

Prediction of Ionic Liquids Heat Capacity by means of their *in silico* Principal Properties

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Experimental

Computational Methods

PLS allows to find relationships between the VolSurf-derived properties matrix (X matrix) and the response, in this case heat capacity values of ILs.

The PLS algorithm computes PLS components for each of the two matrices (X and Y matrices), searching simultaneously for a linear relationship between the X-scores and Y-scores of the PLS components by means of equation (1), where b_a is a proportionality coefficient:

$$y_{ia} = \sum_{i=1}^A b_a t_{ia} + h_{ia} \quad (1)$$

The main statistical parameters provided by the PLS method [29] are R^2X , R^2Y (respectively sum of squares of all the X's and Y's explained by all extracted components) and Q^2 , the fraction of the total variation of the Y's predicted by all PLS components, as estimated by cross validation (CV). Q^2 was computed as: $1 - \text{PRESS}/\text{SS}$, where SS is the residual sum of squares and PRESS is the squared difference between observed and predicted values for the data kept out of the model fitting. CV was performed in the same way than for PCA.

The statistical results obtained by the PLS method are able to detect what variables in the X block are relevant to determine the dependent variables (Y block) by means of the VIP values. SIMCA computes VIP values by summing over all model dimensions the contributions VIN (variable influence). For a given PLS dimension, a , $(\text{VIN})_{ak}^2$ is equal to the squared PLS weight $(w_{ak})^2$ of that term, multiplied by the % explained of residual sum of squares by that PLS dimension. The accumulated (over all PLS dimensions) value, $\text{VIP}_k = \Sigma (\text{VIN})_k^2$ is then divided by the total percent explained of residual sum of squares by the PLS model and multiplied by the number of terms in the model.

Figure S1. Permutation plots

In PLS Q^2 assesses the predictive power of the model and a permutation plot is a further chemoinformatic tool to check the significance of a PLS model and the reliability of its Y-predictions. In fact the purpose of this validation tool is to compare the goodness of fit (R^2 and Q^2) of the original model with the goodness of fit of several models based on data where the order of the Y-observations has been randomly permuted, while the X-matrix has been kept intact. The permutation plot [32] below shows R^2 and Q^2 values on the vertical axis for the parental PLS model (far to the right) and the Y-permuted models parameters on the left. The horizontal axis shows the correlation between the permuted Y-vectors and the original Y-vector. The original parameters have correlation 1 with themselves.

In order to have a valid plot, some important criteria are requested:

1. All Q^2 -values on the left should be lower than the original points to the right.
2. The R^2 intercept should be less than 0.4.
3. The regression line of the Q^2 -points should intersect the vertical axis (on the left) at or below zero.

The plot below was obtained by considering 50 random PLS models, and strongly indicates that Cp correlation model can be considered valid.

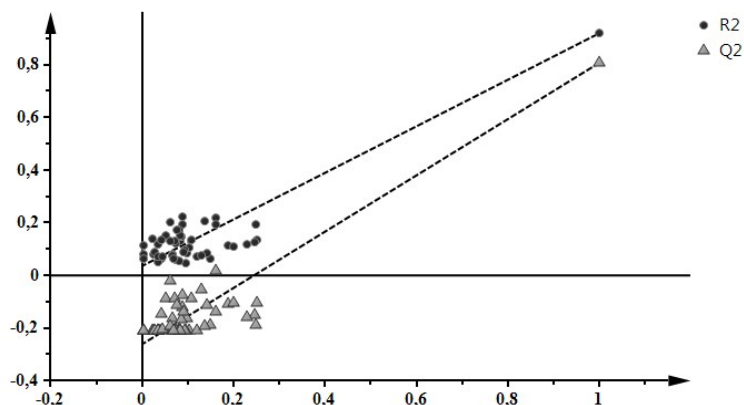


Fig. S1

Synthesis and characterization of test set ILs

Materials

Commercially available compounds were used directly without any preliminary treatment. 1-Butyl-3-methylimidazolium tetrafluoroborate was purchased from Sigma-Aldrich. 1-Butyl-3-methylimidazolium tricyanomethanide, 1-butyl-3-methylimidazolium dimethylphosphate 1-butyl-4-methylpyridinium tricyanomethanide, 1-butyl-4-methylpyridinium chloride and 1-hexyl-3-methylimidazolium chloride were purchased from Io.Li.Tec. Solvents, HBF₄ solution (50/50, w/w) and Amberlite IRA-400 resin were used as purchased without further purification.

Synthesis of 1-butyl-4-methylpyridinium tetrafluoroborate (IL 331). 2 g (10.7 mmol) of 1-butyl-4-methylpyridinium chloride were dissolved in 30 mL of anhydrous CH₂Cl₂ under Argon atmosphere, and 1.17 g (10.7 mmol) of NaBF₄ were added. The solution was stirred for 24h. The suspension was filtered and washed with anhydrous dichloromethane to remove the precipitated sodium chloride salt, then the organic phase was filtered on alumina and charcoal (to remove residual impurities) and washed with small volumes of water. The absence of residual halides was verified by silver nitrate test. The solvent was removed *in vacuo* and no further treatments were needed. The organic salt was recovered with 80.8 % of yield, and the structure confirmed by the NMR spectra in agreement with literature data [34].

Synthesis of 1-butyl-3-methylimidazolium acetate (IL 511) and 1-hexyl-3-methylimidazolium salts (tetrafluoroborate, acetate and trifluoroacetate) (ILs 196, 512, 513). The general procedure for the synthesis of these ionic liquids from the relevant halides is reported below. The Amberlite resin IRA-400 (16 g) was converted from chloride form to hydroxide form by eluting an aqueous solution of NaOH (10 mL, 10% w/v) within a column. Subsequently the resin was washed with water until the eluate was neutral. The halide salt(s) (10 mmol), dissolved in methanol/water (70/30, v/v), was eluted, and the eluate collected into a flask containing a solution of the corresponding acid in stoichiometric amount, until neutralization. The resulting solution was concentrated *in vacuo*, then treated with activated charcoal in ethanol. Filtration and removal of the solvent afforded the ionic liquids as viscous oils in high to quantitative yields. The products structures were confirmed by NMR spectra and are in agreement with literature data [35-38].

1-Hexyl-3-methylimidazolium tetrafluoroborate

Pale yellow oil. Yield: 100%

^1H NMR (300 MHz, CDCl_3): δ =8.70 (s, 1 H), 7.21 (d, J =14 Hz, 2 H), 4.17 (t, J =6 Hz, 2 H), 3.94 (s, 3 H), 1.87 (m, 2 H), 1.31 (m, 6 H), 0.87 (t, J =6 Hz, 3 H) ppm.

^{13}C NMR (300 MHz, CDCl_3): δ = 135.8, 123.4, 121.9, 50.0, 36.2, 31.1, 29.0, 25.9, 22.3, 13.8 ppm [34].

1-Hexyl-3-methylimidazolium acetate

Pale yellow oil. Yield: 99%

^1H NMR (300 MHz, d_6 -DMSO): δ =9.44 (s, 1 H), 7.74 (d, J =24 Hz, 2 H), 4.15 (t, J =7 Hz, 2 H), 3.85 (s, 3 H), 1.77 (quint, J =6.8 Hz, 2 H), 1.56 (s, 3 H), 1.26 (m, 6 H), 0.85 (t, J =7 Hz, 3 H) ppm. ^{13}C NMR (300 MHz, d_6 -DMSO) δ = 173.8, 137.9, 124.1, 122.0, 49.0, 36.0, 31.1, 30.2, 29.8, 25.9, 24.6, 22.4 ppm [38].

1-Hexyl-3-methylimidazolium trifluoroacetate

Pale yellow oil. Yield: 96%

^1H NMR (300 MHz, d_6 -DMSO): δ =9.15 (s, 1 H), 7.74 (d, J =26 Hz, 2 H), 4.13 (t, J =8 Hz, 2 H), 3.82 (s, 3 H), 1.73 (quint, J =8 Hz, 2 H), 1.25 (m, 6 H), 0.85 (t, J =7 Hz, 3 H) ppm. ^{13}C NMR (300 MHz, d_6 -DMSO): δ = 158.0, 137.2, 124.1, 122.1, 49.24, 36.1, 30.9, 30.2, 29.9, 25.6, 22.3, 14.2 ppm [36].

Heat capacity measurements

The heat capacities were measured by means of DSC analysis carrying out experiments on a Linseis STA PT 1600 instrument at atmospheric pressure. over the temperature ranging from. Samples (20.0 ± 0.1 mg) were heated in a platinum sample boat up. In accordance with Chiu [33] a method was created to hold isothermally at the desired starting temperature (298K) for 10 min, then heating at $5^\circ\text{K}/\text{min}$ up to 353°K , then holding at this temperature for 10 min. The purge gas used was nitrogen with a flow rate of 50 cc/min. Water was used as standard to check the heat capacity measurements according to the method reported by Chiu [33].

C_p values measured in the present work are in excellent agreement with values reported in the literature (see Table 1), with differences of 6%, 5% and 2% for ILs 511, 196 and 331 respectively.

Table S1. Cp PLS predictions. DModX values higher than 1.60 corresponding to 95% c.l. [32] marked in red indicate a high distance from the learning set domain.

entry	IL code	PP1+	PP2+	PP3+	PP4+	PP5+	PP1-	PP2-	PP3-	PP4-	Y: Cp J/(K*mol)	Ŷ: Cp pred. J/(K*mol)	DModX	Systematic name
1	Py4-2Me BF4	0.27	-6.91	3.51	0.08	-0.72	1.67	-0.06	-0.33	-3.83		392	0.83	1-Butyl-2-methylpyridinium tetrafluoroborate
2	Py4-2Me Cl	0.27	-6.91	3.51	0.08	-0.72	-0.57	-5.73	-2.31	-1.25		265	0.93	1-Butyl-2-methylpyridinium chloride
3	Pyr12 2OSO3	4.57	-4.49	-4.03	5.55	0.10	1.13	-1.47	-0.18	-0.39		434	1.90	1-Ethyl-1-methylpyrrolidinium ethyl sulfate
4	Pyr11CN (CF3SO2)2N	6.95	0.11	-2.58	2.04	-0.06	-1.19	-2.15	2.86	2.10		430	1.79	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
5	Pyr11CN Cl	6.95	0.11	-2.58	2.04	-0.06	-0.57	-5.73	-2.31	-1.25		151	1.61	1-(Cyanomethyl)-1-methylpyrrolidinium chloride
6	Pyr11COO2 (CF3SO2)2N	7.17	1.90	-2.39	4.75	-1.11	-1.19	-2.15	2.86	2.10		420	2.48	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
7	Pyr11COO2 Br	7.17	1.90	-2.39	4.75	-1.11	-0.52	-5.52	-2.16	-1.13		151	2.35	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide
8	Pyr11COO2 (C2F5)3PF3	7.17	1.90	-2.39	4.75	-1.11	2.83	3.03	4.77	-1.46		534	3.00	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate
9	Pyr13 PF6	3.13	-4.34	-3.85	5.63	-0.10	1.13	-1.14	-0.21	-3.53		416	1.96	1-Methyl-1-propylpyrrolidinium hexafluorophosphate
10	Pyr14 Cl	1.96	-4.12	-3.78	5.67	-0.03	-0.57	-5.73	-2.31	-1.25		329	1.85	1-Butyl-1-methylpyrrolidinium chloride
11	Pyr14 (C2F5)3PF3	1.96	-4.12	-3.78	5.67	-0.03	2.83	3.03	4.77	-1.46	769 ^a	723	2.04	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate
12	Pyr14 (CF3SO2)2N	1.96	-4.12	-3.78	5.67	-0.03	-1.19	-2.15	2.86	2.10	588 ^a	608	1.75	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
13	Pyr14 1OSO3	1.96	-4.12	-3.78	5.67	-0.03	1.36	-1.16	-0.44	-1.31		474	1.84	1-Butyl-1-methylpyrrolidinium methyl sulfate
14	Pyr14 BF4	1.96	-4.12	-3.78	5.67	-0.03	1.67	-0.06	-0.33	-3.83		456	2.00	1-Butyl-1-methylpyrrolidinium tetrafluoroborate
15	Pyr14 Br	1.96	-4.12	-3.78	5.67	-0.03	-0.52	-5.52	-2.16	-1.13		339	1.84	1-Butyl-1-methylpyrrolidinium bromide
16	Pyr14 N(CN)2	1.96	-4.12	-3.78	5.67	-0.03	-2.48	0.49	0.00	0.73		518	1.82	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide
17	Pyr16 (CF3SO2)2N	0.02	-3.63	-3.89	5.63	0.25	-1.19	-2.15	2.86	2.10		660	1.64	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
18	Pyr16 Cl	0.02	-3.63	-3.89	5.63	0.25	-0.57	-5.73	-2.31	-1.25		381	1.87	1-Hexyl-1-methylpyrrolidinium chloride
19	Pyr18 BF4	-2.33	-3.03	-3.71	5.36	0.63	1.67	-0.06	-0.33	-3.83		568	2.03	1-Methyl-1-octylpyrrolidinium tetrafluoroborate
20	Pyr18 Cl	-2.33	-3.03	-3.71	5.36	0.63	-0.57	-5.73	-2.31	-1.25		441	1.85	1-Methyl-1-octylpyrrolidinium chloride
21	Pyr13OH (CF3SO2)2N	10.38	4.48	-2.99	1.65	3.25	-1.19	-2.15	2.86	2.10		432	2.69	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
22	Pyr13OH Cl	10.38	4.48	-2.99	1.65	3.25	-0.57	-5.73	-2.31	-1.25		153	2.59	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride

