Supplementary Material

Enhanced anti-cancer efficacy to cancer cells by a novel monofunctional mononuclear platinum(II) complex containing a mixed *S*,*N*,*S*-donor ligand

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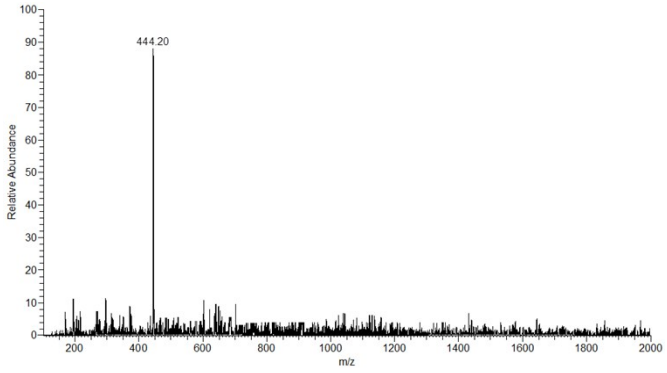


Fig. S1 ESI-MS of *N*-(4-(benzo[d]oxazol-2-yl)phenyl)-2-(bis(2-ethylthioethyl)amino)acetamide (**L**) in methanol.

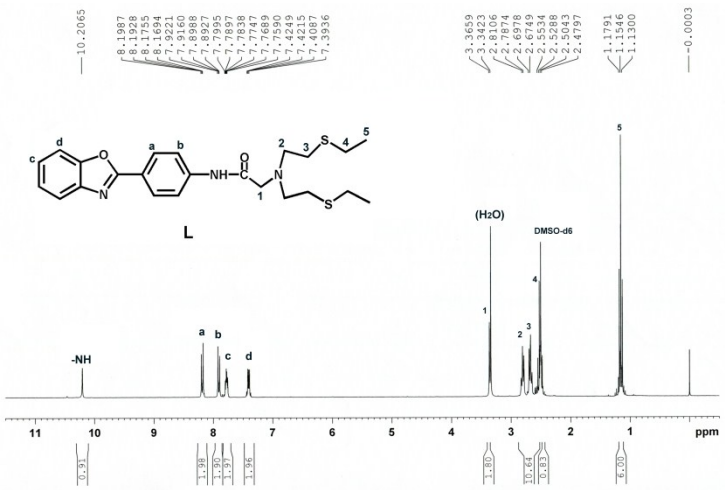


Fig. S2 ^{1}H NMR of *N*-(4-(benzo[d]oxazol-2-yl)phenyl)-2-(bis(2-ethylthioethyl)amino)acetamide (**L**) in DMSO-d^{6}.

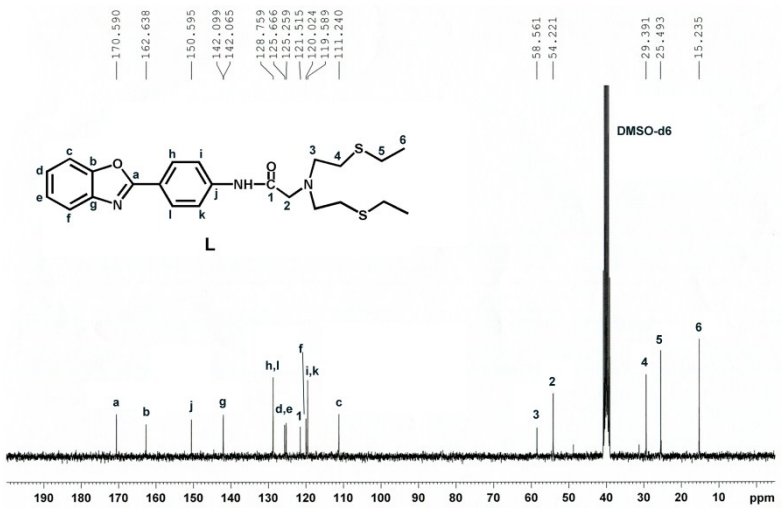


Fig. S3 ^{13}C NMR of *N*-(4-(benzo[d]oxazol-2-yl)phenyl)-2-(bis(2-ethylthioethyl)amino)acetamide (**L**) in DMSO-d^6.

