

Supplementary Information for

Towards reliable quantification of hydroxyl radicals in the Fenton reaction using chemical probes

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In Fig. S1 is shown typical spectra of 7HC standard: the fluorescence intensity increased with the dosage of 7HC. The inset (A) in Fig. S1 depicts the calibration curve constructed using 7HC (concentration ranging from 2×10^{-7} M to 2×10^{-6} M), wherein the fluorescence intensity at 456 nm is linearly correlated ($R^2 = 0.9997$). The limit of detection ($LOD = 3.3 * (SD/S)$) was established at 3.4×10^{-8} M, where SD is the standard deviation of blanks and S is the slope of the linear fit equation

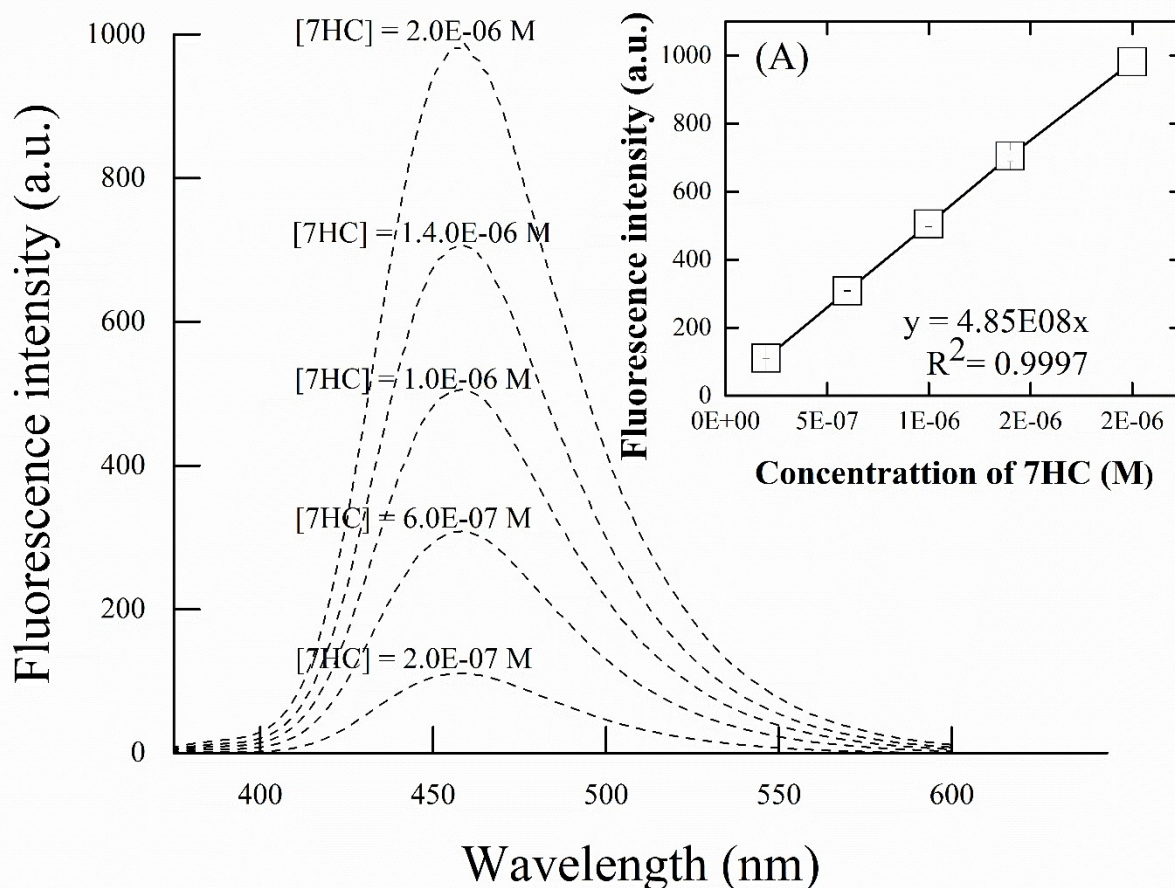


Fig. S1. Fluorescence spectra of umbelliferone (7HC) as a function of increasing the dosage. (A) Inset of the calibration curve ($R^2 = 0.9997$ with 95% confidence interval and 95% prediction band).

