

DNA cleavage and antitumor activity of platinum(II) and copper(II) compounds derived from 4-methyl-2-*N*-(2-pyridylmethyl)aminophenol: spectroscopic, electrochemical and biological investigation

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Table S1. Selected bond lengths [\AA] and bond angles [$^\circ$] for the compound PtL-Cl

Bond lengths	
Pt(1) – N(1)	2.009 (4)
Pt(1) – N(2)	1.946 (4)
Pt(1) – Cl(1)	2.3017 (12)
Pt(1) – O(1)	2.016 (3)
Bond angles	
Cl(1) – Pt(1) – O(1)	94.88 (9)
Cl(1) – Pt(1) – N(1)	99.14 (11)
Cl(1) – Pt(1) – N(2)	177.04 (10)
N(1) – Pt(1) – N(2)	81.74 (15)
O(1) – Pt(1) – N(2)	84.23 (14)
N(1) – Pt(1) – O(1)	165.97(14)

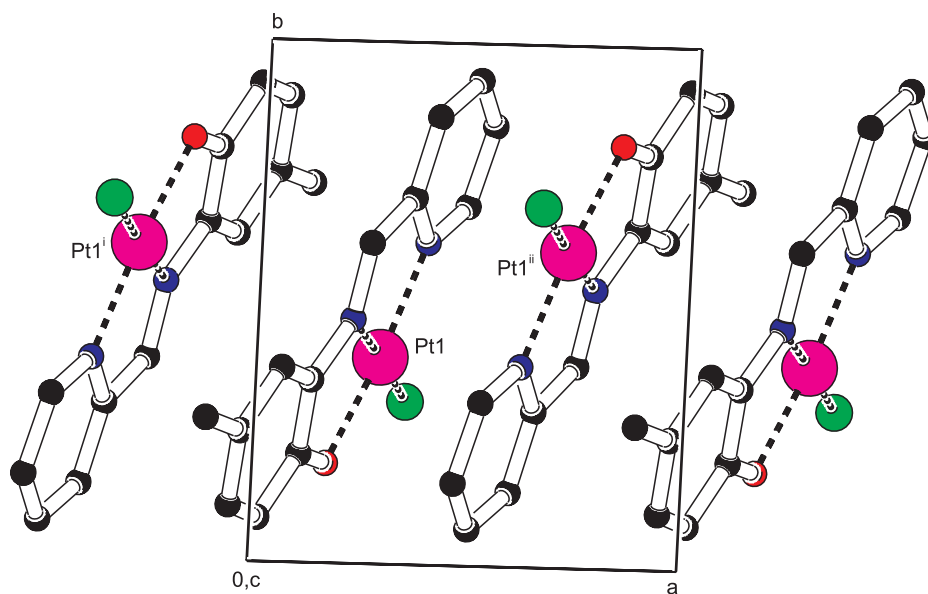


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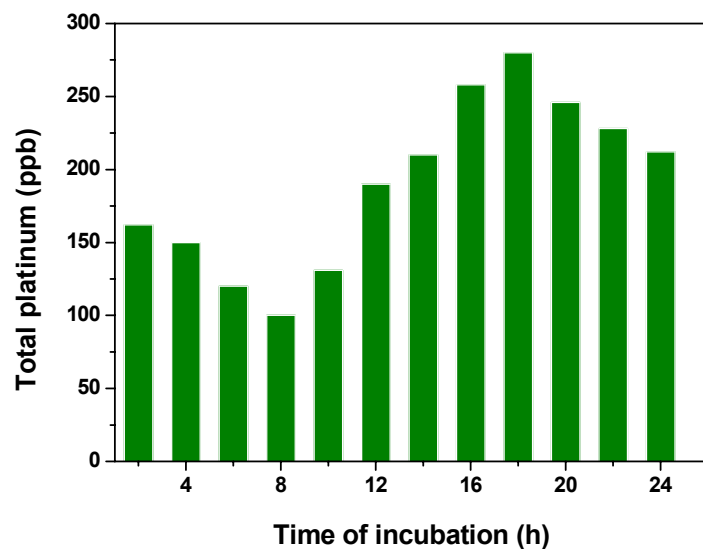


Fig. S2. Time-dependent accumulation of Pt (from PtL-Cl) in the A2780 cell line.

