Electronic Supplementary Material (ESI) for MedChemComm.

Electronic Supporting Information Materials

Synthesis, crystal structure, cytotoxicity and action mechanism of Rh(III) complex with 8-hydroxy-2-methylquinoline as a ligand

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Table S1. Crystal data and structure refinement details for complex **1**.

Empirical formula	$C_{14}H_{20}Cl_2NO_3RhS_2$
Formula weight	488.26
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.9953(9)
b/Å	15.618(2)
c/Å	13.4715(15)
α /°	90
β /°	103.827(12)
γ /°	90
Volume/Å^3	1837.7(4)
Z	4
ρ_{calc}g/cm^3	1.7646
μ /mm^{-1}	1.459
F(000)	982.0
Crystal size/mm^3	0.22 × 0.2 × 0.18
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.22 to 52.74
Index ranges	-8 ⩽ h ⩽ 12, -18 ⩽ k ⩽ 21, -18 ⩽ l ⩽ 17
Reflections collected	7465
Independent reflections	3753 [R_{int} = 0.0903, R_{sigma} = 0.1174]
Data/restraints/parameters	3753/0/212
Goodness-of-fit on F^2	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0956, wR_2 = 0.2539
Final R indexes [all data]	R_1 = 0.1281, wR_2 = 0.2872
Largest diff. peak/hole / e Å^{-3}	3.84/-2.16

[a] $R_1 = \Sigma ||F_o| - |F_c||/\Sigma|F_o|$; [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

Table S2 Selected bond lengths (Å) and bond angles (°) for complex **1**.

Bond lengths (Å) for 1							
Rh1-S0aa	2.295(3)	Rh1-Cl	2.349(3)	Rh1-S1	2.282(3)	Rh1-O1aa	2.010(7)
Rh1-N	2.119(8)	Rh1-Cl8	2.359(3)				
Bond angles (°) for 1							
Cl-Rh1-S0aa	176.33(10)	S1-Rh1-S0aa	96.83(10)	S1-Rh1-Cl	86.83(11)	O1aa-Rh1-S0aa	88.6(2)
O1aa-Rh1-Cl	91.3(2)	O1aa-Rh1-S1	87.5(2)	N-Rh1-S0aa	88.2(2)	N-Rh1-Cl	88.1(2)
N-Rh1-S1	168.2(3)	N-Rh1-O1aa	82.0(3)	Cl8-Rh1-S0aa	89.30(12)	Cl8-Rh1-Cl	91.21(13)
Cl8-Rh1-S1	87.00(12)	Cl8-Rh1-O1aa	173.8(2)	Cl8-Rh1-N	103.8(3)	C4aa-S0aa-Rh1	115.0(5)

Table S3 Inhibition rates of H-MQ, $RhCl_3$, complex **1** and cisplatin towards five selected tumor cell lines and one normal liver cell HL-7702 for 48 h.

Compounds	BEL-7404	Hep-G2	NCI-H460	T-24	A549	HL-7702
H-MQ [a]	32.36±1.32	37.27±0.64	30.98±1.76	27.07±0.76	31.14±1.39	30.47±0.42
1 [a]	60.25±1.81	88.49±0.81	52.13±0.55	61.86±1.25	55.09±2.19	39.44±0.45
$RhCl_3$ [b]	10.58±1.09	18.55±0.56	19.11±0.74	20.18±1.94	14.32±0.83	10.85±1.63
Cisplatin[c]	55.15±1.18	60.63±0.99	50.88±1.29	46.86±1.06	52.18±1.47	68.95±1.42

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. NA represents no activity.

Table S4. IC_{50}[a] (μM) values of H-MQ, $RhCl_3$, complex **1** and cisplatin towards normal liver cell HL-7702 and the selected tumor cell lines.

