

Extraction of Phenol as Pollutant from Aqueous Effluents Using Hydrophobic Deep Eutectic Solvents

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Table S1. Comparison of phenolic compounds extraction efficiency by utilising VOCs, ILs and HDESs as extractants

Solvent	Analytes	Extractant	Efficiency	Refs.
VOCs	Phenol in sebacic acid wastewater	Aliquat-336	96.3 %	[1]
	Phenol in wastewater containing 6000 mg/l phenol and 5 % salts	Octanol	> 99 %	[2]
	Phenol in aqueous solution	50 % v/v mixture of tributyl phosphate and 2-Octanol	99.9 %	[3]
	Phenol in aqueous solution	Cumene	59.22 %	[4]
	Phenol, p-chlorophenol, 2,4-dichlorophenol, 2,4,6-trichlorophenol, and pentachlorophenol in aqueous solutions	Tributyl phosphate	Around 85.94 %	[5]
	Phenol, p-chlorophenol, 2,4-dichlorophenol, 2,4,6-trichlorophenol, and pentachlorophenol in aqueous solutions	1-butyl-3-methylimidazolium tetrafluoroborate	Around 99.42 %	[5]
ILs	Phenolic compounds from cashew and rice industrial wastewater	Phosphonium chloride [PC6C6C6C14][Cl]	100 %	[6]
	Phenol from model oil	1-ethyl-3-methyl imidazolium lactate	99.9 %	[7]
	Phenols from oil mixtures	tetraethylammonium amino acid	99.0 %	[8]
HDESs	2-chlorophenol, 3-chlorophenol, 2,4-dichlorophenol from wastewater	HBA: menthol HBD: hexanoic acid, octanoic acid, decanoic acid, thymol.	> 94 % for all systems.	[9]
	4-chlorophenol, 2,4-dichlorophenol, 2,4,6-trichlorophenol from wastewater	DES composed of methyltrioctylammonium chloride and octanoic acid	90.8 % to 93.0 %	[10]
	Phenol, o-cresol, 2-chlorophenol from water	[Menthol: Octanoic acid] (1:1) [Menthol: Decanoic acid] (1:1)	Phenol: >70 % o-cresol & 2-chlorophenol: > 80 %	[11]

Table S2. Chemical structures of different chemicals investigated in this study.

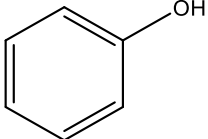
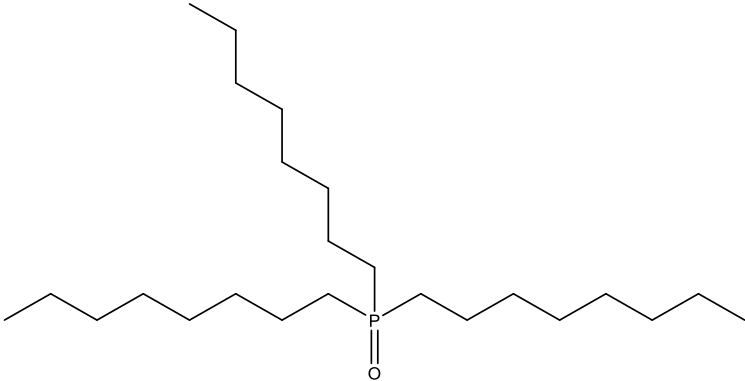
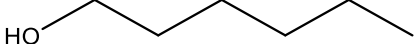
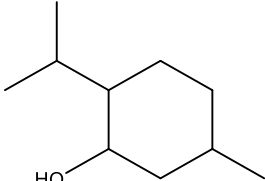
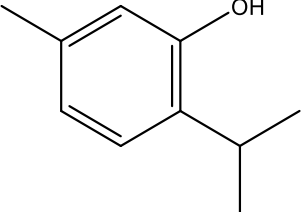
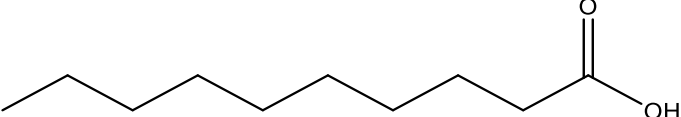
Name	Chemical structure
Phenol	
TOPO	
1-hexanol	
Menthol	
Thymol	
Decanoic acid	

Table S3. COSMO-RS screening results

No	HBA	HBD	Molar ratio	C [∞]	S [∞]	PI [∞]
1	Benzoyltrifluoroacetone	Triphenyl phosphate	2:1	1.98	128.58	254.43
2			2:1	1.99	1.51	3.00
3	Decanoic acid	Lidocaine	3:1	1.65	1.37	2.26
4			4:1	1.48	1.37	2.04
5		Octanoic acid	1:3	1.09	0.89	0.91
6	Dodecanoic acid	Decanoic acid	1:2	0.99	8.13	8.11
7		nonanoic acid	1:3	1.04	7.33	7.61
8	Hydrocinnamic acid	Decanoic acid	1:1	2.55	10.08	25.67
9		Aliquat 336	7:3	6.36	51.72	328.95
10		Lidocaine	5:5	3.95	6.69	26.44
11		ibuprofen	7:3	1.26	20.62	25.97
12		Proton Sponge®	7:3	1.23	46.69	57.39
13		Octanoic acid	1:1	1.29	14.24	18.29
14			1:2	1.23	10.67	13.05
15	Menthol		1:1	1.18	14.77	17.42
16		Decanoic acid	1:2	1.11	11.87	13.13
17			1:3	1.07	10.58	11.35
18		methyl-2,4-pentanediol	2:1	2.13	15.23	32.43
19		1-decanol	2:1	1.83	25.92	47.49
20		Salicylic acid	4:1	1.29	7.56	9.73
21		Propionic acid	1:1	1.40	9.41	13.17
22		Formic acid	1:1	1.19	7.54	9.032
23		Lidocaine	9:1	1.53	7.82	11.95
24	Methyl anthranilate	ibuprofen	9:1	1.27	30.58	38.82
25		Proton Sponge®	9:1	1.24	53.01	65.50
26		DL-menthol	9:1	1.52	40.84	62.07
27	Methyltrioctylammonium	Octanoic acid	1:2	6.73	36.95	248.79
28	bromide	Decanoic acid	1:2	7.89	43.67	344.59
29	Methyltrioctylammonium chloride	Octanoic acid	1:2	2.89	13.16	38.09
30	Tetrabutyl ammonium	Thymol	1:2	5.79	14.48	83.81
31	bromide	octanoic acid	1:2	9.55	32.59	311.41
32	Thenoyltrifluoroacetone	triphenyl phosphate	2:1	1.95	126.09	245.84
33		methyl-2,4-pentanediol	2:1	1.24	3.31	4.0914
34		1-decanol	2:1	1.01	4.54	4.57
35	Thymol	Trioctylphosphine oxide	1:1	6.70	138.02	925.35
36		Decanoic acid	1:3	0.86	4.45	3.84
37		Camphor	1:1	1.68	8.91	14.96
38		Methyl 4-hydroxybenzoate	1:1	3.79	5.35	20.23

