Electronic Supporting Information Materials

Discovery of high *in vitro* and *in vivo* antitumor activities of organometallic ruthenium(II)-arene complexes with 5,7-dihalogenated-2-methyl-8-quinolinol

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Table S1. Crystal data and structure refinement details for **4.**

Empirical formula	$C_{19}H_{17}Br_2ClNORu$
Formula weight	571.67
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.3091(5)
b/Å	7.9928(3)
c/Å	16.1335(5)
α/°	90
β/°	102.4800(10)
γ/°	90
Volume/Å^3	1927.49(11)
Z	4
ρ_{calc}mg/mm^3	1.970
m/mm^{-1}	5.105
F(000)	1108.0
Crystal size/mm^3	0.377 × 0.238 × 0.219
2Θ range for data collection	5.78 to 55.128°
Index ranges	$-19 \leq h \leq 19$, $-10 \leq k \leq 10$, $-20 \leq l \leq 20$
Reflections collected	39514
Independent reflections	4449[R(int) = 0.0313]
Data/restraints/parameters	4449/7/240
Goodness-of-fit on F^2	1.122
Final R indexes [I>=2σ (I)]	$R_1 = 0.0329$, $wR_2 = 0.0785$
Final R indexes [all data]	$R_1 = 0.0418$, $wR_2 = 0.0828$
Largest diff. peak/hole / e Å^{-3}	0.71/-1.23

[a] $R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$; [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2 / \Sigma w(F_o^2)^2]^{½}$.

Table S2. Selected bond lengths (Å) for **4**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	Cl1	2.4217(8)	C4	C5	1.403(6)
Ru1	O1	2.074(2)	C4	C9	1.419(4)
Ru1	N1	2.095(2)	C5	C6	1.365(6)
Ru1	C11	2.201(3)	C6	C7	1.407(5)
Ru1	C12	2.173(3)	C7	C8	1.383(5)
Ru1	C13	2.155(3)	C8	C9	1.424(5)
Ru1	C14	2.178(3)	C10	C11	1.488(5)
Ru1	C15	2.181(3)	C11	C12	1.398(5)
Ru1	C16	2.193(3)	C11	C16	1.429(5)
Br1	C7	1.889(4)	C12	C13	1.411(5)
Br2	C5	1.894(4)	C13	C14	1.408(5)
O1	C8	1.304(4)	C14	C15	1.422(5)
N1	C1	1.324(4)	C14	C17	1.516(5)
N1	C9	1.369(4)	C15	C16	1.388(5)
C1	C2	1.407(5)	C17	C18	1.505(7)
C2	C3	1.345(6)	C17	C19	1.412(9)
C3	C4	1.413(6)	C17	C19'	1.364(10)

Table S3. Selected bond lengths (Å) and bond angles (°) for **4**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	Cl1	86.25(7)	C5	C4	C3	127.0(3)
O1	Ru1	N1	78.68(10)	C5	C4	C9	116.6(3)
O1	Ru1	C11	155.34(11)	C4	C5	Br2	119.9(3)
O1	Ru1	C12	156.40(12)	C6	C5	Br2	118.5(3)
O1	Ru1	C13	118.38(12)	C6	C5	C4	121.7(3)
O1	Ru1	C14	91.10(11)	C5	C6	C7	120.5(4)
O1	Ru1	C15	92.09(11)	C6	C7	Br1	119.7(3)
O1	Ru1	C16	117.60(11)	C8	C7	Br1	118.7(3)
N1	Ru1	Cl1	83.16(7)	C8	C7	C6	121.6(4)
N1	Ru1	C11	125.55(12)	O1	C8	C7	123.9(3)
N1	Ru1	C12	99.18(12)	O1	C8	C9	119.6(3)
N1	Ru1	C13	94.99(12)	C7	C8	C9	116.5(3)
N1	Ru1	C14	116.81(12)	N1	C9	C4	122.3(3)
N1	Ru1	C15	153.75(12)	N1	C9	C8	114.7(3)
N1	Ru1	C16	163.43(12)	C4	C9	C8	123.0(3)
C11	Ru1	Cl1	91.90(9)	C10	C11	Ru1	127.6(2)
C12	Ru1	Cl1	117.02(10)	C12	C11	Ru1	70.29(18)
C12	Ru1	C11	37.28(13)	C12	C11	C10	121.8(3)
C12	Ru1	C14	68.66(13)	C12	C11	C16	117.6(3)
C12	Ru1	C15	79.51(12)	C16	C11	Ru1	70.72(18)

C12	Ru1	C16	67.28(13)	C16	C11	C10	120.5(4)
C13	Ru1	Cl1	154.57(10)	C11	C12	Ru1	72.43(18)
C13	Ru1	C11	68.50(14)	C11	C12	C13	121.6(3)
C13	Ru1	C12	38.05(14)	C13	C12	Ru1	70.27(19)
C13	Ru1	C14	37.91(13)	C12	C13	Ru1	71.68(19)
C13	Ru1	C15	67.67(13)	C14	C13	Ru1	71.9(2)
C13	Ru1	C16	80.18(13)	C14	C13	C12	121.1(3)
C14	Ru1	Cl1	158.95(9)	C13	C14	Ru1	70.15(19)
C14	Ru1	C11	81.87(13)	C13	C14	C15	117.1(3)
C14	Ru1	C15	38.08(13)	C13	C14	C17	122.7(4)
C14	Ru1	C16	68.41(13)	C15	C14	Ru1	71.1(2)
C15	Ru1	Cl1	121.07(10)	C15	C14	C17	120.1(4)
C15	Ru1	C11	67.90(12)	C17	C14	Ru1	127.4(3)
C15	Ru1	C16	36.99(13)	C14	C15	Ru1	70.85(18)
C16	Ru1	Cl1	94.39(9)	C16	C15	Ru1	71.97(19)
C16	Ru1	C11	37.97(13)	C16	C15	C14	122.0(3)
C8	O1	Ru1	113.77(19)	C11	C16	Ru1	71.31(18)
C1	N1	Ru1	127.6(2)	C15	C16	Ru1	71.04(19)
C1	N1	C9	119.1(3)	C15	C16	C11	120.6(3)
C9	N1	Ru1	113.2(2)	C18	C17	C14	113.8(4)
N1	C1	C2	121.5(4)	C19	C17	C14	111.2(5)
C3	C2	C1	120.4(4)	C19	C17	C18	122.8(6)
C2	C3	C4	120.3(3)	C19'	C17	C14	123.3(7)
C3	C4	C9	116.4(4)	C19'	C17	C18	115.9(7)

Table S4. Crystal data and structure refinement details for **9.**

Empirical formula	$C_{19}H_{18}Br_2INORu$
Formula weight	664.13
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	10.6379(5)
b/Å	14.7384(6)
c/Å	13.1395(5)
α/°	90
β/°	101.9650(10)
γ/°	90
Volume/Å^3	2015.33(15)
Z	4
ρ_{calc}mg/mm^3	2.189

m/mm^{-1}	6.282
F(000)	1256.0
Crystal size/mm^3	0.459 × 0.234 × 0.122
2Θ range for data collection	6.178 to 55.08°
Index ranges	-13 ≤ h ≤ 13, -19 ≤ k ≤ 19, -17 ≤ l ≤ 17
Reflections collected	30119
Independent reflections	4627[R(int) = 0.0413]
Data/restraints/parameters	4627/0/229
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R_1 = 0.0288, wR_2 = 0.0601
Final R indexes [all data]	R_1 = 0.0450, wR_2 = 0.0654
Largest diff. peak/hole / e Å^{-3}	0.73/-1.01

Table S5. Selected bond lengths (Å) for **9**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	Ru1	2.7172(4)	C4	C5	1.410(5)
Ru1	O1	2.075(2)	C4	C9	1.415(5)
Ru1	N1	2.090(3)	C5	C6	1.361(5)
Ru1	C13	2.207(3)	C6	C7	1.401(5)
Ru1	C14	2.191(3)	C7	C8	1.385(5)
Ru1	C15	2.190(4)	C8	C9	1.432(5)
Ru1	C16	2.190(4)	C10	C11	1.519(6)
Ru1	C18	2.160(3)	C11	C12	1.528(5)
Ru1	C19	2.177(3)	C11	C13	1.508(5)
Br1	C7	1.880(3)	C13	C14	1.440(5)
Br2	C5	1.893(3)	C13	C19	1.407(5)
O1	C8	1.298(4)	C14	C15	1.380(5)
N1	C1	1.324(5)	C15	C16	1.420(5)
N1	C9	1.368(4)	C16	C17	1.506(6)
C1	C2	1.395(6)	C16	C18	1.403(5)
C2	C3	1.349(6)	C18	C19	1.423(5)
C3	C4	1.407(5)			

Table S6. Selected bond lengths (Å) and bond angles (°) for **9**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	I1	85.12(7)	C3	C4	C5	126.4(3)
O1	Ru1	N1	78.76(10)	C3	C4	C9	116.9(3)
O1	Ru1	C13	159.38(11)	C5	C4	C9	116.6(3)
O1	Ru1	C14	121.20(11)	C4	C5	Br2	119.7(3)
O1	Ru1	C15	94.27(12)	C6	C5	Br2	118.9(3)

O1	Ru1	C16	90.63(12)	C6	C5	C4	121.4(3)
O1	Ru1	C18	115.57(13)	C5	C6	C7	120.7(3)
O1	Ru1	C19	153.43(12)	C6	C7	Br1	118.5(3)
N1	Ru1	I1	85.50(8)	C8	C7	Br1	119.2(3)
N1	Ru1	C13	121.70(12)	C8	C7	C6	122.2(3)
N1	Ru1	C14	159.82(13)	O1	C8	C7	124.8(3)
N1	Ru1	C15	155.85(13)	O1	C8	C9	119.5(3)
N1	Ru1	C16	118.47(14)	C7	C8	C9	115.8(3)
N1	Ru1	C18	94.58(13)	N1	C9	C4	122.1(3)
N1	Ru1	C19	96.05(12)	N1	C9	C8	114.6(3)
C13	Ru1	I1	93.47(9)	C4	C9	C8	123.3(3)
C14	Ru1	I1	92.89(9)	C10	C11	C12	111.0(4)
C14	Ru1	C13	38.23(13)	C13	C11	C10	114.6(3)
C15	Ru1	I1	117.21(10)	C13	C11	C12	108.2(3)
C15	Ru1	C13	68.07(14)	C11	C13	Ru1	131.3(2)
C15	Ru1	C14	36.72(14)	C14	C13	Ru1	70.30(19)
C16	Ru1	I1	154.37(11)	C14	C13	C11	119.7(3)
C16	Ru1	C13	81.76(14)	C19	C13	Ru1	70.14(19)
C16	Ru1	C14	67.85(14)	C19	C13	C11	123.2(3)
C16	Ru1	C15	37.84(14)	C19	C13	C14	117.0(3)
C18	Ru1	I1	158.98(10)	C13	C14	Ru1	71.47(19)
C18	Ru1	C13	68.60(13)	C15	C14	Ru1	71.6(2)
C18	Ru1	C14	79.83(14)	C15	C14	C13	121.5(3)
C18	Ru1	C15	67.38(14)	C14	C15	Ru1	71.7(2)
C18	Ru1	C16	37.63(14)	C14	C15	C16	121.6(3)
C18	Ru1	C19	38.30(14)	C16	C15	Ru1	71.1(2)
C19	Ru1	I1	120.73(10)	C15	C16	Ru1	71.1(2)
C19	Ru1	C13	37.43(13)	C15	C16	C17	120.4(4)
C19	Ru1	C14	67.53(13)	C17	C16	Ru1	126.1(3)
C19	Ru1	C15	79.82(14)	C18	C16	Ru1	70.0(2)
C19	Ru1	C16	68.75(14)	C18	C16	C15	117.5(3)
C8	O1	Ru1	113.8(2)	C18	C16	C17	122.0(4)
C1	N1	Ru1	128.0(3)	C16	C18	Ru1	72.4(2)
C1	N1	C9	118.7(3)	C16	C18	C19	121.5(3)
C9	N1	Ru1	113.2(2)	C19	C18	Ru1	71.51(19)
N1	C1	C2	121.9(4)	C13	C19	Ru1	72.43(19)
C3	C2	C1	120.6(4)	C13	C19	C18	120.9(3)
C2	C3	C4	119.7(4)	C18	C19	Ru1	70.2(2)

Table S7. Crystal data and structure refinement details for **3.**

Empirical formula	$C_{19}H_{18}Cl_2INORu$
Formula weight	575.21
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.2642(5)
b/Å	8.0344(3)
c/Å	15.8749(5)
α/°	90
β/°	100.0110(10)
γ/°	90
Volume/Å^3	1917.23(11)
Z	4
ρ_{calc}mg/mm^3	1.993
m/mm^{-1}	2.714
F(000)	1112.0
Crystal size/mm^3	0.409 × 0.232 × 0.144
2Θ range for data collection	6.116 to 55.088°
Index ranges	$-19 \leq h \leq 19$, $-10 \leq k \leq 10$, $-20 \leq l \leq 20$
Reflections collected	29332
Independent reflections	4415[R(int) = 0.0289]
Data/restraints/parameters	4415/0/229
Goodness-of-fit on F^2	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0316, wR_2 = 0.0780
Final R indexes [all data]	R_1 = 0.0402, wR_2 = 0.0822
Largest diff. peak/hole / e Å^{-3}	1.29/-1.35

Table S8. Selected bond lengths (Å) for **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	C2	2.077(4)	C3	C4	1.363(6)
Ru1	Cl1	2.4414(8)	C4	C5	1.407(5)
Ru1	O1	2.076(2)	C5	C6	1.415(4)
Ru1	N1	2.094(3)	C5	C7	1.413(5)
Ru1	C11	2.204(3)	C7	C8	1.361(6)
Ru1	C12	2.199(3)	C8	C9	1.399(5)
Ru1	C13	2.190(3)	C10	C11	1.500(6)
Ru1	C14	2.193(4)	C11	C12	1.425(5)
Ru1	C15	2.154(4)	C11	C16	1.394(6)
Ru1	C16	2.168(3)	C12	C13	1.394(5)
Cl2	C4	1.743(4)	C13	C14	1.426(5)

O1	C1	1.301(4)	C14	C15	1.405(5)
N1	C6	1.369(4)	C14	C17	1.512(6)
N1	C9	1.325(4)	C15	C16	1.407(6)
C1	C2	1.386(5)	C17	C18	1.397(9)
C1	C6	1.428(4)	C17	C19	1.507(6)
C2	C3	1.405(5)			

Table S9. Selected bond lengths (Å) and bond angles (°) for **3**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	Cl1	85.33(7)	C1	C2	I1	118.7(3)
O1	Ru1	N1	78.26(9)	C1	C2	C3	121.6(3)
O1	Ru1	C11	154.80(12)	C3	C2	I1	119.6(3)
O1	Ru1	C12	117.68(11)	C4	C3	C2	121.0(3)
O1	Ru1	C13	93.24(11)	C3	C4	Cl2	119.6(3)
O1	Ru1	C14	93.42(12)	C3	C4	C5	121.1(3)
O1	Ru1	C15	121.14(13)	C5	C4	Cl2	119.3(3)
O1	Ru1	C16	159.08(14)	C4	C5	C6	117.0(3)
N1	Ru1	Cl1	83.56(8)	C4	C5	C7	126.0(3)
N1	Ru1	C11	126.08(12)	C7	C5	C6	117.0(3)
N1	Ru1	C12	163.84(12)	N1	C6	C1	115.0(3)
N1	Ru1	C13	152.56(12)	N1	C6	C5	122.0(3)
N1	Ru1	C14	115.77(12)	C5	C6	C1	123.0(3)
N1	Ru1	C15	94.76(13)	C8	C7	C5	119.9(3)
N1	Ru1	C16	99.24(12)	C7	C8	C9	119.9(3)
C11	Ru1	Cl1	90.78(11)	N1	C9	C8	122.2(3)
C12	Ru1	Cl1	94.62(10)	C10	C11	Ru1	127.8(3)
C12	Ru1	C11	37.77(13)	C12	C11	Ru1	70.93(19)
C13	Ru1	Cl1	122.10(10)	C12	C11	C10	120.4(4)
C13	Ru1	C11	67.90(13)	C16	C11	Ru1	70.0(2)
C13	Ru1	C12	37.04(13)	C16	C11	C10	122.2(4)
C13	Ru1	C14	37.97(13)	C16	C11	C12	117.4(3)
C14	Ru1	Cl1	160.01(9)	C11	C12	Ru1	71.30(19)
C14	Ru1	C11	81.87(14)	C13	C12	Ru1	71.12(19)
C14	Ru1	C12	68.28(14)	C13	C12	C11	121.0(3)
C15	Ru1	Cl1	152.69(11)	C12	C13	Ru1	71.84(19)
C15	Ru1	C11	68.17(15)	C12	C13	C14	121.9(3)
C15	Ru1	C12	79.48(14)	C14	C13	Ru1	71.12(19)
C15	Ru1	C13	67.17(13)	C13	C14	Ru1	70.9(2)
C15	Ru1	C14	37.71(14)	C13	C14	C17	122.1(3)
C15	Ru1	C16	37.99(16)	C15	C14	Ru1	69.6(2)
C16	Ru1	Cl1	115.21(12)	C15	C14	C13	116.2(3)
C16	Ru1	C11	37.18(15)	C15	C14	C17	121.7(4)

C16	Ru1	C12	66.95(14)	C17	C14	Ru1	129.1(3)
C16	Ru1	C13	79.43(13)	C14	C15	Ru1	72.7(2)
C16	Ru1	C14	68.72(14)	C14	C15	C16	122.2(3)
C1	O1	Ru1	114.45(19)	C16	C15	Ru1	71.5(2)
C6	N1	Ru1	113.1(2)	C11	C16	Ru1	72.8(2)
C9	N1	Ru1	127.7(2)	C11	C16	C15	121.4(3)
C9	N1	C6	119.0(3)	C15	C16	Ru1	70.5(2)
O1	C1	C2	125.1(3)	C18	C17	C14	117.5(5)
O1	C1	C6	118.6(3)	C18	C17	C19	114.6(6)
C2	C1	C6	116.2(3)	C19	C17	C14	113.6(4)

Table S10. Crystal data and structure refinement details for **8.**

Identification code	ClIQ-RuI
Empirical formula	$C_{19}H_{18}ClI_2NORu$
Formula weight	666.66
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pccn
a/Å	20.5287(8)
b/Å	26.6266(10)
c/Å	7.9491(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4345.1(3)
Z	8
ρ_{calc}g/cm^3	2.038
μ/mm^{-1}	3.693
F(000)	2512.0
Crystal size/mm^3	0.26 × 0.21 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.12 to 55.204
Index ranges	-25 ≤ h ≤ 26, -34 ≤ k ≤ 34, -10 ≤ l ≤ 10
Reflections collected	64442
Independent reflections	5029 [R_{int} = 0.0672, R_{sigma} = 0.0360]
Data/restraints/parameters	5029/6/229
Goodness-of-fit on F^2	1.094
Final R indexes [I>=2σ (I)]	R_1 = 0.0443, wR_2 = 0.1159

Final R indexes [all data]	$R_1 = 0.0750$, $wR_2 = 0.1336$
Largest diff. peak/hole / e Å^{-3}	0.65/-1.10

Table S11. Selected bond lengths (Å) for **8**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I2	Ru1	2.7275(6)	C18	C13	1.414(9)
Ru1	O1	2.066(4)	C18	C17	1.389(9)
Ru1	N1	2.092(5)	C13	C14	1.403(10)
Ru1	C16	2.184(6)	C13	C11	1.507(10)
Ru1	C18	2.179(6)	C5	C6	1.415(8)
Ru1	C13	2.200(6)	C5	C9	1.380(10)
Ru1	C17	2.183(6)	C5	C4	1.389(10)
Ru1	C14	2.166(7)	C6	C1	1.432(8)
Ru1	C15	2.166(6)	C7	C8	1.404(10)
I1	C2	2.075(7)	C1	C2	1.386(8)
Cl1	C4	1.748(6)	C14	C15	1.415(10)
O1	C1	1.306(7)	C8	C9	1.349(10)
N1	C6	1.366(8)	C2	C3	1.411(9)
N1	C7	1.341(8)	C4	C3	1.351(10)
C16	C17	1.412(9)	C12	C11	1.516(10)
C16	C15	1.399(9)	C11	C10	1.583(13)
C16	C19	1.520(10)			

Table S12. Selected bond lengths (Å) and bond angles (°) for **8**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	I2	87.60(12)	C15	C16	C17	118.4(6)
O1	Ru1	N1	78.59(18)	C15	C16	C19	120.7(7)
O1	Ru1	C16	88.1(2)	C19	C16	Ru1	125.7(5)
O1	Ru1	C18	124.0(2)	C13	C18	Ru1	72.0(4)
O1	Ru1	C13	161.5(2)	C17	C18	Ru1	71.6(3)
O1	Ru1	C17	94.3(2)	C17	C18	C13	122.4(6)
O1	Ru1	C14	148.7(2)	C18	C13	Ru1	70.3(3)
O1	Ru1	C15	111.3(2)	C18	C13	C11	119.3(6)
N1	Ru1	I2	85.00(13)	C14	C13	Ru1	69.9(4)
N1	Ru1	C16	122.0(2)	C14	C13	C18	116.8(6)
N1	Ru1	C18	157.1(2)	C14	C13	C11	123.9(7)
N1	Ru1	C13	119.9(2)	C11	C13	Ru1	131.5(4)
N1	Ru1	C17	159.4(2)	C9	C5	C6	116.4(7)
N1	Ru1	C14	96.1(2)	C9	C5	C4	126.9(6)
N1	Ru1	C15	96.9(2)	C4	C5	C6	116.8(6)

C16	Ru1	I2	151.10(18)	C16	C17	Ru1	71.1(3)
C16	Ru1	C13	81.5(2)	C18	C17	Ru1	71.3(4)
C16	Ru1	C17	37.7(2)	C18	C17	C16	120.3(6)
C18	Ru1	I2	91.41(17)	N1	C6	C5	122.1(6)
C18	Ru1	C16	67.7(2)	N1	C6	C1	114.5(5)
C18	Ru1	C13	37.7(2)	C5	C6	C1	123.4(6)
C18	Ru1	C17	37.1(2)	N1	C7	C8	120.3(7)
C13	Ru1	I2	94.14(16)	O1	C1	C6	118.9(5)
C17	Ru1	I2	114.26(18)	O1	C1	C2	125.2(6)
C17	Ru1	C13	68.2(2)	C2	C1	C6	115.9(5)
C14	Ru1	I2	122.9(2)	C13	C14	Ru1	72.6(4)
C14	Ru1	C16	68.4(3)	C13	C14	C15	121.4(6)
C14	Ru1	C18	67.0(3)	C15	C14	Ru1	71.0(4)
C14	Ru1	C13	37.5(3)	C9	C8	C7	119.9(7)
C14	Ru1	C17	79.9(2)	C16	C15	Ru1	71.9(3)
C15	Ru1	I2	161.04(19)	C16	C15	C14	120.7(6)
C15	Ru1	C16	37.5(2)	C14	C15	Ru1	70.9(4)
C15	Ru1	C18	79.5(2)	C1	C2	I1	118.8(5)
C15	Ru1	C13	68.5(3)	C1	C2	C3	120.8(6)
C15	Ru1	C17	67.4(2)	C3	C2	I1	120.4(5)
C15	Ru1	C14	38.1(3)	C8	C9	C5	121.8(6)
C1	O1	Ru1	114.3(4)	C5	C4	Cl1	119.7(6)
C6	N1	Ru1	113.5(4)	C3	C4	Cl1	118.8(6)
C7	N1	Ru1	127.0(5)	C3	C4	C5	121.5(6)
C7	N1	C6	119.5(6)	C4	C3	C2	121.7(6)
C17	C16	Ru1	71.1(3)	C13	C11	C12	110.4(6)
C17	C16	C19	120.8(7)	C13	C11	C10	112.9(7)
C15	C16	Ru1	70.6(4)	C12	C11	C10	110.2(7)

Table S13. Crystal data and structure refinement details for **5.**

Identification code	IIQ-RuCl
Empirical formula	$C_{19}H_{17}ClI_2NORu$
Formula weight	665.66
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pbca
a/Å	19.5223(11)
b/Å	8.1342(5)
c/Å	25.6620(14)
α/°	90

β/°	90
γ/°	90
Volume/Å^3	4075.1(4)
Z	8
ρ_{calc}g/cm^3	2.170
μ/mm^{-1}	3.938
F(000)	2504.0
Crystal size/mm^3	0.26 × 0.21 × 0.14
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.286 to 55.12
Index ranges	-25 ≤ h ≤ 25, -10 ≤ k ≤ 10, -33 ≤ l ≤ 33
Reflections collected	56830
Independent reflections	4706 [R_{int} = 0.1129, R_{sigma} = 0.0627]
Data/restraints/parameters	4706/32/229
Goodness-of-fit on F^2	1.067
Final R indexes [I>=2σ (I)]	R_1 = 0.0597, wR_2 = 0.0979
Final R indexes [all data]	R_1 = 0.1460, wR_2 = 0.1194
Largest diff. peak/hole / e Å^{-3}	0.54/-0.73

Table S14. Selected bond lengths (Å) for **5**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	O1	2.080(5)	C18	C17	1.371(10)
Ru1	N1	2.086(5)	C13	C14	1.391(11)
Ru1	C18	2.184(7)	C13	C11	1.540(13)
Ru1	C13	2.153(8)	C15	C14	1.387(11)
Ru1	C15	2.170(8)	C15	C16	1.396(11)
Ru1	C17	2.198(8)	C1	C2	1.393(10)
Ru1	C14	2.144(8)	C6	C7	1.371(10)
Ru1	C16	2.207(8)	C6	C5	1.426(10)
Ru1	Cl1	2.429(2)	C17	C16	1.427(10)
I1	C7	2.100(8)	C5	C4	1.428(10)
I2	C9	2.086(8)	C9	C4	1.398(11)
O1	C6	1.315(8)	C2	C3	1.355(11)
N1	C1	1.324(8)	C4	C3	1.400(11)
N1	C5	1.350(9)	C16	C19	1.530(12)
C8	C7	1.401(11)	C10	C11	1.430(11)
C8	C9	1.378(11)	C11	C12	1.351(10)
C18	C13	1.423(10)			

Table S15. Selected bond lengths (Å) and bond angles (°) for **5**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	N1	78.1(2)	C17	C18	C13	120.6(7)
O1	Ru1	C18	93.7(2)	C18	C13	Ru1	72.0(5)
O1	Ru1	C13	92.5(3)	C18	C13	C11	121.2(8)

O1	Ru1	C15	156.6(3)	C14	C13	Ru1	70.7(5)
O1	Ru1	C17	119.2(2)	C14	C13	C18	117.8(8)
O1	Ru1	C14	119.3(3)	C14	C13	C11	121.0(8)
O1	Ru1	C16	156.7(3)	C11	C13	Ru1	126.9(7)
O1	Ru1	Cl1	85.44(15)	C14	C15	Ru1	70.2(5)
N1	Ru1	C18	153.4(3)	C14	C15	C16	121.0(7)
N1	Ru1	C13	116.0(3)	C16	C15	Ru1	72.8(5)
N1	Ru1	C15	97.9(3)	N1	C1	C2	121.3(8)
N1	Ru1	C17	162.6(3)	O1	C6	C7	124.7(7)
N1	Ru1	C14	94.1(3)	O1	C6	C5	117.9(7)
N1	Ru1	C16	124.8(3)	C7	C6	C5	117.4(7)
N1	Ru1	Cl1	84.80(17)	C8	C7	I1	118.8(6)
C18	Ru1	C17	36.5(3)	C6	C7	I1	119.5(6)
C18	Ru1	C16	67.5(3)	C6	C7	C8	121.6(8)
C18	Ru1	Cl1	120.1(2)	C18	C17	Ru1	71.2(4)
C13	Ru1	C18	38.3(3)	C18	C17	C16	121.3(8)
C13	Ru1	C15	68.3(3)	C16	C17	Ru1	71.4(4)
C13	Ru1	C17	67.8(3)	N1	C5	C6	115.6(7)
C13	Ru1	C16	81.2(3)	N1	C5	C4	123.0(7)
C13	Ru1	Cl1	158.2(2)	C6	C5	C4	121.5(7)
C15	Ru1	C18	79.5(3)	C13	C14	Ru1	71.5(5)
C15	Ru1	C17	67.1(3)	C15	C14	Ru1	72.3(5)
C15	Ru1	C16	37.2(3)	C15	C14	C13	121.8(8)
C15	Ru1	Cl1	117.4(3)	C8	C9	I2	119.6(7)
C17	Ru1	C16	37.8(3)	C8	C9	C4	119.8(8)
C17	Ru1	Cl1	94.3(2)	C4	C9	I2	120.6(7)
C14	Ru1	C18	67.6(3)	C3	C2	C1	120.4(8)
C14	Ru1	C13	37.8(3)	C9	C4	C5	118.4(7)
C14	Ru1	C15	37.5(3)	C9	C4	C3	126.1(8)
C14	Ru1	C17	79.3(3)	C3	C4	C5	115.5(7)
C14	Ru1	C16	67.6(3)	C15	C16	Ru1	70.0(5)
C14	Ru1	Cl1	154.6(3)	C15	C16	C17	117.5(8)
C16	Ru1	Cl1	92.2(3)	C15	C16	C19	122.2(8)
C6	O1	Ru1	114.2(4)	C17	C16	Ru1	70.8(4)
C1	N1	Ru1	126.8(5)	C17	C16	C19	120.3(8)
C1	N1	C5	119.2(6)	C19	C16	Ru1	128.6(7)
C5	N1	Ru1	113.9(5)	C2	C3	C4	120.6(8)
C9	C8	C7	121.3(8)	C10	C11	C13	116.9(8)
C13	C18	Ru1	69.7(4)	C12	C11	C13	115.0(9)
C17	C18	Ru1	72.4(4)	C12	C11	C10	127.7(10)

Table S16. Crystal data and structure refinement details for **10.**

Empirical formula	$C_{19}H_{18}I_3NORu$
Formula weight	758.11
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Pccn
a/Å	21.0592(14)
b/Å	26.7409(18)
c/Å	7.9714(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	4489.0(5)
Z	8
ρ_{calc}g/cm^3	2.243
μ/mm^{-1}	4.832
F(000)	2800.0
Crystal size/mm^3	0.473 × 0.122 × 0.035
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6 to 55.108
Index ranges	-25 ≤ h ≤ 27, -34 ≤ k ≤ 34, -10 ≤ l ≤ 10
Reflections collected	66910
Independent reflections	5180 [R_{int} = 0.0715, R_{sigma} = 0.0357]
Data/restraints/parameters	5180/0/229
Goodness-of-fit on F^2	1.087
Final R indexes [I>=2σ (I)]	R_1 = 0.0383, wR_2 = 0.0740
Final R indexes [all data]	R_1 = 0.0627, wR_2 = 0.0871
Largest diff. peak/hole / e Å^{-3}	0.77/-0.88

Table S17. Selected bond lengths (Å) for **10**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I3	Ru1	2.7316(6)	C5	C6	1.424(7)
Ru1	N1	2.094(4)	C5	C9	1.397(8)
Ru1	C14	2.159(6)	C13	C18	1.418(8)
Ru1	C13	2.210(6)	C13	C11	1.515(9)
Ru1	C18	2.195(5)	C8	C7	1.402(8)
Ru1	C16	2.201(5)	C8	C9	1.358(9)
Ru1	C15	2.180(5)	C6	C1	1.414(7)
Ru1	C17	2.187(5)	C1	C2	1.383(8)
Ru1	O1	2.069(4)	C1	O1	1.304(6)
I1	C2	2.081(5)	C18	C17	1.394(9)
I2	C4	2.094(5)	C16	C15	1.404(8)

N1	C6	1.363(7)	C16	C17	1.421(8)
N1	C7	1.327(7)	C16	C19	1.493(8)
C4	C5	1.389(8)	C2	C3	1.413(7)
C4	C3	1.351(8)	C10	C11	1.512(11)
C14	C13	1.407(9)	C11	C12	1.531(9)
C14	C15	1.412(9)			

Table S18. Selected bond lengths (Å) and bond angles (°) for **10**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Ru1	I3	84.86(12)	C13	C14	C15	122.6(6)
N1	Ru1	C14	96.8(2)	C15	C14	Ru1	71.8(3)
N1	Ru1	C13	120.8(2)	C4	C5	C6	117.1(5)
N1	Ru1	C18	157.9(2)	C4	C5	C9	126.6(5)
N1	Ru1	C16	121.4(2)	C9	C5	C6	116.4(5)
N1	Ru1	C15	96.81(19)	C14	C13	Ru1	69.3(3)
N1	Ru1	C17	158.8(2)	C14	C13	C18	116.6(6)
C14	Ru1	I3	122.79(17)	C14	C13	C11	123.5(6)
C14	Ru1	C13	37.5(2)	C18	C13	Ru1	70.6(3)
C14	Ru1	C18	67.0(2)	C18	C13	C11	119.9(6)
C14	Ru1	C16	68.1(2)	C11	C13	Ru1	131.7(4)
C14	Ru1	C15	38.0(2)	C9	C8	C7	119.7(6)
C14	Ru1	C17	79.3(2)	N1	C6	C5	122.1(5)
C13	Ru1	I3	94.06(16)	N1	C6	C1	114.6(4)
C18	Ru1	I3	91.50(16)	C1	C6	C5	123.3(5)
C18	Ru1	C13	37.6(2)	C2	C1	C6	116.5(5)
C18	Ru1	C16	68.0(2)	O1	C1	C6	119.6(5)
C16	Ru1	I3	151.81(17)	O1	C1	C2	123.8(5)
C16	Ru1	C13	81.4(2)	C13	C18	Ru1	71.8(3)
C15	Ru1	I3	160.76(16)	C17	C18	Ru1	71.1(3)
C15	Ru1	C13	68.6(2)	C17	C18	C13	121.3(6)
C15	Ru1	C18	79.7(2)	C15	C16	Ru1	70.5(3)
C15	Ru1	C16	37.4(2)	C15	C16	C17	117.7(5)
C15	Ru1	C17	67.2(2)	C15	C16	C19	121.1(6)
C17	Ru1	I3	114.91(16)	C17	C16	Ru1	70.6(3)
C17	Ru1	C13	67.8(2)	C17	C16	C19	121.1(6)
C17	Ru1	C18	37.1(2)	C19	C16	Ru1	126.2(4)
C17	Ru1	C16	37.8(2)	C1	C2	I1	119.3(4)
O1	Ru1	I3	87.94(11)	C1	C2	C3	120.1(5)
O1	Ru1	N1	78.35(15)	C3	C2	I1	120.6(4)
O1	Ru1	C14	148.6(2)	N1	C7	C8	121.6(6)
O1	Ru1	C13	160.83(19)	C14	C15	Ru1	70.2(3)
O1	Ru1	C18	123.41(18)	C16	C15	Ru1	72.2(3)
O1	Ru1	C16	87.88(19)	C16	C15	C14	120.2(5)

O1	Ru1	C15	111.2(2)	C18	C17	Ru1	71.8(3)
O1	Ru1	C17	94.09(18)	C18	C17	C16	121.6(5)
C6	N1	Ru1	113.5(3)	C16	C17	Ru1	71.7(3)
C7	N1	Ru1	127.2(4)	C8	C9	C5	121.0(5)
C7	N1	C6	119.3(5)	C4	C3	C2	122.5(5)
C5	C4	I2	121.7(4)	C1	O1	Ru1	113.9(3)
C3	C4	I2	117.8(4)	C13	C11	C12	108.4(6)
C3	C4	C5	120.5(5)	C10	C11	C13	115.4(6)
C13	C14	Ru1	73.2(3)	C10	C11	C12	110.5(6)

Table S19. Crystal data and structure refinement details for **2.**

Empirical formula	$C_{20}H_{20}Br_2ClNORu$
Formula weight	586.71
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.7664(6)
b/Å	8.2019(3)
c/Å	16.9558(7)
α/°	90
β/°	102.769(4)
γ/°	90
Volume/Å^3	2002.77(14)
Z	4
ρ_{calc}mg/mm^3	1.946
m/mm^{-1}	4.916
F(000)	1144.0
Crystal size/mm^3	0.453 × 0.12 × 0.025
2Θ range for data collection	6.632 to 52.744°
Index ranges	$-18 \le h \le 18$, $-10 \le k \le 10$, $-18 \le l \le 21$
Reflections collected	12450
Independent reflections	4091[R(int) = 0.0597]
Data/restraints/parameters	4091/0/239
Goodness-of-fit on F^2	1.073
Final R indexes [I>=2σ (I)]	$R_1 = 0.0441$, $wR_2 = 0.0974$
Final R indexes [all data]	$R_1 = 0.0573$, $wR_2 = 0.1080$
Largest diff. peak/hole / e Å^{-3}	0.70/-1.42

