

Artificial Intelligence as a Catalyst for Scientific Discovery

JupyterCon 2018

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Senior Data Scientist
@modernscientist

BenevolentAI

BenevolentAI

We Are BenevolentAI

Since our foundation in 2013, our mission has been
to bring together the best of technology and
scientific research to enable us to create better
medicines.

BenevolentAI harnesses artificial intelligence to
enhance and accelerate scientific discovery by
making sense of highly fragmented information to
create new insights and usable knowledge that
benefit society.

About Me

Structural Biology

- PhD, Molecular Biophysics & Biochemistry
- Postdoctoral research in biophysics

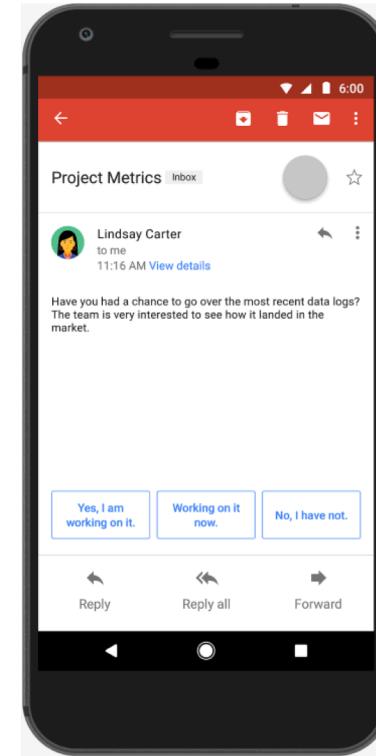
Data Science

- Scientific software developer
- Data science instructor
- Deep learning consultant



Data Scientist & Scientist

AI in Our Daily Lives



Information Accessibility Enables AI in Science



The
**Open
Science**
Prize

ChemRxiv™

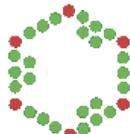
 **EMDataBank**
Unified Data Resource for 3DEM



