Biomolecular simulations in non-aqueous media

Babak Minofar[1,2]

[1] Department of Physical Chemistry, Faculty of Chemistry, University of Lodz, Pomorska 163/165 90-236, Lodz, Poland,
[2] Department of Chemistry, Faculty of Science, University of South Bohemia in České Budějovice, Branišovská 31, 37005 České Budějovice, Czech Republic

Solvation is a crucial aspect of chemistry, particularly in biological contexts, where water, as the native solvent, significantly impacts biomolecules' structure, dynamics, and function. The thermodynamic stability of folded proteins in aqueous environments occurs on the interaction and interplay between hydrophilic and hydrophobic amino acids and the surrounding solvent. Adding co-solvents, including organic solvents, ionic liquids (ILs), and deep eutectic solvents (DESs), can substantially alter these interactions, thus affecting the enzymatic activity, structural integrity, and thermal stability of biomolecules including 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, ILs, and DESs 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*