

Artificial Intelligence as a Catalyst for Scientific Discovery

JupyterCon 2018

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@modernscientist

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

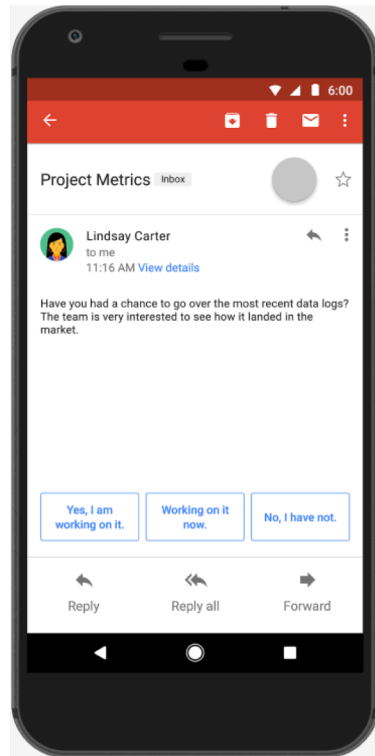
- PhD, Molecular Biophysics & Biochemistry
- Postdoctoral research in biophysics

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



Information Accessibility Enables AI in Science



AI for Automation vs Discovery

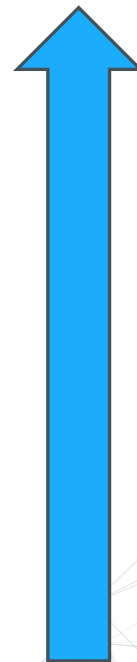
