

Supplementary Information

Experimental and theoretical investigation of cyclometallated platinum(II) complex containing adamantanemethylcyanamide and 1,4-naphthoquinone derivative as ligands: synthesis, characterization, interacting with guanine and cytotoxic activity

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Figure S5. ¹H NMR spectrum of ligand 2-[amino(2-phenylpyridine)]-1,4-naphthoquinone (1,4-NQ) (DMSO-*d*₆).

Figure S6. ¹H NMR spectrum of complex **1**, cis-Pt(1,4-NQ)(1-ADpcyd)(H₂O) (DMSO-*d*₆).

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Figure S8. ¹³C NMR spectrum of ligand 2-[amino(2-phenylpyridine)]-1,4-naphthoquinone (1,4-NQ) (DMSO-*d*₆).

Figure S9. ¹³C NMR spectrum of complex **1**, cis-Pt(1,4-NQ)(1-ADpcyd)(H₂O) (DMSO-*d*₆).

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Figure S11. ¹H NMR spectrum of complex **2**, cis-Pt(1,4-NQ)(1-ADpcyd)(G) (DMSO-*d*₆).

Figure S12. ¹³C NMR spectrum of complex **2**, cis-Pt(1,4-NQ)(1-ADpcyd)(G) (DMSO-*d*₆).

Figure S13. ¹⁹⁵Pt NMR spectrum of complex **2**, cis-Pt(1,4-NQ)(1-ADpcyd)(G) (DMF-*d*₇).

Figure S14. HPLC of the complex **1** in freshly prepared PBS buffer/0.5% DMSO solution recorded during 72 h of incubation time at 37 °C.

Figure S15. Graphs used for IC₅₀ value determinations. Dose-response data points represent the mean value of 3 trials. GraphPad Prism 6 software was used to fit the data.

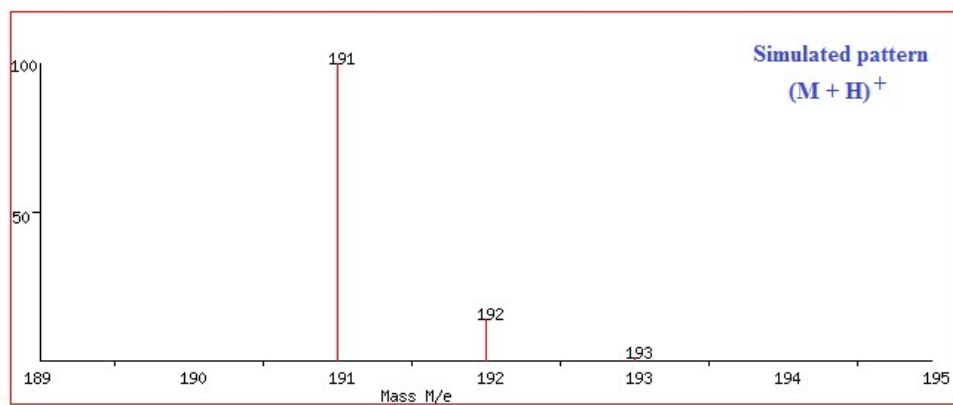
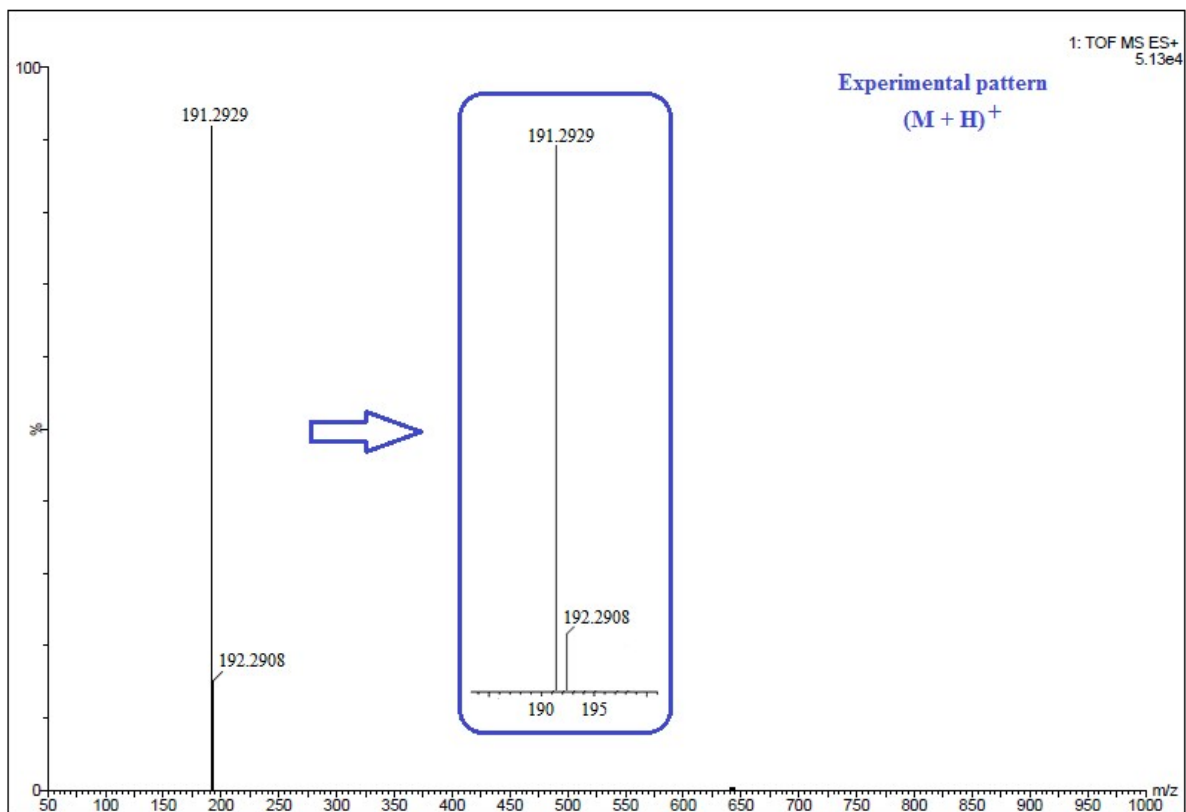


Figure S1. TOF MS spectrum of ligand 1-Adamantanemethylcyanamide (1-ADpcydh).