39	Trioctylmethylammonium chloride	butyl 4-hydroxybenzoate	1:2	2.38	3.08	7.35
40			2:1	4.82	10.31	49.68
41			1:1	4.29	8.06	34.63
42			1:2	2.63	5.35	14.04
43			1:3	1.87	3.69	6.90
44			2:1	5.31	13.58	72.13
45		isobutyl 4-hydroxybenzoate	1:1	3.87	5.85	22.61
46			1:2	2.35	3.56	8.36
47			1:3	1.67	2.36	3.94
48			2:1	4.89	10.98	53.60
49		2-Ethylhexyl 4-hydroxybenzoate	1:1	4.43	7.86	34.87
50			1:2	2.55	5.40	13.76
51			1:3	1.74	3.69	6.43
52			2:1	5.48	13.12	71.79
53		n-octyl 4-hydroxybenzoate	1:1	4.47	9.81	43.83
54			1:2	2.56	7.14	18.27
55			1:3	1.75	4.96	8.67
56			1:4	1.78	3.34	5.95
57			2:1	5.51	15.39	84.79
58			2:1	5.48	28.20	154.51
59		Decanoic acid	1:1	4.66	20.91	97.39
60			1:2	3.02	17.92	54.11
61			2:1	6.06	26.03	157.74
62		Ketoprofen	1:1	5.35	20.13	107.59
63			1:2	3.69	17.69	65.21
64		Gemfibrozil	1:2	3.08	16.58	51.15
65			1:1	4.89	19.80	96.91
66	Trioctylphosphine oxide	Decanoic acid	1:1	9.69	256.07	2483.2
67		menthol	1:1	14.89	215.75	3211.7
68			1:2	5.66	195.19	1103.8
69			1:3	3.88	135.83	527.64
70			1:4	3.19	99.82	318.86
71			1:5	2.78	80.29	222.77
72		1-hexanol	1:1	18.39	186.14	3422.9
73		3,5-Di-tertbutylcatechol	1:1	5.69	80.45	458.24

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Figure S11. ^1H NMR spectra of TOPO:Thy HDES. The peak around 7.25 is the peak of chloroform.

Figure S12. ^1H NMR spectra of TOPO:DecA HDES. The peak around 7.25 is the peak of chloroform.

