Electronic Supplementary Material (ESI) for Analytical Methods.

SUPPLEMENTARY INFORMATION

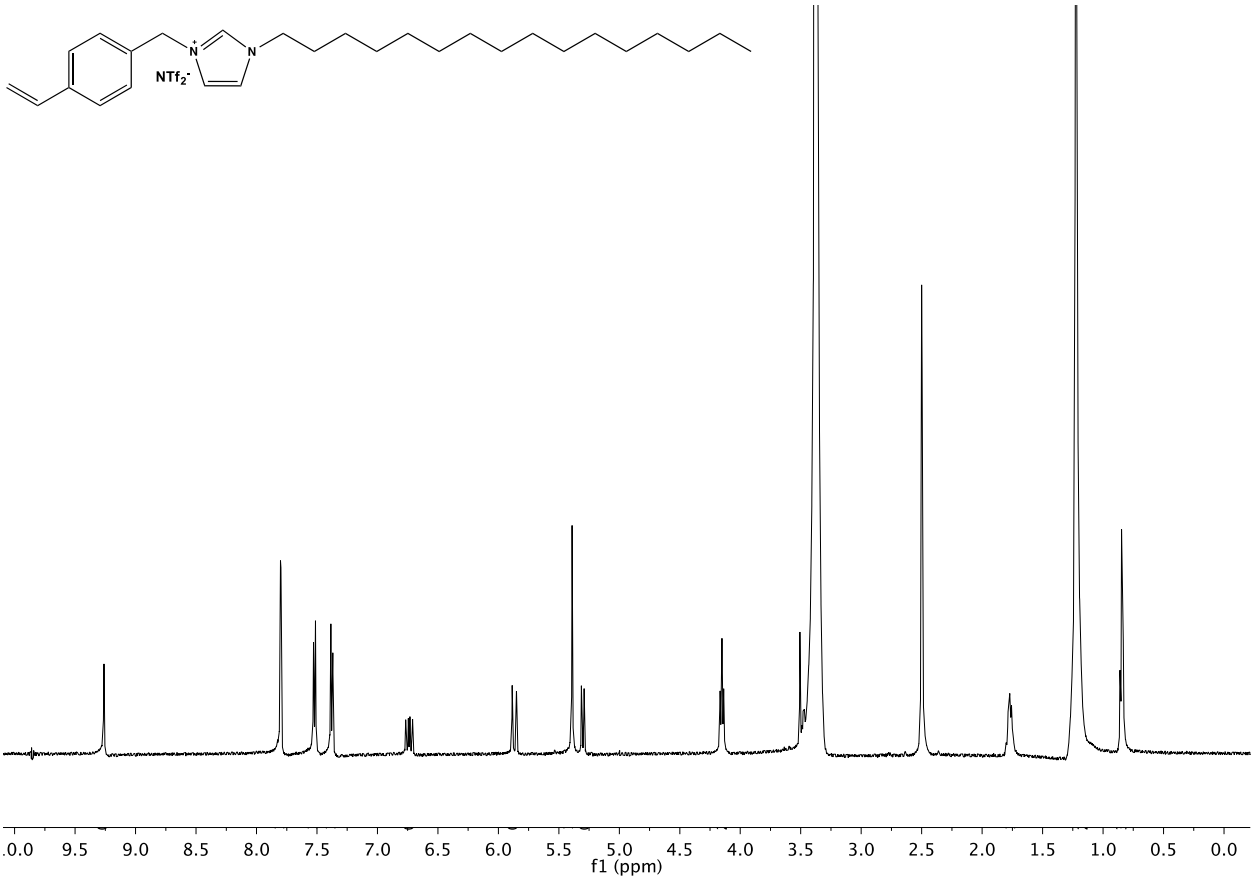
"Determination of compounds with varied volatilities from aqueous samples using a polymeric ionic liquid sorbent coating by direct immersion-headspace solid phase microextraction"

Josias Merib[a,b], Honglian Yu[b], Eduardo Carasek[a], Jared L. Anderson[b]

[a] *Departamento de Química, Universidade Federal de Santa Catarina, Florianópolis 88040-900, SC, Brazil*

