EUROPEAN JOURNAL OF BIOMEDICAL AND PHARMACEUTICAL SCIENCES
http://www.ejbps.com

ISSN 2349-8870
Volume: 9
Issue: 4
427-461
Year: 2022

MOLECULAR DOCKING AND NETWORK PHARMACOLOGY OF BIOACTIVE FROM *AZADIRACHTA INDICA* LEAVES WITH TARGETS RELATED TO BREAST CANCER

Manivannan R.[1], Suresh Kumar G.*, Nivetha B.[3], Dharsan R.[4] and Charan K.[4]

[1]Professor, Department of Pharmaceutical Biotechnology, Excel College of Pharmacy, The Tamilnadu Dr MGR Medical University, Namakkal – 637303.
*Associate Professor, Department of Pharmaceutical Biotechnology, Excel College of Pharmacy, The Tamilnadu Dr MGR Medical University, Namakkal – 637303.
[3]Assistant Professor, Department of Pharmacy Practice, Excel College of Pharmacy, The Tamilnadu Dr MGR Medical University, Namakkal – 637303.
[4]Students, Excel College of Pharmacy, Namakkal – 637303.

***Corresponding Author: Suresh Kumar G.**
Associate Professor, Department of Pharmaceutical Biotechnology, Excel College of Pharmacy, The Tamilnadu Dr MGR Medical University Namakkal – 637303.

Article Received on 16/02/2022 **Article Revised on 07/03/2022** **Article Accepted on 27/03/2022**

ABSTRACT
The neem tree has anti-oxidant, antiseptic, antiviral, antipyretic, anti-inflammatory, cardioprotective, and anti-diabetic properties. Its leaves play an important function in the treatment of breast cancer. We are investigated as active constituents of Nimbin, Gedunin, Nimbolide, Azadirachtin, Mahmoodin, Nimocinol, Meliantriol, Azadirone, Quercetin, Epicatechin, and others in this work. The study's purpose was to create a network pharmacology network of *Azadirachta indica* leaf constituents and breast cancer. Using the SWISS-ADME programme, analyze the pharmacokinetic characteristics of 22 active components of *Azadirachta Indica* leaves. The PharmMapper database was used to find the targets of the active compounds in *Azadirachta Indica* leaves. The potential targets of the disease gene will be added to the GeneCard database. The Venny tool is used to identify the commonly targeted genes of disease and treatments. Using the STRING database, create a protein-protein interaction map. We used Cytoscape to create a visual network to further analyse and comprehend the complicated interactions. BINGO programme is used to examine GO and KEGG enrichment pathways. The PI3K-Akt signalling pathway has been found to play a key regulatory function in tumour therapy. Cell survival, metabolism, angiogenesis, apoptosis, proliferation, and differentiation all rely on the PI3K-Akt signalling pathway. CB- Dock is used to determine the docking molecule's specific binding activity and its targets. The proteins with the greatest interactions revealed that these components have potent anticancer properties. This study provided preliminary confirmation of the pharmacological basis and mechanism of the breast cancer activity of *Azadirachta Indica* leaves, laying the groundwork for future study.

KEYWORDS: Neem, Network pharmacology, Breast cancer, Molecular Docking, *Azadirachta Indica* leaves, CB Dock.

INTRODUCTION
Neem (*Azadirachta indica*) belongs to the Meliaceae family. It is a widespread and popular therapeutic plant in tropical areas across the world. Previously, this plant was known as Melia Azadirachta (L) and Antelaea Azadirachta (L). The term NEEM is derived from the Sanskrit word Nimba, which means "bestower of excellent health." It is also known as Ravisambha - sun ray-like properties in providing health.[1]

The World Health Organization (WHO) cited a study of Neem that showed promising results in the treatment of HIV and cancer. In India, neem is sometimes referred to as a "village pharmacy." The therapeutic virtues of the neem tree can be found in all parts of the tree. Neem is India's fabled medicinal tree that has flourished alongside human settlement throughout the country and has been a vital part of the Indian way of life for ages.[2]

It is indigenous to Myanmar (Burma) and India. However, it may also be found in Bangladesh, Sri Lanka, and African countries. The neem is locally known by several different names, including, English (Indian lilac), Tamil(Vambu, Vaypum), Persian(Azadirakhta), Arabic(Margosa and neeb), Burmese(Tamar), Malaysia(Pokok semambu), Singapore (Kohumba, Nimba), Hindi and Bangla(Neem), Sanskrit and Marathi(Nimba), Malayalam (Aryaveppu, Kaippan, Veppu), Kannada(Bevu), Gujarati(Leemdo), Telugu(Nimtree, Vepu, Vempu, Vepa).[3]

Azadirachta indica has a group of chemical constituents including nimbin, nimbidin, nimbolide, and azadirachtin, and these compounds play an important role in patient care by modulating several genetic pathways and other activities. Several biological and pharmacological actions have been described, including antibacterial, antifungal, and anti- inflammatory properties. Previously, researchers established their role as antioxidant, antiarthritic, antipyretic, hypoglycemic, anti-gastric ulcer, antifungal, antibacterial, and antitumor effects, and a review highlighted the many therapeutic roles of neem.[4]

Breast cancer has become the most prevalent life-threatening malignancy in women and the main cause of cancer death. Over the last two decades, breast cancer research has made incredible advances in our understanding of the disease, resulting in more effective and less damaging treatments. Increased public awareness and greater screening have led to earlier discovery at stages amenable to total surgical resection and curative therapy. As a result, survival rates for breast cancer have significantly improved, especially for younger women. This page describes the numerous forms of breast cancer, their aetiology, clinical symptoms, and the various non-drug (surgery and radiation) and drug therapies (chemotherapy, gene therapy, and so on).[5]

Breast cancer has several causes and risk factors, including family history (hereditary and genetic), obesity, active smoking, early and late childbearing, breastfeeding for less than two weeks, oestrogen exposure, and oral contraceptive pills. The majority of breast cancers are identified by determining oestrogen receptor (ER) positivity, as cells rely on oestrogen for development and survival. There are various traditional breast cancer diagnosis and treatment procedures available, however, they have limitations in terms of accuracy and treatment.[6]

