

Electronic Supplementary Information

Predicting toxicities of ionic liquids in multiple test species – an aid in designing of green chemicals

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Table S1: Two category (class -1 toxic and class -2 non-toxic) qualitative SAR modeling result with descriptor values

IL name	TPSA	Dipole	LogS	Actual Class	GBT-SAR	BDT-SAR	Data sub-sets
Imidazolium acetate	28.680	3.450	-0.212	1	1	1	Training-V. <i>fischeri</i> set
Imidazolium trifluoromethanesulfonate	28.680	3.450	-0.212	1	1	1	Training-V. <i>fischeri</i> set
Methylimidazolium trifluoromethanesulfonate	16.800	4.963	0.568	1	1	1	Training-V. <i>fischeri</i> set
Methylimidazolium caprylate	40.130	21.233	-1.948	2	2	2	Training-V. <i>fischeri</i> set
Methylimidazolium formate	19.070	2.917	-0.742	1	1	1	Training-V. <i>fischeri</i> set
Methylimidazolium	19.070	2.917	-0.742	1	1	1	Training-V. <i>fischeri</i> set
Methylmethylimidazolium methylsulfate	16.800	3.483	0.221	1	1	1	Training-V. <i>fischeri</i> set
(Cyanomethyl)methylimidazolium	32.600	6.964	-0.940	1	1	1	Training-V. <i>fischeri</i> set

bis(trifluoromethanesulfonyl)imide							
(Ethoxymethyl)methylimidazolium chloride	18.040	6.583	-1.422	1	1	1	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium ethylsulfate	8.810	2.639	-1.419	1	1	1	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium chloride	8.810	2.639	-1.419	1	1	1	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium bis(pentafluoroethyl)phosphinate	8.810	2.639	-1.419	1	1	1	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium bis[oxalato(2-)]borate	8.810	2.639	-1.419	1	1	1	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium methylsulfate	8.810	2.639	-1.419	1	1	1	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium tetracyanidoborate	8.810	2.639	-1.419	1	1	1	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium trifluoroacetate	8.810	2.639	-1.419	1	1	1	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium tetrachloroferrate(III)	8.810	2.643	-1.419	2	2	2	Training-V. <i>fischeri</i> set
(Ethoxyethyl)methylimidazolium bromide	18.040	9.554	-1.373	1	1	1	Training-V. <i>fischeri</i> set
(Hydroxyethyl)methylimidazolium iodide	29.040	5.470	-0.518	1	1	1	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	18.040	7.239	-1.025	1	1	1	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium chloride	18.040	7.239	-1.025	1	1	1	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium tetrafluoroborate	16.910	4.581	-0.199	2	2	2	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium dicyanamide	18.040	7.119	-0.910	2	2	2	Training-V. <i>fischeri</i> set
Propylmethylimidazolium tetrafluoroborate	8.810	4.483	-1.703	1	1	1	Training-V. <i>fischeri</i> set
Propylmethylimidazolium bis(trifluoromethanesulfonyl)imide	8.810	4.483	-1.703	1	1	1	Training-V. <i>fischeri</i> set
(Hydroxypropyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	29.040	7.345	-0.820	1	1	1	Training-V. <i>fischeri</i> set
(Hydroxypropyl)methylimidazolium chloride	29.040	7.244	-0.704	1	1	1	Training-V. <i>fischeri</i> set
(Methoxypropyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	18.040	9.209	-1.323	1	1	1	Training-V. <i>fischeri</i> set
(Methoxypropyl)methylimidazolium chloride	18.040	9.103	-1.208	1	1	1	Training-V. <i>fischeri</i> set
Butylimidazolium trifluoroacetate	17.820	3.921	-1.646	1	1	1	Training-V. <i>fischeri</i> set
Butylimidazolium acetate	17.820	3.921	-1.646	1	1	1	Training-V. <i>fischeri</i> set
Butylimidazolium trifluoromethanesulfonate	17.820	3.921	-1.646	1	1	1	Training-V. <i>fischeri</i> set
Butylimidazolium caprylate	40.130	21.233	-1.948	2	2	2	Training-V. <i>fischeri</i> set

Butylimidazolium formate	17.820	3.921	-1.646	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium tetrafluoroborate	8.810	6.703	-2.133	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium bromide	8.810	6.703	-2.133	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium chloride	8.810	6.703	-2.133	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium iodide	8.810	6.703	-2.133	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium dicyanamide	8.810	6.703	-2.133	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium-o-Octylsulfate	66.430	22.819	-2.434	2	2	2	Training-V. <i>fischeri</i> set
Butylmethylimidazolium trifluoromethanesulfonate	8.810	6.703	-2.133	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium bis(trifluoromethyl)amide	8.810	6.703	-2.133	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium methylbenzenesulfonate	8.810	6.703	-2.133	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylimidazolium tetrachloroferrate(III)	8.810	6.703	-2.133	2	1	1	Training-V. <i>fischeri</i> set
Butylethylimidazolium tetrafluoroborate	8.810	4.646	-2.360	1	1	1	Training-V. <i>fischeri</i> set
Pentylmethylimidazolium tetrafluoroborate	8.810	9.181	-2.561	1	1	1	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium bromide	8.810	11.706	-2.987	2	2	2	Training-V. <i>fischeri</i> set
Hexyldimethylimidazolium chloride	12.360	6.584	-1.748	2	2	2	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium hexafluorophosphate	8.810	11.706	-2.987	2	2	2	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium trifluoridotris(pentafluoroethyl)phosphate	0.000	8.338	-9.347	1	1	1	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium-1,1-Dioxo-1,2-dihydrobenzo[d]isothiazol-3-onate	8.810	11.706	-2.987	1	2	2	Training-V. <i>fischeri</i> set
Hexylethylimidazolium tetrafluoroborate	8.810	9.604	-3.210	2	2	2	Training-V. <i>fischeri</i> set
Heptylmethylimidazolium tetrafluoroborate	8.810	14.362	-3.411	1	1	1	Training-V. <i>fischeri</i> set
Octylmethylimidazolium bromide	8.810	17.027	-3.833	2	2	2	Training-V. <i>fischeri</i> set
Octylmethylimidazolium chloride	8.810	17.027	-3.833	2	2	2	Training-V. <i>fischeri</i> set
Octylmethylimidazolium hexafluorophosphate	8.810	17.027	-3.833	2	2	2	Training-V. <i>fischeri</i> set
Octylmethylimidazolium tetrafluoroborate	8.810	17.027	-3.833	2	2	2	Training-V. <i>fischeri</i> set
Octylmethylimidazolium bis(trifluoromethanesulfonyl)imide	8.810	17.027	-3.833	2	2	2	Training-V. <i>fischeri</i> set
Decylmethylimidazolium chloride	8.810	22.525	-4.675	2	2	2	Training-V. <i>fischeri</i> set
Decylmethylimidazolium tetrafluoroborate	8.810	22.525	-4.675	2	2	2	Training-V. <i>fischeri</i> set

Decylmethylimidazolium tetrachloroferrate(III)	8.810	22.525	-4.675	2	2	2	Training-V. <i>fischeri</i> set
Tetradecylmethylimidazolium chloride	8.810	33.825	-5.444	2	2	2	Training-V. <i>fischeri</i> set
Hexadecylmethylimidazolium chloride	8.810	39.570	-6.128	2	2	2	Training-V. <i>fischeri</i> set
Octadecylmethylimidazolium chloride	8.810	45.359	-6.811	2	2	2	Training-V. <i>fischeri</i> set
Methylpyridinium	3.880	1.066	-1.306	1	1	1	Training-V. <i>fischeri</i> set
Hydroxypropylpyridinium bis(trifluoromethanesulfonyl)imide	24.110	6.540	-0.760	1	1	1	Training-V. <i>fischeri</i> set
Butylpyridinium bromide	3.880	5.790	-2.273	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylpyridinium bromide	3.880	4.018	-2.633	1	1	1	Training-V. <i>fischeri</i> set
Butyldimethylpyridinium bromide	3.880	3.496	-2.693	1	1	1	Training-V. <i>fischeri</i> set
Butylpyridinium chloride	3.880	5.790	-2.273	1	1	1	Training-V. <i>fischeri</i> set
Butylpyridinium-m-Chlorohexa chloridodialuminate	3.880	5.790	-2.273	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylpyridinium tetrafluoroborate	3.880	4.018	-2.633	1	1	1	Training-V. <i>fischeri</i> set
Butylpyridinium dicyanamide	3.880	5.790	-2.273	1	1	1	Training-V. <i>fischeri</i> set
Butyldimethylpyridinium dicyanamide	3.880	3.496	-2.693	2	1	1	Training-V. <i>fischeri</i> set
Hexylmethylpyridinium chloride	3.880	9.482	-3.338	2	2	2	Training-V. <i>fischeri</i> set
Octylpyridinium chloride	3.880	16.324	-3.981	2	2	2	Training-V. <i>fischeri</i> set
Octylmethylpyridinium bromide	3.880	14.695	-4.185	2	2	2	Training-V. <i>fischeri</i> set
Octyldimethylpyridinium bromide	3.880	13.254	-4.388	2	2	2	Training-V. <i>fischeri</i> set
Octyldimethylpyridinium bis(trifluoromethanesulfonyl)imide	3.880	13.254	-4.388	2	2	2	Training-V. <i>fischeri</i> set
(Ethoxyethyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	9.230	5.691	-0.397	1	1	1	Training-V. <i>fischeri</i> set
(Hydroxypropyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	20.230	4.806	0.127	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylpyrrolidinium chloride	0.000	4.030	-1.398	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylpyrrolidinium trifluoridotris(pentafluoroethyl)phosphate	0.000	4.030	-1.398	2	1	1	Training-V. <i>fischeri</i> set
Hexylmethylpyrrolidinium chloride	0.000	8.780	-2.227	1	1	1	Training-V. <i>fischeri</i> set
Hexylmethylpyrrolidinium bis(trifluoromethanesulfonyl)imide	0.000	8.780	-2.227	1	1	1	Training-V. <i>fischeri</i> set

Butylmethylpiperidinium bromide	0.000	2.642	-1.717	1	1	1	Training-V. <i>fischeri</i> set
Butylmethylpiperidinium bis(trifluoromethanesulfonyl)imide	0.000	2.642	-1.717	1	1	1	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium bromide	7.120	2.519	-2.433	2	2	2	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium chloride	7.120	2.508	-2.433	1	1	2	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium bis(trifluoromethanesulfonyl)imide	7.120	2.508	-2.433	2	1	2	Training-V. <i>fischeri</i> set
Choline bis(trifluoromethanesulfonyl)imide	20.230	3.646	1.116	1	1	1	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine trifluoroacetate	30.330	3.813	-1.214	2	1	1	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine acetate	30.330	3.813	-1.214	1	1	1	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine trifluoromethanesulfonate	30.330	3.813	-1.214	1	1	1	Training-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine acetate	107.640	3.962	-2.116	1	1	1	Training-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine trifluoromethanesulfonate	107.640	3.968	-2.116	1	1	1	Training-V. <i>fischeri</i> set
Cethyltrimethylammonium bromide	0.000	39.951	-4.612	2	2	2	Training-V. <i>fischeri</i> set
Hexadecylbenzyltrimethylammonium chloride	0.000	27.896	-6.446	2	2	2	Training-V. <i>fischeri</i> set
Benzyltrimethylammonium chloride	0.000	16.981	-5.834	2	2	2	Training-V. <i>fischeri</i> set
Tetrabutylammonium chloride	0.000	1.60 x 10 ⁻⁵	-3.776	1	1	1	Training-V. <i>fischeri</i> set
Tetramethylammonium bromide	0.000	6.13 x 10 ⁻⁶	0.325	1	1	1	Training-V. <i>fischeri</i> set
Tetraethylammonium bromide	0.000	8.08 x 10 ⁻⁶	-1.064	1	1	1	Training-V. <i>fischeri</i> set
Tetrabutylammonium bromide	0.000	1.60 x 10 ⁻⁵	-3.776	1	1	1	Training-V. <i>fischeri</i> set
Butylethyltrimethylammonium bis(trifluoromethanesulfonyl)imide	0.000	4.583	-1.047	1	1	1	Training-V. <i>fischeri</i> set
(Ethoxycarbonylmethyl)ethyltrimethylammonium bis(trifluoromethanesulfonyl)imide	26.300	7.232	-0.090	1	1	1	Training-V. <i>fischeri</i> set
(Hydroxyethyl)trimethylammonium acetate	24.670	4.078	1.132	1	1	1	Training-V. <i>fischeri</i> set
(Hydroxyethyl)trimethylammonium hydroxyacetate	24.670	4.078	1.132	1	1	1	Training-V. <i>fischeri</i> set
(Methoxyethyl)ethyltrimethylammonium bis(trifluoromethanesulfonyl)imide	9.230	3.649	0.286	1	1	1	Training-V. <i>fischeri</i> set
Tetrabutylphosphonium bromide	0.000	4.09 x 10 ⁻⁵	-5.290	1	1	1	Training-V. <i>fischeri</i> set

