# A Quantum-Chemical-Based Guide to Analyze/Quantify the Cytotoxicity of Ionic Liquids

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**Table S1**. Nomenclature.

| **Substituent (R)** | **Abbreviation** |
|---|---|
| Methyl | M |
| Ethyl | E |
| Propyl | Pr |
| Butyl | B |
| Pentyl | Pn |
| Hexyl | Hx |
| Heptyl | Hp |
| Octyl | O |
| Nonyl | N |
| Decyl | D |
| Dodecyl | Dod |
| Tetradecyl | Ted |
| Hexadecyl | Hxd |
| Octadecyl | Ocd |
| Hydroxy | OH |
| 2-Hydroxypropyl | OHPr |
| 2-Hydroxyoctyl | OHO |
| 2-Ethoxyethyl | EOE |
| 2-Methoxyethyl | MeOE |
| 2-Methoxypropyl | MeOPr |
| Phenylethyl | PhE |
| Phenylmethyl | PhM |
| Dimethylamino | $NMe_2$ |
| **Head Group** | **Abbreviation** |
| 1-R-3-methylimidazolium | Mim |
| 1-R-3-ethylimidazolium | Eim |
| 1-R-pyridinium | Pyr |
| 1-R-4-R'-pyridinium | 1R4R'Pyr |
| 1-R-3-R'-pyridinium | 1R3R'Pyr |
| 1-R-1-methylpyrrolidinium | Pyrr |
| 1-R-quinolinium | Quin |
| Phosphonium | P |
| Ammonium | N |
| **Anion** | **Abbreviation** |
| Bis[1,2-benzenediolate(2-)O1,O2] borate | $BBDB^-$ |
| Octylsulfate | $OcSO_4$ |
| Ethylsulfate | $EtSO_4$ |
| Methylsulfate | $MeSO_4$ |
| bis(trifluoromethane sulfonimide) | $NTf_2$ |

