

Supporting Information

Synthesis, Characterization, and Antitumor Mechanism Investigation of Ruthenium(II)/Rhenium(I)-Daminozide Conjugates

Pei-Xin Yang^{1,†}, Kai Xie^{1,†}, Mei-Ru Chen¹, Zheng Zhang¹, Bo Huang^{2,*}, Rong-Tao Li¹ and Rui-Rong Ye^{1,*}

¹ *Faculty of Life Science and Technology, Kunming University of Science and Technology, Kunming 650500, China*

² *Faculty of Chemistry and Chemical Engineering, Yunnan Normal University, Kunming 650500, China*

* Corresponding author.

E-mail addresses: huangbo15@foxmail.com (B.H.); yerr@mail2.sysu.edu.cn (R.-R.Y.)

† These authors contributed equally to this work.

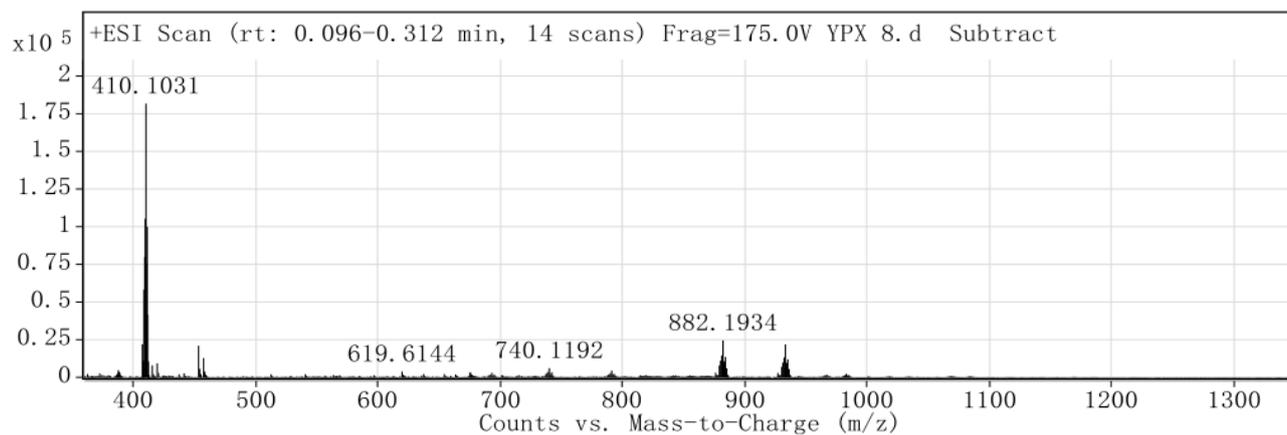


Figure S1. ESI-HRMS characterization of **Ru-1**, 965.1701 [M-PF₆]⁺, 882.1934 [M-2PF₆-H+2CH₃OH]⁺, 410.1031 [M-2PF₆]²⁺.

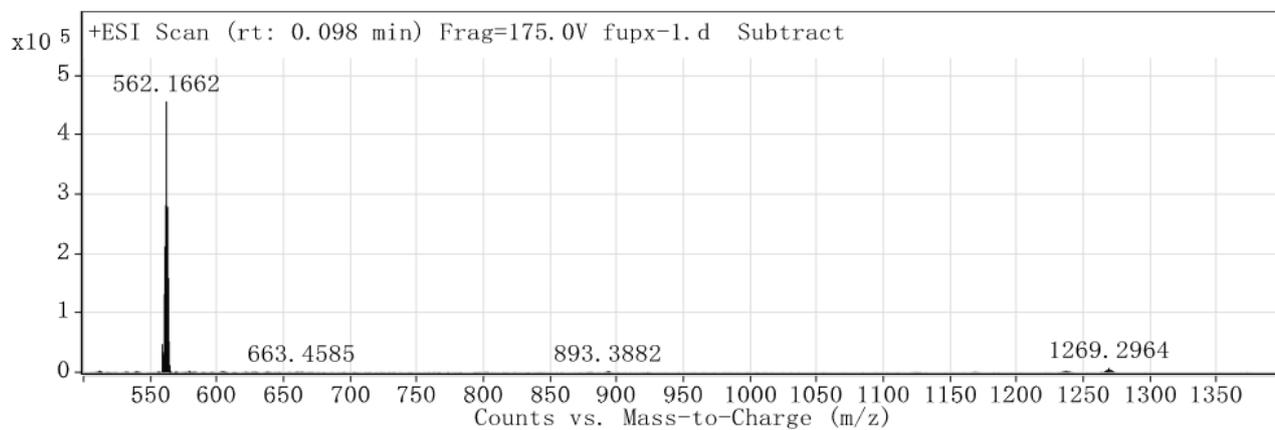


Figure S2. ESI-HRMS characterization of **Ru-2**, 1269.2964 [M-PF₆]⁺, 562.1662 [M-2PF₆]²⁺.

