Synthesis, Structure and Antiproliferative Activity of Ruthenium (II) Arene Complexes of Indenoisoquinoline Derivatives

Nathalie Wambang,[†,‡] Nadège Schifano-Faux,[ξ] Alain Martoriati,[#] Natacha Henry,[†] Brigitte Baldeyrou,[§] Christine Bal-Mahieu,[§] Till Bousquet,[†] Sylvain Pellegrini,[†] Samuel Meignan,[§] Katia Cailliau,[#] Jean-François Goossens,[ξ] Jean-François Bodart,[#] Peter T. Ndifon,[‡] and Lydie Pélinski[†,*]

[†] Univ. Lille, CNRS, ENSCL, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France

[‡] Univ. Yaoundé 1, Laboratoire de Chimie de Coordination, BP 812, Yaoundé, Cameroun

[ξ] Univ. Lille, EA 7365 - GRITA - Groupe de Recherche sur les formes Injectables et les Technologies Associées, F-59000 Lille, France

[#] Univ. Lille, CNRS, UMR 8576 - UGSF - Unité de Glycobiologie Structurale et Fonctionnelle, F-59000 Lille, France

[§] Univ. Lille, Inserm, U908 - CPAC - Cell Plasticity and Cancer, F-59000 Lille, France

Table of Contents

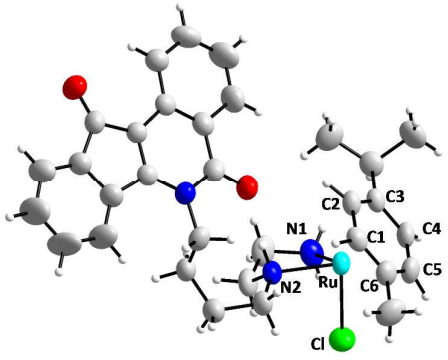

Figure S1. Molecular structure of Ru-complex 9.

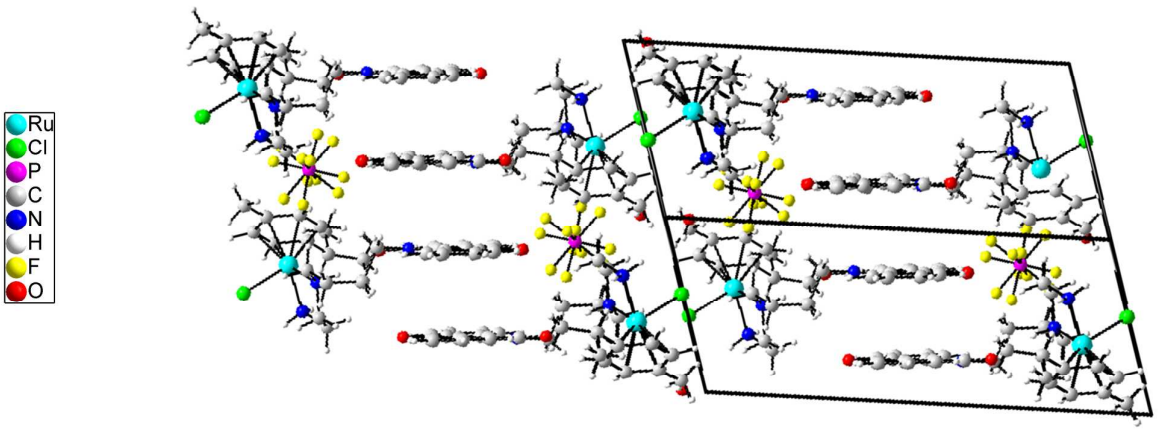

Figure S2. Packing structure of Ru-complex **9** (H atoms were omitted for clarity).

Table S1. Crystal data and structure refinement for Ru-Complex **9**.

