

SUPPORTING INFORMATION FOR

In vitro anticancer activity of α -diimine rhenium dicarbonyl complexes and their reactivity with different functional groups

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NMR spectra

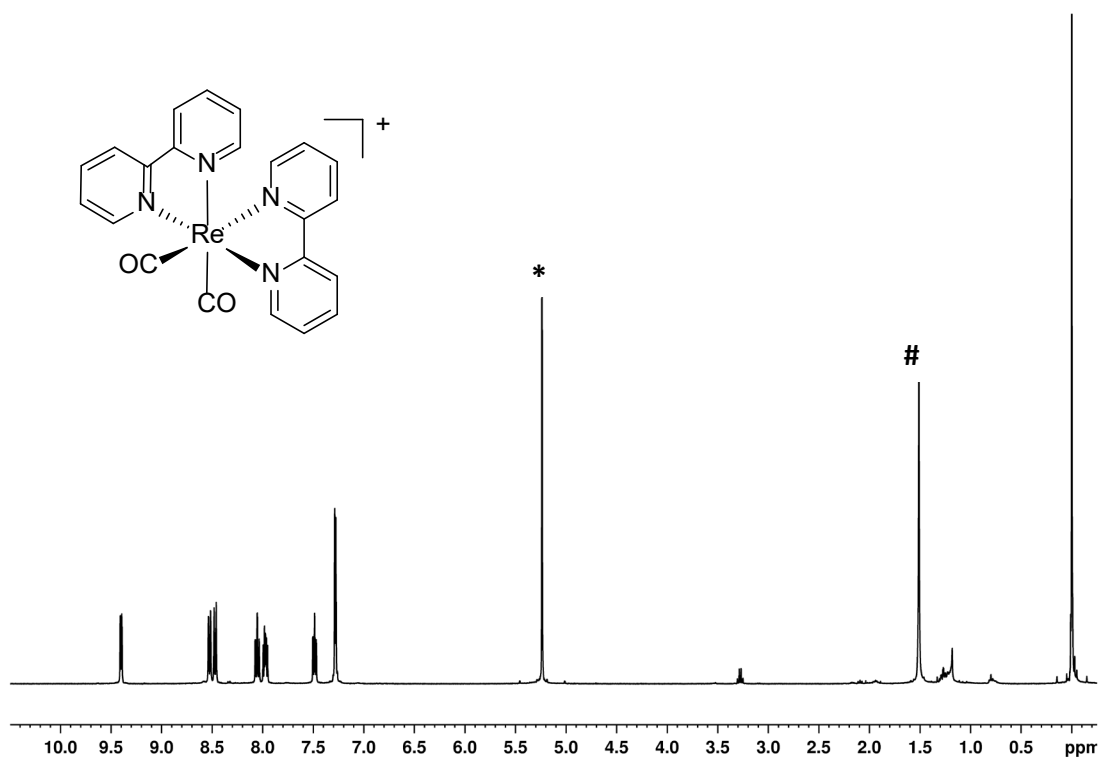


Figure S1. 400 MHz ¹H-NMR of **6a** (in CD₂Cl₂, * = solvent residual peak of DCM, # = solvent residual peaks of water).

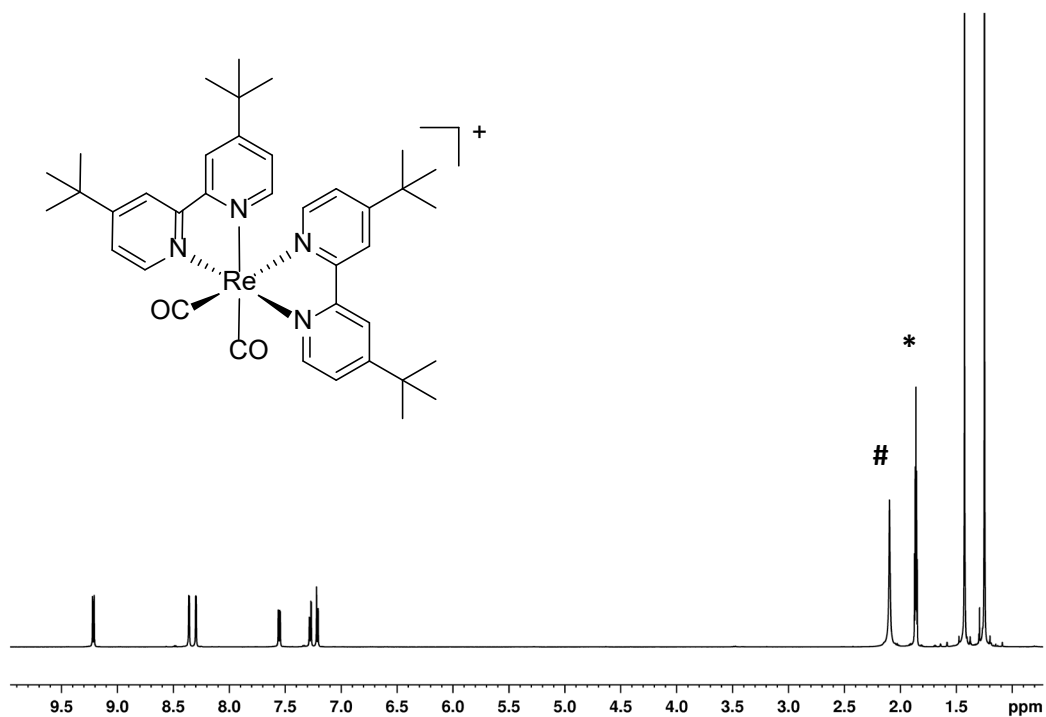


Figure S2. 400 MHz ¹H-NMR of **6b** (in CD₃CN, * = solvent residual peak of CH₃CN, # = solvent residual peaks of water).

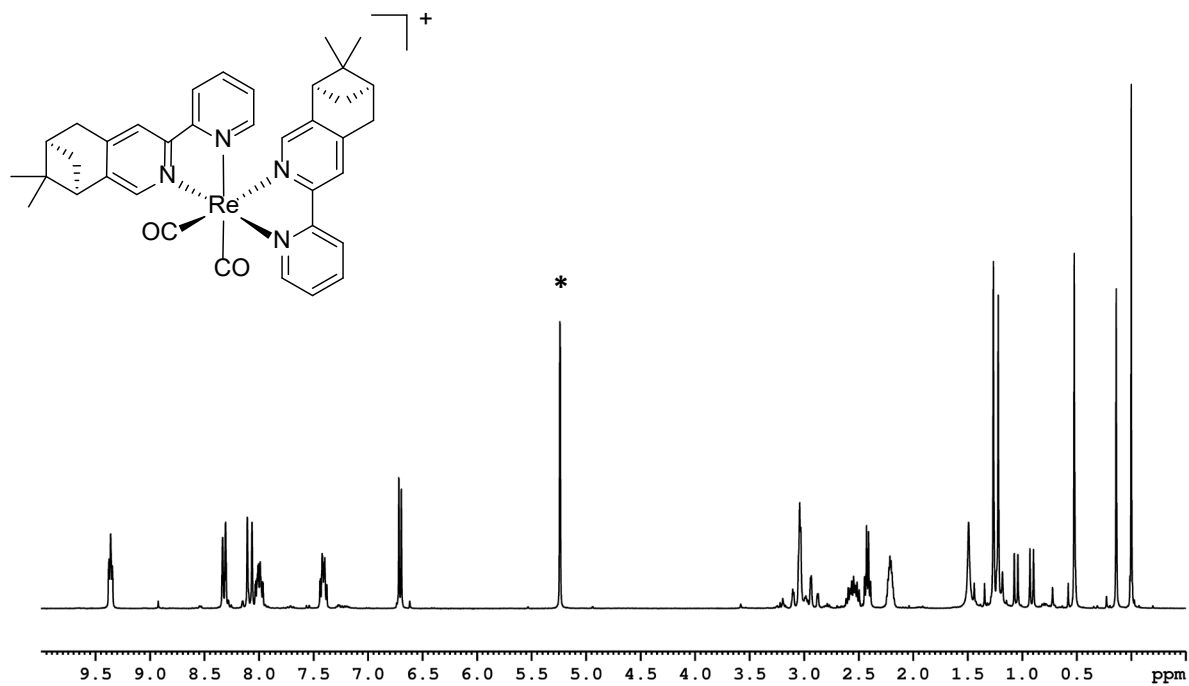


Figure S3. 300 MHz ¹H-NMR of **7a** (in CD₂Cl₂, * = solvent residual peak of DCM).

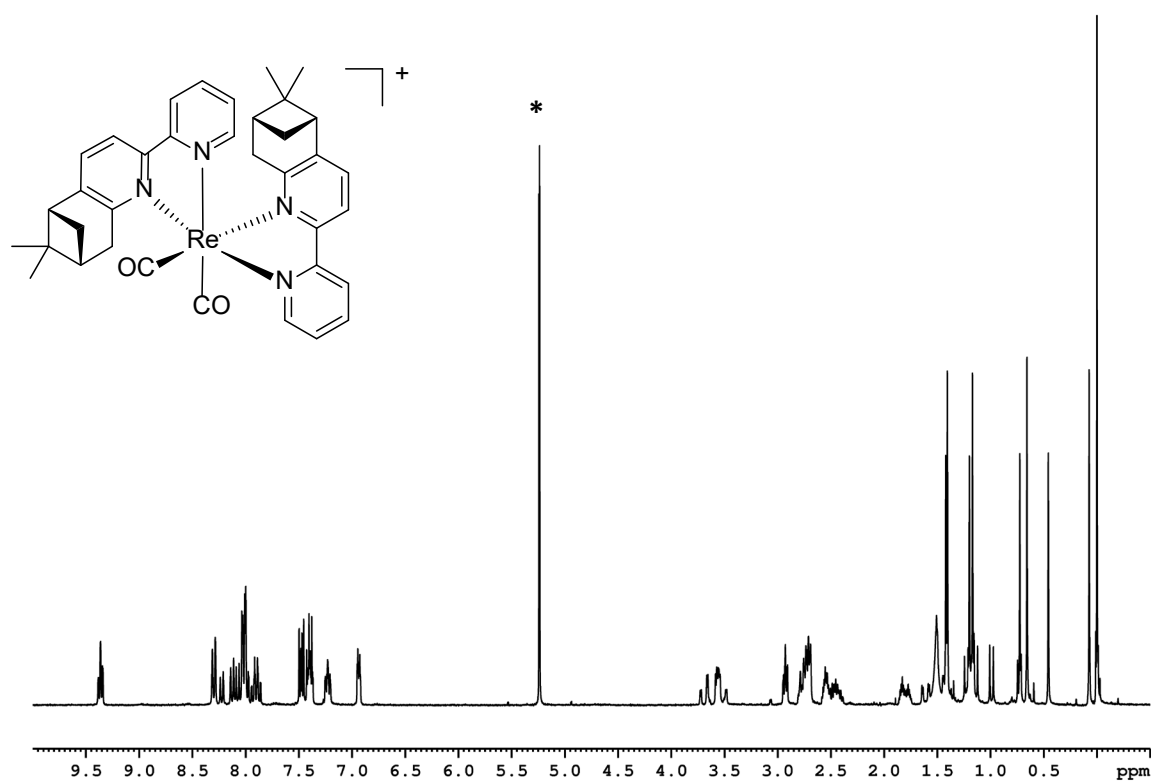


Figure S4. 300 MHz ¹H-NMR of **7b** (in CD₂Cl₂, * = solvent residual peak of DCM).

