Supporting Information for

A novel platinum(II) complex with berberine derivative as potential antitumor agent targeting G-quadruplex DNA

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1. Table S1. Oligomers or primers used in this study

Oligomer	Sequence
bcl-2	5′-GGGCGGGCGCGGGAGGAAGGGGGCGGG-3′
5′-biotin bcl-2	5′-biotin-GGGCGGGCGCGGGAGGAAGGGGGCGGG-3′
c-myc	5′-TTGAGGGTGGGTAGGGTGGGTAAA-3
c-myb	5′-AGGGAGTCGGGCAGGGGTGCTGGGA-3′
VEGF	5′-GGGGCGGGCCGGGGGCGGGG-3′
PDGF-A	5′GGAGGCGGGGGGGGGGGGGCGGGGGCGGGGGCGGGGGAGGGGCGCGGC-3′
DS26	5′-CAATCGGATCGAATTCGATCCGATTG-3′

2. UV–Vis titrations assays of the **Pt1** and various G4s DNA

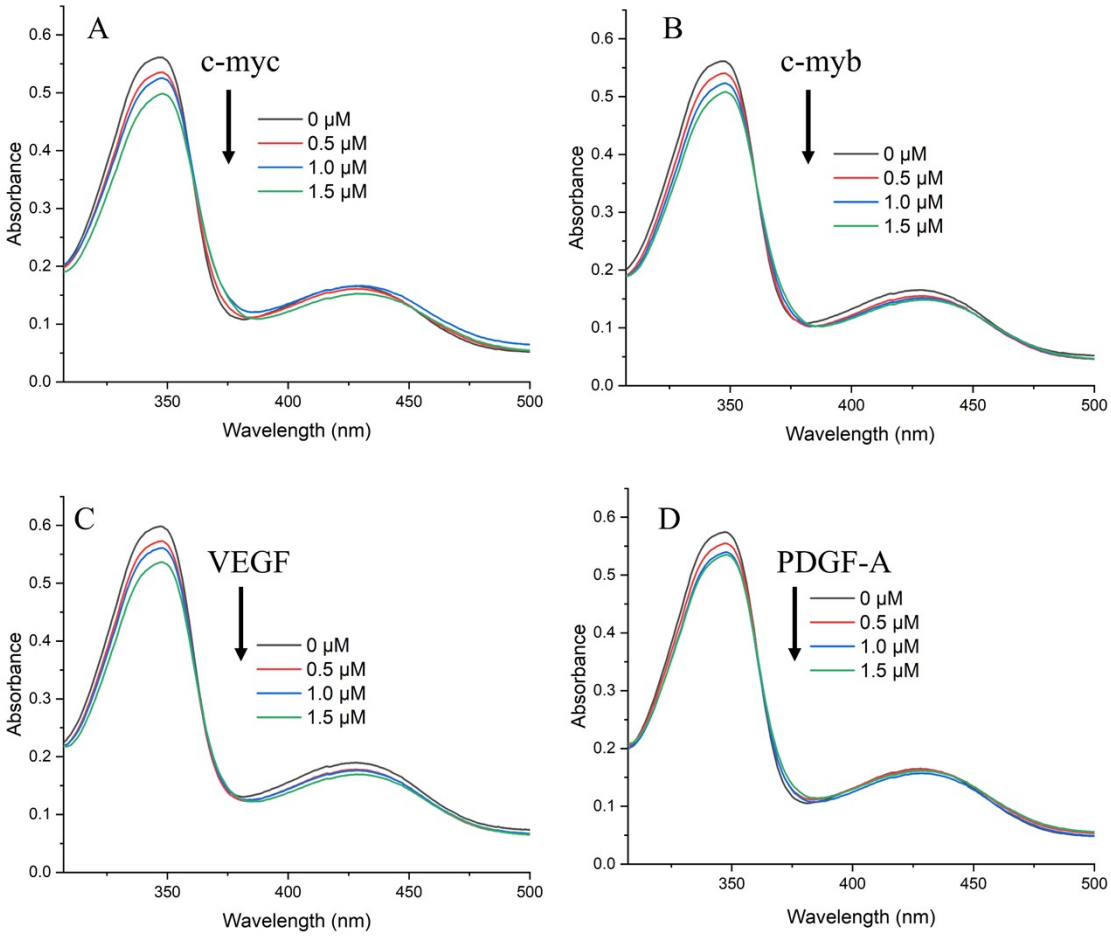

Fig. S1 UV–Vis spectra of the **Pt1** in the absence and presence of increasing amounts of various G4s DNA in 20 mM Tris–HCl, 100 mM KCl buffer at pH 7.4.