Compounds	BEL-7404	Hep-G2	NCI-H460	T-24	A549	HL-7702
H-MQ	152.45±1.04	137.35±0.58	168.92±1.65	187.54±0.69	107.56±1.03	170.65±0.34
1	10.33±1.74	6.52±0.83	17.86±0.65	9.87±1.23	15.07±2.33	28.74±0.38
$RhCl_3$	＞100	＞100	＞100	＞100	＞100	＞100
Cisplatin[c]	12.41±0.38	9.48±0.35	18.89±1.02	28.86±1.05	18.19±1.39	15.67±1.27

[a] IC_{50} values are presented as the mean ± SD (standard error of the mean) from five independent experiments. [b] The concentration unit is μM. [c] Cisplatin was dissolved at a concentration of 1 mM in 0.154 M NaCl.

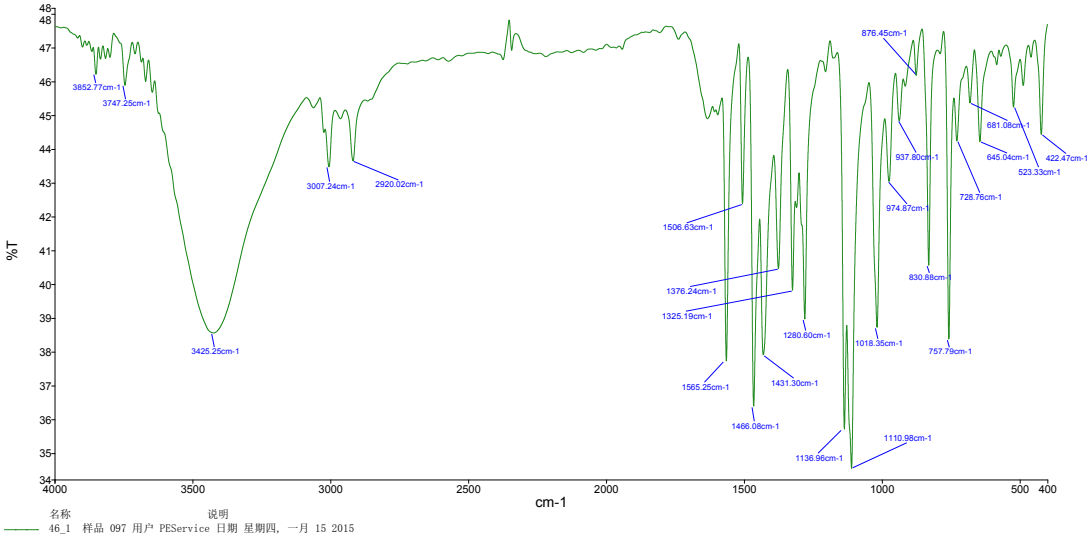

Figure S1. IR (KBr) spectra of complex **1**.

