Solute Descriptors for Free Amino Acids Obtained by Partitioning in ATPS Formed by Different Polymers

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Understanding of how proteins fold into their native state remains the problem continuing to evade researchers. This problem might be solved if it would be possible to characterize the interactions of individual amino acid residues that make up the tertiary structure between themselves and with their environment [1]. The interactions involved are hydrophobic, electrostatic, hydrogen bonding, and van der Waals interactions. The present study is aimed at evaluating these interactions.

It was reported previously [2,3] that solvatochromic solvent features of aqueous media of the coexisting phases can be used to describe partition coefficients of low molecular weight compounds and proteins in ATPS formed by different polymers. On the other hand, the above approach provides values of solute descriptors for the compound examined including solute polarity/polarizability, hydrogen-bond donor acidity, hydrogen-bond acceptor basicity and ion-ion and ion-dipole interactions. In this study partitioning of twelve free amino acids in aqueous two-phase Dextran-Ficoll, Dextran-PEG, Dextran-Ucon, Ficoll-PEG, Ficoll-Ucon, and PEG-Ucon systems with the same ionic composition of 0.15 M NaCl in 0.01 M sodium phosphate buffer, pH 7.4 was studied. Solute descriptors for all amino acids examined were evaluated.

Analysis of lipophilicity/hydrophobicity estimates of the examined amino acids reported in the literature in terms of the obtained solute descriptors was performed. This analysis shows that the combined solute descriptors not only describe the lipophilicity/ hydrophobicity of amino acids in a more general manner than common organic solvent-water partition coefficients or HPLC retention parameters but may also explain the discrepancy between numerous different lipophilicity/hydrophobicity scales for amino acids reported in the literature [1].

The results obtained are discussed in regard to the viewpoint that "one would not expect that any single solvent or physical environment could, except by an occasional coincidence, represent the variety of environments experienced by residues within a protein" [4]. It is suggested that as the solute descriptors under discussion characterize the abilities of the solute to participate in dipole-dipole, induced dipole-dipole, hydrogen bonding and non-polar interactions with any type of environment, they may be used for generalized characterization of amino acids.

References

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