Multiple Molecular Logic Functions and Molecular Calculation Facilitated by Surfactant with its Versatility

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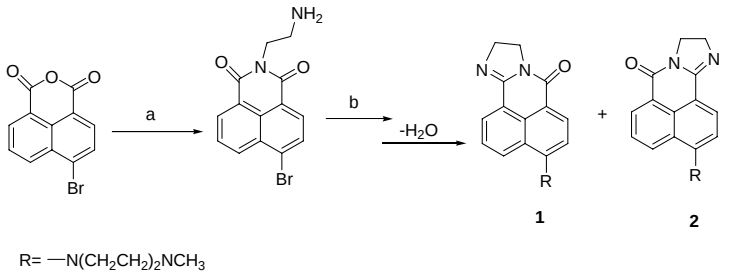
Supporting Information

Materials. All the solvents and reagents were of analytic grade and used as received. Water used was twice distilled. The pH values were adjusted with NaOH and HCl aqueous solution. The pH was determined with a pH meter (Shanghai Rex Instrument Factory, China; model PHS-3C), which was standardized with Aldrich buffers. Absorption measurements were performed with a Varian Cary500 spectrophotometer (1 cm quartz cell) and fluorescent spectra were recorded on a Varian Cary Eclipse fluorescence spectrophotometer (1 cm quartz cell). Mass spectra (MS) were recorded on an MA1212 instrument using standard conditions (ESI, 70 eV). All the experiments were performed at 25.0 °C.

Contents

Synthesis The synthesis of compounds **1** and **2** from commercially available compounds is illustrated in Scheme 1.



Scheme 1 preparation of compounds **1** and **2**

Reagent: (a) $NH_2C_2H_4NH_2$, C_2H_5OH; (b) $NH(CH_2CH_2)_2NCH_3$, $CH_3OC_2H_4OH$.

N-(aminoethyl)-4-bromonaphthalene-1,8-dicarboximide (a): Ethylenediamine (2.0 g, 33.3 mmol) was added to a suspension of 4-bromonaphthalene-1,8-dicarboximide (5.54 g, 20 mmol) in ethanol (50 mL). The mixture was then refluxed for 4 hours, after which the solvent was evaporated under vacuum. The product crystallized from ethanol. Yield 85%. M.p. 154.8 °C; MS: m/z (%) 318 (1%); 1H NMR (500 MHz, $CDCl_3$): δ8.65 (dd, 1H, 7-ArH), 8.56 (dd, 1H, 2-ArH), 8.41 (d, *J* = 7.9 Hz, 1H, 5-ArH), 8.02 (d, *J* = 7.8 Hz, 1H, 5-ArH), 7.82 (dd, 2H, 3,6-ArH), 4.27 (t, *J* = 6.6 Hz, 2H, -N$\underline{CH_2}CH_2NH_2$), 3.07 (t, *J* = 6.6 Hz, 2H, -NCH$_2\underline{CH_2}$NH$_2$).

1: To a solution of 5 mL of ethylene glycol monomethyl ether added 0.2 g (6.3 mmol) of **a** and excess N-methyl piperidine (1 mL). The mixture was refluxed for 5 h under N_2 atmosphere and then the solvent was evaporated under vacuum. The product was purified by chromatography using methanol /dichloromethane (1: 20, v/v) as eluant to give 72 mg (36%) of **1** as yellow solid: 1H-NMR (400MHz, MD_3OD), δ8.06 (d, *J* = 8.4 Hz, 1H), 7.99 (d, *J* = 7.6 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 4.04 (t, *J* = 8.6 Hz, 2H), 3.89 (t, *J* = 8.6 Hz, 2H), 3.17 (s, 4H), 2.78 (s, 4H), 2.46 (s, 3H), ^{13}C NMR (100 MHz, CD_3OD) δ = 160.2, 155.0, 154.5, 129.8, 129.1, 128.2, 126.4, 125.2, 120.0, 117.3, 114.4, 54.7, 52.8, 52.0, 44.7, 43.2 ppm. HR-MS (ES+) Calcd for $([M+H])^+$, 321.1715; Found, 321.1736. **2** was obtained by the same procedure as orange solid 80 mg (40%): 1H-NMR (400MHz, MD_3OD), δ8.03 (d, *J* = 8.0 Hz, 1H), 7.83 (dd, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 8.0 Hz, 1H), 3.97 (t, *J* = 9.2 Hz, 2H), 3.79 (t, *J* = 8.8 Hz, 2H), 3.24 (s, 4H), 3.09 (s, 4H), 2.68 (s, 3H), ^{13}C NMR (100 MHz, CD_3OD) δ = 159.9, 154.2, 153.0, 129.5,