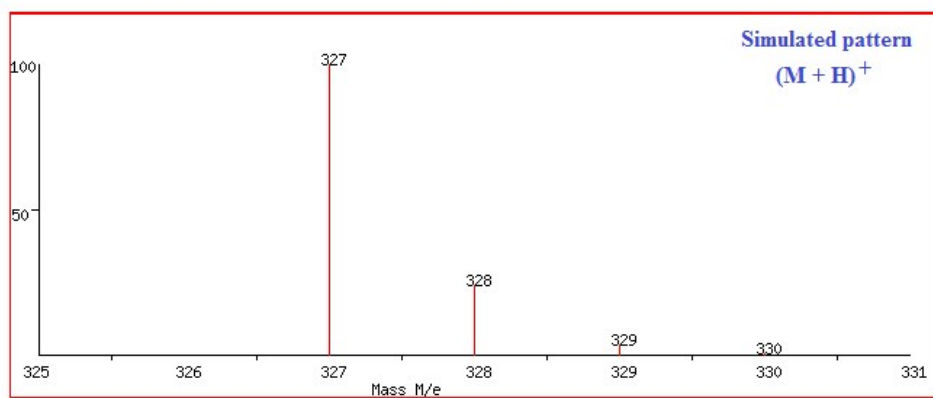
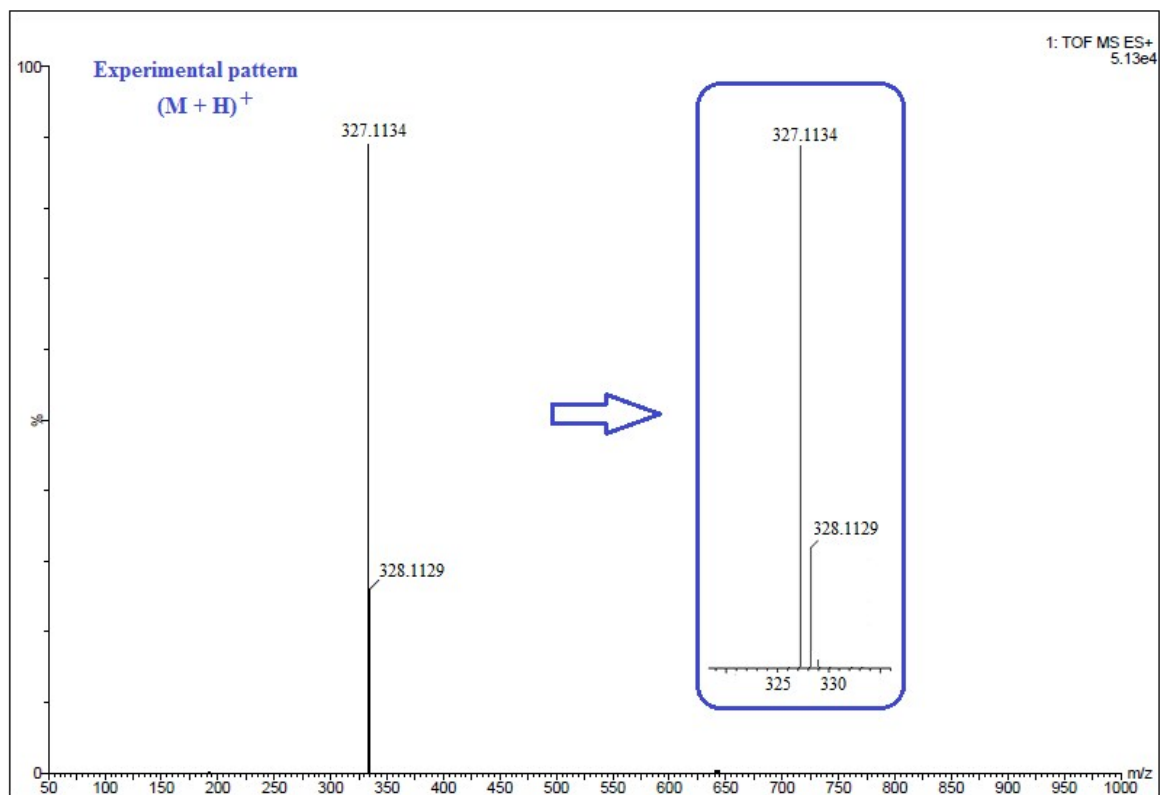


Figure S2. TOF MS spectrum of ligand 2-[amino(2-phenylpyridine)]-1,4-naphthoquinone (1,4-NQ).