3. Fluorescence assays of the **Pt1** and various G4s DNA

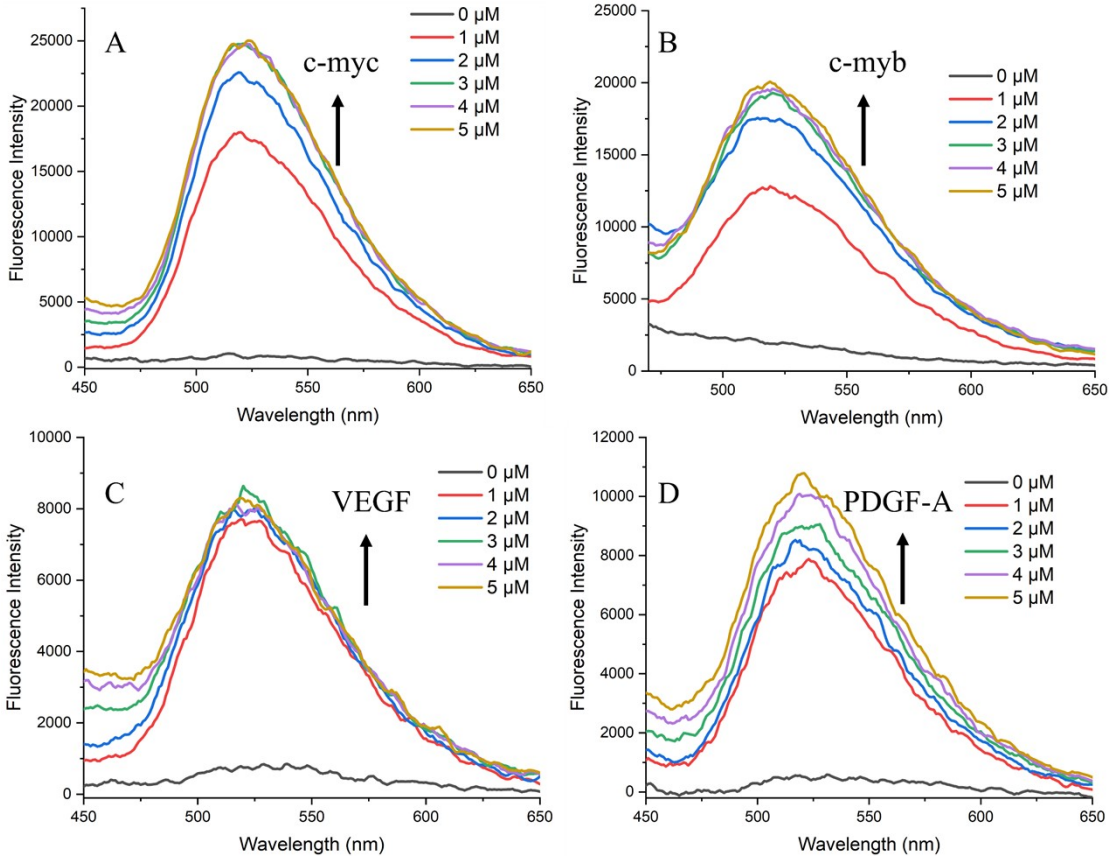

Fig. S2 A) Fluorescence spectra of **Pt1** (1 μM) titrated with increasing amounts of c-myc G4 DNA (0-5 μM) in 20 mM Tris-HCl, 100 mM KCl buffer at pH 7.4, B) Fluorescence spectra of **Pt1** (1 μM) titrated with increasing amounts of c-myb G4 DNA (0-5 μM) in 20 mM Tris-HCl, 100 mM KCl buffer at pH 7.4, C) Fluorescence spectra of **Pt1** (1 μM) titrated with increasing