Electronic Supporting Information for

Towards Rational Chemosensor Design Through Improved Understanding of Experimental Parameter Variation and Tolerance in Cyclodextrin-Promoted Fluorescence Detection

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MATERIALS AND METHODS

All chemicals were obtained from Sigma-Aldrich chemical company or Fisher Scientific and used as received, including compounds **1-6**, **8** and **9**. Compound **7** was synthesized following literature-reported procedures.

REFERENCE: Shepherd, J. L.; Kell, A.; Chung, E.; Sinclar, C. W.; Workentin, M. S.; Bizzotto, D. *J. Am. Chem. Soc.* **2004**, *126*, 8329-8335.

Fluorescence measurements were recorded on a Shimadzu RF 5301 spectrophotometer with 1.5 nm excitation and 1.5 nm emission slit widths. All fluorescence spectra were integrated vs. wavenumber on the X-axis, using OriginPro Version 8.6. For the temperature studies, a Fisher Scientific Isotemp 6200 R20 was used to control the temperature and the spectrophotometer was equipped with a single constant-temperature cell holder.

Select spectra were deconvoluted using OriginPro Version 8.6 fitted to a Gaussian curve.

Array analysis was performed using SYSTAT 13 statistical computing software with the following settings:

(a) Classical Discriminant Analysis

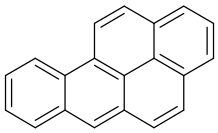
(b) Grouping variable: Analytes

(c) Predictors: γ-cyclodextrin-Bodipy, γ-cyclodextrin-Rhodamine 6G, γ-cyclodextrin-Coumarin 6

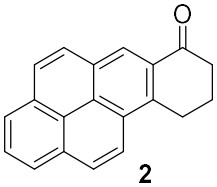
(d) Long-range statistics: Mahal

Computational experiments were performed using Spartan software (Spartan 10, version 1.1.0). All conformations shown were energy-minimized. The red areas represent electron-rich regions and the blue areas represent electron-deficient regions.

ANALYTE DETAILS



1
Benzo[*a*]pyrene



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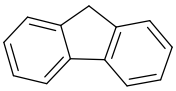
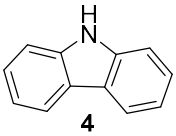
9,10-Dihydrobenzo[*a*]pyrene-7(*8H*)-one



3
Fluorene



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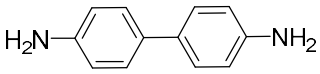
Carbazole



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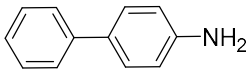
Benzidine



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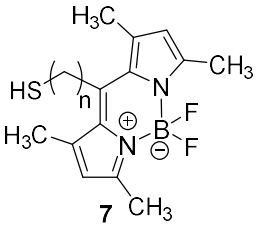
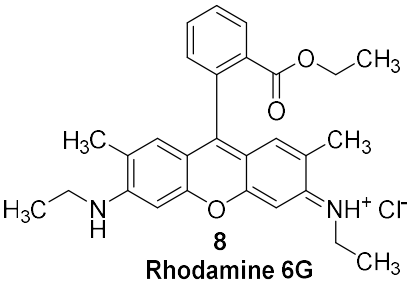
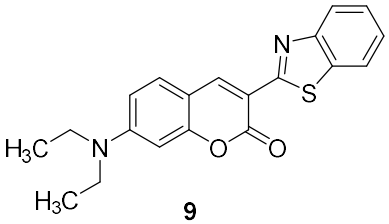
4-Aminobiphenyl



7
BODIPY



8
Rhodamine 6G



9
Coumarin 6

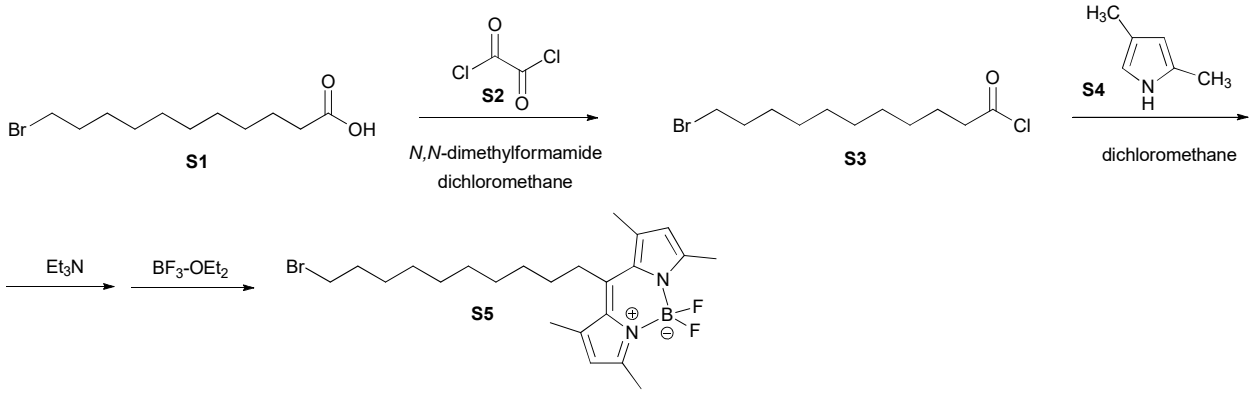
Compound Number	Excitation Wavelength (nm)	Concentration (mg/mL)	Volume Added (µL)	Final Concentration (µM)
1	360	1.0	20	45.5
2	360	1.0	20	41.8
3	270	1.0	20	30.5
4	340	1.0	20	46.0
5	365	1.0	20	28.5
6	290	1.0	20	46.3
7	460	0.1	100	9.5
8	490	0.1	100	8.1
9	420	0.1	100	11.0

SYNTHESIS OF FLUOROPHORE 7

The synthesis of BODIPY **7** was performed according to literature procedures:

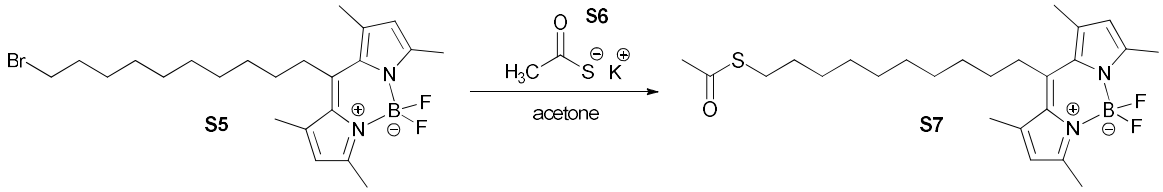
Shepherd, J. L.; Kell, A.; Chung, E.; Sinclar, C. W.; Workentin, M. S.; Bizzotto, D. *J. Am. Chem. Soc.* **2004**, *126*, 8329-8335.

Reaction 1:



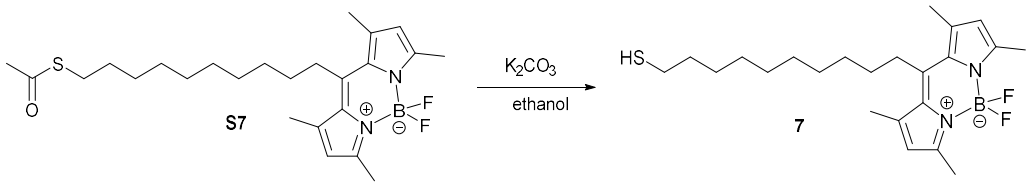
Procedure: 2.0 grams of 11-bromoundecanoic acid **S1** (7.54 mmol, 1.0 eq.) was combined with 2 drops of *N,N*-dimethylformamide in 40 mL of dichloromethane. 1.0 gram of oxalyl chloride **S2** (7.88 mmol, 1.05 eq.) was dissolved in 5.0 mL of dichloromethane and added dropwise. The reaction mixture was stirred for one hour, then the crude mixture was concentrated on the rotary evaporator and dried on a vacuum overnight to remove any unreacted oxalyl chloride. The resulting acid chloride **S3** was dissolved in 50 mL of dichloromethane. 0.772 mL of 2,4-dimethylpyrrole **S4** (7.50 mmol, 0.99 eq.) was dissolved in 5.0 mL of dichloromethane and added to the reaction mixture. The resulting reaction mixture was heated to reflux for 3 hours under a nitrogen atmosphere, during which time the mixture became a dark red color. After three hours, the reaction mixture was cooled to room temperature and solvent was removed on the rotary evaporator until approximately 5.0 mL of the dichloromethane solution remained. 200 mL of *n*-hexanes were added to the flask, and the mixture was cooled overnight in the freezer at -20 ºC. The hexanes were decanted from the insoluble oil and precipitate. The resulting crude product was dissolved in 75 mL of toluene and heated to 80 ºC. 1.0 mL of triethylamine (7.17 mmol, 0.95 eq.) was added and the solution immediately turned light yellow. 1.0 mL of boron trifluoride etherate (8.10 mmol, 1.07 eq.) was then added and the reaction mixture was stirred at 80 ºC for 30 minutes, during which time the color of the mixture darkened and became fluorescent. The reaction mixture was cooled to room temperature, and the product was extracted 3 times with brine (50 mL each time). The organic layer was dried over sodium sulfate, filtered, and concentrated. The crude product was purified by flash chromatography (1:1 dichloromethane: hexanes) to yield the desired product in 28% yield (comparable to the literature-reported 24% yield).

Reaction 2:



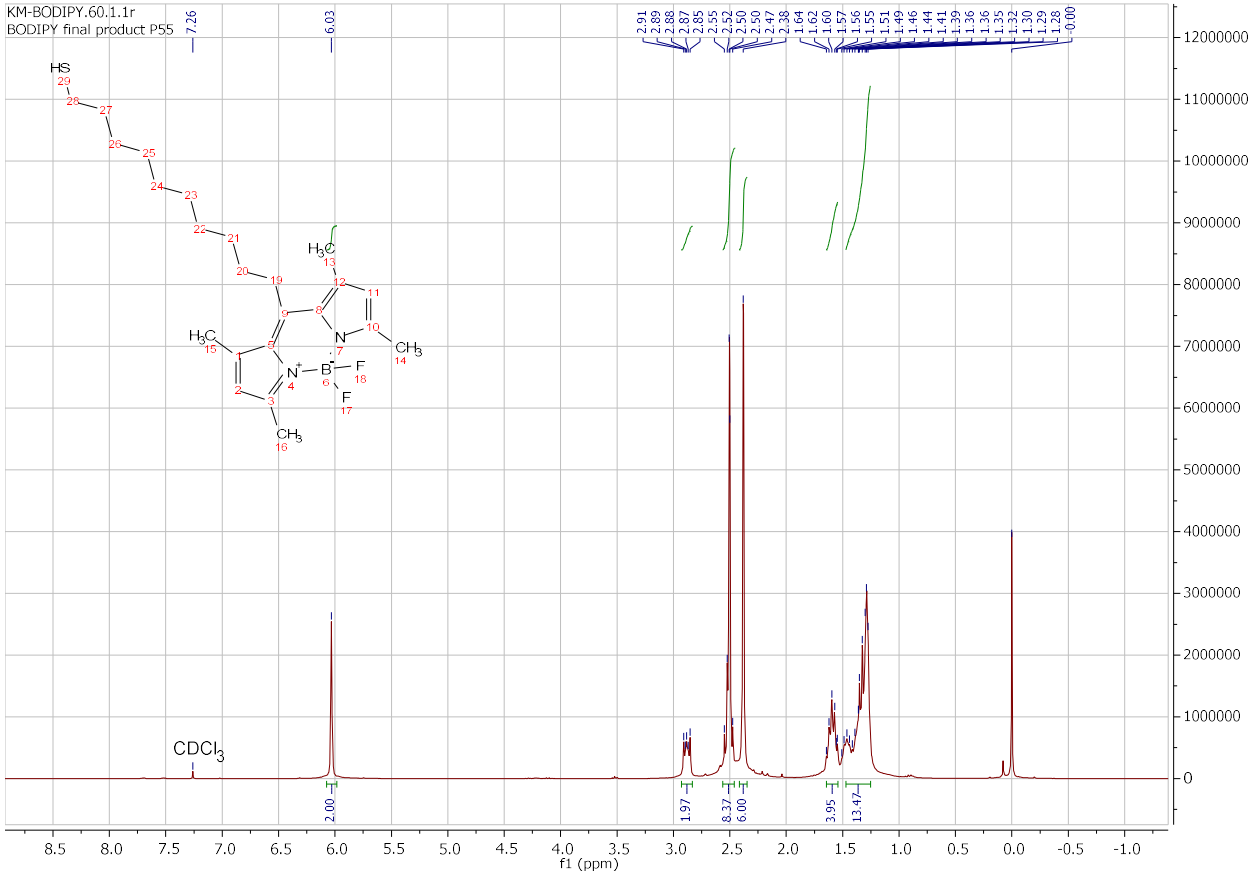
Procedure: Compound **S5** (0.968 g, 2.07 mmol, 1.0 eq.) and compound **S6** (0.27 grams, 2.36 mmol, 1.14 eq.) were dissolved in 50 mL of acetone. The reaction mixture was heated to reflux for two hours. After two hours, the reaction mixture was cooled to room temperature, acetone was removed, and the crude solid was re-dissolved in dichloromethane and washed with water. The organic extract was dried over sodium sulfate, filtered and concentrated, to yield compound **S7** in 97% yield (0.932 grams).

Reaction 3:



Procedure: Compound **S7** (0.932 grams, 2.01 mmol, 1.0 eq.) was dissolved in 150 mL of anhydrous ethanol that was purged with nitrogen. Potassium carbonate was added, and the reaction mixture was warmed to 30 °C. The reaction mixture was stirred under nitrogen for 4 hours at 30 °C. The contents of the flask were poured over 40 mL of aqueous saturated ammonium chloride, at which point the solution turned bright orange. The product was extracted with dichloromethane and washed several times with water. The organic layer was dried over sodium sulfate, filtered, and concentrated. The product was purified via flash chromatography (1:1 dichloromethane: hexanes) to yield compound **7** in 76% yield (674 mg).

[1]H NMR OF FLUOROPHORE 7



EXPERIMENTAL DETAILS FOR ENERGY TRANSFER EXPERIMENTS

Energy transfer experiments. All energy transfer experiments were conducted as follows: 2.5 mL of a 10-mM solution of γ-cyclodextrin dissolved in an aqueous solution (see below) was measured into a quartz cuvette. 20 μL of the analyte (1.0 mg/mL solution in THF) was added and the solution was excited at two wavelengths: near the analyte's absorption maximum (defined as "analyte excitation") and near the fluorophore's absorption maximum (defined as "fluorophore excitation"). Four repeat measurements were taken at each excitation wavelength. 100 μL of the fluorophore (0.1 mg/mL solution in THF) was added and the solution was excited at the analyte and fluorophore wavelengths. Four repeat measurements were taken at each wavelength. The energy transfer efficiencies were calculated according to Equation 1:

$$\% \text{ Energy Transfer} = I_{DA}/I_A \times 100\% \quad (1)$$

where I_{DA} is defined as the integrated fluorophore emission from analyte excitation and I_A is the integrated fluorophore emission from direct excitation.

Control ratio. Control experiments were conducted as follows: (a) The fluorophore was mixed with γ-cyclodextrin and excited at the excitation wavelength of the analyte (but in the absence of any analyte); and (b) the fluorophore and analyte were both mixed in γ-cyclodextrin and excited at the analyte excitation wavelength. The fluorophore emission that resulted from excitation at the analyte wavelength in the absence of the analyte was compared to the fluorophore emission from excitation at the analyte wavelength in the presence of the analyte. The ratio of these two emissions, shown as the "Control ratio" was calculated according to Equation 2:

$$\text{Control ratio} = I_{\text{fluorophore-control}}/I_{\text{fluorophore-analyte}} \quad (2)$$

Where $I_{\text{fluorophore-analyte}}$ is the integration of the fluorophore emission in the presence of the analyte; and $I_{\text{fluorophore-control}}$ is the integration of the fluorophore emission in the absence of the analyte. For ratios less than 0.95, legitimate energy transfer was occurring; for ratios between 0.95-1.05, the observed fluorescence response was the result of exciting the fluorophore at a wavelength where it has non-zero absorbance; and for ratios greater than 1.05, fluorescence quenching was occurring.

Cyclodextrin solutions. For each experiment, different cyclodextrin solutions were prepared and the energy transfer experiments were modified as follows:

a) **Concentration Effects.** Various concentrations of cyclodextrin were used to understand the effect of the host concentration on cyclodextrin-promoted energy transfer. The following concentrations of γ-cyclodextrin were prepared in phosphate buffered saline (PBS): 5 mM, 10 mM, and 15 mM. Energy transfer experiments were conducted using the above procedures.

b) **Temperature Effects.** A 10 mM γ-cyclodextrin solution was prepared in PBS. Energy transfer experiments were then conducted using the above procedures at the following temperatures: 5 °C, 20 °C, 35 °C, 50 °C, 65 °C, and 80 °C. The temperature control system used indicated when the desired temperature was reached, and each sample was allowed to sit in the unit after the desired temperature was reached for approximately 5 minutes before the fluorescence emission spectrum was collected. This was done to ensure the sample was at the correct temperature. Energy transfer experiments were conducted using the above procedures.

c) pH Effects. 10 mM γ-cyclodextrin solutions were prepared using various concentrations of aqueous HCl and NaOH at the following pH levels: 0, 3, 5, 8, 10, 12. Energy transfer experiments were conducted using the above procedures.

d) **Salt Effects.** Sodium chloride and guanidinium hydrochloride were used to investigate the effect of chaotropic and kosmotropic salts on the cyclodextrin-promoted energy transfer. 1 M solutions of each salt were prepared in deionized water. A 10 mM γ-cyclodextrin solution was then prepared using these salt solutions. A control experiment was also performed with a 10 mM γ-cyclodextrin

solution in deionized water in the absence of salt. Energy transfer experiments were then conducted using the above procedures.

e) **Solvent Effects.** The effect of an ethanol co-solvent on cyclodextrin-promoted energy transfer was investigated. A 10 mM γ-cyclodextrin solution was prepared in phosphate buffered saline (PBS). For these experiments, 1.25 mL of γ-cyclodextrin and 1.25 mL of ethanol were used (1:1 v/v). Energy transfer experiments were then conducted using the above procedures.

