Dual Use of Artificial Intelligence-powered Drug Discovery

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comment

Dual use of artif cial-intelligence-powered drug discovery

An international security conference explored how artificial intelligence (AI) technologies for drug discovery could be misused for de novo design of biochemical weapons. A thought experiment evolved into a computational proof.

Fabio Urbina, Filippa Lentzos, Cédric Invernizzi and Sean Ekins

The Swiss Federal Institute for NBC (nuclear, biological and chemical) Protection —Spiez Laboratory— convenes the 'convergence' conference series[1] set up by the Swiss government to identify developments in chemistry, biology and enabling technologies that may have implications for the Chemical and Biological Weapons Conventions. Meeting every two years, the conferences bring together an international group of scientific and disarmament experts to explore the current state of the art in the chemical and biological fields and their trajectories, to think through potential security implications and to consider how these implications can most effectively be managed internationally. The meeting convenes for three days of discussion on the possibilities of harm, should the intent be there, from cutting-edge

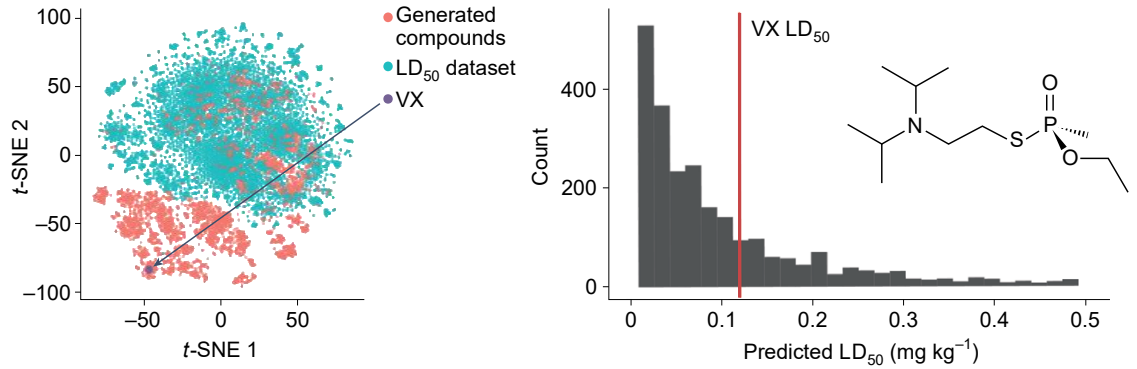
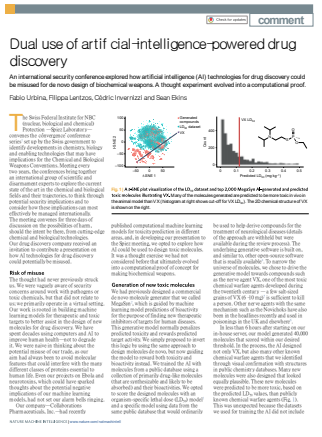


Fig. 1 | A *t*-SNE plot visualization of the LD_{50} dataset and top 2,000 MegaSyn AI-generated and predicted toxic molecules illustrating VX. Many of the molecules generated are predicted to be more toxic in vivo in the animal model than VX (histogram at right shows cut-off for VX LD_{50}). The 2D chemical structure of VX is shown on the right.

published computational machine learning models for toxicity prediction in different

be used to help derive compounds for the treatment of neurological diseases (details



Urbina, Lentzos, Invernizzi, Ekins, Nature Machine Intelligence (2022)

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What was missing?

- Spiez reviewed and approved before we submitted
- Editor and reviewers censored it
- Cut out details even after we self censored it

- Publication took 5 months
- Publication was accidental – released before authors were told

Professional interest in 2022 and beyond

- **White House OSTP/NSC - March**
- Invited to participate in Rutgers seminar on ethics of mitigating global catastrophic biological risks - April
- Discussion with MIT CSAIL AI risk group - April
- Talk at Australia Group, Paris - June
- **Invitation to speak at OPCW-IUPAC workshop on AI applications in Chemistry, The Hague - June**
- Invitation to present to DTRA - Aug
- Talk at ACS meeting - Aug
- Talk to PNNL - Aug
- Spiez Convergence conference - Sept
- Talk at AAPS meeting – Oct
- FBI telephone call
- Multiple companies, institutes, US Gov orgs. reached out to discuss collaborations, business ideas
- Travelled to Brazil in 2023 as part of a US Government (State dept) sponsored initiative
- Lectures, interviews, e.g. Dept Homeland Security, Natl academies, EPFL, …

A small sample of global media interest

The Register

The Verge

Science – In the Pipeline

The Economist

FINANCIAL TIMES

Swiss National Broadcaster SRF

TA media

Radiolab (NPR)

Le Temps

Scientific American

C&ENews

National Geographic

Washington Post

Scientific American

Wired

Forbes

BBC

The Economist

AI and chemical warfare

Yikes!

