Supplementary Material (ESI) for New Journal of Chemistry

Supplementary information

Logic gates from ion-selective bulk optodes

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1. Calculations of threshold values for absorbance outputs

The value chosen for 1 or 0 represents the difference between the corresponding spectra. Threshold values are determined by fix degree of deprotonation (α) at 0.6. The measured absorbance A at a given equilibrium can be related to α by measuring the absorbances of the fully protonated (A_P) and nonprotonated form (A_D) of the chromoionophore:

$$\alpha = \frac{A_P - A}{A_P - A_D}$$

Table S1. Wavelength for outputs O1 and O2

Chromoionophore	Wavelength for output O1 absorbance (nm)	Wavelength for output O2 absorbance (nm)
Chromoionophore I	540	665
Chromoionophore VII	530	670
Chromoionophore XIV	435	660
Nile Blue-urea	540	665

Chromoionophore I

Threshold value for output O1 (540 nm):

$A_D = 0.0957$ $A_P = 0.0256$

$A = A_D - (A_D - A_P)\,\alpha$

$A = 0.0957 - (0.0957 - 0.0256) \times 0.6$
$A = 0.0536$

Threshold value for output O2 (665 nm):

$A_D = 0.0979$ $A_P = 0.0018$
$A = A_P - (A_P - A_D)\ \alpha$
$A = 0.0979 - (0.0979 - 0.0018) \times 0.6$
$A = 0.0402$

Chromoionophore VII

Threshold value for output O1 (530 nm):

$A_D = 0.0584$ $A_P = 0.0039$
$A = A_D - (A_D - A_P)\ \alpha$
$A = 0.0584 - (0.0584 - 0.0039) \times 0.6$
$A = 0.0257$

Threshold value for output O2 (670 nm):

$A_D = 0.0921$ $A_P = 0.0021$
$A = A_P - (A_P - A_D)\ \alpha$
$A = 0.0921 - (0.0921 - 0.0021) \times 0.6$
$A = 0.0381$

Chromoionophore XIV

Threshold value for output O1 (435 nm):

$A_D = 0.0253$ $A_P = 0.0033$
$A = A_D - (A_D - A_P)\ \alpha$
$A = 0.0253 - (0.0253 - 0.0033) \times 0.67$
$A = 0.0105$

Threshold value for output O2 (660 nm):

$A_D = 0.0463$ $A_P = 0.0017$
$A = A_P - (A_P - A_D)\ \alpha$
$A = 0.0463 - (0.0463 - 0.0017) \times 0.6$
$A = 0.0195$

Nile Blue-urea

Threshold value for output O1 (540 nm):

$A_D = 0.0528$ $A_P = 0.0098$
$A = A_D - (A_D - A_P)\ \alpha$
$A = 0.0528 - (0.0528 - 0.0098) \times 0.6$
$A = 0.0270$

Threshold value for output O2 (665 nm):

$A_D = 0.0696$ $A_P = 0.0015$
$A = A_P - (A_P - A_D)\ \alpha$
$A = 0.0696 - (0.0696 - 0.0015) \times 0.6$

$A = 0.0287$

2. Details of non-logic gate operations

Table S2. Truth table for non-logic gates X/X' and Y/Y'

Input A H^+	Input B Na^+	X	X'	Y	Y'
0	0	1	0	0	1
0	1	0	1	0	1
1	0	1	0	1	0
1	1	0	1	1	0

Table S3. pHs and metal concentrations which operated X, X', Y, and Y' logic gates for Na^+ and K^+ selective bulk optodes

pH 1,0	X/X'[a,b,c] Concentration of Na^+ (M)				Y/Y'[a,b,c] Concentration of Na^+ (M)			
	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-1}	10^{-2}	10^{-3}	10^{-4}
3,5	C							
3,6	C							
3,7							C	C
3,8					bc	Bbc	BCbc	BCbc
3,9					bc	Bbc	BCbc	BCbc
3,10					bc	Bbc	BCbc	BCbc
4,6	BC	C						
4,8					b	bc	Bbc	BCbc
4,9					b	bc	BCbc	BCbc
4,10					b	bc	bc	Bc
5,8					bc	bc	bc	Bbc
5,9					bc	bc	bc	Bbc
5,10					bc	bc	bc	Bbc
6,8	AD						bc	bc
6,9	AD						bc	bc
6,10	D						bc	bc
7,9	AD	AD					c	c
7,10	D	D						c
8,10	Dd	D	D	D				

[a] A, B, C and D refer to chromoionophores I, VII, XIV and Nile Blue-urea, respectively in sodium optode.
[b] a, b, c and d refer to chromoionophores I, VII, XIV and Nile Blue-urea, respectively in potassium optode.
[c] X' and Y' operations were obtained from output O2 of the chromoionophores.

