

# 3<sup>rd</sup> Annual East-NMR User Meeting

Preliminary programme (17. 10. 2012)

## Tuesday, November 13<sup>th</sup>

13<sup>00</sup> – 19<sup>00</sup> Arrival and registration

19<sup>00</sup> Welcome dinner

## Wednesday, November 14<sup>th</sup>

1<sup>st</sup> scientific session

Chair: Vladimír Sklenář

9<sup>00</sup> – 9<sup>30</sup> **Harald Schwalbe, Germany** – NMR spectroscopy in drug discovery

9<sup>30</sup> – 10<sup>00</sup> **Christina Redfield, UK** – Oxidation-state-dependent protein-protein interactions in disulfide cascades

10<sup>00</sup> – 10<sup>30</sup> **Jacob Anglister, Israel** – A study of the extra-cellular domain of a GPCR using NMR: CCR5 and its interaction with RANTES and HIV-1 gp120

10<sup>30</sup> – 11<sup>00</sup> Coffee break

11<sup>00</sup> – 11<sup>30</sup> **Rolf Boelens, Netherlands** – Structure and dynamics of DNA repair complexes

11<sup>30</sup> – 12<sup>00</sup> **Jordan Chill, Israel** – NMR 'divide and conquer' investigation of the disordered WASp-interacting protein

12<sup>00</sup> – 12<sup>30</sup> **Ivana Biljan, Croatia** – NMR studies of human prion protein mutants in solution

12<sup>30</sup> – 13<sup>00</sup> **Mirko Cevc, Slovenia** – NMR studies of Noncoding RNAs

13<sup>00</sup> – 14<sup>30</sup> Lunch break

## General assembly

Chair: Harald Schwalbe, Project coordinator

14<sup>30</sup> – 14<sup>50</sup> **Harald Schwalbe, Germany** – Overview of results of the East-NMR project

14<sup>50</sup> – 15<sup>10</sup> **Vladimír Sklenář, Czech Republic** – Presentation of networking activities

15<sup>10</sup> – 15<sup>30</sup> **Rolf Boelens, Netherlands** – Success of the Joint Research Activity

15<sup>30</sup> – 16<sup>00</sup> **Lucia Banci, Italy** – Achievements of transnational access

16<sup>00</sup> – 16<sup>30</sup> **Henriette Molinari, Italy** – Comments from the user community

16<sup>30</sup> – 17<sup>00</sup> Coffee break

17<sup>00</sup> – 18<sup>00</sup> Local operator meeting

17<sup>00</sup> – 19<sup>00</sup> East-NMR MC meeting

18<sup>00</sup> – 19<sup>00</sup> User meeting

19<sup>00</sup> Dinner

## Thursday, November 15<sup>th</sup>

### 2<sup>nd</sup> scientific session

Chair: Christina Redfield

- 9<sup>00</sup> – 9<sup>30</sup> **Lucia Banci, Italy** – NMR in integrated structural biology: From structures to function
- 9<sup>30</sup> – 10<sup>00</sup> **Robert Konrat, Austria** – Experimental demonstration of the condensed matter behaviour of intrinsically disordered proteins
- 10<sup>00</sup> – 10<sup>30</sup> **Sophie Zinn-Justin, France** – Structure, assembly and evolution of phage connector and tail proteins
- 10<sup>30</sup> – 11<sup>00</sup> Coffee break
- 11<sup>00</sup> – 11<sup>30</sup> **Miquel Pons, Spain** – Structure and dynamics of complexation with a flexible protein
- 11<sup>30</sup> – 12<sup>00</sup> **Henriette Molinari, Italy** – NMR investigation of the equilibrium partitioning of a water-soluble bile salt protein carrier in the presence of phospholipid vesicles
- 12<sup>00</sup> – 12<sup>30</sup> **Caroline Montagner, Belgium** – Equilibrium unfolding of Bacillus cereus zinc  $\beta$ -lactamase gives insights into the role of loops in the enzyme activity
- 12<sup>30</sup> – 13<sup>00</sup> **Boris Fürtig, Austria** – Chaperones modulate RNA structural dynamics through anti-folding
- 13<sup>00</sup> – 14<sup>30</sup> Lunch break
- 14<sup>30</sup> – 15<sup>00</sup> **Andrea Bodor, Hungary** – Asymmetric binding of the disordered myosin IIA tail fragment to the metastasis associated S100A4 protein
- 15<sup>00</sup> – 15<sup>30</sup> **Georgios A. Spyroulias, Greece** – NMR structural biology at University of Patras & The SEE-DRUG project
- 15<sup>30</sup> – 18<sup>00</sup> Poster session and final reviews
- 19<sup>00</sup> Dinner