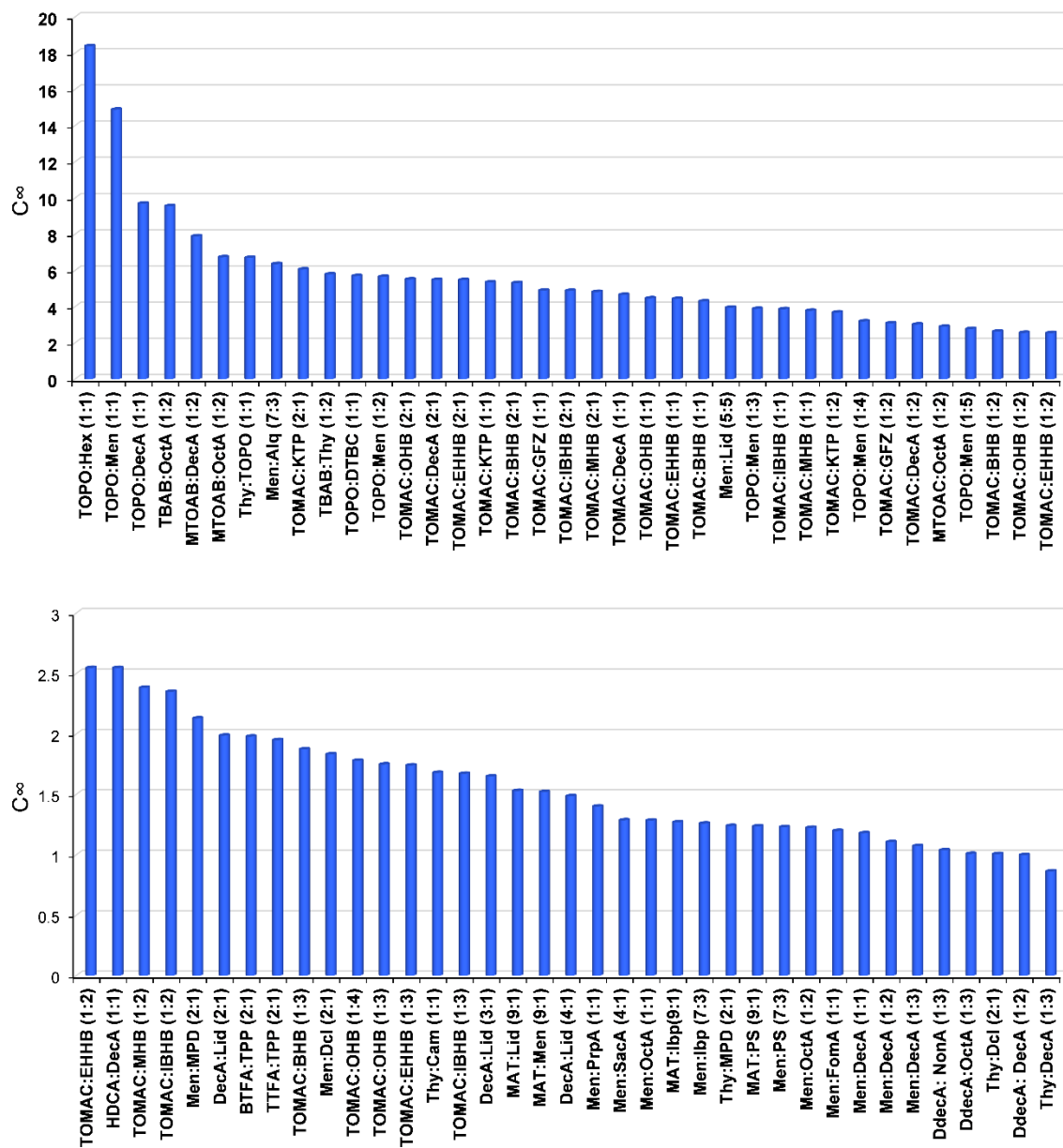


Figure S1. Capacity of HDESs at infinite dilution: A Two-Part Detailed Analysis.

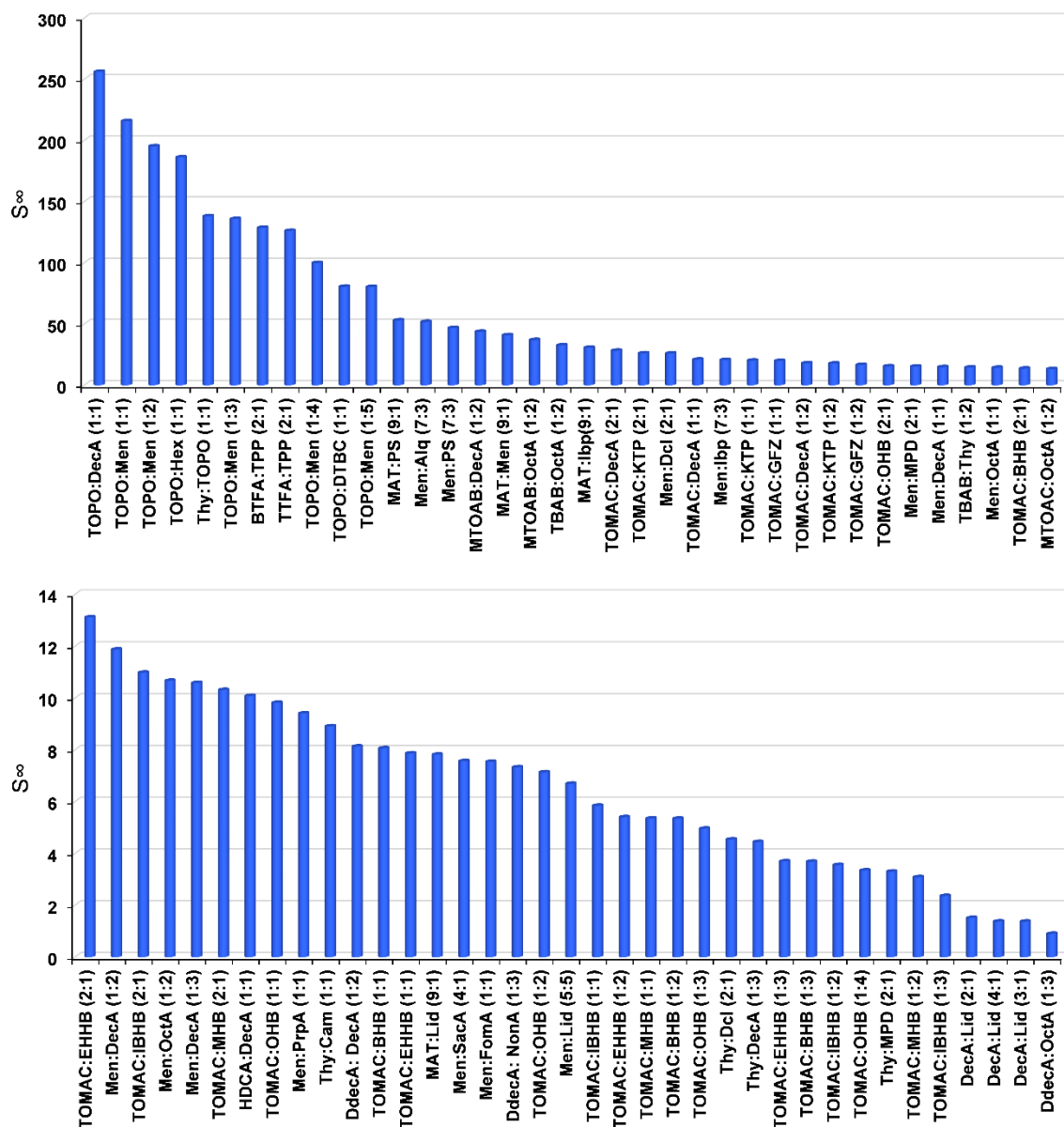


Figure S2. Selectivity of HDESSs at infinite dilution: A Two-Part Detailed Analysis.

