Supporting Information

Poly(*para*-phenyleneethynylene)-Sensor Arrays Discriminate 22 Different Teas

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1. General Information

Chemicals were purchased from commercial laboratory suppliers. Buffer solutions of pH 3 (citric acid/NaOH/NaCl), pH 7 (KH_2PO_4/Na_2HPO) and pH 13 (KCl/NaOH) were purchased from Sigma-Aldrich®. Cucurbituril [8] was purchased from abcr GmbH. Reagents were used without further purification unless otherwise noted.

Solvents were purchased from commercial laboratory suppliers and if necessary distilled prior use. All of the other absolute solvents were dried by a MB SPS-800 using drying columns.

^{1}H NMR spectra was recorded at room temperature on Bruker Avance III 600 (600 MHz). The data was interpreted in first order spectra. The spectra were recorded in D_2O as indicated. Chemical shifts are reported in δ units relative to the solvent residual peak (HDO in D_2O at δ_H = 4.74 ppm).[1] m (multiplet) is used to indicate the signal multiplicity.

Absorption and emission spectra were recorded using a Jasco V660 and Jasco FP6500 spectrometer. Emission data for sensing were recorded on a CLARIOstar (firmware version 1.13) Platereader from BMG Labtech using the corresponding software (software version 5.20 R5). Data were analysed with CLARIOstar MARS Data Analysis Software (software version 3.10 R5) from BMG Labtech.

IR spectra was recorded on a JASCO FT/IR-4100. **P3** was applied as solid. The obtained data was processed with the software JASCO Spectra Manager™ II.

Dialysis was realized with regenerated cellulose tubular membranes (ZelluTrans, Carl Roth®) with a molecular weight cut-off of 3500 Da against deionized (DI) water.

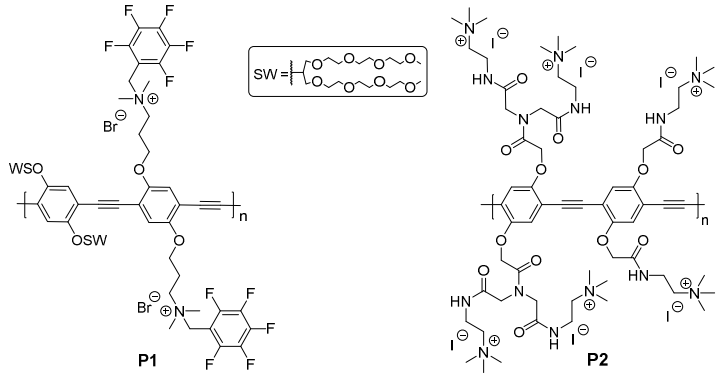
Tea samples within three categories were purchased from local supermarkets in Germany and China. Upon test, tea samples were crashed into powders. 25 mg powders was weighed into 10 mL boiled water for 5 min. The solutions were separated and diluted to 100 mL as final tea infusions with a concentration of 0.25 mg/mL.

Linear discriminant analysis (LDA) and principal component analysis (PCA). Both methods were carried out in this study by using SYSTAT (version 13.0). In LDA, all variables were used in the model (complete mode) and the tolerance was set as 0.001. The fluorescence response patterns were transformed to canonical patterns. The Mahalanobis distances of each individual pattern to the centroid of each group in a multidimensional space were calculated and the assignment of the case was based on the shortest Mahalanobis distance. PCA is a mathematical transformation used to extract variance between entries in a data matrix by reducing the redundancy in the dimensionality of the data. It takes the data points for all analytes and generates a set of orthogonal eigenvectors (principal components, PCs) for maximum variance.[2-3]

Method for Fluorescence response pattern and linear discriminant analysis. Generally, PPEs and the PPE-CB[8] complexes were dissolved in different pH buffer (pH 3, 7 and 13) to give 2.0 μM and 2.0 μM-15.0 μM of stock solutions on the basis of their molecular weights. Each PPE or complex solution (180 μL) in buffer was respectively loaded into a well on a 96-well plate (300 μL microplate). Subsequently, 120 μL tea infusions were added to each well and mixed. Finally, the fluorescence intensity values were recorded with a CLARIOstar (firmware version 1.13) microplate reader. Fluorescence intensity change $((I - I_0) / I_0)$ were calculated and used for linear discriminant analysis. I_0 and I are the fluorescence intensity of the solution (PPE or mixtures of PPE-CB[8]) in the absence and presence of analytes, respectively. The fluorescence intensities (I_0 or I) were recorded at the peak 460 nm with an excitation at 410 nm by using a plate reader.

2. Synthetic Details and Analytical Data

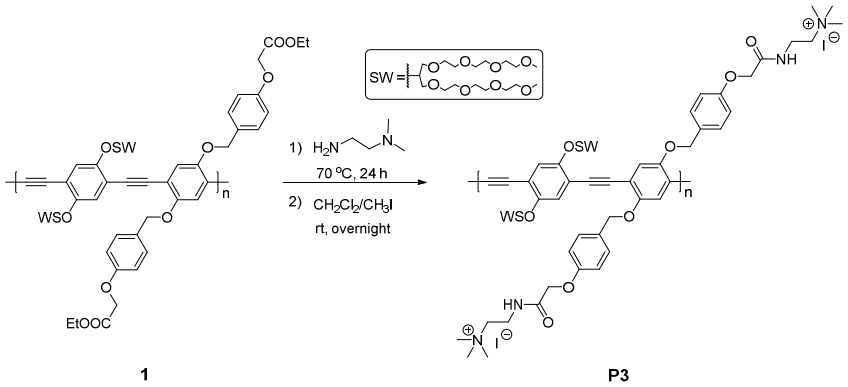
2.1 Syntheses of P1 and P2



P1 *was synthesized according to the literature.*[4]

P2 *was synthesized according to the literature.*[5-6]

2.2 Synthesis of P3



*Polymer **1** was synthesized according to the literature.*[7]

Polymer **1** (75 mg, 54.3 µmol) was dissolved in N, N'-dimethyl-ethylenediamine (20 mL) and stirred at 70 ^{o}C for 24 h. The reaction mixture was evaporated to dryness and washed with copious amounts of *n*-hexane. The crude product was dissolved in CH_2Cl_2 (20 mL). After addition of CH_3I (10 mL), the reaction mixture was stirred overnight at ambient temperature. All volatiles were removed under reduced pressure. The residue was dissolved in H_2O and dialyzed against DI H_2O for 3 d. After freeze-drying, a spongy, yellow solid (75 mg, 92%) was obtained. The M_n and PDI result from polymer **1**, which was 8.3 x 10^3 g/mol and 3.0, respectively. ^{1}H NMR (600 MHz, D_2O): δ = 6.95-7.44 (m, 12 H), 5.16-5.17 (m, 2 H), 4.52-

4.64 (m, 4 H), 3.33-3.58 (m, 68 H) , 3.14-3.18 (m, 30 H) ppm. IR (cm^{-1}): ν 3455, 2870, 2361, 1738, 1671, 1611, 1534, 1510, 1488, 1416, 1351, 1201, 1091, 954, 847, 584, 518, 451. Due to low solubility, ^{13}C NMR spectrum could not be obtained.

3. Screening Process

[1] Screening with individual highly-fluorescent PPEs

Nine highly-fluorescent positively-charged PPEs **P1-9** (Figure S1) were selected for screening. The results showed that similar responses were observed for all positively charged polymers, which indicates the cationic polymers may have similar discrimination ability (Figure S2a). According to the PCA analysis (Figure S2), we finally selected **P1** (positive charge), **P2** (highly positive charge) and **P3** (positive charge) as sensor elements. **P4-P9** were synthesized according to the literature.[2, 4, 6, 8-10]

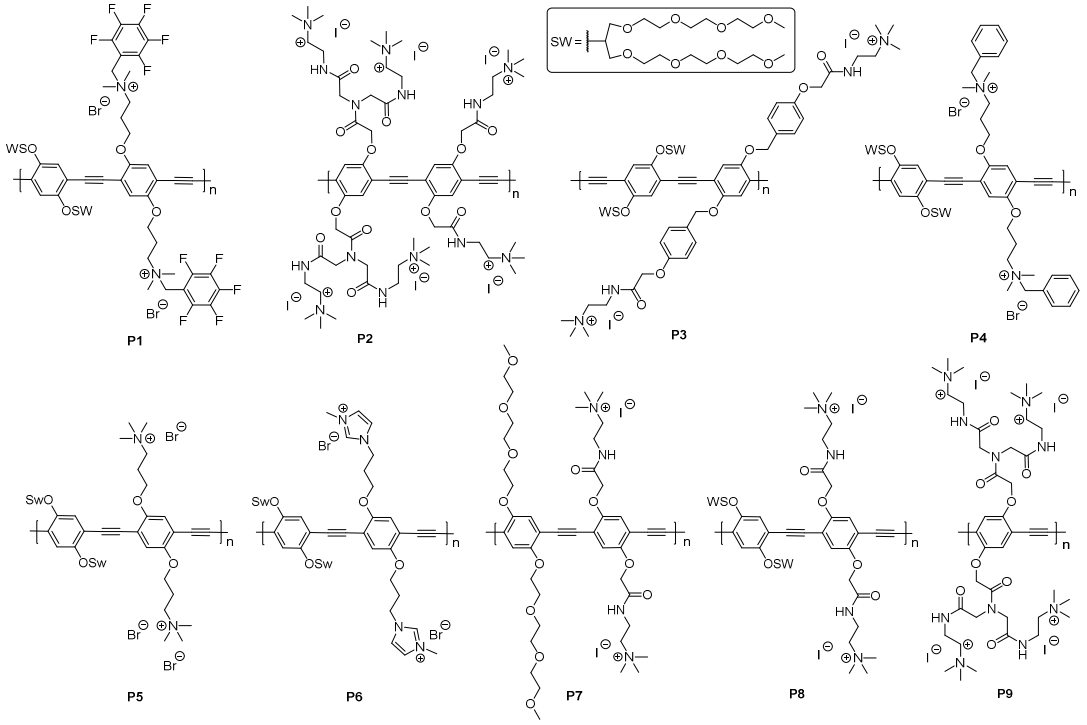
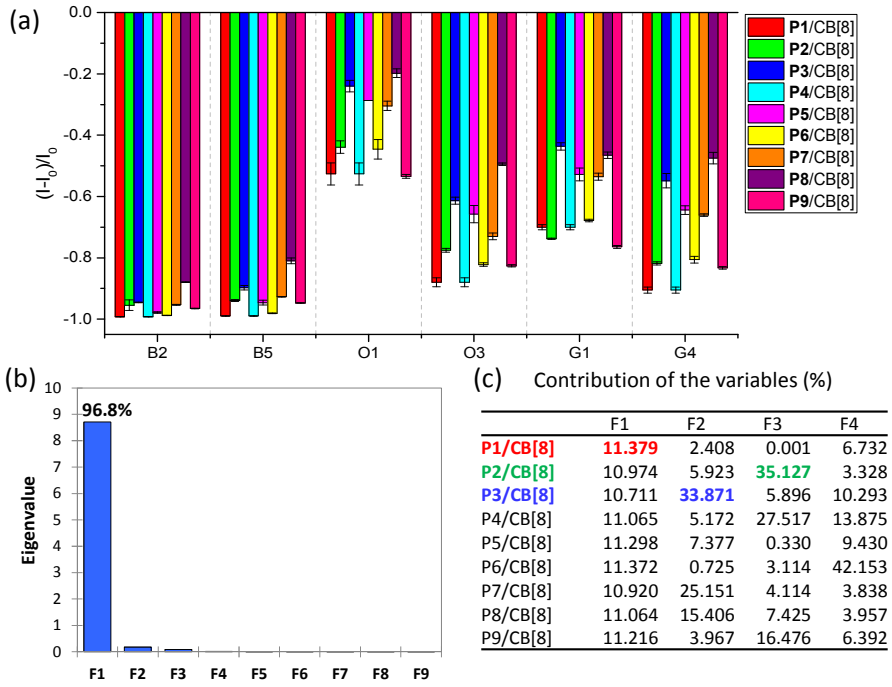


Figure S1. Structures of PPEs used for the screening process.



	F1	F2	F3	F4
P1/CB[8]	11.379	2.408	0.001	6.732
P2/CB[8]	10.974	5.923	35.127	3.328
P3/CB[8]	10.711	33.871	5.896	10.293
P4/CB[8]	11.065	5.172	27.517	13.875
P5/CB[8]	11.298	7.377	0.330	9.430
P6/CB[8]	11.372	0.725	3.114	42.153
P7/CB[8]	10.920	25.151	4.114	3.838
P8/CB[8]	11.064	15.406	7.425	3.957
P9/CB[8]	11.216	3.967	16.476	6.392

Figure S2. (a) Fluorescence response pattern ((I - I_0) / I_0) obtained by **P1-9** (1.2 μM) in the prescence CB[8] (9.0 μM) treated with 6 randomly choosen teas. Each value is the average of two independent measurements. (b) Eigenvalue calculated from principal component analysis, factor 1 represent 96.8% of the total variation. (c) Contribution of each sensor elements to the resulted six factors (F1-F4).

[2] Screening with the suitable concentration and infusion time of tea

Figure S3 (a) shows that the fluorescence of polymer/CB[8] was almost fully quenched when the concentration of tea was over 0.5 mg/mL. The most suitable concentration was 0.1 mg/mL for the discrimination.

25 mg of tea samples were infused with 10 mL distilled boiling water for 5 min, 10 min, 30 min and 60 min, respectively. Then the tea leaves were removed by filtration and the tea infusion were cooled down to room temperature. Afterwards the tea infusions were diluted to 0.1 mg/mL when loaded into a well on a 96-well plate. Figure S3 (b) shows that the fluorescence wasn't further quenched when infusion time was prolonged. Finally, the suitable infusion time was 5 min.

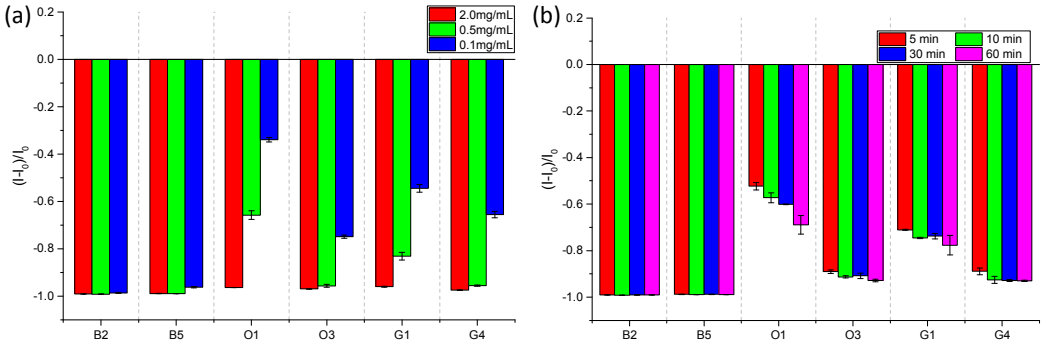


Figure S3. (a) Fluorescence response pattern ((I - I_0) / I_0) obtained by **P1**/CB[8] (1.2 μM/9.0 μM) treated with different concentration of 6 randomly choosen teas. (b) Fluorescence response pattern ((I - I_0) / I_0) obtained by **P1**/CB[8] (1.2 μM/9.0 μM) treated with 6 randomly choosen teas at different infusion time. Each value is the average of two independent measurements.

[3] Screening with different pH values

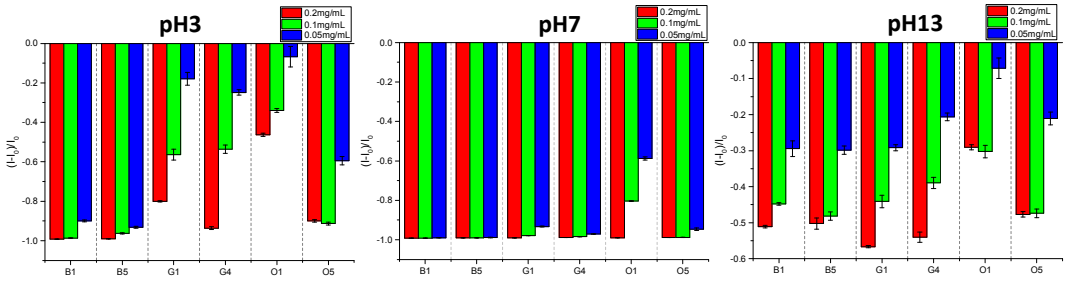


Figure S4. Fluorescence response pattern ((I - I_0) / I_0) obtained by **P1**/CB[8] (1.2 μM/9.0 μM) treated with 6 randomly choosen teas at different pH buffer solutions. Each value is the average of two independent measurements.

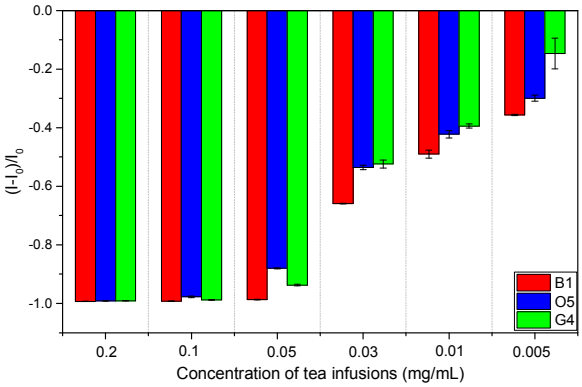


Figure S5. Fluorescence response pattern ((I - I_0) / I_0) obtained by **P1**/CB[8] (1.2 μM/9.0 μM) treated with different concentration of 3 randomly chosen teas at pH 7 buffer solution. Each value is the average of three independent measurements.

4. Complex Titrations and Determination of KSV Constants

All titrations (Figure S6) were performed in water solution. The corresponding emission spectra are shown in the inset of the following figures. The molecular structure of the fluorophore, K_{SV} and log K_{SV} is shown on the right. The fitting of quenching data was performed using the following modified Stern-Volmer equation (eq. 1).

$$I_q = I_0 + \frac{I_{final}-I_0}{2} \times \left\{1 + \frac{[Q]}{[F]} + \frac{1}{K_{SV}[F]} - \left[(1 + \frac{[Q]}{[F]} + \frac{1}{K_{SV}[F]})^2 - 4\frac{[Q]}{[F]}\right]^{1/2}\right\} \quad \textbf{(eq. 1)}$$

Here, I_0 = initial fluorescence intensity of the fluorophore, I_{final} = final fluorescence intensity of the fluorophore, I_q = fluorescence intensity at a given quencher concentration, $[F]$ = concentration of the fluorophore, $[Q]$ = total concentration of the added quencher Q and K_{SV} = Stern-Volmer constant.

