Molecular Modeling as a Strategy for Prioritizing Molecular Targets and Inhibitors in Bacteria

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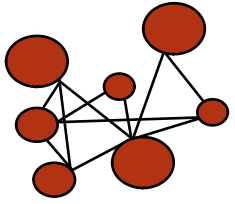
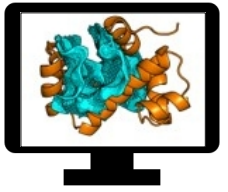
SABIAM-Alvo-Net: Rede Sul-Americana de Bioinformática, Inteligência Artificial e Modelagem na Prospecção de Alvos Moleculares e Inovação Biotecnológica

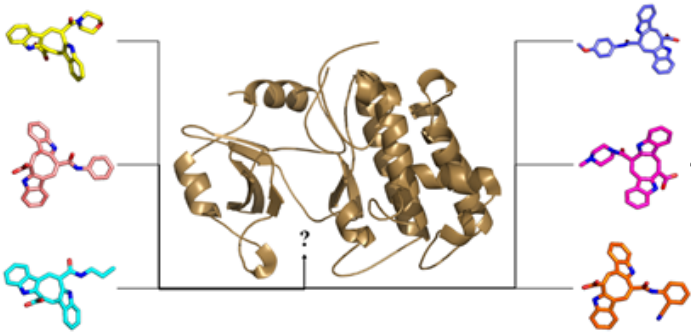




Bioinformatic	Co-expression network	Metabolic modelling	Molecular Modelling	Researchers and students
Ribosome profiling (Ribo-seq) and RNA-seq Bioinformatic analyses of gene translational efficiency	Weighted Correlation Network Analysis (WGCNA) Identification of modules enriched with transcription factors, virulence genes, and resistance genes	Use of metabolic models of Pseudomonas In silico gene knockout (KO) Assessment of bacterial fitness cost	Virtual screening and molecular docking Selection of ligands as promising inhibitors	Development of new tools for analysis Evaluation of in silico results

Drug design new inhibitors

Structural based drug design (SBDD)



Ligand based drug design (LBDD)

Information

Model (ML)

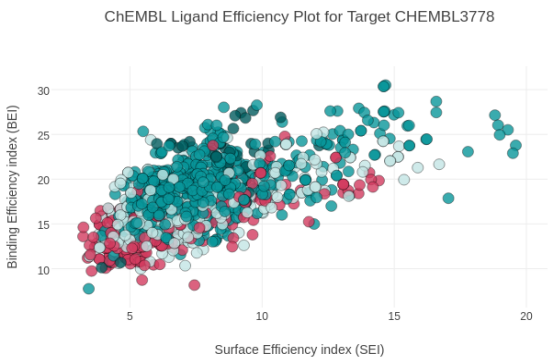
Prediction new inhibitors

Artificial Intelligence: a new era for *in silico* approaches?

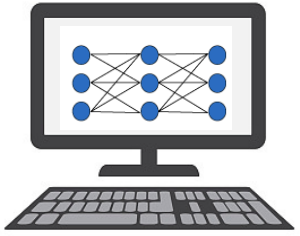
Dataset
Database of bioactivity

Model training
Machine/Deep Learning

Experimental Validation
Drug design



Training set vs. Test set



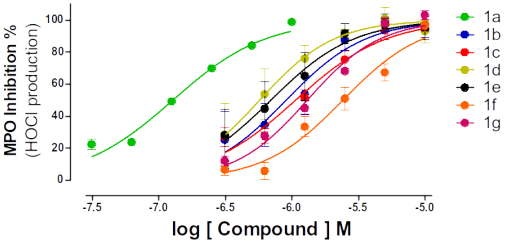
ML models

Molecular descriptors

Classification

Virtual screening

Prediction potential new inhibitors



IC_{50} (μM)
1a: 0.15 ± 0.03
1b: 0.92 ± 0.40
1c: 1.09 ± 0.18
1d: 0.58 ± 0.24
1e: 0.79 ± 0.39
1f: 2.48 ± 0.49
1g: 1.31 ± 0.03