

Accessory Publication

Colorimetric sensor array for qualitative water analysis

Shu Ann Chan^A, Jun-Seok Lee^B, Young-Tae Chang^{A,C,D,E*}

^A Department of Chemistry, National University of Singapore, Singapore 117543

^B Department of Chemistry, New York University, New York, New York 10003

^C NUS MedChem Program of the Office of Life Sciences Institute, National University of Singapore, Singapore 117543

^D Laboratory of Bioimaging Probe Development, Singapore Bioimaging Consortium, Agency for Science, Technology and Research (A*STAR), Biopolis, Singapore 138667, Singapore

^E Corresponding author, Email: chmcyt@nus.edu.sg

Table S1. Selected dyes and working concentrations of Singapore Tongue (SGT) (*: selected probes for 12 bottled water dilution test).

Dye no.	Dye name	λ_0 (nm)	λ_1 (nm)	λ_2 (nm)	[Dye] (mM)	DMSO (%)
15	Methyl orange		460	510	0.07	0.7
19	Alizarin yellow R		370	400	0.50	0.5
25	Eriochrome blue black R		550	510	0.30	3.0
33	Aniline blue black	620			0.04	0.4
35*	Congo red		500	570	0.07	0.7
37	Evans blue	590			0.07	0.7
38*	Brilliant yellow		400	500	0.05	0.5
57*	Aniline blue		480	580	0.42	4.2
64*	Dibromofluorescein	500			0.02	0.2
68	Phloxine B	540			0.03	0.3
75*	Neutral red		530	450	0.07	0.7
85*	Alizarin		430	530	0.42	4.2
86*	Alizarin red S (ARS)		420	520	0.42	4.2
108*	Rosolic acid	480			1.00	1.0
132	Amaranth (acid red 27)		520	460	0.25	2.5
137	Trypan blue	590			0.05	0.5
142	Biebrich scarlet	510			0.12	1.2
143	Ponceau S	520			0.05	0.5
148	Victoria Blue B	610			0.05	0.5
150	Eosin bluish	520			0.03	0.3
163	Bromophenol blue, Na ⁺		590	440	0.05	0.5
166*	Chlorophenol red		430	570	0.08	0.4
176	Rose Bengal	550			0.05	0.5
179	Thymol blue		430	600	0.22	2.2
189	Ethyl violet	590			0.02	0.2
190	Proflavine		440	400	0.05	0.5
200*	Cresol red		430	570	0.15	1.5
201	Metanil yellow	430			0.12	1.2
202	4-Phenylazoaniline		370	490	0.13	1.3
203*	Erythrosin B		530	550	0.10	1.0
206	Ethyl orange, Na ⁺		470	510	0.12	1.2
207*	Bromocresol green, Na ⁺		620	440	0.17	1.7
208*	Resazurin Na ⁺		600	530	0.12	1.2
213*	Bromothymol Blue, Na ⁺		430	620	0.15	1.5
216	m-Cresol Purple		430	570	0.25	2.5
221*	Pyrocatechol violet		440	610	0.20	2.0
222*	Xylenol orange		430	570	0.15	1.5
226	2',7'-Dichlorofluorescein		500	490	0.05	0.5
228*	Bromochlorophenol Blue Na ⁺		590	440	0.03	0.3
229	Quinaldine red	500			0.07	0.7
212*	Nitrazine Yellow		465	590	0.06	0.6

Dye no.	Dye name	λ_0 (nm)	λ_1 (nm)	λ_2 (nm)	[Dye] (mM)	DMSO (%)
232*	4-(p-Ethoxyphenylazo)-m-phenylene-diamine HCl		450	480	0.12	1.2
236*	Methylthymol blue		430	600	0.20	2.0
237	4-(2-Pyridylazo)resorcinol, Na ⁺		410	510	0.10	1.0
239*	Methyl red		520	430	0.02	0.2

Table S2. Nutritional contents of bottled waters and their labels.

