Electronic Supplementary Information for

Development of a functional ruthenium(II) complex for probing hypochlorous acid in living cells

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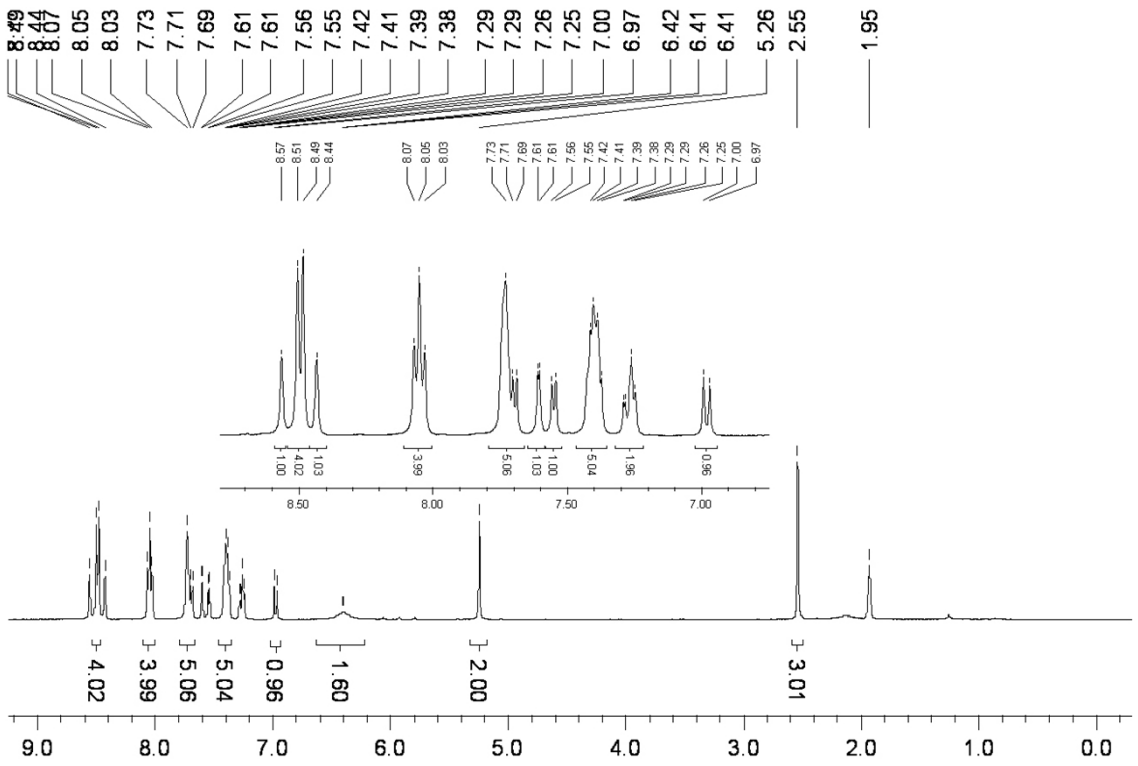

Fig. S1. ^{1}H NMR spectrum (400 MHz) of $[Ru(bpy)(AN\text{-}bpy)_2](PF_6)_2$ in CD_3CN.

