

Electronic Supplementary Information (ESI†)

An antimalarial drug, Tafenoquine, as a fluorescent receptor for ratiometric detection of hypochlorite

Avijit Kumar Das,^a Naoto Hayashi,^a Yasuhiro Shiraishi,^{a,b,*} and Takayuki Hirai^a

^a *Research Center for Solar Energy Chemistry, and Division of Chemical Engineering, Graduate School of Engineering Science, Osaka University, Toyonaka 560-8531, Japan*

^b *PRESTO, JST, Saitama 332-0012, Japan*

shiraish@cheng.es.osaka-u.ac.jp

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Table S1. Calculated excitation energy (E), wavelength (λ), and oscillator strength (f) for low-lying singlet state (S_n) of **TQ**.

	Main orbital transition (CIC ^[a])	E (eV) [λ (nm)]	f
$S_0 \rightarrow S_1$	HOMO \rightarrow LUMO (0.65609)	3.2504 eV [381.45 nm]	0.1279
$S_0 \rightarrow S_2$	HOMO \rightarrow LUMO+1 (0.70067)	3.2837 eV [377.57 nm]	0.0047
$S_0 \rightarrow S_3$	HOMO-2 \rightarrow LUMO (0.25471) HOMO \rightarrow LUMO+2 (0.5941) HOMO \rightarrow LUMO+3 (0.26032)	3.9471 eV [314.11 nm]	0.0387
$S_0 \rightarrow S_4$	HOMO-2 \rightarrow LUMO (0.23814) HOMO \rightarrow LUMO+2 (-0.35569) HOMO \rightarrow LUMO+3 (0.5541)	4.0808 eV [303.82 nm]	0.0164
$S_0 \rightarrow S_5$	HOMO-1 \rightarrow LUMO (0.70656)	4.3939 eV [282.18 nm]	0.0005
$S_0 \rightarrow S_6$	HOMO \rightarrow LUMO+4 (0.67749) HOMO \rightarrow LUMO+7 (-0.13443)	4.5361 eV [273.33 nm]	0.0033

[a] CI expansion coefficients for the main transitions.

Table S2. Calculated excitation energy (E), wavelength (λ), and oscillator strength (f) for low-lying singlet state (S_n) of **TQA**.

	Main orbital transition (CIC ^[a])	E (eV) [λ (nm)]	f
$S_0 \rightarrow S_1$	HOMO-1 \rightarrow LUMO (0.12712) HOMO \rightarrow LUMO (0.68395)	3.2077 eV [386.52 nm]	0.0395
$S_0 \rightarrow S_2$	HOMO-1 \rightarrow LUMO (-0.12354) HOMO-1 \rightarrow LUMO+1 (-0.15968) HOMO \rightarrow LUMO+1 (0.67142)	3.7963 eV [326.59 nm]	0.0018
$S_0 \rightarrow S_3$	HOMO-1 \rightarrow LUMO (0.62457) HOMO \rightarrow LUMO+1 (0.14013)	3.8474 eV [322.25 nm]	0.1162
$S_0 \rightarrow S_4$	HOMO-1 \rightarrow LUMO+1 (0.68184) HOMO \rightarrow LUMO+1 (0.15955)	4.159 eV [298.11 nm]	0.0013
$S_0 \rightarrow S_5$	HOMO-2 \rightarrow LUMO (0.28411) HOMO-1 \rightarrow LUMO (-0.11473) HOMO \rightarrow LUMO+2 (0.44011) HOMO \rightarrow LUMO+3 (-0.4347)	4.2916 eV [288.9 nm]	0.0637

[a] CI expansion coefficients for the main transitions.

