

Ionic liquids with boron-based anions - stability, lipophilicity and toxicity

Euroboron 4

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University of Bremen/D

What are ionic liquids?

Ionic liquids are salts with a low melting point.

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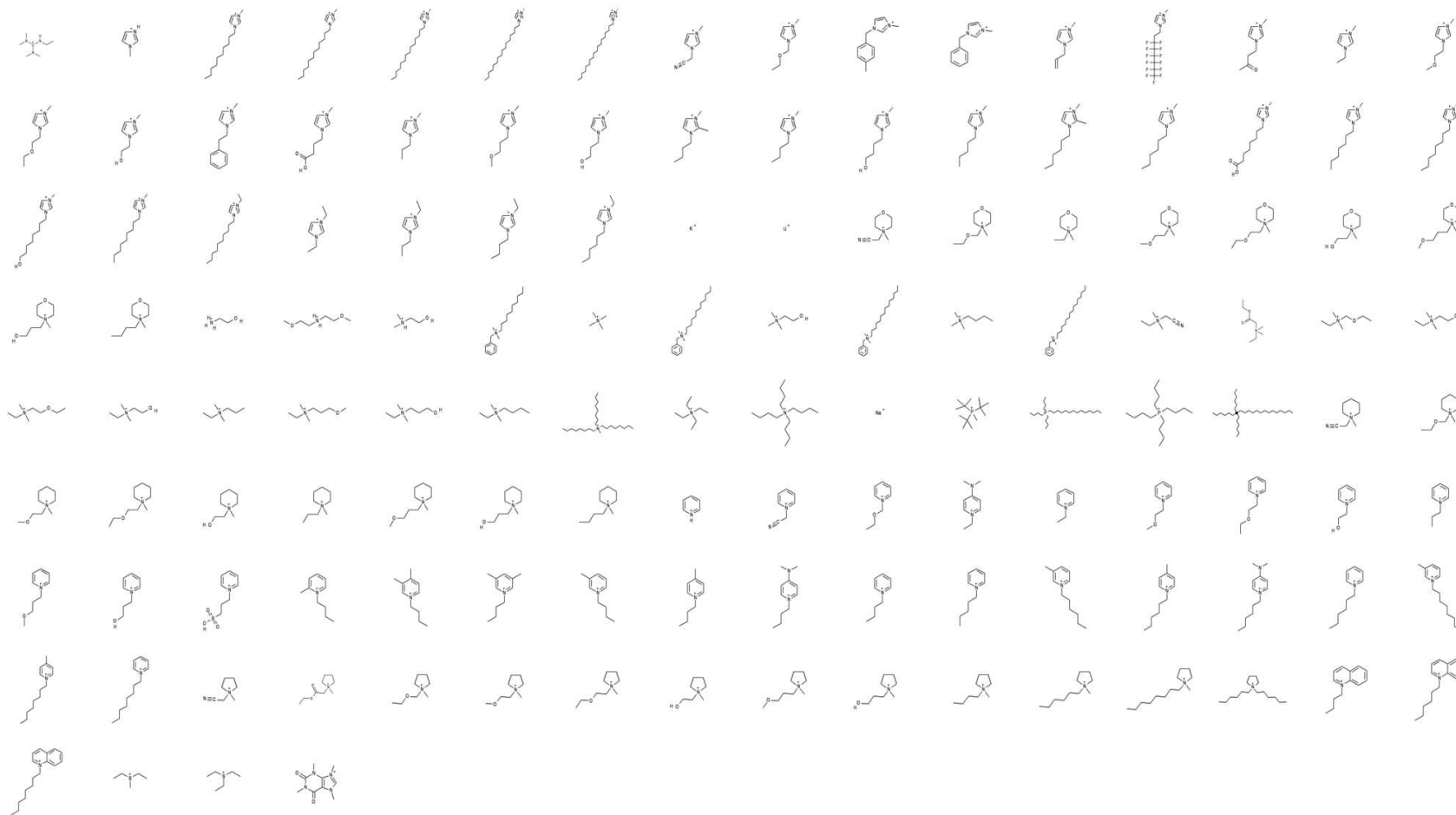
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⇒ Designer solvents of the future?

