Electronic Supplementary Information for
**Sensitive and Selective Detection of Alcohols via Fluorescence
Modulation**
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MATERIALS AND METHODS

All analytes and cyclodextrins were obtained from Sigma-Aldrich chemical company. MCHM was obtained from Tokyo Chemical Company. Fluorophore **14**, BODIPY, was synthesized according to literature procedures. All fluorescence measurements were performed using a Shimadzu RF 5301 spectrophotometer. Both the excitation slit width and the emission slit width were 1.5 nm. All fluorescence spectra were integrated vs. wavenumber on the X-axis using OriginPro Version 9.1. All arrays were generated using SYSTAT Version 13.

DETAILS OF ANALYTES AND FLUOROPHORES

All analytes were prepared at a concentration of 1 mg/mL in tetrahydrofuran (THF). All fluorophores were prepared at 0.1 mg/mL in THF. The final concentrations of all analytes and fluorophores are shown in the tables below.

Final Analyte Concentrations:

Analyte Number	Amount Added	Final Concentration
1	20 μ L	75.3 μ M
2	20 μ L	76.8 μ M
3	20 μ L	241 μ M
4	20 μ L	167 μ M
5	20 μ L	124 μ M
6	20 μ L	104 μ M
7	20 μ L	89.3 μ M
8	20 μ L	59.9 μ M
9	20 μ L	137 μ M
10	20 μ L	81.7 μ M
11	20 μ L	71.1 μ M
12	20 μ L	104 μ M
13	20 μ L	107 μ M

Final Fluorophore Concentrations:

Fluorophore Number	Amount Added	Final Concentration
14	100 μ L	9.5 μ M
15	100 μ L	11 μ M
16	100 μ L	8.1 μ M

SYNTHESIS OF FLUOROPHORE 14:

Synthesis of BODIPY (compound 14):

The synthesis of BODIPY **14** was performed according to literature procedures:

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

Reaction 1:

Procedure: 2.0 grams of 11-bromoundecanoic acid **S1** (7.54 mmol, 1.0 eq.) was combined with 2 drops of *N,N*-dimethylformamide in 40 mL of dichloromethane. 1.0 gram of oxalyl chloride **S2** (7.88 mmol, 1.05 eq.) was dissolved in 5.0 mL of dichloromethane and added dropwise. The reaction mixture was stirred for one hour, then the crude mixture was concentrated on the rotary evaporator and dried on a vacuum overnight to remove any unreacted oxalyl chloride. The resulting acid chloride **S3** was dissolved in 50 mL of dichloromethane. 0.772 mL of 2,4-dimethylpyrrole **S4** (7.50 mmol, 0.99 eq.) was dissolved in 5.0 mL of dichloromethane and added to the reaction mixture. The resulting reaction mixture was heated to reflux for 3 hours under a nitrogen atmosphere, during which time the mixture became a dark red color. After three hours, the reaction mixture was cooled to room temperature and solvent was removed on the rotary evaporator until approximately 5.0 mL of the dichloromethane solution remained. 200 mL of *n*-hexanes were added to the flask, and the mixture was cooled overnight in the freezer at $-20\text{ }^\circ\text{C}$. The hexanes were decanted from the insoluble oil and precipitate. The resulting crude product was dissolved in 75 mL of toluene and heated to $80\text{ }^\circ\text{C}$. 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 $80\text{ }^\circ\text{C}$ 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 (comparable to the literature-reported 24% yield).

Reaction 2:

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

two hours, the reaction mixture was cooled to room temperature, acetone was removed, and the crude solid was re-dissolved in dichloromethane and washed with water. The organic extract was dried over sodium sulfate, filtered and concentrated, to yield compound **S7** in 97% yield (0.932 grams).

Reaction 3:

Procedure: Compound **S7** (0.932 grams, 2.01 mmol, 1.0 eq.) was dissolved in 150 mL of anhydrous ethanol that was purged with nitrogen. Potassium carbonate was added, and the reaction mixture was warmed to 30 °C. The reaction mixture was stirred under nitrogen for 4 hours at 30 °C. The contents of the flask were poured over 40 mL of aqueous saturated ammonium chloride, at which point the solution turned bright orange. The product was extracted with dichloromethane and washed several times with water. The organic layer was dried over sodium sulfate, filtered, and concentrated. The product was purified via flash chromatography (1:1 dichloromethane: hexanes) to yield compound **14** in 76% yield (674 mg).

EXPERIMENTAL DETAILS FOR FLUORESCENCE MODULATION EXPERIMENTS

In a quartz cuvette, 2.5 mL of a 10 mM cyclodextrin solution in phosphate-buffered saline (PBS) and 100 μ L of a fluorophore **14** solution (0.1 mg/mL in THF) were combined. The solution was excited at 460 nm, which is the excitation wavelength to directly excite **14**. 20 μ L of a 1 mg/mL analyte solution in THF was added to the cuvette, and fluorescence measurements were repeated at 460 nm. The experiments were repeated for fluorophore **15** and **16** at excitation wavelengths of 420 nm and 490 nm, respectively. The fluorescence spectra were integrated vs. wavenumber on the X-axis, and fluorescence modulation was determined by quantifying a fluorophore ratio according to Equation 1:

$$\text{Fluorophore Ratio} = (F_{l_{\text{alcohol}}})/F_{l_{\text{blank}}} \quad (\text{Equation 1})$$

where $F_{l_{\text{alcohol}}}$ is the fluorescence emission of the fluorophore in the presence of the alcohol, and $F_{l_{\text{blank}}}$ is the fluorescence emission of the fluorophore in the absence of the alcohol.

Each experiment was repeated four times. The reported values are the average of the results.

EXPERIMENTAL DETAILS FOR LIMIT OF DETECTION EXPERIMENTS

The limit of detection (LOD) is defined as the lowest concentration of analyte at which a signal can be detected. The limit of quantification is defined at the lowest concentration of analyte that can be accurately quantified. These experiments were conducted following literature-reported procedures:

Saute, B.; Premasiri, R.; Ziegler, L.; Narayanan, R. "Gold Nanorods as Surface Enhanced Raman Spectroscopy Substrates for Sensitive and Selective Detection of Ultra-Low Levels of Dithiocarbamate Pesticides." *Analyst* **2012**, *137*, 5082-5087.

To determine the limit of detection (LOD) and limit of quantification (LOQ), each fluorophore-analyte-cyclodextrin combination was examined in the following manner:

1. 2.5 mL of 10 mM cyclodextrin in phosphate-buffered saline (PBS) was measured into a cuvette and 100 μ L of a fluorophore solution (0.1 mg/mL) in THF was added. The solution was excited at the fluorophore's excitation wavelength and the fluorescence emission spectrum was recorded. Six repeat measurements were made for the fluorescence emission spectra.
2. 20 μ L of the analyte was added to the cuvette and the solution was again excited at the fluorophore's excitation wavelength. Six repeat measurements were taken.
3. Step 2 was repeated for 40 μ L of analyte, 60 μ L of analyte, 80 μ L of analyte, and 100 μ L of analyte. In each case, the solution was excited at the fluorophore's excitation wavelength and the fluorescence emission spectrum was recorded four times.
4. All fluorescence emission spectra were integrated vs. wavenumber, and calibration curves were generated with the analyte concentration on the X-axis (in μ M) and the integrated fluorophore emission on the Y-axis. The curve was then fitted to a straight line and an equation for the line was determined.
5. For each case, the fluorophore with cyclodextrin (before any analyte was added) was also excited at its excitation wavelength, and the fluorescence emission spectrum was recorded (as per step 1). These measurements are referred to as the "blank."
6. The limit of the blank is defined according to the following equation:

$$LoBLOD = m_{blank} + 3(SD_{blank})$$

Where m is the mean of the blank integrations and SD is the standard deviation.

7. The limit of the blank was then entered into the equation determined in step 4 (for the y value), and the corresponding X value was determined. This value provided the LOD in μ M.
8. The limit of quantification (LOQ) was calculated in a similar way to the limit of detection. First, the limit of the blank for quantification was determined according to the following equation:

$$LoBLOQ = m_{blank} + 10(SD_{blank})$$

This value was entered into the equation determined in step 4 (for the y value), and the corresponding X value was determined to be the limit of quantification in μ M.

EXPERIMENTAL DETAILS FOR ARRAY GENERATION EXPERIMENTS

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

Arrays were generated for: (a) all analyte-fluorophore-cyclodextrin combinations in one array; and (b) individual cyclodextrin hosts in separate arrays. The results are summarized in the tables.