Tributylethylphosphonium diethylphosphate	0.000	2.755	-4.613	1	1	1	Training-V. <i>fischeri</i> set
Trihexyl(tetradecyl)phosphonium bromide	0.000	14.993	-10.405	1	2	1	Training-V. <i>fischeri</i> set
Trihexyl(tetradecyl)phosphonium trifluoridotris(pentafluoroethyl)phosphate	0.000	14.993	-10.405	2	2	1	Training-V. <i>fischeri</i> set
Bis(trifluoromethanesulfonyl)imide	80.310	1.686	-2.159	1	1	1	Training-V. <i>fischeri</i> set
O-Octylsulfate	66.430	22.819	-2.434	1	1	1	Training-V. <i>fischeri</i> set
Tetrafluoroborate	0.000	2.22 x10 ⁻¹⁶	-0.628	1	1	1	Training-V. <i>fischeri</i> set
Triethylsulfanium bis(trifluoromethanesulfonyl)imide	0.000	3.118	-1.393	1	1	1	Training-V. <i>fischeri</i> set
(Ethoxyoxoethyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	26.300	6.647	-0.441	1	1	1	Training-V. <i>fischeri</i> set
O-Dodecylsulfate	66.430	33.655	-4.091	2	2	2	Training-V. <i>fischeri</i> set
Imidazolium trifluoroacetate	28.970	5.962	0.428	1	1	1	Test-V. <i>fischeri</i> set
Imidazolium caprylate	40.130	21.233	-1.948	2	2	2	Test-V. <i>fischeri</i> set
Methylimidazolium trifluoroacetate	16.800	4.963	0.568	1	1	1	Test-V. <i>fischeri</i> set
Methylimidazolium acetate	17.820	3.906	-0.555	1	1	1	Test-V. <i>fischeri</i> set
(Ethoxymethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	18.040	6.583	-1.422	1	1	1	Test-V. <i>fischeri</i> set
Ethylmethylimidazolium bis[1,2-benzenediolato(2-)]borate	36.920	3.547	-3.831	1	1	1	Test-V. <i>fischeri</i> set
Ethylmethylimidazolium thiocyanate	8.810	2.639	-1.419	1	1	1	Test-V. <i>fischeri</i> set
(Ethoxyethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	18.040	9.554	-1.373	1	1	1	Test-V. <i>fischeri</i> set
(Hydroxyethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	29.040	5.470	-0.518	1	1	1	Test-V. <i>fischeri</i> set
Butylmethylimidazolium hexafluorophosphate	8.810	6.703	-2.133	1	1	1	Test-V. <i>fischeri</i> set
Butylmethylimidazolium bis(trifluoromethanesulfonyl)imide	8.810	6.703	-2.133	1	1	1	Test-V. <i>fischeri</i> set
Hexylmethylimidazolium chloride	8.810	11.706	-2.987	2	2	2	Test-V. <i>fischeri</i> set
Hexylmethylimidazolium tetrafluoroborate	8.810	11.706	-2.987	1	2	2	Test-V. <i>fischeri</i> set
Hexylmethylimidazolium bis(trifluoromethanesulfonyl)imide	8.810	11.706	-2.987	2	2	2	Test-V. <i>fischeri</i> set
Nonylmethylimidazolium tetrafluoroborate	8.810	19.776	-4.255	2	2	2	Test-V. <i>fischeri</i> set

Butylmethylpyridinium dicyanamide	3.880	4.622	-2.484	1	1	1	Test-V. <i>fischeri</i> set
Hexylmethylpyridinium bromide	3.880	9.482	-3.338	2	2	2	Test-V. <i>fischeri</i> set
Butylmethylpyrrolidinium bis(trifluoromethanesulfonyl)imide	0.000	4.030	-1.398	1	1	1	Test-V. <i>fischeri</i> set
(Ethoxymethyl)methylmorpholinium bis(trifluoromethanesulfonyl)imide	18.460	3.380	0.156	1	1	1	Test-V. <i>fischeri</i> set
Butylmethylmorpholinium bromide	9.230	2.469	-0.561	1	1	1	Test-V. <i>fischeri</i> set
Butylmethylmorpholinium bis(trifluoromethanesulfonyl)imide	9.230	2.469	-0.561	1	1	1	Test-V. <i>fischeri</i> set
Hexyl(dimethylamino)pyridinium bis(trifluoromethanesulfonyl)imide	7.120	7.031	-3.280	2	2	1	Test-V. <i>fischeri</i> set
Choline chloride	20.230	3.646	1.116	1	1	1	Test-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine caprylate	40.130	21.233	-1.948	2	2	2	Test-V. <i>fischeri</i> set
Cethyltrimethylammonium chloride	0.000	39.951	-4.612	2	2	2	Test-V. <i>fischeri</i> set
Hexyltriethylammonium bromide	0.000	8.198	-2.571	1	1	1	Test-V. <i>fischeri</i> set
Butylethyldimethylammonium chloride	0.000	4.583	-1.047	1	1	1	Test-V. <i>fischeri</i> set
Bis(2-methoxyethyl)ammonium sulfamate	35.070	2.694	0.831	1	1	1	Test-V. <i>fischeri</i> set
Bis[1,2-benzenediolato(2-)]borate	36.920	3.552	-3.831	1	1	1	Test-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine trifluoroacetate	107.640	3.968	-2.116	2	1	1	Test-V. <i>fischeri</i> set
1-Decyl-3-methylimidazolium chloride	8.810	22.525	-4.675	2	2	2	Test algae set
1-(Cyanomethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	32.600	6.964	-0.940	2	1	2	Test algae set
1-(Cyanomethyl)-3-methylimidazolium chloride	32.600	6.964	-0.940	1	1	2	Test algae set
1-(Ethoxymethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	18.040	6.583	-1.422	2	1	2	Test algae set
1-(Ethoxymethyl)-3-methylimidazolium chloride	18.040	6.583	-1.422	1	1	2	Test algae set
1-Ethyl-3-methylimidazolium-4-Fluoro-1-butanefluoroborate	8.810	2.565	-1.419	2	2	2	Test algae set
1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato(2-)]borate(1-)	36.920	3.547	-3.831	2	2	2	Test algae set
1-Ethyl-3-methylimidazolium-4-Chloro-1-butanefluoroborate	8.810	2.643	-1.419	1	1	1	Test algae set
1-Ethyl-3-methylimidazolium chloride	8.810	2.639	-1.419	1	1	1	Test algae set

1-(2-Methoxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	18.040	7.239	-1.025	2	2	2	Test algae set
1-(2-Methoxyethyl)-3-methylimidazolium chloride	18.040	7.239	-1.025	1	2	2	Test algae set
1-(2-Ethoxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	18.040	9.554	-1.373	2	2	2	Test algae set
1-(2-Ethoxyethyl)-3-methylimidazolium bromide	18.040	9.554	-1.373	1	2	2	Test algae set
1-(2-Hydroxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	29.040	5.470	-0.518	2	2	2	Test algae set
1-(3-Methoxypropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	18.040	9.209	-1.323	2	2	2	Test algae set
1-(3-Hydroxypropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	29.040	7.345	-0.820	2	2	2	Test algae set
1-Butyl-3-methylimidazolium bis(trifluoromethyl)amide(1-)	8.810	6.703	-2.133	1	2	2	Test algae set
1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	8.810	6.703	-2.133	2	2	2	Test algae set
1-Butyl-3-methylimidazolium -O-Octyl sulfate	66.430	22.819	-2.434	2	2	2	Test algae set
1-Butyl-3-methylimidazolium tetrafluoridoboranuide(1-)	8.810	6.703	-2.133	2	2	2	Test algae set
1-Butyl-3-methylimidazolium-4-Chloro-1-butanefulfonate	8.810	6.592	-2.018	1	1	1	Test algae set
1-Butyl-3-methylimidazolium chloride	8.810	6.703	-2.133	2	2	2	Test algae set
1-Hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	8.810	11.706	-2.987	2	2	2	Test algae set
1-Hexyl-3-methylimidazolium trifluoridotris(pentafluoroethyl)phosphate(1-)	8.810	11.706	-2.987	2	2	2	Test algae set
1-Hexyl-3-methylimidazolium hexafluoridophosphate(1-)	8.810	11.706	-2.987	2	2	2	Test algae set
1-Hexyl-3-methylimidazolium chloride	8.810	11.706	-2.987	2	2	2	Test algae set
1-Methyl-3-octylimidazolium tetrafluoridoboranuide(1-)	8.810	17.027	-3.833	2	2	2	Test algae set
1-Methyl-3-octylimidazolium chloride	8.810	17.027	-3.833	2	2	2	Test algae set
4-(Ethoxymethyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)amide(1-)	18.460	3.380	0.156	1	1	1	Test algae set
4-Butyl-4-methylmorpholinium	9.230	2.469	-0.561	2	2	2	Test algae set

bis(trifluoromethylsulfonyl)amide(1-) (Ethoxycarbonylmethyl)ethyl dimethylammonium	26.300	7.232	-0.090	2	1	2	Test algae set
bis(trifluoromethylsulfonyl)amide(1-) (Ethoxycarbonylmethyl)ethyl dimethylammonium bromide	26.300	7.232	-0.090	1	1	2	Test algae set
Butylethyl dimethylammonium bis(trifluoromethylsulfonyl)amide(1-)	0.000	4.583	-1.047	2	2	2	Test algae set
1-(3-Methoxypropyl)-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide(1-)	9.230	5.224	-0.674	2	2	2	Test algae set
1-Butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide(1-)	0.000	2.642	-1.717	2	1	2	Test algae set
1-Butyl-1-methylpiperidinium bromide	0.000	2.642	-1.717	1	1	2	Test algae set
1-Butylpyridinium chloride	3.880	5.790	-2.273	1	1	1	Test algae set
1-Butyl-4-(dimethylamino)pyridinium bis(trifluoromethylsulfonyl)amide(1-)	7.120	2.508	-2.433	2	2	2	Test algae set
1-Butyl-4-(dimethylamino)pyridinium chloride	7.120	2.508	-2.433	2	2	2	Test algae set
1-(Ethoxycarbonylmethyl)-1-methylpyrrolidinium bromide	26.300	6.647	-0.441	1	1	1	Test algae set
1-(2-Methoxyethyl)-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	9.230	4.065	-0.065	2	2	2	Test algae set
1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	0.000	4.030	-1.398	1	1	1	Test algae set
1-Butyl-1-methylpyrrolidinium chloride	0.000	4.030	-1.398	1	1	1	Test algae set
Triethylsulfanium bis(trifluoromethylsulfonyl)amide(1-)	0.000	3.118	-1.393	2	2	2	Test algae set
1-hexyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	0.000	8.780	-2.227	2	2	2	Test algae set
1-butyl-3-methylimidazolium chloride	8.810	6.703	-2.133	2	2	2	Test daphnia set
1-butyl-3-methylimidazolium bromide	8.810	6.703	-2.133	2	2	2	Test daphnia set
1-butyl-3-methylimidazolium tetrafluoroborate	8.810	6.703	-2.133	2	2	2	Test daphnia set
1-butyl-3-methylimidazolium Hexafluorophosphate	8.810	6.703	-2.133	2	2	2	Test daphnia set
1-butyl-3-methylimidazolium bis(trifluoromethyl)sulfonylimide	8.810	6.703	-2.133	2	2	2	Test daphnia set
1-n-Hexyl-3-methylimidazolium Chloride	8.810	11.706	-2.987	2	2	2	Test daphnia set

