Conformational analysis and potential anticancer activity of [Pt(phen)(L^1-κ*S*)$_2$] studied by single crystal X-ray Diffraction and Variable Temperature ^{1}H and ^{195}Pt NMR Spectroscopy. †

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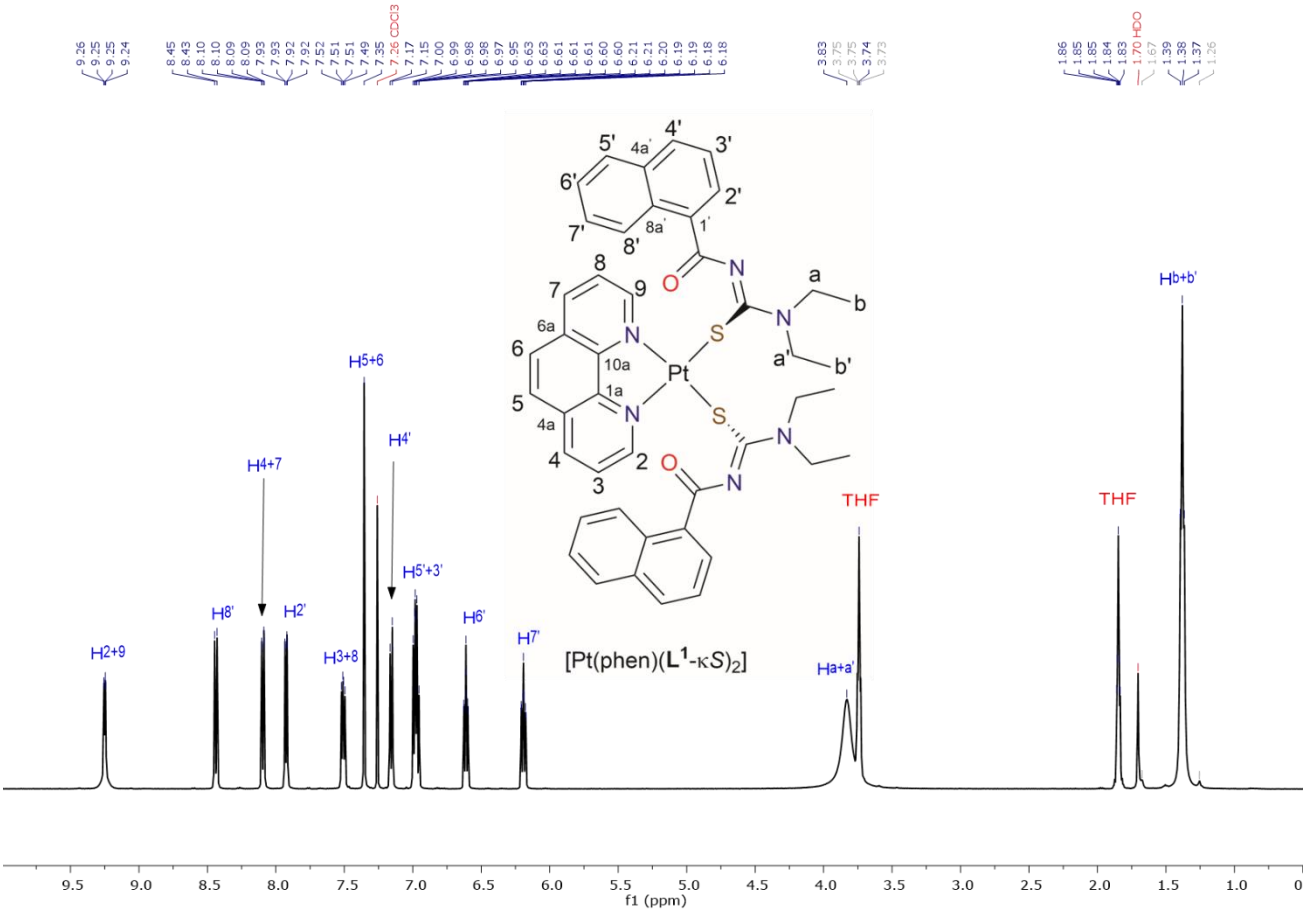

