Electronic Supplementary Material (ESI) for ChemComm.


Electronic Supplementary Information for

# Array-Based Detection of Persistent Organic Pollutants via Cyclodextrin Promoted Energy Transfer

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## MATERIALS AND METHODS

All chemicals were purchased from Sigma-Aldrich Chemical Company and used as received. Urine samples were provided by an anonymous donor and used without any pre-treatment. $^{1}$H NMR spectra were obtained using a Bruker 300 MHz spectrometer. Fluorescence spectra were obtained using a BioTek Synergy Mx Multi-Mode Microplate Reader at 25ºC, with the following settings:

(a) Optics: Top
(b) Gain: 100
(c) Read height: 8 mm
(d) Read speed: Normal
(e) Measured data points at 10 nm increments

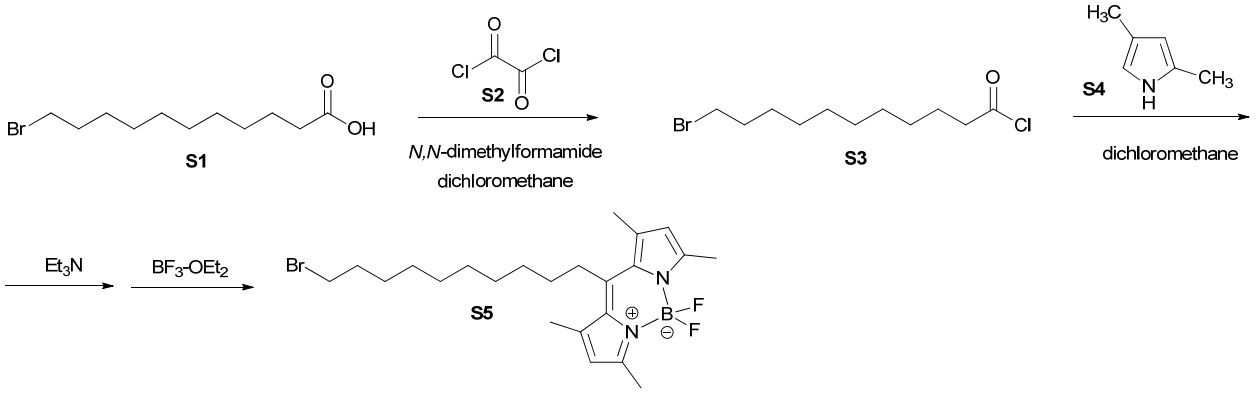
All spectra were integrated versus wavenumber on the X-axis using OriginPro software. The microplates used were black FLUOTRAC™ 200, 96W Microplates, and were purchased from Greiner Bio-One. Array analysis was performed using SYSTAT 13 statistical computing software with the following settings:

(a) Classical Discriminant Analysis
(b) Grouping Variable: Analytes
(c) Predictors: Bodipy, Rhodamine 6G, Coumarin 6
(d) Long-Range Statistics: Mahal

# SYNTHESIS OF BODIPY **31**

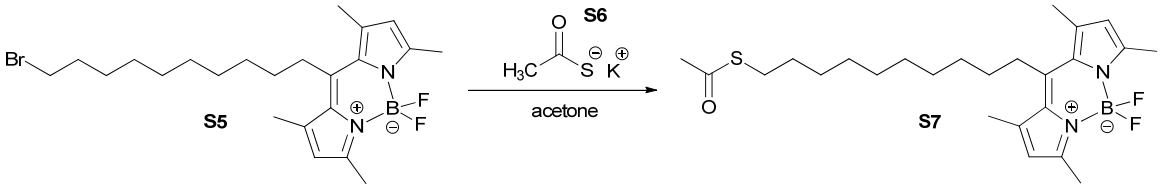
The synthesis of BODIPY 31 was performed according to literature procedures:[1]

**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 mixure 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 $^{o}$C. 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 $^{o}$C. 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 $^{o}$C 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.

**Reaction 2:**

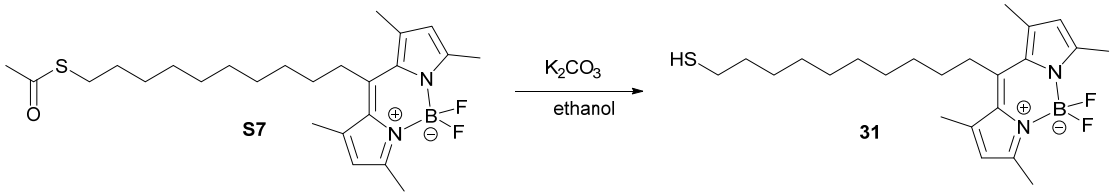



Procedure: Compound **S5** (0.968 g, 2.07 mmol, 1.0 eq.) and compound **S6** (0.27 grams, 2.36 mmol, 1.14 eq.) were dissolved in 50 mL of acetone. The reaction mixture was heated to reflux for two hours. After two

[1] J. L. Shepherd, A. Kell, E. Chung, C. W. Sinclar, M. S. Workentin and D. Bizzotto, *J. Am. Chem. Soc.*, 2004, **126**, 8329.

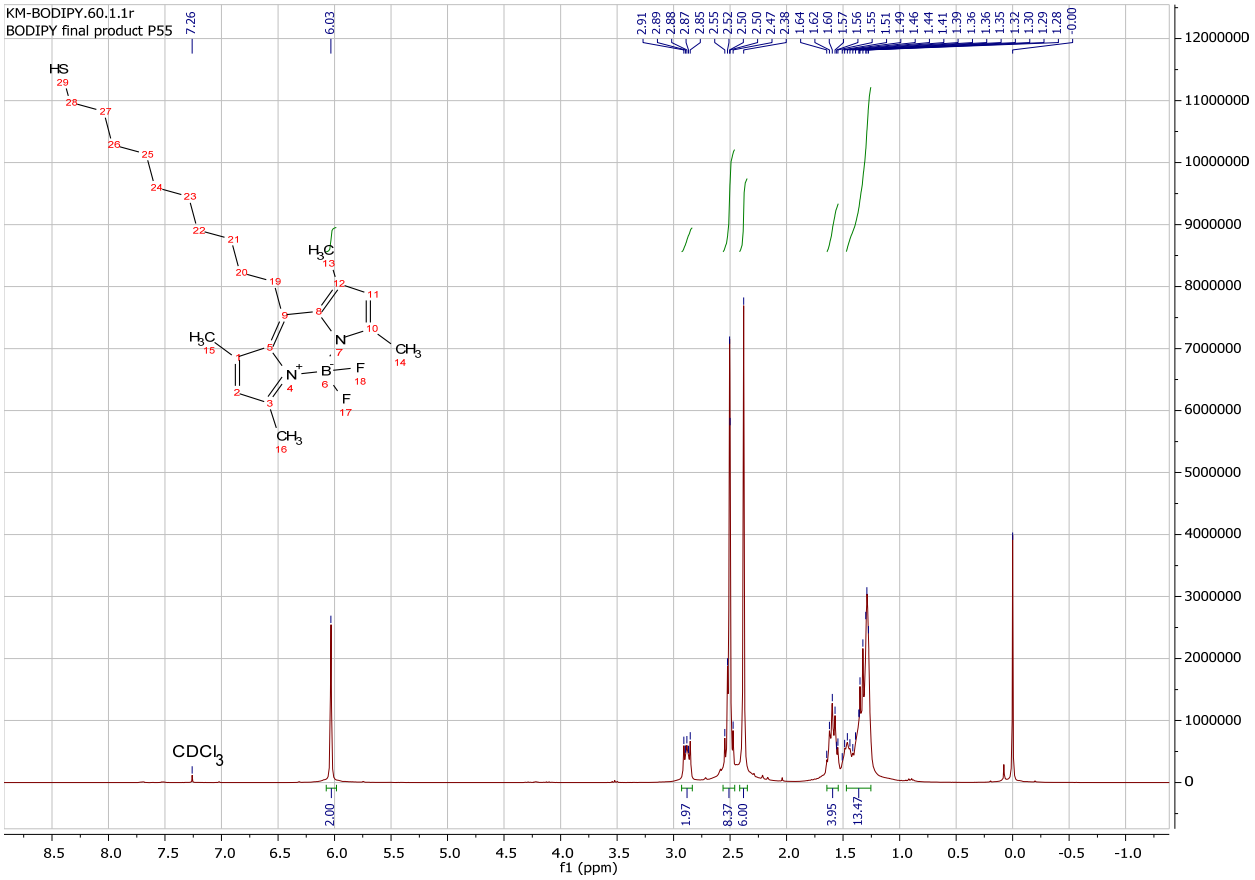
hours, the reaction mixture was cooled to room temperature, acetone was removed, and the crude solid was re-dissolved in dichloromethane and washed with water. The organic extract was dried over sodium sulfate, filtered and concentrated, to yield compound **S7** in 94% yield (0.932 grams).

**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 $^{o}$C. The reaction mixture was stirred under nitrogen for 4 hours at 30 $^{o}$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 **31** in 76% yield (674 mg).

# $^{1}$H NMR FOR BODIPY **31**



# ARRAY PROCEDURES

*General Procedure – Sample Preparation*

The following stock solutions were made:
10 mM γ-cyclodextrin in phosphate buffered saline (PBS) at pH 7.4
1 mg/mL of each analyte (**1**-**30**) in THF
0.1 mg/mL of each fluorophore (**31**-**33**) in THF

Two samples were prepared for each analyte-fluorophore combination: one served as the sample for the training set, and the other served as the unknown. For each sample, 2.5 mL of 10 mM γ-cyclodextrin, 100 μL of fluorophore solution, and 20 μL of analyte solution were added to a vial and vigorously shaken by hand for approximately 30 seconds. The sample remained on a rotary mixer until use to ensure thorough mixing. A 96 well microplate was divided as follows: (a) the first four rows were used for the training array and the remaining four rows were used for the unknowns; and (b) the columns were divided into three sections, one for each of the three dyes. Into each well was pipetted 100 μL of the sample solution, and each solution was repeated four times (*i.e.* each solution was pipetted into four separate wells) to ensure that the results obtained were reproducible.

*General Procedure – Fluorescence Studies*

A BioTek Synergy Mx Multi-Mode Microplate Reader was used to generate the fluorescence data for the array. Each analyte-fluorophore combination was excited at the analyte excitation wavelength (see table below) and the emission was recorded: (a) Fluorophore **31** samples: 470-620 nm; (b) Fluorophore **32** samples: 500-700 nm; (c) Fluorophore **33** samples: 450-700 nm. The fluorescence of the analyte was integrated with respect to wavenumber using OriginPro software.

**Table S1.** Excitation wavelengths used for each analyte.

| Analyte | Excitation Wavelength (nm) |
|---|---|
| **1** | 360 |
| **2** | 360 |
| **3** | 360 |
| **4** | 260 |
| **5** | 360 |
| **6** | 360 |
| **7** | 360 |
| **8** | 360 |
| **9** | 380 |
| **10** | 440 |
| **11** | 270 |
| **12** | 340 |
| **13** | 340 |
| **14** | 320 |
| **15** | 250 |
| **16** | 250 |
| **17** | 250 |
| **18** | 250 |
| **19** | 420 |
| **20** | 420 |
| **21** | 310 |
| **22** | 320 |
| **23** | 340 |
| **24** | 260 |
| **25** | 250 |
| **26** | 250 |
| **27** | 330 |
| **28** | 365 |
| **29** | 290 |
| **30** | 365 |

CLASSIFICATION ANALYSIS FOR BUFFER ARRAY

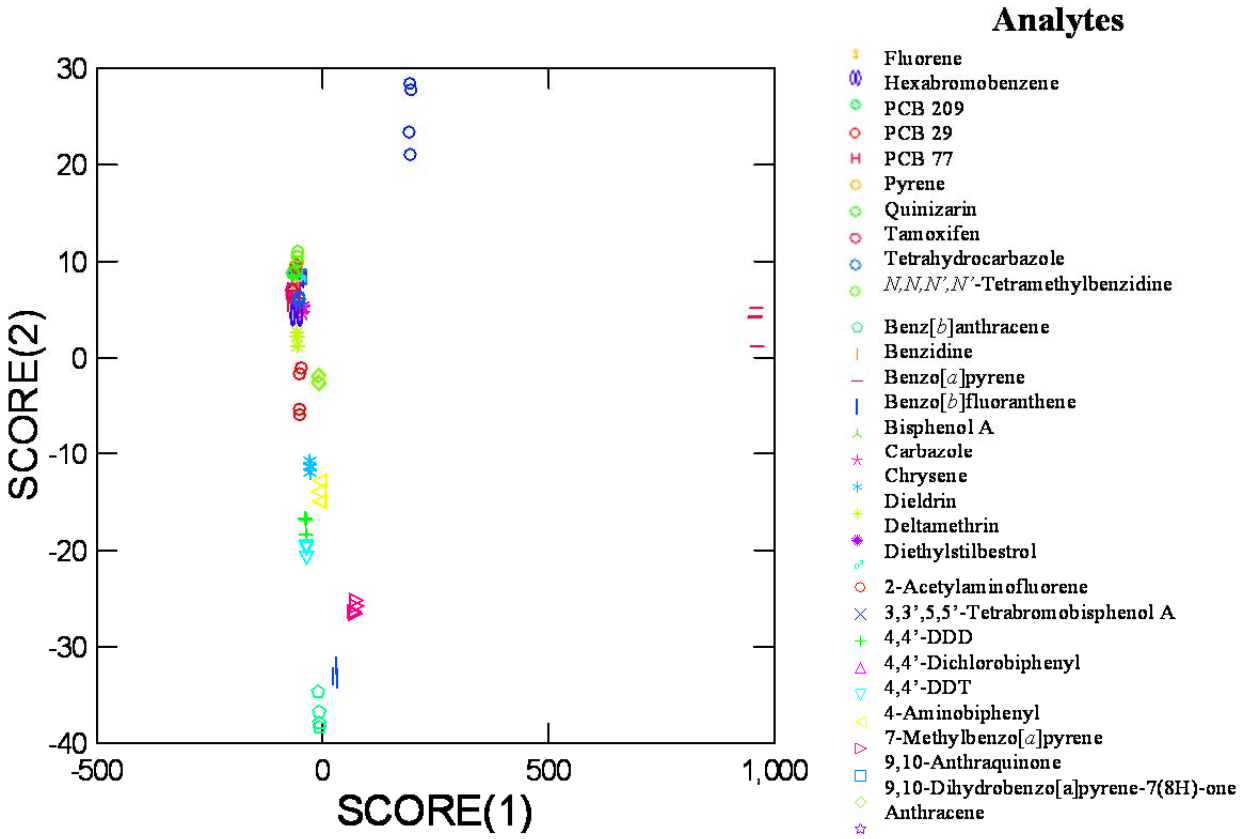



**Figure S1.** LDA score plot for all analytes.

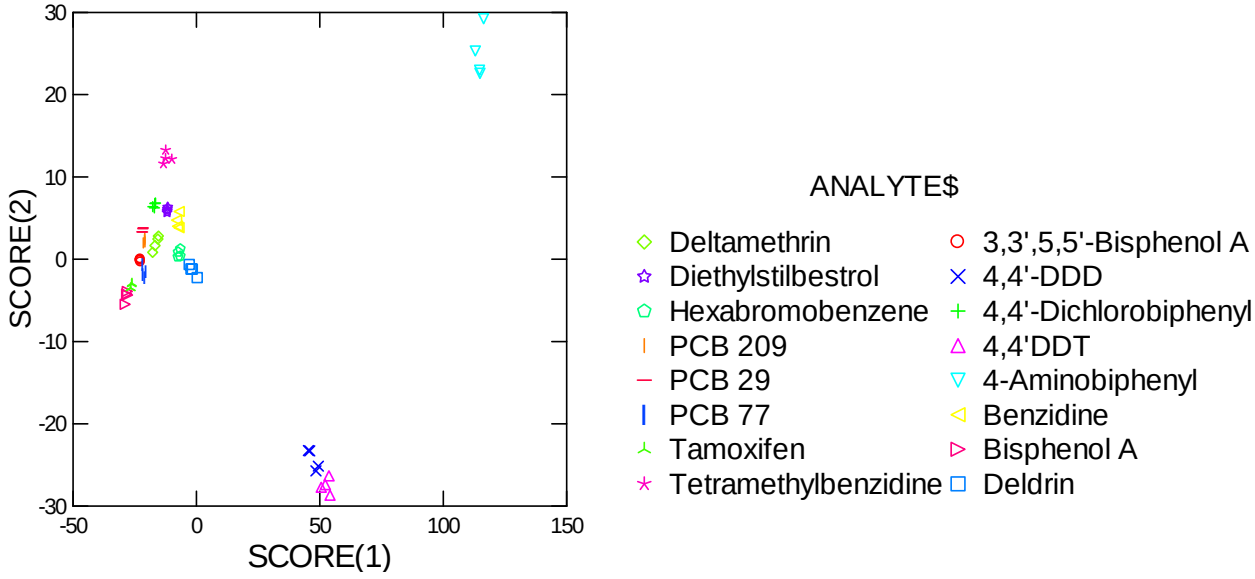



**Figure S2.** LDA score plot for all biphenyl-like analytes.

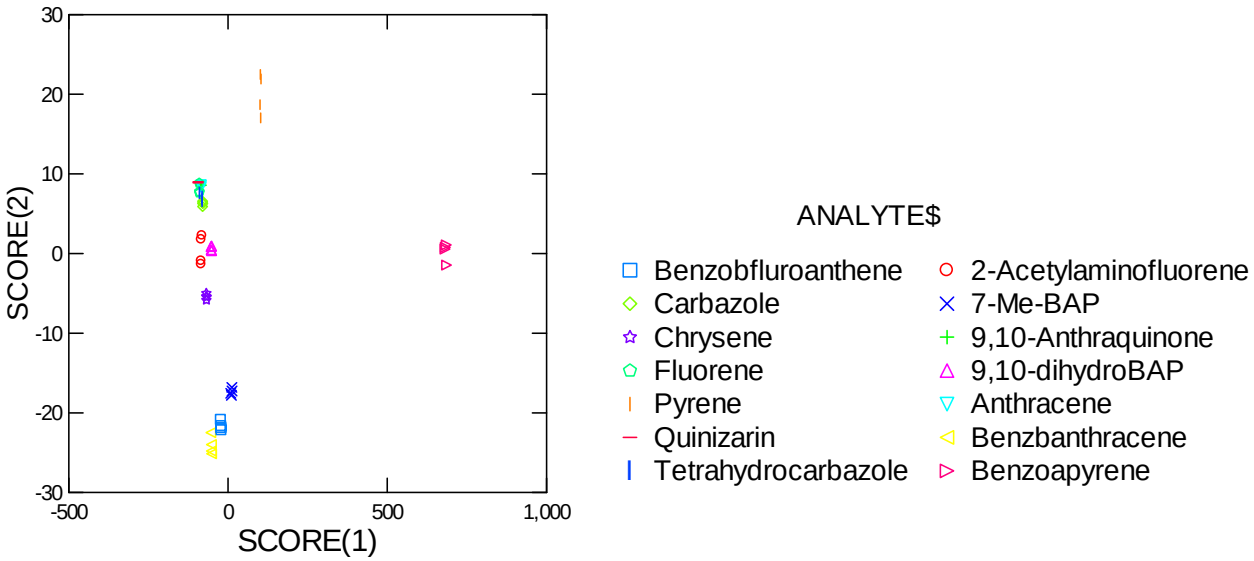



**Figure S3.** LDA score plot for all PAH analytes.

**Table S2.** Jackknifed classification matrix.

| | 14 | 26 | 20 | 15 | 19 | 29 | 7 | 2 | 8 | 1 | 10 | 28 | 6 | 9 | 25 | 12 | 4 | 22 | 21 | 23 | 11 | 27 | 18 | 16 | 17 | 5 | 3 | 24 | 13 | 30 | % Correct |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 14 | 4 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 100 |
| 26 | | 4 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 100 |
| 20 | | | 4 | | | | | | | | | | | | | | | | | | | | | | | | | | | | 100 |
| 15 | | | | 4 | | | | | | | | | | | | | | | | | | | | | | | | | | | 100 |
| 19 | | | | | 4 | | | | | | | | | | | | | | | | | | | | | | | | | | 100 |
| 29 | | | | | | 4 | | | | | | | | | | | | | | | | | | | | | | | | | 100 |
| 7 | | | | | | | 4 | | | | | | | | | | | | | | | | | | | | | | | | 100 |
| 2 | | | | | | | | 4 | | | | | | | | | | | | | | | | | | | | | | | 100 |
| 8 | | | | | | | | | 4 | | | | | | | | | | | | | | | | | | | | | | 100 |
| 1 | | | | | | | | | | 4 | | | | | | | | | | | | | | | | | | | | | 100 |
| 10 | | | | | | | | | | | 4 | | | | | | | | | | | | | | | | | | | | 100 |
| 28 | | | | | | | | | | | | 4 | | | | | | | | | | | | | | | | | | | 100 |
| 6 | | | | | | | | | | | | | 4 | | | | | | | | | | | | | | | | | | 100 |
| 9 | | | | | | | | | | | | | | 4 | | | | | | | | | | | | | | | | | 100 |
| 25 | | | | | | | | | | | | | | | 4 | | | | | | | | | | | | | | | | 100 |
| 12 | | | | | | | | | | | | | | | | 4 | | | | | | | | | | | | | | | 100 |
| 4 | | | | | | | | | | | | | | | | | 4 | | | | | | | | | | | | | | 100 |
| 22 | | | | | | | | | | | | | | | | | | 4 | | | | | | | | | | | | | 100 |
| 21 | | | | | | | | | | | | | | | | | | | 4 | | | | | | | | | | | | 100 |
| 23 | | | | | | | | | | | | | | | | | | | | 4 | | | | | | | | | | | 100 |
| 11 | | | | | | | | | | | | | | | | | | | | | 4 | | | | | | | | | | 100 |
| 27 | | | | | | | | | | | | | | | | | | | | | | 4 | | | | | | | | | 100 |
| 18 | | | | | | | | | | | | | | | | | | | | | | | 4 | | | | | | | | 100 |
| 16 | | | | | | | | | | | | | | | | | | | | | | | | 4 | | | | | | | 100 |
| 17 | | | | | | | | | | | | | | | | | | | | | | | | | 4 | | | | | | 100 |
| 5 | | | | | | | | | | | | | | | | | | | | | | | | | | 4 | | | | | 100 |
| 3 | | | | | | | | | | | | | | | | | | | | | | | | | | | 4 | | | | 100 |
| 24 | | | | | | | | | | | | | | | | | | | | | | | | | | | | 4 | | | 100 |
| 13 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 4 | | 100 |
| 30 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | 4 | 100 |
| TOTAL | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 4 | 100 |

**Table S3.** Cumulative Proportion of Total Dispersion values.

| | | |
|---|---|---|
| 0.993 | 0.999 | 1.000 |

## UNKNOWN CLASSIFICATIONS FOR BUFFER ARRAY

**Table S4.** Classifications of all analytes ("Analyte ID"), including misclassifications of unknowns ("Unknown Classification").

| Score 1 | Score 2 | Score 3 | Analyte ID | Unknown Classification |
|---|---|---|---|---|
| -51.07 | 8.36 | -2.95 | Anthracene | Anthracene |
| -50.96 | 8.49 | -2.95 | Anthracene | Anthracene |
| -50.98 | 8.13 | -2.98 | Anthracene | Anthracene |
| -51.01 | 8.60 | -3.15 | Anthracene | Anthracene |
| 957.26 | 4.29 | -0.23 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 961.95 | 1.17 | 0.98 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 955.47 | 4.15 | -3.58 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 960.07 | 5.14 | -8.47 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 195.50 | 28.32 | 17.92 | Pyrene | Pyrene |
| 197.76 | 27.66 | 16.18 | Pyrene | Pyrene |
| 193.66 | 23.29 | 13.92 | Pyrene | Pyrene |
| 195.99 | 20.95 | 14.88 | Pyrene | Pyrene |
| 75.49 | -25.75 | -16.69 | 7-Methylbenzo[*a*]pyrene | 7-Methylbenzo[*a*]pyrene |
| 72.86 | -26.52 | -16.72 | 7-Methylbenzo[*a*]pyrene | 7-Methylbenzo[*a*]pyrene |
| 74.85 | -25.18 | -15.97 | 7-Methylbenzo[*a*]pyrene | 7-Methylbenzo[*a*]pyrene |
| 70.61 | -26.38 | -12.85 | 7-Methylbenzo[*a*]pyrene | 7-Methylbenzo[*a*]pyrene |
| -51.36 | 8.32 | 0.13 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -52.06 | 8.46 | 0.91 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -51.40 | 8.31 | 0.19 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -51.55 | 8.29 | 0.29 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -9.30 | -2.49 | -2.53 | 9,10-dihydrobenzo[*a*]pyrene | 9,10-dihydrobenzo[*a*]pyrene |
| -7.95 | -1.78 | -3.18 | 9,10-dihydrobenzo[*a*]pyrene | 9,10-dihydrobenzo[*a*]pyrene |
| -9.53 | -1.90 | -2.74 | 9,10-dihydrobenzo[*a*]pyrene | 9,10-dihydrobenzo[*a*]pyrene |
| -7.92 | -2.64 | -2.52 | 9,10-dihydrobenzo[*a*]pyrene | 9,10-dihydrobenzo[*a*]pyrene |
| -7.69 | -36.74 | 4.87 | Benz[*b*]anthracene | Benz[*b*]anthracene |
| -6.88 | -38.35 | 5.36 | Benz[*b*]anthracene | Benz[*b*]anthracene |
| -7.35 | -37.89 | 5.47 | Benz[*b*]anthracene | Benz[*b*]anthracene |
| -9.98 | -34.68 | 4.83 | Benz[*b*]anthracene | Benz[*b*]anthracene |
| -57.71 | 8.18 | -5.03 | 3,3',5,5'-Tetrabromobisphenol A | 3,3',5,5'-Tetrabromobisphenol A |
| -57.93 | 8.00 | -4.81 | 3,3',5,5'-Tetrabromobisphenol A | 3,3',5,5'-Tetrabromobisphenol A |
| -57.67 | 8.20 | -5.03 | 3,3',5,5'-Tetrabromobisphenol A | 3,3',5,5'-Tetrabromobisphenol A |
| -58.08 | 8.13 | -4.77 | 3,3',5,5'-Tetrabromobisphenol A | 3,3',5,5'-Tetrabromobisphenol A |
| -67.71 | 6.62 | 0.90 | Bisphenol A | Bisphenol A |
| -67.48 | 6.93 | 0.96 | Bisphenol A | Bisphenol A |

| Score 1 | Score 2 | Score 3 | Analyte ID | Unknown Classification |
|---|---|---|---|---|
| -67.34 | 6.82 | 0.94 | Bisphenol A | Bisphenol A |
| -67.12 | 7.04 | 0.75 | Bisphenol A | Bisphenol A |
| -5.52 | -12.80 | -2.29 | 4-Aminobiphenyl | 4-Aminobiphenyl |
| -9.83 | -13.87 | -0.01 | 4-Aminobiphenyl | 4-Aminobiphenyl |
| -6.02 | -14.91 | -2.60 | 4-Aminobiphenyl | 4-Aminobiphenyl |
| -7.68 | -14.94 | -1.30 | 4-Aminobiphenyl | 4-Aminobiphenyl |
| -57.79 | 5.52 | -0.07 | Benzidine | Benzidine |
| -57.34 | 6.06 | -0.17 | Benzidine | Benzidine |
| -58.10 | 5.26 | 0.35 | Benzidine | Benzidine |
| -57.84 | 5.90 | -0.13 | Benzidine | Benzidine |
| -28.11 | -10.73 | 8.56 | Chrysene | Chrysene |
| -27.89 | -11.97 | 9.46 | Chrysene | Chrysene |
| -26.92 | -11.42 | 9.14 | Chrysene | Chrysene |
| -28.52 | -11.30 | 8.82 | Chrysene | Chrysene |
| -55.32 | 7.62 | -3.34 | Diethylstilbestrol | Diethylstilbestrol |
| -55.63 | 7.64 | -3.06 | Diethylstilbestrol | Diethylstilbestrol |
| -55.36 | 7.78 | -3.19 | Diethylstilbestrol | Diethylstilbestrol |
| -55.33 | 7.73 | -3.28 | Diethylstilbestrol | Diethylstilbestrol |
| -43.84 | 5.15 | 1.05 | Carbazole | Carbazole |
| -44.39 | 5.53 | 1.65 | Carbazole | Carbazole |
| -44.38 | 5.24 | 0.87 | Carbazole | Carbazole |
| -44.31 | 4.59 | 1.66 | Carbazole | Carbazole |
| -49.28 | 6.00 | -1.05 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -49.80 | 5.59 | -2.05 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -50.44 | 6.23 | -1.72 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -49.81 | 6.04 | -2.12 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -35.16 | -19.79 | -0.15 | 4,4'DDT | 4,4'-DDD |
| -35.78 | -19.85 | -0.16 | 4,4'DDT | 4,4'-DDD |
| -36.40 | -19.60 | -0.18 | 4,4'DDT | 4,4'DDT |
| -35.41 | -20.81 | 0.10 | 4,4'DDT | 4,4'DDT |
| -37.42 | -18.39 | 0.03 | 4,4'-DDD | 4,4'-DDD |
| -37.92 | -16.70 | -0.42 | 4,4'-DDD | 4,4'-DDD |
| -37.57 | -16.81 | -0.55 | 4,4'-DDD | 4,4'-DDD |
| -37.14 | -18.41 | 0.13 | 4,4'-DDD | 4,4'-DDD |
| -53.70 | 10.41 | -4.87 | Tetramethylbenzidine | Tetramethylbenzidine |
| -53.75 | 10.42 | -4.56 | Tetramethylbenzidine | Tetramethylbenzidine |
| -52.78 | 10.91 | -5.29 | Tetramethylbenzidine | Tetramethylbenzidine |

| | | | | |
|---|---|---|---|---|
| -52.52 | 9.84 | -4.75 | Tetramethylbenzidine | Fluorene |
| -55.90 | 9.17 | -4.45 | 4,4'-Dichlorobiphenyl | 4,4'-Dichlorobiphenyl |
| Score 1 | Score 2 | Score 3 | Analyte ID | Unknown Classification |
| -56.35 | 9.35 | -4.30 | 4,4'-Dichlorobiphenyl | 4,4'-Dichlorobiphenyl |
| -55.42 | 9.38 | -4.77 | 4,4'-Dichlorobiphenyl | 4,4'-Dichlorobiphenyl |
| -55.81 | 9.28 | -4.38 | 4,4'-Dichlorobiphenyl | 4,4'-Dichlorobiphenyl |
| -55.12 | 8.93 | -6.47 | PCB 209 | PCB 209 |
| -55.08 | 8.99 | -6.49 | PCB 209 | PCB 209 |
| -55.68 | 8.73 | -6.00 | PCB 209 | PCB 209 |
| -55.62 | 8.89 | -6.27 | PCB 209 | PCB 209 |
| -56.38 | 9.43 | -5.78 | PCB 29 | PCB 29 |
| -56.03 | 9.53 | -5.93 | PCB 29 | PCB 29 |
| -56.09 | 9.51 | -5.83 | PCB 29 | PCB 29 |
| -56.53 | 9.34 | -5.58 | PCB 29 | PCB 29 |
| 31.76 | -34.05 | 8.05 | Benzo[*b*]fluroanthene | Benzo[*b*]fluroanthene |
| 30.68 | -33.29 | 7.20 | Benzo[*b*]fluroanthene | Benzo[*b*]fluroanthene |
| 29.31 | -32.17 | 6.11 | Benzo[*b*]fluroanthene | Benzo[*b*]fluroanthene |
| 31.71 | -33.58 | 6.72 | Benzo[*b*]fluroanthene | Benzo[*b*]fluroanthene |
| -56.38 | 2.67 | 0.11 | Deldrin | Deldrin |
| -55.79 | 2.19 | 0.00 | Deldrin | Deldrin |
| -56.45 | 2.26 | 0.37 | Deldrin | Deldrin |
| -56.06 | 1.22 | 0.81 | Deldrin | Deldrin |
| -55.92 | 4.53 | -1.62 | Hexabromobenzene | Hexabromobenzene |
| -56.05 | 4.42 | -1.23 | Hexabromobenzene | Hexabromobenzene |
| -56.33 | 4.28 | -1.33 | Hexabromobenzene | Hexabromobenzene |
| -55.85 | 4.13 | -1.43 | Hexabromobenzene | Hexabromobenzene |
| -65.66 | 5.50 | 2.26 | PCB 77 | PCB 77 |
| -66.10 | 5.97 | 2.02 | PCB 77 | PCB 77 |
| -66.45 | 6.71 | 2.14 | PCB 77 | PCB 77 |
| -66.34 | 6.22 | 2.04 | PCB 77 | PCB 77 |
| -58.04 | 6.95 | 0.45 | Fluorene | Fluorene |
| -57.81 | 7.14 | 0.55 | Fluorene | Fluorene |
| -58.08 | 7.13 | 0.47 | Fluorene | Fluorene |
| -58.70 | 8.66 | 0.15 | Fluorene | Fluorene |
| -65.73 | 7.06 | 0.25 | Tamoxifen | Tamoxifen |
| -66.15 | 6.92 | 0.42 | Tamoxifen | Tamoxifen |
| -66.29 | 6.92 | 0.53 | Tamoxifen | Tamoxifen |
| -65.53 | 7.07 | 0.07 | Tamoxifen | Tamoxifen |

| | | | | |
|---|---|---|---|---|
| -45.23 | -1.13 | 14.63 | 2-Acetylaminofluorene | Benz[*b*]anthracene |
| -48.66 | -1.74 | 12.74 | 2-Acetylaminofluorene | 2-Acetylaminofluorene |
| Score 1 | Score 2 | Score 3 | Analyte ID | Unknown Classification |
| -48.90 | -5.39 | 11.71 | 2-Acetylaminofluorene | 2-Acetylaminofluorene |
| -48.88 | -5.98 | 11.53 | 2-Acetylaminofluorene | 2-Acetylaminofluorene |
| -64.77 | 6.28 | 2.60 | Deltamethrin | Deltamethrin |
| -64.24 | 6.40 | 2.65 | Deltamethrin | Deltamethrin |
| -64.33 | 6.31 | 2.64 | Deltamethrin | Deltamethrin |
| -64.85 | 6.23 | 2.34 | Deltamethrin | Deltamethrin |
| -62.75 | 8.82 | 0.74 | Quinizarin | Quinizarin |
| -63.18 | 8.74 | 0.77 | Quinizarin | Tamoxifen |
| -62.65 | 8.78 | 0.73 | Quinizarin | Quinizarin |
| -63.72 | 8.61 | 1.21 | Quinizarin | Quinizarin |