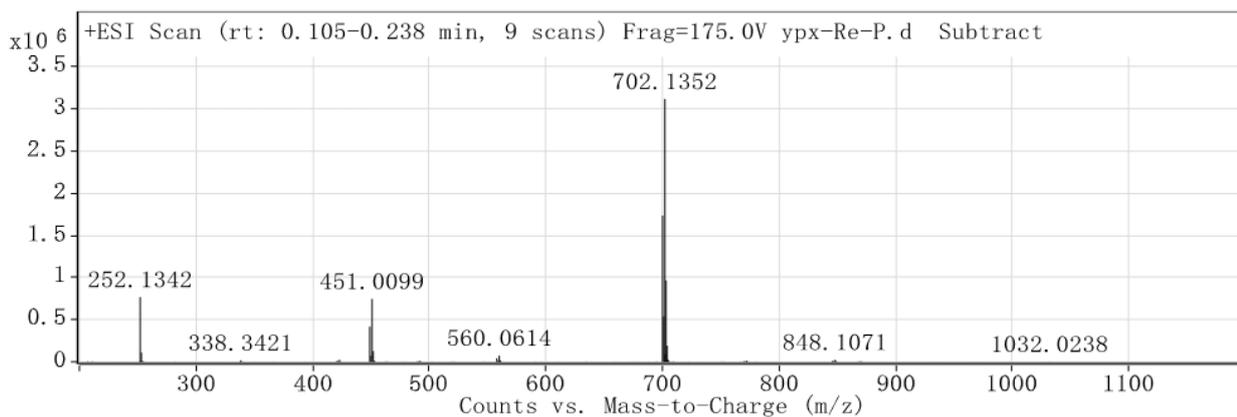


Figure S3. ESI-HRMS characterization of **Re-1**, 702.1352 [M-PF₆]⁺, 451.0099 [Re(phen)(CO)₃]⁺, 252.1342 [M-PF₆-Re(phen)(CO)₃+H]⁺.

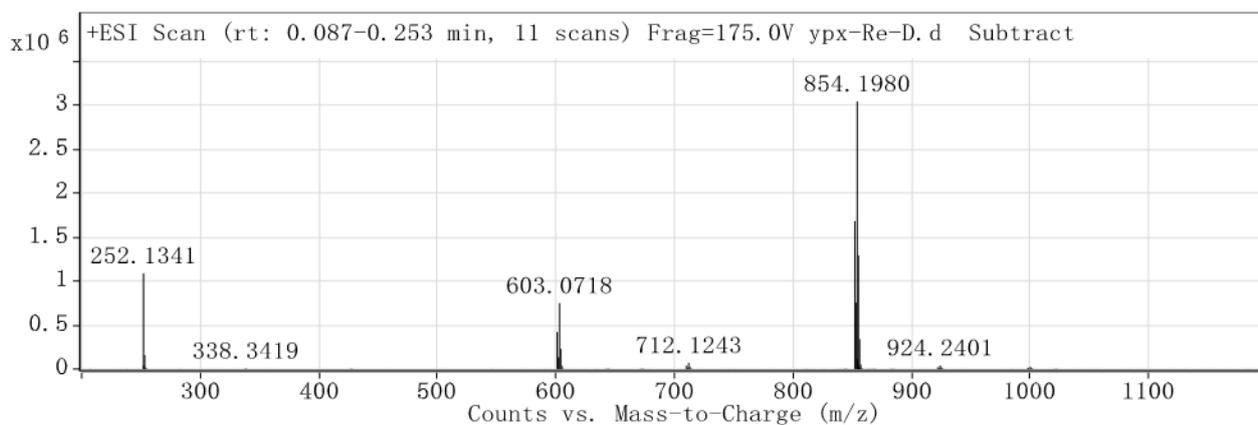


Figure S4. ESI-HRMS characterization of **Re-2**, 854.1980 [M-PF₆]⁺, 603.0718 [Re(DIP)(CO)₃]⁺, 252.1341 [M-PF₆-Re(DIP)(CO)₃+H]⁺.

