Electronic Supplementary Material (ESI) for Metallomics.

Synthesis and antitumor mechanism of a copper(II) complex of anthracene-9-imidazoline hydrazone (9-AIH)

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Table S1. Selected bond lengths (Å) and bond angles (°) for the complex **1**.

bond lengths (Å)		bond angles (°)	
Cu(1)–O(1)	1.902(2)	O(1)– Cu(1)–O(2)	89.61(9)
Cu(1)–N(1)	1.967(2)	O(1)– Cu(1)–O(3)	90.29(9)
Cu(1)–O(2)	1.993(2)	O(1)– Cu(1)–N(1)	93.73(9)
Cu(1)–O(3)	2.322(2)	O(1)– Cu(1)–N(2)	173.51(9)
Cu(1)–N(2)	1.978(2)	O(2)– Cu(1)–O(3)	88.58(9)
Cu(2)–O(6)	1.896(19)	N(1)– Cu(1)–O(2)	168.43(9)
Cu(2)–O(7)	1.972(2)	N(1)– Cu(1)–O(3)	102.47(10)
Cu(2)–N(4)	1.963(2)	N(1)– Cu(1)–N(2)	83.16(9)
Cu(2)–N(5)	1.971(2)	N(2)– Cu(1)–O(2)	92.37(9)
Cu(2)–O(8)	2.413(3)	N(2)– Cu(1)–O(3)	95.93(9)

Table S2. The inhibitive ratios of complex **1** and 9-AIH against five selected tumor cell lines and one normal liver cell line HL-7702 for 48 h.

Compounds	Inhibition ratios (%, uniformly at 20 μM)					
	BEL-7404	HepG2	MGC80-3	NCI-H460	HeLa	HL-7702
9-AIH [a]	80.08±0.57	76.36±0.59	83.91±2.05	71.55±1.94	81.69±0.63	56.10±0.09
Complex **1** [a]	97.23±0.12	88.12±0.41	90.49±0.85	84.62±0.79	83.10±0.62	85.50±0.83
$CuCl_2•2H_2O$ [b]	15.44±1.02	16.33±0.94	10.25±0.78	8.05±0.76	12.84±1.52	11.65±1.01
Cisplatin [c]	65.15±1.08	60.63±0.99	71.35±1.46	61.85±1.69	80.56±0.92	73.58±2.30

Results represent mean ± SD of at least five independent experiments. SD represents the standard deviation. [a] The concentration is 2×10^{-5} mol/L. [b] The concentration is 1×10^{-4} mol/L. [c] Cisplatin was dissolved at a concentration of 1 mM in 0.154 M NaCl.

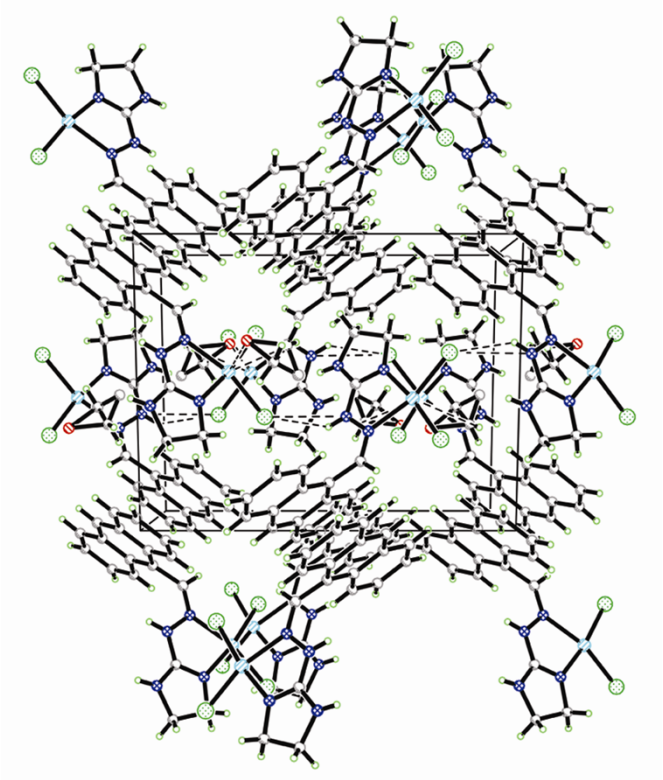


Figure S1. The stacking presentation of complex 1 viewed from the *c*-axis showing the N—H···Cl and C—H···Cl hydrogen bonding and π–π stacking between the neighboring anthracene groups.

