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Supporting Information For

Synthesis, characterization and biological evaluation of labile intercalative ruthenium(II) complexes for anticancer drug screening

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Content

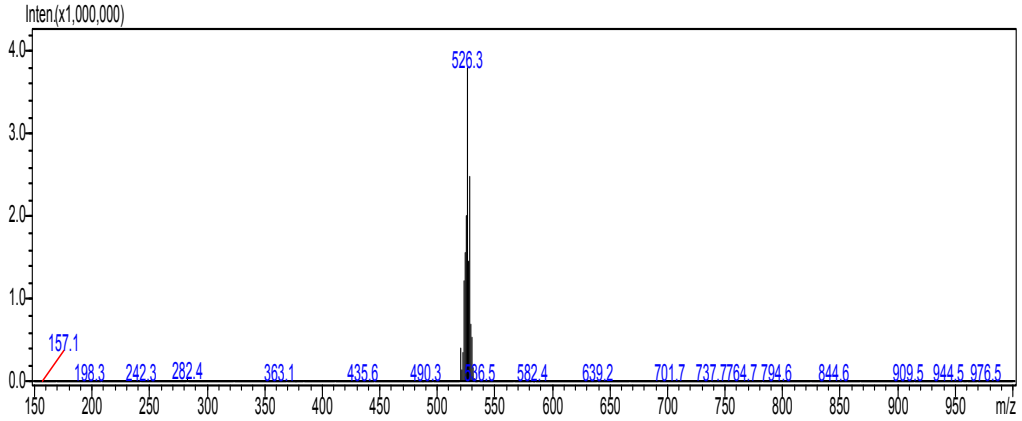

Figure S1 ES-MS (CH_3CN) spectrum of **Ru1**.

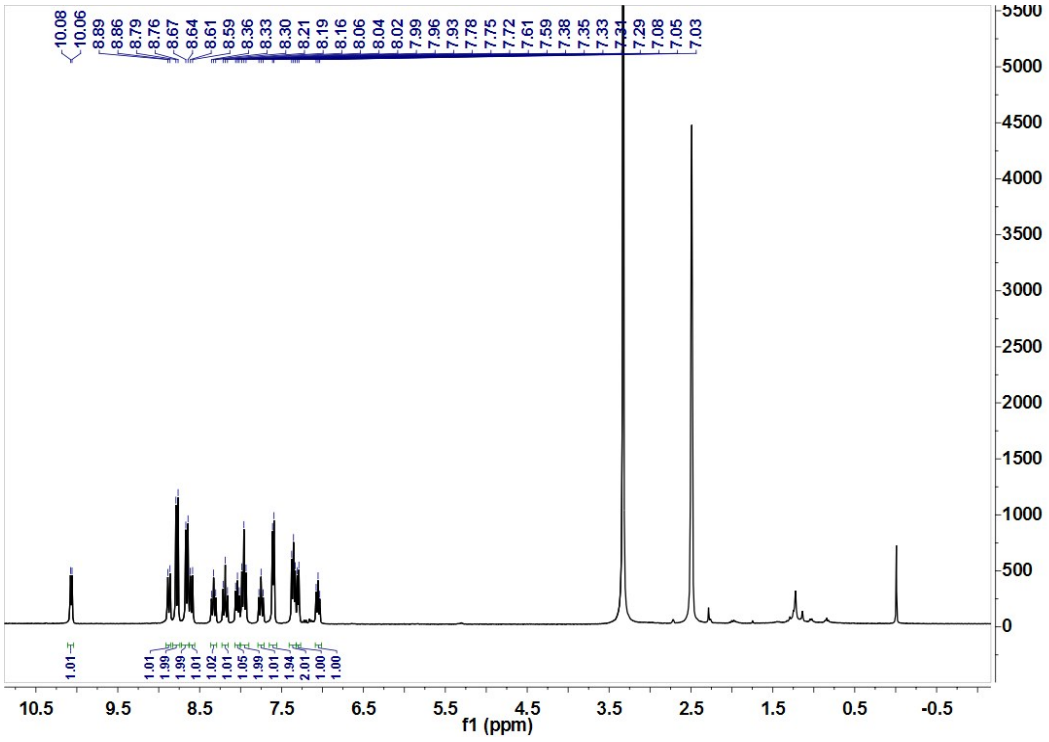

Figure S2 ^{1}H NMR spectrum (300 MHz, DMSO-d_6) spectrum of **Ru1**.

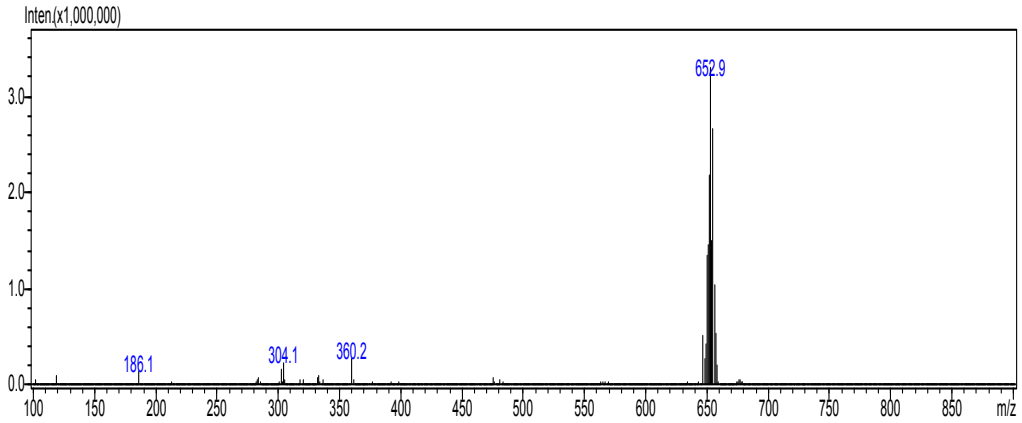

Figure S3 ES-MS (CH_3CN) spectrum of **Ru2**.