Overview of IL cations

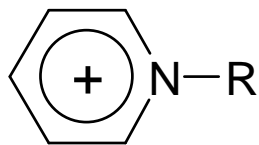


UFT IL substance library

IL cation head groups



1-Methylimidazolium

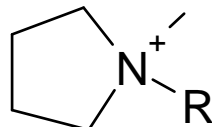


Pyridinium

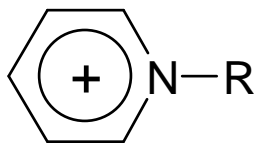
IL cation head groups



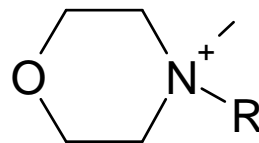
1-Methylimidazolium



N-Methylpyrrolidinium



Pyridinium

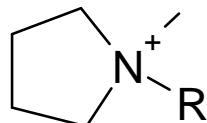


N-Methylmorpholinium

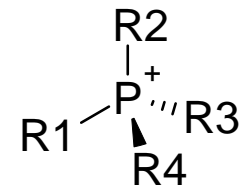
IL cation head groups



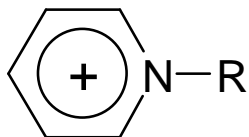
1-Methylimidazolium



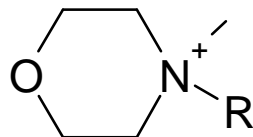
N-Methylpyrrolidinium



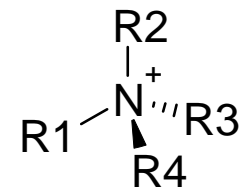
Phosphonium



Pyridinium

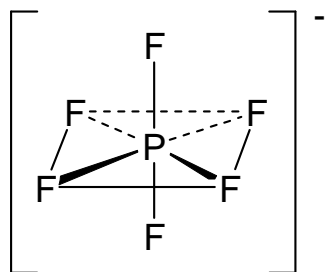


N-Methylmorpholinium

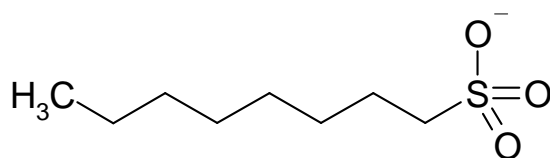


Ammonium

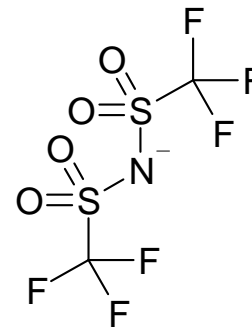
Popular and boron based IL anions



Hexafluorophosphate

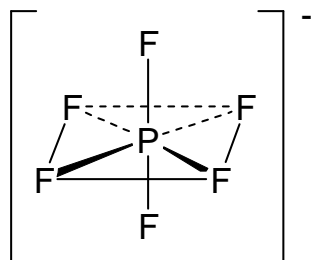


Octylsulfate

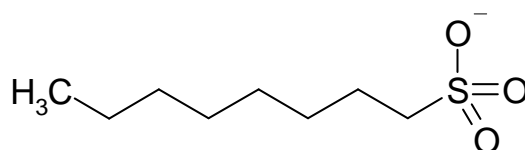


Bistriflamide

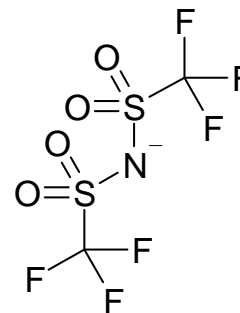
Popular and boron based IL anions



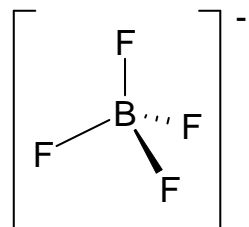
Hexafluorophosphate



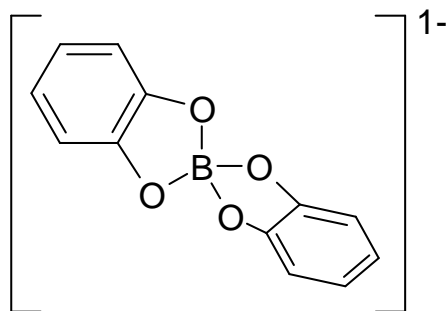
Octylsulfate



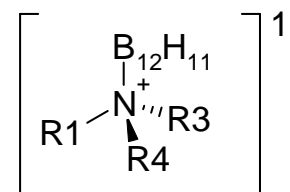
Bistriflamide



Tetrafluoroborate



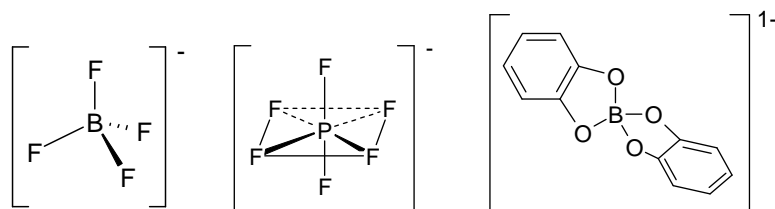
Bis(benzenediolato)borate



Trialkylamino-closo-dodecaborate

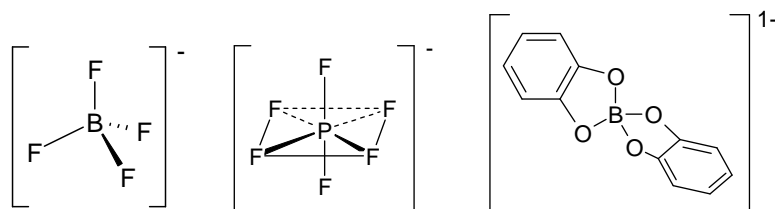
Anion stability

- Some anions are not completely water-stable:

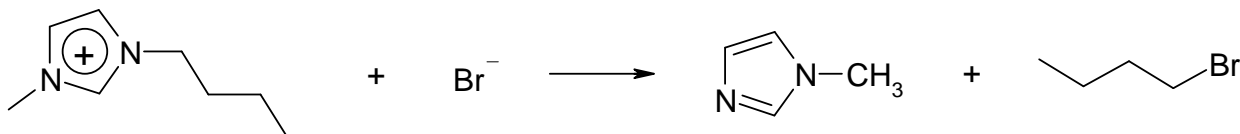


Anion stability

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- Nucleophilic anions have a tendency to cause reverse Menshutkin reactions:

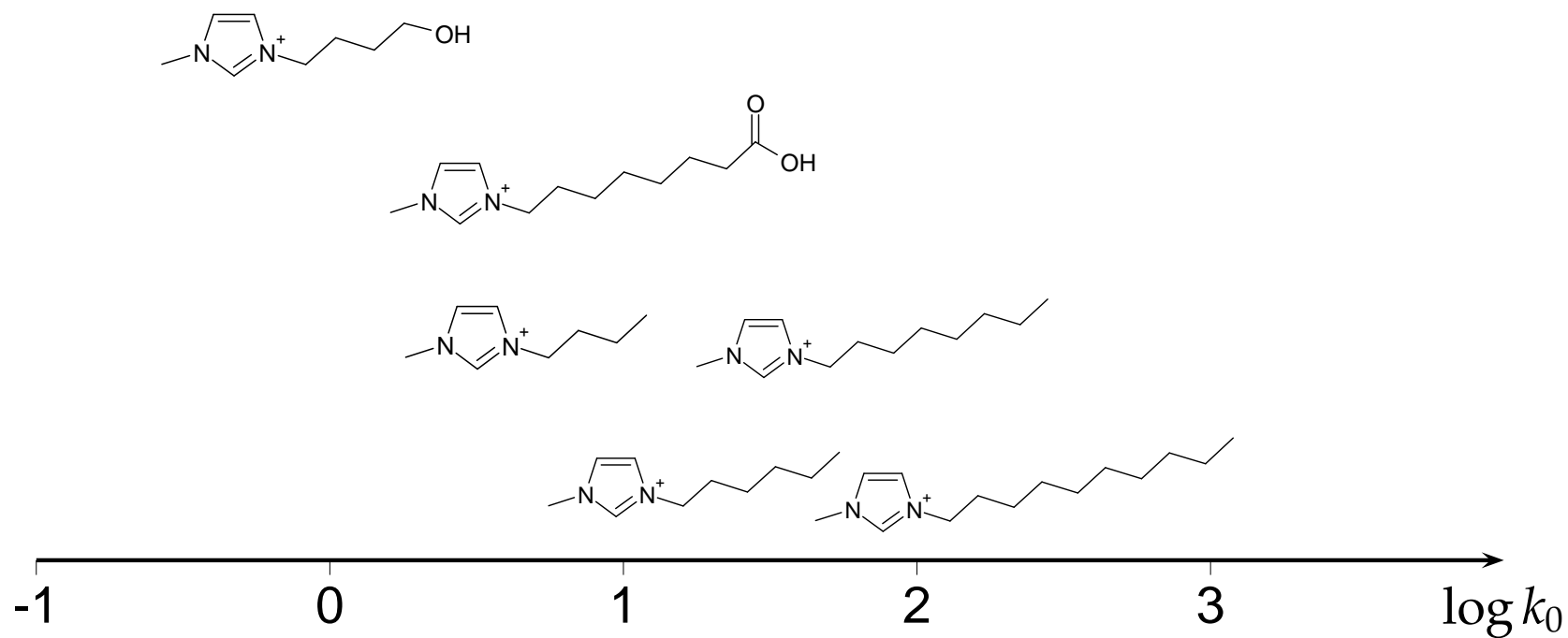


Cation lipophilicity



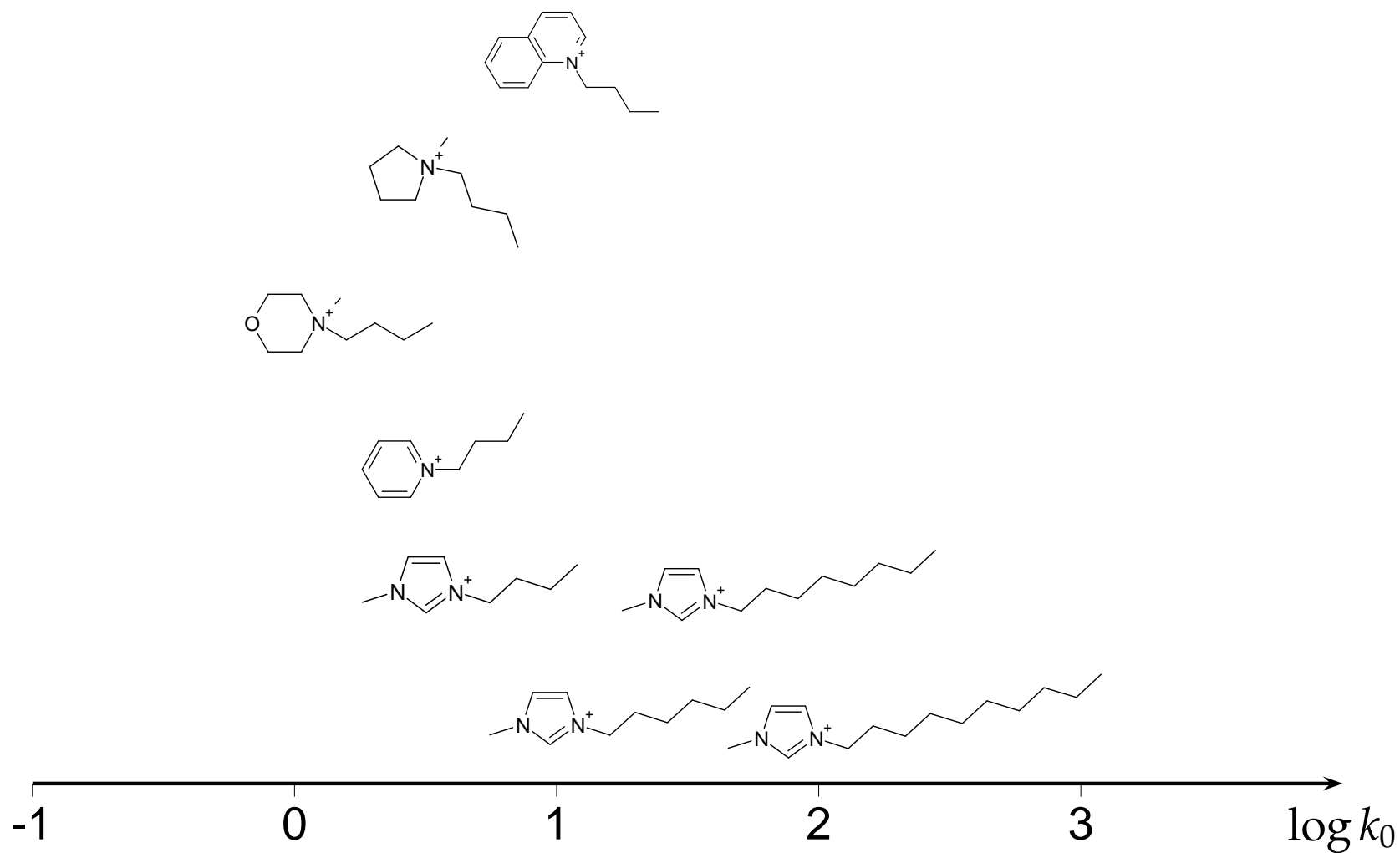
Data from Ranke et al. (2007) *Ecotoxicol Environ Safety* **67** 430

