Supporting information

to

Impact of the Metal Center and Leaving Group on the Anticancer Activity of Organometallic Complexes of Pyridine-2-carbothioamide

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Table of Contents

Table S1. X-ray diffraction parameters for the analysis of single crystals of **3**, **4**, and **6**.

	3·$C_4H_8O_2$	**4**	**6**
CCDC	2050471	2050472	2050473
Formula	$C_{22}H_{23}Br_2FN_2RuS \cdot C_4H_8O_2$	$C_{22}H_{23}FIN_2RuS$	$C_{22}H_{23}FI_2N_2OsS$
Molecular weight / g mol^{-1}	715.48	594.48	810.48
Crystal description	red block	dark red block	dark red block
Crystal size / mm × mm × mm	0.38 × 0.10 × 0.05	0.28 × 0.28 × 0.22	0.35 × 0.34 × 0.10
Wavelength / Å	0.71073	0.71073	0.71073
Temperature / K	99(2)	99(2)	99(4)
Crystal system	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/c$
a / Å	14.1004(4)	6.4580(2)	15.2088(12)
b / Å	8.9443(3)	17.6353(6)	11.3216(9)
c / Å	22.6996(6)	19.1159(7)	13.9552(11)
β / °	91.8909(18)	96.899(2)	94.179(4)
Volume / Å^3	2861.27(15)	2161.32(13)	2396.5(3)
Z	4	4	4
ρ_{calc} / g cm^{-3}	1.661	1.824	2.246
μ / mm^{-1}	3.445	2.269	8.003
F(000)	1424.0	1160.0	1504.0
2Θ range for data collection / °	3.352 to 55.676	5.094 to 55.638	5.252 to 55.728
Index ranges	$-18 \le h \le 17$ $-11 \le k \le 11$ $-29 \le l \le 29$	$-8 \le h \le 8$ $-23 \le k \le 22$ $-24 \le l \le 25$	$-19 \le h \le 19$ $-12 \le k \le 14$ $-17 \le l \le 18$
Reflections collected	32770	25783	26570
Independent reflections	6780 [R_{int} = 0.0968, R_{sigma} = 0.0869]	5098 [R_{int} = 0.0493, R_{sigma} = 0.0456]	5660 [R_{int} = 0.0541, R_{sigma} = 0.0413]
Data/restraints/parameters	6780/0/324	5098/0/256	5660/0/269
Goodness-of-fit on F^2	1.013	1.039	1.084
Final R indexes [$I \ge 2\sigma$ (I)]	R_1 = 0.0436, wR_2 = 0.0811	R_1 = 0.0383, wR_2 = 0.0846	R_1 = 0.0261, wR_2 = 0.0655
Final R indexes [all data]	R_1 = 0.0825, wR_2 = 0.0933	R_1 = 0.0534, wR_2 = 0.0912	R_1 = 0.0284, wR_2 = 0.0668
Largest diff. peak/hole / e Å^{-3}	0.97/-0.70	1.61/-0.65	1.52/-1.46

