Supporting Information

Mechanism and application of halogen bond induced fluorescence enhancement and iodine molecule cleavage in solution

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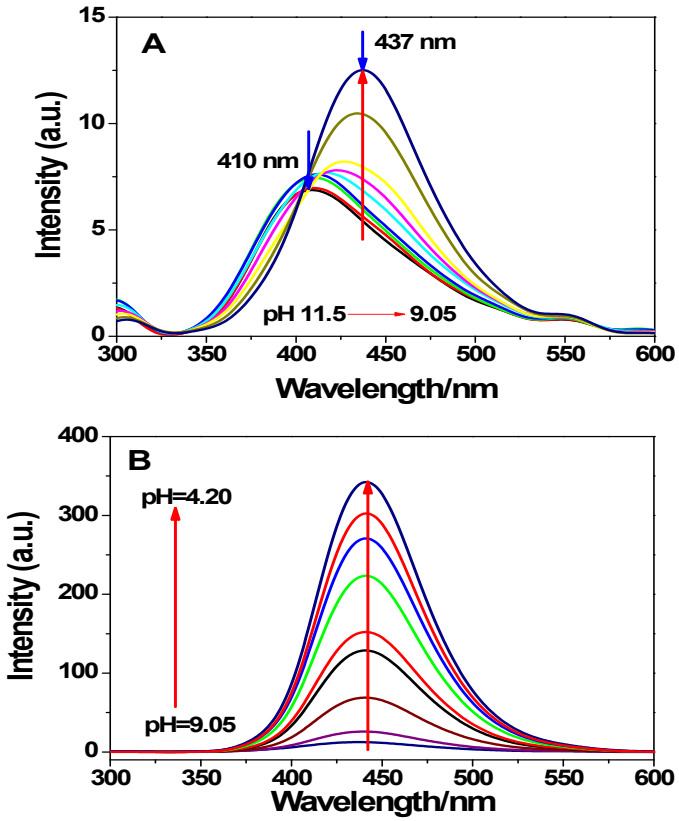

Figure S_1. Proton-dependent fluorescnece spectra of Cip at pH range from 11.5 to 9.05 (A) and from 9.05 to 4.20 (B) in aqueous solution.

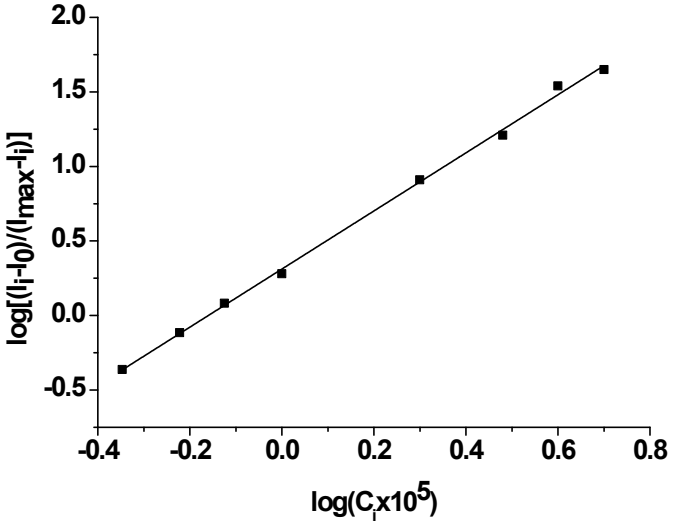

Figure S_2. The line is obtained by fitting the spots of $\log(I_i–I_0)/(I_{max}–I_i)$ versus $\log C_i$. [Cip] = 7.5 μg/mL.