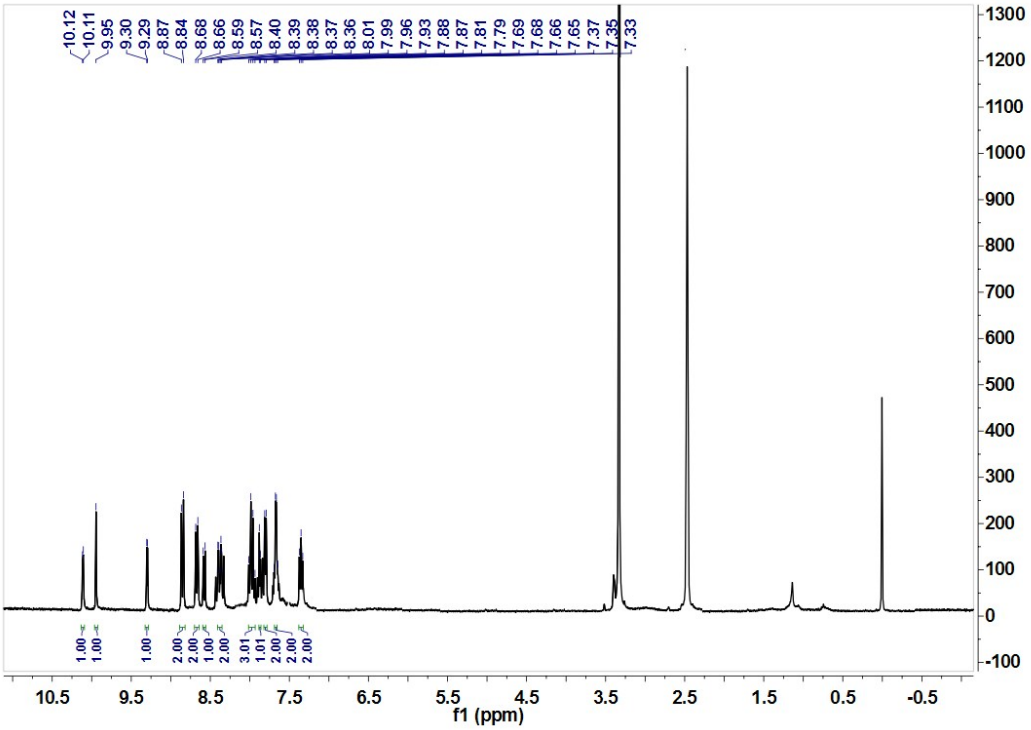

Figure S4 ^{1}H NMR spectrum (300 MHz, DMSO-d_6) spectrum of **Ru2**.

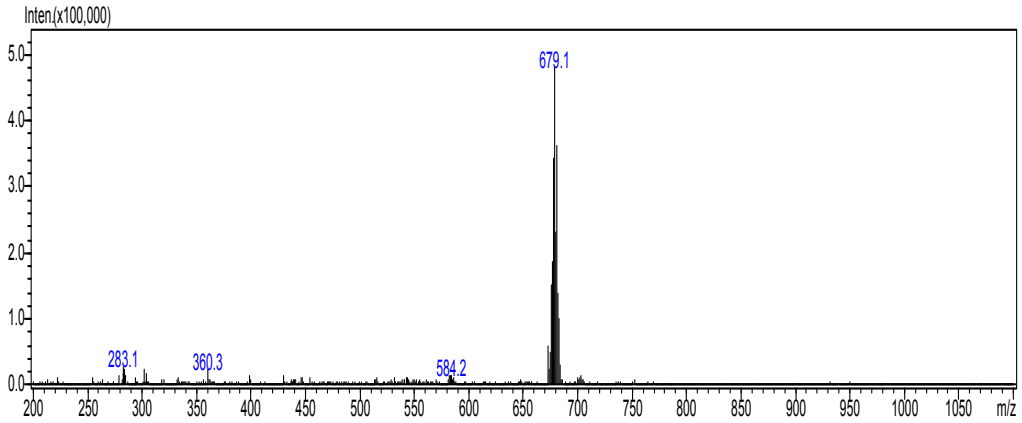

Figure S5 ES-MS (CH_3CN) spectrum of **Ru3**.

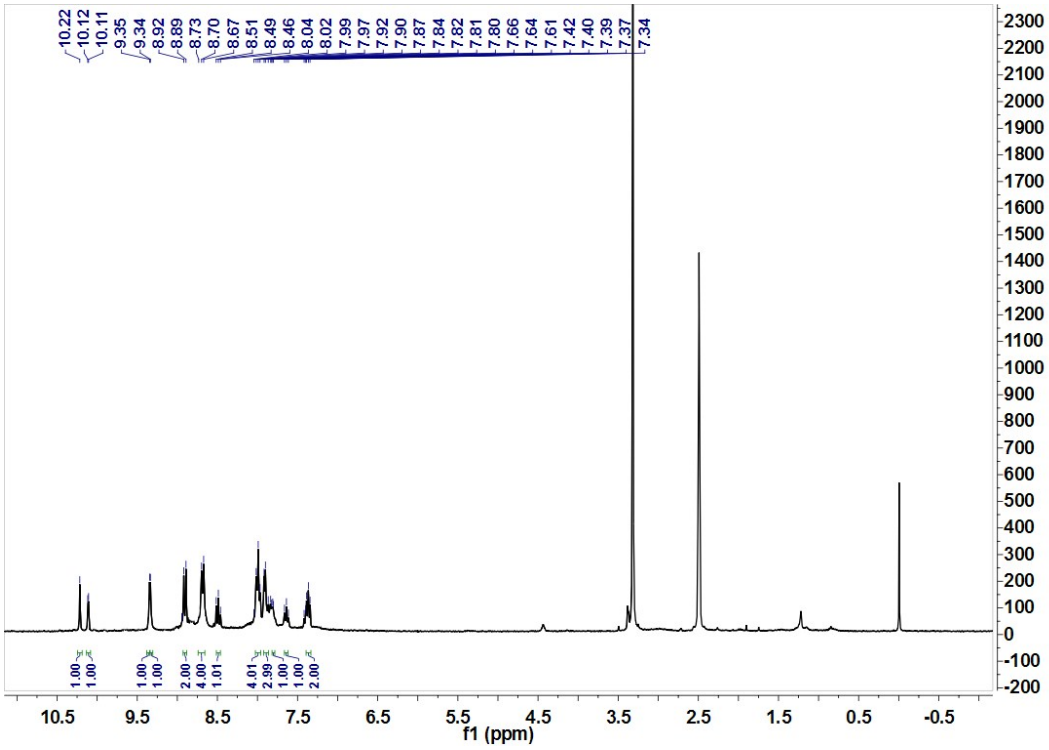

Figure S6 ^{1}H NMR spectrum (300 MHz, DMSO-d_6) spectrum of **Ru3**.