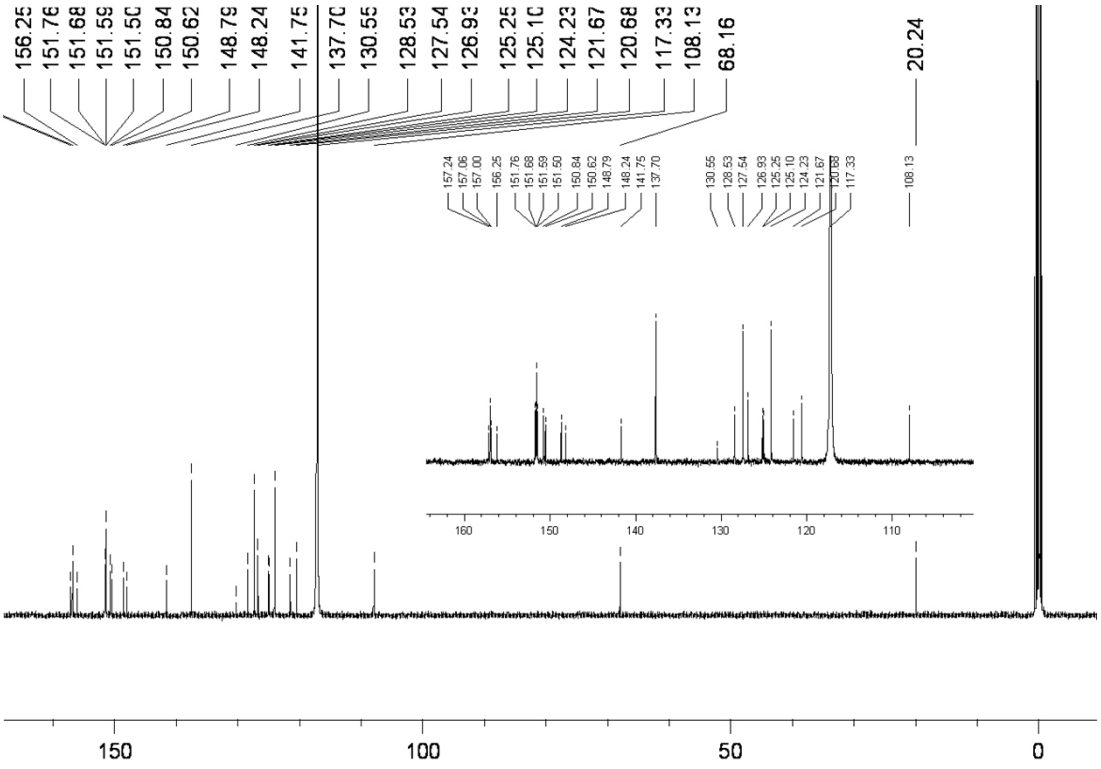

Fig. S2. ^{13}C NMR spectrum (100 MHz) of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ in CD_3CN.

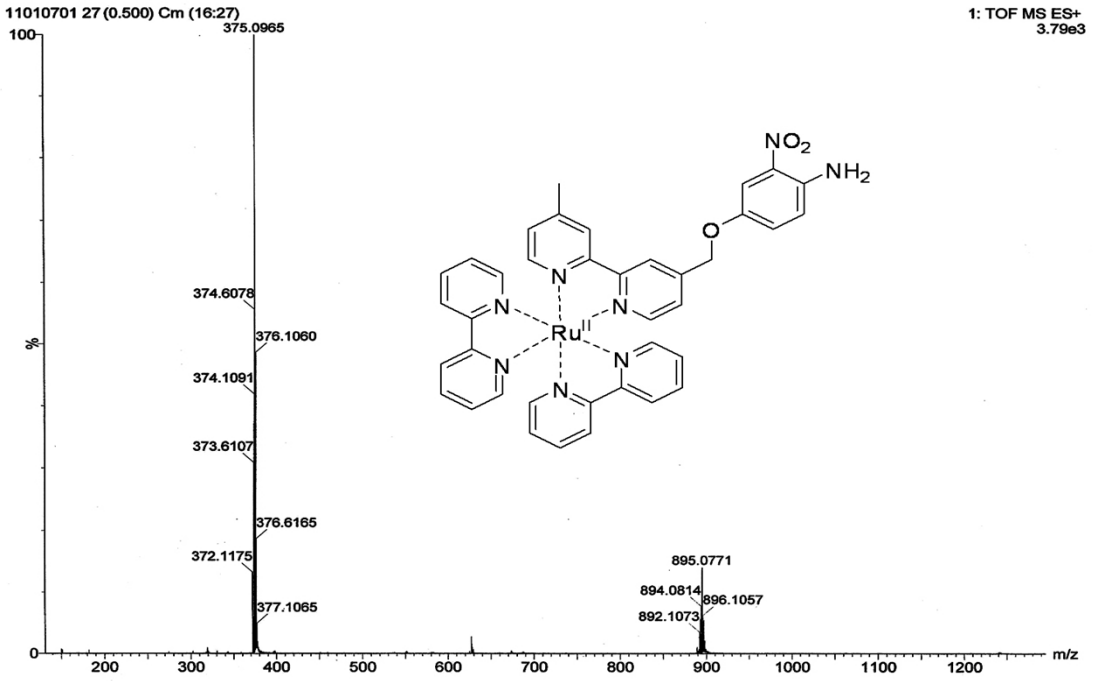

Fig. S3. Mass spectrum of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$.

