

July 2 Sunday

- 11.00- Registration
- 11.30-14.00 EU-OPENSOURCE Partner Site Workshop
- 15.30-15.45 Opening ceremony
- 15.45-16.30 Chair: **Ronald Frank**
PL-1 Herbert Waldmann, Max Planck Institute of Molecular Physiology, Germany
Chemotype-Phenotype-Target
- 16.30-17.00 **Session 1: Screening technologies: assay design, development and hit validation**
Chair: **Gergely Makara**
KL-1 Hans Bräuner-Osborne, Department of Drug Design and Pharmacology, University of Copenhagen, Denmark
Screening technologies: assay design, development and hit validation
- 17.00-17.15 **OL-1 Mercedes Beyna**, Biogen, USA
Discovery of novel transcriptional regulation of NF- κ B signaling via phenotypic screening and chemoproteomics
- 17.15-17.45. **Session 2: Molecular targets and systems**
Chair: **Attila Reményi**
KL-2: Patrick Aloy, Institute for Research in Biomedicine, Spain
A network biology approach to novel therapeutic strategies
- 17.45-18.00 **OL-2 Veronika F.S. Pape**, Hungarian Academy of Sciences, Institute of Enzymology, Hungary
Putting the bite on metals – a ligand based approach to overcome multidrug resistance in cancer
- 18.00-20.00 Welcome reception

July 3 Monday

- 9.00-9.45 Chair: **Bahne Stechmann**
PL-2 Stefan Knapp, Buchmann Institute for Molecular Life Sciences, Frankfurt am Main
Systematic validation of new disease targets by chemical probes
- 9.45-10.15 **Session 3: Chemoinformatics**
Chair: **György Ferenczy**
KL-3 Didier Rognan, CNRS, France
Structure-based discovery of allosteric modulators of receptor tyrosine kinases

10.15-10.30	OL-3 Albert A Antolin , The Institute of Cancer Research, UK <i>Target-Probes Assessment Resource: Objective, Quantitative, Unbiased Assessment of Chemical Probes</i>
10.30-11.00	Coffee break
11.00-11.25	Session 4: Library design and chemical diversity Chair: György Dormán KL-4 Gergely Makara <i>The evolution of library design from combi-chem to in-silico organic chemistry</i>
11.25-11.40	OL-4 Yurii Moroz , Enamine Ltd, Ukraine <i>Real Fragment-Like Covalent Modifiers / Real Arrays – A Comprehensive Database Of Readily Synthesizable Molecules</i>
11.40-11.55	OL-5 Andrea Trabocchi , University of Florence <i>Diversity-Oriented Synthesis of heterocyclic sp³-rich molecular scaffolds through build/couple/pair of carbohydrate and amino acid derivatives</i>
11.55-12.25	Session 5: Manipulation of cellular states and combatting diseases Chair: Gergely Szakács KL-5 Hans Schöler , Max Planck Institute for Molecular Biomedicine, Germany <i>Induction of Pluripotent and Multipotent Stem Cells</i>
12.25-12.40	OL-6 Maria J. Vicent , Centro Investigación Príncipe Felipe, Spain <i>Tumor-derived exosome release as novel target to identify effective anticancer combination therapies for metastatic processes</i>
12.40-14.15	Lunch
14.15-14.45	Session 6: Biocompatible labelling and imaging Chair: Péter Kele KL-6 Hans-Achim Wagenknecht , Karlsruhe Institute of Technology, Germany <i>Bioorthogonal labeling of nucleic acids for fluorescent imaging</i>
15.15-15.30	OL-7 Eszter Kozma , Hungarian Academy of Sciences , Research Centre for Natural Sciences, Hungary <i>Intracellular superresolution microscopy enabled by bioorthogonal double-fluorogenic silicorhodamine-tetrazine probes</i>
15.30-16.00	Coffee Break
16.00-17.15	Poster session
17.15-19.00	Leaving to dinner
19.00-	Dinner

July 4 Tuesday

9.00-9.45	<p>Chair: Philip Gribbon PL-3 John P. Overington, Medicines Discovery Catapult, UK <i>Data Mining in Small Molecule Drug Discovery</i></p>
9.45-10.15	<p>Session 7: Plant biotech and natural products Chair: Gábor Vasas KL-7 Anne Osbourn, John Innes Centre, Norwich, UK <i>Harnessing plant metabolic diversity: from genomes to gram-scale quantities of natural products and analogs</i></p>
10.15-10.30	<p>OL-8 Francisca Vicente, Fundación MEDINA, Centro de Excelencia en Investigación de Medicamentos Innovadores en Andalucía, Spain <i>Application of Labcyte Echo® Liquid Handling to Microbial Natural Product Extracts and Pure Compounds from MEDINA Library in High-Throughput Miniaturized Assays</i></p>
10.30-11.00	Coffee break
11.00-11.30	<p>Session 8: Photochemical applications Chair: Gábor London KL-8 José Luis Mascarenas, Universidad de Santiago de Compostela, Spain <i>Metal-based tools in Chemical Biology</i></p>
11.30-11.45	<p>OL-9 Lilia Reytmán, Institute of Chemistry, The Hebrew University of Jerusalem, Israel <i>Hydrolytically Stable Vanadium(V) Phenolato Antitumor Agents: The role of the ligand in the cytotoxic pathway</i></p>
11.45-12.05	<p>Short talks (5' each) Chair: Katja Herzog ST-1 Frederic Friscourt, Institut Européen de Chimie et Biologie - University of Bordeaux, France <i>A Turn-On Bioorthogonal Probe for the Selective Visualization of Biomolecules in No-Wash Conditions</i> ST-2 Csaba Hetényi, University of Pécs, Hungary <i>Unraveling the histone code by fragment blind docking</i> ST-3 Attila Kormos, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Hungary <i>Double Quenched Fluorogenic Cyanines for bioorthogonal two-point tagging</i> ST-4 Ctibor Skuta, Institute of Molecular Genetics of the ASCR, Czech Republic <i>Probes & Drugs portal: interactive approach to Open Data exploration in chemical biology</i></p>
12.05-13.05	Partner Site Demonstrations
13.05-13.20	Closing ceremony
13.20-	Lunch