Supporting Information

USING COSMO-RS TO PREDICT SOLVATOCHROMIC PARAMETERS FOR DEEP EUTECTIC SOLVENTS

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Table S1. COSMO-RS parameters obtained at 298.2 K for 175 conventional solvents and their solvatochromic parameters from Marcus database.

Solvent	COSMO-RS parameters				Solvatochromic parameters[1]		
	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}	α	β	π^*
Formic acid	1.145	-2.722	1.228	4.630	1.230	0.380	0.650
Acetic acid	1.518	-3.863	2.094	3.785	1.120	0.450	0.640
Propanoic acid	2.005	-4.843	2.628	4.492	1.120	0.450	0.580
Butanoic acid	2.250	-5.886	2.588	4.437	1.100	0.450	0.560
Pentanoic acid	2.396	-6.805	2.647	4.444	1.190	0.450	0.540
Hexanoic acid	2.570	-7.944	2.616	4.409	1.220	0.450	0.520
Heptanoic acid	2.626	-8.649	2.605	4.428	1.200	0.450	0.500
Methanol	1.163	-3.108	4.154	1.905	0.980	0.660	0.600
Ethanol	1.187	-4.176	4.090	1.782	0.860	0.750	0.540
n-Propanol	1.471	-5.109	3.704	1.289	0.840	0.900	0.520
i-Propanol	1.331	-5.139	4.038	1.372	0.760	0.840	0.480
Benzyl alcohol	2.146	-7.281	2.957	1.666	0.600	0.520	0.980
2-Phenylethanol	2.378	-8.224	3.258	1.799	0.640	0.610	0.880
3-Phenylpropanol	2.536	-9.055	3.617	1.633	0.530	0.550	0.950
Allyl alcohol	1.899	-4.390	7.915	3.653	0.840	0.900	0.520
Ethanediol	1.899	-4.390	7.915	3.653	0.900	0.520	0.920
Glycerol	1.479	-5.427	6.549	5.112	1.210	0.510	0.620
Phenol	2.103	-6.291	0.668	3.566	1.650	0.300	0.720
m-Cresol	2.197	-7.234	0.735	3.476	1.130	0.340	0.680
p-Cresol	2.177	-7.238	0.803	3.440	1.640	0.340	0.680
m-Chlorophenol	2.482	-7.769	0.389	4.203	1.570	0.230	0.770
n-Butanol	1.173	-6.220	3.515	1.725	0.840	0.840	0.470
i-Butanol	1.111	-6.097	3.364	1.767	0.790	0.840	0.400
s-Butanol	1.209	-6.127	3.414	1.386	0.690	0.800	0.400
t-Butanol	1.438	-5.978	3.965	1.131	0.420	0.930	0.410
n-Pentanol	1.235	-7.248	3.452	1.715	0.840	0.860	0.400
i-Pentanol	1.512	-7.001	3.716	1.503	0.840	0.860	0.400

Solvent	COSMO-RS parameters				Solvatochromic parameters[1]		
	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}	α	β	π^*
t-Pentanol	1.558	-6.822	3.852	0.928	0.280	0.930	0.400
n-Hexanol	1.643	-8.184	3.660	1.285	0.800	0.840	0.400
Cyclohexanol	1.378	-6.984	3.947	1.338	0.660	0.840	0.450
n-Octanol	1.370	-5.182	3.813	1.536	0.770	0.810	0.400
n-Decanol	1.478	-12.409	3.474	1.713	0.700	0.820	0.450
2-Methylbutane	0.126	-6.814	0.000	0.000	0.000	0.010	-0.080
n-Pentane	0.117	-7.015	0.000	0.000	0.000	0.000	-0.080
n-Hexane	0.135	-8.050	0.000	0.000	0.000	0.000	-0.040
n-Heptane	0.151	-9.085	0.000	0.000	0.000	0.000	-0.080
n-Octane	0.169	-10.116	0.000	0.000	0.000	0.000	0.010
n-Decane	0.198	-12.178	0.000	0.000	0.000	0.000	0.030
n-Dodecane	0.232	-14.222	0.000	0.000	0.000	0.000	0.050
Cyclohexane	0.042	-6.754	0.000	0.000	0.000	0.000	0.000
cis-Decalin	0.070	-9.470	0.000	0.000	0.000	0.080	0.110
Formamide	1.326	-3.414	5.748	3.576	0.710	0.480	0.970
N-Methyl formamide	2.235	-4.515	5.983	2.035	0.620	0.800	0.900
N,N-Dimethyl formamide	3.061	-5.537	2.746	0.000	0.000	0.690	0.880
N-Methyl acetamide	2.822	-5.505	7.274	1.536	0.470	0.800	1.010
N,N-Dimethyl acetamide	4.066	-6.344	7.435	0.000	0.000	0.760	0.880
N,N-Diethyl acetamide	3.808	-8.041	6.563	0.000	0.000	0.780	0.840
2-Pyrrolidinone	3.278	-5.616	7.116	1.494	0.360	0.770	0.850
N-Methyl pyrrolidinone	4.218	-6.674	6.886	0.000	0.000	0.770	0.920
Tetramethyl urea	4.047	-7.885	7.240	0.000	0.000	0.800	0.830
Tetramethyl guanidine	3.614	-7.986	7.376	0.001	0.000	0.860	0.760
Dimethyl cyanamide	3.787	-5.455	3.944	0.000	0.000	0.640	0.720
Butylamine	2.216	-6.323	5.450	0.037	0.000	0.720	0.310
Diaminoethane	2.636	-4.682	9.382	0.122	0.130	1.430	0.470
Pyrrolidine	2.090	-5.660	4.938	0.040	0.160	0.700	0.390
Piperidine	1.518	-6.410	4.190	0.036	0.000	1.040	0.300
Morpholine	2.611	-5.864	6.066	0.104	0.290	0.700	0.390

