AI in Drug Discovery

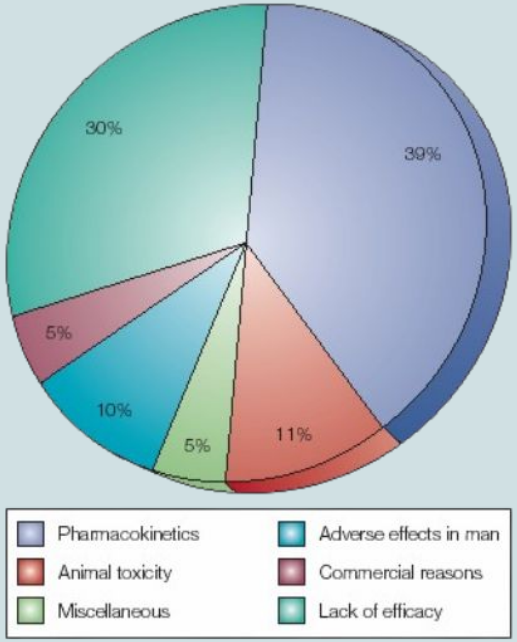
Doelle and Soha

Intro to Drug Discovery

How easy do you think drug discovery is?

Drug discovery is ineffective, slow, and expensive

- 86% of drug candidates between 2000 and 2015 did not meet their goals
- 90% of clinically developed drugs fail
  - lack of clinical efficiency
  - uncontrollable toxicity
  - poor compound make-up
  - lack of strategic planning and consumer demand



Percentages of drug failures

Do you think AI makes drug discovery easier?

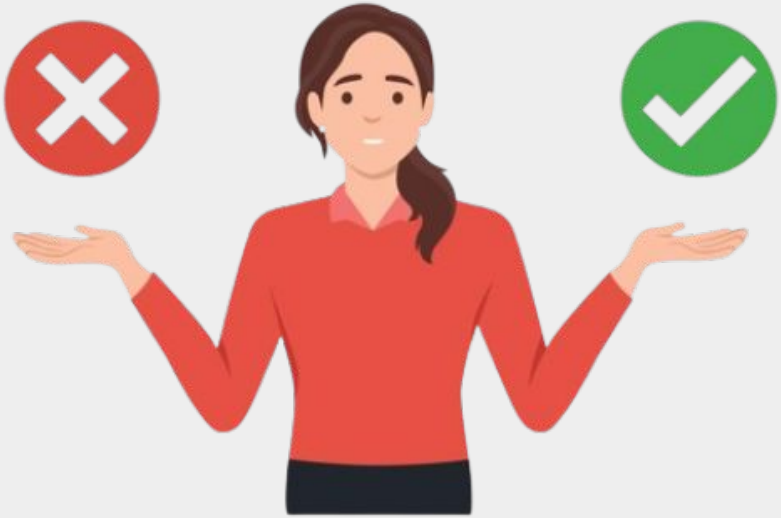
Would you let an AI model prescribe you a drug?

Do you think that AI is trustworthy enough to help humans develop drugs?

Do you think that AI will be better than humans at pharmaceutical research?

Should AI be trusted with drug discovery?

Questions !!



Finding Suitable Drug Candidates

- AI models are able to determine which compounds are necessary for drugs that treat certain conditions
- For example, an AI model was able to find a drug to treat someone's cancer. The doctor initially didn't plan on trying the drug, but it ended up curing the patient's cancer.

