

Supplementary Material

Aquacobalamin accelerates Orange II destruction by peroxymonosulfate via the transient formation of secocorrinoid: a mechanistic study

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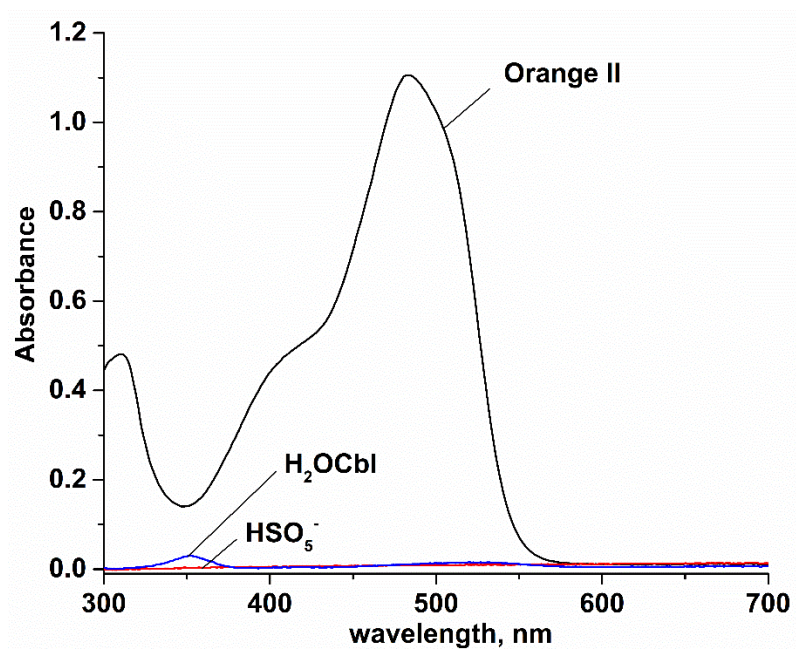


Figure S1. UV-vis spectra of Orange II ($5.7 \cdot 10^{-5}$ M), H₂OCbl ($1.0 \cdot 10^{-6}$ M) and HSO₅⁻ ($5.0 \cdot 10^{-4}$ M) at pH 7.4, 25.0 °C

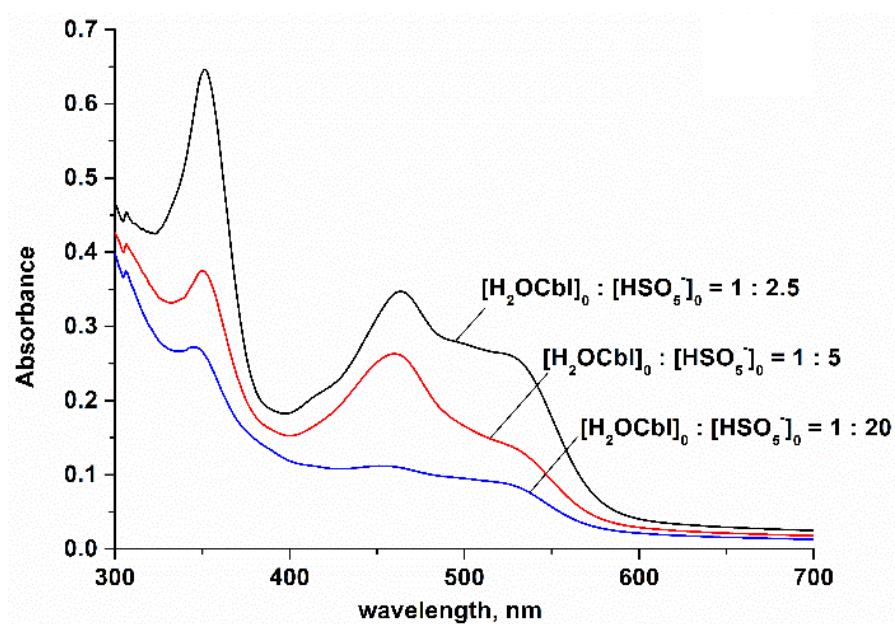


Figure S2. UV-vis spectra of the mixtures of H₂OCbl ($5.0 \cdot 10^{-5}$ M) with different quantities of HSO₅⁻ recorded after 5 hours of incubation at pH 7.4, 25.0 °C

