

Spectral data for dye I (2-((E)-2-((E)-2-Chloro-3-(2-((E)-1-(5-ethoxy-5-oxopentyl)-3,3-dimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1-(5-ethoxy-5-oxopentyl)-3,3-dimethyl-3H-indol-1-ium iodide)

- **Absorption spectrum:** $\lambda_{\max} = 780 \text{ nm}$; $\epsilon = 2.4 \times 10^5 \text{ L/mol cm}$.
- **^1H NMR** (400 MHz, CD_3OD , δ , ppm, J/Hz): 1.21 (t, 6H, $^3J_{\text{HH}} = 7.12$, 2 OCH_2CH_3), 1.74 (s, 12H, $2\text{C}(\text{CH}_3)_2$), 1.75 - 1.81 (m, 4H, 2CH_2), 1.83 - 1.91 (m, 4H, 2CH_2), 1.95 - 1.99 (m, 2H, CH_2), 2.43 (t, 4H, $^3J_{\text{HH}} = 7.00$, $2\text{CH}_2\text{COOEt}$), 2.76 (t, 4H, $^3J_{\text{HH}} = 6.11$, 2CH_2), 4.10 (q, 4H, $^3J_{\text{HH}} = 7.13$, OCH_2CH_3), 4.22 (t, 4H, $^3J_{\text{HH}} = 7.21$, CH_2N^+), 6.32 (d, 2H, $^3J_{\text{HH}} = 14.18$, =CH), 7.27 - 7.33 (m, 2H, Ar), 7.33 - 7.38 (m, 2H, Ar), 7.40 - 7.47 (m, 2H, Ar), 7.54 (d, 2H, $^3J_{\text{HH}} = 7.46$, Ar), 8.45 (d, 2H, $^3J_{\text{HH}} = 14.18$, =CH).
- **^{13}C NMR** (100 MHz, CD_3OD , δ , ppm, J/Hz): 14.11 (s, $2\text{COOCH}_2\text{CH}_3$), 20.57 (s, CH_2), 22.16 (s, 2CH_2), 26.64 (s, 4CH_2), 28.05 (s, $2\text{C}(\text{CH}_3)_2$), 33.47 (s, 2CH_2), 44.65 (s, $2\text{C}(\text{CH}_3)_2$), 49.23 (s, $2\text{CH}_2\text{N}^+$), 60.35 (s, $2\text{COOCH}_2\text{CH}_3$), 93.32 (s, 2CH), 101.30 (s, Ar), 110.85 (s, $\text{C}=\text{C}(\text{Cl})-\text{C}$), 116.55 (s, Ar), 122.16 (s, Ar), 125.25 (s, Ar), 127.46 (s, 2CH), 128.74 (s, Ar), 140.87 (s, Ar), 142.01 (s, Ar), 144.27 (s, Ar), 150.44 (s, CCl), 172.96 (s, $2\text{COOCH}_2\text{CH}_3$), 176.57 (s, $2\text{C}=\text{N}$). IR, ν/cm^{-1} : 714.01 (C-Cl), 1368.25 (N sec.), 1550.01 - 1512.40 (Ar), 1728.87 (C=O).
- **HRMS-ESI:** found m/z: 711.3929, $[\text{M}^+]$ $\text{C}_{44}\text{H}_{56}\text{ClN}_2\text{O}_4^+$, calculated M: 711.3923.

Table S1. Composition of natural water samples (mg/L)

Sample	Color degree	Turbidity*	pH	Hardness (dH)	MnO_4^- index**	F^-	Cl^-	NO_3^-	SO_4^{2-}	Dry residue***
Bor-8	5.8	1	7.4	3.9	2.7	0.3	32	4.8	22	340
Well-4	5.0	1	6.3	2.9	3.0	0.3	0.5	0.5	0.5	380
Spr-6	2.3	1	6.4	8.4	1.2	0.03	120	2.3	62	470

* Formazine turbidity units. ** mg oxygen/L. *** mg/L.

