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AI powered co-ideation for faster patient impact

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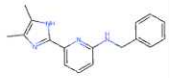
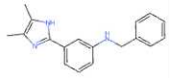
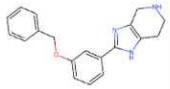
Malaria Libre optimising potency and logD

Molecules | Plots

All | My molecules | Generated molecules

Draw | Generate | Upload new data

Filters | Calculate | Properties | Predict | Columns | Share

	Smiles	Generated with AI	3D7 pIC50	LogD
343			6.87	3.37
1			5.77	3.45
2			7.05	2.77 High Novelty
3			5.93	4.75
Total: 1154		Generated: 800	6.63 ± 0.72	3.06 ± 0.72

Property details

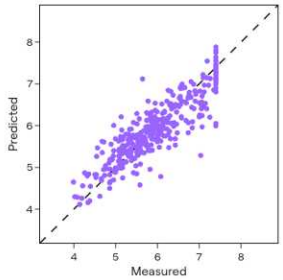
3D7 pIC50

Predicted values ± uncertainty should contain the true value in ~90% of cases.

When sorting for higher or lower **3D7 pIC50** you can expect:
77.1% of the highest predictions to be the true highest values in your dataset.
71.4% of the lowest predictions to be the true lowest values in your dataset.

☐ Add property to all datasets.

Advanced



Comparison between Predicted (y-axis) and Measured (x-axis) values when the measured data was not used for learning. Read more about this validation.
More accurate predictions are closer to the dashed line. Hover over each point for more details.

R-squared: **0.77**
Mean error of predictions: **0.30**
Model ID: **42386**
Molecular features: **2D**

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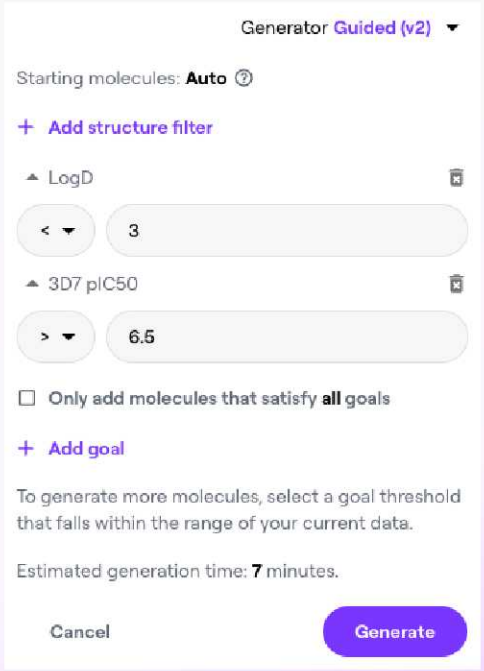
Generator Guided (v2)
Starting molecules: Auto
Add structure filter
LogD
< 3
3D7 pIC50
> 6.5
Only add molecules that satisfy all goals
Add goal
To generate more molecules, select a goal threshold that falls within the range of your current data.
Estimated generation time: 7 minutes.
Cancel
Generate

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Molecules | Plots

All | My molecules | Generated molecules

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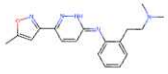
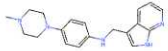
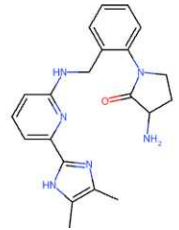
	Smiles	Generated with AI	3D7 pIC50	LogD
356		Generated with 'Guided' Model. Goals: 3D7 pIC50 > 6.5, LogD < 3. Row 343	6.63 High Novelty	2.15 High Novelty
357		Generated with 'Guided' Model. Goals: 3D7 pIC50 > 6.5, LogD < 3. Row 343	6.99 High Novelty	2.61 High Novelty
358		Generated with 'Guided' Model. Goals: 3D7 pIC50 > 6.5, LogD < 3. Row 343	6.90 High Novelty	2.12 High Novelty
Total: 800		Generated: 800	6.94 ± 0.37	2.83 ± 0.48

Molecule Details

Generated

Edit



Generated with AI	Generated with 'Guided' Model. Goals: 3D7 pIC50 > 6.5, LogD < 3. Row 343
3D7 pIC50	6.63 (High Novelty)
LogD	2.15 (High Novelty)