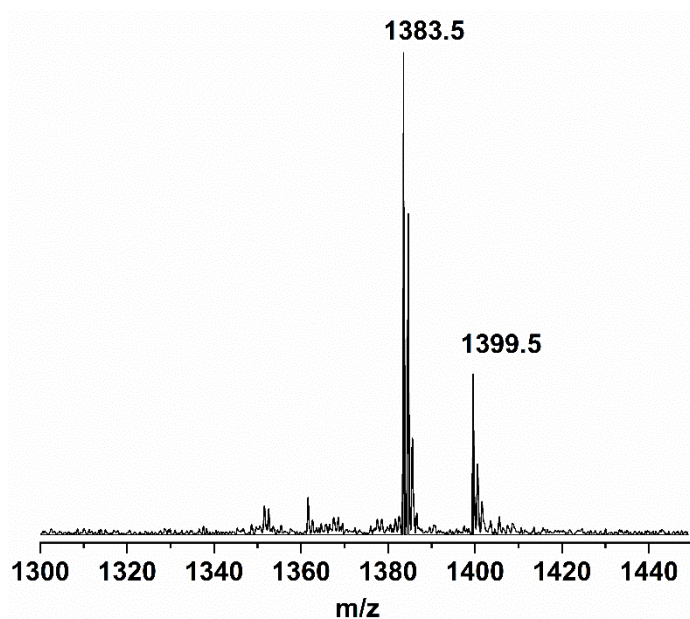


Figure S3. MALDI-mass-spectrum of the products of the reaction between H_2OCbl and two-fold excess of HSO_5^-

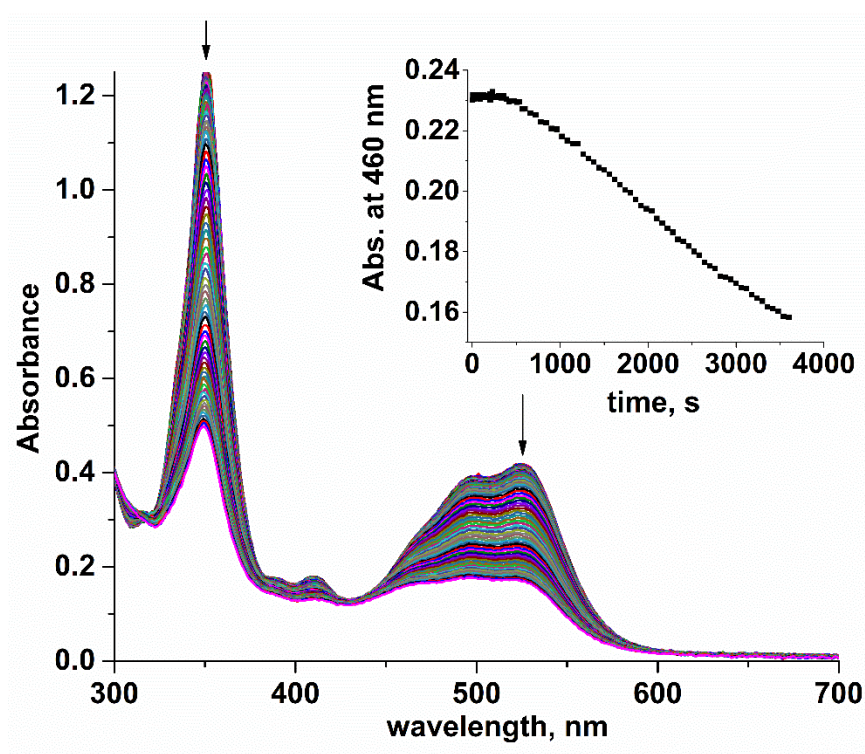


Figure S4. UV-vis spectra of the reaction between H_2OCbl ($5.0 \cdot 10^{-5}$ M) and HSO_5^- ($1.0 \cdot 10^{-3}$ M) at pH 4.5, 25.0 °C. Time intervals between spectra are 10, 30 and 60 s for 0...4, 4.5...10 and 10...60 min of the reaction, respectively. Inset: a time-course curve of the reaction

