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Supporting information

Studies on structures, cytotoxicity and apoptosis mechanism in T-24 cells of 8-hydroxylquinoline rhodium(III) complexes

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Table S1: Crystal data and structure refinement for complexes **1-2**.

Compound	**1**	**2**
Formula	$C_{28}H_{22}N_3O_4Rh$	$C_{19}H_{13}Br_2ClN_2O_3Rh$
Fw	567.40	615.48
T / K	293(2)	293(2)
crystal system	*monoclinic*	*triclinic*
space group	$P2_1/c$	*P-1*
a, *Å*	10.93140(10)	8.0116(6)
b, *Å*	13.1412(2)	11.7397(10)
c, *Å*	18.7929(3)	12.2484(7)
α, º	90.00	78.326(6)
b, º	117.0280(10)	88.221(5)
γ, º	90.00	89.460(6)
V, $Å^3$	2404.79(6)	1127.64(14)
Z	4	2

D_c, g cm^{-3}	1.567	1.863
μ, mm^{-1}	0.751	4.445
GOF on F^2	1.037	1.059
Reflns(collected/unique)	12805/4921	8353/3980
R_{int}	0.0242	0.0236
R_1[a] ($I > 2\sigma(I)$)	0.0288	0.0442
wR_2[b] (all data)	0.0685	0.1228

[a] $R_1 = \Sigma\ ||F_o| - |F_c||/\Sigma|F_o|$; [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)]$

Table S2 IC_{50} (μM) values of ligands and complexes **1**-**2** against five selected tumor cell lines and the normal human liver cell HL-7702 after treatment for 48 h.

Compounds	T-24	BEL7404	HepG2	MGC-803	SK-OV-3	HL-7702
HOQ	76.24±0.11	58.34±0.08	52.70±0.05	33.03±0.03	42.19±0.05	>100
HBrQ	>100	>100	39.53±0.05	43.77±0.04	36.34±0.05	43.77±0.05
Complex **1**	13.42±0.04	25.27±0.03	30.58±0.05	30.21±0.05	27.03±0.06	28.66±0.05
Complex **2**	18.91±0.04	22.93±0.03	25.33±0.04	41.90±0.07	28.67±0.06	25.29±0.04
Cisplatin	15.93±0.06	24.87±0.29	10.34±0.11	4.19±0.05	4.50±0.06	4.93±0.06

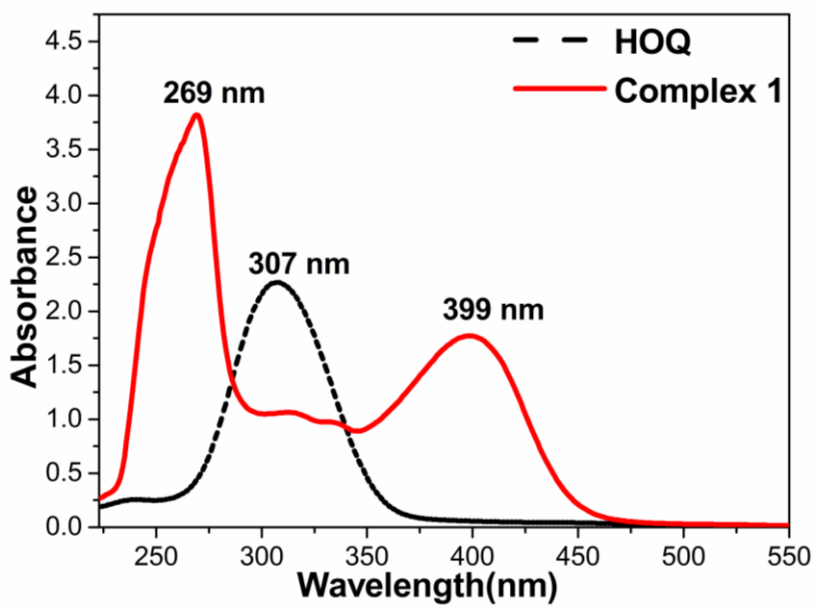

Figure S1. UV-Vis absorption spectra of HOQ and complex **1** (2.0×10^{-5} M).