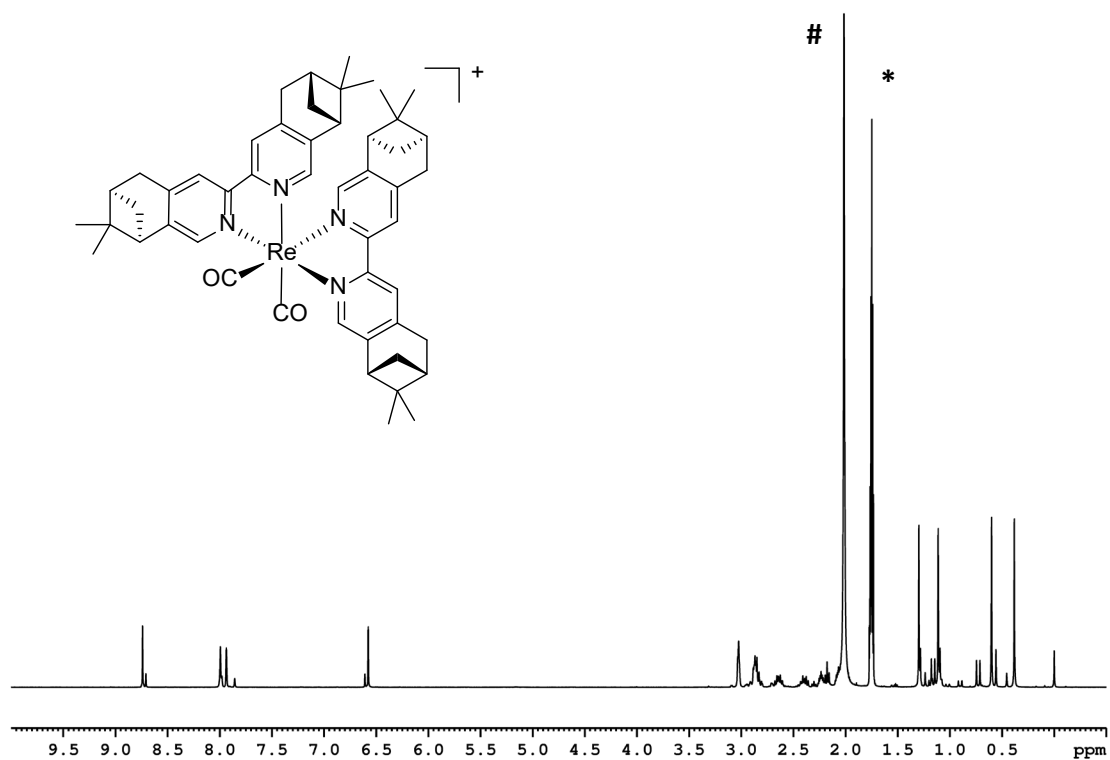


Figure S5. 300 MHz $^1\text{H-NMR}$ of **7c** (in CD_3CN , * = solvent residual peak of CH_3CN , # = solvent residual peaks of water).

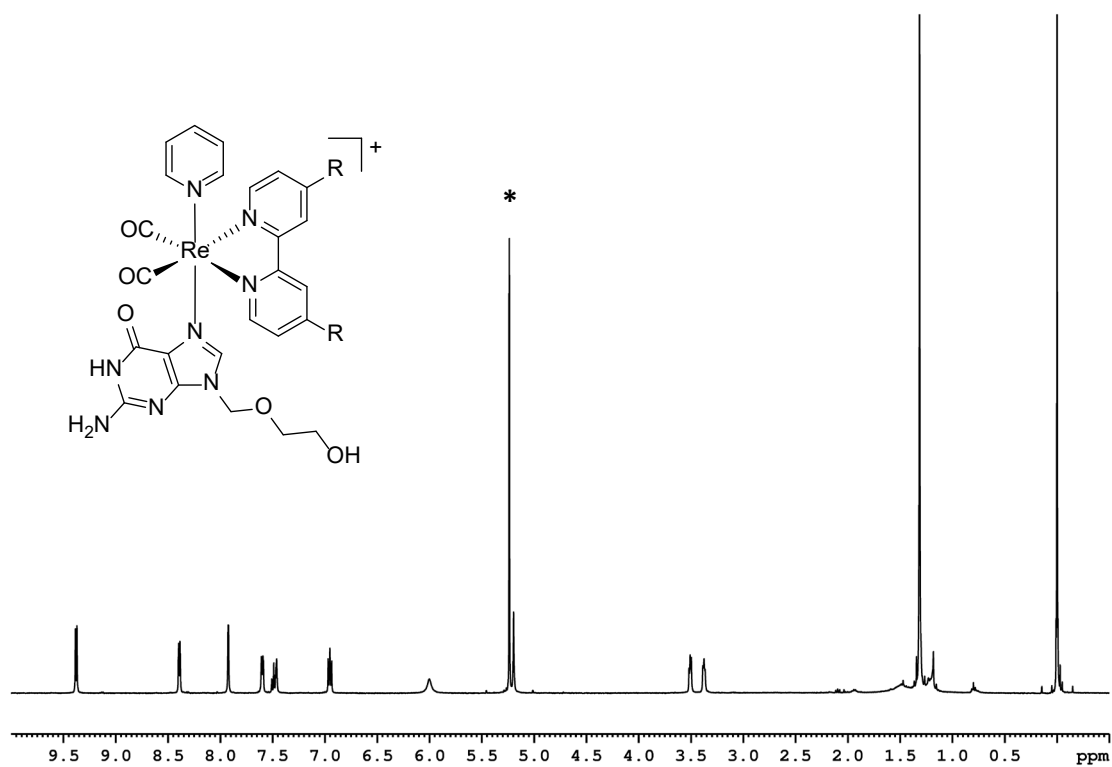


Figure S6. 400 MHz $^1\text{H-NMR}$ of **15** (in CD_2Cl_2 , * = solvent residual peak of DCM).

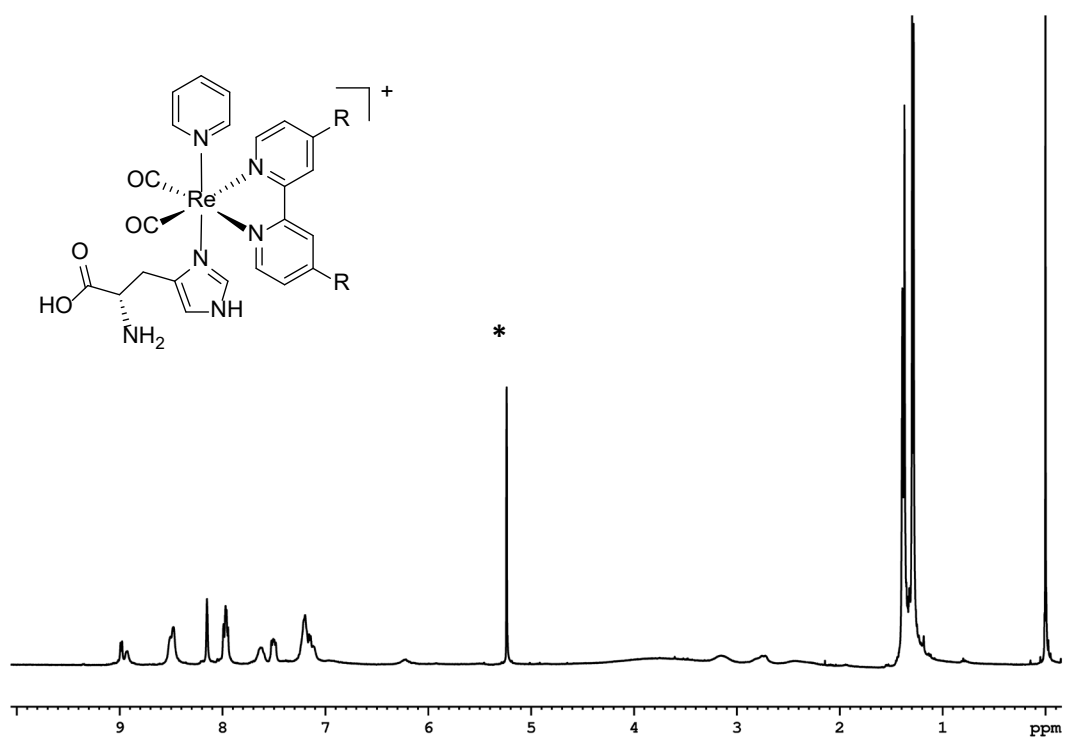


Figure S7. 400 MHz ¹H-NMR of **16** (in CD₂Cl₂, * = solvent residual peak of DCM).

