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Supporting Information

A density model for screening hydrogen bond donors to improve the efficiency of hydrophobic deep eutectic solvents†

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Table S1 4 HDES systems for the extraction of metal*.[1–5]

System 1–Pt(IV)				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η (%)
trioctylphosphine oxide	1-Butanol	1:1	0.810	98.0
	1-Hexanol	1:1	0.814	97.2
	1-Octanol	1:1	0.827	89.0
	L-Menthol	1:1	0.890	94.1
	1-Hexanoic acid	1:1	0.927	82.4
System 2–Cr(VI)				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η (%)
Trioctylmethyl ammonium chloride	2-Ethylhexyl 4-hydroxybenzoate	1:1	1.035	98.3
	n-Octyl 4-hydroxybenzoate	1:1	1.037	96.8
	Isobutyl 4-hydroxybenzoate	1:1	1.105	91.3
	Butyl 4-hydroxybenzoate	1:1	1.280	82.4
	Butyl 4-hydroxybenzoate	1:1	1.460	66.0
System 3–Co(II)				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η
Trioctylmethyl ammonium chloride	1-Hexanol	1:1	0.814	10.1
	1-Octanol	1:1	0.827	9.1
	1-Decanol	1:1	0.829	8.2
	1-Dodecanol	1:1	0.833	7.7
	1-Dodecanol	1:1	0.836	7.1
System 4–Ni(II)				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η
Trioctylmethyl ammonium chloride	1-Hexanol	1:1	0.814	0.112
	1-Octanol	1:1	0.827	0.108
	1-Decanol	1:1	0.829	0.099
	1-Dodecanol	1:1	0.833	0.094
	1-Tetradecanol	1:1	0.836	0.088

*All systems are at room temperature.

Table S2 5 HDES systems for the extraction of organic compounds*.[4–7]

System 1–Artemisinin				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η (mg/g)
Trioctylmethyl ammonium chloride	1-Propanol	1:2	0.804	1.48 ± 0.07
	1-Butanol	1:2	0.810	1.63 ± 0.03
	1-Hexanol	1:2	0.814	1.48 ± 0.07
	1-Octanol	1:2	0.827	1.37 ± 0.02
	L-Menthol	1:2	0.890	0.98 ± 0.03
	1-Decanol	1:2	0.829	1.26 ± 0.06
	1-Dodecanol	1:2	0.833	1.26 ± 0.07
	1-Tetradecanol	1:2	0.836	1.16 ± 0.05
	Cyclohexanol	1:2	0.948	1.07 ± 0.05
	1,2-Butanediol	1:2	1.006	1.42 ± 0.06
	1,3-Propylene glycol	1:2	1.053	1.42 ± 0.01
	Ethylene glycol	1:2	1.113	1.36 ± 0.06
	Elycerol	1:2	1.250	1.28 ± 0.02
System 2–Ciprofloxacin				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η (%)
Tetrabutylammonium bromide	1-Butanol	1:1	0.810	56.3 ± 2.4
	1-Octanol	1:1	0.827	64.2 ± 2.1
	1-Dodecanol	1:1	0.833	61.1 ± 2.1
	1-Octanoic acid	1:1	0.907	55.0 ± 1.1
	Oleyl alcohol	1:1	0.849	62.4 ± 1.3
	Hexanoic acid	1:1	0.927	38.0 ± 2.1
	Decanoic acid	1:1	0.893	45.0 ± 3.2
System 3–Ciprofloxacin				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η (%)
Tetrabutylammonium bromide	1-Butanol	1:1	0.810	73.2 ± 2.3
	1-Octanol	1:1	0.827	81.9 ± 1.8
	1-Dodecanol	1:1	0.833	75.3 ± 1.8
	1-Octanoic acid	1:1	0.907	70.3 ± 2.6
	Oleyl alcohol	1:1	0.849	77.1 ± 2.7
	Hexanoic acid	1:1	0.927	55.3 ± 3.1
	Decanoic acid	1:1	0.893	60.3 ± 2.6
System 4–Levofloxacin				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η (%)
Trioctylmethyl ammonium chloride	1-Butanol	1:1	0.810	68.7 ± 1.1
	1-Octanol	1:1	0.827	78.4 ± 2.2

