

## Synthesis and evaluation of the anticancer activity of [Pt(diimine)(*N,N*-dibutyl-*N'*-acylthiourea)]<sup>+</sup> complexes

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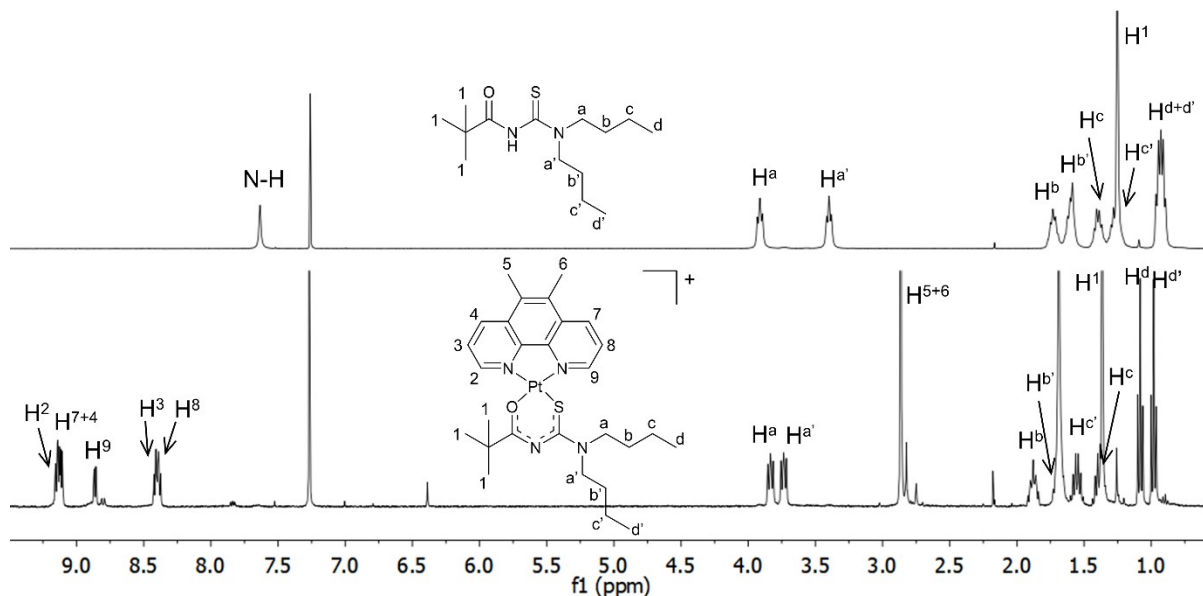


Figure S1: Stacked 1D <sup>1</sup>H NMR spectra of *N,N*-dibutyl-*N'*-pivaloylthiourea ligand with [Pt(dmp)(L<sup>3</sup>-κO,S)]<sup>+</sup> complex in CDCl<sub>3</sub> at 300K with all assignments showing a shift in the proton signals (aliphatic region) upon complexation. Spectra shows pure ligand and complex structure obtained, with residual water and acetone signal observed at 1.59 and 2.17 ppm.