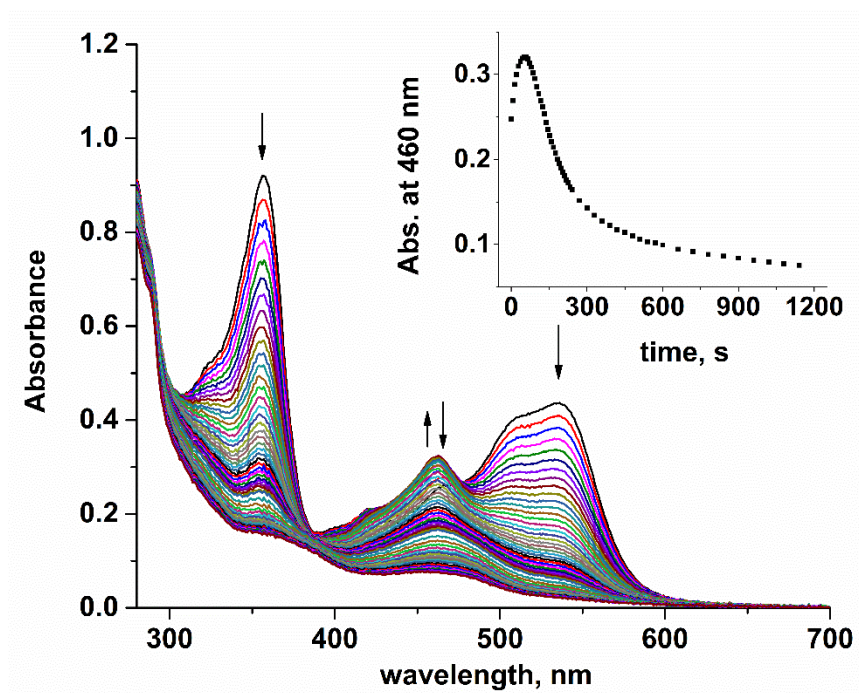


Figure S5. UV-vis spectra of the reaction between H_2OCbl ($5.0 \cdot 10^{-5} \text{ M}$) and HSO_5^- ($1.0 \cdot 10^{-3} \text{ M}$) at pH 9.2, 25.0 °C. Time intervals between spectra are 10, 30 and 60 s for 0...4, 4.5...10 and 10...19 min of the reaction, respectively. Inset: a time-course curve of the reaction