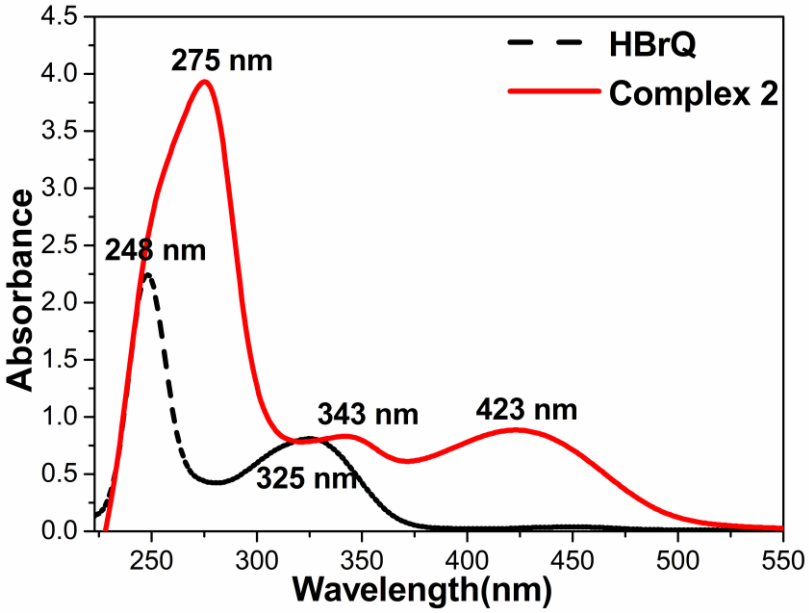

Figure S2. UV-Vis absorption spectra of HBrQ and complex **1** (2.0×10^{-5} M).

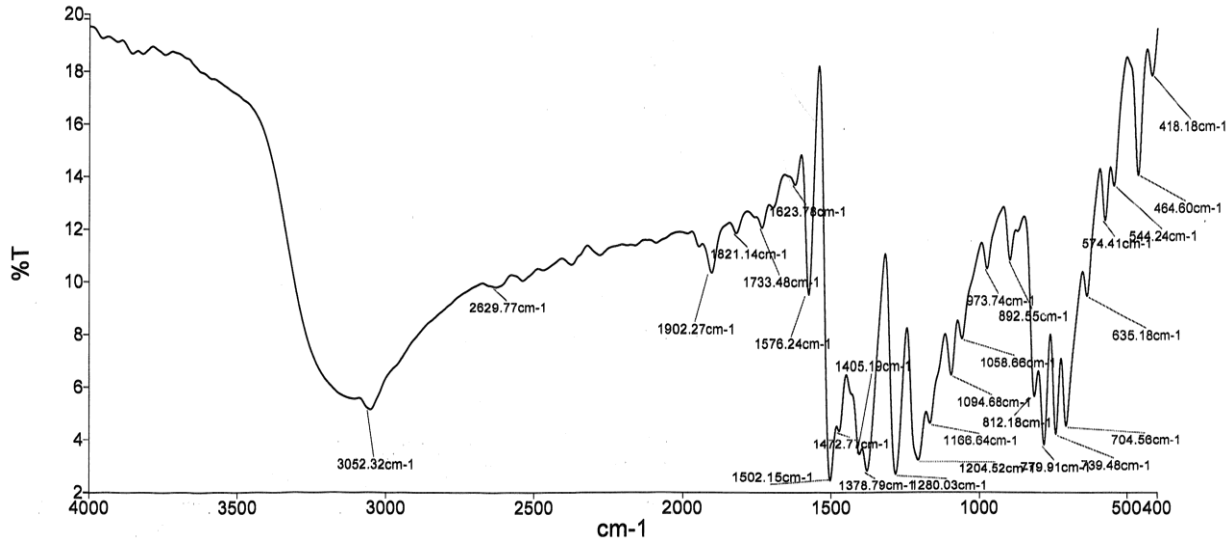

Figure S3. IR spectrum of HOQ.

