

Proposal of next-generation system in big data era based on chemical data science

--- Integrated toxicity research support system adapted to the new era ---

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Introduction:

Changes in toxicity research approach and computer environments.

At present, toxicity research needs to be developed in consideration of the mechanism of AOP, and application of powerful data analysis methods such as artificial intelligence is required. On the other hand, computer technology is rapidly advancing in both hardware and software. As a result, next-generation system is required to apply totally different ideas and technologies from the past.

Purpose:

Current system features, limitations and problems are discussed in this poster.

Most of the systems currently deployed are designed / developed to achieve the best performance according to individual goal. Therefore, as the external / internal environment changes, it becomes difficult to adapt the originally designed function to the new environment.

1. *Changes in toxicity research methods and approaches:*

Toxicity studies themselves also need to consider toxicity mechanisms such as AOP. In such a case, a system that does not consider mechanisms can't be applied to the latest toxicity studies.

2. *Changes in the computer related environment:*

Computer-related environmental changes are extremely rapid. In a short period of time, the conventional technology becomes old, and it is necessary to introduce and adapt a new technology.

Conclusion:

In the latest toxicity evaluation research, an approach considering the toxicity development mechanism such as AOP is important. As a result, in addition to the conventional toxicity prediction software, coordination with a system having a toxicity mechanism analysis function is required.

As described above, the development of toxicological data analysis methods and the advancement of computer-related technologies (including big data and AI) require technologies and approaches that are different from conventional system construction. In this poster, we propose the next-generation system for toxicity research and evaluation by computer.

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