

**“EAST-NMR 2<sup>nd</sup> Young investigators meeting” organized in the frame of 7-th framework programs EAST NMR and EMAR**

Bratislava, Slovakia, May 18-20, 2012

Organized by Institute of Chemistry, Center for Glycomics, Slovak Academy of Sciences

*Scientific Report No 3432*

**Summary**

This conference was organized within the 7 framework program (EAST NMR) with the financial support of EMAR program from ESF. Main goal of the “EAST NMR 2<sup>nd</sup> Young investigators meeting” was to give the opportunity to young researchers and students to present their work in the form of oral and poster communications and to build new links for a future collaboration. This goal is coherent with one of the scopes of the EMAR project. Financial support of EMAR enabled the increasing of the number of young scientist participants from European countries by covering fully their travel and accommodation expenses.

**Scientific content**

The main scope of the conference was NMR spectroscopy but also results of an EPR study were presented in one oral communication. Presentations covered different field of NMR spectroscopy (high resolution NMR, imaging and theoretical calculations). The conference was organized in a traditional way; 5 keynote lectures were delivered by worldwide known senior researchers (Prof. M. Pons, Prof. H. Schwalbe, Prof. A. Perczel, Prof. V. Sklenář and Prof. O. Malkina) and all other oral presentations (20-30 min) were presented only by young scientists and students. There were two poster sessions but also coffee brakes were used for discussions.

**Synopsis of keynote talks**

**Prof. M. Pons, (University of Barcelona, Spain)**

*Biomolecular interactions of the intrinsically disordered unique domain of cSrc*

Results of the research of Prof. Pons group show that a disordered region of non-receptor protein kinases is unique to each member and that it is an important active player in the regulation of the oncogene.

**Prof. H. Schwalbe (Johann Wolfgang Goethe-Universität, Germany)**

*NMR spectroscopic studies of the complementary G-quadruplex and i-motif DNA structures*

In the context of possible development of small molecule drugs based on G-quadruplexes and i-motifs (formed in the presence of cations by guanine-rich strands and cytosine-rich DNA and RNA strands) the NMR characterization of structure and kinetics of i-motif folding and G-quadruplexes binding mode of alkaloids was discussed.

**Prof. A. Perczel (Eötvös Loránd University, Hungary)**

*A dead-end street of protein folding?*

Three dimensional structure of a globular protein having an architecture similar to the aggregated amyloid-state (Alzheimer disease) with low sequence specificity have the common motif of multiple stranded  $\beta$ -pleated sheets. When misfolding becomes possible due to abnormal cellular conditions they tend to adopt such an aggregate. Inter-conversion of the globular form into amyloid like aggregate is coupled with the transformation of the physiologically “healthy” structure into a non-functional and pathogenic conformation. Results of calculations have been presented.

**Prof. V. Sklenář (NCBR National Center for Biomolecular Research, Czech republic)**

*NMR heading high - Assignment strategies for partially disordered proteins*

The lecture reviewed recent developments from Prof. Sklenář laboratory to significantly shorten time needed for thorough description of unstructured or partially disordered proteins.

Prof. O. Malkina (Institut of Inorganic Chemistry, Slovak Academy of Sciences, Slovakia)

*NMR spin-spin couplings trough a hydrogen bond and overlap of densities of localized molecular orbitals*

### **Results and impact**

The main goal of this conference was fulfilled because it has given the opportunity to young scientists, working in the field of magnetic resonance, to present their work and to create new contacts for a future collaboration. At the same time young scientists enriched their knowledge due to keynote lectures given by experienced scientists and discussions with them. Thus a transfer of the knowledge could take place. Financial support of EMAR project helped to increase the quality of the conference by increasing of the number of conference participants of both groups; young scientist/students and senior researcher/lectures which was one of his objectives.

From the total number of participants (49) there were 30% of women from which 79% were young scientist or students. From 61% of male participants 60% were young scientists or students.

