

ATOM3D: Tasks on Molecules in Three Dimensions

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atom3d.ai

Datasets

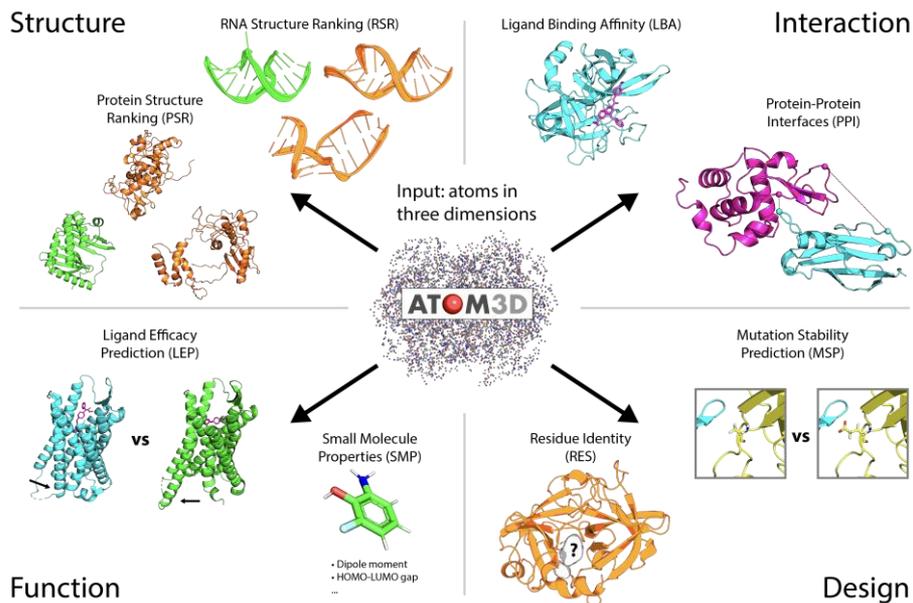
Project goal:

- Make structural biology more accessible for algorithm developers.

Unified framework:

- Standardized formats, splits, and metrics.
- Datasets and data loaders available online.

Check out atom3d.ai and github.com/drorlab/atom3d/



Benchmarking

Prototypical architectures:

- 3D convolutional neural networks.
- Graph neural networks.
- Equivariant neural networks.

Results:

- 3D representations consistently improve upon sequences/graphs.
- No single 3D method dominates all tasks.