Breast cancer will be reported in 12% of women in the United States throughout their lives, with over 250 000 new cases reported in the United States in 2017.[7]

In the United States, breast cancer is the most prevalent cause of cancer in women and the second leading cause of cancer mortality in women. Breast cancer refers to malignancies that develop in breast tissue, most usually in the inner lining of milk ducts or the lobules that supply milk to the ducts. Breast cancer accounts for 10.4 percent of all cancer incidences in women worldwide, making it the second most prevalent type of non-skin cancer (after lung cancer) and the fifth leading cause of cancer death. Breast cancer claimed the lives of 519,000 people globally in 2004. (7 percent of cancer deaths; almost 1 percent of all deaths). Breast cancer is approximately 100 times more common in women than in men, but males have inferior results due to delayed diagnosis. Cancer cells have DNA and RNA that are comparable (but not identical) to cells from the organism from whence they came. This is why they are not always identified by the immune system, especially if it is compromised.[8]

Network pharmacology is a new drug discovery approach developed by Hopkins in 2007 that combines systematic medicine with information science. It highlights the concept of "network target, multicomponent treatments," moving the paradigm away from the concept of one gene, one target, and one disease. Network pharmacology is a strong tool for studying the synergistic impacts and underlying mechanisms of traditional medicine.[9]

ADME is a pharmacokinetic abbreviation that stands for absorption, distribution, metabolism, and excretion, and it is crucial in drug discovery. Caco-2 cell model (Caco-2), a human clone of colorectal cancer cells, is utilised to predict intestinal absorption of the component. Human Intestinal Absorption (HIA) is significant in identifying possible therapeutic candidates since it refers to the sum of bioavailability and absorption as determined by the excretion ratio or cumulative excretion in urine, bile, and faeces. It is used to assess drug absorption capacity in humans. Plasma Protein Binding (PPB) influences drug to function, distribution, and efficacy, and PPB rate is used to predict drug distribution in humans.[9]

Molecular docking is a basic tool in structural molecular biology and computer-aided drug creation. The purpose of ligand-protein docking is to predict the dominant binding mode(s) of a ligand with a known three-dimensional structure of a protein. Docking may be used to perform virtual screening on vast libraries of compounds, rate the results, and provide structural theories for how the ligands inhibit the target, which is extremely useful in lead optimization.[10]

In this study using network pharmacology, the active ingredient of *Azadirachta indica* leaves and the probable mechanism underlying its anti-breast cancer action were investigated. Numerous databases were prepared to identify *Azadirachta indica* leaves target locations, and GO biological process analysis and KEGG pathway enrichment analysis were performed to study the possible processes involved in *Azadirachta indica* leaves anti-breast cancer action. Molecular docking of important targets was employed to validate the network pharmacology of chosen active components.

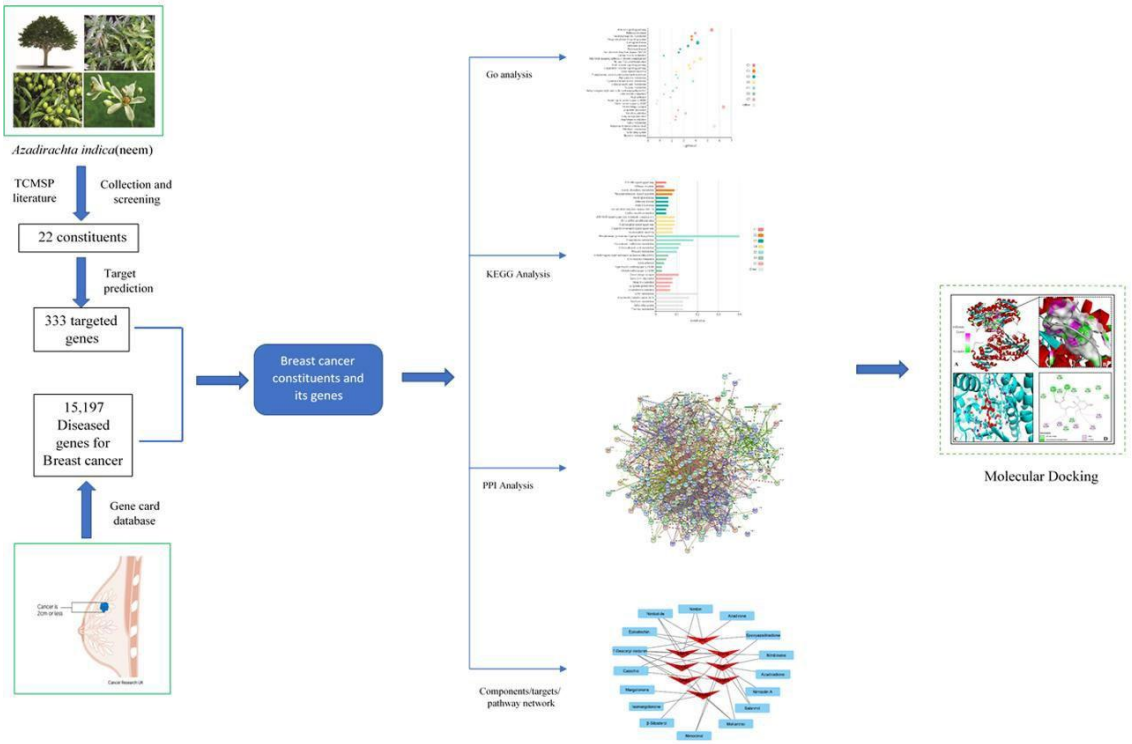


Figure 1: Flow chart of the network pharmacology based study. Go Gene Ontology, KEGG Kyoto encyclopedia of genes and genomes, PPI protein–protein interaction.

