



## DETAILED PROGRAMME

### WEDNESDAY, FEBRUARY 27

|               |                                                |
|---------------|------------------------------------------------|
| 14.00         | <b>Arrival &amp; Registration</b>              |
| 17.00 – 17.15 | <b>Welcome words</b><br><i>Jan Sýkora</i>      |
| 17.15 – 18.00 | <i>Petr Slavíček (I)</i><br>Science of Science |
| 18.00 – 18.30 | <b>Welcome drink</b>                           |
| 18.30 – 21.00 | <b>Dinner</b>                                  |

### THURSDAY, FEBRUARY 28

#### Session 1: BASICS, Chair: Csaba Szántay

|               |                                                                                                      |
|---------------|------------------------------------------------------------------------------------------------------|
| 08.30 – 09.15 | <i>Stan Sykora (T)</i><br>Tutorial on Spin Systems in Magnetic Resonance                             |
| 09.15 – 09.45 | TBA                                                                                                  |
| 09.45 – 10.15 | <i>Klaus Zangger (I)</i><br>Enhancing Time and Frequency Resolution by <i>Restricted Acquisition</i> |
| 10.15 – 10.35 | <i>Małgorzata Rytel</i><br>Accelerated pseudo-2D pure-shift acquisition for serial NMR experiments   |
| 10.35 – 11.00 | <b>Coffee break with ExtraByte</b>                                                                   |

#### Session 2: SMALL MOLECULES, Chair: Radek Pohl

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|---------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 11.00 – 11.45 | <i>Christina M. Thiele (T)</i><br>Opportunities and challenges of using Residual Dipolar Couplings for the Structure Determination of Catalytically Active Species |
| 11.45 – 12.15 | <i>Hélène Freichels (I)</i><br>NMR on your Bench – Possibilities for Structure Elucidation / Confirmation and Reaction Monitoring                                  |
| 12.15 – 12.35 | <i>Dariusz Gołowicz</i><br>Monitoring Hydrogenation Reaction with Enhanced Sensitivity and Resolution using Benchtop NMR                                           |
| 12.35 – 12.55 | <i>Petra Cuřínová</i><br>Dialytic Separation of Anions from DMSO Solution Facilitated by Dendritic Receptors                                                       |
| 12.55 – 14.30 | <b>Lunch</b>                                                                                                                                                       |

#### Session 3: SOFTWARE & HARDWARE NEWS, Chair: Krzysztof Kazimierczuk

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|---------------|-------------------------------------------------------------------------------------------------------------------------|
| 14.30 – 15.15 | <i>Michal Maloň</i><br>JEOL                                                                                             |
| 15.15 – 15.45 | <i>Dimitris Argyropoulos (I)</i><br>Computer Assisted Structure Elucidation (CASE) Workflows, Problems and Capabilities |
| 15.45 – 16.05 | <i>Alexandra Shchukina</i><br>Burst sampling for interferogram pure-shift NMR acquisition                               |
| 16.05 – 16.25 | <i>Nicholle G.A. Bell</i><br>Reduced dimensionality NMR experiments: Reducing overlap in spectra of complex mixtures    |
| 16.25 – 17.00 | <b>Coffee break with ACD/Labs</b>                                                                                       |



**COME TO SEE MY POSTER session, Chair: Wiktor Koźmiński**

17.00 – 18.00 2 min / poster presentations

18.00 – 19.00 **Dinner**

19.00 – 21.00 **Poster Session**

**FRIDAY, MARCH 1**

**Session 4: PHARMACEUTICALS, Chair: Predrag Novak**

08.30 – 09.15 *Petr Váchal (T)*

The Invention of MK-8262, a CETP Inhibitor Backup to Anacetrapib (with best in class properties)

09.15 – 09.45 *Marek J. Potrzebowski (I)*

Solid State NMR Spectroscopy as a Tool Supporting the Mechanochemistry Development

09.45 – 10.15 *Manuel Perez*

Determination of Conformation in Solution: A survival guide for Medicinal and Analytical Chemists