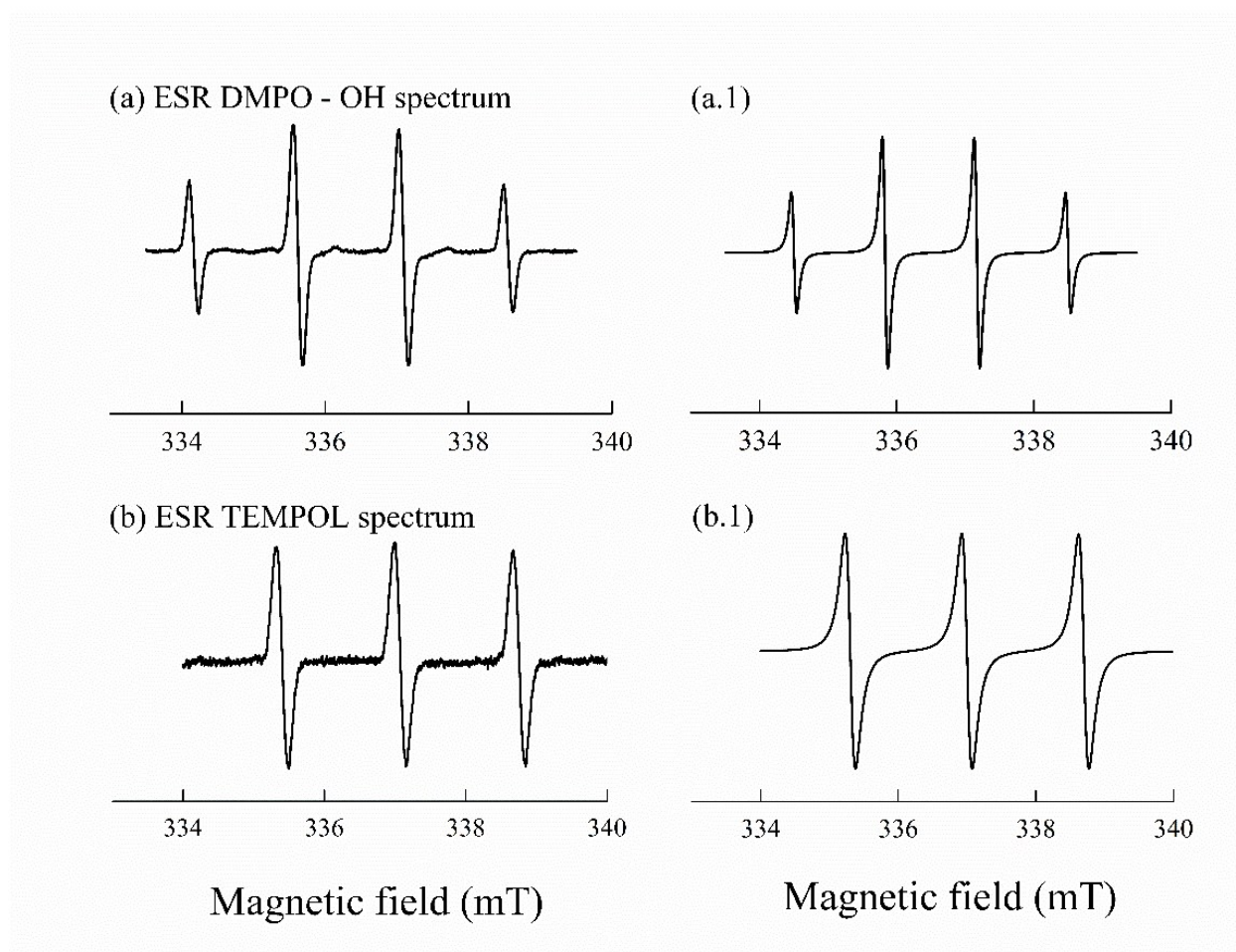


Fig. S2. Electron spin resonance (ESR) spectrum of (a) 5,5-dimethyl-1-pyrroline-N-oxide (DMPO-OH) adduct and (b) 4-hydroxy-2,2,5,5-tetramethyl-piperidine-1-oxyl (TEMPOL). Computer simulation of (a.1) DMPO-OH adduct ($a_H = 1.46 \text{ mT}$; $a_N = 1.47 \text{ mT}$) and (b.1) TEMPOL ($a_N = 1.68 \text{ mT}$).

