

**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:**  $\lambda_{\max} = 780 \text{ nm}$ ;  $\epsilon = 2.4 \times 10^5 \text{ L/mol cm}$ .
- **$^1\text{H NMR}$**  (400 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ , ppm, J/Hz): 1.21 (t, 6H,  $^3J_{\text{HH}} = 7.12$ , 2  $\text{OCH}_2\text{CH}_3$ ), 1.74 (s, 12H, 2C(CH<sub>3</sub>)<sub>2</sub>), 1.75 - 1.81 (m, 4H, 2CH<sub>2</sub>), 1.83 - 1.91 (m, 4H, 2CH<sub>2</sub>), 1.95 - 1.99 (m, 2H, CH<sub>2</sub>), 2.43 (t, 4H,  $^3J_{\text{HH}} = 7.00$ , 2CH<sub>2</sub>COOEt), 2.76 (t, 4H,  $^3J_{\text{HH}} = 6.11$ , 2CH<sub>2</sub>), 4.10 (q, 4H,  $^3J_{\text{HH}} = 7.13$ , OCH<sub>2</sub>CH<sub>3</sub>), 4.22 (t, 4H,  $^3J_{\text{HH}} = 7.21$ , CH<sub>2</sub>N<sup>+</sup>), 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).
- **$^{13}\text{C NMR}$**  (100 MHz,  $\text{CD}_3\text{OD}$ ,  $\delta$ , ppm, J/Hz): 14.11 (s, 2COOCH<sub>2</sub>CH<sub>3</sub>), 20.57 (s, CH<sub>2</sub>), 22.16 (s, 2CH<sub>2</sub>), 26.64 (s, 4CH<sub>2</sub>), 28.05 (s, 2C(CH<sub>3</sub>)<sub>2</sub>), 33.47 (s, 2CH<sub>2</sub>), 44.65 (s, 2C(CH<sub>3</sub>)<sub>2</sub>), 49.23 (s, 2CH<sub>2</sub>N<sup>+</sup>), 60.35 (s, 2COOCH<sub>2</sub>CH<sub>3</sub>), 93.32 (s, 2CH), 101.30 (s, Ar), 110.85 (s, C=C(Cl)-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, 2COOCH<sub>2</sub>CH<sub>3</sub>), 176.57 (s, 2C=N). IR,  $\nu/\text{cm}^{-1}$ : 714.01 (C-Cl), 1368,25 (N sec.), 1550.01 - 1512.40 (Ar), 1728.87 (C=O).
- **HRMS-ESI:** found  $m/z$ : 711.3929,  $[\text{M}^+]$  C<sub>44</sub>H<sub>56</sub>ClN<sub>2</sub>O<sub>4</sub><sup>+</sup>, calculated M: 711.3923.

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

Sample	Color degree	Turbidity*	pH	Hardness (dH)	MnO <sub>4</sub> <sup>-</sup> index**	F <sup>-</sup>	Cl <sup>-</sup>	NO <sub>3</sub> <sup>-</sup>	SO <sub>4</sub> <sup>2-</sup>	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)

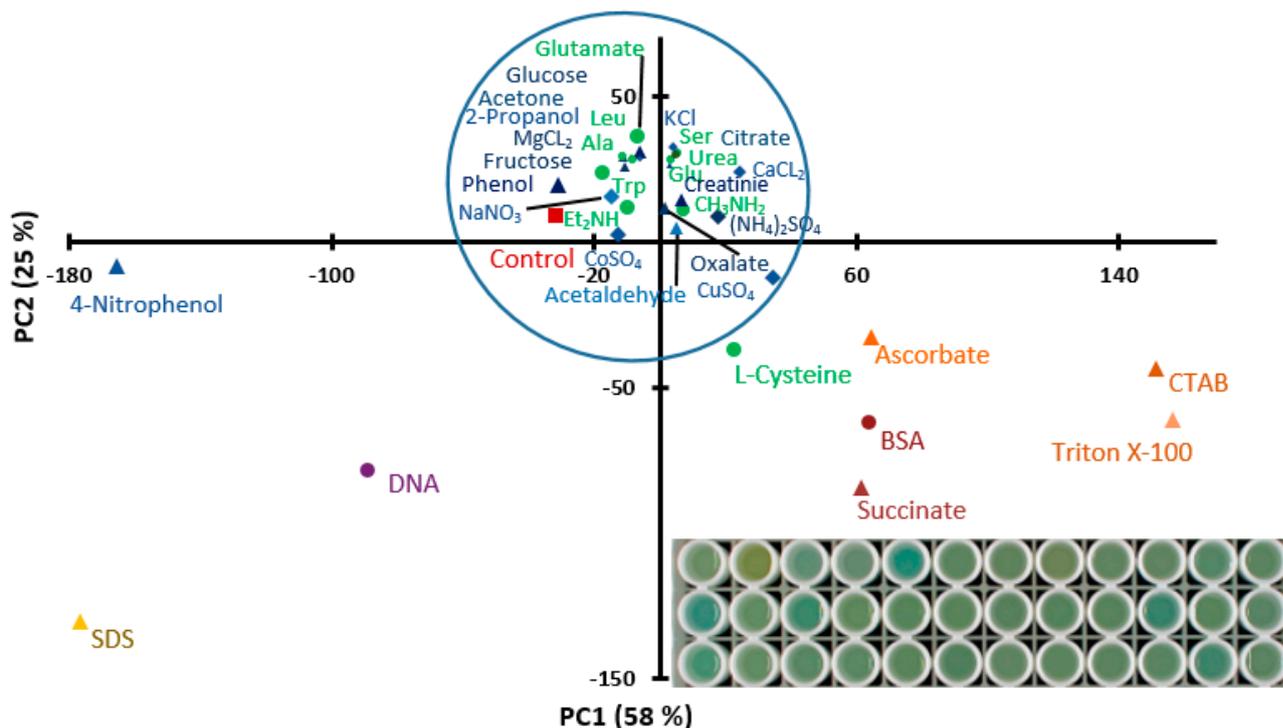
Sample	Mg	K	Ca	Ti	Mn	Fe	Ni	Cu	Zn	Br	Sr
Bor-8	10	1.7	36	0	0.011	0.022	0	0	0.026	0.0096	0.11
Well-4	0	0.8	29	0	0	0.012	0.004	0.014	0.14	0.049	0.08
Spr-6	9.9	1.2	63	0	0	0.011	0	0	0.021	0.036	0.11