SUMMARY TABLES

SUMMARY TABLES FOR CONCENTRATION EXPERIMENTS

Fluorophore **7**

Analyte	Concentration (mM)	Control Ratio	Energy Transfer (%)
1	5	0.04 ± 0.00	851.61 ± 0.05
	10	0.03 ± 0.00	1056.73 ± 0.10
	15	0.03 ± 0.00	1025.58 ± 0.00
2	5	0.47 ± 0.00	75.70 ± 0.00
	10	0.48 ± 0.00	75.67 ± 0.01
	15	0.48 ± 0.00	81.57 ± 0.00
3	5	0.71 ± 0.01	44.05 ± 0.01
	10	0.74 ± 0.03	40.84 ± 0.02
	15	0.79 ± 0.03	40.51 ± 0.02
4	5	0.55 ± 0.03	65.33 ± 0.00
	10	0.73 ± 0.03	50.01 ± 0.02
	15	0.83 ± 0.04	47.74 ± 0.03
5	5	1.08 ± 0.01	38.52 ± 0.00
	10	1.10 ± 0.01	40.13 ± 0.01
	15	1.09 ± 0.01	39.97 ± 0.00
6	5	0.50 ± 0.00	79.66 ± 0.01
	10	0.57 ± 0.01	69.35 ± 0.00
	15	0.55 ± 0.00	75.18 ± 0.00

Fluorophore **8**

Analyte	Concentration (mM)	Control Ratio	Energy Transfer (%)
1	5	0.23 ± 0.00	29.79 ± 0.00
	10	0.13 ± 0.00	55.22 ± 0.00
	15	0.17 ± 0.00	44.10 ± 0.01
2	5	0.74 ± 0.00	9.81 ± 0.00
	10	0.58 ± 0.00	12.30 ± 0.00
	15	0.76 ± 0.01	10.51 ± 0.00
3	5	0.69 ± 0.01	10.48 ± 0.00
	10	0.70 ± 0.01	9.98 ± 0.00
	15	0.72 ± 0.01	11.44 ± 0.00
4	5	0.62 ± 0.01	11.62 ± 0.00
	10	0.64 ± 0.00	11.33 ± 0.00
	15	0.77 ± 0.07	11.01 ± 0.01
5	5	1.39 ± 0.01	5.59 ± 0.00
	10	1.39 ± 0.00	5.50 ± 0.00
	15	1.42 ± 0.01	6.12 ± 0.00
6	5	0.84 ± 0.00	8.98 ± 0.00
	10	1.00 ± 0.02	7.50 ± 0.00
	15	0.99 ± 0.00	9.19 ± 0.00

Fluorophore **9**

Analyte	Concentration (mM)	Control Ratio	Energy Transfer (%)
1	5	0.27 ± 0.00	27.51 ± 0.01
	10	0.28 ± 0.00	22.24 ± 0.00
	15	0.31 ± 0.01	24.36 ± 0.01
2	5	0.41 ± 0.00	45.37 ± 0.00
	10	0.40 ± 0.00	47.93 ± 0.00
	15	0.40 ± 0.00	48.98 ± 0.00
3	5	0.42 ± 0.01	39.69 ± 0.01
	10	0.45 ± 0.00	43.36 ± 0.01
	15	0.53 ± 0.00	43.85 ± 0.00
4	5	0.29 ± 0.01	67.67 ± 0.02
	10	0.41 ± 0.02	48.60 ± 0.02
	15	0.61 ± 0.02	34.18 ± 0.01
5	5	0.93 ± 0.01	23.60 ± 0.00
	10	0.92 ± 0.01	24.68 ± 0.00
	15	0.92 ± 0.01	24.56 ± 0.00
6	5	0.41 ± 0.00	53.66 ± 0.01
	10	0.44 ± 0.01	52.35 ± 0.00
	15	0.43 ± 0.00	54.94 ± 0.00

SUMMARY TABLES FOR CONCENTRATION ARRAYS

5 mM γ-cyclodextrin in PBS

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.949	1.000	1.000

10 mM γ-cyclodextrin in PBS

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.996	1.000	1.000

15 mM γ-cyclodextrin in PBS

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.996	1.000	1.000

SUMMARY TABLES FOR TEMPERATURE EXPERIMENTS

Fluorophore **7**

Analyte	Temperature (°C)	Control Ratio	Energy Transfer (%)
1	5	0.16 ± 0.01	501.12 ± 0.21
	20	0.04 ± 0.00	718.22 ± 0.28
	35	0.07 ± 0.00	313.46 ± 0.04
	50	0.03 ± 0.00	792.62 ± 0.09
	65	0.06 ± 0.00	460.07 ± 0.03
	80	0.08 ± 0.00	290.49 ± 0.02
2	5	0.33 ± 0.00	102.06 ± 0.00
	20	0.43 ± 0.00	61.54 ± 0.00
	35	0.46 ± 0.00	53.94 ± 0.00
	50	0.33 ± 0.00	28.53 ± 0.00
	65	0.10 ± 0.00	224.15 ± 0.01
	80	0.33 ± 0.00	62.21 ± 0.00
3	5	0.86 ± 0.02	34.30 ± 0.01
	20	0.91 ± 0.01	26.00 ± 0.01
	35	0.92 ± 0.01	22.07 ± 0.00
	50	0.97 ± 0.01	28.17 ± 0.00
	65	1.04 ± 0.02	22.48 ± 0.00
	80	1.03 ± 0.02	21.41 ± 0.00
4	5	0.35 ± 0.01	87.27 ± 0.02
	20	0.89 ± 0.00	31.17 ± 0.00
	35	0.94 ± 0.00	27.46 ± 0.00
	50	0.80 ± 0.17	31.33 ± 0.00
	65	1.03 ± 0.22	25.82 ± 0.05
	80	0.94 ± 0.01	26.43 ± 0.00
5	5	1.02 ± 0.00	33.88 ± 0.00
	20	0.99 ± 0.01	29.93 ± 0.00
	35	0.97 ± 0.01	28.47 ± 0.00
	50	0.98± 0.02	29.98 ± 0.00
	65	0.98 ± 0.01	28.06 ± 0.00
	80	0.99 ± 0.01	27.20 ± 0.00
6	5	0.95 ± 0.00	57.93 ± 0.00
	20	1.16 ± 0.01	46.19 ± 0.01
	35	1.10 ± 0.01	35.44 ± 0.00
	50	0.93 ± 0.01	47.64 ± 0.00
	65	0.95 ± 0.01	41.84 ± 0.01
	80	1.02 ± 0.00	37.98 ± 0.01

Fluorophore **8**

Analyte	Temperature (℃)	Control Ratio	Energy Transfer (%)
1	5	0.19 ± 0.00	36.39 ± 0.00
	20	0.21 ± 0.00	37.62 ± 0.00
	35	0.27 ± 0.00	24.78 ± 0.00
	50	0.43 ± 0.00	12.41 ± 0.00
	65	0.55 ± 0.01	14.90 ± 0.00
	80	0.34 ± 0.00	10.51 ± 0.00
2	5	0.56 ± 0.00	15.46 ± 0.00
	20	0.51 ± 0.00	16.19 ± 0.00
	35	0.56 ± 0.00	15.02 ± 0.00
	50	0.79 ± 0.00	10.64 ± 0.00
	65	0.93 ± 0.00	8.45 ± 0.00
	80	0.97 ± 0.00	8.27 ± 0.00
3	5	0.54 ± 0.00	12.95 ± 0.00
	20	0.48 ± 0.00	11.58 ± 0.00
	35	0.40 ± 0.00	8.12 ± 0.00
	50	0.49 ± 0.01	9.47 ± 0.00
	65	0.41 ± 0.00	10.33 ± 0.00
	80	0.43 ± 0.00	8.86 ± 0.07
4	5	1.05 ± 0.00	11.76 ± 0.00
	20	1.03 ± 0.00	11.55 ± 0.00
	35	1.03 ± 0.01	11.23 ± 0.00
	50	1.04 ± 0.00	10.65 ± 0.00
	65	1.05 ± 0.00	10.03 ± 0.00
	80	1.07 ± 0.00	10.02 ± 0.00
5	5	1.09 ± 0.00	6.23 ± 0.00
	20	1.03 ± 0.00	6.02 ± 0.00
	35	1.03 ± 0.01	6.02 ± 0.00
	50	1.01 ± 0.01	5.78 ± 0.00
	65	1.01 ± 0.01	5.34 ± 0.00
	80	1.00 ± 0.00	5.49 ± 0.00
6	5	2.09 ± 0.01	14.26 ± 0.00
	20	2.23 ± 0.02	14.64 ± 0.00
	35	2.41 ± 0.01	12.69 ± 0.00
	50	2.48 ± 0.01	11.27 ± 0.00
	65	3.01 ± 0.02	8.51 ± 0.00
	80	2.83 ± 0.01	7.28 ± 0.00

Fluorophore **9**

Analyte	Temperature (℃)	Control Ratio	Energy Transfer (%)
1	5	0.02 ± 0.00	463.38 ± 0.01
	20	0.02 ± 0.00	459.06 ± 0.01
	35	0.02 ± 0.01	428.74 ± 0.00
	50	0.01 ± 0.00	502.04 ± 0.01
	65	0.05 ± 0.00	211.13 ± 0.00
	80	0.06 ± 0.00	171.00 ± 0.01
2	5	0.22 ± 0.00	88.54 ± 0.00
	20	0.23 ± 0.00	79.44 ± 0.00
	35	0.23 ± 0.00	70.80 ± 0.00
	50	0.16 ± 0.00	117.62 ± 0.00
	65	0.28 ± 0.00	44.61 ± 0.00
	80	0.28 ± 0.00	45.50 ± 0.00
3	5	0.61 ± 0.01	52.91 ± 0.00
	20	0.51 ± 0.02	58.94 ± 0.02
	35	0.48 ± 0.00	49.11 ± 0.01
	50	0.79 ± 0.01	65.68 ± 0.01
	65	0.66 ± 0.01	22.13 ± 0.00
	80	0.64 ± 0.01	21.12 ± 0.00
4	5	0.37 ± 0.00	71.06 ± 0.01
	20	0.69 ± 0.01	34.83 ± 0.01
	35	0.82 ± 0.01	28.34 ± 0.00
	50	0.16 ± 0.00	24.56 ± 0.01
	65	0.89 ± 0.00	18.58 ± 0.00
	80	0.93 ± 0.01	17.53 ± 0.00
5	5	0.70 ± 0.03	33.55 ± 0.01
	20	1.01 ± 0.01	30.87 ± 0.00
	35	1.00 ± 0.01	22.37 ± 0.00
	50	1.03 ± 0.05	35.54 ± 0.02
	65	1.00 ± 0.01	15.94 ± 0.00
	80	1.02 ± 0.01	15.53 ± 0.00
6	5	0.96 ± 0.00	81.42 ± 0.02
	20	0.99 ± 0.00	75.41 ± 0.01
	35	1.09 ± 0.01	68.77 ± 0.00
	50	1.03 ± 0.02	62.41 ± 0.01
	65	1.23 ± 0.01	39.12 ± 0.00
	80	1.50 ± 0.00	37.07 ± 0.01

SUMMARY TABLES FOR TEMPERATURE ARRAYS

5 ºC

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

1.000	1.000	1.000

20 ºC

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.997	1.000	1.000

35 ºC

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.999	1.000	1.000

50 ºC

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.992	1.000	1.000

65 ºC

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.998	1.000	1.000

80 ºC

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.947	0.998	1.000

SUMMARY TABLES FOR PH EXPERIMENTS

Fluorophore **7**

Analyte	pH	Control Ratio	Energy Transfer (%
1	0	0.04 ± 0.00	1250.44 ± 0.21
	3	0.03 ± 0.00	1546.47 ± 0.06
	5	0.03 ± 0.00	1393.07 ± 0.04
	8	0.01 ± 0.00	1163.74 ± 0.13
	10	0.03 ± 0.00	1107.91 ± 0.11
	12	0.04 ± 0.00	648.42 ± 0.22
2	0	1.37 ± 0.01	43.29 ± 0.01
	3	0.36 ± 0.00	103.27 ± 0.00
	5	0.28 ± 0.00	125.87 ± 0.00
	8	0.12 ± 0.00	79.66 ± 0.01
	10	0.47 ± 0.00	80.42 ± 0.00
	12	0.51 ± 0.00	57.47 ± 0.00
3	0	0.93 ± 0.02	63.79 ± 0.02
	3	0.79 ± 0.01	44.86 ± 0.02
	5	0.84 ± 0.01	39.91± 0.01
	8	0.20 ± 0.00	40.83 ± 0.02
	10	0.76 ± 0.02	40.97 ± 0.02
	12	0.80 ± 0.01	46.40 ± 0.01
4	0	0.99 ± 0.02	41.21 ± 0.01
	3	0.85 ± 0.07	44.88 ± 0.03
	5	0.75 ± 0.00	49.47 ± 0.00
	8	0.19 ± 0.01	53.77 ± 0.04
	10	0.82 ± 0.17	47.19 ± 0.08
	12	0.63 ± 0.02	64.12 ± 0.02
5	0	1.09 ± 0.00	35.36 ± 0.00
	3	1.19 ± 0.01	39.68 ± 0.00
	5	1.18 ± 0.00	38.37 ± 0.00
	8	0.26 ± 0.01	42.37 ± 0.00
	10	1.08 ± 0.01	40.05 ± 0.00
	12	1.10 ± 0.03	36.33 ± 0.01
6	0	0.70 ± 0.00	56.11 ± 0.00
	3	0.64 ± 0.01	59.95 ± 0.00
	5	0.54 ± 0.00	73.27 ± 0.01
	8	0.13 ± 0.00	80.94 ± 0.02
	10	0.53 ± 0.00	79.36 ± 0.01
	12	0.58 ± 0.01	71.90 ± 0.01

Fluorophore **8**

Analyte	pH	Control Ratio	Energy Transfer (%
1	0	0.16 ± 0.00	54.96 ± 0.01
	3	0.12 ± 0.01	72.19 ± 0.01
	5	0.16 ± 0.00	46.80 ± 0.01
	8	0.06 ± 0.00	97.41 ± 0.02
	10	0.08 ± 0.00	64.91 ± 0.01
	12	0.10 ± 0.00	116.95 ± 0.03
2	0	1.45 ± 0.00	5.89 ± 0.00
	3	0.76 ± 0.00	10.41 ± 0.00
	5	0.63 ± 0.00	11.73 ± 0.00
	8	0.54 ± 0.00	10.66 ± 0.00
	10	0.61 ± 0.01	8.13 ± 0.00
	12	0.76 ± 0.00	9.22 ± 0.00
3	0	0.69 ± 0.01	11.64 ± 0.00
	3	0.42 ± 0.00	19.20 ± 0.00
	5	0.69 ± 0.01	11.37 ± 0.00
	8	0.54 ± 0.00	10.34 ± 0.00
	10	0.51 ± 0.02	9.59 ± 0.00
	12	0.77 ± 0.01	9.26 ± 0.00
4	0	0.80 ± 0.00	10.80 ± 0.00
	3	0.73 ± 0.02	11.07 ± 0.00
	5	0.67 ± 0.00	11.08 ± 0.00
	8	0.49 ± 0.00	11.25 ± 0.00
	10	0.40 ± 0.00	11.23 ± 0.00
	12	0.64 ± 0.00	11.43 ± 0.00
5	0	1.41 ± 0.00	6.10 ± 0.00
	3	1.34 ± 0.01	5.85 ± 0.00
	5	1.58 ± 0.00	6.17 ± 0.00
	8	0.96 ± 0.01	6.81 ± 0.00
	10	0.89 ± 0.01	5.32 ± 0.00
	12	1.33 ± 0.01	5.62 ± 0.00
6	0	0.54 ± 0.00	15.93 ± 0.00
	3	0.51 ± 0.00	15.69 ± 0.00
	5	0.74 ± 0.00	10.73 ± 0.00
	8	0.64 ± 0.00	9.20 ± 0.00
	10	0.56 ± 0.00	8.71 ± 0.00
	12	0.82 ± 0.00	9.06 ± 0.00

Fluorophore **9**

Analyte	pH	Control Ratio	Energy Transfer (%)
1	0	0.13 ± 0.00	181.37 ± 0.06
	3	0.10 ± 0.00	139.67 ± 0.10
	5	0.27 ± 0.00	123.96 ± 0.00
	8	0.01 ± 0.00	270.92 ± 0.02
	10	0.02 ± 0.00	233.80 ± 0.02
	12	0.02 ± 0.00	299.56 ± 0.03
2	0	1.00 ± 0.01	58.51 ± 0.00
	3	0.34 ± 0.00	48.93 ± 0.00
	5	0.26 ± 0.00	57.55 ± 0.00
	8	0.11 ± 0.00	46.14 ± 0.00
	10	0.43 ± 0.00	48.79 ± 0.00
	12	0.50 ± 0.00	43.91 ± 0.00
3	0	0.77 ± 0.01	63.92 ± 0.01
	3	0.57 ± 0.00	34.70 ± 0.00
	5	0.52 ± 0.01	40.07 ± 0.00
	8	0.12 ± 0.00	49.16 ± 0.00
	10	0.45 ± 0.01	48.65 ± 0.00
	12	0.50 ± 0.00	51.17 ± 0.03
4	0	0.75 ± 0.00	73.66 ± 0.08
	3	0.62 ± 0.00	29.50 ± 0.00
	5	0.55 ± 0.01	30.69 ± 0.00
	8	0.13 ± 0.01	42.68 ± 0.01
	10	0.58 ± 0.02	31.63 ± 0.01
	12	0.45 ± 0.02	52.90 ± 0.02
5	0	0.87 ± 0.05	66.05 ± 0.04
	3	0.82 ± 0.01	23.65 ± 0.00
	5	0.82 ± 0.00	24.78 ± 0.00
	8	0.24 ± 0.00	26.26 ± 0.01
	10	0.93 ± 0.01	25.02 ± 0.00
	12	1.07 ± 0.00	24.40 ± 0.00
6	0	0.54 ± 0.00	106.92 ± 0.01
	3	0.35 ± 0.00	56.07 ± 0.00
	5	0.36 ± 0.00	52.23 ± 0.00
	8	0.10 ± 0.00	65.61 ± 0.00
	10	0.52 ± 0.00	54.20 ± 0.01
	12	0.49 ± 0.00	57.48 ± 0.00

SUMMARY TABLE FOR PH ARRAYS

pH 0

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	1	3	0	0	75
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	5	3	4	4	96

Cumulative Proportion of Total Dispersion

0.895	1.000	1.000

pH 3

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.999	1.000	1.000

pH 5

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.996	1.000	1.000

pH 8

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.998	1.000	1.000

pH 10

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

1.000	1.000	1.000

pH 12

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

1.000	1.000	1.000

SUMMARY TABLES FOR SALT EXPERIMENTS

Fluorophore **7**

Analyte	Salt	Control Ratio	Energy Transfer (%)
1	NaCl	0.07 ± 0.00	500.76 ± 0.28
	GuHCl	0.04 ± 0.00	882.51 ± 0.14
	No Salt	0.02 ± 0.00	1094.05 ± 0.05
2	NaCl	0.44 ± 0.00	89.19 ± 0.00
	GuHCl	0.44 ± 0.00	80.12 ± 0.01
	No Salt	0.22 ± 0.00	88.40 ± 0.00
3	NaCl	0.94 ± 0.01	41.51 ± 0.01
	GuHCl	0.85 ± 0.03	37.63 ± 0.02
	No Salt	0.35 ± 0.01	39.73 ± 0.02
4	NaCl	0.78 ± 0.01	51.44 ± 0.01
	GuHCl	0.89 ± 0.02	41.41 ± 0.01
	No Salt	0.32 ± 0.02	58.79 ± 0.05
5	NaCl	1.14 ± 0.00	40.01 ± 0.00
	GuHCl	1.07 ± 0.01	37.30 ± 0.00
	No Salt	0.54 ± 0.01	40.11 ± 0.00
6	NaCl	0.58 ± 0.00	72.17 ± 0.01
	GuHCl	0.51 ± 0.01	76.37 ± 0.01
	No Salt	0.27 ± 0.00	75.63 ± 0.01

Fluorophore **8**

Analyte	Salt	Control Ratio	Energy Transfer (%)
1	NaCl	0.33 ± 0.00	24.04 ± 0.00
	GuHCl	0.20 ± 0.00	36.22 ± 0.01
	No Salt	0.08 ± 0.00	77.94 ± 0.01
2	NaCl	0.76 ± 0.00	10.61 ± 0.00
	GuHCl	0.73 ± 0.00	10.53 ± 0.00
	No Salt	0.66 ± 0.00	8.74 ± 0.00
3	NaCl	0.74 ± 0.01	11.04 ± 0.00
	GuHCl	0.69 ± 0.01	10.76 ± 0.00
	No Salt	0.61 ± 0.01	9.63 ± 0.00
4	NaCl	0.69 ± 0.01	11.52 ± 0.00
	GuHCl	0.68 ± 0.00	11.38 ± 0.00
	No Salt	0.60 ± 0.05	9.73 ± 0.01
5	NaCl	1.40 ± 0.00	6.03 ± 0.00
	GuHCl	1.37 ± 0.01	5.76 ± 0.00
	No Salt	1.56 ± 0.01	4.07 ± 0.00
6	NaCl	1.07 ± 0.01	7.73 ± 0.00
	GuHCl	0.94 ± 0.01	8.37 ± 0.00
	No Salt	0.88 ± 0.01	6.93 ± 0.00

Fluorophore **9**

Analyte	Salt	Control Ratio	Energy Transfer (%)
1	NaCl	0.32 0.02	30.65 ± 0.02
	GuHCl	0.03	382.72 ± 0.03
	No Salt	0.01 0.00	403.41 ± 0.00
2	NaCl	0.43 0.01	49.70 ± 0.00
	GuHCl	0.41 0.00	44.76 ± 0.00
	No Salt	0.20 0.00	49.35 ± 0.00
3	NaCl	0.77 0.02	27.22 ± 0.00
	GuHCl	0.55 0.01	33.27 ± 0.01
	No Salt	0.20 0.01	55.56 ± 0.02
4	NaCl	0.57 0.02	36.55 ± 0.01
	GuHCl	0.64 0.05	29.92 ± 0.03
	No Salt	0.21 0.03	58.75 ± 0.08
5	NaCl	0.96 0.02	23.79 ± 0.00
	GuHCl	0.92 0.00	22.53 ± 0.00
	No Salt	0.47 0.01	27.42 ± 0.00
6	NaCl	0.49 0.01	46.42 ± 0.00
	GuHCl	0.42 0.00	49.09 ± 0.00
	No Salt	0.21 0.00	57.50 ± 0.00

SUMMARY TABLE FOR SALT ARRAYS

1 M NaCl

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.971	0.988	1.000

1 M GuHCl

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	1	3	0	0	75
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	5	3	4	4	96

Cumulative Proportion of Total Dispersion

0.994	1.000	1.000

DI H_2O

Jackknifed Classification Matrix

	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	1	2	0	1	50
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	5	2	4	5	92

Cumulative Proportion of Total Dispersion

0.999	1.000	1.000

SUMMARY TABLE FOR SOLVENT EXPERIMENTS

Analyte	Fluorophore	Control Ratio	Energy Transfer (%
1	7	1.51 ± 0.01	12.73 ± 0.00
	8	1.06 ± 0.00	6.97 ± 0.00
	9	0.17 ± 0.00	25.53 ± 0.00
2	7	1.02 ± 0.01	18.85 ± 0.00
	8	0.91 ± 0.00	7.93 ± 0.00
	9	0.82 ± 0.00	5.76 ± 0.00
3	7	7.70 ± 0.04	2.50 ± 0.00
	8	0.77 ± 0.00	9.38 ± 0.00
	9	0.62 ± 0.00	7.24 ± 0.00
4	7	1.24 ± 0.01	15.19 ± 0.00
	8	0.65 ± 0.00	11.10 ± 0.00
	9	0.89 ± 0.00	5.06 ± 0.00
5	7	1.05 ± 0.01	18.13 ± 0.00
	8	1.47 ± 0.00	5.00 ± 0.00
	9	0.82 ± 0.00	5.47 ± 0.00
6	7	3.37 ± 0.01	5.58 ± 0.00
	8	1.10 ± 0.00	6.27 ± 0.00
	9	0.42 ± 0.00	10.21 ± 0.00