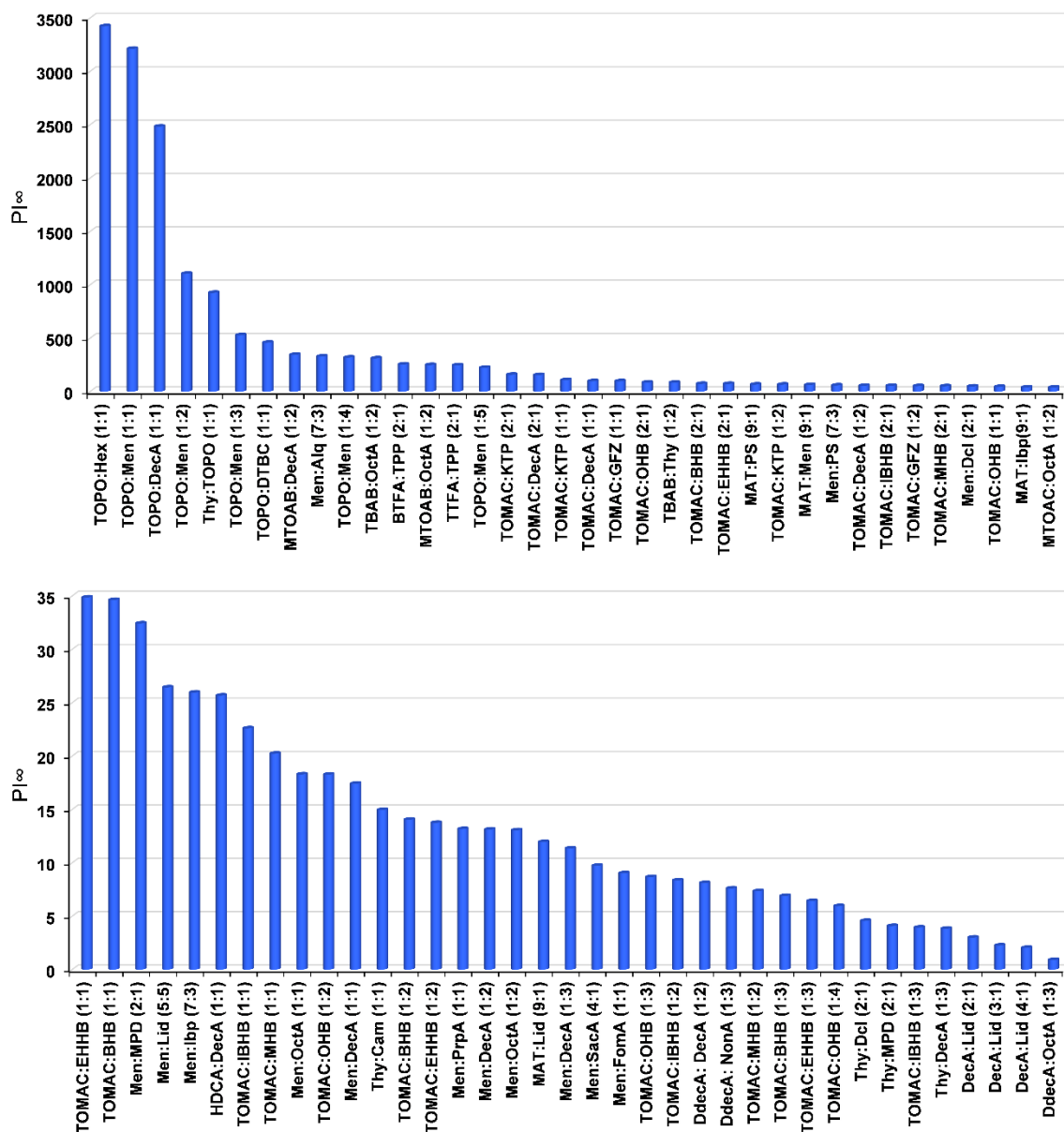


Figure S3. Performance index of HDESs at infinite dilution: A Two-Part Detailed Analysis.

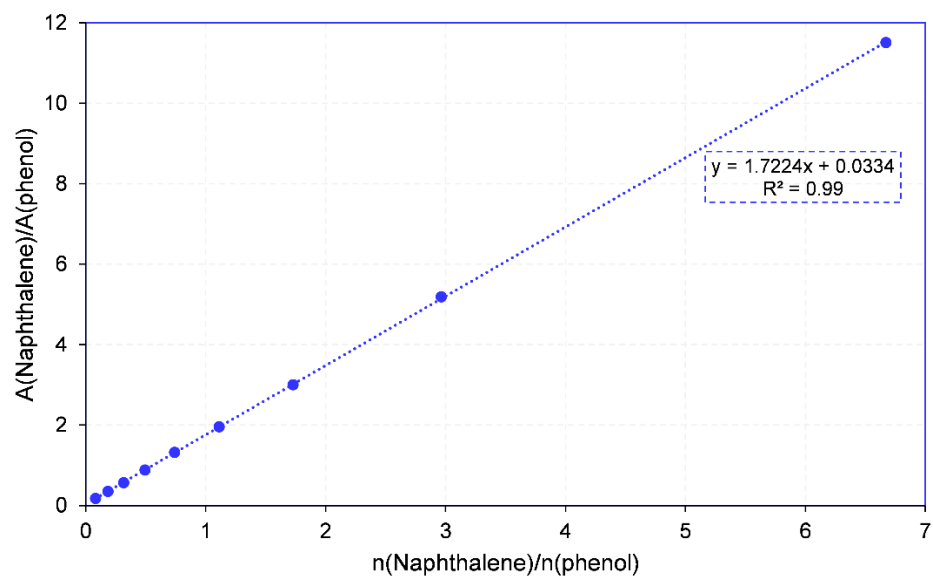


Figure S4. GC calibration curve of naphthalene/phenol.