Machine Automation

- *Previously observed outcomes*
- *Focused on learning salient features*

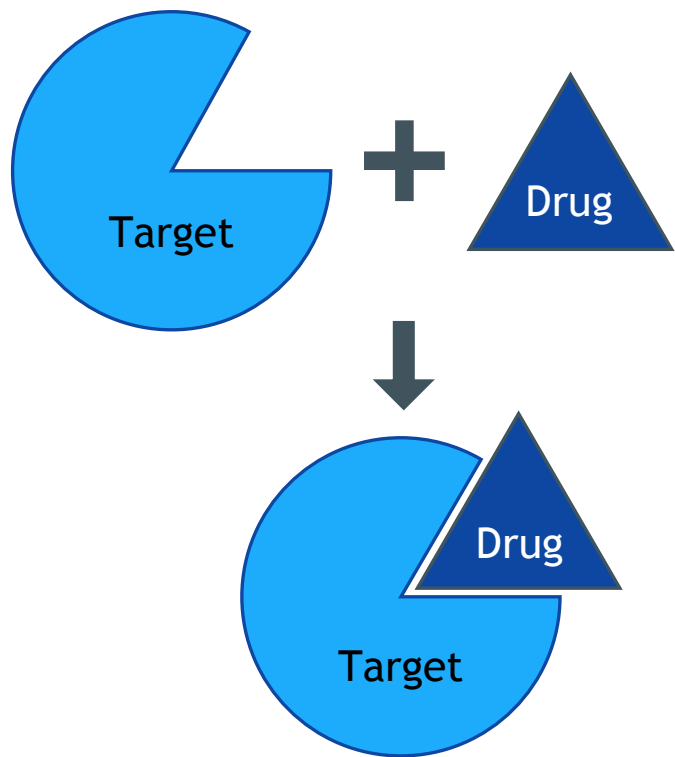
Machine Discovery

- *Must search for novel or unknown outcomes*
- *Uses deductive reasoning*

Increased Data and Complexity

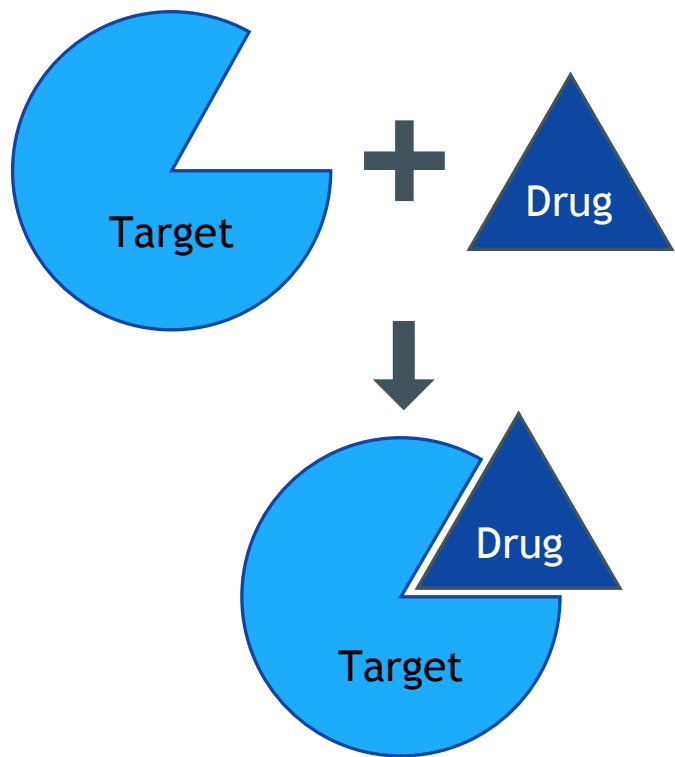


AI-Assisted Automation of Drug Discovery



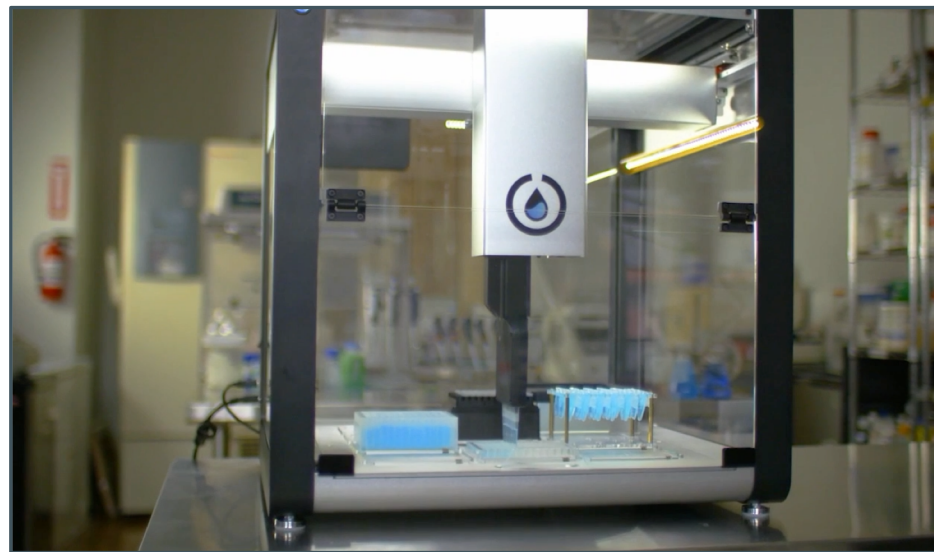
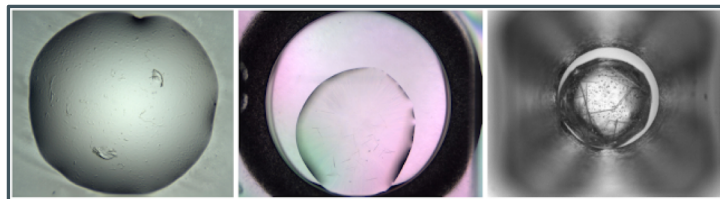
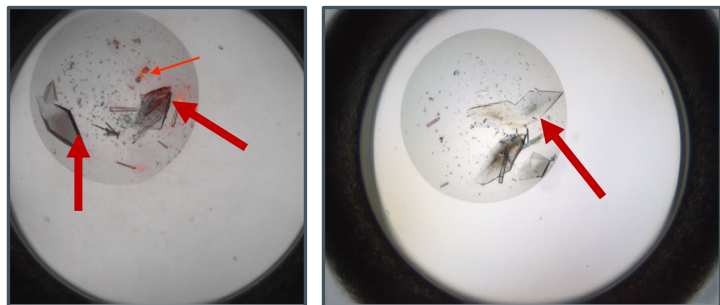
Tray of Crystallization Trials