Label	Brand	Ion concentration (ppm)								
		Ca ²⁺	Mg ²⁺	Na ⁺	K ⁺	Silica	Cl ⁻	NO ₃ ⁻	SO ₄ ²⁻	HCO ₃ ⁻
N1	NTUC	-	-	-	-	-	-	-	-	-
N2	Evian	80.0	26.0	6.5	1.0	15.0	6.8	3.7	12.6	360.0
N3	Ice Mountain	34.0	7.0	22.0	2.0	-	3.0	-	4.0	124.0
N4	Perrier	15.5	6.8	11.8	-	-	25.0	-	46.1	44.5
N5	Cool Rhino	-	-	-	-	-	-	-	-	-
N6	Life	-	-	-	-	-	-	-	-	-
N7	Aqua	-	10.0	17.0	2.3	-	2.3	-	7.2	84.0
N8	Newater	-	-	0.7	-	-	-	-	-	-
N9	Volvic	11.5	8.0	11.6	6.2	31.7	13.5	6.3	8.1	71.0
N10	Fiji Natural Artesian Water	17.0	13.0	18.0	4.9	85.0	8.6	-	-	140.0
N11	Vittel	94.0	20.0	7.7	5.0	-	4.0	< 0.5	120.0	248.0
N12	First Choice Eau de Source French Spring Water	58.0	24.0	3.0	0.8	-	5.0	1.0	8.0	280.0

Table S3. Representative CCD images of dyes toward MRT waters.

Dye no.	Dye name	Colour change of respective dyes in Control, C1 representative and C2 representative detected by naked eye
213	Bromothymol Blue, Sodium Salt	
236	Methylthymol blue (MTB)	
86	Alizarin red S (ARS)	
85	Alizarin	
222	Xylenol Orange (XO)	
212	Nitrazine Yellow	
200	Cresol red	
166	Chlorophenol red (CPR)	
57	Aniline blue (AB)	
108	Rosolic acid	

Figure S1. PCA plot of tap waters from 4 Asian countries (TIn: tap water from India, TJ: tap water from Japan, TM: tap water from Malaysia, TS: tap water from Singapore).

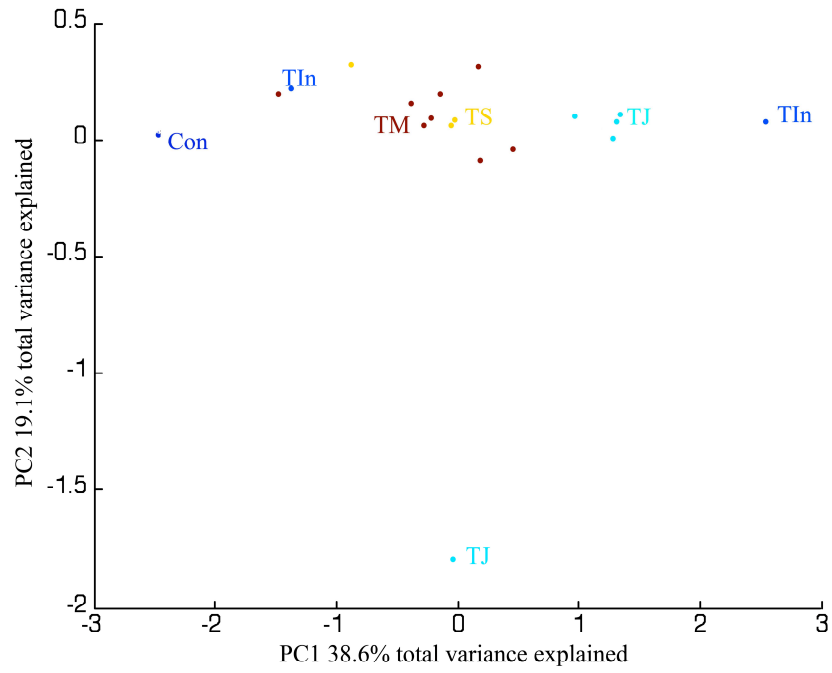
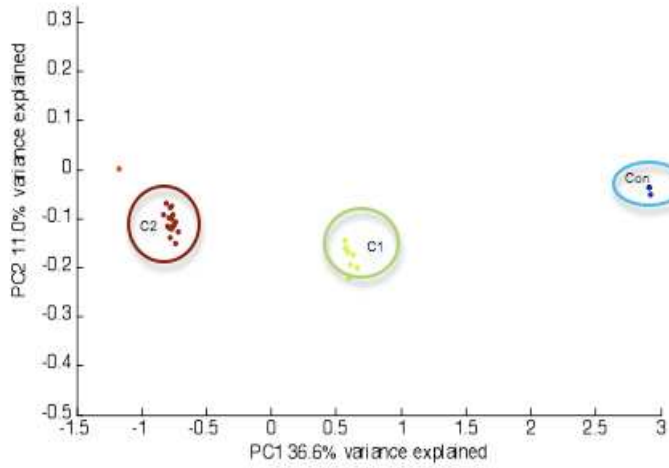


