

Supporting Information

Machine Learning-Assisted Pattern Recognition and Imaging of Multiplexed Cancer Cells via Porphyrin-Embedded Dendrimer Array

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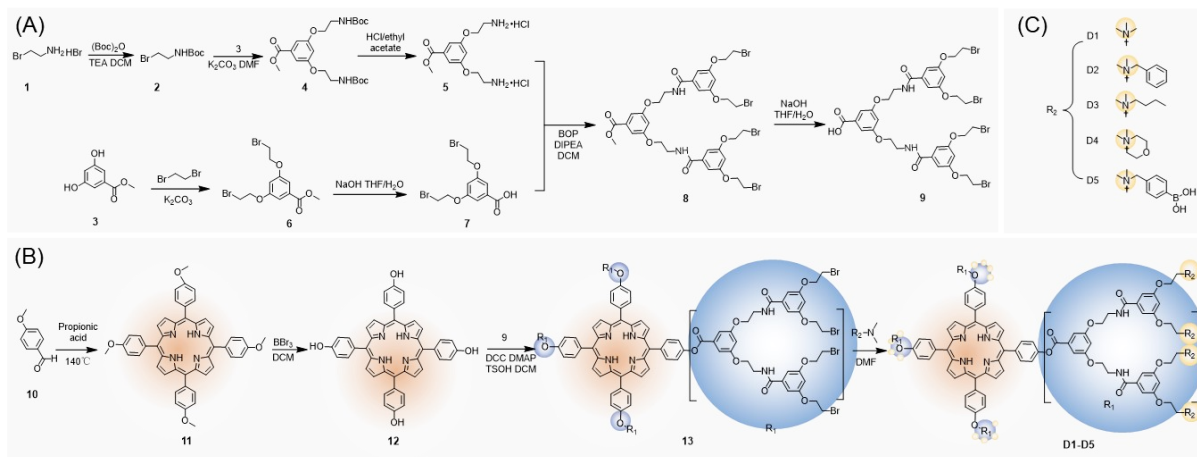
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1. Synthesis of D1-D5

Scheme S1. Synthetic route of D1-D5

To a solution of 2-bromoethylamine hydrobromide salt (**1**) (556.0 mg, 2.7 mmol) in dichloromethane (20 mL) were added di-*tert*-butyl dicarbonate (Boc₂O) (651.0 mg, 3.0 mmol), triethylamine was added dropwise slowly (754.0 μL, 5.4 mmol). After stirring for overnight at room temperature, a precipitate formed and then was filtered. The mixture was extracted with dichloromethane (30 mL×3). The combined organic layers were dried over anhydrous sodium sulfate and concentrated under reduced pressure to give the crude product **2**, which was used directly for the next step without further purification. ¹H NMR (400 MHz, Chloroform-*d*) δ 4.97 (s, 1H), 3.56 (q, *J* = 5.9 Hz, 2H), 3.48 (t, *J* = 5.9 Hz, 2H), 1.47 (s, 9H).

A mixture of **2** (6.7 g, 30.0 mmol), methyl 3,5-dihydroxybenzoate (**3**) (2.0 g, 12.0 mmol), K₂CO₃ (4.2 g, 30.0 mmol) dissolve in dimethylformamide (50 mL) was stirred at 80 °C for 8 h, the mixture was poured into ice water (200 mL), and then extracted with ethyl acetate (50 mL×3). The combined organic layers were dried over anhydrous sodium sulfate, filtrated, then concentrated to afford **4**, the crude product was purified by silica gel column chromatography using petroleum ether/ethyl acetate (*v/v* = 10:1) as eluent to give white solid product **4** (4.5 g) in 83.7% yield. ¹H NMR (300 MHz, Chloroform-*d*) δ 7.14 (d, *J* = 2.3 Hz, 2H), 6.61 (t, *J* = 2.3 Hz, 1H), 5.10 (d, *J* = 6.1 Hz, 2H), 4.02 (t, *J* = 5.1 Hz, 4H), 3.88 (s, 3H), 3.52 (q, *J* = 5.4 Hz, 4H), 1.44 (s, 18H).

The solid **4** (300.0 mg, 0.7 mmol) was added to 10 mL ethyl acetate solution with hydrochloride. After stirring for overnight at room temperature, a precipitate formed and then was filtered. The suspension was concentrated under reduced pressure to give the crude product **5**, which was used directly for the next step without further purification.

A suspension of methyl 3,5-dihydroxybenzoate (**3**, 1.0 g, 6.0 mmol), K₂CO₃ (2.1 g, 15.0 mmol) and 18-crown-6 (100.0 mg) in 10 mL of 1,2-dibromoethane was heated at 80 °C for 36 h. The reaction mixture was cooled, filtered, extracted with ethyl acetate (30 mL×3) and then the filtrate was evaporated under vacuum giving a residue that was purified by column chromatography using petroleum ether/ethyl acetate (v/v = 10:1) as eluent to give white solid product **6**; Yield: 731.0 mg (45.7%). ¹H NMR (300 MHz, Chloroform-*d*) δ 7.23 (d, *J* = 2.4 Hz, 2H), 6.72 (t, *J* = 2.4 Hz, 1H), 4.34 (t, *J* = 6.1 Hz, 4H), 3.93 (s, 3H), 3.67 (t, *J* = 6.1 Hz, 4H).

The product **6** (1.0 g, 2.6 mmol) was dissolved in THF (20 mL) and 1 M LiOH (5 mL) was added to the above solution. The mixture was stirred at room temperature for 5 h, and then filtered and concentrated to about 10 mL. The resulting residue was neutralized by diluted hydrochloric acid to pH = 5. The precipitation was filtered and dried to afford **7** as a white solid, which was used directly for the next step without further purification. ¹H NMR (400 MHz, Chloroform-*d*) δ 7.30 (d, *J* = 2.4 Hz, 2H), 6.78 (t, *J* = 2.4 Hz, 1H), 4.36 (t, *J* = 6.1 Hz, 4H), 3.68 (t, *J* = 6.1 Hz, 4H).

To a suspension of the acid **7** (260.0 mg, 0.7 mmol), hydrochloride salt **5** (100.0 mg, 0.3 mmol) and BOP (318.0 mg, 0.7 mmol) in dry dichloromethane (10 mL) was slowly added DIPEA (270 μL, 2.0 mmol). The mixture was stirred at room temperature for 4 h, extracted with ethyl acetate (30 mL×3). Then the filtrate was evaporated under vacuum giving a residue that was purified by column chromatography using petroleum ether/dichloromethane (v/v = 1:1) as eluent to give white solid product **8** (484.0 mg,

72.5%); ¹H NMR (300 MHz, Chloroform-*d*) δ 7.19 (d, *J* = 2.3 Hz, 2H), 6.97 (d, *J* = 2.2 Hz, 4H), 6.73 - 6.65 (m, 3H), 6.62 (t, *J* = 2.3 Hz, 2H), 4.32 (t, *J* = 6.0 Hz, 8H), 4.16 (dd, *J* = 6.2, 3.8 Hz, 4H), 3.92 (s, 3H), 3.90 - 3.82 (m, 4H), 3.65 (t, *J* = 6.0 Hz, 8H).

The product **8** (200.0 mg, 2.1 mmol) was dissolved in THF (5 mL) and 1 M LiOH (2 mL) was added to the above solution. The mixture was stirred at room temperature for 5 h, and then filtered and concentrated to about 2 mL. The resulting residue was neutralized by diluted hydrochloric acid to pH = 5. The precipitation was filtered and dried to afford **9** as a white solid, which was used directly for the next step without further purification. ¹H NMR (400 MHz, DMSO-*d*₆) δ 8.74 (t, *J* = 5.6 Hz, 2H), 7.14 (d, *J* = 2.3 Hz, 2H), 7.11 - 7.04 (m, 4H), 6.72 (t, *J* = 2.3 Hz, 2H), 6.67 (t, *J* = 2.4 Hz, 1H), 4.36 (dd, *J* = 6.3, 4.4 Hz, 8H), 4.13 (t, *J* = 5.8 Hz, 4H), 3.81 (dd, *J* = 6.2, 4.4 Hz, 8H), 3.62 (q, *J* = 5.7 Hz, 4H).