Table S20. Selected bond lengths (Å) for **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	Cl1	2.4143(12)	C4	C5	1.408(7)
Ru1	O1	2.057(3)	C5	C6	1.401(7)
Ru1	N1	2.152(4)	C5	C10	1.420(6)
Ru1	C14	2.185(5)	C6	C7	1.364(7)
Ru1	C15	2.163(5)	C7	C8	1.391(6)
Ru1	C16	2.210(5)	C8	C9	1.391(6)
Ru1	C17	2.216(4)	C9	C10	1.413(6)
Ru1	C19	2.188(5)	C11	C12	1.513(8)
Ru1	C20	2.169(4)	C12	C13	1.513(8)
Br1	C8	1.887(5)	C12	C14	1.509(7)
Br2	C6	1.902(5)	C14	C15	1.402(7)
O1	C9	1.304(5)	C14	C20	1.414(7)
N1	C2	1.332(6)	C15	C16	1.443(7)
N1	C10	1.379(6)	C16	C17	1.387(7)
C1	C2	1.479(7)	C17	C18	1.497(7)
C2	C3	1.414(7)	C17	C19	1.427(7)
C3	C4	1.343(7)	C19	C20	1.399(7)

Table S21. Selected bond lengths (Å) and bond angles (°) for **2**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	Cl1	87.72(10)	C3	C4	C5	120.1(5)
O1	Ru1	N1	78.52(13)	C4	C5	C10	116.4(4)
O1	Ru1	C14	88.60(16)	C6	C5	C4	126.1(4)
O1	Ru1	C15	117.02(16)	C6	C5	C10	117.5(4)
O1	Ru1	C16	155.44(16)	C5	C6	Br2	119.6(4)
O1	Ru1	C17	152.33(16)	C7	C6	Br2	118.7(4)
O1	Ru1	C19	114.58(16)	C7	C6	C5	121.7(4)
O1	Ru1	C20	88.49(16)	C6	C7	C8	119.7(5)
N1	Ru1	Cl1	82.39(10)	C7	C8	Br1	119.3(4)
N1	Ru1	C14	118.34(16)	C9	C8	Br1	118.6(3)
N1	Ru1	C15	98.45(16)	C9	C8	C7	122.1(5)
N1	Ru1	C16	103.63(17)	O1	C9	C8	123.1(4)
N1	Ru1	C17	128.80(17)	O1	C9	C10	119.8(4)
N1	Ru1	C19	166.09(18)	C8	C9	C10	117.1(4)
N1	Ru1	C20	153.89(17)	N1	C10	C5	122.6(4)
C14	Ru1	Cl1	157.70(13)	N1	C10	C9	115.8(4)
C14	Ru1	C16	68.64(18)	C9	C10	C5	121.5(4)
C14	Ru1	C17	81.66(18)	C13	C12	C11	113.8(5)
C14	Ru1	C19	68.57(18)	C14	C12	C11	113.1(5)
C15	Ru1	Cl1	155.02(14)	C14	C12	C13	108.1(5)
C15	Ru1	C14	37.61(18)	C12	C14	Ru1	126.6(3)

C15	Ru1	C16	38.50(18)	C15	C14	Ru1	70.3(3)
C15	Ru1	C17	68.31(18)	C15	C14	C12	124.3(5)
C15	Ru1	C19	80.09(18)	C15	C14	C20	117.0(5)
C15	Ru1	C20	67.32(18)	C20	C14	Ru1	70.4(3)
C16	Ru1	Cl1	116.84(14)	C20	C14	C12	118.6(5)
C16	Ru1	C17	36.51(18)	C14	C15	Ru1	72.0(3)
C17	Ru1	Cl1	91.58(13)	C14	C15	C16	121.2(4)
C19	Ru1	Cl1	93.13(13)	C16	C15	Ru1	72.5(3)
C19	Ru1	C16	66.61(18)	C15	C16	Ru1	69.0(3)
C19	Ru1	C17	37.81(18)	C17	C16	Ru1	72.0(3)
C20	Ru1	Cl1	119.99(13)	C17	C16	C15	120.7(5)
C20	Ru1	C14	37.89(17)	C16	C17	Ru1	71.5(3)
C20	Ru1	C16	79.22(19)	C16	C17	C18	121.1(5)
C20	Ru1	C17	68.01(18)	C16	C17	C19	118.3(5)
C20	Ru1	C19	37.45(18)	C18	C17	Ru1	128.9(3)
C9	O1	Ru1	114.8(3)	C19	C17	Ru1	70.0(3)
C2	N1	Ru1	130.2(3)	C19	C17	C18	120.7(5)
C2	N1	C10	118.7(4)	C17	C19	Ru1	72.1(3)
C10	N1	Ru1	110.9(3)	C20	C19	Ru1	70.5(3)
N1	C2	C1	120.3(4)	C20	C19	C17	120.4(4)
N1	C2	C3	120.7(5)	C14	C20	Ru1	71.7(3)
C3	C2	C1	119.0(5)	C19	C20	Ru1	72.0(3)
C4	C3	C2	121.4(5)	C19	C20	C14	122.3(5)

Table S22. Crystal data and structure refinement details for **7.**

Empirical formula	$C_{20}H_{20}Br_2INORu$
Formula weight	678.16
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.1403(6)
b/Å	14.1963(9)
c/Å	14.3901(8)
α/°	86.310(5)
β/°	71.536(5)
γ/°	84.761(5)
Volume/Å^3	2148.1(2)
Z	4
ρ_{calc}mg/mm^3	2.097
m/mm^{-1}	5.896

F(000)	1288.0
Crystal size/mm^3	? × ? × ?
2Θ range for data collection	6.594 to 52.742°
Index ranges	-13 ≤ h ≤ 12, -17 ≤ k ≤ 17, -17 ≤ l ≤ 16
Reflections collected	24876
Independent reflections	8702[R(int) = 0.0305]
Data/restraints/parameters	8702/0/477
Goodness-of-fit on F^2	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0343, wR_2 = 0.0696
Final R indexes [all data]	R_1 = 0.0528, wR_2 = 0.0779
Largest diff. peak/hole / e Å^{-3}	0.67/-0.79

Table S23. Selected bond lengths (Å) for **7**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	Ru1	2.7205(5)	C6	C7	1.366(7)
I2	Ru2	2.7251(5)	C7	C8	1.389(7)
Ru1	O1	2.066(3)	C8	C9	1.383(6)
Ru1	N1	2.131(4)	C9	C10	1.428(6)
Ru1	C12	2.213(4)	C11	C20	1.511(7)
Ru1	C13	2.154(4)	C12	C13	1.406(6)
Ru1	C14	2.174(5)	C12	C20	1.393(6)
Ru1	C18	2.161(5)	C13	C14	1.417(7)
Ru1	C19	2.192(5)	C14	C15	1.522(8)
Ru1	C20	2.225(5)	C14	C18	1.429(7)
Ru2	O2	2.059(3)	C15	C16	1.517(10)
Ru2	N2	2.133(4)	C15	C17	1.521(9)
Ru2	C34	2.187(5)	C18	C19	1.365(7)
Ru2	C35	2.167(5)	C19	C20	1.423(7)
Ru2	C36	2.206(4)	C21	C22	1.408(7)
Ru2	C37	2.236(4)	C21	C30	1.387(6)
Ru2	C39	2.186(5)	C22	C23	1.351(8)
Ru2	C40	2.155(5)	C23	C24	1.412(7)
Br1	C8	1.910(4)	C24	C25	1.392(7)
Br2	C6	1.901(5)	C24	C29	1.420(6)
Br3	C21	1.885(5)	C25	C26	1.361(7)
Br4	C23	1.912(5)	C26	C27	1.422(6)
O1	C9	1.309(5)	C27	C28	1.496(6)
O2	C30	1.318(5)	C29	C30	1.415(7)
N1	C2	1.349(5)	C31	C32	1.512(11)
N1	C10	1.387(6)	C32	C33	1.520(10)
N2	C27	1.324(6)	C32	C34	1.530(8)
N2	C29	1.382(5)	C34	C35	1.412(7)
C1	C2	1.497(7)	C34	C40	1.396(8)

C2	C3	1.394(7)	C35	C36	1.404(7)
C3	C4	1.362(7)	C36	C37	1.398(7)
C4	C5	1.420(6)	C37	C38	1.486(7)
C5	C6	1.402(6)	C37	C39	1.420(7)
C5	C10	1.406(6)	C39	C40	1.406(8)

Table S24. Selected bond lengths (Å) and bond angles (°) for **7**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	I1	85.19(9)	C5	C6	Br2	119.5(4)
O1	Ru1	N1	79.00(13)	C7	C6	Br2	119.7(4)
O1	Ru1	C12	160.52(16)	C7	C6	C5	120.8(5)
O1	Ru1	C13	124.04(16)	C6	C7	C8	120.1(5)
O1	Ru1	C14	92.25(16)	C7	C8	Br1	118.4(3)
O1	Ru1	C18	87.57(17)	C9	C8	Br1	118.6(4)
O1	Ru1	C19	109.66(16)	C9	C8	C7	122.9(4)
O1	Ru1	C20	146.46(15)	O1	C9	C8	124.2(4)
N1	Ru1	I1	84.96(10)	O1	C9	C10	120.0(4)
N1	Ru1	C12	105.08(16)	C8	C9	C10	115.8(4)
N1	Ru1	C13	94.49(17)	N1	C10	C5	122.9(4)
N1	Ru1	C14	110.77(18)	N1	C10	C9	114.8(4)
N1	Ru1	C18	146.3(2)	C5	C10	C9	122.3(4)
N1	Ru1	C19	171.24(16)	C13	C12	Ru1	68.9(3)
N1	Ru1	C20	134.03(16)	C20	C12	Ru1	72.2(3)
C12	Ru1	I1	113.98(13)	C20	C12	C13	121.1(4)
C12	Ru1	C20	36.58(16)	C12	C13	Ru1	73.5(3)
C13	Ru1	I1	150.20(14)	C12	C13	C14	121.8(4)
C13	Ru1	C12	37.52(17)	C14	C13	Ru1	71.7(3)
C13	Ru1	C14	38.22(18)	C13	C14	Ru1	70.1(3)
C13	Ru1	C18	67.78(19)	C13	C14	C15	123.6(5)
C13	Ru1	C19	79.64(19)	C13	C14	C18	115.4(5)
C13	Ru1	C20	67.63(18)	C15	C14	Ru1	126.8(4)
C14	Ru1	I1	163.32(15)	C18	C14	Ru1	70.2(3)
C14	Ru1	C12	68.40(18)	C18	C14	C15	120.9(5)
C14	Ru1	C19	68.4(2)	C16	C15	C14	113.6(5)
C14	Ru1	C20	81.56(19)	C16	C15	C17	112.1(7)
C18	Ru1	I1	124.83(15)	C17	C15	C14	109.7(6)
C18	Ru1	C12	78.67(18)	C14	C18	Ru1	71.3(3)
C18	Ru1	C14	38.5(2)	C19	C18	Ru1	72.9(3)
C18	Ru1	C19	36.6(2)	C19	C18	C14	122.9(5)
C18	Ru1	C20	67.2(2)	C18	C19	Ru1	70.5(3)
C19	Ru1	I1	96.88(14)	C18	C19	C20	120.9(5)
C19	Ru1	C12	66.33(18)	C20	C19	Ru1	72.5(3)
C19	Ru1	C20	37.58(18)	C11	C20	Ru1	129.2(4)
C20	Ru1	I1	91.47(13)	C12	C20	Ru1	71.3(3)

O2	Ru2	I2	86.98(10)	C12	C20	C11	120.8(5)
O2	Ru2	N2	78.82(13)	C12	C20	C19	117.7(5)
O2	Ru2	C34	92.57(17)	C19	C20	Ru1	69.9(3)
O2	Ru2	C35	124.55(17)	C19	C20	C11	121.5(4)
O2	Ru2	C36	160.43(17)	C22	C21	Br3	119.7(4)
O2	Ru2	C37	144.71(17)	C30	C21	Br3	118.9(4)
O2	Ru2	C39	108.08(18)	C30	C21	C22	121.3(5)
O2	Ru2	C40	86.20(16)	C23	C22	C21	120.6(5)
N2	Ru2	I2	84.23(10)	C22	C23	Br4	118.7(4)
N2	Ru2	C34	110.14(19)	C22	C23	C24	121.3(5)
N2	Ru2	C35	94.92(17)	C24	C23	Br4	120.0(4)
N2	Ru2	C36	106.56(17)	C23	C24	C29	117.5(5)
N2	Ru2	C37	135.98(17)	C25	C24	C23	125.6(5)
N2	Ru2	C39	172.90(17)	C25	C24	C29	116.8(4)
N2	Ru2	C40	143.9(2)	C26	C25	C24	120.3(5)
C34	Ru2	I2	165.27(17)	C25	C26	C27	120.5(5)
C34	Ru2	C36	67.87(19)	N2	C27	C26	121.1(4)
C34	Ru2	C37	81.17(19)	N2	C27	C28	120.5(4)
C35	Ru2	I2	147.80(14)	C26	C27	C28	118.4(5)
C35	Ru2	C34	37.85(19)	N2	C29	C24	122.7(5)
C35	Ru2	C36	37.45(18)	N2	C29	C30	115.6(4)
C35	Ru2	C37	67.67(19)	C30	C29	C24	121.7(4)
C35	Ru2	C39	79.9(2)	O2	C30	C21	123.0(5)
C36	Ru2	I2	112.07(14)	O2	C30	C29	119.5(4)
C36	Ru2	C37	36.67(18)	C21	C30	C29	117.5(4)
C37	Ru2	I2	90.71(13)	C31	C32	C33	111.5(8)
C39	Ru2	I2	97.60(16)	C31	C32	C34	112.8(6)
C39	Ru2	C34	68.5(2)	C33	C32	C34	109.7(6)
C39	Ru2	C36	66.38(19)	C32	C34	Ru2	128.3(4)
C39	Ru2	C37	37.44(19)	C35	C34	Ru2	70.3(3)
C40	Ru2	I2	127.87(18)	C35	C34	C32	123.6(6)
C40	Ru2	C34	37.5(2)	C40	C34	Ru2	70.0(3)
C40	Ru2	C35	67.1(2)	C40	C34	C32	119.8(6)
C40	Ru2	C36	78.59(19)	C40	C34	C35	116.5(5)
C40	Ru2	C37	67.7(2)	C34	C35	Ru2	71.9(3)
C40	Ru2	C39	37.8(2)	C36	C35	Ru2	72.8(3)
C9	O1	Ru1	114.2(3)	C36	C35	C34	121.1(5)
C30	O2	Ru2	114.4(3)	C35	C36	Ru2	69.8(3)
C2	N1	Ru1	130.3(3)	C37	C36	Ru2	72.9(3)
C2	N1	C10	117.8(4)	C37	C36	C35	122.2(5)
C10	N1	Ru1	111.8(3)	C36	C37	Ru2	70.5(3)
C27	N2	Ru2	129.8(3)	C36	C37	C38	121.0(5)
C27	N2	C29	118.6(4)	C36	C37	C39	117.1(5)
C29	N2	Ru2	111.6(3)	C38	C37	Ru2	130.1(3)
N1	C2	C1	119.9(4)	C39	C37	Ru2	69.3(3)

N1	C2	C3	121.1(4)	C39	C37	C38	121.8(5)
C3	C2	C1	118.9(4)	C37	C39	Ru2	73.2(3)
C4	C3	C2	122.2(4)	C40	C39	Ru2	69.9(3)
C3	C4	C5	118.4(5)	C40	C39	C37	120.1(5)
C6	C5	C4	124.6(5)	C34	C40	Ru2	72.5(3)
C6	C5	C10	117.9(4)	C34	C40	C39	123.0(5)
C10	C5	C4	117.5(4)	C39	C40	Ru2	72.3(3)

Table S25. Crystal data and structure refinement details for **1.**

Empirical formula	$C_{20}H_{20}Cl_3NORu$
Formula weight	497.79
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	14.5834(3)
b/Å	8.19777(16)
c/Å	16.7486(4)
α/°	90
β/°	102.210(2)
γ/°	90
Volume/Å^3	1957.03(7)
Z	4
ρ_{calc}mg/mm^3	1.689
m/mm^{-1}	1.220
F(000)	1000.0
Crystal size/mm^3	? × ? × ?
2Θ range for data collection	6.486 to 52.744°
Index ranges	$-18 \le h \le 18$, $-10 \le k \le 10$, $-20 \le l \le 18$
Reflections collected	14458
Independent reflections	3995[R(int) = 0.0265]
Data/restraints/parameters	3995/0/239
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	$R_1 = 0.0270$, $wR_2 = 0.0607$
Final R indexes [all data]	$R_1 = 0.0339$, $wR_2 = 0.0649$
Largest diff. peak/hole / e Å^{-3}	0.77/-0.43

Table S26. Selected bond lengths (Å) for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	Cl3	2.4189(7)	C3	C4	1.364(4)
Ru1	O1	2.0652(18)	C4	C5	1.406(4)
Ru1	N1	2.156(2)	C5	C6	1.410(4)
Ru1	C14	2.184(3)	C5	C10	1.413(4)
Ru1	C15	2.172(2)	C6	C7	1.345(4)
Ru1	C16	2.183(3)	C7	C8	1.416(4)
Ru1	C17	2.223(3)	C8	C9	1.488(4)
Ru1	C19	2.208(3)	C11	C12	1.514(5)
Ru1	C20	2.164(3)	C12	C13	1.495(5)
Cl1	C2	1.738(3)	C12	C14	1.508(4)
Cl2	C4	1.743(3)	C14	C15	1.428(4)
O1	C1	1.304(3)	C14	C20	1.412(4)
N1	C8	1.331(3)	C15	C16	1.388(4)
N1	C10	1.376(3)	C16	C17	1.421(4)
C1	C2	1.387(4)	C17	C18	1.496(4)
C1	C10	1.424(4)	C17	C19	1.398(4)
C2	C3	1.396(4)	C19	C20	1.415(4)

Table S27. Selected bond lengths (Å) and bond angles (°) for **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	Cl3	87.65(5)	C1	C2	C3	122.5(3)
O1	Ru1	N1	78.31(7)	C3	C2	Cl1	119.2(2)
O1	Ru1	C14	88.96(9)	C4	C3	C2	119.6(3)
O1	Ru1	C15	88.14(9)	C3	C4	Cl2	119.2(2)
O1	Ru1	C16	113.66(9)	C3	C4	C5	121.5(3)
O1	Ru1	C17	151.15(9)	C5	C4	Cl2	119.3(2)
O1	Ru1	C19	155.93(9)	C4	C5	C6	125.7(3)
O1	Ru1	C20	118.34(9)	C4	C5	C10	117.9(3)
N1	Ru1	Cl3	82.09(6)	C6	C5	C10	116.4(3)
N1	Ru1	C14	117.64(9)	C7	C6	C5	119.9(3)
N1	Ru1	C15	153.27(10)	C6	C7	C8	121.5(3)
N1	Ru1	C16	167.25(10)	N1	C8	C7	120.4(3)
N1	Ru1	C17	130.11(9)	N1	C8	C9	120.5(2)
N1	Ru1	C19	104.45(9)	C7	C8	C9	119.1(3)
N1	Ru1	C20	98.58(9)	N1	C10	C1	115.5(2)
C14	Ru1	Cl3	158.80(7)	N1	C10	C5	123.0(2)
C14	Ru1	C17	81.61(10)	C5	C10	C1	121.5(3)
C14	Ru1	C19	68.37(10)	C13	C12	C11	115.9(3)
C15	Ru1	Cl3	120.64(8)	C13	C12	C14	109.7(3)

C15	Ru1	C14	38.28(10)	C14	C12	C11	113.2(3)
C15	Ru1	C16	37.18(10)	C12	C14	Ru1	126.9(2)
C15	Ru1	C17	67.66(10)	C15	C14	Ru1	70.39(15)
C15	Ru1	C19	79.09(10)	C15	C14	C12	118.4(3)
C16	Ru1	Cl3	93.66(8)	C20	C14	Ru1	70.27(15)
C16	Ru1	C14	68.66(10)	C20	C14	C12	125.2(3)
C16	Ru1	C17	37.61(10)	C20	C14	C15	116.4(3)
C16	Ru1	C19	66.62(10)	C14	C15	Ru1	71.32(14)
C17	Ru1	Cl3	91.41(7)	C16	C15	Ru1	71.85(15)
C19	Ru1	Cl3	116.41(8)	C16	C15	C14	121.9(2)
C19	Ru1	C17	36.78(10)	C15	C16	Ru1	70.97(15)
C20	Ru1	Cl3	153.72(8)	C15	C16	C17	121.2(3)
C20	Ru1	C14	37.91(10)	C17	C16	Ru1	72.75(15)
C20	Ru1	C15	67.67(10)	C16	C17	Ru1	69.65(15)
C20	Ru1	C16	79.92(10)	C16	C17	C18	121.2(3)
C20	Ru1	C17	67.93(10)	C18	C17	Ru1	128.6(2)
C20	Ru1	C19	37.76(10)	C19	C17	Ru1	71.00(15)
C1	O1	Ru1	114.91(16)	C19	C17	C16	117.6(3)
C8	N1	Ru1	129.54(19)	C19	C17	C18	121.2(3)
C8	N1	C10	118.8(2)	C17	C19	Ru1	72.22(15)
C10	N1	Ru1	111.39(16)	C17	C19	C20	121.2(2)
O1	C1	C2	123.5(2)	C20	C19	Ru1	69.44(15)
O1	C1	C10	119.8(2)	C14	C20	Ru1	71.82(15)
C2	C1	C10	116.7(2)	C14	C20	C19	121.6(2)
C1	C2	Cl1	118.4(2)	C19	C20	Ru1	72.81(15)

Table S28. Crystal data and structure refinement details for **6.**

Empirical formula	$C_{20}H_{20}Cl_2INORu$
Formula weight	589.24
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.9010(5)
b/Å	14.1378(5)
c/Å	14.1674(8)
α/°	87.431(4)
β/°	73.597(5)
γ/°	86.195(3)
Volume/Å^3	2089.16(18)
Z	4

ρ_{calc}mg/mm^3	1.873
m/mm^{-1}	2.493
F(000)	1144.0
Crystal size/mm^3	? × ? × ?
2Θ range for data collection	6.582 to 52.744°
Index ranges	-11 ≤ h ≤ 13, -17 ≤ k ≤ 16, -17 ≤ l ≤ 16
Reflections collected	14252
Independent reflections	8526[R(int) = 0.0313]
Data/restraints/parameters	8526/0/477
Goodness-of-fit on F^2	1.005
Final R indexes [I>=2σ (I)]	R_1 = 0.0423, wR_2 = 0.0669
Final R indexes [all data]	R_1 = 0.0759, wR_2 = 0.0800
Largest diff. peak/hole / e Å^{-3}	0.74/-0.60

Table S29. Selected bond lengths (Å) for **6**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	Ru1	2.7290(6)	C5	C10	1.411(7)
I2	Ru2	2.7317(6)	C7	C8	1.479(7)
Ru1	O1	2.063(3)	C7	C9	1.411(7)
Ru1	N1	2.142(4)	C9	C10	1.348(7)
Ru1	C14	2.185(6)	C11	C12	1.528(9)
Ru1	C15	2.152(6)	C12	C13	1.518(10)
Ru1	C16	2.189(5)	C12	C14	1.495(7)
Ru1	C17	2.234(5)	C14	C15	1.413(7)
Ru1	C19	2.219(5)	C14	C20	1.416(7)
Ru1	C20	2.154(5)	C15	C16	1.382(7)
Ru2	O2	2.063(4)	C16	C17	1.428(7)
Ru2	N2	2.142(4)	C17	C18	1.493(7)
Ru2	C24	2.210(6)	C17	C19	1.402(7)
Ru2	C25	2.147(5)	C19	C20	1.418(7)
Ru2	C26	2.182(5)	C21	C22	1.513(9)
Ru2	C27	2.220(5)	C22	C23	1.535(10)
Ru2	C29	2.210(5)	C22	C24	1.508(8)
Ru2	C30	2.158(5)	C24	C25	1.434(8)
Cl1	C2	1.736(5)	C24	C30	1.402(8)
Cl2	C4	1.741(5)	C25	C26	1.389(8)
Cl3	C38	1.721(6)	C26	C27	1.414(8)
Cl4	C36	1.743(5)	C27	C28	1.497(7)
O1	C1	1.251(5)	C27	C29	1.402(7)
O2	C39	1.306(5)	C29	C30	1.400(7)
N1	C6	1.379(6)	C31	C32	1.481(7)
N1	C7	1.325(6)	C32	C33	1.413(6)
N2	C32	1.314(6)	C33	C34	1.350(8)
N2	C40	1.384(6)	C34	C35	1.402(8)

C1	C2	1.368(6)	C35	C36	1.401(8)
C1	C6	1.463(6)	C35	C40	1.431(6)
C2	C3	1.422(7)	C36	C37	1.349(8)
C3	C4	1.357(7)	C37	C38	1.402(7)
C4	C5	1.395(7)	C38	C39	1.382(7)
C5	C6	1.427(6)	C39	C40	1.417(7)

Table S30. Selected bond lengths (Å) and bond angles (°) for **6**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	I1	85.32(11)	C3	C4	C5	122.9(5)
O1	Ru1	N1	78.65(14)	C5	C4	Cl2	118.1(5)
O1	Ru1	C14	93.21(17)	C4	C5	C6	116.8(5)
O1	Ru1	C15	87.24(18)	C4	C5	C10	126.1(5)
O1	Ru1	C16	108.65(17)	C10	C5	C6	117.0(5)
O1	Ru1	C17	145.21(16)	N1	C6	C1	115.6(4)
O1	Ru1	C19	161.85(18)	N1	C6	C5	121.5(5)
O1	Ru1	C20	125.37(18)	C5	C6	C1	122.9(5)
N1	Ru1	I1	84.75(11)	N1	C7	C8	121.6(5)
N1	Ru1	C14	109.44(19)	N1	C7	C9	119.7(5)
N1	Ru1	C15	144.0(2)	C9	C7	C8	118.7(5)
N1	Ru1	C16	172.34(18)	C10	C9	C7	122.4(5)
N1	Ru1	C17	135.53(18)	C9	C10	C5	119.2(5)
N1	Ru1	C19	105.83(17)	C13	C12	C11	112.9(7)
N1	Ru1	C20	94.24(18)	C14	C12	C11	114.2(6)
C14	Ru1	I1	165.20(15)	C14	C12	C13	110.0(6)
C14	Ru1	C16	68.5(2)	C12	C14	Ru1	127.1(4)
C14	Ru1	C17	81.8(2)	C15	C14	Ru1	69.7(4)
C14	Ru1	C19	68.66(19)	C15	C14	C12	120.7(5)
C15	Ru1	I1	127.20(16)	C15	C14	C20	115.3(5)
C15	Ru1	C14	38.0(2)	C20	C14	Ru1	69.7(3)
C15	Ru1	C16	37.12(19)	C20	C14	C12	123.9(6)
C15	Ru1	C17	67.7(2)	C14	C15	Ru1	72.3(3)
C15	Ru1	C19	79.0(2)	C16	C15	Ru1	72.9(3)
C15	Ru1	C20	67.4(2)	C16	C15	C14	123.4(5)
C16	Ru1	I1	97.98(16)	C15	C16	Ru1	70.0(3)
C16	Ru1	C17	37.65(18)	C15	C16	C17	120.8(5)
C16	Ru1	C19	66.51(19)	C17	C16	Ru1	72.9(3)
C17	Ru1	I1	91.02(15)	C16	C17	Ru1	69.5(3)
C19	Ru1	I1	112.42(15)	C16	C17	C18	122.1(5)
C19	Ru1	C17	36.71(17)	C18	C17	Ru1	130.2(4)
C20	Ru1	I1	148.58(15)	C19	C17	Ru1	71.1(3)
C20	Ru1	C14	38.10(19)	C19	C17	C16	117.3(5)
C20	Ru1	C16	79.7(2)	C19	C17	C18	120.6(5)
C20	Ru1	C17	67.9(2)	C17	C19	Ru1	72.2(3)

C20	Ru1	C19	37.82(18)	C17	C19	C20	120.7(5)
O2	Ru2	I2	86.75(10)	C20	C19	Ru1	68.6(3)
O2	Ru2	N2	79.26(15)	C14	C20	Ru1	72.2(3)
O2	Ru2	C24	93.4(2)	C14	C20	C19	122.4(5)
O2	Ru2	C25	85.60(19)	C19	C20	Ru1	73.6(3)
O2	Ru2	C26	106.7(2)	C21	C22	C23	110.5(7)
O2	Ru2	C27	143.1(2)	C24	C22	C21	109.4(6)
O2	Ru2	C29	161.11(18)	C24	C22	C23	112.0(6)
O2	Ru2	C30	125.83(19)	C22	C24	Ru2	128.2(4)
N2	Ru2	I2	83.89(10)	C25	C24	Ru2	68.4(3)
N2	Ru2	C24	108.81(19)	C25	C24	C22	119.7(7)
N2	Ru2	C25	143.0(2)	C30	C24	Ru2	69.3(3)
N2	Ru2	C26	173.5(2)	C30	C24	C22	125.6(6)
N2	Ru2	C27	137.0(2)	C30	C24	C25	114.6(6)
N2	Ru2	C29	107.11(19)	C24	C25	Ru2	73.2(3)
N2	Ru2	C30	94.91(18)	C26	C25	Ru2	72.7(3)
C24	Ru2	I2	167.12(16)	C26	C25	C24	123.0(6)
C24	Ru2	C27	81.6(2)	C25	C26	Ru2	69.9(3)
C24	Ru2	C29	67.8(2)	C25	C26	C27	120.7(6)
C25	Ru2	I2	128.93(18)	C27	C26	Ru2	72.7(3)
C25	Ru2	C24	38.4(2)	C26	C27	Ru2	69.8(3)
C25	Ru2	C26	37.4(2)	C26	C27	C28	122.2(6)
C25	Ru2	C27	67.8(2)	C28	C27	Ru2	131.4(4)
C25	Ru2	C29	78.8(2)	C29	C27	Ru2	71.2(3)
C25	Ru2	C30	67.3(2)	C29	C27	C26	117.3(5)
C26	Ru2	I2	98.82(17)	C29	C27	C28	120.6(6)
C26	Ru2	C24	68.8(2)	C27	C29	Ru2	71.9(3)
C26	Ru2	C27	37.5(2)	C30	C29	Ru2	69.3(3)
C26	Ru2	C29	66.4(2)	C30	C29	C27	121.2(6)
C27	Ru2	I2	90.61(15)	C24	C30	Ru2	73.3(3)
C29	Ru2	I2	111.36(15)	C29	C30	Ru2	73.4(3)
C29	Ru2	C27	36.90(19)	C29	C30	C24	123.1(6)
C30	Ru2	I2	146.73(17)	N2	C32	C31	120.8(5)
C30	Ru2	C24	37.4(2)	N2	C32	C33	120.5(5)
C30	Ru2	C26	79.6(2)	C33	C32	C31	118.7(5)
C30	Ru2	C27	67.8(2)	C34	C33	C32	121.2(6)
C30	Ru2	C29	37.38(18)	C33	C34	C35	120.5(5)
C1	O1	Ru1	116.3(3)	C34	C35	C40	116.0(5)
C39	O2	Ru2	114.0(4)	C36	C35	C34	126.8(5)
C6	N1	Ru1	110.6(3)	C36	C35	C40	117.3(6)
C7	N1	Ru1	129.2(4)	C35	C36	Cl4	118.9(5)
C7	N1	C6	120.2(4)	C37	C36	Cl4	119.3(5)
C32	N2	Ru2	129.8(4)	C37	C36	C35	121.8(5)
C32	N2	C40	119.6(4)	C36	C37	C38	120.2(6)
C40	N2	Ru2	110.5(3)	C37	C38	Cl3	119.1(5)

O1	C1	C2	127.3(5)	C39	C38	Cl3	118.6(4)
O1	C1	C6	118.8(4)	C39	C38	C37	122.3(6)
C2	C1	C6	113.9(4)	O2	C39	C38	123.3(5)
C1	C2	Cl1	117.4(4)	O2	C39	C40	119.9(5)
C1	C2	C3	124.8(5)	C38	C39	C40	116.7(5)
C3	C2	Cl1	117.7(4)	N2	C40	C35	122.0(5)
C4	C3	C2	118.5(5)	N2	C40	C39	116.2(4)
C3	C4	Cl2	119.0(5)	C39	C40	C35	121.7(5)

Table S31. Crystal data and structure refinement details for **p-cymene-RuCl.**

Empirical formula	$C_{30}H_{42}Cl_6Ru_3$
Formula weight	918.54
Temperature/K	293(2)
Crystal system	orthorhombic
Space group	Fdd2
a/Å	47.198(3)
b/Å	15.9275(10)
c/Å	18.8189(11)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	14146.9(15)
Z	16
ρ_{calc}g/cm^3	1.725
μ/mm^{-1}	1.737
F(000)	7296.0
Crystal size/mm^3	0.26 × 0.21 × 0.15
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.172 to 55.11
Index ranges	$-61 \le h \le 61$, $-20 \le k \le 20$, $-24 \le l \le 24$
Reflections collected	48743
Independent reflections	8111 [R_{int} = 0.0412, R_{sigma} = 0.0361]
Data/restraints/parameters	8111/37/339
Goodness-of-fit on F^2	1.051
Final R indexes [I>=2σ (I)]	R_1 = 0.0654, wR_2 = 0.1670
Final R indexes [all data]	R_1 = 0.0889, wR_2 = 0.1930
Largest diff. peak/hole / e Å^{-3}	4.39/-0.98
Flack parameter	0.43(14)

Table S32. Selected bond lengths (Å) for **p-cymene-RuCl**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru3	Cl6	2.451(3)	C25	C24	1.39(3)
Ru3	Cl5	2.450(3)	C25	C26	1.42(2)
Ru3	Cl7	2.392(3)	C27	C26	1.42(2)
Ru3	C28	2.153(15)	C27	C30	1.48(3)
Ru3	C25	2.147(15)	C29	C24	1.43(3)
Ru3	C27	2.176(16)	C22	C24	1.51(3)
Ru3	C29	2.143(15)	C22	C23	1.55(3)
Ru3	C24	2.175(17)	C22	C21	1.58(4)
Ru3	C26	2.162(14)	C8	C9	1.3900
Ru1	Cl2	2.442(4)	C8	C7	1.3900
Ru1	Cl1	2.444(4)	C9	C4	1.3900
Ru1	Cl3	2.398(4)	C4	C5	1.3900
Ru1	C8	2.181(10)	C4	C2	1.54(3)
Ru1	C9	2.165(11)	C5	C6	1.3900
Ru1	C4	2.140(10)	C6	C7	1.3900
Ru1	C5	2.132(10)	C7	C10	1.56(2)
Ru1	C6	2.149(11)	C2	C3	1.45(3)
Ru1	C7	2.174(10)	C2	C1	1.49(3)
Ru2	Cl2	2.450(4)	C12	C14	1.56(2)
Ru2	Cl1	2.455(4)	C12	C11	1.54(3)
Ru2	Cl4	2.392(4)	C12	C13	1.50(3)
Ru2	C15	2.141(10)	C15	C14	1.3900
Ru2	C14	2.136(9)	C15	C16	1.3900
Ru2	C19	2.149(10)	C14	C19	1.3900
Ru2	C18	2.166(9)	C19	C18	1.3900
Ru2	C17	2.170(10)	C18	C17	1.3900
Ru2	C16	2.158(11)	C17	C16	1.3900
C28	C27	1.42(3)	C17	C20	1.56(3)
C28	C29	1.38(3)			

Table S33. Selected bond lengths (Å) and bond angles (°) for **p-cymene-RuCl**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl5	Ru3	Cl6	82.43(11)	C18	Ru2	Cl1	109.9(3)
Cl7	Ru3	Cl6	85.75(11)	C18	Ru2	Cl4	162.1(3)
Cl7	Ru3	Cl5	87.37(12)	C18	Ru2	C17	37.39(15)
C28	Ru3	Cl6	163.3(6)	C17	Ru2	Cl2	123.2(4)
C28	Ru3	Cl5	96.5(5)	C17	Ru2	Cl1	88.8(3)
C28	Ru3	Cl7	110.9(6)	C17	Ru2	Cl4	148.8(4)
C28	Ru3	C27	38.3(7)	C16	Ru2	Cl2	160.7(4)