**Table S2**. Calculated values of $S_{\sigma\text{-profile}}$ parameters for cations included in QSAR studies.

| **Cation** | **S (-0.011 e/Å$^2$)** | **S(-0.008 e/Å$^2$)** | **S(-0.006 e/Å$^2$)** | **S(-0.002 e/Å$^2$)** |
|---|---|---|---|---|
| Emim | 6.81 | 13.01 | 16.37 | 6.09 |
| Prmim | 6.70 | 13.41 | 15.59 | 9.64 |
| Bmim | 6.77 | 11.97 | 14.90 | 13.39 |
| Pnmim | 6.70 | 12.06 | 14.56 | 17.77 |
| Hmim | 6.69 | 12.45 | 14.13 | 22.10 |
| Hpmim | 6.73 | 12.44 | 14.10 | 25.94 |
| Omim | 6.80 | 12.38 | 14.15 | 29.47 |
| Nmim | 6.77 | 12.37 | 14.08 | 33.02 |
| Dcmim | 6.67 | 12.55 | 14.29 | 36.60 |
| Tetradmim | 6.69 | 12.23 | 14.40 | 50.36 |
| HexDmim | 6.70 | 12.22 | 14.42 | 57.23 |
| OctDmim | 6.70 | 12.24 | 14.46 | 63.99 |
| Heim | 7.18 | 15.48 | 15.14 | 23.17 |
| Beim | 6.38 | 11.33 | 16.63 | 16.17 |
| Dceim | 6.20 | 11.65 | 15.80 | 39.18 |
| EtOemim | 7.30 | 12.72 | 19.54 | 11.74 |
| MeOemim | 7.47 | 12.55 | 20.87 | 9.64 |
| MeOprmim | 7.66 | 12.46 | 20.45 | 12.81 |
| OHomim | 7.74 | 12.92 | 15.02 | 27.96 |
| OHprmim | 7.89 | 13.77 | 18.48 | 6.19 |
| PhEtmim | 7.05 | 16.74 | 21.44 | 10.15 |
| PhMemim | 7.44 | 17.59 | 18.37 | 8.36 |
| Epyr | 10.61 | 12.51 | 14.16 | 11.05 |
| Prpyr | 10.12 | 11.99 | 13.53 | 13.94 |
| Bpyr | 10.03 | 11.60 | 12.61 | 17.54 |
| Pnpyr | 10.03 | 11.57 | 12.15 | 21.85 |
| Hxpyr | 10.05 | 11.52 | 12.12 | 26.00 |
| Hppyr | 10.06 | 11.51 | 12.06 | 30.07 |
| Opyr | 10.03 | 11.50 | 12.15 | 33.67 |
| 1O4MPyr | 7.72 | 12.23 | 15.94 | 37.19 |
| 1B4MPyr | 7.93 | 12.21 | 16.76 | 21.05 |
| 1B3MPyr | 7.75 | 11.92 | 16.92 | 20.66 |
| NM4 | 11.62 | 14.05 | 12.51 | 0.29 |
| NE4 | 4.62 | 17.46 | 26.49 | 10.72 |
| NPr4 | 3.70 | 13.45 | 24.28 | 21.17 |
| NB4 | 3.22 | 12.38 | 21.51 | 36.27 |
| NPn4 | 3.93 | 10.73 | 21.46 | 52.26 |
| NHx4 | 3.72 | 10.79 | 20.66 | 70.79 |
| OH-EM2N | 9.69 | 12.44 | 10.21 | 1.57 |
| BuM3N | 9.00 | 14.76 | 14.85 | 9.35 |
| BuEM2N | 6.84 | 16.18 | 18.12 | 12.19 |
| Et4P | 3.75 | 17.58 | 22.49 | 12.21 |
| Pr4P | 5.49 | 12.64 | 22.20 | 22.19 |
| But4P | 5.08 | 11.02 | 19.34 | 36.91 |
| Pn4P | 4.92 | 11.09 | 17.99 | 54.75 |
| Hx4P | 4.92 | 10.96 | 17.65 | 70.75 |
| Hx3MP | 4.14 | 10.56 | 18.23 | 100.72 |
| Bquin | 8.35 | 16.22 | 15.46 | 20.18 |
| Hxquin | 8.38 | 16.15 | 14.82 | 28.55 |
| Oquin | 8.34 | 16.10 | 14.76 | 36.73 |
| Bpyrr | 8.56 | 7.21 | 10.15 | 13.80 |
| Morpholinium | 6.95 | 16.42 | 14.23 | 10.94 |
| Na | 38.08 | 0.00 | 0.00 | 0.00 |

**Table S3**. Calculated values of $S_{\sigma\text{-profile}}$ parameters for anion included in QSAR studies.

| Anion | S (-0.002 e/Å$^2$) | S(0.009 e/Å$^2$) | S(0.011 e/Å$^2$) | S(0.015 e/Å$^2$) | S(0.017 e/Å$^2$) | S(0.019 e/Å$^2$) |
|---|---|---|---|---|---|---|
| BBDB | 20.32 | 1.98 | 0.00 | 0.00 | 0.00 | 0.00 |
| BF4 | 0.00 | 5.36 | 26.15 | 0.00 | 0.00 | 0.00 |
| Br | 0.00 | 0.00 | 0.00 | 0.27 | 29.11 | 0.06 |
| $CF_3CO_2$ | 0.38 | 2.55 | 1.81 | 4.14 | 8.47 | 3.53 |
| CF3SO3 | 0.35 | 1.40 | 6.13 | 9.61 | 0.30 | 0.00 |
| $CH_3CO_2$ | 3.89 | 0.99 | 1.35 | 1.57 | 2.24 | 6.16 |
| CH3SO3 | 3.21 | 1.14 | 3.50 | 5.93 | 14.95 | 6.32 |
| (C2F5)3PF3 | 31.93 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| Cl | 0.00 | 0.00 | 0.00 | 0.00 | 0.28 | 26.02 |
| Co(CO)4 | 6.05 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| DCN | 0.05 | 3.33 | 4.46 | 8.12 | 6.74 | 0.97 |
| $EtSO_4$ | 6.09 | 2.35 | 3.63 | 15.49 | 6.24 | 0.01 |
| F | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| HSO4 | 0.36 | 2.73 | 2.90 | 17.04 | 4.91 | 0.00 |
| MeSO4 | 4.33 | 2.55 | 3.67 | 15.69 | 5.67 | 0.01 |
| N(CF3)2 | 4.21 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| $NTf_2$ | 2.57 | 12.29 | 17.35 | 0.00 | 0.00 | 0.00 |
| OctSO4 | 29.96 | 2.36 | 3.50 | 15.45 | 6.24 | 0.01 |
| PF6 | 0.00 | 38.55 | 6.54 | 0.00 | 0.00 | 0.00 |
| SCN | 0.00 | 6.52 | 7.58 | 5.07 | 3.79 | 1.64 |

