

Supplementary Information

**A QSPR approach to the ecotoxicity of ionic liquids (*Vibrio fischeri*) using VolSurf
Principal Properties†**

Table S1. PLS model parameters derived by 55x9 matrix correlation model.

Comp.	R2X	R2X(cum)	Eigenvalue	R2Y	R2Y(cum)	Q2	Q2(cum)	Significance
1	0.187	0.187	1.69	0.602	0.602	0.527	0.527	R1
2	0.176	0.364	1.59	0.167	0.769	0.326	0.681	R1

Table S2. PLS model parameters derived by 55x3 matrix correlation model.

Comp.	R2X	R2X(cum)	Eigenvalue	R2Y	R2Y(cum)	Q2	Q2(cum)	Significance
1	0.493	0.493	1.48	0.554	0.554	0.537	0.537	R1
2	0.239	0.732	0.716	0.236	0.789	0.502	0.77	R1

Table S3. List of the 520 ionic liquids with their experimental and predicted *Vibrio fischeri* ecotoxicity values and corresponding PPs.¹⁹ Red DModX indicates a value higher than 2.33 (default value). L: learning set; T: test set; U: unknown log(EC₅₀).

entry	Systematic name	Set	Y = log (EC ₅₀) <i>Vibrio f.</i> µg/L	Ŷ = log (EC ₅₀) <i>Vibrio f.</i>	Y-Ŷ	DModX	PP ₁₊	PP ₂₊	PP ₃₋
1	1-Butyl-2-methylpyridinium tetrafluoroborate	U		3.00		0.51	0.27	-6.91	-0.33
2	1-Butyl-2-methylpyridinium chloride	U		3.48		0.07	0.27	-6.91	-2.31
3	1-Ethyl-1-methylpyrrolidinium ethyl sulfate	U		3.88		0.37	4.57	-4.49	-0.18
4	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.36		0.29	6.95	0.11	2.86
5	1-(Cyanomethyl)-1-methylpyrrolidinium chloride	U		4.60		1.21	6.95	0.11	-2.31
6	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.23	3.25	-0.02	0.18	7.17	1.90	2.86
7	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide	U		4.46		1.63	7.17	1.90	-2.16
8	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	U		2.79		0.38	7.17	1.90	4.77
9	1-Methyl-1-propylpyrrolidinium hexafluorophosphate	U		3.49		0.16	3.13	-4.34	-0.21
10	1-Butyl-1-methylpyrrolidinium chloride	L	4.65	3.67	0.99	0.65	1.96	-4.12	-2.31
11	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	U		1.96		1.42	1.96	-4.12	4.77
12	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.42		0.87	1.96	-4.12	2.86

13	1-Butyl-1-methylpyrrolidinium methyl sulfate	U		3.22	0.09	1.96	-4.12	-0.44	
14	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	U		3.19	0.06	1.96	-4.12	-0.33	
15	1-Butyl-1-methylpyrrolidinium bromide	U		3.63	0.59	1.96	-4.12	-2.16	
16	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	U		3.11	0.04	1.96	-4.12	0.00	
17	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.40	1.87	0.53	0.52	0.02	-3.63	2.86
18	1-Hexyl-1-methylpyrrolidinium chloride	U		3.11	0.98	0.02	-3.63	-2.31	
19	1-Methyl-1-octylpyrrolidinium tetrafluoroborate	U		1.96	0.82	-2.33	-3.03	-0.33	
20	1-Methyl-1-octylpyrrolidinium chloride	U		2.43	1.40	-2.33	-3.03	-2.31	
21	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.91	3.86	0.04	0.52	10.38	4.48	2.86
22	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride	U		5.11	2.01	10.38	4.48	-2.31	
23	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.08	0.23	5.81	-0.16	2.86	
24	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	U		4.32	1.27	5.81	-0.16	-2.31	
25	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		4.15	0.39	11.45	4.49	2.86	
26	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	U		5.22	1.69	11.45	4.49	-1.63	
27	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.49	0.41	7.36	-0.19	2.86	
28	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	U		3.03	0.96	7.36	-0.19	4.77	
29	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	U		4.74	1.09	7.36	-0.19	-2.31	
30	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.97	3.10	-0.13	0.34	5.75	-0.56	2.86
31	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	U		4.31	1.12	5.75	-0.56	-2.16	
32	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.01	0.48	5.12	-1.38	2.86	
33	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	U		4.25	1.02	5.12	-1.38	-2.31	
34	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.05	0.13	5.85	0.24	2.86	
35	1-(Cyanomethyl)-1-methylpiperidinium chloride	U		4.30	1.37	5.85	0.24	-2.31	
36	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.49	0.91	2.18	-4.18	2.86	
37	1-Methyl-1-propylpiperidinium hexafluorophosphate	U		3.23	0.02	2.18	-4.18	-0.21	
38	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.57	2.20	0.37	0.76	1.15	-3.97	2.86
39	1-Butyl-1-methylpiperidinium bromide	T	4.32	3.40	0.92	0.72	1.15	-3.97	-2.16
40	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.55	0.69	9.27	4.69	2.86	
41	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	U		4.80	2.19	9.27	4.69	-2.31	
42	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-	U		2.82	0.08	4.88	0.03	2.86	

	[(trifluoromethyl)sulfonyl]methanesulfonamide								
43	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	U		4.06		1.42	4.88	0.03	-2.31
44	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.92		0.53	10.68	4.70	2.86
45	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	U		5.00		1.84	10.68	4.70	-1.63
46	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.15		0.49	5.73	-1.14	2.86
47	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	U		4.36		0.97	5.73	-1.14	-2.16
48	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.84		0.17	4.83	-0.32	2.86
49	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	U		4.04		1.29	4.83	-0.32	-2.16
50	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.64		0.29	3.80	-1.20	2.86
51	1-(Ethoxymethyl)-1-methylpiperidinium chloride	U		3.89		1.21	3.80	-1.20	-2.31
52	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	U		4.00		0.50	8.90	-0.32	2.48
53	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.66		0.37	9.29	3.51	2.86
54	4-(Cyanomethyl)-4-methylmorpholinium chloride	U		4.91		1.87	9.29	3.51	-2.31
55	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	2.48	3.17	-0.69	0.22	6.23	0.06	2.86
56	4-Butyl-4-methylmorpholinium bromide	L	4.30	4.38	-0.08	1.27	6.23	0.06	-2.16
57	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		4.04		1.16	12.12	7.62	2.86
58	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	U		5.28		2.66	12.12	7.62	-2.31
59	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.38		0.21	7.79	2.32	2.86
60	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	U		4.62		1.72	7.79	2.32	-2.31
61	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		4.28		1.06	13.05	7.64	2.86
62	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	U		5.36		2.37	13.05	7.64	-1.63
63	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.67		0.18	9.02	2.70	2.86
64	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	U		4.91		1.68	9.02	2.70	-2.31
65	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.45		0.27	8.20	2.70	2.86
66	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	U		4.66		1.73	8.20	2.70	-2.16
67	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.38	3.49	-0.10	0.22	8.27	2.53	2.86
68	4-(Ethoxymethyl)-4-methylmorpholinium chloride	U		4.73		1.72	8.27	2.53	-2.31