## INTEGRATIONS FOR BUFFER ARRAY

**Table S5.** All integration values used for the training set ("Array Inttegrations") and unknowns ("Unknown Integrations").

| | ARRAY INTEGRATIONS | | | UNKNOWN INTEGRATIONS | | |
|---|---|---|---|---|---|---|
| **Analyte** | **Bodipy** | **Rhodamine** | **Coumarin 6** | **Bodipy** | **Rhodamine** | **Coumarin 6** |
| Anthracene | 2344330 | 5788640 | 2837790 | 2935710 | 5941930 | 2554070 |
| Anthracene | 2389360 | 5807720 | 2792760 | 2528110 | 5786270 | 2689250 |
| Anthracene | 2313910 | 5795470 | 2980850 | 2431180 | 5372210 | 2719030 |
| Anthracene | 2328730 | 5858840 | 2706150 | 2492970 | 5863640 | 2643950 |
| Benzo[*a*]pyrene | 197135000 | 135687000 | 221909000 | 213389000 | 143601000 | 231367000 |
| Benzo[*a*]pyrene | 197935000 | 135825000 | 224692000 | 200380000 | 144479000 | 232252000 |
| Benzo[*a*]pyrene | 195618000 | 136329000 | 221301000 | 204588000 | 145191000 | 232944000 |
| Benzo[*a*]pyrene | 194993000 | 138260000 | 221322000 | 205116000 | 142745000 | 239354000 |
| Pyrene | 60395800 | 33249500 | 46980800 | 56544000 | 31845600 | 45106900 |
| Pyrene | 60125600 | 33969800 | 47668500 | 56669700 | 33357600 | 45520300 |

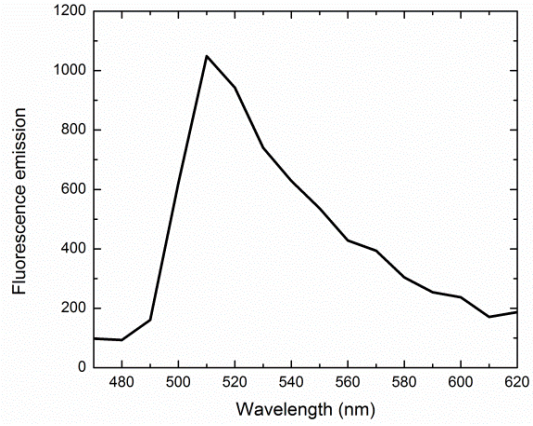
| | | | | | | |
|---|---|---|---|---|---|---|
| Pyrene | 57829500 | 33822300 | 48926400 | 50957700 | 33475500 | 46952500 |
| Pyrene | 58216400 | 33757800 | 50765000 | 54997000 | 34222200 | 48875700 |
| 7-Methylbenzo[*a*]pyrene | 16368100 | 24170300 | 47076500 | 16340800 | 25085700 | 46688100 |
| 7-Methylbenzo[*a*]pyrene | 15723400 | 23798700 | 46922800 | 16514600 | 23922200 | 46562500 |
| 7-Methylbenzo[*a*]pyrene | 16589800 | 23923600 | 46696200 | 16891600 | 24203300 | 47867000 |
| 7-Methylbenzo[*a*]pyrene | 16639300 | 22494900 | 46705700 | 16714700 | 24432300 | 47920800 |
| 9,10-Anthraquinone | 3339760 | 4938430 | 3070680 | 3711370 | 5064900 | 3196160 |
| 9,10-Anthraquinone | 3493350 | 4649630 | 2913540 | 3729870 | 5110870 | 3119300 |
| 9,10-Anthraquinone | 3350860 | 4914250 | 3074480 | 3557800 | 4990940 | 3051800 |
| 9,10-Anthraquinone | 3351850 | 4868730 | 3062140 | 3693370 | 4935830 | 3703960 |
| 9,10-dihydrobenzo[*a*]pyrene | 8740320 | 10569400 | 17659200 | 9433050 | 10578700 | 18685200 |
| 9,10-dihydrobenzo[*a*]pyrene | 8894640 | 10951500 | 17515900 | 9251610 | 10844000 | 19914200 |
| 9,10-dihydrobenzo[*a*]pyrene | 8722630 | 10622700 | 17278200 | 9196540 | 10951700 | 18259600 |
| 9,10-dihydrobenzo[*a*]pyrene | 8985250 | 10738800 | 18037400 | 9198960 | 10884400 | 17920300 |
| Benz[*b*]anthracene | 5880480 | 7171510 | 37002100 | 6044890 | 7176490 | 36988600 |
| Benz[*b*]anthracene | 5934610 | 7071350 | 38082400 | 6005150 | 7038890 | 36116900 |
| Benz[*b*]anthracene | 5960310 | 7002950 | 37747100 | 6170620 | 7046430 | 36752600 |
| Benz[*b*]anthracene | 5768110 | 6985040 | 35402900 | 5944810 | 7042520 | 35179400 |
| 3,3',5,5'-Tetrabromobisphenol A | 321517.9473 | 5464500 | 1321330 | 372599.737 | 5680820 | 1421620 |
| 3,3',5,5'-Tetrabromobisphenol A | 326051.9081 | 5369600 | 1392180 | 377280.7686 | 5320190 | 1378000 |
| 3,3',5,5'-Tetrabromobisphenol A | 332000.834 | 5471080 | 1325050 | 369755.9172 | 5588710 | 1332650 |
| 3,3',5,5'-Tetrabromobisphenol A | 332338.5885 | 5346170 | 1295350 | 352995.9294 | 5379570 | 1291410 |
| Bisphenol A | 164975.9969 | 2530060 | 537570.5586 | 273596.3212 | 2501340 | 478510.0797 |
| Bisphenol A | 281422.7581 | 2560330 | 424763.8135 | 202756.0464 | 2633190 | 447133.9969 |
| Bisphenol A | 284783.3698 | 2578150 | 514330.4449 | 293299.0857 | 2577770 | 433039.421 |
| Bisphenol A | 296819.8954 | 2667980 | 429165.557 | 316476.6339 | 2776620 | 428135.4458 |
| 4-Aminobiphenyl | 7831380 | 10498200 | 24016000 | 7802810 | 10079600 | 23786300 |
| 4-Aminobiphenyl | 7603120 | 9287820 | 23865700 | 7425880 | 10137200 | 23818700 |
| 4-Aminobiphenyl | 7278220 | 10411900 | 25010100 | 7327080 | 10208100 | 23891800 |
| 4-Aminobiphenyl | 7399990 | 9853030 | 24785600 | 7263830 | 9208620 | 24715800 |
| Benzidine | 1562180 | 4019660 | 3172210 | 1586620 | 3871930 | 3070850 |
| Benzidine | 1706970 | 4130440 | 2973910 | 1575380 | 4053890 | 3012020 |
| Benzidine | 1603230 | 3857790 | 3284810 | 1671020 | 3908980 | 3062950 |
| Benzidine | 1594700 | 4049410 | 2955540 | 2348740 | 3892300 | 3262240 |
| Chrysene | 7537630 | 4812970 | 19016500 | 7509190 | 4725880 | 23090000 |
| Chrysene | 7683220 | 4545150 | 19808600 | 8078330 | 4966370 | 22046200 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Chrysene | 7850840 | 4780890 | 19695700 | 7913350 | 4863150 | 20544000 |
| Chrysene | 7454590 | 4662210 | 19260200 | 8115170 | 5035080 | 21757400 |
| Diethylstilbestrol | 1268840 | 5302150 | 2286780 | 1353590 | 5476050 | 2170590 |
| Diethylstilbestrol | 1308000 | 5188480 | 2237310 | 1435710 | 5204210 | 2150480 |
| Diethylstilbestrol | 1337990 | 5266390 | 2204900 | 1423790 | 5411600 | 2162530 |
| Diethylstilbestrol | 1307120 | 5290210 | 2233740 | 1436290 | 5650180 | 2274210 |
| Carbazole | 4577100 | 5518380 | 6466370 | 4760750 | 5339300 | 4968150 |
| Carbazole | 4739950 | 5305900 | 6198730 | 4154560 | 5204710 | 5229600 |
| Carbazole | 4425730 | 5498990 | 6284480 | 4154680 | 5463700 | 6960520 |
| Carbazole | 4601260 | 5268360 | 6716870 | 4336350 | 5513090 | 6020140 |
| Tetrahydrocarbazole | 2947180 | 5405470 | 4656030 | 2406100 | 5409130 | 3828440 |
| Tetrahydrocarbazole | 2436650 | 5580550 | 4676770 | 2444380 | 5543350 | 4090740 |
| Tetrahydrocarbazole | 2532740 | 5441970 | 4224090 | 2574520 | 5477720 | 3920220 |
| Tetrahydrocarbazole | 2487310 | 5620380 | 4423620 | 2563120 | 5470260 | 3904700 |
| 4,4'DDT | 1684430 | 5750210 | 21581900 | 1569440 | 5398940 | 20560200 |
| 4,4'DDT | 1552330 | 5668870 | 21478600 | 1420310 | 5333340 | 20717100 |
| 4,4'DDT | 1465720 | 5607960 | 21206100 | 1480460 | 5350550 | 21148500 |
| 4,4'DDT | 1552510 | 5604360 | 22093900 | 1448620 | 5259280 | 22511200 |
| 4,4'-DDD | 1544780 | 5477630 | 20363600 | 1510440 | 5503750 | 18707800 |
| 4,4'-DDD | 1572200 | 5613880 | 19310700 | 1527160 | 5377520 | 20269200 |
| 4,4'-DDD | 1577740 | 5688070 | 19430800 | 1530450 | 5560140 | 19007300 |
| 4,4'-DDD | 1627870 | 5488470 | 20441100 | 1551580 | 5528360 | 19237100 |
| Tetramethylbenzidine | 1520860 | 6051990 | 1005620 | 1507530 | 6050120 | 972035.2017 |
| Tetramethylbenzidine | 1621030 | 5962580 | 1018130 | 1629050 | 5981870 | 1196920 |
| Tetramethylbenzidine | 1638950 | 6304710 | 901313.882 | 1666980 | 6048750 | 1005620 |
| Tetramethylbenzidine | 1694570 | 6145490 | 1573940 | 1737030 | 4616090 | 1057190 |
| 4,4'-Dichlorobiphenyl | 1032410 | 5595980 | 1235560 | 1047250 | 5872250 | 1224060 |
| 4,4'-Dichlorobiphenyl | 1029590 | 5505390 | 1057460 | 1021190 | 5643030 | 1168530 |
| 4,4'-Dichlorobiphenyl | 1052180 | 5751210 | 1196530 | 1106760 | 5842740 | 1174750 |
| 4,4'-Dichlorobiphenyl | 1094530 | 5591980 | 1200720 | 1113730 | 5894820 | 1317250 |
| PCB 209 | 453048.1818 | 6215530 | 1348670 | 425377.2386 | 6065550 | 1241850 |
| PCB 209 | 465323.4285 | 6228530 | 1323530 | 418902.5815 | 6226550 | 1266380 |
| PCB 209 | 472454.3332 | 6011080 | 1380230 | 455185.4721 | 5822230 | 1821660 |
| PCB 209 | 418976.8646 | 6095100 | 1285890 | 435157.7603 | 6233700 | 1324280 |
| PCB 29 | 531875.0924 | 5895110 | 873247.0627 | 547290.0987 | 5820520 | 858283.8289 |
| PCB 29 | 561504.8833 | 5983200 | 884011.5299 | 498319.8173 | 5781790 | 858396.816 |
| PCB 29 | 581818.1567 | 5947780 | 889432.5626 | 513385.6741 | 5848900 | 841238.0276 |
| PCB 29 | 555030.4344 | 5817370 | 909945.7993 | 534392.9553 | 5971290 | 929443.2662 |
| Benzo[*b*]fluroanthene | 15028200 | 11584400 | 44323100 | 15313900 | 11959500 | 42064300 |
| Benzo[*b*]fluroanthene | 14658700 | 11704300 | 43608500 | 14782800 | 11409300 | 40213100 |
| Benzo[*b*]fluroanthene | 14204900 | 11868800 | 42615900 | 14883100 | 10798300 | 43469800 |

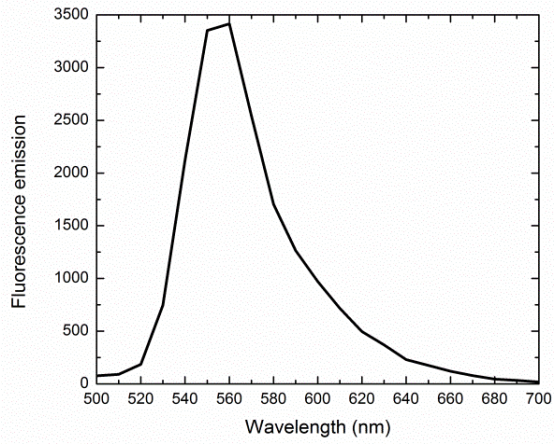
| | | | | | | |
|---|---|---|---|---|---|---|
| Benzo[*b*]fluroanthene | 14641200 | 11952100 | 43943200 | 14748900 | 10718900 | 50475500 |
| Deldrin | 1420940 | 4018030 | 5019670 | 1511320 | 3876690 | 5263270 |
| Deldrin | 1417390 | 4101580 | 5391480 | 1467690 | 3823220 | 5413300 |
| Deldrin | 1427990 | 3922020 | 5246670 | 1174600 | 4118590 | 5618500 |
| Deldrin | 1481490 | 3804410 | 5922460 | 1364000 | 4051710 | 5914470 |
| Hexabromobenzene | 1226440 | 4624300 | 3967040 | 1141920 | 4595150 | 4079280 |
| Hexabromobenzene | 1317660 | 4497900 | 4034300 | 1233090 | 4479410 | 4201520 |
| Hexabromobenzene | 1205930 | 4481260 | 4037890 | 1164920 | 4579230 | 4374870 |
| Hexabromobenzene | 1240100 | 4560780 | 4214460 | 1155290 | 4499770 | 4863190 |
| PCB 77 | 839704.8676 | 2385080 | 1695620 | 708245.2612 | 2582700 | 1312410 |
| PCB 77 | 752580.4947 | 2412310 | 1328760 | 793938.1268 | 2466290 | 825571.5808 |
| PCB 77 | 847562.3788 | 2373710 | 870507.7246 | 756997.1851 | 2489550 | 698702.8582 |
| PCB 77 | 753622.9896 | 2390630 | 1147010 | 695711.5765 | 2564760 | 728611.2761 |
| Fluorene | 1929270 | 3920640 | 2397860 | 1712520 | 4043990 | 2183210 |
| Fluorene | 2041240 | 3934310 | 2354073 | 1628840 | 4249530 | 1375090 |
| Fluorene | 1959650 | 3918550 | 2295910 | 1720450 | 4172670 | 1510360 |
| Fluorene | 1986020 | 3995590 | 1315300 | 1780330 | 4157860 | 1428680 |
| Tamoxifen | 398750.892 | 2979600 | 673227.4786 | 504065.9217 | 3099830 | 668913.8956 |
| Tamoxifen | 350659.0438 | 2875130 | 666478.4343 | 503315.9529 | 3128320 | 622361.4476 |
| Tamoxifen | 362062.5407 | 2825900 | 651469.0481 | 440452.5467 | 3154710 | 684194.4508 |
| Tamoxifen | 376278.625 | 3054260 | 693753.737 | 435331.8377 | 3138070 | 632823.8573 |
| 2-Acetylaminofluorene | 7918440 | 1458300 | 10738000 | 10241600 | 1333740 | 39288100 |
| 2-Acetylaminofluorene | 6503530 | 1482600 | 10159300 | 10700200 | 1409470 | 13209700 |
| 2-Acetylaminofluorene | 5496760 | 1546390 | 11974600 | 7817160 | 1476840 | 14139600 |
| 2-Acetylaminofluorene | 5339970 | 1566620 | 12276800 | 6216200 | 1438910 | 14806300 |
| Deltamethrin | 1258470 | 2448830 | 1501340 | 1698110 | 2615940 | 1531940 |
| Deltamethrin | 1397070 | 2508850 | 1557710 | 1726650 | 2797710 | 1681840 |
| Deltamethrin | 1362940 | 2495350 | 1584280 | 1686410 | 2615400 | 1454640 |
| Deltamethrin | 1143880 | 2505770 | 1486960 | 1899690 | 2587410 | 1400020 |
| Quinizarin | 1434650 | 3323740 | 412845.2934 | 1406390 | 2807450 | 336652.3436 |
| Quinizarin | 1346530 | 3256000 | 362591.0776 | 673941.8402 | 2873090 | 372959.104 |
| Quinizarin | 1442520 | 3338080 | 453065.5186 | 1372640 | 2926220 | 369444.6492 |
| Quinizarin | 1372830 | 3063820 | 358199.4948 | 1426810 | 3061840 | 333778.2161 |