C28	Ru3	C24	69.7(8)	C16	Ru2	Cl1	95.8(3)
C28	Ru3	C26	68.7(7)	C16	Ru2	Cl4	112.2(4)
C25	Ru3	Cl6	90.4(4)	C16	Ru2	C18	67.7(2)
C25	Ru3	Cl5	146.6(5)	C16	Ru2	C17	37.47(17)
C25	Ru3	Cl7	124.8(5)	Ru3	Cl6	Ru3[1]	97.54(18)
C25	Ru3	C28	81.3(6)	Ru3	Cl5	Ru3[1]	97.61(18)
C25	Ru3	C27	69.5(6)	Ru1	Cl2	Ru2	97.61(15)
C25	Ru3	C24	37.6(7)	Ru1	Cl1	Ru2	97.44(16)
C25	Ru3	C26	38.4(6)	C27	C28	Ru3	71.7(9)
C27	Ru3	Cl6	125.1(5)	C29	C28	Ru3	70.9(9)
C27	Ru3	Cl5	88.1(4)	C29	C28	C27	120.0(15)
C27	Ru3	Cl7	147.8(5)	C24	C25	Ru3	72.3(10)
C27	Ru3	C24	83.0(7)	C24	C25	C26	122.3(17)
C29	Ru3	Cl6	149.5(5)	C26	C25	Ru3	71.3(8)
C29	Ru3	Cl5	127.5(5)	C28	C27	Ru3	70.0(9)
C29	Ru3	Cl7	89.7(5)	C28	C27	C26	117.8(16)
C29	Ru3	C28	37.5(7)	C28	C27	C30	119.4(19)
C29	Ru3	C25	67.7(6)	C26	C27	Ru3	70.3(9)
C29	Ru3	C27	68.3(7)	C26	C27	C30	123(2)
C29	Ru3	C24	38.6(8)	C30	C27	Ru3	128.7(12)
C29	Ru3	C26	80.3(7)	C28	C29	Ru3	71.7(9)
C24	Ru3	Cl6	111.7(7)	C28	C29	C24	123.7(17)
C24	Ru3	Cl5	165.8(7)	C24	C29	Ru3	71.9(10)
C24	Ru3	Cl7	94.4(5)	C24	C22	C23	108.0(18)
C26	Ru3	Cl6	95.9(4)	C24	C22	C21	110(2)
C26	Ru3	Cl5	109.7(5)	C23	C22	C21	110(2)
C26	Ru3	Cl7	163.0(5)	C25	C24	Ru3	70.1(9)
C26	Ru3	C27	38.3(7)	C25	C24	C29	115.9(19)
C26	Ru3	C24	69.2(6)	C25	C24	C22	125(2)
Cl2	Ru1	Cl1	82.67(11)	C29	C24	Ru3	69.5(10)
Cl3	Ru1	Cl2	85.28(16)	C29	C24	C22	118.8(19)
Cl3	Ru1	Cl1	87.11(18)	C22	C24	Ru3	129.2(13)
C8	Ru1	Cl2	94.7(3)	C25	C26	Ru3	70.2(9)
C8	Ru1	Cl1	111.7(4)	C25	C26	C27	120.3(16)
C8	Ru1	Cl3	161.1(4)	C27	C26	Ru3	71.4(10)
C9	Ru1	Cl2	90.7(3)	C9	C8	Ru1	70.7(4)
C9	Ru1	Cl1	147.9(4)	C9	C8	C7	120.0
C9	Ru1	Cl3	123.8(4)	C7	C8	Ru1	71.1(4)
C9	Ru1	C8	37.30(16)	C8	C9	Ru1	72.0(3)
C9	Ru1	C7	67.4(2)	C4	C9	Ru1	70.2(3)
C4	Ru1	Cl2	114.1(3)	C4	C9	C8	120.0
C4	Ru1	Cl1	163.2(3)	C9	C4	Ru1	72.1(4)
C4	Ru1	Cl3	95.0(3)	C9	C4	C2	116.8(13)
C4	Ru1	C8	67.7(2)	C5	C4	Ru1	70.7(4)
C4	Ru1	C9	37.67(17)	C5	C4	C9	120.0

C4	Ru1	C6	68.3(2)	C5	C4	C2	123.2(13)
C4	Ru1	C7	80.2(2)	C2	C4	Ru1	129.9(10)
C5	Ru1	Cl2	151.4(3)	C4	C5	Ru1	71.3(4)
C5	Ru1	Cl1	125.5(3)	C4	C5	C6	120.0
C5	Ru1	Cl3	90.7(3)	C6	C5	Ru1	71.7(4)
C5	Ru1	C8	80.2(2)	C5	C6	Ru1	70.4(3)
C5	Ru1	C9	68.1(2)	C7	C6	Ru1	72.2(3)
C5	Ru1	C4	37.97(15)	C7	C6	C5	120.0
C5	Ru1	C6	37.89(17)	C8	C7	Ru1	71.7(4)
C5	Ru1	C7	68.0(2)	C8	C7	C10	124.7(18)
C6	Ru1	Cl2	160.3(4)	C6	C7	Ru1	70.3(4)
C6	Ru1	Cl1	95.6(3)	C6	C7	C8	120.0
C6	Ru1	Cl3	114.3(4)	C6	C7	C10	115.2(18)
C6	Ru1	C8	67.6(2)	C10	C7	Ru1	127.3(11)
C6	Ru1	C9	80.2(2)	C3	C2	C4	116.8(18)
C6	Ru1	C7	37.51(17)	C3	C2	C1	114(2)
C7	Ru1	Cl2	122.8(4)	C1	C2	C4	110(2)
C7	Ru1	Cl1	89.9(3)	C11	C12	C14	108(2)
C7	Ru1	Cl3	151.2(4)	C13	C12	C14	112.8(14)
C7	Ru1	C8	37.23(15)	C13	C12	C11	114(2)
Cl2	Ru2	Cl1	82.28(10)	C14	C15	Ru2	70.9(4)
Cl4	Ru2	Cl2	87.02(16)	C14	C15	C16	120.0
Cl4	Ru2	Cl1	87.97(18)	C16	C15	Ru2	71.8(4)
C15	Ru2	Cl2	151.1(3)	C12	C14	Ru2	129.2(9)
C15	Ru2	Cl1	126.3(3)	C15	C14	Ru2	71.2(4)
C15	Ru2	Cl4	89.5(3)	C15	C14	C12	119.0(10)
C15	Ru2	C19	68.3(2)	C19	C14	Ru2	71.6(3)
C15	Ru2	C18	80.4(2)	C19	C14	C12	121.0(10)
C15	Ru2	C17	67.9(2)	C19	C14	C15	120.0
C15	Ru2	C16	37.73(17)	C14	C19	Ru2	70.6(3)
C14	Ru2	Cl2	113.9(3)	C14	C19	C18	120.0
C14	Ru2	Cl1	163.7(3)	C18	C19	Ru2	71.9(3)
C14	Ru2	Cl4	95.0(3)	C19	C18	Ru2	70.5(4)
C14	Ru2	C15	37.93(16)	C19	C18	C17	120.0
C14	Ru2	C19	37.85(16)	C17	C18	Ru2	71.5(4)
C14	Ru2	C18	68.1(2)	C18	C17	Ru2	71.1(4)
C14	Ru2	C17	80.4(2)	C18	C17	C20	118.5(16)
C14	Ru2	C16	68.2(2)	C16	C17	Ru2	70.8(3)
C19	Ru2	Cl2	90.5(3)	C16	C17	C18	120.0
C19	Ru2	Cl1	146.2(3)	C16	C17	C20	121.4(16)
C19	Ru2	Cl4	124.8(3)	C20	C17	Ru2	128.1(11)
C19	Ru2	C18	37.58(15)	C15	C16	Ru2	70.5(3)
C19	Ru2	C17	67.8(2)	C17	C16	Ru2	71.8(3)
C19	Ru2	C16	80.4(2)	C17	C16	C15	120.0
C18	Ru2	Cl2	94.7(3)				

Table S34. Crystal data and structure refinement details for **13.**

Empirical formula	$C_{19}H_{17}Cl_2NO_3Ru$
Formula weight	479.31
Temperature/K	293(2)
Crystal system	monoclinic
Space group	P2/c
a/Å	16.2187(6)
b/Å	5.9701(2)
c/Å	22.2623(12)
α/°	90
β/°	121.786(3)
γ/°	90
Volume/Å^3	1832.30(14)
Z	4
ρ_{calc}mg/mm^3	1.737
m/mm^{-1}	1.166
F(000)	960.0
Crystal size/mm^3	? × ? × ?
2Θ range for data collection	6.824 to 52.742°
Index ranges	$-20 \le h \le 20$, $-7 \le k \le 7$, $-27 \le l \le 23$
Reflections collected	12936
Independent reflections	3755[R(int) = 0.0662]
Data/restraints/parameters	3755/763/238
Goodness-of-fit on F^2	1.098
Final R indexes [I>=2σ (I)]	R_1 = 0.0578, wR_2 = 0.1244
Final R indexes [all data]	R_1 = 0.0847, wR_2 = 0.1383
Largest diff. peak/hole / e Å^{-3}	1.10/-0.78

Table S35. Selected bond lengths (Å) for **13**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	Cl1	2.4059(18)	C2	C3	1.438(9)
Ru1	O1	2.095(4)	C3	C4	1.533(10)
Ru1	N14	2.089(5)	C4	C5	1.469(9)
Ru1	C11	2.160(7)	C5	C6	1.387(9)
Ru1	C12	2.205(7)	C5	C9	1.382(9)
Ru1	C13	2.177(7)	C6	C7	1.371(9)
Ru1	C14	2.156(7)	C7	C8	1.382(9)
Ru1	C15	2.187(7)	C10	C12	1.493(11)
Ru1	C16	2.153(7)	C11	C12	1.396(11)

Cl2	C2	1.723(7)	C11	C16	1.391(11)
O1	C1	1.280(7)	C12	C13	1.415(10)
O2	C3	1.225(8)	C13	C14	1.379(10)
O3	C4	1.207(8)	C14	C15	1.400(11)
N14	C8	1.343(8)	C15	C16	1.397(11)
N14	C9	1.346(8)	C15	C17	1.497(12)
C1	C2	1.366(8)	C17	C18	1.498(12)
C1	C9	1.479(9)	C17	C19	1.397(12)

Table S36. Selected bond lengths (Å) and bond angles (°) for **13**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	Cl1	85.79(13)	C1	C2	C3	123.7(6)
O1	Ru1	C11	156.8(3)	C3	C2	Cl2	117.3(5)
O1	Ru1	C12	156.8(2)	O2	C3	C2	124.0(7)
O1	Ru1	C13	119.5(2)	O2	C3	C4	119.6(7)
O1	Ru1	C14	94.0(2)	C2	C3	C4	116.4(6)
O1	Ru1	C15	93.4(2)	O3	C4	C3	118.7(7)
O1	Ru1	C16	119.4(3)	O3	C4	C5	122.0(7)
N14	Ru1	Cl1	83.99(15)	C5	C4	C3	119.3(6)
N14	Ru1	O1	76.88(18)	C6	C5	C4	122.7(6)
N14	Ru1	C11	99.4(2)	C9	C5	C4	118.4(6)
N14	Ru1	C12	125.7(3)	C9	C5	C6	118.9(6)
N14	Ru1	C13	163.2(2)	C7	C6	C5	118.5(6)
N14	Ru1	C14	154.2(3)	C6	C7	C8	120.0(7)
N14	Ru1	C15	117.9(3)	N14	C8	C7	121.8(6)
N14	Ru1	C16	95.8(2)	N14	C9	C1	114.3(5)
C11	Ru1	Cl1	116.8(2)	N14	C9	C5	122.5(6)
C11	Ru1	C12	37.3(3)	C5	C9	C1	123.2(6)
C11	Ru1	C13	67.2(3)	C12	C11	Ru1	73.1(4)
C11	Ru1	C15	67.9(3)	C16	C11	Ru1	70.9(4)
C12	Ru1	Cl1	91.2(2)	C16	C11	C12	121.7(7)
C13	Ru1	Cl1	93.0(2)	C10	C12	Ru1	128.7(6)
C13	Ru1	C12	37.7(3)	C11	C12	Ru1	69.6(4)
C13	Ru1	C15	67.7(3)	C11	C12	C10	122.4(8)
C14	Ru1	Cl1	119.8(2)	C11	C12	C13	117.3(7)
C14	Ru1	C11	79.4(3)	C13	C12	Ru1	70.1(4)
C14	Ru1	C12	67.6(3)	C13	C12	C10	120.3(8)
C14	Ru1	C13	37.1(3)	C12	C13	Ru1	72.3(4)
C14	Ru1	C15	37.6(3)	C14	C13	Ru1	70.6(4)
C15	Ru1	Cl1	157.4(2)	C14	C13	C12	120.6(7)
C15	Ru1	C12	80.7(3)	C13	C14	Ru1	72.3(4)
C16	Ru1	Cl1	154.2(2)	C13	C14	C15	122.1(7)

C16	Ru1	C11	37.6(3)	C15	C14	Ru1	72.4(4)
C16	Ru1	C12	67.9(3)	C14	C15	Ru1	70.0(4)
C16	Ru1	C13	79.8(3)	C14	C15	C17	127.7(8)
C16	Ru1	C14	67.4(3)	C16	C15	Ru1	69.9(4)
C16	Ru1	C15	37.5(3)	C16	C15	C14	117.4(7)
C1	O1	Ru1	116.9(4)	C16	C15	C17	114.9(8)
C8	N14	Ru1	126.1(4)	C17	C15	Ru1	132.9(6)
C8	N14	C9	118.3(5)	C11	C16	Ru1	71.4(4)
C9	N14	Ru1	115.6(4)	C11	C16	C15	121.0(7)
O1	C1	C2	124.9(6)	C15	C16	Ru1	72.5(4)
O1	C1	C9	116.3(5)	C15	C17	C18	111.6(8)
C2	C1	C9	118.7(6)	C19	C17	C15	118.8(9)
C1	C2	Cl2	118.9(5)	C19	C17	C18	109.3(10)

Table S37. Crystal data and structure refinement details for **11**.

Empirical formula	$C_{20}H_{22}INORu$
Formula weight	520.35
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.1740(8)
b/Å	16.6484(19)
c/Å	13.7808(17)
α/°	90
β/°	93.707(12)
γ/°	90
Volume/Å^3	1871.4(4)
Z	4
ρ_{calc}mg/mm^3	1.847
m/mm^{-1}	2.493
F(000)	1016.0
Crystal size/mm^3	? × ? × ?
2Θ range for data collection	6.994 to 52.742°
Index ranges	$-10 \leq h \leq 10$, $-20 \leq k \leq 19$, $-17 \leq l \leq 17$
Reflections collected	12797
Independent reflections	3816[R(int) = 0.1884]
Data/restraints/parameters	3816/672/221
Goodness-of-fit on F^2	0.931
Final R indexes [I>=2σ (I)]	$R_1 = 0.0943$, $wR_2 = 0.2046$
Final R indexes [all data]	$R_1 = 0.1942$, $wR_2 = 0.2623$
Largest diff. peak/hole / e Å^{-3}	1.70/-1.27

Table S38. Selected bond lengths (Å) for **11**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	Ru1	2.7434(15)	C5	C6	1.38(2)
Ru1	O1	2.033(9)	C5	C10	1.398(18)
Ru1	N1	2.102(11)	C6	C7	1.339(19)
Ru1	C14	2.151(14)	C7	C8	1.398(19)
Ru1	C15	2.224(14)	C8	C9	1.403(19)
Ru1	C16	2.119(15)	C9	C10	1.46(2)
Ru1	C17	2.179(15)	C11	C12	1.46(2)
Ru1	C18	2.234(14)	C12	C13	1.50(2)
Ru1	C19	2.186(13)	C12	C15	1.48(2)
O1	C9	1.285(16)	C14	C15	1.397(19)
N1	C2	1.371(17)	C14	C19	1.42(2)
N1	C10	1.395(16)	C15	C16	1.394(19)
C1	C2	1.494(18)	C16	C17	1.385(19)
C2	C3	1.42(2)	C17	C18	1.41(2)
C3	C4	1.34(2)	C18	C19	1.36(2)
C4	C5	1.40(2)	C18	C20	1.49(2)

Table S39. Selected bond lengths (Å) and bond angles (°) for **11**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	I1	86.3(3)	C3	C2	C1	121.6(14)
O1	Ru1	N1	78.3(4)	C4	C3	C2	122.1(15)
O1	Ru1	C14	132.6(5)	C3	C4	C5	119.8(15)
O1	Ru1	C15	98.9(4)	C6	C5	C4	124.1(15)
O1	Ru1	C16	86.6(5)	C6	C5	C10	119.8(15)
O1	Ru1	C17	103.4(5)	C10	C5	C4	116.0(14)
O1	Ru1	C18	137.7(5)	C7	C6	C5	119.9(15)
O1	Ru1	C19	164.7(5)	C6	C7	C8	123.4(16)
N1	Ru1	I1	84.9(3)	C7	C8	C9	119.8(15)
N1	Ru1	C14	93.9(5)	O1	C9	C8	125.8(15)
N1	Ru1	C15	103.9(5)	O1	C9	C10	118.0(13)
N1	Ru1	C16	135.5(5)	C8	C9	C10	116.1(13)
N1	Ru1	C17	171.8(5)	N1	C10	C5	126.2(14)
N1	Ru1	C18	143.2(5)	N1	C10	C9	112.9(12)
N1	Ru1	C19	111.5(5)	C5	C10	C9	120.9(14)
C14	Ru1	I1	140.1(4)	C11	C12	C13	110.4(15)
C14	Ru1	C15	37.2(5)	C11	C12	C15	113.1(14)
C14	Ru1	C17	79.0(5)	C15	C12	C13	113.7(15)
C14	Ru1	C18	67.8(6)	C15	C14	Ru1	74.2(8)
C14	Ru1	C19	38.3(5)	C15	C14	C19	121.7(15)
C15	Ru1	I1	170.5(4)	C19	C14	Ru1	72.2(8)
C15	Ru1	C18	81.0(6)	C12	C15	Ru1	130.9(10)
C16	Ru1	I1	136.1(4)	C14	C15	Ru1	68.6(8)

C16	Ru1	C14	66.5(6)	C14	C15	C12	121.6(14)
C16	Ru1	C15	37.3(5)	C16	C15	Ru1	67.2(8)
C16	Ru1	C17	37.6(5)	C16	C15	C12	124.4(14)
C16	Ru1	C18	67.7(6)	C16	C15	C14	114.0(14)
C16	Ru1	C19	78.2(6)	C15	C16	Ru1	75.4(9)
C17	Ru1	I1	103.2(4)	C17	C16	Ru1	73.6(9)
C17	Ru1	C15	67.9(5)	C17	C16	C15	124.6(15)
C17	Ru1	C18	37.2(5)	C16	C17	Ru1	68.9(9)
C17	Ru1	C19	65.2(6)	C16	C17	C18	120.6(15)
C18	Ru1	I1	89.8(4)	C18	C17	Ru1	73.5(9)
C19	Ru1	I1	105.7(4)	C17	C18	Ru1	69.3(8)
C19	Ru1	C15	67.9(6)	C17	C18	C20	119.8(15)
C19	Ru1	C18	35.9(5)	C19	C18	Ru1	70.2(8)
C9	O1	Ru1	117.2(9)	C19	C18	C17	116.2(14)
C2	N1	Ru1	132.0(9)	C19	C18	C20	124.1(15)
C2	N1	C10	114.6(12)	C20	C18	Ru1	130.4(11)
C10	N1	Ru1	113.3(9)	C14	C19	Ru1	69.5(8)
N1	C2	C1	117.1(13)	C18	C19	Ru1	74.0(8)
N1	C2	C3	121.2(14)	C18	C19	C14	122.6(15)

Table S40. Crystal data and structure refinement details for **12**.

Empirical formula	$C_{19}H_{20}INO_2Ru$
Formula weight	522.33
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	9.3758(3)
b/Å	14.4693(4)
c/Å	13.6980(4)
α/°	90
β/°	100.3030(10)
γ/°	90
Volume/Å^3	1828.32(9)
Z	4
ρ_{calc}mg/mm^3	1.898
m/mm^{-1}	2.557
F(000)	1016.0
Crystal size/mm^3	0.425 × 0.172 × 0.067
2Θ range for data collection	6.046 to 55.014°
Index ranges	$-12 \le h \le 12$, $-18 \le k \le 18$, $-16 \le l \le 17$
Reflections collected	28457
Independent reflections	4205[R(int) = 0.0375]

Data/restraints/parameters	4205/0/221
Goodness-of-fit on F^2	1.044
Final R indexes [I>=2σ (I)]	R_1 = 0.0256, wR_2 = 0.0512
Final R indexes [all data]	R_1 = 0.0371, wR_2 = 0.0543
Largest diff. peak/hole / e $Å^{-3}$	1.01/-0.57

Table S41. Selected bond lengths (Å) for **12**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
I1	Ru1	2.7410(3)	C4	C5	1.409(4)
Ru1	O1	2.0861(19)	C4	C9	1.403(4)
Ru1	N1	2.123(2)	C5	C6	1.369(4)
Ru1	C11	2.177(3)	C6	C7	1.395(4)
Ru1	C12	2.195(3)	C7	C8	1.380(4)
Ru1	C13	2.176(3)	C8	C9	1.421(4)
Ru1	C14	2.181(3)	C10	C12	1.506(4)
Ru1	C15	2.220(3)	C11	C12	1.418(5)
Ru1	C16	2.171(3)	C11	C16	1.398(5)
O1	C8	1.338(3)	C12	C13	1.410(4)
O2	C1	1.317(3)	C13	C14	1.422(4)
N1	C1	1.327(3)	C14	C15	1.402(4)
N1	C9	1.380(3)	C15	C16	1.426(4)
C1	C2	1.425(4)	C15	C17	1.506(4)
C2	C3	1.343(4)	C17	C18	1.519(6)
C3	C4	1.423(4)	C17	C19	1.513(5)

Table S42. Selected bond lengths (Å) and bond angles (°) for **12**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Ru1	I1	86.39(6)	N1	C1	C2	120.7(3)
O1	Ru1	N1	78.04(8)	C3	C2	C1	120.8(3)
O1	Ru1	C11	161.95(11)	C2	C3	C4	120.2(3)
O1	Ru1	C12	124.18(11)	C5	C4	C3	124.5(3)
O1	Ru1	C13	95.58(10)	C9	C4	C3	116.1(3)
O1	Ru1	C14	91.03(10)	C9	C4	C5	119.4(3)
O1	Ru1	C15	113.09(9)	C6	C5	C4	119.5(3)
O1	Ru1	C16	150.15(10)	C5	C6	C7	121.6(3)
N1	Ru1	I1	84.47(6)	C8	C7	C6	120.5(3)
N1	Ru1	C11	101.40(10)	O1	C8	C7	123.9(2)
N1	Ru1	C12	93.09(10)	O1	C8	C9	117.4(2)

N1	Ru1	C13	112.65(10)	C7	C8	C9	118.7(3)
N1	Ru1	C14	148.21(10)	N1	C9	C4	123.4(2)
N1	Ru1	C15	168.85(10)	N1	C9	C8	116.3(2)
N1	Ru1	C16	131.01(10)	C4	C9	C8	120.3(3)
C11	Ru1	I1	111.59(9)	C12	C11	Ru1	71.76(18)
C11	Ru1	C12	37.85(12)	C16	C11	Ru1	70.97(17)
C11	Ru1	C14	80.04(11)	C16	C11	C12	120.7(3)
C11	Ru1	C15	68.30(11)	C10	C12	Ru1	128.8(2)
C12	Ru1	I1	148.22(9)	C11	C12	Ru1	70.39(18)
C12	Ru1	C15	81.25(11)	C11	C12	C10	121.0(3)
C13	Ru1	I1	162.83(8)	C13	C12	Ru1	70.42(17)
C13	Ru1	C11	67.76(12)	C13	C12	C10	120.8(3)
C13	Ru1	C12	37.64(11)	C13	C12	C11	118.2(3)
C13	Ru1	C14	38.09(11)	C12	C13	Ru1	71.94(18)
C13	Ru1	C15	68.24(11)	C12	C13	C14	120.6(3)
C14	Ru1	I1	124.99(8)	C14	C13	Ru1	71.15(17)
C14	Ru1	C12	68.39(11)	C13	C14	Ru1	70.76(16)
C14	Ru1	C15	37.15(11)	C15	C14	Ru1	72.96(16)
C15	Ru1	I1	95.26(8)	C15	C14	C13	121.7(3)
C16	Ru1	I1	89.67(9)	C14	C15	Ru1	69.90(16)
C16	Ru1	C11	37.52(12)	C14	C15	C16	117.0(3)
C16	Ru1	C12	68.19(13)	C14	C15	C17	123.1(3)
C16	Ru1	C13	80.13(12)	C16	C15	Ru1	69.17(16)
C16	Ru1	C14	67.32(11)	C16	C15	C17	119.9(3)
C16	Ru1	C15	37.88(11)	C17	C15	Ru1	131.2(2)
C8	O1	Ru1	115.20(16)	C11	C16	Ru1	71.51(18)
C1	N1	Ru1	128.34(19)	C11	C16	C15	121.9(3)
C1	N1	C9	118.7(2)	C15	C16	Ru1	72.96(17)
C9	N1	Ru1	112.96(16)	C15	C17	C18	109.0(3)
O2	C1	N1	116.8(2)	C15	C17	C19	114.0(3)
O2	C1	C2	122.5(2)	C19	C17	C18	111.0(3)

Table S43. ROS generation assay (OD value) in HeLa cells after treatment with **1** and **2** for 24 h, respectively.

	OD_1	OD_2	OD_3	mean value of OD	SD
Control	24.573	26.322	21.869	24.255	2.244
2	36.772	38.564	33.481	36.272	2.578
1	57.635	54.816	55.147	55.866	1.541

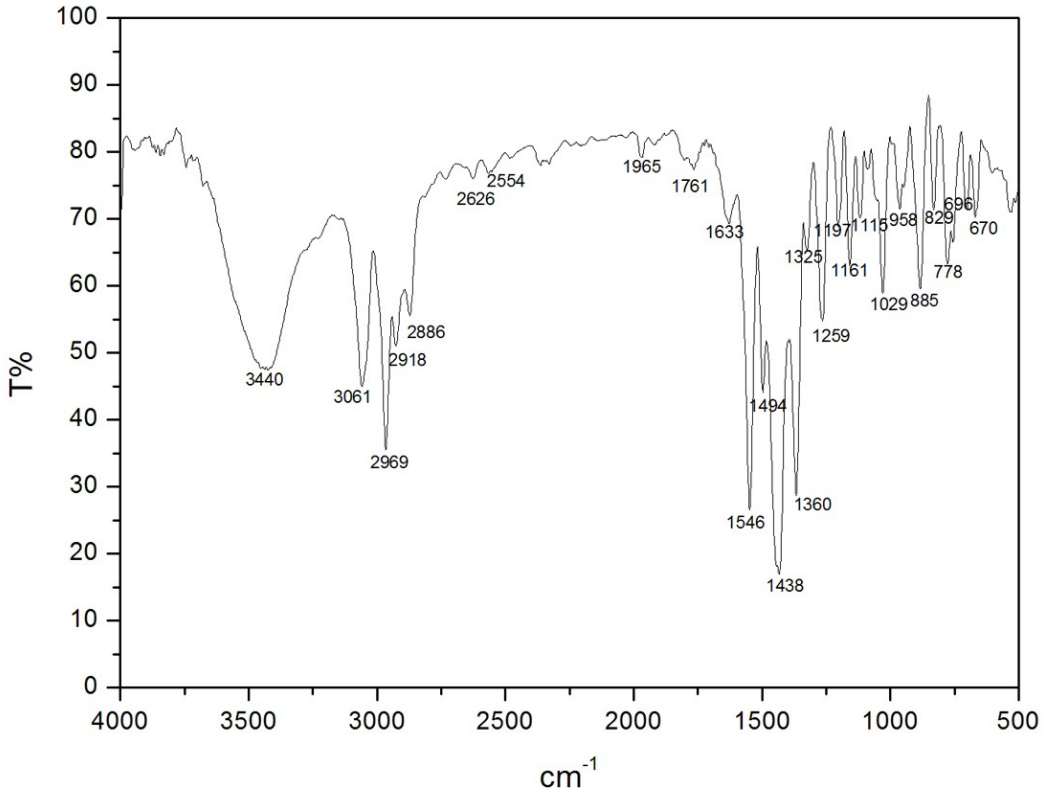

Figure S1. IR (KBr) spectra of **6**.

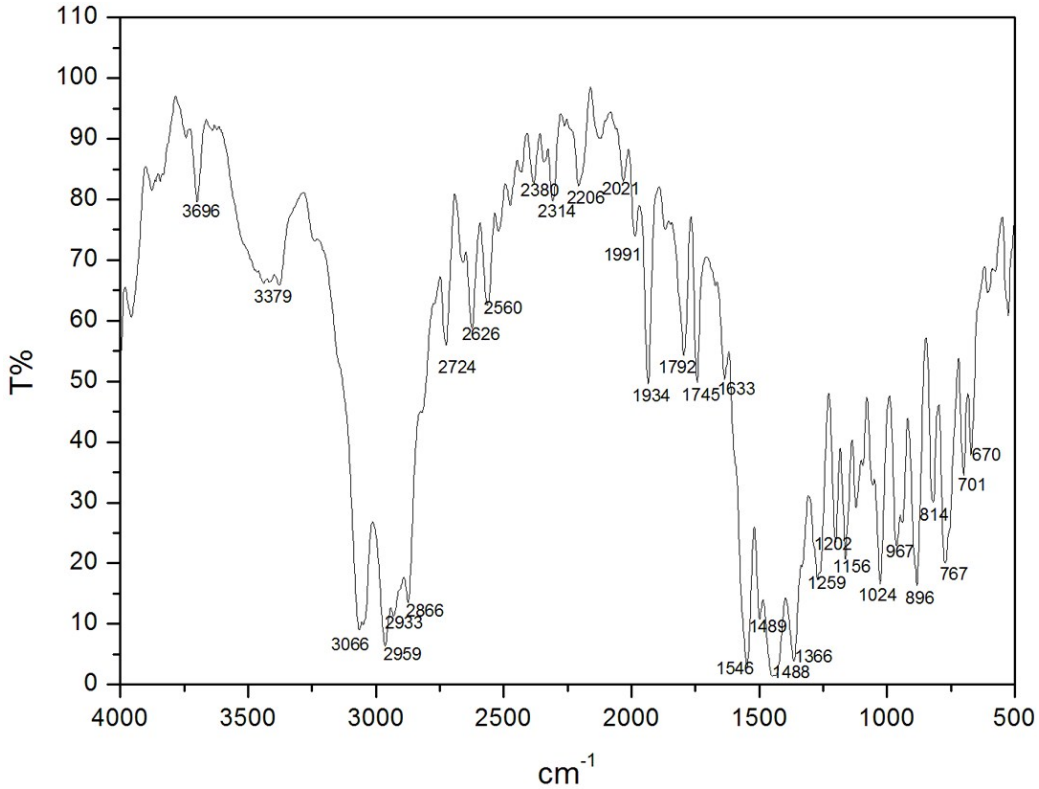

Figure S2. IR (KBr) spectra of **1**.

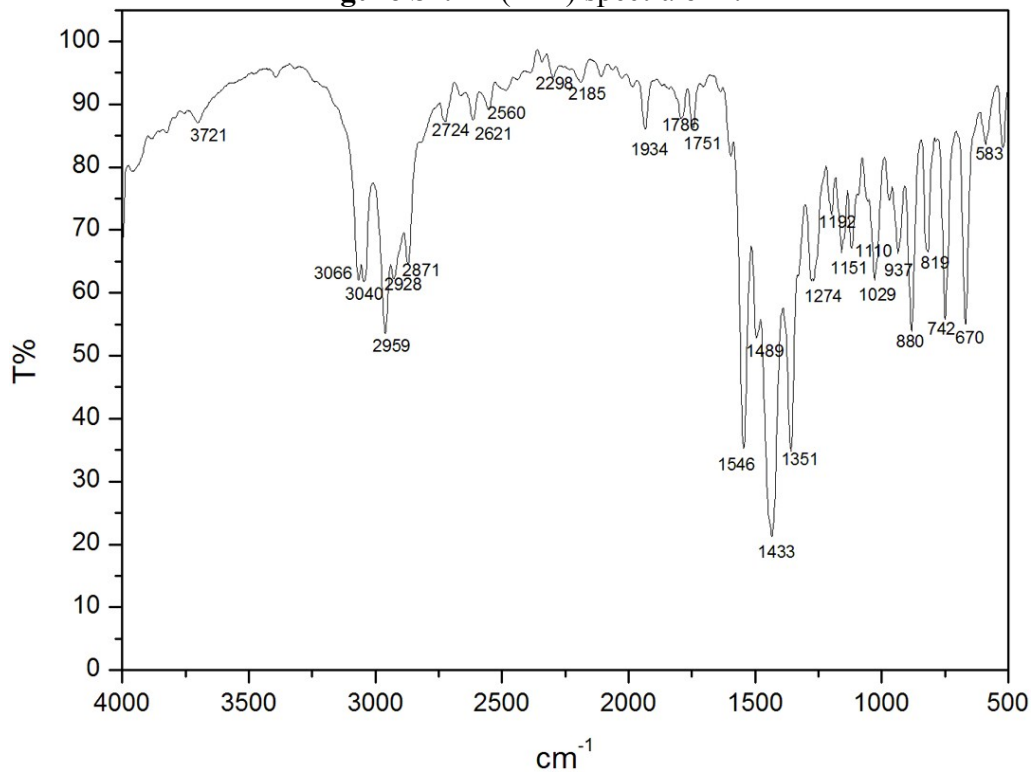

Figure S3. IR (KBr) spectra of **2.**

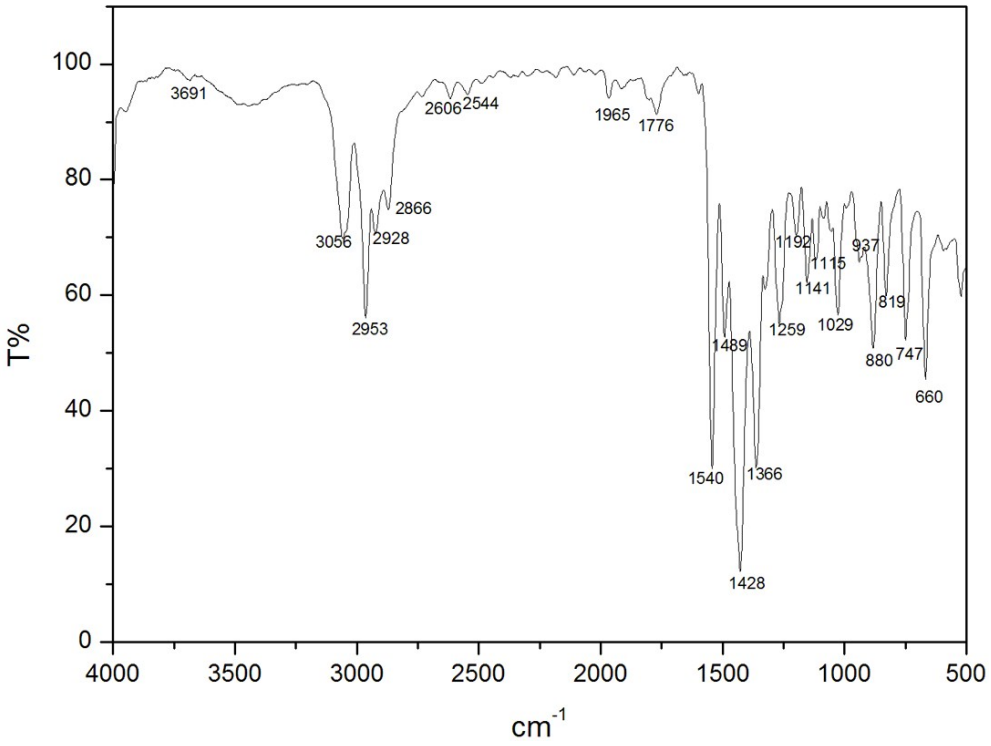

Figure S4. IR (KBr) spectra of **7**.

