THE TRANSFORMATION OF FREE AMINO ACIDS TO PROTEIN RESIDUES – A STUDY ON DISSOLVENCE

Andrzej J. Bojarski (a), Mateusz Nowak (a), Bernard Testa (b)
(a) Institute of Pharmacology of the Polish Academy of Sciences, PL-31343 Kraków, Poland
(b) Pharmacy Dept, University Medical Centre, CH-1001 Lausanne-CHUV, Switzerland

The formation of complex systems is accompanied by the emergence of properties that are non-existent in the components. At the same time the properties and behavior of integrated components undergo substantial changes (constraints) when compared to their free (unbound) state. This phenomenon, termed downward causation or dissolvence, has recently gained increasing interest, since it may be considered as a process generating information which drives self-organization of complex systems [1].
Due to their fundamental importance in living systems, proteins and their monomers appear as particularly interesting objects in the study of dissolvence. Thus, a recent study was focused on the conformational behavior of the side chain of residues in a model protein (profilin Ib) compared to the free amino acids [2]. MD simulations indeed revealed strong conformational constraints in residue "chi space" of residues. These constrains were quantified using the Shannon Entropy of the chi dihedral angles, showing a clear gain in information content. As a sequel to this study, new developments will be presented, including an analysis of:

- a prolonged MD simulation (10 ns) of the model protein (profilin Ib);
- a conformation comparison between free amino acids and residues at the center of an alpha-helical nonapeptide, revealing constraints of intermediate intensity;
- a chemically functional protein (trypsin).

[1] B. Testa, L.B. Kier. Emergence and dissolvence in the self-organization of complex systems. *Entropy* **2000**, *2*, 1-25. http://www.mdpi.org/entropy/list00.htm
[2] A. Bojarski, M. Nowak, B. Testa. Conformational constraints on side chains in protein residues increase their information content. *Cell. Mol. Life Sci.* **2003**, *60*, 2526-2531.