Electronic Supplementary Information

DNA-polyfluorophore Chemosensors for Environmental Remediation: Vapor-phase Identification of Petroleum Products in Contaminated Soil

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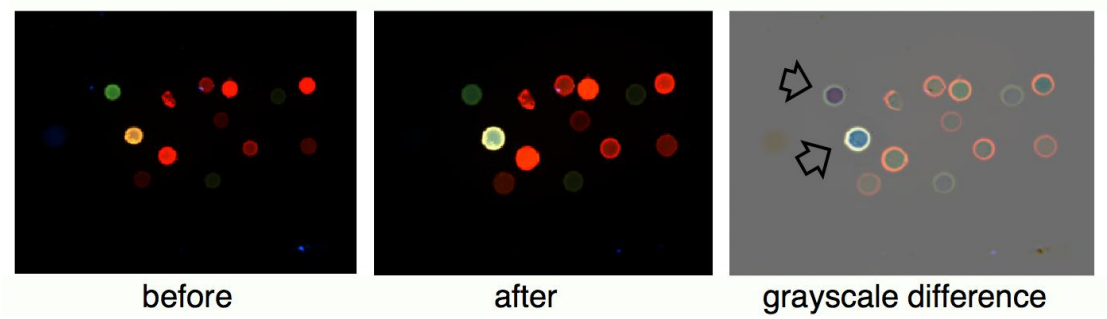


Figure S1: Examples of images used in screening for candidate chemosensors on beads. (Arrows point to two strongly-responding sequences)

Table S1. MALDI-MS data for ODF chemosensors.

Sequence	$MW_{(calc)}$	$MW_{(found)}$
5'-YYVF-3'	1931.9	1932.5
5'-EKHV-3'	1716.5	1715.6
5'-FVYE-3'	1981.9	1981.3
5'-EYYY-3'	1589.4	1590.6
5'-YYSK-3'	1440.2	1440.7
5'-FEYF-3'	2174.2	2175.3
5'-FHVS-3'	1657.5	1658.8
5'-YKFY-3'	1932.8	1935.3
5'-FESV-3'	1781.7	1780.2
5'-EVFF-3'	2274.3	NA[b]
5'-SSEK-3'	1290.0	1319.3
5'-FQSH-3'	1681.5	1681.8
5'-HQHY-3'	1515.2	1515.5
5'-HQHF-3'	1807.6	1807.3
5'-YQFS-3'	1755.6	1757.3
5'-YHYH-3'[a]	1390.3	1391.0
5'-SSYE-3'[a]	1190.2	1190.0
5'-HSYE-3'[a]	1313.3	1313.2
5'-YSES-3'[a]	1188.2	1189.9
5'-EHSE-3'[a]	1364.3	1365.2

[a]Compound made and characterized previously: F. Samain, N. Dai, E. T. Kool, *Chemistry* **2011**, *17*, 174-183.
[b]parent ion not observed.

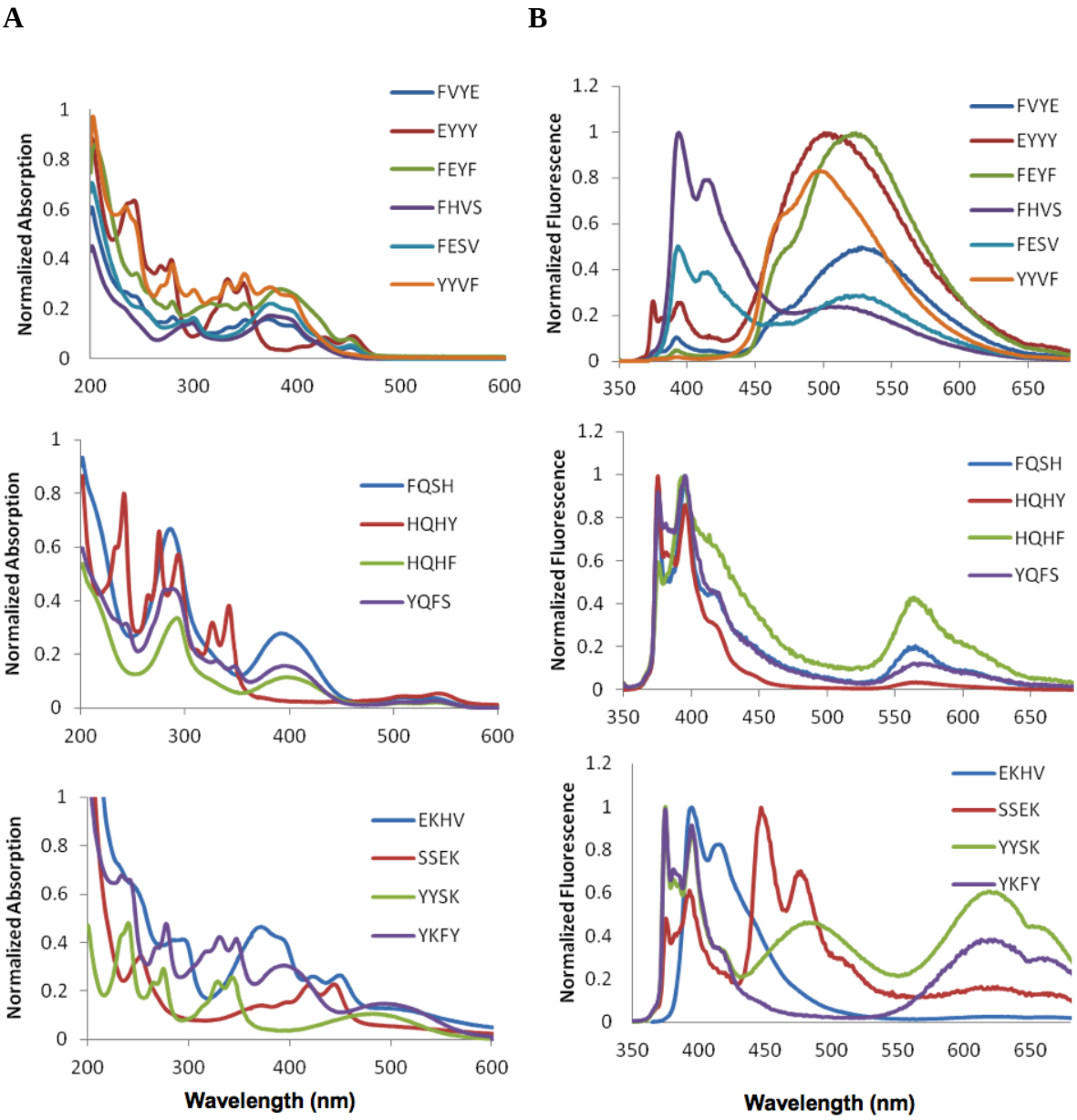


Figure S2: Optical spectra of new ODF chemosensors synthesized for this study (concentration = 1 μM in PBS buffer). (A) Normalized absorption spectra; (B) Normalized emission spectra (excitation 345 nm). Spectra of the last five sequences (Table S1) were published previously.