IR spectra

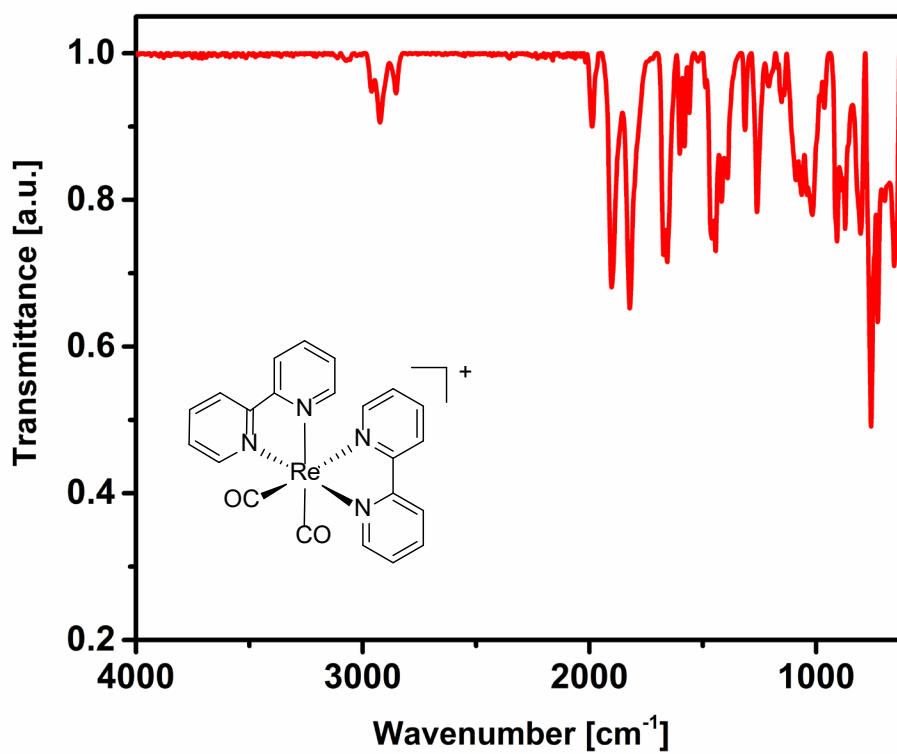


Figure S8. IR spectrum (solid) of 6a.

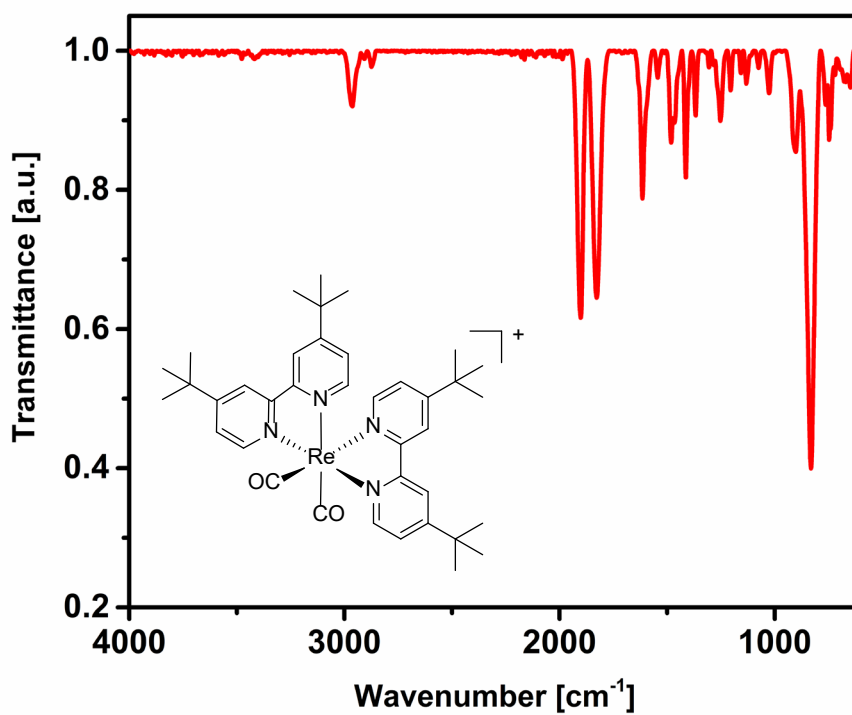


Figure S9. IR spectrum (solid) of 6b.

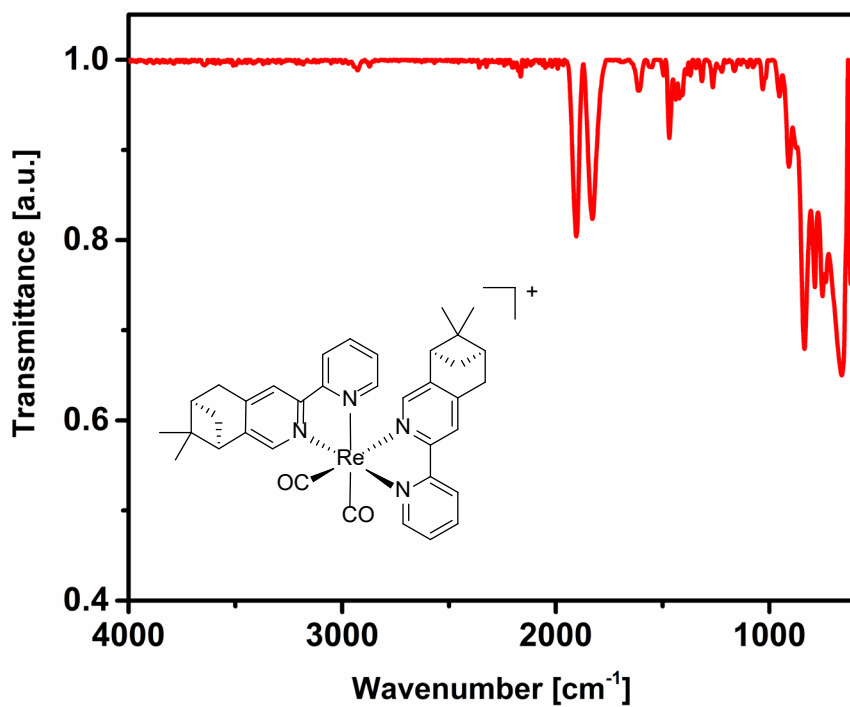


Figure S10. IR spectrum (solid) of 7a.

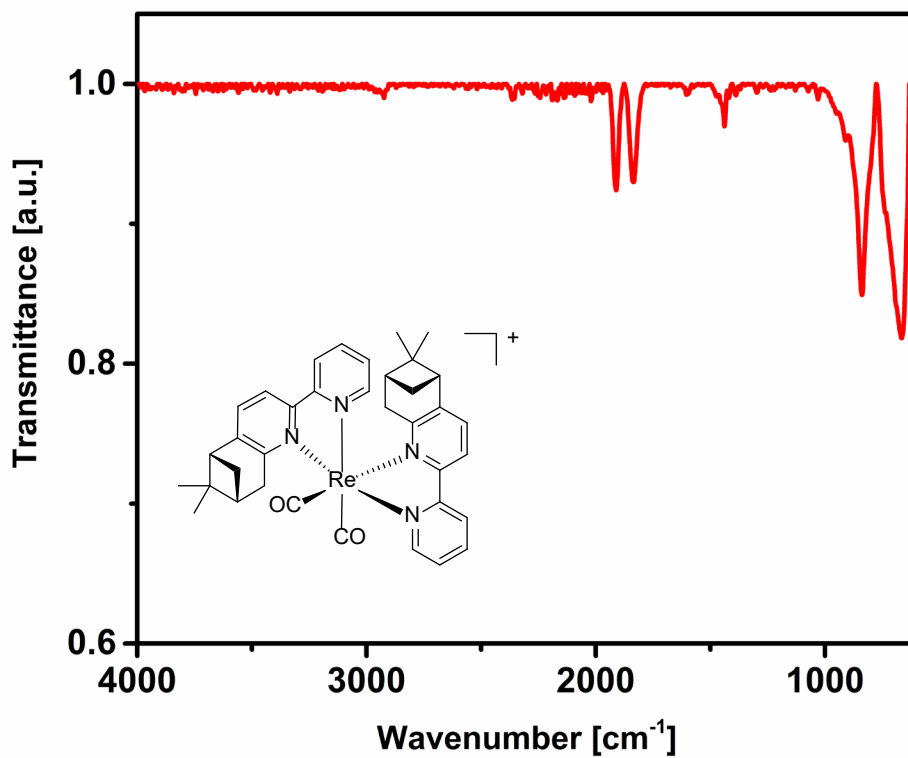


Figure S11. IR spectrum (solid) of 7b.

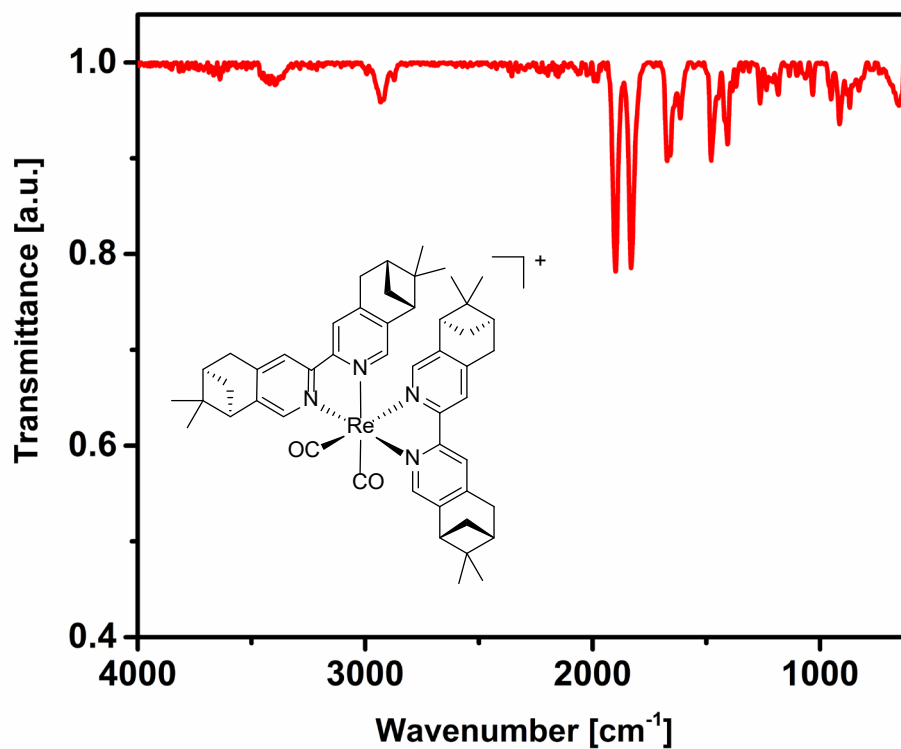


Figure S12. IR spectrum (solid) of 7c.