Solvent	COSMO-RS parameters				Solvatochromic parameters[1]		
	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}	α	β	π^*
Diethylamine	1.634	-6.631	3.984	0.009	0.030	0.700	0.240
Triethylamine	0.877	-8.232	3.076	0.000	0.000	0.710	0.140
Tributylamine	0.384	-14.151	0.000	0.000	0.000	0.620	0.160
Dimethylcyclohexylamine	1.417	-9.058	3.060	0.000	0.000	0.840	0.230
Dimethylbenzylamine	2.047	-9.436	1.919	0.000	0.000	0.640	0.450
Aniline	2.300	-6.506	0.032	1.579	0.260	0.500	0.730
N-Methylaniline	2.328	-7.601	0.000	0.822	0.170	0.470	0.820
N,N-Dimethylaniline	2.234	-8.470	0.009	0.000	0.000	0.430	0.730
o-Chloroaniline	2.344	-7.895	0.641	1.357	0.250	0.400	0.830
Acetic anhydride	2.874	-6.085	1.192	0.000	0.000	0.290	0.760
Benzene	1.505	-6.142	0.000	0.000	0.000	0.100	0.590
Toluene	1.566	-7.089	0.000	0.000	0.000	0.110	0.540
m-Xylene	1.597	-8.040	0.000	0.000	0.000	0.120	0.470
p-Xylene	1.588	-8.049	0.000	0.000	0.000	0.120	0.430
Mesitylene	1.595	-9.021	0.000	0.000	0.000	0.130	0.410
Dimethyl carbonate	2.544	-5.555	1.458	0.000	0.000	0.320	0.550
Diethyl carbonate	2.790	-7.602	1.359	0.000	0.000	0.400	0.450
Propylene carbonate	2.669	-5.630	1.748	0.000	0.000	0.400	0.830
Ethylene carbonate	1.962	-4.638	1.618	0.000	0.000	0.320	0.990
Ethyl benzoate	2.641	-9.333	1.529	0.000	0.000	0.410	0.740
Dimethyl phthalate	3.656	-10.202	2.052	0.000	0.000	0.780	0.820
Methyl formate	1.948	-4.159	1.397	0.000	0.000	0.370	0.620
Ethyl formate	2.266	-5.195	1.573	0.000	0.000	0.360	0.610
Methyl acetate	2.481	-5.184	2.029	0.000	0.000	0.420	0.600
Ethyl acetate	2.715	-6.267	2.294	0.000	0.000	0.450	0.550
Butyl acetate	2.844	-8.197	2.208	0.000	0.000	0.450	0.460
4-Butyrolactone	3.233	-5.297	2.651	0.000	0.000	0.490	0.870
Ethyl chloroacetate	2.365	-7.708	0.903	0.008	0.000	0.350	0.700
Ethyl trichloroacetate	2.059	-10.231	0.185	0.000	0.000	0.250	0.610
Diethyl ether	1.717	-6.450	2.565	0.000	0.000	0.470	0.270

Solvent	COSMO-RS parameters				Solvatochromic parameters[1]		
	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}	α	β	π^*
Di-n-propyl ether	1.847	-8.390	2.685	0.000	0.000	0.460	0.270
Di-i-propyl ether	1.917	-7.963	3.186	0.000	0.000	0.490	0.270
Di-n-butyl ether	1.776	-10.548	2.602	0.000	0.000	0.460	0.270
Di-(2-chloroethyl) ether	2.266	-7.891	1.835	0.000	0.000	0.400	0.820
Dimethoxyethane	3.482	-6.657	5.170	0.000	0.000	0.410	0.530
bis-(2-Methoxyethyl) ether	4.083	-9.154	5.949	0.000	0.000	0.400	0.640
Dibenzyl ether	2.956	-12.124	1.441	0.000	0.000	0.410	0.800
Diphenyl ether	2.422	-10.574	0.067	0.000	0.000	0.130	0.660
Tetrahydrofuran	2.227	-5.471	3.449	0.000	0.000	0.550	0.580
2-Methyltetrahydrofuran	2.133	-6.479	3.421	0.000	0.000	0.580	0.530
Tetrahydropyran	2.227	-5.471	3.449	0.000	0.000	0.540	0.510
Eucalyptol	1.826	-9.664	3.374	0.000	0.000	0.610	0.360
1,3-Dioxane	2.441	-5.712	3.236	0.000	0.000	0.370	0.550
1,3-Dioxolane	2.392	-4.850	3.029	0.000	0.000	0.450	0.690
Anisole	2.037	-7.423	0.414	0.000	0.000	0.320	0.730
Phenetole	2.127	-8.323	0.465	0.000	0.000	0.300	0.690
2-Chloroethanol	1.630	-5.546	2.621	1.259	1.280	0.530	0.460
Trifluoroethanol	1.807	-4.025	1.308	3.080	1.510	0.000	0.730
Hexafluoroisopropanol	2.284	-5.137	0.183	4.560	1.960	0.000	0.650
1-Chlorobutane	1.431	-7.355	0.000	0.000	0.000	0.000	0.390
Dichloromethane	1.721	-6.029	0.000	0.197	0.130	0.100	0.820
1,1-Dichloroethane	1.559	-6.855	0.000	0.073	0.100	0.100	0.480
1,2-Dichloroethane	2.049	-8.630	0.000	0.001	0.000	0.100	0.810
Chloroform	1.552	-7.509	0.000	1.270	0.200	0.100	0.580
1,1,1-Trichloroethane	1.206	-8.152	0.000	0.000	0.000	0.000	0.490
Carbon tetrachloride	0.408	-8.780	0.000	0.000	0.000	0.100	0.280
1,1,2,2-Tetrachloroethane	2.330	-9.518	0.000	1.671	0.000	0.000	0.950
1-Bromobutane	1.493	-7.898	0.000	0.000	0.000	0.130	0.500
Dibromomethane	1.700	-8.134	0.000	0.222	0.000	0.000	0.920
1,2-Dibromoethane	1.726	-6.970	0.000	0.000	0.000	0.000	0.750

