A comprehensive dataset on cytotoxicity of ionic liquids

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Supporting Information

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Table S1. Diversity of unique structures, cations, anions, cell lines and methods in the dataset and four most populated groups of ILs[a]

	All ILs	**Imidazolium ILs**	**Phosphonium ILs**	**Polycharged ILs**	**Ammonium ILs**
Total count of IL	3837	1366 (36%)	572 (15%)	478 (12%)	312 (8%)
Unique structures	1227	314	98	184	127
Unique cations	657	130	66	94	67
Unique anions	156	63	21	51	36
Cell lines	155	104	104	27	93
Methods	24	13	11	7	11

[a] Percentage of the total count is shown in parentheses.

Table S2. Diversity of unique structures, cations, anions, cell lines and methods in all other groups of ILs[a]

	All	Pyridinium	Benzimidazolium	Cholinium	Guanidium	Thiazolium	Pyrrolidinium	Piperazinium	Morpholinium	Piperidinium	Quinolinium	Triazolium	Pyrimidinium	Other
Total count of ILs	3837	255 (6%)	229 (5%)	131 (3%)	73 (2%)	64 (1%)	59 (1%)	36 (<1%)	36 (<1%)	35 (<1%)	34 (<1%)	21(<1%)	8 (<1%)	128 (3%)
Unique structures	1227	136	51	65	43	26	32	12	36	25	13	12	3	56
Unique cations	657	85	45	20	36	14	14	8	12	13	11	10	1	43
Unique anions	156	17	5	38	11	6	8	5	20	7	3	5	3	20
Cell lines	155	43	13	35	13	7	16	2	2	6	8	7	3	23
Methods	24	10	3	11	3	2	5	1	2	3	2	4	1	8

[a] Percentage of the total count is shown in parentheses.

Table S3. Most popular cell lines and measurement methods for all groups of ILs and imidazolium ILs in particular

Cell name	Cell type (tissue)/disease	Count of entries for all groups of ILs	Count of entries for imidazolium ILs	Assays for all groups of ILs	Assays for imidazolium ILs
IPC-81	Bone marrow/Leukemia	308	141	WST-1	WST-1
MCF-7	Epithelial cells (mammary gland)/Adenocarcinoma	273	74	MTT MTS SRB HCT/MTT	MTT MTS SRB
A549/ATCC	Epithelial cells (lung)/Carcinoma	201	63	Prestoblue MTT MTS SRB WST-8	PrestoBlue MTT MTS SRB
HeLa	Epithelial cells (cervix)/Adenocarcinoma	180	72	WST-1 MTT MTS	WST-1 MTT
CaCo-2	Epithelial cells (colon)/Colorectal adenocarcinoma	174	110	MTT MTS WST-1	MTT MTS
T-47D	Epithelial cells (mammary gland)/Carcinoma (ductal)	93	34	MTT SRB	MTT SRB
HaCat	Keratinocytes (skin)	93	20	MTT MTS WST-1 WST-8 AlamarBlue	MTT MTS AlamarBlue