Chemoinformatics
Ph.D. course
Danish University of Pharmaceutical Sciences (DFU),
Technical University of Denmark (DTU) & Drug Research Academy

Course director: Associate Professor Flemming Steen Jørgensen
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Monday 27. September 2004

9.15 - 9.30 Welcome and Practical Information
Flemming Steen Jørgensen
DFU

9.30 - 10.00 Introduction to Chemoinformatics (History, Overview)
Johnny Gasteiger
Universität Erlangen-Nürnberg

10.00 - 10.15 Discussion

10.15 - 10.30 Coffee

10.30 - 11.15 Molecules are like Humans (Representation of Chemical Structures)
Johnny Gasteiger
Universität Erlangen-Nürnberg

11.15 - 11.30 Discussion

11.30 - 12.15 Electronic Laboratory Notebook
Gorm Kruse
Novo Nordisk A/S

12.15 - 12.30 Discussion

12.30 - 13.30 Lunch

13.30 - 14.15 Chemoinformatics at Novo Nordisk
Henrik Sune Andersen
Novo Nordisk A/S

14.15 - 14.30 Discussion

14.30 - 15.15 3D Descriptors
Lars Olsen
DFU

15.15 - 15.30 Discussion

15.30 - 16.15 in silico ADME
Flemming Steen Jørgensen
DFU

16.15 - 16.30 Discussion

Lectures, except Wednesday, takes place in the Benzon Auditorium,
Danish University of Pharmaceutical Sciences.
The lectures are open to all interested.

Tuesday 28. September 2004

9.15 - 10.00 Virtual Screening
Matthias Rarey
Universität Hamburg

10.00 - 10.15 Discussion

10.15 - 10.30 Coffee

10.30 - 11.15 Large Datasets
Mads Norregaard-Madsen
Nuevolution A/S

11.15 - 11.30 Discussion

11.30 - 12.15 Practical Chemoinformatics
Sanne Glad
Nuevolution A/S

12.15 - 12.30 Discussion

12.30 - 13.30 Lunch
13.30 - 16.30  **Practical Exercises**  
Department of Medicinal Chemistry

16.30 -  **Get-together-Party**  
Department of Medicinal Chemistry

**Wednesday 29. September 2004**

9.15 - 10.00  **From Bioinformatics to Chemoinformatics**  
Søren Brunak  
DTU

10.00 - 10.15  Discussion

10.15 - 10.30  Coffee

10.30 - 11.15  **GPCR Ligands**  
Thomas Frimurer  
7TM Pharma A/S

11.15 - 11.30  Discussion

11.30 - 12.15  **Databases**  
Svava Jónsdóttir  
DTU

12.15 - 12.30  Discussion

12.30 - 13.30  Lunch

13.30 - 16.30  **Practical Exercises**  
Room 007, building 208, DTU

All lectures and practical exercises Wednesday 29. September takes place in room 007, building 208 at the Technical University of Denmark

**Thursday 30. September 2004**

9.15 - 10.00  **Multivariate Data Analysis and Modelling in QSAR and Triomics**  
Lennart Eriksson  
Umetrics AB, Umeå

10.00 - 10.15  Discussion

10.15 - 10.30  Coffee

10.30 - 11.15  **Fingerprints and Pharmacophores**  
Inge Thøger Christensen  
Novo Nordisk A/S

11.15 - 11.30  Discussion

11.30 - 12.15  **Metabonomics**  
Dan Stærk  
DFU

12.15 - 12.30  Discussion

12.30 - 13.30  Lunch

13.30 - 16.30  **Practical Exercises**  
Department of Medicinal Chemistry

**Friday 1. October 2004**

9.15 - 10.15  **Preparation for student presentations**  
Department of Medicinal Chemistry

10.15 - 10.30  Coffee

10.30 - 12.30  **Preparation for student presentations**  
Department of Medicinal Chemistry

12.30 - 13.30  Lunch

13.30 - 16.00  **Student Presentations**  
Benzon Auditorium

16.00 - 16.30  **Evaluation of the course and Closing Remarks**  
Benzon Auditorium