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

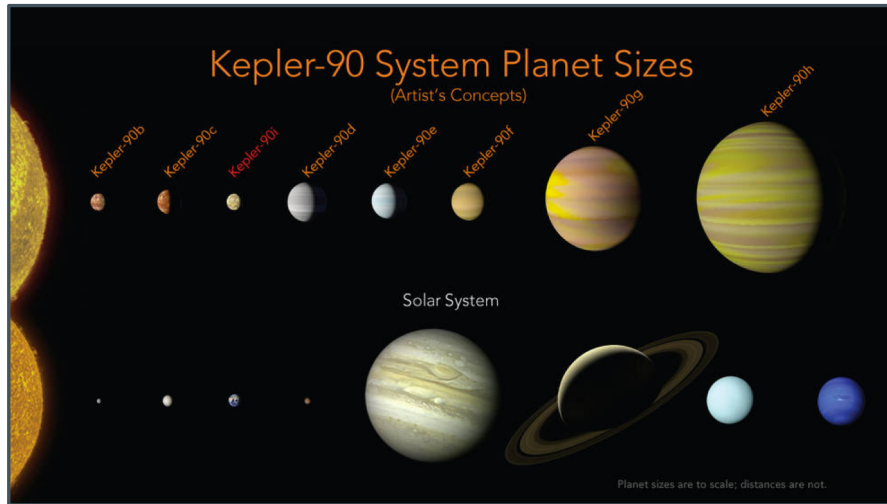
AI-Assisted Automation of Drug Discovery



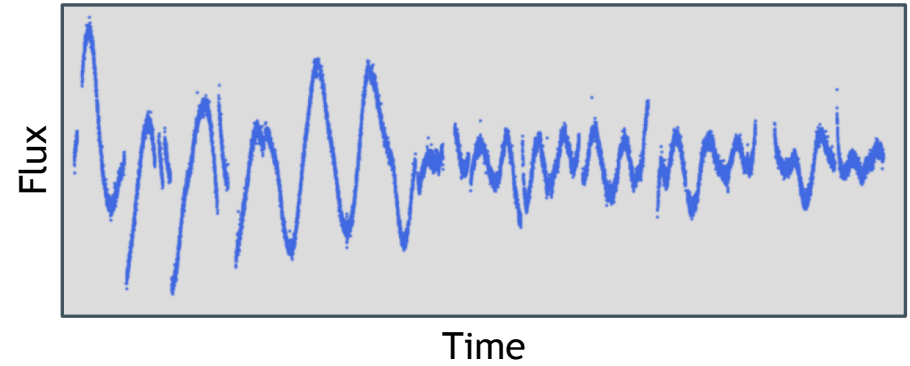
A screenshot of a GitHub repository page for `tensorflow/models`. The repository is owned by `vincentvanhoucke` and has 2,538 watchers, 40,142 stars, and 23,847 forks. The current branch is `master`. The repository contains a `models/research/marco/README.md` file. The README content includes the title "Automating the Evaluation of Crystallization Experiments" and a description: "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." Below the text is a circular image showing a crystallization experiment.

A screenshot of a GitHub repository page for `Opentrons/opentrons`. The repository has 21 watchers, 63 stars, and 41 forks. The current branch is `edge`. The repository contains a `opentrons/README.md` file. The README content includes the title "Opentrons Platform" and a description: "Easily upload a protocol, calibrate positions, and run your experiment from your computer." Below the text is a screenshot of the Opentrons software interface, showing a "Prepare for Run" dialog box with a "ROBOT" section and a "PROTOCOL" section. The "ROBOT" section shows "PIPETTE CALIBRATION" with a "TIPRACK-200UL" button and a "MOVE TO NEXT LABWARE" button. The "PROTOCOL" section shows "Left Multi-channel p300_multi_v1" and "Right Single-channel p300_single_v1".

