

Computational Studies of the interactions between Glycine and Choline Chloride-Based Deep Eutectic Solvents

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For the last two decades, research on ionic liquids has increased dramatically as chemistry trends are pointing towards “green” solvents. Deep eutectic solvents (DESs) have emerged as the green solvents of choice considering their properties, ease of synthesis and tunability to a wide array of biochemical applications. First described in 2003 [1], these solvents are eutectic mixtures of ammonium salts (such as choline chloride) and hydrogen bond donors (such as urea, ethylene glycol and glycerol) with melting points lower than any of their individual components. Among these, Deep eutectic solvents of the choline chloride analogues have attracted much attention during the past decade for their capability to dissolve biomass. Besides experimental work, numerous computational studies have been conducted on DESs to study the interaction of these solvents with different solutes.

Many studies and publications have already tried to validate the properties of DESs complexes while comparing experimental results to molecular dynamics simulations using adapted force fields. Starting from the OLPS-AA force field model [2], a number of improved force fields variants were created to adapt to DESs complexes [3] allowing to study the effect of hydration as well as bring more clarity to the physicochemical properties of DESs.

In this work, we studied the complex of the DES Reline (Choline Chloride + urea) - Glycine amino acid with or without water by conducting molecular dynamics simulations using OPLS force field. The simulations were carried out using GROMACS software package. Generated center of mass radial functions and hydrogen bonds around Glycine were analyzed. These results bring more precision on the interaction of the amino acid with the DES-water complex. The ultimate objective of the study is to be able to simulate the interactions of DESs with large biomolecules such as lipases. Thus, coarsed-grain force field molecular dynamics have to be realized as current DES all-atom force fields lack many parameters to adapt big proteins.

[1] Abbott, A. P., Capper, G., Davies, D. L., Rasheed, R. K., & Tambyrajah, V. (2003). Novel solvent properties of choline chloride/urea mixtures. *Chemical Communications*, 9(1), 70–71.

[2] Doherty, B., & Acevedo, O. (2018). OPLS Force Field for Choline Chloride-Based Deep Eutectic Solvents. *Journal of Physical Chemistry B*, 122(43), 9982–9993.

[3] Ferreira, E. S. C., Voroshylova, I. V., Pereira, C. M., & Cordeiro, M. N. D. S. (2016). Improved force field model for the deep eutectic solvent ethaline: Reliable physicochemical properties. *Journal of Physical Chemistry B*, 120(38), 10124–10137.