1-n-Hexyl-3-methylimidazolium bromide	8.810	11.706	-2.987	2	2	2	Test daphnia set
1-n-Hexyl-3-methylimidazolium tetrafluoroborate	8.810	11.706	-2.987	2	2	2	Test daphnia set
1-n-Octyl-3-methylimidazolium chloride	8.810	17.027	-3.833	2	2	2	Test daphnia set
1-n-Octyl-3-methylimidazolium bromide	8.810	17.027	-3.833	2	2	2	Test daphnia set
1-n-Octyl-3-methylimidazolium tetrafluoroborate	8.810	17.027	-3.833	2	2	2	Test daphnia set
Decylmethylimidazolium Bromide	8.810	22.525	-4.675	2	2	2	Test daphnia set
1-dodecyl-3-methylimidazolium chloride	8.810	28.136	-5.514	2	2	2	Test daphnia set
1-dodecyl-3-methylimidazolium bromide	8.810	28.136	-5.514	2	2	2	Test daphnia set
1-hexadecyl-3-methylimidazolium chloride	8.810	39.570	-6.128	2	2	2	Test daphnia set
Octadecylmethylimidazolium Chloride	8.810	45.359	-6.811	2	2	2	Test daphnia set
1-n-Hexyl-2,3-dimethylimidazolium bromide	8.810	10.773	-3.200	2	2	2	Test daphnia set
Butylpyridinium Chloride	3.880	5.790	-2.273	2	2	2	Test daphnia set
Butylpyridinium bis(trifluoromethyl)sulfonylimide	3.880	5.790	-2.273	2	2	2	Test daphnia set
Butylmethylpyridinium bromide	3.880	4.622	-2.484	2	2	2	Test daphnia set
Butylmethylmethylpyridinium bromide	3.880	3.496	-2.693	2	2	2	Test daphnia set
Hexylpyridinium bromide	3.880	10.936	-3.131	2	2	2	Test daphnia set
Hexylmethylpyridinium bromide	3.880	9.482	-3.338	2	2	2	Test daphnia set
1-n-Hexyl-4-piperidinopyridinium bromide	7.120	3.534	-4.273	2	2	2	Test daphnia set
Octylmethylpyridinium bromide	3.880	14.695	-4.185	2	2	2	Test daphnia set
1-n-Hexyl-4-dimethylaminopyridinium bromide	7.120	7.035	-3.280	2	2	2	Test daphnia set
1-n-Hexyl-3-methyl-4-dimethylaminopyridinium bromide	7.120	6.225	-3.483	2	2	2	Test daphnia set
N,N-methylbutylpyrrolidinium bis(trifluoromethyl)sulfonylimide	0.000	4.030	-1.398	2	2	2	Test daphnia set
Dodecyltrimethylammonium bromide	0.000	28.380	-4.013	2	2	2	Test daphnia set
Tetradecyltrimethylammonium bromide	0.000	34.143	-3.935	2	2	2	Test daphnia set
Hexadecyltrimethylammonium bromide	0.000	39.951	-4.612	2	2	2	Test daphnia set
Tetrabutylphosphonium bromide	0.000	4.09 x10 ⁻⁵	-5.290	2	2	2	Test daphnia set
Tetrabutylammonium bromide	0.000	1.36 x10 ⁻⁵	-3.776	2	2	2	Test daphnia set
Dodecylbenzyltrimethylammonium bromide	0.000	16.981	-5.834	2	2	2	Test daphnia set

Tributylethylphosphonium diethyl phosphate	0.000	2.755	-4.613	2	2	2	Test daphnia set
Trihexyltetradecylphosphonium chloride	0.000	14.993	-10.405	2	2	2	Test daphnia set
Methyltrioctylammonium bis(trifluoromethylsulfonyl)amide(1-)	0.000	7.911	-6.512	2	2	2	Test daphnia set
Picolinium bromide	3.880	1.066	-1.306	2	2	2	Test daphnia set
1-(2-methoxyethyl)-3-methyl-1H-imidazolium tetrafluoroborate	18.040	7.239	-1.025	1	1	1	Test daphnia set
1-(2-methoxyethyl)-3-methyl-1H-imidazolium N-cyanocynamide	18.040	7.239	-1.025	1	1	1	Test daphnia set
3-(2-chloroethyl)-1-methylimidazolium chloride	8.810	8.674	-1.831	1	1	1	Test daphnia set
3-(2-chloroethyl)-1-methylimidazolium bis(trifluoromethyl)sulfonylimide	8.810	8.674	-1.831	1	1	1	Test daphnia set
3-(2-hydroxyethyl)-1-methylimidazolium bis(trifluoromethyl)sulfonylimide	29.040	5.470	-0.518	1	1	1	Test daphnia set
3-(2-chloropropyl)-1-methylimidazolium chloride	8.810	6.332	-2.992	1	1	2	Test daphnia set
1-methyl-3-[(trimethylsilyl)methyl]-imidazolium bromide	8.810	7.777	-3.217	2	2	2	Test daphnia set
Methylimidazolium chloride	28.200	4.300	-1.498	1	1	1	Test daphnia set
1-(2-Chloroethyl)imidazolium chloride	19.030	11.445	-1.599	1	1	1	Test daphnia set
1,10-(1,2-ethanediyl)bis-imidazolium chloride	35.640	1.764	-1.417	1	1	1	Test daphnia set
Choline hexafluorophosphate	20.230	3.646	1.116	1	1	1	Test daphnia set
Ethyl-methylmorpholiniumbromide	9.230	4.169	0.117	1	1	1	Test daphnia set
Butylethyl-morpholiniumbromide	13.670	6.203	-1.149	1	1	1	Test daphnia set
Ethyltetrahydrothiopheniumbromide	0.000	3.393	-1.378	1	1	1	Test daphnia set
Triethylsulfoniumbromide	0.000	3.118	-1.393	1	1	1	Test daphnia set

Table S2: Four category (class -1 very highly toxic; class -2 highly toxic; class -3 moderately toxic; class -4 low toxic) qualitative modeling result with descriptor values

Ionic liquid name	Dipole	LogS	InertiaX	Actual Class	GBT-SAR	BDT-SAR	Data sub-sets
Imidazolium trifluoroacetate	5.962	0.428	53.695	4	4	4	Training-V. <i>fischeri</i> set
Imidazolium acetate	3.450	-0.212	50.371	3	4	4	Training-V. <i>fischeri</i> set
Imidazolium trifluoromethanesulfonate	3.450	-0.212	50.371	4	4	4	Training-V. <i>fischeri</i> set
Imidazolium caprylate	21.233	-1.948	77.689	3	3	3	Training-V. <i>fischeri</i> set
Methylimidazolium acetate	3.906	-0.555	54.412	4	4	4	Training-V. <i>fischeri</i> set
Methylimidazolium formate	2.917	-0.742	55.589	3	4	4	Training-V. <i>fischeri</i> set
Methylimidazolium	2.917	-0.742	55.589	4	4	4	Training-V. <i>fischeri</i> set
Methylmethylimidazolium methylsulfate	3.483	0.221	74.347	4	4	4	Training-V. <i>fischeri</i> set
(Cyanomethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	6.964	-0.940	121.712	4	4	4	Training-V. <i>fischeri</i> set
(Ethoxymethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	6.583	-1.422	133.279	3	3	4	Training-V. <i>fischeri</i> set
(Ethoxymethyl)methylimidazolium chloride	6.583	-1.422	133.279	4	3	4	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium bis[1,2-benzenediolato(2-)]borate	3.547	-3.831	291.682	3	3	3	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium chloride	2.639	-1.419	97.815	4	4	4	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium bis(pentafluoroethyl)phosphinate	2.639	-1.419	97.815	3	4	4	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium bis[oxalato(2-)]borate	2.639	-1.419	97.815	4	4	4	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium tetracyanidoborate	2.639	-1.419	97.815	3	4	4	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium thiocyanate	2.639	-1.419	97.815	4	4	4	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium trifluoroacetate	2.639	-1.419	97.815	4	4	4	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium tetrachloroferrate(III)	2.643	-1.419	97.804	2	2	2	Training-V. <i>fischeri</i> set
(Ethoxyethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	9.554	-1.373	131.427	3	3	3	Training-V. <i>fischeri</i> set
(Hydroxyethyl)methylimidazolium	5.470	-0.518	104.691	4	4	4	Training-V. <i>fischeri</i> set

bis(trifluoromethanesulfonyl)imide							
(Methoxyethyl)methylimidazolium chloride	7.239	-1.025	126.819	4	4	4	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium tetrafluoroborate	4.581	-0.199	136.752	2	2	2	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium dicyanamide	7.119	-0.910	126.628	2	2	2	Training-V. <i>fischeri</i> set
Propylmethylimidazolium tetrafluoroborate	4.483	-1.703	106.359	4	4	4	Training-V. <i>fischeri</i> set
Propylmethylimidazolium bis(trifluoromethanesulfonyl)imide	4.483	-1.703	106.350	3	3	3	Training-V. <i>fischeri</i> set
(Hydroxypropyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	7.345	-0.820	128.316	4	4	4	Training-V. <i>fischeri</i> set
(Hydroxypropyl)methylimidazolium chloride	7.244	-0.704	128.117	4	4	4	Training-V. <i>fischeri</i> set
(Methoxypropyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	9.209	-1.323	134.505	3	3	3	Training-V. <i>fischeri</i> set
Butylimidazolium acetate	3.921	-1.646	96.448	3	3	3	Training-V. <i>fischeri</i> set
Butylimidazolium trifluoromethanesulfonate	3.921	-1.646	96.448	3	3	3	Training-V. <i>fischeri</i> set
Butylimidazolium caprylate	21.233	-1.948	77.689	2	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium hexafluorophosphate	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium tetrafluoroborate	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium bromide	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium chloride	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium iodide	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium dicyanamide	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium- <i>O</i> -Octylsulfate	22.819	-2.434	141.512	2	2	2	Training-V. <i>fischeri</i> set
Butylmethylimidazolium bis(trifluoromethanesulfonyl)imide	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium bis(trifluoromethyl)amide	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium methylbenzenesulfonate	6.703	-2.133	133.278	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylimidazolium tetrachloroferrate(III)	6.703	-2.133	133.278	2	3	3	Training-V. <i>fischeri</i> set
Butylethylimidazolium tetrafluoroborate	4.646	-2.360	156.036	3	3	3	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium bromide	11.706	-2.987	162.821	2	3	3	Training-V. <i>fischeri</i> set

Hexylmethylimidazolium chloride	11.706	-2.987	162.821	3	3	3	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium hexafluorophosphate	11.706	-2.987	162.821	3	3	3	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium tetrafluoroborate	11.706	-2.987	162.821	3	3	3	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium trifluoridotris(pentafluoroethyl)phosphate	8.338	-9.347	2903.910	3	3	3	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium-1,1-Dioxo-1,2-dihydrobenzo[d]isothiazol-3-onate	11.706	-2.987	162.821	3	3	3	Training-V. <i>fischeri</i> set
Hexylethylimidazolium tetrafluoroborate	9.604	-3.210	187.824	3	3	3	Training-V. <i>fischeri</i> set
Heptylmethylimidazolium tetrafluoroborate	14.362	-3.411	167.033	3	3	3	Training-V. <i>fischeri</i> set
Octylmethylimidazolium bromide	17.027	-3.833	188.399	2	2	2	Training-V. <i>fischeri</i> set
Octylmethylimidazolium chloride	17.027	-3.833	188.399	2	2	2	Training-V. <i>fischeri</i> set
Octylmethylimidazolium tetrafluoroborate	17.027	-3.833	188.399	2	2	2	Training-V. <i>fischeri</i> set
Octylmethylimidazolium bis(trifluoromethanesulfonyl)imide	17.027	-3.833	188.399	2	2	2	Training-V. <i>fischeri</i> set
Decylmethylimidazolium chloride	22.525	-4.675	211.379	2	1	1	Training-V. <i>fischeri</i> set
Decylmethylimidazolium tetrafluoroborate	22.525	-4.675	211.379	1	1	1	Training-V. <i>fischeri</i> set
Decylmethylimidazolium tetrachloroferrate(III)	22.525	-4.675	211.379	1	1	1	Training-V. <i>fischeri</i> set
Tetradecylmethylimidazolium chloride	33.825	-5.444	252.397	1	1	1	Training-V. <i>fischeri</i> set
Hexadecylmethylimidazolium chloride	39.570	-6.128	271.225	2	2	2	Training-V. <i>fischeri</i> set
Octadecylmethylimidazolium chloride	45.359	-6.811	289.252	2	2	2	Training-V. <i>fischeri</i> set
Methylpyridinium	1.066	-1.306	87.034	3	3	3	Training-V. <i>fischeri</i> set
Hydroxypropylpyridinium bis(trifluoromethanesulfonyl)imide	6.540	-0.760	129.391	4	4	4	Training-V. <i>fischeri</i> set
Butylpyridinium bromide	5.790	-2.273	134.365	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylpyridinium bromide	4.018	-2.633	148.517	3	3	3	Training-V. <i>fischeri</i> set
Butyldimethylpyridinium bromide	3.496	-2.693	334.343	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylpyridinium tetrafluoroborate	4.018	-2.633	148.517	3	3	3	Training-V. <i>fischeri</i> set
Butylpyridinium dicyanamide	5.790	-2.273	134.365	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylpyridinium dicyanamide	4.622	-2.484	211.731	3	3	3	Training-V. <i>fischeri</i> set
Hexylmethylpyridinium bromide	9.482	-3.338	243.628	3	2	3	Training-V. <i>fischeri</i> set
Hexylmethylpyridinium chloride	9.482	-3.338	243.628	2	2	3	Training-V. <i>fischeri</i> set