In Fig. S3 are depicted the EPR spectra of TEMPOL. The inset (A) describes the calibration curve constructed using the peak-to-peak intensity of the TEMPOL signal ($R^2 = 0.9879$) with the concentration ranging from 2.5×10^{-6} M to 12.5×10^{-6} M

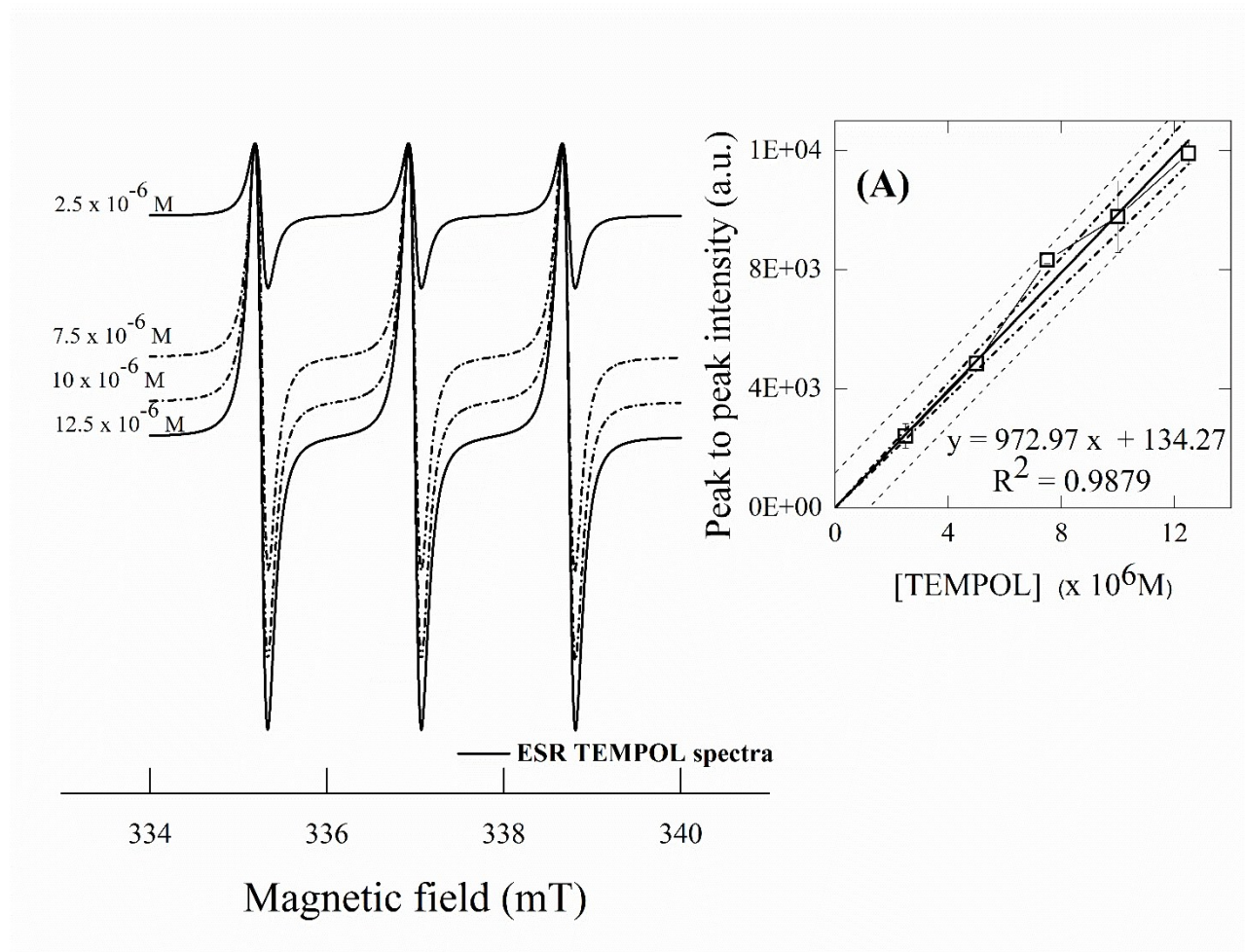


Fig. S3. Simulated electron spin resonance (ESR) spectrum of 4-hydroxy-2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPOL) radical as a function of increasing the dosage. (A) Inset of the calibration curve ($R^2 = 0.9879$ with 95% confidence interval and 95% prediction band).

