**Project 5**

**In-Silico Analysis of Protein-Ligand Interaction Using Docking Platforms**

**Objective:** Perform molecular docking of a drug molecule against a target protein.

**Data Source:**

* Target protein: PDB (e.g., **COX-2 enzyme, PDB ID: 5IKR**).
* Ligand: PubChem (e.g., aspirin or ibuprofen structure).

**Steps:**

1. Download protein structure (PDB) and ligand structure (SDF).
2. Use **SwissDock (online)** or **AutoDock Vina GUI** for docking.
3. Analyze docking results: binding affinity, top docking pose.
4. Visualize binding pocket with **PyMOL/ChimeraX**.
5. Interpret: does the ligand fit the active site?

**Deliverables:**

* Docking output files
* 2–3 images of protein–ligand complex
* Short report (binding energy, possible interactions, drug relevance)