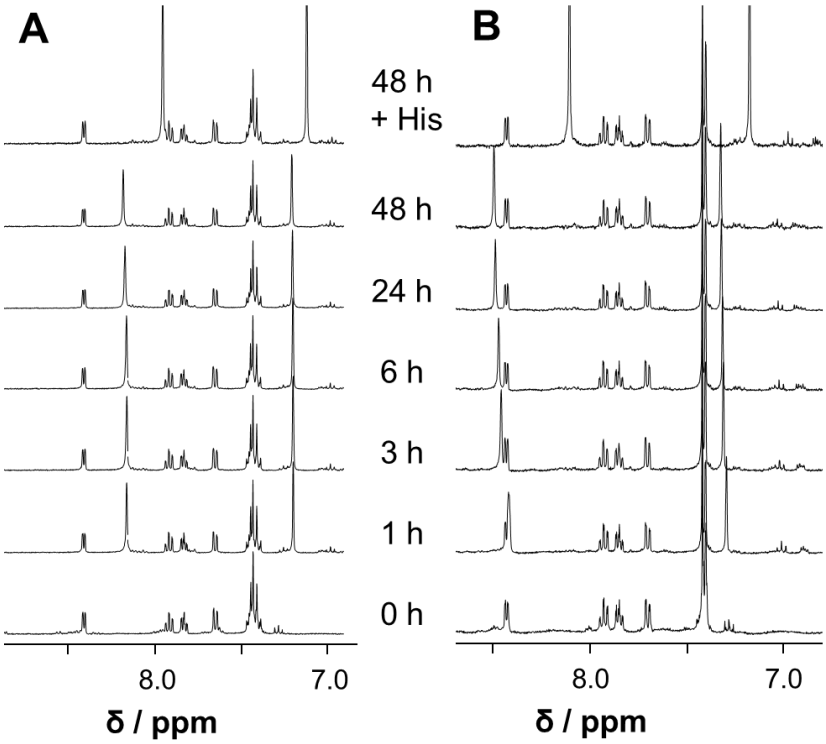

Figure S1. The reactions of **7** (A) and **8** (B) with His (1 : 1) in D_2O over a period of 48 h by ^1H NMR spectroscopy. After 48 h, another equivalent of His was added.

NMR spectra

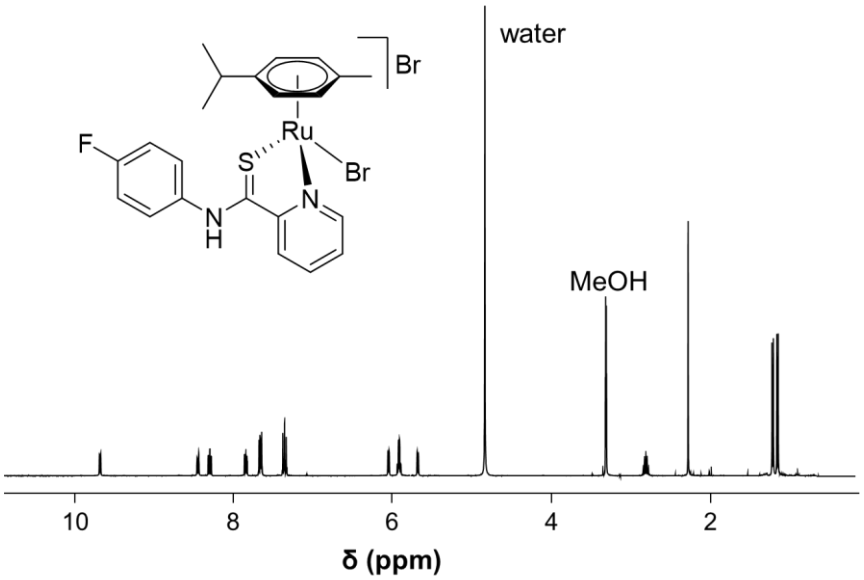

Figure S2. ^{1}H NMR spectrum of **3** in d_4-MeOD.

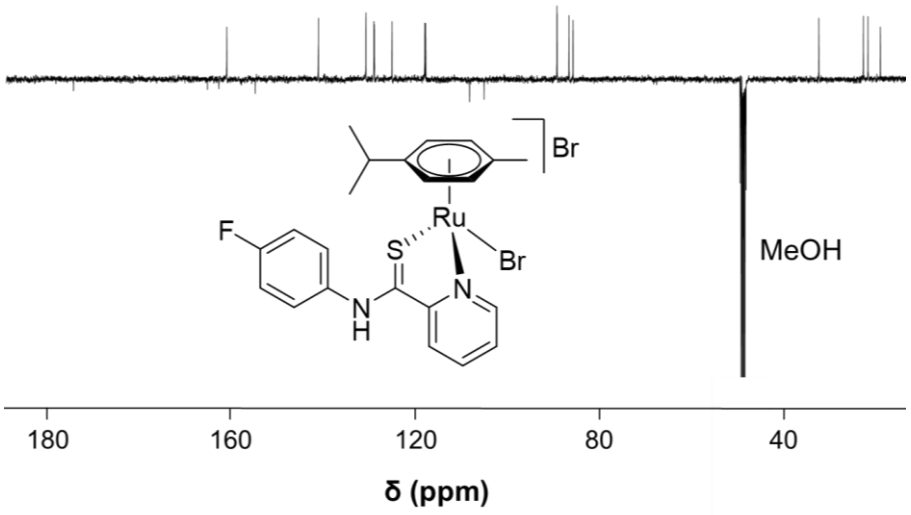

Figure S3. ^{13}C{^{1}H} NMR spectrum of **3** in d_4-MeOD.

