

Supplementary Informations

S1: The 403 heterocyclic ILs in the Overall toxicity model.

	CAS no.	Name
1	151200-14-5	1-Methylimidazolium hydrogen tetrafluoroborate
2	615538-92-6	1-Methylimidazolium 2-hydroxypropanoate
3	1010075-76-9	1-Methylimidazolium (2S)-2-hydroxypropanoate
4	615539-01-0	1-Decylimidazolium 2-hydroxypropanoate
5	898223-27-3	1-Decylimidazolium (2S)-2-hydroxypropanoate
6	615539-02-1	1-Undecylimidazolium 2-hydroxypropanoate
7	885224-27-1	1-Undecylimidazolium (2S)-2-hydroxypropanoate
8	615539-03-2	1-Dodecylimidazolium 2-hydroxypropanoate
9	898558-89-9	1-Dodecylimidazolium (2S)-2-hydroxypropanoate
10	615539-10-1	1-[(Decyloxy)methyl]imidazolium 2-hydroxypropanoate
11	885224-30-6	1-[(Decyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
12	615539-11-2	1-[(Undecyloxy)methyl]imidazolium 2-hydroxypropanoate
13	none (2013-09-19)	1-[(Undecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
14	615539-12-3	1-[(Dodecyloxy)methyl]imidazolium 2-hydroxypropanoate
15	898558-92-4	1-[(Dodecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
16	615539-04-3	1-(Butoxymethyl)imidazolium 2-hydroxypropanoate
17	885224-28-2	1-(Butoxymethyl)imidazolium (2S)-2-hydroxypropanoate
18	615539-05-4	1-[(Pentyloxy)methyl]imidazolium 2-hydroxypropanoate
19	none (2013-09-19)	1-[(Pentyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
20	615539-06-5	1-[(Hexyloxy)methyl]imidazolium 2-hydroxypropanoate
21	885224-29-3	1-[(Hexyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
22	615539-07-6	1-[(Heptyloxy)methyl]imidazolium 2-hydroxypropanoate
23	none (2013-09-19)	1-[(Heptyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
24	615539-08-7	1-[(Octyloxy)methyl]imidazolium 2-hydroxypropanoate
25	898558-90-2	1-[(Octyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
26	615539-09-8	1-[(Nonyloxy)methyl]imidazolium 2-hydroxypropanoate
27	898558-91-3	1-[(Nonyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
28	615538-93-7	1-Ethylimidazolium 2-hydroxypropanoate
29	none (2013-09-19)	1-Ethylimidazolium (2S)-2-hydroxypropanoate
30	615538-94-8	1-Propylimidazolium 2-hydroxypropanoate
31	none (2013-09-19)	1-Propylimidazolium (2S)-2-hydroxypropanoate
32	885224-25-9	1-Butylimidazolium (2S)-2-hydroxypropanoate
33	615538-96-0	1-Pentylimidazolium 2-hydroxypropanoate

34	none (2013-09-19)	1-Pentylimidazolium (2S)-2-hydroxypropanoate
35	615538-97-1	1-Hexylimidazolium 2-hydroxypropanoate
36	885224-26-0	1-Hexylimidazolium (2S)-2-hydroxypropanoate
37	615538-98-2	1-Heptylimidazolium 2-hydroxypropanoate
38	none (2013-09-19)	1-Heptylimidazolium (2S)-2-hydroxypropanoate
39	615538-99-3	1-Octylimidazolium 2-hydroxypropanoate
40	898558-87-7	1-Octylimidazolium (2S)-2-hydroxypropanoate
41	615539-00-9	1-Nonylimidazolium 2-hydroxypropanoate
42	898558-88-8	1-Nonylimidazolium (2S)-2-hydroxypropanoate
43	847335-66-4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate
44	637348-60-8	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride
45	952429-66-2	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate
46	1310460-36-6	1,3-Didecyl-2-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
47	174899-81-1	1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
48	1241842-81-8	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride
49	1241842-26-1	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide
50	244193-56-4	1-Decyl-3-methylimidazolium tetrafluoroborate
51	188589-32-4	1-Decyl-3-methylimidazolium bromide
52	171058-18-7	1-Decyl-3-methylimidazolium chloride
53	362043-46-7	1-Decyl-3-methylimidazolium hexafluorophosphate
54	none (2013-09-19)	1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide
55	171058-21-2	1-Methyl-3-tetradecylimidazolium chloride
56	61546-01-8	1-Hexadecyl-3-methylimidazolium chloride
57	171058-19-8	1-Methyl-3-octadecylimidazolium chloride
58	937720-90-6	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
59	154312-63-7	1-(Cyanomethyl)-3-methylimidazolium chloride
60	503439-24-5	1-[2-(Butylamino)-2-oxoethyl]-3-methylimidazolium bromide
61	503439-25-6	1-[2-(Butylmethylamino)-2-oxoethyl]-3-methylimidazolium bromide
62	109833-17-2	1-(2-Methoxy-2-oxoethyl)-3-methylimidazolium bromide
63	1241842-28-3	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide
64	503439-30-3	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium tetrafluoroborate
65	109833-18-3	1-(2-Ethoxy-2-oxoethyl)-3-methylimidazolium bromide
66	503439-64-3	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
67	911066-07-4	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate
68	503439-32-5	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium tetrafluoroborate
69	503439-21-2	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide
70	1065248-59-0	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium N-cyanocyanamide
71	503439-51-8	1-Methyl-3-(2-oxo-2-propoxyethyl)imidazolium hexafluorophosphate
72	911066-16-5	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium octylsulfate
73	911066-10-9	1,2-Dimethyl-3-(2-oxo-2-propoxyethyl)imidazolium bromide

74	808184-31-8	1-(2-Butoxy-2-oxoethyl)-3-methylimidazolium bromide
75	911066-18-7	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate
76	808184-34-1	1-Methyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide
77	911066-21-2	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium octylsulfate
78	911066-13-2	1,2-Dimethyl-3-[2-oxo-2-(pentyloxy)ethyl]imidazolium bromide
79	503439-22-3	1-[2-(Hexyloxy)-2-oxoethyl]-3-methylimidazolium bromide
80	503439-23-4	1-Methyl-3-[2-(octyloxy)-2-oxoethyl]imidazolium bromide
81	945996-13-4	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
82	945996-02-1	1-(Ethoxymethyl)-3-methylimidazolium chloride
83	500996-04-3	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate
84	36443-80-8	1-Methyl-3-(phenylmethyl)imidazolium chloride
85	433337-11-2	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate
86	376650-04-3	1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato-O1,O2]borate
87	852616-00-3	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate
88	878005-11-9	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate
89	174899-82-2	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
90	376650-06-5	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate
91	143314-17-4	1-Ethyl-3-methylimidazolium acetate
92	790663-77-3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate
93	516474-01-4	1-Ethyl-3-methylimidazolium methyl sulfate
94	145022-45-3	1-Ethyl-3-methylimidazolium methanesulfonate
95	342573-75-5	1-Ethyl-3-methylimidazolium ethyl sulfate
96	328090-25-1	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate
97	790663-79-5	1-Ethyl-3-methylimidazolium octylsulfate
98	742099-80-5	1-Ethyl-3-methylimidazolium tetracyanoborate
99	143314-16-3	1-Ethyl-3-methylimidazolium tetrafluoroborate
100	666823-18-3	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile (1:1)
101	174899-65-1	1-Ethyl-3-methylimidazolium trifluoroacetate
102	145022-44-2	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate
103	65039-09-0	1-Ethyl-3-methylimidazolium chloride
104	412009-61-1	1-Ethyl-3-methylimidazolium hydrogen sulfate
105	370865-89-7	1-Ethyl-3-methylimidazolium N-cyanocyanamide
106	331717-63-6	1-Ethyl-3-methylimidazolium thiocyanate
107	65039-10-3	1-Methyl-3-(2-propenyl)imidazolium chloride
108	313475-50-2	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate
109	952429-67-3	1-Methyl-3-(3-oxobutyl)imidazolium bromide
110	1739-84-0	1,2-Dimethylimidazolium
111	178631-01-1	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
112	474972-46-8	1-(2-Methoxyethyl)-3-methylimidazolium chloride
113	778593-17-2	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide

114	1012793-99-5	1-(2-Ethoxyethyl)-3-methylimidazolium bromide
115	474972-49-1	1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride
116	174899-86-6	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
117	374564-83-7	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate
118	1012794-00-1	1-(2-Hydroxyethyl)-3-methylimidazolium iodide
119	845835-00-9	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate
120	187332-85-0	1-Methyl-3-(2-phenylethyl)imidazolium chloride
121	433337-12-3	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate
122	216299-72-8	1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
123	244193-48-4	1-Methyl-3-propylimidazolium tetrafluoroborate
124	79917-89-8	1-Methyl-3-propylimidazolium chloride
125	216300-12-8	1-Methyl-3-propylimidazolium hexafluorophosphate
126	805228-35-7	3-(3-Carboxypropyl)-1-methylimidazolium chloride
127	1015254-36-0	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
128	1012794-06-7	1-(3-Methoxypropyl)-3-methylimidazolium chloride
129	827027-30-5	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
130	355011-34-6	1-(3-Hydroxypropyl)-3-methylimidazolium chloride
131	917762-91-5	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate
132	710336-91-7	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminat
133	174899-83-3	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
134	595565-54-1	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate
135	401788-98-5	1-Butyl-3-methylimidazolium methyl sulfate
136	342789-81-5	1-Butyl-3-methylimidazolium methanesulfonate
137	410522-18-8	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate
138	445473-58-5	1-Butyl-3-methylimidazolium octylsulfate
139	174501-65-6	1-Butyl-3-methylimidazolium tetrafluoroborate
140	85100-77-2	1-Butyl-3-methylimidazolium bromide
141	174899-66-2	1-Butyl-3-methylimidazolium trifluoromethanesulfonate
142	79917-90-1	1-Butyl-3-methylimidazolium chloride
143	385384-39-4	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate
144	359845-21-9	1-Butyl-3-methylimidazolium tetrachloroferrate
145	262297-13-2	1-Butyl-3-methylimidazolium hydrogen sulfate
146	65039-05-6	1-Butyl-3-methylimidazolium iodide
147	448245-52-1	1-Butyl-3-methylimidazolium N-cyanocyanamide
148	none (2013-09-19)	1-Butyl-3-methylimidazolium hexafluorophosphate
149	174645-81-9	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate
150	344790-87-0	1-Butyl-3-methylimidazolium thiocyanate
151	350493-08-2	1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
152	402846-78-0	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate
153	765910-73-4	1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate

154	864665-30-5	1-(4-Hydroxybutyl)-3-methylimidazolium chloride
155	280779-53-5	1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
156	244193-49-5	1-Methyl-3-pentylimidazolium tetrafluoroborate
157	171058-22-3	1-Methyl-3-pentylimidazolium chloride
158	280779-52-4	1-Methyl-3-pentylimidazolium hexafluorophosphate
159	697248-62-7	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)
160	713512-19-7	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate
161	943229-71-8	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate
162	382150-50-7	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
163	1196206-01-5	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide (1:1)
164	244193-50-8	1-Hexyl-3-methylimidazolium tetrafluoroborate
165	85100-78-3	1-Hexyl-3-methylimidazolium bromide
166	171058-17-6	1-Hexyl-3-methylimidazolium chloride
167	304680-35-1	1-Hexyl-3-methylimidazolium hexafluorophosphate
168	384347-21-1	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate
169	425382-14-5	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
170	244193-51-9	1-Heptyl-3-methylimidazolium tetrafluoroborate
171	581101-92-0	1-Heptyl-3-methylimidazolium chloride
172	357915-04-9	1-Heptyl-3-methylimidazolium hexafluorophosphate
173	952429-64-0	1-(7-Carboxyheptyl)-3-methylimidazolium bromide
174	178631-04-4	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
175	817575-02-3	3-Methyl-1-octylimidazolium octylsulfate
176	244193-52-0	1-Methyl-3-octylimidazolium tetrafluoroborate
177	61545-99-1	1-Methyl-3-octylimidazolium bromide
178	403842-84-2	1-Methyl-3-octylimidazolium trifluoromethanesulfonate
179	64697-40-1	1-Methyl-3-octylimidazolium chloride
180	304680-36-2	1-Methyl-3-octylimidazolium hexafluorophosphate
181	952429-65-1	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide
182	244193-55-3	1-Methyl-3-nonylimidazolium tetrafluoroborate
183	171058-20-1	1-Methyl-3-nonylimidazolium chloride
184	343952-29-4	1-Methyl-3-nonylimidazolium hexafluorophosphate
185	none (2013-09-19)	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
186	761410-66-6	1,3-Bis[(decyloxy)methyl]imidazolium chloride
187	761410-67-7	1,3-Bis[(undecyloxy)methyl]imidazolium chloride
188	761410-68-8	1,3-Bis[(dodecyloxy)methyl]imidazolium chloride
189	none (2013-09-19)	1,3-Bis[(tetradecyloxy)methyl]imidazolium chloride
190	none (2013-09-19)	1,3-Bis[(hexadecyloxy)methyl]imidazolium chloride
191	126049-85-2	1,3-Bis(propoxymethyl)imidazolium chloride
192	761410-60-0	1,3-Bis(butoxymethyl)imidazolium chloride
193	761410-61-1	1,3-Bis[(pentyloxy)methyl]imidazolium chloride

194	761410-62-2	1,3-Bis[(hexyloxy)methyl]imidazolium chloride
195	761410-63-3	1,3-Bis[(heptyloxy)methyl]imidazolium chloride
196	761410-64-4	1,3-Bis[(octyloxy)methyl]imidazolium chloride
197	761410-65-5	1,3-Bis[(nonyloxy)methyl]imidazolium chloride
198	581101-93-1	1-Decyl-3-ethylimidazolium bromide
199	174899-88-8	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
200	54304-66-4	1,3-Diethylimidazolium bromide
201	347882-21-7	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
202	637348-59-5	1-Ethyl-3-propylimidazolium bromide
203	581101-91-9	1-Butyl-3-ethylimidazolium tetrafluoroborate
204	174899-96-8	1-Butyl-3-ethylimidazolium trifluoroacetate
205	145022-48-6	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate
206	393550-29-3	1-Ethyl-3-hexylimidazolium tetrafluoroborate
207	547719-00-6	1-Ethyl-3-hexylimidazolium bromide
208	none (2013-09-19)	1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
209	749921-07-1	1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
210	none (2013-09-19)	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
211	none (2013-09-19)	1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
212	68039-12-3	1H-Imidazolium, 1-ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)-, ethyl sulfate
213	1040381-03-0	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
214	1012794-13-6	4-(Cyanomethyl)-4-methylmorpholinium chloride
215	1049751-90-7	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
216	1012794-15-8	4-(Ethoxymethyl)-4-methylmorpholinium chloride
217	445497-25-6	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate
218	796039-07-1	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
219	1012794-10-3	4-(2-Methoxyethyl)-4-methylmorpholinium chloride
220	663628-48-6	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
221	1012794-09-0	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide
222	868742-24-9	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
223	53875-78-8	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide
224	1049751-91-8	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
225	1012794-12-5	4-(3-Methoxypropyl)-4-methylmorpholinium chloride
226	1026019-24-8	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
227	1012794-11-4	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride
228	324574-95-0	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
229	75174-77-5	4-Butyl-4-methylmorpholinium bromide
230	1309983-34-3	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
231	194986-67-9	1-(Cyanomethyl)-1-methylpiperidinium chloride
232	1049751-93-0	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
233	1012794-08-9	1-(Ethoxymethyl)-1-methylpiperidinium chloride

234	873583-83-6	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
235	886439-37-8	1-(2-Methoxyethyl)-1-methylpiperidinium bromide
236	663628-45-3	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
237	663628-44-2	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide
238	757212-03-6	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
239	67889-35-4	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide
240	608140-12-1	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
241	none (2013-09-19)	1-Methyl-1-propylpiperidinium hexafluorophosphate
242	1049751-95-2	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
243	1012794-04-5	1-(3-Methoxypropyl)-1-methylpiperidinium chloride
244	1049751-96-3	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
245	1334291-67-6	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride
246	623580-02-9	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
247	94280-72-5	1-Butyl-1-methylpiperidinium bromide
248	628-13-7	Pyridine hydrochloride
249	1241842-94-3	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide
250	1241840-01-6	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride
251	1424967-13-4	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide
252	7538-79-6	4-(Dimethylamino)-1-methylpyridinium iodide
253	1017553-46-6	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
254	17281-59-3	1-(Cyanomethyl)pyridinium chloride
255	1241839-96-2	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide
256	1241842-60-3	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide
257	435346-40-0	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride
258	435346-66-0	3-[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride
259	435346-34-2	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride
260	435346-58-0	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate
261	435346-54-6	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorocobaltate
262	435346-55-7	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorocuprate
263	435346-57-9	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachloromagnesate
264	435346-56-8	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorozincate
265	435346-76-2	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride
266	435346-35-3	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride
267	1127350-84-8	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)
268	1127350-78-0	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate (1:1)
269	454234-78-7	3-Hydroxy-1-[(undecyloxy)methyl]pyridinium chloride
270	435346-77-3	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride
271	435346-53-5	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate
272	435346-52-4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate
273	435346-41-1	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide

274	435346-36-4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride
275	435346-45-5	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate
276	435346-42-2	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide
277	435346-44-4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate
278	435346-78-4	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride
279	1277184-36-7	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)
280	1277184-26-5	3-Hydroxy-1-[(octadecyloxy)methyl]pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate (1:1)
281	1049751-98-5	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
282	21379-36-2	1-(Ethoxymethyl)pyridinium chloride
283	1127350-79-1	3-Hydroxy-1-(propoxymethyl)pyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)
284	1127350-73-5	3-Hydroxy-1-(propoxymethyl)pyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate (1:1)
285	454234-70-9	3-Hydroxy-1-(propoxymethyl)pyridinium chloride
286	1127350-80-4	1-(Butoxymethyl)-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)
287	1127350-74-6	1-(Butoxymethyl)-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate (1:1)
288	1127350-82-6	1-[(Hexyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)
289	1127350-76-8	1-[(Hexyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate (1:1)
290	435346-63-7	3-[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride
291	1127350-83-7	1-[(Heptyloxy)methyl]-3-hydroxypyridinium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)
292	1127350-77-9	1-[(Heptyloxy)methyl]-3-hydroxypyridinium 6-methyl-2,2-dioxo-1,2,3-oxathiazin-4(3H)-onate (1:1)
293	454234-74-3	1-[(Heptyloxy)methyl]-3-hydroxypyridinium chloride
294	435346-64-8	3-[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride
295	435346-65-9	3-[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride
296	2294-38-4	1-Ethylpyridinium chloride
297	900797-77-5	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
298	114203-57-5	4-(Dimethylamino)-1-ethylpyridinium bromide
299	863663-01-8	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
300	209679-88-9	1-(2-Methoxyethyl)pyridinium chloride
301	849418-12-8	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
302	108153-25-9	1-(2-Ethoxyethyl)pyridinium bromide
303	752260-02-9	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
304	69095-13-2	1-(2-Hydroxyethyl)pyridinium iodide
305	1104525-90-7	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
306	873-71-2	1-Propylpyridinium bromide
307	1049752-00-2	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
308	1012794-07-8	1-(3-Methoxypropyl)pyridinium chloride
309	827027-29-2	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
310	187863-16-7	1-(3-Hydroxypropyl)pyridinium chloride
311	941580-56-9	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate
312	885456-20-2	1-Butylpyridinium methyl sulfate
313	67226-45-3	1-Butylpyridinium μ -chlorohexachlorodialuminate

314	203389-28-0	1-Butylpyridinium tetrafluoroborate
315	874-80-6	1-Butylpyridinium bromide
316	390423-43-5	1-Butylpyridinium trifluoromethanesulfonate
317	1124-64-7	1-Butylpyridinium chloride
318	827033-71-6	1-Butylpyridinium N-cyanocyanamide
319	186088-50-6	1-Butylpyridinium hexafluorophosphate
320	286453-46-1	1-Butyl-2-methylpyridinium tetrafluoroborate
321	112400-85-8	1-Butyl-2-methylpyridinium chloride
322	597581-48-1	1-Butyl-3-methylpyridinium tetrafluoroborate
323	26576-85-2	1-Butyl-3-methylpyridinium bromide
324	125652-55-3	1-Butyl-3-methylpyridinium chloride
325	712355-12-9	1-Butyl-3-methylpyridinium N-cyanocyanamide
326	845835-03-2	1-Butyl-3-methylpyridinium hexafluorophosphate
327	952429-71-9	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate
328	916730-30-8	1-Butyl-3,4-dimethylpyridinium chloride
329	952429-72-0	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate
330	26576-98-7	1-Butyl-3,5-dimethylpyridinium bromide
331	916730-31-9	1-Butyl-3,5-dimethylpyridinium chloride
332	877678-54-1	1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide
333	883860-38-6	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate
334	742099-83-8	1-Butyl-4-methylpyridinium tetracyanoborate
335	343952-33-0	1-Butyl-4-methylpyridinium tetrafluoroborate
336	112400-86-9	1-Butyl-4-methylpyridinium chloride
337	401788-99-6	1-Butyl-4-methylpyridinium hexafluorophosphate
338	900797-79-7	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
339	82522-15-4	1-Butyl-4-(dimethylamino)pyridinium chloride
340	890532-45-3	1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
341	53385-72-1	1-Pentylpyridinium bromide
342	460983-97-5	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
343	623167-81-7	1-Hexylpyridinium trifluoromethanesulfonate
344	6220-15-1	1-Hexylpyridinium chloride
345	797789-00-5	1-Hexylpyridinium hexafluorophosphate
346	67021-56-1	1-Hexyl-3-methylpyridinium bromide
347	916730-40-0	1-Hexyl-3-methylpyridinium chloride
348	952429-73-1	1-Hexyl-4-methylpyridinium tetrafluoroborate
349	62409-49-8	1-Hexyl-4-methylpyridinium chloride
350	872672-57-6	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
351	1012794-14-7	4-(Dimethylamino)-1-hexylpyridinium chloride
352	384347-06-2	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
353	4086-73-1	1-Octylpyridinium chloride