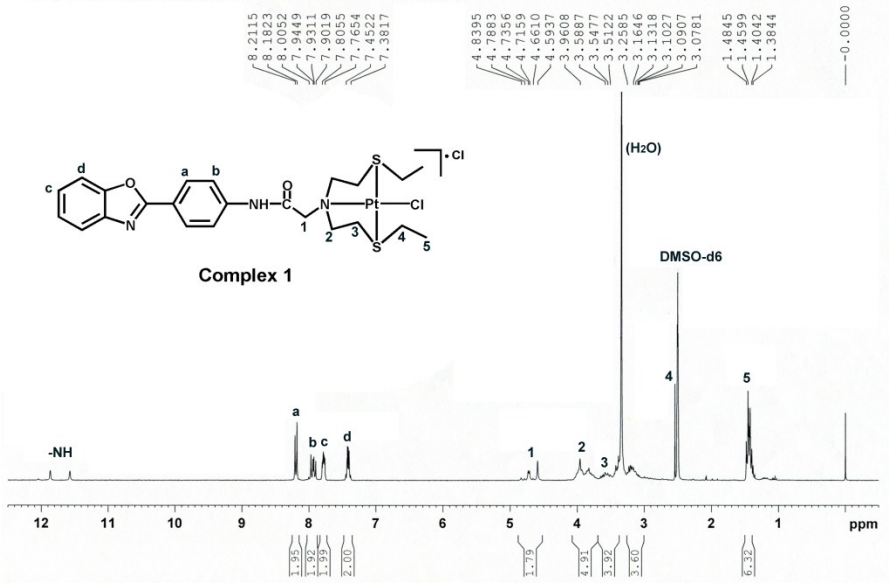


Fig. S4 ^{1}H NMR of complex **1** ([Pt**L**Cl]Cl) in DMSO-d^6.

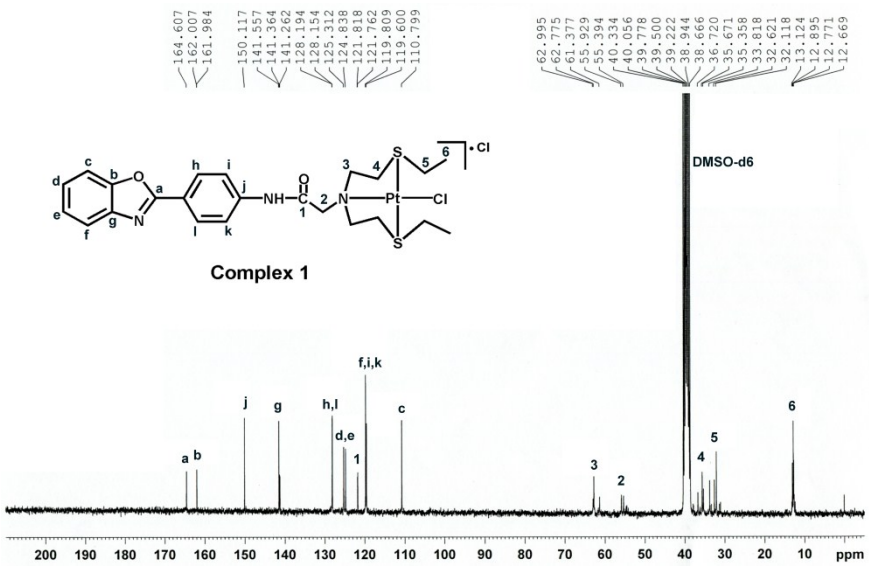


Fig. S5 ^{13}C NMR of complex **1** ([Pt**L**Cl]Cl) in DMSO-d^6.