MATERIALS AND METHODS

A. Materials

PubChem, PharmMapper, STRING, Swiss ADME, UniProt, GeneCards, Autodock vina, Venny 2.1.0, SystemsDock, Swiss Target Prediction, and CB-Dock were among the databases investigated in this work. Bingo, David Database, Open Babel, Swiss Dock, Drug Discovery Studio, Cytoscape 3.7.1 (Cytoscape) were among the software programmes used.

Plant Profile

Taxonomical Classification

Order	Rutales
Suborder	Rutinae
Family	Meliaceae
Subfamily	Melioideae
Genus	Azadirachta
Specie	Indica
Latin	*Azadirachta indica*
Class	Magnoliopsida
Kingdom	Plantae

Origin and botanical distribution

Neem can be seen on the plains and up to 1850 metres in elevation. In its native region, neem is grown from sea level to 1500 metres above sea level. Neem is tolerant of most soil types, including dry, stony, shallow soils, lateritic crusts, severely leached sands, and clays. Because of its extensive and deep root system, the tenacious Neem can grow and thrive even in marginal and leached soils. The drought resistance of the Neem tree is widely documented. It flourishes in sub-arid to sub-humid climates with annual rainfall ranging from 400 to 1200 mm. It can grow in locations with less than 400 mm of yearly rainfall, however, it is largely dependent on groundwater levels in these areas. Neem may be grown in many soil types, but it likes deep, sandy, well-drained soils (pH 6.2-7.0). It is a tropical/subtropical tree that thrives in annual temperatures ranging from 21 to 32 degrees Celsius. It can tolerate temperatures ranging from hot to extremely hot. Temperatures below 4°C are insufficient (leaf shedding and death may ensue).

Chemical constituents

It demonstrates a therapeutic role in health management because of its rich sources of numerous types of components. Azadirachtin is the most active ingredient, followed by nimbolinin, nimbin, nimbidin, nimbidol, sodium nimbinate, gedunin, salannin, and quercetin. The leaves contain nimbin, nimbanene, 6-desacetylnimbinene, nimbandiol, nimbolide, ascorbic acid, n-hexacosanol, and amino acid, 7-deacetyl-7-benzoylgedunin, 17- hydroxyazadiradione, and nimbiol. Quercetin and ß-sitosterol, polyphenolic flavonoids isolated from neem fresh leaves and known to have antibacterial and antifungal activities, and seeds include important compounds such as gedunin and azadirachtin.

Uses

It has been specified that it is an antibacterial, anthelmintic, antiviral, anticancer, and, most critically, immunomodulatory agent.

B. METHODS

Collection of Active Constituents and Chemical Structures

Screening of active chemicals found in *Azadirachta Indica* leaves utilising literature research; the 2D or 3D structure of the targeting compound was located in the PubChem database (https://pubchem.ncbi.nlm.nih.gov/) however, some of the compounds should not be included in the database.[11]

PubChem is a free and open database that offers valuable information resources including drug discovery and chemical biology research. To acquire the chemical formula and the Canonical Smiles of active chemicals, we typed the compound's term into the search box.[12]

Evaluation of Pharmacokinetics by SWISSADME

This site (http://www.swissadme.ch/) assists in the determination of physicochemical parameters as well as the estimation of ADME parameters, pharmacokinetic features, drug properties, and drug chemistry compatibility of one or more small molecules. We were able to compute the pharmacokinetic characteristics and drug-like nature of the target molecules using this platform. This database includes five rule-based filters for determining how drug-like a chemical is. All of these filters, which include Lipinski, Ghose, Veber, Egan, and Muegge, are from big pharmaceutical corporations looking to improve the quality of their medication research.[13] As a result, compounds that met at least four criteria were designated as active ingredients and used in the following phases.

Screening of Potential targets and target gene of Breast cancer

The Pharm Mapper (http://www.lilab-ecust.cn/pharmmapper/) online database is a web server that employs reversed pharmacophore matching to find potential drug targets by comparing the query molecule to an in-house pharmacophore model database.[14]

To search and pick a 3D structure of active constituents and provide a mail id to obtain job results through email, identify a specific target prediction. The PharmMapper database was used to retrieve the targets of *Azadirachta Indica* leaves active ingredients, and targets with Z-score 1 were tested as prospective *Azadirachta Indica* leaves active ingredient targets.[15] Using the term "Breast cancer" in the human gene database GeneCards, the cancer target genes with the highest interaction with breast cancer were picked, and the first 500 genes (in descending order of correlation score) were recognized as disease genes.[16]

Acquisition of Intersection Target and Topological analysis of target protein

The *Azadirachta indica* leaves constituent targets and the breast cancer-related targets were uploaded to Venny 2.1.0 (https://bioinfogp.cnb.csic.es/tools/venny/) for the intersection to acquire the possible targets of *Azadirachta indica* leaves for the treatment of breast cancer.

The STRING database (https://string-db.org/) is a web-based resource for evaluating protein- protein interaction (PPI). Computational predictions can be used to complement the existing understanding of protein-protein interactions.[17] [18] [19]

Construction of Network

The species for building a protein interaction network was set to Homo sapiens, and the minimum interaction score was 0.4. The data was saved as a "TSV" file and then imported into Cytoscape 3.6.0 for visual analysis. Set the node's size, colour, and edge thickness based on the degree value and combination score. We used Cytoscape to create a visual network to further analyse and comprehend the complicated interactions between *Azadirachta indica* leaves and breast targets and pathways. Besides, four topological attributes of the hub network were determined, including "Degree" and "Betweenness Centrality," to screen the prospective targets of topological importance.[20]

GO & KEGG pathway enrichment analysis

GO is a free and open public resource that provides a standardised vocabulary for defining the functional features of gene products from all species. It consists of three ontologies: biological process (BP), cellular component (CC), and molecular functional (MF).[21] KEGG is a highly efficient network structure that has acted as a comprehensive location for describing metabolic pathways, gene signalling networks, and the practical use of genomic information.[22]

A BINGO plugin in Cytoscape, which is used to depict nonrepetitive biological concepts as functionally grouped networks, was utilised to perform GO and KEGG pathway enrichment analysis on the hub genes in the core network. It is worth mentioning that the threshold in both the GO and KEGG functional categories was set to less than or equal to 0.01.

