

# 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. 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)

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

**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)

**18:25 Take Home message**

**18:40 Final Conclusions**

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