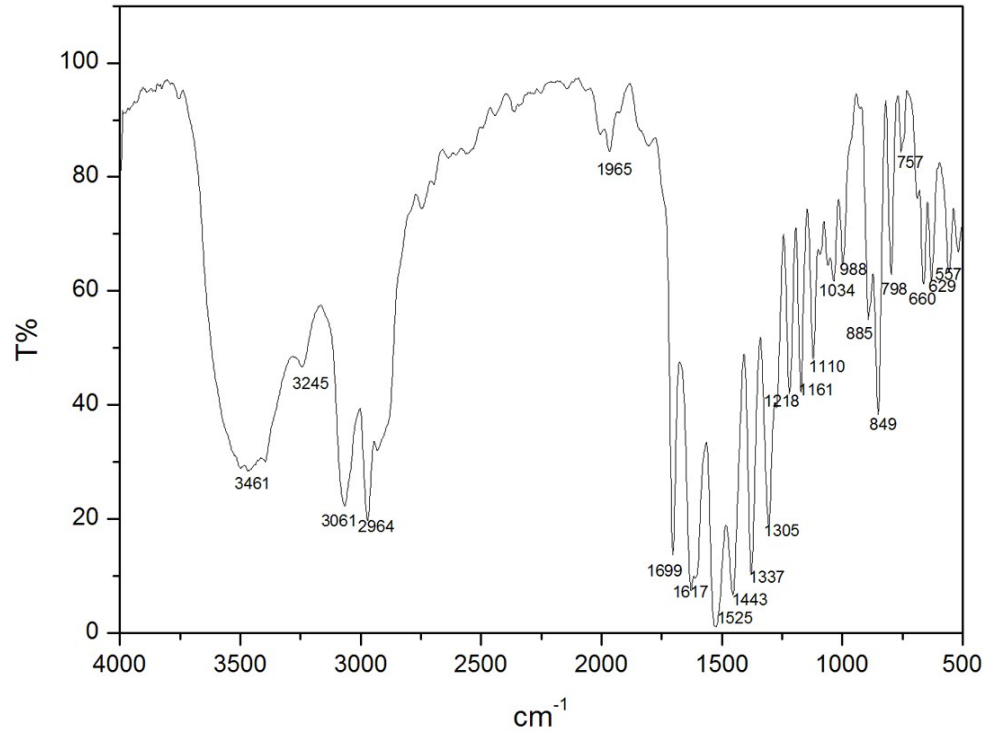

Figure S5. IR (KBr) spectra of **13.**

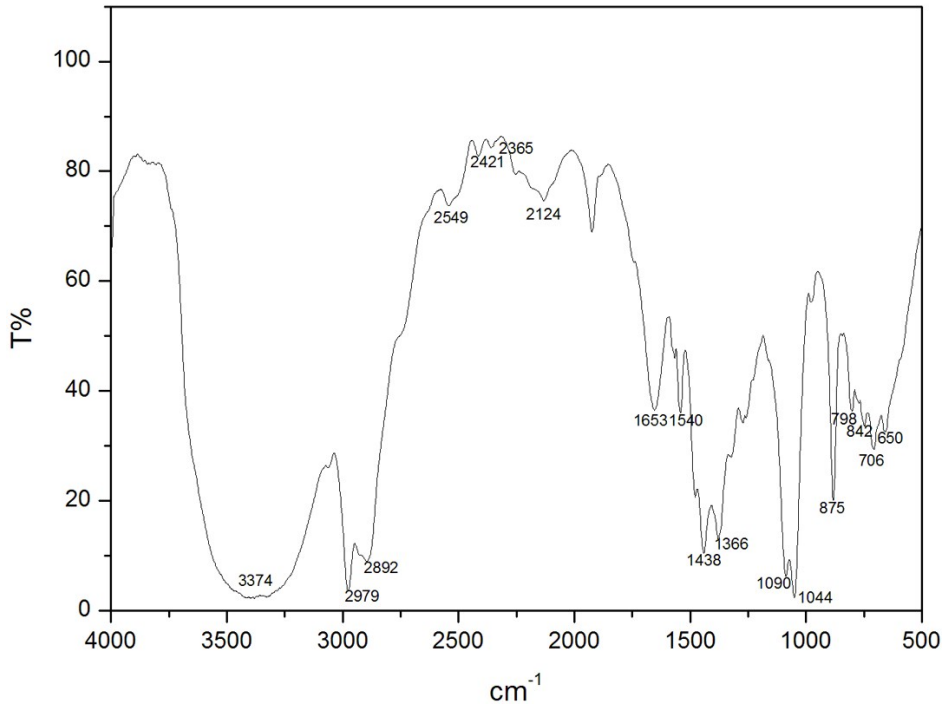

Figure S6. IR (KBr) spectra of **3**.

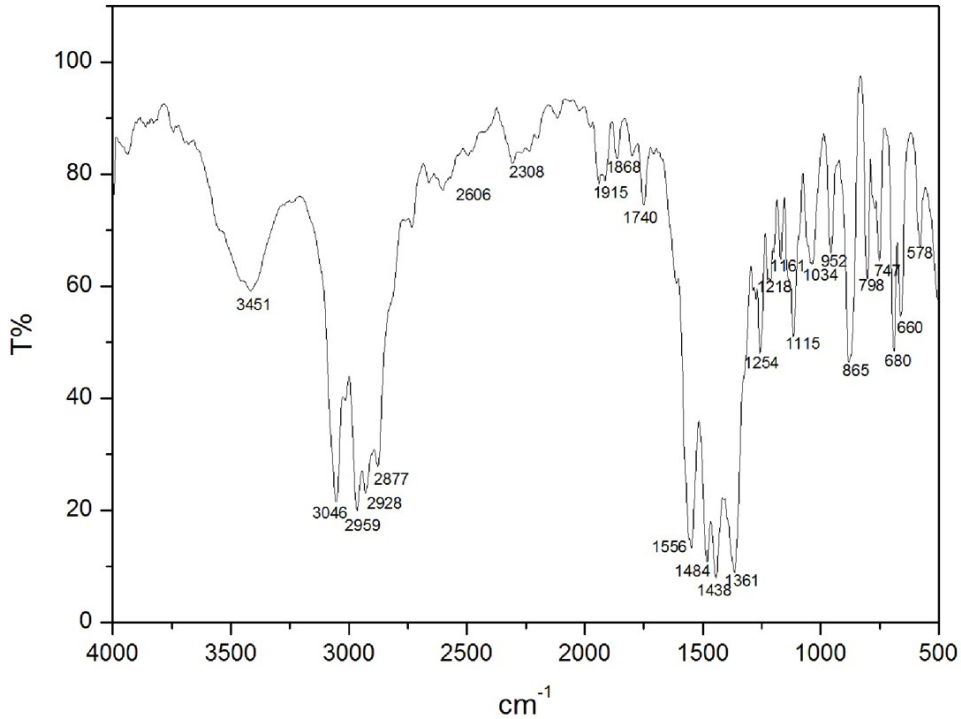

Figure S7. IR (KBr) spectra of **4.**

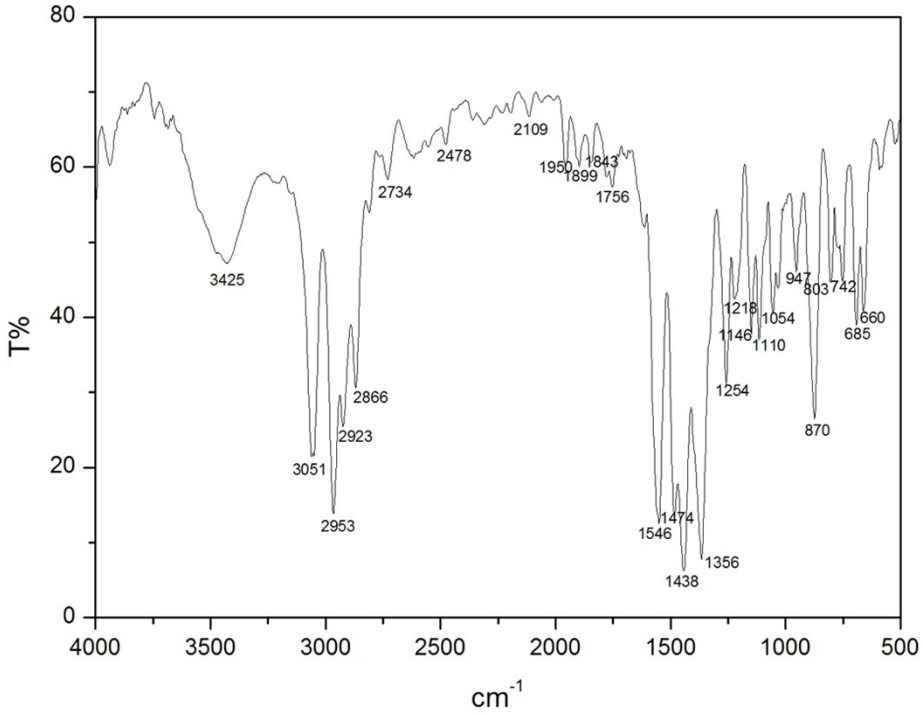

Figure S8. IR (KBr) spectra of **9**.

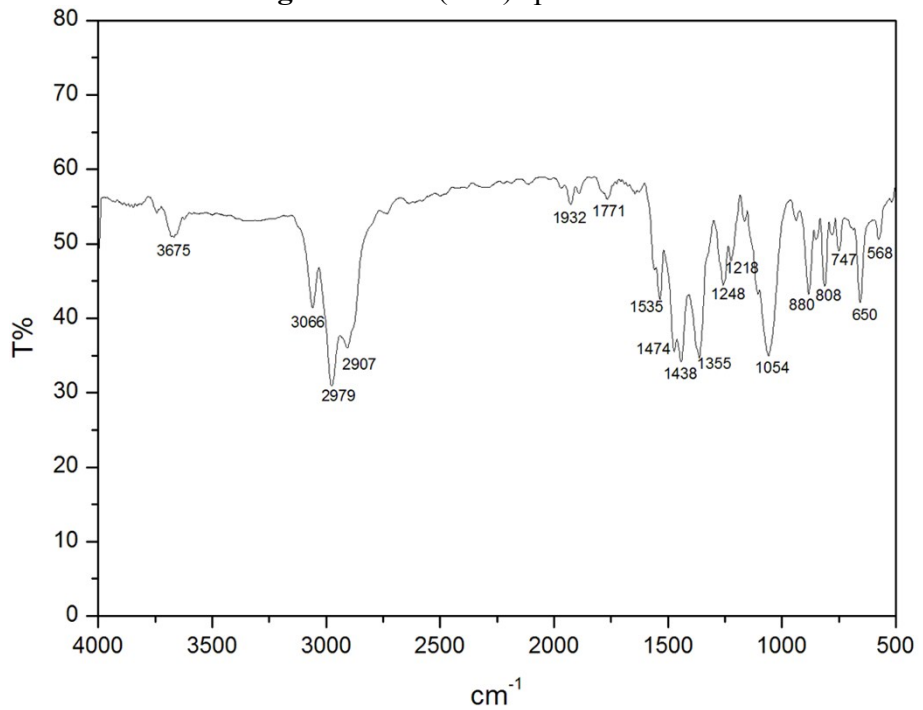

Figure S9. IR (KBr) spectra of **5.**

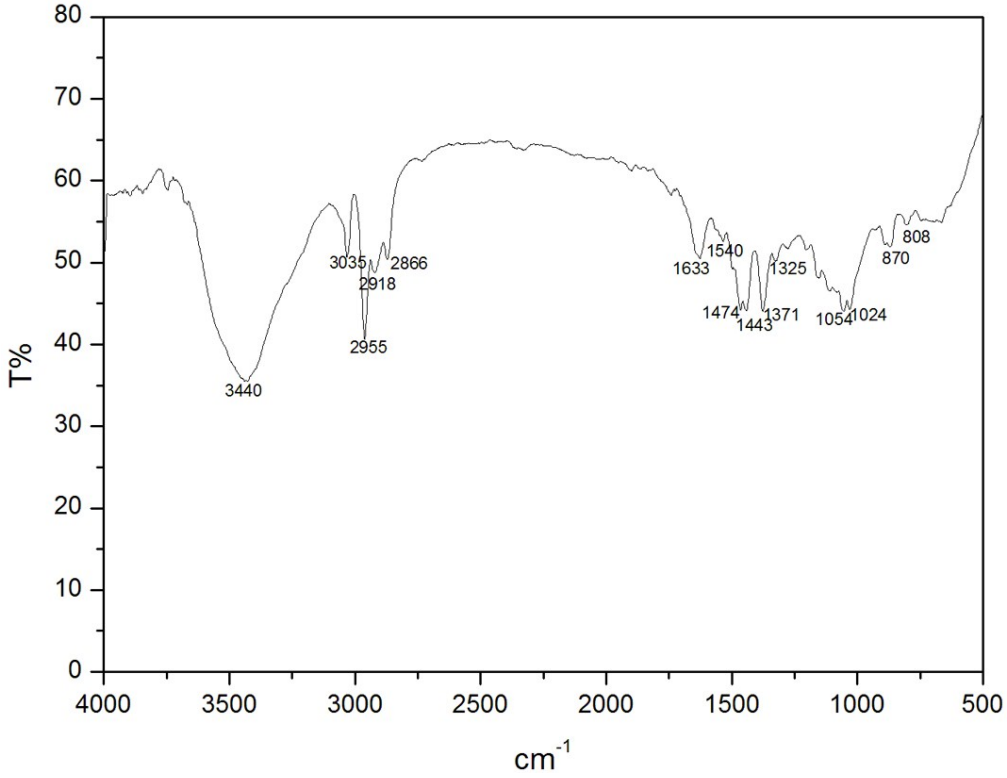

Figure S10. IR (KBr) spectra of **10**.

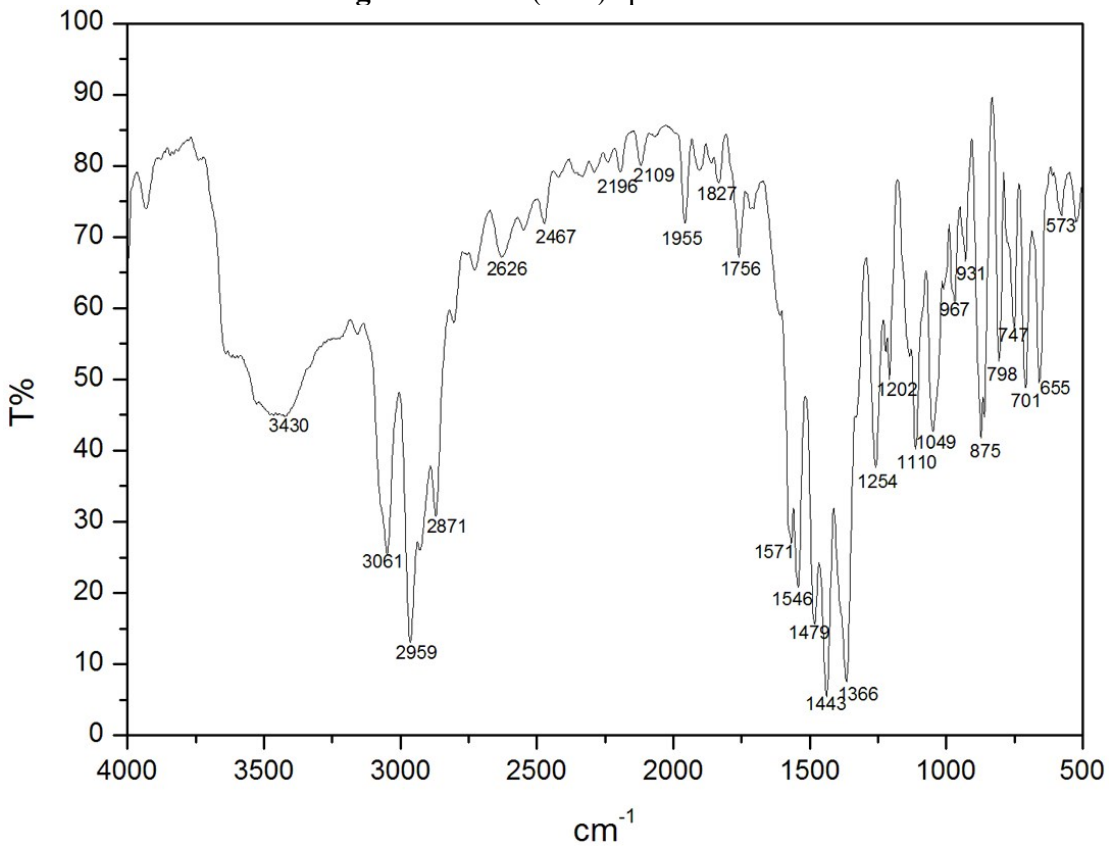

Figure S11. IR (KBr) spectra of **8.**

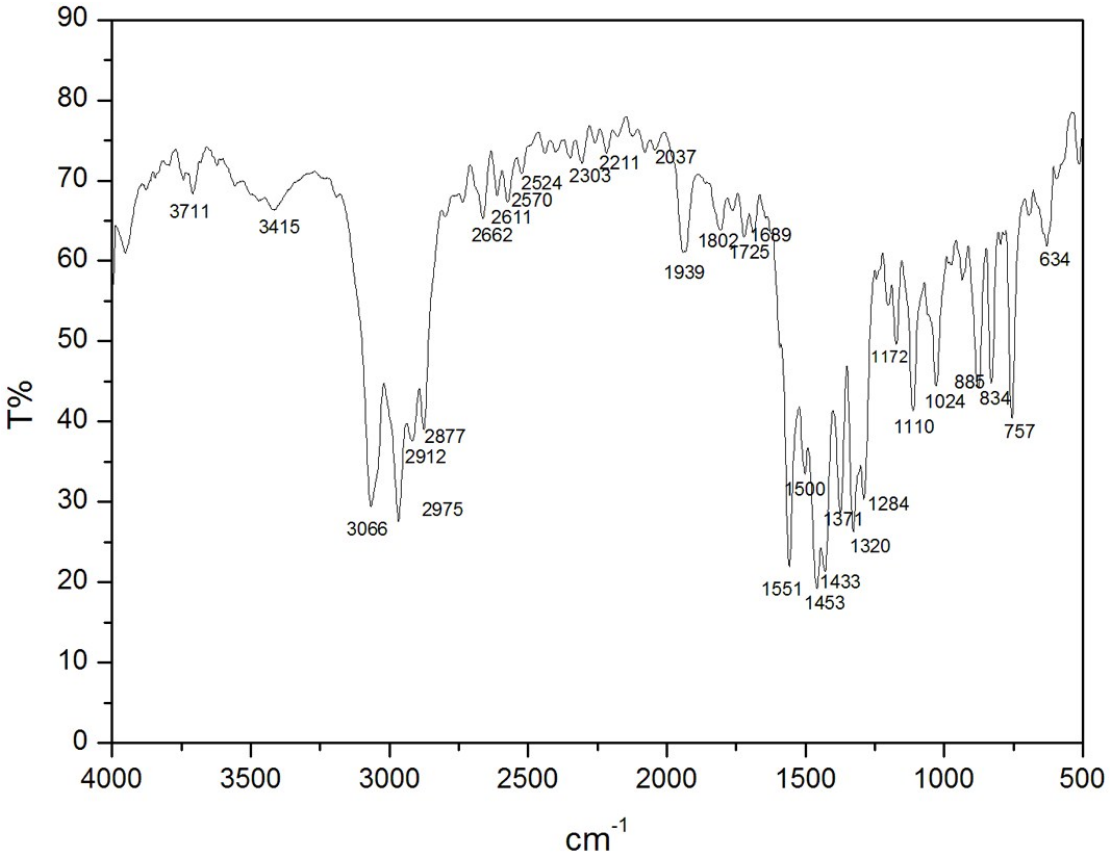

Figure S12. IR (KBr) spectra of **11**.

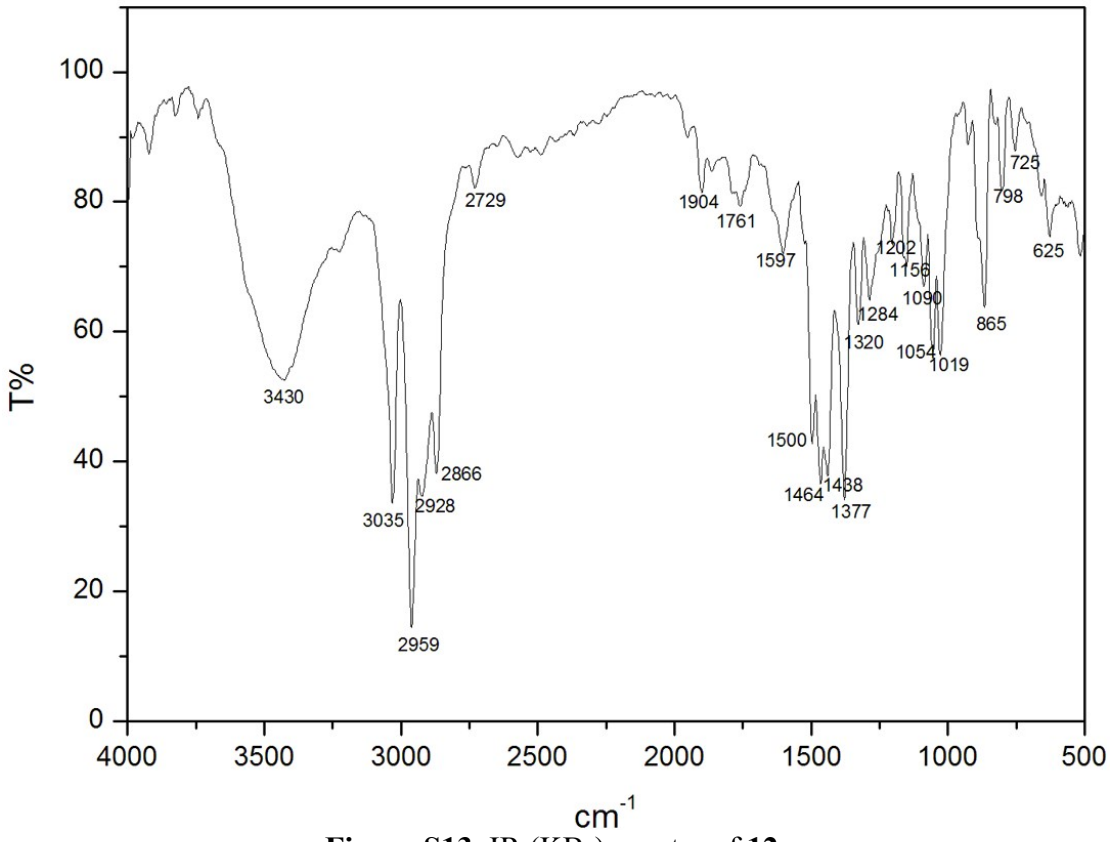

Figure S13. IR (KBr) spectra of **12**.

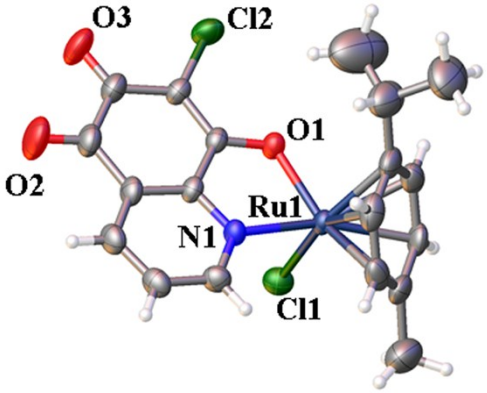

Figure S14. Molecular structure of **13**.

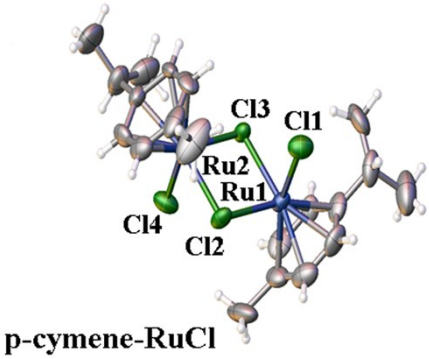

Figure S15. Molecular structure of **p-cymene-RuCl**.

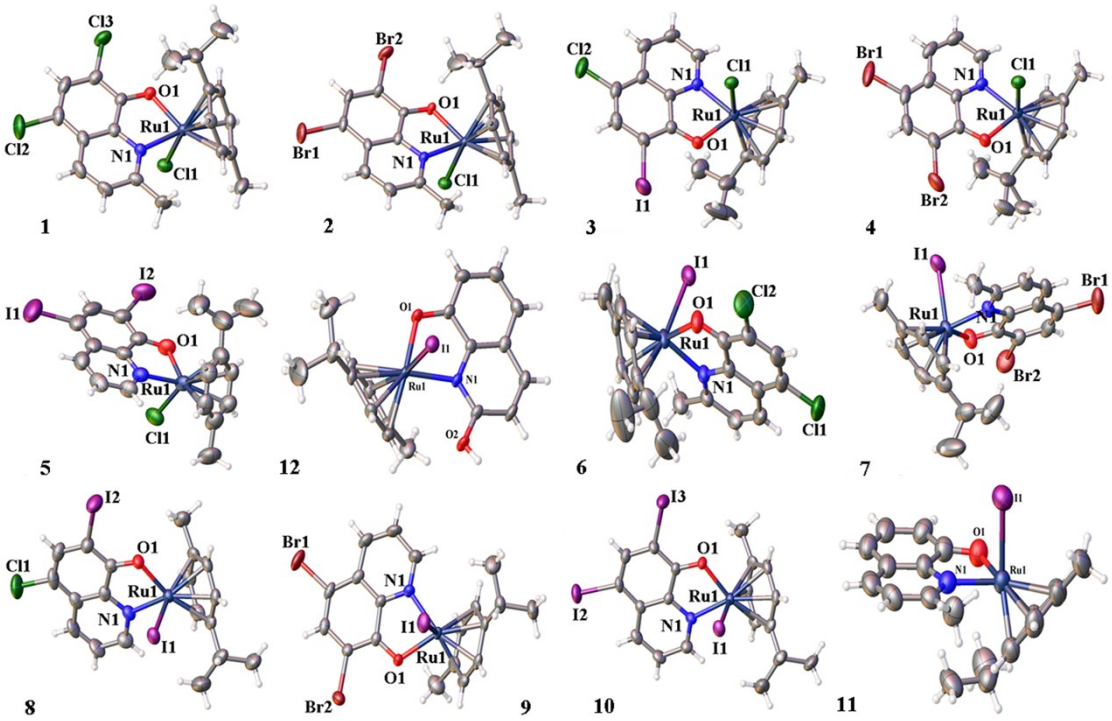

Figure S16. Molecular structure of 13 organometallic Ru(II)-arene complexes **1**−**13**, respectively.

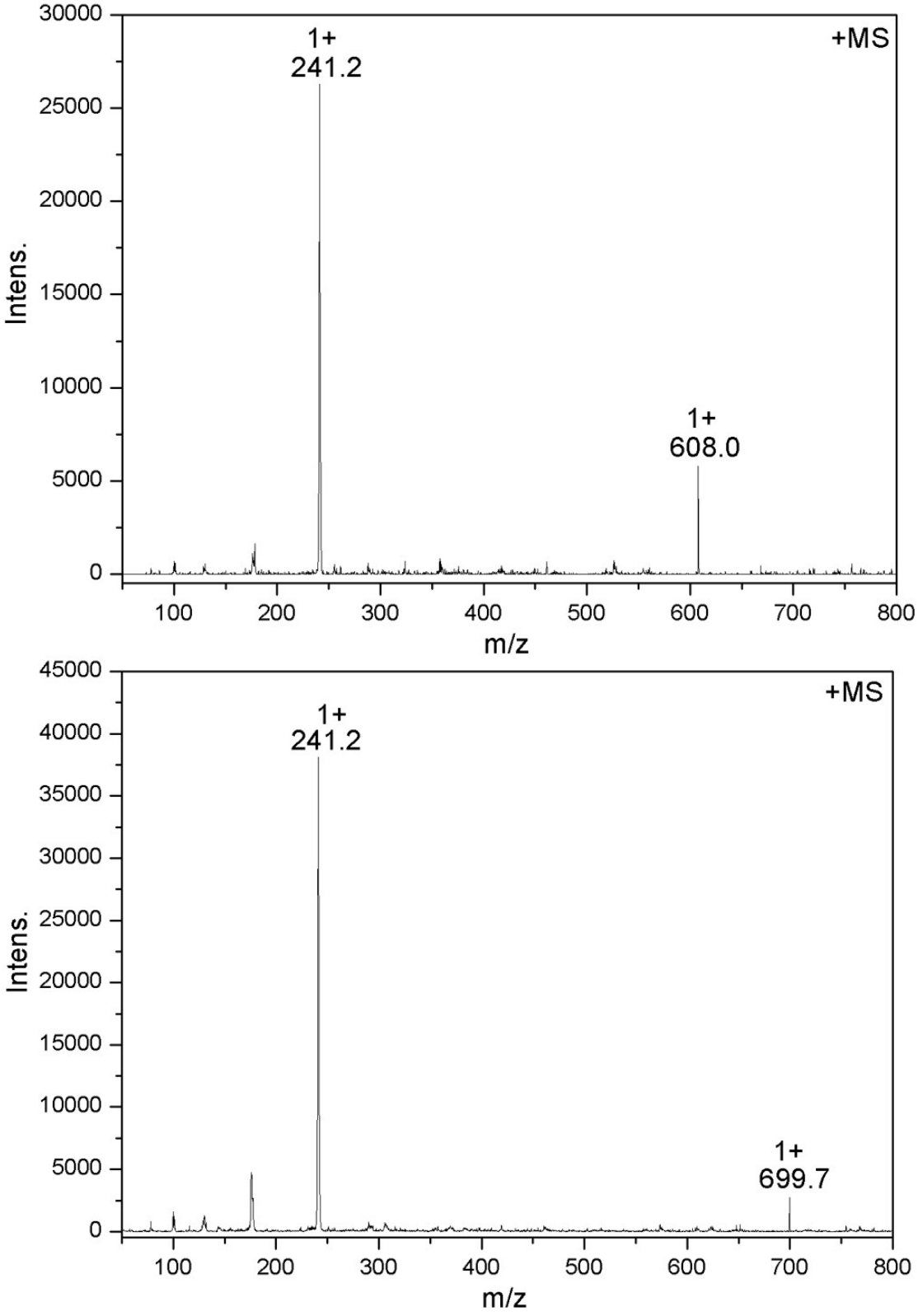

Figure S17. The mass spectra of L8 (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

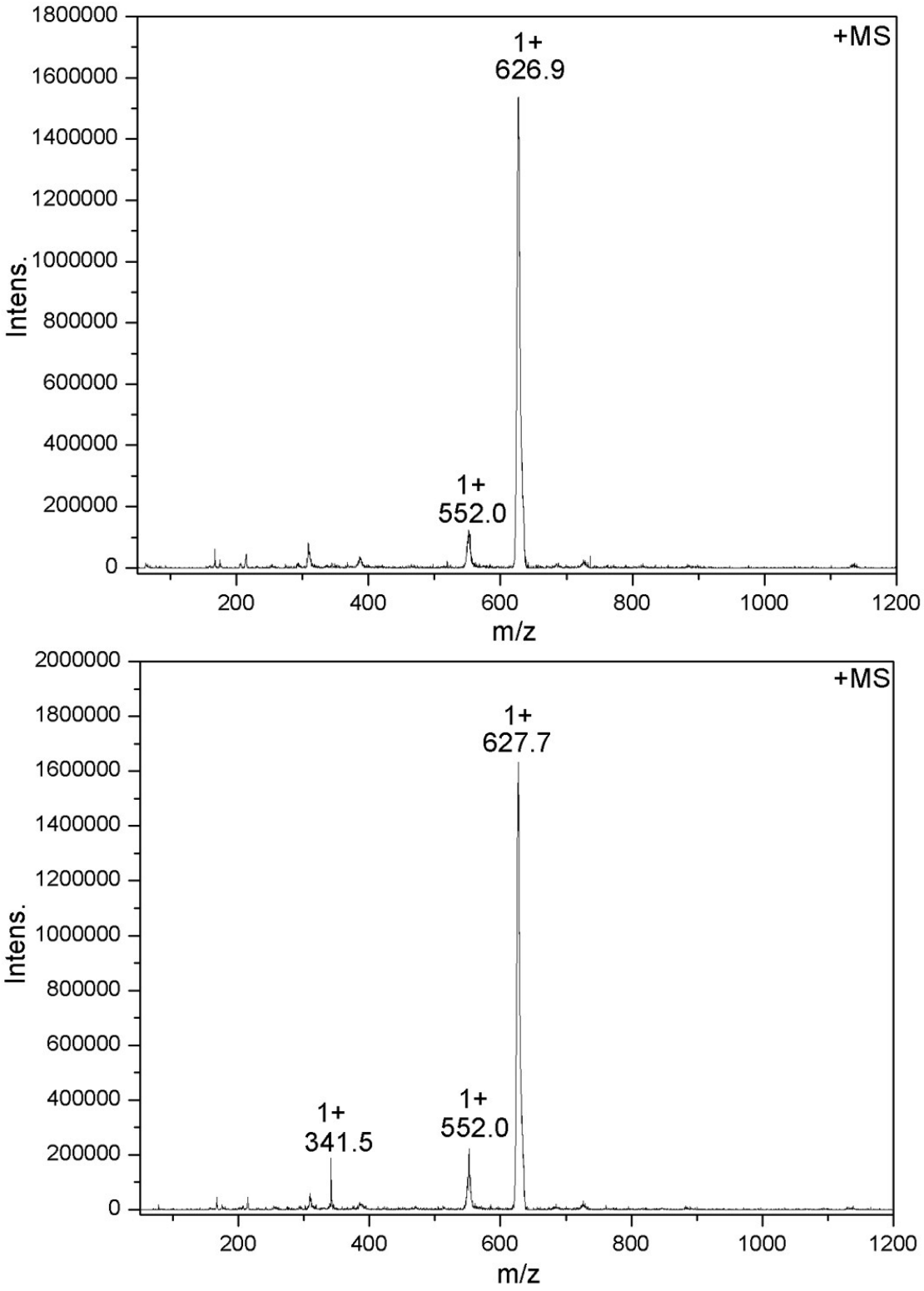

Figure S18. The mass spectra of **2** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

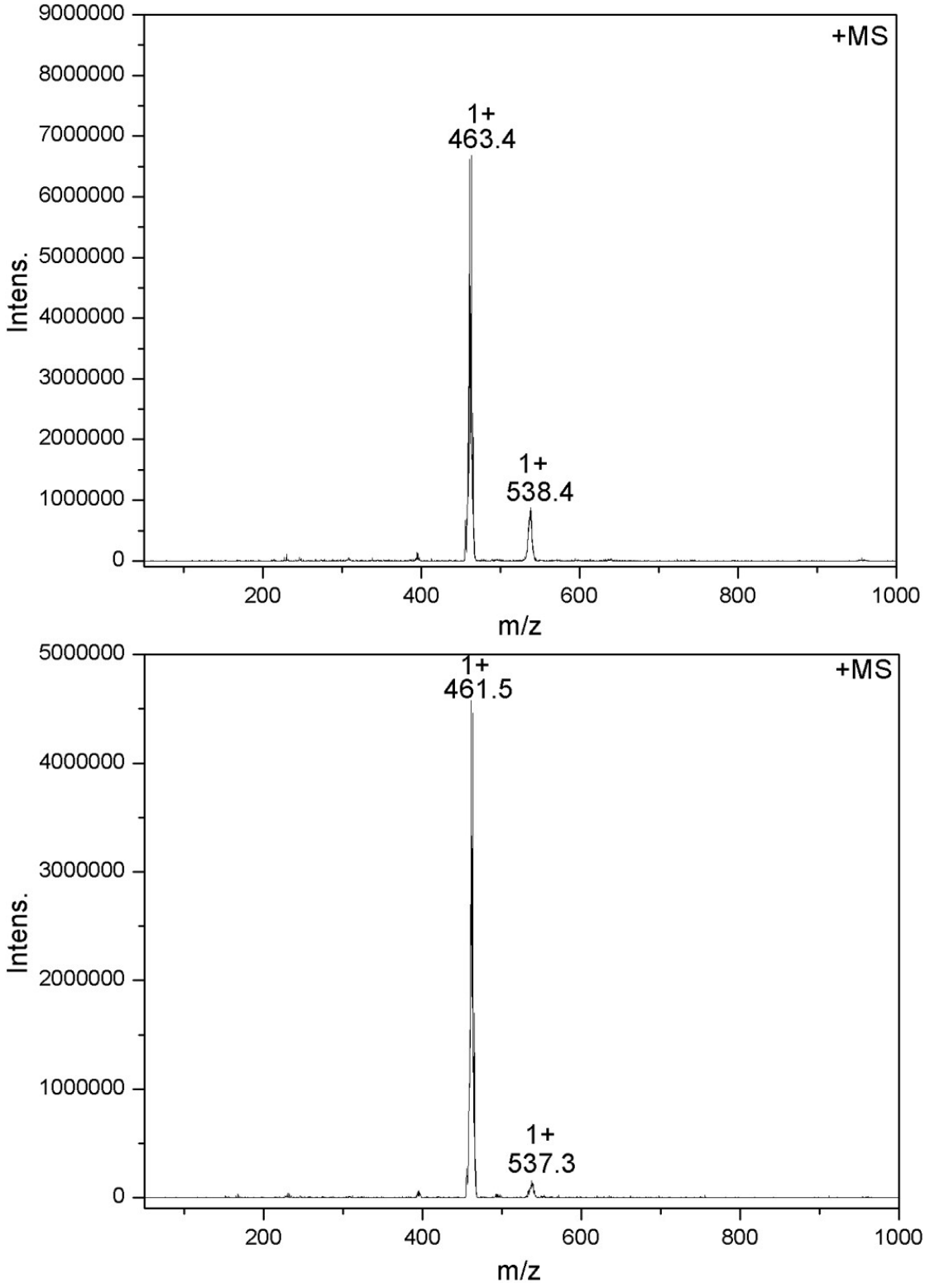

Figure S19. The mass spectra of **1** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

