



PostEra

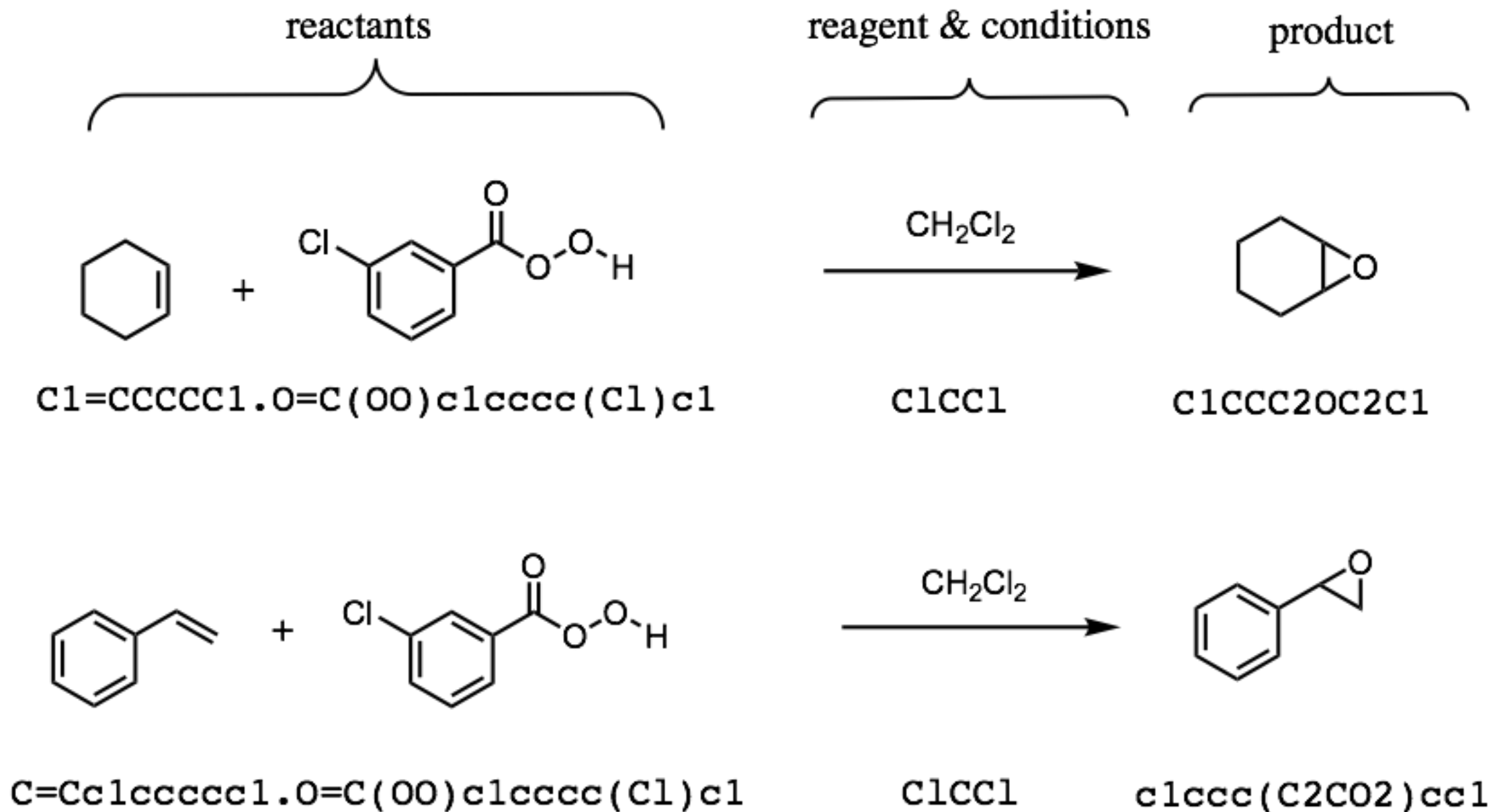
Medicinal Chemistry as a Service powered by Machine Learning

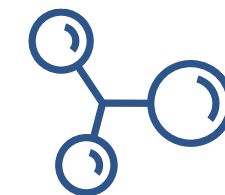


Backed by Y Combinator



We learn the rules of chemistry using a natural language processing approach





Organic reaction prediction using a machine translation approach

	Jin et al. (2017)	IBM (2018)	Coley et al. (2019)	Molecular Transformer
Test set accuracy	79.6%	80.3%	85.6%	90.4%

Molecular Transformer matches human performance and augments chemistry expertise

Using Molecular Transformer to accelerate Moonshot



Picking out quick wins from many great suggestions

HOW YOU CAN HELP

Fund Us

Funds go toward making and testing the most promising antiviral candidates.

