YDS Medicine, Inc

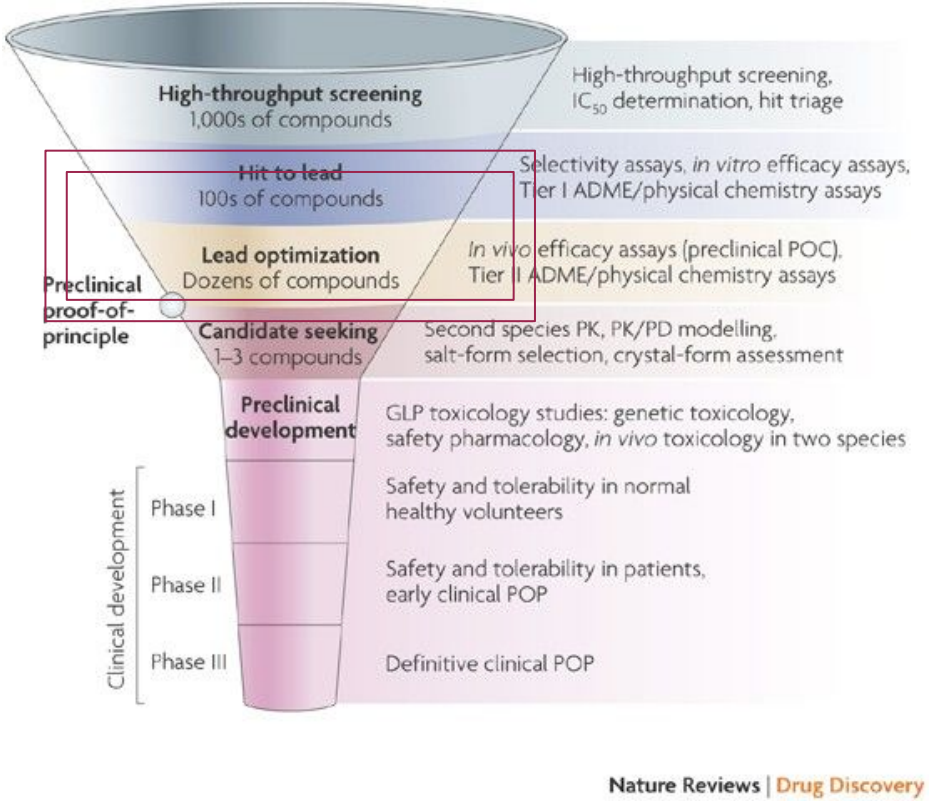
Leading computational engine for drug design, leveraging AI+biophysics

AI for Pharmaceutical Science

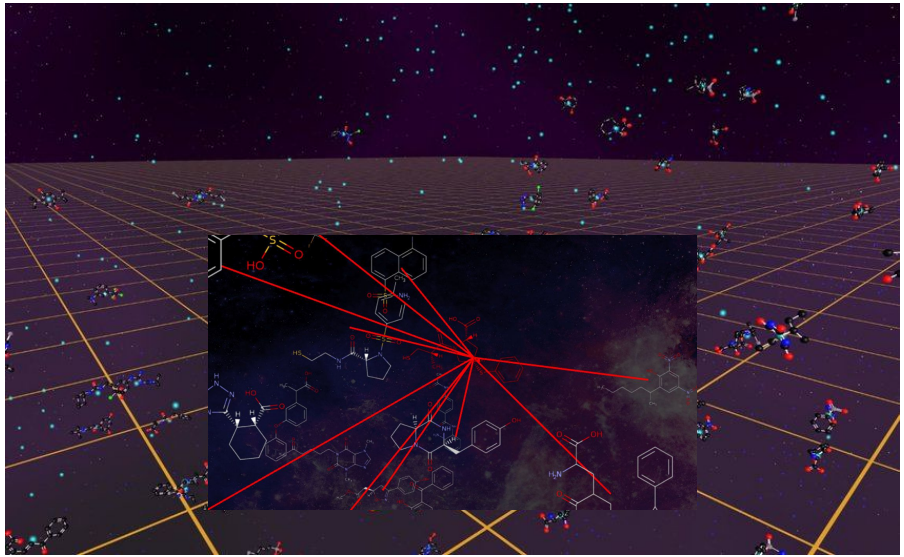
Albany, NY

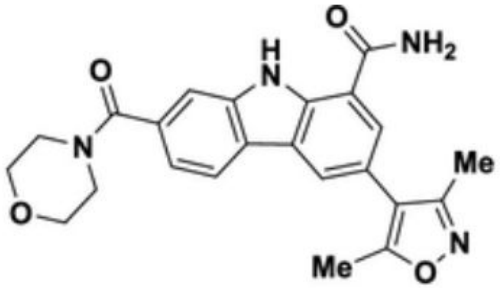
Pain point and our solution

Drug discovery-find the best key



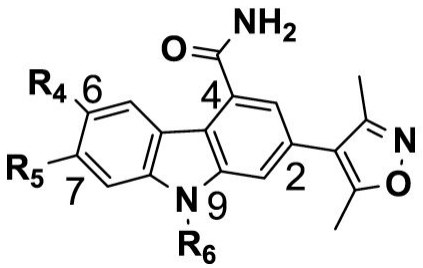
Pain point-Which modifications to choose for hit compounds?