 **open
access**

 **isaexplorer**
a data discovery tool

ChEMBL



arXiv

WORLDWIDE
 **PDB**
PROTEIN DATA BANK

NIH U.S. National Library of Medicine

ClinicalTrials.gov

PeptideAtlas


 **PubChem**
 **CANCER
IMAGING ARCHIVE**



 **OpenNEURO**

 **PLOS**

TOXNET TOXICOLOGY
DATA NETWORK

OPEN 
bioRxiv

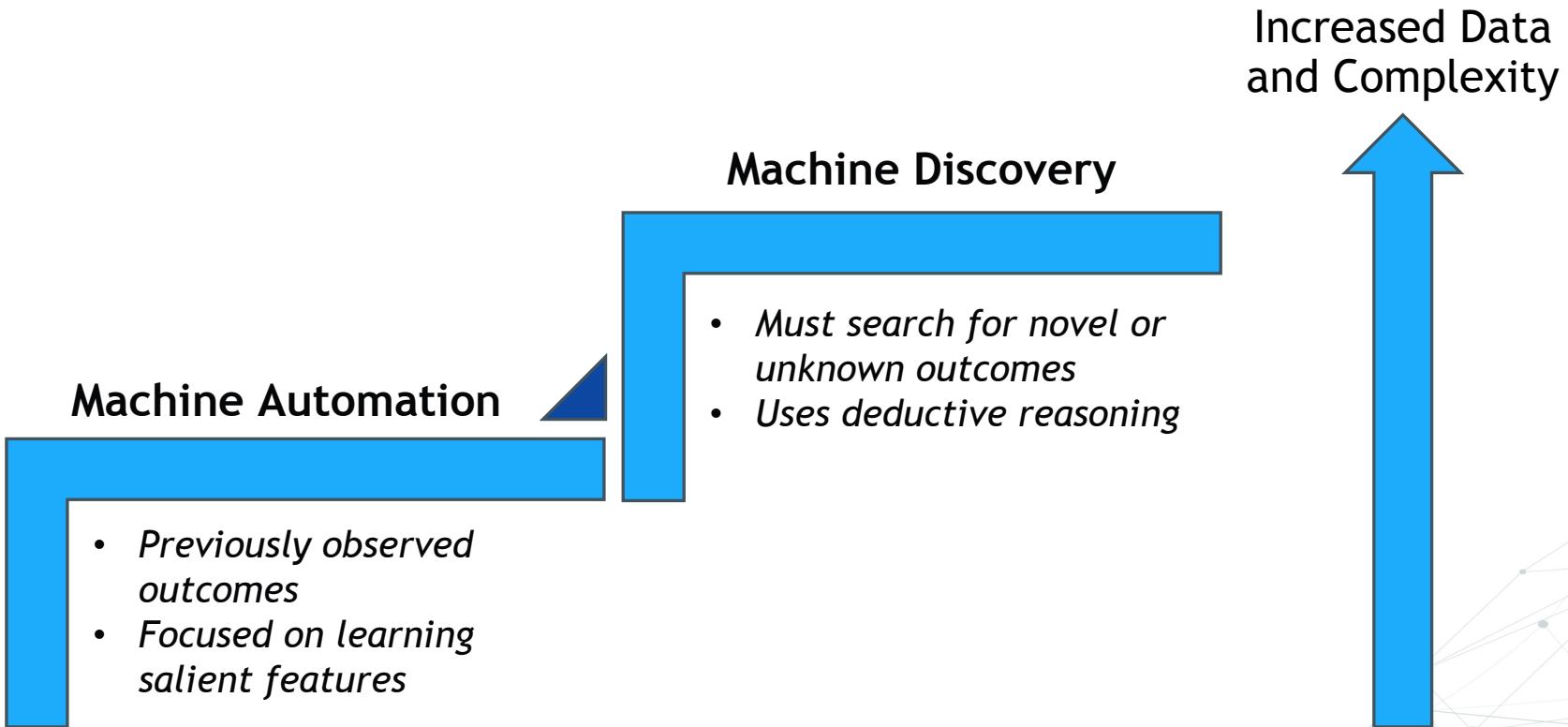




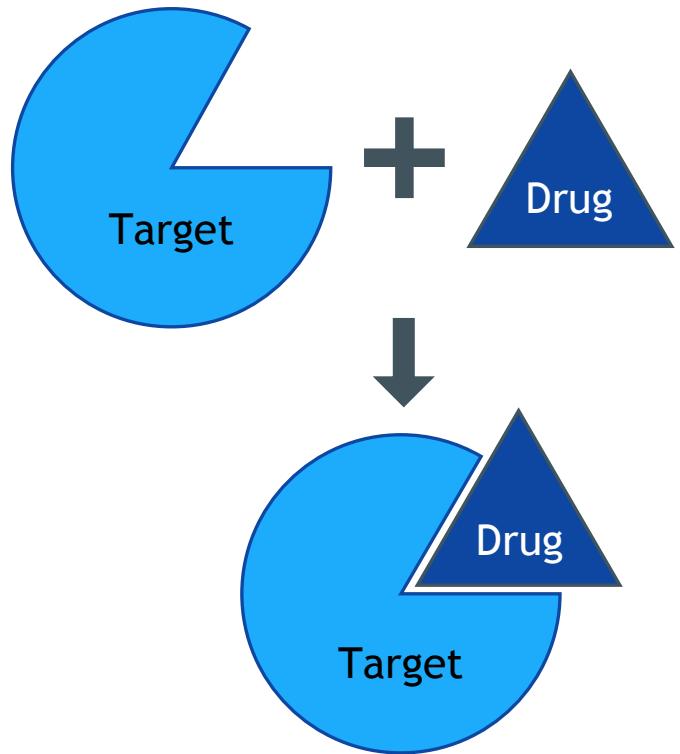
Information Accessibility Enables AI in Science



AI for Automation vs Discovery

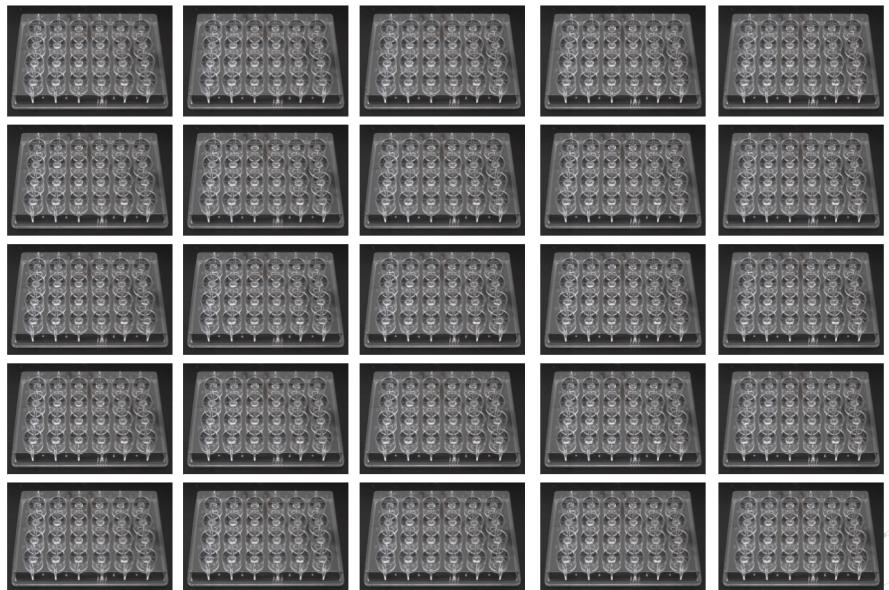
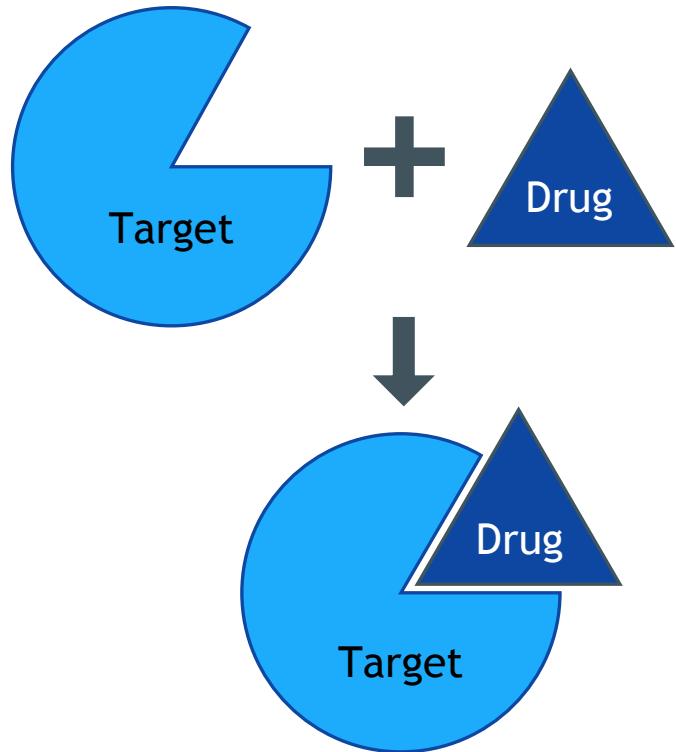