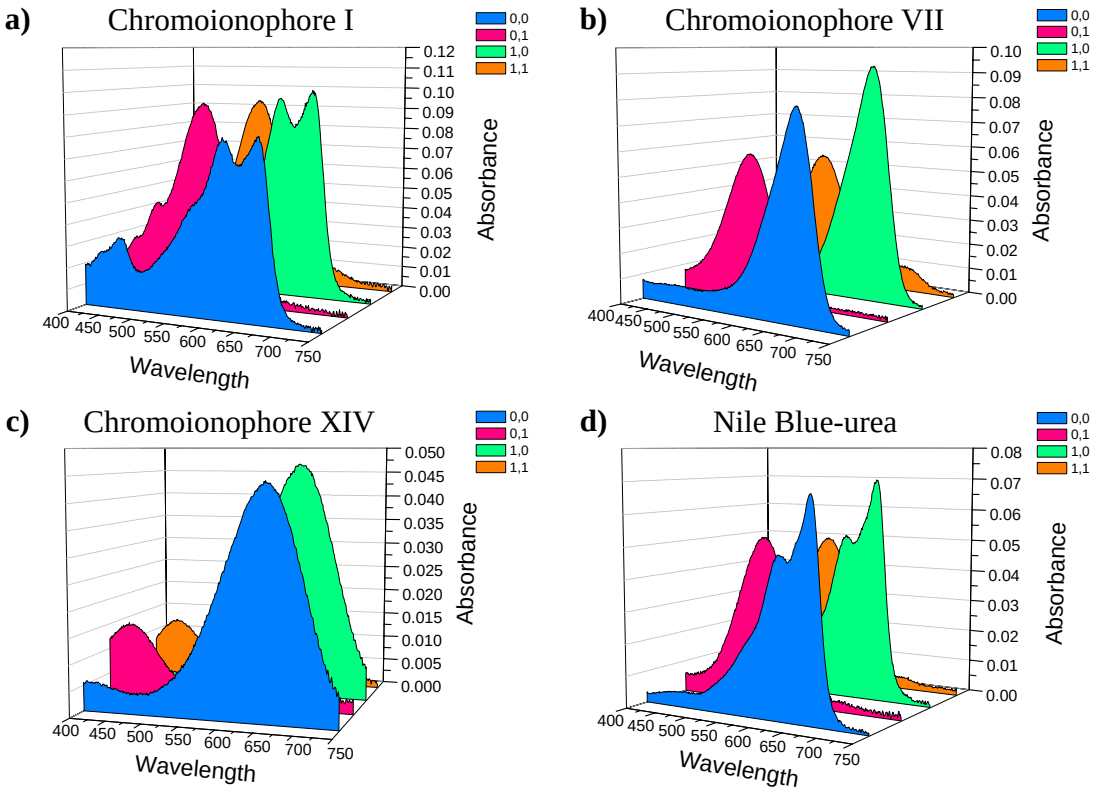

Figure S1. Absorbance features of the X and X' of sodium optode of studied chromoionophores: (a) Chromoionophore I (10^{-1} M $NaNO_3$ pH7, pH9) (b) Chromoionophore VII (10^{-1} M $NaNO_3$ pH4, pH6) (c) Chromoionophore XIV (10^{-1} M $NaNO_3$ pH3, pH5) (d) Nile Blue-urea (10^{-1} M $NaNO_3$ pH7, pH9) Input combination 0,0: blue; 0,1: pink; 1,0: green and 1,1: orange.

