

## ***Supplementary Information:***

### **An array sensor consisting of a single indicator with multiple concentrations and its application in ions discrimination†**

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## 1. Experimental

Deionized water was used throughout the whole work. The indicators and metal salts ( $\text{NiCl}_2$ ,  $\text{CoCl}_2$ ,  $\text{CuCl}_2$ ,  $\text{ZnCl}_2$ ,  $\text{PbCl}_2$ ,  $\text{CdCl}_2$ , and  $\text{HgCl}_2$ ) used were analytical-reagent grade, obtained from Alfa Aesar Co., and used without further purification unless otherwise specified. All anion salts ( $\text{NaF}$ ,  $\text{NaCl}$ ,  $\text{NaBr}$ ,  $\text{NaI}$ ,  $\text{Na}_2\text{S}$ ,  $\text{Na}_3\text{PO}_4$ ,  $\text{Na}_2\text{CrO}_4$ , and  $\text{Na}_2\text{C}_2\text{O}_4$ ) were purchased from Shanghai Jingchun Reagent Co., P. R. China, and were metals basis (99.99%). UV-Vis spectra were obtained from TU-1901 UV/Vis spectrometer (Beijing Perkinje General Instrument Co., Ltd, P. R. China).

All stock solutions of anions were prepared using deionized water and were adjusted to pH 6.5 by the addition of  $\text{NaOH}$  or  $\text{HCl}$  utilizing a Titrator T50 (Mettler Toledo Co.) and all the solutions were used immediately after preparation. The heavy-metal ions stock solutions were prepared using acetic acid buffer (0.01 M, pH=5.6). The sensor array composition is listed separately as below.

Sensor array for $\text{SO}_4^{2-}$ and $\text{PO}_4^{3-}$ sensing			Sensor array for eight anions sensing			Sensor array for seven heavy-metal ions sensing	
Indicator #	1-(2-pyridylazo)-2-naphthol ( $\mu\text{M}$ )	$\text{Pb}^{2+}$ (mM)	Indicator #	3,5-diBr-PADAP ( $\mu\text{M}$ )	$\text{Hg}^{2+}$ ( $\mu\text{M}$ )	Indicator #	1-(2-pyridylazo)-2-naphthol ( $\mu\text{M}$ )
1	35	0.05	1	25	3	1	5
2	35	0.10	2	25	6	2	10
3	35	0.15	3	25	9	3	20
4	35	0.20	4	25	12	4	40
5	35	0.25	5	25	15	5	60
6	35	0.30	6	25	18	6	80
7	35	0.35	7	25	21	7	100
8	35	0.40	8	25	24	8	200
9	35	0.45	9	25	27	9	300
10	35	0.50	10	25	30	10	400
11	35	0.55	11	25	45	11	500
12	35	0.60	12	25	60	12	600

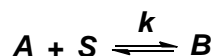
198  $\mu\text{L}$  aqueous solutions (for anion sensing: ethanol/water = 50%, v/v, pH 6.5; for heavy-metal ions sensing: ethanol/acetic acid buffer (0.01 M) = 50%, v/v, pH 5.6) of 12 indicators were loaded in a  $6 \times 2$  polystyrene well plate (from 96-well plate). Each well was an individual cylinder with 10 mm tall (the inner diameter = 6 mm; the out diameter = 8 mm). The wells were then sealed immediately by plastic film to prevent the solvent evaporation. The “before” image was acquired. The Epson V200 flatbed scanner with a built-in transparency unit was utilized to collect the full digital images of the array from the bottom of the  $6 \times 2$  well plate. The transparency scan unit was used (usually for negative scan) to avoid the light reflection of solutions. Uniform images of solutions were obtained.

2  $\mu\text{L}$  individual corresponding anions or heavy-metal ions stock solutions were separately added to the corresponding  $6 \times 2$  array to reach the desired concentrations. After three minutes mixing, the “after” image was acquired.

Digitization of the color differences was performed using Adobe Photoshop software package. Difference maps were obtained by taking the difference of average red, green, and blue (RGB) values from the center ( $\phi = 4$  mm, 80% of the total size) of each individual well from the “before” and “after” images. The chemometric analysis was carried out on the color difference vectors using the Multi-Variate Statistical Package; in all cases, minimum variance (i.e., “Ward’s Method”) was used for hierarchical clustering analysis (HCA).

## 2. Schemes

**Scheme S1. The deduction of the initial concentration of indicator A.**



let 0 and 1 denote different chemical species (analytes) with different equilibrium coefficients;

let x and y denote the same indicator at different concentrations;

let  $k$  denote the equilibrium coefficient when the indicator reacts with an analyte;

let  $[A]$  denote the initial concentration of the indicator A;

let  $[B]$  denote the concentration of product produced by the reaction of the indicator and the analyte;

let  $[S]$  denote the initial concentration of the analyte;

For the same indicator at different concentrations  $A_x$  and  $A_y$

$$k = \frac{[B]}{([A] - [B])([S] - [B])}$$

Thus, the concentration of indicator A could be deduced as follow:

$$[A] = \frac{[B]}{k([S] - [B])} + [B]$$

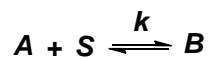
If the final color of analyte 0 and 1 are same after the reaction with  $A_x$ , that is,  $[B]_{0x} = [B]_{1x} = [B]_x$ , then,

$$[A]_x = \frac{[B]_{0x}}{k_0([S]_0 - [B]_{0x})} + [B]_{0x} = \frac{[B]_{1x}}{k_1([S]_1 - [B]_{1x})} + [B]_{1x}$$

Similarly, if the final color of analyte 0 and 1 are same after the reaction with  $A_y$ , that is,  $[B]_{0y} = [B]_{1y} = [B]_y$ , then,

$$[A]_y = \frac{[B]_{0y}}{k_0([S]_0 - [B]_{0y})} + [B]_{0y} = \frac{[B]_{1y}}{k_1([S]_1 - [B]_{1y})} + [B]_{1y}$$

