
Program

Wednesday, 11. 02. 2009

- Arrival
- 16.00 - 21.00 Registration
- Pre-conference lectures
- 17.30 - 18.00 **Ago Samoson:** *NMR Fringe Phenomena*
- 18.00 - 19.00 **Marc Baldus:** *Studying Protein Function and Disease by High-Resolution Solid-State NMR*
- 19.30 - 20.00 Reception at Otočec Castle
- 20.00 - 22.00 Dinner

Thursday, 12. 02. 2009

- 9.00 Opening
Janez Plavec
Gregor Golobič, minister, Ministry of Higher Education, Science and Technology
Janko Jamnik, director, National Institute of Chemistry
- 9.30 - 10.30 **Ivano Bertini:** *Mechanistic Systems Biology by NMR: Cellular Copper as an Example*
- 10.30 - 11.00 Coffee break
- 11.00 - 12.00 **Harald Schwalbe:** *Biomolecular Dynamics Characterized by NMR: From Fast Local Motions to Slow Global Folding*

Residual Dipolar Couplings

Chair: **Tibor Liptaj**

- 12.00 - 13.00 **Dušan Uhrín:** *Residual Dipolar Coupling Constants in NMR Structure Elucidation*
- 13.00 - 14.30 Lunch
- 14.30 - 15.00 **Perttu Permi:** *NMR Methods for Studying Protein Structure by Residual Dipolar Couplings*
- 15.00 - 15.30 **Christina M. Thiele:** *The Use of RDCs in the Structure Determination of Organic Compounds*
- 15.30 - 15.50 **Georg Kontaxis:** *Residual Dipolar Couplings in Protein Structure Determination*
- 15.50 - 16.10 **Nicholle G. A. Bell:** *Measurement of Proton-Carbon Residual Dipolar Coupling Constants Using Carbon Detection*
- 16.10 - 16.40 Coffee break

Biomolecular NMR I

Chair: **Robert Konrat**

16.40 - 17.40 **Bernhard Brutscher**: *New Tools for Parallel Screening of Protein Constructs, Fast NMR Resonance Assignment, and Real-Time Studies of Molecular Kinetics*

17.40 - 18.10 **Igor Zhukov**: *Three-Dimensional Structure of CsPin Protein from Archaeon *C. symbiosum* as Determined by NMR Spectroscopy*

18.10 - 18.40 **András Perczel**: *Calcium-Induced Tripartite Binding of Intrinsically Disordered Calpastatin to Its Cognate Enzyme, Calpain*

18.40 - 19.00 **Klaus Zangger**: *Structural Studies on Peptides and Proteins by Relaxation Enhancements Induced by an Inert and Soluble Paramagnetic Agent*

19.00 - 20.30 Dinner

20.30 - **Poster session**, drinks, courtesy of ARMAR AG

Friday, 13. 02. 2009

Biomolecular NMR II

Chair: **András Perczel**

9.00 - 10.00 **Oscar Millet**: *Structural Basis for the Aminoacid Composition of Proteins from Halophilic Archea*

10.00 - 10.30 **Simona Golič Grdadolnik**: *Conformational Preferences of Unfolded Polypeptide Chain – Protein Folding Problem*

10.30 - 10.50 **Zoltán Gáspári**: *Assessing the Compliance of Protein Structural Ensembles with Experimental NMR Data*

10.50 - 11.10 **Miloš Hricovíni**: *Explorations of Heparin-Oligosaccharides-Proteins Interactions by NMR*

11.10 - 11.40 Coffee break

11.40 - 12.10 **Claudio Dalvit**: *A Comparison of Different NMR Techniques Applied to Fragment Based Screening*

12.10 - 12.40 **Mirko Cevec**: *Investigation of 3D Structure of let-7 miRNA:lin-41 mRNA Constructs*

12.40 - 13.00 **Sabine Schultes**: *NMR Studies of the Leader Protease of the Foot-and-Mouth Disease Virus*