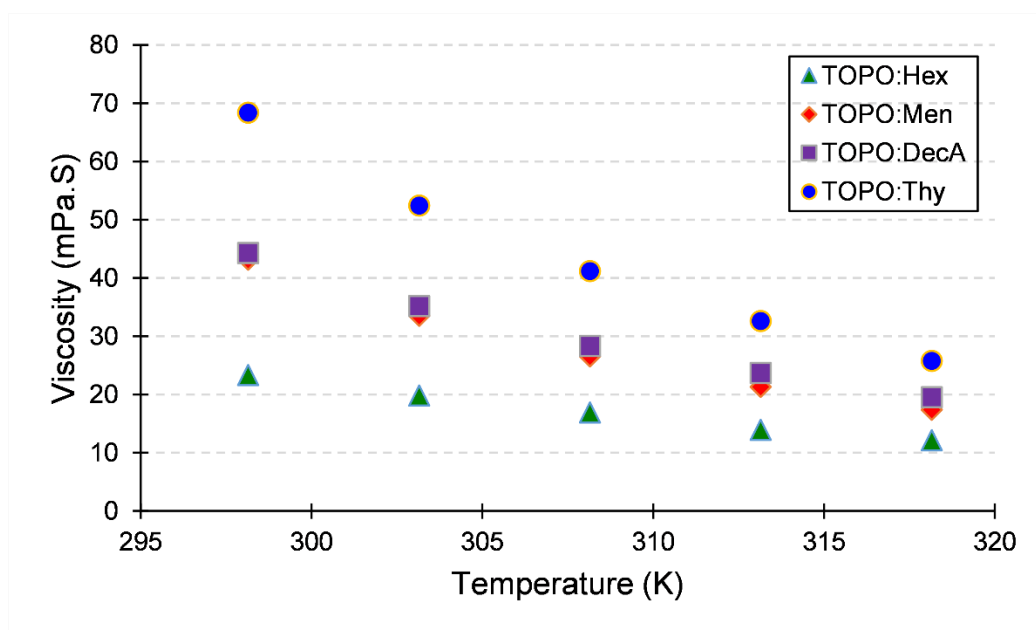


Figure S5. Viscosity of HDESs at different temperatures.

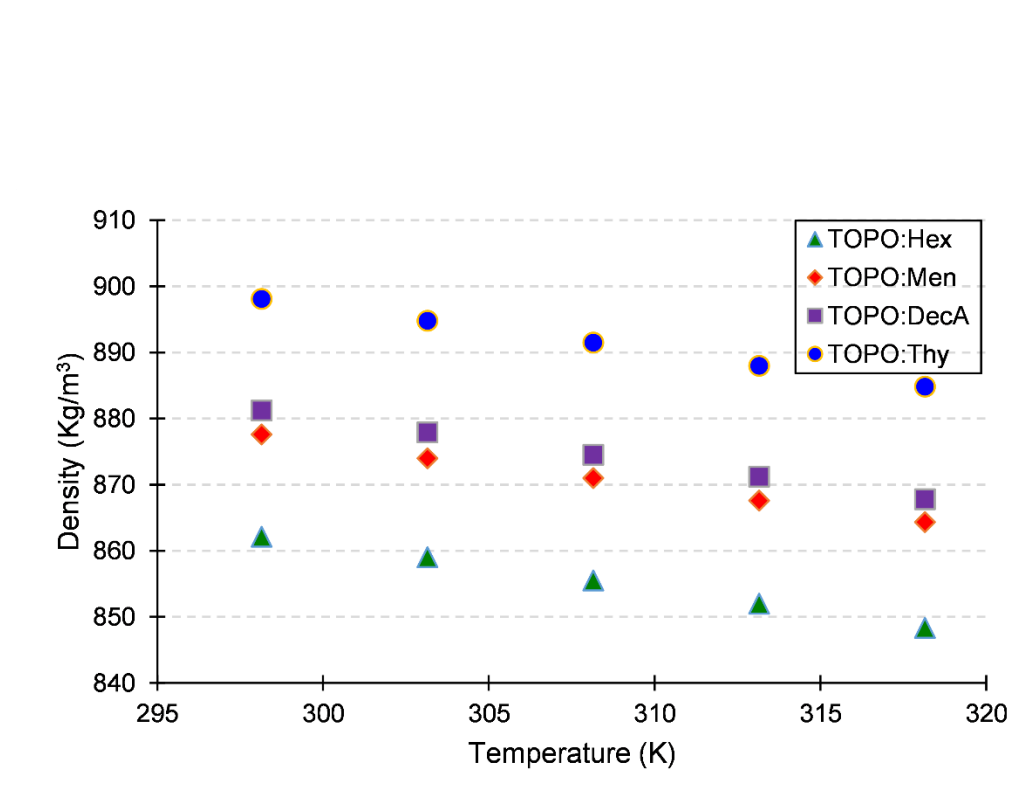


Figure S6. Density of HDESs at different temperatures.