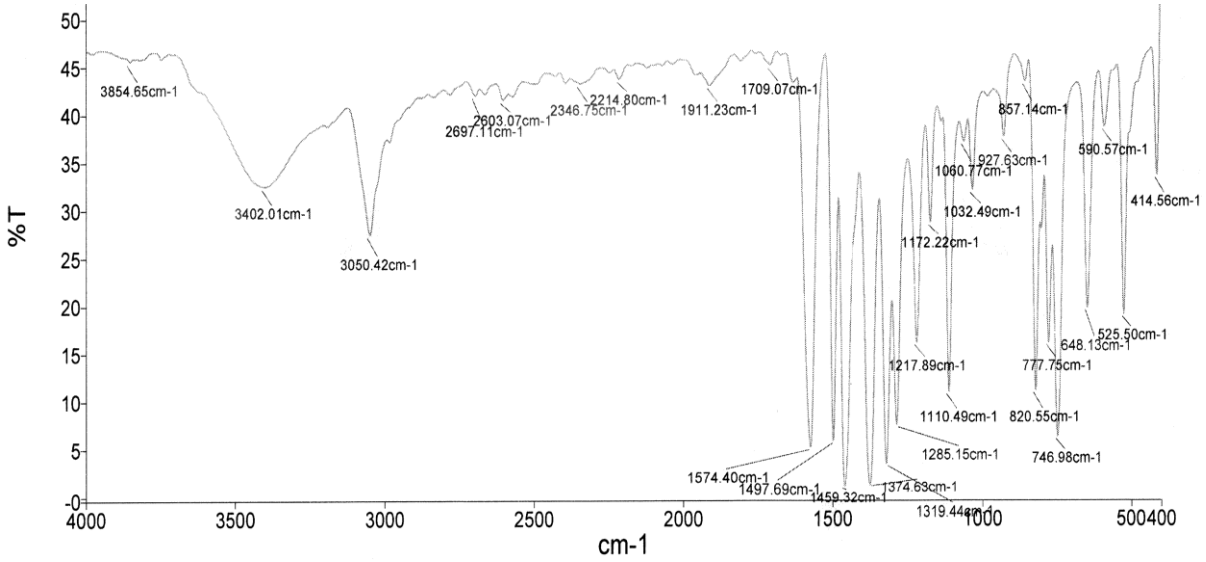

Figure S4. IR spectrum of complex **1**.

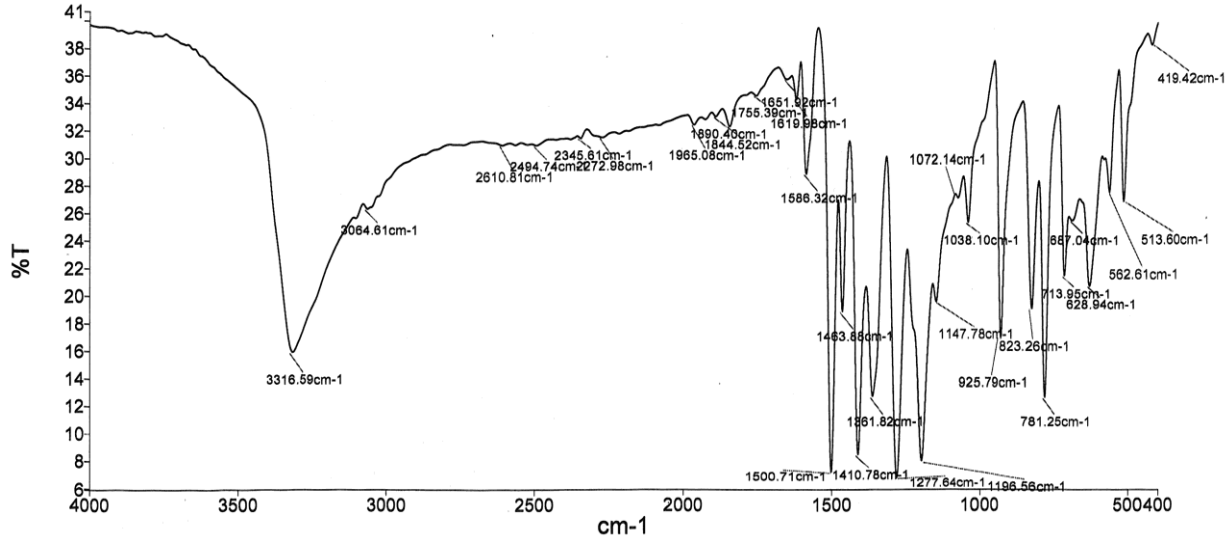

Figure S5. IR spectrum of HBrQ.

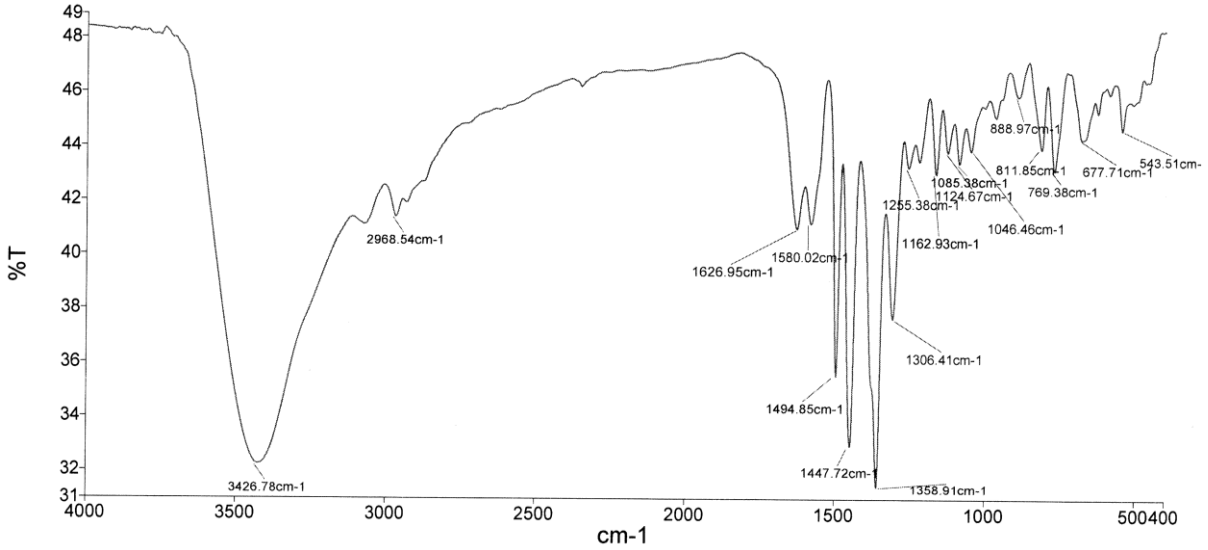

Figure S6. IR spectrum of complex **2**.

