

Supporting information

Role of the auxiliary ligand in determining the genotoxicity and mode of cell death of Pd(II) complexes with thiosemicarbazone

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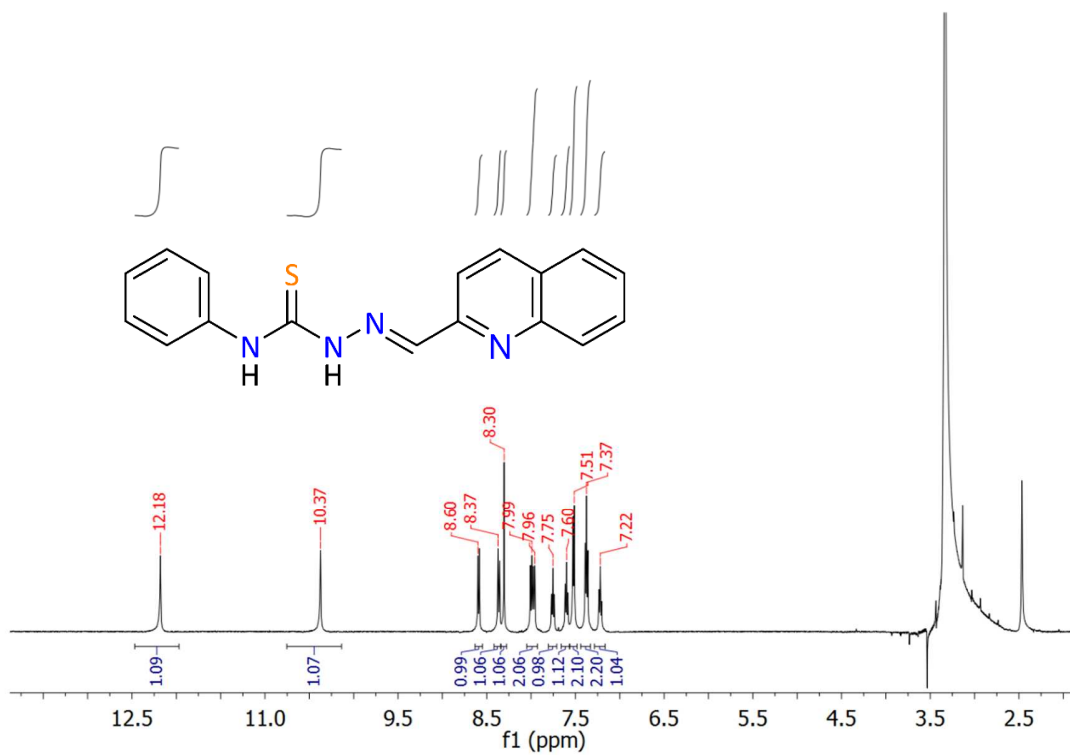
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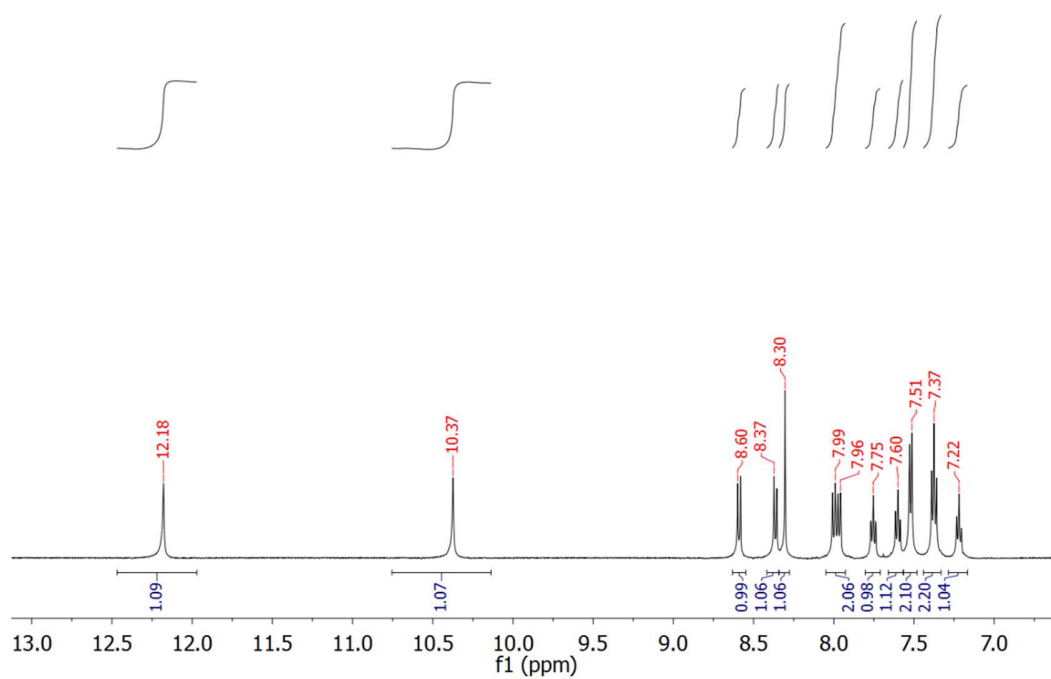
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¹ equal contribution.

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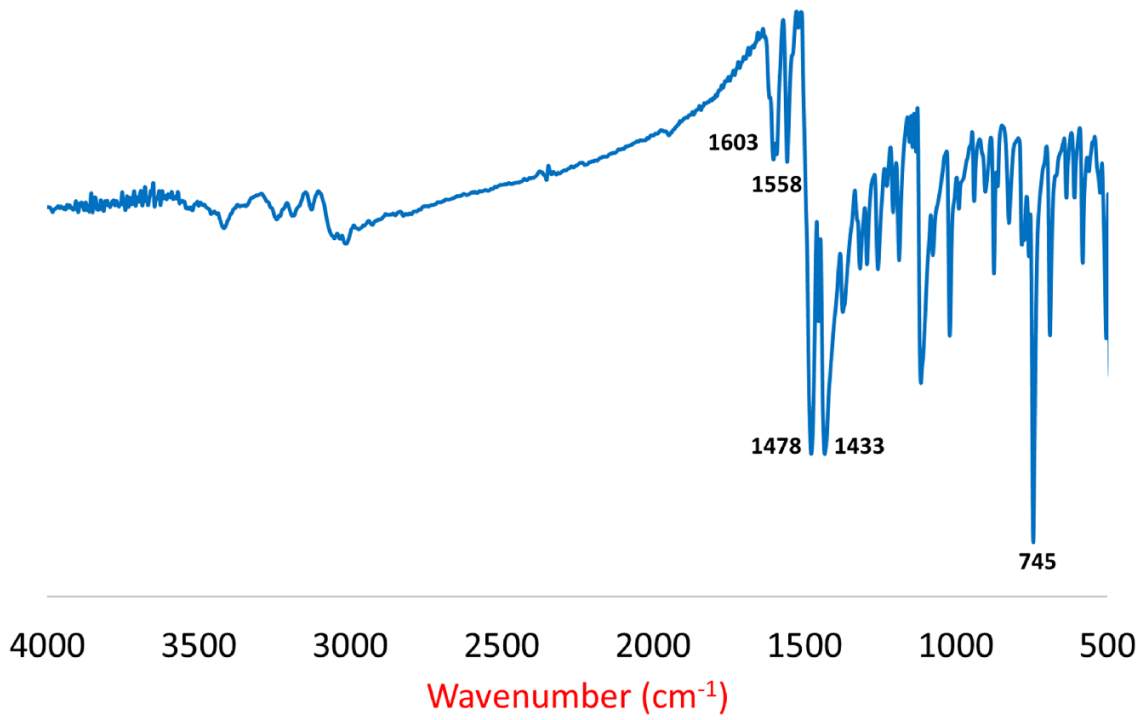


a)