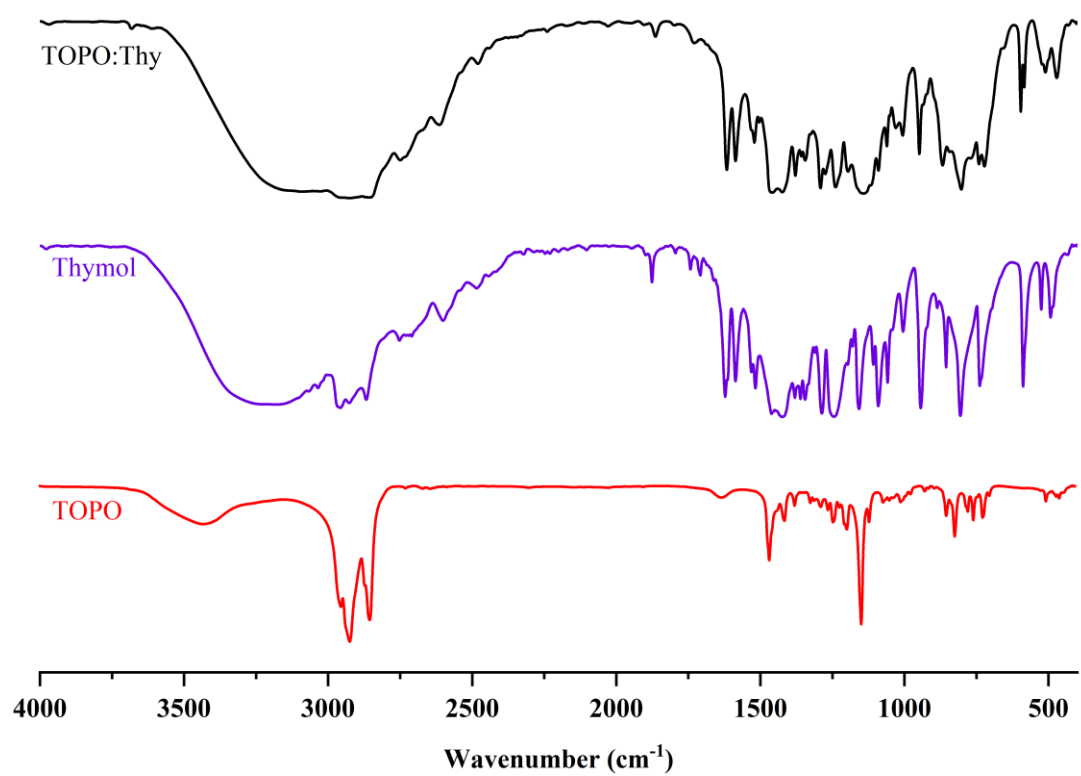


Figure S7. FTIR analysis of TOPO:Thy HDES and its individual components.

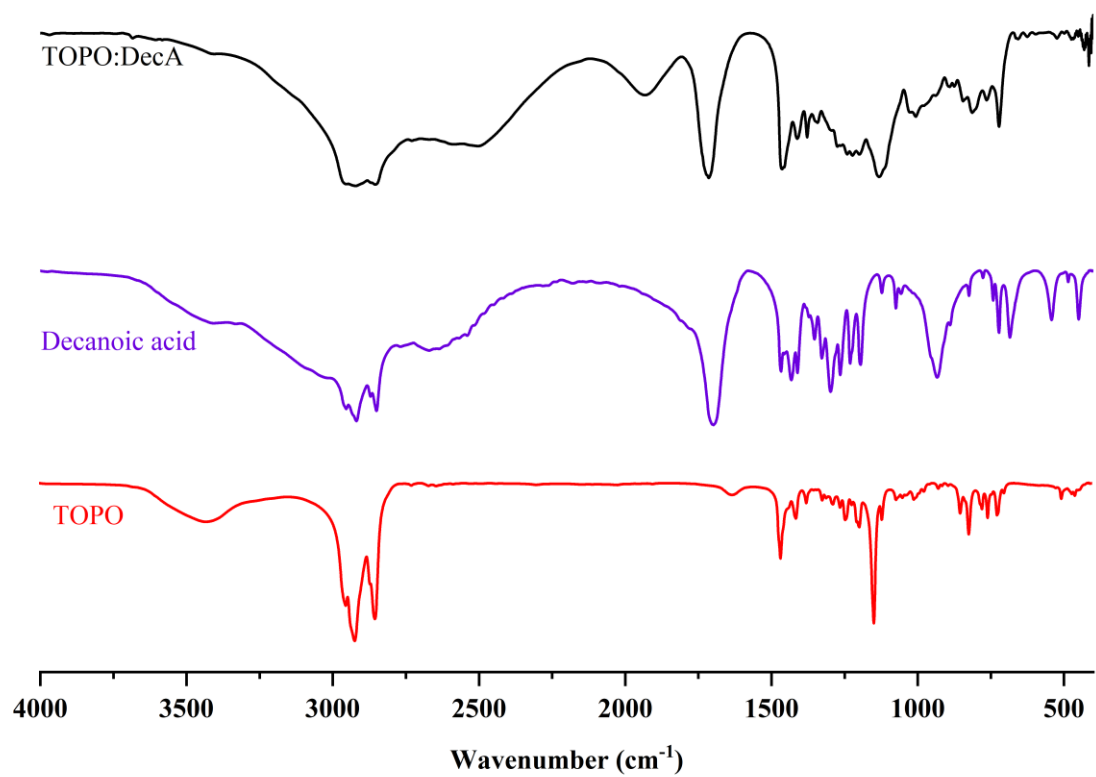


Figure S8. FTIR analysis of TOPO:DecA HDES and its individual components.