Cation lipophilicity



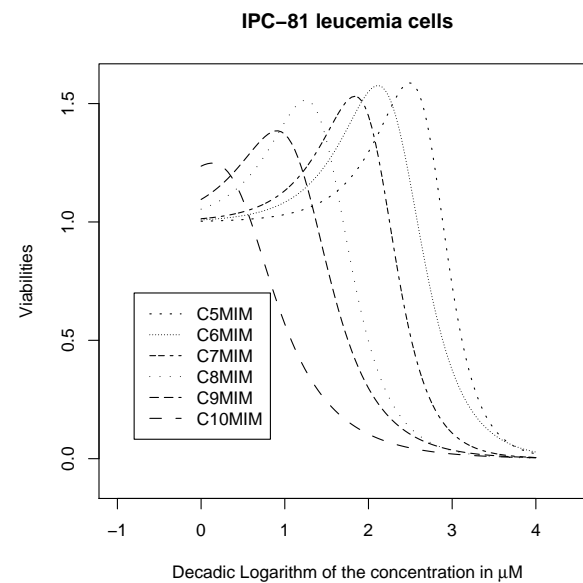
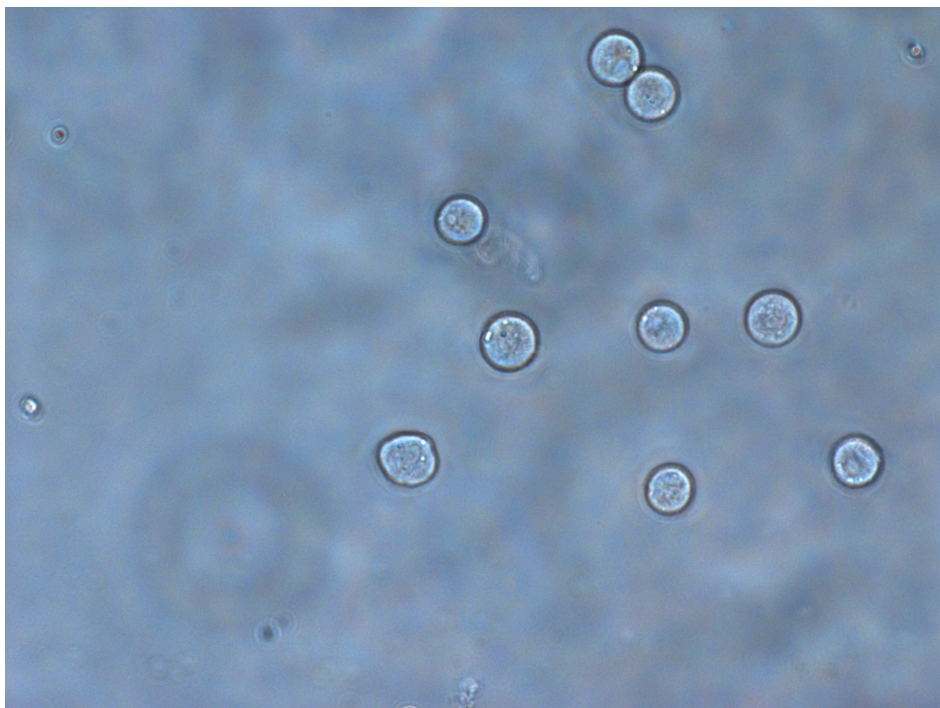
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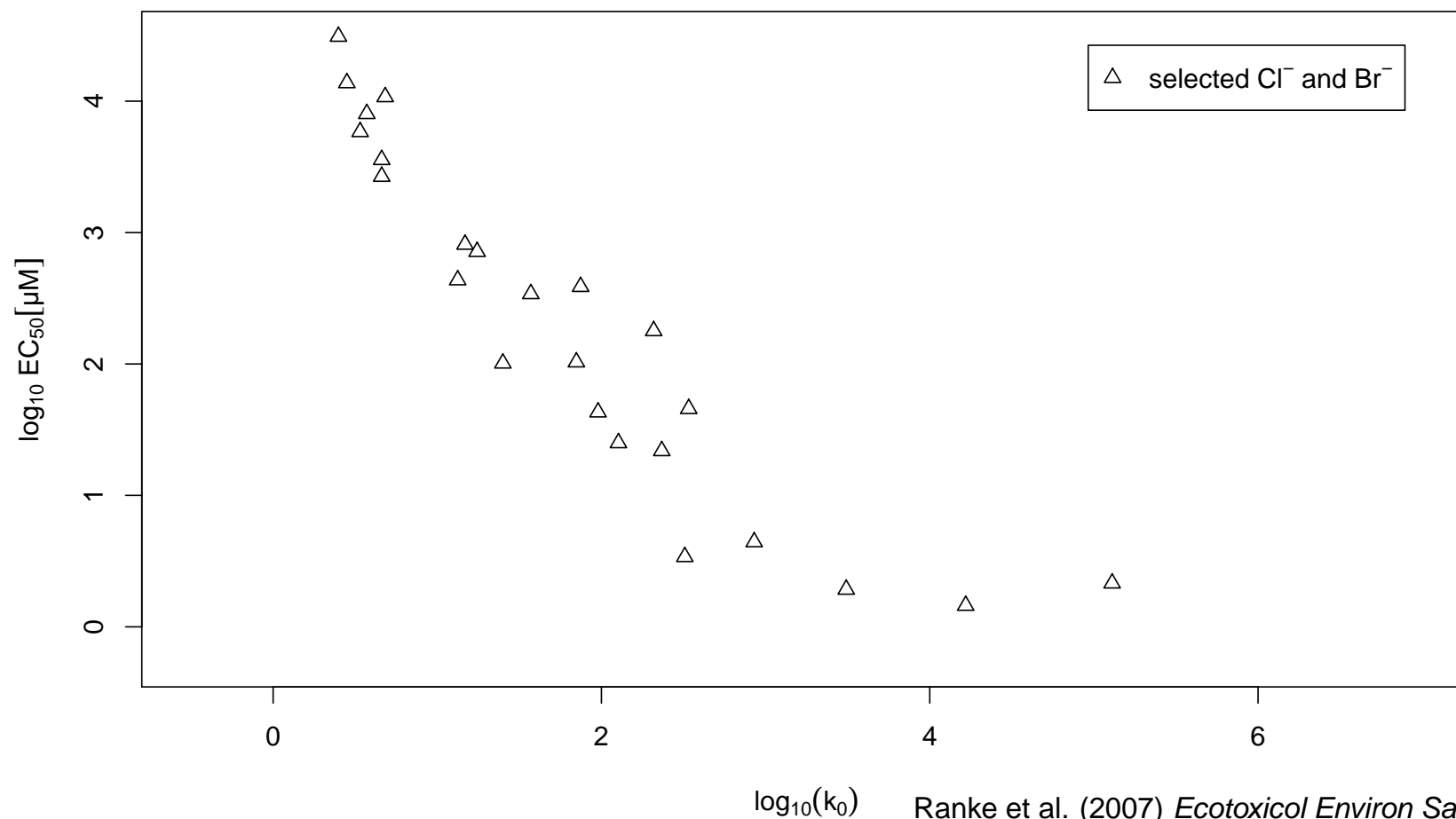
Cell viability assay