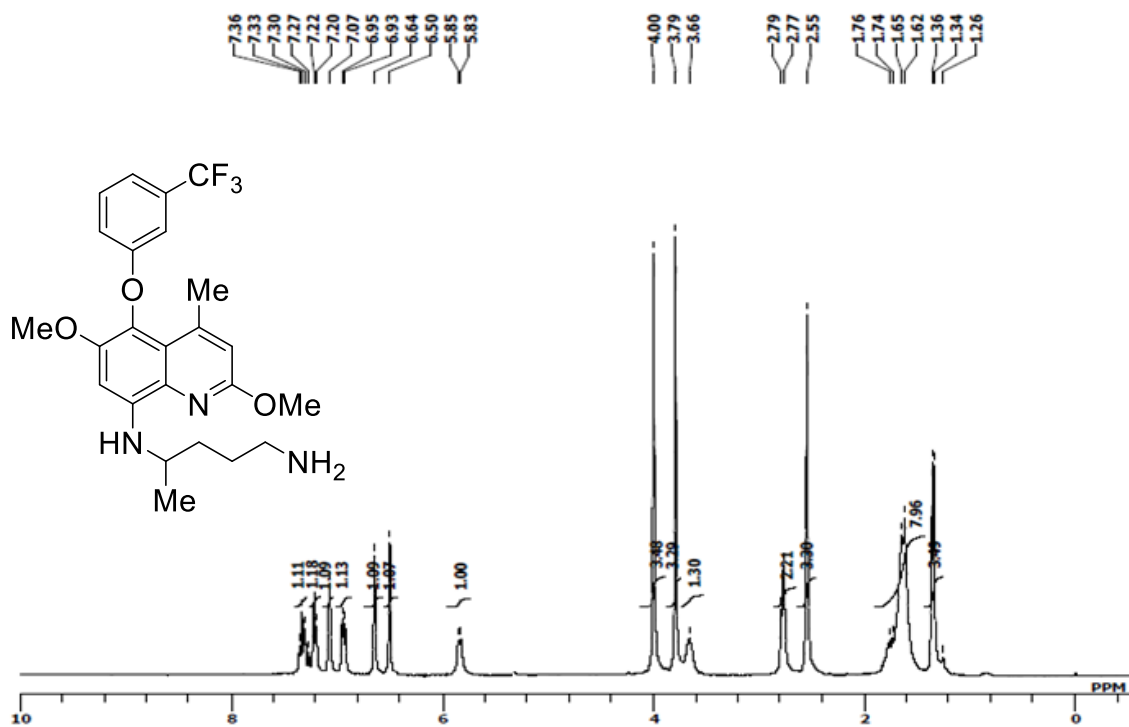


Fig. S1 ¹H NMR spectra of TQ

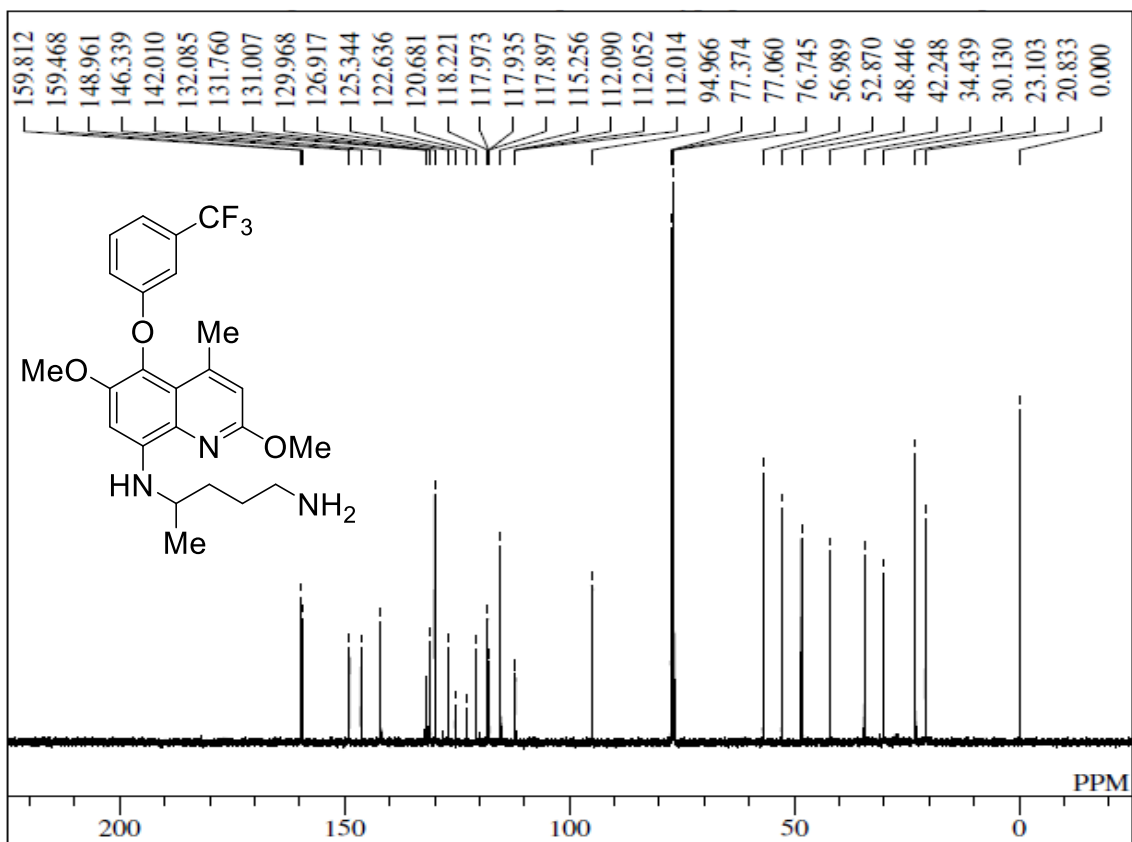


Fig. S2 ¹³C NMR spectra of TQ

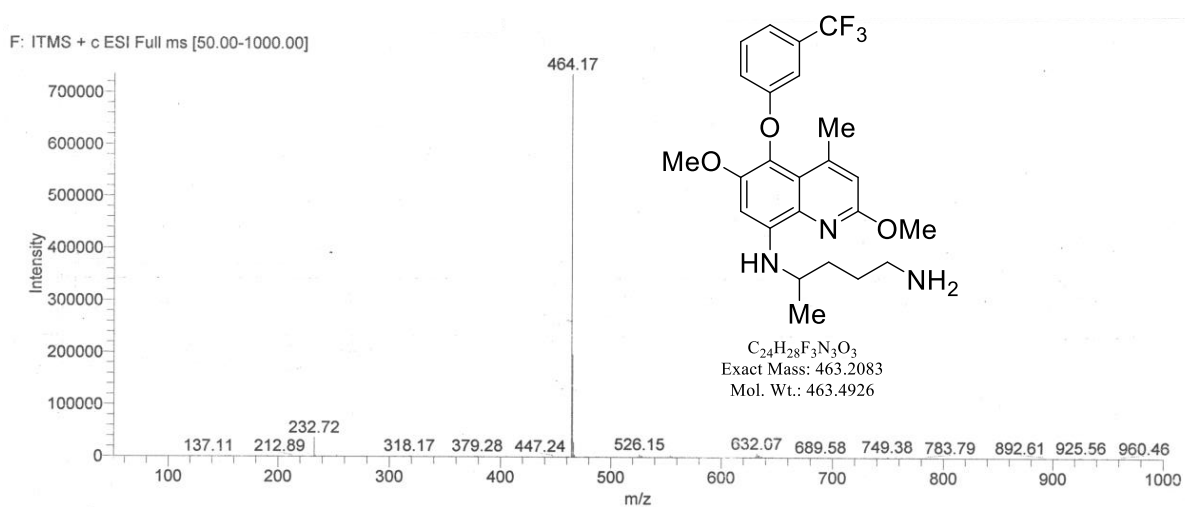


Fig. S3 ESI-MS chart of TQ

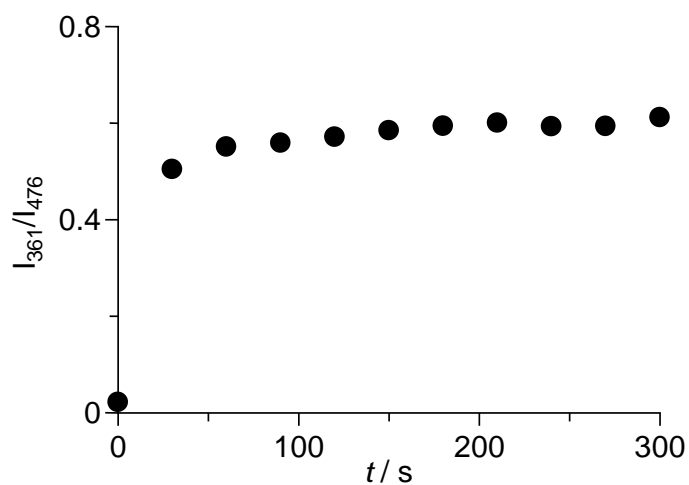


Fig. S4 Time-dependent change in the ratio of fluorescence intensity (I_{361}/I_{476}) of TQ after addition of OCl^- to a buffered water/MeCN (3/7 v/v) mixture (HEPES, 0.1 M, pH 7.4) at 25 °C, where I_{361} is the intensity at $\lambda_{\text{em}} = 361$ nm and I_{476} is the intensity at $\lambda_{\text{em}} = 476$ nm, respectively.