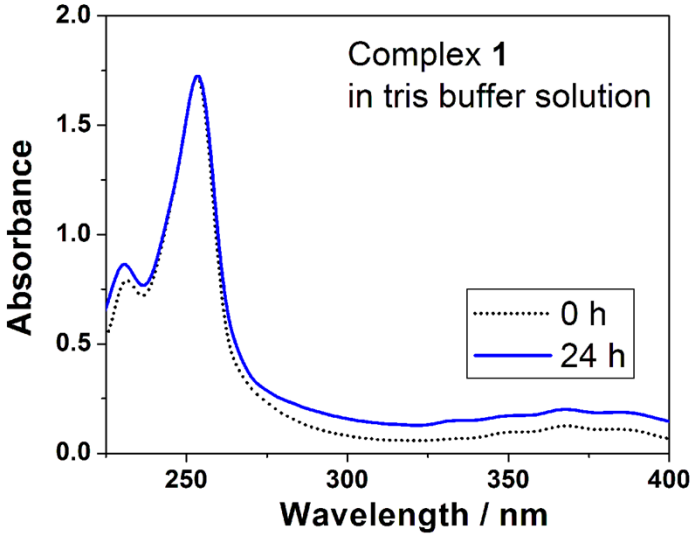


Figure S2. UV-vis spectrum of complex **1** in tris buffer solution (containing 5% DMSO) for 0 h

(dashed line) and for 24 h (solid line), respectively.

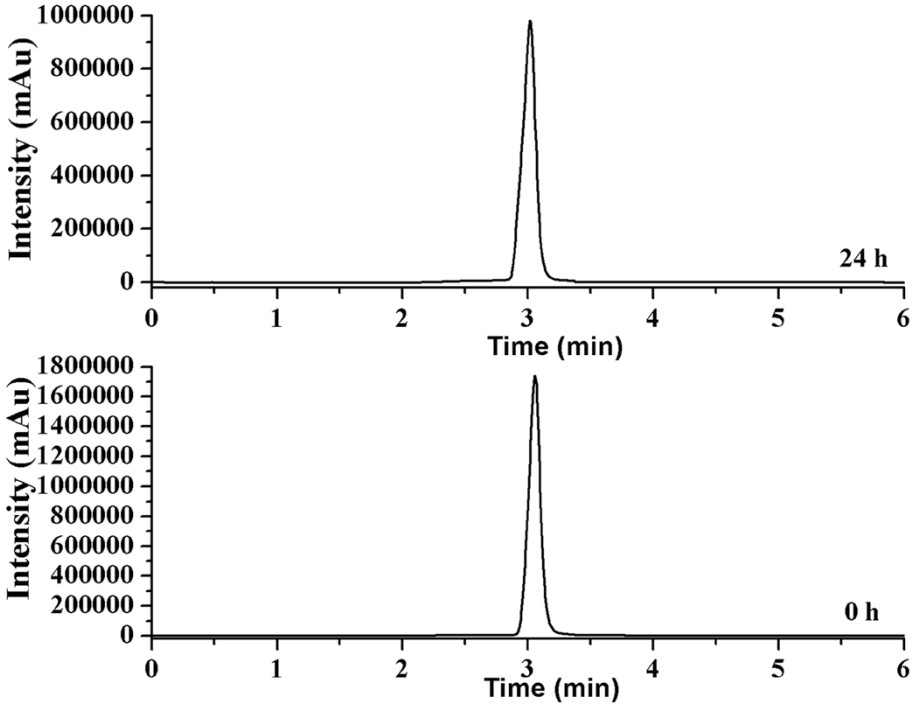
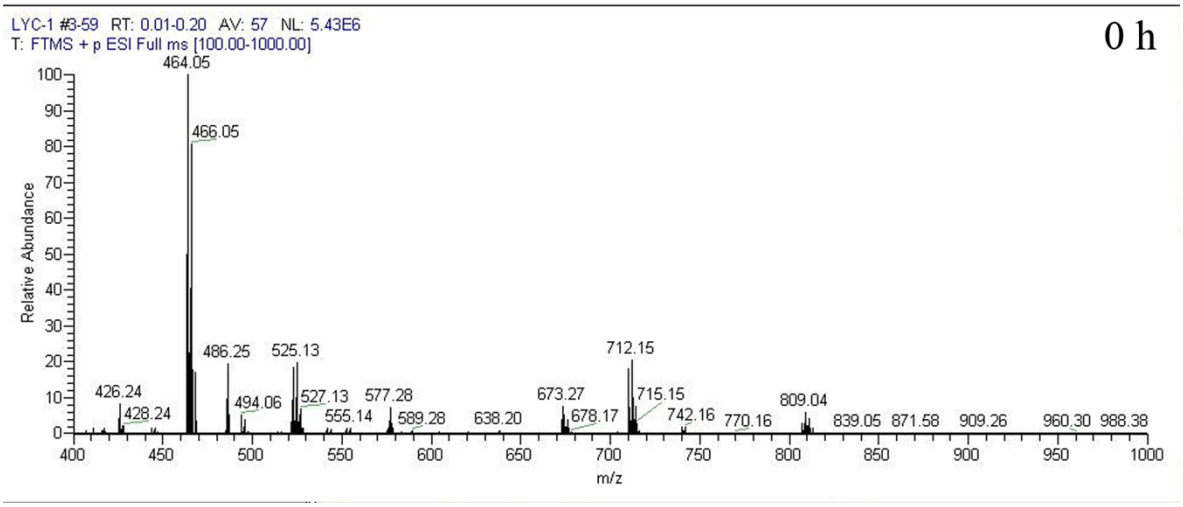