Solvent	COSMO-RS parameters				Solvatochromic parameters[1]		
	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}	α	β	π^*
Bromoform	1.521	-10.674	0.000	1.097	0.050	0.050	0.620
Iodobutane	1.486	-9.284	0.000	0.000	0.000	0.230	0.470
Diiodomethane	1.648	-10.518	0.000	0.147	0.000	0.000	0.650
trans-Dichloroethylene	1.370	-6.782	0.000	0.144	0.000	0.000	0.440
Trichloroethylene	0.995	-8.148	0.000	0.197	0.000	0.050	0.530
Tetrachloroethylene	0.427	-9.452	0.000	0.000	0.000	0.050	0.280
Fluorobenzene	1.554	-5.959	0.000	0.000	0.000	0.070	0.620
p-Difluorobenzene	1.673	-9.094	0.000	0.000	0.000	0.030	0.580
Hexafluorobenzene	1.256	-5.907	0.000	0.000	0.000	0.020	0.330
Chlorobenzene	1.563	-7.627	0.000	0.000	0.000	0.070	0.710
o-Dichlorobenzene	1.556	-8.908	0.000	0.000	0.000	0.030	0.800
m-Dichlorobenzene	1.550	-9.107	0.000	0.002	0.000	0.030	0.750
Bromobenzene	1.642	-8.765	0.000	0.000	0.000	0.060	0.790
Iodobenzene	1.659	-9.884	0.000	0.000	0.000	0.060	0.810
Acetone	2.673	-4.817	2.768	0.000	0.080	0.430	0.710
2-Butanone	2.792	-5.740	2.726	0.000	0.060	0.480	0.670
2-Pentanone	2.883	-6.580	2.785	0.000	0.050	0.500	0.650
3-Pentanone	2.789	-6.698	2.767	0.000	0.000	0.450	0.720
Methyl i-butyl ketone	2.642	-11.824	2.298	0.000	0.020	0.480	0.650
2-Heptanone	3.036	-8.820	2.793	0.000	0.050	0.480	0.610
Cyclopentanone	2.926	-5.915	2.641	0.000	0.000	0.520	0.760
Cyclohexanone	3.043	-6.691	3.042	0.000	0.000	0.530	0.760
Acetophenone	2.705	-7.877	2.041	0.000	0.040	0.490	0.900
Acetonitrile	1.975	-3.797	1.344	0.000	0.190	0.400	0.750
Propanenitrile	2.459	-4.750	1.305	0.000	0.000	0.390	0.710
Butanenitrile	2.599	-5.619	1.302	0.000	0.000	0.400	0.710
Chloroacetonitrile	1.970	-5.396	0.385	1.036	0.000	0.340	1.010
Benzyl cyanide	2.958	-7.916	1.040	0.011	0.000	0.410	1.000
Benzonitrile	2.536	-7.088	0.855	0.000	0.000	0.370	0.900
Nitromethane	1.119	-3.509	0.216	0.039	0.220	0.060	0.850

Solvent	COSMO-RS parameters				Solvatochromic parameters[1]		
	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}	α	β	π^*
Nitrobenzene	2.092	-6.796	0.244	0.000	0.000	0.300	1.010
Perfluoro-n-hexane	-0.021	-8.192	0.000	0.000	0.000	-0.080	-0.410
Perfluoromethylcyclohexane	0.036	-7.844	0.000	0.000	0.000	-0.060	-0.400
Perfluorodecalin	-0.030	-9.482	0.000	0.000	0.000	-0.050	-0.320
Pyridine	2.246	-5.753	3.363	0.000	0.000	0.640	0.870
4-Methylpyridine	2.547	-6.619	3.680	0.000	0.000	0.670	0.840
2-Fluoropyridine	2.027	-5.553	1.738	0.000	0.000	0.510	0.840
Perfluoropyridine	1.640	-5.641	0.078	0.000	0.000	0.160	0.530
3,4-Lutidine	2.766	-7.442	3.860	0.000	0.000	0.780	0.730
2,6-Lutidine	2.146	-7.679	3.393	0.000	0.000	0.760	0.800
2-Cyanopyridine	2.543	-6.825	1.880	0.007	0.000	0.290	1.200
Quinoline	2.538	-8.167	2.972	0.000	0.000	0.640	0.920
Tetramethylsilane	0.445	-7.680	0.000	0.000	0.000	0.020	0.000
Dimethyl sulphide	1.653	-5.973	0.546	0.000	0.000	0.340	0.570
Diethyl sulphide	1.799	-7.814	0.668	0.000	0.000	0.370	0.460
Diisopropyl sulphide	1.782	-9.183	0.648	0.000	0.000	0.380	0.360
Dibutyl sulphide	1.887	-11.576	0.592	0.000	0.000	0.380	0.360
Carbon disulphide	0.131	-7.431	0.000	0.000	0.000	0.070	0.610
Dimethyl sulphoxide	4.165	-5.713	9.638	0.003	0.000	0.760	1.000
Sulpholane	3.899	-6.407	4.071	0.000	0.000	0.390	0.980
Tetrahydrothiophene	1.797	-7.000	0.680	0.000	0.000	0.440	0.620
Thiane	1.763	-7.685	0.624	0.000	0.000	0.360	0.610
Dimethyl sulphate	1.939	-5.933	0.058	0.000	0.000	0.360	0.780
Water	0.290	-0.941	5.695	3.856	1.170	0.470	1.090
Trimethyl phosphate	3.654	-7.493	4.558	0.000	0.000	0.770	0.720
Triethyl phosphate	4.006	-10.421	4.324	0.000	0.000	0.770	0.720
Tributyl phosphate	5.451	-16.125	5.924	0.000	0.000	0.800	0.650
Hexamethyl phosphoramide	4.853	-10.380	9.074	0.000	0.000	1.050	0.870

Table S2. Solvatochromic parameters for different deep eutectic solvents (DES).

