Review Article

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A ROLE OF AYURINFORMATICS COMPUTATIONAL TOXICOLOGY STUDY IN AGADATANTRA: A REVIEW

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ABSTRACT

Ayurveda the heart of Indian medical system consists of eight branches and Agadatantra is one of them which on the whole deal with poison and their therapeutic management. The Ayurveda toxicology (Agadatantra) help to identify poison, described type of poison and secernate minerals, plant and animal poison along with their treatment methodology. Ayurveda acknowledges the presences of toxic substances, called Visha Dravya. Many Ayurvedic texts outline methods for detoxifying or purifying these substances before they are used in medicine e.g., Shodhana processes. However, traditional methods of detoxification require scientific validation to confirm their efficacy in removing or neutralizing toxins. Toxicity testing is done on animal models. Animal ethical committee always suggests reducing the number of animals or replacing the animals in safety and toxicity profiling. A computational toxicology approach is a better option for toxicity prediction based on chemical structure of the compound, as it offers a promising alternative to traditional methods. This technique is highly reliable because it limits the animal testing and provides precision in study of toxicity of various phytochemicals. This technique is highly efficient, accurate and reliable for toxicity assessment without animal testing.

Keywords: Ayurinformatics, Computational toxicology, Agadatantra, Toxicology, Ayurveda.

INTRODUCTION

Agadatantra, one of the eight branches of Ayurveda (Ashtanga Ayurveda), specializes in the science of toxicology. This branch is dedicated to the comprehensive study and management of poisons, covering various aspects such as poison identification, symptom assessment and treatment of poisoning cases[1].

In Ayurveda, diseases are classified as either Nija (internal) Agantuja diseases include those caused by outside factors like poisons (Visha), weapons (Shastra) and burns (Agni). The Visha comes from the root vis, meaning "This refers to how poison quickly spreads throughout the body after ingestion. In Ayurveda, Visha also includes anything that harms or threatens life, making people unwell. Visha Dravya are substances that, in small amount, can be life-threatening or cause serious issues[2].

Interestingly, Ayurveda uses some Visha Dravyas (toxic substance) as medicine (Aushadha Dravya) once they have been properly processed. Ayurveda believes that the difference between a medicine and a poison is dosage. A small amount may heal, while a larger amount may harm. Ayurvedic texts describe the properties of poisons, showing how they can be dangerous even in small doses[3].

Scientific validation of these Visha, Aushadha Dravya is essential to ensure their safety, efficacy and global acceptance4. Traditional toxicological studies often rely heavily on animal testing, which can be time-consuming, costly and ethical challenging. With growing ethical and logistical concerns, there is a rising demand for innovative technologies to complement or replace animal testing.

Computational Toxicology: A New Era In Toxicity Prediction

Computational toxicology offers a promising alternative to traditional methods. This approach minimizes the need for extensive animal testing and provides a powerful tool for predicting the toxicity of various phytochemicals[5]. Drawing from diverse fields such as medicine, biology, chemistry and mathematics computational toxicology uses computer-based models to analyse and detect patterns within large biological and chemical data sets[6]. By integrating data from multiple disciplines, computational toxicology enables researchers to identify potential toxic effects of chemicals more efficiently. Simulate biological interactions and predict toxicological outcomes. enhance the accuracy and reliability of toxicity assessments without animal testing. This interdisciplinary method has become an invaluable resource in toxicology, paving the way for more ethical, efficient and data-driven approaches in toxicity research.

In Silico Models In Ayurvedic Toxicology: A New Frontier For Herbo-Mineral Safety And Interactions

In the field of toxicology, advanced software tools such as TOPKAT (Toxicity prediction by komputer Assisted Technology) by Accelrys Inc., Cambridge, UK, offer a valuable alternative to tradition testing. These tools, based on biostatistics and QSAR (Quantitative Structure-Activity Relationship) methods, assist in predicting the toxicity of various compounds[7].

Given Ayurveda rich history of using herbal, herbo-mineral, and mineral formulations, these in silico models hold significant promise in assessing the safety and toxicity of these traditional treatment.

Table 1: Summary of various computational toxicology approaches[8]

Approach	Technology Variants	Methodology	Reference
Linear free energy relationship	Quantitative Structure Toxicity Relationship (QSTR)	The toxicity of various novel molecules can be determined by studying the function group present in the molecule.	9
	Toxicity prediction by Komputer Assisted Technology (TOPKAT)	This technique helps in determining the 16 toxicity endpoints from QSTR, by studying the shape and symmetry descriptors and electro-topological rich information.	10
	ADMET predictor	It helps in predicting various same toxicity endpoints available in TOPKAT by employing different modelling methodologies.	11
	CSGenoTox	It uses similar modelling methods as TOPKAT, namely connectivity indexes, electro topological state indexes and shape indices.	12
	Admensa Interactive	It is similar to ADMET predictor but also predict cardiotoxicity	13
Expert Systems	Hazard Expert	It helps in predicting the toxicity endpoints such as irritations, mutagenicity, teratogenicity, immunotoxicity, carcinogenicity and neurotoxicity.	14
	Oncologic	It is used to determine the carcinogenicity of fibres, metals and polymers, and in determination of toxicity of organic excipient.	14
	Deductive Estimation of Risk from Existing Knowledge	This helps to determine the toxicities such as carcinogenicity, skin irritation, genotoxicity, and other toxicological risks.	15
Machine learning approaches	Computer Automated Structure Evaluation (CASE/MultiCASE)	Principally works on structural fragmentation at the atomic level.	16
	Tox Boxes	This helps in determining the toxicity, upon the fragmentation of the structure at atomic level and then to study the toxicity carried by each individual atom.	17
Web-based toxicity predictor	No variants	This is a web-based software and doesn't require installation of any software. This helps in determination of salmonella, rodent carcinogenicity, human maximum therapeutic dose and LC50 at no cost.	18

The Future Of *In Silico* Toxicity Studies In Agadatantra

In silico modelling could provide a non-invasive and efficient way to study these Visha Aushadh Dravya[19], Researcher can gain inside into the potential toxicity and safety of these traditional formulations. This could help to advance the understanding of Ayurvedic pharmaceutical. The computational approaches have the potential to bridge the gap between Ayurvedic knowledge and modern scientific practice.

CONCLUSION

Incorporating computational toxicology into Ayurvedic research can significantly enhance the safety and efficacy of traditional formulations. While Ayurveda has a rich history of herbal and herbo-minerals remedies, the integration of omics technologies and computational methods can offer a more precise understanding of toxicity mechanisms, which is crucial for their modern application. By utilizing in silico models to predict the toxicity of Ayurvedic compounds, researchers can better evaluate their safety and optimize their therapeutic potential. The combination of traditional Ayurvedic knowledge with modern computational tools will lead to more reliable and effective treatments, ensuring Ayurveda remains relevant in today's scientific landscape.

Challenges And Future Prospect Of Computational Toxicology In Agadatantra

Ayurvedic researchers need foundational training in medical informatics to fully leverage modern technologies and promote the growth of this ancient system of medicine. Many Ayurvedic scholars, physicians and researchers lack formal training in areas like computer science, information technology and bioinformatics, which presents a significant challenge when exploring in silico biology in Ayurveda[7]. In today's scientific landscape, conducting research without information technology is nearly unthinkable. The major hurdle in this field is the shortage of professionals with expertise in both traditional medicine and information technology. Global collaboration in Ayurvedic research, particularly for exploring newer research methodologies, is essential to address the challenges of Ayurveda in a modern context.

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