**Software/ Online Tools/ Modules used during the present study:**

* **Protein Structure Preparation:** 
  + Protein preparation wizard of Glide Module of Schrödinger Suite – available from :<https://www.schrodinger.com/platform/products/glide/>
* **Protein Receptor Grid Generation:** 
  + Receptor grid generation tool of Glide Module of Schrödinger Suite – available from :<https://www.schrodinger.com/platform/products/glide/>
* **Protein binding site prediction:**
  + SiteMap tool of the Schrödinger Suite – available from :

<https://www.schrodinger.com/platform/products/sitemap/>

* **Reverse Docking of Ligands & Proteins:**
  + Maestro Module of Schrödinger Suite – available from :<https://www.schrodinger.com/platform/products/maestro/>
* **Optimization of Force field:**
  + OPLS5 product of Schrödinger Suite – available from : <https://www.schrodinger.com/platform/products/opls4/>
* **Chemical Bond Assignment & orientation of water molecules:**
  + ‘Protassign’ utility of Schrödinger Suite – available from : <https://learn.schrodinger.com/public/python_api/2025-2/api/schrodinger.protein.protassign.utils.html>
* **2D interactions: using Discovery studio:** 
  + <https://discover.3ds.com/discovery-studio-visualizer-download>
  + <https://3ds-download-eu-west-1.s3.eu-west-1.amazonaws.com/public/BIOVIA/BIOVIA_DS2025Client.exe>
* **Molecular Dynamics (MD) Simulation:**
  + GROMACS version 2023.2 – available from :
  + <https://ftp.gromacs.org/gromacs/gromacs-2023.2.tar.gz>
* **Data visualization, plotting, & Molecular plot generation:** 
  + PyMOL available from: (https://www.pymol.org/
  + <https://storage.googleapis.com/pymol-storage/installers/PyMOL-3.1.6.1-Windows-x86_64.exe>)
  + UCSF Chimera available from: <https://www.cgl.ucsf.edu/chimera/download.html>
  + GNUPlot available from : <http://www.gnuplot.info/>