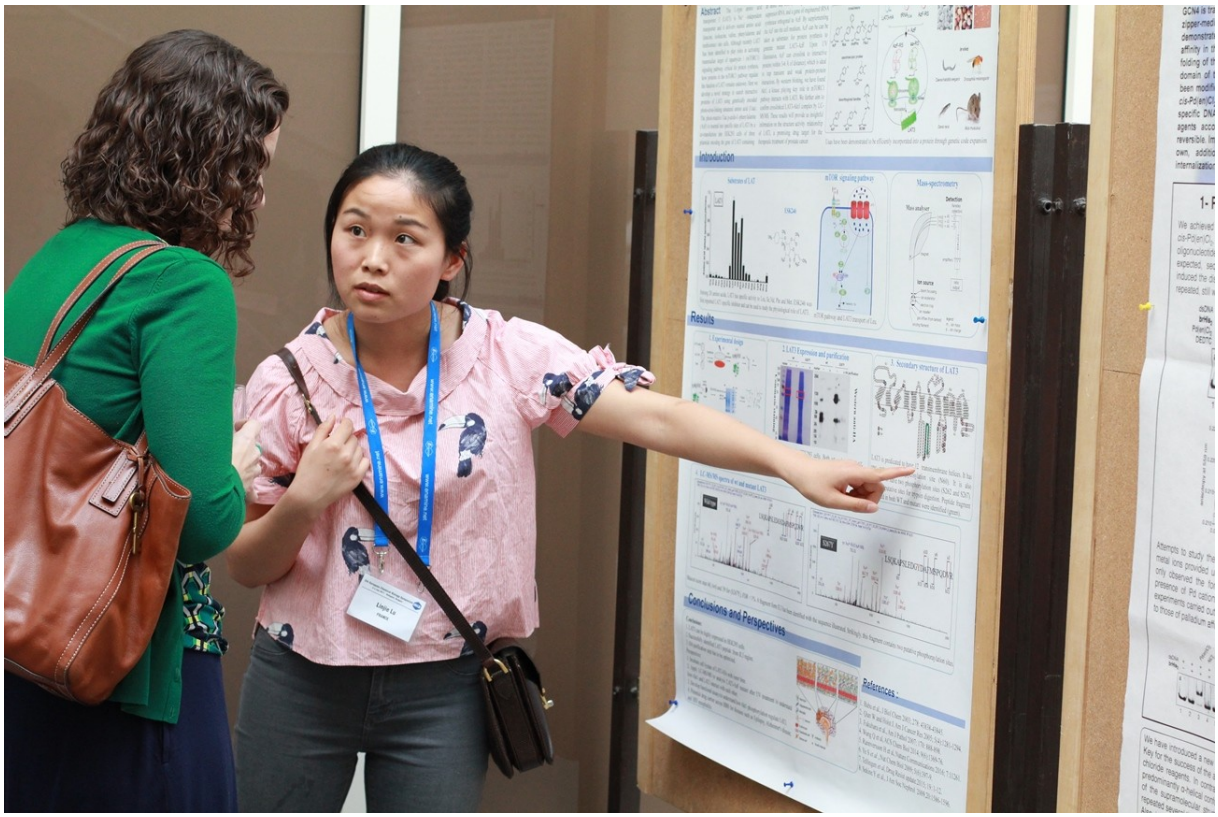
Report of the ECBS2017 meeting and the chemical biology workshop on library design and bioprofiling and databases

ECBS2017 and EU-OPENSCREEN partners in Budapest: a fruitful meeting!

The EU-OPENSCREEN community met in Budpest- Hungary, July 2nd – 4th, during the 5th European Chemical Biology Symposium.

Hosting more than 100 participants from 22 countries in Europe, Asia and America, the meeting featured three keynote lectures, eight plenary talks, nine oral presentations, four short talks and over 50 posters.



The conference keynotes presented different perspectives on chemical biology. Herbert Waldmann from the Max-Planck-Institut für molekulare Physiologie in Dortmund – Germany presented small molecule library design inspired by natural products and biological evolution, Stefan Knapp from the Johann Wolfgang Goethe-University in Frankfurt am Main – Germany talked about the systemic validation of new disease targets, and John P. Overington from Medicines Discovery Catapult in Cheshire – United Kingdom talked about the development of chemical biology databases and ongoing challenges in data mining.

The conference also hosted an EU-OPENSCREEN workshop for nominated partner sites as well as potential commercial vendors to discuss a range of topics related to the set-up of the EU-OPENSCREEN ERIC.

The full breadth of EU-OPENSCREEN resources and technologies was highlighted during a session dedicated to partner site demonstrations, in a special part in the program booklet and an EU-OPENSCREEN poster corner.