DES	HBA*	HBD	Molar ratio	α	β	π^*	Reference
1	$[N_{2222}]Cl$	Butanoic acid	1:2	0.990	0.760	0.920	
2	$[N_{2222}]Cl$	Hexanoic acid	1:2	0.970	0.850	0.860	
3	$[N_{2222}]Cl$	Octanoic acid	1:2	0.960	0.870	0.810	
4	$[N_{3333}]Cl$	Butanoic acid	1:2	0.940	0.840	0.930	
5	$[N_{3333}]Cl$	Hexanoic acid	1:2	0.910	0.920	0.850	
6	$[N_{3333}]Cl$	Octanoic acid	1:2	0.900	0.960	0.800	
7	$[N_{4444}]Cl$	Butanoic acid	1:2	0.920	0.990	0.860	
8	$[N_{4444}]Cl$	Hexanoic acid	1:2	0.900	1.020	0.810	
9	$[N_{4444}]Cl$	Octanoic acid	1:2	0.840	1.190	0.800	
10	$[N_{4444}]Cl$	Decanoic acid	1:2	0.850	1.280	0.690	2
11	$[N_{4444}]Cl$	Decanoic acid	1:1	0.910	1.210	0.860	
12	$[N_{3333}]Br$	Butanoic acid	1:2	1.070	0.800	0.930	
13	$[N_{3333}]Br$	Hexanoic acid	1:2	1.020	0.860	0.870	
14	$[N_{4444}]Br$	Butanoic acid	1:2	1.020	0.810	0.930	
15	$[N_{4444}]Br$	Butanoic acid	1:1	1.090	0.840	0.900	
16	$[N_{4444}]Br$	Butanoic acid	2:1	0.940	0.820	0.950	
17	$[N_{4444}]Br$	Hexanoic acid	1:2	1.020	0.930	0.920	
18	$[N_{4444}]Br$	Octanoic acid	1:2	0.980	1.090	0.840	
19	$[N_{4444}]Br$	Decanoic acid	1:2	0.950	1.050	0.710	
20	[Ch]Cl	urea:glycerol	1:1:1	0.893	0.583	1.170	
21	[Ch]Cl	urea: ethylene glycol	1:1:1	0.862	0.000	1.165	
22	[Ch]Cl	urea:formamide	1:1:1	0.846	0.593	1.159	
23	[Ch]Cl	urea:thiourea	1:1:1	0.840	0.486	1.245	3
24	[Ch]Cl	glycerol:ethylene glycol	1:1:1	0.897	0.625	1.127	
25	[Ch]Cl	glycerol:formamide	1:1:1	0.891	0.598	1.131	
26	[Ch]Cl	glycerol:thiourea	1:1:1	0.889	0.539	1.217	

DES	HBA*	HBD	Molar ratio	α	β	π^*	Reference
27	[Ch]Cl	ethylene glycol:formamide	1:1:1	0.872	0.000	1.113	4–6
28	[Ch]Cl	ethylene glycol:thiourea	1:1:1	0.864	0.601	1.207	
29	[Ch]Cl	formamide:thiourea	1:1:1	0.843	0.549	1.209	
30	[Ch]Cl	Urea	1:2	1.420	0.500	1.140	
31	[Ch]Cl	malonic acid	1:2	1.390	0.420	1.080	
32	[Ch]Cl	Ethylene glycol	1:2	1.470	0.570	1.070	
33	[Ch]Cl	Glycerol	1:2	1.490	0.520	1.110	
34	[Ch]Cl	Latic acid	1:1	1.305	1.025	1.003	
35	[Ch]Cl	D-sorbitol	1:2	2.216	0.493	1.244	
36	[Ch]Cl	Citric acid	1:1	2.248	0.714	1.373	
37	[Ch]Cl	Zinc chloride	1:2	1.543	1.253	1.406	
38	Betaine	Glycerol	1:2	2.236	0.587	1.253	7
39	Betaine	Citric acid	1:1	2.216	0.012	1.671	
40	Betaine	Urea	1:2	2.133	1.035	1.288	
41	Menthol	acetic acid	1:1	1.640	0.600	0.530	6
42	Menthol	levulinic acid	1:1	1.560	0.580	0.660	
43	Menthol	Octanoic acid	1:1	1.770	0.500	0.410	
44	Menthol	dodecanoic acid	1:2	1.790	0.570	0.370	

*$[N_{2222}]$Cl: Tetraethylammonium Chloride; $[N_{3333}]$Cl: Tetrapropylammonium Chloride; $[N_{4444}]$Cl: Tetrabuthylammonium Chloride; $[N_{3333}]$Br: Tetrapropylammonium Bromide; $[N_{4444}]$Br: Tetrabuthylammonium Bromide; [Ch]Cl: choline chloride.

Table S3. COSMO-RS parameters obtained at 298.2 K for 44 deep eutectic solvents (DES).

DES (HBA:HBD)	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}
1	7.221	-10.890	24.438	0.000
	2.832	-6.193	2.588	4.437
2	6.877	-10.929	24.438	0.000
	3.236	-8.217	2.616	4.409
3	6.667	-10.959	24.438	0.000
	3.585	-10.278	2.618	4.431
4	8.004	-14.551	24.867	0.001
	2.784	-6.209	2.588	4.437
5	7.656	-14.596	24.867	0.001
	3.174	-8.234	2.616	4.409
6	7.409	-14.633	24.867	0.001
	3.512	-10.294	2.618	4.431
7	8.339	-18.667	23.616	0.000
	2.725	-6.226	2.588	4.437
8	8.016	-18.713	23.616	0.000
	3.096	-8.253	2.616	4.409
9	7.767	-18.751	23.616	0.000
	3.420	-10.314	2.618	4.431
10	7.554	-18.782	23.616	0.000
	3.690	-12.334	2.599	4.414
11	9.097	-18.946	23.616	0.000
	3.966	-12.432	2.599	4.414
12	7.896	-15.024	20.241	0.002
	2.718	-6.201	2.588	4.437
13	7.570	-15.062	20.241	0.002
	3.120	-8.227	2.616	4.409

DES (HBA:HBD)	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}
14	8.532	-18.804	20.410	0.001
	2.691	-6.214	2.588	4.437
15	9.636	-19.058	20.410	0.001
	2.843	-6.310	2.588	4.437
16	10.354	-19.231	20.410	0.001
	2.949	-6.376	2.588	4.437
17	8.214	-18.845	20.410	0.001
	3.072	-8.240	2.616	4.409
18	7.968	-18.880	20.410	0.001
	3.406	-10.301	2.618	4.431
19	7.761	-18.907	20.410	0.001
	3.685	-12.322	2.599	4.414
20	4.406	-8.725	15.949	0.170
	1.494	-4.102	8.133	5.244
	2.139	-5.771	6.549	5.112
21	4.789	-8.767	15.949	0.170
	1.576	-4.099	8.133	5.244
	2.031	-4.588	6.092	4.023
22	5.110	-8.774	15.949	0.170
	1.651	-4.075	8.133	5.244
	1.635	-3.514	5.748	3.576
23	4.224	-9.096	15.949	0.170
	1.478	-4.133	8.133	5.244
	1.436	-5.457	3.723	8.539
24	4.388	-8.742	15.949	0.170
	2.051	-5.753	6.549	5.112
	1.818	-4.562	6.092	4.023
25	4.609	-8.766	15.949	0.170