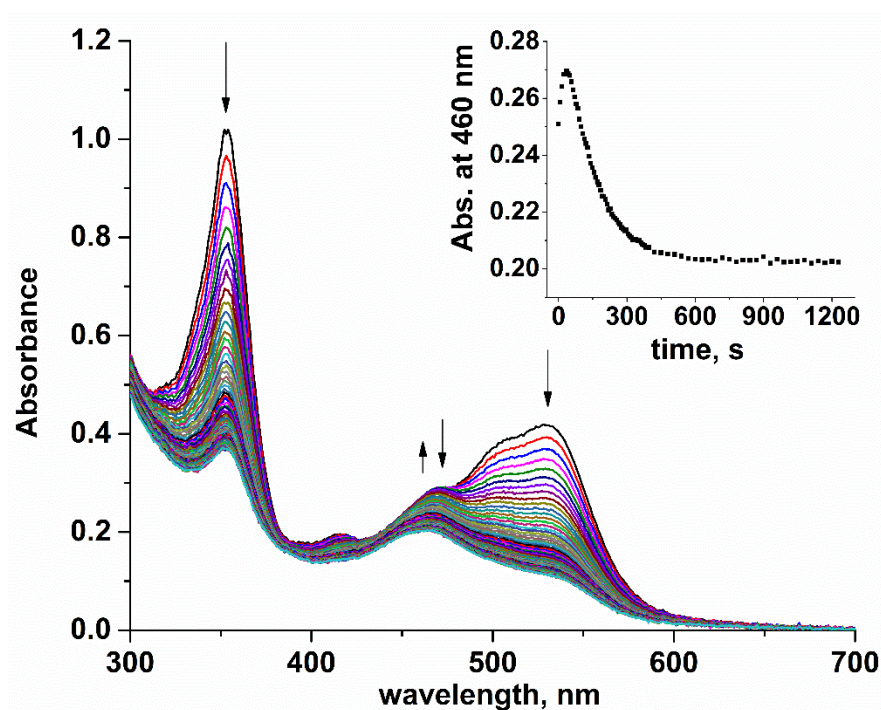


Figure S6. UV-vis spectra for the reaction between H_2OCbl ($5.0 \cdot 10^{-5} \text{ M}$) with HSO_5^- ($1.0 \cdot 10^{-3} \text{ M}$) at pH 7.4, 25.0 °C in the presence of ethanol ($5.0 \cdot 10^{-2} \text{ M}$). Time intervals between spectra are 10 and 30 s for 0...6.5 and 7 ...21 min of the reaction, respectively. Inset: a time-course curve of the reaction

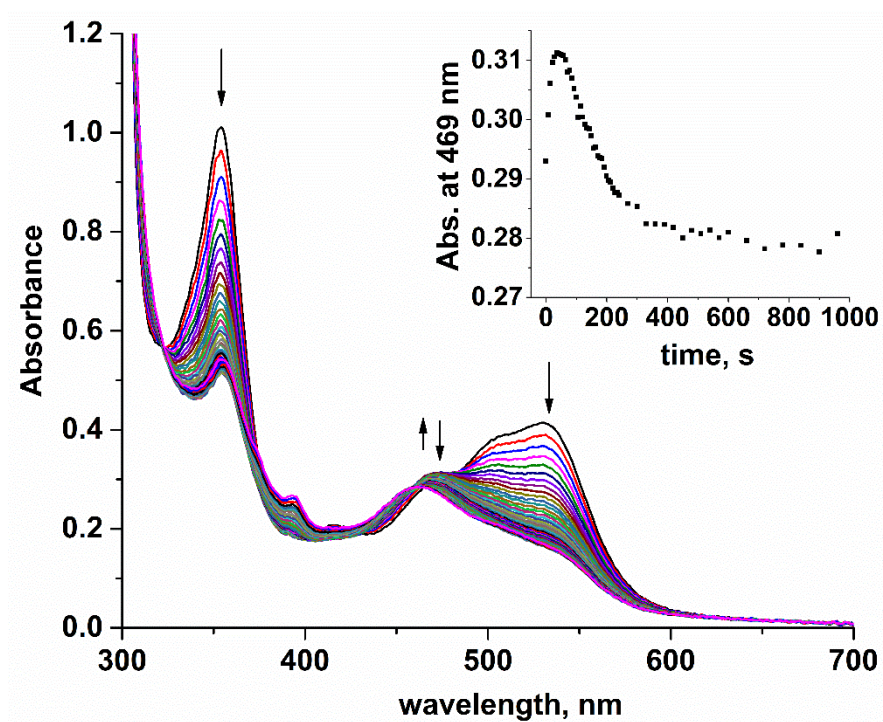


Figure S7. UV-vis spectra for the reaction between H_2OCbl ($5.0 \cdot 10^{-5} \text{ M}$) with HSO_5^- ($1.0 \cdot 10^{-3} \text{ M}$) at pH 7.4, 25.0°C in the presence of tryptophan ($5.0 \cdot 10^{-3} \text{ M}$). Final spectra of the reaction are contributed by absorbance of tryptophan oxidation products. Time intervals between spectra are 10, 30 and 60 s for 0...4, 4.5...10 and 10...16 min of the reaction, respectively. Inset: a time-course curve of the reaction

