

Supplementary Information

A Potential Visible-Light NO Releaser: Synthesis, Reactivity and Vasodilator Properties

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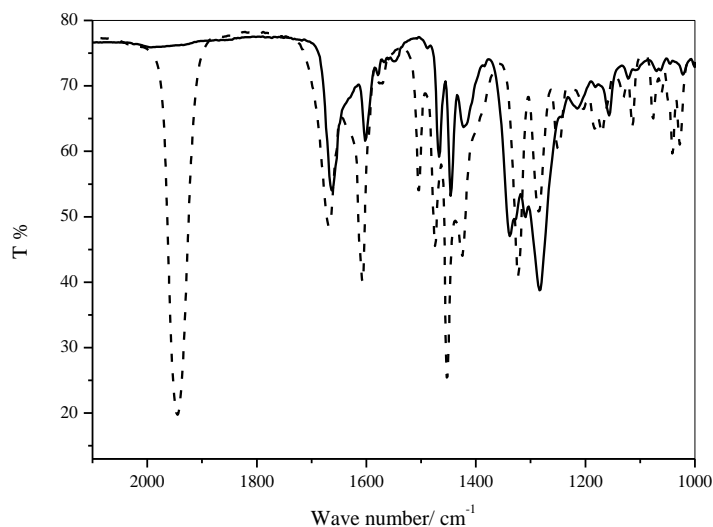


Figure S1. Infrared spectra of the complexes *cis*-[Ru(bpy)₂(4-bzpy)NO₂](PF₆) (solid line) and *cis*-[Ru(bpy)₂(4-bzpy)(NO)](PF₆)₃ (dashed line) dispersed in KBr.

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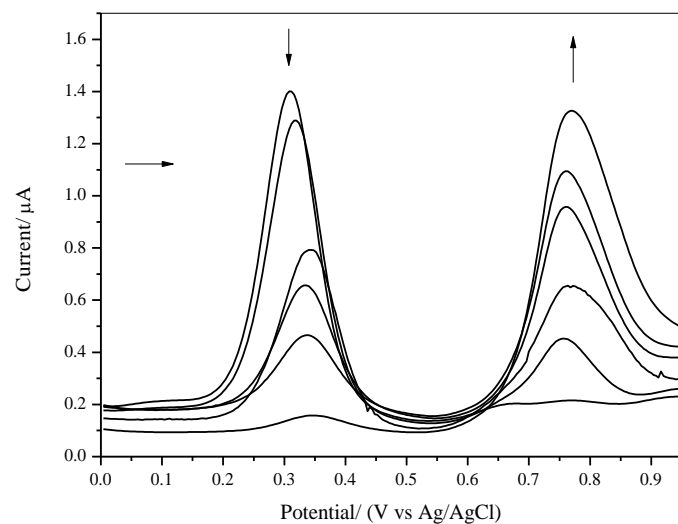


Figure S2. Square wave voltammogram at 0.10 V s^{-1} of the $\text{cis-}[\text{Ru}(\text{bpy})_2(4\text{-bzpy})(\text{NO})]^{3+}$ complex in 0.1 M KCl aqueous solution, $\text{pH} = 2.0$, scans starting at 0.0 V .

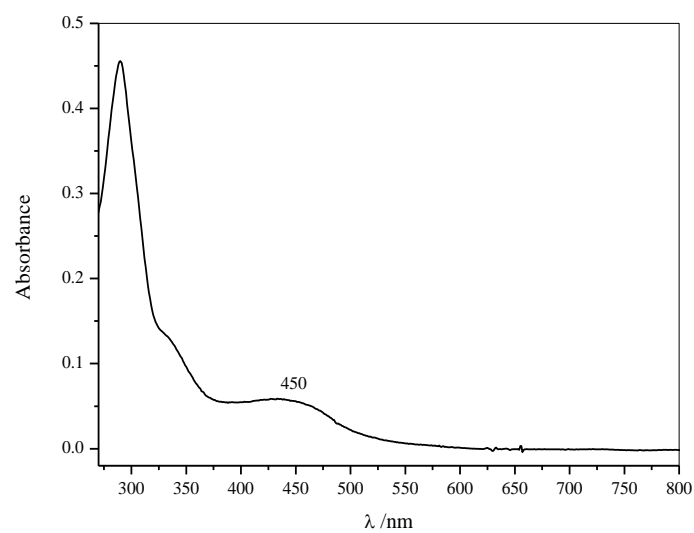


Figure S3. Electronic spectra in aqueous solution of $\text{cis-}[\text{Ru}(\text{bpy})_2(4\text{-bzpy})(\text{H}_2\text{O})]^{2+}$, $c = 6.0 \times 10^{-6} \text{ mol L}^{-1}$.

