

Electronic Supplementary Information:

## Syntheses, crystal structures, and biological evaluations of new dinuclear platinum(II) complexes with 1,2,4-triazole derivate as bridging ligands

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**Fig. S3** ESI-MS of **3** in the negative ion mode. Insert graph shows the base peaks of **3**.

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**Fig. S6** (a) Partial packing diagram of **2**, showing Cl<sup>⋯</sup>π stacking interactions, and C-H<sup>⋯</sup>π interactions (black dashes) (symmetry code: A -x, 1 - y, -z; B x - 1, y + 1, z; C -1-x, 3-y, -z; D x-1, y, z+1; E -1-x, 3-y, -z). (b) View down the sheets of **2**, showing interlinking via p<sup>⋯</sup>π interactions to form 2D stair-step chain.

**Fig. S7** (a) Dimers structures of **4**, showing C-H<sup>⋯</sup>O and C-H<sup>⋯</sup>S interactions (black dashes) (symmetry code: B -x, -y, 1-z; C x, 1+y, z; D -x, 1-y, 1-z). (b) The extended 1D chain structure.

**Fig. S8** (a) 1D chain of **2** extend through free DMSO along the a axis. (b) View perpendicular to the solvent-filled (DMSO) channels of **2**. (c) 1D chain of **3** assembled from hydrogen bonds from solvent DMSO. (d) Solvated DMSO molecules are encapsulated in the channels of **3**. (e) The antiparallel chains of **4** assembled by intermolecular interactions from solvent DMSO. (f) The packed structure with combination of A and B channels in **4**.

**Fig. S9** Kinetic stability of **3** in PBS buffer solution including 10% DMSO within 72 h at 310K.

**Fig. S10** Antiproliferation activities of **1-4** with different concentration (from left to right: 0 μM, 5 μM, 10 μM, and 50 μM) against HepG2 cell lines for 48 and 72 h.

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**Fig. S15** Emission spectra of EB bound to DNA in the absence and presence of increasing concentrations of **3** (0-20 μM) in Tris-HCl buffer. [EB]=0.2 μM, [DNA]=1 μM.

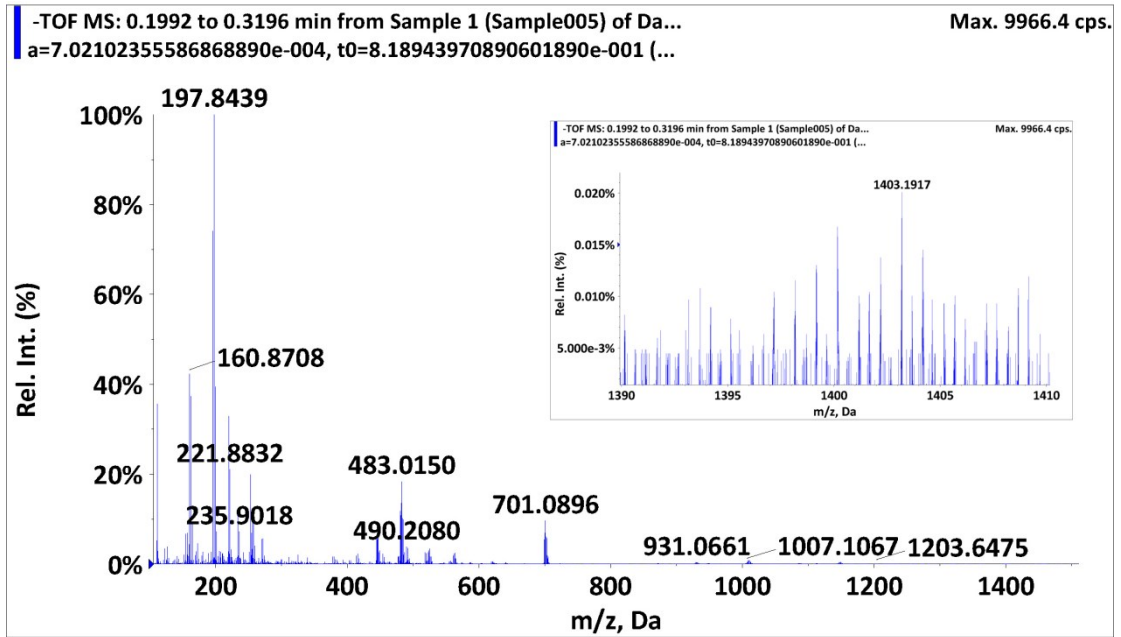


Fig. S1 ESI-MS of **1** in the negative ion mode. Insert graph shows the base peaks of **1**.

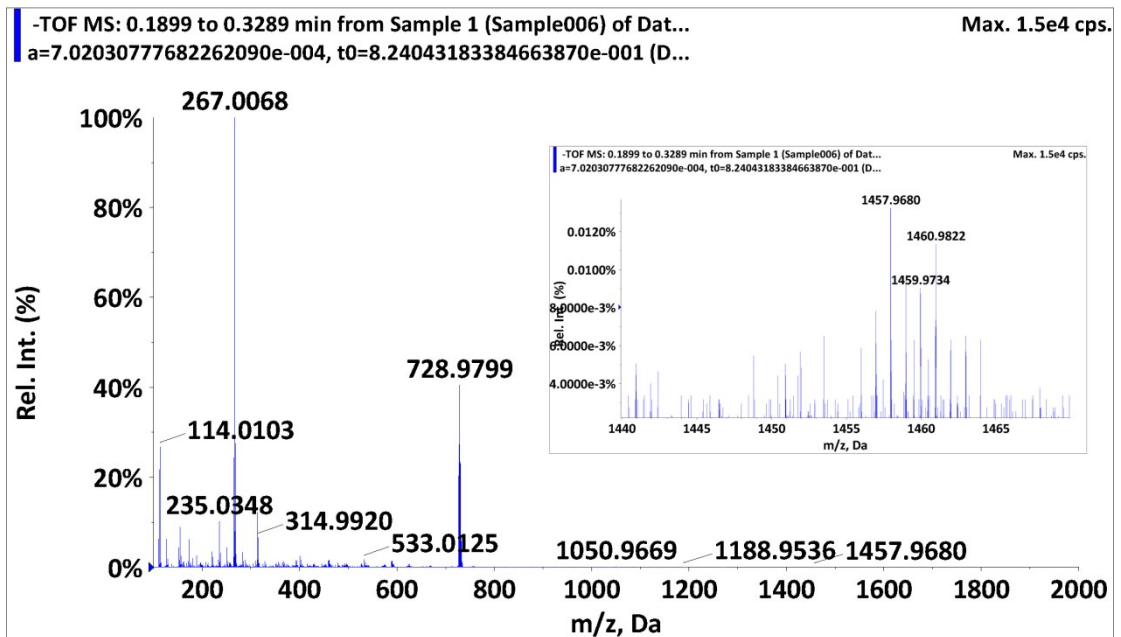


Fig. S2 ESI-MS of **2** in the negative ion mode. Insert graph shows the base peaks of **2**.