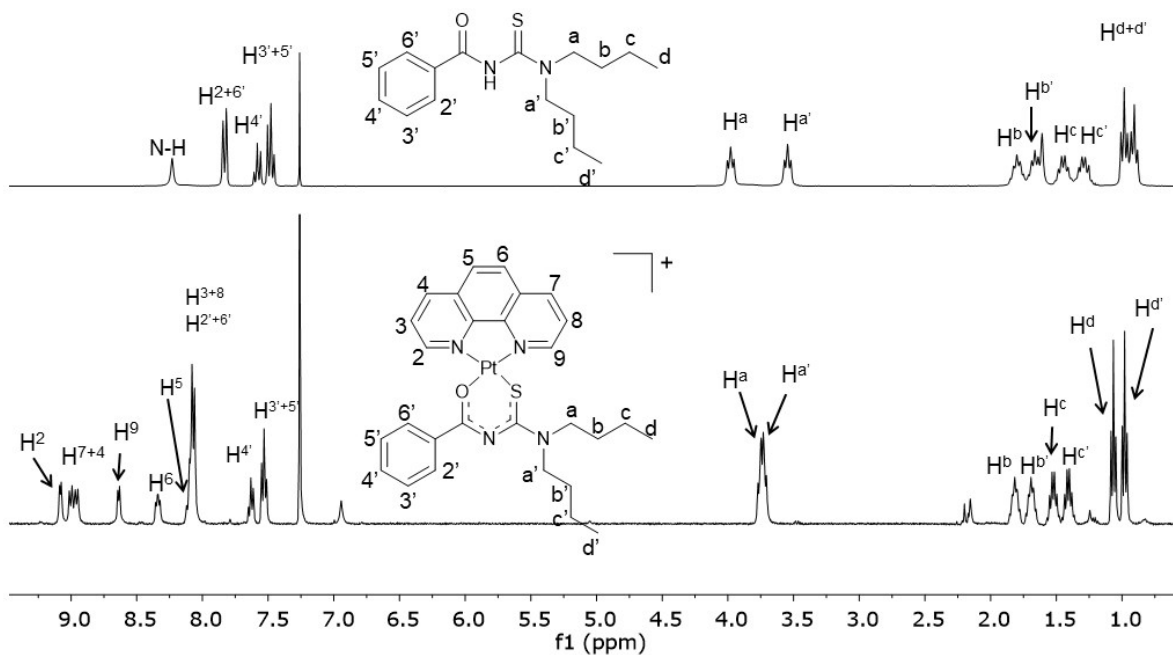


Figure S2: Stacked 1D <sup>1</sup>H NMR spectra of *N,N*-dibutyl-*N'*-benzoylthiourea with [Pt(phen)(L<sup>1</sup>-κO,S)]<sup>+</sup> complex in CDCl<sub>3</sub> at 300K with all assignments showing a shift in the proton signals (aliphatic and aromatic region) upon complexation.



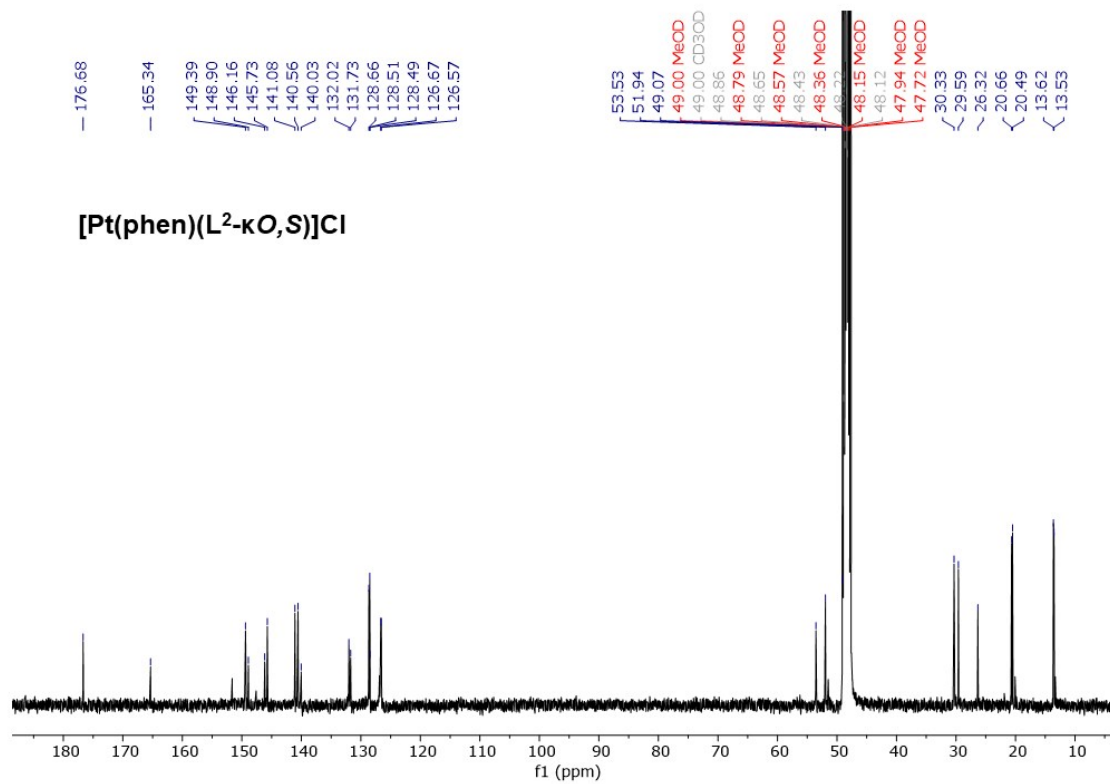


Fig S4: <sup>13</sup>C NMR spectrum of [Pt(phen)(L<sup>2</sup>-κO,S)]<sup>+</sup> complex in CD<sub>3</sub>OD at 300K.