SUMMARY TABLE FOR SOLVENT ARRAYS

Ethanol

Jackknifed Classification Matrix

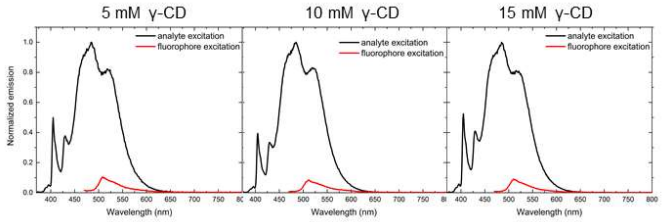
	Analyte 1	Analyte 2	Analyte 3	Analyte 4	Analyte 5	Analyte 6	%correct
Analyte 1	4	0	0	0	0	0	100
Analyte 2	0	4	0	0	0	0	100
Analyte 3	0	0	4	0	0	0	100
Analyte 4	0	0	0	4	0	0	100
Analyte 5	0	0	0	0	4	0	100
Analyte 6	0	0	0	0	0	4	100
Total	4	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

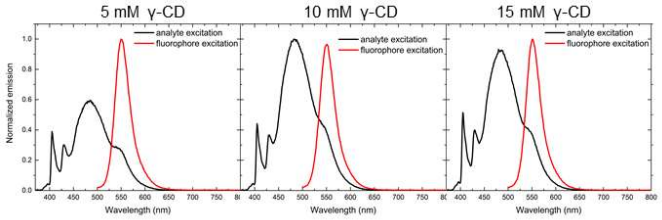
0.538	0.990	1.000

SUMMARY FIGURES
SUMMARY FIGURES FOR CONCENTRATION EXPERIMENTS
Energy Transfer

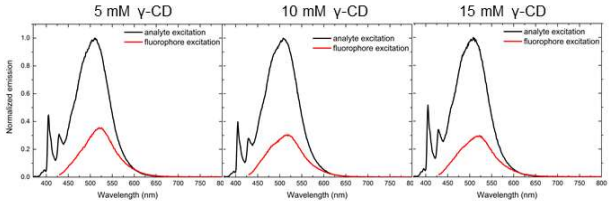
Analyte **1** – Fluorophore **7**



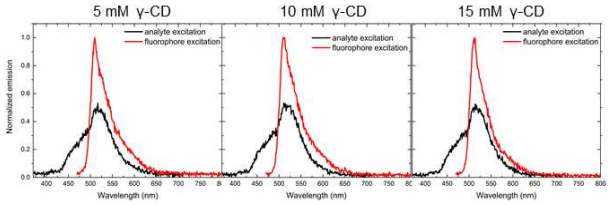
Analyte **1** – Fluorophore **8**



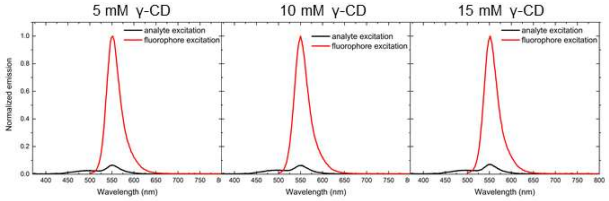
Analyte **1** – Fluorophore **9**



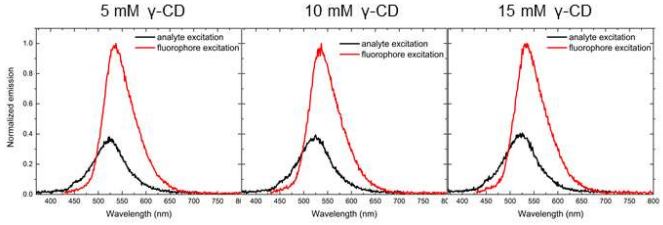
Analyte **2** – Fluorophore **7**



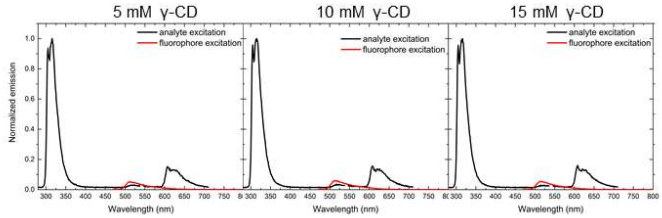
Analyte **2** – Fluorophore **8**



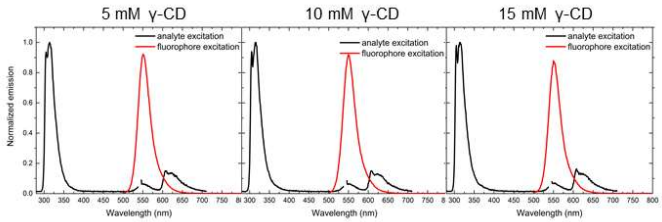
Analyte **2** – Fluorophore **9**



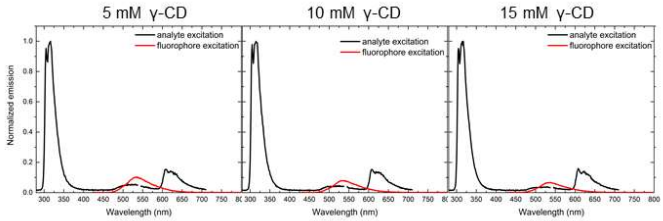
Analyte **3** – Fluorophore **7**



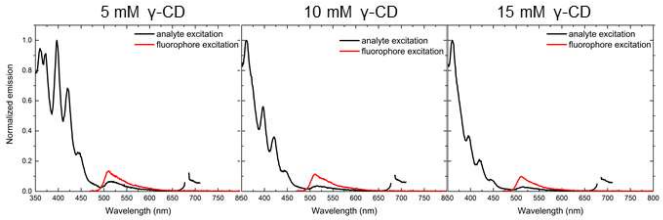
Analyte **3** – Fluorophore **8**



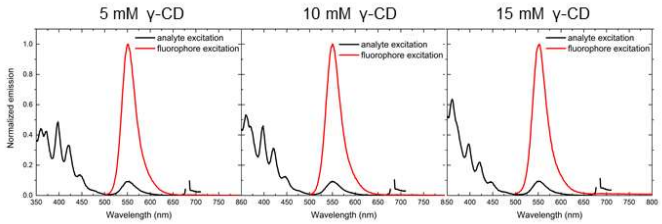
Analyte **3** – Fluorophore **9**



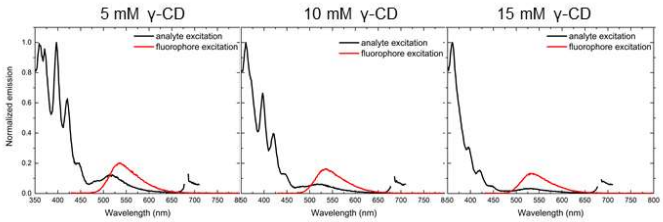
Analyte **4** – Fluorophore **7**



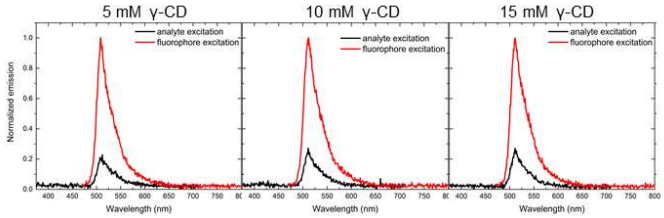
Analyte **4** – Fluorophore **8**



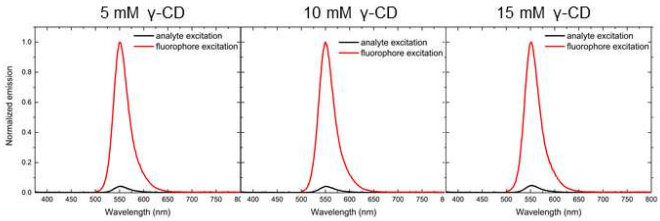
Analyte **4** – Fluorophore **9**



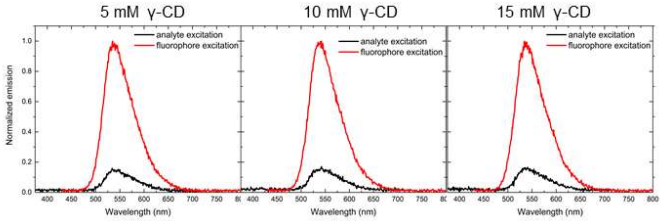
Analyte **5** – Fluorophore **7**



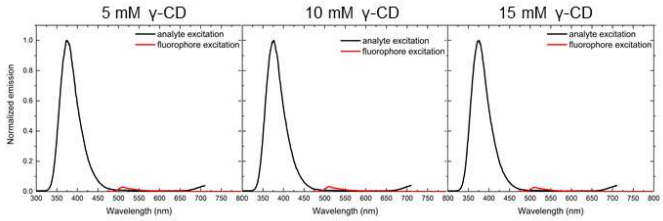
Analyte **5** – Fluorophore **8**



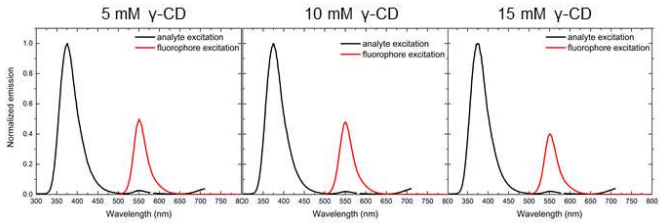
Analyte **5** – Fluorophore **9**



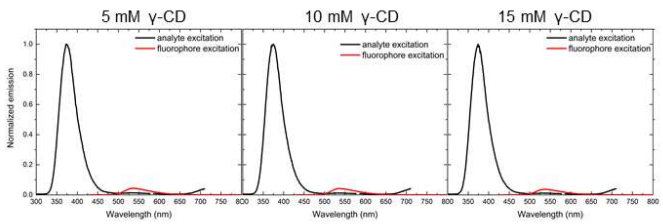
Analyte **6** – Fluorophore **7**



Analyte **6** – Fluorophore **8**

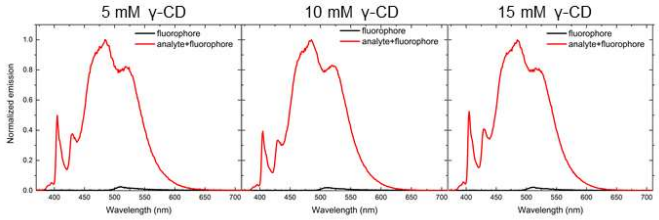


Analyte **6** – Fluorophore **9**

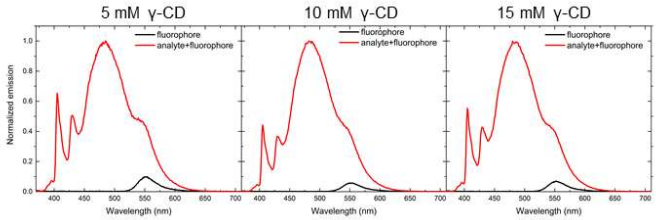


Control Ratio

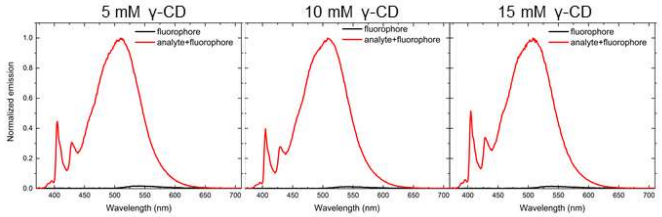
Analyte **1** – Fluorophore **7**



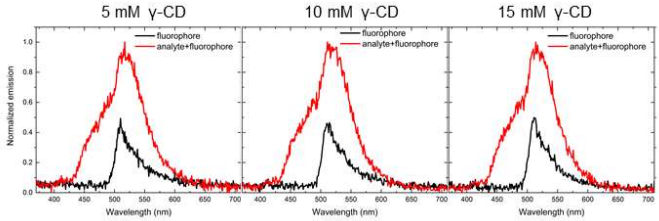
Analyte **1** – Fluorophore **8**



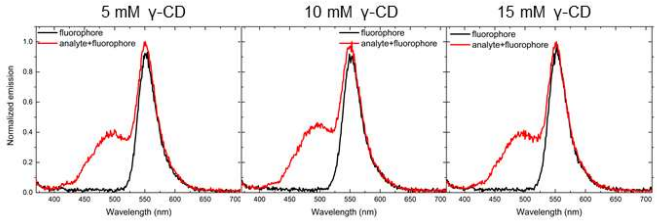
Analyte **1** – Fluorophore **9**



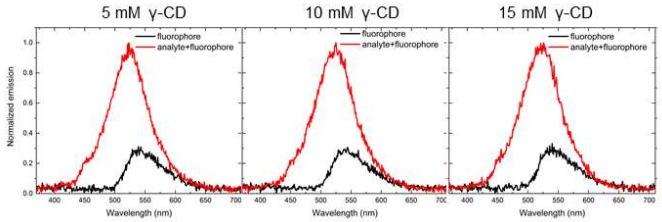
Analyte **2** – Fluorophore **7**



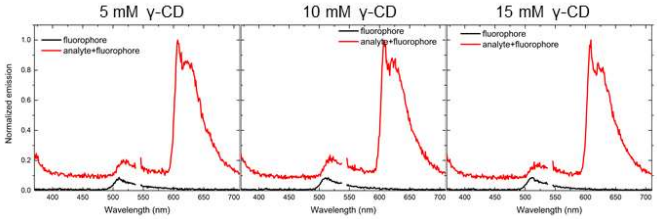
Analyte **2** – Fluorophore **8**



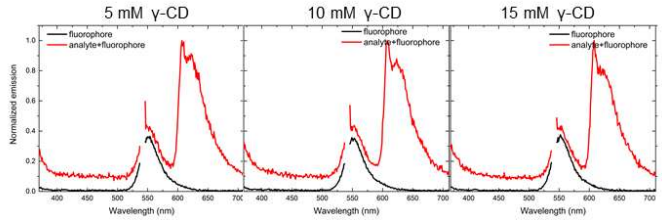
Analyte **2** – Fluorophore **9**



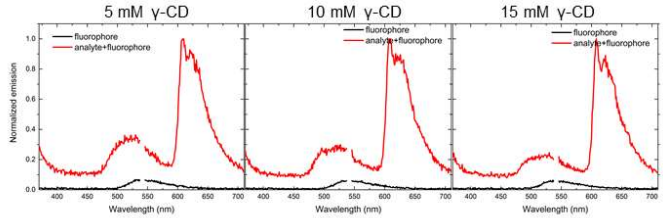
Analyte **3** – Fluorophore **7**



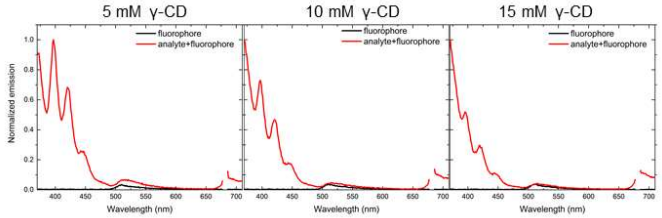
