SUPPORTING INFORMATION FOR

Synthesis, characterization, and *in vivo* evaluation of the anticancer activity of a series of 5- and 6-(halomethyl)-2,2'-bipyridine rhenium tricarbonyl complexes.

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Table 1. Crystallographic details of complexes.

	2	**3**	**5**	**6**	**7**	**9**	**10**
Formula	$C_{14}H_9$ $BrClN_2O_3Re$	$C_{14}H_{10}$ BrN_2O_4Re	$C_{14}H_8$ $BrF_2N_2O_3Re$	$C_{14}H_9$ $Br_2N_2O_3Re$	$C_{14}H_9$ $BrClN_3O_3Re$	$ReC_{14}H_{10}$ BrN_2O_3	$C_{14}H_8$ $BrF_2N_2O_3Re$
M_W	554.79	536.35	556.33	599.25	554.79	520.35	556.33
T [K]	200	200	200	200	200	200	200
Lattice	monoclinic	triclinic	orthorombic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	C2/c	P -1	Pca21	P21/c	P21/c	Pc	P21/c
Z	8	2	4	4	4	4	4
a [Å]	12.8442(3)	7.7857(3)	14.1812(2)	10.9912(4)	10.9380(6)	14.9333(5)	14.7874(5)
b [Å]	11.1458(3)	8.4162(3)	7.8891(1)	12.2942(4)	12.1342(11)	11.3306(2)	11.5066(2)
c [Å]	21.9911(5)	11.3670(4)	13.6693(2)	12.4352(5)	12.3961(7)	9.2074(3)	8.8657(3)
α [°]	90	92.440(3)	90	90	90	90	90
β [°]	92.621(2)	95.136(3)	90	97.928(3)	97.486(5)	106.894(2)	92.420(3)
γ [°]	90	92.303(3)	90	90	90	90	90
V [Å^3]	3144.93(13)	740.45(5)	1529.28(4)	1664.28(11)	1631.2(2)	1490.69(8)	1507.18(8)
d_{calcd} [g/cm^3]	2.343	2.406	2.416	2.392	2.259	2.319	2.452
R_1, wR_2	0.0443, 0.1169	0.0199, 0.0480	0.0147, 0.0387	0.0648, 0.1665	0.0829, 0.2252	0.0418, 0.1204	0.0241, 0.0624

NMR spectra

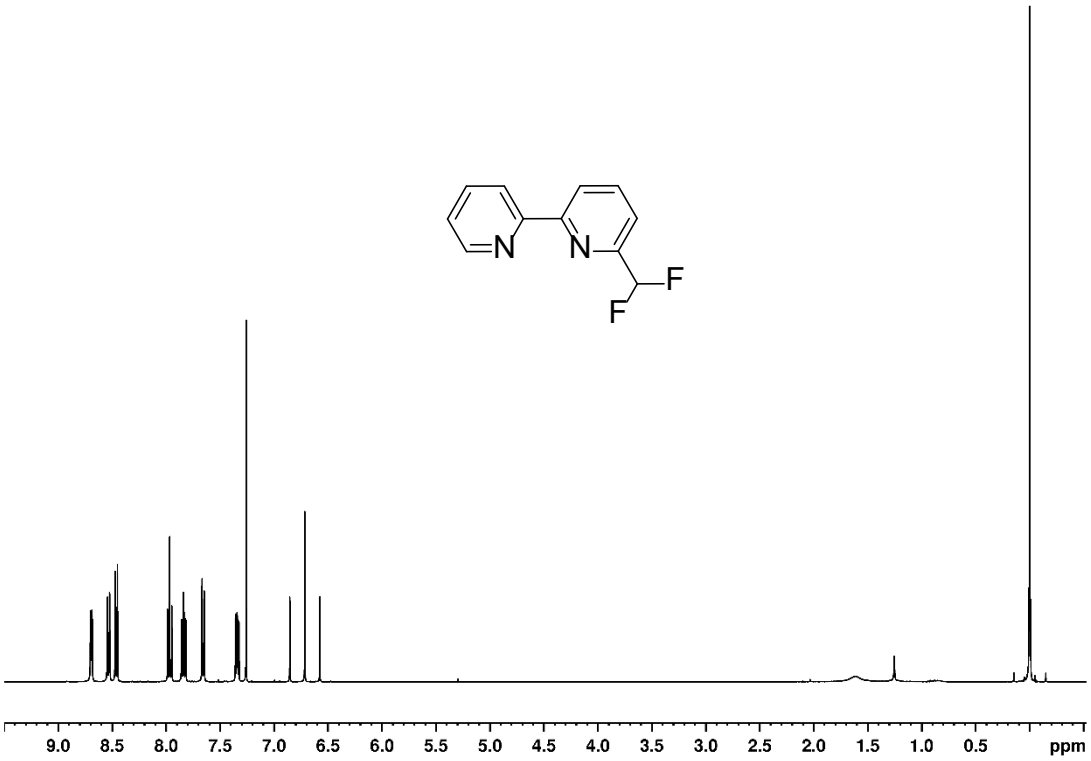


Figure S0a. 400 MHz ^{1}H-NMR of **L_5** in $CDCl_3$.

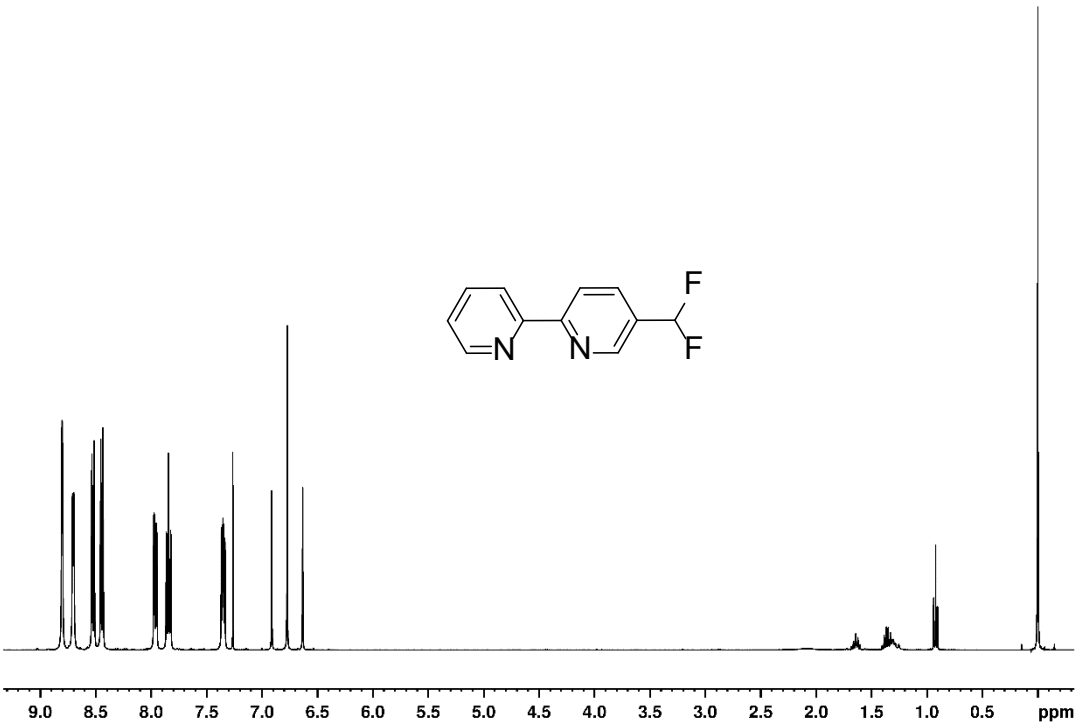


Figure S0a. 400 MHz ^{1}H-NMR of **L_{10}** in $CDCl_3$.

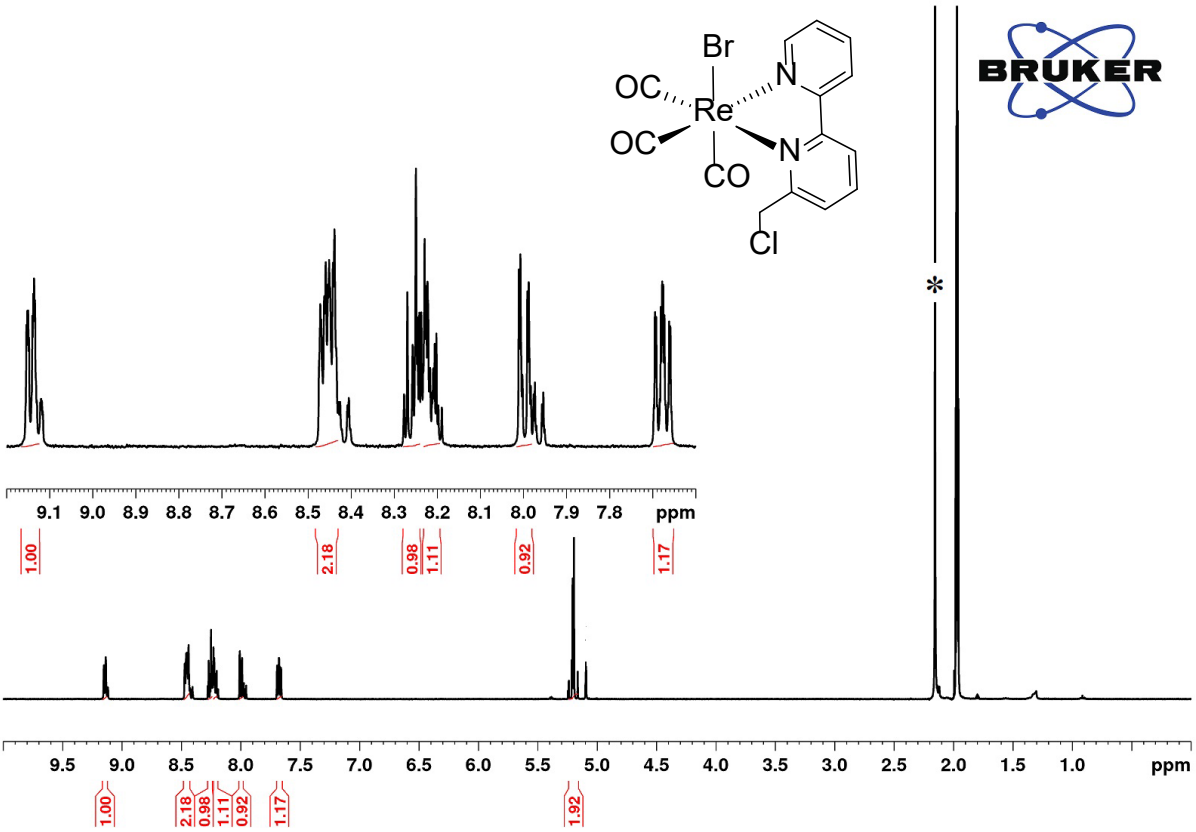


Figure S1. 400 MHz ^{1}H-NMR of **2** (in acetonitrile-d3, ✻= solvent residual peak).

