Workshop Chemoinformatics in Europe: Research and Teaching

Obernai, France, 29 May – 1 June 2006

Monday May, 29th

15:00-18:00 Registration

18:00-19:00 ***Opening Remarks*** (A. Varnek, D. Rognan)

18:10-19:10 ***Opening Lecture*** J. Gasteiger (U. Erlangen, Germany):*Chemoinformatics in Europe: Achievements and perspectives.*

19.10 Welcome party

Tuesday May, 30th

Session 1: Encoding Chemical Structures

Chairman: P. Willett

8:30-09:00 R. Glen (UCMSI, Cambridge, UK):*Chemical informatics: where are we headed?*

9:00-09:20 Christoph Steinbeck (U. of Cologne, Germany): *Open Source Components for Chemoinformatics Education*

9:20-09:40 R. Todeschini (U. Milano-Bicocca, Italy):*On the characterization of DNA primary sequences by a new algorithm for similarity/diversity measures.*

9:40-10:00 ***Coffee break***

10:00-10:30 G. Schneider (U. Frankfurt, Germany): *"Fuzzy" pharmacophores for virtual database screening and library design*

10:30-10:50 R.D. Clark and E. Metwally *Pharmacophores, Pharmacosteres, Flexibility and Fast Feature Multiplets* (Tripos Discovery Informatics Research Center, St. Louis, MO, USA)

10:50 – 12.00 Round Table 1 (leader J. Gasteiger)

Chemoinformatics community in Europe: How should we get organized ?

- Do we need a separate European Chemoinformatics Society given that there exists the International QSAR and Cheminformatics Society ?
- Shall we organize regular European workshops, or conferences, or summer schools ? If "yes", how often ?

- Funding of Chemoinformatics in Academia and Industry.
- Availability and exchange of data.

12:00-13:30 ***Lunch***

Session 2: Predicting physicochemical properties

Chairman: R. Todeschini

13:30-14.00 G. Cruciani (U. Perugia, Italy): *Predicting metabolism by human Cytochromes P450.*

14.00-14:20 P.Vayer (Technologie SERVIER, France): *Application of molecular modelling to biopharmaceutical properties screening.*

14:20-14:40 N. T. Hansen (Danish University of Pharmaceutical Sciences, Denmark): *Prediction of pH-dependent aqueous solubility of drug-like molecules.*

14:40-15:00 I.V. Tetko (Institute for Bioinformatics, Germany): *Estimation of the accuracy of ADMET predictions and secure sharing of information are two sides of the same coin.*

15*:00-15:20** ***Coffee break

Session 3: Chemoinformatics in Academic and Industrial Settings

Chairman: T. Oprea

15:20-15:50 P. Willett (U. Sheffield, U.K.): *Post-graduate education programmes in chemoinformatics*

15:50-16:10 J. Pansanel (Aptonomics S.A., France): *The information system in a small biotech company : Overview of the cheminformatics developments at Aptonomics.*

16:10-16:30 A. Klamt (COSMOlogic GmbH&Co KG, Germany): *From quantum chemistry to chemoinformatics.*

16:30-17:30 Round Table 2 (leader P. Willett)

Teaching of Chemoinformatics at the graduate and post-graduate level

- Which topics should be covered in the Master and PhD programs on chemoinformatics ?
- Wow many such programs do we need in Europe ?
- What is the job outlook for chemoinformatics specialists ?

17:30-18:30 Poster Session

Wednesday May, 31st

Session 4: Navigating in Chemical Space

Chairman: G. Cruciani

8:30-09:00 T. Oprea (U. New Mexico, USA): *How does Cheminformatics Contribute to Lead and Drug Discovery ?*

9:00 -09:20 C. Laggner (U. Insbrück, Austria): *Reproducing bio-active conformations with CATALYST and OMEGA*

9:20-09:40 A. Clark, (Chemical Computing Group, Inc): *The 2D Depiction Algorithm in MOE*

***9:40-10:00* Coffee break**

10:00-10:30 A. Tropsha (U. North Carolina, USA): *Cheminformatics Analysis of Protein-Ligand Interface*

10:30-10:50 J. Bajorath (U. Bonn, Germany): *Novel Algorithms for Molecular Similarity Analysis and Virtual Screening*

10:50-11:10 D. Horvath (CNRS UMR 8576, France): *Comprehensive variable selection strategies in linear and non-linear QSAR.*

11:10-11:30 A.G. Maldonado (U. Paris 7, France): *A new structural approach for molecular similarity and diversity in chemoinformatics.*

11:30-11:50 N. Brown (Novartis, Basel): *The application of consensus modelling and genetic algorithms in interpretable discriminant analysis.*

***12:00-13:30* Lunch**

Session 5: Assisting Rational Drug Design

Chairman: A. Tropsha

13:30-14:00 Dr. P. M. Selzer (Intervet Innovation GmbH, Germany): *Bio- and Chemoinformatics: Key Technologies within the Drug Discovery Process.*

14:00-14:20 F. Barbault (CNRS UMR 7086, France): *RNA as drug target in docking studies.*

14:20-14:40 M. Ford (U. Porsmouth, U.K.): *Identifying GPCR/ligand binding sites using consensus regression.*

14:40-15:00 F. Moriaud (MEDIT S.A., France): *MED-SuMo: From target based drug design to innovative cheminformatics tools.*

***15:00-15:20* Coffee break**

15:20-15:40 E. Van de Water (Accelrys): *A Data Pipelining Approach to Data Retrieval Organization and Reporting*

15:40-16:00 C. Daul **(**U. Fribourg, Switzerland)The self-consistent perturbed projection method for high order response

16:00-16:20 T. Nyronen (Finnish IT Center for Science, Finland): *SOMA - Environment for Integrating Molecular Modeling Workflows on a Multiplatform Computing Grid*

16:20-16:40 G. Pirok (ChemAxon) *Standardizer: Molecular cosmetics for cheminformatics*

16:40-17:40 **Round Table 3 (leaders A. Varnek, D. Rognan, J. Gasteiger, P. Willett)**

- Future of Chemoinformatics in Europe,
- Summary of all Round Tables,
- Organization issues, action plan.

17:40-17:50 **Concluding remarks (A. Varnek, D. Rognan)**

18:00 ***Departure to the Conference Dinner (Barr)***

Thursday, June 1st

Departure at 9:00