The poster prizes went to Zoeisha S. Chinoy from the European Institute for Chemistry and Biology in Bordeaux – France for her work on novel glycan-reporters for metabolic oligosaccharide engineering and to Saba Nojoumi from the Technical University of Berlin – Germany for engineering modular biopolymers as functional multivalent scaffolds.

EU-OPENSCREEN and the Hungarian Society of Chemical Biology would like to thank all speakers and participants of the conference - for their insightful talks and inspiring discussions!

A special thank you also goes to the local organisers Attila Reményi, Görgy Dorman, Panna Korispataky, Beata Androsits, Eszter Kortvelyessy and Andrea Gonusz.

There was a worshop on the different aspects of the EU-OPENSCREEN project where experts discussed library formats, bioprofiling and data analyis.

The program of this venue is seen below.

EU-OPENSCREEN Partner Site Workshop
2nd July 2017

Venue: Research Center for Natural Sciences of the Hungarian Academy of Sciences, Budapest, Magyar tudósok körútja 2)

DAY 1 - Sunday, July 2nd 2017

11:30 **TOP 1 – Welcome & Introduction**

Philip Gribbon

- Current status of EU-OPENSCREEN
- EU-OPENSCREEN ERIC: Inauguration, prospective ERIC members and observers
- Overview of the Partner Site Evaluation (screening, assay adaptation and chemistry sites)

11:45 ***COMPANY TALK: David Booth – Titian*** *(www.titian.co.uk)*

- Multi-site inventory (MOSAICS) http://www.titian.co.uk/mosaic-products/

COMPANY TALK: **Vladimir Ivanov –** ***Enamine*** *(http://www.enamine.net/)*

11:55 **TOP 2 – Library formats and practical aspects**

Bahne Stechmann

- Design principles for the design of the commercial compound collection
- Past experiences with vendors
- Selection criteria for academic compounds

12:25 **TOP 3 – Bioprofiling assays**

Petr Bartunek

- Bioprofiling: Concept, budget and next steps

12:45 **TOP 4 – Data analysis and ECBD**

Bahne Stechmann

- Update on the evaluation procedure for the host of the EU-OPENSCREEN Database (ECBD, European Chemical Biology Database)
- Main characteristics and uses of the ECBD