Figure S3. The time-dependent HPLC spectra for complex **1** (6.0×10^{-3} M stock solution in DMSO) with 0 h and 24 h. Column: Inertsustain C18 column (LC-20AT, SPD-20A HPLC Column, 150mm×5.0μm I. D.). Column temperature: 40ºC. Mobile phase: methanol/H_2O containing 0.01% TFA (85/15 as methanol/H_2O). Flow rate: 1.0 mL/min. Injection volume: 3.0×10^{-4} M.



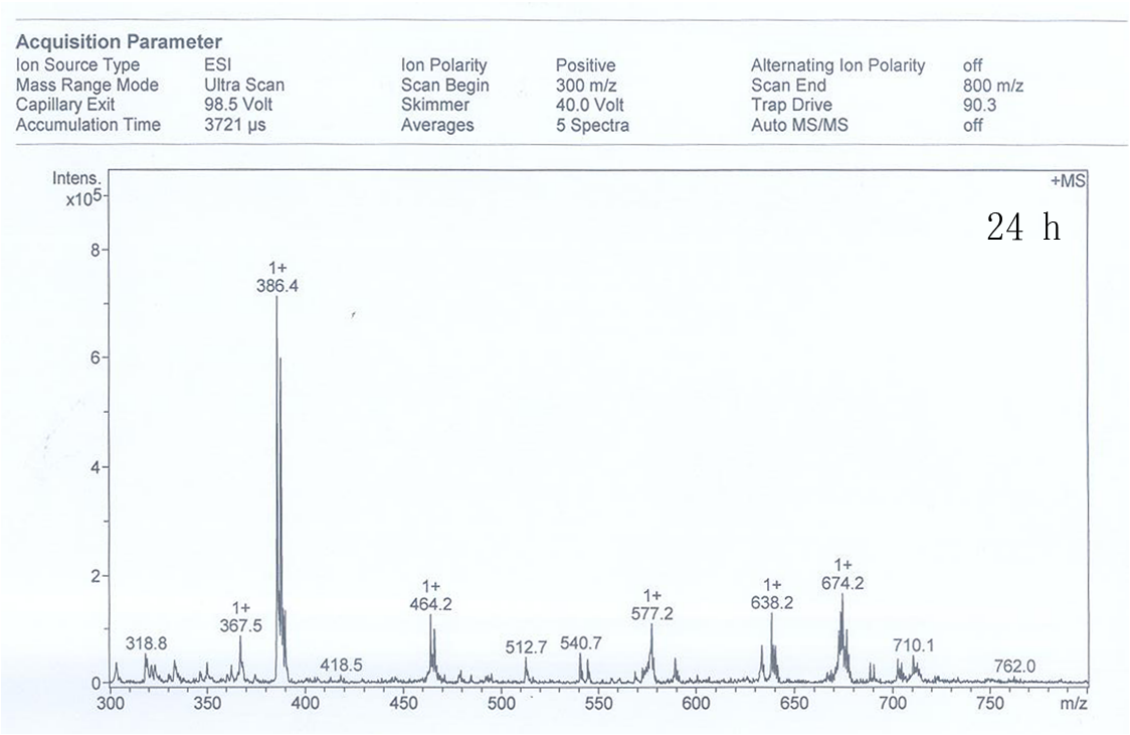


Figure S4. The mass spectra of complex **1** in tris buffer solution (containing 5% DMSO) for 0 h (top) and 24 h (down), respectively.