69	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	U		2.40	0.34	5.13	2.76	3.86	
70	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	U		3.84	2.08	5.13	2.76	-2.16	
71	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate	U		1.68	0.76	2.60	3.30	3.86	
72	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide	U		3.13	2.51	2.60	3.30	-2.16	
73	1,2-dimethyl-3-glycerylimidazolium dicyanamide	U		4.71	2.49	12.79	9.75	0.00	
74	1,2-dimethyl-3-glycerylimidazolium bis(trifluoromethylsulphonyl)imide	U		4.02	1.66	12.79	9.75	2.86	
75	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.31	1.16	1.01	-5.58	2.86	
76	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	U		3.07	0.23	1.01	-5.58	-0.33	
77	1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate	U		2.98	0.35	1.01	-5.58	0.07	
78	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	U		2.15	0.02	-2.67	-6.14	-0.33	
79	1-hexyl-2,3-dimethylimidazolium bis(trifluoromethylsulphonyl)imide	U		1.38	0.90	-2.67	-6.14	2.86	
80	1-(2-hydroxyethyl)-2,3-dimethylimidazolium chloride	U		5.00	1.54	9.21	2.25	-2.31	
81	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.26	1.85	4.18	-6.87	2.86	
82	1,3-dimethylimidazolium methylsulfate	U		4.05	0.90	4.18	-6.87	-0.44	
83	1,3-dimethylimidazolium p-toluenesulfonate	U		3.35	1.74	4.18	-6.87	2.48	
84	1-methyl-3-methylimidazolium N-cyanocyanamide	U		3.95	1.02	4.18	-6.87	0.00	
85	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride	U		2.80	3.32	2.18	6.00	-2.31	
86	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide	U		2.11	3.86	0.12	7.31	-2.16	
87	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	L	1.68	2.54	-0.86	2.33	3.24	-6.75	4.77
88	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	L	3.05	3.03	0.02	1.73	3.24	-6.75	2.75
89	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile	L	3.59	4.16	-0.57	0.33	3.24	-6.75	-1.96
90	1-Ethyl-3-methylimidazolium tetracyanoborate	L	3.56	3.82	-0.26	0.76	3.24	-6.75	-0.53
91	1-Ethyl-3-methylimidazolium N-cyanocyanamide	L	4.00	3.69	0.31	0.91	3.24	-6.75	0.00
92	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.11	3.00	0.11	1.77	3.24	-6.75	2.86
93	1-Ethyl-3-methylimidazolium chloride	L	4.32	4.25	0.08	0.22	3.24	-6.75	-2.31
94	1-Ethyl-3-methylimidazolium ethyl sulfate	T	4.28	3.73	0.55	0.83	3.24	-6.75	-0.18
95	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate	U		3.69	0.89	3.24	-6.75	0.02	
96	1-Ethyl-3-methylimidazolium acetate	U		5.10	0.81	3.24	-6.75	-5.87	
97	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	U		2.81	1.95	3.24	-6.75	3.67	
98	1-Ethyl-3-methylimidazolium methylsulfate	U		3.79	0.76	3.24	-6.75	-0.44	
99	1-Ethyl-3-methylimidazolium methanesulfonate	U		3.90	0.64	3.24	-6.75	-0.86	
100	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	U		3.09	1.61	3.24	-6.75	2.48	
101	1-Ethyl-3-methylimidazolium octylsulfate	U		2.76	2.01	3.24	-6.75	3.86	
102	1-Ethyl-3-methylimidazolium tetrafluoroborate	U		3.77	0.79	3.24	-6.75	-0.33	
103	1-Ethyl-3-methylimidazolium trifluoroacetate	U		4.24	0.22	3.24	-6.75	-2.30	
104	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	U		3.67	0.91	3.24	-6.75	0.07	
105	1-Ethyl-3-methylimidazolium hydrogen sulfate	U		4.03	0.48	3.24	-6.75	-1.42	

106	1-Ethyl-3-methylimidazolium hexafluorophosphate	U		3.74	0.83	3.24	-6.75	-0.21	
107	1-Ethyl-3-methylimidazolium thiocyanate	U		4.44	0.01	3.24	-6.75	-3.10	
108	1-Ethyl-3-methylimidazolium bromide	U		4.21	0.26	3.24	-6.75	-2.16	
109	1-Ethyl-3-methylimidazolium nitrate	U		4.26	0.20	3.24	-6.75	-2.37	
110	1-ethyl-3-methylimidazolium tetrachloroferrate	U		3.80	0.75	3.24	-6.75	-0.46	
111	1-(Cyanomethyl)-3-methylimidazolium chloride	U		4.56	0.47	5.65	-3.19	-2.31	
112	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.81	3.31	0.50	1.06	5.65	-3.19	2.86
113	1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		3.22	2.11	2.43	1.73	-2.16	
114	1-[2-(Diethylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		3.58	1.83	3.60	1.16	-2.16	
115	1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium bromide	U		3.26	2.32	2.91	2.71	-2.16	
116	1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium bromide	U		4.53	1.71	7.61	2.40	-2.16	
117	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide	U		1.24	5.47	-1.26	12.75	-2.16	
118	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	U		3.81	1.39	6.71	2.81	-0.33	
119	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium bromide	U		4.25	1.92	6.71	2.81	-2.16	
120	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.65	0.44	4.93	1.96	2.86	
121	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate	U		2.41	0.15	4.93	1.96	3.86	
122	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium tetrafluoroborate	U		3.42	1.36	4.93	1.96	-0.33	
123	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide	U		3.86	1.89	4.93	1.96	-2.16	
124	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium N-cyanocyanamide	U		3.34	1.26	4.93	1.96	0.00	
125	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium hexafluorophosphate	U		3.39	1.33	4.93	1.96	-0.21	
126	3-(2-Butoxy-2-oxoethyl)-1-methylimidazolium N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.35	0.81	4.15	3.03	2.86	
127	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium octylsulfate	U		2.11	0.52	4.15	3.03	3.86	
128	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate	U		3.12	1.73	4.15	3.03	-0.33	
129	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium bromide	U		3.56	2.27	4.15	3.03	-2.16	
130	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium N-cyanocyanamide	U		3.04	1.64	4.15	3.03	0.00	
131	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium hexafluorophosphate	U		3.09	1.70	4.15	3.03	-0.21	
132	1-Methyl-3-[2-oxo-2-(pentylloxy)ethyl]imidazolium octylsulfate	U		1.61	0.65	2.15	2.70	3.86	
133	1-Methyl-3-[2-oxo-2-(pentylloxy)ethyl]imidazolium bromide	U		3.06	2.40	2.15	2.70	-2.16	
134	1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium bromide	U		2.90	2.52	1.62	2.95	-2.16	
135	1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazolium bromide	U		2.13	2.83	-1.30	2.89	-2.16	
136	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.45	1.31	1.42	-5.98	2.86	
137	1-methyl-3-glycerylrylimidazolium chloride	U		5.20	3.23	12.59	9.92	-2.31	
138	1-methyl-3-glycerylimidazolium dicyanamide	U		4.64	2.56	12.59	9.92	0.00	
139	1-methyl-3-glycerylimidazolium bis(trifluoromethylsulphonyl)imide	U		3.95	1.73	12.59	9.92	2.86	
140	1-Methyl-3-(2-propenyl)imidazolium chloride	U		3.80	0.06	1.49	-6.89	-2.31	

