**67457\_Retrieving and Importing Protein Structures.mp4**

* **2.1.2:** **All Apps** menu being selected, the list being scrolled to locate the **Schrodinger** folder, the folder being opened, the **Maestro** icon followed by **Open** being clicked to launch the software **00:00:00-00:00:21**
* **2.2.1:** The **File** tab being clicked, the **Get PDB** option being selected from the pop-up menu, the PDB code being entered in the text box, and the **Download** button being clicked **00:00:22-00:00:31**
* **2.2.2:** The downloaded PDB file appearing in the project window. **00:00:32-00:00:48**
* **2.3.1:** **Protein Data Bank** website being opened. The PDB ID being entered in the **Protein Data Bank** search box, and the **Download** button being clicked **00:00:49-00:01:15**
* **2.3.2:** The **File** tab being clicked in **Maestro**, and **Import Structures** being selected **00:01:16-00:01:19**
* **2.3.3:** The downloaded PDB file being located in the **Import** interface and the **Import** button being clicked **00:01:20:00:01:53**
* **2.4.1:** The protein structure being selected and right-clicked **00:01:53-00:01:55**
* **2.4.2:** The **Split Ligand** option being selected, followed by choosing the option to split into ligands, water, and other components **00:01:56-00:02:01** (Splitting of already prepared protein structure).

**67457\_Ligand Preparation.mp4**

* **3.1.1:** The **PubChem** database being opened. The compound name being entered in the **PubChem** search bar **00:00:00-00:00:11**
* **3.1.2:** A list of available structures being reviewed, with **3D structures** being selected & **3.1.3:** The **Download** button being clicked and the structure being saved in **SDF** format. **00:00:11-00:01:55 (Steps 3.1.1-3.1.2 is repeated to download all the 6 NNRTI ligands)**
* **3.2.1:** The **File** tab being clicked in **Schrodinger**, and **Import Structures** being selected. The SDF file location being accessed, and the **SDF** file being loaded **00:01:56-00:02:41**
* **3.3.1:** The **Task** button being clicked in the **Schrodinger** software. **LigPrep** being typed into the search bar. **LigPrep** being selected from the right window **00:0:42-00:02:48**
* **3.4.1-3.4.2:** The **Use Structures From** option being selected and then the files being chosen from the Workspace or Project Table & The preferred option being selected from the **LigPrep** window and then the file being saved. **00:02:49- 00:02:57**
* **Run** button being clicked to start ligand preparation (Visualizing the prepared ligands in the SOFTWARE Window) **00:02:58-00:03:20**

**67457\_Geometry and Optimization of Ligands.mp4**

* **4.1.1:** The software being opened for geometry optimization **00:00:00-00:00:16**
* **4.1.2:** The **File** tab being clicked, and the **Open** option being selected. The **SDF** file being loaded. **00:00:17-00:00:31**
* **4.2.1:** The **Calculate** tab being clicked, and **Gaussian Calculation Setup** being selected. The **Job Type** tab being accessed, and **Optimization** or **Opt+Freq** being selected **00:00:32-00:00:39**
* **4.3.1:** The **Method** tab being clicked, and a quantum chemistry method being selected. The **Kohn–Sham** **global-hybrid exchange-correlation density functional**, basis set, charge, and spin being chosen from dropdown menus. **00:00:40-00:01:05**
* **4.4.1:** The **Title** tab being accessed, and a name being entered for the compound (Navigate to the **Link 0** *(zero)* tab and specify the **Memory Limit** and **Shared Processors**. Untick the **Full Path** boxes ) **00:01:06-00:01:55**
* **4.45.1:** The **Edit** button being clicked to save the **Gaussian input file. 00:01:56-00:02:34 (Steps 4.1.1 – 4.4.1 repeated for the rest of the ligands 00:02:35-00:03:10**
* **4.5.2:** The file being named and saved as a **Gaussian job file (GJF)** in the preferred location. **00:03:11-00:03:35**

**67457\_Receptor Grid Generation and Molecular Docking.mp4**

* **5.1.1:** The **Tasks** menu being accessed and **Receptor Grid Generation** being selected. **00:00:00-00:00:14**
* **5.1.2:** The **Pick** **to identify the ligand** is checked , and the notification being checked for a co-crystallized ligand. **00:00:15-00:00:00:39 (Includes submitting the Glid gride for generation by clicking Run)**
* **5.2.1:** The **Tasks** menu being accessed, and **Docking > Ligand Docking (Glide Docking)** being selected. **00:00:40-00:00:53**
* **5.2.2:** The **Grid File** being loaded. **00:00:53-00:01:07**
* **5.2.3:** Ligands being selected from the workspace using **Use Ligand From** option. **00:01:07-00:02:15**
* The **Settings** tab being accessed, and the docking precision method being selected **00:02:16-00:02:20**
* **5.3.3:** The **Constraints** tab being accessed, and constraints such as hydrogen bonds being configured. **00:02:21-00:02:24**
* **5.4.1:** Docking settings being reviewed and saved. **00:02:21-00:02:24 (same process as 5.3.3).**
* **5.4.2:** The **RUN** button being clicked to initiate docking. **00:02:24-00:02:25 (Reviewing docking results comparing the docking scores before optimizing the ligands and after optimizing the ligands (00:02:26-00:02:56))**

**674576\_Enumeration and Molecular Mechanics with Generalized Born and Surface Area MMGBSA.mp4**

* **6.1.1:** A docked protein-ligand complex being selected in the Workspace Navigator. **00:00:00-00:00:21**
* **6.1.2:** The **Analyze Workspace** button being clicked in the **Ligand Designer** window. **00:00:22-00:00:35**
* **6.2.1:** Isostere Scanning being selected from the workflow list. **00:00:36-00:00:44**
* **6.2.2:** Ligand structure being extended by adding molecular fragments. **00:00:44-00:01:05 (**Analyzing the docking results from the enumerated compounds and searching for a compound that has a more negative value than the Co-crystalized compound **-9.242, 00:01:05-00:02:45)**

**674576\_Enumeration\_Molecular Dynamics and Molecular Mechanics with Generalized Born and Surface Area\_MM\_GBSA.mp4**

* **6.1.1:** The **Task** button being clicked and **Desmond System Builder** being selected. **00:00:00-00:00:**