1

BRD4 IC_{50} (nM) 712



https://pubs.acs.org/doi/10.1021/acs.jmedchem.1c00625

How to automatically and efficiently find the best key? The missing piece -- roadmap to navigate chemical universe

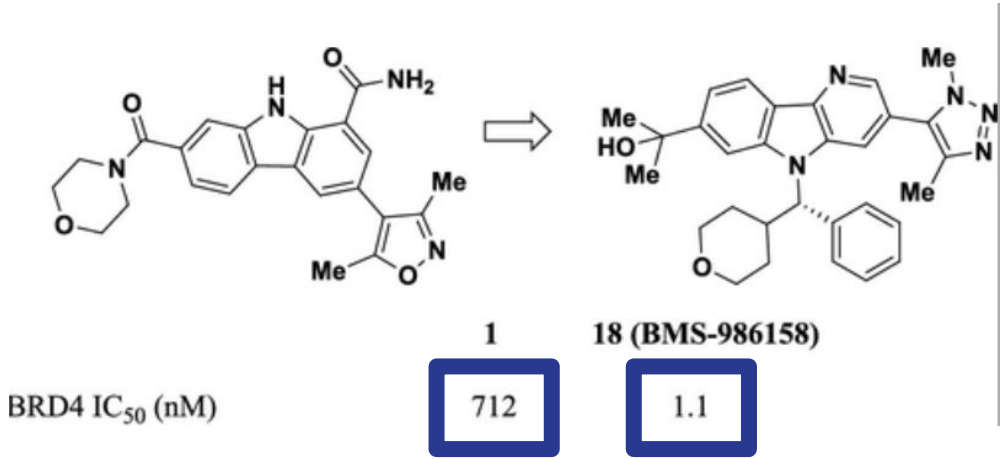
Weak binder

↓

Millions of ways to modify molecules
Huge trial-and-error costs

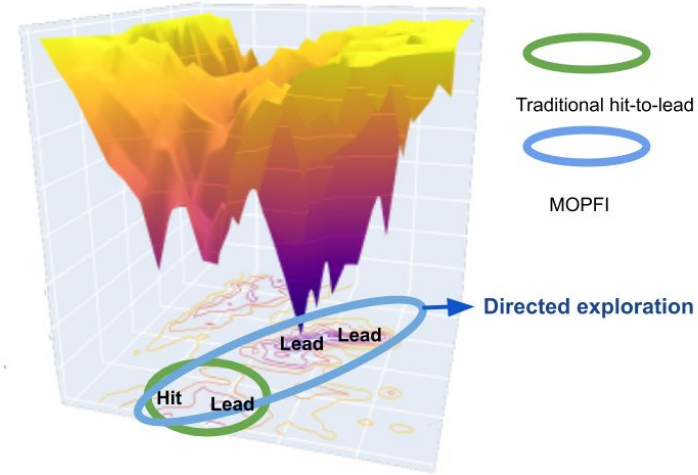
↓

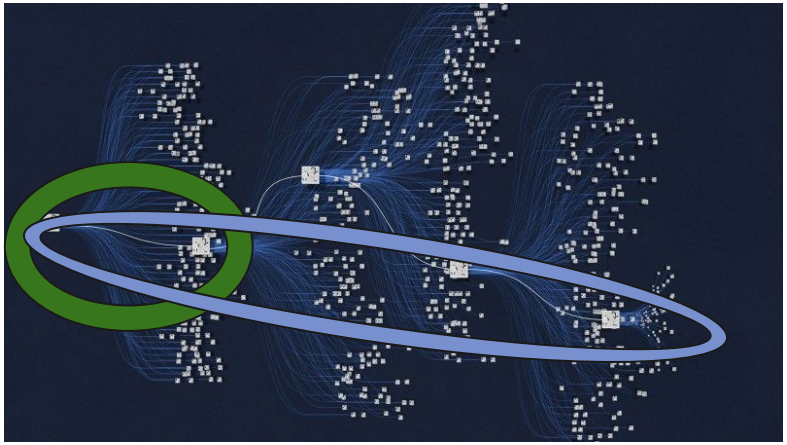
Strong binder



Our solution- Alpha Zero for drug design: AI+biophysics platform

Better candidates in shorter time, reduce trial-and-error costs





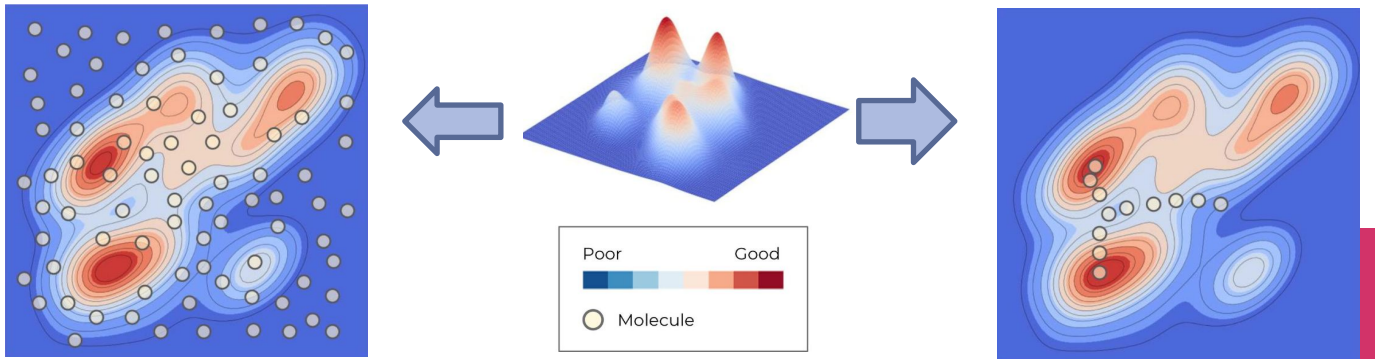
MOPFI (Modification- Optimization-Prediction-Feedback-Interaction)

