

# Chemoinformatics

## Ph.D. course

Danish University of Pharmaceutical Sciences (DFU),  
Technical University of Denmark (DTU) & Drug Research Academy

	Monday 27. September 2004 DFU	Tuesday 28. September 2004 DFU	Wednesday 29. September 2004 DTU	Thursday 30. September 2004 DFU	Friday 1. October 2004 DFU	
9.15	Flemming Jørgensen	Matthias Rarey	Søren Brunak	Lennart Eriksson	Preparation for student presentations	9.30
9.30	Introduction	Virtual Screening	From Bioinformatics to Chemoinformatics	Multivariate Statistics		9.45
9.45	Johnny Gasteiger	Discussion	Discussion	Discussion		10.00
10.00	Chemoinformatics I					10.15
10.15	Discussion	Coffee	Coffee	Coffee	Coffee	10.30
10.30	Coffee	Mads	Thomas Frimurer	Inge T. Christensen	Preparation for student presentations	10.45
10.45	Johnny Gasteiger	Nørregaard-Madsen	GPCR Ligands	Fingerprints and Pharmacophores		11.00
11.00	Chemoinformatics II	Large Datasets	Discussion	Discussion		11.15
11.15	Discussion	Discussion				11.30
11.30	Gorm Kruse	Sanne Glad	Svava Jonsdottir	Dan Stærk	11.45	
11.45	Electronic Laboratory	Practical	Databases	Metabonomics	12.00	
12.00	Notebook	Chemoinformatics	Discussion	Discussion	12.15	
12.15	Discussion	Discussion			12.30	
12.30	Lunch	Lunch	Lunch	Lunch	Lunch	12.45
12.45						13.00
13.00						13.15
13.15						13.30
13.30	Henrik Sune Andersen	Exercises DFU	Exercises DTU	Exercises DFU	Student presentations	13.45
13.45	Chemoinformatics at					14.00
14.00	Novo Nordisk					14.15
14.15	Discussion					14.30
14.30	Lars Olsen	Practical Exercises	Practical Exercises	Practical Exercises		14.45
14.45	3D Descriptors					15.00
15.00						15.15
15.15	Discussion					15.30
15.30	Flemming Jørgensen					15.45
15.45	in silico ADME					16.00
16.00					Course evaluation	16.15
16.15	Discussion					16.30

Social party

Course director: Associate Professor Flemming Steen Jørgensen  
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