\$51,270 raised of \$1,500,000

GoFundMe

Share Your Compute Power

Run molecular simulations on your computer when idle to help us find new molecules to test.

100.0% of sprint completed

Sprint 5 : Started Sat Nov 7 20:00:21 UTC 2020

Folding@home

Contribute Your Expertise

Submit drug design ideas using the form below.

15,016 molecules submitted

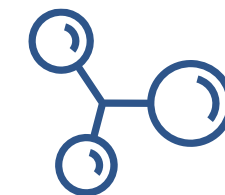
1,476 synthesized and tested

211 structures

Submit Molecule(s)

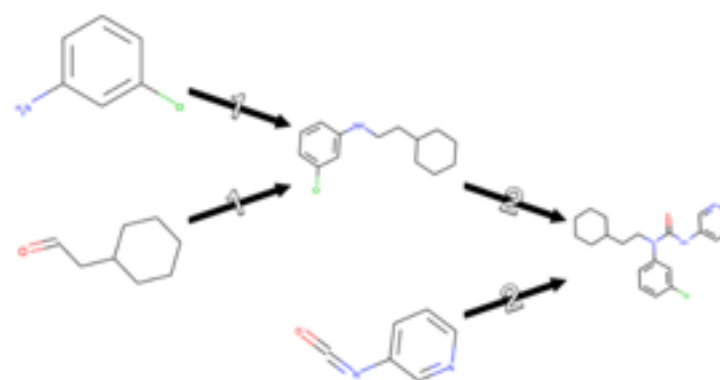
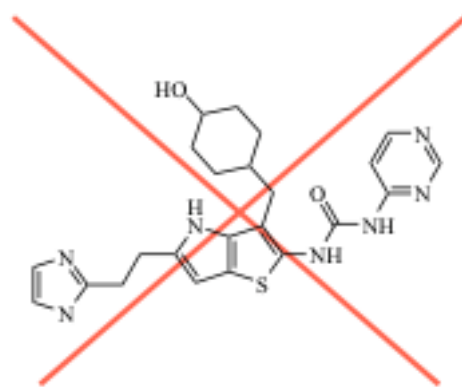
Please feel free to [email us](#) if you think you can be of additional help.

Machine learning triages compounds at scale

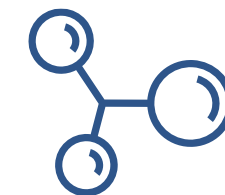


2000 submissions
in the first week

Less than a weekend to automatically filter
to ~200 compounds with <3 steps
synthesis



Machine learning leverages vast chemical inventory



BUILDING BLOCK CATALOGUE



225 Thousand compounds in stock
Original and unique

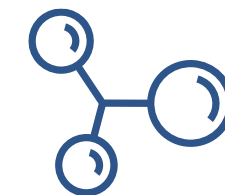
MAKE-ON-DEMAND BUILDING BLOCKS



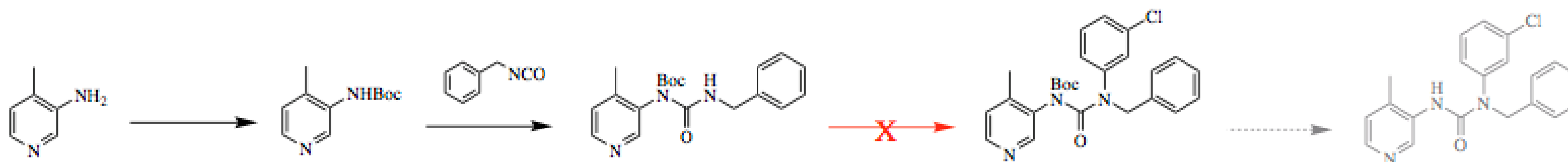
210 Million novel building blocks
Reliable supply

Complex molecules can be made easily, if we can keep track of all the building blocks and reactivity

