

**A large-scale study of ionic liquids employed in chemistry and energy research to reveal
cytotoxicity mechanisms and to develop safe design guide**

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Supporting Information

Table S1. Dataset of cytotoxic activity of ILs measured in the present study.

#	Substance name	Mw, g·mol ⁻¹	Cell line	24-h CC ₅₀ , mM	Jurkat cells			
					Apoptotic cells, % ^a	Mitochondrial damage, % ^a (%)	Cytochrome loss, % ^b	Dead cells, % ^a
1	1-Ethyl-3-methylimidazolium chloride C ₂ MIm Cl	146.618	U937	110.31 (104.51-116.11)	5.69	18.43	63.33	68.17
			Jurkat	102.14 (95.94-108.34)				
			HL60	33.17 (31.27-35.07)				
			K562	143.22 (137.82-148.62)				
			HEK293	393.37 (372.07-414.67)				
			A549	188.18 (175.78-200.58)				
A2780	187.41 (173.31-201.51)							
2	1-Ethyl-3-methylimidazolium acetate C ₂ MIm OAc	170.212	U937	150.88 (143.48-158.28)	1.35	20.53	36.69	0.60
			Jurkat	146.76 (141.06-152.46)				
			HL60	72.50 (70.00-75.00)				
			K562	178.25 (170.15-186.35)				
			HEK293	651.6 (605-698.2)				
			A549	271.01 (249.61-292.41)				
A2780	174.60 (159.1-190.1)							
3	1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide C ₂ MIm NTf ₂	391.303	U937	6.13 (5.63-6.63)	6.49	8.83	25.27	2.75
			Jurkat	4.64 (4.34-4.94)				
			HL60	3.07 (2.77-3.37)				
			K562	6.64 (6.04-7.24)				
			HEK293	13.19 (12.59-13.79)				
			A549	4.3 (4.1-4.5)				
A2780	13.39 (12.49-14.29)							
4	1-Ethyl-3-methylimidazolium tetrafluoroborate C ₂ MIm BF ₄	197.972	U937	73.24 (69.84-76.64)	8.15	27.15	40.88	0.69
			Jurkat	75.77 (72.97-78.57)				
			HL60	25.26 (23.76-26.76)				
			K562	106.07 (101.47-110.67)				
			HEK293	478.12 (444.92-511.32)				
A549	151.23 (139.08-163.38)							

			A2780	241.76 (239.54-243.98)				
5	1-Methyl-3-propylimidazolium chloride C ₃ MIm Cl	160.645	U937	93.37 (89.57-97.17)	3.91	7.05	N/A	0.82
			Jurkat	62.25 (59.05-65.45)				
			HL60	31.13 (28.63-33.63)				
			K562	124.49 (118.19-130.79)				
			HEK293	342.23 (316.43-368.03)				
			A549	101 (89.7-112.3)				
			A2780	174.4 (162-186.8)				
6	1-Butyl-3-methylimidazolium chloride C ₄ MIm Cl	174.672	U937	57.25 (53.45-61.05)	5.67	6.54	N/A	41.36
			Jurkat	28.62 (24.92-32.32)				
			HL60	14.31 (13.11-15.51)				
			K562	85.87 (82.17-89.57)				
			HEK293	322.38 (303.68-341.08)				
			A549	185.61 (173.71-197.51)				
			A2780	101.62 (91.52-111.72)				
7	1-Butyl-3-methylimidazolium acetate C ₄ MIm OAc	198.266	U937	32.78 (30.08-35.48)	8.26	99.85	87.93	43.43
			Jurkat	37.82 (36.42-39.22)				
			HL60	20.17 (19.07-21.27)				
			K562	80.69 (77.29-84.09)				
			HEK293	284.11 (264.21-304.01)				
			A549	130.05 (117.95-142.15)				
			A2780	123.58 (111.28-135.88)				
8	1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide C ₄ MIm NTf ₂	419.357	U937	3.81 (3.01-4.61)	4.98	6.09	N/A	1.84
			Jurkat	2.38 (1.78-2.98)				
			HL60	1.90 (1.7-2.1)				
			K562	5.24 (4.64-5.84)				
			HEK293	21.70 (19.3-24.1)				
			A549	13.10 (11.6-14.6)				
			A2780	12.16 (11.06-13.26)				
9	1-Butyl-3-methylimidazolium	226.026	U937	31.18 (29.38-32.98)	8.11	18.76	30.02	40.64

