

Structural Biochemistry Course IBPC

From Protein Identification by Mass Spectrometry to Crystal Structure Determination and Molecular Dynamic Analysis.

8-16 March 2018



**Master
In Silico
Drug Design**



Organizers :

Karine Moncoq, Daniel Picot, Valérie Biou

Intervenants :

Marc Baaden, Sandrine Masscheleyn, Franck Brachet, Mathilde Piel, Serena Sirigu, Leo Chavas

We announce the third Structural Biochemistry Course organized in collaboration with the Labex Dynamo with the UMR 7099 and UPR 9080 of the Institute of Physico-Chemical Biology (IBPC) and University of Paris Diderot.

The course is principally aimed to « *In Silico* Drug Design » Master 1 students of University of Paris Diderot, but applications from mature graduate students are encouraged in the limit of a maximum number of 10 participants.

The goal of this course is to provide students with a better knowledge of available structural data in the scientific community and the importance of how a 3D structure is obtained, which is in perfect agreement with the objectives of the Master.

This course consists of lectures given on principles and limitations of the different techniques and practical training on robot-assisted protein crystallisation, data analysis, structure refinement and molecular dynamics programs. The availability of mass spectrometry and crystallography facilities at IBPC and the unique opportunity to visit the SOLEIL synchrotron will introduce students to advanced and modern techniques in structural biology.

Throughout this course, the students will have the opportunity to face some of the current challenges in structural biology and have a grasp at the importance of critical analysis of experimental data.

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8-16 March 2018

Thursday, March 8

9h15-9h30	General presentation of the course
9h30-11h00	An overview of mass spectrometry and introduction to MALDI-TOF (Sandrine Masscheleyn) <i>Break</i>
11h30-12h	Short Exam for M1 ISDD students <i>Lunch Break</i>
13h-17h	Protein crystallisation : how to make well-diffracting crystals (Karine Moncoq)

Friday, March 9

9h-12h	Practical session – Protein identification by mass spectrometry (MALDI-TOF) (Sandrine Masscheleyn, Mathilde Piel, Karine Moncoq) <i>Lunch Break</i>
13h-17h	Practical session – Protein crystallisation with Dragonfly and Mosquito robots (Franck Brachet, Valerie Biou, Daniel Picot)

Monday, March 12

9h-12h	Principles of protein crystallography : from diffraction data to model building (Daniel Picot) <i>Lunch Break</i>
13h-17h	Practical session – Crystals visualisation and freezing (Franck Brachet, Valerie Biou, Karine Moncoq)

Tuesday, March 13

9h-12h	Practical session – Molecular dynamics analysis with Gromacs programs (Marc Baaden) <i>Lunch Break</i>
13h-17h	Practical session – Data analysis and phasing with CCP4 and Phenix programs (Karine Moncoq, Valerie Biou, Daniel Picot)

Thursday, March 15 (SOLEIL Synchrotron)

10h-11h30	General presentation of the SOLEIL synchrotron <i>Lunch Break</i>
13h30-17h	Practical session – Diffraction experiments and data collections at PX1 beamline (Leo Chavas, Serena Sirigu)

Friday, March 16

9h-10h	Principles of structure refinement (Valerie Biou)
10h-12h	Practical session – Model building and refinement with Phenix programs (Karine Moncoq, Valerie Biou, Daniel Picot) <i>Lunch Break</i>
13h-14h	How to validate a 3D structure (Valerie Biou)
14h-17h	Practical session – Structure validation and analysis (Karine Moncoq, Valerie Biou, Daniel Picot)