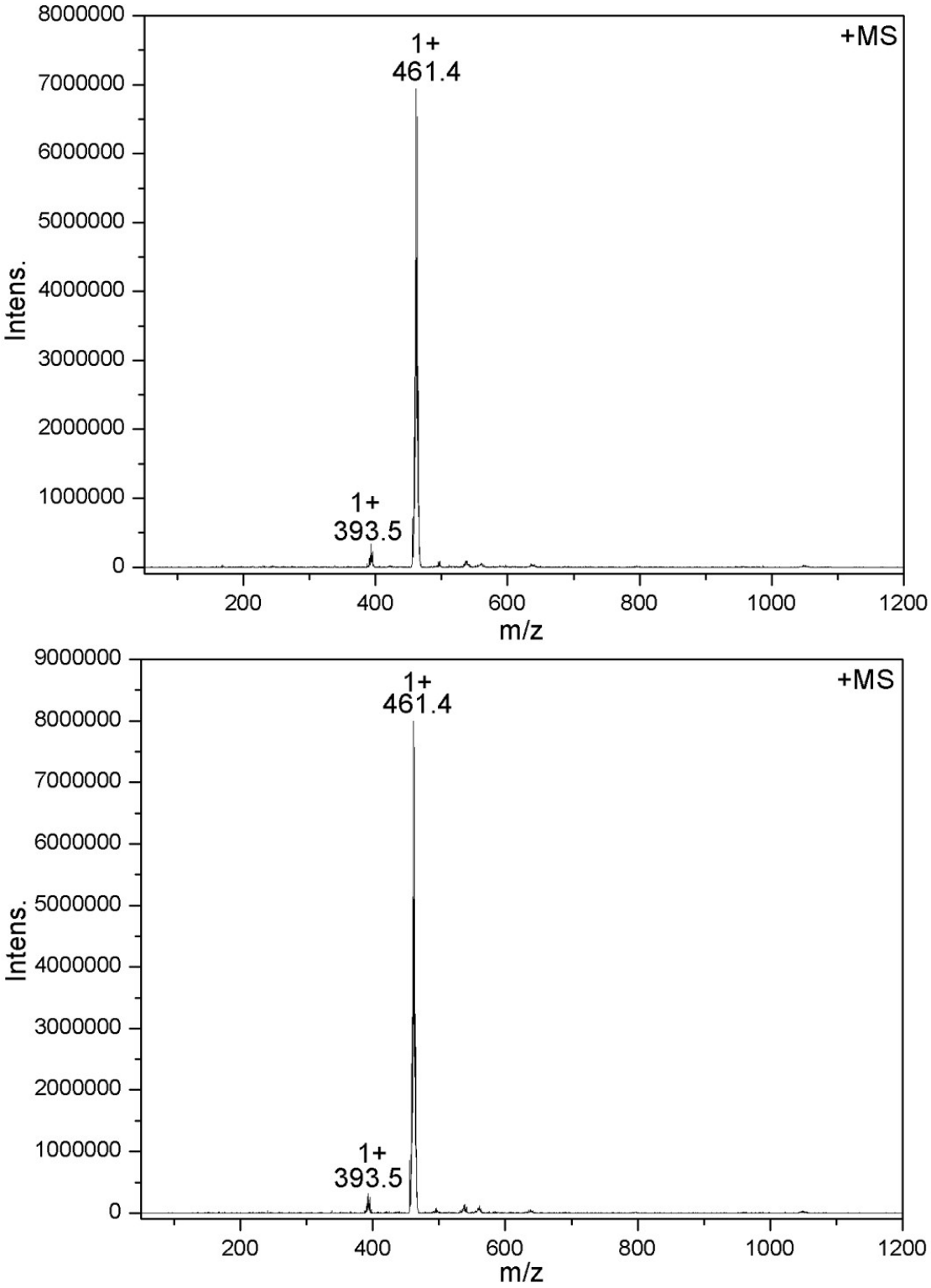

Figure S20. The mass spectra of **6** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

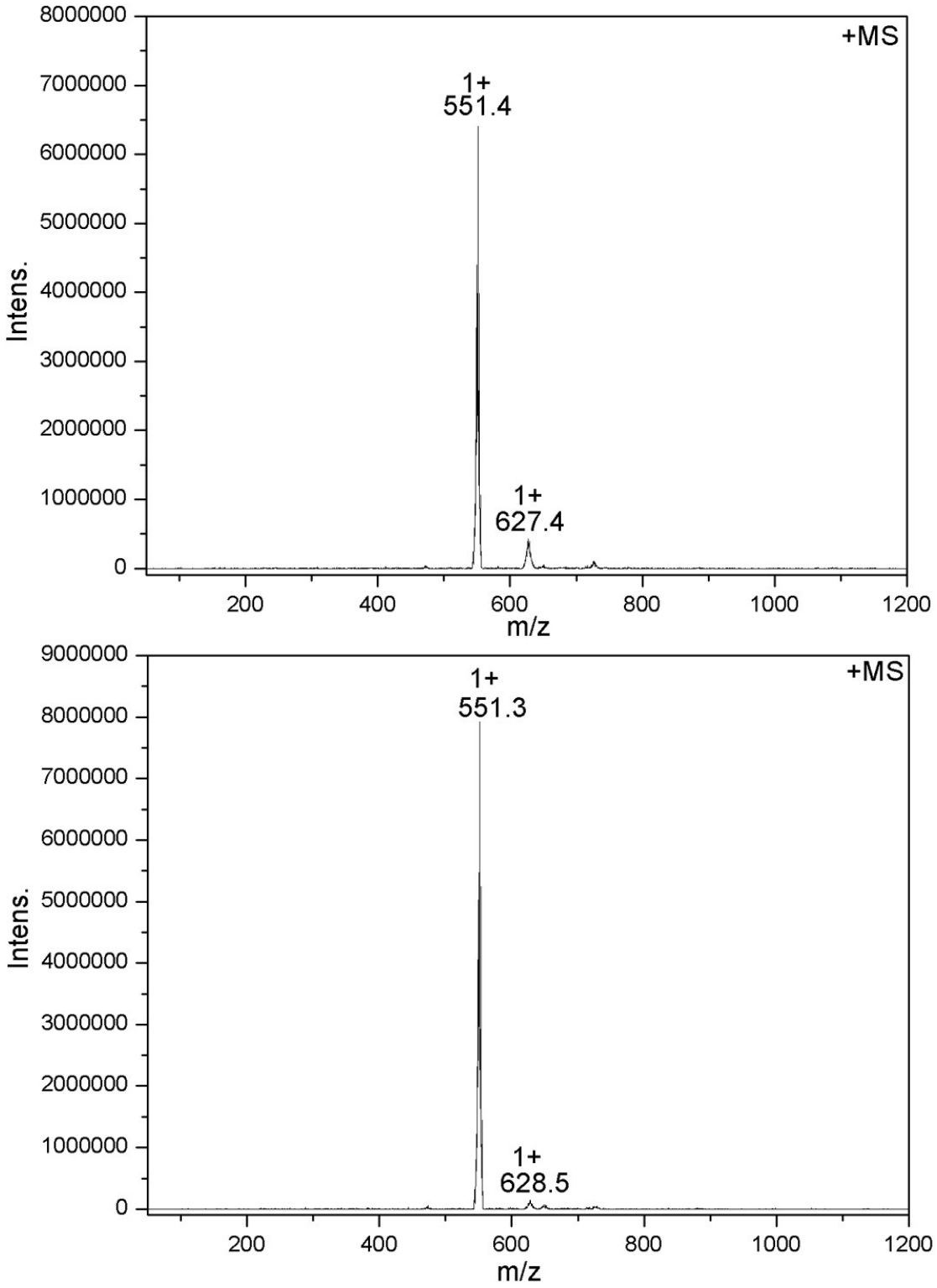

Figure S21. The mass spectra of **7** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

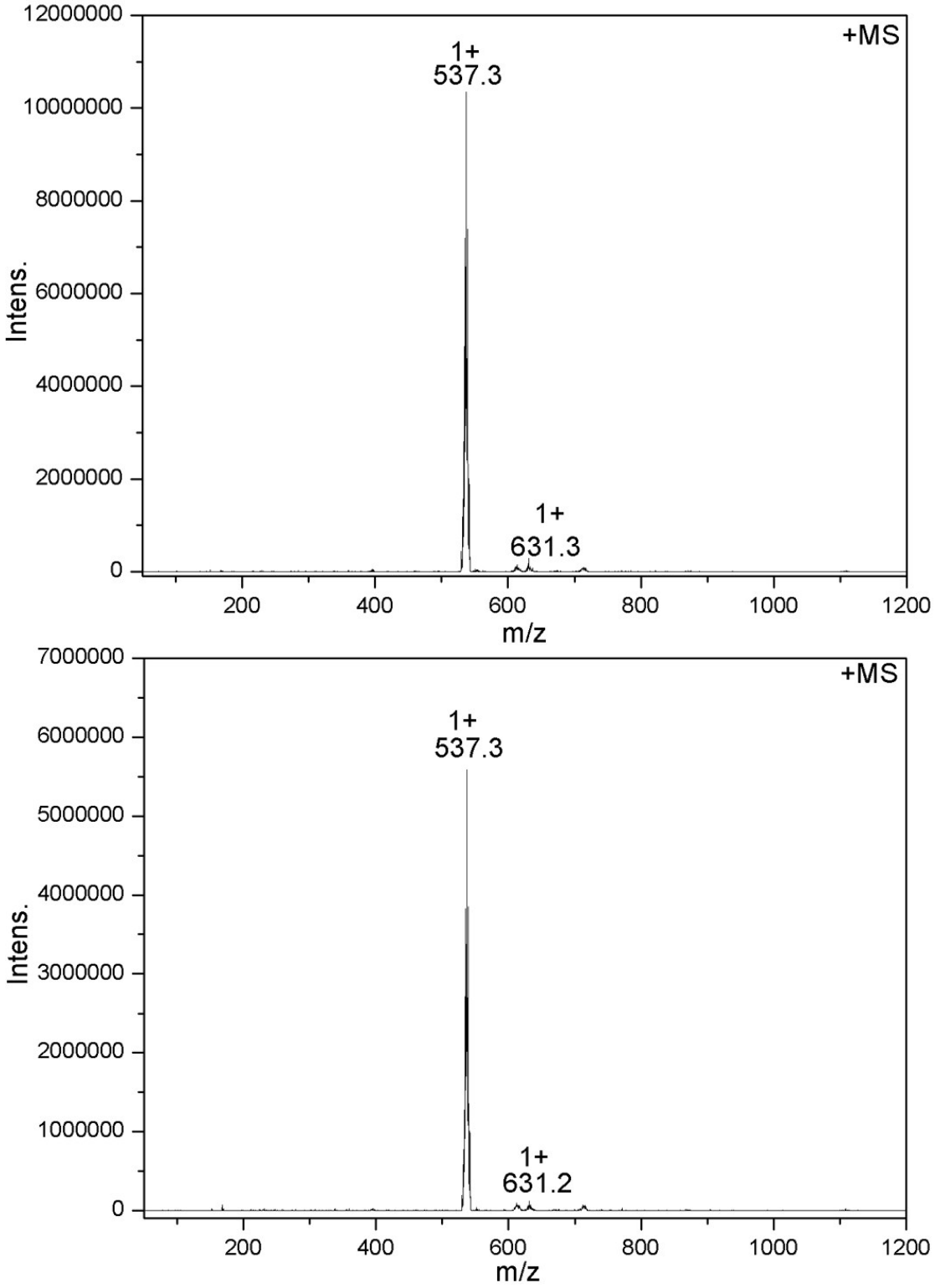

Figure S22. The mass spectra of **4** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

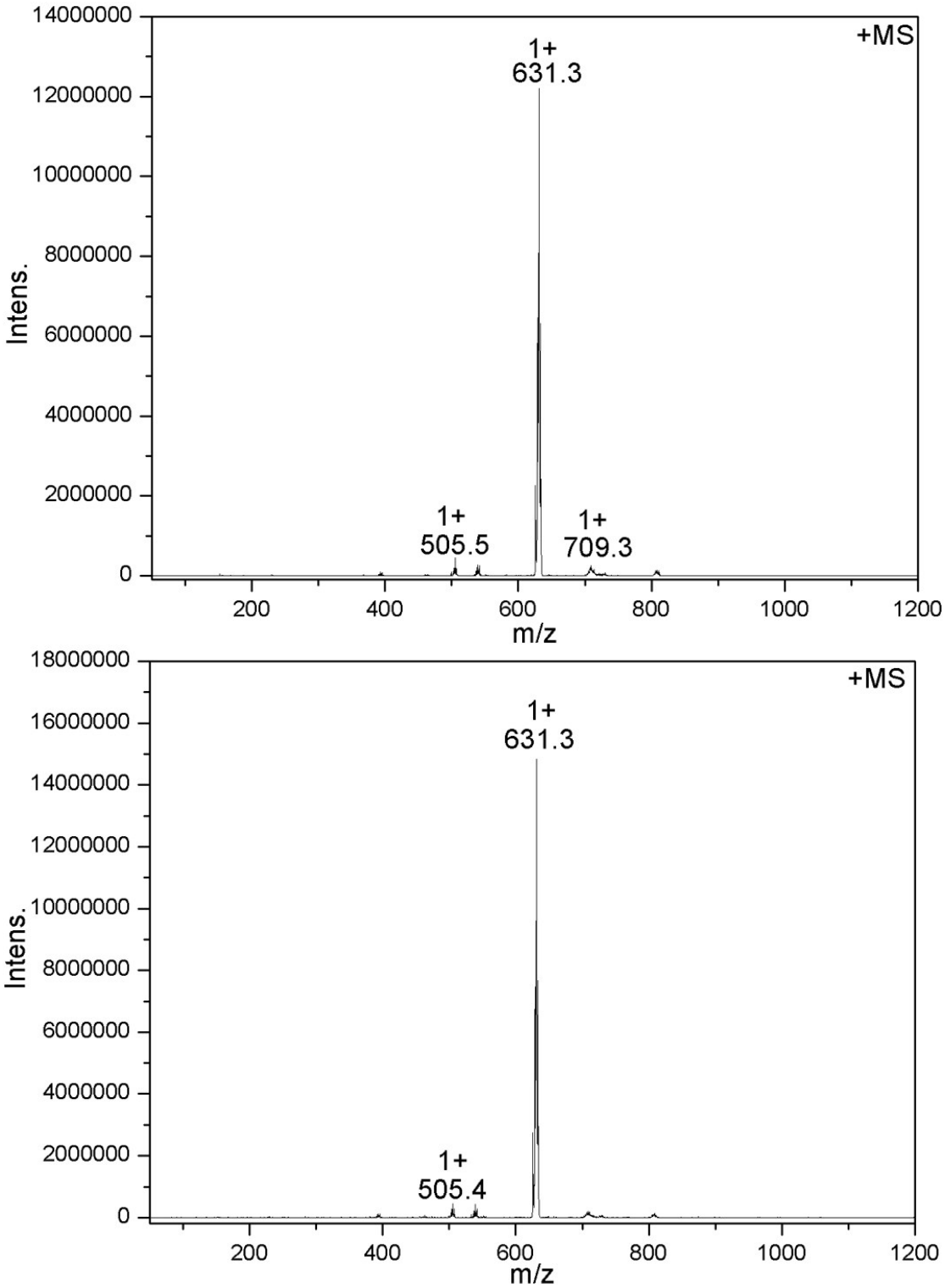

Figure S23. The mass spectra of **5** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

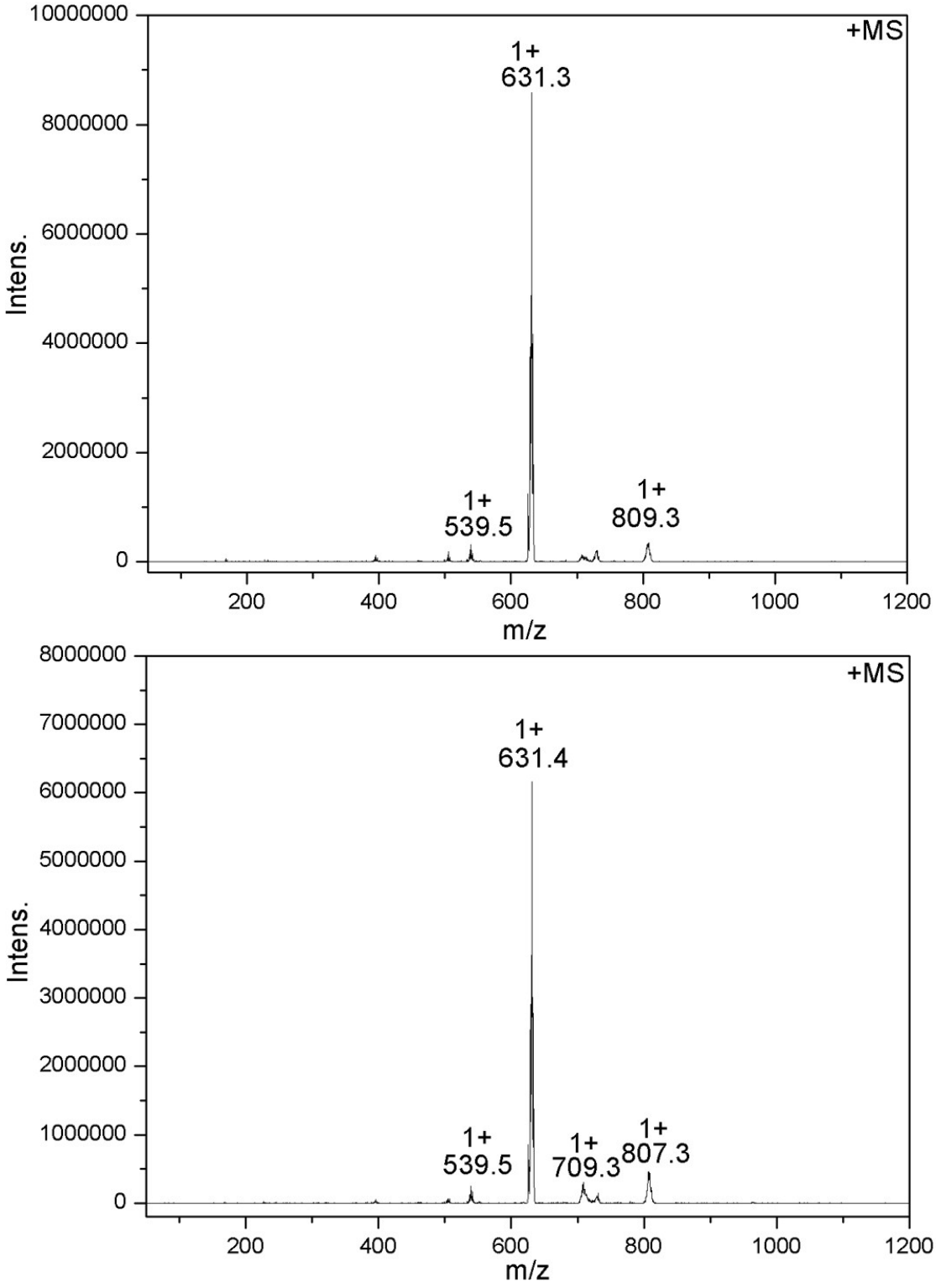

Figure S24. The mass spectra of **10** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

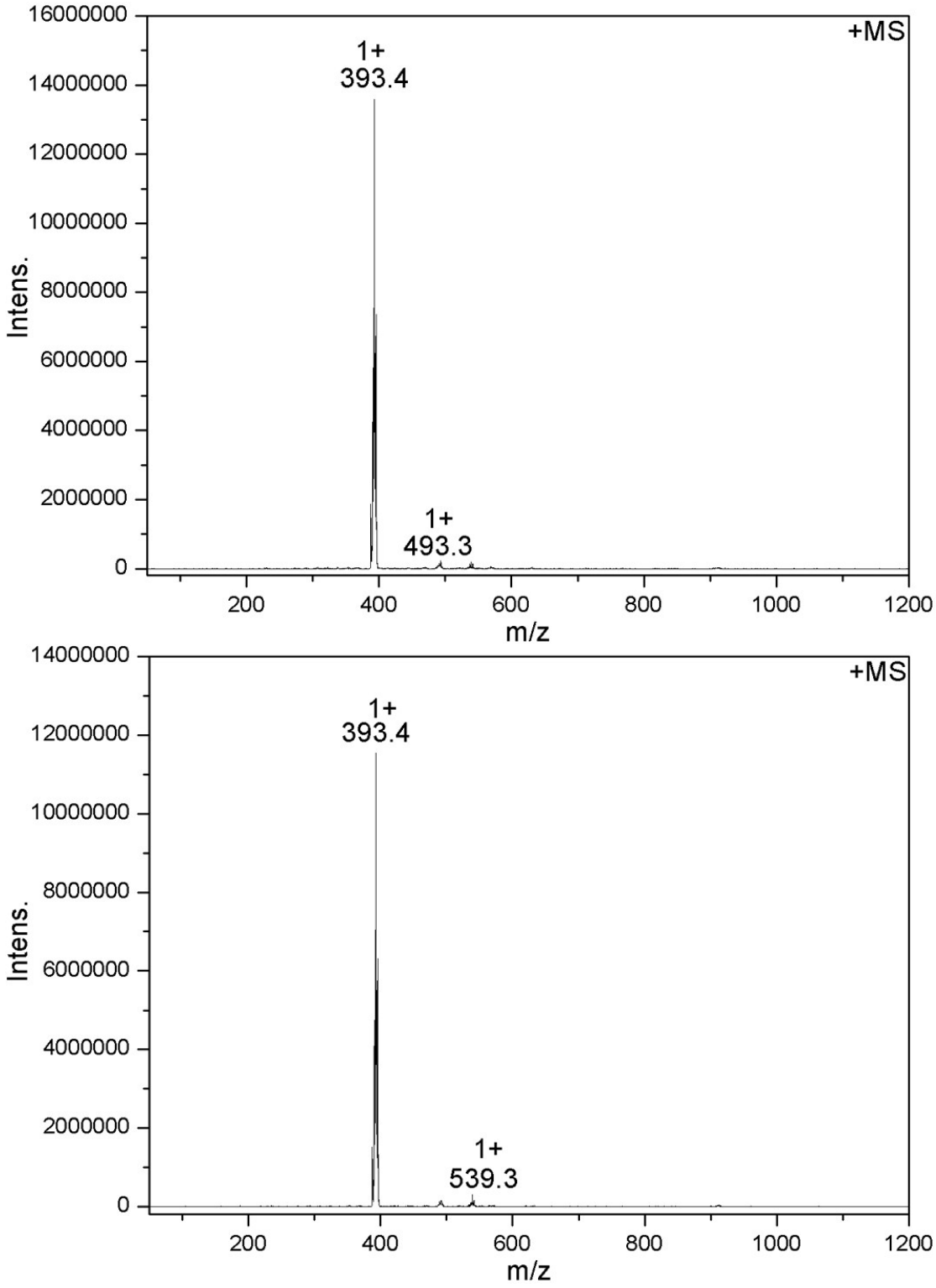

Figure S25. The mass spectra of **11** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

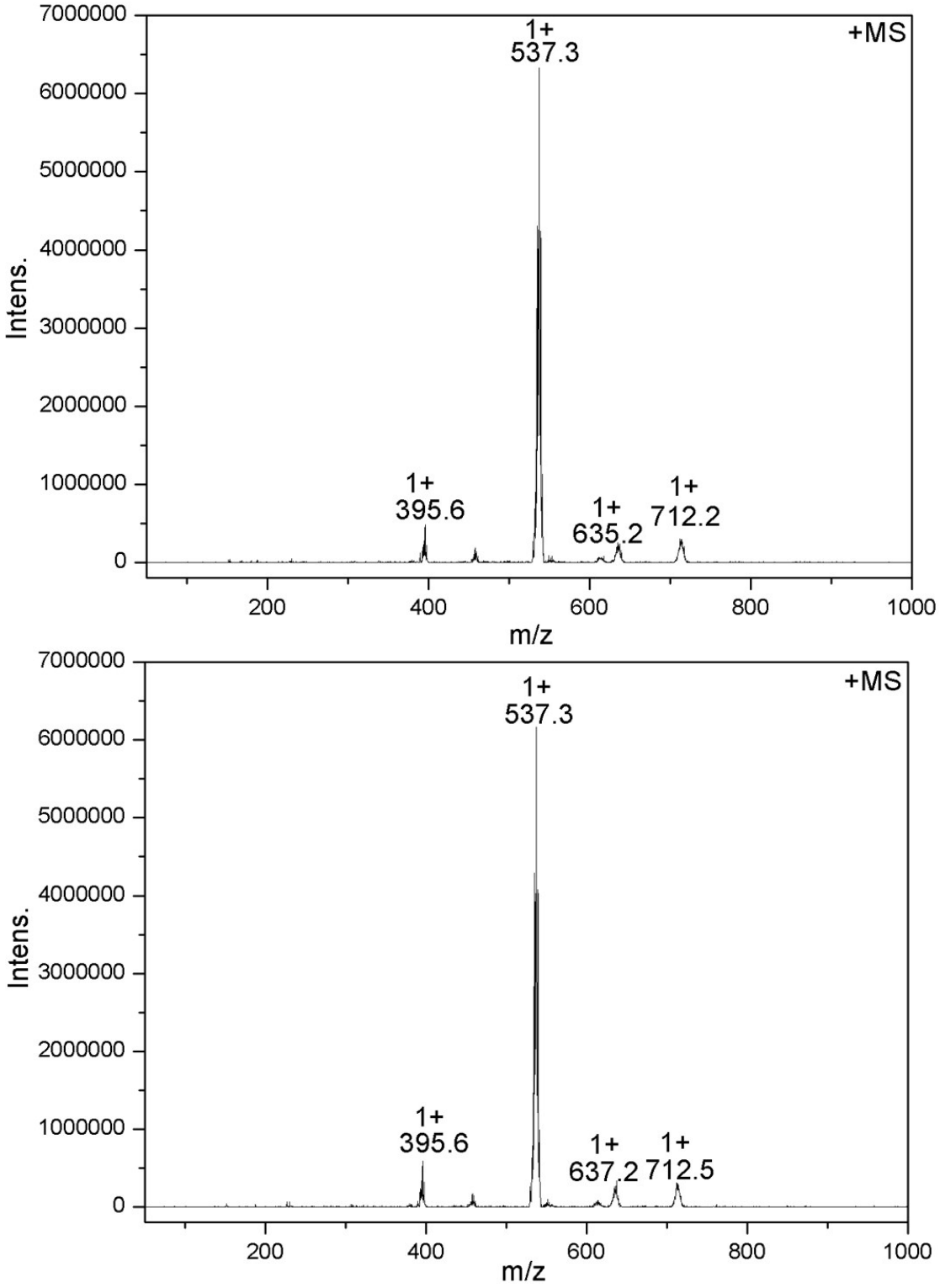

Figure S26. The mass spectra of **9** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

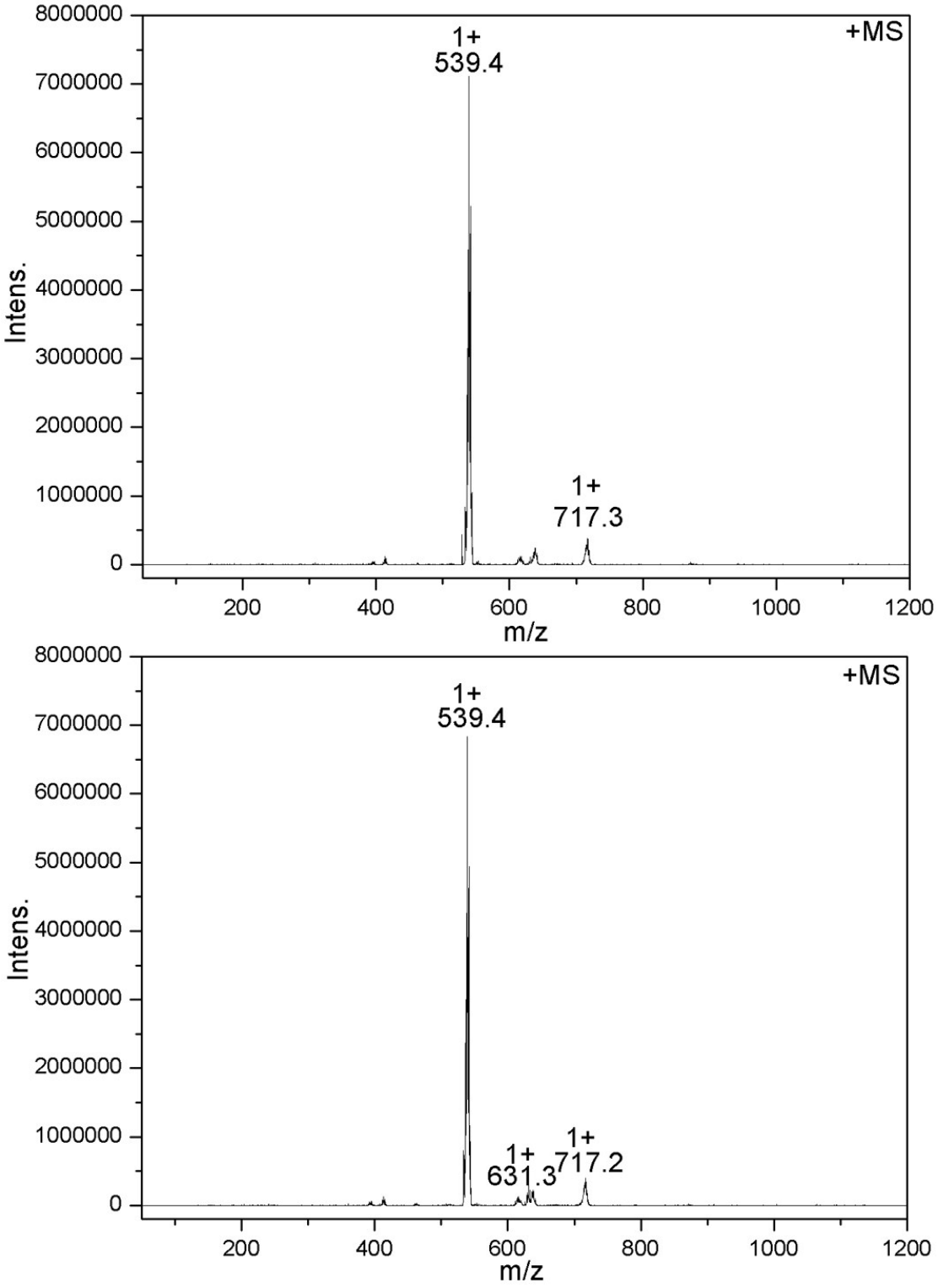

Figure S27. The mass spectra of **8** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

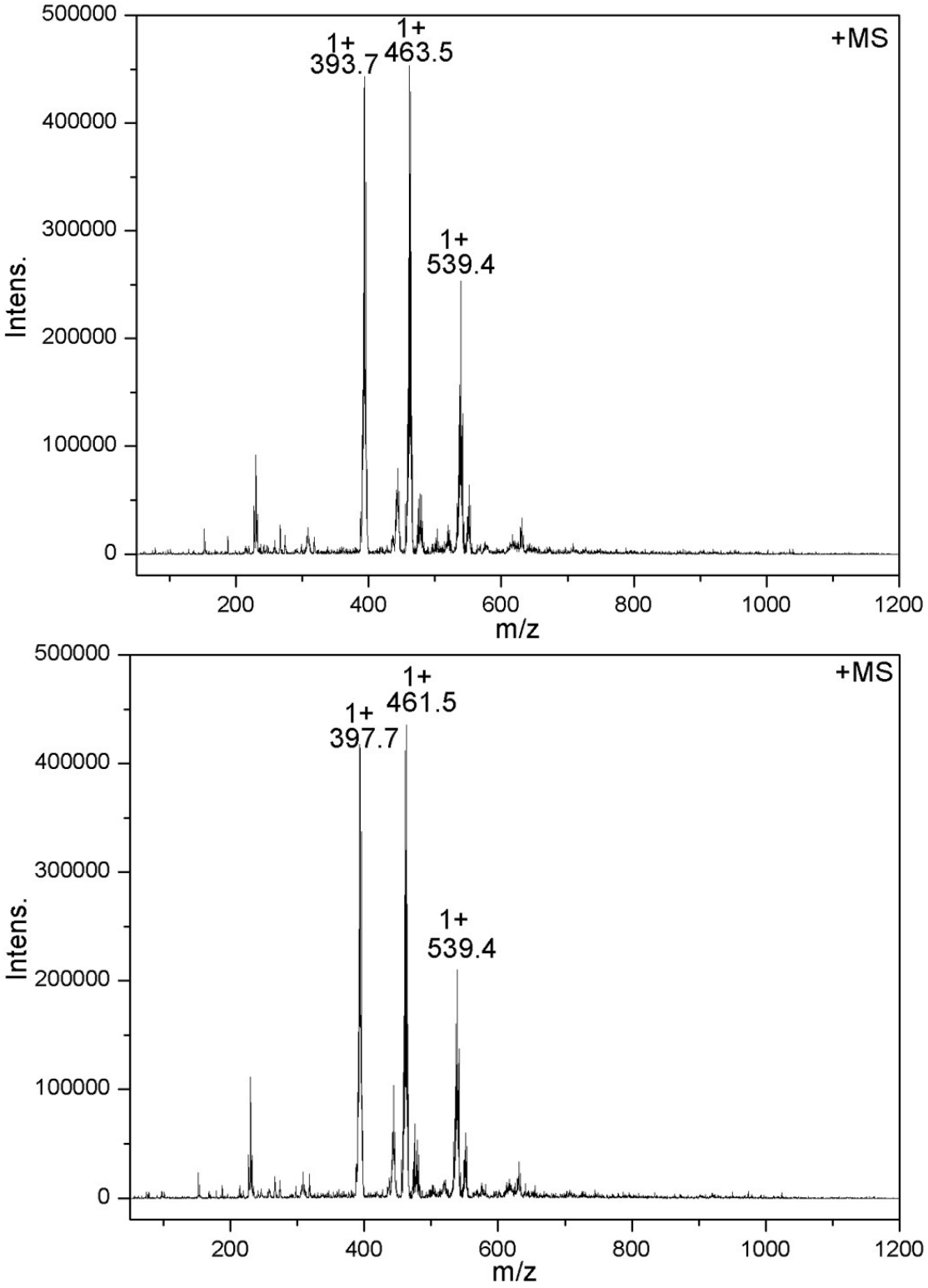

Figure S28. The mass spectra of **13** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

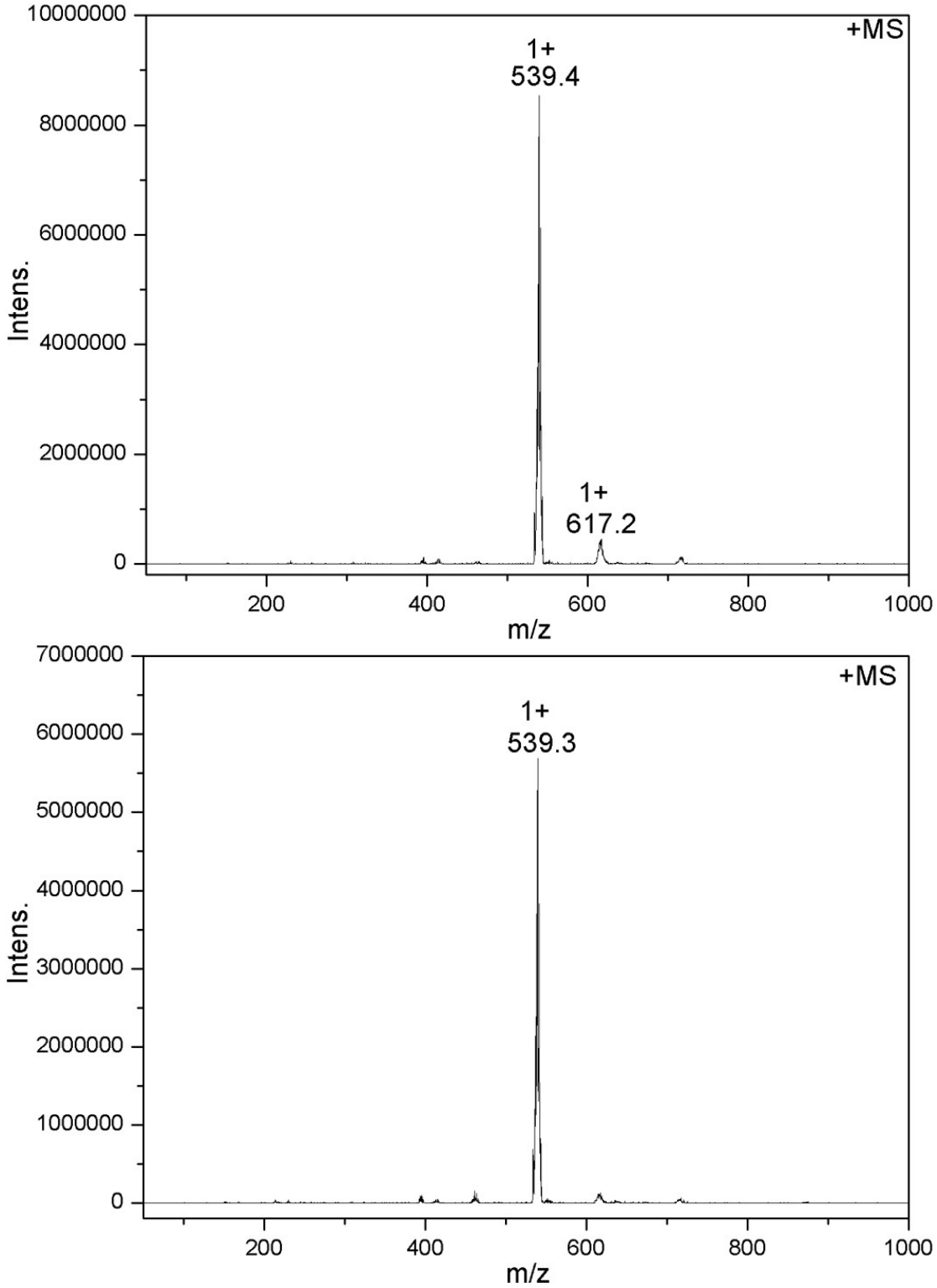

Figure S29. The mass spectra of **3** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

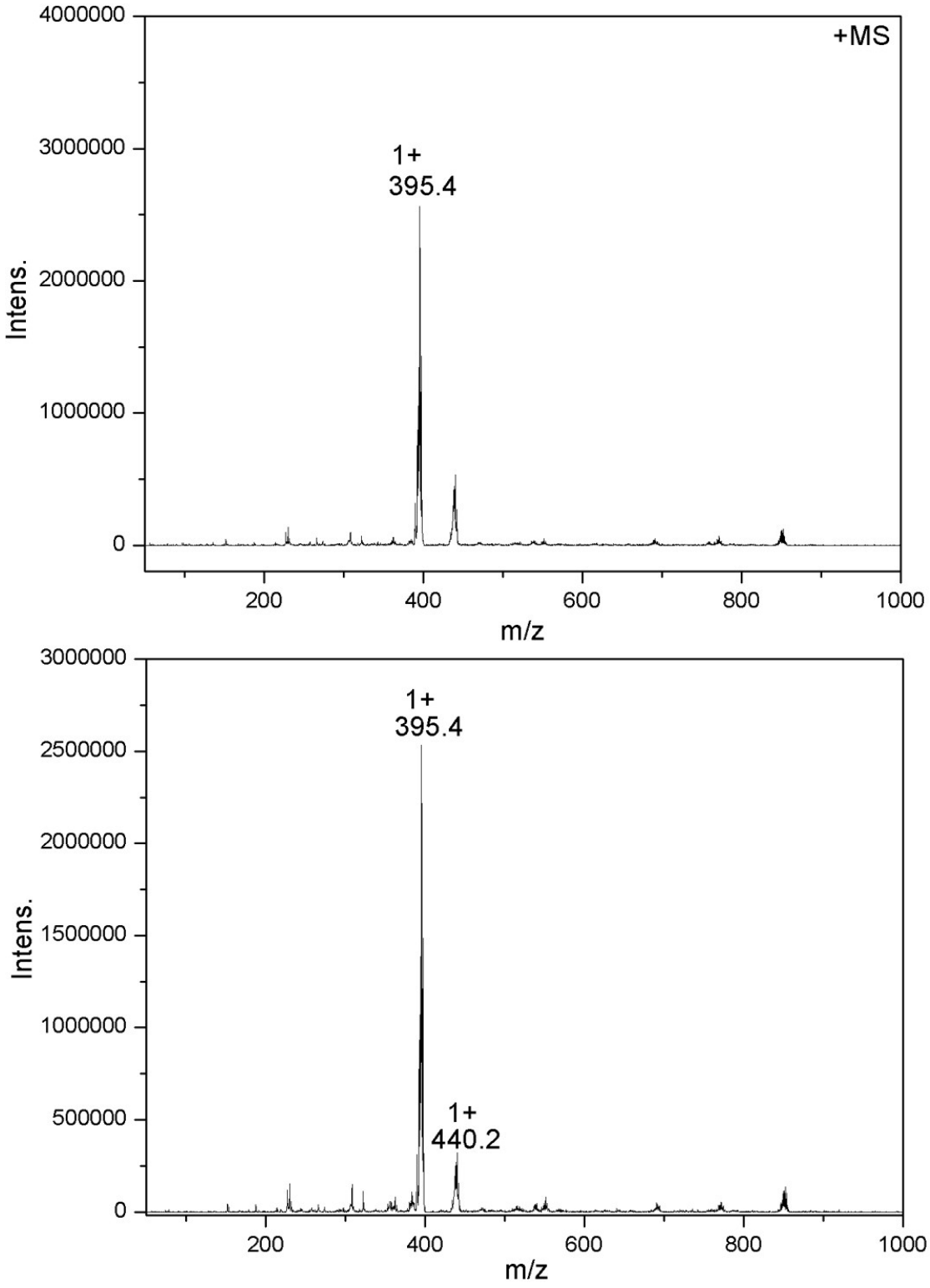

Figure S30. The mass spectra of **12** (3.0×10^{-5} M) in Tris-HCl buffer solution (containing 5% DMSO) for 0 h (top) and 48 h (down), respectively.