MOPFI-Directed exploring chemical space

- **No priori big data dependent**——think out of box, generate novel scaffold which leads to new IPs, no concern disclosing your assay data
- **Customize** designs based on your target——Integrating 3D info of targets, focus on related chemical space

Pattern learning+Virtual Screening

MOPFI Goal directed learning

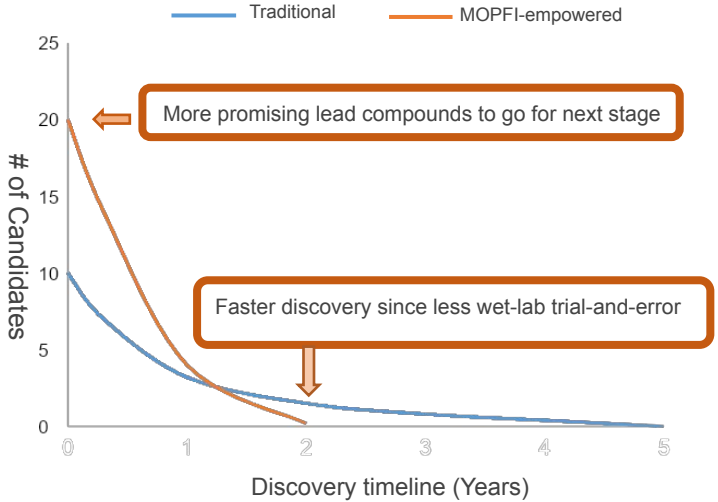


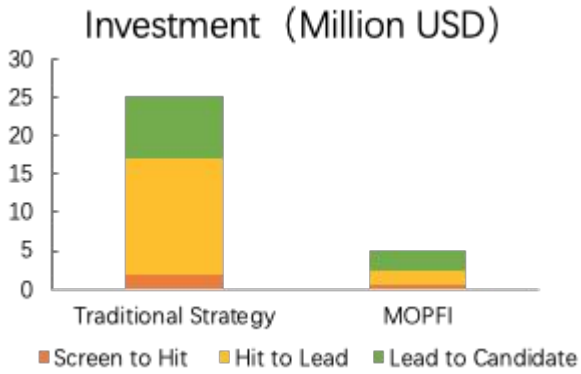
MOPFI- Increase success rates by generating more promising candidates