Empirical formula	$C_{32}H_{38}ClF_6N_3O_{2.5}PRu$
Formula weight	786.14
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	8.0477(4)
b/Å	12.1034(6)
c/Å	18.7685(10)
α/°	71.477(3)
β/°	79.560(3)
γ/°	74.539(3)
Volume/Å^3	1661.36(15)
Z	2
ρ_{calc}g/cm^3	1.572
μ/mm^{-1}	0.670
F(000)	802.0
Crystal size/mm^3	0.30 × 0.05 × 0.02
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.642 to 53.088
Index ranges	-10 ≤ h ≤ 10, -15 ≤ k ≤ 15, -23 ≤ l ≤ 23
Reflections collected	38112
Independent reflections	6806 [R_{int} = 0.0871, R_{sigma} = 0.0878]
Data/restraints/parameters	6806/0/485
Goodness-of-fit on F^2	1.014
Final R indexes [I>=2σ (I)]	R_1 = 0.0554, wR_2 = 0.1104
Final R indexes [all data]	R_1 = 0.1117, wR_2 = 0.1294
Largest diff. peak/hole / e Å^{-3}	1.06/-0.46

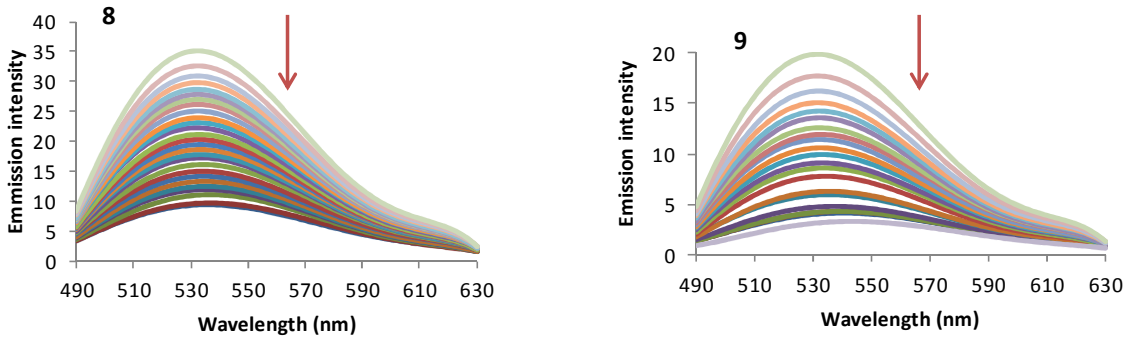

Figure S3. Emission spectra of EB bound to DNA in the presence of the compounds **8** and **9**. Arrow indicates that the emission changes upon increasing compound concentration.

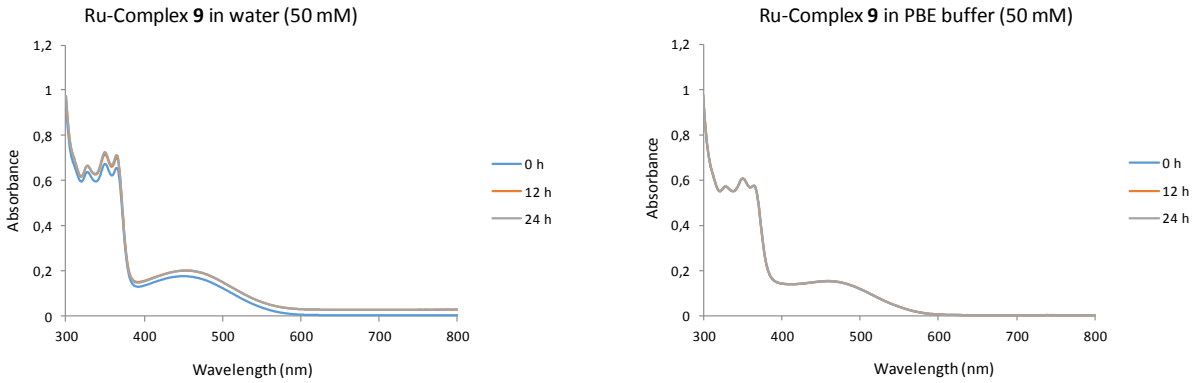

Figure S4. UV-Vis spectra for complex **9** in water and in PBE buffer at 25°C. The UV-Vis profiles were monitored over 24 hours.