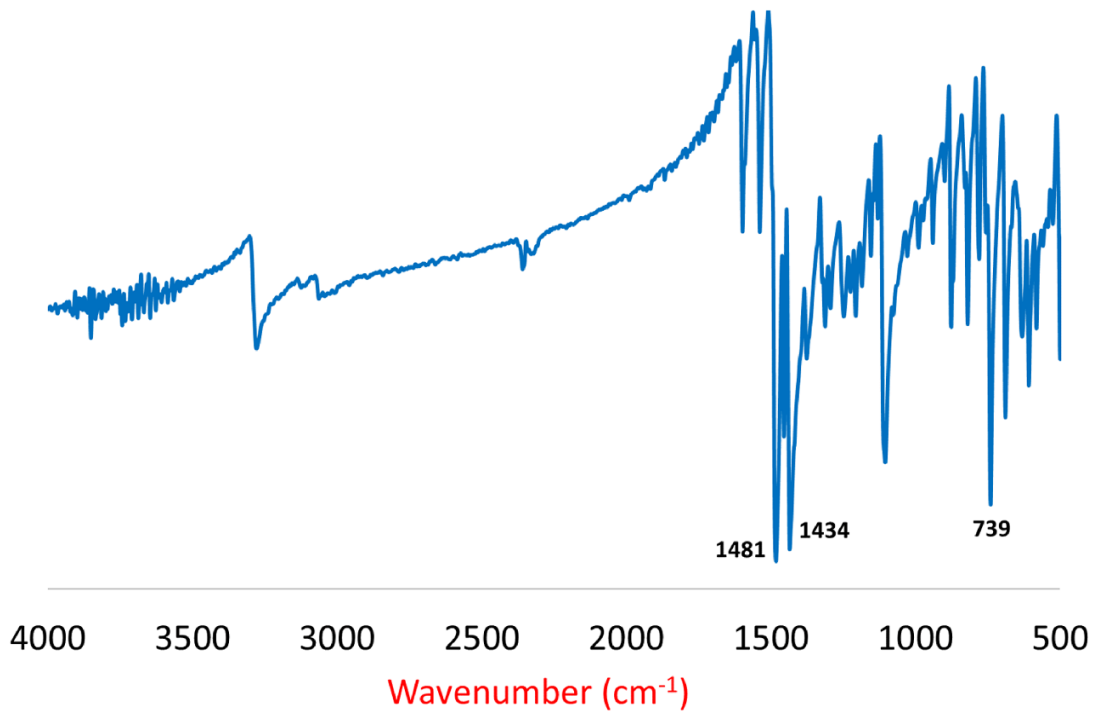


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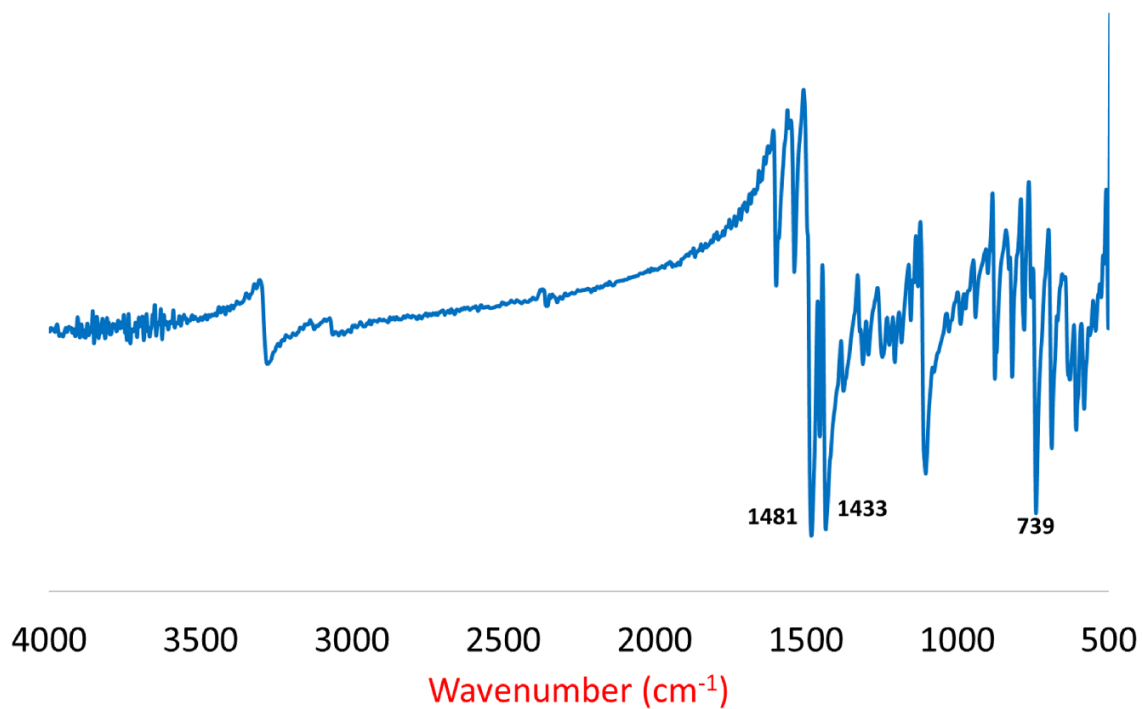
Fig. S1 ^1H NMR spectrum of thiosemicarbazone ligand **a)** whole spectrum and **b)** zoomed spectrum.



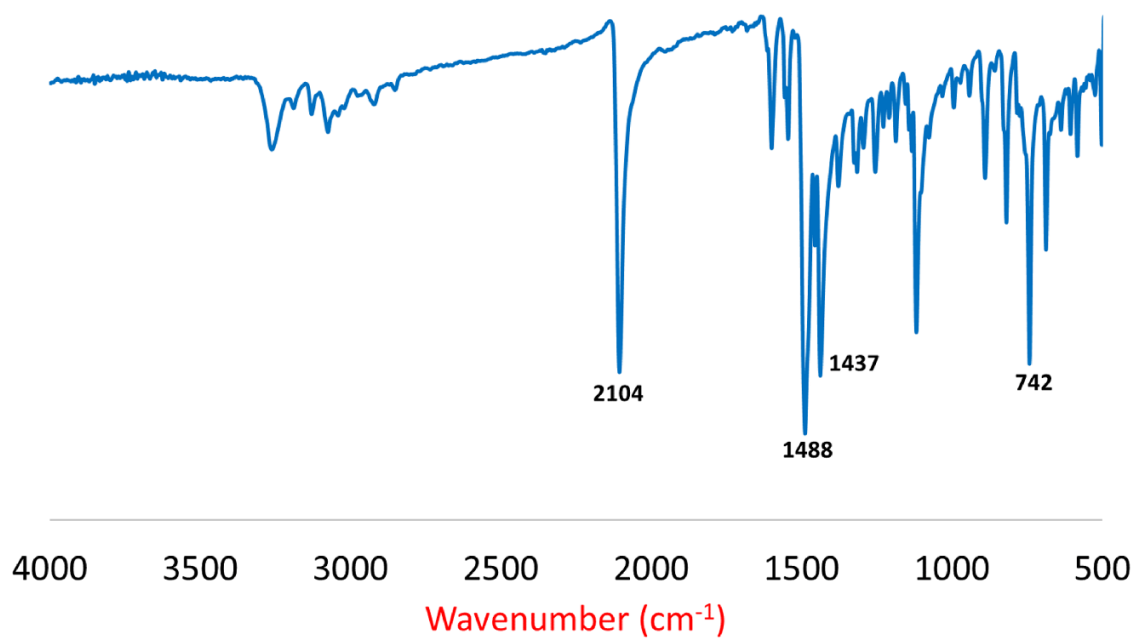
a)



b)



c)



d)

Fig. S2 IR spectra of the Pd(II) complexes a) 3, b) 4, c) 5, and d) 6.