Analyte **3** – Fluorophore **8**



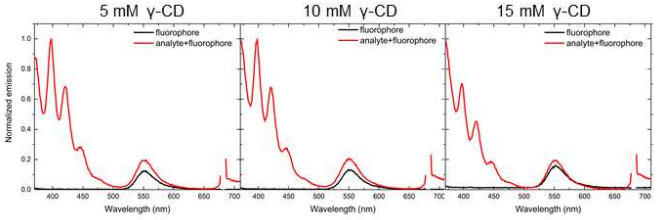
Analyte **3** – Fluorophore **9**



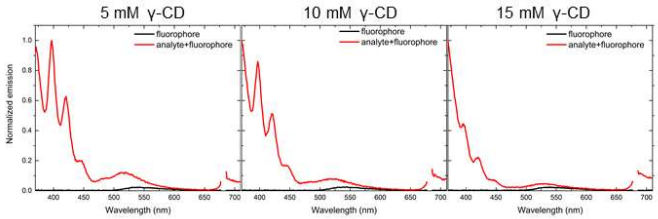
Analyte **4** – Fluorophore **7**



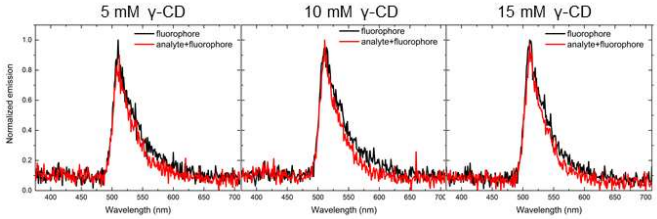
Analyte **4** – Fluorophore **8**



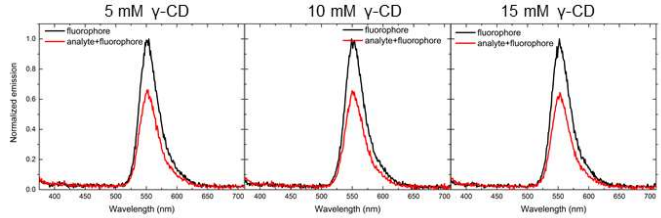
Analyte **4** – Fluorophore **9**



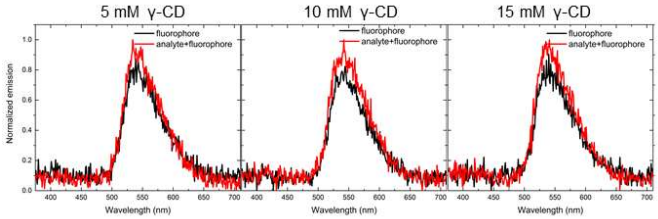
Analyte **5** – Fluorophore **7**



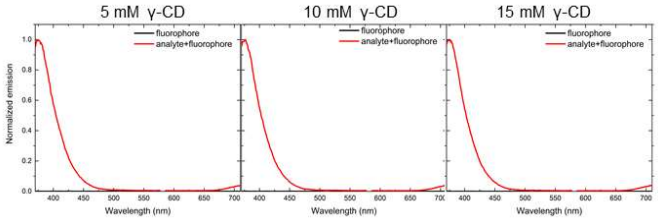
Analyte **5** – Fluorophore **8**



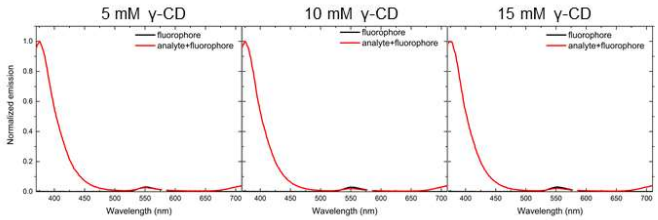
Analyte **5** – Fluorophore **9**



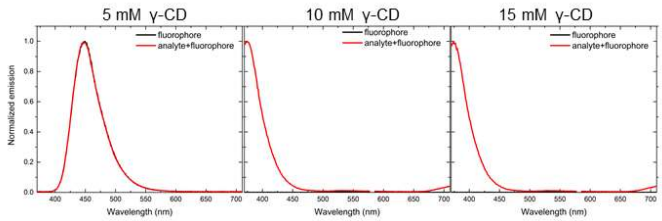
Analyte **6** – Fluorophore **7**



Analyte **6** – Fluorophore **8**

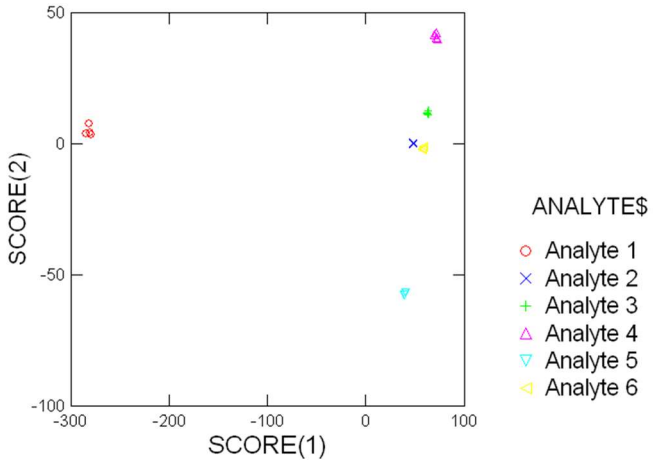


Analyte **6** – Fluorophore **9**

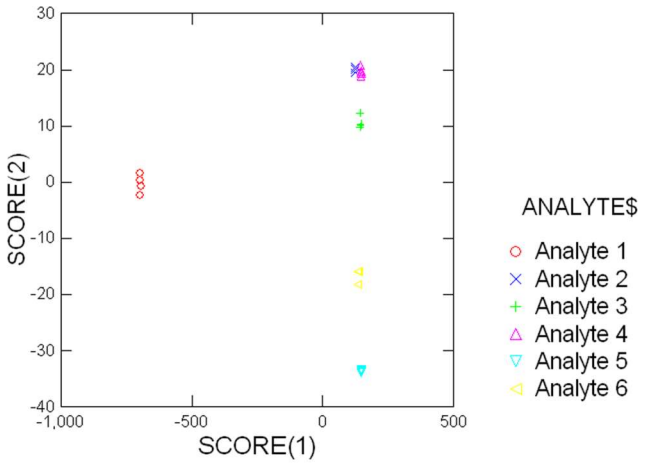


SUMMARY FIGURES FOR CONCENTRATION ARRAYS

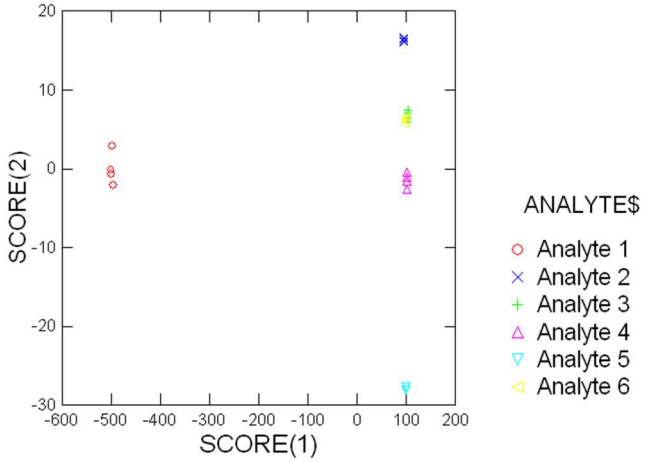
5 mM γ-cyclodextrin in PBS



10 mM γ-cyclodextrin in PBS



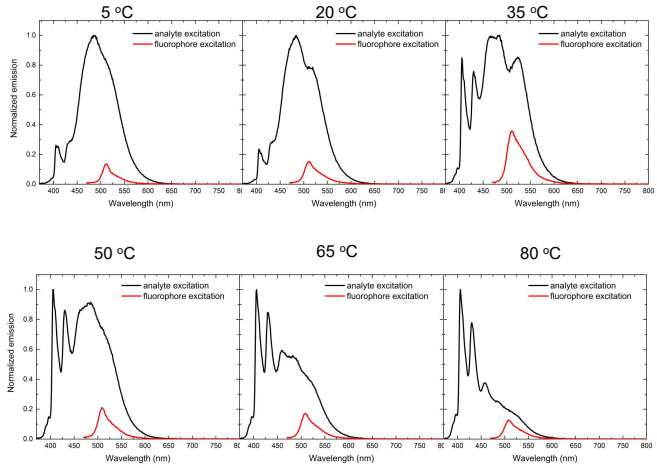
15 mM γ-cyclodextrin in PBS



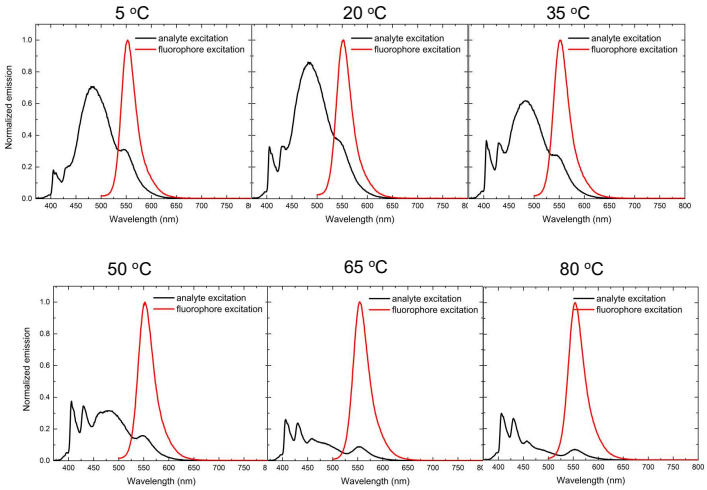
SUMMARY FIGURES FOR TEMPERATURE EXPERIMENTS

Energy Transfer

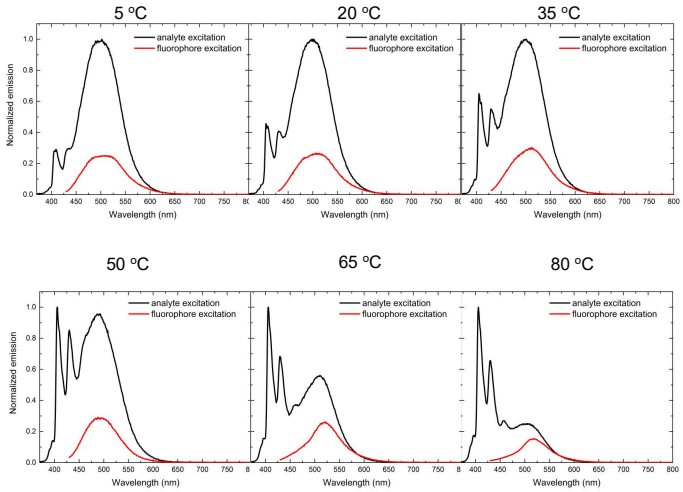
Analyte **1** – Fluorophore **7**



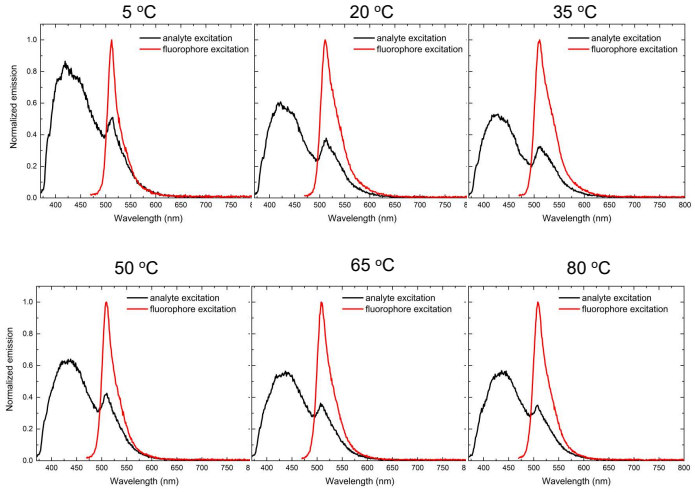
Analyte **1** – Fluorophore **8**



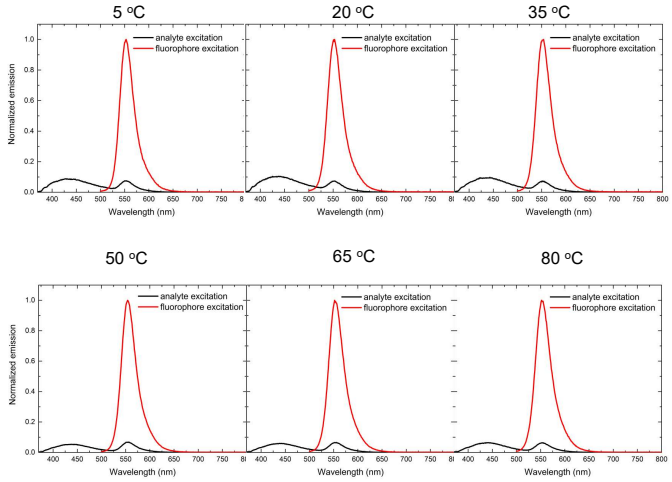
Analyte **1** – Fluorophore **9**



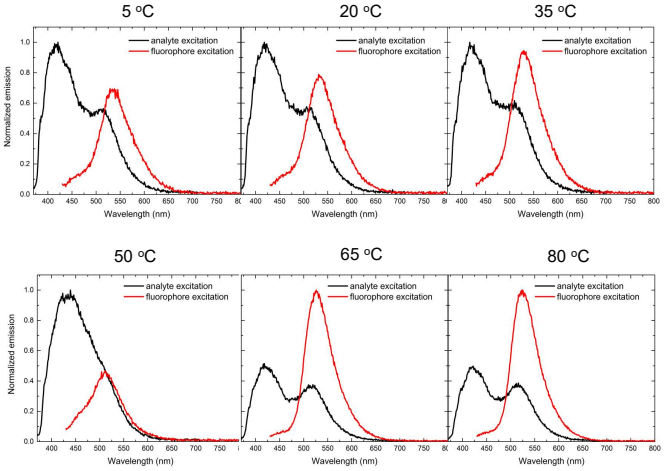
Analyte **2** – Fluorophore **7**



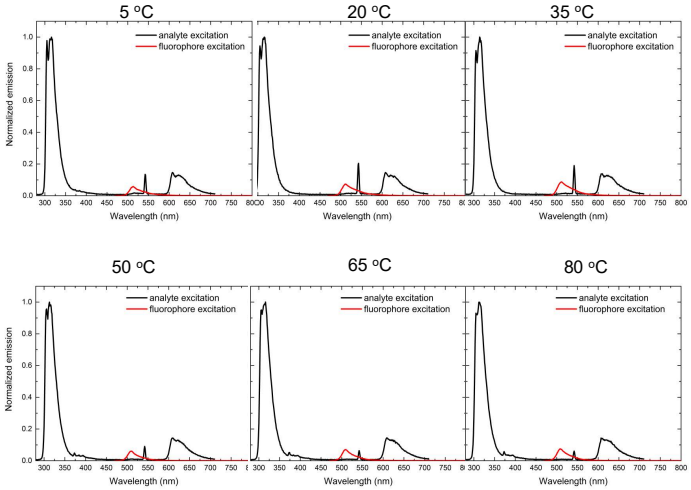
Analyte **2** – Fluorophore **8**



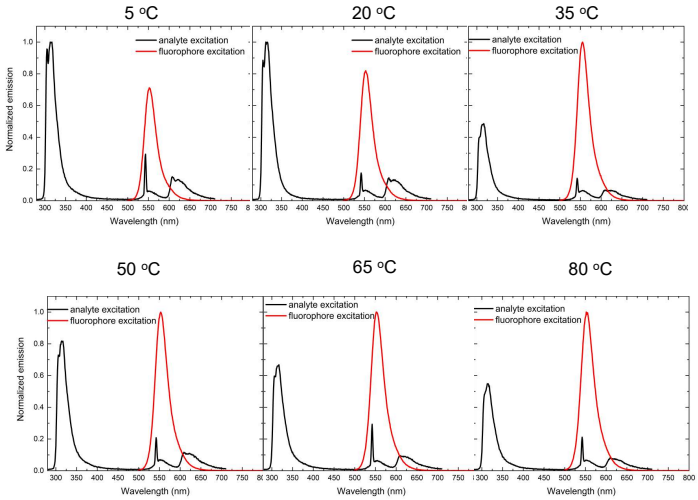
Analyte **2** – Fluorophore **9**



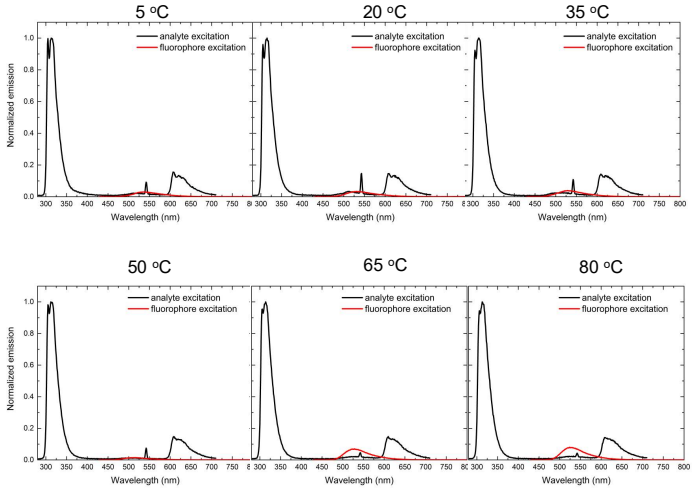
Analyte **3** – Fluorophore **7**



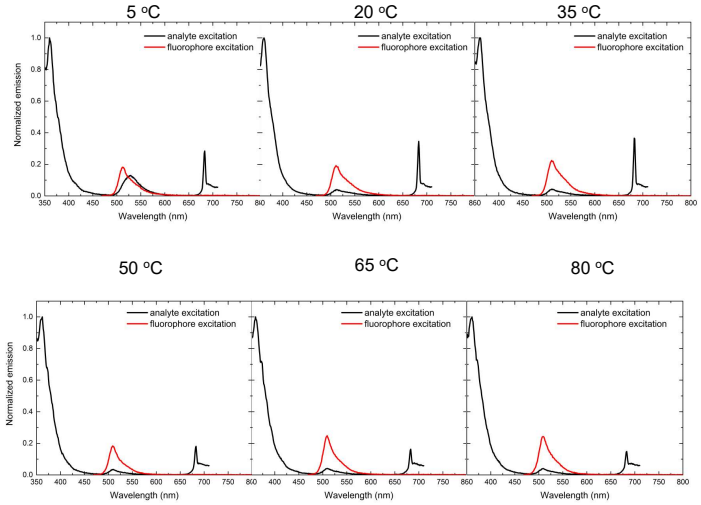
Analyte **3** – Fluorophore **8**



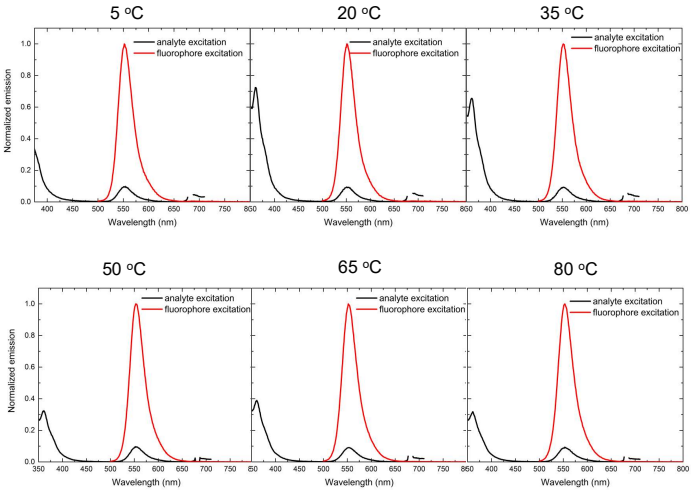
Analyte **3** – Fluorophore **9**



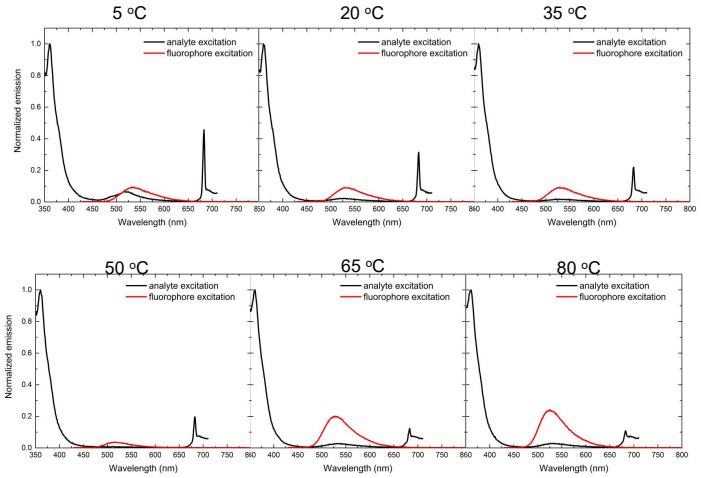
Analyte **4** – Fluorophore **7**



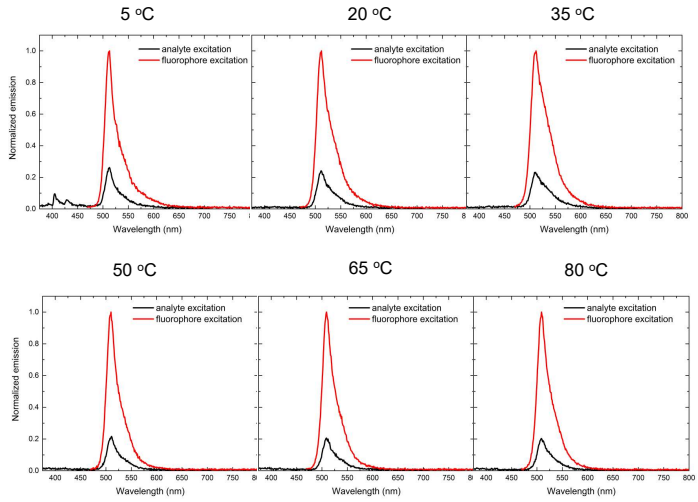
Analyte **4** – Fluorophore **8**



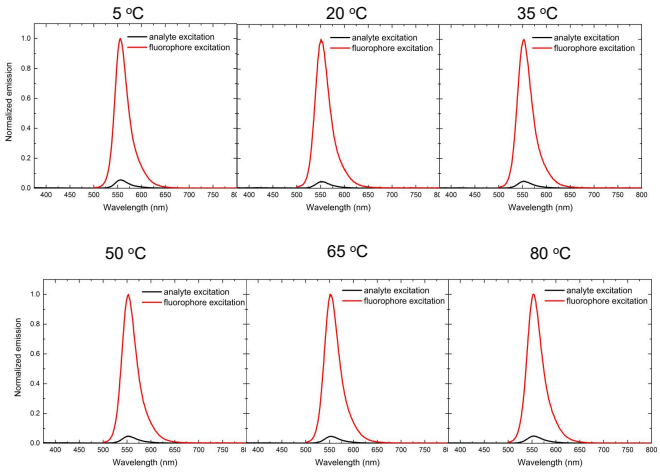
Analyte **4** – Fluorophore **9**



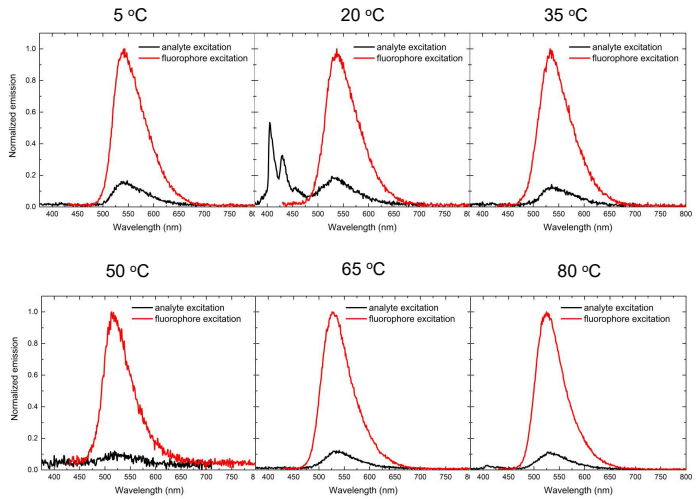
Analyte **5** – Fluorophore **7**



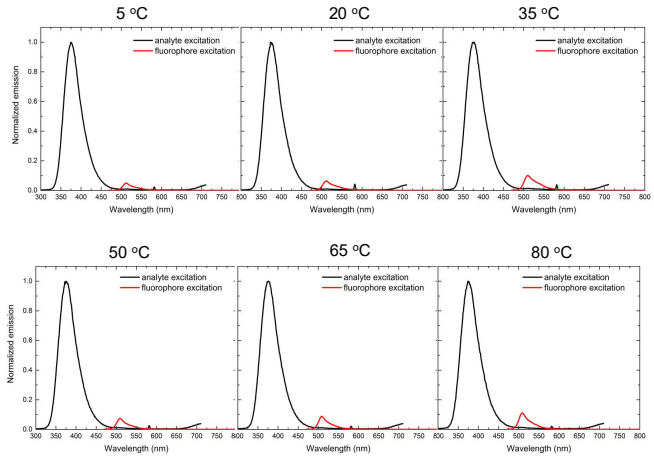
Analyte **5** – Fluorophore **8**



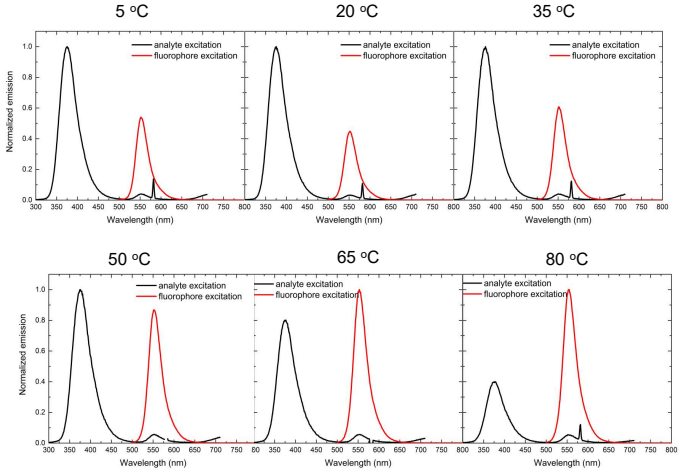
Analyte **5** – Fluorophore **9**



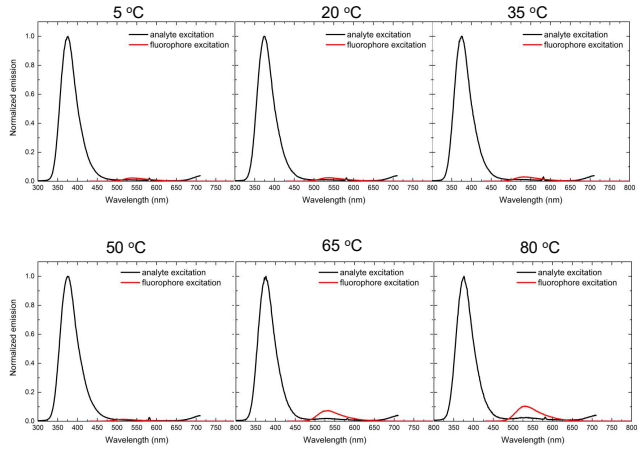
Analyte **6** – Fluorophore **7**



Analyte **6** – Fluorophore **8**

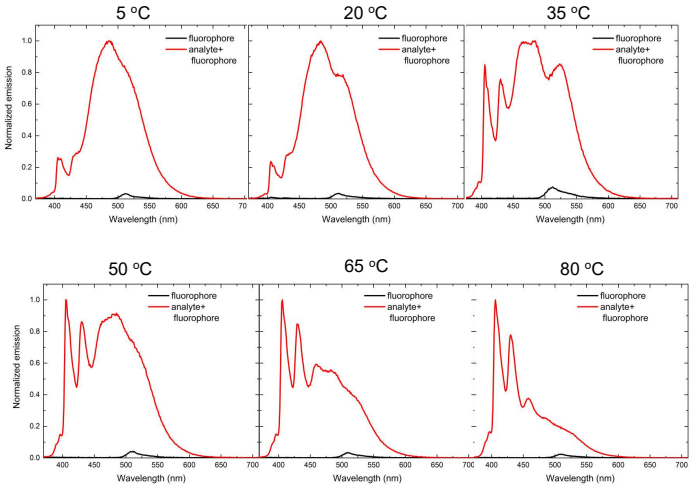


Analyte **6** – Fluorophore **9**

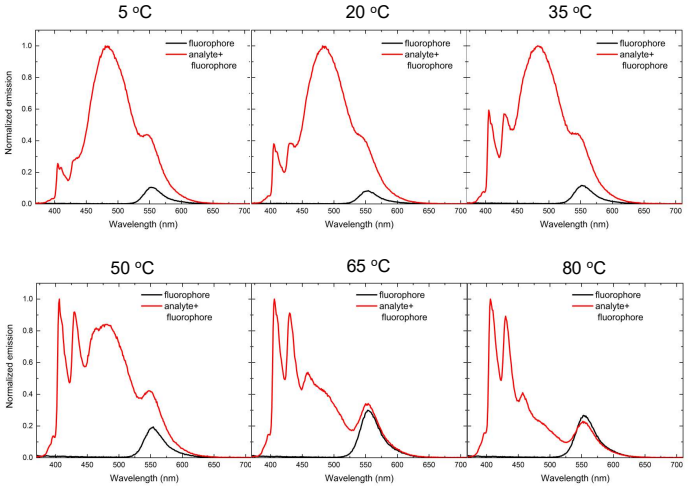


Control Ratio.

