

The interaction of room temperature ionic liquids with phospholipid bilayers: a computational investigation

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Abstract

A vast number of new chemical compounds are screened every year to assess their toxicity or to search for new pharmaceutical principles. In this respect, the first relevant aspect arguably is the interaction of the new compound with biological membranes. A case in point is represented by the interaction between biomembranes and room temperature ionic liquids (IL), which are a large class of organic ionic compounds whose melting temperature falls below 100 °C. As well as their potential for use as pharmacological agents, these compounds are the crucial ingredient of innovative approaches (Green chemistry) meant to decrease the environmental impact of industrial processes. However, recent experiments carried out on model bio-membranes have shown that, at sufficiently high concentration, several IL's damage or even destroy phospholipid bilayers. The observation refers to concentrations far above those expected from industrial processes, but the interaction of IL's and phospholipids remains an important issue to be explored in detail.

Biomembrane simulations are at present one of the most active subjects of computational biophysics. Computer simulations, in particular, are being used to determine the phase diagram, mechanical and dynamical properties and even the formation process of lipid bilayers. For reasons of computational complexity, much less has been done to investigate the interaction of membranes and third chemical species in solution, which, however, is a crucial aspect for many biotechnology and health applications. The proposed simulations of a phospholipid bilayer in contact with ionic liquid aqueous solutions will complement ongoing lab experiments and could pave the way to important new applications.