Octyldimethylpyridinium bis(trifluoromethanesulfonyl)imide	13.254	-4.388	391.341	2	2	2	Training-V. <i>fischeri</i> set
(Ethoxyethyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	5.691	-0.397	260.221	3	3	3	Training-V. <i>fischeri</i> set
(Hydroxypropyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	4.806	0.127	166.646	4	4	4	Training-V. <i>fischeri</i> set
Butylmethylpyrrolidinium chloride	4.030	-1.398	170.283	4	3	4	Training-V. <i>fischeri</i> set
Butylmethylpyrrolidinium bis(trifluoromethanesulfonyl)imide	4.030	-1.398	170.283	3	3	4	Training-V. <i>fischeri</i> set
(Ethoxymethyl)methylmorpholinium bis(trifluoromethanesulfonyl)imide	3.380	0.156	187.117	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylmorpholinium bis(trifluoromethanesulfonyl)imide	2.469	-0.561	186.507	3	4	4	Training-V. <i>fischeri</i> set
Butylmethylpiperidinium bromide	2.642	-1.717	191.445	4	3	4	Training-V. <i>fischeri</i> set
Butylmethylpiperidinium bis(trifluoromethanesulfonyl)imide	2.642	-1.717	191.445	3	3	4	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium bromide	2.519	-2.433	216.473	3	3	3	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium chloride	2.508	-2.433	215.752	3	3	3	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium bis(trifluoromethanesulfonyl)imide	2.508	-2.433	215.752	2	3	3	Training-V. <i>fischeri</i> set
Hexyl(dimethylamino)pyridinium bis(trifluoromethanesulfonyl)imide	7.031	-3.280	264.557	2	2	2	Training-V. <i>fischeri</i> set
Choline chloride	3.646	1.116	121.187	4	4	4	Training-V. <i>fischeri</i> set
Choline bis(trifluoromethanesulfonyl)imide	3.646	1.116	121.187	4	4	4	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine trifluoroacetate	3.813	-1.214	167.118	2	3	3	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine trifluoromethanesulfonate	3.813	-1.214	167.118	3	3	3	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine caprylate	21.233	-1.948	77.689	3	3	3	Training-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine trifluoroacetate	3.968	-2.116	244.595	3	3	3	Training-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine acetate	3.962	-2.116	244.367	3	3	3	Training-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine trifluoromethanesulfonate	3.968	-2.116	244.595	3	3	3	Training-V. <i>fischeri</i> set
Cethyltrimethylammonium bromide	39.951	-4.612	201.761	2	2	2	Training-V. <i>fischeri</i> set
Cethyltrimethylammonium chloride	39.951	-4.612	201.761	2	2	2	Training-V. <i>fischeri</i> set

Hexadecylbenzyltrimethylammonium chloride	27.896	-6.446	341.551	1	1	1	Training-V. <i>fischeri</i> set
Tetrabutylammonium chloride	1.60 x10 ⁻⁵	-3.776	1473.200	3	3	3	Training-V. <i>fischeri</i> set
Tetramethylammonium bromide	6.13 x10 ⁻⁶	0.325	104.705	4	4	4	Training-V. <i>fischeri</i> set
Tetraethylammonium bromide	8.08 x10 ⁻⁶	-1.064	294.625	4	4	4	Training-V. <i>fischeri</i> set
Tetrabutylammonium bromide	1.60 x10 ⁻⁵	-3.776	1473.200	3	3	3	Training-V. <i>fischeri</i> set
Hexyltriethylammonium bromide	8.198	-2.571	322.666	3	3	3	Training-V. <i>fischeri</i> set
Butylethyldimethylammonium bis(trifluoromethanesulfonyl)imide	4.583	-1.047	125.073	3	4	4	Training-V. <i>fischeri</i> set
Butylethyldimethylammonium chloride	4.583	-1.047	125.073	4	4	4	Training-V. <i>fischeri</i> set
(Ethoxycarbonylmethyl)ethyldimethylammonium bis(trifluoromethanesulfonyl)imide	7.232	-0.090	146.951	3	3	3	Training-V. <i>fischeri</i> set
(Hydroxyethyl)dimethylammonium acetate	4.078	1.132	85.566	4	4	4	Training-V. <i>fischeri</i> set
Bis(2-methoxyethyl)ammonium sulfamate	2.694	0.831	152.366	4	4	4	Training-V. <i>fischeri</i> set
(Methoxyethyl)ethyldimethylammonium bis(trifluoromethanesulfonyl)imide	3.649	0.286	142.994	3	3	3	Training-V. <i>fischeri</i> set
Trihexyl(tetradecyl)phosphonium bromide	14.993	-10.405	4815.100	3	3	3	Training-V. <i>fischeri</i> set
Bis(trifluoromethanesulfonyl)imide	1.686	-2.159	534.205	4	4	4	Training-V. <i>fischeri</i> set
Bis[1,2-benzenediolato(2-)]borate	3.552	-3.831	291.770	3	3	3	Training-V. <i>fischeri</i> set
O-Dodecylsulfate	33.655	-4.091	167.857	2	2	2	Training-V. <i>fischeri</i> set
O-Octylsulfate	22.819	-2.434	141.512	3	3	3	Training-V. <i>fischeri</i> set
Triethylsulfanium bis(trifluoromethanesulfonyl)imide	3.118	-1.393	171.988	3	3	3	Training-V. <i>fischeri</i> set
(Ethoxyoxoethyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	6.647	-0.441	191.895	3	3	3	Training-V. <i>fischeri</i> set
Butylmethylmorpholinium bromide	2.469	-0.561	186.507	4	4	4	Training-V. <i>fischeri</i> set
Butylmethylpyrrolidinium trifluoridotrakis(pentafluoroethyl)phosphate	4.030	-1.398	170.283	2	3	4	Training-V. <i>fischeri</i> set
Methylimidazolium trifluoroacetate	4.963	0.568	66.488	3	3	3	Training-V. <i>fischeri</i> set
Methylimidazolium trifluoromethanesulfonate	4.963	0.568	66.488	4	3	3	Test-V. <i>fischeri</i> set
Methylimidazolium caprylate	21.233	-1.948	77.689	3	3	3	Test-V. <i>fischeri</i> set
Ethylmethylimidazolium ethylsulfate	2.639	-1.419	97.815	4	4	4	Test-V. <i>fischeri</i> set
Ethylmethylimidazolium methylsulfate	2.639	-1.419	97.815	4	4	4	Test-V. <i>fischeri</i> set

(Ethoxyethyl)methylimidazolium bromide	9.554	-1.373	131.427	4	3	3	Test-V. <i>fischeri</i> set
(Hydroxyethyl)methylimidazolium iodide	5.470	-0.518	104.691	4	4	4	Test-V. <i>fischeri</i> set
(Methoxypropyl)methylimidazolium chloride	9.103	-1.208	134.245	4	3	3	Test-V. <i>fischeri</i> set
Butylimidazolium trifluoroacetate	3.921	-1.646	96.448	3	3	3	Test-V. <i>fischeri</i> set
Butylimidazolium formate	3.921	-1.646	96.448	3	3	3	Test-V. <i>fischeri</i> set
Butylmethylimidazolium trifluoromethanesulfonate	6.703	-2.133	133.278	3	3	3	Test-V. <i>fischeri</i> set
Pentylmethylimidazolium tetrafluoroborate	9.181	-2.561	138.841	3	3	3	Test-V. <i>fischeri</i> set
Hexyldimethylimidazolium chloride	6.584	-1.748	248.666	2	3	3	Test-V. <i>fischeri</i> set
Hexylmethylimidazolium bis(trifluoromethanesulfonyl)imide	11.706	-2.987	162.821	3	3	3	Test-V. <i>fischeri</i> set
Octylmethylimidazolium hexafluorophosphate	17.027	-3.833	188.399	2	2	2	Test-V. <i>fischeri</i> set
Nonylmethylimidazolium tetrafluoroborate	19.776	-4.255	191.975	2	2	2	Test-V. <i>fischeri</i> set
Butylpyridinium chloride	5.790	-2.273	134.365	3	3	3	Test-V. <i>fischeri</i> set
Butylpyridinium-m-Chlorohexachloridodialuminate	5.790	-2.273	134.365	3	3	3	Test-V. <i>fischeri</i> set
Butyldimethylpyridinium dicyanamide	3.496	-2.693	334.343	3	3	3	Test-V. <i>fischeri</i> set
Octylmethylpyridinium bromide	14.695	-4.185	270.780	2	2	2	Test-V. <i>fischeri</i> set
Octyldimethylpyridinium bromide	13.254	-4.388	391.341	2	2	2	Test-V. <i>fischeri</i> set
Hexylmethylpyrrolidinium chloride	8.780	-2.227	188.343	3	3	3	Test-V. <i>fischeri</i> set
Hexylmethylpyrrolidinium bis(trifluoromethanesulfonyl)imide	8.780	-2.227	188.343	3	3	3	Test-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine acetate	3.813	-1.214	167.118	3	3	3	Test-V. <i>fischeri</i> set
Benzyldimethyldodecylammonium chloride	16.981	-5.834	306.223	1	1	1	Test-V. <i>fischeri</i> set
Tetrabutylphosphonium bromide	4.09 x10 ⁻⁵	-5.290	1736.710	3	3	3	Test-V. <i>fischeri</i> set
Tributylethylphosphonium diethylphosphate	2.755	-4.613	1008.390	3	3	3	Test-V. <i>fischeri</i> set
Trihexyl(tetradecyl)phosphonium trifluoridotris(pentafluoroethyl)phosphate	14.993	-10.405	4815.100	2	3	3	Test-V. <i>fischeri</i> set
Tetrafluoroborate	2.22x10 ⁻¹⁶	-0.628	95.089	4	4	4	Test-V. <i>fischeri</i> set
(Hydroxyethyl)dimethylammonium hydroxyacetate	4.078	1.132	85.566	4	4	4	Test-V. <i>fischeri</i> set
Octylpyridinium chloride	16.324	-3.981	180.312	2	2	2	Test-V. <i>fischeri</i> set

(Methoxyethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	7.239	-1.025	126.819	3	4	4	Test-V. <i>fischeri</i> set
1-Decyl-3-methylimidazolium chloride	22.525	-4.675	211.379	1	1	1	Test algae set
1-(Cyanomethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	6.964	-0.940	121.712	3	4	3	Test algae set
1-(Cyanomethyl)-3-methylimidazolium chloride	6.964	-0.940	121.712	4	4	3	Test algae set
1-(Ethoxymethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	6.583	-1.422	133.279	2	3	3	Test algae set
1-(Ethoxymethyl)-3-methylimidazolium chloride	6.583	-1.422	133.279	3	3	3	Test algae set
1-Ethyl-3-methylimidazolium-4-Fluoro-1-butanesulfonate	2.565	-1.419	97.778	2	2	2	Test algae set
1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato(2-)]borate(1-)	3.547	-3.831	291.682	2	2	2	Test algae set
1-Ethyl-3-methylimidazolium-4-Chloro-1-butanesulfonate	2.643	-1.419	97.804	3	3	3	Test algae set
1-Ethyl-3-methylimidazolium chloride	2.639	-1.419	97.815	3	3	3	Test algae set
1-(2-Methoxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	7.239	-1.025	126.819	2	3	3	Test algae set
1-(2-Methoxyethyl)-3-methylimidazolium chloride	7.239	-1.025	126.819	3	3	3	Test algae set
1-(2-Ethoxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	9.554	-1.373	131.427	2	3	3	Test algae set
1-(2-Ethoxyethyl)-3-methylimidazolium bromide	9.554	-1.373	131.427	3	3	3	Test algae set
1-(2-Hydroxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	5.470	-0.518	104.691	3	3	3	Test algae set
1-(3-Methoxypropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	9.209	-1.323	134.505	3	3	3	Test algae set
1-(3-Hydroxypropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	7.345	-0.820	128.316	2	2	2	Test algae set
1-Butyl-3-methylimidazolium bis(trifluoromethyl)amide(1-)	6.703	-2.133	133.278	3	3	3	Test algae set
1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	6.703	-2.133	133.278	2	3	3	Test algae set
1-Butyl-3-methylimidazolium-O-Octyl sulfate	22.819	-2.434	141.512	2	2	2	Test algae set
1-Butyl-3-methylimidazolium	6.703	-2.133	133.278	3	3	3	Test algae set