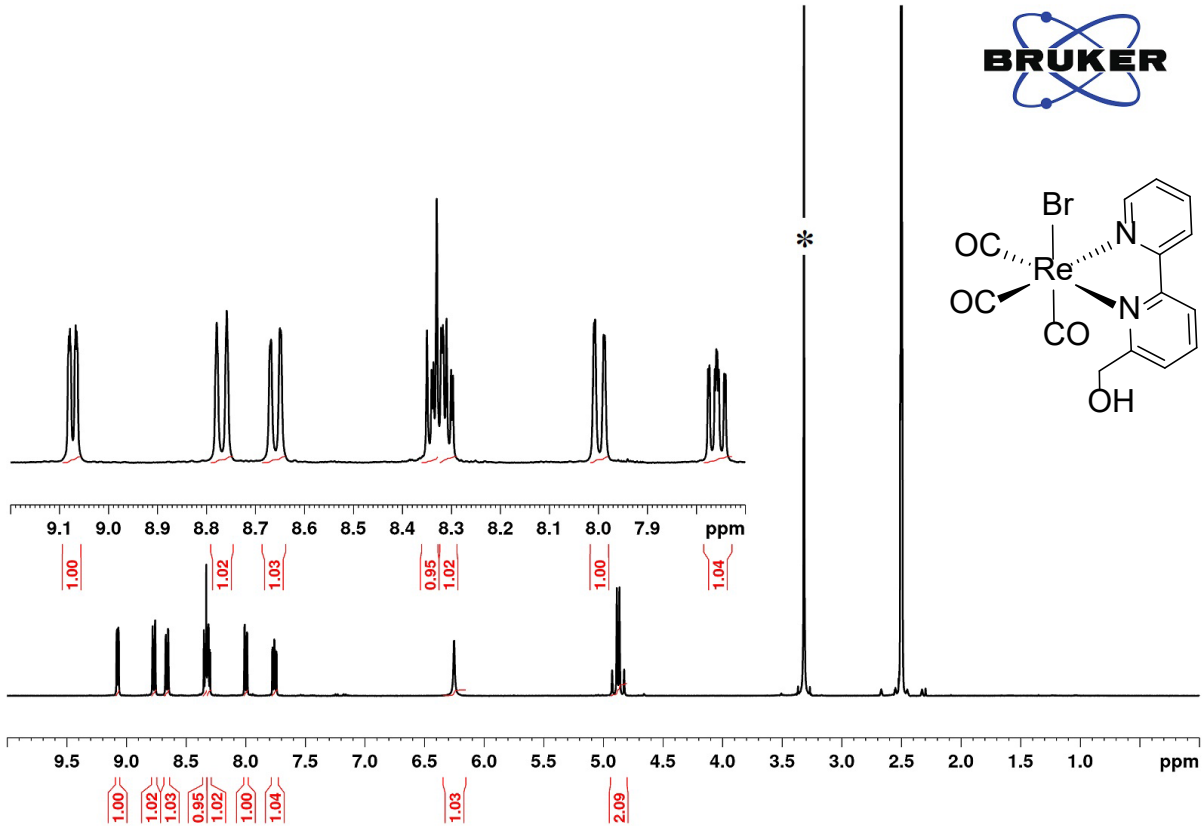


Figure S2. 400 MHz ^{1}H-NMR of **3** (in DMSO, ✻= solvent residual peak).

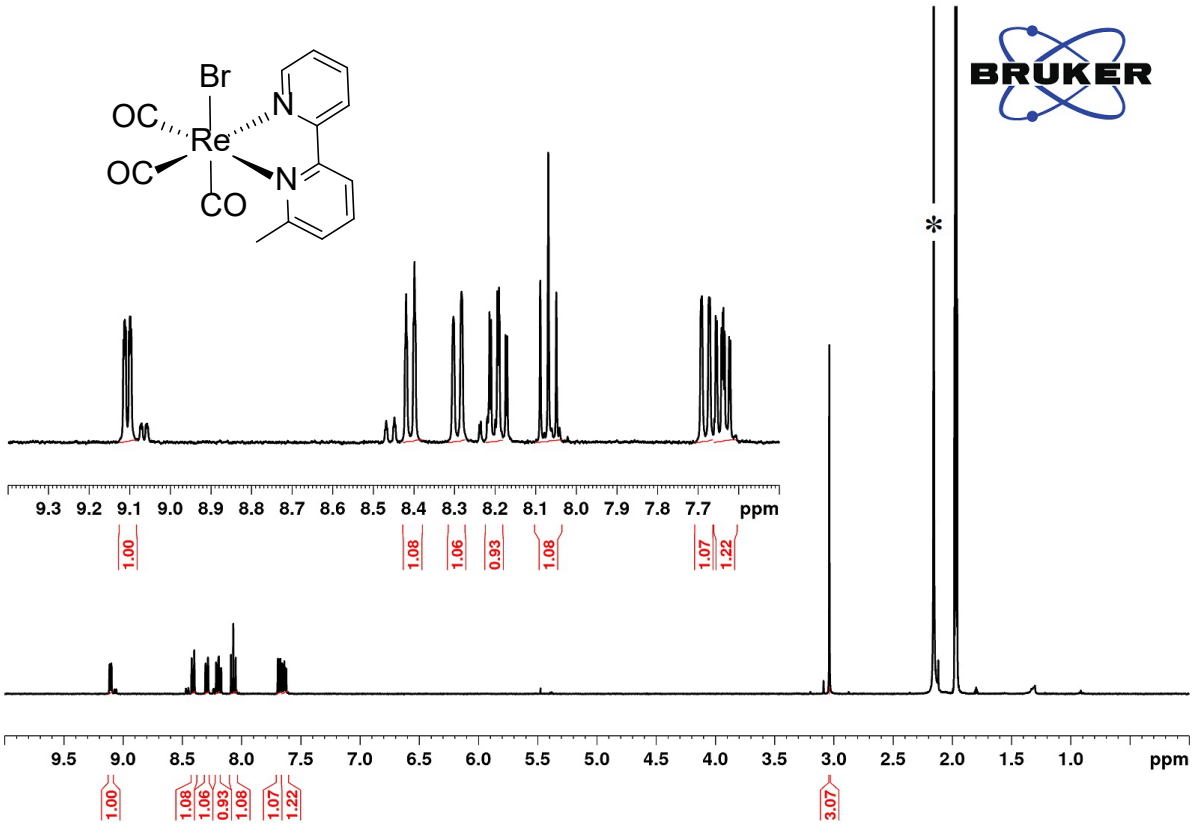


Figure S3. 400 MHz ^{1}H-NMR of **4** (in acetonitrile-d3, ✻= solvent residual peak).

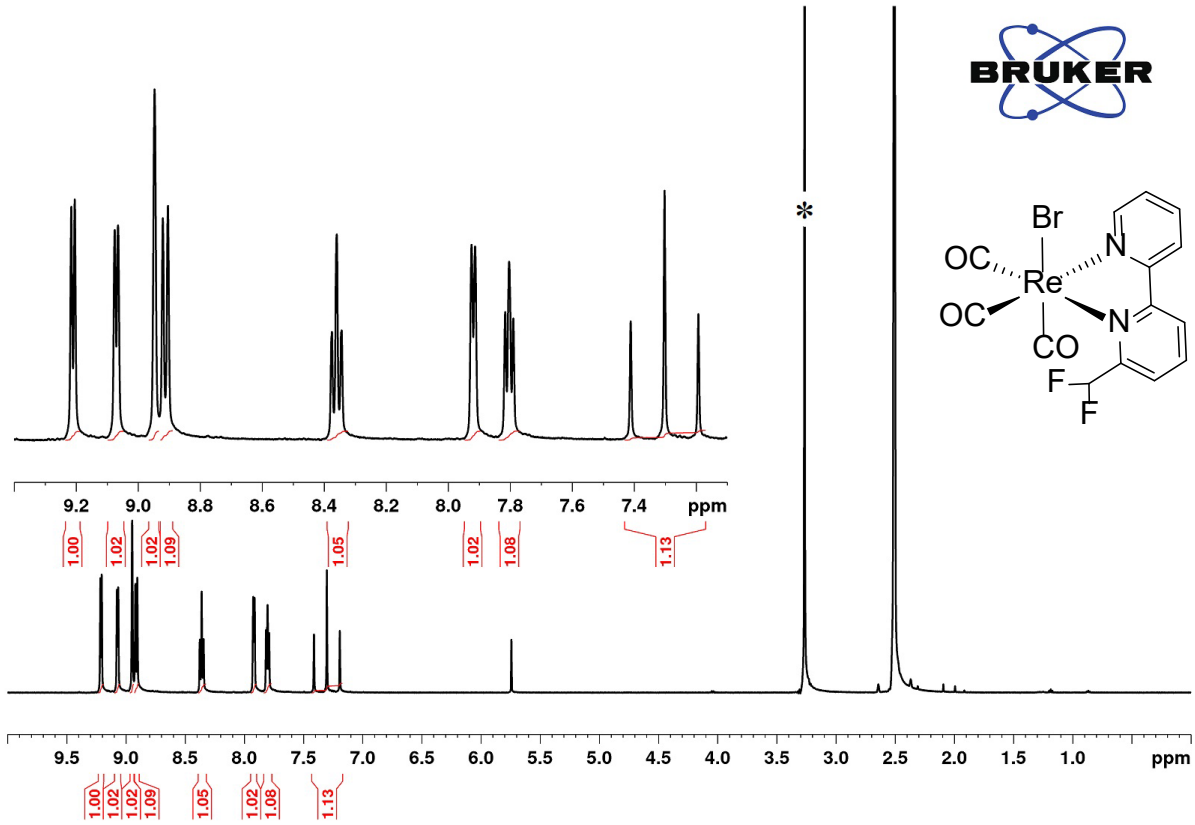


Figure S4. 400 MHz ^{1}H-NMR of **5** (in DMSO, ✻= solvent residual peak).

