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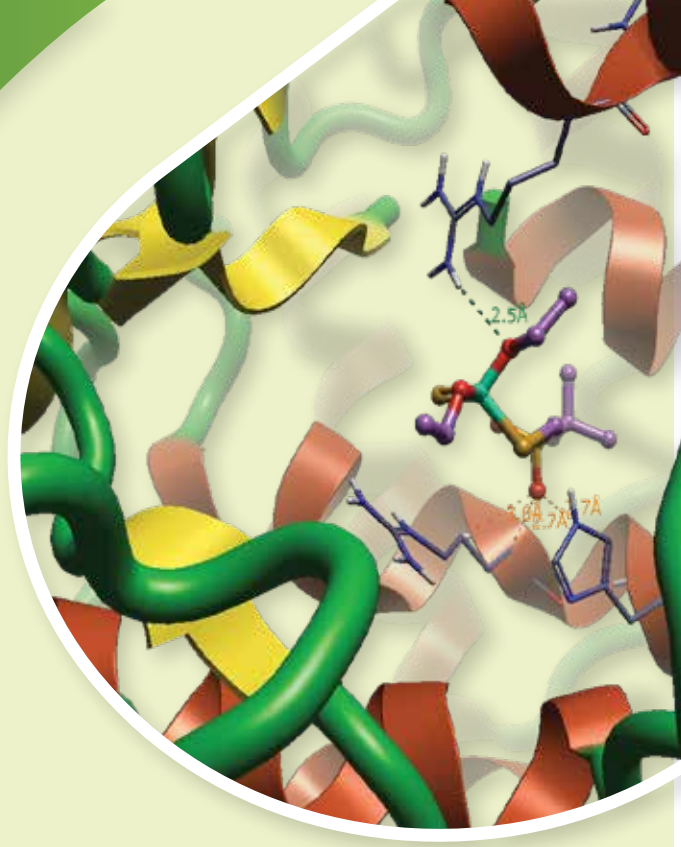
In-silico Methods in Toxicity Prediction



Dr. Bharath BR

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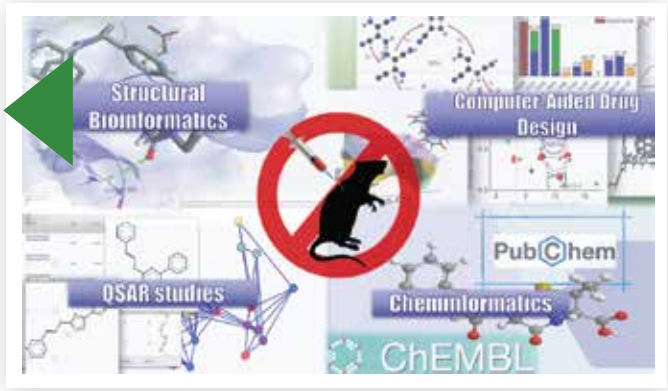
Computational chemist, with proficiency in molecular modelling and simulation of micro and macromolecules. Involved in screening small molecules for different toxicity endpoints in compliance with OECD and ICH guidelines. Development of QSAR/ statistical models for toxicological endpoints using machine learning concepts. Understanding of the mechanism of action involved in the development of toxicity using omics approach.

Welcome to the latest edition of our newsletter on *in-silico* methods in the prediction of toxicity.

In recent years, there has been an increasing interest in using ***in-silico*** methods such as computational models and machine learning algorithms to predict the toxicity of chemicals and products. These approaches have the potential to reduce the need for animal testing and provide faster and more cost-effective ways to evaluate chemical safety.