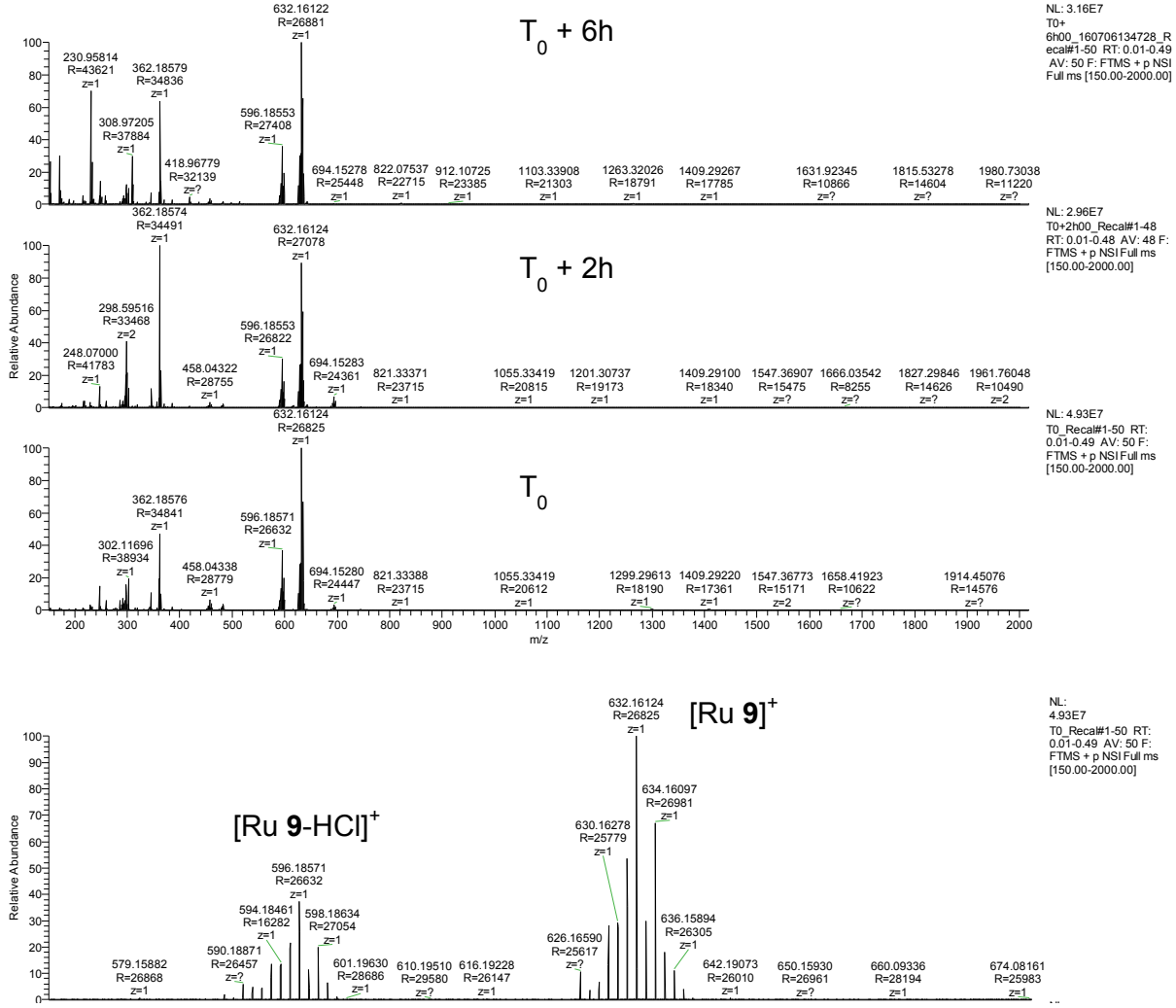

Figure S5. ESI-MS for complex **9** in water.

