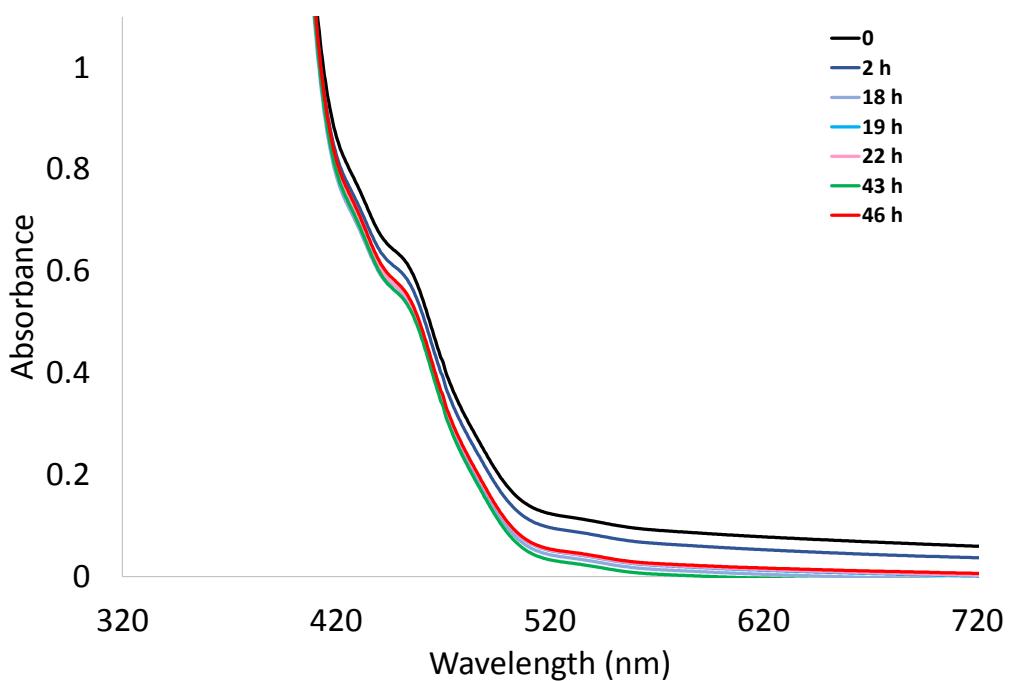


Fig. S26 UV-Vis spectra of **2** (0.17 mM) in DMSO recorded as a function of time during the incubation for 46 h. (Note: the absolute scale on the left Y-axis)