Compare to similar molecules

See how this molecule compares to similar molecules from your uploaded dataset

View comparisons →

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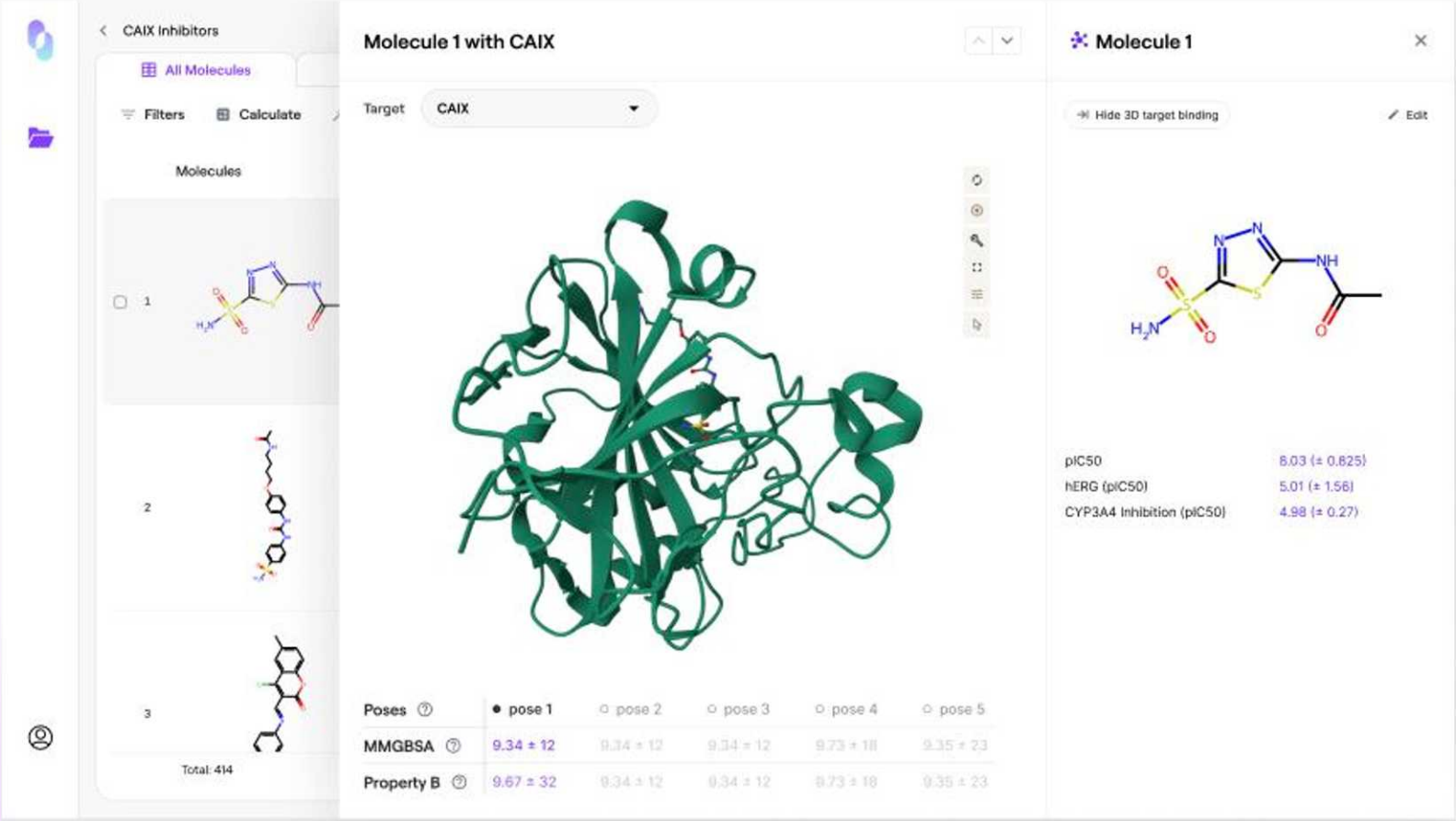
CAIX Inhibitors
All Molecules
Filters
Calculate
Molecules
1
2
3
Total: 414
Molecule 1 with CAIX
Target
CAIX
Poses
pose 1
pose 2
pose 3
pose 4
pose 5
MMGBSA
9.34 ± 12
Property B
9.67 ± 32
Molecule 1
Hide 3D target binding
Edit
pIC50
8.03 (± 0.825)
hERG (pIC50)
5.01 (± 1.56)
CYP3A4 Inhibition (pIC50)
4.98 (± 0.27)