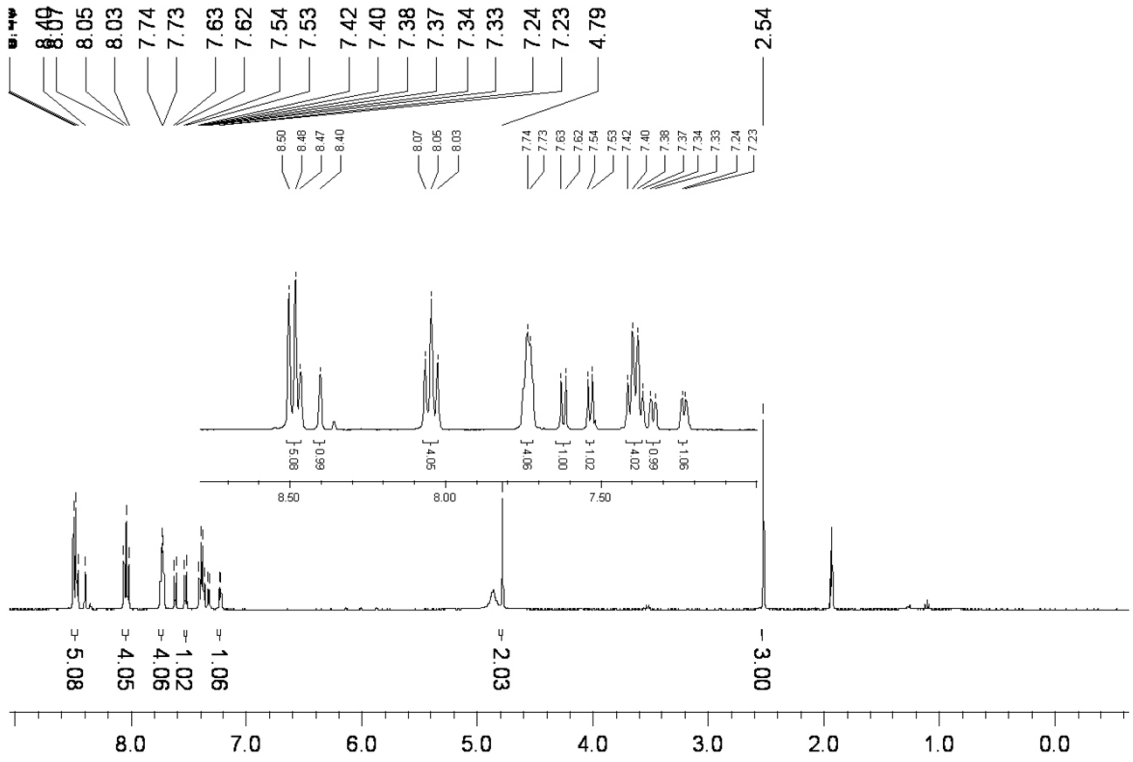

Fig. S4. ^{1}H NMR spectrum (400 MHz) of $[Ru(bpy)(HM\text{-}bpy)_2](PF_6)_2$ in CD_3CN.