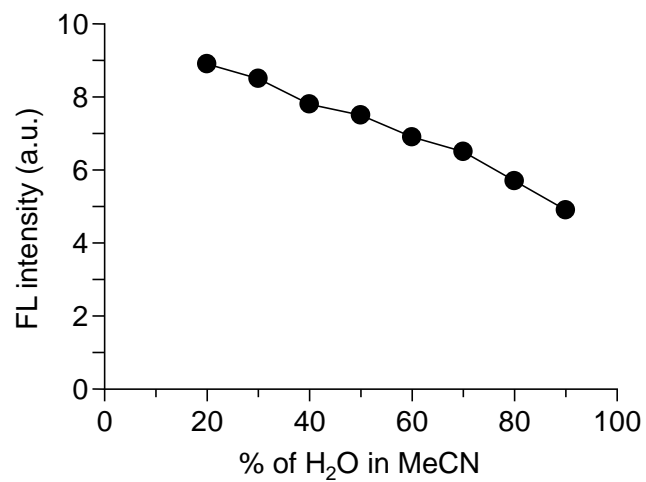


Fig. S5 Effect of water content in solution on the fluorescence intensity of **TQ** with 100 equiv of OCI^- at 361 nm.

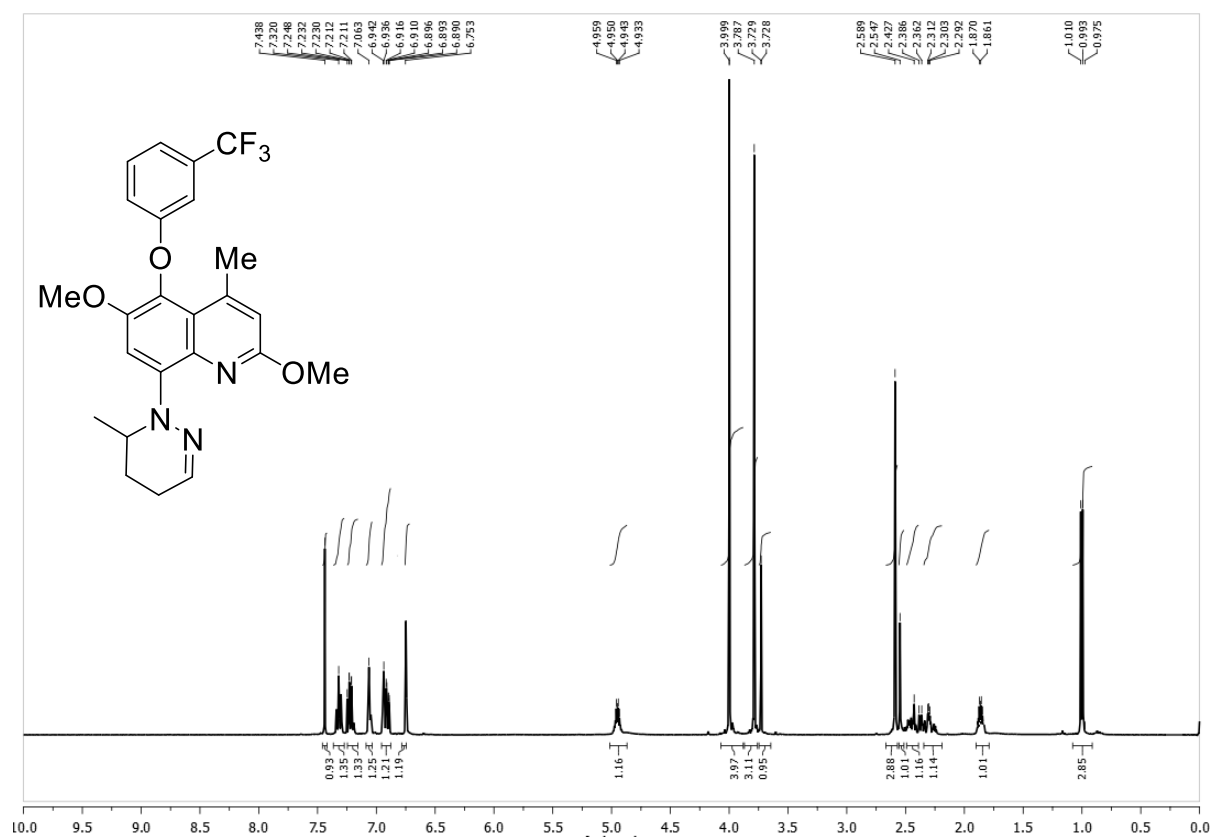


