

## **Applicability of heuristic rules defining structure-ecotoxicity relationships of ionic liquids: an integrative assessment using species sensitivity distributions (SSD)**

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**Table S1.** EC<sub>20</sub> and EC<sub>10</sub> values, with the respective 95% confidence intervals (CI), obtained in the ecotoxicological tests performed in the present study.

IL	Species	Exposure period	Endpoint		EC <sub>x</sub> value (mg.L <sup>-1</sup> )	95% CI	Notes
[Chol]CI	<i>Chlorella vulgaris</i>	96h	Yield	EC <sub>20</sub>	4724	3768-5681	
				EC <sub>10</sub>	4086	2652-5215	
	<i>Lemna gibba</i>	7d	Yield	EC <sub>20</sub>	359.2	300.7-417.6	fronds number
				EC <sub>10</sub>	300.6	234.1-367.0	
				EC <sub>20</sub>	510.9	0.1239-1022	dry weight
				EC <sub>10</sub>	214.4	0-522.1	
	<i>Daphnia magna</i>	24h + 4h	Post-exposure feeding inhibition	EC <sub>20</sub>	467.5	326.0-609.1	
				EC <sub>10</sub>	408.0	244.5-571.5	
	<i>Corbicula fluminea</i>	2h	Feeding inhibition	EC <sub>20</sub>	2853	1628-4078	
				EC <sub>10</sub>	2012	870-3154	
	<i>Danio rerio</i>	96h	Hatching	EC <sub>20</sub>	427.2	72.71-781.6	
			Yolk sac absorption	EC <sub>20</sub>	1.372x10 <sup>4</sup>	1.175x10 <sup>4</sup> -1.570x10 <sup>4</sup>	
				EC <sub>10</sub>	1.177x10 <sup>4</sup>	9.572x10 <sup>3</sup> -1.397x10 <sup>4</sup>	
	<i>Brachionus calyciflorus</i>	48h	Population growth	EC <sub>20</sub>	1500	23.50-2977	
				EC <sub>10</sub>	1673	468.2-2877	
[Chol][DHCit]	<i>Chlorella vulgaris</i>	96h	Yield	EC <sub>20</sub>	1469	95.93-2842	
				EC <sub>10</sub>	238.3	137.8-338.7	
	<i>Lemna gibba</i>	7d	Yield	EC <sub>20</sub>	150.2	64.14-236.2	fronds number
				EC <sub>20</sub>	329.9	191.2-468.7	
				EC <sub>10</sub>	185.6	83.24-288.0	dry weight
				EC <sub>20</sub>	479.6	0-965.9	
	<i>Daphnia magna</i>	24h+4h	Post-exposure feeding inhibition	EC <sub>10</sub>	199.7	0-469.0	
				EC <sub>20</sub>	450.7	365.2-536.3	
	<i>Danio rerio</i>	96h	Hatching	EC <sub>10</sub>	392.9	285.2-500.5	
				EC <sub>20</sub>	1385	1344-1425	
			Heart edema	EC <sub>10</sub>	1378	1378-1378	
				EC <sub>20</sub>	1385	1344-1425	
	<i>Brachionus calyciflorus</i>	48h	Population growth	EC <sub>10</sub>	1378	1378-1378	
				EC <sub>20</sub>	205.3	147.5-263.1	
	[C <sub>2</sub> mim]CI	<i>Aliivibrio fischeri</i>	30min	Luminescence	EC <sub>10</sub>	181.4	114.2-248.6
EC <sub>20</sub>					1366	969.9-1761	
<i>Raphidocelis subcapitata</i>		96h	Yield	EC <sub>20</sub>	559.2	342.0-776.4	
				EC <sub>10</sub>	46.27	15.82-76.72	
<i>Chlorella vulgaris</i>		96h	Yield	EC <sub>10</sub>	16.66	8.452x10 <sup>-2</sup> -33.23	
				EC <sub>20</sub>	38.15	26.59-49.71	
				EC <sub>10</sub>	24.77	14.60-34.94	