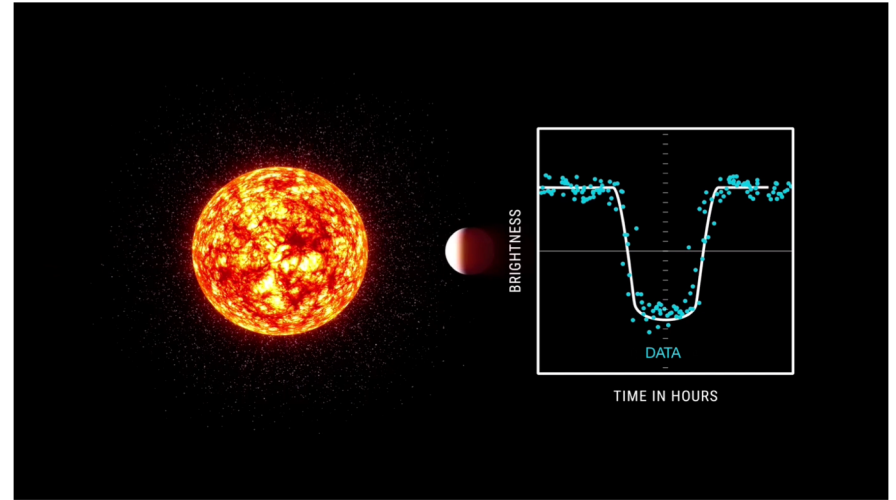
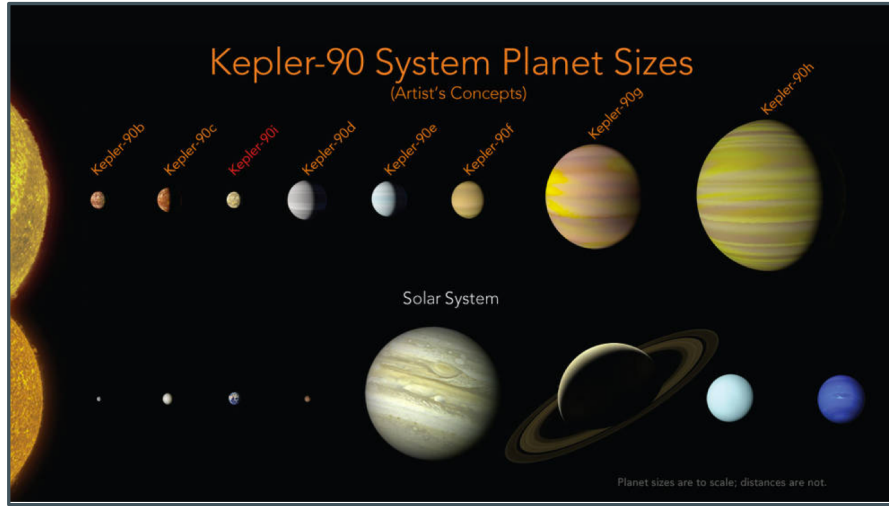
Discovering New Planets with AI



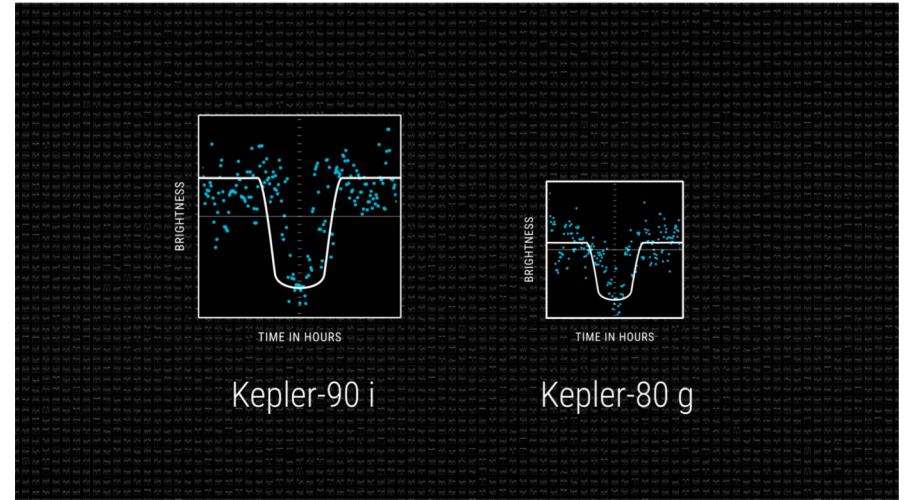
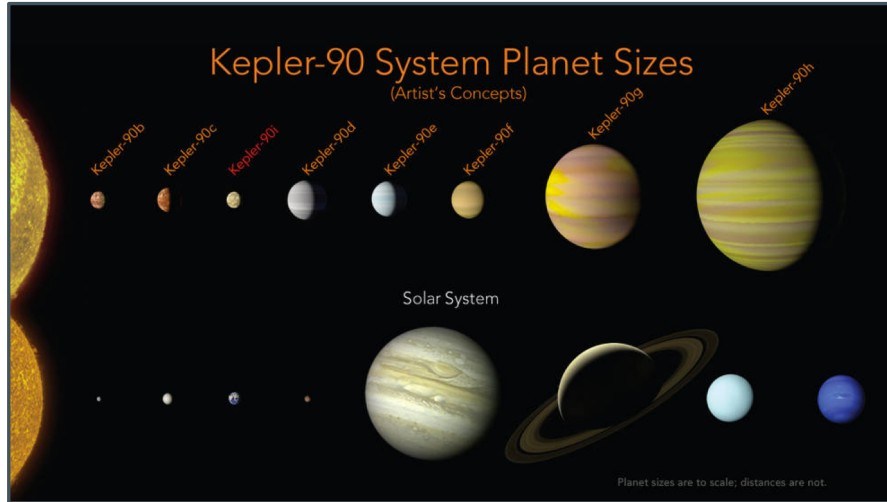
Kepler Raw Light Curve