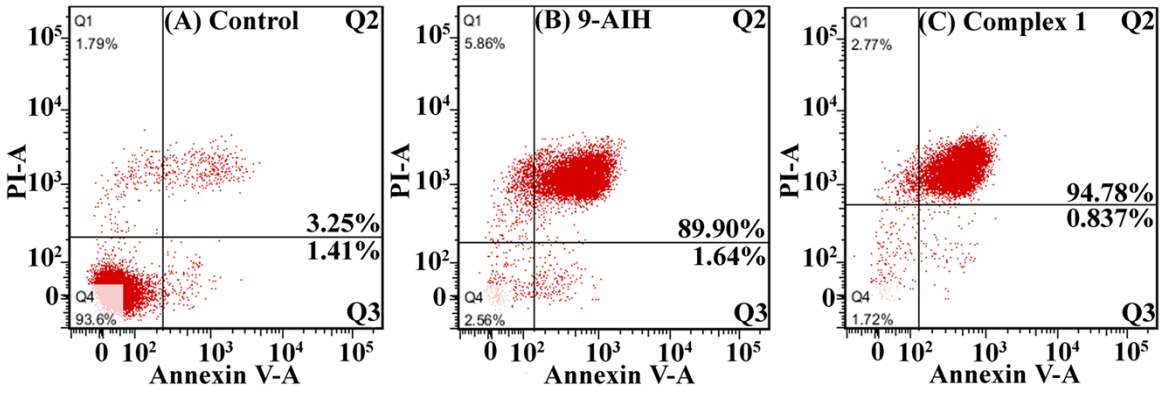


Figure S5. The significant cell apoptosis in BEL-7404 cells induced by 20 µM of 9-AIH and complex **1** for 24 h, respectively, which clearly showed that the apoptotic BEL-7404 cells in the late stage was predominant under the incubation of both compounds in such a high concentration.

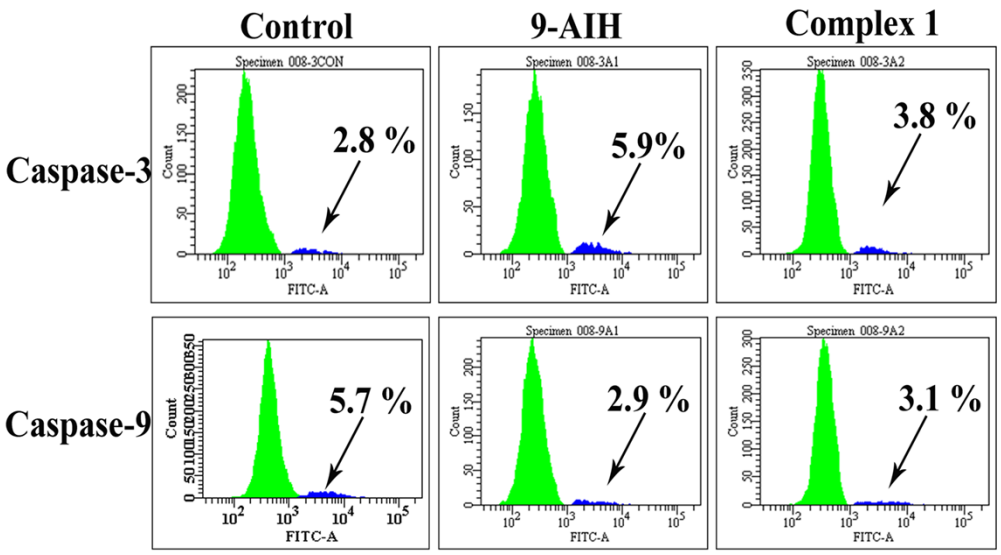


Figure S6. The expression level of caspase-9 and caspase-3 pro-apoptotic protein enhanced in BEL-7404 cells under the treatment of complex **1** and 9-AIH at 1.0 μM for 12 h. Caspase-3 was assessed using the CasPGLOW^{TM} Fluorescein Activite Caspase-3 Staining kit by flow cytometry.