

Synthesis and Analysis of the Anticancer Activity of Ru(II) Complexes

Incorporating 2-Hydroxymethylidene-indene-1,3-diones Ligands

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Table S1. Human ovarian cancer cell lines to be used for the *in vitro* analysis of the compounds biological activity

Cancer Type	Human Cell line designation	Oncogenes	Special Characteristics
Ovarian Adenocarcinoma	SK-OV-3 (SKOV-3)		Tumor Necrosis Factor; Diphtheria Toxin; Cis-platinum and Adriamycin resistant
Epithelial Ovarian Adenocarcinoma	NIH:OVCAR-5		Cisplatin resistant
Ovarian Carcinoma	UWB1.289	p53 + BRCA1 -	Estrogen/Progesterone receptor negative
Ovarian Carcinoma	UWB1.289+BRCA1	p53 + BRCA1 +	Estrogen/Progesterone receptor negative

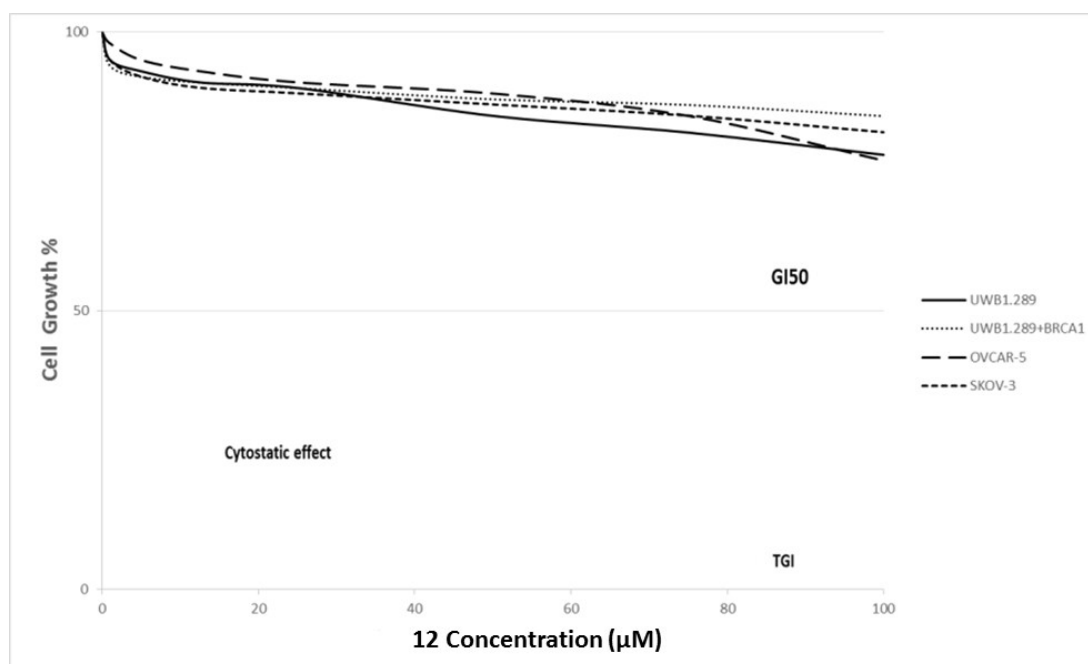


Figure S1

Table S2. Growth inhibition/cytostatic (GI_{50} and TGI μM) and cytocidal/cytotoxic (IC_{50} μM) anticancer effects induced by **12** on OVCAR-5, SKOV-3, UWB1.289 and UWB1.289+BRCA1 human cancer ovarian cell lines

Human ovarian cancer cell	12		
	GI_{50}	TGI	IC_{50}
OVCAR-5	>100	>100	>100
SKOV-3	>100	>100	>100
UWB1.289	>100	>100	>100
UWB1.289+BRCA1	>100	>100	>100

Figure S2. Growth inhibition/cytostatic (GI_{50} and TGI μM) and cytocidal/cytotoxic (IC_{50} μM) anticancer effects induced by **cisplatin** on SKOV-3, and UWB1.289+BRCA1 human cancer ovarian cell lines

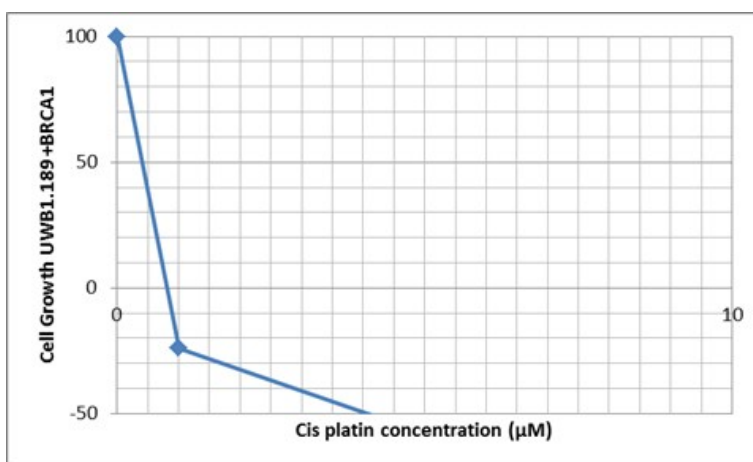
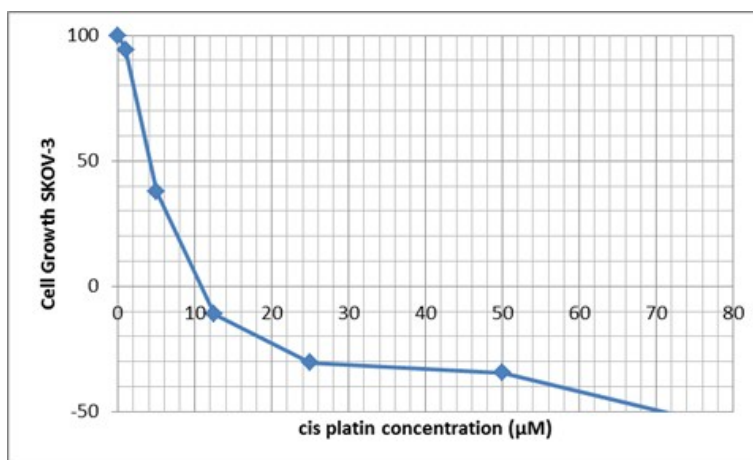


Table S3. Crystallographic and refinement details.

Structure	11a	11c	11d·0.25(CH₂Cl₂)	13a·0.5(CH₂Cl₂)
Formula	C ₂₆ H ₂₉ ClO ₄ Ru	C ₂₄ H ₂₅ ClO ₄ Ru	C ₉₇ H ₉₄ Cl ₆ O ₁₆ Ru ₄	C ₅₉ H ₅₄ Cl ₄ N ₂ O ₆ Ru ₂
Fw	542.04	513.98	2132.80	1231.04
T (K)	295(2)	295(2)	295(2)	295(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	P -1	P -1	P -1	P -1
Crystal size (mm)	0.36 × 0.24 × 0.08	0.23 × 0.19 × 0.08	0.24 × 0.11 × 0.09	0.21 × 0.15 × 0.13
Unit cell lengths, a, b, c (Å)	9.3961(10), 14.3704(15), 18.598(2)	7.7108(3), 12.7742(4), 12.7925(3)	12.1381(5), 12.9005(5), 15.6604 (6)	11.3428(7), 11.6272(8), 12.1199(11)
Unit cell angles, α, β, γ (°)	99.204(5), 91.117(5), 94.615(5)	64.6825(15), 74.5158(17), 83.476(2)	104.149(2), 90.794(2), 107.642(2)	65.746(6), 76.952(5), 80.911(4)
Unit cell volume (Å ³)	2469.4(3)	1097.68(3)	2255.72(9)	1415.89 (13)
Z	4	2	1	1
T _{min} , T _{max}	0.83, 0.94	0.85, 0.93	0.91, 0.92	0.89, 0.90
Calculated density (g cm ⁻³)	1.458	1.555	1.570	1.444
μ (mm ⁻¹)	0.77	0.864	0.90	0.77
F (000)	1112	524	1082	626
θ range (°)	1.110 - 25.533	1.764 - 27.212	1.347 - 27.289	1.848 – 25.811
Completeness to θ _{max}	98.3%	99.5%	99.1%	95.9%
h, k, l min / h, k, l max	-11, -17, -22 / 11, 16, 22	-9, -16, -16 / 9, 16, 16	-15, -16, -20 / 15, 16, 20	-13, -14, -14 / 13, 14, 14
No. of measured, independent, observed [I > 2.0σ(I)] reflections	32640, 9088, 6480	18999, 4878, 3692	62962, 9943, 5792	36116, 5232, 3500
no. of parameters / restraints	572 / 26	271 / 0	568 / 0	343 / 0
R _{int}	0.025	0.0103	0.041	0.038
Goodness of fit on F ²	1.0001	1.0000	0.9999	1.0000
R indices [I > 2σ(I)]	R1 = 0.0386, wR2 = 0.0895	R1 = 0.0219, wR2 = 0.0469	R1 = 0.0451, wR2 = 0.0786	R1 = 0.0537, wR2 = 0.1469
R indices (all data)	R1 = 0.0624, wR2 = 0.0988	R1 = 0.0370, wR2 = 0.0500	R1 = 0.0969, wR2 = 0.0834	R1 = 0.0882, wR2 = 0.1646