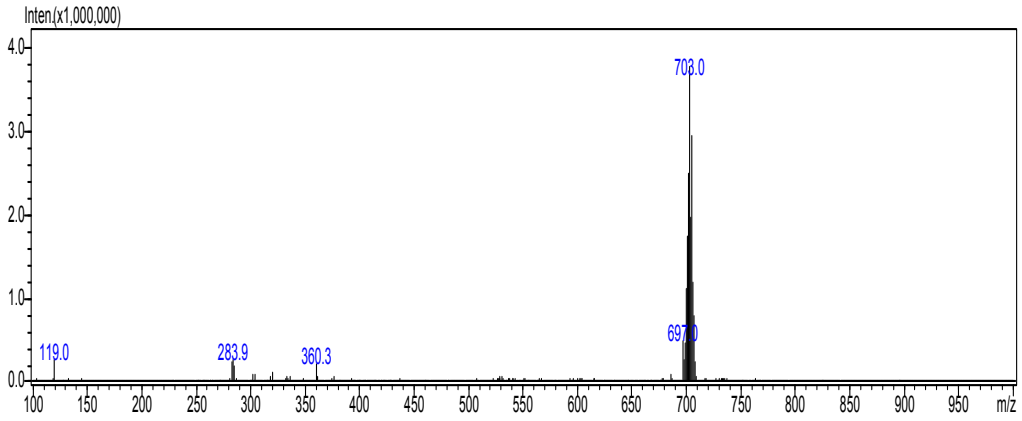

Figure S7 ES-MS (CH_3CN) spectrum of **Ru4**.

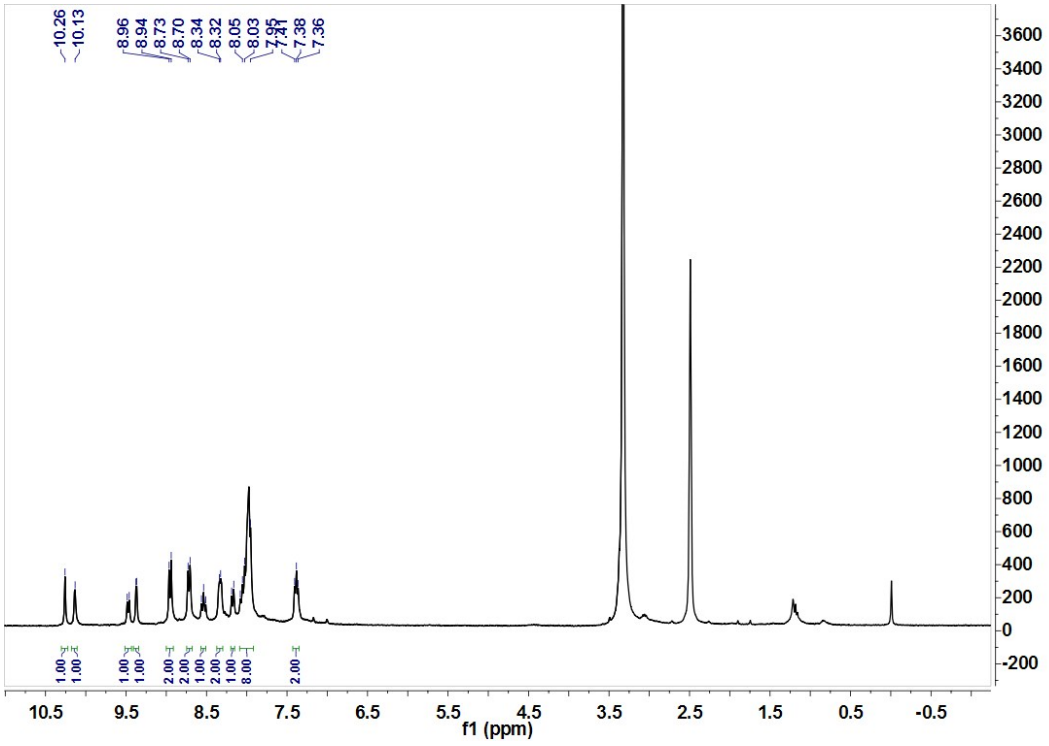

Figure S8 ^{1}H NMR spectrum (300 MHz, DMSO-d_6) spectrum of **Ru4**.