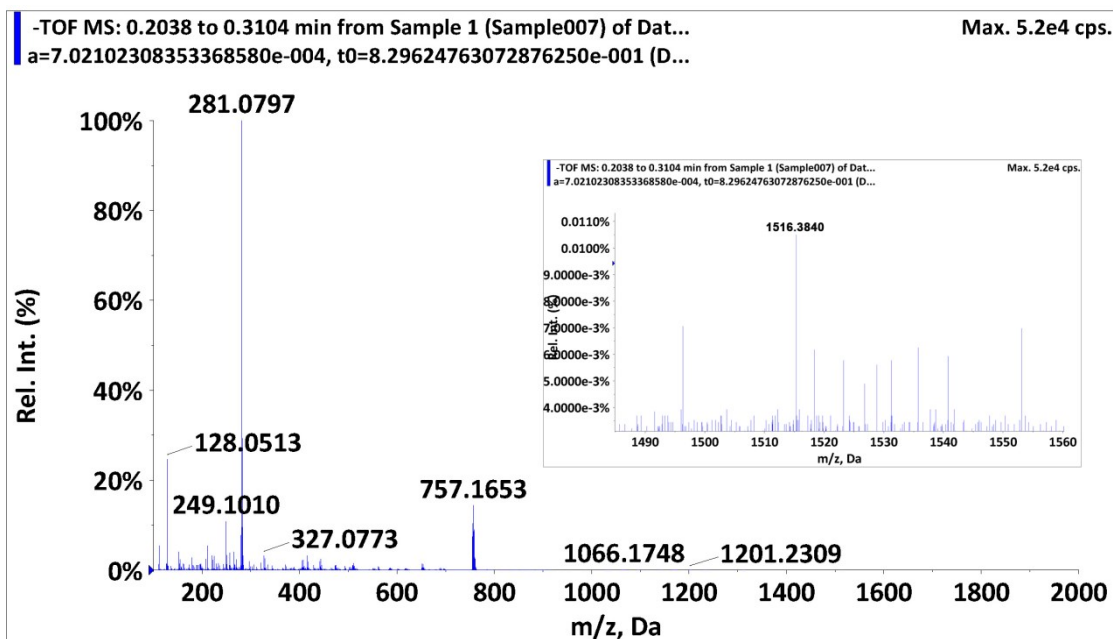


Fig. S3 ESI-MS of **3** in the negative ion mode. Insert graph shows the base peaks of **3**.