Table S2. Inorganic components of natural water samples according to total reflectance X-ray fluorescence (TXRF)* (mg/L)

Sample	Mg	K	Ca	Ti	Mn	Fe	Ni	Cu	Zn	Br	Sr
Bor-8	10	1.7	36	0	0.011	0.022	0	0	0.026	0.0096	0.11
Well-4	0	0.8	29	0	0	0.012	0.004	0.014	0.14	0.049	0.08
Spr-6	9.9	1.2	63	0	0	0.011	0	0	0.021	0.036	0.11

* TXRF spectra of samples were measured on Picofox S2 spectrometer (Bruker Nano GmbH, Germany). A 5 μL aliquot of the water sample was pipetted on a quartz reflector and dried. Mo K-L3 line was used for excitation of X-ray fluorescence, the spectrum acquisition time was 250 s. The concentrations were calculated by internal calibration. The reflectors were treated with 10% nitric acid, water and acetone before use.

*Carbonate buffer (pH 5.6); Glyc: glycinate buffer; NIR: near-IR images. Concentrations: NaOCl 2.5×10^{-4} M, Dye 0.01 g/L.

Time	Images of the reaction mixture at various pH values												
1 min	HCl	Acetate					Phosphate		Glyc	Borate			
pH	2.1	3.6	4.8	5.6	5.6*	6.1	7.4	8.4	9.4	10.8	11.5	12.5	
Dye													
Dye + NaOCl													
2 min													
3 min													
5 min													
7 min													
10 min													
13 min													
16 min													
35 min													
NIR 1 min													
NIR 3 min													
NIR 12 min													
NIR 20 min													

