Artificial Intelligence

Evaluate, Develop and Apply AI models to all types of data in drug discovery and development

Description

We review, test, benchmark, train and run various AI/ML models applicable to all types of data

- CBDD – Computational Biology methods for Drug Discovery: implementation of the best advanced AI approaches
- ABC – Algorithm Benchmarking Consortium: Ease algorithm and data selection
- Custom AI projects

State-of-the-art AI approaches

Classical ML and statistics – Exploratory and predictive analysis

NLP and Large Language Models for text mining and interactive response generation

Deep Learning / Neural Networks, including **Graph-based** approaches for predictive modeling

Foundation Models and GenAI for interrogating structured and unstructured data

Multi-modal approaches for evaluation of complex predictors

Methodology

Inputs

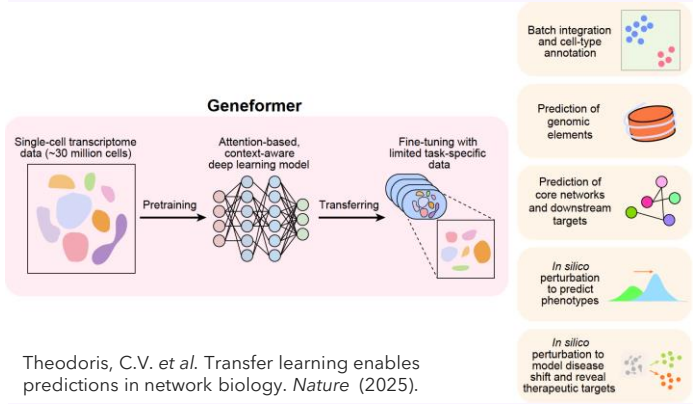
- Structured and un-structured public and customer-owned data: OMICS, text, audio, images, chemical structures
- Clarivate content sources from molecular evidence to competitive intelligence, safety alerts and Real-World-Data
- Knowledge Graphs (KGs), biological networks

Workflows

- AI predictive models for network- and graph-based applications in drug discovery
- LLM-based text data retrieval, i.e. for KGs
- LLM-enabled systems to power (graph) Retrieval Augmented Generation (RAG) applications
- Deep Learning, Foundation models and GenAI for OMICs data analysis
- AI-Driven Molecular Docking
- Deep learning for (acoustic) image classification
- Biomarker discovery and precision medicine, including multi-modal biomarker predictions
- Comprehensive review of existing AI models

Output

- AI application results, predictive models, workflows



Theodoris, C.V. *et al.* Transfer learning enables predictions in network biology. *Nature* (2025).

- Exploratory/ interactive reports, result visualization and interpretation
- Benchmarking of algorithms, code review

Typical Project Timeline

From 4 weeks, subject to complexity

Select case studies available upon request

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