Cureline
BALTIC PRECLINICAL CRO

Your *in silico* Support in Translational Medicine

Virtual HTS: Hit Identification

Our approach is characterized by state-of-the-art software with a unique deep learning system that trains on large proprietary database consisting of thousands of curated High Throughput Screening results covering most therapeutic areas.

The system is:

- **Proven:** tested by independent laboratories
- **Accurate:** unprecedented prediction precision, on par with experiments
- **Fast:** with >10k molecules per second
- **Versatile:** applicable in any therapeutic area

The technology can extend any HTS to a vast chemical space including millions of purchasable molecules and billions of synthesizable compounds.

The libraries are organized by potential compound approval speed:

- **FDA-approved natural products:** direct inclusion in nutraceutical and cosmetic products.
- **Natural compounds:** a significant proportion will lead to fast clinical studies that will not require FDA approval.
- **Existing or experimental drugs:** drug repurposing bypasses most preclinical and clinical phase I experiments.
- **Physical libraries:** quick order with the option to choose the library containing most hits

Virtual ADMET: Hit-to-Lead

Our in silico system bridges the gap between a promising hit and developing lead candidates ready for lead optimization and preclinical development. The technology we apply alleviates the overall attrition rates during the drug discovery pipeline with high accuracy predictions of absorption, distribution, metabolism, excretion, and toxicity (ADMET). This predictive capacity enables the identification of hits with favorable pharmacological properties.

Off-Target Prediction: Lead Optimization

Drug-like compounds are most of the time denied approval and use owing to the unexpected clinical side effects and cross-reactivity observed during clinical trials. This is generally linked to several factors, including incomplete knowledge on the drug targets and off-target effects. By capitalizing on large amounts of biochemical data, our off-target prediction service is an essential tool that steers us clear from the undesirable side-effects that impede drugs from getting into the market.

De Novo Prediction: Lead Optimization

Our system can screen virtual new compounds or analogs to existing hit compounds for hit-to-lead and lead optimization. This enables the virtual selection of many more hit analogs prior to costly syntheses and experiments, which drastically accelerates the hit-to-lead and lead optimization process.

Therapeutic Area Agnostic

Independent research projects guided by the system's predictions have led to new drug candidates along with proof of concepts in the field of virology and oncology. Given that our system's learning only depends on the amount and quality of data it trains from, the highest accuracies it can achieve are in therapeutic areas for which substantial data is available. Its performance across virology, bacteriology, parasitology, oncology, cardiology, neurology, and metabolic disorders reaches experimental accuracy, whenever HTS data is available.