Figure S3. 11a d_6 -DMSO adduct

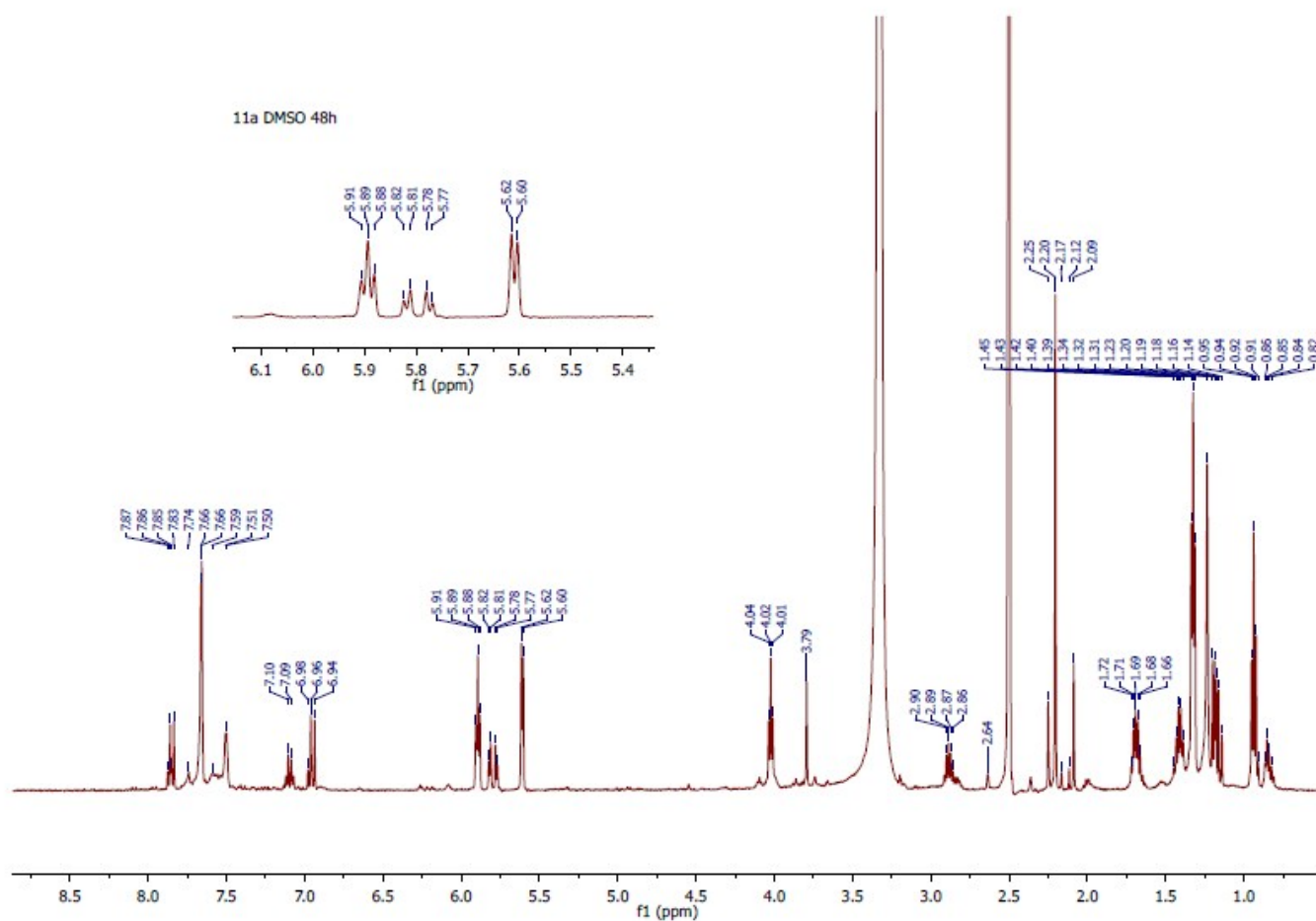
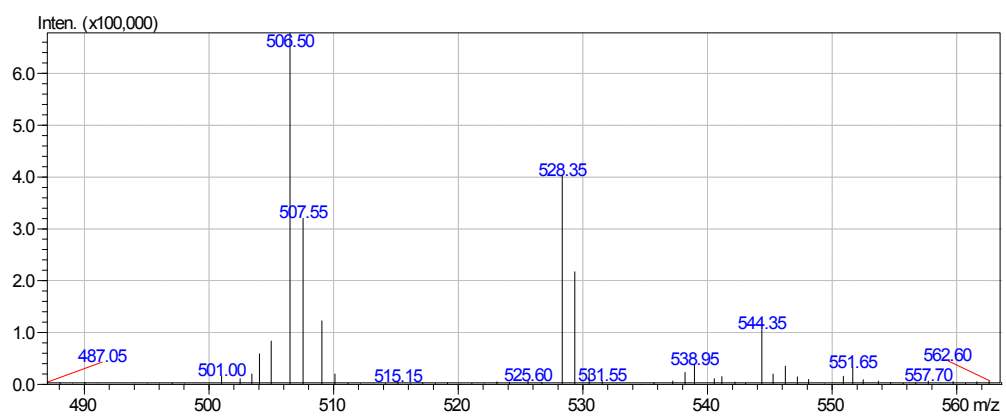


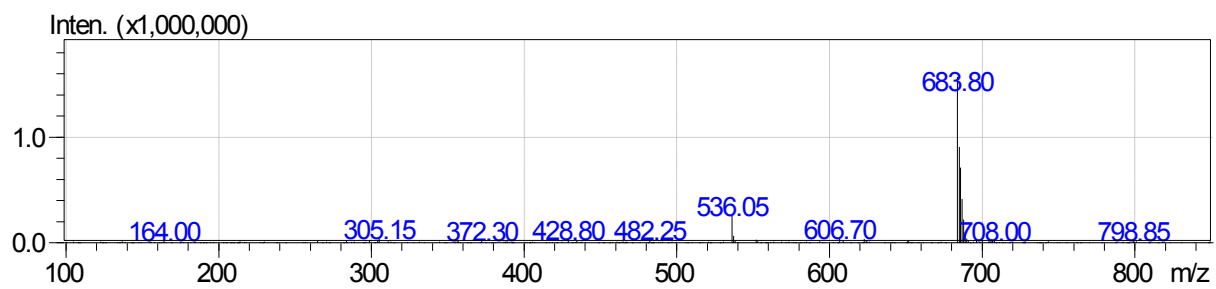
Figure S4. ESI-MS analysis-Hydrolysis studies