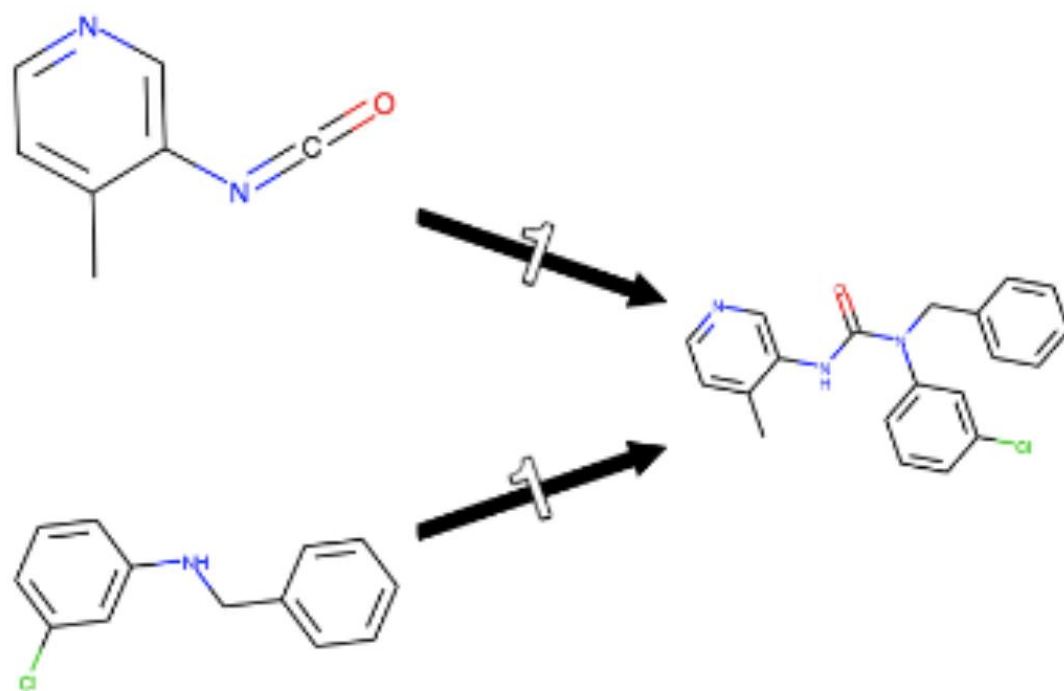
Examples of machine learning in action



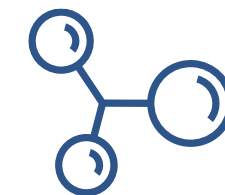
Attempted route



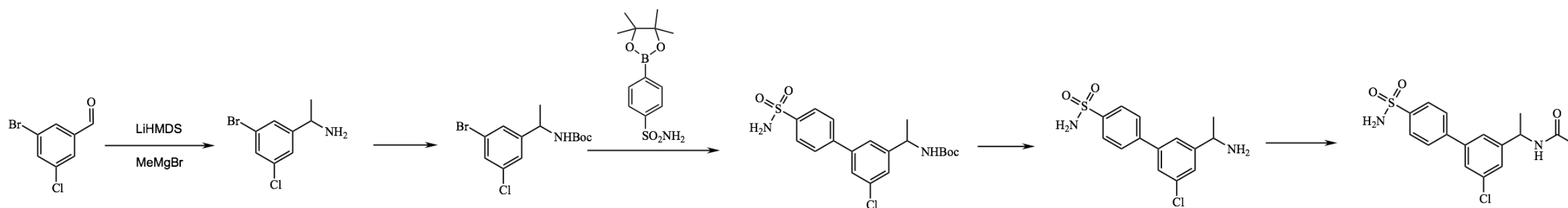
Manifold Route



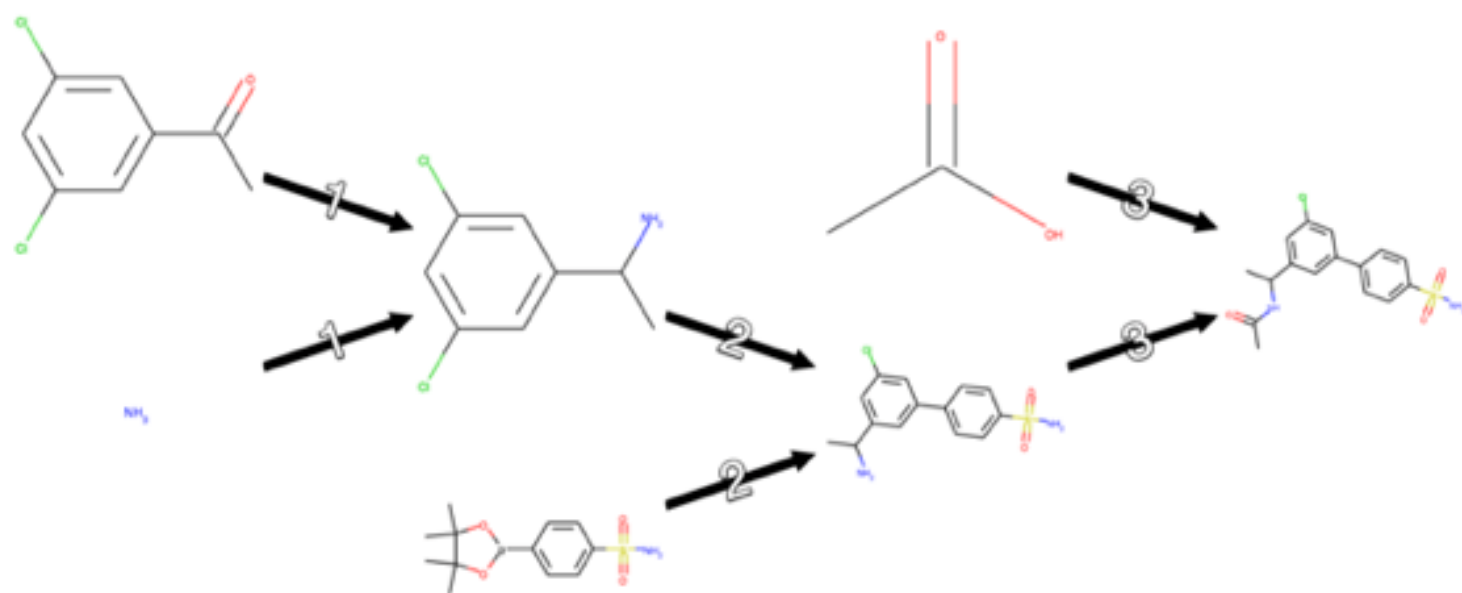
Examples of machine learning in action