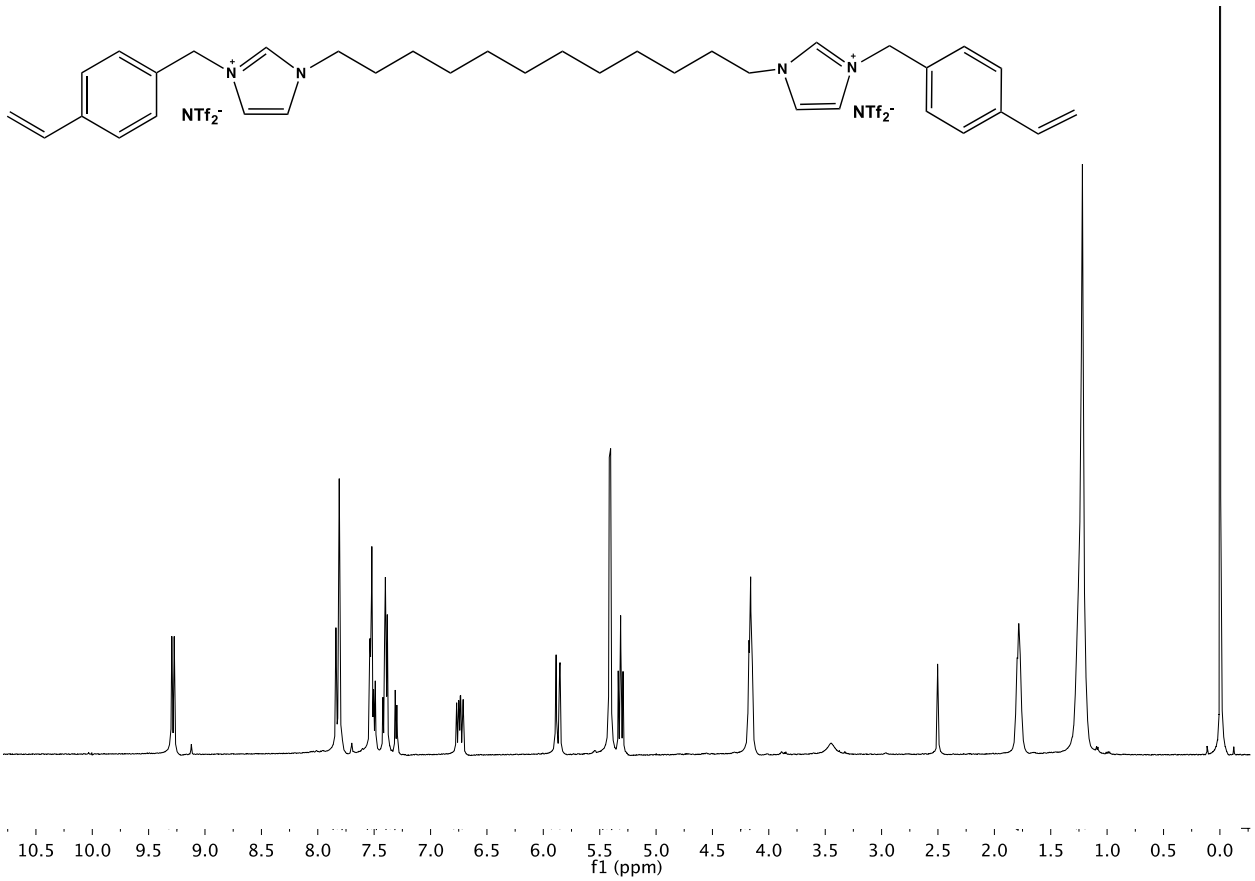
[b] *Department of Chemistry, Iowa State University, Ames IA 50011, USA*

Figure S1. ^{1}H-NMR for the [VBC$_{16}$IM][NTf$_2$] monomer (Fiber **1**)