**Scheme S2. The calculation for equilibrium constants.**



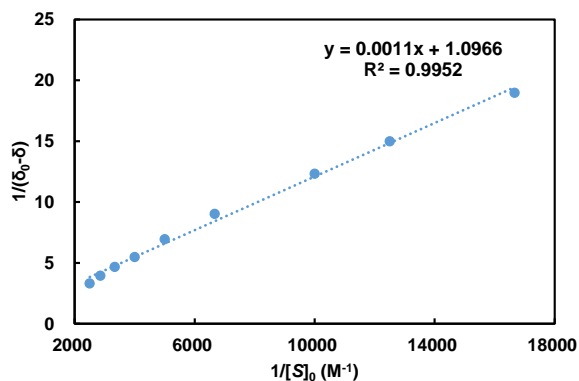
Then the following equation is valid <sup>[1]</sup>,

$$\frac{1}{\delta_0 - \delta} = \frac{1}{[A]_0 \Delta \varepsilon L} + \frac{1}{[A]_0 \Delta \varepsilon L k [S]_0}$$

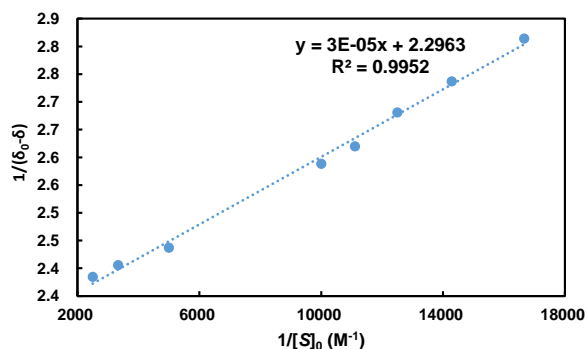
Where  $\delta_0$  and  $\delta$  are the absorbance of A and mixed solution, respectively.  $[A]_0$  and  $[S]_0$  are initial concentration of A and S.  $L$  is the path length.  $k$  is the equilibrium constant, which can be very approximately calculated from the slope of the straight line obtained by plotting  $\frac{1}{\delta_0 - \delta}$  vs

$$\frac{1}{[S]_0}.$$

For sulphate anions,  $k=995 \text{ M}^{-1}$ . ( $\delta_0=0.4247$ )

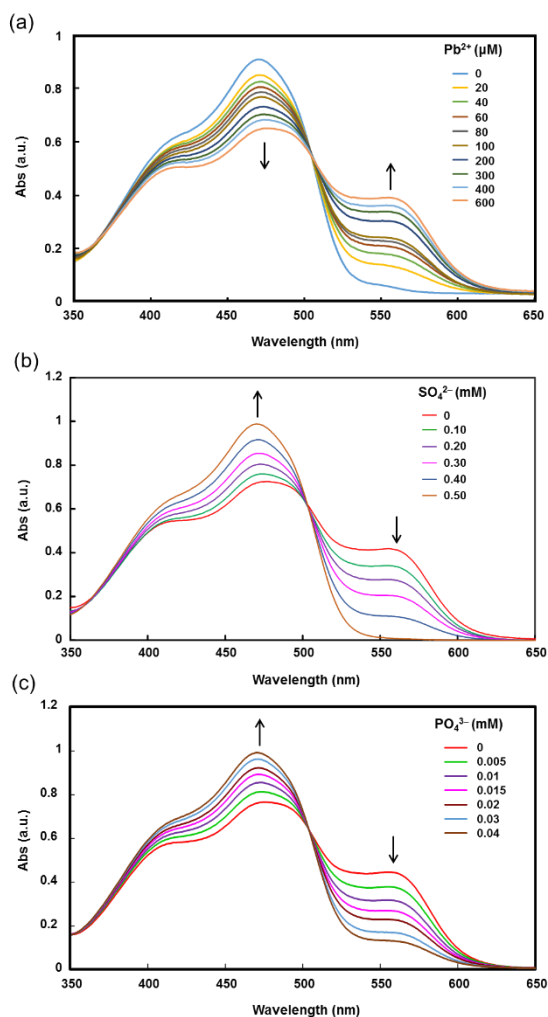


For phosphate anions,  $k=76543 \text{ M}^{-1}$ . ( $\delta_0=0.4247$ )

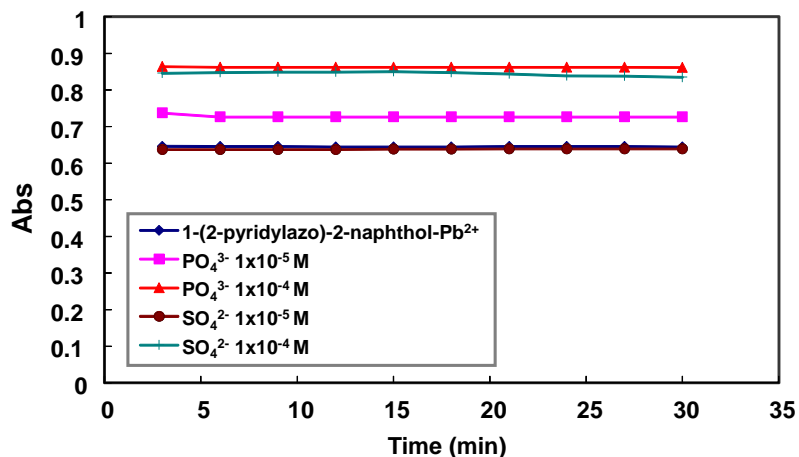


<sup>[1]</sup> Ohga, K.; Takashima, Y.; Takahashi, H.; Kawaguchi, Y.; Yamaguchi, H.; Harada, A. *Macromolecules*, **2005**, *38*, 5897-5904.