23	Pyr13O1 (CF3SO2)2N	5.81	-0.16	-3.72	4.31	0.62	-1.19	-2.15	2.86	2.10	509	1.95	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
24	Pyr13O1 Cl	5.81	-0.16	-3.72	4.31	0.62	-0.57	-5.73	-2.31	-1.25	229	1.92	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	
25	Pyr12OH (CF3SO2)2N	11.45	4.49	-2.64	1.01	3.23	-1.19	-2.15	2.86	2.10	398	2.74	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
26	Pyr12OH I	11.45	4.49	-2.64	1.01	3.23	-0.65	-5.31	-1.63	-1.12	150	2.61	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	
27	Pyr12O1 (CF3SO2)2N	7.36	-0.19	-3.63	4.10	0.85	-1.19	-2.15	2.86	2.10	477	2.01	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
28	Pyr12O1 (C2F5)3PF3	7.36	-0.19	-3.63	4.10	0.85	2.83	3.03	4.77	-1.46	592	2.64	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	
29	Pyr12O1 Cl	7.36	-0.19	-3.63	4.10	0.85	-0.57	-5.73	-2.31	-1.25	198	1.94	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	
30	Pyr12O2 (CF3SO2)2N	5.75	-0.56	-3.73	5.02	0.54	-1.19	-2.15	2.86	2.10	518	2.00	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
31	Pyr12O2 Br	5.75	-0.56	-3.73	5.02	0.54	-0.52	-5.52	-2.16	-1.13	249	2.00	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	
32	Pyr11O2 (CF3SO2)2N	5.12	-1.38	-4.24	5.38	0.11	-1.19	-2.15	2.86	2.10	528	2.04	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
33	Pyr11O2 Cl	5.12	-1.38	-4.24	5.38	0.11	-0.57	-5.73	-2.31	-1.25	249	2.05	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	
34	Pip11CN (CF3SO2)2N	5.85	0.24	-2.52	1.66	0.09	-1.19	-2.15	2.86	2.10	455	1.69	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
35	Pip11CN Cl	5.85	0.24	-2.52	1.66	0.09	-0.57	-5.73	-2.31	-1.25	175	1.54	1-(Cyanomethyl)-1-methylpiperidinium chloride	
36	Pip13 (CF3SO2)2N	2.18	-4.18	-3.94	5.90	-0.26	-1.19	-2.15	2.86	2.10	607 ^a	600	1.84	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
37	Pip13 PF6	2.18	-4.18	-3.94	5.90	-0.26	1.13	-1.14	-0.21	-3.53	436	2.00	1-Methyl-1-propylpiperidinium hexafluorophosphate	
38	Pip14 (CF3SO2)2N	1.15	-3.97	-3.95	5.81	-0.09	-1.19	-2.15	2.86	2.10	627	1.73	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
39	Pip14 Br	1.15	-3.97	-3.95	5.81	-0.09	-0.52	-5.52	-2.16	-1.13	358	1.90	1-Butyl-1-methylpiperidinium bromide	
40	Pip13OH (CF3SO2)2N	9.27	4.69	-2.96	1.70	3.21	-1.19	-2.15	2.86	2.10	457	2.63	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
41	Pip13OH Cl	9.27	4.69	-2.96	1.70	3.21	-0.57	-5.73	-2.31	-1.25	177	2.55	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	
42	Pip13O1 (CF3SO2)2N	4.88	0.03	-3.74	4.40	0.67	-1.19	-2.15	2.86	2.10	532	1.92	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
43	Pip13O1 Cl	4.88	0.03	-3.74	4.40	0.67	-0.57	-5.73	-2.31	-1.25	253	1.93	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	
44	Pip12OH (CF3SO2)2N	10.68	4.70	-2.87	1.16	3.53	-1.19	-2.15	2.86	2.10	427	2.74	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
45	Pip12OH I	10.68	4.70	-2.87	1.16	3.53	-0.65	-5.31	-1.63	-1.12	179	2.65	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	
46	Pip12O1 (CF3SO2)2N	5.73	-1.14	-3.80	5.03	0.34	-1.19	-2.15	2.86	2.10	514	1.97	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
47	Pip12O1 Br	5.73	-1.14	-3.80	5.03	0.34	-0.52	-5.52	-2.16	-1.13	245	1.95	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	
48	Pip12O2 (CF3SO2)2N	4.83	-0.32	-3.71	5.03	0.45	-1.19	-2.15	2.86	2.10	536	1.97	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	

49	Pip12O2 Br	4.83	-0.32	-3.71	5.03	0.45	-0.52	-5.52	-2.16	-1.13	267	1.99	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide
50	Pip11O2 (CF3SO2)2N	3.80	-1.20	-4.17	5.21	0.01	-1.19	-2.15	2.86	2.10	553	1.95	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
51	Pip11O2 Cl	3.80	-1.20	-4.17	5.21	0.01	-0.57	-5.73	-2.31	-1.25	273	2.00	1-(Ethoxymethyl)-1-methylpiperidinium chloride
52	Mor12 4MePhSO3	8.90	-0.32	-3.78	4.51	0.50	-1.66	-1.59	2.48	3.83	456	2.23	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate
53	Mor11CN (CF3SO2)2N	9.29	3.51	-1.23	1.82	-0.65	-1.19	-2.15	2.86	2.10	340	2.54	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
54	Mor11CN Cl	9.29	3.51	-1.23	1.82	-0.65	-0.57	-5.73	-2.31	-1.25	61	2.29	4-(Cyanomethyl)-4-methylmorpholinium chloride
55	Mor14 (CF3SO2)2N	6.23	0.06	-3.73	3.90	0.91	-1.19	-2.15	2.86	2.10	502	1.94	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
56	Mor14 Br	6.23	0.06	-3.73	3.90	0.91	-0.52	-5.52	-2.16	-1.13	233	1.91	4-Butyl-4-methylmorpholinium bromide
57	Mor13OH (CF3SO2)2N	12.12	7.62	-1.88	2.42	2.48	-1.19	-2.15	2.86	2.10	364	3.32	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
58	Mor13OH Cl	12.12	7.62	-1.88	2.42	2.48	-0.57	-5.73	-2.31	-1.25	85	3.17	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride
59	Mor13O1 (CF3SO2)2N	7.79	2.32	-2.66	5.24	-0.19	-1.19	-2.15	2.86	2.10	438	2.53	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
60	Mor13O1 Cl	7.79	2.32	-2.66	5.24	-0.19	-0.57	-5.73	-2.31	-1.25	159	2.43	4-(3-Methoxypropyl)-4-methylmorpholinium chloride
61	Mor12OH (CF3SO2)2N	13.05	7.64	-1.48	2.13	2.17	-1.19	-2.15	2.86	2.10	329	3.38	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
62	Mor12OH I	13.05	7.64	-1.48	2.13	2.17	-0.65	-5.31	-1.63	-1.12	81	3.21	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide
63	Mor12O1 (CF3SO2)2N	9.02	2.70	-2.46	5.23	-0.32	-1.19	-2.15	2.86	2.10	404	2.67	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
64	Mor12O1 Cl	9.02	2.70	-2.46	5.23	-0.32	-0.57	-5.73	-2.31	-1.25	125	2.54	4-(2-Methoxyethyl)-4-methylmorpholinium chloride
65	Mor12O2 (CF3SO2)2N	8.20	2.70	-2.65	4.89	0.06	-1.19	-2.15	2.86	2.10	431	2.54	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
66	Mor12O2 Br	8.20	2.70	-2.65	4.89	0.06	-0.52	-5.52	-2.16	-1.13	162	2.44	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide
67	Mor11O2 (CF3SO2)2N	8.27	2.53	-3.27	4.62	-0.47	-1.19	-2.15	2.86	2.10	413	2.61	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
68	Mor11O2 Cl	8.27	2.53	-3.27	4.62	-0.47	-0.57	-5.73	-2.31	-1.25	133	2.47	4-(Ethoxymethyl)-4-methylmorpholinium chloride
69	IM11COO3-2Me 8OSO3	5.13	2.76	0.82	1.26	-2.57	-1.48	-1.82	3.86	4.62	445	2.68	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate
70	IM11COO3-2Me Br	5.13	2.76	0.82	1.26	-2.57	-0.52	-5.52	-2.16	-1.13	99	2.34	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide
71	IM11COO5-2Me 8OSO3	2.60	3.30	0.45	1.76	-2.70	-1.48	-1.82	3.86	4.62	505	2.75	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate
72	IM11COO5-2Me Br	2.60	3.30	0.45	1.76	-2.70	-0.52	-5.52	-2.16	-1.13	159	2.52	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide
73	IM1gly-2Me N(NC)2	12.79	9.75	2.58	-6.27	5.14	-2.48	0.49	0.00	0.73	212	4.31	1,2-dimethyl-3-glycerylimidazolium dicyanamide
74	IM1gly-2Me (CF3SO2)2N	12.79	9.75	2.58	-6.27	5.14	-1.19	-2.15	2.86	2.10	302	4.24	1,2-dimethyl-3-glycerylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide

75	IM14-2Me (CF3SO2)2N	1.01	-5.58	0.95	1.99	-0.19	-1.19	-2.15	2.86	2.10	570	0.51	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide	
76	IM14-2Me BF4	1.01	-5.58	0.95	1.99	-0.19	1.67	-0.06	-0.33	-3.83	418	0.81	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	
77	IM14-2Me CF3SO3	1.01	-5.58	0.95	1.99	-0.19	1.41	-0.86	0.07	-2.60	437	0.60	1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate	
78	IM16-2Me BF4	-2.67	-6.14	4.17	-0.99	0.57	1.67	-0.06	-0.33	-3.83	482	1.41	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	
79	IM16-2Me (CF3SO2)2N	-2.67	-6.14	4.17	-0.99	0.57	-1.19	-2.15	2.86	2.10	686 ^a	634	1.21	1-hexyl-2,3-dimethylimidazolium bis(trifluoromethylsulphonyl)imide
80	IM12OH-2Me Cl	9.21	2.25	3.25	-4.16	2.37	-0.57	-5.73	-2.31	-1.25	71	2.31	1-(2-hydroxyethyl)-2,3-dimethylimidazolium chloride	
81	IM11 (CF3SO2)2N	4.18	-6.87	0.65	1.98	-1.80	-1.19	-2.15	2.86	2.10	454	1.10	1,3-Dimethylimidazolium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide	
82	IM11 1OSO3	4.18	-6.87	0.65	1.98	-1.80	1.36	-1.16	-0.44	-1.31	319	0.52	1,3-dimethylimidazolium methylsulfate	
83	IM11 4MePhSO3	4.18	-6.87	0.65	1.98	-1.80	-1.66	-1.59	2.48	3.83	473	1.26	1,3-dimethylimidazolium 4-methylbenzenesulfonate	
84	IM11 N(CN)2	4.18	-6.87	0.65	1.98	-1.80	-2.48	0.49	0.00	0.73	363	1.04	1,3-dimethylimidazolium N-cyanocyanamide	
85	IM11(COO1)(Ph-(3,4- OCH2O-)) Cl	2.18	6.00	3.93	-0.16	-6.28	-0.57	-5.73	-2.31	-1.25	8	4.19	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3- methylimidazolium chloride	
86	IM11(COO4)(Ph-(3,4- OCH2O-)) Br	0.12	7.31	1.19	2.24	-4.78	-0.52	-5.52	-2.16	-1.13	144	4.03	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide	
87	IM12 (C2F5)3PF3	3.24	-6.75	0.93	1.70	-1.60	2.83	3.03	4.77	-1.46	591	0.93	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	
88	IM12 (C2F5)2PO2	3.24	-6.75	0.93	1.70	-1.60	1.54	0.08	2.75	-1.62	466	0.65	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	
89	IM12 C(CN)3	3.24	-6.75	0.93	1.70	-1.60	-13.16	6.89	-1.96	-0.13	324	3.30	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile	
90	IM12 B(CN)4	3.24	-6.75	0.93	1.70	-1.60	-10.53	7.57	-0.53	-2.02	373	2.95	1-Ethyl-3-methylimidazolium tetracyanoborate	
91	IM12 N(CN)2	3.24	-6.75	0.93	1.70	-1.60	-2.48	0.49	0.00	0.73	314.6 ^b	386	0.96	1-Ethyl-3-methylimidazolium N-cyanocyanamide
92	IM12 (CF3SO2)2N	3.24	-6.75	0.93	1.70	-1.60	-1.19	-2.15	2.86	2.10	506.5 ^a	477	1.00	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
93	IM12 Cl	3.24	-6.75	0.93	1.70	-1.60	-0.57	-5.73	-2.31	-1.25	235 ^b	197	0.73	1-Ethyl-3-methylimidazolium chloride
94	IM12 2OSO3	3.24	-6.75	0.93	1.70	-1.60	1.13	-1.47	-0.18	-0.39	382.8 ^a	358	0.43	1-Ethyl-3-methylimidazolium ethyl sulfate
95	IM12 (OOCOO)2B	3.24	-6.75	0.93	1.70	-1.60	4.60	5.52	0.02	-0.26	494	1.10	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate	
96	IM12 1COO	3.24	-6.75	0.93	1.70	-1.60	4.20	2.41	-5.87	3.73	321.9 ^b	304	1.54	1-Ethyl-3-methylimidazolium acetate
97	IM12 1O2O2OSO3	3.24	-6.75	0.93	1.70	-1.60	1.54	0.57	3.67	1.93	561	0.84	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	
98	IM12 1OSO3	3.24	-6.75	0.93	1.70	-1.60	1.36	-1.16	-0.44	-1.31	331 ^b	342	0.37	1-Ethyl-3-methylimidazolium methylsulfate
99	IM12 1SO3	3.24	-6.75	0.93	1.70	-1.60	1.32	-1.45	-0.86	-1.35	345.5 ^b	322	0.35	1-Ethyl-3-methylimidazolium methanesulfonate
100	IM12 4MePhSO3	3.24	-6.75	0.93	1.70	-1.60	-1.66	-1.59	2.48	3.83	496	1.15	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	