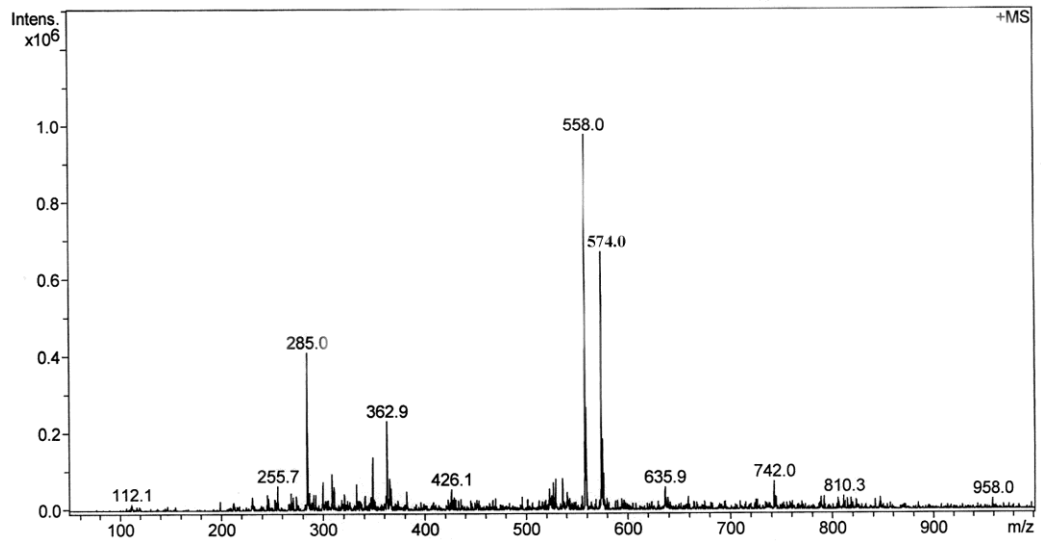

Figure S7. ESI-MS spectrum of complex **1**.

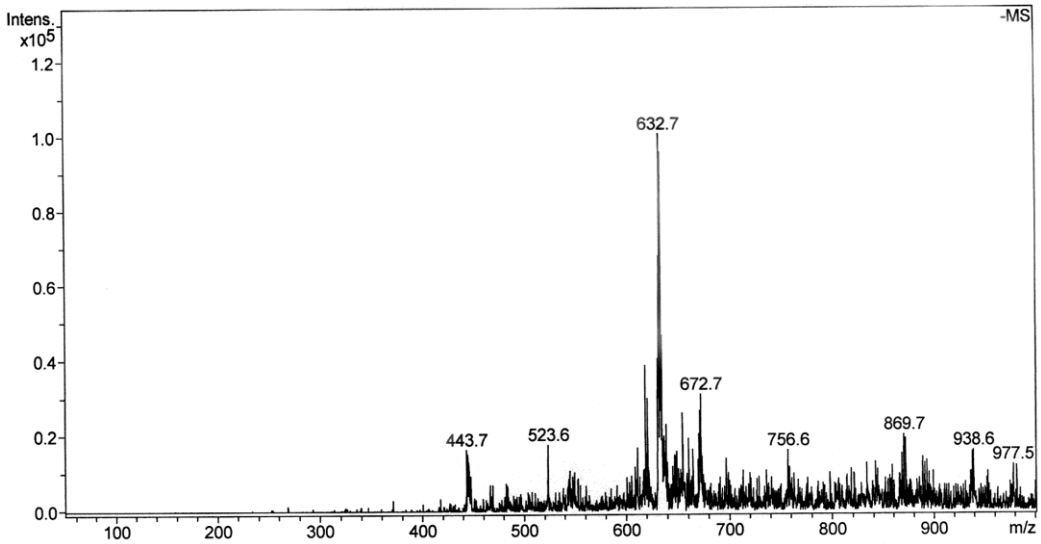

Figure S8. ESI-MS spectrum of complex **2**.