	1-Dodecanol	1:1	0.833	74.2 ± 2.7
	1-Octanoic acid	1:1	0.907	66.2 ± 3.6
	Oleyl alcohol	1:1	0.849	76.1 ± 1.6
	Hexanoic acid	1:1	0.927	55.3 ± 3.1
	Decanoic acid	1:1	0.893	59.0 ± 2.6
System 5–Levofloxacin				
HBA	HBD	Molar ratio	ρ (g/cm^3)	η (%)
Trioctylmethyl ammonium chloride	1-Butanol	1:1	0.810	78.2 ± 1.6
	1-Octanol	1:1	0.827	84.5 ± 0.8
	1-Dodecanol	1:1	0.833	79.0 ± 2.1
	1-Octanoic acid	1:1	0.907	75.5 ± 2.4
	Oleyl alcohol	1:1	0.849	80.0 ± 1.9
	Hexanoic acid	1:1	0.927	59.2 ± 2.9
	Decanoic acid	1:1	0.893	65.3 ± 2.4

*All systems are at room temperature.

Table S3 6 HDES systems for the extraction of organic compounds*.[4,5,8]

System 1–PFOA			System 2–PFOS	
HBDs	ρ (g/cm^3)	η	HBDs	η
1-Hexadecanol	0.838	4.466	1-Hexadecanol	5.624
1-Tetradecanol	0.836	4.518	1-Tetradecanol	5.679
Dodecanol	0.833	4.560	Dodecanol	5.72
1-Undecanol	0.830	4.610	1-Undecanol	5.778
1-Decanol	0.829	4.628	1-Decanol	5.791
1-Nonanol	0.828	4.674	1-Nonanol	5.843
1-Octanol	0.827	4.691	1-Octanol	5.855
Oleyl alcohol	0.849	4.389	Oleyl alcohol	5.499
1-Heptanol	0.822	4.692	1-Heptanol	5.848
Cinnamyl alcohol	1.044	4.198	Cinnamyl alcohol	5.145
Cyclohexanol	0.948	4.360	Cyclohexanol	5.438
2-Phenylethanol	1.020	4.149	2-Phenylethanol	5.088
System 3–PFOA			System 4–PFOS	
HBDs	ρ (g/cm^3)	η	HBDs	η
Ricinoleic acid	0.940	4.240	Ricinoleic acid	5.216
Decanoic acid	0.918	4.012	Decanoic acid	4.793
Dodecanoic acid	0.883	3.993	Dodecanoic acid	4.694
Nonanoic acid	0.906	4.033	Nonanoic acid	4.816
Undecanoic acid	0.890	3.963	Undecanoic acid	4.727
Caprylic acid	0.907	4.059	Caprylic acid	4.848
10-Undecenoic-acid	0.912	3.975	10-Undecenoic-acid	4.728
Tetradecanoic acid	0.862	3.852	Tetradecanoic acid	4.591
Hexadecanoic acid	0.852	3.787	Hexadecanoic acid	4.518
n-Heptanoic acid	0.918	4.041	n-Heptanoic acid	4.827
n-Hexanoic acid	0.927	3.955	n-Hexanoic acid	4.729
Benzoic acid	1.080	3.337	Benzoic acid	3.943
System 5–PFOA			System 6–PFOS	
HBDs	ρ (g/cm^3)	η	HBDs	η
4-Methylphenol	1.034	3.434	4-Methylphenol	3.982
Phenylacetic acid	1.091	3.197	Phenylacetic acid	3.776
4-Ethylphenol	1.011	3.622	4-Ethylphenol	4.199
4-Propylphenol	0.983	3.705	4-Propylphenol	4.292
2-Methylphenol	1.048	3.499	2-Methylphenol	4.037
Methylsalicylate	1.147	3.169	Methylsalicylate	3.837

*All systems are at room temperature.

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