128.8, 127.9, 127.2, 126.2, 125.4, 123.4, 115.0, 114.1, 54.2, 52.5, 51.1, 43.8, 43.1ppm.

HR-MS (ES+) Calcd for $([M+H])^{+}$, 321.1715; Found, 321.1714.

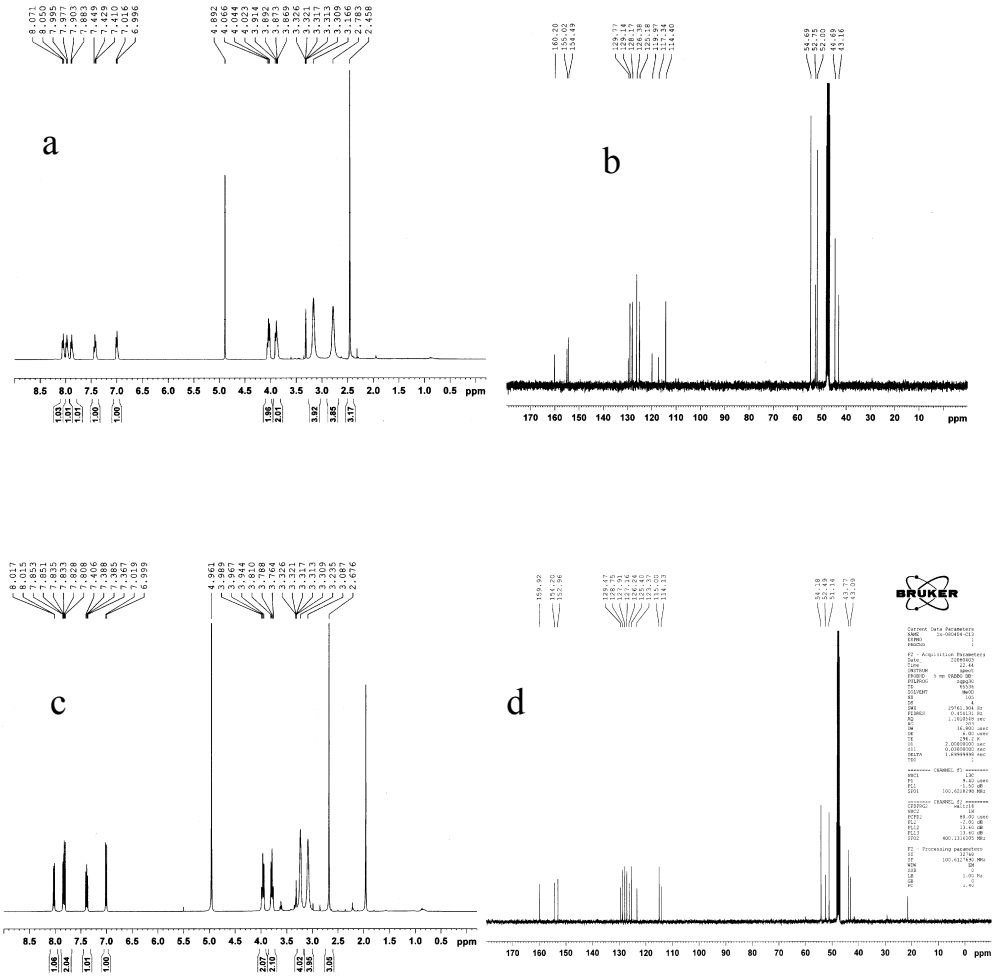


Figure 1 ^{1}H-NMR and ^{13}C-NMR spectra of **1** (a, b) and **2** (c, d)