101	IM12 8OSO3	3.24	-6.75	0.93	1.70	-1.60	-1.48	-1.82	3.86	4.62		553	1.30	1-Ethyl-3-methylimidazolium octylsulfate
102	IM12 BF4	3.24	-6.75	0.93	1.70	-1.60	1.67	-0.06	-0.33	-3.83	308.1 ^a	324	0.60	1-Ethyl-3-methylimidazolium tetrafluoroborate
103	IM12 CF3COO	3.24	-6.75	0.93	1.70	-1.60	3.18	2.08	-2.30	-0.22	316.5 ^b	354	0.74	1-Ethyl-3-methylimidazolium trifluoroacetate
104	IM12 CF3SO3	3.24	-6.75	0.93	1.70	-1.60	1.41	-0.86	0.07	-2.60	363 ^a	344	0.47	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate
105	IM12 HSO4	3.24	-6.75	0.93	1.70	-1.60	2.60	1.36	-1.42	-2.11	295.5 ^b	341	0.55	1-Ethyl-3-methylimidazolium hydrogen sulfate
106	IM12 PF6	3.24	-6.75	0.93	1.70	-1.60	1.13	-1.14	-0.21	-3.53		313	0.54	1-Ethyl-3-methylimidazolium hexafluorophosphate
107	IM12 SCN	3.24	-6.75	0.93	1.70	-1.60	0.65	-2.07	-3.10	1.46	281.4 ^b	274	0.67	1-Ethyl-3-methylimidazolium thiocyanate
108	IM12 Br	3.24	-6.75	0.93	1.70	-1.60	-0.52	-5.52	-2.16	-1.13	207.5 ^b	208	0.71	1-Ethyl-3-methylimidazolium bromide
109	IM12 NO3	3.24	-6.75	0.93	1.70	-1.60	-6.94	-0.46	-2.37	-1.73		221	1.56	1-Ethyl-3-methylimidazolium nitrate
110	[C2MIM][FeCl4] 1.51	3.24	-6.75	0.93	1.70	-1.60	-4.01	-4.57	-0.46	0.67		284	1.08	1-ethyl-3-methylimidazolium tetrachloroferrate
111	IM11CN Cl	5.65	-3.19	5.25	-4.99	-2.61	-0.57	-5.73	-2.31	-1.25		5	2.05	1-(Cyanomethyl)-3-methylimidazolium chloride
112	IM11CN (CF3SO2)2N	5.65	-3.19	5.25	-4.99	-2.61	-1.19	-2.15	2.86	2.10		284	2.45	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
113	IM11CONMeBu Br	2.43	1.73	1.93	0.17	-1.17	-0.52	-5.52	-2.16	-1.13		190	1.79	1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium bromide
114	IM11CONEt2 Br	3.60	1.16	2.52	-0.30	-1.47	-0.52	-5.52	-2.16	-1.13		149	1.75	1-[2-(Diethylamino)-2-oxoethyl]-3-methylimidazolium bromide
115	IM11CONHBu Br	2.91	2.71	3.36	-1.67	-1.72	-0.52	-5.52	-2.16	-1.13		133	2.26	1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium bromide
116	IM11COO1 Br	7.61	2.40	0.08	1.03	-2.04	-0.52	-5.52	-2.16	-1.13		58	2.17	1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium bromide
117	IM11COO1(COO4)(Ph-(3,4-OCH2O-)) Br	-1.26	12.75	4.21	0.45	-9.43	-0.52	-5.52	-2.16	-1.13		-12	6.63	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide
118	IM11COO2 BF4	6.71	2.81	-0.50	1.76	-1.59	1.67	-0.06	-0.33	-3.83		219	2.68	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate
119	IM11COO2 Br	6.71	2.81	-0.50	1.76	-1.59	-0.52	-5.52	-2.16	-1.13		102	2.19	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium bromide
120	IM11COO3 (CF3SO2)2N	4.93	1.96	-0.19	1.96	-2.50	-1.19	-2.15	2.86	2.10		389	2.40	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
121	IM11COO3 8OSO3	4.93	1.96	-0.19	1.96	-2.50	-1.48	-1.82	3.86	4.62		466	2.52	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate
122	IM11COO3 BF4	4.93	1.96	-0.19	1.96	-2.50	1.67	-0.06	-0.33	-3.83		237	2.58	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium tetrafluoroborate
123	IM11COO3 Br	4.93	1.96	-0.19	1.96	-2.50	-0.52	-5.52	-2.16	-1.13		120	2.20	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide
124	IM11COO3 N(CN)2	4.93	1.96	-0.19	1.96	-2.50	-2.48	0.49	0.00	0.73		299	2.41	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium N-cyanocyanamide
125	IM11COO3 PF6	4.93	1.96	-0.19	1.96	-2.50	1.13	-1.14	-0.21	-3.53		226	2.49	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium hexafluorophosphate
126	IM11COO4 (CF3SO2)2N	4.15	3.03	-0.57	1.95	-1.69	-1.19	-2.15	2.86	2.10		429	2.39	3-(2-Butoxy-2-oxoethyl)-1-methylimidazolium N-[(trifluoromethyl)sulfonyl]methanesulfonamide

127	IM11COO4 8OSO3	4.15	3.03	-0.57	1.95	-1.69	-1.48	-1.82	3.86	4.62	506	2.48	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium octylsulfate	
128	IM11COO4 BF4	4.15	3.03	-0.57	1.95	-1.69	1.67	-0.06	-0.33	-3.83	277	2.69	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	
129	IM11COO4 Br	4.15	3.03	-0.57	1.95	-1.69	-0.52	-5.52	-2.16	-1.13	160	2.24	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium bromide	
130	IM11COO4 N(CN)2	4.15	3.03	-0.57	1.95	-1.69	-2.48	0.49	0.00	0.73	338	2.44	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium N-cyanocyanamide	
131	IM11COO4 PF6	4.15	3.03	-0.57	1.95	-1.69	1.13	-1.14	-0.21	-3.53	266	2.59	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium hexafluorophosphate	
132	IM11COO5 8OSO3	2.15	2.70	-0.08	2.28	-2.61	-1.48	-1.82	3.86	4.62	528	2.61	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	
133	IM11COO5 Br	2.15	2.70	-0.08	2.28	-2.61	-0.52	-5.52	-2.16	-1.13	182	2.40	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	
134	IM11COO6 Br	1.62	2.95	-0.77	2.59	-2.31	-0.52	-5.52	-2.16	-1.13	209	2.42	1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium bromide	
135	IM11COO8 Br	-1.30	2.89	0.41	1.89	-1.69	-0.52	-5.52	-2.16	-1.13	283	2.25	1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazolium bromide	
136	IM1i4 (CF3SO2)2N	1.42	-5.98	0.77	1.78	-0.34	-1.19	-2.15	2.86	2.10	556	0.58	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
137	IM1gly Cl	12.59	9.92	2.10	-6.03	2.96	-0.57	-5.73	-2.31	-1.25	-34	3.88	1-methyl-3-glycerylymidazolium chloride	
138	IM1gly N(CN)2	12.59	9.92	2.10	-6.03	2.96	-2.48	0.49	0.00	0.73	155	4.17	1-methyl-3-glycerylimidazolium dicyanamide	
139	IM1gly (CF3SO2)2N	12.59	9.92	2.10	-6.03	2.96	-1.19	-2.15	2.86	2.10	245	4.12	1-methyl-3-glycerylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
140	IM1-2=1 Cl	1.49	-6.89	2.60	0.50	-0.78	-0.57	-5.73	-2.31	-1.25	243	0.73	1-Methyl-3-(2-propenyl)imidazolium chloride	
141	IM1-(1Ph-4Me) BF4	-1.72	-6.38	3.34	-0.01	-1.50	1.67	-0.06	-0.33	-3.83	413	0.90	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	
142	IM1-(1Ph-4Me) Cl	-1.72	-6.38	3.34	-0.01	-1.50	-0.57	-5.73	-2.31	-1.25	286	1.07	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	
143	IM1-(1Ph-4Me) PF6	-1.72	-6.38	3.34	-0.01	-1.50	1.13	-1.14	-0.21	-3.53	402	0.88	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	
144	IM1-1Ph BF4	-0.98	-6.53	3.48	-0.20	-1.45	1.67	-0.06	-0.33	-3.83	395	0.88	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	
145	IM1-3Ph Cl	-0.98	-6.53	3.48	-0.20	-1.45	-0.57	-5.73	-2.31	-1.25	268	1.03	1-Methyl-3-(phenylmethyl)imidazolium chloride	
146	IM1-1Ph PF6	-0.98	-6.53	3.48	-0.20	-1.45	1.13	-1.14	-0.21	-3.53	384	0.86	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	
147	IM13 BF4	1.85	-6.45	1.37	1.24	-0.80	1.67	-0.06	-0.33	-3.83	373	0.60	1-Methyl-3-propylimidazolium tetrafluoroborate	
148	IM13 (CF3SO2)2N	1.85	-6.45	1.37	1.24	-0.80	-1.19	-2.15	2.86	2.10	535 ^b	525	0.73	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
149	IM13 PF6	1.85	-6.45	1.37	1.24	-0.80	1.13	-1.14	-0.21	-3.53	362	0.51	1-Methyl-3-propylimidazolium hexafluorophosphate	
150	IM13 Br	1.85	-6.45	1.37	1.24	-0.80	-0.52	-5.52	-2.16	-1.13	281 ^b	256	0.58	1-Methyl-3-propylimidazolium bromide
151	IM13 Cl	1.85	-6.45	1.37	1.24	-0.80	-0.57	-5.73	-2.31	-1.25	246	0.59	1-Methyl-3-propylimidazolium chloride	
152	IM13 I	1.85	-6.45	1.37	1.24	-0.80	-0.65	-5.31	-1.63	-1.12	277	0.55	1-Methyl-3-propylimidazolium iodide	

153	IM1-2CO-1 Br	5.91	1.45	2.73	-1.85	0.18	-0.52	-5.52	-2.16	-1.13	124	1.71	1-Methyl-3-(3-oxobutyl)imidazolium bromide	
154	IM1-2C6F13 PF6	1.89	7.73	-2.78	3.01	0.18	1.13	-1.14	-0.21	-3.53	379	3.54	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate	
155	IM12(2Pin-1R) Cl	-3.71	-4.44	1.54	1.20	1.21	-0.57	-5.73	-2.31	-1.25	427	1.05	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium chloride	
156	IM12(2Pin-1R) NO3	-3.71	-4.44	1.54	1.20	1.21	-6.94	-0.46	-2.37	-1.73	451	1.48	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium nitrate	
157	IM1-2Ph BF4	-3.43	-6.10	4.96	-1.28	0.61	1.67	-0.06	-0.33	-3.83	494	1.59	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate	
158	IM1-2Ph Cl	-3.43	-6.10	4.96	-1.28	0.61	-0.57	-5.73	-2.31	-1.25	367	1.55	1-Methyl-3-(2-phenylethyl)imidazolium chloride	
159	IM1-2Ph PF6	-3.43	-6.10	4.96	-1.28	0.61	1.13	-1.14	-0.21	-3.53	483	1.54	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	
160	IM14 8OSO3	0.58	-5.91	1.21	1.20	-0.39	-1.48	-1.82	3.86	4.62	635 ^a	642	0.90	1-Butyl-3-methylimidazolium octylsulfate
161	IM14 CF3SO3	0.58	-5.91	1.21	1.20	-0.39	1.41	-0.86	0.07	-2.60	427.7 ^a	432	0.50	1-Butyl-3-methylimidazolium trifluoromethanesulfonate
162	IM14 (CF3)2N	0.58	-5.91	1.21	1.20	-0.39	1.11	-1.38	-0.04	-2.50	420	0.45	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminat	
163	IM14 BF4	0.58	-5.91	1.21	1.20	-0.39	1.67	-0.06	-0.33	-3.83	367.1 ^a	413	0.73	1-Butyl-3-methylimidazolium tetrafluoroborate
164	IM14 (CF3SO2)2N	0.58	-5.91	1.21	1.20	-0.39	-1.19	-2.15	2.86	2.10	565.1 ^a	565	0.54	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
165	IM14 PF6	0.58	-5.91	1.21	1.20	-0.39	1.13	-1.14	-0.21	-3.53	408.7 ^a	402	0.63	1-Butyl-3-methylimidazolium hexafluorophosphate
166	IM14 Cl	0.58	-5.91	1.21	1.20	-0.39	-0.57	-5.73	-2.31	-1.25	317 ^a	286	0.62	1-Butyl-3-methylimidazolium chloride
167	IM14 I	0.58	-5.91	1.21	1.20	-0.39	-0.65	-5.31	-1.63	-1.12	314 ^a	317	0.55	1-Butyl-3-methylimidazolium iodide
168	IM14 Br	0.58	-5.91	1.21	1.20	-0.39	-0.52	-5.52	-2.16	-1.13	311.4 ^a	296	0.58	1-Butyl-3-methylimidazolium bromide
169	IM14 N(CN)2	0.58	-5.91	1.21	1.20	-0.39	-2.48	0.49	0.00	0.73	375.7 ^a	475	0.67	1-Butyl-3-methylimidazolium N-cyanocyanamide
170	IM14 4MePhSO3	0.58	-5.91	1.21	1.20	-0.39	-1.66	-1.59	2.48	3.83	412.7 ^b	584	0.75	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate
171	IM14 1SO3	0.58	-5.91	1.21	1.20	-0.39	1.32	-1.45	-0.86	-1.35	410	0.33	1-Butyl-3-methylimidazolium methanesulfonate	
172	IM14 (2-SO2PhCO)N	0.58	-5.91	1.21	1.20	-0.39	-0.91	-0.17	1.38	3.13	561	0.60	1-Butyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	
173	IM14 (C2F5)3PF3	0.58	-5.91	1.21	1.20	-0.39	2.83	3.03	4.77	-1.46	680	0.84	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	
174	IM14 1O2O2OSO3	0.58	-5.91	1.21	1.20	-0.39	1.54	0.57	3.67	1.93	643 ^a	649	0.52	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate
175	IM14 1OSO3	0.58	-5.91	1.21	1.20	-0.39	1.36	-1.16	-0.44	-1.31	416 ^a	430	0.33	1-Butyl-3-methylimidazolium methyl sulfate
176	IM14 AC	0.58	-5.91	1.21	1.20	-0.39	0.38	-0.22	0.92	2.67	546	0.49	3-Butyl-1-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	
177	IM14 Co(CO)4	0.58	-5.91	1.21	1.20	-0.39	-0.43	-2.12	-1.00	3.57	460	0.69	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate	
178	IM14 FeCl4	0.58	-5.91	1.21	1.20	-0.39	-4.01	-4.57	-0.46	0.67	415 ^a	373	0.76	1-Butyl-3-methylimidazolium tetrachloroferrate