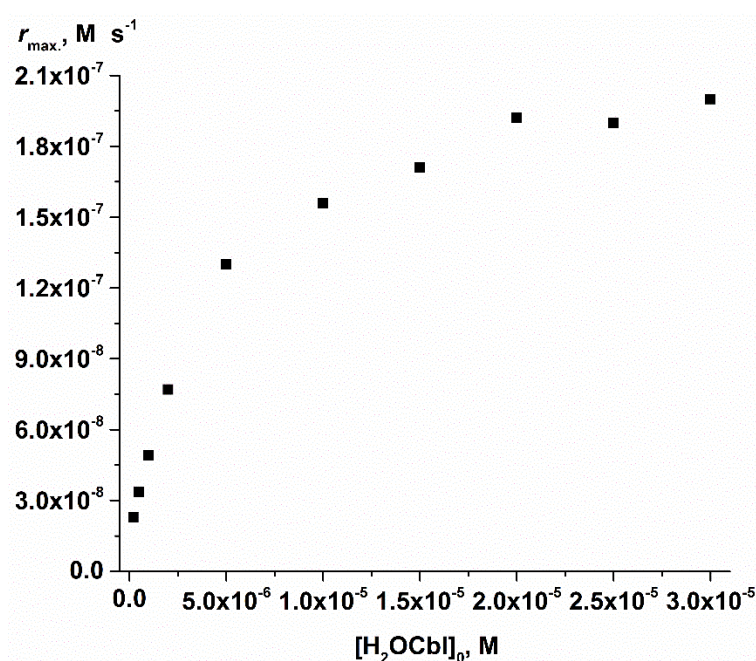


Figure S8. Plot of the maximum rate of the reaction between Orange II ($5.7 \cdot 10^{-5} \text{ M}$) and HSO_5^- ($5.0 \cdot 10^{-4} \text{ M}$) in the presence of H_2OCbl versus initial concentration of H_2OCbl at pH 7.4, 25.0°C

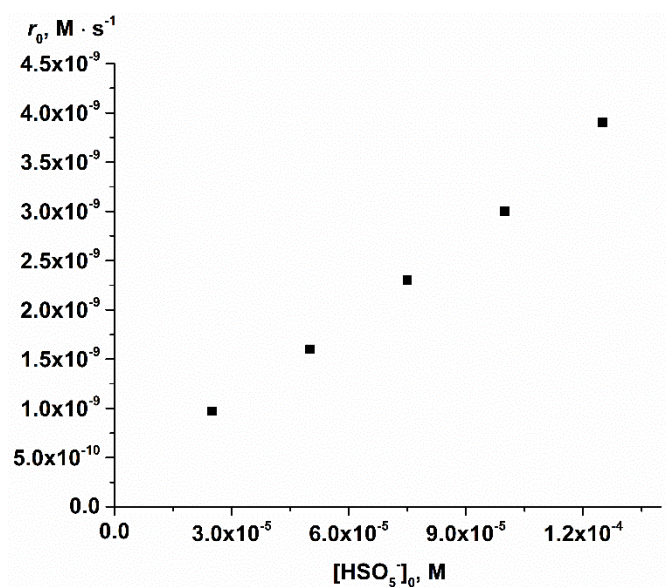


Figure S9. Plot of the initial rate of the reaction between Orange II ($5.7 \cdot 10^{-5}$ M) and HSO_5^- in the presence of H_2OCbl ($1.0 \cdot 10^{-6}$ M) versus initial concentration of HSO_5^- at pH 7.4, 25.0 °C