To a stirred suspension solution of 4-methoxybenzaldehyde (**10**, 680.0 mg, 5.0 mmol) in propionic acid (10 mL) being heated to 135 °C, pyrrole (335.0 mg, 5.0 mmol) in propionic acid (5 mL) was added drop wise under a nitrogen atmosphere for 1 min via constant pressure drop funnel. The mixture was stirred at 135 °C for 1 h. The reaction system was cooled to room temperature by slow cooling. Extracted with dichloromethane (50 mL) three times, and dried with anhydrous Na₂SO₄. The solvent was removed under vacuum getting crude product. The crude product was subjected to column chromatography using petroleum ether/dichloromethane (v/v = 1:1) as eluent to give purple solid product **11** (232.1 mg, 25.3%); ¹H NMR (300 MHz, Chloroform-*d*) δ 8.89 (s, 8H), 8.15 (s, 8H), 7.33 (d, *J* = 2.2 Hz, 8H), 4.03 (s, 12H), -2.73 (s, 2H).

To a stirred suspension solution of **11** (1.0 g, 1.4 mmol) in CH₂Cl₂ (20 mL) being cooled to 0 °C, BBr₃ was added drop via constant pressure drop funnel. The mixture was stirred at room temperature overnight. After completion of the reaction, the reaction was quenched with saturation NH₄Cl and stirred at room temperature for another 10 min. Extracted with ethyl acetate (20 mL) three times, and dried with

anhydrous Na₂SO₄. The solvent was removed under vacuum. The residue was purified by column chromatography using petroleum ether/ethyl acetate (v/v = 3:1) as eluent to give purple solid product **12** (612.4 mg, 66.3%); ¹H NMR (400 MHz, DMSO-*d*₆) δ 10.00 (s, 4H), δ 8.99 (s, 8H), 8.03 (s, 8H), 7.23 (s, 8H), -2.88 (s, 2H).

In a flash bottle, **9** (1128.3 mg, 1.2 mmol), DCC (247.6 mg, 1.2 mmol) and DMAP (146.6 mg, 1.2 mmol) were dissolved in 10 mL dried dichloromethane. After stirring for 0.5 h at 0 °C, **12** (100.0 mg, 0.2 mmol) and TsOH (206.6 mg, 1.2 mmol) were added into the flask and the mixture was heated to room temperature. After stirred overnight, the mixture was poured into 30 mL water and extracted with dichloromethane (3×25 mL). The collected organic layer was dried over anhydrous Na₂SO₄. After solvent evaporation, the crude product was purified by a silica gel column using petroleum ether/ethyl acetate (v/v = 1:2) as eluent to give purple solid product **13** (319.5 mg, 53.7%); ¹H NMR (400 MHz, Chloroform-*d*) δ 8.97 (s, 8H), 8.32 (dd, *J* = 8.6, 2.6 Hz, 8H), 7.73 - 7.63 (m, 24 H), 7.59 (d, *J* = 2.3 Hz, 8H), 6.89 (t, *J* = 2.4 Hz, 12H), 4.36 (dd, *J* = 6.2, 4.5 Hz, 32H), 4.16 (t, *J* = 5.8 Hz, 16H), 3.81 (dd, *J* = 6.2, 4.4 Hz, 32H), 3.62 (q, *J* = 5.8 Hz, 16H), -2.75 (s, 2H).

Synthesis of **D1**

A mixture of compound **12** (1 eq.) and the trimethylamine (64 eq.) was stirred and heated to reflux in dimethylformamide for 24 h. The solvent was removed under vacuum and the solution was allowed to cool to room temperature, filtered and washed with copious amounts of acetone and ethyl acetate to give a deep red filter cake, Yield 57.2%. ¹H NMR (400 MHz, DMSO-*d*₆) δ 9.10 - 8.46 (m, 12H), 8.39 - 8.11 (m, 8H), 7.99 (s, 8H), 7.67 (d, *J* = 8.3 Hz, 8H), 7.45 (s, 8H), 7.30 - 6.90 (m, 20H), 6.85 - 6.47 (m, 8H), 4.46 - 4.21 (m, 48H), 4.08 (s, 144H), 3.89 - 3.43 (m, 48H), -2.90 (s, 2H). HRMS (ESI): calcd. For C₂₂₅H₃₁₂N₂₈O₄₀¹⁶⁺ [M]¹⁶⁺/16: 252.8947, found 252.8429.

Synthesis of **D2**

The preparation method of compound **D2** was analogous to that used for **D1**. Yield 76.1%. ¹H NMR (400 MHz, Methanol-*d*₄) δ 8.74 (s, 8H), 7.79 (d, *J* = 5.91 Hz, 4H), 7.66 - 7.38 (m, 72H), 7.17 (dt, *J* = 60.3, 21.0 Hz, 52H), 6.87 - 6.45 (m, 16H), 4.67 (s, 96H), 4.60 (s, 8H), 3.37 (s, 32H), 3.15 (s, 48H), 2.94 (s, 48H), -2.75 (s, 2H). HRMS (ESI): calcd. For: C₃₂₀H₃₇₄N₂₈O₄₀¹⁶⁺ [M]¹⁶⁺/16: 328.0500, found 328.0543.

Synthesis of **D3**

The preparation method of compound **D3** was analogous to that used for **D1**. Yield 58.8%. ¹H NMR (400 MHz, Methanol-*d*₄) δ 8.82 (s, 8H), 7.96 (d, *J* = 23.6 Hz, 15H), 7.28 - 6.95 (m, 24H), 6.91 - 6.44 (m, 12H), 4.60 - 4.31 (m, 32H), 3.76 (ddt, *J* = 27.7, 17.9, 9.3 Hz, 96H), 3.25 - 3.07 (m, 48H), 2.99 (s, 32H), 2.86 (s, 16H), 1.91 - 1.61 (m, 32H), 1.53 - 1.19 (m, 32H), 1.07 - 0.85 (m, 48H), -2.77 (s, 2H). HRMS (ESI): calcd. For: C₂₇₂H₄₀₆N₂₈O₄₀¹⁶⁺ [M]¹⁶⁺/16: 294.0657, found 294.0681.

Synthesis of **D4**

The preparation method of compound **D4** was analogous to that used for **D1**. Yield 43.9%. ¹H NMR (400 MHz, Methanol-*d*₄) δ 8.89 (s, 8H), 8.03 - 8.00 (m, 4H), 7.28 - 7.21 (m, 8H), 7.18 - 7.15 (m, 4H), 7.10 (s, 8H), 7.04 - 7.00 (m, 8H), 6.78 (d, *J* = 9.5 Hz, 8H), 6.73 - 6.65 (m, 8H), 6.58 (s, 4H), 4.18 (d, *J* = 5.5 Hz, 64H), 3.74 (t, *J* = 4.7 Hz, 64H), 3.51 (d, *J* = 1.9 Hz, 48H), 3.28 (s, 80H), 3.23 (s, 16H), -2.77 (s, 2H). HRMS (ESI): calcd. For: C₂₅₅H₃₄₀N₂₈O₅₆¹⁶⁺ [M]¹⁶⁺/16: 293.1533, found 293.1533.

Synthesis of **D5**

The preparation method of compound **D5** was analogous to that used for **D1**. Yield 28.3%. ¹H NMR (400 MHz, Methanol-*d*₄) δ 8.90 (s, 8H), 7.95 - 8.25 (m, 4H), 7.20 - 7.12 (m, 56H), 6.88 - 6.58 (m, 24H), 4.57 (s, 1H), 4.36 - 4.26 (m, 96H), 3.82 - 3.74 (m, 32H), 3.25 (d, *J* = 1.0 Hz, 80H), 2.79 - 2.70 (m, 16H), -2.77 (s, 2H). HRMS (ESI): calcd. for: C₃₂₂H₃₉₄B₁₆N₂₈O₇₀¹⁶⁺ [M]¹⁶⁺/16: 371.8096, found 371.8047.