141	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	U		2.42		0.15	-1.72	-6.38	-0.33
142	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	U		2.90		0.43	-1.72	-6.38	-2.31
143	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	U		2.40		0.18	-1.72	-6.38	-0.21
144	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	U		2.63		0.27	-0.98	-6.53	-0.33
145	1-Methyl-3-(phenylmethyl)imidazolium chloride	U		3.11		0.31	-0.98	-6.53	-2.31
146	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	U		2.61		0.30	-0.98	-6.53	-0.21
147	1-Methyl-3-propylimidazolium tetrafluoroborate	L	3.94	3.37	0.57	0.58	1.85	-6.45	-0.33
148	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.61		1.48	1.85	-6.45	2.86
149	1-Methyl-3-propylimidazolium hexafluorophosphate	U		3.35		0.59	1.85	-6.45	-0.21
150	1-Methyl-3-propylimidazolium bromide	U		3.82		0.03	1.85	-6.45	-2.16
151	1-Methyl-3-propylimidazolium chloride	U		3.85		0.02	1.85	-6.45	-2.31
152	1-Methyl-3-propylimidazolium iodide	U		3.69		0.18	1.85	-6.45	-1.63
153	1-Methyl-3-(3-oxobutyl)imidazolium bromide	U		4.17		1.65	5.91	1.45	-2.16
154	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate	U		2.07		3.21	1.89	7.73	-0.21
155	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium chloride	U		2.20		1.17	-3.71	-4.44	-2.31
156	1-[2-[(1R,5S)-6,6-Dimethylbicyclo[3.1.1]hept-2-en-2-yl]ethyl]-3-methylimidazolium nitrate	U		2.21		1.19	-3.71	-4.44	-2.37
157	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate	U		1.95		0.12	-3.43	-6.10	-0.33
158	1-Methyl-3-(2-phenylethyl)imidazolium chloride	U		2.43		0.69	-3.43	-6.10	-2.31
159	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	U		1.92		0.08	-3.43	-6.10	-0.21
160	1-Butyl-3-methylimidazolium octylsulfate	L	1.83	1.98	-0.15	1.53	0.58	-5.91	3.86
161	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	L	3.60	2.89	0.70	0.40	0.58	-5.91	0.07
162	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminat	L	3.46	2.92	0.54	0.36	0.58	-5.91	-0.04
163	1-Butyl-3-methylimidazolium tetrafluoroborate	L	3.55	2.99	0.56	0.28	0.58	-5.91	-0.33
164	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.47	2.22	0.25	1.23	0.58	-5.91	2.86
165	1-Butyl-3-methylimidazolium hexafluorophosphate	T	3.51	2.96	0.55	0.30	0.58	-5.91	-0.21
166	1-Butyl-3-methylimidazolium chloride	L	3.47	3.47	0.01	0.31	0.58	-5.91	-2.31
167	1-Butyl-3-methylimidazolium iodide	L	3.59	3.30	0.29	0.11	0.58	-5.91	-1.63
168	1-Butyl-3-methylimidazolium bromide	L	3.07	3.43	-0.36	0.27	0.58	-5.91	-2.16
169	1-Butyl-3-methylimidazolium N-cyanocyanamide	U		2.91		0.37	0.58	-5.91	0.00
170	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	L	3.53	2.31	1.21	1.12	0.58	-5.91	2.48
171	1-Butyl-3-methylimidazolium methanesulfonate	U		3.12		0.12	0.58	-5.91	-0.86
172	1-Butyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		2.58		0.77	0.58	-5.91	1.38
173	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	U		1.76		1.75	0.58	-5.91	4.77
174	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	U		2.03		1.43	0.58	-5.91	3.67
175	1-Butyl-3-methylimidazolium methyl sulfate	U		3.02		0.24	0.58	-5.91	-0.44
176	3-Butyl-1-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		2.69		0.63	0.58	-5.91	0.92
177	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate	U		3.15		0.08	0.58	-5.91	-1.00

178	1-Butyl-3-methylimidazolium tetrachloroferrate	U		3.02	0.23	0.58	-5.91	-0.46	
179	1-Butyl-3-methylimidazolium hydrogen sulfate	U		3.25	0.04	0.58	-5.91	-1.42	
180	1-Butyl-3-methylimidazolium nitrate	U		3.48	0.32	0.58	-5.91	-2.37	
181	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	U		2.94	0.33	0.58	-5.91	-0.12	
182	1-Butyl-3-methylimidazolium thiocyanate	U		3.66	0.53	0.58	-5.91	-3.10	
183	1-butyl-3-methylimidazolium dimethyl phosphate	U		2.86	0.43	0.58	-5.91	0.20	
184	1-butyl-3-methylimidazolium tricyanomethanide	U		3.38	0.20	0.58	-5.91	-1.96	
185	1-Butyl-3-Methylimidazolium trifluoroacetate	U		3.46	0.30	0.58	-5.91	-2.30	
186	3-(3-Carboxypropyl)-1-methylimidazolium chloride	U		5.13	2.22	10.77	5.41	-2.31	
187	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.87	0.97	-0.64	-5.56	2.86	
188	1-Methyl-3-pentylimidazolium tetrafluoroborate	L	3.14	2.63	0.51	0.05	-0.64	-5.56	-0.33
189	1-Methyl-3-pentylimidazolium chloride	U		3.11	0.53	-0.64	-5.56	-2.31	
190	1-Methyl-3-pentylimidazolium hexafluorophosphate	U		2.61	0.08	-0.64	-5.56	-0.21	
191	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.05	1.65	0.40	0.96	-1.54	-5.78	2.86
192	1-Hexyl-3-methylimidazolium bromide	U		2.86	0.53	-1.54	-5.78	-2.16	
193	1-Hexyl-3-methylimidazolium chloride	L	2.93	2.89	0.04	0.59	-1.54	-5.78	-2.31
194	1-Hexyl-3-methylimidazolium hexafluorophosphate	U		2.39	0.04	-1.54	-5.78	-0.21	
195	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	L	2.67	2.01	0.66	0.51	-1.54	-5.78	1.38
196	1-Hexyl-3-methylimidazolium tetrafluoroborate	L	3.18	2.42	0.76	0.00	-1.54	-5.78	-0.33
197	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	U		1.19	1.48	-1.54	-5.78	4.77	
198	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate	U		0.72	2.05	-1.54	-5.78	6.72	
199	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	U		1.39	1.24	-1.54	-5.78	3.93	
200	1-hexyl-3-methylimidazolium dicyanamide	U		2.34	0.10	-1.54	-5.78	0.00	
201	1-hexyl-3-methylimidazolium nitrate	U		2.91	0.59	-1.54	-5.78	-2.37	
202	1-hexyl-3-methylimidazolium hexafluoroantimonate	U		2.37	0.06	-1.54	-5.78	-0.12	
203	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.27	0.55	-2.66	-4.82	2.86	
204	1-Heptyl-3-methylimidazolium tetrafluoroborate	L	2.44	2.03	0.41	0.39	-2.66	-4.82	-0.33
205	1-Heptyl-3-methylimidazolium chloride	U		2.51	0.95	-2.66	-4.82	-2.31	
206	1-Heptyl-3-methylimidazolium hexafluorophosphate	U		2.01	0.35	-2.66	-4.82	-0.21	
207	1-Methyl-3-octylimidazolium tetrafluoroborate	T	1.40	1.91	-0.51	0.46	-3.07	-4.67	-0.33
208	1-Methyl-3-octylimidazolium bromide	U		2.35	0.99	-3.07	-4.67	-2.16	
209	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	0.83	1.15	-0.32	0.48	-3.07	-4.67	2.86
210	3-Methyl-1-octylimidazolium octylsulfate	U		0.91	0.75	-3.07	-4.67	3.86	
211	1-Methyl-3-octylimidazolium trifluoromethanesulfonate	U		1.82	0.35	-3.07	-4.67	0.07	
212	1-Methyl-3-octylimidazolium chloride	L	1.05	2.39	-1.34	1.07	-3.07	-4.67	-2.31
213	1-Methyl-3-octylimidazolium hexafluorophosphate	U		1.88	0.43	-3.07	-4.67	-0.21	
214	1-(7-Carboxyheptyl)-3-methylimidazolium bromide	U		3.83	2.72	6.03	5.48	-2.16	