Compound-Target Molecular Docking

SwissDock is a molecular docking website, analyses ligand selectivity and action using docking simulation and molecular route mapping before evaluating the potential of protein- ligand interaction based on its complete features. Because the stronger the affinity with which the protein and small molecules attach, the more energy is released and the lower the G value, the docking model with the lowest G value is chosen.[23]

For the docking simulation, CB- Dock (http://cao.labshare.cn/cb-dock/), a new blind docking approach based on cavity detection, was employed. It can automatically locate binding sites in a given protein, calculate the centre and size, adjust the docking box size based on the query ligands, and then execute molecular docking with AutoDock Vina. The crystal structures of these targets were collected from the protein data bank

(http://www.rcsb.org). In addition, the chemical's 3D structure was retrieved from the PubChem compound database (https://pubchem.ncbi.nlm.nih.gov/).[24][25]

RESULTS

Collection of Active Ingredients and Their Chemical Structures

The PubChem database was searched for all compounds' 2D or 3D structures, and sdf files were saved. PubChem scanned the database for the compounds' structures and obtained their chemical formulae and accession numbers (PubChem CID). Table 1 provides the information about the 22 active constituents of *Azadirachta indica* leaves. (Supplementary File 1)

Identification of Pharmacokinetic Properties

We used the online website SwissADME to do an in-depth analysis of the ADME-related features of the 22 bioactive substances. SwissADME prediction found that all of the bioactive compounds met Lipinski's rule of five, and other chemical and pharmacological parameters such as topological polar surface area (TPSA) and solubility (LogS) were also assessed (Table 2). These findings imply that these chemicals have high permeability across cell membranes.(Supplementary File 2)

Screening of Targets

The PharmMapper database was used to obtain the targets of *Azadirachta indica* leaves active components, and targets with a Z-score of >1 were regarded prospective targets of *Azadirachta indica* leaves active constituents. "Fit Score" and "z'-score" are scores generated by the metric's Fit score, which is a pre-calculated library score matrix, and a large positive z'score signals the target-to-query combination, according to the database website. There are 1141 target genes in the database. After eliminating duplicate genes, there were 257 targeted genes left. (Supplementary File 3)

Prediction of Common Genes

A total of 15,197 genes finding from the Genecards database were related with breast cancer using the keyword "Breast Cancer," and the genes associated with the chemicals were compared to the breast cancer genes in the Venny 2.1.0 database, creating a gene interaction chart. (See Fig.2) A total of 125 breast cancer genes, as well as the target genes of *Azadirachta Indica* leaves components against breast cancer, were identified. (Supplementary File 4)

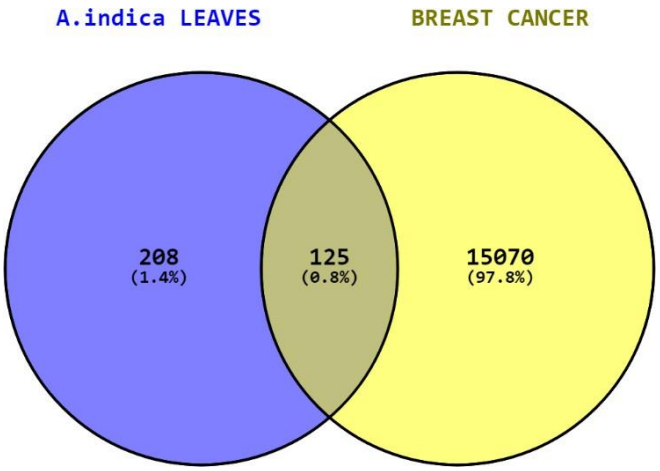


Figure 2: Identification of common genes from Venny 2.1.0 database.

Network Construction

The 125 breast cancer targets identified as component targets of *Azadirachta Indica* leaves were integrated into the STRING database to form a protein interaction network. The target protein network was topologically analysed using Cytoscape. The topological analysis findings are provided in Tab. 5. The colour depth and size of the nodes show the level of interaction between the gene and other genes. The interaction network included 145 nodes in total. The average node degree was 13.4, with 971 edges connected with the target protein and a p-value (PPI enrichment p-value) of 1.0e—16. Target genes with degrees more than or equal to 70 in the *Azadirachta Indica* leaves component and breast cancer cross-linking network topology analysis were consecutively inserted into Cytoscape to acquire the protein type corresponding to the target. The results revealed that these proteins belonged to the protein kinase superfamily, peptidase C14A, nuclear hormone receptor, cyclin, Rho, annexin, MDM2/MDM4, CMGC Ser/Thr protein kinase, CAMK Ser/Thr protein kinase, heme oxygenase, Tyr protein kinase, AGC Ser/Thr protein kinase, NOS, heat shock protein 70, type. (Supplementary File 5)

Cytoscape network interaction analysis

Regarding medications and diseases, there is a genetic relationship. This is typical of multi- component and multi-target network pharmacology studies. An "*Azadirachta Indica* leaves - compound class-active ingredient-gene" interaction network was discovered using Cytoscape network visualisation analysis. Table 6

shows the compound and target information for nodes with more than 20 nodes, where the Average Shortest Path Length is the average shortest path, Closeness Centrality is the centre proximity, and Radiality is the radial degree.