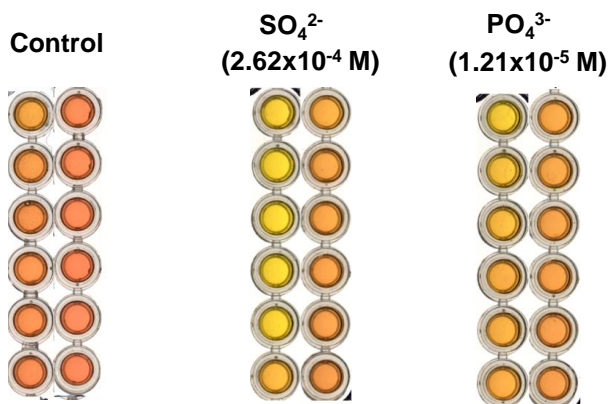
### 3. Figures and tables



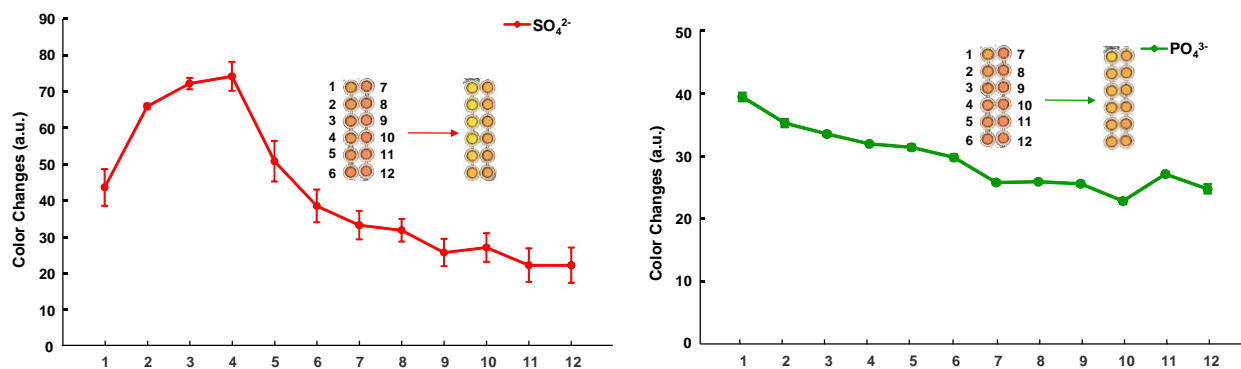
**Fig. S1.** (a) Absorption spectra of 1-(2-pyridylazo)-2-naphthol ( $3.5 \times 10^{-5}$  M) after 3 min upon the addition of  $Pb^{2+}$  at increasing concentrations in ethanol/acetic acid buffer solution (50% v/v, 0.01 M, pH 5.6); (b) Absorption spectra of 1-(2-pyridylazo)-2-naphthol ( $3.5 \times 10^{-5}$  M) -  $Pb^{2+}$  ( $5 \times 10^{-4}$  M) chelating compound after 3 min upon the addition of increasing concentrations of sulfate anion in ethanol/water solution (50% v/v, pH 6.5); (c) Absorption spectra of 1-(2-pyridylazo)-2-naphthol ( $3.5 \times 10^{-5}$  M) -  $Pb^{2+}$  ( $5 \times 10^{-4}$  M) chelating compound after 3 min upon the addition of increasing concentrations of phosphate anion in ethanol/water solution (50% v/v, pH 6.5).



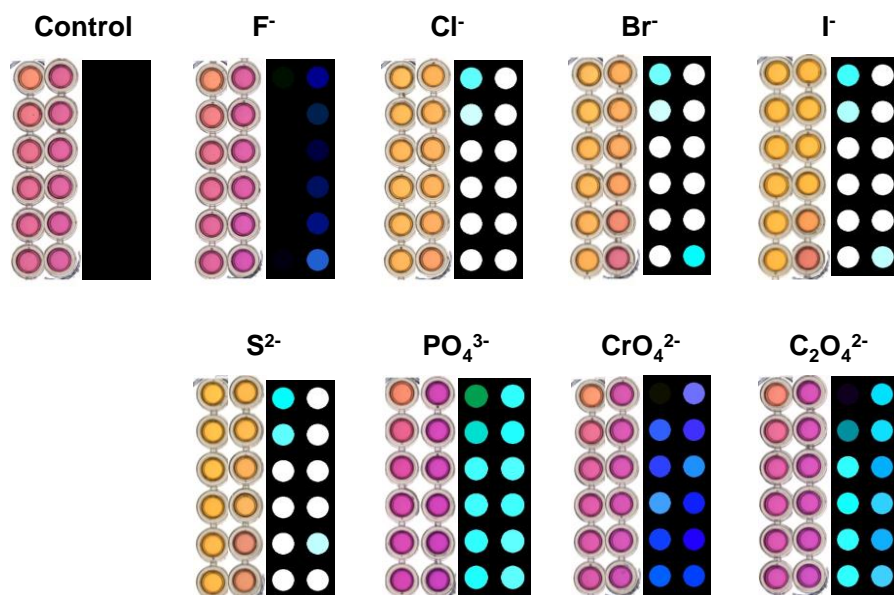
**Fig. S2.** The final color of 1-(2-pyridylazo)-2-naphthol-Pb<sup>2+</sup> displacement reaction versus response time for sulfate and phosphate at different concentrations in ethanol/water solution (50% v/v, pH 6.5). As shown, three minute is enough to get equilibrium for both sulfate and phosphate anions.



**Fig. S3.** Images of 6×2 sensor array after 3 min upon the addition of SO<sub>4</sub><sup>2-</sup> and PO<sub>4</sub><sup>3-</sup> anions.

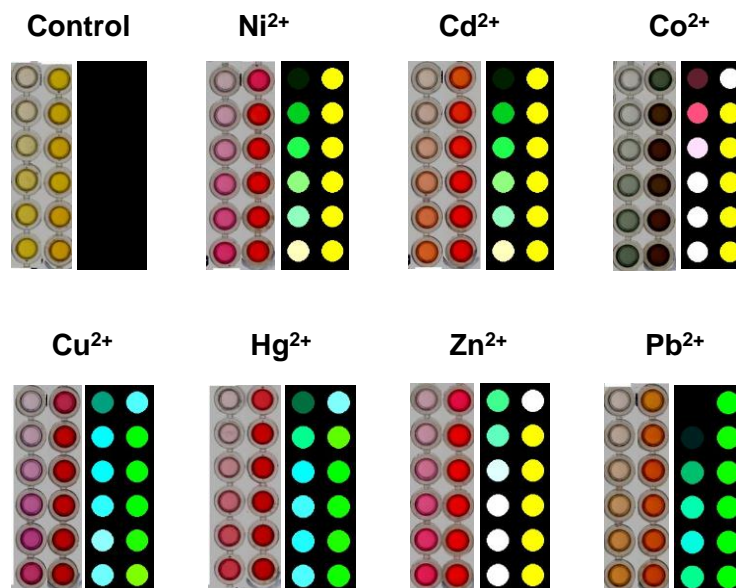


**Fig. S4.** The color changes (defined as  $\sqrt{\Delta R^2 + \Delta G^2 + \Delta B^2}$ ) of each individual sensing unit for 1-(2-pyridylazo)-2-naphthol- $\text{Pb}^{2+}$  sensor array. All experiments were run in quintuplicate.