Discovering New Planets with AI



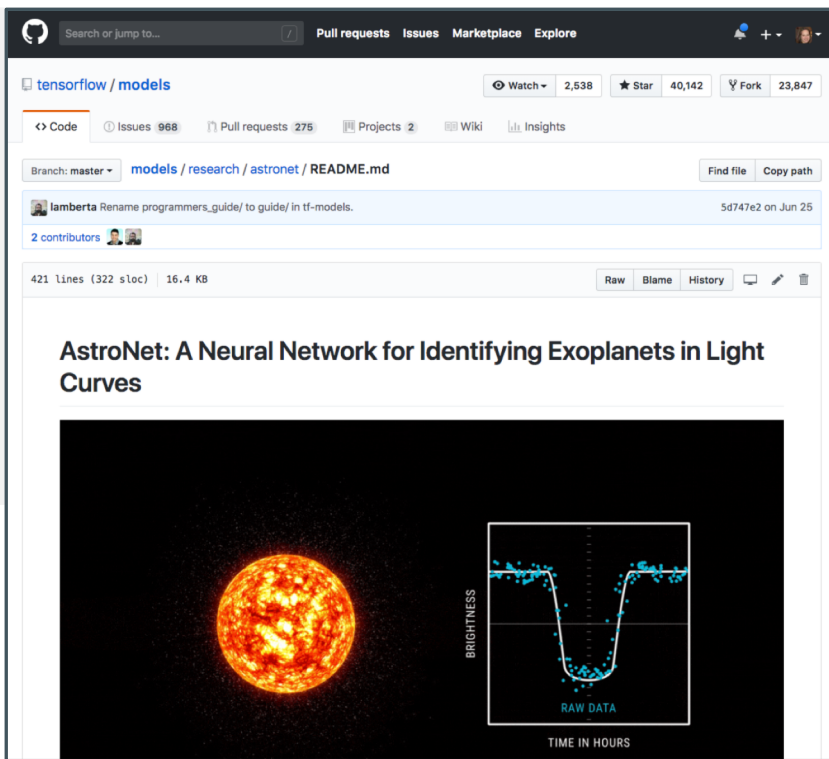
Discovering New Planets with AI



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

BenevolentAI

Discovering New Planets with AI



Search or jump to... Pull requests Issues Marketplace Explore

tensorflow / models Watch 2,538 Star 40,142 Fork 23,847

Code Issues 968 Pull requests 275 Projects 2 Wiki Insights