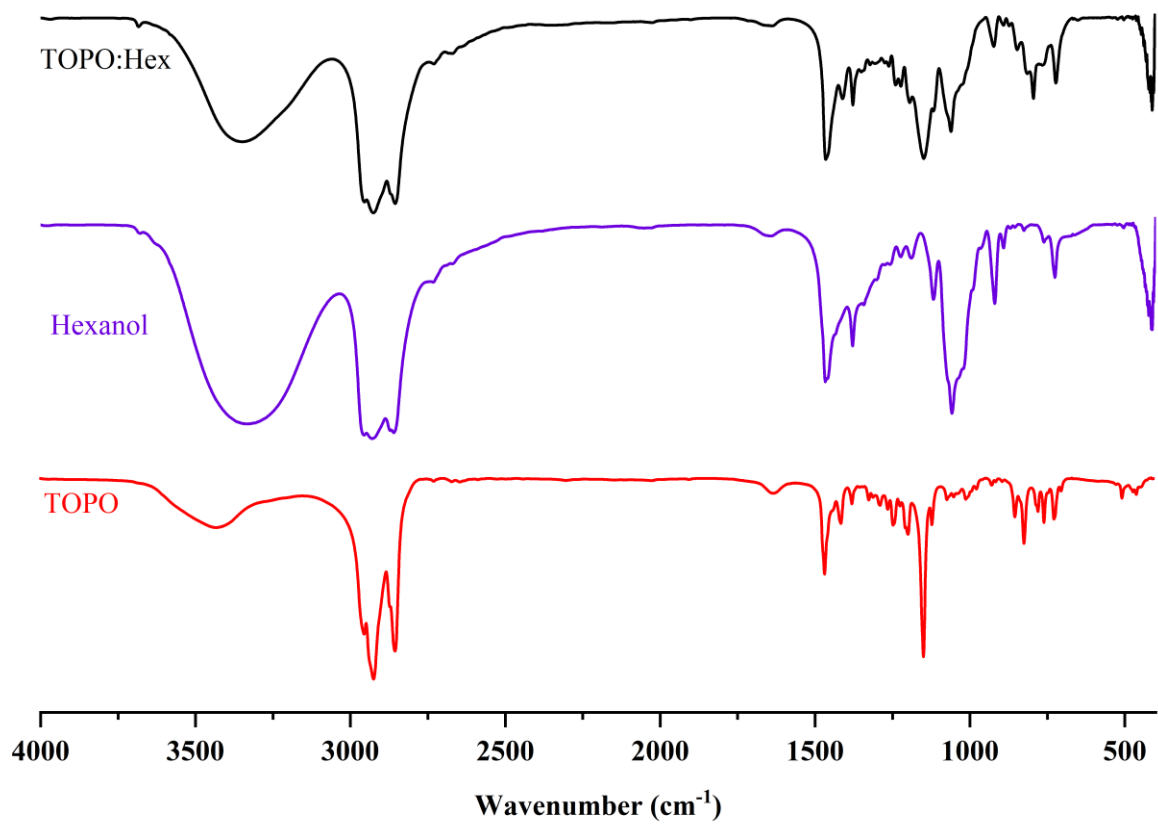


Figure S9. FTIR analysis of TOPO:Hex HDES and its individual components.

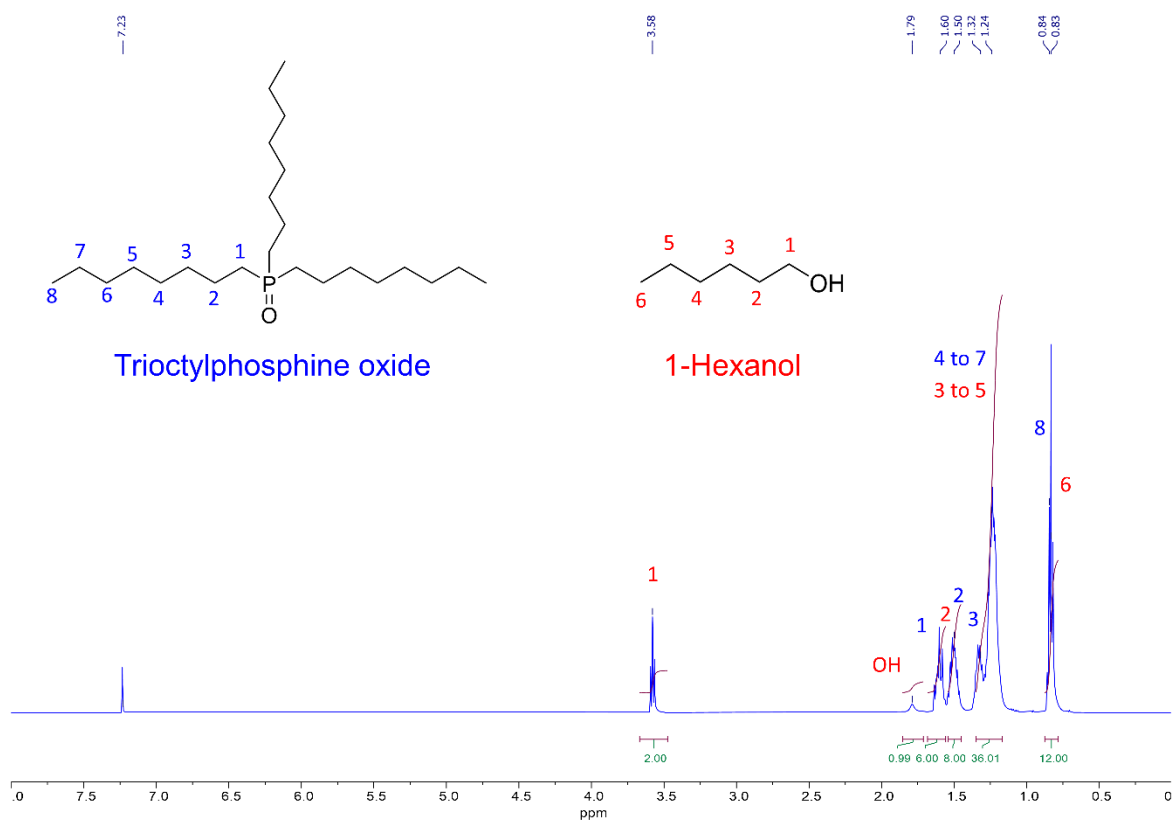


Figure S10. ^1H NMR spectra of TOPO:Hex HDES. The peak around 7.25 is the peak of chloroform.