As shown in Fig. 3 and Table 6, the compounds found in *Azadirachta Indica* leaves that interacted strongly with breast cancer were 7-Deacetyl dedunin, -Sitosterol, Gedunin, Nimbin, Nimbolide, Nimocinol, Meliantriol, Nimbolin A, Margolonone, Isomargolonone, Catechin, Epicatechin, Azadirone, Azadiradione. (Supplementary File 6,7)

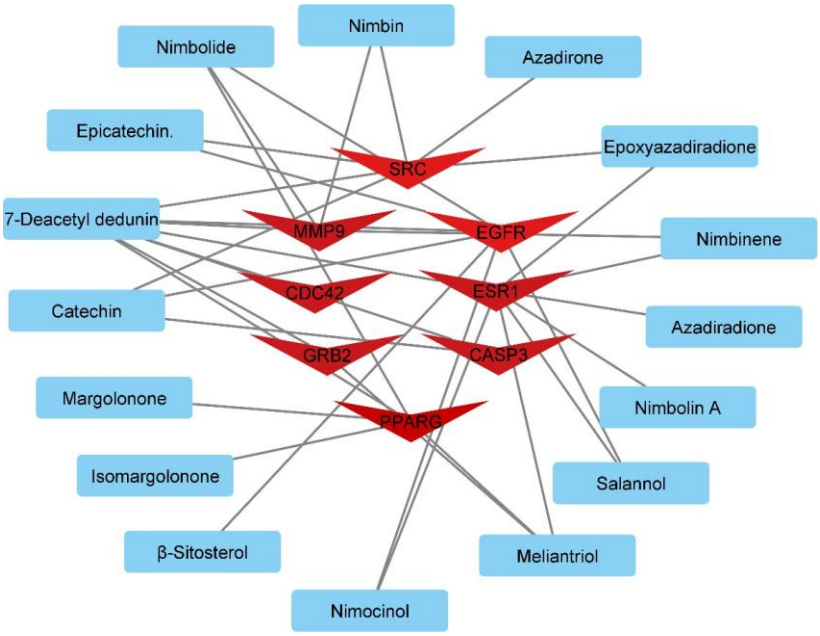


Figure 3: Interaction network of Target and Genetic information of Compounds (Degree >20).

GO and KEGG enrichment analysis

BINGO analysis identified 853 GO biological processes with 2253 interactions between them; 269 molecular functions with 311 molecular interactions; and 38 GO Cellular processes with 50 interactions with cellular components. Tab.8 displays the top ten enriched biological processes. The PI3K-Akt signalling pathway, for example, has been found to play a key regulatory function in tumour therapy. Cell survival, metabolism, angiogenesis, apoptosis, proliferation, and differentiation all rely on the PI3K-Akt signalling pathway. The substrate is utilised to govern essential cellular processes, and several targets are implicated in this route, including AKT, which plays an important role in its regulation. (Supplementary File 8,9,10)

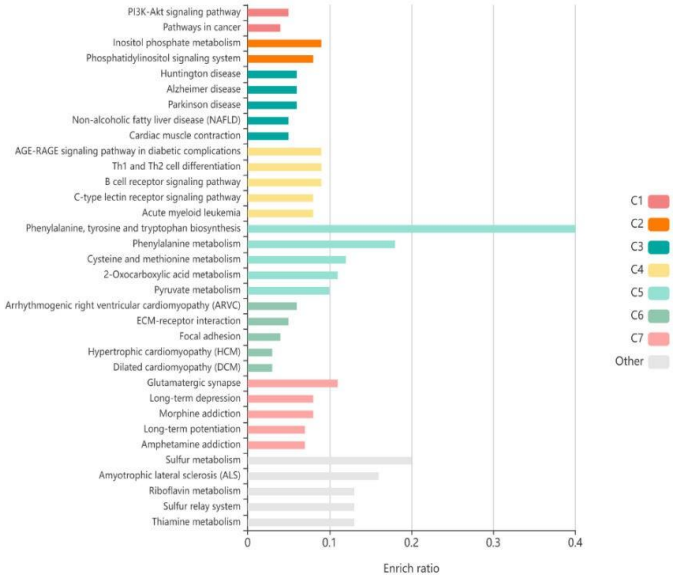


Figure 4: GO and KEGG analysis of '*Azadirachta Indica* leaves-breast cancer' interaction gene.

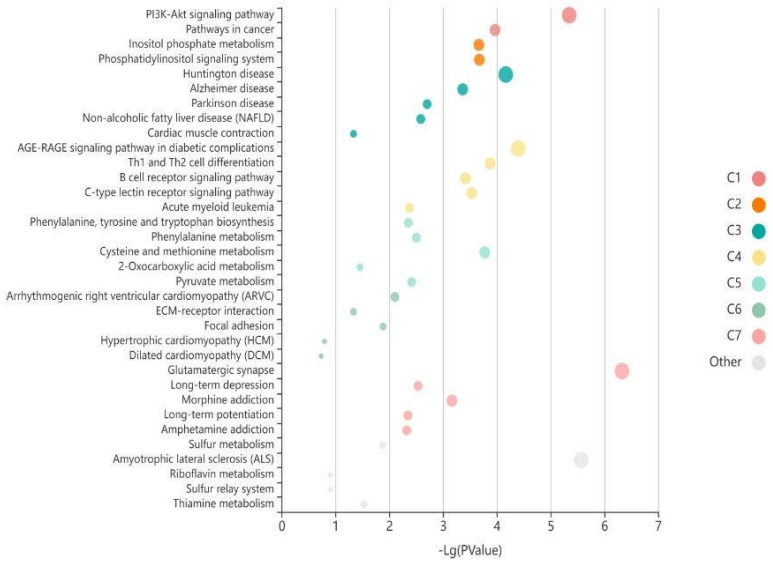


Figure 5: GO and KEGG analysis of '*Azadirachta indica* leaves – breast cancer' interactive gene with P-values.