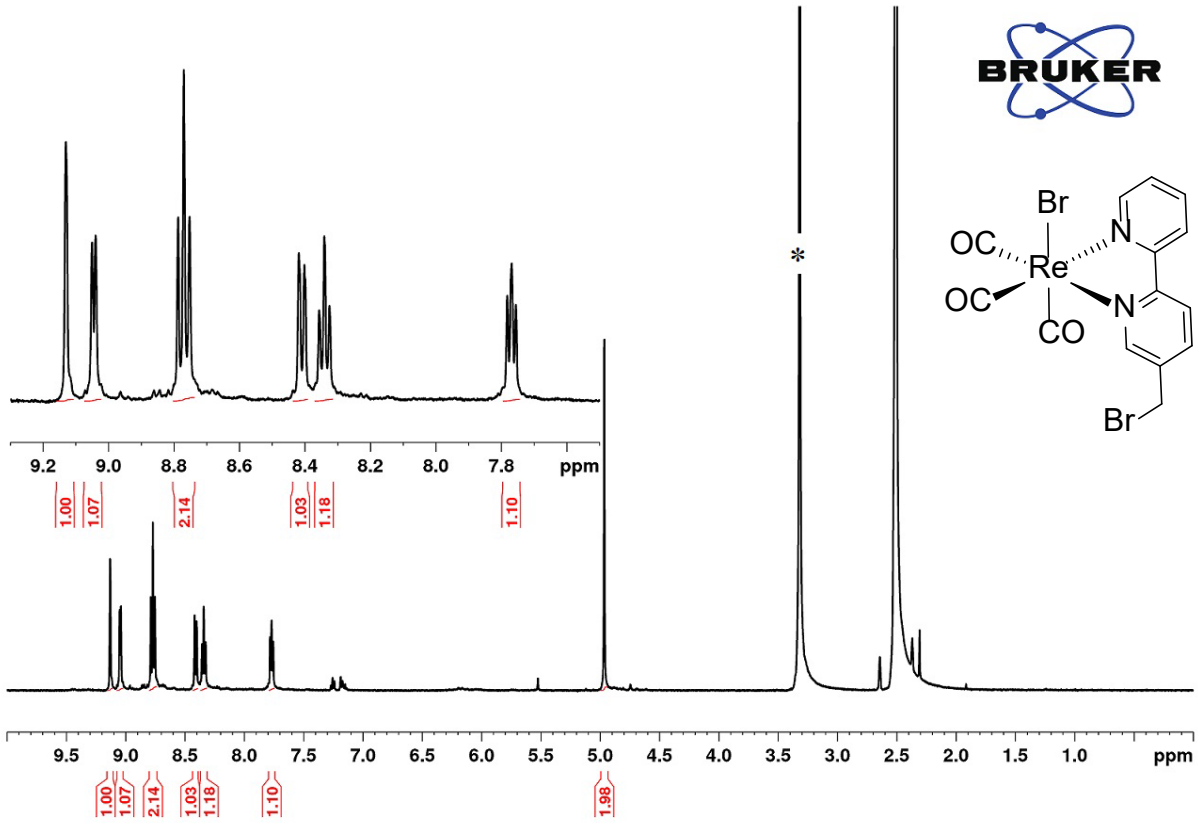


Figure S5. 400 MHz ^{1}H-NMR of **6** (in DMSO, ✻= solvent residual peak).

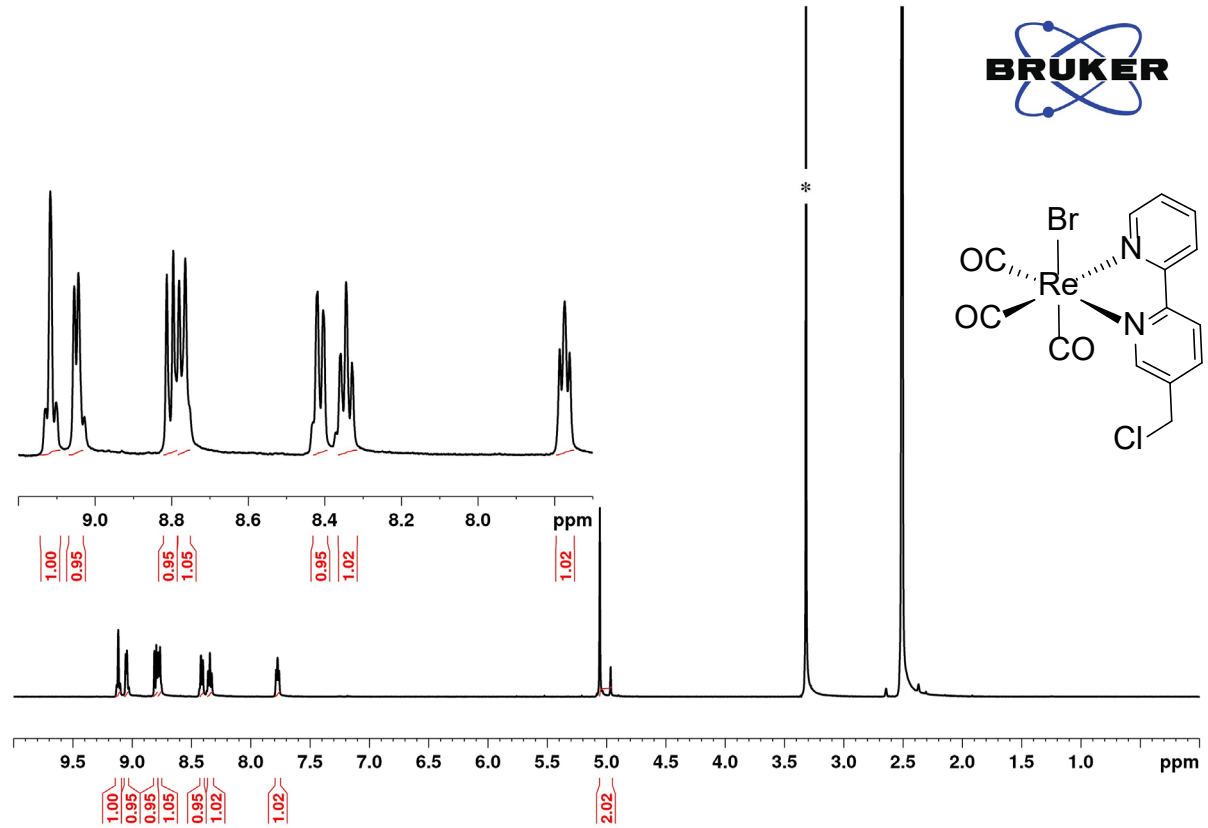


Figure S6. 400 MHz ^{1}H-NMR of **7** (in DMSO, ✻= solvent residual peak).

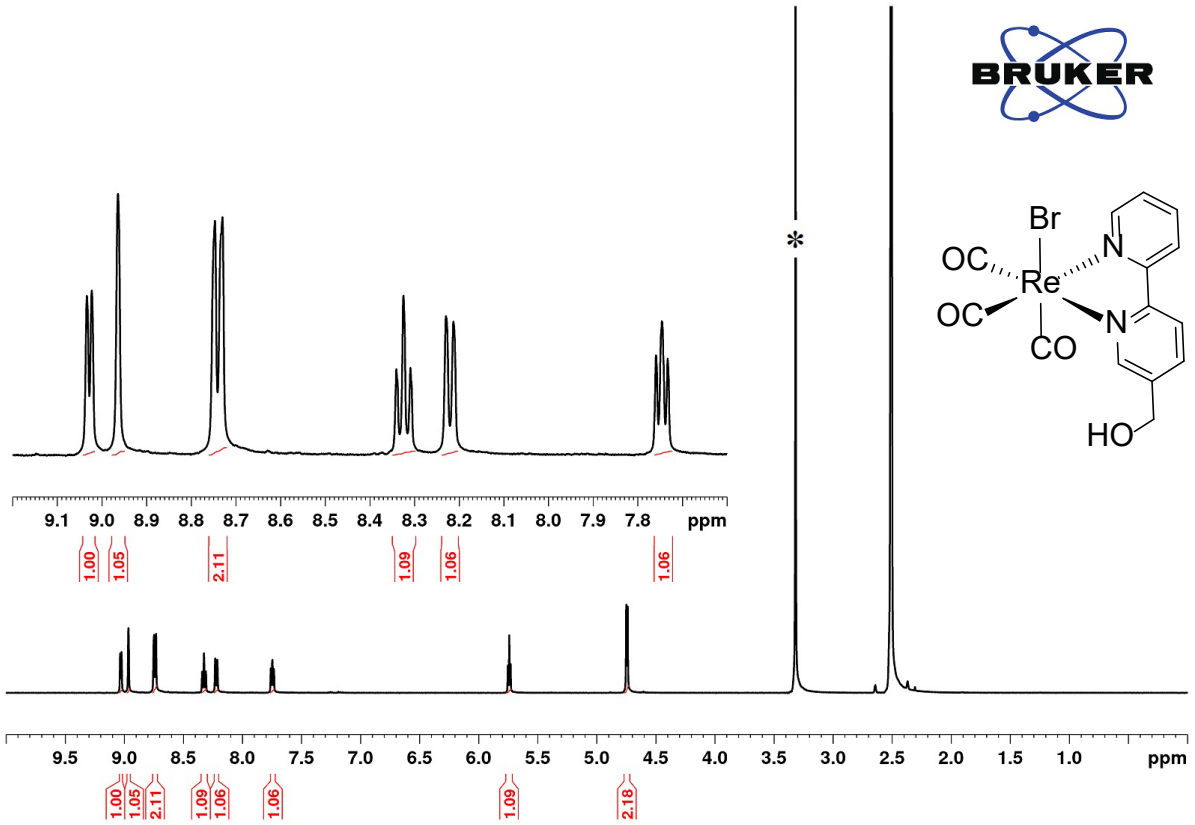


Figure S7. 400 MHz ^{1}H-NMR of **8** (in DMSO, ✻= solvent residual peak).

