Supporting Information

Photoinduced cytotoxic activity of a rare ruthenium nitrosyl phenanthroline complex showing NO generation in human cells

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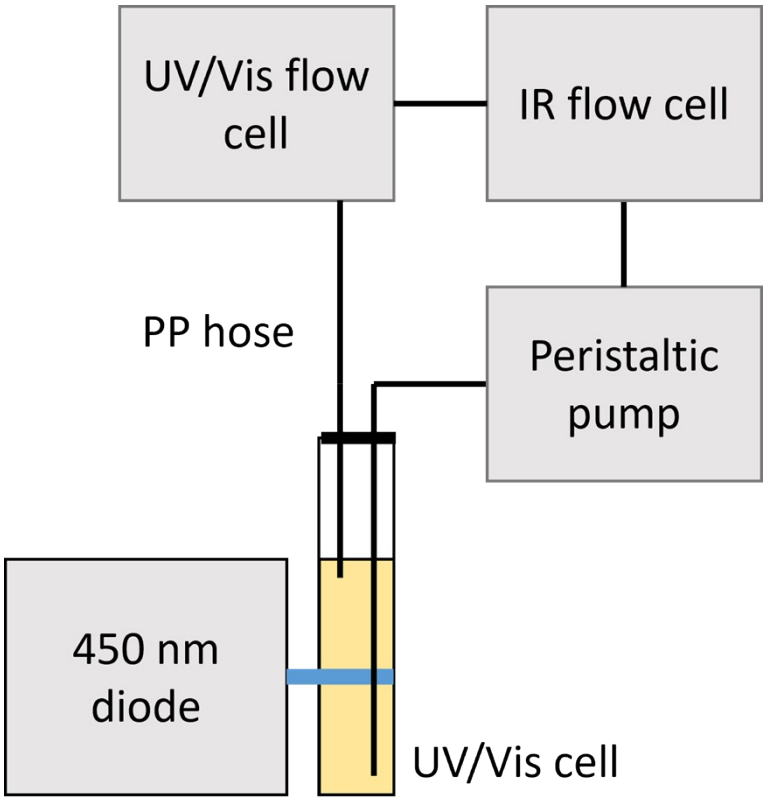
Table S1. Crystal data and refinement details.

Identification code	[RuNO(Phen)$(NO_2)_2$OH]·DMF **(1a)**	[RuNO(Phen)$(NO_2)_2$OH] **(1)**
Empirical formula	$C_{15}H_{16}N_6O_7Ru_1$	$C_{12}H_9N_5O_6Ru_1$
Formula weight	493.4	420.3
Temperature/K	150	296
Crystal system	triclinic	monoclinic
Space group	P-1	$P2_1/n$
a/Å	7.0875(1)	10.6515(8)
b/Å	10.3691(2)	7.2960(6)
c/Å	12.6632(3)	18.6158(11)
α/°	92.948(1)	90
β/°	93.662(1)	90.038(3)
γ/°	103.612(1)	90
Volume/Å^3	900.52(3)	1446.70(18)
Z	2	4
ρ_{calc}g/cm^3	1.82	1.93
μ/mm^{-1}	0.926	1.127
F(000)	493.9	832

Crystal size/mm^3	1 × 0.8 × 0.4	0.04 × 0.08 × 0.19
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	3.24 to 63.1	4.404 to 52.854
Index ranges	-10 ≤ h ≤ 10, -14 ≤ k ≤ 14, -18 ≤ l ≤ 17	-11 ≤ h ≤ 13, -9 ≤ k ≤ 9, -22 ≤ l ≤ 18
Reflections collected	19478	8183
Independent reflections	5591 [R_{int} = 0.0245, R_{sigma} = 0.0263]	2844 [R_{int} = 0.0565, R_{sigma} = 0.0656]
Data/restraints/parameters	5591/0/266	2844/0/219
Goodness-of-fit on F^2	1.006	1.16
Final R indexes [I>=2σ (I)]	R_1 = 0.0243, wR_2 = 0.0687	R_1 = 0.0609, wR_2 = 0.1286
Final R indexes [all data]	R_1 = 0.0289, wR_2 = 0.0776	R_1 = 0.0831, wR_2 = 0.1381
Largest diff. peak/hole/e Å^{-3}	0.86/-0.51	1.01/-1.10



Scheme S1. UV-vis-IR-flow-through system.