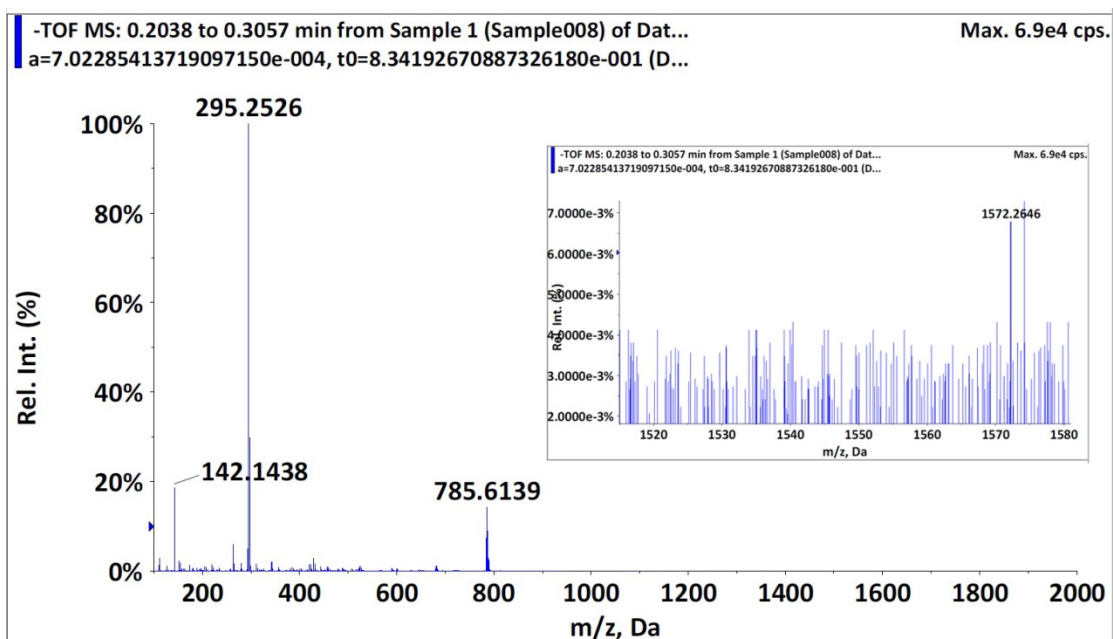
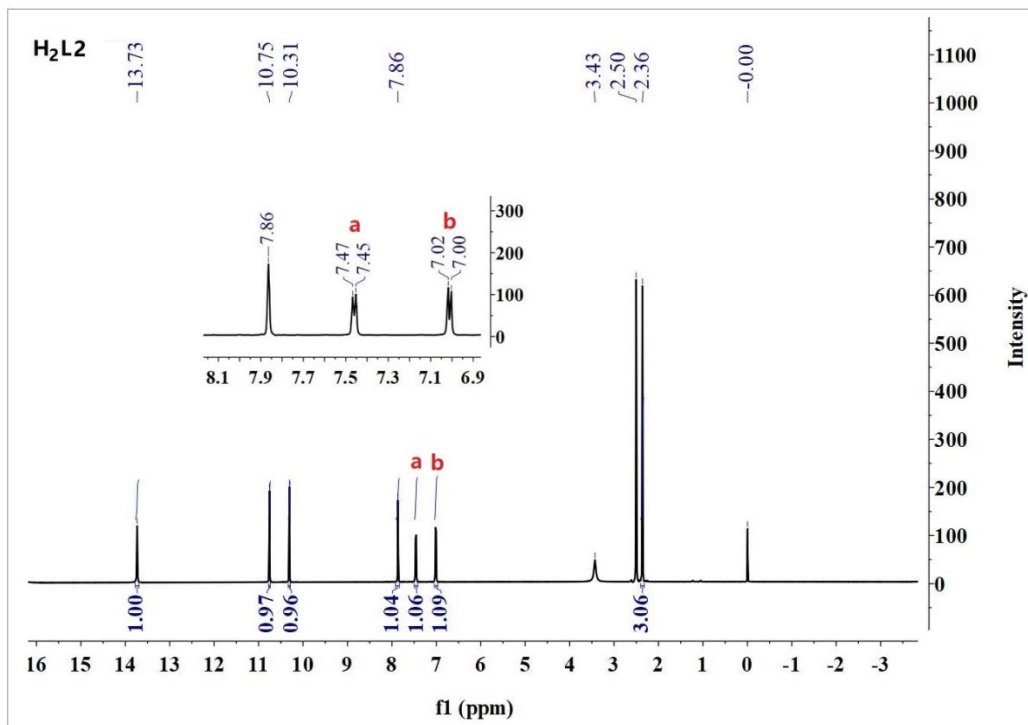
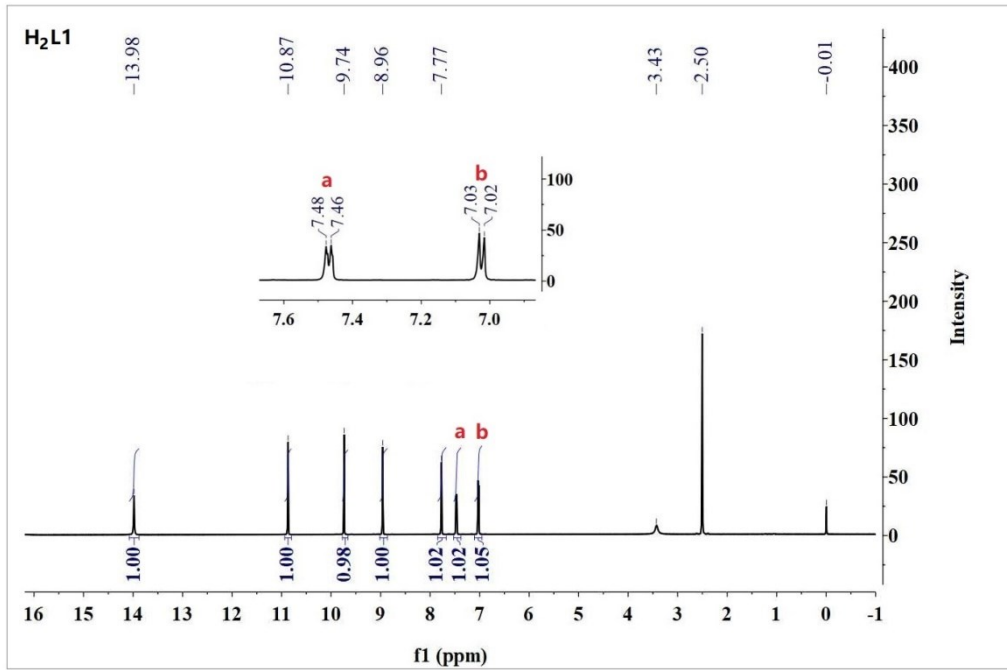
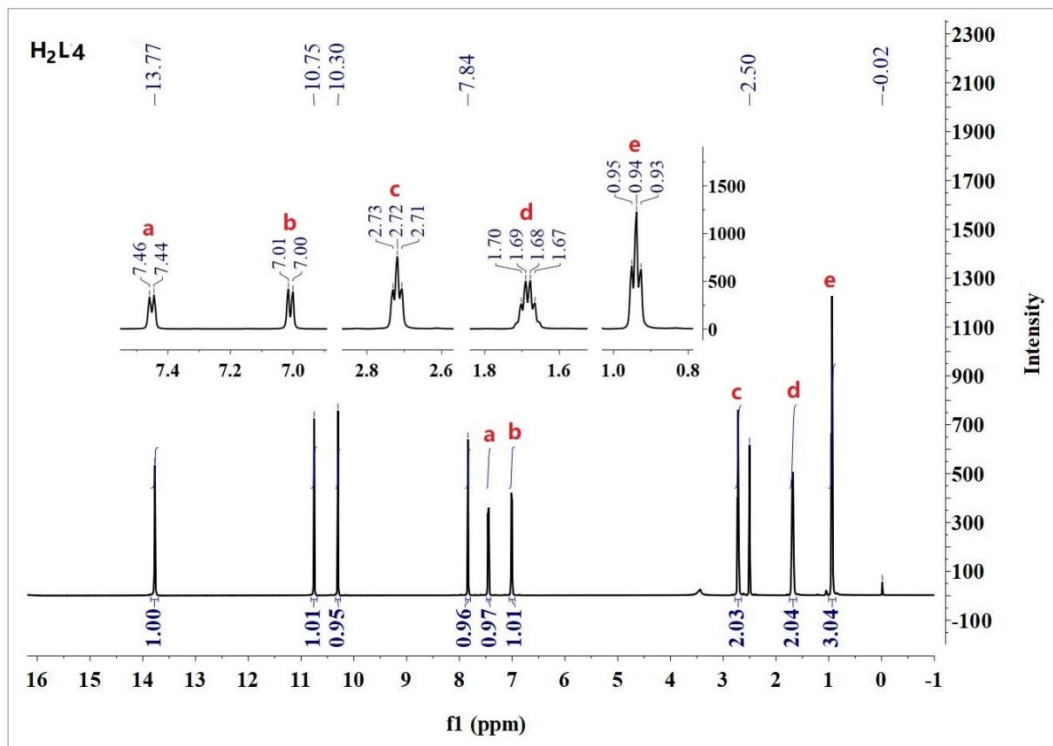