A graphic showing a possible future of drug discovery

Tool spotlight **DeepChem**

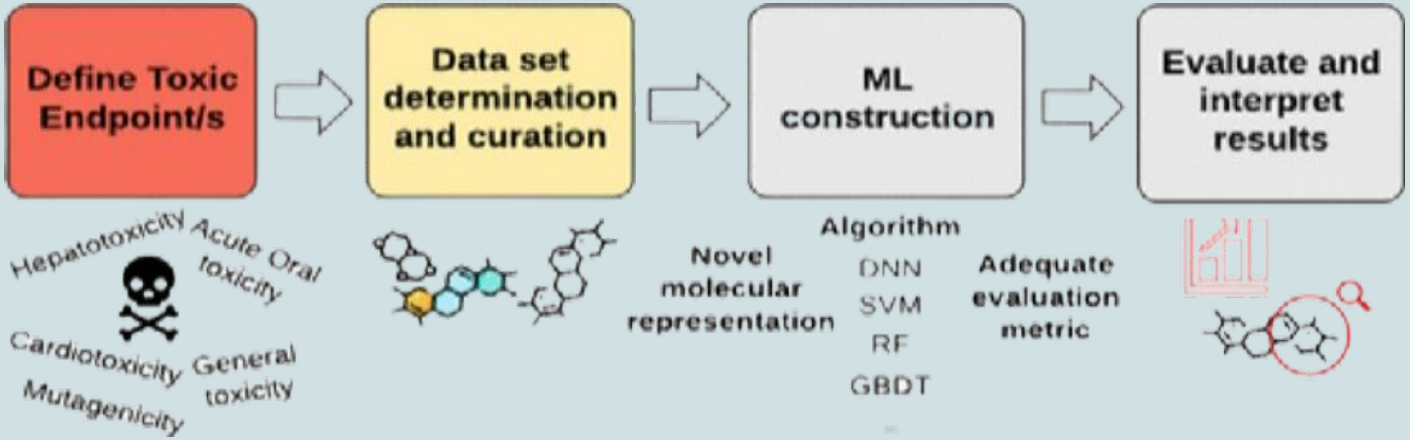
DeepChem is an MLP (multi-layer perceptron) model that uses an AI system to find a suitable candidate in drug discovery. It is python-based.

DeepChem

(GitHub link is embedded in the image)

Predicting Drug Toxicity

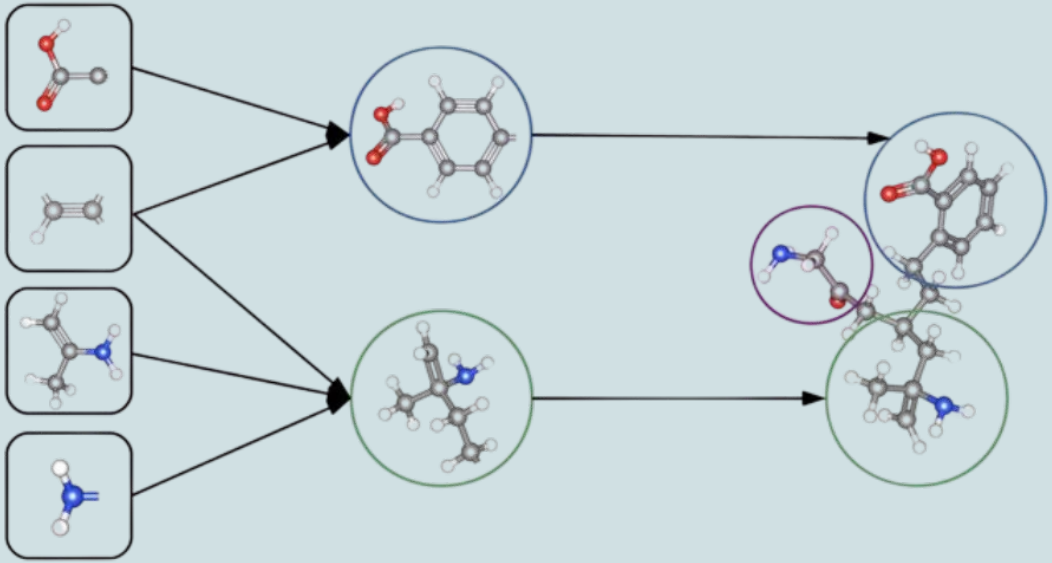
- AI models can also be used to predict the toxicity of a drug, which could be the difference between whether a drug fails or succeeds
- Using AI to predict the toxicity of drugs would prevent researchers from wasting their time developing unusable drugs