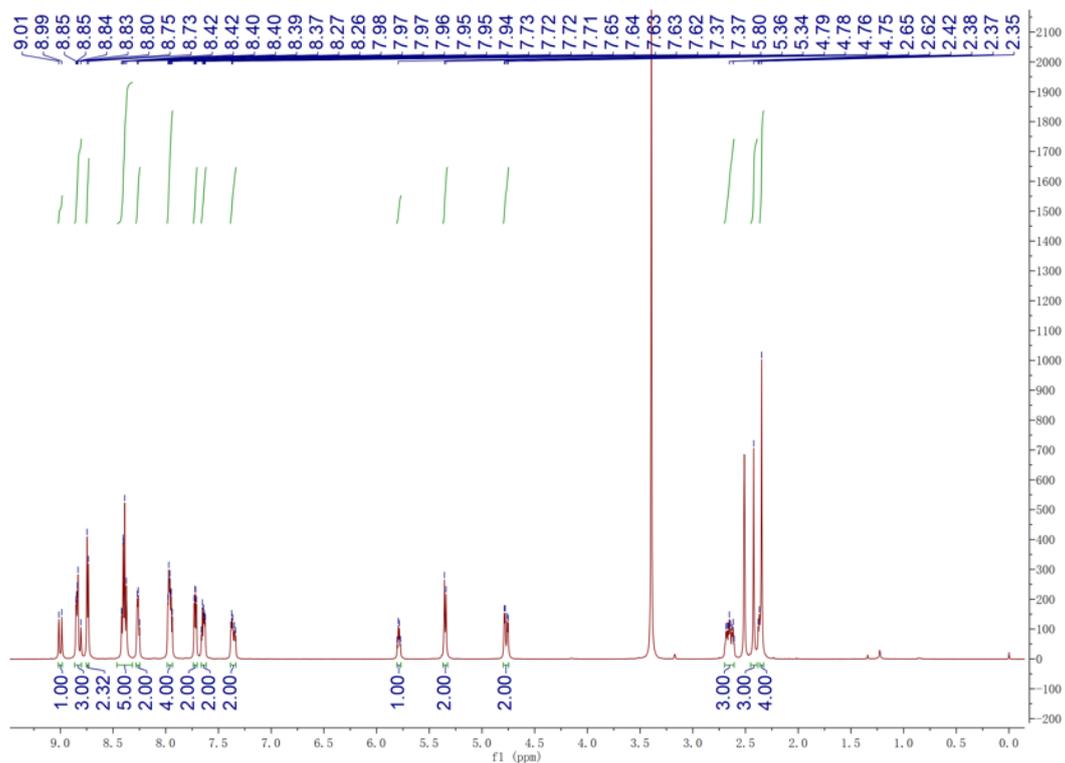


Figure S5. ^1H NMR spectrum of Ru-1.

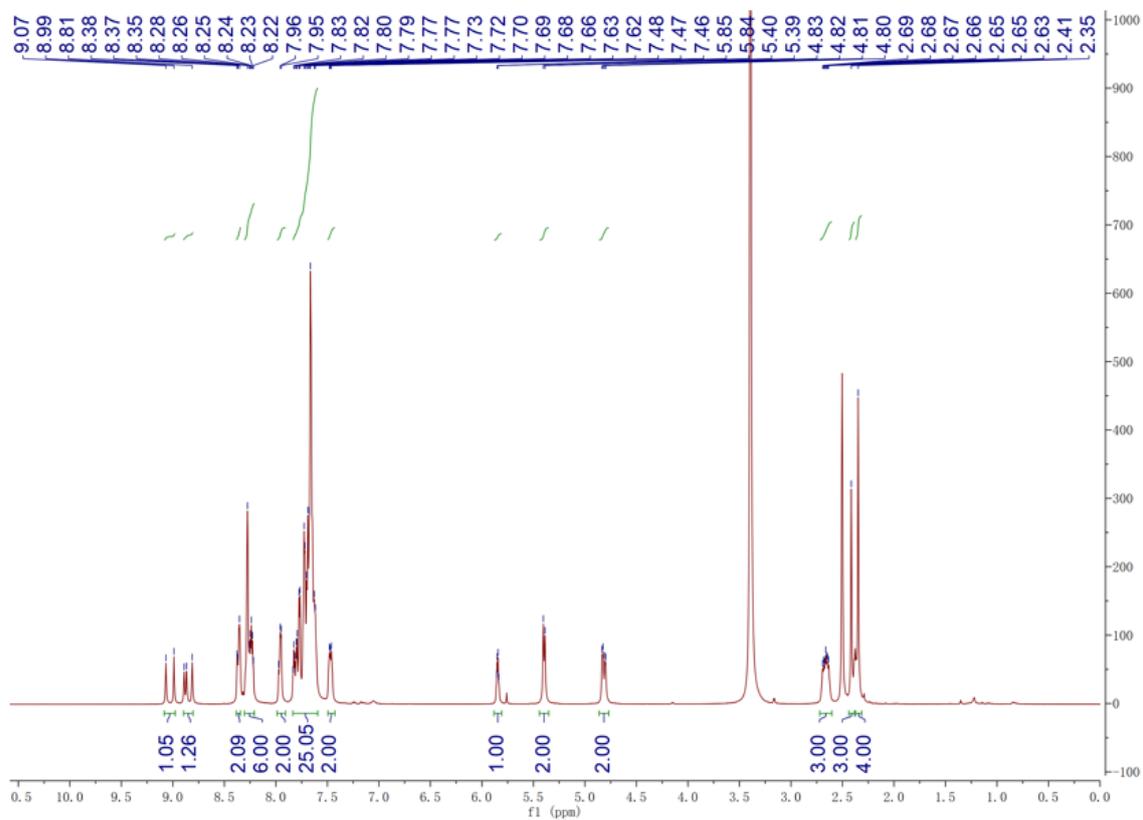


Figure S6. ^1H NMR spectrum of Ru-2.