2. Fluorescence Spectra

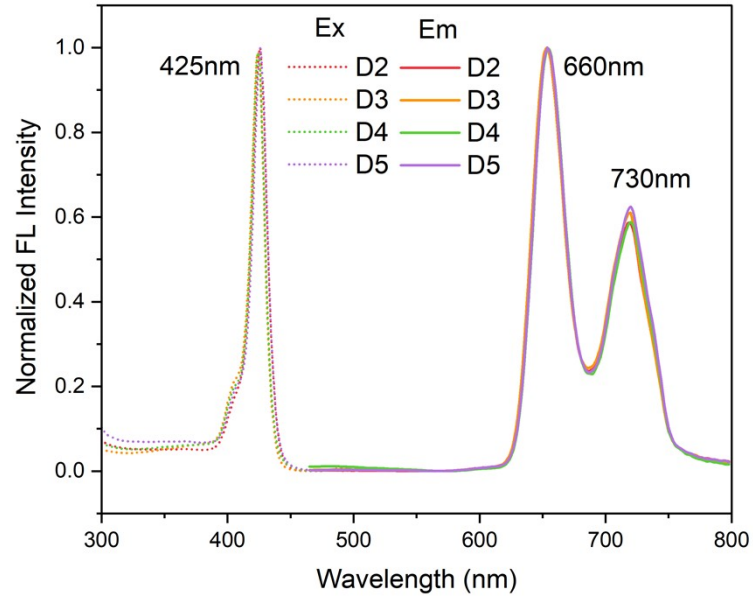


Fig. S1 Normalized excitation and emission spectra of **D2-D5**.

Table S1. Quantum yield and lifetime of the array.

	Lifetime (ns)	quantum yield (%)
D1	7.80	7.46
D2	8.57	0.53
D3	7.97	3.19
D4	8.47	2.07
D5	8.52	4.62

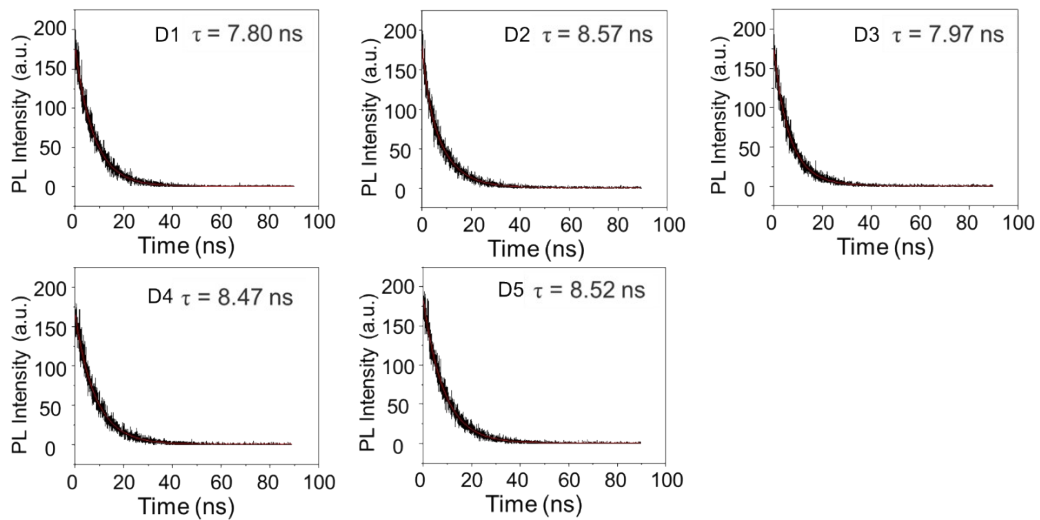


Fig. S2 Fluorescence lifetime of the array.

3. Linear Discriminant Analysis Data

Table S2 LDA was carried out and resulted in 3 factors of the canonical scores.

Analyte	Results LDA			
Cell	Factor 1	Factor 2	Factor 3	Group
PANC-1	11.64	-5.50	-0.62	11.64
PANC-1	14.15	-8.52	-0.72	14.15
PANC-1	14.11	-7.92	0.39	14.11
PANC-1	12.70	-6.39	-0.45	12.70
PANC-1	10.98	-7.10	-0.88	10.98
PANC-1	13.86	-6.87	-3.06	13.86
PANC02	2.53	3.83	3.46	2.53
PANC02	2.69	3.01	6.10	2.69
PANC02	3.30	3.75	3.87	3.30
PANC02	3.36	3.85	4.07	3.36
PANC02	4.96	5.23	5.59	4.96
PANC02	4.01	5.72	2.65	4.01
NIH/3T3	1.07	6.33	-3.31	1.07
NIH/3T3	0.11	6.66	-3.62	0.11
NIH/3T3	0.66	6.42	-3.36	0.66
NIH/3T3	-0.67	7.45	-3.13	-0.67
NIH/3T3	1.37	7.78	-3.97	1.37
NIH/3T3	1.69	7.34	-3.36	1.69
HPDE6-C7	-17.49	-5.44	-0.59	-17.49
HPDE6-C7	-17.78	-2.34	0.70	-17.78
HPDE6-C7	-17.39	-5.38	-1.55	-17.39
HPDE6-C7	-15.82	-3.40	0.51	-15.82
HPDE6-C7	-16.49	-4.06	0.49	-16.49

HPDE6-C7	-17.53	-4.45	0.77	-17.53
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Canonical Scores Plot

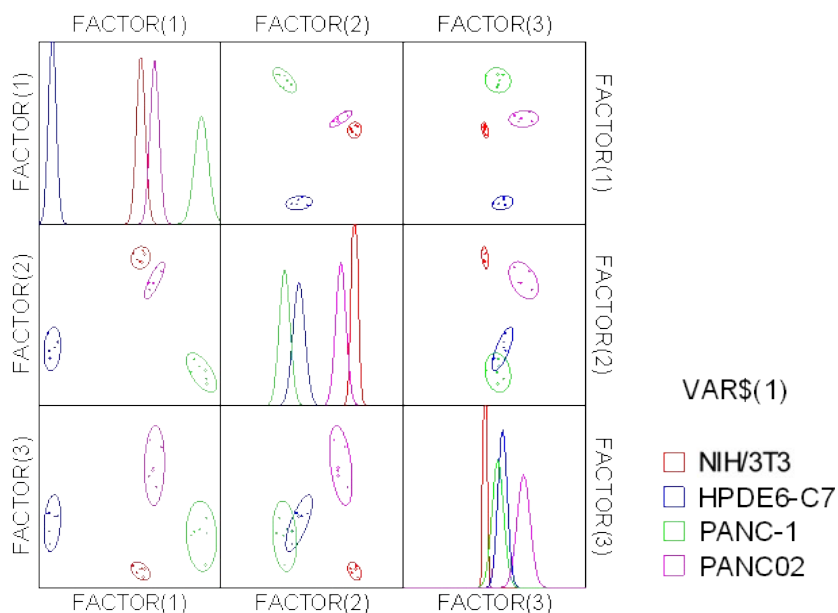


Fig. S3 Correlations of canonical fluorescence response patterns from the array of channel 1-channel 10 against 4 cell lines. The 95% confidence ellipses for the individual analytes are shown.

Table S3 LDA was carried out and resulted in 6 factors of the canonical scores.

Analyte	Results LDA						
Cell	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Group
Du145	12.75	-5.37	2.55	-0.14	-0.95	0.80	4
Du145	11.84	-4.66	2.15	-0.44	-1.98	-0.25	4
Du145	12.56	-5.39	1.55	-2.02	-0.59	-0.27	4
Du145	11.27	-5.68	3.09	-1.49	-2.57	-0.91	4
Du145	11.75	-5.25	3.08	-0.99	-1.62	-1.71	4
Du145	12.72	-3.65	2.85	0.74	0.42	-2.00	4
A549	6.53	4.92	2.82	0.96	0.84	-2.98	2
A549	6.78	3.93	2.12	1.25	1.28	-1.31	2
A549	5.22	7.38	3.17	2.85	1.78	-3.17	2
A549	5.16	7.04	1.23	1.26	1.68	0.59	2
A549	6.14	5.89	0.84	1.33	1.12	0.05	2
A549	5.56	6.68	2.29	2.21	-0.02	0.27	2
PANC-1	1.89	3.33	-0.14	-2.34	-0.46	0.52	6
PANC-1	2.72	4.70	0.95	-3.53	0.59	0.73	6