215	1-Methyl-3-nonylimidazolium tetrafluoroborate	T	0.72	1.38	-0.66	0.78	-4.95	-4.26	-0.33
216	1-Methyl-3-nonylimidazolium chloride	U		1.86		1.35	-4.95	-4.26	-2.31
217	1-Methyl-3-nonylimidazolium hexafluorophosphate	U		1.35		0.75	-4.95	-4.26	-0.21
218	1-Decyl-3-methylimidazolium tetrafluoroborate	L	-0.18	1.14	-1.31	0.94	-5.83	-4.13	-0.33
219	1-Decyl-3-methylimidazolium bromide	U		1.58		1.44	-5.83	-4.13	-2.16
220	1-Decyl-3-methylimidazolium chloride	L	0.50	1.61	-1.11	1.53	-5.83	-4.13	-2.31
221	1-Decyl-3-methylimidazolium hexafluorophosphate	U		1.11		0.88	-5.83	-4.13	-0.21
222	1-decyl-3-methylimidazolium bis(trifluoromethylsulphonyl)imide	U		0.37		0.01	-5.83	-4.13	2.86
223	1-decyl-3-methylimidazolium tetrachloroferrate	U		1.17		0.95	-5.83	-4.13	-0.46
224	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide	U		1.31		3.43	-4.00	4.03	-2.16
225	1-Dodecyl-3-methylimidazolium bromide	U		1.04		1.86	-7.55	-3.29	-2.16
226	1-dodecyl-3-methylimidazolium chloride	U		1.08		1.90	-7.55	-3.29	-2.31
227	1-Methyl-3-tetradecylimidazolium chloride	L	-0.14	0.40	-0.54	2.43	-9.86	-2.51	-2.31
228	1-Methyl-3-tetradecylimidazolium bromide	U		0.36		2.32	-9.86	-2.51	-2.16
229	1-Hexadecyl-3-methylimidazolium chloride	L	0.23	-0.03	0.26	2.71	-11.34	-2.14	-2.31
230	1-Hexadecyl-3-methylimidazolium bromide	U		-0.06		2.59	-11.34	-2.14	-2.16
231	1-Methyl-3-octadecylimidazolium chloride	T	1.26	-0.74	1.99	3.12	-13.76	-1.31	-2.31
232	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide	U		3.02		2.65	2.36	3.73	-2.16
233	1-(4-Hydroxybutyl)-3-methylimidazolium chloride	U		4.39		1.82	6.92	2.34	-2.31
234	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	L	4.30	4.71	-0.41	1.67	8.05	2.08	-2.31
235	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	T	3.89	3.47	0.42	0.12	8.05	2.08	2.86
236	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.24	2.90	0.34	0.45	4.71	-1.38	2.86
237	1-(3-Methoxypropyl)-3-methylimidazolium chloride	L	4.30	4.15	0.16	1.09	4.71	-1.38	-2.31
238	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	L	3.89	4.93	-1.05	1.45	9.73	2.71	-1.63
239	1-(2-Hydroxyethyl)-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U		4.21		0.54	9.73	2.71	1.38
240	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.85		0.11	9.73	2.71	2.86
241	1-(2-Hydroxyethyl)-3-methylimidazolium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U		4.32		0.67	9.73	2.71	0.92
242	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	U		4.62		1.03	9.73	2.71	-0.33
243	1-(2-Hydroxyethyl)-3-methylimidazolium hexafluorophosphate	U		4.59		1.00	9.73	2.71	-0.21
244	1-(2-hydroxyethyl)-3-methylimidazolium chloride	U		5.10		1.61	9.73	2.71	-2.31
245	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.84	3.31	-0.47	0.72	6.12	-1.79	2.86
246	1-(2-Methoxyethyl)-3-methylimidazolium chloride	L	4.18	4.55	-0.37	0.82	6.12	-1.79	-2.31
247	1-(2-Methoxyethyl)-3-methylimidazolium tetrafluoroborate	U		4.08		0.22	6.12	-1.79	-0.33

248	1-(2-Methoxyethyl)-3-methylimidazolium dicyanamide	U		4.00		0.13	6.12	-1.79	0.00
249	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	2.96	2.78	0.18	0.55	4.04	-2.03	2.86
250	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	L	4.30	3.99	0.31	0.95	4.04	-2.03	-2.16
251	1-(2-Ethoxyethyl)-3-methylimidazolium chloride	U		4.03		0.96	4.04	-2.03	-2.31
252	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride	U		4.03		1.80	5.30	1.60	-2.31
253	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	3.00	3.02	-0.02	0.61	5.01	-1.83	2.86
254	1-(Ethoxymethyl)-3-methylimidazolium chloride	L	4.33	4.26	0.06	0.93	5.01	-1.83	-2.31
255	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride	U		1.71		4.36	-1.11	8.51	-2.31
256	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	U		1.66		4.27	-1.45	8.05	-2.31
257	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate	U		1.21		3.74	-1.45	8.05	-0.46
258	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	U		1.11		4.61	-3.36	8.53	-2.31
259	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate	U		1.76		6.00	-3.72	9.72	-5.87
260	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate	U		0.43		4.40	-3.72	9.72	-0.33
261	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide	U		0.87		4.93	-3.72	9.72	-2.16
262	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	U		0.91		4.97	-3.72	9.72	-2.31
263	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate	U		0.38		4.34	-3.72	9.72	-0.12
264	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide	U		0.74		4.77	-3.72	9.72	-1.63
265	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate	U		0.92		4.99	-3.72	9.72	-2.37
266	1-Butyl-3-[(butylamino)carbonyl]pyridinium octyl sulfate	U		1.02		0.64	-0.50	1.56	3.86
267	1-Butyl-3-[(butylamino)carbonyl]pyridinium iodide	U		2.34		2.23	-0.50	1.56	-1.63
268	3-[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride	U		-0.43		5.99	-8.10	11.70	-2.31
269	3-[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride	U		-0.87		6.56	-9.18	13.37	-2.31
270	3-[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride	U		-1.59		7.20	-11.41	14.87	-2.31
271	3-[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride	U		-2.33		7.65	-14.01	15.45	-2.31
272	3-(Butoxycarbonyl)-1-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.13		0.52	2.74	1.39	2.86
273	3-(Butoxycarbonyl)-1-methylpyridinium octyl sulfate	U		1.89		0.24	2.74	1.39	3.86
274	3-(Butoxycarbonyl)-1-methylpyridinium iodide	U		3.21		1.83	2.74	1.39	-1.63
275	3-(Butoxycarbonyl)-1-methylpyridinium hexafluorophosphate	U		2.87		1.42	2.74	1.39	-0.21
276	3-(Butoxycarbonyl)-1-butylpyridinium octyl sulfate	U		0.97		0.69	-0.63	1.72	3.86
277	3-(Butoxycarbonyl)-1-butylpyridinium iodide	U		2.29		2.28	-0.63	1.72	-1.63
278	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate	U		2.40		0.16	-1.83	-6.48	-0.33
279	1-Butyl-3,4-dimethylpyridinium chloride	U		2.88		0.42	-1.83	-6.48	-2.31
280	1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide	U		1.94		0.13	-3.35	-6.65	0.00
281	1-Butyl-3,5-dimethylpyridinium bromide	U		2.46		0.49	-3.35	-6.65	-2.16

