

Evaluating DiffDock - Comparisons between SOTA models

Project Group Members

Student 1:

Name: Anh Dao

Student Number: 102503023

Student 2:

Name: Huy Trinh

Student Number: 102789290

Student 3:

Name: Ting Fu

Student Number: 103766678

Abstract

In this project, we focus on studying and evaluating DiffDock, a diffusion-based model for molecular docking published at ICLR 2023. DiffDock frames molecular docking as a generative modeling problem, using diffusion processes to predict the binding structure of small molecule ligands to proteins. The method achieves a 38% top-1 success rate on the PDBBind benchmark, significantly outperforming traditional search-based methods and previous deep learning approaches.

Source: Corso, G., Stärk, H., Jing, B., Barzilay, R., & Jaakkola, T. (2023). DiffDock: Diffusion Steps, Twists, and Turns for Molecular Docking. *ICLR 2023*.

Paper available at: https://openreview.net/pdf?id=kKF8_K-mBbS