Natural Resources for Human Health
eISSN: 2583-1194

**Original Research**

**Received** 18 March 2026
**Revised** 25 April 2026
**Accepted** 15 May 2026

Natural Resources for Human Health 2026, Vol. 6 (3): 226–234

**KEYWORDS**:
Computational toxicology; Functional foods; Herbal products; Artificial intelligence; Machine learning; QSAR; Molecular docking; ADMET prediction; Network toxicology; Multi-omics; Toxicogenomics; Risk assessment.

# Computational Toxicology of Functional Foods and Herbal Products: Current Advances and Future Directions

Dr. S. Sasikumar[1], Dr. Gurpreet Singh[2], Mohit Sanduja[3], Ibrokhim Sapaev[4], Aishwarya D. Jagtap[5*], Drishti Patel[6], Nilufar Mamatkulova[7], Joshua S[8]

[1] Professor, Department of Forensic Medicine, Vinayaka Mission's Kirupananda Variyar Medical College & Hospitals, Vinayaka Mission's Research Foundation (DU), Salem, Tamil Nadu, India. sasikumarfm@gmail.com, 0000-0001-7179-3413

[2] Associate Professor, Department of Pharmacy, Vivekananda Global University, Jaipur, India, Email Id-gurpreet.singh@vgu.ac.in, Orcid id- 0000-0002-1421-3782

[3]School of Pharmacy and Research, Dev Bhoomi Uttarakhand University, sopr.mohitsanduja@dbuu.ac.in, 0000-0003-3139-8835

[4]1. Head of the Department of Physics and Chemistry, "Tashkent Institute of Irrigation and Agricultural Mechanization Engineers" National Research University, Tashkent, Uzbekistan; 2. Scientific Researcher, University of Tashkent for Applied Science; 3. School of Engineering, Central Asian University, Tashkent, Uzbekistan. sapaevibrokhim@gmail.com, 0000-0003-2365-1554

[5]Krishna Institute of Science and Technology, Krishna Vishwa Vidyapeeth "Deemed to be University", Taluka-Karad, Dist-Satara, Pin-415 539, Maharashtra, India. aishwarya22999@gmail.com

[6]Department of Forensic Medicine , Noida international University, Greater Noida, Uttar Pradesh 203201, India., drishtipatel@yahoo.in

[7]Jizzakh State Pedagogical University, Uzbekistan. nilufar.mamatkulova78@mail.ru 0009-0009-1487-4933

[8]Meenakshi College of Allied Health Sciences, Meenakshi Medical College Hospital & Research Institute, Meenakshi Academy of Higher Education and Research, joshuasahs@maher.ac.in

**ABSTRACT:** Computational toxicology, which integrates computational modelling, artificial intelligence (AI), and systems biology, is a powerful tool for improving the safety assessment of functional foods and herbal medicines. The review focuses on recent advances in computational tools such as quantitative structure–activity relationship (QSAR) modeling, molecular docking, molecular dynamics simulation, read-across methods, and prediction of ADMET and network toxicology for predicting the toxicological profile of bioactive compounds. The role of machine learning, deep learning, explainable AI, and predictive toxicology platforms in enhancing the accuracy of toxicity prediction is discussed. In addition, the review emphasizes the use of multi-omics approaches such as toxicogenomics, proteomics, metabolomics, and integrated systems toxicology to gain insights into mechanisms of toxicity. The current regulatory perspectives, such as OECD, FDA and EFSA guidelines, are also discussed along with validation strategies for models. Finally, the existing challenges, future research directions, and the potential of AI-driven precision toxicology are discussed. It is envisioned that computational toxicology will be a game-changer in the rate of risk assessment, minimizing animal testing, improving the science of regulatory decision-making, and

providing a scientific blueprint for safe and effective functional foods and herbal therapeutics.

