

Electronic Supplementary Information for

A Highly Selective Phosphorescence Probe for Histidine in Living Bodies

Quankun Gao, Bo Song, Zhiqiang Ye,* Liu Yang, Ruoyang Liu, Jingli Yuan

State Key Laboratory of Fine Chemicals, Department of Chemistry, Dalian University of Technology, Dalian 116024, China

*Corresponding author

Tel./Fax: +86-411-84986042;

E-mail: yezq@dlut.edu.cn

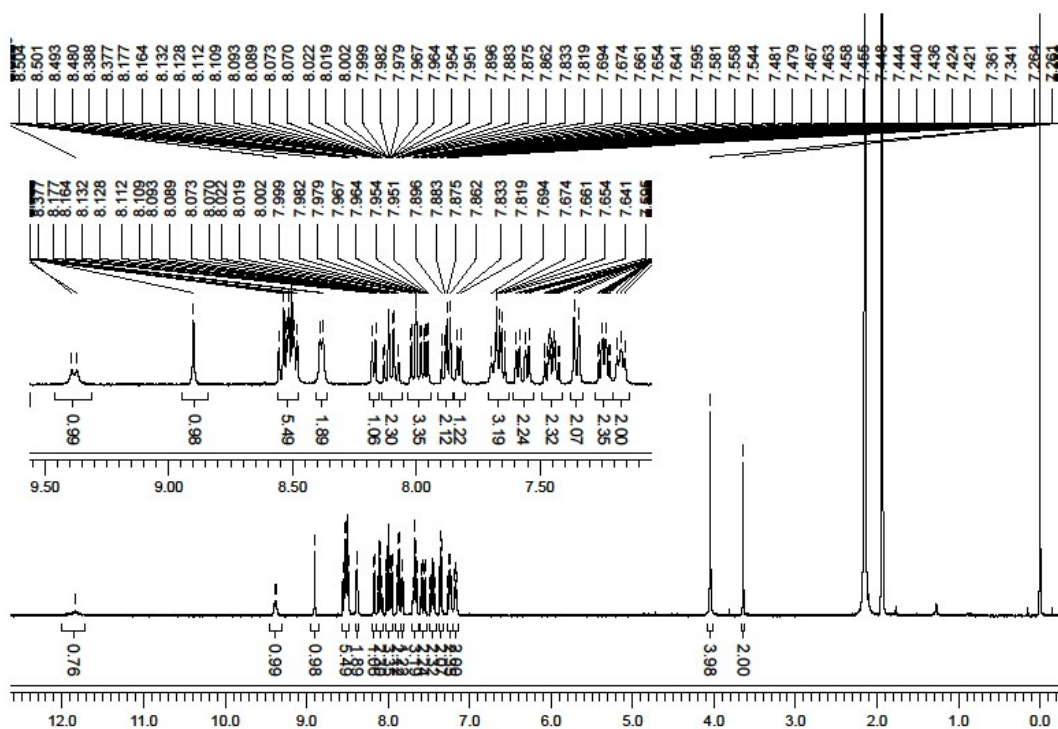


Figure S1. ^1H NMR of $[\text{Ru}(\text{bpy})_2(\text{phen-DPA})](\text{PF}_6)_2$ (CD_3CN , 400MHz).