DES (HBA:HBD)	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}
	2.165	-5.788	6.549	5.112
	1.492	-3.538	5.748	3.576
	3.870	-9.088	15.949	0.170
26	2.038	-5.933	6.549	5.112
	1.443	-5.583	3.723	8.539
	5.002	-8.813	15.949	0.170
27	2.065	-4.609	6.092	4.023
	1.591	-3.547	5.748	3.576
	4.169	-9.146	15.949	0.170
28	1.899	-4.724	6.092	4.023
	1.471	-5.580	3.723	8.539
	4.438	-9.153	15.949	0.170
29	1.460	-5.542	3.723	8.539
	1.494	-3.627	5.748	3.576
30	4.894	-8.720	15.949	0.170
	1.627	-4.022	8.133	5.244
31	3.023	-8.368	15.949	0.170
	1.679	-5.045	1.932	10.637
32	-7.943	15.949	4.727	-8.790
	-7.272	6.092	1.943	-4.587
33	4.094	-8.699	15.949	0.170
	1.927	-5.718	6.549	5.112
34	4.893	-8.824	15.949	0.170
	2.246	-5.347	3.046	5.362
35	3.798	-8.554	15.949	0.170
	2.960	-8.660	10.946	8.422
36	3.846	-8.513	15.949	0.170
	2.916	-7.796	4.158	13.958

DES (HBA:HBD)	E_{MF} (kcal/mol)	E_{vdW} (kcal/mol)	M_{Hba}	M_{Hbd}
37	3.480	-9.658	15.949	0.170
	1.351	-6.179	0.000	0.000
38	4.028	-6.904	21.430	0.088
	2.075	-5.567	6.549	5.112
39	3.717	-6.724	21.430	0.088
	3.092	-7.449	4.158	13.958
40	5.264	-6.929	21.430	0.088
	1.844	-3.873	8.133	5.244
41	1.860	-10.032	3.323	1.076
	1.528	-4.104	2.094	3.785
42	2.238	-10.013	3.323	1.076
	2.845	-6.789	3.509	3.702
43	1.765	-10.139	3.323	1.076
	2.675	-10.130	2.618	4.431
44	1.639	-10.177	3.323	1.076
	3.054	-14.183	2.569	4.423

Table S4 – Correlations models between K-T parameters and COSMO-RS descriptors for organic solvents

Number	Equation for K-T parameters																R^2
1	$\alpha =$	-4.878E-03	×	M_{HBA}	+	4.944E-02											0.024
2	$\alpha =$	2.615E-01	×	M_{HBD}	+	2.774E-02											0.864
3	$\alpha =$	-2.631E-04	×	E_{vdW}	+	2.826E-02											0.081
4	$\alpha =$	-2.610E-04	×	E_{MF}	+	4.071E-02											0.005
5	$\alpha =$	8.704E-03	×	M_{HBA}	+	2.626E-01	×	M_{HBD}	+	-3.157E-08							0.864
6	$\alpha =$	8.199E-03	×	M_{HBA}	+	5.798E-03	×	E_{vdW}	+	6.893E-02							0.072
7	$\alpha =$	-5.012E-03	×	M_{HBA}	+	3.161E-04	×	E_{MF}	+	4.945E-02							0.025
8	$\alpha =$	2.601E-01	×	M_{HBD}	+	2.833E-03	×	E_{vdW}	+	5.348E-02							0.866
9	$\alpha =$	2.622E-01	×	M_{HBD}	+	1.176E-02	×	E_{MF}	+	8.184E-03							0.860
10	$\alpha =$	9.652E-03	×	M_{HBA}	+	2.563E-01	×	M_{HBD}	+	1.995E-03	×	E_{vdW}	+	2.141E-02			0.864
11	$\alpha =$	5.799E-03	×	M_{HBA}	+	2.615E-01	×	M_{HBD}	+	8.420E-03	×	E_{MF}	+	-9.101E-03			0.861
12	$\beta =$	1.555E-01	×	M_{HBA}	+	5.000E-02											0.636
13	$\beta =$	8.827E-02	×	M_{HBD}	+	5.660E-02											0.022
14	$\beta =$	1.143E-02	×	E_{vdW}	+	1.604E-01											0.026
15	$\beta =$	9.857E-02	×	E_{MF}	+	-2.450E-03											0.197
16	$\beta =$	1.608E-01	×	M_{HBA}	+	8.828E-03	×	M_{HBD}	+	3.001E-02							0.634
17	$\beta =$	1.574E-01	×	M_{HBA}	+	8.828E-03	×	E_{vdW}	+	3.371E-02							0.635
18	$\beta =$	1.332E-01	×	M_{HBA}	+	8.828E-03	×	E_{MF}	+	4.329E-03							0.623
19	$\beta =$	9.021E-02	×	M_{HBD}	+	8.828E-03	×	E_{vdW}	+	3.033E-02							0.020
20	$\beta =$	6.014E-02	×	M_{HBD}	+	8.828E-03	×	E_{MF}	+	1.225E-03							0.173
21	$\beta =$	1.540E-01	×	M_{HBA}	+	8.828E-03	×	M_{HBD}	+	3.080E-02	×	E_{vdW}	+	1.104E-01			0.632
22	$\beta =$	1.342E-01	×	M_{HBA}	+	4.204E-02	×	M_{HBD}	+	1.637E-02	×	E_{MF}	+	4.690E-03			0.627
23	$\pi^* =$	1.073E-01	×	M_{HBA}	+	5.274E-02											0.045
24	$\pi^* =$	1.183E-01	×	M_{HBD}	+	2.690E-01											0.006
25	$\pi^* =$	5.595E-02	×	E_{vdW}	+	8.456E-01											0.073
26	$\pi^* =$	2.741E-01	×	E_{MF}	+	2.430E-02											0.386
27	$\pi^* =$	9.688E-02	×	M_{HBA}	+	5.262E-02	×	M_{HBD}	+	5.000E-02							0.048
28	$\pi^* =$	5.741E-02	×	M_{HBA}	+	4.227E-02	×	E_{vdW}	+	6.511E-01							0.094
29	$\pi^* =$	-3.657E-02	×	M_{HBA}	+	3.229E-01	×	E_{MF}	+	-3.073E-02							0.419
30	$\pi^* =$	1.806E-01	×	M_{HBD}	+	-8.637E-03	×	E_{vdW}	+	3.421E-02							0.003
31	$\pi^* =$	5.249E-02	×	M_{HBD}	+	2.538E-01	×	E_{MF}	+	-2.029E-02							0.391
32	$\pi^* =$	9.947E-02	×	M_{HBA}	+	5.819E-02	×	M_{HBD}	+	-4.525E-03	×	E_{vdW}	+	-1.630E-02			0.044
33	$\pi^* =$	-3.955E-02	×	M_{HBA}	+	7.810E-02	×	M_{HBD}	+	3.033E-01	×	E_{MF}	+	-2.828E+01			0.427

Table S5. Experimental and predicted solvatochromic parameters (α, β and π^*) for different organic solvents.