354	872672-72-5	3-Methyl-1-octylpyridinium bromide
355	864461-36-9	3-Methyl-1-octylpyridinium chloride
356	936239-96-2	4-Methyl-1-octylpyridinium tetrafluoroborate
357	141645-91-2	4-Methyl-1-octylpyridinium chloride
358	1017553-47-7	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
359	194986-69-1	1-(Cyanomethyl)-1-methylpyrrolidinium chloride
360	1187194-44-0	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate
361	1107545-20-9	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
362	129412-64-2	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide
363	1373334-02-1	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
364	151263-00-2	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride
365	1195983-48-2	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate
366	757240-24-7	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
367	1012794-01-2	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride
368	663628-46-4	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
369	833446-39-2	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide
370	757212-04-7	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
371	54770-67-1	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide
372	327022-58-2	1-Methyl-1-propylpyrrolidinium hexafluorophosphate
373	1373334-04-3	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
374	1012794-05-6	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride
375	1332694-08-2	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
376	941584-15-2	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride
377	851856-47-8	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate
378	223437-11-4	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
379	345984-11-4	1-Butyl-1-methylpyrrolidinium tetrafluoroborate
380	93457-69-3	1-Butyl-1-methylpyrrolidinium bromide
381	479500-35-1	1-Butyl-1-methylpyrrolidinium chloride
382	370865-80-8	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide
383	380497-19-8	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
384	909398-59-0	1-Hexyl-1-methylpyrrolidinium chloride
385	952429-74-2	1-Methyl-1-octylpyrrolidinium tetrafluoroborate
386	909398-60-3	1-Methyl-1-octylpyrrolidinium chloride
387	13501-50-3	1-[(Decyloxy)methyl]quinolinium chloride
388	97166-43-3	1-[(Decyloxy)methyl]-6-methylquinolinium chloride
389	97166-47-7	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride
390	41063-22-3	1-[(Dodecyloxy)methyl]quinolinium chloride
391	97166-44-4	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride
392	97166-48-8	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride
393	97166-39-7	1-[(Hexyloxy)methyl]quinolinium chloride

394	97166-41-1	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride
395	97166-45-5	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride
396	97166-40-0	1-[(Octyloxy)methyl]quinolinium chloride
397	97166-42-2	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride
398	97166-46-6	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride
399	952429-68-4	1-Butylquinolinium tetrafluoroborate
400	31537-79-8	1-Butylquinolinium bromide
401	952429-69-5	1-Hexylquinolinium tetrafluoroborate
402	952429-70-8	1-Octylquinolinium tetrafluoroborate
403	14848-21-6	1-Octylquinolinium bromide

S2: The 35 variables in the Overall toxicity model.

	Variables	unit
1	<i>Candida albicans</i> ATCC 10231 (growth inhibition) 48h	log(MIC)
2	<i>Candida albicans</i> ATCC 10231 (death) 5d	log(MBC)
3	<i>Enterococcus hirae</i> ATCC 10541 (growth inhibition) 24h	log(MIC)
4	<i>Enterococcus hirae</i> ATCC 10541 (death) 48h	log(MBC)
5	<i>Escherichia coli</i> ATCC 25922 (growth inhibition) 24h	log(MIC)
6	<i>Escherichia coli</i> ATCC 25922 (death) 48h	log(MBC)
7	<i>Klebsiella pneumoniae</i> ATCC 4352 (growth inhibition) 24h	log(MIC)
8	<i>Klebsiella pneumoniae</i> ATCC 4352 (death) 48h	log(MBC)
9	<i>Lemna minor</i> (frond area) 7d	log(EC50)
10	<i>Lemna minor</i> (frond number) 7d	log(EC50)
11	<i>Micrococcus luteus</i> ATCC 9341 (growth inhibition) 24h	log(MIC)
12	<i>Micrococcus luteus</i> ATCC 9341 (death) 48h	log(MBC)
13	<i>Proteus vulgaris</i> NCTC 4635 (growth inhibition) 24h	log(MIC)
14	<i>Proteus vulgaris</i> NCTC 4635 (death) 48h	log(MBC)
15	<i>Pseudomonas aeruginosa</i> ATCC 27853 (growth inhibition) 24h	log(MIC)
16	<i>Pseudomonas aeruginosa</i> ATCC 27853 (death) 48h	log(MBC)
17	<i>Pseudomonas aeruginosa</i> NCTC 6749 (growth inhibition) 24h	log(MIC)
18	<i>Rhodotorula rubra</i> PhB (growth inhibition) 48h	log(MIC)
19	<i>Rhodotorula rubra</i> PhB (death) 5d	log(MBC)
20	<i>Scenedesmus vacuolatus</i> (cell count) 24h	log(EC50)
21	<i>Serratia marcescens</i> ATCC 8100 (growth inhibition) 24h	log(MIC)
22	<i>Serratia marcescens</i> ATCC 8100 (death) 48h	log(MBC)
23	<i>Staphylococcus aureus</i> ATCC 6538 (growth inhibition) 24h	log(MIC)
24	<i>Staphylococcus aureus</i> ATCC 6538 (death) 48h	log(MBC)
25	<i>Staphylococcus aureus</i> (MRSA) (growth inhibition) 24h	log(MIC)
26	<i>Staphylococcus aureus</i> (MRSA) (death) 48h	log(MBC)
27	<i>Staphylococcus aureus</i> NCTC 4163 (growth inhibition) 24h	log(MIC)
28	<i>Staphylococcus epidermidis</i> ATCC 12228 (growth inhibition) 24h	log(MIC)
29	<i>Staphylococcus epidermidis</i> ATCC 12228 (death) 48h	log(MBC)
30	<i>Vibrio fischeri</i> 5'	log(EC50)
31	<i>Vibrio fischeri</i> 15'	log(EC50)
32	<i>Vibrio fischeri</i> 30'	log(EC50)
33	Acetylcholinesterase inhibition	log(EC50)
34	IPC-81 leukemia cells cytotoxicity	log(EC50)
35	BOD 28 d	%

S3: The 104 ILs in the Aquatic toxicity model.

CAS no.	Name
1	174899-81-1 1,3-Dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
2	1241842-81-8 1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]-3-methylimidazolium chloride
3	1241842-26-1 1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]-3-methylimidazolium bromide
4	244193-56-4 1-Decyl-3-methylimidazolium tetrafluoroborate
5	none (2013-09-19) 1-(11-Ethoxy-11-oxoundecyl)-3-methylimidazolium bromide
6	171058-21-2 1-Methyl-3-tetradecylimidazolium chloride
7	61546-01-8 1-Hexadecyl-3-methylimidazolium chloride
8	171058-19-8 1-Methyl-3-octadecylimidazolium chloride
9	937720-90-6 1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
10	154312-63-7 1-(Cyanomethyl)-3-methylimidazolium chloride
11	1241842-28-3 1-[2-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl]-3-methylimidazolium bromide
12	945996-13-4 1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
13	945996-02-1 1-(Ethoxymethyl)-3-methylimidazolium chloride
14	376650-04-3 1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato(2-)-O1,O2]borate
15	852616-00-3 1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate
16	878005-11-9 1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate
17	174899-82-2 1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
18	342573-75-5 1-Ethyl-3-methylimidazolium ethyl sulfate
19	742099-80-5 1-Ethyl-3-methylimidazolium tetracyanoborate
20	666823-18-3 1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile (1:1)
21	65039-09-0 1-Ethyl-3-methylimidazolium chloride
22	370865-89-7 1-Ethyl-3-methylimidazolium N-cyanocyanamide
23	178631-01-1 1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
24	474972-46-8 1-(2-Methoxyethyl)-3-methylimidazolium chloride
25	778593-17-2 1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
26	1012793-99-5 1-(2-Ethoxyethyl)-3-methylimidazolium bromide
27	474972-49-1 1-[2-(2-Methoxyethoxy)ethyl]-3-methylimidazolium chloride
28	1012794-00-1 1-(2-Hydroxyethyl)-3-methylimidazolium iodide
29	216299-72-8 1-Methyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
30	244193-48-4 1-Methyl-3-propylimidazolium tetrafluoroborate
31	216300-12-8 1-Methyl-3-propylimidazolium hexafluorophosphate
32	1015254-36-0 1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
33	1012794-06-7 1-(3-Methoxypropyl)-3-methylimidazolium chloride
34	827027-30-5 1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
35	355011-34-6 1-(3-Hydroxypropyl)-3-methylimidazolium chloride
36	710336-91-7 1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanamine
37	174899-83-3 1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
38	342789-81-5 1-Butyl-3-methylimidazolium methanesulfonate
39	410522-18-8 1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate
40	445473-58-5 1-Butyl-3-methylimidazolium octylsulfate
41	174501-65-6 1-Butyl-3-methylimidazolium tetrafluoroborate
42	85100-77-2 1-Butyl-3-methylimidazolium bromide
43	174899-66-2 1-Butyl-3-methylimidazolium trifluoromethanesulfonate
44	79917-90-1 1-Butyl-3-methylimidazolium chloride
45	65039-05-6 1-Butyl-3-methylimidazolium iodide
46	448245-52-1 1-Butyl-3-methylimidazolium N-cyanocyanamide
47	none (2013-09-19) 1-Butyl-3-methylimidazolium hexafluorophosphate
48	350493-08-2 1-Butyl-2,3-dimethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
49	280779-53-5 1-Methyl-3-pentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
50	244193-49-5 1-Methyl-3-pentylimidazolium tetrafluoroborate
51	697248-62-7 1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)
52	382150-50-7 1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
53	244193-50-8 1-Hexyl-3-methylimidazolium tetrafluoroborate
54	85100-78-3 1-Hexyl-3-methylimidazolium bromide
55	171058-17-6 1-Hexyl-3-methylimidazolium chloride

56	304680-35-1	1-Hexyl-3-methylimidazolium hexafluorophosphate
57	425382-14-5	1-Heptyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
58	244193-51-9	1-Heptyl-3-methylimidazolium tetrafluoroborate
59	178631-04-4	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
60	244193-52-0	1-Methyl-3-octylimidazolium tetrafluoroborate
61	61545-99-1	1-Methyl-3-octylimidazolium bromide
62	244193-55-3	1-Methyl-3-nonylimidazolium tetrafluoroborate
63	none (2013-09-19)	1-Methyl-3-(2-methylpropyl)imidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
64	174899-88-8	1,3-Diethylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
65	347882-21-7	1-Ethyl-3-propylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
66	393550-29-3	1-Ethyl-3-hexylimidazolium tetrafluoroborate
67	none (2013-09-19)	1,3-Dipropylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
68	749921-07-1	1,3-Dibutylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
69	none (2013-09-19)	1,3-Dipentylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
70	none (2013-09-19)	1,3-Dihexylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
71	1049751-90-7	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
72	324574-95-0	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
73	75174-77-5	4-Butyl-4-methylmorpholinium bromide
74	608140-12-1	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
75	none (2013-09-19)	1-Methyl-1-propylpiperidinium hexafluorophosphate
76	1049751-95-2	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
77	623580-02-9	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
78	94280-72-5	1-Butyl-1-methylpiperidinium bromide
79	1241842-94-3	1-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethyl]pyridinium bromide
80	1241840-01-6	1-[1-(3,4-Dimethoxyphenyl)-2-methoxy-2-oxoethyl]pyridinium chloride
81	1424967-13-4	1-[1-(1,3-Benzodioxol-5-yl)-2-butoxy-2-oxoethyl]pyridinium bromide
82	1241839-96-2	1-[2-[1-(1,3-Benzodioxol-5-yl)-2-methoxy-2-oxoethoxy]-2-oxoethyl]pyridinium bromide
83	827027-29-2	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
84	67226-45-3	1-Butylpyridinium μ -chlorohexachlorodialuminate
85	874-80-6	1-Butylpyridinium bromide
86	1124-64-7	1-Butylpyridinium chloride
87	827033-71-6	1-Butylpyridinium N-cyanocyanamide
88	26576-85-2	1-Butyl-3-methylpyridinium bromide
89	712355-12-9	1-Butyl-3-methylpyridinium N-cyanocyanamide
90	26576-98-7	1-Butyl-3,5-dimethylpyridinium bromide
91	877678-54-1	1-Butyl-3,5-dimethylpyridinium N-cyanocyanamide
92	343952-33-0	1-Butyl-4-methylpyridinium tetrafluoroborate
93	460983-97-5	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
94	67021-56-1	1-Hexyl-3-methylpyridinium bromide
95	872672-57-6	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
96	4086-73-1	1-Octylpyridinium chloride
97	872672-72-5	3-Methyl-1-octylpyridinium bromide
98	1107545-20-9	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
99	129412-64-2	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide
100	757240-24-7	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
101	663628-46-4	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
102	1332694-08-2	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide
103	479500-35-1	1-Butyl-1-methylpyrrolidinium chloride
104	380497-19-8	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide

S4: The 6 Variables in the Aquatic toxicity model.