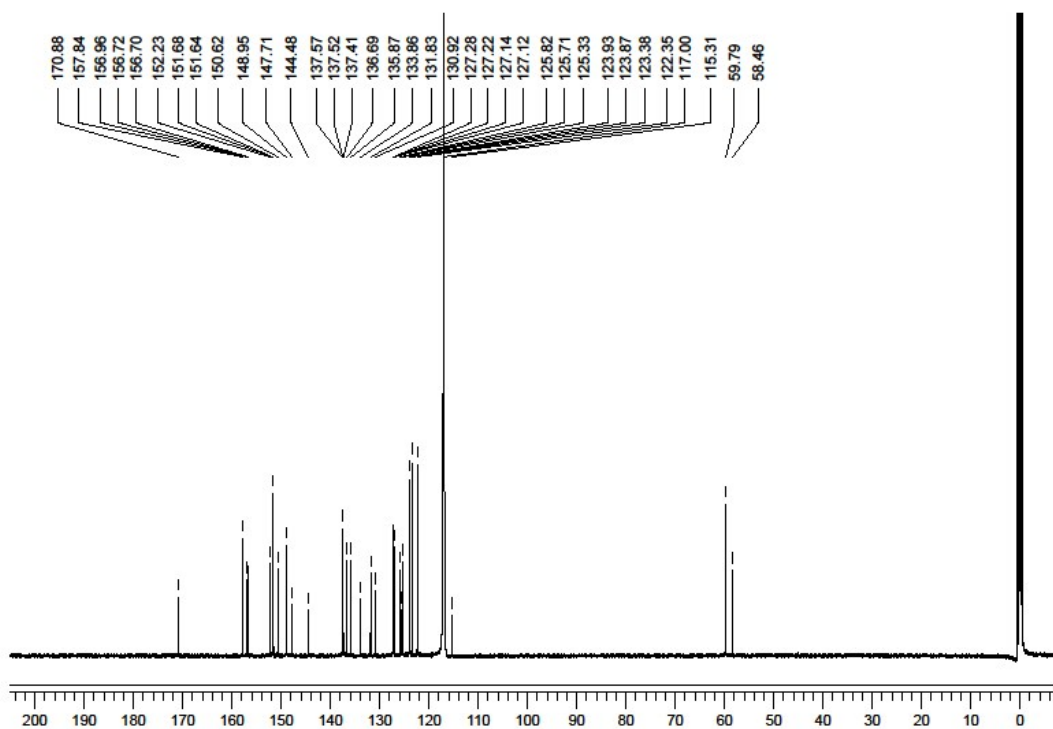


Figure S2. ^{13}C NMR of $[\text{Ru}(\text{bpy})_2(\text{phen-DPA})](\text{PF}_6)_2$ (CD_3CN , 100MHz).

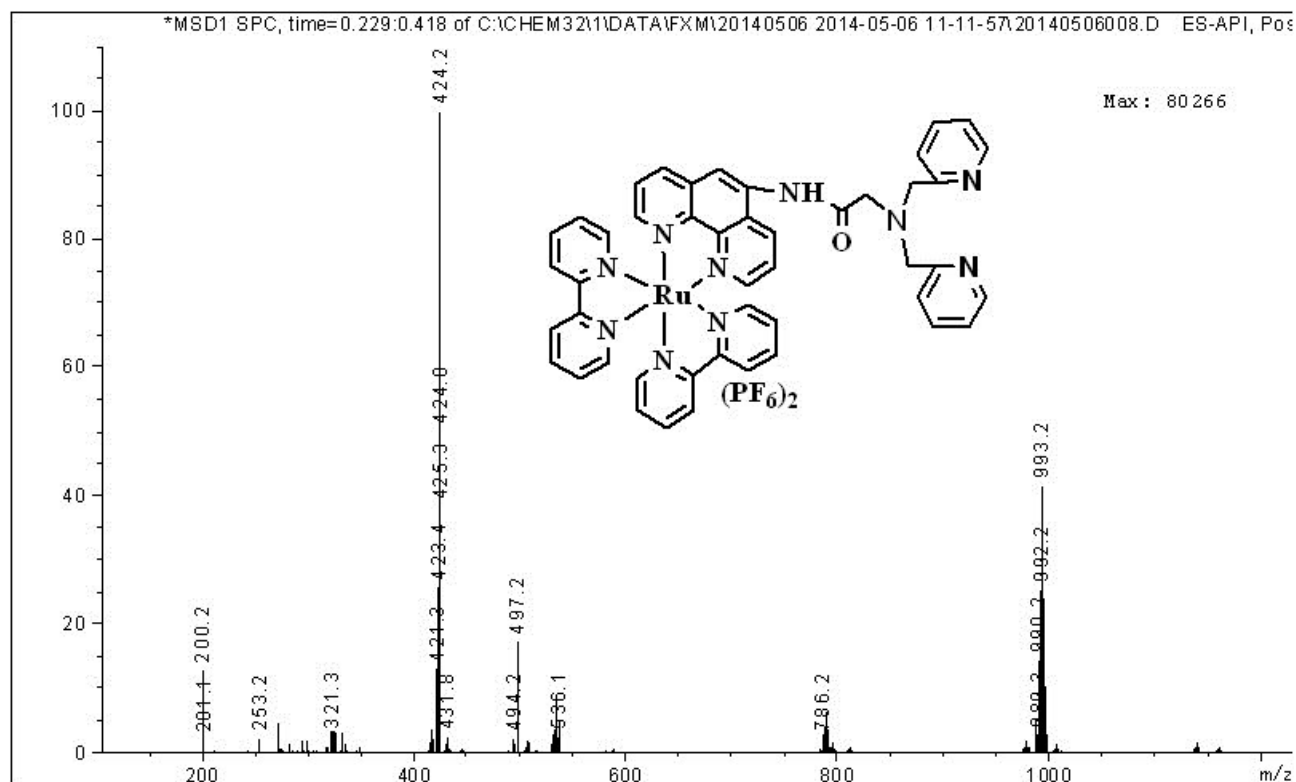


Figure S3. ESI-MS of $[\text{Ru}(\text{bpy})_2(\text{phen-DPA})](\text{PF}_6)_2$.

