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SCIENTIFIC MODULE
OF THE GRADUATE SCHOOL OF SFB1423

Generation of publication quality molecular figures with PyMOL

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February 17TH-19TH (Beginners), February 20TH (Beginners and Advanced students)

Leipzig University, BBZ (Deutscher Platz 5, 04103 Leipzig), Seminarroom 2

The workshop aims to introduce to the use of the software PyMOL to generate publication quality molecular figures. It is intended for beginners, but advanced users may benefit as well from some topics. The course material is provided as freely accessible webpages, so advanced users will easily find out if certain topics are of interest and require participation in presence or if the provided web page info suffices. We will send the web link around shortly before the course starts. In addition to generating molecular figures, PyMOL can also be used to analyze (interpret) molecular structures.

The 3-day beginner workshop will cover the following topics:

- Introduction to the PyMOL GUI
- Generation of figures: Overview, GPCR-ligand interactions
- Avoid common mistakes in showing erroneous polar interactions
- PML script files: The better way to generate and handle molecular images.
- PyMOL selection algebra
- Visualization of large complexes
- Depiction and analysis of experimental X-ray or CryoEM maps
- Superposition of molecular structures: Some points to consider
- Map properties (electrostatic potential, conservation, ...) onto the protein fold or molecular surface
- Generating, analyzing and displaying AlphaFold models
- Generate simple movies
- Labeling and arranging composite figures in inkscape

The fourth day will probably be a Q&A session (if there is enough interest). So please send your questions, problems or suggestions to: jenny.leopold@medizin.uni-leipzig.de

PLACES AVAILABLE: 20

PARTICIPANTS: Members of SFB1423 graduate school
(everyone else will be placed on a waiting list)

REGISTRATION: email to jenny.leopold@medizin.uni-leipzig.de