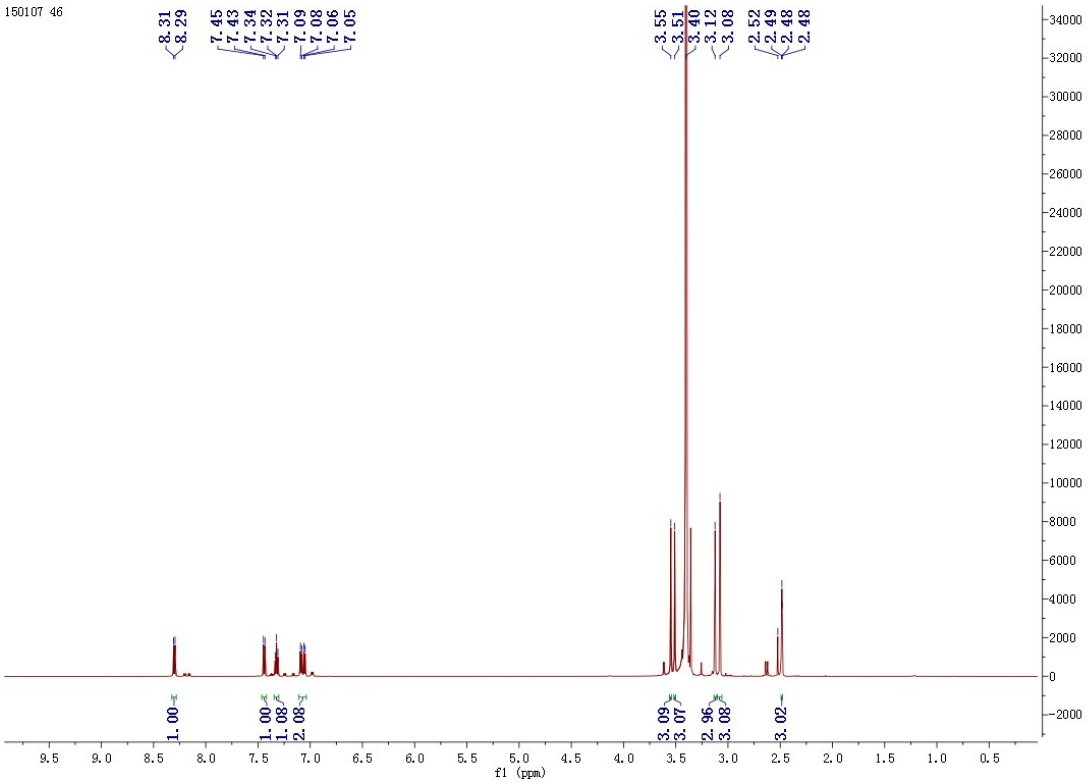

Figure S2. ^{1}H NMR (600 MHz, DMSO-d_6) for complex **1.**

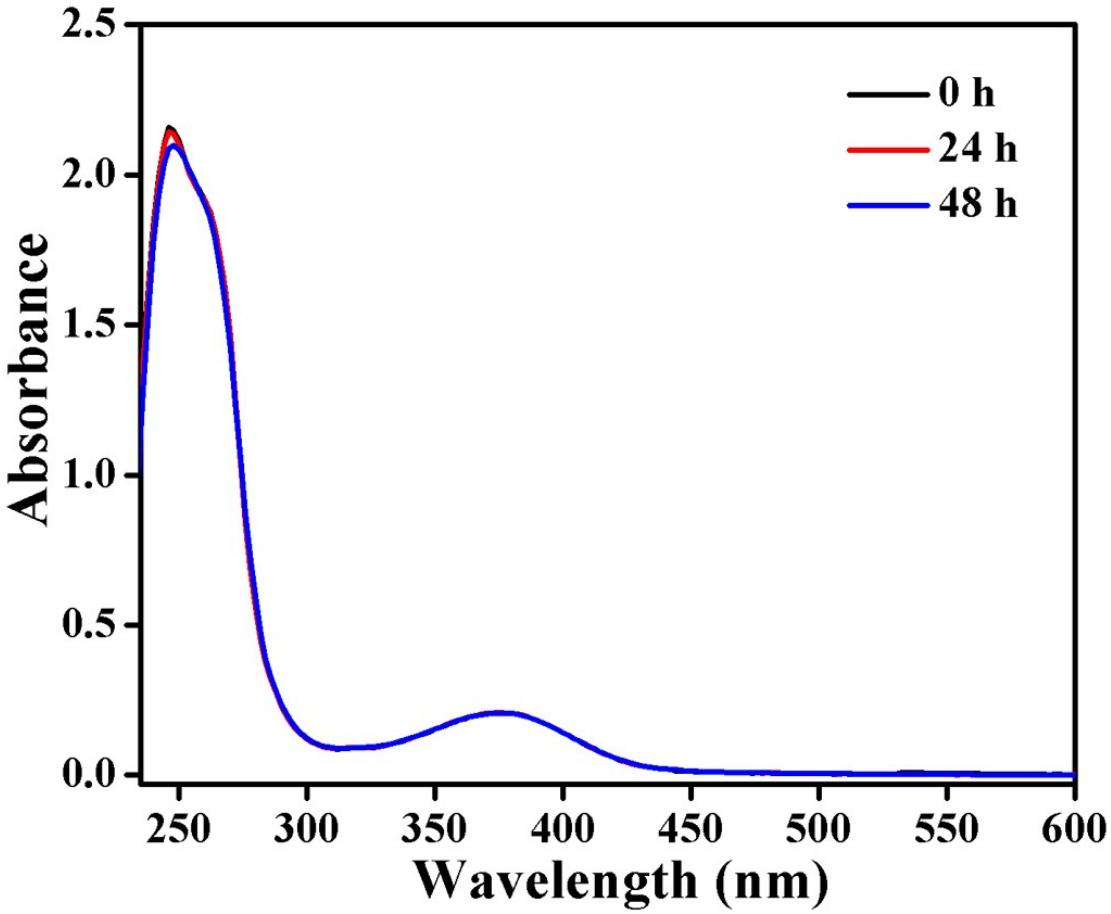

Figure S3. UV-Vis absorption spectra of complex **1** (4.0×10^{-5} M) in Tris-HCl