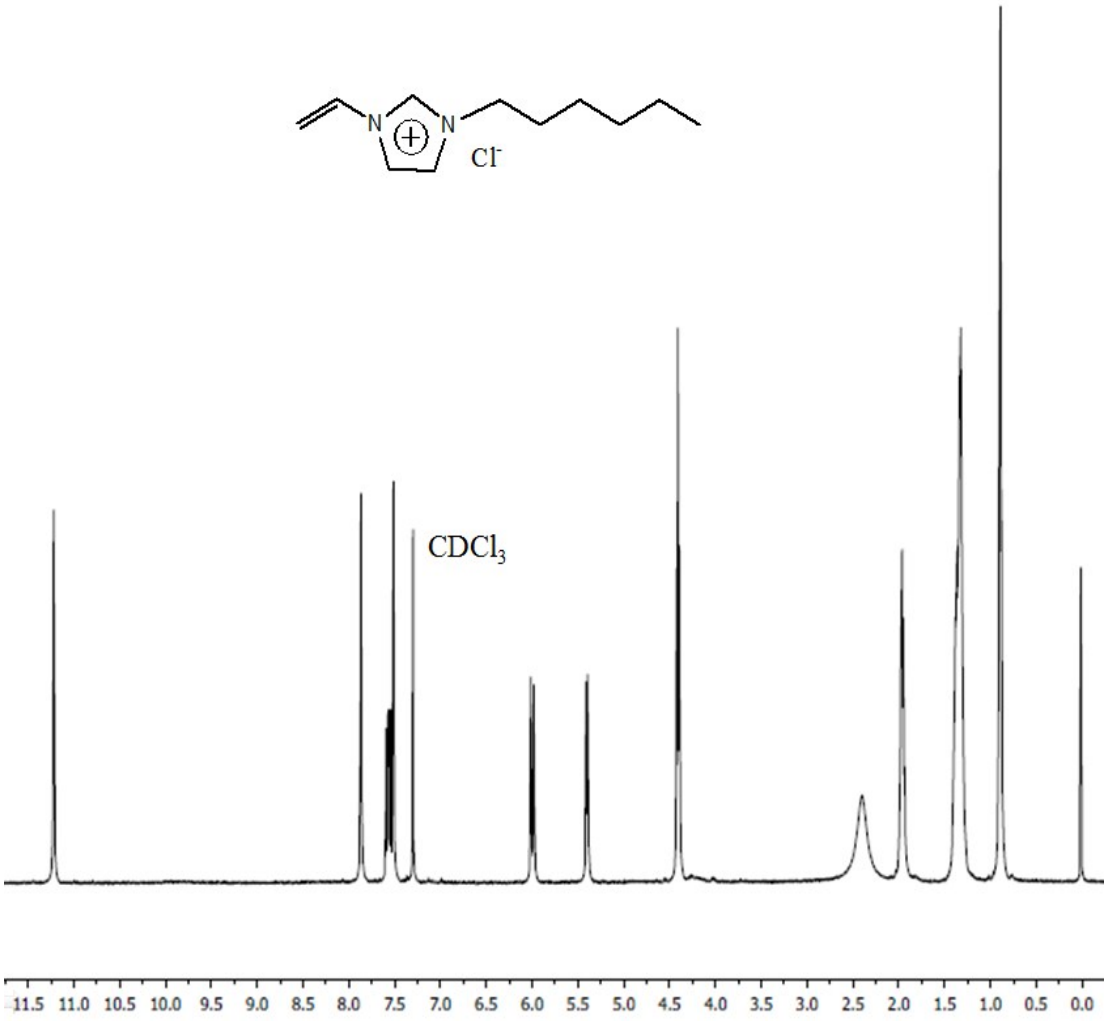
^{1}H NMR (500 MHz, DMSO-d_6): 9.26 (s, 1H), 7.80 (d, 2H), 7.61 – 7.45 (m, 2H), 7.38 (d, 2H), 6.74 (dd, 1H), 5.87 (dd, 1H), 5.39 (s, 2H), 5.30 (d, 1H), 4.15 (t, 2H), 1.84 – 1.68 (m, 2H), 1.22 (d, 26H), 0.95 – 0.74 (m, 3H).

Figure S2. ^{1}H-NMR for the [(VBIM)$_2$C$_{12}$] 2[NTf$_2$] IL crosslinker (Fiber **1**)