amounts of VEGF G4 DNA (0-5 μM) in 20 mM Tris-HCl, 100 mM KCl buffer at pH 7.4, D) Fluorescence spectra of **Pt1** (1 μM) titrated with increasing amounts of PDGF-A G4 DNA (0-5 μM) in 20 mM Tris-HCl, 100 mM KCl buffer at pH 7.4.

4. CD spectra of the **Pt1** and various G4s DNA and DS26

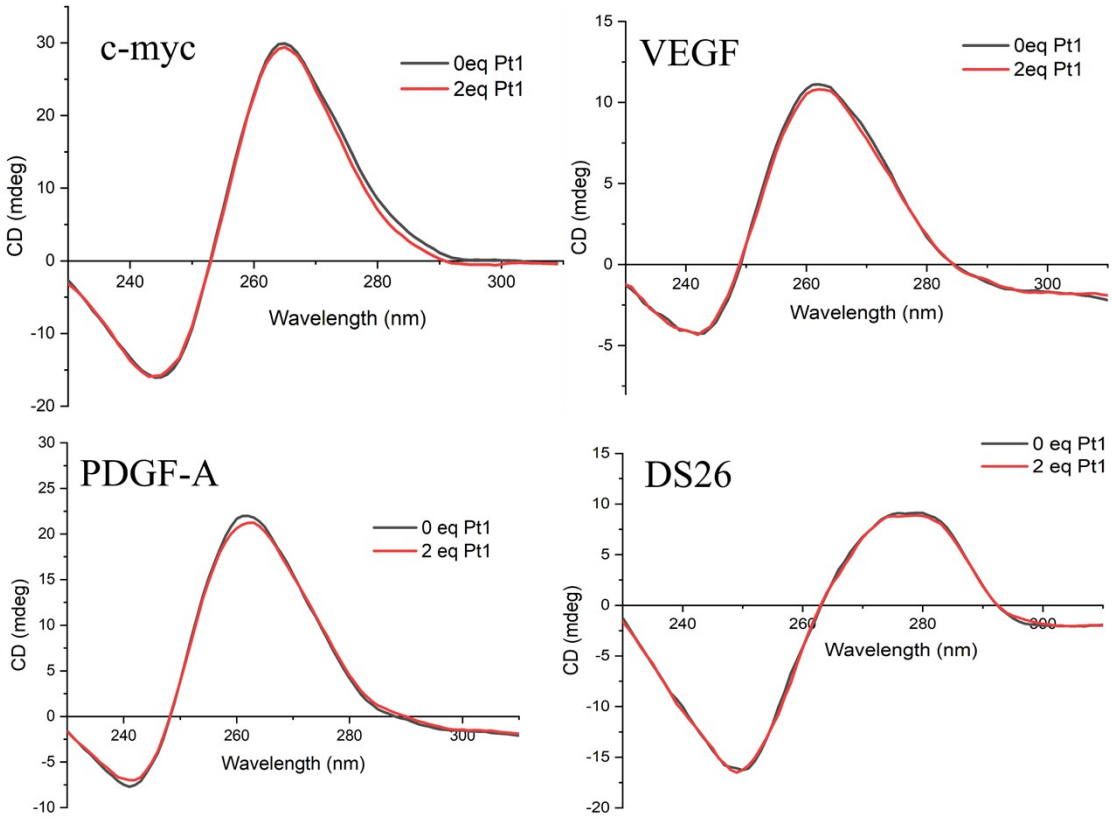

Fig. S3 CD spectra of different G4s and DS26 in the absence and presence of 2eq **Pt1** in 20 mM Tris-HCl, 100 mM KCl buffer at pH 7.4.