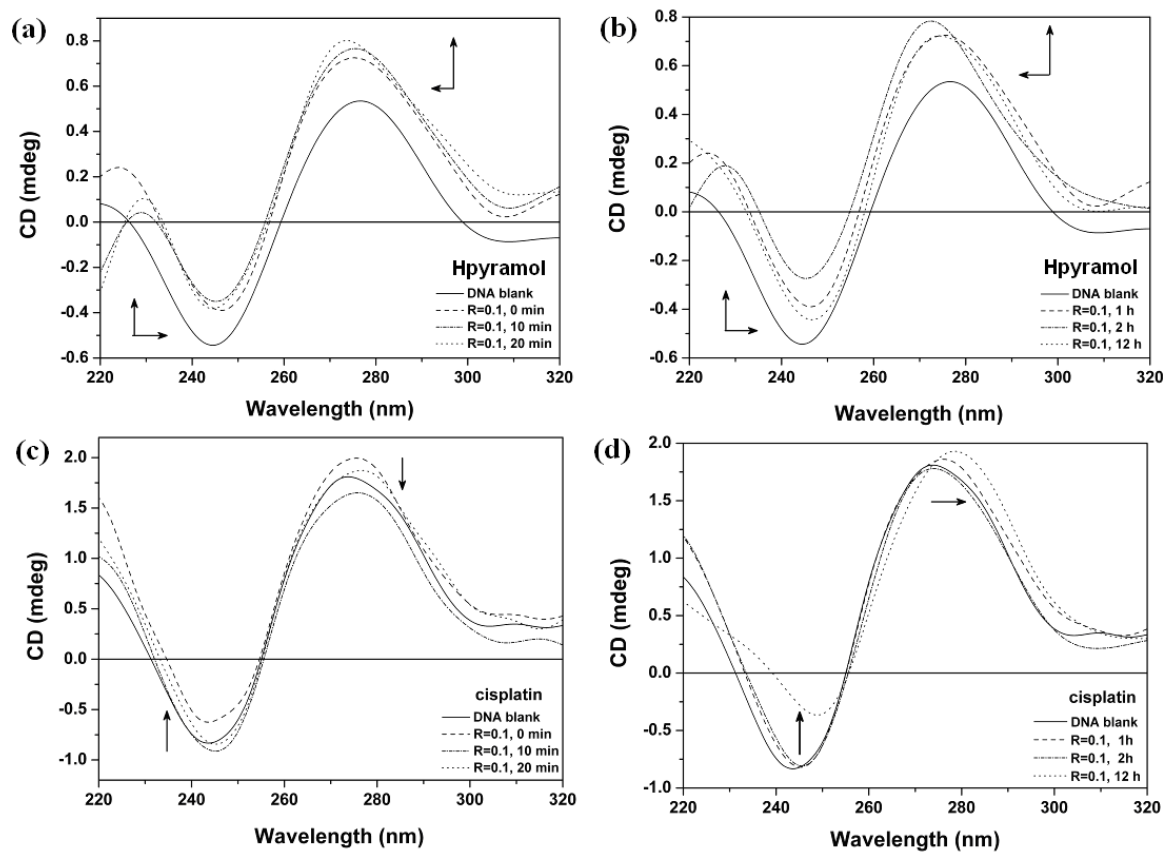


Fig. S3. Time-dependent conformational changes of right-handed DNA upon addition of Hpyramol and cisplatin in phosphate buffer (10 mM) at pH = 7.2 at 37 °C with R=0.1.