# FLUORESCENCE EMISSION GRAPHS FOR BUFFER ARRAY

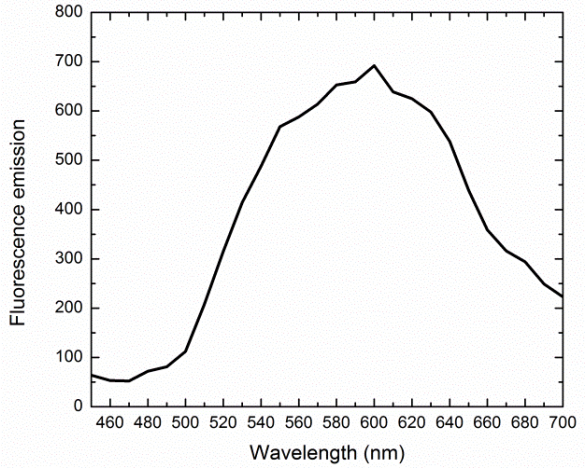
Analyte **1** – Fluorophore **31**



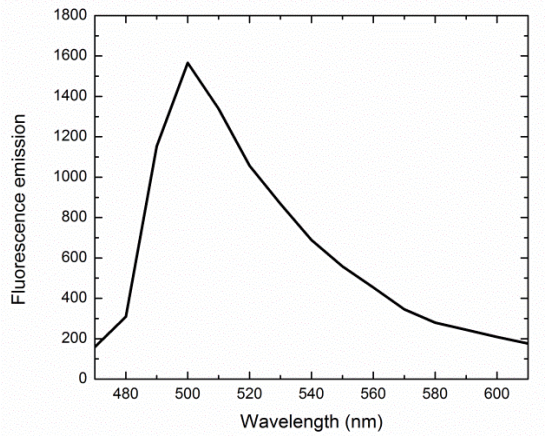

Analyte **1** – Fluorophore **32**



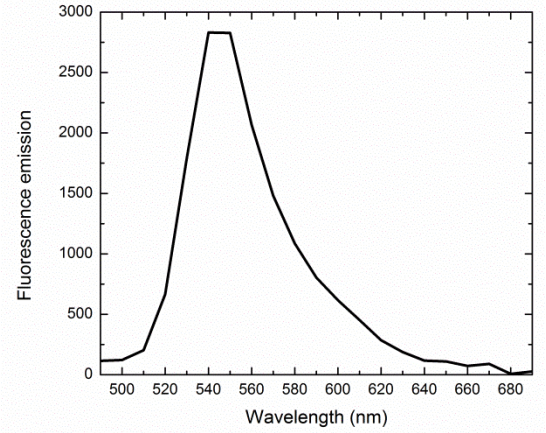

Analyte **1** – Fluorophore **33**



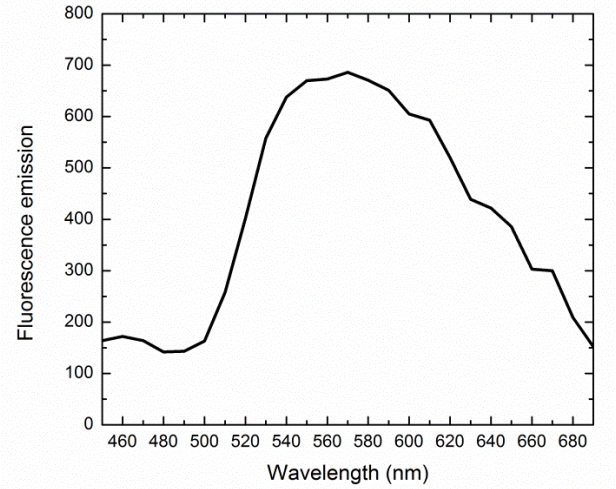
Analyte **2** – Fluorophore **31**



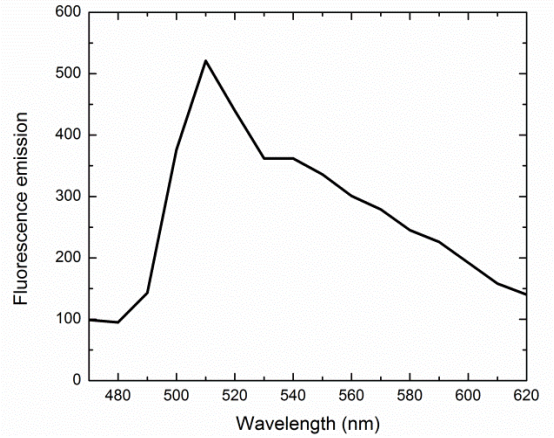

Analyte **2** – Fluorophore **32**



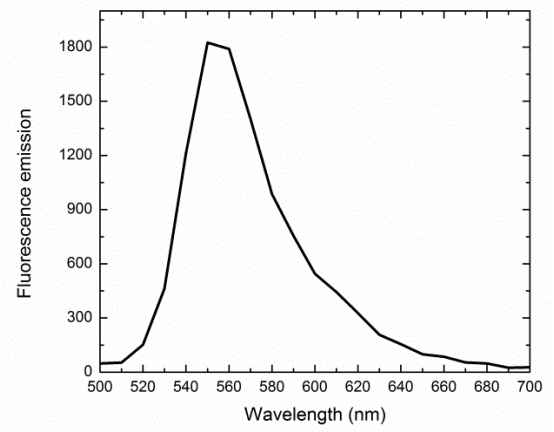

Analyte **2** – Fluorophore **33**



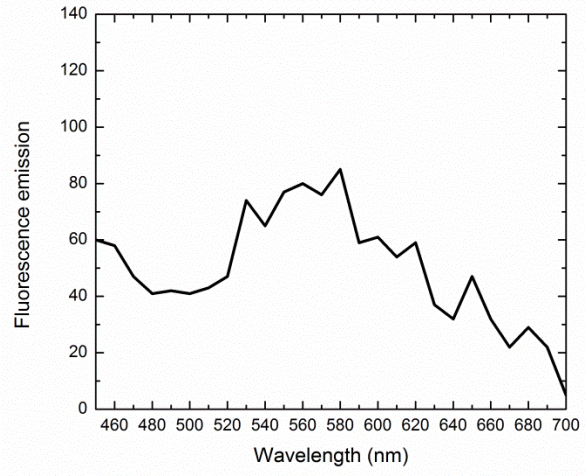
Analyte **3** – Fluorophore **31**



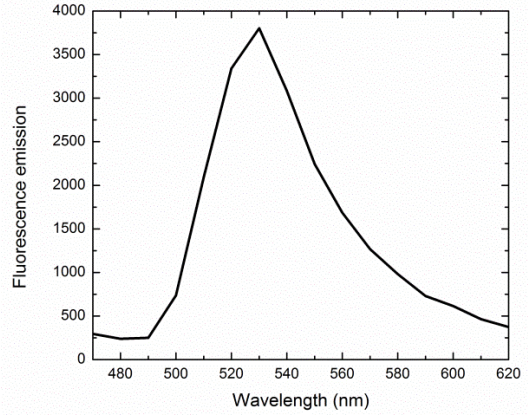

Analyte **3** – Fluorophore **32**



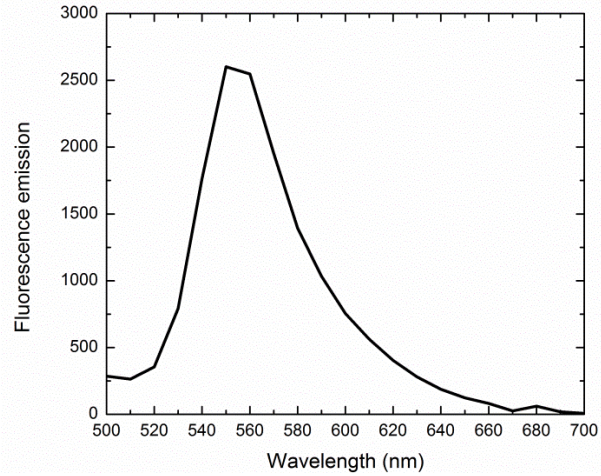

Analyte **3** – Fluorophore **33**



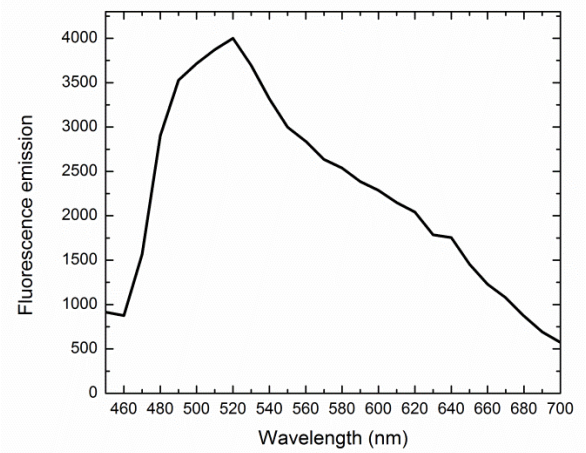
Analyte **4**- Fluorophore **31**



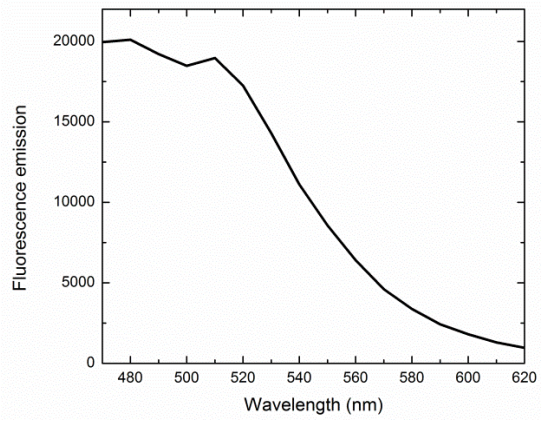

Analyte **4** – Fluorophore **32**



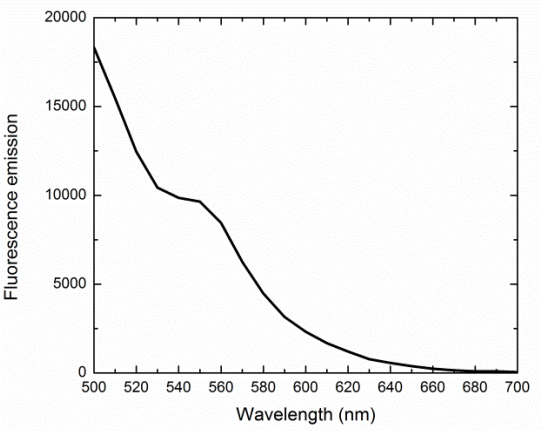

Analyte **4** – Fluorophore **33**



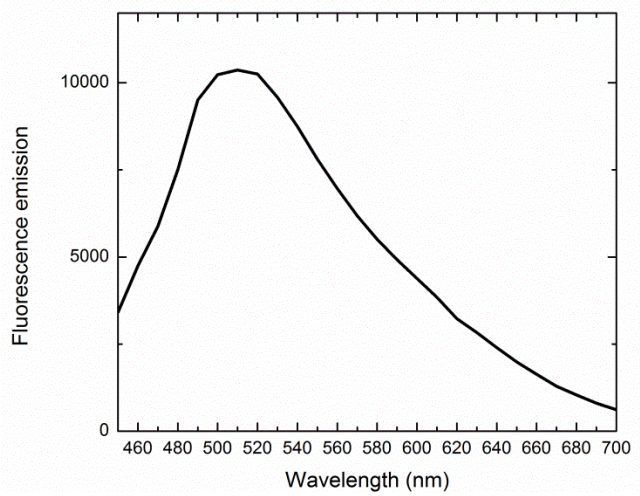
Analyte **5**- Fluorophore **31**



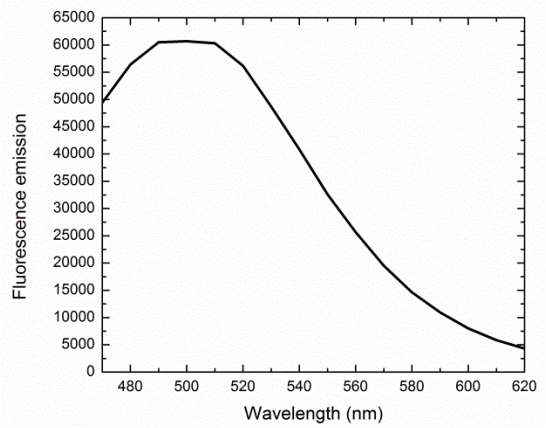

Analyte **5** – Fluorophore **32**



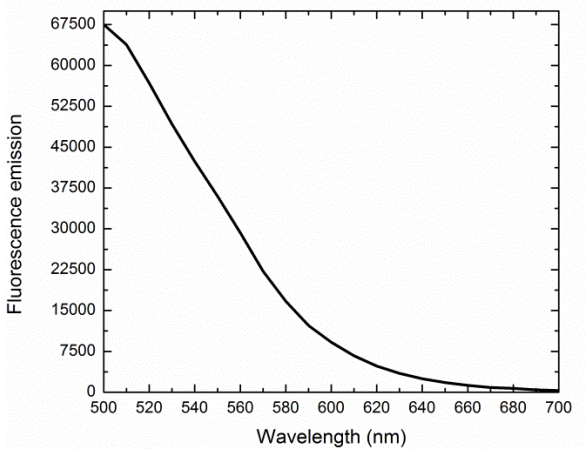

Analyte **5** – Fluorophore **33**



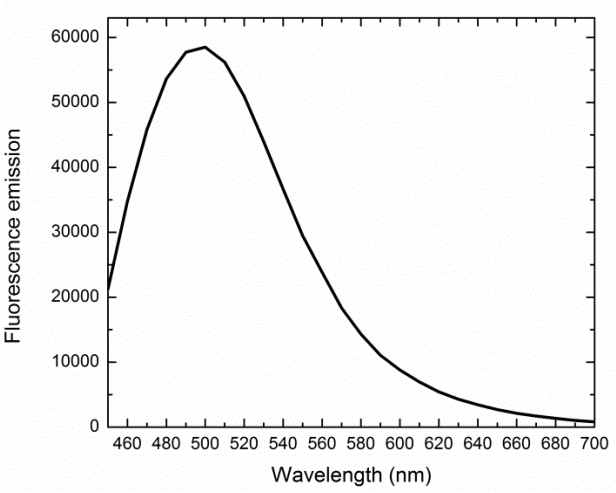
Analyte **6** – Fluorophore **31**



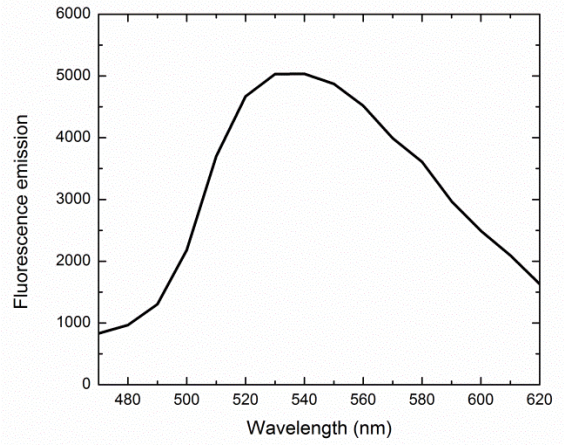

Analyte **6** – Fluorophore **32**



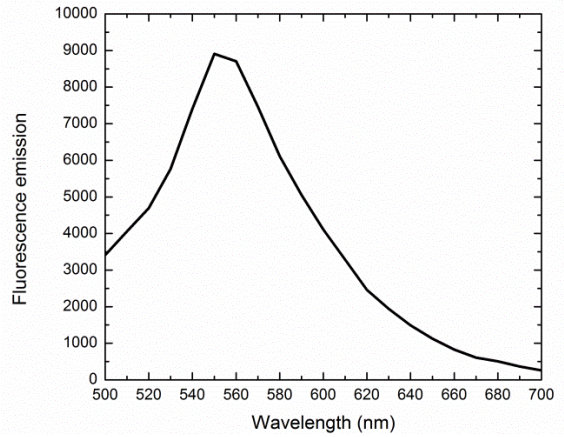

Analyte **6** – Fluorophore **33**



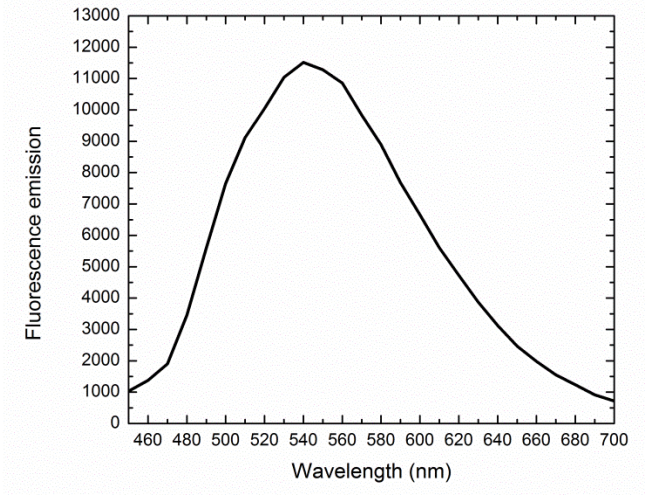
Analyte **7** – Fluorophore **31**



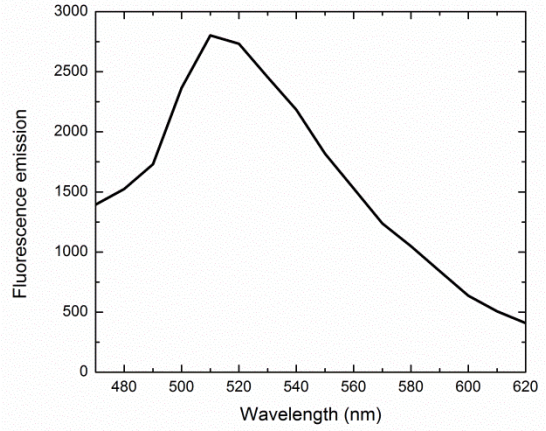

Analyte **7** – Fluorophore **32**



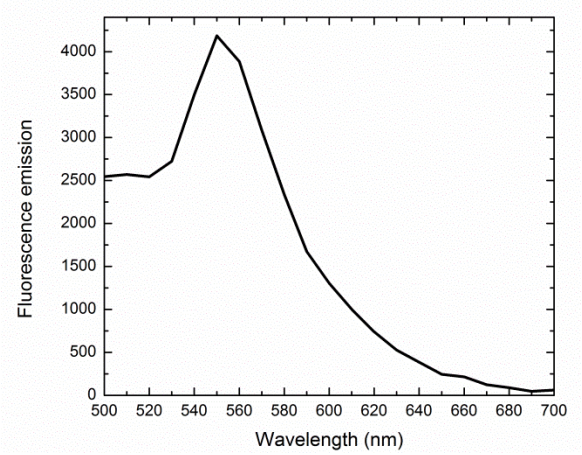

Analyte **7** – Fluorophore **33**



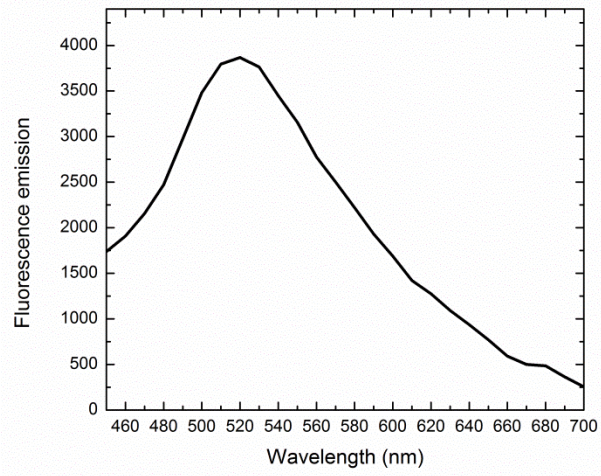
Analyte **8** – Fluorophore **31**



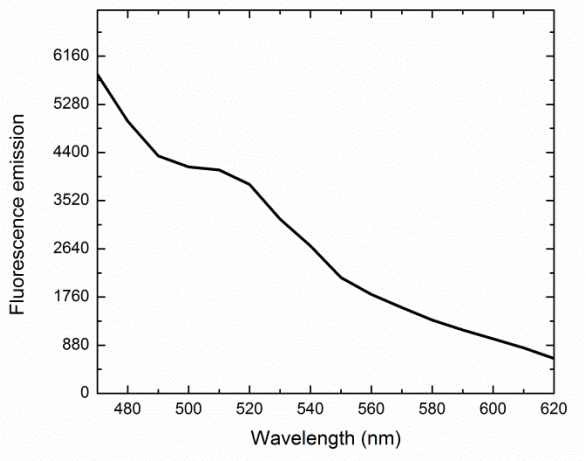

Analyte **8** – Fluorophore **32**



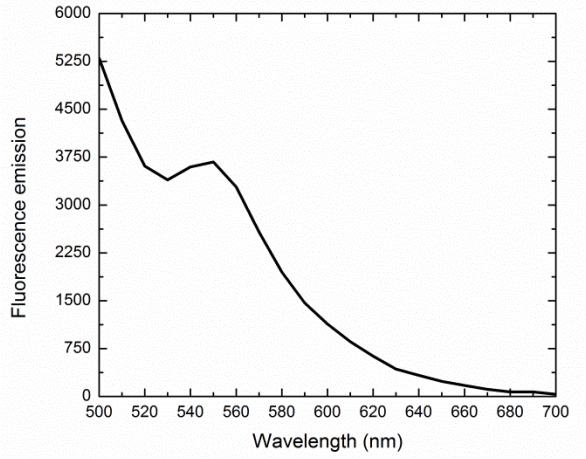

Analyte **8** – Fluorophore **33**



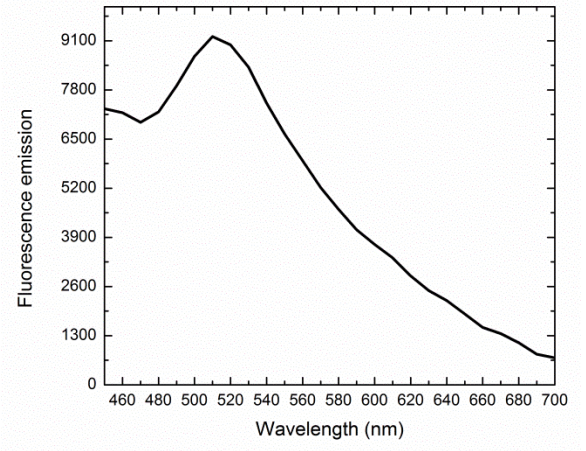
Analyte **9** – Fluorophore **31**



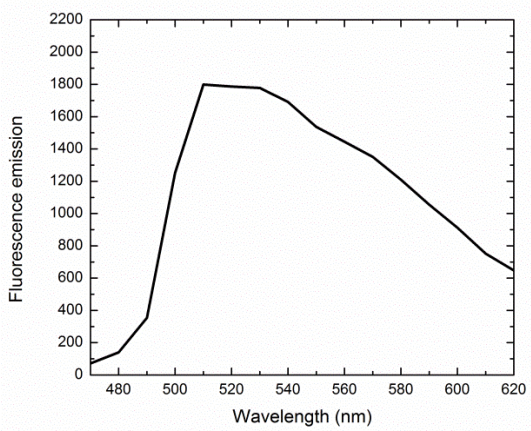

Analyte **9** – Fluorophore **32**



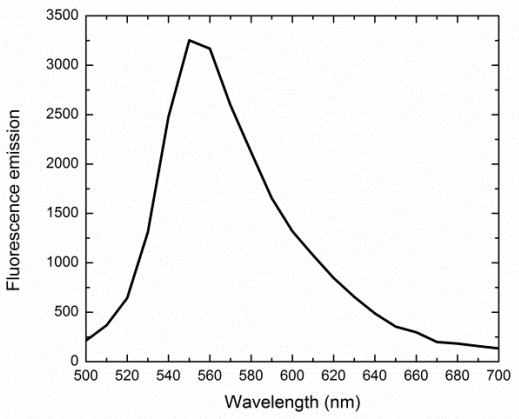

Analyte **9** – Fluorophore **33**



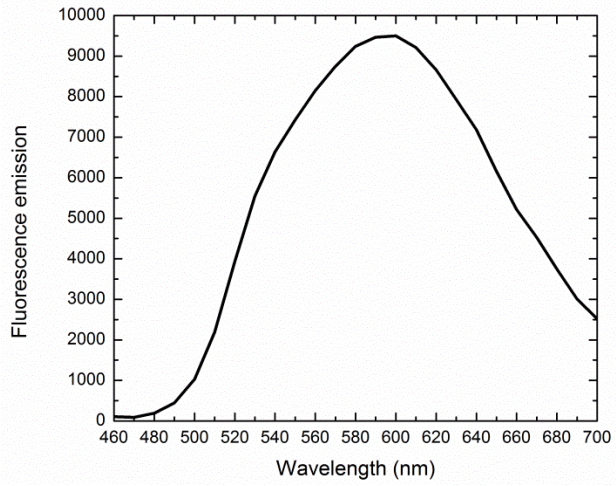
Analyte **10** – Fluorophore **31**



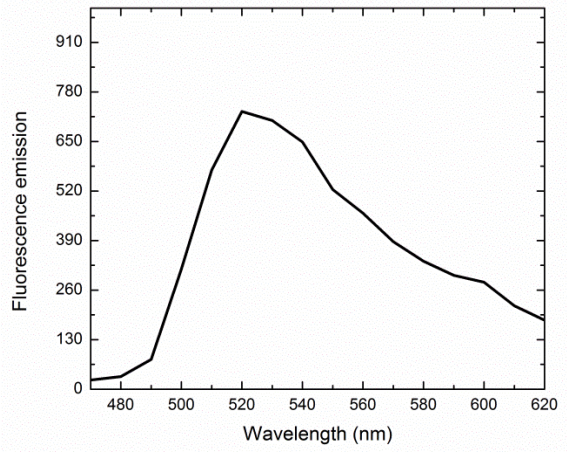

Analyte **10** – Fluorophore **32**



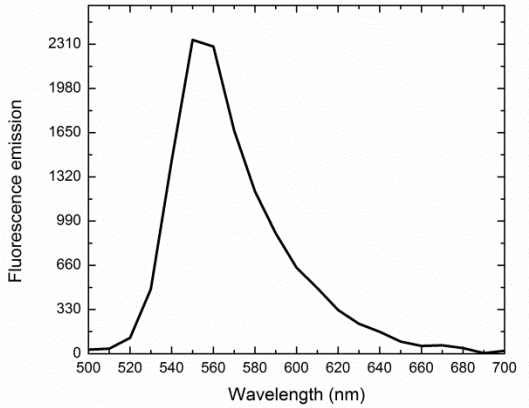

Analyte **10** – Fluorophore **33**



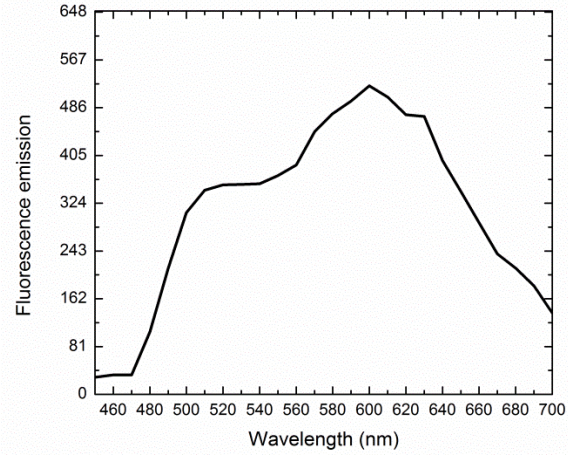
Analyte **11** – Fluorophore **31**



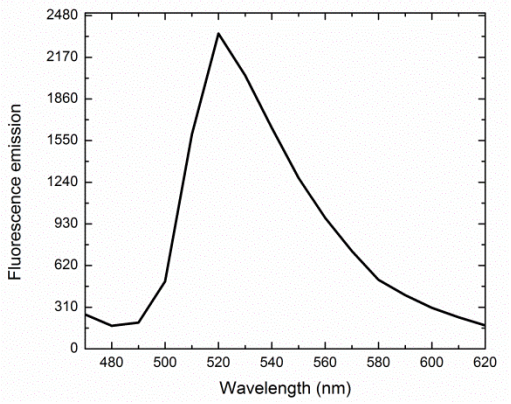

Analyte **11** – Fluorophore **32**



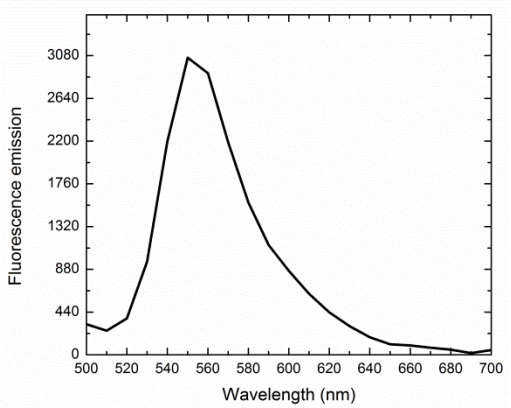

Analyte **11** – Fluorophore **33**



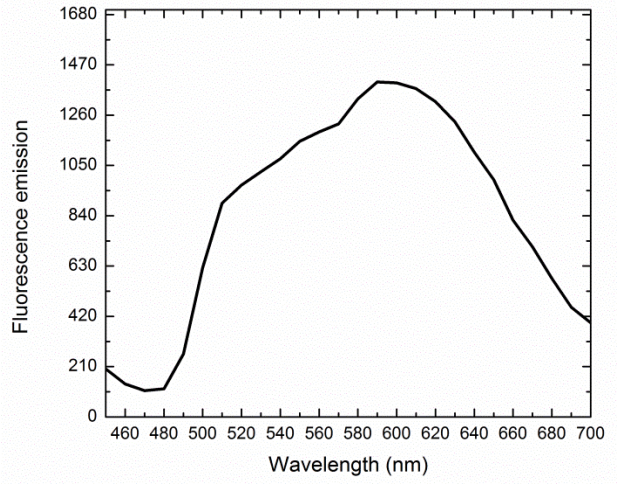
Analyte **12** – Fluorophore **31**



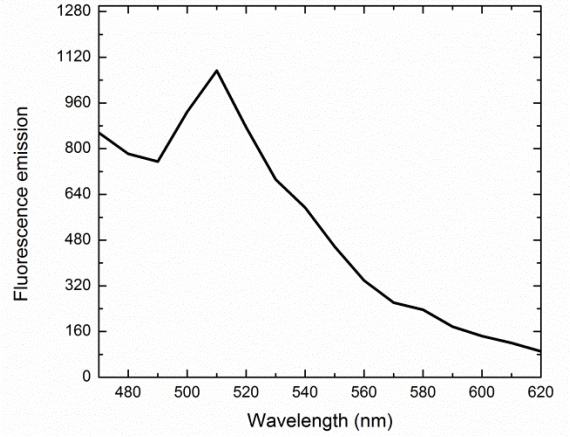

Analyte **12** – Fluorophore **32**



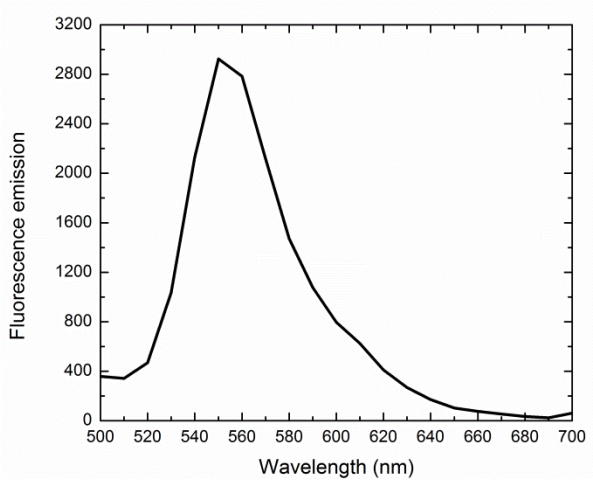

Analyte **12** – Fluorophore **33**



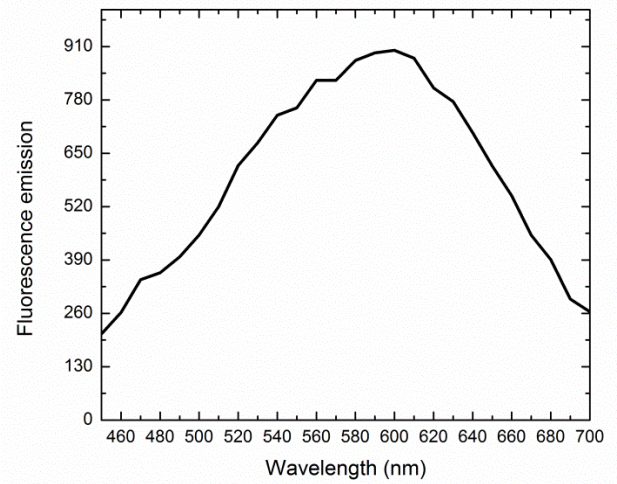
Analyte **13** – Fluorophore **31**



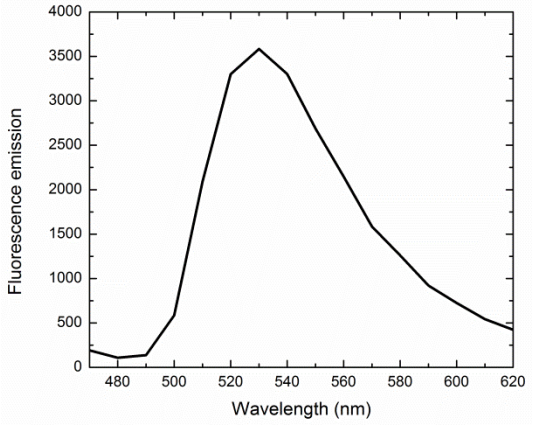

Analyte **13** – Fluorophore **32**



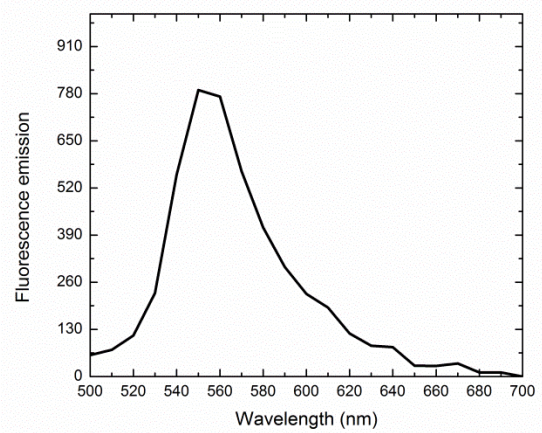

Analyte **13** – Fluorophore **33**



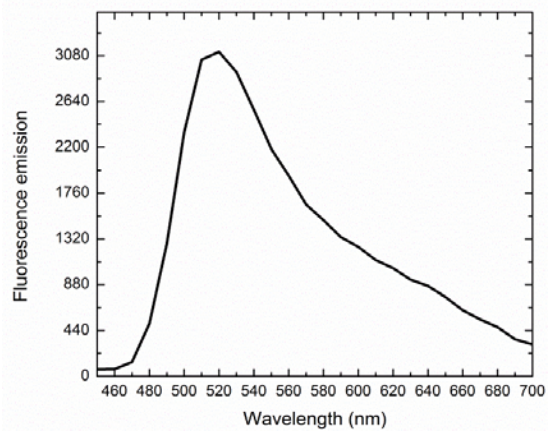
Analyte **14** – Fluorophore **31**



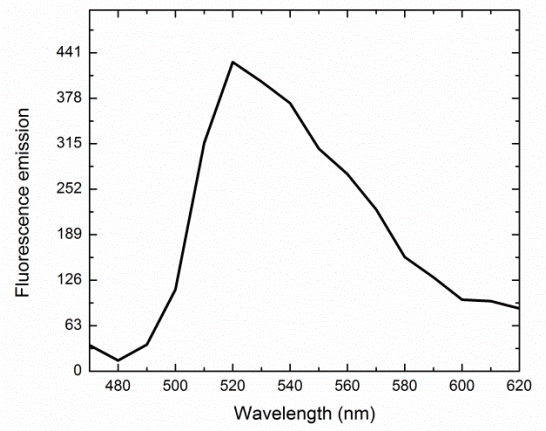

Analyte **14** – Fluorophore **32**



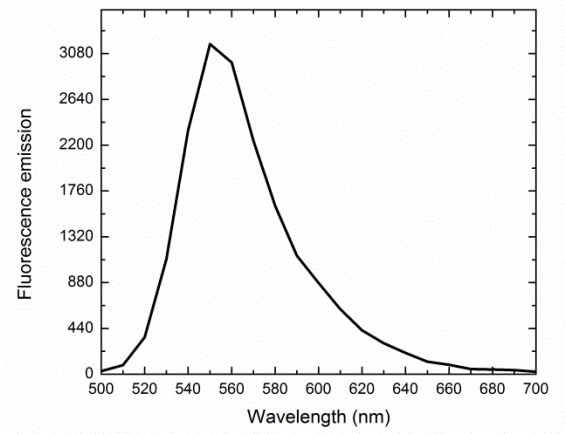

Analyte **14** – Fluorophore **33**



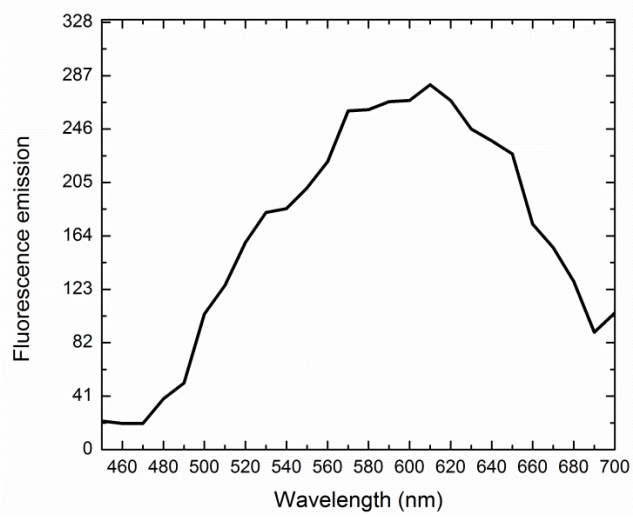
Analyte **15** – Fluorophore **31**



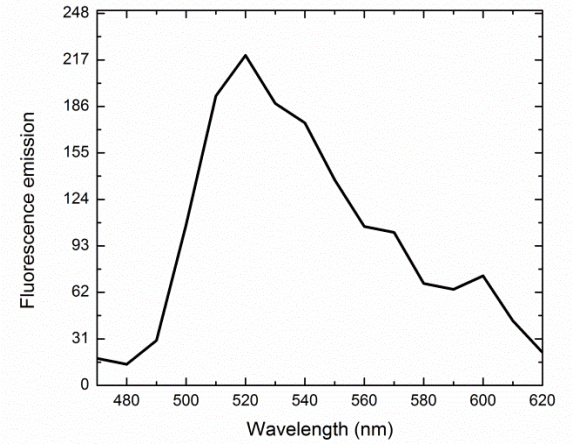

Analyte **15** – Fluorophore **32**



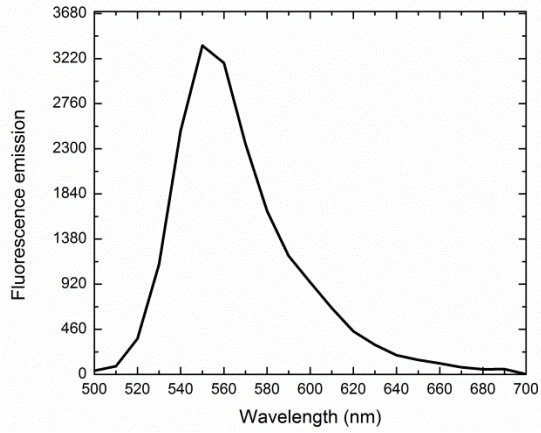

Analyte **15** – Fluorophore **33**



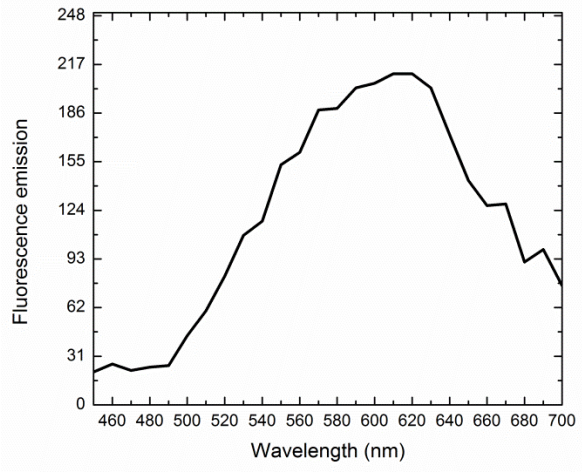
Analyte **16** – Fluorophore **31**



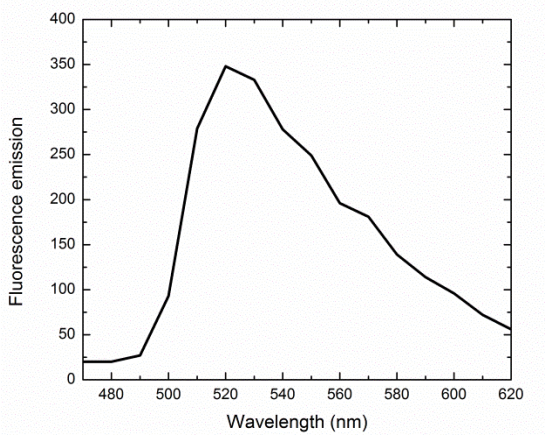

Analyte **16** – Fluorophore **32**



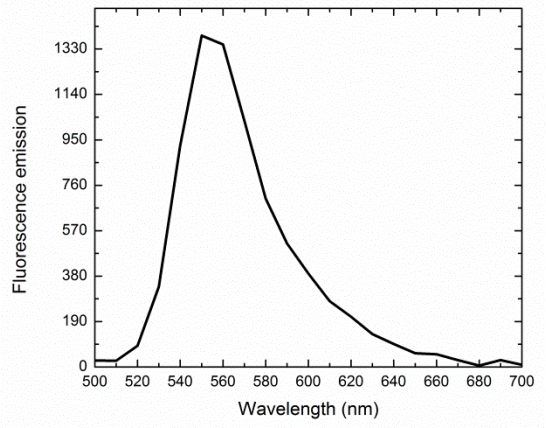

Analyte **16** – Fluorophore **33**



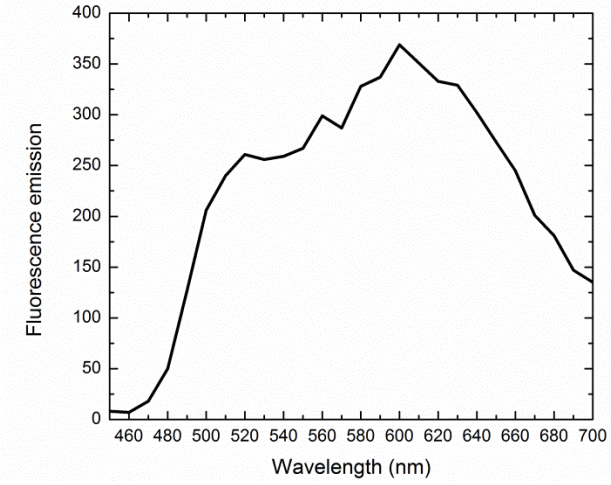
Analyte **17** – Fluorophore **31**



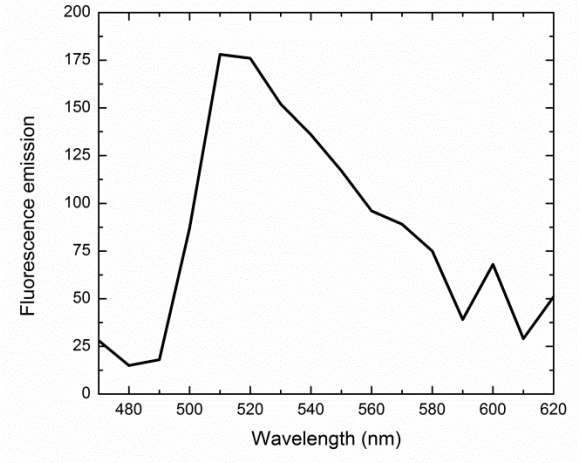

Analyte **17** – Fluorophore **32**



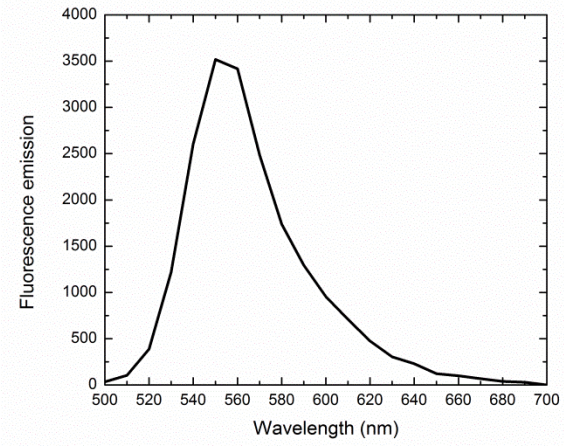

Analyte **17** – Fluorophore **33**



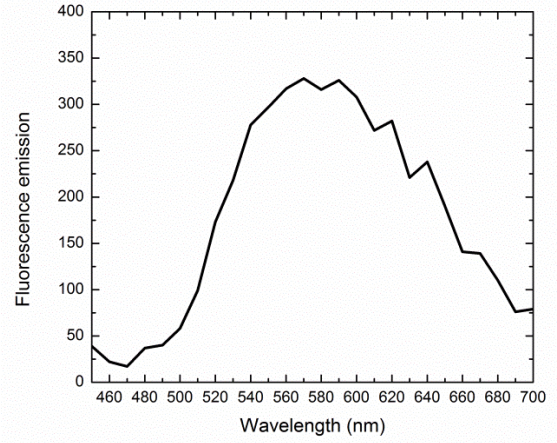
Analyte **18** – Fluorophore **31**