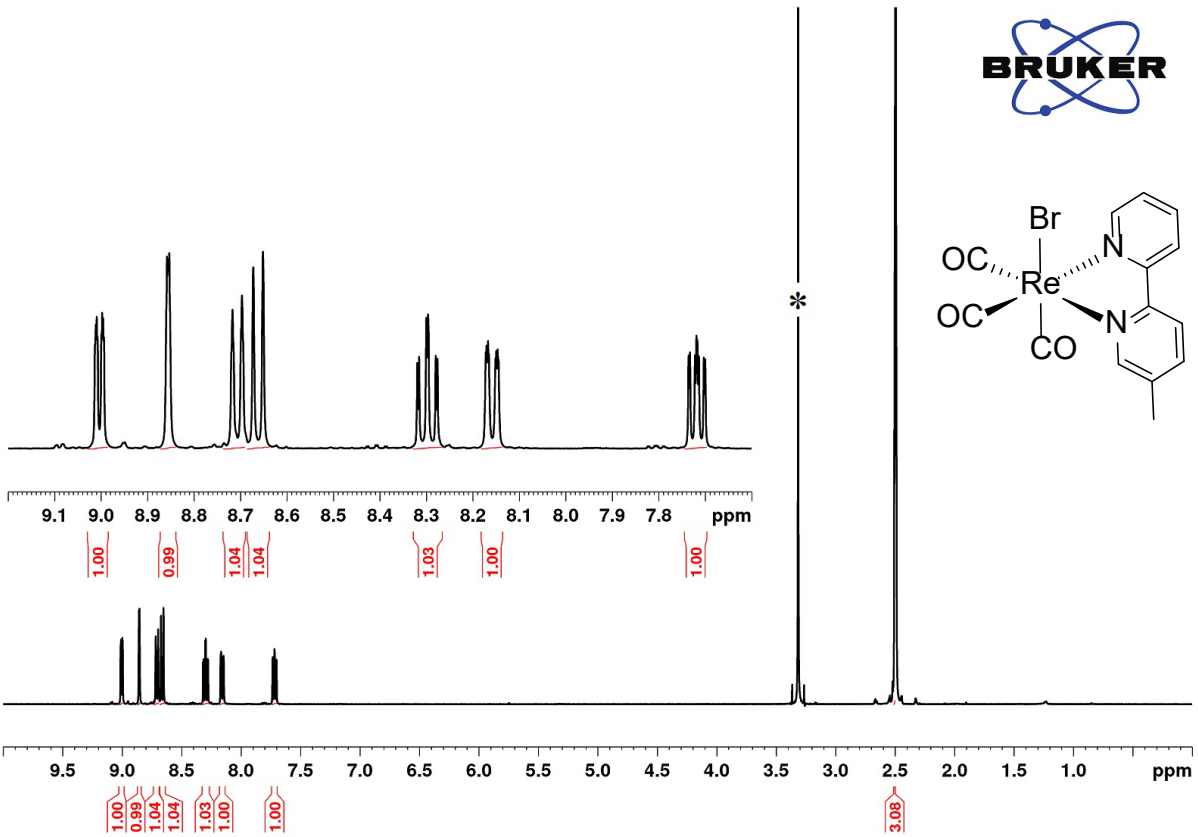


Figure S8. 400 MHz ^{1}H-NMR of **9** (in DMSO, ✻= solvent residual peak)

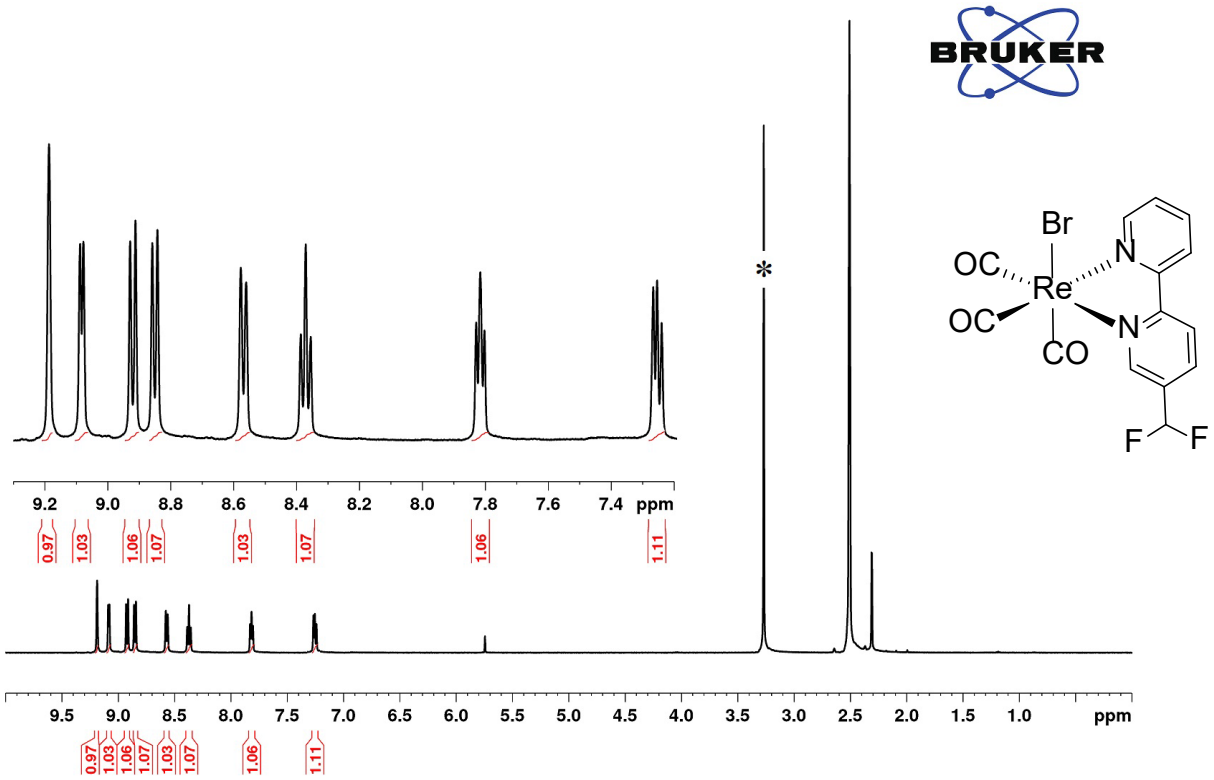


Figure S9. 400 MHz ^{1}H-NMR of **10** (in DMSO, ✻= solvent residual peak).

^{13}C-NMR spectra

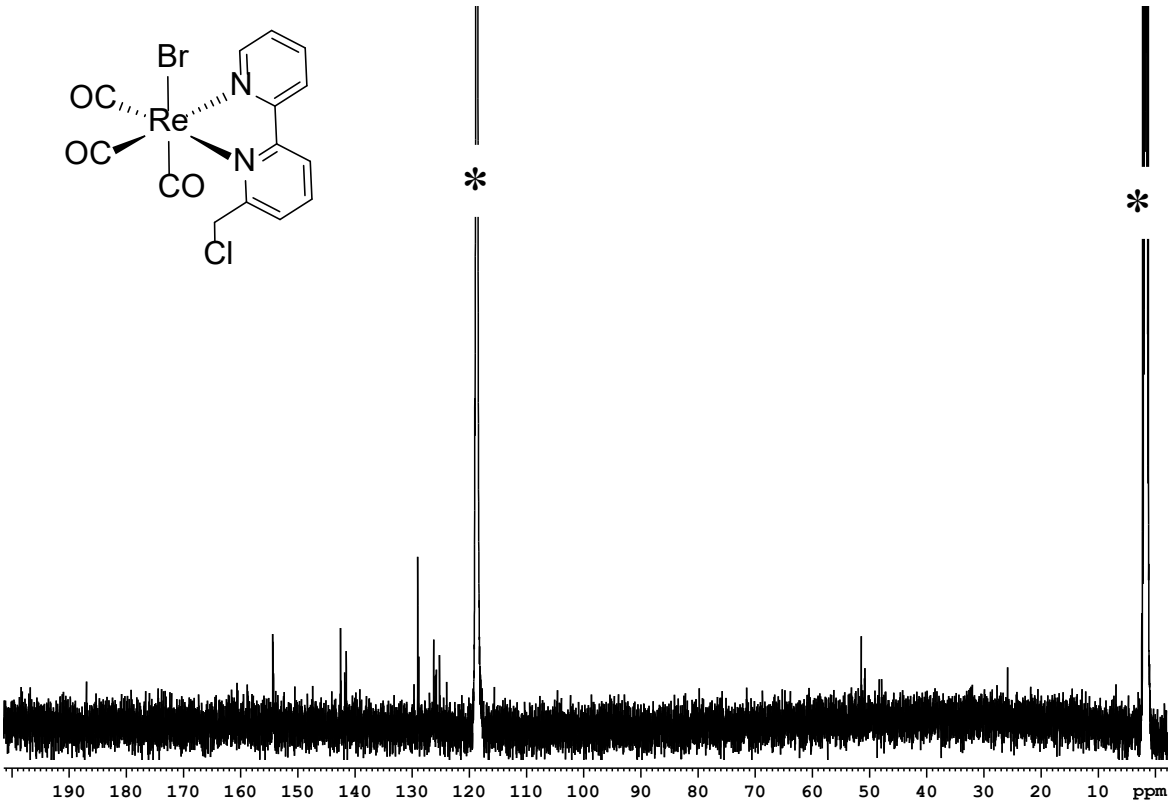


Figure S10. 126 MHz ^{13}C-NMR of **2** (in acetonitrile-d3, ✻= solvent residual peak).