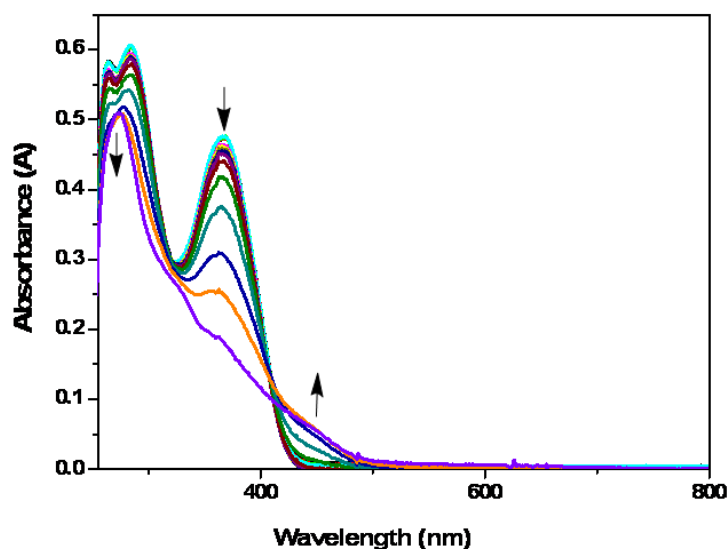


Fig. S4. UV-Vis spectral changes accompanying the oxidation of Hpyrimol ligand at the electrode potential O₂ (Fig. 8b) to an assumed phenoxyl radical species in DMF at room temperature, using an OTTLE cell.

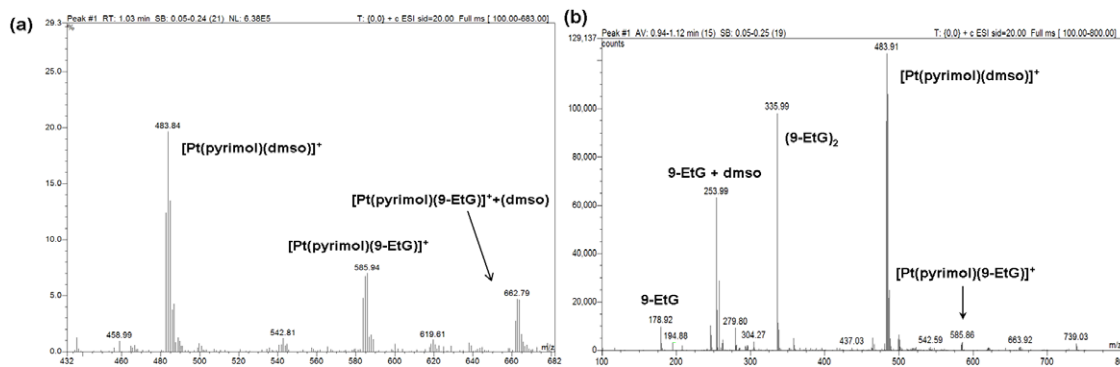


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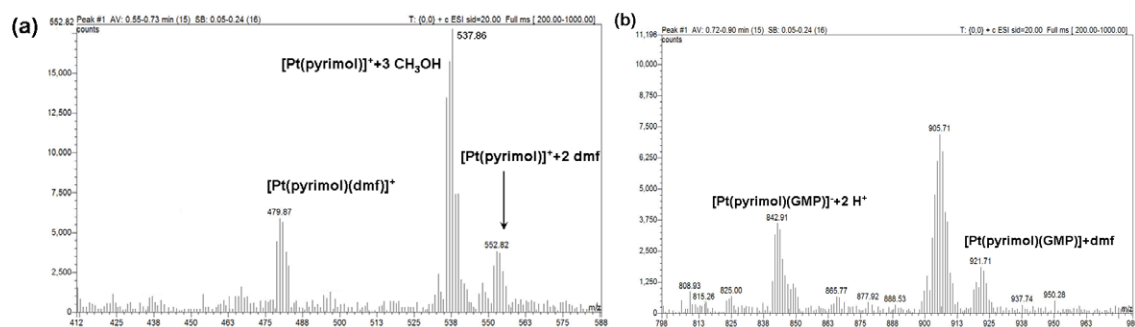


Fig. S6. ESI-MS spectra of platinum moieties detected during the reaction in presence of PtL-Cl with 5'-GMP in DMSO-H₂O with (a) mainly solvated products and (b) some GMP-adducts after selected part zoomed out.