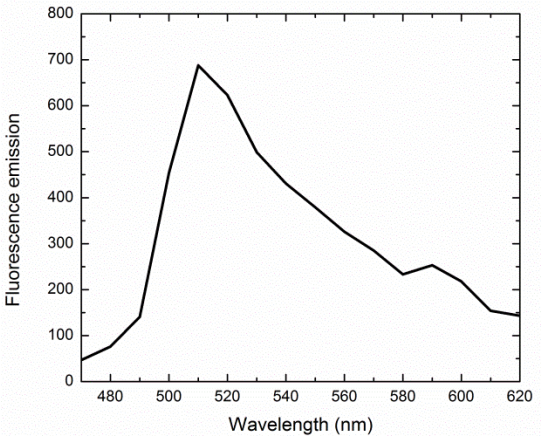

Analyte **18** – Fluorophore **32**



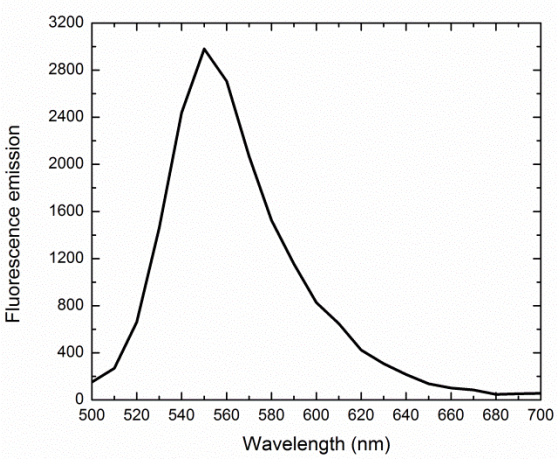

Analyte **18** – Fluorophore **33**



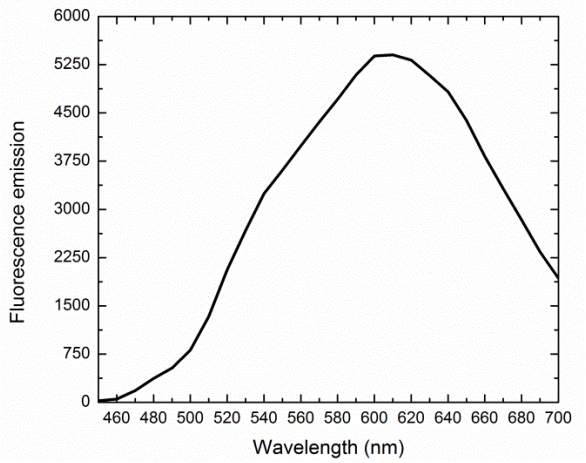
Analyte **19** – Fluorophore **31**



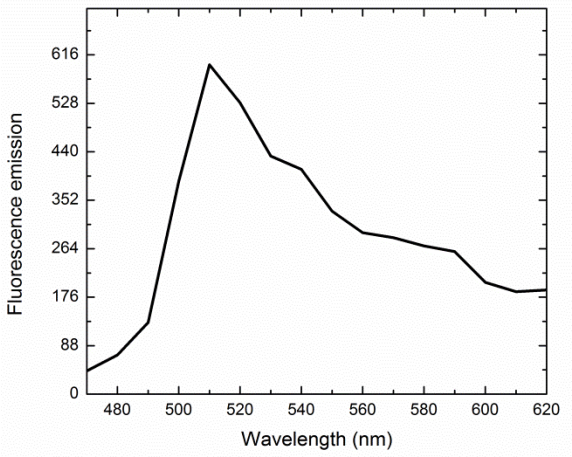

Analyte **19** – Fluorophore **32**



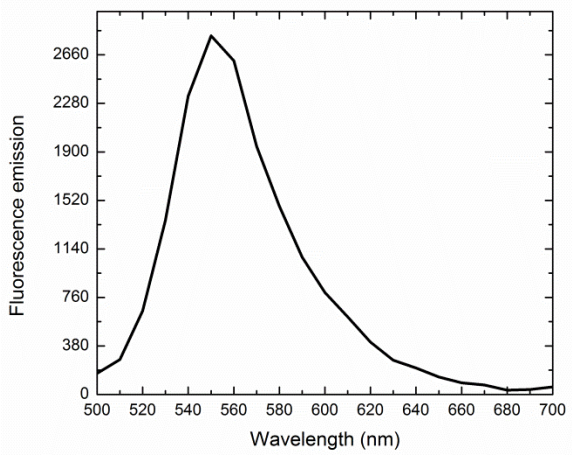

Analyte **19** – Fluorophore **33**



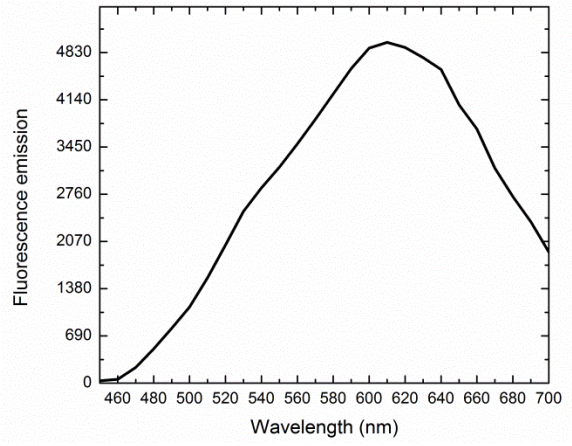
Analyte **20** – Fluorophore **31**



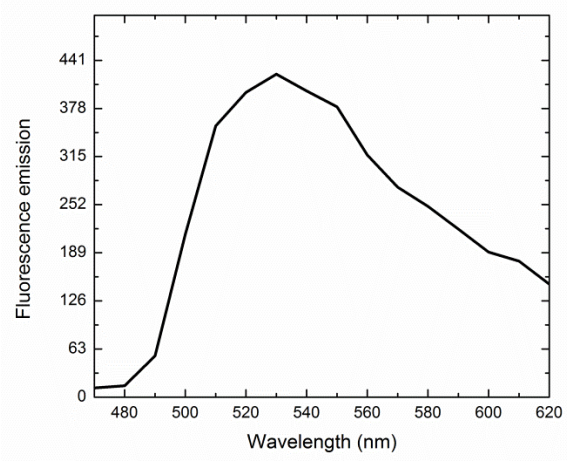

Analyte **20** – Fluorophore **32**



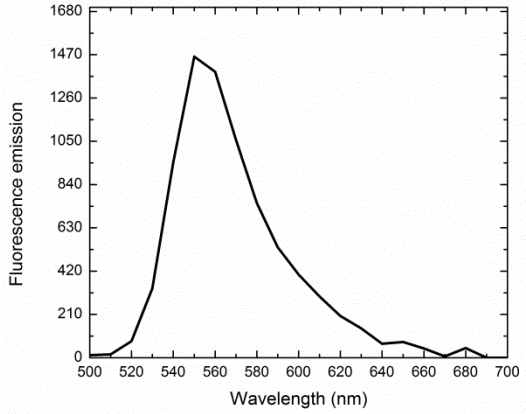

Analyte **20** – Fluorophore **33**



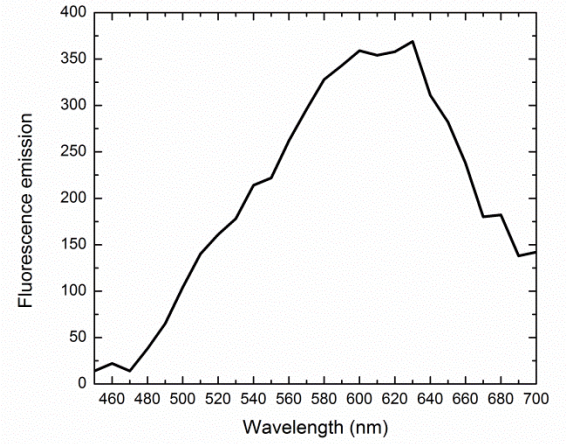
Analyte **21** – Fluorophore **31**



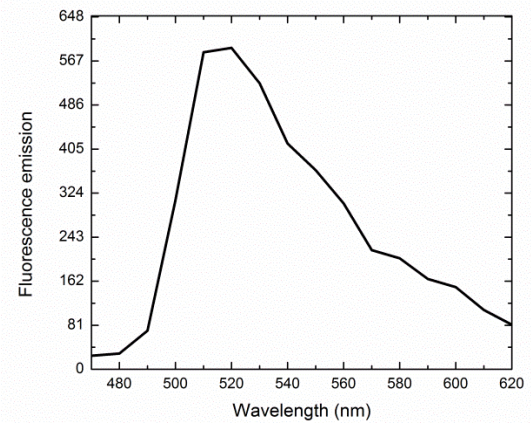

Analyte **21** – Fluorophore **32**



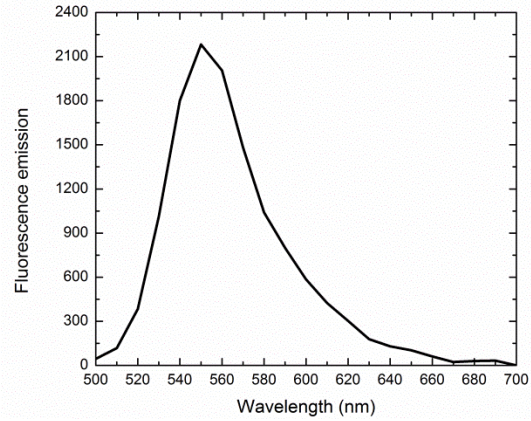

Analyte **21** – Fluorophore **33**



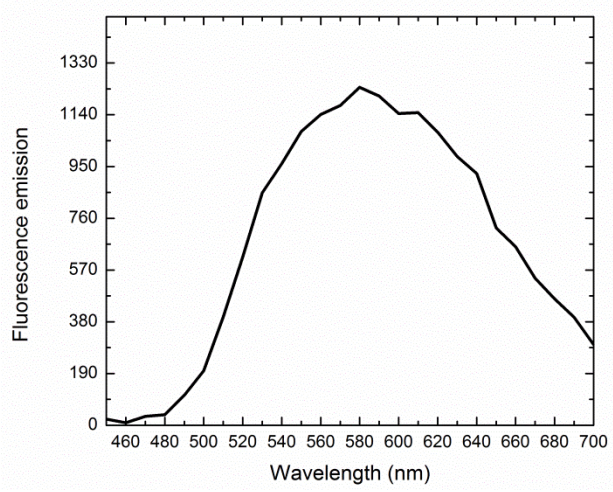
Analyte **22** – Fluorophore **31**



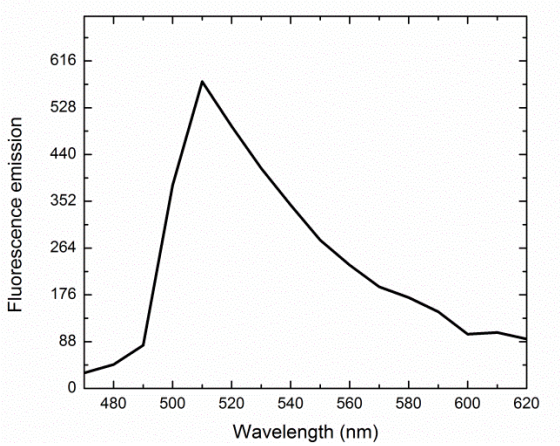

Analyte **22** – Fluorophore **32**



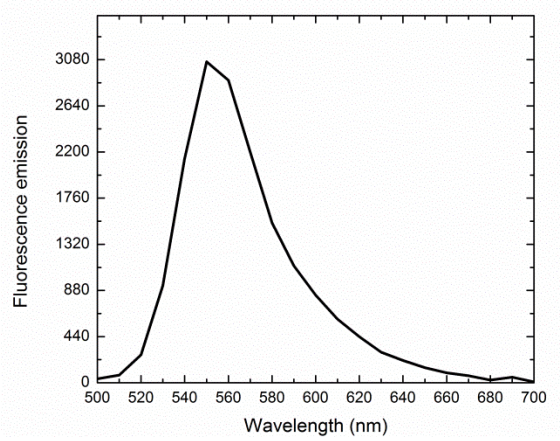

Analyte **22** – Fluorophore **33**



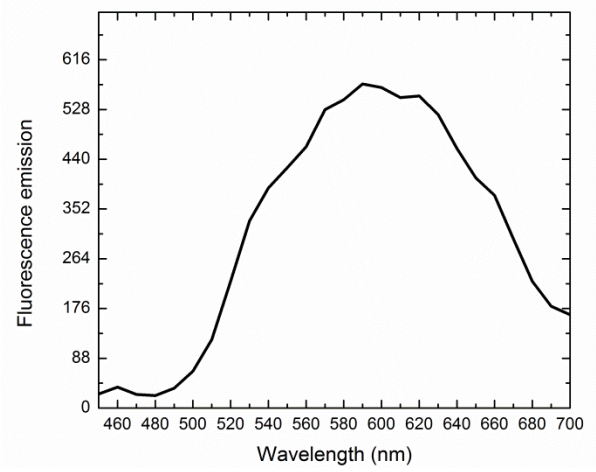
Analyte **23** – Fluorophore **31**



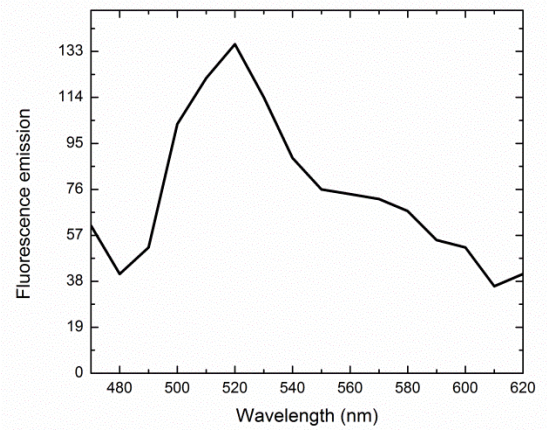

Analyte **23** – Fluorophore **32**



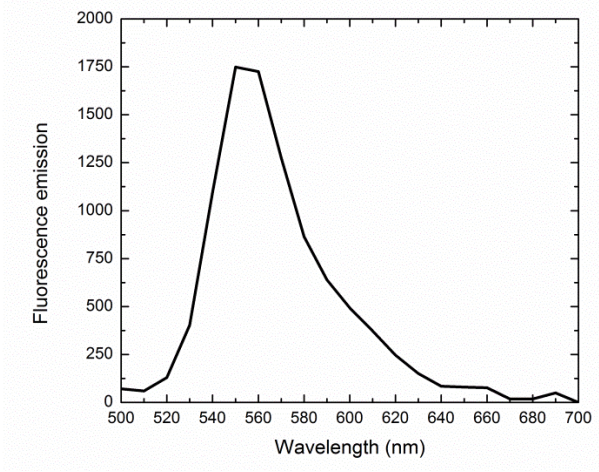

Analyte **23** – Fluorophore **33**



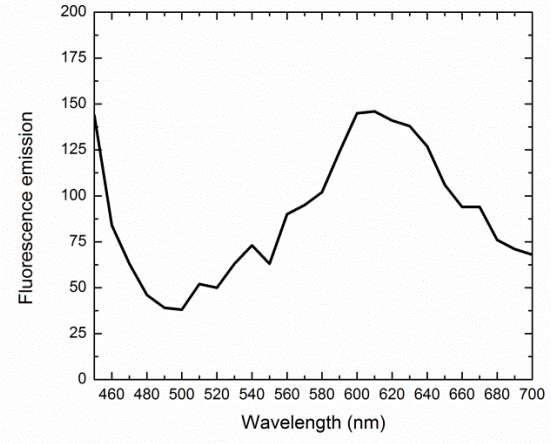
Analyte **24** – Fluorophore **31**



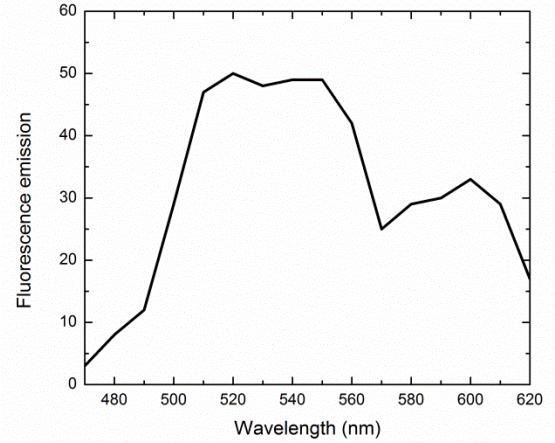

Analyte **24** – Fluorophore **32**



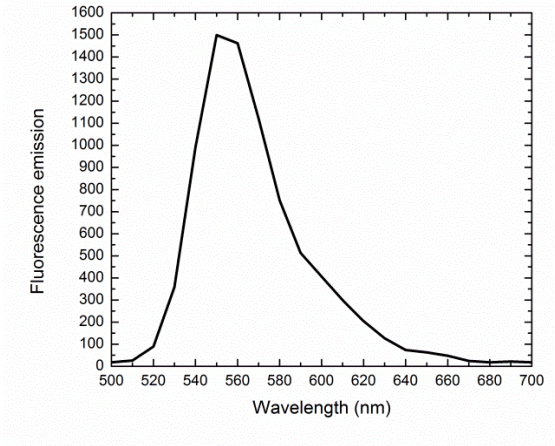

Analyte **24** – Fluorophore **33**



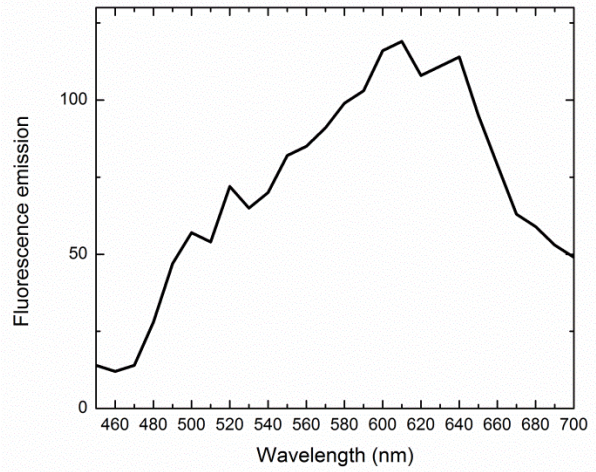
Analyte **25** – Fluorophore **31**



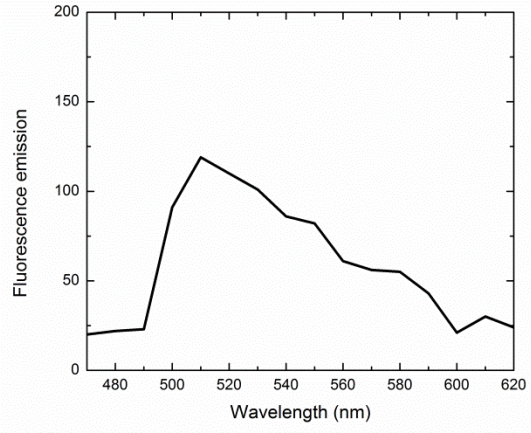

Analyte **25** – Fluorophore **32**



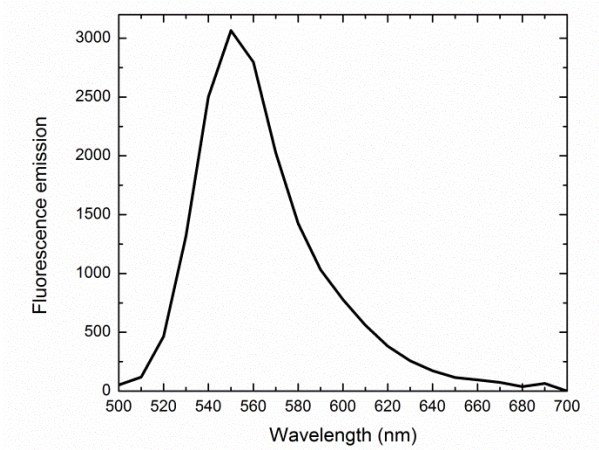

Analyte **25** – Fluorophore **33**



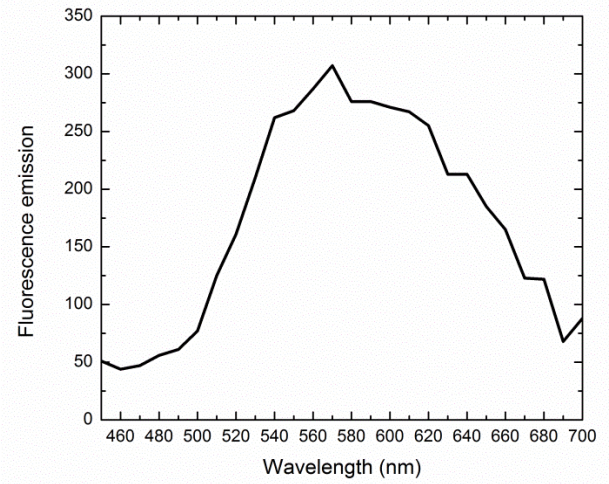
Analyte **26** – Fluorophore **31**



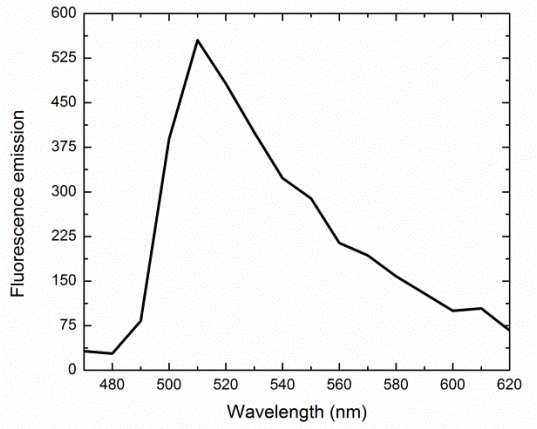

Analyte **26** – Fluorophore **32**



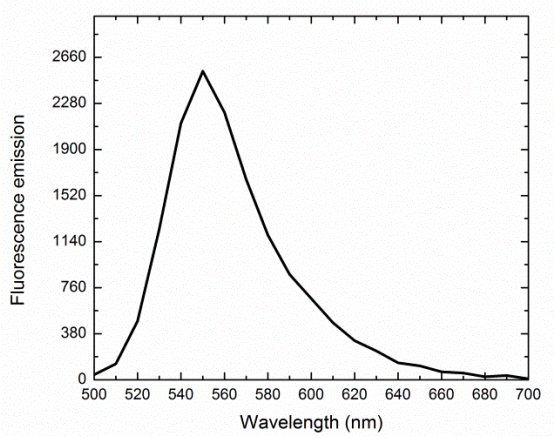

Analyte **26** – Fluorophore **33**



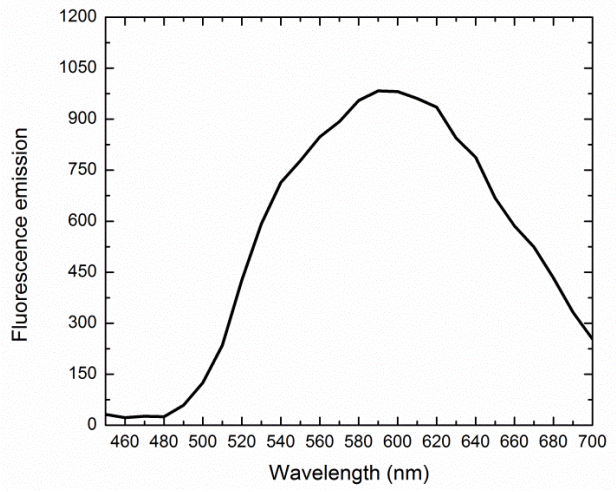
Analyte **27** – Fluorophore **31**



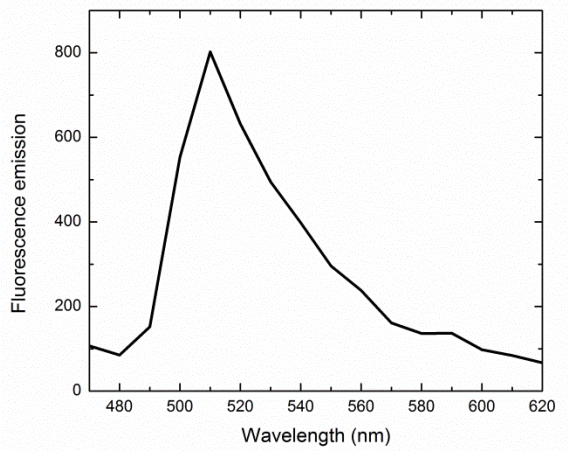

Analyte **27** – Fluorophore **32**



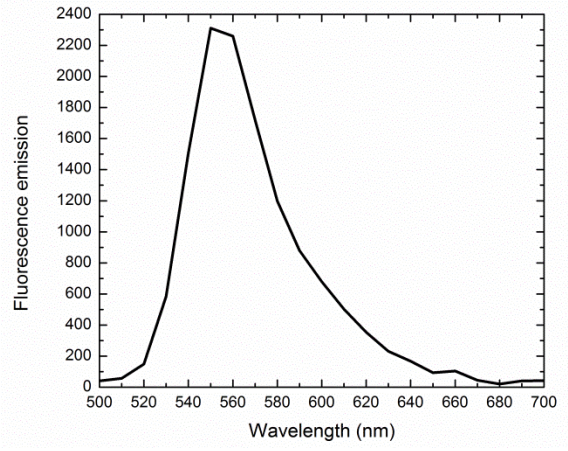

Analyte **27** – Fluorophore **33**



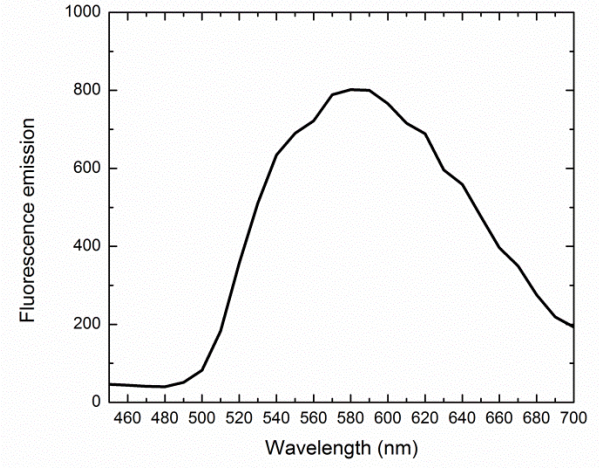
Analyte **28** – Fluorophore **31**



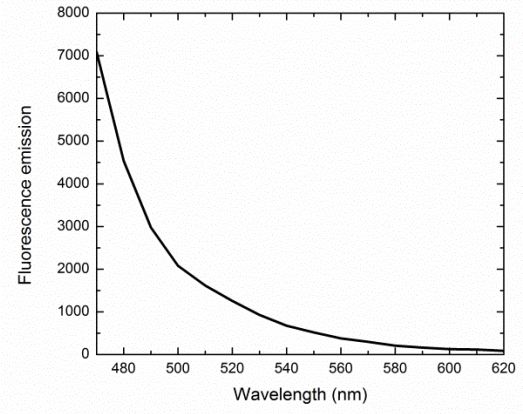

Analyte **28** – Fluorophore **32**



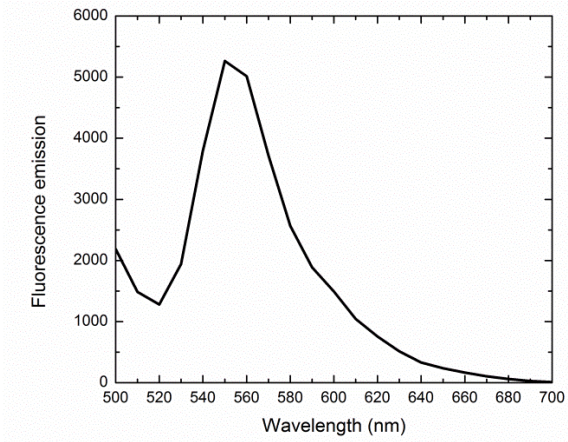

Analyte **28** – Fluorophore **33**



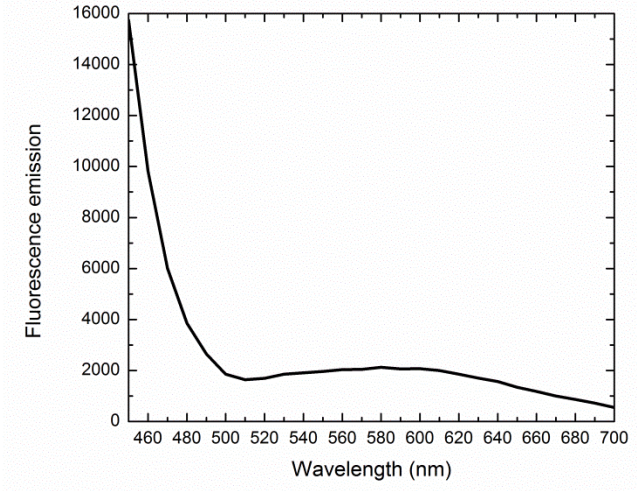
Analyte **29** – Fluorophore **31**



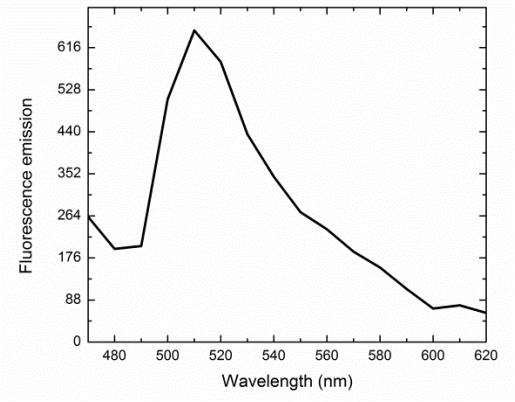

Analyte **29** – Fluorophore **32**



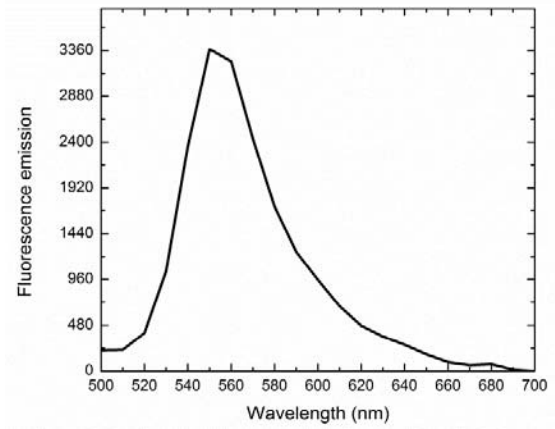

Analyte **29** – Fluorophore **33**



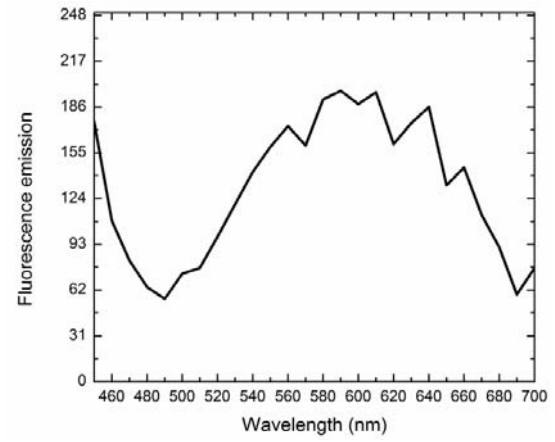
Analyte **30** – Fluorophore **31**




Analyte **30** – Fluorophore **32**




Analyte **30** – Fluorophore **33**



# CONTROL EXPERIMENTS PROCEDURE

## CONTROL 1: Blanks

*General Procedure – Sample Preparation*

Two samples were prepared for each fluorophore: one served as the sample for the training set, and the other served as the unknown. For each sample, 2.5 mL of 10 mM γ-cyclodextrin and 100 μL of fluorophore were added to a vial and vigorously shaken by hand for approximately 30 seconds. The sample remained on a rotary mixer until use to ensure thorough mixing. A 96 well microplate was used, and into each well was pipetted 100 μL of the sample solution, and each solution was repeated four times (*i.e.* each solution was pipetted into four separate wells) to ensure data reproducibility.

*General Procedure – Fluorescence Studies*

A BioTek Synergy Mx Multi-Mode Microplate Reader was used to generate the fluorescence data for the array. The samples were excited at one of four excitation wavelengths: 250, 300, 360, and 400 nm. The emission of each was recorded as follows: (a) Fluorophore **31** samples: 470-620 nm; (b) Fluorophore **32** samples: 500-700 nm; (c) Fluorophore **33** samples: 450-700 nm. The fluorescence emission was integrated with respect to wavenumber using OriginPro software.