	Variables	unit
1	<i>Lemna minor</i> (frond area) 7d	log(EC50)
2	<i>Lemna minor</i> (frond number) 7d	log(EC50)
3	<i>Scenedesmus vacuolatus</i> (cell count) 24h	log(EC50)
4	<i>Vibrio fischeri</i> 5'	log(EC50)
5	<i>Vibrio fischeri</i> 15'	log(EC50)
6	<i>Vibrio fischeri</i> 30'	log(EC50)

S5: Ranking of the 245 IPC-81 variables according to decreasing values.

	CAS no.	Name	IPC-81 log (EC50)
1	941584-15-2	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride	4,30
2	67889-35-4	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	4,01
3	1012794-05-6	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	3,99
4	886439-37-8	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	3,98
5	1012794-07-8	1-(3-Methoxypropyl)pyridinium chloride	3,88
6	194986-67-9	1-(Cyanomethyl)-1-methylpiperidinium chloride	3,82
7	1012794-12-5	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	3,80
8	873-71-2	1-Propylpyridinium bromide	3,78
9	1012794-06-7	1-(3-Methoxypropyl)-3-methylimidazolium chloride	3,77
10	1334291-67-6	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	3,76
11	53875-78-8	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	3,74
12	1012794-04-5	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	3,72
13	54770-67-1	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	3,71
14	663628-44-2	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	3,71
15	1012794-00-1	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	3,71
16	1012794-09-0	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	3,71
17	75174-77-5	4-Butyl-4-methylmorpholinium bromide	3,68
18	833446-39-2	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	3,68
19	108153-25-9	1-(2-Ethoxyethyl)pyridinium bromide	3,61
20	1012794-10-3	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	3,59
21	1012794-11-4	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	3,59
22	1309983-34-3	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,57
23	1012794-01-2	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	3,56
24	69095-13-2	1-(2-Hydroxyethyl)pyridinium iodide	3,55
25	370865-80-8	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	3,55
26	479500-35-1	1-Butyl-1-methylpyrrolidinium chloride	3,55
27	474972-46-8	1-(2-Methoxyethyl)-3-methylimidazolium chloride	3,55
28	355011-34-6	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	3,55
29	1012794-13-6	4-(Cyanomethyl)-4-methylmorpholinium chloride	3,55
30	516474-01-4	1-Ethyl-3-methylimidazolium methyl sulfate	3,54
31	209679-88-9	1-(2-Methoxyethyl)pyridinium chloride	3,54
32	187863-16-7	1-(3-Hydroxypropyl)pyridinium chloride	3,54
33	1012794-08-9	1-(Ethoxymethyl)-1-methylpiperidinium chloride	3,52
34	1012793-99-5	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	3,51

35	79917-89-8	1-Methyl-3-propylimidazolium chloride	3,51
36	937720-90-6	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,51
37	145022-44-2	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	3,50
38	154312-63-7	1-(Cyanomethyl)-3-methylimidazolium chloride	3,50
39	143314-17-4	1-Ethyl-3-methylimidazolium acetate	3,46
40	331717-63-6	1-Ethyl-3-methylimidazolium thiocyanate	3,45
41	796039-07-1	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,45
42	941580-56-9	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate	3,45
43	194986-69-1	1-(Cyanomethyl)-1-methylpyrrolidinium chloride	3,44
44	1049751-91-8	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,43
45	1017553-47-7	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,41
46	94280-72-5	1-Butyl-1-methylpiperidinium bromide	3,41
47	1373334-04-3	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,40
48	752260-02-9	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,40
49	2294-38-4	1-Ethylpyridinium chloride	3,38
50	174899-86-6	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,37
51	174899-65-1	1-Ethyl-3-methylimidazolium trifluoroacetate	3,35
52	663628-48-6	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,35
53	790663-77-3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	3,34
54	757212-04-7	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,33
55	885456-20-2	1-Butylpyridinium methyl sulfate	3,31
56	412009-61-1	1-Ethyl-3-methylimidazolium hydrogen sulfate	3,31
57	342573-75-5	1-Ethyl-3-methylimidazolium ethyl sulfate	3,30
58	186088-50-6	1-Butylpyridinium hexafluorophosphate	3,30
59	445497-25-6	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	3,29
60	145022-45-3	1-Ethyl-3-methylimidazolium methanesulfonate	3,29
61	827027-30-5	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,29
62	757212-03-6	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,28
63	328090-25-1	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	3,26
64	1107545-20-9	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,25
65	1049751-96-3	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,25
66	129412-64-2	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium bromide	3,25
67	874-80-6	1-Butylpyridinium bromide	3,24
68	1332694-08-2	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,23
69	1196206-01-5	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide (1:1)	3,20
70	1026019-24-8	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,19
71	67226-45-3	1-Butylpyridinium μ -chlorohexachlorodialuminate	3,18
72	778593-17-2	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,18
73	827027-29-2	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,17
74	65039-09-0	1-Ethyl-3-methylimidazolium chloride	3,16

75	1040381-03-0	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,16
76	125652-55-3	1-Butyl-3-methylpyridinium chloride	3,12
77	390423-43-5	1-Butylpyridinium trifluoromethanesulfonate	3,12
78	93457-69-3	1-Butyl-1-methylpyrrolidinium bromide	3,11
79	1017553-46-6	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,10
80	324574-95-0	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,07
81	370865-89-7	1-Ethyl-3-methylimidazolium N-cyanocyanamide	3,07
82	1049751-90-7	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,06
83	1049751-93-0	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,05
84	623580-02-9	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,05
85	1049752-00-2	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,02
86	112400-85-8	1-Butyl-2-methylpyridinium chloride	3,02
87	663628-45-3	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	3,00
88	1015254-36-0	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,98
89	17281-59-3	1-(Cyanomethyl)pyridinium chloride	2,98
90	952429-64-0	1-(7-Carboxyheptyl)-3-methylimidazolium bromide	2,96
91	203389-28-0	1-Butylpyridinium tetrafluoroborate	2,95
92	845835-03-2	1-Butyl-3-methylpyridinium hexafluorophosphate	2,94
93	757240-24-7	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,93
94	1049751-95-2	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,92
95	174899-82-2	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,91
96	145022-48-6	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	2,91
97	65039-05-6	1-Butyl-3-methylimidazolium iodide	2,91
98	849418-12-8	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,90
99	873583-83-6	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,89
100	1373334-02-1	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,89
101	342789-81-5	1-Butyl-3-methylimidazolium methanesulfonate	2,88
102	178631-01-1	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,88
103	742099-80-5	1-Ethyl-3-methylimidazolium tetracyanoborate	2,86
104	945996-02-1	1-(Ethoxymethyl)-3-methylimidazolium chloride	2,85
105	952429-67-3	1-Methyl-3-(3-oxobutyl)imidazolium bromide	2,84
106	663628-46-4	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,84
107	628-13-7	Pyridine hydrochloride	2,83
108	945996-13-4	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,83
109	868742-24-9	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,82
110	374564-83-7	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate	2,81
111	1012794-15-8	4-(Ethoxymethyl)-4-methylmorpholinium chloride	2,81
112	863663-01-8	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,81
113	1104525-90-7	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,81
114	79917-90-1	1-Butyl-3-methylimidazolium chloride	2,80

115	712355-12-9	1-Butyl-3-methylpyridinium N-cyanocyanamide	2,79
116	805228-35-7	3-(3-Carboxypropyl)-1-methylimidazolium chloride	2,79
117	244193-48-4	1-Methyl-3-propylimidazolium tetrafluoroborate	2,78
118	410522-18-8	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	2,78
119	608140-12-1	1-Methyl-1-propylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,78
120	445473-58-5	1-Butyl-3-methylimidazolium octylsulfate	2,77
121	85100-77-2	1-Butyl-3-methylimidazolium bromide	2,77
122	864665-30-5	1-(4-Hydroxybutyl)-3-methylimidazolium chloride	2,76
123	1049751-98-5	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,74
124	174899-96-8	1-Butyl-3-ethylimidazolium trifluoroacetate	2,74
125	143314-16-3	1-Ethyl-3-methylimidazolium tetrafluoroborate	2,73
126	790663-79-5	1-Ethyl-3-methylimidazolium octylsulfate	2,73
127	916730-31-9	1-Butyl-3,5-dimethylpyridinium chloride	2,72
128	359845-21-9	1-Butyl-3-methylimidazolium tetrachloroferrate	2,70
129	1187194-44-0	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	2,70
130	595565-54-1	1-Butyl-3-methylimidazolium-2-(2-methoxyethoxy)ethyl sulfate	2,69
131	597581-48-1	1-Butyl-3-methylpyridinium tetrafluoroborate	2,68
132	262297-13-2	1-Butyl-3-methylimidazolium hydrogen sulfate	2,66
133	952429-72-0	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate	2,65
134	637348-59-5	1-Ethyl-3-propylimidazolium bromide	2,64
135	581101-91-9	1-Butyl-3-ethylimidazolium tetrafluoroborate	2,64
136	223437-11-4	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,63
137	286453-46-1	1-Butyl-2-methylpyridinium tetrafluoroborate	2,62
138	401788-98-5	1-Butyl-3-methylimidazolium methyl sulfate	2,61
139	1739-84-0	1,2-Dimethylimidazolium	2,61
140	666823-18-3	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile (1:1)	2,60
141	112400-86-9	1-Butyl-4-methylpyridinium chloride	2,59
142	21379-36-2	1-(Ethoxymethyl)pyridinium chloride	2,56
143	none (2013-09-19)	1-Butyl-3-methylimidazolium hexafluorophosphate	2,55
144	460983-97-5	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,52
145	53385-72-1	1-Pentylpyridinium bromide	2,51
146	433337-11-2	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	2,50
147	890532-45-3	1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,49
148	174899-66-2	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	2,48
149	280779-52-4	1-Methyl-3-pentylimidazolium hexafluorophosphate	2,47
150	401788-99-6	1-Butyl-4-methylpyridinium hexafluorophosphate	2,47
151	174501-65-6	1-Butyl-3-methylimidazolium tetrafluoroborate	2,47
152	448245-52-1	1-Butyl-3-methylimidazolium N-cyanocyanamide	2,47
153	433337-12-3	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	2,45
154	852616-00-3	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	2,45