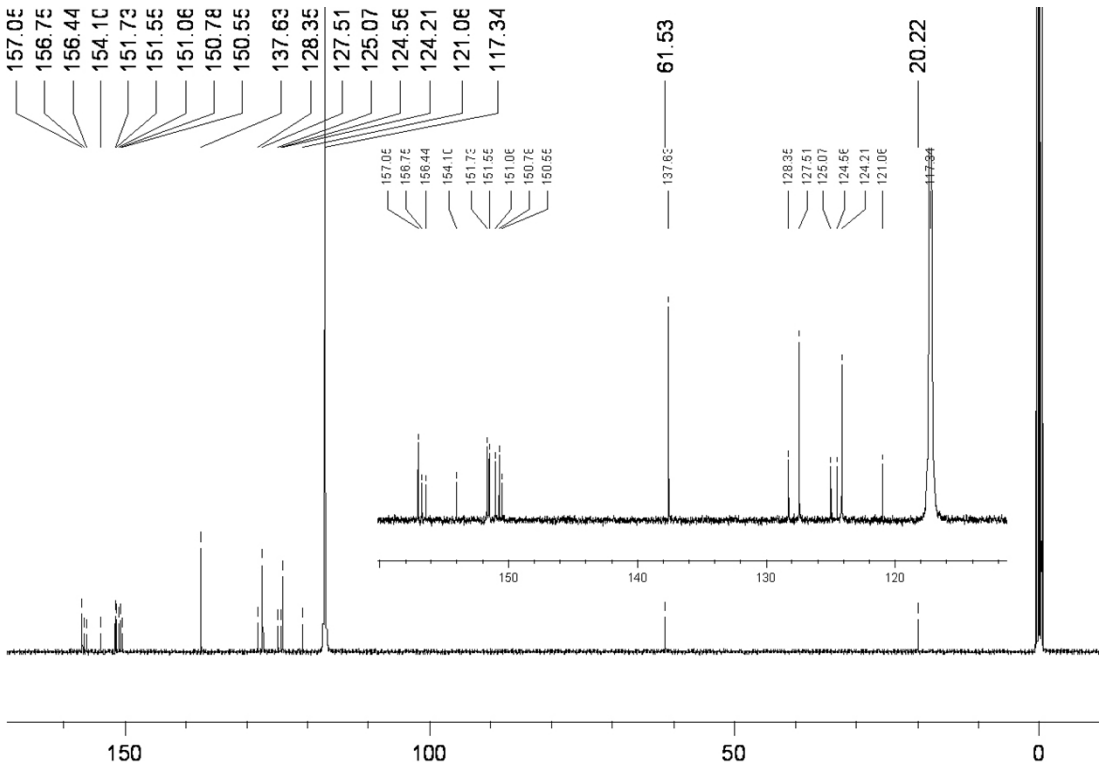

Fig. S5. ^{13}C NMR spectrum (100 MHz) of $[Ru(bpy)_2(HM\text{-}bpy)](PF_6)_2$ in CD_3CN.

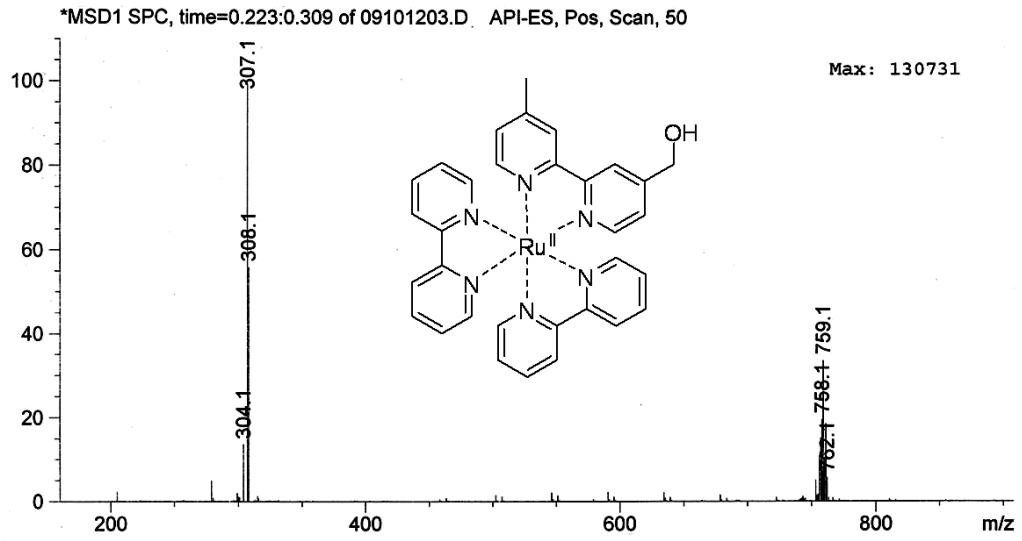

Fig. S6. Mass spectrum of $[Ru(bpy)_2(HM\text{-}bpy)](PF_6)_2$.