$[M-Cl]^+ = 507.5$

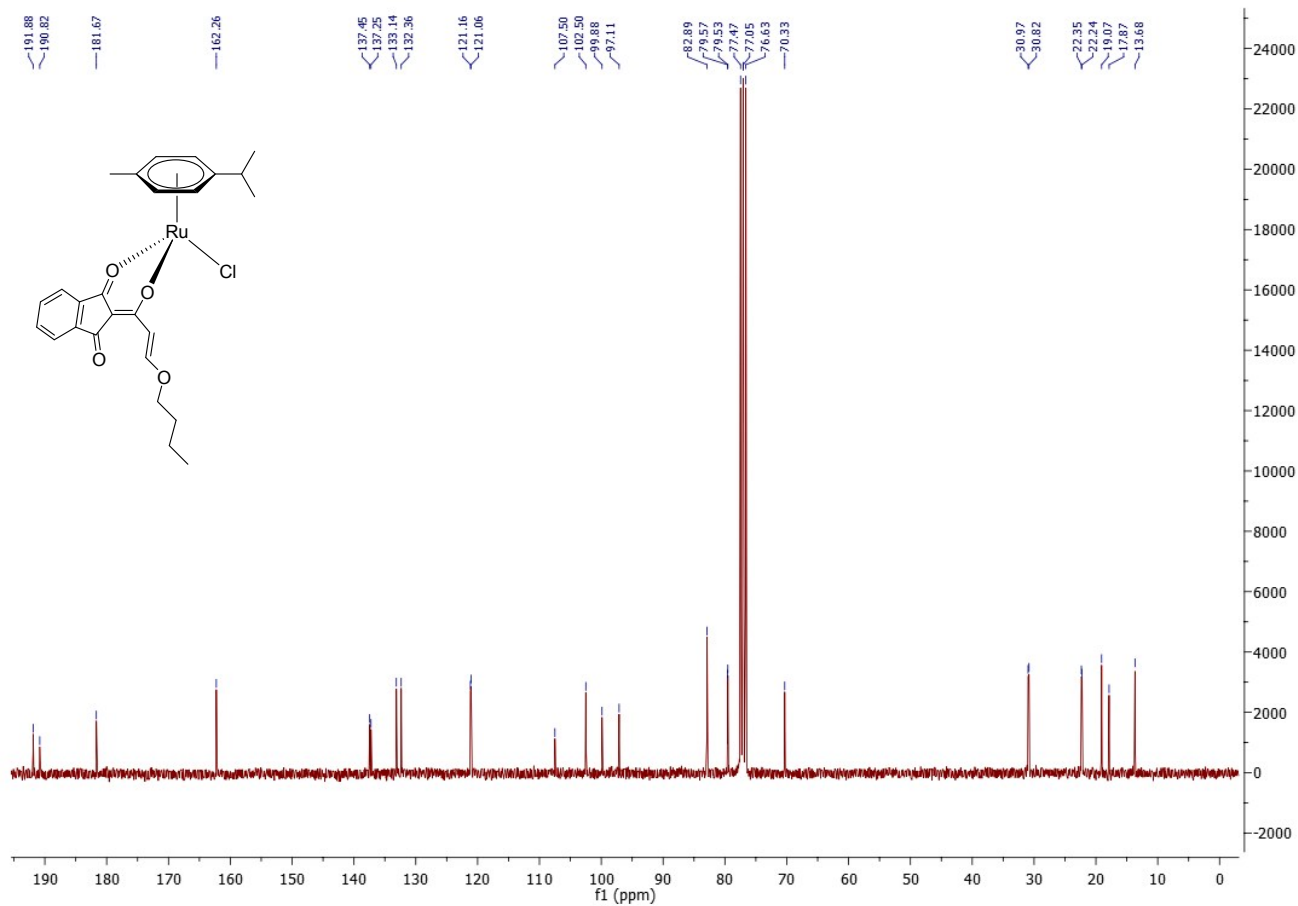
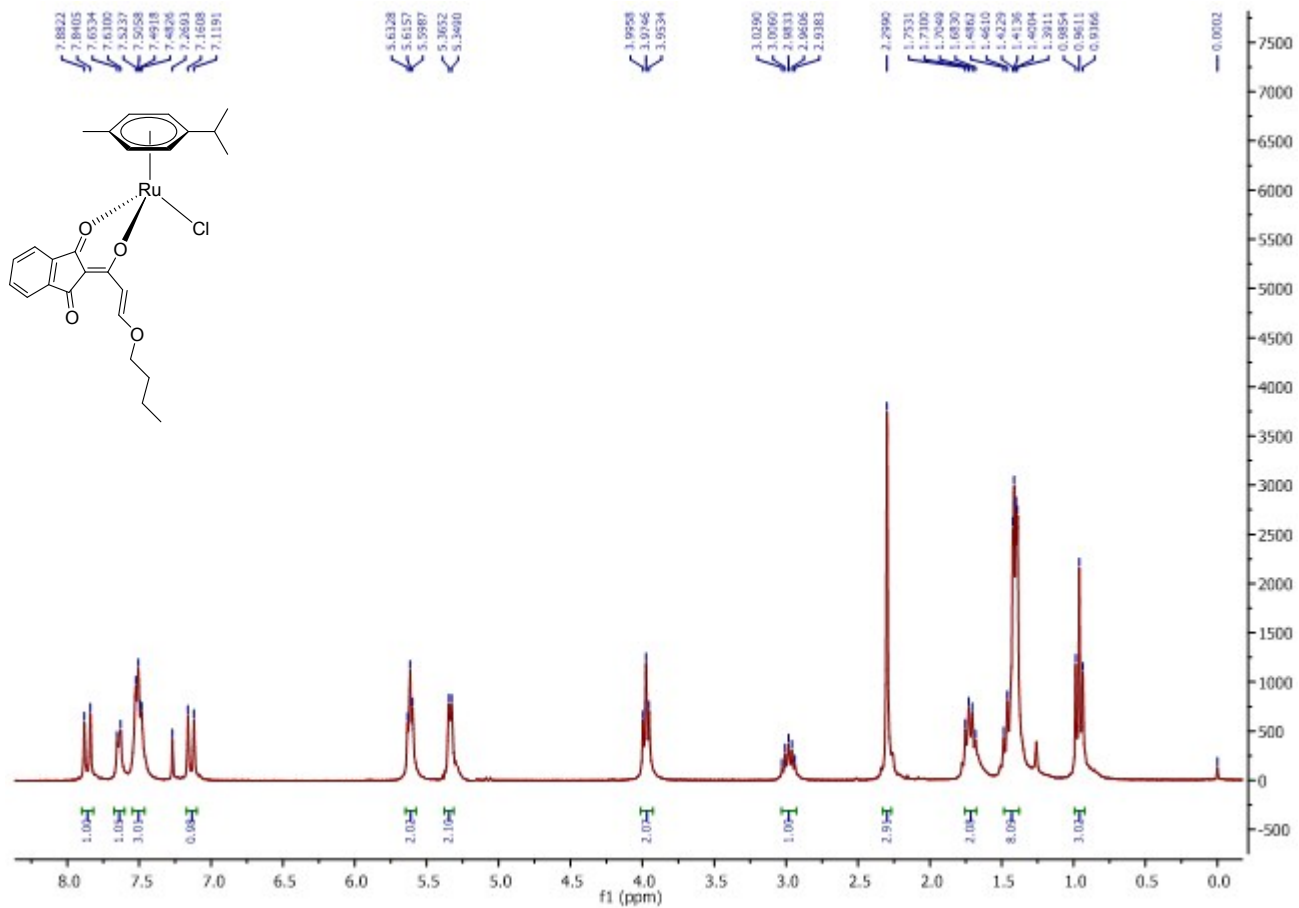
$[M-Cl+H_2O]^+ = 525.5$

