Video Summary for **In Silico Simulation of HDP-2P Interaction with PI and phosphoinositides Using Molecular Modeling Software**

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- **68594_screenshot_1.mp4**
  - **2.1.1** (Install the chemical drawing editor & Chem3D) **00:00–01:42**
  - **2.1.2** (Install molecular modeling software) **01:43–02:16**
  - **2.1.3** (Install Auto Dock Tools) **02:17–02:36**
  - **2.1.4** (Install Python) **02:37–03:08**

- **68594_screenshot_2.mp4**
  - **2.2.1** (Show built phosphatidylinositol **(PI),** PI-4-P, PI-4,5-P_2 in the chemical drawing editor) **00:00–00:25**
  - **2.2.2** (Save the structure as a PDB file by chem3D) **00:26–01:07**

- **68594_screenshot_3.mp4**
  - **2.3.1** (Open the PI PDB file in Auto Dock Tools) **00:00–00:15**
  - **2.3.2** (Add hydrogen atoms – polar or all – to the ligand) **00:16–00:32**

- **68594_screenshot_4.mp4**
  - **2.4.1** Set the ligand, make all bonds rotatable, and save as PDBQT) **00:00–00:40**

- **68594_screenshot_5.mp4**
  - **2.5.1** (Download phospholipase A2 HDP-2 (2I0U) from the Protein Data Bank database) **00:00–00:34**
  - **2.5.2** (Open 2I0U in the molecular modeling software showing monomers A & E) **00:35–00:52**
  - **2.5.3** (Highlight all atoms belonging to monomer A using the selection tool) **00:53–01:03**
  - **2.5.4** (Remove monomer A, leaving only monomer E) **01:04–01:44**

- **68594_screenshot_6.mp4**
  - **2.6.1** (Open the HDP-2P receptor file) **00:00–00:20**
  - **2.6.2** (remove all water molecules) **00:21–00:26**

- **68594_screenshot_7.mp4**
  - **2.7.1** (Add polar hydrogens to the receptor) **00:00–00:14**
  - **2.7.2** (Select polar hydrogens for the receptor) **00:15–00:20**

- **68594_screenshot_8.mp4**
  - **2.8.1** (Set HDP-2P as receptor) **00:00–00:13**
  - **2.8.2** (Save HDP-2P as receptor as PDBQT file with no rotatable bonds) **00:14–00:35**

- **68594_screenshot_9.mp4**
  - **2.9.1** (Load ligand and receptor PDBQT files in the docking software) **00:00–00:51**

- **68594_screenshot_10.mp4**
  - **2.10.1** (Define the grid box size and center coordinates around the receptor) **00:00–01:36**

- **68594_screenshot_11.mp4**
  - **2.11.1** (Close the grid setup) **00:00–00:07**
  - **2.11.2** (Save parameters as config.txt) **00:08–00:52**

- **68594_screenshot_12.mp4**
  - **2.12.1** (Run docking using config.txt) **00:00–00:10**
  - **2.12.2** (Show docking progress) **00:11–00:12**

- **68594_screenshot_13.mp4**
  - **2.13.1** (Open docking_log.txt file) **00:00–00:21**
  - **2.13.2** (identify the lowest energy pose) **00:22–00:27**

- **68594_screenshot_14.mp4**
  - **2.14.1** (Open docking result PDBQT in Auto Dock Tools) **00:00–01:38**

- **68594_screenshot_15.mp4**
  - **2.15.1** (Visualize ligand–receptor interactions at the active site) **00:00–02:21**
  - **2.15.2** (Populate the results table with binding affinities, residues, and bond types) **02:22–03:07**