155	216300-12-8	1-Methyl-3-propylimidazolium hexafluorophosphate	2,43
156	900797-77-5	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,43
157	952429-71-9	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate	2,42
158	376650-06-5	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate	2,41
159	304680-35-1	1-Hexyl-3-methylimidazolium hexafluorophosphate	2,40
160	500996-04-3	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	2,39
161	244193-50-8	1-Hexyl-3-methylimidazolium tetrafluoroborate	2,39
162	244193-49-5	1-Methyl-3-pentylimidazolium tetrafluoroborate	2,38
163	343952-33-0	1-Butyl-4-methylpyridinium tetrafluoroborate	2,35
164	916730-30-8	1-Butyl-3,4-dimethylpyridinium chloride	2,35
165	187332-85-0	1-Methyl-3-(2-phenylethyl)imidazolium chloride	2,35
166	36443-80-8	1-Methyl-3-(phenylmethyl)imidazolium chloride	2,32
167	151200-14-5	1-Methylimidazolium hydrogen tetrafluoroborate	2,32
168	54304-66-4	1,3-Diethylimidazolium bromide	2,31
169	7538-79-6	4-(Dimethylamino)-1-methylpyridinium iodide	2,31
170	174899-83-3	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,31
171	151263-00-2	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	2,31
172	742099-83-8	1-Butyl-4-methylpyridinium tetracyanoborate	2,30
173	171058-22-3	1-Methyl-3-pentylimidazolium chloride	2,28
174	114203-57-5	4-(Dimethylamino)-1-ethylpyridinium bromide	2,26
175	345984-11-4	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	2,26
176	909398-59-0	1-Hexyl-1-methylpyrrolidinium chloride	2,24
177	380497-19-8	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,21
178	952429-66-2	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium hexafluorophosphate	2,18
179	851856-47-8	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	2,18
180	171058-17-6	1-Hexyl-3-methylimidazolium chloride	2,13
181	847335-66-4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	2,11
182	6220-15-1	1-Hexylpyridinium chloride	2,10
183	623167-81-7	1-Hexylpyridinium trifluoromethanesulfonate	2,04
184	244193-51-9	1-Heptyl-3-methylimidazolium tetrafluoroborate	2,01
185	797789-00-5	1-Hexylpyridinium hexafluorophosphate	2,00
186	62409-49-8	1-Hexyl-4-methylpyridinium chloride	2,00
187	637348-60-8	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	1,99
188	909398-60-3	1-Methyl-1-octylpyrrolidinium chloride	1,96
189	1195983-48-2	1-(2-Methoxyethyl)-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphate	1,93
190	765910-73-4	1-Butyl-2,3-dimethylimidazolium trifluoromethanesulfonate	1,91
191	382150-50-7	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,89
192	581101-92-0	1-Heptyl-3-methylimidazolium chloride	1,87
193	697248-62-7	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)	1,85
194	174645-81-9	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	1,83

195	952429-65-1	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide	1,82
196	357915-04-9	1-Heptyl-3-methylimidazolium hexafluorophosphate	1,82
197	31537-79-8	1-Butylquinolinium bromide	1,74
198	916730-40-0	1-Hexyl-3-methylpyridinium chloride	1,73
199	313475-50-2	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate	1,70
200	393550-29-3	1-Ethyl-3-hexylimidazolium tetrafluoroborate	1,69
201	710336-91-7	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanamine	1,65
202	952429-68-4	1-Butylquinolinium tetrafluoroborate	1,60
203	952429-73-1	1-Hexyl-4-methylpyridinium tetrafluoroborate	1,60
204	304680-36-2	1-Methyl-3-octylimidazolium hexafluorophosphate	1,50
205	900797-79-7	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,49
206	547719-00-6	1-Ethyl-3-hexylimidazolium bromide	1,41
207	343952-29-4	1-Methyl-3-nonylimidazolium hexafluorophosphate	1,40
208	64697-40-1	1-Methyl-3-octylimidazolium chloride	1,38
209	384347-21-1	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	1,33
210	178631-04-4	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,32
211	952429-74-2	1-Methyl-1-octylpyrrolidinium tetrafluoroborate	1,28
212	82522-15-4	1-Butyl-4-(dimethylamino)pyridinium chloride	1,27
213	713512-19-7	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	1,21
214	344790-87-0	1-Butyl-3-methylimidazolium thiocyanate	1,18
215	917762-91-5	1-Butyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	1,14
216	817575-02-3	3-Methyl-1-octylimidazolium octylsulfate	1,13
217	244193-55-3	1-Methyl-3-nonylimidazolium tetrafluoroborate	1,12
218	362043-46-7	1-Decyl-3-methylimidazolium hexafluorophosphate	1,06
219	244193-52-0	1-Methyl-3-octylimidazolium tetrafluoroborate	1,04
220	141645-91-2	4-Methyl-1-octylpyridinium chloride	1,02
221	936239-96-2	4-Methyl-1-octylpyridinium tetrafluoroborate	0,95
222	864461-36-9	3-Methyl-1-octylpyridinium chloride	0,85
223	171058-20-1	1-Methyl-3-nonylimidazolium chloride	0,79
224	171058-18-7	1-Decyl-3-methylimidazolium chloride	0,75
225	402846-78-0	1-Butyl-2,3-dimethylimidazolium tetrafluoroborate	0,75
226	878005-11-9	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	0,75
227	872672-57-6	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0,70
228	4086-73-1	1-Octylpyridinium chloride	0,63
229	403842-84-2	1-Methyl-3-octylimidazolium trifluoromethanesulfonate	0,62
230	952429-69-5	1-Hexylquinolinium tetrafluoroborate	0,55
231	376650-04-3	1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato-O1,O2]borate	0,55
232	1012794-14-7	4-(Dimethylamino)-1-hexylpyridinium chloride	0,32
233	244193-56-4	1-Decyl-3-methylimidazolium tetrafluoroborate	0,26
234	581101-93-1	1-Decyl-3-ethylimidazolium bromide	0,03

235	943229-71-8	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate	-0,12
236	883860-38-6	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	-0,23
237	68039-12-3	1H-Imidazolium, 1-ethyl-2-(8-heptadecenyl)-4,5-dihydro-3-(2-hydroxyethyl)imidazolium ethyl sulfate	-0,23
238	188589-32-4	1-Decyl-3-methylimidazolium bromide	-0,25
239	952429-70-8	1-Octylquinolinium tetrafluoroborate	-0,31
240	1310460-36-6	1,3-Didecyl-2-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0,32
241	384347-06-2	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	-0,33
242	171058-19-8	1-Methyl-3-octadecylimidazolium chloride	-0,42
243	14848-21-6	1-Octylquinolinium bromide	-0,52
244	61546-01-8	1-Hexadecyl-3-methylimidazolium chloride	-0,71
245	171058-21-2	1-Methyl-3-tetradecylimidazolium chloride	-0,92

S6: Ranking of the 232 AChE variables according to decreasing values

	CAS no.	Name	Acetylcholinesterase inhibition
			log(EC50)
1	713512-19-7	1-Hexyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	2,79
2	851856-47-8	1-Butyl-1-methylpyrrolidinium trifluorotris(pentafluoroethyl)phosphate	2,77
3	663628-48-6	4-(2-Ethoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,66
4	1049751-91-8	4-(3-Methoxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,66
5	1107545-20-9	1-(2-Ethoxy-2-oxoethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,66
6	1026019-24-8	4-(3-Hydroxypropyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,64
7	1040381-03-0	4-(Cyanomethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,62
8	868742-24-9	4-(2-Hydroxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,56
9	941580-56-9	1-(3-Sulfopropyl)pyridinium trifluoromethanesulfonate	2,55
10	796039-07-1	4-(2-Methoxyethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,54
11	1049751-90-7	4-(Ethoxymethyl)-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,53
12	174899-86-6	1-(2-Hydroxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,49
13	952429-64-0	1-(7-Carboxyheptyl)-3-methylimidazolium bromide	2,48
14	937720-90-6	1-(Cyanomethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,48
15	1017553-47-7	1-(Cyanomethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,44
16	313475-50-2	1-Methyl-3-(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)imidazolium hexafluorophosphate	2,42
17	324574-95-0	4-Butyl-4-methylmorpholinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,42
18	1012794-09-0	4-(2-Ethoxyethyl)-4-methylmorpholinium bromide	2,40
19	1332694-08-2	1-(3-Hydroxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,40
20	53875-78-8	4-(2-Hydroxyethyl)-4-methylmorpholinium iodide	2,40
21	1012794-00-1	1-(2-Hydroxyethyl)-3-methylimidazolium iodide	2,37
22	827027-30-5	1-(3-Hydroxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,36
23	1373334-04-3	1-(3-Methoxypropyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,35
24	1012794-12-5	4-(3-Methoxypropyl)-4-methylmorpholinium chloride	2,32
25	805228-35-7	3-(3-Carboxypropyl)-1-methylimidazolium chloride	2,31
26	1012794-11-4	4-(3-Hydroxypropyl)-4-methylmorpholinium chloride	2,29
27	943229-71-8	1-Hexyl-3-methylimidazolium trifluorotris(heptafluoropropyl)phosphate	2,28
28	1012794-10-3	4-(2-Methoxyethyl)-4-methylmorpholinium chloride	2,28
29	752260-02-9	1-(2-Hydroxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,26
30	380497-19-8	1-Hexyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,26
31	1012794-15-8	4-(Ethoxymethyl)-4-methylmorpholinium chloride	2,26
32	1012794-13-6	4-(Cyanomethyl)-4-methylmorpholinium chloride	2,25
33	355011-34-6	1-(3-Hydroxypropyl)-3-methylimidazolium chloride	2,23
34	151200-14-5	1-Methylimidazolium hydrogen tetrafluoroborate	2,23

35	1015254-36-0	1-(3-Methoxypropyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,22
36	757212-04-7	1-(2-Hydroxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,22
37	663628-45-3	1-(2-Ethoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,21
38	1049751-96-3	1-(3-Hydroxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,20
39	663628-46-4	1-(2-Ethoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,20
40	827027-29-2	1-(3-Hydroxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,18
41	1196206-01-5	1-Hexyl-3-methylimidazolium tris[(trifluoromethyl)sulfonyl]methide (1:1)	2,16
42	952429-67-3	1-Methyl-3-(3-oxobutyl)imidazolium bromide	2,16
43	878005-11-9	1-Ethyl-3-methylimidazolium trifluorotris(pentafluoroethyl)phosphate	2,14
44	941584-15-2	1-(3-Hydroxypropyl)-1-methylpyrrolidinium chloride	2,12
45	1017553-46-6	1-(Cyanomethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,11
46	178631-01-1	1-(2-Methoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,10
47	69095-13-2	1-(2-Hydroxyethyl)pyridinium iodide	2,09
48	194986-69-1	1-(Cyanomethyl)-1-methylpyrrolidinium chloride	2,09
49	154312-63-7	1-(Cyanomethyl)-3-methylimidazolium chloride	2,09
50	75174-77-5	4-Butyl-4-methylmorpholinium bromide	2,09
51	945996-13-4	1-(Ethoxymethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,07
52	1309983-34-3	1-(Cyanomethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	2,07
53	445497-25-6	4-Ethyl-4-methylmorpholinium 4-methylbenzenesulfonate	2,06
54	628-13-7	Pyridine hydrochloride	2,06
55	54770-67-1	1-(2-Hydroxyethyl)-1-methylpyrrolidinium iodide	2,04
56	1012794-05-6	1-(3-Methoxypropyl)-1-methylpyrrolidinium chloride	2,03
57	663628-44-2	1-(2-Ethoxyethyl)-1-methylpiperidinium bromide	2,00
58	864665-30-5	1-(4-Hydroxybutyl)-3-methylimidazolium chloride	1,98
59	833446-39-2	1-(2-Ethoxyethyl)-1-methylpyrrolidinium bromide	1,98
60	757212-03-6	1-(2-Hydroxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,96
61	385384-39-4	1-Butyl-3-methylimidazolium (T-4)-tetracarbonylcobaltate	1,93
62	1049751-95-2	1-(3-Methoxypropyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,92
63	1012794-06-7	1-(3-Methoxypropyl)-3-methylimidazolium chloride	1,89
64	187863-16-7	1-(3-Hydroxypropyl)pyridinium chloride	1,89
65	945996-02-1	1-(Ethoxymethyl)-3-methylimidazolium chloride	1,86
66	1373334-02-1	1-(Ethoxymethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,85
67	666823-18-3	1-Ethyl-3-methylimidazolium, salt with methanetricarbonitrile (1:1)	1,84
68	474972-46-8	1-(2-Methoxyethyl)-3-methylimidazolium chloride	1,83
69	1334291-67-6	1-(3-Hydroxypropyl)-1-methylpiperidinium chloride	1,82
70	1104525-90-7	1-Propylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,82
71	382150-50-7	1-Hexyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,80
72	1049751-93-0	1-(Ethoxymethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,80
73	909398-59-0	1-Hexyl-1-methylpyrrolidinium chloride	1,79
74	370865-89-7	1-Ethyl-3-methylimidazolium N-cyanocyanamide	1,79