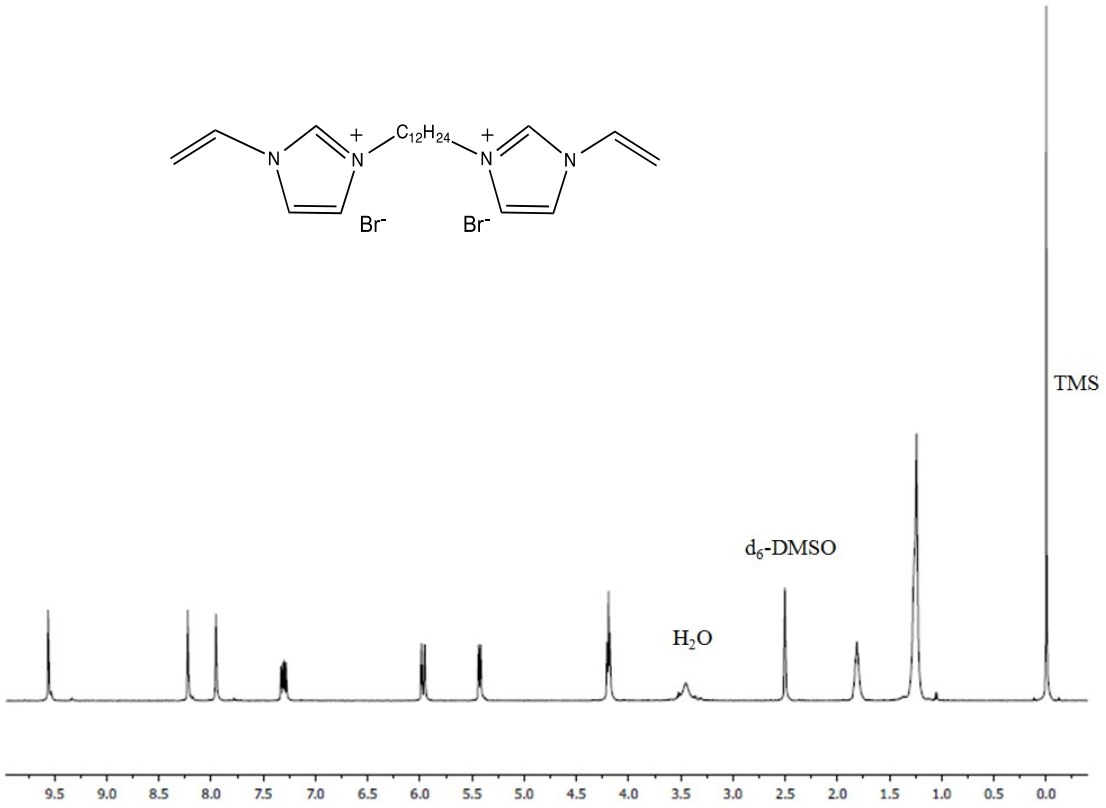
^{1}H NMR (500 MHz, DMSO-d_6): 9.28 (dt, 2H), 7.90 – 7.74 (m, 4H), 7.58 – 7.45 (m, 4H), 7.45 – 7.25 (m, 4H), 6.74 (ddd, 2H), 5.87 (ddd, 2H), 5.41 (d, 4H), 5.31 (ddd, 2H), 4.16 (td, 4H), 1.78 (s, 4H), 1.23 (d, 16H).

Figure S3. ^{1}H-NMR for the ([VC_6IM][Cl]) IL monomer (Fiber **2**)