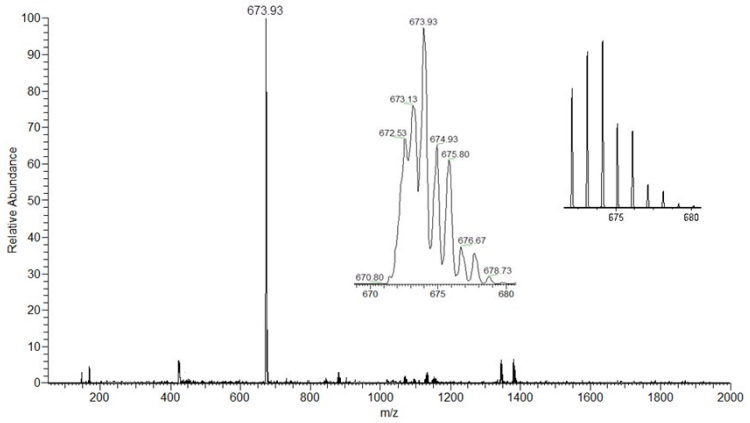


Fig. S6 ESI-MS of complex **1** ([Pt**L**Cl]Cl) in methanol.

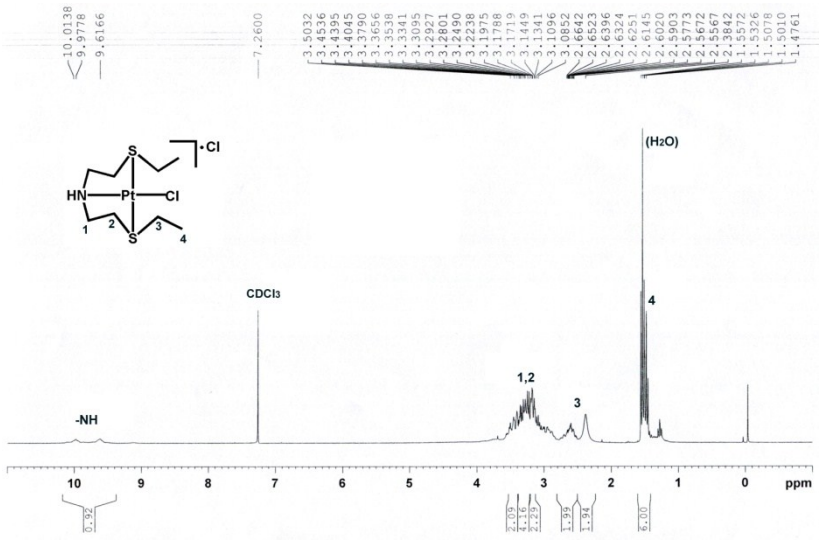


Fig. S7 ^{1}H NMR of complex **2** ([Pt**L′**Cl]Cl) in $CDCl_3$.