### **Final Program**

#### **Wednesday, May 16, 2012**

10:00-12:30 *Registration*

12:30-14:00 *Lunch*

14:00-14:10 *Welcome*

#### **Session I,**

chair V. Sklenář

14:10-14:40 **Keynote 1 H. Schwalbe:** NMR spectroscopic studies of the complementary G-quadruplex and i-motif DNA structures.

14:40-15:00 **Szymon Żerko:** 7D NMR experiments for protein backbone assignment.

15:00-15:20 **Kristaps Jaudzems:** Structural studies of spider silk N-terminal domain: insights into the mechanism of fibre formation.

15:20-16:00 *Coffee Break*

#### **Session II,** chair H. Schwalbe

16:00-16:20 **Stefano Elli:** Conformational and dynamic properties of Human (26) and Avian (23) sialylated receptors of influenza A virus haemagglutinin.

16:20-16:40 **Saurabh Saxena:** The sequential analysis of intrinsically disordered proteins using a set of multidimensional (5D) NMR experiments acquired with non-uniform sampling.  
16:40-17:00 **Mateusz Urbanczyk:** Iterative Thresholding Algorithm for Multi-exponential Decay applied to PFG NMR data.  
18:30 *Dinner*

## Thursday, May 17, 2012

### *Session III,*

chair A. Perczel

9:00-9:30 Keynote 2 **M. Pons:** Biomolecular interactions of the intrinsically disordered Unique domain of cSrc.  
9:30-9:50 **Ivica Kukurová Just:** Comparison of 31P GOIA-1D-ISIS/2D-CSI to conventional 2D-CSI at 7T: Pulse profile and localization performance.  
9:50-10:10 **Michal Štjber:** NMR Structural Analysis of a Novel Triterpenoid Saponin Extracted from *Bellis Perennis* L.  
10:10-10:50 *Coffee Break*

### *Session IV,*

chair S. Bekiroglu

10:50-11:10 **Min-Ji Shin:** 1H Nuclear magnetic resonance spectroscopy based Human serum Metabolic profiling in Type 2 diabetes and controls.  
11:10-11:30 **Andrea Gálisová:** Animal model of vascular dementia studied by *ex vivo* magnetic resonance microimaging and histology.  
11:30-11:50 **Michal Kaliňák:** Changes in intracellular metabolites during life cycle of *Trichodermaviride*.  
12:15-14:00 *Lunch*

### *Session V,*

chair M. Pons

14:00-14:30 Keynote 3 **A. Perczel:** A dead-end street of protein folding?  
14:30-14:50 **Zuzana Barbieriková:** EPR Spectroscopy Application in the Studies of Photoinduced Processes.  
14:50-15:10 **Miroslava Bobeničová:** Reactive Oxygen Species in Irradiated Titanium Dioxide Suspensions (An EPR Study).  
15:10-15:40 Keynote 4 **V. Sklenář:** NMR heading high - Assignment strategies for partially disordered proteins.  
15:40-16:15 *Coffee Break*  
16:15-17:00 Poster Session I  
17:30-22:00 *Social Programme*

## Friday, May 18, 2012

### *Session VI,*

chair M. Hricovíni

09:00-9:30 Keynote 5 **O. Malkina:** NMR spin-spin couplings through a hydrogen bond. and overlap of densities of localized molecular orbitals.  
9:30-9:50 **James Asher:** Calculation of Benzosemiquinone EPR properties with inclusion of Dynamical Effects.

9:50-10:10 **Anežka Křístková:** Efficient implementation of NMR spin-spin coupling in the framework of four-component mDKS method.

10:10-10:40 *Coffee Break*

***Session VII,***

chair V.G. Malkin

10:40-11:00 **Peter Bystrický:** NMR Study of *Ralstonia Solanacearum* lectin interactions.

11:00-11:20 **Mária Vilková:** Definitive assignment of allobetulin chemical shifts.

11:20-12:20 Poster Session II

12:20-12:30 Closing

12:30-14:00 *Lunch*