Table S2. Volatile organic analytes used in screening for chemosensors.

Analyte	Saturated Vapor Pressure (ppm)	Temperature (°C)
Acrylamide	9.2	25
Acrylonitrile	12,800	25
Benzene	131,000	25
Decane	1,700	25
Dibromoethane	15,400	25
Dichlorobenzene	1,900	25
MTBE	322,000	25
Naphthalene	110	25
Phenanthrene	1.2	25
Styrene	5,900	25
Thiophene	107,000	25
Xylene	8,000	25

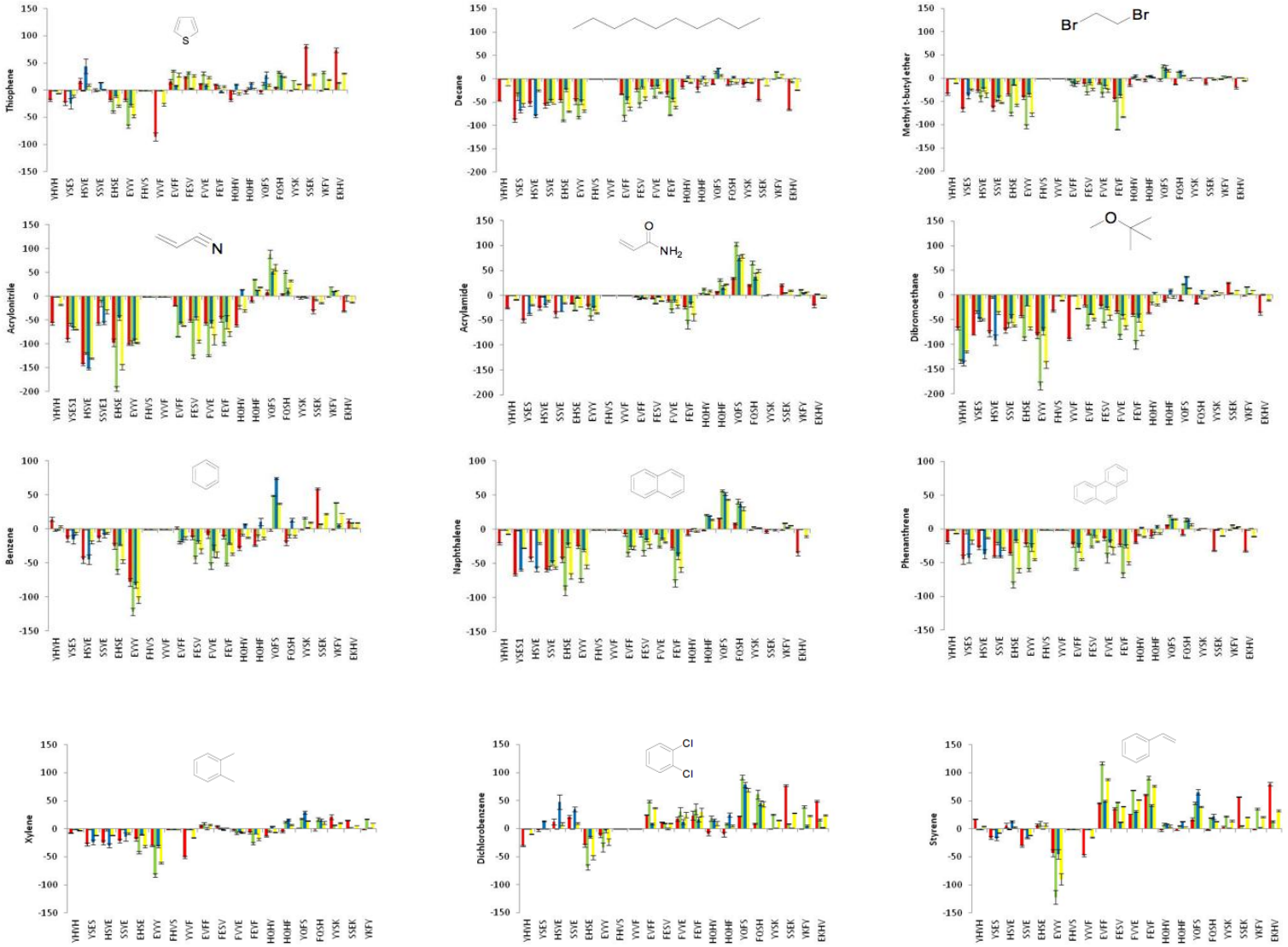
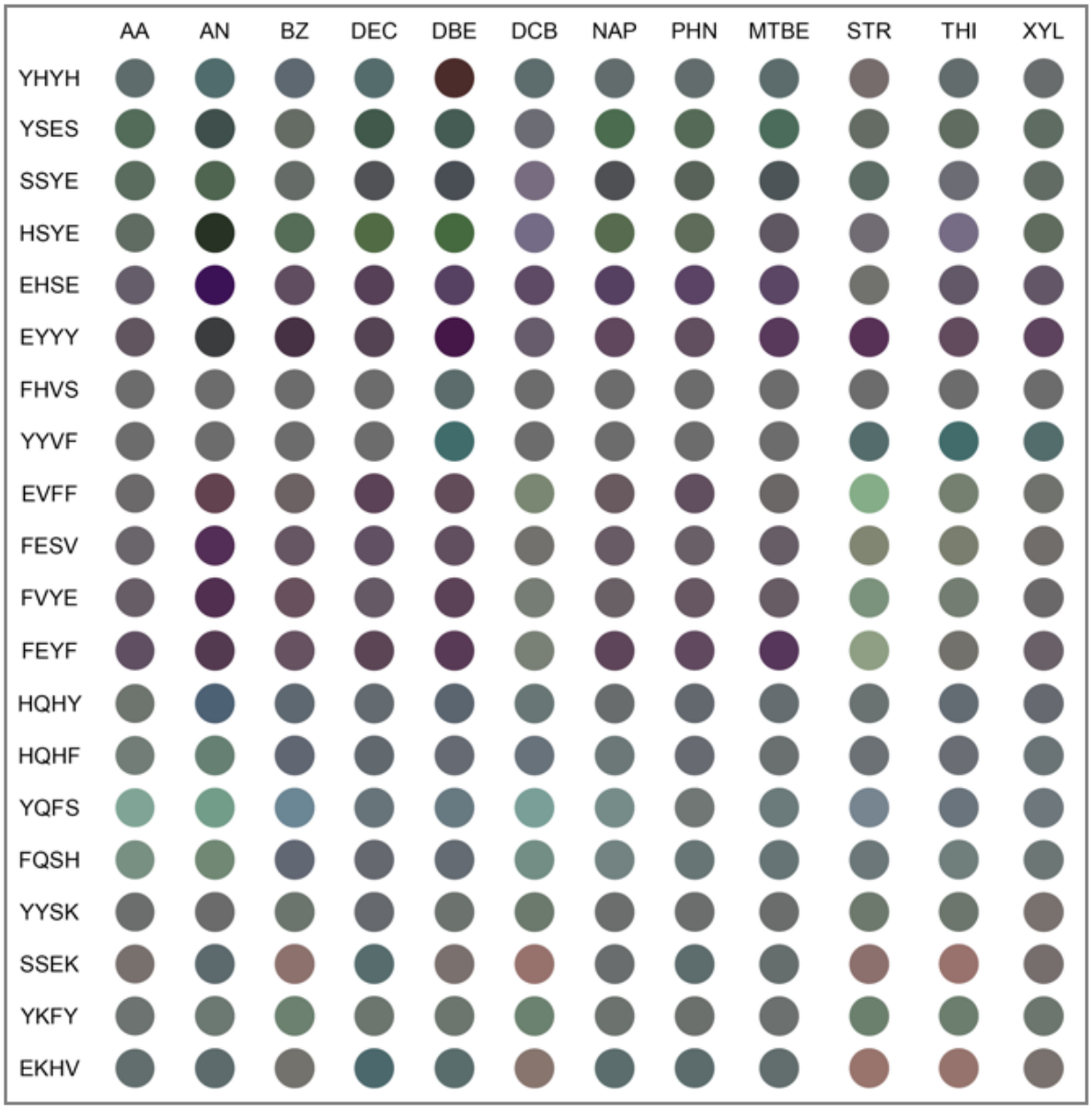
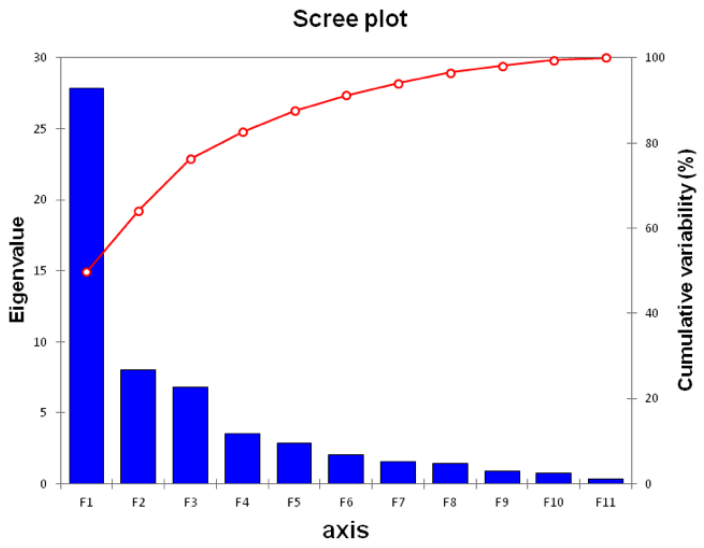