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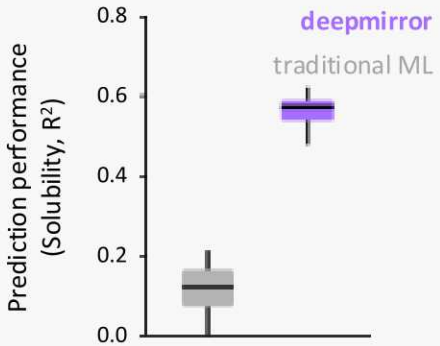
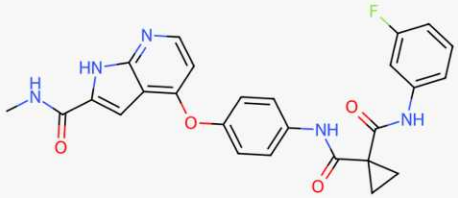
Foundation Models for Molecular Properties

Step up performance in potency, ADMET, and more



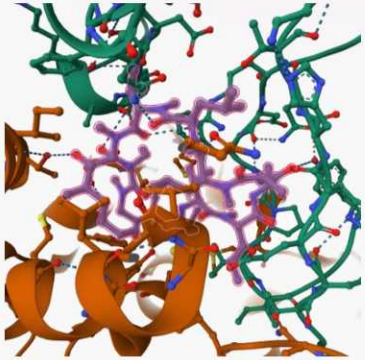
Generative AI Tailored to Medicinal Chemistry

Design novel, viable molecules that address multiple design goal



Protein-Ligand Structure Predictions

Accurate AlphaFold3-style predictions for biomolecular complexes



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autoML for chemistry

User Dataset

Build the best model

Make predictions

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Expert

Graph

Text

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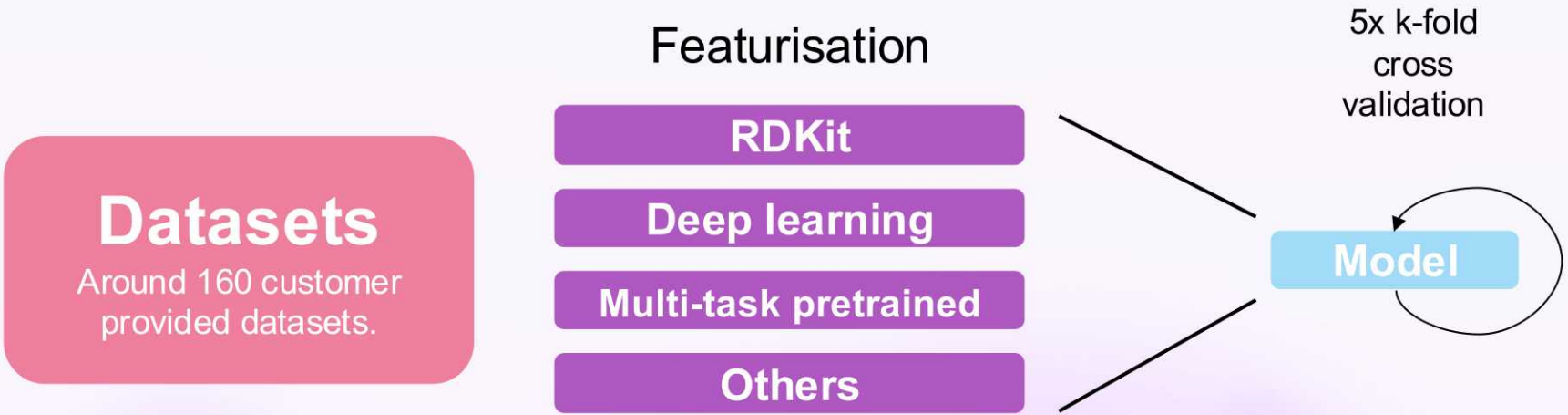

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autoML for chemistry

- RDKit-based models (e.g., Morgan, RDKit2D)
- Deep Learning-based models (e.g., ChemBERTa, Mol2Vec)
- Multi-task pretrained models (trained on large portions of ChEMBL / private data)
- Other (e.g., Pharmacophore-based models)