Molecular Docking

The previous drug-disease interaction gene network topological study revealed that the eight genes with the strongest connection were SRC, MMP9, PPARG, EGFR, ESR1, GRB2, CASP3, and CDC42, which are effective in the "*Azadirachta Indica* leaves –breast cancer – constituent category" network. The Cytoscape interaction network of component-genes revealed that the 17 compounds with strong interactions between *Azadirachta Indica* leaves constituents and breast cancer genes were Gedunin, Nimbin, Nimbolide, Nimocinol, Meliantriol, Nimbolin A, Margolonone, Isomargolonone, Catechin, Epicatechin, Azadirone, Azadiradione, Epoxyazadiradione, 7-Deacetyl dedunine. The 17 chemicals and 8 target proteins were molecularly docked utilising the CB-Dock website's online molecular docking. The docking score in the database ranged from 0 to 10. The docking score indicates the docking effect and binding activity between the docking molecule and the target. A docking score greater than 4.25 shows that a ligand has specific binding activity with a receptor; a score greater than 5.0 implies improved binding activity; and a score greater than 7.0 indicates robust binding activity. The eight genes' PDB IDs were molecularly docked with the seventeen chemicals. All chemicals and proteins had docking scores more than 4.25, indicating the presence of binding activity. Table 11 displays the molecular docking results. The results of molecular docking reveal that the essential bioactive components have great binding to the core targets for breast cancer treatment. (Supplementary File 11)

DISCUSSION

Natural product research has received increased attention in recent years. The network pharmacology approach fosters an understanding of the complex interactions between drugs and their targets, as well as potential mechanisms of action. Similarly, the complexity of developing drugs for *Azadirachta indica* natural sources introduces methodological issues. *Azadirachta indica* leaves are medicinal herbs with various pharmacological effects and a wide range of research and development significance. It also has certain antitumor effects.

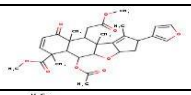
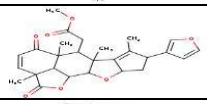
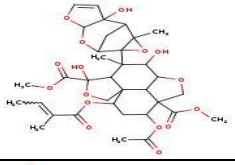
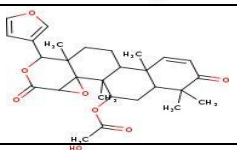
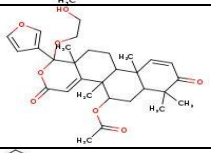
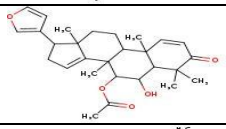
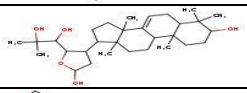
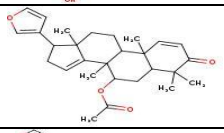
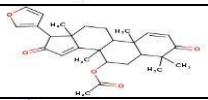
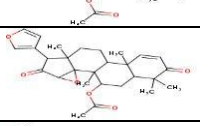
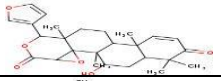
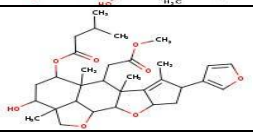
From the research point of view, examination of the potential intersection of *Azadirachta indica* leaves potential target and breast cancer genes revealed 125 common genes, and the interaction between SRC, EGFR, CASP3, ESR1, and CCND1and PPAR was the strongest. Using the 22 compounds in *Azadirachta indica* leaves and the 125 genes, we constructed an '*Azadirachta indica* leaves -constituent category active constituent-gene" network, and our results showed that the compounds 7-Deacetyl dedunin, β-Sitosterol, Gedunin, Nimbin, Mahmoodin, Salannol, Epoxyazadiradione, Nimbolin A, Meliantriol, Azadirone, Nimocinol, Nimbolide, Catechin, Nimbinene, and Epicatechin showed the strongest effect against breast cancer. The proteins with the strongest interaction were SRC, MMP9, PPARG, EGFR, MMP9, ESR1, EGFR, GRB2, CASP3, and CDC42 indicating that these genes interacted with most constituents of neem leaves, showing that these constituents have high antitumor activities.

GO annotation is an important means to examine the function of gene products Through GO analysis, in biological processes, enrichment information includes regulation of cell proliferation, positive regulation of cell proliferation and positive regulation of the cellular process, etc.; in terms of cellular components, enrichment Information includes intracellular part, membrane raft, cytosol, intracellular axon, etc.; in terms of molecular function, it is mainly reflected in protein tyrosine kinase activity, protein kinase activity, kinase activity, and retinoic acid receptor activity.

KEGG enrichment analysis provides information on integrated metabolic pathways including metabolism, membrane trafficking, signal processing, and cell cycle. From the molecular docking analysis, the *Azadirachta*

indica leaves constituents have been reported to exert inhibitory effects against BC. Gedunin's proapoptotic effects were confirmed by morphological changes associated with apoptosis, DNA fragmentation, and increased caspase 3/7 activities. By targeting the PI3K/Akt pathway, oxyazadiradione inhibits breast tumor growth via mitochondrial depolarization and caspase-dependent apoptosis. Azadirone, a Limonoid Tetranortriterpene, activates death receptors and sensitises human cancer cells to Tumor Necrosis Factor-related Apoptosis-inducing Ligand (TRAIL) via a p53-independent mechanism. Reactive Oxygen Species Mediate (-)-Epicatechin-Induced Apoptosis in Human Breast Cancer Cells.

Table 1: Molecular information of *Azadirachta indica* leaves constituents. The first column is the compound name, the second column is the molecular formula. The molecular structure, the PubChem ID for compound retrieved from the database, and the Pharmmapper JOB ID (the search number of targets in the Pharmmapper database) were listed from third to five.