tetrafluoridoboranuide(1-)							
1-Butyl-3-methylimidazolium-4-Chloro-1-butanesulfonate	6.592	-2.018	133.279	3	3	3	Test algae set
1-Butyl-3-methylimidazolium chloride	6.703	-2.133	133.278	3	3	3	Test algae set
1-Hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	11.706	-2.987	162.821	2	2	2	Test algae set
1-Hexyl-3-methylimidazolium trifluoridotris(pentafluoroethyl)phosphate(1-)	11.706	-2.987	162.821	1	2	2	Test algae set
1-Hexyl-3-methylimidazolium hexafluoridophosphate(1-)	11.706	-2.987	162.821	2	2	2	Test algae set
1-Hexyl-3-methylimidazolium chloride	11.706	-2.987	162.821	2	2	2	Test algae set
1-Methyl-3-octylimidazolium tetrafluoridoboranuide(1-)	17.027	-3.833	188.399	1	1	1	Test algae set
1-Methyl-3-octylimidazolium chloride	17.027	-3.833	188.399	1	1	1	Test algae set
4-(Ethoxymethyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)amide(1-)	3.380	0.156	187.117	3	3	3	Test algae set
4-Butyl-4-methylmorpholinium bis(trifluoromethylsulfonyl)amide(1-)	2.469	-0.561	186.507	2	2	2	Test algae set
(Ethoxycarbonylmethyl)ethyl dimethylammonium bis(trifluoromethylsulfonyl)amide(1-)	7.232	-0.090	146.951	3	3	3	Test algae set
(Ethoxycarbonylmethyl)ethyl dimethylammonium bromide	7.232	-0.090	146.951	3	3	3	Test algae set
Butylethyldimethylammonium bis(trifluoromethylsulfonyl)amide(1-)	4.583	-1.047	125.073	2	2	2	Test algae set
1-(3-Methoxypropyl)-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide(1-)	5.224	-0.674	191.141	2	2	2	Test algae set
1-Butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide(1-)	2.642	-1.717	191.445	3	3	3	Test algae set
1-Butyl-1-methylpiperidinium bromide	2.642	-1.717	191.445	3	3	3	Test algae set
1-Butylpyridinium chloride	5.790	-2.273	134.365	3	3	3	Test algae set
1-Butyl-4-(dimethylamino)pyridinium bis(trifluoromethylsulfonyl)amide(1-)	2.508	-2.433	215.752	1	1	1	Test algae set
1-Butyl-4-(dimethylamino)pyridinium chloride	2.508	-2.433	215.752	1	1	1	Test algae set
1-(Ethoxycarbonylmethyl)-1-methylpyrrolidinium bromide	6.647	-0.441	191.895	3	3	3	Test algae set

1-(2-Methoxyethyl)-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	4.065	-0.065	205.910	3	3	3	Test algae set
1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	4.030	-1.398	170.283	3	3	3	Test algae set
1-Butyl-1-methylpyrrolidinium chloride	4.030	-1.398	170.283	3	3	3	Test algae set
Triethylsulfanium bis(trifluoromethylsulfonyl)amide(1-)	3.118	-1.393	171.988	2	2	2	Test algae set
1-hexyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	8.780	-2.227	188.343	2	2	2	Test algae set
1-butyl-3-methylimidazolium chloride	6.703	-2.133	133.278	2	2	2	Test daphnia set
1-butyl-3-methylimidazolium bromide	6.703	-2.133	133.278	2	2	2	Test daphnia set
1-butyl-3-methylimidazolium tetrafluoroborate	6.703	-2.133	133.278	2	2	2	Test daphnia set
1-butyl-3-methylimidazolium Hexafluorophosphate	6.703	-2.133	133.278	2	2	2	Test daphnia set
1-butyl-3-methylimidazolium bis(trifluoromethyl)sulfonylimide	6.703	-2.133	133.278	2	2	2	Test daphnia set
1-n-Hexyl-3-methylimidazolium Chloride	11.706	-2.987	162.821	2	2	2	Test daphnia set
1-n-Hexyl-3-methylimidazolium bromide	11.706	-2.987	162.821	2	2	2	Test daphnia set
1-n-Hexyl-3-methylimidazolium tetrafluoroborate	11.706	-2.987	162.821	2	2	2	Test daphnia set
1-n-Octyl-3-methylimidazolium chloride	17.027	-3.833	188.399	2	2	2	Test daphnia set
1-n-Octyl-3-methylimidazolium bromide	17.027	-3.833	188.399	2	2	2	Test daphnia set
1-n-Octyl-3-methylimidazolium tetrafluoroborate	17.027	-3.833	188.399	2	2	2	Test daphnia set
decylmethylimidazolium Bromide	22.525	-4.675	211.379	1	1	1	Test daphnia set
1-dodecyl-3-methylimidazolium chloride	28.136	-5.514	232.552	1	1	1	Test daphnia set
1-dodecyl-3-methylimidazolium bromide	28.136	-5.514	232.552	1	1	1	Test daphnia set
1-hexadecyl-3-methylimidazolium chloride	39.570	-6.128	271.225	1	1	1	Test daphnia set
Octadecylmethylimidazolium Chloride	45.359	-6.811	289.252	1	1	1	Test daphnia set
1-n-Hexyl-2,3-dimethylimidazolium bromide	10.773	-3.200	238.624	2	2	2	Test daphnia set
Butylpyridinium Chloride	5.790	-2.273	134.365	3	2	2	Test daphnia set
Butylpyridinium bis(trifluoromethyl) sulfonylimide	5.790	-2.273	134.365	2	2	2	Test daphnia set
Butylmethylpyridinium bromide	4.622	-2.484	211.731	2	2	2	Test daphnia set
Butylmethylmethylpyridinium bromide	3.496	-2.693	334.343	2	2	2	Test daphnia set

Hexylpyridinium bromide	10.936	-3.131	158.943	2	2	2	Test daphnia set
Hexylmethylpyridinium bromide	9.482	-3.338	243.628	2	2	2	Test daphnia set
1-n-Hexyl-4-piperidinopyridinium bromide	3.534	-4.273	315.487	1	1	1	Test daphnia set
Octylmethylpyridinium bromide	14.695	-4.185	270.780	2	2	2	Test daphnia set
1-n-Hexyl-4-dimethylaminopyridinium bromide	7.035	-3.280	265.625	1	1	1	Test daphnia set
1-n-Hexyl-3-methyl-4-dimethylaminopyridinium bromide	6.225	-3.483	363.746	2	2	2	Test daphnia set
N,N-methylbutylpyrrolidinium bis(trifluoromethyl)sulfonylimide	4.030	-1.398	170.283	2	2	2	Test daphnia set
Dodecyltrimethylammonium bromide	28.380	-4.013	175.582	2	2	2	Test daphnia set
Tetradecyltrimethylammonium bromide	34.143	-3.935	188.703	1	1	1	Test daphnia set
Hexadecyltrimethylammonium bromide	39.951	-4.612	201.761	1	1	1	Test daphnia set
Tetrabutylphosphonium bromide	4.090x10 ⁻⁵	-5.290	1736.710	3	3	3	Test daphnia set
Tetrabutylammonium bromide	1.360x10 ⁻⁵	-3.776	1473.210	3	3	3	Test daphnia set
Dodecylbenzyltrimethylammonium bromide	16.981	-5.834	306.223	2	2	2	Test daphnia set
Tributylethylphosphonium diethyl phosphate	2.755	-4.613	1008.390	2	2	2	Test daphnia set
Trihexyltetradecylphosphonium chloride	14.993	-10.405	4815.100	1	1	1	Test daphnia set
Methyltrioctylammonium bis(trifluoromethylsulfonyl)amide(1-)	7.911	-6.512	3716.760	1	1	1	Test daphnia set
Picolinium bromide	1.066	-1.306	87.034	3	3	3	Test daphnia set
1-(2-methoxyethyl)-3-methyl-1H-imidazolium tetrafluoroborate	7.239	-1.025	126.819	3	3	3	Test daphnia set
1-(2-methoxyethyl)-3-methyl-1H-imidazolium N-cyanocynamide	7.239	-1.025	126.819	3	3	3	Test daphnia set
3-(2-chloroethyl)-1-methylimidazolium chloride	8.674	-1.831	105.244	3	3	3	Test daphnia set
3-(2-chloroethyl)-1-methylimidazolium bis(trifluoromethyl)sulfonylimide	8.674	-1.831	105.244	3	3	3	Test daphnia set
3-(2-hydroxyethyl)-1-methylimidazolium bis(trifluoromethyl)sulfonylimide	5.470	-0.518	104.691	3	3	3	Test daphnia set
3-(2-chloropropyl)-1-methylimidazolium chloride	6.332	-2.992	218.221	3	3	3	Test daphnia set
1-methyl-3-[(trimethylsilyl)methyl]-imidazolium bromide	7.777	-3.217	255.884	2	2	2	Test daphnia set

Methylimidazolium chloride	4.300	-1.498	57.064	3	3	3	Test daphnia set
1-(2-Chloroethyl)imidazolium chloride	11.445	-1.599	68.855	3	3	3	Test daphnia set
1,10-(1,2-ethanediyl)bis-imidazolium chloride	1.764	-1.417	126.890	3	3	3	Test daphnia set
Choline hexafluorophosphate	3.646	1.116	121.187	3	3	3	Test daphnia set
Ethyl-methylmorpholiniumbromide	4.169	0.117	165.785	3	3	3	Test daphnia set
Butylethyl-morpholiniumbromide	6.203	-1.149	157.427	3	3	3	Test daphnia set
Ethyltetrahydrothiopheniumbromide	3.393	-1.378	123.624	3	3	3	Test daphnia set
Triethylsulfoniumbromide	3.118	-1.393	171.988	3	3	3	Test daphnia set

Table S3: Quantitative SAR modeling result with descriptor values

Ionic liquid name	XlogP	Dipole	InertiaX	log EC ₅₀ (μM)	GBT-SAR	BDT-SAR	Data sub-sets
Imidazolium trifluoroacetate	-0.620	5.962	53.695	4.07	4.02	3.95	Training-V. <i>fischeri</i> set
Imidazolium acetate	-0.017	3.450	50.371	3.61	3.62	3.76	Training-V. <i>fischeri</i> set
Imidazolium caprylate	2.497	21.233	77.689	2.29	2.19	2.19	Training-V. <i>fischeri</i> set
Methylimidazolium trifluoroacetate	-0.662	4.963	66.488	3.57	3.95	3.94	Training-V. <i>fischeri</i> set
Methylimidazolium acetate	0.298	3.906	54.412	4.07	3.97	3.68	Training-V. <i>fischeri</i> set
Methylimidazolium trifluoromethanesulfonate	-0.662	4.963	66.488	4.35	3.95	3.94	Training-V. <i>fischeri</i> set
Methylimidazolium caprylate	2.497	21.233	77.689	2.13	2.19	2.19	Training-V. <i>fischeri</i> set
Methylimidazolium formate	0.255	2.917	55.589	2.83	3.40	3.51	Training-V. <i>fischeri</i> set
Methylimidazolium	0.255	2.917	55.589	4.17	3.40	3.51	Training-V. <i>fischeri</i> set
(Cyanomethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	0.084	6.964	121.712	3.81	3.74	3.49	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium ethylsulfate	0.998	2.639	97.815	4.02	3.79	3.80	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium bis[1,2-benzenediolato(2-)]borate	3.817	3.547	291.682	2.98	2.95	2.84	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium bis(pentafluoroethyl)phosphinate	0.998	2.639	97.815	3.05	3.79	3.80	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium tetracyanidoborate	0.998	2.639	97.815	3.56	3.79	3.80	Training-V. <i>fischeri</i> set

Ethylmethylimidazolium thiocyanate	0.998	2.639	97.815	4.15	3.79	3.80	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium trifluoroacetate	0.998	2.639	97.815	4.28	3.79	3.80	Training-V. <i>fischeri</i> set
Ethylmethylimidazolium tetrachloroferrate(III)	0.998	2.643	97.804	1.51	1.66	2.34	Training-V. <i>fischeri</i> set
(Hydroxyethyl)methylimidazolium iodide	-0.136	5.470	104.691	3.89	3.89	3.84	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	0.387	7.239	126.819	2.84	3.44	3.54	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium tetrafluoroborate	0.375	4.581	136.752	1.15	1.30	1.93	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium dicyanamide	0.224	7.119	126.628	1.07	1.18	2.01	Training-V. <i>fischeri</i> set
(Hydroxypropyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	0.204	7.345	128.316	3.89	3.79	3.51	Training-V. <i>fischeri</i> set
(Methoxypropyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	0.727	9.209	134.505	3.24	3.23	2.95	Training-V. <i>fischeri</i> set
Butylimidazolium trifluoroacetate	1.618	3.921	96.448	3.28	3.10	3.09	Training-V. <i>fischeri</i> set
Butylimidazolium acetate	1.618	3.921	96.448	3.32	3.10	3.09	Training-V. <i>fischeri</i> set
Butylimidazolium trifluoromethanesulfonate	1.618	3.921	96.448	2.77	3.10	3.09	Training-V. <i>fischeri</i> set
Butylimidazolium caprylate	2.497	21.233	77.689	2.00	2.19	2.19	Training-V. <i>fischeri</i> set
Butylmethylimidazolium hexafluorophosphate	1.890	6.703	133.278	3.29	3.27	3.18	Training-V. <i>fischeri</i> set
Butylmethylimidazolium tetrafluoroborate	1.890	6.703	133.278	3.43	3.27	3.18	Training-V. <i>fischeri</i> set
Butylmethylimidazolium bromide	1.890	6.703	133.278	3.45	3.27	3.18	Training-V. <i>fischeri</i> set
Butylmethylimidazolium chloride	1.890	6.703	133.278	3.41	3.27	3.18	Training-V. <i>fischeri</i> set
Butylmethylimidazolium dicyanamide	1.890	6.703	133.278	3.67	3.27	3.18	Training-V. <i>fischeri</i> set
Butylmethylimidazolium trifluoromethanesulfonate	1.890	6.703	133.278	3.60	3.27	3.18	Training-V. <i>fischeri</i> set
Butylmethylimidazolium bis(trifluoromethanesulfonyl)imide	1.890	6.703	133.278	2.78	3.27	3.18	Training-V. <i>fischeri</i> set
Butylmethylimidazolium methylbenzenesulfonate	1.890	6.703	133.278	3.52	3.27	3.18	Training-V. <i>fischeri</i> set
Butylmethylimidazolium tetrachloroferrate(III)	1.890	6.703	133.278	1.51	3.27	3.18	Training-V. <i>fischeri</i> set
Butylethylimidazolium tetrafluoroborate	2.155	4.646	156.036	2.80	2.81	2.76	Training-V. <i>fischeri</i> set
Pentylmethylimidazolium tetrafluoroborate	2.443	9.181	138.841	3.14	3.08	2.91	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium chloride	2.996	11.706	162.821	2.15	2.26	2.26	Training-V. <i>fischeri</i> set
Hexyldimethylimidazolium chloride	1.942	6.584	248.666	1.74	1.81	2.12	Training-V. <i>fischeri</i> set