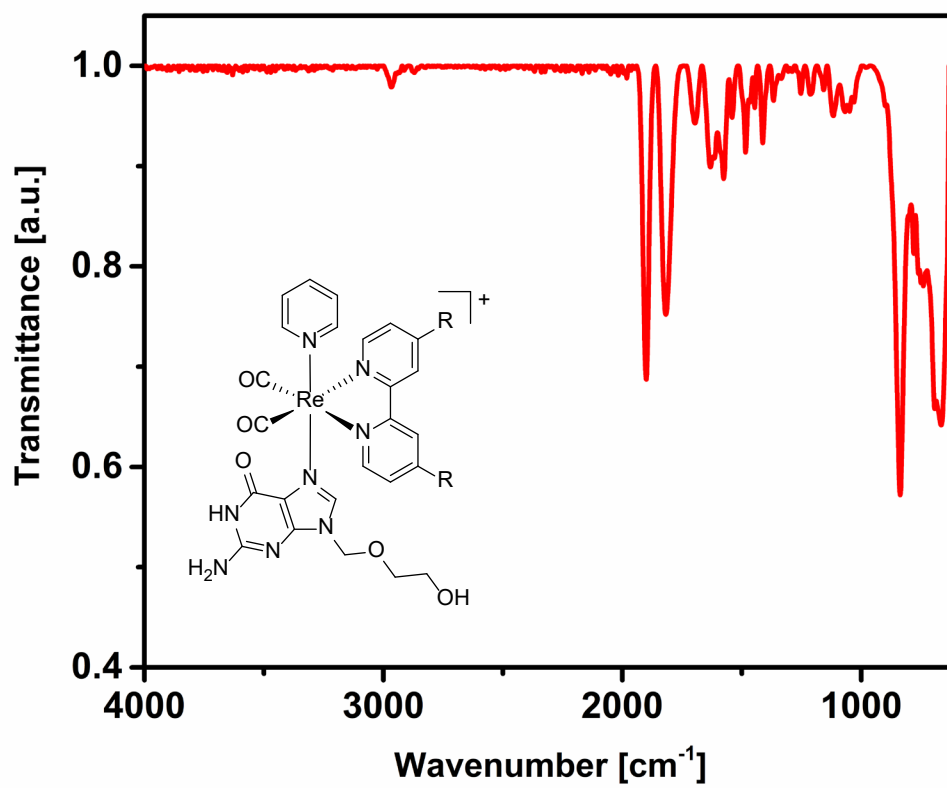


Figure S13. IR spectrum (solid) of 15.

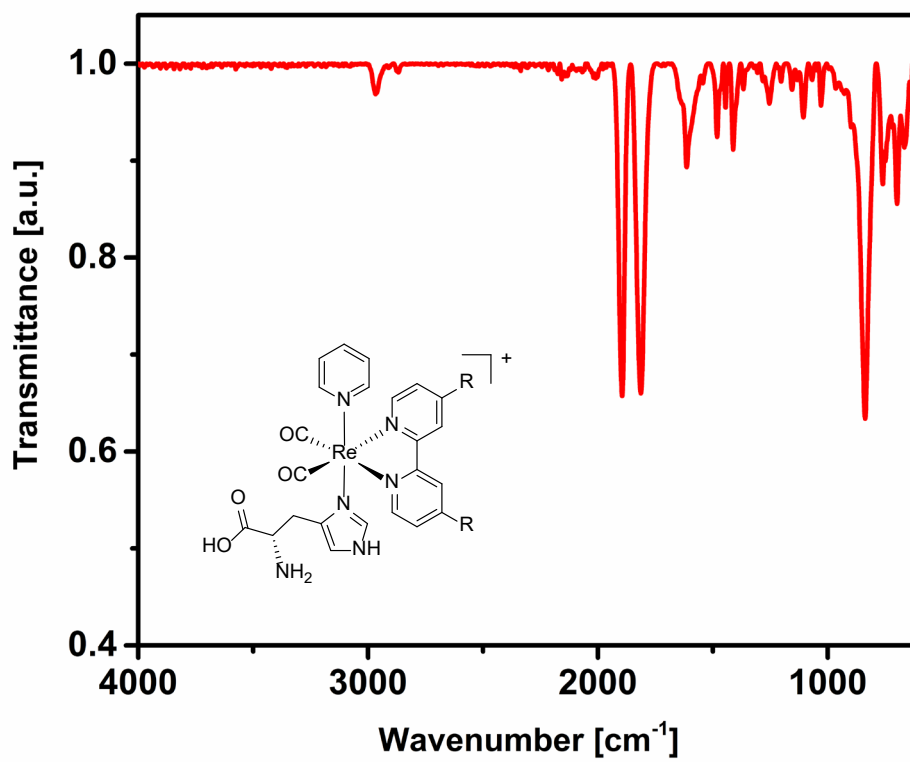


Figure S14. IR spectrum (solid) of 16.

UV-Vis spectra

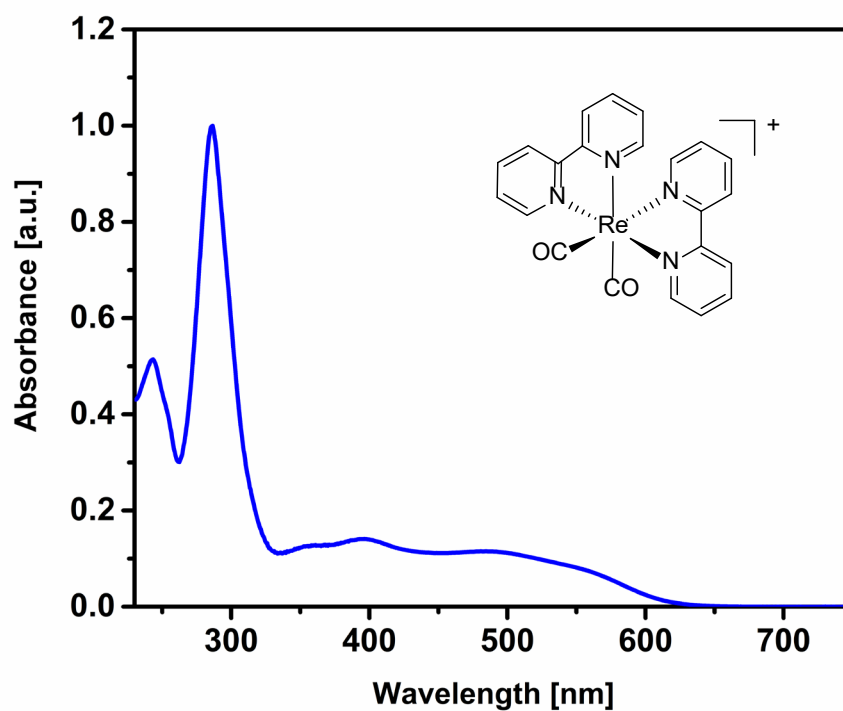


Figure S15. UV-Vis spectrum (in MeOH) of 6a.

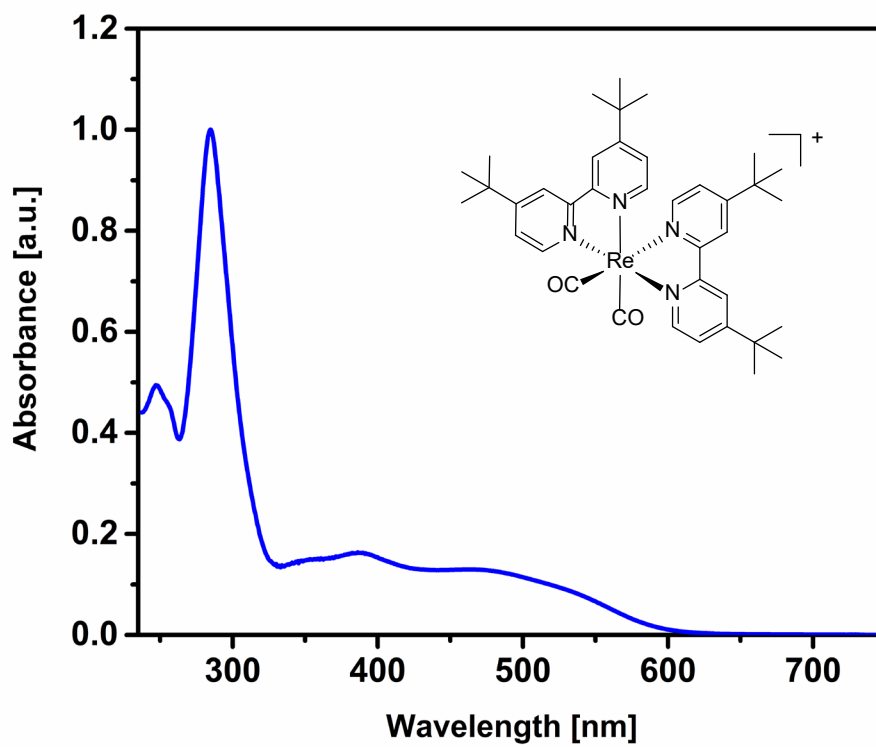


Figure S16. UV-Vis spectrum (in MeCN) of 6b.