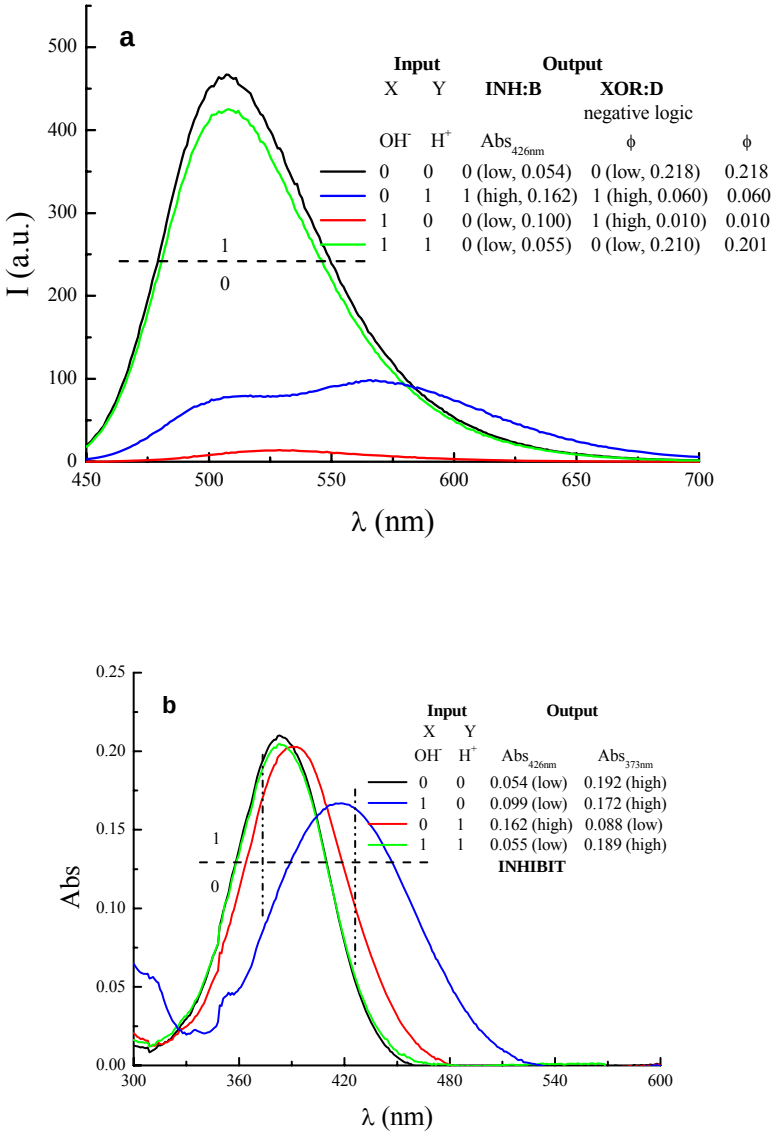


Figure 2 Fluorescence, UV-vis spectra and truth table of **1** in water in the presence of chemical inputs (excited at 410 nm).