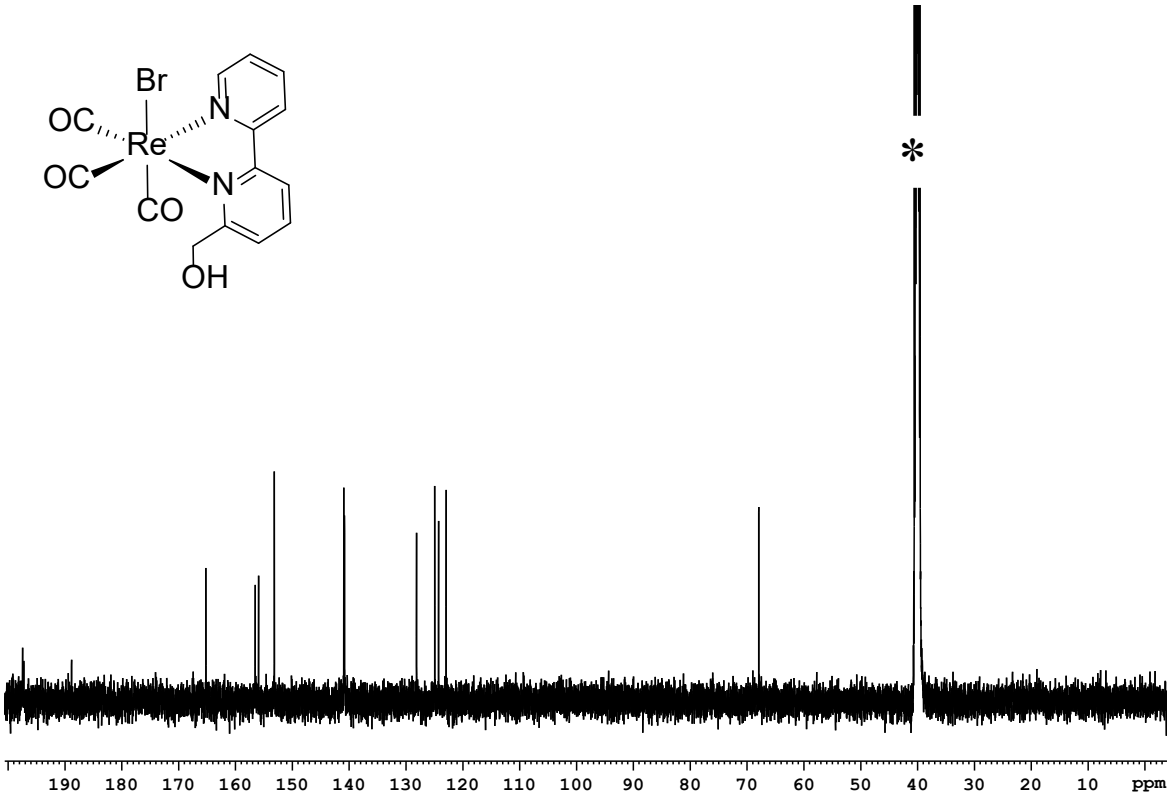


Figure S11. 126 MHz ^{13}C-NMR of **3** (in DMSO, ✻= solvent residual peak).

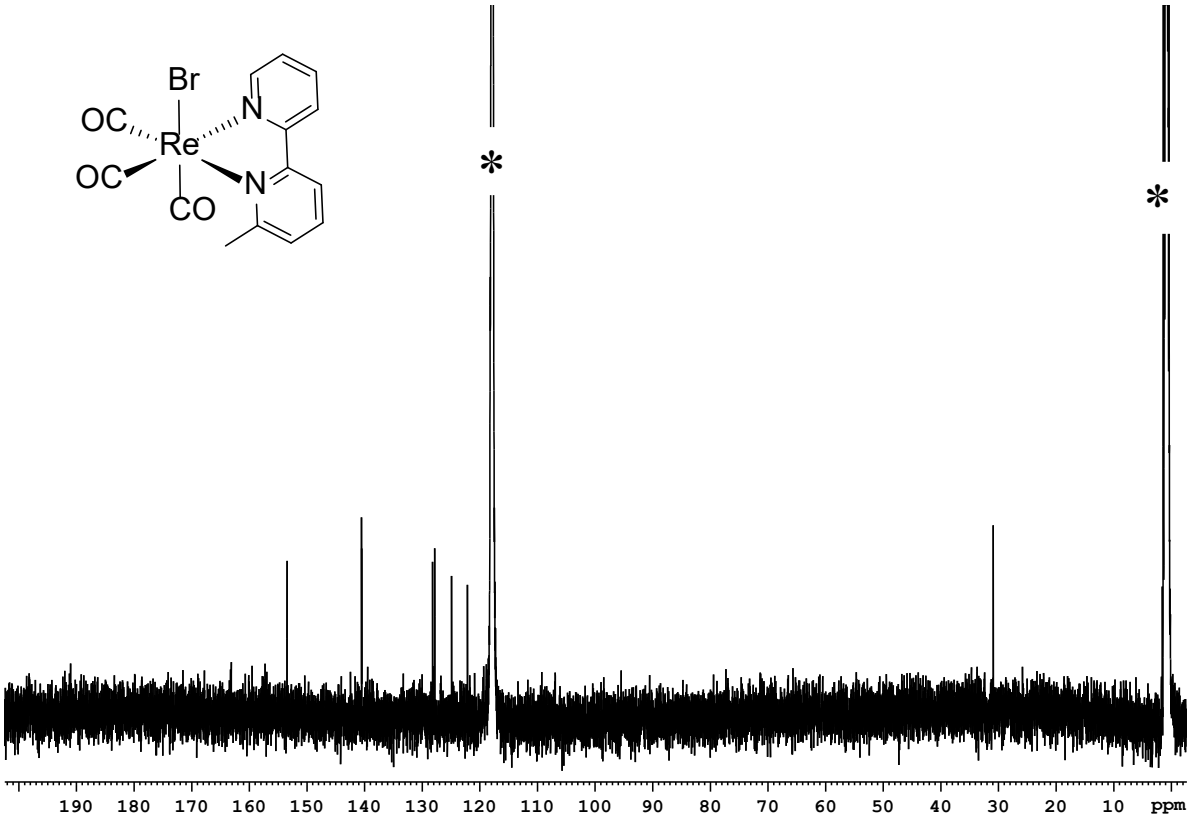


Figure S12. 126 MHz ^{13}C-NMR of **4** (in acetonitrile-d3, ✻= solvent residual peak).

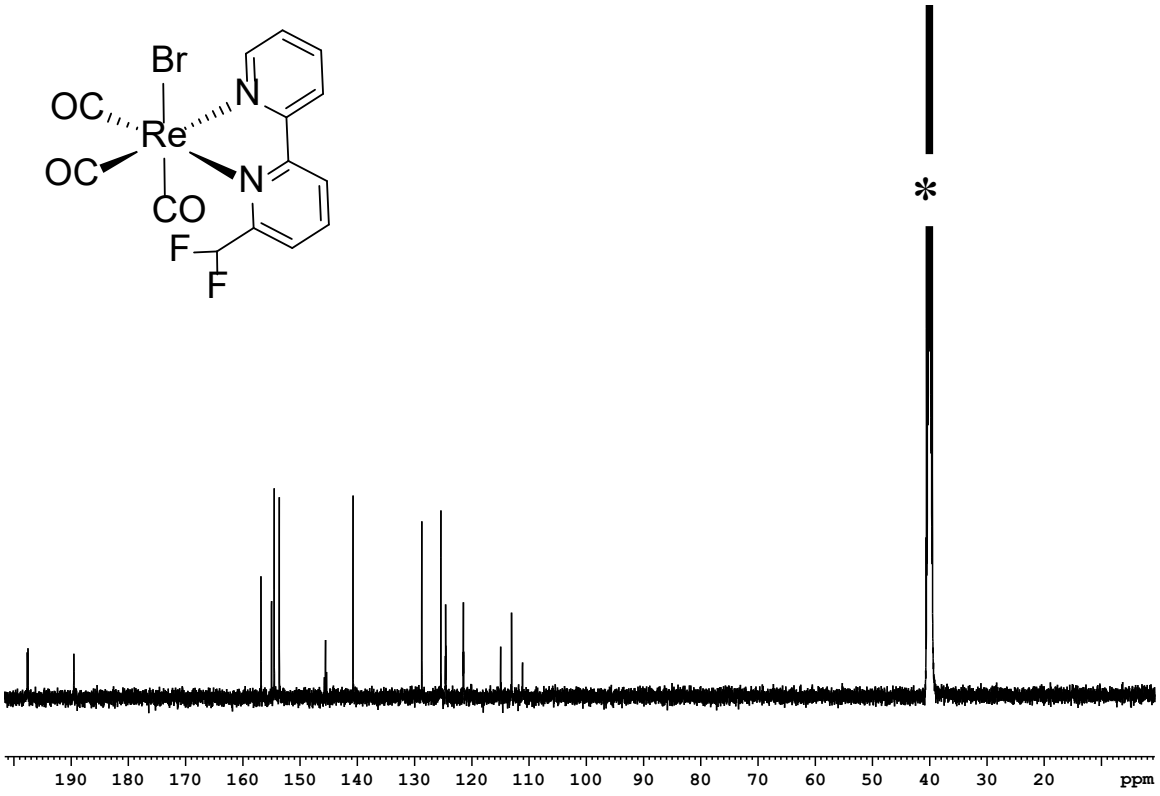


Figure S13. 126 MHz ^{13}C-NMR of **5** (in DMSO, ✻= solvent residual peak).

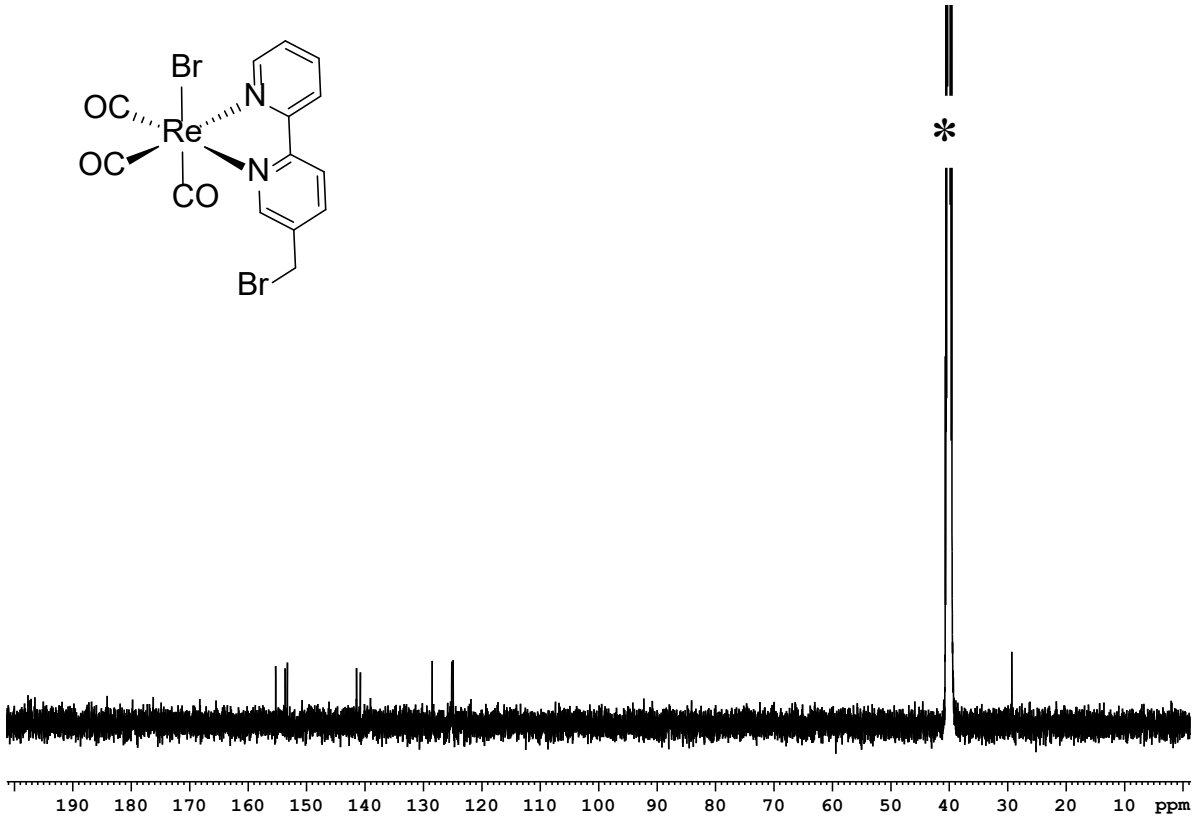


Figure S14. 126 MHz ^{13}C-NMR of **6** (in DMSO, ✻= solvent residual peak).