## 1. INTRODUCTION

Due to their nutritional properties and a wide range of biological activities like anti-inflammatory, antimicrobial, antioxidant, immunomodulatory, and anticancer, functional foods and herbal products are becoming significant players in the healthcare industry and are viable therapeutic agents for the prevention and management of chronic diseases like cardiovascular disorders, diabetes, obesity, and cancer (1). These products are rich in various bioactive phytochemicals, such as polyphenols, flavonoids, alkaloids, terpenoids, phenolic acids, and glycosides, which have therapeutic efficacy but can also be toxic under specific circumstances (2). While functional foods and herbal medicines are generally considered safe, they can be highly dangerous because of the presence of natural toxicants, heavy metals, herbicide residues, mycotoxins, microbial organisms and pathogens, use of synthetic pharmaceutical drugs, and overuse or clinically important drug–herb interactions (3). Comprehensive toxicological evaluation has become necessary; therefore, to assure product quality, efficacy, and consumer safety (4). The traditional toxicity testing approaches are based on in vitro assays, animal experiments, and clinical trials, but these are costly, labor-intensive, ethically questionable, and unsuitable for the rapid screening of thousands of natural compounds identified annually (5). Given these limitations, computational toxicology has developed into a state-of-the-art multidisciplinary science that integrates cheminformatics, bioinformatics, quantitative structure–activity relationship (QSAR) modeling, molecular docking, molecular dynamics simulations, read-across strategies, network toxicology, and artificial intelligence (AI)-based predictive algorithms to estimate the toxicological outcome efficiently without the need to sacrifice animal use (6). The prediction of hepatotoxicity, nephrotoxicity, cardiotoxicity, genotoxicity, carcinogenicity, reproductive toxicity, and endocrine disruption of phytochemicals and functional food ingredients has been significantly improved by the increased development of machine learning, deep learning, and multi-omics integration (7). Moreover, there has been increasing acceptance of in silico chemical hazard identification, risk assessment, and regulatory decision-making methods by internationally recognized regulatory agencies like the Organisation for Economic Co-operation and Development (OECD), European Food Safety Authority (EFSA) and the U.S. Food and Drug Administration (FDA) (8). As a result, computational toxicology is emerging as an essential and valuable tool for rapid safety evaluation, precision nutrition, standardization of herbal products and facilitating the development of safer functional foods using reliable, cost-effective, and mechanism-based predictive approaches (9).

## 2. FUNCTIONAL FOODS AND HERBAL PRODUCTS: SAFETY AND TOXICOLOGICAL CONCERNS

Apart from nutrition, the active ingredients in functional foods, nutraceuticals, and herbal health products have proven to be of great value in the field of health care and disease prevention (6). The concept of functional foods includes concentrated foods (foods containing high levels of dietary fibre, probiotics, omega-3 fatty acids, vitamins, minerals, and polyphenols), which are added to food products for health purposes, and naturally occurring or fortified foods with high levels of bioactive substances for a particular health application (nutraceuticals) (7). Medicinal plants used in herbal medicine are rich in a variety of phytochemicals like flavonoids, alkaloids, terpenoids, phenolic acids, tannins, glycosides, and saponins, which have antioxidant, anti-inflammatory, antimicrobial, anticancer, immunomodulatory, and cardioprotective properties (8). While they have beneficial properties, it is still crucial to consider the safety of natural products due to the presence of toxic phytoconstituents in natural sources or the possibility of contamination during cultivation, harvesting, processing, storage, and commercialization. Some frequent contaminants found in food that can cause hepatotoxicity, nephrotoxicity, neurotoxicity, reproductive toxicity, carcinogenicity, and affect product quality are heavy metals (such as lead, cadmium, mercury, and arsenic), pesticide residues, mycotoxins, microbial pathogens, residual solvents, and adulterants (9). Moreover, medicinal plants may be misidentified, some are intentionally adulterated with synthetic medicines, and there may be other health risks involved (10). Herb–drug interactions are another important area of concern, where the phytochemicals of the herb can interact with conventional drugs by binding to and inhibiting cytochrome P450 enzyme(s), drug transporters or metabolic pathways, which results in reduced efficacy of the conventional medication or enhanced toxicity (11). There are well-documented interactions between the herbals St. John's wort, ginkgo, garlic, ginseng, turmeric, and green tea with prescription drugs that highlight the clinical significance of the need to monitor herbal product use when a patient is taking a prescription medication (12). Therefore,

it is important to use strict quality control, standardization, toxicological studies, and risk assessment calculations when assessing the human health impact of functional food products and herbal products, to ensure their safety, efficacy, and regulatory compliance.