Figure S2. (a) PCA plot of representative C1, C2 with EW28 and EW29 (red dots) (b) Singapore MRT map with different color code (Blue line: C1 cluster, Dark red line: C2 cluster)

(a)



(b)

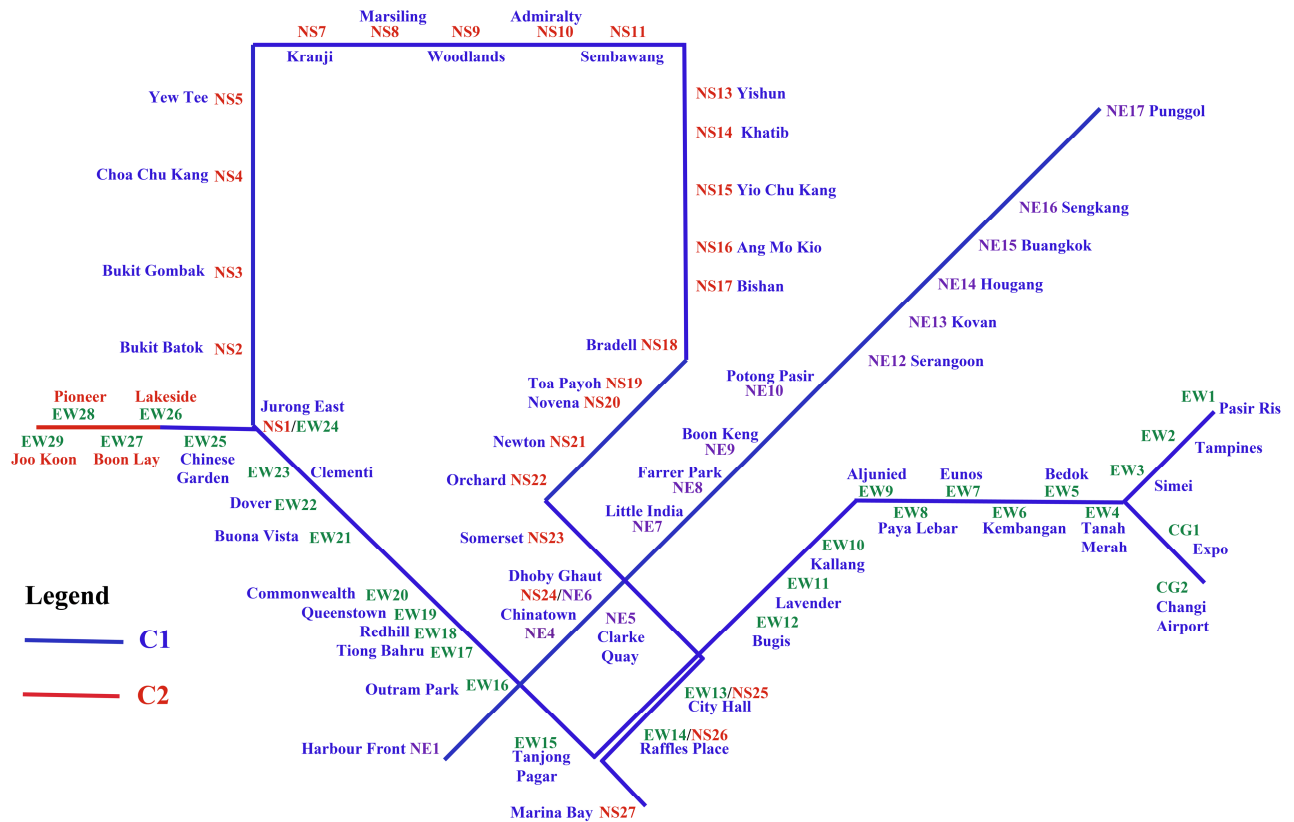


Figure S3. General Singapore Tongue (SGT) plate layout.