A possible process that an ML model could use to predict drug toxicity

Tool spotlight: DeepTox

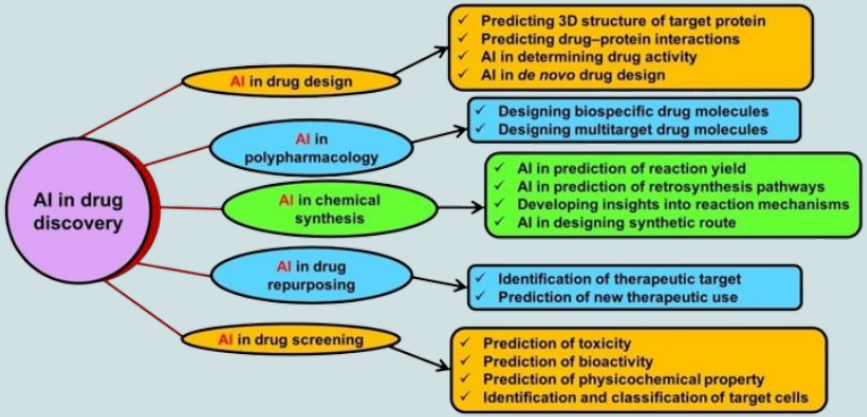
DeepTox is a software program that can predict the toxicity of 12,000 drugs.



An example of a DeepTox neural network, which breaks up molecules and combines them

Predicting Drug Effectiveness

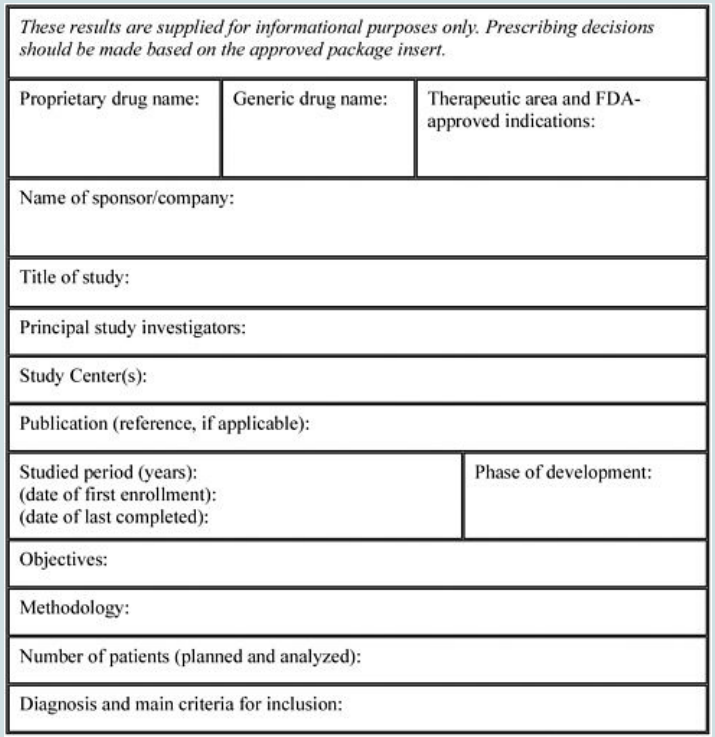
- AI can look at drug compounds and how molecules will react to biochemical assays
- AI can predict the structures of newly formed proteins
- AI can predict the properties of novel molecules (newly formed molecules)



The process AI uses in drug discovery

Formatting Drug Reports

- Formatting scientific reports properly is one of the most tedious parts of research, and there have been tools made to make the process easier
- AI can speed up the writing of these reports even more, letting researchers spend more of their time working on a drug