5. Molecular docking of **Pt1** with c-myc G4 DNA

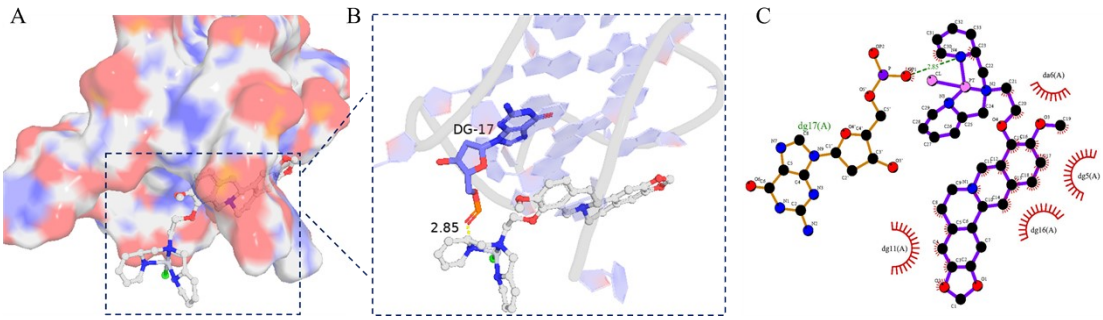

Fig. S4 A) Overall surface diagram of **Pt1** binding to c-myc G4 DNA (PDB code: 2L7V). B) the detailed cartoon diagram of **Pt1** binding to c-myc G4 DNA (PDB code: 2L7V). C) Two-dimensional (2D) interaction diagrams of **Pt1** binding to c-myc G4 DNA (PDB code: 2L7V).

6. NMR spectra of compounds

^{1}H and ^{13}C NMR of **L**:

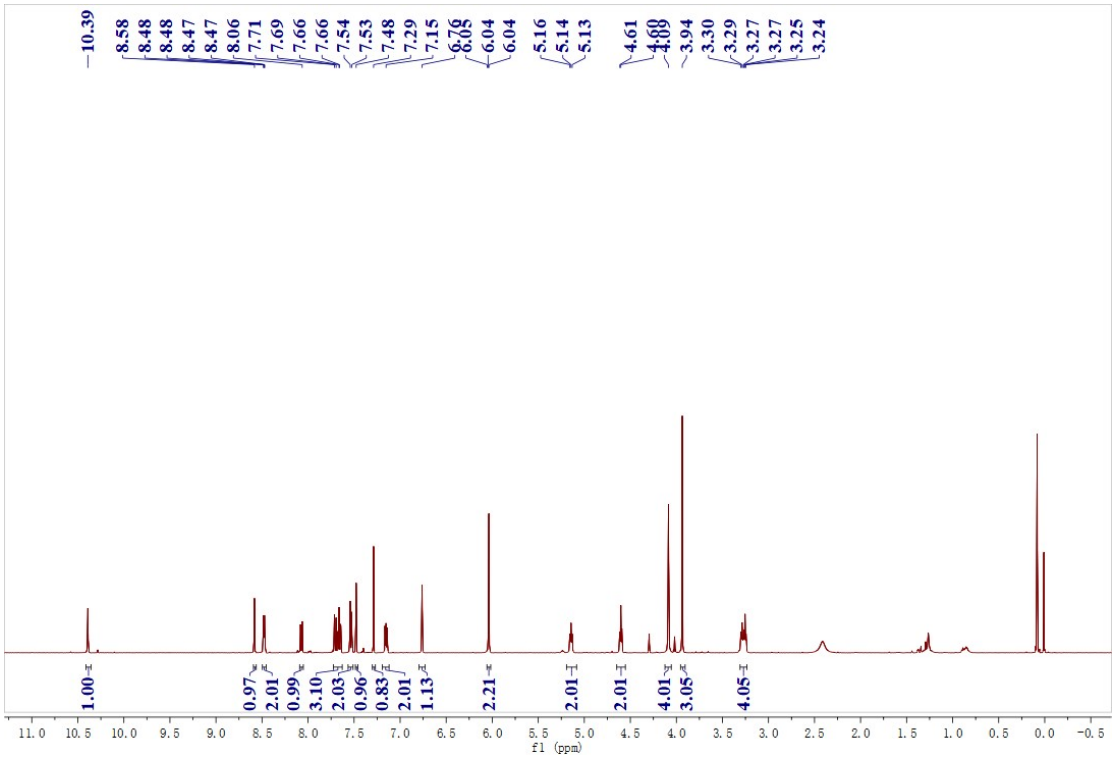

Fig.S5 ^{1}H NMR spectrum of **L**.

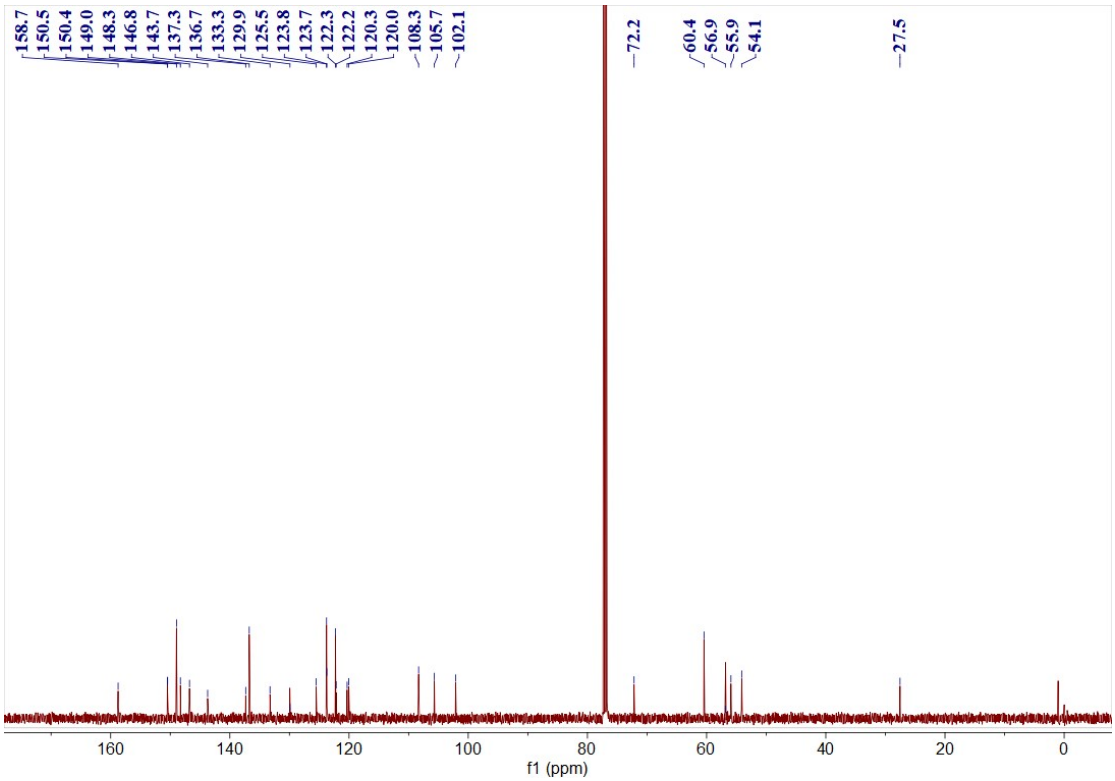

Fig.S6 ^{13}C NMR spectrum of **L**.