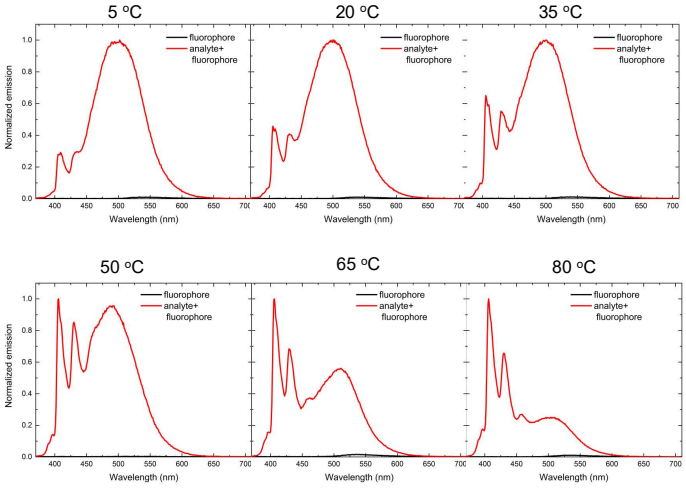
Analyte **1** – Fluorophore **7**



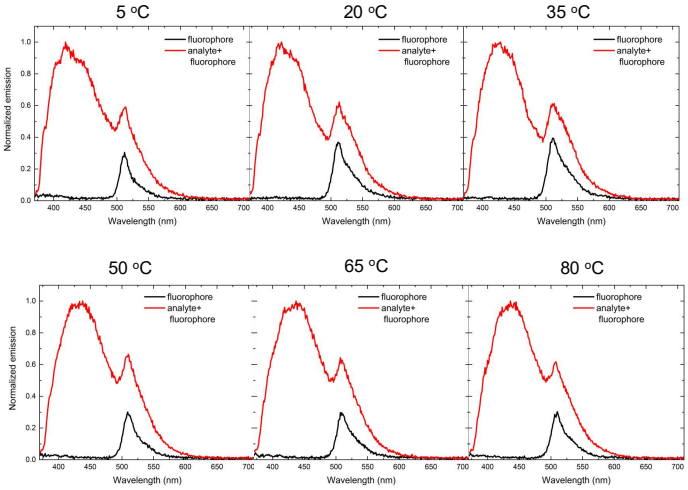
Analyte **1** – Fluorophore **8**



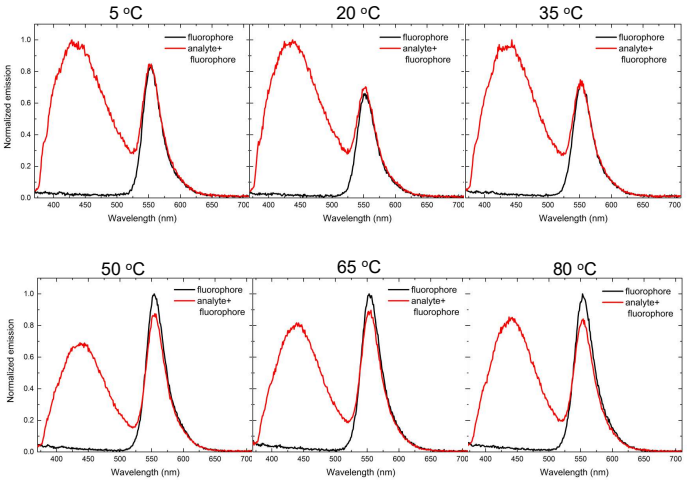
Analyte **1** – Fluorophore **9**



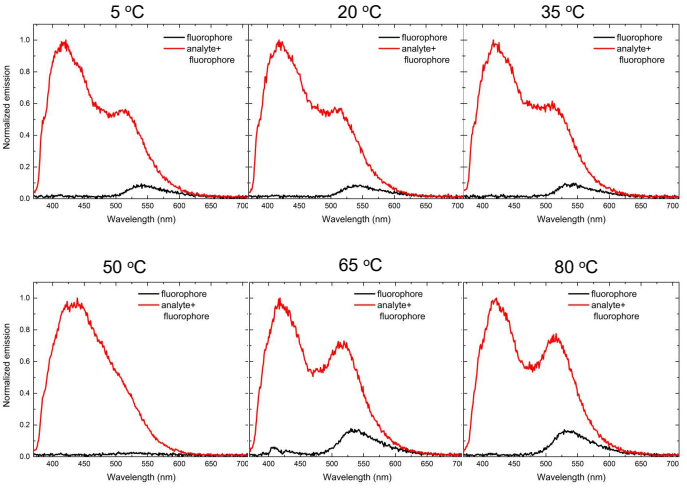
Analyte **2** – Fluorophore **7**



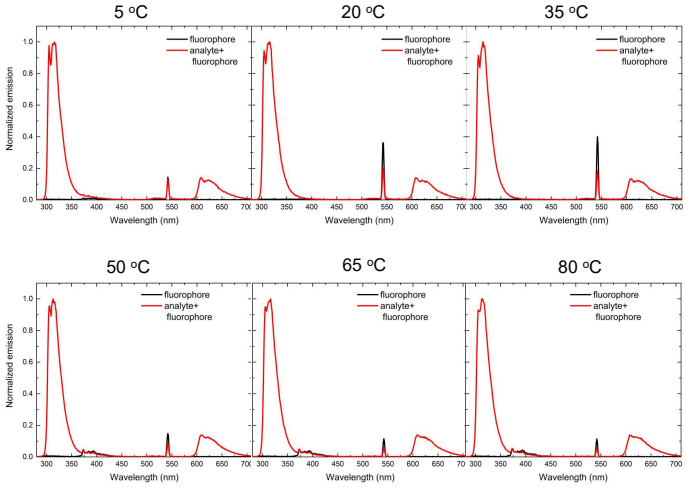
Analyte **2** – Fluorophore **8**



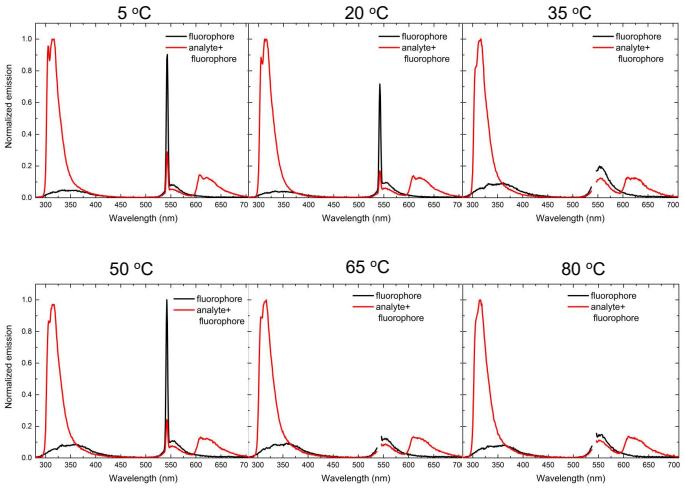
Analyte **2** – Fluorophore **9**



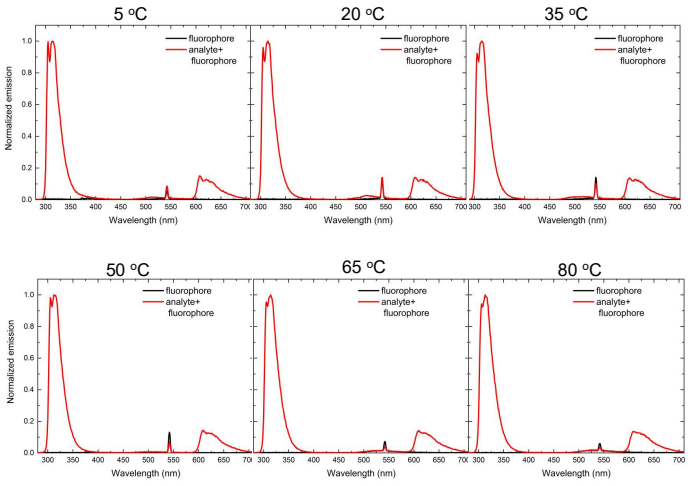
Analyte **3** – Fluorophore **7**



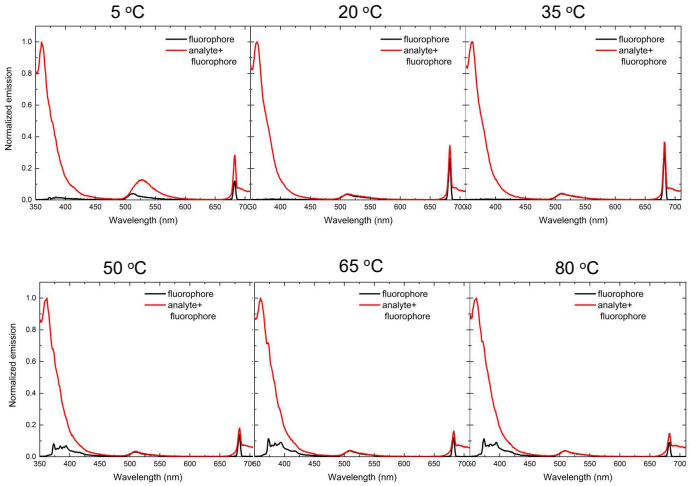
Analyte **3** – Fluorophore **8**



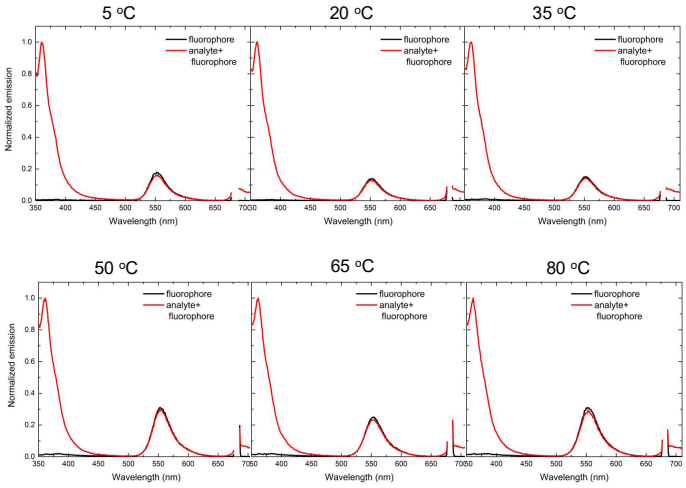
Analyte **3** – Fluorophore **9**



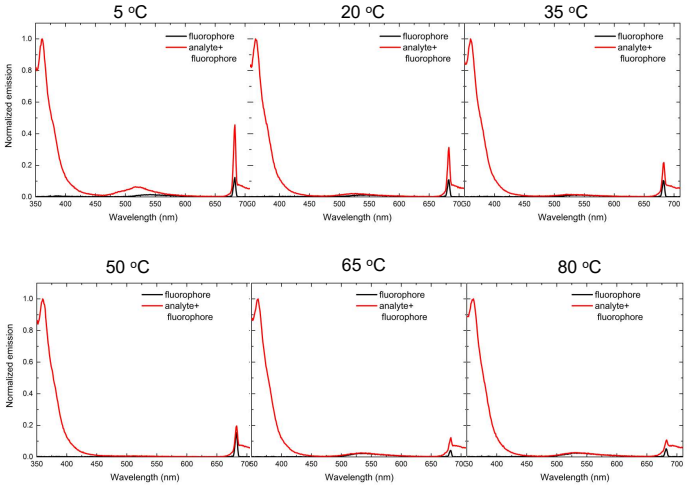
Analyte **4** – Fluorophore **7**



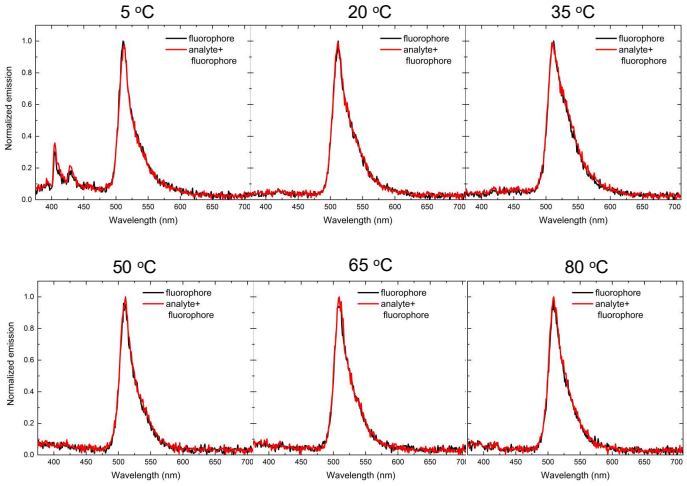
Analyte **4** – Fluorophore **8**



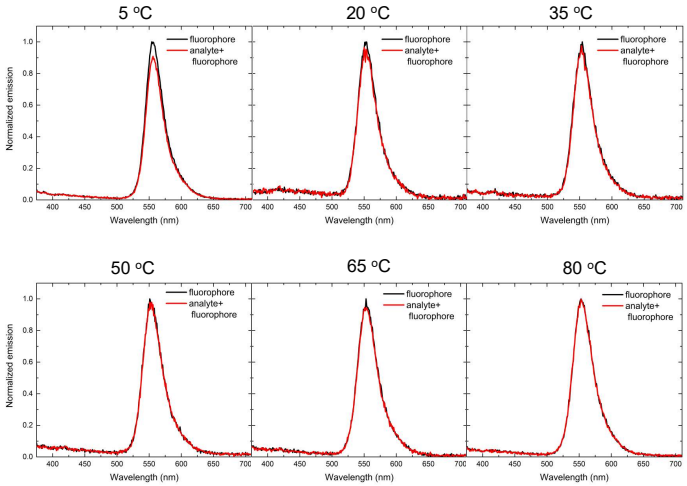
Analyte **4** – Fluorophore **9**



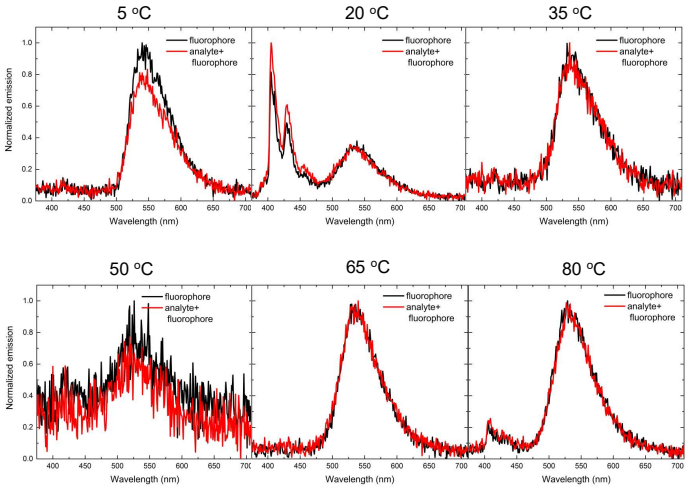
Analyte **5** – Fluorophore **7**



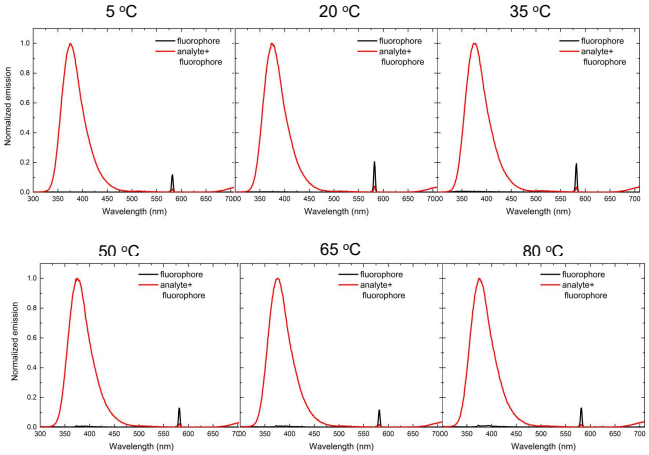
Analyte **5** – Fluorophore **8**



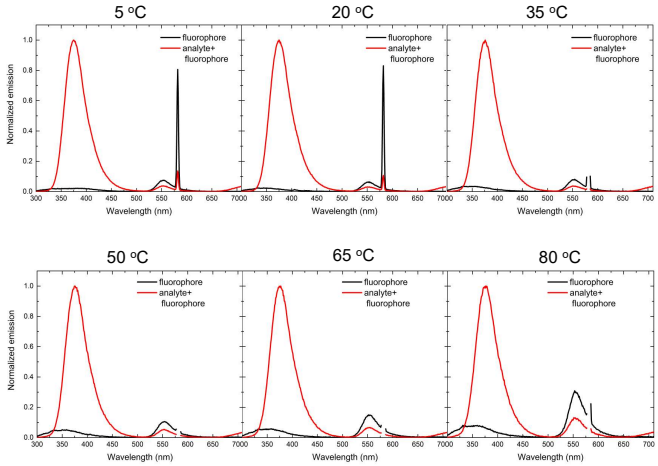
Analyte **5** – Fluorophore **9**



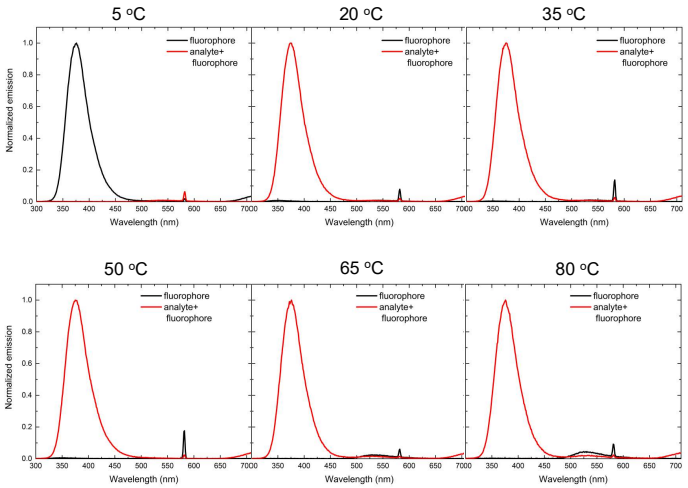
Analyte **6** – Fluorophore **7**



Analyte **6** – Fluorophore **8**

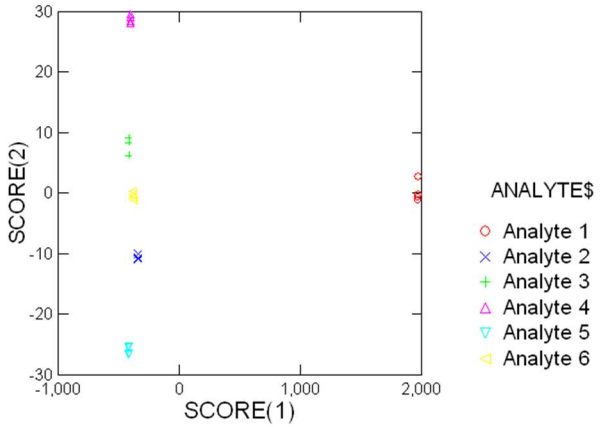


Analyte **6** – Fluorophore **9**

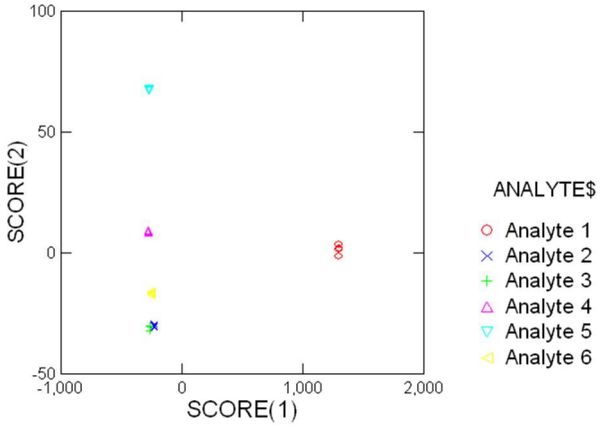


SUMMARY FIGURES FOR TEMPERATURE ARRAYS

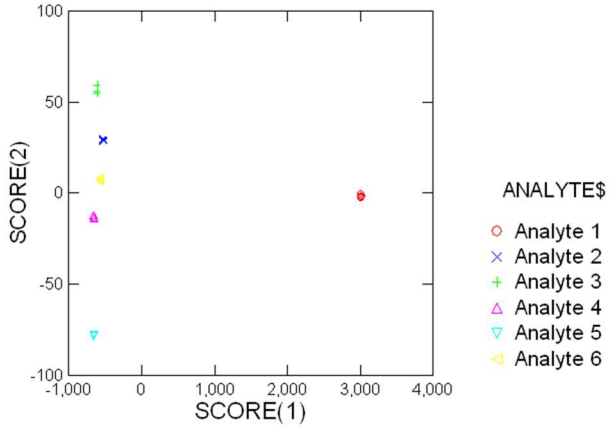
5 ºC



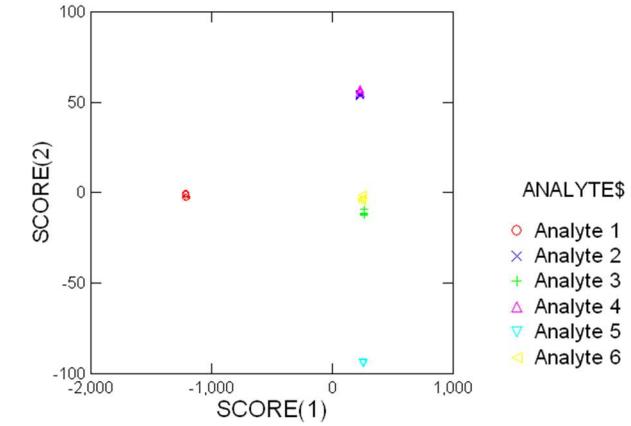
20 ºC



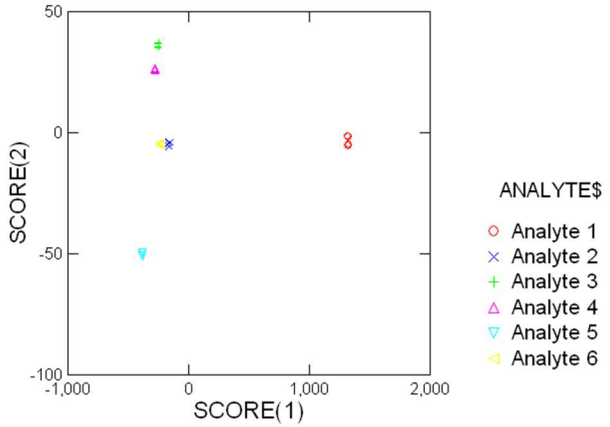
35 ºC



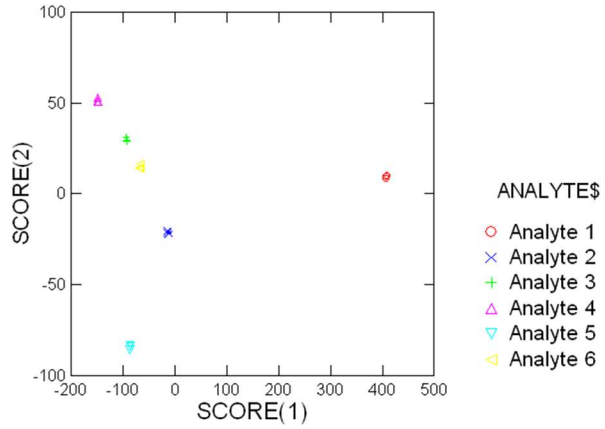
50 ºC



65 ºC



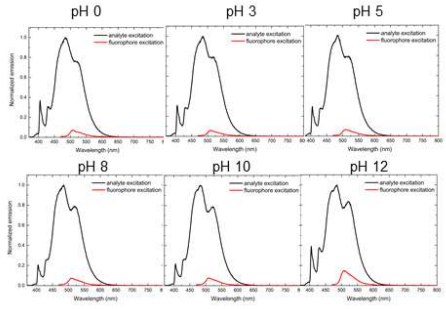
80 ºC



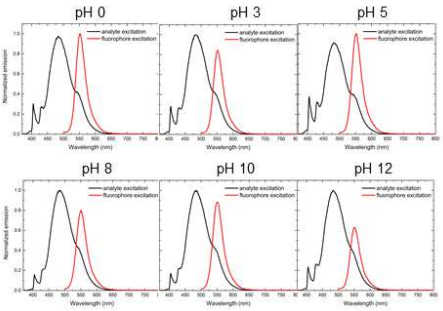
SUMMARY FIGURES FOR PH EXPERIMENTS

Energy Transfer

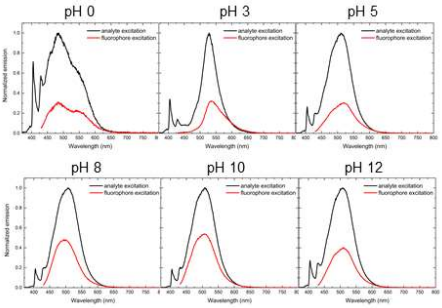
Analyte **1** – Fluorophore **7**



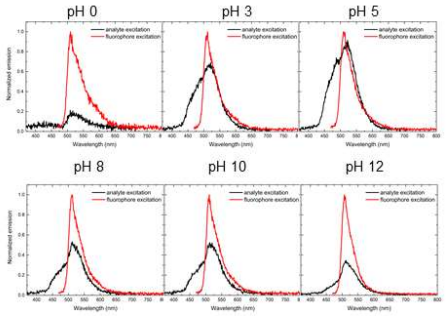
Analyte **1** – Fluorophore **8**



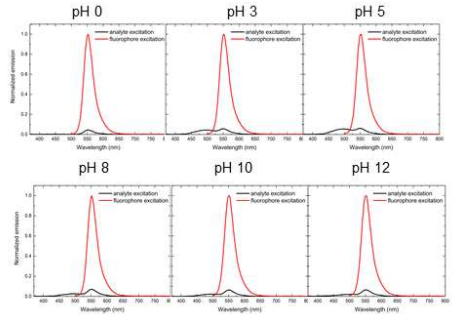
Analyte **1** – Fluorophore **9**



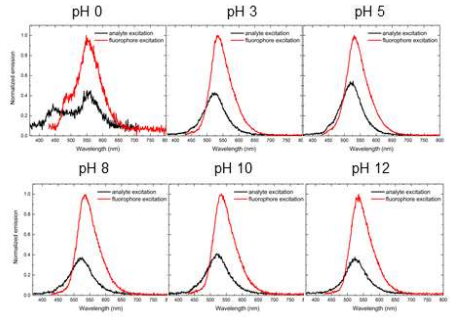
Analyte **2** – Fluorophore **7**



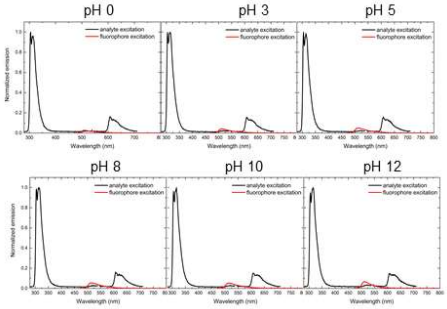
Analyte **2** – Fluorophore **8**



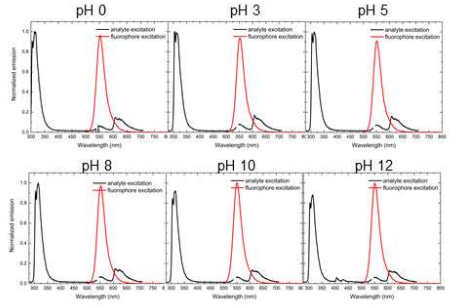
Analyte **2** – Fluorophore **9**



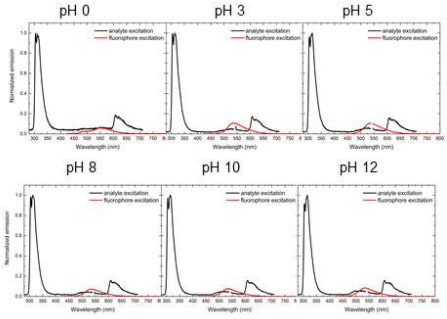
Analyte **3** – Fluorophore **7**



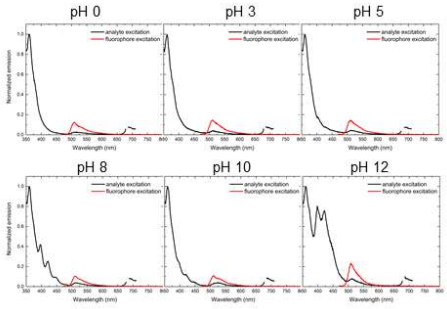