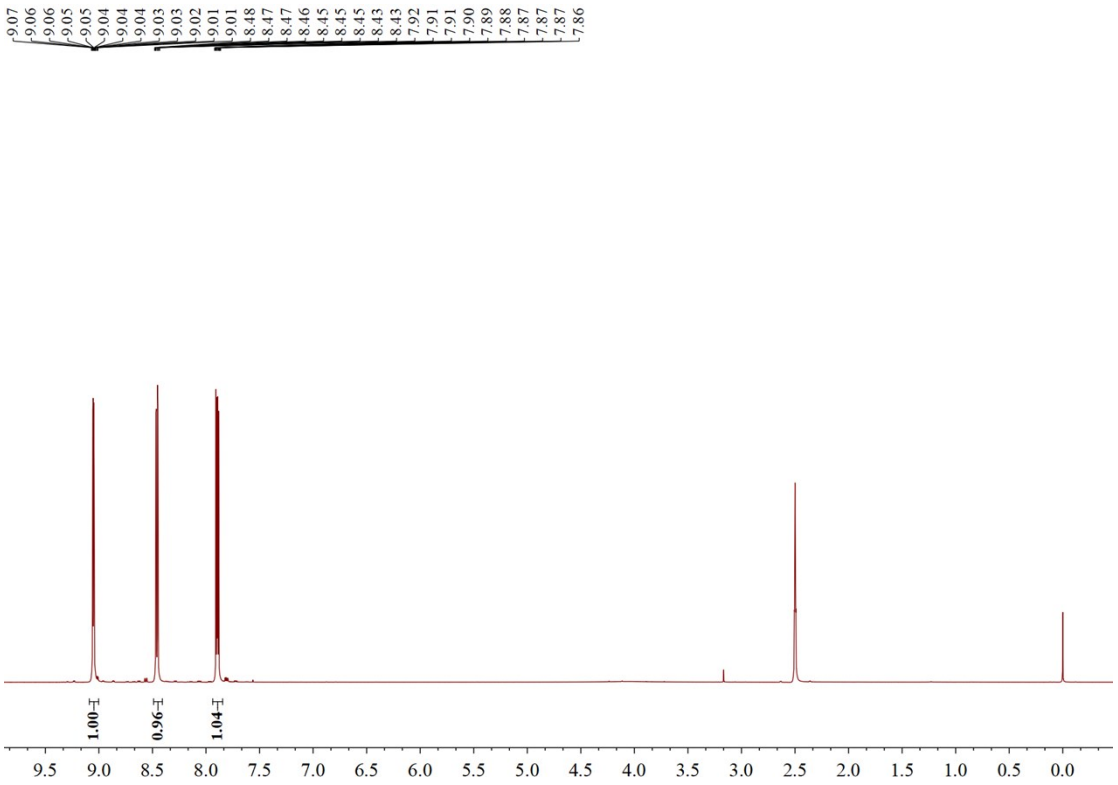

Figure S31. ^{1}H NMR (500MHz, DMSO-d_6) for H-L8.

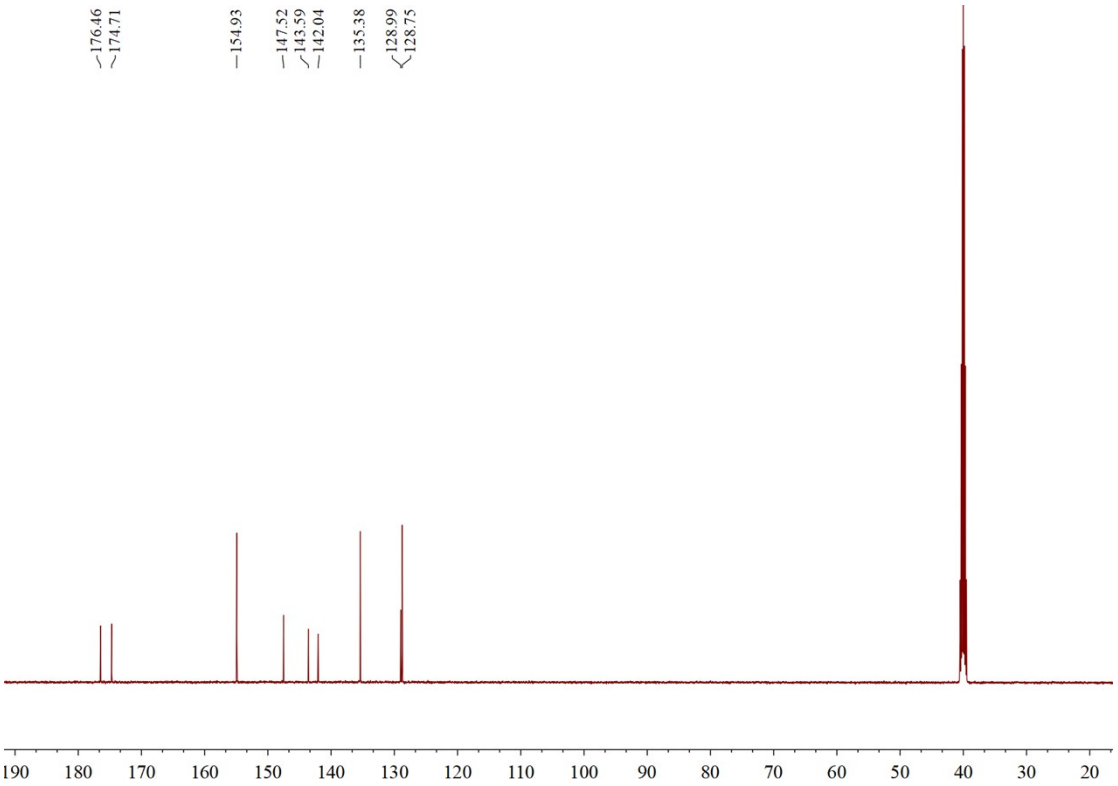

Figure S32. ^{13}C NMR (126MHz, DMSO-d_6) for H-L8.

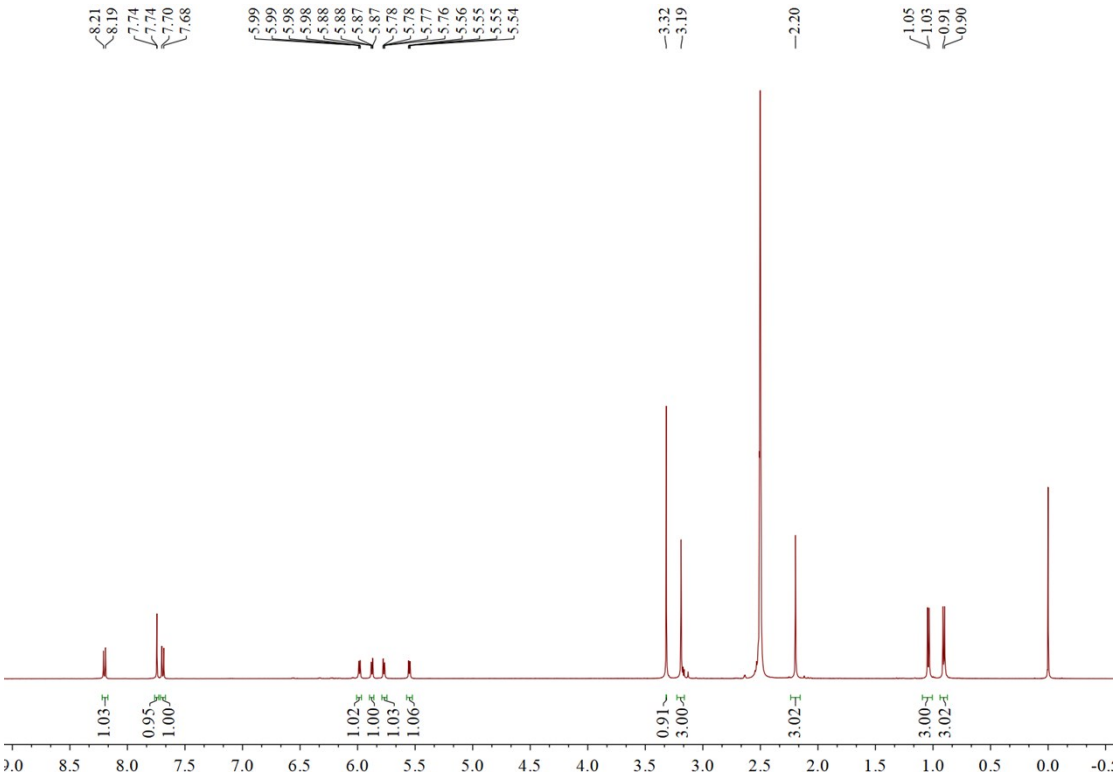

Figure S33. ^{1}H NMR (500MHz, DMSO-d_6) for complex **2**.

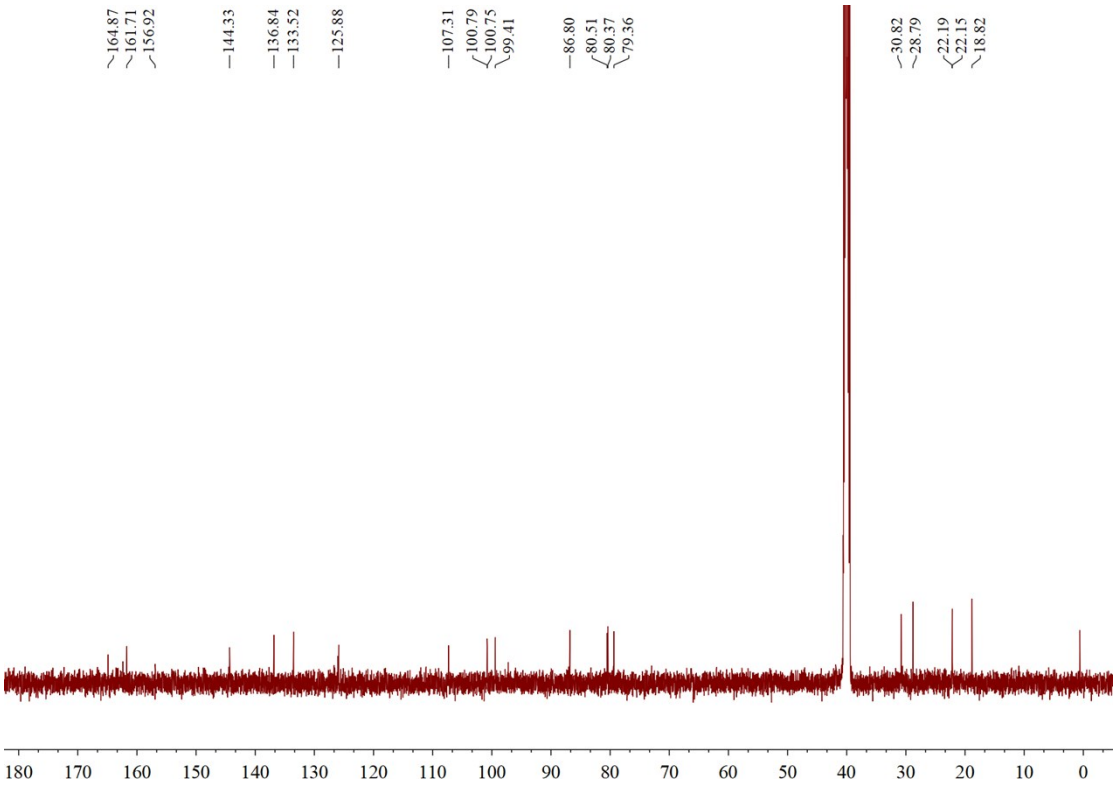

Figure S34. ^{13}C NMR (126MHz, DMSO-d_6) for complex **2**.

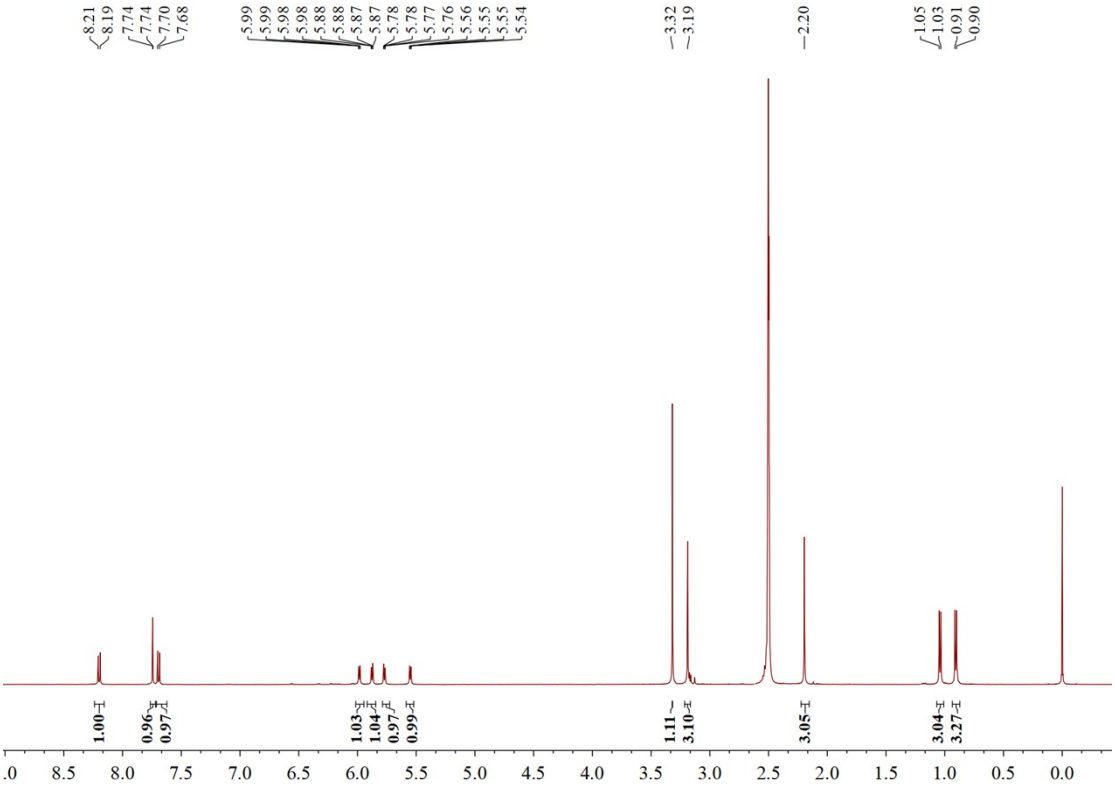

Figure S35. ^{1}H NMR (500MHz, DMSO-d_6) for complex **1**.

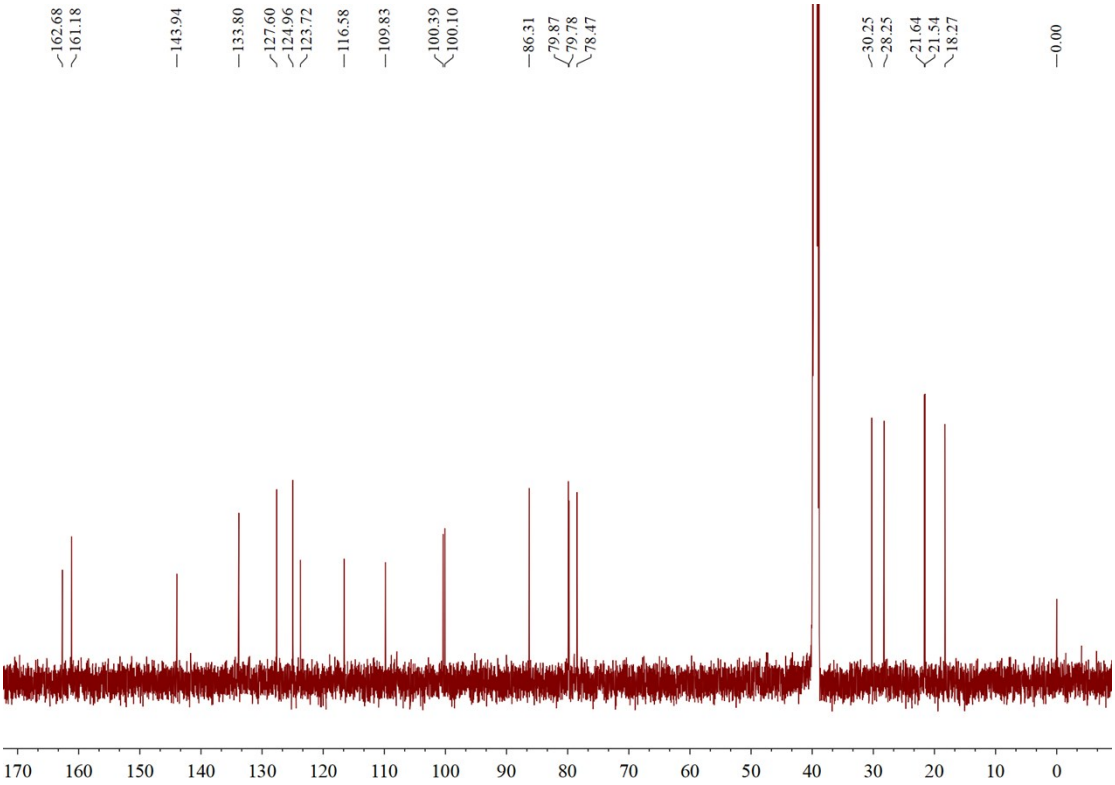

Figure S36. ^{13}C NMR (126MHz, DMSO-d_6) for complex **1**.

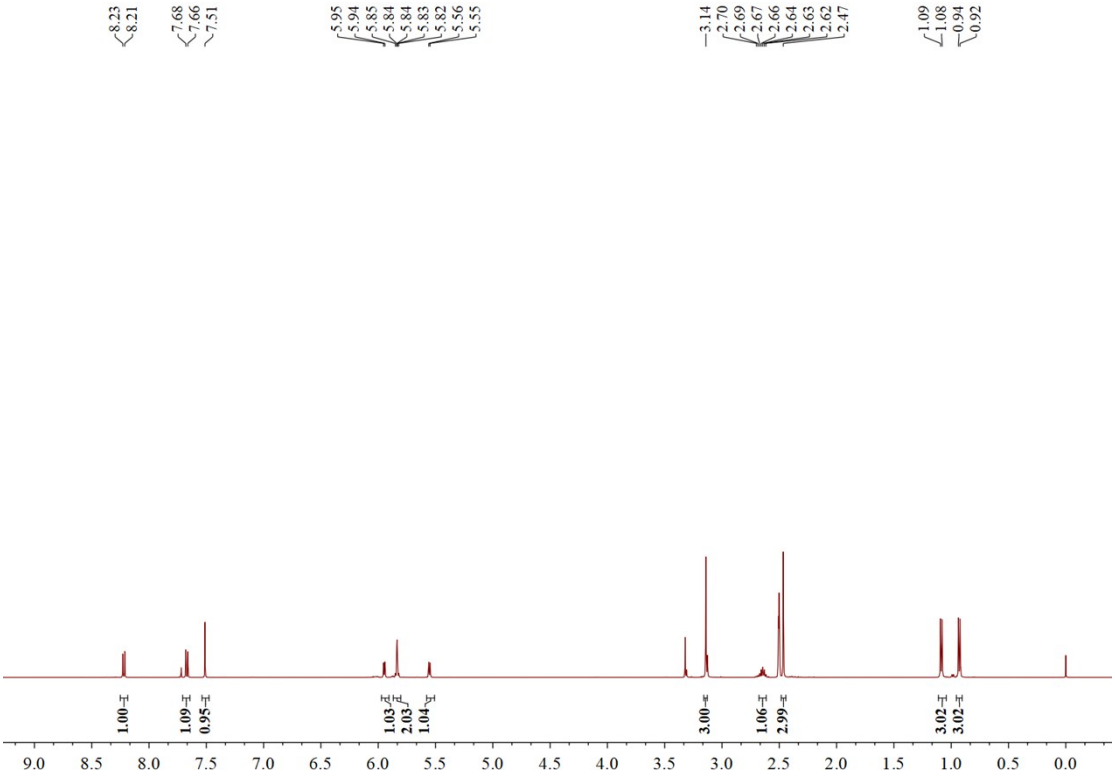

Figure S37. ^{1}H NMR (500MHz, DMSO-d_6) for complex **6**.

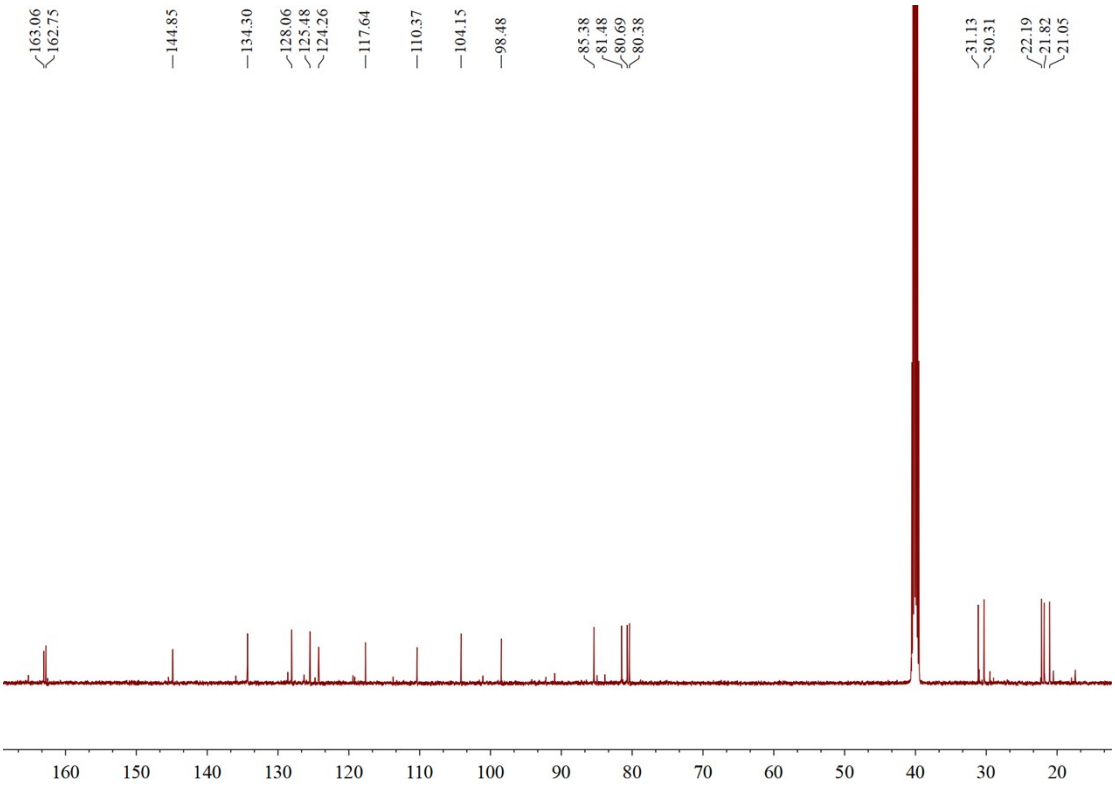

Figure S38. ^{13}C NMR (126MHz, DMSO-d_6) for complex **6**.

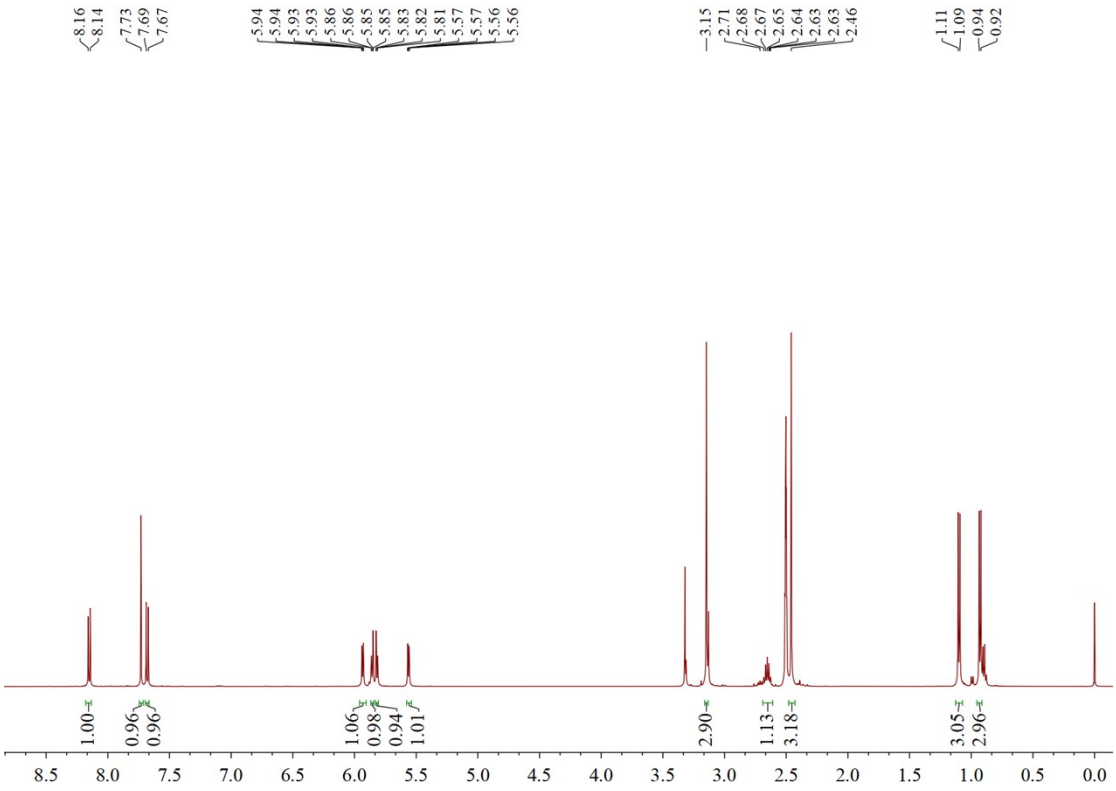

Figure S39. ^{1}H NMR (500MHz, DMSO-d_6) for complex **7**

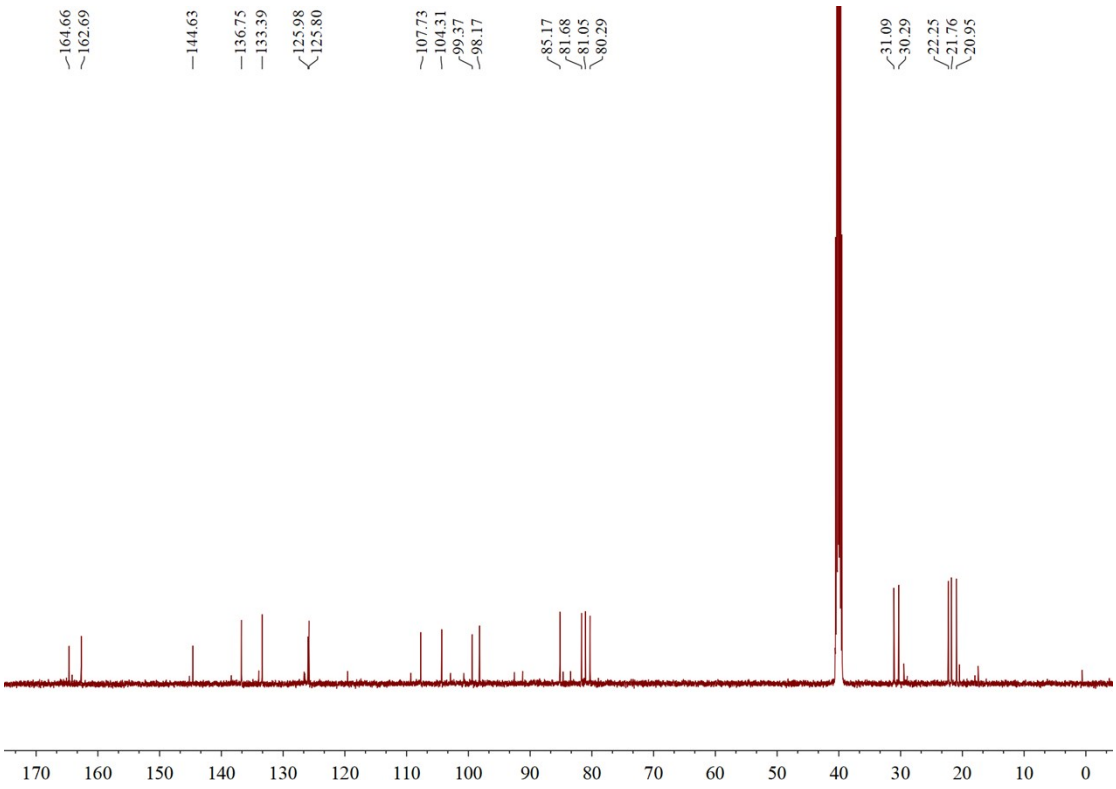

Figure S40. ^{13}C NMR (126MHz, DMSO-d_6) for complex **7**.

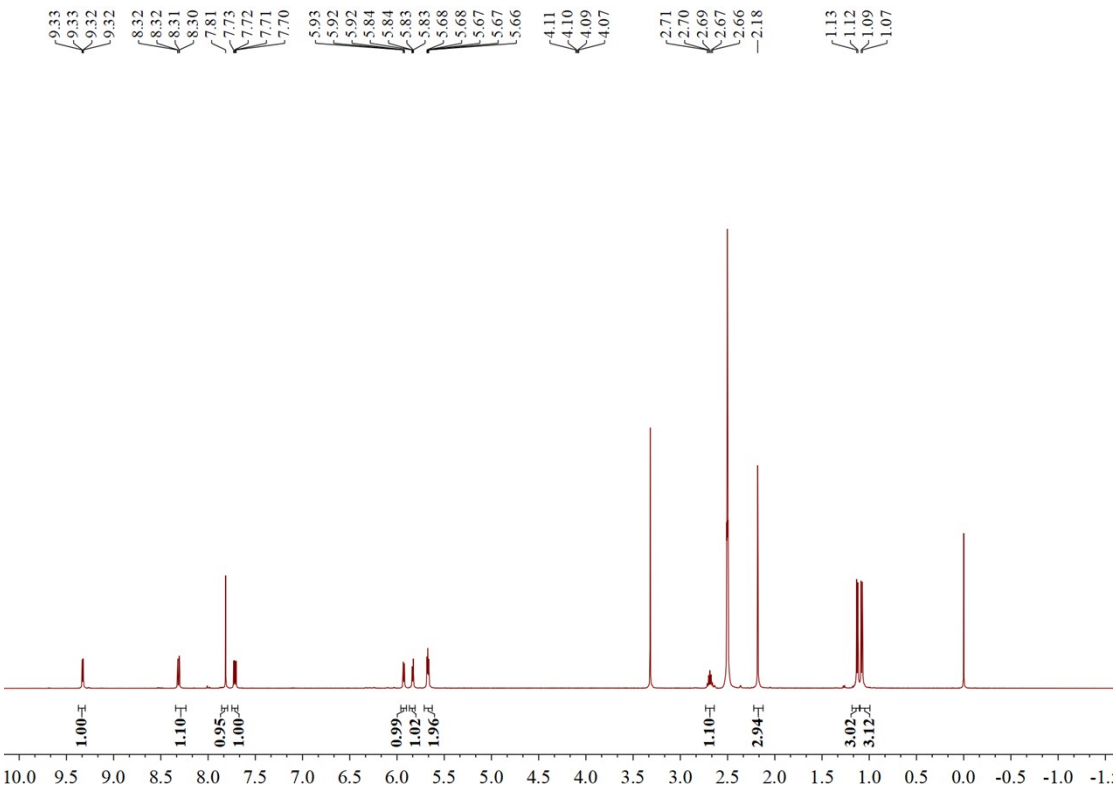

Figure S41. ^{1}H NMR (500MHz, DMSO-d_6) for complex **4**.