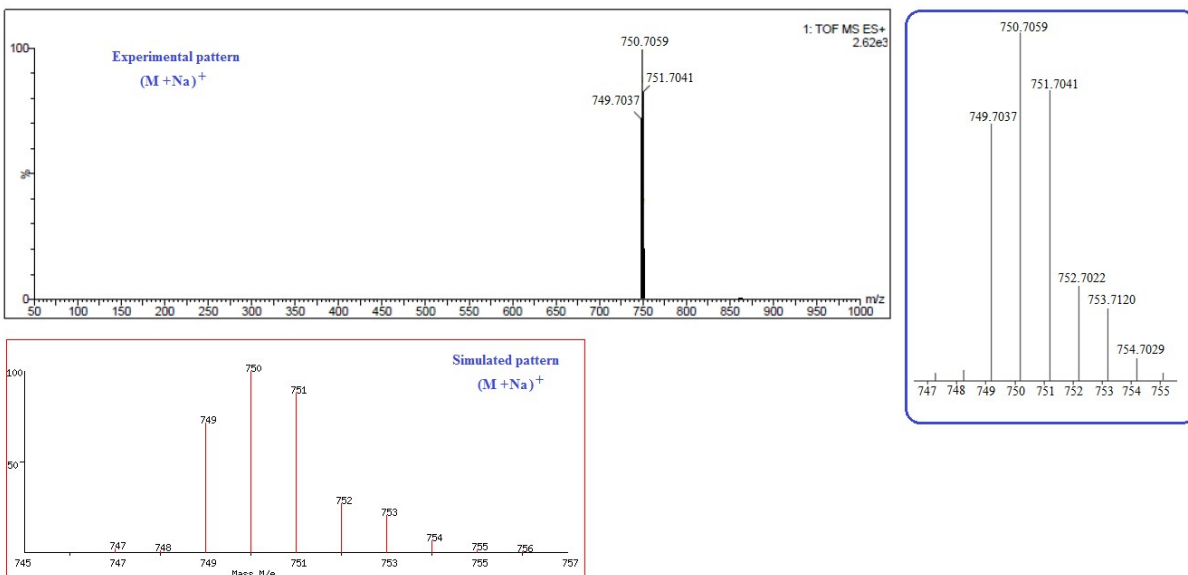


Figure S3. TOF MS spectrum of complex **1**, cis-Pt(1,4-NQ)(1-ADpcyd)(H₂O).

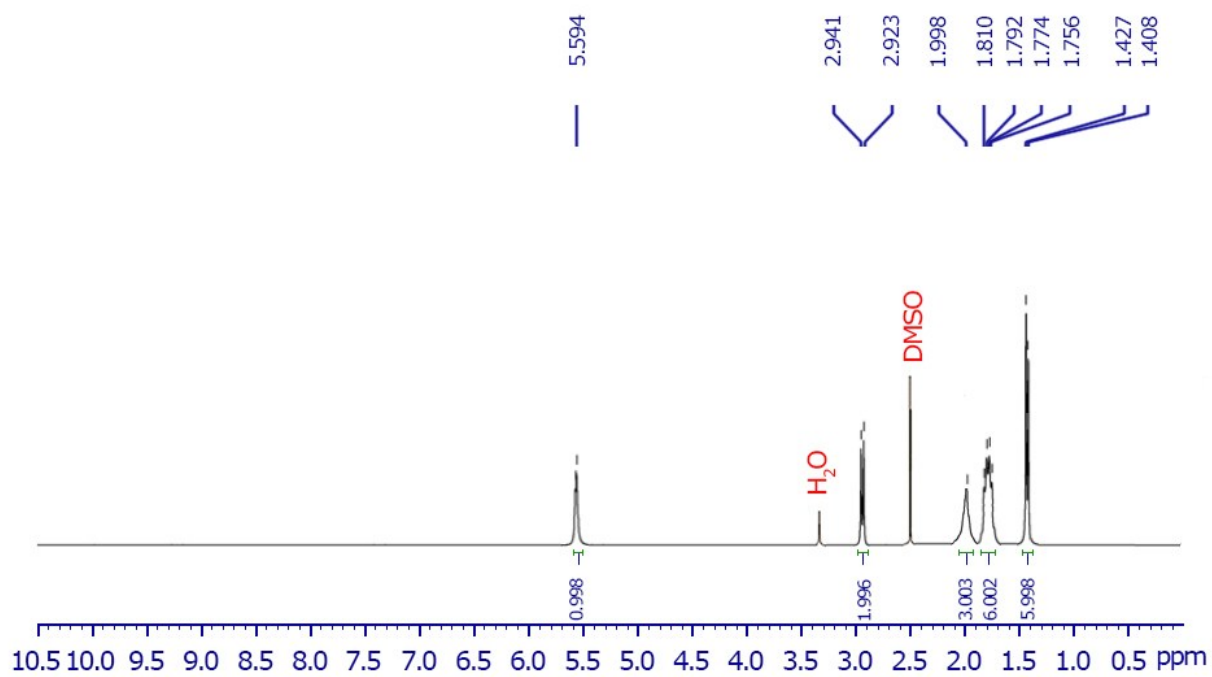


Figure S4. ¹H NMR spectrum of ligand 1-Adamantanemethylcyanamide (1-ADpcydh) (DMSO-*d*₆).

