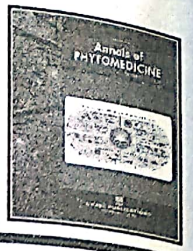
Annals of Phytomedicine 15(1): 290-303, 2026
DOI: http://dx.doi.org/10.54085/ap.2026.15.1.25
Annals of Phytomedicine: An International Journal
http://www.ukaazpublications.com/publications/index.php
Print ISSN : 2278-9839
Online ISSN : 2393-9885



Review Article : Open Access

Therapeutic potential of fruit crop phytochemicals: An *in silico* drug discovery perspective

Sindhuja Balaraman*, Kavino Mathiyazhagan*◆, Nakkeeran Sevugapperumal, Auxcilia Jone*, Saranya Nallusamy*** and Raghu Rajasekaran*****

* *Department of Fruit Science, Horticultural College and Research Institute, Tamil Nadu Agricultural University, Coimbatore-641003, Tamil Nadu, India*

** *Department of Plant Biotechnology, Centre for Plant Molecular Biology and Biotechnology, Tamil Nadu Agricultural University, Coimbatore-641003, Tamil Nadu, India*

*** *Department of Plant Molecular Biology and Bioinformatics, Tamil Nadu Agricultural University, Coimbatore-641003, Tamil Nadu, India*

Article Info

Article history
Received 3 March 2026
Revised 8 April 2026
Accepted 9 April 2026
Published Online 30 June 2026

Keywords
Computational pharmacology
Drug discovery
Fruit phytochemicals
Antioxidant compounds
Molecular docking

Abstract

Fruit crops serve as a vital natural source of biologically active phytochemicals that play an important role in enhancing human health. These naturally occurring substances are widely studied because of their potential in preventing and treating a variety of diseases. With advancement in computational approaches in drug discovery, scientists can now more effectively identify and analyze bioactive molecules derived from fruits. Phytochemicals such as polyphenols, flavonoids, terpenoids, carotenoids, alkaloids and sulfur-based compounds exhibit a broad spectrum of pharmacological properties. Many of these compounds possess antioxidant, anti-inflammatory, antiviral, anticancer and neuroprotective activities. They affect numerous molecular targets and cellular signalling pathways involved in the initiation and progression of diseases. In recent years, advanced *in silico* drug discovery techniques, including molecular docking, molecular dynamics simulations, pharmacokinetic analysis and network pharmacology, have enabled rapid screening and evaluation of natural compounds to evaluate their potential therapeutic benefits. These computational methodsenable researchers to predict ligand-protein interactions, drug-likeness and toxicity profiles before conducting experimental studies, thereby reducing the time and cost associated with traditional drug discovery processes. Several fruit crops, such as *Musa acuminata* (banana), *Vitis vinifera* (grape), *Punica granatum* (pomegranate), *Mangifera indica* (mango) and *Citrus sinensis* (orange) are rich in bioactive compounds including dopamine, resveratrol, ellagitannins, mangiferin and hesperidin. These molecules have demonstrated promising biological activities against key disease targets such as viral enzymes, inflammatory mediators, metabolic regulators, and cancer-related signalling pathways. Although, phytochemical research has been accelerated by various approaches, difficulties persist in ensuring accuracy of predictions and validating experimental findings. Even so, artificial intelligence, metabolomics and advanced molecular modelling are anticipated to contribute to the development of more efficient natural product-based drug discovery from fruit crops in the future.

Scanned with OKEN Scanner