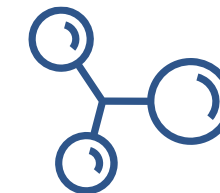
Route suggested based on experience with a similar product



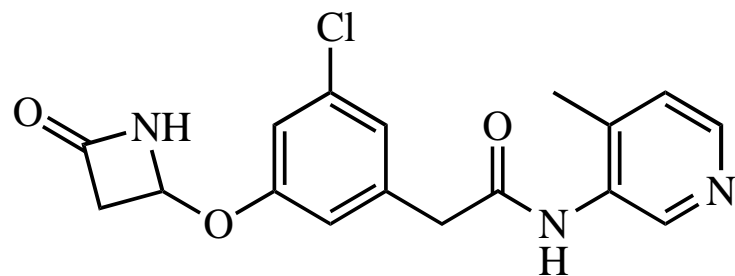
Manifold Route



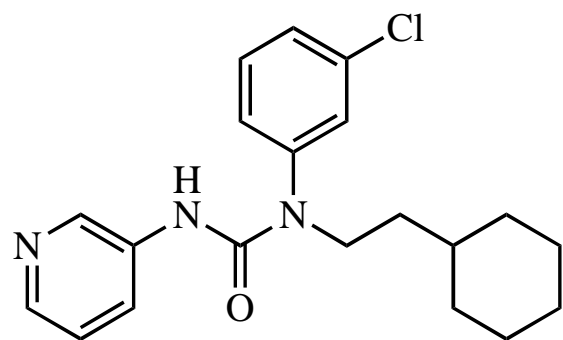
Generative Design augmented by synthesis prediction