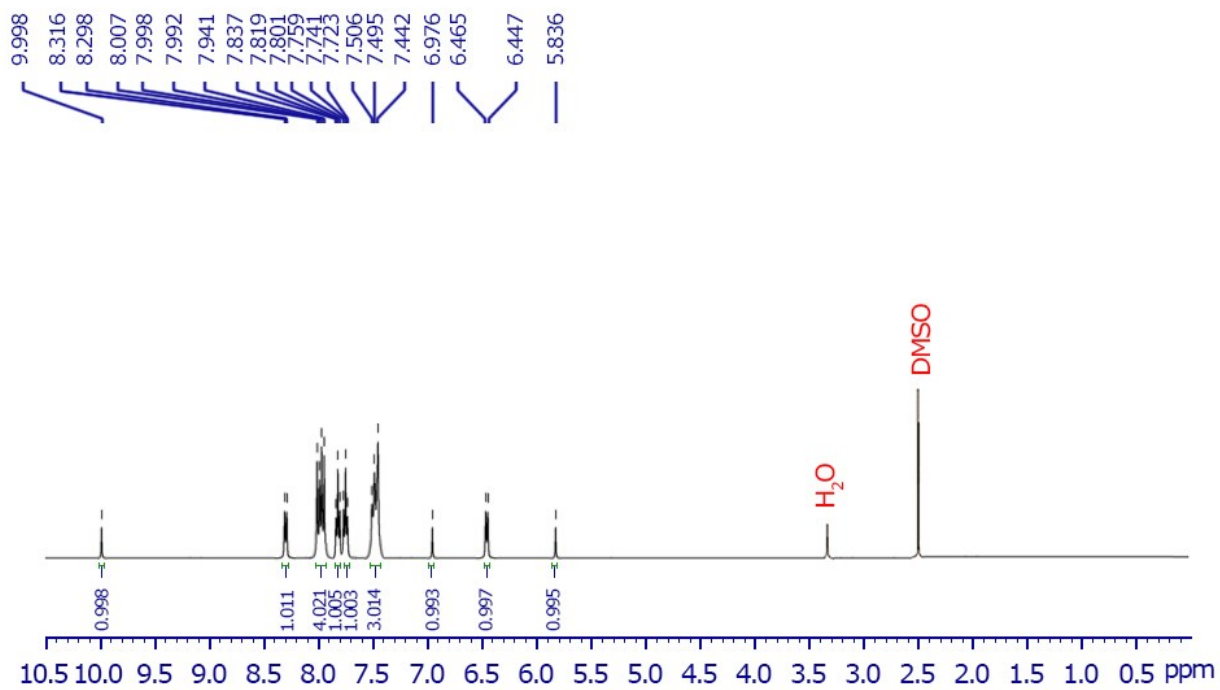


Figure S5. ¹H NMR spectrum of ligand 2-[amino(2-phenylpyridine)]-1,4-naphthoquinone (1,4-NQ) (DMSO-*d*₆).

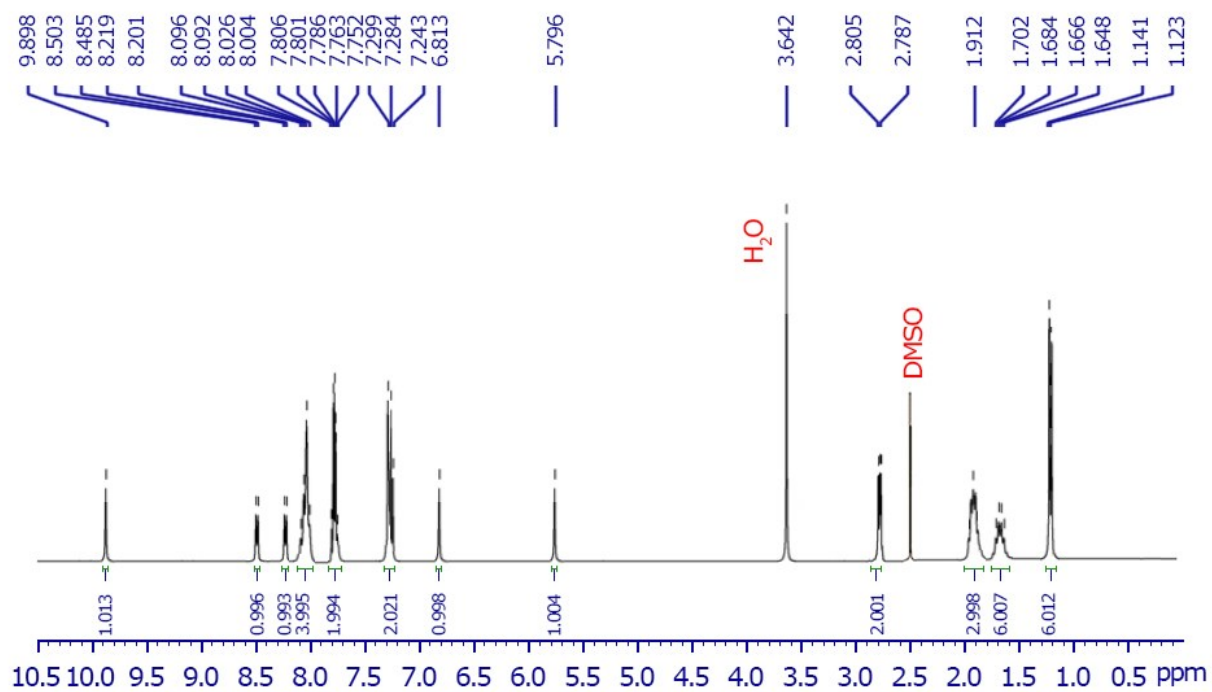


Figure S6. ¹H NMR spectrum of complex **1**, cis-Pt(1,4-NQ)(1-ADpcyd)(H₂O) (DMSO-*d*₆).

