Machine Learning and Multi-Omics for Predicting Chemical Toxicity

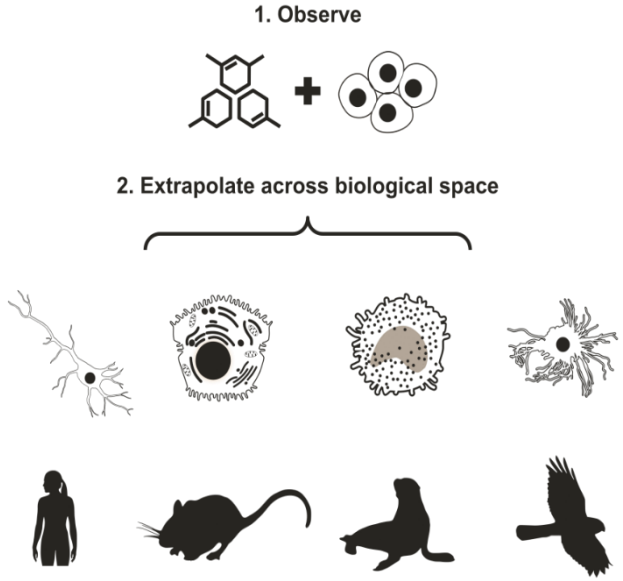
Challenge

- Traditional animal-based toxicity tests are too costly, slow, and ethically concerning to assess the safety of all chemicals used in society.
- Borrowing from drug discovery, scientists are exploring high-throughput screening methods to identify the most hazardous chemicals efficiently. These approaches leverage computational models and cellular testing to prioritize resource-intensive evaluations.
- Rather than testing every compound across all cell types and species, researchers aim to develop computational strategies that use existing knowledge of biology to design targeted screens and extrapolate toxicity across diverse biological systems.

Technology

Imaging and omics data helps us study thousands of molecular and structural changes in cells when exposed to chemicals. When we collect this data from lab-based cell tests, it's called "cell profiling." Using this data, we can:

- Estimates the lowest chemical exposure that causes molecular and morphological perturbations in different tissues of living organisms (including humans) for thousands of compounds;
- Predict toxicity mechanisms using machine learning, transfer learning, and multi-omics analysis of exposed cell images;
- Create user-friendly web-tools that connect cell profiles to toxicity data from diverse *in silico*, *in vitro*, and *in vivo* sources.



Internal EMBLEM Reference

2026-008

Key Inventors

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Applications

- **Toxicology Screening**: Assesses chemical toxicity in pharmaceuticals, chemicals, and cosmetics.
- **Drug Development**: Identifies toxic compounds early, reducing late-stage failures.
- **Regulatory Risk Assessment**: Helps evaluate risks of chemicals and pollutants on health and ecosystems.
- **Personalized Medicine**: Identifies patients at higher risk of adverse reactions.
- **Environmental and Public Health**: Assesses pollutants and chemicals to protect public health.

Keywords

New Approach Methods (NAMs)
Omics data
High-throughput screening
Mode-of-action analysis
Adverse outcome pathways

Benefits

- **Early Detection**
  Identifies toxicity risks at low exposure levels.
- **Predictive Modeling**
  Uses machine learning to predict toxicity mechanisms.
- **Cost-Effective**
  Reduces reliance on animal studies with scalable screening.
- **Informed Decision-Making**
  Integrates diverse data for better research and regulatory decisions.
- **Real-World Relevance**
  Bridges lab research with real-world chemical exposure scenarios.

Further Reading

[1] doi:10.1038/s41596-023-00950-4

[2] doi:10.1038/s41467-024-50613-5

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Intellectual Property

☒ Know-how based

☒ Copyright

Commercial Opportunity

We value collaboration with stakeholders from government, industry, and academia, we aim to ensure our work drives meaningful, real-world impact and advances environmental health research.

We offer special rates for academics and SMEs.

Seeking:

☒ Collaborations

☒ Commercial partner

☒ Licensing

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