Figure S1: Full proton assignments in the ^{1}H NMR spectrum of [Pt(phen)(**L**^{1}-κ*S*)$_2$] in $CDCl_3$

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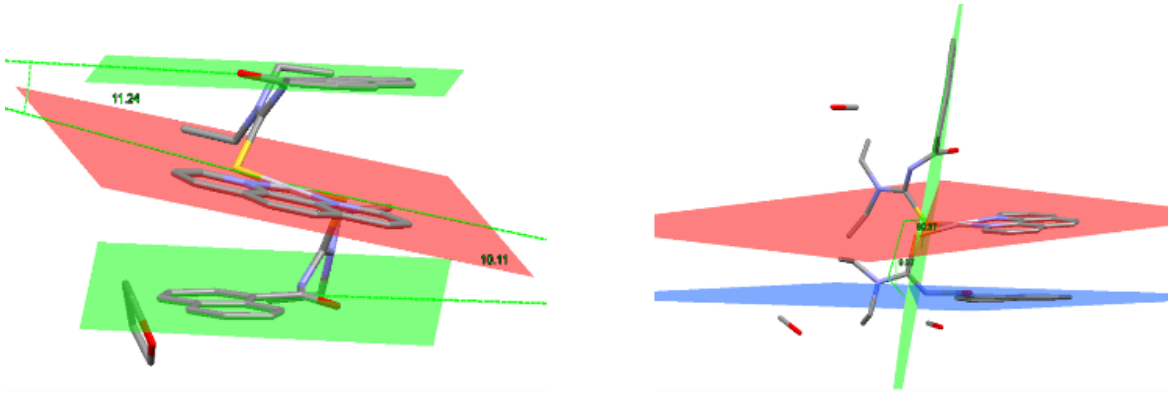

Figure S2: Orientation of naphthyl rings of the acylthioureato ligands with respect to the phenanthroline ring in the two solvates (a) Form I and (b) Form II respectively.

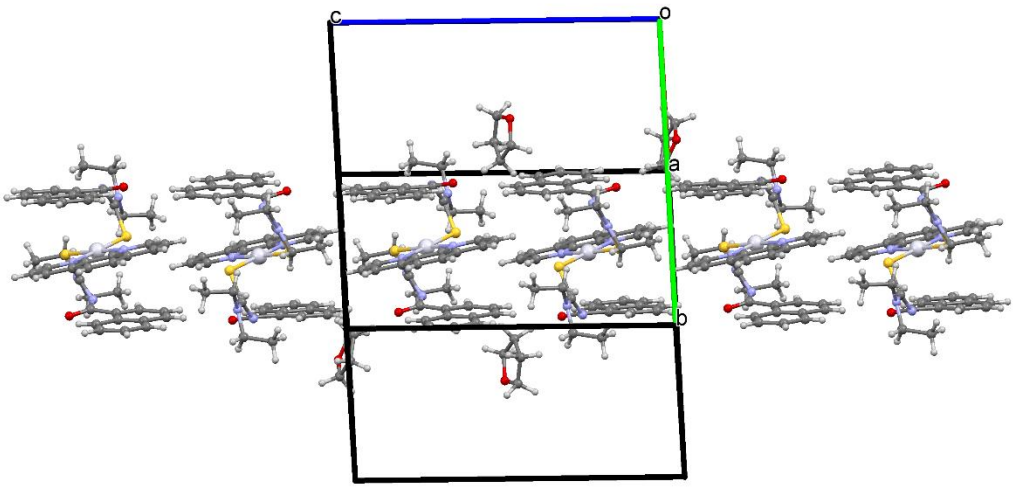

Figure S3(a). Projections of crystal structure showing one-dimensional packing for the Form I solvate.