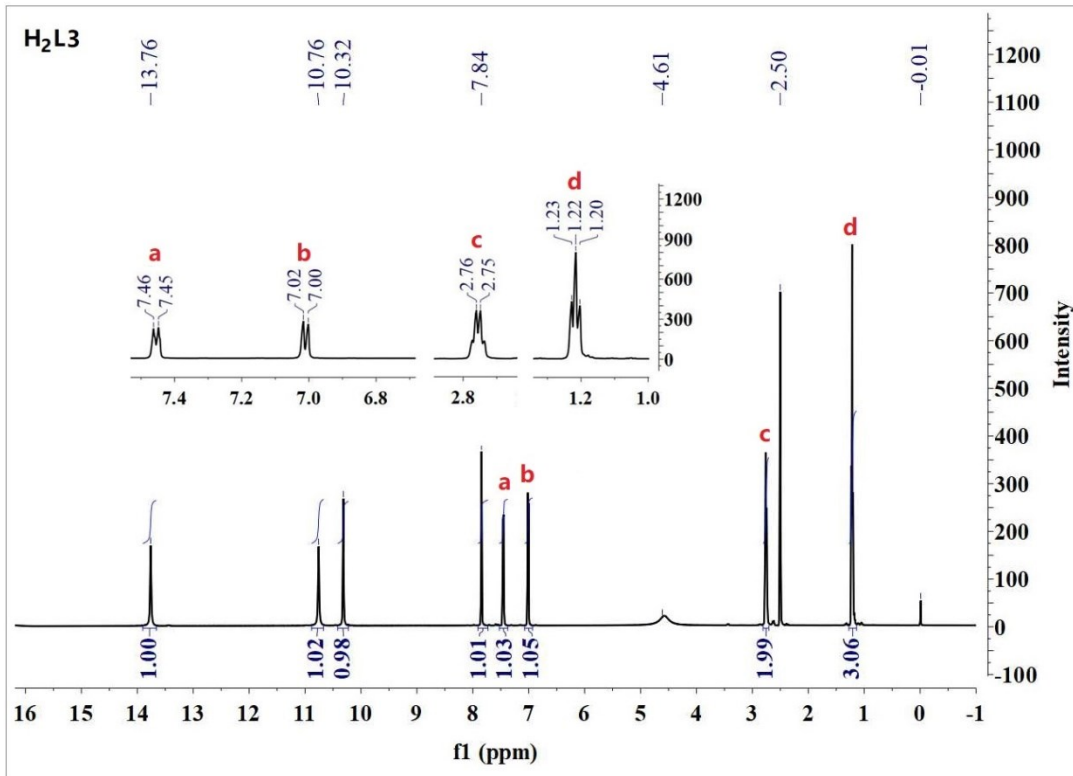
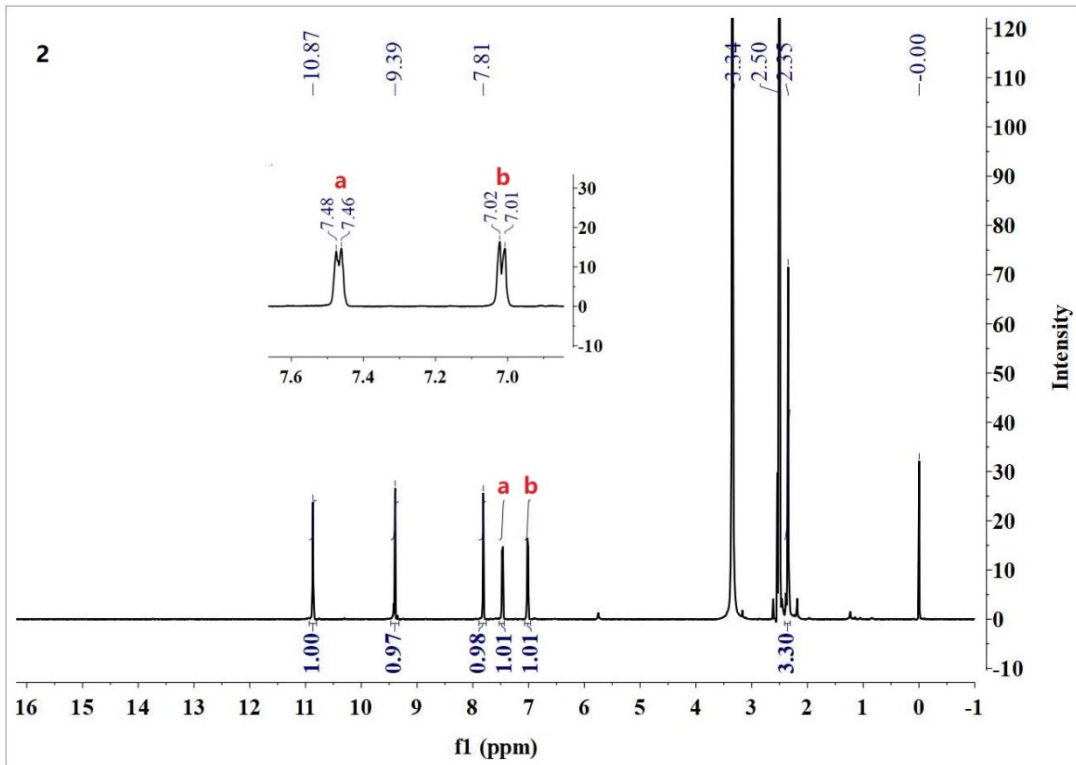
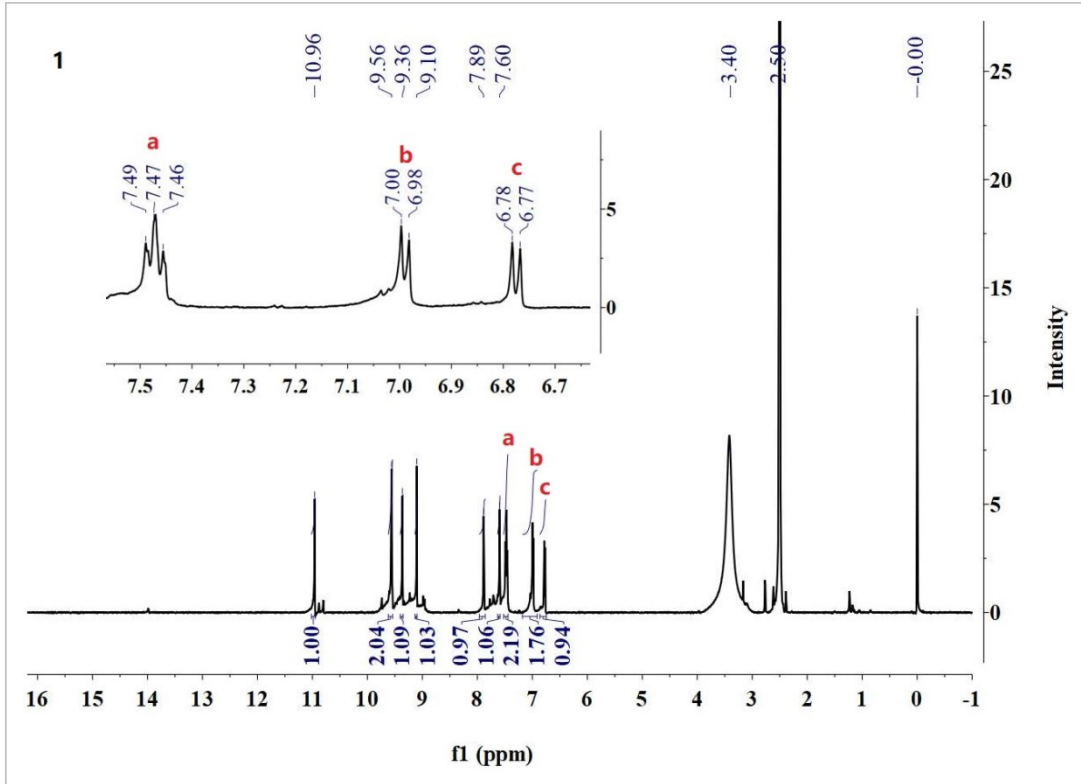