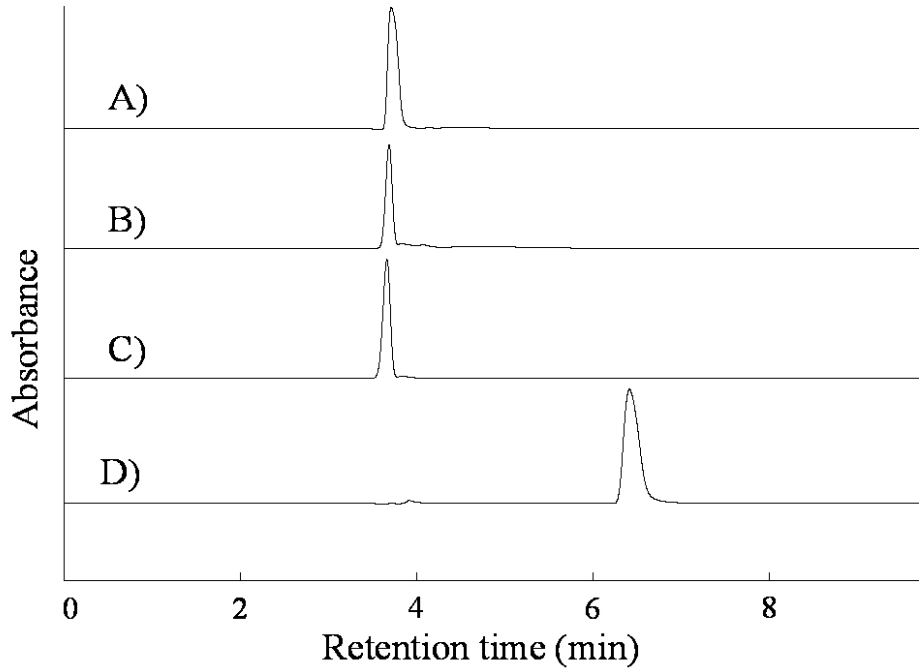

Fig. S7. HPLC analysis of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ after reaction with HOCl. Hypochlorous acid (4.0 mM) was added to a solution of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ (2.0 mM) in CH_3CN-borate buffer (50 mM, pH 7.4) (1: 50, v/v). The mixture was stirred at room temperature for 1 h, and then subjected to HPLC analysis with aqueous CH_3OH (50%)/HAc (1%) as eluent. The wavelength of the UV-vis detector was 456 nm. A: pure $[Ru(bpy)_2(HM\text{-}bpy)](PF_6)_2$ (2.0 mM); B: the product of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ (2.0 mM) reacted with HOCl (4.0 mM); C: a mixed solution of A (10 μL) and B (10 μL); D: pure $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ (2.0 mM).