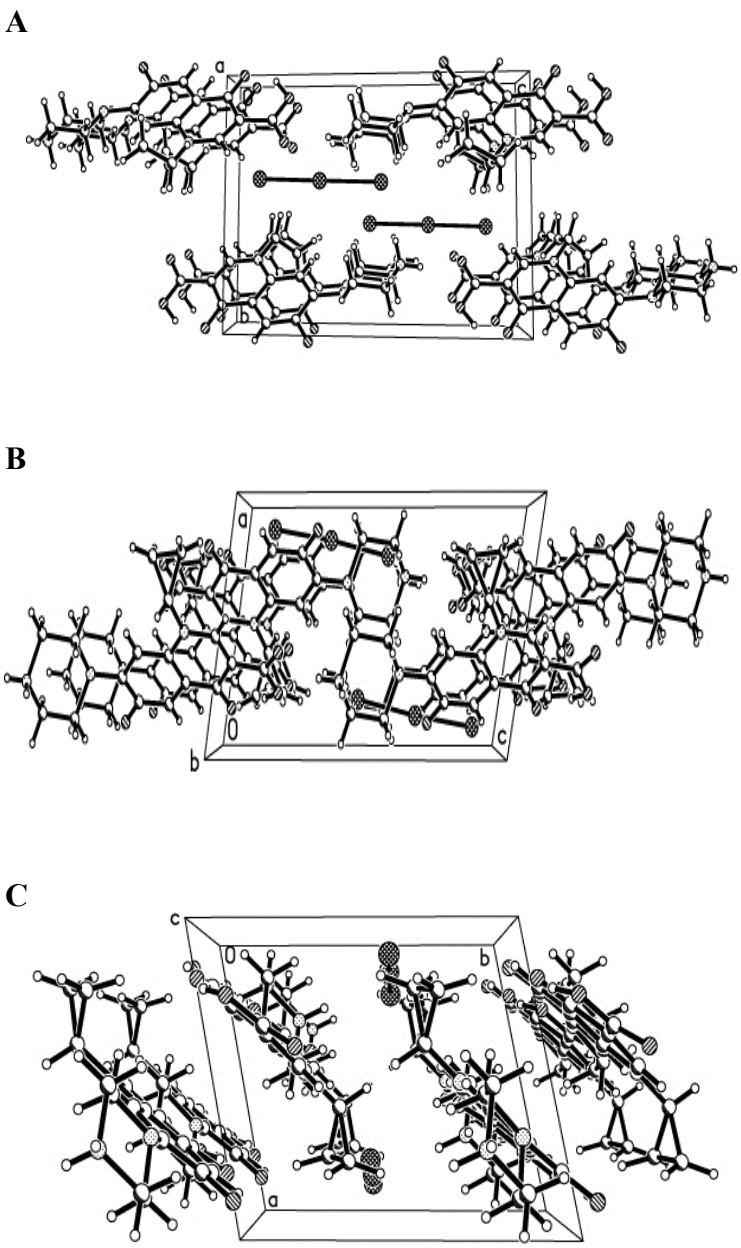

Figure S_3. The packing diagram along *a* (A), *b* (B) and *c* (C) axes in crystal constructed by Cip and iodine molecule.

Table S_1. Crystal data and structure refinement

	Crystal
Formula	C17 H19 F N3 O3 I3
Formula weight	713.05
Crystal system	Triclinic
Space group	P-1
a [Å]	8.1001(7)
b [Å]	9.6437(8)
c [Å]	13.9228(12)
α [°]	87.481(1)
β [°]	77.694(2)
γ [°]	77.279(1)
V [Å^3]	1036.50(15)
Dc Mgm^{-3}	2.285
F [000]	668
μ mm^{-1}	4.555
Crystal size mm	0.18 × 0.18 × 0.22
Reflns collected	5717
Independent refln	3996
R_{int}	0.023
GoF (F^2)	1.056
Final R_1 [I>2σ(I)]	2436
Final wR_2	0.1159

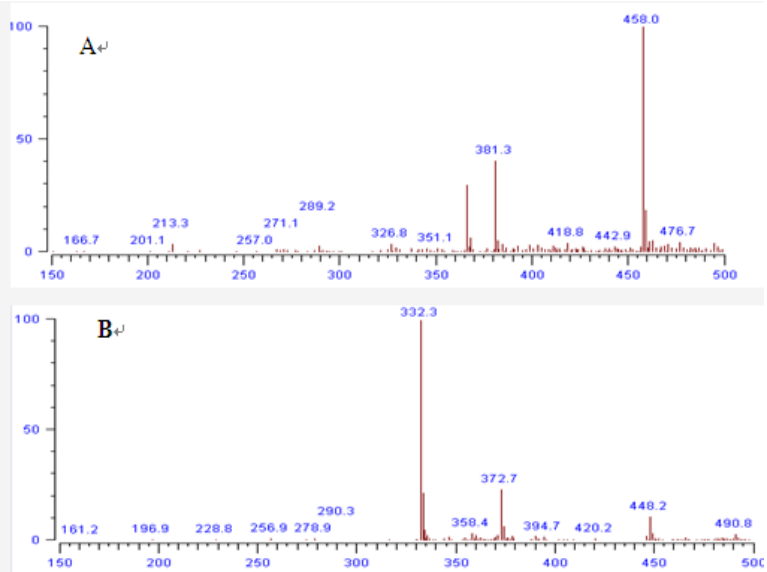

Figure S_4. ESI-MS spectra of mixture of Cip·HCl and iodine (Cip+I_2) in negative- (A) and positive-ion modes (B). Concentration: 100 μg/mL each. Full scan: 150~500 amu.

Table S_2. Analytical results for the determination of Cip in real samples

Manufacturers	Certified (mg/grain)	Determined (mg/grain, mean±sd, n=3)
Yangtze River	250	249 ± 12
Zhejiang Jolly	250	243 ± 27
Shandong Taiyi	250	249 ± 2
Hangzhou Tiancheng	250	262 ± 25
Jingxin	250	247 ± 18