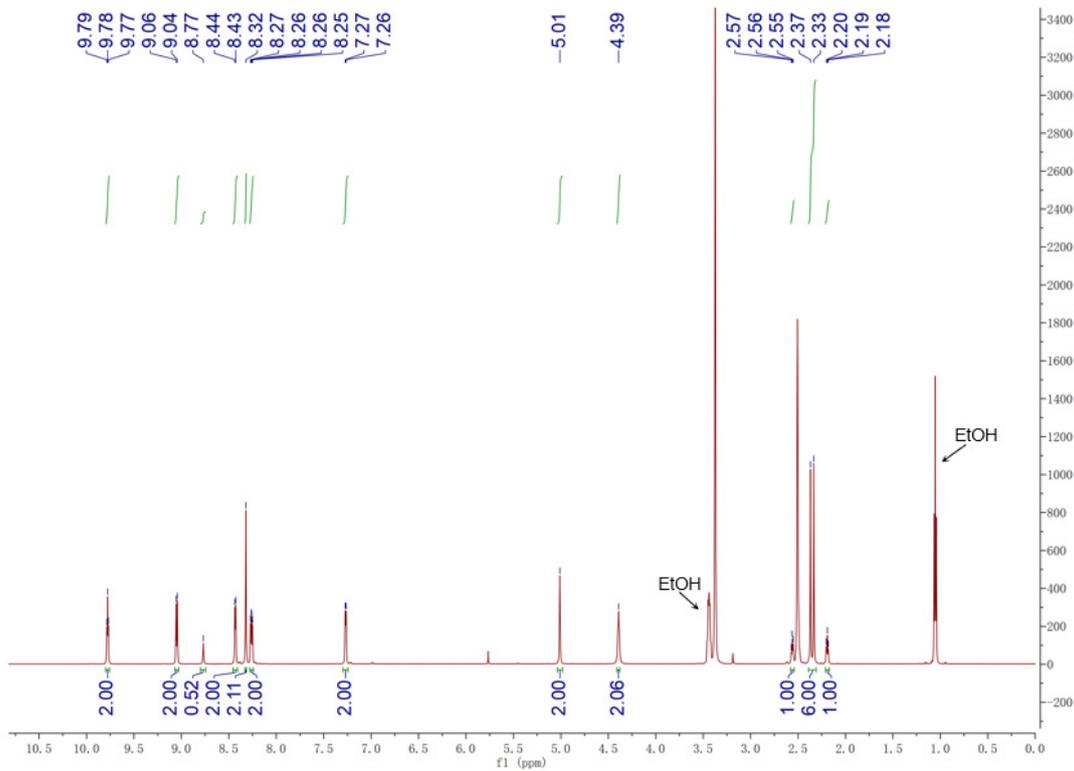


Figure S7. ^1H NMR spectrum of Re-1.