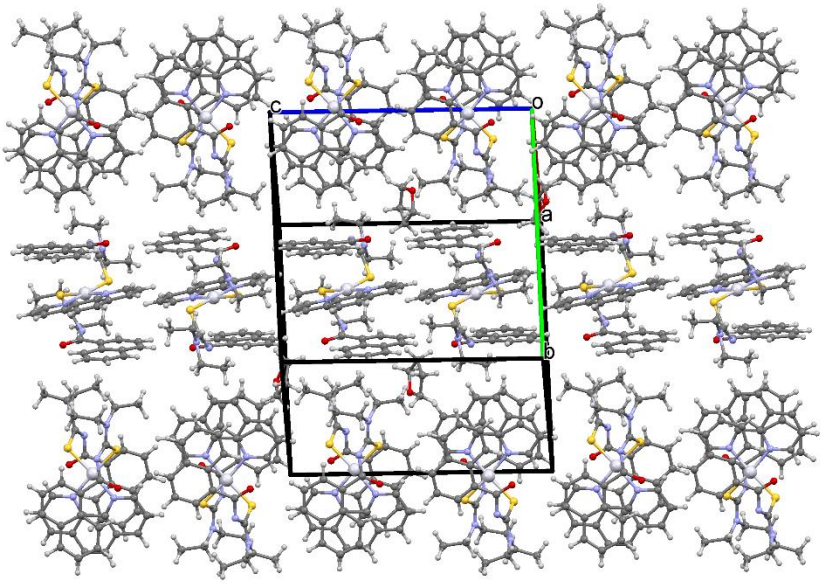

Figure S3(b). Projections of crystal structure showing two-dimensional packing for the Form I solvate (with one-dimensional ribbons arranging alternately perpendicular to each other).

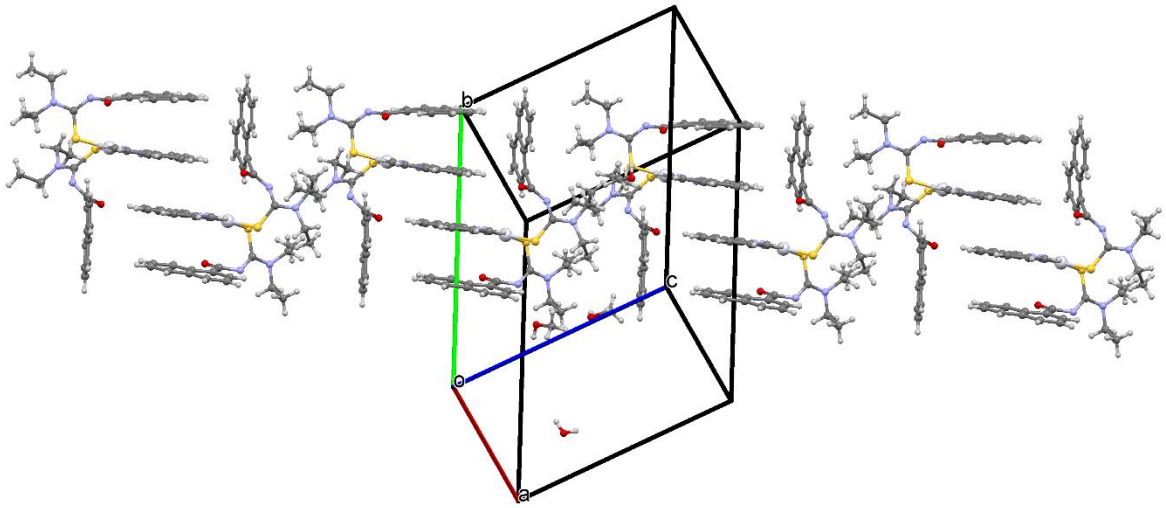

Figure S4(a). Projections of crystal structure showing one-dimensional packing for the Form II solvate.

