Chemistry Central Journal

Poster presentation

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A theoretical investigation of microhydration of cationic amino acids

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from 4th German Conference on Chemoinformatics
Goslar, Germany. 9–11 November 2008

Published: 5 June 2009

Chemistry Central Journal 2009, **3**(Suppl 1):P50 doi:10.1186/1752-153X-3-S1-P50

This abstract is available from: http://www.journal.chemistrycentral.com/content/3/S1/P50

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Hydration of biological macromolecules has a crucial role as it modifies their structures, stabilities, and functions [1]. Water molecules preferentially occupy sites either inside the macromolecules or on the surface, where hydrogen bonds with the amino acids (AA) of the protein are built up and stabilize its specific fold [2]. Investigating the interactions of AA with water is therefore an essential first step to understand the solvation process that opens insights into fields as human health, biomedicine, biotechnology, protein engineering or drug design.

In this work, we describe the microhydration of AA, and particularly of protonated glycine (GlyH+), alanine (AlaH+) and proline (ProH+). First a high-level theoretical method was setting up in order to compute the structures and properties of GlyH+water complexes, Gly being the simplest AA and a suitable model for such a study [3]. Then complexes with more than one water molecule [4] as well as other amino acids (Ala and Pro) [5] were investigated, to extend the validity domain of our computational procedure. Using a MP2/6-311++G(d,p) approach combined with a full counterpoise correction, we obtained theoretical hydration enthalpies that are in perfect agreement with the most recent experimental investigations. Gly/Ala/ProH+-(H2O)n complexes (n: 0–4) have been systematically classified in a family tree, based on their structures and energetics. A Darwinian-like logic can be used to build such protonated AA complexes, as the most stable complex at any stage gives the best structure at the next generation.

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