S.No	Compound Name	Molecular Formula	Structure	Pubchem Id	PharmMapper Job Id
1	Nimbin	C30H36O9		108058	220128045922
2	Nimbolide	C27H30O7		12313376	220128050906
3	Azadirachtin	C35H44O16		5281303	220128051254
4	Gedunin	C28H34O7		12004512	220128051512
5	Mahmoodin	C30H38O8		126566	220128051939
6	Nimocinol	C28H36O5		178770	220302152813
7	Meliantriol	C30H50O5		46173826	220128052623
8	Azadirone	C28H36O4		10906239	220128052900
9	Azadiradione/ nimolicin	C28H34O5		12308714	220128053247
10	Epoxyazadiradione	C28H34O6		49863985	220128053950
11	7-Deacetyl gedunin	C26H32O6		1885	220128055239
12	Salannol	C32H44O8		157144	220128060157

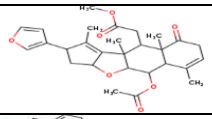
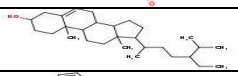
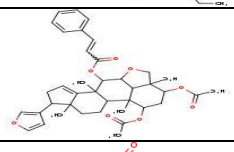
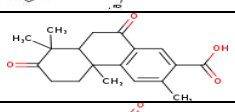
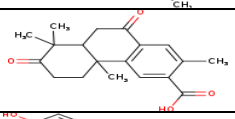
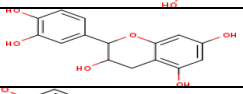
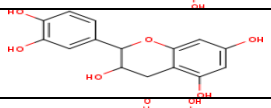
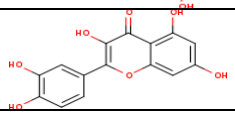
13	Nimbinene	C28H34O7		44715635	220128055432
14	β-Sitosterol	C29H50O		222284	220128061254
15	Nimbolin A	C39H46O8		6443004	220128061531
16	Margolonone	C19H22O4		189726	220128061812
17	Isomargolonone	C19H22O4		189727	220128062033
20	Catechin	C15H14O6		9064	220128062638
21	Epicatechin	C15H14O6		72276	220128062840
22	Quercetin	C15H10O7		5280343	220128063156

Table 2: Phytochemical Properties of *Azadirachta Indica* Leaves.

Compounds	Lipinski's Violations				Lipinski's Violation s	Bioavailability Score
	MW	HB A	HB D	Mlog P		
	<500	<10	≤5	≤4.15	≤1	>1
Nimbin	540.60	9	0	2.04	1	0.55
Nimbolide	466.52	7	0	2.28	0	0.55
Azadirachtin	720.71	16	3	-0.47	2	0.17
Gedunin	482.57	7	0	2.56	0	0.55
Mahmoodin	526.62	8	1	2.75	1	0.55
Nimocinol	452.58	5	1	3.36	0	0.55
Meliantriol	490.72	5	4	3.84	0	0.55
Azadirone	436.58	4	0	4.19	1	0.55
Azadiradione/ nimolicin	450.57	5	0	3.28	0	0.55
Epoxyazadiradione	466.57	6	0	2.54	0	0.55
7-Deacetyl dedunin	440.53	6	1	2.23	0	0.55
Salannol	556.69	8	1	2.62	1	0.55
Nimbinene	482.57	7	0	2.48	0	0.55
β-Sitosterol	414.71	1	1	6.73	1	0.55
Nimbolin A	642.78	8	0	4.3	2	0.17
Margolonone	314.38	4	1	2.59	0	0.85
Isomargolonone	314.38	4	1	2.59	0	0.85
Catechin	290.27	6	5	0.98	0	0.55
Epicatechin	290.27	6	5	0.98	0	0.55
Quercetin	302.24	7	5	-0.56	0	0.55

Table 3: Bioactive Compounds *of Azadirachta indica* leaves and its target genes obtained from PharmMapper database.

Compound	Target	Genes
7-deacetylgedunin	Vitamin D-binding protein	GC
7-deacetylgedunin	Progesterone receptor	PGR
7-deacetylgedunin	Collagenase 3	MMP13
7-deacetylgedunin	Mineralocorticoid receptor	MCR
7-deacetylgedunin	3-phosphoinositide-dependent protein kinase 1	PDPK1

7-deacetylgedunin	Estradiol 17-beta-dehydrogenase 1	HSD17B1
7-deacetylgedunin	Nuclear receptor ROR-alpha	RORA
7-deacetylgedunin	Mitogen-activated protein kinase 14	MAPK14
7-deacetylgedunin	Serine/threonine-protein kinase Chk1	CHEK1
7-deacetylgedunin	Complement factor D	CFD
7-deacetylgedunin	Serine/threonine-protein phosphatase 5	PPP5C
7-deacetylgedunin	TGF-beta receptor type-1	TGFBR1
7-deacetylgedunin	Epidermal growth factor receptor	EGFR
7-deacetylgedunin	Alpha-tocopherol transfer protein	TTPA
7-deacetylgedunin	Bile salt sulfotransferase	SULT2A1
7-deacetylgedunin	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
7-deacetylgedunin	Hepatocyte growth factor receptor	MET
7-deacetylgedunin	Heat shock protein HSP 90-alpha	HSP90AA1
7-deacetylgedunin	SEC14-like protein 2	SEC14L2
7-deacetylgedunin	cAMP-specific 3,5-cyclic phosphodiesterase 4B	PDE4B
7-deacetylgedunin	Sex hormone-binding globulin	SHBG
7-deacetylgedunin	Cell division protein kinase 2	CDK2
7-deacetylgedunin	Catenin alpha-1	CTNNA1
7-deacetylgedunin	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
7-deacetylgedunin	Sulfotransferase family cytosolic 2B member 1	SULT2B1
7-deacetylgedunin	Bile acid receptor	NR1H4
7-deacetylgedunin	Aldo-keto reductase family 1 member C1	AKR1C1
7-deacetylgedunin	cAMP-specific 3,5-cyclic phosphodiesterase 4D	PDE4D
7-deacetylgedunin	Glycogen synthase kinase-3 beta	GSK3B
7-deacetylgedunin	Sorbitol dehydrogenase	SORD
7-deacetylgedunin	Cell division protein kinase 6	CDK6
7-deacetylgedunin	Cyclin-A2	CCNA2
7-deacetylgedunin	Adenosine kinase	ADK
7-deacetylgedunin	Coagulation factor X	F10
7-deacetylgedunin	Cytochrome P450 2C9	CYP2C9
7-deacetylgedunin	Placenta growth factor	PGF
7-deacetylgedunin	Alcohol dehydrogenase class-3	ADH5
7-deacetylgedunin	Glutathione-requiring prostaglandin D synthase	HPGDS
7-deacetylgedunin	Trafficking protein particle complex subunit 3	TRAPPC3
7-deacetylgedunin	Fatty acid-binding protein, brain	FABP7
7-deacetylgedunin	Oxysterols receptor LXR-alpha	NR1H3
7-deacetylgedunin	Tyrosine-protein kinase JAK3	JAK3
7-deacetylgedunin	Thyroid hormone receptor beta	THRB
7-deacetylgedunin	Histo-blood group ABO system transferase	ABO
7-deacetylgedunin	Cytochrome P450 2C8	CYP2C8
7-deacetylgedunin	Gastrotropin	FABP6
7-deacetylgedunin	Hepatocyte nuclear factor 4-gamma	HNF4G
7-deacetylgedunin	Fatty acid-binding protein, adipocyte	FABP4
7-deacetylgedunin	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
7-deacetylgedunin	Ferrochelatase, mitochondrial	FECH
7-deacetylgedunin	Macrophage metalloelastase	MMP12
7-deacetylgedunin	Interleukin-2	IL2
7-deacetylgedunin	Protein-glutamine gamma-glutamyltransferase E	TGM3
7-deacetylgedunin	Retinoic acid receptor gamma	RARG
7-deacetylgedunin	72 kDa type IV collagenase	MMP2
7-deacetylgedunin	Retinoic acid receptor beta	RARB
7-deacetylgedunin	Proto-oncogene tyrosine-protein kinase ABL1	ABL1
7-deacetylgedunin	S-adenosylmethionine decarboxylase proenzyme	AMD1
7-deacetylgedunin	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
7-deacetylgedunin	Amine oxidase [flavin-containing] A	MAOA
Azadirachtin	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Azadirachtin	Bile salt sulfotransferase	SULT2A1
Azadirachtin	Mitogen-activated protein kinase 14	MAPK14