Speedy

Directed

Little data



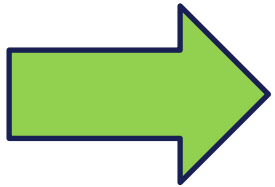


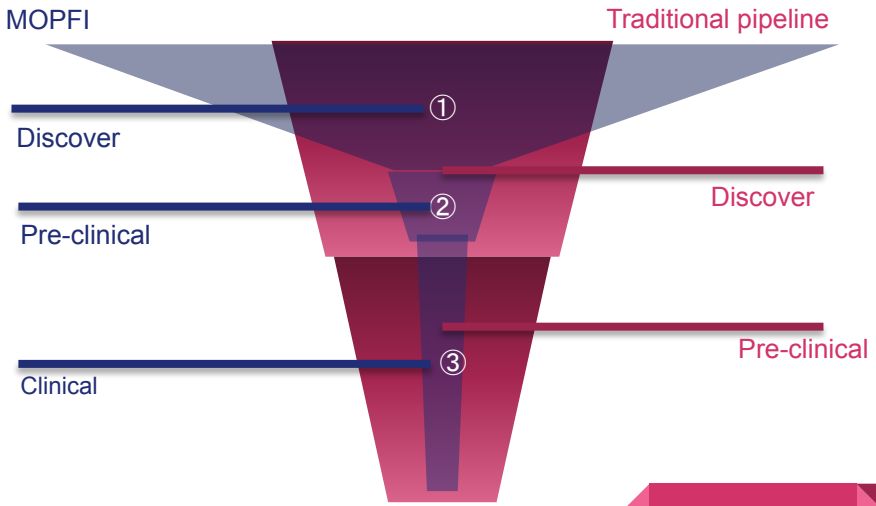
MOPFI-Reshape drug discovery

Speedy

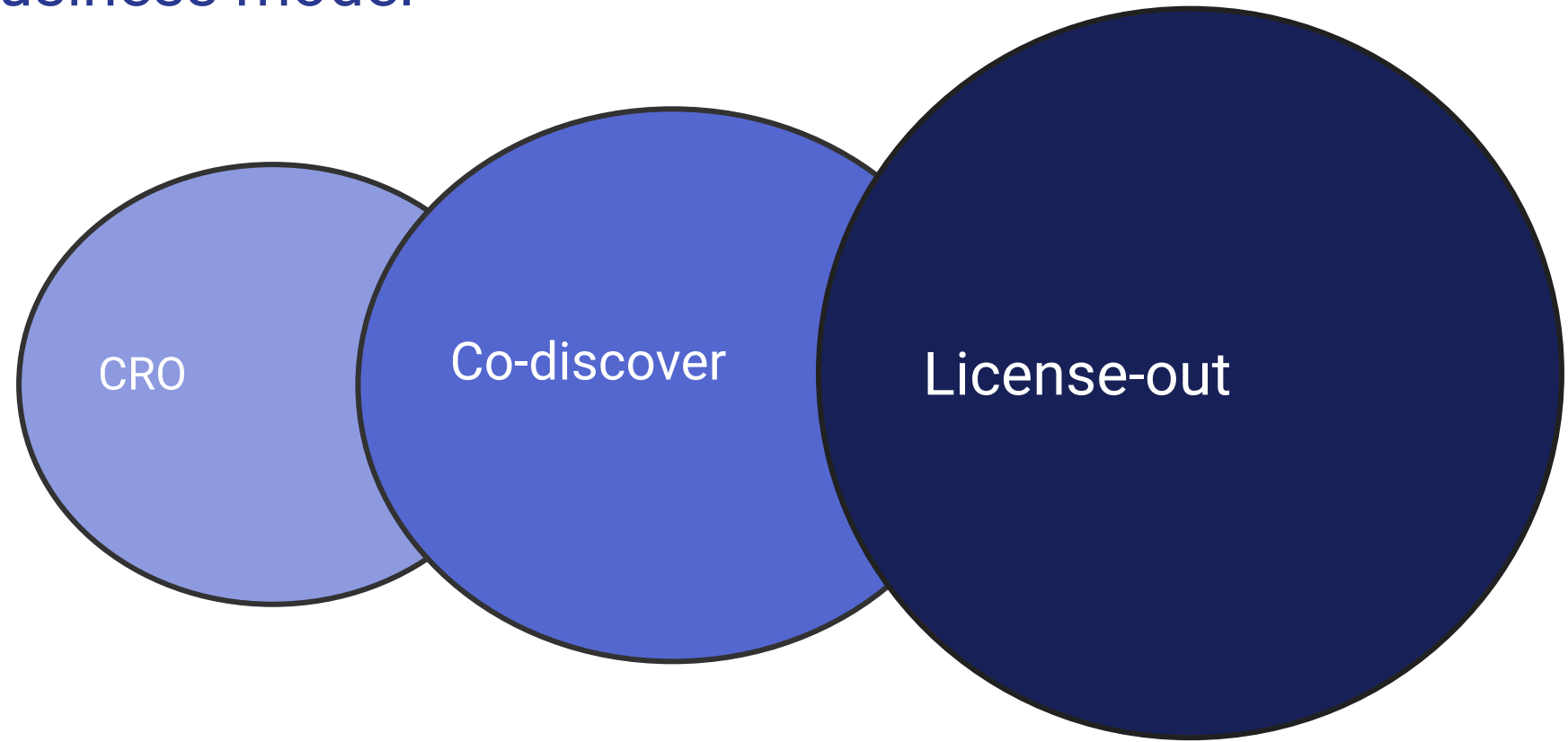
Directed

Little data