282	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate	U	2.02	0.04	-3.35	-6.65	-0.33
283	1-Butyl-3,5-dimethylpyridinium chloride	U	2.50	0.54	-3.35	-6.65	-2.31
284	1-butyl-3,5-dimethyl pyridinium bistrifluoromethanesulfonamide	U	1.25	0.96	-3.35	-6.65	2.86
285	1-octyl-3,5-dimethylpyridinium bromide	U	1.23	1.41	-7.40	-4.91	-2.16
286	1-octyl-3,5-dimethylpyridinium bromide 1,1,1-trifluoro-N- [(trifluoromethyl)sulfonyl]methanesulfonamide	U	0.02	0.05	-7.40	-4.91	2.86
287	3-Methyl-1-propylpyridinium bromide	U	3.43	0.01	0.18	-7.09	-2.16
288	3-Methyl-1-propylpyridinium hexafluorophosphate	U	2.96	0.58	0.18	-7.09	-0.21
289	1-Butyl-3-methylpyridinium N-cyanocyanamide	U	2.56	0.41	-1.02	-6.72	0.00
290	1-Butyl-3-methylpyridinium bromide	U	3.08	0.22	-1.02	-6.72	-2.16
291	1-Butyl-3-methylpyridinium octyl sulfate	U	1.63	1.53	-1.02	-6.72	3.86
292	1-Butyl-3-methylpyridinium tetrafluoroborate	U	2.64	0.31	-1.02	-6.72	-0.33
293	1-Butyl-3-methylpyridinium chloride	U	3.12	0.26	-1.02	-6.72	-2.31
294	1-Butyl-3-methylpyridinium hexafluorophosphate	U	2.61	0.35	-1.02	-6.72	-0.21
295	1-Hexyl-3-methylpyridinium bromide	U	2.45	0.73	-3.03	-5.66	-2.16
296	1-Hexyl-3-methylpyridinium chloride	U	2.49	0.77	-3.03	-5.66	-2.31
297	3-Methyl-1-octylpyridinium bromide	U	1.77	1.13	-5.44	-5.13	-2.16
298	3-Methyl-1-octylpyridinium chloride	U	1.81	1.18	-5.44	-5.13	-2.31
299	3-Hydroxy-1-(propoxymethyl)pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	4.04	0.56	9.04	2.53	1.38
300	3-Hydroxy-1-(propoxymethyl)pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	4.16	0.70	9.04	2.53	0.92
301	3-Hydroxy-1-(propoxymethyl)pyridinium chloride	U	4.93	1.63	9.04	2.53	-2.31
302	1-(Butoxymethyl)-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	3.68	0.78	7.76	2.79	1.38
303	1-(Butoxymethyl)-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	3.79	0.91	7.76	2.79	0.92
304	1-[(Hexyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	3.02	1.19	5.49	3.42	1.38
305	1-[(Hexyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	3.14	1.33	5.49	3.42	0.92
306	1-[(Heptyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	2.82	1.26	4.71	3.35	1.38
307	1-[(Heptyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	2.94	1.40	4.71	3.35	0.92
308	1-[(Heptyloxy)methyl]-3-hydroxypyridinium chloride	U	3.71	2.33	4.71	3.35	-2.31
309	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	1.45	2.05	-0.18	4.26	1.38
310	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	1.56	2.18	-0.18	4.26	0.92
311	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium chloride	U	2.34	3.12	-0.18	4.26	-2.31
312	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide	U	-0.60	3.53	-7.03	6.97	1.38
313	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate	U	-0.49	3.66	-7.03	6.97	0.92
314	1-Butyl-1-ethylpyrrolidinium ethyl sulfate	U	2.95	0.15	1.25	-3.90	-0.18
315	1-ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)imidazolium ethyl sulfate	U	-1.54	4.36	-12.25	6.23	-0.18
316	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.66	1.53	2.03	-6.56	2.86
317	1,3-Diethylimidazolium bromide	U	3.87	0.07	2.03	-6.56	-2.16

318	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U			2.40		1.36	1.10	-6.31	2.86
319	1-Ethyl-3-propylimidazolium bromide	U			3.60		0.09	1.10	-6.31	-2.16
320	1-Butyl-3-ethylimidazolium tetrafluoroborate	L	2.80		2.81	-0.01	0.22	-0.12	-5.99	-0.33
321	1-Butyl-3-ethylimidazolium trifluoroacetate	U			3.28		0.36	-0.12	-5.99	-2.30
322	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	U			2.72		0.33	-0.12	-5.99	0.07
323	1-Ethyl-3-hexylimidazolium tetrafluoroborate	L	2.15		2.05	0.10	0.29	-2.72	-5.19	-0.33
324	1-Ethyl-3-hexylimidazolium bromide	U			2.49		0.82	-2.72	-5.19	-2.16
325	1-Decyl-3-ethylimidazolium bromide	U			1.32		1.52	-6.83	-4.25	-2.16
326	1-benzyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U			1.91		1.21	-0.83	-6.52	2.86
327	1-benzyl-3-butylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U			0.95		0.62	-4.16	-5.71	2.86
328	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride	U			1.76		4.38	-0.84	8.71	-2.31
329	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride	U			1.41		4.66	-1.97	9.29	-2.31
330	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride	U			1.07		4.83	-3.23	9.40	-2.31
331	1-Butyl-4-methylpyridinium tetrafluoroborate	L	3.02		2.87	0.15	0.48	-0.22	-6.95	-0.33
332	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	U			1.65		1.94	-0.22	-6.95	4.77
333	1-Butyl-4-methylpyridinium tetracyanoborate	U			2.92		0.40	-0.22	-6.95	-0.53
334	1-Butyl-4-methylpyridinium chloride	U			3.35		0.11	-0.22	-6.95	-2.31
335	1-Butyl-4-methylpyridinium hexafluorophosphate	U			2.84		0.49	-0.22	-6.95	-0.21
336	1-butyl-4-methylpyridinium tricyanomethanide	U			3.26		0.01	-0.22	-6.95	-1.96
337	1-Hexyl-4-methylpyridinium tetrafluoroborate	U			2.08		0.09	-2.88	-5.97	-0.33
338	1-Hexyl-4-methylpyridinium chloride	U			2.56		0.67	-2.88	-5.97	-2.31
339	4-Methyl-1-octylpyridinium tetrafluoroborate	U			1.52		0.52	-4.69	-5.10	-0.33
340	4-Methyl-1-octylpyridinium chloride	U			2.00		1.10	-4.69	-5.10	-2.31
341	4-(Dimethylamino)-1-methylpyridinium iodide	U			3.88		0.67	1.97	-8.24	-1.63
342	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U			2.65		1.82	1.55	-7.82	2.86
343	4-(Dimethylamino)-1-ethylpyridinium bromide	U			3.86		0.36	1.55	-7.82	-2.16
344	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U			1.97		1.33	-0.73	-6.95	2.86
345	1-Butyl-4-(dimethylamino)pyridinium bromide	U			3.18		0.12	-0.73	-6.95	-2.16
346	1-Butyl-4-(dimethylamino)pyridinium chloride	L	2.55		3.22	-0.67	0.17	-0.73	-6.95	-2.31
347	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	1.38		1.22	0.16	0.94	-3.42	-6.49	2.86
348	4-(Dimethylamino)-1-hexylpyridinium chloride	U			2.46		0.59	-3.42	-6.49	-2.31
349	1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U			2.03		1.12	-0.15	-5.93	2.86
350	1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U			1.44		0.75	-2.22	-5.41	2.86
351	1-butyl-3-(2-hydroxyethyl)imidazolium chloride	U			4.25		2.00	6.56	2.86	-2.31
352	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride	U			1.92		2.00	-3.71	-1.36	-2.31
353	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride	U			1.15		2.63	-6.17	-0.01	-2.31
354	1-[(Decyloxy)methyl]-6-methylquinolinium chloride	U			0.60		2.79	-8.33	-0.33	-2.31