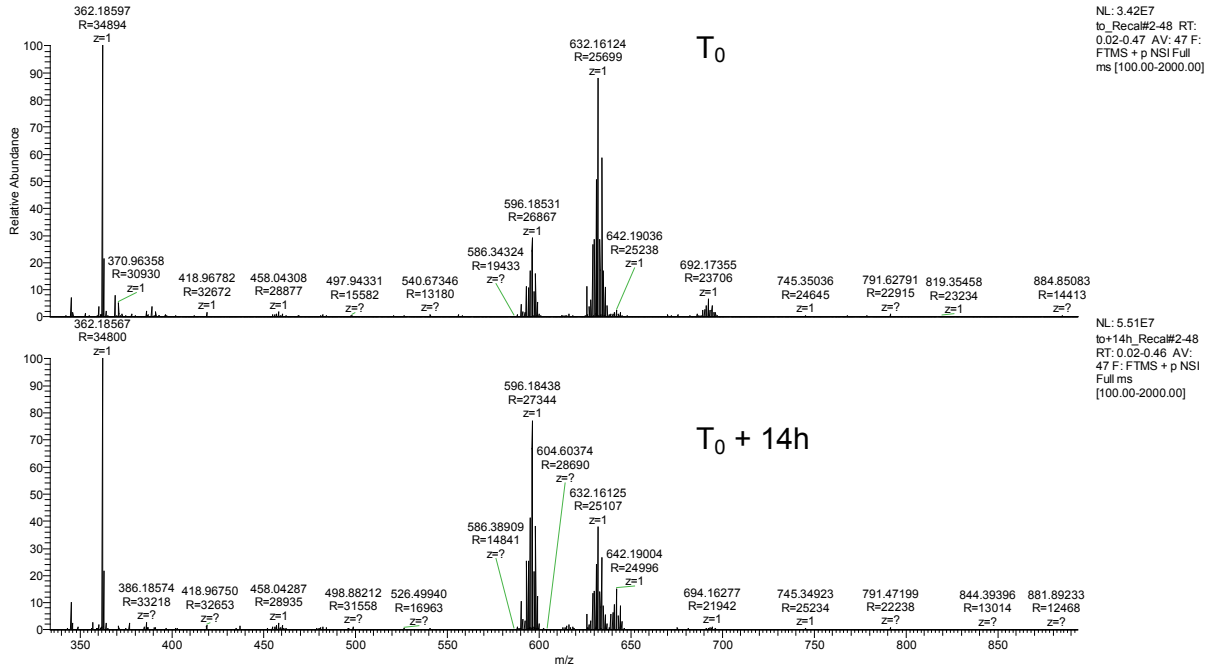

Figure S6. ESI-MS for complex **9** at pH = 2.7 in 0.1% Formic acid.