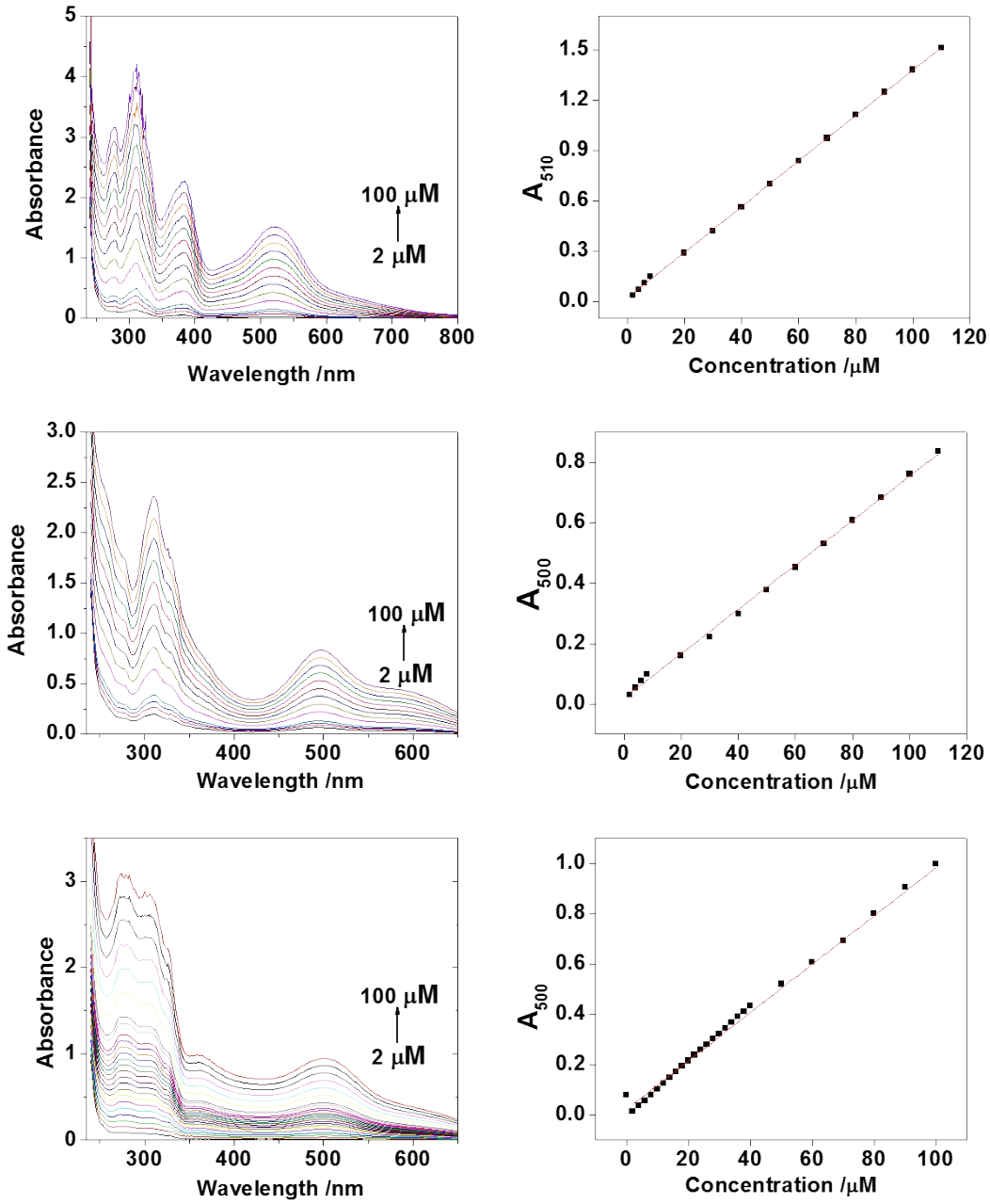

Figure S9 UV-visspectra of **Ru2-Ru4** by gradually increasing concentration in Tris-HCl buffer (5 mM Tris, 100 mM NaCl, pH = 7.4).

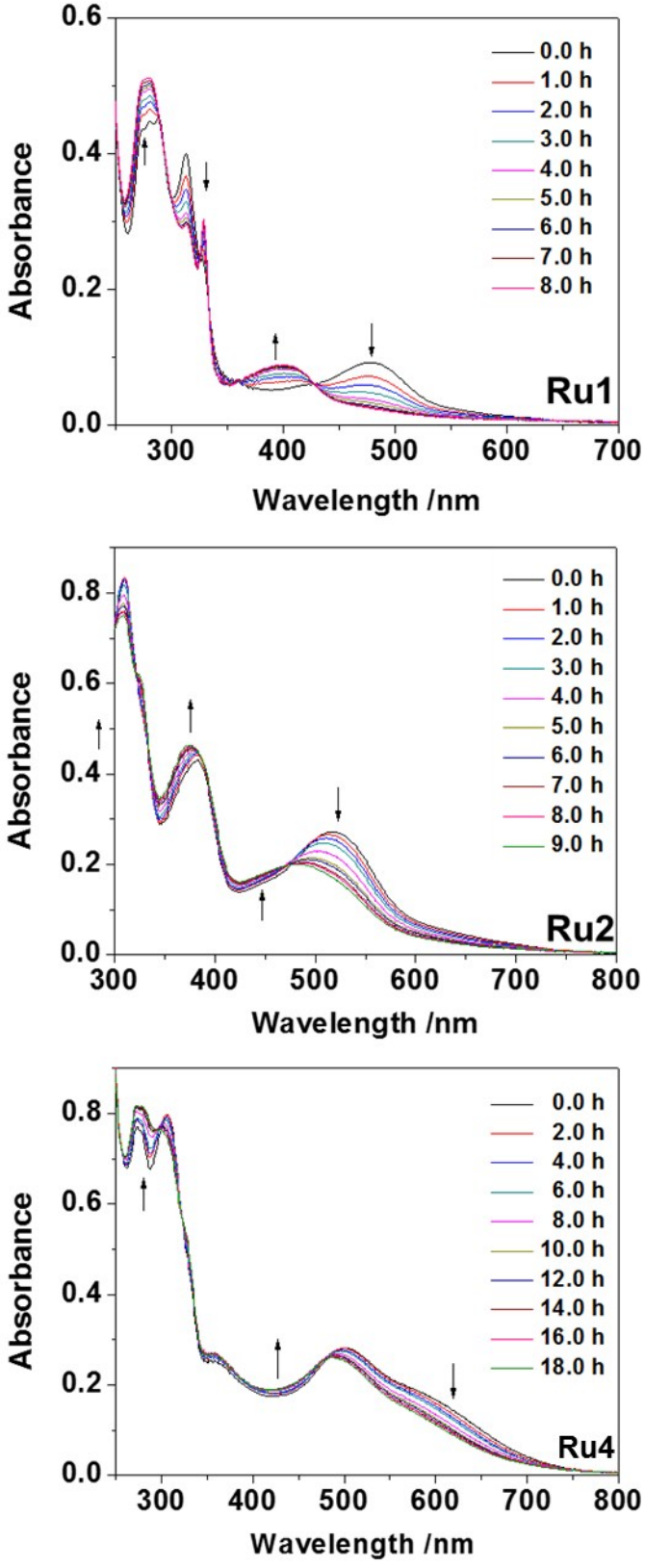

Figure S10 The UV–Visible spectral changes of **Ru1**, **Ru2** and **Ru4** (10 μM) in water at 37 °C measured at different time points. The arrows indicate the change of the absorption spectrum.