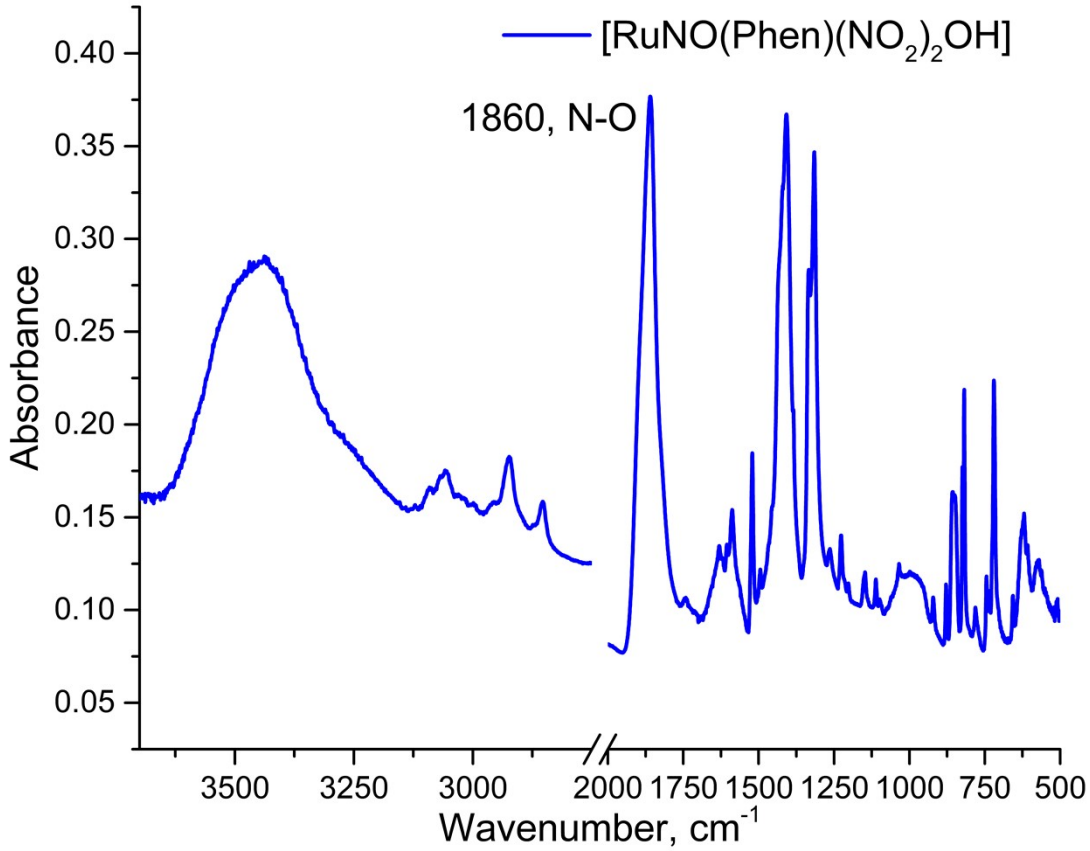


Figure S1. IR-spectrum of [RuNO(Phen)$(NO_2)_2$OH] **(1)**.

