P021 Protein structure and dynamics in ionic liquids. Insights from molecular dynamics simulation studies

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We present in this work a molecular modelling study of an enzyme, the serine protease named cutinase from Fusarium solani pisi, in two room temperature ionic liquids (RTILs): 1-butyl-3-methylimidazolium hexafluorophosphate and 1-butyl-3-methylimidazolium nitrate. RTILs are organic salts that are liquid at room temperature and are composed solely by an organic cation and an organic or inorganic anion. A united atom model of these two RTILs has been developed in the framework of the GROMOS96 43A11 force field. In the outline of our molecular modelling research studies of enzymes in nonaqueous solvents we have recently addressed the molecular details of protein structure and dynamics in RTILs by means of molecular modelling methodologies.

It has been recently shown that enzymes are fully active in RTILs and in some case they show enhanced catalytic properties relative to the conventional organic solvents. We tested different enzyme hydration conditions in these two ionic liquids at room (298 K) and high temperature (343 K) conditions. We show that the enzyme is highly stable in [BMIM][PF6] especially at 5-10% (w/w) (weight of water over protein) water content at room temperature, whereas [BMIM][NO3] is shown to have a detrimental effect on enzyme structure confirming previous experimental observations.