179	IM14 HSO4	0.58	-5.91	1.21	1.20	-0.39	2.60	1.36	-1.42	-2.11		429	0.72	1-Butyl-3-methylimidazolium hydrogen sulfate
180	IM14 NO3	0.58	-5.91	1.21	1.20	-0.39	-6.94	-0.46	-2.37	-1.73	353.5 ^a	309	1.43	1-Butyl-3-methylimidazolium nitrate
181	IM14 SbF6	0.58	-5.91	1.21	1.20	-0.39	1.35	-0.70	-0.12	-3.68		411	0.66	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate
182	IM14 SCN	0.58	-5.91	1.21	1.20	-0.39	0.65	-2.07	-3.10	1.46	385 ^b	363	0.59	1-Butyl-3-methylimidazolium thiocyanate
183	IM14 (10)2PO2	0.58	-5.91	1.21	1.20	-0.39	1.30	-1.22	0.20	-0.78		459	0.26	1-butyl-3-methylimidazolium dimethyl phosphate
184	IM14 C(CN)3	0.58	-5.91	1.21	1.20	-0.39	-13.16	6.89	-1.96	-0.13		413	3.15	1-butyl-3-methylimidazolium tricyanomethanide
185	IM14 CF3COO	0.58	-5.91	1.21	1.20	-0.39	3.18	2.08	-2.30	-0.22	408.2 ^a	443	0.89	1-Butyl-3-Methylimidazolium trifluoroacetate
186	IM13COOH Cl	10.77	5.41	3.56	-2.44	0.51	-0.57	-5.73	-2.31	-1.25		-12	2.74	3-(3-Carboxypropyl)-1-methylimidazolium chloride
187	IM15 (CF3SO2)2N	-0.64	-5.56	1.33	1.08	0.30	-1.19	-2.15	2.86	2.10	596 ^b	611	0.39	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
188	IM15 BF4	-0.64	-5.56	1.33	1.08	0.30	1.67	-0.06	-0.33	-3.83		459	0.91	1-Methyl-3-pentylimidazolium tetrafluoroborate
189	IM15 Cl	-0.64	-5.56	1.33	1.08	0.30	-0.57	-5.73	-2.31	-1.25		332	0.72	1-Methyl-3-pentylimidazolium chloride
190	IM15 PF6	-0.64	-5.56	1.33	1.08	0.30	1.13	-1.14	-0.21	-3.53		448	0.80	1-Methyl-3-pentylimidazolium hexafluorophosphate
191	IM16 (CF3SO2)2N	-1.54	-5.78	1.66	0.51	-0.75	-1.19	-2.15	2.86	2.10	631.6 ^a	593	0.64	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
192	IM16 Br	-1.54	-5.78	1.66	0.51	-0.75	-0.52	-5.52	-2.16	-1.13	344 ^a	324	0.77	1-Hexyl-3-methylimidazolium bromide
193	IM16 Cl	-1.54	-5.78	1.66	0.51	-0.75	-0.57	-5.73	-2.31	-1.25	381 ^b	314	0.80	1-Hexyl-3-methylimidazolium chloride
194	IM16 PF6	-1.54	-5.78	1.66	0.51	-0.75	1.13	-1.14	-0.21	-3.53	424 ^b	430	0.73	1-Hexyl-3-methylimidazolium hexafluorophosphate
195	IM16 (2-SO2PhCO)N	-1.54	-5.78	1.66	0.51	-0.75	-0.91	-0.17	1.38	3.13		589	0.67	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
196	IM16 BF4	-1.54	-5.78	1.66	0.51	-0.75	1.67	-0.06	-0.33	-3.83	429.8 ^a	441	0.80	1-Hexyl-3-methylimidazolium tetrafluoroborate
197	IM16 (C2F5)3PF3	-1.54	-5.78	1.66	0.51	-0.75	2.83	3.03	4.77	-1.46	730 ^b	708	0.83	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate
198	IM16 (C3F7)3PF3	-1.54	-5.78	1.66	0.51	-0.75	4.00	5.68	6.72	-0.31		840	1.08	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate
199	IM16 (CF3SO2)3C	-1.54	-5.78	1.66	0.51	-0.75	-0.58	-1.39	3.93	0.50		621	0.57	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide
200	IM16 N(CN)2	-1.54	-5.78	1.66	0.51	-0.75	-2.48	0.49	0.00	0.73	534 ^b	503	0.77	1-hexyl-3-methylimidazolium dicyanamide
201	IM16 NO	-1.54	-5.78	1.66	0.51	-0.75	-6.94	-0.46	-2.37	-1.73		337	1.49	1-hexyl-3-methylimidazolium nitrate
202	IM16 SbF6	-1.54	-5.78	1.66	0.51	-0.75	1.35	-0.70	-0.12	-3.68		439	0.74	1-hexyl-3-methylimidazolium hexafluoroantimonate
203	IM17 (CF3SO2)2N	-2.66	-4.82	0.99	1.12	0.77	-1.19	-2.15	2.86	2.10		671	0.24	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
204	IM17 BF4	-2.66	-4.82	0.99	1.12	0.77	1.67	-0.06	-0.33	-3.83		519	1.12	1-Heptyl-3-methylimidazolium tetrafluoroborate

205	IM17 Cl	-2.66	-4.82	0.99	1.12	0.77	-0.57	-5.73	-2.31	-1.25		392	0.89	1-Heptyl-3-methylimidazolium chloride
206	IM17 PF6	-2.66	-4.82	0.99	1.12	0.77	1.13	-1.14	-0.21	-3.53		508	1.01	1-Heptyl-3-methylimidazolium hexafluorophosphate
207	IM18 BF4	-3.07	-4.67	0.46	1.44	0.28	1.67	-0.06	-0.33	-3.83	497.8 ^a	519	1.09	1-Methyl-3-octylimidazolium tetrafluoroborate
208	IM18 Br	-3.07	-4.67	0.46	1.44	0.28	-0.52	-5.52	-2.16	-1.13	392 ^a	402	0.88	1-Methyl-3-octylimidazolium bromide
209	IM18 (CF3SO2)2N	-3.07	-4.67	0.46	1.44	0.28	-1.19	-2.15	2.86	2.10	692.7 ^a	671	0.23	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
210	IM18 8OSO3	-3.07	-4.67	0.46	1.44	0.28	-1.48	-1.82	3.86	4.62		748	0.53	3-Methyl-1-octylimidazolium octylsulfate
211	IM18 CF3SO3	-3.07	-4.67	0.46	1.44	0.28	1.41	-0.86	0.07	-2.60		538	0.86	1-Methyl-3-octylimidazolium trifluoromethanesulfonate
212	IM18 Cl	-3.07	-4.67	0.46	1.44	0.28	-0.57	-5.73	-2.31	-1.25		392	0.89	1-Methyl-3-octylimidazolium chloride
213	IM18 PF6	-3.07	-4.67	0.46	1.44	0.28	1.13	-1.14	-0.21	-3.53	851 ^a	508	0.97	1-Methyl-3-octylimidazolium hexafluorophosphate
214	IM17COOH Br	6.03	5.48	3.42	-1.70	1.31	-0.52	-5.52	-2.16	-1.13		141	2.55	1-(7-Carboxyheptyl)-3-methylimidazolium bromide
215	IM19 BF4	-4.95	-4.26	1.20	0.99	1.25	1.67	-0.06	-0.33	-3.83		582	1.36	1-Methyl-3-nonylimidazolium tetrafluoroborate
216	IM19 Cl	-4.95	-4.26	1.20	0.99	1.25	-0.57	-5.73	-2.31	-1.25		455	1.15	1-Methyl-3-nonylimidazolium chloride
217	IM19 PF6	-4.95	-4.26	1.20	0.99	1.25	1.13	-1.14	-0.21	-3.53		571	1.26	1-Methyl-3-nonylimidazolium hexafluorophosphate
218	IM1-10 BF4	-5.83	-4.13	1.06	0.96	1.33	1.67	-0.06	-0.33	-3.83		605	1.43	1-Decyl-3-methylimidazolium tetrafluoroborate
219	IM1-10 Br	-5.83	-4.13	1.06	0.96	1.33	-0.52	-5.52	-2.16	-1.13		488	1.20	1-Decyl-3-methylimidazolium bromide
220	IM1-10 Cl	-5.83	-4.13	1.06	0.96	1.33	-0.57	-5.73	-2.31	-1.25		477	1.23	1-Decyl-3-methylimidazolium chloride
221	IM1-10 PF6	-5.83	-4.13	1.06	0.96	1.33	1.13	-1.14	-0.21	-3.53		594	1.34	1-Decyl-3-methylimidazolium hexafluorophosphate
222	IM1-10 (CF3SO2)2N	-5.83	-4.13	1.06	0.96	1.33	-1.19	-2.15	2.86	2.10	754 ^b	757	0.53	1-decyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
223	IM1-10 FeCl4	-5.83	-4.13	1.06	0.96	1.33	-4.01	-4.57	-0.46	0.67		565	0.90	1-decyl-3-methylimidazolium tetrachloroferrate
224	IM1-10COO2 Br	-4.00	4.03	0.76	-0.19	0.44	-0.52	-5.52	-2.16	-1.13		380	2.20	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide
225	IM1-12 Br	-7.55	-3.29	0.51	1.23	1.51	-0.52	-5.52	-2.16	-1.13		536	1.38	1-Dodecyl-3-methylimidazolium bromide
226	1201IMCL	-7.55	-3.29	0.51	1.23	1.51	-0.57	-5.73	-2.31	-1.25		525	1.41	1-dodecyl-3-methylimidazolium chloride
227	IM1-14 Cl	-9.86	-2.51	0.38	1.23	2.54	-0.57	-5.73	-2.31	-1.25		607	1.76	1-Methyl-3-tetradecylimidazolium chloride
228	IM1-14 Br	-9.86	-2.51	0.38	1.23	2.54	-0.52	-5.52	-2.16	-1.13		618	1.73	1-Methyl-3-tetradecylimidazolium bromide
229	IM1-16 Cl	-11.34	-2.14	0.02	1.34	2.01	-0.57	-5.73	-2.31	-1.25		627	1.84	1-Hexadecyl-3-methylimidazolium chloride
230	IM1-16 Br	-11.34	-2.14	0.02	1.34	2.01	-0.52	-5.52	-2.16	-1.13		638	1.82	1-Hexadecyl-3-methylimidazolium bromide

231	IM1-18 Cl	-13.76	-1.31	-0.02	1.21	2.84	-0.57	-5.73	-2.31	-1.25	704	2.18	1-Methyl-3-octadecylimidazolium chloride
232	IM18OH Br	2.36	3.73	-0.11	-1.86	3.95	-0.52	-5.52	-2.16	-1.13	321	2.19	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide
233	IM14OH Cl	6.92	2.34	1.31	-2.68	2.61	-0.57	-5.73	-2.31	-1.25	154	1.99	1-(4-Hydroxybutyl)-3-methylimidazolium chloride
234	IM13OH Cl	8.05	2.08	2.12	-3.44	2.47	-0.57	-5.73	-2.31	-1.25	113	2.09	1-(3-Hydroxypropyl)-3-methylimidazolium chloride
235	IM13OH (CF3SO2)2N	8.05	2.08	2.12	-3.44	2.47	-1.19	-2.15	2.86	2.10	393	2.31	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
236	IM13O1 (CF3SO2)2N	4.71	-1.38	0.08	0.80	0.67	-1.19	-2.15	2.86	2.10	485	1.09	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
237	IM13O1 Cl	4.71	-1.38	0.08	0.80	0.67	-0.57	-5.73	-2.31	-1.25	205	0.92	1-(3-Methoxypropyl)-3-methylimidazolium chloride
238	IM12OH I	9.73	2.71	2.15	-3.96	2.49	-0.65	-5.31	-1.63	-1.12	98	2.34	1-(2-Hydroxyethyl)-3-methylimidazolium iodide
239	IM12OH (2-SO2PhCO)N	9.73	2.71	2.15	-3.96	2.49	-0.91	-0.17	1.38	3.13	342	2.70	1-(2-Hydroxyethyl)-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
240	IM12OH (CF3SO2)2N	9.73	2.71	2.15	-3.96	2.49	-1.19	-2.15	2.86	2.10	346	2.57	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
241	IM12OH AC	9.73	2.71	2.15	-3.96	2.49	0.38	-0.22	0.92	2.67	327	2.79	1-(2-Hydroxyethyl)-3-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
242	IM12OH BF4	9.73	2.71	2.15	-3.96	2.49	1.67	-0.06	-0.33	-3.83	194	3.03	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate
243	IM12OH PF6	9.73	2.71	2.15	-3.96	2.49	1.13	-1.14	-0.21	-3.53	183	2.89	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate
244	IM12OH Cl	9.73	2.71	2.15	-3.96	2.49	-0.57	-5.73	-2.31	-1.25	67	2.32	1-(2-hydroxyethyl)-3-methylimidazolium chloride
245	IM12O1 (CF3SO2)2N	6.12	-1.79	1.00	-0.25	-0.03	-1.19	-2.15	2.86	2.10	417	1.25	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
246	IM12O1 Cl	6.12	-1.79	1.00	-0.25	-0.03	-0.57	-5.73	-2.31	-1.25	138	0.88	1-(2-Methoxyethyl)-3-methylimidazolium chloride
247	IM12O1 BF4	6.12	-1.79	1.00	-0.25	-0.03	1.67	-0.06	-0.33	-3.83	265	1.57	1-(2-Methoxyethyl)-3-methylimidazolium tetrafluoroborate
248	IM12O1 N(CN)2	6.12	-1.79	1.00	-0.25	-0.03	-2.48	0.49	0.00	0.73	327	1.30	1-(2-Methoxyethyl)-3-methylimidazolium dicyanamide
249	IM12O2 (CF3SO2)2N	4.04	-2.03	1.37	0.09	0.45	-1.19	-2.15	2.86	2.10	484	1.00	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
250	IM12O2 Br	4.04	-2.03	1.37	0.09	0.45	-0.52	-5.52	-2.16	-1.13	215	0.78	1-(2-Ethoxyethyl)-3-methylimidazolium bromide
251	IM12O2 Cl	4.04	-2.03	1.37	0.09	0.45	-0.57	-5.73	-2.31	-1.25	204	0.77	1-(2-Ethoxyethyl)-3-methylimidazolium chloride
252	IM12O2O1 Cl	5.30	1.60	0.58	1.08	0.99	-0.57	-5.73	-2.31	-1.25	194	1.53	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride
253	IM11O2 (CF3SO2)2N	5.01	-1.83	-0.67	1.85	0.11	-1.19	-2.15	2.86	2.10	478	1.15	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
254	IM11O2 Cl	5.01	-1.83	-0.67	1.85	0.11	-0.57	-5.73	-2.31	-1.25	199	0.98	1-(Ethoxymethyl)-3-methylimidazolium chloride
255	Py1O(Cdd)-3CONH2 Cl	-1.11	8.51	2.67	-2.27	-1.31	-0.57	-5.73	-2.31	-1.25	204	3.52	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride
256	Py1O-10-3CONH2 Cl	-1.45	8.05	2.07	-2.56	-0.26	-0.57	-5.73	-2.31	-1.25	243	3.24	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride

257	Py10-10-3CONH2 FeCl4	-1.45	8.05	2.07	-2.56	-0.26	-4.01	-4.57	-0.46	0.67	330	3.00	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate
258	Py10-11-3CONH2 Cl	-3.36	8.53	2.80	-2.69	-0.26	-0.57	-5.73	-2.31	-1.25	282	3.44	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride
259	Py10-12-3CONH2 1COO	-3.72	9.72	2.10	-2.74	0.54	4.20	2.41	-5.87	3.73	419	4.46	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate
260	Py10-12-3CONH2 BF4	-3.72	9.72	2.10	-2.74	0.54	1.67	-0.06	-0.33	-3.83	439	4.11	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate
261	Py10-12-3CONH2 Br	-3.72	9.72	2.10	-2.74	0.54	-0.52	-5.52	-2.16	-1.13	322	3.58	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide
262	Py10-12-3CONH2 Cl	-3.72	9.72	2.10	-2.74	0.54	-0.57	-5.73	-2.31	-1.25	312	3.57	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride
263	Py10-12-3CONH2 ClO4	-3.72	9.72	2.10	-2.74	0.54	2.67	3.01	-0.12	-1.50	535	4.26	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate
264	Py10-12-3CONH2 I	-3.72	9.72	2.10	-2.74	0.54	-0.65	-5.31	-1.63	-1.12	343	3.57	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide
265	Py10-12-3CONH2 NO3	-3.72	9.72	2.10	-2.74	0.54	-6.94	-0.46	-2.37	-1.73	336	3.54	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate
266	Py4-3CONHBu 8OSO3	-0.50	1.56	3.74	-1.41	-2.27	-1.48	-1.82	3.86	4.62	546	2.47	1-Butyl-3-[(butylamino)carbonyl]pyridinium octyl sulfate
267	Py4-3CONHBu I	-0.50	1.56	3.74	-1.41	-2.27	-0.65	-5.31	-1.63	-1.12	222	2.23	1-Butyl-3-[(butylamino)carbonyl]pyridinium iodide
268	Py107-3CONH(MeO- MeO-Hp) Cl	-8.10	11.70	3.19	0.15	-1.79	-0.57	-5.73	-2.31	-1.25	368	4.52	3-[[[(Heptyloxy)methoxy)methyl]amino]carbonyl]-1-[[heptyloxy)methyl]pyridinium chloride
269	Py108-3CONH(MeO- MeO-Oc) Cl	-9.18	13.37	1.88	0.56	-3.29	-0.57	-5.73	-2.31	-1.25	352	5.21	3-[[[(Octyloxy)methoxy)methyl]amino]carbonyl]-1-[[octyloxy)methyl]pyridinium chloride
270	Py109-3CONH(MeO- MeO-No) Cl	-11.41	14.87	2.97	0.32	-6.01	-0.57	-5.73	-2.31	-1.25	311	6.34	3-[[[(Nonyloxy)methoxy)methyl]amino]carbonyl]-1-[[nonyloxy)methyl]pyridinium chloride
271	Py10-10- 3CONH(MeO-MeO- De) Cl	-14.01	15.45	3.67	-0.31	-4.11	-0.57	-5.73	-2.31	-1.25	417	6.12	3-[[[(Decyloxy)methoxy)methyl]amino]carbonyl]-1-[[decyloxy)methyl]pyridinium chloride
272	Py1-3COOBu (CF3SO2)2N	2.74	1.39	1.45	0.46	-2.32	-1.19	-2.15	2.86	2.10	424	2.16	3-(Butoxycarbonyl)-1-methylpyridinium 1,1,1-trifluoro-N-[[trifluoromethyl]sulfonyl]methanesulfonamide
273	Py1-3COOBu 8OSO3	2.74	1.39	1.45	0.46	-2.32	-1.48	-1.82	3.86	4.62	500	2.28	3-(Butoxycarbonyl)-1-methylpyridinium octyl sulfate
274	Py1-3COOBu I	2.74	1.39	1.45	0.46	-2.32	-0.65	-5.31	-1.63	-1.12	175	1.97	3-(Butoxycarbonyl)-1-methylpyridinium iodide
275	Py1-3COOBu PF6	2.74	1.39	1.45	0.46	-2.32	1.13	-1.14	-0.21	-3.53	260	2.26	3-(Butoxycarbonyl)-1-methylpyridinium hexafluorophosphate
276	Py4-3COOBu 8OSO3	-0.63	1.72	1.77	0.78	-1.80	-1.48	-1.82	3.86	4.62	596	2.13	3-(Butoxycarbonyl)-1-butylpyridinium octyl sulfate
277	Py4-3COOBu I	-0.63	1.72	1.77	0.78	-1.80	-0.65	-5.31	-1.63	-1.12	271	1.98	3-(Butoxycarbonyl)-1-butylpyridinium iodide
278	Py4-3Me-4Me BF4	-1.83	-6.48	3.18	-0.01	-0.44	1.67	-0.06	-0.33	-3.83	448	0.94	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate
279	Py4-3Me-4Me Cl	-1.83	-6.48	3.18	-0.01	-0.44	-0.57	-5.73	-2.31	-1.25	321	1.01	1-Butyl-3,4-dimethylpyridinium chloride
280	Py4-3Me-5Me N(CN)2	-3.35	-6.65	3.68	-0.65	0.01	-2.48	0.49	0.00	0.73	550	1.19	1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide
281	Py4-3Me-5Me Br	-3.35	-6.65	3.68	-0.65	0.01	-0.52	-5.52	-2.16	-1.13	371	1.26	1-Butyl-3,5-dimethylpyridinium bromide

282	Py4-3Me-5Me BF4	-3.35	-6.65	3.68	-0.65	0.01	1.67	-0.06	-0.33	-3.83		488	1.23	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate
283	Py4-3Me-5Me Cl	-3.35	-6.65	3.68	-0.65	0.01	-0.57	-5.73	-2.31	-1.25		361	1.29	1-Butyl-3,5-dimethylpyridinium chloride
284	Py4-3Me-5Me (CF3SO2)2N	-3.35	-6.65	3.68	-0.65	0.01	-1.19	-2.15	2.86	2.10		640	1.09	1-butyl-3,5-dimethyl pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
285	Py8-3Me-5Me Br	-7.40	-4.91	2.82	-0.43	1.31	-0.52	-5.52	-2.16	-1.13		504	1.54	1-octyl-3,5-dimethylpyridinium bromide
286	Py8-3Me-5Me (CF3SO2)2N	-7.40	-4.91	2.82	-0.43	1.31	-1.19	-2.15	2.86	2.10		773	1.07	1-octyl-3,5-dimethylpyridinium bromide 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
287	Py3-3Me Br	0.18	-7.09	3.15	0.16	-0.85	-0.52	-5.52	-2.16	-1.13		277	0.88	3-Methyl-1-propylpyridinium bromide
288	Py3-3Me PF6	0.18	-7.09	3.15	0.16	-0.85	1.13	-1.14	-0.21	-3.53		382	0.72	3-Methyl-1-propylpyridinium hexafluorophosphate
289	Py4-3Me N(CN)2	-1.02	-6.72	3.14	0.02	-0.45	-2.48	0.49	0.00	0.73		492	0.96	1-Butyl-3-methylpyridinium N-cyanocyanamide
290	Py4-3Me Br	-1.02	-6.72	3.14	0.02	-0.45	-0.52	-5.52	-2.16	-1.13		313	0.94	1-Butyl-3-methylpyridinium bromide
291	Py4-3Me 8OSO3	-1.02	-6.72	3.14	0.02	-0.45	-1.48	-1.82	3.86	4.62		659	1.15	1-Butyl-3-methylpyridinium octyl sulfate
292	Py4-3Me BF4	-1.02	-6.72	3.14	0.02	-0.45	1.67	-0.06	-0.33	-3.83	388 ^a	430	0.91	1-Butyl-3-methylpyridinium tetrafluoroborate
293	Py4-3Me Cl	-1.02	-6.72	3.14	0.02	-0.45	-0.57	-5.73	-2.31	-1.25		303	0.96	1-Butyl-3-methylpyridinium chloride
294	Py4-3Me PF6	-1.02	-6.72	3.14	0.02	-0.45	1.13	-1.14	-0.21	-3.53		419	0.84	1-Butyl-3-methylpyridinium hexafluorophosphate
295	Py6-3Me Br	-3.03	-5.66	2.50	0.25	0.50	-0.52	-5.52	-2.16	-1.13	343 ^a	390	1.03	1-Hexyl-3-methylpyridinium bromide
296	Py6-3Me Cl	-3.03	-5.66	2.50	0.25	0.50	-0.57	-5.73	-2.31	-1.25		379	1.03	1-Hexyl-3-methylpyridinium chloride
297	Py8-3Me Br	-5.44	-5.13	2.92	-0.28	1.42	-0.52	-5.52	-2.16	-1.13		464	1.39	3-Methyl-1-octylpyridinium bromide
298	Py8-3Me Cl	-5.44	-5.13	2.92	-0.28	1.42	-0.57	-5.73	-2.31	-1.25		453	1.41	3-Methyl-1-octylpyridinium chloride
299	Py1O3-3OH (2-SO2PhCO)N	9.04	2.53	1.71	1.07	2.30	-0.91	-0.17	1.38	3.13		415	2.30	3-Hydroxy-1-(propoxymethyl)pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
300	Py1O3-3OH AC	9.04	2.53	1.71	1.07	2.30	0.38	-0.22	0.92	2.67		400	2.40	3-Hydroxy-1-(propoxymethyl)pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
301	Py1O3-3OH Cl	9.04	2.53	1.71	1.07	2.30	-0.57	-5.73	-2.31	-1.25		139	1.98	3-Hydroxy-1-(propoxymethyl)pyridinium chloride
302	Py1O4-3OH (2-SO2PhCO)N	7.76	2.79	1.60	1.11	2.48	-0.91	-0.17	1.38	3.13		450	2.25	1-(Butoxymethyl)-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
303	Py1O4-3OH AC	7.76	2.79	1.60	1.11	2.48	0.38	-0.22	0.92	2.67		435	2.36	1-(Butoxymethyl)-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
304	Py1O6-3OH (2-SO2PhCO)N	5.49	3.42	1.24	1.23	3.06	-0.91	-0.17	1.38	3.13		521	2.24	1-[(Hexyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
305	Py1O6-3OH AC	5.49	3.42	1.24	1.23	3.06	0.38	-0.22	0.92	2.67		506	2.37	1-[(Hexyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate
306	Py1O7-3OH (2-SO2PhCO)N	4.71	3.35	1.30	1.26	2.71	-0.91	-0.17	1.38	3.13		529	2.15	1-[(Heptyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide
307	Py1O7-3OH AC	4.71	3.35	1.30	1.26	2.71	0.38	-0.22	0.92	2.67		514	2.28	1-[(Heptyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate

308	Py1O7-3OH Cl	4.71	3.35	1.30	1.26	2.71	-0.57	-5.73	-2.31	-1.25	253	1.98	1-[(Heptyloxy)methyl]-3-hydroxypyridinium chloride	
309	Py1O-11-3OH (2-SO ₂ PhCO)N	-0.18	4.26	1.07	0.69	4.01	-0.91	-0.17	1.38	3.13	672	2.21	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	
310	Py1O-11-3OH AC	-0.18	4.26	1.07	0.69	4.01	0.38	-0.22	0.92	2.67	657	2.38	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	
311	Py1O-11-3OH Cl	-0.18	4.26	1.07	0.69	4.01	-0.57	-5.73	-2.31	-1.25	396	2.23	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium chloride	
312	Py1O-18-3OH (2-SO ₂ PhCO)N	-7.03	6.97	-0.02	0.65	4.92	-0.91	-0.17	1.38	3.13	852	2.70	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	
313	Py1O-18-3OH AC	-7.03	6.97	-0.02	0.65	4.92	0.38	-0.22	0.92	2.67	837	2.88	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	
314	Pyr24 2OSO ₃	1.25	-3.90	-3.89	5.76	0.08	1.13	-1.47	-0.18	-0.39	511	1.83	1-Butyl-1-ethylpyrrolidinium ethyl sulfate	
315	IMi022OH-2-(8=9)2OSO ₃	-12.25	6.23	-6.24	-8.83	3.20	1.13	-1.47	-0.18	-0.39	716	4.27	1-ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)imidazolium ethyl sulfate	
316	IM22 (CF ₃ SO ₂) ₂ N	2.03	-6.56	1.57	1.51	-0.99	-1.19	-2.15	2.86	2.10	518	0.77	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
317	IM22 Br	2.03	-6.56	1.57	1.51	-0.99	-0.52	-5.52	-2.16	-1.13	249	0.60	1,3-Diethylimidazolium bromide	
318	IM23 (CF ₃ SO ₂) ₂ N	1.10	-6.31	1.51	1.58	-0.99	-1.19	-2.15	2.86	2.10	540	0.70	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
319	IM23 Br	1.10	-6.31	1.51	1.58	-0.99	-0.52	-5.52	-2.16	-1.13	271	0.62	1-Ethyl-3-propylimidazolium bromide	
320	IM24 BF ₄	-0.12	-5.99	1.68	1.39	-0.48	1.67	-0.06	-0.33	-3.83	427	0.71	1-Butyl-3-ethylimidazolium tetrafluoroborate	
321	IM24 CF ₃ COO	-0.12	-5.99	1.68	1.39	-0.48	3.18	2.08	-2.30	-0.22	457	0.84	1-Butyl-3-ethylimidazolium trifluoroacetate	
322	IM24 CF ₃ SO ₃	-0.12	-5.99	1.68	1.39	-0.48	1.41	-0.86	0.07	-2.60	447	0.49	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	
323	IM26 BF ₄	-2.72	-5.19	1.84	0.95	0.87	1.67	-0.06	-0.33	-3.83	520	1.14	1-Ethyl-3-hexylimidazolium tetrafluoroborate	
324	IM26 Br	-2.72	-5.19	1.84	0.95	0.87	-0.52	-5.52	-2.16	-1.13	403	0.94	1-Ethyl-3-hexylimidazolium bromide	
325	IM2-10 Br	-6.83	-4.25	2.07	0.24	1.15	-0.52	-5.52	-2.16	-1.13	494	1.35	1-Decyl-3-ethylimidazolium bromide	
326	IM1-(1Ph)(CF ₃ SO ₂) ₂ N	-0.83	-6.52	3.35	-0.20	-1.72	-1.19	-2.15	2.86	2.10	536	1.12	1-benzyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
327	IM4-(1Ph)(CF ₃ SO ₂) ₂ N	-4.16	-5.71	3.48	-0.32	-0.57	-1.19	-2.15	2.86	2.10	643	1.02	1-benzyl-3-butylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	
328	Py1O-10-4CONH ₂ Cl	-0.84	8.71	2.60	-2.76	0.20	-0.57	-5.73	-2.31	-1.25	236	3.35	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	
329	Py1O-11-4CONH ₂ Cl	-1.97	9.29	2.71	-2.72	0.30	-0.57	-5.73	-2.31	-1.25	264	3.49	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	
330	Py1O-12-4CONH ₂ Cl	-3.23	9.40	3.02	-3.16	0.39	-0.57	-5.73	-2.31	-1.25	289	3.58	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	
331	Py4-4Me BF ₄	-0.22	-6.95	3.85	-0.06	-0.45	1.67	-0.06	-0.33	-3.83	414 ^a	409	0.98	1-Butyl-4-methylpyridinium tetrafluoroborate
332	Py4-4Me (C ₂ F ₅) ₃ PF ₃	-0.22	-6.95	3.85	-0.06	-0.45	2.83	3.03	4.77	-1.46	676	1.04	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	
333	Py4-4Me B(CN) ₄	-0.22	-6.95	3.85	-0.06	-0.45	-10.53	7.57	-0.53	-2.02	458	2.97	1-Butyl-4-methylpyridinium tetracyanoborate	

334	Py4-4Me Cl	-0.22	-6.95	3.85	-0.06	-0.45	-0.57	-5.73	-2.31	-1.25	282	1.04	1-Butyl-4-methylpyridinium chloride	
335	Py4-4Me PF6	-0.22	-6.95	3.85	-0.06	-0.45	1.13	-1.14	-0.21	-3.53	398	0.92	1-Butyl-4-methylpyridinium hexafluorophosphate	
336	Py4-4Me C(CN)3	-0.22	-6.95	3.85	-0.06	-0.45	-13.16	6.89	-1.96	-0.13	409	3.31	1-butyl-4-methylpyridinium tricyanomethanide	
337	Py6-4Me BF4	-2.88	-5.97	3.94	-0.40	1.13	1.67	-0.06	-0.33	-3.83	511	1.45	1-Hexyl-4-methylpyridinium tetrafluoroborate	
338	Py6-4Me Cl	-2.88	-5.97	3.94	-0.40	1.13	-0.57	-5.73	-2.31	-1.25	384	1.36	1-Hexyl-4-methylpyridinium chloride	
339	Py8-4Me BF4	-4.69	-5.10	3.21	0.18	1.30	1.67	-0.06	-0.33	-3.83	564	1.47	4-Methyl-1-octylpyridinium tetrafluoroborate	
340	Py8-4Me Cl	-4.69	-5.10	3.21	0.18	1.30	-0.57	-5.73	-2.31	-1.25	437	1.34	4-Methyl-1-octylpyridinium chloride	
341	Py1-4NMe2 I	1.97	-8.24	4.64	-1.89	-2.88	-0.65	-5.31	-1.63	-1.12	169	1.49	4-(Dimethylamino)-1-methylpyridinium iodide	
342	Py2-4NMe2 (CF3SO2)2N	1.55	-7.82	4.30	-1.27	-2.67	-1.19	-2.15	2.86	2.10	441	1.60	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide	
343	Py2-4NMe2 Br	1.55	-7.82	4.30	-1.27	-2.67	-0.52	-5.52	-2.16	-1.13	172	1.32	4-(Dimethylamino)-1-ethylpyridinium bromide	
344	Py4-4NMe2 (CF3SO2)2N	-0.73	-6.95	4.30	-1.12	-1.38	-1.19	-2.15	2.86	2.10	531	1.32	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide	
345	Py4-4NMe2 Br	-0.73	-6.95	4.30	-1.12	-1.38	-0.52	-5.52	-2.16	-1.13	262	1.22	1-Butyl-4-(dimethylamino)pyridinium bromide	
346	Py4-4NMe2 Cl	-0.73	-6.95	4.30	-1.12	-1.38	-0.57	-5.73	-2.31	-1.25	251	1.23	1-Butyl-4-(dimethylamino)pyridinium chloride	
347	Py6-4NMe2 (CF3SO2)2N	-3.42	-6.49	5.27	-1.90	-0.04	-1.19	-2.15	2.86	2.10	628 ^a	619	1.58	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
348	Py6-4NMe2 Cl	-3.42	-6.49	5.27	-1.90	-0.04	-0.57	-5.73	-2.31	-1.25	340	1.64	4-(Dimethylamino)-1-hexylpyridinium chloride	
349	IM33 (CF3SO2)2N	-0.15	-5.93	1.74	1.28	-0.21	-1.19	-2.15	2.86	2.10	587	0.50	1,3-Dipropylimidazolium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide	
350	IM44 (CF3SO2)2N	-2.22	-5.41	1.53	1.53	-0.31	-1.19	-2.15	2.86	2.10	634	0.43	1,3-Dibutylimidazolium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide	
351	IM42OH Cl	6.56	2.86	1.24	-2.46	1.82	-0.57	-5.73	-2.31	-1.25	140	1.96	1-butyl-3-(2-hydroxyethyl)imidazolium chloride	
352	Quin1O6-6Me Cl	-3.71	-1.36	2.43	-0.72	-0.06	-0.57	-5.73	-2.31	-1.25	353	1.33	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride	
353	Quin1O8-6Me Cl	-6.17	-0.01	1.74	-0.12	0.87	-0.57	-5.73	-2.31	-1.25	443	1.58	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride	
354	Quin1O-10-6Me Cl	-8.33	-0.33	2.01	-0.49	0.96	-0.57	-5.73	-2.31	-1.25	492	1.76	1-[(Decyloxy)methyl]-6-methylquinolinium chloride	
355	Quin1O-12-6Me Cl	-10.30	0.77	1.45	0.40	1.01	-0.57	-5.73	-2.31	-1.25	547	2.01	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride	
356	Quin1O6-8OH Cl	-0.56	0.61	4.16	-2.65	1.01	-0.57	-5.73	-2.31	-1.25	277	1.81	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride	
357	Quin1O8-8OH Cl	-2.66	1.72	3.00	-1.66	2.18	-0.57	-5.73	-2.31	-1.25	373	1.86	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride	
358	Quin1O-10-8OH Cl	-4.64	2.67	2.11	-0.97	2.53	-0.57	-5.73	-2.31	-1.25	437	2.00	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride	
359	Quin1O-12-8OH Cl	-7.05	3.58	1.77	-1.52	3.02	-0.57	-5.73	-2.31	-1.25	499	2.30	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride	

360	Quin4 BF4	-3.22	-7.41	6.68	-2.67	-0.32	1.67	-0.06	-0.33	-3.83	443	1.91	1-Butylquinolinium tetrafluoroborate
361	Quin4 Br	-3.22	-7.41	6.68	-2.67	-0.32	-0.52	-5.52	-2.16	-1.13	327	1.98	1-Butylquinolinium bromide
362	Quin6 BF4	-5.56	-6.58	6.69	-2.83	0.73	1.67	-0.06	-0.33	-3.83	525	2.18	1-Hexylquinolinium tetrafluoroborate
363	Quin8 BF4	-7.55	-5.95	6.77	-3.00	1.19	1.67	-0.06	-0.33	-3.83	580	2.39	1-Octylquinolinium tetrafluoroborate
364	Quin8 Br	-7.55	-5.95	6.77	-3.00	1.19	-0.52	-5.52	-2.16	-1.13	463	2.36	1-Octylquinolinium bromide
365	Quin106 Cl	-3.19	-1.99	3.20	-1.15	0.26	-0.57	-5.73	-2.31	-1.25	345	1.31	1-[(Hexyloxy)methyl]quinolinium chloride
366	Quin108 Cl	-5.27	-1.84	2.22	-0.10	0.66	-0.57	-5.73	-2.31	-1.25	421	1.32	1-[(Octyloxy)methyl]quinolinium chloride
367	Quin10-10 Cl	-7.56	-0.68	2.47	-0.62	1.53	-0.57	-5.73	-2.31	-1.25	489	1.70	1-[(Decyloxy)methyl]quinolinium chloride
368	Quin10-12 Cl	-9.13	0.23	2.06	-0.80	1.46	-0.57	-5.73	-2.31	-1.25	520	1.91	1-[(Dodecyloxy)methyl]quinolinium chloride
369	IM55 (CF3SO2)2N	-4.42	-4.59	1.39	1.41	0.75	-1.19	-2.15	2.86	2.10	713	0.36	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
370	Py1(COO1)(Ph-3-OMe-4-OMe) Cl	2.48	4.98	2.05	1.69	-4.39	-0.57	-5.73	-2.31	-1.25	89	3.36	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride
371	Py1(COO1)(Ph-(3,4-OCH2O-)) Br	3.15	5.90	2.96	0.51	-4.03	-0.52	-5.52	-2.16	-1.13	75	3.46	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide
372	Py1(COO4)(Ph-(3,4-OCH2O-)) Br	-0.04	6.08	1.97	1.50	-4.27	-0.52	-5.52	-2.16	-1.13	156	3.60	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide
373	Py2 Cl	3.56	-7.36	2.26	1.22	-1.59	-0.57	-5.73	-2.31	-1.25	182	0.74	1-Ethylpyridinium chloride
374	Py1CN (CF3SO2)2N	5.10	-3.86	6.39	-5.86	-2.84	-1.19	-2.15	2.86	2.10	278	2.71	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
375	Py1CN Cl	5.10	-3.86	6.39	-5.86	-2.84	-0.57	-5.73	-2.31	-1.25	-1	2.34	1-(Cyanomethyl)pyridinium chloride
376	Py1COO1(COO1)(Ph-(3,4-OCH2O-)) Br	-0.87	11.80	5.15	-1.25	-8.30	-0.52	-5.52	-2.16	-1.13	-8	6.12	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide
377	Py1COO1(COO4)(Ph-(3,4-OCH2O-)) Br	-4.31	12.32	4.51	-0.39	-7.74	-0.52	-5.52	-2.16	-1.13	100	6.11	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide
378	Py1COO2 (CF3SO2)2N	4.31	2.25	-0.36	0.90	-2.53	-1.19	-2.15	2.86	2.10	389	2.43	1-(2-Ethoxy-2-oxoethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
379	Py1COO2 8OSO3	4.31	2.25	-0.36	0.90	-2.53	-1.48	-1.82	3.86	4.62	466	2.55	1-(2-Ethoxy-2-oxoethyl)pyridinium octyl sulfate
380	Py1COO2 Br	4.31	2.25	-0.36	0.90	-2.53	-0.52	-5.52	-2.16	-1.13	120	2.23	1-(2-Ethoxy-2-oxoethyl)pyridinium bromide
381	Py1COO2 PF6	4.31	2.25	-0.36	0.90	-2.53	1.13	-1.14	-0.21	-3.53	226	2.54	1-(2-Ethoxy-2-oxoethyl)pyridinium hexafluorophosphate
382	Py3 (CF3SO2)2N	1.68	-7.24	3.58	0.18	-0.27	-1.19	-2.15	2.86	2.10	528	1.04	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
383	Py3 Br	1.68	-7.24	3.58	0.18	-0.27	-0.52	-5.52	-2.16	-1.13	259	0.93	1-Propylpyridinium bromide
384	Py4 Cl	0.96	-6.71	2.76	0.70	-0.52	-0.57	-5.73	-2.31	-1.25	265	0.76	1-Butylpyridinium chloride
385	Py4 Al2Cl7	0.96	-6.71	2.76	0.70	-0.52	-5.66	-3.72	1.43	2.02	439	1.31	1-Butylpyridinium μ -chlorohexachlorodialuminate