75	67889-35-4	1-(2-Hydroxyethyl)-1-methylpiperidinium iodide	1,78
76	778593-17-2	1-(2-Ethoxyethyl)-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,76
77	1049751-98-5	1-(Ethoxymethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,76
78	223437-11-4	1-Butyl-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,75
79	757240-24-7	1-(2-Methoxyethyl)-1-methylpyrrolidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,73
80	909398-60-3	1-Methyl-1-octylpyrrolidinium chloride	1,73
81	178631-04-4	1-Methyl-3-octylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,71
82	863663-01-8	1-(2-Methoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,71
83	852616-00-3	1-Ethyl-3-methylimidazolium bis(pentafluoroethyl)phosphinate	1,71
84	1049752-00-2	1-(3-Methoxypropyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,70
85	328090-25-1	1-Ethyl-3-methylimidazolium 4-methylbenzenesulfonate	1,67
86	194986-67-9	1-(Cyanomethyl)-1-methylpiperidinium chloride	1,67
87	17281-59-3	1-(Cyanomethyl)pyridinium chloride	1,66
88	216300-12-8	1-Methyl-3-propylimidazolium hexafluorophosphate	1,66
89	1012793-99-5	1-(2-Ethoxyethyl)-3-methylimidazolium bromide	1,64
90	174899-82-2	1-Ethyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,63
91	1012794-01-2	1-(2-Methoxyethyl)-1-methylpyrrolidinium chloride	1,63
92	376650-04-3	1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato-O1,O2]borate	1,62
93	244193-48-4	1-Methyl-3-propylimidazolium tetrafluoroborate	1,62
94	none (2013-09-19)	1-Butyl-3-methylimidazolium hexafluorophosphate	1,60
95	174899-83-3	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,59
96	790663-77-3	1-Ethyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	1,57
97	873583-83-6	1-(2-Methoxyethyl)-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,57
98	304680-36-2	1-Methyl-3-octylimidazolium hexafluorophosphate	1,56
99	637348-59-5	1-Ethyl-3-propylimidazolium bromide	1,55
100	145022-44-2	1-Ethyl-3-methylimidazolium trifluoromethanesulfonate	1,55
101	244193-51-9	1-Heptyl-3-methylimidazolium tetrafluoroborate	1,55
102	359845-21-9	1-Butyl-3-methylimidazolium tetrachloroferrate	1,54
103	445473-58-5	1-Butyl-3-methylimidazolium octylsulfate	1,52
104	873-71-2	1-Propylpyridinium bromide	1,52
105	595565-54-1	1-Butyl-3-methylimidazolium 2-(2-methoxyethoxy)ethyl sulfate	1,52
106	847335-66-4	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	1,52
107	1012794-04-5	1-(3-Methoxypropyl)-1-methylpiperidinium chloride	1,52
108	697248-62-7	1-Hexyl-3-methylimidazolium, salt with 1,2-benzisothiazol-3(2H)-one 1,1-dioxide (1:1)	1,50
109	460983-97-5	1-Hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,50
110	65039-10-3	1-Methyl-3-(2-propenyl)imidazolium chloride	1,50
111	145022-48-6	1-Butyl-3-ethylimidazolium trifluoromethanesulfonate	1,49
112	410522-18-8	1-Butyl-3-methylimidazolium 4-methylbenzenesulfonate	1,49
113	376650-06-5	1-Ethyl-3-methylimidazolium bis[ethanedioato-O1,O2]borate	1,48
114	79917-89-8	1-Methyl-3-propylimidazolium chloride	1,47

115	952429-74-2	1-Methyl-1-octylpyrrolidinium tetrafluoroborate	1,47
116	412009-61-1	1-Ethyl-3-methylimidazolium hydrogen sulfate	1,45
117	342573-75-5	1-Ethyl-3-methylimidazolium ethyl sulfate	1,44
118	65039-05-6	1-Butyl-3-methylimidazolium iodide	1,44
119	174899-96-8	1-Butyl-3-ethylimidazolium trifluoroacetate	1,44
120	886439-37-8	1-(2-Methoxyethyl)-1-methylpiperidinium bromide	1,43
121	1012794-08-9	1-(Ethoxymethyl)-1-methylpiperidinium chloride	1,43
122	623580-02-9	1-Butyl-1-methylpiperidinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,42
123	581101-91-9	1-Butyl-3-ethylimidazolium tetrafluoroborate	1,42
124	357915-04-9	1-Heptyl-3-methylimidazolium hexafluorophosphate	1,42
125	1012794-07-8	1-(3-Methoxypropyl)pyridinium chloride	1,42
126	433337-12-3	1-Methyl-3-(2-phenylethyl)imidazolium hexafluorophosphate	1,42
127	883860-38-6	1-Butyl-4-methylpyridinium trifluorotris(pentafluoroethyl)phosphate	1,41
128	845835-00-9	1-Methyl-3-(2-phenylethyl)imidazolium tetrafluoroborate	1,41
129	581101-92-0	1-Heptyl-3-methylimidazolium chloride	1,41
130	500996-04-3	1-Methyl-3-(phenylmethyl)imidazolium tetrafluoroborate	1,40
131	174899-66-2	1-Butyl-3-methylimidazolium trifluoromethanesulfonate	1,39
132	54304-66-4	1,3-Diethylimidazolium bromide	1,39
133	174645-81-9	1-Butyl-3-methylimidazolium (OC-6-11)-hexafluoroantimonate	1,38
134	174899-65-1	1-Ethyl-3-methylimidazolium trifluoroacetate	1,38
135	790663-79-5	1-Ethyl-3-methylimidazolium octylsulfate	1,37
136	304680-35-1	1-Hexyl-3-methylimidazolium hexafluorophosphate	1,37
137	36443-80-8	1-Methyl-3-(phenylmethyl)imidazolium chloride	1,36
138	342789-81-5	1-Butyl-3-methylimidazolium methanesulfonate	1,36
139	331717-63-6	1-Ethyl-3-methylimidazolium thiocyanate	1,35
140	401788-98-5	1-Butyl-3-methylimidazolium methyl sulfate	1,35
141	262297-13-2	1-Butyl-3-methylimidazolium hydrogen sulfate	1,34
142	143314-16-3	1-Ethyl-3-methylimidazolium tetrafluoroborate	1,34
143	174501-65-6	1-Butyl-3-methylimidazolium tetrafluoroborate	1,34
144	742099-80-5	1-Ethyl-3-methylimidazolium tetracyanoborate	1,33
145	623167-81-7	1-Hexylpyridinium trifluoromethanesulfonate	1,33
146	390423-43-5	1-Butylpyridinium trifluoromethanesulfonate	1,33
147	280779-52-4	1-Methyl-3-pentylimidazolium hexafluorophosphate	1,32
148	1739-84-0	1,2-Dimethylimidazolium	1,32
149	209679-88-9	1-(2-Methoxyethyl)pyridinium chloride	1,31
150	67226-45-3	1-Butylpyridinium μ -chlorohexachlorodialuminate	1,31
151	21379-36-2	1-(Ethoxymethyl)pyridinium chloride	1,30
152	85100-77-2	1-Butyl-3-methylimidazolium bromide	1,30
153	370865-80-8	1-Butyl-1-methylpyrrolidinium N-cyanocyanamide	1,29
154	344790-87-0	1-Butyl-3-methylimidazolium thiocyanate	1,29

155	186088-50-6	1-Butylpyridinium hexafluorophosphate	1,29
156	244193-50-8	1-Hexyl-3-methylimidazolium tetrafluoroborate	1,28
157	93457-69-3	1-Butyl-1-methylpyrrolidinium bromide	1,28
158	393550-29-3	1-Ethyl-3-hexylimidazolium tetrafluoroborate	1,27
159	345984-11-4	1-Butyl-1-methylpyrrolidinium tetrafluoroborate	1,26
160	187332-85-0	1-Methyl-3-(2-phenylethyl)imidazolium chloride	1,26
161	2294-38-4	1-Ethylpyridinium chloride	1,26
162	362043-46-7	1-Decyl-3-methylimidazolium hexafluorophosphate	1,25
163	797789-00-5	1-Hexylpyridinium hexafluorophosphate	1,25
164	65039-09-0	1-Ethyl-3-methylimidazolium chloride	1,25
165	433337-11-2	1-Methyl-3-(phenylmethyl)imidazolium hexafluorophosphate	1,24
166	448245-52-1	1-Butyl-3-methylimidazolium N-cyanocyanamide	1,24
167	244193-49-5	1-Methyl-3-pentylimidazolium tetrafluoroborate	1,24
168	171058-22-3	1-Methyl-3-pentylimidazolium chloride	1,24
169	171058-17-6	1-Hexyl-3-methylimidazolium chloride	1,22
170	637348-60-8	1-Methyl-3-[(4-methylphenyl)methyl]imidazolium chloride	1,20
171	94280-72-5	1-Butyl-1-methylpiperidinium bromide	1,20
172	547719-00-6	1-Ethyl-3-hexylimidazolium bromide	1,18
173	890532-45-3	1-Pentylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,18
174	343952-29-4	1-Methyl-3-nonylimidazolium hexafluorophosphate	1,17
175	479500-35-1	1-Butyl-1-methylpyrrolidinium chloride	1,17
176	79917-90-1	1-Butyl-3-methylimidazolium chloride	1,16
177	885456-20-2	1-Butylpyridinium methyl sulfate	1,15
178	203389-28-0	1-Butylpyridinium tetrafluoroborate	1,15
179	849418-12-8	1-(2-Ethoxyethyl)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,12
180	151263-00-2	1-(Ethoxymethyl)-1-methylpyrrolidinium chloride	1,11
181	874-80-6	1-Butylpyridinium bromide	1,10
182	384347-06-2	1-Octylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	1,08
183	710336-91-7	1-Butyl-3-methylimidazolium 1,1,1-trifluoro-N-(trifluoromethyl)methanaminat	1,07
184	6220-15-1	1-Hexylpyridinium chloride	1,02
185	817575-02-3	3-Methyl-1-octylimidazolium octylsulfate	0,98
186	244193-52-0	1-Methyl-3-octylimidazolium tetrafluoroborate	0,98
187	64697-40-1	1-Methyl-3-octylimidazolium chloride	0,96
188	4086-73-1	1-Octylpyridinium chloride	0,96
189	1124-64-7	1-Butylpyridinium chloride	0,93
190	343952-33-0	1-Butyl-4-methylpyridinium tetrafluoroborate	0,92
191	108153-25-9	1-(2-Ethoxyethyl)pyridinium bromide	0,92
192	244193-55-3	1-Methyl-3-nonylimidazolium tetrafluoroborate	0,90
193	952429-73-1	1-Hexyl-4-methylpyridinium tetrafluoroborate	0,90
194	401788-99-6	1-Butyl-4-methylpyridinium hexafluorophosphate	0,90