Figure S5. ESI-MS analysis-Formation of histidine adduct peaks

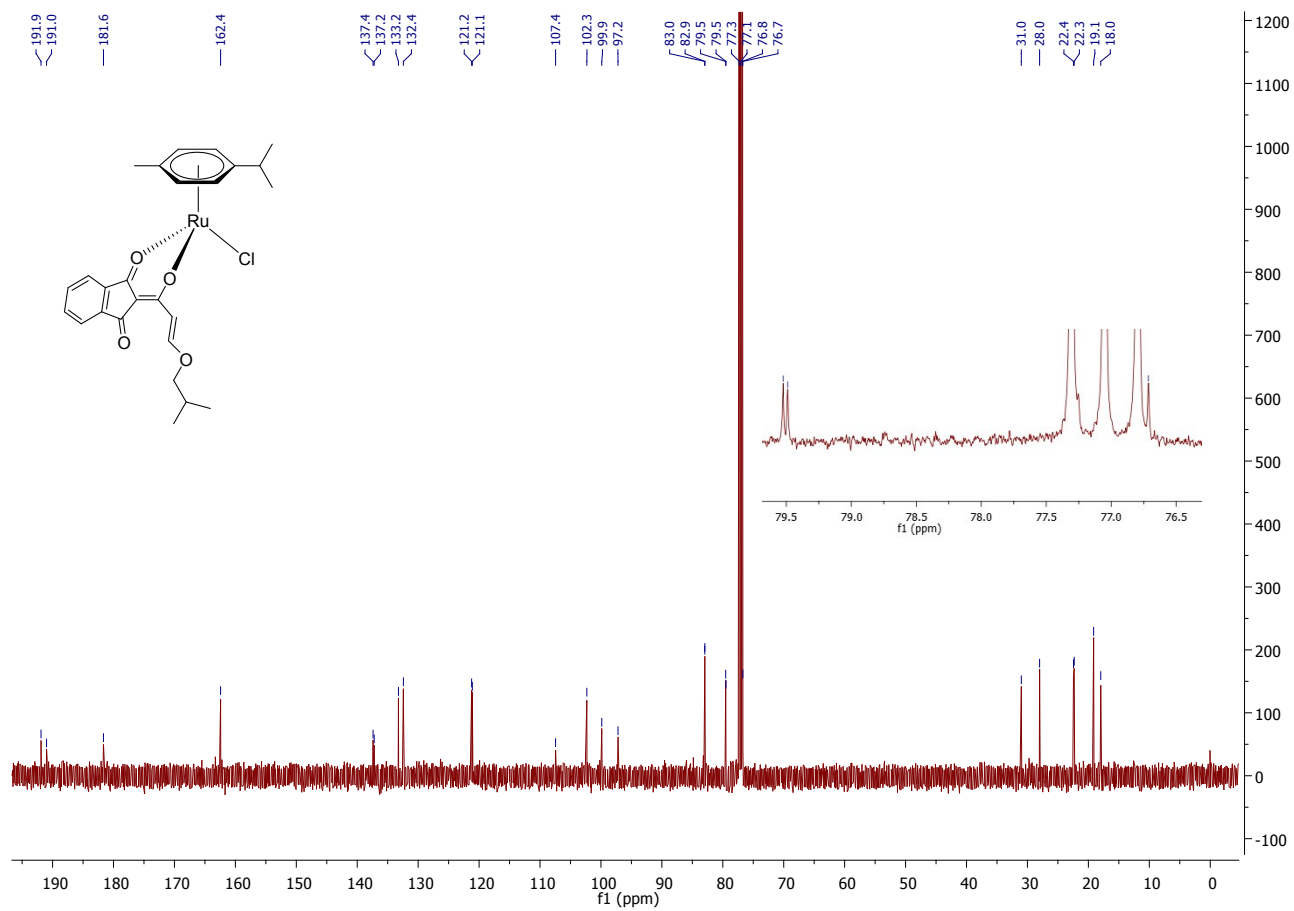
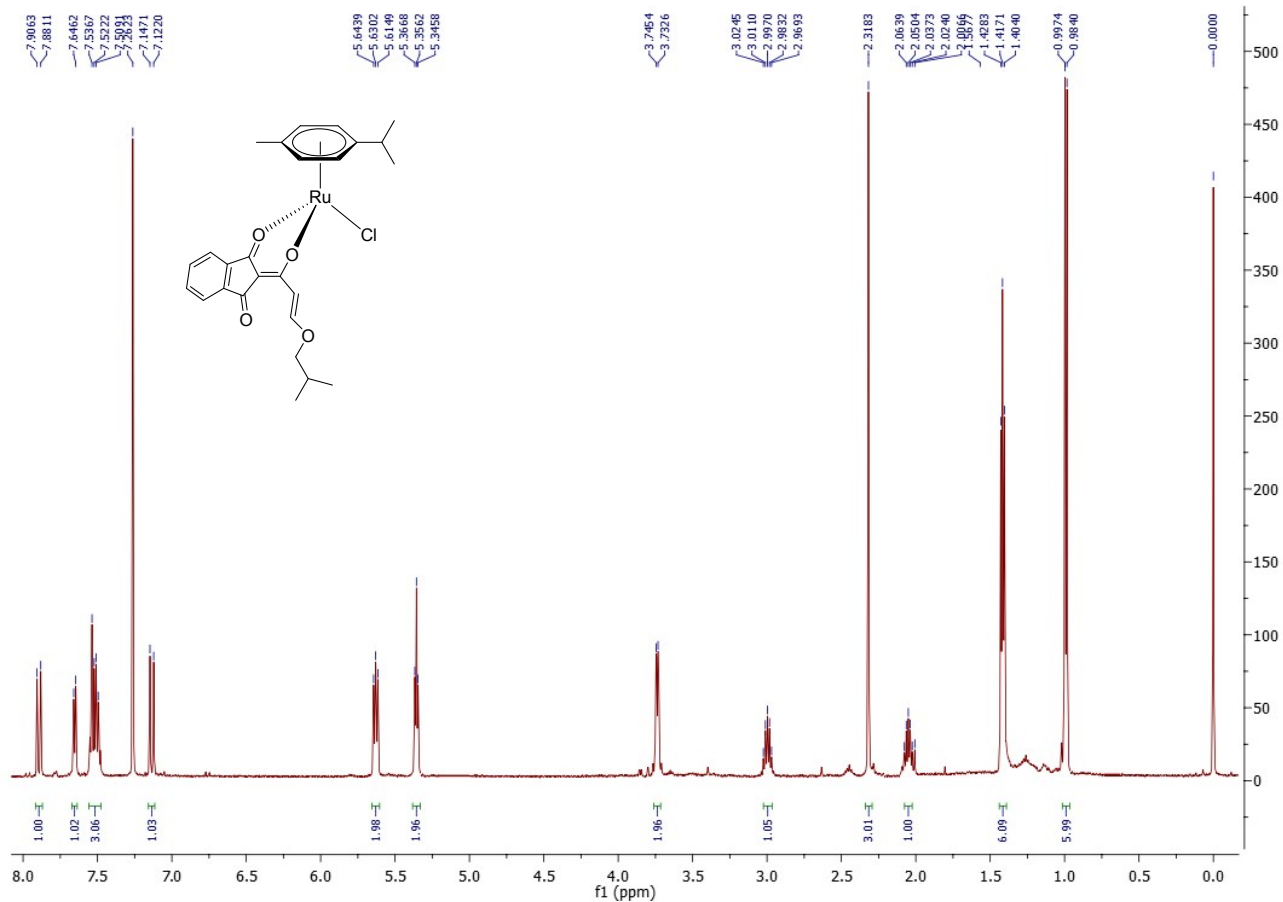