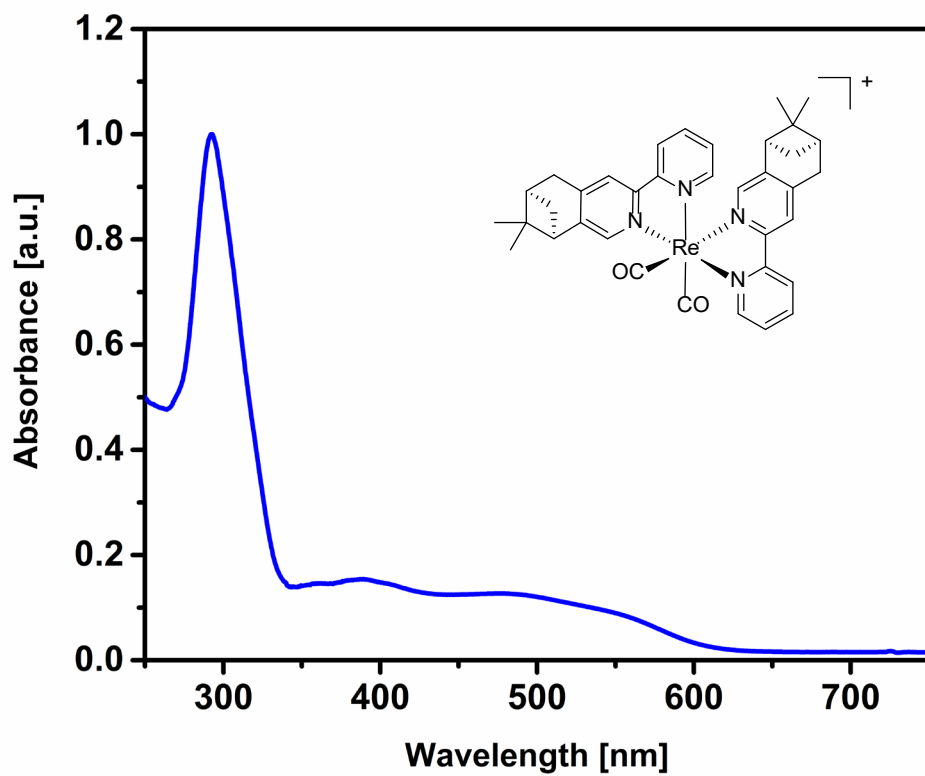


Figure S17. UV-Vis spectrum (in MeOH) of **7a**.

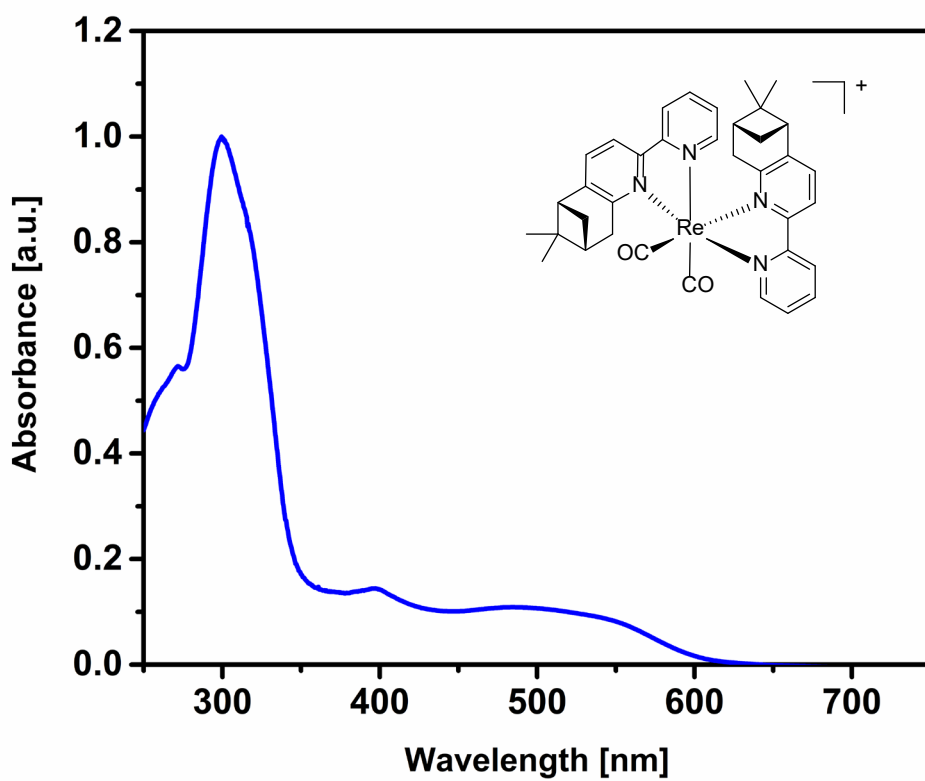


Figure S18. UV-Vis spectrum (in MeOH) of **7b**.

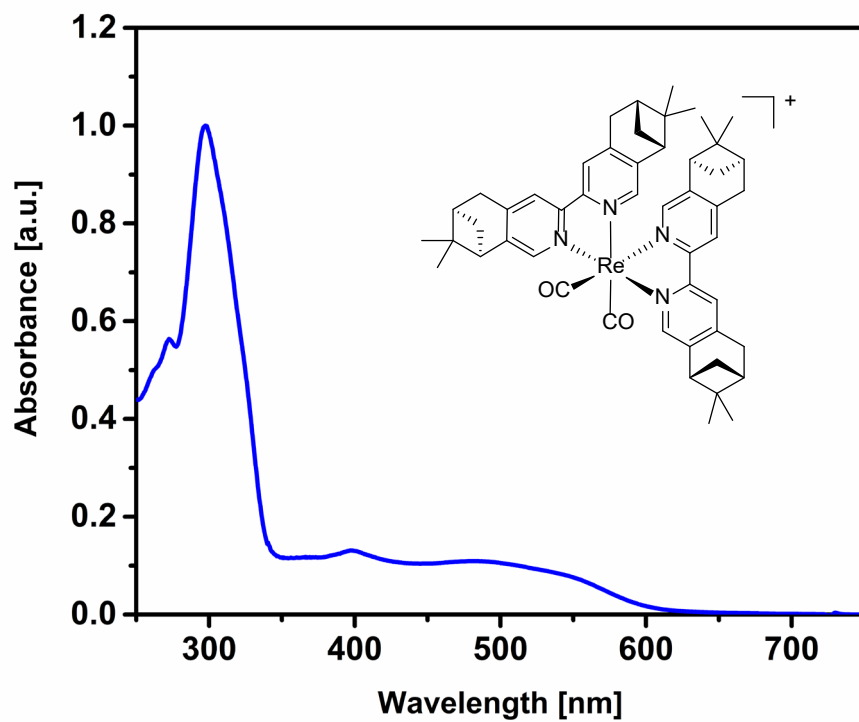


Figure S19. UV-Vis spectrum (in MeOH) of **7c**.

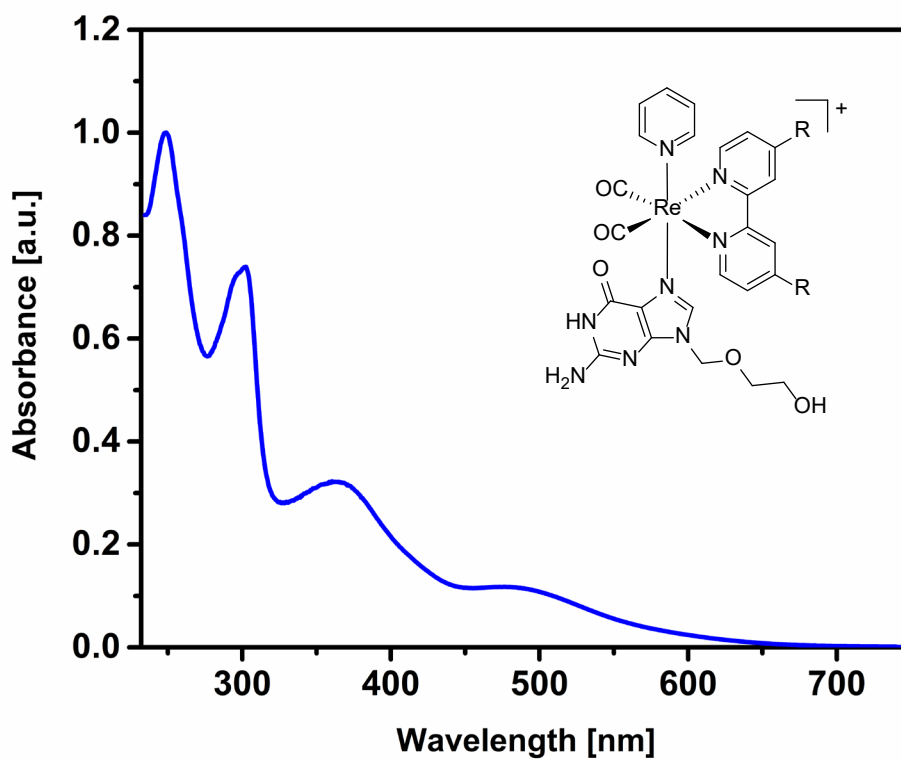


Figure S20. UV-Vis spectrum (in MeOH) of **15**.

ESI-MS

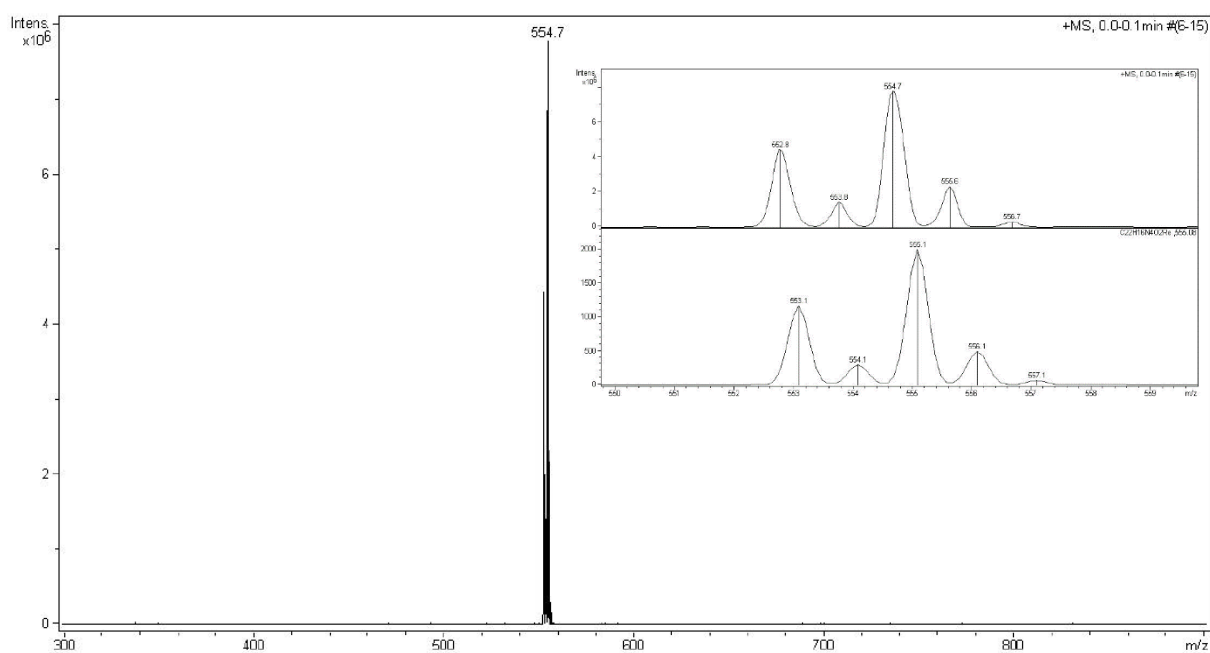


Figure S21. ESI-MS spectrum (in MeOH) of **6a**.