SUMMARY TABLES

SUMMARY TABLES FOR FLUORESCENCE MODULATION EXPERIMENTS

Fluorophore ratios of analytes 1-13 in combination with fluorophore 15^a

Analyte	α -CD	β -CD	Me- β -CD	2-HPCD
1	1.09 $\pm$ 0.01	1.01 $\pm$ 0.01	0.60 $\pm$ 0.14	0.99 $\pm$ 0.02
2	1.08 $\pm$ 0.01	1.04 $\pm$ 0.01	0.68 $\pm$ 0.14	0.17 $\pm$ 0.04
3	1.09 $\pm$ 0.00	0.98 $\pm$ 0.01	0.71 $\pm$ 0.14	0.21 $\pm$ 0.06
4	1.13 $\pm$ 0.01	1.08 $\pm$ 0.03	0.75 $\pm$ 0.06	1.04 $\pm$ 0.07
5	1.01 $\pm$ 0.01	1.00 $\pm$ 0.02	0.83 $\pm$ 0.08	0.97 $\pm$ 0.02
6	1.05 $\pm$ 0.01	0.95 $\pm$ 0.01	0.92 $\pm$ 0.00	0.88 $\pm$ 0.01
7	0.92 $\pm$ 0.02	0.87 $\pm$ 0.02	0.90 $\pm$ 0.01	0.86 $\pm$ 0.01
8	1.02 $\pm$ 0.02	0.92 $\pm$ 0.01	0.81 $\pm$ 0.01	0.85 $\pm$ 0.01
9	0.95 $\pm$ 0.00	0.26 $\pm$ 0.07	0.97 $\pm$ 0.00	0.65 $\pm$ 0.05
10	1.22 $\pm$ 0.01	0.37 $\pm$ 0.12	0.94 $\pm$ 0.00	0.73 $\pm$ 0.06
11	1.07 $\pm$ 0.01	0.53 $\pm$ 0.20	0.96 $\pm$ 0.00	0.81 $\pm$ 0.04
12	1.03 $\pm$ 0.01	0.49 $\pm$ 0.21	0.97 $\pm$ 0.00	0.75 $\pm$ 0.04
13	1.07 $\pm$ 0.01	0.88 $\pm$ 0.01	0.98 $\pm$ 0.00	0.97 $\pm$ 0.01

^a All values were calculated according to Equation 1 and represent the average of 4 trials.

Fluorophore ratios of analytes 1-13 in combination with fluorophore 16^a

Analyte	α -CD	β -CD	Me- β -CD	2-HPCD
1	1.00 $\pm$ 0.01	1.03 $\pm$ 0.01	1.00 $\pm$ 0.00	1.01 $\pm$ 0.01
2	1.01 $\pm$ 0.01	0.98 $\pm$ 0.02	1.17 $\pm$ 0.02	1.02 $\pm$ 0.01
3	1.01 $\pm$ 0.01	1.03 $\pm$ 0.01	1.39 $\pm$ 0.03	1.09 $\pm$ 0.00
4	1.03 $\pm$ 0.02	1.00 $\pm$ 0.02	1.17 $\pm$ 0.01	0.99 $\pm$ 0.01
5	1.03 $\pm$ 0.02	1.00 $\pm$ 0.01	1.08 $\pm$ 0.01	1.07 $\pm$ 0.01
6	1.01 $\pm$ 0.01	1.05 $\pm$ 0.02	1.14 $\pm$ 0.03	1.03 $\pm$ 0.01
7	0.97 $\pm$ 0.01	0.96 $\pm$ 0.02	1.00 $\pm$ 0.01	0.98 $\pm$ 0.01
8	0.97 $\pm$ 0.01	0.99 $\pm$ 0.01	0.99 $\pm$ 0.02	0.99 $\pm$ 0.01
9	1.01 $\pm$ 0.00	1.00 $\pm$ 0.00	0.99 $\pm$ 0.00	1.01 $\pm$ 0.00
10	1.00 $\pm$ 0.00	1.00 $\pm$ 0.00	0.99 $\pm$ 0.00	1.00 $\pm$ 0.00
11	0.97 $\pm$ 0.00	0.98 $\pm$ 0.00	0.99 $\pm$ 0.00	1.00 $\pm$ 0.00
12	0.99 $\pm$ 0.00	0.98 $\pm$ 0.00	0.98 $\pm$ 0.00	0.99 $\pm$ 0.01
13	0.98 $\pm$ 0.00	0.98 $\pm$ 0.00	0.98 $\pm$ 0.00	0.99 $\pm$ 0.01

^a All values were calculated according to Equation 1 and represent the average of 4 trials.

SUMMARY TABLE FOR DIFFERENT SOLVENT SYSTEMS USING ANALYTE 8 IN β -CYCLODEXTRIN

	Fluorophore 14	Fluorophore 15	Fluorophore 16
1 M NaCl	1.02 ± 0.01	0.97 ± 0.01	0.99 ± 0.00
ultrapure water	1.02 ± 0.01	0.89 ± 0.00	0.96 ± 0.00
seawater	1.06 ± 0.01	1.03 ± 0.01	0.98 ± 0.00
PBS	1.06 ± 0.01	1.03 ± 0.01	0.96 ± 0.00

SUMMARY TABLES FOR LOD EXPERIMENTS

Analyte	Fluorophore	CD	LOD (μM)	LOQ (μM)	Equation	R^2
1	14	α -CD	102.2	204.6	$y = 52.897x + 35048$	0.9972
1	14	β -CD	<i>a</i>	43.8	$y = 55.104x + 49523$	0.9846
1	14	Me- β -CD	<i>a</i>	77.0	$y = 77.26x + 82316$	0.9999
1	14	2-HPCD	109.2	200.4	$y = 76.811x + 43207$	0.9984
1	14	PBS	8.0	46.7	$y = 87.498x + 43572$	0.9976
2	14	α -CD	18.0	192.3	$y = 42.312x + 46434$	0.9784
2	14	β -CD	30.1	71.2	$y = 73.443x + 49933$	0.9923
2	14	Me- β -CD	401.6	427.9	$y = 13.153x + 85888$	0.9639
2	14	2-HPCD	21.5	82.1	$y = 62.827x + 52136$	0.9994
2	14	PBS	12.2	15.4	$y = 103.59x + 42017$	0.9998
3	14	α -CD	<i>a</i>	14256.0	$y = 2.0296x + 107479$	0.9079
3	14	β -CD	<i>a</i>	221.0	$y = 26.049x + 63193$	0.9988
3	14	Me- β -CD	2298.0	2383.0	<i>b</i>	<i>b</i>
3	14	2-HPCD	352.0	677.0	$y = 25.508x + 61113$	0.9963
3	14	PBS	<i>a</i>	185.0	$y = 38.138x + 49325$	0.9888
3	15	α -CD	151.0	264.0	$y = 22.966x + 66914$	0.9951
3	15	β -CD	<i>a</i>	<i>a</i>	$y = -24.062x + 135707$	0.9448
3	15	Me- β -CD	<i>a</i>	<i>a</i>	$y = -463.38x + 1\text{E}6$	0.9999
3	15	2-HPCD	223.0	170.0	$y = -251.97x + 407239$	0.9825
3	15	PBS	201.0	291.0	$y = 23.444x + 62467$	0.9970
3	16	α -CD	<i>a</i>	<i>a</i>	$y = -67.888x + 1\text{E}6$	0.9943
3	16	β -CD	<i>a</i>	<i>a</i>	$y = -67.49x + 1\text{E}6$	0.9760
3	16	Me- β -CD	<i>a</i>	<i>a</i>	$y = -44.365x + 1\text{E}6$	0.9879
3	16	2-HPCD	<i>a</i>	<i>a</i>	$y = -25.44x + 1\text{E}6$	0.8746
3	16	PBS	<i>a</i>	<i>a</i>	$y = -31.313x + 770331$	0.7262
4	14	α -CD	178.0	1204.0	$y = 23.887X + 55946$	0.9779
4	14	β -CD	4.0	192.0	$y = 40.425x + 55708$	0.9979
4	14	Me- β -CD	115.0	19.0	$y = -13.83x + 112839$	0.8195
4	14	2-HPCD	183.0	318.0	$y = 44.927x + 52002$	0.9842
4	14	PBS	51.0	278.0	$y = 58.209x + 41162$	0.9992
4	15	α -CD	80.0	123.0	$y = 35.54x + 57762$	0.9841
4	15	β -CD	<i>a</i>	<i>a</i>	$y = -25.176x + 121103$	0.8862
4	15	Me- β -CD	<i>a</i>	<i>a</i>	$y = -743.59x + 835393$	0.9735
4	15	2-HPCD	128.0	26.0	$y = -262.47x + 433210$	0.9981
4	15	PBS	111.0	121.0	$y = 46.214x + 63696$	0.9686
4	16	α -CD	18.0	<i>a</i>	$y = -35.189x + 391701$	0.9991
4	16	β -CD	<i>a</i>	<i>a</i>	$y = -18.992x + 400576$	0.9957
4	16	Me- β -CD	<i>a</i>	<i>a</i>	$y = -9.7123x + 388109$	0.7445
4	16	2-HPCD	1119104.0	1124473.0	$y = -39.323x + 1\text{E}6$	0.9875
4	16	PBS	1113038.0	1148325.0	$y = -66.674x + 1\text{E}6$	0.9982