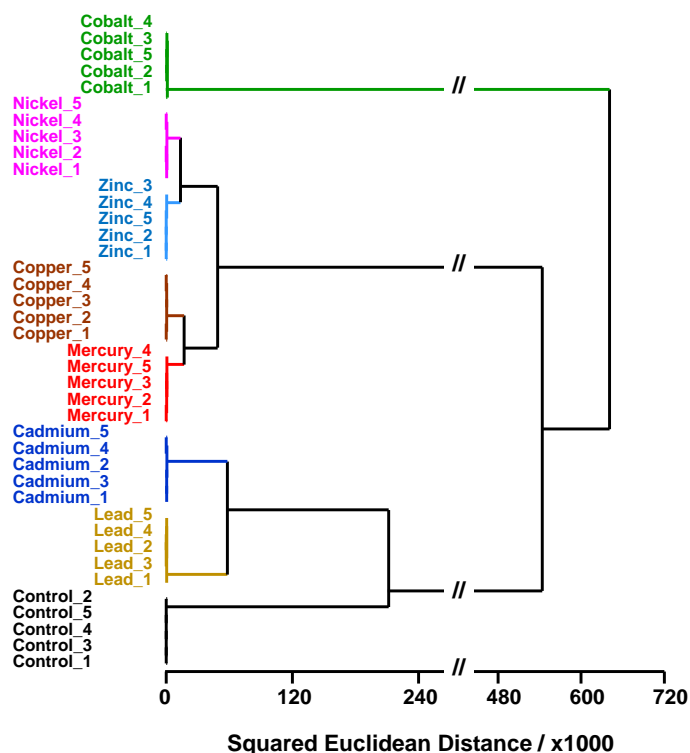


**Fig. S5.** Images and color difference maps of eight anions at their wastewater discharge standard concentrations after 2 min of exposure. For display purposes, the color ranges of these difference maps are expanded from 4 to 8 bits per color (RGB range of 4-19 expanded to 0-255).





**Fig. S6.** Images and color difference maps of seven heavy-metal ions at 50  $\mu\text{M}$  after 2 min of exposure. For display purposes, the color ranges of these difference maps are expanded from 4 to 8 bits per color (RGB range of 4-19 expanded to 0-255).



**Fig. S7.** Hierarchical cluster analysis for seven heavy-metal ions at equal concentrations (50  $\mu\text{M}$ ) and a control. All experiments were run in quintuplicate; no confusions or errors in classification were observed in 40 trials.

**Table S1.** The Chinese wastewater discharge standard concentration for eight anions. <sup>[2]</sup>

Anions	Concentration (M)
F <sup>-</sup>	$5.60 \times 10^{-4}$
Cl <sup>-</sup>	$7.05 \times 10^{-3}$
Br <sup>-</sup>	$5.00 \times 10^{-5}$
I <sup>-</sup>	$5.00 \times 10^{-5}$
S <sup>2-</sup>	$3.00 \times 10^{-5}$
CrO <sub>4</sub> <sup>2-</sup>	$2.88 \times 10^{-5}$
PO <sub>4</sub> <sup>3-</sup>	$1.00 \times 10^{-4}$
C <sub>2</sub> O <sub>4</sub> <sup>2-</sup>	$5.00 \times 10^{-4}$

- <sup>[2]</sup> (a) Feng, L.; Li, H.; Li, X.; Chen, L.; Shen, Z.; Guan, Y. F. *Anal. Chim. Acta*, **2012**, 743, 1;  
(b) Chinese National Standard, Integrated Wastewater-Discharge Standard. GB 8978, **1996**.