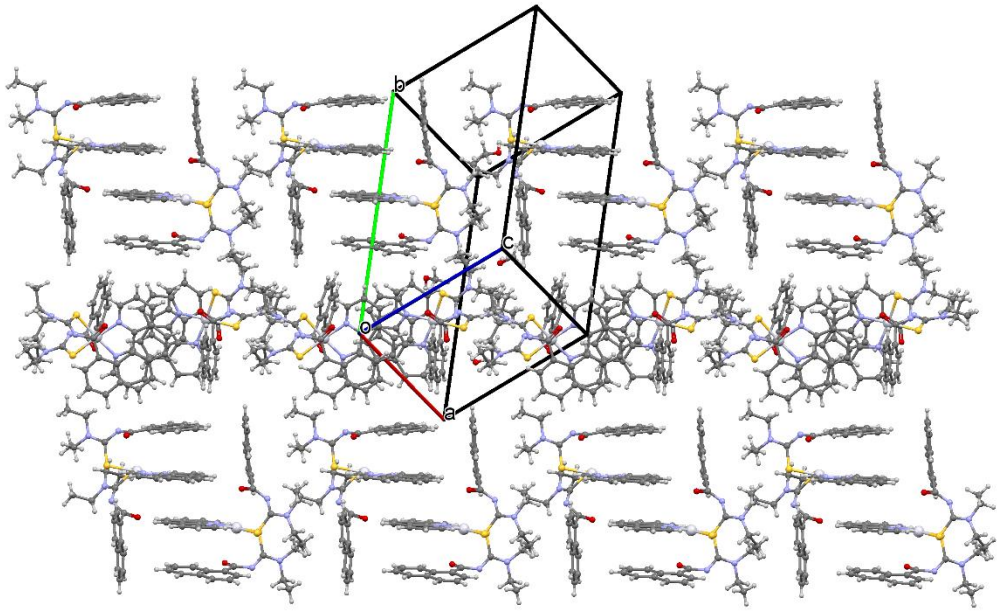

Figure S4(b). Projections of crystal structure showing two-dimensional packing for the Form II solvate (with one-dimensional ribbons arranging alternately perpendicular to each other).