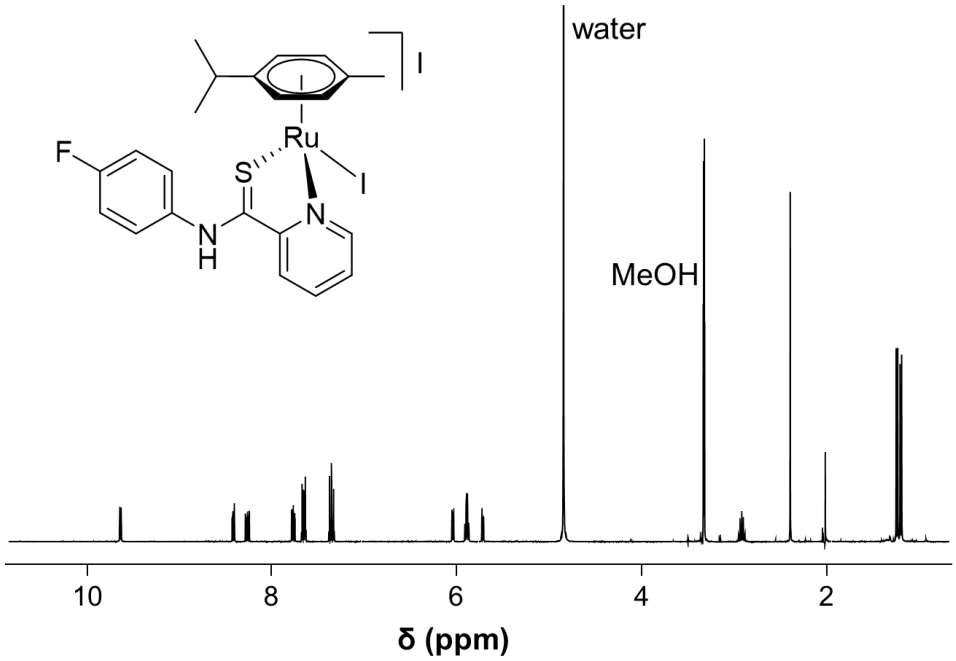

Figure S4. ^{1}H NMR spectrum of **4** in *d*$_4$-MeOD.

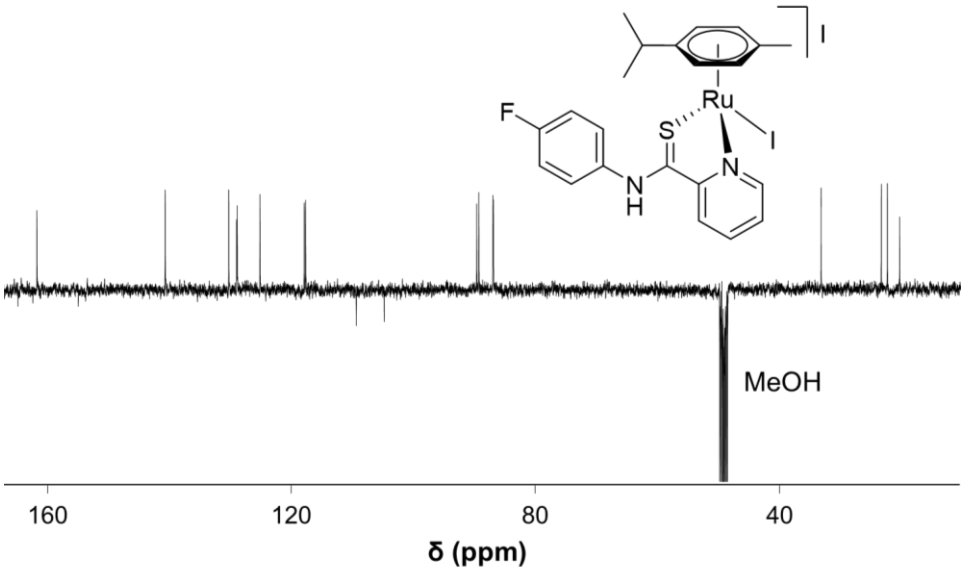

Figure S5. ^{13}C{^{1}H} NMR spectrum of **4** in *d*$_4$-MeOD.

