



EMBO-Course

“Methods for protein simulations and drug design”

Time: Mon, 13/09/2004 – Fri, 24/09/2004

Place: Drug Discovery and Design Center (DDDC), Shanghai Institute of
Materia Medica, Chinese Academy of Sciences, Shanghai

L: lecture (lecture hall ‘Chenggu Ting’), P: practical (computer lab)

Mon, September 13

Registration and Introduction

9.00 – 11.00 am Registration

11.00 – 12.00 am Frauke Meyer and Hualiang Jiang

Welcome and Introduction

Lunch break (lunch 12.30 daily)

2.00 – 3.30 pm Jeremy Smith

L: Introduction to Protein simulations and drug design

 &  break

4.00 – 5.00 pm Frauke Meyer, Yu Kunqian

Introduction to the computer lab

6.00 pm Welcome dinner

Tue, September 14**Module I: MD**

9.00 – 10.30 am Self-introduction of participants, oral presentations

 &  break

11.00 – 12.00 am Bert de Groot, Phil Biggin

L: Introduction to Molecular Dynamics (MD) simulations

Lunch break

2.00 – 5.00 pm Bert de Groot, Phil Biggin

P: MD simulations with Gromacs

Wed, September 15**Module I: MD**

9.00 – 10.30 am Daan van Aalten

L: MD for drug design

 &  break

11.00 – 12.00 am Daan van Aalten

L: MD for drug design

Lunch break

2.00 – 5.00 pm Daan van Aalten

P: MD for drug design (Gromacs)

7.00 – 9.00 pm Gerhard Klebe

Evening Lecture: Prediction of active sites

Thu, September 16**Module I: MD**

9.00 – 9.30 am Short presentations

9.30 – 10.30 am Jeremy Smith

L: Protein dynamics and function

 &  break

11.00 – 12.00 am Jeremy Smith
L: Protein dynamical transition

Lunch break

2.00 – 3.30 am Phil Biggin/Bert de Groot
L: Membrane protein simulations

3.30 – 5.00 pm Phil Biggin/Bert de Groot
P: Membrane protein simulations

Fri, September 17

Module I: MD

9.00 – 10.00 am Phil Biggin
L: BioSimGrid

10.00 – 11.00 am Bert de Groot
L: Essential Dynamics

 &  break

11.20 – 12.00 am Short presentations

Lunch break

2.00 – 3.00 pm Poster session

3.30 – 5.00 pm Jianpeng Ma
L: Normal mode analysis

7.00 – 9.00 pm Evening Lecture: Wilfried van Gunsteren:
Validating MD simulations through comparison
with experimental data

Sat, September 18**Module I: MD**

9.00 – 12.00 am Jianpeng Ma

P: Normal mode analysis

4.00 pm

Tea time: “Chinese Ink Paintings”

Shanghai Institute of Advanced Sciences

Sun, September 19**EXCURSION**

Excursion to Hangzhou (West Lake, Buddhist Temple, Longjing Green Tea...)

Mon, September 20**Module II:CADD**

9.00 – 10.30 am Johan Åqvist

L: Free energy calculation: FEP

 &  break

11.00 – 12.00 am Johan Åqvist

L: Free energy calculation: LIE

Lunch break

2.00 – 4.00 pm Martin Stahl

L: Conformational analyses with the Cambridge Structural Database (CSD)

 &  break

4.30 – 5.00 pm Short presentations / Poster session

Tue, September 21**Module II:CADD**

9.00 – 12.00 am Martin Stahl

P: Conformational analyses with the CSD

Lunch break

2.00 – 3.30 pm Qi Chen
L: Docking and scoring

 &  break

4.00 – 5.00 pm Martin Stahl
L: Similarity search

Wed, September 22

Module II:CADD

9.00 – 12.00 am Qi Chen
P: Docking and scoring

Lunch break

2.00 – 3.30 pm Jonathan Essex
L: Flexible docking

 &  break

4.00 – 5.00 pm Short presentations / Poster session

7.00 – 9.00 pm William N. Lipscomb
Evening Lecture: Drug design for diabetes type II

Thu September 23

Module II/III: CADD and QM/MM

9.00 – 12.00 am Jonathan Essex
P: Flexible docking

Lunch break

2.00 – 3.30 pm Gerrit Groenhof
L: Hybrid QM/MM simulations with Gromacs

 &  break

4.00 – 5.00 pm Gerrit Groenhof

L: QM/MM application: photoactive yellow protein

Fri, September 24

Module III: QM/MM

9.00 – 12.00 am	Gerrit Groenhof
	P: Hybrid QM/MM (Gromacs)
Lunch break	
2.00 – 3.30 pm	Ursula Roethlisberger
	L: CPMD basics
3.30 – 4.30 pm	Ursula Roethlisberger
	L: CPMD for enzymatic reactions
4.30 – 5.30 pm	Closing session
6.00 pm	Farewell dinner