# Strasbourg Summer School on Chemoinformatics

## Obernai, France, 22 - 25 June 2008

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## Sunday, 22 June

**14:00-17:00** Registration

**17:00-17:10** ***Opening Remarks*** *(A. Varnek, D. Rognan)*

**17:10-17:40** **T. Fujita**

QSAR: discovery and first steps

**17:40-18:20** **J. Gasteiger**

History and challenges of chemoinformatics.

**18:20-19:00** **W. Warr**

Current trends in chemoinformatics

**19:00** ***Welcome party***

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## Monday, 23 June (morning session)

***Molecular Similarity Analysis in Virtual Screening***

*Chairman:* *J. Gasteiger*

**8:30-09:30** **J. Bajorath**

Fingerprint Design and Molecular Complexity Effects

**9:30-10:30** **V. Gillet**

Diversity Analysis and Library Design

**10:30 10:45** ***Coffee break***

**10:45-11:45** **G. Schneider**

*De novo* Design

## Monday, 23 June (after-noon session)

*Chairman: J. Bajorath*

**14:00 – 15:00** **R. Glen**

Lessons learned from modelling bioactivity - what works and what doesn't

**15:00 – 16:00** **T. Oprea**

Exploring novel estrogen receptors and more...

**16:00 – 16:15** ***Coffee break***

**16:15 – 17:30** **N. Weill, G. Marcou, D. Horvath, A. Varnek and D. Rognan**

Tutorial: Impact of dataset composition on models performance

**17:45-19:00** Meeting SFCi (*Albert Schweitzer hall*)

**17:45-19:00** Software demonstration (*Hansi hall*)

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## Tuesday, 24 June (morning session)

***QSAR/QSPR strategies, ADME/Tox predictions***

*Chairwoman: W. Warr*

**8:30-09:30** **R. Todeschini**

Molecular descriptors: an overview

**9:30-10:30** **A. Tropsha**

The good, the bad and the ugly practices of QSAR modelling

**10:30 10:45** ***Coffee break***

**10:45-11:45** **T. Langer**

Pharmacophore Approach in Drug Discovery

## Tuesday, 24 June (after-noon session)

*Chairman: R. Glen*

**14:00 – 15:00** **J. Aires-de-Sousa**

Classification of chemical resactions

**15:00 – 16:00** **I. Tetko, I. Baskin**

Machine learning methods in QSAR

**16:00 – 17:00** **I. Baskin, I. Tetko and A. Varnek**

Tutorial on application of non-linear methods in chemistry (neural networks, support vector machines)

**17:00 17:15** ***Coffee break***

**17:00 - 18:00** ***Poster session*** *(Bertoldi hall)*

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## Wednesday, 25 June (morning session)

***Bio- and Chemoinformatics: Key Technologies within the Drug Discovery Process***

*Chairman: R. Todeschini*

**8:30-09:15** **J. Mestres**

*In silico* target profiling

**9:15--10:15** **D. Rognan**

Docking and post-docking strategies

**10:15 10:30** ***Coffee break***

**10:30- 11:15** **M. Stahl**

What Crystal Structure Databases Tell us about Conformational Preferences of Drug-like Molecules

**11:15 – 12:00** **P. Ertl (Novartis)**

The Role of Cheminformatics in the Modern Drug Discovery Process

## Wednesday, 25 June (after-noon session)

**14:00 – 16:00** **Round Table** *(A. Tropsha, P. Vayer, L. Morin-Allory)*

- ***Hot topics in chemoinformatics***
- ***Teaching chemoinformatics***

**16:00** **Closing Remarks** *(A. Varnek, D. Rognan)*