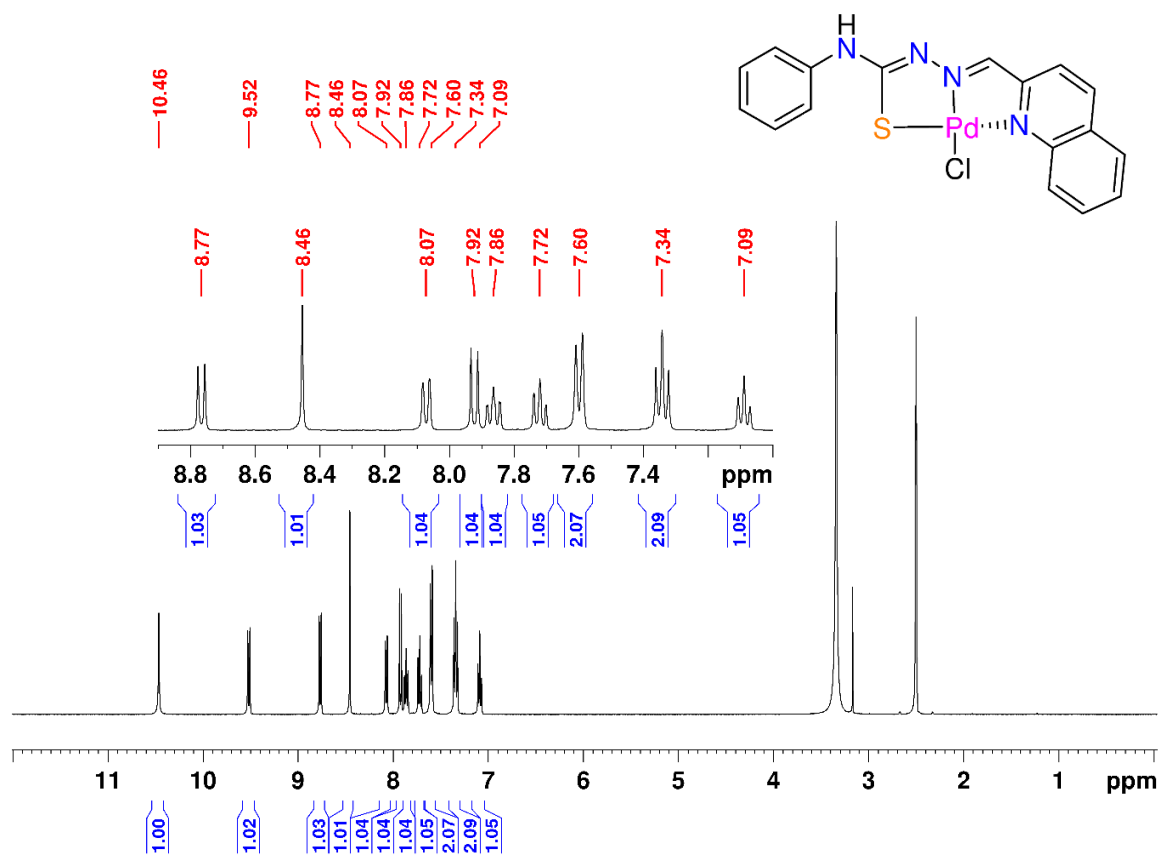


Fig. S3. ¹H NMR spectrum of 3.

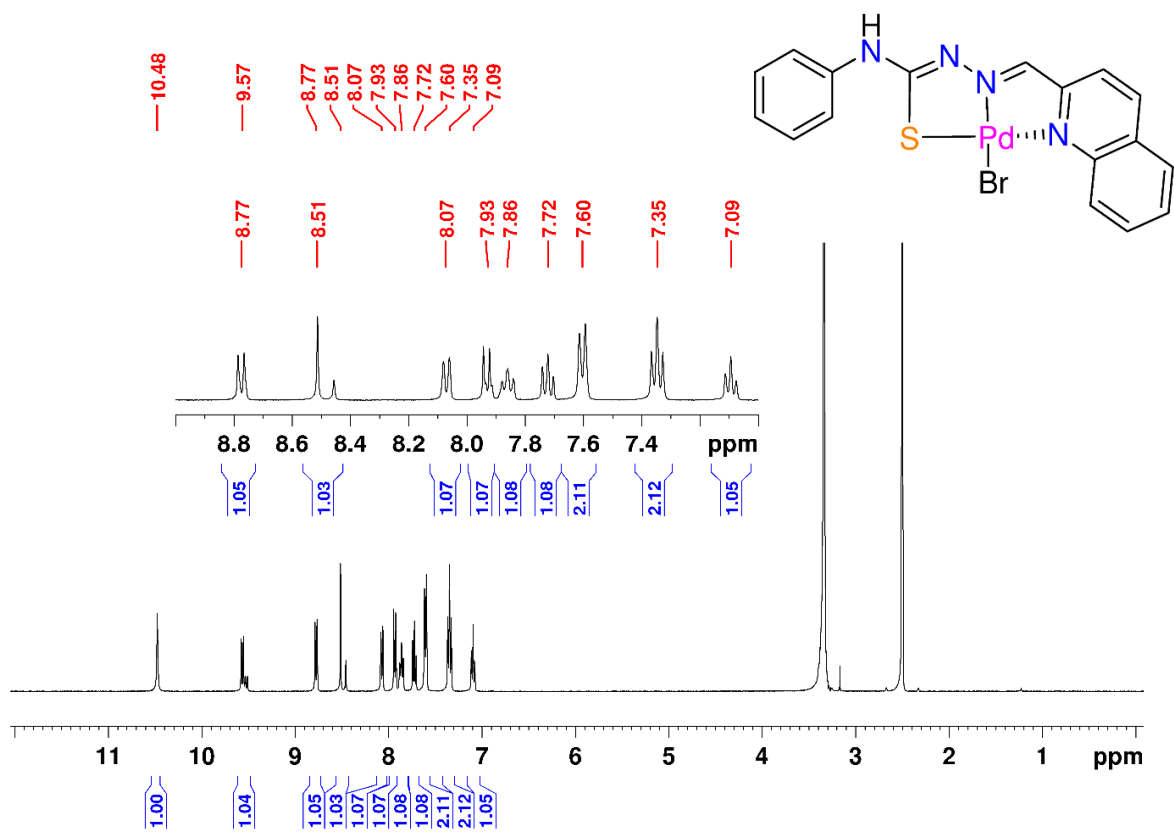


Fig. S4. ¹H NMR spectrum of 4.

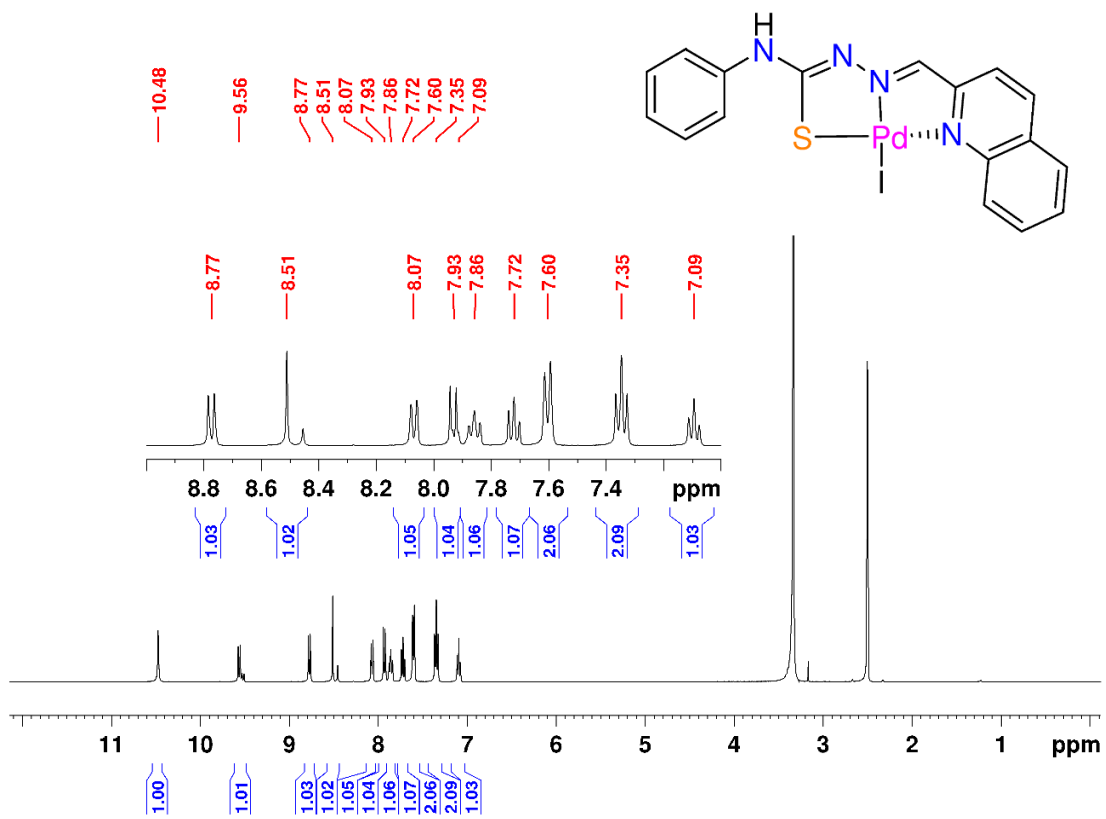


Fig. S5. ¹H NMR spectrum of 5.