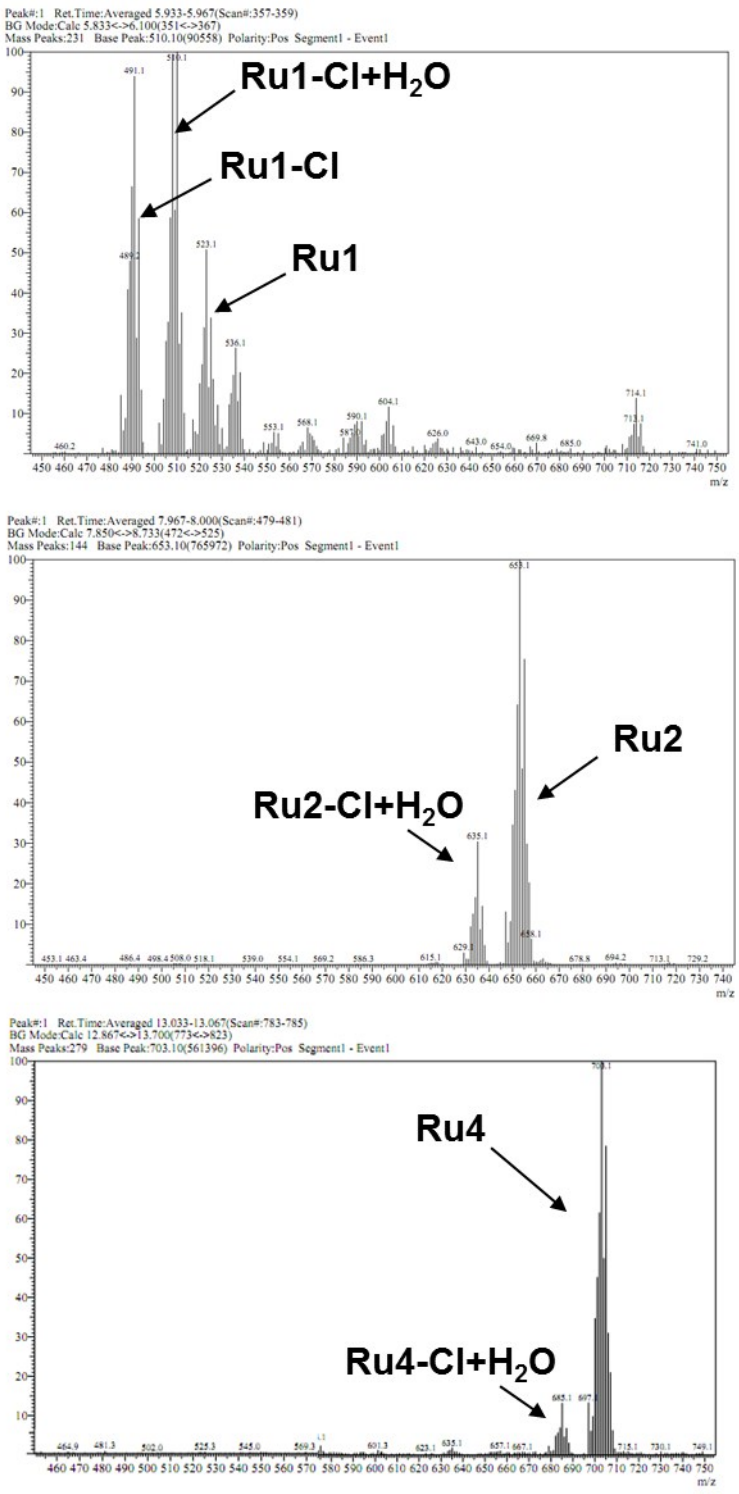

Figure 11 ES-MS spectrum of **Ru1**, **Ru2** and **Ru4** after hydrolysis.

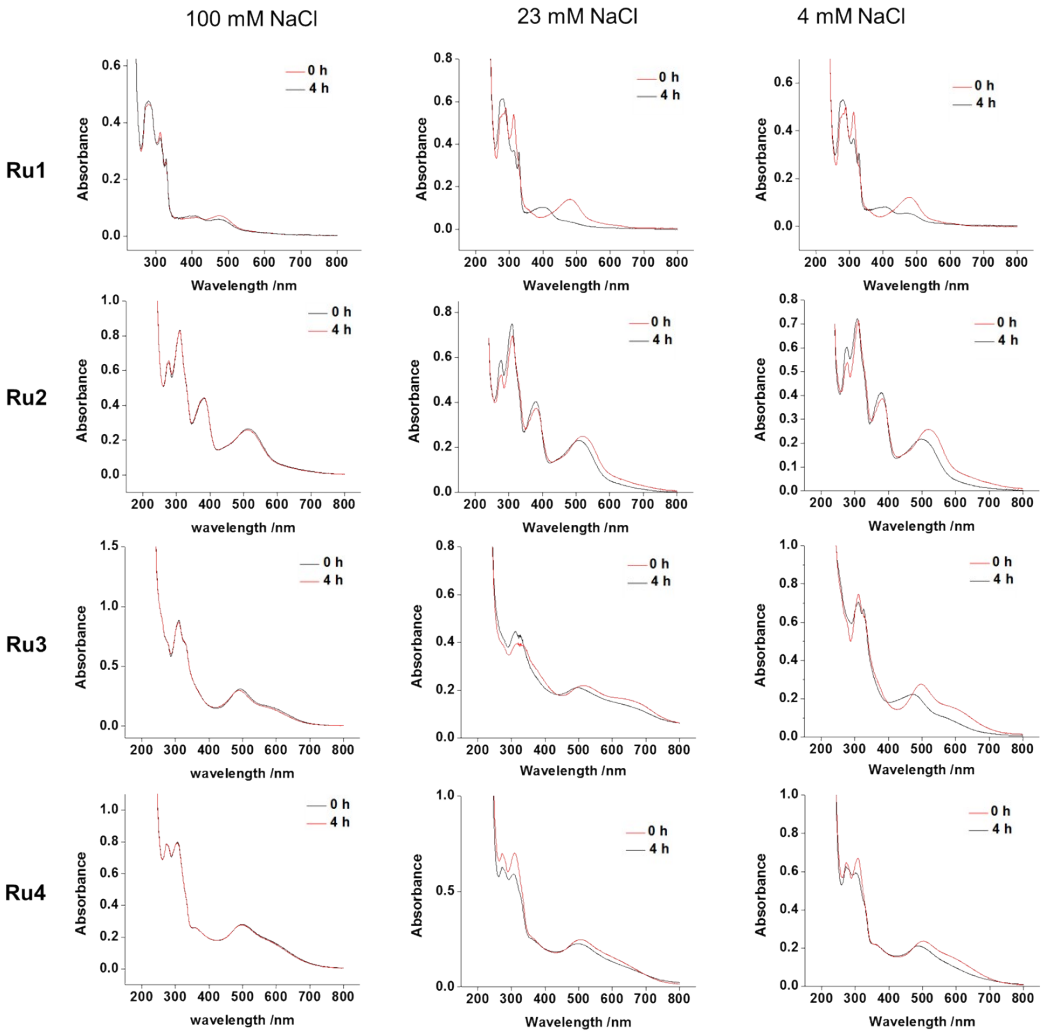

Figure S12 Aquation of **Ru1-Ru4** in present of different NaCl concentration detected by UV-vis spectra.