PANC-1	6.07	6.37	2.53	-3.18	-1.07	2.61	6
PANC-1	3.74	4.98	1.01	-3.83	-0.28	1.09	6
PANC-1	4.41	3.98	1.73	-1.90	-0.43	2.09	6
PANC-1	1.95	2.84	2.44	-1.37	-1.45	2.65	6
BT549	1.49	0.20	-7.46	-2.91	0.12	-1.97	3
BT549	-1.25	-0.34	-6.13	-1.15	1.90	0.88	3
BT549	0.78	-2.20	-6.24	-2.44	-0.83	-1.31	3
BT549	-0.12	0.23	-6.05	-2.67	0.15	0.65	3
BT549	0.69	0.36	-7.69	-3.63	0.61	-0.55	3
BT549	0.40	-0.07	-7.31	-2.75	0.55	-1.44	3
A375	-12.25	-2.71	3.45	-1.60	1.16	0.13	1
A375	-12.91	-3.44	3.64	-1.97	0.88	-0.50	1
A375	-12.80	-4.22	3.37	-2.02	1.72	-0.39	1
A375	-14.17	-3.89	4.08	-1.81	1.65	-0.48	1
A375	-13.92	-3.59	3.30	-1.24	0.77	0.59	1
A375	-13.83	-3.71	3.92	-1.19	1.10	0.22	1
SK-OV-3	3.03	-2.49	-4.12	2.47	0.29	1.31	7
SK-OV-3	4.11	-3.42	-3.07	4.72	1.97	1.66	7
SK-OV-3	2.62	-3.29	-0.41	2.17	0.11	0.50	7
SK-OV-3	4.79	-3.30	0.74	2.48	2.45	1.80	7
SK-OV-3	4.66	-3.20	-3.00	5.22	-0.73	0.65	7
SK-OV-3	5.51	-4.20	-2.18	5.59	0.66	1.35	7
HPDE6-C7	-13.12	2.54	-0.54	2.84	-0.29	-0.84	5
HPDE6-C7	-12.18	0.25	-0.99	2.99	-0.05	-0.39	5
HPDE6-C7	-13.75	3.96	-0.62	3.28	-3.55	-1.11	5
HPDE6-C7	-11.27	1.34	-2.26	2.42	-2.46	-0.32	5
HPDE6-C7	-12.21	1.66	0.46	1.59	-3.55	0.38	5
HPDE6-C7	-13.34	1.49	-1.15	0.22	-0.91	0.42	5

Canonical Scores Plot

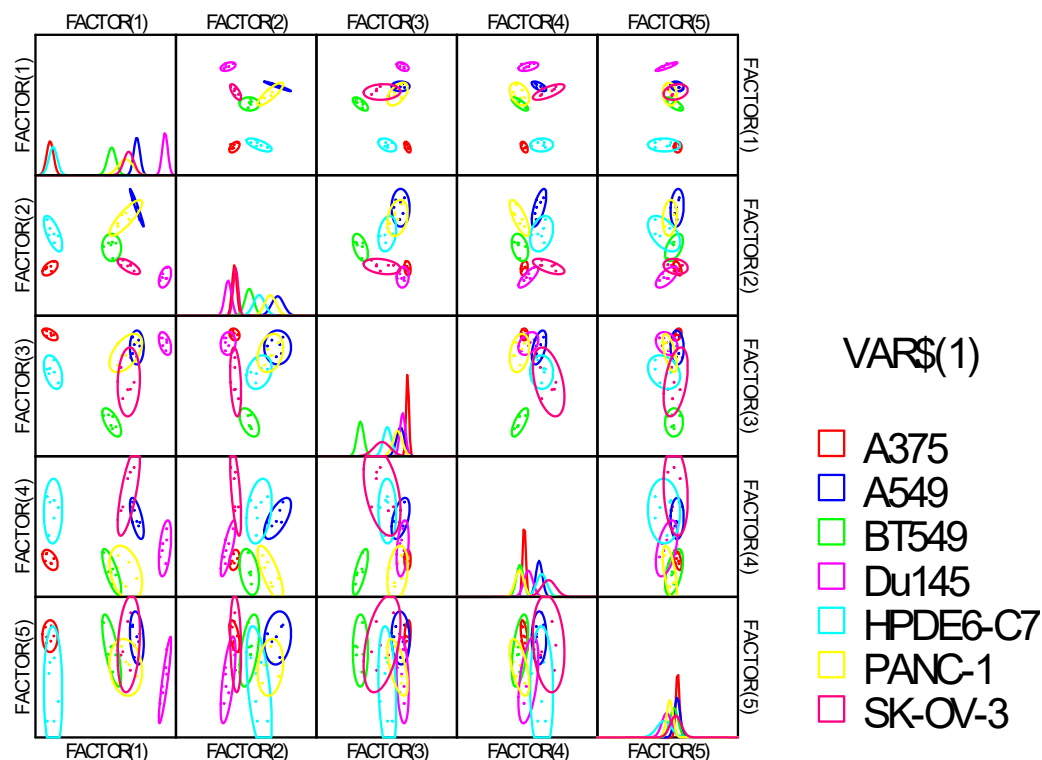


Fig. S4 Correlations of canonical fluorescence response patterns from the array of channel 1-channel 10 against 7 cell lines. The 95% confidence ellipses for the individual analytes are shown.

Table S4 Training matrix of fluorescence response pattern from an array of channel 1-channel 10 against different proportion of the HPDE6-C7 to PANC-1. LDA was carried out and resulted in 5 factors of the canonical scores.

Analyte	Fluorescence Response Pattern									
Concentration	CH1	CH2	CH3	CH4	CH5	CH6	CH7	CH8	CH9	CH10
100%:0	0.28	0.10	0.05	0.11	-0.05	-0.06	-0.03	0.07	-0.16	-0.18
100%:0	0.27	0.09	0.00	0.10	-0.11	-0.08	-0.06	0.04	-0.19	-0.22
100%:0	0.23	0.03	-0.01	0.08	-0.12	-0.09	-0.07	-0.07	-0.20	-0.23
100%:0	0.22	0.03	-0.03	0.03	-0.12	-0.09	-0.08	-0.11	-0.21	-0.23
100%:0	0.19	0.02	-0.05	-0.06	-0.14	-0.13	-0.09	-0.18	-0.22	-0.26
100%:0	0.19	-0.01	-0.08	-0.09	-0.20	-0.20	-0.11	-0.20	-0.22	-0.30
80%:20%	0.13	0.09	0.03	-0.17	-0.18	-0.12	-0.09	-0.06	-0.22	-0.21
80%:20%	0.12	-0.03	0.02	-0.17	-0.20	-0.13	-0.10	-0.09	-0.23	-0.24
80%:20%	0.12	-0.03	0.02	-0.17	-0.21	-0.15	-0.12	-0.16	-0.23	-0.25
80%:20%	0.11	-0.03	0.00	-0.18	-0.24	-0.20	-0.12	-0.18	-0.23	-0.27
80%:20%	0.09	-0.05	-0.02	-0.25	-0.27	-0.22	-0.13	-0.24	-0.25	-0.27

80%:20%	0.06	-0.12	-0.07	-0.30	-0.28	-0.23	-0.14	-0.25	-0.30	-0.32
60%:40%	0.02	0.02	-0.03	0.02	-0.16	-0.16	-0.06	-0.07	-0.17	-0.25
60%:40%	0.01	-0.02	-0.03	0.00	-0.16	-0.18	-0.07	-0.08	-0.21	-0.27
60%:40%	0.00	-0.03	-0.05	-0.02	-0.22	-0.19	-0.07	-0.09	-0.22	-0.27
60%:40%	-0.01	-0.04	-0.05	-0.03	-0.22	-0.20	-0.08	-0.13	-0.22	-0.30
60%:40%	-0.04	-0.08	-0.06	-0.14	-0.23	-0.24	-0.08	-0.15	-0.27	-0.34
60%:40%	-0.06	-0.10	-0.08	-0.17	-0.23	-0.24	-0.08	-0.25	-0.28	-0.34
40%:60%	-0.01	0.00	-0.03	-0.01	-0.17	-0.17	-0.05	0.02	-0.27	-0.28
40%:60%	-0.05	-0.06	-0.05	-0.04	-0.18	-0.18	-0.08	-0.06	-0.28	-0.30
40%:60%	-0.07	-0.15	-0.07	-0.04	-0.20	-0.22	-0.15	-0.09	-0.29	-0.31
40%:60%	-0.08	-0.15	-0.07	-0.05	-0.20	-0.24	-0.16	-0.09	-0.29	-0.32
40%:60%	-0.09	-0.15	-0.08	-0.12	-0.25	-0.28	-0.16	-0.22	-0.30	-0.33
40%:60%	-0.09	-0.16	-0.12	-0.14	-0.26	-0.29	-0.21	-0.24	-0.30	-0.34
20%:80%	-0.08	-0.05	-0.04	0.07	-0.18	-0.19	-0.10	0.10	-0.21	-0.25
20%:80%	-0.11	-0.11	-0.04	0.05	-0.18	-0.23	-0.12	0.06	-0.21	-0.30
20%:80%	-0.11	-0.12	-0.05	0.05	-0.21	-0.25	-0.13	0.04	-0.22	-0.30
20%:80%	-0.14	-0.16	-0.13	-0.03	-0.23	-0.28	-0.14	0.03	-0.23	-0.31
20%:80%	-0.15	-0.17	-0.14	-0.09	-0.24	-0.28	-0.15	0.03	-0.24	-0.34
20%:80%	-0.15	-0.20	-0.17	-0.13	-0.29	-0.28	-0.24	0.03	-0.24	-0.34
0:100%	-0.10	-0.03	-0.07	0.16	-0.15	-0.13	-0.08	-0.02	-0.22	-0.26
0:100%	-0.11	-0.04	-0.07	0.06	-0.15	-0.13	-0.09	-0.10	-0.22	-0.27
0:100%	-0.12	-0.06	-0.10	0.05	-0.17	-0.14	-0.09	-0.13	-0.24	-0.27
0:100%	-0.13	-0.08	-0.11	0.04	-0.19	-0.14	-0.13	-0.16	-0.24	-0.31
0:100%	-0.20	-0.10	-0.11	0.01	-0.21	-0.19	-0.15	-0.16	-0.25	-0.31
0:100%	-0.22	-0.13	-0.12	-0.03	-0.22	-0.29	-0.15	-0.23	-0.30	-0.31