## 3. PRINCIPLES OF COMPUTATIONAL TOXICOLOGY

Computational toxicology is an interdisciplinary science, bringing together toxicology, chemistry, bioinformatics, computational biology, artificial intelligence (AI), and data science to predict, understand, and assess the toxic potential of chemicals, phytochemicals, functional food ingredients, and herbal products without the sole application of traditional animal testing (12). The goal of computational toxicology is to use in silico tools and quantitative structure–activity relationship (QSAR) modeling, molecular docking, molecular dynamics simulation, read-across techniques, physiologically based pharmacokinetic (PBPK) modeling, network toxicology, and machine learning algorithms to enhance the efficiency, accuracy, and cost-effectiveness of chemical safety evaluation (13). These computational methods can predict many toxicity endpoints, including acute and chronic toxicity, hepatotoxicity, nephrotoxicity, cardiotoxicity, neurotoxicity, genotoxicity, mutagenicity, carcinogenicity, reproductive toxicity, developmental toxicity, immunotoxicity, and endocrine disruption, before experimental validation (13). In recent years, the power of computational toxicology to predict toxicity, to provide explanations of the toxicity mechanism, and to become an important tool in the assessment of chemical and food safety has been rapidly increasing, especially with the advent of deep learning and explainable artificial intelligence (14). High quality toxicological databases that include the chemical structure, biological activity, exposure data, and toxicological outcomes of chemicals—all confirmed by experiments- are critical to reliable toxicity prediction. Many resources are available, such as PubChem, ChEMBL, ToxCast, Tox21, Comparative Toxicogenomics Database (CTD), OECD QSAR Toolbox, LiverTox, and DrugBank, that can be used for model development, validation, and regulatory decision-making (15). These databases can facilitate integration, discovery, and analysis of biomarkers, pathways, and risk assessments of regulations, and provide transparency and reproducibility of computational research. Thus, computational toxicology has become an important means to evaluate the safety of functional foods, nutraceuticals, and herbal medicines to accelerate hazard identification, reduce costs of experiments, animal usage, and aid the regulatory process based on solid evidence to safeguard public health.

## 4. COMPUTATIONAL APPROACHES FOR TOXICITY PREDICTION

Computational approach has revolutionized toxicity assessment, allowing a rapid, cost-effective, and mechanistic prediction of the safety of functional foods, nutraceuticals, and herbal products before experimental testing. Among these, a quantitative structure–activity relationship (QSAR) model can be developed that can predict the biological and toxicological properties of chemical substances based on their structural and physicochemical properties, which can help to reduce the use of animals in testing and the evaluation of chemical hazards as early as possible (15). Along with QSAR, molecular docking is another tool to predict the interaction between phytochemicals and molecular targets that are related to toxicity, which provides important information regarding the binding affinity, molecular recognition, and adverse biological responses (16). These interactions can further be validated by molecular dynamics (MD) simulation to help gain more confidence in predictions of the toxic behavior of protein–ligand complexes under physiological conditions (17). Another popular computational approach that is widely used is the read-across method, where the toxicity of a compound that is not tested can be estimated by comparing it to other compounds with similar structures and/or mechanisms of action on which validated toxicological data have been obtained, and it is an important tool for chemical safety assessment in regulatory decision making (18). Furthermore, Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) prediction is now a necessity to describe the pharmacokinetic properties and to help identify potential toxic liability, such as hepatotoxicity, cardiotoxicity, mutagenicity, carcinogenicity, and reproductive toxicity, during product development (19). Recently, a systems biology approach called network toxicology was introduced to elucidate the complex pathways involved in natural product and functional food-induced toxicity, which integrates molecular targets, signaling pathways, protein–protein interactions and multi-omics (20). The set of these complementary computational tools can be used for predicting toxicity, to speed up safety assessment, to reduce the number of experiments, to minimize animal use, and to guide regulatory decisions. The entire process of these integrated computational methods for the safety evaluation of functional foods and herbal products is highlighted in Figure 1, indicating the sequential process from compound identification through computational analysis, toxicity prediction, and risk assessment.

