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FuncBind:
Unified all-atom molecule generation with neural fields

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NeurIPS 2025

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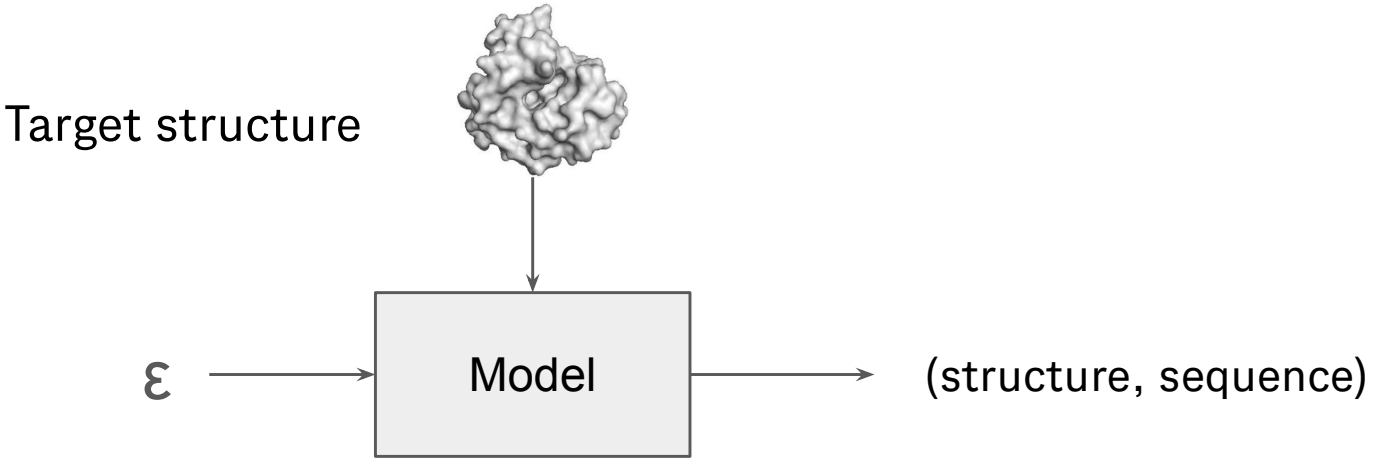
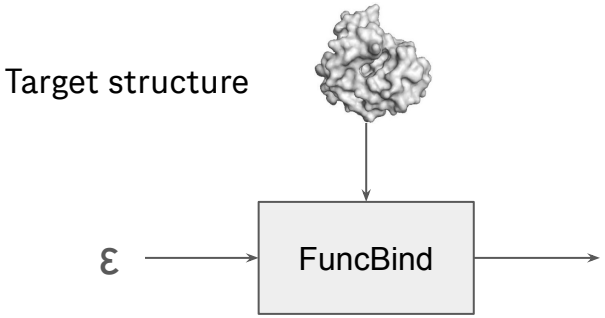
Context: structure-conditioned de novo generation



Many existing models ***usually***

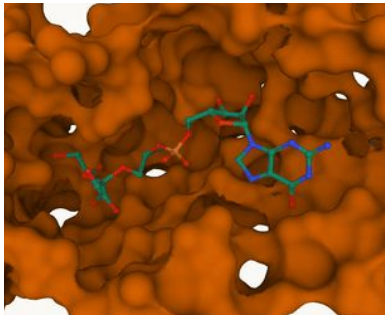
- inspired by AF style architectures
- limited to sequences of canonical AAs and pre-defined sequence lengths

An unified structure conditioned generative model

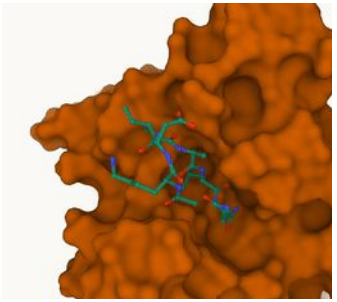


CDR loop structure given framework dock

small molecule



macrocyclic peptides (with ncAA)



- Single unified model trained across data modalities (small molecule, antibody CDR loop, cyclic peptide)
- All-atom modelling
- Variable sequence lengths
- Handles constraints such as non-canonical amino acids, cyclized peptides etc.