Hexylmethylimidazolium hexafluorophosphate	2.996	11.706	162.821	2.14	2.26	2.26	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium tetrafluoroborate	2.996	11.706	162.821	3.18	2.26	2.26	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium bis(trifluoromethanesulfonyl)imide	2.996	11.706	162.821	2.05	2.26	2.26	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium trifluoridotris(pentafluoroethyl)phosphate	8.978	8.338	2903.910	2.65	2.65	2.58	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium-1,1-Dioxo-1,2-dihydrobenzo[d]isothiazol-3-onate	2.996	11.706	162.821	2.67	2.26	2.26	Training-V. <i>fischeri</i> set
Hexylethylimidazolium tetrafluoroborate	3.261	9.604	187.824	2.15	2.16	2.13	Training-V. <i>fischeri</i> set
Heptylmethylimidazolium tetrafluoroborate	3.549	14.362	167.033	2.44	2.40	2.16	Training-V. <i>fischeri</i> set
Octylmethylimidazolium bromide	4.102	17.027	188.399	0.63	1.01	0.98	Training-V. <i>fischeri</i> set
Octylmethylimidazolium chloride	4.102	17.027	188.399	1.05	1.01	0.98	Training-V. <i>fischeri</i> set
Octylmethylimidazolium tetrafluoroborate	4.102	17.027	188.399	1.40	1.01	0.98	Training-V. <i>fischeri</i> set
Octylmethylimidazolium bis(trifluoromethanesulfonyl)imide	4.102	17.027	188.399	0.83	1.01	0.98	Training-V. <i>fischeri</i> set
Nonylmethylimidazolium tetrafluoroborate	4.655	19.776	191.975	0.72	0.72	0.43	Training-V. <i>fischeri</i> set
Decylmethylimidazolium chloride	5.208	22.525	211.379	0.13	0.02	-0.01	Training-V. <i>fischeri</i> set
Decylmethylimidazolium tetrafluoroborate	5.208	22.525	211.379	-0.18	0.02	-0.01	Training-V. <i>fischeri</i> set
Tetradecylmethylimidazolium chloride	6.139	33.825	252.397	-0.15	-0.07	0.03	Training-V. <i>fischeri</i> set
Hexadecylmethylimidazolium chloride	7.032	39.570	271.225	0.23	0.32	0.40	Training-V. <i>fischeri</i> set
Octadecylmethylimidazolium chloride	7.925	45.359	289.252	1.35	1.30	0.89	Training-V. <i>fischeri</i> set
Hydroxypropylpyridinium bis(trifluoromethanesulfonyl)imide	0.196	6.540	129.391	4.01	3.97	3.85	Training-V. <i>fischeri</i> set
Butylmethylpyridinium bromide	2.320	4.018	148.517	2.75	2.85	2.85	Training-V. <i>fischeri</i> set
Butylpyridinium chloride	1.883	5.790	134.365	3.29	3.19	3.19	Training-V. <i>fischeri</i> set
Butylpyridinium-m-Chlorohexa chloridodialuminate	1.883	5.790	134.365	3.01	3.19	3.19	Training-V. <i>fischeri</i> set
Butylmethylpyridinium tetrafluoroborate	2.320	4.018	148.517	3.02	2.85	2.85	Training-V. <i>fischeri</i> set
Butylpyridinium dicyanamide	1.883	5.790	134.365	3.30	3.19	3.19	Training-V. <i>fischeri</i> set
Butylmethylpyridinium dicyanamide	2.107	4.622	211.731	2.66	2.62	2.48	Training-V. <i>fischeri</i> set
Hexylmethylpyridinium bromide	3.212	9.482	243.628	2.07	1.74	1.74	Training-V. <i>fischeri</i> set
Hexylmethylpyridinium chloride	3.212	9.482	243.628	1.44	1.74	1.74	Training-V. <i>fischeri</i> set
Octylmethylpyridinium bromide	4.318	14.695	270.780	0.79	0.81	0.87	Training-V. <i>fischeri</i> set

Octyldimethylpyridinium bis(trifluoromethanesulfonyl)imide	4.542	13.254	391.341	0.36	0.45	0.95	Training-V. <i>fischeri</i> set
(Ethoxyethyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	0.563	5.691	260.221	2.97	2.89	2.74	Training-V. <i>fischeri</i> set
(Hydroxypropyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	-0.048	4.806	166.646	3.91	3.85	3.49	Training-V. <i>fischeri</i> set
Butylmethylpyrrolidinium bis(trifluoromethanesulfonyl)imide	1.638	4.030	170.283	2.54	2.17	2.19	Training-V. <i>fischeri</i> set
Butylmethylpyrrolidinium trifluoridotris(pentafluoroethyl)phosphate	1.638	4.030	170.283	1.70	2.17	2.19	Training-V. <i>fischeri</i> set
Hexylmethylpyrrolidinium chloride	2.744	8.780	188.343	3.00	2.70	2.61	Training-V. <i>fischeri</i> set
Hexylmethylpyrrolidinium bis(trifluoromethanesulfonyl)imide	2.744	8.780	188.343	2.40	2.70	2.61	Training-V. <i>fischeri</i> set
(Ethoxymethyl)methylmorpholinium bis(trifluoromethanesulfonyl)imide	-0.160	3.380	187.117	3.38	3.39	3.34	Training-V. <i>fischeri</i> set
Butylmethylmorpholinium bis(trifluoromethanesulfonyl)imide	0.777	2.469	186.507	2.49	2.52	2.66	Training-V. <i>fischeri</i> set
Butylmethylpiperidinium bromide	1.978	2.642	191.445	4.27	3.30	3.28	Training-V. <i>fischeri</i> set
Butylmethylpiperidinium bis(trifluoromethanesulfonyl)imide	1.978	2.642	191.445	2.56	3.30	3.28	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium bromide	2.107	2.519	216.473	2.32	2.36	2.41	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium chloride	2.107	2.508	215.752	2.52	2.20	2.26	Training-V. <i>fischeri</i> set
Butyl(dimethylamino)pyridinium bis(trifluoromethanesulfonyl)imide	2.107	2.508	215.752	1.85	2.20	2.26	Training-V. <i>fischeri</i> set
Hexyl(dimethylamino)pyridinium bis(trifluoromethanesulfonyl)imide	3.213	7.031	264.557	1.38	1.49	1.77	Training-V. <i>fischeri</i> set
Choline bis(trifluoromethanesulfonyl)imide	-0.875	3.646	121.187	4.15	4.15	4.06	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine trifluoroacetate	1.433	3.813	167.118	0.47	2.51	2.40	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine acetate	1.433	3.813	167.118	3.17	2.51	2.40	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine trifluoromethanesulfonate	1.433	3.813	167.118	3.52	2.51	2.40	Training-V. <i>fischeri</i> set
1,1,3,3-Tetramethylguanidine caprylate	2.497	21.233	77.689	2.29	2.19	2.19	Training-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine trifluoromethanesulfonate	0.643	3.968	244.595	2.45	2.45	2.45	Training-V. <i>fischeri</i> set
Hexadecylbenzyltrimethylammonium chloride	8.014	27.896	341.551	-0.31	-0.17	0.17	Training-V. <i>fischeri</i> set

Benzyldimethyldodecylammonium chloride	7.296	16.981	306.223	-0.23	-0.17	0.09	Training-V. <i>fischeri</i> set
Butylethyldimethylammonium bis(trifluoromethanesulfonyl)imide	1.579	4.583	125.073	3.21	3.21	3.10	Training-V. <i>fischeri</i> set
(Hydroxyethyl)dimethylammonium acetate	-0.832	4.078	85.566	4.29	4.23	4.03	Training-V. <i>fischeri</i> set
Tetrabutylphosphonium bromide	7.025	4.09x10 ⁻⁵	1736.710	2.71	2.69	2.64	Training-V. <i>fischeri</i> set
Tributylethylphosphonium diethylphosphate	6.132	2.755	1008.390	3.07	3.02	2.92	Training-V. <i>fischeri</i> set
Trihexyl(tetradecyl)phosphonium bromide	13.738	14.993	4815.100	3.41	2.32	2.31	Training-V. <i>fischeri</i> set
Trihexyl(tetradecyl)phosphonium trifluoridotris(pentafluoroethyl)phosphate	13.738	14.993	4815.100	1.70	2.32	2.31	Training-V. <i>fischeri</i> set
Bis[1,2-benzenediolato(2-)]borate	3.817	3.552	291.770	2.76	2.76	2.74	Training-V. <i>fischeri</i> set
O-Dodecylsulfate	4.458	33.655	167.857	1.50	1.49	1.24	Training-V. <i>fischeri</i> set
O-Octylsulfate	2.246	22.819	141.512	2.46	2.42	2.23	Training-V. <i>fischeri</i> set
Triethylsulfanium bis(trifluoromethanesulfonyl)imide	2.591	3.118	171.988	3.26	3.20	3.06	Training-V. <i>fischeri</i> set
(Ethoxyoxoethyl)methylpyrrolidinium bis(trifluoromethanesulfonyl)imide	0.449	6.647	191.895	3.23	3.19	2.95	Training-V. <i>fischeri</i> set
(Methoxyethyl)methylimidazolium chloride	0.387	7.239	126.819	4.18	3.44	3.54	Training-V. <i>fischeri</i> set
Hexylmethylimidazolium bromide	2.996	11.706	162.821	1.42	2.26	2.26	Training-V. <i>fischeri</i> set
Butylmethylimidazolium-O-Octylsulfate	2.246	22.819	141.512	1.83	1.90	2.05	Training-V. <i>fischeri</i> set
Imidazolium trifluoromethanesulfonate	-0.017	3.450	50.371	3.81	3.62	3.76	Test-V. <i>fischeri</i> set
(Ethoxymethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	0.953	6.583	133.279	3.00	3.28	3.11	Test-V. <i>fischeri</i> set
Ethylmethylimidazolium chloride	0.998	2.639	97.815	4.44	3.79	3.80	Test-V. <i>fischeri</i> set
(Ethoxyethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	0.815	9.554	131.427	2.96	2.78	2.82	Test-V. <i>fischeri</i> set
(Hydroxyethyl)methylimidazolium bis(trifluoromethanesulfonyl)imide	-0.136	5.470	104.691	4.08	3.89	3.84	Test-V. <i>fischeri</i> set
Propylmethylimidazolium tetrafluoroborate	1.337	4.483	106.359	3.94	3.20	3.17	Test-V. <i>fischeri</i> set
Propylmethylimidazolium bis(trifluoromethanesulfonyl)imide	1.337	4.483	106.350	2.77	3.20	3.17	Test-V. <i>fischeri</i> set
Butylimidazolium formate	1.618	3.921	96.448	3.19	3.10	3.09	Test-V. <i>fischeri</i> set
Butylmethylimidazolium iodide	1.890	6.703	133.278	3.59	3.27	3.18	Test-V. <i>fischeri</i> set
Butylmethylimidazolium bis(trifluoromethyl)amide	1.890	6.703	133.278	3.47	3.27	3.18	Test-V. <i>fischeri</i> set