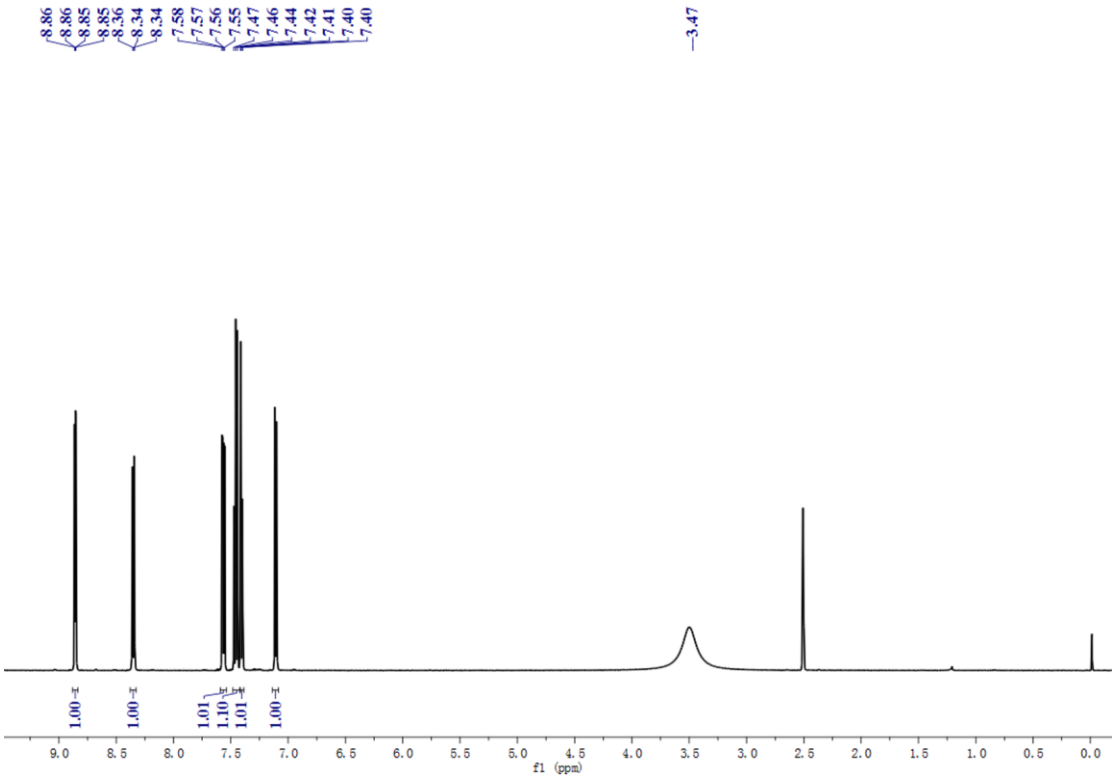

Figure S9. ^{1}H NMR spectrum of HOQ. (^{1}H NMR (600 MHz, DMSO-d_6) δ 8.86 (dd, J = 4.2, 1.6 Hz, 1H), 8.35 (dd, J = 8.3, 1.6 Hz, 1H), 7.57 (dd, J = 8.3, 4.2 Hz, 1H), 7.48 – 7.42 (m, 1H), 7.41 (dd, J = 8.2, 1.4 Hz, 1H), 7.11 (dd, J = 7.4, 1.4 Hz, 1H).)

