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...
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.

**Literature and links:**

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- Picture of Igor Omilaev auf Unsplash