1. A. J. Oakley, Z. Prokop, M. Boháč, J. Kmuníček, T. Jedlička, M. Monincová, I. Kutá Smatanová, Y. Nagata, J. Damborský, M. C. J. Wilce. *Biochemistry US*, **41** (2002) 4847-4855.

MOLECULAR MODELING AS A TOOL IN MOLECULAR BIOLOGY OF MEMBRANE-BOUND RECEPTORS

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The importance of computer modeling of membrane proteins in molecular biology is worked out. We give three examples that models gained by a combined approach of homology and energetic modeling with vibrational spectroscopy are a useful help in site-directed mutagenesis, truncation, binding-studies and even in crystallography. The study of the vanilloid receptor is a successful application of a computer model in the construction of truncations that served for the identification of functionally important protein parts. In the case of CD69 computer docking helped to identify the Ca^{2+}–binding site that was not observed in the crystal structure of this protein due to the non-physiological conditions of crystallisation.

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PROTON TRANSFER IN SHORT OLIGOPEPTIDES

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Peptides belong to key biomolecules. Their activity can be influenced by several impacts and the interaction with protons is one of them. Such a type of interaction can also influence behaviour of peptides in gas phase, which can lead to different way of fragmentation during mass spectroscopy analysis [1].

Our quantum-chemical study has been focused on detailed analysis of proton interaction with short oligopeptides. Density functional theory employing hybrid functional B3LYP and 6-31G(d',p') basis set was used. The study was performed on terminally blocked diglycine and triglycine models. It implies that the proton can only interact with the oxygen and nitrogen atoms of the amidic groups. Because of appropriate geometry, the proton transfer can occur between these positions [2, 3].

In general, the proton transfer process consists of two repeating steps. In the first step, the proton is moved around the double bond of the carbonyl group by isomerization from *E* to *Z* configuration. Then the process continues by proton jump between adjacent carbonyl oxygens. The isomerization processes have significantly higher activation barriers than the jump steps [3]. Also changes in proton transfer were examined when a single water molecule was presented in the system. Strong influence to all steps, and also active participation of the water molecule due to proton exchange processes was found.

1. C. F. Rodriquez, A. Cunje, T. Shoeib, I. K. Chu, A. C. Hopkinson & K. W. M. Siu, *J. Am. Chem. Soc.*, **123** (2001) 3006-3012.
2. C. F. Rodriquez, A. Cunje, T. Shoeib, I. K. Chu, A. C. Hopkinson & K. W. M. Siu, *J. Phys. Chem. A*, **104** (2000) 5023-5028.
3. B. Paizs, I. P. Csonka, G. Lendvay & S. Suhai, *Rapid Commun. Mass Spectrom.*, **15** (2001) 637-650.

APPLICATION OF POWDER DIFFRACTION IN BIOLOGY? THE EGG-SHELL MICROSTRUCTURE

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In last years, renaissance of rather old and traditional technique - X-ray powder diffraction can be observed. This was initiated by both the interest in design of new materials (in materials science, physics and chemistry, where it plays the role of a basic method), and also by fast development in instrumental techniques - X-ray optics and detection which enhanced its possibilities.

Powder diffraction pattern contains different kind of information. Peak positions and intensities are related to crystal (atomic) structure, i.e. the type and size of lattice cell and atomic positions and consequently it can be used for structure refinement and even structure determination in some cases. As a finger print of each individual phase, the diffraction pattern can be an ideal tool for phase analysis.

However, there is much more hidden in the pattern. Variations of lattice parameters and intensitites can detect lattice defects. This is related to the so-called real structure of material, the term which is also used for structural features in the scale of nanometers, i.e. grains or subgrains. The topics which is now of great interest because of intense