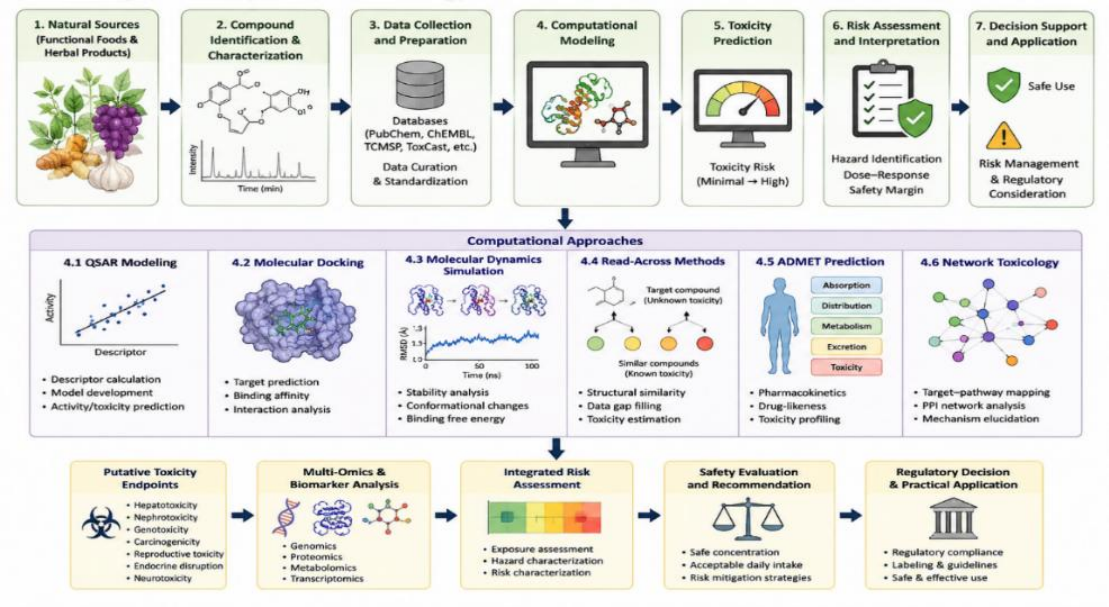


**Figure 1.** Computational Toxicology Workflow for Functional Foods and Herbal Products

## 5. ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN COMPUTATIONAL TOXICOLOGY

The computational toxicology field has been revolutionized by the advent of artificial intelligence (AI) and machine learning (ML), which enable the prediction of the toxicological profile of functional food ingredients, nutraceuticals, and herbal phytochemicals to be performed rapidly, accurately, and in a high-throughput manner (21). Using machine learning models (random forest, support vector machine (SVM), decision tree, k-nearest neighbor (k-NN), gradient boosting, artificial neural networks, etc.), complex chemical descriptors, and biological data sets allow for multiple toxicity endpoints to be predicted, including hepatotoxicity, nephrotoxicity, cardiotoxicity, genotoxicity, carcinogenicity, and endocrine disruption (22). In more recent times, deep learning methods such as convolutional neural networks (CNNs), recurrent neural networks (RNNs), graph neural networks (GNNs), and transformer-based models have been shown to outperform traditional machine learning techniques, as they can automatically learn complex molecular features from vast chemical databases (23). Many AI models, however, remain "black-box," which is not accepted by regulators and/or biological interpretation. To tackle this issue, Explainable Artificial Intelligence (XAI) has emerged as a crucial strategy for enhancing the transparency of AI models and elucidating the molecular descriptors, structural alerts, and biological pathways contributing to toxicity predictions, thereby fostering trust among researchers and regulators (24). Today, several platforms have enabled the ability to integrate the capabilities of AI with cheminformatics and bioinformatics to support chemical hazard identification, virtual screening, ADMET prediction, and regulatory risk assessment. The platforms that are widely used include VEGA, OECD QSAR Toolbox (25), ProTox-3.0, DeepTox, ToxCast, and Tox21, which offer wide computational resources to assess the safety of natural products and also cut down on testing on animals and reduce costs. AI algorithms will play a crucial role in precision toxicology, personalized nutrition, and evidence-based safety assessment of functional foods and herbal medicine as they are further developed and connected with multi-omics data, cloud computing, and big-data analytics.