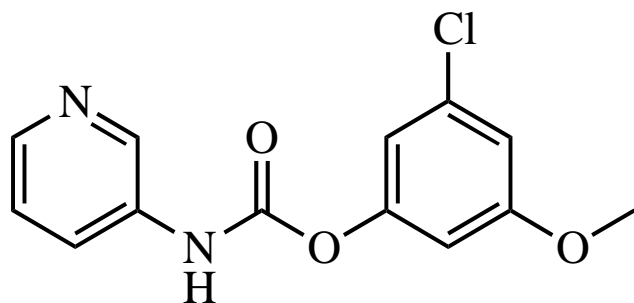
Top 3 compounds in July



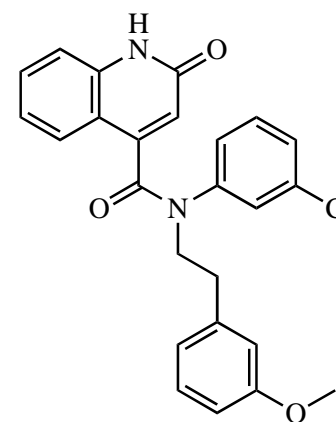
IC50 = 3.6 μ M



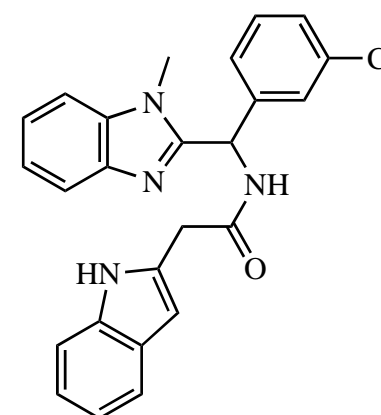
IC50 = 3.1 μ M



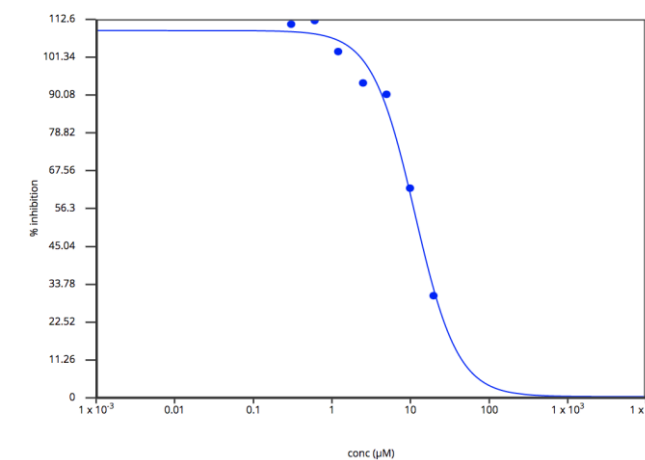
IC50 = 6.6 μ M



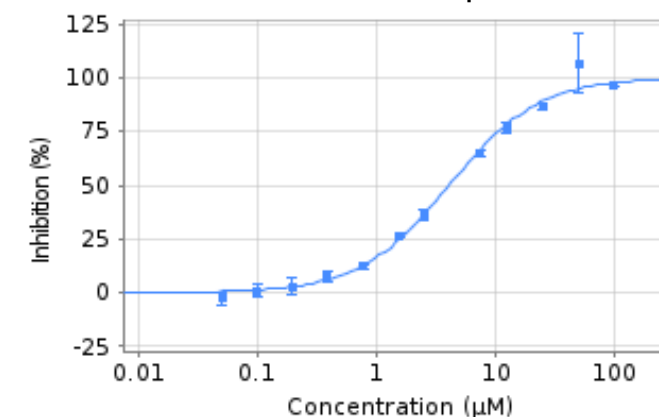
Generative Model



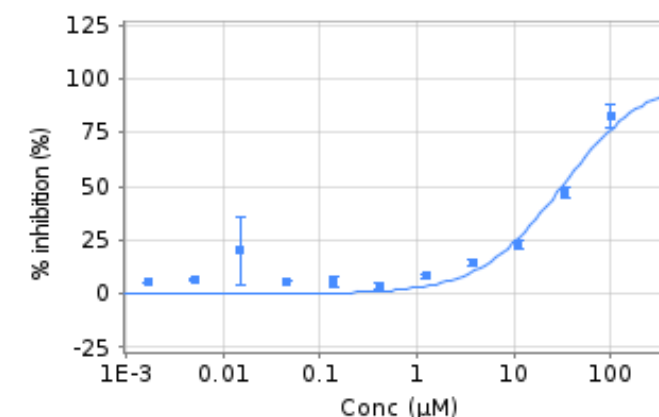
Viral EC50 (OC43) = 10 μ M



IC50 = 4.1 μ M



IC50 = 30 μ M (racemic)





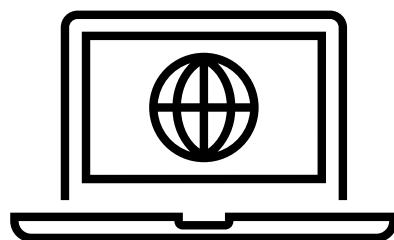
MANIFOLD

Synthesis and Search
across every available molecule



Introducing Manifold

- ✓ The world's largest chemical space to make and order compounds
- ✓ Integrated with many of the world's top CROs to get your compounds made
- ✓ Manifold combines retrosynthesis and search technology to give you the best selection of compound options



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