10.15 – 10.35 *Václav Veverka*

Disentangling the LEDGF/p75 Interactome

10.35 – 11.00 **Coffee break with Magritek**

**Session 5: METABOLOMICS, Chair: Jan Sýkora**

11.00 – 11.45 *Leonardo Tenori (T)*

NMR-based metabolomics in biomedicine

11.45 – 12.15 *Ana Gil (I)*

Human and *in vitro* NMR Metabolomics Impacting on Health Research

12.15 – 12.35 *Michal Kaliňák*

An Investigation of Cerebral Metabolic Profile in the Rat Model of Age-Related Dementia

12.35 – 12.55 *Lenka Michálková*

Metabolomic Study of the Association between Pancreatic Cancer and Diabetes Mellitus

12.55 – 14.30 **Lunch**

**Session 6: SOLIDS, Chair: Martin Dračinský**

14.30 – 15.15 *Beat Meier (T)*

Protein dynamics: from local motions to molecular machines

15.15 – 15.45 *Yusuke Nishiyama (I)*

Internuclear distance measurements in rigid solids at natural abundance

15.45 – 16.05 *Jan Stanek*

Hyperdimensionality and shared-time acquisition – new hope for protein resonance assignment in solids?

16.05 – 16.25 *Marta K. Dudek*

Solid-state NMR and crystal structure prediction: a perfect alliance? A difficult case of solvate-hydrate of catechin

16.25 – 16.45 *Eliška Procházková*

Polymorphic Transformation of Drugs Loaded into Glycopolymetric Micelles Probed by Solid-State NMR

16.45 – 17.15 **Coffee break with PharmaCan**

17.15 **Departure by bus**

18.00 – 22.00 **Excursion to Unětice brewery / Dinner**



## SATURDAY, MARCH 2

### Session 7: BIOMOLECULES I, Chair: Václav Veverka

- 08.40 – 09.25 *Lukáš Žídek* (T)  
NMR as a window to the dynamic microcosmos of (disordered) proteins
- 09.25 – 09.55 *Paul Schanda* (I)  
Solid-state NMR combined with cryo-EM to determine the structure and functional dynamics of a large enzyme
- 09.55 – 10.15 *Katarína Pšenáková*  
Structural characterization of protein kinase ASK1 and its interaction with thioredoxin
- 10.15 – 10.35 *Bertalan Kovács*  
Interdomain mobility in PDZ tandem captured by externally restrained MD simulation
- 10.35 – 11.00 **Coffee break with Jeol**

### Session 8: BIOMOLECULES II, Chair: Georg Kontaxis

- 11.00 – 11.45 *Katja Petzold* (T)  
When Artifacts turn out to be Real Data: Discoveries of RNA Dynamics
- 11.45 – 12.15 *Hana Macíčková Cahová* (I)  
How to find needle in a haystack? (New RNA modifications)
- 12.15 – 12.35 *Martina Lenarčič Živković*  
Adenine-Dependent G-Quadruplex Structural Switch
- 12.35 – 12.55 *Witold Andraśjć*  
Unravelling the structural basis for the exceptional stability of RNA G-quadruplexes capped by a uridine tetrad at the 3' terminus
- 12.55 – 14.30 **Lunch**

### MESTRELAB USERS' MEETING, Chair: Manuel Perez

- 14.30 – 16.45 Mestrelab Users' Meeting
- 16.45 – 17.15 **Coffee break with Mestrelab**
- 17.15 **Departure by tram**
- 18.00 – 18.45 **Organ resonances**
- 19.00 – 22.00 **Conference Dinner**

## SUNDAY, MARCH 3

### Session 9: CALCULATIONS, Chair: Ján Tarábek

- 09.00 – 09.45 *Trygve Helgaker* (T)  
Quantum-Chemical Calculations of NMR parameters
- 09.45 – 10.15 *Martin Dračinský* (I)  
Towards Accurate Predictions of NMR Parameters
- 10.15 – 10.45 *Torsten Herrmann* (I)  
Bioinformatics-driven NMR structure determination
- 10.45 – 11.05 *Krzysztof Kazimierczuk*  
How to Collect and Process Data in Serial NMR Experiments?
- 11.05 – 11.30 **Coffee break with Spin-Doc**
- 11.30 – 11.50 **Closing Remarks**
- 11.50 – 13.00 **Lunch**