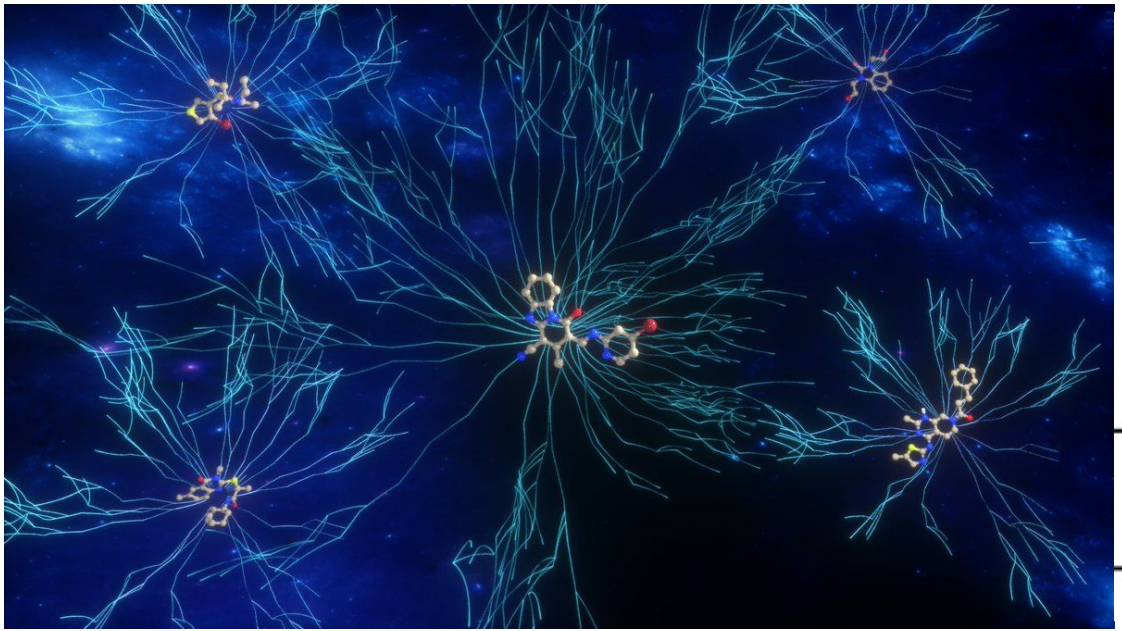
Business model

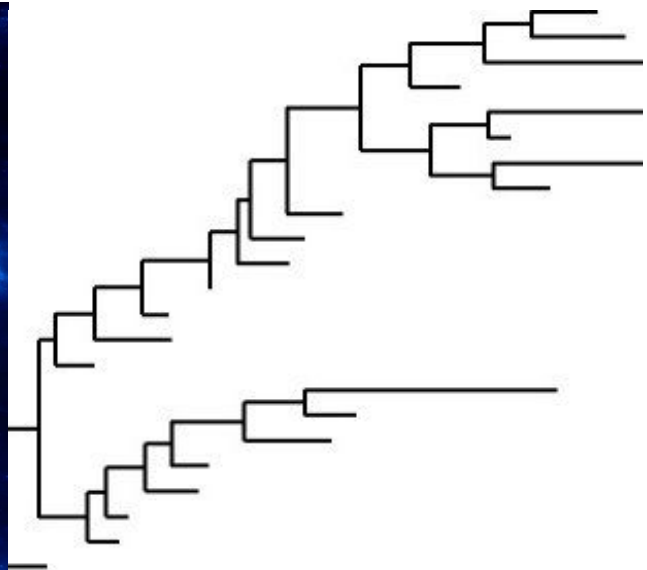


How we are different

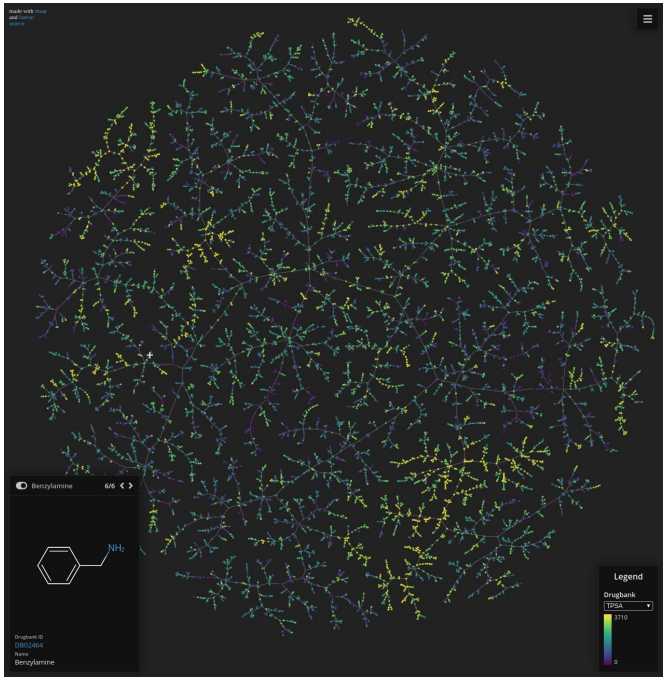
Zero data-learning from scratch | Self Evolve