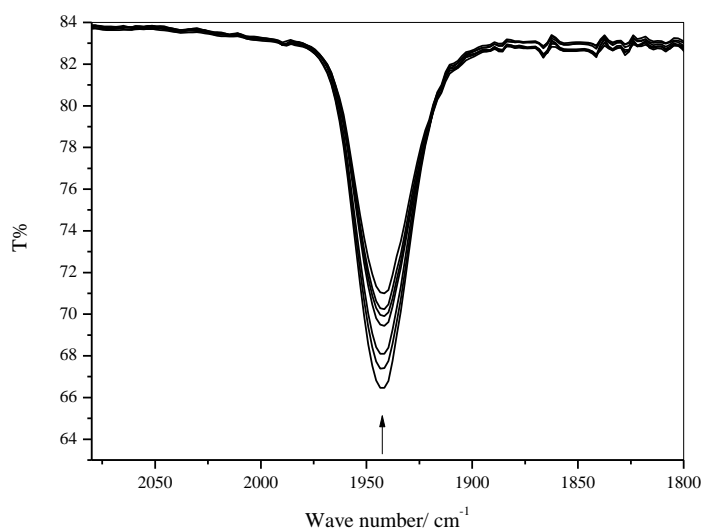


Figure S4. Infrared spectral changes of *cis*-[Ru(bpy)₂(4-bzpy)(NO)](PF₆)₃ dispersed in KBr upon irradiation using light at 505 nm.

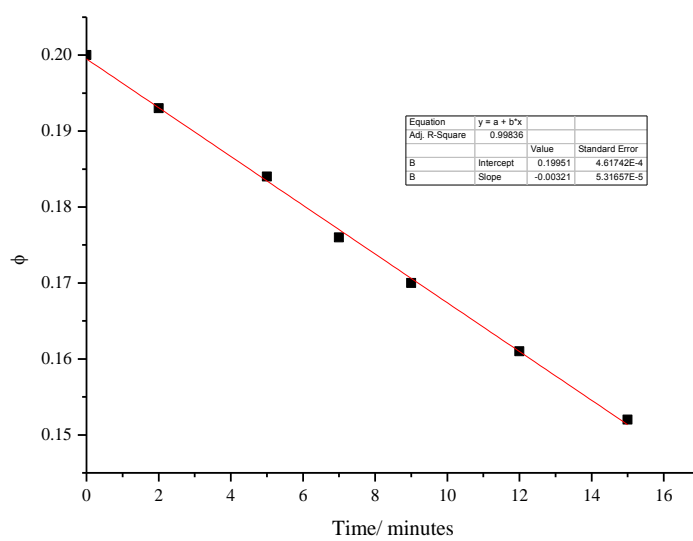


Figure S5. Measured quantum yields *versus* time of the photoreaction $\lambda_{\text{irradiation}} = 365$ nm.