Ranke et al. *Ecotoxicol Environ Safety* **2004** 58 396-404

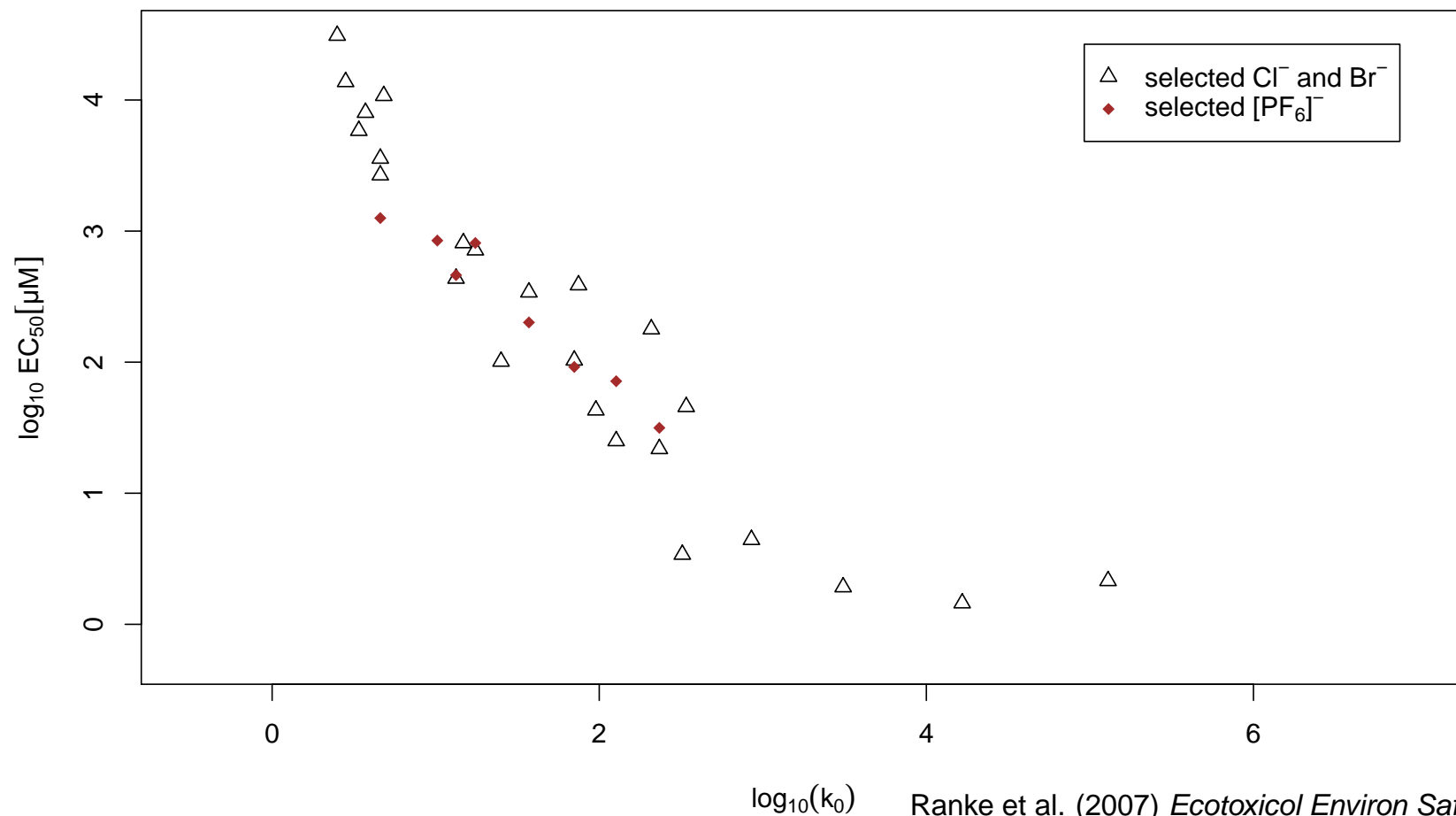
Stolte et al. *Green Chem* **2006** 8 621-629