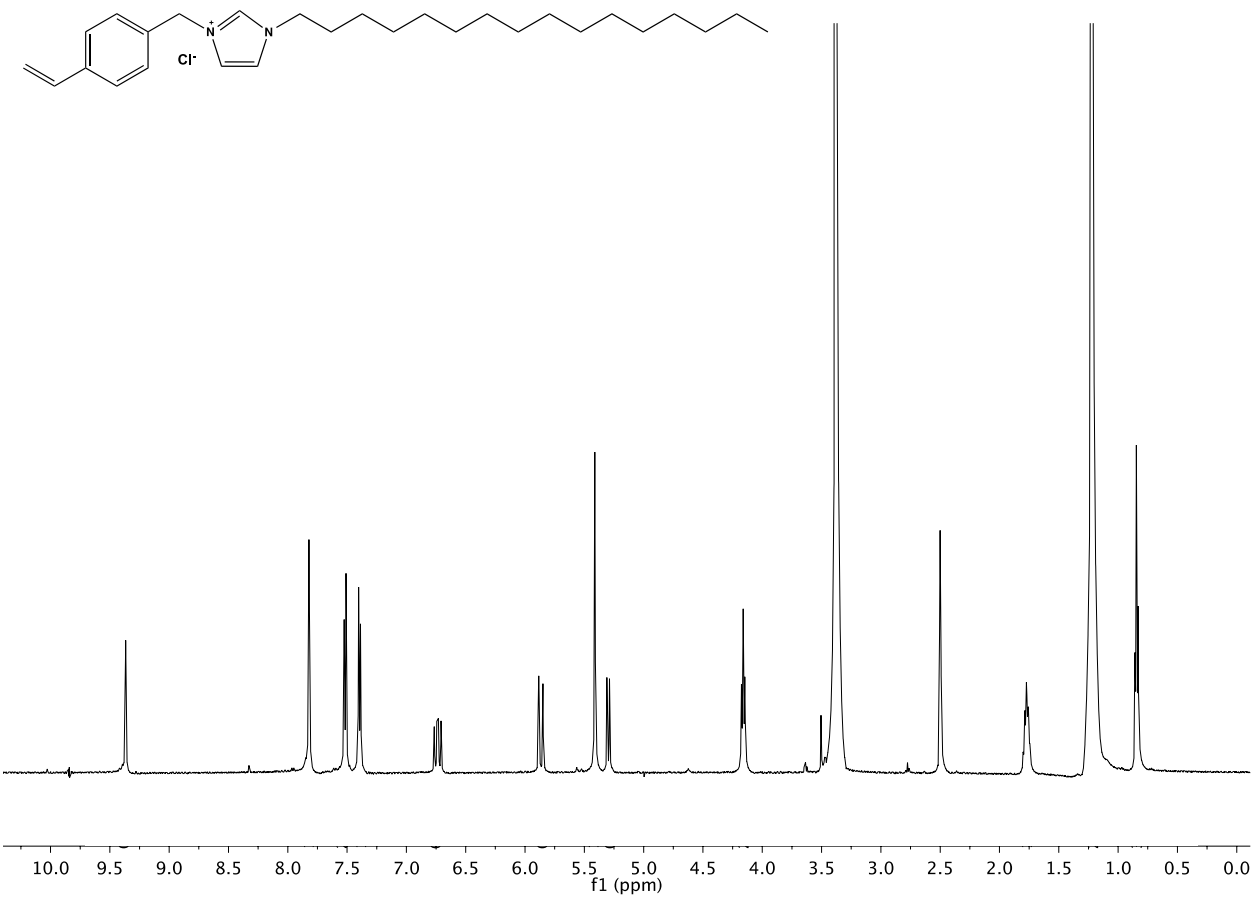
^{1}H NMR (500 MHz, $CDCl_3$): 11.21 (s, 1H), 7.86 (s, 1H), 7.55 (m, 1H), 7.49 (s, 1H), 5.98 (s, 1H), 5.38 (s, 1H), 4.40 (t, 2H), 1.96 (m, 2H), 1.35 (m, 6H), 0.87 (t, 3H).

Figure S4. ^{1}H-NMR for the [$(VIM)_2C_{12}$] 2[Br] IL crosslinker (Fiber **2**)



