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Effect of alkyl chain length on aggregation behavior of amino acid ionic liquid surfactant by molecular dynamics simulation

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Amino acid ionic liquids (AAILs) with the amino acids as anion or cation have attracted a considerable attention in green chemistry and environmental engineering. The ion pairs possess good biodegradability and biocompatibility that may shed light on the synthesis of specialized solvents for medical, biological, and pharmaceutical sciences [1]. The effect of alkyl chain length on the structure of cation aggregation in $[C_nH_{2n+2}NO_2][C_4H_6NO_3]$ AAIL was studied by molecular dynamics (MD) simulation at different alkyl chain lengths (n= 8, 12, and 16) at 300 K. The anion is N-acyl glycinate and the cation is n-alkyl betaine.

The radial distribution functions (RDFs) of cation-cation, cation-anion and anion-anion demonstrated that the position of RDF for three alkyl chain lengths is almost similar because of the same interactions in spite of different heights due to the interaction strength. In addition, the root-mean-square deviation (RMSD) was studied. Figure 1 indicates RMSD for micelles. As the figure shows the AAILs follow n8 > n16 > n12 trend that demonstrates dodecyl betaine N-acyl glycinate is the most stable micelle while octyl betaine N-acyl glycinate is the least stable [2].

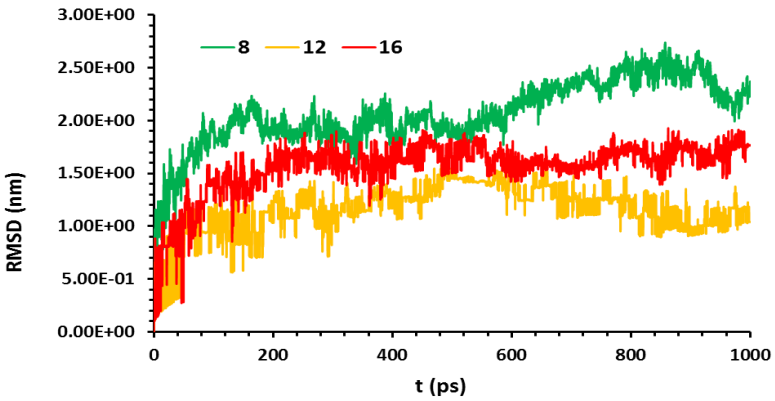

Figure 1: RMSD compare for octyl (green), dodecyl (yellow), and hexyldecyl (red) betaine N-acyl glycinate AAILs.

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