solution (TBS) in the time course 0, 24 and 48 h, respectively.

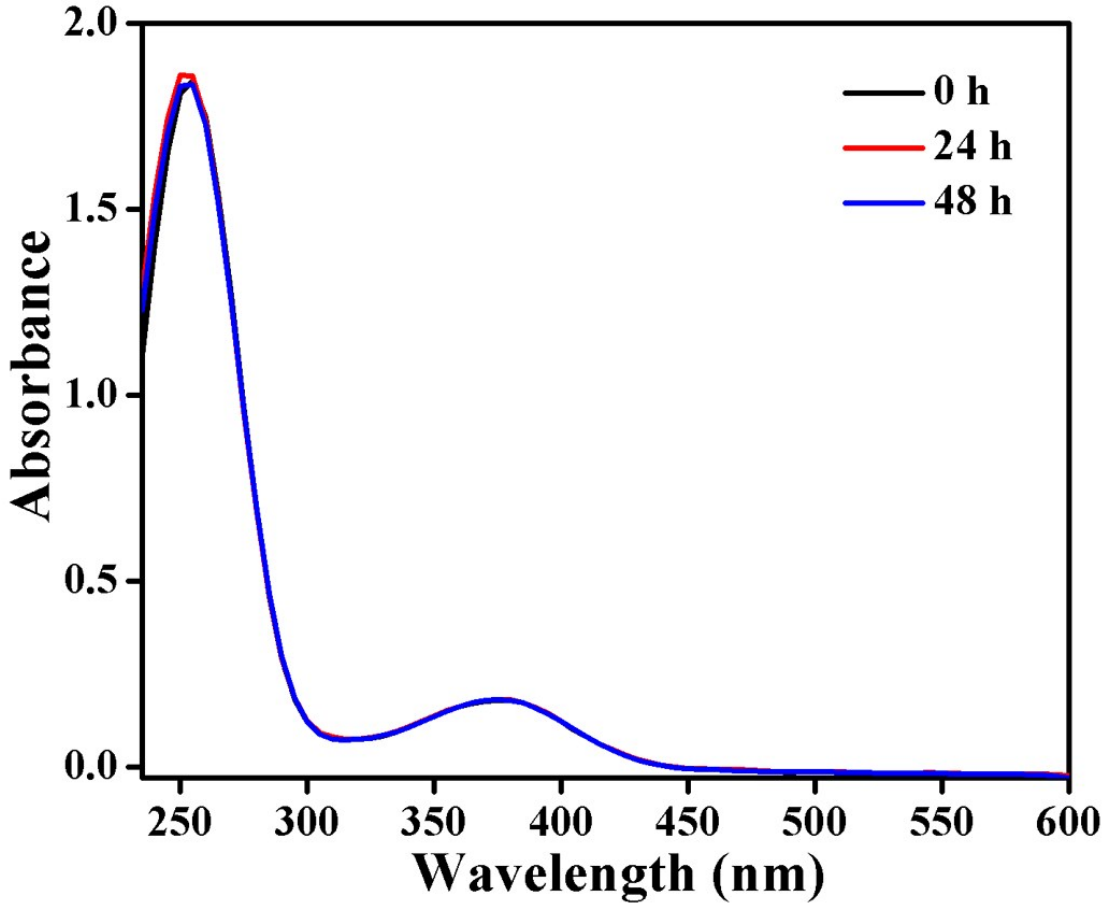

Figure S4. UV-Vis absorption spectra of complex **1** (4.0×10^{-5} M) in water in the time course 0, 24 and 48 h, respectively.