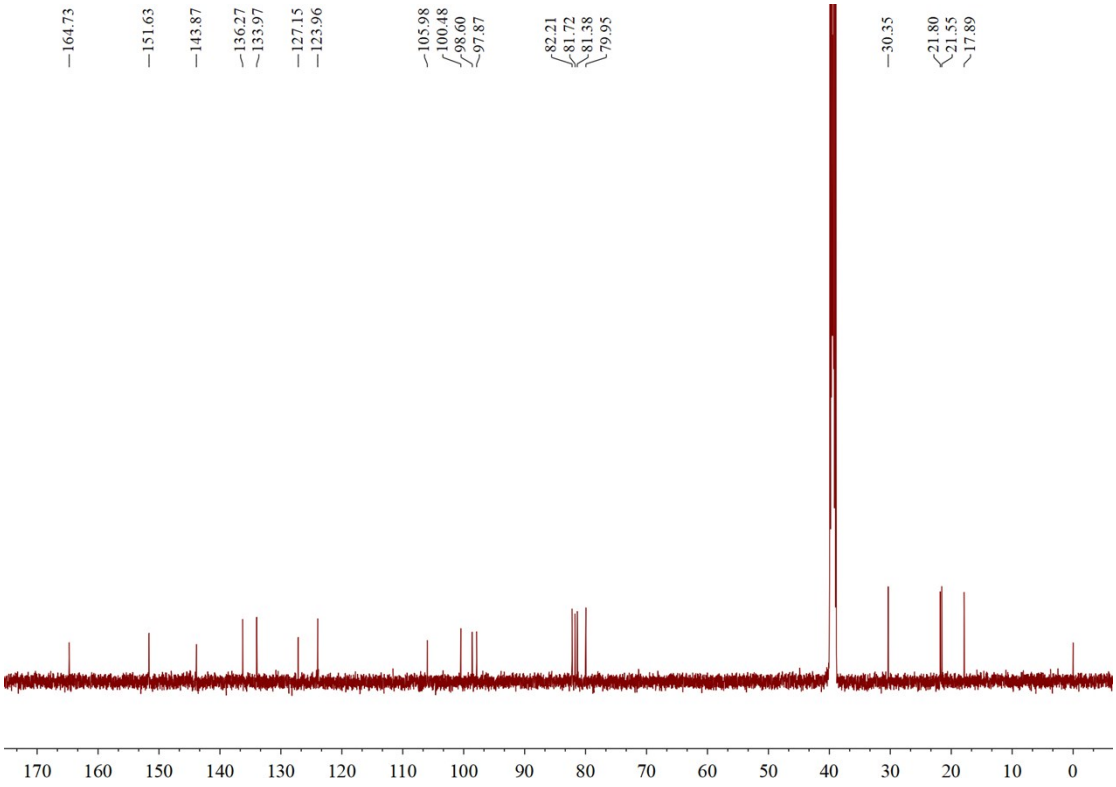

Figure S42. ^{13}C NMR (126MHz, DMSO-d_6) for complex **4**.

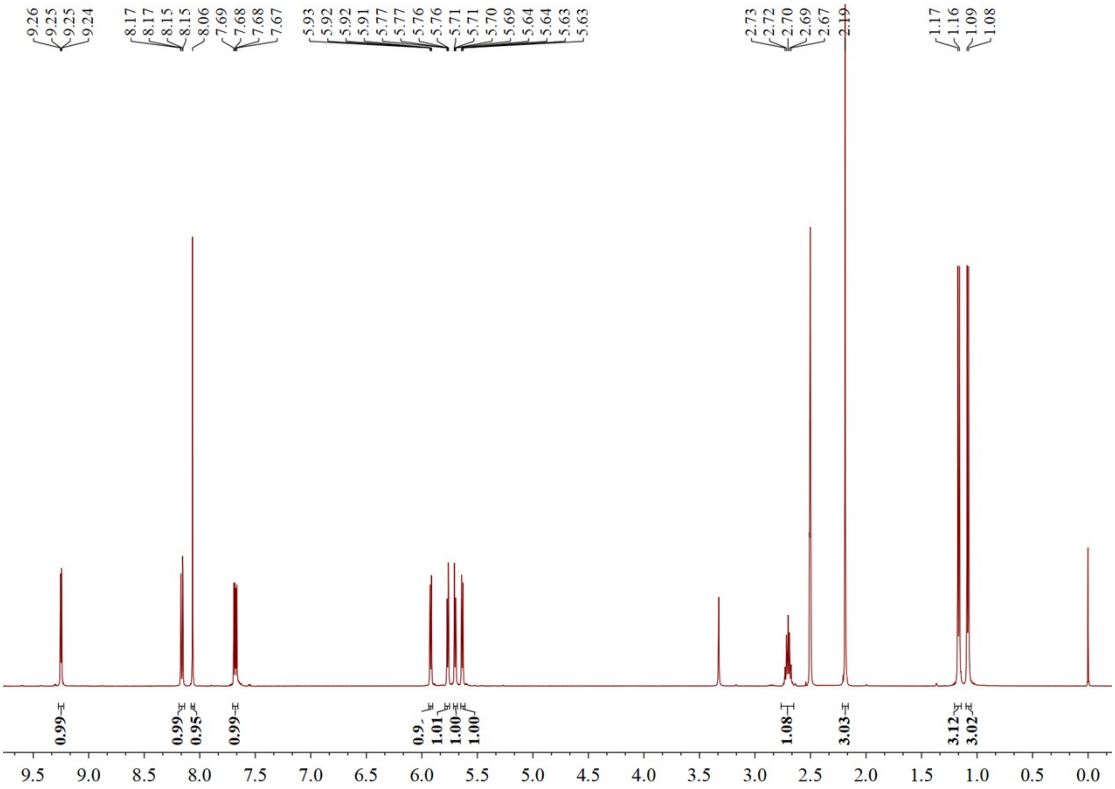

Figure S43. ^{1}H NMR (500MHz, DMSO-d_6) for complex **5**.

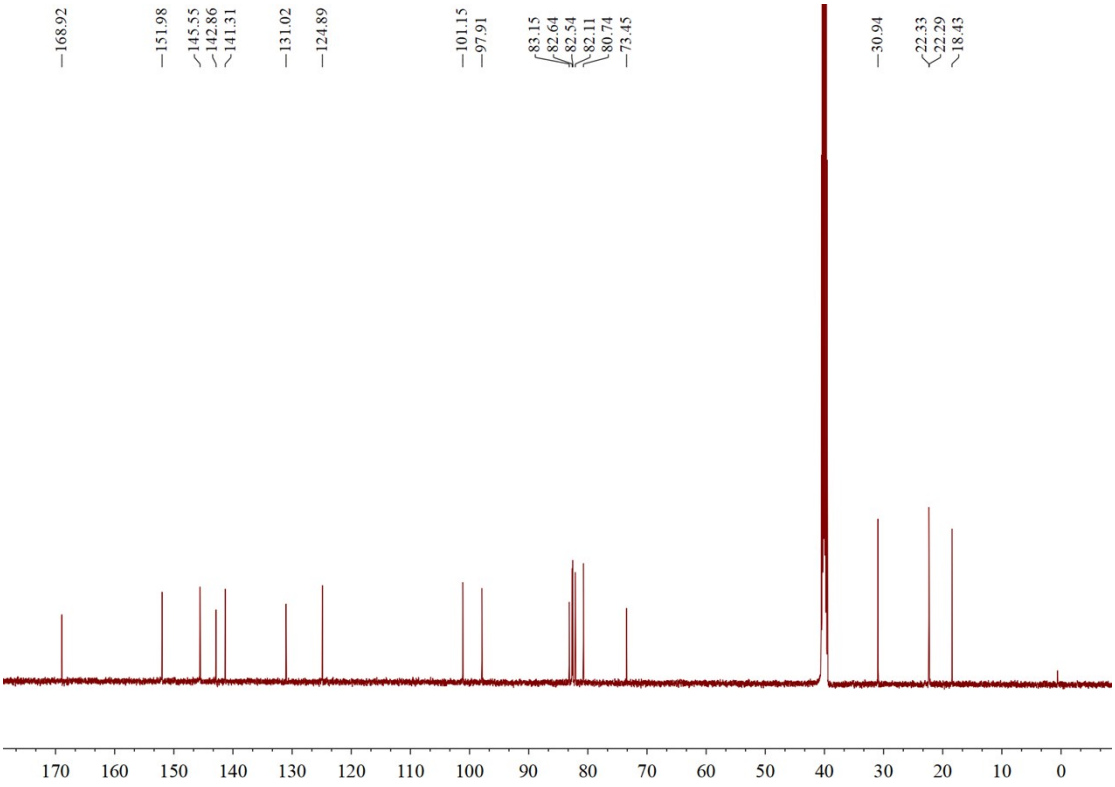

Figure S44. ^{13}C NMR (126MHz, DMSO-d_6) for complex **5**.

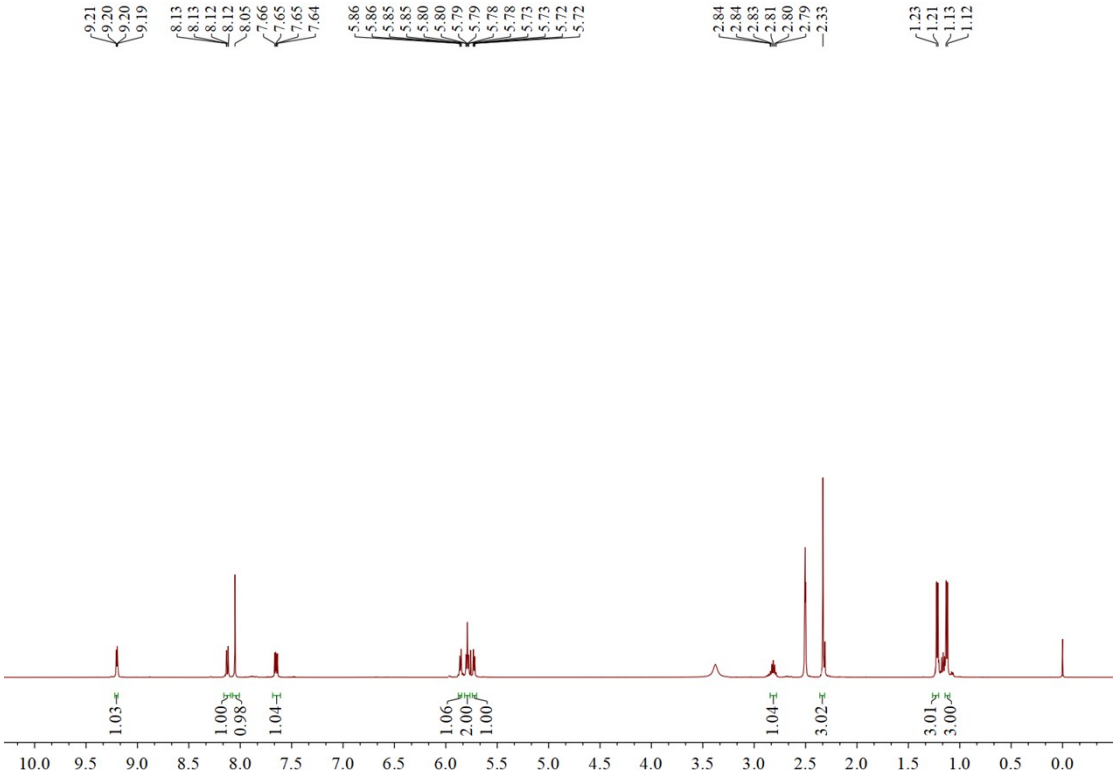

Figure S45. ^{1}H NMR (500MHz, DMSO-d_6) for complex **10**.

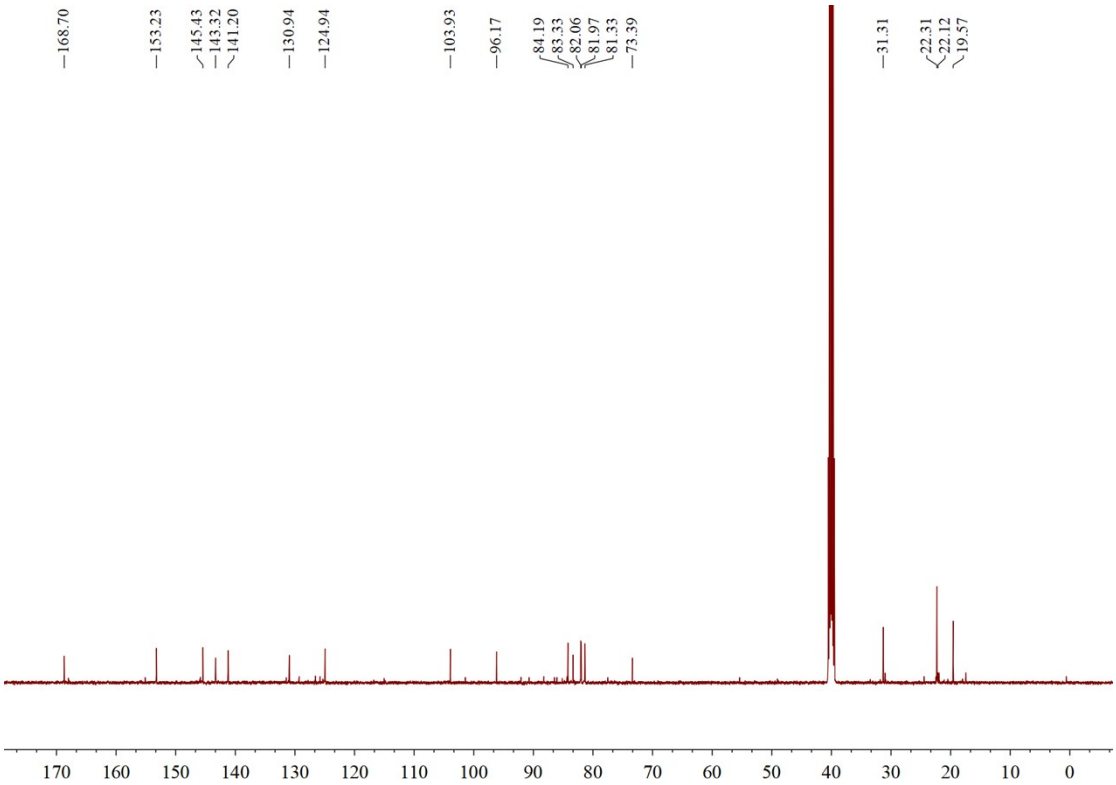

Figure S46. ^{13}C NMR (126MHz, DMSO-d_6) for complex **10**.

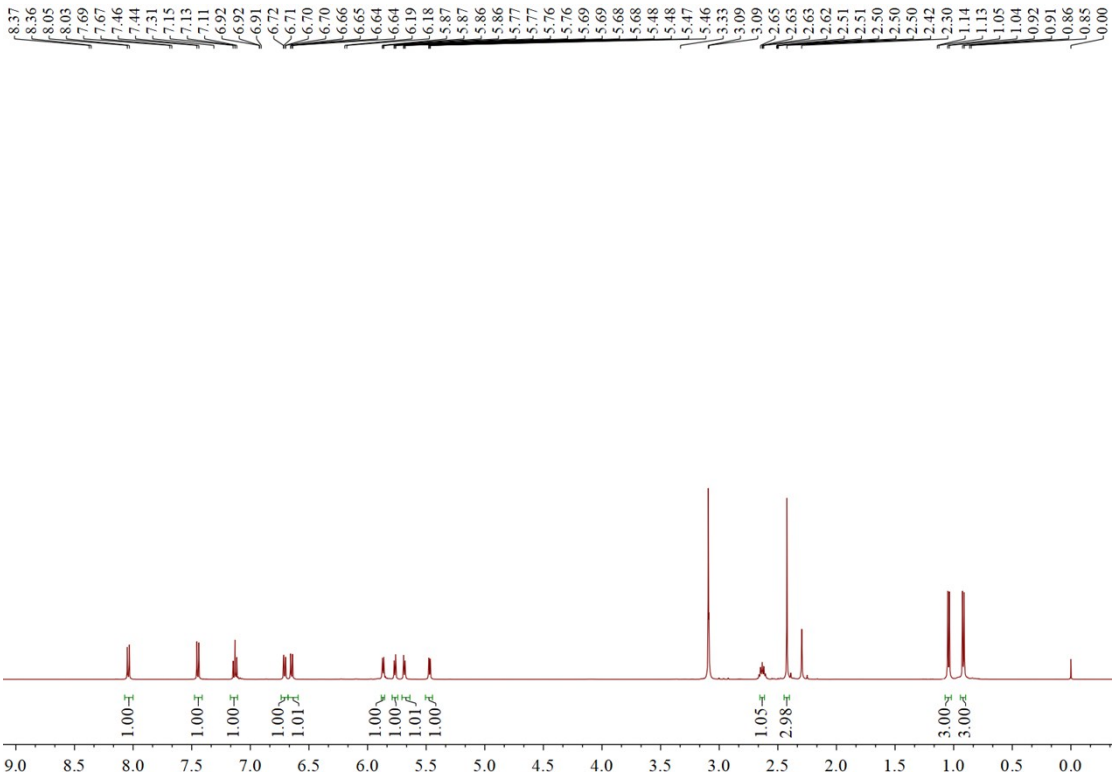

Figure S47. ^{1}H NMR (500MHz, DMSO-d_6) for complex **11**.

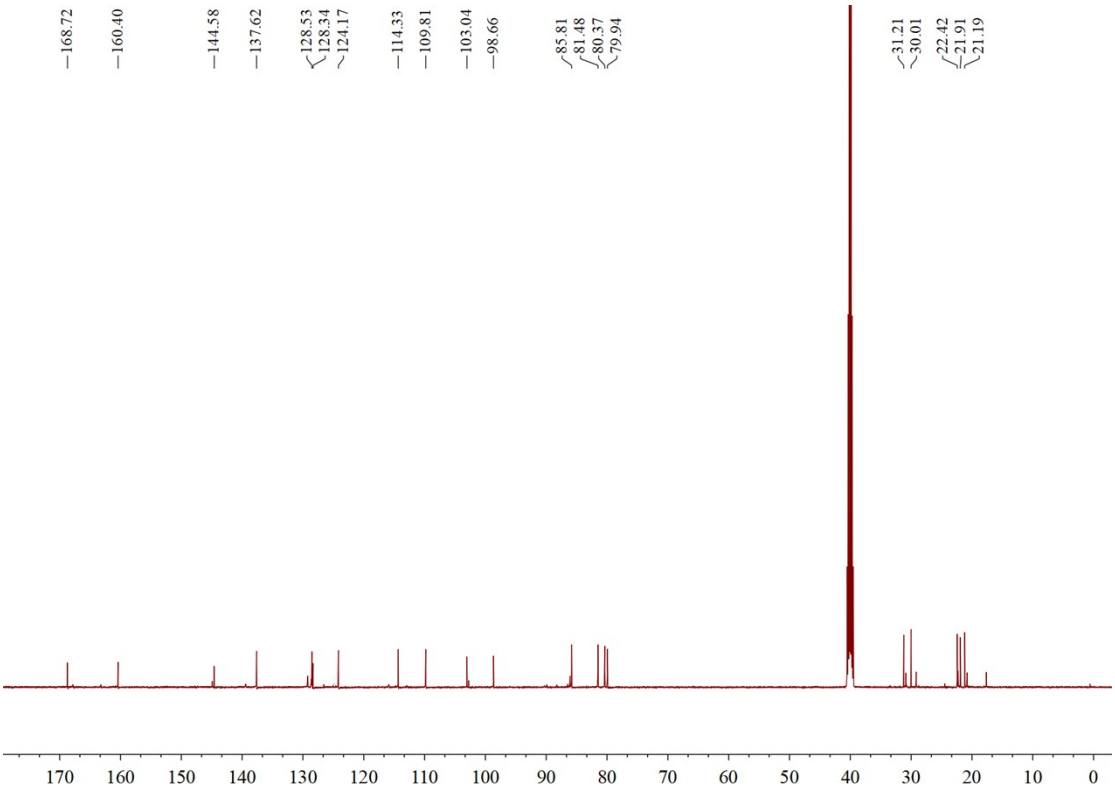

Figure S48. ^{13}C NMR (126MHz, DMSO-d_6) for complex **11**.

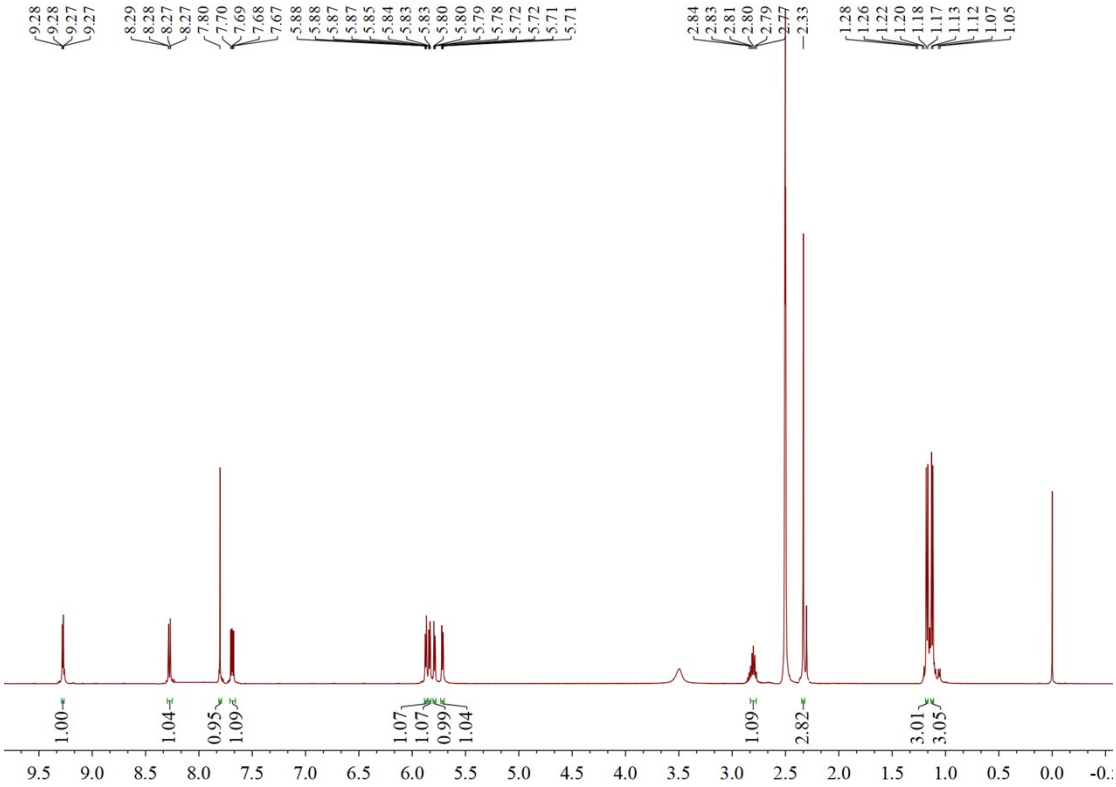

Figure S49. ^{1}H NMR (500MHz, DMSO-d_6) for complex **9**.

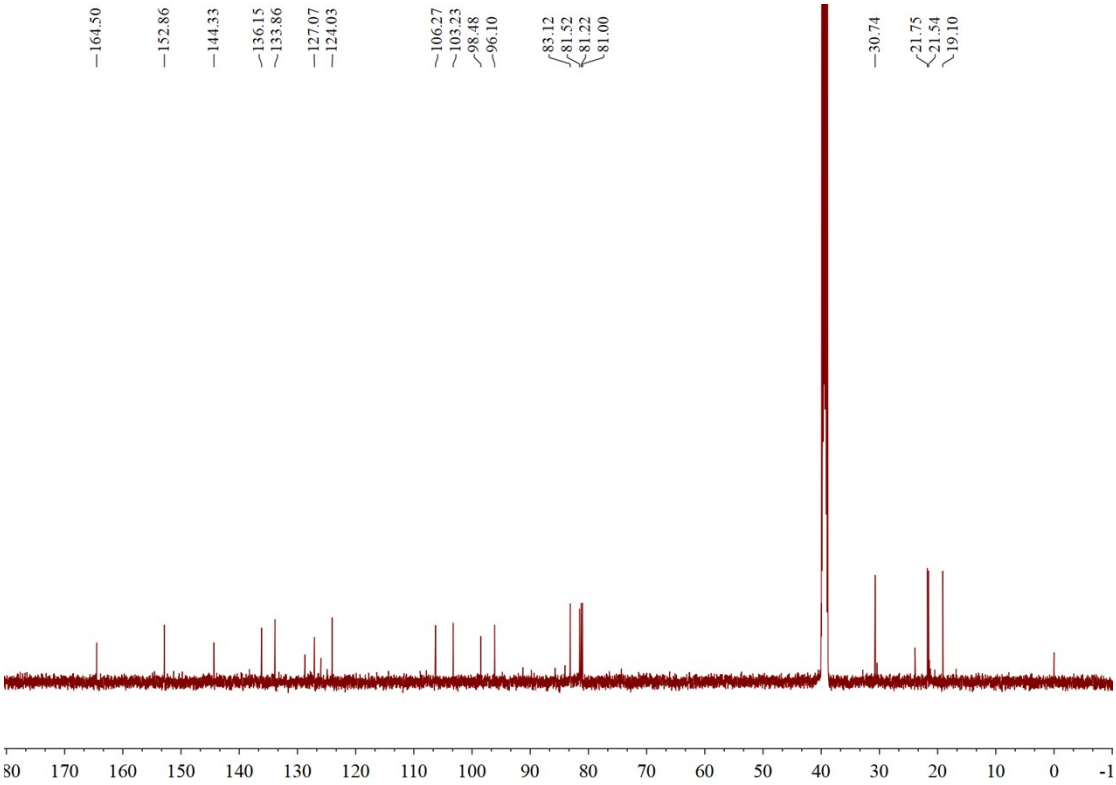

Figure S50. ^{13}C NMR (126MHz, DMSO-d_6) for complex **9**.

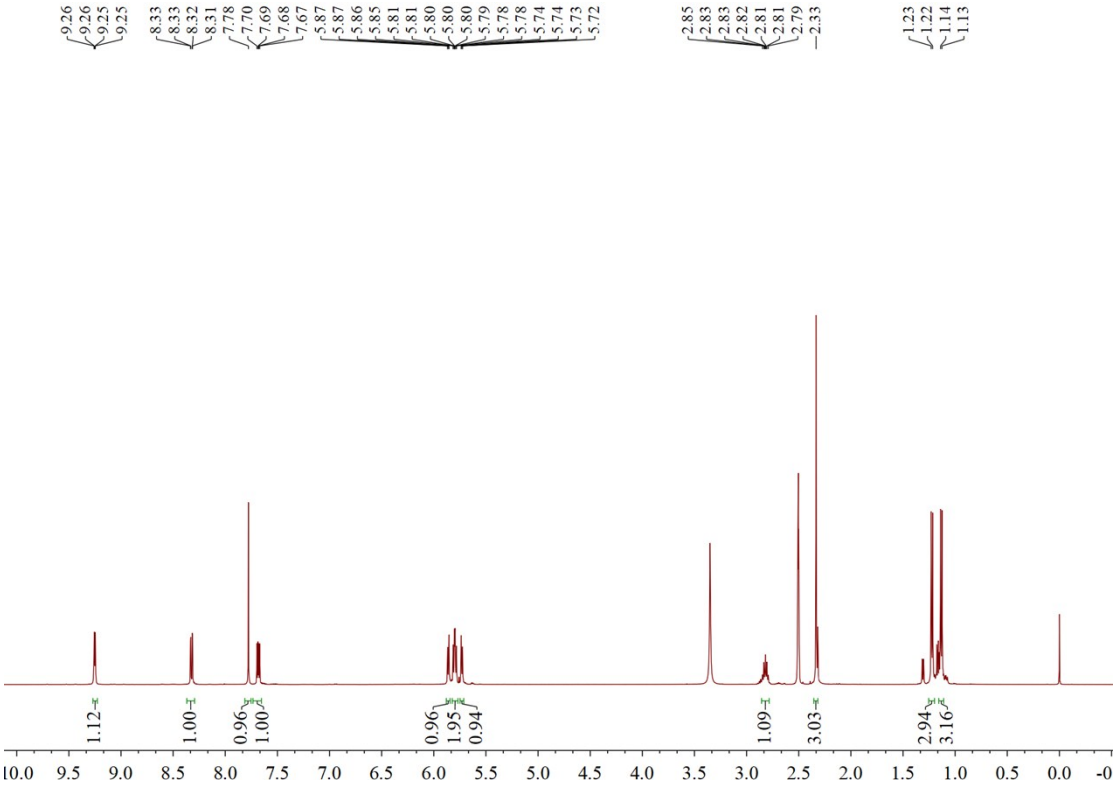

Figure S51. ^{1}H NMR (500MHz, DMSO-d_6) for complex **8**.

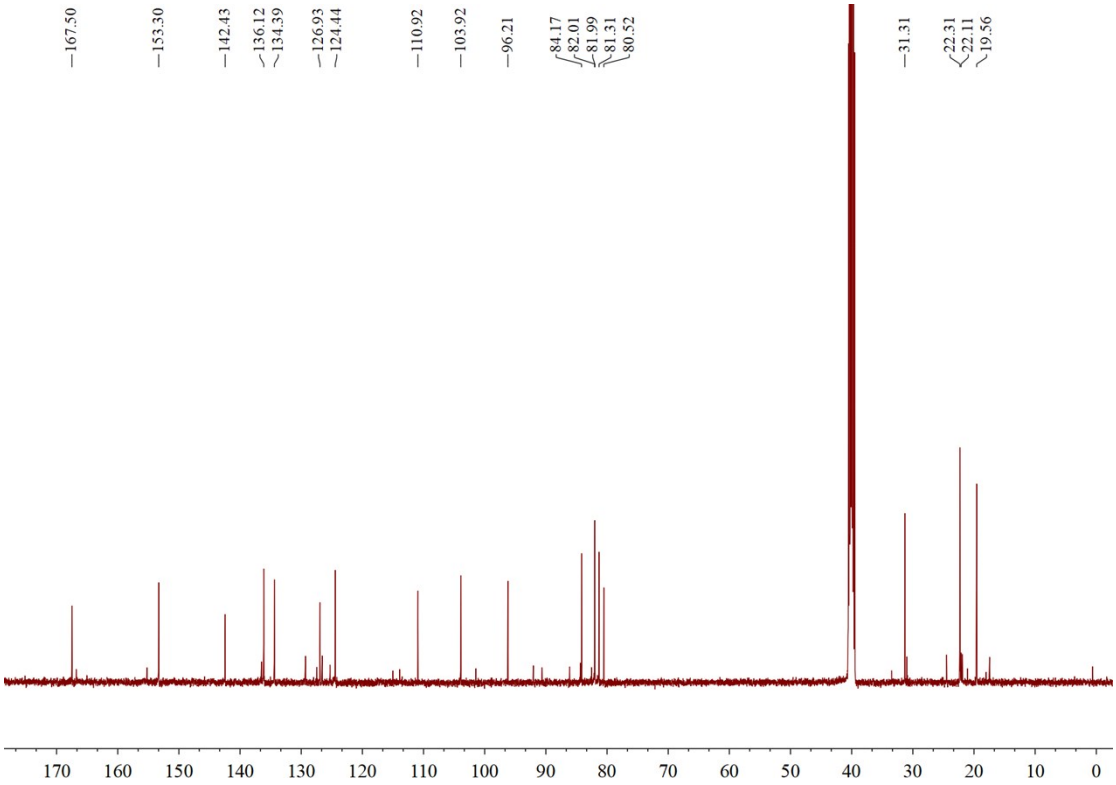

Figure S52. ^{13}C NMR (126MHz, DMSO-d_6) for complex **8**.

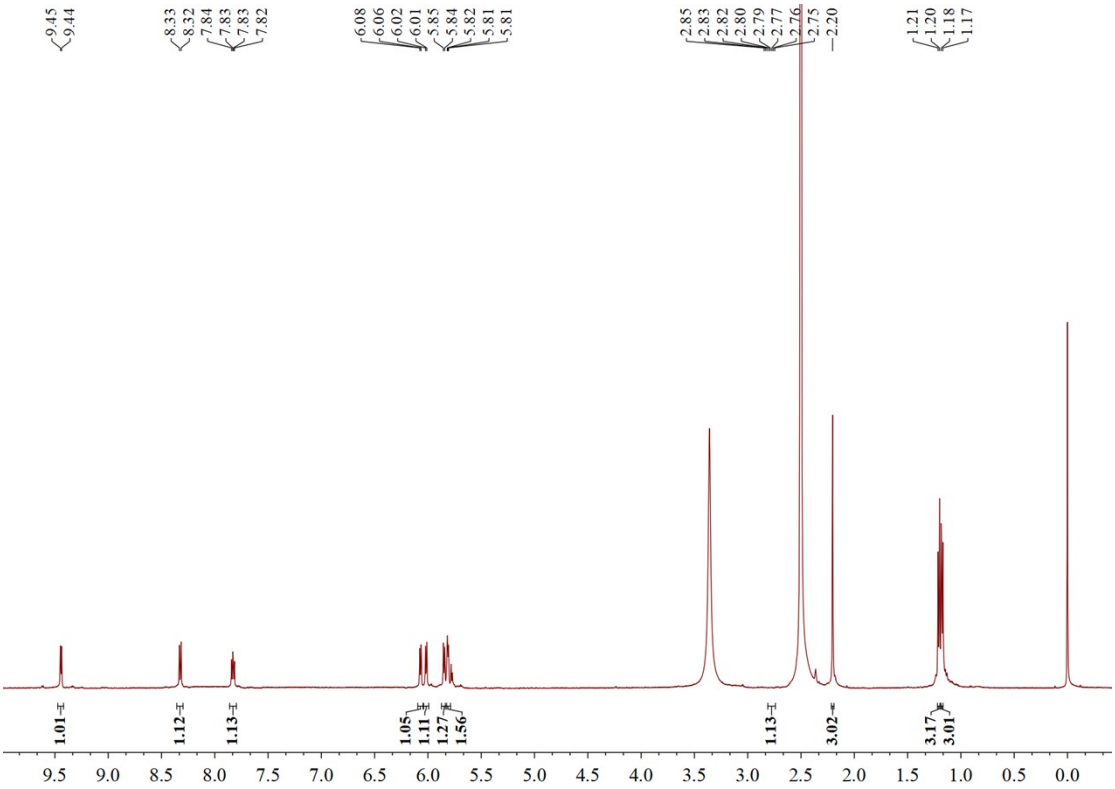

Figure S53. ^{1}H NMR (500MHz, DMSO-d_6) for complex **13**.

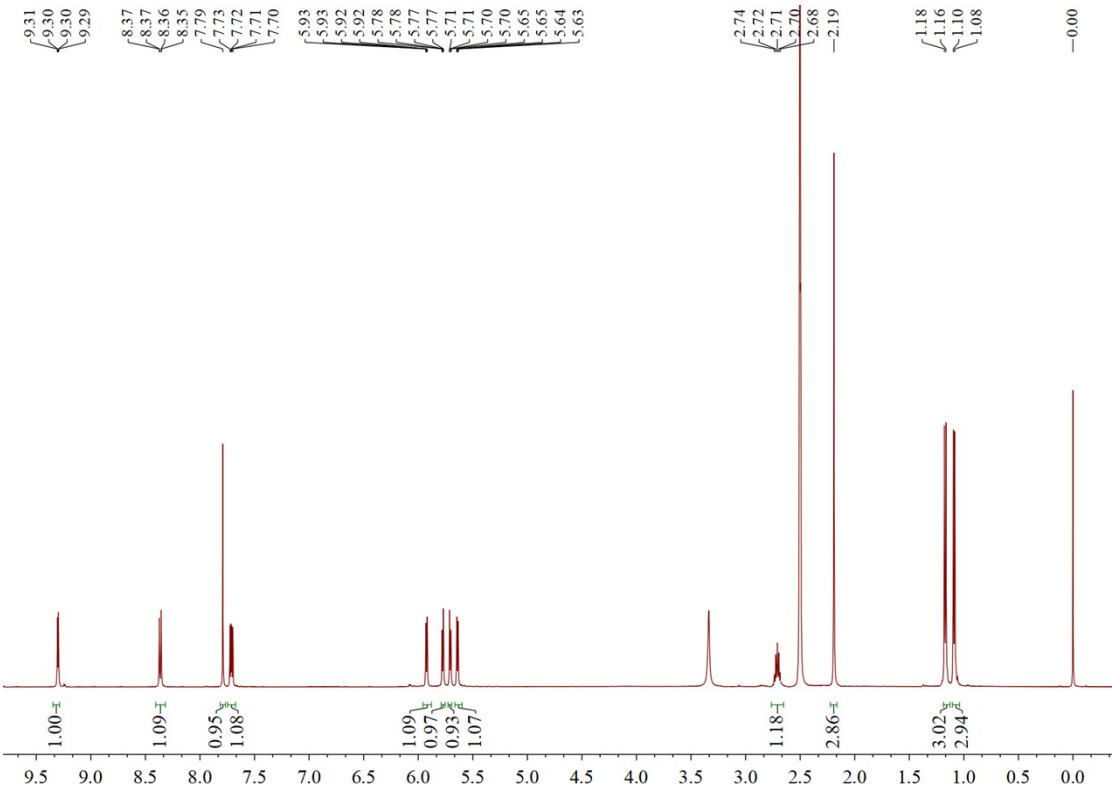

Figure S54. ^{1}H NMR (500MHz, DMSO-d_6) for complex **3**.