Powerful first-in-class drug design engine



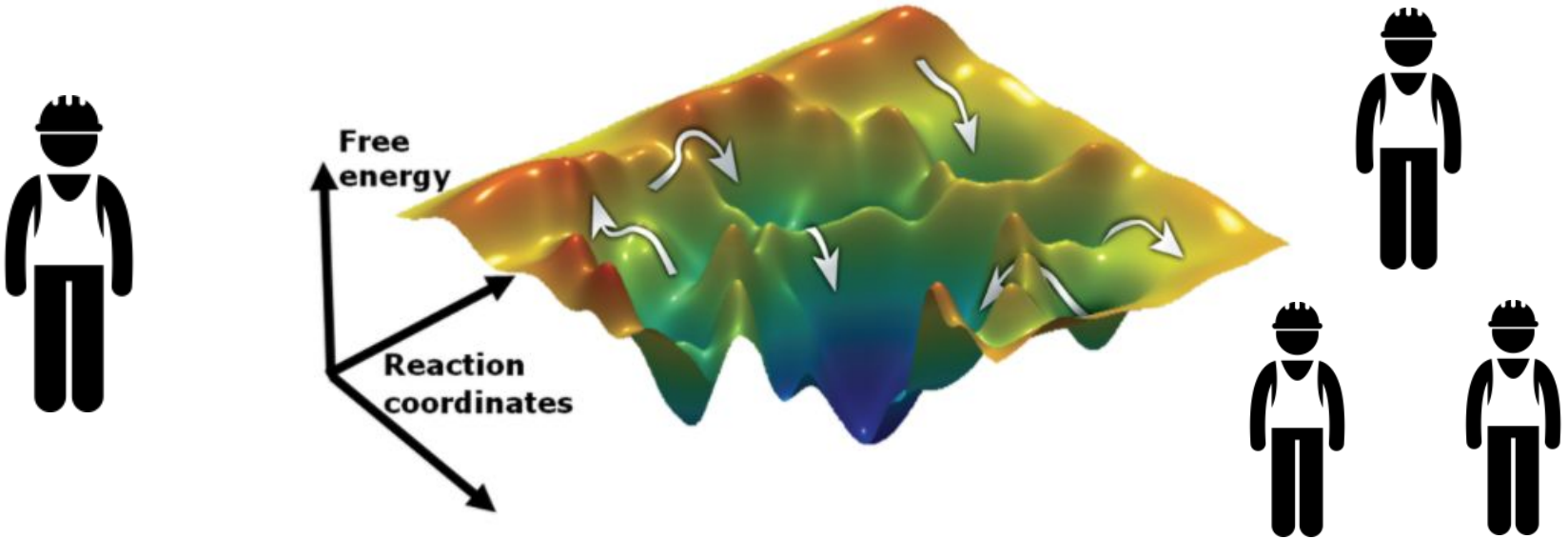


Sample relevant chemical space | Integrating protein structure information into AI engine