Cation lipophilicity and cytotoxicity



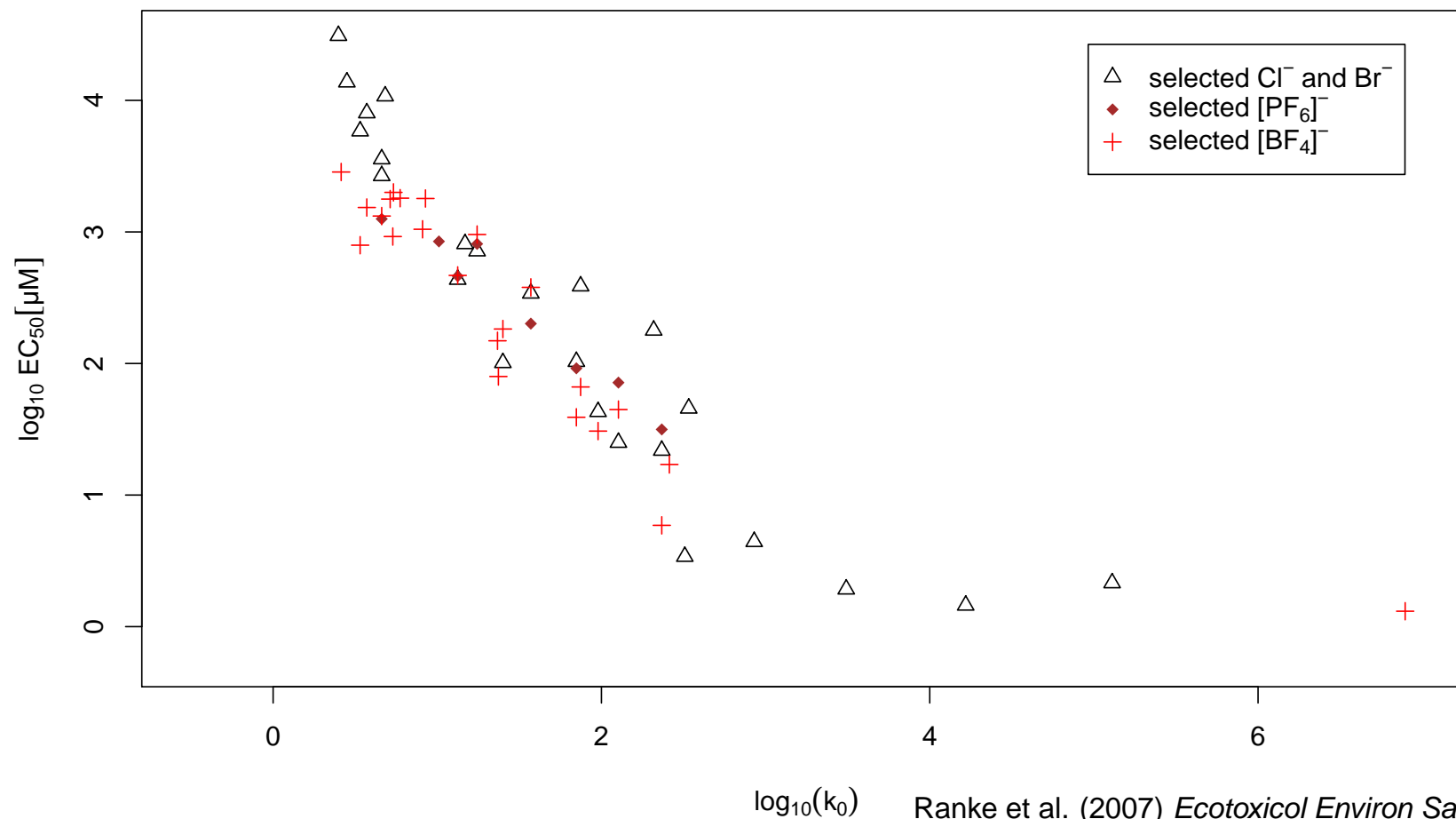
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Stolte et al. (2007) *Green Chem* **9** 760