**Table S2.** A full digital database for eight anions sensing.

	R1	G1	B1	R2	G2	B2	R3	G3	B3	R4	G4	B4	R5	G5	B5	R6	G6	B6	R7	G7	B7	R8	G8	B8	R9	G9	B9	R10	G10	B10	R11	G11	B11	R12	G12	B12
<b>Fluoride_1</b>	6.19101	7.98875	-2.2022	-2.2247	-8.4944	6.8427	3.88763	1.26967	-5.4045	-0.7978	-6.9393	9.96629	2.80899	-2.7079	-1.3483	-3.4382	-3.8989	6.55055	1	-1.2921	2.69663	-3.7865	-10.101	6.49439	0.30338	-2.6292	3.97752	-0.6966	-4.3034	13.8539	-1.4831	-7.7303	3.70786	-3.3596	-6.8876	20.9775
<b>Fluoride_2</b>	3.34831	5.47191	-2.1798	-0.2135	-2.7753	13.5056	-0.2809	0.96629	-4.2359	-2.4832	-6.7528	5.95951	-1.6292	-1.1461	-0.573	-2.2135	-4.5506	8.89663	-1.1573	-3.8539	2.62921	-2.3371	-5.9651	10.6067	-2.3708	-4.2247	3.55055	-2.8202	-5.4607	12.9438	-6.9666	-4.9551	5.52809	-6.3371	-10.73	17.5393
<b>Fluoride_3</b>	9.39325	10.3708	3.52809	0.5618	-2.2247	14.1461	5.44943	6.11237	0.46068	1.51685	-1.3483	15.1124	5.31462	2.32584	4.93259	-1.427	-5.2135	9.77528	-1.1012	-3.5281	1.88763	-3.8539	-7.1655	8.33708	1.86517	3.20225	9.04494	-0.6292	-3.382	14.6854	-1	-1.8676	6.10112	-5.1461	-10.899	18.1236
<b>Fluoride_4</b>	3.67415	6.4382	-0.3034	-0.0225	-3.0899	13.955	2.47191	2.1573	-3.4607	-0.9326	-0.4494	13.1124	3.30338	2.39326	4.50562	-3.3258	-8	8.41573	1.22472	-2.1685	4.16853	-3.1461	-8.1124	9.61798	1.93259	0.8764	8.76404	-0.8202	-3.764	14.1011	-1.1124	-7.2921	6.19101	-4.7528	-10.416	19.2247
<b>Fluoride_5</b>	7.11235	11.5168	3.88764	2.37079	0.04495	12.3595	4.42696	7.4045	-0.6629	0.79775	-1.8427	10.3146	6.7191	5.13483	5.29213	-1.3595	-3.6966	8.8427	5.16855	2.22472	3.98875	-2.7753	-9.2472	5.52809	2.78651	1.19101	5.62921	-2	-3.5506	13.0112	0.78651	-5.191	5.29213	-5.2921	-13.775	15.3146
<b>Chloride_1</b>	10.5281	48.4607	-27.067	33.1348	89.1236	-56.303	17.1798	72.9326	-46.944	31.9438	89.7079	-55.348	21.9775	79.3034	-51.596	29.8877	85.3708	-66.427	26.6966	85.2697	-58.36	28.7641	84.4607	-65.764	27.618	89.7753	-56.034	34.5393	83.8315	-64.079	29.8652	81.8989	-61.528	34.1685	62.4944	-54.708
<b>Chloride_2</b>	9.79775	45.9663	-23.281	33.0899	82.5281	-56.966	17.1461	68.3034	-43.966	31.9438	84.382	-57.652	23.9214	75.427	-51.169	30	85.618	-60.393	26.8202	82.4831	-52.73	28.7978	79.2135	-66.719	27.4719	85.1685	-56.292	34.7303	78.4831	-67.157	29.8652	75.6854	-65.292	33.9888	62.8315	-58.944
<b>Chloride_3</b>	11.4607	46.6067	-20.978	32.8427	79.8202	-60.596	17.2584	65.1348	-45.416	31.8876	80.5618	-59.067	22.6292	71.7303	-51.865	29.9663	81.7079	-62.876	26.9326	81.3483	-54.034	28.7978	78.4719	-68.135	27.618	82.0449	-58.416	34.6741	78.3483	-63.494	29.7753	76.6067	-60.64	33.1798	62.0899	-53.584
<b>Chloride_4</b>	11.5056	47.573	-21.753	33.1348	77.1236	-59.315	17.1798	65.809	-44.303	31.7977	78.0449	-59.101	23.9551	71.5506	-50.112	29.9214	78.1011	-61.258	26.809	79.9775	-51.618	28.809	76.1685	-66.82	27.618	80.7191	-55.236	34.7079	76.9438	-61.618	29.8652	73.5056	-57.427	33.6741	62.3483	-51.91
<b>Chloride_5</b>	8.70786	45.7079	-21.584	32.9213	74.7528	-55.697	17.2135	66.4494	-44.09	31.809	73.6742	-53.472	22.7753	71.9551	-50.36	29.8989	80.3371	-59.719	26.9214	83.4494	-51.112	28.7079	78.6742	-66.292	27.5393	82.5618	-55.101	34.6629	80.9663	-62.798	29.8539	75.9663	-57.157	33.9438	69.4157	-49.955
<b>Bromide_1</b>	11.2921	50.0899	-28.989	30.4382	70.3371	-61	17.1573	66.3708	-50.64	31.8966	74.0225	-58.011	23.7303	69.8482	-54.933	29.3483	70.3146	-60.124	26.4944	78.8989	-54.079	27.2584	81.3258	-63.225	27.3146	77.9101	-57.528	22.8202	48.3933	-48.461	29.4607	68.9326	-61.584	4.88763	20.8315	-26.371
<b>Bromide_2</b>	11.5056	42.1573	-24.169	30.8315	71.7978	-50.831	17.2584	67.1236	-43	30.9101	69.0112	-53.876	23.9551	76.0112	-44.685	26.8652	65.0449	-58.888	26.9326	76.9663	-51.371	24.2584	59.5618	-58.281	27.1685	71.2584	-57.292	20.382	45.8989	-44.157	28.1124	66.5955	-60.292	3.82022	14.775	-22.854
<b>Bromide_3</b>	3.10112	35.7079	-33.652	31.3371	70.1685	-53.697	16.6292	66.9775	-44.719	30.8989	68.8652	-53.798	21.7753	68.6854	-51.079	29.2921	67.3258	-53.528	26.7416	74.8764	-55.663	26.8764	60.3596	-53.73	27.2472	73.2135	-56.809	20.382	42.9101	-43.056	29.3259	70.236	-55.045	1.76404	14.8652	-24.933