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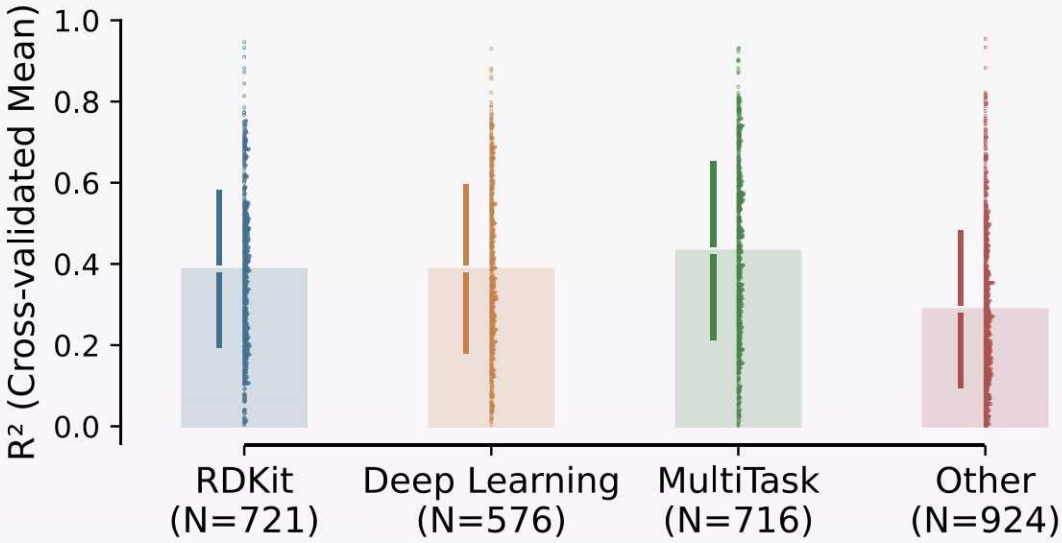
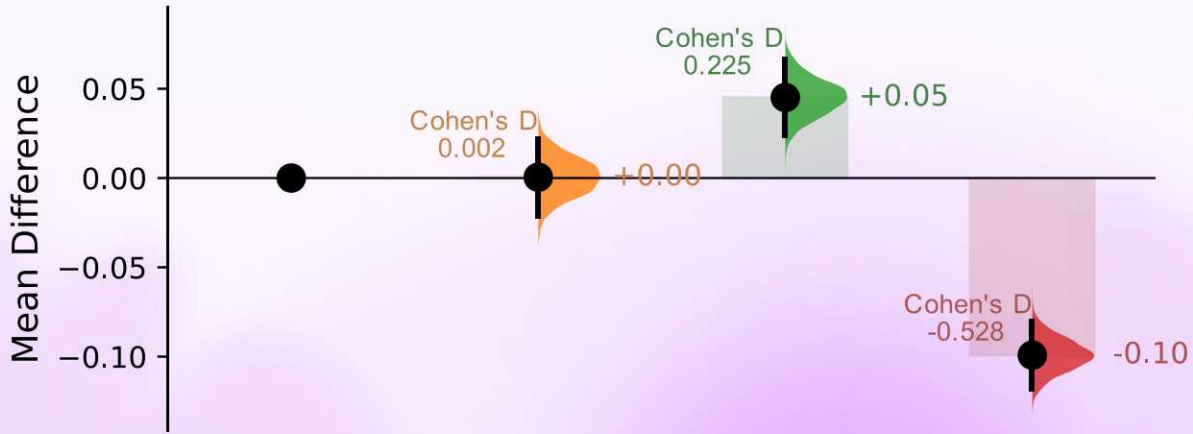

R² (Cross-validated Mean)
1.0
0.8
0.6
0.4
0.2
0.0
RDKit
(N=721)
Deep Learning
(N=576)
MultiTask
(N=716)
Other
(N=924)


Mean Difference
0.05
0.00
−0.05
−0.10
Cohen's D
0.225
+0.05
Cohen's D
0.002
+0.00
Cohen's D
-0.528
-0.10