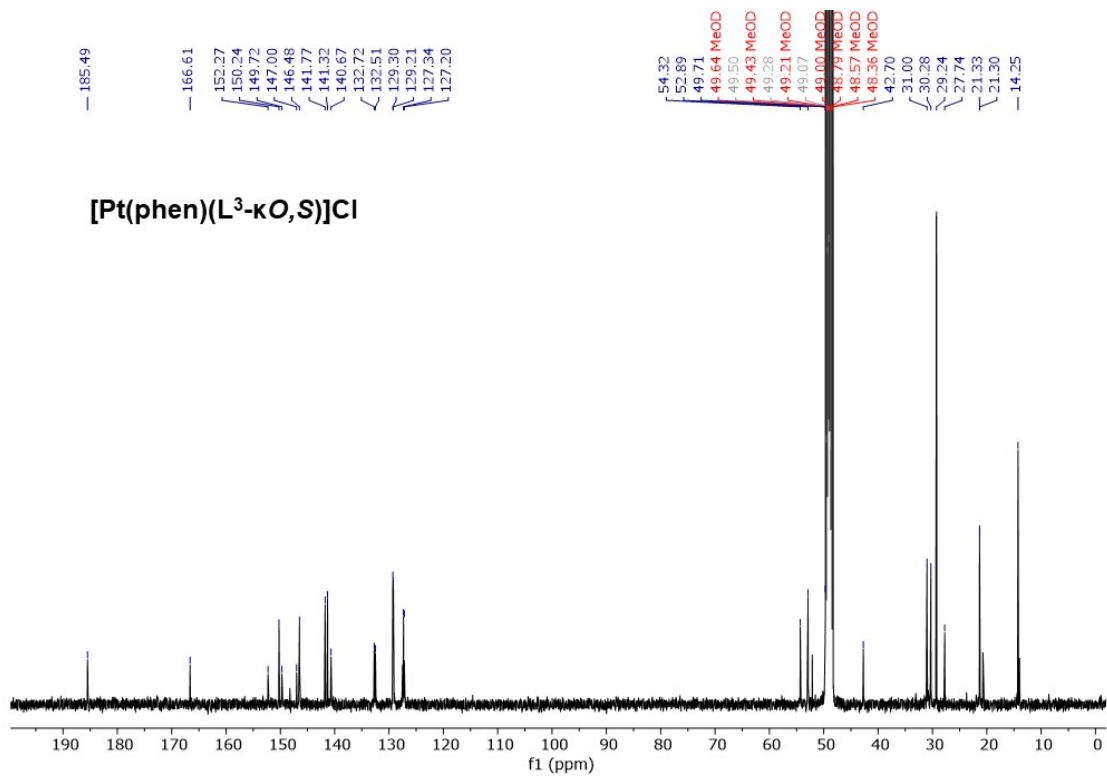


Fig S5: <sup>13</sup>C NMR spectrum of [Pt(phen)(L<sup>3</sup>-κO,S)]<sup>+</sup> complex in CD<sub>3</sub>OD at 300K.