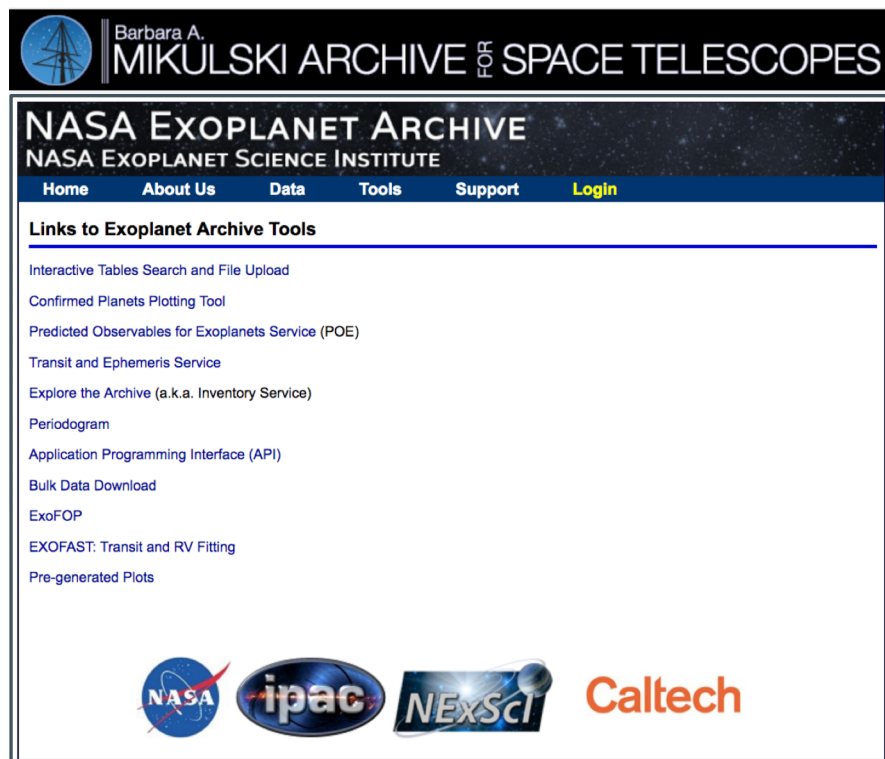
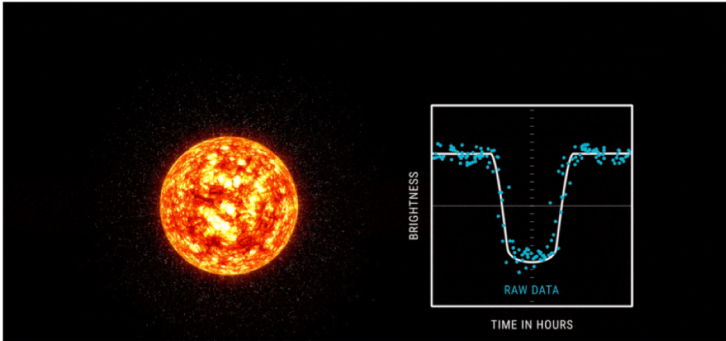
Branch: master models / research / astronnet / README.md Find file Copy path

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

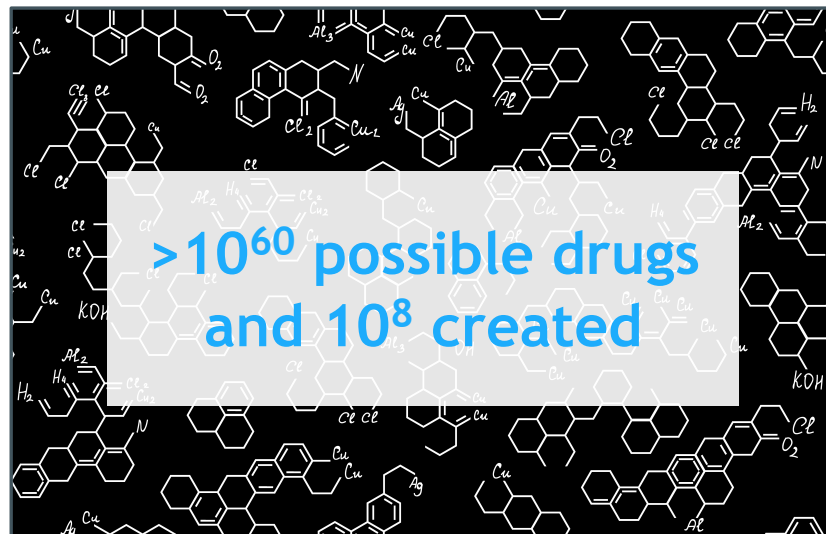
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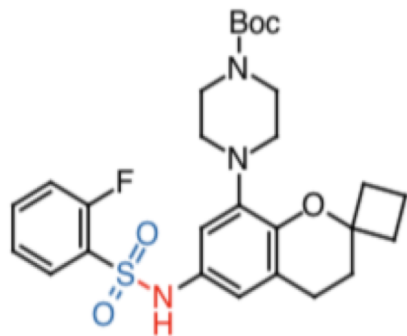
Synthesizing New Drugs with AI