Analyte **3** – Fluorophore **8**



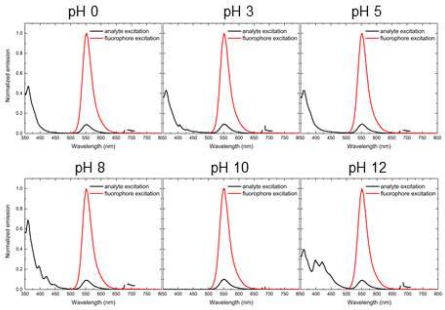
Analyte **3** – Fluorophore **9**



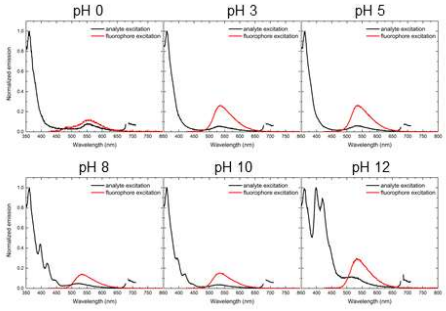
Analyte **4** – Fluorophore **7**



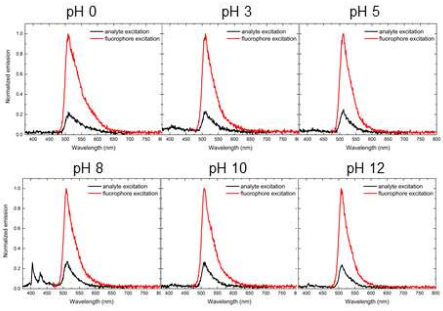
Analyte **4** – Fluorophore **8**



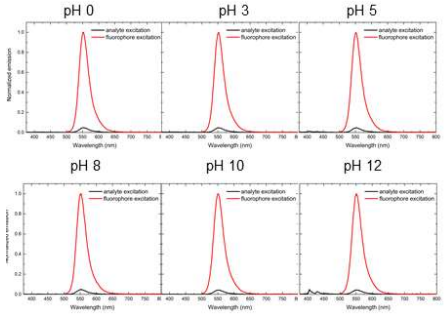
Analyte **4** – Fluorophore **9**



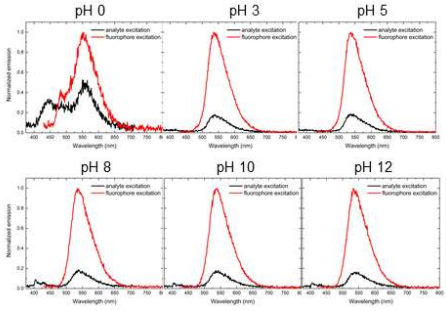
Analyte **5** – Fluorophore **7**



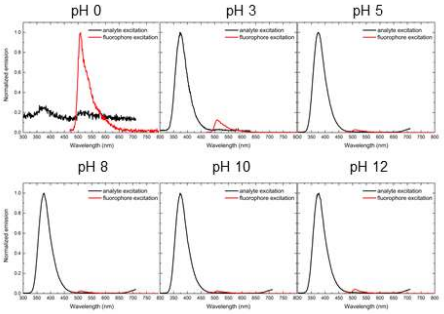
Analyte **5** – Fluorophore **8**



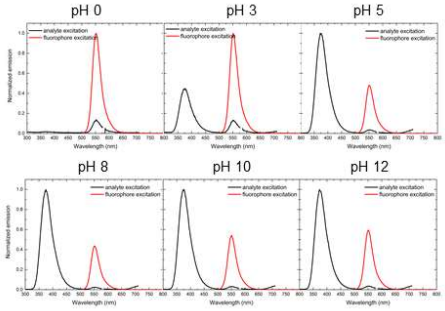
Analyte **5** – Fluorophore **9**



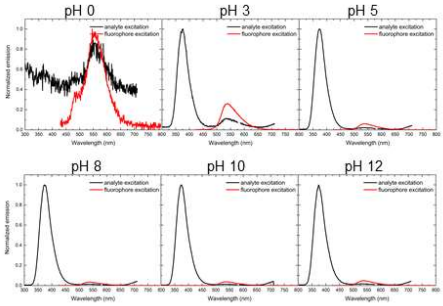
Analyte **6** – Fluorophore **7**



Analyte **6** – Fluorophore **8**

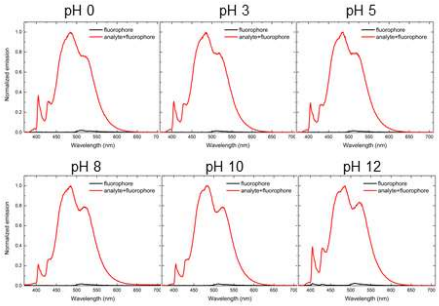


Analyte **6** – Fluorophore **9**

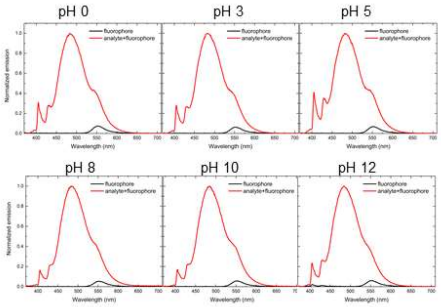


Control Ratio

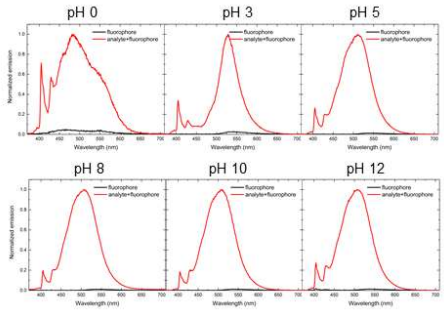
Analyte **1** – Fluorophore **7**



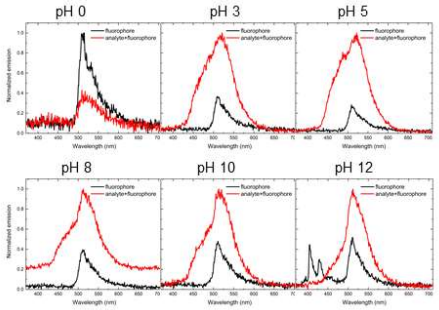
Analyte **1** – Fluorophore **8**



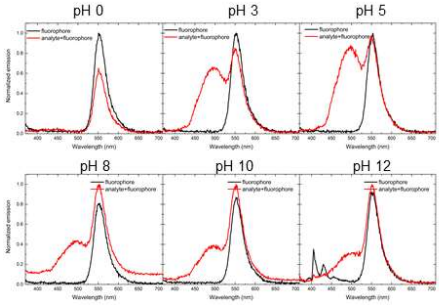
Analyte **1** – Fluorophore **9**



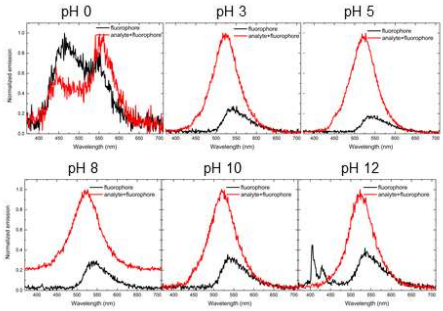
Analyte **2** – Fluorophore **7**



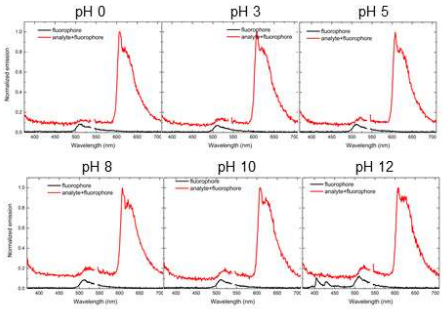
Analyte **2** – Fluorophore **8**



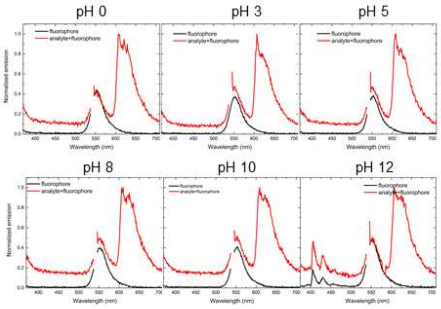
Analyte **2** – Fluorophore **9**



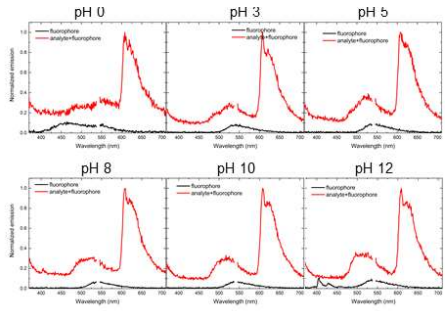
Analyte **3** – Fluorophore **7**



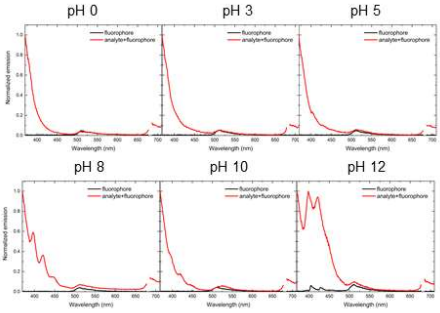
Analyte **3** – Fluorophore **8**



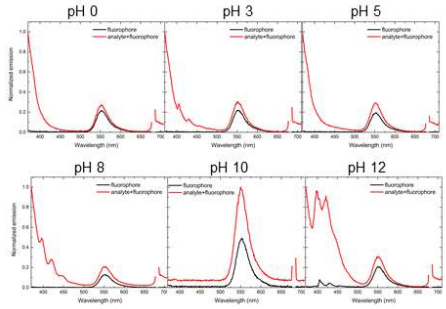
Analyte **3** – Fluorophore **9**



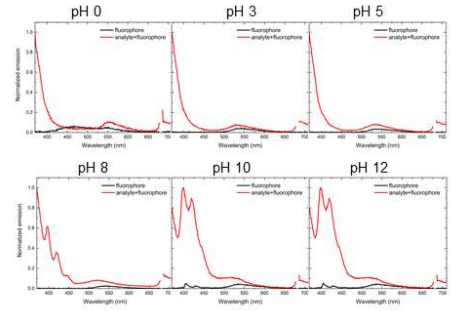
Analyte **4** – Fluorophore **7**



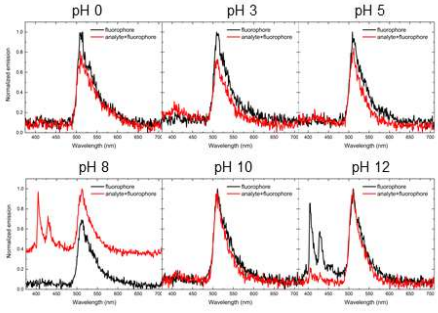
Analyte **4** – Fluorophore **8**



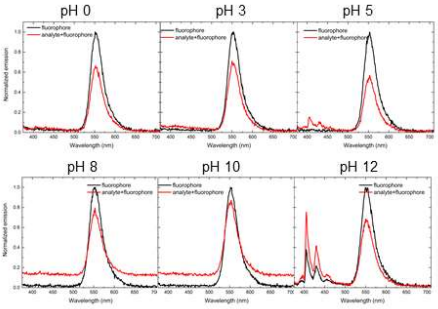
Analyte **4** – Fluorophore **9**



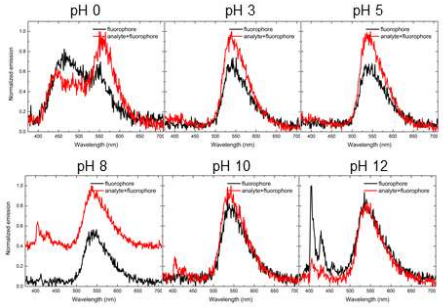
Analyte **5** – Fluorophore **7**



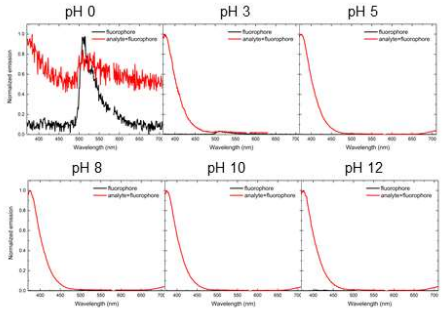
Analyte **5** – Fluorophore **8**



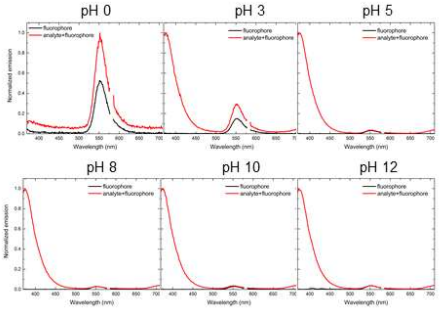
Analyte **5** – Fluorophore **9**



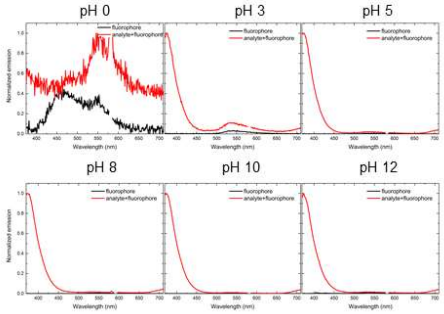
Analyte **6** – Fluorophore **7**



Analyte **6** – Fluorophore **8**

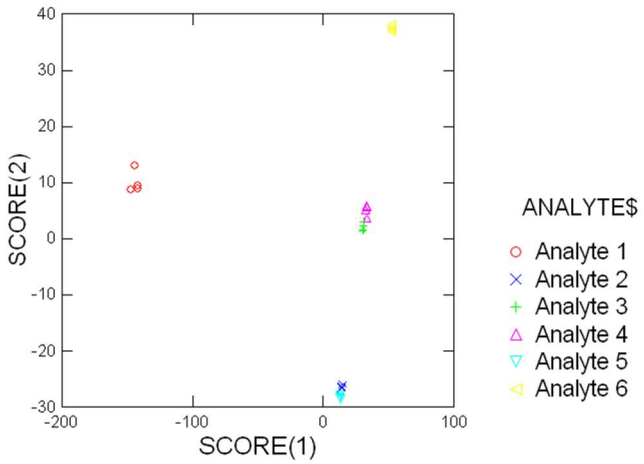


Analyte **6** – Fluorophore **9**

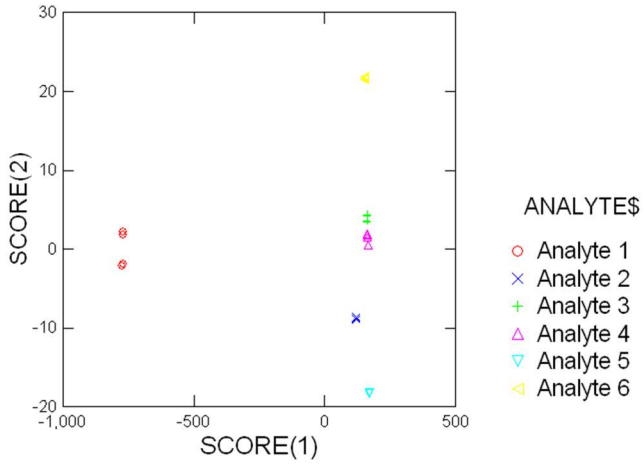


SUMMARY FIGURES FOR PH ARRAYS

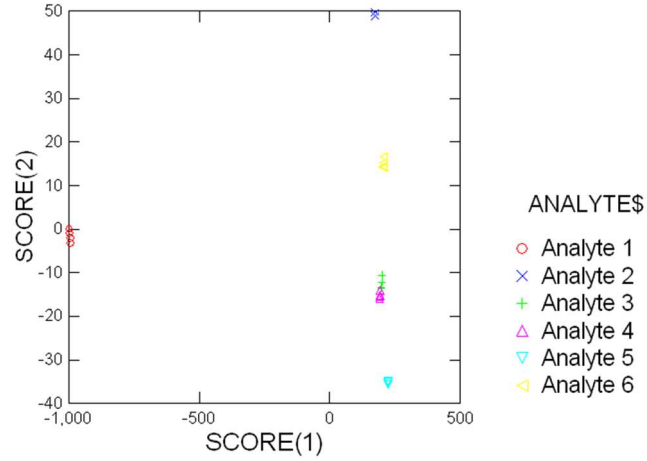
pH 0



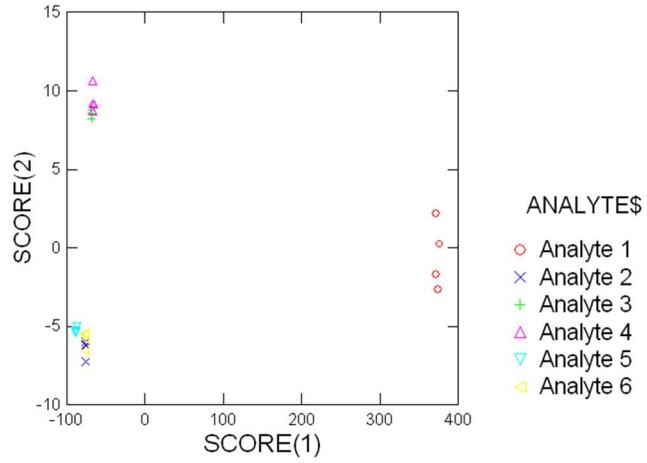
pH 3



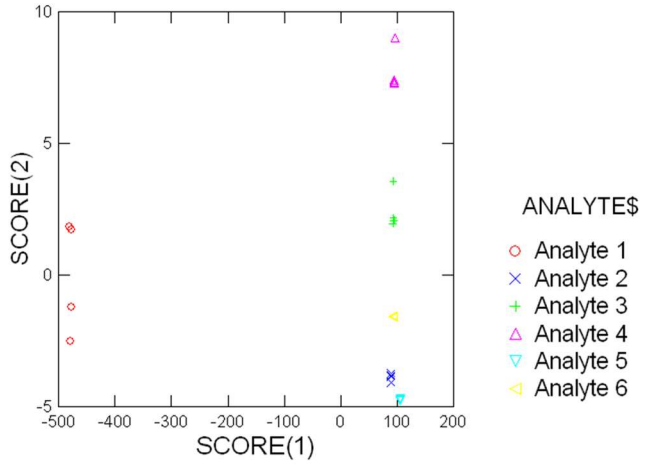