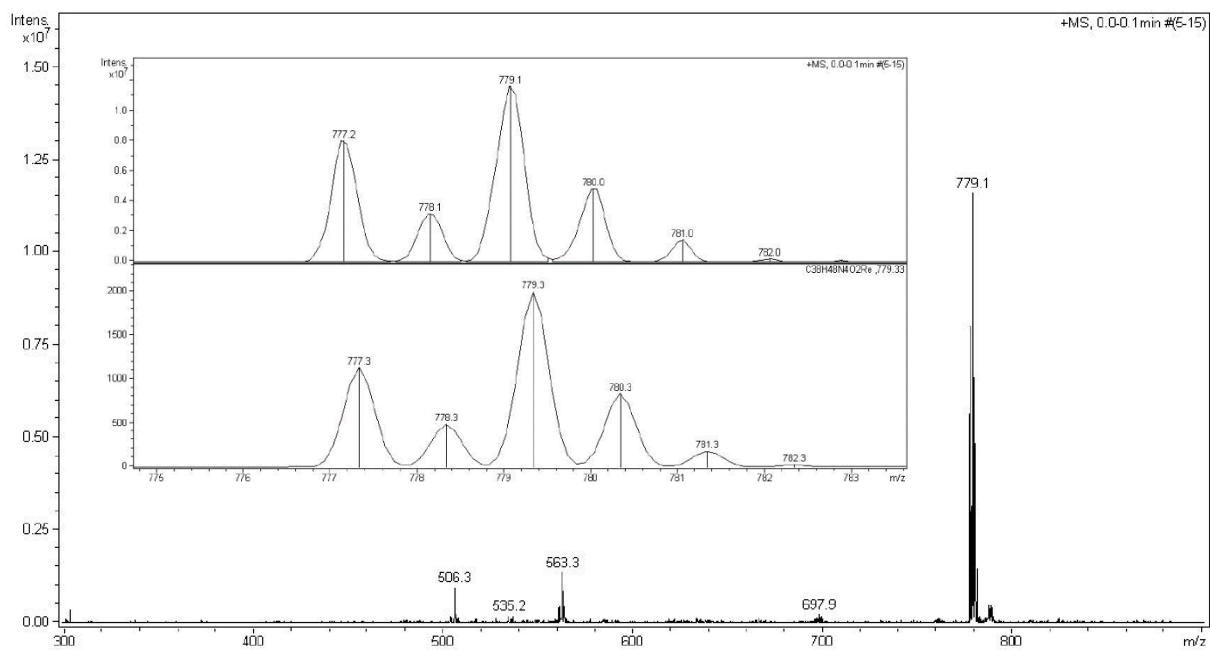


Figure S22. ESI-MS spectrum (in MeOH) of **6b**.

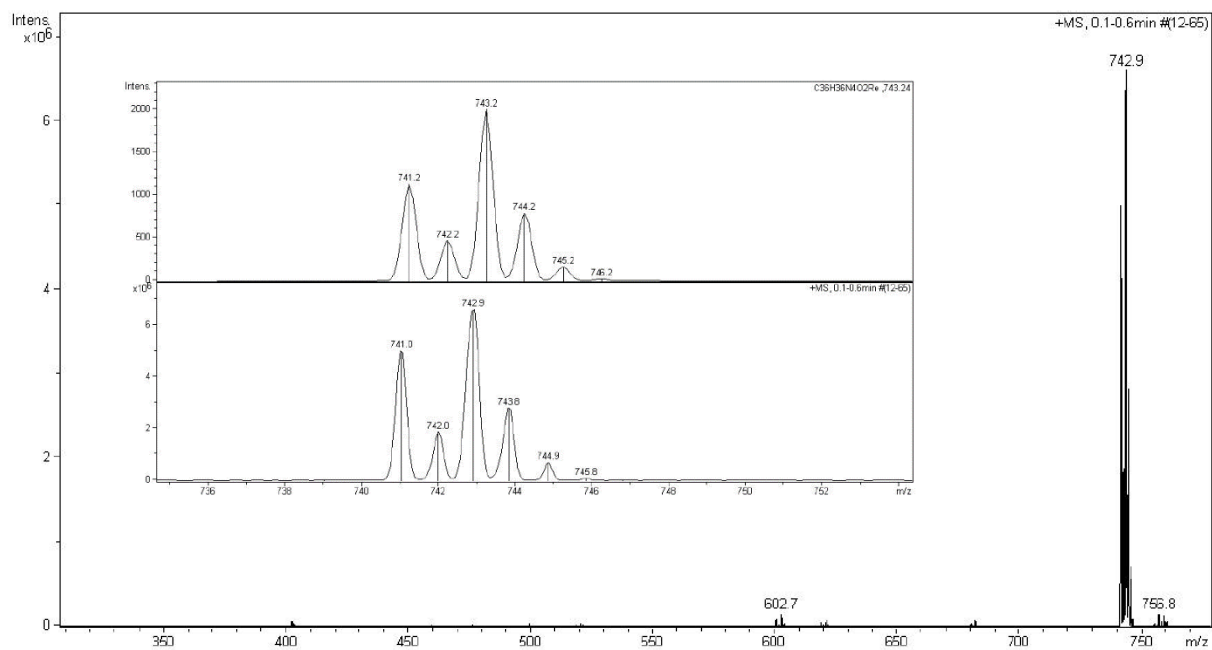


Figure S23. ESI-MS spectrum (in MeOH) of 7a.

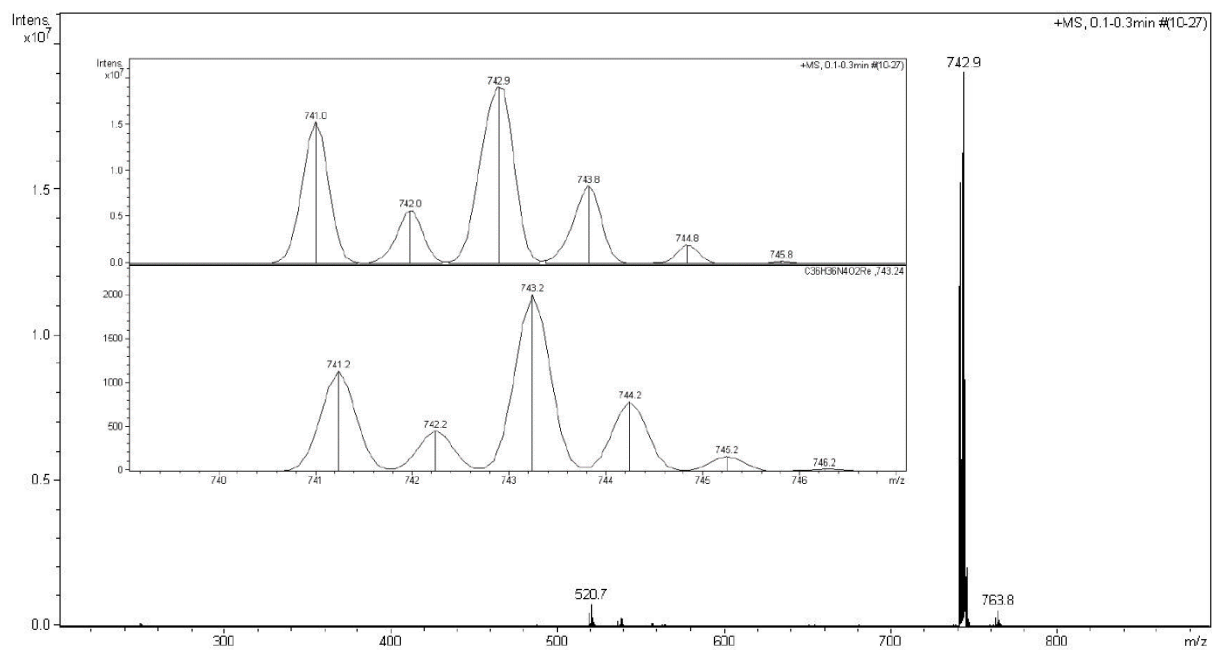


Figure S24. ESI-MS spectrum (in MeOH) of 7b.

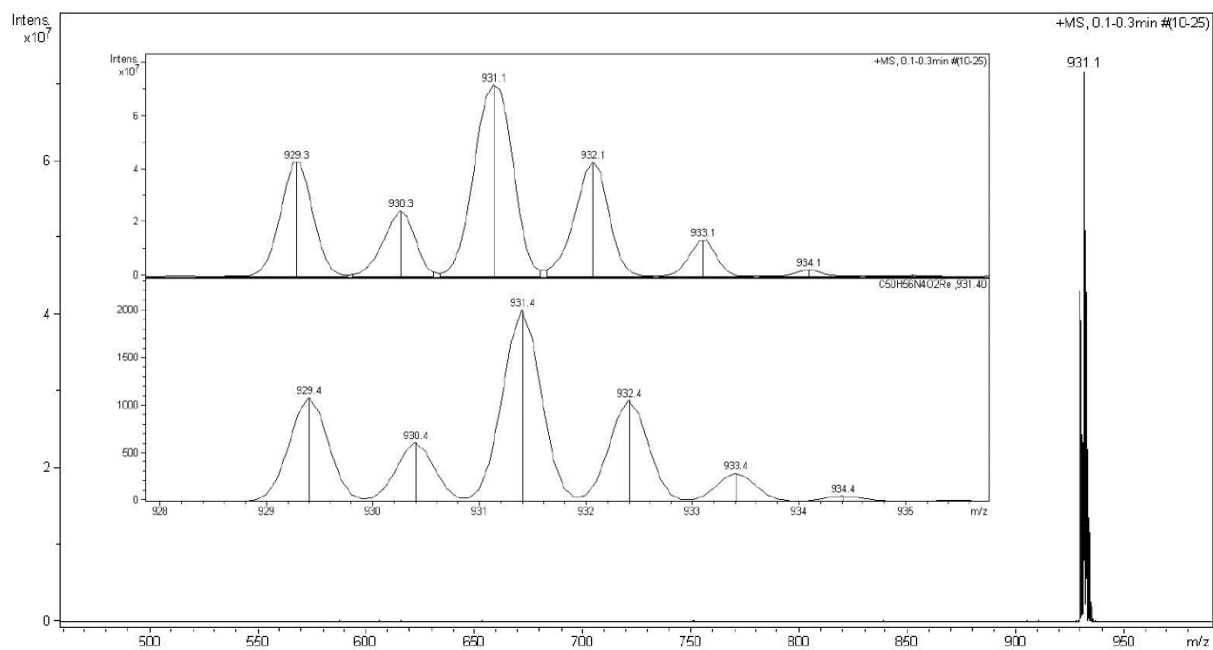


Figure S25. ESI-MS spectrum (in MeOH) of 7c.