355	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride	U		-0.02	3.30	-10.30	0.77	-2.31	
356	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride	U		2.57	2.18	-0.56	0.61	-2.31	
357	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride	U		1.91	2.71	-2.66	1.72	-2.31	
358	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride	U		1.31	3.18	-4.64	2.67	-2.31	
359	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride	U		0.59	3.69	-7.05	3.58	-2.31	
360	1-Butylquinolinium tetrafluoroborate	U		2.12	0.26	-3.22	-7.41	-0.33	
361	1-Butylquinolinium bromide	U		2.56	0.28	-3.22	-7.41	-2.16	
362	1-Hexylquinolinium tetrafluoroborate	U		1.43	0.22	-5.56	-6.58	-0.33	
363	1-Octylquinolinium tetrafluoroborate	U		0.84	0.61	-7.55	-5.95	-0.33	
364	1-Octylquinolinium bromide	U		1.29	1.15	-7.55	-5.95	-2.16	
365	1-[(Hexyloxy)methyl]quinolinium chloride	U		2.11	1.77	-3.19	-1.99	-2.31	
366	1-[(Octyloxy)methyl]quinolinium chloride	U		1.55	2.04	-5.27	-1.84	-2.31	
367	1-[(Decyloxy)methyl]quinolinium chloride	U		0.84	2.61	-7.56	-0.68	-2.31	
368	1-[(Dodecyloxy)methyl]quinolinium chloride	U		0.34	3.02	-9.13	0.23	-2.31	
369	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		0.78	0.29	-4.42	-4.59	2.86	
370	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride	U		2.98	3.02	2.48	4.98	-2.31	
371	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide	U		3.03	3.15	3.15	5.90	-2.16	
372	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide	U		2.17	3.55	-0.04	6.08	-2.16	
373	1-Ethylpyridinium chloride	U		4.38	0.41	3.56	-7.36	-2.31	
374	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.23	1.14	5.10	-3.86	2.86	
375	1-(Cyanomethyl)pyridinium chloride	U		4.47	0.36	5.10	-3.86	-2.31	
376	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	U		1.43	5.17	-0.87	11.80	-2.16	
377	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide	U		0.48	5.69	-4.31	12.32	-2.16	
378	1-(2-Ethoxy-2-oxoethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.46	0.58	4.31	2.25	2.86	
379	1-(2-Ethoxy-2-oxoethyl)pyridinium octyl sulfate	U		2.23	0.29	4.31	2.25	3.86	
380	1-(2-Ethoxy-2-oxoethyl)pyridinium bromide	U		3.67	2.04	4.31	2.25	-2.16	
381	1-(2-Ethoxy-2-oxoethyl)pyridinium hexafluorophosphate	U		3.20	1.47	4.31	2.25	-0.21	
382	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.63	1.68	1.68	-7.24	2.86	
383	1-Propylpyridinium bromide	U		3.84	0.22	1.68	-7.24	-2.16	
384	1-Butylpyridinium chloride	L	3.18	3.64	-0.46	0.05	0.96	-6.71	-2.31
385	1-Butylpyridinium μ -chlorohexachlorodialuminate	T	3.01	2.74	0.27	1.04	0.96	-6.71	1.43
386	1-Butylpyridinium N-cyanocyanamide	U		3.08	0.63	0.96	-6.71	0.00	
387	1-Butylpyridinium bromide	U		3.60	0.00	0.96	-6.71	-2.16	
388	1-Butylpyridinium methyl sulfate	U		3.19	0.50	0.96	-6.71	-0.44	
389	1-Butylpyridinium octyl sulfate	U		2.16	1.74	0.96	-6.71	3.86	
390	1-Butylpyridinium tetrafluoroborate	U		3.16	0.53	0.96	-6.71	-0.33	
391	1-Butylpyridinium trifluoromethanesulfonate	U		3.07	0.65	0.96	-6.71	0.07	

392	1-Butylpyridinium hexafluorophosphate	U		3.13	0.56	0.96	-6.71	-0.21	
393	1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.03	1.19	-0.24	-6.22	2.86	
394	1-Pentylpyridinium bromide	U		3.24	0.27	-0.24	-6.22	-2.16	
395	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.82	1.03	-0.95	-5.90	2.86	
396	1-Hexylpyridinium trifluoromethanesulfonate	U		2.49	0.22	-0.95	-5.90	0.07	
397	1-Hexylpyridinium chloride	U		3.06	0.47	-0.95	-5.90	-2.31	
398	1-Hexylpyridinium hexafluorophosphate	U		2.56	0.13	-0.95	-5.90	-0.21	
399	1-Octylpyridinium chloride	L	1.69	2.34	-0.65	0.99	-3.41	-5.10	-2.31
400	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		1.09	0.54	-3.41	-5.10	2.86	
401	1-Decylpyridinium bromide	U		1.71	1.32	-5.41	-4.43	-2.16	
402	1-Hexadecylpyridinium bromide	U		-0.13	2.50	-11.79	-2.66	-2.16	
403	1-Hexadecylpyridinium chloride	U		-0.10	2.54	-11.79	-2.66	-2.31	
404	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	L	4.01	3.77	0.24	0.08	9.31	2.44	2.86
405	1-(3-Hydroxypropyl)pyridinium chloride	U		5.01	1.58	9.31	2.44	-2.31	
406	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		2.92	0.71	4.39	-2.54	2.86	
407	1-(3-Methoxypropyl)pyridinium chloride	U		4.17	0.79	4.39	-2.54	-2.31	
408	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate	U		5.40	1.69	14.74	7.66	0.07	
409	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		4.01	0.01	10.28	2.57	2.86	
410	1-(2-Hydroxyethyl)pyridinium iodide	U		5.09	1.31	10.28	2.57	-1.63	
411	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.48	0.93	6.51	-2.48	2.86	
412	1-(2-Methoxyethyl)pyridinium chloride	U		4.72	0.57	6.51	-2.48	-2.31	
413	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.02	0.74	4.79	-2.48	2.86	
414	1-(2-Ethoxyethyl)pyridinium bromide	U		4.23	0.72	4.79	-2.48	-2.16	
415	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		3.22	0.72	5.70	-2.01	2.86	
416	1-(Ethoxymethyl)pyridinium chloride	U		4.46	0.78	5.70	-2.01	-2.31	
417	1,1-Dihexylpyrrolidinium tetrafluoroborate	U		1.16	1.27	-5.18	-2.55	-0.33	
418	1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		0.13	0.04	-6.81	-4.32	2.86	
419	1,3-Didecyl-2-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U		-2.03	1.61	-13.99	-1.46	2.86	
420	1-Dodecyl-1-(2-hydroxyethyl)pyrrolidinium chloride	U		1.66	3.88	-2.02	6.35	-2.31	
421	1-(2-Hydroxyethyl)-2-methyl-3-tetradecylimidazolium chloride	U		0.90	3.87	-5.40	4.92	-2.31	
422	1-Hexadecyl-3-(2-hydroxyethyl)-2-methylimidazolium chloride	U		0.21	4.26	-7.84	5.39	-2.31	
423	1-(2-hydroxyethyl)-3-(2-phenylethyl)imidazolium chloride	U		3.17	2.40	2.41	2.66	-2.31	
424	1,3-di-(2-hydroxyethyl)imidazolium chloride	U		4.93	3.28	11.50	9.67	-2.31	
425	1,3-Bis(propoxymethyl)imidazolium chloride	U		2.99	2.37	1.60	2.22	-2.31	
426	1,3-Bis(butoxymethyl)imidazolium chloride	U		2.44	2.65	-0.46	2.39	-2.31	
427	1,3-Bis[(pentyloxy)methyl]imidazolium chloride	U		1.87	3.04	-2.37	3.08	-2.31	
428	1,3-Bis[(hexyloxy)methyl]imidazolium chloride	U		1.22	3.50	-4.54	3.90	-2.31	