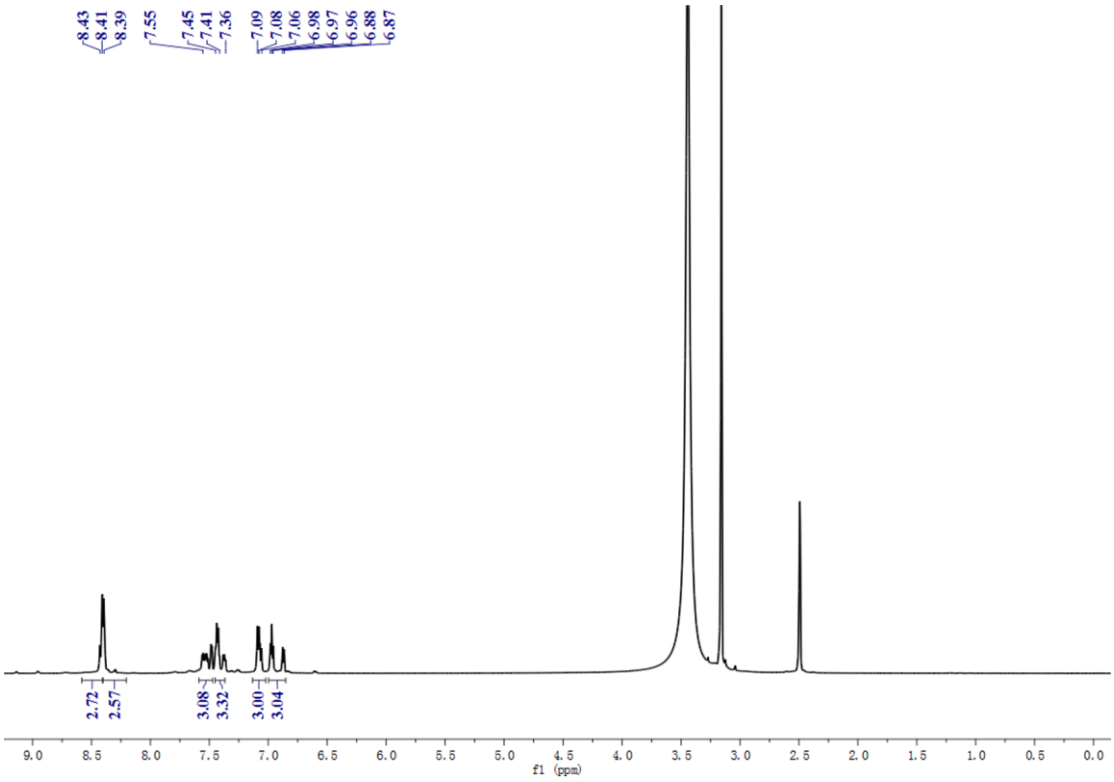

Figure S10. ^{1}H NMR spectrum of complex **1**.

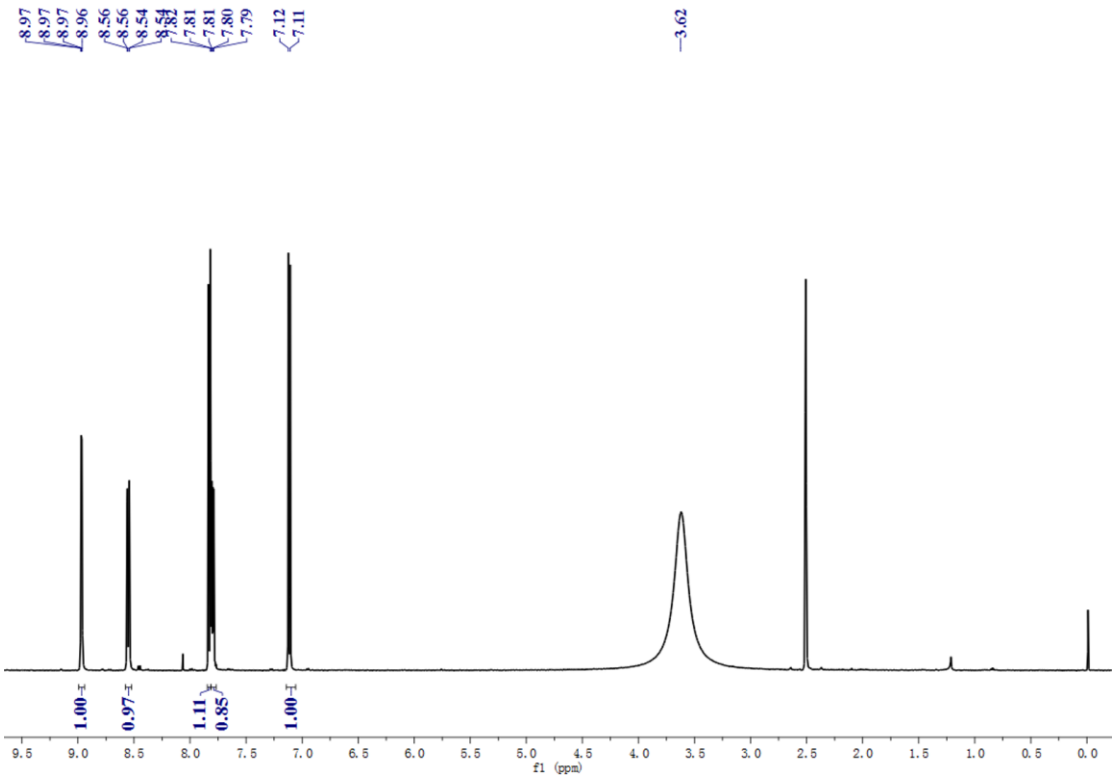

Figure S11. ^{1}H NMR spectrum of HBrQ. (^{1}H NMR (600 MHz, DMSO-d_6) 8.97 (dd, J = 4.3, 1.4 Hz, 1H), 8.55 (dd, J = 8.6, 1.2 Hz, 1H), 7.85 – 7.81 (m, 1H), 7.81 – 7.77 (m, 1H), 7.12 (d, J = 8.3 Hz, 1H).)