AI-Assisted Automation of Drug Discovery



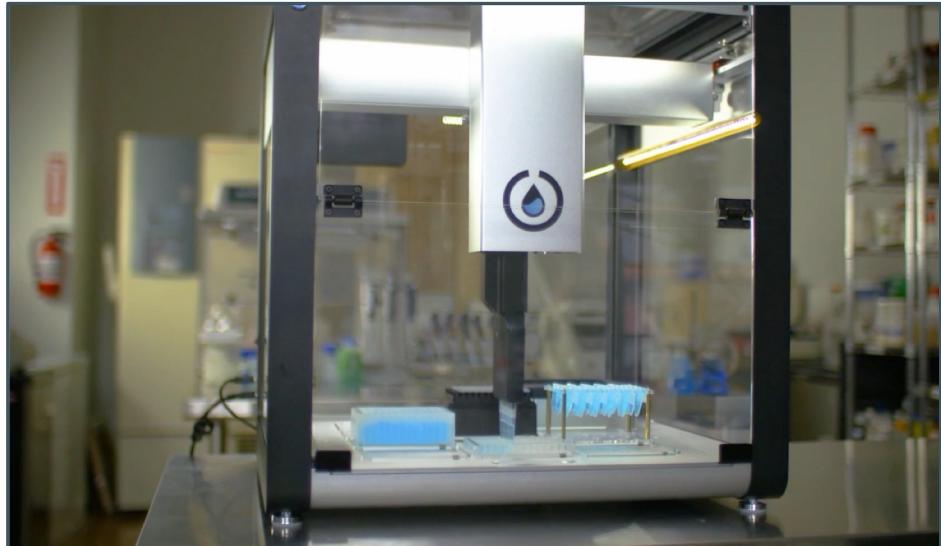
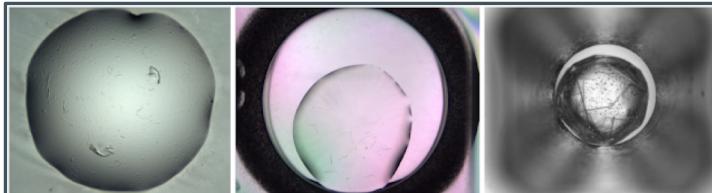
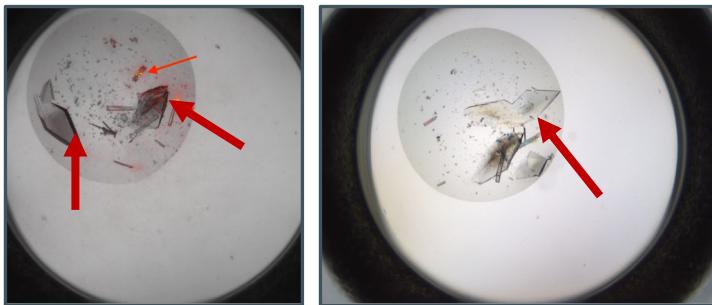
Tray of Crystallization Trials

AI-Assisted Automation of Drug Discovery



(Many) Trays of Crystallization Trials

AI-Assisted Automation of Drug Discovery



Bruno, A., Charbonneau, P., Newman, J., Snell, E., So, D., Vanhoucke, V., Watkins, C., Williams, S., Wilson, J., *PLoS One*, 2018, v13.

Video Credit: Opentrons.com

AI-Assisted Automation of Drug Discovery



MARCO About Browse Images Download

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vincentvanhoucke Fix width / height. d89e528 on Apr 30

1 contributor

79 lines (48 sloc) 2.32 KB

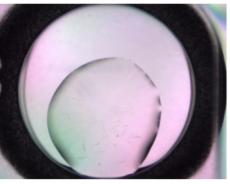
Raw Blame History

Automating the Evaluation of Crystallization Experiments

This is a pretrained model described in the paper:

Classification of crystallization outcomes using deep convolutional neural networks.

This model takes images of crystallization experiments as an input:



Download The MARCO Image dataset (BY 4.0). By downloading, you agree to the terms of the license.

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Kadee80 docs(docs): Update header and footer navigation (#1542) 697a2b8 on May 25

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Protocol Library

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- Cell Plating
- Dilution
- Media Exchange
- Plate Consolidation
- Plate Filling
- Plate Mapping
- Septum Plate

CELL CULTURE

- Media Exchange

CHEMISTRY

- Dilution

DEMONS

Opentrons Platform

*nix build error windows build passing coverage 33%

Opentrons App

Easily upload a protocol, calibrate positions, and run your experiment from your computer.