	tetrafluoroborate C ₄ MIm BF ₄		Jurkat	23.11 (21.61-24.61)				
			HL60	7.04 (5.84-8.24)				
			K562	41.24 (38.84-43.64)				
			HEK293	148.15 (126.55-169.75)				
			A549	136.60 (125.00-148.2)				
			A2780	114.47 (103.57-125.37)				
10	1-Hexyl-3-methylimidazolium chloride C ₆ MIm Cl	202.726	U937	9.76 (8.96-10.56)	3.09	3.59	N/A	1.36
			Jurkat	5.13 (4.73-5.53)				
			HL60	1.23 (1.14-1.32)				
			K562	7.39 (6.69-8.09)				
			HEK293	16.76 (14.88-18.64)				
			A549	17.87 (16.67-19.07)				
			A2780	11.9 (10.6-13.2)				
11	1-Hexyl-3-methylimidazolium tetrafluoroborate C ₆ MIm BF ₄	254.08	U937	3.94 (3.64-4.24)	5.56	4.75	N/A	0.66
			Jurkat	4.26 (3.86-4.66)				
			HL60	1.57 (1.37-1.77)				
			K562	7.08 (6.38-7.78)				
			HEK293	27.25 (24.75-29.75)				
			A549	14.8 (13.36-16.24)				
			A2780	12.38 (11.3-13.46)				
12	1-Methyl-3-octylimidazolium tetrafluoroborate C ₈ MIm BF ₄	282.134	U937	0.35 (0.3-0.4)	8.17	6.29	24.51	1.19
			Jurkat	0.53 (0.46-0.6)				
			HL60	0.07 (0.06-0.08)				
			K562	0.78 (0.69-0.87)				
			HEK293	2.14 (1.81-2.47)				
			A549	1.1 (1.01-1.19)				
			A2780	0.89 (0.81-0.97)				
13	1-Decyl-3-methylimidazolium chloride C ₁₀ MIm Cl	258.834	U937	0.04 (0.031-0.049)	16.71	3.03	N/A	1.33
			Jurkat	0.08 (0.075-0.085)				
			HL60	0.007 (0.006-0.008)				
			K562	0.081 (0.073-0.089)				

			HEK293	0.19 (0.174-0.206)				
			A549	0.12 (0.109-0.131)				
			A2780	0.93 (0.858-1.002)				
14	1-Hexadecyl-3-methylimidazolium chloride C ₁₆ MIm Cl	342.996	U937	0.012 (0.01-0.014)	18.93	41.07	30.76	12.23
			Jurkat	0.015 (0.013-0.017)				
			HL60	0.003 (0.002-0.004)				
			K562	0.007 (0.006-0.008)				
			HEK293	0.045 (0.042-0.048)				
			A549	0.022 (0.02-0.024)				
A2780	0.012 (0.011-0.013)							
15	1-(2-Hydroxyethyl)-3-methylimidazolium tetrafluoroborate HOC ₂ MIm BF ₄	213.971	U937	72.12 (68.72-75.52)	8.52	15.55	28.12	0.39
			Jurkat	51.41 (48.91-53.91)				
			HL60	64.10 (61.00-67.20)				
			K562	74.78 (70.68-78.88)				
			HEK293	128.45 (116.67-140.23)				
			A549	125.39 (113.85-136.93)				
A2780	97.10 (89.97-104.23)							
16	1-Butylpyridinium chloride C ₄ Py Cl	171.668	U937	96.12 (91.82-100.42)	3.96	6.57	79.36	0.93
			Jurkat	37.86 (35.76-39.96)				
			HL60	29.13 (26.93-31.33)				
			K562	87.38 (83.78-90.98)				
			HEK293	251.48 (226.78-276.18)				
			A549	133.57 (120.24-146.9)				
A2780	118.31 (106.15-130.47)							
17	1-Butylpyridinium tetrafluoroborate C ₄ Py BF ₄	223.022	U937	17.94 (16.74-19.14)	6.63	92.20	40.58	1.53
			Jurkat	22.42 (21.52-23.32)				
			HL60	4.48 (4.08-4.88)				
			K562	8.96 (8.26-9.66)				
			HEK293	35.81 (32.53-39.09)				
A549	22.82 (20.86-24.78)							