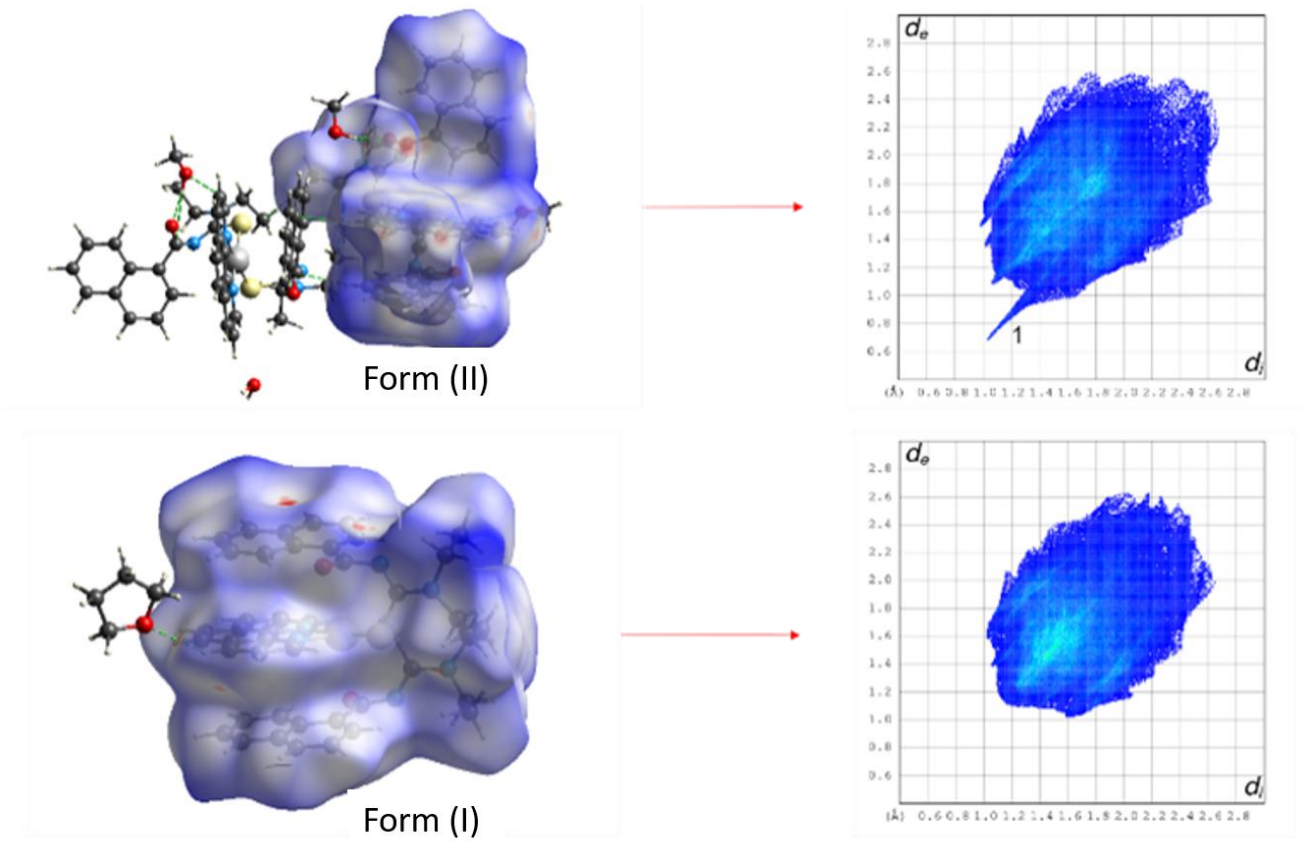

Figure S5. Hirshfeld surfaces and 2D fingerprint plots for the two solvates Form I and Form II.