Cation lipophilicity and cytotoxicity



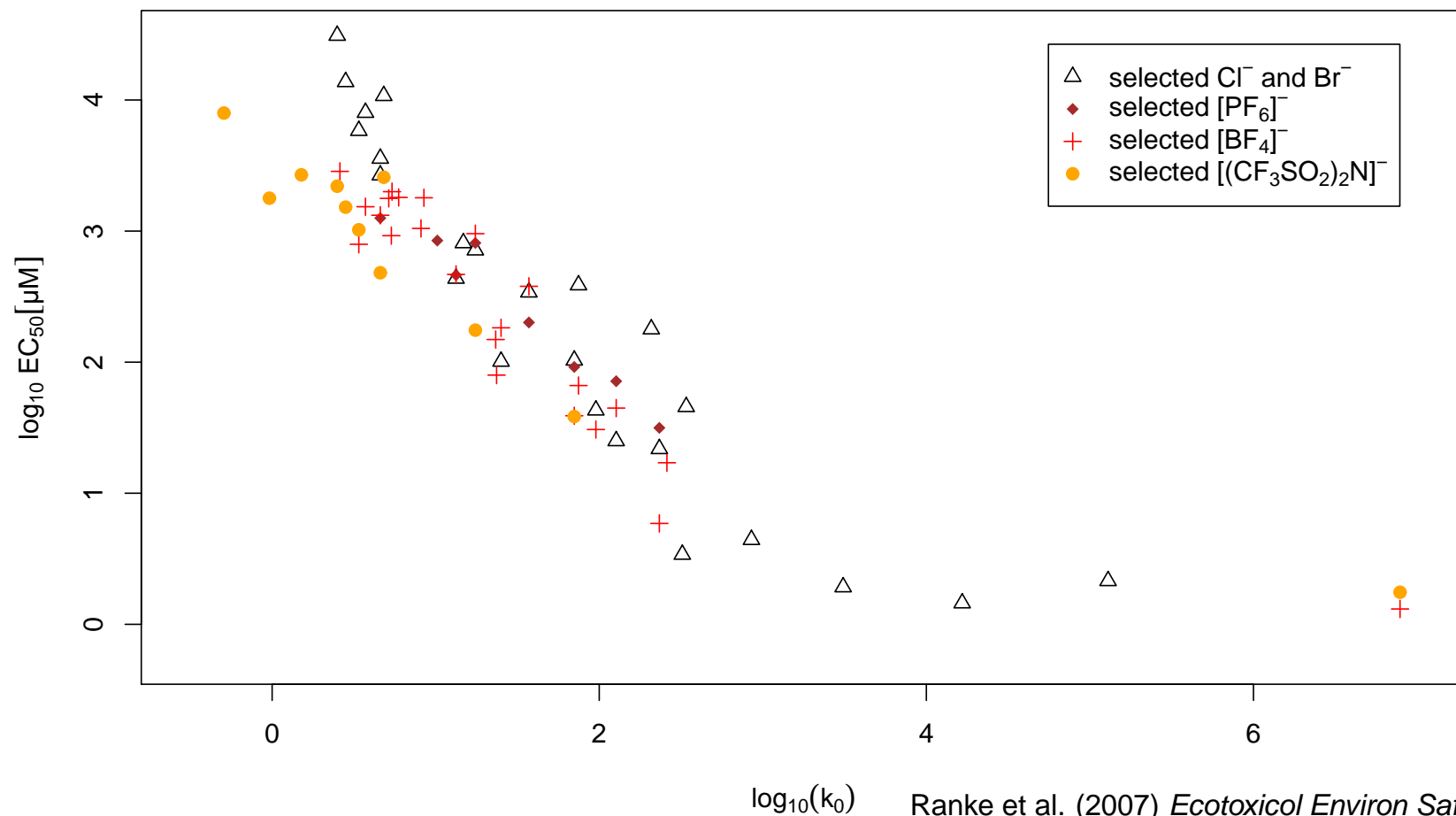
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Cation lipophilicity and cytotoxicity



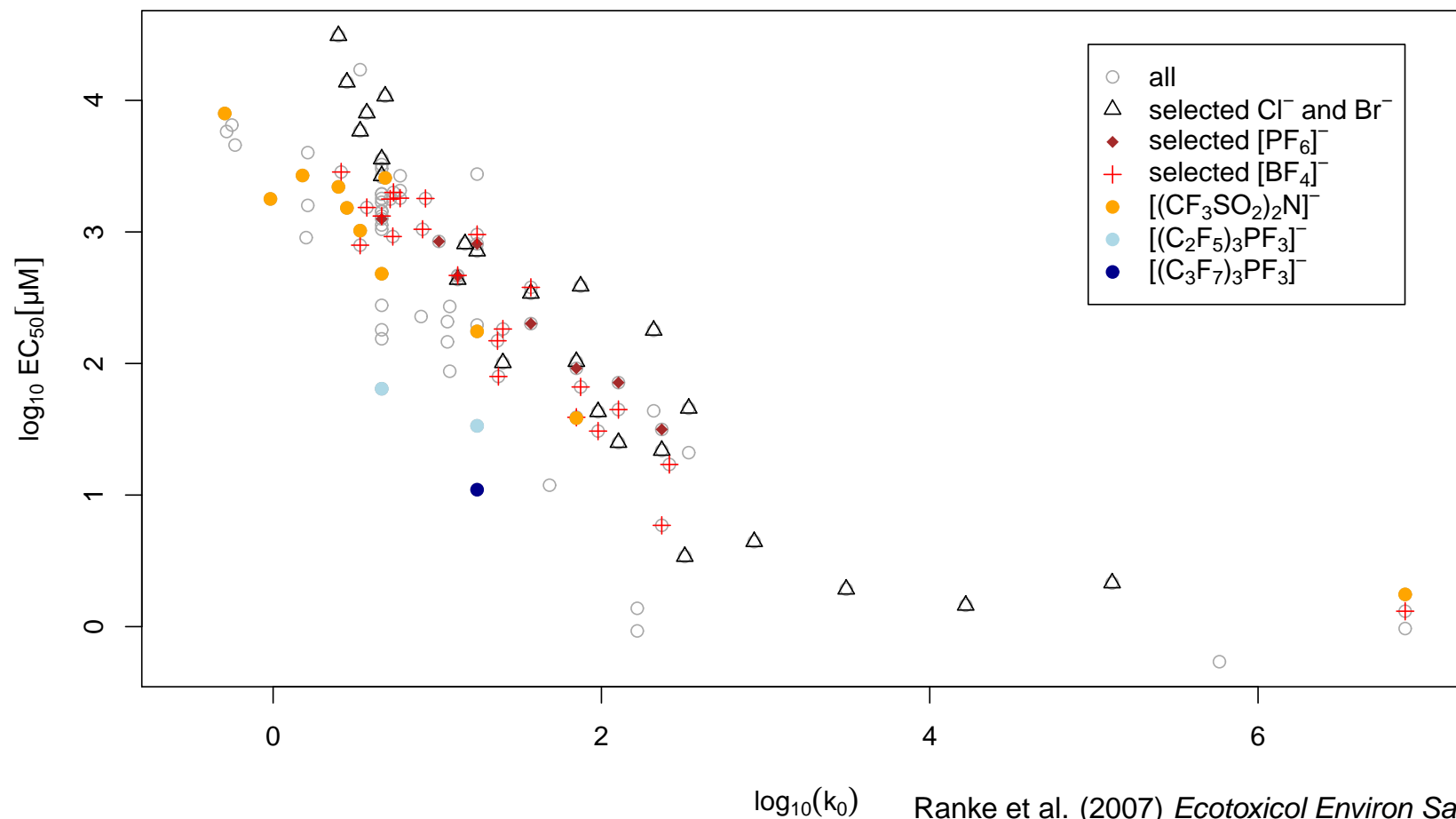
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Cation lipophilicity and cytotoxicity