195	742099-83-8	1-Butyl-4-methylpyridinium tetracyanoborate	0,88
196	53385-72-1	1-Pentylpyridinium bromide	0,88
197	62409-49-8	1-Hexyl-4-methylpyridinium chloride	0,77
198	171058-20-1	1-Methyl-3-nonylimidazolium chloride	0,75
199	952429-65-1	1-(8-Hydroxyoctyl)-3-methylimidazolium bromide	0,74
200	845835-03-2	1-Butyl-3-methylpyridinium hexafluorophosphate	0,71
201	112400-86-9	1-Butyl-4-methylpyridinium chloride	0,71
202	384347-21-1	1-Hexyl-2,3-dimethylimidazolium tetrafluoroborate	0,69
203	936239-96-2	4-Methyl-1-octylpyridinium tetrafluoroborate	0,69
204	597581-48-1	1-Butyl-3-methylpyridinium tetrafluoroborate	0,64
205	244193-56-4	1-Decyl-3-methylimidazolium tetrafluoroborate	0,58
206	952429-72-0	1-Butyl-3,5-dimethylpyridinium tetrafluoroborate	0,56
207	900797-77-5	4-(Dimethylamino)-1-ethylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0,56
208	712355-12-9	1-Butyl-3-methylpyridinium N-cyanocyanamide	0,55
209	171058-19-8	1-Methyl-3-octadecylimidazolium chloride	0,53
210	171058-18-7	1-Decyl-3-methylimidazolium chloride	0,50
211	952429-71-9	1-Butyl-3,4-dimethylpyridinium tetrafluoroborate	0,50
212	872672-57-6	4-(Dimethylamino)-1-hexylpyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0,50
213	141645-91-2	4-Methyl-1-octylpyridinium chloride	0,50
214	581101-93-1	1-Decyl-3-ethylimidazolium bromide	0,42
215	125652-55-3	1-Butyl-3-methylpyridinium chloride	0,42
216	916730-40-0	1-Hexyl-3-methylpyridinium chloride	0,39
217	114203-57-5	4-(Dimethylamino)-1-ethylpyridinium bromide	0,36
218	916730-31-9	1-Butyl-3,5-dimethylpyridinium chloride	0,29
219	900797-79-7	1-Butyl-4-(dimethylamino)pyridinium 1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]methanesulfonamide	0,25
220	61546-01-8	1-Hexadecyl-3-methylimidazolium chloride	0,22
221	31537-79-8	1-Butylquinolinium bromide	0,22
222	286453-46-1	1-Butyl-2-methylpyridinium tetrafluoroborate	0,20
223	916730-30-8	1-Butyl-3,4-dimethylpyridinium chloride	0,15
224	952429-68-4	1-Butylquinolinium tetrafluoroborate	0,05
225	171058-21-2	1-Methyl-3-tetradecylimidazolium chloride	0,04
226	864461-36-9	3-Methyl-1-octylpyridinium chloride	0,02
227	112400-85-8	1-Butyl-2-methylpyridinium chloride	-0,03
228	952429-69-5	1-Hexylquinolinium tetrafluoroborate	-0,04
229	82522-15-4	1-Butyl-4-(dimethylamino)pyridinium chloride	-0,07
230	1012794-14-7	4-(Dimethylamino)-1-hexylpyridinium chloride	-0,12
231	952429-70-8	1-Octylquinolinium tetrafluoroborate	-0,18
232	14848-21-6	1-Octylquinolinium bromide	-0,20

S7: The 87 ILs in Bacteria and Fungi toxicity model

	CAS no.	Name
1	615538-92-6	1-Methylimidazolium 2-hydroxypropanoate
2	1010075-76-9	1-Methylimidazolium (2S)-2-hydroxypropanoate
3	615539-01-0	1-Decylimidazolium 2-hydroxypropanoate
4	898223-27-3	1-Decylimidazolium (2S)-2-hydroxypropanoate
5	615539-02-1	1-Undecylimidazolium 2-hydroxypropanoate
6	885224-27-1	1-Undecylimidazolium (2S)-2-hydroxypropanoate
7	615539-03-2	1-Dodecylimidazolium 2-hydroxypropanoate
8	898558-89-9	1-Dodecylimidazolium (2S)-2-hydroxypropanoate
9	615539-10-1	1-[(Decyloxy)methyl]imidazolium 2-hydroxypropanoate
10	885224-30-6	1-[(Decyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
11	615539-11-2	1-[(Undecyloxy)methyl]imidazolium 2-hydroxypropanoate
12	none (2013-09-19)	1-[(Undecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
13	615539-12-3	1-[(Dodecyloxy)methyl]imidazolium 2-hydroxypropanoate
14	898558-92-4	1-[(Dodecyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
15	615539-04-3	1-(Butoxymethyl)imidazolium 2-hydroxypropanoate
16	885224-28-2	1-(Butoxymethyl)imidazolium (2S)-2-hydroxypropanoate
17	615539-05-4	1-[(Pentyloxy)methyl]imidazolium 2-hydroxypropanoate
18	none (2013-09-19)	1-[(Pentyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
19	615539-06-5	1-[(Hexyloxy)methyl]imidazolium 2-hydroxypropanoate
20	885224-29-3	1-[(Hexyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
21	615539-07-6	1-[(Heptyloxy)methyl]imidazolium 2-hydroxypropanoate
22	none (2013-09-19)	1-[(Heptyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
23	615539-08-7	1-[(Octyloxy)methyl]imidazolium 2-hydroxypropanoate
24	898558-90-2	1-[(Octyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
25	615539-09-8	1-[(Nonyloxy)methyl]imidazolium 2-hydroxypropanoate
26	898558-91-3	1-[(Nonyloxy)methyl]imidazolium (2S)-2-hydroxypropanoate
27	615538-93-7	1-Ethylimidazolium 2-hydroxypropanoate
28	none (2013-09-19)	1-Ethylimidazolium (2S)-2-hydroxypropanoate
29	615538-94-8	1-Propylimidazolium 2-hydroxypropanoate
30	none (2013-09-19)	1-Propylimidazolium (2S)-2-hydroxypropanoate
31	885224-25-9	1-Butylimidazolium (2S)-2-hydroxypropanoate
32	615538-96-0	1-Pentylimidazolium 2-hydroxypropanoate
33	none (2013-09-19)	1-Pentylimidazolium (2S)-2-hydroxypropanoate
34	615538-97-1	1-Hexylimidazolium 2-hydroxypropanoate
35	885224-26-0	1-Hexylimidazolium (2S)-2-hydroxypropanoate