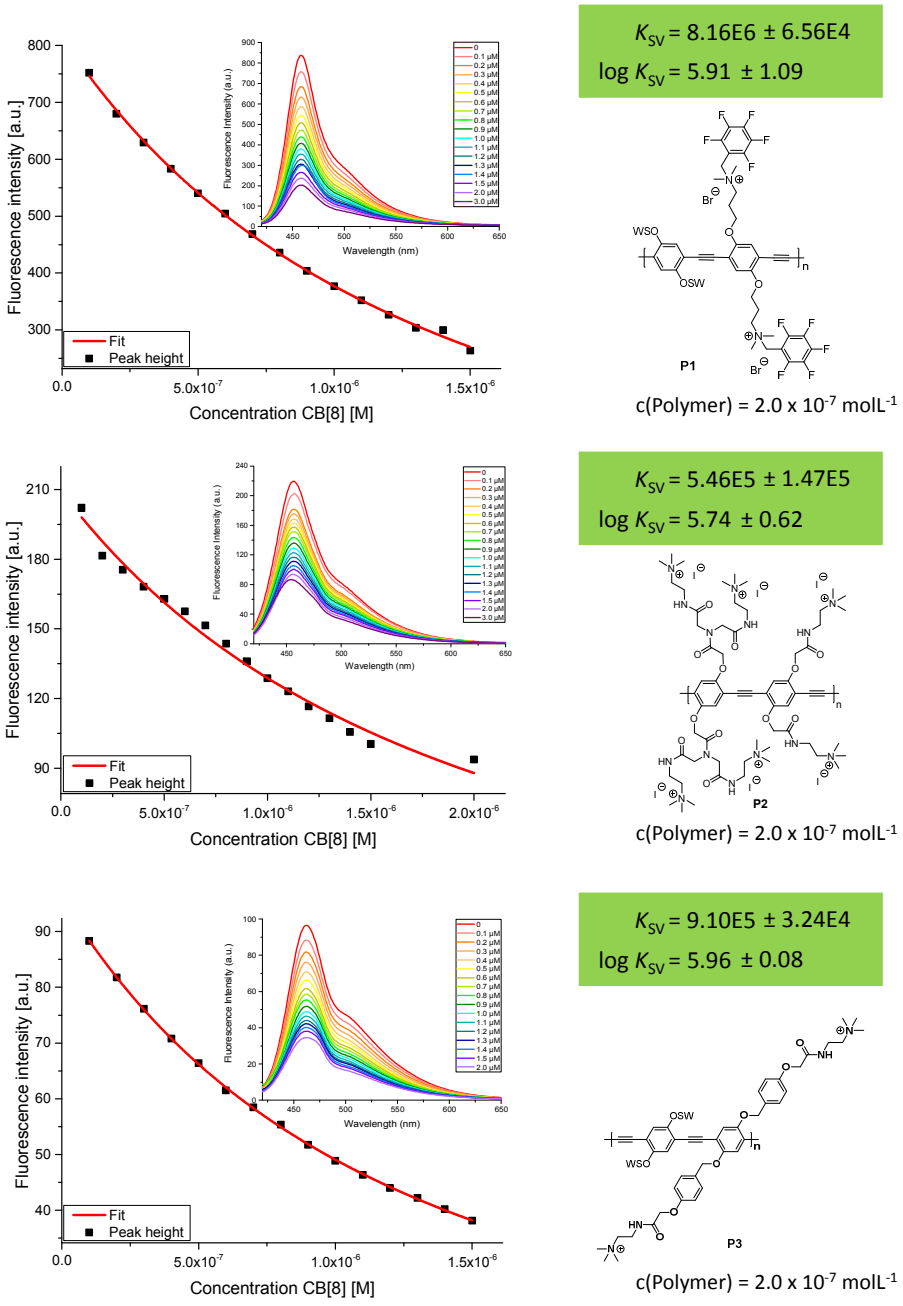


Figure S6. Volmer plots using a modified Stern–Volmer equation for fluorescence quenching of **P1-3** (2.0×10^{-7} M) with CB[8]. The inset shows the emission quenching data.

5. Fluorescence Response Patterns

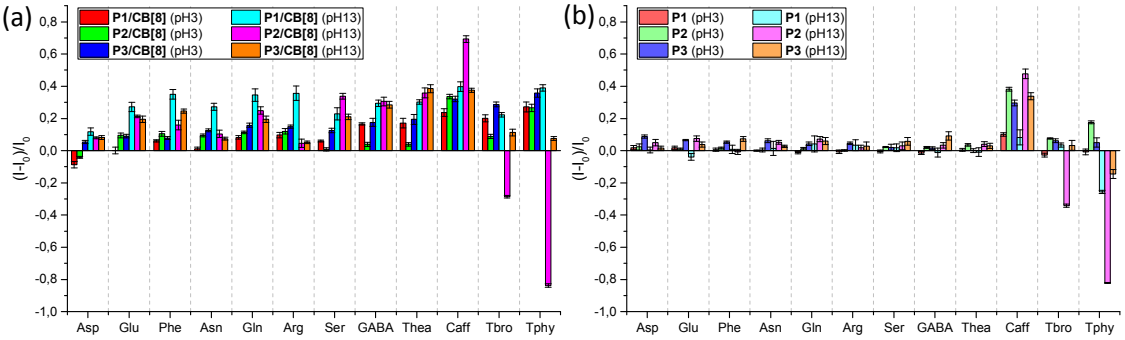


Figure S7. Fluorescence response pattern ($(I - I_0)/I_0$) obtained by (a) PPE/CB[8] tongue (1.2 μM/9.0 μM, at pH 3 and 13, buffered) and (b) PPE tongue (1.2 μM, at pH 3 and 13, buffered) treated with tea related analytes (c = 10 mM). Each value is the average of six independent measurements; each error bar shows the standard deviation (SD) of these measurements.

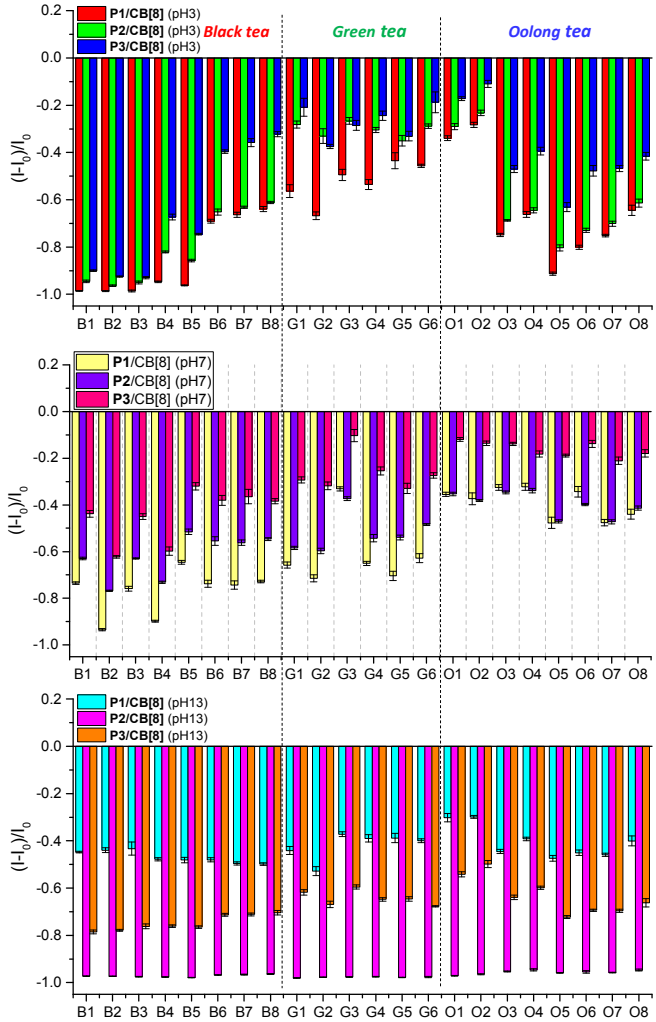


Figure S8. Fluorescence response patterns ($(I - I_0)/I_0$) obtained by PPE/CB[8] tongue (1.2 μM/9.0 μM, at pH 3, 7 and 13, buffered) treated with 22 kinds of teas (0.1 mg/mL at pH 3 and 13, 0.01 mg/mL at pH 7, respectively). Each value is the average of six independent measurements; each error bar shows the standard deviation (SD) of these measurements.

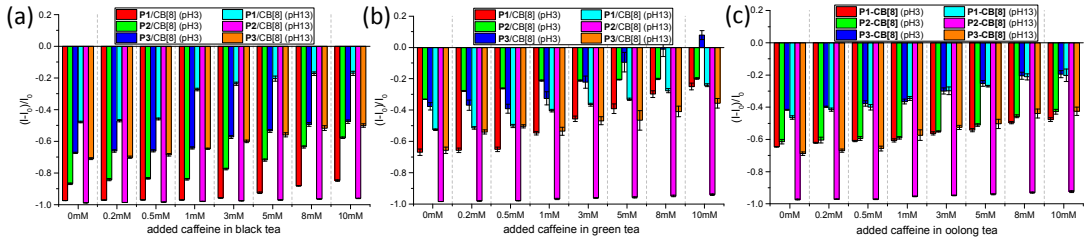


Figure S9. Fluorescence response patterns ($(I - I_0)/I_0$) obtained by PPE/CB[8] tongue (1.2 μM/9.0 μM, at pH 3 and 13, buffered) treated with different concentrations of caffeine (0-10 mM) in (a) black tea, (b) green tea, (c) oolong tea infusions.

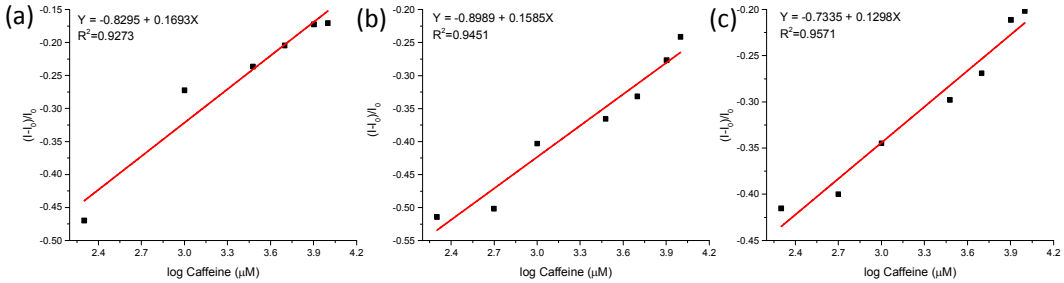


Figure S10. Linear relationship between fluorescence response ($(I - I_0) / I_0$) vs log concentration of caffeine obtained by P**1**/CB[8] (1.2 μM/9.0 μM) in (a) black tea, (b) green tea and (c) oolong tea at pH 13 buffer solutions.

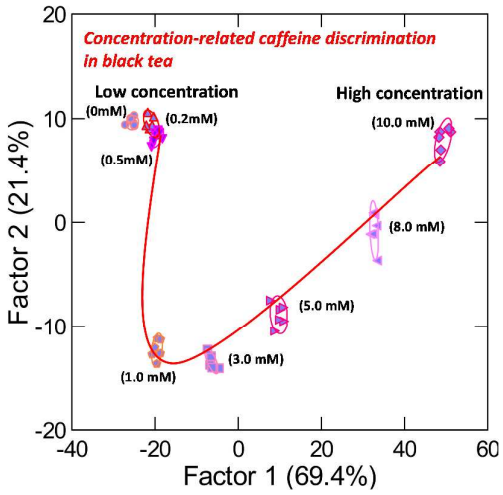


Figure S11. 2D canonical score plot for the first two factors obtained with an array of PPE-CB[8] (1.2 μM/9.0 μM, at pH 3 and 13, buffered) treated with different concentrations of caffeine (0-10 mM) with 95% confidence ellipses in black tea infusions. Cross-validated LDA showed 94% correct accuracy.

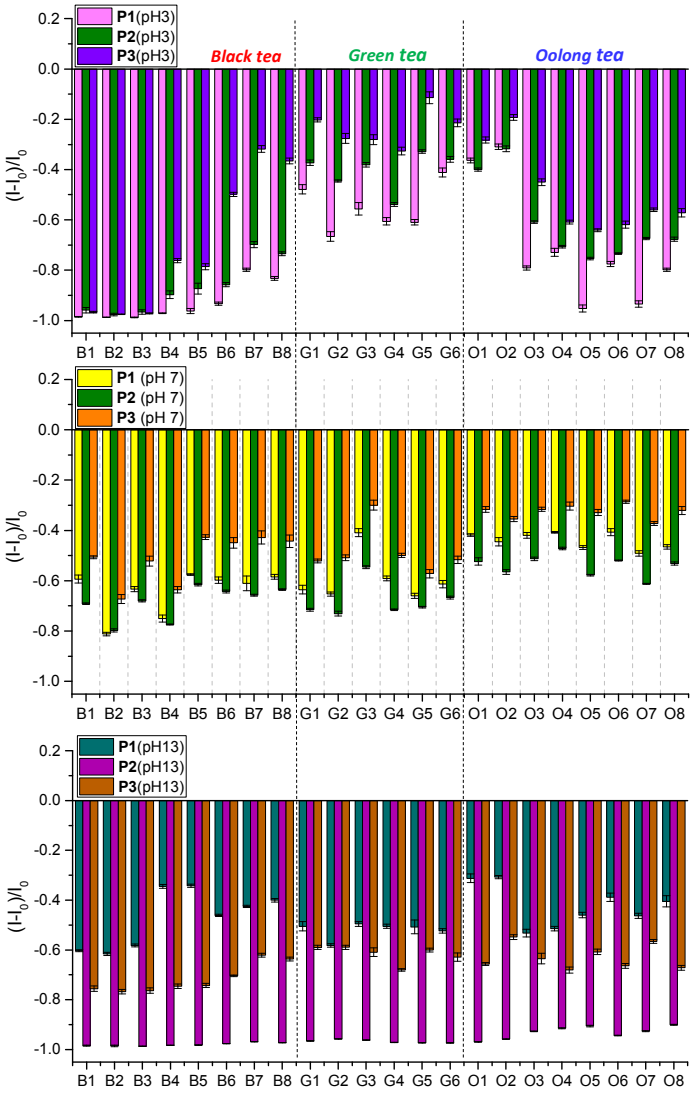


Figure S12. Fluorescence response patterns ($(I - I_0)/I_0$) obtained by PPE tongue (1.2 μM, at pH 3, 7 and 13, buffered) treated with 22 kinds of teas (0.1 mg/mL at pH 3 and 13, 0.01 mg/mL at pH 7, respectively). Each value is the average of six independent measurements; each error bar shows the standard deviation (SD) of these measurements.

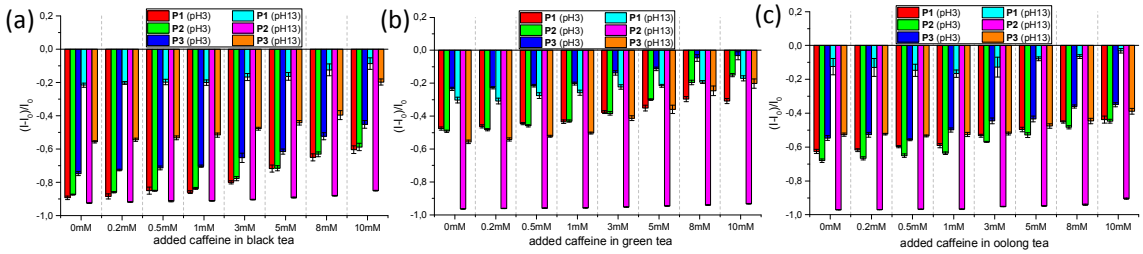


Figure S13. Fluorescence response patterns ($(I - I_0)/I_0$) obtained by PPE tongue (1.2 μM, at pH 3 and 13, buffered) treated with different concentrations of caffeine (0-10 mM) in (a) black tea, (b) green tea, (c) oolong tea infusions.

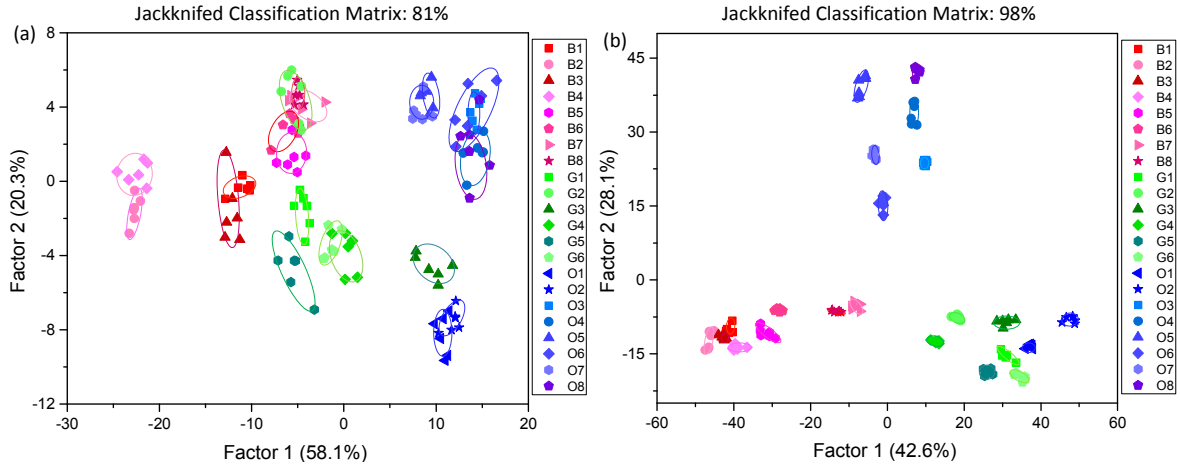


Figure S14. 2D canonical score plot obtained by an array of (a) three elements (**P3**/CB[8] (pH 7), **P1**/CB[8] (pH 13), and **P2**/CB[8] (pH 13)) and (b) six elements (**P3**/CB[8] (pH 7), **P1**/CB[8] (pH 13), **P2**/CB[8] (pH 13), and **P1** (pH 3), **P2** (pH 3), **P2** (pH 13)).

Screening process for the minimal elements: first, the data of 18 sensing elements for 22 teas were calculated with PCA, **P3**/CB[8] (pH 7), **P1**/CB[8] (pH 13), and **P2**/CB[8] (pH 13) contributed most. The LDA-plot with the selected three elements show oolong teas O3-O8 group together (Fig S14a). Then, the left 15 elements with the 6 oolong teas lying close together were calculated with PCA again and we found that the sensing elements of **P1** (pH 3), **P2** (pH 3) and **P2** (pH 13) show best discrimination power to the 6 oolong teas. However, the black teas are still very close to each other (Fig S14b). The left 12 elements with 8 black teas lying close together were calculated with PCA again and **P3** (pH 3) show best discrimination power. Thus, seven elements (**P1** (pH 3), **P2** (pH 3), **P2** (pH 13), **P3**/CB[8] (pH 7), **P1**/CB[8] (pH 13), **P2**/CB[8] (pH 13) and **P3** (pH 3)) were selected. Finally, good discrimination results with minimal elements were observed in LDA (see Figure 7 in the manuscript).

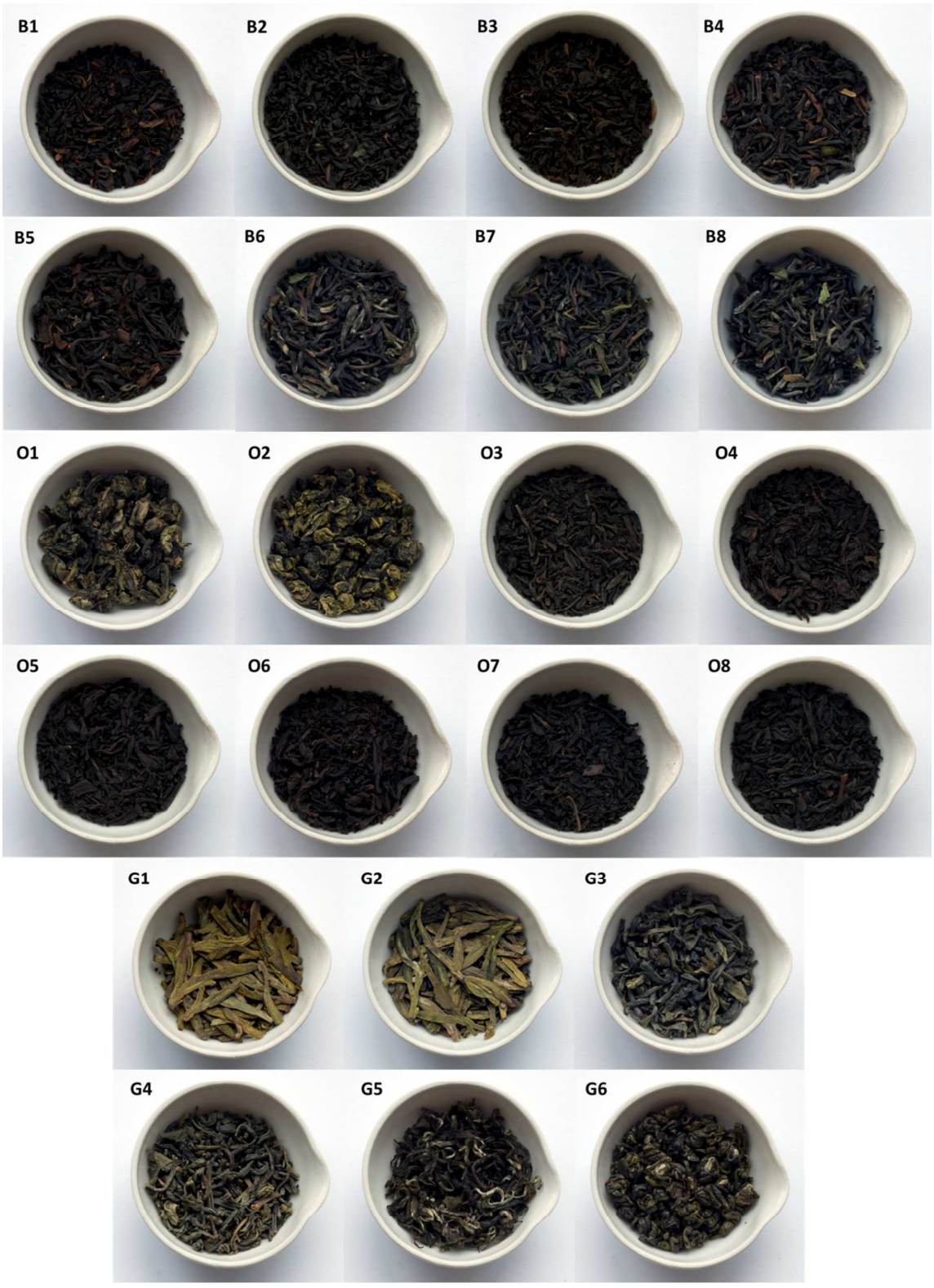


Figure S15. The appearance of the investigated teas (black teas B1-B8, green teas G1-G6 and oolong teas O1-O8).

