Preliminary assesment of the bioaccumulation of ionic liquids using *in vitro* method

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Bioaccumulation is of the highest concern for environmental risk assessment of chemicals, since it is known to cause far-reaching hazards to wildlife and human health. Generally, the experimental measurement of bioaccumulation is time-consuming, expensive, and due to ethical concerns regarding animal welfare not feasible for large sets of chemicals. Thus prediction models - mainly based on easily determinable physicochemical properties such as the octanol-water partition coefficient - are usually used. However the existing prediction models often give inappropriate and inaccurate results for ionogenic compounds and permanently charged organic chemicals. This is due to the fact that classical bioaccumulation models neither sufficiently consider ion–macromolecule interactions nor interactions of cations and anions in solution - both strongly influencing the transport, uptake and bioavailability of ions.
Ionic liquids (ILs) have become a very interesting alternative to conventional organic solvents due to their unique feature. This is their possibility to be “designed for the process” for certain chemical/technological requirements. Hence, properties of ILs such as viscosity, density, miscibility with water or other solvents, can be tuned by the appropriate modification of cation and anion. Moreover, the majority of ILs are generally thermally stable, have insignificantly negligible volatility and are non-flammable. It leads to application in a variety of industrial processes; they are used as media for organic synthesis and biocatalysis, as alternative electrolytes, as phases and phase modifications in separation techniques, dissolution and recovery of cellulose, separation of products in biphasic systems, and as alternative lubricants. However, the current implementation of ILs on technological scale causes a danger of possible contamination of natural environment by these compounds.
Therefore the main aim of this study was to understand and predict the interactions of organic ions, and ion pairs in particular, with *in vitro* biological systems and their consequences in terms of bioaccumulation. Since lipids are generally regarded as the predominant biomolecules involved in the absorption and accumulation processes of chemicals the assessment of membrane lipids was performed for different cations, anions and various combinations. The experiment was performed using commercially available systems consist of unilamellar lipid membranes that are non-covalently bound to porous silica beads (SSLM).