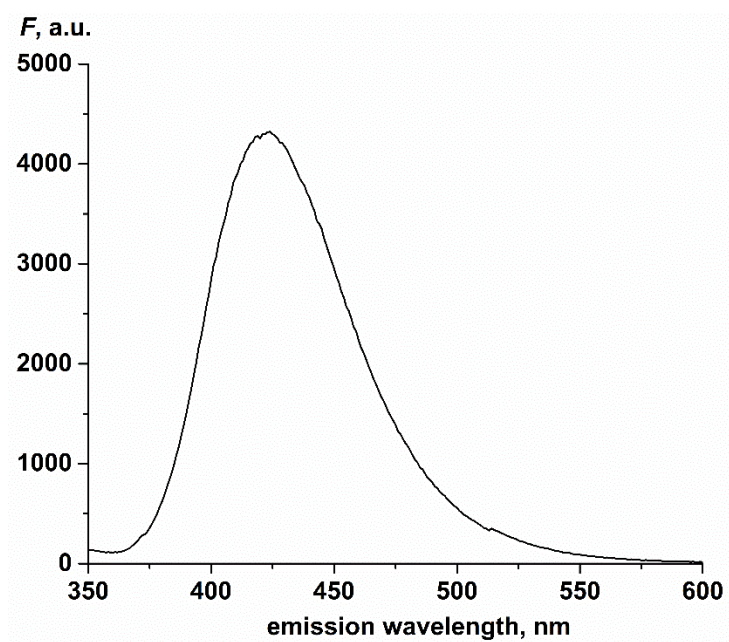


Figure S10. Fluorescence emission spectrum of 2-hydroxyterephthalic acid ($1.0 \cdot 10^{-6}$ M) at pH 7.4, 25.0 °C

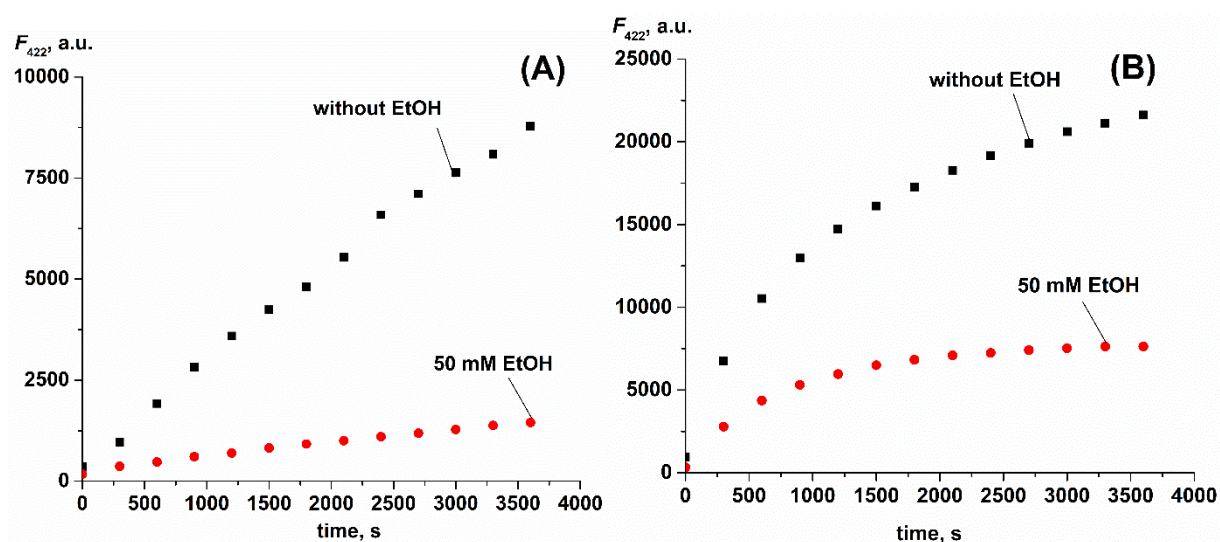


Figure S11. Plots of fluorescence intensity at 422 nm versus time for mixtures of terephthalic acid ($1.0 \cdot 10^{-3}$ M) with HSO_5^- ($5.0 \cdot 10^{-4}$ M; A) and with HSO_5^- ($5.0 \cdot 10^{-4}$ M) and H_2OCbl ($1.0 \cdot 10^{-6}$ M; B) in the absence and in the presence of ethanol (50 mM) at pH 7.4, 25.0 °C

