

FEBS Practical Course 2020 | Macromolecule MD Simulations for Interdisciplinary Beginners

Sunday, 2020/9/6

18:00 - 22:00	Lobby	Welcome reception (including dinner)	Networking
18:00 - 22:00	Blue Hall	Installation of the posters Instalation of the poster for the whole duration of course	Poster

Monday, 2020/9/7

08:50 - 10:30	Theater Hall	Introduction to MD simulations - basic principles	Lectures
08:50 - 09:00		Opening remarks	
09:00 - 10:30		Introduction to MD simulations - basic principles	
10:30 - 10:50	Lobby	Cofee break	Networking
10:50 - 12:10	Theater Hall	Introduction to practical implementation of MD	Lectures
12:10 - 13:00	Rotunda	Lunch	Networking
13:00 - 17:45	PC room	Introduction to MD programs	Practical Session
17:45 - 18:30	Theater Hall	Invited Lecture	Lectures
17:45 - 18:30		TBA Carol B. Post	
18:30 - 19:30	Rotunda	Dinner	Networking

FEBS Practical Course 2020 | Macromolecule MD Simulations for Interdisciplinary Beginners

19:30 - 22:00 Lobby
Social hours Networking

19:30 - 22:00 Blue Hall
Formal poster viewing Poster

Tuesday, 2020/9/8

09:00 - 10:30 Theater Hall
Forcefield parametrization Lectures
Forcefield parametrization

09:00 - 09:45 **Principals of forcefield parametrization**

09:45 - 10:30 **Forcefield parametrization of ligands (implementations)**

10:30 - 10:50 Lobby
Cofee break Networking

10:50 - 12:00 Theater Hall
Introduction of QM calculations Lectures

12:00 - 13:00 Rotunda
Lunch Networking

13:00 - 19:30 PC room
Forcefield parametrization in practice Practical Session

18:30 - 19:30 Rotunda
Dinner Networking

20:00 - 22:00 Lobby
Round Tabels + social hours Networking
Round Tables will consist of three groups (at lobby and adjacent rooms) with 3 topics: 1. Advance parametrization ; 2. Ligand-protein simulations; 3. Membrane protein simulations >Refreshments will be available.

20:00 - 22:00 Blue Hall
Informal discussions Poster

Wednesday, 2020/9/9

08:40 - 10:30 Theater Hall
Ligand - protein interactions Lectures

08:40 - 09:30 **Introduction to molecular docking**
 08:40 - 09:40 **Ligand binding theory**
 Jannette Carey

10:30 - 10:50 Lobby
Coffee break Networking

10:50 - 12:30 Theater Hall
Ligand - protein simulations Lectures

12:30 - 13:30 Rotunda
Lunch Networking

13:30 - 19:00 PC room
Ligand - protein simulations and molecular docking Practical Session

13:30 - 16:00 **Molecular Docking**
 16:00 - 19:00 **Ligand - protein simulations**

19:00 - 20:00 Rotunda
Dinner Networking

20:00 - 22:00 Lobby
Round Tables + social hours Networking
 Round Tables will consist of three groups (at lobby and adjacent rooms) with 3 topics: 1. Advance parametrization ; 2. Ligand-protein simulations; 3. Membrane protein simulations >Refreshments will be available.

20:00 - 22:00 Blue Hall
Informal discussions Poster

Thursday, 2020/9/10

09:00 - 10:40 Theater Hall
Coarse-grained simulations with membranes Lectures

09:00 - 09:45 **Introduction to MD simulations with membranes**

FEBS Practical Course 2020 | Macromolecule MD Simulations for Interdisciplinary Beginners

09:45 - 10:40	Introduction to coarse-grained simulations Luca Monticelli	
10:40 - 11:00	Lobby Coffee break	Networking
11:00 - 12:00	Theater Hall Student talks	Lectures
12:00 - 13:00	Rotunda Lunch	Networking
13:00 - 17:00	PC room Coarse-grained simulations with membranes	Practical Session
17:00 - 19:00	PC room Individual projects	Practical Session
19:00 - 20:00	Rotunda Dinner	Networking
20:00 - 22:00	Lobby Round Tables + social hours Round Tables will consist of three groups (at lobby and adjacent rooms) with 3 topics: 1. Advance parametrization ; 2. Ligand-protein simulations; 3. Membrane protein simulations >Refreshments will be available.	Networking

Friday, 2020/9/11

09:00 - 10:30	Theater Hall Applications of MD simulations	Lectures
10:30 - 11:00	Lobby Coffee break	Networking
11:00 - 12:00	Theater Hall Student talks	Lectures

FEBS Practical Course 2020 | Macromolecule MD Simulations for Interdisciplinary Beginners

12:00 - 13:00	Rotunda Lunch	Networking
13:00 - 15:00	PC room Advanced analysis of MD simulation	Practical Session
15:00 - 19:00	PC room Individual projects	Practical Session
19:00 - 22:00	Lobby Farewell party (including dinner)	Networking

Saturday, 2020/9/12

09:00 - 10:00	Theater Hall Students talks	Lectures
10:00 - 10:30	Theater Hall Closing remarks	Lectures