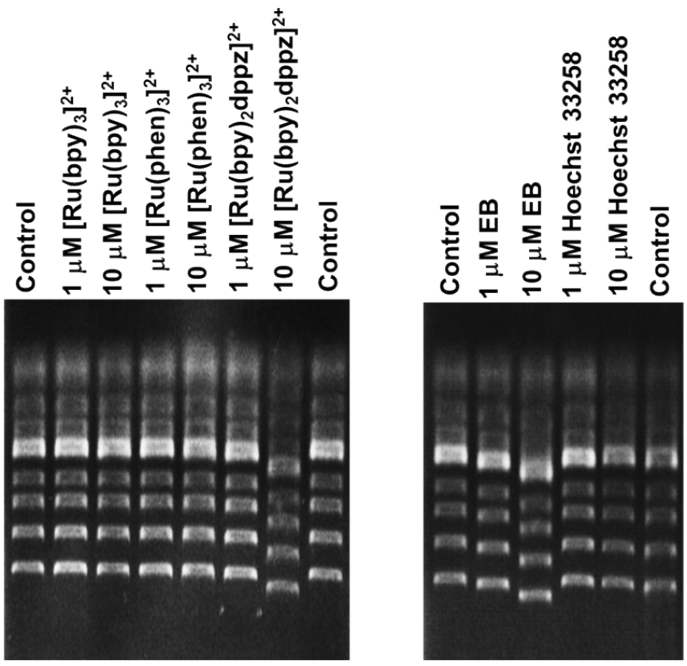

Figure 13 Gel electrophoresis of DL5000 DNA marker by diferent compound.

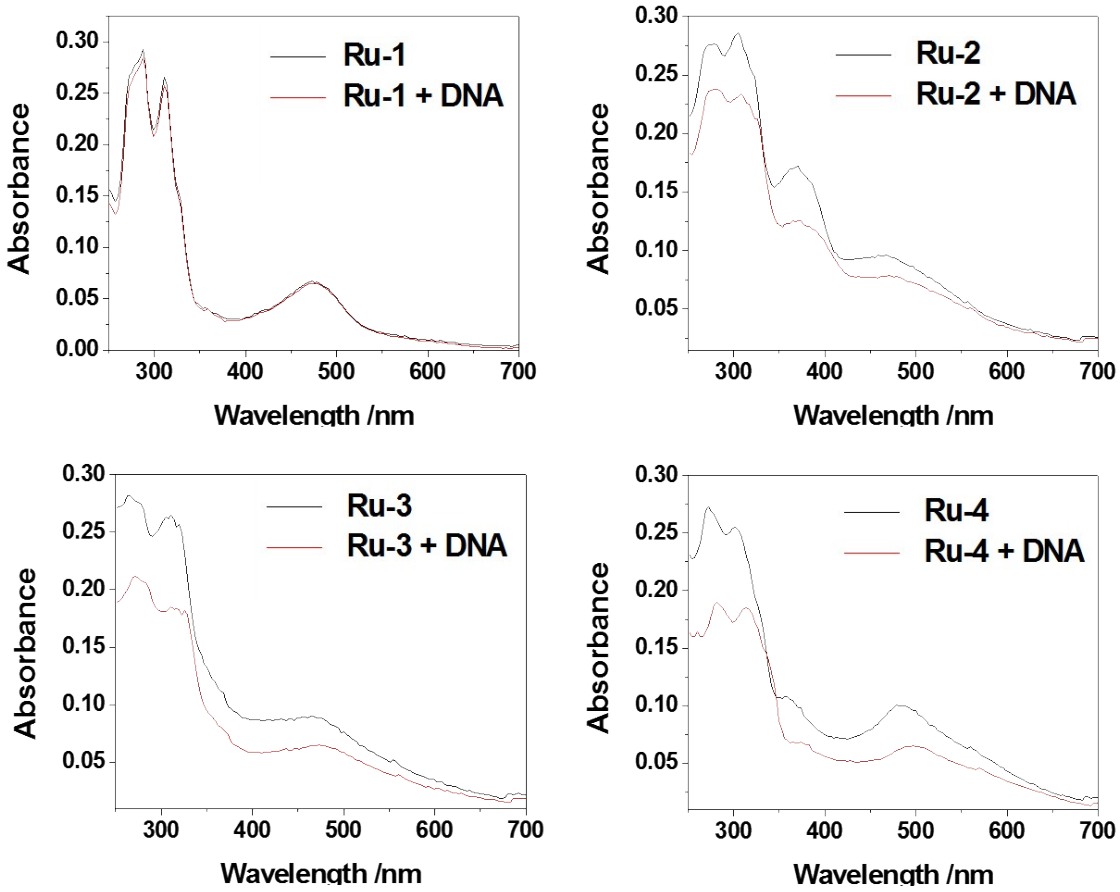

Figure 14 Change of UV-vis spectra of **Ru1-Ru4** after adding CT-DNA into the solution.

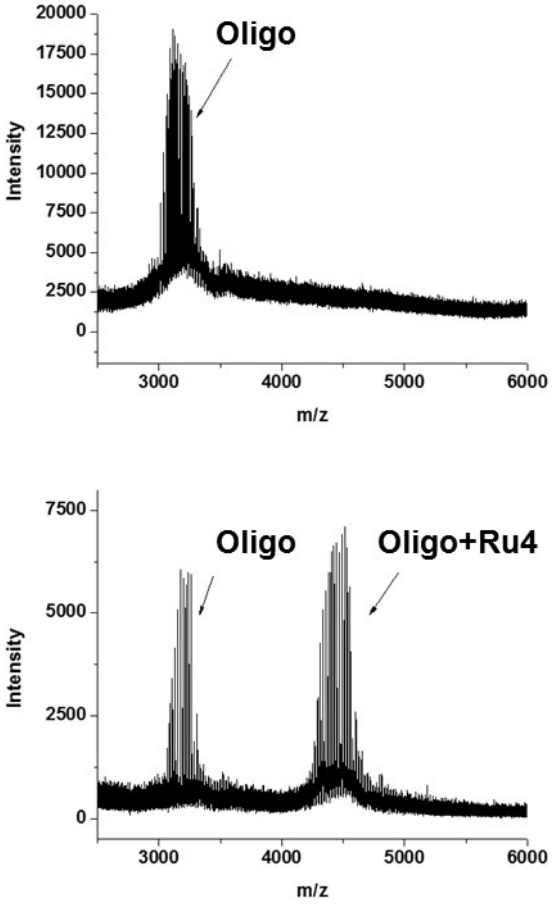

Figure S15 MALDI-TOF mass spectra of free oligonucleotides and oligonucleotides + **Ru4**.