Fig. S4 ESI-MS of **4** in the negative ion mode. Insert graph shows the base peaks of **4**.







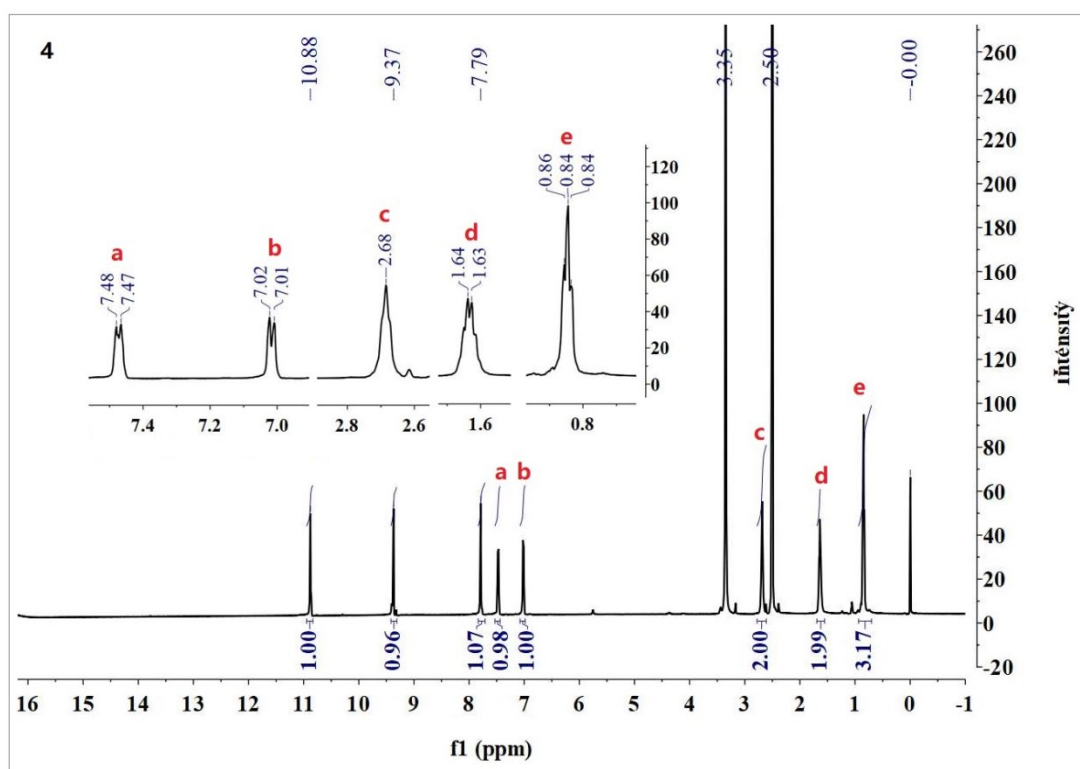
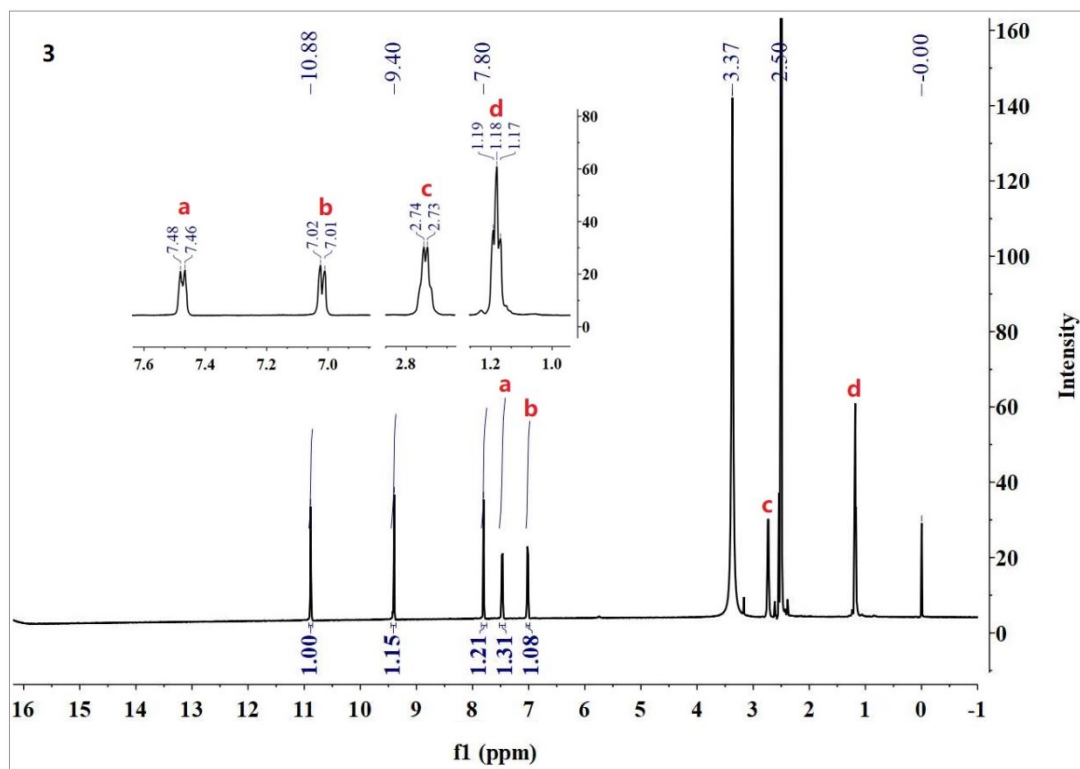


Fig. S5  $^1\text{H}$ NMR spectra of the ligands  $\text{H}_2\text{L1}$ – $\text{H}_2\text{L4}$  (left) and **1**–**4** (right)