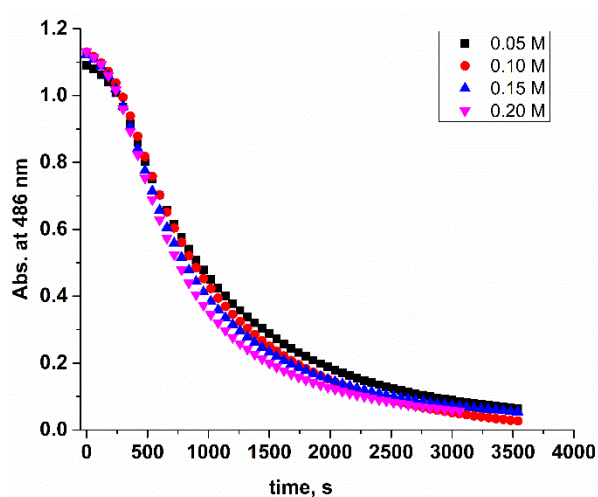


Figure S12. Time-course curves for the destruction of Orange II ($5.5 \cdot 10^{-5}$ M) by the mixture of H_2OCbl ($1.0 \cdot 10^{-6}$ M) with HSO_5^- ($5.0 \cdot 10^{-4}$ M) at pH 7.4, 25.0 °C in the presence of different phosphate buffer concentrations

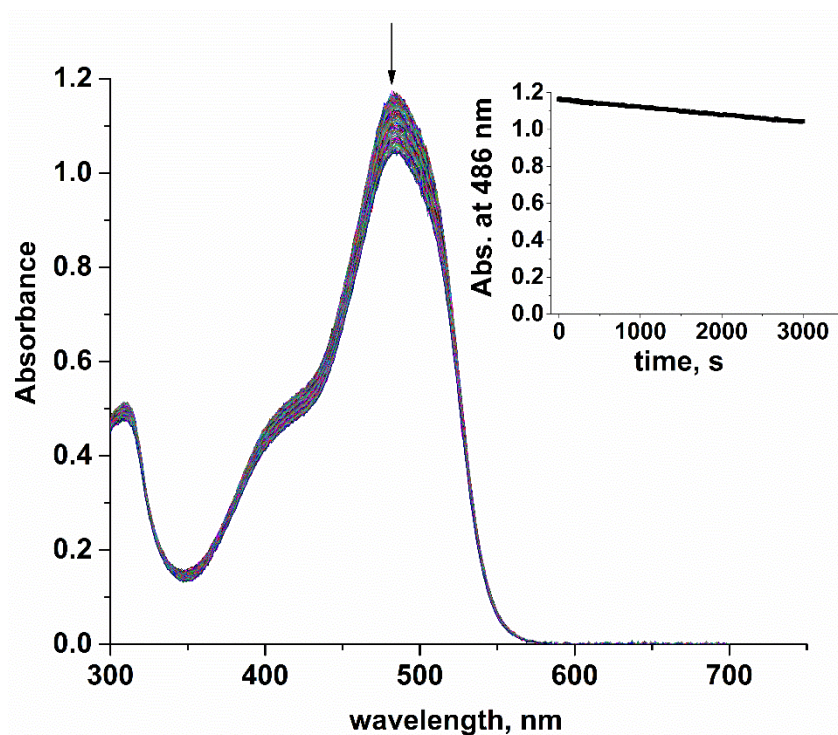


Figure S13. UV-vis spectra for the destruction of Orange II ($5.7 \cdot 10^{-5}$ M) by the mixture of H_2OCbl ($1.0 \cdot 10^{-6}$ M) with HSO_5^- ($5.0 \cdot 10^{-4}$ M) at pH 7.4, 25.0 °C in the presence of HCO_3^- ($5.0 \cdot 10^{-2}$ M). Time interval between spectra is 60 s. Inset: a time-course curve of the reaction