Figure S3. Cross-screening results for assessing candidate chemosensors. Shown are R,G,B,L responses of twenty candidate chemosensors to all twelve petrochemical analytes.



AA: acrylamide, AN: acrylonitrile, BZ: benzene, DEC: decane, DBE: dibromoethane, DCB: dichlorobenzene, NAP: naphthalene, PHN: phenanthrene, MEBE: methyl t-butyl ether, STR: stryrene, THI: thiophene, XYL: xylene.

Figure S4. Differential bead images from cross screening, showing diversity of responses to pure petrochemical analyte vapors.



	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10	F11
Eigenvalue	27.872	8.031	6.787	3.546	2.814	2.009	1.589	1.411	0.870	0.756	0.315
Variability (%)	49.772	14.341	12.120	6.332	5.026	3.588	2.837	2.520	1.553	1.349	0.563

Figure S5. Eigenvalues and variability from cross screening of twenty chemosensors with twelve VOC analytes, showing high dispersion of the data over several dimensions.

Figure S6. Syringe pump and optical cell used for analyzing headgas from contaminated soils.

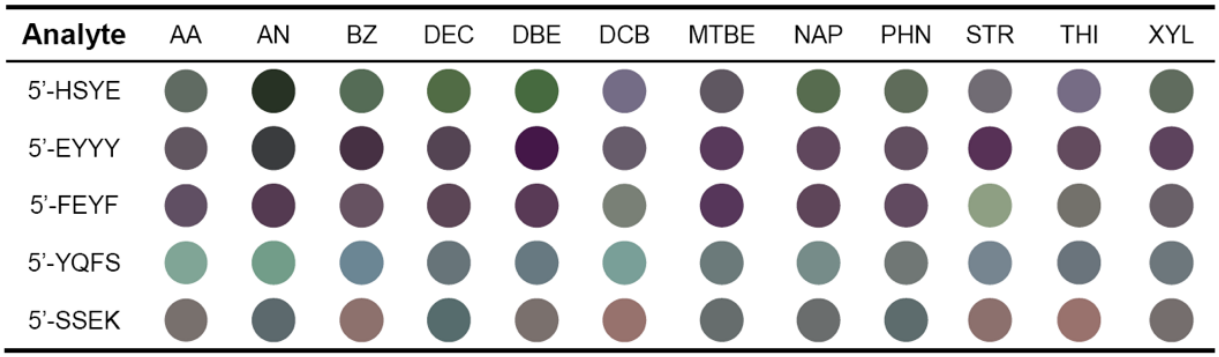


Figure S7. Differential bead images, showing high diversity of responses of five optimal chemosensors to the pure petrochemical analytes.

