Electronic Supplementary Information to "Effects of different head groups and functionalised side chains on the cytotoxicity of ionic liquids"

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Table 1: All fitted EC_{50} values, their base 10 log and their confidence intervals.
The definitions of mtype, a, b, and c are given in the documentation of the R package drfit:
http://cran.r-project.org/src/contrib/Descriptions/drfit.html

Acronym	mtype	EC_{50} [μM]	$log_{10}\,EC_{50}$	b	c
IM1-14 Cl	linlogit	0.379	-0.421 ± 0.049	2.11	2.21
IM11CN (CF3SO2)2N	linlogit	7950	3.9 ± 0.032	3.51	0.000194
IM11CN Cl	inactive	> 20000	> 4.3		
IM11O2 (CF3SO2)2N	linlogit	1590	3.2 ± 0.04	3.85	0.000542
IM11O2 Cl	linlogit	4010	$3.6 \pm NA$	6.67	-5.72e-05
IM12O1 (CF3SO2)2N	linlogit	1780	3.25 ± 0.078	5.88	0.000424
IM12O1 Cl	inactive	> 20000	> 4.3		
IM12O2 (CF3SO2)2N	linlogit	1520	3.18 ± 0.056	2.9	0.000925
IM12O2 Br	linlogit	13800	4.14 ± 0.045	2.37	5.77e-05
IM12OH (CF3SO2)2N	linlogit	5800	3.76 ± 0.024	3.52	0.000158
IM12OH I	inactive	> 20000	> 4.3		
IM13O1 (CF3SO2)2N	linlogit	2200	3.34 ± 0.025	3.5	0.000563
IM13O1 Cl	linlogit	31000	4.49 ± 0.049	2.56	6.55e-05
IM13OH (CF3SO2)2N	linlogit	4570	3.66 ± 0.038	2.97	0.000251
IM13OH Cl	inactive	> 20000	> 4.3		
IM14 (CF3SO2)2N	linlogit	481	2.68 ± 0.041	3.9	0.00188
IM14 Cl	linlogit	3580	3.55 ± 0.072	1.92	0.000679
Mor11CN (CF3SO2)2N	linlogit	3400	3.53 ± 0.074	2.01	0.000363
Mor11CN Cl	inactive	> 20000	> 4.3		
Mor11O2 (CF3SO2)2N	linlogit	2320	$3.37 \pm NA$	1.72	-8.16e-05
Mor11O2 Cl	probit	3310	$3.52 \pm NA$	0.128	0
Mor12O1 (CF3SO2)2N	linlogit	6470	$3.81 \pm NA$	4.8	6.1e-05
Mor12O1 Cl	inactive	> 20000	> 4.3		
Mor12O2 (CF3SO2)2N	linlogit	4910	3.69 ± 0.043	5.12	-1.93e-05
Mor12O2 Br	inactive	> 20000	> 4.3		
Mor12OH (CF3SO2)2N	linlogit	1540	3.19 ± 0.11	1.47	0.000497
Mor12OH I	inactive	> 20000	> 4.3		
Mor13O1 (CF3SO2)2N	linlogit	5910	3.77 ± 0.053	3.22	2.07e-05
Mor13O1 Cl	inactive	> 30000	> 4.48		
Mor13OH (CF3SO2)2N	probit	3360	3.53 ± 0.03	0.191	0
Mor13OH Cl	inactive	> 20000	> 4.3		
Mor14 (CF3SO2)2N	linlogit	2690	3.43 ± 0.1	1.12	-5.29e-05
Mor14 Br	inactive	> 20000	> 4.3		
N1121CN (CF3SO2)2N	probit	7340	3.87 ± 0.057	0.21	0
N1121CN Cl	inactive	> 20000	> 4.3		
N1121O2 (CF3SO2)2N	linlogit	6300	3.8 ± 0.033	3.66	0.000247
N1121O2 Cl	linlogit	3900	$3.59 \pm NA$	9.62	2.59e-05
N1122O1 (CF3SO2)2N	linlogit	2040	3.31 ± 0.041	3.01	0.000469
N1122O1 Cl	inactive	> 20000	> 4.3		
N1122OH (CF3SO2)2N	manual fit	6310	$3.8 \pm NA$	0	0
N1122OH I	inactive	> 20000	> 4.3		
N1123O1 (CF3SO2)2N	linlogit	3430	3.54 ± 0.038	6.14	-1.91e-05
N1123O1 Cl	inactive	> 40000	> 4.6		
N1123OH (CF3SO2)2N	linlogit	6730	3.83 ± 0.034	3.82	0.000142
N1124 (CF3SO2)2N	probit	2680	3.43 ± 0.081	0.163	0
N1124 Cl	inactive	> 20000	> 4.3		