## Friday, November 16<sup>th</sup>

### 3<sup>rd</sup> scientific session

Chair: Rolf Boelens

- 9<sup>00</sup> – 9<sup>30</sup> **Vladimír Sklenář, Czech Republic** – NMR heading high – Strategies for studies of partially disordered proteins
- 9<sup>30</sup> – 10<sup>00</sup> **Ago Samoson, UK** – Fast (enough?) MAS
- 10<sup>00</sup> – 10<sup>30</sup> **Fabien Ferrage, France** – Uncovering the dynamics of disordered proteins by multiple-magnetic field nuclear spin relaxation
- 10<sup>30</sup> – 11<sup>00</sup> Coffee break
- 11<sup>00</sup> – 11<sup>30</sup> **Roberta Pierattelli, Italy** – Direct <sup>13</sup>C detection NMR to characterize intrinsic disorder in proteins
- 11<sup>30</sup> – 12<sup>00</sup> **Wiktor Koźmiński, Poland** – New high dimensionality experiments for intrinsically disordered proteins
- 12<sup>00</sup> – 12<sup>30</sup> **András Perczel, Hungary** – Unfolding of a miniprotein; structures and intermediates at atomic level
- 12<sup>30</sup> – 13<sup>00</sup> **Torsten Hermann, France** – Modelling of protein structures with UNIO
- 13<sup>00</sup> – 14<sup>30</sup> Lunch break

## 4<sup>th</sup> scientific session

Chair: Ago Samoson

- 14<sup>30</sup> – 15<sup>00</sup> **Katalin E. Kövér, Hungary** – Measuring heteronuclear couplings with improved resolution – <sup>n</sup>J(<sup>77</sup>Se, <sup>1</sup>H) – based conformational and stereochemical analysis of selenosugars
- 15<sup>00</sup> – 15<sup>30</sup> **Somer Bekiroğlu, Turkey** – Use of hydroxyl protons in NMR spectroscopy: Is there anything in common for sweet molecules?
- 15<sup>30</sup> – 16<sup>00</sup> **Miloš Hricovíni, Slovakia** – NMR and theoretical analysis of saccharides: Influence of counter-ions upon 3D structure
- 16<sup>00</sup> – 16<sup>30</sup> Coffee break
- 16<sup>30</sup> – 17<sup>00</sup> **Sabine Hediger, France** – Structure and interactions of the bacterial cell wall by solid-state NMR and DNP
- 17<sup>00</sup> – 17<sup>30</sup> **Mark Lorch, UK** – Dynamic nuclear polarization enhanced solid state NMR of a <sup>13</sup>C labeled signal peptide bound to lipid reconstituted Sec translocon
- 17<sup>30</sup> – 18<sup>00</sup> **Lena Mäler, Sweden** – Lipid interactions of glycosyltransferases
- 18<sup>00</sup> – 18<sup>30</sup> **Thomas Mavromostakos, Greece** – Exploring the molecular basis of interactions of candesartan cilexetil (TCV-116) in lipid bilayers using solid state NMR spectroscopy
- 18<sup>30</sup> Concluding remarks
- 19<sup>00</sup> Dinner