

Supplementary Information

High-Throughput Toxicity Screening of Novel Azepanium and 3-Methylpiperidinium Ionic Liquids

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Table S1. CHNS data for ionic liquids studied in this work.

Ionic liquid		C	H	N	S
[C ₄ mazp][NTf ₂]	Found	34.7	5.1	6.2	14.3
	Calcd.	34.66	5.37	6.22	14.24
[C ₆ mazp][I]	Found	47.9	8.2	4.2	-
	Calcd.	48	8.68	4.31	-
[C ₆ mazp][TFA]	Found	57	8.9	4.45	
	Calcd.	57.86	9.06	4.5	
[MeOC ₂ mazp][TFA]	Found	50	7.6	4.95	-
	Calcd.	50.52	7.77	4.91	-
[MeOC ₂ mazp][CF ₃ SO ₃]	Found	41.2	6.6	4.6	10.3
	Calcd.	41.11	6.9	4.36	10
[MeOC ₂ mazp][NTf ₂]	Found	32.1	5.2	6.1	14.5
	Calcd.	31.86	4.9	6.19	14.17
[MeOC ₂ OC ₂ mazp][I]	Found	42.35	7.3	4.1	-
	Calcd.	41.99	7.63	4.08	-
[MeOC ₂ OC ₂ mazp][CF ₃ SO ₃]	Found	42.4	6.8	4.2	8.75
	Calcd.	42.73	7.17	3.83	8.78
[MeOC ₂ OC ₂ mazp][NTf ₂]	Found	34	5.2	5.8	13.2
	Calcd.	33.87	5.28	5.64	12.92
[C ₄ mm _β pip][I]	Found	44.2	7.6	4.7	-
	Calcd.	44.45	8.14	4.71	-
[C ₄ mm _β pip][NTf ₂]	Found	34.9	5.4	6.2	14.9
	Calcd.	34.66	5.37	6.22	14.24
[C ₆ mm _β pip][I]	Found	48	8.4	4.3	-
	Calcd.	48	8.68	4.31	-
[C ₆ mm _β pip][NTf ₂]	Found	37.6	5.9	5.9	13.3
	Calcd.	37.65	5.9	5.85	13.4
[MeOC ₂ mm _β pip][TFA]	Found	50	8.05	5.1	-
	Calcd.	50.52	7.77	4.91	-
[MeOC ₂ mm _β pip][CF ₃ SO ₃]	Found	40.7	7.4	4.2	9.9
	Calcd.	41.11	6.9	4.36	9.98
[MeOC ₂ OC ₂ mm _β pip][I]	Found	41.7	7.95	4	-
	Calcd.	41.99	7.63	4.08	-

[MeOC ₂ OC ₂ mm _β pip][TFA]	Found	49.5	8.6	4.1	-
	Calcd.	51.05	7.96	4.25	-
[MeOC ₂ OC ₂ mm _β pip][CF ₃ SO ₃]	Found	42.3	6.8	3.6	8.9
	Calcd.	42.73	7.17	3.83	8.78
[MeOC ₂ OC ₂ mm _β pip][NTf ₂]	Found	34	5.4	5.2	13.3
	Calcd.	33.87	5.28	5.64	12.92