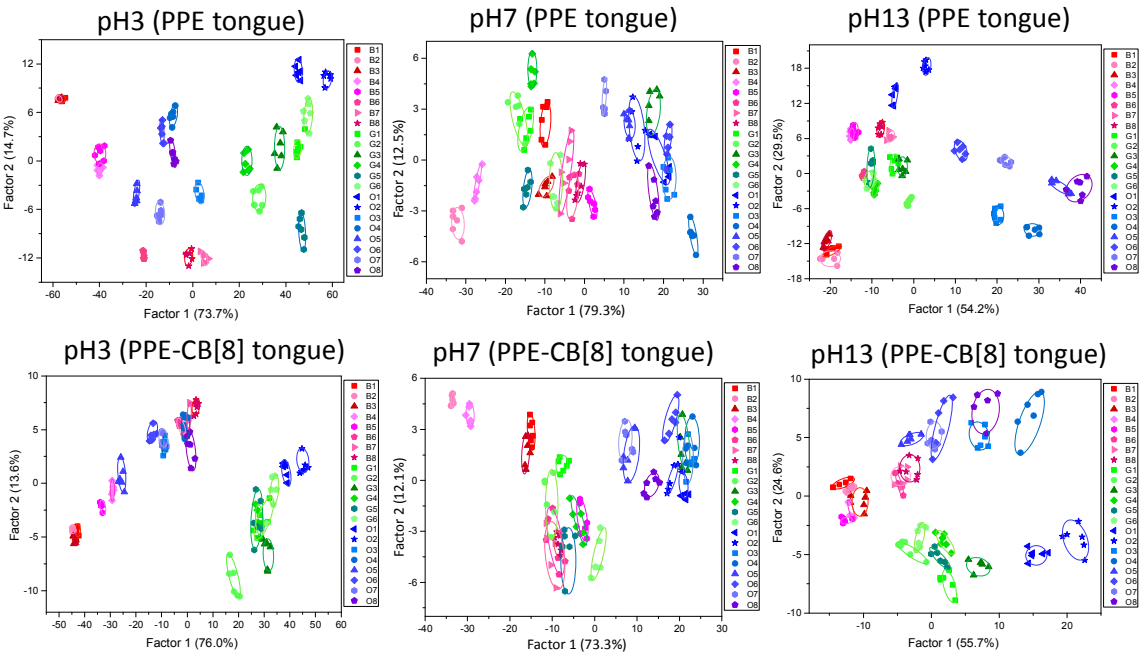


Figure S16. 2D canonical score plot obtained by PPE tongue or PPE-CB[8] tongue at different pH values (pH 3, 7 and 13) treated with 22 kinds of teas with 95% confidence ellipses. Each point represents the response pattern for a single analyte to the array.

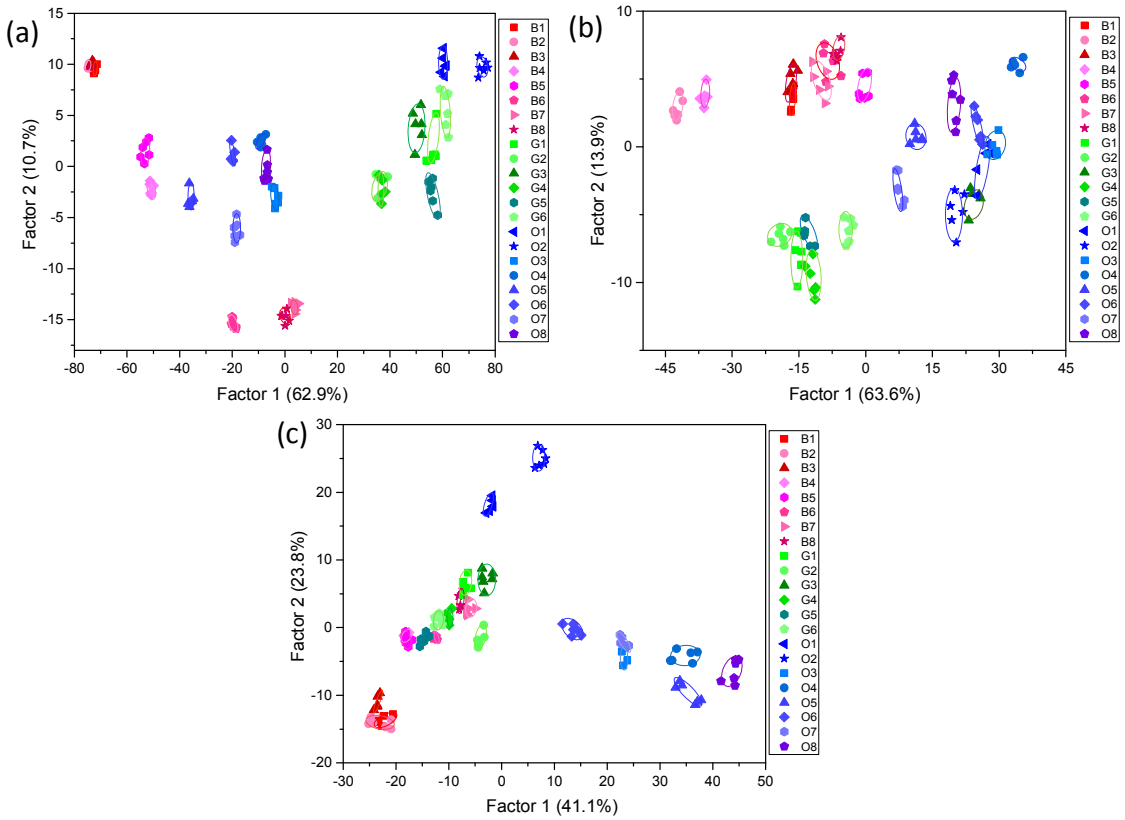


Figure S17. 2D canonical score plot obtained by combined tongue of the PPE/CB[8] tongue and the PPE-only-tongue at (a) pH 3, (b) pH 7 and (c) pH 13 buffer solution treated with 22 kinds of teas with 95% confidence ellipses. Each point represents the response pattern for a single analyte to the array.

6. Linear Discriminant Analysis

Table S1. Training matrix of fluorescence response pattern from an array of **P1**/CB[8], **P2**/CB[8] and **P3**/CB[8] (each at pH 3 and 13, buffered) against 12 analytes. LDA was carried out and resulting in 6 factors of the canonical scores (the first three scores were shown here) and group generation.

Analytes	Fluorescence Response Pattern						Results LDA (the first three scores)			
	P1/CB[8] (pH3)	**P2**/CB[8] (pH3)	**P3**/CB[8] (pH3)	**P1**/CB[8] (pH13)	**P2**/CB[8] (pH13)	**P3**/CB[8] (pH13)	Factor 1	Factor 2	Factor 3	Group
Asp	-0.10	-0.04	0.05	0.12	0.08	0.10	-3.65	-15.79	-2.64	3
Asp	-0.10	-0.04	0.05	0.10	0.08	0.08	-4.13	-15.92	-3.41	3
Asp	-0.09	-0.04	0.05	0.10	0.08	0.07	-3.91	-15.79	-3.78	3
Asp	-0.10	-0.05	0.04	0.12	0.07	0.07	-4.37	-16.87	-3.27	3
Asp	-0.06	-0.04	0.07	0.10	0.08	0.10	-3.69	-14.37	-1.84	3
Asp	-0.06	-0.05	0.05	0.16	0.09	0.08	-3.50	-15.70	-2.55	3
Glu	0.03	0.10	0.10	0.30	0.22	0.21	4.98	-3.05	-1.42	7
Glu	0.01	0.12	0.09	0.28	0.22	0.21	5.06	-2.53	-2.41	7
Glu	0.01	0.10	0.08	0.24	0.22	0.21	4.87	-3.92	-1.46	7
Glu	0.00	0.08	0.07	0.28	0.20	0.17	3.48	-5.72	-2.77	7
Glu	-0.03	0.10	0.09	0.23	0.21	0.17	3.68	-4.45	-4.45	7
Glu	-0.01	0.08	0.10	0.30	0.22	0.21	4.79	-5.04	-1.68	7
Phe	0.07	0.12	0.07	0.39	0.13	0.27	2.34	-1.49	2.42	8
Phe	0.06	0.08	0.07	0.37	0.19	0.25	4.88	-3.75	2.44	8
Phe	0.07	0.10	0.09	0.36	0.18	0.24	4.10	-2.22	1.26	8
Phe	0.05	0.09	0.07	0.31	0.18	0.24	4.23	-3.46	1.40	8
Phe	0.06	0.10	0.08	0.33	0.16	0.23	3.26	-2.71	0.86	8
Phe	0.05	0.12	0.09	0.35	0.12	0.25	1.31	-1.93	1.54	8
Asn	0.02	0.09	0.13	0.26	0.13	0.09	-1.30	-4.19	-6.19	2
Asn	0.02	0.08	0.13	0.31	0.10	0.08	-2.69	-4.77	-6.13	2
Asn	0.01	0.10	0.13	0.28	0.12	0.06	-2.13	-3.71	-7.93	2
Asn	0.02	0.10	0.12	0.29	0.11	0.07	-2.25	-3.65	-7.49	2
Asn	-0.01	0.10	0.11	0.26	0.07	0.08	-4.24	-4.48	-6.68	2
Asn	0.01	0.10	0.13	0.24	0.09	0.07	-3.51	-3.52	-7.03	2
Gln	0.09	0.12	0.17	0.34	0.25	0.21	6.26	0.71	-1.57	6
Gln	0.10	0.11	0.18	0.40	0.22	0.18	4.65	0.20	-2.08	6
Gln	0.08	0.12	0.15	0.34	0.24	0.16	5.23	0.04	-3.74	6
Gln	0.07	0.12	0.16	0.38	0.26	0.20	6.63	0.52	-3.05	6
Gln	0.07	0.11	0.14	0.30	0.24	0.21	6.15	-0.36	-1.06	6
Gln	0.09	0.10	0.15	0.32	0.29	0.21	8.05	-0.46	-1.41	6
Arg	0.08	0.14	0.15	0.37	0.03	0.05	-6.24	0.24	-7.77	1
Arg	0.11	0.14	0.17	0.40	0.04	0.04	-5.64	1.08	-7.54	1
Arg	0.11	0.11	0.14	0.37	0.07	0.05	-4.39	-1.05	-6.46	1
Arg	0.07	0.10	0.14	0.31	0.07	0.07	-4.05	-2.42	-5.93	1
Arg	0.10	0.12	0.15	0.39	0.06	0.04	-4.80	-0.53	-7.35	1
Arg	0.11	0.11	0.14	0.29	0.00	0.06	-7.26	-1.27	-5.15	1
Ser	0.07	0.02	0.14	0.27	0.34	0.22	10.71	-5.64	1.31	9
Ser	0.06	0.00	0.14	0.27	0.33	0.19	9.51	-7.26	0.83	9
Ser	0.06	0.02	0.12	0.19	0.32	0.20	9.56	-6.59	1.18	9
Ser	0.06	0.00	0.11	0.20	0.33	0.20	9.91	-7.81	1.52	9
Ser	0.05	0.01	0.12	0.19	0.37	0.20	11.51	-7.12	0.63	9
Ser	0.05	0.00	0.13	0.25	0.35	0.24	11.21	-7.08	2.52	9
GABA	0.16	0.06	0.18	0.32	0.32	0.30	11.49	-0.45	5.80	5

GABA	0.18	0.04	0.17	0.32	0.33	0.31	11.92	-1.58	7.38	5
GABA	0.16	0.03	0.22	0.28	0.33	0.27	10.75	-1.53	5.08	5
GABA	0.17	0.05	0.17	0.27	0.27	0.26	8.19	-1.47	5.24	5
GABA	0.16	0.04	0.14	0.29	0.31	0.28	10.49	-2.59	6.03	5
GABA	0.16	0.03	0.18	0.30	0.28	0.30	9.40	-2.54	7.63	5
Thea	0.19	0.05	0.21	0.30	0.39	0.38	15.55	0.74	9.77	11
Thea	0.19	0.04	0.22	0.29	0.32	0.41	13.20	0.18	12.59	11
Thea	0.18	0.05	0.20	0.32	0.37	0.40	15.06	0.22	10.90	11
Thea	0.20	0.03	0.22	0.30	0.36	0.35	14.02	-0.31	9.65	11
Thea	0.15	0.02	0.18	0.32	0.32	0.40	12.89	-2.49	11.70	11
Thea	0.12	0.05	0.14	0.29	0.39	0.36	15.58	-2.35	8.00	11
Caff	0.21	0.32	0.33	0.43	0.69	0.37	28.65	21.12	-4.35	4
Caff	0.23	0.35	0.34	0.43	0.67	0.39	28.22	23.48	-3.61	4
Caff	0.26	0.34	0.31	0.39	0.68	0.37	28.55	22.92	-3.67	4
Caff	0.27	0.35	0.32	0.38	0.68	0.38	28.73	24.31	-3.15	4
Caff	0.24	0.33	0.33	0.36	0.72	0.38	30.29	22.45	-3.71	4
Caff	0.21	0.32	0.29	0.39	0.72	0.36	30.04	20.66	-4.89	4
Tbro	0.21	0.07	0.28	0.23	-0.29	0.13	-19.94	0.25	5.02	10
Tbro	0.22	0.10	0.27	0.23	-0.28	0.11	-20.03	2.33	3.22	10
Tbro	0.16	0.09	0.29	0.20	-0.27	0.13	-19.60	0.88	2.64	10
Tbro	0.20	0.10	0.32	0.23	-0.29	0.13	-20.10	2.49	3.71	10
Tbro	0.21	0.08	0.29	0.21	-0.29	0.10	-20.91	0.76	3.09	10
Tbro	0.20	0.09	0.28	0.24	-0.29	0.08	-21.11	0.98	1.57	10
Tphy	0.26	0.29	0.35	0.41	-0.84	0.07	-46.12	13.52	0.86	12
Tphy	0.24	0.29	0.35	0.41	-0.83	0.09	-45.33	13.49	1.18	12
Tphy	0.29	0.26	0.38	0.36	-0.84	0.08	-45.93	13.05	2.87	12
Tphy	0.31	0.23	0.40	0.40	-0.85	0.06	-47.02	11.93	3.41	12
Tphy	0.29	0.26	0.35	0.38	-0.82	0.08	-45.07	12.81	2.82	12
Tphy	0.24	0.26	0.32	0.38	-0.85	0.07	-46.43	10.60	1.57	12

Table S2. LDA jackknifed classification matrix table obtained from an array of **P1**/CB[8], **P2**/CB[8] and **P3**/CB[8] (each at pH 3 and 13, buffered) against 12 analytes. The jackknifed classification matrix with cross-validation reveals a 99% accuracy.

	Arg	Asn	Asp	Caff	GABA	Gln	Glu	Phe	Ser	Tbro	Thea	Tphy	%correct
Arg	5	1	0	0	0	0	0	0	0	0	0	0	83
Asn	0	6	0	0	0	0	0	0	0	0	0	0	100
Asp	0	0	6	0	0	0	0	0	0	0	0	0	100
Caff	0	0	0	6	0	0	0	0	0	0	0	0	100
GABA	0	0	0	0	6	0	0	0	0	0	0	0	100
Gln	0	0	0	0	0	6	0	0	0	0	0	0	100
Glu	0	0	0	0	0	0	6	0	0	0	0	0	100
Phe	0	0	0	0	0	0	0	6	0	0	0	0	100
Ser	0	0	0	0	0	0	0	0	6	0	0	0	100
Tbro	0	0	0	0	0	0	0	0	0	6	0	0	100
Thea	0	0	0	0	0	0	0	0	0	0	6	0	100
Tphy	0	0	0	0	0	0	0	0	0	0	0	6	100
Total	5	7	6	6	6	6	6	6	6	6	6	6	**99**

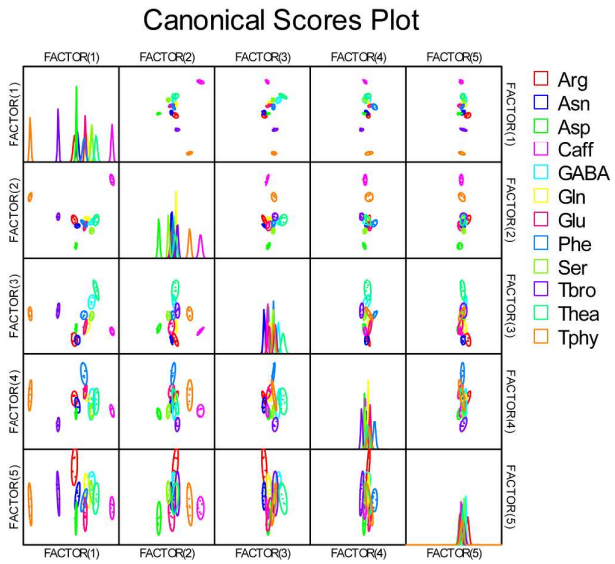


Figure S18. Correlations of canonical fluorescence response patterns from an array of **P1**/CB[8], **P2**/CB[8] and **P3**/CB[8] (each at pH 3 and 13, buffered) against 12 analytes. The 95% confidence ellipses for the individual analytes are shown.

Table S3. Detection and identification of unknown samples using LDA from an array of **P1**/CB[8], **P2**/CB[8] and **P3**/CB[8] (each at pH 3 and 13, buffered). According to the verification, 46 among 48 unknown sample were correctly identified, representing an accuracy of 95.8%.