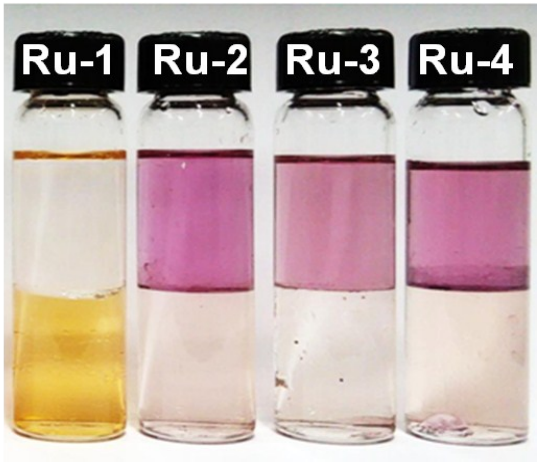

Figure S16 The distribuction of **Ru1-Ru4** in octanol/water solution.

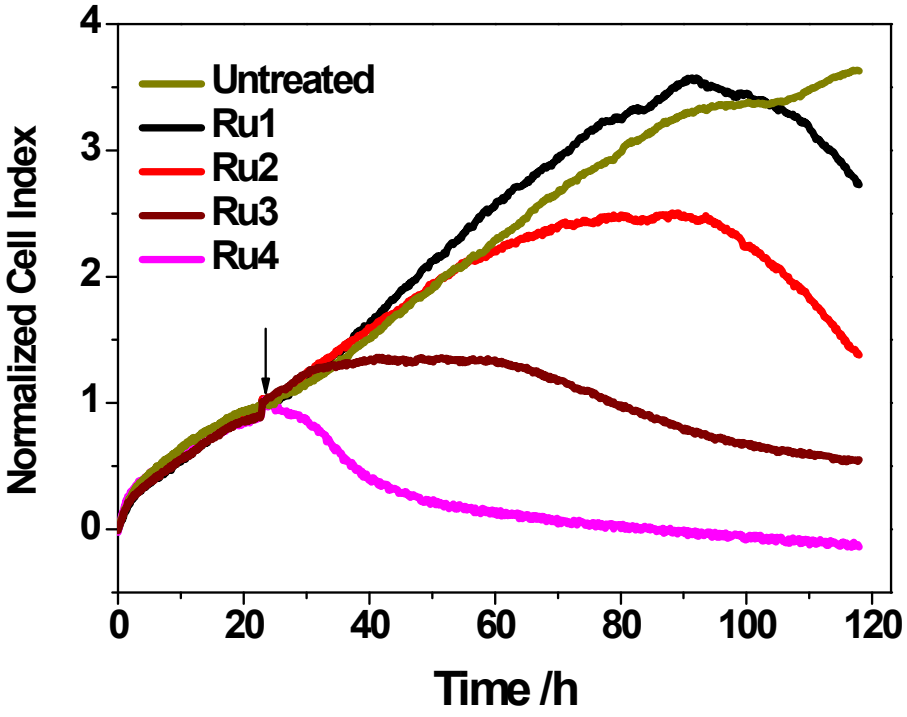

Figure S17 Kinetics of cytotoxicity responded for **Ru1-Ru4** (15 μM) in cells monitored by the xCELLigence System.

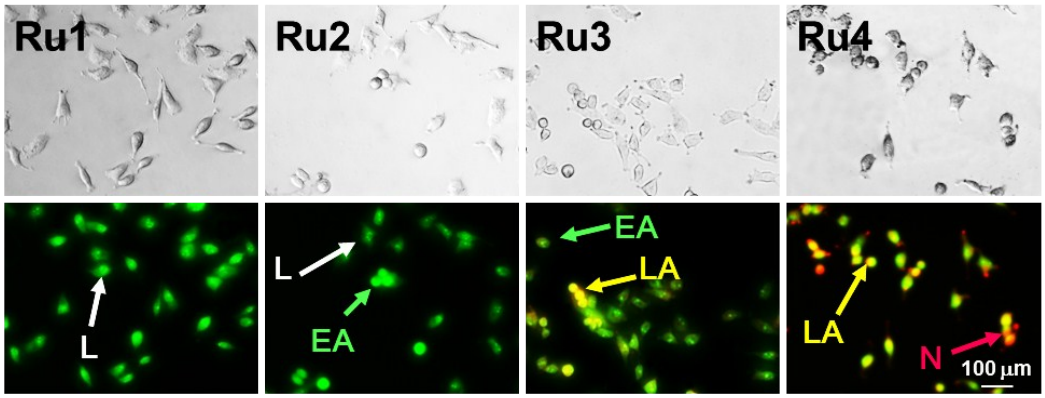

Figure 18 HeLa cells were stained by AO/EB and observed under a fluorescence microscope after 48 h drug exposure (15 μM). L: live cells; EA: early-stage apoptotic cells, LA: late-stage apoptotic cells, N: necrotic cells.