$[M-Cl + His+Na]^+ = 683.8$

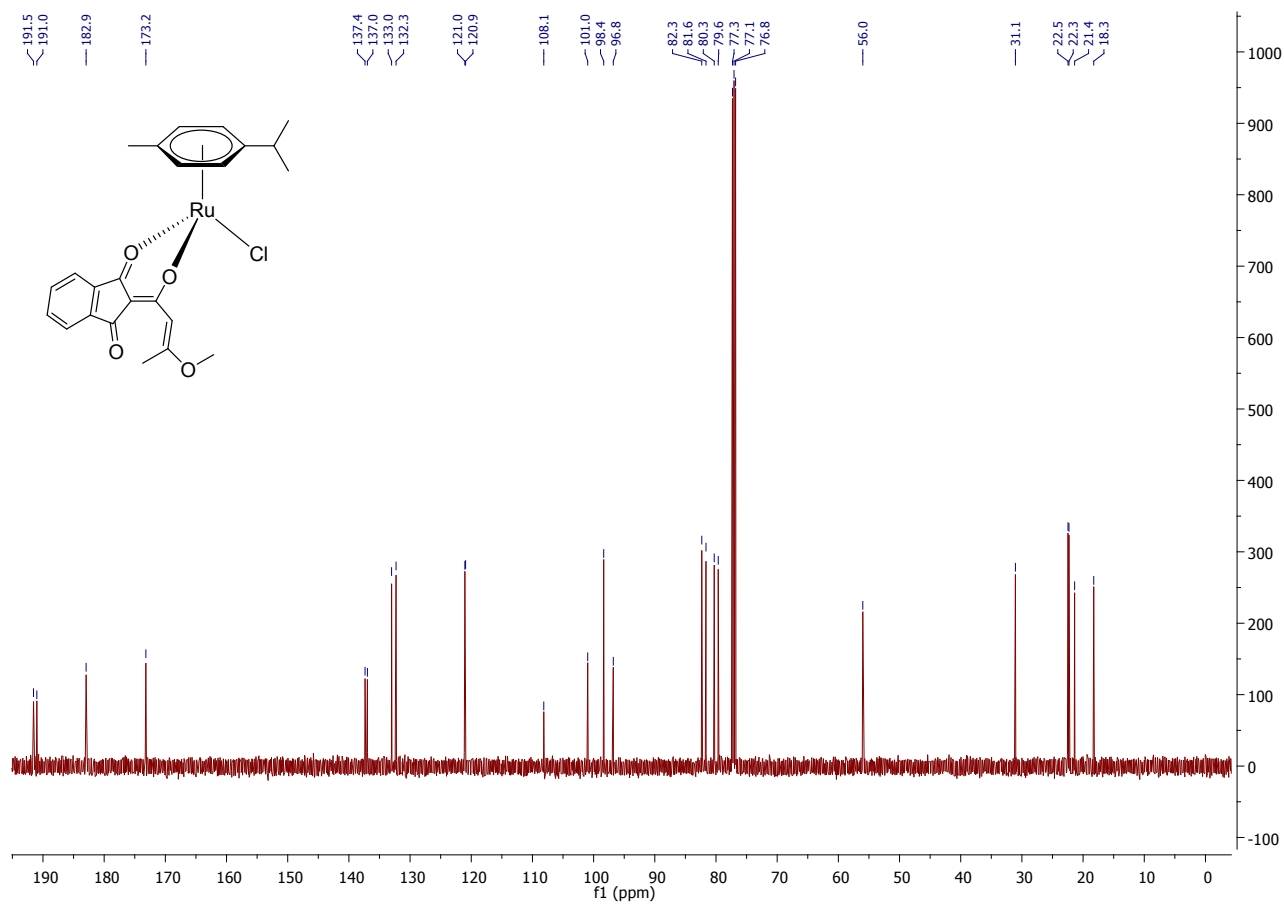
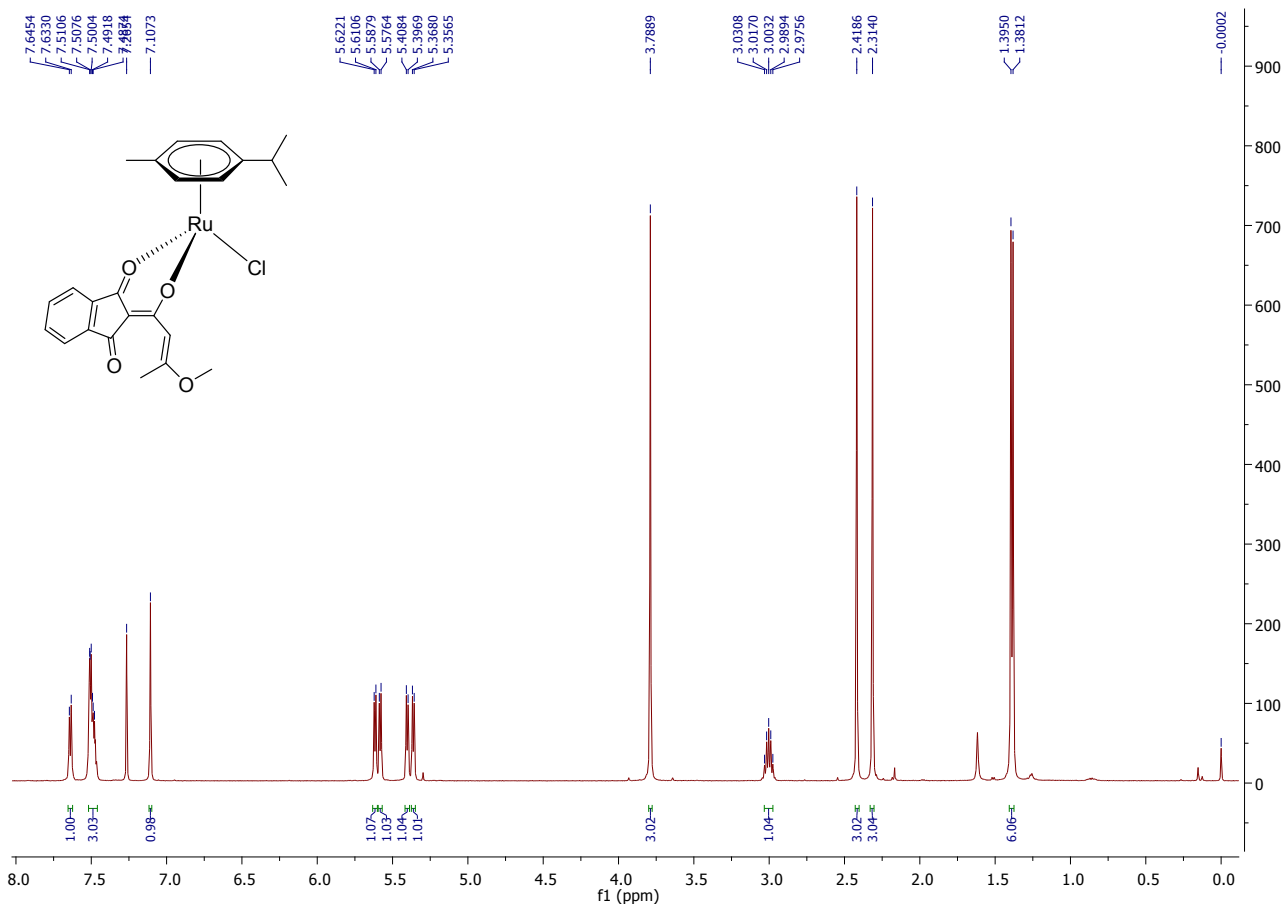
Compound 11a