Unknown samples	Fluorescence Response Pattern						Results LDA (the first three scores)					
	P1/ CB[8] (pH3)	**P2**/ CB[8] (pH3)	**P3**/ CB[8] (pH3)	**P1**/ CB[8] (pH13)	**P2**/ CB[8] (pH13)	**P3**/ CB[8] (pH13)	Factor 1	Factor 2	Factor 3	Group	Identification	Verification
1	-0.01	0.09	0.08	0.19	0.21	0.19	4.18	-4.90	-2.35	7	Glu	Glu
2	-0.07	-0.03	0.07	0.12	0.10	0.09	-3.05	-13.99	-3.04	3	Asp	Asp
3	0.05	0.10	0.09	0.27	0.12	0.22	0.70	-3.27	0.95	8	Phe	Phe
4	0.01	0.08	0.12	0.22	0.08	0.07	-4.11	-4.92	-6.37	2	Asn	Asn
5	0.05	0.04	0.13	0.21	0.37	0.24	12.10	-4.82	1.08	9	Ser	Ser
6	-0.07	-0.03	0.05	0.12	0.09	0.07	-3.40	-14.68	-3.44	3	Asp	Asp
7	-0.03	0.09	0.08	0.17	0.20	0.21	3.68	-5.29	-1.38	7	Glu	Glu
8	0.06	0.10	0.08	0.28	0.12	0.25	1.29	-2.92	2.55	8	Phe	Phe
9	0.03	0.07	0.11	0.24	0.12	0.07	-1.95	-5.34	-6.14	2	Asn	Asn
10	0.10	0.09	0.11	0.33	0.03	0.06	-5.66	-3.04	-4.77	1	Arg	Arg
11	0.24	0.36	0.33	0.44	0.73	0.36	30.62	24.58	-6.23	4	Caff	Caff
12	0.15	0.03	0.14	0.29	0.33	0.27	11.41	-3.54	5.65	5	GABA	GABA
13	0.06	0.02	0.11	0.21	0.34	0.22	10.82	-6.65	1.66	9	Ser	Ser
14	0.24	0.32	0.34	0.38	0.69	0.37	28.70	21.82	-3.28	4	Caff	Caff
15	0.19	0.08	0.31	0.20	-0.29	0.13	-20.41	1.26	4.16	10	Tbro	Tbro
16	0.12	0.04	0.14	0.31	0.36	0.41	15.17	-2.76	10.37	11	Thea	Thea
17	0.17	0.10	0.31	0.22	-0.31	0.14	-20.87	1.63	3.78	10	Tbro	Tbro
18	0.07	0.12	0.10	0.29	0.03	0.05	-6.15	-2.25	-6.57	1	Arg	Arg
19	0.16	0.06	0.14	0.30	0.30	0.29	10.34	-1.07	5.80	5	GABA	GABA
20	0.22	0.33	0.37	0.37	0.73	0.40	30.85	23.02	-3.50	4	Caff	Caff
21	0.05	0.11	0.14	0.26	0.26	0.21	6.58	-1.01	-1.68	6	Gln	Gln
22	0.06	0.09	0.13	0.28	0.22	0.22	5.35	-2.07	0.30	7	Glu	Gln
23	0.10	0.14	0.12	0.32	0.06	0.05	-4.71	0.09	-7.05	1	Arg	Arg
24	0.19	0.25	0.28	0.31	-0.84	0.04	-46.62	8.09	0.06	12	Tphy	Tphy
25	0.12	0.05	0.14	0.30	0.33	0.39	13.17	-2.44	10.13	11	Thea	Thea

26	0.09	0.13	0.11	0.31	0.02	0.07	-6.27	-1.05	-5.77	1	Arg	Arg
27	0.22	0.07	0.30	0.22	-0.30	0.13	-20.52	0.75	5.09	10	Tbro	Tbro
28	0.23	0.26	0.28	0.32	-0.83	0.08	-45.22	9.66	2.27	12	Tphy	Tphy
29	0.03	0.10	0.08	0.24	0.14	0.23	1.65	-3.93	0.90	8	Phe	Phe
30	0.02	0.07	0.15	0.23	0.10	0.05	-3.28	-4.86	-6.91	2	Asn	Asn
31	0.12	0.02	0.14	0.28	0.35	0.40	14.16	-3.84	11.24	11	Thea	Thea
32	0.11	0.04	0.15	0.29	0.38	0.40	15.75	-2.71	9.71	11	Thea	Thea
33	0.00	0.07	0.11	0.21	0.07	0.08	-4.40	-5.98	-5.22	2	Asn	Asn
34	0.04	0.11	0.14	0.25	0.23	0.18	4.86	-1.57	-3.03	7	Glu	Gln
35	0.06	0.09	0.13	0.28	0.24	0.18	5.47	-2.46	-1.90	6	Gln	Gln
36	0.16	0.08	0.28	0.18	-0.30	0.11	-21.31	-0.25	2.88	10	Tbro	Tbro
37	0.23	0.23	0.30	0.34	-0.83	0.07	-45.67	8.32	2.82	12	Tphy	Tphy
38	0.22	0.24	0.27	0.34	-0.84	0.04	-46.23	8.15	0.67	12	Tphy	Tphy
39	-0.10	-0.03	0.05	0.08	0.07	0.07	-4.45	-15.71	-3.60	3	Asp	Asp
40	0.00	0.13	0.12	0.20	0.21	0.18	4.02	-1.57	-4.02	7	Glu	Glu
41	0.05	0.01	0.11	0.21	0.34	0.24	11.01	-6.80	2.58	9	Ser	Ser
42	0.16	0.03	0.18	0.28	0.28	0.30	9.42	-2.23	7.39	5	GABA	GABA
43	0.21	0.33	0.32	0.41	0.67	0.40	28.22	21.45	-2.98	4	Caff	Caff
44	0.05	0.00	0.12	0.22	0.36	0.23	11.71	-7.17	2.11	9	Ser	Ser
45	0.16	0.03	0.18	0.27	0.35	0.31	12.74	-2.30	7.47	5	GABA	GABA
46	0.06	0.10	0.08	0.28	0.15	0.20	1.81	-3.01	0.03	8	Phe	Phe
47	0.00	0.07	0.10	0.20	0.21	0.17	3.66	-5.34	-2.47	7	Glu	Glu
48	-0.07	-0.05	0.07	0.12	0.10	0.10	-2.68	-15.20	-1.58	3	Asp	Asp

Table S4. Training matrix of fluorescence response pattern from an array of **P1**/CB[8], **P2**/CB[8] and **P3**/CB[8] (each at pH 3, 7 and 13, buffered) against 22 teas. LDA was carried out and resulting in 9 factors of the canonical scores (the first three scores were shown here) and group generation. The jackknifed classification matrix with cross-validation reveals a 100% accuracy.

Analytes	Fluorescence Response Pattern									Results LDA(the first three scores)			
	P1/CB[8](pH3)	**P2**/CB[8](pH3)	**P3**/CB[8](pH3)	**P1**/CB[8](pH7)	**P2**/CB[8](pH7)	**P3**/CB[8](pH7)	**P1**/CB[8](pH13)	**P2**/CB[8](pH13)	**P3**/CB[8](pH13)	Factor 1	Factor 2	Factor 3	Group
B1	-0.98	-0.95	-0.89	-0.73	-0.64	-0.43	-0.44	-0.97	-0.78	-47.36	-0.06	3.41	1
B1	-0.98	-0.93	-0.90	-0.73	-0.64	-0.45	-0.45	-0.97	-0.78	-46.63	-0.35	3.40	1
B1	-0.99	-0.95	-0.90	-0.73	-0.63	-0.46	-0.44	-0.97	-0.80	-47.89	0.22	2.30	1
B1	-0.99	-0.95	-0.90	-0.74	-0.63	-0.45	-0.45	-0.97	-0.79	-47.36	-0.13	2.06	1
B1	-0.99	-0.95	-0.91	-0.73	-0.63	-0.43	-0.45	-0.97	-0.79	-47.64	-0.64	3.44	1
B1	-0.99	-0.95	-0.90	-0.74	-0.63	-0.42	-0.45	-0.97	-0.78	-47.55	-0.53	3.09	1
B2	-0.99	-0.96	-0.92	-0.93	-0.77	-0.62	-0.44	-0.97	-0.78	-54.76	19.57	1.75	2
B2	-0.98	-0.97	-0.92	-0.93	-0.77	-0.62	-0.44	-0.97	-0.78	-55.29	19.57	1.82	2
B2	-0.99	-0.96	-0.93	-0.93	-0.77	-0.61	-0.45	-0.97	-0.78	-54.87	19.10	1.40	2
B2	-0.99	-0.97	-0.92	-0.93	-0.76	-0.63	-0.42	-0.97	-0.78	-55.31	19.70	2.37	2
B2	-0.99	-0.96	-0.93	-0.94	-0.77	-0.63	-0.44	-0.97	-0.78	-55.09	19.62	2.29	2
B2	-0.99	-0.96	-0.92	-0.94	-0.77	-0.63	-0.45	-0.97	-0.77	-54.86	19.25	2.25	2
B3	-0.99	-0.94	-0.92	-0.75	-0.63	-0.43	-0.43	-0.98	-0.75	-48.16	0.71	3.81	3
B3	-0.98	-0.95	-0.93	-0.75	-0.63	-0.45	-0.44	-0.98	-0.75	-48.23	0.81	2.76	3
B3	-0.99	-0.94	-0.93	-0.76	-0.63	-0.46	-0.42	-0.97	-0.76	-48.20	1.37	2.63	3
B3	-0.99	-0.96	-0.93	-0.75	-0.63	-0.46	-0.41	-0.98	-0.78	-49.07	1.16	2.14	3
B3	-0.99	-0.95	-0.94	-0.77	-0.63	-0.45	-0.40	-0.97	-0.76	-48.51	1.30	2.06	3
B3	-0.99	-0.96	-0.93	-0.77	-0.63	-0.45	-0.48	-0.98	-0.77	-49.07	0.71	2.25	3
B4	-0.94	-0.82	-0.67	-0.90	-0.73	-0.58	-0.47	-0.98	-0.76	-39.00	22.11	1.02	4
B4	-0.95	-0.82	-0.68	-0.89	-0.73	-0.61	-0.47	-0.98	-0.76	-39.82	22.18	1.80	4
B4	-0.94	-0.82	-0.68	-0.90	-0.73	-0.63	-0.48	-0.98	-0.76	-39.43	22.42	2.59	4

B4	-0.95	-0.82	-0.69	-0.90	-0.73	-0.59	-0.48	-0.98	-0.76	-39.55	21.78	1.07	4
B4	-0.95	-0.83	-0.66	-0.90	-0.73	-0.59	-0.48	-0.98	-0.77	-39.29	21.36	2.28	4
B4	-0.95	-0.82	-0.66	-0.91	-0.74	-0.59	-0.49	-0.98	-0.77	-39.22	22.50	1.82	4
B5	-0.96	-0.86	-0.74	-0.65	-0.51	-0.30	-0.48	-0.98	-0.77	-34.23	-9.01	4.79	5
B5	-0.96	-0.85	-0.74	-0.64	-0.53	-0.33	-0.48	-0.98	-0.77	-34.83	-7.23	4.87	5
B5	-0.96	-0.85	-0.75	-0.64	-0.51	-0.32	-0.48	-0.98	-0.76	-33.71	-9.13	4.79	5
B5	-0.97	-0.86	-0.74	-0.65	-0.50	-0.34	-0.48	-0.98	-0.77	-34.97	-8.24	3.27	5
B5	-0.96	-0.86	-0.75	-0.64	-0.53	-0.31	-0.47	-0.98	-0.77	-35.45	-7.33	5.63	5
B5	-0.96	-0.86	-0.74	-0.66	-0.52	-0.32	-0.50	-0.98	-0.76	-34.92	-7.81	4.39	5
B6	-0.69	-0.64	-0.38	-0.72	-0.53	-0.36	-0.48	-0.97	-0.71	-3.07	7.76	8.00	6
B6	-0.69	-0.66	-0.39	-0.73	-0.55	-0.36	-0.48	-0.97	-0.70	-5.11	9.21	7.93	6
B6	-0.69	-0.66	-0.40	-0.75	-0.54	-0.38	-0.49	-0.97	-0.71	-4.78	8.66	9.26	6
B6	-0.70	-0.66	-0.39	-0.72	-0.57	-0.37	-0.49	-0.97	-0.71	-6.54	9.28	6.82	6
B6	-0.68	-0.66	-0.40	-0.74	-0.57	-0.41	-0.47	-0.97	-0.71	-6.08	11.69	9.32	6
B6	-0.68	-0.63	-0.40	-0.76	-0.57	-0.40	-0.48	-0.97	-0.72	-4.25	12.11	8.38	6
B7	-0.65	-0.64	-0.34	-0.71	-0.55	-0.35	-0.48	-0.97	-0.71	-1.16	9.25	8.86	7
B7	-0.66	-0.63	-0.33	-0.75	-0.55	-0.32	-0.50	-0.97	-0.71	-1.15	10.59	8.35	7
B7	-0.68	-0.63	-0.36	-0.74	-0.55	-0.39	-0.50	-0.97	-0.70	-2.04	10.05	8.79	7
B7	-0.66	-0.63	-0.36	-0.76	-0.56	-0.36	-0.50	-0.97	-0.72	-2.08	12.00	8.39	7
B7	-0.66	-0.64	-0.37	-0.75	-0.57	-0.38	-0.50	-0.96	-0.71	-2.41	11.64	9.48	7
B7	-0.68	-0.63	-0.38	-0.75	-0.58	-0.40	-0.50	-0.96	-0.72	-2.91	11.80	8.39	7
B8	-0.63	-0.61	-0.31	-0.72	-0.54	-0.37	-0.49	-0.97	-0.69	2.72	10.38	10.66	8
B8	-0.63	-0.62	-0.32	-0.72	-0.54	-0.39	-0.49	-0.96	-0.69	1.88	10.18	11.50	8
B8	-0.65	-0.61	-0.31	-0.73	-0.54	-0.38	-0.50	-0.97	-0.72	2.00	10.51	10.61	8
B8	-0.64	-0.62	-0.32	-0.73	-0.55	-0.38	-0.50	-0.96	-0.71	1.39	10.56	10.58	8
B8	-0.63	-0.61	-0.34	-0.73	-0.55	-0.40	-0.50	-0.96	-0.70	2.13	10.09	11.11	8
B8	-0.66	-0.61	-0.34	-0.74	-0.55	-0.40	-0.51	-0.96	-0.71	1.07	10.27	10.46	8
G1	-0.52	-0.27	-0.16	-0.64	-0.58	-0.27	-0.45	-0.98	-0.60	25.49	21.88	6.69	9
G1	-0.55	-0.26	-0.19	-0.65	-0.58	-0.28	-0.43	-0.98	-0.61	25.09	21.78	-7.96	9
G1	-0.58	-0.27	-0.20	-0.67	-0.58	-0.31	-0.45	-0.98	-0.63	22.23	22.46	7.46	9
G1	-0.60	-0.30	-0.24	-0.66	-0.58	-0.29	-0.45	-0.98	-0.62	19.60	19.99	8.71	9
G1	-0.57	-0.29	-0.20	-0.66	-0.59	-0.30	-0.46	-0.98	-0.62	21.35	21.89	7.72	9
G1	-0.56	-0.29	-0.26	-0.67	-0.59	-0.30	-0.41	-0.98	-0.62	20.89	22.03	7.38	9
G2	-0.66	-0.34	-0.37	-0.71	-0.58	-0.31	-0.51	-0.98	-0.64	12.10	17.80	10.37	10
G2	-0.68	-0.35	-0.38	-0.73	-0.58	-0.30	-0.50	-0.98	-0.67	10.33	18.20	10.36	10
G2	-0.64	-0.38	-0.38	-0.69	-0.60	-0.30	-0.54	-0.98	-0.68	10.28	16.90	9.75	10
G2	-0.68	-0.30	-0.37	-0.73	-0.60	-0.33	-0.55	-0.98	-0.68	12.86	19.51	12.69	10
G2	-0.67	-0.29	-0.36	-0.72	-0.61	-0.34	-0.53	-0.98	-0.68	13.48	20.37	12.42	10
G2	-0.67	-0.32	-0.39	-0.72	-0.61	-0.33	-0.55	-0.98	-0.67	11.47	18.96	12.47	10
G3	-0.47	-0.28	-0.29	-0.33	-0.36	-0.09	-0.36	-0.98	-0.59	34.97	-8.82	9.15	11
G3	-0.51	-0.25	-0.29	-0.33	-0.37	-0.08	-0.37	-0.98	-0.60	34.55	-8.31	13.83	11
G3	-0.48	-0.26	-0.32	-0.34	-0.38	-0.07	-0.37	-0.98	-0.59	34.84	-8.14	12.87	11
G3	-0.53	-0.28	-0.26	-0.33	-0.38	-0.11	-0.37	-0.98	-0.58	32.94	-8.27	11.12	11
G3	-0.47	-0.26	-0.28	-0.31	-0.38	-0.13	-0.39	-0.98	-0.59	35.78	-7.54	9.90	11
G3	-0.51	-0.28	-0.27	-0.34	-0.37	-0.13	-0.38	-0.98	-0.61	33.64	-7.69	9.66	11
G4	-0.54	-0.30	-0.25	-0.64	-0.53	-0.25	-0.37	-0.98	-0.64	24.15	16.52	4.75	12
G4	-0.53	-0.29	-0.27	-0.65	-0.53	-0.23	-0.37	-0.98	-0.65	24.73	16.46	5.27	12
G4	-0.55	-0.32	-0.22	-0.64	-0.54	-0.25	-0.40	-0.98	-0.65	22.85	16.06	4.31	12
G4	-0.50	-0.29	-0.25	-0.66	-0.56	-0.25	-0.40	-0.97	-0.65	25.48	18.93	4.36	12
G4	-0.54	-0.31	-0.25	-0.66	-0.57	-0.26	-0.40	-0.97	-0.65	23.03	18.36	5.02	12
G4	-0.55	-0.31	-0.22	-0.66	-0.54	-0.28	-0.40	-0.97	-0.66	23.68	17.47	2.75	12
G5	-0.39	-0.36	-0.31	-0.70	-0.55	-0.32	-0.40	-0.98	-0.63	23.65	23.05	3.92	13