- Documentation
- Source code

Opentrons

Robot

Protocol

Prepare for Run

BRADFORD_ASSAY.PY

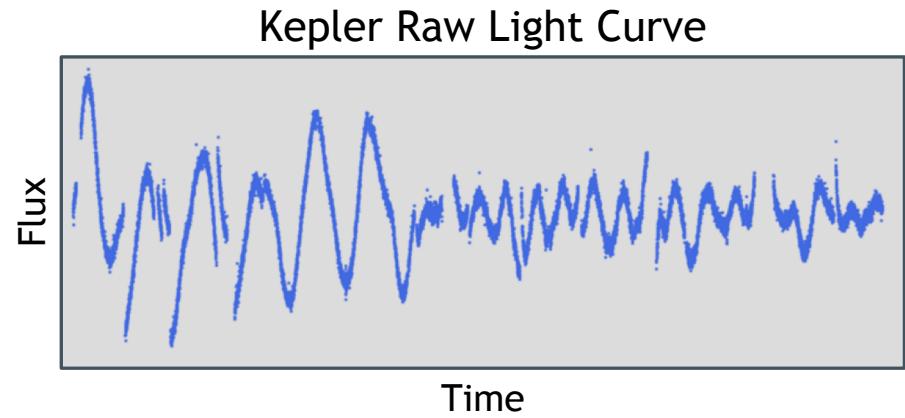
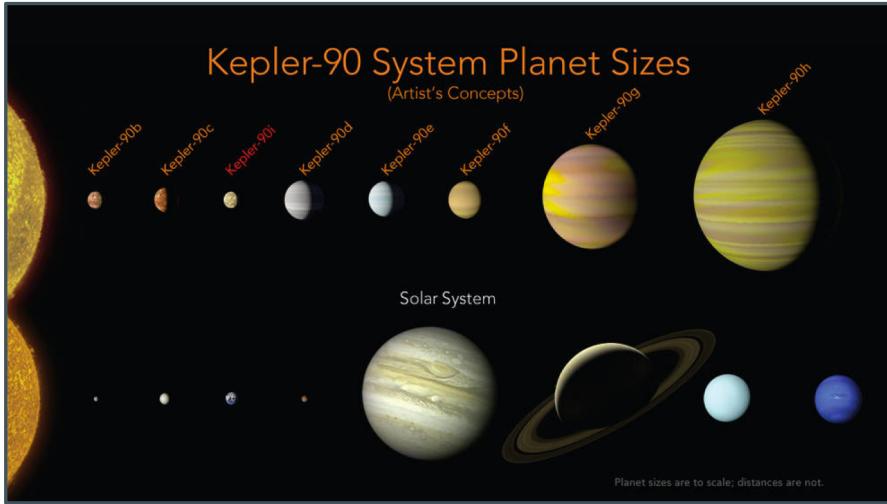
PIPETTE CALIBRATION

TIPRACK-200UL

Tiprack is calibrated

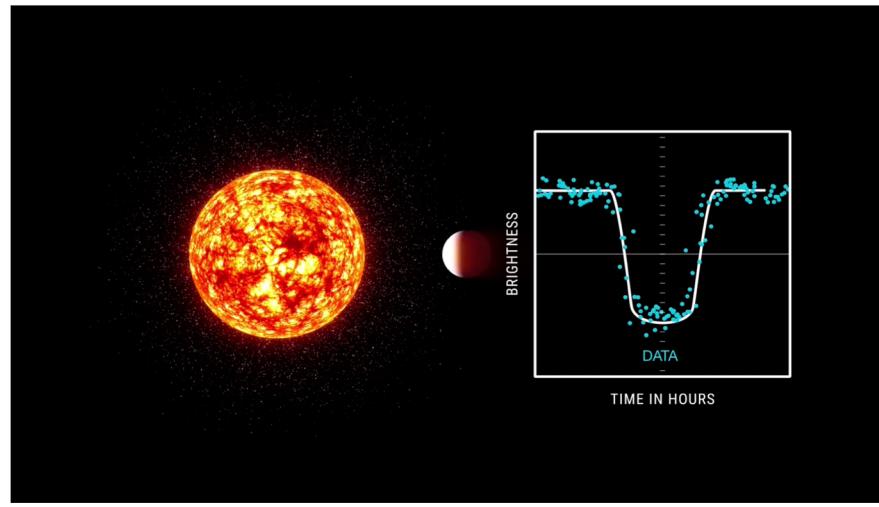
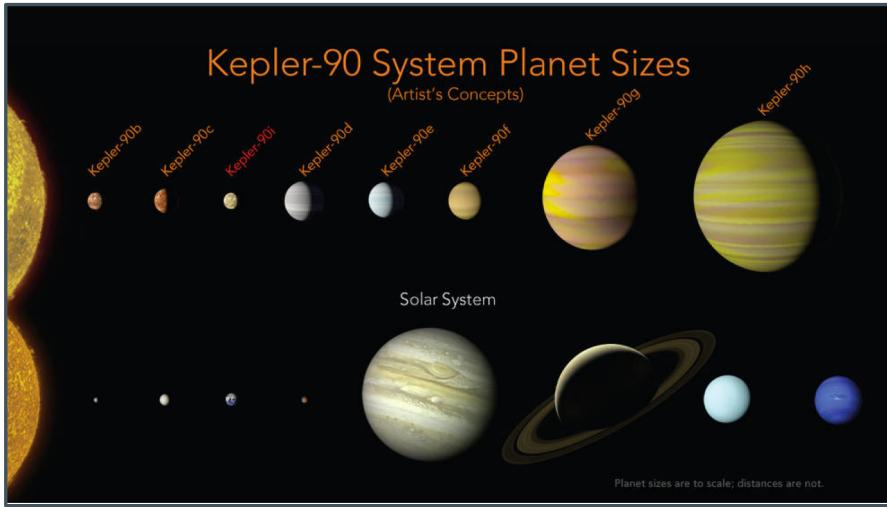
MOVE TO NEXT LABWARE