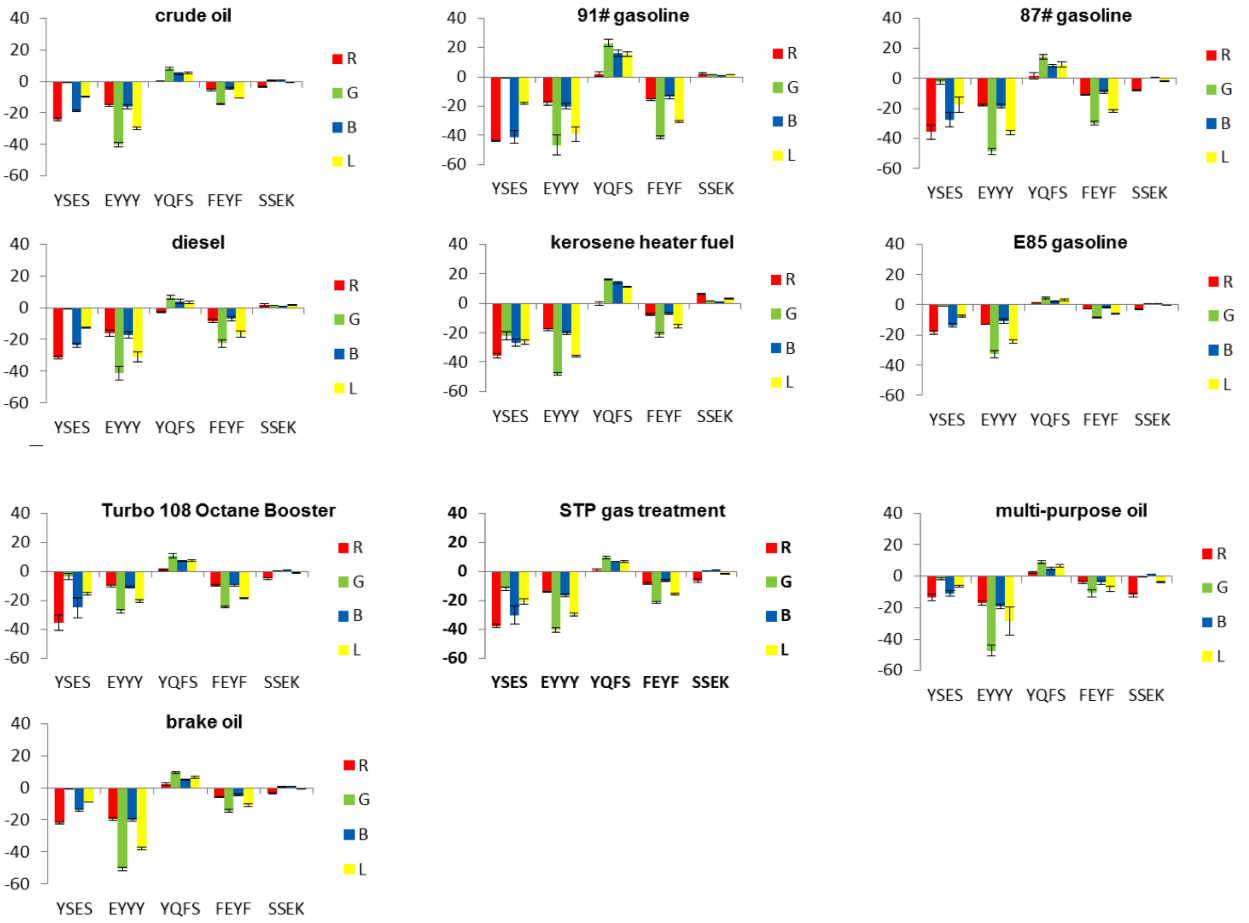


Figure S8. Quantitative R,G,B,L responses of five sensors with 1000 ppm petroleum product contamination in soil