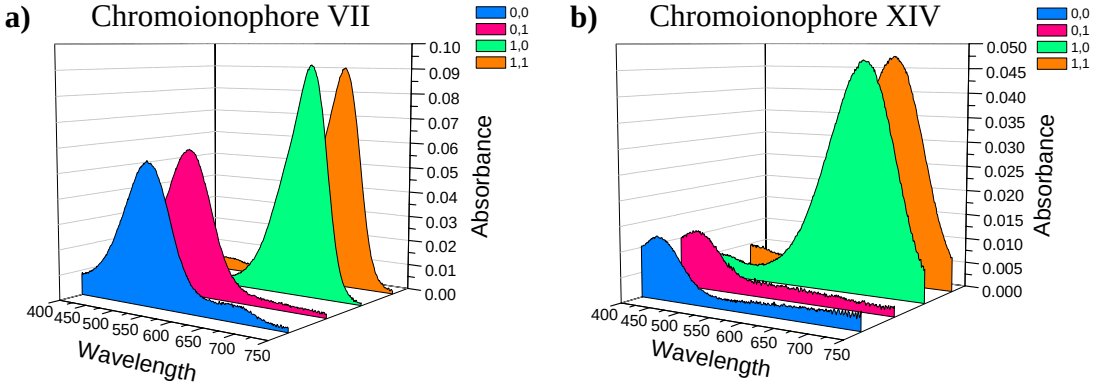

Figure S2. Absorbance features of the Y and Y' of sodium optode of studied chromoionophores: (a) Chromoionophore VII (10^{-4} M $NaNO_3$ pH3, pH10) (b) Chromoionophore XIV (10^{-4} M $NaNO_3$ pH3, pH10) Input combination 0,0: blue; 0,1: pink; 1,0: green and 1,1: orange.

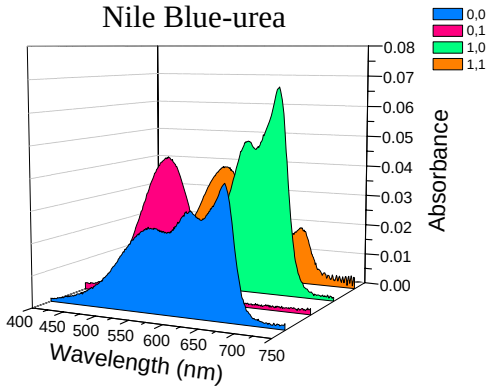

Figure S3. Absorbance features of the X and X' of potassium optode of studied Chromoionophores I (10^{-1} M $NaNO_3$ pH8, pH10) Input combination 0,0: blue; 0,1: pink; 1,0: green and 1,1: orange.

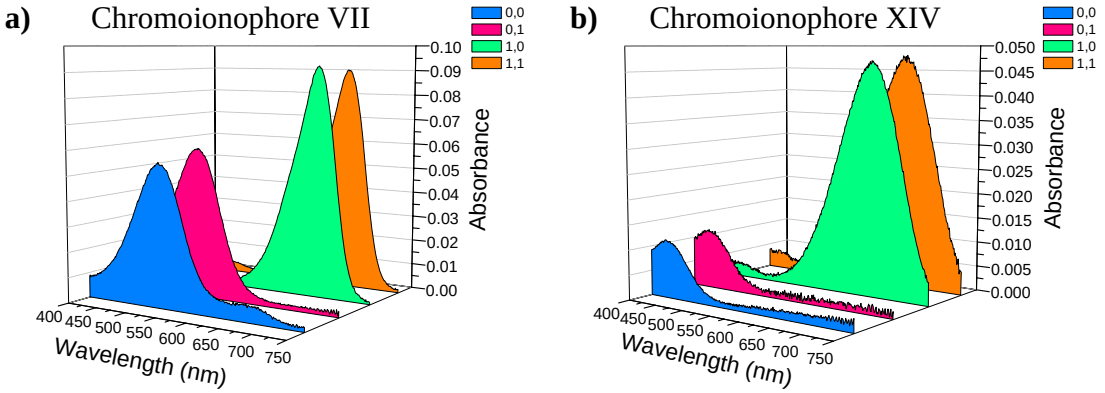

Figure S4. Absorbance features of the Y and Y' of potassium optode of studied chromoionophores: (a) Chromoionophore VII (10^{-1} M $NaNO_3$ pH3, pH8) (b) Chromoionophore XIV (10^{-1} M $NaNO_3$ pH3, pH8) Input combination 0,0: blue; 0,1: pink; 1,0: green and 1,1: orange.