Microhydration of protonated amino acids with *ab initio* tools

C. Michaux, J. Wouters, E.A. Perpète and D. Jacquemin

Groupe de Chimie Physique Théorique et Structurale, Facultés Universitaires Notre-Dame de la Paix, rue de Bruxelles, 61, B-5000 Namur, Belgium
e-mail : denis.jacquemin@fundp.ac.be

Hydration of biological macromolecules has a crucial role as it modifies their structures, stabilities, and functions.[1] Investigating the interactions of AA with water is therefore an essential first step to understand the solvation process and related properties, that allows to open insights into fields as human health, biomedicine, biotechnology, protein engineering or drug design.

In this work, we describe the microhydration of several protonated AA. First an adequate theoretical method was set up in order to compute the structures and properties of GlyH+-water complexes.[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 very good agreement with the most recent experimental investigations. Gly/Ala/ProH+-$(H_2O)n$ complexes (n: 0-4) have been systematically classified in a family tree, based on their structures and energetics. It appears that an evolutionary logic can be used to build such protonated AA complexes, as the most stable complex at any stage systematically yields the “best” structure at the next generation.

[1] Chaplin M.F. *Nat Rev Mol Cell Biol* **2006**, *7*, 861; Israelachvili J., Wennerström H. *Nature* **1996**, *379*, 219-25; Levy Y., Onuchic J.N. *Annu Re*V *Biophys Biomol Struct* **2006**, *35*, 389; Baldwin R.L. *J Mol Biol* **2007**, *371*, 283.
[3] Michaux C., Wouters J., Jacquemin D., Perpète E.A. *Chem Phys Lett* **2007**, *445*, 57.
[4] Michaux C., Wouters J., Perpète E.A., Jacquemin D. *J Phys Chem B* **2008**, *112*, 2430.
[5] Michaux C.,Wouters J., Perpète E.A., Jacquemin D. *J Phys Chem B* **2008**, *112*, 9896; Michaux C., Wouters J., Perpète E.A., Jacquemin D. *J Phys Chem B* **2008**, *112*, 7702.