Lead Identification

Accelerate and validate lead identification for lead development

Time: Lead identification can be time-consuming and complex

Design: Optimize drug design utilizing ADME principles

Bias: Insights can often be skewed by biased data and siloed data sets

Complexity: Infinite dynamic molecular interactions obfuscate clear pathway

Harness AI to empower data analytics and in-silico validation

Lead identification & validation

Mine text and contextualize data from upto 95% world wide web to identify and validate drug leads with natural language processing (NLP) that understands life sciences

Online data sources include

Academic literature: In-silico studies and published reports

Published chemicals and their preclinical studies
In-silico published reports, Pharmacophore designs

Experimental studies with chemical for:
DMPK studies, Screening studies, Medicinal Chemistry, Cytotoxicity studies, ADME studies etc.

Targets	Drugs	Binding score	HD:HA
Target-1	Drug-1	2.86E-12	Glu286:OE2:: N4(2.92), Met318:N:: N1 (2.97), Asp381:O1:: N(3.32), Asp381:N4:: O (2.72)
Target-2	Drug-2	2.91E-11	Glu286:Oe2:: N5(2.81), Glu381:N5:: O (2.73), Met318:O:: N3(3.08)
Target-3	Drug-3	1.22E-07	Glu286:OE2:: O1(2.79), Met381:O2:: O(2.96), Glu316:O: N2 (3.41), Met318:N:: N3(3.07)
Target-4	Drug-4	5.87E-12	Glu286:OE2::O5(2.78), Met318: N:: O2 (3.07), Met318:N::O1(3.33)
Target-5	Drug-5	3.81E-10	Asn322 ND2: O1 (2.79)

Rank targets based on their predicted binding scores

Biological network analytics

Understand disease mechanism in relation to lead

- Mechanism of Action
- Identify alternative drugs/chemical

Drug prioritization based on:

Druglikeness:

- MW 500, ClogP 5, H–bond donors, 5 H–bond acceptors (sum of N and O atoms) 10
- Polar surface area 140, sum of H–bond donors, and acceptors 12, rotatable bonds 10

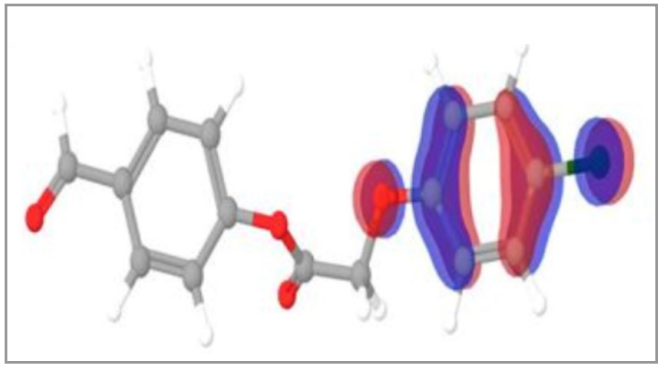
Structure-based drug/lead identification

Lead Identification

- Structure and substructure library screening
- Scaffold hopping
- Pharmacophore and shape-based virtual screening
- Fragment based drug design modelling

Ligand-based drugs design

- Lead Optimization
- QSAR modelling and analysis
- 3D-QSAR modeling
- Structure based optimization



Model and predict drug-protein interactions based on their pharmacokinetic and pharmacodynamic properties

Genetic profile and gene expression using public, and/or client data

Biomarker based drug identification

Drug response biomarker

- Which drugs are affecting which disease?
- Which biological targets are getting triggered?
- Drug toxicity
- Drug efficacy

Benefits

Identify optimal lead:
Efficacious, safe, meets clinical and commercial requirements, lead prioritization

Narrow lead selection:
Researchers must sift through seemingly endless potential targets

Accelerate lead identification:
Lead identification can be time-consuming and complex

Data-driven decision-making:
Insights can often be skewed by biased data and siloed data sets

info@innoplexus.com
www.innoplexus.com