429	1,3-Bis[(heptyloxy)methyl]imidazolium chloride	U	0.70	3.73	-6.51	3.95	-2.31
430	1,3-Bis[(octyloxy)methyl]imidazolium chloride	U	0.16	4.13	-8.29	4.70	-2.31
431	1,3-Bis[(nonyloxy)methyl]imidazolium chloride	U	-0.56	4.54	-10.86	5.16	-2.31
432	1,3-Bis[(decyloxy)methyl]imidazolium chloride	U	-0.94	4.64	-12.39	4.91	-2.31
433	1,3-Bis[(undecyloxy)methyl]imidazolium chloride	U	-1.49	5.15	-14.03	6.14	-2.31
434	1,3-Bis[(dodecyloxy)methyl]imidazolium chloride	U	-2.15	5.61	-16.24	6.96	-2.31
435	1,3-Bis[(tetradecyloxy)methyl]imidazolium chloride	U	-3.21	6.45	-19.66	8.67	-2.31
436	1,3-Bis[(hexadecyloxy)methyl]imidazolium chloride	U	-3.76	6.77	-21.63	9.04	-2.31
437	1-Methylimidazole hydrogen tetrafluoroborate	U	4.14	0.71	5.03	-5.69	-0.33
438	1-Methylimidazole 2-hydroxypropanoate	U	5.07	0.41	5.03	-5.69	-4.18
439	1-Methylimidazole (2S)-2-hydroxypropanoate	U	5.15	0.51	5.03	-5.69	-4.51
440	1-methylimidazolium acetate	U	5.48	0.90	5.03	-5.69	-5.87
441	1-methylimidazolium trifluoroacetate	U	4.62	0.13	5.03	-5.69	-2.30
442	1-methylimidazolium 1,1,1-trifluoromethanesulfonate	U	4.05	0.82	5.03	-5.69	0.07
443	1-Ethylimidazole 2-hydroxypropanoate	U	4.78	0.57	3.99	-5.53	-4.18
444	1-Ethylimidazole (2S)-2-hydroxypropanoate	U	4.86	0.67	3.99	-5.53	-4.51
445	1-Propylimidazole 2-hydroxypropanoate	U	4.33	0.76	2.28	-5.50	-4.18
446	1-Propylimidazole (2S)-2-hydroxypropanoate	U	4.41	0.86	2.28	-5.50	-4.51
447	1-Butylimidazole 2-hydroxypropanoate	U	3.94	1.05	1.00	-4.97	-4.18
448	1-Butylimidazole (2S)-2-hydroxypropanoate	U	4.02	1.14	1.00	-4.97	-4.51
449	1-butylimidazolium acetate	U	4.35	1.54	1.00	-4.97	-5.87
450	1-butylimidazolium trifluoroacetate	U	3.49	0.50	1.00	-4.97	-2.30
451	1-butylimidazolium 1,1,1-trifluoromethanesulfonate	U	2.92	0.18	1.00	-4.97	0.07
452	1-Pentylimidazole 2-hydroxypropanoate	U	3.52	1.30	-0.48	-4.65	-4.18
453	1-Pentylimidazole (2S)-2-hydroxypropanoate	U	3.60	1.39	-0.48	-4.65	-4.51
454	1-Hexylimidazole 2-hydroxypropanoate	U	3.32	1.49	-1.08	-4.19	-4.18
455	1-Hexylimidazole (2S)-2-hydroxypropanoate	U	3.40	1.58	-1.08	-4.19	-4.51
456	1-Heptylimidazole 2-hydroxypropanoate	U	2.88	1.72	-2.69	-4.01	-4.18
457	1-Heptylimidazole (2S)-2-hydroxypropanoate	U	2.96	1.81	-2.69	-4.01	-4.51
458	1-Octylimidazole 2-hydroxypropanoate	U	2.60	1.95	-3.55	-3.47	-4.18
459	1-Octylimidazole (2S)-2-hydroxypropanoate	U	2.68	2.05	-3.55	-3.47	-4.51
460	1-Nonylimidazole 2-hydroxypropanoate	U	2.30	2.13	-4.64	-3.28	-4.18
461	1-Nonylimidazole (2S)-2-hydroxypropanoate	U	2.38	2.22	-4.64	-3.28	-4.51
462	1-Decylimidazole 2-hydroxypropanoate	U	1.96	2.36	-5.78	-2.89	-4.18
463	1-Decylimidazole (2S)-2-hydroxypropanoate	U	2.04	2.45	-5.78	-2.89	-4.51
464	1-Undecylimidazole 2-hydroxypropanoate	U	1.72	2.54	-6.55	-2.51	-4.18
465	1-Undecylimidazole (2S)-2-hydroxypropanoate	U	1.80	2.64	-6.55	-2.51	-4.51

466	1-Dodecylimidazole 2-hydroxypropanoate	U	1.48	2.72	-7.34	-2.19	-4.18
467	1-Dodecylimidazole (2S)-2-hydroxypropanoate	U	1.56	2.81	-7.34	-2.19	-4.51
468	1-(Butoxymethyl)imidazole 2-hydroxypropanoate	U	3.62	2.24	1.36	-0.40	-4.18
469	1-(Butoxymethyl)imidazole (2S)-2-hydroxypropanoate	U	3.70	2.33	1.36	-0.40	-4.51
470	1-[(Pentyloxy)methyl]imidazole 2-hydroxypropanoate	U	3.29	2.38	0.12	-0.39	-4.18
471	1-[(Pentyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	3.37	2.47	0.12	-0.39	-4.51
472	1-[(Hexyloxy)methyl]imidazole 2-hydroxypropanoate	U	3.07	2.66	-0.43	0.45	-4.18
473	1-[(Hexyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	3.15	2.76	-0.43	0.45	-4.51
474	1-[(Heptyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.74	2.76	-1.75	0.26	-4.18
475	1-[(Heptyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.82	2.85	-1.75	0.26	-4.51
476	1-[(Octyloxy)methyl]imidazole 2-hydroxypropanoate	U	2.36	3.08	-2.94	0.97	-4.18
477	1-[(Octyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.44	3.17	-2.94	0.97	-4.51
478	1-[(Nonyloxy)methyl]imidazole 2-hydroxypropanoate	U	1.94	3.23	-4.56	0.87	-4.18
479	1-[(Nonyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	2.02	3.33	-4.56	0.87	-4.51
480	1-[(Decyloxy)methyl]imidazole 2-hydroxypropanoate	U	1.79	3.32	-5.09	0.97	-4.18
481	1-[(Decyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	1.87	3.41	-5.09	0.97	-4.51
482	1-[(Undecyloxy)methyl]imidazole 2-hydroxypropanoate	U	1.33	3.67	-6.60	1.67	-4.18
483	1-[(Undecyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	1.41	3.77	-6.60	1.67	-4.51
484	1-[(Dodecyloxy)methyl]imidazole 2-hydroxypropanoate	U	1.09	3.89	-7.33	2.17	-4.18
485	1-[(Dodecyloxy)methyl]imidazole (2S)-2-hydroxypropanoate	U	1.17	3.98	-7.33	2.17	-4.51
486	Pyridine hydrochloride	U	4.25	0.13	3.78	-5.25	-2.31
487	1-hexyl-1,4-diaza[2.2.2]bicyclooctanium bis(trifluoromethylsulfonyl)imide	U	2.42	0.30	3.71	0.96	2.86
488	1H-Imidazol-1-ium acetate	U	5.87	1.29	7.34	-3.31	-5.87
489	1H-Imidazol-1-ium trifluoroacetate	U	5.01	0.25	7.34	-3.31	-2.30
490	1H-Imidazol-1-ium 1,1,1-trifluoromethanesulfonate	U	4.44	0.44	7.34	-3.31	0.07
491	1,2-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	3.30	1.60	4.73	-5.69	2.86
492	1-hexyl-2,3-dimethyl imidazolium chloride midazolium chloride	U	2.73	0.59	-2.23	-6.01	-2.31
493	1,2-dimethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.62	1.56	1.81	-6.77	2.86
494	1-Methyl-3-octylimidazolium dicyanamide	U	1.83	0.37	-3.07	-4.67	0.00
495	1-buthyl-3-methylpyridinium1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.87	1.24	-1.02	-6.72	2.86
496	1-methyl-3-octylimidazolium hexafluoroantimonate	U	1.86	0.40	-3.07	-4.67	-0.12
497	1,3-dimethyl imidazolium dimethyl phopsphate	U	3.90	1.08	4.18	-6.87	0.20
498	1-methyl-3-octylimidazolium trifluoroacetate	U	2.39	1.03	-3.07	-4.67	-2.30
499	1-(2-hydroxyethyl)-3-methylimidazolium acetate	U	5.95	2.64	9.73	2.71	-5.87
500	1-(2-hydroxyethyl)-3-methylimidazolium dicyanamide	U	4.54	0.94	9.73	2.71	0.00
501	1-(2-hydroxyethyl)-3-methylimidazolium nitrate	U	5.11	1.62	9.73	2.71	-2.37