Discovering New Planets with AI



Media Credits: NASA Ames Laboratory
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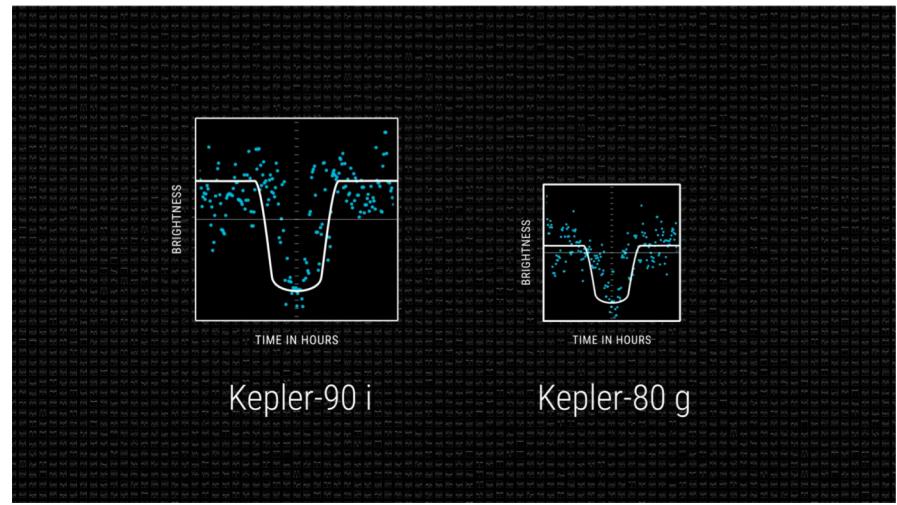
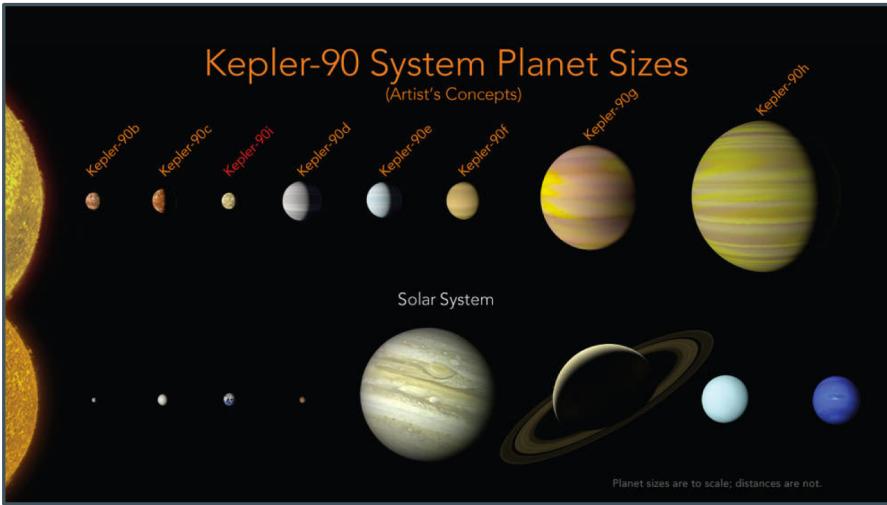
Discovering New Planets with AI



Shallue, C., and Vanderburg, A., AJ, 2018, v155.
Media Credits: NASA Ames Laboratory

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Discovering New Planets with AI

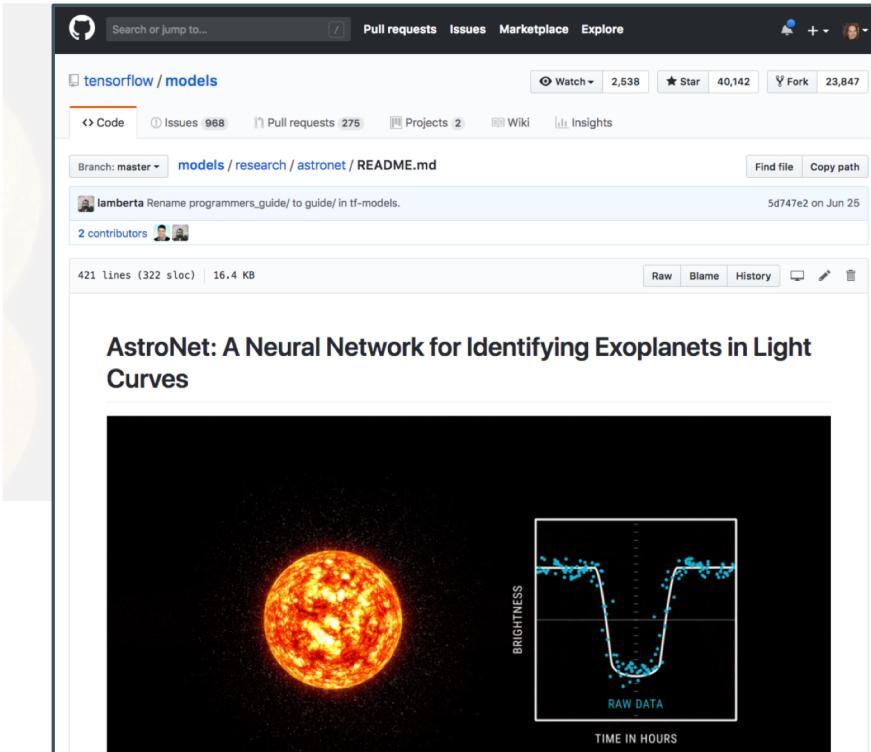


Shallue, C., and Vanderburg, A., AJ, 2018, v155.