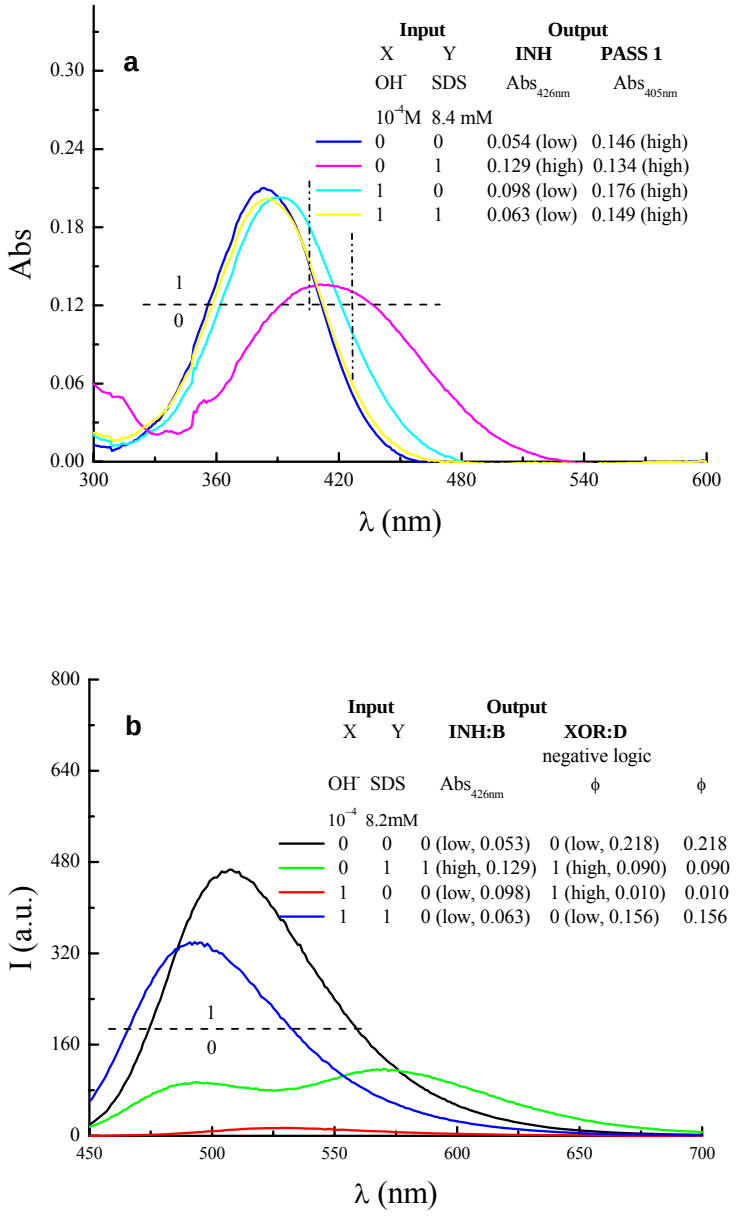


Figure 3 Fluorescence, UV-vis spectra and truth table of **1** in the presence of chemical inputs (excited at 410 nm).