Solvents	α_{exp}	α_{pred}	β_{exp}	β_{pred}	π^*_{exp}	π^*_{pred}
Formic acid	1.230	1.215	0.380	0.257	0.650	0.632
Propanoic acid	1.120	1.188	0.450	0.406	0.580	0.827
Benzyl alcohol	0.600	0.462	0.520	0.356	0.980	0.636
Glycerol	1.210	1.384	0.510	0.997	0.620	0.561
n-Butanol	0.840	0.485	0.840	0.475	0.470	0.323
n-Pentanol	0.840	0.480	0.860	0.434	0.400	0.344
n-Hexanol	0.800	0.370	0.840	0.434	0.400	0.426
n-Pentane	0.000	0.007	0.000	-0.106	-0.080	0.007
n-Heptane	0.000	0.003	0.000	-0.169	-0.080	0.017
n-Octane	0.000	0.001	0.000	-0.201	0.010	0.023
Cyclohexane	0.000	0.008	0.000	-0.098	0.000	-0.015
Formamide	0.710	0.987	0.480	0.922	0.970	0.426
N-Methyl acetamide	0.470	0.474	0.800	1.075	1.010	0.660
N,N-Diethyl acetamide	0.000	0.069	0.780	0.874	0.840	0.867
2-Pyrrolidinone	0.360	0.462	0.770	1.047	0.850	0.801
Tetramethyl guanidine	0.000	0.077	0.860	1.001	0.760	0.776
Dimethyl cyanamide	0.000	0.049	0.640	0.550	0.720	0.964
Butylamine	0.000	0.071	0.720	0.756	0.310	0.431
Diaminoethane	0.130	0.134	1.430	1.413	0.470	0.410
Pyrrolidine	0.160	0.068	0.700	0.697	0.390	0.414
Piperidine	0.000	0.058	1.040	0.559	0.300	0.269
Morpholine	0.290	0.095	0.700	0.865	0.390	0.532
Dimethylbenzylamine	0.000	0.021	0.640	0.115	0.450	0.517
N,N-Dimethylaniline	0.000	0.005	0.430	-0.149	0.730	0.649
Acetic anhydride	0.000	0.021	0.290	0.107	0.760	0.796
m-Xylene	0.000	0.005	0.120	-0.137	0.470	0.456
Mesitylene	0.000	0.003	0.130	-0.167	0.410	0.455
Ethylene carbonate	0.000	0.028	0.320	0.217	0.990	0.503
Dimethyl phthalate	0.000	0.021	0.780	0.112	0.820	0.999
Methyl acetate	0.000	0.031	0.420	0.263	0.600	0.644
4-Butyrolactone	0.000	0.036	0.490	0.356	0.870	0.847

Solvents	α_{exp}	α_{pred}	β_{exp}	β_{pred}	π^*_{exp}	π^*_{pred}
Diethyl ether	0.000	0.033	0.470	0.307	0.270	0.391
Di-(2-chloroethyl) ether	0.000	0.023	0.400	0.150	0.820	0.586
Dibenzyl ether	0.000	0.011	0.410	-0.041	0.800	0.811
Diphenyl ether	0.000	0.001	0.130	-0.205	0.660	0.704
Tetrahydrofuran	0.000	0.044	0.550	0.473	0.580	0.511
Eucalyptol	0.000	0.035	0.610	0.332	0.360	0.392
Anisole	0.000	0.011	0.320	-0.054	0.730	0.573
2-Chloroethanol	1.280	0.358	0.530	0.355	0.460	0.461
Hexafluoroisopropanol	1.960	1.182	0.000	0.021	0.650	1.014
1-Chlorobutane	0.000	0.007	0.000	-0.116	0.390	0.406
1,1,1-Trichloroethane	0.000	0.005	0.000	-0.141	0.490	0.337
1-Bromobutane	0.000	0.006	0.130	-0.133	0.500	0.425
1,2-Dibromoethane	0.000	0.008	0.000	-0.104	0.750	0.495
trans-Dichloroethylene	0.000	0.045	0.000	-0.097	0.440	0.399
Tetrachloroethylene	0.000	0.003	0.050	-0.181	0.280	0.101
Hexafluorobenzene	0.000	0.010	0.020	-0.072	0.330	0.353
Bromobenzene	0.000	0.004	0.060	-0.160	0.790	0.470
3-Pentanone	0.000	0.035	0.450	0.330	0.720	0.708
Cyclopentanone	0.000	0.035	0.520	0.335	0.760	0.755
Acetonitrile	0.190	0.027	0.400	0.201	0.750	0.517
Butanenitrile	0.000	0.023	0.400	0.138	0.710	0.708
Benzonitrile	0.000	0.016	0.370	0.024	0.900	0.707
Perfluoromethylcyclohexane	0.000	0.006	-0.060	-0.131	-0.400	-0.017
Tetramethylsilane	0.000	0.006	0.020	-0.126	0.000	0.107
Sulpholane	0.000	0.048	0.390	0.540	0.980	0.993
Thiane	0.000	0.012	0.360	-0.030	0.610	0.482
Water	1.170	1.063	0.470	0.993	1.090	0.136

	α	β	π^*
R^2	0.827	0.659	0.546
MSE	0.037	0.076	0.046
MAE	0.088	0.229	0.135

Table S6 – Correlations models between K-T parameters and COSMO-RS descriptors for acid DES