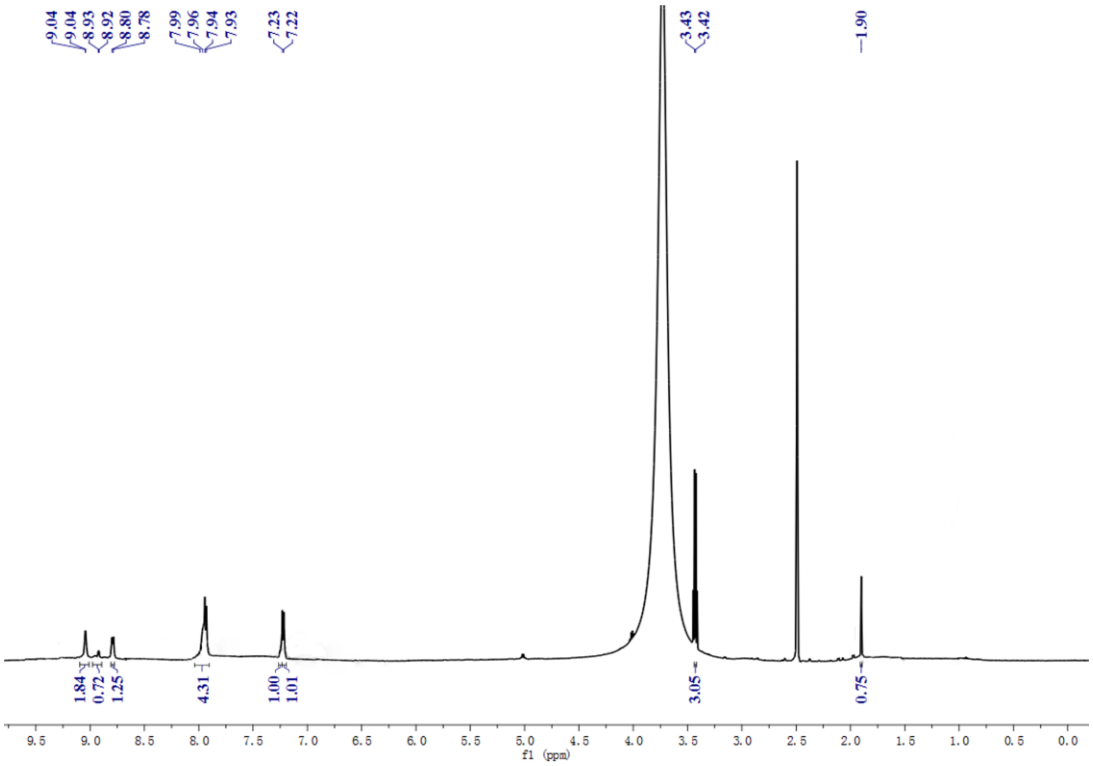

Figure S12. ^{1}H NMR spectrum of complex **2**.