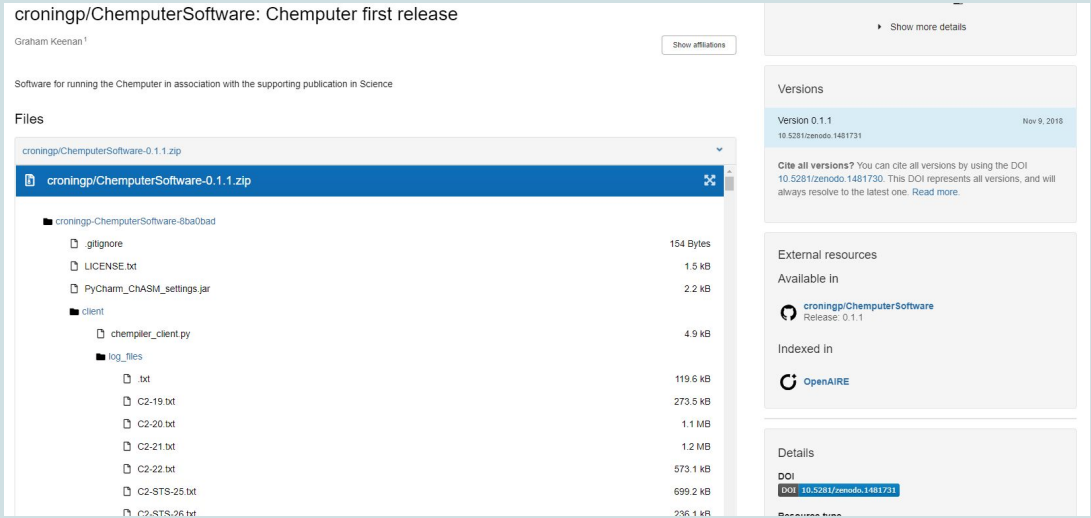
These results are supplied for informational purposes only. Prescribing decisions should be made based on the approved package insert.

Proprietary drug name:	Generic drug name:	Therapeutic area and FDA-approved indications:
Name of sponsor/company:		
Title of study:		
Principal study investigators:		
Study Center(s):		
Publication (reference, if applicable):		
Studied period (years): (date of first enrollment): (date of last completed):		Phase of development:
Objectives:		
Methodology:		
Number of patients (planned and analyzed):		
Diagnosis and main criteria for inclusion:		

An example of a clinical report template

Tool spotlight: Chemputer

Chemputer helps to report procedure for chemical synthesis in standardized format