Table S1 Crystal data and structure details of **Ru3.**

Identification code	**Ru3**
Empirical formula	$C_{34}H_{22}Cl_2N_8O_4Ru$
Formula weight	778.56
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	8.5691(5)
b/Å	22.4491(13)
c/Å	16.5370(11)
α/°	90
β/°	104.962(2)
γ/°	90
Volume/Å^3	3073.3(3)
Z	4
ρ_{calc}g/cm^3	1.683
μ/mm^{-1}	0.740
F(000)	1568.0
Crystal size/mm^3	0.191 × 0.093 × 0.086
Radiation	MoKα (λ = 0.71073)
Range for data collection/	6.012 to 54.966
Index ranges	$-11 \leq h \leq 10$, $-29 \leq k \leq 29$, $-21 \leq l \leq 19$
Reflections collected	25278
Independent reflections	6926 [R_{int} = 0.0925, R_{sigma} = 0.0825]
Data/restraints/parameters	6926/0/442
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0458, wR_2 = 0.0952
Final R indexes [all data]	R_1 = 0.0837, wR_2 = 0.1210
Largest diff. peak/hole / e Å^{-3}	0.93/-0.65

Table S2 Bond Lengths for **Ru3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ru1	Cl1	2.4011(11)	C10	C11	1.464(6)
Ru1	N2	1.981(3)	C10	C9	1.390(6)
Ru1	N4	2.037(3)	C2	C1	1.402(6)
Ru1	N5	2.014(4)	C2	C3	1.336(7)
Ru1	N1	2.062(4)	C7	C6	1.389(6)
Ru1	N3	2.072(3)	C5	C6	1.479(5)
Cl2	O1	1.439(4)	C5	C4	1.375(6)
Cl2	O4	1.432(3)	C17	C16	1.378(6)
Cl2	O3	1.443(4)	C20	C18	1.468(6)
Cl2	O2	1.430(3)	N8	C21	1.360(5)
N2	C10	1.348(5)	C33	C34	1.412(7)
N2	C6	1.344(6)	C33	C32	1.380(6)
N4	C20	1.337(5)	C11	C12	1.392(5)
N4	N8	1.342(4)	C23	C22	1.448(6)
N5	C16	1.346(5)	C23	C24	1.420(7)
N5	C18	1.353(5)	C23	C28	1.430(6)
N6	C17	1.346(6)	C4	C3	1.403(6)
N6	C19	1.340(5)	C18	C19	1.390(6)
N1	C5	1.378(5)	C22	C21	1.394(6)
N1	C1	1.351(5)	C34	C21	1.456(6)
N3	C15	1.307(6)	C34	C29	1.400(6)
N3	C11	1.385(5)	C32	C31	1.391(7)
C14	C13	1.390(7)	C24	C25	1.351(7)
C14	C15	1.390(6)	C28	C27	1.389(7)
N7	C20	1.360(6)	C28	C29	1.475(7)
N7	C22	1.336(5)	C31	C30	1.368(7)
C8	C7	1.399(6)	C27	C26	1.377(7)
C8	C9	1.373(7)	C29	C30	1.398(6)
C13	C12	1.366(7)	C25	C26	1.387(7)

Table S3 Bond Angles for **Ru3**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N2	Ru1	Cl1	88.77(10)	N1	C1	C2	120.6(4)
N2	Ru1	N4	177.88(13)	N6	C17	C16	123.8(4)
N2	Ru1	N5	99.01(14)	N4	C20	N7	125.9(4)
N2	Ru1	N1	79.23(14)	N4	C20	C18	113.5(4)
N2	Ru1	N3	79.64(14)	N7	C20	C18	120.6(4)
N4	Ru1	Cl1	93.21(10)	N2	C6	C7	120.0(4)
N4	Ru1	N1	99.90(13)	N2	C6	C5	113.2(4)
N4	Ru1	N3	101.17(14)	C7	C6	C5	126.8(4)
N5	Ru1	Cl1	171.07(11)	N4	N8	C21	117.6(3)
N5	Ru1	N4	79.07(14)	C32	C33	C34	119.9(5)
N5	Ru1	N1	92.69(14)	N3	C15	C14	124.2(4)
N5	Ru1	N3	89.05(13)	N5	C16	C17	119.6(4)
N1	Ru1	Cl1	93.08(10)	N3	C11	C10	115.7(3)
N1	Ru1	N3	158.81(14)	N3	C11	C12	119.9(4)
N3	Ru1	Cl1	88.03(10)	C12	C11	C10	124.4(4)
O1	Cl2	O3	110.2(3)	C24	C23	C22	121.9(4)
O4	Cl2	O1	109.4(2)	C24	C23	C28	118.4(4)
O4	Cl2	O3	109.2(3)	C28	C23	C22	119.7(4)
O2	Cl2	O1	110.0(2)	C5	C4	C3	119.1(5)
O2	Cl2	O4	109.6(2)	N5	C18	C20	115.3(4)
O2	Cl2	O3	108.3(2)	N5	C18	C19	120.6(4)
C10	N2	Ru1	118.7(3)	C19	C18	C20	124.0(4)
C6	N2	Ru1	118.8(2)	C8	C9	C10	119.1(4)
C6	N2	C10	122.2(4)	N7	C22	C23	119.2(4)
C20	N4	Ru1	116.2(3)	N7	C22	C21	121.2(4)
C20	N4	N8	119.2(3)	C21	C22	C23	119.6(4)
N8	N4	Ru1	124.6(3)	C13	C12	C11	120.4(4)
C16	N5	Ru1	126.7(3)	N6	C19	C18	122.1(5)
C16	N5	C18	118.0(4)	C33	C34	C21	121.0(4)
C18	N5	Ru1	115.2(3)	C29	C34	C33	120.8(4)
C19	N6	C17	115.8(4)	C29	C34	C21	118.3(4)
C5	N1	Ru1	114.1(2)	C33	C32	C31	119.1(5)
C1	N1	Ru1	126.7(3)	N8	C21	C22	121.3(4)
C1	N1	C5	119.0(4)	N8	C21	C34	116.4(4)
C15	N3	Ru1	128.9(3)	C22	C21	C34	122.4(4)
C15	N3	C11	118.5(4)	C25	C24	C23	121.4(4)
C11	N3	Ru1	112.6(3)	C23	C28	C29	119.2(4)

C15	C14	C13	117.7(5)	C27	C28	C23	118.2(5)
C22	N7	C20	114.6(4)	C27	C28	C29	122.6(4)
C9	C8	C7	120.4(4)	C30	C31	C32	121.3(4)
C12	C13	C14	119.2(4)	C26	C27	C28	121.5(4)
N2	C10	C11	113.2(4)	C34	C29	C28	120.7(4)
N2	C10	C9	119.7(4)	C30	C29	C34	117.6(4)
C9	C10	C11	127.1(4)	C30	C29	C28	121.6(4)
C3	C2	C1	120.6(4)	C2	C3	C4	119.6(5)
C6	C7	C8	118.4(4)	C24	C25	C26	120.1(5)
N1	C5	C6	114.3(4)	C31	C30	C29	121.3(5)
C4	C5	N1	121.2(4)	C27	C26	C25	120.4(5)
C4	C5	C6	124.4(4)				