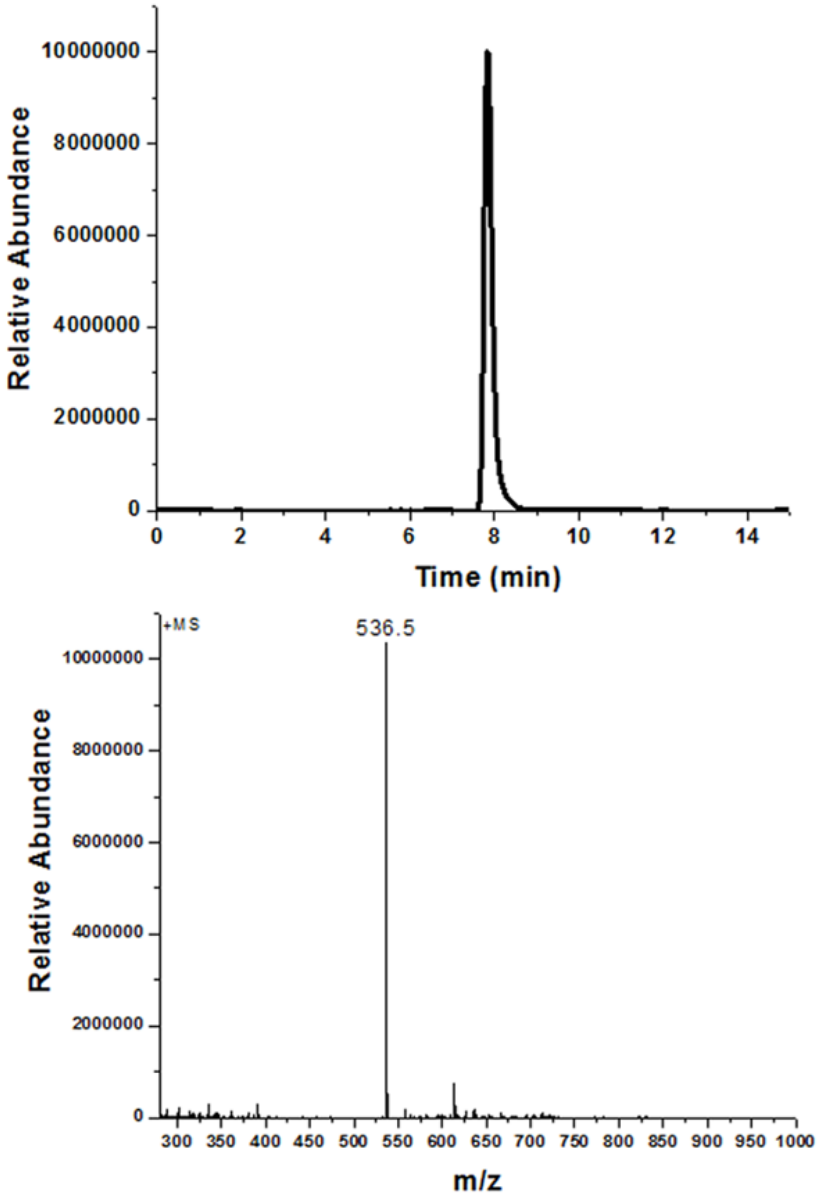

Figure S13. HPLC-MS spectra for complex **1** after keeping in water for 72 h. (2.0×10^{-3} M in aqueous solution containing 1% DMSO). Column: reversed-phase C18 column (YMC HPLC COLUMN, 150×4.6 mm I. D.). Column temperature: 30 ºC. Mobile phase: Methol/H_2O (70:30). Flow rate: 1.0 ml/min. Injection volume: 20 μM.

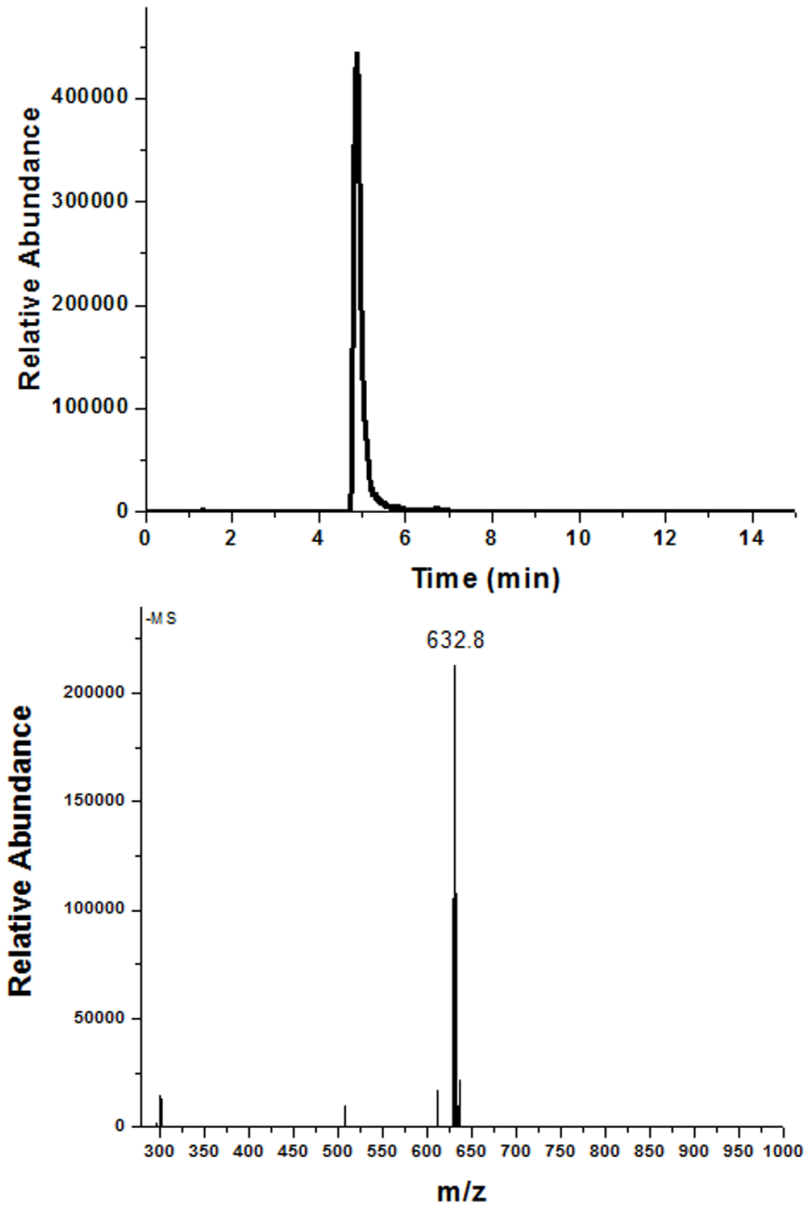

Figure S14. HPLC-MS spectra for complex **2** after keeping in water for 72 h. (2.0×10^{-3} M in aqueous solution containing 1% DMSO). Column: reversed-phase C18 column (YMC HPLC COLUMN, 150×4.6 mm I. D.). Column temperature: 30 ºC. Mobile phase: Methol/H_2O (60:40). Flow rate: 1.0 ml/min. Injection volume: 20 μM.