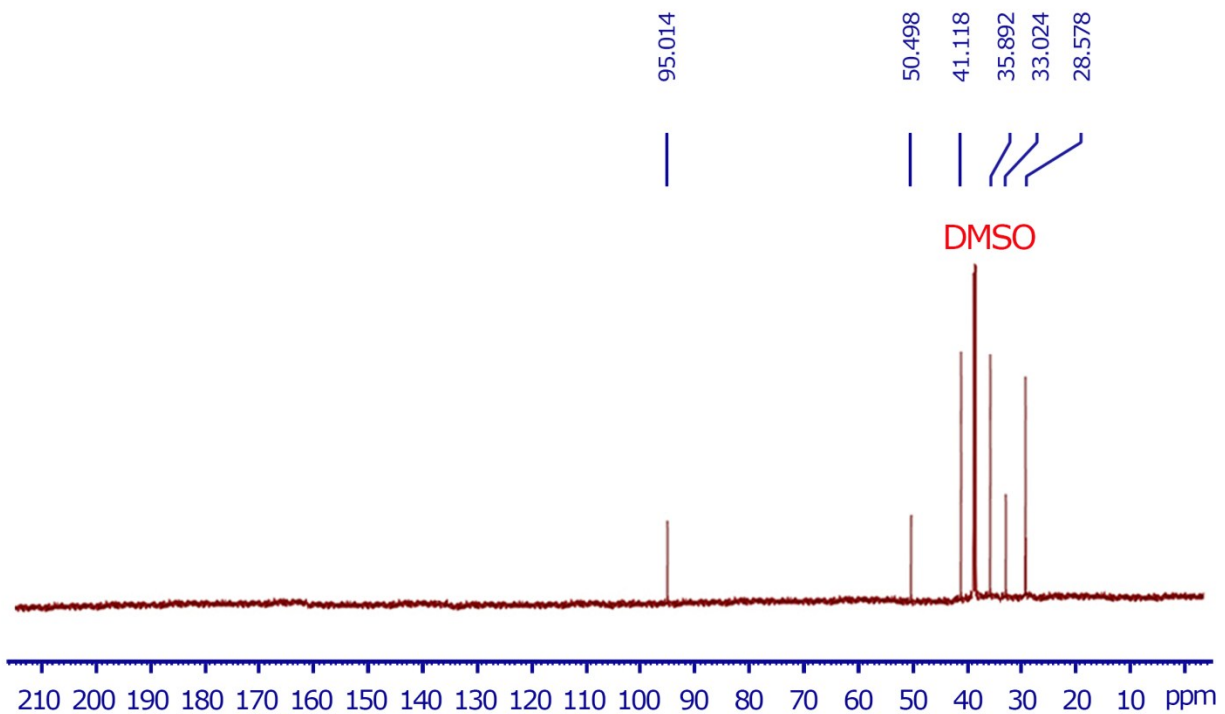


Figure S7. ^{13}C NMR spectrum of ligand 1-Adamantanemethylecyanamide (1-ADpcydH) ($\text{DMSO-}d_6$).

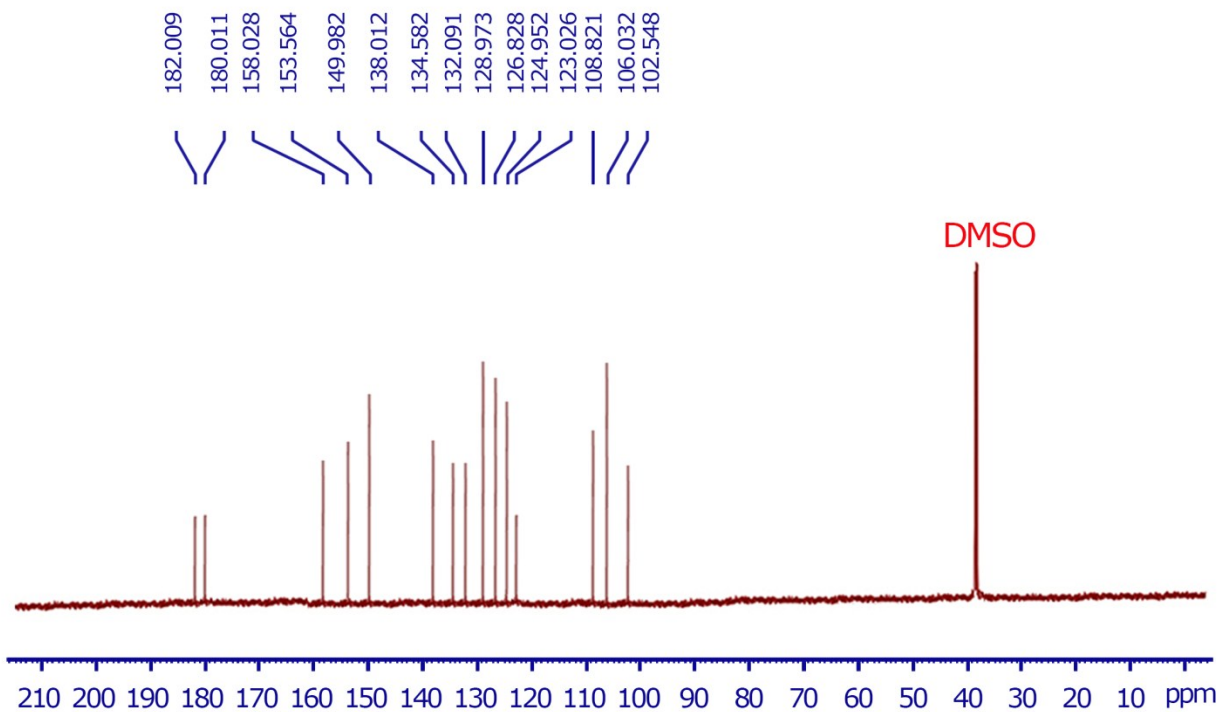


Figure S8. ^{13}C NMR spectrum of ligand 2-[amino(2-phenylpyridine)]-1,4-naphthoquinone (1,4-NQ) ($\text{DMSO-}d_6$).