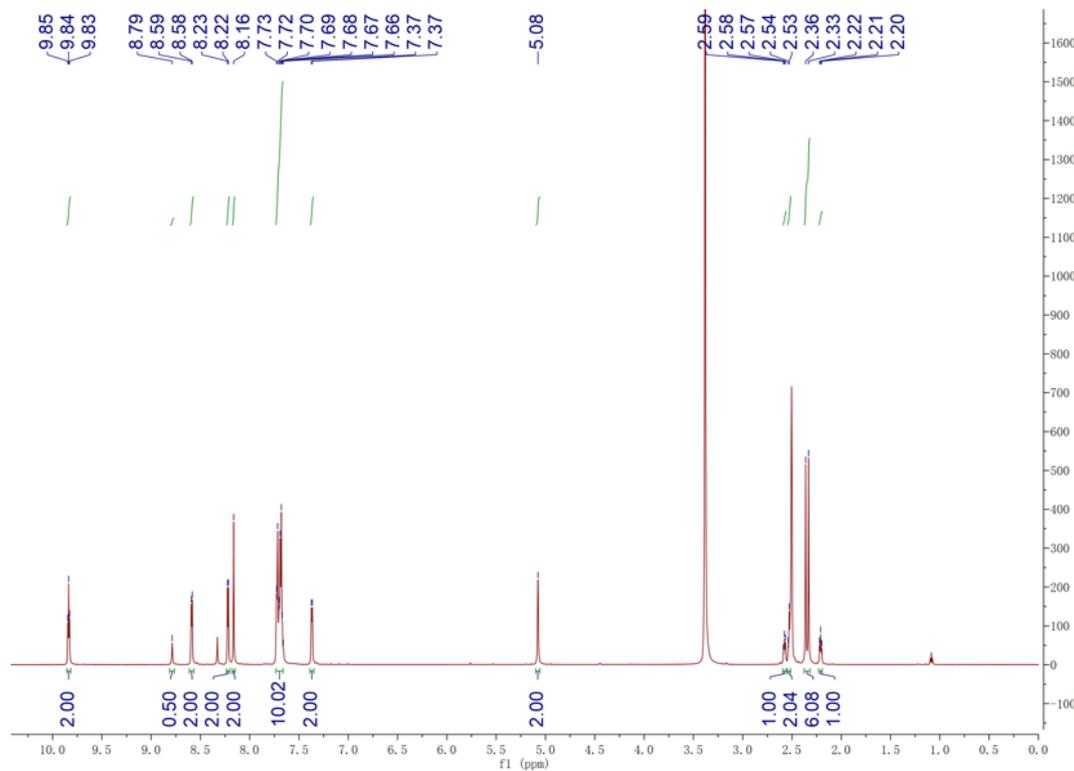


Figure S8. ^1H NMR spectrum of Re-2.

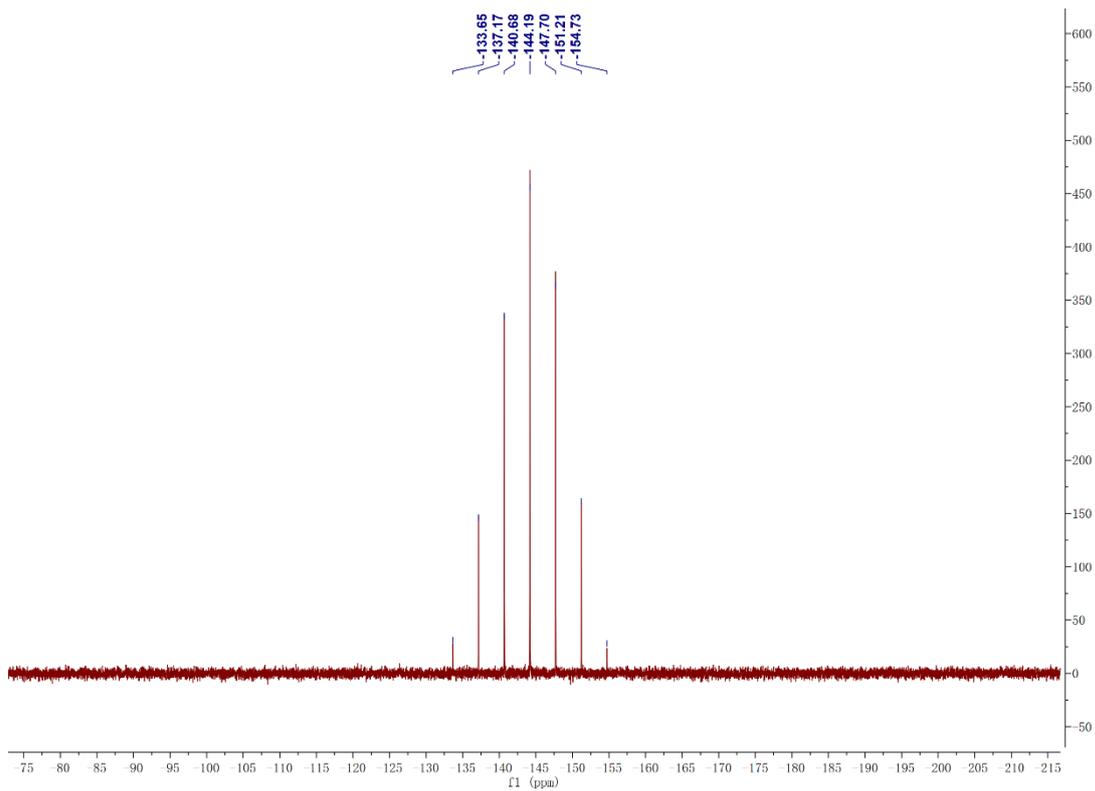


Figure S9. ^{31}P NMR spectrum of Ru-1.