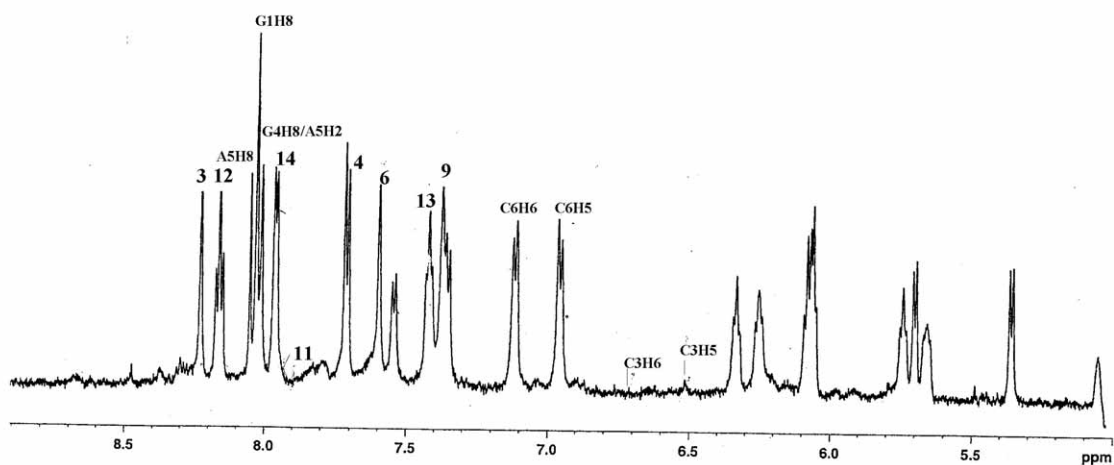


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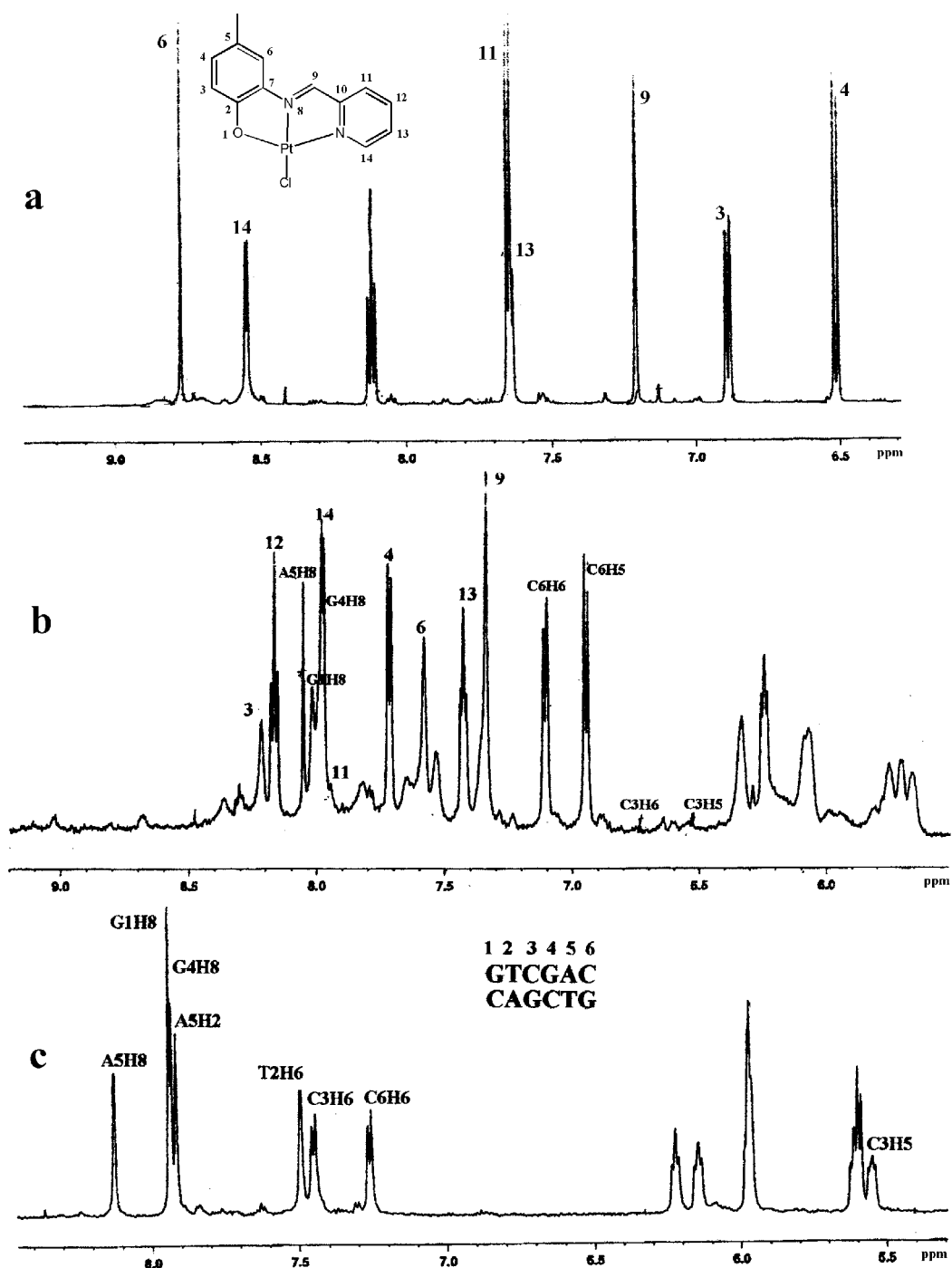