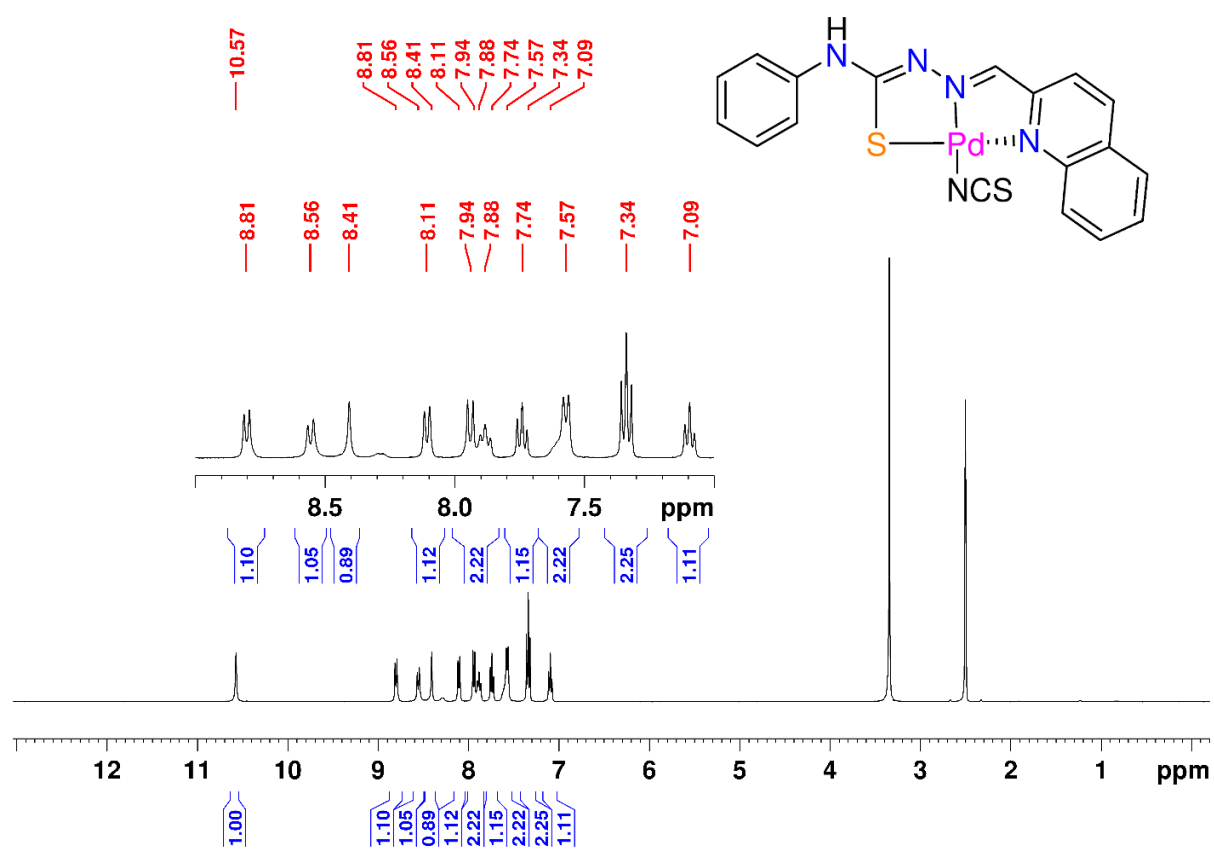


Fig. S6. ^1H NMR spectrum of 6.

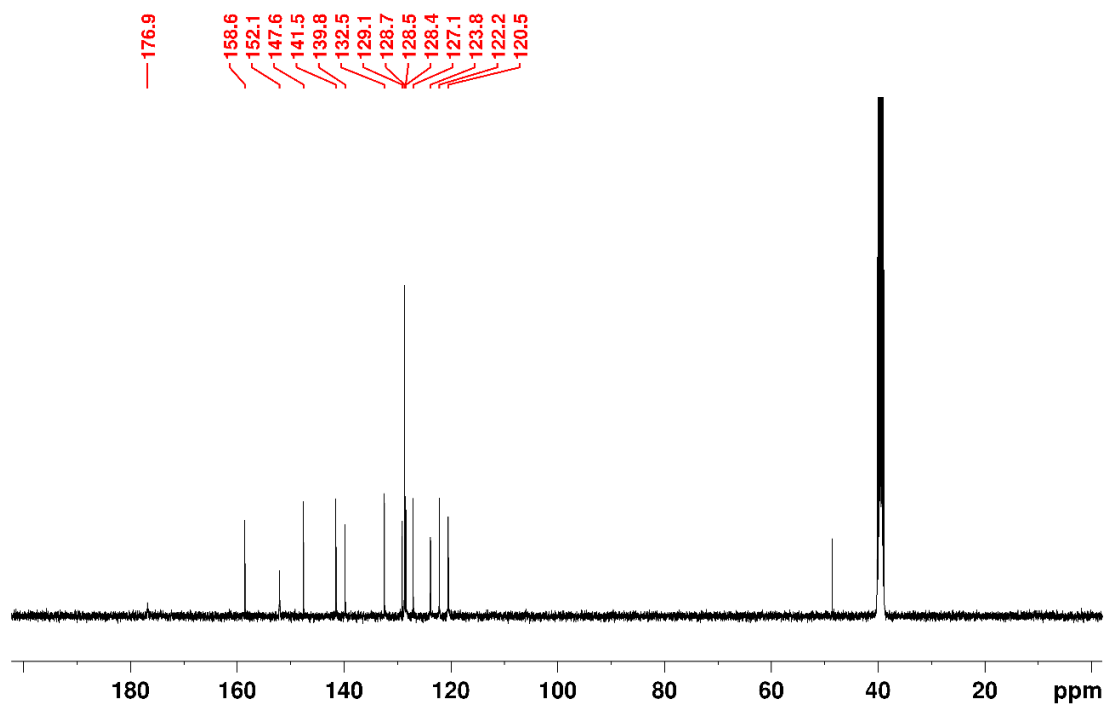


Fig. S7. ^{13}C NMR spectrum of **3**.

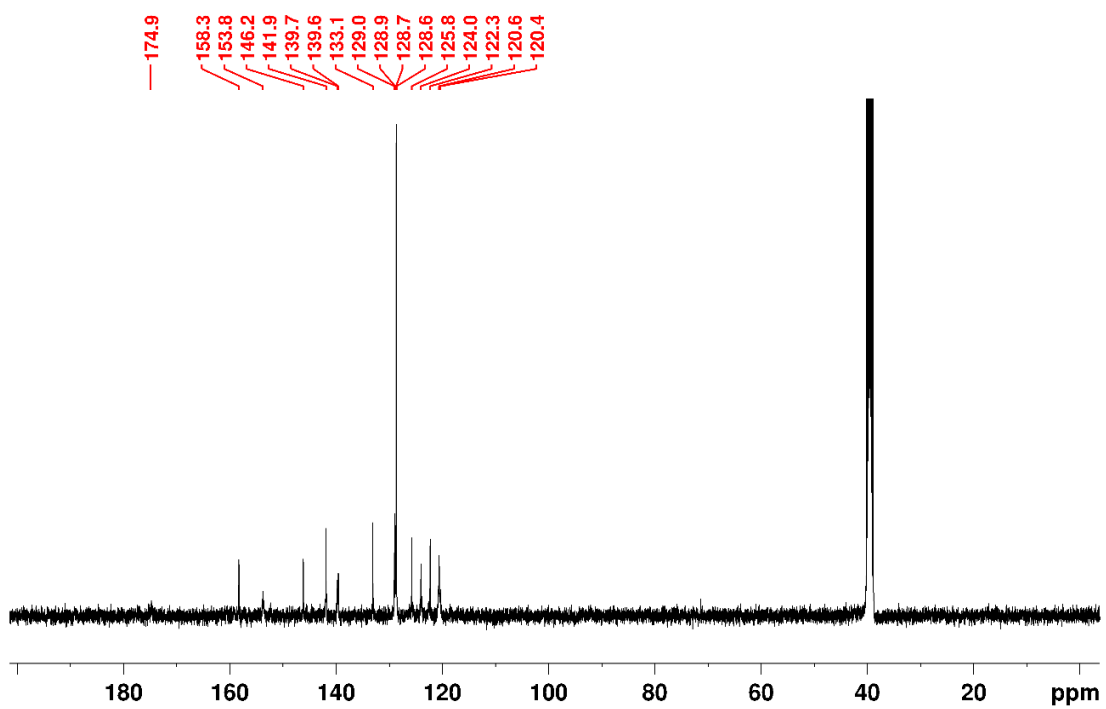


Fig. S8. ^{13}C NMR spectrum of **6**.

