VOKA
by innowise

AI-driven virtual screening white-label pipeline for drug discovery

Our ML ensemble pipeline and professional molecular modeling efficiently filter and prioritize lead compounds from vast chemical libraries. Trained on known true/false candidates for specific target proteins, this solution dramatically reduces screening time while maintaining exceptional accuracy.

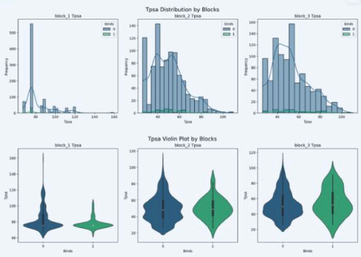
It achieves 90% precision and 80% recall across multiple targets. Researchers can rapidly process millions of compounds and informed reduce candidate pools by up to 85% without losing viable leads.

Problems addressed

CHALLENGE	HOW WE SOLVE IT
High costs and time-intensive manual screening processes	Reduced database size by up to 85%, preserving true lead candidates.
Low hit rates	Reasonably rank candidates by quality and relevance selected for further screening, increasing the success rate.
Difficulty in targeting specific proteins	Our solution is specifically trained on data for target proteins, enabling highly accurate predictions tailored to research needs.

Probability distribution for class 0 and class 1 (Threshold = 0.5)

Tpsa Distribution



Technical highlights

Efficient computational processing

Completed reviews in just 40 minutes on mid-level hardware.

Versatile data handling

Processes molecular fingerprints, SMILES strings, and molecular descriptors.

Advanced model architecture

Combines CNN, LSTM, BERT, and XGBoost models for comprehensive analysis.

Optimized performance

Employs model quantization, batch processing, and parallelization.

Scalable design

Successfully tested across multiple target proteins with consistent performance.

Key benefits

Reduced chemical search space

Capable of filtering out up to 85% of non-viable compounds.

Accelerated discovery

Automation of time-consuming manual filtering processes.

Improved success rates

Better early-stage filtering increases viable candidate advancement.

Lower computational costs

Optimized architecture reduces hardware requirements.

Scalability across targets

Adaptable to different protein targets with high performance.

Related services

1. **Structure-based virtual screening**
   Target protein structure analysis for predicting drug candidate binding.
2. **Ligand-based virtual screening**
   Known active compound analysis for identifying essential chemical features for drug discovery.
3. **Molecular docking and dynamics**
   Drug-target interaction prediction and binding stability assessment.
4. **ADMET prediction**
   Early assessment of drug-likeness and potential toxicity risks.
5. **Pharmacophore modeling**
   Essential chemical feature identification for target interaction and drug design.
6. **Compound library screening**
   Virtual screening of chemical databases for potential drug candidate identification.

Get started

Contact us today for a demonstration or consultation on how our Binding candidate selection pipeline can accelerate your drug discovery workflows.

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