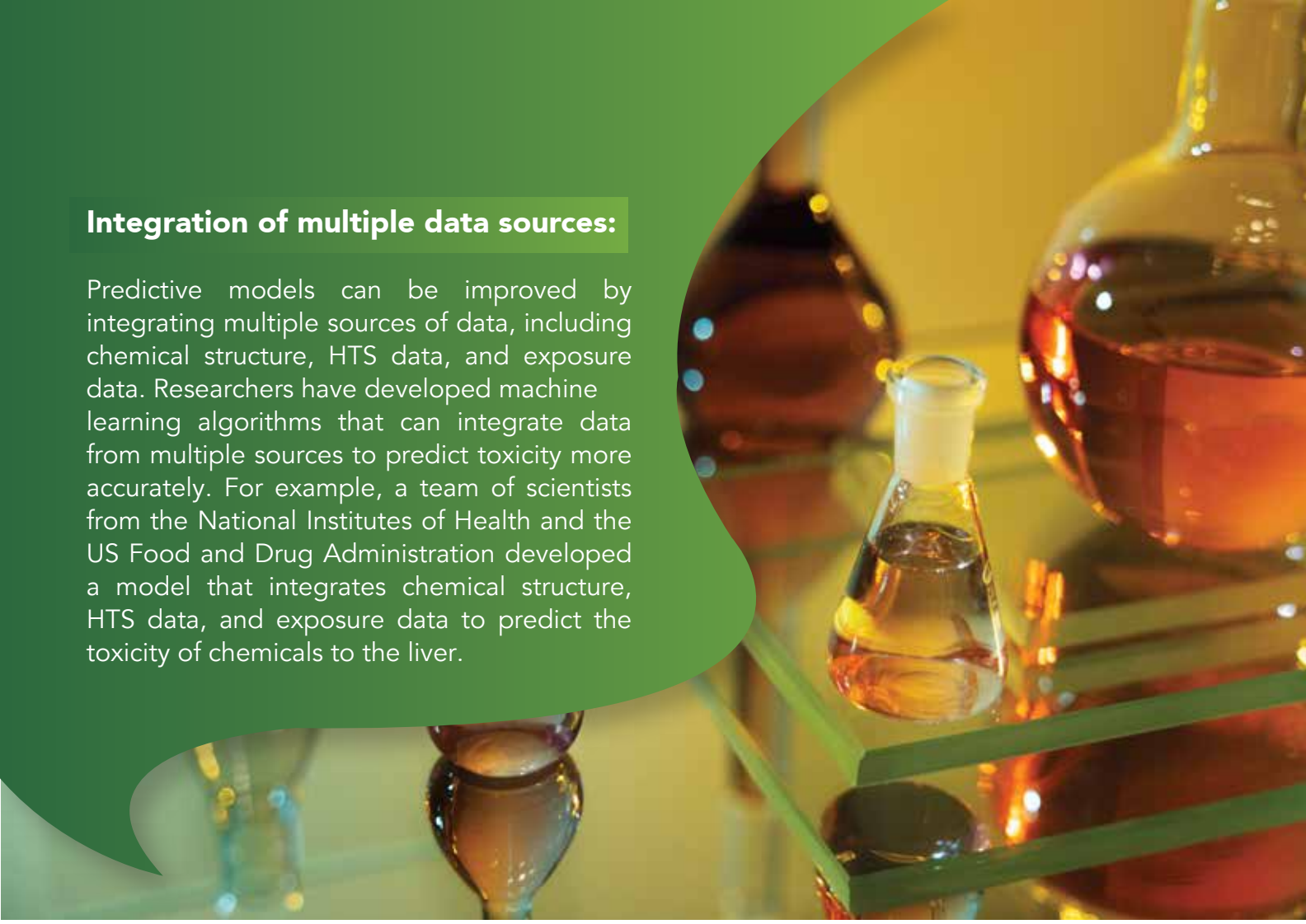
Development of new computational models:

Researchers have been developing new computational models to predict toxicity based on chemical structure and other properties. For example, a team of scientists from the University of California, San Diego, and the University of Iowa developed a machine learning model that predicts the toxicity of chemicals to fish. The model is based on the chemical structure of the compounds and can predict the toxicity of chemicals that have not been tested in fish. Use of high-throughput screening data.

High-throughput screening (HTS) data from in vitro assays can be used to develop computational models for toxicity prediction. The US Environmental Protection Agency's Tox Cast program has generated a large amount of HTS data for thousands of chemicals. Researchers have used this data to develop predictive models for a range of toxicity endpoints, including reproductive toxicity and carcinogenicity.

Integration of multiple data sources:

Predictive models can be improved by integrating multiple sources of data, including chemical structure, HTS data, and exposure data. Researchers have developed machine learning algorithms that can integrate data from multiple sources to predict toxicity more accurately. For example, a team of scientists from the National Institutes of Health and the US Food and Drug Administration developed a model that integrates chemical structure, HTS data, and exposure data to predict the toxicity of chemicals to the liver.



Regulatory Acceptance

Regulatory agencies around the world are starting to accept *in-silico* methods for toxicity prediction. For example, the European Chemicals Agency's (ECHA) guidance on the Application of the Classification, Labelling and Packaging (CLP) Criteria includes provisions for the use of *in-silico* methods for hazard identification and classification. In addition, the US Environmental Protection Agency's Strategic Plan to Promote the Development and Implementation of Alternative Test Methods includes a commitment to promoting the use of computational models for toxicity prediction.

in-silico **methods have the potential to revolutionize the way we evaluate chemical safety. As research in this area continues to progress, we can expect to see more accurate and reliable predictive models for toxicity.**

In that regard, Jai Research Foundation is also equipped with *in-silico* methods are catering the predictive toxicology, NGS data analysis, cheminformatics, molecular modeling, and MD simulation services to clients from pharmaceutical, agrochemical, and crop care sectors. Eventually, contributing to save the animals in pre-clinical research.