

1st SCT Workshop on Biologically Relevant Molecular Diversity

Programme

Thursday April 4, 2013

08:30 Registration

09:10 Introductory Remarks

Dr Pascal GEORGE
(SCT & INDEPENDENT SCIENTIFIC EXPERT & ADVISER, Longvilliers, France)

Chemspace Session

Session Chair

Prof. Benoit DEPREZ
(UNIVERSITY OF LILLE 2, Lille, France)

09:20 The Chemical Space Project

Prof. Jean-Louis REYMOND
(UNIVERSITY OF BERN, Bern, Switzerland)

10:00 Feature-based Pharmacophores for Molecular Profiling

Prof. Dr Thierry LANGER
(PRESTWICK CHEMICAL, Vienna, Austria)

10:40 Coffee Break and Exhibition

11:10 Navigation in Chemistry Space Towards Biological Activity

Dr Peter ERTL
(NOVARTIS INSTITUTE FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

11:50 Chemspace Session - Roundtable Discussion

12:30 Lunch and Exhibition

Biospace Session

Session Chair

Dr Gerhard MÜLLER
(MERCACHEM, Nijmegen, The Netherlands)

14:00 Molecular Diversity : Why Do We Want it? What Do We Get?

Dr Ansgar SCHUFFENHAUER
(NOVARTIS INSTITUTES FOR BIOMEDICAL RESEARCH, Basel, Switzerland)

14:40 Merging Chemical and Biological Spaces

Prof. Gabriele CRUCIANI
(UNIVERSITY OF PERUGIA, Perugia, Italy)

15:20 Systematic Mapping of Target-Ligand Interactions Using Compound Activity Data

Prof. Jürgen BAJORATH
(UNIVERSITY OF BONN, Bonn, Germany)

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16:00 **Biospace Session - Roundtable Discussion**

16:40 **Coffee Break and Exhibition**

Perspectives

Session Chair

Dr Bruno VILLOUTREIX
(INSERM / UNIVERSITY PARIS DIDEROT, Paris, France)

17:05 **Macrocycles Approaches for Protein-protein Interactions**

Dr Daniel OBRECHT
(POLYPHOR, Allschwil, Switzerland)

17:45 **Enriching Chemical Space by Diversity–Oriented Synthesis of Natural Product-Like Compounds**

Dr David SPRING
(UNIVERSITY OF CAMBRIDGE, Cambridge, United Kingdom)

Session Chair

Dr Gerhard MÜLLER (MERCACHEM, Nijmegen, The Netherlands)

18:25 **Take Home message**

18:40 **Final Conclusions**

Dr Pascal GEORGE
(SCT & INDEPENDENT SCIENTIFIC EXPERT & ADVISER, Longvilliers, France)