**Table S1** Selected bond length, angles intermolecular interaction for three crystals

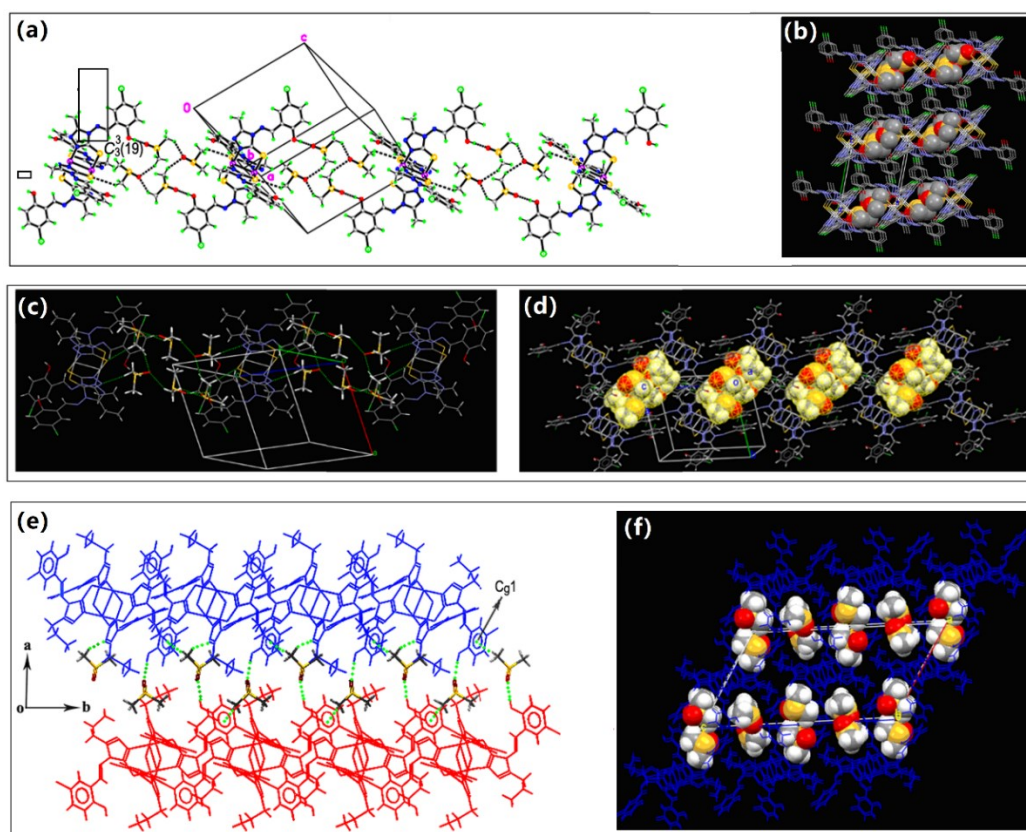
Complex 2				
Pt–Pt	Pt(1)–Pt(1) <sup>i</sup>	2.7597(5)		
Pt–N	Pt(1)–N(1) <sup>i</sup>	2.044(5)	Pt(1)–N(5) <sup>i</sup>	2.041(5)
Pt–S	Pt(1)–S(1)	2.2945(16)	Pt(1)–S(2)	2.2983(17)
	N(5) <sup>i</sup> –Pt(1)–N(1) <sup>i</sup>	88.09(19)	N(1) <sup>i</sup> –Pt(1)–S(1)	178.28(14)
	N(5) <sup>i</sup> –Pt(1)–S(1)	90.32(14)	N(5) <sup>#1</sup> –Pt(1)–S(2)	178.19(14)
	N(1) <sup>i</sup> –Pt(1)–S(2)	90.25(14)	S(1)–Pt(1)–S(2)	91.32(7)
	N(5) <sup>i</sup> –Pt(1)–Pt(1) <sup>i</sup>	86.51(14)	N(1) <sup>i</sup> –Pt(1)–Pt(1) <sup>i</sup>	86.52(14)
	S(1)–Pt(1)–Pt(1) <sup>i</sup>	92.71(4)	S(2)–Pt(1)–Pt(1) <sup>i</sup>	92.67(5)
	symmetry code: i –x, –y+2, –z			
Intermolecular interactions	O(1)–H(1)•••N(6) <sup>ii</sup>	2.747(7)	C(21)–H(21A)•••O(4) <sup>iii</sup>	3.345(2)
	O(2)–H(2)•••O(3)	2.563(2)	C(22)–H(22C)•••O(4)	3.412(2)
	C(24)–H(24C)•••S(1)	3.793(2)	Cl(2)•••Cg(1) <sup>iv</sup>	3.333(5)
	Cl(1)•••Cg(2) <sup>v</sup>	3.448(4)		
	symmetry code: ii 1+x, y, z; iii 1–x, 2–y, 1–z; iv –1+x, y, 1+z; v 1–x, 1–y, –z			
Complex 3				
Pt–Pt	Pt(1)–Pt(1) <sup>i</sup>	2.7733(10)		
Pt–N	Pt(1)–N(1)	2.052(6)	Pt(1)–N(5)	2.052(6)
Pt–S	Pt(1)–S(1)	2.3004(19)	Pt(1)–S(2)	2.288(2)
	N(1)–Pt(1)–N(5)	91.4(2)	N(1)–Pt(1)–S(1)	179.15(16)
	N(5)–Pt(1)–S(1)	88.10(17)	N(5)–Pt(1)–S(2)	178.68(17)
	N(1)–Pt(1)–S(2)	89.32(17)	S(2)–Pt(1)–S(1)	91.16(7)
	N(5)–Pt(1)–Pt(1) <sup>i</sup>	85.80(18)	N(1)–Pt(1)–Pt(1) <sup>i</sup>	85.32(16)
	S(1)–Pt(1)–Pt(1) <sup>i</sup>	93.95(5)	S(2)–Pt(1)–Pt(1) <sup>i</sup>	93.16(6)
	symmetry code: i –x, 1–y, 1–z			
Intermolecular interactions	O(1)–H(1)•••O(3) <sup>ii</sup>	2.629(1)	C(20)–H(20)•••O(1)	3.346(2)
	O(2)–H(2)•••O(4) <sup>iii</sup>	2.595(9)	C(14)–H(14C)•••Cl(1)	3.501(1)
	C(24)–H(24A)•••O(5) <sup>iv</sup>	3.344(5)	C(24)–H(24B)•••O(2) <sup>v</sup>	3.254(5)
	C(24)–H(24C)•••S(1) <sup>iv</sup>	3.755(2)	C(25)–H(25B)•••O(5) <sup>vi</sup>	3.242(6)
	C(26)–H(26B)•••O(5) <sup>vi</sup>	3.197(5)	C(26)–H(26C)•••O(5) <sup>vii</sup>	3.290(4)
	C(27)–H(27B)•••N(2)	3.493(7)	Cg1•••Cg1 <sup>viii</sup>	3.337(4)
	symmetry code: ii –1+x, y, 1+z; iii x, 1+y, z; iv 1+x, y, z; v 1–x, 1–y, 1–z; vi x, y, 1+z; vii –x, –y, 1–z; viii –x, 1–y, 2–z			
Complex 4				
Pt–Pt	Pt(1)–Pt(1) <sup>i</sup>	2.7684(9)		
Pt–N	Pt(1)–N(1) <sup>i</sup>	2.027(9)	Pt(1)–N(5) <sup>i</sup>	2.044(9)
Pt–S	Pt(1)–S(1)	2.296(3)	Pt(1)–S(2)	2.281(3)
	N(1) <sup>i</sup> –Pt(1)–N(5) <sup>i</sup>	85.8(3)	N(1) <sup>i</sup> –Pt(1)–S(1)	177.1(3)
	N(5) <sup>i</sup> –Pt(1)–S(1)	91.5(2)	N(5) <sup>i</sup> –Pt(1)–S(2)	176.7(2)
	N(1) <sup>i</sup> –Pt(1)–S(2)	90.6(3)	S(2)–Pt(1)–S(1)	91.71(12)
	N(5) <sup>i</sup> –Pt(1)–Pt(1) <sup>i</sup>	86.9(2)	N(1) <sup>i</sup> –Pt(1)–Pt(1) <sup>i</sup>	86.5(3)
	S(1)–Pt(1)–Pt(1) <sup>i</sup>	92.07(8)	S(2)–Pt(1)–Pt(1) <sup>i</sup>	92.67(8)
	symmetry code: i –x, –y, 1–z			
Intermolecular interactions	O(1)–H(1)•••O(3) <sup>ii</sup>	2.591(2)	O(2)–H(2)•••O(4)	2.556(2)
	C(25)–H(25A)•••N(8)	3.430(2)	C(28)–H(28A)•••N(2) <sup>iii</sup>	3.360(2)
	C(21)–H(21)•••S(1) <sup>iv</sup>	3.52(2)	C(21)–H(21)•••O(1) <sup>iv</sup>	3.38(2)
	C(27)–H(27C)•••Cg1 <sup>v</sup>	3.808(2)		
	symmetry code: ii x, 1+y, z; iii 1/2+x, 1/2–y, –1/2+z; iv x, –1+y, z; v 1/2–x, 1/2+y, 1/2–z			