Analyte	Results LDA					
Concentration	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Group
100%:0	17.46	5.27	3.03	0.29	-0.91	2.00
100%:0	16.48	7.30	3.23	0.96	-0.13	2.00
100%:0	15.13	6.78	1.19	0.22	-0.66	2.00
100%:0	15.81	7.92	0.15	0.53	-0.98	2.00
100%:0	15.80	6.95	0.31	-0.83	-0.39	2.00
100%:0	16.77	5.90	2.62	-1.54	0.73	2.00
80%:20%	13.01	-6.30	-3.46	0.66	-1.21	6.00
80%:20%	13.08	-7.96	-2.18	0.83	-1.59	6.00
80%:20%	13.63	-6.79	-2.59	0.12	-1.08	6.00
80%:20%	13.61	-6.05	-1.01	-0.77	0.00	6.00
80%:20%	13.92	-7.88	-2.58	-0.94	-0.51	6.00
80%:20%	13.14	-5.39	-1.80	0.92	0.67	6.00
60%:40%	-1.90	-0.12	0.77	-4.30	-0.35	5.00
60%:40%	-0.71	0.79	0.72	-2.00	0.71	5.00
60%:40%	-1.64	-2.27	0.14	-2.58	0.38	5.00
60%:40%	-2.08	-0.76	0.28	-3.19	1.47	5.00

60%:40%	-0.03	-1.89	0.25	-1.36	3.28	5.00
60%:40%	-0.72	-1.09	-1.61	-2.35	2.51	5.00
40%:60%	-2.59	0.20	-0.32	1.99	2.38	4.00
40%:60%	-4.05	0.90	-1.38	1.83	1.95	4.00
40%:60%	-3.12	0.44	-0.07	3.86	0.74	4.00
40%:60%	-3.92	0.65	0.26	4.12	0.98	4.00
40%:60%	-1.90	-0.96	-1.31	1.94	1.20	4.00
40%:60%	-1.95	1.88	-0.96	3.03	-0.10	4.00
20%:80%	-10.32	-3.38	1.92	0.50	-0.91	3.00
20%:80%	-11.14	-3.23	4.17	-0.27	0.59	3.00
20%:80%	-10.71	-2.90	4.19	0.14	0.66	3.00
20%:80%	-11.81	-2.22	5.39	-0.65	-1.15	3.00
20%:80%	-11.64	-3.53	5.44	-0.48	-0.47	3.00
20%:80%	-10.24	-4.79	4.72	2.06	-2.70	3.00
0:100%	-14.59	4.48	-1.96	-0.32	-0.87	1.00
0:100%	-12.98	3.13	-3.00	-1.80	-1.31	1.00
0:100%	-13.32	4.13	-3.77	-1.09	-1.49	1.00
0:100%	-13.44	5.17	-3.88	-0.38	-1.11	1.00
0:100%	-17.74	2.11	-3.66	-0.81	-1.10	1.00
0:100%	-15.30	3.52	-3.27	1.66	0.77	1.00

Canonical Scores Plot

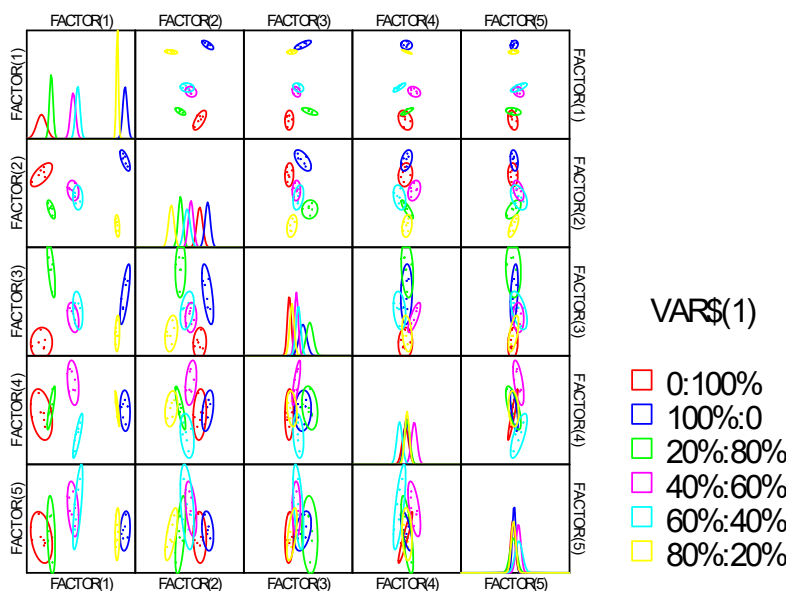


Fig. S5 Correlations of canonical fluorescence response patterns from the array of channel 1-channel 10 against different proportion of the HPDE6-C7 to PANC-1. The 95% confidence ellipses for the individual analytes are shown.

Table S5 Training matrix of fluorescence response pattern from an array of 10 channels against 9 cell lines. LDA was carried out and resulted in 8 factors of the canonical scores.