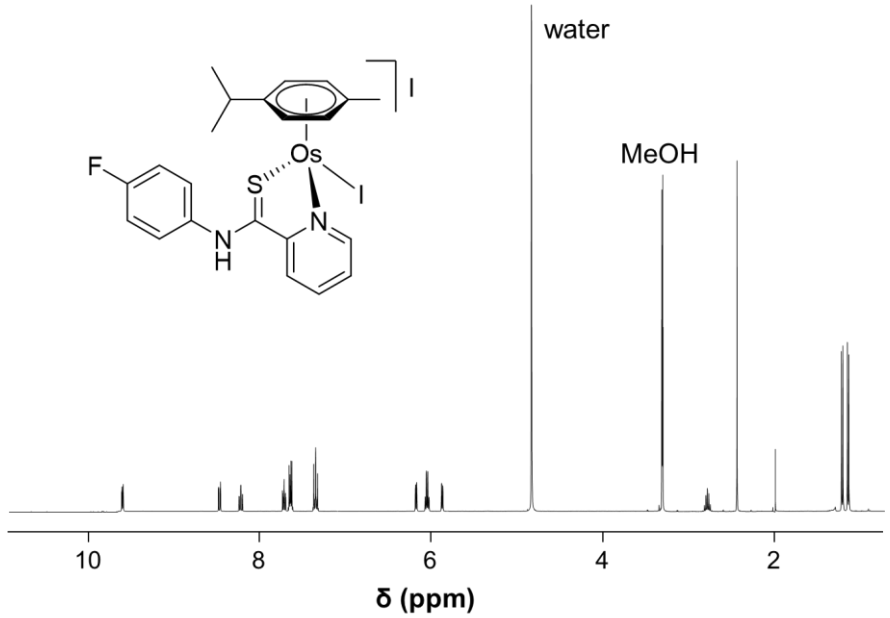

Figure S6. ^{1}H NMR spectrum of **6** in d_4-MeOD.

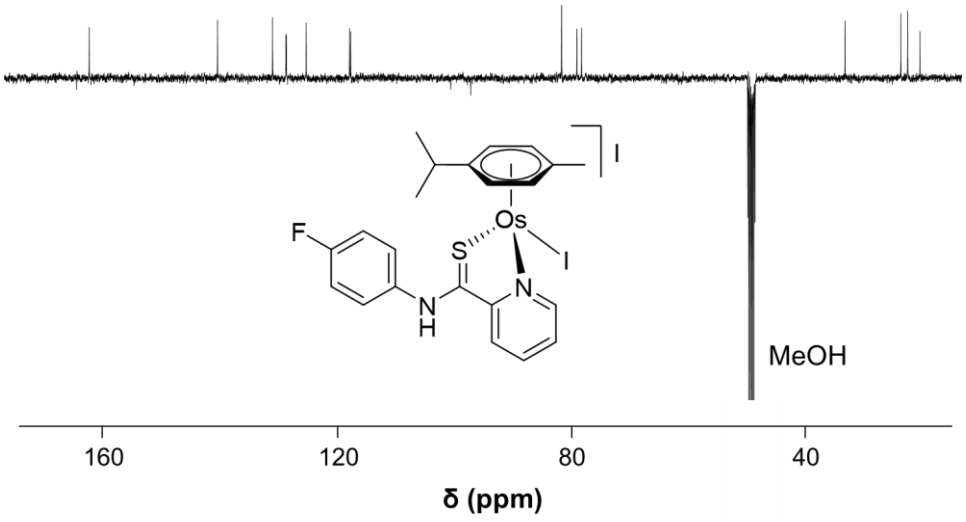

Figure S7. ^{13}C{^{1}H} NMR spectrum of **6** in d_4-MeOD.