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Discovering New Planets with AI



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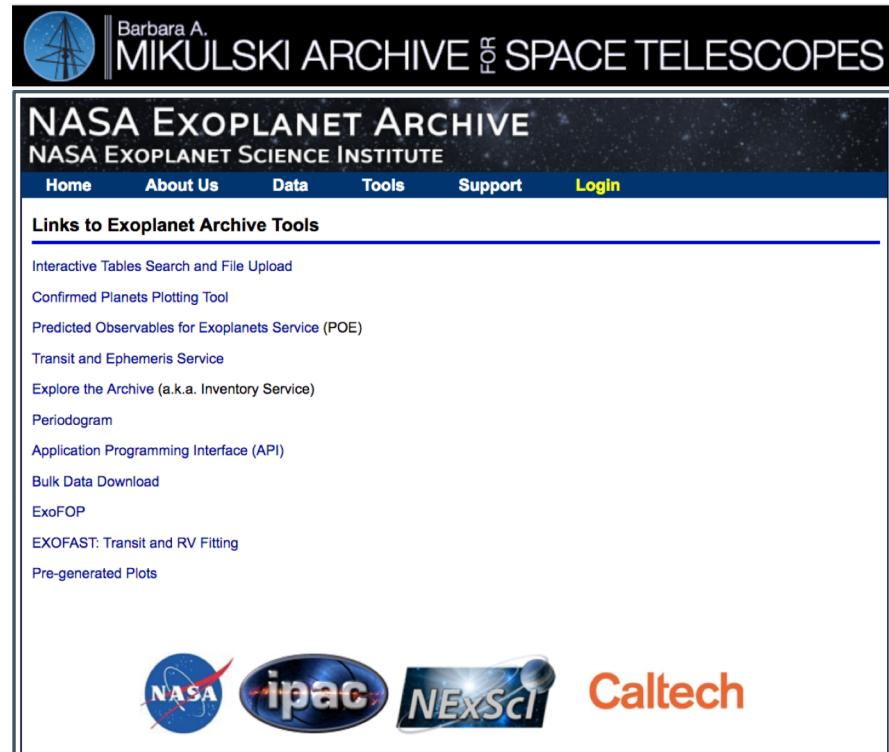
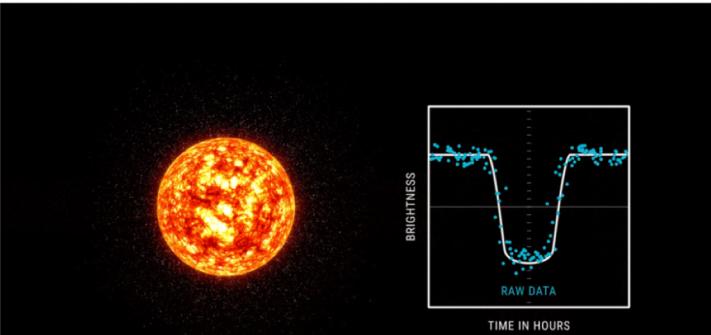
lamberta Rename programmers_guide/ to guide/ in tf-models. 5d747e2 on Jun 25

2 contributors

421 lines (322 sloc) | 16.4 KB

Raw Blame History

AstroNet: A Neural Network for Identifying Exoplanets in Light Curves



Barbara A. MIKULSKI ARCHIVE FOR SPACE TELESCOPES

NASA EXOPLANET ARCHIVE

NASA EXOPLANET SCIENCE INSTITUTE

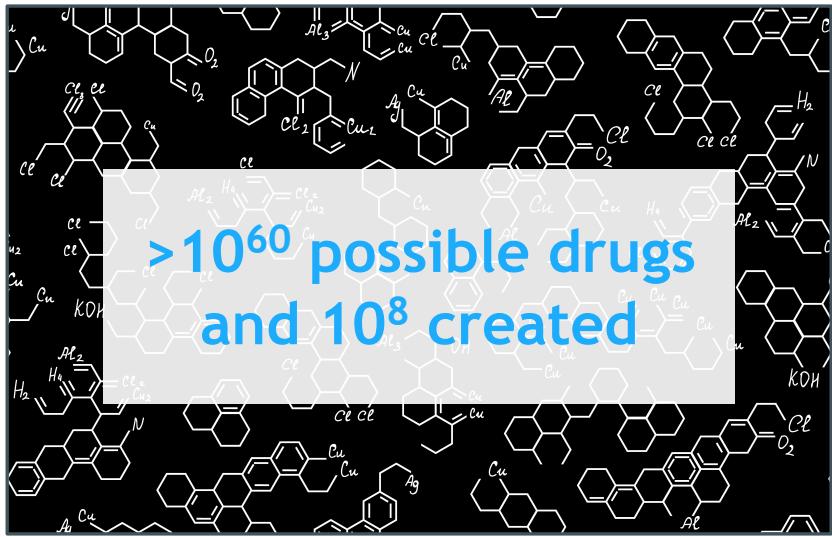
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- Bulk Data Download
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- EXOFAST: Transit and RV Fitting
- Pre-generated Plots

NASA ipac NExSci Caltech

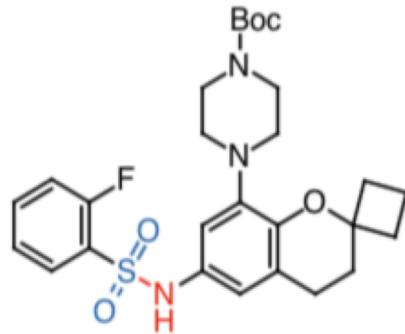
Synthesizing New Drugs with AI



Less than the area of a NYC cab on the surface of the earth!