Fig. S6 ^1H NMR spectra of **TQA**

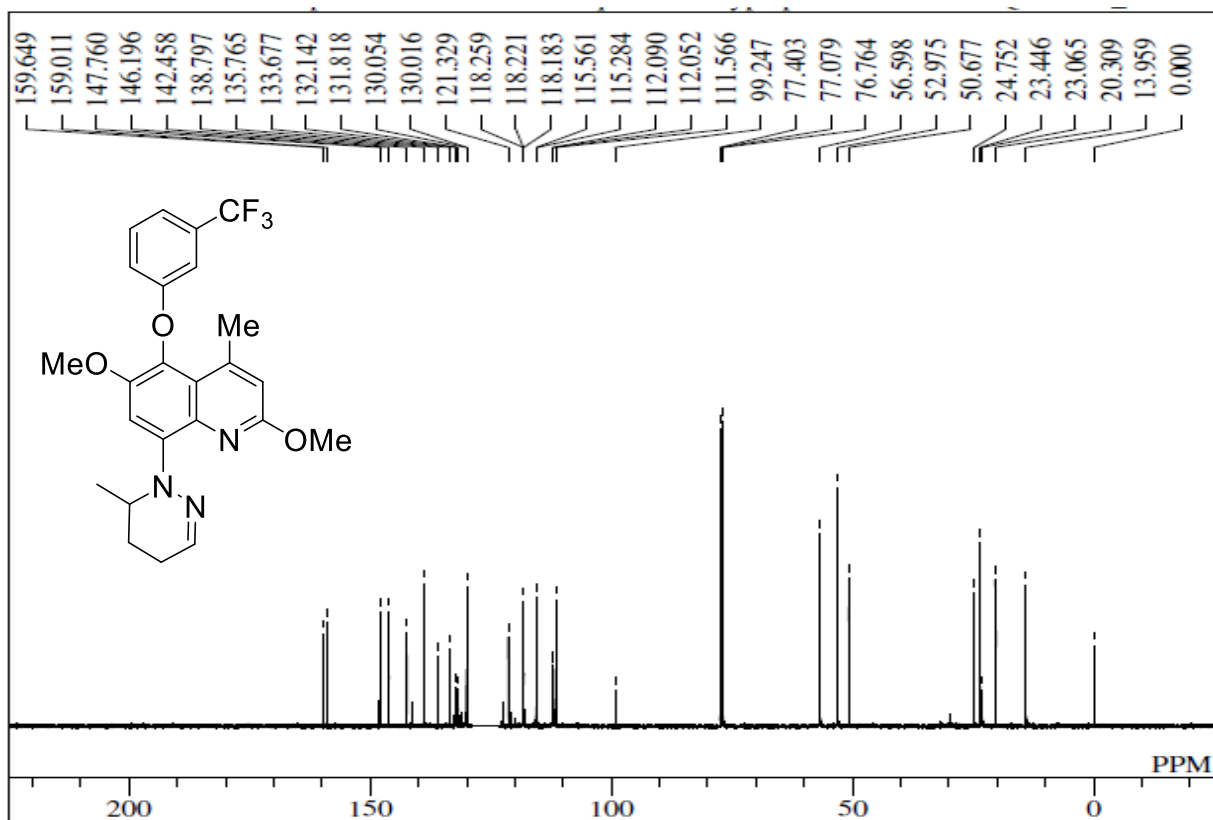


Fig. S7 ¹³C NMR spectra of TQA

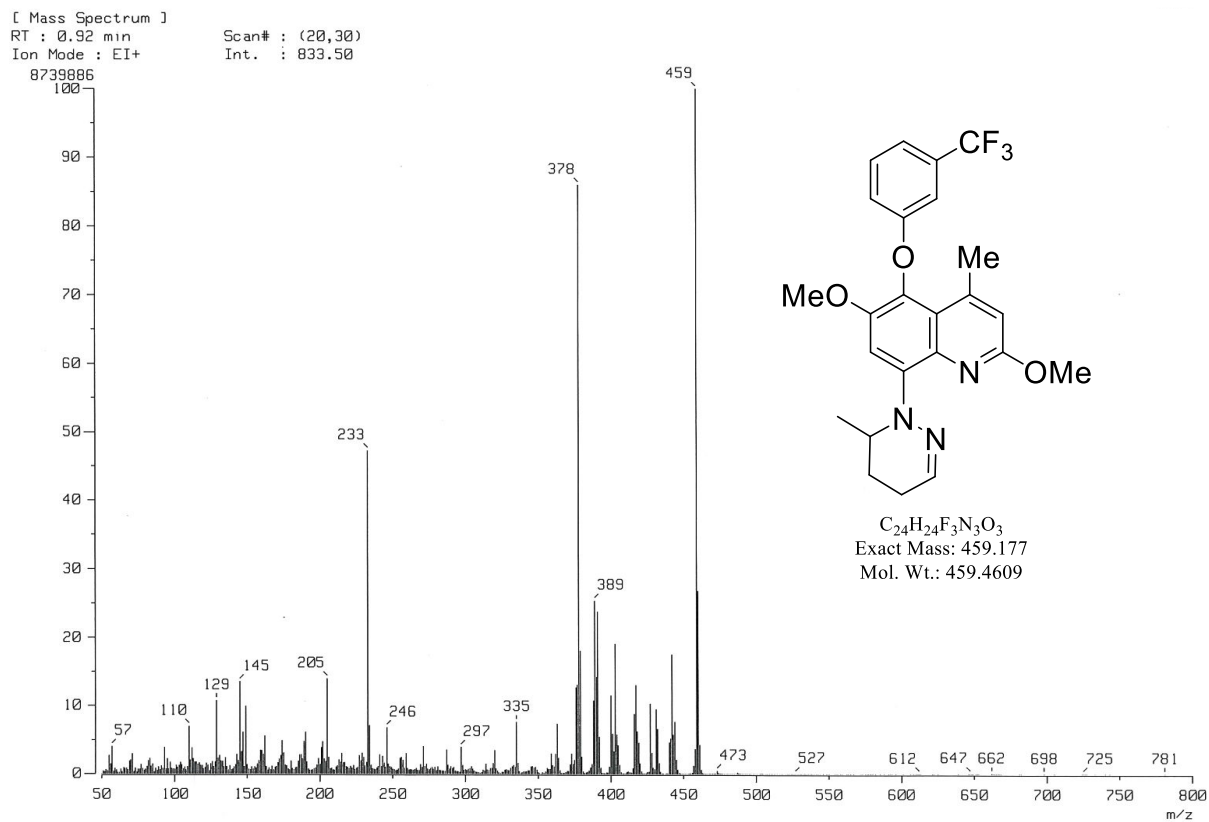


Fig. S8 EI-MS chart of TQA

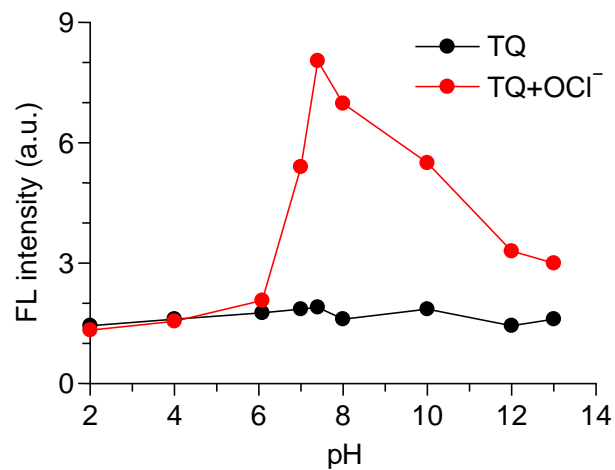


Fig. S9 Fluorescence intensity of **TQ** (20 μM) at 361 nm under different pH conditions (red) with and (black) without OCl⁻ (2 mM).