Octylmethylimidazolium hexafluorophosphate	4.102	17.027	188.399	0.82	1.01	0.98	Test-V. <i>fischeri</i> set
Decylmethylimidazolium tetrachloroferrate(III)	5.208	22.525	211.379	-0.43	0.02	-0.01	Test-V. <i>fischeri</i> set
Methylpyridinium	0.725	1.066	87.034	3.07	2.98	3.03	Test-V. <i>fischeri</i> set
Butylpyridinium bromide	1.883	5.790	134.365	3.39	3.19	3.19	Test-V. <i>fischeri</i> set
Butyldimethylpyridinium bromide	2.330	3.496	334.343	2.59	2.69	2.63	Test-V. <i>fischeri</i> set
Butyldimethylpyridinium dicyanamide	2.330	3.496	334.343	2.12	2.69	2.63	Test-V. <i>fischeri</i> set
Octylpyridinium chloride	4.095	16.324	180.312	1.69	1.25	1.12	Test-V. <i>fischeri</i> set
Octyldimethylpyridinium bromide	4.542	13.254	391.341	1.12	0.45	0.95	Test-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine trifluoroacetate	0.643	3.968	244.595	2.24	2.45	2.45	Test-V. <i>fischeri</i> set
1,3,5-Triazine-2,4,6-triamine acetate	0.643	3.962	244.367	2.39	2.45	2.45	Test-V. <i>fischeri</i> set
Cethyltrimethylammonium bromide	6.293	39.951	201.761	0.04	0.20	0.19	Test-V. <i>fischeri</i> set
Cethyltrimethylammonium chloride	6.293	39.951	201.761	0.40	0.20	0.19	Test-V. <i>fischeri</i> set
Tetrabutylammonium chloride	5.113	1.60 x10 ⁻⁵	1473.200	2.69	2.76	2.68	Test-V. <i>fischeri</i> set
Tetrabutylammonium bromide	5.113	1.60 x10 ⁻⁵	1473.200	3.27	2.76	2.68	Test-V. <i>fischeri</i> set
Hexyltriethylammonium bromide	3.541	8.198	322.666	2.46	2.28	2.30	Test-V. <i>fischeri</i> set
(Ethoxycarbonylmethyl)ethyl dimethylammonium bis(trifluoromethanesulfonyl)imide	0.390	7.232	146.951	3.32	3.12	2.99	Test-V. <i>fischeri</i> set
(Methoxyethyl)ethyl dimethylammonium bis(trifluoromethanesulfonyl)imide	0.077	3.649	142.994	3.35	3.51	3.05	Test-V. <i>fischeri</i> set
1-Decyl-3-methylimidazolium chloride	5.208	22.525	211.379	-3.57	-3.37	-2.88	Test algae set
1-(Cyanomethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	0.084	6.964	121.712	2.07	2.71	2.87	Test algae set
1-(Cyanomethyl)-3-methylimidazolium chloride	0.084	6.964	121.712	4.01	2.71	2.87	Test algae set
1-(Ethoxymethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	0.953	6.583	133.279	1.93	2.36	2.37	Test algae set
1-(Ethoxymethyl)-3-methylimidazolium chloride	0.953	6.583	133.279	2.80	2.36	2.37	Test algae set
1-Ethyl-3-methylimidazolium-4-Fluoro-1-butanesulfonate	0.998	2.565	97.778	1.59	1.67	2.08	Test algae set
1-Ethyl-3-methylimidazolium bis[1,2-benzenediolato(2-)]borate(1-)	3.817	3.547	291.682	1.42	1.28	0.37	Test algae set
1-Ethyl-3-methylimidazolium-4-Chloro-1-butanesulfonate	0.998	2.643	97.804	2.98	2.92	2.73	Test algae set
1-Ethyl-3-methylimidazolium chloride	0.998	2.639	97.815	2.78	2.80	2.70	Test algae set

1-(2-Methoxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	0.387	7.239	126.819	1.98	2.45	2.53	Test algae set
1-(2-Methoxyethyl)-3-methylimidazolium chloride	0.387	7.239	126.819	3.26	2.45	2.53	Test algae set
1-(2-Ethoxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	0.815	9.554	131.427	1.88	2.20	2.13	Test algae set
1-(2-Ethoxyethyl)-3-methylimidazolium bromide	0.815	9.554	131.427	2.52	2.20	2.13	Test algae set
1-(2-Hydroxyethyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	-0.136	5.470	104.691	2.15	2.16	2.36	Test algae set
1-(3-Methoxypropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	0.727	9.209	134.505	2.06	2.09	2.07	Test algae set
1-(3-Hydroxypropyl)-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	0.204	7.345	128.316	1.98	2.00	2.11	Test algae set
1-Butyl-3-methylimidazolium bis(trifluoromethyl)amide(1-)	1.890	6.703	133.278	2.83	2.25	2.25	Test algae set
1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	1.890	6.703	133.278	1.80	2.25	2.25	Test algae set
1-Butyl-3-methylimidazolium-O-Octyl sulfate	2.246	22.819	141.512	1.72	1.68	1.05	Test algae set
1-Butyl-3-methylimidazolium tetrafluoridoboranuide(1-)	1.890	6.703	133.278	2.13	2.25	2.25	Test algae set
1-Butyl-3-methylimidazolium-4-Chloro-1-butanesulfonate	1.727	6.592	133.279	2.39	2.40	2.38	Test algae set
1-Butyl-3-methylimidazolium chloride	1.890	6.703	133.278	2.25	2.25	2.25	Test algae set
1-Hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide(1-)	2.996	11.706	162.821	0.04	0.06	0.01	Test algae set
1-Hexyl-3-methylimidazolium trifluoridotris(pentafluoroethyl)phosphate(1-)	2.996	11.706	162.821	-0.37	0.06	0.01	Test algae set
1-Hexyl-3-methylimidazolium hexafluoridophosphate(1-)	2.996	11.706	162.821	0.34	0.06	0.01	Test algae set
1-Hexyl-3-methylimidazolium chloride	2.996	11.706	162.821	0.08	0.06	0.01	Test algae set
1-Methyl-3-octylimidazolium tetrafluoridoboranuide(1-)	4.102	17.027	188.399	-2.24	-2.43	-2.30	Test algae set
1-Methyl-3-octylimidazolium chloride	4.102	17.027	188.399	-2.76	-2.43	-2.30	Test algae set
4-(Ethoxymethyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)amide(1-)	-0.160	3.380	187.117	2.34	2.34	2.40	Test algae set

4-Butyl-4-methylmorpholinium bis(trifluoromethylsulfonyl)amide(1-)	0.777	2.469	186.507	2.00	1.93	1.93	Test algae set
(Ethoxycarbonylmethyl)ethyl dimethylammonium bis(trifluoromethylsulfonyl)amide(1-)	0.390	7.232	146.951	2.18	2.41	2.38	Test algae set
(Ethoxycarbonylmethyl)ethyl dimethylammonium bromide	0.390	7.232	146.951	2.63	2.41	2.38	Test algae set
Butylethyl dimethylammonium bis(trifluoromethylsulfonyl)amide(1-)	1.579	4.583	125.073	1.79	1.86	2.04	Test algae set
1-(3-Methoxypropyl)-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide(1-)	0.815	5.224	191.141	1.87	1.91	2.02	Test algae set
1-Butyl-1-methylpiperidinium bis(trifluoromethylsulfonyl)amide(1-)	1.978	2.642	191.445	2.09	2.55	2.57	Test algae set
1-Butyl-1-methylpiperidinium bromide	1.978	2.642	191.445	3.28	2.55	2.57	Test algae set
1-Butylpyridinium chloride	1.883	5.790	134.365	2.59	2.55	2.51	Test algae set
1-Butyl-4-(dimethylamino)pyridinium bis(trifluoromethylsulfonyl)amide(1-)	2.107	2.508	215.752	-0.43	-0.26	-0.12	Test algae set
1-Butyl-4-(dimethylamino)pyridinium chloride	2.107	2.508	215.752	-0.27	-0.26	-0.12	Test algae set
1-(Ethoxycarbonylmethyl)-1-methylpyrrolidinium bromide	0.449	6.647	191.895	3.16	3.09	2.55	Test algae set
1-(2-Methoxyethyl)-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	0.136	4.065	205.910	2.03	2.05	1.88	Test algae set
1-Butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	1.638	4.030	170.283	2.53	2.93	2.89	Test algae set
1-Butyl-1-methylpyrrolidinium chloride	1.638	4.030	170.283	3.39	2.93	2.89	Test algae set
Triethylsulfanium bis(trifluoromethylsulfonyl)amide(1-)	2.591	3.118	171.988	1.97	2.00	1.74	Test algae set
1-hexyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide(1-)	2.744	8.780	188.343	1.57	1.55	1.06	Test algae set
1-butyl-3-methylimidazolium chloride	1.890	6.703	133.278	1.85	1.81	1.82	Test daphnia set
1-butyl-3-methylimidazolium bromide	1.890	6.703	133.278	1.84	1.81	1.82	Test daphnia set
1-butyl-3-methylimidazolium tetrafluoroborate	1.890	6.703	133.278	1.79	1.81	1.82	Test daphnia set
1-butyl-3-methylimidazolium Hexafluorophosphate	1.890	6.703	133.278	1.95	1.81	1.82	Test daphnia set
1-butyl-3-methylimidazolium bis(trifluoromethyl)sulfonylimide	1.890	6.703	133.278	1.65	1.81	1.82	Test daphnia set

1-n-Hexyl-3-methylimidazolium Chloride	2.996	11.706	162.821	1.09	1.10	1.07	Test daphnia set
1-n-Hexyl-3-methylimidazolium bromide	2.996	11.706	162.821	1.06	1.10	1.07	Test daphnia set
1-n-Hexyl-3-methylimidazolium tetrafluoroborate	2.996	11.706	162.821	1.13	1.10	1.07	Test daphnia set
1-n-Octyl-3-methylimidazolium chloride	4.102	17.027	188.399	0.54	0.60	0.52	Test daphnia set
1-n-Octyl-3-methylimidazolium bromide	4.102	17.027	188.399	0.54	0.60	0.52	Test daphnia set
1-n-Octyl-3-methylimidazolium tetrafluoroborate	4.102	17.027	188.399	0.66	0.60	0.52	Test daphnia set
Decylmethylimidazolium Bromide	5.208	22.525	211.379	-0.31	-0.26	-0.42	Test daphnia set
1-dodecyl-3-methylimidazolium chloride	6.314	28.136	232.552	-1.82	-1.31	-1.27	Test daphnia set
1-dodecyl-3-methylimidazolium bromide	6.314	28.136	232.552	-0.82	-1.31	-1.27	Test daphnia set
1-hexadecyl-3-methylimidazolium chloride	7.032	39.570	271.225	-2.00	-1.91	-1.74	Test daphnia set
Octadecylmethylimidazolium Chloride	7.925	45.359	289.252	-2.34	-2.20	-1.94	Test daphnia set
1-n-Hexyl-2,3-dimethylimidazolium bromide	3.216	10.773	238.624	0.81	0.81	0.80	Test daphnia set
Butylpyridinium Chloride	1.883	5.790	134.365	2.07	1.16	1.49	Test daphnia set
Butylpyridinium bis(trifluoromethyl)sulfonylimide	1.883	5.790	134.365	0.62	1.16	1.49	Test daphnia set
Butylmethylpyridinium bromide	2.107	4.622	211.731	1.76	1.80	1.85	Test daphnia set
Butylmethylmethylpyridinium bromide	2.330	3.496	334.343	1.99	1.99	1.76	Test daphnia set
Hexylpyridinium bromide	2.989	10.936	158.943	1.07	1.08	1.10	Test daphnia set
Hexylmethylpyridinium bromide	3.212	9.482	243.628	0.59	0.62	0.64	Test daphnia set
1-n-Hexyl-4-piperidinopyridinium bromide	4.040	3.534	315.487	-0.66	-0.55	0.02	Test daphnia set
Octylmethylpyridinium bromide	4.318	14.695	270.780	0.40	0.41	0.29	Test daphnia set
1-n-Hexyl-4-dimethylaminopyridinium bromide	3.213	7.035	265.625	-0.28	-0.14	0.25	Test daphnia set
1-n-Hexyl-3-methyl-4-dimethylaminopyridinium bromide	3.437	6.225	363.746	0.21	0.20	0.45	Test daphnia set
N,N-methylbutylpyrrolidinium bis(trifluoromethyl)sulfonylimide	1.638	4.030	170.283	1.94	1.92	2.02	Test daphnia set
Dodecyltrimethylammonium bromide	5.575	28.380	175.582	0.09	0.10	-0.07	Test daphnia set
Tetradecyltrimethylammonium bromide	5.401	34.143	188.703	-0.38	-0.31	-0.45	Test daphnia set
Hexadecyltrimethylammonium bromide	6.293	39.951	201.761	-0.45	-0.48	-0.83	Test daphnia set
Tetrabutylphosphonium bromide	7.025	4.09 x10 ⁻⁵	1736.710	2.11	2.06	1.42	Test daphnia set