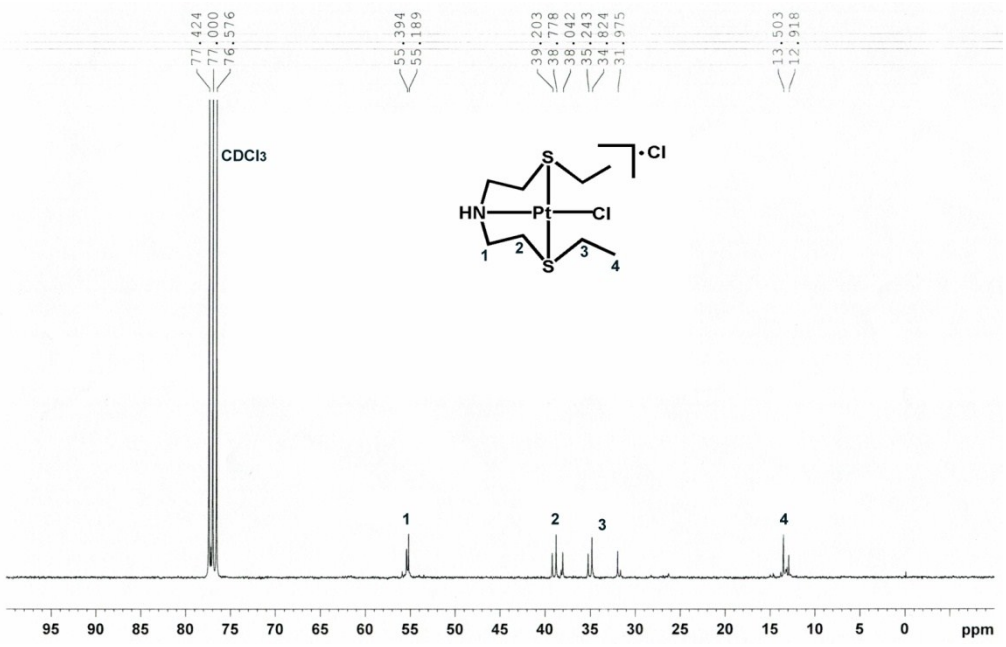


Fig. S8 ^{13}C NMR of complex **2** ([Pt**L′**Cl]Cl) in $CDCl_3$.

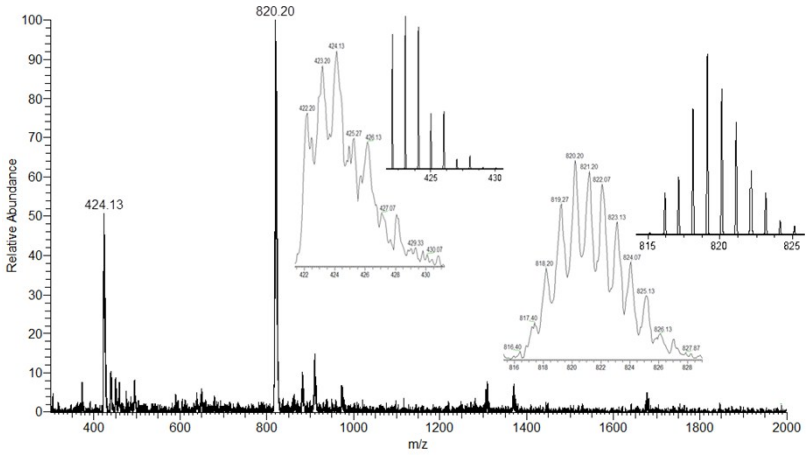


Fig. S9 ESI-MS of complex **2** ([Pt**L′**Cl]Cl) in methanol.

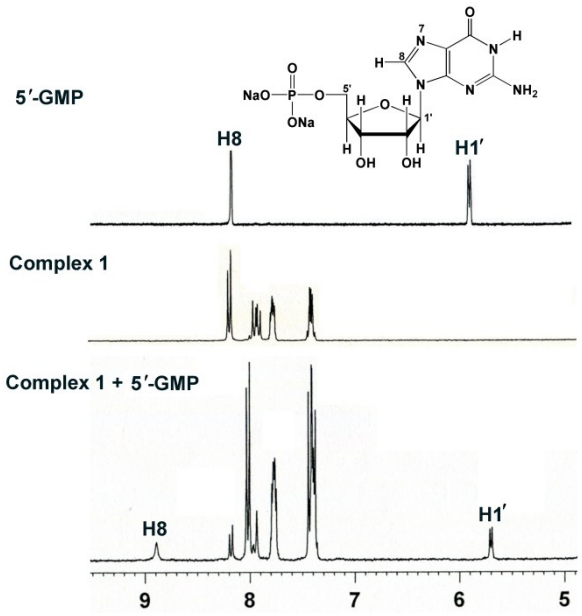


Fig. S10 ^{1}H NMR spectra of 5′-GMP, complex **1**, and the reaction of complex **1** with equimolar 5′-GMP for 24 h in DMSO-d^6 at room temperature.