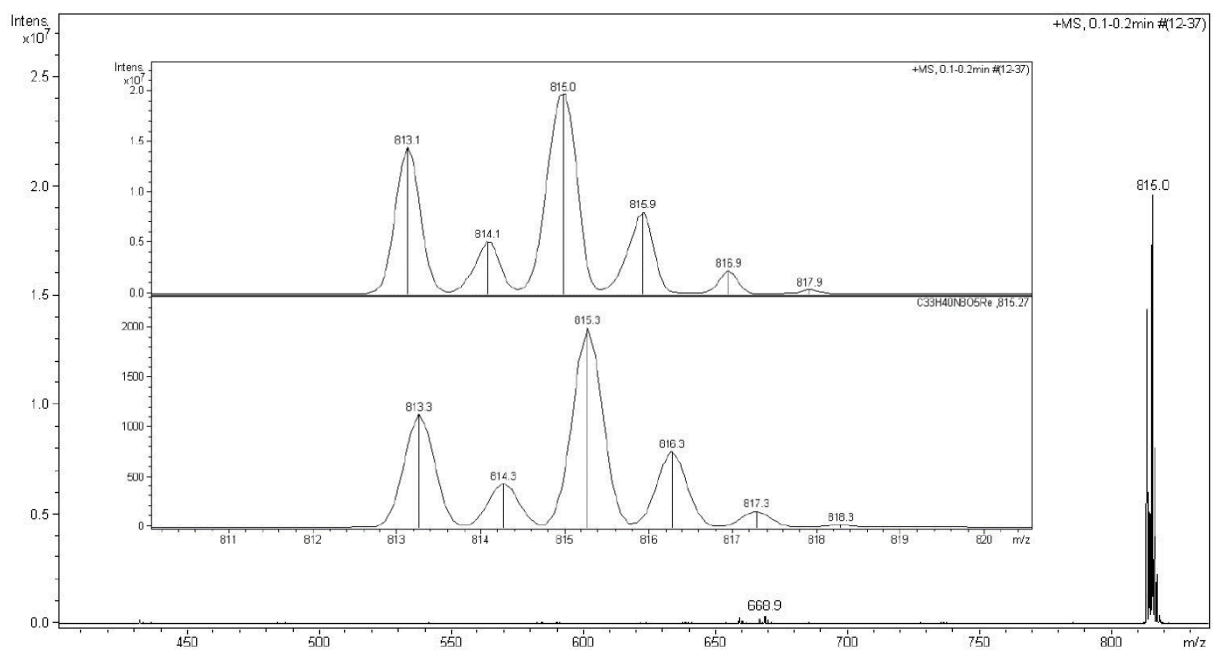


Figure S26. ESI-MS spectrum (in MeOH) of 15.

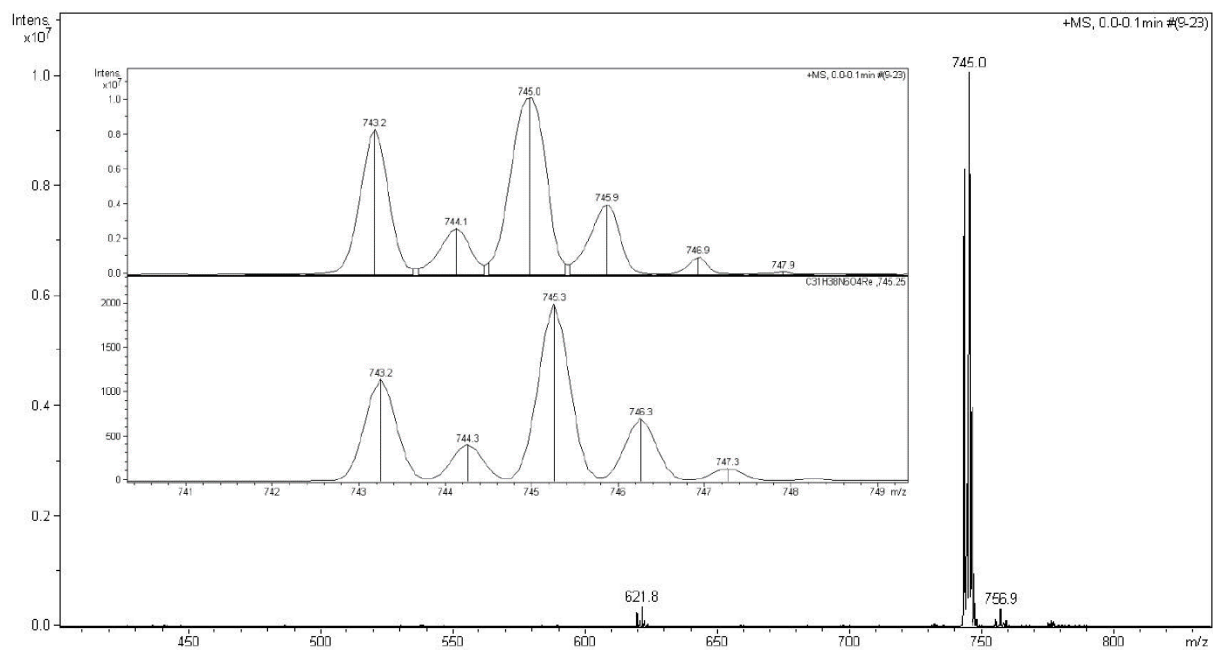


Figure S27. ESI-MS spectrum (in MeOH) of **16**.

Crystallography

Table S1. Crystallographic details of **6a**, **7c**, **11** and **13**.

Compound	6a	7c	11	13
formula	C ₄₄ H ₃₂ Br ₂ N ₈ O ₁₂ Re ₂	C ₅₀ H ₅₆ FeN ₄ O ₂ Pre	C ₁₇ H ₁₃ N ₃ O ₆ Re ₂	C ₃₀ H ₃₆ BrN ₄ O ₂ Re
fw	1396.99	1076.15	727.70	750.74
T, K	250	250	200(2)	250(2)
Crystal system	triclinic	trigonal	monoclinic	monoclinic
Space group	P-1	P ₃ 121	P ₂ ₁ /c	P ₂ ₁ /c
a, Å	12.3721(3)	11.28990(10)	8.3343(2)	12.9550(5)
b, Å	12.7016(3)	11.28990(10)	8.3947(2)	21.4764(6)
c, Å	14.5759(3)	30.9494(5)	26.6358(5)	10.9068(4)
α, deg	101.448(2)	90	90	90
β, deg	96.251(2)	90	92.336(2)	101.144(3)
γ, deg	90.415(2)	120	90	90
V, Å ³	2230.64(9)	3416.35(8)	1862.00(7)	2977.35(18)
Z	2	3	4	4
ρ _{calc} , g/cm ³	2.080	1.569	2.596	1.675
Crystal size, mm ³	0.06 × 0.06 × 0.06	0.13 × 0.103 × 0.06	0.36 × 0.16 × 0.06	0.32 × 0.24 × 0.05
Radiation	Cu Kα (λ = 1.54186)	Cu Kα (λ = 1.54186)	Cu Kα (λ = 1.54186)	Cu Kα (λ = 1.54186)
R1 ^a , (wR2) ^a	0.0696, 0.1673	0.0620, 0.1772	0.0708, 0.1691	0.0766, 0.2157
Largest diff. peak/hole (e Å ⁻³)	9.78/-8.37	5.13/-1.28	3.98/-3.13	2.84/-0.87

^a[I >= 2σ (I)]

Cytotoxicity

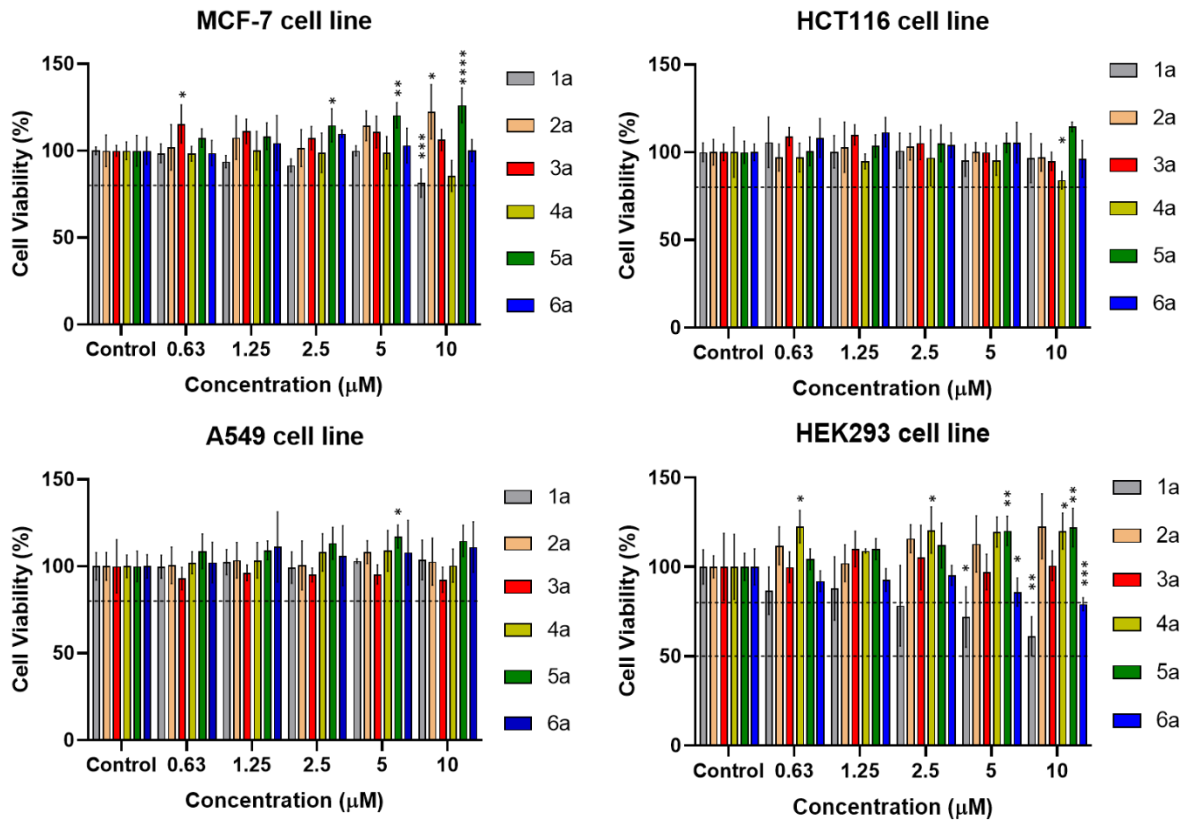


Figure S28. Cytotoxicity of complexes 1a-6a.