## CONTROL 2: 0 mM γ-Cyclodextrin

*General Procedure – Sample Preparation*

Two samples were prepared for each analyte-fluorophore combination: one served as the sample for the training set, and the other served as the unknown. For each sample, 2.5 mL of 0 mM γ-cyclodextrin (pure PBS), 20 μL of analyte, and 100 μL of fluorophore were added to a vial and vigorously shaken by hand for approximately 30 seconds. The sample remained on a rotary mixer until use to ensure thorough mixing. A 96W microplate was used, and into each well was pipetted 100 μL of the sample solution, and each solution was repeated four times (*ie* each solution was pipetted into four separate wells) to ensure data reproducibility.

*General Procedure – Fluorescence Studies*

A BioTek Synergy Mx Multi-Mode Microplate Reader was used to generate the fluorescence data for the array. The samples were excited at the excitation of the analyte (see Table S1). The emission of each was recorded: (a) Fluorophore **31** samples: 470-620 nm; (b) Fluorophore **32** samples: 500-700 nm; (c) Fluorophore **33** samples: 450-700 nm. The fluorescence emission was integrated with respect to wavenumber using OriginPro software.

# CONTROL EXPERIMENTS INTEGRATIONS

CONTROL 1: Blanks

| Knowns | | | | Unknowns | | |
|---|---|---|---|---|---|---|
| Wavelength | Bodipy | Rhodamine | Coumarin 6 | Bodipy | Rhodamine | Coumarin 6 |
| 250 | 372296.3208 | 8005010 | 1088930 | 624669.4718 | 6028250 | 985322.4188 |
| 250 | 364274.9589 | 7175490 | 1059720 | 602870.012 | 5677540 | 987655.7596 |
| 250 | 389946.2043 | 7425510 | 991672.0112 | 609527.6932 | 6113680 | 1075740 |
| 250 | 369808.7176 | 7461030 | 1091510 | 609505.1152 | 6017940 | 904644.4853 |
| 300 | 2080150 | 16260800 | 6851360 | 6308020 | 12133500 | 6421880 |
| 300 | 2137460 | 14574700 | 6765780 | 6063120 | 11466800 | 6344850 |
| 300 | 2092890 | 14963700 | 6644190 | 6168140 | 12274900 | 6825700 |
| 300 | 2086280 | 15069800 | 7067660 | 6195200 | 11972100 | 6253280 |
| 360 | 2718670 | 11550600 | 4378570 | 3577090 | 8504470 | 3317110 |
| 360 | 2830390 | 10505500 | 2679090 | 3577580 | 8171070 | 3413320 |
| 360 | 2813720 | 10554200 | 2781460 | 3646400 | 8720680 | 3533840 |
| 360 | 2819660 | 10807800 | 3152400 | 8504470 | 8511800 | 2481550 |
| 400 | 1307740 | 5863200 | 17172000 | 1720830 | 4417480 | 18434700 |
| 400 | 1360190 | 5366240 | 16453800 | 1679840 | 4294770 | 19928500 |
| 400 | 1362280 | 5449980 | 16616700 | 1678630 | 4536020 | 20285300 |
| 400 | 1341170 | 5476460 | 19066200 | 1720680 | 4429490 | 16203200 |

**Table S6.** Integration values for the training set ("Knowns") and unknowns.

CONTROL 2: 0 mM γ-Cyclodextrin

| Analyte | Bodipy | Rhodamine | Coumarin 6 |
|---|---|---|---|
| Benzo[*a*]pyrene | 5758820 | 7521340 | 12942700 |
| Benzo[*a*]pyrene | 6833050 | 7872950 | 10241700 |
| Benzo[*a*]pyrene | 4598340 | 7245710 | 9968350 |
| Benzo[*a*]pyrene | 4386190 | 7789140 | 10133300 |
| 9,10-Dihydrobenzo[*a*]pyrene-7(8*H*)-one | 4573660 | 7723020 | 16148000 |
| 9,10-Dihydrobenzo[*a*]pyrene-7(8*H*)-one | 4902520 | 7247860 | 9387400 |
| 9,10-Dihydrobenzo[*a*]pyrene-7(8*H*)-one | 4066790 | 7779200 | 11938400 |
| 9,10-Dihydrobenzo[*a*]pyrene-7(8*H*)-one | 3816500 | 6952350 | 14603600 |
| DDT | 1450020 | 4258930 | 26781300 |
| DDT | 1441210 | 4225630 | 17924300 |
| DDT | 1489210 | 3293770 | 20601400 |
| DDT | 1278440 | 3007230 | 22219700 |
| DDD | 1564800 | 4464790 | 55265100 |

| | | | |
|---|---|---|---|
| DDD | 1383280 | 4298270 | 26197900 |
| DDD | 1602050 | 4597650 | 29861300 |
| DDD | 1350870 | 4206070 | 18636700 |
| PCB 209 | 397604.2584 | 5711010 | 1407550 |
| PCB 209 | 363958.8922 | 5662200 | 765442.5262 |
| PCB 209 | 305887.249 | 4154680 | 730244.4856 |
| PCB 209 | 391847.242 | 3168990 | 890504.5502 |
| PCB 77 | 538580.0305 | 3526120 | 2210040 |
| PCB 77 | 483943.1419 | 4179010 | 2165330 |
| PCB 77 | 411699.3966 | 3601880 | 2391340 |
| PCB 77 | 431592.1488 | 3647470 | 1601120 |
| Fluorene | 1905920 | 6447090 | 2315410 |
| Fluorene | 1356500 | 7120630 | 2235370 |
| Fluorene | 1391630 | 5655180 | 2394580 |
| Fluorene | 1791050 | 4611910 | 1912250 |
| 2-Acetylaminofluorene | 1441620 | 5322710 | 1980660 |
| 2-Acetylaminofluorene | 1432210 | 5974870 | 1741540 |
| 2-Acetylaminofluorene | 917835.9426 | 5357840 | 1627910 |
| 2-Acetylaminofluorene | 1132240 | 5393120 | 2020750 |
| Benzidine | 652418.5509 | 4342870 | 1420600 |
| Benzidine | 619185.8684 | 4097810 | 1415510 |
| Benzidine | 521028.2375 | 3733890 | 1256380 |
| Benzidine | 637791.0903 | 4092930 | 1458850 |
| *N*,*N*,*N*′,*N*′-Tetramethylbenzidine | 1603540 | 5701460 | 2187540 |
| *N*,*N*,*N*′,*N*′-Tetramethylbenzidine | 887503.5283 | 6163350 | 1931860 |
| *N*,*N*,*N*′,*N*′-Tetramethylbenzidine | 836781.317 | 4943420 | 3443980 |
| *N*,*N*,*N*′,*N*′-Tetramethylbenzidine | 909186.2311 | 5694810 | 2163850 |

**Table S7.** Integration values for the training set. NOTE: Unknowns were not tested with this system due to the low JCA plot value (53%).

# CONTROL EXPERIMENTS CLASSIFICATIONS ANALYSIS

CONTROL 1: Blanks

| Analyte | % Correct | Misclassified ID |
|---|---|---|
| Anthracene | 100 | |
| Benzo[*a*]pyrene | 100 | |
| Pyrene | 100 | |
| 7-Methylbenzo[*a*]pyrene | 100 | |
| 9,10-Anthraquinone | 100 | |
| 9,10-Dihydrobenzo[*a*]pyrene | 100 | |
| Benz[*b*]anthracene | 100 | |
| 3,3',5,5'-Tetrabromobisphenol A | 100 | |
| Bisphenol A | 100 | |
| 4-Aminobiphenyl | 100 | |
| Benzidine | 100 | |
| Chrysene | 100 | |
| Diethylstilbestrol | 100 | |
| Carbazole | 100 | |
| Tetrahydrocarbazole | 100 | |
| 4,4'-DDT | 100 | |
| 4,4'-DDD | 100 | |
| *N*,*N*,*N'*,*N'*-Tetramethylbenzidine | 100 | |
| 4,4'-Dichlorobiphenyl | 100 | |
| PCB 209 | 100 | |
| PCB 29 | 100 | |
| Benzo[*b*]fluroanthene | 100 | |
| Deldrin | 100 | |
| Hexabromobenzene | 100 | |
| PCB 77 | 100 | |
| Fluorene | 100 | |
| Tamoxifen | 100 | |
| 2-Acetylaminofluorene | 100 | |
| Deltamethrin | 100 | |
| Quinizarin | 100 | |
| Blank 250 | 100 | |
| Blank 300 | 100 | |
| Blank 360 | 100 | |
| Blank 400 | 75 | 4,4'-DDD |

**Table S8.** Jackknifed classification matrix summary.

| | | |
|---|---|---|
| 0.991 | 0.998 | 1.000 |

**Table S9.** Cumulative Proportion of Total Dispersion values.

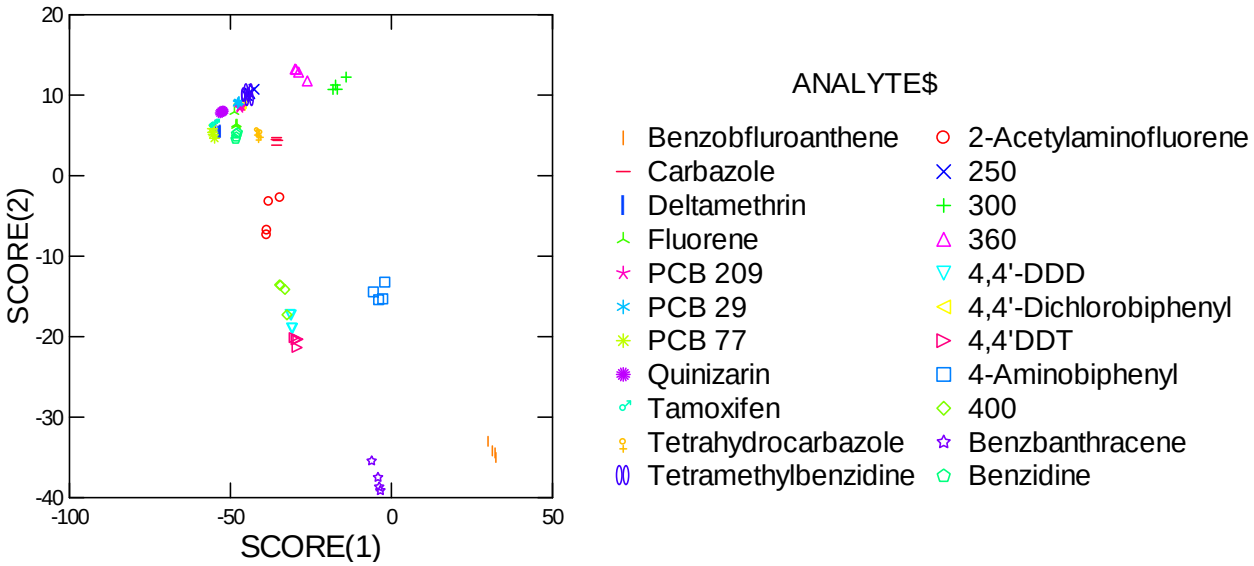



**Figure 4.** LDA score plot for selected analytes (all analytes were used to generate the array; select analytes are shown here for more clarity).

| Score 1 | Score 2 | Score 3 | Analyte ID | Unknown Classification |
|---|---|---|---|---|
| -42.4073 | 7.833422 | -0.8291 | Anthracene | Anthracene |
| -42.2978 | 7.961798 | -0.81187 | Anthracene | Anthracene |
| -42.3435 | 7.601337 | -0.87479 | Anthracene | Anthracene |
| -42.374 | 8.081937 | -1.00098 | Anthracene | Anthracene |
| 875.2862 | 3.889797 | 0.07794 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 879.5816 | 0.715296 | 0.999882 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 873.0585 | 3.97038 | -3.25862 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 876.4355 | 5.278348 | -8.03613 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 186.7615 | 26.36654 | 21.31852 | Pyrene | Pyrene |
| 188.4797 | 25.82204 | 19.52655 | Pyrene | Pyrene |
| 184.097 | 21.62687 | 16.89587 | Pyrene | Pyrene |
| 186.2442 | 19.2375 | 17.63893 | Pyrene | Pyrene |
| 68.35616 | -25.1252 | -17.668 | 7-Methylbenzo[a]pyrene | 7-Methylbenzo[a]pyrene |

| | | | | |
|---|---|---|---|---|
| 65.91507 | -25.8914 | -17.7582 | 7-Methylbenzo[a]pyrene | 7-Methylbenzo[a]pyrene |
| 67.93517 | -24.6026 | -16.8935 | 7-Methylbenzo[a]pyrene | 7-Methylbenzo[a]pyrene |
| 64.55376 | -26.0031 | -13.8977 | 7-Methylbenzo[a]pyrene | 7-Methylbenzo[a]pyrene |
| -42.1273 | 7.593467 | 2.230692 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -42.6231 | 7.681316 | 3.015133 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -42.1592 | 7.574272 | 2.295031 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -42.2782 | 7.547622 | 2.388995 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -4.95885 | -2.96318 | -1.42334 | 9,10-Dihydrobenzo[*a*]pyrene | 9,10-Dihydrobenzo[*a*]pyrene |
| -3.79988 | -2.22147 | -2.0133 | 9,10-Dihydrobenzo[*a*]pyrene | 9,10-Dihydrobenzo[*a*]pyrene |
| -5.16942 | -2.36802 | -1.57747 | 9,10-Dihydrobenzo[*a*]pyrene | 9,10-Dihydrobenzo[*a*]pyrene |
| -3.70856 | -3.11269 | -1.42881 | 9,10-Dihydrobenzo[*a*]pyrene | 9,10-Dihydrobenzo[*a*]pyrene |
| -4.1777 | -37.4786 | 2.902889 | Benz[*b*]anthracene | Benz[*b*]anthracene |
| -3.44718 | -39.1112 | 3.240548 | Benz[*b*]anthracene | Benz[*b*]anthracene |
| -3.82453 | -38.6635 | 3.395429 | Benz[*b*]anthracene | Benz[*b*]anthracene |
| -6.14898 | -35.4288 | 3.047464 | Benz[*b*]anthracene | Benz[*b*]anthracene |
| -48.8266 | 7.790947 | -2.89746 | 3,3',5,5'-Tetrabromobisphenol A | 3,3',5,5'-Tetrabromobisphenol A |
| -48.9928 | 7.596153 | -2.69284 | 3,3',5,5'-Tetrabromobisphenol A | 3,3',5,5'-Tetrabromobisphenol A |
| -48.7847 | 7.802154 | -2.89703 | 3,3',5,5'-Tetrabromobisphenol A | 3,3',5,5'-Tetrabromobisphenol A |
| -49.1132 | 7.72064 | -2.64206 | 3,3',5,5'-Tetrabromobisphenol A | 3,3',5,5'-Tetrabromobisphenol A |
| -56.9738 | 5.84433 | 2.872213 | Bisphenol A | Bisphenol A |
| -56.7347 | 6.151828 | 2.956098 | Bisphenol A | Bisphenol A |
| -56.6126 | 6.041615 | 2.929032 | Bisphenol A | Bisphenol A |
| -56.434 | 6.268204 | 2.755688 | Bisphenol A | Bisphenol A |
| -2.07545 | -13.2271 | -2.10558 | 4-Aminobiphenyl | 4-Aminobiphenyl |
| -5.65654 | -14.4407 | 0.069877 | 4-Aminobiphenyl | 4-Aminobiphenyl |

| | | | | |
|---|---|---|---|---|
| -2.70712 | -15.302 | -2.59596 | 4-Aminobiphenyl | 4-Aminobiphenyl |
| -3.98706 | -15.417 | -1.30302 | 4-Aminobiphenyl | 4-Aminobiphenyl |
| -48.182 | 4.817026 | 1.794863 | Benzidine | Benzidine |
| -47.7516 | 5.357883 | 1.745841 | Benzidine | Benzidine |
| -48.3991 | 4.528824 | 2.187002 | Benzidine | Benzidine |
| -48.21 | 5.195773 | 1.764086 | Benzidine | Benzidine |
| -20.6017 | -11.8854 | 8.887372 | Chrysene | Chrysene |
| -20.3103 | -13.176 | 9.672242 | Chrysene | Chrysene |
| -19.4564 | -12.613 | 9.401632 | Chrysene | Chrysene |
| -20.9589 | -12.4737 | 9.101787 | Chrysene | Chrysene |
| -46.3867 | 7.12122 | -1.26992 | Diethylstilbestrol | Diethylstilbestrol |
| -46.6186 | 7.11722 | -0.98833 | Diethylstilbestrol | Diethylstilbestrol |
| -46.388 | 7.271717 | -1.11074 | Diethylstilbestrol | Diethylstilbestrol |
| -46.3743 | 7.223727 | -1.19835 | Diethylstilbestrol | Diethylstilbestrol |
| -35.3076 | 4.383817 | 2.853235 | Carbazole | Carbazole |
| -35.6841 | 4.719177 | 3.48697 | Carbazole | Carbazole |
| -35.8304 | 4.485828 | 2.684589 | Carbazole | Carbazole |
| -35.668 | 3.788734 | 3.411918 | Carbazole | Carbazole |
| -40.5842 | 5.361187 | 0.84905 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -41.2553 | 5.016751 | -0.17698 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -41.7437 | 5.633557 | 0.207301 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -41.248 | 5.476507 | -0.20676 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -29.0683 | -20.3213 | -0.54887 | 4,4'DDT | 4,4'-DDD |
| -29.6382 | -20.3782 | -0.56076 | 4,4'DDT | 4,4'-DDD |
| -30.1929 | -20.1229 | -0.56465 | 4,4'DDT | 4,4'DDT |

| | | | | |
|---|---|---|---|---|
| -29.3074 | -21.345 | -0.39325 | 4,4'DDT | 4,4'DDT |
| -31.0077 | -18.9426 | -0.24172 | 4,4'-DDD | 4,4'-DDD |
| -31.4499 | -17.2357 | -0.54514 | 4,4'-DDD | 4,4'-DDD |
| -31.1609 | -17.332 | -0.68324 | 4,4'-DDD | 4,4'-DDD |
| -30.738 | -18.9656 | -0.15082 | 4,4'-DDD | 4,4'-DDD |
| -45.017 | 9.994155 | -2.55097 | Tetramethylbenzidine | Tetramethylbenzidine |
| -45.007 | 9.982159 | -2.23578 | Tetramethylbenzidine | Tetramethylbenzidine |
| -44.223 | 10.51406 | -2.92074 | Tetramethylbenzidine | Tetramethylbenzidine |
| -43.9573 | 9.421374 | -2.48315 | Tetramethylbenzidine | Fluorene |
| -47.0187 | 8.730675 | -2.24174 | 4,4'-Dichlorobiphenyl | 4,4'-Dichlorobiphenyl |
| -47.3879 | 8.898169 | -2.06973 | 4,4'-Dichlorobiphenyl | 4,4'-Dichlorobiphenyl |
| -46.6264 | 8.962688 | -2.53649 | 4,4'-Dichlorobiphenyl | 4,4'-Dichlorobiphenyl |
| -46.9203 | 8.837337 | -2.15422 | 4,4'-Dichlorobiphenyl | 4,4'-Dichlorobiphenyl |
| -46.679 | 8.630931 | -4.26428 | PCB 209 | PCB 209 |
| -46.6403 | 8.692617 | -4.27631 | PCB 209 | PCB 209 |
| -47.112 | 8.398046 | -3.81773 | PCB 209 | PCB 209 |
| -47.0981 | 8.569406 | -4.06541 | PCB 209 | PCB 209 |
| -47.6683 | 9.08199 | -3.5309 | PCB 29 | PCB 29 |
| -47.3793 | 9.183057 | -3.6722 | PCB 29 | PCB 29 |
| -47.4173 | 9.159041 | -3.57266 | PCB 29 | PCB 29 |
| -47.7788 | 8.972359 | -3.33905 | PCB 29 | PCB 29 |
| 32.43383 | -35.0073 | 6.238009 | Benzo[*b*]fluroanthene | Benzo[*b*]fluroanthene |
| 31.35236 | -34.1937 | 5.467942 | Benzo[*b*]fluroanthene | Benzo[*b*]fluroanthene |
| 29.97514 | -33.0085 | 4.480282 | Benzo[*b*]fluroanthene | Benzo[*b*]fluroanthene |
| 32.18629 | -34.4525 | 4.955776 | Benzo[*b*]fluroanthene | Benzo[*b*]fluroanthene |

| | | | | |
|---|---|---|---|---|
| -47.0286 | 1.971102 | 1.718342 | Deldrin | Deldrin |
| -46.5367 | 1.506408 | 1.563446 | Deldrin | Deldrin |
| -47.068 | 1.548657 | 1.937399 | Deldrin | Deldrin |
| -46.7026 | 0.491065 | 2.287043 | Deldrin | Deldrin |
| -46.8052 | 3.936478 | 0.160446 | Hexabromobenzene | Hexabromobenzene |
| -46.8618 | 3.79849 | 0.542907 | Hexabromobenzene | Hexabromobenzene |
| -47.1439 | 3.669336 | 0.431032 | Hexabromobenzene | Hexabromobenzene |
| -46.7344 | 3.523048 | 0.322669 | Hexabromobenzene | Hexabromobenzene |
| -54.9345 | 4.648135 | 4.118344 | PCB 77 | PCB 77 |
| -55.3495 | 5.129786 | 3.927635 | PCB 77 | PCB 77 |
| -55.6 | 5.854059 | 4.105069 | PCB 77 | PCB 77 |
| -55.5445 | 5.375509 | 3.963143 | PCB 77 | PCB 77 |
| -48.2363 | 6.205165 | 2.434353 | Fluorene | Fluorene |
| -47.9928 | 6.390506 | 2.55035 | Fluorene | Fluorene |
| -48.2559 | 6.381693 | 2.472603 | Fluorene | Fluorene |
| -48.7879 | 7.922118 | 2.293374 | Fluorene | Fluorene |
| -55.2547 | 6.320948 | 2.263754 | Tamoxifen | Tamoxifen |
| -55.6209 | 6.179839 | 2.414724 | Tamoxifen | Tamoxifen |
| -55.7284 | 6.163369 | 2.529773 | Tamoxifen | Tamoxifen |
| -55.1048 | 6.344237 | 2.082372 | Tamoxifen | Tamoxifen |
| -34.5507 | -2.74939 | 15.79638 | 2-Acetylaminofluorene | Benzbanthracene |
| -38.0439 | -3.23387 | 13.86209 | 2-Acetylaminofluorene | 2-Acetylaminofluorene |
| -38.6481 | -6.79732 | 12.51691 | 2-Acetylaminofluorene | 2-Acetylaminofluorene |
| -38.7016 | -7.37052 | 12.28741 | 2-Acetylaminofluorene | 2-Acetylaminofluorene |
| -54.0171 | 5.398725 | 4.524543 | Deltamethrin | Deltamethrin |

| | | | | |
|---|---|---|---|---|
| -53.5224 | 5.509288 | 4.586007 | Deltamethrin | Deltamethrin |
| -53.609 | 5.424036 | 4.570545 | Deltamethrin | Deltamethrin |
| -54.1396 | 5.367035 | 4.256978 | Deltamethrin | Deltamethrin |
| -52.3542 | 8.041959 | 2.898656 | Quinizarin | Quinizarin |
| -52.7525 | 7.963107 | 2.919433 | Quinizarin | Tamoxifen |
| -52.2699 | 8.004931 | 2.881826 | Quinizarin | Quinizarin |
| -53.1689 | 7.801866 | 3.347795 | Quinizarin | Quinizarin |
| -42.6814 | 10.73059 | -8.05525 | 250 | PCB 29 |
| -44.7526 | 9.933045 | -6.36591 | 250 | PCB 29 |
| -44.1385 | 10.30842 | -6.84902 | 250 | PCB 209 |
| -44.0163 | 10.17837 | -6.94256 | 250 | PCB 29 |
| -14.071 | 12.24854 | -22.5075 | 300 | 300 |
| -18.1704 | 10.71435 | -18.9501 | 300 | 360 |
| -17.3919 | 11.26372 | -19.8362 | 300 | 300 |
| -16.8203 | 10.72729 | -20.0256 | 300 | 300 |
| -26.1399 | 11.76479 | -12.1717 | 360 | 360 |
| -29.9373 | 13.26036 | -9.86583 | 360 | 360 |
| -29.6497 | 13.19813 | -10.0871 | 360 | 360 |
| -28.8535 | 12.86209 | -10.4685 | 360 | 360 |
| -33.0929 | -14.1444 | -1.52253 | 400 | 400 |
| -34.7502 | -13.5666 | -0.47431 | 400 | 4,4'-DDD |
| -34.4613 | -13.6271 | -0.63766 | 400 | 4,4'-DDD |
| -32.4586 | -17.2864 | -0.57756 | 4,4'-DDD | 400 |

**Table S10.** Classifications of all analytes ("Analyte ID"), including classifications of unknowns ("Unknown Classification")

CONTROL 2: 0 mM γ-Cyclodextrin

| Jackknifed Classification Matrix | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | **14** | **8** | **28** | **6** | **20** | **19** | **11** | **18** | **17** | **30** | %correct |
| **14** | 2 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 50 |
| **8** | 0 | 3 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 75 |
| **28** | 0 | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 75 |
| **6** | 0 | 2 | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 50 |
| **20** | 0 | 0 | 0 | 0 | 2 | 2 | 0 | 0 | 0 | 0 | 50 |
| **19** | 0 | 0 | 0 | 0 | 1 | 3 | 0 | 0 | 0 | 0 | 75 |
| **11** | 2 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 25 |
| **18** | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 1 | 2 | 0 |
| **17** | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 3 | 0 | 75 |
| **30** | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 0 | 2 | 50 |
| Total | 4 | 5 | 5 | 3 | 3 | 5 | 3 | 1 | 5 | 6 | 53 |

**Table S11.** Jackknifed classification matrix for 0 mM γ-Cyclodextrin array.

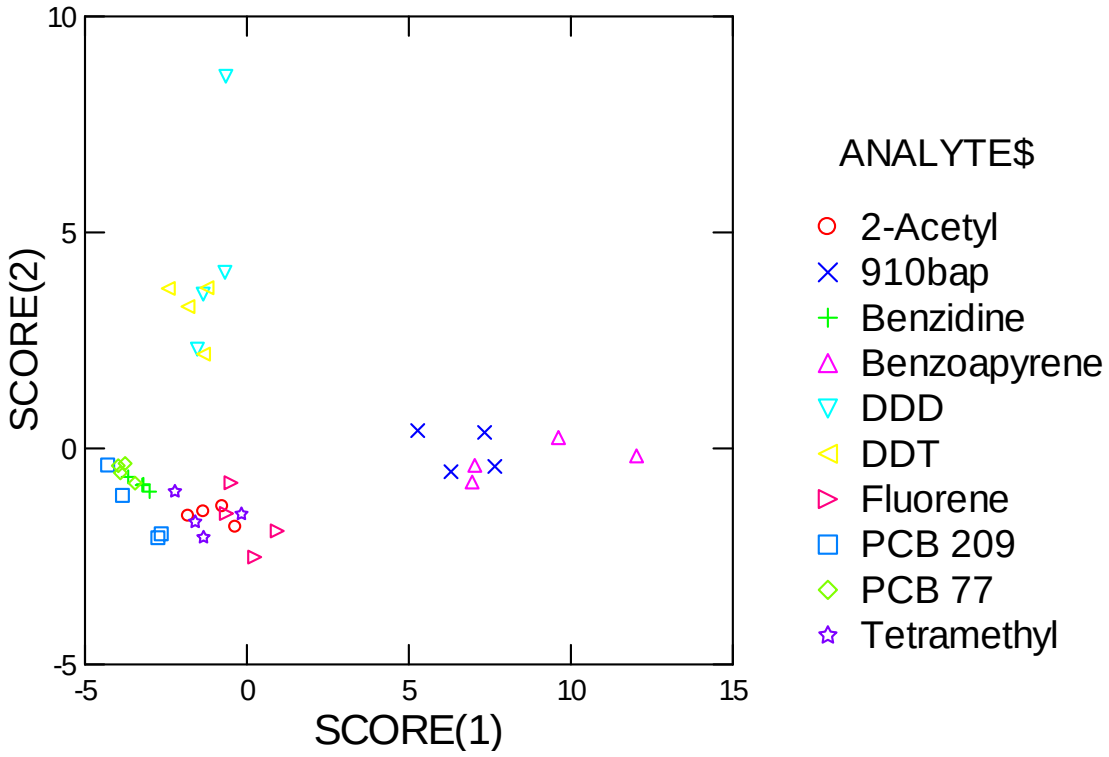



**Figure S5.** LDA score plot for 0 mM γ-Cyclodextrin array.

| | | |
|---|---|---|
| 0.778 | 0.976 | 1.000 |

**Table S12.** Cumulative Proportion of Total Dispersion.

| Analyte | Score 1 | Score 2 | Score 3 |
|---|---|---|---|
| Benzo[*a*]pyrene | 9.616227 | 0.251158 | 1.124543 |
| Benzo[*a*]pyrene | 12.02777 | -0.17525 | 2.046879 |

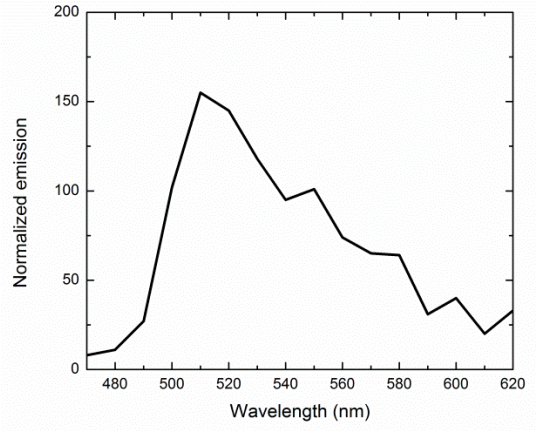
| | | | |
|---|---|---|---|
| Benzo[*a*]pyrene | 7.034479 | -0.39227 | 0.417812 |
| Benzo[*a*]pyrene | 6.951427 | -0.77957 | -0.548059 |
| 9,10-Dihydrobenzo[*a*]pyrene | 7.33825 | 0.36984 | -0.689067 |
| 9,10-Dihydrobenzo[*a*]pyrene | 7.655771 | -0.41606 | 0.79446 |
| 9,10-Dihydrobenzo[*a*]pyrene | 6.302991 | -0.53958 | -1.020094 |
| 9,10-Dihydrobenzo[*a*]pyrene | 5.275016 | 0.411785 | -0.39761 |
| DDT | -1.23079 | 3.718547 | -0.34382 |
| DDT | -1.33638 | 2.182706 | 0.333001 |
| DDT | -1.81997 | 3.283997 | 1.424297 |
| DDT | -2.42557 | 3.703215 | 1.45206 |
| DDD | -0.65 | 8.614843 | -2.555191 |
| DDD | -1.34669 | 3.572486 | -0.427535 |
| DDD | -0.67702 | 4.074514 | -0.846581 |
| DDD | -1.52911 | 2.297152 | 0.206995 |
| PCB 209 | -2.64148 | -1.97754 | -1.590378 |
| PCB 209 | -2.74684 | -2.06674 | -1.516562 |
| PCB 209 | -3.84023 | -1.08753 | 0.415114 |
| PCB 209 | -4.29944 | -0.38262 | 1.802284 |
| PCB 77 | -3.75776 | -0.34947 | 1.39702 |
| PCB 77 | -3.44841 | -0.80498 | 0.476297 |
| PCB 77 | -3.96785 | -0.40114 | 1.142969 |
| PCB 77 | -3.90346 | -0.56498 | 1.162072 |
| Fluorene | 0.936172 | -1.91158 | -0.956863 |
| Fluorene | 0.243216 | -2.5166 | -2.451058 |
| Fluorene | -0.63027 | -1.50676 | -0.485755 |
| Fluorene | -0.4882 | -0.79439 | 1.371811 |
| 2-Acetylaminofluorene | -0.74557 | -1.34569 | 0.039368 |
| 2-Acetylaminofluorene | -0.34532 | -1.82302 | -0.816129 |
| 2-Acetylaminofluorene | -1.8004 | -1.56816 | -0.562386 |
| 2-Acetylaminofluorene | -1.33468 | -1.46642 | -0.39976 |
| Benzidine | -3.00236 | -1.00042 | 0.500482 |
| Benzidine | -3.22892 | -0.84736 | 0.78806 |
| Benzidine | -3.66665 | -0.65947 | 1.171988 |
| Benzidine | -3.19357 | -0.83163 | 0.812003 |
| Tetramethylbenzidine | -0.16704 | -1.51834 | -0.296921 |
| Tetramethylbenzidine | -1.33997 | -2.05737 | -1.683273 |
| Tetramethylbenzidine | -2.22094 | -0.99535 | -0.236006 |
| Tetramethylbenzidine | -1.59645 | -1.69996 | -1.056465 |