Synthesizing New Drugs with AI

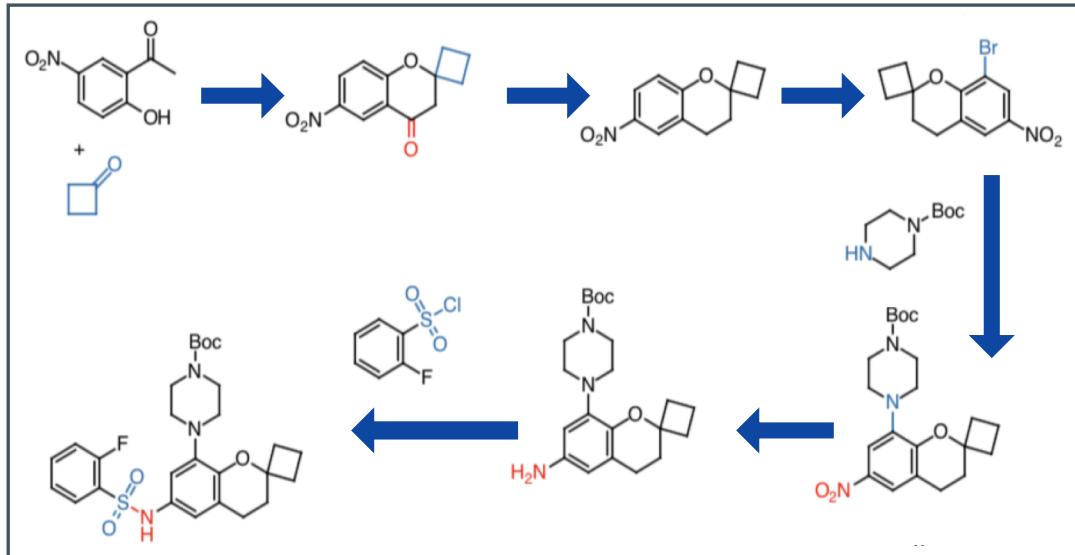
Alzheimer's Drug Intermediate



Nirogi, R., Badange, R., Rebali, V., Khagga, M., *Asian Journal of Chemistry*, 2015, v.27.

Synthesizing New Drugs with AI

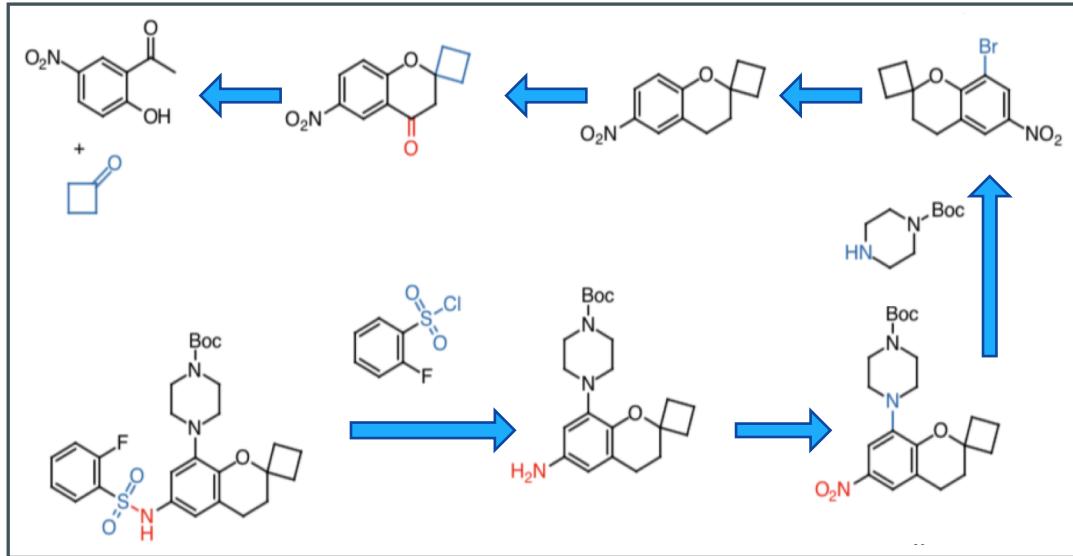
Synthesis of Alzheimer's Drug Intermediate



Nirogi, R., Badange, R., Rebali, V., Khagga, M., *Asian Journal of Chemistry*, 2015, v.27.