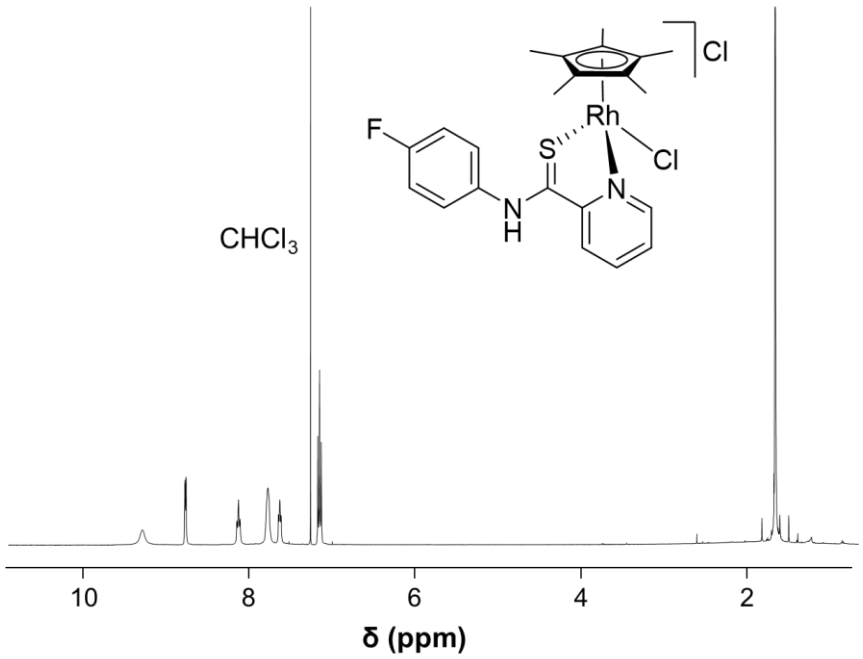

Figure S8. ^{1}H NMR spectrum of **7** in $CDCl_3$.

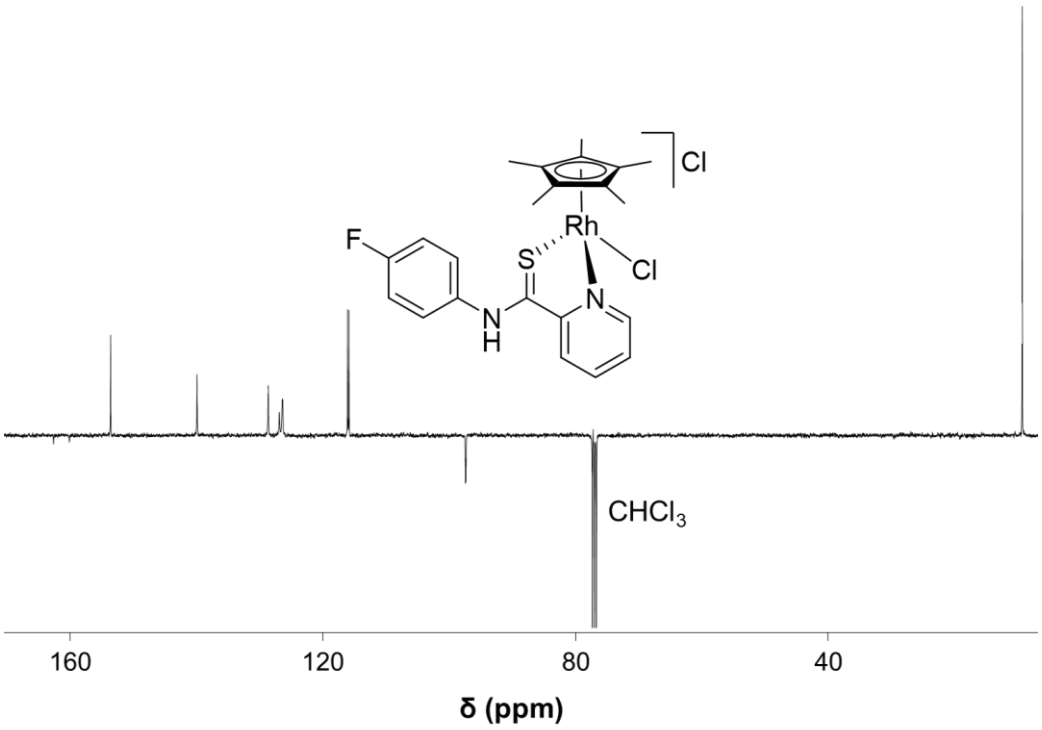

Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of **7** in *d*$_4$-MeOD.