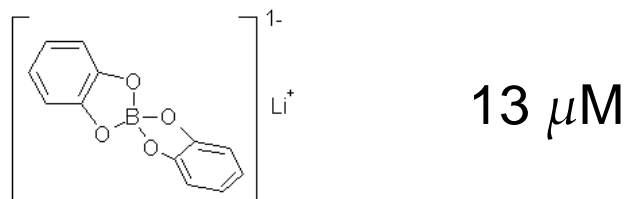
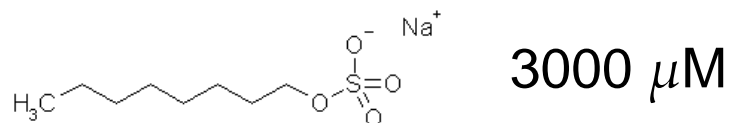
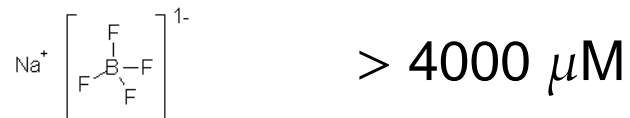


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Cation lipophilicity and cytotoxicity

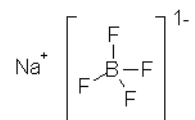


Anion cytotoxicities

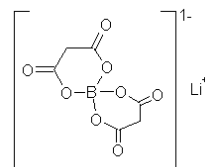


Stolte et al. (2006) *Green Chem* **8** 621

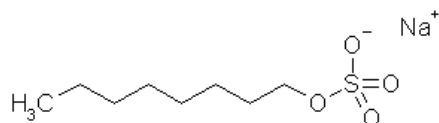
Anion cytotoxicities



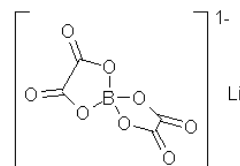
> 4000 μM



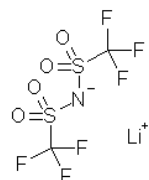
2700 μM



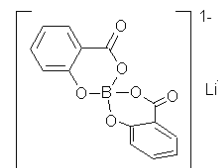
3000 μM



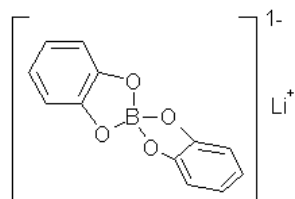
740 μM



2200 μM



210 μM

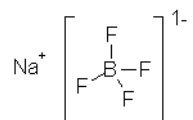


13 μM

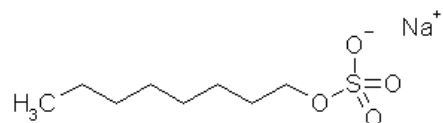
Stolte et al. (2006) *Green Chem* **8** 621

plus unpublished data

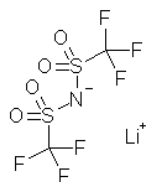
Anion cytotoxicities



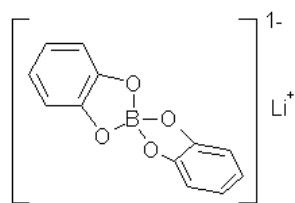
> 4000 μM



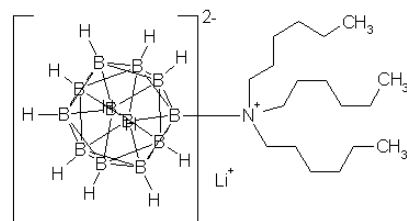
3000 μM



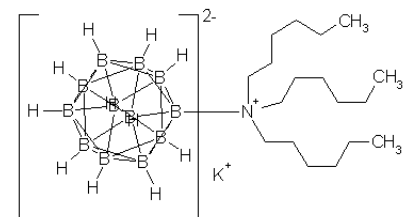
2200 μM



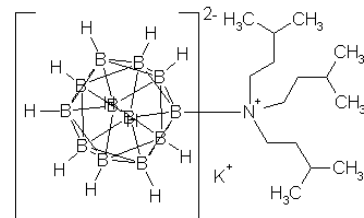
13 μM



51 μM



54 μM



59 μM

Stolte et al. (2006) *Green Chem* **8** 621

plus unpublished data

Conclusions

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- the tetrafluoroborate anion has only a moderate influence on cytotoxicity
- with borate ester or anhydride anions, cytotoxicity is difficult to predict
- with trialkylammonio-undecahydro-closo-dodecaborate anions a considerable contribution of the anion to cytotoxicity is to be expected

Acknowledgments

- Coauthors
- Prof. Detlev Gabel and his group
- Merck KGaA, Darmstadt
- FSU Jena
- IOLITEC, Solvent innovation and other cooperation partners

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