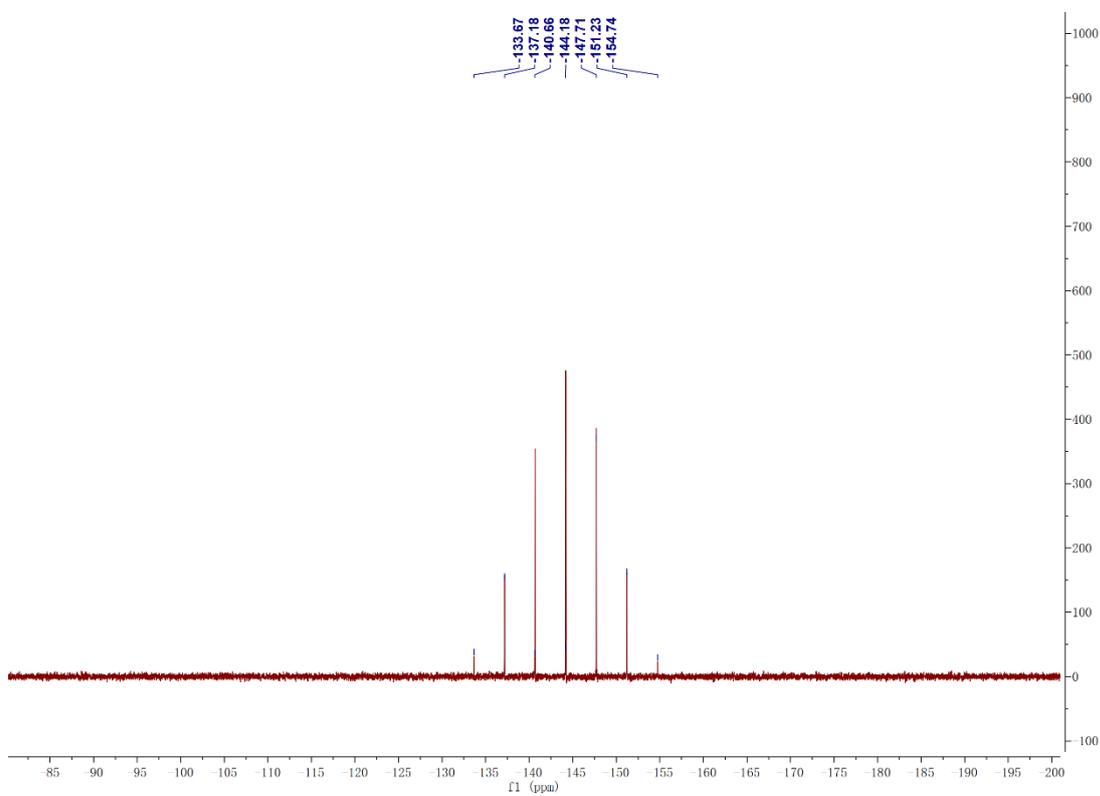


Figure S10. ^{31}P NMR spectrum of Ru-2.