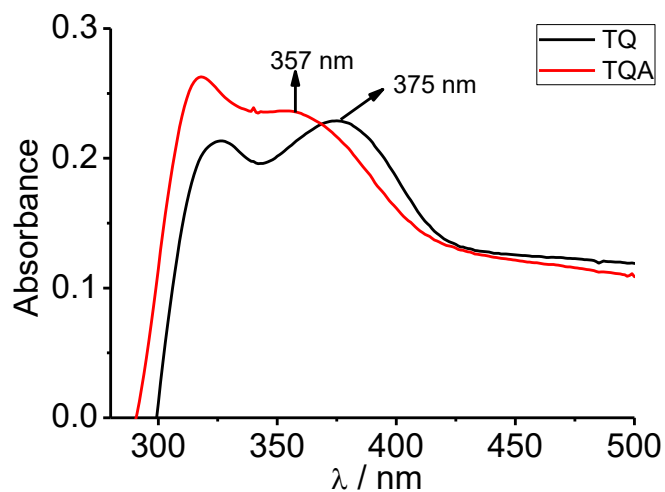
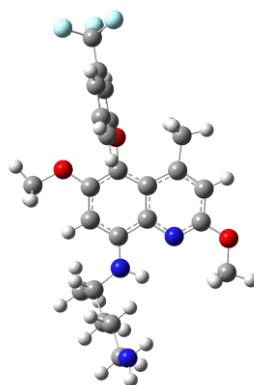
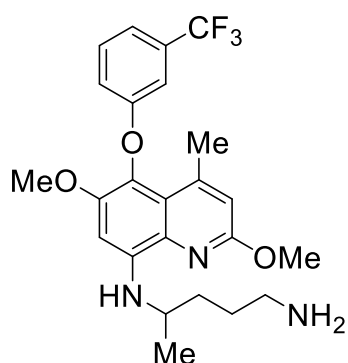


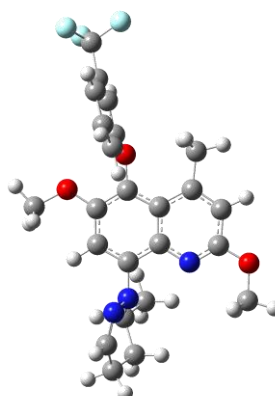
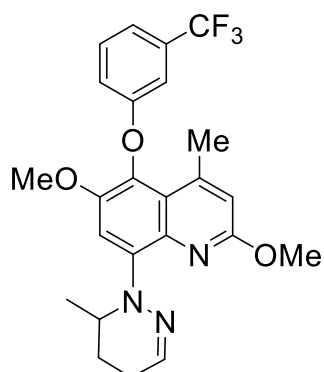
Fig. S10 UV-vis spectra of **TQ** and **TQA** (20 μM) in a buffered water/MeCN (3/7 v/v) mixture (HEPES 0.1 M, pH 7.4) at 25 °C.

Cartesian Coordinates (in Å^o) of TQ
(DFT/B3LYP/6-31+G, PCM: water)