502	4-(Dimethylamino)-1-hexylpyridinium bromide	U	2.43	0.55	-3.42	-6.49	-2.16
503	1-octyl-4-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	0.76	0.40	-4.69	-5.10	2.86
504	1-butylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.40	1.46	0.96	-6.71	2.86
505	1-(2-hydroxyethyl)-1-methylpiperidinium N-cyanocyanamide	U	4.61	1.36	10.68	4.70	0.00
506	1-methyl-1-octylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.19	0.10	-2.33	-3.03	2.86
507	4-butyl-4-methylmorpholinium dicyanamide	U	3.86	0.61	6.23	0.06	0.00
508	4-(2-hydroxyethyl)-4-methylmorpholinium dicyanamide	U	4.97	1.89	13.05	7.64	0.00
509	1-ethyl-1-methylmorpholinium dicyanamide	U	4.60	0.21	8.90	-0.32	0.00
510	1-ethyl-1-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	3.91	0.62	8.90	-0.32	2.86
511	1-butyl-3-methylimidazolium acetate	U	4.32	1.33	0.58	-5.91	-5.87
512	1-hexyl-3-methylimidazolium acetate	U	3.75	1.60	-1.54	-5.78	-5.87
513	1-hexyl-3-methylimidazolium trifluoroacetate	U	2.89	0.57	-1.54	-5.78	-2.30
514	1-butyl-1-methylpyrrolidinium acetate	U	4.52	1.66	1.96	-4.12	-5.87
515	1-methyl-3-octylimidazolium nitrate	U	2.40	1.05	-3.07	-4.67	-2.37
516	1-butyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide	U	1.97	1.51	0.58	-5.91	3.93
517	1-methyl-3-octadecylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	-1.98	1.62	-13.76	-1.31	2.86
518	1-butyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.87	1.24	-1.02	-6.72	2.86
519	1-hexyl-3-methylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	1.25	0.73	-3.03	-5.66	2.86
520	1-methyl-1-propylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	U	2.75	1.06	3.13	-4.34	2.86

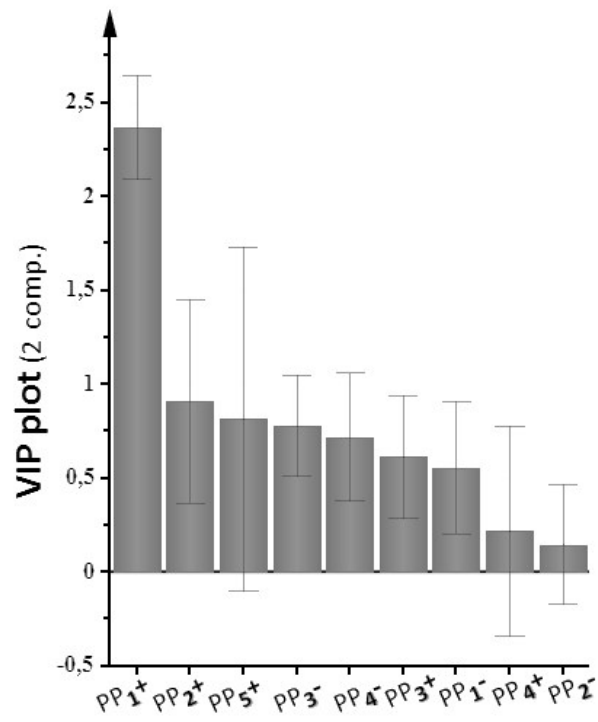


Figure S1. VIP plot resulting in 55x9 matrix correlation model.

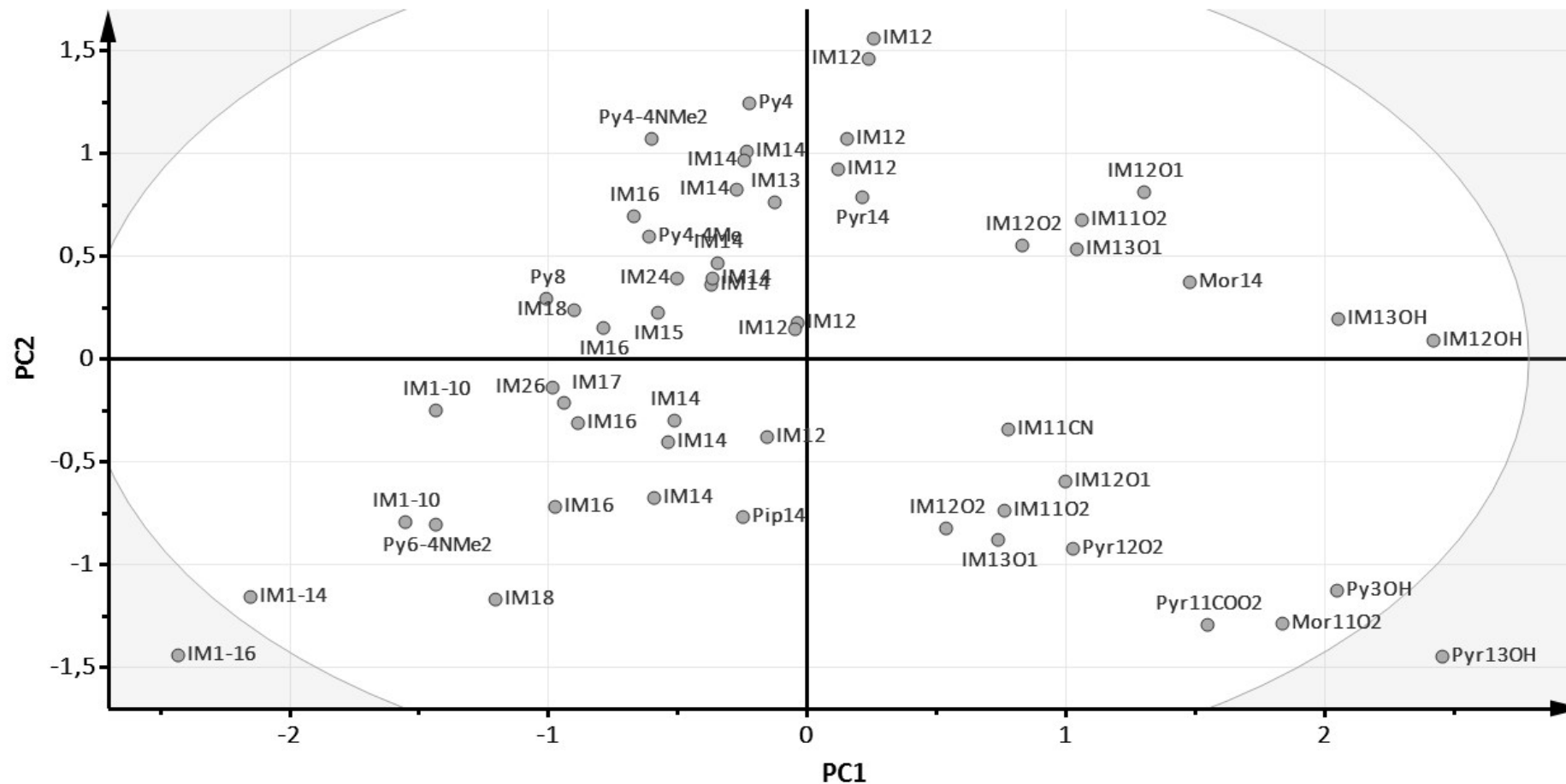


Figure S2 PC 1 vs PC 2 scores plot for *Vibrio fischeri* toxicity PLS model. Log(EC_{50}) increases from the bottom left to the upper right. The scores plot is a window in the X space displaying how the object are situated with respect to each other. In this plot labels refer to their cationic substituents:

- for imidazolium-based ILs (IM): the first value refers to the first *N*-substituent; the second values (and the following molecular group) refers to the second one (*i. e.*: "12" means "*N*-methyl-*N*-ethyl"; "1-16" means "*N*-methyl-*N*-hexadecyl"; "12O1" means "*N*-methyl-*N*-(methoxyethyl)").
- for pyrrolidinium, piperidinium and morpholinium-based ILs (PYR, PIP, MOR): the first value refers to the first *N*-substituent; the second values (and the following molecular group) refers to the second one in the same nitrogen atom (*i. e.*: 14 means "*N*-butyl-*N*-methyl");
- for pyridinium-based ILs (PY): the first value refers to the *N*-substituent; if present, the second values (and the following molecular group) refers to the second one and its *C*-position (*i. e.*: Py4-4NMe2 means "1-methyl-4-dimethylaminopyridinium").

In PLS Q^2 assesses the predictive power of the model and a permutation plot⁴⁰ 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 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, the fulfilment of some important criteria is 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 reported in Figure S4 was obtained by considering 50 random PLS models, and strongly indicates that the PLS correlation model can be considered valid.