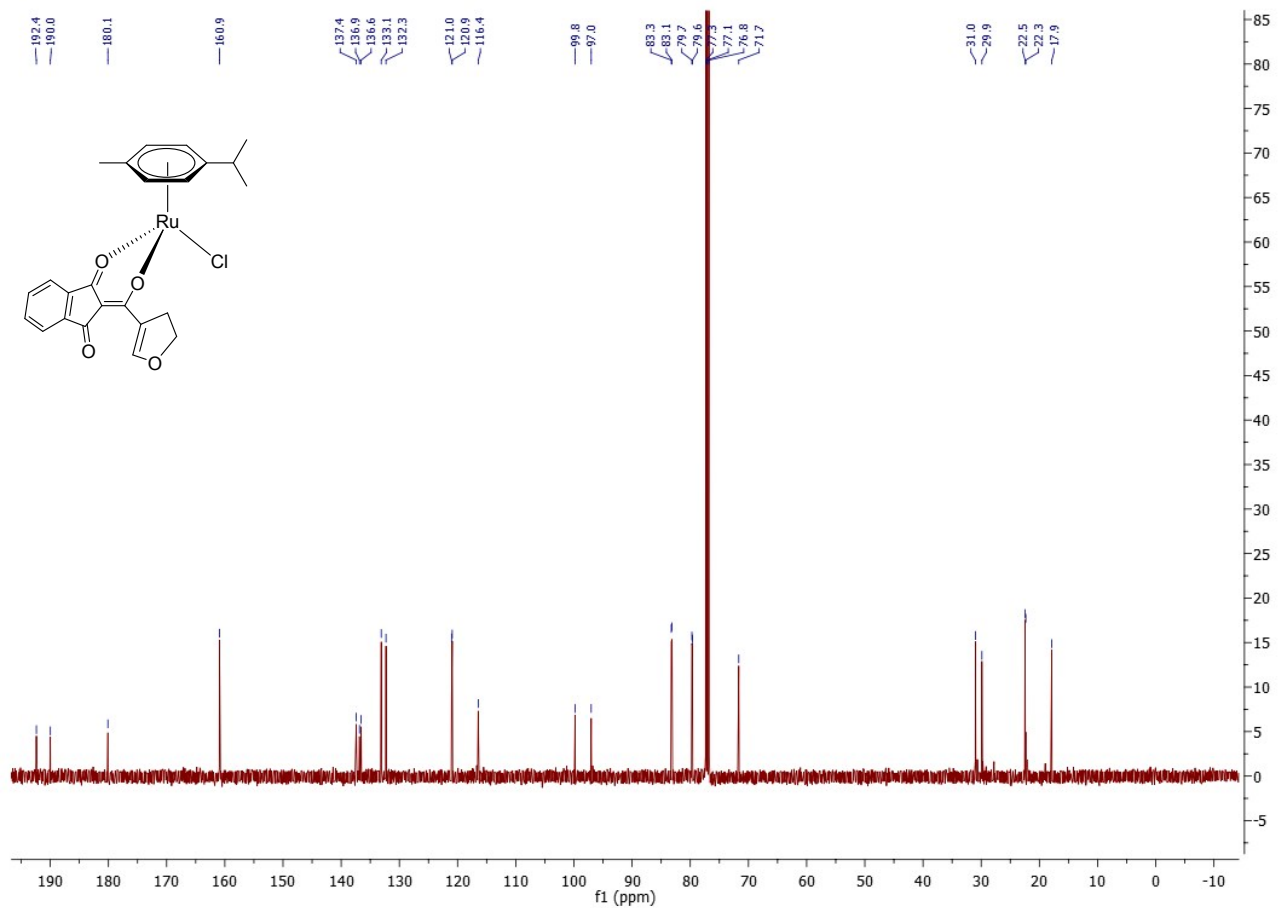
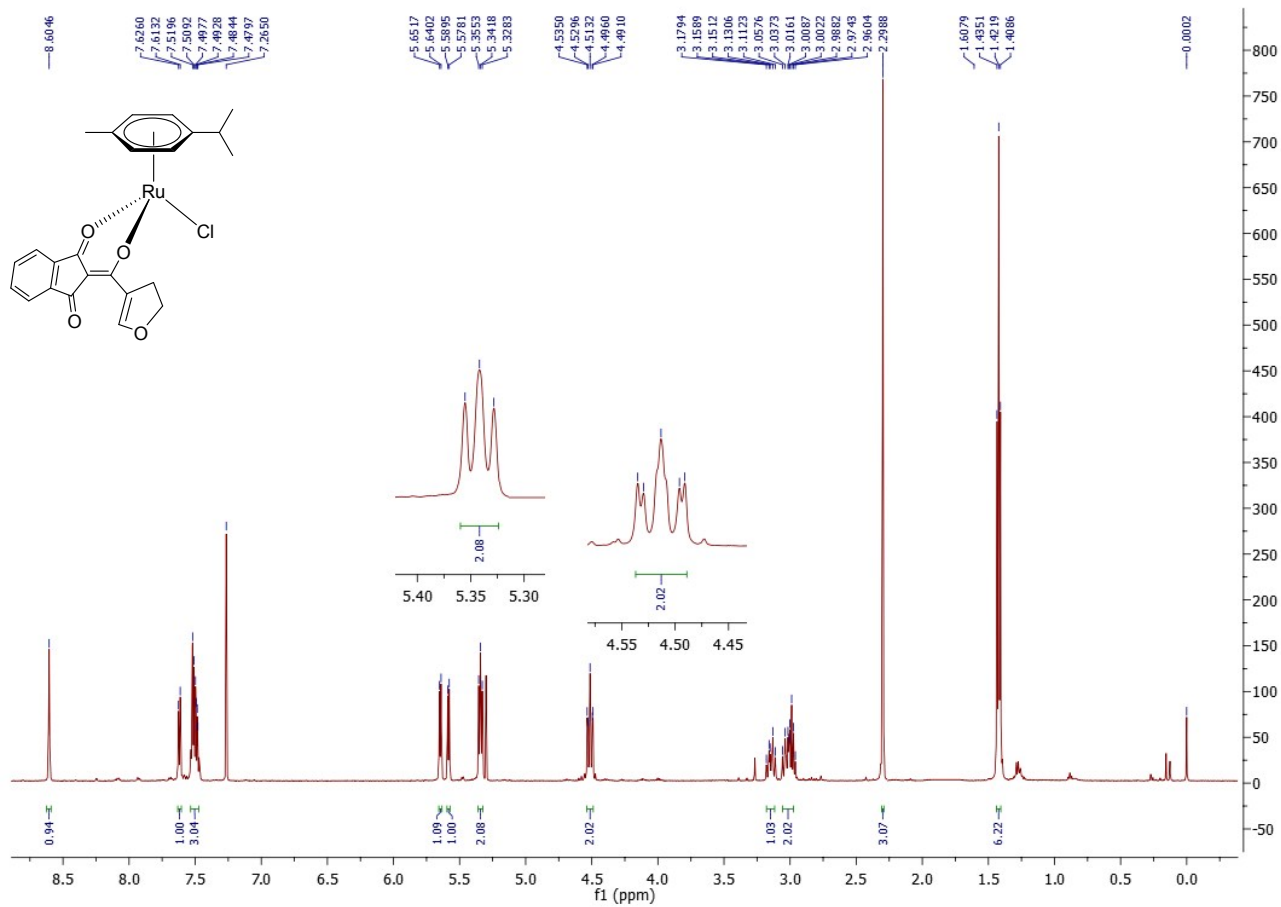
Compound 11b