13:10 **TOP 5 – Organisation and next steps**

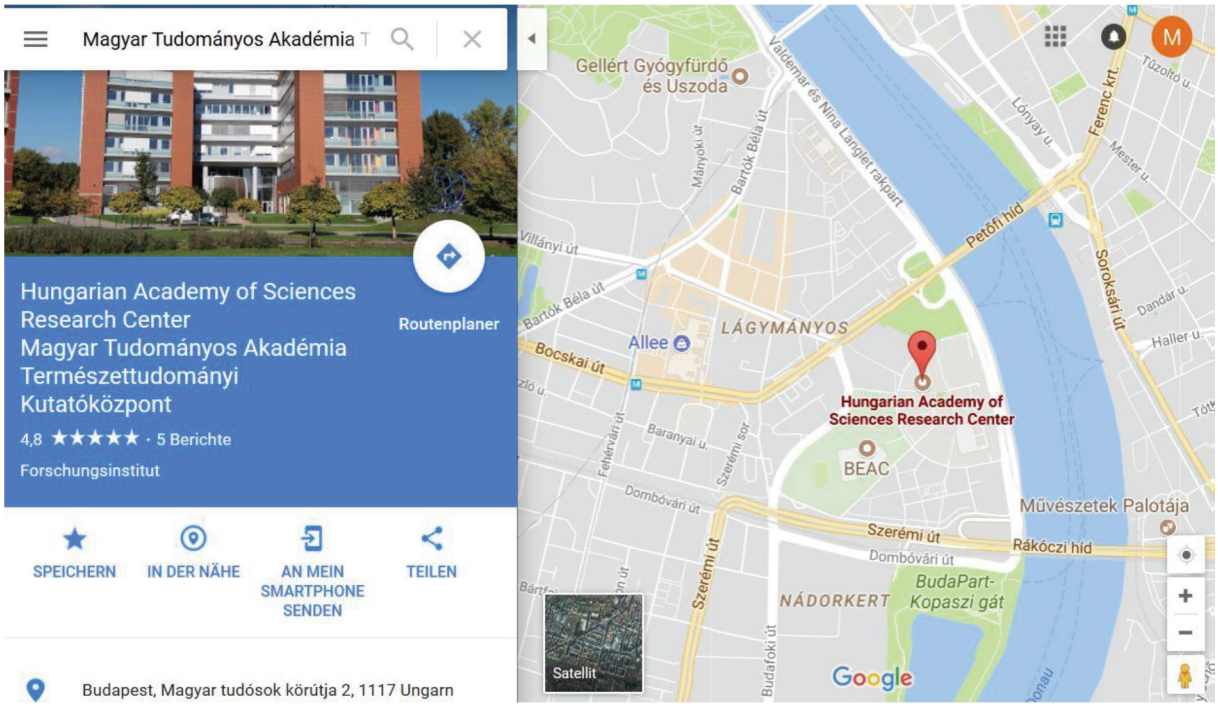
Phil Gribbon

- Partner Site Evaluation: Next steps towards formal approval

- EU-OPENSCREEN Working Groups (Library Design Group, Bioprofiling Group)
- The next six months until the ERIC Inauguration

13:20 **TOP 6 – AOB**
Philip Gribbon

13:30 *Snack Lunch*



July 2 Sunday

11.00-	Registration
11.30-14.00	EU-OPENSCREEN 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-kB 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 multidrog 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 *Target-Probes Assessment Resource: Objective, Quantitative, Unbiased Assessment of Chemical Probes*
10.30-11.00	Coffee break
11.00-11.25	**Session 4: Library design and chemical diversity** Chair: **György Dormán** **KL-4 Gergely Makara** *The evolution of library design from combichem to in-silico organic chemistry*
11.25-11.40	**OL-4 Yurii Moroz**, Enamine Ltd, Ukraine *Real Fragment-Like Covalent Modifiers / Real Arrays – A Comprehensive Database Of Readily Synthesizable Molecules*
11.40-11.55	**OL-5 Andrea Trabocchi**, University of Florence *Diversity-Oriented Synthesis of heterocyclic sp3-rich molecular scaffolds through build/couple/pair of carbohydrate and amino acid derivatives*
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 *Induction of Pluripotent and Multipotent Stem Cells*
12.25-12.40	**OL-6 Maria J. Vicent**, Centro Investigación Príncipe Felipe, Spain *Tumor-derived exosome release as novel target to identify effective anticancer combination therapies for metastatic processes*
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 *Bioorthogonal labeling of nucleic acids for fluorescent imaging*
15.15-15.30	**OL-7 Eszter Kozma**, Hungarian Academy of Sciences , Research Centre for Natural Sciences, Hungary *Intracellular superresolution microscopy enabled by bioorthogonal double-fluorogenic silicorhodamine-tetrazine probes*
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	Chair: **Philip Gribbon** **PL-3 John P. Overington**, Medicines Discovery Catapult, UK *Data Mining in Small Molecule Drug Discovery*
9.45-10.15	**Session 7: Plant biotech and natural products** Chair: **Gábor Vasas**
	KL-7 Anne Osbourn, John Innes Centre, Norwich, UK *Harnessing plant metabolic diversity: from genomes to gram-scale quantities of natural products and analogs*
10.15-10.30	**OL-8 Francisca Vicente**, Fundación MEDINA, Centro de Excelencia en Investigación de Medicamentos Innovadores en Andalucía, Spain *Application of Labcyte Echo® Liquid Handling to Microbial Natural Product Extracts and Pure Compounds from MEDINA Library in High-Throughput Miniaturized Assays*
10.30-11.00	Coffee break
11.00-11.30	**Session 8: Photochemical applications** Chair: **Gábor London**
	KL-8 José Luis Mascarenas, Universidad de Santiago de Compostela, Spain *Metal-based tools in Chemical Biology*
11.30-11.45	**OL-9 Lilia Reytman**, Institute of Chemistry, The Hebrew University of Jerusalem, Israel *Hydrolytically Stable Vanadium(V) Phenolato Antitumor Agents: The role of the ligand in the cytotoxic pathway*
11.45-12.05	**Short talks (5' each)** Chair: **Katja Herzog**
	ST-1 Frederic Friscourt, Institut Européen de Chimie et Biologie - University of Bordeaux, France *A Turn-On Bioorthogonal Probe for the Selective Visualization of Biomolecules in No-Wash Conditions*
	ST-2 Csaba Hetényi, University of Pécs, Hungary *Unraveling the histone code by fragment blind docking*
	ST-3 Attila Kormos, Research Centre for Natural Sciences, Hungarian Academy of Sciences, Hungary *Double Quenched Fluorogenic Cyanines for bioorthogonal two-point tagging*
	ST-4 Ctibor Skuta, Institute of Molecular Genetics of the ASCR, Czech Republic *Probes & Drugs portal: interactive approach to Open Data exploration in chemical biology*
12.05-13.05	Partner Site Demonstrations
13.05-13.20	Closing ceremony
13.20-	Lunch