### The description of the hydrogen-bonding between the guest molecules and the subject stock part

The Guest DMSO molecules play an important role in the crystallization process of the complexes. As shown in Fig. S8a, the dinuclear units of **2** associate the DMSO molecules to generate a 1D chain through intermolecular hydrogen bonds (O–H...O, C–H...O, and C–H...S, Table S1), which consist in  $C_3^3(19)$  motifs. The guest DMSO molecules in **2** occupy channels viewed toward *b* axis (Fig. S8b). The channels are stabilized by a combination of Cl... $\pi$  stacking, and O–H...N interactions, with no specific packing motif dominating. For **3**, DMSO clusters occupy in the channels from the layers parallel packing (Fig. S8c and S8d). Unlike **2**, an extended 1D wave-like chain is formed through the  $\pi$ ... $\pi$  interactions along the *c* axis in **3**. The distance of  $\pi$ ... $\pi$  interactions between two phenol planes (Cg1...Cg1<sup>viii</sup> symmetry code: viii –*x*, 1–*y*, 2–*z*) is 3.337(4) Å in adjacent dinuclear units. For **4**, there are guest DMSO molecules between the antiparallel chains. The chains are linked into a 2D sheet by hydrogen bonds (Fig. S8e). Interestingly, the free DMSO molecules in the crystal lattice form an infinite ribbon-like chain along the *b* axis. It is the guest DMSO molecules that not only act as hydrogen bond donors to form C–H...N and C–H... $\pi$  interactions (C...N 3.360(2) Å, C...Cg1 3.808(2) Å, respectively, Table S1), but also act as acceptors to produce O–H...O (O...O 2.556(2) Å) hydrogen bonds. Finally, the packed structure shares the favorable combination of A and B channels due to existence of the propyl group along the *b* axis (Fig. S8f).



**Fig. S8** (a) 1D chain of **2** extend through free DMSO along the *a* axis. (b) View perpendicular to the solvent-filled (DMSO) channels of **2**. (c) 1D chain of **3** assembled from hydrogen bonds from solvent DMSO. (d) Solvated DMSO molecules are encapsulated in the channels of **3**. (e) The antiparallel chains of **4** assembled by intermolecular interactions from solvent DMSO. (f) The packed structure with combination of A and B channels in the channels of **4**.

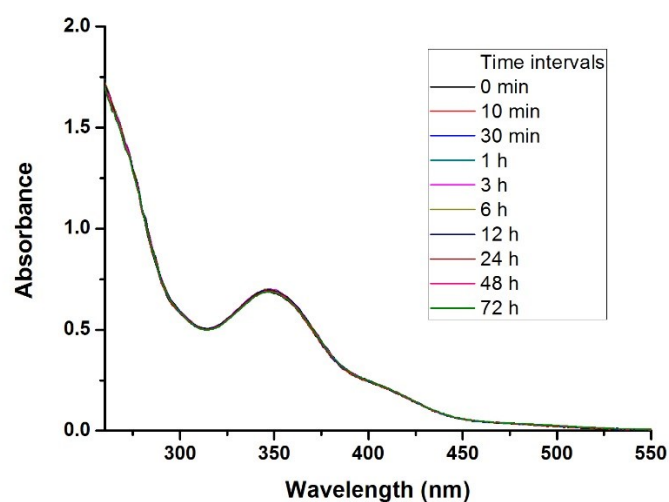


Fig. S9 Kinetic stability of 3 in PBS buffer solution including 10% DMSO within 72 h at 310K.

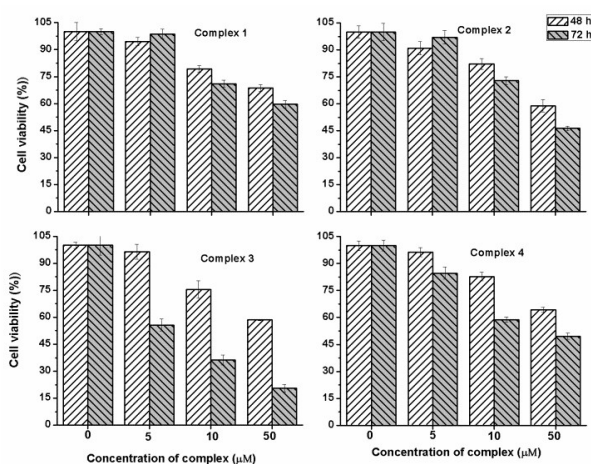


Fig. S10 Antiproliferation activities of 1–4 with different concentration (from left to right: 0 μM, 5 μM, 10 μM, and 50 μM) against HepG2 cell lines for 48 and 72 h.