pH 5



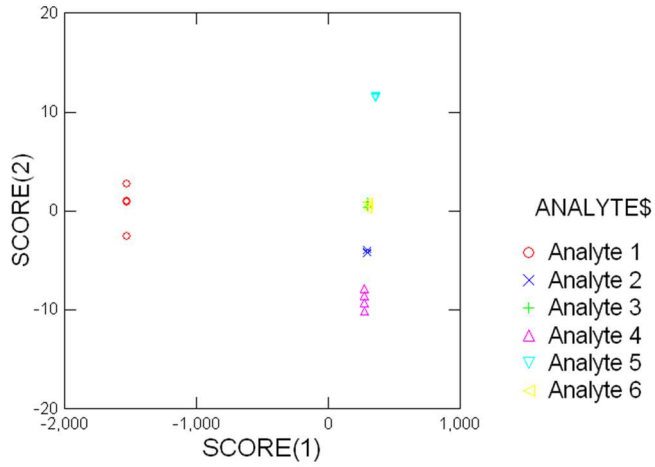
pH 8



pH 10



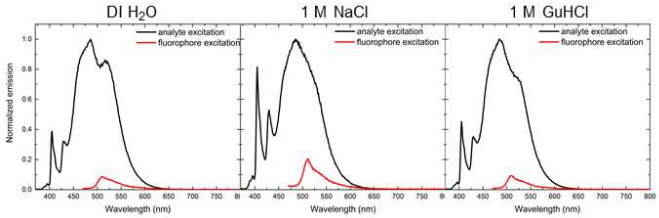
pH 12



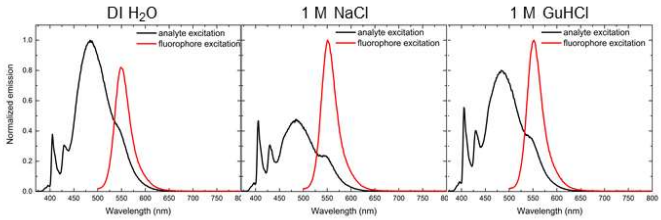
SUMMARY FIGURES FOR SALT EXPERIMENTS

Energy Transfer

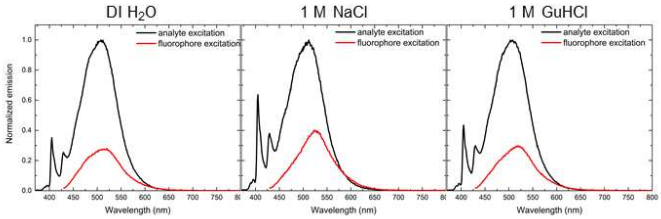
Analyte **1** – Fluorophore **7**



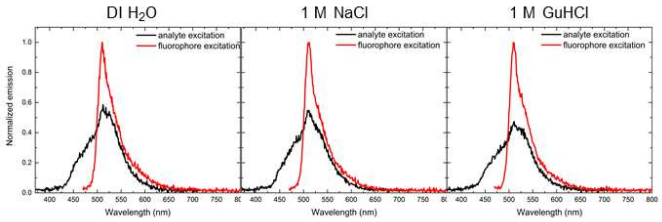
Analyte **1** – Fluorophore **8**



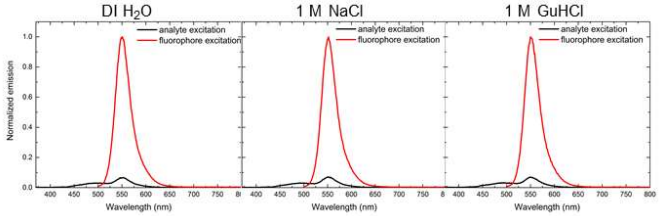
Analyte **1** – Fluorophore **9**



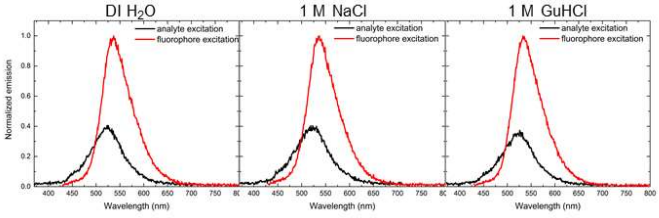
Analyte **2** – Fluorophore **7**



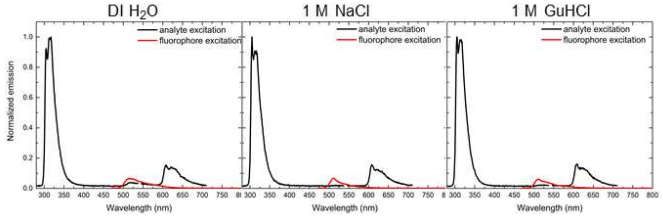
Analyte **2** – Fluorophore **8**



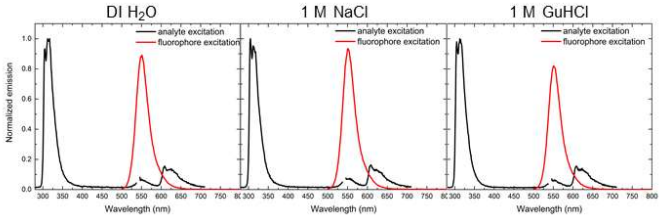
Analyte **2** – Fluorophore **9**



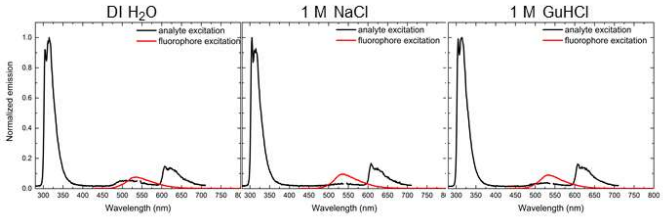
Analyte **3** – Fluorophore **7**



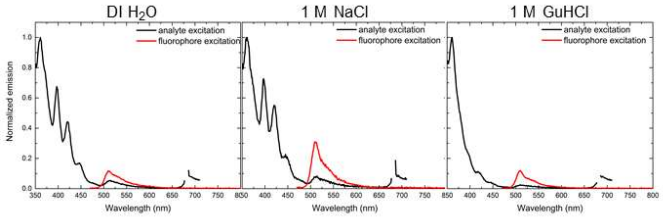
Analyte **3** – Fluorophore **8**



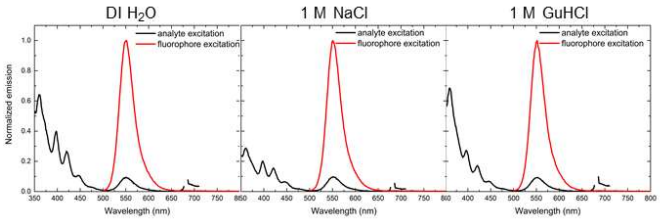
Analyte **3** – Fluorophore **9**



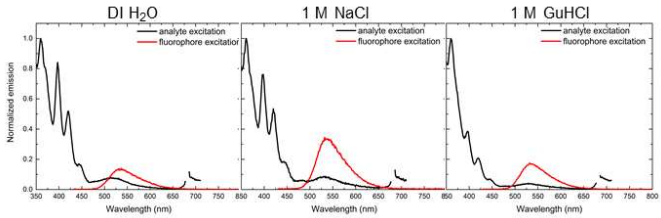
Analyte **4** – Fluorophore **7**



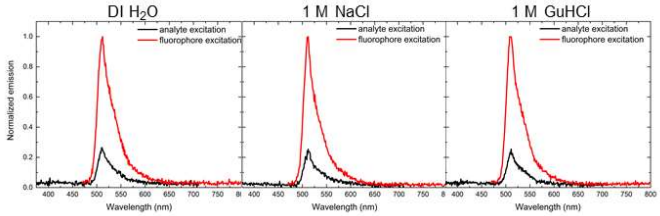
Analyte **4** – Fluorophore **8**



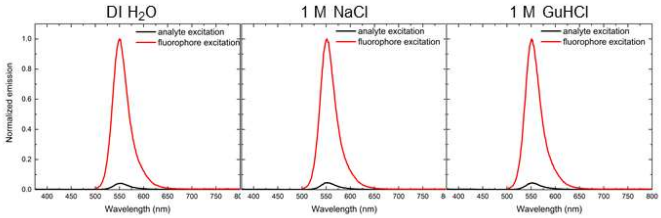
Analyte **4** – Fluorophore **9**



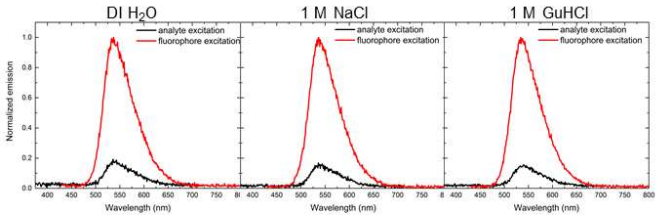
Analyte **5** – Fluorophore **7**



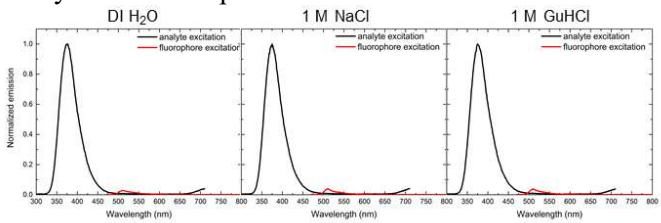
Analyte **5** – Fluorophore **8**



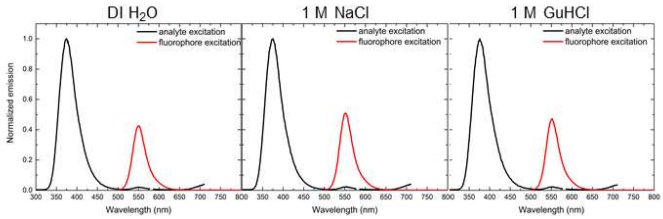
Analyte **5** – Fluorophore **9**



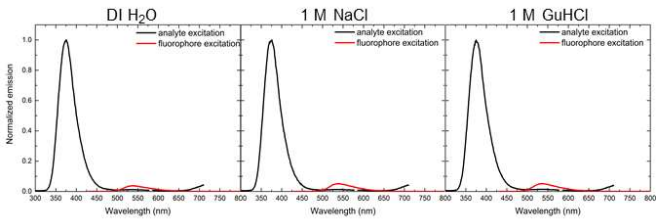
Analyte **6** – Fluorophore **7**



Analyte **6** – Fluorophore **8**

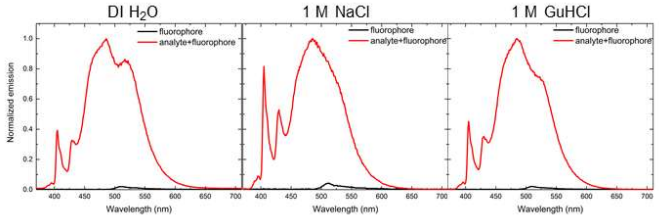


Analyte **6** – Fluorophore **9**

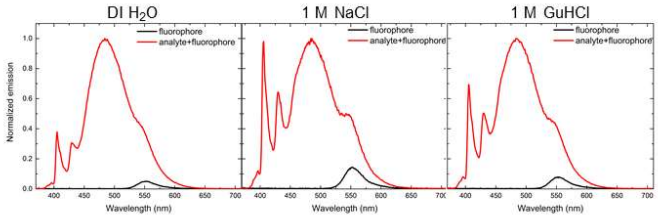


Control Ratio

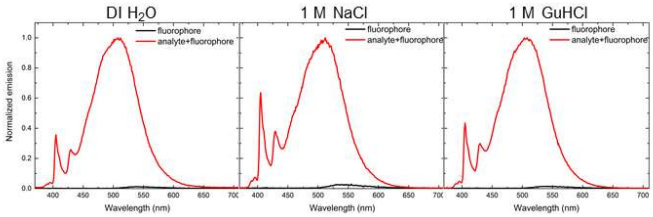
Analyte **1** – Fluorophore **7**



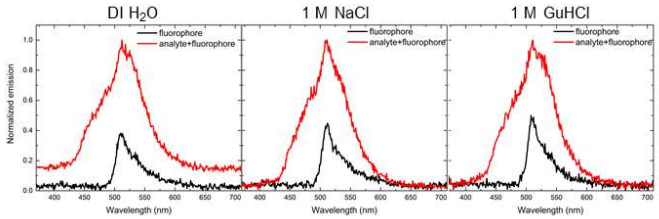
Analyte **1** – Fluorophore **8**



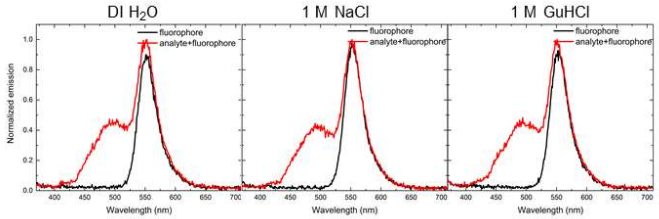
Analyte **1** – Fluorophore **9**



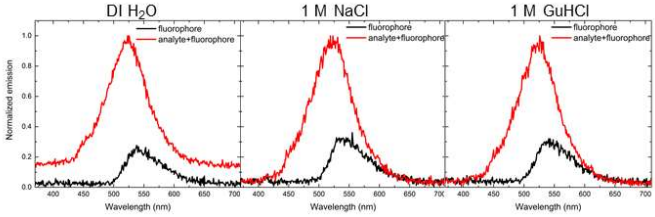
Analyte **2** – Fluorophore **7**



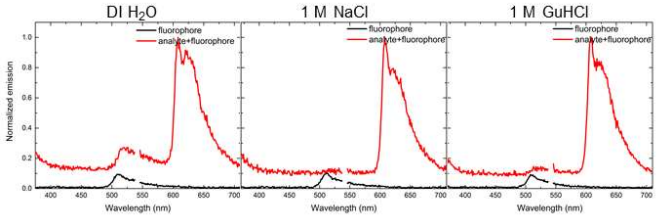
Analyte **2** – Fluorophore **8**



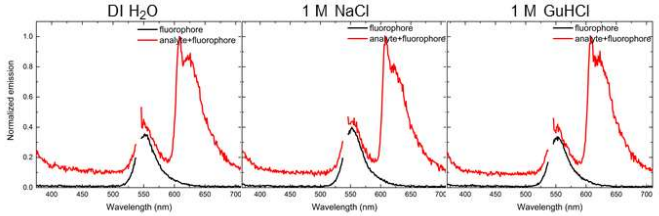
Analyte **2** – Fluorophore **9**



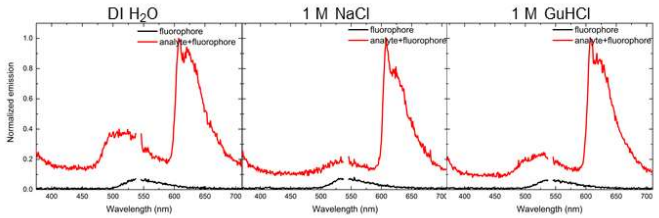
Analyte **3** – Fluorophore **7**



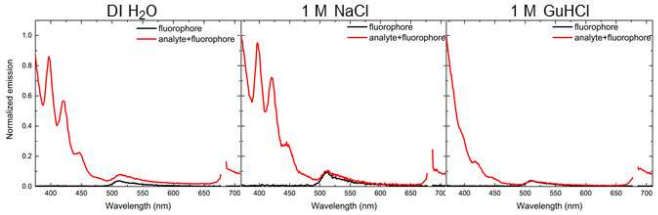
Analyte **3** – Fluorophore **8**



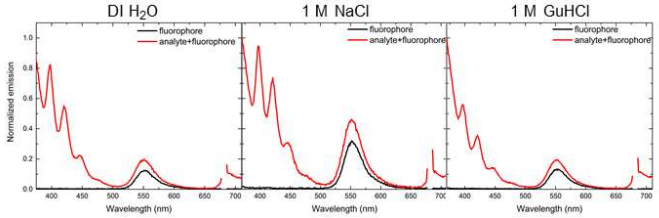
Analyte **3** – Fluorophore **9**



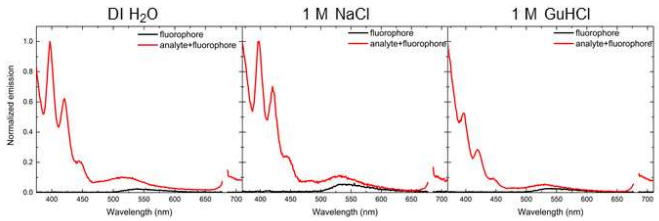