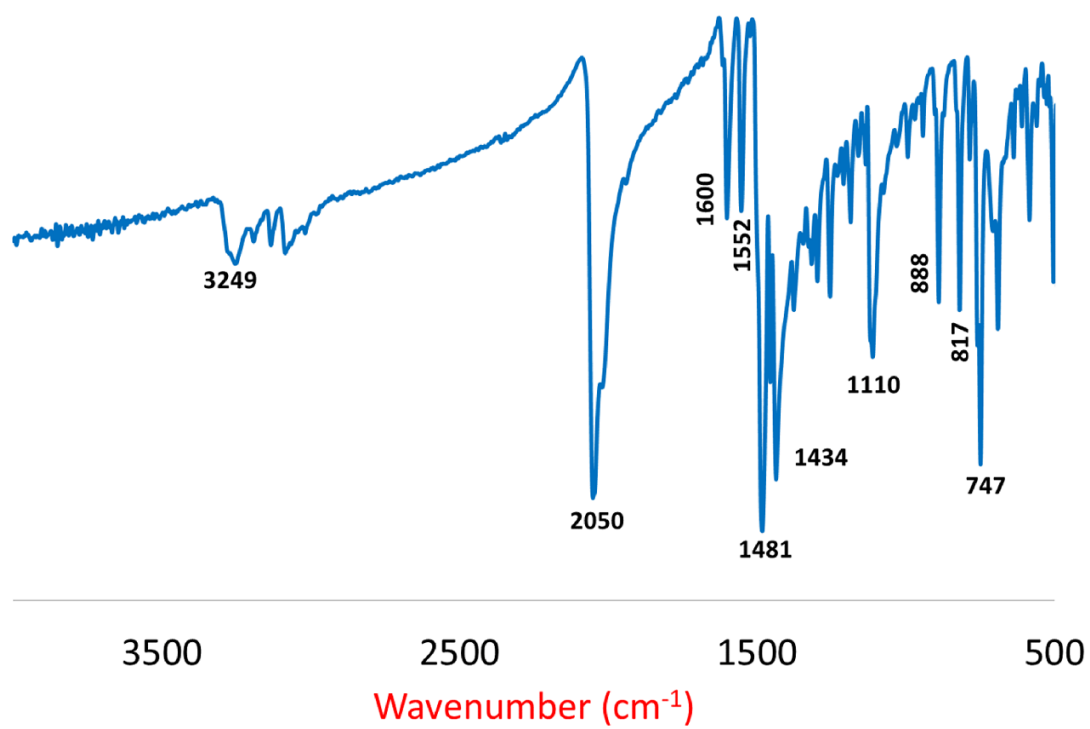
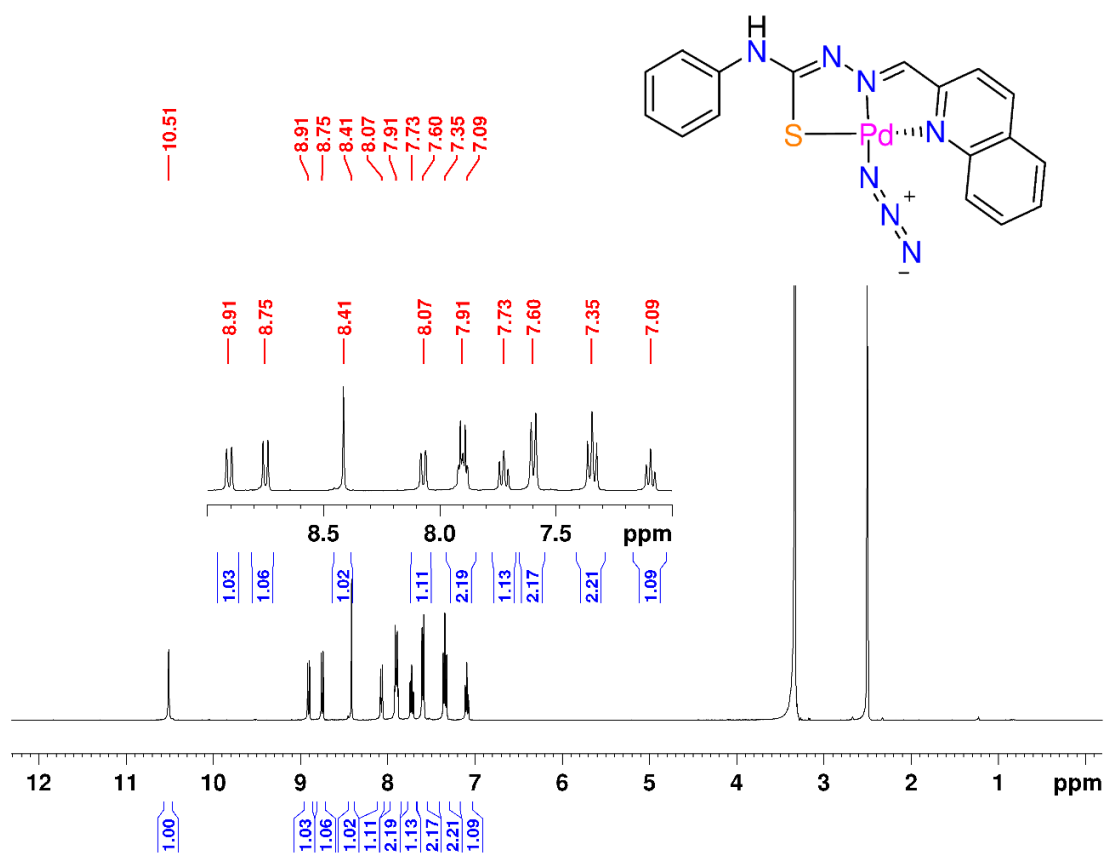
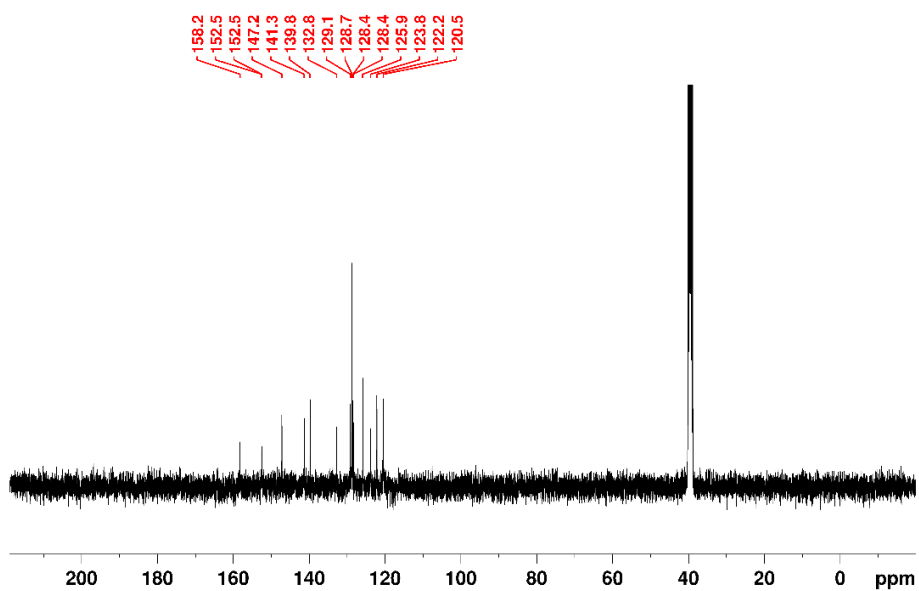


Fig. S9 IR spectrum of 7.



a)



b)

Fig. S10. NMR spectra of 7 a) ¹H and b) ¹³C.

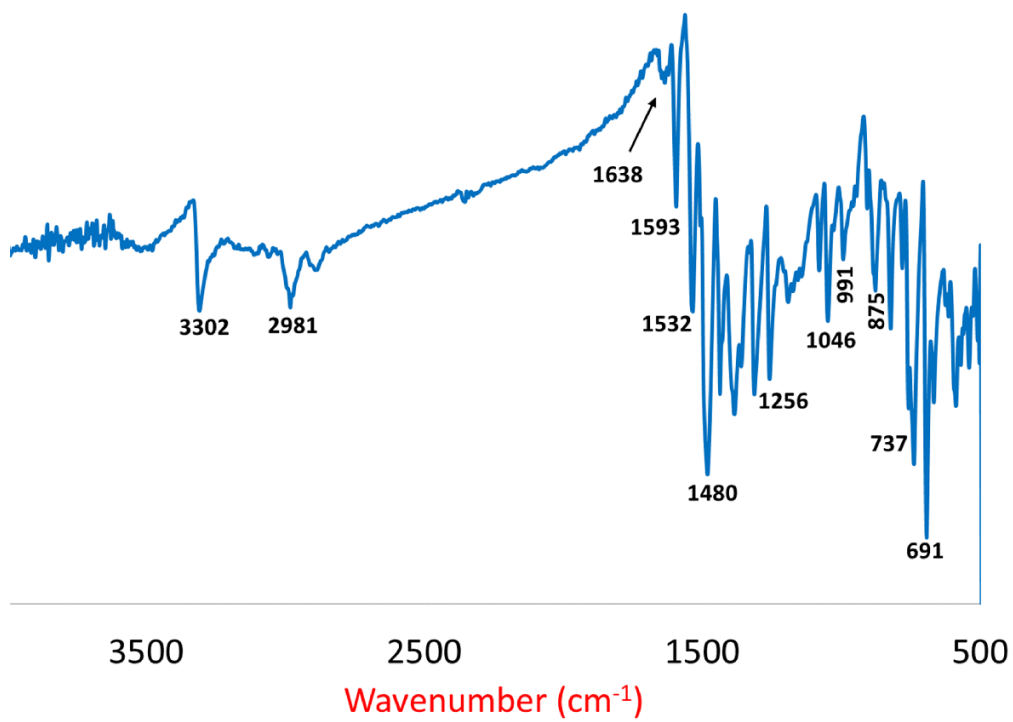


Fig. S11 IR spectrum of **8**.

