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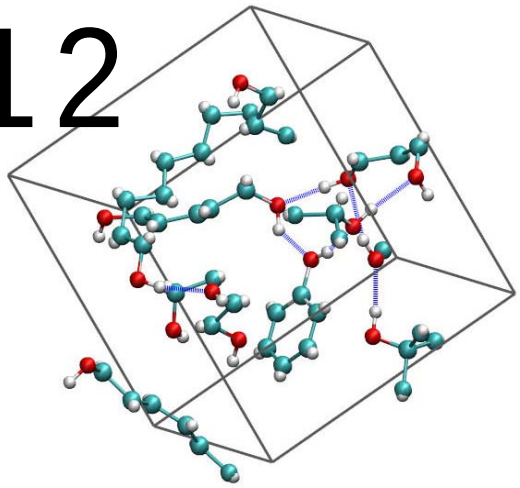

19-20 March 2012 - Lyon, France

Industrial use of
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Program and Book of Abstracts

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Summary

Ref P-049

The Cation Effect on the aqueous Solubility of amino Acids in the Presence of Salts: experimental and molecular Dynamics Simulation Studies.

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The study of the solubility behavior of amino acids and proteins in aqueous electrolyte solutions is of utmost importance to understand the biochemistry of natural systems, develop medical and pharmaceutical responses to diseases induced by biochemical disorders and improve the efficiency of biotechnological processes. Although the effect of common salts on the aqueous solubility of amino acids and proteins is phenomenologically well described [1], the underlying molecular-level mechanisms are far from being elucidated and consensual, in spite of the several explanations proposed during the past century. In order to contribute to the interpretation of the solubility behaviour of (amino acids+salts +water) ternary mixtures, we have previously studied the anion effect on the aqueous solubilities of amino acids using molecular dynamics (MD) simulation methods [2]. Aiming at further understanding the molecular interactions governing the behavior of these systems, experimental and MD studies were performed in this work for aqueous solutions of three amino acids, taken as model systems – alanine, valine and isoleucine – in the presence of salts such as $MgCl_2$, $MgSO_4$, NH_4Cl and $(NH_4)_2SO_4$, at T=298.15 K and different concentrations. The ions were selected in order to evaluate the cation effect on the aqueous solubility of the amino acids. The combined analysis of the thermodynamic data and of the radial distribution functions of the various groups and moieties, as well as of their respective energy of interaction, insight into the molecular interactions established in solution will be provided.

References:
[1] Hofmeister, F. Arch. Exp. Pathol. Pharmakol. ***1888****, XXV, 1*
[2] Tomé, L. I. N.; Jorge, M.; Gomes, J. R. B.; Coutinho, J. A. P. J. Phys. Chem. B ***2010****, 114, 16450.*

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