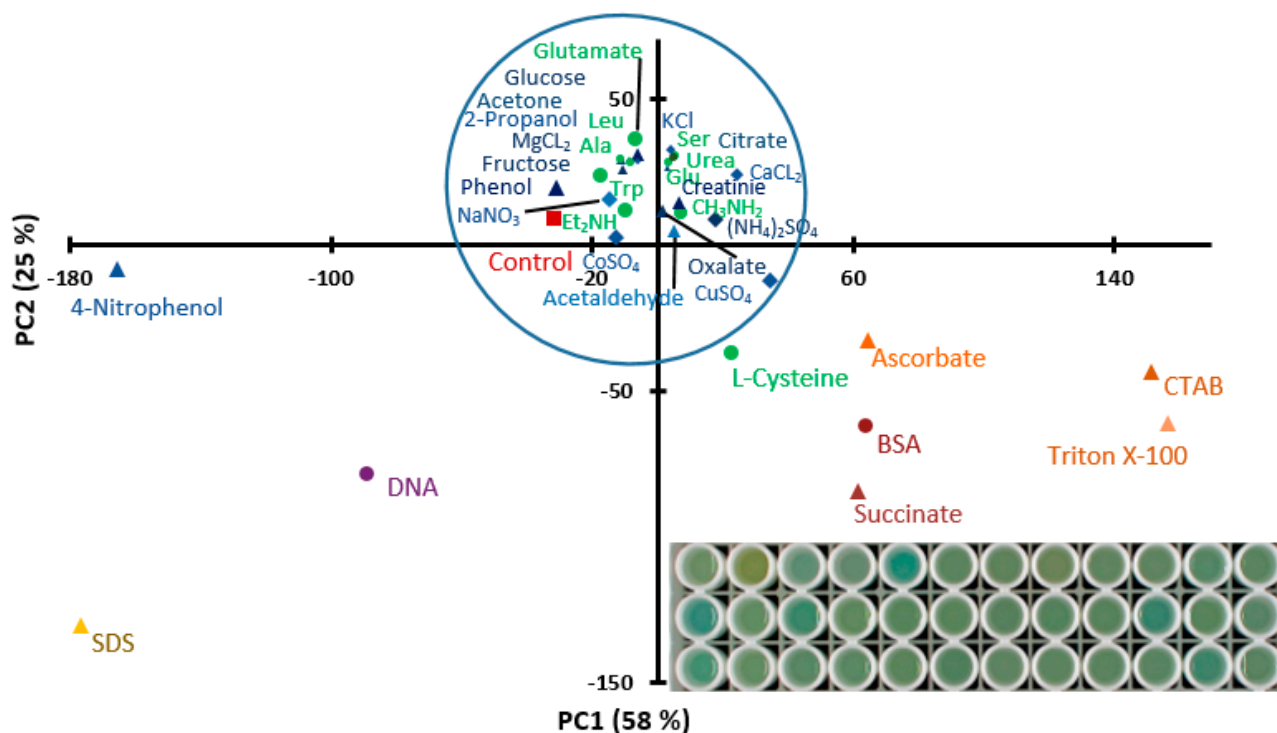


Figure S1. Principal component analysis (PCA) score plot constructed using the images of mixtures of dye I with model analytes (shown in the plot) **without NaOCl**. The signal was observed during 30 min in acetate buffer solution (pH 5.6). **Inset:** image of the plate at 8 min after mixing the reactants. Model compounds: 1st row: control, 4-nitrophenol, Triton X-100, CTAB, SDS, fructose, glucose, phenol, isopropanol, acetone, acetaldehyde, control; 2nd row: succinate, oxalate, ascorbate, citrate, serine, glutamate, leucine, glutamine, alanine, cysteine, tryptophan, BSA; 3rd row: DNA, diethylamine, methylamine, creatinine, urea, CaCl_2 , NaNO_3 , KCl , MgCl_2 , $(\text{NH}_4)_2\text{SO}_4$, CuSO_4 , CoSO_4 . Concentrations of organic analytes in the well were 0.5 mM, inorganic compounds 1 mM, Cu and Co 0.1 mM, BSA 0.3 g/L, DNA 0.025 g/L.

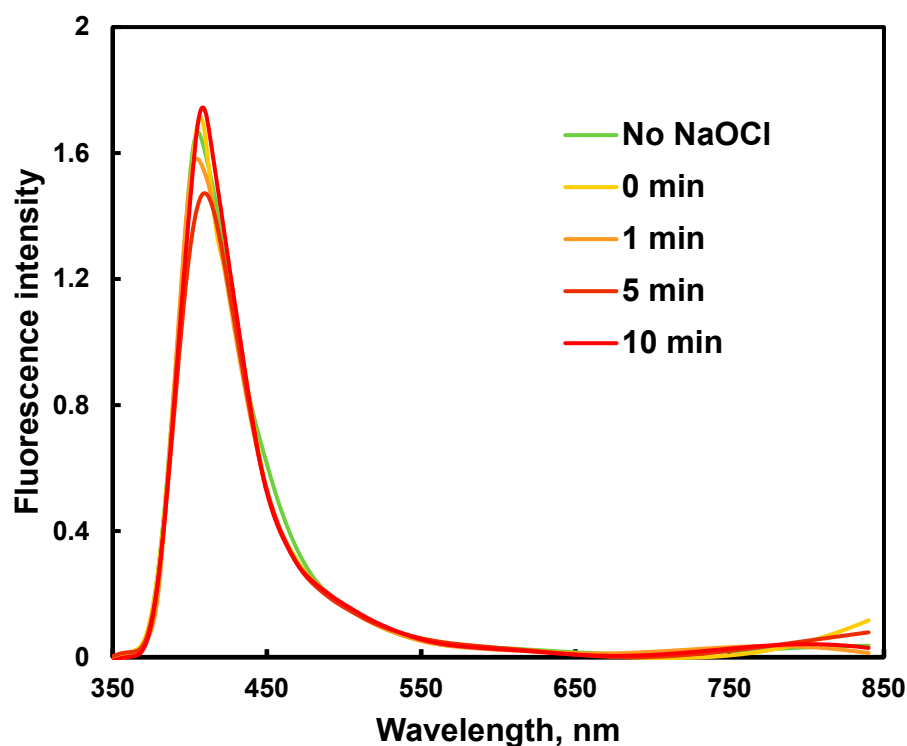




























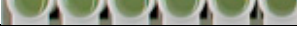
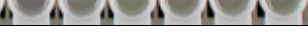


Figure S2. Fluorescence spectra of dye I (no NaOCl) and its reaction products with NaOCl at various reaction times. Excitation at 300 nm.