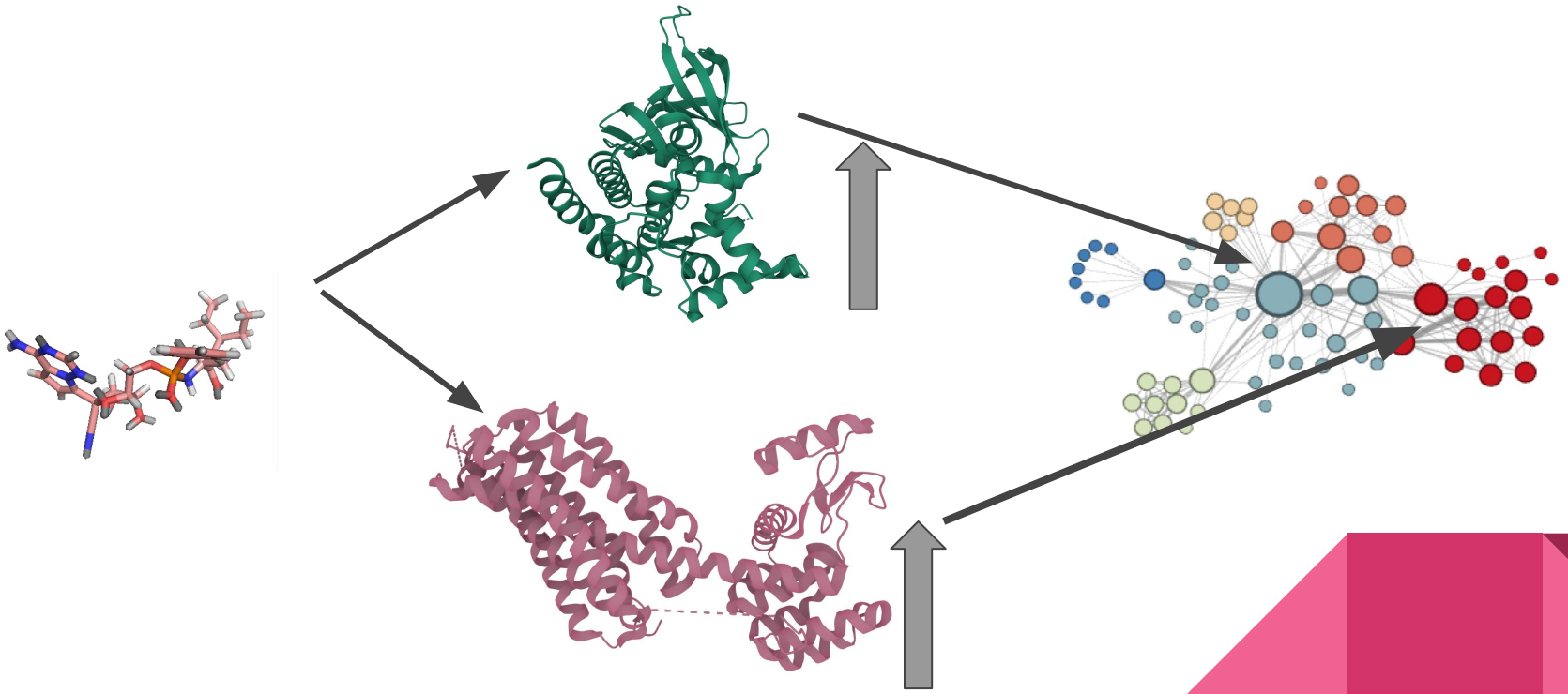


Novel scaffold | diversified designs

Single exploration engine VS. MOPFI **Multiple** exploration engine

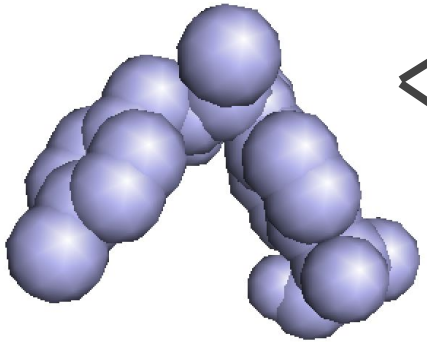


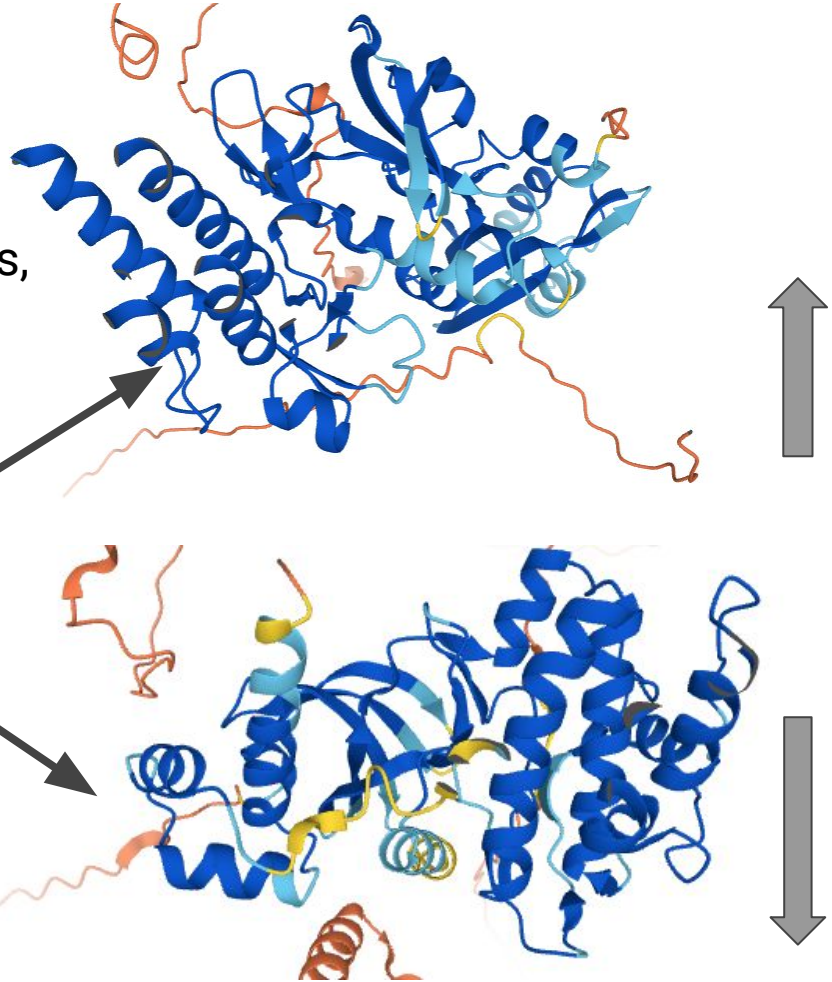
Bispecifics



Drug specificity

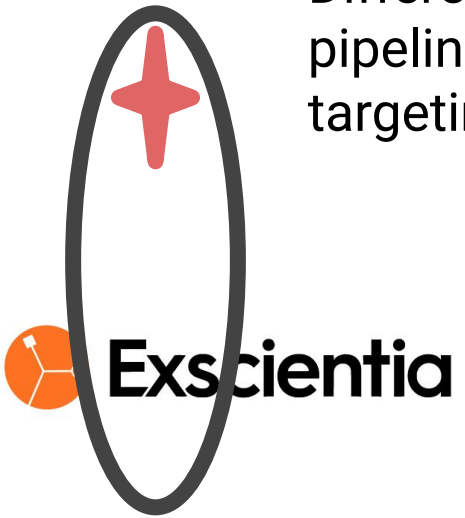
Design molecules towards two goals, increasing binding affinity towards protein A while decreasing binding affinity towards protein B





Competitors

Differentiate in technologies, pipelines, indications and targeting collaborators



neoX BIOTECH

XtalPi

Benevolent AI

Peptide

Bigger small molecules (PROTAC)

Traditional small molecules

On-the-fly

modeling data

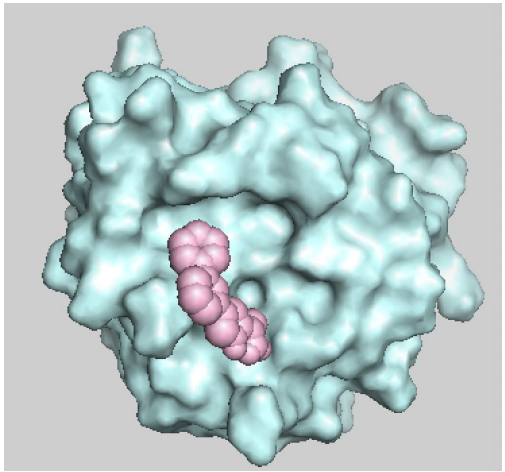
wet-lab data

Literature

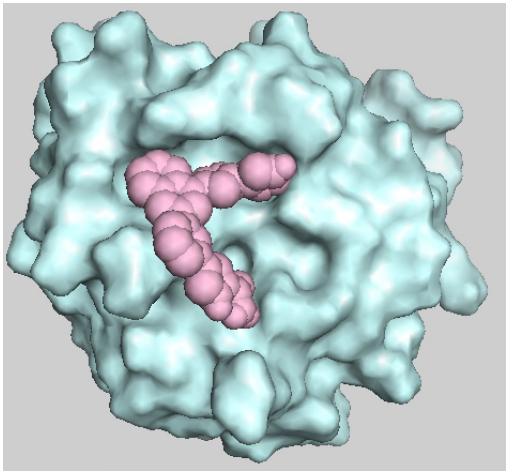
Priori Data

Case studies

Case study- Targeting undruggable



20 uM



200 nM

Tractions-Case study

A **novel** lead compound was designed that bypasses the current patent in **40 days**, not 12-15 months

