**COURSE AIM**

Computational biochemistry is an extremely important and complementary tool to modern structural biology. In this 2.5 day workshop, you will learn how to use python via a jupyter notebook and how to perform homology modelling, molecular dynamics and small-molecule docking. The whole course will be delivered remotely and advice will be give prior on how to install the required software (all of which is freeware).

We assume very little prior knowledge of either python or computational biochemistry.

**COURSE DESCRIPTION**

The course is divided into four sessions:

1. Introduction to python and jupyter notebooks (2-3 hours with 30 min lecture)
2. Introduction to homology modelling (2-3 hours with 30 min lecture)
3. Introduction to molecular dynamics (4-5 hours including 1 hour lecture)
4. Introduction to small-molecule docking (2-3 hours with 20 min lecture)

Each session will commence with a live-lecture designed to provide some necessary background to the practical components. The four sessions are designed to be done semi-independently (so if you are already very familiar with python, then one could omit that session).

**Please make sure you read all of the sections below relating to how the course will work, the survey and the attendance certificate.**

**COURSE OBJECTIVES**

At the end of the course, participants will be able to

* Understand some basic python commands and a jupyter notebook
* Understand how homology modelling works and how to go about building quite complex homology models
* Understand how molecular dynamics works and perform a simulation of a soluble protein
* Understand how docking works and how to interpret the results

**PARTICIPANT NUMBERS**

Maximum 30

**HOW IT WILL WORK**

The course is designed such that participants should be able to work through things at their own pace on their own. However, there will be live lectures introducing the course and the background to each component during Monday 14th – Wednesday 16th December (week 10). During this period, demonstrators will also be available via zoom/teams breakout rooms to help with any issues.

To facilitate the smooth running of the course, participants are requested to ensure they have installed the relevant software on their laptop/desktop in the week **BEFORE**. Demonstrators will be available during the Thursday and Friday of week 9 to help with installation issues. They will not be able to help with installation during the course proper. You must ensure the software is installed and is functioning before starting the course proper. To summarise:-

Thursday 10th/Friday 11th December – Demonstrators available to advise on installation issues.

Monday 14th to Wednesday 16th December – Live course lectures and demonstrators available to help on course progression.

Booking confirmation and reminder emails will send you the link for the live interactive session (held in Zoom) and joining instructions. To join the session, you can click on the link 15 minutes before the session. Arrangements for the optional live workshop will be made following the scheduled online session.

**WHAT YOU WILL NEED**

You will need a good laptop/desktop running either linux, Mac OSX or windows 10. The preferred option is linux as that is what most scientific labs use these days, however, the practical sessions should work on all platforms. A good internet connection will be essential.

**ATTENDANCE CERTIFICATE ON SURVEY COMPLETION**

It is now a requirement that you complete the three short questions in the survey you receive after attending the course. Once you have submitted the survey, you will be sent an email with a link to your attendance certificate. This is to ensure we receive the feedback we need to evaluate and improve our courses. Survey results are downloaded and stored anonymously.

**PLEASE NOTE**

Where no cost is indicated in the shopping trolley, no deposit is required. However, more than two consecutive non-attendances or late cancellations without good reason will be logged and may mean you cannot attend any further MSD training that term. Please refer to our Terms and Conditions for further information.