

Supporting Information

Deterpenation of Citrus Essential Oils using Glycerol-based Deep Eutectic Solvents

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Experimental extraction methodology validation of model mixture with aq. ethanol (wt. 70%)

Table S1: Experimental solute distribution coefficient (β) and selectivity (S) for the system {limonene(1) + linalool(2) + aq.ethanol (70 wt. %) (3)} at T=298.15 K and P=101.3 kPa

Terpene rich phase		Ethanol rich phase		Selection Parameter			
w ₁	w ₂	w ₁	w ₂	δ (%)	β_1	β_2	S
0.932	0.022	0.038	0.021	0.050	0.040	0.950	23.310
0.928	0.027	0.040	0.022	0.110	0.040	0.820	19.120
0.923	0.032	0.041	0.024	0.110	0.040	0.770	17.130
0.893	0.061	0.040	0.026	0.090	0.050	0.430	9.410
0.863	0.068	0.055	0.039	0.120	0.060	0.570	8.960
0.810	0.090	0.051	0.043	0.140	0.060	0.480	7.670
0.742	0.121	0.057	0.066	0.140	0.080	0.540	7.050
0.701	0.138	0.061	0.075	0.080	0.090	0.550	6.260

Standard uncertainties u are u(T)=0.05 K, u(P)=0.5 kPa and u(w)=0.005.

COSMO-RS predicted extraction results of model mixture with DES

Table S2: COSMO-RS predicted solute distribution coefficient (β) and selectivity (S) for the system {limonene(1) + linalool(2) + DES 1(3)} at T=298.15 K

Terpene rich phase		DES rich phase		Selection Parameter		
w ₁	w ₂	w ₁	w ₂	β_1	β_2	S
0.947	0.052	0.008	0.005	0.008	0.092	11.060
0.889	0.110	0.008	0.009	0.009	0.078	9.010
0.750	0.247	0.007	0.015	0.009	0.063	6.649
0.570	0.420	0.006	0.023	0.011	0.055	5.126
0.670	0.324	0.007	0.019	0.010	0.058	5.859
0.824	0.174	0.007	0.012	0.009	0.069	7.660
0.537	0.451	0.006	0.024	0.011	0.054	4.928
0.494	0.492	0.005	0.027	0.011	0.055	5.077

Table S3: COSMO-RS predicted solute distribution coefficient (β) and selectivity (S) for the system {limonene(1) + linalool(2) + DES 2(3)} at T=298.15 K

Terpene rich phase		DES rich phase		Selection Parameter		
w_1	w_2	w_1	w_2	β_1	β_2	S
0.947	0.052	0.008	0.005	0.009	0.090	10.228
0.888	0.110	0.008	0.008	0.009	0.077	8.336
0.823	0.174	0.008	0.012	0.010	0.068	7.085
0.749	0.246	0.008	0.015	0.010	0.063	6.138
0.665	0.327	0.007	0.019	0.011	0.058	5.367
0.568	0.418	0.007	0.023	0.012	0.056	4.723
0.536	0.449	0.006	0.025	0.012	0.055	4.536
0.668	0.324	0.007	0.019	0.011	0.059	5.397

Table S4: COSMO-RS predicted solute distribution coefficient (β) and selectivity (S) for the system {limonene(1) + linalool(2) + DES 3(3)} at T=298.15 K

Terpene rich phase		DES rich phase		Selection Parameter		
w_1	w_2	w_1	w_2	β_1	β_2	S
0.937	0.052	0.006	0.004	0.006	0.078	12.333
0.889	0.110	0.008	0.009	0.009	0.084	9.768
0.750	0.246	0.007	0.016	0.009	0.066	7.198
0.667	0.328	0.006	0.020	0.010	0.061	6.312
0.571	0.420	0.006	0.024	0.010	0.057	5.557
0.670	0.324	0.006	0.020	0.010	0.061	6.343
0.824	0.174	0.007	0.013	0.009	0.074	8.322

Table S5: COSMO-RS predicted solute distribution coefficient (β) and selectivity (S) for the system {limonene(1) + linalool(2) + DES 4(3)} at T=298.15 K

Terpene rich phase		DES rich phase		Selection Parameter		
w_1	w_2	w_1	w_2	β_1	β_2	S
0.947	0.052	0.007	0.004	0.007	0.080	10.960
0.889	0.110	0.007	0.008	0.008	0.070	8.940
0.823	0.175	0.007	0.011	0.008	0.060	7.600
0.749	0.247	0.006	0.014	0.008	0.060	6.590
0.665	0.328	0.006	0.017	0.009	0.050	5.780
0.823	0.175	0.007	0.011	0.008	0.060	7.590

Characterisation of crude orange essential oil (COEO) on GC-MS

In the following figure, the characterisation of used real crude orange essential oil is shown by the GC-MS spectrum, where the peaks were identified by NIST library and retention time confirmation of limonene and linalool standards

Figure S1: The GC-MS spectrum of crude orange essential oil (COEO)