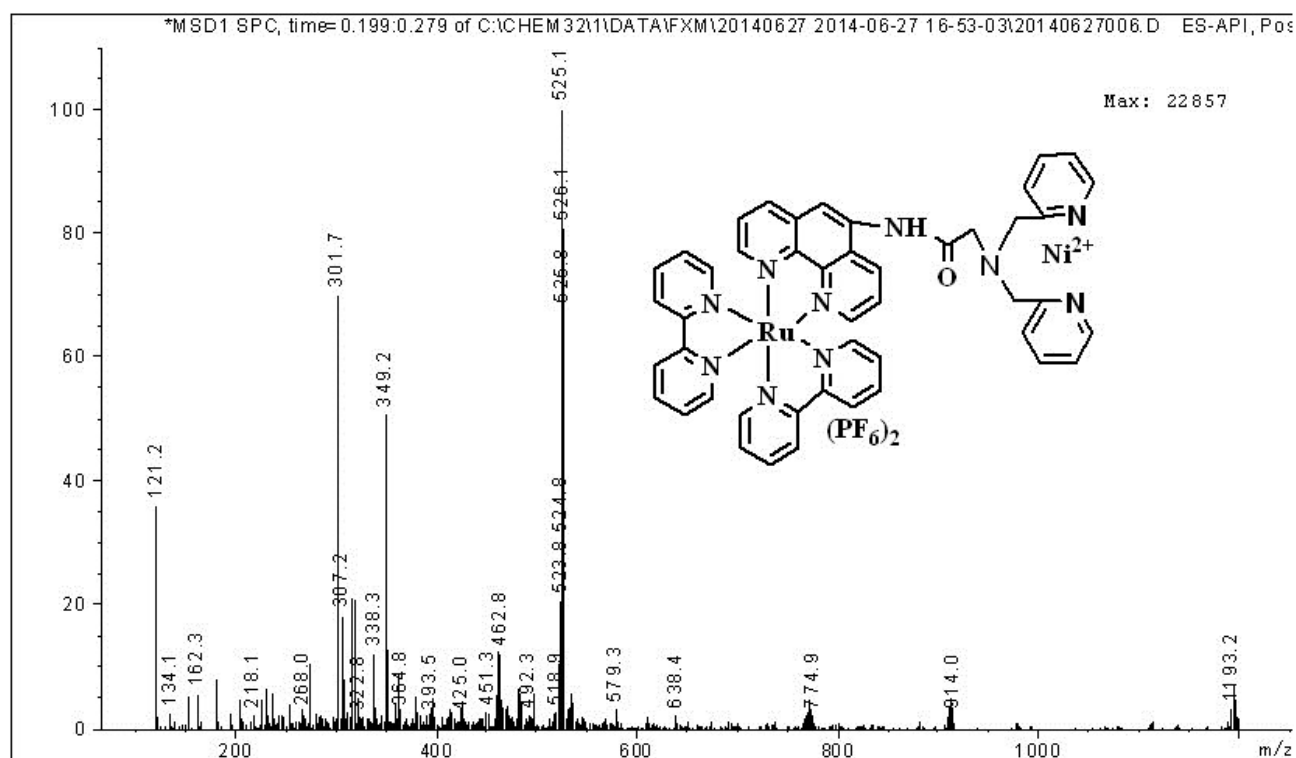


Figure S4. ESI-MS of Ru-Ni.