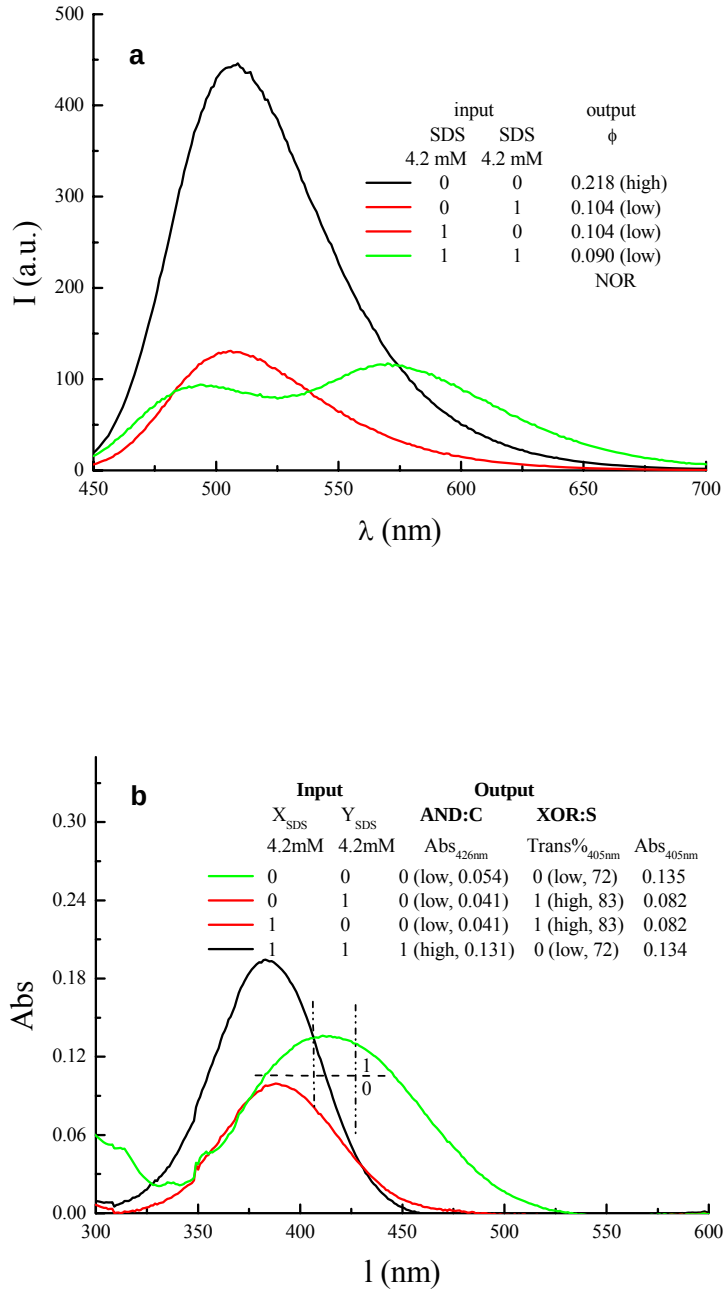
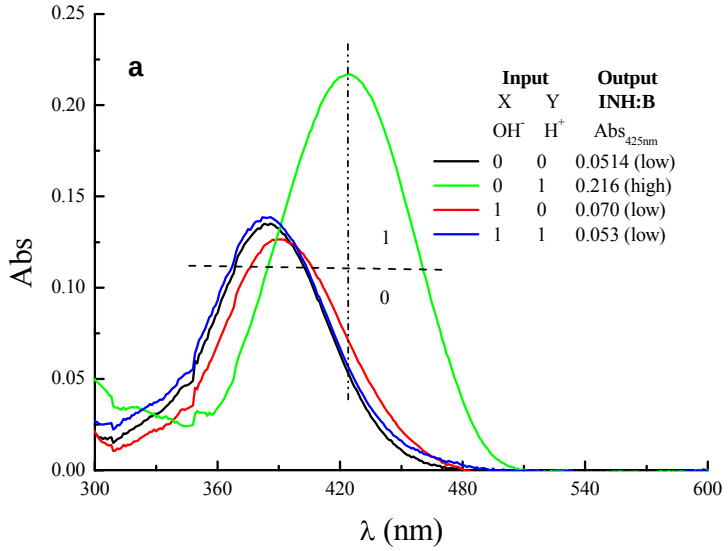
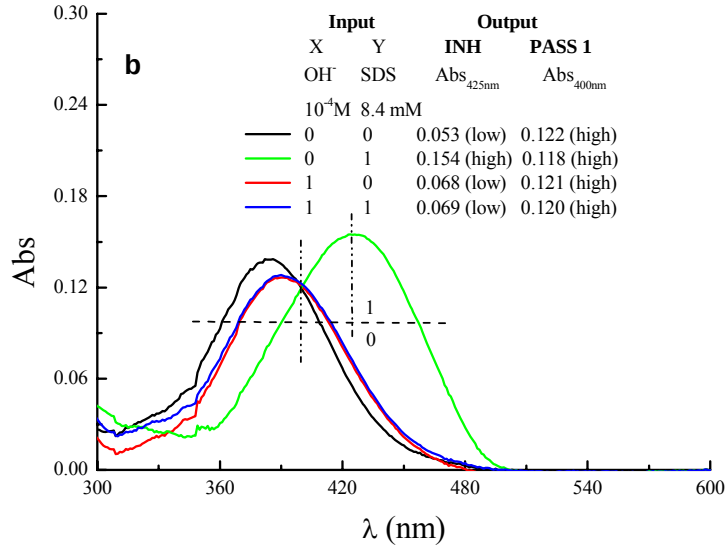