Analyte **4** – Fluorophore **7**



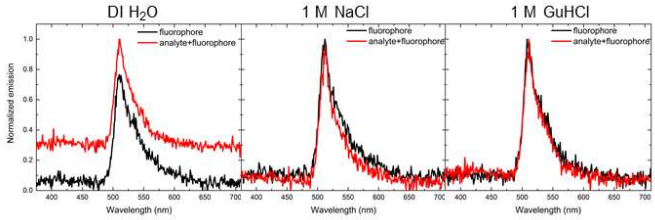
Analyte **4** – Fluorophore **8**



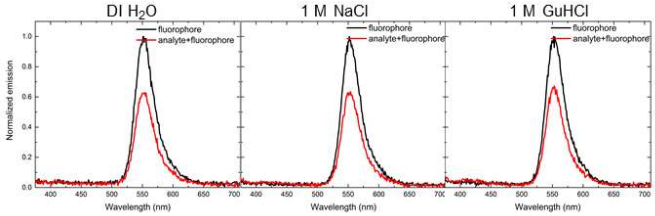
Analyte **4** – Fluorophore **9**



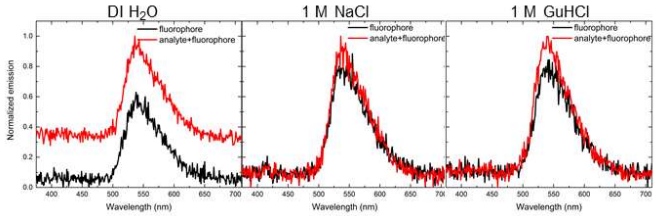
Analyte **5** – Fluorophore **7**



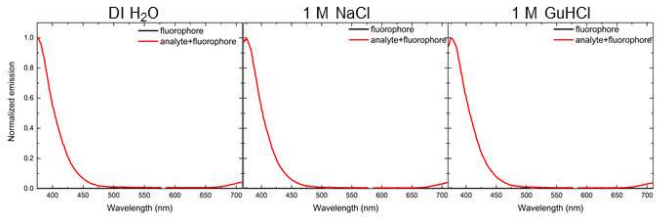
Analyte **5** – Fluorophore **8**



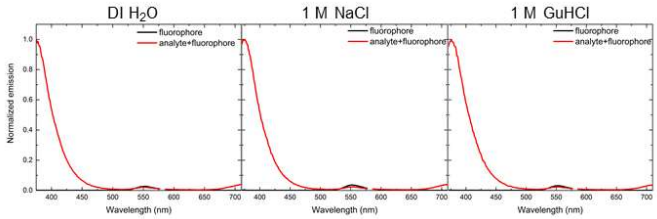
Analyte **5** – Fluorophore **9**



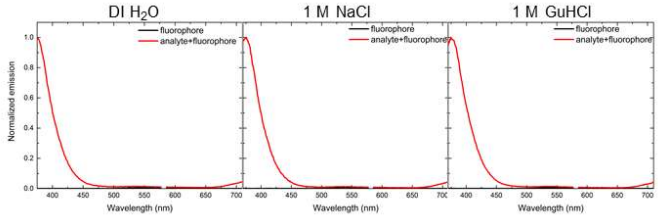
Analyte **6** – Fluorophore **7**



Analyte **6** – Fluorophore **8**

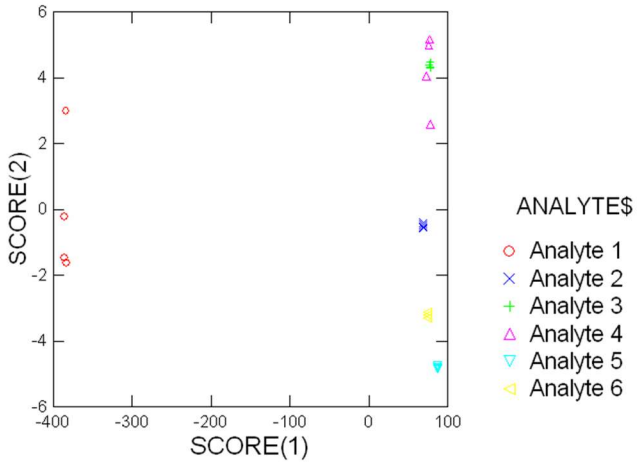


Analyte **6** – Fluorophore **9**

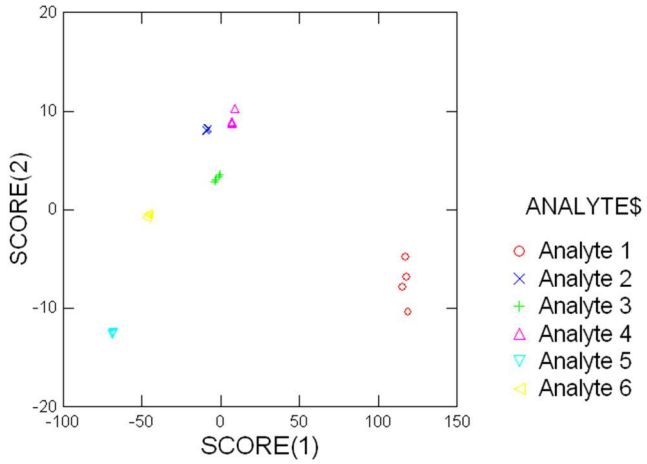


SUMMARY FIGURES FOR SALT ARRAYS

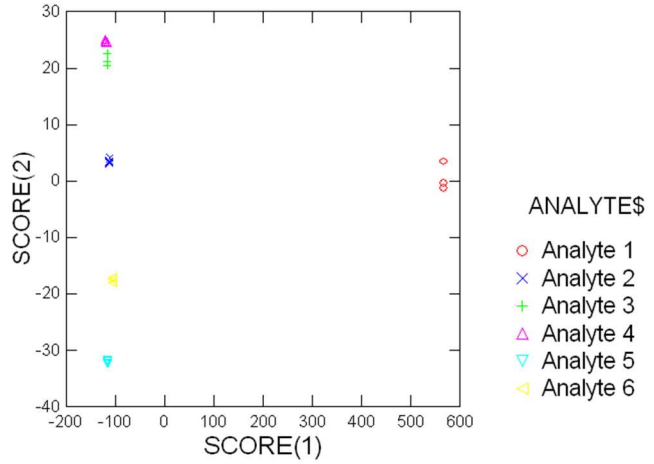
DI H_2O



1 M NaCl



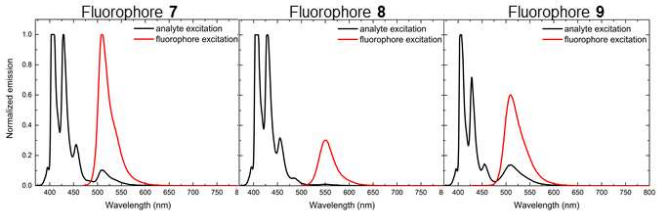
1 M GuHCl



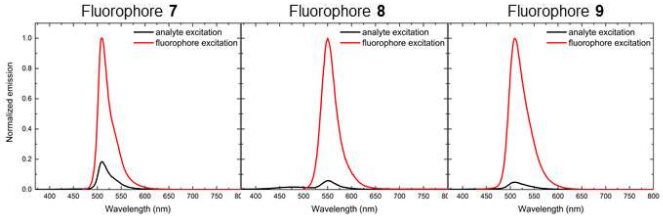
SUMMARY FIGURES FOR SOLVENT EXPERIMENTS

Energy Transfer

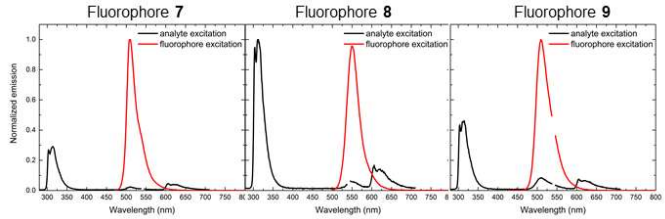
Analyte **1**



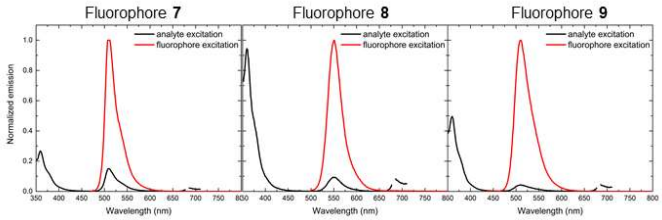
Analyte **2**



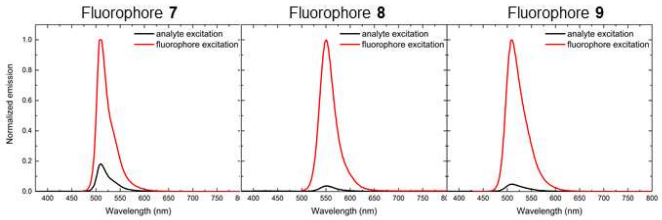
Analyte **3**



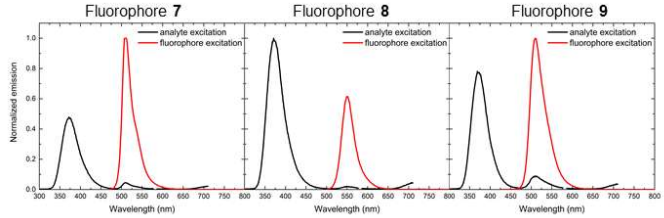
Analyte **4**



Analyte **5**

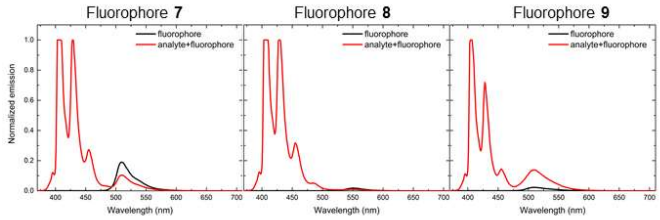


Analyte **6**

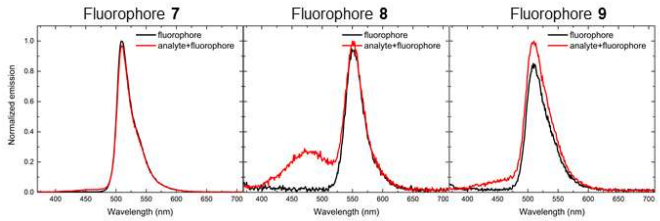


Control Ratio

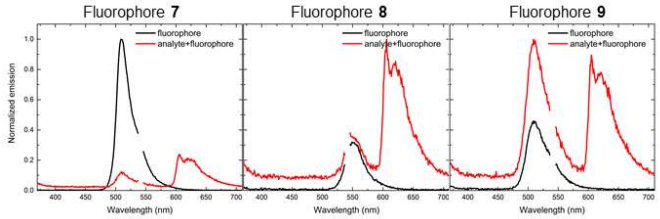
Analyte **1**



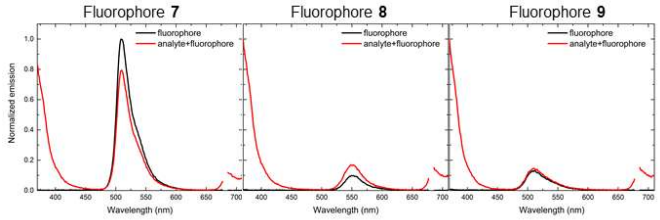
Analyte **2**



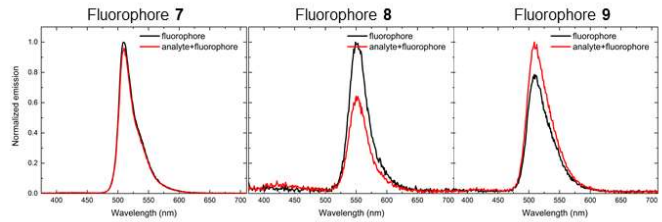
Analyte **3**



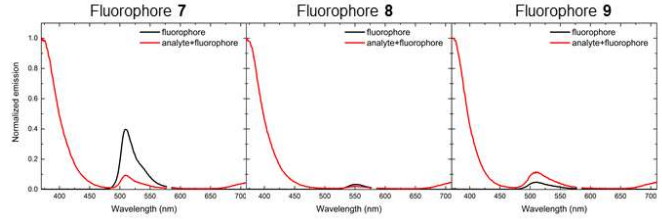
Analyte **4**



Analyte **5**

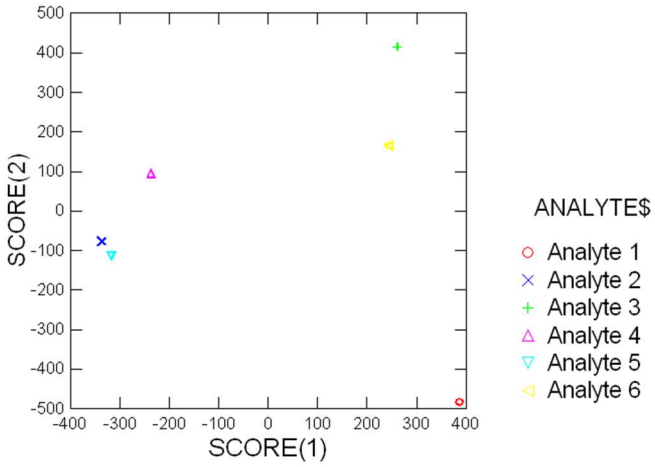


Analyte **6**



SUMMARY FIGURES FOR SOLVENT ARRAYS

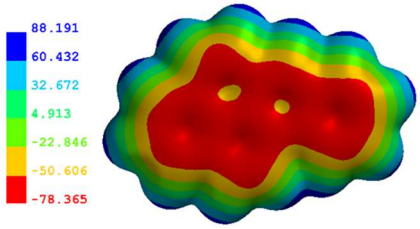
10 mM y-cyclodextrin in ethanol



ELECTROSTATIC POTENTIAL MAPPING FIGURES

All conformations shown were energy-minimized. The red areas represent electron-rich regions and the blue areas represent electron-deficient regions.

Analyte **1**



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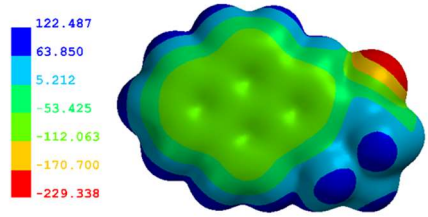

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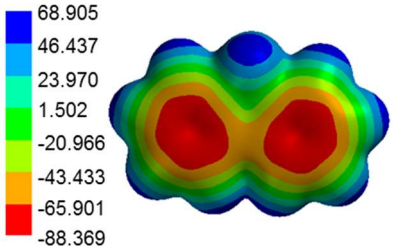
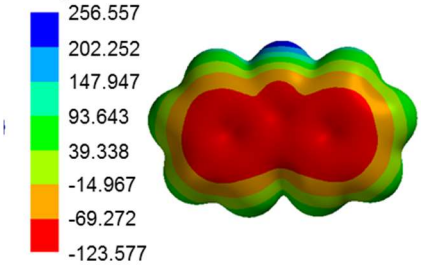
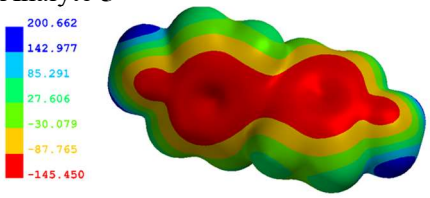


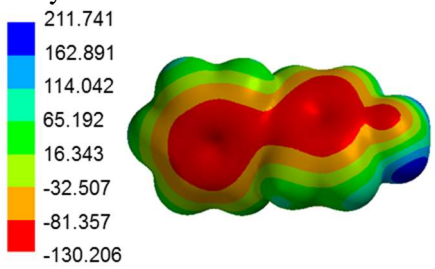
Analyte **4**



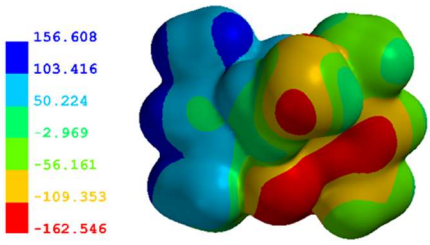
Analyte **5**



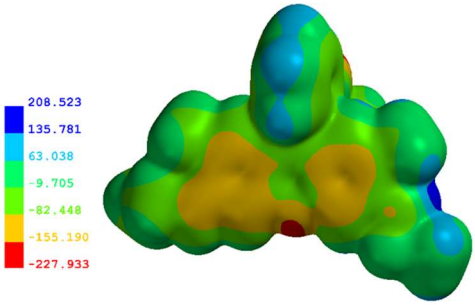
Analyte **6**



Fluorophore **7**



Fluorophore **8**



Fluorophore **9**