\* TXRF spectra of samples were measured on Picofox S2 spectrometer (Bruker Nano GmbH, Germany). A 5  $\mu\text{L}$  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.

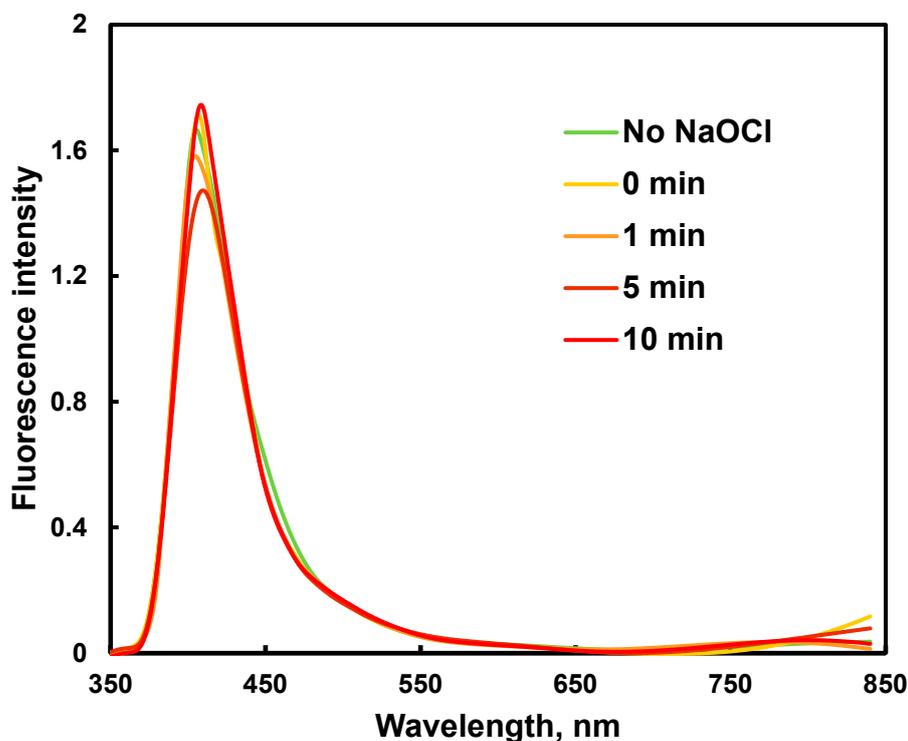
**Table S3.** Effect of pH on the color of the reaction system *dye I* – *NaOCl*.

\*Carbonate buffer (pH 5.6); Glyc: glycinate buffer; NIR: near-IR images. Concentrations: NaOCl  $2.5 \times 10^{-4}$  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
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: 1<sup>st</sup> row: control, 4-nitrophenol, Triton X-100, CTAB, SDS, fructose, glucose, phenol, isopropanol, acetone, acetaldehyde, control; 2<sup>nd</sup> row: succinate, oxalate, ascorbate, citrate, serine, glutamate, leucine, glutamine, alanine, cysteine, tryptophan, BSA; 3<sup>rd</sup> row: DNA, diethylamine, methylamine, creatinine, urea, CaCl<sub>2</sub>, NaNO<sub>3</sub>, KCl, MgCl<sub>2</sub>, (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, CuSO<sub>4</sub>, CoSO<sub>4</sub>. 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