**Table 1.** Major Computational Toxicology Tools and Their Applications

| Computational Tool | Methodology | Primary Application | Major Toxicity Endpoints |
|---|---|---|---|
| QSAR Models | Structure–activity relationship | Chemical toxicity prediction | Acute, chronic, mutagenicity |
| Molecular Docking | Protein–ligand interaction | Target-based toxicity analysis | Hepatotoxicity, endocrine disruption |
| Molecular Dynamics | Dynamic simulation | Stability of protein–ligand complexes | Mechanistic toxicity |
| Random Forest | Machine learning | Toxicity classification | Multi-endpoint toxicity |
| Support Vector Machine (SVM) | Machine learning | Chemical hazard prediction | Carcinogenicity, mutagenicity |
| Deep Neural Networks (DNN) | Deep learning | Large-scale toxicity prediction | Organ-specific toxicity |
| Graph Neural Networks (GNN) | Deep learning | Molecular graph analysis | Drug-induced toxicity |
| ProTox-3.0 | AI platform | Toxicity and LD50 prediction | Acute toxicity, organ toxicity |
| VEGA Platform | QSAR-based platform | Regulatory risk assessment | Multiple toxicity endpoints |
| OECD QSAR Toolbox | Read-across/QSAR | Chemical safety evaluation | Regulatory hazard assessment |
| ToxCast & Tox21 | High-throughput screening | Toxicity pathway prediction | Biological pathway perturbation |
| SwissADME | ADMET prediction | Pharmacokinetic evaluation | Absorption, metabolism, toxicity |

## 6. MULTI-OMICS AND SYSTEMS TOXICOLOGY

In the era of multi-omics and systems toxicology, the functional assessment of foods and herbal products could be improved considerably by computers, as new and extensive data on multi-level mechanisms of toxicity have become available. Toxicogenomics studies the molecular fingerprinting of the expression of thousands of genes after exposure to bioactive compounds and toxicants to identify molecular biomarkers, mechanism of toxicity and adverse outcome pathways of hepatotoxicity, nephrotoxicity, carcinogenicity and endocrine disruption, etc. (27). While transcriptomic analysis is underway, proteomic analysis will be conducted to identify changes in protein levels, modifications, and protein–protein interactions, which will give insights into changes in protein function that cannot be gained from genomic analysis alone (28). Similarly, metabolomics can provide an overall metabolic profile of the endogenous metabolites and metabolic pathways affected, which allows for the early detection of biochemical changes and organ-specific toxicity resulting from exposure to functional food components and herbal phytochemicals (29).