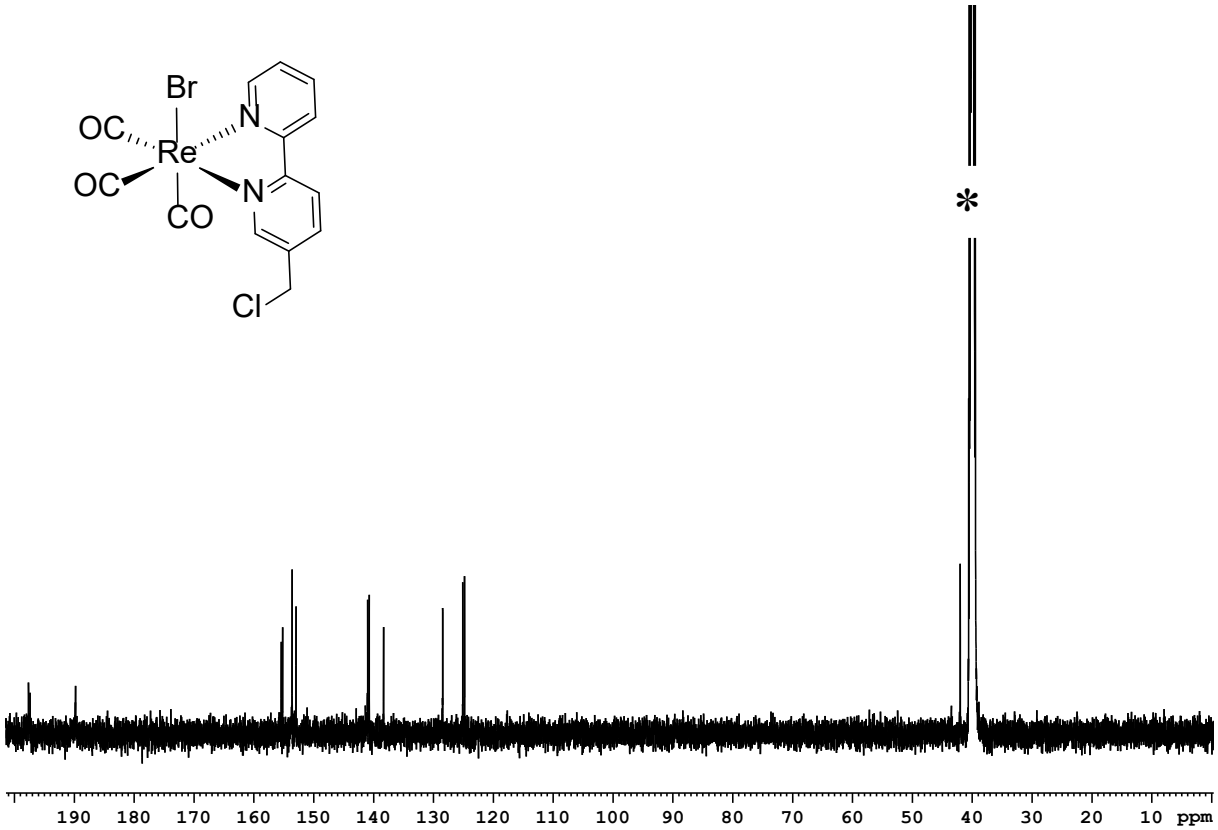


Figure S15. 126 MHz ^{13}C-NMR of **7** (in DMSO, ✻= solvent residual peak).

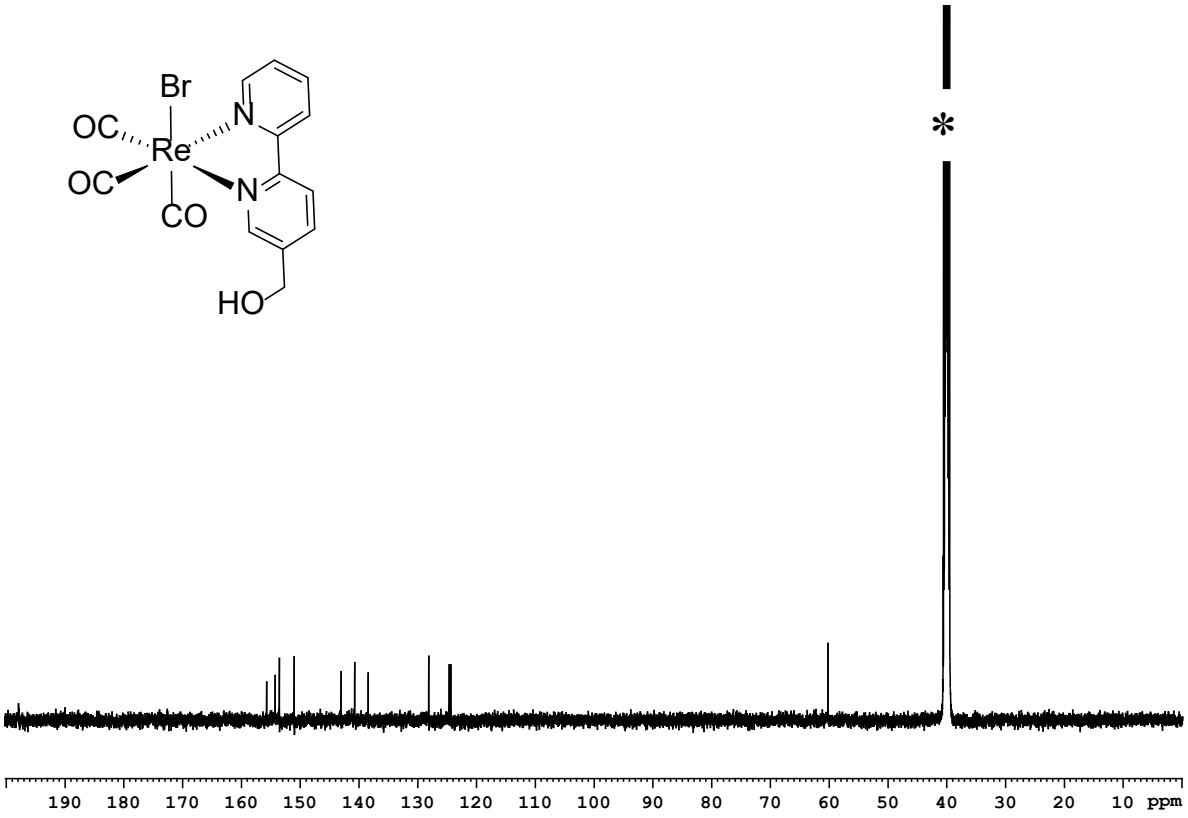


Figure S16. 126 MHz ^{13}C-NMR of **8** (in DMSO, ✻= solvent residual peak).

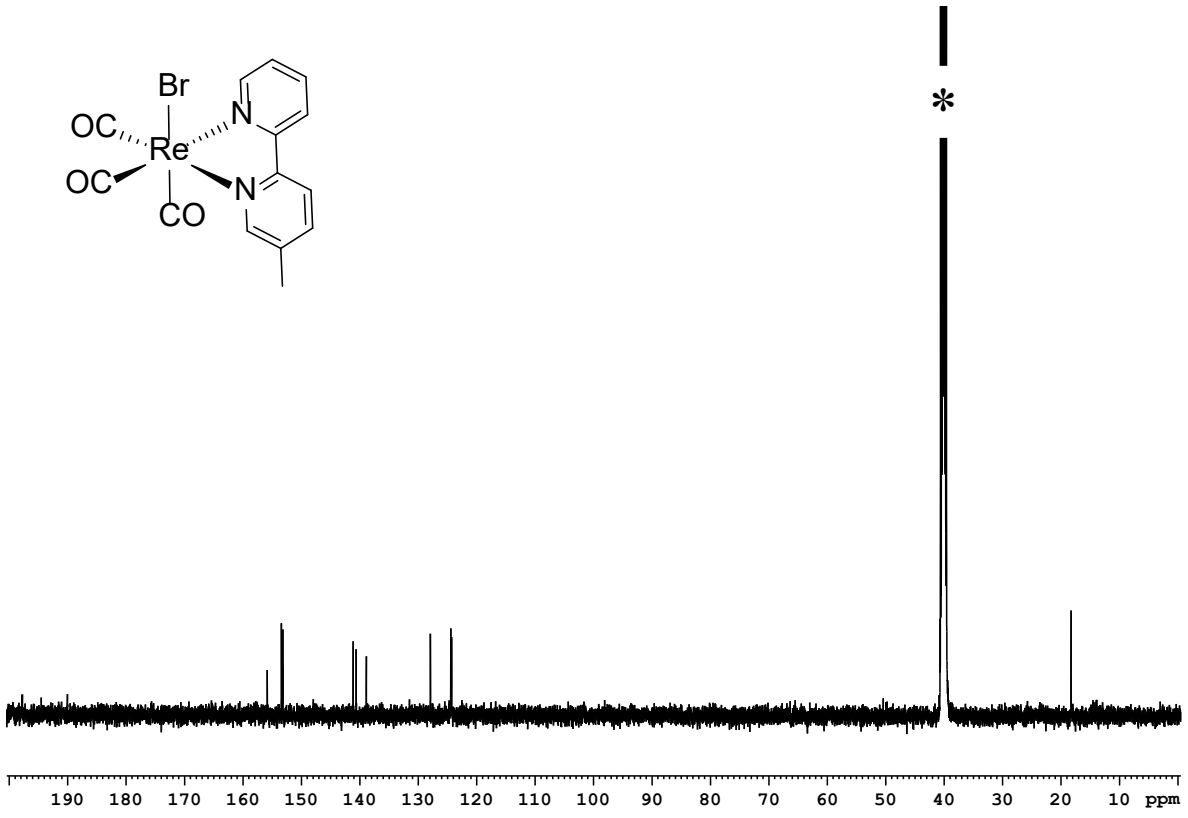


Figure S17. 126 MHz ^{13}C-NMR of **9** (in DMSO, ✻= solvent residual peak).