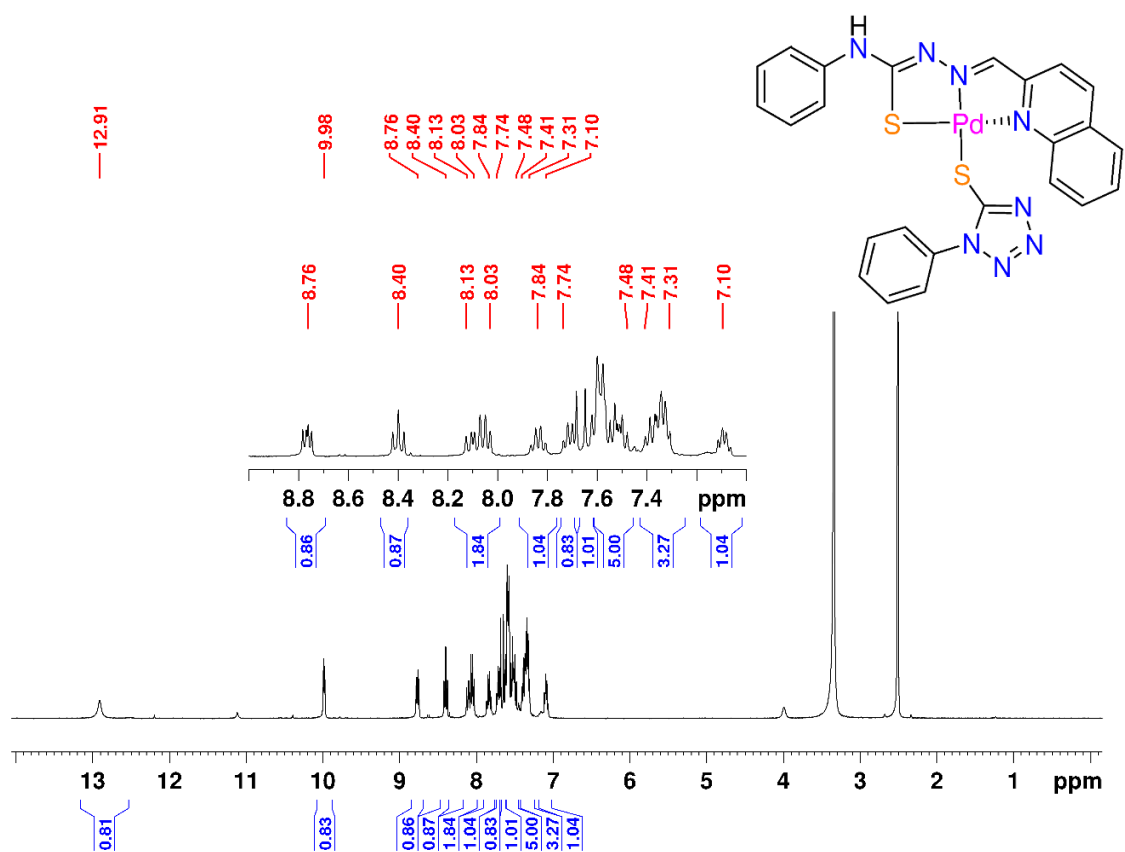


Fig. S12. ^1H NMR spectrum of 8.

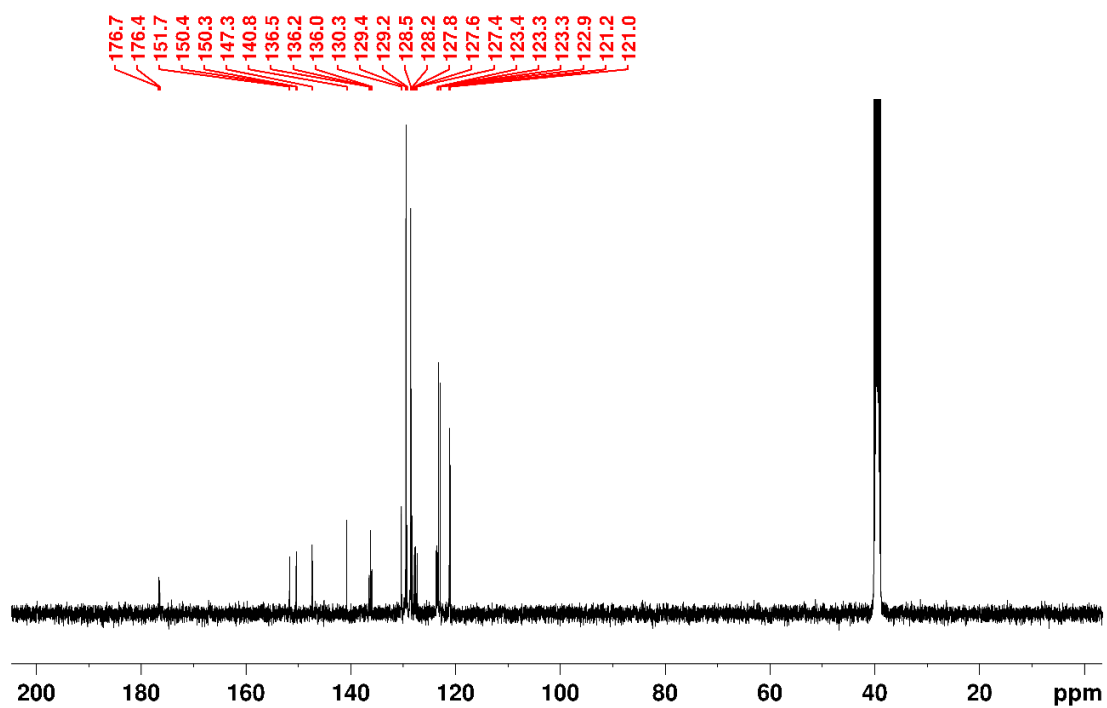


Fig. S13. ^{13}C NMR spectrum of **8**.

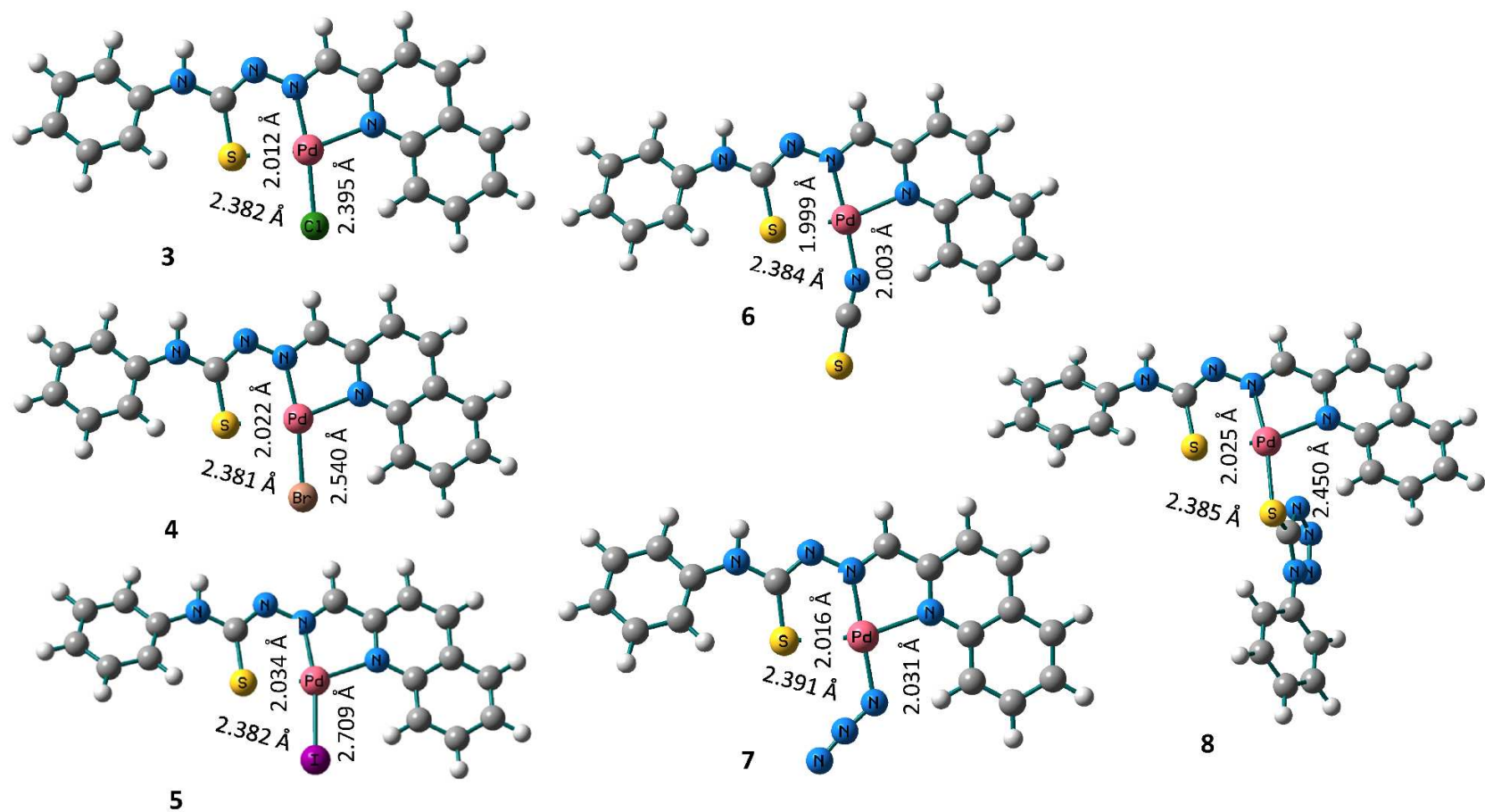


Fig. S14. The local minimum structures of **3–8** calculated at B3LYP/LANL2DZ level of theory. (Hydrogen-atoms were omitted for the clarity).