<b>Bromide_4</b>	11.4932	45.955	-20.843	32.9213	74.9551	-52.09	16.4944	67.5056	-43.966	31.6517	71.382	-53.494	23.7641	72.0225	-51.685	30.0899	71.7641	-54.404	25.7753	75.6741	-54.202	27.3034	59.3506	-60.809	27.4832	75.4157	-53.539	23.3146	43.7303	-46.73	28.6405	67.6742	-63.843	9.31461	16.9663	-24.09
<b>Bromide_5</b>	11.5056	54.1573	-21.674	31.3933	73.8202	-55.742	17.2022	70.6629	-44.899	30.8876	74.2135	-57.067	23.9551	77.5281	-50.101	29.6742	70.6966	-62.18	26.5056	77.382	-58.292	26.2697	64.7079	-60.764	26.6629	76.9438	-53.697	21.4719	47.8584	-50.011	28.8427	70.0337	-61.292	6.97752	19.4157	-28.618
<b>Iodide_1</b>	8.78889	51.32	-20.4	30.4444	95.0311	-58.796	15.5956	75.9422	-35.196	32.4178	93.6533	-61.902	20.9422	81.6133	-47.058	30.0133	93.5733	-62.951	23.84	87.4267	-54.649	30.2356	95.9822	-61.484	25.0978	91.6844	-51.449	31.6533	64.3733	-56.431	30.4	90.0311	-56.64	16.4889	35.5333	-35.6
<b>Iodide_2</b>	4.10223	44.2311	-20.542	33.96	91.6444	-59.769	15.5911	73.1778	-36.2	32.3644	91.8445	-62.84	20.3911	79.16	-47.787	30.0222	90.0178	-59.293	23.7422	88.6267	-49.187	30.2667	92.9022	-62.113	24.7111	88.2178	-55.32	32.32	66.36	-60.276	80.0711	-58.37	32.744	-35.338		
<b>Iodide_3</b>	8.88001	50.28	-16.129	34.04	92.9778	-57.991	15.5289	73.8844	-34.276	32.4267	92.72	-61.178	21.0044	78.88	-48.231	30.0222	98.04	-60.591	23.7689	87.3867	-49.218	30.3244	93.08	-65.751	25.12	89.5289	-53.996	32.3156	60.5422	-60.111	30.5422	86.72	-59.018	13.3467	27.3422	-29.502
<b>Iodide_4</b>	8.89334	49.4978	-19.311	33.9667	94.1778	-55.889	15.4667	71.0444	-38.862	32.3911	91.5022	-61.724	20.5867	78.6489	-45.582	29.8578	97.5644	-60.24	23.84	85.96	-50.142	30.1689	95.8667	-60.227	25.0978	87.12	-54.049	31.0755	63.4089	-54.133	30.4844	90.3556	-51.338	11.0844	27.5867	-25.004
<b>Iodide_5</b>	8.84445	61.7511	-7.0356	34.0622	102.902	-48.96	15.5956	82.08	-29.649	32.4044	92.5822	-56.209	21.0844	89.1689	-41.813	29.6511	92.9689	-57.644	23.8222	93.6489	-41.889	30.1956	86.8711	-62.364	25.0755	98.5511	-45.342	29.8711	59.2133	-55.671	30.4111	94.9156	-49.129	11.5111	29.0267	-25.889
<b>Phosphate_1</b>	-1.4692	-14.517	9.26617	-7.0737	-23.371	41.1429	-4.2451	-18.43	17.4556	-6.7699	-22.956	42.4601	-8.8602	-26.223	35.6556	-9.2195	-23.465	39.1353	-8.9447	-26.988	41.4812	-8.606	-22.528	41.8812	-7.8932	-25.998	42.6511	-10.066	-21.466	38.7985	-6.9594	-23.023	42.2526	-10.162	-19.415	36.4632
<b>Phosphate_2</b>	-3.3068	-16.241	8.98647	-8.5053	-23.208	39.8406	-4.8406	-15.681	14.7835	-8.5203	-22.934	41.1459	-9.397	-24.738	33.9023	-10.848	-24.421	37.8556	-13.732	-28.448	33.9624	-10.098	-23.653	40.9549	-10.316	-25.086	38.0827	-10.332	-22.015	39.0286	-8.5534	-24.087	40.5519	-10.731	-19.086	36.3113
<b>Phosphate_3</b>	-2.8586	-20.519	6.89625	-7.1865	-22.329	41.3669	-3.5263	-17.167	16.5594	-7.4105	-20.063	42.1022	-7.1323	-21.474	37.8677	-11.478	-27.847	36.5549	-9.1414	-28.8	39.0165	-7.412	-17.427	44.7459	-7.6105	-24.059	42.4722	-7.7053	-16.502	42.4932	-6.5684	-19.361	44.197	-8.8406	-16.612	39.1744
<b>Phosphate_4</b>	-0.821	-15.937	9.87219	-5.7383	-19.227	43.3128	-2.9098	-12.923	18.6617	-5.415	-20.34	44.4586	-5.9113	-17.94	38.8301	-8.2256	-22.952	40.6571	-6.7654	-25.597	41.218	-6.2241	-16.226	46.2601	-6.8165	-23.971	41.9083	-6.8887	-16.023	43.7474	-4.5308	-17.525	45.4331	-7.9338	-16.066	39.5248
<b>Phosphate_5</b>	-0.821	-20.798	10.8316	-7.4	-22.023	40.3128	-3.3278	-15.138	16.3865	-6.8662	-19.432	42.382	-6.6511	-19.067	36.9774	-9.7624	-23.952	38.1173	-8.9384	-27.74	37.3098	-7.609	-16.621	43.782	-7.1805	-20.027	42.3128	-7.3383	-17.364	41.8436	-5.7504	-17.215	44.1203	-8.6572	-16.208	38.1143
<b>Chromate_1</b>	7.51128	13.3158	-8.5414	-9.3459	-14.977	17.6466	-0.5414	-8.218	7.49623	-4.7143	-9.1128	21.2481	-2.7293	-12.466	17.609	-6.6241	-15.414	14.7218	-3.8045	-14.293	16.3835	-6.4962	-12.812	16.0376	-2.3008	-9.797										

