

# Polaris Challenge Ligand Poses 2025

## Report

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For the ligand pose challenge, we employed DiffDock-L [1], a diffusion generative model for blind docking. Using the pretrained DiffDock-L model (v1.1)<sup>1</sup>, we performed inference on the test data, sampling 40 poses per test sample and selecting the top1-ranked prediction based on the confidence model for submission.

Since the 3D protein structures were not provided for the test set, we used the reference structure for docking with MERS-CoV Mpro. For SARS-CoV-2 Mpro, we utilized protein structures from the training set when the amino acid sequence of a protein matched a test sample; otherwise, we also used the reference structure.

## References

- [1] Gabriele Corso et al. “Deep Confident Steps to New Pockets: Strategies for Docking Generalization”. In: *International Conference on Learning Representations (ICLR)*. 2024.

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<sup>1</sup><https://github.com/gcorso/DiffDock/releases/tag/v1.1>