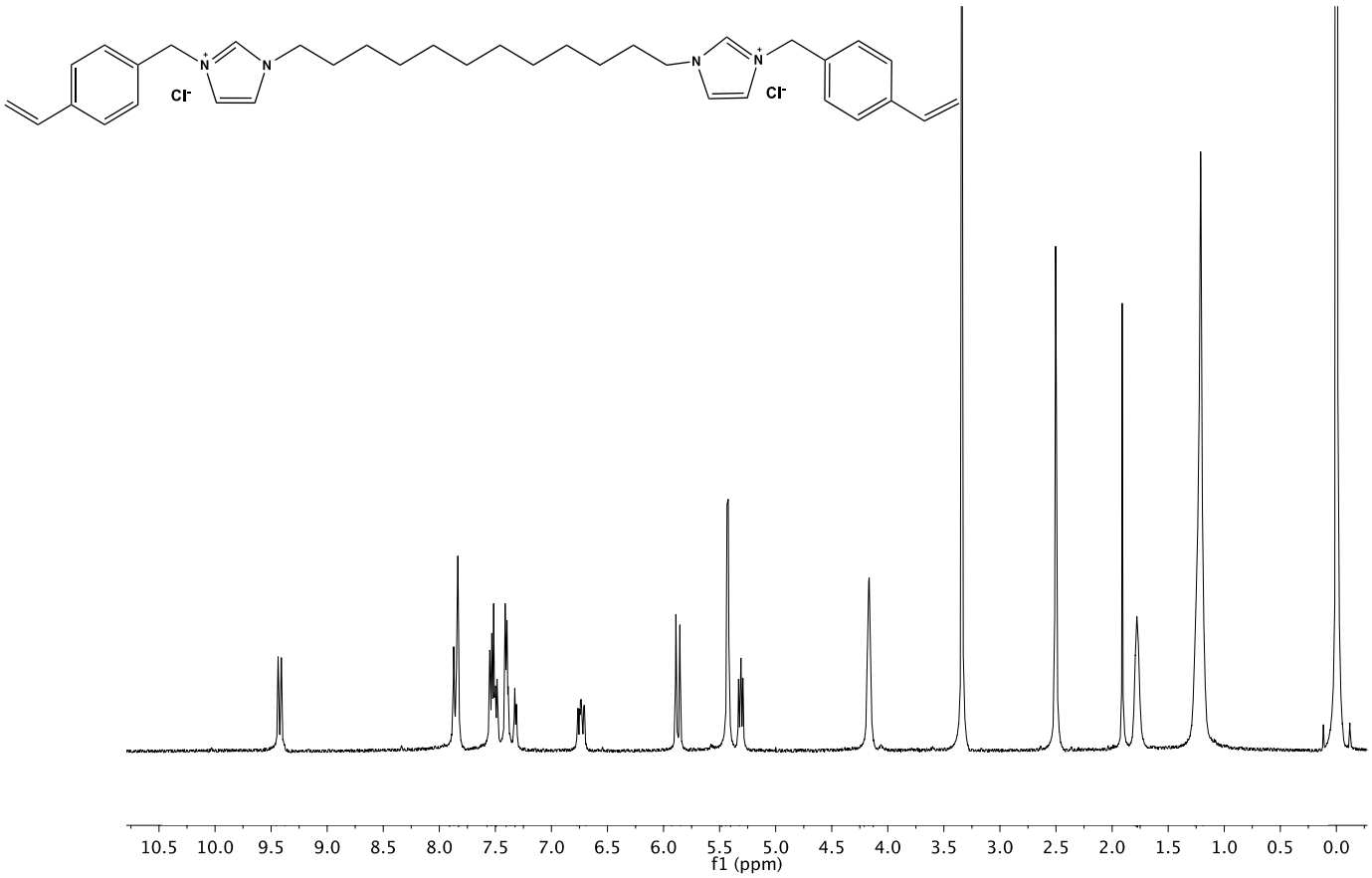
^{1}H NMR (500 MHz, d_6-DMSO): 9.55 (s, 2H), 8.22 (s, 2H), 7.95 (s, 2H), 7.30 (m, 2H), 5.97 (d, 2H), 5.42 (d, 2H), 4.18 (t, 4H), 1.80 (t, 4H), 1.24 (m, 16H).

Figure S5. ^{1}H-NMR for the [VBC$_{16}$IM][Cl] monomer (Fiber **3**)



^{1}H NMR (500 MHz, DMSO-d_6): 9.37 (s, 1H), 7.82 (p, 2H), 7.62 – 7.45 (m, 2H), 7.40 (d, 2H), 6.74 (dd, 1H), 5.87 (dd, 1H), 5.41 (s, 2H), 5.30 (dd, 1H), 4.16 (t, 2H), 1.78 (q, 2H), 1.22 (d, 26H), 0.89 – 0.78 (m, 3H).

Figure S6. ^{1}H-NMR for the [$(VBIM)_2C_{12}$] 2[Cl] IL crosslinker (Fiber **3**)



^{1}H NMR (500 MHz, DMSO-d_6): 9.42 (d, 2H), 7.95 – 7.77 (m, 4H), 7.60 – 7.45 (m, 4H), 7.40 (dt, 4H), 6.74 (ddd, 2H), 5.87 (d, 2H), 5.43 (d, 4H), 5.31 (dd, 2H), 4.17 (td, 4H), 1.78 (s, 4H), 1.21 (s, 16H).

Figure S7. Scanning electron micrograph showing the cross-section of the PIL-based sorbent coating (Fiber **1)** after approximately 110 extraction cycles.