Figure 4 Fluorecence, UV-vis spectra and truth table of **1** in water in the presence of chemical inputs (excited at 410 nm).


a
Input
Output
X
Y
INH:B
OH-
H+
Abs425nm
0 0 0.0514 (low)
0 1 0.216 (high)
1 0 0.070 (low)
1 1 0.053 (low)
1
0
Abs
λ (nm)


b
Input
Output
X
Y
INH
PASS 1
OH-
SDS
Abs425nm
Abs400nm
10-4M 8.4 mM
0 0 0.053 (low) 0.122 (high)
0 1 0.154 (high) 0.118 (high)
1 0 0.068 (low) 0.121 (high)
1 1 0.069 (low) 0.120 (high)
1
0
Abs
λ (nm)

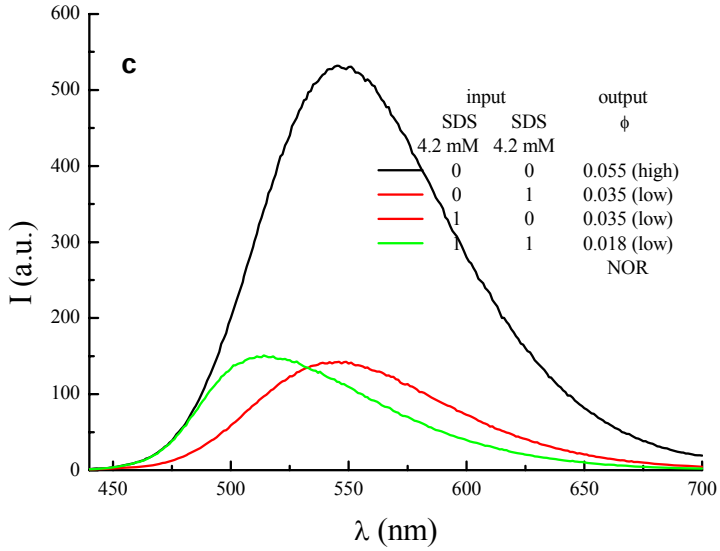


Figure 5 UV-vis, fluorescence spectra and truth table of **2** in water in the presence of chemical inputs (excited at 395 nm).