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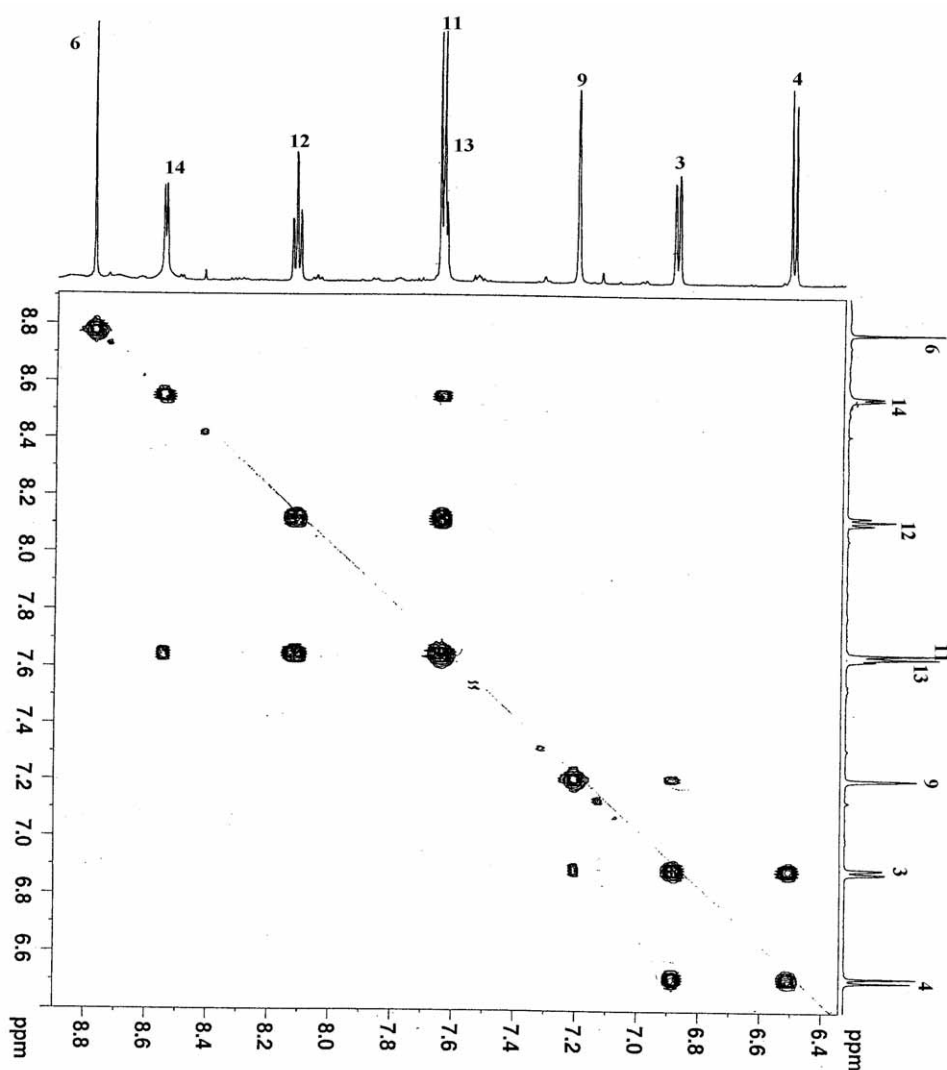