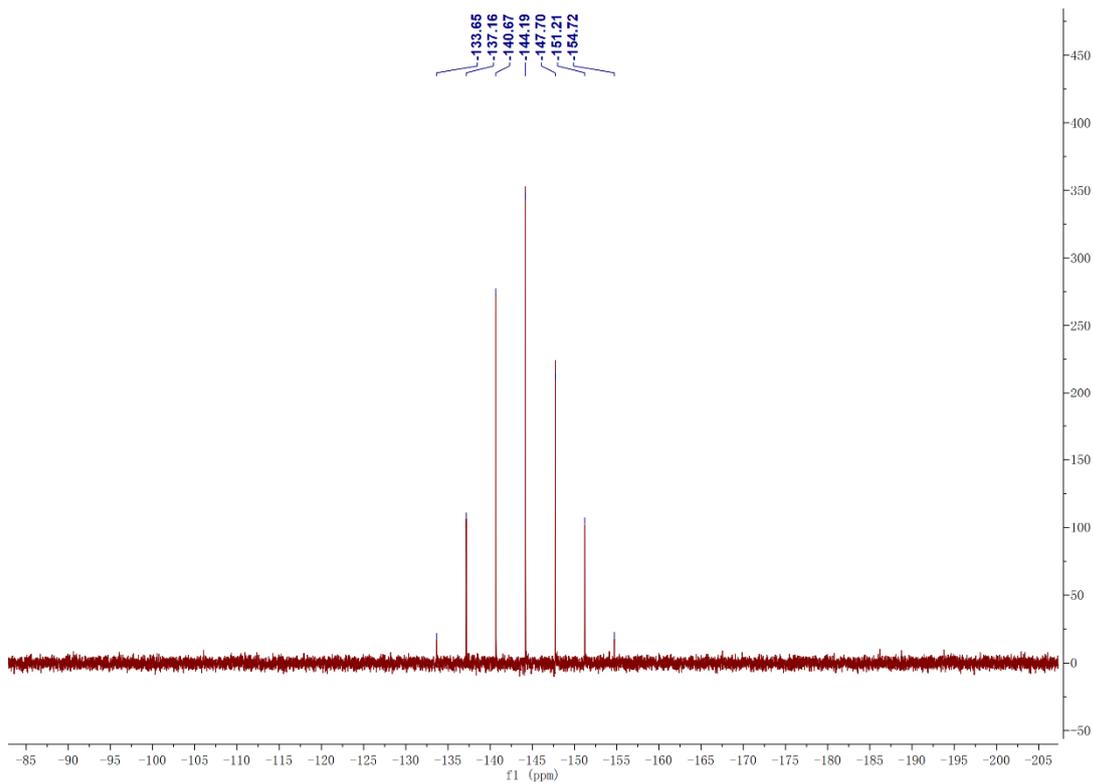


Figure S11. ^{31}P NMR spectrum of Re-1.

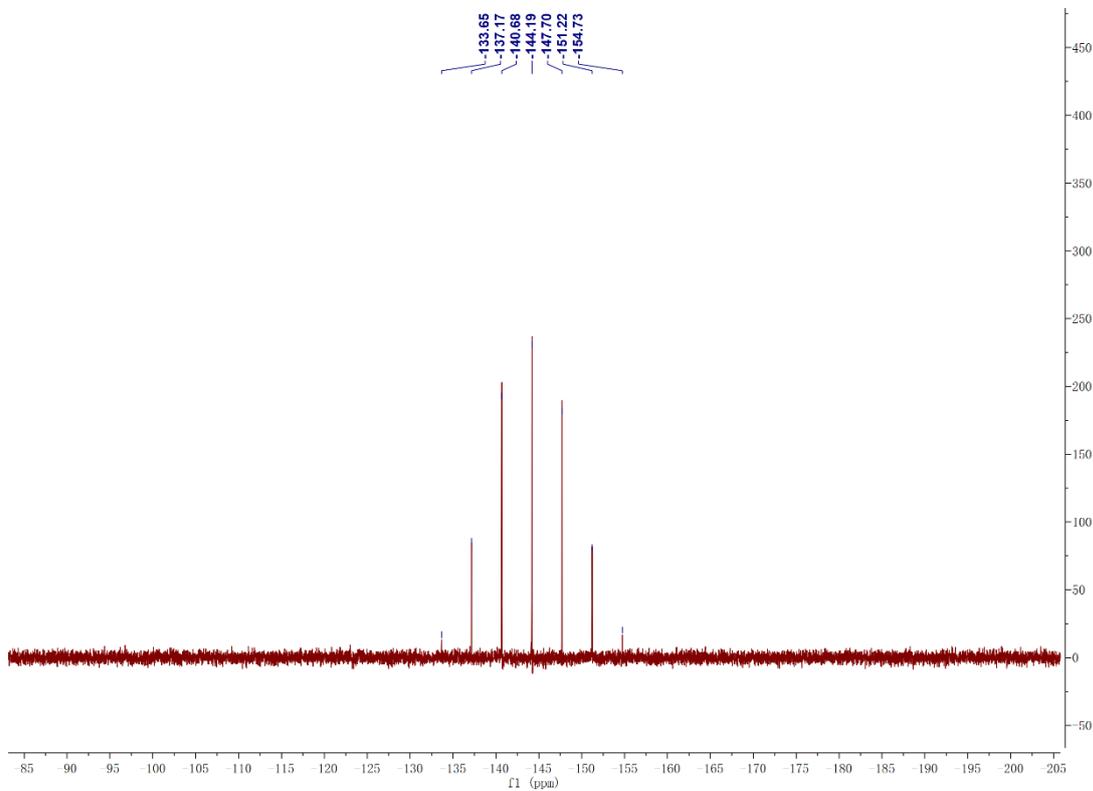


Figure S12. ^{31}P NMR spectrum of Re-2.

