

# Evaluating DiffDock - Comparisons between SOTA models

## Project Group Members

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## 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](https://openreview.net/pdf?id=kKF8_K-mBbS)