Fig. S9. ^1H NMR, 2-D DQF-COSY for the pure compound PtL-Cl in $\text{DMSO-}d_6$ at 27°C . The assignments were done according to through-bond interactions.

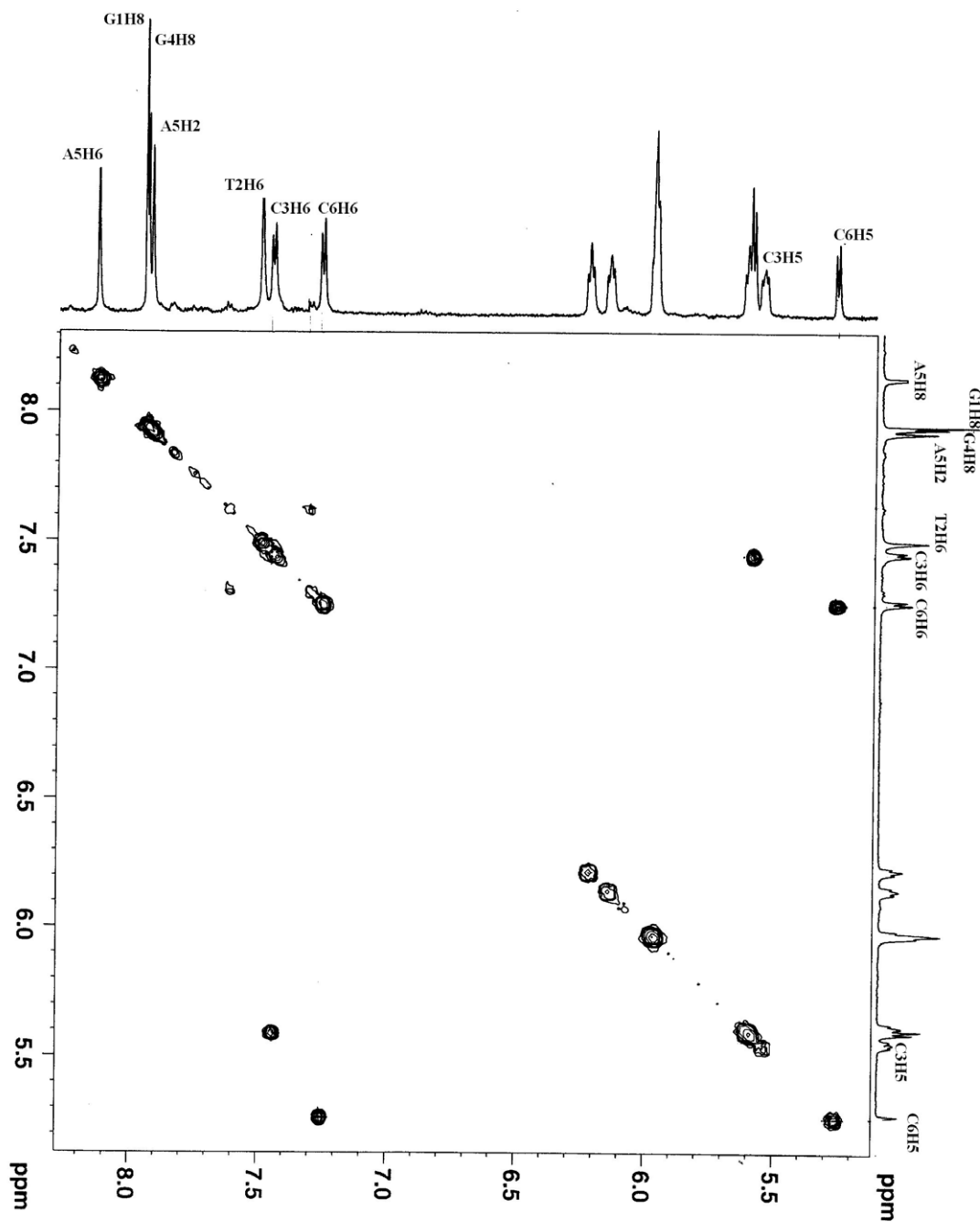


Fig. S10. ¹H NMR, 2-D DQF-COSY for the pure d(GTCGAC)₂ in 90% H₂O and 10% D₂O at 27 °C. The assignments were done according to through-bond interactions.

