

Supplementary Information

Ciprofloxacin degradation from aqueous solution by Fenton oxidation: Reaction kinetics and degradation mechanisms

Ardhendu Sekhar Giri and Animes Kumar Golder

Table S1

Daughter ions formation in CIP degradation by FO.

Daughter ions	Molecular Formula	m/z (MH ⁺)	Degradation route
D ₁	C ₁₅ H ₁₆ O ₃ N ₃ F	305	Partial piperazine ring cleavage
D ₂	C ₁₅ H ₁₇ O ₄ N ₃	304	Defluorination followed by hydroxylation of D ₁
D ₃	C ₁₃ H ₁₁ O ₄ N	239	Complete piperazine ring cleavage of D ₂
D ₄	C ₁₃ H ₁₅ O ₂ N ₃ F	304	Decarboxylation of CIP
D ₅	C ₁₃ H ₁₆ O ₃ N ₃	301	Defluorination followed by hydroxylation of D ₄
D ₆	C ₁₆ H ₁₆ ON ₃ F	287	Dehydroxylation of D ₁
D ₇	C ₁₁ H ₁₀ ON ₂	186	Partial piperazine ring breaking followed by defluorination of D ₆
D ₈	C ₁₁ H ₁₂ O ₂ N ₂	205	Hydroxylation of D ₇
D ₉	C ₁₁ H ₁₂ ON ₂	198	Cleavage of cyclic amine of D ₇
D ₁₀	C ₁₁ H ₁₀ O ₂ N ₂	217	Hydroxylation of D ₉
D ₁₁	C ₁₄ H ₁₄ O ₂ N ₂	242	Partial piperazine ring breaking followed by defluorination of D ₁
D ₁₂	C ₁₄ H ₁₄ O ₂ N ₂ F	261	Partially piperazine ring cleavage of D ₁
D ₁₃	C ₁₄ H ₁₆ O ₃ N ₂ F	279	Hydroxylation followed by protonation of D ₁₂

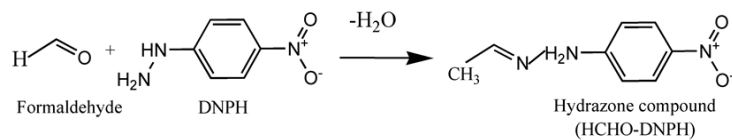


Fig. S1 Formation of hydrazone colored derivative by the reaction between HCHO and DNPH.

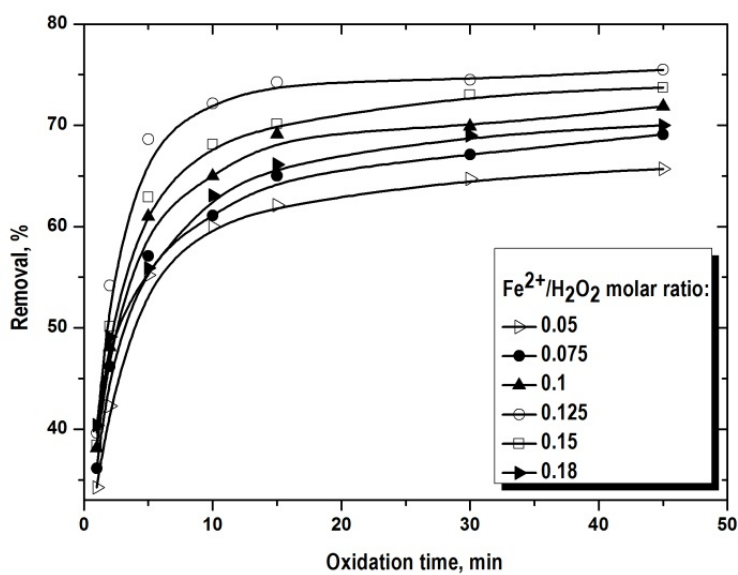


Fig. S2 Dynamics of drug degradation with the variation of $\text{Fe}^{2+}/\text{H}_2\text{O}_2$ molar ratio. Experimental conditions: $[\text{CIP}]_0 = 15 \text{ mg/L}$, $\text{pH} = 3.5$ and temperature = 25°C

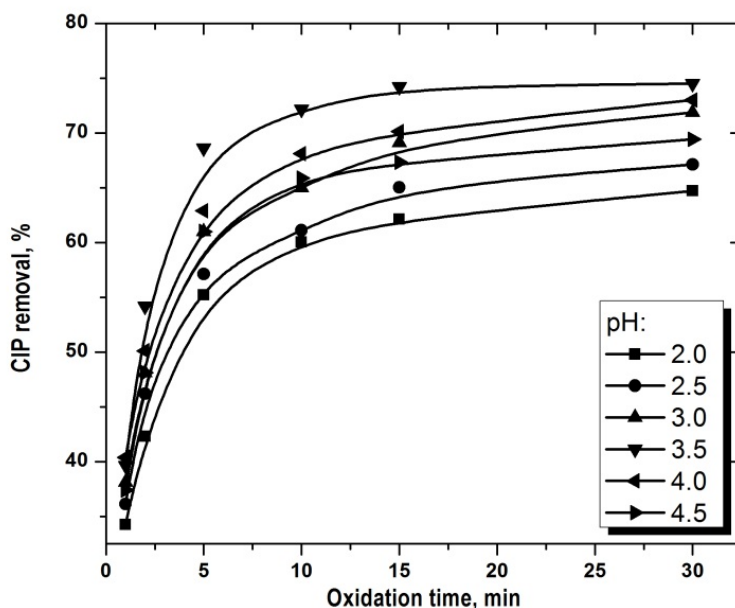


Fig. S3 Effect of pH on % CIP degradation at 3.5 pH. Experimental conditions: $[CIP]_0 = 15$ mg/L, Fe^{2+}/H_2O_2 molar ratio = 0.125 and temperature = 25°C.