**Table S13.** LDA Score values for an array generated in 0 mM γ-cyclodextrin.

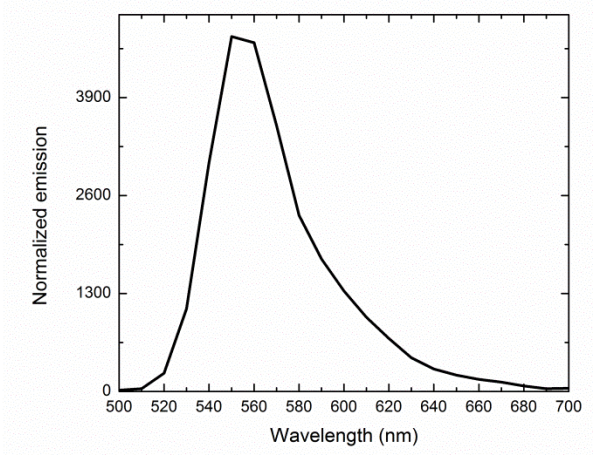
# CONTROL FLUORESCENCE EMISSION GRAPHS

## CONTROL 1: 10 mM γ-Cyclodextrin

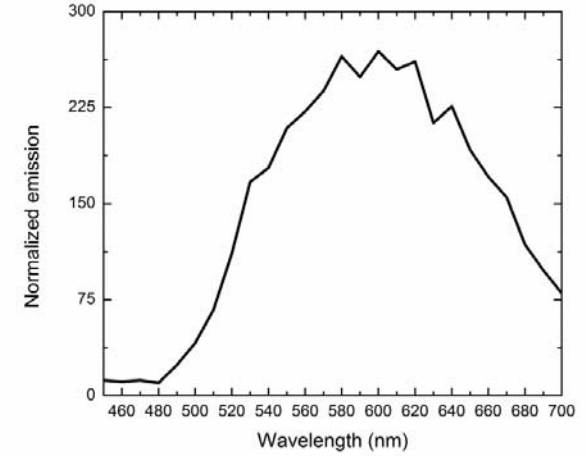
250 nm – Fluorophore **31**



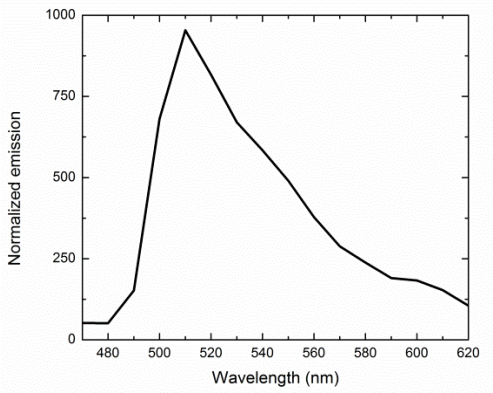

250 nm – Fluorophore **32**



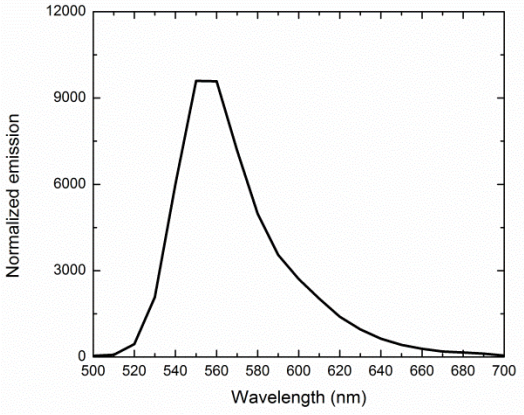

250 nm – Fluorophore **33**



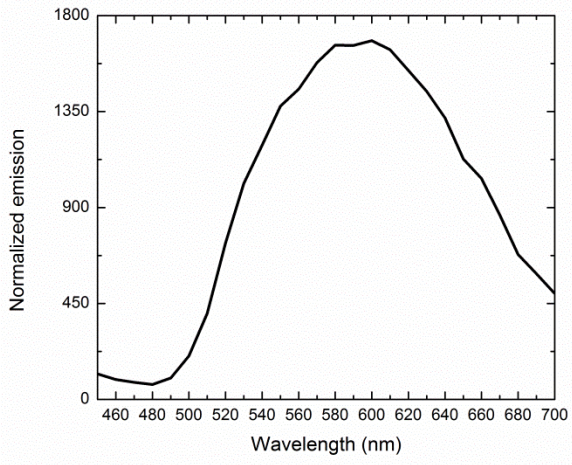
300 nm – Fluorophore **31**



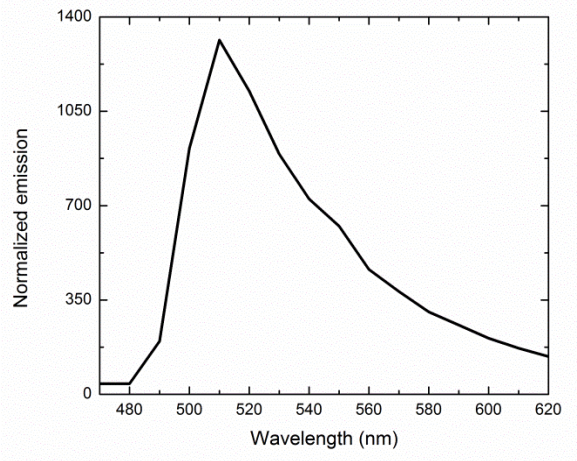

300 nm – Fluorophore **32**



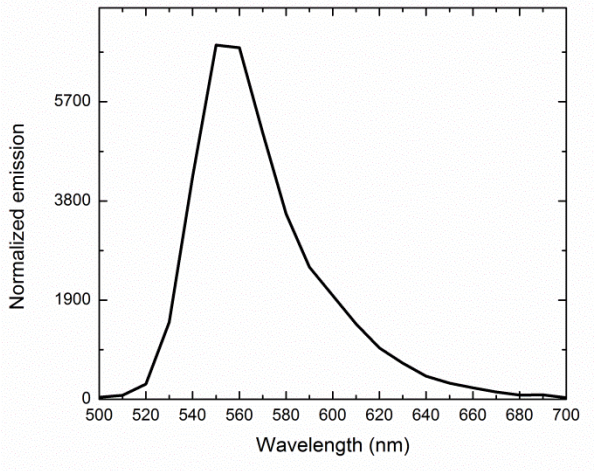

300 nm – Fluorophore **33**



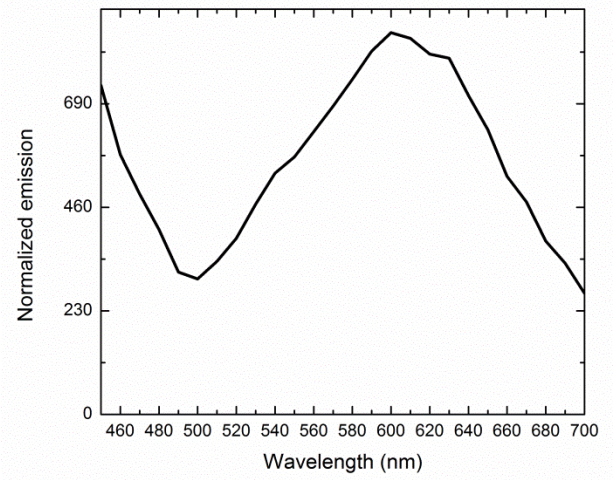
360 nm – Fluorophore **31**



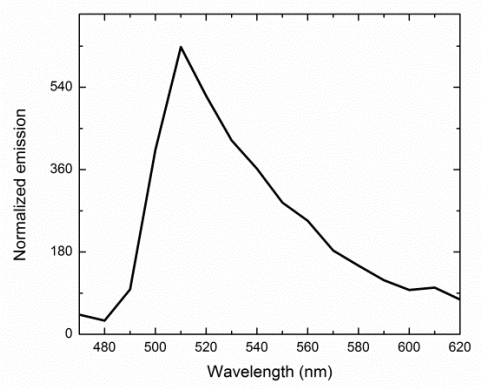

360 nm – Fluorophore **32**



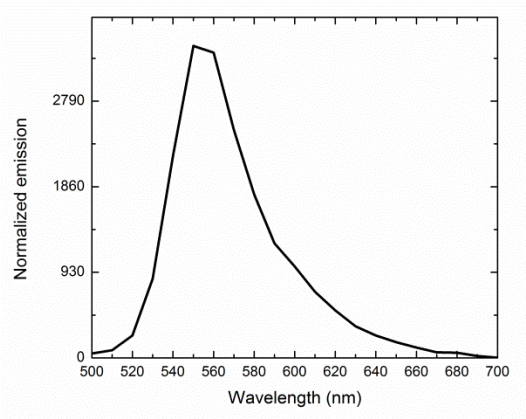

360 nm – Fluorophore **33**



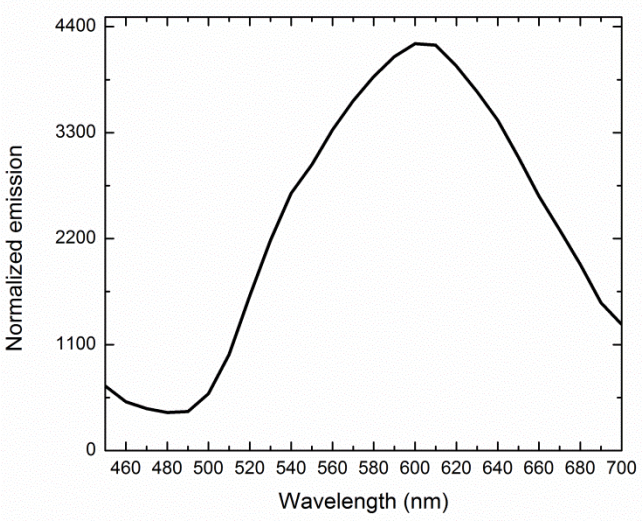
400 nm – Fluorophore **31**




400 nm – Fluorophore **32**

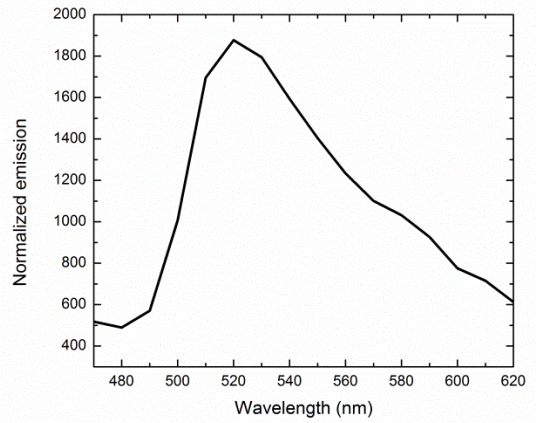



400 nm – Fluorophore **33**

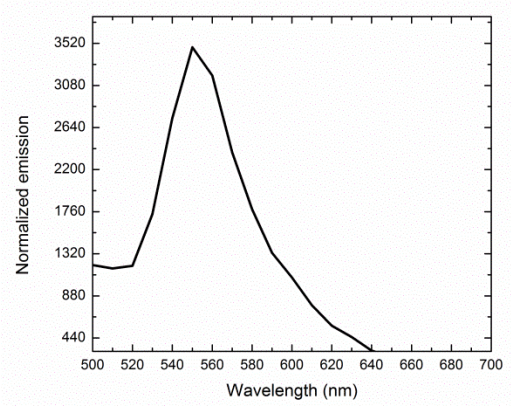


CONTROL 2: 0 mM γ-Cyclodextrin

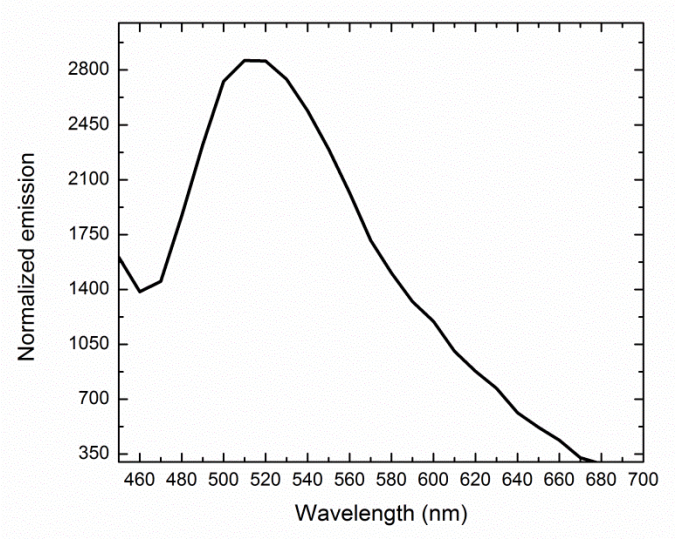
Analyte **6** – Fluorophore **31**



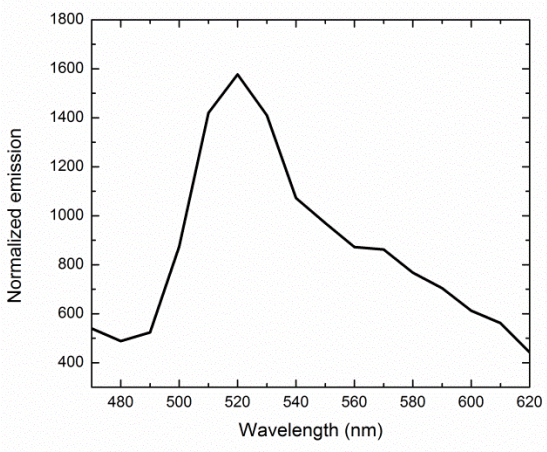

Analyte **6** – Fluorophore **32**



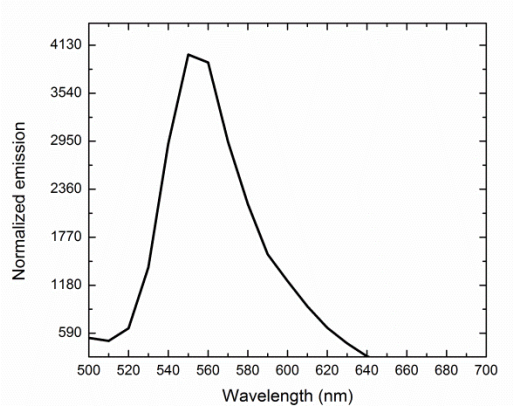

Analyte **6** – Fluorophore **33**



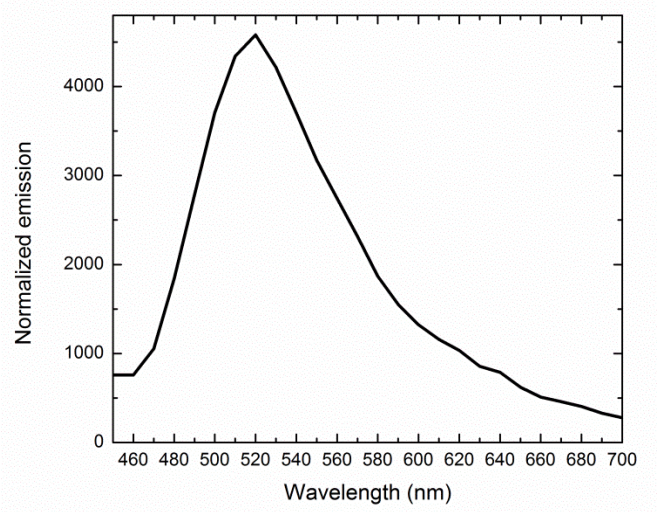
Analyte **8** – Fluorophore **31**



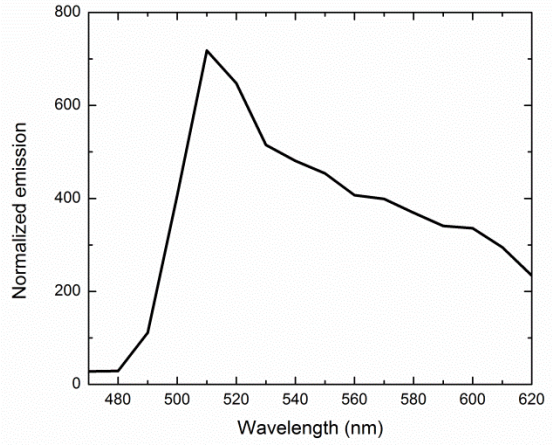

Analyte **8** – Fluorophore **32**



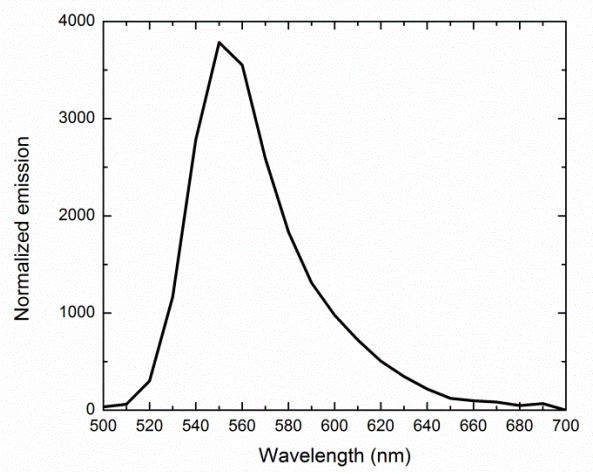

Analyte **8** – Fluorophore **33**



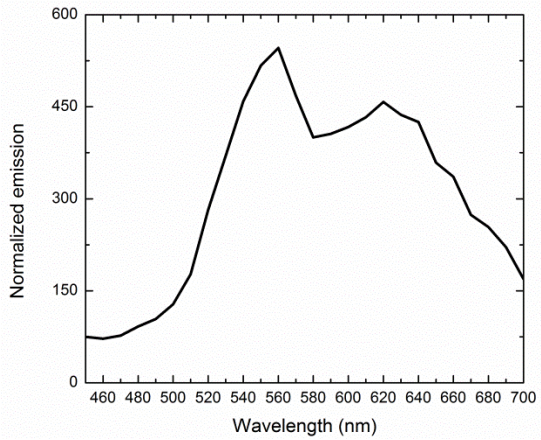
Analyte **11** – Fluorophore **31**



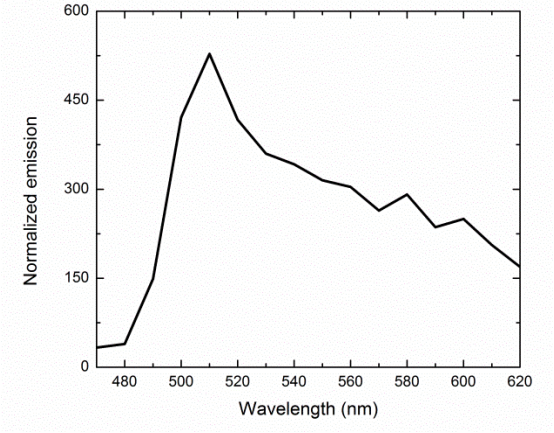

Analyte **11** – Fluorophore **32**



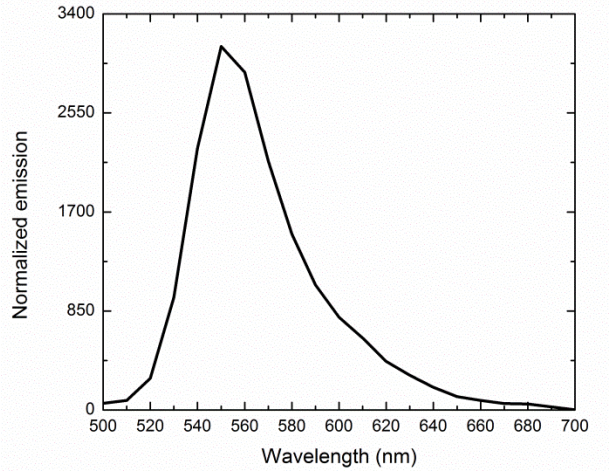

Analyte **11** – Fluorophore **33**



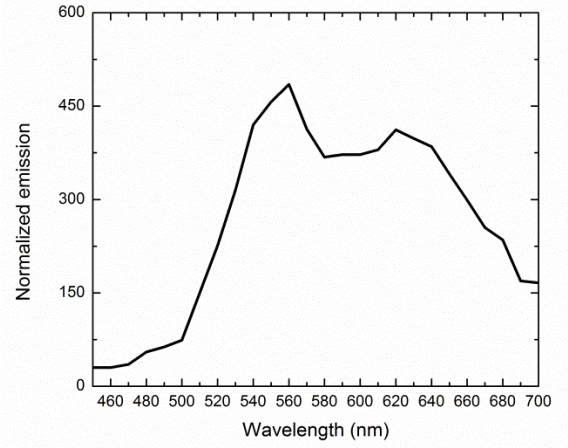
Analyte **14** – Fluorophore **31**



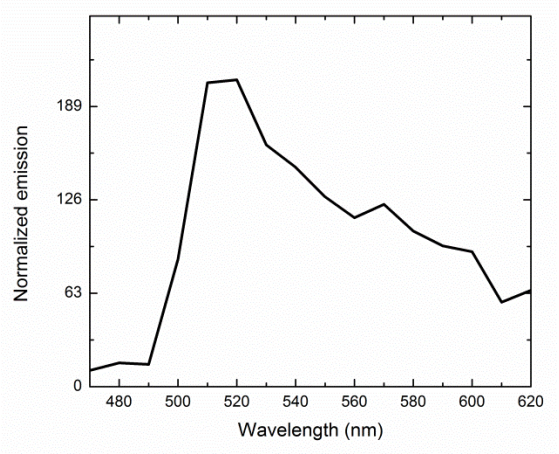

Analyte **14** – Fluorophore **32**



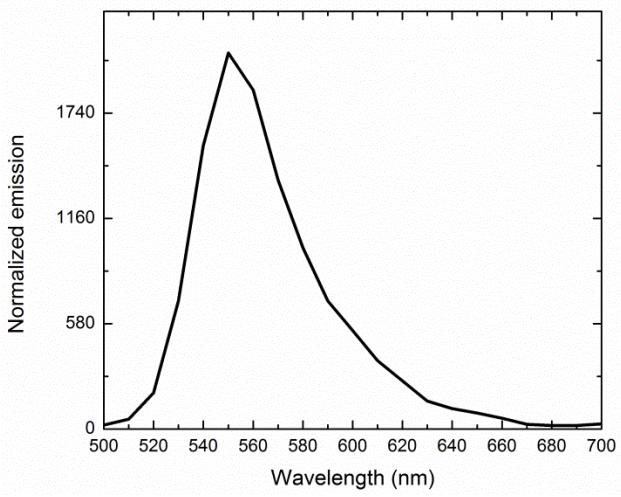

Analyte **14** – Fluorophore **33**



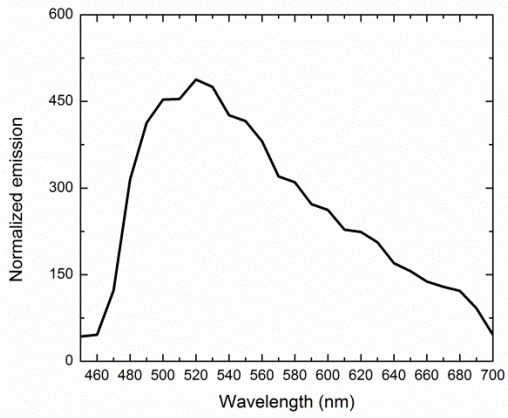
Analyte **17** – Fluorophore **31**



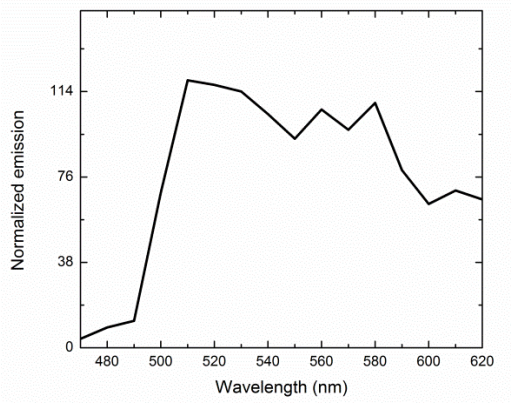

Analyte **17** – Fluorophore **32**



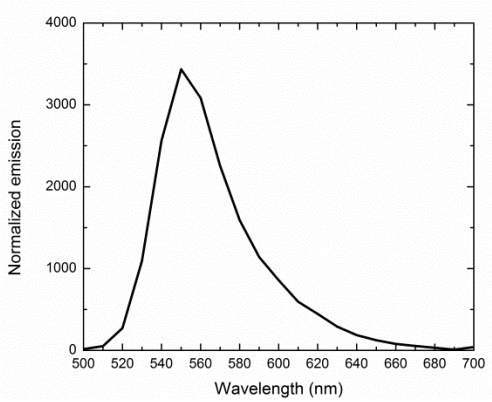

Analyte **17** – Fluorophore **33**



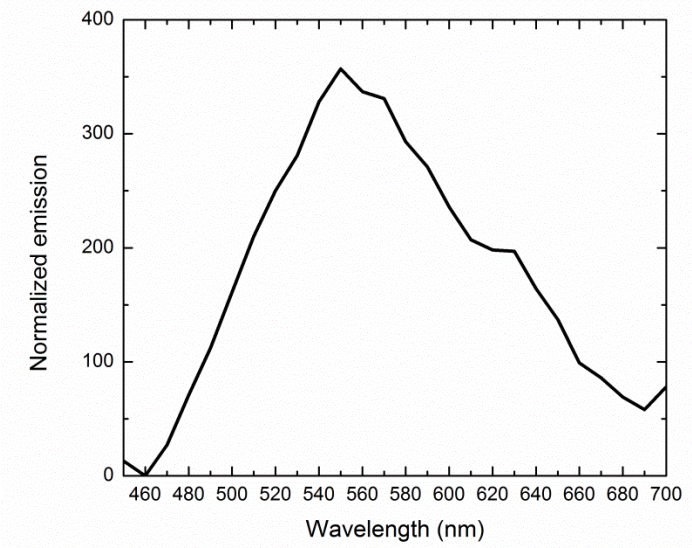
Analyte **18** – Fluorophore **31**



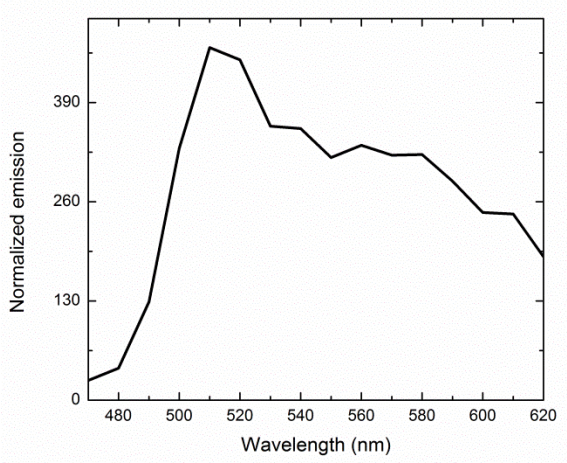

Analyte **18** – Fluorophore **32**



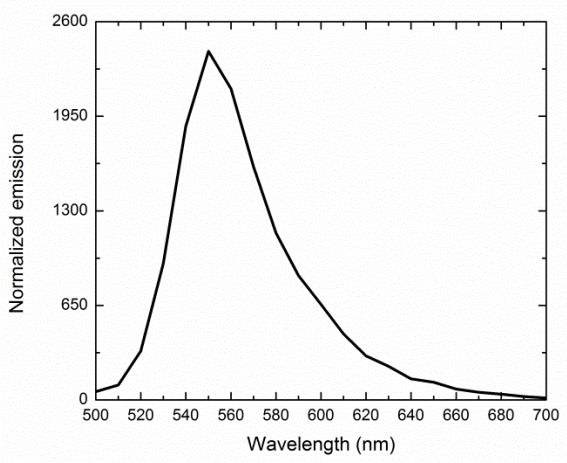

Analyte **18** – Fluorophore **33**



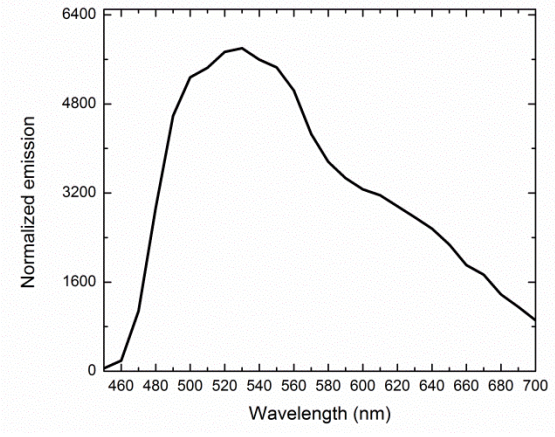
Analyte **19** – Fluorophore **31**



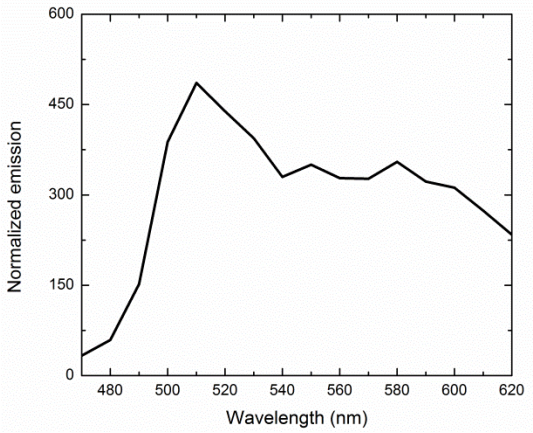

Analyte **19** – Fluorophore **32**



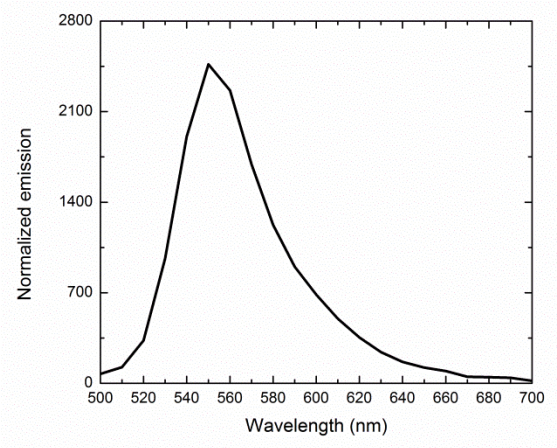

Analyte **19** – Fluorophore **33**



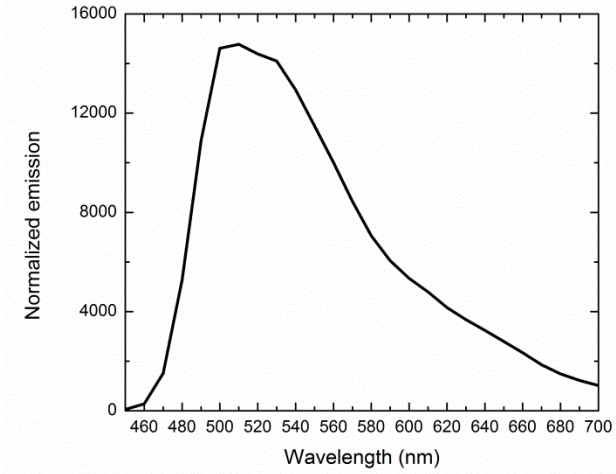
Analyte **20** – Fluorophore **31**



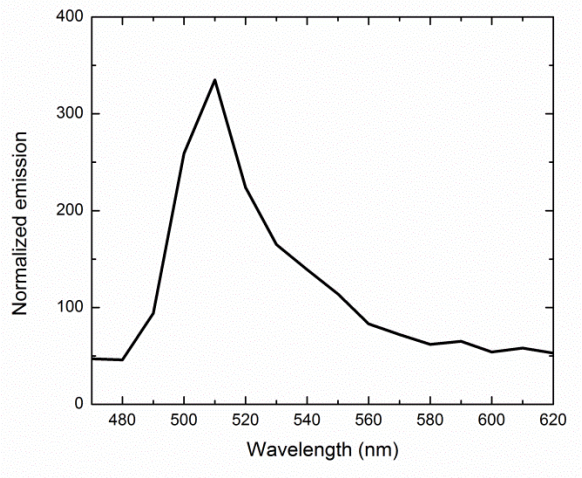

Analyte **20** – Fluorophore **32**



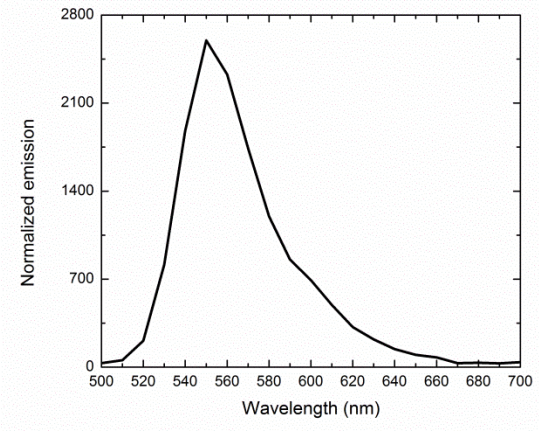

Analyte **20** – Fluorophore **33**



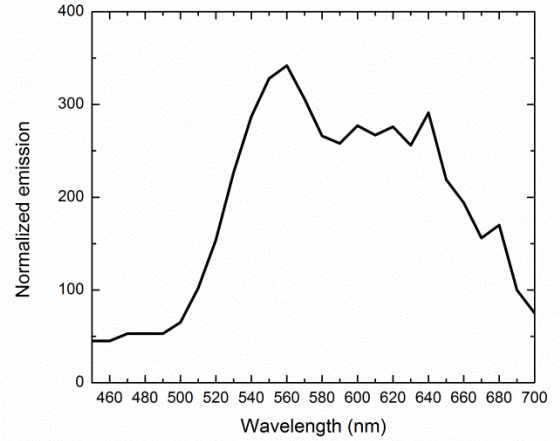
Analyte **28** – Fluorophore **31**



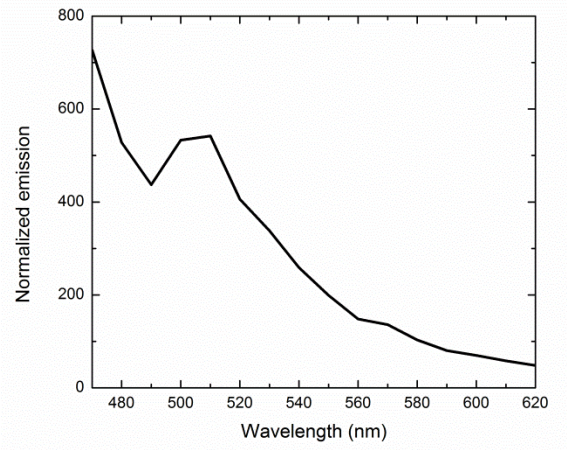

Analyte **28** – Fluorophore **32**



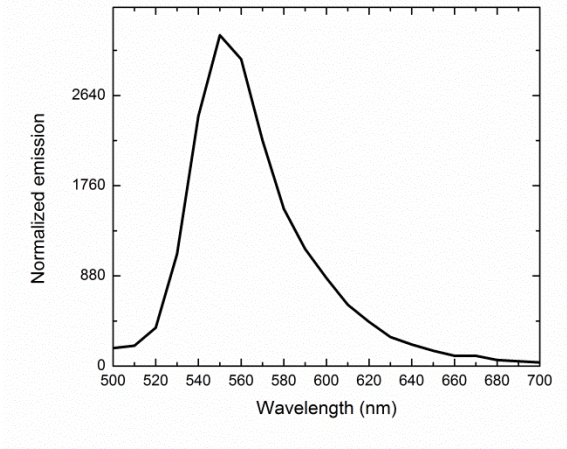

Analyte **28** – Fluorophore **33**



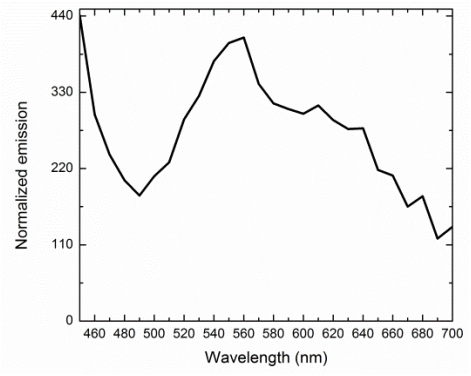
Analyte **30** – Fluorophore **31**




Analyte **30** – Fluorophore **32**




Analyte **30** – Fluorophore **33**



## URINE EXPERIMENTS PROCEDURE

*General Procedure – Sample Preparation*

Two samples were prepared for each fluorophore: one served as the sample for the training set, and the other served as the unknown. For each sample, 1.25 mL of 10 mM γ-cyclodextrin and 1.25 mL of urine were combined and mixed in a vial. Then, 100 μL of fluorophore was added and vigorously shaken by hand for approximately 30 seconds. The sample remained on a rotary mixer until use to ensure thorough mixing. A 96 well microplate was used, and into each well was pipetted 100 μL of the sample solution, and each solution was repeated four times (*i.e.* each solution was pipetted into four separate wells) to ensure data reproducibility.