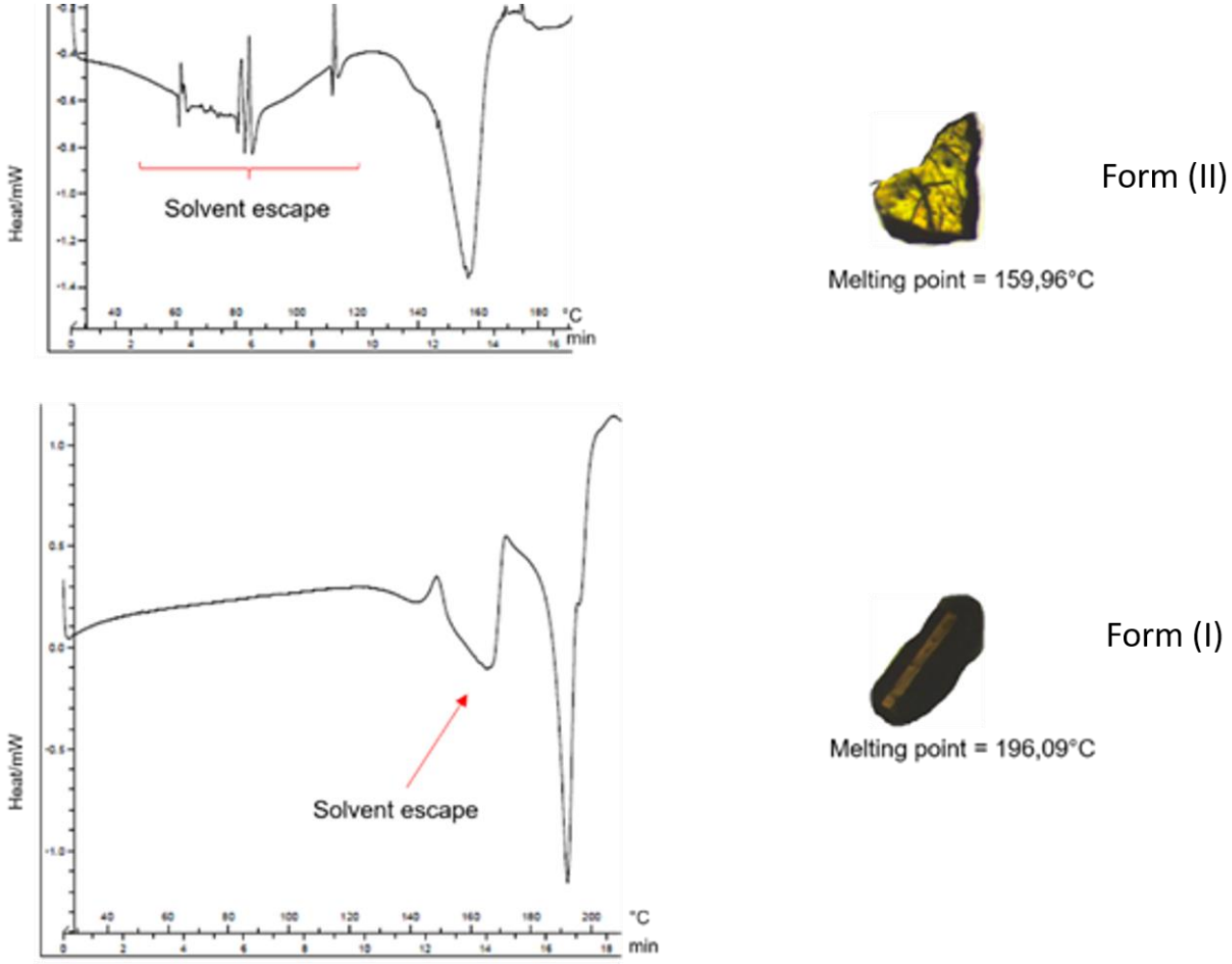

Figure S6. Differential scanning calorimetry (DSC) plots indicating the melting points for Form I and Form II