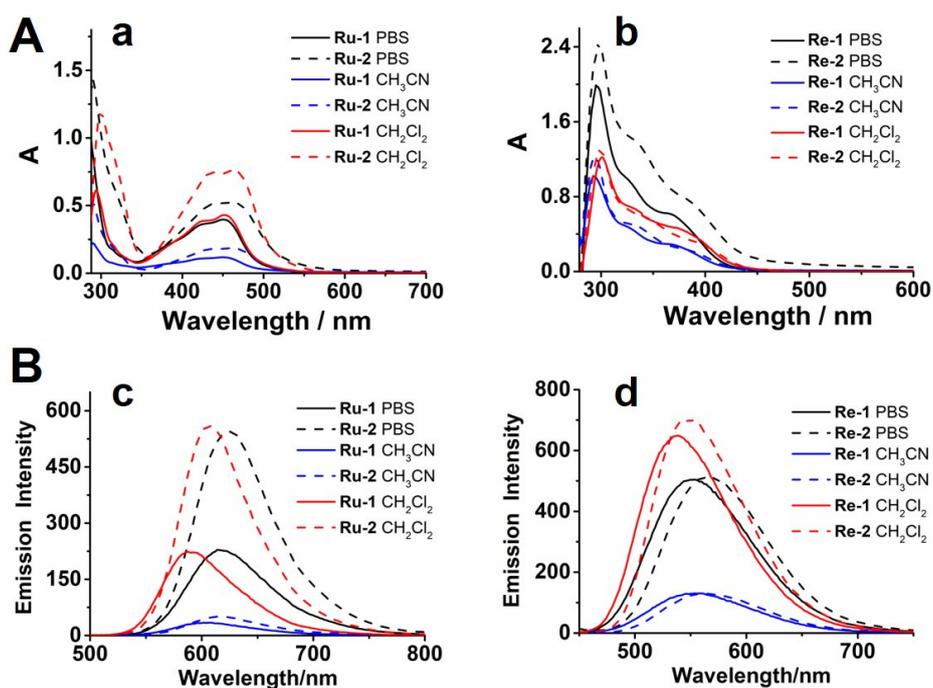


Figure S13. (A) UV/Vis spectra of Ru(II) (a) and Re(I) complexes (b) measured in PBS, CH₃CN and CH₂Cl₂ at 298 K. (B) Emission spectra of Ru(II) (a) and Re(I) complexes (b) measured in PBS, CH₃CN and CH₂Cl₂ at 298 K.

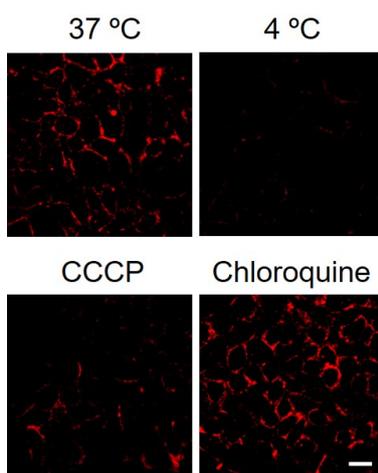


Figure S14. Cellular uptake mechanisms of **Ru-2**. HeLa cells were incubated with **Ru-2** (20 μ M, 2 h) under different conditions (37 $^{\circ}$ C, 4 $^{\circ}$ C, pre-treated HeLa cells with CCCP (30 μ M) or chloroquine (50 μ M)).

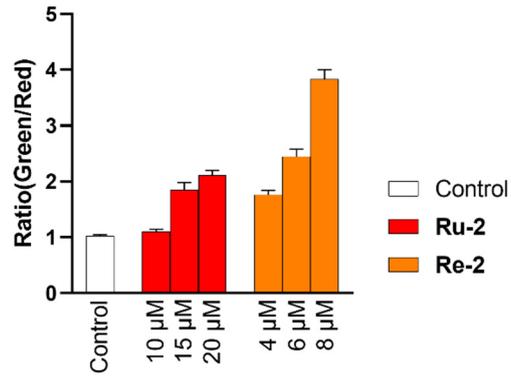


Figure S15. Ratio of green to red fluorescence intensity.

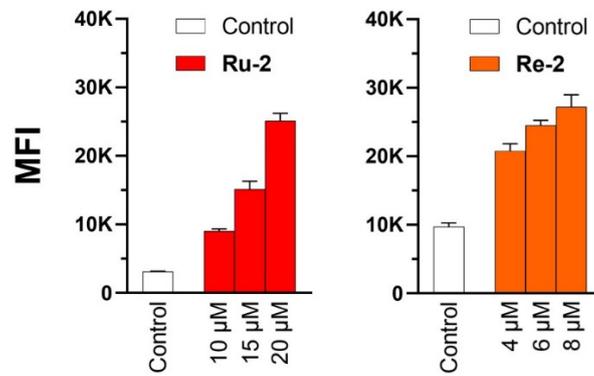


Figure S16. Quantitative data of MFI.

Table S1. Photophysical data of Ru(II) and Re(I) complexes

Compounds	Medium	$\lambda_{\text{abs, max}}$ (nm)	$\lambda_{\text{em, max}}$ (nm)
Ru-1	PBS	452	616
	CH ₃ CN	454	603
	CH ₂ Cl ₂	454	590
Ru-2	PBS	460	624
	CH ₃ CN	461	616
	CH ₂ Cl ₂	464	606
Re-1	PBS	367	550
	CH ₃ CN	377	553
	CH ₂ Cl ₂	380	537
Re-2	PBS	388	565
	CH ₃ CN	377	562
	CH ₂ Cl ₂	394	547