	<i>Lemna minor</i>	7 d	Yield	EC <sub>20</sub>	38.03	31.85-44.22	fronds number
				EC <sub>10</sub>	28.21	22.12-34.29	
				EC <sub>20</sub>	10.46	8.61-18.88	dry weight (mg)
	<i>Lemna gibba</i>	7d	Yield	EC <sub>20</sub>	23.36	17.57-29.15	fronds number
				EC <sub>10</sub>	14.74	9.848-19.64	
				EC <sub>20</sub>	36.63	0.3491-72.91	dry weight (mg)
				EC <sub>10</sub>	11.80	0-29.40	
	<i>Daphnia magna</i>	24h + 4h	Post-exposure feeding inhibition	EC <sub>20</sub>	256.2	214.9-297.5	
				EC <sub>10</sub>	228.7	179.7-277.7	
	<i>Corbicula fluminea</i>		Feeding inhibition	EC <sub>20</sub>	2737	641.6-4832	
	<i>Danio rerio</i>	96h	Yolk sac absorption	EC <sub>20</sub>	7782	7277-8288	
				EC <sub>10</sub>	1.402x10 <sup>4</sup>	1.399x10 <sup>4</sup> -1.405x10 <sup>4</sup>	
			Tail deformities (spinal curvature)	EC <sub>20</sub>	6716	6128-7305	
				EC <sub>10</sub>	1.371x10 <sup>4</sup>	1.371x10 <sup>4</sup> -1.372x10 <sup>4</sup>	
			Balance (sideways <sup>2</sup> )	EC <sub>20</sub>	7798	5776-9819	
				EC <sub>10</sub>	6409	4179-8638	
	<i>Brachionus calyciflorus</i>	48h	Population growth	EC <sub>20</sub>	46.73	28.98-64.48	
				EC <sub>10</sub>	35.81	16.92-54.70	
	[C <sub>12</sub> mim]Cl	<i>Aliivibrio fischeri</i>	30min	Luminescence	EC <sub>20</sub>	0.1835	0.1642-0.2028
EC <sub>10</sub>					0.1210	0.1042-0.1379	
<i>Raphidocelis subcapitata</i>		96h	Yield	EC <sub>20</sub>	3.794×10 <sup>-3</sup>	1.915×10 <sup>-3</sup> - 5.673×10 <sup>-3</sup>	
				EC <sub>10</sub>	1.424×10 <sup>-3</sup>	4.670×10 <sup>-4</sup> -2.381×10 <sup>-3</sup>	
<i>Chlorella vulgaris</i>		96h	Yield	EC <sub>20</sub>	0.1214	8.939×10 <sup>-2</sup> -0.1533	
				EC <sub>10</sub>	8.450×10 <sup>-2</sup>	5.175×10 <sup>-2</sup> -0.1173	
<i>Lemna minor</i>		7d	Yield	EC <sub>20</sub>	1.4577	1.088-1.827	fronds number
				EC <sub>10</sub>	0.9198	0.6086-1.231	
				EC <sub>20</sub>	1.892	1.105-2.680	dry weight (mg)
				EC <sub>10</sub>	0.8298	0.3546-1.305	
<i>Lemna gibba</i>		7d	Yield	EC <sub>20</sub>	1.0477	0.6519-1.444	fronds number
				EC <sub>10</sub>	0.5079	0.2419-0.7738	
				EC <sub>20</sub>	0.3944	0-1.002	dry weight (mg)
				EC <sub>10</sub>	6.960×10 <sup>-2</sup>	0-0.2281	
<i>Daphnia magna</i>		24h + 4h	Post-exposure feeding inhibition	EC <sub>20</sub>	4.122	6.288×10 <sup>-2</sup> -8.181	
<i>Danio rerio</i>			Yolk sac absorption	EC <sub>20</sub>	9880	177-1.958x10 <sup>4</sup>	
				EC <sub>10</sub>	11033	8538-1.353x10 <sup>4</sup>	
			Tail deformities (spinal curvature)	EC <sub>20</sub>	13249	1.102x10 <sup>4</sup> -1.548x10 <sup>4</sup>	
				EC <sub>10</sub>	11033	8538-1.353x10 <sup>4</sup>	
Balance (sideways <sup>2</sup> )	EC <sub>20</sub>	8356	7265-9466				
	EC <sub>10</sub>	6988	5770-8207				
<i>Brachionus calyciflorus</i>	48h	Population growth	EC <sub>20</sub>	0.1775	0.1409-0.2142		

				EC <sub>10</sub>	0.1587	0.1155-0.2018	
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embryo showing signs of unbalance but dorsally positioned; <sup>2</sup> embryo positioned sideways