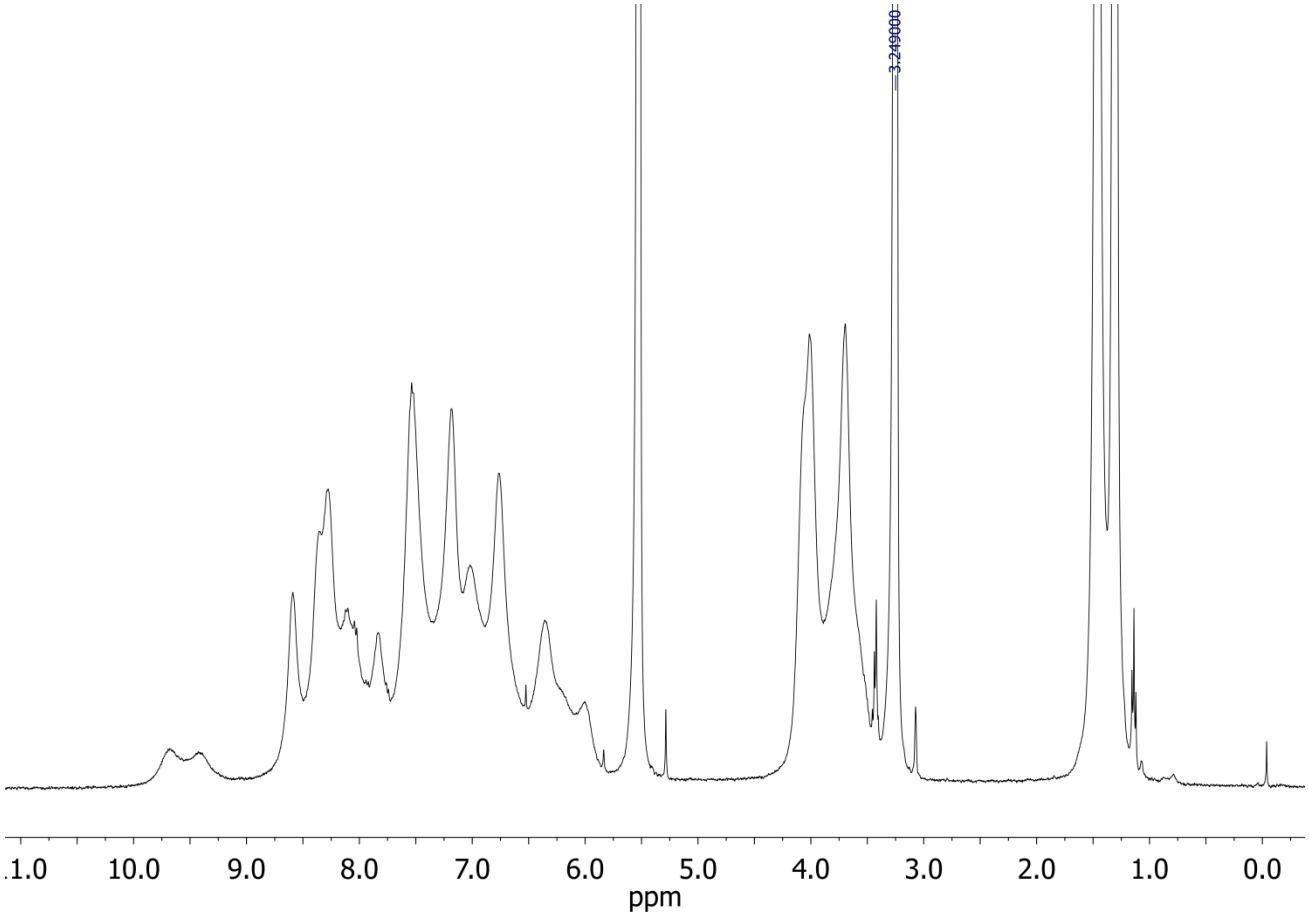

Figure S7 ^{1}H NMR spectrum of [Pt(phen)(**L**^{1}-κ*S*)$_2$] in CD_3OD recorded at -50 °C