C	-0.11522	-1.16043	-1.08311	F	-7.37193	0.535166	1.255029
C	1.272883	-1.39498	-1.03072	F	-7.31674	-1.59012	0.5674
C	2.157034	-0.34313	-0.76691	H	1.655798	-2.39133	-1.19808
C	1.620175	0.979845	-0.56272	H	0.452574	4.598648	-0.02743
C	0.208542	1.22245	-0.61193	H	4.036154	0.358566	-0.52408
C	-0.64472	0.110113	-0.8619	H	3.708585	-2.57218	-0.51123
N	2.54053	1.977823	-0.32446	H	6.230748	-2.52834	-0.58997
C	2.104625	3.206075	-0.13983	H	6.17559	-0.76761	-0.61747
C	0.733307	3.559615	-0.17926	H	4.980296	-0.79675	1.625574
C	-0.22668	2.592889	-0.41239	H	5.060324	-2.55976	1.633816
O	-2.04554	0.282064	-1.00521	H	7.546393	-2.47928	1.63815
N	3.51853	-0.49712	-0.68525	H	7.506273	-0.71314	1.531716
C	4.267643	-1.73295	-0.95544	H	7.769891	-1.69657	3.870911
C	5.641351	-1.6623	-0.2571	H	6.379806	-0.76263	3.768415
C	5.575436	-1.65506	1.280446	H	-4.58168	0.268784	-1.28361
C	6.966395	-1.59319	1.927208	H	-5.53455	-1.08829	2.727737
N	6.869881	-1.5817	3.402167	H	-3.10173	-1.1896	3.243549
C	-2.91475	-0.11774	0.021339	H	-1.42203	-0.56844	1.52156
C	-4.27738	-0.05073	-0.291	H	-1.74262	4.108048	-0.32797
C	-5.21058	-0.40173	0.691276	H	-2.14925	2.752756	-1.40362
C	-4.80108	-0.81624	1.971491	H	-2.26382	2.553258	0.339493
C	-3.43424	-0.87241	2.257474	H	4.919	4.861474	0.350825
C	-2.48244	-0.52288	1.288554	H	4.625276	3.197279	0.964611
C	-1.67548	3.023539	-0.45568	H	4.757955	3.48521	-0.79546
O	2.996718	4.234092	0.103637	H	-1.48782	-4.11924	-1.68444
C	4.42939	3.907812	0.15748	H	0.082377	-3.63251	-2.38973
O	-1.04032	-2.16288	-1.35771	H	-0.06966	-3.89151	-0.61606
C	-0.5782	-3.5423	-1.52086	H	4.899064	-2.95408	-2.65432
C	4.42274	-1.98316	-2.47119	H	3.450592	-1.97809	-2.97642
C	-6.66674	-0.34404	0.398071	H	5.045406	-1.20067	-2.92254
F	-6.97249	0.069672	-0.90317				

Cartesian Coordinates (in Å°) of TQA
(DFT/B3LYP/6-31+G, PCM: water)



C	0.067493	-1.38024	-0.50439	C	-6.48167	-0.07116	-0.18872
C	1.417475	-1.69865	-0.26337	F	-6.56678	-0.32712	-1.56591
C	2.353487	-0.69793	-0.04445	F	-7.03099	1.229052	-0.02461
C	1.958235	0.671595	-0.04926	F	-7.4086	-0.92898	0.427049
C	0.579059	1.017121	-0.30092	H	1.752869	-2.73025	-0.25706
C	-0.33938	-0.04618	-0.51487	H	1.030635	4.410696	-0.07281
N	2.91695	1.631699	0.201359	H	-4.13555	0.233622	-1.54527
C	2.555986	2.894387	0.188554	H	-5.78096	-0.63168	2.377136
C	1.235116	3.343279	-0.07133	H	-3.47135	-0.73426	3.294496
C	0.232255	2.427865	-0.31434	H	-1.51082	-0.35619	1.821344
O	-1.68098	0.228385	-0.85209	H	4.416936	-2.34162	-1.32981
C	-2.72239	-0.04261	0.052481	H	6.772816	-1.49555	-1.2544
C	-4.00955	0.023624	-0.48647	H	6.294166	-0.28642	-0.05358
C	-5.10486	-0.19465	0.358877	H	7.143186	-2.0956	1.303325
C	-4.92629	-0.4656	1.726191	H	6.443837	-3.33349	0.273857
C	-3.62597	-0.52307	2.238686	H	5.107358	-2.91499	2.533427
C	-2.51604	-0.30999	1.409799	H	4.623759	0.698128	-1.76355
N	3.721329	-1.05249	0.193512	H	5.120531	-0.5679	-2.91515
C	4.633804	-1.3195	-0.95835	H	3.410311	-0.36524	-2.50465
C	6.079795	-1.2955	-0.42845	H	-1.14439	4.047152	-0.58635
C	6.259027	-2.33245	0.694219	H	-1.54684	2.607062	-1.54646
C	5.044825	-2.37812	1.587916	H	-1.87341	2.628352	0.181199
N	3.90432	-1.78958	1.365681	H	5.409795	4.395903	0.89
C	4.427357	-0.32343	-2.10178	H	4.912428	2.810053	1.582262
C	-1.16024	2.953232	-0.58387	H	5.285956	2.938211	-0.1579
O	3.49047	3.880663	0.439728	H	-1.52907	-4.26393	-0.8323
C	4.876608	3.463626	0.707716	H	0.159305	-4.03925	-1.38181
O	-0.91755	-2.32487	-0.75959	H	-0.23471	-3.97673	0.37228
C	-0.58967	-3.7479	-0.63808				