Table S4. Images of the wells for selected reaction times. Each concentration was run in 6 replicate runs (6 wells of the plate in a row). The concentrations refer to the reaction mixture in the well.

a – varying concentration of tryptophan and urea (separately):

Time, min / concentration, M		Tryptophan	Urea
1	0		
	$5 \cdot 10^{-7}$		
	$5 \cdot 10^{-6}$		
	$5 \cdot 10^{-5}$		
	$5 \cdot 10^{-4}$		
2	0		
	$5 \cdot 10^{-7}$		
	$5 \cdot 10^{-6}$		
	$5 \cdot 10^{-5}$		
	$5 \cdot 10^{-4}$		
5	0		
	$5 \cdot 10^{-7}$		
	$5 \cdot 10^{-6}$		
	$5 \cdot 10^{-5}$		
	$5 \cdot 10^{-4}$		

b – varying concentration of tryptophan in a mixture with a constant concentration of urea ($5 \cdot 10^{-5}$ M):
















Time, min / composition of mixture		Tryptophan + urea mixture
1	0	
	$5 \cdot 10^{-7}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-6}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-5}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-4}$ M trp + $5 \cdot 10^{-5}$ M urea	
2	0	
	$5 \cdot 10^{-7}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-6}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-5}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-4}$ M trp + $5 \cdot 10^{-5}$ M urea	
5	0	
	$5 \cdot 10^{-7}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-6}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-5}$ M trp + $5 \cdot 10^{-5}$ M urea	
	$5 \cdot 10^{-4}$ M trp + $5 \cdot 10^{-5}$ M urea	

Table S5. Images of the wells with four model analytes in reaction *dye I* – *NaOCl* started different time after adding NaOCl (0, 1, and 24 h). In the left column, time after the reaction start (min) is given. All experiments were conducted in 6 replicates (6 wells in a row). The final concentrations of model analytes were: diethylamine 1 mM, DNA 0.025 g/L, proteins 0.1 g/L.










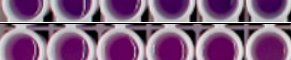









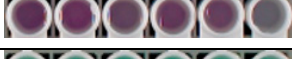










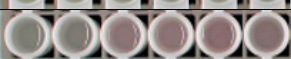










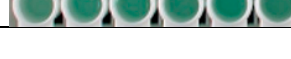



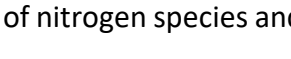
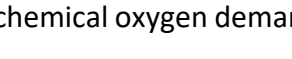
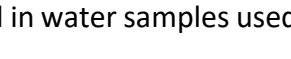
Reaction time, min / Model analyte		Time between adding NaOCl and the dye, h		
		0	1	24
1	Diethylamine			
	DNA			
	Lysozyme			
	BSA			
3	Diethylamine			
	DNA			
	Lysozyme			
	BSA			
15	Diethylamine			
	DNA			
	Lysozyme			
	BSA			
30	Diethylamine			
	DNA			
	Lysozyme			
	BSA			

Table S6. Concentration of nitrogen species and chemical oxygen demand in water samples used in this study

Sample code	Water type	Ammonia, mg/L	NO_3^- , mg/L	NO_2^- , mg/L	Total N, mg/L	MnO_4^- index, mg oxygen/L
WW-7	Sewage	4.4±0.6	0.34±0.05	0.06±0.01	40±5	10±2
WW-4	Sewage	<0.1	11±1	>1.0	30±3	28±3
WW-1	Sewage	0.79±0.16	9.2±0.9	0.094±0.016	30±3	62±4
Bor-8	Borehole	–	5.0±0.5	<0.01	21±3	2.7±0.3
Well-4	Well	0.26±0.05	<0.1	<0.01	16±2	3.0±0.4
Spr-6	Spring	0.23±0.05	<0.1	0.015±0.005	18±2	1.2±0.1