## 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   |
|-------------------------------|-----|-----|-----|-----|
| [C₄mazp][NTf₂]                |     |     |     |     |
| Found                         | 34.7| 5.1 | 6.2 | 14.3|
| Calcd.                        | 34.66| 5.37| 6.22| 14.24|
| [C₆mazp][I]                   |     |     |     |     |
| Found                         | 47.9| 8.2 | 4.2 | -   |
| Calcd.                        | 48  | 8.68| 4.31| -   |
| [C₆mazp][TFA]                 |     |     |     |     |
| Found                         | 57  | 8.9 | 4.45| -   |
| Calcd.                        | 57.86| 9.06| 4.5 | -   |
| [MeOC₂mazp][TFA]              |     |     |     |     |
| Found                         | 50  | 7.6 | 4.95| -   |
| Calcd.                        | 50.52| 7.77| 4.91| -   |
| [MeOC₂mazp][CF₃SO₃]           |     |     |     |     |
| Found                         | 41.2| 6.6 | 4.6 | 10.3|
| Calcd.                        | 41.11| 6.9 | 4.36| 10  |
| [MeOC₂mazp][NTf₂]             |     |     |     |     |
| Found                         | 32.1| 5.2 | 6.1 | 14.5|
| Calcd.                        | 31.86| 4.9 | 6.19| 14.17|
| [MeOC₂OC₂mazp][I]             |     |     |     |     |
| Found                         | 42.35| 7.3 | 4.1 | -   |
| Calcd.                        | 41.99| 7.63| 4.08| -   |
| [MeOC₂OC₂mazp][CF₃SO₃]        |     |     |     |     |
| Found                         | 42.4| 6.8 | 4.2 | 8.75|
| Calcd.                        | 42.73| 7.17| 3.83| 8.78|
| [MeOC₂OC₂mazp][NTf₂]          |     |     |     |     |
| Found                         | 34  | 5.2 | 5.8 | 13.2|
| Calcd.                        | 33.87| 5.28| 5.64| 12.92|
| [C₄mmₜpip][I]                |     |     |     |     |
| Found                         | 44.2| 7.6 | 4.7 | -   |
| Calcd.                        | 44.45| 8.14| 4.71| -   |
| [C₄mmₜpip][NTF₂]              |     |     |     |     |
| Found                         | 34.9| 5.4 | 6.2 | 14.9|
| Calcd.                        | 34.66| 5.37| 6.22| 14.24|
| [C₆mmₜpip][I]                |     |     |     |     |
| Found                         | 48  | 8.4 | 4.3 | -   |
| Calcd.                        | 48  | 8.68| 4.31| -   |
| [C₆mmₜpip][NTF₂]              |     |     |     |     |
| Found                         | 37.6| 5.9 | 5.9 | 13.3|
| Calcd.                        | 37.65| 5.9 | 5.85| 13.4|
| [MeOC₂mmₜpip][TFA]            |     |     |     |     |
| Found                         | 50  | 8.05| 5.1 | -   |
| Calcd.                        | 50.52| 7.77| 4.91| -   |
| [MeOC₂mmₜpip][CF₃SO₃]         |     |     |     |     |
| Found                         | 40.7| 7.4 | 4.2 | 9.9 |
| Calcd.                        | 41.11| 6.9 | 4.36| 9.98|
| [MeOC₂OC₂mmₜpip][I]           |     |     |     |     |
| Found                         | 41.7| 7.95| 4  | -   |
| Calcd.                        | 41.99| 7.63| 4.08| -   |
| Compound                  | Found  | Calcd. | | | |
|---------------------------|--------|--------|--------|--------|--------|
| [MeOC₂OC₂mm₃pip][TFA]     | 49.5   | 51.05  | 8.6    | 7.96   | 4.1    | 4.25   | -      |
| [MeOC₂OC₂mm₃pip][CF₃SO₃] | 42.3   | 42.73  | 6.8    | 7.17   | 3.6    | 3.83   | 8.9    |
| [MeOC₂OC₂mm₃pip][NTf₂]   | 34     | 33.87  | 5.4    | 5.28   | 5.2    | 5.64   | 13.3   |
|                           |        |        |        |        |        |        | 12.92  |