Spring School on Digital Chemistry

Applied to Drug & Crop Protection Discovery

Les Diablerets, 16.-20. April 2023

# *Beyond software: CADD behind the scenes*

#### Wednesday, 19.04.2023, 14:00-18:30

In contrast to the other sessions, where you learned about different concepts & technologies and how to apply them in a CADD setting, we will focus now on the discussion of results you obtain from those tools in a concrete project-like setting. Nowadays, computational tools have evolved a lot in the sense, that their application is often just a button click away, and by keeping "standard settings" almost everybody can retrieve some "computational results/ predictions" on their target. But actually, that's only when the work of a CADD scientists starts: We will have different examples ready to analyse those initial results, which aspects could be considered or discussed in depth and how to derive working hypotheses from them.

# Installations

Please install **PyMol**:

Follow the instructions here:

Linux: <https://pymolwiki.org/index.php/Linux_Install>

MAC: <https://pymolwiki.org/index.php/MAC_Install>

Windows: [https://pymolwiki.org/index.php/Windows\_Install](https://pymolwiki.org/index.php/Windows_Install" \o "Original URL: https://pymolwiki.org/index.php/Windows_Install. Click or tap if you trust this link." \t "_blank)

download the exact files mentioned under “Example of filenames 2023-01-12”:

* pymol\_launcher-2.5-cp311-cp311-win\_amd64.whl
* pymol-2.6.0a0-cp311-cp311-win\_amd64.whl
* numpy-1.22.4+mkl-cp311-cp311-win\_amd64.whl

AND (Win)**Coot**:

[https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/binaries/release/](https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/binaries/release/" \o "Original URL: https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/binaries/release/. Click or tap if you trust this link." \t "_blank)

OR:

<http://bernhardcl.github.io/coot/wincoot-download.html>

# Introduction to Coot

Graphical user interface, text, application

Description automatically generated

Graphical user interface, text, application

Description automatically generated

Graphical user interface, text, application

Description automatically generated

Graphical user interface, application, Word

Description automatically generated

# Introduction to PyMol

Graphical user interface, application

Description automatically generated

Graphical user interface, application

Description automatically generated

Text

Description automatically generated with low confidence

Graphical user interface

Description automatically generatedpp