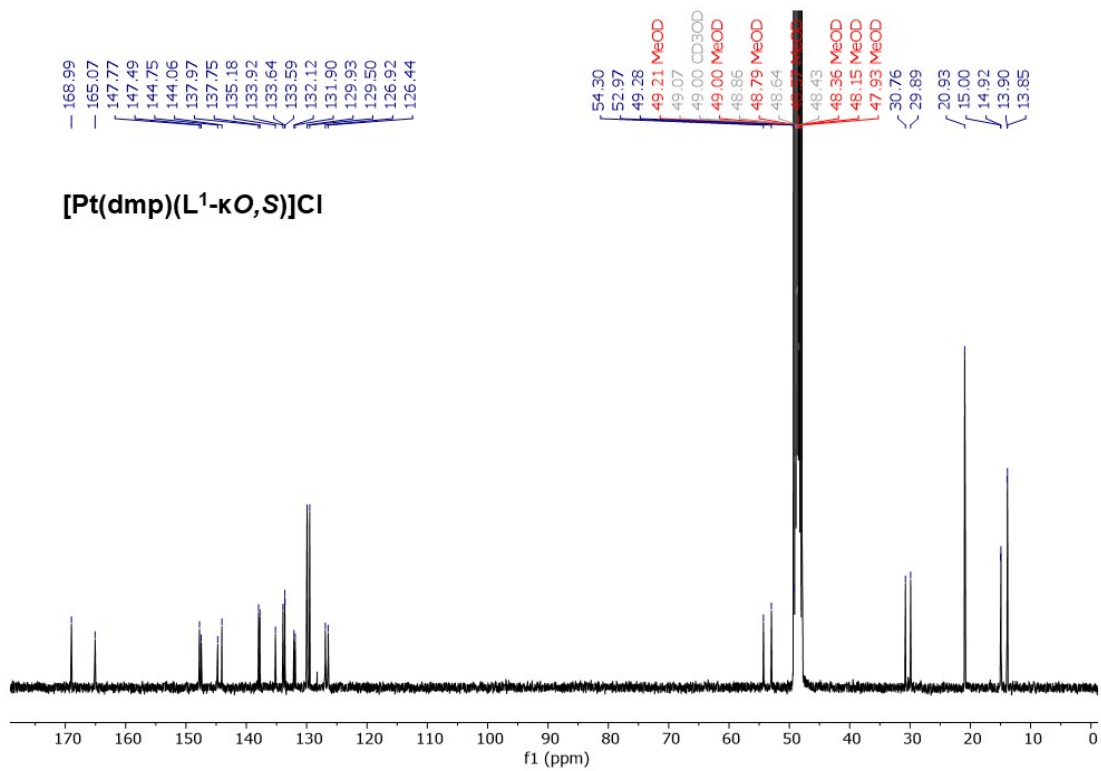


Fig S6:  $^{13}\text{C}$  NMR spectrum of  $[\text{Pt}(\text{dmp})(\text{L}^1\text{-}\kappa\text{O,S})]^+$  complex in  $\text{CD}_3\text{OD}$  at 300K.

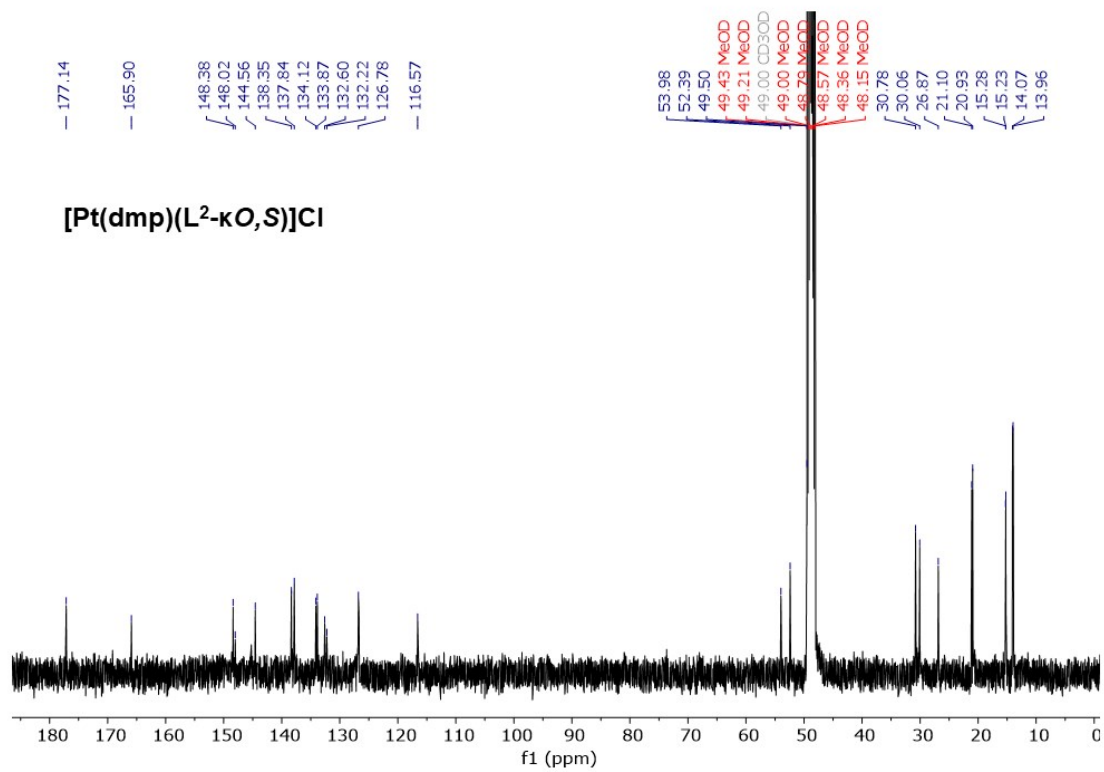


Fig S7: <sup>13</sup>C NMR spectrum of [Pt(dmp)(L<sup>2</sup>-κO,S)]<sup>+</sup> complex in CD<sub>3</sub>OD at 300K.