Analyte	Fluorescence Response Pattern									
Cell	CH1	CH2	CH3	CH4	CH5	CH6	CH7	CH8	CH9	CH10
Du145	0.21	0.26	0.16	0.10	-0.04	0.01	0.16	0.24	0.19	0.20
Du145	0.18	0.26	0.16	0.09	-0.04	-0.03	0.12	0.19	0.18	0.18
Du145	0.17	0.26	0.15	-0.02	-0.04	-0.05	0.11	0.14	0.16	0.13
Du145	0.13	0.25	0.14	-0.03	-0.12	-0.07	0.10	0.08	0.15	0.09
Du145	0.12	0.25	0.13	-0.06	-0.13	-0.09	0.09	0.05	0.15	0.04
Du145	0.12	0.21	0.09	-0.07	-0.14	-0.13	0.09	-0.02	0.12	-0.04
A549	0.18	0.24	0.13	0.12	0.06	0.04	0.14	0.11	0.33	0.19
A549	0.18	0.20	0.13	0.11	0.05	0.02	0.14	0.10	0.28	0.17
A549	0.13	0.18	0.12	0.10	0.02	-0.03	0.12	-0.07	0.28	0.07
A549	0.12	0.06	0.11	0.03	-0.02	-0.03	0.08	-0.07	0.22	0.06
A549	0.09	0.05	0.11	-0.02	-0.09	-0.06	0.05	-0.09	0.19	-0.01
A549	0.07	0.03	0.02	-0.04	-0.12	-0.10	0.02	-0.19	0.16	-0.03
PANC-1	0.14	0.08	0.10	0.03	-0.02	0.02	0.10	0.24	0.30	0.22
PANC-1	0.14	0.07	0.09	-0.04	-0.03	-0.04	0.09	0.11	0.30	0.21
PANC-1	0.13	0.05	0.08	-0.07	-0.09	-0.06	0.03	-0.06	0.26	0.19
PANC-1	0.07	0.03	0.07	-0.18	-0.12	-0.07	0.02	-0.06	0.23	0.08
PANC-1	0.06	0.02	0.01	-0.18	-0.12	-0.09	0.02	-0.16	0.14	0.03
PANC-1	0.03	-0.02	-0.06	-0.20	-0.16	-0.14	0.02	-0.20	0.09	0.01
BT549	0.09	0.13	0.06	-0.07	0.17	0.10	0.01	0.27	0.16	0.10
BT549	0.15	0.18	0.15	0.11	0.31	0.30	0.18	0.45	0.22	0.27
BT549	0.04	0.06	-0.04	-0.18	0.03	0.02	-0.01	0.21	0.09	0.00
BT549	0.02	-0.01	-0.04	-0.21	0.02	0.01	-0.02	0.11	0.08	-0.01
BT549	0.02	-0.04	-0.05	-0.23	0.00	-0.10	-0.07	0.10	0.07	-0.05
BT549	0.00	-0.06	-0.06	-0.23	-0.06	-0.17	-0.08	0.07	0.04	-0.12
PANC02	0.15	0.18	0.24	0.16	0.19	0.31	0.26	0.33	0.21	0.34
PANC02	0.05	0.06	0.14	-0.03	-0.11	-0.06	0.11	0.21	0.08	0.09
PANC02	0.02	0.01	0.11	-0.05	-0.12	-0.08	0.04	0.07	0.07	0.06
PANC02	0.02	0.00	0.09	-0.10	-0.12	-0.09	0.02	0.07	0.07	0.03
PANC02	-0.03	-0.01	0.07	-0.17	-0.13	-0.16	0.00	0.00	0.03	-0.06
PANC02	-0.04	-0.18	0.06	-0.19	-0.15	-0.30	-0.04	-0.01	-0.01	-0.06
A375	0.04	0.06	-0.05	-0.05	-0.02	-0.02	0.31	0.30	0.24	0.21
A375	0.04	0.08	-0.04	-0.04	-0.02	-0.02	0.32	0.35	0.26	0.23
A375	0.05	0.09	-0.04	-0.04	-0.01	-0.01	0.35	0.39	0.27	0.24
A375	0.05	0.09	-0.04	-0.01	-0.01	-0.01	0.37	0.41	0.29	0.26
A375	0.05	0.09	0.20	0.18	0.00	0.00	0.39	0.41	0.29	0.27
A375	0.06	0.11	0.22	0.20	0.00	0.00	0.41	0.42	0.30	0.28

SK-OV-3	0.05	0.12	-0.01	-0.07	0.13	0.15	0.07	0.06	-0.01	-0.03
SK-OV-3	0.09	0.13	0.00	0.01	0.13	0.15	0.14	0.12	-0.01	-0.02
SK-OV-3	0.11	0.14	0.15	0.13	0.01	0.03	0.18	0.21	0.12	0.09
SK-OV-3	0.15	0.14	0.15	0.13	0.02	0.03	0.23	0.22	0.14	0.12
SK-OV-3	0.10	0.20	0.27	0.28	0.13	0.16	0.16	0.19	0.05	0.04
SK-OV-3	0.13	0.21	0.28	0.29	0.14	0.17	0.21	0.21	0.06	0.05
NIH/3T3	0.01	0.00	-0.06	-0.07	0.10	0.14	0.07	0.06	0.01	-0.02
NIH/3T3	0.01	0.00	-0.05	-0.06	0.11	0.14	0.08	0.07	0.05	0.01
NIH/3T3	0.02	0.03	-0.04	-0.03	0.11	0.14	0.08	0.08	0.06	0.02
NIH/3T3	0.02	0.03	-0.04	-0.01	0.11	0.15	0.10	0.09	0.06	0.05
NIH/3T3	0.05	0.03	0.19	0.20	0.14	0.15	0.10	0.10	0.12	0.06
NIH/3T3	0.06	0.05	0.05	0.06	0.02	0.05	0.07	0.04	0.15	0.17
HPDE6-C7	-0.01	0.02	0.04	0.12	0.06	0.08	0.22	0.19	0.18	0.08
HPDE6-C7	-0.02	0.02	0.03	0.10	0.04	0.04	0.21	0.18	0.13	0.04
HPDE6-C7	0.06	0.12	0.11	0.35	0.18	0.26	0.25	0.44	0.32	0.30
HPDE6-C7	0.05	0.11	0.11	0.26	0.17	0.24	0.23	0.41	0.24	0.23
HPDE6-C7	0.00	0.10	0.10	0.16	0.09	0.23	0.23	0.26	0.23	0.20
HPDE6-C7	0.00	0.04	0.10	0.12	0.09	0.09	0.22	0.24	0.20	0.16

Note: CH: channel;

LDA was carried out and resulted in 8 factors of the canonical scores.

Analyte	Results LDA								
	Factor	Factor	Factor	Factor	Factor	Factor	Factor	Factor	Group
	1	2	3	4	5	6	7	8	
Du145	11.41	-3.35	3.36	1.48	-0.44	-0.44	-0.89	1.46	5.00
Du145	10.70	-3.05	2.84	1.49	-0.29	-1.66	-0.86	0.08	5.00
Du145	11.95	-4.22	3.21	-0.08	0.42	-0.66	-0.56	-0.88	5.00
Du145	9.74	-3.88	3.83	0.29	-0.34	-2.51	-0.57	-0.52	5.00
Du145	10.25	-3.05	4.22	0.51	0.60	-2.19	-0.19	-0.38	5.00
Du145	11.51	-0.92	4.49	1.86	1.35	-0.66	0.28	-0.14	5.00
A549	6.03	5.84	2.89	0.38	2.50	-1.03	-0.02	-0.80	3.00
A549	6.56	4.68	2.38	0.89	1.36	0.21	0.05	-0.50	3.00
A549	4.94	8.34	3.07	1.82	1.95	-0.31	0.80	-2.12	3.00
A549	5.40	6.74	0.95	-0.35	-0.31	1.46	0.98	0.23	3.00
A549	6.06	6.04	0.80	-0.50	0.02	0.73	1.64	1.40	3.00
A549	5.13	7.14	1.21	0.88	-1.30	0.19	0.15	0.02	3.00
PANC-1	2.18	2.59	-0.01	-3.29	0.63	-0.26	0.34	2.53	7.00
PANC-1	3.28	3.40	1.18	-4.40	0.30	0.68	0.16	0.56	7.00
PANC-1	5.91	4.70	1.06	-4.36	-2.60	0.35	-0.74	0.23	7.00
PANC-1	3.89	3.58	0.76	-5.60	-0.62	0.08	0.62	1.03	7.00
PANC-1	4.40	3.21	1.04	-2.85	-2.15	0.68	-0.59	-0.38	7.00
PANC-1	1.85	2.42	1.29	-1.41	-3.43	0.43	-1.71	-1.43	7.00