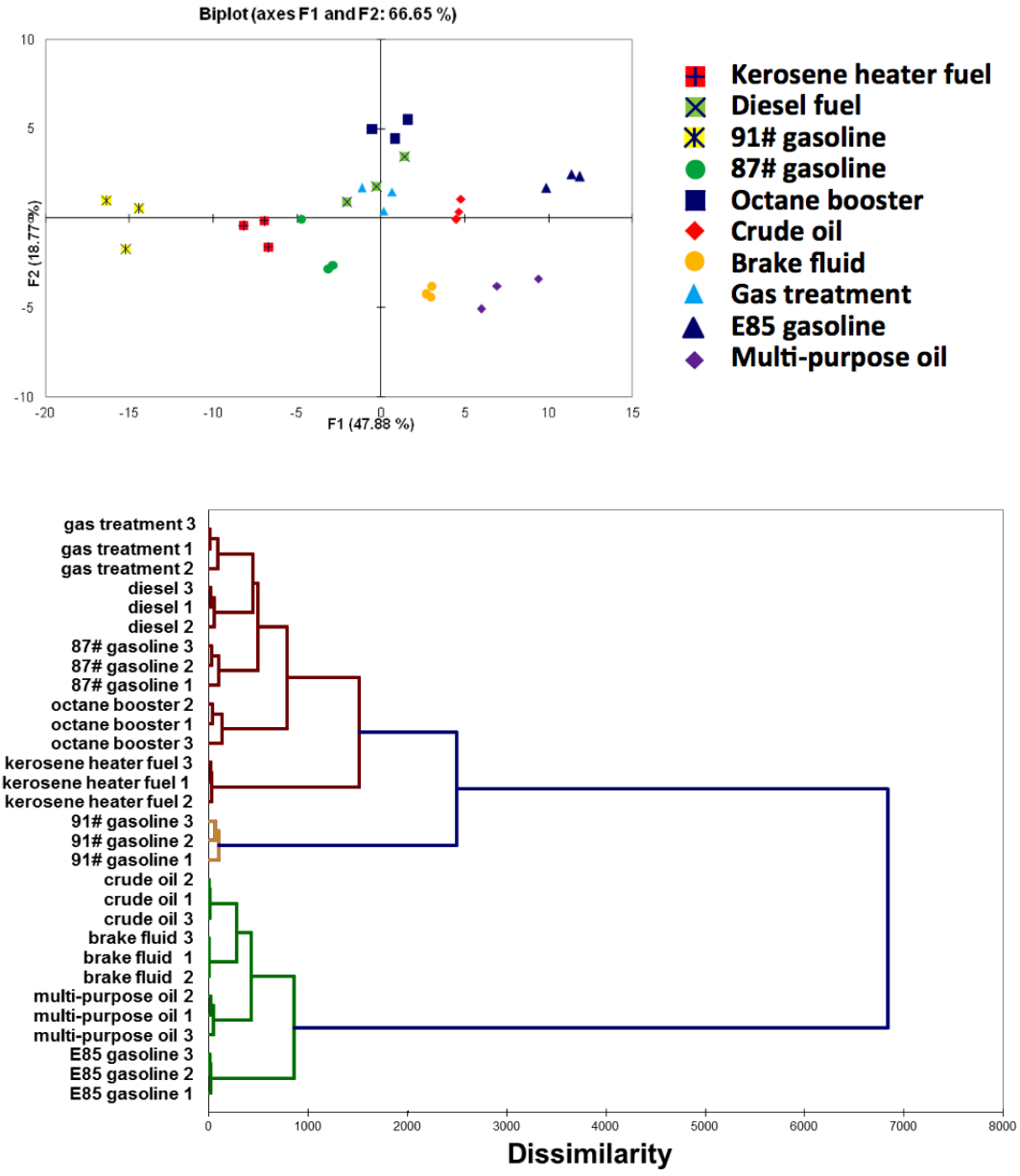


Figure S9. (top) PCA scatterplot and (bottom) AHC clustering dendrogram of five sensor responses to 1000 ppm oil products in soil .

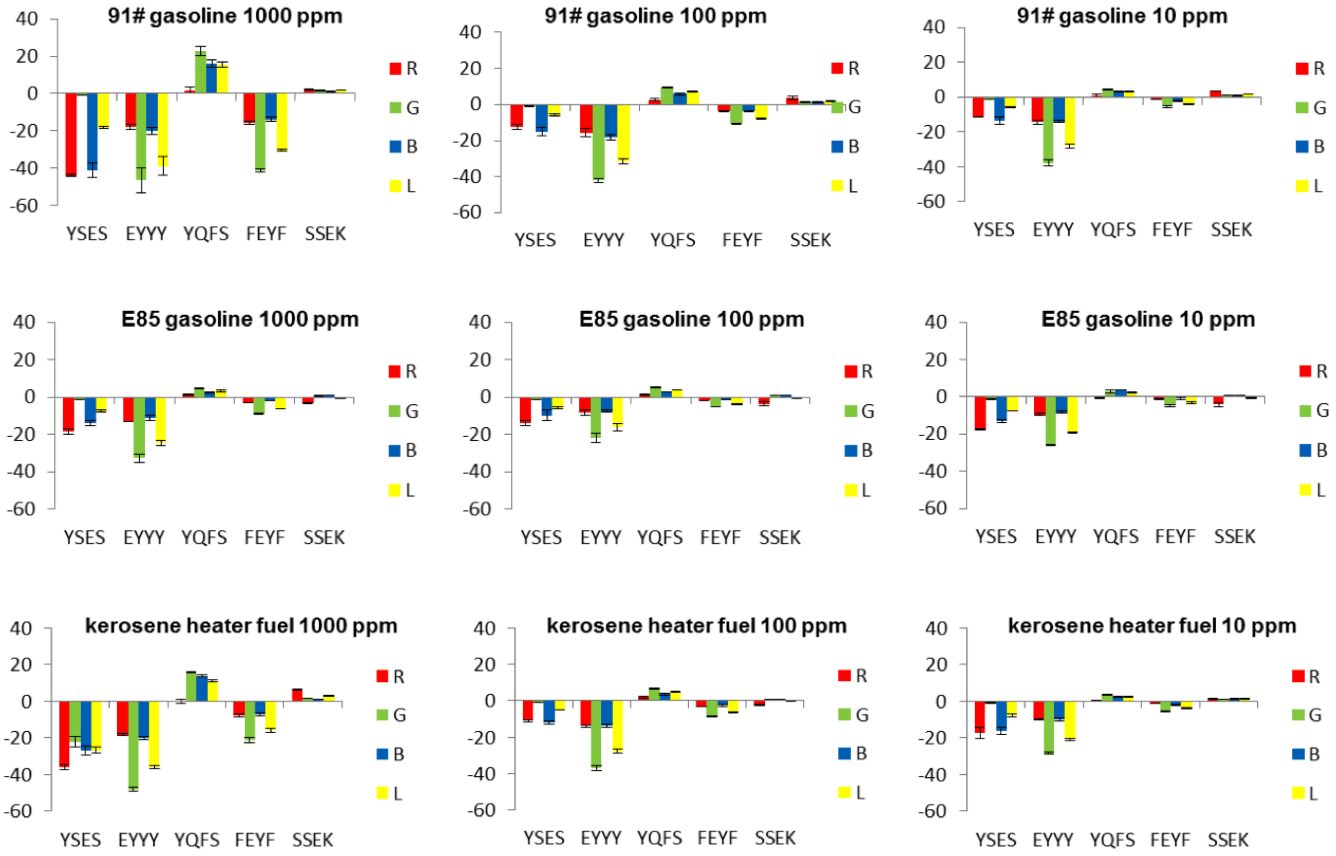


Figure S10. Comparison of RGBL responses of five chemosensors at 1000, 100, and 10 ppm petroleum contaminants.