13.00 - 14.30 Lunch

Fast and Novel Methods

Chair: **Janez Dolinšek**

- 14.30 - 15.30 **Lucio Frydman:** *Principles and Applications of "Ultrafast" Multidimensional NMR*
- 15.30 - 16.00 **Krzysztof Kazimierczuk:** *Narrow Peaks and High Dimensionalities: Exploiting the Advantages of Random Sampling*
- 16.00 - 16.30 **Martin Billeter:** *"Fast" NMR: Protein Characterization Using Projection Spectroscopy*
- 16.30 - 17.00 **Wiktor Koźmiński:** *Multidimensional NMR Spectroscopy Beyond Sampling Limitations*
- 17.00 - 17.30 Coffee break

Hardware and Software News

Chair: **Gregor Mali**

- 17.30 - 18.00 **Péter Sándor:** *The OneNMR Probe: A Unique Probe for the NMR of Small Molecules*
- 18.00 - 18.30 **Vadim E. Zorin:** *Probes for Solid-State NMR*
- 18.30 - 18.50 **Vratislav Blechta:** *Decoupling During Gradient Pulses?*
- 18.50 - 19.10 **Stanislav Sykora:** *Peak Shapes in NMR Spectroscopy*
- 19.10 - 21.00 Dinner at Struga Castle
- 21.00 - **Poster session**, drinks, courtesy of ARMAR AG

Saturday, 14. 02. 2009

The Application of NMR to Small Molecules

Chair: **Jan Schraml**

- 9.00 - 10.00 **Vladimír Sychrovský:** *Theoretical Methods for Reliable Interpretation of NMR Spectroscopy Parameters*
- 10.00 - 10.30 **Predrag Novak:** *Ribosome-Macrolide Interactions Monitored by NMR*
- 10.30 - 11.00 **Csaba Szántay:** *On the "Philosophy" of Small-Molecule Structure Elucidation by NMR: the Human Factor*
- 11.00 - 11.20 **Marta Bugaj:** *Carbon-Carbon Spin-Spin Couplings $^nJ(CC)$ ($n = 1-3$) and ^{13}C CP MAS Spectra of Enaminoketones with a Steric Hindrance*
- 11.20 - 11.50 Coffee break
- 11.50 - 12.20 **Gábor Tárkányi:** *The Story of an Intriguing Molecular Self-Recognition Phenomenon in Bifunctional Organocatalysis*

12.20 - 12.40 **Agnieszka Sadlej:** *Diamines as Ligands in Adducts of Dimeric Rhodium(II) Salts: NMR Investigation in Solid State and Liquid Phase*

12.40 - 13.00 **Zoltán Szakács:** *Is NMR-Based Small-Molecule Structure Elucidation Becoming "Routine"? Tales of the Unexpected!*

13.00 - 13.20 **Michal Straka:** *What Can Relativistic Effects in ¹H NMR Tell Us About Structure of Polyalcohol Amine Complexes*

13.20 - 13.30 Announcement of the best poster award (short presentation)

13.30 - 15.00 Lunch

15.30 - Social program:

- Excursion to Pleterje and Kostanjevica
or
- Visit to wellness centre

followed by St. Valentine's dinner

Sunday, 15. 02. 2009

Polymorphism and Solid-State NMR

Chair: **Csaba Szántay**

9.00 - 10.00 **Robin K. Harris:** *NMR Crystallography & Polymorphism*

10.00 - 10.30 **Ádám Demeter:** *Solid-State NMR from a Pharmaceutical Perspective*

10.30 - 10.50 **Jiri Brus:** *Poly(a)morphism of Pharmaceutical Solids: Simvastatin vs. Atorvastatin*

10.50 - 11.20 Coffee break

11.20 - 11.50 **Gábor Szalontai:** *ssNMR: The Effect of Rotor Size on Resolution, Sensitivity and Choice of Method. Benefits of High Speed Rotation. Practical Aspects, Applications.*

11.50 - 12.10 **Nonappa:** *Solid-State NMR Studies on Low Molecular Mass Organogelators: Insights Into the Gelation, Formation of Inclusion Complexes and Solvates*

12.10 - 12.30 **Zvonko Trontelj:** *Study of Polymorphism in Some Pharmaceutically Interesting Materials by Nuclear Quadrupole Resonance (NQR)*

12.30 - 14.00 Lunch

14.00 - 15.00 Meeting of the Scientific Committee of MMCE 2011

Departure