Analyte	Fluorophore	CD	LOD (μM)	LOQ (μM)	Equation	R^2
8	14	α -CD	63.6	189.2	$y = 18.494x + 25641$	0.9248
8	14	β -CD	6.3	27.7	$y = 76.95x + 39029$	0.9957
8	14	Me- β -CD	<i>a</i>	<i>a</i>	$y = -26.172x + 88805$	0.9205
8	14	2-HPCD	164.6	353.7	$y = 26.306x + 46582$	0.9414
8	14	PBS	12.5	73.4	$y = 68.756x + 39383$	0.9979
9	14	α -CD	<i>a</i>	1158.8	$y = 10.276x + 75615$	0.8908
9	14	β -CD	27.1	98.3	$y = 32.857x + 74297$	0.9988
9	14	Me- β -CD	46.7	368.7	$y = 21.225x + 74017$	0.9990
9	14	2-HPCD	<i>a</i>	257.8	$y = 38.874x + 71234$	0.9982
9	14	PBS	<i>a</i>	225.4	$y = 26.092x + 69625$	0.9893
10	14	α -CD	108.9	302.5	$y = 51.534x + 63540$	0.9955
10	14	β -CD	63.3	172.1	$y = 87.661x + 46279$	0.9952
10	14	Me- β -CD	40.8	81.9	$y = 44.784x + 58935$	0.9986
10	14	2-HPCD	94.4	233.4	$y = 112.43x + 48688$	0.9911
10	14	PBS	109.9	263.8	$y = 40.689x + 62051$	0.9945
11	14	α -CD	0.2	84.7	$y = 75.754x + 51142$	1.0000
11	14	β -CD	23.8	89.2	$y = 99.09x + 36149$	0.9998
11	14	Me- β -CD	534.1	573.7	$y = 14.777x + 51151$	0.9743
11	14	2-HPCD	63.7	150.2	$y = 106.59x + 44981$	0.9984
11	14	PBS	<i>a</i>	61.0	$y = 98.664x + 42088$	0.9975
12	14	α -CD	123.5	231.5	$y = 54.457x + 70545$	0.964
12	14	β -CD	<i>a</i>	159.0	$y = 75.572x + 68689$	0.9924
12	14	Me- β -CD	29.1	115.1	$y = 82.904x + 65333$	1
12	14	2-HPCD	<i>a</i>	159.7	$y = 45.603x + 70779$	0.9985
12	14	PBS	<i>a</i>	294.5	$y = 25.25x + 65219$	0.9835
<i>a</i> = nonsensical values obtained						
<i>b</i> = non-linear fit						

SUMMARY TABLES FOR ARRAY DATA

ARRAY 1: SINGLE COMPOUNDS ENTERED INTO ARRAY

All cyclodextrin hosts in a single array:

Jackknifed Classification Matrix

	2HPCD1-hexanol	2HPCDMCHM	2HPCDTHF	2HPCDbenzylalco- hol	2HPCDcyclohexan- ol	2HPCDethanol	2HPCDethylenegl- ycol
2HPCD1-hexanol	4	0	0	0	0	0	0
2HPCDMCHM	0	4	0	0	0	0	0
2HPCDTHF	0	0	4	0	0	0	0
2HPCDbenzylalcohol	0	0	0	4	0	0	0
2HPCDcyclohexanol	0	0	0	0	4	0	0
2HPCDethanol	0	0	0	0	0	4	0
2HPCDethyleneglycol	0	0	0	0	0	0	4
2HPCDmethanol	0	0	0	0	0	0	0
2HPCDphenol	0	0	0	0	0	0	0
2HPCDpropargylalcohol	0	0	0	0	0	0	0
2HPCDtertiarybutanol	0	0	0	0	0	0	0
ACD1-hexanol	0	0	0	0	0	0	0
ACDMCHM	0	0	0	0	0	0	0
ACDTHF	0	0	0	0	0	0	0
ACDbenzylalcohol	0	0	0	0	0	0	0
ACDcyclohexanol	0	0	0	0	0	0	0
ACDethanol	0	0	0	0	0	0	0
ACDethyleneglycol	0	0	0	0	0	0	0
ACDmethanol	0	0	0	0	0	0	0
ACDphenol	0	0	0	0	0	0	0
ACDpropargylalcohol	0	0	0	0	0	0	0
ACDtertiarybutanol	0	0	0	0	0	0	0
BCD1-hexanol	0	0	0	0	0	0	0
BCDMCHM	0	0	0	0	0	0	0
BCDTHF	0	0	0	0	0	0	0
BCDbenzylalcohol	0	0	0	0	0	0	0
BCDcyclohexanol	0	0	0	0	0	0	0
BCDethanol	0	0	0	0	0	0	0
BCDethyleneglycol	0	0	0	0	0	0	0
BCDmethanol	0	0	0	0	0	0	0
BCDphenol	0	0	0	0	0	0	0
BCDpropargylalcohol	0	0	0	0	0	0	0
BCDtertiarybutanol	0	0	0	0	0	0	0
MeBCD1-hexanol	0	0	0	0	0	0	0
MeBCDMCHM	0	0	0	0	0	0	0
MeBCDTHF	0	0	0	0	0	0	0
MeBCDbenzylalcohol	0	0	0	0	0	0	0
MeBCDcyclohexanol	0	0	0	0	0	0	0
MeBCDethanol	0	0	0	0	0	0	0
MeBCDethyleneglycol	0	0	0	0	0	0	0
MeBCDmethanol	0	0	0	0	0	0	0
MeBCDphenol	0	0	0	0	0	0	0
MeBCDpropargylalcohol	0	0	0	0	0	0	0
MeBCDtertiarybutanol	0	0	0	0	0	0	0
PBS1-hexanol	0	0	0	0	0	0	0
PBSMCHM	0	0	0	0	0	0	0
PBSTHF	0	0	0	0	0	0	0
PBSbenzylalcohol	0	0	0	0	0	0	0
PBSscyclohexanol	0	0	0	0	0	0	0
PBSethanol	0	0	0	0	0	0	0
PBSethyleneglycol	0	0	0	0	0	0	0
PBSmethanol	0	0	0	0	0	0	0
PBSphenol	0	0	0	0	0	0	0
PBSpropargylalcohol	0	0	0	0	0	0	0
PBStertiarybutanol	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	2HPCDmethanol	2HPCDphenol	2HPCDpropargylalcohol	2HPCDtertiarybutanol	ACD1-hexanol	ACDMCHM	ACDTHF	ACDbenzylalcohol
2HPCD1-hexanol	0	0	0	0	0	0	0	0
2HPCDMCHM	0	0	0	0	0	0	0	0
2HPCDTHF	0	0	0	0	0	0	0	0
2HPCDbenzylalcohol	0	0	0	0	0	0	0	0
2HPCDcyclohexanol	0	0	0	0	0	0	0	0
2HPCDethanol	0	0	0	0	0	0	0	0
2HPCDethyleneglycol	0	0	0	0	0	0	0	0
2HPCDmethanol	4	0	0	0	0	0	0	0
2HPCDphenol	0	4	0	0	0	0	0	0
2HPCDpropargylalcohol	0	0	4	0	0	0	0	0
2HPCDtertiarybutanol	0	0	0	4	0	0	0	0
ACD1-hexanol	0	0	0	0	4	0	0	0
ACDMCHM	0	0	0	0	0	4	0	0
ACDTHF	0	0	0	0	0	0	4	0
ACDbenzylalcohol	0	0	0	0	0	0	0	4
ACDcyclohexanol	0	0	0	0	0	0	0	0
ACDethanol	0	0	0	0	0	0	0	0
ACDethyleneglycol	0	0	0	0	0	0	0	0
ACDmethanol	0	0	0	0	0	0	0	0
ACDphenol	0	0	0	0	0	0	0	0
ACDpropargylalcohol	0	0	0	0	0	0	0	0
ACDtertiarybutanol	0	0	0	0	0	0	0	0
BCD1-hexanol	0	0	0	0	0	0	0	0
BCDMCHM	0	0	0	0	0	0	0	0
BCDTHF	0	0	0	0	0	0	0	0
BCDbenzylalcohol	0	0	0	0	0	0	0	0
BCDcyclohexanol	0	0	0	0	0	0	0	0
BCDethanol	0	0	0	0	0	0	0	0
BCDethyleneglycol	0	0	0	0	0	0	0	0
BCDmethanol	0	0	0	0	0	0	0	0
BCDphenol	0	0	0	0	0	0	0	0
BCDpropargylalcohol	0	0	0	0	0	0	0	0
BCDtertiarybutanol	0	0	0	0	0	0	0	0
MeBCD1-hexanol	0	0	0	0	0	0	0	0
MeBCDMCHM	0	0	0	0	0	0	0	0
MeBCDTHF	0	0	0	0	0	0	0	0
MeBCDbenzylalcohol	0	0	0	0	0	0	0	0
MeBCDcyclohexanol	0	0	0	0	0	0	0	0
MeBCDethanol	0	0	0	0	0	0	0	0
MeBCDethyleneglycol	0	0	0	0	0	0	0	0
MeBCDmethanol	0	0	0	0	0	0	0	0
MeBCDphenol	0	0	0	0	0	0	0	0
MeBCDpropargylalcohol	0	0	0	0	0	0	0	0
MeBCDtertiarybutanol	0	0	0	0	0	0	0	0
PBS1-hexanol	0	0	0	0	0	0	0	0
PBSMCHM	0	0	0	0	0	0	0	0
PBSTHF	0	0	0	0	0	0	0	0
PBSbenzylalcohol	0	0	0	0	0	0	0	0
PBSscyclohexanol	0	0	0	0	0	0	0	0
PBSethanol	0	0	0	0	0	0	0	0
PBSethyleneglycol	0	0	0	0	0	0	0	0
PBSmethanol	0	0	0	0	0	0	0	0
PBSphenol	0	0	0	0	0	0	0	0
PBSpropargylalcohol	0	0	0	0	0	0	0	0
PBStertiarybutanol	0	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	ACDcyclohexanol	ACDethanol	ACDethyleneglycol	ACDmethanol	ACDphenol	ACDpropargylalcohol	ACDtertiarybutanol
2HPCD1-hexanol	0	0	0	0	0	0	0
2HPCDMCHM	0	0	0	0	0	0	0
2HPCDTHF	0	0	0	0	0	0	0
2HPCDbenzylalcohol	0	0	0	0	0	0	0
2HPCDcyclohexanol	0	0	0	0	0	0	0
2HPCDethanol	0	0	0	0	0	0	0
2HPCDethyleneglycol	0	0	0	0	0	0	0
2HPCDmethanol	0	0	0	0	0	0	0
2HPCDphenol	0	0	0	0	0	0	0
2HPCDpropargylalcohol	0	0	0	0	0	0	0
2HPCDtertiarybutanol	0	0	0	0	0	0	0
ACD1-hexanol	0	0	0	0	0	0	0
ACDMCHM	0	0	0	0	0	0	0
ACDTHF	0	0	0	0	0	0	0
ACDbenzylalcohol	0	0	0	0	0	0	0
ACDcyclohexanol	4	0	0	0	0	0	0
ACDethanol	0	4	0	0	0	0	0
ACDethyleneglycol	0	0	4	0	0	0	0
ACDmethanol	0	0	0	4	0	0	0
ACDphenol	0	0	0	0	4	0	0
ACDpropargylalcohol	0	0	0	0	0	4	0
ACDtertiarybutanol	0	0	0	0	0	0	4
BCD1-hexanol	0	0	0	0	0	0	0
BCDMCHM	0	0	0	0	0	0	0
BCDTHF	0	0	0	0	0	0	0
BCDbenzylalcohol	0	0	0	0	0	0	0
BCDcyclohexanol	0	0	0	0	0	0	0
BCDethanol	0	0	0	0	0	0	0
BCDethyleneglycol	0	0	0	0	0	0	0
BCDmethanol	0	0	0	0	0	0	0
BCDphenol	0	0	0	0	0	0	0
BCDpropargylalcohol	0	0	0	0	0	0	0
BCDtertiarybutanol	0	0	0	0	0	0	0
MeBCD1-hexanol	0	0	0	0	0	0	0
MeBCDMCHM	0	0	0	0	0	0	0
MeBCDTHF	0	0	0	0	0	0	0
MeBCDbenzylalcohol	0	0	0	0	0	0	0
MeBCDcyclohexanol	0	0	0	0	0	0	0
MeBCDethanol	0	0	0	0	0	0	0
MeBCDethyleneglycol	0	0	0	0	0	0	0
MeBCDmethanol	0	0	0	0	0	0	0
MeBCDphenol	0	0	0	0	0	0	0
MeBCDpropargylalcohol	0	0	0	0	0	0	0
MeBCDtertiarybutanol	0	0	0	0	0	0	0
PBS1-hexanol	0	0	0	0	0	0	0
PBSMCHM	0	0	0	0	0	0	0
PBSTHF	0	0	0	0	0	0	0
PBSbenzylalcohol	0	0	0	0	0	0	0
PBSscyclohexanol	0	0	0	0	0	0	0
PBSethanol	0	0	0	0	0	0	0
PBSethyleneglycol	0	0	0	0	0	0	0
PBSmethanol	0	0	0	0	0	0	0
PBSphenol	0	0	0	0	0	0	0
PBSpropargylalcohol	0	0	0	0	0	0	0
PBStertiarybutanol	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	BCD1-hexanol	BCDMCHM	BCDTHF	BCDbenzylalcohol	BCDcyclohexanol	BCDethanol	BCDethyleneglycol	BCDmethanol
2HPCD1-hexanol	0	0	0	0	0	0	0	0
2HPCDMCHM	0	0	0	0	0	0	0	0
2HPCDTHF	0	0	0	0	0	0	0	0
2HPCDbenzylalcohol	0	0	0	0	0	0	0	0
2HPCDcyclohexanol	0	0	0	0	0	0	0	0
2HPCDethanol	0	0	0	0	0	0	0	0
2HPCDethyleneglycol	0	0	0	0	0	0	0	0
2HPCDmethanol	0	0	0	0	0	0	0	0
2HPCDphenol	0	0	0	0	0	0	0	0
2HPCDpropargylalcohol	0	0	0	0	0	0	0	0
2HPCDtertiarybutanol	0	0	0	0	0	0	0	0
ACD1-hexanol	0	0	0	0	0	0	0	0
ACDMCHM	0	0	0	0	0	0	0	0
ACDTHF	0	0	0	0	0	0	0	0
ACDbenzylalcohol	0	0	0	0	0	0	0	0
ACDcyclohexanol	0	0	0	0	0	0	0	0
ACDethanol	0	0	0	0	0	0	0	0
ACDethyleneglycol	0	0	0	0	0	0	0	0
ACDmethanol	0	0	0	0	0	0	0	0
ACDphenol	0	0	0	0	0	0	0	0
ACDpropargylalcohol	0	0	0	0	0	0	0	0
ACDtertiarybutanol	0	0	0	0	0	0	0	0
BCD1-hexanol	4	0	0	0	0	0	0	0
BCDMCHM	0	3	0	0	0	0	0	0
BCDTHF	0	0	4	0	0	0	0	0
BCDbenzylalcohol	0	0	0	4	0	0	0	0
BCDcyclohexanol	0	0	0	0	4	0	0	0
BCDethanol	0	0	0	0	0	4	0	0
BCDethyleneglycol	0	0	0	0	0	0	4	0
BCDmethanol	0	0	0	0	0	0	0	4
BCDphenol	0	0	0	0	0	0	0	0
BCDpropargylalcohol	0	0	0	0	0	0	0	0
BCDtertiarybutanol	0	0	0	0	0	0	0	0
MeBCD1-hexanol	0	0	0	0	0	0	0	0
MeBCDMCHM	0	0	0	0	0	0	0	0
MeBCDTHF	0	0	0	0	0	0	0	0
MeBCDbenzylalcohol	0	0	0	0	0	0	0	0
MeBCDcyclohexanol	0	0	0	0	0	0	0	0
MeBCDethanol	0	0	0	0	0	0	0	0
MeBCDethyleneglycol	0	0	0	0	0	0	0	0
MeBCDmethanol	0	0	0	0	0	0	0	0
MeBCDphenol	0	0	0	0	0	0	0	0
MeBCDpropargylalcohol	0	0	0	0	0	0	0	0
MeBCDtertiarybutanol	0	0	0	0	0	0	0	0
PBS1-hexanol	0	0	0	0	0	0	0	0
PBSMCHM	0	1	0	0	0	0	0	0
PBSTHF	0	0	0	0	0	0	0	0
PBSbenzylalcohol	0	0	0	0	0	0	0	0
PBScyclohexanol	0	0	0	0	0	0	0	0
PBSethanol	0	0	0	0	0	0	0	0
PBSethyleneglycol	0	0	0	0	0	0	0	0
PBSmethanol	0	0	0	0	0	0	0	0
PBSphenol	0	0	0	0	0	0	0	0
PBSpropargylalcohol	0	0	0	0	0	0	0	0
PBSTertiarybutanol	0	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	BCDphenol	BCDpropargylalcohol	BCDtertiarybutanol	MeBCD1-hexanol	MeBCDMCHM	MeBCDTHF	MeBCDbenzylalcohol
2HPCD1-hexanol	0	0	0	0	0	0	0
2HPCDMCHM	0	0	0	0	0	0	0
2HPCDTHF	0	0	0	0	0	0	0
2HPCDbenzylalcohol	0	0	0	0	0	0	0
2HPCDcyclohexanol	0	0	0	0	0	0	0
2HPCDethanol	0	0	0	0	0	0	0
2HPCDethyleneglycol	0	0	0	0	0	0	0
2HPCDmethanol	0	0	0	0	0	0	0
2HPCDphenol	0	0	0	0	0	0	0
2HPCDpropargylalcohol	0	0	0	0	0	0	0
2HPCDtertiarybutanol	0	0	0	0	0	0	0
ACD1-hexanol	0	0	0	0	0	0	0
ACDMCHM	0	0	0	0	0	0	0
ACDTHF	0	0	0	0	0	0	0
ACDbenzylalcohol	0	0	0	0	0	0	0
ACDcyclohexanol	0	0	0	0	0	0	0
ACDethanol	0	0	0	0	0	0	0
ACDethyleneglycol	0	0	0	0	0	0	0
ACDmethanol	0	0	0	0	0	0	0
ACDphenol	0	0	0	0	0	0	0
ACDpropargylalcohol	0	0	0	0	0	0	0
ACDtertiarybutanol	0	0	0	0	0	0	0
BCD1-hexanol	0	0	0	0	0	0	0
BCDMCHM	0	0	0	0	0	0	0
BCDTHF	0	0	0	0	0	0	0
BCDbenzylalcohol	0	0	0	0	0	0	0
BCDcyclohexanol	0	0	0	0	0	0	0
BCDethanol	0	0	0	0	0	0	0
BCDethyleneglycol	0	0	0	0	0	0	0
BCDmethanol	0	0	0	0	0	0	0
BCDphenol	4	0	0	0	0	0	0
BCDpropargylalcohol	0	4	0	0	0	0	0
BCDtertiarybutanol	0	0	4	0	0	0	0
MeBCD1-hexanol	0	0	0	4	0	0	0
MeBCDMCHM	0	0	0	0	4	0	0
MeBCDTHF	0	0	0	0	0	4	0
MeBCDbenzylalcohol	0	0	0	0	0	0	4
MeBCDcyclohexanol	0	0	0	0	0	0	0
MeBCDethanol	0	0	0	0	0	0	0
MeBCDethyleneglycol	0	0	0	0	0	0	0
MeBCDmethanol	0	0	0	0	0	0	0
MeBCDphenol	0	0	0	0	0	0	0
MeBCDpropargylalcohol	0	0	0	0	0	0	0
MeBCDtertiarybutanol	0	0	0	0	0	0	0
PBS1-hexanol	0	0	0	0	0	0	0
PBSMCHM	0	0	0	0	0	0	0
PBSTHF	0	0	0	0	0	0	0
PBSbenzylalcohol	0	0	0	0	0	0	0
PBScyclohexanol	0	0	0	0	0	0	0
PBSethanol	0	0	0	0	0	0	0
PBSethyleneglycol	0	0	0	0	0	0	0
PBSmethanol	0	0	0	0	0	0	0
PBSphenol	0	0	0	0	0	0	0
PBSpropargylalcohol	0	0	0	0	0	0	0
PBStertiarybutanol	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	MeBCDtertiarybutanol	PBS1-hexanol	PBSMCHM	PBSTHF	PBSbenzylalcohol	PBScyclohexanol	PBSethanol	PBSethyleneglycol
2HPCD1-hexanol	0	0	0	0	0	0	0	0
2HPCDMCHM	0	0	0	0	0	0	0	0
2HPCDTHF	0	0	0	0	0	0	0	0
2HPCDbenzylalcohol	0	0	0	0	0	0	0	0
2HPCDcyclohexanol	0	0	0	0	0	0	0	0
2HPCDethanol	0	0	0	0	0	0	0	0
2HPCDethyleneglycol	0	0	0	0	0	0	0	0
2HPCDmethanol	0	0	0	0	0	0	0	0
2HPCDphenol	0	0	0	0	0	0	0	0
2HPCDpropargylalcohol	0	0	0	0	0	0	0	0
2HPCDtertiarybutanol	0	0	0	0	0	0	0	0
ACD1-hexanol	0	0	0	0	0	0	0	0
ACDMCHM	0	0	0	0	0	0	0	0
ACDTHF	0	0	0	0	0	0	0	0
ACDbenzylalcohol	0	0	0	0	0	0	0	0
ACDcyclohexanol	0	0	0	0	0	0	0	0
ACDethanol	0	0	0	0	0	0	0	0
ACDethyleneglycol	0	0	0	0	0	0	0	0
ACDmethanol	0	0	0	0	0	0	0	0
ACDphenol	0	0	0	0	0	0	0	0
BCD1-hexanol	0	0	0	0	0	0	0	0
BCDMCHM	0	0	0	0	0	0	0	0
BCDTHF	0	0	0	0	0	0	0	0
BCDbenzylalcohol	0	0	0	0	0	0	0	0
BCDcyclohexanol	0	0	0	0	0	0	0	0
BCDethanol	0	0	0	0	0	0	0	0
BCDethyleneglycol	0	0	0	0	0	0	0	0
BCDmethanol	0	0	0	0	0	0	0	0
BCDphenol	0	0	0	0	0	0	0	0
BCDpropargylalcohol	0	0	0	0	0	0	0	0
BCDtertiarybutanol	0	0	0	0	0	0	0	0
MeBCD1-hexanol	0	0	0	0	0	0	0	0
MeBCDMCHM	0	0	0	0	0	0	0	0
MeBCDTHF	0	0	0	0	0	0	0	0
MeBCDbenzylalcohol	0	0	0	0	0	0	0	0
MeBCDcyclohexanol	0	0	0	0	0	0	0	0
MeBCDethanol	0	0	0	0	0	0	0	0
MeBCDethyleneglycol	0	0	0	0	0	0	0	0
MeBCDmethanol	0	0	0	0	0	0	0	0
MeBCDphenol	0	0	0	0	0	0	0	0