A vision-based model for molecule generation

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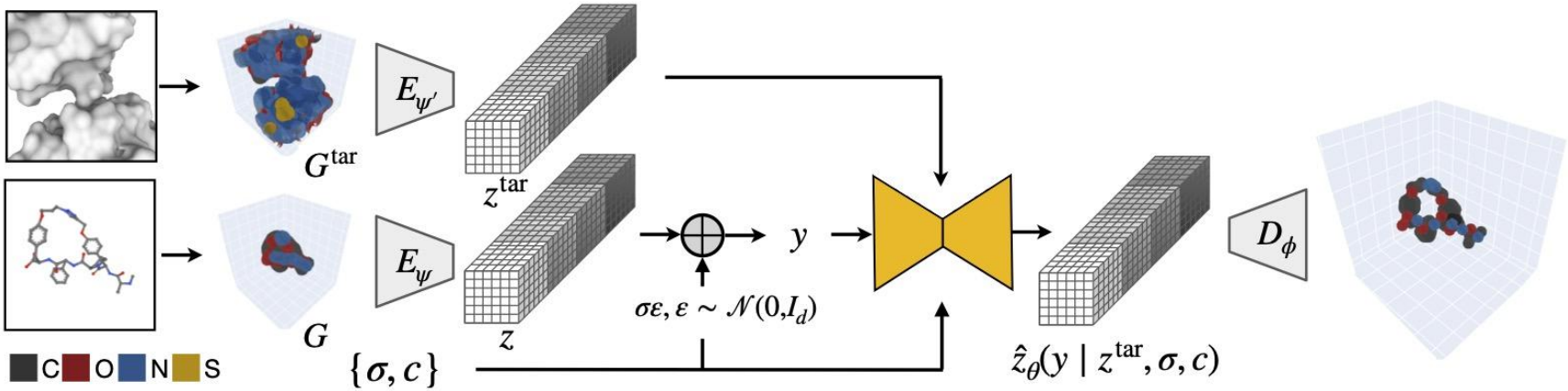
- Vision-based approach that represents molecules as 3D densities.
  - Auto-encoder of input molecules based on neural fields Kirchmeyer et al., NeurIPS 2024
  - UNet-based conditional denoiser scaled up to 5B parameters Karras et al., CVPR 2024



- Postprocessing to recover point cloud from generated 3D density

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Sampling with score based approaches

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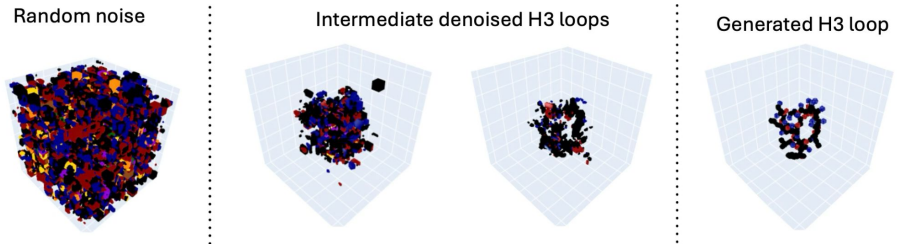
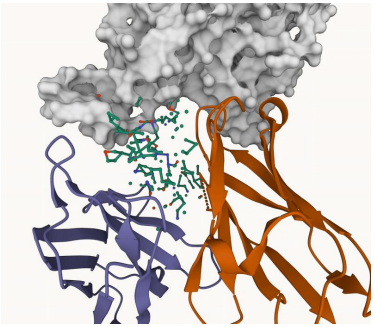
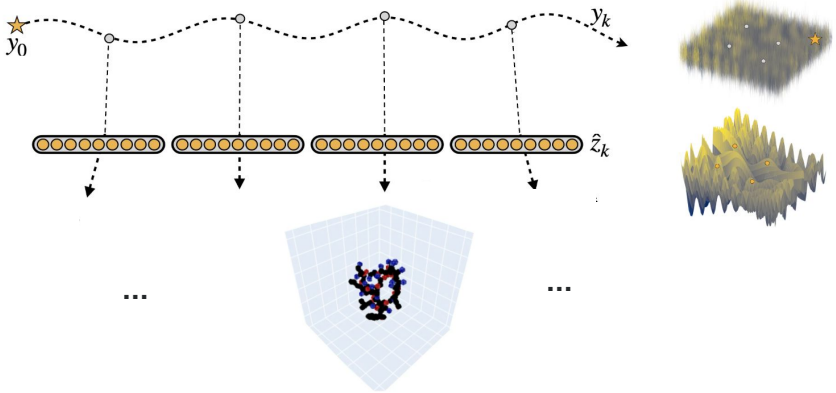
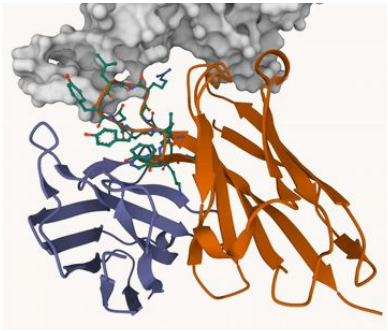
Diffusion
Ho et al., 2020





Walk Jump Sampling
Saremi et al., 2019





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Conclusion

- Check the paper for the following
  - In-silico benchmarking against standard baselines for small molecule, antibody CDR loop and macrocyclic peptide generation.
  - Wetlab validation for CDR H3 redesign for 2 anonymized targets.

- Code and weights (Apache 2.0) to be released
  - https://github.com/prescient-design/funcbind

- Dataset of macro-cyclic peptide - protein complexes to be released

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