Electronic Supplementary Information to "The influence of anion species on the toxicity of ionic liquids observed in an (eco)toxicological test battery"

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The substances used in this study are listed in Table 1. EC_{50} values for the various test systems are listed in tables 2, 3, 4, 5 and 6. The statistical parameters listed in the tables are as given by the drfit package [1] of the R software [2].

Table 1: Acronyms and chemical names

UFT No.	Acronym	Chemical name
78	IM12 (2-OPhO)2B	1-Ethyl-3-methyl-imidazolium bis(1,2-benzenediolato)borate
87	IM14 (CF3)2N	1-Butyl-3-methyl-imidazolium bis(trifluoromethyl)imide
88	IM14 (CF3SO2)2N	1-Butyl-3-methyl-imidazolium bis(trifluoromethylsulfonyl)imide
66	IM14 8OSO3	1-Butyl-3-methyl-imidazolium octylsulfate
7	IM14 BF4	1-Butyl-3-methyl-imidazolium tetrafluoroborate
5	IM14 Cl	1-Butyl-3-methyl-imidazolium chloride
25	IM18 BF4	1-Methyl-3-octyl-imidazolium tetrafluoroborate
156	Li (2-OPhO)2B	Lithium bis(1,2-benzenediolato)borate
142	Li (CF3SO2)2N	Lithium bis(trifluoromethylsulfonyl)imide
67	Na 8OSO3	Sodium octyl sulfate
44	Na BF4	Sodium tetrafluoroborate

Table 2: Acetylcholinesterase inhibition

	mtype	EC_{50}	unit	log EC_{50}	sigma	a	b
IM12 (2-OPhO)2B	probit	120	μM	2.09 ± 0.04	0.06866	2.094	0.7754
IM14 (CF3)2N	probit	40	μM	1.6 ± 0.033	0.04793	1.603	0.6448
IM14 (CF3SO2)2N	probit	92	μM	1.96 ± 0.021	0.02857	1.964	0.7637
IM14 8OSO3	probit	95	μM	1.98 ± 0.031	0.06143	1.979	0.8483
IM14 BF4	probit	97	μM	1.98 ± 0.018	0.03577	1.985	0.7849
IM14 Cl	probit	82	μM	1.91 ± 0.04	0.0503	1.915	0.8415
IM18 BF4	probit	34	μM	1.53 ± 0.025	0.05752	1.531	0.9032
Li (2-OPhO)2B	inactive	> 1000	μM	> 3			
Li (CF3SO2)2N	inactive	> 1000	μM	> 3			
Na 8OSO3	inactive	> 5000	μM	> 3.7			
Na BF4	inactive	> 1000	μM	> 3			

Table 3: Cytotoxicity in the WST-1 assay with IPC-81 cells

	mtype	EC_{50}	unit	log EC_{50}	sigma	a	b	c
IM12 (2-OPhO)2B	linlogit	11	μM	1.02 ± 0.058	0.09308	1.023	1.113	-0.008171
IM14 (CF3)2N	linlogit	150	μM	2.19 ± 0.079	0.2052	2.188	2.162	-0.0003866
IM14 (CF3SO2)2N	linlogit	480	μM	2.68 ± 0.054	0.1941	2.682	3.903	0.001878
IM14 8OSO3	linlogit	1700	μM	3.23 ± 0.045	0.1971	3.226	4.562	0.001511
IM14 BF4	linlogit	1300	μM	3.12 ± 0.021	0.1231	3.121	3.458	0.0002377
IM14 Cl	linlogit	3600	μM	3.55 ± 0.079	0.1748	3.554	1.921	0.0006786
IM18 BF4	linlogit	39	μM	1.59 ± 0.054	0.2373	1.591	2.187	0.05746
Li (2-OPhO)2B	linlogit	13	μM	1.13 ± 0.11	0.1514	1.128	1.052	-0.002347
Li (CF3SO2)2N	linlogit	2200	μM	3.33	0.1584	3.335	1.013	-5.239e-05
Na 8OSO3	linlogit	3000	μM	3.48 ± 0.081	0.2343	3.481	2.498	0.0009449
Na BF4	inactive	> 2000	μM	> 3.3				

Table 4: Acute toxicity toward *Vibrio fischeri*

	mtype	EC_{50}	unit	log EC_{50}	sigma	a	b	c
IM12 (2-OPhO)2B	linlogit	910	μM	2.96 ± 0.036	0.03067	2.959	1.434	-0.0001212
IM14 (CF3)2N	linlogit	2900	μM	3.46 ± 0.083	0.05726	3.456	0.9362	-3.01e-05
IM14 (CF3SO2)2N	linlogit	300	μM	2.47 ± 0.036	0.03602	2.472	2.215	-0.0003319
IM14 8OSO3	linlogit	67	μM	1.82 ± 0.036	0.02828	1.824	1.397	-0.0005529
IM14 BF4	probit	3500	μM	3.55 ± 0.026	0.05672	3.548	0.5708	
IM14 Cl	probit	3000	μM	3.47 ± 0.043	0.04062	3.473	0.6795	
IM18 BF4	probit	25	μM	1.4 ± 0.087	0.05611	1.402	0.8009	
Li (2-OPhO)2B	linlogit	580	μM	2.76 ± 0.044	0.03982	2.764	1.488	-0.0003218
Li (CF3SO2)2N	inactive	> 20000	μM	> 4.3				
Na 8OSO3	linlogit	290	μM	2.46 ± 0.039	0.03339	2.456	0.7746	-2.139e-05
Na BF4	inactive	> 20000	μM	> 4.3				