Tetrabutylammonium bromide	5.113	1.36 x10 ⁻⁵	1473.210	2.33	2.30	2.03	Test daphnia set
Dodecylbenzyltrimethylammonium bromide	7.296	16.981	306.223	0.47	0.38	-0.09	Test daphnia set
Tributylethylphosphonium diethyl phosphate	6.132	2.755	1008.390	1.46	1.45	1.26	Test daphnia set
Trihexyltetradecylphosphonium chloride	13.738	14.993	4815.100	-0.83	-0.74	-0.58	Test daphnia set
Methyltrioctylammonium bis(trifluoromethylsulfonyl)amide(1-)	8.721	7.911	3716.760	-0.51	-0.49	-0.14	Test daphnia set
Picolinium bromide	0.725	1.066	87.034	2.01	2.04	2.23	Test daphnia set
1-(2-methoxyethyl)-3-methyl-1H-imidazolium tetrafluoroborate	0.387	7.239	126.819	2.99	2.97	2.88	Test daphnia set
1-(2-methoxyethyl)-3-methyl-1H-imidazolium N-cyanocynamide	0.387	7.239	126.819	3.00	2.97	2.88	Test daphnia set
3-(2-chloroethyl)-1-methylimidazolium chloride	1.327	8.674	105.244	2.74	2.52	2.50	Test daphnia set
3-(2-chloroethyl)-1-methylimidazolium bis(trifluoromethyl)sulfonylimide	1.327	8.674	105.244	2.37	2.52	2.50	Test daphnia set
3-(2-hydroxyethyl)-1-methylimidazolium bis(trifluoromethyl)sulfonylimide	-0.136	5.470	104.691	2.39	2.39	2.48	Test daphnia set
3-(2-chloropropyl)-1-methylimidazolium chloride	2.901	6.332	218.221	2.53	2.44	1.91	Test daphnia set
1-methyl-3-[(trimethylsilyl)methyl]-imidazolium bromide	3.307	7.777	255.884	1.85	1.78	1.36	Test daphnia set
Methylimidazolium chloride	0.896	4.300	57.064	2.93	2.89	2.76	Test daphnia set
1-(2-Chloroethyl)imidazolium chloride	1.057	11.445	68.855	2.78	2.75	2.55	Test daphnia set
1,10-(1,2-ethanediyl)bis-imidazolium chloride	0.403	1.764	126.890	2.63	2.60	2.47	Test daphnia set
Choline hexafluorophosphate	-0.875	3.646	121.187	2.60	2.56	2.62	Test daphnia set
Ethyl-methylmorpholiniumbromide	-0.116	4.169	165.785	2.68	2.63	2.52	Test daphnia set
Butylethyl-morpholiniumbromide	1.925	6.203	157.427	2.60	2.55	2.35	Test daphnia set
Ethyltetrahydrothiopheniumbromide	2.222	3.393	123.624	2.71	2.66	2.53	Test daphnia set
Triethylsulfoniumbromide	2.591	3.118	171.988	2.70	2.67	2.31	Test daphnia set

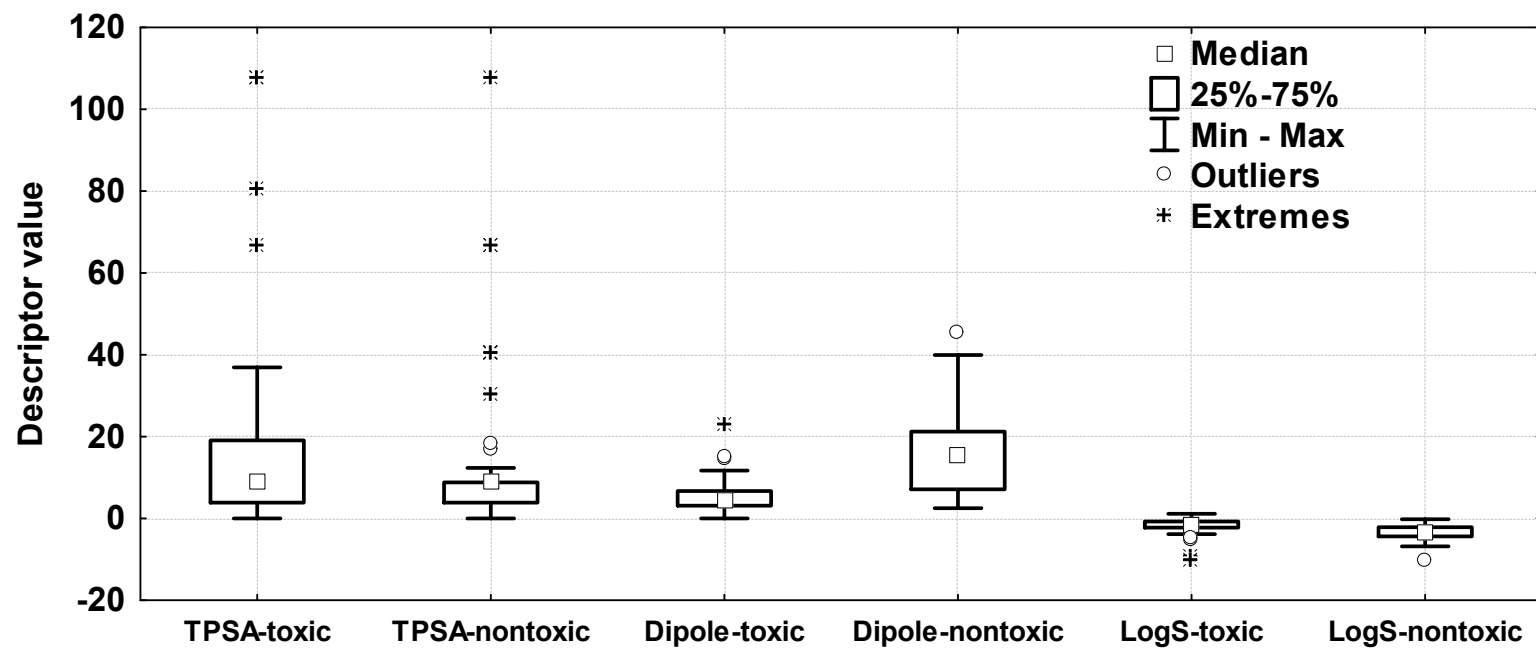


Figure S1: Box-Whisker plots of the input descriptors (*V.fischeri*) in two-category qualitative SARs.

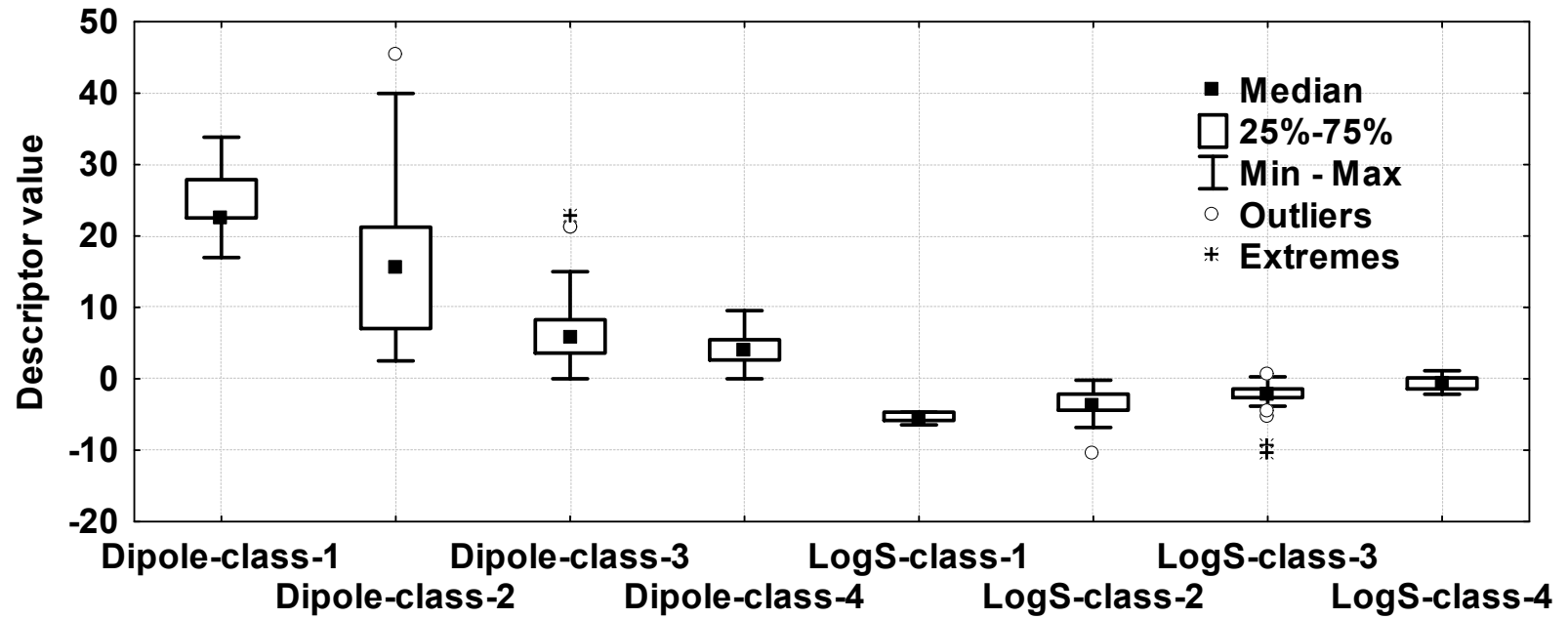


Figure S2a: Box-Whisker plots of the input descriptors (*V.fischeri*) in four-category qualitative SARs.

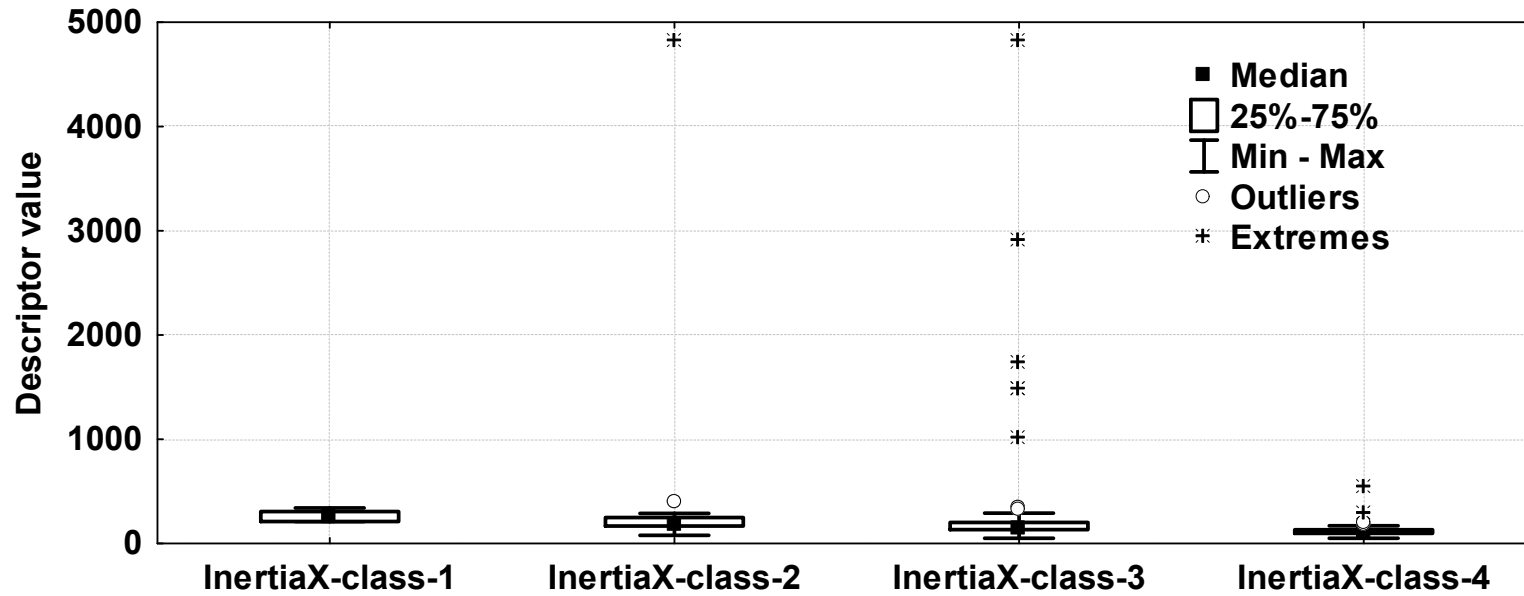


Figure S2b: *V. fischeri* plot

Figure S2b: Box-Whisker plots of the input descriptor (*V.fischeri*) in four-category qualitative SARs.