Number	Equation for K-T parameters																R^2
1	$\alpha =$	-9.441E-02	×	M_{HBA}	+	1.885E+00											0.151
2	$\alpha =$	9.713E-02	×	M_{HBD}	+	6.956E-01											0.300
3	$\alpha =$	4.603E-02	×	E_{vdW}	+	1.504E+00											0.378
4	$\alpha =$	-1.932E-01	×	E_{MF}	+	1.909E+00											0.367
5	$\alpha =$	-9.500E-02	×	M_{HBA}	+	3.001E-02	×	M_{HBD}	+	1.803E+00							0.223
6	$\alpha =$	-8.248E-02	×	M_{HBA}	+	2.924E-02	×	E_{vdW}	+	2.070E+00							0.241
7	$\alpha =$	-5.323E-02	×	M_{HBA}	+	-1.054E-01	×	E_{MF}	+	1.966E+00							0.324
8	$\alpha =$	7.155E-02	×	M_{HBD}	+	1.573E-02	×	E_{vdW}	+	9.757E-01							0.392
9	$\alpha =$	-3.385E-02	×	M_{HBD}	+	-2.073E-01	×	E_{MF}	+	2.074E+00							0.435
10	$\alpha =$	-8.414E-02	×	M_{HBA}	+	1.753E-02	×	M_{HBD}	+	2.371E-02	×	E_{vdW}	+	1.967E+00			0.797
11	$\alpha =$	-5.950E-02	×	M_{HBA}	+	3.970E-03	×	M_{HBD}	+	-8.937E-02	×	E_{MF}	+	1.945E+00			0.307
12	$\beta =$	-6.076E-02	×	M_{HBA}	+	7.893E-01											0.066
13	$\beta =$	-2.037E-01	×	M_{HBD}	+	1.443E+00											0.220
14	$\beta =$	-1.954E-01	×	E_{vdW}	+	-1.372E+00											0.534
15	$\beta =$	3.829E-01	×	E_{MF}	+	-1.292E+00											0.330
16	$\beta =$	4.919E-02	×	M_{HBA}	+	-2.453E-01	×	M_{HBD}	+	1.105E+00							0.307
17	$\beta =$	-5.860E-02	×	M_{HBA}	+	-1.439E-01	×	E_{vdW}	+	-2.582E-01							0.487
18	$\beta =$	-1.062E-01	×	M_{HBA}	+	3.937E-01	×	E_{MF}	+	3.079E-02							0.453
19	$\beta =$	-1.281E-01	×	M_{HBD}	+	-9.167E-02	×	E_{vdW}	+	2.621E-01							0.487
20	$\beta =$	-1.719E-01	×	M_{HBD}	+	1.219E-01	×	E_{MF}	+	8.042E-01							0.362
21	$\beta =$	3.589E-02	×	M_{HBA}	+	-2.071E-01	×	M_{HBD}	+	-4.494E-02	×	E_{vdW}	+	6.885E-01			0.816
22	$\beta =$	-6.406E-02	×	M_{HBA}	+	-5.542E-02	×	M_{HBD}	+	3.044E-01	×	E_{MF}	+	1.845E-01			0.435
23	$\pi^* =$	4.791E-02	×	M_{HBA}	+	4.002E-01											0.406
24	$\pi^* =$	5.986E-02	×	M_{HBD}	+	6.521E-01											0.544
25	$\pi^* =$	4.792E-03	×	E_{vdW}	+	9.037E-01											0.056
26	$\pi^* =$	7.868E-02	×	E_{MF}	+	4.521E-01											0.021
27	$\pi^* =$	3.673E-02	×	M_{HBA}	+	1.459E-01	×	M_{HBD}	+	7.573E-02							0.832
28	$\pi^* =$	7.508E-02	×	M_{HBA}	+	5.601E-02	×	E_{vdW}	+	7.546E-01							0.421
29	$\pi^* =$	1.148E-01	×	M_{HBA}	+	-1.596E-01	×	E_{MF}	+	4.893E-01							0.785
30	$\pi^* =$	1.456E-01	×	M_{HBD}	+	-3.261E-02	×	E_{vdW}	+	2.701E-02							0.580
31	$\pi^* =$	1.202E-01	×	M_{HBD}	+	8.703E-02	×	E_{MF}	+	9.021E-02							0.787
32	$\pi^* =$	6.315E-02	×	M_{HBA}	+	6.157E-02	×	M_{HBD}	+	3.432E-02	×	E_{vdW}	+	4.340E-01			0.487
33	$\pi^* =$	2.737E-02	×	M_{HBA}	+	9.214E-02	×	M_{HBD}	+	3.157E-02	×	E_{MF}	+	1.784E-01			0.831

Table S7 – Correlations models between K-T parameters and COSMO-RS descriptors for non-acid DES