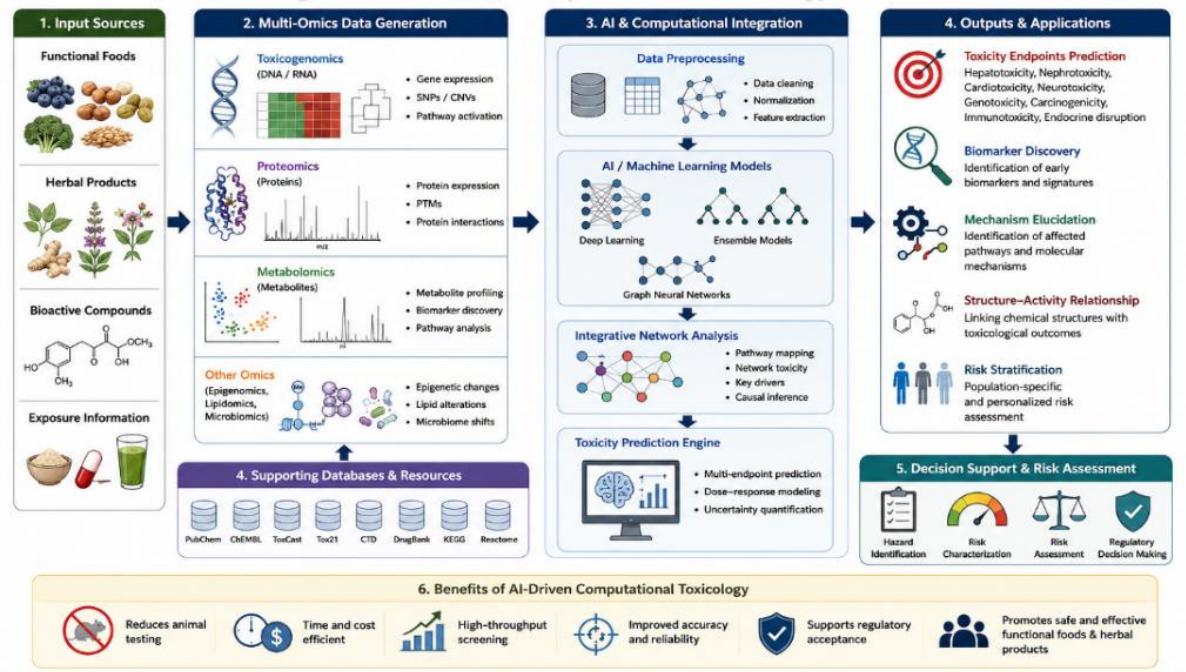


**Figure 2.** AI-Driven Computational Toxicology Framework

In a systems biology approach, multi-omics integration is being employed by combining information from different omic technologies and artificial intelligence (AI) and machine learning with network analysis to enhance the ability to predict toxicity, discover new biomarkers, and unravel complicated molecular interactions and adverse biological responses (30). This is complemented by the introduction of AI-driven computational frameworks, which combine chemical structures, molecular descriptors, omics data, signaling pathways and predictive algorithms, all connected to a single platform to enable more robust hazard identification and individualized risk assessment. These integrated approaches result in increased prediction accuracy, decreased experimental expenses, decreased animal use, and aid precision toxicology and regulatory decision-making. The proposed integration of AI into multi-omics technologies for computational toxicity prediction and functional food/herbal safety assessment is summarized in Figure 2, showcasing the shift from generating vast amounts of biological data to intelligent predictions of toxicity and risk assessment for functional food and herbal products.

## 7. REGULATORY PERSPECTIVES AND RISK ASSESSMENT

As the field of in silico continues to grow, the acceptance of this approach by regulators is gaining momentum, from the ability to aid rapid hazard identification and data-gap filling to aid in chemical prioritization and reduce the use of animals. The Organisation for Economic Co-operation and Development (OECD) provides agreed guidelines in the field of chemical safety assessment for the assessment of quantitative structure–activity relationship (QSAR) models. The principles set out here are that the regulatory QSAR model should have a specified endpoint, an unambiguous algorithm, a specified applicability domain, appropriate measures of robustness and predictivity, and, if possible, it should be mechanistic (31). The OECD QSAR Assessment Framework also contributes to the consistent and transparent evaluation of each prediction, multiple predictions from different models and the capacity to apply the predictions for regulatory purposes (32). The U.S. Food and Drug Administration has issued a call for development of new approach methodologies along the Predictive Toxicology Roadmap, which involve the use of computational modeling, high-throughput screening, and mechanistic approaches as complementary tools to be used in product safety evaluation (33). Similarly, EMA has been increasingly employing new approach methodologies (NAM), such as QSAR, PBPK modeling, read-across, and omics data in food and feed risk assessment (34).EFSA guidance emphasizes the importance of interpreting computational evidence within the framework of a weight-of-evidence approach and integrating adequate chemical similarity, biological plausibility, exposure data, and uncertainty analysis. Therefore, a crucial step of model validation is needed before using the in silico model for predicting the function of a functional food or a herbal product. To assess data quality, reproduction, sensitivity, specificity, goodness of fit, external predictivity, applicability domain,

and uncertainty, model validation should be considered. It is also important that the testing datasets used are independent of the model datasets and that they are also reported separately to ensure transparency and prevent biased or unreliable conclusions (35). Use of a single computational result for making a regulatory decision should be avoided; instead, computational prediction should be used in conjunction with experimental data, exposure assessment, toxicokinetic data, and expert judgment. This comprehensive approach can improve consumer protection and enable the safety assessment of multi-component natural products by efficient, ethical, and scientifically sound procedures.

## 8. CHALLENGES AND LIMITATIONS

However, CT still has many scientific and technical problems that hinder the application of CT to the safety evaluation of functional food and herbal products. Data quality, standardization and experimental validation of computational models are very important. Natural products are extremely chemically diverse and variable, and as such are hard to build and validate models. Furthermore, many AI models are "black boxes" that are hard to interpret and to regulate from a biological viewpoint. Chronic exposure effects and inter-individual variability, as well as complex metabolic transformations, can also be overlooked in computational predictions. Hence, computational methods need to be coupled with experimental and clinical studies for reliable and comprehensive toxicological evaluation.

## 9. FUTURE PERSPECTIVES

The future of computational toxicology will involve various technologies, including AI, machine learning, multi-omics integration, and high-performance computing. New technologies such as explainable AI, graph neural networks, and foundation models are expected to increase prediction accuracy, improve the transparency of models, and increase trust in them for regulatory purposes. Integration of genomics, proteomics, metabolomics, exposures, and clinical data will enable precision toxicology and personalised risk assessment. The building of standardised databases, international collaborative platforms, and harmonised regulatory frameworks will further consolidate computational safety evaluation, promote innovations, minimise animal testing, and facilitate the development of safer functional foods, nutraceuticals, and herbal medicines.

