LiveDesign ML

Complete solution for rapid AI/ML molecular property predictions

LiveDesign ML is a module in LiveDesign for training and deploying state-of-the-art AI/ML models for small molecule drug discovery. By treating datasets as dynamic information feeds that evolve as scientists explore new chemistry, LiveDesign ML delivers AI/ML models that are optimized to the most relevant project compounds and provides users with the critical information needed to determine if the models are sufficiently accurate for prospective use. The technology allows teams to streamline the optimization and validation of AI/ML models, expanding their application within drug discovery programs.

Democratize AI/ML model generation with a fully automated workflow to build and monitor molecular property and multi-parameter optimization (MPO) predictions

Deploy models prospectively with confidence via data visualizations and performance metrics that monitor a model's predictive power in evolving chemistry

Easily integrate models into team decision-making and design workflows via a centralized collaborative platform

Benefit from highly scalable AI/ML pipelines based on a modern cloud infrastructure to model hundreds of properties and make millions of predictions

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Seamless integration of cutting-edge AI/ML models into a centralized design platform

Input:
Experimental and/or *in silico* data

LiveDesign ML:
Automated AI/ML creation, optimization, and validation

Output:
Updated AI/ML predictions and performance statistics

Examples of properties predicted with LiveDesign ML

- **Experimental data:** Potency (on- and off-target), ADME, DMPK, and safety endpoints
- ***In silico* physics data:** Any properties stored in LiveDesign, i.e. FEP+

Key Features

- Rapid property predictions in an interactive design environment
- Simple user interface for generating AI/ML models and retraining them as the chemistry evolves
- Ability to triage hundreds of thousands of compound ideas in minutes for large library screening
- Built-in transfer learning across AI/ML models to improve low-data performance
- Leverages DeepAutoQSAR to train and tune state-of-the art model ensembles
- Visual representation of atom-level attribution
- Integrated model management to track ML performance over time

References

Benchmark study of DeepAutoQSAR, ChemProp, and DeepPurpose on the ADMET subset of the Therapeutic Data Commons

Contact us: sales@schrodinger.com

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Learn more about LiveDesign ML