Jackknifed Classification Matrix (Contd.)

	PBSmethanol	PBSphenol	PBSpropargylalcohol	PBStertiarybutanol	%correct
2HPCD1-hexanol	0	0	0	0	100
2HPCDMCHM	0	0	0	0	100
2HPCDTHF	0	0	0	0	100
2HPCDbenzylalcohol	0	0	0	0	100
2HPCDcyclohexanol	0	0	0	0	100
2HPCDethanol	0	0	0	0	100
2HPCDethyleneglycol	0	0	0	0	100
2HPCDmethanol	0	0	0	0	100
2HPCDphenol	0	0	0	0	100
2HPCDpropargylalcohol	0	0	0	0	100
2HPCDtertiarybutanol	0	0	0	0	100
ACD1-hexanol	0	0	0	0	100
ACDMCHM	0	0	0	0	100
ACDTHF	0	0	0	0	100
ACDbenzylalcohol	0	0	0	0	100
ACDcyclohexanol	0	0	0	0	100
ACDethanol	0	0	0	0	100
ACDethyleneglycol	0	0	0	0	100

ACDmethanol	0	0	0	0	100
ACDphenol	0	0	0	0	100
ACDpropargylalcohol	0	0	0	0	100
ACDtertiarybutanol	0	0	0	0	100
BCD1-hexanol	0	0	0	0	100
BCDMCHM	0	0	0	0	75
BCDTHF	0	0	0	0	100
BCDbenzylalcohol	0	0	0	0	100
BCDcyclohexanol	0	0	0	0	100
BCDethanol	0	0	0	0	100
BCDethyleneglycol	0	0	0	0	100
BCDmethanol	0	0	0	0	100
BCDphenol	0	0	0	0	100
BCDpropargylalcohol	0	0	0	0	100
BCDtertiarybutanol	0	0	0	0	100
MeBCD1-hexanol	0	0	0	0	100
MeBCDMCHM	0	0	0	0	100
MeBCDTHF	0	0	0	0	100
MeBCDbenzylalcohol	0	0	0	0	100
MeBCDcyclohexanol	0	0	0	0	100
MeBCDethanol	0	0	0	0	100
MeBCDethyleneglycol	0	0	0	0	100

MeBCDmethanol	0	0	0	0	100
MeBCDphenol	0	0	0	0	100
MeBCDpropargylalcohol	0	0	0	0	100
MeBCDtertiarybutanol	0	0	0	0	100
PBS1-hexanol	0	0	0	0	100
PBSMCHM	0	0	0	0	75
PBSTHF	0	0	0	0	100
PBSbenzylalcohol	0	0	0	0	100
PBScyclohexanol	0	0	0	0	100
PBSethanol	0	0	0	0	100
PBSethyleneglycol	0	0	0	0	100
PBSmethanol	4	0	0	0	100
PBSphenol	0	4	0	0	100
PBSpropargylalcohol	0	0	4	0	100
PBStertiarybutanol	0	0	0	4	100
Total	4	4	4	4	99

Cumulative Proportion of Total Dispersion

0.884	0.998	1.000

α -Cyclodextrin array:

Jackknifed Classification Matrix

	ACD1-hexanol	ACDMCHM	ACDTHF	ACDbenzylalcohol	ACDcyclohexanol	ACDethanol	ACDethyleneglycol	ACDmethanol
ACD1-hexanol	4	0	0	0	0	0	0	0
ACDMCHM	0	4	0	0	0	0	0	0
ACDTHF	0	0	4	0	0	0	0	0
ACDbenzylalcohol	0	0	0	4	0	0	0	0
ACDcyclohexanol	0	0	0	0	4	0	0	0
ACDethanol	0	0	0	0	0	4	0	0
ACDethyleneglycol	0	0	0	0	0	0	4	0
ACDmethanol	0	0	0	0	0	0	0	4
ACDphenol	0	0	0	0	0	0	0	0
ACDpropargylalcohol	0	0	0	0	0	0	0	0
ACDtertiarybutanol	0	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	ACDphenol	ACDpropargylalcohol	ACDtertiarybutanol	%correct
ACD1-hexanol	0	0	0	100
ACDMCHM	0	0	0	100
ACDTHF	0	0	0	100
ACDbenzylalcohol	0	0	0	100
ACDcyclohexanol	0	0	0	100
ACDethanol	0	0	0	100
ACDethyleneglycol	0	0	0	100
ACDmethanol	0	0	0	100
ACDphenol	4	0	0	100
ACDpropargylalcohol	0	4	0	100
ACDtertiarybutanol	0	0	4	100
Total	4	4	4	100

Cumulative Proportion of Total Dispersion

0.989	0.999	1.000

β -Cyclodextrin array:

Jackknifed Classification Matrix

	BCD1-hexanol	BCDMCHM	BCDTHF	BCDbenzylalcohol	BCDcyclohexanol	BCDethanol	BCDethyleneglycol	BCDmethanol
BCD1-hexanol	4	0	0	0	0	0	0	0
BCDMCHM	0	4	0	0	0	0	0	0
BCDTHF	0	0	4	0	0	0	0	0
BCDbenzylalcohol	0	0	0	4	0	0	0	0
BCDcyclohexanol	0	0	0	0	4	0	0	0
BCDethanol	0	0	0	0	0	4	0	0
BCDethyleneglycol	0	0	0	0	0	0	4	0
BCDmethanol	0	0	0	0	0	0	0	4
BCDphenol	0	0	0	0	0	0	0	0
BCDpropargylalcohol	0	0	0	0	0	0	0	0
BCDtertiarybutanol	0	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	BCDphenol	BCDpropargylalcohol	BCDtertiarybutanol	%correct
BCD1-hexanol	0	0	0	100
BCDMCHM	0	0	0	100
BCDTHF	0	0	0	100
BCDbenzylalcohol	0	0	0	100
BCDcyclohexanol	0	0	0	100
BCDethanol	0	0	0	100
BCDethyleneglycol	0	0	0	100
BCDmethanol	0	0	0	100
BCDphenol	4	0	0	100
BCDpropargylalcohol	0	4	0	100
BCDtertiarybutanol	0	0	4	100
Total	4	4	4	100

Cumulative Proportion of Total Dispersion

0.975	1.000	1.000

Methyl- β -cyclodextrin array:

Jackknifed Classification Matrix

	MeBCD1-hexanol	MeBCDMCHM	MeBCDTHF	MeBCDbenzylalcohol	MeBCDcyclohexanol	MeBCDethanol	MeBCDethyleneglycol
MeBCD1-hexanol	4	0	0	0	0	0	0
MeBCDMCHM	0	4	0	0	0	0	0
MeBCDTHF	0	0	4	0	0	0	0
MeBCDbenzylalcohol	0	0	0	4	0	0	0
MeBCDcyclohexanol	0	0	0	0	4	0	0
MeBCDethanol	0	0	0	0	0	4	0
MeBCDethyleneglycol	0	0	0	0	0	0	4
MeBCDmethanol	0	0	0	0	0	0	0
MeBCDphenol	0	0	0	0	0	0	0
MeBCDpropargylalcohol	0	0	0	0	0	0	0
MeBCDtertiarybutanol	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	MeBCDmethanol	MeBCDphenol	MeBCDpropargylalcohol	MeBCDtertiarybutanol	%correct
MeBCD1-hexanol	0	0	0	0	100
MeBCDMCHM	0	0	0	0	100
MeBCDTHF	0	0	0	0	100
MeBCDbenzylalcohol	0	0	0	0	100
MeBCDcyclohexanol	0	0	0	0	100
MeBCDethanol	0	0	0	0	100
MeBCDethyleneglycol	0	0	0	0	100
MeBCDmethanol	4	0	0	0	100
MeBCDphenol	0	4	0	0	100
MeBCDpropargylalcohol	0	0	4	0	100
MeBCDtertiarybutanol	0	0	0	4	100
Total	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.925	1.000	1.000

2-Hydroxypropyl-β-cyclodextrin array:

Jackknifed Classification Matrix

	2HPCD1-hexanol	2HPCDMCHM	2HPCDTHF	2HPCDbenzylalcohol	2HPCDcyclohexanol	2HPCDethanol	2HPCDethyleneglycol
2HPCD1-hexanol	4	0	0	0	0	0	0
2HPCDMCHM	0	4	0	0	0	0	0
2HPCDTHF	0	0	4	0	0	0	0
2HPCDbenzylalcohol	0	0	0	4	0	0	0
2HPCDcyclohexanol	0	0	0	0	4	0	0
2HPCDethanol	0	0	0	0	0	4	0
2HPCDethyleneglycol	0	0	0	0	0	0	4
2HPCDmethanol	0	0	0	0	0	0	0
2HPCDphenol	0	0	0	0	0	0	0
2HPCDpropargylalcohol	0	0	0	0	0	0	0
2HPCDtertiarybutanol	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	2HPCDmethanol	2HPCDphenol	2HPCDpropargylalcohol	2HPCDtertiarybutanol	%correct
2HPCD1-hexanol	0	0	0	0	100
2HPCDMCHM	0	0	0	0	100
2HPCDTHF	0	0	0	0	100
2HPCDbenzylalcohol	0	0	0	0	100
2HPCDcyclohexanol	0	0	0	0	100
2HPCDethanol	0	0	0	0	100
2HPCDethyleneglycol	0	0	0	0	100
2HPCDmethanol	4	0	0	0	100
2HPCDphenol	0	4	0	0	100
2HPCDpropargylalcohol	0	0	4	0	100
2HPCDtertiarybutanol	0	0	0	4	100
Total	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.827	1.000	1.000

PBS array:

Jackknifed Classification Matrix

	PBS1-hexanol	PBSMCHM	PBSTHF	PBSbenzylalcohol	PBSscyclohexanol	PBSethanol	PBSethyleneglycol	PBSmethanol
PBS1-hexanol	4	0	0	0	0	0	0	0
PBSMCHM	0	4	0	0	0	0	0	0
PBSTHF	0	0	4	0	0	0	0	0
PBSbenzylalcohol	0	0	0	4	0	0	0	0
PBSscyclohexanol	0	0	0	0	4	0	0	0
PBSethanol	0	0	0	0	0	4	0	0
PBSethyleneglycol	0	0	0	0	0	0	4	0
PBSmethanol	0	0	0	0	0	0	0	4
PBSphenol	0	0	0	0	0	0	0	0
PBSpropargylalcohol	0	0	0	0	0	0	0	0
PBStertiarybutanol	0	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	PBSphenol	PBSpropargylalcohol	PBStertiarybutanol	%correct
PBS1-hexanol	0	0	0	100
PBSMCHM	0	0	0	100
PBSTHF	0	0	0	100
PBSbenzylalcohol	0	0	0	100
PBScyclohexanol	0	0	0	100
PBSethanol	0	0	0	100
PBSethyleneglycol	0	0	0	100
PBSmethanol	0	0	0	100
PBSphenol	4	0	0	100
PBSpropargylalcohol	0	4	0	100
PBStertiarybutanol	0	0	4	100
Total	4	4	4	100

Cumulative Proportion of Total Dispersion

0.984	0.994	1.000

ARRAY 2: MIXED ANALYTES (2 AND 8) ENTERED INTO ARRAY:

All cyclodextrin hosts in a single array:

Jackknifed Classification Matrix

	2HPCD 1:1 CH:MCHM	2HPCD 1:2 CH:MCHM	2HPCD 2:1 CH:MCHM	2HPCDMCHM	2HPCDcyclohexanol	ACD 1:1 CH:MCHM	ACD 1:2 CH:MCHM	ACD 2:1 CH:MCHM
2HPCD 1:1 CH:MCHM	4	0	0	0	0	0	0	0
2HPCD 1:2 CH:MCHM	0	4	0	0	0	0	0	0
2HPCD 2:1 CH:MCHM	0	0	4	0	0	0	0	0
2HPCDMCHM	0	0	0	4	0	0	0	0
2HPCDcyclohexanol	0	0	0	0	4	0	0	0
ACD 1:1 CH:MCHM	0	0	0	0	0	4	0	0
ACD 1:2 CH:MCHM	0	0	0	0	0	0	4	0
ACD 2:1 CH:MCHM	0	0	0	0	0	0	0	4
ACDMCHM	0	0	0	0	0	0	0	0
ACDcyclohexanol	0	0	0	0	0	0	0	0
BCD 1:1 CH:MCHM	0	0	0	0	0	0	0	0
BCD 1:2 CH:MCHM	0	0	0	0	0	0	0	0
BCD 2:1 CH:MCHM	0	0	0	0	0	0	0	0
BCDMCHM	0	0	0	0	0	0	0	0
BCDcyclohexanol	0	0	0	0	0	0	0	0
MeBCD 1:1 CH:MCHM	0	0	0	0	0	0	0	0
MeBCD 1:2 CH:MCHM	0	0	0	0	0	0	0	0
MeBCD 2:1 CH:MCHM	0	0	0	0	0	0	0	0
MeBCDMCHM	0	0	0	0	0	0	0	0
MeBCDcyclohexanol	0	0	0	0	0	0	0	0
PBS 1:1 CH:MCHM	0	0	0	0	0	0	0	0
PBS 1:2 CH:MCHM	0	0	0	0	0	0	0	0
PBS 2:1 CH:MCHM	0	0	0	0	0	0	0	0
PBSMCHM	0	0	0	0	0	0	0	0
PBScyclohexanol	0	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	ACDMCHM	ACDcyclohexanol	BCD 1:1 CH:MCHM	BCD 1:2 CH:MCHM	BCD 2:1 CH:MCHM	BCDMCHM	BCDcyclohexanol	MeBCD 1:1 CH:MCHM
2HPCD 1:1 CH:MCHM	0	0	0	0	0	0	0	0
2HPCD 1:2 CH:MCHM	0	0	0	0	0	0	0	0
2HPCD 2:1 CH:MCHM	0	0	0	0	0	0	0	0
2HPCDMCHM	0	0	0	0	0	0	0	0
2HPCDcyclohexanol	0	0	0	0	0	0	0	0
ACD 1:1 CH:MCHM	0	0	0	0	0	0	0	0
ACD 1:2 CH:MCHM	0	0	0	0	0	0	0	0
ACD 2:1 CH:MCHM	0	0	0	0	0	0	0	0
ACDMCHM	4	0	0	0	0	0	0	0
ACDcyclohexanol	0	4	0	0	0	0	0	0
BCD 1:1 CH:MCHM	0	0	4	0	0	0	0	0
BCD 1:2 CH:MCHM	0	0	0	4	0	0	0	0
BCD 2:1 CH:MCHM	0	0	0	0	4	0	0	0
BCDMCHM	0	0	0	0	0	3	0	0
BCDcyclohexanol	0	0	0	0	0	0	4	0
MeBCD 1:1 CH:MCHM	0	0	0	0	0	0	0	4
MeBCD 1:2 CH:MCHM	0	0	0	0	0	0	0	0
MeBCD 2:1 CH:MCHM	0	0	0	0	0	0	0	0
MeBCDMCHM	0	0	0	0	0	0	0	0
MeBCDcyclohexanol	0	0	0	0	0	0	0	0
PBS 1:1 CH:MCHM	0	0	0	0	0	0	0	0
PBS 1:2 CH:MCHM	0	0	0	0	0	0	0	0
PBS 2:1 CH:MCHM	0	0	0	0	0	0	0	0
PBSMCHM	0	0	0	0	0	1	0	0
PBScyclohexanol	0	0	0	0	0	0	0	0
Total	4	4	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	MeBCD 1:2 CH:MCHM	MeBCD 2:1 CH:MCHM	MeBCDMCHM	MeBCDcyclohexanol	PBS 1:1 CH:MCHM	PBS 1:2 CH:MCHM	PBS 2:1 CH:MCHM	PBSMCHM
2HPCD 1:1 CH:MCHM	0	0	0	0	0	0	0	0
2HPCD 1:2 CH:MCHM	0	0	0	0	0	0	0	0
2HPCD 2:1 CH:MCHM	0	0	0	0	0	0	0	0
2HPCDMCHM	0	0	0	0	0	0	0	0
2HPCDcyclohexanol	0	0	0	0	0	0	0	0
ACD 1:1 CH:MCHM	0	0	0	0	0	0	0	0
ACD 1:2 CH:MCHM	0	0	0	0	0	0	0	0
ACD 2:1 CH:MCHM	0	0	0	0	0	0	0	0
ACDMCHM	0	0	0	0	0	0	0	0
ACDcyclohexanol	0	0	0	0	0	0	0	0
BCD 1:1 CH:MCHM	0	0	0	0	0	0	0	0
BCD 1:2 CH:MCHM	0	0	0	0	0	0	0	0
BCD 2:1 CH:MCHM	0	0	0	0	0	0	0	0
BCDMCHM	0	0	0	0	0	0	0	1
BCDcyclohexanol	0	0	0	0	0	0	0	0
MeBCD 1:1 CH:MCHM	0	0	0	0	0	0	0	0
MeBCD 1:2 CH:MCHM	4	0	0	0	0	0	0	0
MeBCD 2:1 CH:MCHM	1	3	0	0	0	0	0	0
MeBCDMCHM	0	0	4	0	0	0	0	0
MeBCDcyclohexanol	0	0	0	4	0	0	0	0
PBS 1:1 CH:MCHM	0	0	0	0	4	0	0	0
PBS 1:2 CH:MCHM	0	0	0	0	0	4	0	0
PBS 2:1 CH:MCHM	0	0	0	0	0	0	4	0
PBSMCHM	0	0	0	0	0	0	0	3
PBScyclohexanol	0	0	0	0	0	0	0	0
Total	5	3	4	4	4	4	4	4

Jackknifed Classification Matrix (Contd.)

	PBScyclohexanol	%correct
2HPCD 1:1 CH:MCHM	0	100
2HPCD 1:2 CH:MCHM	0	100
2HPCD 2:1 CH:MCHM	0	100
2HPCDMCHM	0	100
2HPCDcyclohexanol	0	100
ACD 1:1 CH:MCHM	0	100
ACD 1:2 CH:MCHM	0	100
ACD 2:1 CH:MCHM	0	100
ACDMCHM	0	100
ACDcyclohexanol	0	100
BCD 1:1 CH:MCHM	0	100
BCD 1:2 CH:MCHM	0	100
BCD 2:1 CH:MCHM	0	100
BCDMCHM	0	75
BCDcyclohexanol	0	100
MeBCD 1:1 CH:MCHM	0	100
MeBCD 1:2 CH:MCHM	0	100
MeBCD 2:1 CH:MCHM	0	75
MeBCDMCHM	0	100
MeBCDcyclohexanol	0	100
PBS 1:1 CH:MCHM	0	100
PBS 1:2 CH:MCHM	0	100
PBS 2:1 CH:MCHM	0	100
PBSMCHM	0	75
PBScyclohexanol	4	100
Total	4	97

Cumulative Proportion of Total Dispersion

0.986	0.999	1.000

α -Cyclodextrin array:

Jackknifed Classification Matrix

	ACD 1:1 CH:MCHM	ACD 1:2 CH:MCHM	ACD 2:1 CH:MCHM	ACDMCHM	ACDcyclohexanol	%correct
ACD 1:1 CH:MCHM	4	0	0	0	0	100
ACD 1:2 CH:MCHM	0	4	0	0	0	100
ACD 2:1 CH:MCHM	0	0	4	0	0	100
ACDMCHM	0	0	0	4	0	100
ACDcyclohexanol	0	0	0	0	4	100
Total	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.998	1.000	1.000

β -Cyclodextrin array:

Jackknifed Classification Matrix

	BCD 1:1 CH:MCHM	BCD 1:2 CH:MCHM	BCD 2:1 CH:MCHM	BCDMCHM	BCDcyclohexanol	%correct
BCD 1:1 CH:MCHM	4	0	0	0	0	100
BCD 1:2 CH:MCHM	0	4	0	0	0	100
BCD 2:1 CH:MCHM	0	0	4	0	0	100
BCDMCHM	0	0	0	4	0	100
BCDcyclohexanol	0	0	0	0	4	100
Total	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

1.000	1.000	1.000

Methyl- β -cyclodextrin array:

Jackknifed Classification Matrix

	MeBCD 1:1 CH:MCHM	MeBCD 1:2 CH:MCHM	MeBCD 2:1 CH:MCHM	MeBCDMCHM	MeBCDcyclohexanol	%correct
MeBCD 1:1 CH:MCHM	4	0	0	0	0	100
MeBCD 1:2 CH:MCHM	0	4	0	0	0	100
MeBCD 2:1 CH:MCHM	0	1	3	0	0	75
MeBCDMCHM	0	0	0	4	0	100
MeBCDcyclohexanol	0	0	0	0	4	100
Total	4	5	3	4	4	95

Cumulative Proportion of Total Dispersion

0.977	1.000	1.000

2-Hydroxypropyl- β -cyclodextrin array:

Jackknifed Classification Matrix

	2HPCD 1:1 CH:MCHM	2HPCD 1:2 CH:MCHM	2HPCD 2:1 CH:MCHM	2HPCDMCHM	2HPCDcyclohexanol	%correct
2HPCD 1:1 CH:MCHM	4	0	0	0	0	100
2HPCD 1:2 CH:MCHM	0	4	0	0	0	100
2HPCD 2:1 CH:MCHM	0	0	4	0	0	100
2HPCDMCHM	0	0	0	4	0	100
2HPCDcyclohexanol	0	0	0	0	4	100
Total	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.996	1.000	1.000

PBS array:

Jackknifed Classification Matrix

	PBS 1:1 CH:MCHM	PBS 1:2 CH:MCHM	PBS 2:1 CH:MCHM	PBSMCHM	PBScyclohexanol	%correct
PBS 1:1 CH:MCHM	4	0	0	0	0	100
PBS 1:2 CH:MCHM	0	4	0	0	0	100
PBS 2:1 CH:MCHM	0	0	4	0	0	100
PBSMCHM	0	0	0	4	0	100
PBScyclohexanol	0	0	0	0	4	100
Total	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.998	1.000	1.000

ARRAY 3 – ANALYTE 8 IN β -CYCLODEXTRIN IN DIFFERENT SOLVENT SYSTEMS:

Jackknifed Classification Matrix

	1M NaCl MCHM	PB MCHM	PBS MCHM	PureWater MCHM	Seawater MCHM	%correct
1M NaCl MCHM	4	0	0	0	0	100
PB MCHM	0	4	0	0	0	100
PBS MCHM	0	0	4	0	0	100
PureWater MCHM	0	0	0	4	0	100
Seawater MCHM	0	0	0	0	4	100
Total	4	4	4	4	4	100

Cumulative Proportion of Total Dispersion

0.955	1.000	1.000

SUMMARY FIGURES

SUMMARY FIGURES FOR FLUORESCENCE MODULATION

Analyte 1 – Fluorophore 14

Analyte 1 – Fluorophore 15

Analyte 1 – Fluorophore 16

Analyte 2 – Fluorophore 14

Analyte 2 – Fluorophore 15

Analyte 2 – Fluorophore 16

Analyte 3 – Fluorophore 14

Analyte 3 – Fluorophore 15

Analyte 3 – Fluorophore 16

Analyte 4 – Fluorophore 14

Analyte 4 – Fluorophore 15

Analyte 4 – Fluorophore 16

Analyte 5 – Fluorophore 14

Analyte 5 – Fluorophore 15

Analyte 5 – Fluorophore 16

Analyte 6 – Fluorophore 14

Analyte 6 – Fluorophore 15

Analyte 6 – Fluorophore 16

Analyte 7 – Fluorophore 14

Analyte 7 – Fluorophore 15

Analyte 7 – Fluorophore 16

Analyte 8 – Fluorophore 14

Analyte 8 – Fluorophore 15

Analyte 8 – Fluorophore 16

Analyte 9 – Fluorophore 14

Analyte 9 – Fluorophore 15

Analyte 9 – Fluorophore 16

Analyte 10 – Fluorophore 14

Analyte 10 – Fluorophore 15

Analyte 10 – Fluorophore 16

Analyte 11 – Fluorophore 14

Analyte 11 – Fluorophore 15

Analyte 11 – Fluorophore 16

Analyte 12 – Fluorophore 14

Analyte 12 – Fluorophore 15

Analyte 12 – Fluorophore 16

Analyte 13 – Fluorophore 14

Analyte 13 – Fluorophore 15

Analyte 13 – Fluorophore 16

Analytes **2** and **8** (2:1) – Fluorophore **14**

Analytes **2** and **8** (2:1) – Fluorophore **15**

Analytes **2** and **8** (2:1) – Fluorophore **16**

Analytes **2** and **8** (1:1) – Fluorophore **14**

Analytes **2** and **8** (1:1) – Fluorophore **15**

Analytes **2** and **8** (1:1) – Fluorophore **16**

Analytes **2** and **8** (1:2) – Fluorophore **14**

Analytes **2** and **8** (1:2) – Fluorophore **15**

Analytes **2** and **8** (1:2) – Fluorophore **16**

Different solvent systems using analyte **8** in β -cyclodextrin:
With fluorophore **14**:

With fluorophore **15**:

With fluorophore **16**:

SUMMARY FIGURES FOR ARRAY-BASED DETECTION

ARRAY 1: SINGLE COMPOUNDS ENTERED INTO ARRAY

All analyte-fluorophore-host combinations:

In α -CD:

In β -CD:

In Me- β -CD:

In 2-HPCD:

In PBS:

ARRAY 2: MIXED ANALYTES (2 AND 8) ENTERED INTO ARRAY:

All analyte-fluorophore-host combinations:

In α -CD:

In β -CD:

In Me- β -CD:

In 2-HPCD:

In PBS:

ARRAY 3: ANALYTE 8 IN β -CYCLODEXTRIN IN DIFFERENT SOLVENT SYSTEMS:

ARRAY WITH DIFFERENT SOLVENT SYSTEMS USING ANALYTE 8 AND FLUOROPHORE 14 IN β -CYCLODEXTRIN

SUMMARY FIGURES FOR LIMITS OF DETECTION

Analyte **1** – Fluorophore **14** – α -CD

Analyte **1** – Fluorophore **14** – β -CD

Analyte **1** – Fluorophore **14** – Me- β -CD

Analyte 1 – Fluorophore 14 – 2-HPCD

Analyte 1 – Fluorophore 14 – PBS

Analyte 2 – Fluorophore 14 – α-CD

Analyte **2** – Fluorophore **14** – β -CD

Analyte **2** – Fluorophore **14** – Me- β -CD

Analyte **2** – Fluorophore **14** – 2-HPCD

Analyte **2** – Fluorophore **14** – PBS

Analyte **3** – Fluorophore **14** – α -CD

Analyte **3** – Fluorophore **14** – β -CD

Analyte **3** – Fluorophore **14** – Me- β -CD

Analyte **3** – Fluorophore **14** – 2HPCD

Analyte **3** – Fluorophore **14** – PBS

Analyte **3** – Fluorophore **15** – α -CD

Analyte **3** – Fluorophore **15** – β -CD

Analyte **3** – Fluorophore **15** – Me- β -CD

Analyte **3** – Fluorophore **15** – 2-HPCD

Analyte **3** – Fluorophore **15** – PBS

Analyte **3** – Fluorophore **16** – α -CD

Analyte **3** – Fluorophore **16** – β -CD

Analyte **3** – Fluorophore **16** – Me- β -CD

Analyte **3** – Fluorophore **16** – 2-HPCD

Analyte **3** – Fluorophore **16** – PBS

Analyte **4** – Fluorophore **14** – α -CD

Analyte **4** – Fluorophore **14** – β -CD

Analyte **4** – Fluorophore **14** – Me- β -CD

Analyte **4** – Fluorophore **14** – 2HPCD

Analyte **4** – Fluorophore **14** – PBS

Analyte **4** – Fluorophore **15** – α -CD

Analyte **4** – Fluorophore **15** – β -CD

Analyte **4** – Fluorophore **15** – Me- β -CD

Analyte **4** – Fluorophore **15** – 2-HPCD

Analyte **4** – Fluorophore **15** – PBS

Analyte **4** – Fluorophore **16** – α -CD

Analyte **4** – Fluorophore **16** – β -CD

Analyte **4** – Fluorophore **16** – Me- β -CD

Analyte **4** – Fluorophore **16** – 2-HPCD

Analyte **4** – Fluorophore **16** – PBS

Analyte **8** – Fluorophore **14** – α -CD

Analyte **8** – Fluorophore **14** – β -CD

Analyte **8** – Fluorophore **14** – Me- β -CD

Analyte **8** – Fluorophore **14** – 2-HPCD

Analyte **8** – Fluorophore **14** – PBS

Analyte **9** – Fluorophore **14** – α -CD

Analyte **9** – Fluorophore **14** – β -CD

Analyte **9** – Fluorophore **14** – Me- β -CD

Analyte **9** – Fluorophore **14** – 2-HPCD

Analyte **9** – Fluorophore **14** – PBS

Analyte **10** – Fluorophore **14** – α-CD

Analyte **10** – Fluorophore **14** – β -CD

Analyte **10** – Fluorophore **14** – Me- β -CD

Analyte **10** – Fluorophore **14** – 2-HPCD

Analyte **10** – Fluorophore **14** – PBS

Analyte **11** – Fluorophore **14** – α -CD

Analyte **11** – Fluorophore **14** – β -CD

Analyte **11** – Fluorophore **14** – Me- β -CD

Analyte **11** – Fluorophore **14** – 2-HPCD

Analyte **11** – Fluorophore **14** – PBS

Analyte **12** – Fluorophore **14** – α -CD

Analyte **12** – Fluorophore **14** – β -CD

Analyte **12** – Fluorophore **14** – Me- β -CD

Analyte **12** – Fluorophore **14** – 2-HPCD

Analyte **12** – Fluorophore **14** – PBS