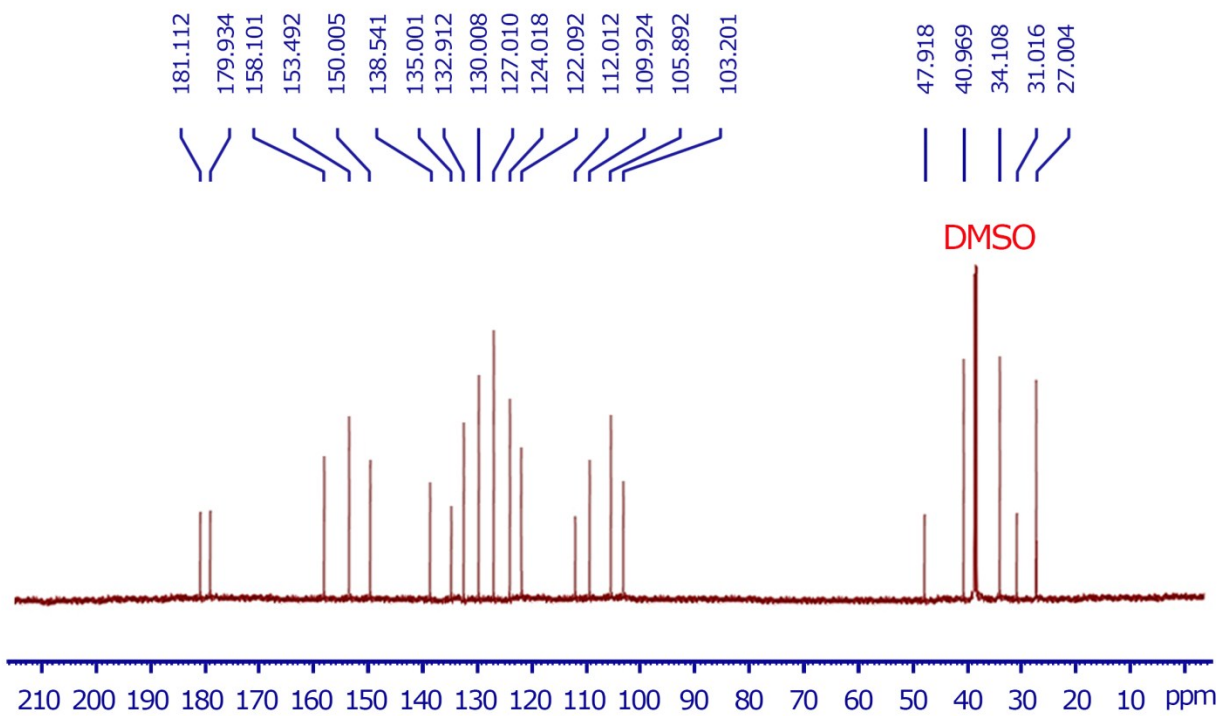


Figure S9. ^{13}C NMR spectrum of complex **1**, $\text{cis-Pt}(1,4\text{-NQ})(1\text{-ADpcyd})(\text{H}_2\text{O})$ ($\text{DMSO-}d_6$).

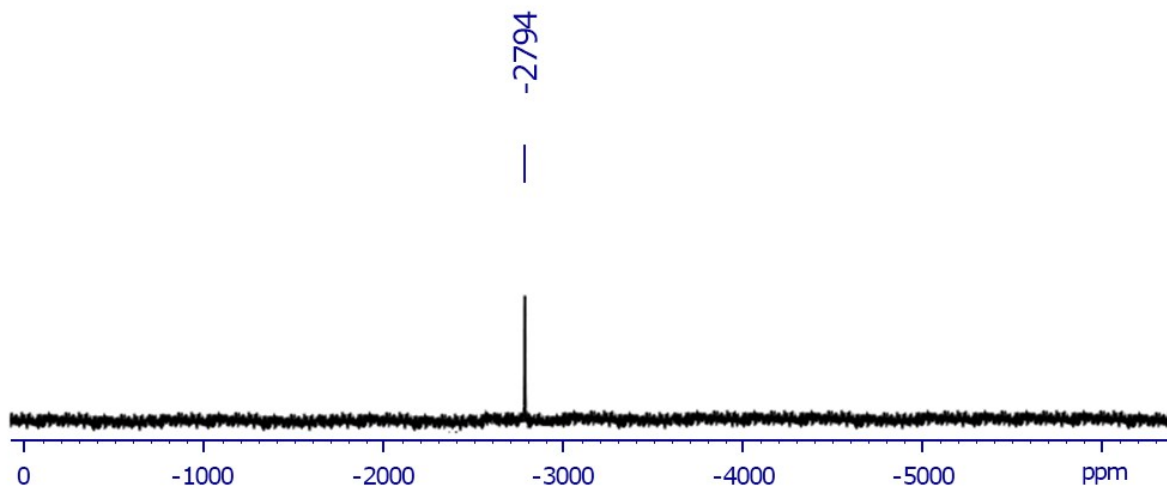


Figure S10. ^{195}Pt NMR spectrum of complex **1**, $\text{cis-Pt}(1,4\text{-NQ})(1\text{-ADpcyd})(\text{H}_2\text{O})$ ($\text{DMF-}d_7$).

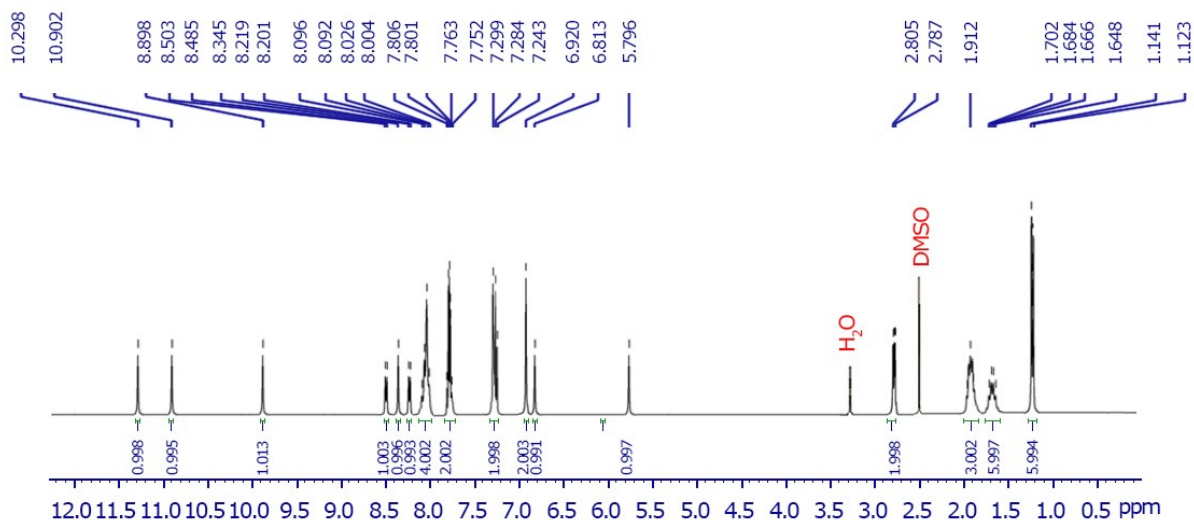


Figure S11. ^1H NMR spectrum of complex **2**, $\text{cis-Pt}(1,4\text{-NQ})(1\text{-ADpcyd})(\text{G})$ ($\text{DMSO-}d_6$).