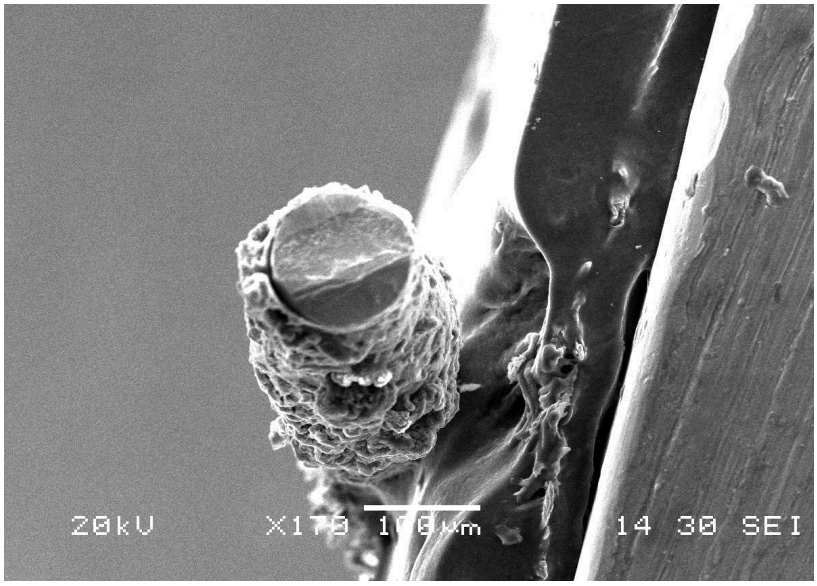


Table S1. ANOVA tables for the compounds ethyl benzene, m-xylene, naphthalene, acenaphthene, heptachlor, aldrin, heptachlor epoxide, and fluorene

ANOVA (ethyl benzene)

Source	SS	df	MS	F	P-value	F critic
Between groups	9,27224E+13	2	4,6361E+13	41,6334137	0,00030366	5,143253
Within groups	6,68134E+12	6	1,1136E+12			
Total	9,94037E+13	8				

ANOVA (m-xylene)

Source	*SS*	*df*	*MS*	*F*	*P-value*	*F critic*
Between groups	1,21151E+14	2	6,0575E+13	12,9493384	0,00665481	5,143253
Within groups	2,80672E+13	6	4,6779E+12			
Total	1,49218E+14	8				

ANOVA (naphthalene)

Source	*SS*	*df*	*MS*	*F*	*P-value*	*F critic*
Between groups	5,07986E+14	2	2,5399E+14	34,5768358	0,00050887	5,143253
Within groups	4,40746E+13	6	7,3458E+12			
Total	5,52061E+14	8				

ANOVA (acenaphthene)

Source	*SS*	*df*	*MS*	*F*	*P-value*	*F critic*
Between groups	1,00664E+15	2	5,0332E+14	2,47222809	0,16476736	5,143253
Within groups	1,22154E+15	6	2,0359E+14			
Total	2,22819E+15	8				

ANOVA (heptachlor)

Source	*SS*	*df*	*MS*	*F*	*P-value*	*F critic*
Between groups	2,56265E+16	2	1,2813E+16	37,4063989	0,00040927	5,143253
Within groups	2,05525E+15	6	3,4254E+14			
Total	2,76818E+16	8				

ANOVA (aldrin)

Source	*SS*	*df*	*MS*	*F*	*P-value*	*F critic*
Between groups	6,12798E+16	2	3,064E+16	60,3290577	0,00010631	5,143253
Within groups	3,04728E+15	6	5,0788E+14			
Total	6,43271E+16	8				

ANOVA (heptachlor epoxide)

Source	*SS*	*df*	*MS*	*F*	*P-value*	*F critic*
Between groups	1,5552E+15	2	7,776E+14	169,257759	5,2824E-06	5,143253
Within groups	2,75651E+13	6	4,5942E+12			
Total	1,58277E+15	8				

ANOVA (fluorene)

Source	*SS*	*df*	*MS*	*F*	*P-value*	*F critic*
Between groups	4,1201E+15	2	2,0601E+15	7,37470721	0,02417888	5,143253
Within groups	1,67604E+15	6	2,7934E+14			
Total	5,79614E+15	8				