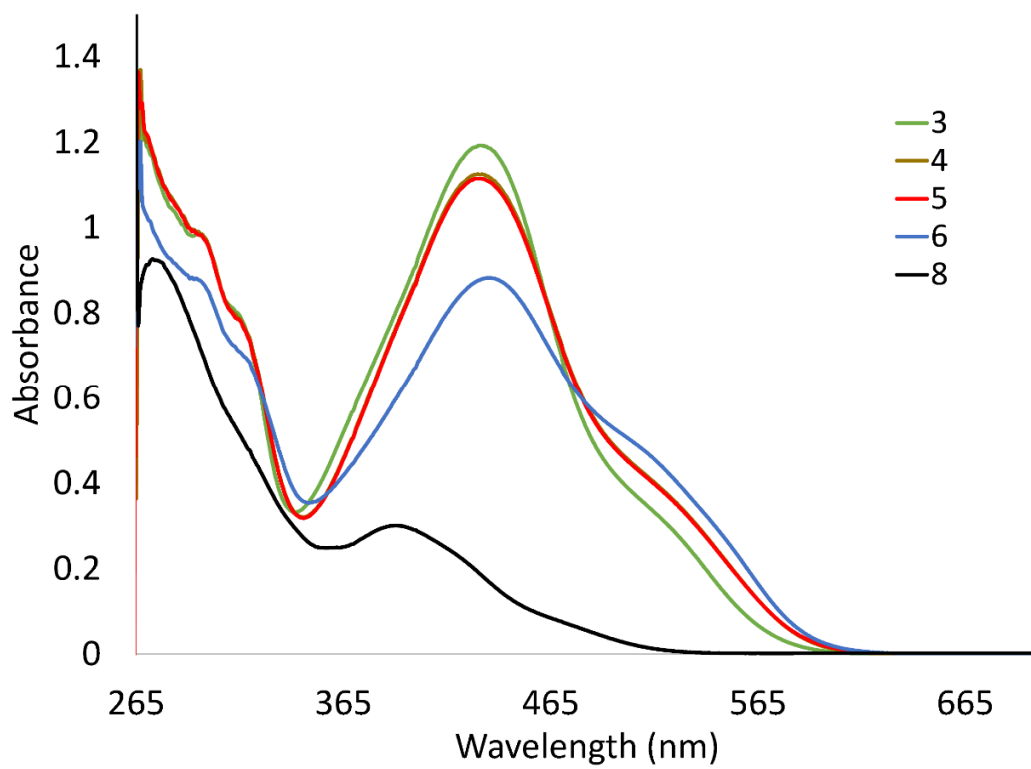
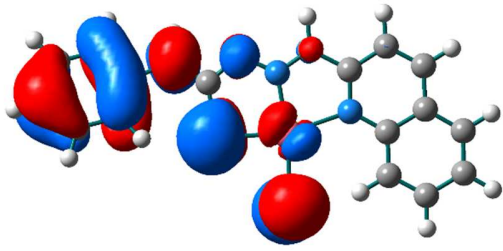
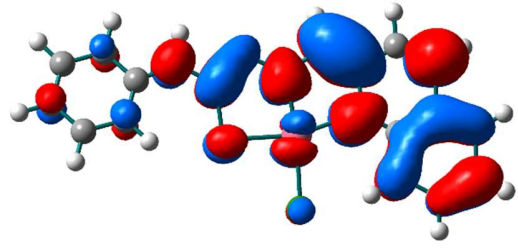


Fig. S15 Electronic absorption spectra of **3–8** in DMF.

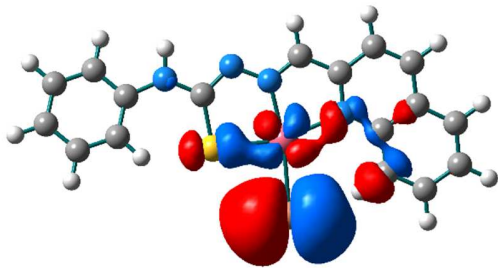
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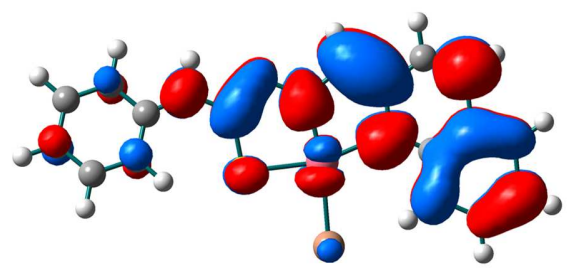
3: LUMO