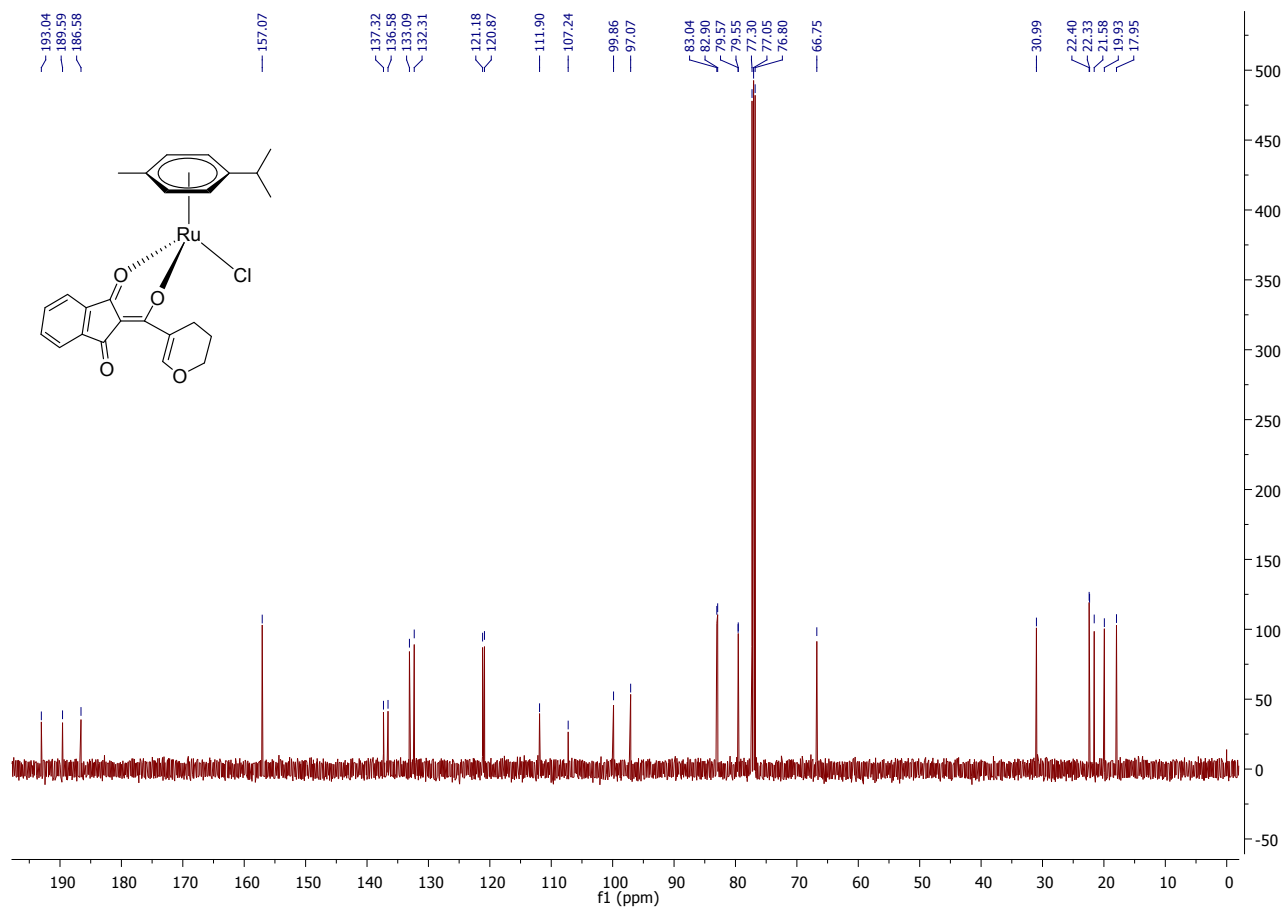
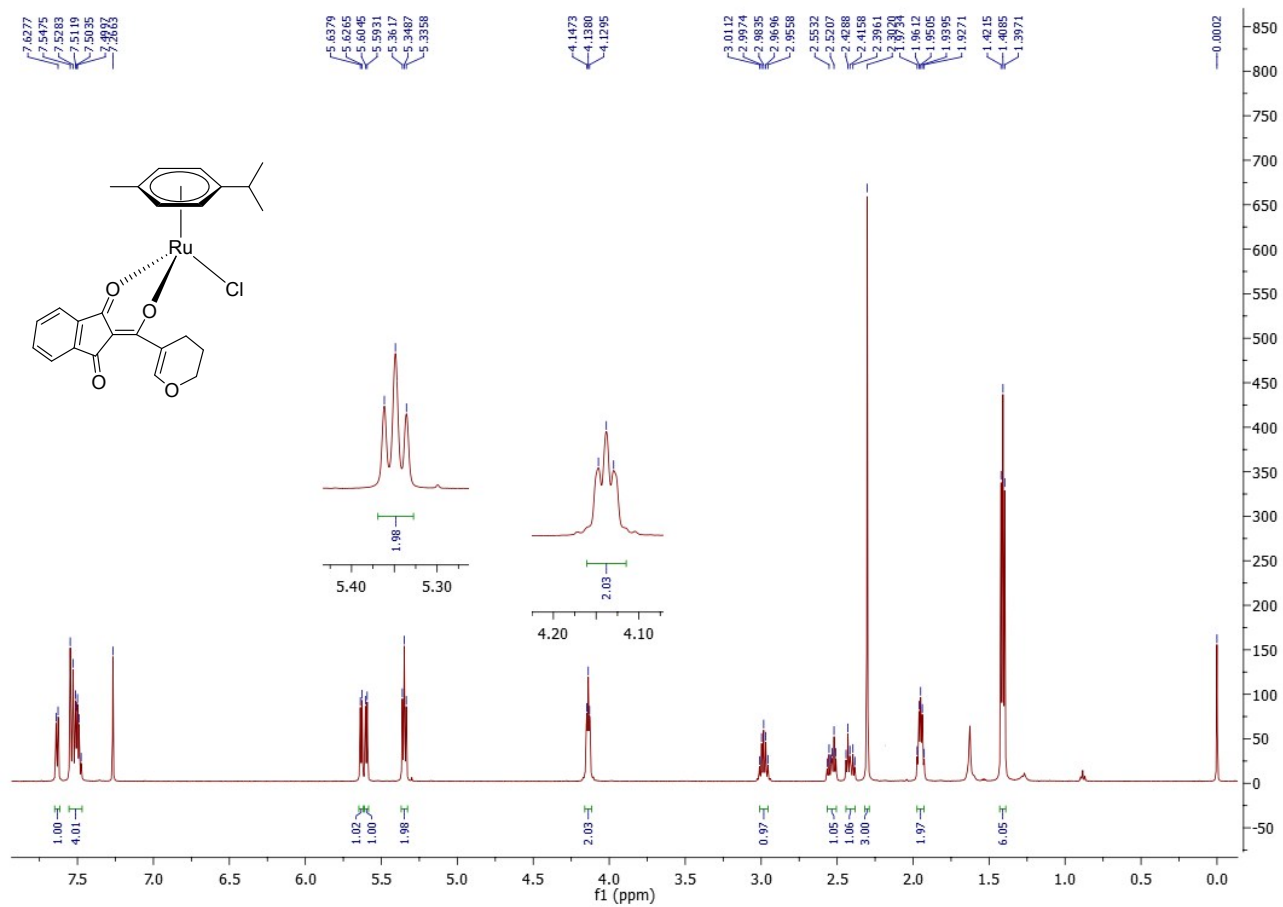
Compound 11c