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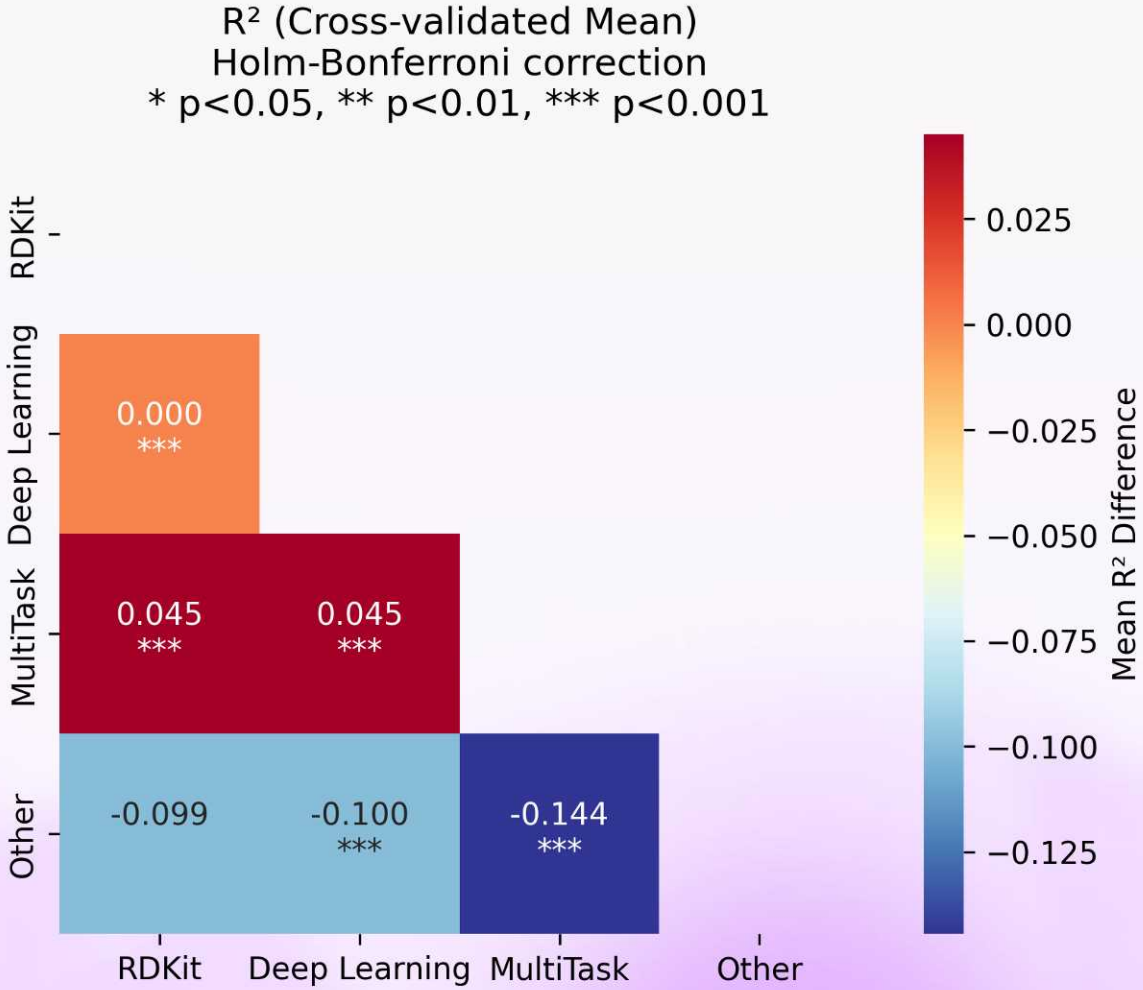
R² (Cross-validated Mean)
Holm-Bonferroni correction
* p<0.05, ** p<0.01, *** p<0.001
RDKit
Deep Learning
MultiTask
Other
0.000
***
0.045
***
0.045
***
-0.099
-0.100
***
-0.144
***
RDKit
Deep Learning
MultiTask
Other
0.025
0.000
−0.025
−0.050
−0.075
−0.100
−0.125
Mean R² Difference

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Lessons Learned from our autoML Pipeline:

1. Classical fingerprints (RDKit-based) are a very strong baseline and are often comparable to deep learning models.

2. Multi-task pretrained models consistently deliver strong results, validating their practical effectiveness.

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Thank you for listening

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Sanford Burnham Prebys

Santero therapeutics

UBC

AMPHISTA THERAPEUTICS

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Tes Pharma

and more...