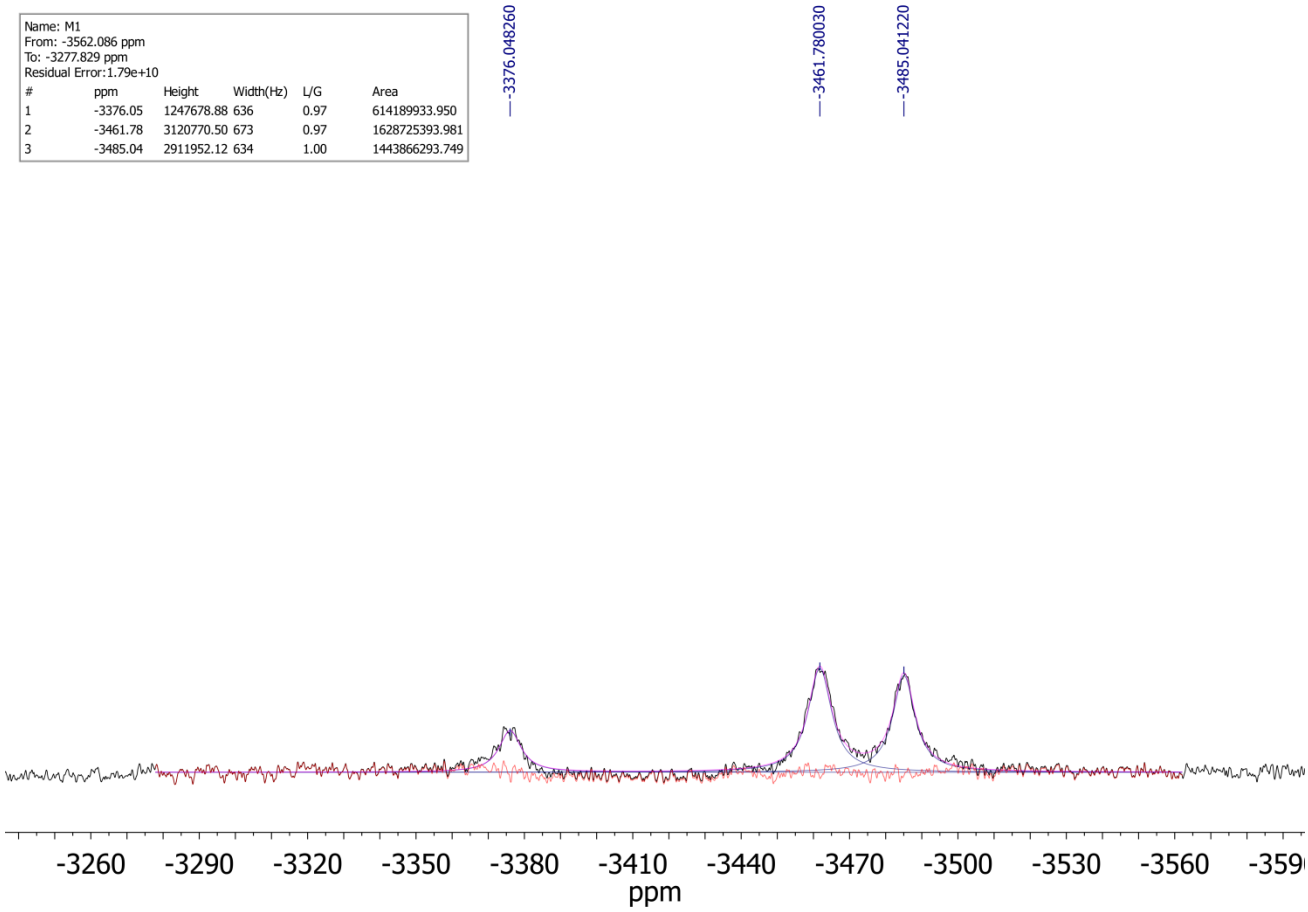

Figure S8: ^{195}Pt NMR spectrum of [Pt(phen)(**L**$^{\mathbf{1}}$-κ*S*)$_2$] in CD_3OD recorded at -50 °C with peak fit areas

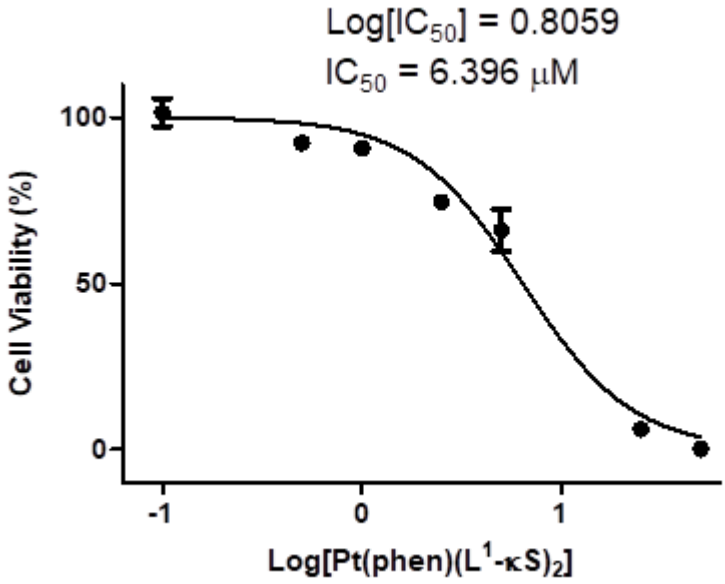

Figure S9**.** A representative dose–response curve of Log[Pt(phen)(**L**^{1}-κ*S*)$_2$] versus percentage cell viability of A549 cancer cell line treated for 46 hours.