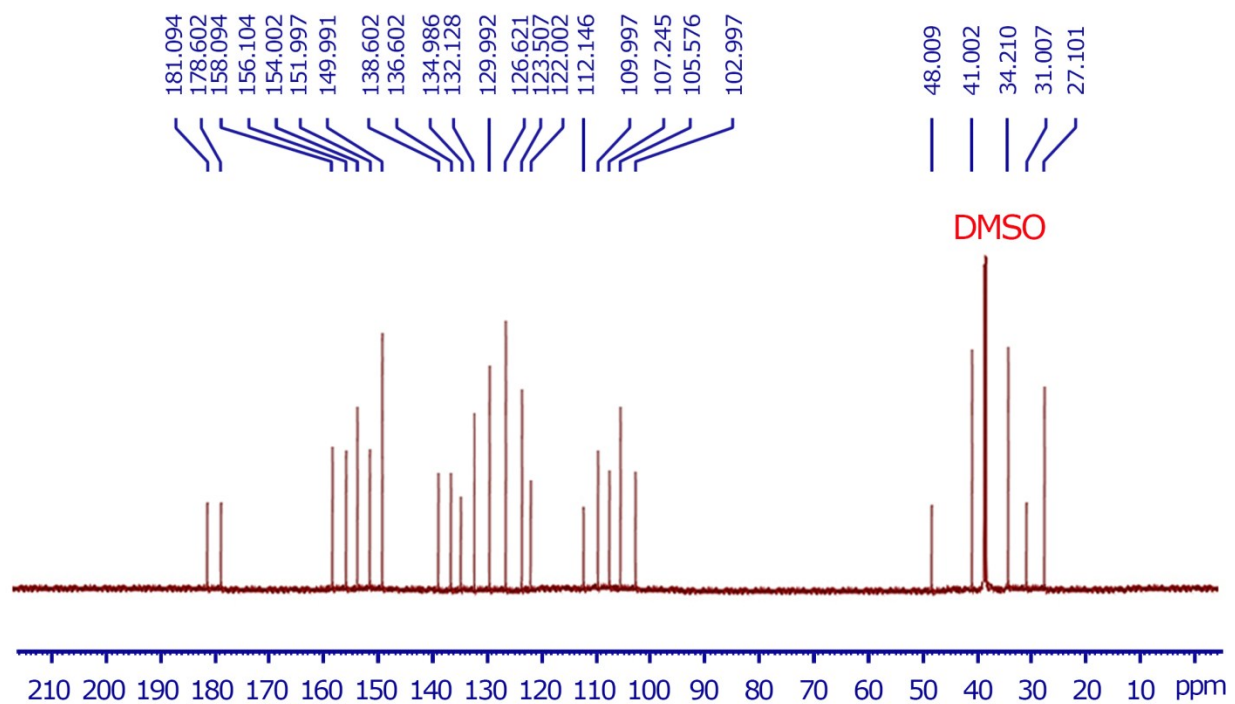


Figure S12. ^{13}C NMR spectrum of complex **2**, cis-Pt(1,4-NQ)(1-ADpcyd)(G) (DMSO- d_6).

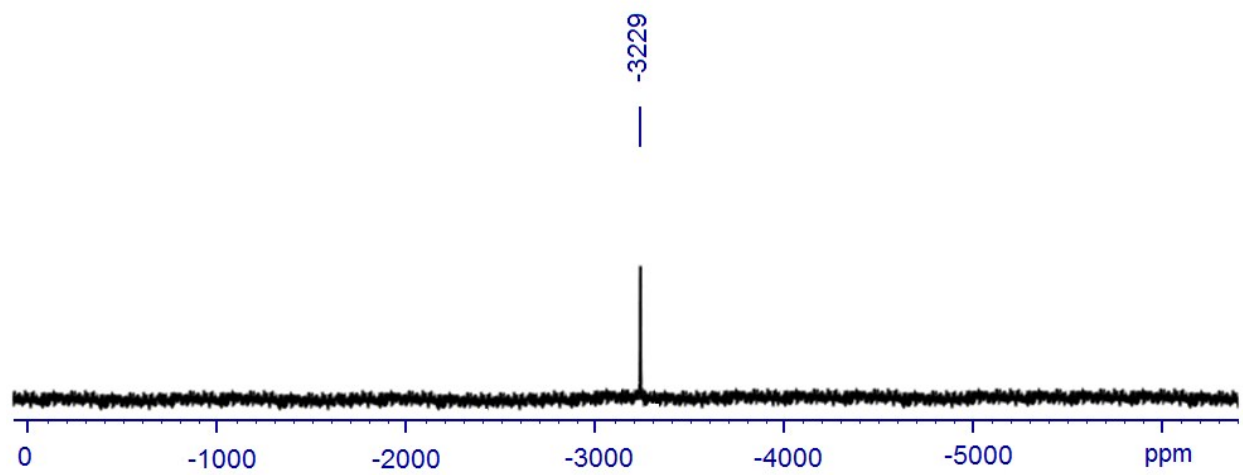


Figure S13. ^{195}Pt NMR spectrum of complex **2**, $\text{cis-Pt}(1,4\text{-NQ})(1\text{-ADpcyd})(\text{G})$ ($\text{DMF-}d_7$).