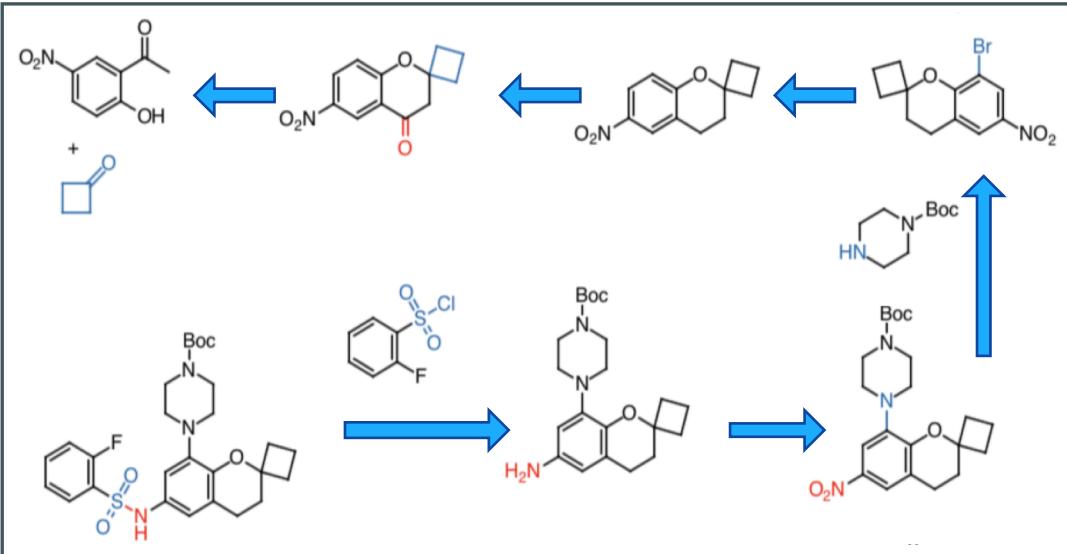
Synthesizing New Drugs with AI

Retro-Synthesis of Alzheimer's Drug Intermediate



Synthesizing New Drugs with AI

AI Derived Retro-Synthesis of Alzheimer's Drug Intermediate



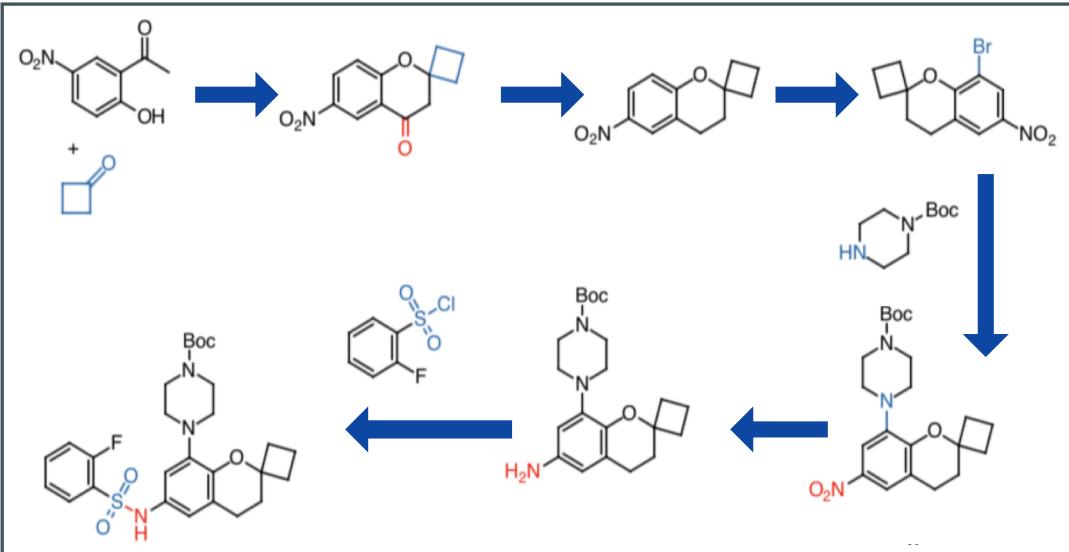
Chemists have tried to automate the logic of chemical synthesis for over 60 years...

There are too many edge cases and exceptions for a human to capture.

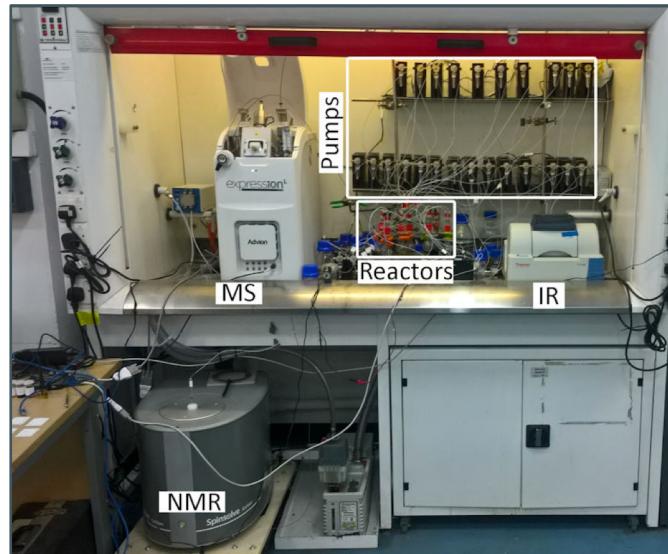
Segler, M., Preuss, M., Waller, M., *Nature*, 2018, v555.

Synthesizing New Drugs with AI

AI Derived Retro-Synthesis of Alzheimer's Drug Intermediate



On-Demand Compound Synthesis



Segler, M., Preuss, M., Waller, M., *Nature*, 2018, v555.
Granda, J., Donina, L., Dragone, V., Long, D.L., Cronin, L., *Nature*, 2018, v559.

AI, Open Data, and the Nobel Turing Challenge

*“I propose the launch of a grand challenge ...
to develop an AI system that can make major
scientific discoveries in biomedical sciences and
that is worthy of a Nobel Prize and far beyond.”*

Hiroaki Kitano

Head of Systems Biology Institute

President & CEO of Sony Computer Science Laboratories

Association for Advancement of Artificial Intelligence, Spring 2016



Thank You

Michelle L. Gill
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