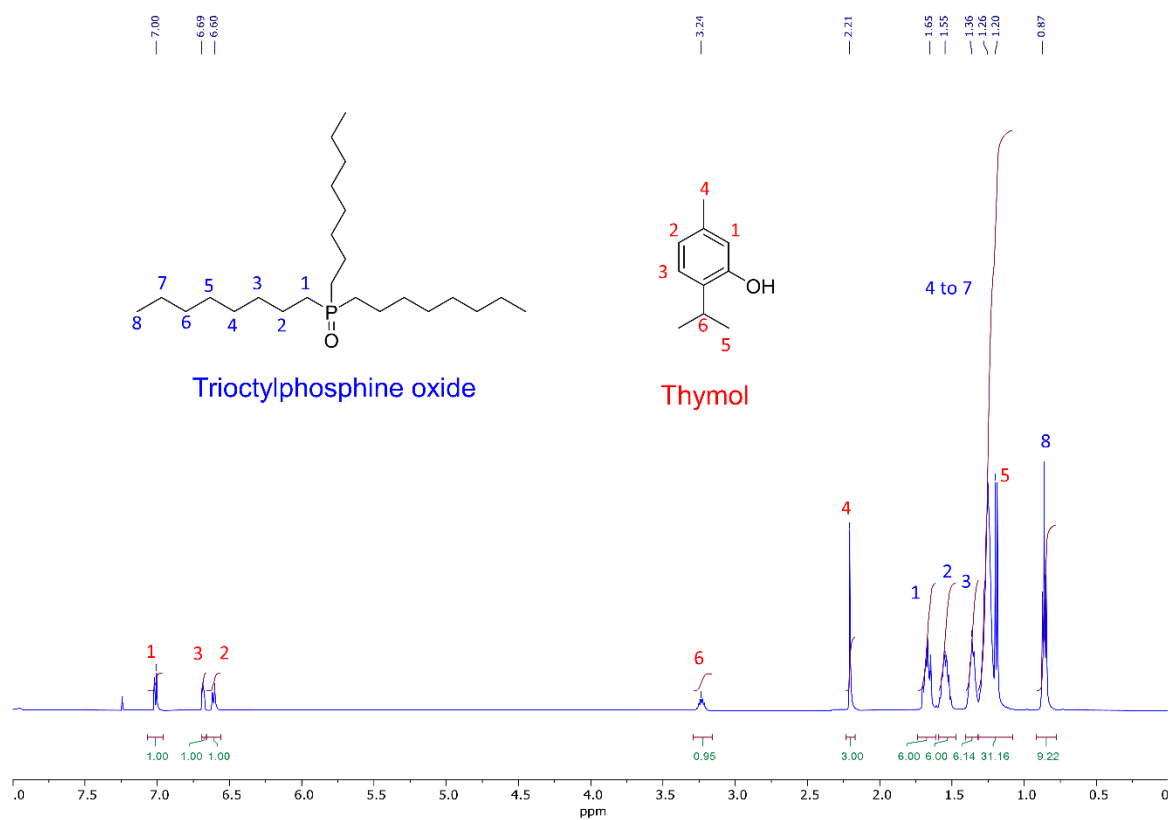


Figure S11. ^1H NMR spectra of TOPO:Thy HDES. The peak around 7.25 is the peak of chloroform.

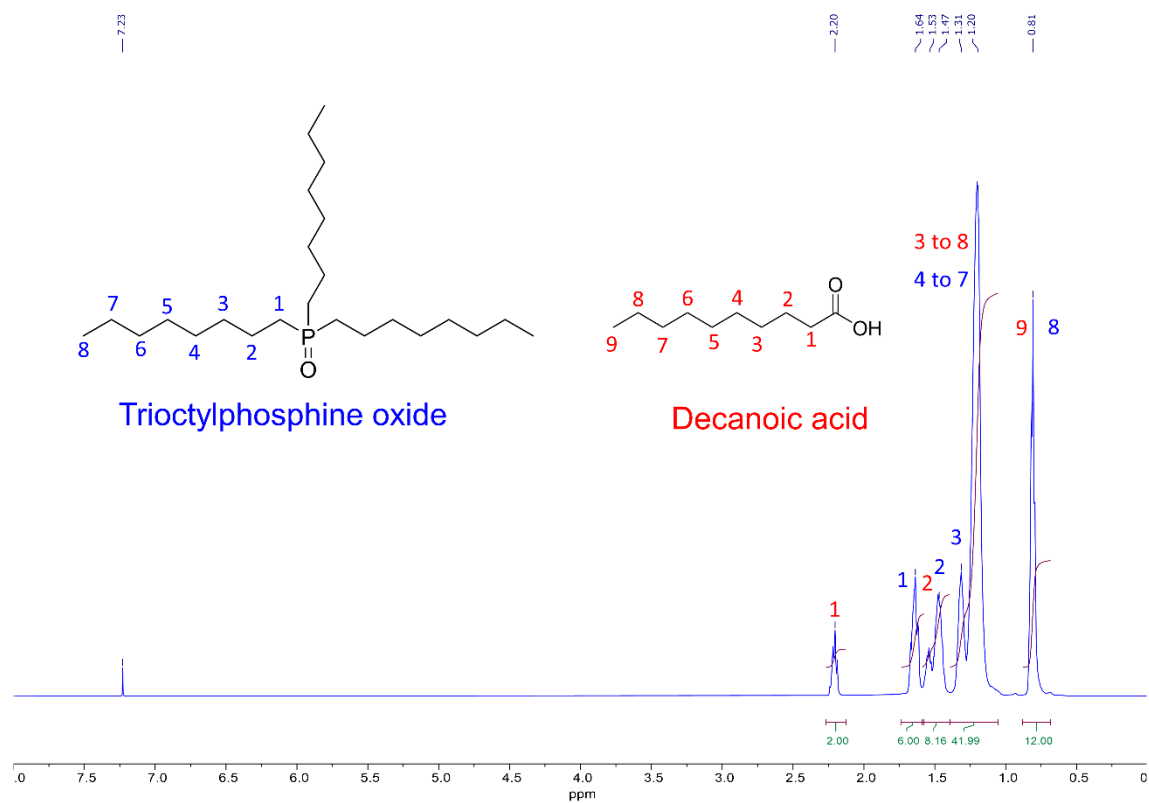


Figure S12. ^1H NMR spectra of TOPO:DecA HDES. The peak around 7.25 is the peak of chloroform.

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