MS18-P1 **Electronic structure of the nickel(II) complex of the Schiff base and glycine.** Marek Fronc[a], Peter Herich[a], Alexander Popkov[b] and Jozef Kozisek[a] [a]*Slovak University of Technology in Bratislava, Faculty of Chemical and Food Technology, Radlinskeho 9, 812 37 Bratislava 1, Slovak Republic*, [b]*Department of Cognitive Research and Tomographic Imaging Methods, SamoUniversity in Pardubice, Na Klínku 1082, 530 06 Pardubice, Czech Republic*
E-mail: marek.fronc@stuba.sk

Our interest in structural research of Ni(II) complexes of Schiff bases of (S)-N-(2-benzoylphenyl)-1-benzyl-prolinamide and its derivatives with α-amino acids is driven by growing number of successful applications of these chiral synthons of α-amino acids to achieve the preparation of carbon-11 and fluorine-18 labelled radiodiagnostics for positron emission tomography (PET).

Complex presented in this contribution was studied in the terms of the charge density analysis [1] – data were collected at F1 beamline at Hasylab/DESY in Hamburg.

With the aim of set-up a solid benchmark for the electron density studies of this complex and its derivatives, we have decided to re-evaluate the electron density distribution.

Data were collected at Oxford Diffraction GEMINI R diffractometer with Ruby CCD detector at the temperature 100 K. Data reduction was done by CrysAlis171.35.19 package. An electronic structure analysis was performed with XD software package. The results of the topological analysis of electron density will be discussed together with the comparison of the previous experiment.

This work has been supported by Slovak Grant Agency APVV and VEGA (APVV-0202-10 and 1/0679/11).

[1] Kozisek, J., Fronc, M., Skubak, P., Popkov, A., Breza, M., Fuess, H. & Paulmann, C. (2004). *Acta Cryst.,* A60, 510-516

Keywords: charge density; chiral synthon; nickel complex

MS18-P2 **Electrostatic interactions and sequence recognition by Zinc Fingers.** Anna M. Goral[a], Katarzyna N. Jarzembska[a], Paulina M. Dominiak[a] [a] *Department of Chemistry, University of Warsaw, Poland*
E-mail: annamariagoral@gmail.com

The specific sequence recognition is crucial for the use of Zinc Fingers e.g. in gene therapy. Several studies have already been performed to establish the recognition pattern. A mechanism based on hydrogen bonding was proposed: Zinc Finger domain, folded into two anti-parallel beta-strands and an alpha-helix, recognizes DNA via hydrogen bonding with the helix outer side. However, according to our studies, this recognition code is not as simple as described in the literature [1]. The complexity of the problem is well visible on the example of the aminoacid at the position 2 [1]. This residue participates in the recognition of the secondary strand, but its action is highly sequence dependent, and thus not universal. The quantitative characterization of particular electrostatic interactions for the selected structures will be presented and discussed. Our results were obtained by the application of the University at Buffalo Databank (UBDB) [2], which contains aspherical atomic electron density fragments represented by more than 200 atom types, corresponding to the atoms found in proteins and nucleic acids. The electron density of the protein molecule and the DNA fragment was reconstructed via the *LSBD* program applied to the experimentally obtained geometries deposited in the PDB databank. Subsequently, the electrostatic energy of interaction was calculated with the EPMM (Exact Potential and Multipole Method) method developed by A. Volkov [3]. This allowed for evaluating not only the total interaction energy of the studied macromolecular complexes, but also for estimating contributions atributed to single aminoacid residues.

[1] Elrod-Erickson M., Benson T.E. & Pabo C. O. (1998) *Structure* **6**, 451-464.
[2] Jarzembska, K. N. & Dominiak, P. M. (2012) *Acta Cryst.* **A68**, 139-147.
[3] Volkov, A., Koritsanszky, T. & Coppens, P. (2004) *Chem. Phys. Lett.* **391**, 170-175.

Keywords: electrostatic interactions; protein; DNA