386	Py4 N(CN)2	0.96	-6.71	2.76	0.70	-0.52	-2.48	0.49	0.00	0.73		453	0.85	1-Butylpyridinium N-cyanocyanamide
387	Py4 Br	0.96	-6.71	2.76	0.70	-0.52	-0.52	-5.52	-2.16	-1.13		275	0.73	1-Butylpyridinium bromide
388	Py4 1OSO3	0.96	-6.71	2.76	0.70	-0.52	1.36	-1.16	-0.44	-1.31		409	0.45	1-Butylpyridinium methyl sulfate
389	Py4 8OSO3	0.96	-6.71	2.76	0.70	-0.52	-1.48	-1.82	3.86	4.62		621	1.11	1-Butylpyridinium octyl sulfate
390	Py4 BF4	0.96	-6.71	2.76	0.70	-0.52	1.67	-0.06	-0.33	-3.83	383^a	392	0.74	1-Butylpyridinium tetrafluoroborate
391	Py4 CF3SO3	0.96	-6.71	2.76	0.70	-0.52	1.41	-0.86	0.07	-2.60		411	0.56	1-Butylpyridinium trifluoromethanesulfonate
392	Py4 PF6	0.96	-6.71	2.76	0.70	-0.52	1.13	-1.14	-0.21	-3.53		381	0.66	1-Butylpyridinium hexafluorophosphate
393	Py5 (CF3SO2)2N	-0.24	-6.22	2.71	0.59	0.14	-1.19	-2.15	2.86	2.10		589	0.70	1-Pentylpyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
394	Py5 Br	-0.24	-6.22	2.71	0.59	0.14	-0.52	-5.52	-2.16	-1.13		320	0.81	1-Pentylpyridinium bromide
395	Py6 (CF3SO2)2N	-0.95	-5.90	2.50	0.55	0.12	-1.19	-2.15	2.86	2.10	612^a	604	0.64	1-Hexylpyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
396	Py6 CF3SO3	-0.95	-5.90	2.50	0.55	0.12	1.41	-0.86	0.07	-2.60		471	0.74	1-Hexylpyridinium trifluoromethanesulfonate
397	Py6 Cl	-0.95	-5.90	2.50	0.55	0.12	-0.57	-5.73	-2.31	-1.25		324	0.83	1-Hexylpyridinium chloride
398	Py6 PF6	-0.95	-5.90	2.50	0.55	0.12	1.13	-1.14	-0.21	-3.53		440	0.84	1-Hexylpyridinium hexafluorophosphate
399	Py8 Cl	-3.41	-5.10	2.61	0.39	1.43	-0.57	-5.73	-2.31	-1.25		416	1.19	1-Octylpyridinium chloride
400	Py8 (CF3SO2)2N	-3.41	-5.10	2.61	0.39	1.43	-1.19	-2.15	2.86	2.10	629^b	695	0.77	1-Octylpyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
401	Py-10 Br	-5.41	-4.43	2.31	0.46	1.66	-0.52	-5.52	-2.16	-1.13		479	1.31	1-Decylpyridinium bromide
402	Py-16 Br	-11.79	-2.66	2.50	0.08	3.09	-0.52	-5.52	-2.16	-1.13		659	2.11	1-Hexadecylpyridinium bromide
403	Py-16 Cl	-11.79	-2.66	2.50	0.08	3.09	-0.57	-5.73	-2.31	-1.25		649	2.13	1-Hexadecylpyridinium chloride
404	Py3OH (CF3SO2)2N	9.31	2.44	2.69	-3.75	1.97	-1.19	-2.15	2.86	2.10		342	2.49	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
405	Py3OH Cl	9.31	2.44	2.69	-3.75	1.97	-0.57	-5.73	-2.31	-1.25		62	2.21	1-(3-Hydroxypropyl)pyridinium chloride
406	Py3O1 (CF3SO2)2N	4.39	-2.54	2.94	-0.77	0.87	-1.19	-2.15	2.86	2.10		474	1.19	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
407	Py3O1 Cl	4.39	-2.54	2.94	-0.77	0.87	-0.57	-5.73	-2.31	-1.25		195	0.96	1-(3-Methoxypropyl)pyridinium chloride
408	Py3SO3H CF3SO3	14.74	7.66	6.06	-4.40	3.17	1.41	-0.86	0.07	-2.60		83	4.28	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate
409	Py2OH (CF3SO2)2N	10.28	2.57	3.54	-4.42	2.59	-1.19	-2.15	2.86	2.10		327	2.75	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
410	Py2OH I	10.28	2.57	3.54	-4.42	2.59	-0.65	-5.31	-1.63	-1.12		79	2.51	1-(2-Hydroxyethyl)pyridinium iodide
411	Py2O1 (CF3SO2)2N	6.51	-2.48	1.93	-0.46	-0.20	-1.19	-2.15	2.86	2.10		400	1.27	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide

412	Py2O1 Cl	6.51	-2.48	1.93	-0.46	-0.20	-0.57	-5.73	-2.31	-1.25	120	0.83	1-(2-Methoxyethyl)pyridinium chloride
413	Py2O2 (CF3SO2)2N	4.79	-2.48	2.51	-0.28	0.17	-1.19	-2.15	2.86	2.10	451	1.13	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
414	Py2O2 Br	4.79	-2.48	2.51	-0.28	0.17	-0.52	-5.52	-2.16	-1.13	182	0.82	1-(2-Ethoxyethyl)pyridinium bromide
415	Py1O2 (CF3SO2)2N	5.70	-2.01	-0.01	1.57	0.11	-1.19	-2.15	2.86	2.10	457	1.15	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
416	Py1O2 Cl	5.70	-2.01	-0.01	1.57	0.11	-0.57	-5.73	-2.31	-1.25	178	0.90	1-(Ethoxymethyl)pyridinium chloride
417	Pyr66 BF4	-5.18	-2.55	-3.71	5.26	0.71	1.67	-0.06	-0.33	-3.83	633	2.11	1,1-Dihexylpyrrolidinium tetrafluoroborate
418	IM66 (CF3SO2)2N	-6.81	-4.32	1.77	1.22	1.01	-1.19	-2.15	2.86	2.10	771	0.65	1,3-Dihexylimidazolium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
419	IM-10-10-2Me (CF3SO2)2N	-13.99	-1.46	0.53	1.86	2.47	-1.19	-2.15	2.86	2.10	984	1.45	1,3-Didecyl-2-methylimidazolium 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide
420	Pyr-12-2OH Cl	-2.02	6.35	-2.97	0.68	3.83	-0.57	-5.73	-2.31	-1.25	440	2.61	1-Dodecyl-1-(2-hydroxyethyl)pyrrolidinium chloride
421	IM-14-2OH-2Me Cl	-5.40	4.92	-0.25	-1.53	4.03	-0.57	-5.73	-2.31	-1.25	493	2.45	1-(2-Hydroxyethyl)-2-methyl-3-tetradecylimidazolium chloride
422	IM-16-2OH-2Me Cl	-7.84	5.39	0.95	-2.31	4.75	-0.57	-5.73	-2.31	-1.25	557	2.78	1-Hexadecyl-3-(2-hydroxyethyl)-2-methylimidazolium chloride
423	IM2OH-(2Ph) Cl	2.41	2.66	3.93	-4.66	3.40	-0.57	-5.73	-2.31	-1.25	249	2.49	1-(2-hydroxyethyl)-3-(2-phenylethyl)imidazolium chloride
424	IM2OH-(2OH) Cl	11.50	9.67	5.76	-7.07	5.63	-0.57	-5.73	-2.31	-1.25	48	4.36	1,3-di-(2-hydroxyethyl)imidazolium chloride
425	IM1O3-1O3 Cl	1.60	2.22	-0.33	2.43	0.25	-0.57	-5.73	-2.31	-1.25	274	1.76	1,3-Bis(propoxymethyl)imidazolium chloride
426	IM1O4-1O4 Cl	-0.46	2.39	-1.08	3.65	-0.28	-0.57	-5.73	-2.31	-1.25	323	2.03	1,3-Bis(butoxymethyl)imidazolium chloride
427	IM1O5-1O5 Cl	-2.37	3.08	-1.21	3.28	0.15	-0.57	-5.73	-2.31	-1.25	374	2.12	1,3-Bis[(pentyloxy)methyl]imidazolium chloride
428	IM1O6-1O6 Cl	-4.54	3.90	-1.41	3.31	-0.06	-0.57	-5.73	-2.31	-1.25	416	2.40	1,3-Bis[(hexyloxy)methyl]imidazolium chloride
429	IM1O7-1O7 Cl	-6.51	3.95	-2.25	3.80	0.56	-0.57	-5.73	-2.31	-1.25	489	2.49	1,3-Bis[(heptyloxy)methyl]imidazolium chloride
430	IM1O8-1O8 Cl	-8.29	4.70	-2.62	3.95	0.51	-0.57	-5.73	-2.31	-1.25	529	2.75	1,3-Bis[(octyloxy)methyl]imidazolium chloride
431	IM1O9-1O9 Cl	-10.86	5.16	-1.92	3.61	0.67	-0.57	-5.73	-2.31	-1.25	586	2.90	1,3-Bis[(nonyloxy)methyl]imidazolium chloride
432	IM1O-10-10-10 Cl	-12.39	4.91	-2.50	3.87	0.83	-0.57	-5.73	-2.31	-1.25	632	2.97	1,3-Bis[(decyloxy)methyl]imidazolium chloride
433	IM1O-11-10-11 Cl	-14.03	6.14	-3.22	4.48	0.64	-0.57	-5.73	-2.31	-1.25	670	3.38	1,3-Bis[(undecyloxy)methyl]imidazolium chloride
434	IM1O-12-10-12 Cl	-16.24	6.96	-2.08	3.57	0.63	-0.57	-5.73	-2.31	-1.25	704	3.57	1,3-Bis[(dodecyloxy)methyl]imidazolium chloride
435	IM1O-14-10-14 Cl	-19.66	8.67	-3.30	4.57	1.51	-0.57	-5.73	-2.31	-1.25	820	4.09	1,3-Bis[(tetradecyloxy)methyl]imidazolium chloride
436	IM1O-16-10-16 Cl	-21.63	9.04	-1.98	3.39	2.77	-0.57	-5.73	-2.31	-1.25	884	4.09	1,3-Bis[(hexadecyloxy)methyl]imidazolium chloride
437	IM01 BF4	5.03	-5.69	-6.83	-6.30	-3.04	1.67	-0.06	-0.33	-3.83	165	3.09	1-Methylimidazolium hydrogen tetrafluoroborate

438	IM01 HO1(1)COO	5.03	-5.69	-6.83	-6.30	-3.04	4.48	3.75	-4.18	2.80	211	3.40	1-Methylimidazolium 2-hydroxypropanoate
439	IM01 HO1(1)COO-S	5.03	-5.69	-6.83	-6.30	-3.04	4.81	4.31	-4.51	3.25	216	3.47	1-Methylimidazolium (2S)-2-hydroxypropanoate
440	IM01 1COO	5.03	-5.69	-6.83	-6.30	-3.04	4.20	2.41	-5.87	3.73	145	3.41	1-methylimidazolium acetate
441	IM01 CF3COO	5.03	-5.69	-6.83	-6.30	-3.04	3.18	2.08	-2.30	-0.22	195	3.16	1-methylimidazolium trifluoroacetate
442	IM01 CF3SO3	5.03	-5.69	-6.83	-6.30	-3.04	1.41	-0.86	0.07	-2.60	184	3.06	1-methylimidazolium 1,1,1-trifluoromethanesulfonate
443	IM02 HO1(1)COO	3.99	-5.53	-6.71	-5.77	-2.93	4.48	3.75	-4.18	2.80	243	3.28	1-Ethylimidazolium 2-hydroxypropanoate
444	IM02 HO1(1)COO-S	3.99	-5.53	-6.71	-5.77	-2.93	4.81	4.31	-4.51	3.25	249	3.36	1-Ethylimidazolium (2S)-2-hydroxypropanoate
445	IM03 HO1(1)COO	2.28	-5.50	-5.68	-6.45	-2.21	4.48	3.75	-4.18	2.80	293	3.18	1-Propylimidazolium 2-hydroxypropanoate
446	IM03 HO1(1)COO-S	2.28	-5.50	-5.68	-6.45	-2.21	4.81	4.31	-4.51	3.25	299	3.26	1-Propylimidazolium (2S)-2-hydroxypropanoate
447	IM04 HO1(1)COO	1.00	-4.97	-6.24	-6.11	-1.76	4.48	3.75	-4.18	2.80	340	3.21	1-Butylimidazolium 2-hydroxypropanoate
448	IM04 HO1(1)COO-S	1.00	-4.97	-6.24	-6.11	-1.76	4.81	4.31	-4.51	3.25	346	3.28	1-Butylimidazolium (2S)-2-hydroxypropanoate
449	IM04 1COO	1.00	-4.97	-6.24	-6.11	-1.76	4.20	2.41	-5.87	3.73	274	3.23	1-butylimidazolium acetate
450	IM04 CF3COO	1.00	-4.97	-6.24	-6.11	-1.76	3.18	2.08	-2.30	-0.22	325	2.95	1-butylimidazolium trifluoroacetate
451	IM04 CF3SO3	1.00	-4.97	-6.24	-6.11	-1.76	1.41	-0.86	0.07	-2.60	314	2.82	1-butylimidazolium 1,1,1-trifluoromethanesulfonate
452	IM05 HO1(1)COO	-0.48	-4.65	-6.13	-6.17	-1.31	4.48	3.75	-4.18	2.80	386	3.21	1-Pentylimidazolium 2-hydroxypropanoate
453	IM05 HO1(1)COO-S	-0.48	-4.65	-6.13	-6.17	-1.31	4.81	4.31	-4.51	3.25	392	3.28	1-Pentylimidazolium (2S)-2-hydroxypropanoate
454	IM06 HO1(1)COO	-1.08	-4.19	-6.92	-5.73	-1.42	4.48	3.75	-4.18	2.80	403	3.29	1-Hexylimidazolium 2-hydroxypropanoate
455	IM06 HO1(1)COO-S	-1.08	-4.19	-6.92	-5.73	-1.42	4.81	4.31	-4.51	3.25	409	3.36	1-Hexylimidazolium (2S)-2-hydroxypropanoate
456	IM07 HO1(1)COO	-2.69	-4.01	-6.24	-6.38	-0.74	4.48	3.75	-4.18	2.80	450	3.30	1-Heptylimidazolium 2-hydroxypropanoate
457	IM07 HO1(1)COO-S	-2.69	-4.01	-6.24	-6.38	-0.74	4.81	4.31	-4.51	3.25	456	3.38	1-Heptylimidazolium (2S)-2-hydroxypropanoate
458	IM08 HO1(1)COO	-3.55	-3.47	-6.97	-6.04	-0.63	4.48	3.75	-4.18	2.80	478	3.39	1-Octylimidazolium 2-hydroxypropanoate
459	IM08 HO1(1)COO-S	-3.55	-3.47	-6.97	-6.04	-0.63	4.81	4.31	-4.51	3.25	484	3.47	1-Octylimidazolium (2S)-2-hydroxypropanoate
460	IM09 HO1(1)COO	-4.64	-3.28	-6.83	-6.04	-0.24	4.48	3.75	-4.18	2.80	514	3.40	1-Nonylimidazolium 2-hydroxypropanoate
461	IM09 HO1(1)COO-S	-4.64	-3.28	-6.83	-6.04	-0.24	4.81	4.31	-4.51	3.25	520	3.47	1-Nonylimidazolium (2S)-2-hydroxypropanoate
462	IM0-10 HO1(1)COO	-5.78	-2.89	-7.12	-5.67	0.06	4.48	3.75	-4.18	2.80	554	3.43	1-Decylimidazolium 2-hydroxypropanoate
463	IM0-10 HO1(1)COO-S	-5.78	-2.89	-7.12	-5.67	0.06	4.81	4.31	-4.51	3.25	560	3.50	1-Decylimidazolium (2S)-2-hydroxypropanoate