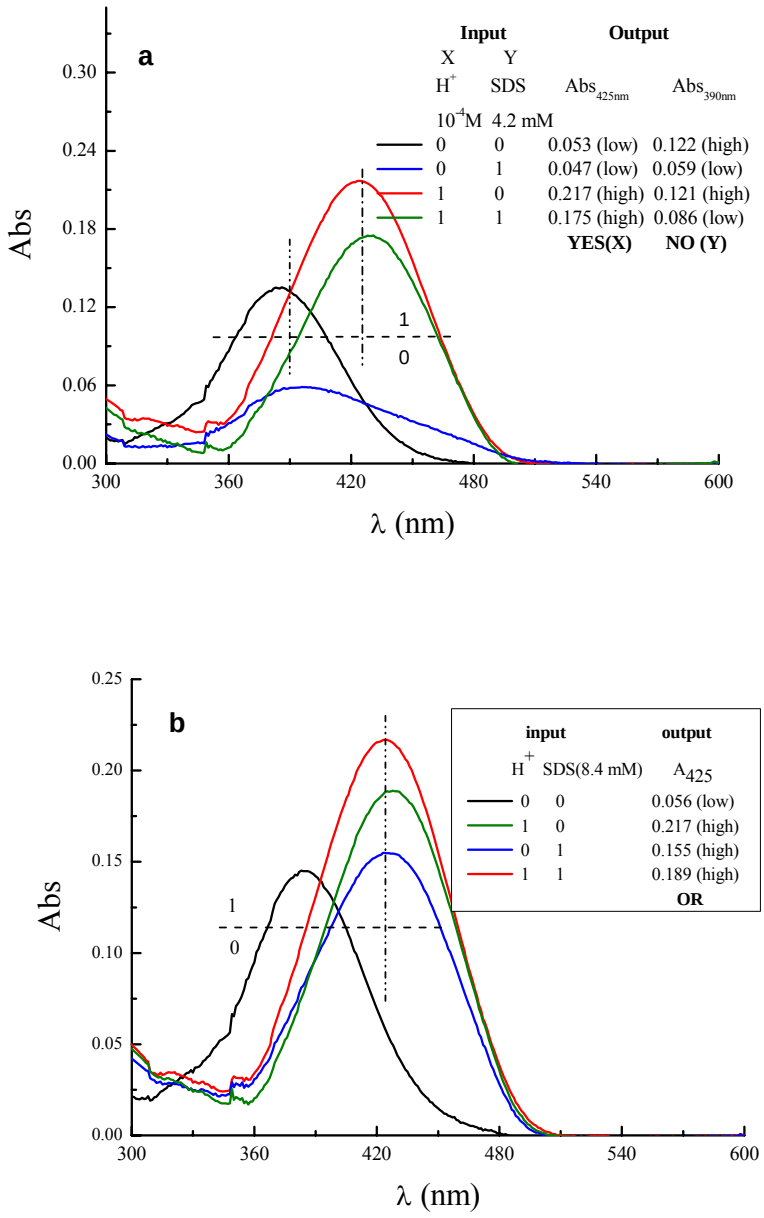


Figure 6 UV-vis spectra and truth table of **2** in water in the presence of chemical inputs.