Table S3. A full digital database for seven heavy-metal ions sensing.

	R1	G1	B1	R2	G2	B2	R3	G3	B3	R4	G4	B4	R5	G5	B5	R6	G6	B6	R7	G7	B7	R8	G8	B8	R9	G9	B9	R10	G10	B10	R11	G11	B11	R12	G12	B12
Pb <sup>2+</sup> _1	2.73044	-5.4087	5.23187	2.97682	-49.313	9.56812	6.27246	-2.2	12.8261	8.77683	-67.145	-0.5652	4.11304	-14.133	11.4319	1.84638	-79.235	-0.8319	1.67535	-25.417	15.5739	3.59421	-79.878	0.36812	3.50435	-37.322	17.5391	1.95653	-77.504	0.03478	11.287	-35.788	15.9101	5.12465	-80.041	0.36232
Pb <sup>2+</sup> _2	2.58261	-3.7275	4.32753	3.83479	-48.881	3.31594	0.83478	-6.7942	7.71304	5.10436	-67.194	-1.0377	3.4261	-16.241	11.4406	6	-88.339	-0.5739	2.93044	-28.223	16.6725	4.08406	-84.125	0.55073	4.19421	-38.22	16.3971	4.55942	-82.383	-0.6406	5.02899	-41.73	14.0609	6.50725	-79.557	-1.7275
Pb <sup>2+</sup> _3	-2.4377	-7.1333	4.48406	2.24348	-52.751	4.11015	-0.4319	-10.62	7.21739	3.45218	-67.351	-0.5362	2.28406	-17.609	9.14782	2.88985	-65.017	-2.1159	1.41159	-28.035	16.2667	1.25508	-81.003	-0.4087	1.56812	-39.255	15.9217	2.51015	-82.328	-0.7391	2.62318	-43.91	14.571	1.22609	-81.484	-0.7449
Pb <sup>2+</sup> _4	-0.771	-7.8783	0.59711	3.57391	-52.701	4.51884	-0.3855	-10.562	7.25508	3.51305	-65.42	0.24928	1.58841	-18.168	8.82899	5.30724	-70.328	0.1942	0.23769	-28.962	16.2203	3.43478	-81.328	0.85217	3.55074	-37.519	16.7101	1.81448	-79.267	1.55362	4.84638	-44.267	16.2058	3.29855	-77.997	-0.6783
Pb <sup>2+</sup> _5	-0.629	-7.5188	3.86957	3.59129	-53.281	10.2609	0.77971	-8.9681	5.75362	2.91014	-61.052	-1.1014	4.71594	-14.78	10.3333	4.70435	-73.304	-0.4087	1.44928	-28.861	15.5217	4.10436	-71.446	1.13913	2.59131	-40.588	19.1565	2.56522	-80.258	-0.6841	6.95651	-42.922	13.9768	3.44493	-80.067	-0.6522
Cd <sup>2+</sup> _1	3.07866	-6.4831	6.14607	26.2022	-83.146	10.6405	5.77528	-12.831	5.14607	31.6629	-112.62	-2.764	10.0787	-21.674	11.8989	34.4719	-126.58	-0.5281	10.7303	-42.944	12.764	32.7865	-134.91	-1.1685	15.7079	-55.146	17.1798	32.2921	-142.31	-0.1573	16.9775	-66.461	16.5169	30.1124	-136.2	-0.5618
Cd <sup>2+</sup> _2	1.26666	-11.649	3.22609	21.3246	-80.667	-0.1768	4.23189	-16.31	7.53333	32.3768	-113.72	-0.8899	8.39131	-27.606	7.45218	30.5159	-125.84	-0.4232	13.3565	-42.939	17.1072	33.3275	-137.46	0.37681	17.6087	-58.258	16.3275	37.1536	-142.3	0.46087	22.7159	-75.713	15.8986	39.4957	-134.66	-1.3333
Cd <sup>2+</sup> _3	6.89275	-4.5942	5.68115	25.4493	-81.849	9.77681	6.90434	-11.699	6.89887	32.9044	-114.94	-0.9855	10.5333	-22.122	11.2464	27.287	-111.27	-0.0261	12.2435	-39.322	12.0493	34.2406	-131.53	1.3913	16.5884	-56.049	18.7275	35.5072	-140.32	-0.4986	19.6319	-73.855	15.2841	35.6464	-139.39	-0.9826
Cd <sup>2+</sup> _4	-0.229	-8.8174	1.67537	28.7072	-78.012	4.84638	3.72754	-13.316	4.23189	34.0116	-113.95	-1.487	7.63478	-23.565	11.0783	37.6696	-137.99	-0.1594	13.171	-41.368	14.2232	36.4029	-137.46	0.21159	15.5188	-55.591	18.8174	35.7536	-130.79	0.71304	20.9971	-71.635	18.3217	36.8811	-129.55	-0.1478
Cd <sup>2+</sup> _5	2.96233	-7.6609	7.2029	26.3855	-83.235	10.8696	7.45796	-12.148	5.33334	31.884	-113.79	-1.1536	7.91884	-21.551	10.5884	37.9043	-142.43	0.22319	11.5246	-38.913	14.7507	35.742	-133.82	0.46667	15.4783	-55.852	19.2928	34.5304	-132.36	-0.2783	19.9971	-70.977	16.2232	36.7217	-140.75	-0.3072
Hg <sup>2+</sup> _1	0.97102	-11.194	8.52464	11.7478	-127.13	37.6551	1.75362	-20.49	16.0812	8.86377	-153.07	-1.0029	4.89565	-37.258	22.3536	3.23769	-153.48	-0.2899	8.14203	-64.548	35.6406	-4.4145	-147.44	0.23478	8.40581	-86.464	42.9942	-4.2464	-144.78	0.15652	11.2232	-107.72	47.6522	-5.4928	-142.34	1.35362
Hg <sup>2+</sup> _2	-0.0464	-13.067	3.04349	12.8435	-123.37	40.3681	8.11884	-13.299	20.5072	8.78261	-153.5	-0.5594	7.36232	-36.878	22.0812	4.91596	-154.15	-0.3101	7.46956	-63.316	32.8	4.71014	-147.3	0.03768	9.68697	-84.751	40.6638	-1.6667	-144.55	1.21159	13.6	-106.49	42.258	-3.2623	-142.81	-0.1768
Hg <sup>2+</sup> _3	1.32584	-10.843	8.60674	8.05618	-114.73	41.3258	4.79776	-16.865	14.0899	12.4382	-140.92	-3.2809	3.20226	-28.876	23.0787	11.7528	-155.28	-0.0449	8.80899	-59.539	33.0112	-147.5	0.50562	7.91013	-85.753	37.9326	1.20224	-140.7	1.03371	14.0899	-94.326	48.7753	-2.4382	-138.9	-0.0337	
