



How to prepare for the Advanced Gromacs + HADDOCK + PMX Workshop 9-11 October 2019

Flash talks

All participants coming on-site **must** provide a one slide presentation of themselves before the Workshop. The slides will be used in 3 minute (max, strict) informal flash talks on Wednesday evening to facilitate networking among participants. You are free to create the slide any way you like, but the result should be one slide with aspect ratio 16:9. Here are templates for ([pptx](#)) and ([odp](#)), and an example ([odp](#)). Send your slide to [atte.sillanpaa \(ät\) csc.fi](mailto:atte.sillanpaa@csc.fi) named *firstname_lastname.[pptx|odt|pdf]*.

Basic Gromacs understanding

If you're not familiar with Gromacs (based on registration data, most of you are), please complete at least the "Lysozyme in Water" online tutorial made by Justin Lemkul *before* participating. This is an *advanced* Gromacs workshop, and we will assume the participants know the basic things. You'll benefit much more of the content if you know the basics in advance. The tutorials are in here:
<http://www.mdtutorials.com/gmx/>

Basic HADDOCK understanding

If you're not familiar with HADDOCK, please complete this tutorial before participating:
<http://www.bonvinlab.org/education/HADDOCK24/HADDOCK24-protein-protein-basic/>

Basic Linux command line skills

The workshop will include hands on using the Linux command line, so to maximally benefit from your time, it will be important to learn the very basics *before* you come the course.

In the course, you'll only need to be able to move around in the directory hierarchy (**cd**, **ls**, **pwd**), create directories, copy, rename, delete files (**mkdir**, **cp**, **mv**, **rm**), uncompress files (**tar**, **unzip**), edit files (any text editor, e.g. **gedit**, **nano**, **emacs**), look at file contents (**more**, **less**, **grep**), use some environment variables (**\$HOME**, ...), download files (**wget**, **curl**).

Here are some links for easy self-study:

<https://linuxsurvival.com/> (Linux command line and tutorials that you can do in your browser)

https://www.csc.fi/web/training/-/linux1_spring2018 (check the materials links)

<http://www.ee.surrey.ac.uk/Teaching/Unix/> (the first two topics are a good start, try also some editor)

https://www.youtube.com/watch?v=uFPly_nGBMg (sit back and watch)

[CSC Linux Cheat Sheet](#) (one page summary of most important Linux commands and then some

Q & A – help on your own systems

If you have questions related to your own systems, zip up some data and bring it with you. We have dedicated the end of the workshop to open questions, but there will be other opportunities as well. For example, mutations in a small protein could be done on the fly with PMX.

A temporary discussion forum will be set up in here, <https://ask.bioexcel.eu/c/workshop-tutorials> which will be hopefully useful also for remote participants.