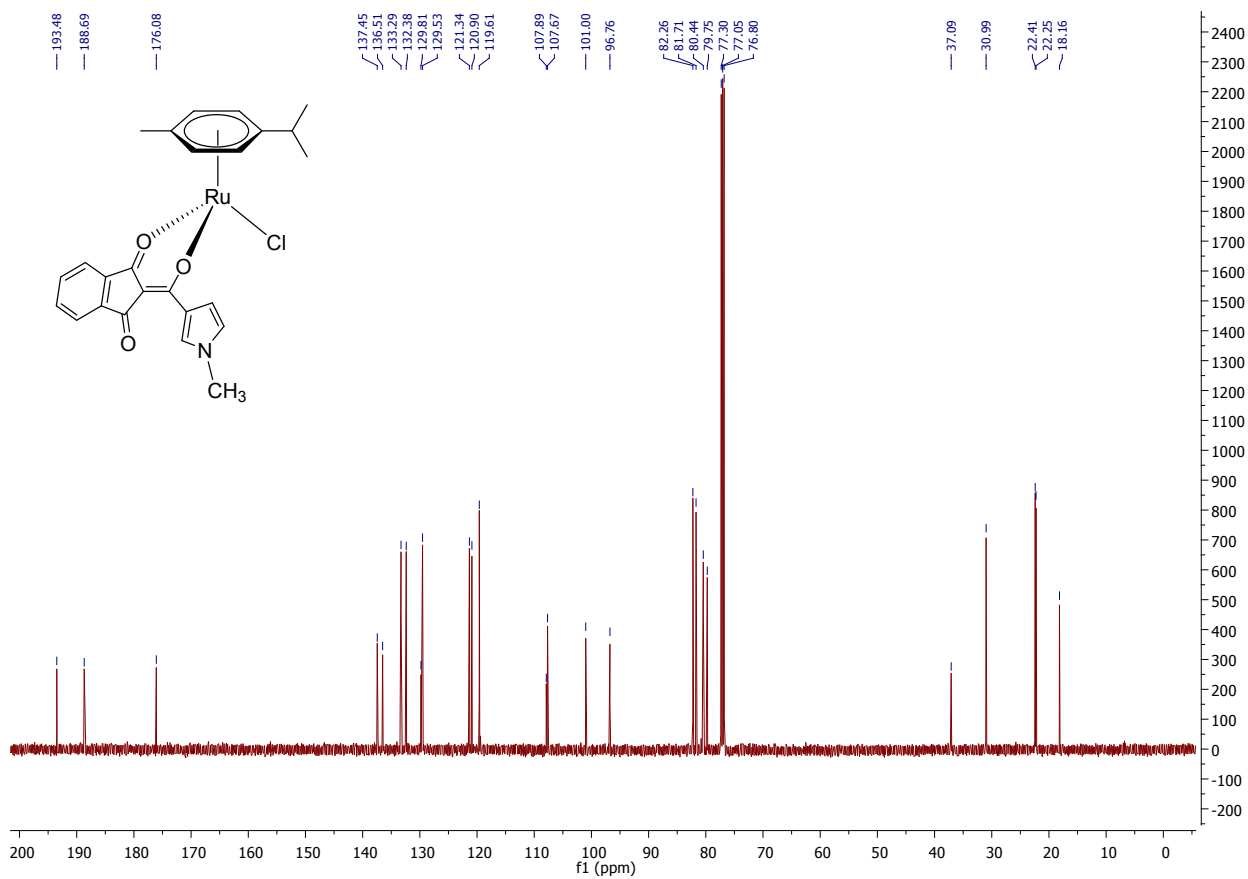
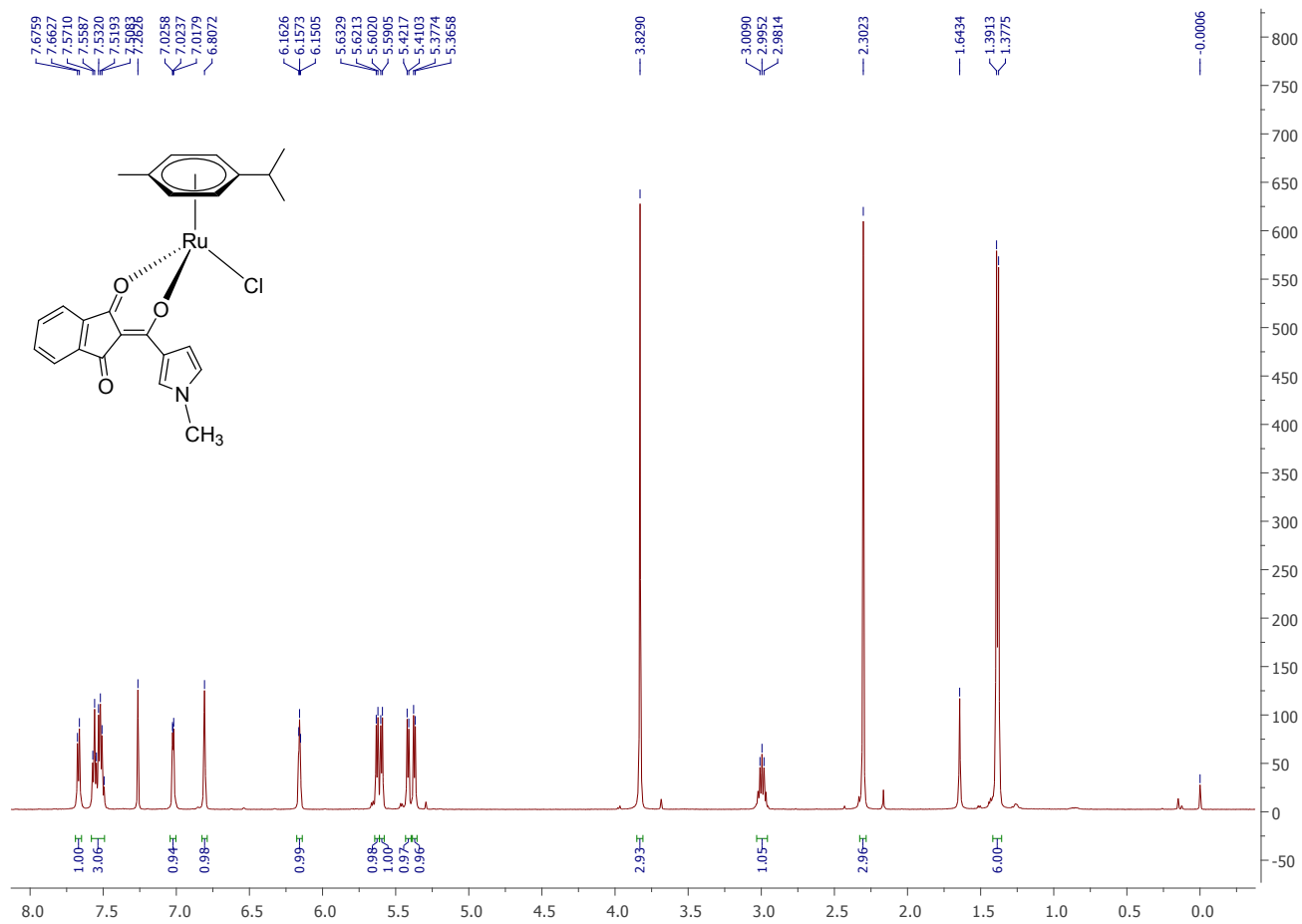
Compound 11d



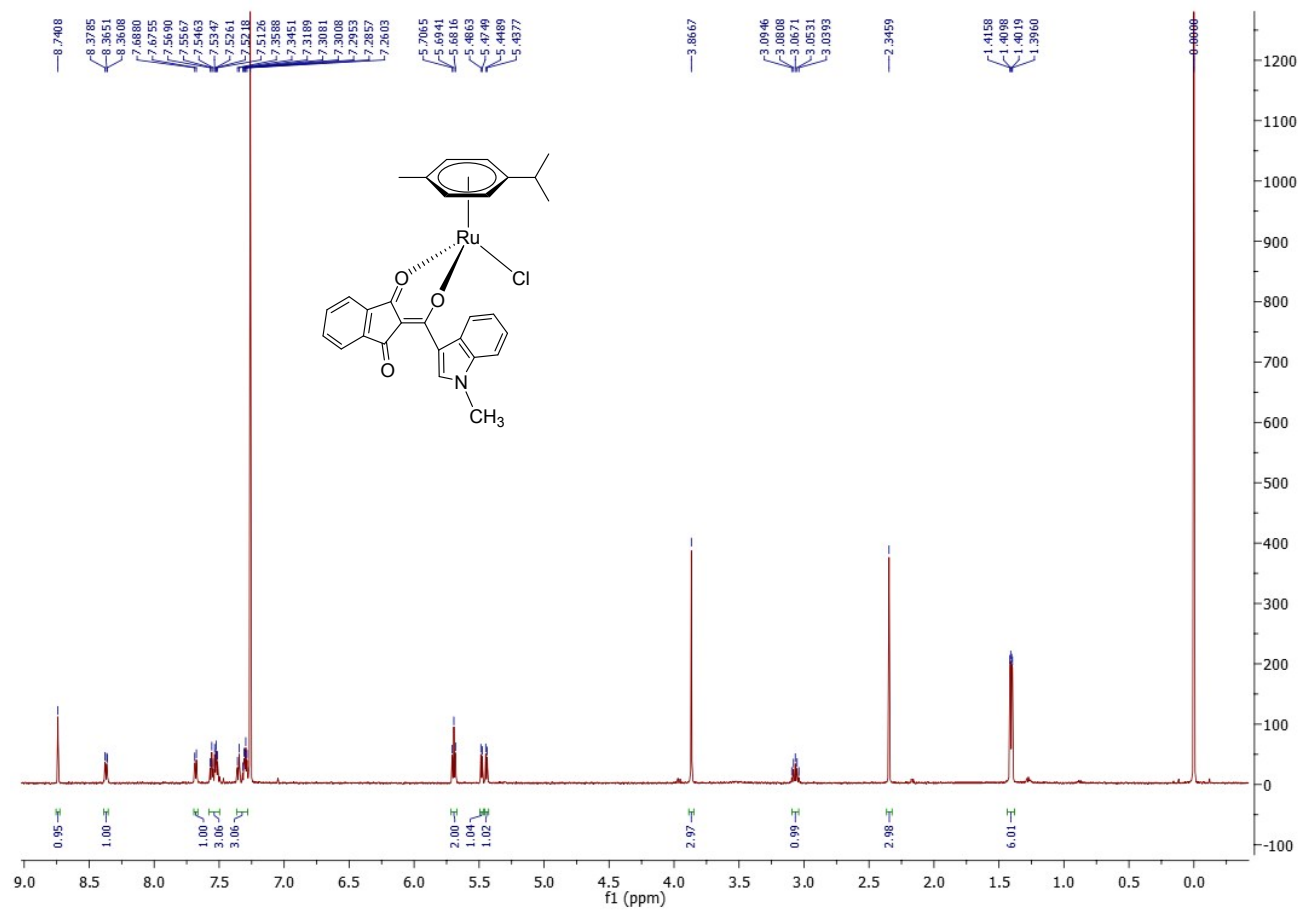
Compound 11e



Compound 12



Compound 13a



Compound 13b