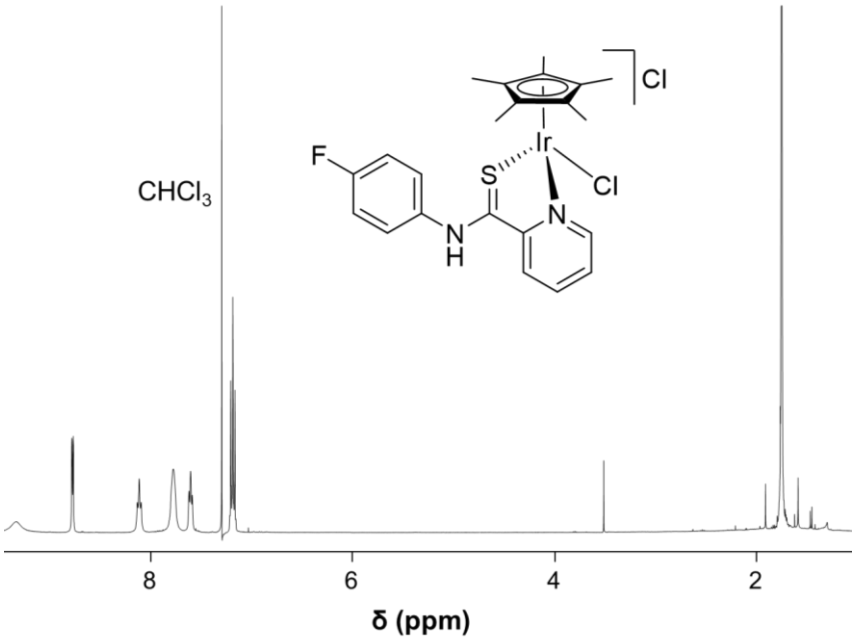

Figure S10. ^{1}H NMR spectrum of **8** in $CDCl_3$.

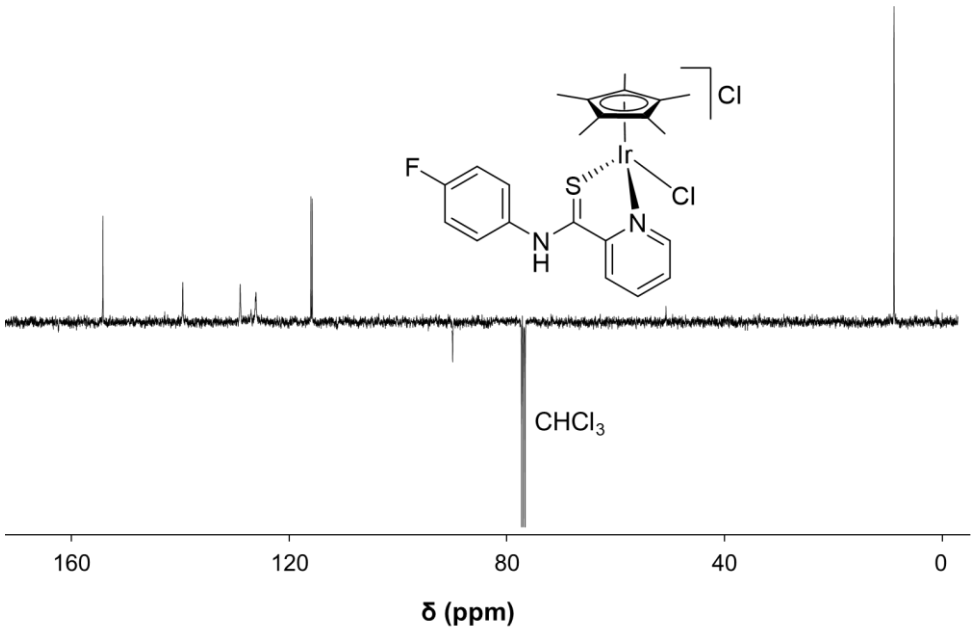

Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$.