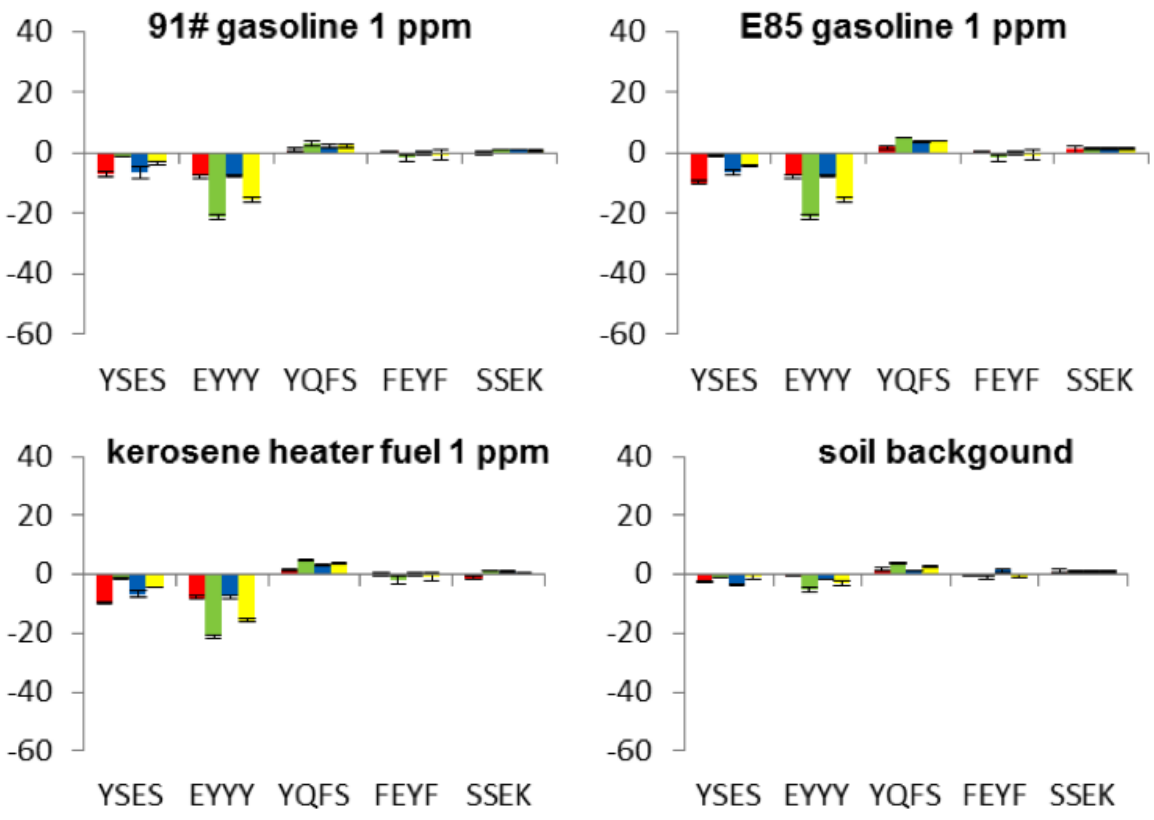
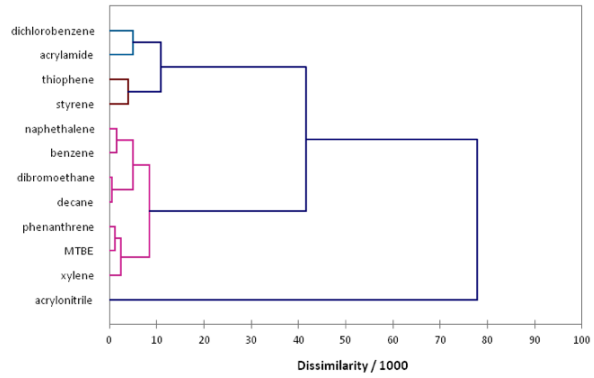


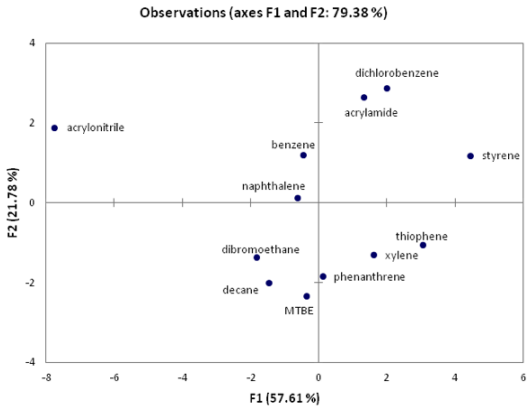
Figure S11. RGBL chemosensor responses to 1 ppm contaminants in soil.

Figure S12. AHC and PCA plots for different combinations of five sensors.

Combination # 1

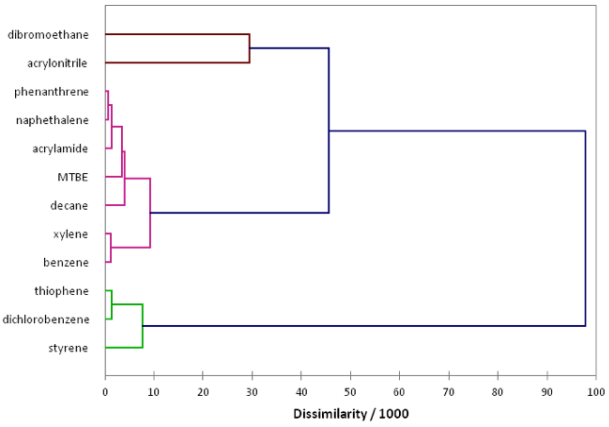
#	Sequence
1	HSYE
2	FESV
3	EHSE
4	YKFY
5	YQFS