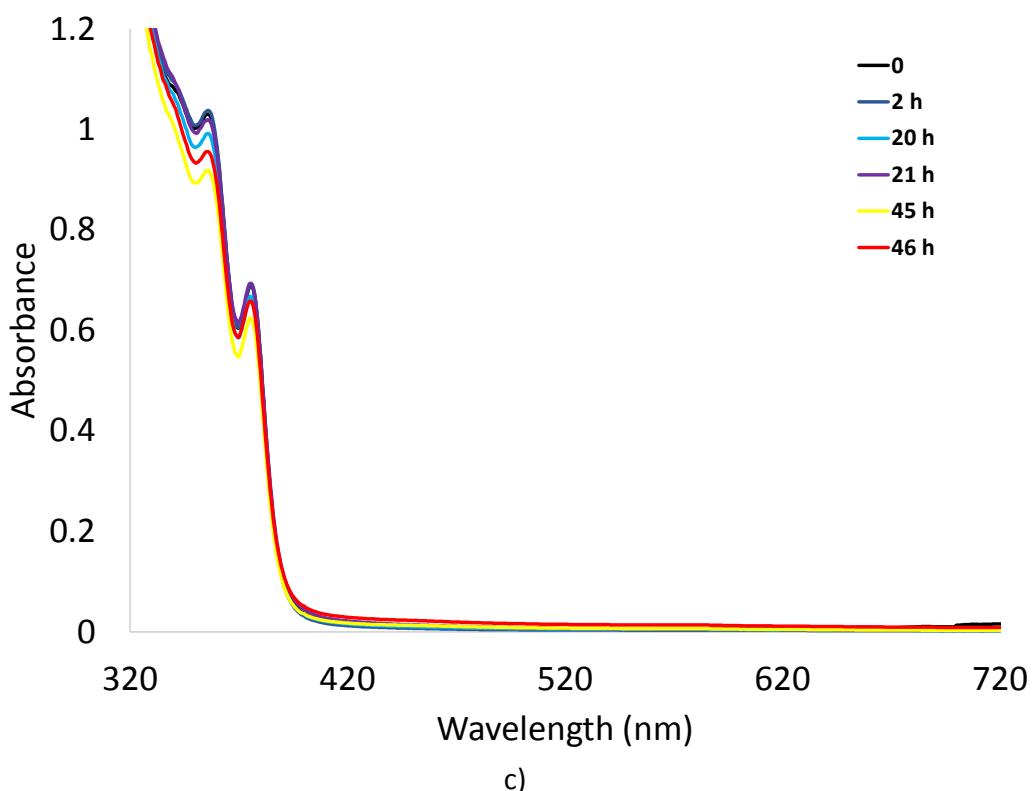


Fig. S27 UV-Vis spectra of **3** (0.17 mM) in DMSO recorded as a function of time during the incubation for 46 h. (Note: the absolute scale on the left Y-axis)

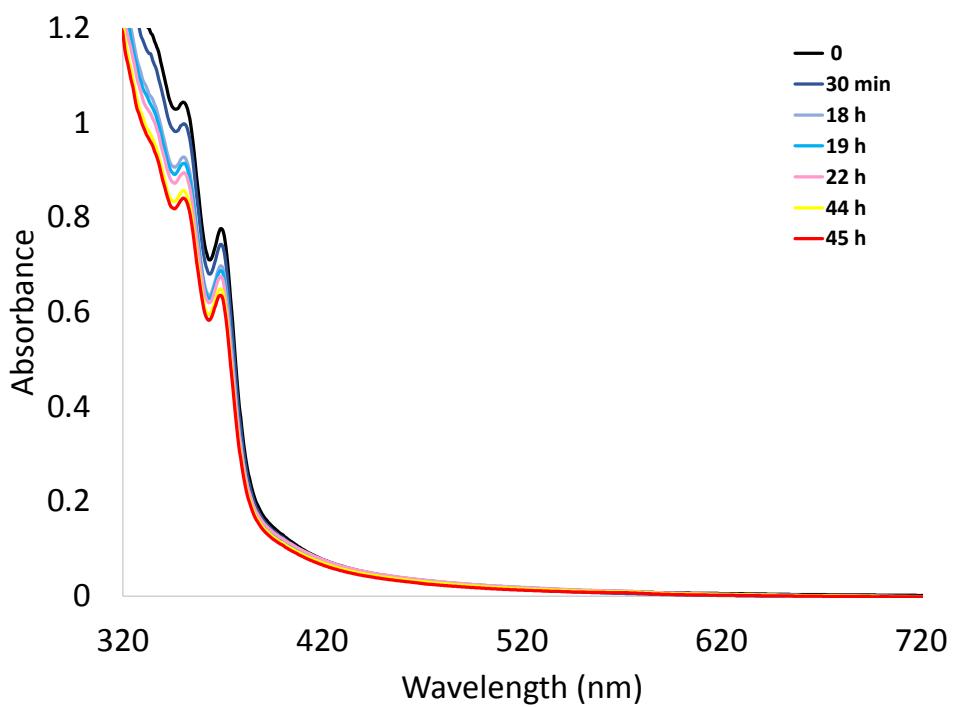


Fig. S28 UV-Vis spectra of **1** (0.17 mM) in 2% (v/v) DMSO/H₂O mixture recorded as a function of time during the incubation for 45 h. (Note: the absolute scale on the left Y-axis)