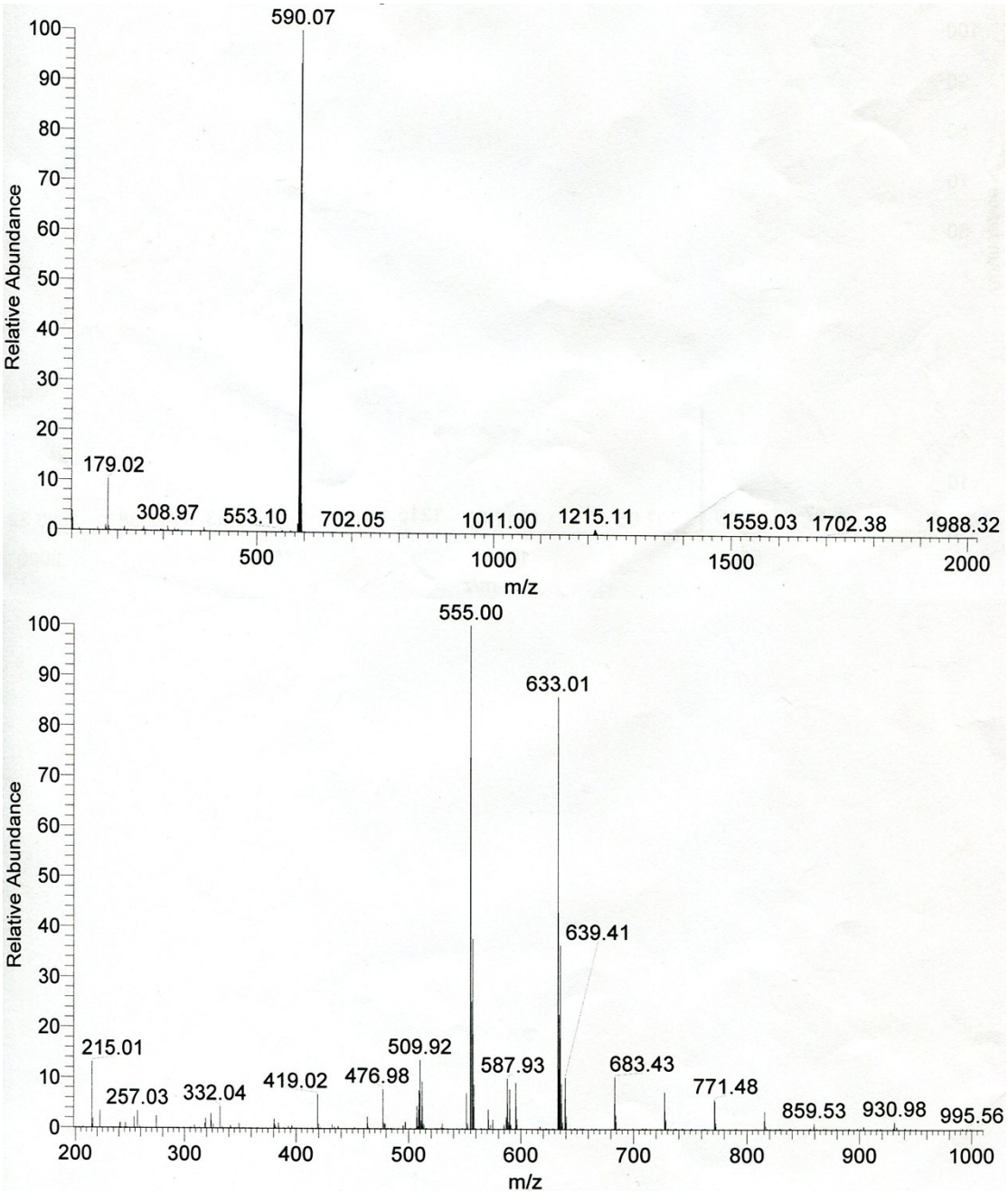

Figure S5. The mass spectra of complex **1** in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.