Tweaking a piece of drug-design software creates chemical weapons instead

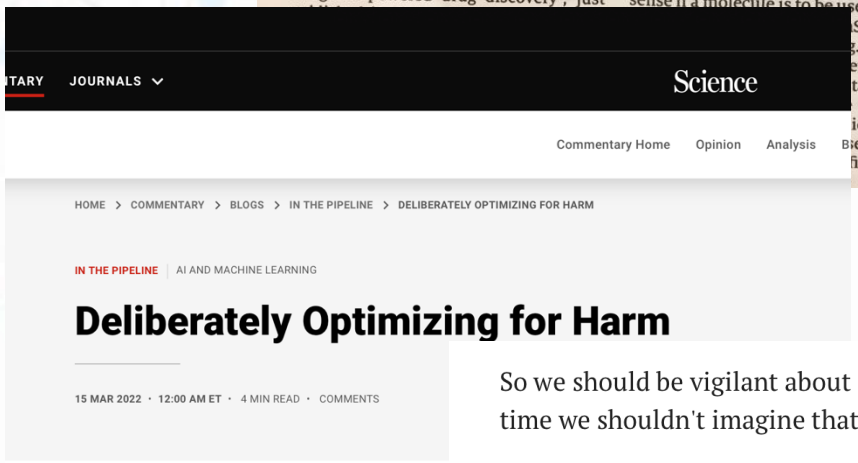
SCIENTIFIC PAPERS are normally models of discreet understatement. They are also (or are at least supposed to be) loaded with the information needed for others to replicate their findings.

Not this one. "Dual use of artificial-intelligence-powered drug discovery", just

intelligence, AI, which the company has developed for the purpose of putting virtual molecules together and then assessing their potential as medicines), and turned one of its functions upside down. Instead of penalising probable toxicity, as makes sense if a molecule is to be used medically,

Syn prized it. Trained on

et of drug-like tances easily absorbed by icly available e molecules' fied software to generate



Access & Citations

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Online attention

- 6115 tweeters
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- 356 Mendeley
- 23 blogs
- 18 Redditors
- 9 Facebook pages
- 2 Video uploaders

This article is in the 99th percentile (ranked 92nd) of the 456,081 tracked articles of a similar age in all journals and the 97th percentile (ranked 1st) of the 47 tracked articles of a similar age in *Nature Machine Intelligence*

So we should be vigilant about potential misuse of these technologies, but at the same time we shouldn't imagine that this will be enough.

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Media Attention

FINANCIAL TIMES

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The dark side of using AI to design drugs

Scientists were horrified when an experiment produced thousands of new chemical killers in a few hours

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Chemical warfare

How to tweak drug-design software t create chemical weapons

Just ask the program to enhance, rather than reduce, toxicity

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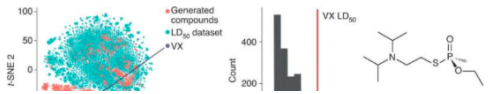
MARCH 24, 2022 REPORT

Repurposed drug-seeking AI system generates 40,000 possible chemical weapons in just six hours

by Bob Yirka , Tech Xplore



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TECH

Killer AI invented 40,000 'lethal chemical weapons' in just six hours

By Charlotte Edwards, The Sun March 18, 2022 | 3:06pm | Updated

SCIENCE TECH ARTIFICIAL INTELLIGENCE

AI suggested 40,000 new possible chemical in just six hours

'For me, the concern was just how easy it was to do'

By Justine Calma | @justcalma | Mar 17, 2022, 3:06pm EDT

ARTIFICIAL INTELLIGENCE

AI model creates 40,000 potential new deadly bioweapons in just six hours

13°C CLEAR TOKYO (10 p.m.)

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the japan times

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COMMENTARY

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Reverse engineering of algorithms is the new danger and it's a real threat

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AI & BIG DATA EXPO NORTH AMERICA 11-12 SANTA CLARA C REGIS

AI drug research algorithm flipped to invent 40,000 biochemical weapons

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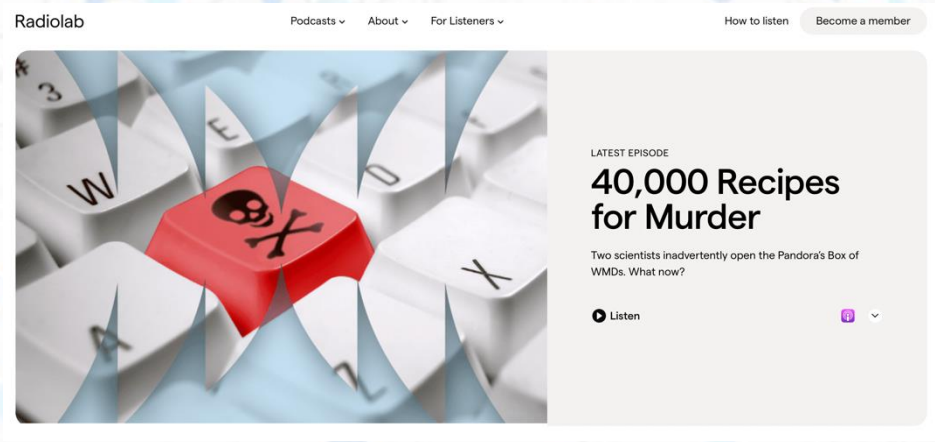

