Contribution ID: **25** Type: **not specified**

Modeling Biomolecular Structures through Generative Models

Friday, October 25, 2024 11:50 AM (40 minutes)

Predicting the binding structure of a small molecule ligand to a protein – a task known as molecular docking – is critical to biological research and drug design. Framing molecular docking as a generative modeling problem we developed DiffDock, a diffusion model over the non-Euclidean manifold of ligand poses. Empirically, DiffDock was the first ML model to outperform traditional docking methods on blind docking and it has since been integrated in the drug discovery pipelines of many pharma and biotech companies. In this talk I will give an overview of DiffDock as well as recent improvements we made to its generalization across the proteome and its ability to model the protein flexibility.

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