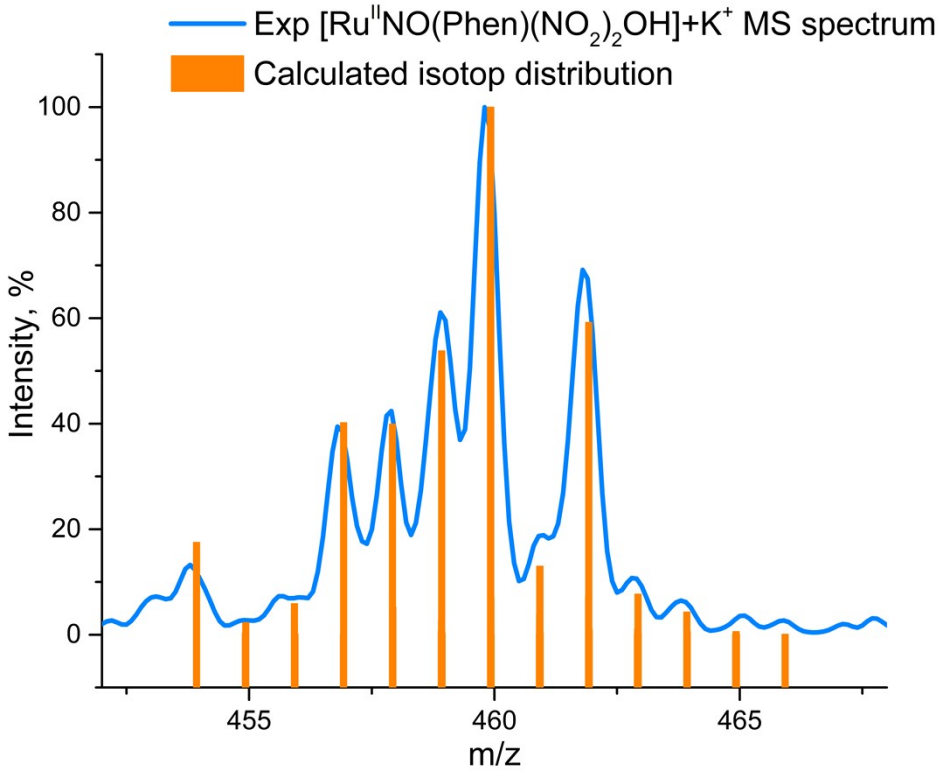


Figure S2. Experimental ESI-MS spectrum of {[RuNO(Phen)$(NO_2)_2$OH]+K^+} and calculated isotope distribution.

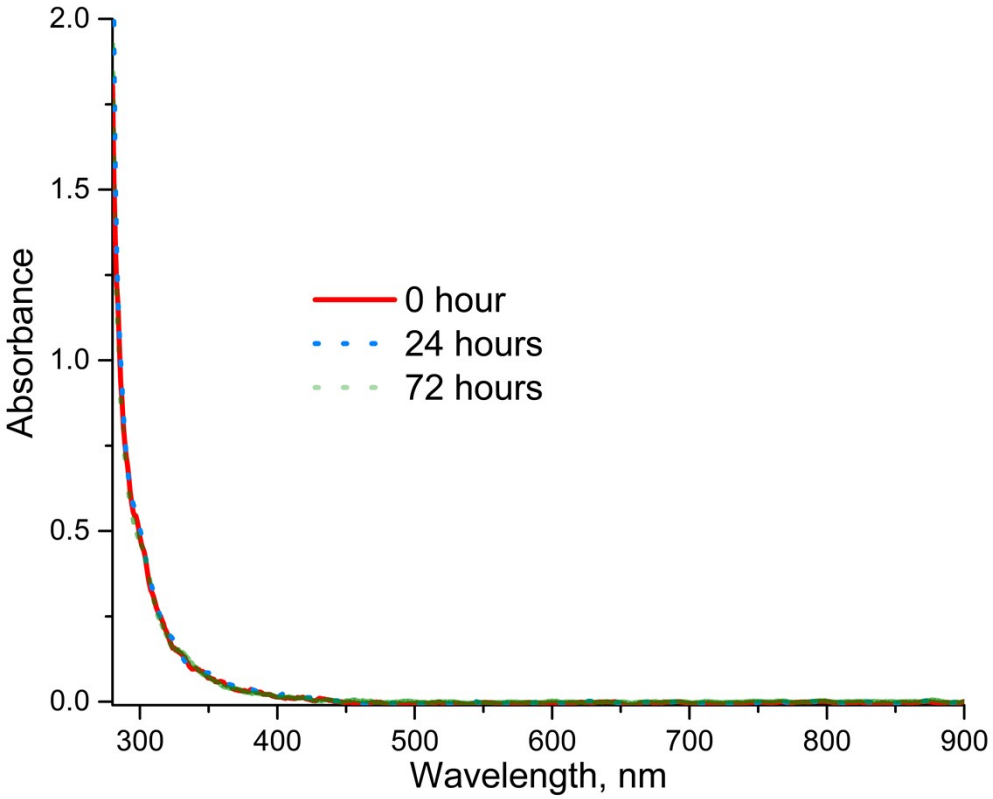


Figure S3. Stability test of [RuNO(Phen)$(NO_2)_2$OH in PBS ($5*10^{-5}$ M).