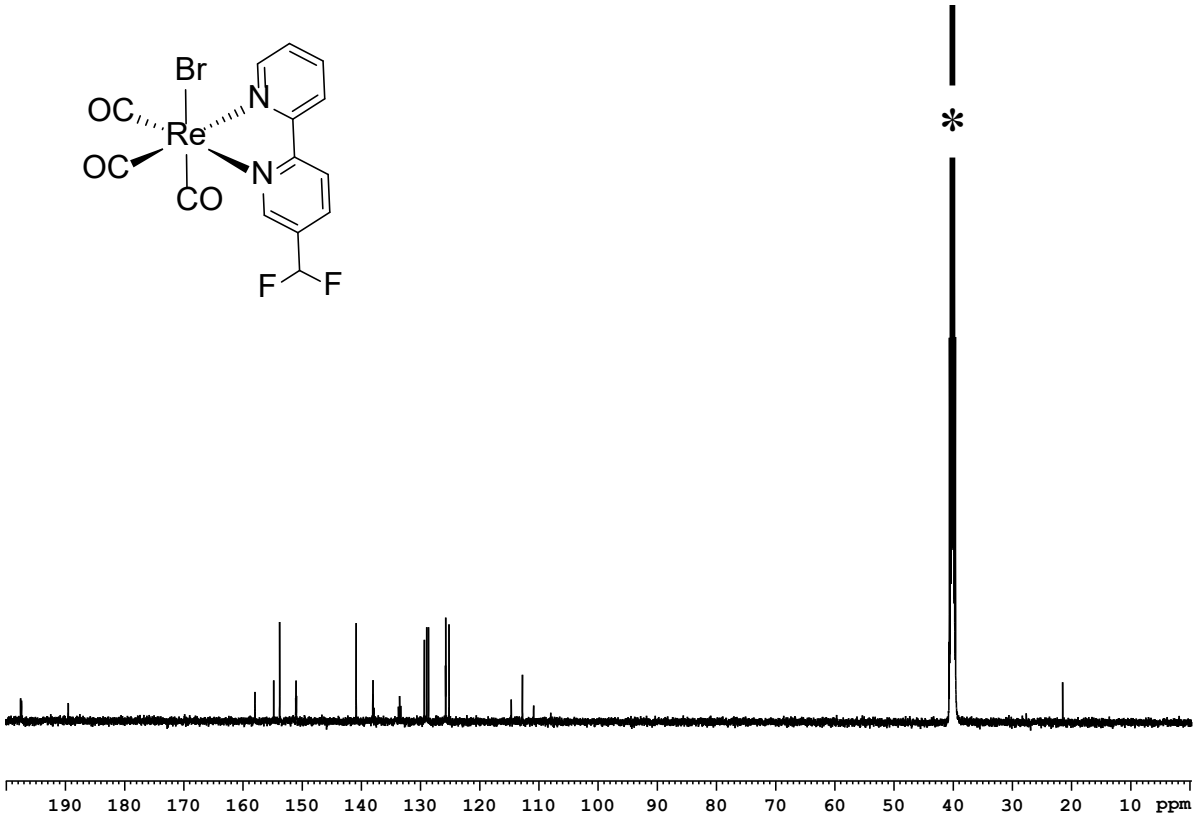


Figure S18. 126 MHz ^{13}C-NMR of **10** (in DMSO, ✻= solvent residual peak).

IR spectra

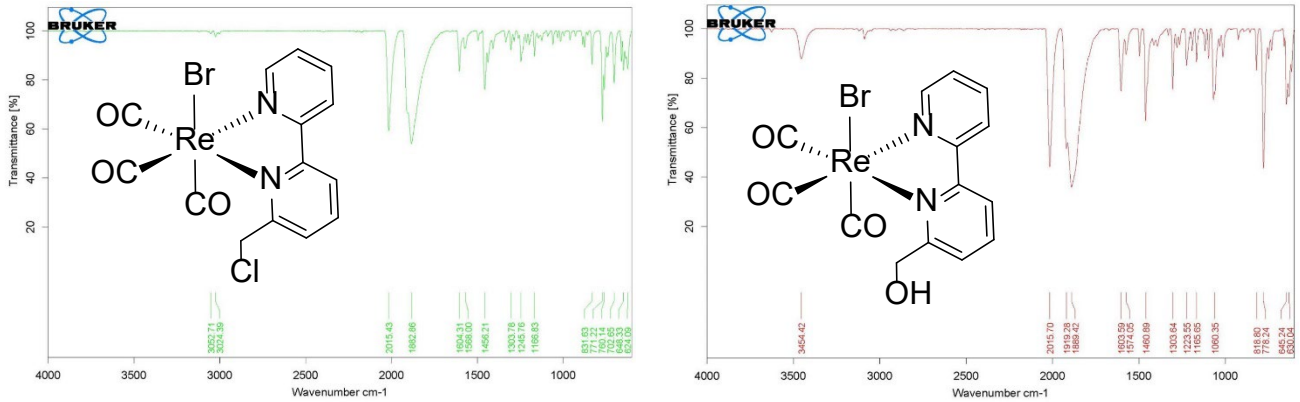


Figure S19. IR spectra of **2** (left) and **3**.

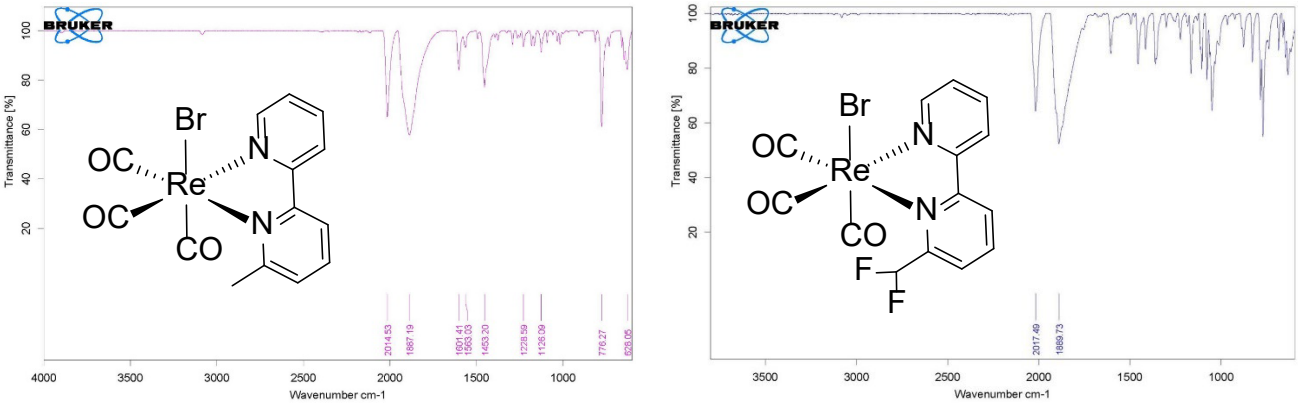


Figure S20. IR spectra of **4** (left) and **5**.

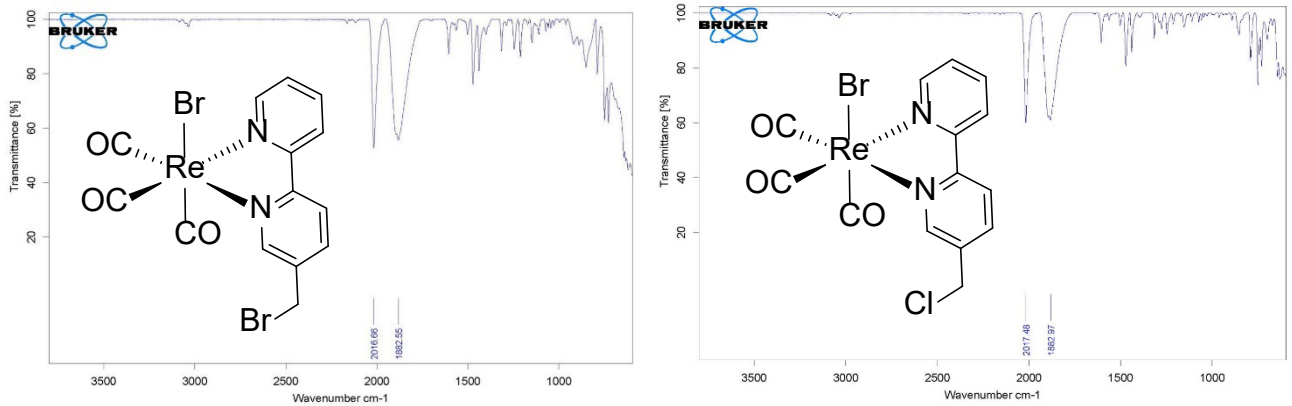


Figure S21. IR spectra of **6** (left) and **7**.

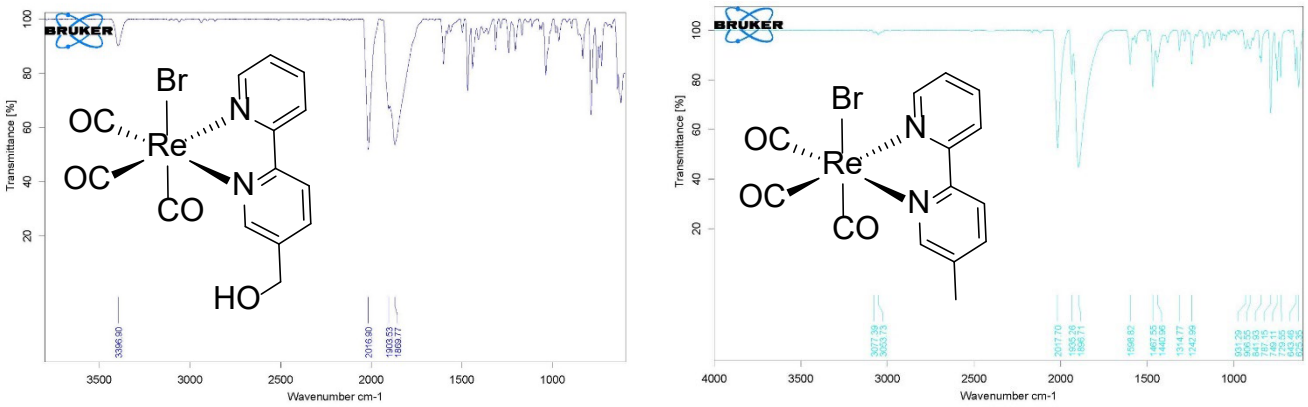


Figure S22. IR spectra of **8** (left) and **9**.