G5	-0.40	-0.39	-0.32	-0.69	-0.54	-0.29	-0.35	-0.98	-0.64	22.23	21.65	4.33	13
G5	-0.46	-0.36	-0.34	-0.68	-0.52	-0.33	-0.38	-0.98	-0.64	21.88	19.54	1.77	13
G5	-0.42	-0.33	-0.33	-0.73	-0.53	-0.33	-0.39	-0.98	-0.66	24.44	23.25	3.07	13
G5	-0.47	-0.33	-0.37	-0.72	-0.54	-0.36	-0.39	-0.98	-0.65	21.44	22.24	0.79	13
G5	-0.46	-0.33	-0.32	-0.70	-0.55	-0.34	-0.41	-0.98	-0.65	22.74	21.65	1.19	13
G6	-0.45	-0.27	-0.16	-0.60	-0.49	-0.27	-0.40	-0.98	-0.68	31.81	16.80	0.15	14
G6	-0.46	-0.30	-0.16	-0.61	-0.48	-0.28	-0.39	-0.98	-0.67	30.49	16.29	1.63	14
G6	-0.45	-0.29	-0.15	-0.62	-0.48	-0.26	-0.40	-0.98	-0.68	31.89	16.45	2.29	14
G6	-0.47	-0.29	-0.18	-0.63	-0.49	-0.26	-0.41	-0.98	-0.68	30.40	15.90	1.08	14
G6	-0.45	-0.28	-0.20	-0.64	-0.48	-0.28	-0.39	-0.97	-0.68	31.48	16.58	1.82	14
G6	-0.46	-0.30	-0.27	-0.66	-0.49	-0.29	-0.41	-0.97	-0.68	28.75	16.25	1.27	14
O1	-0.34	-0.28	-0.17	-0.35	-0.34	-0.12	-0.28	-0.97	-0.56	44.51	-5.42	1.50	15
O1	-0.33	-0.29	-0.17	-0.35	-0.36	-0.12	-0.28	-0.97	-0.55	43.35	-4.00	1.53	15
O1	-0.35	-0.30	-0.16	-0.35	-0.35	-0.11	-0.32	-0.97	-0.54	42.78	-5.84	1.32	15
O1	-0.35	-0.30	-0.17	-0.36	-0.36	-0.12	-0.32	-0.97	-0.54	42.30	-4.22	1.54	15
O1	-0.32	-0.30	-0.18	-0.37	-0.36	-0.13	-0.30	-0.97	-0.53	43.24	-4.37	3.52	15
O1	-0.34	-0.27	-0.18	-0.36	-0.35	-0.12	-0.31	-0.97	-0.53	44.61	-5.41	1.15	15
O2	-0.27	-0.21	-0.10	-0.36	-0.37	-0.14	-0.29	-0.97	-0.49	52.57	-1.43	3.27	16
O2	-0.27	-0.23	-0.11	-0.37	-0.38	-0.13	-0.30	-0.97	-0.52	50.87	-0.94	2.98	16
O2	-0.28	-0.25	-0.09	-0.34	-0.38	-0.12	-0.29	-0.96	-0.51	50.03	-2.78	3.36	16
O2	-0.30	-0.24	-0.13	-0.40	-0.38	-0.15	-0.30	-0.97	-0.48	48.44	0.46	3.00	16
O2	-0.29	-0.24	-0.13	-0.40	-0.38	-0.15	-0.31	-0.96	-0.50	50.14	-1.10	4.33	16
O2	-0.29	-0.23	-0.11	-0.39	-0.38	-0.14	-0.30	-0.96	-0.49	50.71	-0.56	3.38	16
O3	-0.75	-0.69	-0.46	-0.32	-0.34	-0.13	-0.43	-0.96	-0.64	1.72	-31.29	0.03	17
O3	-0.76	-0.69	-0.47	-0.35	-0.35	-0.13	-0.45	-0.95	-0.63	1.33	-31.21	0.08	17
O3	-0.74	-0.68	-0.47	-0.31	-0.34	-0.14	-0.44	-0.95	-0.63	2.41	-32.17	0.19	17
O3	-0.74	-0.69	-0.48	-0.32	-0.34	-0.14	-0.45	-0.96	-0.64	1.69	-31.55	0.21	17
O3	-0.75	-0.69	-0.45	-0.32	-0.36	-0.15	-0.44	-0.95	-0.64	1.84	-31.93	0.54	17
O3	-0.75	-0.69	-0.49	-0.33	-0.35	-0.15	-0.45	-0.95	-0.66	1.22	-32.11	0.37	17
O4	-0.66	-0.65	-0.39	-0.30	-0.34	-0.19	-0.38	-0.94	-0.60	11.73	-31.03	7.60	18
O4	-0.65	-0.63	-0.37	-0.32	-0.33	-0.16	-0.38	-0.95	-0.59	11.35	-28.21	5.20	18
O4	-0.68	-0.64	-0.39	-0.31	-0.33	-0.19	-0.40	-0.95	-0.61	10.28	-29.92	6.07	18
O4	-0.66	-0.66	-0.39	-0.33	-0.35	-0.18	-0.40	-0.95	-0.59	9.80	-28.75	7.08	18
O4	-0.65	-0.65	-0.42	-0.34	-0.34	-0.18	-0.39	-0.94	-0.61	10.50	-28.96	7.05	18
O4	-0.68	-0.63	-0.41	-0.33	-0.34	-0.19	-0.40	-0.94	-0.60	11.24	-30.25	5.79	18
O5	-0.91	-0.78	-0.64	-0.45	-0.46	-0.20	-0.45	-0.96	-0.71	-19.34	-24.02	6.32	19
O5	-0.91	-0.81	-0.65	-0.45	-0.47	-0.19	-0.48	-0.96	-0.73	-21.67	-24.05	6.23	19
O5	-0.91	-0.80	-0.64	-0.48	-0.47	-0.19	-0.48	-0.96	-0.72	-20.95	-22.47	5.64	19
O5	-0.92	-0.81	-0.65	-0.49	-0.46	-0.18	-0.46	-0.96	-0.73	-21.99	-22.79	5.24	19
O5	-0.92	-0.80	-0.61	-0.50	-0.48	-0.18	-0.49	-0.96	-0.72	-20.62	-21.52	5.48	19
O5	-0.91	-0.82	-0.61	-0.49	-0.48	-0.20	-0.48	-0.96	-0.72	-21.75	-21.09	3.79	19
O6	-0.79	-0.72	-0.46	-0.34	-0.39	-0.13	-0.44	-0.96	-0.69	-4.23	-28.35	2.95	20
O6	-0.81	-0.73	-0.48	-0.33	-0.40	-0.13	-0.44	-0.96	-0.69	-6.91	-28.41	3.73	20
O6	-0.80	-0.74	-0.50	-0.31	-0.40	-0.12	-0.46	-0.95	-0.70	-5.62	-32.63	3.08	20
O6	-0.79	-0.74	-0.50	-0.35	-0.40	-0.15	-0.45	-0.96	-0.69	-6.12	-28.20	2.08	20
O6	-0.81	-0.73	-0.45	-0.38	-0.41	-0.15	-0.45	-0.95	-0.69	-4.47	-28.42	0.26	20
O6	-0.81	-0.72	-0.47	-0.36	-0.40	-0.15	-0.47	-0.95	-0.70	-4.61	-28.71	1.09	20
O7	-0.75	-0.71	-0.48	-0.47	-0.48	-0.22	-0.46	-0.96	-0.69	-6.25	-14.67	0.32	21
O7	-0.75	-0.70	-0.48	-0.47	-0.46	-0.20	-0.46	-0.96	-0.69	-5.17	-16.49	0.06	21
O7	-0.75	-0.71	-0.46	-0.47	-0.46	-0.19	-0.45	-0.96	-0.70	-5.18	-16.53	0.24	21
O7	-0.75	-0.71	-0.46	-0.48	-0.47	-0.23	-0.46	-0.96	-0.69	-5.18	-15.22	1.93	21
O7	-0.76	-0.68	-0.46	-0.47	-0.48	-0.21	-0.46	-0.96	-0.70	-4.43	-14.39	0.88	21

O7	-0.76	-0.71	-0.46	-0.50	-0.48	-0.22	-0.47	-0.95	-0.71	-5.51	-14.84	1.83	21
O8	-0.62	-0.59	-0.42	-0.42	-0.42	-0.16	-0.37	-0.95	-0.65	9.99	-17.04	2.06	22
O8	-0.63	-0.62	-0.42	-0.42	-0.40	-0.16	-0.38	-0.95	-0.65	10.24	-21.03	5.21	22
O8	-0.64	-0.63	-0.40	-0.43	-0.40	-0.19	-0.41	-0.95	-0.65	9.53	-19.82	6.07	22
O8	-0.64	-0.63	-0.42	-0.46	-0.42	-0.19	-0.40	-0.95	-0.67	7.91	-17.72	6.27	22
O8	-0.65	-0.59	-0.44	-0.45	-0.42	-0.19	-0.42	-0.95	-0.67	8.73	-17.20	2.64	22
O8	-0.68	-0.61	-0.39	-0.47	-0.42	-0.20	-0.43	-0.94	-0.69	8.63	-18.85	5.30	22

Table S5. Training matrix of fluorescence response pattern from an array of **P1-3** (each at pH 3, 7 and 13, buffered) against 22 teas. LDA was carried out and resulting in 9 factors of the canonical scores (the first three scores were shown here) and group generation. The jackknifed classification matrix with cross-validation reveals a 100% accuracy.

Analytes	Fluorescence Response Pattern									Results LDA (the first three scores)			
	P1 (pH3)	**P2** (pH3)	**P3** (pH3)	**P1** (pH7)	**P2** (pH7)	**P3** (pH7)	**P1** (pH13)	**P2** (pH13)	**P3** (pH13)	Factor 1	Factor 2	Factor 3	Group
B1	-0.99	-0.95	-0.97	-0.57	-0.69	-0.50	-0.60	-0.98	-0.74	-57.03	12.88	5.73	1
B1	-0.99	-0.96	-0.97	-0.58	-0.69	-0.50	-0.60	-0.98	-0.76	-58.29	14.39	7.27	1
B1	-0.98	-0.94	-0.97	-0.59	-0.70	-0.51	-0.60	-0.98	-0.75	-56.42	14.54	5.59	1
B1	-0.99	-0.96	-0.97	-0.61	-0.69	-0.51	-0.60	-0.99	-0.77	-58.77	14.97	7.53	1
B1	-0.98	-0.97	-0.96	-0.60	-0.70	-0.50	-0.60	-0.98	-0.75	-58.38	15.35	6.79	1
B1	-0.99	-0.96	-0.97	-0.61	-0.69	-0.52	-0.61	-0.99	-0.77	-58.12	15.59	6.57	1
B2	-0.99	-0.98	-0.98	-0.80	-0.79	-0.64	-0.61	-0.98	-0.75	-60.81	25.96	-8.87	2
B2	-0.99	-0.97	-0.98	-0.81	-0.79	-0.68	-0.61	-0.98	-0.76	-59.71	26.39	-8.82	2
B2	-0.99	-0.97	-0.98	-0.81	-0.80	-0.68	-0.62	-0.98	-0.77	-59.37	26.66	-10.38	2
B2	-0.99	-0.98	-0.98	-0.81	-0.80	-0.69	-0.61	-0.99	-0.78	-60.36	30.21	-7.96	2
B2	-0.99	-0.97	-0.98	-0.82	-0.80	-0.66	-0.61	-0.99	-0.78	-60.59	29.85	-8.47	2
B2	-0.99	-0.98	-0.97	-0.82	-0.80	-0.69	-0.62	-0.99	-0.76	-60.04	30.37	-8.43	2
B3	-0.99	-0.97	-0.97	-0.62	-0.67	-0.49	-0.57	-0.99	-0.75	-59.89	13.33	8.87	3
B3	-0.99	-0.97	-0.98	-0.63	-0.68	-0.54	-0.58	-0.99	-0.76	-59.71	14.92	8.01	3
B3	-0.99	-0.96	-0.97	-0.63	-0.68	-0.52	-0.58	-0.99	-0.78	-59.08	14.69	8.34	3
B3	-0.99	-0.96	-0.97	-0.65	-0.68	-0.51	-0.58	-0.99	-0.76	-59.29	14.96	8.07	3
B3	-0.99	-0.98	-0.97	-0.63	-0.68	-0.52	-0.59	-0.99	-0.77	-60.48	15.24	8.59	3
B3	-0.99	-0.96	-0.97	-0.65	-0.69	-0.55	-0.58	-0.99	-0.76	-58.41	15.70	6.31	3
B4	-0.97	-0.91	-0.76	-0.73	-0.77	-0.62	-0.34	-0.98	-0.74	-46.21	22.37	-4.05	4
B4	-0.97	-0.91	-0.75	-0.74	-0.78	-0.64	-0.36	-0.98	-0.74	-44.83	24.05	-5.00	4
B4	-0.97	-0.90	-0.77	-0.74	-0.77	-0.64	-0.35	-0.98	-0.76	-46.06	23.14	-4.51	4
B4	-0.97	-0.90	-0.77	-0.76	-0.78	-0.65	-0.34	-0.98	-0.74	-45.83	24.04	-5.31	4
B4	-0.97	-0.87	-0.76	-0.76	-0.77	-0.63	-0.34	-0.98	-0.75	-44.01	23.60	-6.18	4
B4	-0.97	-0.90	-0.76	-0.76	-0.78	-0.64	-0.34	-0.98	-0.74	-45.56	23.95	-5.27	4
B5	-0.97	-0.90	-0.80	-0.57	-0.61	-0.43	-0.35	-0.98	-0.73	-47.49	3.26	14.78	5
B5	-0.97	-0.85	-0.77	-0.58	-0.61	-0.41	-0.35	-0.98	-0.75	-44.11	4.15	13.95	5
B5	-0.97	-0.86	-0.80	-0.57	-0.62	-0.42	-0.34	-0.98	-0.75	-45.71	5.40	14.11	5
B5	-0.95	-0.89	-0.79	-0.58	-0.61	-0.43	-0.34	-0.98	-0.74	-46.30	4.47	15.92	5
B5	-0.97	-0.89	-0.77	-0.57	-0.62	-0.44	-0.35	-0.98	-0.75	-45.63	5.10	14.59	5
B5	-0.95	-0.85	-0.79	-0.58	-0.62	-0.43	-0.33	-0.98	-0.74	-43.46	5.65	14.02	5
B6	-0.93	-0.86	-0.49	-0.59	-0.64	-0.45	-0.46	-0.98	-0.70	-23.95	8.14	7.16	6
B6	-0.94	-0.84	-0.51	-0.59	-0.64	-0.42	-0.47	-0.98	-0.70	-24.96	7.85	6.69	6
B6	-0.93	-0.86	-0.50	-0.60	-0.64	-0.43	-0.46	-0.98	-0.71	-24.70	8.97	6.71	6
B6	-0.92	-0.87	-0.50	-0.59	-0.65	-0.47	-0.47	-0.98	-0.71	-24.02	9.56	6.26	6
B6	-0.93	-0.86	-0.49	-0.61	-0.65	-0.46	-0.46	-0.98	-0.70	-23.92	9.54	5.47	6
B6	-0.94	-0.86	-0.49	-0.62	-0.64	-0.47	-0.45	-0.98	-0.70	-24.56	8.82	5.95	6
B7	-0.80	-0.70	-0.34	-0.59	-0.66	-0.38	-0.42	-0.97	-0.62	0.53	7.91	1.45	7

B7	-0.80	-0.69	-0.33	-0.58	-0.65	-0.43	-0.43	-0.97	-0.62	3.18	7.82	0.47	7
B7	-0.80	-0.68	-0.31	-0.59	-0.65	-0.44	-0.42	-0.97	-0.61	5.36	8.71	0.40	7
B7	-0.80	-0.71	-0.31	-0.62	-0.66	-0.46	-0.42	-0.97	-0.63	2.73	8.73	-0.01	7
B7	-0.80	-0.70	-0.31	-0.62	-0.66	-0.44	-0.42	-0.97	-0.62	3.23	8.91	-0.86	7
B7	-0.79	-0.71	-0.31	-0.66	-0.66	-0.43	-0.43	-0.97	-0.62	2.20	9.97	0.03	7
B8	-0.83	-0.73	-0.35	-0.58	-0.64	-0.41	-0.39	-0.97	-0.63	-3.07	7.08	5.06	8
B8	-0.82	-0.72	-0.37	-0.57	-0.63	-0.41	-0.40	-0.97	-0.63	-2.91	6.49	5.65	8
B8	-0.83	-0.73	-0.37	-0.58	-0.63	-0.44	-0.41	-0.97	-0.65	-3.48	6.89	4.92	8
B8	-0.84	-0.74	-0.38	-0.59	-0.64	-0.46	-0.40	-0.97	-0.62	-4.73	7.66	4.75	8
B8	-0.84	-0.74	-0.35	-0.59	-0.64	-0.46	-0.40	-0.97	-0.64	-3.88	8.23	4.65	8
B8	-0.84	-0.74	-0.37	-0.60	-0.64	-0.47	-0.41	-0.97	-0.64	-4.99	8.19	4.36	8
G1	-0.48	-0.37	-0.22	-0.65	-0.73	-0.52	-0.49	-0.96	-0.58	47.89	18.21	-11.28	9
G1	-0.49	-0.37	-0.20	-0.64	-0.71	-0.52	-0.52	-0.97	-0.59	48.63	18.19	-10.25	9
G1	-0.49	-0.38	-0.20	-0.61	-0.71	-0.52	-0.53	-0.96	-0.58	49.01	17.38	-9.73	9
G1	-0.50	-0.38	-0.19	-0.62	-0.71	-0.53	-0.50	-0.96	-0.59	48.34	16.60	-10.16	9
G1	-0.47	-0.38	-0.19	-0.66	-0.72	-0.53	-0.49	-0.96	-0.61	48.99	17.91	-9.44	9
G1	-0.45	-0.35	-0.21	-0.63	-0.71	-0.51	-0.49	-0.97	-0.59	51.19	17.93	-7.80	9
G2	-0.65	-0.45	-0.28	-0.65	-0.73	-0.49	-0.58	-0.96	-0.58	31.23	14.78	-17.84	10
G2	-0.66	-0.44	-0.25	-0.65	-0.73	-0.50	-0.58	-0.96	-0.60	32.56	15.23	-17.43	10
G2	-0.68	-0.44	-0.26	-0.66	-0.72	-0.51	-0.58	-0.96	-0.59	31.45	13.76	-17.30	10
G2	-0.69	-0.45	-0.28	-0.65	-0.73	-0.51	-0.59	-0.96	-0.59	29.43	15.17	-18.80	10
G2	-0.64	-0.45	-0.28	-0.67	-0.75	-0.51	-0.59	-0.96	-0.59	32.70	16.92	-19.15	10
G2	-0.68	-0.44	-0.31	-0.65	-0.73	-0.52	-0.58	-0.96	-0.58	29.29	13.93	-18.65	10
G3	-0.53	-0.37	-0.29	-0.40	-0.54	-0.28	-0.48	-0.96	-0.60	41.47	-6.16	10.75	11
G3	-0.56	-0.38	-0.26	-0.39	-0.54	-0.30	-0.50	-0.96	-0.61	41.15	-5.78	11.05	11
G3	-0.58	-0.38	-0.29	-0.42	-0.55	-0.30	-0.51	-0.96	-0.60	37.87	-3.70	9.05	11
G3	-0.54	-0.38	-0.31	-0.43	-0.54	-0.32	-0.49	-0.96	-0.63	38.41	-5.78	10.31	11
G3	-0.54	-0.39	-0.27	-0.41	-0.55	-0.28	-0.49	-0.96	-0.59	39.98	-3.46	10.87	11
G3	-0.59	-0.38	-0.26	-0.42	-0.55	-0.33	-0.50	-0.96	-0.63	39.14	-4.36	8.51	11
G4	-0.61	-0.53	-0.31	-0.60	-0.72	-0.50	-0.49	-0.97	-0.67	25.68	17.49	-4.87	12
G4	-0.61	-0.54	-0.33	-0.59	-0.72	-0.51	-0.50	-0.97	-0.68	23.97	18.23	-4.02	12
G4	-0.60	-0.54	-0.31	-0.60	-0.72	-0.51	-0.52	-0.97	-0.68	25.39	18.03	-4.24	12
G4	-0.63	-0.55	-0.32	-0.58	-0.71	-0.50	-0.50	-0.97	-0.68	23.02	17.35	-3.52	12
G4	-0.60	-0.54	-0.35	-0.58	-0.72	-0.49	-0.52	-0.97	-0.68	23.48	17.72	-4.04	12
G4	-0.58	-0.54	-0.33	-0.60	-0.71	-0.49	-0.50	-0.97	-0.69	24.87	17.19	-2.89	12
G5	-0.62	-0.33	-0.13	-0.65	-0.71	-0.55	-0.56	-0.97	-0.59	48.71	21.92	-12.33	13
G5	-0.62	-0.32	-0.10	-0.65	-0.70	-0.56	-0.51	-0.97	-0.59	50.93	21.19	-11.82	13
G5	-0.60	-0.33	-0.13	-0.65	-0.70	-0.58	-0.50	-0.97	-0.60	49.16	21.33	-11.38	13
G5	-0.62	-0.34	-0.08	-0.68	-0.71	-0.58	-0.50	-0.97	-0.60	50.23	22.16	-12.82	13
G5	-0.61	-0.33	-0.11	-0.66	-0.70	-0.59	-0.47	-0.97	-0.61	49.30	21.87	-10.90	13
G5	-0.59	-0.32	-0.14	-0.66	-0.71	-0.58	-0.50	-0.97	-0.61	49.76	22.07	-11.64	13
G6	-0.43	-0.37	-0.21	-0.59	-0.66	-0.49	-0.53	-0.97	-0.60	51.87	15.96	0.18	14
G6	-0.41	-0.34	-0.21	-0.61	-0.68	-0.51	-0.52	-0.97	-0.63	54.09	17.32	-1.84	14
G6	-0.44	-0.35	-0.19	-0.63	-0.67	-0.51	-0.52	-0.97	-0.62	53.17	17.20	-1.76	14
G6	-0.39	-0.36	-0.23	-0.63	-0.66	-0.52	-0.54	-0.97	-0.64	53.11	17.32	1.00	14
G6	-0.40	-0.36	-0.22	-0.61	-0.66	-0.53	-0.52	-0.97	-0.64	53.41	17.47	1.66	14
G6	-0.42	-0.37	-0.23	-0.62	-0.67	-0.53	-0.52	-0.97	-0.65	51.04	16.67	-0.14	14
O1	-0.37	-0.40	-0.28	-0.42	-0.51	-0.31	-0.29	-0.97	-0.65	45.60	-6.01	24.07	15
O1	-0.36	-0.40	-0.27	-0.42	-0.51	-0.31	-0.29	-0.97	-0.65	46.46	-5.90	24.54	15
O1	-0.37	-0.39	-0.26	-0.41	-0.51	-0.31	-0.33	-0.97	-0.65	47.15	-5.62	23.45	15
O1	-0.37	-0.41	-0.28	-0.42	-0.52	-0.33	-0.33	-0.97	-0.66	45.19	-4.87	23.37	15
O1	-0.35	-0.40	-0.29	-0.42	-0.54	-0.32	-0.31	-0.97	-0.66	46.04	-3.24	22.69	15