BT549	4.18	-1.76	-4.76	-2.48	4.15	-0.92	-0.14	-1.23	4.00
BT549	1.10	-1.95	-4.04	-1.52	2.86	1.52	-0.25	0.54	4.00
BT549	2.59	-2.83	-3.86	-2.02	3.16	-1.19	-0.47	0.83	4.00
BT549	2.04	-1.25	-4.14	-2.99	1.69	0.51	-0.32	0.81	4.00
BT549	3.73	-1.68	-4.64	-3.12	2.85	0.49	0.33	-0.44	4.00
BT549	3.26	-1.41	-4.01	-1.96	3.17	0.14	0.80	-0.37	4.00
PANC02	0.07	-3.05	-1.05	-1.63	-2.76	1.66	-0.45	1.30	8.00
PANC02	0.71	-7.04	0.18	-1.46	-2.16	-0.74	0.72	1.01	8.00
PANC02	0.56	-3.71	-1.35	-1.82	-3.06	-1.25	0.42	0.18	8.00
PANC02	1.58	-3.65	-1.46	-2.19	-2.05	-0.77	0.55	0.32	8.00
PANC02	-0.04	-4.03	-1.33	-2.31	-0.99	-1.10	1.11	-1.62	8.00
PANC02	-1.23	-4.59	-3.19	-3.55	-1.88	1.85	1.98	-2.46	8.00
A375	-12.09	-1.17	4.43	-0.80	0.80	1.07	-1.30	-0.18	2.00
A375	-12.86	-1.73	4.78	-0.96	1.30	0.53	-1.28	-0.20	2.00
A375	-12.60	-2.33	5.00	-0.95	1.78	1.21	-1.13	0.19	2.00
A375	-14.09	-1.87	5.48	-0.72	1.65	1.13	-1.19	0.08	2.00
A375	-13.72	-2.77	4.58	-0.45	-0.21	0.72	1.80	-0.12	2.00
A375	-13.79	-2.69	5.32	-0.45	0.07	0.73	2.11	-0.24	2.00
SK-OV-3	4.17	-2.02	-2.99	2.98	0.17	0.92	-1.68	-0.94	9.00
SK-OV-3	4.88	-1.60	-1.58	5.33	0.38	2.41	-1.38	0.37	9.00
SK-OV-3	2.66	-1.88	0.85	3.07	0.00	0.31	0.70	0.76	9.00
SK-OV-3	4.77	-1.44	2.39	3.20	-0.14	2.72	0.66	1.55	9.00
SK-OV-3	4.96	-2.24	-2.03	5.86	-0.65	-0.46	1.66	-0.15	9.00
SK-OV-3	5.68	-2.70	-0.83	6.31	-0.69	0.93	1.70	0.32	9.00
NIH/3T3	-1.85	0.51	-4.21	2.03	-0.56	1.20	-1.31	0.22	1.00
NIH/3T3	-3.35	1.13	-4.01	1.11	-0.56	0.97	-1.25	-0.22	1.00
NIH/3T3	-2.78	1.50	-3.68	1.69	-0.31	0.55	-1.34	-0.11	1.00
NIH/3T3	-3.55	1.20	-3.48	1.82	-1.09	0.63	-1.71	-0.35	1.00
NIH/3T3	-2.02	3.08	-4.48	1.96	-1.30	0.37	1.74	-0.13	1.00
NIH/3T3	-1.64	2.17	-1.79	-0.13	-3.17	-1.30	-1.46	-1.32	1.00
HPDE6-C7	-12.33	3.03	-0.57	2.10	0.56	-0.63	0.69	-0.29	6.00
HPDE6-C7	-11.22	1.04	-0.42	3.08	0.27	-0.09	0.56	-0.73	6.00
HPDE6-C7	-13.69	4.01	-2.45	2.18	0.28	-3.49	-0.21	1.40	6.00
HPDE6-C7	-10.66	1.25	-2.88	1.77	0.48	-2.24	0.05	1.31	6.00
HPDE6-C7	-12.51	1.63	-1.32	0.31	-1.29	-2.88	-0.23	0.76	6.00
HPDE6-C7	-12.09	0.61	-1.05	-0.05	-0.36	-0.57	0.65	-1.21	6.00

Canonical Scores Plot

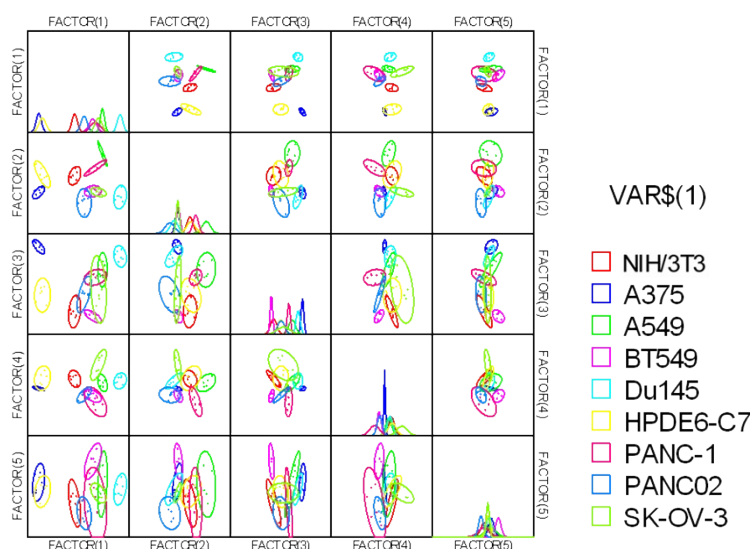


Fig. S6 Correlations of canonical fluorescence response patterns from the array of channel 1-channel 10 against 9 cell lines. The 95% confidence ellipses for the individual analytes are shown.

Table S6 Detection and identification of unknown samples in PBS using LDA from the array of 10 channels. According to the verification, 35 of 36 unknown samples were correctly identified, representing an accuracy of 97.2%.

Unknown Samples	Fluorescence Response Pattern									
	CH1	CH2	CH3	CH4	CH5	CH6	CH7	CH8	CH9	CH10
1	0.26	0.33	0.24	0.21	0.08	0.14	0.29	0.52	0.31	0.35
2	0.25	0.33	0.22	0.17	0.00	0.13	0.20	0.41	0.30	0.28
3	0.23	0.27	0.22	0.16	-0.02	0.07	0.19	0.28	0.26	0.23
4	0.22	0.26	0.18	0.12	-0.02	0.04	0.19	0.26	0.20	0.22
5	0.28	0.31	0.32	0.38	0.15	0.13	0.28	0.42	0.44	0.27
6	0.27	0.28	0.29	0.26	0.14	0.11	0.26	0.33	0.41	0.27
7	0.21	0.25	0.22	0.18	0.13	0.10	0.23	0.26	0.39	0.24
8	0.20	0.24	0.20	0.16	0.12	0.10	0.20	0.18	0.38	0.21
9	0.20	0.33	0.24	0.10	0.11	0.21	0.21	0.43	0.37	0.47
10	0.20	0.28	0.23	0.07	0.09	0.17	0.20	0.37	0.37	0.39
11	0.18	0.12	0.20	0.05	0.05	0.07	0.16	0.30	0.34	0.32
12	0.16	0.09	0.10	0.04	-0.02	0.04	0.11	0.25	0.34	0.32
13	0.05	0.06	0.06	-0.09	0.14	0.05	-0.01	0.22	0.12	0.09
14	0.15	0.18	0.12	0.04	0.30	0.22	0.10	0.43	0.22	0.22
15	0.12	0.14	0.11	0.02	0.25	0.15	0.08	0.39	0.21	0.18
16	0.10	0.13	0.10	-0.03	0.19	0.11	0.07	0.36	0.20	0.15
17	0.07	0.12	0.17	-0.01	-0.03	-0.04	0.12	0.24	0.09	0.12

18	0.13	0.17	0.23	0.08	0.09	0.08	0.25	0.29	0.15	0.26
19	0.11	0.14	0.22	0.08	0.03	0.07	0.22	0.29	0.12	0.21
20	0.07	0.13	0.22	0.01	-0.03	0.05	0.13	0.27	0.10	0.18
21	0.03	0.07	0.06	0.04	-0.08	-0.08	0.25	0.29	0.21	0.21
22	0.03	0.08	0.06	0.06	-0.08	-0.08	0.27	0.32	0.21	0.22
23	0.04	0.08	0.06	0.07	-0.08	-0.08	0.27	0.33	0.23	0.26
24	0.04	0.09	0.07	0.07	-0.08	-0.08	0.27	0.34	0.29	0.27
25	0.09	0.12	0.13	0.12	0.00	0.02	0.15	0.15	0.01	0.01
26	0.10	0.13	0.14	0.13	0.01	0.02	0.17	0.19	0.01	0.01
27	0.09	0.17	0.01	0.03	0.13	0.15	0.15	0.12	0.00	-0.01
28	0.10	0.20	0.04	0.03	0.13	0.16	0.16	0.16	0.03	0.03
29	0.03	0.03	0.05	0.04	0.01	0.02	0.05	0.03	0.11	0.06
30	0.04	0.04	0.05	0.05	0.01	0.03	0.05	0.04	0.13	0.11
31	0.04	0.05	0.05	0.05	0.01	0.04	0.06	0.04	0.15	0.14
32	0.05	0.03	0.20	0.20	0.14	0.16	0.14	0.10	0.13	0.10
33	-0.02	-0.02	0.03	0.09	0.03	0.03	0.20	0.18	0.12	0.04
34	-0.02	-0.05	0.02	0.06	0.00	0.01	0.19	0.03	0.10	0.03
35	-0.02	-0.11	0.01	-0.01	-0.01	-0.06	0.15	0.00	0.10	0.00
36	-0.04	-0.13	-0.01	-0.09	-0.02	-0.17	0.11	-0.09	0.07	-0.02