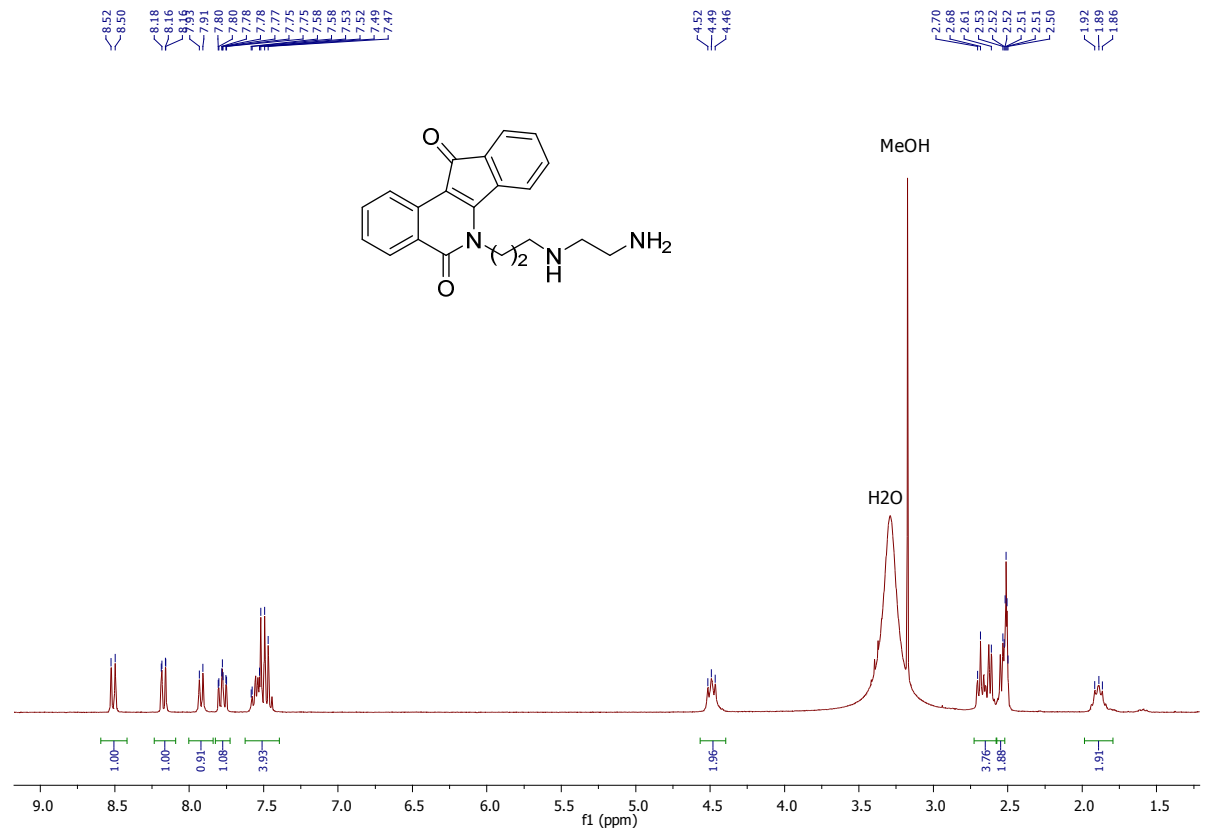

Figure S7. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound **11**

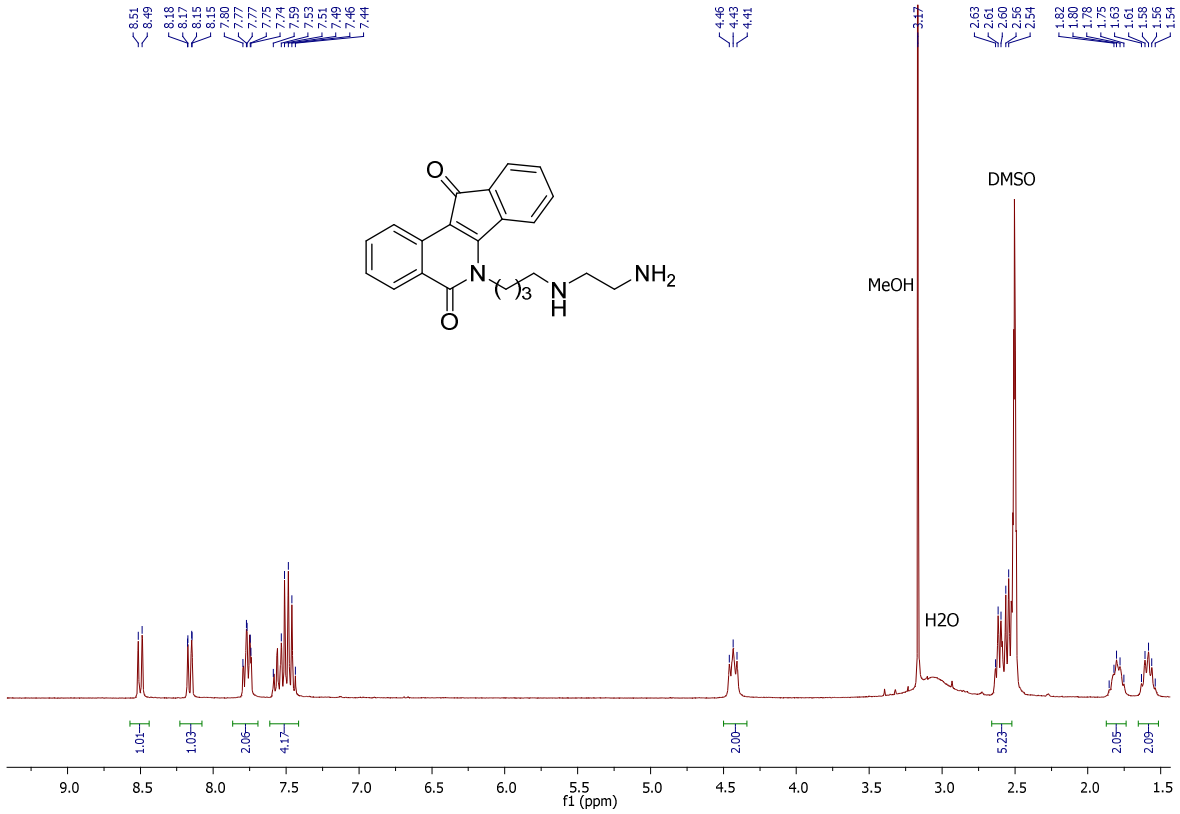

Figure S8. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of compound **12**