**Table S4**. Ionic liquids included in the external validation sample

| | | $S_{\sigma\text{-profile}}$ cation | | | | $S_{\sigma\text{-profile}}$ anion | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Cation** | **Anion** | **-0.011** | **-0.008** | **-0.006** | **-0.002** | **-0.002** | **0.009** | **0.011** | **0.015** | **0.017** | **0.019** |
| 1Bu4N$Me_2$Pyr | NTf2 | 7.0 | 15.7 | 16.9 | 25.9 | 2.6 | 12.3 | 17.4 | 0.0 | 0.0 | 0.0 |
| 1Bu4N$Me_2$Pyr | Cl | 7.0 | 15.7 | 16.9 | 25.9 | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 26.0 |
| 1Hx4N$Me_2$Pyr | NTf2 | 6.9 | 15.7 | 16.4 | 34.6 | 2.6 | 12.3 | 17.4 | 0.0 | 0.0 | 0.0 |
| 1Hx4N$Me_2$Pyr | Cl | 6.9 | 15.7 | 16.4 | 34.6 | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 26.0 |
| 1Et4N$Me_2$Pyr | NTf2 | 7.2 | 16.6 | 18.2 | 18.8 | 2.6 | 12.3 | 17.4 | 0.0 | 0.0 | 0.0 |
| 1Et4N$Me_2$Pyr | Br | 7.2 | 16.6 | 18.2 | 18.8 | 0.0 | 0.0 | 0.0 | 0.3 | 29.1 | 0.1 |
| Bmim | Toluene-4-SO3 | 6.8 | 12.0 | 14.9 | 13.4 | 5.8 | 2.2 | 2.4 | 9.2 | 12.9 | 2.5 |
| Emim | Toluene-4-SO3 | 6.8 | 13.0 | 16.4 | 6.1 | 5.8 | 2.2 | 2.4 | 9.2 | 12.9 | 2.5 |
| Na | Toluene-4-SO3 | 38.1 | 0.0 | 0.0 | 0.0 | 5.8 | 2.2 | 2.4 | 9.2 | 12.9 | 2.5 |
| 1Hx4Mepyr | BF4 | 8.0 | 12.0 | 16.1 | 29.3 | 0.0 | 5.4 | 26.2 | 0.0 | 0.0 | 0.0 |
| Octpyrr | BF4 | 8.3 | 7.3 | 9.2 | 30.7 | 0.0 | 5.4 | 26.2 | 0.0 | 0.0 | 0.0 |
| Octpyrr | Cl | 8.3 | 7.3 | 9.2 | 30.7 | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 26.0 |
| Hxpyrr | Cl | 8.5 | 7.3 | 9.3 | 22.5 | 0.0 | 0.0 | 0.0 | 0.0 | 0.3 | 26.0 |
| 1Me3Him | BF4 | 6.1 | 9.1 | 9.5 | 3.5 | 0.0 | 5.4 | 26.2 | 0.0 | 0.0 | 0.0 |
| 1Et3Prim | Br | 6.3 | 11.4 | 17.8 | 12.1 | 0.0 | 0.0 | 0.0 | 0.3 | 29.1 | 0.1 |