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

Synthesizing New Drugs with AI

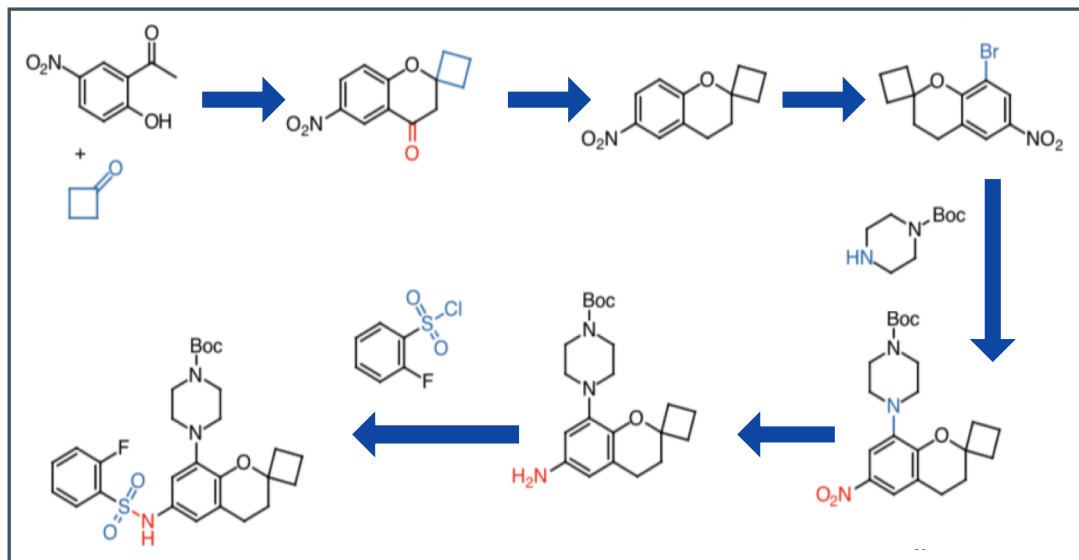
Alzheimer's Drug Intermediate



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

Synthesizing New Drugs with AI

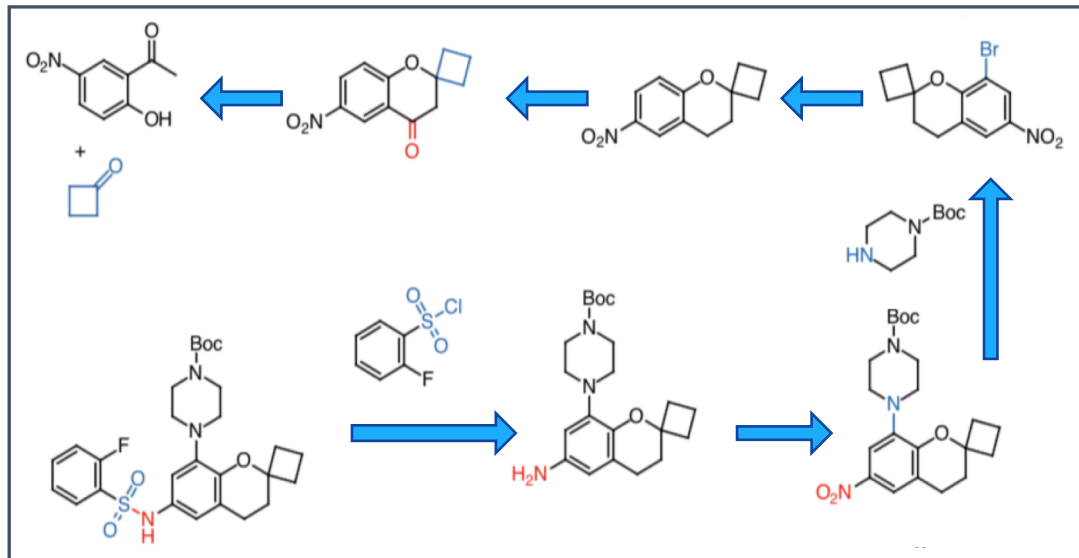
Synthesis of Alzheimer's Drug Intermediate