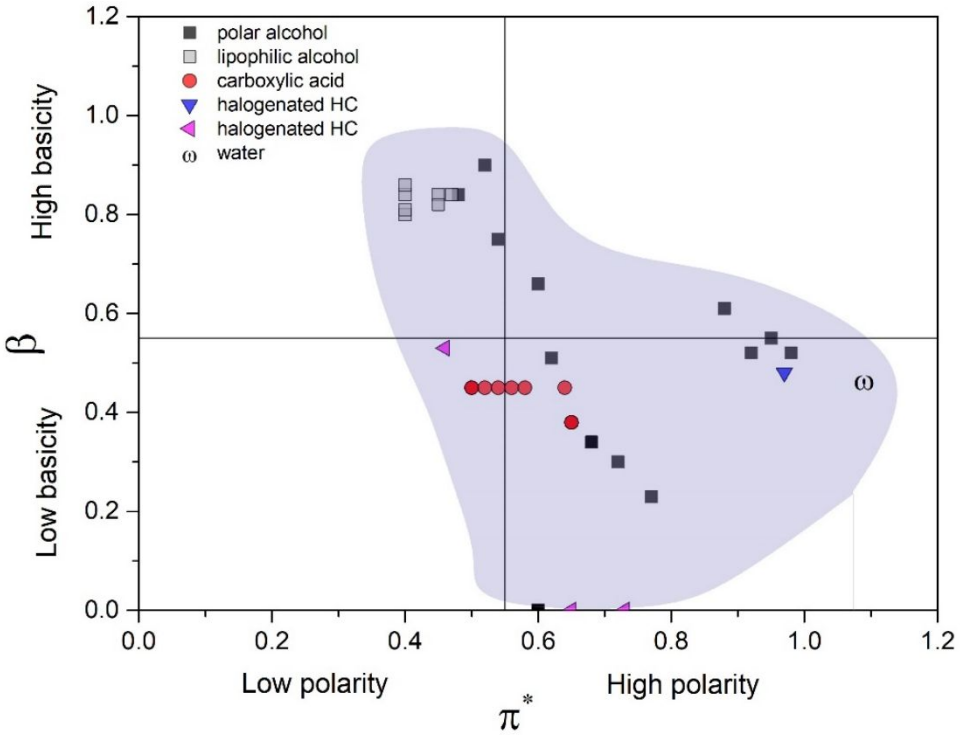
Number	Equation for K-T parameters																R²
1	$\alpha =$	2.059E-01	×	M_{HBA}	+	-9.099E-01											0.675
2	$\alpha =$	-2.093E-02	×	M_{HBD}	+	9.528E-01											0.292
3	$\alpha =$	-2.572E-02	×	E_{vdW}	+	7.124E-01											0.116
4	$\alpha =$	1.769E-01	×	E_{MF}	+	4.191E-01											0.638
5	$\alpha =$	8.623E-02	×	M_{HBA}	+	3.585E-02	×	M_{HBD}	+	-2.671E-02							0.635
6	$\alpha =$	6.278E-02	×	M_{HBA}	+	-5.355E-02	×	E_{vdW}	+	-2.303E-02							0.727
7	$\alpha =$	1.547E-01	×	M_{HBA}	+	1.612E-01	×	E_{MF}	+	-8.697E-01							0.684
8	$\alpha =$	-4.054E-02	×	M_{HBD}	+	-7.248E-02	×	E_{vdW}	+	5.736E-01							0.022
9	$\alpha =$	3.330E-01	×	M_{HBD}	+	1.676E+00	×	E_{MF}	+	-4.712E+00							0.696
10	$\alpha =$	2.654E-01	×	M_{HBA}	+	-6.948E-02	×	M_{HBD}	+	-3.735E-01	×	E_{vdW}	+	-3.622E+00			0.867
11	$\alpha =$	1.194E-01	×	M_{HBA}	+	3.503E-02	×	M_{HBD}	+	-6.798E-02	×	E_{MF}	+	-1.490E-01			0.631
12	$\beta =$	4.392E-02	×	M_{HBA}	+	1.563E-01											0.749
13	$\beta =$	-1.618E-02	×	M_{HBD}	+	6.143E-01											0.247
14	$\beta =$	2.448E-02	×	E_{vdW}	+	7.071E-01											0.221
15	$\beta =$	1.940E-01	×	E_{MF}	+	5.013E-02											0.782
16	$\beta =$	-1.667E-02	×	M_{HBA}	+	-4.504E-02	×	M_{HBD}	+	8.694E-01							0.671
17	$\beta =$	5.270E-02	×	M_{HBA}	+	-1.115E-02	×	E_{vdW}	+	1.806E-03							0.755
18	$\beta =$	-4.732E-02	×	M_{HBA}	+	2.974E-01	×	E_{MF}	+	2.171E-01							0.609
19	$\beta =$	-1.868E-02	×	M_{HBD}	+	-5.035E-03	×	E_{vdW}	+	5.905E-01							0.228
20	$\beta =$	2.300E-02	×	M_{HBD}	+	1.759E-01	×	E_{MF}	+	2.069E-03							0.890
21	$\beta =$	-1.489E-02	×	M_{HBA}	+	-7.062E-02	×	M_{HBD}	+	-5.987E-02	×	E_{vdW}	+	5.833E-01			0.707
22	$\beta =$	-5.890E-02	×	M_{HBA}	+	2.567E-02	×	M_{HBD}	+	3.910E-01	×	E_{MF}	+	-2.056E-02			0.672
23	$\pi^* =$	2.600E-02	×	M_{HBA}	+	9.035E-01											0.144
24	$\pi^* =$	5.886E-02	×	M_{HBD}	+	9.572E-01											0.166
25	$\pi^* =$	-4.378E-02	×	E_{vdW}	+	9.163E-01											0.006
26	$\pi^* =$	-1.575E-01	×	E_{MF}	+	1.600E+00											0.341
27	$\pi^* =$	3.023E-02	×	M_{HBA}	+	6.900E-02	×	M_{HBD}	+	6.439E-01							0.712
28	$\pi^* =$	4.035E-02	×	M_{HBA}	+	-1.180E-01	×	E_{vdW}	+	5.426E-02							0.158
29	$\pi^* =$	7.905E-02	×	M_{HBA}	+	-3.347E-01	×	E_{MF}	+	1.309E+00							0.611
30	$\pi^* =$	7.344E-02	×	M_{HBD}	+	4.393E-02	×	E_{vdW}	+	1.179E+00							0.307
31	$\pi^* =$	1.159E-01	×	M_{HBD}	+	2.534E-01	×	E_{MF}	+	7.835E-02							0.779
32	$\pi^* =$	3.863E-02	×	M_{HBA}	+	6.447E-02	×	M_{HBD}	+	-3.570E-02	×	E_{vdW}	+	3.522E-01			0.417
33	$\pi^* =$	2.024E-02	×	M_{HBA}	+	9.036E-02	×	M_{HBD}	+	9.426E-02	×	E_{MF}	+	4.129E-01			0.823

Table S8. Experimental and predicted solvatochromic parameters (α, β and π*) for DES obtained by this and other works.

DES	α_{exp}	α_{pred}	α_{pred_2} [8]	β_{exp}	β_{pred}	β_{pred_2} [8,9]	π^*_{exp}	$\pi^*_{pred_2}$	π^*_{pred} [9]
1	0.990	1.004	0.988	0.760	0.779	0.7556 ,0.790	0.920	0.857	0.790
5	0.910	0.931	0.921	0.920	0.905	0.919			
8	0.900	0.931	0.885	1.020	0.953	1.020	0.810	0.862	
14	1.020	1.054	1.011	0.810	0.850	0.828	0.930	0.831	
19	0.950	0.956	0.959	1.050	1.038	1.089	0.710	0.842	
38	2.236	2.239	1.284	0.587	0.565	0.455	1.253	1.219	
44	1.790	1.483	1.779	0.570	0.682	0.563	0.370	0.642	

Note: α_{pred}, β_{pred} and π^*_{pred} values were obtained by this work; α_{pred_2}, β_{pred_2} and $\pi^*_{pred_2}$ values were obtained from cited literature; for DES composition, please check Table S2.

Figure S1. The protic conventional solvents plotted according to their π^* and β values. The shaded area represents the range of properties possessed by the set of Marcus database solvents.



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