Table 1: *(continued)*

Acronym	mtype	EC_{50}	$log_{10} EC_{50}$	b	c
Pip11CN (CF3SO2)2N	linlogit	10000	4 ± 0.11	1.98	6.42e-05
Pip11CN Cl	linlogit	38000	4.58 ± 0.064	-0.286	-1.27e-05
Pip11O2 (CF3SO2)2N	linlogit	2590	3.41 ± 0.054	3.37	0.000303
Pip11O2 Cl	linlogit	17200	4.24 ± 0.063	0.397	-3.81e-05
Pip12O1 (CF3SO2)2N	linlogit	1890	$3.28 \pm NA$	2.44	-1.15e-05
Pip12O1 Br	inactive	> 40000	> 4.6		
Pip12O2 (CF3SO2)2N	probit	2210	$3.35 \pm NA$	0.105	0
Pip12O2 Br	linlogit	20200	4.31 ± 0.07	2.21	9.65e-05
Pip12OH (CF3SO2)2N	linlogit	4500	3.65 ± 0.028	3.96	0.000242
Pip12OH I	linlogit	23400	4.37 ± 0.055	-0.0796	-1.9e-05
Pip13O1 (CF3SO2)2N	linlogit	1860	3.27 ± 0.035	4.25	0.000385
Pip13O1 Cl	linlogit	25200	4.4 ± 0.071	2.04	6.52e-05
Pip13OH (CF3SO2)2N	linlogit	4240	$3.63 \pm NA$	3.5	-4.45e-06
Pip13OH Cl	inactive	> 40000	> 4.6		
Pip14 (CF3SO2)2N	linlogit	2570	3.41 ± 0.065	2.68	0.000442
Pip14 Br	linlogit	10800	4.03 ± 0.039	2.22	0.000219
Py1CN (CF3SO2)2N	linlogit	3150	3.5 ± 0.047	2.59	0.000305
Py1CN Cl	linlogit	6140	$3.79 \pm NA$	1.48	4.16e-05
Py1O2 (CF3SO2)2N	linlogit	1330	3.12 ± 0.034	3.67	0.000302
Py1O2 Cl	linlogit	2100	$3.32 \pm NA$	5.53	0.000194
Py2-4NMe2 (CF3SO2)2N	linlogit	697	2.84 ± 0.11	1.67	0.00604
Py2-4NMe2 Br	linlogit	788	2.9 ± 0.068	1.86	0.00798
Py2O1 (CF3SO2)2N	linlogit	1540	3.19 ± 0.017	4.92	5.5e-05
Py2O1 Cl	inactive	> 20000	> 4.3		
Py2O2 (CF3SO2)2N	linlogit	1840	3.26 ± 0.049	4.09	0.000326
Py2O2 Br	linlogit	17500	4.24 ± 0.067	1.71	6.76e-05
Py2OH (CF3SO2)2N	linlogit	6200	3.79 ± 0.045	4.5	4.66e-05
Py2OH I	probit	14300	4.15 ± 0.12	1.75	0
Py3O1 (CF3SO2)2N	linlogit	2400	$3.38 \pm NA$	12	0.000191
Py3O1 Cl	inactive	> 40000	> 4.6		
Py3OH (CF3SO2)2N	linlogit	3530	3.55 ± 0.08	2.8	0.000195
Py3OH Cl	inactive	> 20000	> 4.3		
Py4 Br	linlogit	8020	3.9 ± 0.058	1.79	0.000448
Py4-4NMe2 (CF3SO2)2N	linlogit	48.5	1.69 ± 0.12	1.42	0.0361
Py4-4NMe2 Cl	linlogit	87.3	1.94 ± 0.081	1.86	0.118
Py6-4NMe2 (CF3SO2)2N	linlogit	8.5	$0.93 \pm NA$	1.68	0.127
Py6-4NMe2 Cl	linlogit	8.45	0.927 ± 0.078	2.04	0.366
Pyr11CN (CF3SO2)2N	linlogit	6370	$3.8 \pm NA$	3.69	0.000254
Pyr11CN Cl	probit	17100	$4.23 \pm NA$	0.137	0
Pyr11O2 (CF3SO2)2N	linlogit	1810	3.26 ± 0.044	4.5	0.000426
Pyr11O2 Cl	probit	830	$2.92 \pm NA$	0.11	0
Pyr12O1 (CF3SO2)2N	linlogit	1990	3.3 ± 0.037	5.11	0.000397
Pyr12O1 Cl	inactive	> 20000	> 4.3		
Pyr12O2 (CF3SO2)2N	linlogit	1580	3.2 ± 0.053	3.32	0.000425
Pyr12O2 Br	inactive	> 20000	> 4.3		
Pyr12OH (CF3SO2)2N	linlogit	5240	3.72 ± 0.048	3.03	0.000568
Pyr12OH I	inactive	> 20000	> 4.3		
Pyr13O1 (CF3SO2)2N	linlogit	2530	$3.4 \pm NA$	7.11	0.000233
Pyr13O1 Cl	inactive	> 50000	> 4.7		
Pyr13OH (CF3SO2)2N	linlogit	4010	3.6 ± 0.055	3.15	0.000505
Pyr13OH Cl	inactive	> 20000	> 4.3		
Pyr14 (CF3SO2)2N	probit	1020	3.01 ± 0.047	0.23	0
Pyr14 Cl	inactive	> 20000	> 4.3		
DCOIT	probit	1.15	0.0608 ± 0.051	0.511	0.0514
Carbendazim	probit	7.12	0.852 ± 0.036	0.46	0.0365

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Table 1: *(continued)*

Acronym	mtype	EC_{50}	log_{10} EC_{50}	b	c
Methanol	linlogit	1567000	6.20 ± 0.032	NA	NA
Ethanol	probit	683000	5.83 ± 0.098	0.646	0.0984
Propanol	probit	104000	5.02 ± 0.18	1.44	0.183