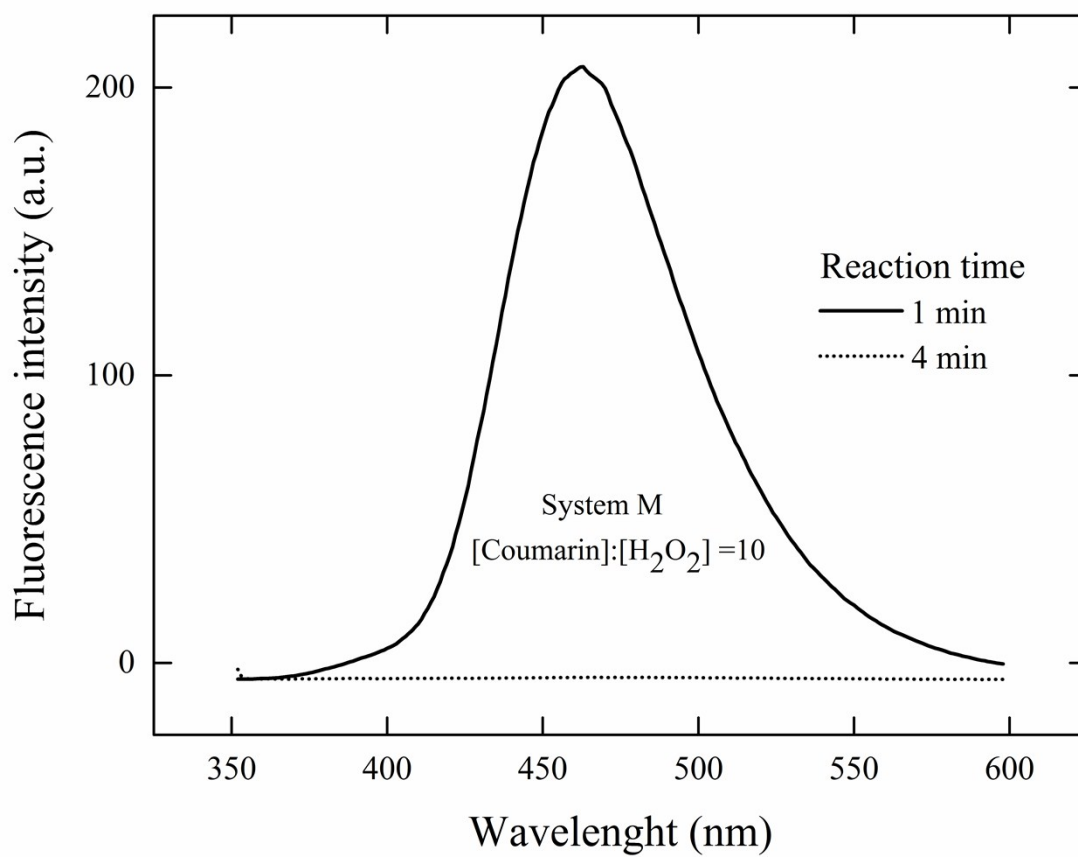


Fig. S4. Effect of [Coumarin]: [H₂O₂] ratio on molar formation of [•]OH (using 1 mM coumarin concentration) at [H₂O₂]: [Fe²⁺] ratio = 10.