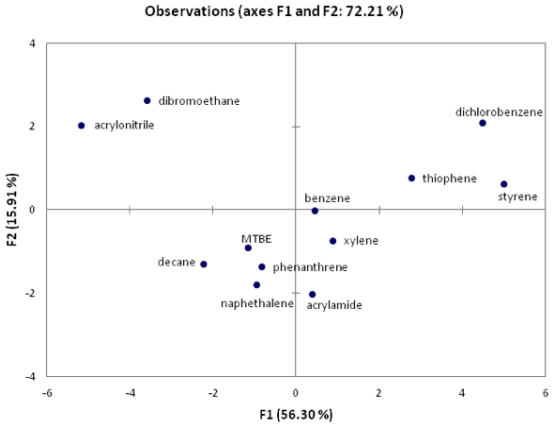




Combination # 2

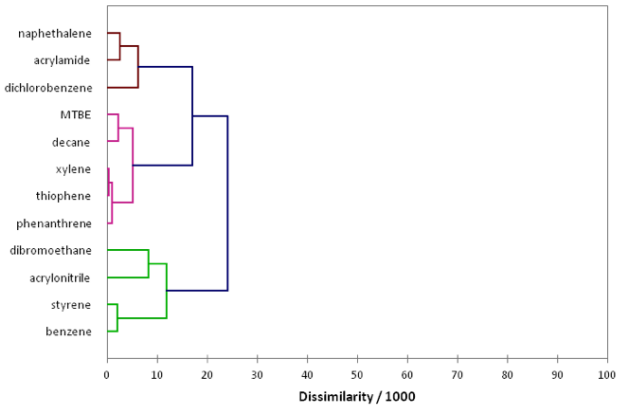
#	Sequence
1	HSYE
2	YHYH
3	FEYF
4	EKHV
5	HQHY

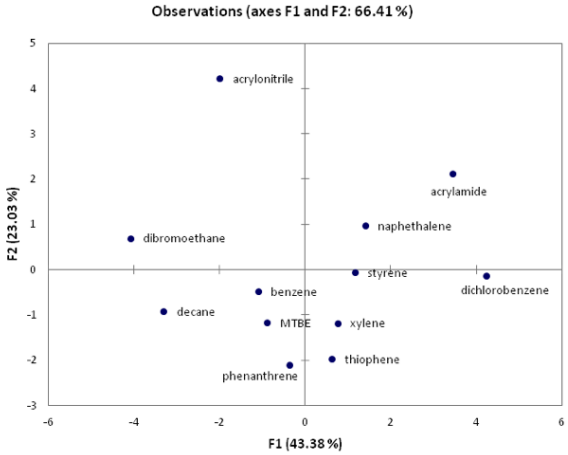




Combination # 3

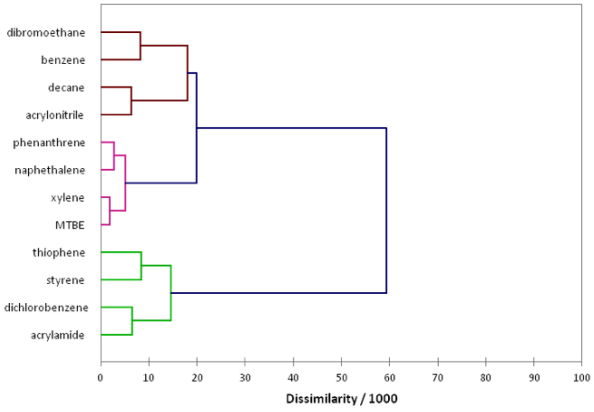
#	Sequence
1	YSES
2	EYYY
3	FHVS
4	HQHF
5	YQFS

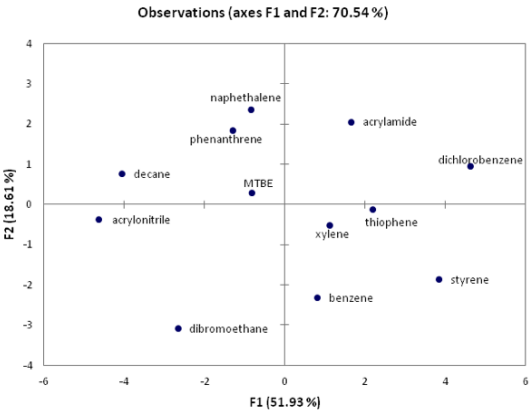




Combination # 4

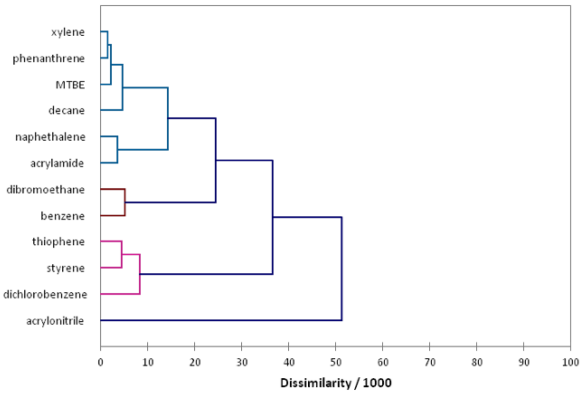
#	Sequence
1	YSES
2	EYYY
3	EVFF
4	YQFS
5	SSEK

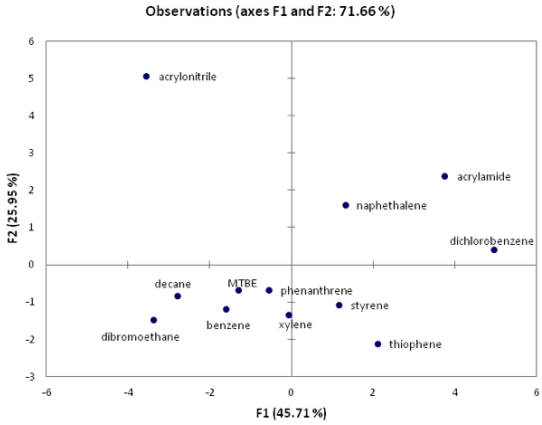




Combination # 5

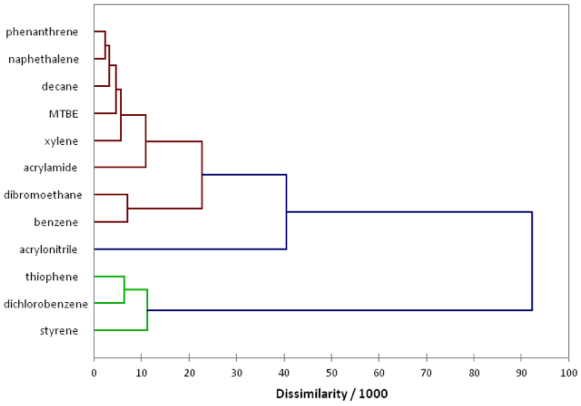
#	Sequence
1	HSYE
2	EYYY
3	FQSH
4	YQFS
5	SSEK