*General Procedure – Fluorescence Studies*

A BioTek Synergy Mx Multi-Mode Microplate Reader was used to generate the fluorescence data for the array. The samples were excited at the excitation wavelength of the analyte under investigation. The emission of each was recorded: (a) Fluorophore **31** samples: 470-620 nm; (b) Fluorophore **32** samples: 500-700 nm; (c) Fluorophore **33** samples: 450-700 nm. The fluorescence emission was integrated with respect to wavenumber using OriginPro software.

URINE ARRAY INTEGRATIONS

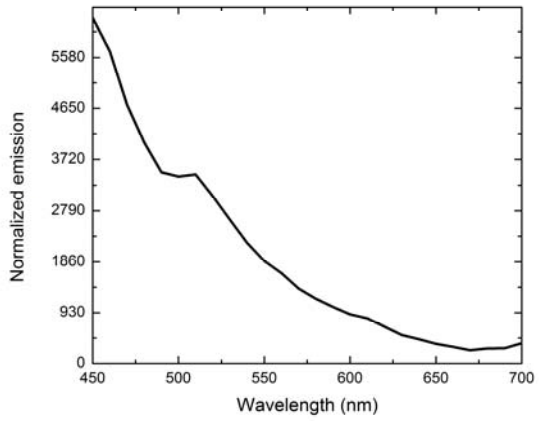
| | KNOWNS | | | UNKNOWNS | | |
|---|---|---|---|---|---|---|
| Analyte | Bodipy | Rhodamine | Coumarin 6 | Bodipy | Rhodamine | Coumarin 6 |
| Carbazole | 9977290 | 16811800 | 16303100 | 9519830 | 17126500 | 16401700 |
| Carbazole | 9852340 | 16444500 | 16239700 | 9196440 | 17292500 | 16145300 |
| Carbazole | 9106740 | 17552400 | 16603600 | 9403130 | 16030500 | 15614200 |
| Carbazole | 9681010 | 17570700 | 16344200 | 9494670 | 17399900 | 16434700 |
| Tetrahydrocarbazole | 8277820 | 16966300 | 15793300 | 8095290 | 16471800 | 15595600 |
| Tetrahydrocarbazole | 8594330 | 15501800 | 15394500 | 8587960 | 14453900 | 15441100 |
| Tetrahydrocarbazole | 8575630 | 15322300 | 14710500 | 8627270 | 15991400 | 24755000 |
| Tetrahydrocarbazole | 8879900 | 17405700 | 15102100 | 8774730 | 9754300 | 15060400 |
| PCB77 | 458486.5485 | 1128480 | 699145.051 | 446208.2553 | 1135840 | 721275.9881 |
| PCB77 | 458156.7682 | 1108510 | 774457.07 | 521717.0157 | 1107960 | 649362.6781 |
| PCB77 | 471364.335 | 1120730 | 672999.245 | 446451.4 | 1089950 | 660855.2029 |
| PCB77 | 478491.2669 | 1108540 | 684801.371 | 465035.3352 | 1137570 | 682521.2137 |
| PCB29 | 375105.8244 | 1273260 | 667093.201 | 350579.3925 | 1258180 | 654064.0535 |
| PCB29 | 374221.3044 | 1240720 | 629378.778 | 357590.5784 | 1272190 | 640527.6095 |
| PCB29 | 376168.7531 | 1285790 | 638077.116 | 352731.6064 | 1263390 | 627272.8804 |
| PCB29 | 357327.551 | 1258660 | 664245.009 | 350317.9046 | 1290240 | 652694.6157 |
| PCB209 | 371591.6112 | 1394320 | 682179.077 | 364223.1518 | 1399990 | 716362.7391 |
| PCB209 | 372541.1789 | 1383950 | 719301.534 | 372381.885 | 1414600 | 732976.7629 |
| PCB209 | 370172.9025 | 1372500 | 696218.142 | 378861.2475 | 1401340 | 727616.3371 |
| PCB209 | 381633.5472 | 1446430 | 709404.557 | 354174.4774 | 1423750 | 687678.1119 |
| Anthracene | 12540800 | 23396900 | 20035600 | 12671800 | 23837800 | 21430000 |
| Anthracene | 13102300 | 23446200 | 20693100 | 12261700 | 23057600 | 20819200 |
| Anthracene | 13052500 | 23404400 | 21372400 | 12486700 | 22817400 | 21757500 |
| Anthracene | 13028500 | 23417800 | 20531900 | 12436000 | 24154500 | 21282900 |
| Benzo[*a*]pyprene | 116544000 | 109414000 | 150526000 | 112705000 | 116477000 | 143198000 |
| Benzo[*a*]pyprene | 104606000 | 94858500 | 187876000 | 109114000 | 110113000 | 158249000 |
| Benzo[*a*]pyprene | 92678500 | 96047000 | 176276000 | 95653300 | 110299000 | 174174000 |
| Benzo[*a*]pyprene | 115363000 | 66477200 | 183083000 | 120603000 | 98948800 | 188271000 |
| Pyrene | 34096700 | 30870700 | 26617000 | 33031400 | 34470000 | 27154500 |
| Pyrene | 32108500 | 35617200 | 26017700 | 26917300 | 34632100 | 25994300 |
| Pyrene | 31490400 | 27374100 | 26321400 | 29044200 | 35350200 | 28874100 |
| Pyrene | 30055800 | 34439300 | 26927000 | 27755100 | 32789300 | 28991400 |
| 7-Methylbenzo[*a*]pyrene | 24169400 | 37208900 | 53380400 | 26248900 | 38892300 | 53509100 |
| 7-Methylbenzo[*a*]pyrene | 26587700 | 38204900 | 51236300 | 26747700 | 38815200 | 52882200 |
| 7-Methylbenzo[*a*]pyrene | 27357000 | 36968900 | 45199000 | 25226400 | 37907800 | 54423800 |
| 7-Methylbenzo[*a*]pyrene | 23497600 | 34547100 | 41173900 | 22095400 | 38397500 | 52524600 |
| 9,10-Anthraquinone | 11147900 | 24398800 | 18068000 | 10947000 | 24463400 | 19391800 |
| 9,10-Anthraquinone | 11226500 | 23849900 | 18476600 | 11080900 | 24720900 | 18042800 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 9,10-Anthraquinone | 11676000 | 24553800 | 17363800 | 11097300 | 24587700 | 19216400 |
| 9,10-Anthraquinone | 11657800 | 24829300 | 18211300 | 10937400 | 25197700 | 18588800 |
| Quinizarin | 11925000 | 24554400 | 18587600 | 11383900 | 24701900 | 19118300 |
| Quinizarin | 11769400 | 25013500 | 18308200 | 11181800 | 25633900 | 18276400 |
| Quinizarin | 12345900 | 24730200 | 17827700 | 11436900 | 22692000 | 18453500 |
| Quinizarin | 12285500 | 24203200 | 17895200 | 11899500 | 26029100 | 18786000 |
| 9,10-dihydrobenzo[*a*]pyrene | 14778500 | 20718100 | 32570200 | 15378200 | 20907400 | 31204500 |
| 9,10-dihydrobenzo[*a*]pyrene | 15554100 | 21220200 | 36107600 | 14615400 | 20908700 | 32470400 |
| 9,10-dihydrobenzo[*a*]pyrene | 15044400 | 21103200 | 34842400 | 15145500 | 19672200 | 30999700 |
| 9,10-dihydrobenzo[*a*]pyrene | 15105500 | 20987900 | 34859200 | 15829100 | 21620100 | 36323400 |
| DDT | 11419700 | 25228800 | 77255500 | 10869700 | 26023900 | 79950200 |
| DDT | 11129000 | 26048100 | 74556400 | 11088900 | 25316400 | 80106900 |
| DDT | 11217500 | 25956500 | 77026300 | 10520600 | 26528800 | 79200400 |
| DDT | 10540700 | 26174300 | 74846500 | 10662900 | 26962100 | 76053600 |
| DDD | 10890700 | 28021000 | 70042900 | 9982200 | 29808000 | 79851000 |
| DDD | 10585200 | 25190100 | 64952000 | 10604100 | 27437800 | 72577100 |
| DDD | 10898900 | 23753200 | 74658800 | 10773000 | 22987000 | 70179200 |
| DDD | 11341200 | 28149900 | 72083400 | 10637100 | 27523800 | 78118500 |
| Deldrin | 6174160 | 4547020 | 12814100 | 5577860 | 5237860 | 12968500 |
| Deldrin | 5942320 | 4801120 | 11884600 | 5782650 | 3832920 | 12002600 |
| Deldrin | 6064750 | 5837520 | 12609100 | 5748400 | 4309740 | 12269900 |
| Deldrin | 5599550 | 6170930 | 12985000 | 5416730 | 5612480 | 12931000 |

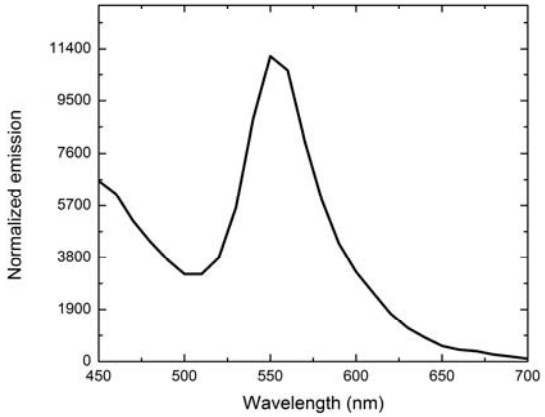
**TABLE S14.** Integration data for all analytes tested in a 1:1 v/v matrix of urine and 10 mM γ-cyclodextrin.

