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Society of Toxicology
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AI will only replace toxicologists, who don't use it

The advent of Artificial Intelligence (AI) in daily life is also impacting on toxicology. In fact, it prompts a scientific and technological revolution. You just heard examples of what is happening and what is likely to come. Let's use a real case to sharpen our discussions:

The Elk River chemical spill occurred on January 9, 2014, in Charleston, West Virginia, when a storage tank at Freedom Industries leaked a chemical mixture, primarily consisting of 4-methylcyclohexanemethanol (MCHM), into the Elk River. This spill contaminated the water supply for over 300,000 residents, leading to widespread panic, water use restrictions, and a significant public health emergency. The incident highlighted the vulnerabilities in chemical storage and water safety regulations and underscored the need for improved emergency response and contaminant detection methods. The use of AI in toxicology could greatly enhance the speed and accuracy of detecting and analyzing chemical spills, aiding in quicker decision-making and potentially mitigating the impact of such environmental disasters.

At the time of the incident, toxicological information on MCHM was limited, leading to challenges in assessing the chemical's health risks and setting safe exposure levels. Available data primarily came from material safety data sheets (MSDS) and essentially one LD_{50} study in rats, but these offered insufficient detail on the compound's effects on human health, highlighting the need for more comprehensive toxicological evaluations and rapid evidence integration in such emergencies. In response to the Elk River chemical spill, risk assessment efforts were initiated despite the sparse toxicological data on MCHM. These efforts involved gathering all available information on MCHM, including any existing studies and its MSDS, to estimate potential health risks. Agencies like the CDC and local health departments worked to establish provisional guidelines for safe water use, based on conservative estimates of toxicity and exposure levels. This approach aimed to protect public health while acknowledging the limitations and uncertainties due to the lack of comprehensive toxicological data on MCHM.

Discussion Questions:

1. What was the risk assessment that was possible with this data in 2014? What could be done to support decisions with *in vivo* and *in vitro* tests?
2. How can AI help information retrieval in such cases nowadays? What are the problems?
3. Information is often contradictory and comes from very different sources. How does this impede emergency risk assessments? How can AI help to integrate information?
4. How can AI fill data gaps and predict toxicity by automated read-across in such cases?
5. Why are big data and transfer learning superior to traditional computational methods?
6. What are hallucinations in AI? How can these be mitigated? What would this mean in an emergency case?
7. What is the black box problem of AI and how can it be mitigated? Is this important in an emergency risk assessment?
8. Can AI support mechanistic and systems toxicology? Is this important for emergency situations?
9. How fast can we expect AI to develop in toxicology? How can it be used already?
10. What are the bottlenecks for AI use? How can we overcome them?