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Mutual Exclusion of Urea and Trimethylamine N-oxide from Amino Acids in Mixed Solvent Environment PRITAM GANGULY, Univ of California - Santa Barbara, TIMIR HAJARI, TU Darmstadt, Germany, JOAN-EMMA SHEA, Univ of California - Santa Barbara, NICO F. A. VAN DER VEGT, TU Darmstadt, Germany — We study the solvation thermodynamics of individual amino acids in mixed urea and trimethylamine N-oxide (TMAO) solutions using molecular dynamics simulations and the Kirkwood-Buff theory. Our results on the preferential interactions between the amino acids and the cosolvents (urea and TMAO) show a mutual exclusion of both the cosolvents from the amino acid surface in the mixed cosolvent condition which is followed by an increase in the cosolvent-cosolvent aggregation away from the amino acid surface. The effects of the mixed cosolvents on the association of the amino acids and the preferential solvation of the amino acids by water are found to be highly non-linear in terms of the effects of the individual cosolvents. A similar result has been found for the association of the protein backbone, mimicked by triglycine. Our results have been confirmed by different TMAO force-fields and the mutual exclusions of the cosolvents from the amino acids are found to be independent of the choice of the strength of the TMAO-water interactions. Based on our data, a general mechanism can potentially be proposed for the effects of the mixed cosolvents on the preferential solvations of the solutes including the case of cononsolvency.

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