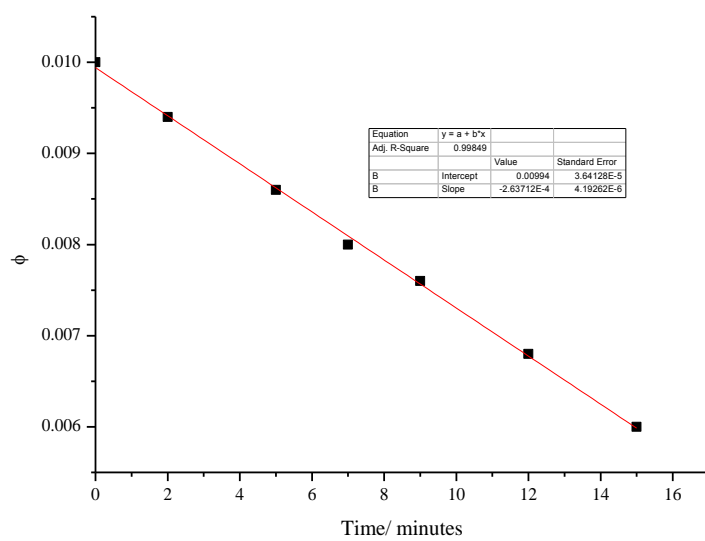


Figure S6. Measured quantum yields *versus* time of the photoreaction $\lambda_{\text{irradiation}} = 453 \text{ nm}$.

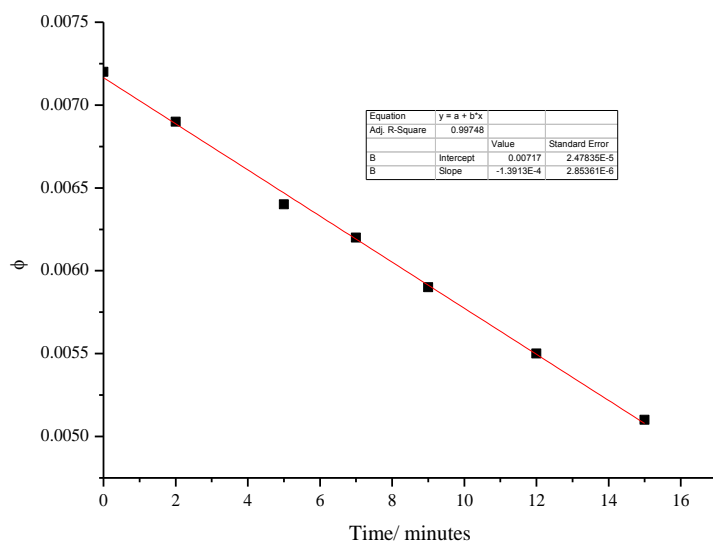


Figure S7. Measured quantum yields *versus* time of the photoreaction $\lambda_{\text{irradiation}} = 505 \text{ nm}$.

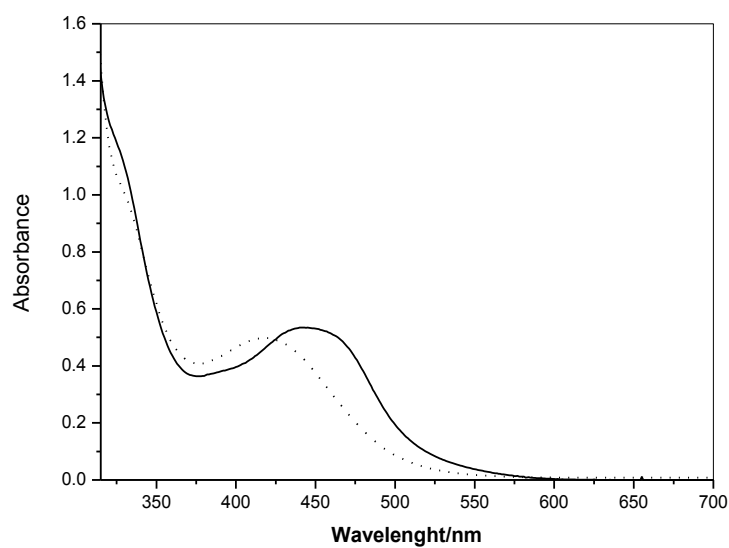


Figure S8. Electronic spectra in aqueous solution of *cis*-[Ru(bpy)₂(4-bzpy)(NO₂)]⁺, $c = 1.0 \times 10^{-4} \text{ mol L}^{-1}$, pH adjusted to 7.4. Solid line: starting material, dot line: after irradiation, $\lambda_{\text{irradiation}} = 453 \text{ nm}$.

