Pre-Workshop Requirement: Software Installation Checklist

Dear Participant,

To ensure a smooth experience during our upcoming "Drug Designing, Molecular Docking & MD Simulation" workshop, please install the following software packages on your laptop **before Day 1**.

System Requirements:

- **OS:** Windows 10/11 (64-bit), macOS, or Linux.
- **RAM:** Minimum 8GB (16GB recommended for MD Simulation).
- **Storage:** At least 20GB free space.

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1. Visualization & Protein Preparation (Days 1–2)

These tools are essential for viewing 3D structures and preparing PDB files.

- **UCSF Chimera (v1.17 or newer)**
    - *Purpose:* Protein cleaning, minimization, and visualization.
    - *Note:* Download the "Production Release."
- **PyMOL (Educational/Open Source)**
    - *Purpose:* High-quality rendering and structural analysis.
- **BIOVIA Discovery Studio Visualizer**
    - *Purpose:* 2D interaction plotting and visualizing docking results.
    - *Note:* Requires a free account registration to download.

2. Ligand Preparation & Utilities (Day 3)

Tools to sketch chemical structures and convert file formats.

- **ChemSketch (Freeware)**
    - *Purpose:* Drawing 2D chemical structures.
    - *Alternative:* MarvinSketch (requires academic license).
- **OpenBabel GUI**
    - *Purpose:* Converting chemical file formats (e.g., .sdf to .pdbqt).

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3. Molecular Docking Suite (Days 4–6)

We will use these for the actual docking and virtual screening.

- **AutoDock Tools (MGLTools 1.5.6)**
  - *Purpose:* Preparing grid boxes and PDBQT files.
  - *Warning:* If you are on a Mac or newer Windows, MGLTools can be buggy. Please also install **PyRx** as a backup.
- **AutoDock Vina**
  - *Purpose:* The docking engine.
- **PyRx (Version 0.8)**
  - *Purpose:* A user-friendly GUI for running Vina and managing multiple ligands.
- **LigPlot+**
  - *Purpose:* Generating 2D interaction diagrams.
  - *Requirement:* You must have **Java** installed for this to run.

4. Molecular Dynamics (Days 7–9)

CRITICAL: This is the most complex installation.

- **GROMACS**
  - *Linux Users:* Install via terminal (sudo apt install gromacs).
  - *Windows Users:* You **must** enable WSL (Windows Subsystem for Linux) and install Ubuntu from the Microsoft Store. Then, install GROMACS inside the Ubuntu terminal.
  - *MacOS Users:* Install via Homebrew (brew install gromacs).

Troubleshooting Tips

- **Admin Rights:** Ensure you have administrator permissions on your laptop to install software.
- **Mouse:** A **3-button mouse (with scroll wheel)** is highly recommended. navigating 3D protein structures with a trackpad is very difficult.
- **Paths:** Avoid installing software in folders with spaces in the name (e.g., avoid C:\Program Files\). Use simple paths like C:\BioTools\ to prevent script errors.

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