

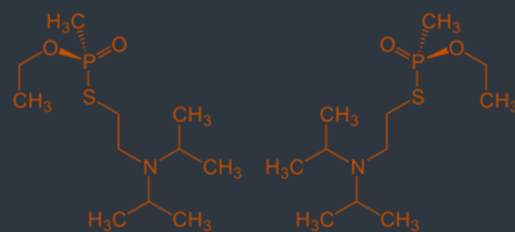
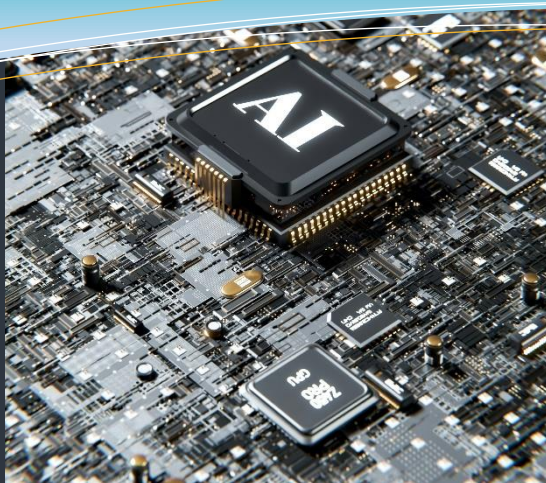
## The proposal to designate "Misuse of AI" as this month's poison...

... was suggested by the Computational Toxicology Working Group of the GT. Computational Toxicology now plays an important role in all areas of toxicology. Through the development and application of computer-based models, predictions can be made about how chemicals affect biological systems and what potential health risks they could pose. Furthermore, the use of such prediction models can reduce the number of animal experiments. Thus, the use of *in silico* models and *in vitro* tests enables scientists to gather information about the toxicity of a molecule without having to rely on laboratory animals.

Additionally, computer-based methods assist in the identification of chemical safety profiles. By analyzing large amounts of data, the toxicity of a chemical can be characterized, and safety profiles can be established. Moreover, the results from computational toxicity analyses contribute to the chemical risk assessment, which defines the potential hazards of chemicals to human health and the environment.

### *In silico*

The term is derived from the Latin word "silicium," which represents the element silicon. Silicon is the most abundant chemical element in computer chips. Therefore, "*in silico*" roughly translates to "in the computer" and describes computer-based approaches distinguishing itself from "*in vitro*" (in cell culture) and "*in vivo*" (in living organisms).



VX (racemic mixture)

## Misuse of AI and computational chemistry to develop new chemical weapons - a rapidly growing threat

The use and continuous development of computer-based methods and artificial intelligence (AI) have been one of the driving forces behind chemical and pharmaceutical research and development in recent decades. Both the quantity and quality of globally available data are steadily increasing. Large international databases are now available, in which scientific research findings are processed in such a way that they can be used for knowledge generation with the help of advanced algorithms. These algorithms enable, for example, the rapid analysis of complex molecular structures or the prediction of chemical properties through pattern recognition in chemical structures. AI can also be used in areas such as the development of new synthesis pathways and the process optimization of chemical analyses.

An important area where the use of computer-based methods and AI has increased significantly is pharmaceutical research. Their use offers numerous advantages for the discovery and development of new drugs. The AI technologies used have been and are being developed with the intention of generating insights for the benefit of humanity, in order to save time, money, and resources in the development and manufacturing of new active substances.

However, these programs can be misused and thus become dangerous tools. This was demonstrated for the first time by Sean Ekins and his team in 2022 when they provided computational evidence of the misuse of AI technologies for drug development. The researchers reversed the logic of their designed *de novo* molecule generator, MegaSyn. This program makes predictions about the bioactivity of molecules derived from machine learning models. For drug development, the program was configured to penalize calculated toxicity while rewarding target activity. They now reconfigured the program to reward both high toxicity and

## Chemical weapons

Chemical weapons consist of chemical substances that can harm, injure, or kill humans, animals, or plants. The effects of chemical weapons can vary and depend on the type of chemicals used. For example, some chemical weapons may irritate the respiratory system, leading to breathing difficulties or suffocation, while others may have neurotoxic effects that attack the nervous system, resulting in paralysis, convulsions, or even death. Others may cause skin burns or severe chronic health damage. Chemical weapons can exist as gases, vapors, liquids, or solids and can be dispersed in various ways.

## Prohibition of chemical weapons

The use of chemical weapons is internationally condemned due to their potentially devastating effects. The use of chemical weapons is regulated by the international Chemical Weapons Convention of 1997, which prohibits the use, development, production, storage, and transfer of chemical weapons. Despite these prohibitions, chemical weapons have been and continue to be used, sometimes with devastating consequences.

## VX

VX is a chemical nerve agent developed in the 1950s. The effect of VX is based on its ability to block the enzyme acetylcholinesterase, which results in excessive stimulation of nerve endings. This can lead to a variety of symptoms, including muscle cramps, respiratory paralysis, and ultimately death due to respiratory failure. The treatment for VX poisoning involves the use of atropine.

bioactivity resembling the mechanism of the known nerve agent VX in molecules.

Within a few hours, their model generated 40,000 molecules that met these criteria. The AI not only designed VX itself but also various other known chemical warfare agents, which were confirmed by public chemical databases. Furthermore, new molecules were created that seemed plausible and, based on their predicted toxicity (LD<sub>50</sub> values), were expected to be more toxic than already known chemical warfare agents. Even more alarming was, that the researchers had not previously trained the AI on this question, and the datasets used to train the AI did not contain nerve agents but rather came from publicly available data on drug-like molecules.

With the publication of the study, the potential dangers posed by computer-based methods and AI became tangible in case they are abused for the development of chemical weapons.

Reality shows that calling for sanity alone is not enough to minimize this danger. It requires the establishment of ethical standards and codes of conduct in this area of science, as well as an active dialogue among experts from industry, academia, and political decision-makers regarding the impact of the application of computer-based tools. Queries to publicly accessible AIs should be made available to gain security and control over how published models are used. Furthermore, restrictions on applicability could increase safety.

*Text: Ute Haßmann*

## Literature and links:

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- Urbina, F., Lentzos, F., Invernizzi, C., Ekins S. Preventing AI From Cre Preventing AI From Creating Biochemical Threats *Journal of Chemical Information and Modeling* 2023 63 (3), 691-694 DOI: [10.1021/acs.jcim.2c01616](https://doi.org/10.1021/acs.jcim.2c01616)
- [VX – Wikipedia](#)
- [Chemical Weapons: Protect Integrity of Global Ban | Human Rights Watch \(hrw.org\)](#)
- [Picture of Igor Omilaev auf Unsplash](#)