Tractions-Collaborative biopharma companies

ST** A+ $22.22 M raised

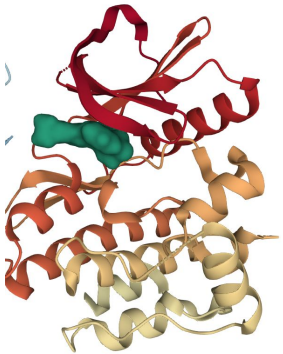
UA** A $10.5 M raised

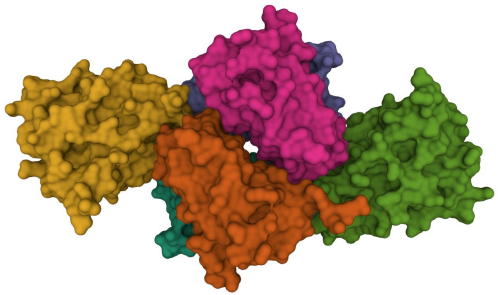
A World-leading lab

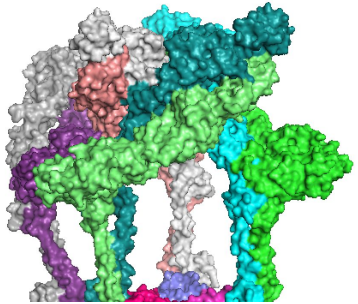
Allosteric Inhibitor

Bispecifics

Antiviral

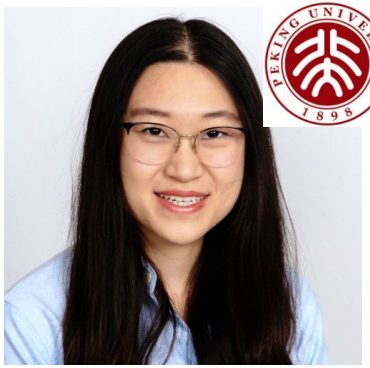






One drug, two targets

The Team -- Core



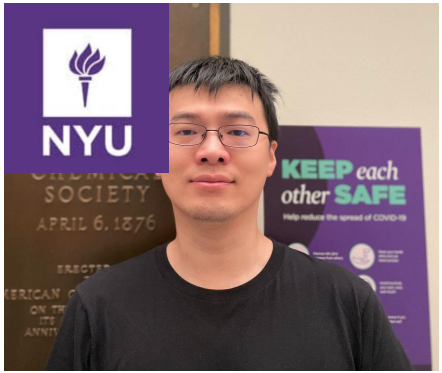
Xing Che, Ph. D.,
Co-founder/CEO

A computational chemist and biophysicist, focused on developing new algorithms to study thermodynamics and kinetics of ligand-drug interaction

Renming Wang,
Co-founder/Chief Operating Officer

Serial successful entrepreneur

Raised $400k and secured $10M acquisition



Zhuoran Long, Ph.D.

Machine Learning Scientist

Shengmin Zhou, Ph.D.

Quantum mechanics/Molecular mechanics scientist

RUTGERS

The Team-- Advisors

curia

Peter Guzzo, PhD,

Former director of drug discovery at Curia, one of the world's largest CROs. Generated innovative intellectual property in the areas of metabolic, CNS, oncology and gastrointestinal diseases etc. with 40 patents and led three license deals

Wharton

TRYP THERAPEUTICS

ImmunoPrecise

James Kuo, MD. MBA

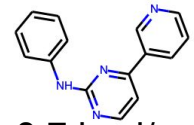
CEO and Co-founder of TRYP Therapeutics (CSE TRYP.CN)

Chairman of the Board ImmunoPrecise Antibodies LTD (NASDAQ IPA)

2X 0-> IPO

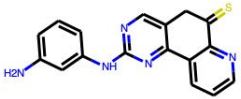
Thank You

How it works

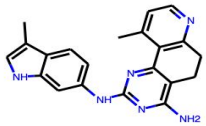


-8.7 kcal/mol

Molecular modifier



-10.3 kcal/mol



-11.6 kcal/mol

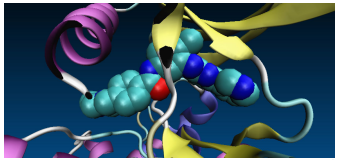
MOPFI

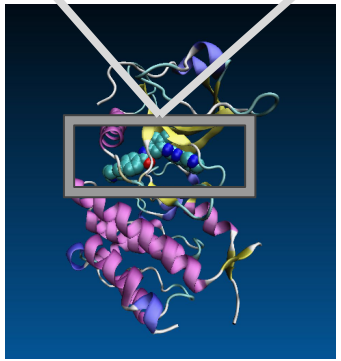
Property calculator

Feedback--
Binding affinity scores

Learning engine

Learn to obtain stronger binding





Results

The learning engine learnt how to generate molecules with stronger binding affinities

1 kcal/mol ~ **5.4X**
3 kcal/mol ~ **157X**

FDA approved inhibitor: Imatinib (-9.9 kcal/mol, commercial name: Gleevec)