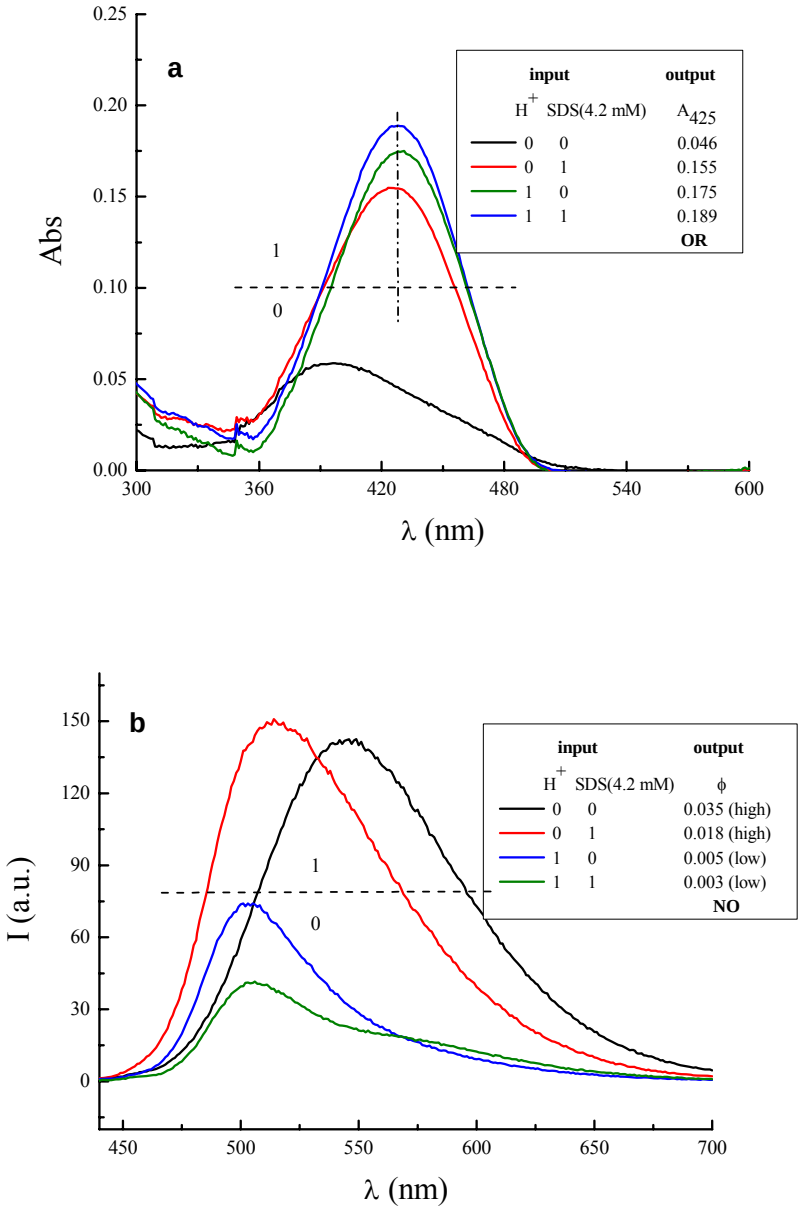


Figure 7 Fluorescence, UV-vis spectra and truth table of **2** in 4.2 mM SDS aqueous solution in the presence of chemical inputs (excited at 395 nm).

Table 1 Two-input logic truth table of **2**

Input 1 SDS (4.2 mM)	Input 2 OH^- (pH 9.5)	Output 1 A_{400}	Output 2 A_{426}	Output 3 Φ
0	0	1 (0.117)	0 (0.051)	1 (0.055)
0	1	1 (0.123)	0 (0.071)	0 (0.016)
1	0	0 (0.059)	0 (0.047)	0 (0.035)
1	1	1 (0.118)	0 (0.069)	0 (0.020)
			Pass 0	**NOR**

Table 2 Two-input logic truth table of **2** in 4.2 mM SDS aqueous solution

Input 1 SDS (4.2 mM)	Input 2 OH^- (pH 9.5)	Output 1 A_{400}	Output 2 A_{426}	Output 3 Φ
0	0	0 (0.059)	0 (0.047)	0 (0.035)
0	1	1 (0.118)	0 (0.069)	0 (0.020)
1	0	1 (0.120)	1 (0.155)	0 (0.018)
1	1	1 (0.122)	0 (0.072)	1 (0.057)
		NAND	**INH**	**AND**

Table 3 Three-input NOR logic truth table of **1**

Input 1 SDS (4.2 mM)	Input 2 SDS (4.2 mM)	Input 3 H^+ (pH 3.5)	Output 1 A_{373}	Output 2 A_{426}	Output 3 Φ
0	0	0	1 (0.192)	0 (0.054)	1 (0.218)
0	0	1	0 (0.084)	1 (0.163)	0 (0.060)
0	1	0	0 (0.084)	0 (0.043)	0 (0.104)
0	1	1	0 (0.040)	1 (0.113)	0 (0.011)
1	0	0	0 (0.084)	0 (0.043)	0 (0.104)
1	0	1	0 (0.040)	1 (0.114)	0 (0.011)
1	1	0	0 (0.090)	1 (0.127)	0 (0.090)
1	1	1	0 (0.083)	1 (0.130)	0 (0.080)
					NOR

Table 4 Three-input INHIBIT logic truth table 0f **1**

Input 1 SDS (4.2 mM)	Input 2 SDS (4.2 mM)	Input 3 OH^- (pH 9.5)	Output 1 A_{373}	Output 2 A_{426}	Output 3 Φ
0	0	0	1 (0.192)	0 (0.054)	1 (0.218)
0	0	1	1 (0.188)	0 (0.056)	0 (0.010)
0	1	0	0 (0.084)	0 (0.043)	0 (0.104)
0	1	1	1 (0.174)	0 (0.098)	0 (0.010)
1	0	0	0 (0.084)	0 (0.043)	0 (1049)
1	0	1	1 (0.174)	0 (0.098)	0 (0.010)
1	1	0	0 (0.090)	1 (0.127)	0 (0.090)
1	1	1	1 (0.152)	0 (0.096)	1 (0.156)
				INH	

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