464	IM0-11 HO1(1)COO	-6.55	-2.51	-7.31	-5.72	-0.03	4.48	3.75	-4.18	2.80	567	3.50	1-Undecylimidazolium 2-hydroxypropanoate
465	IM0-11 HO1(1)COO-S	-6.55	-2.51	-7.31	-5.72	-0.03	4.81	4.31	-4.51	3.25	573	3.58	1-Undecylimidazolium (2S)-2-hydroxypropanoate
466	IM0-12 HO1(1)COO	-7.34	-2.19	-7.84	-5.07	-0.29	4.48	3.75	-4.18	2.80	586	3.54	1-Dodecylimidazolium 2-hydroxypropanoate
467	IM0-12 HO1(1)COO-S	-7.34	-2.19	-7.84	-5.07	-0.29	4.81	4.31	-4.51	3.25	592	3.61	1-Dodecylimidazolium (2S)-2-hydroxypropanoate
468	IM0104 HO1(1)COO	1.36	-0.40	-9.16	-3.36	-1.19	4.48	3.75	-4.18	2.80	377	3.66	1-(Butoxymethyl)imidazolium 2-hydroxypropanoate
469	IM0104 HO1(1)COO-S	1.36	-0.40	-9.16	-3.36	-1.19	4.81	4.31	-4.51	3.25	383	3.74	1-(Butoxymethyl)imidazolium (2S)-2-hydroxypropanoate
470	IM0105 HO1(1)COO	0.12	-0.39	-8.73	-4.18	-1.24	4.48	3.75	-4.18	2.80	393	3.67	1-[(Pentyloxy)methyl]imidazolium 2-hydroxypropanoate
471	IM0105 HO1(1)COO-S	0.12	-0.39	-8.73	-4.18	-1.24	4.81	4.31	-4.51	3.25	399	3.75	1-[(Pentyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
472	IM0106 HO1(1)COO	-0.43	0.45	-9.42	-3.76	-1.21	4.48	3.75	-4.18	2.80	411	3.83	1-[(Hexyloxy)methyl]imidazolium 2-hydroxypropanoate
473	IM0106 HO1(1)COO-S	-0.43	0.45	-9.42	-3.76	-1.21	4.81	4.31	-4.51	3.25	417	3.91	1-[(Hexyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
474	IM0107 HO1(1)COO	-1.75	0.26	-9.61	-3.55	-0.93	4.48	3.75	-4.18	2.80	453	3.80	1-[(Heptyloxy)methyl]imidazolium 2-hydroxypropanoate
475	IM0107 HO1(1)COO-S	-1.75	0.26	-9.61	-3.55	-0.93	4.81	4.31	-4.51	3.25	459	3.88	1-[(Heptyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
476	IM0108 HO1(1)COO	-2.94	0.97	-9.30	-3.78	-0.63	4.48	3.75	-4.18	2.80	484	3.84	1-[(Octyloxy)methyl]imidazolium 2-hydroxypropanoate
477	IM0108 HO1(1)COO-S	-2.94	0.97	-9.30	-3.78	-0.63	4.81	4.31	-4.51	3.25	490	3.92	1-[(Octyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
478	IM0109 HO1(1)COO	-4.56	0.87	-8.72	-4.46	-0.49	4.48	3.75	-4.18	2.80	516	3.82	1-[(Nonyloxy)methyl]imidazolium 2-hydroxypropanoate
479	IM0109 HO1(1)COO-S	-4.56	0.87	-8.72	-4.46	-0.49	4.81	4.31	-4.51	3.25	522	3.90	1-[(Nonyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
480	IM010-10 HO1(1)COO	-5.09	0.97	-9.44	-3.89	-0.65	4.48	3.75	-4.18	2.80	533	3.90	1-[(Decyloxy)methyl]imidazolium 2-hydroxypropanoate
481	IM010-10 HO1(1)COO-S	-5.09	0.97	-9.44	-3.89	-0.65	4.81	4.31	-4.51	3.25	539	3.98	1-[(Decyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
482	IM010-11 HO1(1)COO	-6.60	1.67	-9.05	-4.06	-0.50	4.48	3.75	-4.18	2.80	567	3.96	1-[(Undecyloxy)methyl]imidazolium 2-hydroxypropanoate
483	IM010-11 HO1(1)COO-S	-6.60	1.67	-9.05	-4.06	-0.50	4.81	4.31	-4.51	3.25	573	4.04	1-[(Undecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
484	IM010-12 HO1(1)COO	-7.33	2.17	-9.65	-4.12	0.13	4.48	3.75	-4.18	2.80	602	4.09	1-[(Dodecyloxy)methyl]imidazolium 2-hydroxypropanoate
485	IM010-12 HO1(1)COO-S	-7.33	2.17	-9.65	-4.12	0.13	4.81	4.31	-4.51	3.25	608	4.17	1-[(Dodecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
486	Py0 Cl	3.78	-5.25	-7.66	-7.06	-2.26	-0.57	-5.73	-2.31	-1.25	82	3.14	pyridinium hydrochloride
487	0600NN (CF3SO2)2N	3.71	0.96	-4.42	2.25	-1.41	-1.19	-2.15	2.86	2.10	470	2.23	1-hexyl-1,4-diaza[2.2.2]bicyclooctanium bis(trifluoromethylsulfonyl)imide
488	IM00 1COO	7.34	-3.31	-7.65	-5.38	-2.63	4.20	2.41	-5.87	3.73	109	3.53	1H-Imidazol-1-ium acetate
489	IM00 CF3COO	7.34	-3.31	-7.65	-5.38	-2.63	3.18	2.08	-2.30	-0.22	160	3.30	1H-Imidazol-1-ium trifluoroacetate

490	IM00 CFSO3	7.34	-3.31	-7.65	-5.38	-2.63	1.41	-0.86	0.07	-2.60		149	3.15	1H-Imidazol-1-ium 1,1,1-trifluoromethanesulfonate
491	IM01-2Me (CF3SO2)2N	4.73	-5.69	-5.54	-6.03	-3.20	-1.19	-2.15	2.86	2.10		319	2.99	1,2-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
492	IM16-2Me Cl	-2.23	-6.01	3.61	-0.45	0.11	-0.57	-5.73	-2.31	-1.25		338	1.13	1-hexyl-2,3-dimethyl imidazolium chloride imidazolium chloride
493	IM13-2Me (CF3SO2)2N	1.81	-6.77	2.84	0.66	-0.92	-1.19	-2.15	2.86	2.10	555 ^a	512	0.91	1,2-dimethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
494	IM18 N(CN)2	-3.07	-4.67	0.46	1.44	0.28	-2.48	0.49	0.00	0.73		581	0.68	1-Methyl-3-octylimidazolium dicyanamide
495	Py4-3Me (CF3SO2)2N	-1.02	-6.72	3.14	0.02	-0.45	-1.19	-2.15	2.86	2.10	548 ^b	582	0.91	1-butyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
496	IM18 SbF6	-3.07	-4.67	0.46	1.44	0.28	1.35	-0.70	-0.12	-3.68		517	1.00	1-methyl-3-octylimidazolium hexafluoroantimonate
497	IM11 (10)2PO2	4.18	-6.87	0.65	1.98	-1.80	1.30	-1.22	0.20	-0.78		348	0.57	1,3-dimethyl imidazolium dimethyl phosphite
498	IM18 CF3COO	-3.07	-4.67	0.46	1.44	0.28	3.18	2.08	-2.30	-0.22	544 ^b	549	1.21	1-methyl-3-octylimidazolium trifluoroacetate
499	IM12OH 1COO	9.73	2.71	2.15	-3.96	2.49	4.20	2.41	-5.87	3.73		173	3.47	1-(2-hydroxyethyl)-3-methylimidazolium acetate
500	IM12OH N(CN)2	9.73	2.71	2.15	-3.96	2.49	-2.48	0.49	0.00	0.73	231.8 ^b	256	2.69	1-(2-hydroxyethyl)-3-methylimidazolium dicyanamide
501	IM12OH NO3	9.73	2.71	2.15	-3.96	2.49	-6.94	-0.46	-2.37	-1.73		90	2.41	1-(2-hydroxyethyl)-3-methylimidazolium nitrate
502	Py6-4NMe2 Br	-3.42	-6.49	5.27	-1.90	-0.04	-0.52	-5.52	-2.16	-1.13		350	1.62	4-(Dimethylamino)-1-hexylpyridinium bromide
503	Py8-4Me (CF3SO2)2N	-4.69	-5.10	3.21	0.18	1.30	-1.19	-2.15	2.86	2.10		717	0.91	1-octyl-4-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
504	Py4 (CF3SO2)2N	0.96	-6.71	2.76	0.70	-0.52	-1.19	-2.15	2.86	2.10		544	0.80	1-butylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
505	Pip12OH N(CN)2	10.68	4.70	-2.87	1.16	3.53	-2.48	0.49	0.00	0.73		336	2.85	1-(2-hydroxyethyl)-1-methylpiperidinium N-cyanocyanamide
506	Pyr18 (CF3SO2)2N	-2.33	-3.03	-3.71	5.36	0.63	-1.19	-2.15	2.86	2.10	642 ^b	720	1.53	1-methyl-1-octylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
507	Mor14 N(CN)2	6.23	0.06	-3.73	3.90	0.91	-2.48	0.49	0.00	0.73		412	2.05	4-butyl-4-methylmorpholinium dicyanamide
508	Mor12OH N(CN)2	13.05	7.64	-1.48	2.13	2.17	-2.48	0.49	0.00	0.73		238	3.45	4-(2-hydroxyethyl)-4-methylmorpholinium dicyanamide
509	Mor12 N(CN)2	8.90	-0.32	-3.78	4.51	0.50	-2.48	0.49	0.00	0.73		346	2.27	1-ethyl-1-methylmorpholinium dicyanamide
510	Mor12 (CF3SO2)2N	8.90	-0.32	-3.78	4.51	0.50	-1.19	-2.15	2.86	2.10		437	2.20	1-ethyl-1-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
511	IM14 1COO	0.58	-5.91	1.21	1.20	-0.39	4.20	2.41	-5.87	3.73	383.2 ^a	392	1.64	1-butyl-3-methylimidazolium acetate
512	IM16 1COO	-1.54	-5.78	1.66	0.51	-0.75	4.20	2.41	-5.87	3.73		420	1.62	1-hexyl-3-methylimidazolium acetate
513	IM16 CF3COO	-1.54	-5.78	1.66	0.51	-0.75	3.18	2.08	-2.30	-0.22		471	0.90	1-hexyl-3-methylimidazolium trifluoroacetate
514	Pyr14 1COO	1.96	-4.12	-3.78	5.67	-0.03	4.20	2.41	-5.87	3.73		436	2.50	1-butyl-1-methylpyrrolidinium acetate
515	IM18 NO3	-3.07	-4.67	0.46	1.44	0.28	-6.94	-0.46	-2.37	-1.73		415	1.43	1-methyl-3-octylimidazolium nitrate

516	IM14 (CF ₃ SO ₂) ₃ C	0.58	-5.91	1.21	1.20	-0.39	-0.58	-1.39	3.93	0.50	783^a	593	0.50	1-butyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide
517	IM1-18 (CF ₃ SO ₂) ₂ N	-13.76	-1.31	-0.02	1.21	2.84	-1.19	-2.15	2.86	2.10	1052^a	984	1.49	1-methyl-3-octadecylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
518	Py4-3Me (CF ₃ SO ₂) ₂ N	-1.02	-6.72	3.14	0.02	-0.45	-1.19	-2.15	2.86	2.10	622^a	582	0.91	1-butyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
519	Py6-3Me (CF ₃ SO ₂) ₂ N	-3.03	-5.66	2.50	0.25	0.50	-1.19	-2.15	2.86	2.10	624^a	659	0.69	1-hexyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
520	Pyr13 (CF ₃ SO ₂) ₂ N	3.13	-4.34	-3.85	5.63	-0.10	-1.19	-2.15	2.86	2.10	554^a	580	1.81	1-methyl-1-propylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide

^a Ref. [13]; ^b Ref. [12]

Table S2. Statistical parameters of the PLS model

Component	R ² X	R ² X(cum)	Eigenvalue	R ² Y	R ² Y(cum)	Q ²	Q ² (cum)
1	0.27	0.27	2.43	0.779	0.779	0.709	0.709
2	0.135	0.405	1.22	0.141	0.919	0.338	0.807

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