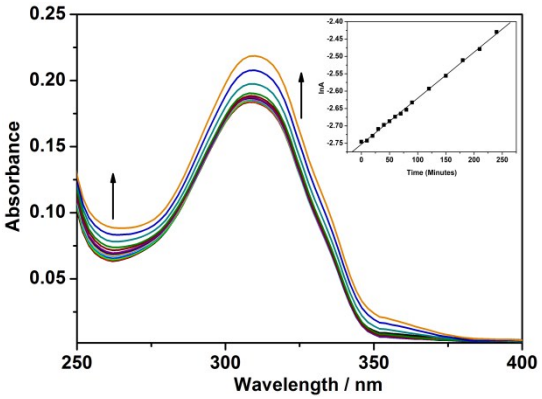
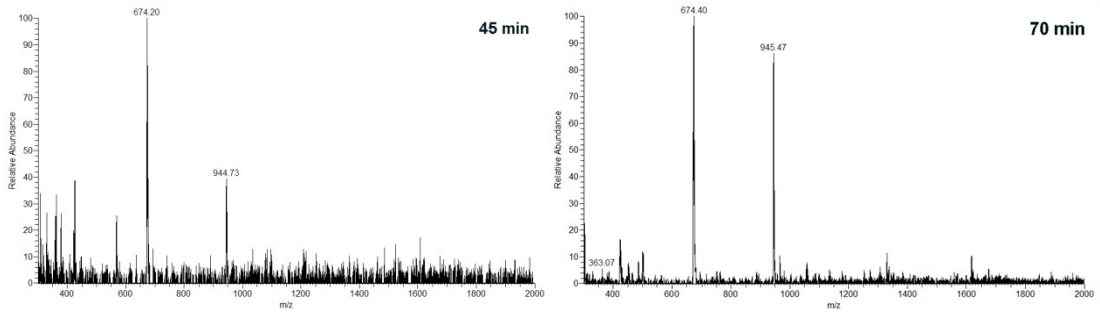
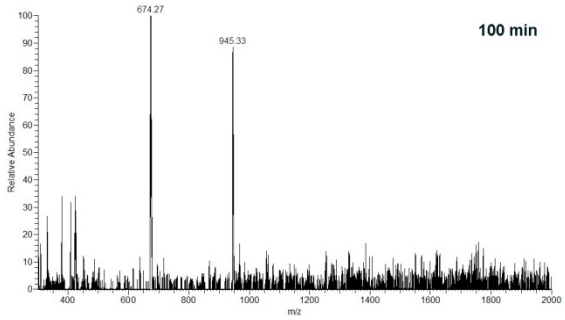
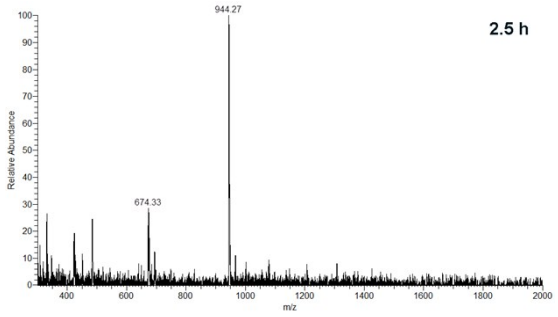
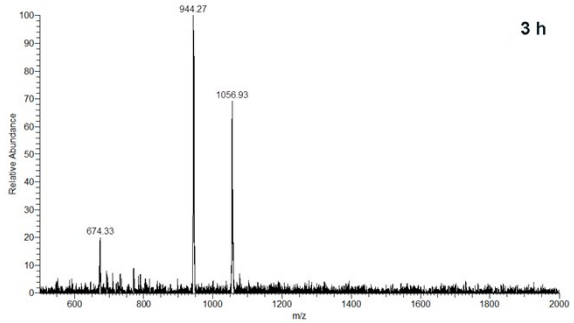


