CompBioMed

A Centre of Excellence in Computational Biomedicine

E-Seminar Series

Seminar #14
Molecular visualisation using PyMOL

2 December 2020
2pm CET / 1pm GMT (1h duration)

Register for free here: https://register.gotowebinar.com/register/2624223503575523341

PyMOL, developed and maintained by Warren L. DeLano as of 1998, has become the most popular tool for preparing publication-ready renderings of three-dimensional biomolecular structures. This online tutorial provides hands-on introduction on how to visualize molecular structures in PyMOL, aiming at the generation of state-of-the-art ray-traced images. We will learn to operate PyMOL both by using the graphical user interface and from the command line. The tutorial is set up for researchers working in the biomedical field and individuals with a general interest in effectively applying PyMOL. Attendees should ideally have basic Python and Linux shell (bash) knowledge.

This is the 14th of a series of online seminars organised by CompBioMed.

Watch the full series on www.compbiomed.eu/training!

Dr. David Wifling received his licensure as pharmacist in 2011 and his PhD degree in Medicinal Chemistry in 2015 from the University of Regensburg. As a postdoctoral researcher, he focussed on computational chemistry and high-performance computing, with an emphasis on structure-based drug design as well as long time-scale molecular dynamics simulations. He has authored over 15 publications in renowned international journals. Since 2020, he works as a computational scientist at the Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities (LRZ) in Munich. Within the CompBioMed2 Centre of Excellence he leads both the work package on "Data Management and Analytics" and the task "Route to the Exascale". His research interests are at the intersection of high-performance computing, pharmaceutical/ biomedical and data sciences.

Moderated by Gavin Pringle, **EPCC**

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