O1	-0.37	-0.40	-0.30	-0.42	-0.54	-0.33	-0.32	-0.97	-0.66	44.82	-2.83	20.79	15
O2	-0.30	-0.32	-0.18	-0.45	-0.56	-0.36	-0.30	-0.96	-0.56	61.32	-4.82	12.67	16
O2	-0.30	-0.31	-0.19	-0.43	-0.55	-0.34	-0.31	-0.96	-0.55	61.81	-4.78	14.33	16
O2	-0.31	-0.30	-0.18	-0.47	-0.57	-0.36	-0.30	-0.96	-0.55	61.48	-2.65	10.93	16
O2	-0.32	-0.33	-0.18	-0.46	-0.56	-0.36	-0.31	-0.96	-0.54	59.13	-3.88	12.52	16
O2	-0.32	-0.31	-0.21	-0.43	-0.57	-0.34	-0.32	-0.96	-0.55	59.66	-3.42	11.31	16
O2	-0.31	-0.33	-0.20	-0.44	-0.57	-0.37	-0.30	-0.96	-0.54	59.07	-3.19	12.09	16
O3	-0.78	-0.61	-0.47	-0.41	-0.51	-0.31	-0.53	-0.93	-0.65	4.90	-28.75	-0.92	17
O3	-0.80	-0.61	-0.44	-0.43	-0.52	-0.31	-0.52	-0.93	-0.65	4.75	-26.42	-1.61	17
O3	-0.80	-0.60	-0.44	-0.41	-0.52	-0.31	-0.53	-0.93	-0.65	6.22	-27.17	-1.50	17
O3	-0.79	-0.61	-0.44	-0.43	-0.51	-0.33	-0.54	-0.93	-0.60	6.99	-27.84	-2.37	17
O3	-0.80	-0.61	-0.44	-0.41	-0.50	-0.32	-0.52	-0.93	-0.63	5.31	-28.25	0.02	17
O3	-0.80	-0.61	-0.47	-0.43	-0.52	-0.32	-0.56	-0.93	-0.62	4.40	-27.23	-2.64	17
O4	-0.72	-0.71	-0.60	-0.41	-0.48	-0.28	-0.51	-0.91	-0.67	-6.26	-40.47	1.97	18
O4	-0.71	-0.70	-0.61	-0.41	-0.47	-0.28	-0.52	-0.92	-0.69	-5.53	-39.47	4.17	18
O4	-0.72	-0.71	-0.61	-0.41	-0.46	-0.32	-0.50	-0.92	-0.70	-6.24	-39.45	5.37	18
O4	-0.75	-0.70	-0.62	-0.41	-0.47	-0.31	-0.52	-0.92	-0.67	-7.22	-38.48	2.86	18
O4	-0.75	-0.70	-0.60	-0.41	-0.47	-0.31	-0.52	-0.91	-0.68	-6.21	-40.89	1.09	18
O4	-0.73	-0.71	-0.61	-0.40	-0.47	-0.32	-0.52	-0.91	-0.67	-6.34	-39.82	2.28	18
O5	-0.96	-0.74	-0.64	-0.46	-0.58	-0.32	-0.44	-0.91	-0.61	-23.76	-33.46	-14.68	19
O5	-0.97	-0.76	-0.64	-0.48	-0.57	-0.32	-0.45	-0.90	-0.63	-24.72	-36.71	-17.41	19
O5	-0.96	-0.75	-0.64	-0.46	-0.58	-0.34	-0.46	-0.91	-0.60	-23.52	-33.73	-15.93	19
O5	-0.93	-0.76	-0.65	-0.47	-0.58	-0.32	-0.47	-0.90	-0.61	-23.15	-36.31	-16.72	19
O5	-0.94	-0.76	-0.64	-0.47	-0.58	-0.34	-0.47	-0.90	-0.61	-22.52	-35.96	-18.24	19
O5	-0.95	-0.76	-0.64	-0.46	-0.57	-0.34	-0.46	-0.91	-0.60	-23.15	-33.36	-14.64	19
O6	-0.77	-0.74	-0.63	-0.41	-0.52	-0.29	-0.36	-0.94	-0.68	-14.72	-23.56	12.32	20
O6	-0.76	-0.73	-0.63	-0.40	-0.52	-0.29	-0.37	-0.94	-0.66	-14.19	-22.10	12.71	20
O6	-0.79	-0.73	-0.60	-0.39	-0.52	-0.28	-0.39	-0.94	-0.66	-13.25	-22.85	11.83	20
O6	-0.79	-0.74	-0.60	-0.42	-0.52	-0.28	-0.41	-0.94	-0.66	-13.87	-22.99	10.56	20
O6	-0.77	-0.73	-0.63	-0.40	-0.52	-0.29	-0.40	-0.95	-0.66	-14.38	-22.04	12.88	20
O6	-0.78	-0.74	-0.62	-0.43	-0.52	-0.30	-0.40	-0.94	-0.66	-14.14	-23.49	10.47	20
O7	-0.91	-0.68	-0.57	-0.47	-0.62	-0.38	-0.44	-0.93	-0.58	-12.75	-19.68	-13.05	21
O7	-0.95	-0.67	-0.57	-0.50	-0.61	-0.38	-0.46	-0.92	-0.57	-14.21	-20.76	-15.22	21
O7	-0.94	-0.68	-0.56	-0.50	-0.61	-0.38	-0.48	-0.93	-0.56	-13.43	-19.71	-14.79	21
O7	-0.93	-0.66	-0.56	-0.50	-0.61	-0.36	-0.46	-0.93	-0.56	-12.88	-18.83	-13.64	21
O7	-0.93	-0.68	-0.55	-0.50	-0.61	-0.38	-0.47	-0.92	-0.56	-12.41	-20.45	-15.25	21
O7	-0.95	-0.67	-0.55	-0.48	-0.61	-0.36	-0.46	-0.93	-0.56	-13.47	-19.20	-13.71	21
O8	-0.79	-0.67	-0.60	-0.45	-0.53	-0.32	-0.38	-0.90	-0.67	-8.87	-43.13	-11.57	22
O8	-0.80	-0.68	-0.56	-0.46	-0.54	-0.30	-0.39	-0.90	-0.68	-7.84	-40.34	-11.50	22
O8	-0.80	-0.66	-0.56	-0.46	-0.53	-0.32	-0.39	-0.90	-0.67	-6.53	-41.90	-11.35	22
O8	-0.81	-0.68	-0.56	-0.48	-0.52	-0.30	-0.42	-0.90	-0.68	-7.78	-42.52	-11.59	22
O8	-0.79	-0.69	-0.57	-0.47	-0.53	-0.34	-0.43	-0.90	-0.65	-7.13	-41.91	-11.95	22
O8	-0.80	-0.68	-0.58	-0.47	-0.53	-0.34	-0.42	-0.90	-0.67	-7.89	-39.47	-9.24	22

Table S6. Training matrix of fluorescence response pattern from an array of **P1**/CB[8], **P2**/CB[8] and **P3**/CB[8] (each at pH 3 and 13, buffered) against different concentrations of caffeine (0-10 mM) in three kinds of teas (B-black tea, G-green tea and O-oolong tea). LDA was carried out and resulting in 6 factors of the canonical scores (the first three scores were shown here) and group generation. The jackknifed classification matrix with cross-validation reveals a 96% accuracy.

Analytes	Fluorescence Response Pattern						Results LDA (the first three scores)			
	P1/CB[8] (pH3)	**P2**/CB[8] (pH3)	**P3**/CB[8] (pH3)	**P1**/CB[8] (pH13)	**P2**/CB[8] (pH13)	**P3**/CB[8] (pH13)	Factor 1	Factor 2	Factor 3	Group

Control	0.07	0.00	0.04	0.04	0.10	0.08	53.95	-75.72	1.00	9
Control	0.03	0.03	0.00	-0.03	0.05	-0.03	58.53	-70.48	-3.55	9
Control	-0.01	0.00	0.02	-0.04	-0.03	-0.03	55.32	-65.24	-2.38	9
Control	0.04	0.00	0.06	0.03	-0.03	0.04	55.53	-64.84	3.24	9
Control	-0.04	-0.01	-0.04	-0.01	-0.01	-0.02	52.54	-68.20	-2.39	9
Control	-0.10	-0.01	-0.07	0.00	-0.08	-0.05	52.90	-64.74	-2.27	9
B-0mM	-0.97	-0.86	-0.67	-0.48	-0.99	-0.70	-48.82	-0.98	-8.05	3
B-0mM	-0.97	-0.86	-0.68	-0.48	-0.99	-0.70	-48.64	-1.10	-8.08	3
B-0mM	-0.97	-0.88	-0.68	-0.48	-0.99	-0.71	-50.21	-1.03	-7.73	3
B-0mM	-0.97	-0.87	-0.67	-0.48	-0.99	-0.71	-49.62	-0.94	-7.79	3
B-0mM	-0.97	-0.87	-0.67	-0.47	-0.99	-0.72	-49.15	-1.18	-7.53	3
B-0mM	-0.97	-0.87	-0.67	-0.47	-0.99	-0.71	-49.17	-1.17	-7.60	3
B-0.2mM	-0.97	-0.83	-0.65	-0.46	-0.98	-0.70	-45.29	-1.82	-7.73	2
B-0.2mM	-0.97	-0.84	-0.67	-0.47	-0.99	-0.69	-46.17	-1.53	-8.05	1
B-0.2mM	-0.97	-0.84	-0.67	-0.47	-0.99	-0.71	-46.24	-1.51	-7.93	1
B-0.2mM	-0.97	-0.84	-0.67	-0.47	-0.99	-0.71	-45.74	-1.33	-8.33	1
B-0.2mM	-0.97	-0.85	-0.66	-0.48	-0.99	-0.71	-47.32	-1.18	-8.08	1
B-0.2mM	-0.97	-0.85	-0.66	-0.47	-0.99	-0.69	-47.05	-1.39	-7.98	1
B-0.5mM	-0.97	-0.83	-0.65	-0.45	-0.98	-0.68	-45.18	-2.00	-7.23	2
B-0.5mM	-0.97	-0.84	-0.66	-0.45	-0.98	-0.68	-46.55	-2.02	-7.19	2
B-0.5mM	-0.97	-0.84	-0.67	-0.46	-0.98	-0.69	-45.75	-1.93	-7.65	2
B-0.5mM	-0.97	-0.83	-0.66	-0.46	-0.98	-0.68	-44.41	-1.80	-8.21	2
B-0.5mM	-0.97	-0.83	-0.66	-0.46	-0.99	-0.68	-45.43	-1.71	-7.91	2
B-0.5mM	-0.97	-0.83	-0.65	-0.46	-0.98	-0.70	-45.30	-1.74	-8.05	2
B-1.0mM	-0.97	-0.83	-0.63	-0.27	-0.98	-0.64	-49.16	-6.36	1.65	4
B-1.0mM	-0.97	-0.84	-0.64	-0.26	-0.98	-0.65	-50.01	-6.49	2.18	4
B-1.0mM	-0.97	-0.84	-0.65	-0.28	-0.98	-0.65	-49.92	-6.25	1.11	4
B-1.0mM	-0.97	-0.83	-0.64	-0.28	-0.98	-0.65	-49.06	-6.10	1.07	4
B-1.0mM	-0.97	-0.84	-0.65	-0.27	-0.98	-0.64	-50.38	-6.28	1.78	4
B-1.0mM	-0.97	-0.84	-0.64	-0.28	-0.98	-0.65	-49.93	-6.20	1.35	4
B-2.0mM	-0.95	-0.77	-0.57	-0.22	-0.97	-0.59	-41.75	-7.73	2.77	6
B-2.0mM	-0.96	-0.78	-0.57	-0.23	-0.98	-0.60	-42.95	-7.39	2.49	6
B-2.0mM	-0.96	-0.78	-0.57	-0.23	-0.98	-0.61	-42.83	-7.44	2.44	6
B-2.0mM	-0.96	-0.78	-0.57	-0.23	-0.98	-0.61	-42.93	-7.54	2.76	6
B-2.0mM	-0.96	-0.77	-0.58	-0.25	-0.97	-0.59	-41.68	-7.35	1.53	6
B-2.0mM	-0.96	-0.78	-0.59	-0.25	-0.98	-0.60	-42.38	-7.14	1.43	6
B-5.0mM	-0.92	-0.72	-0.53	-0.19	-0.97	-0.54	-35.39	-8.05	4.21	7
B-5.0mM	-0.93	-0.72	-0.54	-0.20	-0.97	-0.57	-35.87	-8.08	3.58	7
B-5.0mM	-0.92	-0.72	-0.54	-0.19	-0.97	-0.56	-36.24	-8.04	4.07	7
B-5.0mM	-0.92	-0.72	-0.52	-0.20	-0.97	-0.57	-36.15	-7.66	3.86	7
B-5.0mM	-0.93	-0.71	-0.53	-0.22	-0.97	-0.55	-33.86	-7.65	2.48	7
B-5.0mM	-0.93	-0.72	-0.54	-0.23	-0.97	-0.56	-35.27	-7.27	1.92	7
B-8.0mM	-0.88	-0.63	-0.48	-0.15	-0.96	-0.49	-24.84	-8.58	5.11	8
B-8.0mM	-0.88	-0.63	-0.49	-0.18	-0.96	-0.52	-24.66	-7.97	3.64	8
B-8.0mM	-0.88	-0.64	-0.49	-0.18	-0.96	-0.52	-25.60	-7.65	4.01	8
B-8.0mM	-0.88	-0.64	-0.49	-0.18	-0.96	-0.52	-25.48	-7.94	3.95	8
B-8.0mM	-0.88	-0.63	-0.51	-0.18	-0.96	-0.50	-23.91	-8.02	3.14	8
B-8.0mM	-0.88	-0.64	-0.51	-0.17	-0.97	-0.54	-25.81	-7.50	4.30	8
B-10.0mM	-0.84	-0.58	-0.50	-0.16	-0.96	-0.49	-17.12	-7.68	4.08	5
B-10.0mM	-0.85	-0.58	-0.47	-0.16	-0.96	-0.51	-18.08	-7.88	4.16	5
B-10.0mM	-0.85	-0.58	-0.48	-0.16	-0.96	-0.51	-18.11	-7.78	3.88	5
B-10.0mM	-0.85	-0.58	-0.47	-0.18	-0.96	-0.49	-17.23	-7.27	2.88	5

B-10.0mM	-0.85	-0.57	-0.47	-0.18	-0.96	-0.49	-16.02	-7.37	2.82	5
B-10.0mM	-0.85	-0.58	-0.47	-0.18	-0.96	-0.51	-17.30	-7.38	2.72	5
G-0mM	-0.68	-0.33	-0.38	-0.53	-0.98	-0.68	23.32	7.58	-14.83	12
G-0mM	-0.66	-0.33	-0.38	-0.52	-0.98	-0.63	23.67	7.91	-13.55	12
G-0mM	-0.65	-0.33	-0.37	-0.52	-0.99	-0.65	24.04	8.47	-13.25	12
G-0mM	-0.66	-0.33	-0.35	-0.53	-0.98	-0.67	23.73	8.29	-13.68	12
G-0mM	-0.67	-0.33	-0.37	-0.52	-0.99	-0.65	23.64	7.69	-14.30	12
G-0mM	-0.70	-0.33	-0.42	-0.53	-0.98	-0.67	23.10	6.79	-16.33	12
G-0.2mM	-0.67	-0.28	-0.42	-0.53	-0.98	-0.53	30.44	6.34	-16.59	10
G-0.2mM	-0.67	-0.28	-0.38	-0.50	-0.98	-0.53	30.19	6.14	-14.93	10
G-0.2mM	-0.64	-0.28	-0.35	-0.51	-0.98	-0.54	30.55	7.47	-13.90	10
G-0.2mM	-0.65	-0.28	-0.38	-0.51	-0.98	-0.57	30.36	7.29	-14.68	10
G-0.2mM	-0.65	-0.28	-0.37	-0.51	-0.98	-0.54	29.71	7.11	-14.50	10
G-0.2mM	-0.67	-0.28	-0.32	-0.51	-0.98	-0.53	30.15	6.24	-14.94	10
G-0.5mM	-0.67	-0.26	-0.42	-0.49	-0.98	-0.52	31.35	5.32	-15.09	11
G-0.5mM	-0.64	-0.26	-0.40	-0.49	-0.98	-0.51	32.82	6.40	-14.11	11
G-0.5mM	-0.65	-0.27	-0.38	-0.50	-0.98	-0.49	31.95	6.45	-14.58	11
G-0.5mM	-0.66	-0.26	-0.34	-0.51	-0.98	-0.50	31.79	6.21	-14.62	11
G-0.5mM	-0.63	-0.26	-0.40	-0.51	-0.98	-0.50	32.50	7.02	-14.67	11
G-0.5mM	-0.66	-0.26	-0.41	-0.51	-0.98	-0.50	32.81	6.21	-15.95	11
G-1.0mM	-0.56	-0.21	-0.28	-0.41	-0.97	-0.51	38.93	7.21	-8.07	13
G-1.0mM	-0.54	-0.21	-0.35	-0.40	-0.96	-0.53	39.17	6.67	-8.03	13
G-1.0mM	-0.54	-0.21	-0.29	-0.40	-0.97	-0.54	39.12	7.33	-7.38	13
G-1.0mM	-0.54	-0.21	-0.31	-0.41	-0.97	-0.52	38.67	7.48	-7.95	13
G-1.0mM	-0.54	-0.22	-0.33	-0.41	-0.97	-0.53	38.33	7.48	-7.85	13
G-1.0mM	-0.57	-0.22	-0.39	-0.39	-0.97	-0.58	37.35	6.85	-8.38	13
G-2.0mM	-0.47	-0.21	-0.18	-0.38	-0.96	-0.48	40.18	8.77	-2.91	15
G-2.0mM	-0.45	-0.21	-0.18	-0.36	-0.96	-0.47	40.41	8.98	-1.62	15
G-2.0mM	-0.45	-0.21	-0.22	-0.38	-0.96	-0.48	40.29	9.31	-2.58	15
G-2.0mM	-0.44	-0.21	-0.29	-0.35	-0.96	-0.46	39.98	9.36	-1.48	15
G-2.0mM	-0.45	-0.22	-0.22	-0.36	-0.96	-0.42	39.32	8.56	-1.84	15
G-2.0mM	-0.49	-0.21	-0.24	-0.36	-0.96	-0.50	38.71	8.00	-3.31	15
G-5.0mM	-0.41	-0.20	-0.07	-0.32	-0.95	-0.54	40.31	9.08	1.88	16
G-5.0mM	-0.34	-0.20	-0.02	-0.33	-0.95	-0.39	42.13	10.83	4.70	16
G-5.0mM	-0.37	-0.21	-0.04	-0.34	-0.96	-0.49	41.32	11.00	2.86	16
G-5.0mM	-0.39	-0.21	-0.19	-0.33	-0.96	-0.40	41.00	10.11	2.06	16
G-5.0mM	-0.43	-0.21	-0.12	-0.33	-0.96	-0.46	40.11	9.01	0.96	16
G-5.0mM	-0.40	-0.21	-0.13	-0.33	-0.96	-0.52	40.82	10.36	1.65	16
G-8.0mM	-0.28	-0.20	0.02	-0.29	-0.95	-0.37	42.93	11.63	8.90	17
G-8.0mM	-0.27	-0.20	0.02	-0.26	-0.94	-0.39	42.75	10.98	10.08	17
G-8.0mM	-0.30	-0.20	0.05	-0.26	-0.95	-0.44	42.16	11.32	9.96	17
G-8.0mM	-0.33	-0.20	-0.04	-0.28	-0.95	-0.45	41.96	10.75	6.98	17
G-8.0mM	-0.31	-0.21	-0.03	-0.28	-0.95	-0.43	41.47	11.33	8.15	17
G-8.0mM	-0.29	-0.20	-0.08	-0.29	-0.95	-0.38	42.58	11.76	7.49	17
G-10.0mM	-0.28	-0.20	0.08	-0.25	-0.93	-0.31	42.59	9.69	10.82	14
G-10.0mM	-0.24	-0.19	0.12	-0.24	-0.94	-0.35	43.37	11.41	13.12	14
G-10.0mM	-0.23	-0.20	0.10	-0.23	-0.94	-0.38	42.75	12.22	13.98	14
G-10.0mM	-0.22	-0.20	0.06	-0.23	-0.95	-0.37	43.54	12.55	13.65	14
G-10.0mM	-0.26	-0.20	0.05	-0.25	-0.93	-0.39	42.97	10.85	11.39	14
G-10.0mM	-0.27	-0.21	0.06	-0.25	-0.94	-0.33	41.62	10.36	11.40	14
O-0mM	-0.64	-0.60	-0.42	-0.46	-0.97	-0.68	-9.83	7.62	-2.35	20
O-0mM	-0.64	-0.62	-0.42	-0.46	-0.98	-0.69	-11.80	8.35	-2.11	20