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NETFLIX

Unknown: Killer Robots

2023 · TV-14 · 1h 8m

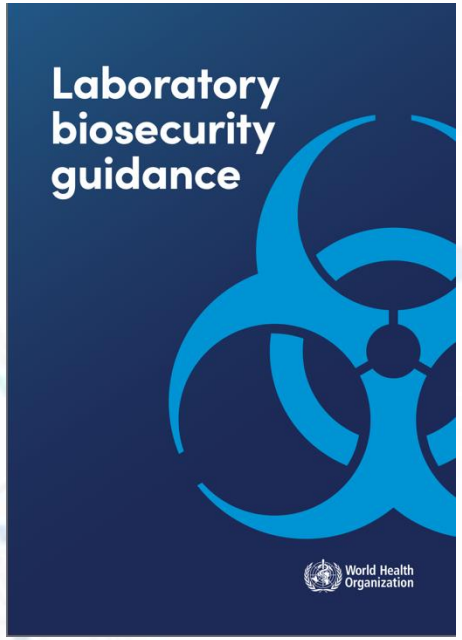
IMDb RATING
6.5/10
185

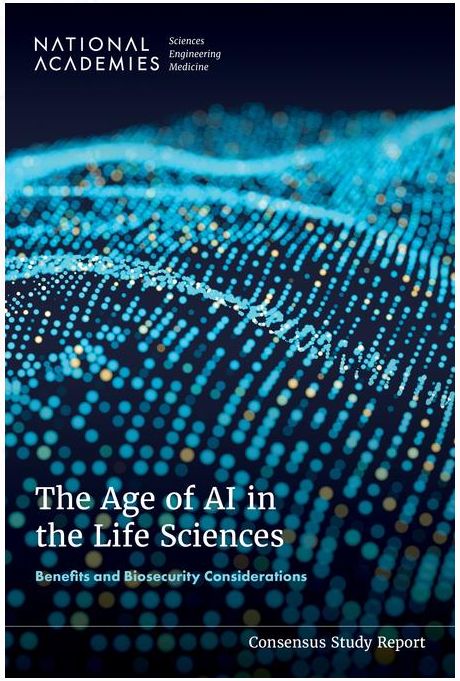
Documentary

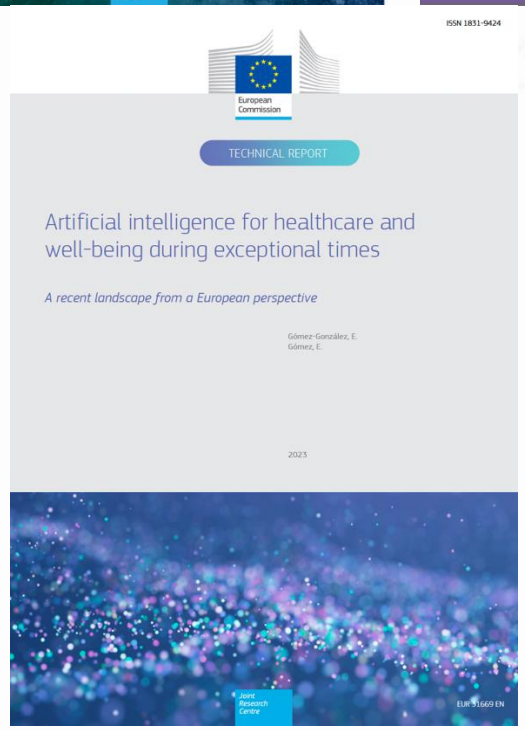
Follows the terrifying behind-the-scenes of military-funded scientists racing to build this technology, as Artificial intelligence infiltrates every level of the armed forces.

Watch on Netflix
with subscription

Policy Documents







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10 Recommendations for generative AI: Preventing AI from creating chemical threats

1. Learn from The Hague Ethical Guidelines
2. Engage numerous AI ethics institutes or other experts to provide guidance
3. Increase ethical training for computing students and raise awareness
4. Increase training of scientists in companies to recognize potential for dual use of generative AI
5. Keep a human in the loop
6. Waitlist restriction (e.g. like GPT-3 was initially) to limit access
7. Use a public facing API to control access and how models are used
8. Federated learning - use encrypted data to train model without decrypting data
9. Disclosure of potential for dual use in publications to encourage recognition of this potential and visibility
10. Regulation of software and applications in industry/academia: limit access to tools, knowledge and expertise

+ Self regulation, anyone?

Urbina, Lentzos, Invernizzi, Ekins, J Chem Inf Model. 2023 Feb 13;63(3):691-694

Key take-home points

- **Publishing** led to increased engagement on dual use, but should it have even happened?
- Need for oversight of in silico research that could be used for dual use models
- Especially in the design of biological, chemical agents or other toxins
- Need for Benefit- risk assessment before you start - Ask yourself - Should the work even be done?
- Need for Risk mitigation plan - How to share and communicate the data related to biological / chemical toxins (or not)

- **Would any restrictions on AI be used as a broader attack on science**
- **Current administration attacks on science may be more dangerous than anything that AI could do?**

- P.S. More ethics training?