## 10. CONCLUSION

The recent advancement of computational toxicology for functional foods and herbal product safety assessment is a powerful and innovative tool combining QSAR modeling, molecular docking, molecular dynamics simulation, network toxicology, artificial intelligence, and multi-omics technologies. These computational methods offer quick, inexpensive, and mechanistically meaningful toxicity predictions and reduce reliance on traditional animal testing. While data quality, model validation, and regulatory acceptance are still issues to address, ongoing advancements in computational science and AI are likely to overcome these limitations. This synergy between the computational prediction and experimental validation will help to better describe the risk, to ensure consumer safety, to aid in regulatory decision-making, and to aid the development of safe, effective, and evidence-based functional foods and herbal therapeutics.

## DECLARATIONS

**Funding:** The authors received no specific funding for this work.

**Conflict of Interest:** The authors declare that they have no competing interests.

**Author Contributions:** All authors contributed to the conceptualization, literature review, writing, revision, and final approval of the manuscript.

## REFERENCES

[1] Liu RH. Health benefits of fruit and vegetables are from additive and synergistic combinations of phytochemicals. *American Journal of Clinical Nutrition*. 2003;78(3 Suppl):517S–520S. https://doi.org/10.1093/ajcn/78.3.517S

[2] Pan MH, Ho CT. Chemopreventive effects of natural dietary compounds on cancer development. *Chemical Society Reviews*. 2008;37(11):2558–2574. https://doi.org/10.1039/B801558A

[3] Ekor M. The growing use of herbal medicines: Issues relating to adverse reactions and challenges in monitoring safety. *Frontiers in Pharmacology*. 2014;4:177. https://doi.org/10.3389/fphar.2013.00177

[4] World Health Organization. *WHO Guidelines on Good Herbal Processing Practices for Herbal Medicines*. Geneva: World Health Organization; 2018.
[5] National Research Council. *Toxicity Testing in the 21st Century: A Vision and a Strategy*. Washington, DC: National Academies Press; 2007. https://doi.org/10.17226/11970
[6] Roberfroid MB. Concepts and strategy of functional food science: The European perspective. *American Journal of Clinical Nutrition*. 2000;71(6 Suppl):1660S–1664S. https://doi.org/10.1093/ajcn/71.6.1660S
[7] Santini A, Cammarata SM, Capone G, et al. Nutraceuticals: Opening the debate for a regulatory framework. *British Journal of Clinical Pharmacology*. 2018;84(4):659–672. https://doi.org/10.1111/bcp.13496
[8] Pan SY, Litscher G, Gao SH, et al. Historical perspective of traditional indigenous medical practices: The current renaissance and conservation of herbal resources. *Evidence-Based Complementary and Alternative Medicine*. 2014;2014:525340. https://doi.org/10.1155/2014/525340
[9] World Health Organization. *WHO Guidelines for Assessing Quality of Herbal Medicines with Reference to Contaminants and Residues*. Geneva: World Health Organization; 2007.
[10] Izzo AA, Ernst E. Interactions between herbal medicines and prescribed drugs: An updated systematic review. *Drugs*. 2009;69(13):1777–1798. https://doi.org/10.2165/11317010-000000000-00000
[11] Williamson EM, Driver S, Baxter K. *Stockley's Herbal Medicines Interactions*. 2nd ed. London: Pharmaceutical Press; 2013.
[12] National Research Council. *Toxicity Testing in the 21st Century: A Vision and a Strategy*. Washington, DC: National Academies Press; 2007. https://doi.org/10.17226/11970
[13] Cherkasov A, Muratov EN, Fourches D, et al. QSAR modeling: Where have you been? Where are you going to? *Journal of Medicinal Chemistry*. 2014;57(12):4977–5010. https://doi.org/10.1021/jm4004285
[14] Hartung T. Artificial intelligence in toxicology. *Frontiers in Artificial Intelligence*. 2023;6:1269932. https://doi.org/10.3389/frai.2023.1269932
[15] Richard AM, Judson RS, Houck KA, et al. ToxCast chemical landscape: Paving the road to 21st-century toxicology. *Chemical Research in Toxicology*. 2016;29(8):1225–1251. https://doi.org/10.1021/acs.chemrestox.6b00135
[16] Pinzi L, Rastelli G. Molecular docking: Shifting paradigms in drug discovery. *International Journal of Molecular Sciences*. 2019;20(18):4331. https://doi.org/10.3390/ijms20184331
[17] Hollingsworth SA, Dror RO. Molecular dynamics simulation for all. *Neuron*. 2018;99(6):1129–1143. https://doi.org/10.1016/j.neuron.2018.08.011
[18] OECD. *Guidance on Grouping of Chemicals, Second Edition*. OECD Series on Testing and Assessment No. 194. Paris: OECD Publishing; 2017.
[19] Daina A, Michielin O, Zoete V. SwissADME: A free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Scientific Reports*. 2017;7:42717. https://doi.org/10.1038/srep42717
[20] Hopkins AL. Network pharmacology: The next paradigm in drug discovery. *Nature Chemical Biology*. 2008;4(11):682–690. https://doi.org/10.1038/nchembio.118
[21] Vamathevan J, Clark D, Czodrowski P, et al. Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery*. 2019;18(6):463–477. https://doi.org/10.1038/s41573-019-0024-5
[22] Wu Z, Ramsundar B, Feinberg EN, et al. MoleculeNet: A benchmark for molecular machine learning. *Chemical Science*. 2018;9(2):513–530. https://doi.org/10.1039/C7SC02664A
[23] Mayr A, Klambauer G, Unterthiner T, Hochreiter S. DeepTox: Toxicity prediction using deep learning. *Frontiers in Environmental Science*. 2016;3:80. https://doi.org/10.3389/fenvs.2015.00080
[24] Arrieta AB, Díaz-Rodríguez N, Del Ser J, et al. Explainable Artificial Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI. *Information Fusion*. 2020;58:82–115. https://doi.org/10.1016/j.inffus.2019.12.012
[25] Banerjee P, Eckert AO, Schrey AK, Preissner R. ProTox-3.0: A comprehensive webserver for the prediction of toxicity of small molecules. *Nucleic Acids Research*. 2024;52(W1):W653–W661. https://doi.org/10.1093/nar/gkae436
[26] Krewski D, Acosta D Jr, Andersen M, et al. Toxicity testing in the 21st century: A vision and a strategy. *Journal of Toxicology and Environmental Health, Part B*. 2010;13(2–4):51–138. https://doi.org/10.1080/10937404.2010.483176
[27] Fielden MR, Zacharewski TR. Challenges and limitations of gene expression profiling in mechanistic and predictive toxicology. *Toxicological Sciences*. 2001;60(1):6–10. https://doi.org/10.1093/toxsci/60.1.6