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

Synthesizing New Drugs with AI

AI Derived Retro-Synthesis of Alzheimer's Drug Intermediate



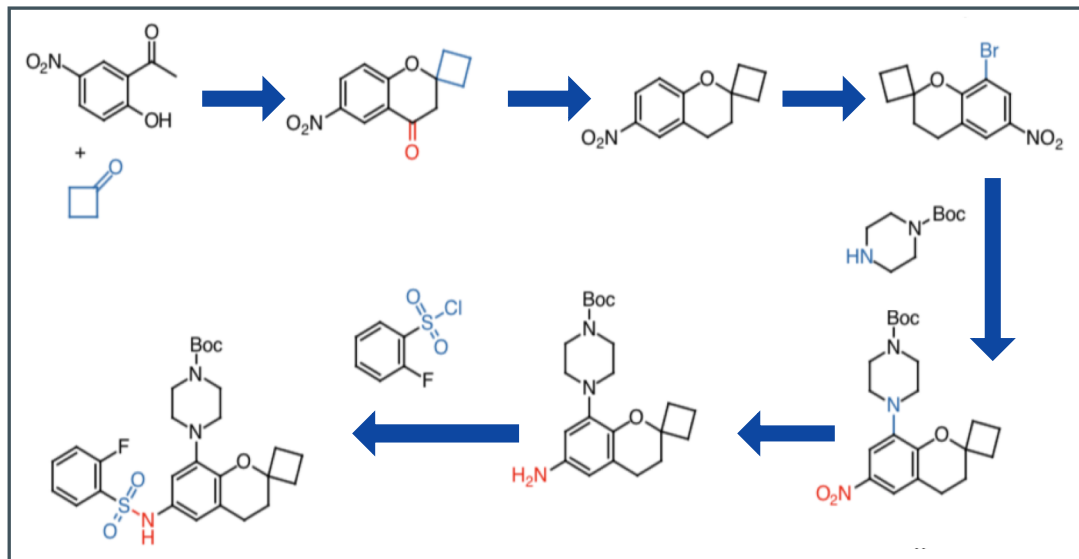
Chemists have tried to automate the logic of chemical synthesis for over 60 years...

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

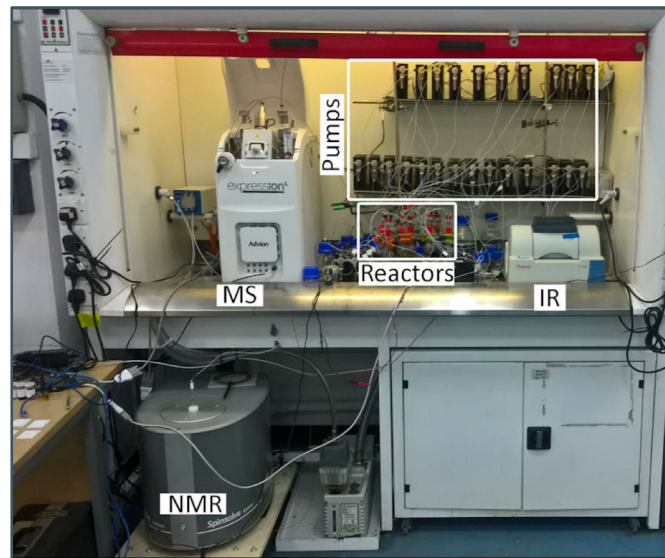
Segler, M., Preuss, M., Waller, M., *Nature*, 2018, v555.

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

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