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Molecular dynamics / quantum mechanics modelling of aqueous mixtures of choline tryptophanate ionic liquid

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Choline tryptophanate [Cho][Trp] is a biocompatible, biodegradable ionic liquid belonging to choline-aminoacid family of ionic liquids ([Cho][AA] ILs). The potential for applying [Cho][AA] ILs in biomass processing and pharmaceutical fields stems from their ability to effectively solubilize some macromolecules (e.g. lignin [1]) and drugs (e.g. glibenclamide [2]) in aqueous medium. Nanoheterogeneity of [Cho][AA] IL-water mixtures is believed to be an important feature in solubilization process. Choline lysinate [Cho][Lys] was expected to not have nanodomain-like structure, shown by X-ray diffraction measurements [3], but neutron scattering and our theoretical study supported the formation of polar and nonpolar domains [1,4]. Therefore we aim to scrutinize the intermolecular structure of aqueous mixtures of another [Cho][AA] IL – choline tryptophanate, which should also be non-nanosegregated, according to X-ray diffraction experiments [3].

In order to get information about local coordination around each moiety of Cho^+, Trp^- and H_2O, and aggregate size distribution, we performed molecular dynamics (MD) simulations of two [Cho][Trp]:H_2O mixtures (one having 10 % [Cho][Trp] molar fraction and another having a single ionic pair surrounded by 4000 water molecules). ^{1}H NMR shielding constants of some nuclei in Cho^+ and Trp^- were calculated with qualitative precision by conducting quantum mechanics / molecular mechanics (QM/MM) calculations on 100 configurations extracted from MD trajectories.

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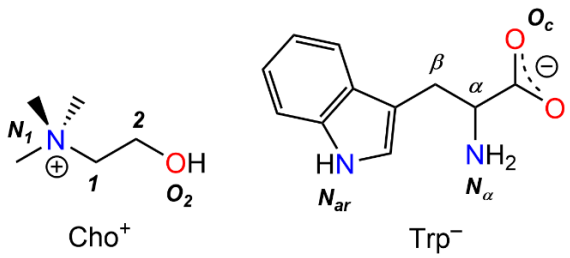

Fig. 1. Choline tryptophanate [Cho][Trp] chemical structure and important atomic labels.

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