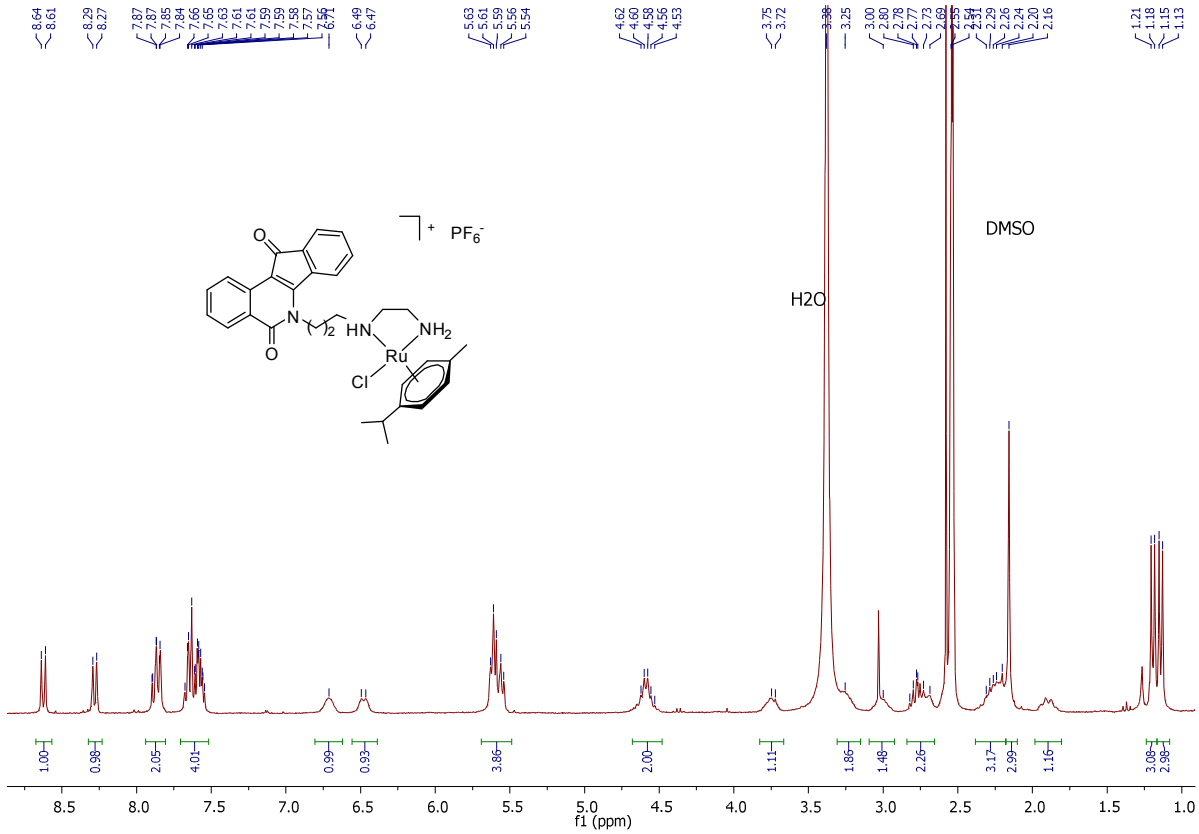

Figure S9. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of Ru-complex **8**