[28] Aebersold R, Mann M. Mass-spectrometric exploration of proteome structure and function. *Nature*. 2016;537(7620):347–355. https://doi.org/10.1038/nature19949
[29] Johnson CH, Ivanisevic J, Siuzdak G. Metabolomics: Beyond biomarkers and towards mechanisms. *Nature Reviews Molecular Cell Biology*. 2016;17(7):451–459. https://doi.org/10.1038/nrm.2016.25
[30] Hasin Y, Seldin M, Lusis A. Multi-omics approaches to disease. *Genome Biology*. 2017;18:83. https://doi.org/10.1186/s13059-017-1215-1
[31] Jagtap AD, Singh S, Karanje P, Dash S, Roselin Jenifer D. Monitoring the changing pest scenario in major grain crops: A longitudinal study. *Journal of Entomological Research*. 2025;49:1134–1140. https://doi.org/10.5958/0974-4576.2025.00199.6
[32] Minh NP. Functional beverage prepared from watermelon (*Citrullus lanatus*) blended green tangerine (*Citrus reticulata*) juice. *Journal of Entomological Research*. 2025;49(3):722–726. https://doi.org/10.5958/0974-4576.2025.00127.6
[33] Nanaware J, Geevarghese JA, Datta D, Patel KG, Hasan F. Predicting pest outbreak patterns in response to global climate change: An overview. *Journal of Entomological Research*. 2025;49(3):804–811. https://doi.org/10.5958/0974-4576.2025.00141.4
[34] Shamli, Bajaj K, Thakur J, Singh A. Comparative evaluation of selected bio-pesticides for insect pest management in tomato. *Journal of Entomological Research*. 2025;49:1176–1179. https://doi.org/10.5958/0974-4576.2025.00207.3
[35] Ghodekar KS, Devi YK, Sonawane VK. Species composition, richness and diversity studies of tephritid fruit flies captured on cucurbit crops from central plain zone of Punjab. *Journal of Entomological Research*. 2025;49(2):449–453. https://doi.org/10.5958/0974-4576.2025.00074.4