Modelling of biomolecules in non-aqueous media

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Solvation is a crucial aspect of chemistry, particularly in biological contexts, where water, as the most prevalent native solvent, significantly impacts protein structure, dynamics, and function. The thermodynamic stability of folded proteins in aqueous environments occurs through the interaction and interplay between hydrophilic and hydrophobic amino acids and the surrounding solvent. The addition of co-solvents, including organic solvents and ionic liquids (ILs), can substantially alter these interactions, thereby affecting the enzymatic activity, structural integrity, and thermal stability of proteins. These effects have potential applications in the pharmaceutical industry, particularly in drug development, but a comprehensive understanding of micro-solvent behavior at the molecular level is essential. Investigating the role of organic solvents and ILs at this level provides valuable insights into the activation or deactivation of biomolecules such as proteins, enzymes, DNA, and RNA.

Classical molecular dynamics (MD) simulations have been employed to explore the solvation structure and dynamics of ions and biomolecules in aqueous solutions containing these co-solvents. Simulation results indicate that organic molecules and IL cations exhibit specific orientations on biomolecular surfaces, which can significantly influence biomolecular stability and activity.

In this context, the present contribution explains the effects of organic solvents, ionic liquids, and deep eutectic solvents on the solvation structure and dynamics of various biomolecules, such as DNA and proteins, using molecular dynamics simulations to elucidate complex phenomena observed in experimental findings. [1-5]

[1] ZE Eremenko, VA Pashynska, KS Kuznetsova, A Shaposhnikova, B. Minofar, *Journal of Molecular Liquids 364, 119981*.
[2] F Fadaei, M Tortora, A Gessini, C Masciovecchio, S Catalini, J Vigna, B. Minofar, *Journal of Molecular Liquids 347, 118350*
[3] A Shaposhnikova, M Kuty, R Chaloupkova, J Damborsky, B. Minofar, *Crystals 11 (9), 1052*
[4] Berta, M.; Sedl, D.; Du, E.; Dzurillov, V.; Minofar, B.; Shaposhnikova, A.; Fadaei, F.; Sedl, E., *Biophys Chem. 2022, 287*
[5] Dusekov´E. , Garajova K. , Yavaser R., Tomkova M., Sedlakova D. Dzurillova V., Kulik N., Fadaei F., Shaposhnikova A., Minofar B., Sedlak E.,*Biophysical Chemistry 288 (2022) 106856*