O-0mM	-0.65	-0.62	-0.41	-0.46	-0.97	-0.70	-13.04	7.85	-1.91	20
O-0mM	-0.65	-0.63	-0.42	-0.47	-0.97	-0.67	-13.91	8.15	-2.23	20
O-0mM	-0.64	-0.60	-0.41	-0.45	-0.97	-0.70	-10.46	7.91	-2.04	20
O-0mM	-0.64	-0.61	-0.42	-0.48	-0.97	-0.70	-10.94	8.15	-3.36	20
O-0.2mM	-0.62	-0.57	-0.40	-0.40	-0.97	-0.66	-7.00	7.17	0.17	19
O-0.2mM	-0.62	-0.61	-0.40	-0.41	-0.97	-0.66	-11.85	7.67	1.52	18
O-0.2mM	-0.62	-0.62	-0.39	-0.42	-0.97	-0.68	-13.16	7.78	1.03	18
O-0.2mM	-0.62	-0.61	-0.39	-0.43	-0.97	-0.66	-11.02	7.74	0.15	18
O-0.2mM	-0.62	-0.60	-0.40	-0.41	-0.97	-0.68	-10.44	7.44	0.59	18
O-0.2mM	-0.62	-0.61	-0.40	-0.42	-0.97	-0.67	-11.55	7.85	0.50	18
O-0.5mM	-0.60	-0.59	-0.36	-0.39	-0.97	-0.67	-8.89	7.49	2.35	19
O-0.5mM	-0.61	-0.57	-0.38	-0.37	-0.97	-0.67	-7.80	7.03	2.12	19
O-0.5mM	-0.61	-0.60	-0.36	-0.40	-0.97	-0.67	-10.82	7.65	2.00	19
O-0.5mM	-0.61	-0.60	-0.39	-0.40	-0.97	-0.65	-10.24	7.03	1.36	19
O-0.5mM	-0.60	-0.60	-0.38	-0.42	-0.97	-0.65	-10.44	8.29	1.31	18
O-0.5mM	-0.61	-0.60	-0.40	-0.42	-0.97	-0.64	-9.43	8.06	0.74	19
O-1.0mM	-0.60	-0.59	-0.37	-0.33	-0.95	-0.57	-10.93	4.52	5.10	21
O-1.0mM	-0.61	-0.60	-0.39	-0.34	-0.95	-0.58	-11.68	4.42	3.99	21
O-1.0mM	-0.60	-0.58	-0.37	-0.33	-0.95	-0.61	-9.18	4.92	4.55	21
O-1.0mM	-0.62	-0.59	-0.34	-0.36	-0.95	-0.53	-10.02	3.77	2.91	21
O-1.0mM	-0.60	-0.58	-0.36	-0.34	-0.95	-0.61	-9.33	4.97	3.92	21
O-1.0mM	-0.60	-0.59	-0.36	-0.36	-0.95	-0.54	-10.44	4.86	3.83	21
O-2.0mM	-0.55	-0.55	-0.27	-0.29	-0.95	-0.52	-5.68	4.49	8.17	23
O-2.0mM	-0.57	-0.55	-0.32	-0.28	-0.95	-0.52	-6.30	3.52	7.13	23
O-2.0mM	-0.55	-0.55	-0.31	-0.29	-0.94	-0.55	-6.06	4.33	7.63	23
O-2.0mM	-0.57	-0.55	-0.28	-0.32	-0.95	-0.51	-5.67	4.25	6.04	23
O-2.0mM	-0.57	-0.54	-0.30	-0.27	-0.94	-0.53	-5.32	3.36	7.86	23
O-2.0mM	-0.56	-0.55	-0.31	-0.34	-0.95	-0.53	-3.98	5.38	5.05	23
O-5.0mM	-0.54	-0.51	-0.24	-0.27	-0.94	-0.46	-0.84	3.49	8.13	24
O-5.0mM	-0.54	-0.51	-0.27	-0.26	-0.94	-0.53	-1.41	3.76	8.54	24
O-5.0mM	-0.53	-0.50	-0.25	-0.27	-0.94	-0.49	0.82	3.92	8.24	24
O-5.0mM	-0.55	-0.51	-0.25	-0.27	-0.94	-0.49	-1.48	2.56	7.63	24
O-5.0mM	-0.54	-0.51	-0.24	-0.27	-0.94	-0.52	-0.55	3.97	8.29	24
O-5.0mM	-0.55	-0.52	-0.28	-0.27	-0.94	-0.53	-2.29	3.23	7.49	24
O-8.0mM	-0.50	-0.46	-0.19	-0.23	-0.93	-0.44	5.07	2.54	9.89	25
O-8.0mM	-0.48	-0.45	-0.21	-0.21	-0.93	-0.39	6.93	2.32	11.05	25
O-8.0mM	-0.49	-0.47	-0.19	-0.22	-0.93	-0.43	4.57	2.64	10.91	25
O-8.0mM	-0.50	-0.45	-0.18	-0.19	-0.93	-0.45	5.17	2.25	12.23	25
O-8.0mM	-0.50	-0.46	-0.21	-0.23	-0.93	-0.46	4.73	3.06	10.30	25
O-8.0mM	-0.50	-0.45	-0.24	-0.19	-0.93	-0.47	6.20	2.26	11.04	25
O-10.0mM	-0.47	-0.40	-0.18	-0.15	-0.92	-0.43	11.27	1.17	12.99	22
O-10.0mM	-0.46	-0.42	-0.20	-0.16	-0.91	-0.42	9.10	1.18	13.35	22
O-10.0mM	-0.47	-0.44	-0.19	-0.20	-0.92	-0.37	7.74	2.04	11.54	22
O-10.0mM	-0.48	-0.42	-0.17	-0.23	-0.92	-0.44	10.06	2.63	9.27	22
O-10.0mM	-0.49	-0.44	-0.18	-0.23	-0.93	-0.44	8.26	3.08	10.09	22
O-10.0mM	-0.49	-0.44	-0.24	-0.24	-0.93	-0.44	8.12	3.29	8.96	22

Table S7. Training matrix of fluorescence response pattern from an array of **P1**/CB[8], **P2**/CB[8] and **P3**/CB[8] (each at pH 3 and 13, buffered) against different concentrations of caffeine (0-10 mM) in black tea. LDA was carried out and resulting in 6 factors of the canonical scores (the first three scores were shown here) and group generation.

Analytes	Fluorescence Response Pattern						Results LDA (the first three scores)			
	P1/CB[8] (pH3)	**P2**/CB[8] (pH3)	**P3**/CB[8] (pH3)	**P1**/CB[8] (pH13)	**P2**/CB[8] (pH13)	**P3**/CB[8] (pH13)	Factor 1	Factor 2	Factor 3	Group
B-0mM	-0.97	-0.86	-0.67	-0.48	-0.99	-0.70	-24.90	10.24	0.43	3
B-0mM	-0.97	-0.86	-0.68	-0.48	-0.99	-0.70	-25.11	9.57	0.38	3
B-0mM	-0.97	-0.88	-0.68	-0.48	-0.99	-0.71	-27.01	9.36	1.33	3
B-0mM	-0.97	-0.87	-0.67	-0.48	-0.99	-0.71	-25.75	9.99	0.88	3
B-0mM	-0.97	-0.87	-0.67	-0.47	-0.99	-0.72	-24.81	9.25	1.11	3
B-0mM	-0.97	-0.87	-0.67	-0.47	-0.99	-0.71	-24.86	9.33	0.72	3
B-0.2mM	-0.97	-0.83	-0.65	-0.46	-0.98	-0.70	-18.95	8.48	-1.48	2
B-0.2mM	-0.97	-0.84	-0.67	-0.47	-0.99	-0.69	-21.35	9.05	-0.20	1
B-0.2mM	-0.97	-0.84	-0.67	-0.47	-0.99	-0.71	-20.68	9.39	-0.06	1
B-0.2mM	-0.97	-0.84	-0.67	-0.47	-0.99	-0.71	-20.30	10.19	-0.50	1
B-0.2mM	-0.97	-0.85	-0.66	-0.48	-0.99	-0.71	-21.74	10.60	-0.67	1
B-0.2mM	-0.97	-0.85	-0.66	-0.47	-0.99	-0.69	-22.10	9.37	-1.27	1
B-0.5mM	-0.97	-0.83	-0.65	-0.45	-0.98	-0.68	-18.22	8.08	-0.92	2
B-0.5mM	-0.97	-0.84	-0.66	-0.45	-0.98	-0.68	-20.84	7.30	-0.81	2
B-0.5mM	-0.97	-0.84	-0.67	-0.46	-0.98	-0.69	-20.31	7.84	-0.15	2
B-0.5mM	-0.97	-0.83	-0.66	-0.46	-0.98	-0.68	-18.93	8.63	-1.59	2
B-0.5mM	-0.97	-0.83	-0.66	-0.46	-0.99	-0.68	-20.09	8.63	-1.19	2
B-0.5mM	-0.97	-0.83	-0.65	-0.46	-0.98	-0.70	-19.30	8.91	-1.74	2
B-1.0mM	-0.97	-0.83	-0.63	-0.27	-0.98	-0.64	-18.73	-12.64	2.71	4
B-1.0mM	-0.97	-0.84	-0.64	-0.26	-0.98	-0.65	-19.57	-13.65	3.52	4
B-1.0mM	-0.97	-0.84	-0.65	-0.28	-0.98	-0.65	-19.44	-11.21	3.45	4
B-1.0mM	-0.97	-0.83	-0.64	-0.28	-0.98	-0.65	-18.69	-11.28	2.72	4
B-1.0mM	-0.97	-0.84	-0.65	-0.27	-0.98	-0.64	-20.71	-12.73	4.66	4
B-1.0mM	-0.97	-0.84	-0.64	-0.28	-0.98	-0.65	-20.07	-12.08	3.21	4
B-2.0mM	-0.95	-0.77	-0.57	-0.22	-0.97	-0.59	-4.60	-14.07	-2.11	6
B-2.0mM	-0.96	-0.78	-0.57	-0.23	-0.98	-0.60	-6.62	-13.38	-1.74	6
B-2.0mM	-0.96	-0.78	-0.57	-0.23	-0.98	-0.61	-6.77	-13.75	-2.00	6
B-2.0mM	-0.96	-0.78	-0.57	-0.23	-0.98	-0.61	-6.29	-14.02	-1.90	6
B-2.0mM	-0.96	-0.77	-0.58	-0.25	-0.97	-0.59	-6.51	-12.91	-2.28	6
B-2.0mM	-0.96	-0.78	-0.59	-0.25	-0.98	-0.60	-7.40	-12.25	-1.75	6
B-5.0mM	-0.92	-0.72	-0.53	-0.19	-0.97	-0.54	11.04	-9.48	-0.87	7
B-5.0mM	-0.93	-0.72	-0.54	-0.20	-0.97	-0.57	8.85	-10.47	-0.99	7
B-5.0mM	-0.92	-0.72	-0.54	-0.19	-0.97	-0.56	9.96	-9.34	0.42	7
B-5.0mM	-0.92	-0.72	-0.52	-0.20	-0.97	-0.57	10.16	-8.36	-1.11	7
B-5.0mM	-0.93	-0.71	-0.53	-0.22	-0.97	-0.55	10.91	-8.14	-3.34	7
B-5.0mM	-0.93	-0.72	-0.54	-0.23	-0.97	-0.56	7.81	-7.48	-2.82	7
B-8.0mM	-0.88	-0.63	-0.48	-0.15	-0.96	-0.49	33.43	-3.66	-1.10	8
B-8.0mM	-0.88	-0.63	-0.49	-0.18	-0.96	-0.52	33.29	-0.32	-0.92	8
B-8.0mM	-0.88	-0.64	-0.49	-0.18	-0.96	-0.52	32.84	0.75	0.25	8
B-8.0mM	-0.88	-0.64	-0.49	-0.18	-0.96	-0.52	31.77	-1.14	-0.96	8
B-8.0mM	-0.88	-0.63	-0.51	-0.18	-0.96	-0.50	32.27	-1.12	-1.03	8
B-8.0mM	-0.88	-0.64	-0.51	-0.17	-0.97	-0.54	32.52	0.91	2.37	8
B-10.0mM	-0.84	-0.58	-0.50	-0.16	-0.96	-0.49	51.08	8.73	4.27	5
B-10.0mM	-0.85	-0.58	-0.47	-0.16	-0.96	-0.51	48.51	5.87	1.21	5
B-10.0mM	-0.85	-0.58	-0.48	-0.16	-0.96	-0.51	48.73	7.00	1.82	5
B-10.0mM	-0.85	-0.58	-0.47	-0.18	-0.96	-0.49	48.50	8.73	0.36	5
B-10.0mM	-0.85	-0.57	-0.47	-0.18	-0.96	-0.49	50.69	9.06	-0.19	5
B-10.0mM	-0.85	-0.58	-0.47	-0.18	-0.96	-0.51	48.28	8.23	-0.13	5

Table S8. Detection and identification of unknown samples of different concentrations of caffeine (0-10 mM) in black tea using LDA from an array of **P1**/CB[8], **P2**/CB[8] and **P3**/CB[8] (each at pH 3 and 13, buffered). According to the verification, 30 among 32 unknown sample were correctly identified, representing an accuracy of 93.8%.

Unknown samples	Fluorescence Response Pattern						Results LDA (the first three scores)					
	P1/ CB[8] (pH3)	**P2**/ CB[8] (pH3)	**P3**/ CB[8] (pH3)	**P1**/ CB[8] (pH13)	**P2**/ CB[8] (pH13)	**P3**/ CB[8] (pH13)	Factor 1	Factor 2	Factor 3	Group	Identification	Verification
1	-0.96	-0.78	-0.61	-0.22	-0.98	-0.62	-7.31	-13.84	1.81	6	B-2.0mM	B-2.0mM
2	-0.93	-0.71	-0.55	-0.21	-0.97	-0.57	9.38	-8.91	-1.69	7	B-5.0mM	B-5.0mM
3	-0.97	-0.85	-0.68	-0.47	-0.99	-0.70	-23.05	9.19	1.13	1	B-0.2mM	B-0.2mM
4	-0.93	-0.72	-0.55	-0.22	-0.97	-0.58	8.53	-7.47	-1.17	7	B-5.0mM	B-5.0mM
5	-0.88	-0.64	-0.53	-0.19	-0.97	-0.54	30.76	1.37	1.86	8	B-8.0mM	B-8.0mM
6	-0.97	-0.83	-0.66	-0.28	-0.98	-0.65	-19.08	-11.26	4.19	4	B-1.0mM	B-1.0mM
7	-0.88	-0.63	-0.52	-0.21	-0.97	-0.55	33.55	5.12	2.21	8	B-8.0mM	B-8.0mM
8	-0.97	-0.83	-0.67	-0.47	-0.98	-0.71	-18.66	9.62	-1.05	2	B-0.5mM	B-0.5mM
9	-0.97	-0.85	-0.67	-0.48	-0.99	-0.71	-22.14	10.42	0.37	1	B-0.2mM	B-0.2mM
10	-0.85	-0.58	-0.48	-0.17	-0.96	-0.54	49.51	8.63	2.76	5	B-10.0mM	B-10.0mM
11	-0.97	-0.87	-0.68	-0.48	-0.99	-0.73	-25.69	10.30	1.59	3	B-0mM	B-0mM
12	-0.97	-0.85	-0.68	-0.46	-0.98	-0.72	-20.31	9.93	1.48	1	B-0.2mM	B-0.5mM
13	-0.97	-0.82	-0.68	-0.48	-0.98	-0.70	-18.56	10.52	-0.81	2	B-0.5mM	B-0.5mM
14	-0.97	-0.84	-0.63	-0.28	-0.98	-0.65	-19.17	-11.29	2.60	4	B-1.0mM	B-1.0mM
15	-0.96	-0.78	-0.62	-0.25	-0.98	-0.61	-9.26	-11.72	0.62	6	B-2.0mM	B-2.0mM
16	-0.88	-0.64	-0.53	-0.24	-0.97	-0.55	31.60	6.39	0.42	8	B-8.0mM	B-8.0mM
17	-0.97	-0.87	-0.68	-0.49	-0.99	-0.73	-25.85	11.04	1.57	3	B-0mM	B-0mM
18	-0.85	-0.57	-0.50	-0.20	-0.96	-0.49	48.27	10.10	1.01	5	B-10.0mM	B-10.0mM
19	-0.97	-0.86	-0.67	-0.48	-0.99	-0.72	-24.51	10.01	0.66	3	B-0mM	B-0mM
20	-0.97	-0.84	-0.66	-0.28	-0.98	-0.66	-20.51	-11.47	4.58	4	B-1.0mM	B-1.0mM
21	-0.88	-0.64	-0.52	-0.23	-0.96	-0.53	30.24	4.34	-0.52	8	B-8.0mM	B-8.0mM
22	-0.84	-0.58	-0.46	-0.18	-0.96	-0.53	51.87	11.85	2.14	5	B-10.0mM	B-10.0mM
23	-0.97	-0.87	-0.67	-0.48	-0.99	-0.72	-25.03	9.65	0.97	3	B-0mM	B-0mM
24	-0.97	-0.84	-0.67	-0.47	-0.99	-0.71	-20.39	9.85	-0.08	1	B-0.2mM	B-0.2mM
25	-0.97	-0.84	-0.66	-0.29	-0.98	-0.65	-20.85	-10.22	4.16	4	B-1.0mM	B-1.0mM
26	-0.96	-0.78	-0.60	-0.24	-0.97	-0.61	-8.43	-13.18	-0.27	6	B-2.0mM	B-2.0mM
27	-0.97	-0.84	-0.66	-0.47	-0.99	-0.70	-20.86	8.91	-0.59	1	B-0.2mM	B-0.5mM
28	-0.85	-0.58	-0.48	-0.19	-0.96	-0.49	48.36	9.15	0.34	5	B-10.0mM	B-10.0mM
29	-0.93	-0.72	-0.57	-0.23	-0.97	-0.58	8.21	-6.57	0.07	7	B-5.0mM	B-5.0mM
30	-0.97	-0.85	-0.68	-0.48	-0.99	-0.72	-21.87	10.92	1.26	1	B-0.2mM	B-0.2mM
31	-0.96	-0.78	-0.60	-0.25	-0.98	-0.61	-7.09	-11.36	0.26	6	B-2.0mM	B-2.0mM
32	-0.93	-0.71	-0.55	-0.22	-0.97	-0.58	8.40	-8.45	-2.66	7	B-5.0mM	B-5.0mM

Table S9. Training matrix of fluorescence response pattern from an array of **P1-P3** (each at pH 3, 7 and 13, buffered) against different concentrations of caffeine (0-10 mM) in three kinds of teas (B-black tea, G-green tea and O-oolong tea). LDA was carried out and resulting in 6 factors of the canonical scores (the first three scores were shown here) and group generation. The jackknifed classification matrix with cross-validation reveals a 91% accuracy.