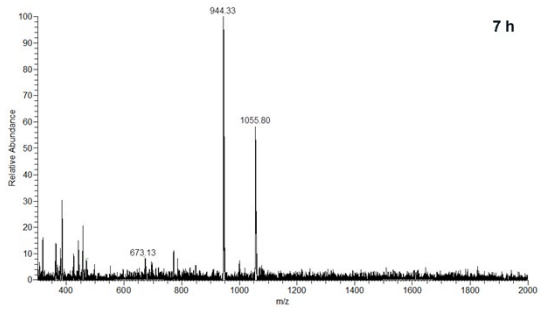
Fig. S11 Time-dependent absorption spectra of complex **1** (16 μM) in the presence GSH (8 mM) (incubated time: 0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 120, 150, 180, 210, 240 min, respectively) at 37 °C in Tris-HCl/NaCl buffer (pH 7.40). The inset shows the plot of the linear fit of lnA *vs.* time (A is the absorbance of 260 nm).

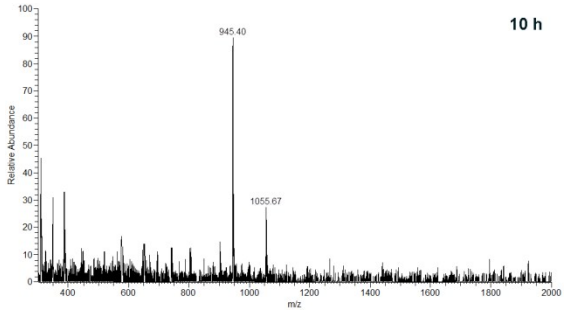



100 min
674.27
945.33
Relative Abundance
m/z


2.5 h
944.27
674.33
Relative Abundance
m/z


3 h
944.27
1056.93
674.33
Relative Abundance
m/z


7 h
944.33
1055.80
673.13
Relative Abundance
m/z


10 h
945.40
1055.67
Relative Abundance
m/z

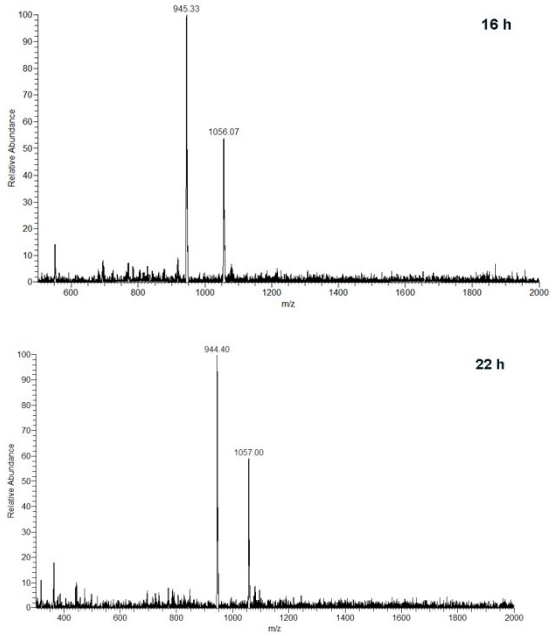


Fig. S12 ESI-MS spectra (positive mode) of the competitive reaction of complex **1** with GSH and 5′-GMP (1:1:1) recorded in methanol/water/water (v/v/v, 1:1:1) at 37 °C for the different incubated time. Assignments: 674, $[Pt\mathbf{L}Cl]^+$ ($C_{23}H_{29}N_3O_2S_2ClPt$, calcd 674.17); 945, $[Pt\mathbf{L}(GS)]^+$ ($C_{33}H_{45}N_6O_8S_3Pt$, calcd 945.03); 1056, $[Pt\mathbf{L}(GMP) - Na + CH_3OH]^+$ ($C_{34}H_{45}N_8O_{11}S_2PNaPt$, calcd 1054.95).