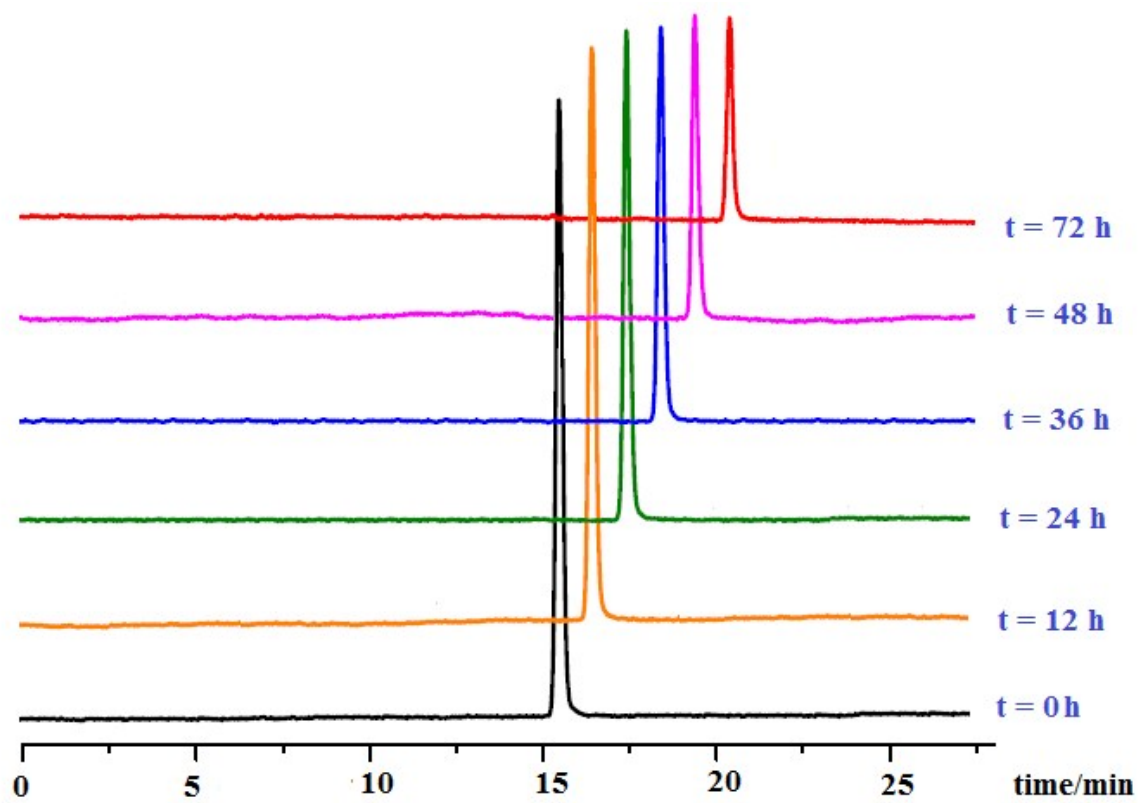


Figure S14. HPLC of the complex **1** in freshly prepared PBS buffer/0.5% DMSO solution recorded during 72 h of incubation time at 37 °C.

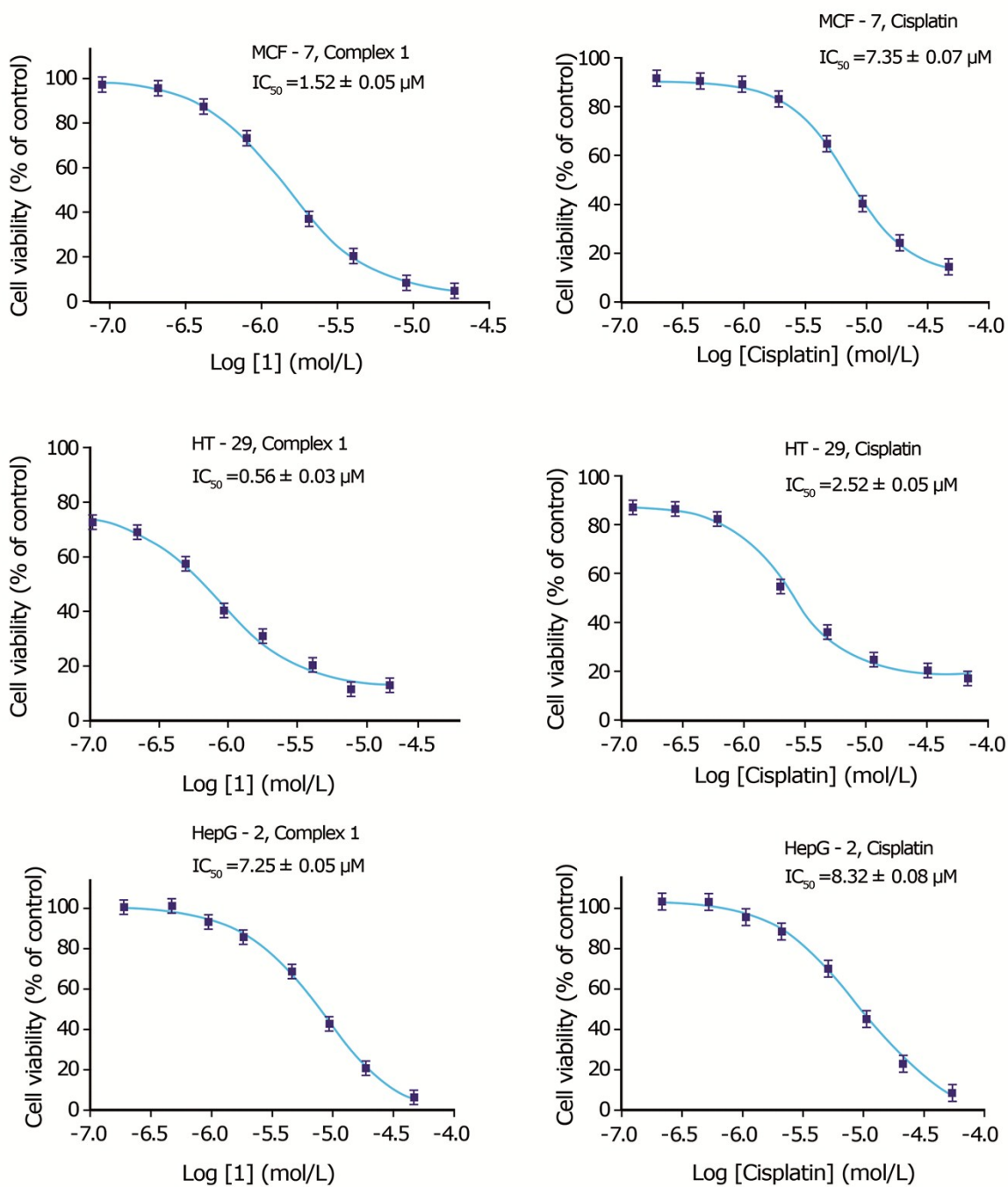


Figure S15. Graphs used for IC_{50} value determinations. Dose-response data points represent the mean value of 3 trials. GraphPad Prism 6 software was used to fit the data.