Analytes	Fluorescence Response Pattern						Results LDA(the first three scores)			
	P1(pH3)	**P2**(pH3)	**P3**(pH3)	**P1**(pH13)	**P2**(pH13)	**P3**(pH13)	Factor 1	Factor 2	Factor 3	Group
Control	0.00	0.04	0.03	0.03	-0.01	0.02	294.80	5.75	1.48	9
Control	0.00	0.01	0.02	0.02	0.01	0.03	298.80	1.83	2.19	9
Control	0.00	-0.01	0.02	-0.01	0.01	0.02	298.55	1.05	3.06	9
Control	0.00	-0.01	-0.01	-0.02	-0.02	-0.04	289.48	1.01	5.68	9

Control	-0.01	0.02	0.00	-0.04	0.01	-0.03	299.51	0.99	4.61	9
Control	-0.03	0.01	-0.01	-0.02	0.00	0.00	296.15	0.86	2.72	9
B-0mM	-0.88	-0.87	-0.74	-0.20	-0.92	-0.55	-13.30	-42.64	-0.78	3
B-0mM	-0.88	-0.87	-0.75	-0.20	-0.92	-0.55	-13.04	-43.01	-0.76	3
B-0mM	-0.89	-0.87	-0.76	-0.22	-0.92	-0.56	-13.26	-43.53	-0.59	3
B-0mM	-0.89	-0.87	-0.76	-0.22	-0.92	-0.56	-13.66	-43.31	-0.55	3
B-0mM	-0.91	-0.87	-0.73	-0.22	-0.93	-0.55	-14.57	-42.26	-1.80	3
B-0mM	-0.91	-0.88	-0.73	-0.23	-0.93	-0.56	-14.04	-42.94	-0.72	3
B-0.2mM	-0.87	-0.86	-0.72	-0.20	-0.92	-0.53	-10.96	-40.59	-1.54	1
B-0.2mM	-0.87	-0.86	-0.72	-0.19	-0.92	-0.55	-11.51	-41.04	-0.67	1
B-0.2mM	-0.89	-0.85	-0.72	-0.20	-0.92	-0.54	-11.44	-40.74	-1.89	1
B-0.2mM	-0.87	-0.86	-0.73	-0.21	-0.92	-0.55	-11.27	-41.54	-0.64	1
B-0.2mM	-0.90	-0.86	-0.72	-0.21	-0.92	-0.54	-12.05	-41.58	-1.82	1
B-0.2mM	-0.90	-0.86	-0.73	-0.20	-0.92	-0.56	-12.19	-41.87	-1.07	1
B-0.5mM	-0.84	-0.85	-0.72	-0.19	-0.91	-0.52	-9.37	-39.82	-0.83	2
B-0.5mM	-0.84	-0.85	-0.70	-0.20	-0.91	-0.54	-9.16	-39.20	0.49	2
B-0.5mM	-0.84	-0.85	-0.73	-0.22	-0.92	-0.52	-10.84	-39.78	-1.46	2
B-0.5mM	-0.84	-0.85	-0.71	-0.17	-0.91	-0.54	-7.77	-39.81	0.36	2
B-0.5mM	-0.88	-0.85	-0.71	-0.20	-0.92	-0.52	-10.61	-39.65	-2.35	1
B-0.5mM	-0.87	-0.85	-0.71	-0.20	-0.92	-0.54	-11.28	-39.61	-0.95	1
B-1.0mM	-0.85	-0.83	-0.70	-0.20	-0.91	-0.50	-9.46	-37.53	-2.97	4
B-1.0mM	-0.85	-0.84	-0.70	-0.22	-0.91	-0.53	-8.02	-38.64	-1.11	4
B-1.0mM	-0.86	-0.83	-0.69	-0.21	-0.91	-0.52	-7.98	-37.84	-1.88	4
B-1.0mM	-0.86	-0.84	-0.71	-0.19	-0.91	-0.52	-8.86	-39.08	-2.29	4
B-1.0mM	-0.85	-0.84	-0.70	-0.20	-0.91	-0.53	-9.61	-38.86	-1.25	2
B-1.0mM	-0.87	-0.83	-0.71	-0.17	-0.91	-0.50	-9.31	-38.46	-3.79	4
B-2.0mM	-0.80	-0.78	-0.70	-0.17	-0.90	-0.47	-6.09	-33.08	-4.57	6
B-2.0mM	-0.79	-0.79	-0.63	-0.17	-0.90	-0.47	-5.25	-31.09	-2.74	6
B-2.0mM	-0.79	-0.78	-0.66	-0.17	-0.90	-0.48	-5.05	-31.20	-3.12	6
B-2.0mM	-0.80	-0.78	-0.64	-0.16	-0.90	-0.49	-5.18	-31.23	-2.51	6
B-2.0mM	-0.82	-0.78	-0.63	-0.20	-0.91	-0.49	-6.42	-30.68	-2.93	6
B-2.0mM	-0.80	-0.75	-0.66	-0.14	-0.90	-0.47	-5.30	-30.08	-4.21	6
B-5.0mM	-0.69	-0.71	-0.63	-0.16	-0.89	-0.44	-0.54	-24.04	-3.27	7
B-5.0mM	-0.72	-0.75	-0.62	-0.19	-0.90	-0.42	-2.56	-25.89	-4.33	7
B-5.0mM	-0.71	-0.71	-0.60	-0.17	-0.89	-0.44	0.17	-23.16	-3.12	7
B-5.0mM	-0.71	-0.71	-0.60	-0.14	-0.89	-0.45	-0.16	-22.99	-3.00	7
B-5.0mM	-0.75	-0.71	-0.62	-0.13	-0.89	-0.46	-0.13	-25.15	-3.84	7
B-5.0mM	-0.72	-0.71	-0.63	-0.19	-0.89	-0.44	-1.64	-24.10	-3.82	7
B-8.0mM	-0.64	-0.63	-0.53	-0.13	-0.88	-0.38	3.58	-13.21	-5.70	8
B-8.0mM	-0.67	-0.66	-0.55	-0.10	-0.88	-0.37	4.51	-16.70	-6.71	8
B-8.0mM	-0.64	-0.62	-0.49	-0.13	-0.88	-0.40	4.19	-11.18	-4.26	8
B-8.0mM	-0.64	-0.62	-0.51	-0.09	-0.88	-0.40	3.52	-12.34	-4.18	8
B-8.0mM	-0.68	-0.64	-0.53	-0.11	-0.88	-0.37	3.47	-15.05	-6.99	8
B-8.0mM	-0.63	-0.62	-0.53	-0.19	-0.88	-0.44	3.87	-12.99	-1.54	8
B-10.0mM	-0.58	-0.59	-0.45	-0.07	-0.85	-0.18	13.24	-5.73	-15.06	5
B-10.0mM	-0.62	-0.62	-0.45	-0.11	-0.85	-0.19	14.28	-9.36	-14.38	5
B-10.0mM	-0.58	-0.58	-0.43	-0.04	-0.85	-0.20	13.87	-4.90	-13.65	5
B-10.0mM	-0.60	-0.60	-0.43	-0.07	-0.85	-0.19	13.49	-5.66	-13.96	5
B-10.0mM	-0.64	-0.58	-0.46	-0.09	-0.85	-0.19	13.62	-6.76	-16.43	5
B-10.0mM	-0.59	-0.55	-0.49	-0.14	-0.85	-0.23	13.96	-5.92	-13.36	5
G-0mM	-0.48	-0.49	-0.24	-0.29	-0.96	-0.54	-20.31	16.18	7.77	12
G-0mM	-0.48	-0.48	-0.23	-0.29	-0.96	-0.55	-19.83	16.79	8.66	12

G-0mM	-0.46	-0.50	-0.24	-0.29	-0.97	-0.55	-20.51	15.96	9.53	12
G-0mM	-0.47	-0.50	-0.25	-0.32	-0.96	-0.56	-19.90	14.97	9.71	12
G-0mM	-0.49	-0.49	-0.24	-0.30	-0.97	-0.57	-20.87	15.99	9.34	12
G-0mM	-0.48	-0.49	-0.22	-0.33	-0.97	-0.56	-20.48	16.80	9.37	12
G-0.2mM	-0.46	-0.48	-0.22	-0.29	-0.96	-0.54	-18.71	17.67	8.43	10
G-0.2mM	-0.46	-0.48	-0.22	-0.30	-0.96	-0.54	-19.11	18.08	8.27	10
G-0.2mM	-0.45	-0.49	-0.23	-0.31	-0.96	-0.53	-18.97	16.65	8.56	10
G-0.2mM	-0.47	-0.48	-0.22	-0.31	-0.96	-0.54	-18.96	17.17	8.56	10
G-0.2mM	-0.46	-0.48	-0.23	-0.32	-0.96	-0.56	-19.19	17.60	9.49	10
G-0.2mM	-0.48	-0.48	-0.24	-0.34	-0.96	-0.55	-18.81	16.48	8.33	10
G-0.5mM	-0.44	-0.46	-0.20	-0.26	-0.96	-0.52	-18.07	20.41	7.71	11
G-0.5mM	-0.45	-0.47	-0.21	-0.26	-0.96	-0.52	-18.37	19.43	7.43	11
G-0.5mM	-0.45	-0.46	-0.22	-0.26	-0.96	-0.52	-18.61	19.14	7.65	11
G-0.5mM	-0.44	-0.46	-0.21	-0.27	-0.96	-0.53	-17.76	19.72	8.18	11
G-0.5mM	-0.44	-0.45	-0.22	-0.29	-0.96	-0.51	-18.47	20.72	6.88	11
G-0.5mM	-0.45	-0.46	-0.22	-0.30	-0.96	-0.52	-18.40	19.28	7.13	11
G-1.0mM	-0.44	-0.43	-0.20	-0.25	-0.96	-0.50	-17.58	22.43	5.88	13
G-1.0mM	-0.42	-0.43	-0.21	-0.24	-0.96	-0.51	-17.57	22.69	6.63	13
G-1.0mM	-0.44	-0.44	-0.19	-0.25	-0.96	-0.50	-17.72	22.73	5.95	13
G-1.0mM	-0.44	-0.42	-0.20	-0.26	-0.96	-0.51	-17.25	22.91	6.33	13
G-1.0mM	-0.42	-0.42	-0.21	-0.26	-0.96	-0.50	-17.21	23.06	6.31	13
G-1.0mM	-0.45	-0.44	-0.20	-0.28	-0.96	-0.50	-17.07	21.94	5.86	13
G-2.0mM	-0.39	-0.39	-0.13	-0.20	-0.95	-0.42	-15.59	29.97	2.49	15
G-2.0mM	-0.37	-0.38	-0.14	-0.22	-0.95	-0.43	-15.14	30.28	3.61	15
G-2.0mM	-0.38	-0.39	-0.13	-0.23	-0.95	-0.42	-14.50	29.85	3.45	15
G-2.0mM	-0.37	-0.37	-0.12	-0.22	-0.95	-0.40	-15.23	32.55	2.04	15
G-2.0mM	-0.38	-0.40	-0.15	-0.23	-0.95	-0.40	-15.60	29.30	1.89	15
G-2.0mM	-0.37	-0.37	-0.15	-0.24	-0.95	-0.40	-15.49	31.15	1.23	15
G-5.0mM	-0.35	-0.31	-0.10	-0.21	-0.95	-0.39	-12.13	37.60	0.38	16
G-5.0mM	-0.37	-0.30	-0.12	-0.21	-0.95	-0.37	-12.46	37.09	-1.97	16
G-5.0mM	-0.36	-0.30	-0.12	-0.22	-0.94	-0.38	-11.80	36.96	-0.65	16
G-5.0mM	-0.36	-0.29	-0.11	-0.22	-0.95	-0.36	-12.88	38.92	-2.05	16
G-5.0mM	-0.32	-0.30	-0.11	-0.21	-0.94	-0.34	-11.68	38.93	-1.74	16
G-5.0mM	-0.35	-0.30	-0.12	-0.23	-0.95	-0.33	-12.74	38.48	-3.61	16
G-8.0mM	-0.31	-0.19	-0.02	-0.19	-0.94	-0.28	-8.61	50.56	-6.32	17
G-8.0mM	-0.31	-0.21	-0.06	-0.18	-0.94	-0.24	-10.26	48.59	-8.94	17
G-8.0mM	-0.31	-0.17	-0.07	-0.19	-0.94	-0.28	-9.52	50.04	-7.11	17
G-8.0mM	-0.29	-0.21	-0.04	-0.20	-0.94	-0.22	-8.43	49.96	-9.27	17
G-8.0mM	-0.27	-0.20	-0.03	-0.21	-0.94	-0.23	-9.31	50.75	-8.06	17
G-8.0mM	-0.29	-0.19	-0.07	-0.20	-0.94	-0.23	-9.20	49.77	-9.44	17
G-10.0mM	-0.31	-0.16	-0.03	-0.17	-0.93	-0.21	-6.60	52.85	-11.56	14
G-10.0mM	-0.29	-0.16	-0.06	-0.16	-0.93	-0.23	-6.86	51.48	-9.74	14
G-10.0mM	-0.33	-0.15	-0.03	-0.16	-0.93	-0.23	-7.38	52.88	-11.02	14
G-10.0mM	-0.30	-0.14	-0.04	-0.17	-0.93	-0.16	-6.23	54.34	-14.31	14
G-10.0mM	-0.30	-0.15	0.01	-0.20	-0.93	-0.20	-6.47	55.73	-11.06	14
G-10.0mM	-0.32	-0.14	-0.05	-0.17	-0.93	-0.18	-6.15	53.34	-14.40	14
O-0mM	-0.61	-0.67	-0.55	-0.14	-0.97	-0.52	-24.78	-11.52	2.31	20
O-0mM	-0.61	-0.69	-0.55	-0.11	-0.97	-0.53	-24.53	-12.97	3.27	20
O-0mM	-0.63	-0.70	-0.52	-0.07	-0.97	-0.53	-25.37	-12.86	3.19	20
O-0mM	-0.63	-0.67	-0.56	-0.08	-0.97	-0.54	-25.49	-12.29	2.26	20
O-0mM	-0.64	-0.67	-0.56	-0.14	-0.97	-0.51	-25.49	-12.38	0.73	20
O-0mM	-0.63	-0.68	-0.53	-0.21	-0.97	-0.53	-25.74	-11.53	2.86	18

O-0.2mM	-0.61	-0.66	-0.54	-0.09	-0.97	-0.52	-24.71	-10.12	2.03	18
O-0.2mM	-0.63	-0.68	-0.54	-0.07	-0.97	-0.52	-24.96	-12.08	2.01	20
O-0.2mM	-0.62	-0.68	-0.51	-0.19	-0.97	-0.53	-25.10	-10.19	3.29	18
O-0.2mM	-0.62	-0.66	-0.51	-0.11	-0.97	-0.53	-24.84	-9.29	2.74	18
O-0.2mM	-0.60	-0.66	-0.53	-0.13	-0.97	-0.52	-25.01	-9.87	2.38	18
O-0.2mM	-0.63	-0.66	-0.53	-0.20	-0.97	-0.52	-24.52	-10.44	2.12	18
O-0.5mM	-0.59	-0.66	-0.55	-0.18	-0.97	-0.53	-23.57	-10.80	3.05	19
O-0.5mM	-0.60	-0.66	-0.56	-0.10	-0.97	-0.53	-23.97	-11.21	2.61	19
O-0.5mM	-0.61	-0.64	-0.55	-0.11	-0.97	-0.53	-23.59	-9.68	2.40	19
O-0.5mM	-0.60	-0.64	-0.56	-0.15	-0.97	-0.54	-23.74	-9.81	3.12	19
O-0.5mM	-0.59	-0.66	-0.57	-0.17	-0.97	-0.53	-24.43	-10.94	3.24	19
O-0.5mM	-0.59	-0.65	-0.55	-0.17	-0.97	-0.54	-23.78	-10.07	3.60	19
O-1.0mM	-0.59	-0.63	-0.49	-0.15	-0.96	-0.51	-22.51	-5.87	2.44	21
O-1.0mM	-0.58	-0.64	-0.49	-0.14	-0.97	-0.53	-23.63	-6.77	3.72	21
O-1.0mM	-0.61	-0.63	-0.49	-0.15	-0.97	-0.51	-23.24	-6.61	1.65	21
O-1.0mM	-0.57	-0.63	-0.51	-0.17	-0.97	-0.54	-23.73	-6.50	4.15	21
O-1.0mM	-0.59	-0.65	-0.49	-0.18	-0.97	-0.53	-23.72	-7.12	3.91	21
O-1.0mM	-0.60	-0.64	-0.51	-0.20	-0.97	-0.53	-23.78	-7.82	3.20	21
O-2.0mM	-0.53	-0.57	-0.44	-0.25	-0.95	-0.52	-17.02	0.68	4.80	23
O-2.0mM	-0.54	-0.57	-0.47	-0.11	-0.95	-0.51	-17.92	-0.70	2.55	23
O-2.0mM	-0.53	-0.57	-0.43	-0.09	-0.95	-0.52	-17.43	0.55	4.09	23
O-2.0mM	-0.52	-0.57	-0.46	-0.11	-0.95	-0.51	-17.71	-0.63	3.79	23
O-2.0mM	-0.54	-0.57	-0.42	-0.11	-0.95	-0.53	-16.92	0.51	4.61	23
O-2.0mM	-0.54	-0.57	-0.44	-0.10	-0.95	-0.53	-17.89	-0.36	4.02	23
O-5.0mM	-0.49	-0.53	-0.43	-0.08	-0.95	-0.48	-16.78	4.85	2.17	24
O-5.0mM	-0.49	-0.54	-0.42	-0.09	-0.95	-0.46	-16.97	4.86	1.12	24
O-5.0mM	-0.51	-0.54	-0.43	-0.08	-0.95	-0.47	-16.79	3.42	1.43	24
O-5.0mM	-0.50	-0.54	-0.41	-0.06	-0.95	-0.48	-16.25	4.23	2.35	24
O-5.0mM	-0.52	-0.52	-0.46	-0.07	-0.95	-0.47	-15.27	3.68	-0.15	24
O-5.0mM	-0.49	-0.51	-0.45	-0.08	-0.95	-0.50	-14.88	4.82	2.40	24
O-8.0mM	-0.45	-0.48	-0.35	-0.08	-0.94	-0.42	-11.75	11.62	0.23	25
O-8.0mM	-0.45	-0.49	-0.36	-0.07	-0.94	-0.44	-12.35	10.86	1.27	25
O-8.0mM	-0.44	-0.48	-0.35	-0.06	-0.94	-0.44	-12.77	11.85	1.40	25
O-8.0mM	-0.45	-0.50	-0.36	-0.05	-0.95	-0.44	-14.76	10.60	1.15	25
O-8.0mM	-0.46	-0.47	-0.37	-0.08	-0.94	-0.46	-14.00	11.46	1.41	25
O-8.0mM	-0.45	-0.47	-0.37	-0.05	-0.94	-0.47	-12.72	11.03	2.08	25
O-10.0mM	-0.42	-0.44	-0.36	-0.01	-0.90	-0.38	0.04	12.76	-1.81	22
O-10.0mM	-0.42	-0.44	-0.33	-0.03	-0.91	-0.36	-2.83	14.47	-2.57	22
O-10.0mM	-0.46	-0.44	-0.36	-0.01	-0.91	-0.41	-3.18	11.92	-1.36	22
O-10.0mM	-0.47	-0.47	-0.35	-0.04	-0.90	-0.40	-0.56	9.97	-1.36	22
O-10.0mM	-0.45	-0.45	-0.36	-0.04	-0.90	-0.40	-0.15	11.50	-1.49	22
O-10.0mM	-0.42	-0.44	-0.35	-0.04	-0.90	-0.39	-0.09	12.94	-1.40	22

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