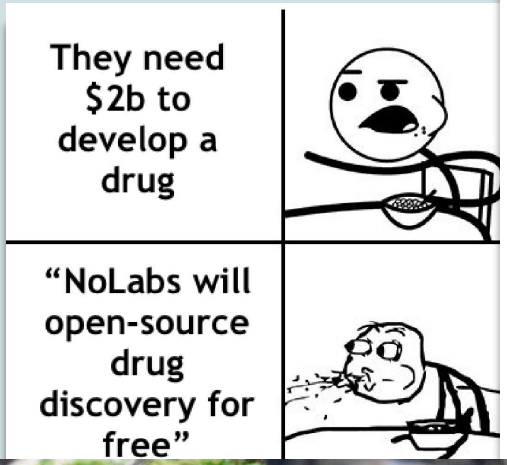
A screenshot of
Chemputer's files

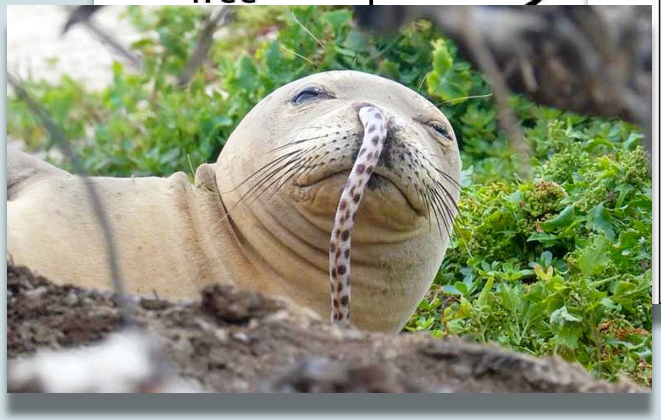
Exit Ticket

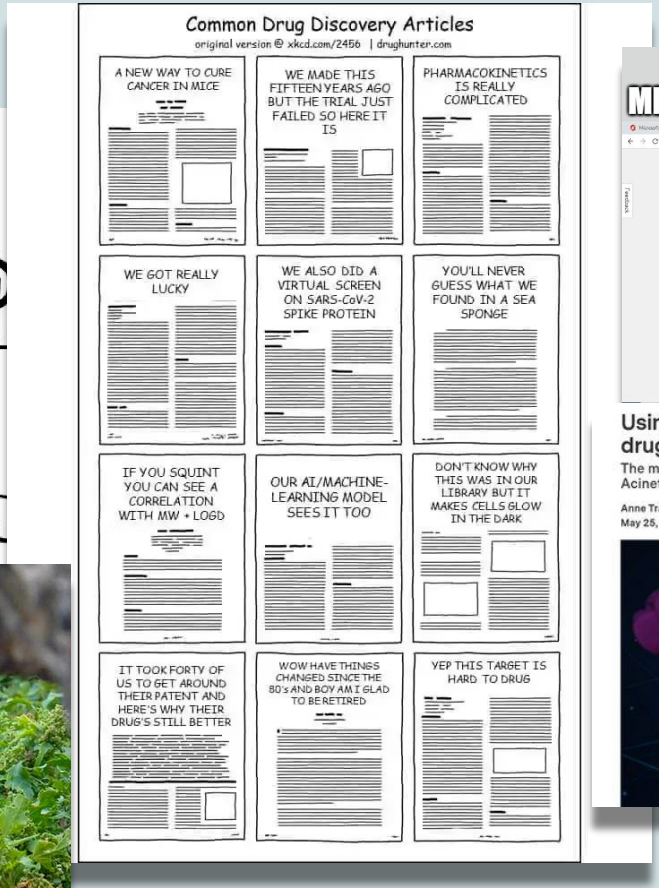
What are some ways that AI can help drug development?

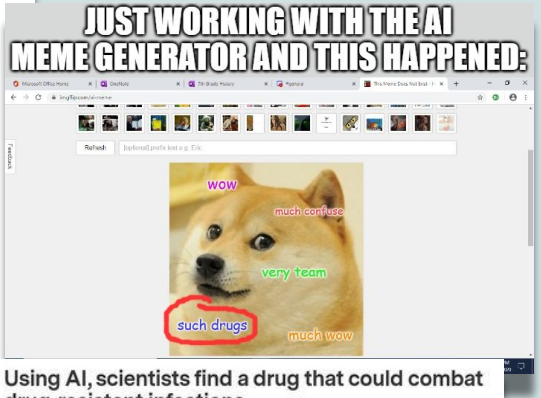
- yusss

Questions


They need $2b to develop a drug
"NoLabs will open-source drug discovery for free"




Common Drug Discovery Articles
original version © xkcd.com/2456 | drughunter.com
A NEW WAY TO CURE CANCER IN MICE
WE MADE THIS FIFTEEN YEARS AGO BUT THE TRIAL JUST FAILED SO HERE IT IS
PHARMACOKINETICS IS REALLY COMPLICATED
WE GOT REALLY LUCKY
WE ALSO DID A VIRTUAL SCREEN ON SARS-CoV-2 SPIKE PROTEIN
YOU'LL NEVER GUESS WHAT WE FOUND IN A SEA SPONGE
IF YOU SQUINT YOU CAN SEE A CORRELATION WITH MW * LOGD
OUR AI/MACHINE-LEARNING MODEL SEES IT TOO
DON'T KNOW WHY THIS WAS IN OUR LIBRARY BUT IT MAKES CELLS GLOW IN THE DARK
IT TOOK FORTY OF US TO GET AROUND THEIR PATENT AND HERE'S WHY THEIR DRUG'S STILL BETTER
WOW HAVE THINGS CHANGED SINCE THE 80'S AND BOY AM I GLAD TO BE RETIRED
YEP THIS TARGET IS HARD TO DRUG


JUST WORKING WITH THE AI MEME GENERATOR AND THIS HAPPENED:
wow
much confuse
very team
such drugs
much wow


Using AI, scientists find a drug that could combat drug-resistant infections
The machine-learning algorithm identified a compound that kills Acinetobacter baumannii, a bacterium that lurks in many hospital settings.
Anne Trafton | MIT News Office
May 25, 2023

Citations

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Klambauer, Günter. “DeepTox.” *DeepTox: Deep Learning for Toxicity Prediction*, www.bioinf.jku.at/research/DeepTox/. Accessed 5 Aug. 2024.

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