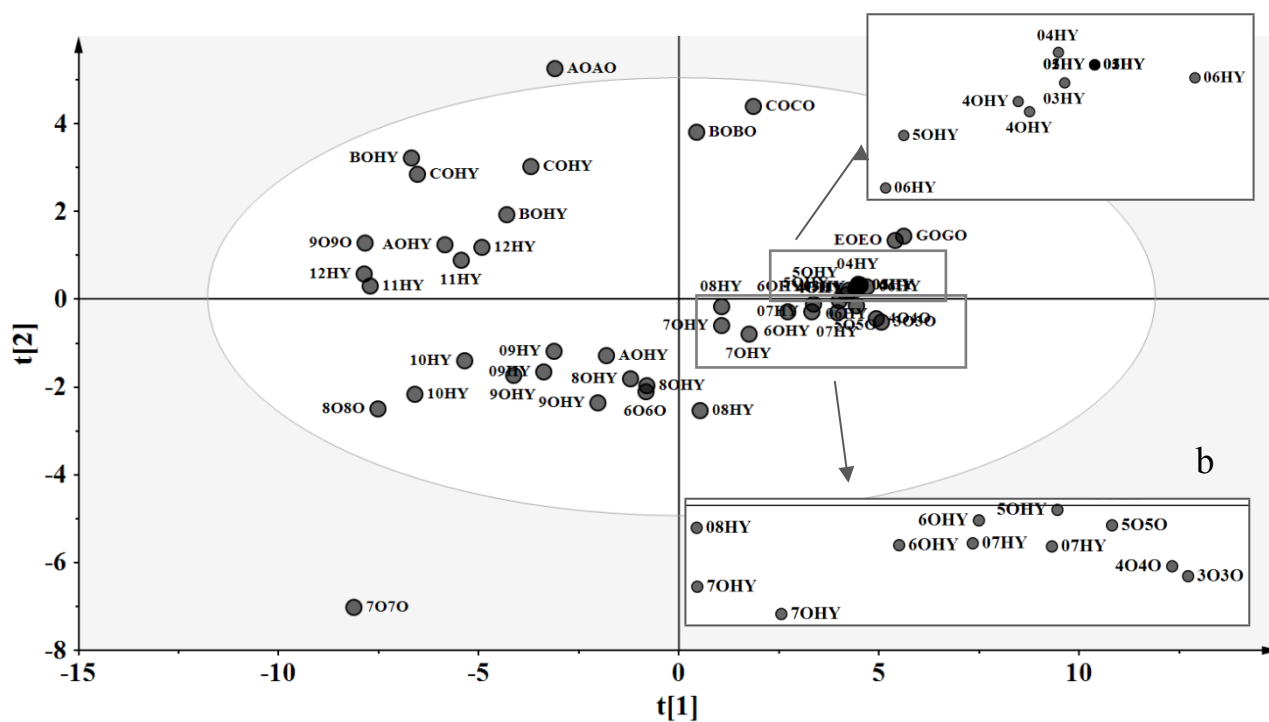
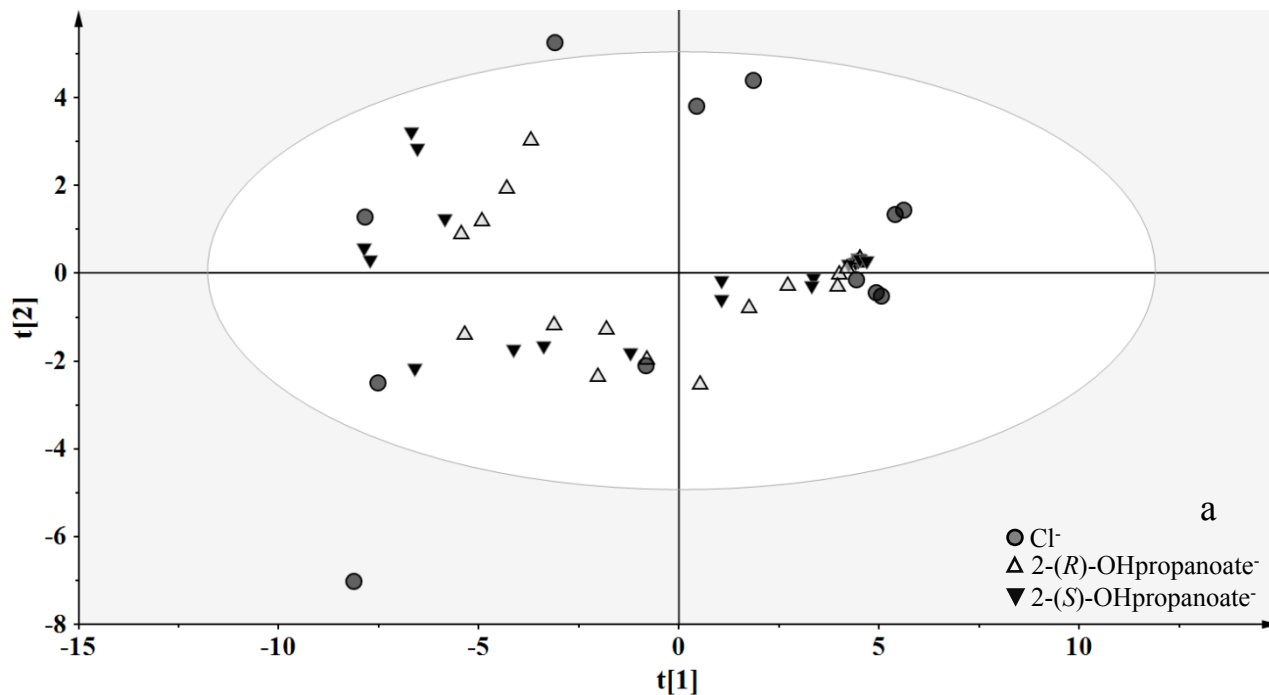
36	615538-98-2	1-Heptylimidazolium 2-hydroxypropanoate
37	none (2013-09-19)	1-Heptylimidazolium (2S)-2-hydroxypropanoate
38	615538-99-3	1-Octylimidazolium 2-hydroxypropanoate
39	898558-87-7	1-Octylimidazolium (2S)-2-hydroxypropanoate
40	615539-00-9	1-Nonylimidazolium 2-hydroxypropanoate
41	898558-88-8	1-Nonylimidazolium (2S)-2-hydroxypropanoate
42	761410-66-6	1,3-Bis[(decyloxy)methyl]imidazolium chloride
43	761410-67-7	1,3-Bis[(undecyloxy)methyl]imidazolium chloride
44	761410-68-8	1,3-Bis[(dodecyloxy)methyl]imidazolium chloride
45	none (2013-09-19)	1,3-Bis[(tetradecyloxy)methyl]imidazolium chloride
46	none (2013-09-19)	1,3-Bis[(hexadecyloxy)methyl]imidazolium chloride
47	126049-85-2	1,3-Bis(propoxymethyl)imidazolium chloride
48	761410-60-0	1,3-Bis(butoxymethyl)imidazolium chloride
49	761410-61-1	1,3-Bis[(pentyloxy)methyl]imidazolium chloride
50	761410-62-2	1,3-Bis[(hexyloxy)methyl]imidazolium chloride
51	761410-63-3	1,3-Bis[(heptyloxy)methyl]imidazolium chloride
52	761410-64-4	1,3-Bis[(octyloxy)methyl]imidazolium chloride
53	761410-65-5	1,3-Bis[(nonyloxy)methyl]imidazolium chloride
54	435346-40-0	3-(Aminocarbonyl)-1-[(cyclododecyloxy)methyl]pyridinium chloride
55	435346-66-0	3-[[[(Decyloxy)methoxy]methyl]amino]carbonyl]-1-[(decyloxy)methyl]pyridinium chloride
56	435346-34-2	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride
57	435346-58-0	3-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium (T-4)-tetrachloroferrate
58	435346-54-6	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorocobaltate
59	435346-55-7	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorocuprate
60	435346-57-9	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachloromagnesate
61	435346-56-8	Bis[3-(aminocarbonyl)-1-[(decyloxy)methyl]pyridinium] (T-4)-tetrachlorozincate
62	435346-76-2	4-(Aminocarbonyl)-1-[(decyloxy)methyl]pyridinium chloride
63	435346-35-3	3-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride
64	435346-77-3	4-(Aminocarbonyl)-1-[(undecyloxy)methyl]pyridinium chloride
65	435346-53-5	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium acetate
66	435346-52-4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium tetrafluoroborate
67	435346-41-1	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium bromide
68	435346-36-4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride
69	435346-45-5	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium perchlorate
70	435346-42-2	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium iodide
71	435346-44-4	3-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium nitrate
72	435346-78-4	4-(Aminocarbonyl)-1-[(dodecyloxy)methyl]pyridinium chloride
73	435346-63-7	3-[[[(Heptyloxy)methoxy]methyl]amino]carbonyl]-1-[(heptyloxy)methyl]pyridinium chloride
74	435346-64-8	3-[[[(Octyloxy)methoxy]methyl]amino]carbonyl]-1-[(octyloxy)methyl]pyridinium chloride
75	435346-65-9	3-[[[(Nonyloxy)methoxy]methyl]amino]carbonyl]-1-[(nonyloxy)methyl]pyridinium chloride

76	13501-50-3	1-[(Decyloxy)methyl]quinolinium chloride
77	97166-43-3	1-[(Decyloxy)methyl]-6-methylquinolinium chloride
78	97166-47-7	1-[(Decyloxy)methyl]-8-hydroxyquinolinium chloride
79	41063-22-3	1-[(Dodecyloxy)methyl]quinolinium chloride
80	97166-44-4	1-[(Dodecyloxy)methyl]-6-methylquinolinium chloride
81	97166-48-8	1-[(Dodecyloxy)methyl]-8-hydroxyquinolinium chloride
82	97166-39-7	1-[(Hexyloxy)methyl]quinolinium chloride
83	97166-41-1	1-[(Hexyloxy)methyl]-6-methylquinolinium chloride
84	97166-45-5	1-[(Hexyloxy)methyl]-8-hydroxyquinolinium chloride
85	97166-40-0	1-[(Octyloxy)methyl]quinolinium chloride
86	97166-42-2	6-Methyl-1-[(octyloxy)methyl]quinolinium chloride
87	97166-46-6	8-Hydroxy-1-[(octyloxy)methyl]quinolinium chloride

S8: The 26 Variables in Bacteria and Fungi toxicity model

	Variables	unit
1	<i>Candida albicans</i> ATCC 10231 (growth inhibition) 48h	log(MIC)
2	<i>Candida albicans</i> ATCC 10231 (death) 5d	log(MBC)
3	<i>Enterococcus hirae</i> ATCC 10541 (growth inhibition) 24h	log(MIC)
4	<i>Enterococcus hirae</i> ATCC 10541 (death) 48h	log(MBC)
5	<i>Escherichia coli</i> ATCC 25922 (growth inhibition) 24h	log(MIC)
6	<i>Escherichia coli</i> ATCC 25922 (death) 48h	log(MBC)
7	<i>Klebsiella pneumoniae</i> ATCC 4352 (growth inhibition) 24h	log(MIC)
8	<i>Klebsiella pneumoniae</i> ATCC 4352 (death) 48h	log(MBC)
9	<i>Micrococcus luteus</i> ATCC 9341 (growth inhibition) 24h	log(MIC)
10	<i>Micrococcus luteus</i> ATCC 9341 (death) 48h	log(MBC)
11	<i>Proteus vulgaris</i> NCTC 4635 (growth inhibition) 24h	log(MIC)
12	<i>Proteus vulgaris</i> NCTC 4635 (death) 48h	log(MBC)
13	<i>Pseudomonas aeruginosa</i> ATCC 27853 (growth inhibition) 24h	log(MIC)
14	<i>Pseudomonas aeruginosa</i> ATCC 27853 (death) 48h	log(MBC)
15	<i>Pseudomonas aeruginosa</i> NCTC 6749 (growth inhibition) 24h	log(MIC)
16	<i>Rhodotorula rubra</i> PhB (growth inhibition) 48h	log(MIC)
17	<i>Rhodotorula rubra</i> PhB (death) 5d	log(MBC)
18	<i>Serratia marcescens</i> ATCC 8100 (growth inhibition) 24h	log(MIC)
19	<i>Serratia marcescens</i> ATCC 8100 (death) 48h	log(MBC)
20	<i>Staphylococcus aureus</i> ATCC 6538 (growth inhibition) 24h	log(MBC)
21	<i>Staphylococcus aureus</i> ATCC 6538 (death) 48h	log(MIC)
22	<i>Staphylococcus aureus</i> (MRSA) (growth inhibition) 24h	log(MIC)
23	<i>Staphylococcus aureus</i> (MRSA) (death) 48h	log(MBC)
24	<i>Staphylococcus aureus</i> NCTC 4163 (growth inhibition) 24h	log(MIC)
25	<i>Staphylococcus epidermidis</i> ATCC 12228 (growth inhibition) 24h	log(MIC)
26	<i>Staphylococcus epidermidis</i> ATCC 12228 (death) 48h	log(MBC)

S10: PCA Scores Plot in the Bacteria and Fungi toxicity model for imidazolium-based ILs. S10a: anions distribution; S10b: side chains distribution. Imidazolium side chains labels in S11.



S11: Imidazolium side chains labels

	Side chain	label
<i>none</i>	hydrogen	HY
	methyl	01
	ethyl	02
	propyl	03
	2-propenyl (<i>allyl</i>)	AL
	2-methylpropyl (<i>isobutyl</i>)	14
	butyl	04
	pentyl	05
	hexyl	06
	heptyl	07
	octyl	08
	nonyl	09
	decyl	10
	undecyl	11
	dodecyl	12
	tridecyl	13
	tetradecyl	14
	pentadecyl	15
	hexadecyl	16
heptadecyl	17	
octadecyl	18	
nonadecyl	19	
<i>alkylic</i>	phenylmethyl	PM
	phenylethyl	PE
	(4-methylphenyl)methyl	MP
	(1,3-benzodioxol-5-yl)-2-methoxy-2-oxoethyl	ZM
	1-(1,3-benzodioxol-5-yl)-2-butoxy-2-oxoethyl	ZB
	2-[1-(1,3-benzodioxol-5-yl)-2-butoxy-2-oxoethoxy]-2-oxoethyl	ZX
<i>aromatic</i>	metoxymethyl	1O
	etoxymethyl	2O
	propoxymethyl	3O
	butoxymethyl	4O
	pentoxymethyl	5O
	hexyloxymethyl	6O
	heptyloxymethyl	7O
	octyloxymethyl	8O
	nonyloxymethyl	9O
	decyloxymethyl	AO
	undecyloxymethyl	BO
	dodecyloxymethyl	CO
	tetradecyloxymethyl	EO
	hexadecyloxymethyl	GO
<i>alkyloxymethyl ether</i>	2-metoxyethyl	1E
	2-etoxethyl	2E
	2-(2-methoxyethoxy)ethyl	ME
	3-methoxypropyl	1P
<i>ether</i>	2-hydroxyethyl	ET
	3-hydroxypropyl	PR
<i>alcoholic</i>	4-hydroxypropyl	BL
	3-carboxypropyl	C3
<i>carboxylic</i>		
<i>ester</i>	11-ethoxy-11-oxoundecyl	EU
<i>amidic</i>	2-(diethylamino)-2-oxoethyl	EE
<i>nitrile</i>	cyanomethyl	CM