Hg <sup>2+</sup> _4	7.09566	-5.2406	16.8377	11.8927	-117.03	41.3072	11.6145	-9.8348	20.3304	8.73792	-148.29	-0.7101	12.1536	-31.461	25.3015	0.9971	-141.96	0.89565	17.2464	-51.745	40.0812	-2.571	-142.25	0.28406	10.829	-80.991	43.7275	-5.3565	-140.25	-0.1362	16.6754	-98.383	46.913	-5.2145	-133.41	-1.6406
Hg <sup>2+</sup> _5	2.09856	-9.9971	11.9246	12.0319	-121.45	45.3449	5.56812	-14.846	15.8927	11.9652	-154.88	-0.8377	7.50435	-32.026	25.6667	11.5478	-156.43	-1.0696	9.51593	-57.788	34.9623	-2.1333	-148.45	0.4029	10.2058	-84.89	45.0609	-0.8406	-144.4	-1.1623	14.8754	-99.554	45.8551	-3.913	-137.91	-0.3768
Cu <sup>2+</sup> _1	1.88115	-11.58	14.6	-9.5884	-128.84	55.3449	7.24059	-17.272	28.1014	-2.5913	-148.93	-0.3623	-0.3362	-47.577	39.6609	-3.1362	-146.86	-0.1043	-3.3594	-78.612	60.5101	-2.4058	-153.14	-1.658	-12.835	-109.56	77.5797	-7.2754	-142.81	-1.3101	-7.058	-113.79	66.6522	-10.365	-141.7	-1.1913
Cu <sup>2+</sup> _2	4.86667	-9.6133	13.7333	-9.3111	-120.37	60.1956	7.08888	-16.2	26.68	0.97778	-150.49	-1.2489	-2.5022	-46.36	37.3911	-6.2533	-148.72	0.34222	-7.3022	-78.16	55.3911	-3.9289	-153.92	-1.0622	-13.551	-102.54	71.12	-6.7956	-142.75	-1.4667	-8.7333	-114.19	64.72	-10.627	-141.6	-1.0667
Cu <sup>2+</sup> _3	-0.6711	-20.569	16.6	-7.6889	-127.21	56.0578	0.91556	-24.542	21.3378	-4.6133	-146.15	-0.2356	-0.8533	-51.698	39.2578	-7.8133	-146.71	-3.1333	-7.8489	-86.596	57.3822	-1.9733	-155.68	-0.6844	-12.511	-110.68	72.9644	-9.9156	-143.44	2.03111	-10.956	-122.84	65.7556	-10.933	-141.01	-0.2311
Cu <sup>2+</sup> _4	1.12889	-14.929	16.4311	-8.1867	-132.13	55.8222	0.8889	-24.64	24.5511	-3.36	-154.34	-0.4933	-1.6222	-52.04	39.7911	-8.0711	-149.77	-0.8667	-8.12	-88.609	63.6933	-5.3822	-154.92	0.48	-15.689	-108.08	70.9556	-13.196	-144.92	-0.9333	-7.8711	-116.88	67.84	-14.031	-141.72	-0.1867
Cu <sup>2+</sup> _5	-2	-18.796	13.3555	-12.138	-138.76	63.4756	1.38222	-23.173	24.4756	-3.24	-154.23	-0.9244	-1.7378	-52.436	38.1555	-7.3822	-150.89	-2.1289	-7.0844	-87.849	62.12	-7.0356	-155.95	-0.2178	-16.204	-110.4	75.8	-8.755	-145.02	-1.4756	-12.529	-120.83	64.8444	-13.067	-142.93	0.33333
Zn <sup>2+</sup> _1	11.5338	-16.797	15.6241	41.3008	-145.96	66.7895	12.3534	-27.128	17.8571	43.1805	-154.27	-0.3083	18.2556	-56.203	29.0602	42.5338	-150.84	0.06767	27.5263	-92.647	48.1429	41.2331	-156.65	0.29323	35.0075	-115.77	55.0301	39.4887	-145.59	0.67669	36.8722	-132.47	60.2256	34.3308	-143.14	-0.391
Zn <sup>2+</sup> _2	7.04445	-19.827	12.4089	41.0711	-144.04	66.9111	12.04	-27.364	17.2889	42.9867	-154.48	-0.6533	20.8533	-58.333	30.76	41.1822	-150.8	-1.1822	29.7689	-92.062	47.8489	41.5956	-156.81	-1.4267	34.8489	-116	56.8133	40.5422	-144.45	-0.1022	37.1733	-131.71	66.1378	38.4355	-143.88	1.45778
Zn <sup>2+</sup> _3	4.46243	-21.844	6.2948	36.9827	-143.3	62.0058	17.526	-24.503	22.2601	42.1156	-152.42	-0.1908	19.1676	-57.168	28.4335	40.3526	-148.9	0.50289	28.6416	-91.364	50.4277	43.8844	-154.75	0.09827	35.237	-114.89	56.4682	38.7861	-143.85	0.82659	41.5607	-126.75	63.9884	37.9249	-141.13	0.6474
Zn <sup>2+</sup> _4	15.4382	-11.067	18.0899	39.7641	-145.91	67.0337	11.382	-27.101	17.4382	43.1124	-152.36	0.19101	17.5169	-56.393	28.5843	38.8539	-148.85	1.57303	27.8539	-93.843	47.4607	42.1124	-154.96	0.13483	32.7191	-114.25	54.9101	37	-142.18	-1.5506	34.3933	-131.61	63.3596	36.191	-140.38	-0.3708
Zn <sup>2+</sup> _5	8.39327	-19.506	13.618	38.1124	-141.69	65.3034	12.8539	-25.753	18.1798	42.0112	-154.17	1.70787	20.573	-55.427	29.3371	42.0562	-150.13	-0.3034	29.3034	-89.955	43.8427	43.0112	-153.64	1.08989	34.4045	-113.12	55.5843	42.8315	-146.26	1.16854	38.427	-128.03	60.4944	38.8315	-142.36	-1.573
Co <sup>2+</sup> _1	-7.7865	0.21349	13.2135	-115.83	-79.831	53.8989	-15.337	-4.2247	22.0225	-120.03	-114.71	-0.5169	-39.079	-23.427	25.4157	-122.8	-121.19	-1.9213	-39.82	34.8539	-111.19	-103.29	0.8427	-90.079	-55.674	45.6966	-121.56	-113.18</								