Unknown Samples	Results LDA								Analyte	
	Factor 1	Factor 2	Factor 3	Factor 4	Factor 5	Factor 6	Factor 7	Factor 8	Group	Verification
1	8.28	-4.62	3.90	0.64	1.83	0.20	-0.18	3.10	5.00	Du145
2	11.78	-2.58	3.31	0.14	1.58	-1.25	0.08	4.65	5.00	Du145
3	11.29	-0.99	3.64	0.84	0.37	0.00	0.29	3.16	5.00	Du145
4	11.27	-3.31	3.58	1.54	-0.62	0.20	-0.73	2.03	5.00	Du145
5	7.43	5.54	3.57	2.38	5.43	0.54	3.03	2.63	3.00	A549
6	8.62	4.93	3.75	0.31	4.31	1.96	2.38	1.82	3.00	A549
7	4.70	4.98	3.08	-0.72	3.91	0.62	1.53	0.40	3.00	A549
8	5.03	6.82	2.83	-0.43	3.84	0.41	1.31	-0.19	3.00	A549
9	3.39	-4.24	1.73	-5.49	-0.23	-2.98	-1.55	0.04	8.00	PANC02
10	4.15	-2.13	2.03	-5.37	0.77	-1.34	-0.39	1.11	7.00	PANC-1
11	3.72	0.71	0.62	-5.30	0.31	1.36	0.79	2.04	7.00	PANC-1
12	2.48	2.60	0.35	-4.77	-0.82	-0.42	-0.57	2.48	7.00	PANC-1
13	1.71	-2.40	-5.28	-3.07	2.57	-0.59	0.01	-1.96	4.00	BT549
14	3.86	-2.15	-4.93	-2.27	4.89	0.94	-0.01	-0.51	4.00	BT549
15	1.96	-1.81	-4.67	-2.46	4.64	0.11	0.30	-1.02	4.00	BT549
16	2.55	-2.49	-3.92	-3.22	4.77	0.20	0.61	-0.75	4.00	BT549
17	2.12	-7.76	-0.23	-1.40	-0.97	-0.63	0.56	-0.73	8.00	PANC02
18	1.30	-6.76	1.71	-1.04	-1.88	2.29	0.13	-1.33	8.00	PANC02
19	2.18	-7.19	0.95	-0.62	-2.37	1.52	0.38	0.34	8.00	PANC02
20	1.40	-8.38	-0.79	-2.54	-2.53	-1.20	0.51	0.61	8.00	PANC02

21	-9.84	-3.37	3.46	-0.49	-0.98	-1.08	-0.44	-0.81	2.00	A375
22	-10.55	-3.49	3.62	-0.13	-0.78	-1.24	-0.34	-0.61	2.00	A375
23	-11.25	-3.68	3.73	-0.74	-1.18	-1.49	-0.65	-0.99	2.00	A375
24	-11.99	-1.54	4.04	-1.49	-0.06	-2.04	-0.22	-0.62	2.00	A375
25	5.09	-3.78	0.13	5.11	-1.25	1.13	0.40	0.68	9.00	SK-OV-3
26	4.99	-4.40	0.37	5.41	-0.73	1.37	0.57	0.90	9.00	SK-OV-3
27	5.20	-1.72	-0.83	5.74	0.54	1.78	-1.53	-0.07	9.00	SK-OV-3
28	5.22	-2.80	-0.49	4.83	0.77	1.04	-1.57	-0.28	9.00	SK-OV-3
29	-1.35	2.03	-2.54	0.73	-1.83	-1.31	-0.42	-0.75	1.00	NIH/3T3
30	-2.27	1.97	-2.30	0.22	-2.47	-1.88	-0.96	-1.34	1.00	NIH/3T3
31	-2.17	2.20	-2.14	-0.11	-2.75	-1.68	-1.12	-1.11	1.00	NIH/3T3
32	-3.59	2.81	-3.53	1.59	-2.09	0.92	1.49	-0.62	1.00	NIH/3T3
33	-11.07	1.23	-0.89	2.62	0.14	0.45	0.82	-0.24	6.00	HPDE6-C7
34	-10.30	3.17	-0.27	2.54	-2.27	1.37	0.33	-0.61	6.00	HPDE6-C7
35	-8.89	3.36	-0.99	0.86	-1.62	2.96	0.98	-1.14	6.00	HPDE6-C7
36	-9.11	2.28	-0.45	-0.06	-1.62	3.17	0.65	-4.31	6.00	HPDE6-C7

4. Various Data Split Ratios

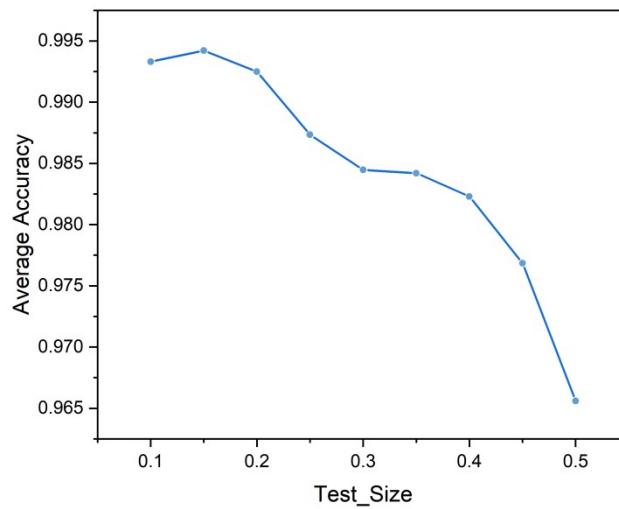


Fig. S7 The curve depicting the relationship between average accuracy and the percentage of the test set.

5. Train and Test Accuracy in Different Model.

Table S7 Training and test accuracy in different model.

Signal Channel (RF-RFE-MLP)										Accuracy
1	2	3	4	5	6	7	8	9	10	0.96
1	2	3	4	5	7	8	9	10	/	0.98
1	2	4	5	7	8	9	10	/	/	0.97
1	2	4	5	7	8	9	/	/	/	0.95

1	2	5	7	8	9	/	/	/	/	0.89
1	2	5	7	9	/	/	/	/	/	0.84
2	5	7	9	/	/	/	/	/	/	0.82
2	7	9	/	/	/	/	/	/	/	0.66
2	7	/	/	/	/	/	/	/	/	0.52
7	/	/	/	/	/	/	/	/	/	0.28

Table S8 Train and test accuracy in different model.

Model Name	10 Features Model		7 Features Model		6 PC Model	
	Train Accuracy (%)	Test Accuracy (%)	Train Accuracy (%)	Test Accuracy (%)	Train Accuracy (%)	Test Accuracy (%)
RF	100.0	83.7	100.0	82.0	100.0	92.7
LRG	100.0	96.0	98.2	92.1	100.0	96.9
SVM	99.0	88.3	97.5	84.8	100.0	98.8
KNN	91.3	71.8	89.7	74.6	97.5	90.6
DT	100.0	63.6	100.0	65.4	100.0	85.1
GNB	85.8	68.4	82.2	64.7	99.1	89.7
LDA	100.0	99.4	98.4	94.3	98.8	97.7
BNB	68.1	54.5	69.3	55.8	89.2	78.2
GPC	100.0	91.6	99.7	89.7	100.0	97.2

6.CCK-8 Assay

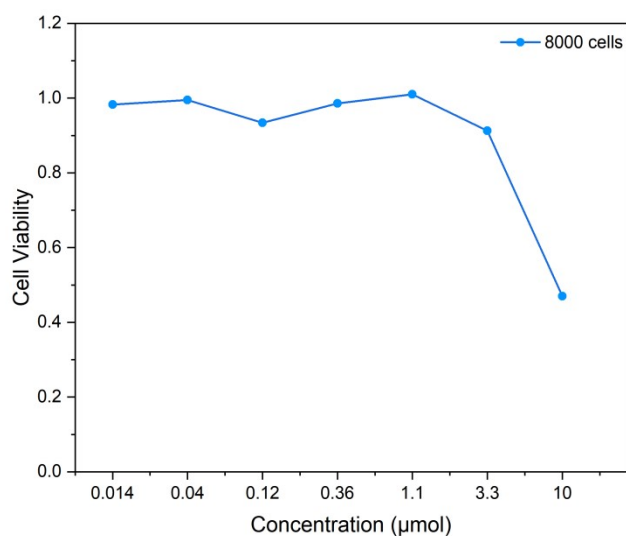


Fig. S8 Curve of cell viability versus cell concentration in CCK-8 assay.