**Step1:** Download the files ‘davis targ\_info.csv’, ‘filtered davis targ\_info.csv’, ‘kiba targ\_info.csv’, ‘metz targ\_info.csv’, ‘toxcast targ\_info.csv’ from the URL ‘https://github.com/LiZhang30/GPCNDTA’.

**Step2:** Obtain the ID information of proteins in the Protein Data Bank Database or the AlphaFold Protein Structure Database from the downloaded five files.

**Step3:** Download the 3D structure files of proteins from the Protein Data Bank Database or the AlphaFold Protein Structure Database according to their ID information.”