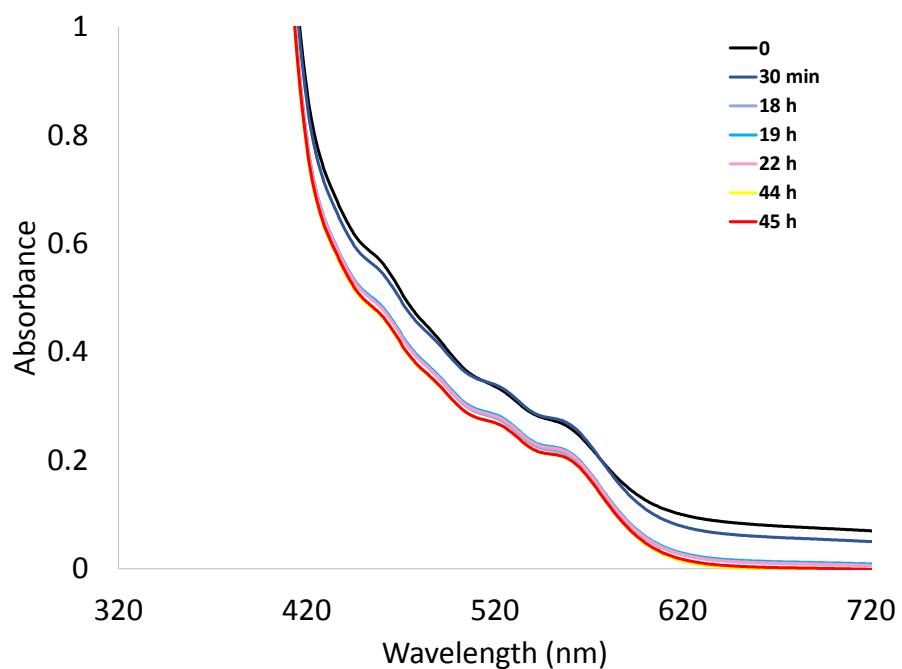


Fig. S29 UV-Vis spectra of **2** (0.17 mM) in 2% (v/v) DMSO/H₂O mixture recorded as a function of time during the incubation for 45 h. (Note: the absolute scale on the left Y-axis)

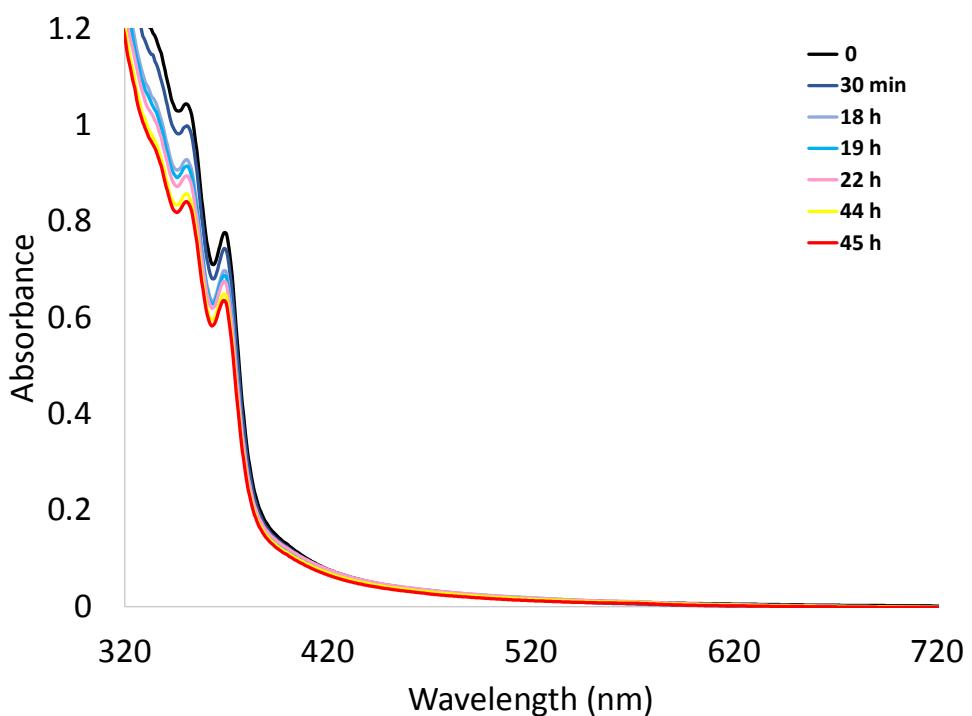


Fig. S30 UV-Vis spectra of **3** (0.17 mM) in 2% (v/v) DMSO/H₂O mixture recorded as a function of time during the incubation for 45 h. (Note: the absolute scale on the left Y-axis)