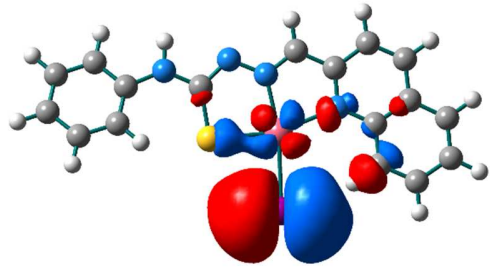
4: HOMO-1



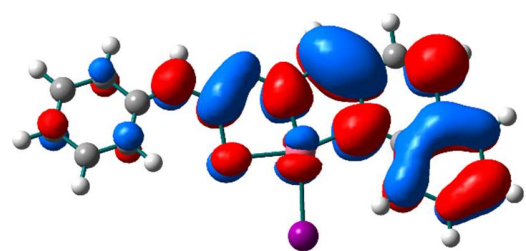
4: LUMO



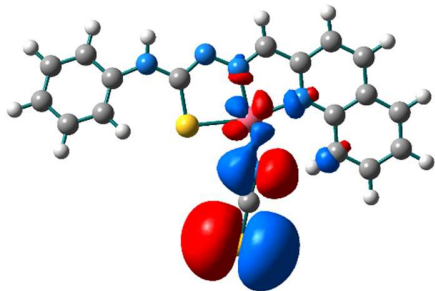
5: HOMO-1



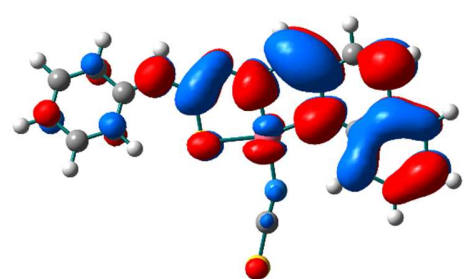
5: LUMO



6: HOMO-1



6: LUMO



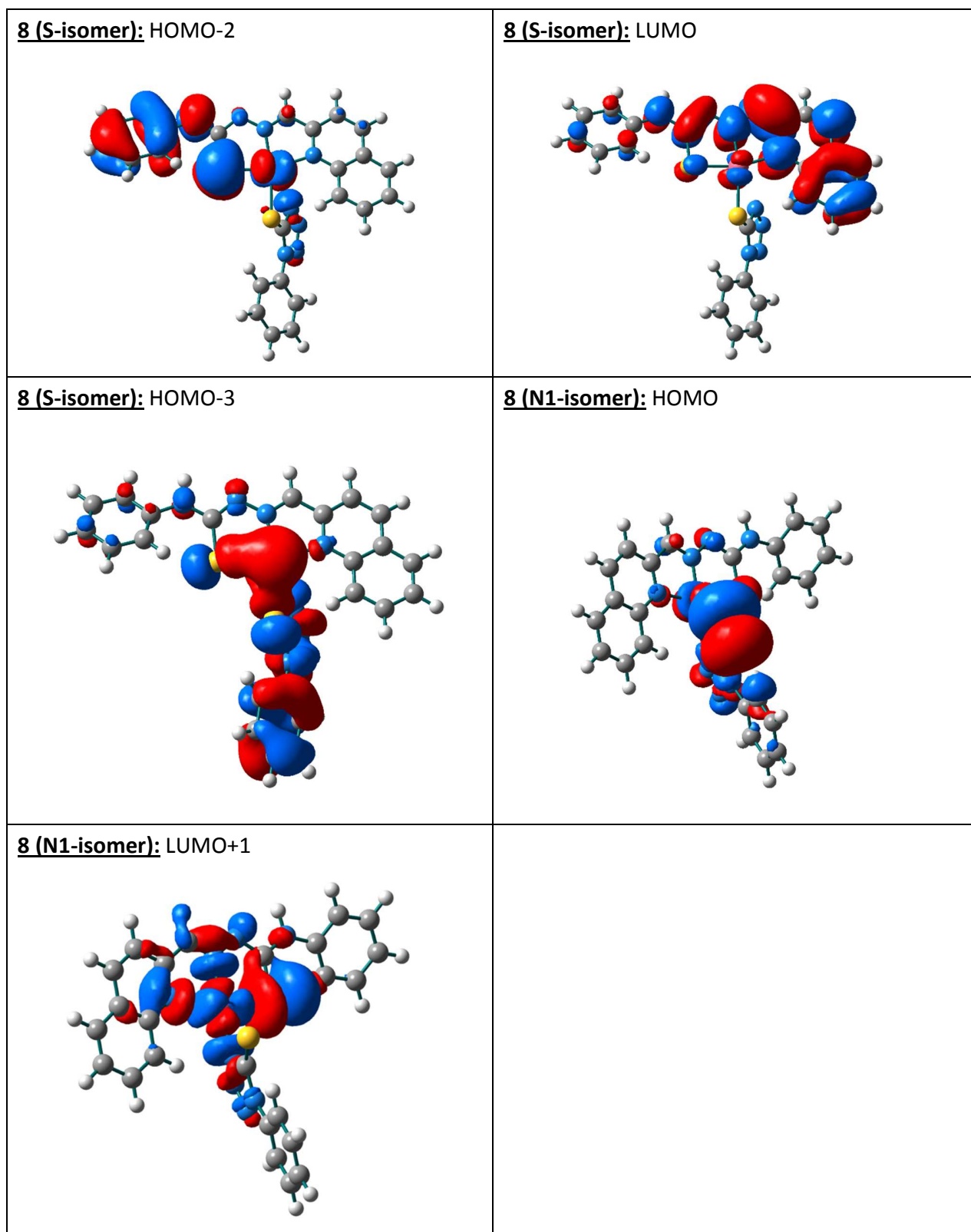


Fig. S16 Selective frontiers molecular orbitals of **3–8**.

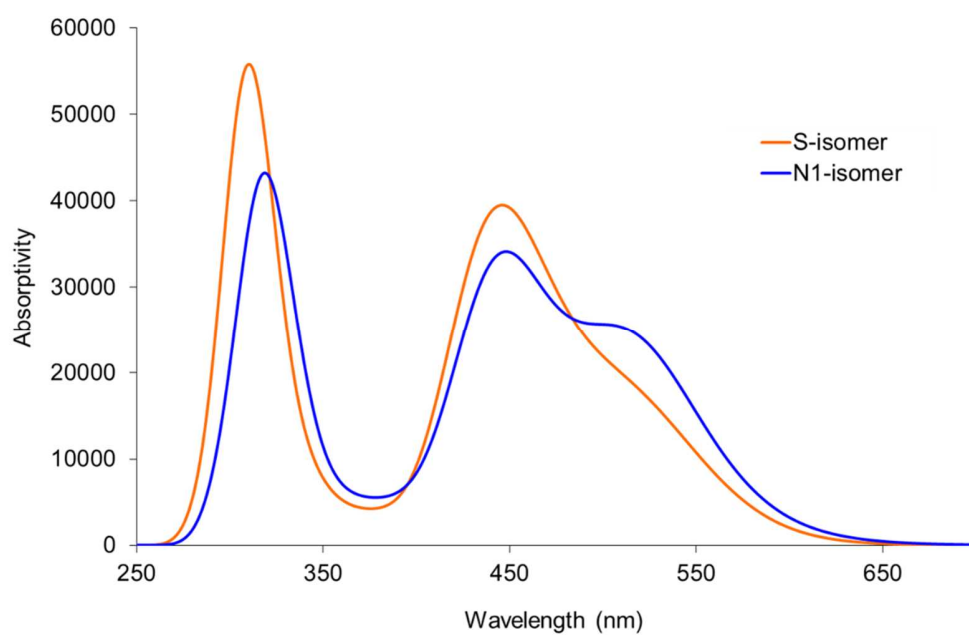


Fig. S17 TDDFT spectra of S- and N1 isomers of **8**.

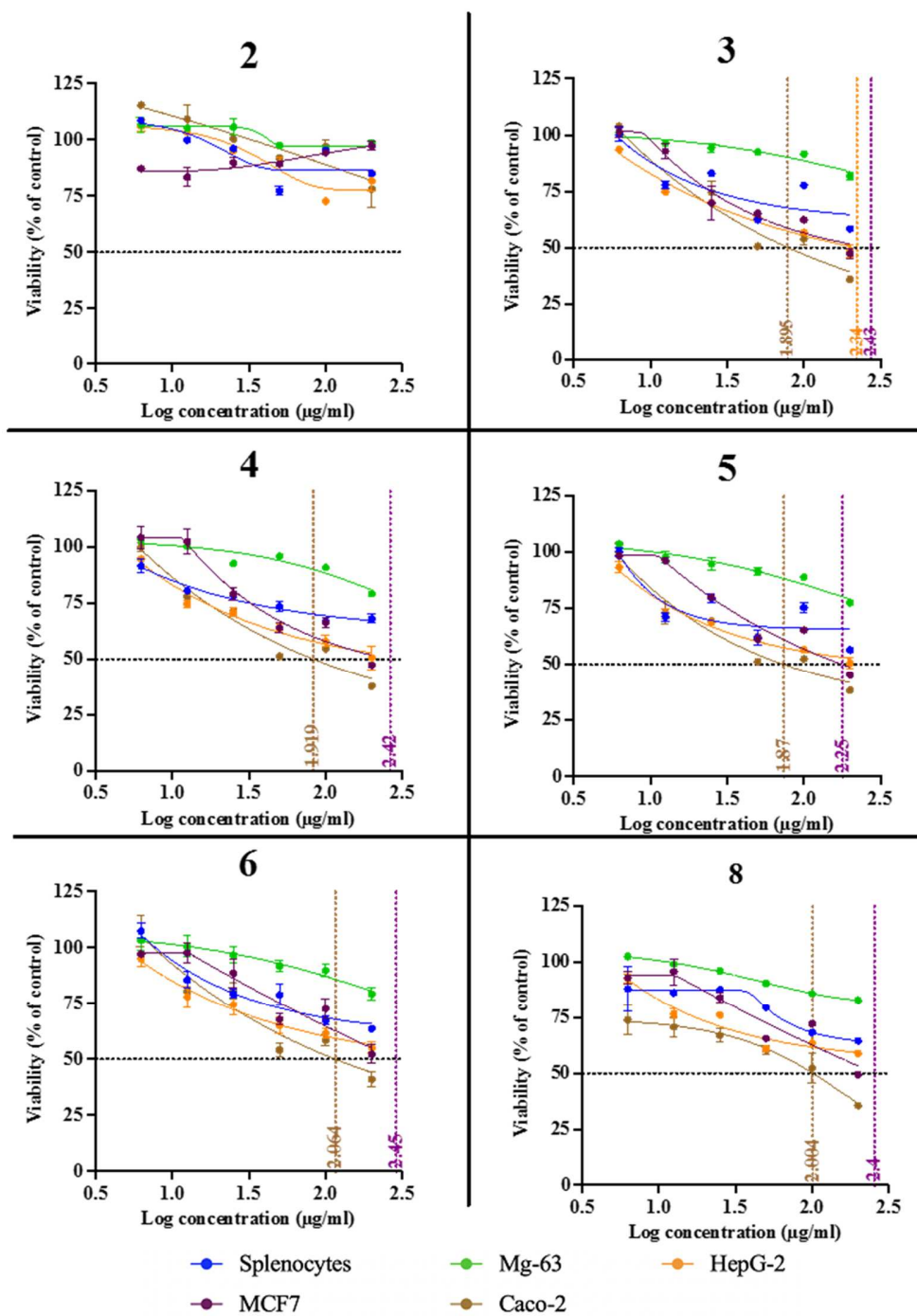


Fig. S18 The dose response curves of 2–8 on five different cell lines.