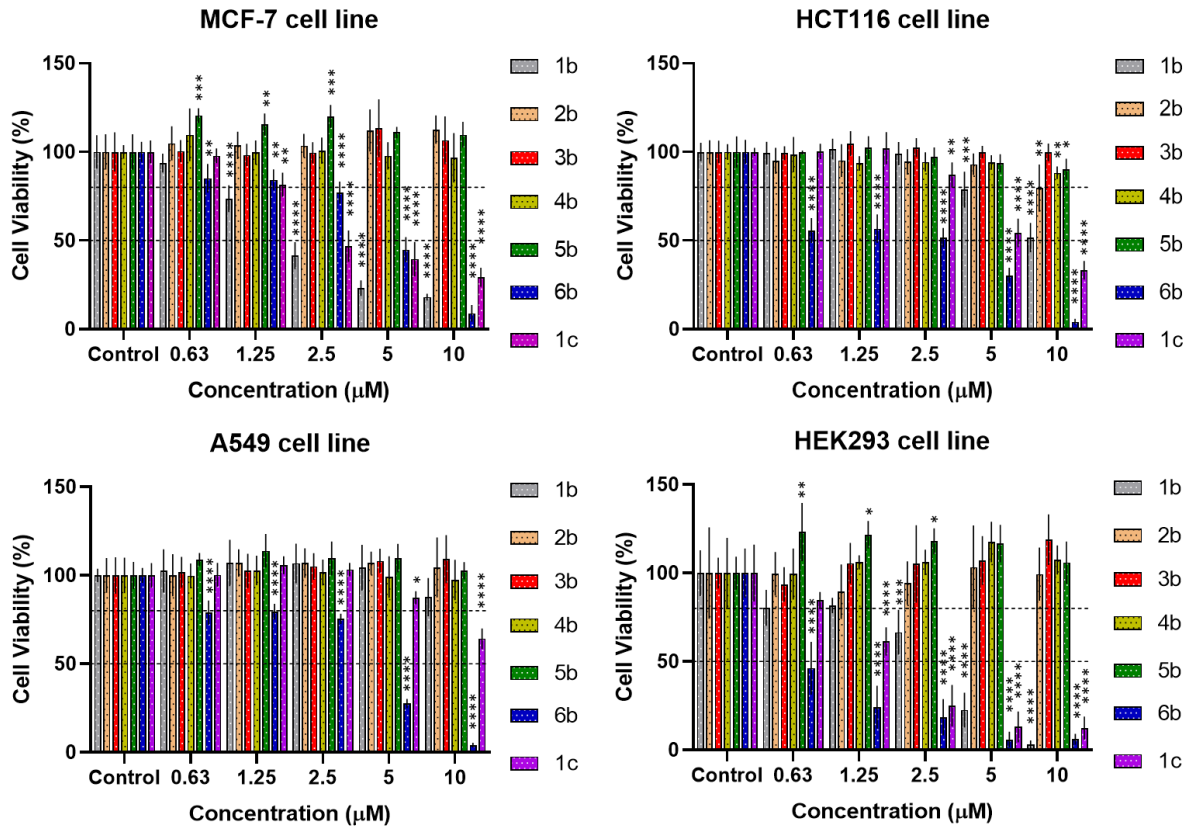


Figure S29. Cytotoxicity of complexes 1b-6b and 1c.

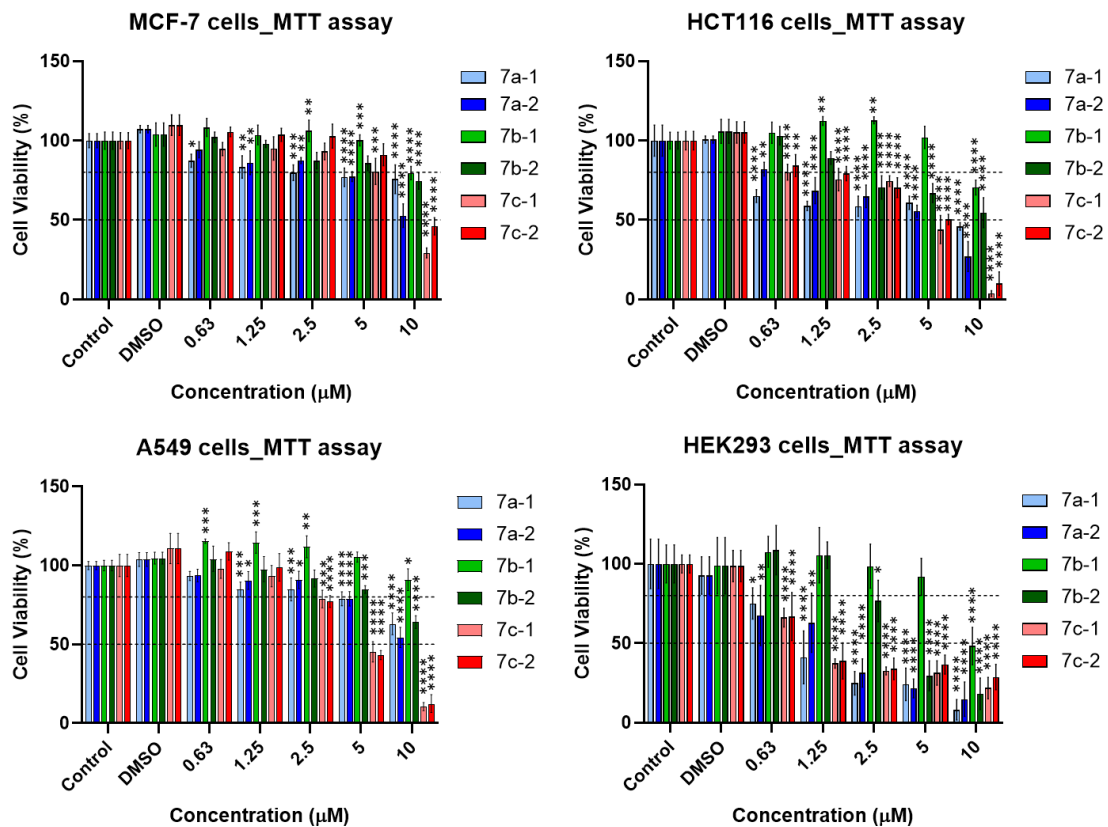


Figure S30. Cytotoxicity of complexes 7a-7c.

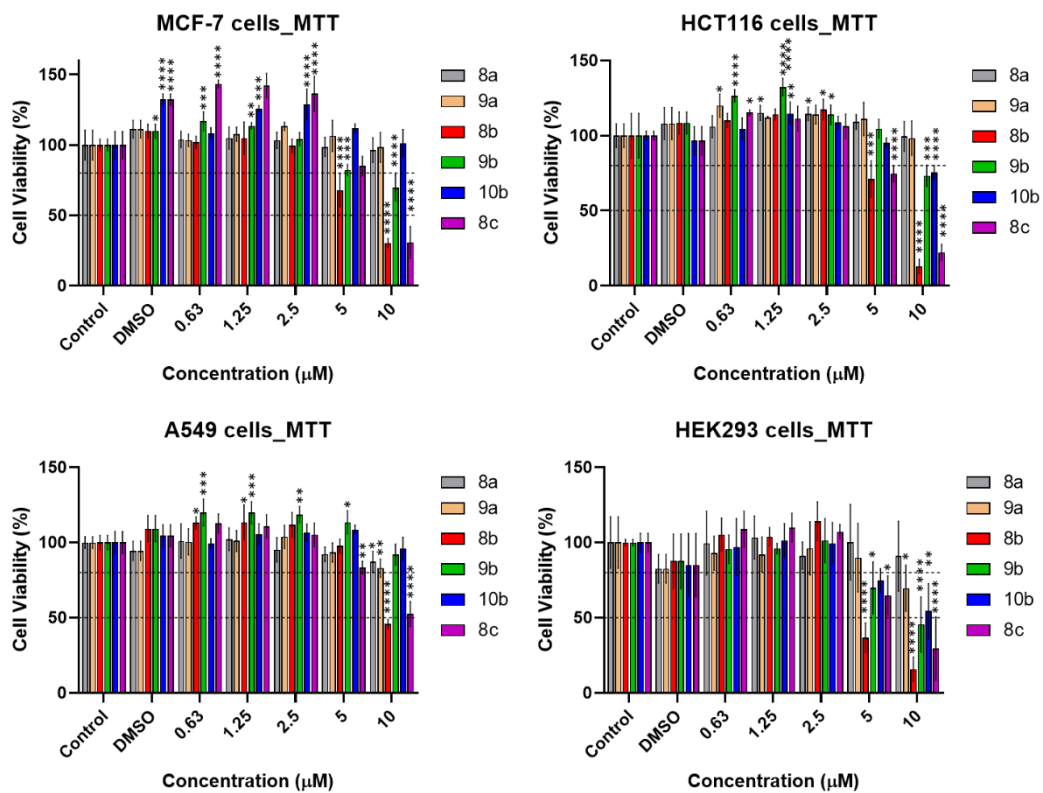


Figure S31. Cytotoxicity of complexes 8-10.