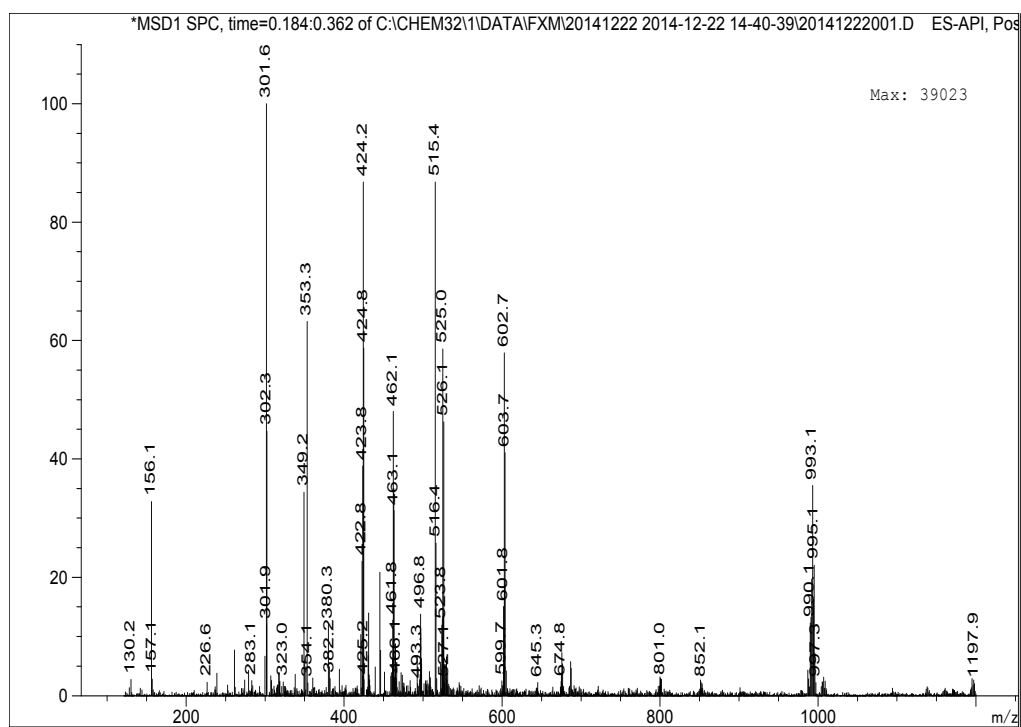


Figure S5. ESI-MS of the product of **Ru-Ni** reacted with Histidine.

Table S1. Photophysical parameters of the Ru complexes^[a].

complex	$\lambda_{\text{ex,max}}$ (nm)	ϵ_{450} ($\text{cm}^{-1}\text{M}^{-1}$)	$\lambda_{\text{em,max}}$ (nm)	ϕ (%)	τ (ns) ^[b]
[Ru(bpy) ₂ (phen-DPA)](PF ₆) ₂	450	1.64×10^4	603	4.17	683
Ru-Ni	450	1.77×10^4	603	0.35	655

[a] All data were obtained in EtOH/HEPES buffer (50 mM, pH 7.2, 2 : 3, v/v). [b] Phosphorescence lifetime, measured with the phosphorescence method.

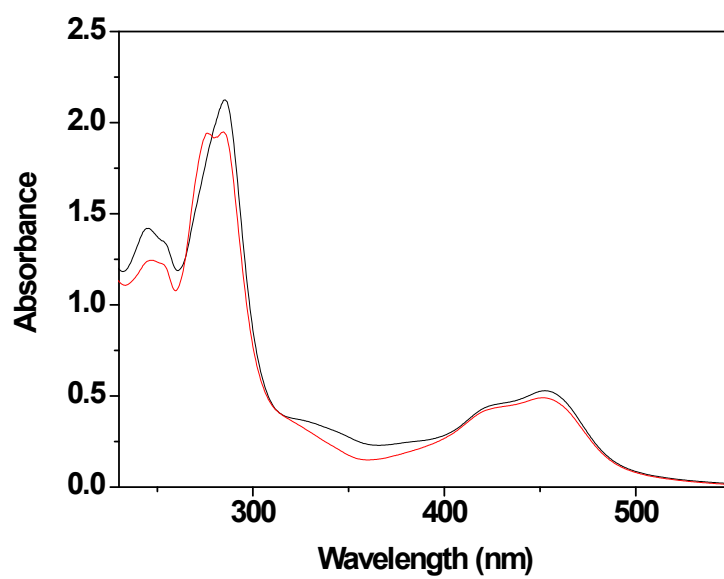


Figure S6. UV/Vis absorption spectra of the Ru complexes (30 μ M) in EtOH/HEPES buffer (50 mM, pH 7.2, 2 : 3, v/v). [Ru(bpy)₂(phen-DPA)](PF₆)₂: black line; **Ru-Ni**: red line