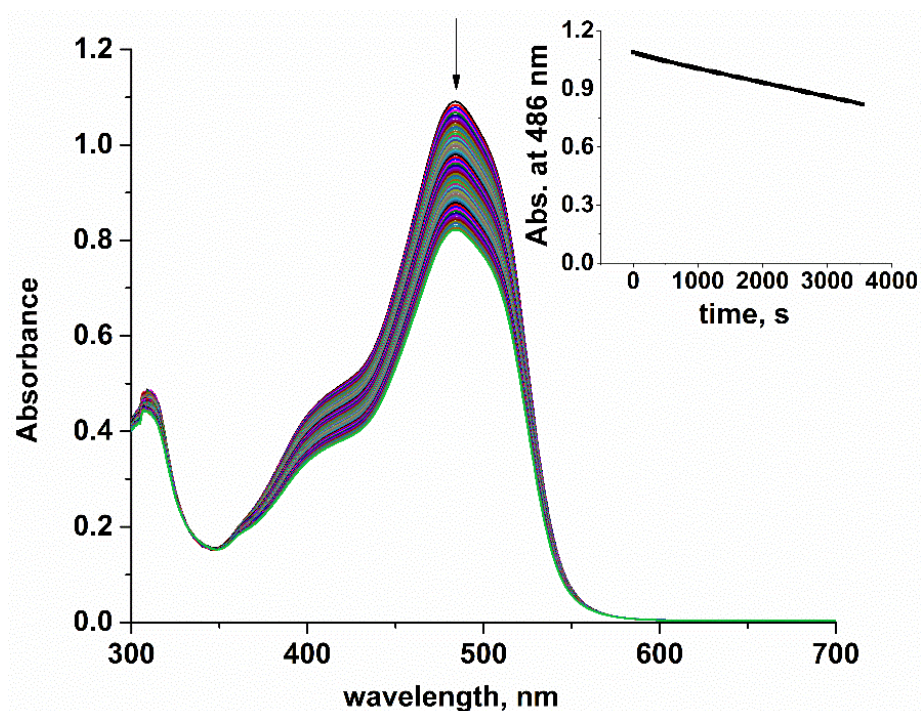


Figure S14. UV-vis spectra of the reaction between Orange II ($5.5 \cdot 10^{-5}$ M) and HSO_5^- ($5.0 \cdot 10^{-4}$ M) in the presence of CNCbl ($1.0 \cdot 10^{-6}$ M) at pH 7.4, 25.0 °C. Time interval between spectra is 60 s. Inset: a time-course curve of the reaction

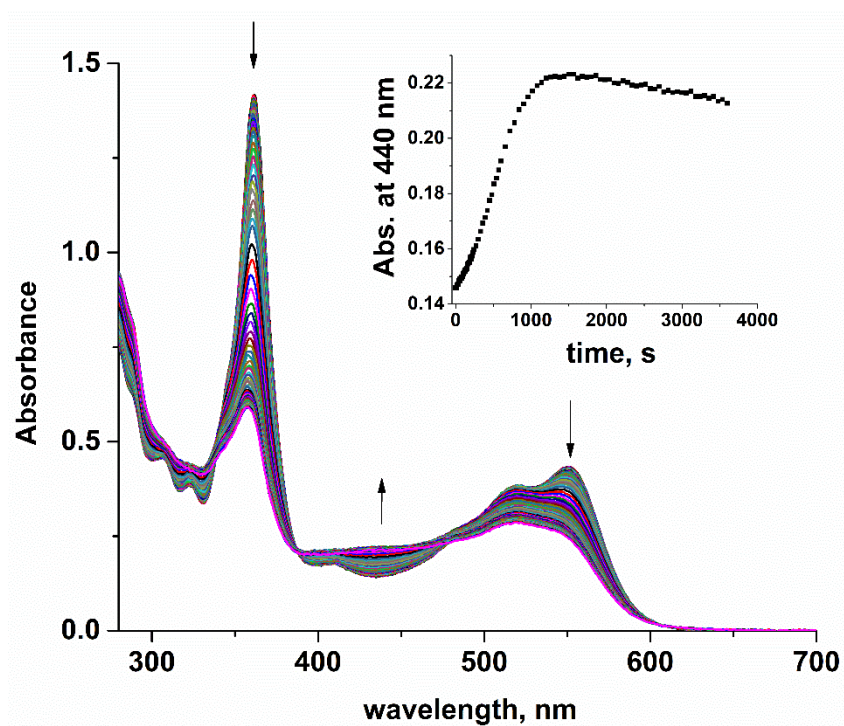


Figure S15. UV-vis spectra for the reaction between CNCbl ($5.0 \cdot 10^{-5}$ M) with HSO_5^- ($5.0 \cdot 10^{-4}$ M) at pH 7.0, 25.0 °C. Time interval between spectra is 60 s. Inset: a time-course curve of the reaction