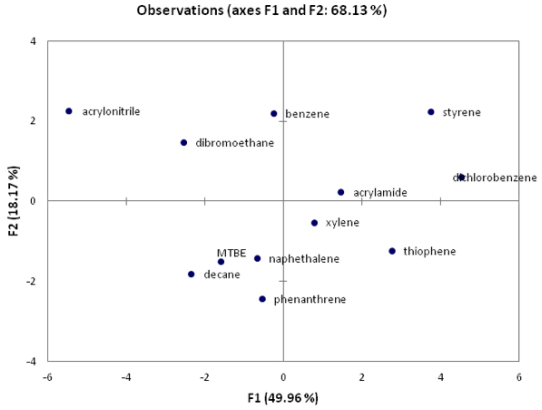




Combination # 6

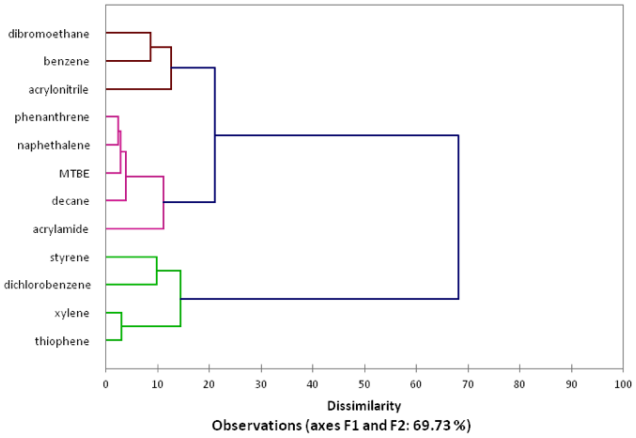
#	Sequence
1	HSYE
2	EYYY
3	FEYF
4	YQFS
5	SSEK

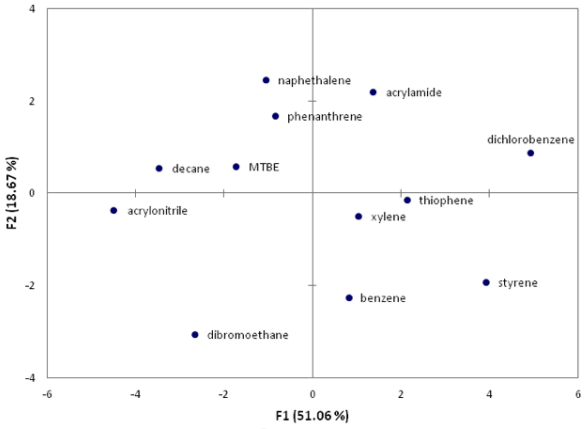




Combination # 7

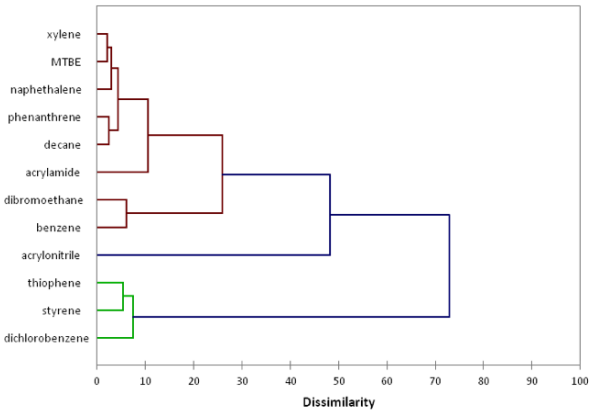
#	Sequence
1	YSES
2	EYYY
3	FEYF
4	YQFS
5	SSEK

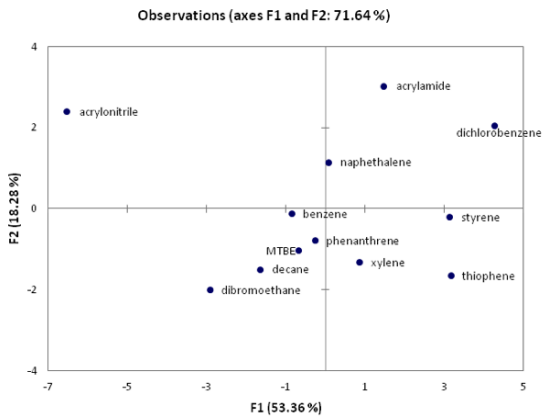




Combination # 8

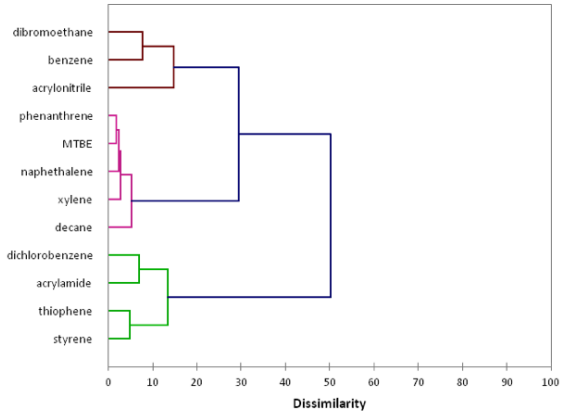
#	Sequence
1	HSYE
2	EYYY
3	FVYE
4	YQFS
5	SSEK

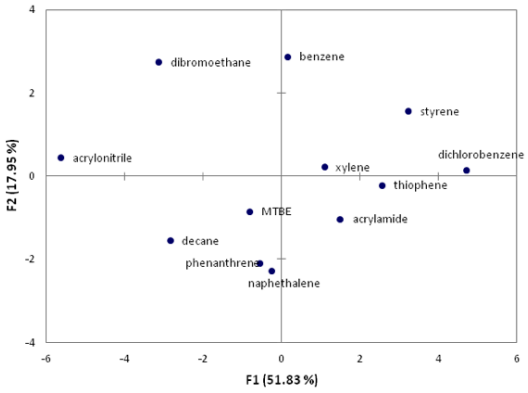




Combination # 9

#	Sequence
1	YSES
2	EYYY
3	FVYE
4	YQFS
5	SSEK





Combination # 10

#	Sequence
1	YSES
2	EYYY
3	FVYE
4	YQFS
5	YKFY