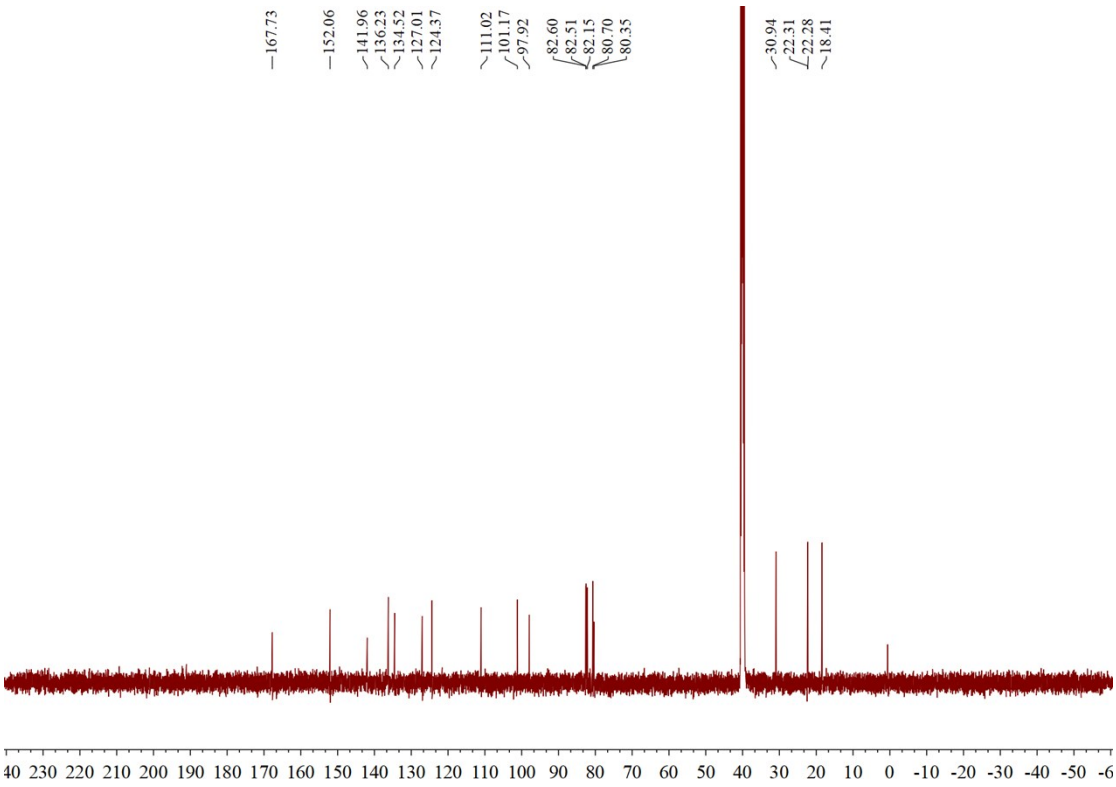

Figure S55. ^{13}C NMR (126MHz, DMSO-d_6) for complex **3**.

In Vivo Anti-cancer Activity toward HeLa Xenograft Tumor.

Table S44. The tumor volume in treated and non-treated mice from the date of surgery to the study end point in the Hela xenograft model.

Group	Tumor Volume (mm^3)		T/C (%)
	(start)	(end)	
Control	82.4±27.0	1127.8±180.7	-
1 (10.0 mg/kg)	82.9±19.0	410.8±113.0	35.6[a]

[a] mean $p<0.05$, *p vs* vehicle control

Table S45. Average body weight in treated and non-treated mice from the date of surgery to the study end point in the Hela xenogfart model.

Group	Body Weight (g)		RBW (%)
	(start)	(end)	(end)
Control	18.7±1.2	20.7±1.4	110.7
1 (10.0 mg/kg)	18.8±0.9	20.6±1.0	109.6

Table S46. In Vivo Anticancer Activity of **1** (10.0 mg/kg) toward Hela Tumor Xenograft.

Group	average tumor weight(mean ± SD g)	inhibition of tumor growth(%)
Control	1.562±0.148	-
1 (10.0 mg/kg)	0.648±0.101	58.5

[a] mean $p<0.05$, *pvs* control.

Experimental section

Synthesis of 6,7-dichloro-5,8-quinolinedione (H-L8)

Sodium chlorate (53.0 g, 500.0 mmol) was added portionwise over a period of 1.0 h into a stirred mixture of 8-hydroxyquinoline (14.5 g, 100.0 mmol) in HCl (38.0%, ca. 600 mL) at 40.0 °C and the reaction mixture was stirred for 2 h. The reaction mixture was then diluted, filtered to remove the white precipitate and the filtrate was extracted with CH_2Cl_2 (6 × 250.0 mL). The organic layers were combined, dried with Na_2SO_4 and concentrated in reduced pressure to afford the crude product as a yellow-orange solid. Recrystallization in various alkyl alcohols (MeOH, EtOH, i-PrOH or n-BuOH)

afforded 6,7-dichloro-5,8-quinolinedione (H-L8) as a bright yellow powder (3.89 g, 17.0%).

Synthesis and characterization of 13 organometallic Ru(II)-arene complexes

A total of 0.049 mmol of dichloro(p-cymene) Ru(II) dimer (**p-cymene-RuCl**) or diiodo(p-cymene) Ru(II) dimer (**p-cymene-RuI**) and 0.098 mmol of 5,7-dichloro-2-methyl-8-quinolinol (H-L1), 5,7-dibromo-2-methyl-8-quinolinol (H-L2), 5-chloro-7-iodo-8-hydroxy-quinoline (H-L3), 5,7-dibromo-8-quinolinol (H-L4), 5,7-diiodo-8-hydroxyquinoline (H-L5), 8-hydroxy-2-methylquinoline (H-L6), 2,8-quinolinediol (H-L7), or 6,7-dichloro-5,8-quinolinedione (H-L8) were dissolved in 10.0 mL of CH_3OH/CH_2Cl_2 mixture (v:v = 1:1), and the solution was refluxed for 6.0 h. The solvent was rotary evaporated, replaced by CH_3OH/CH_2Cl_2 (5.0 mL, v:v = 1:1), and was removed by filtration. The red-brown precipitate solution of organometallic Ru(II)-arene complexes were collected by filtration and washed with n-hexane (5.0 mL, yield: 85.1%−95.2%). Crystals of 13 organometallic Ru(II)-arene complexes **1**−**13** suitable for X-ray analysis were obtained by slow evaporation of a CH_3OH/CH_2Cl_2 (6.0 mL, v:v = 5:2) solution (Scheme 1).

*Data for **6**:* Yield (95.2%). IR (KBr): 3440, 3061, 2969, 2918, 2886, 2626, 2554, 1965, 1761, 1633, 1546, 1494, 1438, 1360, 1325, 1259, 1197, 1161, 1115, 1029, 958, 885, 829, 778, 696, 670 cm^{-1}. Elemental analysis calcd (%) for $C_{20}H_{20}Cl_2INORu$: C 40.77, H 3.42, N 2.38. Found: C 40.72, H 3.45, N 2.34. ESI-MS: m/z = 461.4 for $[M - Cl]^+$. ^1H NMR (500 MHz, DMSO-d_6) δ 8.22 (d, J = 8.6 Hz, 1H), 7.67 (d, J = 8.7 Hz, 1H), 7.51 (s, 1H), 5.95 (d, J = 5.9 Hz, 1H), 5.87 – 5.80 (m, 2H), 5.55 (d, J = 5.9 Hz, 1H), 3.14 (s, 3H), 2.65 (dq, J = 13.9,

6.9 Hz, 1H), 2.47 (s, 3H), 1.09 (d, J = 6.9 Hz, 3H), 0.93 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 163.06, 162.75, 144.85, 134.30, 128.06, 125.48, 124.26, 117.64, 110.37, 104.15, 98.48, 85.38, 81.48, 80.69, 80.38, 31.13, 30.31, 22.19, 21.82, 21.05.

*Data for **1**:* Yield (85.1%). IR (KBr): 3696, 3397, 3066, 2959, 2933, 2866, 2724, 2626, 2560, 2380, 2314, 2206, 2021, 1991, 1934, 1792, 1745, 1633, 1546, 1489, 1488, 1366, 1259, 1202, 1156, 1024, 967, 896, 814, 767, 701, 670 cm^{-1}. Elemental analysis calcd (%) for $C_{20}H_{20}Cl_3NORu$: C 48.25, H 4.05, N 2.81. Found: C 48.28, H 4.07, N 2.78. ESI-MS: m/z = 463.4 for $[M - Cl]^+$. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.20 (d, J = 8.6 Hz, 1H), 7.74 (s, 1H), 7.69 (d, J = 8.7 Hz, 1H), 5.98 (dd, J = 5.9, 1.1 Hz, 1H), 5.88 (dd, J = 6.1, 1.2 Hz, 1H), 5.77 (dd, J = 6.2, 1.2 Hz, 1H), 5.55 (dd, J = 5.9, 1.2 Hz, 1H), 3.32 (s, 1H), 3.19 (s, 3H), 2.20 (s, 3H), 1.04 (d, J = 7.0 Hz, 3H), 0.91 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 162.68, 161.18, 143.94, 133.80, 127.60, 124.96, 123.72, 116.58, 109.83, 100.39, 100.10, 86.31, 79.87, 79.78, 78.47, 30.25, 28.25, 21.64, 21.54, 18.27

*Data for **2**:* Yield (87.5%). IR (KBr): 3721, 3066, 3040, 2959, 2928, 2871, 2724, 2621, 2560, 2298, 2185, 1934, 1786, 1751, 1546, 1489, 1433, 1351, 1274, 1192, 1151, 1110, 1029, 937, 880, 819, 742, 670, 583 cm^{-1}. Elemental analysis calcd (%) for $C_{20}H_{20}Br_2ClNORu$: C 40.94, H 3.44, N 2.39. Found: C 40.90, H 3.47, N 2.36. ESI-MS: m/z = 626.9 for $[M - Cl + DMSO]^+$. ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.20 (d, J = 8.6 Hz, 1H), 7.74 (s, 1H), 7.69 (d, J = 8.7 Hz, 1H), 5.98 (dd, J = 5.9, 1.1 Hz, 1H), 5.88 (dd, J = 6.1, 1.1 Hz, 1H), 5.77 (dd, J = 6.1, 1.2 Hz, 1H), 5.55 (dd, J = 5.9, 1.2 Hz, 1H), 3.19 (s, 3H), 2.20 (s, 3H), 1.04 (d, J = 7.0 Hz, 3H), 0.91 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-

d_6) δ 164.87, 161.71, 156.92, 144.33, 136.84, 133.52, 125.88, 107.31, 100.79, 100.75, 99.41, 86.80, 80.51, 80.37, 79.36, 30.82, 28.79, 22.19, 22.15, 18.82.

*Data for **7**:* Yield (90.1%). IR (KBr): 3691, 3056, 2953, 2928, 2866, 2606, 2544, 1965, 1776, 1540, 1489, 1428, 1366, 1259, 1192, 1141, 1115, 1029, 937, 880, 819, 747, 660 cm^{-1}. Elemental analysis calcd (%) for $C_{20}H_{20}Br_2INORu$: C 35.42, H 2.97, N 2.07. Found: C 35.45, H 2.94, N 2.02. ESI-MS: m/z = 551.4 for $[M - Cl]^+$. ^1H NMR (500 MHz, DMSO-d_6) δ 8.15 (d, J = 8.6 Hz, 1H), 7.73 (s, 1H), 7.68 (d, J = 8.7 Hz, 1H), 5.93 (dd, J = 5.9, 1.2 Hz, 1H), 5.86 (dd, J = 6.3, 1.2 Hz, 1H), 5.83 – 5.81 (m, 1H), 5.56 (dd, J = 6.0, 1.2 Hz, 1H), 3.15 (s, 3H), 2.65 (p, J = 7.0 Hz, 1H), 2.46 (s, 3H), 1.10 (d, J = 7.0 Hz, 3H), 0.93 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.66, 162.69, 144.63, 136.75, 133.39, 125.98, 125.80, 107.73, 104.31, 99.37, 98.17, 85.17, 81.68, 81.05, 80.29, 31.09, 30.29, 22.25, 21.76, 20.95.

*Data for **13**:* Yield (93.5%). IR (KBr): 3461, 3245, 3061, 2964, 1965, 1699, 1617, 1525, 1443, 1337, 1305, 1218, 1161, 1110, 1034, 988, 885, 849, 798, 757, 660, 629, 557 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{19}Cl_2NO_3Ru$: C 47.41, H 3.98, N 2.91. Found: C 47.36, H 4.03, N 2.88. ESI-MS: m/z = 463.5 for $[M - Cl]^+$. ^1H NMR (500 MHz, DMSO-d_6) δ 9.44 (d, J = 5.6 Hz, 1H), 8.32 (d, J = 7.8 Hz, 1H), 7.83 (dd, J = 7.8, 5.6 Hz, 1H), 6.07 (d, J = 6.1 Hz, 1H), 6.02 (d, J = 6.0 Hz, 1H), 5.85 (d, J = 6.2 Hz, 1H), 5.84 – 5.79 (m, 2H), 2.77 (q, J = 6.9 Hz, 1H), 2.20 (s, 3H), 1.21 (d, J = 7.0 Hz, 3H), 1.17 (s, 3H).

*Data for **3**:* Yield (89.6%). IR (KBr): 3374, 2979, 2892, 2549, 2421, 2365, 2124, 1653, 1540, 1438, 1366, 1090, 1044, 875, 798, 842, 706, 650 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{18}Cl_2INORu$: C 39.67, H 3.15, N 2.43.

Found: C 39.63, H 3.19, N 2.41. ESI-MS: m/z = 539.4 for $[M - Cl]^+$. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.30 (dd, J = 4.9, 1.3 Hz, 1H), 8.36 (dd, J = 8.6, 1.2 Hz, 1H), 7.79 (s, 1H), 7.71 (dd, J = 8.6, 4.9 Hz, 1H), 5.92 (dd, J = 6.1, 1.1 Hz, 1H), 5.78 (dd, J = 6.0, 1.1 Hz, 1H), 5.71 (dd, J = 6.0, 1.1 Hz, 1H), 5.64 (dd, J = 6.1, 1.1 Hz, 1H), 2.71 (hept, J = 6.9 Hz, 1H), 2.19 (s, 3H), 1.17 (d, J = 6.9 Hz, 3H), 1.09 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.73, 152.06, 141.96, 136.23, 134.52, 127.01, 124.37, 111.02, 101.17, 97.92, 82.60, 82.51, 82.15, 80.70, 80.35, 30.94, 22.31, 22.28, 18.41.

*Data for **4**:* Yield (92.3%). IR (KBr): 3451, 3046, 2959, 2928, 2877, 2606, 2308, 1915, 1868, 1740, 1556, 1484, 1438, 1361, 1254, 1218, 1161, 1115, 1034, 952, 865, 798, 747, 680, 660, 578 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{18}Br_2ClNORu$: C 39.85, H 3.17, N 2.45. Found: C 39.81, H 3.20, N 2.43. ESI-MS: m/z = 537.3 for $[M - Cl]^+$. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.33 (dd, J = 5.0, 1.2 Hz, 1H), 8.31 (dd, J = 8.6, 1.2 Hz, 1H), 7.81 (s, 1H), 7.72 (dd, J = 8.6, 5.0 Hz, 1H), 5.96 – 5.90 (m, 1H), 5.83 (dd, J = 6.1, 1.2 Hz, 1H), 5.71 – 5.63 (m, 2H), 2.69 (p, J = 6.9 Hz, 1H), 2.18 (s, 3H), 1.13 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 164.73, 151.63, 143.87, 136.27, 133.97, 127.15, 123.96, 105.98, 100.48, 98.60, 97.87, 82.21, 81.72, 81.38, 79.95, 30.35, 21.80, 21.55, 17.89.

*Data for **9**:* Yield (88.3%). IR (KBr): 3425, 3051, 2953, 2923, 2866, 2734, 2478, 2109, 1950, 1899, 1843, 1756, 1546, 1474, 1438, 1356, 1254, 1218, 1146, 1110, 1054, 947, 870, 803, 742, 685, 660 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{18}Br_2INORu$: C 34.36, H 2.73, N 2.11. Found: C 34.40, H 2.71, N 2.13. ESI-MS: m/z = 537.3 for $[M - Cl]^+$. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.28 (dd, J = 5.0, 1.2 Hz, 1H), 8.28 (dd, J = 8.6, 1.2 Hz, 1H), 7.80 (s, 1H), 7.69

(dd, J = 8.6, 5.0 Hz, 1H), 5.87 (dd, J = 6.1, 1.2 Hz, 1H), 5.84 (dd, J = 6.0, 1.3 Hz, 1H), 5.79 (dd, J = 6.0, 1.2 Hz, 1H), 5.72 (dd, J = 5.9, 1.2 Hz, 1H), 2.83 – 2.78 (m, 1H), 2.33 (s, 3H), 1.17 (d, J = 7.0 Hz, 3H), 1.12 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) 164.50, 152.86, 144.33, 136.15, 133.86, 127.07, 124.03, 106.27, 103.23, 98.48, 96.10, 83.12, 81.52, 81.22, 81.00, 30.74, 21.75, 21.54, 19.10.

*Data for **5**:* Yield (87.0%). IR (KBr): 3675, 3066, 2979, 2907, 1932, 1771, 1535, 1474, 1438, 1355, 1248, 1218, 1054, 880, 747, 650, 568 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{18}ClI_2INORu$: C 34.23, H 2.72, N 2.10. Found: C 34.20, H 2.75, N 2.08. ESI-MS: m/z = 631.3 for $[M - Cl]^+$. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.25 (dd, J = 4.9, 1.2 Hz, 1H), 8.16 (dd, J = 8.6, 1.2 Hz, 1H), 8.06 (s, 1H), 7.68 (dd, J = 8.6, 4.9 Hz, 1H), 5.92 (dd, J = 6.1, 1.2 Hz, 1H), 5.77 (dd, J = 5.9, 1.2 Hz, 1H), 5.70 (dd, J = 5.9, 1.2 Hz, 1H), 5.64 (dd, J = 6.1, 1.2 Hz, 1H), 2.70 (hept, J = 6.9 Hz, 1H), 2.19 (s, 3H), 1.17 (d, J = 6.9 Hz, 3H), 1.08 (d, J = 7.0 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 168.92, 151.98, 145.55, 142.86, 141.31, 131.02, 124.89, 101.15, 97.91, 83.15, 82.64, 82.54, 82.11, 80.74, 73.45, 30.94, 22.33, 22.29, 18.43.

*Data for **10**:* Yield (91.0%). IR (KBr): 3440, 3035, 2955, 2918, 2866, 1633, 1540, 1474, 1443, 1371, 1325, 1054, 1024, 870, 808 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{18}I_3INORu$: C 30.10, H 2.39, N 2.11. Found: C 30.05, H 2.43, N 2.09. ESI-MS: m/z = 631.3 for $[M - Cl]^+$. ^{1}H NMR (500 MHz, DMSO-d_6) δ 9.20 (dd, J = 4.9, 1.2 Hz, 1H), 8.12 (dd, J = 8.6, 1.2 Hz, 1H), 8.05 (s, 1H), 7.65 (dd, J = 8.6, 5.0 Hz, 1H), 5.86 (dd, J = 6.1, 1.3 Hz, 1H), 5.79 (td, J = 6.5, 1.2 Hz, 2H), 5.73 (dd, J = 6.0, 1.2 Hz, 1H), 2.81 (p, J = 6.9 Hz, 1H), 2.33 (s, 3H), 1.22 (d, J = 7.0 Hz, 3H), 1.13 (d, J = 6.9 Hz, 4H). ^{13}C NMR

(126 MHz, DMSO-d_6) δ 168.70, 153.23, 145.43, 143.32, 141.20, 130.94, 124.94, 103.93, 96.17, 84.19, 83.33, 82.06, 81.97, 81.33, 73.39, 31.31, 22.31, 22.12, 19.57.

*Data for **8**:* Yield (88.9%). IR (KBr): 3430, 3061, 2959, 2871, 2626, 2467, 2196, 2109, 1955, 1827, 1756, 1571, 1546, 1479, 1443, 1366, 1254, 1202, 1110, 1049, 967, 931, 875, 798, 747, 701, 655, 573 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{18}Cl_2INORu$: C 34.23, H 2.72, N 2.10. Found: C 34.19, H 2.74, N 2.07. ESI-MS: m/z = 539.4 for $[M - Cl]^+$. ^1H NMR (500 MHz, DMSO-d_6) δ 9.25 (dd, J = 5.0, 1.3 Hz, 1H), 8.32 (dd, J = 8.6, 1.2 Hz, 1H), 7.78 (s, 1H), 7.68 (dd, J = 8.6, 5.0 Hz, 1H), 5.86 (dd, J = 6.0, 1.2 Hz, 1H), 5.80 (ddd, J = 9.1, 6.0, 1.2 Hz, 2H), 5.73 (dd, J = 5.9, 1.2 Hz, 1H), 2.82 (p, J = 6.9 Hz, 1H), 2.33 (s, 3H), 1.22 (d, J = 6.9 Hz, 3H), 1.13 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 167.50, 153.30, 142.43, 136.12, 134.39, 126.93, 124.44, 110.92, 103.92, 96.21, 84.17, 82.01, 81.99, 81.31, 80.52, 31.31, 22.31, 22.11, 19.56.

*Data for **11**:* Yield (85.8%). IR (KBr): 3711, 3415, 3066, 2975, 2912, 2877, 2662, 2611, 2570, 2524, 2303, 2211, 2037, 1939, 1802, 1725, 1689, 1551, 1500, 1453, 1433, 1371, 1320, 1284, 1172, 1110, 1024, 885, 834, 757, 634 cm^{-1}. Elemental analysis calcd (%) for $C_{20}H_{22}INORu$: C 46.16, H 4.26, N 2.69. Found: C 46.12, H 4.30, N 2.67. ESI-MS: m/z = 393.4 for $[M - Cl]^+$. ^1H NMR (500 MHz, DMSO-d_6) δ 8.04 (d, J = 8.5 Hz, 1H), 7.45 (d, J = 8.5 Hz, 1H), 7.13 (t, J = 7.9 Hz, 1H), 6.71 (dd, J = 7.9, 1.2 Hz, 1H), 6.65 (dd, J = 7.8, 1.1 Hz, 1H), 5.87 (dd, J = 5.8, 1.2 Hz, 1H), 5.77 (dd, J = 6.2, 1.2 Hz, 1H), 5.69 (dd, J = 6.1, 1.2 Hz, 1H), 5.47 (dd, J = 5.8, 1.2 Hz, 1H), 2.63 (td, J = 6.9, 2.5 Hz, 1H), 2.42 (s, 3H), 1.04 (d, J = 6.9 Hz, 3H), 0.92 (d, J = 6.9 Hz, 3H). ^{13}C NMR (126 MHz, DMSO-d_6) δ 168.72, 160.40, 144.58, 137.62, 128.53, 128.34,

124.17, 114.33, 109.81, 103.04, 98.66, 85.81, 81.48, 80.37, 79.94, 31.21, 30.01, 22.42, 21.91, 21.19.

Data for ***12****:* Yield (90.1%). IR (KBr): 3430, 3035, 2959, 2928, 2866, 2729, 1904, 1761, 1597, 1500, 1464, 1438, 1377, 1320, 1284, 1202, 1156, 1090, 1054, 1019, 865, 798, 725, 625 cm^{-1}. Elemental analysis calcd (%) for $C_{19}H_{20}INO_2Ru$: C 43.69, H 3.86, N 2.68. Found: C 43.67, H 3.90, N 2.66. ESI-MS: m/z = 395.4 for $[M - Cl]^+$.

Cell Culture

Human HeLa (human cervical cancer), T-24 (human bladder cancer), SK-OV-3 (human ovarian carcinoma cancer) and HL-7702 normal cells were obtained from the Shanghai Institute for Biological Science (China). HeLa (human cervical cancer), T-24 (human bladder cancer), SK-OV-3 (human ovarian carcinoma cancer) and HL-7702 normal cells were grown in DMEM medium, both containing heat-inactivated fetal calf serum (FCS, Sigma, USA) (10%) and antibiotics (penicillin/streptomycin) at 37 °C and CO_2 (5%).

MTT assay

Cytotoxicity was determined using the MTT assay (MTT = 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl-2Htetrazolium bromide). Cells were seeded in 96-well plates as monolayers with 100 μL of cell solution (approximately 20000 cells) per well and preincubated for 24 h in medium supplemented with 10% FCS. The 13 organometallic Ru(II)-arene complexes **1**−**13**, H-L1, H-L2, H-L3, H-L4, H-L5, H-L6, H-L7, H-L8, and cisplatin, were prepared as 0.5% DMSO solution. Then 100 μL of 13 organometallic Ru(II)-arene complexes **1**−**13**, H-L1, H-L2, H-L3, H-L4, H-L5, H-L6, H-L7, H-L8, and cisplatin solution was added to each well and the plates were

incubated for another 48 h. Subsequently, MTT (5.0 mg/mL solution) was added to the cells and the plates were incubated for a further 4 h. The culture medium was aspirated, and the purple formazan crystals formed by the mitochondrial dehydrogenase activity of vital cells were dissolved in DMSO. The optical density, directly proportional to the number of surviving cells, was quantified at 540 nm using a multiwell plate reader and the fraction of surviving cells was calculated from the absorbance of untreated control cells.

In vitro transwell migration assay

The inhibition of tumor cell migration was assessed by the Boyden chamber (Corning Falcon) migration assay in 24-well cell culture plate with 8.0 μm pore. Briefly, HeLa cancer cells were collected, centrifuged, and re-suspended with serum-free medium. The top chambers were seeded with 1×10^5 cells in 200 μL of serum-free 1640 medium containing different dose of **1** (2.0 nM) and **2** (25.0 nM). The bottom chambers were filled with 600 μL of complete medium supplemented with different dose of **1** (2.0 nM) and **2** (25.0 nM). After 24 h incubation, non-migrated cells were removed with cotton swabs, and migrated cells were fixed with cold 4% paraformaldehyde and stained with 0.2% crystal violet for 1 min. Then the chambers were washed using water, and the membrane was left to dry. Images were taken with an inverted microscope (Olympus) and cells from three random areas per filter were counted.

Cell cycle analysis

HeLa cancer cells were seeded in 6-well plates (3×10^5 cells/well) and incubated in the presence or absence of **1** (2.0 nM) and **2** (25.0 nM) for 24 h. Then, cells were harvested by centrifugation and fixed in ice-cold 70% ethanol overnight. After the ethanol was removed the next day, the cells were resuspended in the ice-cold PBS and

treated with RNase A (Keygen Biotech, China) at 37 °C for 30 min, followed by incubated with the DNA staining solution propidium iodide (PI) (Keygen Biotech, China) at 4 °C for 30 min. About 10,000 events were detected by flow cytometry (BECKMAN-COULTER) at 488 nm. The data regarding the number of cells in different phases of the cell cycle were analyzed by EXPO32 ADC analysis software.

Apoptosis analysis

HeLa cells were seeded in 6-well plates (3×10^5 cells/well) and incubated in the presence or absence of **1** (2.0 nM) and **2** (25.0 nM) for 24 h to induce cancer cell apoptosis. After incubation, the cancer cells were harvested and incubated with 5.0 μL of Annexin-V/FITC (Keygen Biotech, China) in binding buffer (10 mM HEPES, 140 mM NaCl, and 2.5 mM $CaCl_2$ at pH 7.4) at room temperature for 30.0 min. PI solution was then added to the medium for another 5.0 min of incubation. Almost 10,000 events were collected for each sample and analyzed by flow cytometry (BECKMAN-COULTER). The percentage of apoptotic cells was calculated with EXPO32 ADC Analysis software.

Immunofluorescence assay

The HeLa cancer cells were grown on polylysine-coated coverslips, treated with **1** (2.0 nM) and **2** (25.0 nM), these cells rinsed in phosphate-buffered saline, fixed in cold methanol for 20 min, permeabilized for 10 min in 0.5% Triton X-100 on ice, and blocked in 5% BSA for 30 min at room temperature. The coverslips were incubated with rabbit monoclonal anti-H2A.X (Abcam) primary antibodies for 240 min at 25 °C. The coverslips were washed and incubated with fluorescein conjugated goat anti-secondary antibodies (Alexa Fluor® 488 Goat Anti- Rabbit IgG, green) for 30.0 min. Finally, these cells stained with 0.1 mg/mL DAPI. Fluorescence images were visualized by LeicaTCS-SP5 confocal microscope (Germany, magnification 400×).

Mitochondrial membrane potential (MMP) assay

A lipophilic cationic dye, 5,5′,6,6′-tetrachloro-1,1′,3,3′-tetraethylbenzimidazolcarbocyanine (JC-1, Beyotime, China) was used to monitor the level of MMP in the cells. At normal state, the MMP is high, and JC-1 appears as aggregates, which is indicated by red fluorescence. However, when apoptosis occurs, the MMP reduced and JC-1 displayed as monomers, which is indicated by green fluorescence. For flow cytometry analysis, HeLa cancer cells were plated in 6-well plates (3×10^5 cells/well) and grown for 24.0 h and treated with **1** (2.0 nM) and **2** (25.0 nM) for 24 h. Then the cells were harvested by centrifugation and incubated with JC-1 solution for 30 min. After briefly washing, the proportion of green and red fluorescence intensity was immediately detected and analyzed by flow cytometry.

Western blot analysis

HeLa cancer cells seeded in 60.0 mm dishes at a density of 6×10^5 cells/well were incubated with or without **1** (2.0 nM) and **2** (25.0 nM) for 24 h. After incubation, these cells were washed twice with ice-cold PBS and then lysed in RIPA lysis buffer containing 150 mM NaCl, 50 mM Tris (pH 7.4), 1% (w/v) sodium deoxycholate, 1% (v/v) Triton X-100, 0.1% (w/v) SDS, and 1 mM EDTA (Beyotime, China). The lysates were incubated at 0 °C for 30 min and vortexed every 10.0 min intermittently, and then the total protein was harvested by centrifuging at 12,500 g for 35.0 min. After the protein concentrations were determined by a BCA Protein Assay Kit (Beyotime, China), the protein extracts were reconstituted in loading buffer containing 62 mM Tris-HCl, 2% SDS, 10% glycerol, and 5% β-mercaptoethanol (Beyotime, China) and boiled at 100 °C for 5.0 min. An equal amount of the proteins (40.0 μg) was separated by 8−12% sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) and was transferred to nitrocellulose membranes

(Amersham Biosciences, Little Chalfont, Buckinghamshire, UK). After blocking with 5% nonfat dried milk in TBS containing 1% Tween-20 for 90 min at room temperature, the membranes were incubated overnight with specific primary antibodies (CST, USA) at 4 °C. After three washes in TBST, the membranes were incubated with the appropriate HRP-conjugated secondary antibodies at room temperature for 2.5 h. The blots were developed with enhanced chemiluminescence and were detected by an imager.

Measurement of reactive oxygen species (ROS) generation

DCFH-DA is a freely permeable tracer specific for ROS. DCFH-DA can be deacetylated by intracellular esterase to the non-fluorescent DCFH which is oxidized by ROS to the fluorescent compound 2',7'-dichloroflorescein (DCF). Thus, the fluorescence intensity of DCF is proportional to the amount of ROS produced by the cells. 6×10^5 cells were exposed to **1** (2.0 nM) and **2** (25.0 nM) for 24 h. After exposure, the cells were harvested, washed once with ice-cold PBS and incubated with DCFH-DA (100 μM in a final concentration) at 37 °C for 30.0 min in the dark. Then the cells were washed again and maintained in 1 mL PBS. The ROS generation was assessed from 10,000 cells each sample by fluorescence photometer (GC126N, China) with excitation and emission wavelengths of 488 and 525 nm, respectively. The experiment was performed at least three times.

TRAP assay

Telomerase extract was prepared from HeLa cells. A modified version of the TRAP assay was used. PCR was performed in a final 50 μL reaction volume composed of reaction mix (45 μL) containing Tris-HCl (20 mM, pH 8.0), deoxynucleotide triphosphates (50 mM), $MgCl_2$ (1.5 mM), KCl (63 mM), EGTA (1 mM), Tween-20 (0.005%), BSA (20 μg/mL), primer HTG21 (3.5 pmol; 5'-

G3ACHTUNGTRENUNG[T2AG3]3-3'), primer TS (18 pmol; 5'-AATCCG TCGAGC AGAGTT-3'), primer CXext (22.5 pmol; 5'-GTGCCCT TACCCTT ACCCTTA CCCTAA-3'), primer NT (7.5 pmol; 5'-ATCGCT TCTCGG CCTTTT-3'), TSNT internal control (0.01 amol; 5'-ATTCCG TCGAGC AGAGTT AAAAGG CCGAGA AGCGAT-3'), Taq DNA polymerase (2.5 U), and telomerase (100 ng). **1** (2.0 nM) and **2** (25.0 nM) or distilled water were added (5 μL). PCR was performed in an Eppendorf Master cycler equipped with a hot lid and incubated for 30 min at 30°C, followed by 92°C 30 s, 52°C 30 s, and 72°C 30 s for 30 cycles. After amplification, loading buffer (8 μL; 5×TBE buffer, 0.2% bromophenol blue, and 0.2% xylene cyanol) was added to the reaction. An aliquot (15.0 μL) was loaded onto a nondenaturing acrylamide gel (16%; 19:1) in 1×TBE buffer and resolved at 200.0 V for 1.0 h. Gels were fixed and then stained with $AgNO_3$.

Animale Used. The male and female KM mice, 5-6 weeks old, weight 20-23 g, six-week-old athymic BALB/cA nu/nufemale mice (18-20 g) were purchased from Guangxi Medical University Laboratory Animal Centre (Guangxi, China), the Acute toxicity studies and in vivo antitumor study were carried out in there. Animals were housed at a sterile environment with conditions of constant photoperiod (12 h light/ 12 h dark at 23-24 °C and 65-85% humidity).

In addition, HeLa xenograft mouse models were purchased from Beijing HFK Bioscience Co., Ltd (Beijing, China, approval No. SCXK 2014-004). The animal procedures were approved by the Institute of Radiation Medicine Chinese Academy of Medical Sciences (Tian Jin, China, approval No. SYXK 2014-0002). And all of the experimental procedures were carried out in accordance with the NIH Guidelines for the Care and Use of Laboratory Animals. Animal experiments were approved by the Animal Care and Use Committee of Institute of Radiation Medicine Chinese

Academy of Medical Sciences. In addition, statistical analysis and abbreviations used have been reported.

Anti-cancer activity toward HeLa *in Vivo*. The HeLa cells were harvested and injected subcutaneously into the right flank of nude mice with 5×10^6 cells in 200 μL of serum-free medium. When the xenograft tumor growth to the volume about 1000 mm^3, the mice were killed and the tumor tissue were cut into about 1.5 mm^3 small pieces, and then transplanted into the right flank of female nude mice, When tumors reach a volume of 80-190 mm^3 on all mice, the mice were randomized into vehicle control and treatment groups (n=6/group), received the following treatments: (a) control, 10% v/v DMSO/saline vehicle, (b) complex **1** at dose 10 mg/kg every two day (10% v/v DMSO/saline). The tumor volumes were determined every three days by measuring length (*l*) and width (*w*) and calculating volume, tumor volume and inhibition of tumor growth were calculated using formulas $1-3:1^{-3}$

Tumor volume: $V = (w^2\times l)/2$ (1)

The tumor relative increment rate: $T/C\ (\%) = T_{RTV}/C_{RTV}\times100\%$ (2)

inhibition of tumor growth: $IR(\%) = (W_c - W_t)/W_c\times100\%$ (3)

Where w and l mean the shorter and the longer diameter of the tumor respectively; T_{RTV} and C_{RTV} was the RTV of treated group and control group respectively. (RTV: relative tumor volume, $RTV= V_t /V_0$); W_t and W_c mean the average tumor weight of complex-treated and vehicle controlled group respectively.

X-ray Crystallographic Determination. All reflection data were collected on an Agilent Supernova diffractometer (Mo, λ = 0.71073Å) at room temperature. A semiempirical absorption correction by using the SADABS program was applied, and the raw data frame integration was performed with SAINT [4]. The crystal structures were solved by the direct method using the program SHELXS-97[5] and refined by the

full-matrix least-squares method on F^2 for all non-hydrogen atoms using SHELXL-97[6] with anisotropic thermal parameters. All hydrogen atoms were located in calculated positions and refined isotropically. The details of the crystal data were summarized in Tables S1–S42, and selected bond lengths and angles for 13 organometallic Ru(II)-arene complexes **1**−**13**, and **p-cymene-RuCl** are listed in the Tables S1–S42. The crystallographic data of 13 organometallic Ru(II)-arene complexes **1**−**13**, and **p-cymene-RuCl** in CIF format has been deposited in the Cambridge Crystallographic Data Center. The CCDC number for **4**, **9**, **3**, **8**, **5**, **10**, **2**, **7**, **1**, **6**, **p-cymene-RuCl**, **13**, **11** and **12** were 1895279, 1895411, 1895280, 1895281, 1895282, 1895283, 1895284, 1895285, 1895412, 1895286, 1895287, 1895288, 1896981 and 1896982.

Statistical Analysis. The experiments have been repeated from three to five times, and the results obtained are presented as means ± standard deviation (SD). Significant changes were assesses by using Student's *t* test for unpaired data, and p values of <0.05 were considered significant.

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