



High resolution tools to understand the functional role of protein intrinsic disorder

21 – 26 September 2014

Castiglione della Pescaia, Italy

Scientific Programme





Organizers

**Isabella C. Felli
Roberta Pierattelli
Francesca Di Gloria
Francesca Morelli**

IDPbyNMR partners

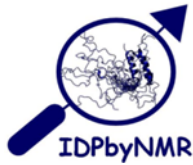
**Isabella C. Felli
Roberta Pierattelli
Martin Blackledge
Bernhard Brutscher
Dmitri Svergun
Peter Tompa
Michele Vendruscolo
András Dinnyés
Tatiana Kozyreva
Rainer Kümmerle
Andrea Degen**

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Priyanka Joshi
Mikhail Kachala
Magdalena Korsak
Jaka Kragelj
Alexandra Louka
Anna Lovrics
Hadas Raveh-Amit
Zsófia Sólyom
Erica Valentini**

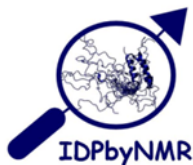
Thanks to

**Lorenzo Baronti
Azzurra Carlon
Tomáš Hošek
Magdalena Korsak
Tatiana Kozyreva
Alexandra Louka
Marcela Nogueira
Talita Pagani
Alessandro Piai**



Sunday 21st September

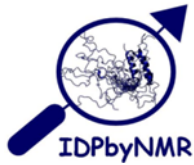
16:00 – 18:00	Registration
18:00 – 18:20	Isabella C. Felli & Roberta Pierattelli <i>Opening</i>
18:20 – 18:50	Vladimir N. Uversky <i>Intrinsically disordered proteins: Past, present, and future.</i>
19:00 – 20:00	Aperitif
20:00 – 22:00	Dinner



Monday 22nd September

9:00 – 9:30	Peter Tompa <i>The pE-DB database: a tool for approaching IDP function by dynamic structural ensembles.</i>
9:40 – 10:10	Isabella C. Felli <i>New methods to study intrinsically disordered proteins based on ¹³C direct detection.</i>
10:20 – 10:40	John L. Markley <i>Serial functional conversions between disordered and ordered states in the scaffold protein for iron-sulfur cluster biosynthesis.</i>
10:45 – 11:15	Coffee
11:15 – 11:45	Michele Vendruscolo <i>Structure and dynamics of intrinsically disordered proteins.</i>

11:55 – 12:25	Rainer Kümmerle <i>NMR hardware.</i>
12:35 – 12:55	Priyanka Joshi <i>Targeting IDPs: A fragment-based strategy for the screening of small drug-like molecules for intrinsically disordered proteins.</i>
13:00 – 16:00	Seaside & Sandwich
16:00 – 16:30	András Dinnyés <i>Neuronal differentiation from human induced pluripotent stem cells.</i>
16:40 - 17:00	Kyou-Hoon Han <i>The Pre-Structured Motifs (PreSMos) in IDPs.</i>
17:05 – 17:25	Magdalena Korsak <i>From IDP to Alzheimer's disease - insight into beta amyloid protein.</i>
17:30 – 18:00	Coffee
18:00 – 18:20	Jaka Kragelj <i>Role of intrinsically disordered regions in MAP kinase signaling pathways: Substrate recognition in the c-Jun N-terminal kinase (JNK) pathway.</i>
18:25 – 18:45	Frans A.A. Mulder <i>Unambiguous sequential assignments by correlating the backbone chemical shifts of seven contiguous residues in a 3D spectrum.</i>
18:50 – 19:20	Ad Bax <i>New methods and parameters for defining IDP structure and dynamics.</i>
19:45 – 21:00	Dinner
21:00 – 23:00	Posters



Tuesday 23rd September

9:00 – 9:30

Martin Blackledge

Complex dynamics and dynamics complexes: Visualizing the molecular recognition trajectories of intrinsically disordered proteins.

9:40 – 10:10

Dmitri I. Svergun

Small-angle X-ray scattering to study the structure and flexibility of biological macromolecules in solution.

10:20 – 10:40

Erica Valentini

SASBDB: a curated repository of biological small angle scattering data and models.

10:45 – 11:15

Coffee

11:15 – 11:45

Monika Fuxreiter

Genome-wide analysis of fuzzy complexes.

11:55 – 12:25

Toby J. Gibson

IDP and cell regulation by molecular switching.