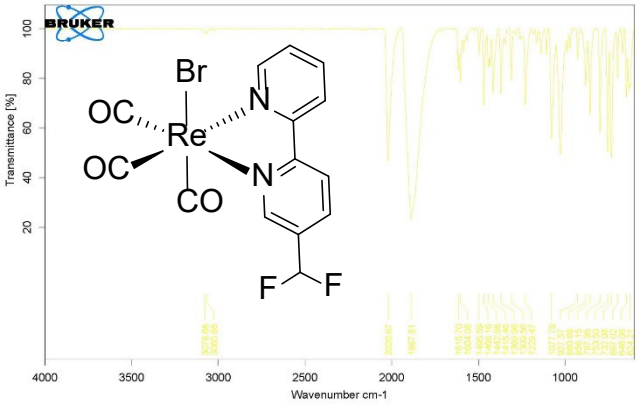


Figure S23. IR spectrum of **10**.

UV-Vis spectra

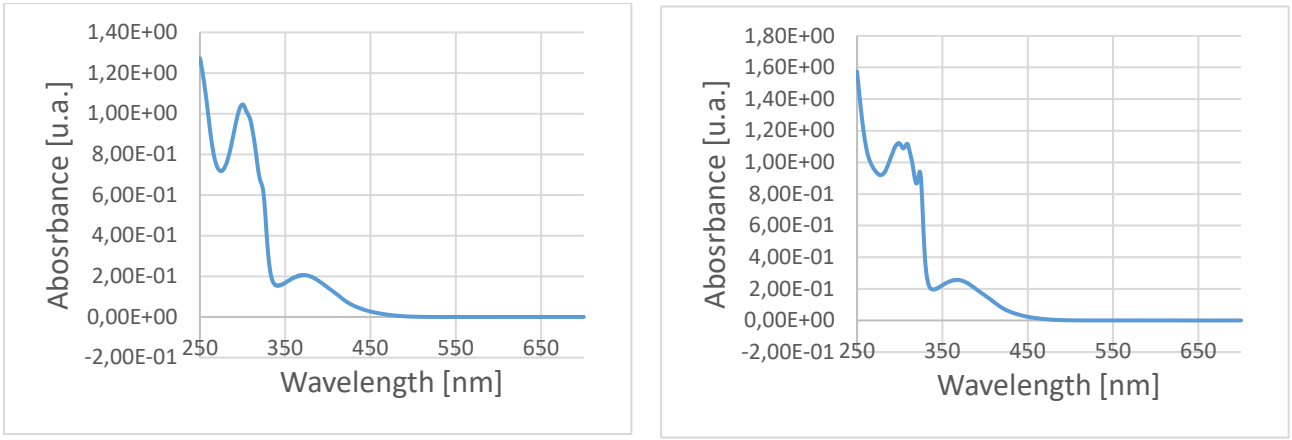


Figure S24. UV-Vis spectrum of **2** (left) and **3** in Acetonitrile.

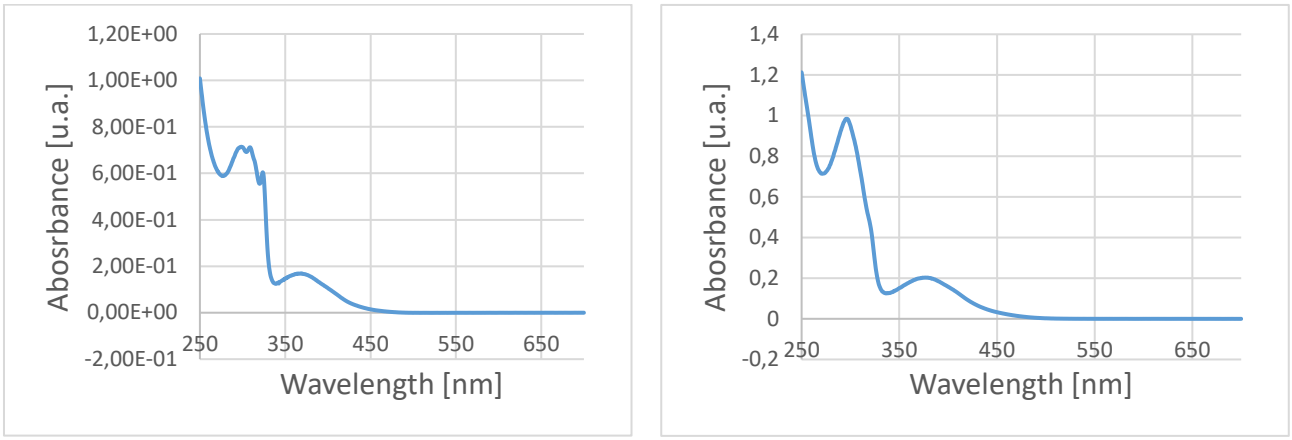


Figure S25. UV-Vis spectrum of **4** (left) and **5** in Acetonitrile.

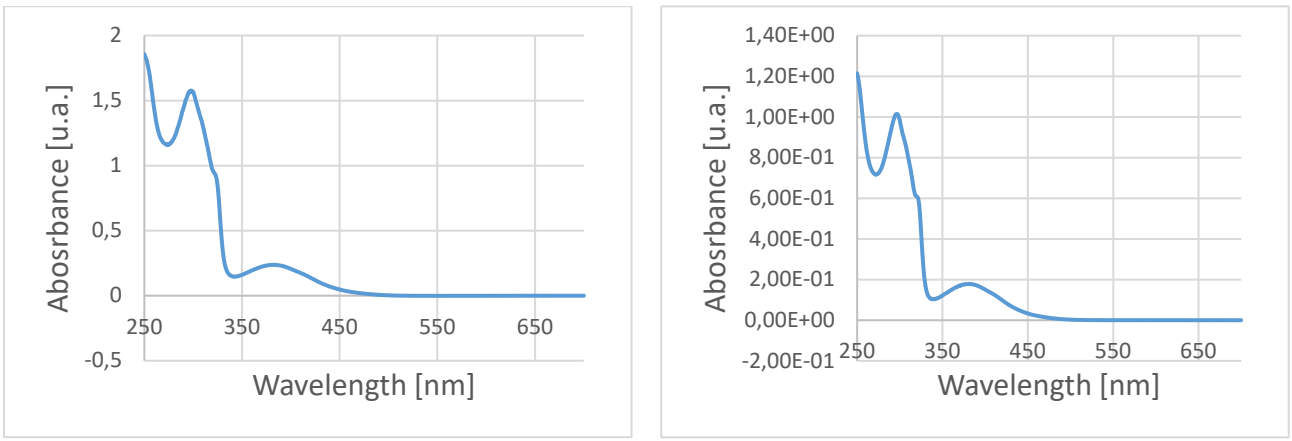
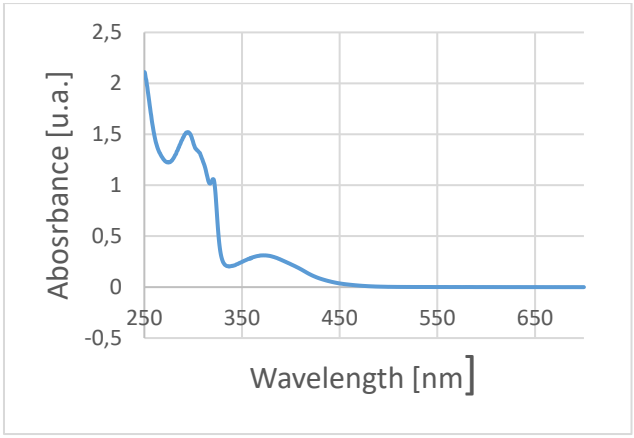


Figure S26. UV-Vis spectrum of **6** (left) and **7** in Acetonitrile.



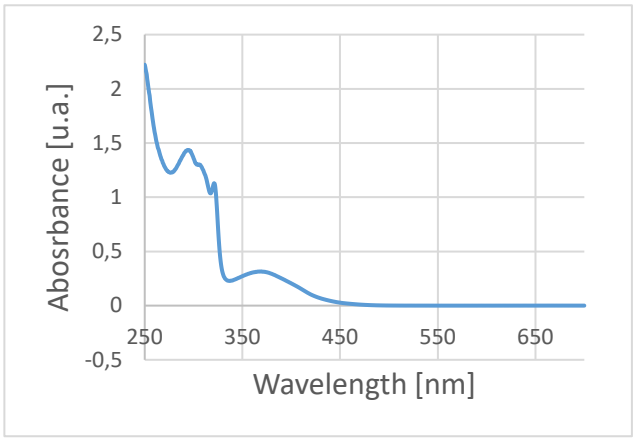


Figure S27. UV-Vis spectrum of **8** (left) and **9** in Acetonitrile.

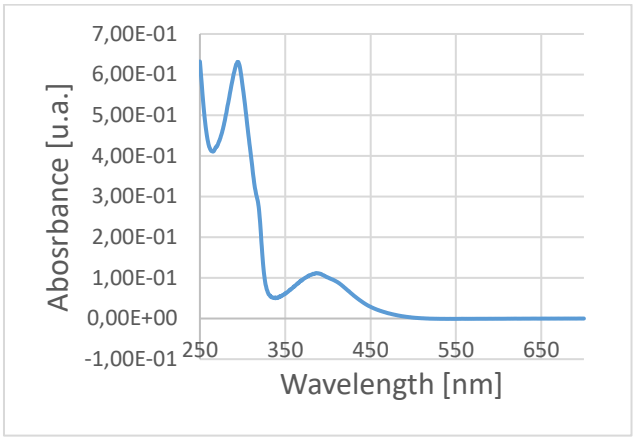


Figure S28. UV-Vis spectrum of **10** in Acetonitrile.