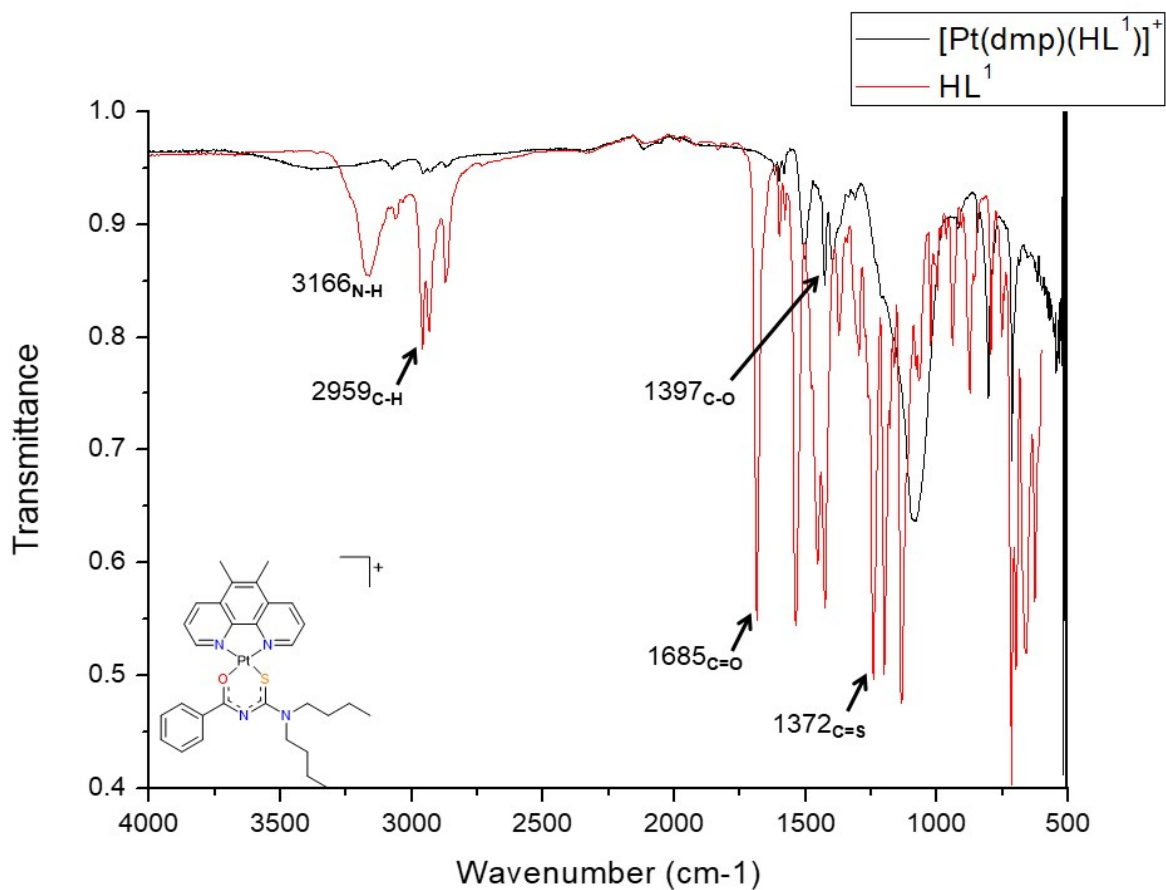


Figure S8: Infra-Red spectra of a *N,N*-dibutyl-*N'*-benzoylthiourea ( $\text{HL}^1$ ) free ligand and  $[\text{Pt}(\text{dmp})(\text{L}^1-\kappa\text{O}, \text{S})]^+$  complex showing the assigned functional groups present in their molecular structure. The spectra shows the absence of the N-H signal and a change in the bond order of C=O to C-O upon co-ordination.



### ***In vitro* anticancer cytotoxicity evaluation**

Table S1: Cell viability of H1975 cells (%) treated with *N,N*-di(butyl)-*N'*-benzoylthiourea (HL<sup>1</sup>), *N,N*-di(butyl)-*N'*-acetylthiourea (HL<sup>2</sup>) and *N,N*-di(butyl)-*N'*-pivaloylthiourea (HL<sup>3</sup>) at 50  $\mu$ M for 48 hours. A minimum of three independent repeats of the experiment were conducted (N=3).

<b>HL<sup>n</sup></b>	<b>HL<sup>1</sup></b>	<b>HL<sup>2</sup></b>	<b>HL<sup>3</sup></b>
Cell Viability (%)	70.5 $\pm$ 3.7	94.4 $\pm$ 3.3	89.60 $\pm$ 0.85