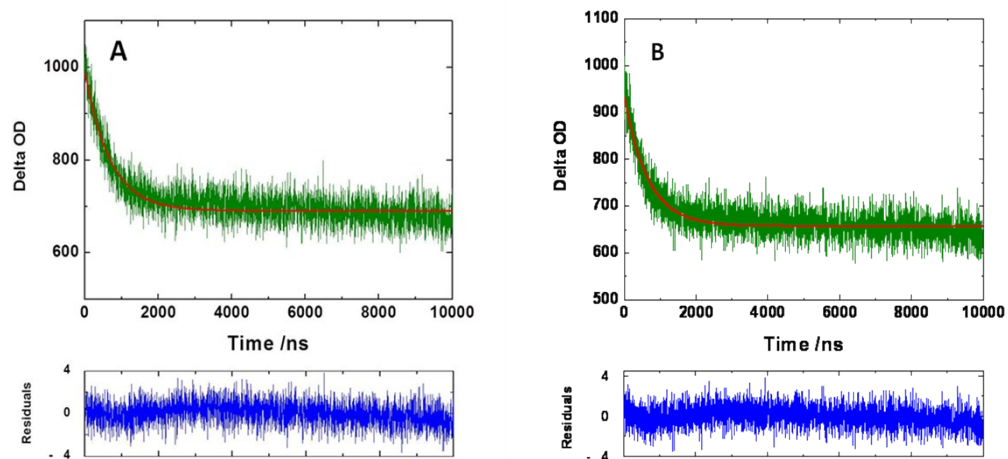


Figure S7. Decay traces of the Ru(II) complexes solutions. (A) $[\text{Ru}(\text{bpy})_2(\text{phen-DPA})](\text{PF}_6)_2$; (B)

Ru-Ni

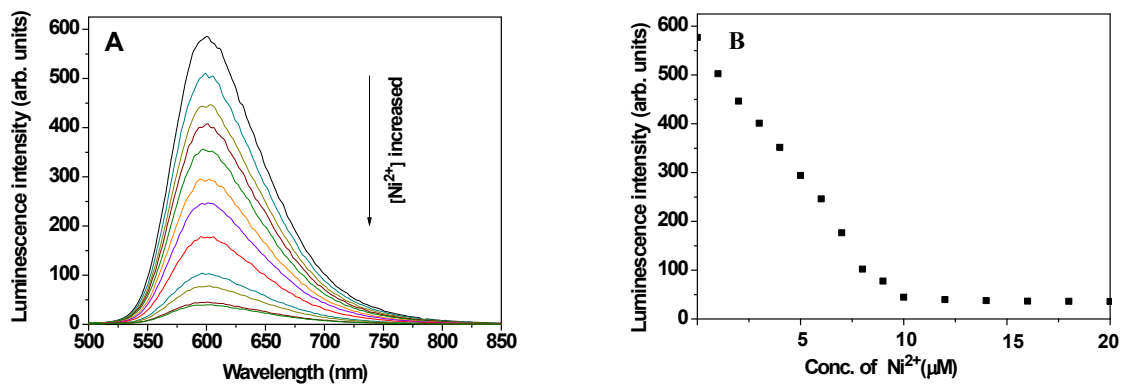


Figure S8. (A) Emission spectra of $[\text{Ru}(\text{bpy})_2(\text{phen-DPA})](\text{PF}_6)_2$ ($10 \mu\text{M}$) in the presence of different concentrations of Ni^{2+} in EtOH/HEPES buffer (50 mM , $\text{pH } 7.2$, $2 : 3$, v/v) (Ni^{2+} concentrations: 0.0 , 1.0 , 2.0 , 3.0 , 4.0 , 5.0 , 6.0 , 7.0 , 8.0 , 9.0 , 10 and $12 \mu\text{M}$). (B) The change in luminescence intensity of $[\text{Ru}(\text{bpy})_2(\text{phen-DPA})](\text{PF}_6)_2$ at 603 nm in the presence of different concentrations of Ni^{2+} (0 - $20 \mu\text{M}$). Excitation wavelength: 450 nm .

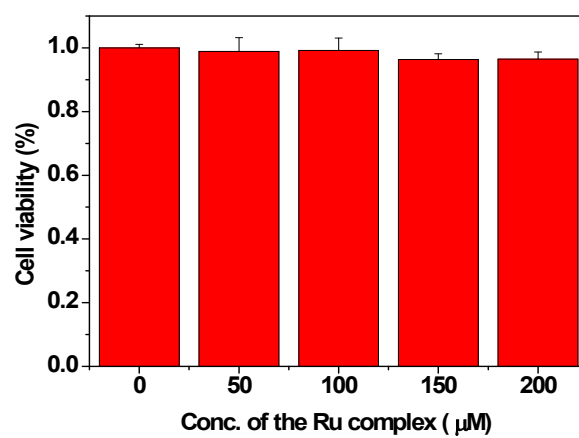


Figure S9. Viabilities of the HeLa cells after incubated with different concentrations of **Ru-Ni** for 3 h.