Table 5: Acute toxicity towards *Scenedesmus vacuolatus*

	mtype	EC_{50}	unit	log EC_{50}	sigma	a	b	c
IM12 (2-OPhO)2B	linlogit	26	μM	1.42	0.1331	1.418	1.87	0.0006587
IM14 (CF3)2N	linlogit	670	μM	2.83	0.2471	2.829	5.516	-0.0006244
IM14 (CF3SO2)2N	linlogit	63	μM	1.8 ± 0.15	0.1632	1.802	1.379	0.0003504
IM14 8OSO3	linlogit	53	μM	1.72	0.2702	1.723	2.512	0.01128
IM14 BF4	linlogit	130	μM	2.13 ± 0.11	0.1893	2.129	1.59	-0.000799
IM18 BF4	probit	0.0058	μM	-2.24	0.3683		0.4077	
Li (2-OPhO)2B	probit	27	μM	1.43 ± 0.27	0.2441	1.432	0.8954	
Li (CF3SO2)2N	linlogit	120	μM	2.1 ± 0.12	0.1884	2.096	2.14	0.003092
Na 8OSO3	probit	2300	μM	3.36 ± 0.49	0.1133	3.358	1.334	
Na BF4	inactive	> 5000	μM	> 3.7				

References

[1] J. Ranke. *drfit: Dose-response data evaluation*, 2007. R package version 0.05-89.

[2] R Development Core Team. *R: A Language and Environment for Statistical Computing, version 2.5.1.* R Foundation for Statistical Computing, Vienna, Austria, 2007. ISBN 3-900051-07-0.

Table 6: Acute toxicity towards *Lemna minor*

	mtype	EC_{50}	unit	log EC_{50}	sigma	a	b	c
IM12 (2-OPhO)2B	weibull	150	μM	2.17	0.06149	3.116	6.998	
IM14 (CF3)2N	linlogit	180	μM	2.25	0.05412	2.25	0.9527	-0.003255
IM14 (CF3SO2)2N	linlogit	330	μM	2.52 $\pm$ 0.023	0.04487	2.516		-0.001479
IM14 8OSO3	linlogit	400	μM	2.61	0.07278	2.605	2.049	-0.000809
IM14 BF4	linlogit	310	μM	2.49 $\pm$ 0.051	0.06063	2.494	1.701	0.003201
IM18 BF4	active	< 35	μM	> 1.55				
Li (2-OPhO)2B	linlogit	310	μM	2.5 $\pm$ 0.12	0.05818	2.498	4.292	-0.0001656
Li (CF3SO2)2N	probit	6300	μM	3.8 $\pm$ 0.076	0.05341	3.799	0.5825	
Na 8OSO3	manual fit	3000	μM	3.5				
Na BF4	weibull	2000	μM	3.31	0.08751	4.206	3.43	

Table 7: Growth inhibition towards *Lepidium sativum*

	mtype	EC_{50}	unit	$logEC_{50}$	sigma	a	b	c
IM14 BF4	linlogit	1912	µM	3.28	0.06433053	3.28154	3.091371	0.0006495855
IM18 BF4	probit	297	µM	2.47	0.02340937	2.472644	0.081723	
IM 14 (CF3SO2)2N	probit	397	µM	2.60	0.1121726	2.598722	0.256964	
Li (CF3SO2)2N	linlogit	1243	µM	3.09	0.1125764	3.094799	0.126186	-0.000305172

Table 8: Growth inhibition towards *Triticum aestivum*

	mtype	EC_{50}	unit	$logEC_{50}$	sigma	a	b	c
IM14 BF4	probit	1703	µM	3.23	0.0839606	3.231396	0.423951	
IM18 BF4	probit	288	µM	2.46	0.09241839	2.459274	0.655758	
IM 14 (CF3SO2)2N	linlogit	111	µM	2.04	0.105597	2.043581	2.329599	0.0065875
Li (CF3SO2)2N	linlogit	99	µM	1.99	0.0909517	1.997819	2.084733	0.0168228

Table 9: Reproduction inhibition towards *Folsomia candida*

	mtype	EC_{50}	unit	log EC_{50}	sigma	a	b	c
Li (CF3SO2)2N	probit	18	µM	1.244	0.05541865	1.243996	0.3487042	
IM14 (CF3SO2)2N	probit	28	µM	1.442	0.1239894	1.441875	0.3635762	
IM18 BF4	probit	103	µM	-0.985	0,08839852	-0,09858	1,128338	
IM14 8OSO3	probit	1122	µM	3.050	0.09664819	3.050246	0.0269984	