^{1}H and ^{13}C NMR of **Pt1**:

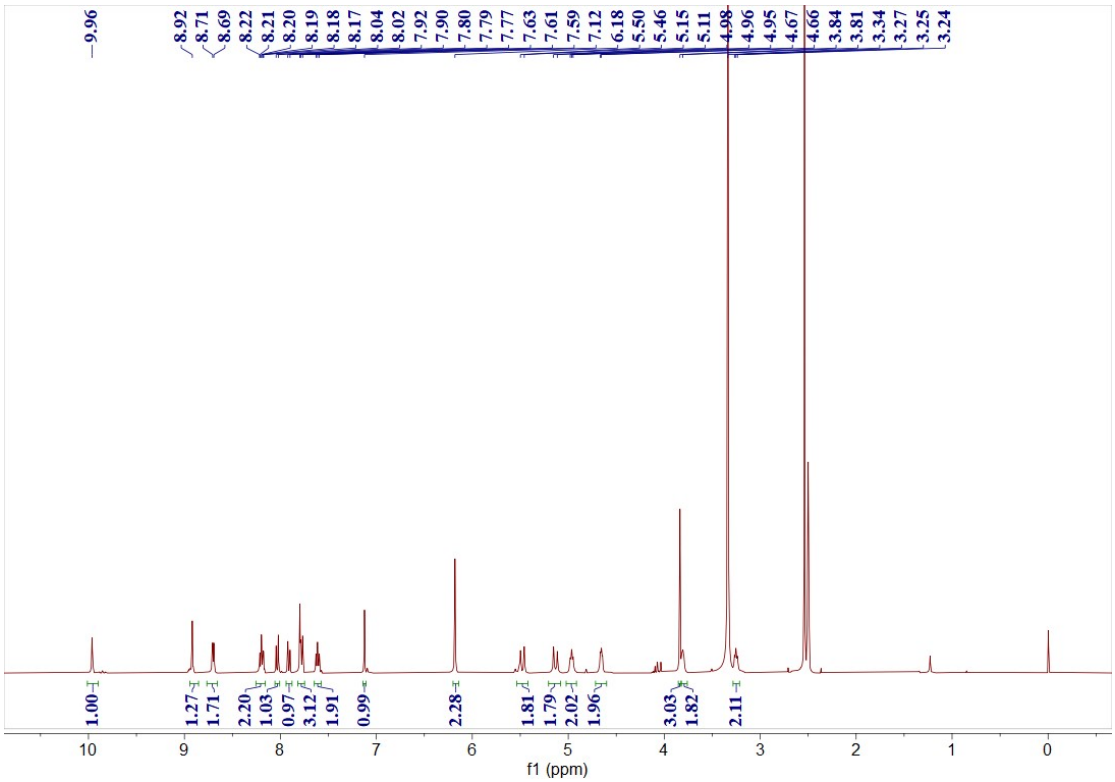

Fig.S7 ^{1}H NMR spectrum of **Pt1**.