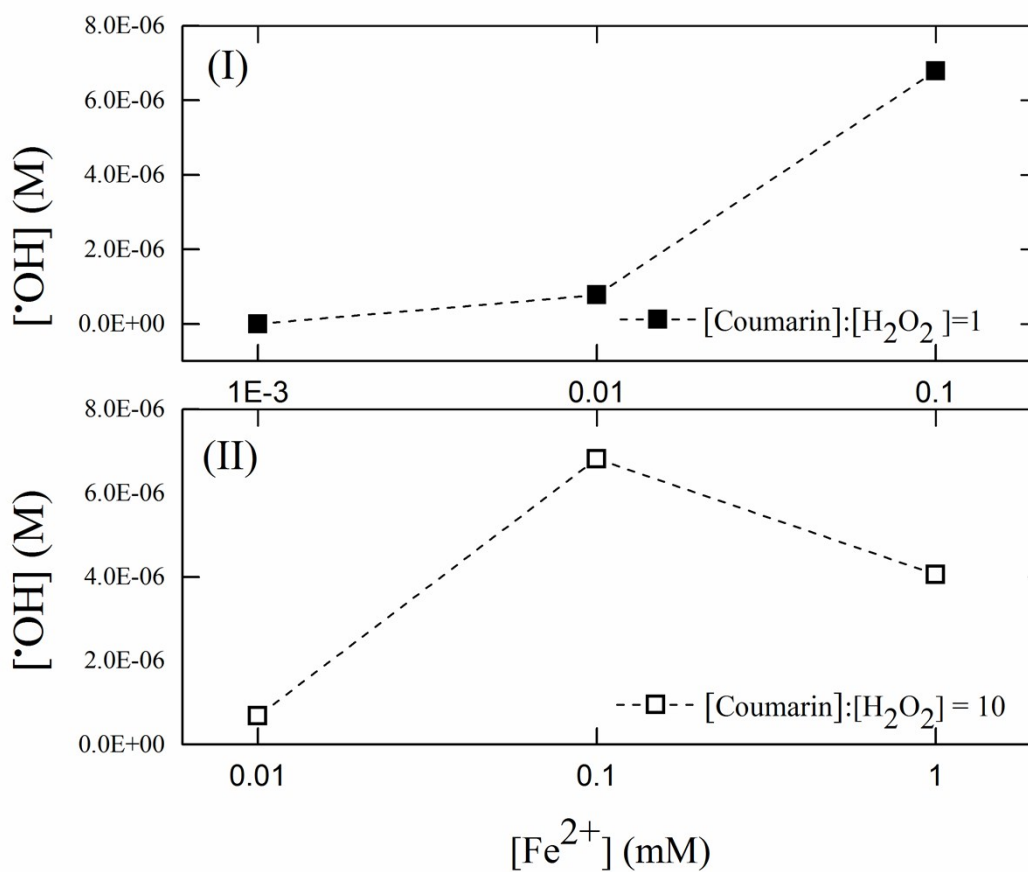


Fig. S5. Highlighted effect of $[\text{coumarin}]:[\text{H}_2\text{O}_2]$ ratio on molar formation of $\cdot\text{OH}$ at constant 1 mM coumarin and different initial $[\text{H}_2\text{O}_2]$ of (I) 1 mM and (II) 10 mM. The x -axis is shown on a logarithm scale.

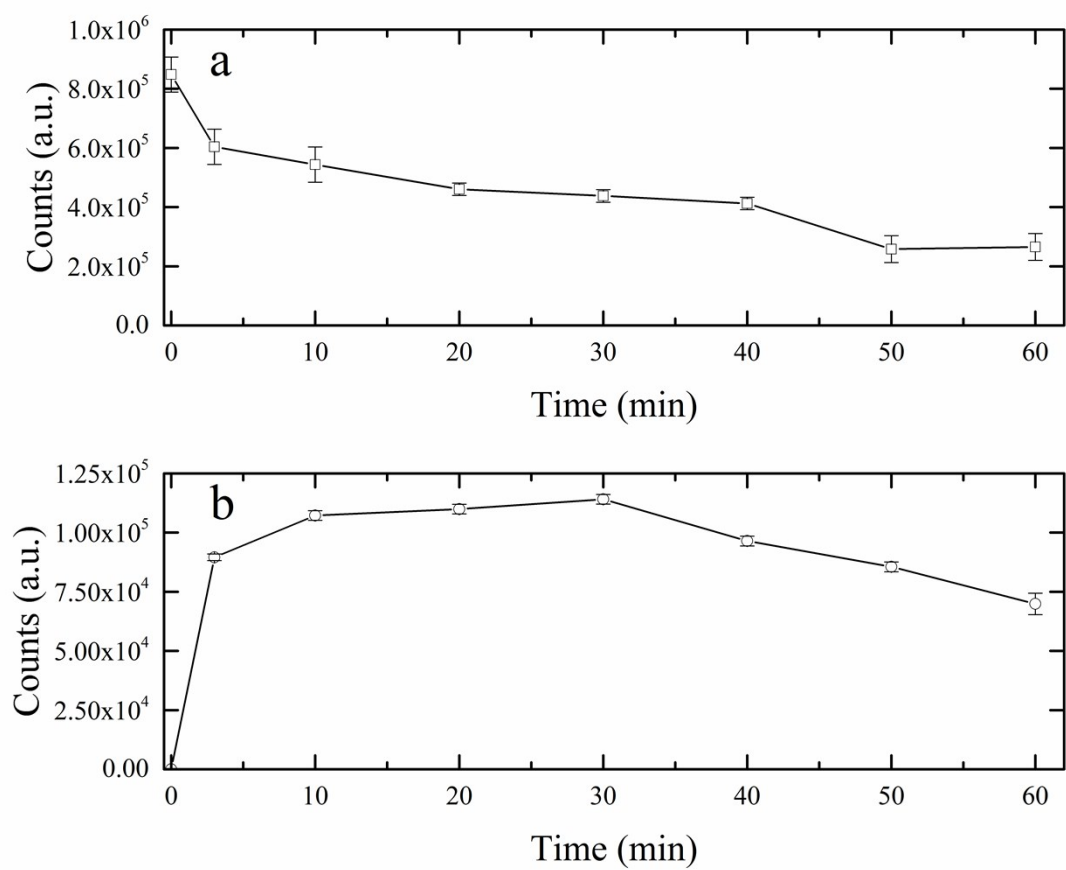


Fig. S6. Decomposition of coumarin (Fig. S6-a) and accumulation of 7HC (Fig.S6-b) using initial concentration of 1 mM coumarin; 1 mM H_2O_2 and 0.1 mM Fe^{2+} .