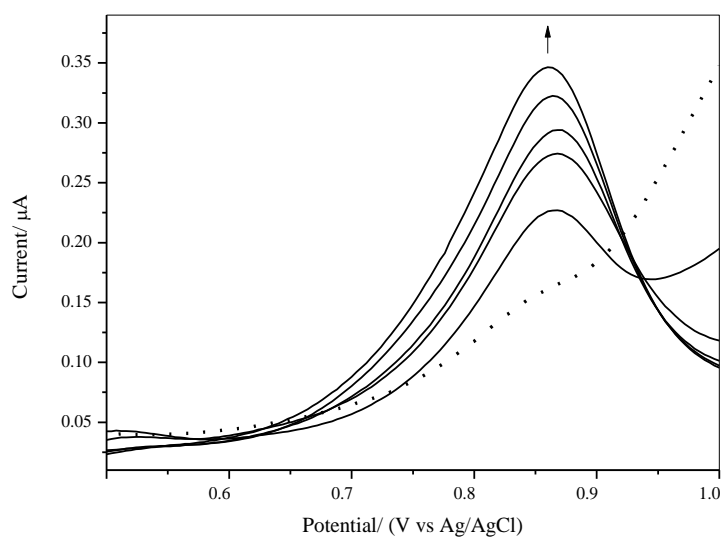


Figure S9. Square wave voltammograms for Au/*trans*-[Fe(cyclam)(NCS)₂]⁺ electrode in 0.1 M KCl solution, pH = 2.0, containing *cis*-[Ru(bpy)₂(4-bzpy)NO]³⁺ complex ($8.5 \times 10^{-4} \text{ mol L}^{-1}$) and cysteine ($8.5 \times 10^{-3} \text{ mol L}^{-1}$), followed over time. Dashed line: before the addition of cysteine and solid lines after addition for a total time 20 min.

Table S1. Crystal data and structure refinement

Empirical formula	$(\text{C}_{32}\text{H}_{25}\text{N}_6\text{O}_3\text{Ru})^+\text{PF}_6^-\cdot 1/2(\text{CH}_3\text{CH}_2\text{OH})$
Formula weight	810.65
Crystal system	monoclinic
Space group	$P2_1/c$
Unit cell dimensions	$a = 11.4456(4) \text{ \AA}$ $b = 21.4796(11) \text{ \AA}; \beta = 102.702(2)^\circ$ $c = 15.6031(8) \text{ \AA}$
Volume / \AA^3	3742.1(3)
Z	4
Absorption coefficient / mm^{-1}	0.533
F (000)	1636
Reflections collected	39409
Independent reflections	7231 [R(int) = 0.0774]
Final R indices [I > 2 σ (I)]	$R_1 = 0.0630, wR_2 = 0.1636$
R indices (all data)	$R_1 = 0.1458, wR_2 = 0.1781$
CCDC ref. number	1475460

Table S2. Bond lengths and angles for the complex *cis*-[Ru(bpy)₂(4-bzpy)(NO₂)](PF₆)

Bond length / Å		Bond angle / degree	
Ru–N(3)	2.061(4)	N(3)–Ru–N(1)	96.39(19)
Ru–N(2)	2.077(4)	N(6)–Ru–N(4)	175.0(2)
Ru–N(1)	2.061(4)	N(3)–Ru–N(6)	96.0(2)
Ru–N(4)	2.091(5)	N(2)–Ru–N(4)	98.09(18)
Ru–N(6)	2.075(6)	N(1)–Ru–N(6)	91.14(19)
Ru–N(5)	2.099(4)	N(3)–Ru–N(5)	89.40(18)
N(6)–O(2)	1.210(6)	N(3)–Ru–N(2)	174.20(19)
N(6)–O(1)	1.212(6)	N(1)–Ru–N(5)	173.94(17)
		N(1)–Ru–N(2)	78.39(19)
		N(6)–Ru–N(5)	90.0(2)
		N(6)–Ru–N(2)	86.70(18)
		N(2)–Ru–N(5)	95.74(18)
		N(3)–Ru–N(4)	79.1(2)
		N(4)–Ru–N(5)	90.75(18)
		N(1)–Ru–N(4)	88.59(17)
		C(1)–N(1)–C(5)	118.8(5)
		C(11)–N(3)–Ru	126.8(5)
		C(15)–N(3)–Ru	115.5(4)
		O(2)–N(6)–O(1)	121.6(6)
		O(2)–N(6)–Ru	118.9(4)
		O(1)–N(6)–Ru	119.3(5)