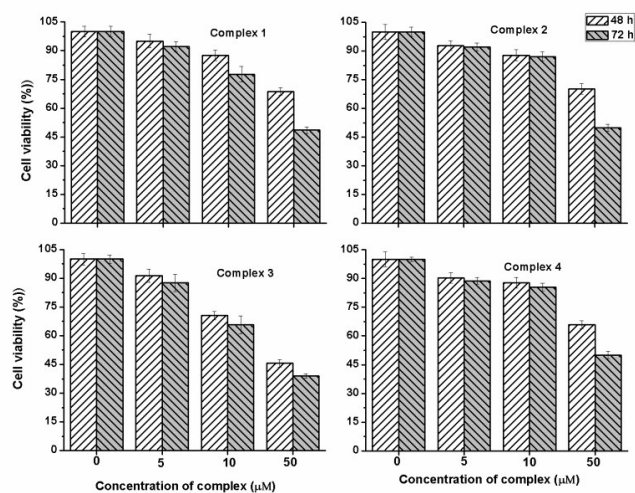
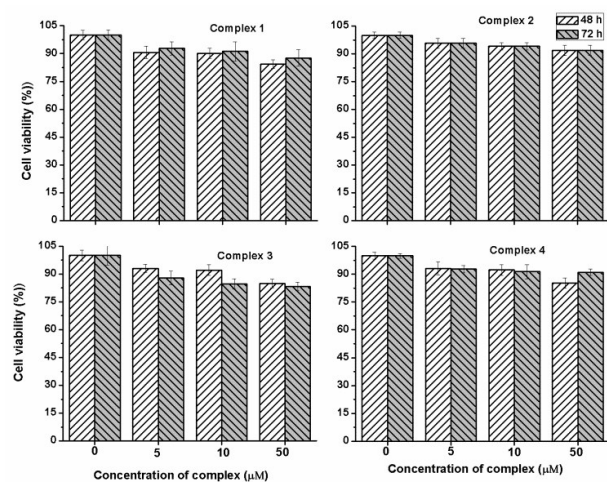
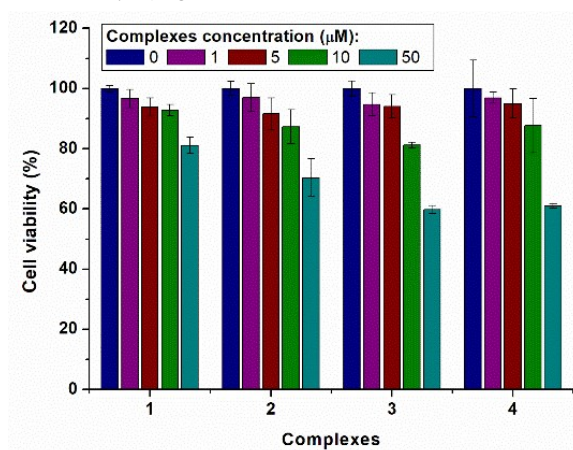


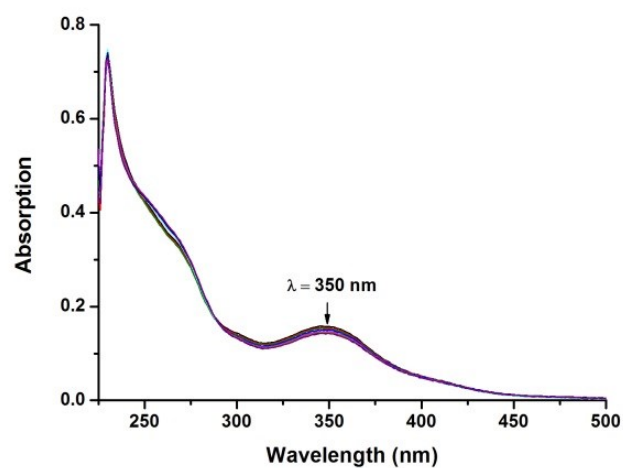
Fig. S11 Antiproliferation activities of 1–4 with different concentration (from left to right: 0 μM, 5 μM, 10 μM, and 50 μM) against MCF7 cell lines for 48 and 72 h.



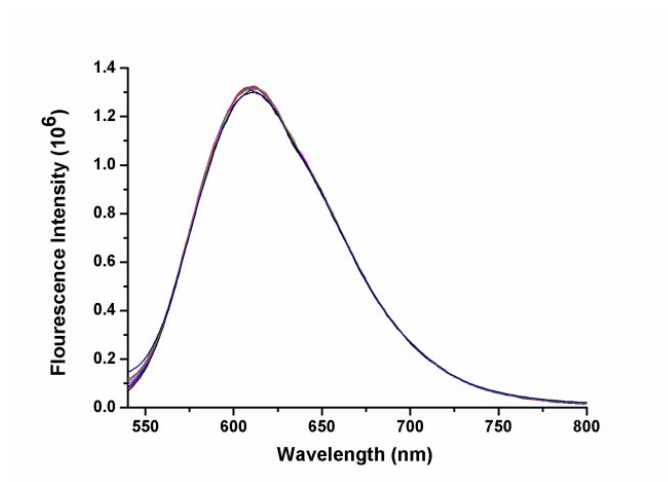
**Fig. S12** Antiproliferation activities of 1–4 with different concentration (from left to right: 0  $\mu\text{M}$ , 5  $\mu\text{M}$ , 10  $\mu\text{M}$ , and 50  $\mu\text{M}$ ) against A549 cell lines for 48 and 72 h.



**Fig. S13** Antiproliferation activities of 1–4 with different concentration (0  $\mu\text{M}$ , 5  $\mu\text{M}$ , 10  $\mu\text{M}$ , and 50  $\mu\text{M}$ ) against HL-7702 cell lines for 72 h.



**Fig. S14** Electronic absorption spectra of 3 (5  $\mu\text{M}$ ) upon the titration of CT-DNA (0–10  $\mu\text{M}$ ) in Tris-HCl buffer.



**Fig. S15** Emission spectra of EB bound to DNA in the absence and presence of increasing concentrations of **3** (0–20  $\mu\text{M}$ ) in Tris-HCl buffer.  $[\text{EB}] = 0.2 \mu\text{M}$ ,  $[\text{DNA}] = 1 \mu\text{M}$ .