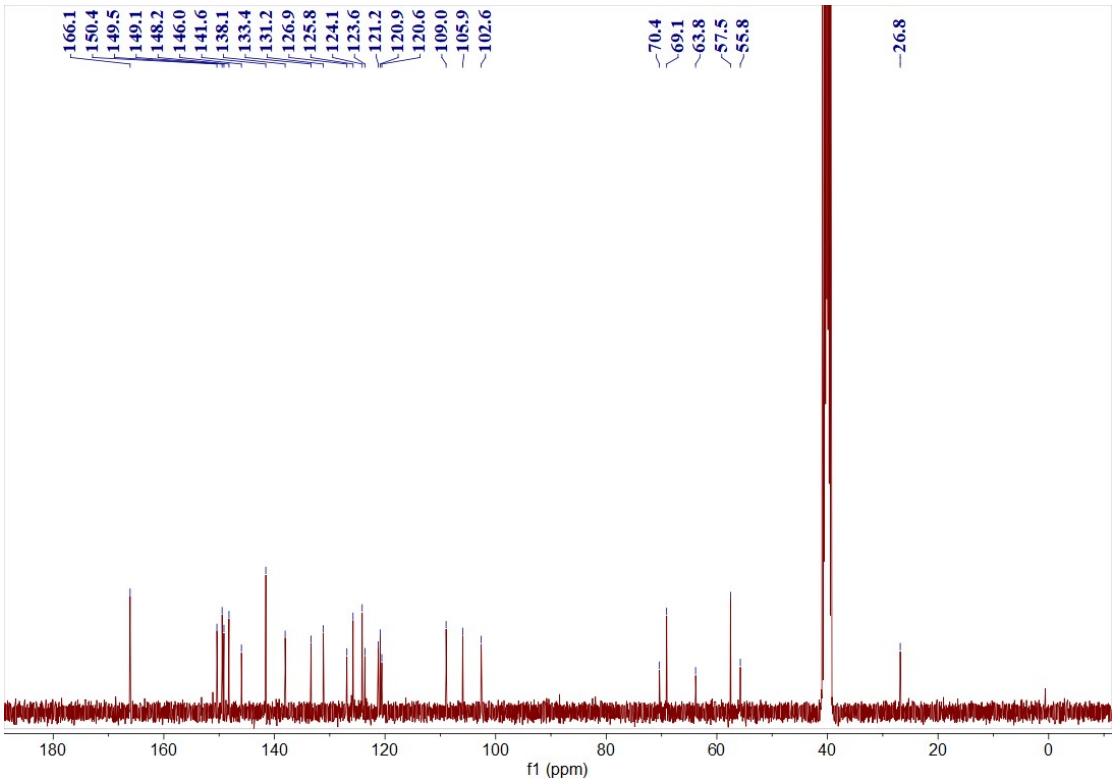

Fig.S8 ^{13}C NMR spectrum of **Pt1**.

7. IR spectra of compounds

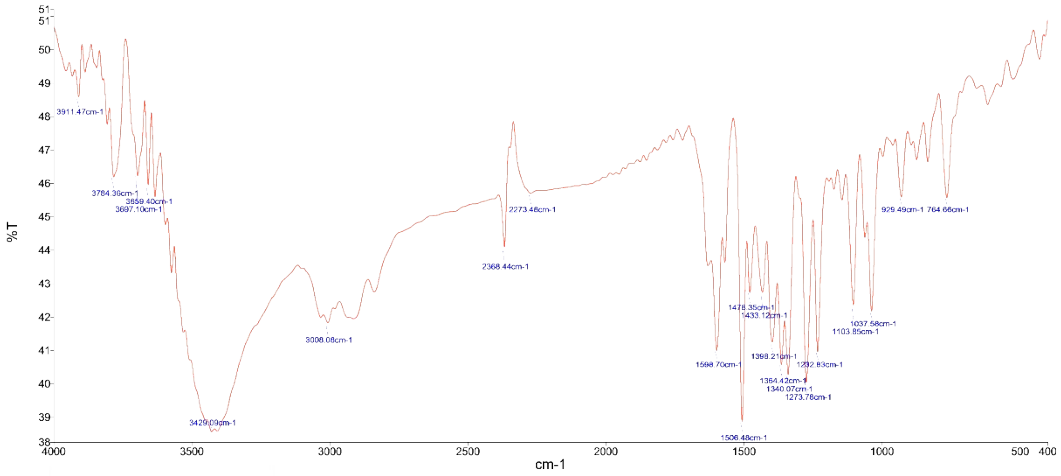

Fig.S9 IR spectrum of **L**.