12:35 – 12:55

Pallab Bhowmick

Tripartite degrons impart diversity, specificity and multi-layered regulability to ubiquitin-mediated proteasomal degradation.

13:00 – 16:00

Seaside & Sandwich

16:00 – 16:30

Andrea Degen

Graduate curricula: Support towards academic careers and beyond.

16:30 - 17:30

Round table on pE-DB

17:30 – 18:00

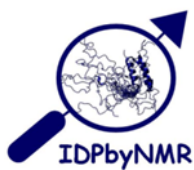
Coffee

18:00 – 18:20

Elisar Barbar

Protein disorder in dynein regulation by dynactin.

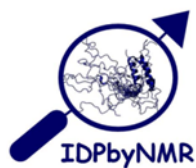
18:25 – 18:45	Biao Fu <i>Molecular dynamics simulations of intrinsically disordered proteins with replica-averaged chemical shift restraints.</i>
18:50 – 19:20	Peter E. Wright <i>Intrinsic disorder, posttranslational modification, and signaling complexity.</i>
20:00 – 22:00	BBQ and music



Wednesday 24th September

9:00 – 9:30	Christian Griesinger <i>Dynamics of biomolecular systems studied by NMR and further biophysical techniques.</i>
9:40 – 10:10	Robert Konrat <i>NMR spin relaxation approaches to structural dynamics of intrinsically disordered proteins.</i>
10:20 – 10:40	Tomáš Hošek <i>¹³C detected experiments to monitor ¹H^N and ¹H^α longitudinal relaxation: Hints on protein compactness and solvent accessibility.</i>
10:45 – 11:15	Coffee
11:15 – 11:45	H. Jane Dyson <i>NMR studies of structure and flexibility in the NFκB-IκBα system.</i>
11:55 – 12:25	Sonia Longhi <i>Order and disorder within the replicative complex of paramyxoviruses.</i>
12:35 – 12:55	Eduardo O. Calçada <i>Characterization of flexible linkers: the case of ID4 from CBP.</i>
13:00 – 16:00	Seaside & Sandwich
16:00 – 17:30	Posters

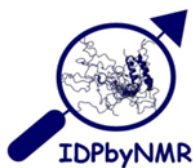
17:30 – 18:00	Coffee
18:00 – 18:20	Mikhail Kachala <i>Monte-Carlo based approach for simultaneous determination of form and structure factors for mono- and polydisperse solutions in small angle scattering data analysis.</i>
18:25 – 18:45	Cesyen Cedeño <i>Towards an in-cell NMR experiment for plants. Dos and don'ts.</i>
18:50 – 19:20	Philipp Selenko <i>Atomic resolution insights into the structure of a human amyloid protein in neuronal and non-neuronal cells.</i>
20:00 – 22:00	Dinner



Thursday 25th September

9:00 – 9:30	Bernhard Brutscher <i>Fast sensitivity-enhanced NMR experiments for the study of intrinsically disordered proteins (IDPs).</i>
9:40 – 10:00	Vladislav Yu. Orekhov <i>Causality principle in reconstruction of sparse NMR spectra.</i>
10:05 – 10:25	Fabien Ferrage <i>A new approach for the Interpretation of NMR relaxation rates to characterize dynamics in intrinsically disordered proteins.</i>
10:30 – 10:50	Sergio Gil <i>NMR studies of intrinsically disordered proteins at near physiological conditions.</i>
10:55 – 11:25	Coffee

11:25 – 11:55	Xavier Salvatella <i>Order disorder transitions in the androgen receptor: implications for the onset and treatment of prostate cancer.</i>
12:05 – 12:35	Roberta Pierattelli <i>The heterogeneous structural behaviour of viral intrinsically disordered proteins revealed by NMR spectroscopy.</i>
12:45 – 13:05	Tatiana Kozyreva <i>Potential SOD1 fALS mutants toxic species precursor revealed by in-cell NMR.</i>
13:10 – 16:00	Seaside & Sandwich
16:00 – 16:20	Zsófia Sólyom <i>Transient structure and dynamics of the intrinsically disordered region of HCV protein NS5A.</i>
16:25 – 16:55	A. Keith Dunker <i>Intrinsically disordered protein and multicellular organisms.</i>
17:05 – 17:30	Closing
17:30 - night	Sunset in Castiglione and Closing dinner



Friday 26th September

Departure