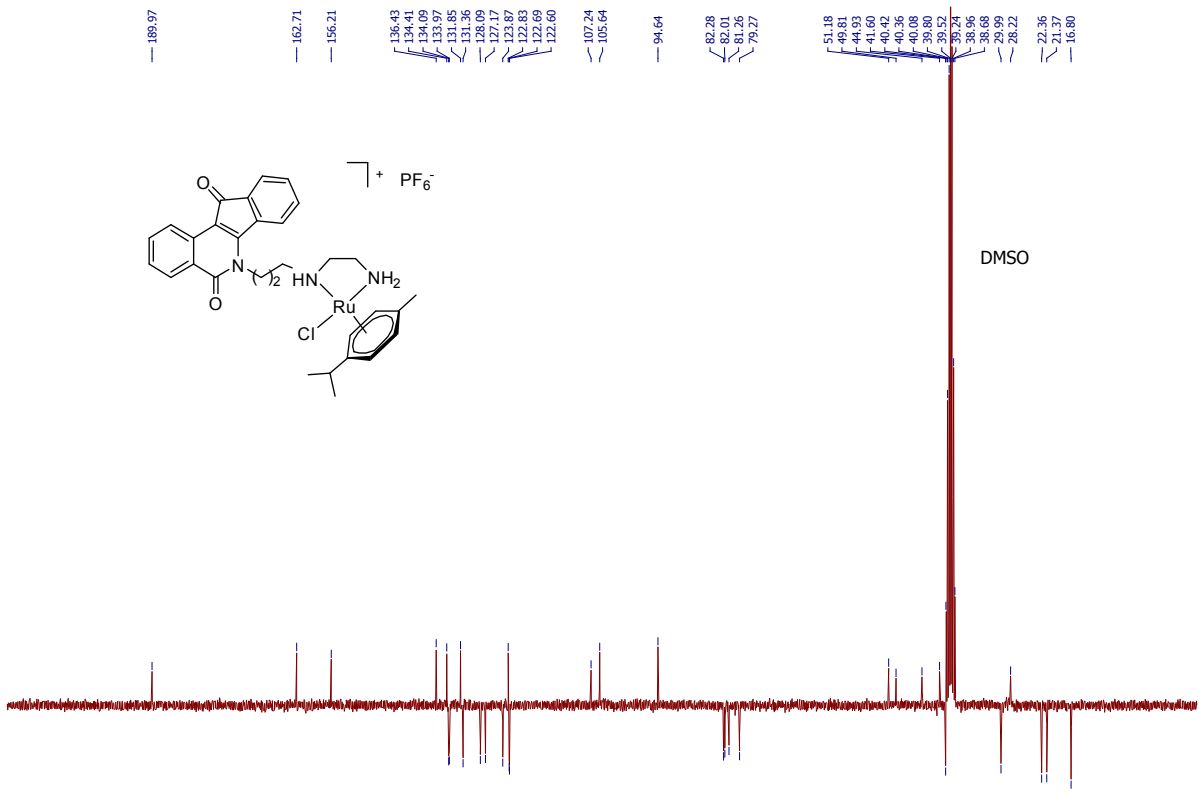

Figure S10. ^{13}C NMR spectrum (75.5 MHz, DMSO-d6) of Ru-Complex **8**

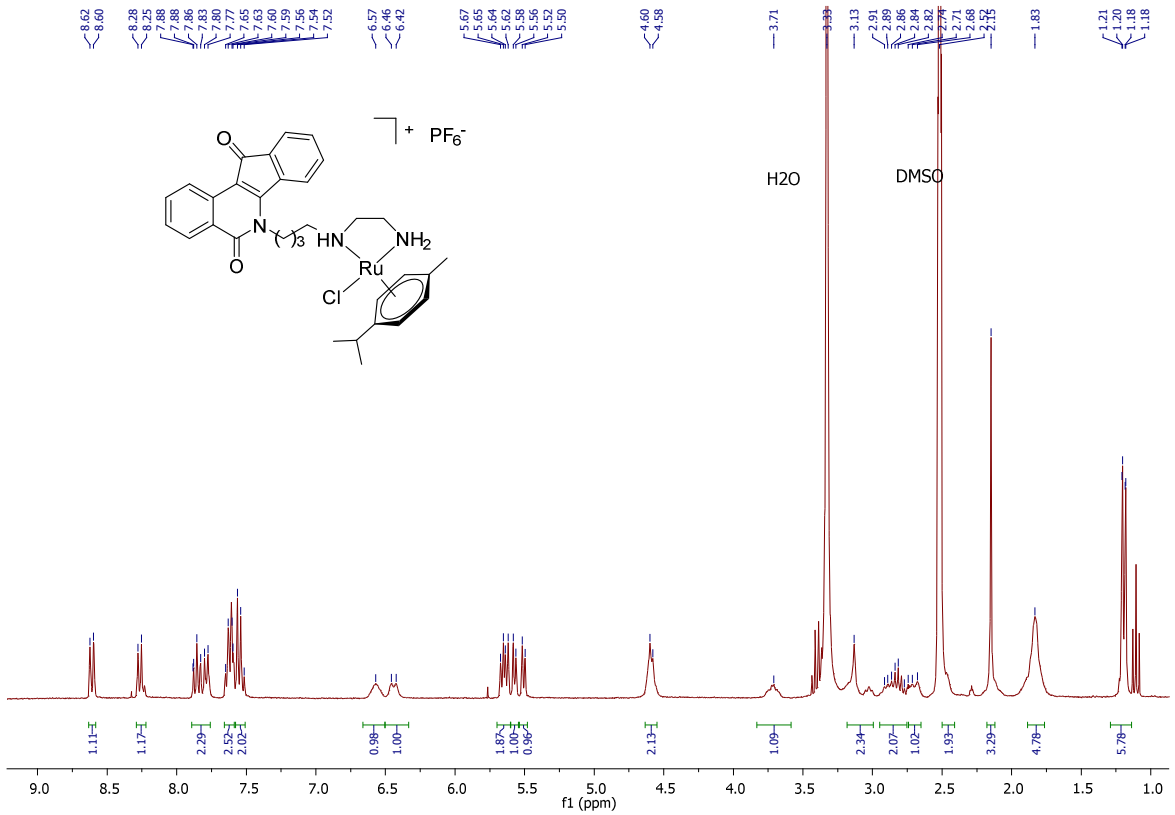