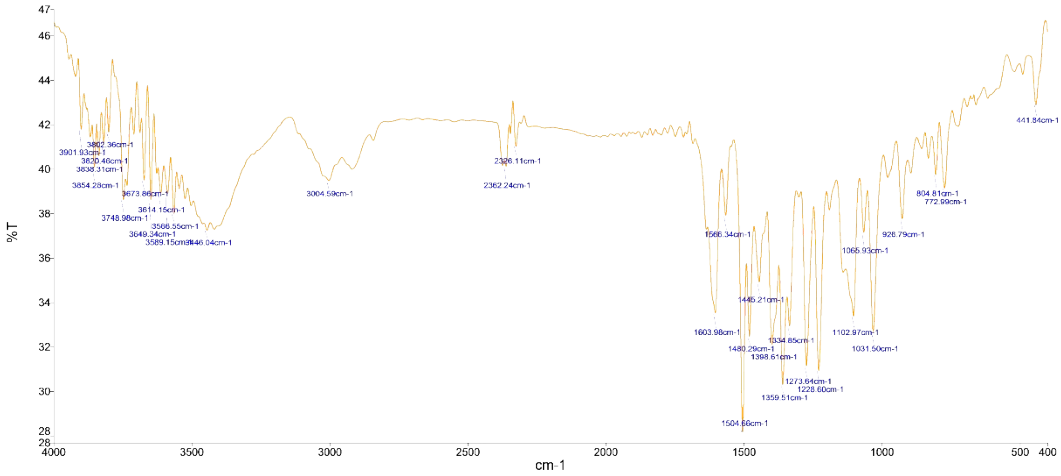

Fig.S10 IR spectrum of **Pt1**.

8. ESI-ME spectra of compounds

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Std/Enhanced	Scan Begin	50 m/z	Scan End	1500 m/z
Capillary Exit	132.0 Volt	Skimmer	40.0 Volt	Trap Drive	58.3
Accumulation Time	28 µs	Averages	5 Spectra	Auto MS/MS	off

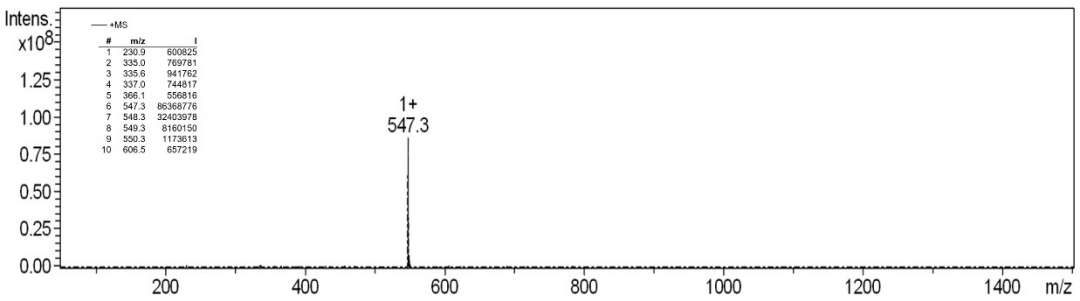

Fig.S11 ESI-MS spectrum of **L**.

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Std/Enhanced	Scan Begin	50 m/z	Scan End	1500 m/z
Capillary Exit	149.3 Volt	Skimmer	40.0 Volt	Trap Drive	74.6
Accumulation Time	5769 µs	Averages	5 Spectra	Auto MS/MS	off

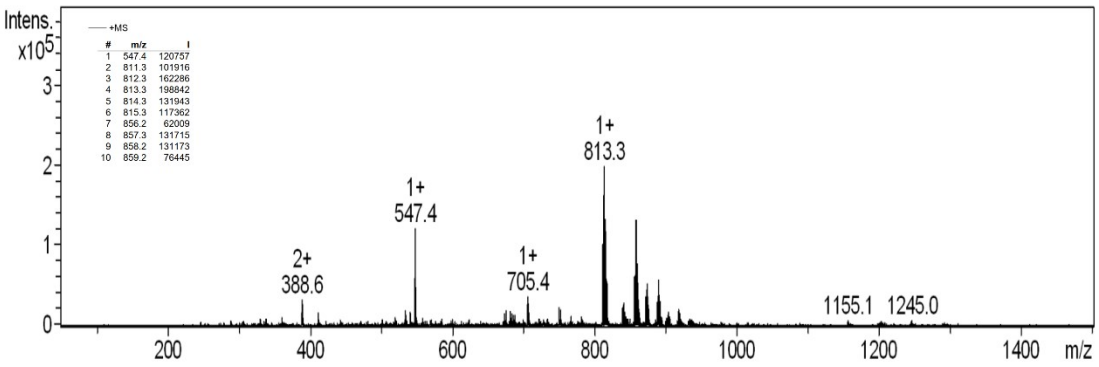

Fig.S12 ESI-MS spectrum of **Pt1**.