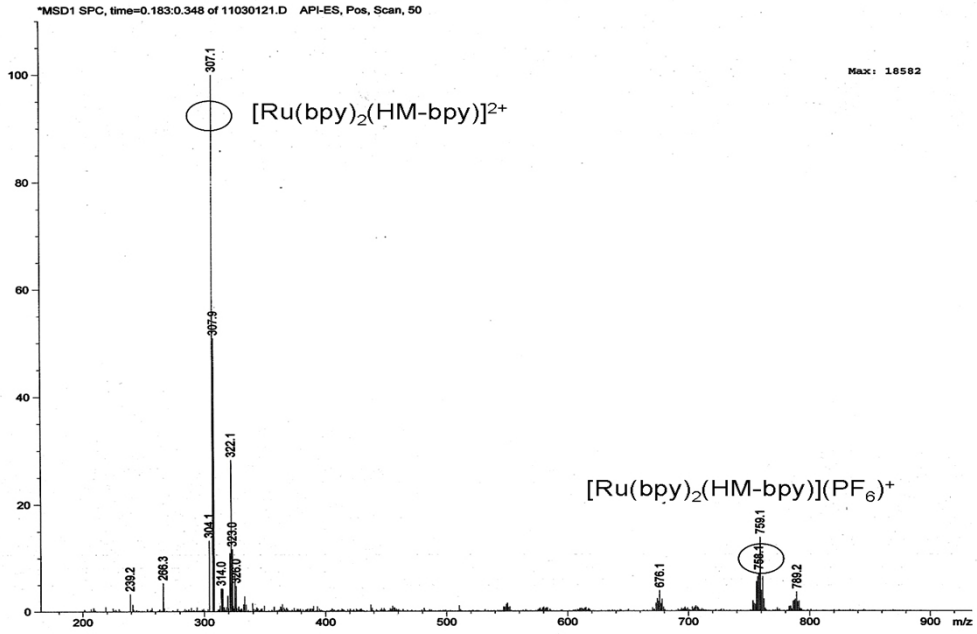

Fig. S8. Mass spectrum of the reaction solution of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ plus HOCl. Hypochlorous acid (4.0 mM) was added to a solution of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ (2.0 mM) in CH_3CN-borate buffer (50 mM, pH 7.4) (1: 50, v/v). The mixture was stirred at room temperature for 1 h, and then subjected to the mass spectrum measurement.

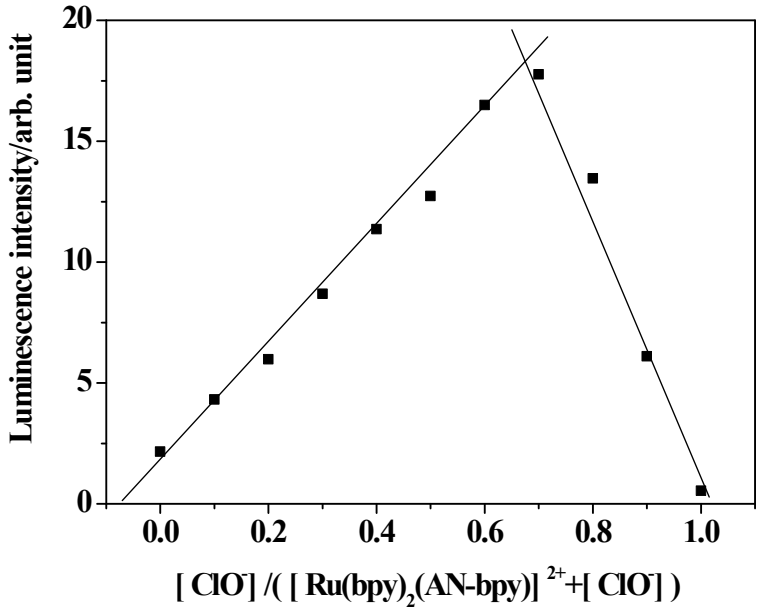

Fig. S9. Job's plot of the reaction between $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ and hypochlorite in 50 mM borate buffer of pH 7.4. The total concentrations of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ and hypochlorite were kept at 100 μM.

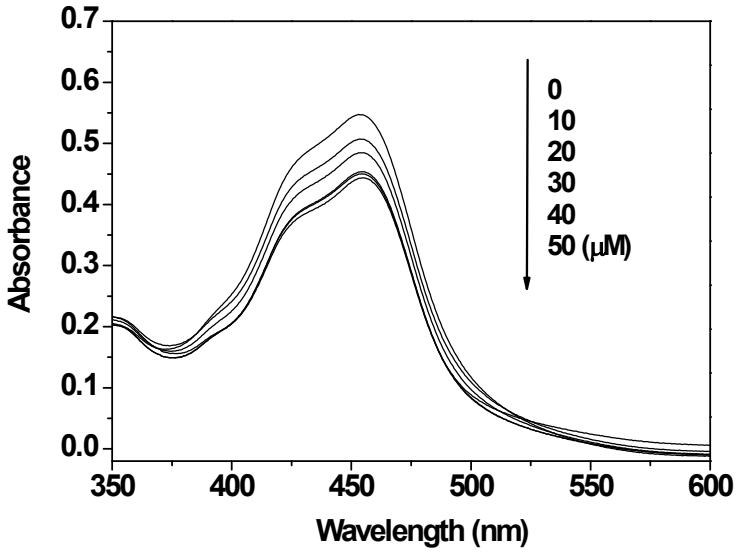

Fig. S10. The absorption spectrum changes of $[Ru(bpy)_2(AN\text{-}bpy)](PF_6)_2$ (30 μM) upon reaction with different concentrations (0.0, 10, 20, 30, 40, and 50 μM) of HOCl in 50 mM borate buffer of pH 7.4.