# FLUORESCENCE EMISSION GRAPHS IN URINE

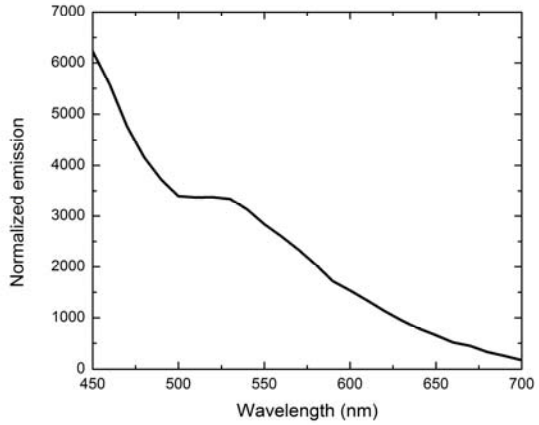
Analyte **1** – Fluorophore **31**



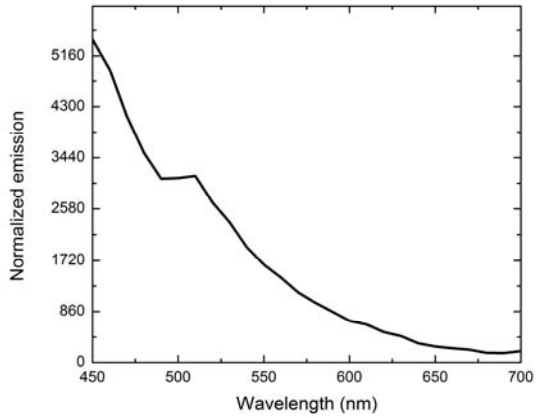

Analyte **1** – Fluorophore **32**



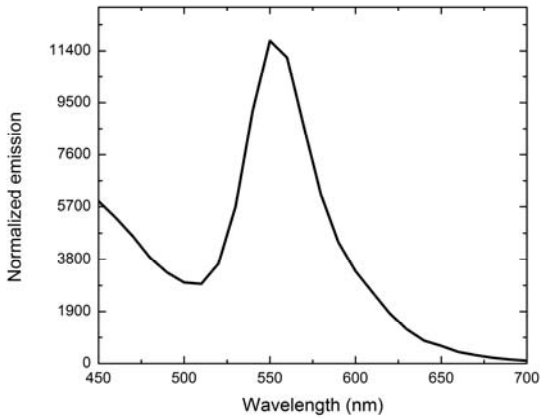

Analyte **1** – Fluorophore **33**



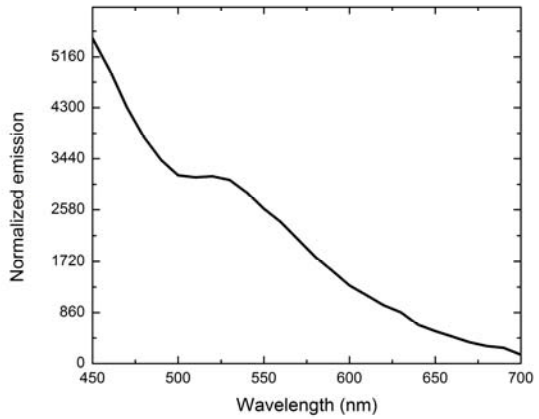
Analyte **2** – Fluorophore **31**



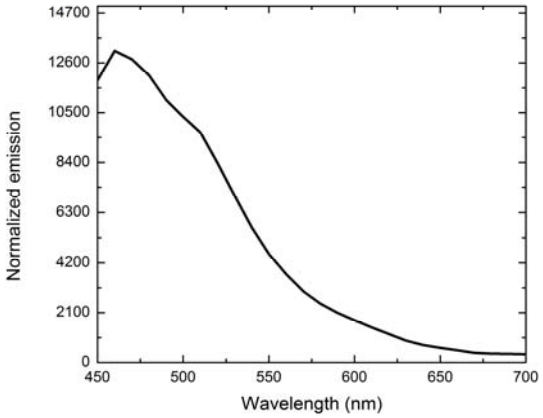

Analyte **2** – Fluorophore **32**



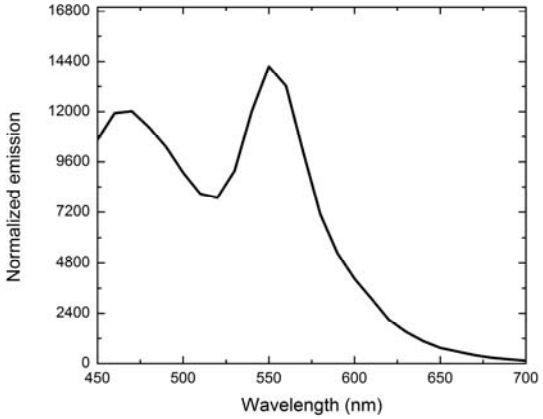

Analyte **2** – Fluorophore **33**



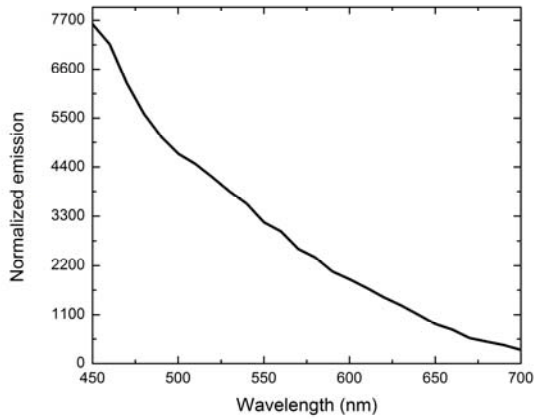
Analyte **5** – Fluorophore **31**



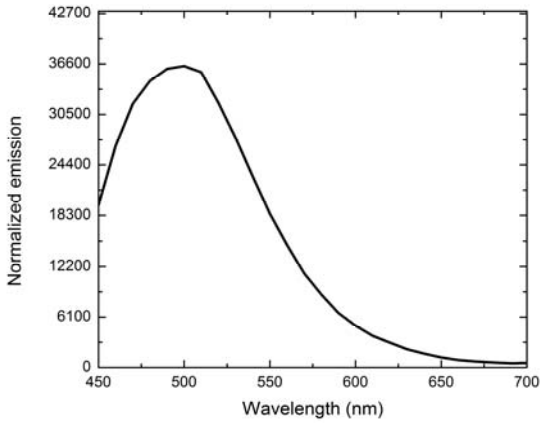

Analyte **5** – Fluorophore **32**



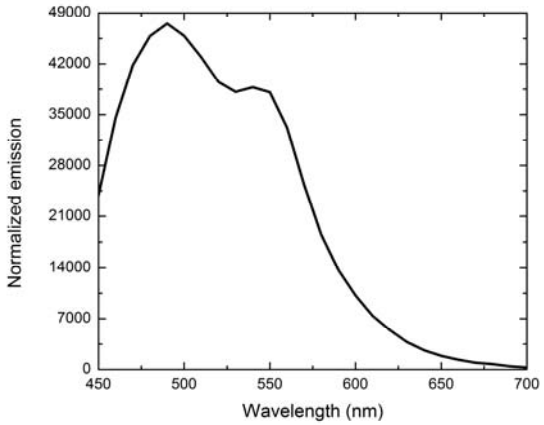

Analyte **5** – Fluorophore **33**



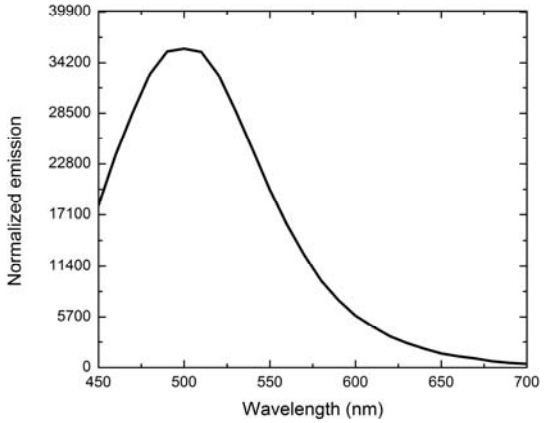
Analyte **6** – Fluorophore **31**



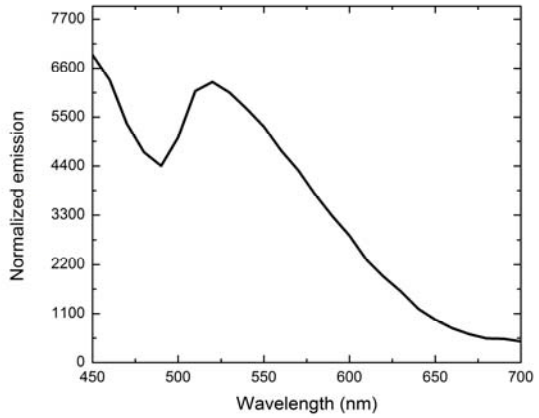

Analyte **6** – Fluorophore **32**



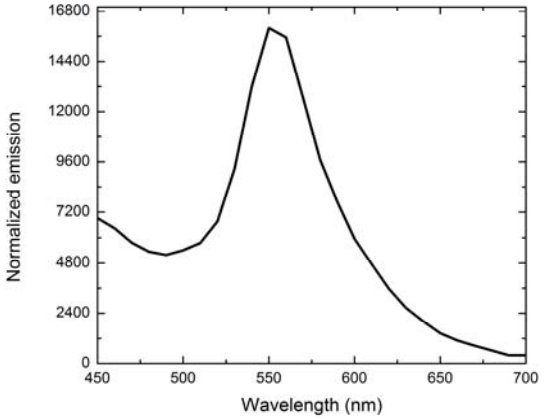

Analyte **6** – Fluorophore **33**



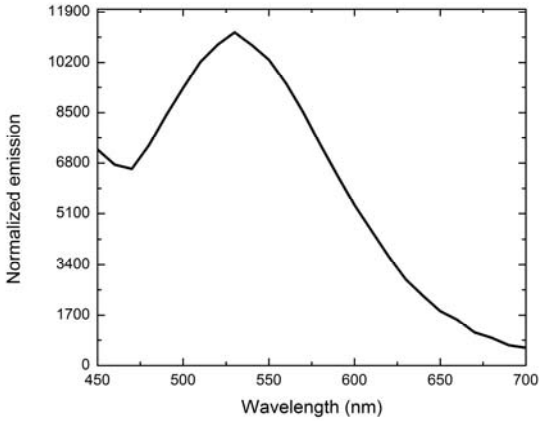
Analyte **7** – Fluorophore **31**



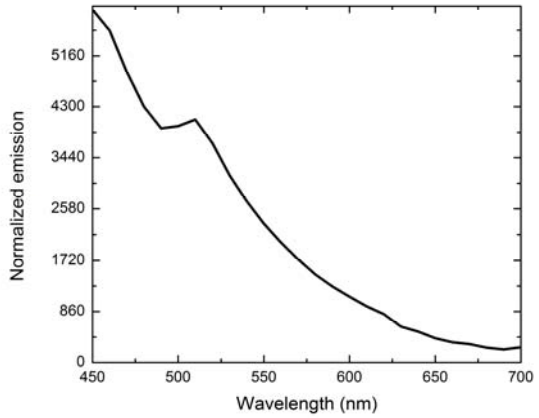

Analyte **7** – Fluorophore **32**



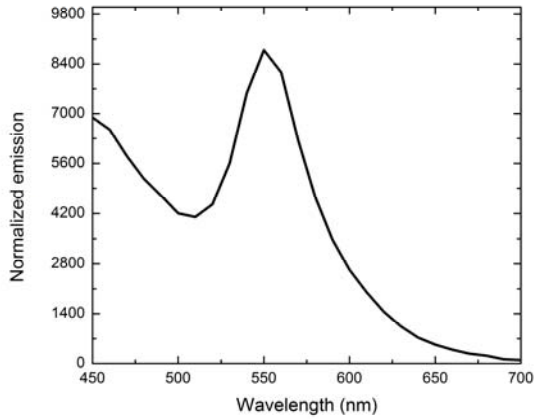

Analyte **7** – Fluorophore **33**



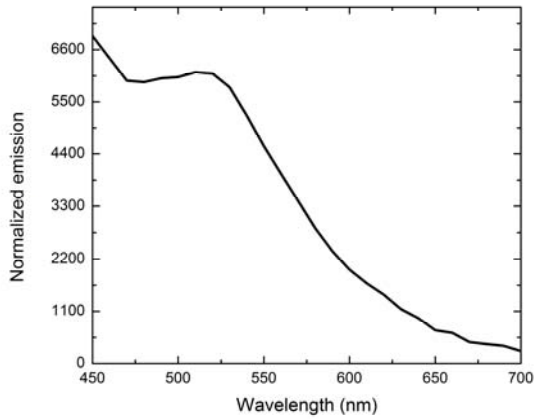
Analyte **8** – Fluorophore **31**



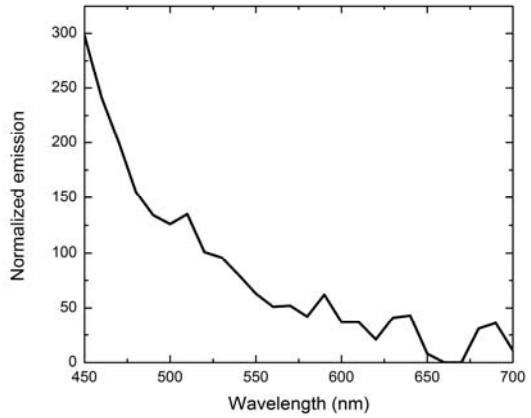

Analyte **8** – Fluorophore **32**



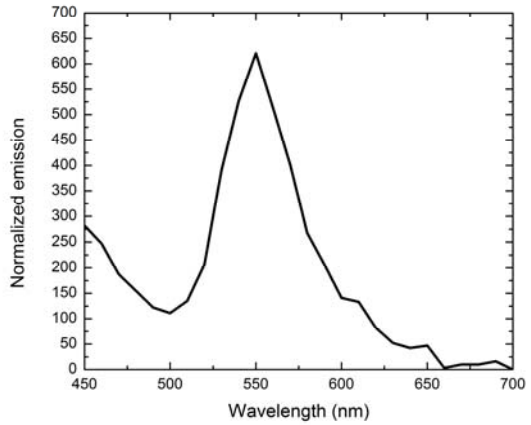

Analyte **8** – Fluorophore **33**



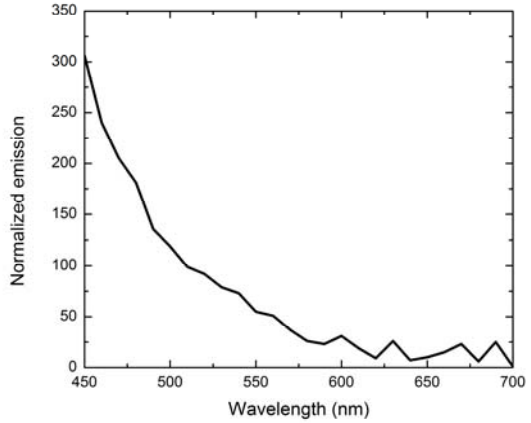
Analyte **11** – Fluorophore **31**



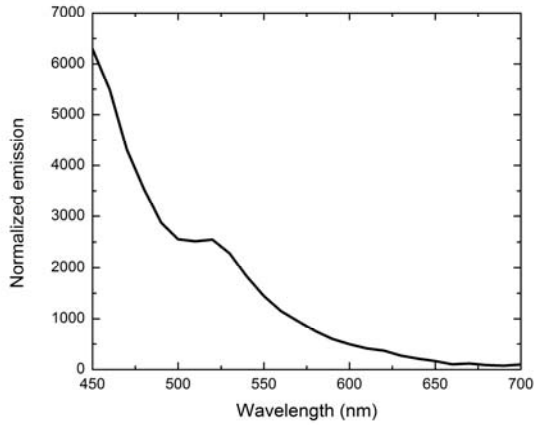

Analyte **11** – Fluorophore **32**



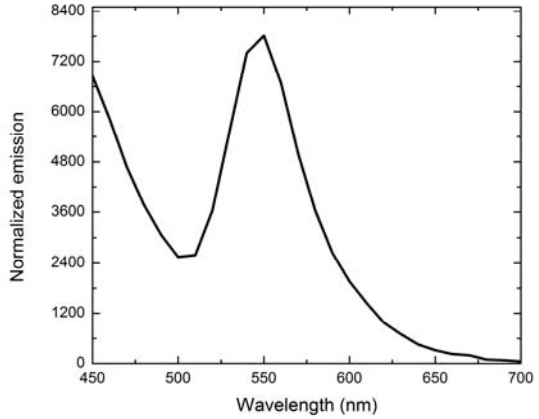

Analyte **11** – Fluorophore **33**



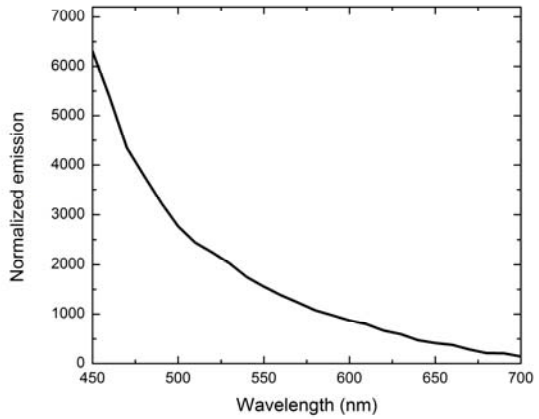
Analyte **12** – Fluorophore **31**



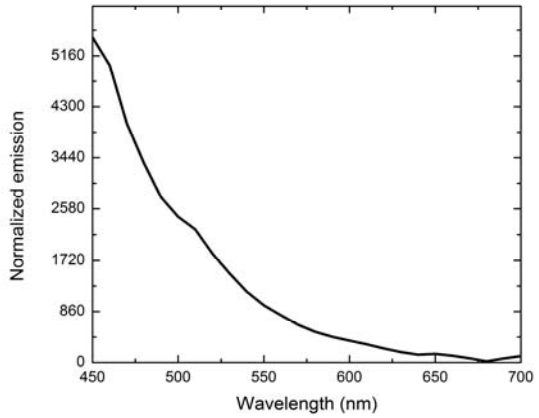

Analyte **12** – Fluorophore **32**



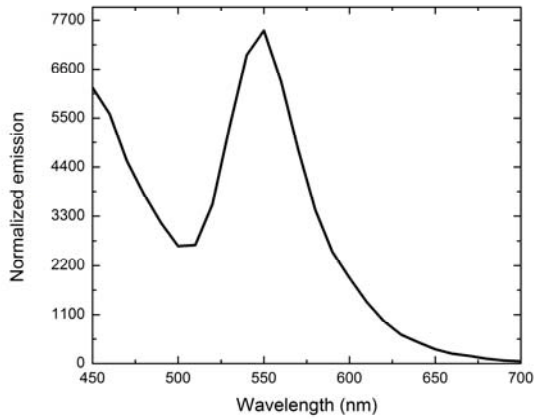

Analyte **12** – Fluorophore **33**



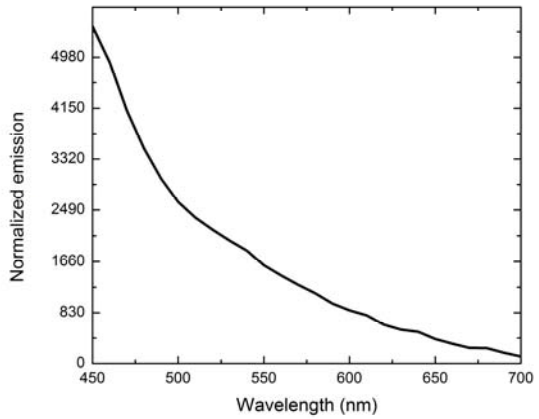
Analyte **13** – Fluorophore **31**



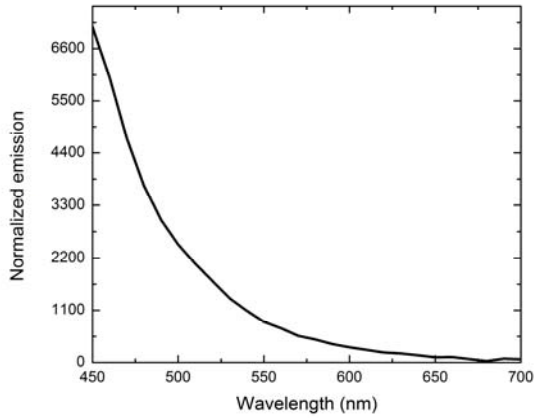

Analyte **13** – Fluorophore **32**



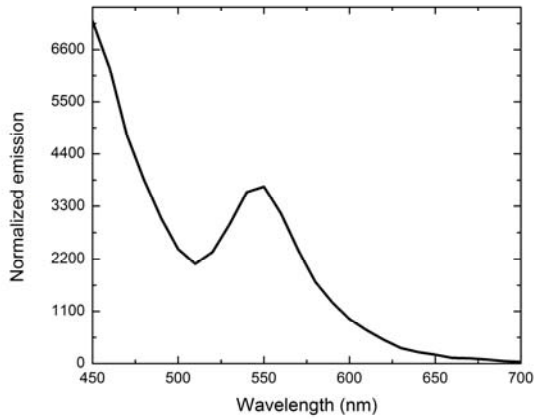

Analyte **13** – Fluorophore **33**



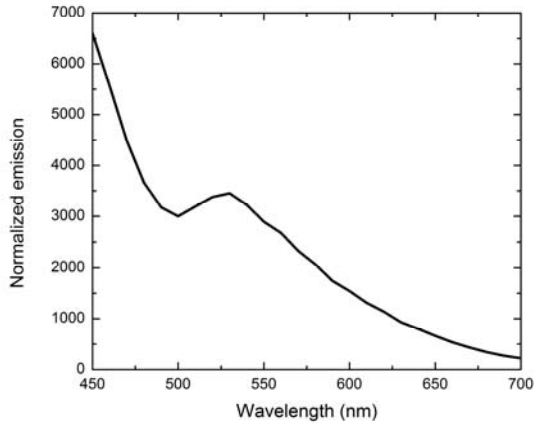
Analyte **14** – Fluorophore **31**



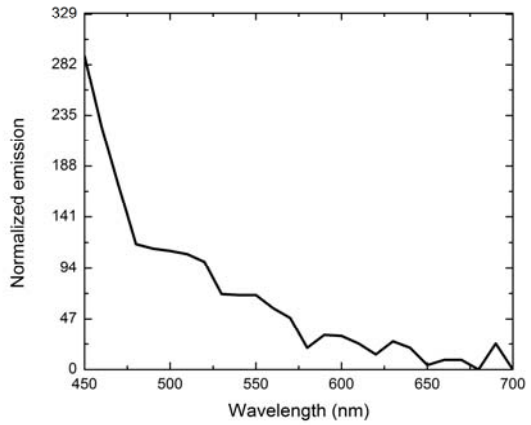

Analyte **14** – Fluorophore **32**



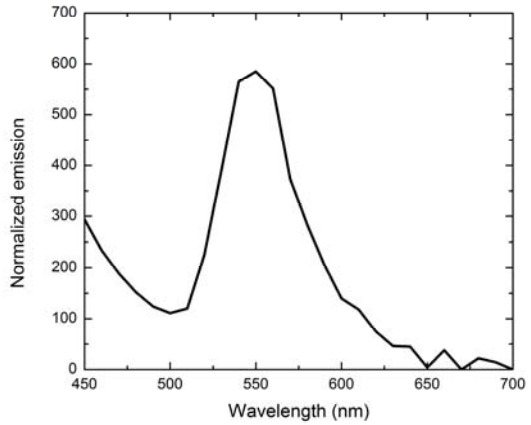

Analyte **14** – Fluorophore **33**



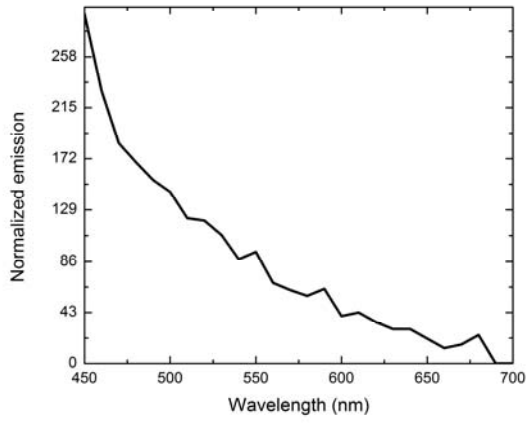
Analyte **15** – Fluorophore **31**



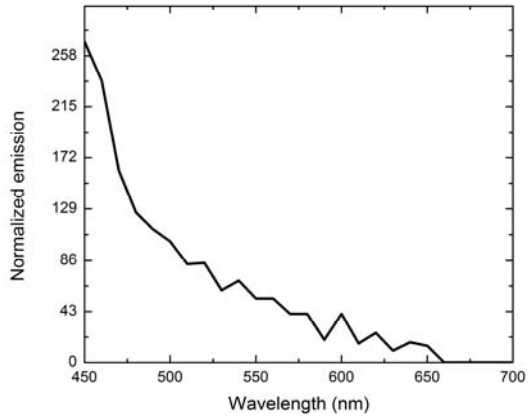

Analyte **15** – Fluorophore **32**



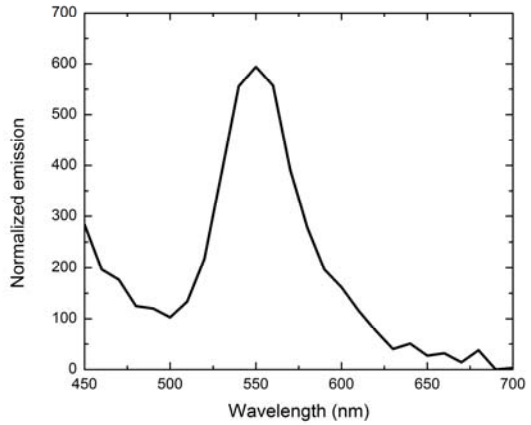

Analyte **15** – Fluorophore **33**



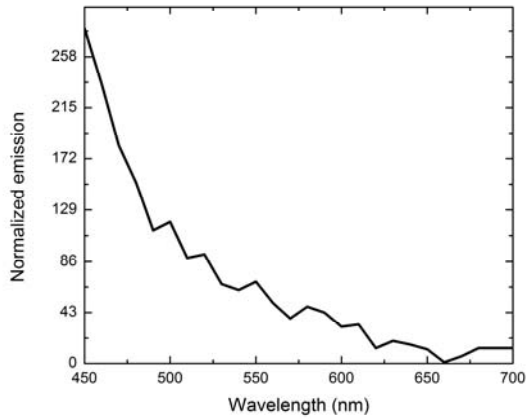
Analyte **16** – Fluorophore **31**



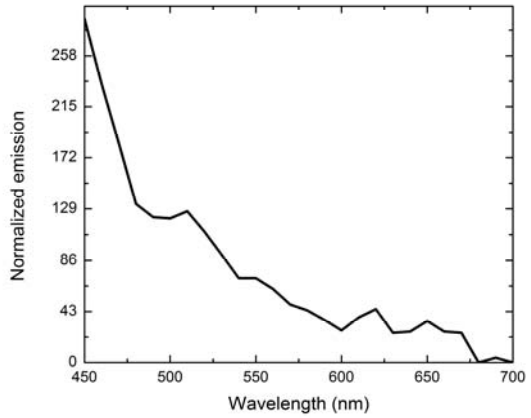

Analyte **16** – Fluorophore **32**



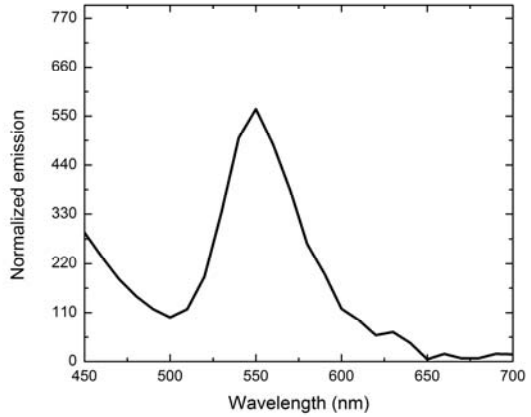

Analyte **16** – Fluorophore **33**



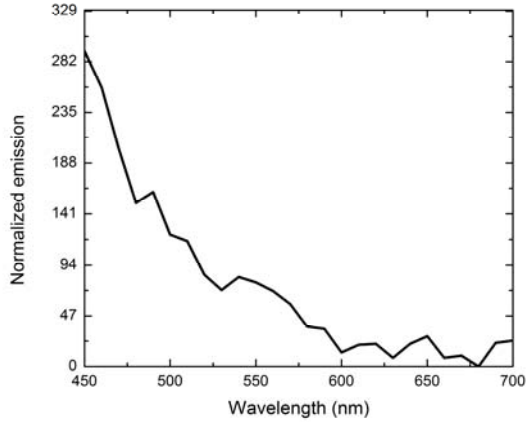
Analyte **17** – Fluorophore **31**



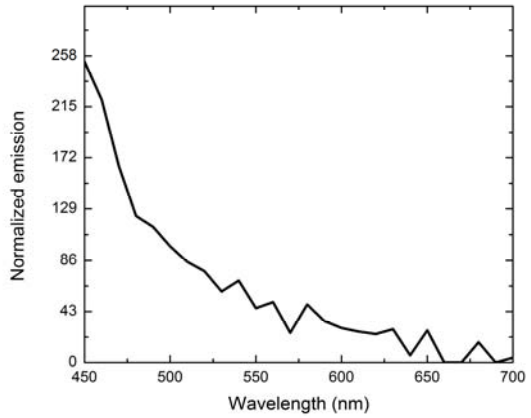

Analyte **17** – Fluorophore **32**



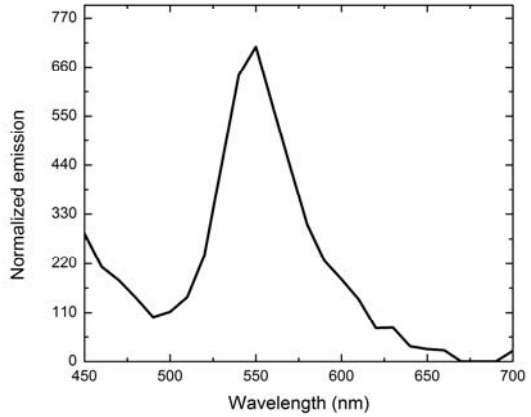

Analyte **17** – Fluorophore **33**



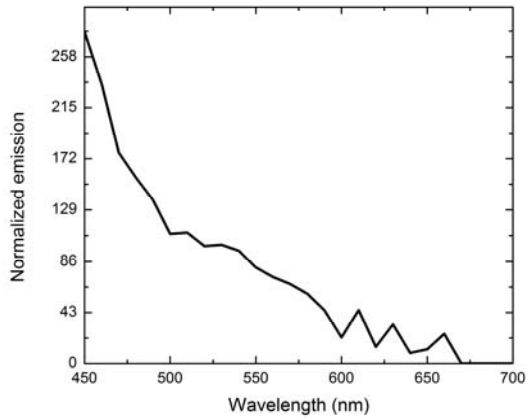
Analyte **18** – Fluorophore **31**



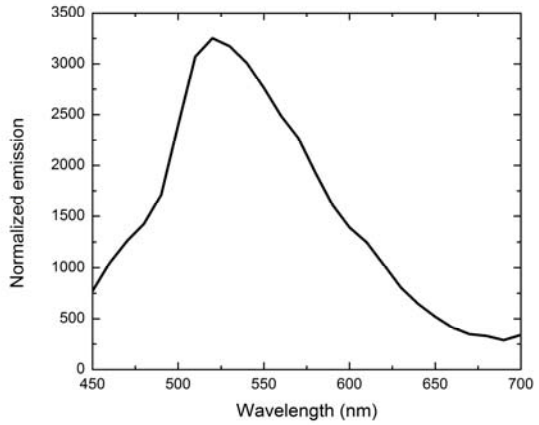

Analyte **18** – Fluorophore **32**



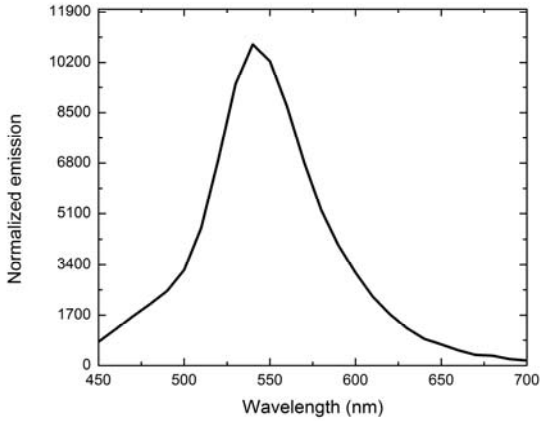

Analyte **18** – Fluorophore **33**



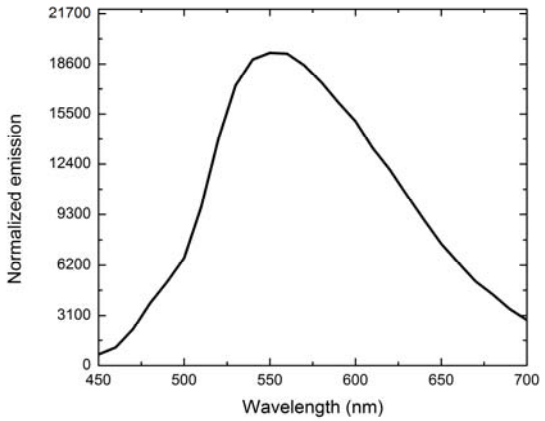
Analyte **19** – Fluorophore **31**



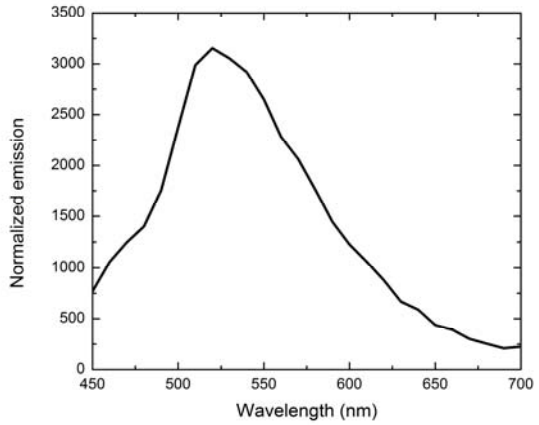

Analyte **19** – Fluorophore **32**



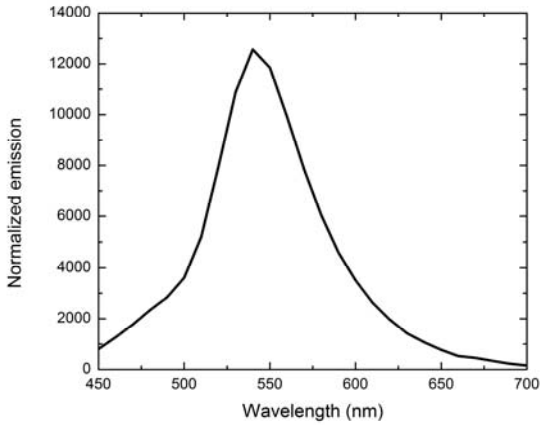

Analyte **19** – Fluorophore **33**



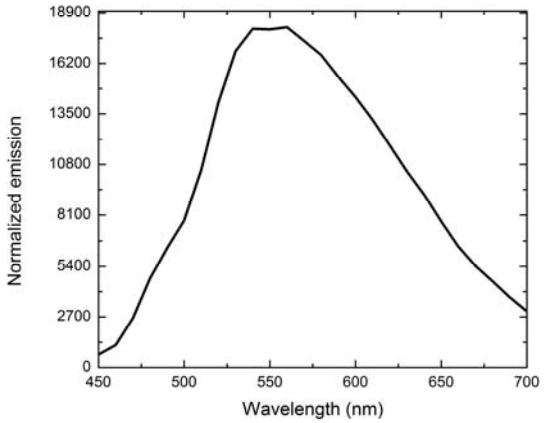
Analyte **20** – Fluorophore **31**



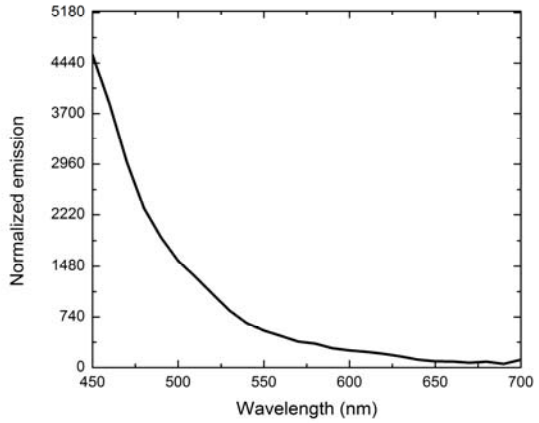

Analyte **20** – Fluorophore **32**



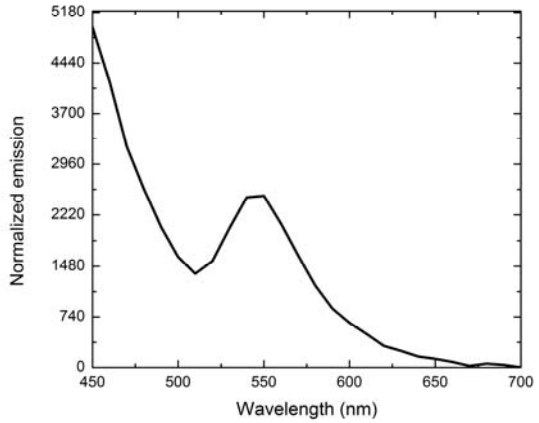

Analyte **20** – Fluorophore **33**



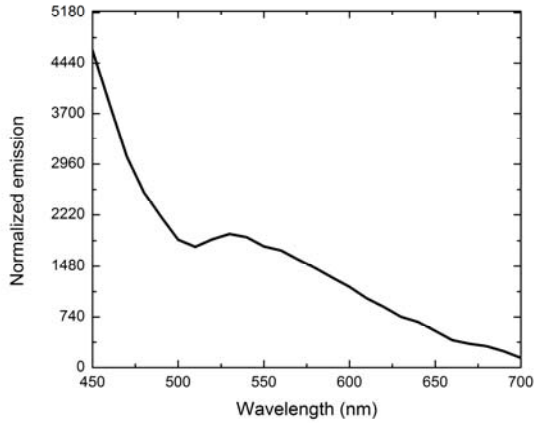
Analyte **21** – Fluorophore **31**



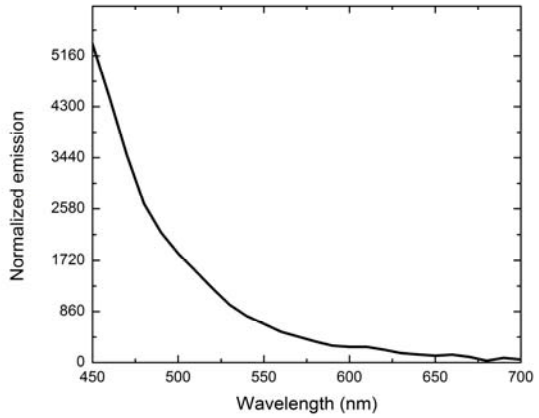

Analyte **21** – Fluorophore **32**



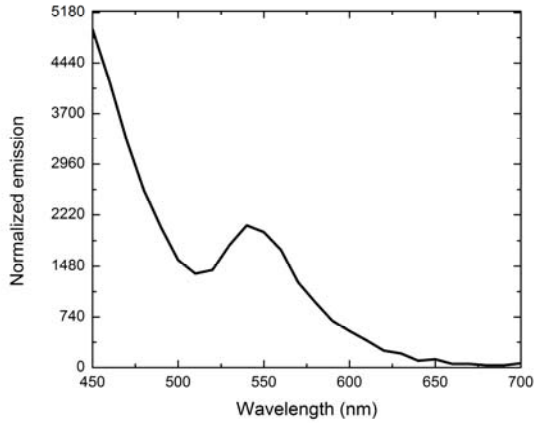

Analyte **21** – Fluorophore **33**



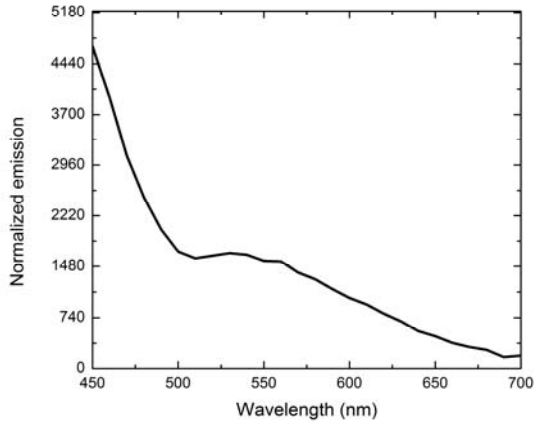
Analyte **22** – Fluorophore **31**




Analyte **22** – Fluorophore **32**




Analyte **22** – Fluorophore **33**



URINE ARRAY CLASSIFICATION ANALYSIS

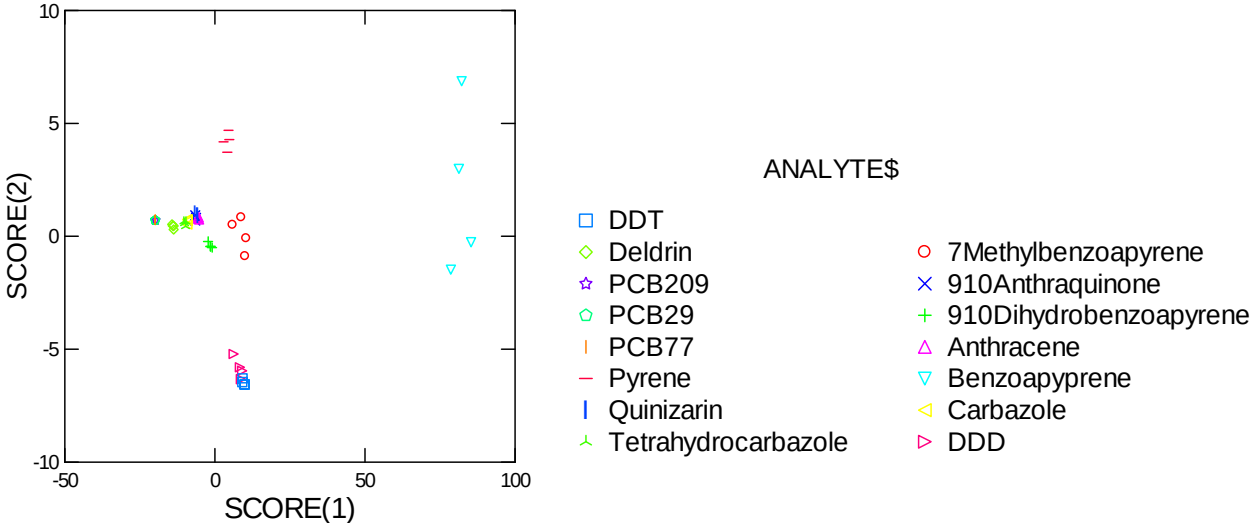



**Figure S6.** LDA Score plot of 15 analytes tested in a 1:1 v/v matrix of urine and 10 mM γ-cyclodextrin.

**Table S15**. Jackknifed classification matrix of 15 analytes tested in a 1:1 v/v matrix of urine and 10 mM γ-cyclodextrin.

| | **7** | **2** | **8** | **1** | **6** | **12** | **20** | **19** | **22** | **18** | **16** | **17** | **5** | **3** | **13** | %correct |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **7** | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 75 |
| **2** | 0 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 75 |
| **8** | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| **1** | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| **6** | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| **12** | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| **20** | 0 | 0 | 0 | 0 | 0 | 0 | 2 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 50 |
| **19** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| **22** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| **18** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 0 | 100 |
| **16** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 0 | 100 |
| **17** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 0 | 100 |
| **5** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 0 | 100 |
| **3** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 0 | 100 |
| **13** | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | 100 |
| Total | 3 | 3 | 4 | 4 | 4 | 4 | 2 | 6 | 4 | 4 | 4 | 4 | 5 | 5 | 4 | 93 |

**Table S16.** Cumulative proportion of total dispersion values.

| | | |
|---|---|---|
| 0.987 | 0.999 | 1.000 |

## URINE UNKNOWN CLASSIFICATION

**Table S17.** LDA Score values for each analyte ("Analyte ID") and the unknown classification identities ("Unknown Classification").

| Score 1 | Score 2 | Score 3 | Analyte ID | Unknown Classification |
|---|---|---|---|---|
| -9.1054548 | 0.756718249 | -0.182720436 | Carbazole | Tetrahydrocarbazole |
| -9.243637707 | 0.740388335 | -0.132672994 | Carbazole | Carbazole |
| -9.140747219 | 0.519515068 | -0.38834831 | Carbazole | Carbazole |
| -9.022878737 | 0.678719826 | -0.342976678 | Carbazole | Carbazole |
| -9.757566263 | 0.441749371 | -0.390803807 | Tetrahydrocarbazole | Carbazole |
| -10.08634234 | 0.575262349 | -0.115856847 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -10.31870806 | 0.657523289 | -0.106367092 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -9.656283869 | 0.656556425 | -0.428863697 | Tetrahydrocarbazole | Tetrahydrocarbazole |
| -19.87616018 | 0.729168476 | 1.167700303 | PCB77 | PCB77 |
| -19.86006961 | 0.719961447 | 1.173358423 | PCB77 | PCB77 |
| -19.88086477 | 0.735333587 | 1.169547405 | PCB77 | PCB77 |
| -19.87802358 | 0.735568165 | 1.172717833 | PCB77 | PCB77 |
| -19.87994901 | 0.713275761 | 1.133333328 | PCB29 | PCB29 |
| -19.89768646 | 0.718060321 | 1.137823784 | PCB29 | PCB29 |
| -19.88478529 | 0.716984212 | 1.130400647 | PCB29 | PCB29 |
| -19.88965283 | 0.709828148 | 1.134060242 | PCB29 | PCB29 |
| -19.85037159 | 0.709472276 | 1.112296995 | PCB209 | PCB209 |
| -19.84219815 | 0.705185473 | 1.115286635 | PCB209 | PCB209 |
| -19.85178296 | 0.707628142 | 1.116378377 | PCB209 | PCB209 |
| -19.82825713 | 0.707828739 | 1.10497862 | PCB209 | PCB209 |
| -5.814613075 | 0.799740692 | -0.972399713 | Anthracene | Anthracene |
| -5.44346416 | 0.842293035 | -0.906854684 | Anthracene | Anthracene |
| -5.283017304 | 0.747548729 | -0.884546932 | Anthracene | Anthracene |
| -5.517496756 | 0.846168898 | -0.913831327 | Anthracene | Anthracene |
| 82.19449476 | 6.868831096 | -1.999495187 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 85.36506846 | -0.262116452 | 0.467214228 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 78.61883341 | -1.480427087 | -1.246148356 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 81.28307897 | 2.986362869 | 6.333567677 | Benzo[*a*]pyrene | Benzo[*a*]pyrene |
| 4.559783717 | 4.690369497 | 0.023421172 | Pyrene | Pyrene |
| 4.798744352 | 4.278616481 | -1.017169865 | Pyrene | Pyrene |
| 2.872694459 | 4.182809927 | 0.370322234 | Pyrene | Pyrene |
| 4.128228618 | 3.722395659 | -0.985659052 | Pyrene | Pyrene |
| 10.0722822 | -0.883871018 | -1.270610905 | 7-Methylbenzo[*a*]pyrene | 7-Methylbenzo[*a*]pyrene |
| 10.48300485 | -0.092005484 | -1.270751938 | 7-Methylbenzo[*a*]pyrene | 7-Methylbenzo[*a*]pyrene |
| 8.809116384 | 0.837797802 | -1.156433777 | 7-Methylbenzo[*a*]pyrene | 7-Methylbenzo[*a*]pyrene |
| 5.935696225 | 0.504041614 | -1.228855724 | 7-Methylbenzo[*a*]pyrene | 7-Methylbenzo[*a*]pyrene |
| -6.580414377 | 0.725109916 | -1.341103353 | 9,10-Anthraquinone | 9,10-Anthraquinone |

| | | | | |
|---|---|---|---|---|
| -6.564001984 | 0.697182536 | -1.225634123 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -6.568938996 | 0.927849852 | -1.337128783 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -6.282678944 | 0.816250453 | -1.362201304 | 9,10-Anthraquinone | 9,10-Anthraquinone |
| -6.154250477 | 0.83149894 | -1.27706798 | Quinizarin | 9,10-Anthraquinone |
| -6.179844698 | 0.827223813 | -1.380608951 | Quinizarin | Quinizarin |
| -6.187915716 | 1.017180411 | -1.288837822 | Quinizarin | Quinizarin |
| -6.304629728 | 1.000473862 | -1.200767295 | Quinizarin | Quinizarin |
| -2.257423388 | -0.230747393 | 0.080918036 | 9,10-Dihydrobenzo[*a*]pyrene | 9,10-Dihydrobenzo[*a*]pyrene |
| -0.930911084 | -0.5016518 | 0.172635181 | 9,10-Dihydrobenzo[*a*]pyrene | 9,10-Dihydrobenzo[*a*]pyrene |
| -1.466342294 | -0.456835418 | 0.106189511 | 9,10-Dihydrobenzo[*a*]pyrene | 9,10-Dihydrobenzo[*a*]pyrene |
| -1.467415439 | -0.444273554 | 0.132784785 | 9,10-Dihydrobenzo[*a*]pyrene | 9,10-Dihydrobenzo[*a*]pyrene |
| 9.864724835 | -6.55090804 | 0.272761912 | DDT | DDT |
| 9.213487032 | -6.288968348 | 0.022312127 | DDT | DDT |
| 9.896843993 | -6.5742923 | 0.119241935 | DDT | DDT |
| 9.131227759 | -6.456464218 | -0.048759279 | DDT | DDT |
| 8.336580052 | -5.801789774 | -0.477504735 | DDD | DDT |
| 6.225329147 | -5.212107051 | -0.162162712 | DDD | DDT |
| 8.663483139 | -6.330708606 | 0.403442101 | DDD | DDD |
| 9.06746279 | -5.95583299 | -0.396235736 | DDD | DDD |
| -13.97580639 | 0.463114034 | 1.48439872 | Deldrin | Deldrin |
| -14.24861212 | 0.52439495 | 1.390164465 | Deldrin | Deldrin |
| -13.78363083 | 0.451918187 | 1.242409515 | Deldrin | Deldrin |
| -13.7573368 | 0.299098618 | 1.149713201 | Deldrin | Deldrin |