Figure S11. ^{1}H NMR spectrum (300 MHz, DMSO-d6) of Ru-Complex **9**

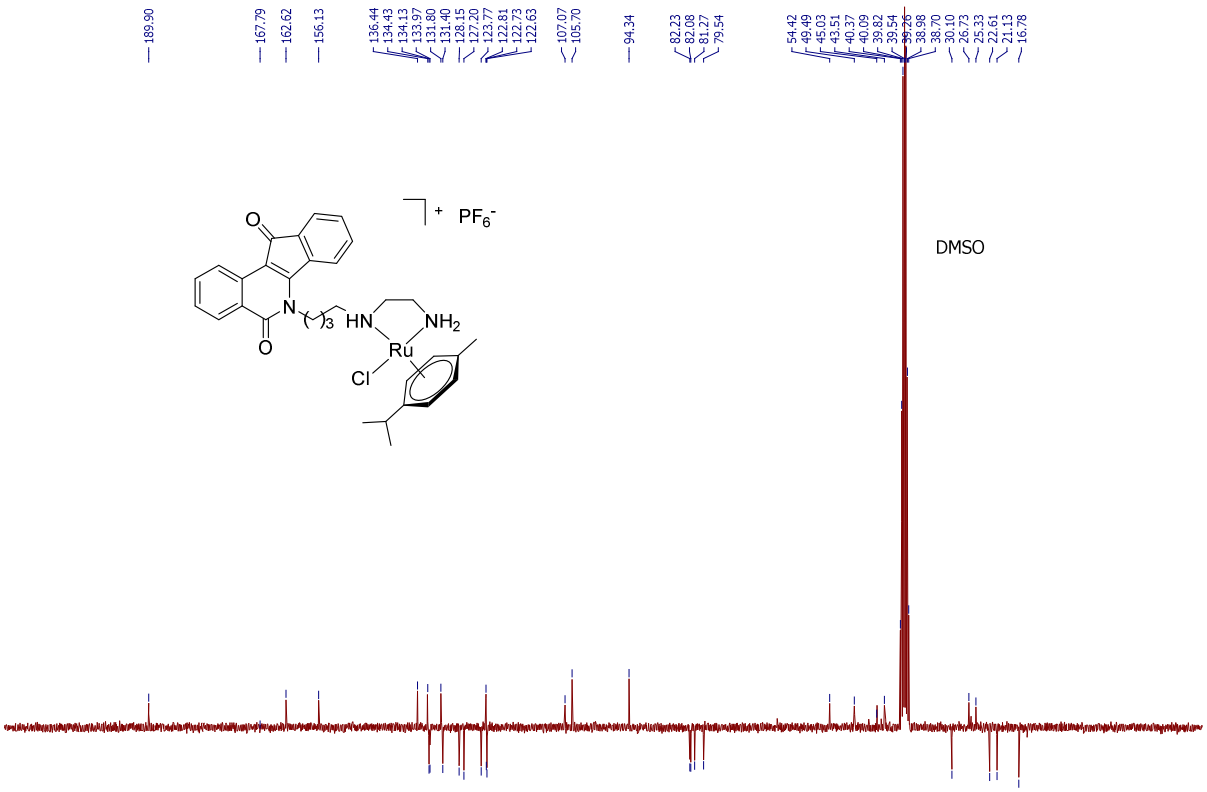

Figure S12. ^{13}C NMR spectrum (75.5 MHz, DMSO-d6) of Ru-Complex **9**