			A2780	20.62 (19.53-21.71)				
18	1-Butyl-2-methylpyridinium chloride C ₄ M(2)Py Cl	185.695	U937	18.69 (16.97-20.41)	3.55	8.43	27.08	1.45
			Jurkat	29.62 (27.72-31.52)				
			HL60	13.46 (12.16-14.76)				
			K562	35.01 (32.51-37.51)				
			HEK293	93.38 (84.5-102.26)				
			A549	54.63 (49.64-59.62)				
A2780	47.18 (42.61-51.75)							
19	1-Butyl-3-methylpyridinium chloride C ₄ M(3)Py Cl	185.695	U937	10.77 (9.67-11.87)	5.20	11.57	25.06	2.79
			Jurkat	9.08 (8.28-9.88)				
			HL60	4.13 (3.73-4.53)				
			K562	5.38 (4.68-6.08)				
			HEK293	21.08 (18.88-23.28)				
			A549	15.12 (13.66-16.58)				
A2780	12.81 (11.67-13.95)							
20	1-Butyl-1-methylpyrrolidinium chloride C ₄ C ₁ Pyr Cl	177.716	U937	41.20 (38.5-43.9)	7.23	16.31	74.03	0.59
			Jurkat	89.47 (85.57-93.37)				
			HL60	55.27 (51.97-58.57)				
			K562	119.54 (113.64-125.44)				
			HEK293	251.48 (227.33-275.63)				
			A549	140.05 (126.52-153.58)				
A2780	132.22 (119.24-145.2)							
21	Tetraethylammonium tetrafluoroborate (C ₂) ₄ N BF ₄	217.059	U937	13.16 (12.46-13.86)	3.66	6.25	25.57	1.13
			Jurkat	11.08 (10.18-11.98)				
			HL60	10.21 (9.61-10.81)				
			K562	14.62 (13.52-15.72)				
			HEK293	42.05 (38.38-45.72)				
A549	27.07 (24.08-31.99)							

			A2780	29.44 (26.79-32.09)				
22	Tetrabutylammonium chloride (C ₄) ₄ N Cl	277.921	U937	8.99 (7.89-10.09)	1.95	9.48	27.41	0.74
			Jurkat	5.39 (4.69-6.09)				
			HL60	1.79 (1.59-1.99)				
			K562	12.59 (11.39-13.79)				
			HEK293	25.34 (23.21-27.47)				
			A549	12.95 (11.81-14.09)				
			A2780	12.97 (11.82-14.12)				
23	Tetrabutylammonium tetrafluoroborate (C ₄) ₄ N BF ₄	329.275	U937	8.54 (7.94-9.14)	4.69	22.07	39.20	0.59
			Jurkat	4.96 (4.56-5.36)				
			HL60	2.23 (2.13-2.33)				
			K562	8.37 (7.77-8.97)				
			HEK293	27.52 (24.81-30.23)				
			A549	16.76 (15.48-18.04)				
A2780	11.65 (10.65-12.74)							
24	Cholinium acetate Chol OAc	163.21	U937	137.77 (130.87-144.67)	5.50	37.71	60.75	0.88
			Jurkat	153.09 (146.34-159.84)				
			HL60	100.40 (94.59-106.21)				
			K562	86.62 (82.94-90.3)				
			HEK293	256.15 (232.39-279.91)				
			A549	143.14 (127.96-158.32)				
A2780	149.1 (133.79-164.41)							
25	Cholinium bis(trifluoromethylsulfonyl)imide Chol NTf ₂	384.308	U937	7.24 (6.74-7.74)	7.66	13.64	44.32	1.15
			Jurkat	5.21 (4.81-5.61)				
			HL60	3.12 (2.82-3.42)				
			K562	7.28 (6.78-7.78)				
			HEK293	24.33 (22.96-25.7)				
			A549	13.40 (12.16-14.64)				
A2780	15.15 (14.03-16.27)							
	Valinomycin		Jurkat	0.002	34.52	5.87	N/A	25.36
	CCCP			0.050	17.37	92.20	N/A	1.10
	Staurosporine			0.002	63.74	70.34	30.82	0.24

	Living cells		-	1.52	1.49	5.82	0.18
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^a Incubation time – 2 h.

^b Incubation time – 4 h.

CC₅₀, half-maximal cytotoxicity concentration; CCCP, carbonyl cyanide *m*-chlorophenyl hydrazone; N/A, data not available.