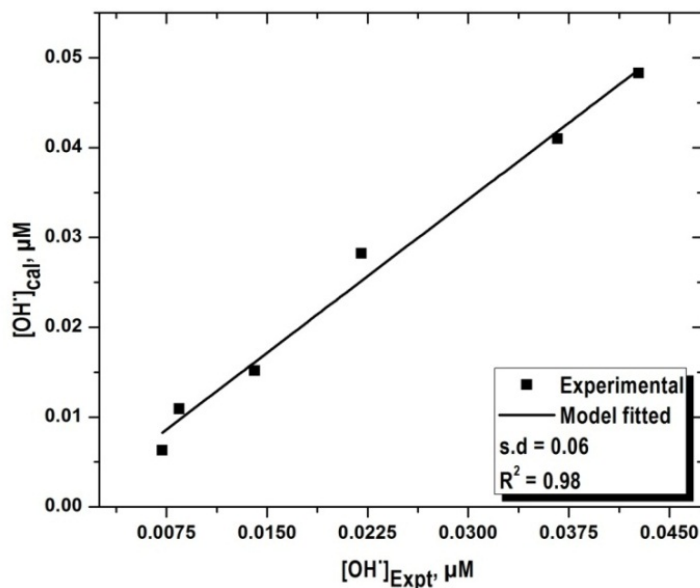


Fig. S4 Experimental vs. model predicted (eqns (17) to (20)) concentration of OH^\cdot . Experimental conditions: $[CIP]_0 = 15$ mg/L, Fe^{2+}/H_2O_2 molar ratio = 0.125, pH = 3.5 and temperature = 25°C.

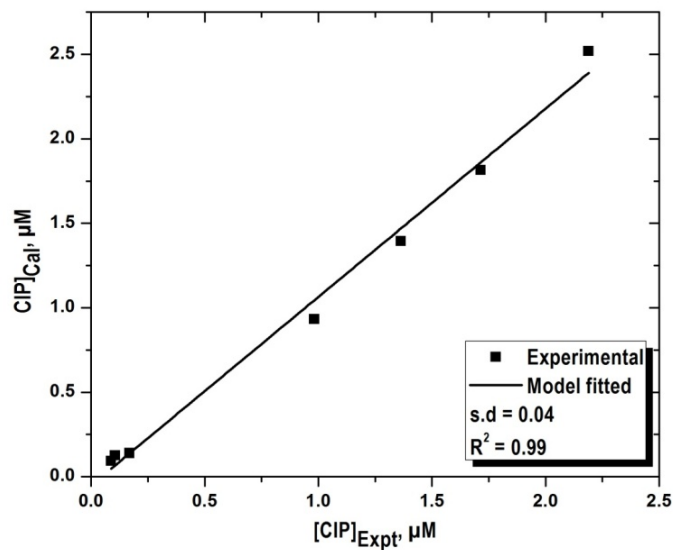


Fig. S5 Experimental vs. model predicted (eqns (17) to (20)) CIP degradation. Experimental conditions: $[CIP]_0=15$ mg/L, Fe^{2+}/H_2O_2 molar ratio = 0.125, pH = 3.5 and temperature = 25°C.

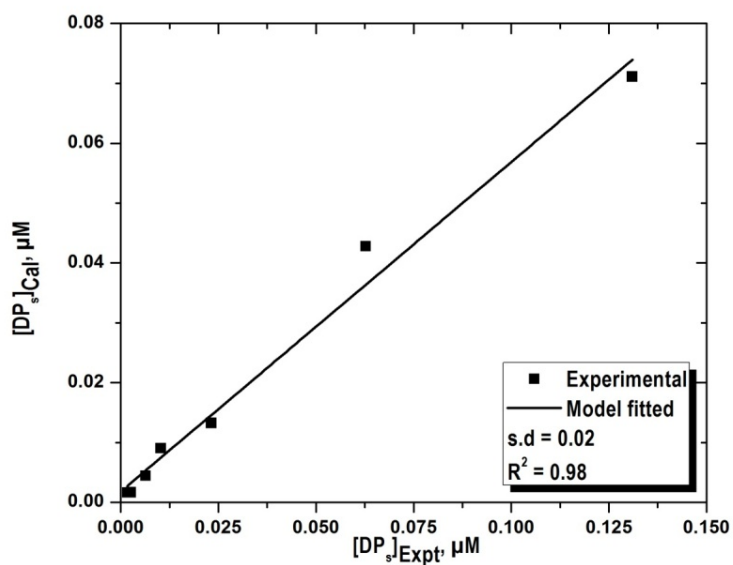


Fig. S6 Experimental vs. model predicted (eqns (17) to (20)) degradation products (DPs). Experimental conditions: $[CIP]_0 = 15$ mg/L, Fe^{2+}/H_2O_2 molar ratio = 0.125, pH = 3.5 and temperature = 25°C.