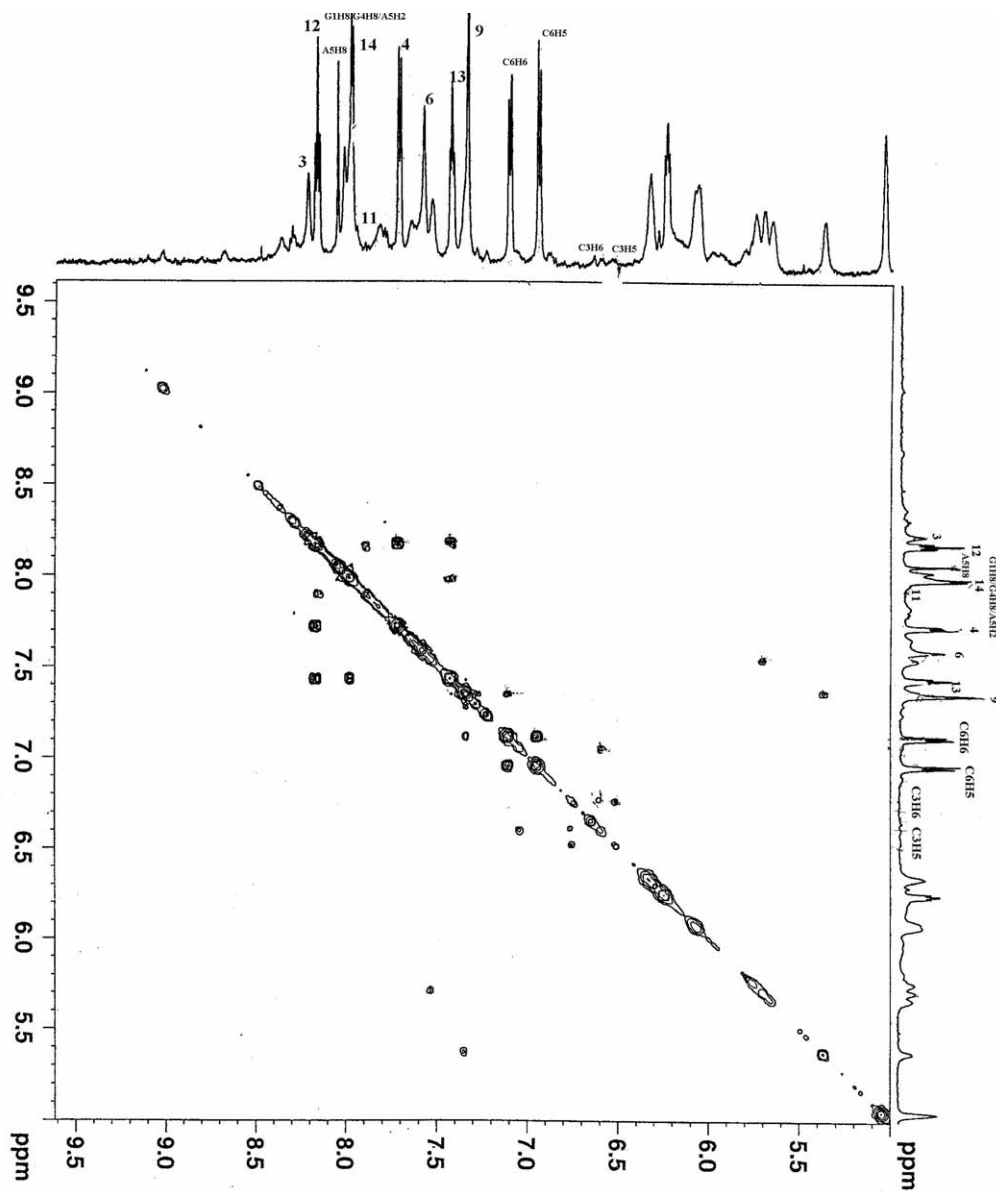


Fig. S11. ¹H NMR, 2-D COSY spectrum of PtL-Cl (in DMSO-*d*₆ + D₂O) at 27 °C in the presence of d(GTCGAC)₂ in H₂O at 1:1 ratio (PtL-Cl : oligonucleotide).

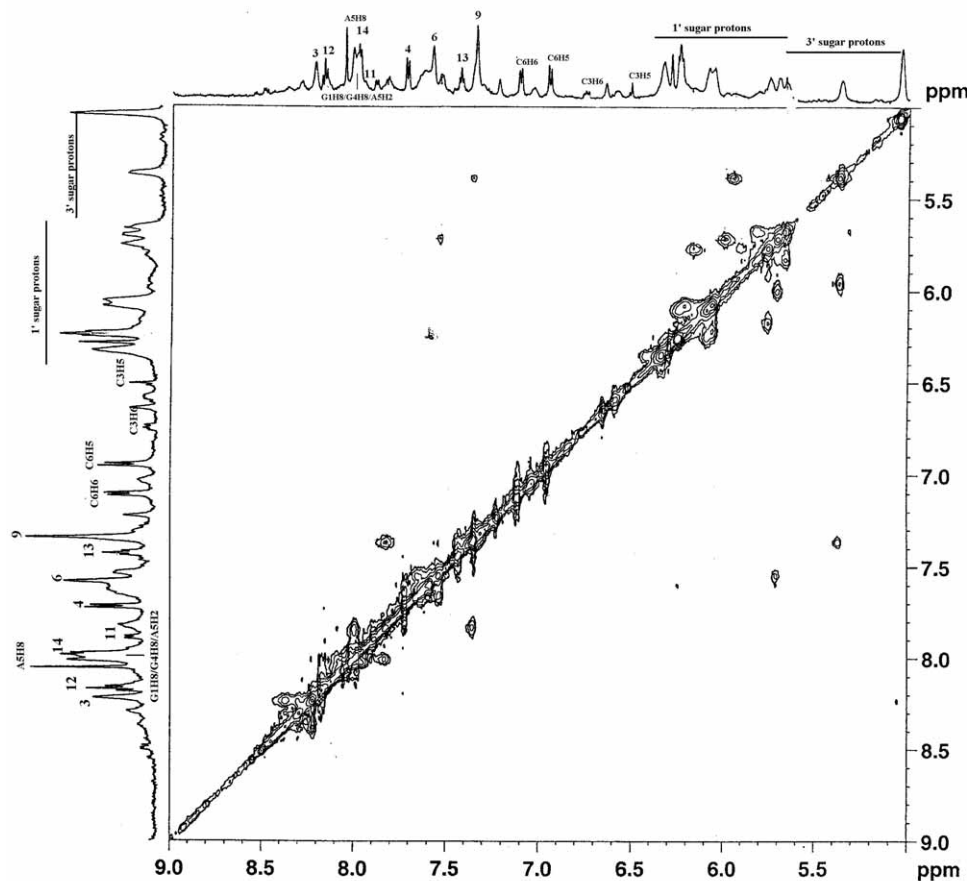


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