Azadirachtin	Liver carboxylesterase 1	EST1
Azadirachtin	Serum albumin	ALB
Azadirachtin	cAMP-specific 3,5-cyclic phosphodiesterase 4D	PDE4D
Azadirachtin	Coagulation factor X	F10
Azadirachtin	Catenin alpha-1	CTNNA1
Azadirachtin	Aldo-keto reductase family 1 member C3	AKR1C3
Azadirachtin	Oxysterols receptor LXR-alpha	NR1H3
Azadirachtin	Aldo-keto reductase family 1 member C1	AKR1C1
Azadirachtin	Hepatocyte growth factor receptor	MET
Azadirachtin	cAMP-specific 3,5-cyclic phosphodiesterase 4B	PDE4B
Azadirachtin	E3 ubiquitin-protein ligase Mdm2	MDM2
Azadirachtin	Estrogen-related receptor gamma	ESRRG
Azadirachtin	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Azadirachtin	Proto-oncogene tyrosine-protein kinase Src	SRC
Azadirachtin	Nuclear receptor subfamily 1 group I member 3	NR1I3
Azadirachtin	[Pyruvate dehydrogenase [lipoamide]] kinase isozyme 2, mitochondrial	PDK2
Azadirachtin	Histone deacetylase 8	HDAC8
Azadirachtin	Cyclin-A2	CCNA2
Azadirachtin	Superoxide dismutase [Mn], mitochondrial	SOD2
Azadirachtin	Proto-oncogene tyrosine-protein kinase LCK	LCK
Azadirachtin	Tyrosine-protein kinase JAK3	JAK3
Azadirachtin	Tyrosine-protein kinase ITK/TSK	ITK
Azadirachtin	Integrin alpha-L	ITGAL
Azadirachtin	Cytochrome P450 2C9	CYP2C9
Azadirachtin	NONE	NONE
Azadirachtin	Peroxisome proliferator-activated receptor gamma	PPARG
Azadirachtin	Leukocyte elastase	ELANE
Azadirachtin	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
Azadirachtin	Fatty acid-binding protein, brain	FABP7
Azadirachtin	NAD(P)H dehydrogenase [quinone] 1	NQO1
Azadirachtin	Gastrotropin	FABP6
Azadirachtin	Fatty acid-binding protein, heart	FABP3
Azadirachtin	Glycogen synthase kinase-3 beta	GSK3B
Azadirachtin	Dihydroorotate dehydrogenase, mitochondrial	PYRD
Azadirachtin	cAMP-dependent protein kinase, alpha-catalytic subunit	PRKACA
Azadirachtin	Nuclear receptor subfamily 1 group I member 2	NR1I2
Azadirachtin	Retinoic acid receptor gamma	RARG
Azadirachtin	MAP kinase-activated protein kinase 2	MAPKAPK2
Azadirachtin	Hepatocyte nuclear factor 4-gamma	HNF4G
Azadirachtin	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Azadirachtin	Flavin reductase	BLVRB
Azadirachtin	Thyroid hormone receptor alpha	THRA
Azadirachtin	Cathepsin G	CTSG
Azadirachtin	Glucocorticoid receptor	GCR
Azadirachtin	Proactivator polypeptide	PSAP
Azadirachtin	Tyrosine-protein kinase ZAP-70	ZAP70
Azadirachtin	Methionine aminopeptidase 2	METAP2
Azadirachtin	Histo-blood group ABO system transferase	ABO
Azadirachtin	Neutrophil gelatinase-associated lipocalin	LCN2
Azadirachtin	Bile acid receptor	NR1H4
Azadirachtin	Histamine N-methyltransferase	HNMT
Azadirachtin	Deoxycytidine kinase	DCK
Azadirachtin	Phospholipase A2, membrane associated	PLA2G2A
Azadirachtin	B-Raf proto-oncogene serine/threonine-protein kinase	BRAF1
Azadirachtin	Baculoviral IAP repeat-containing protein 4	XIAP
Azadirachtin	Cathepsin S	CATS
Azadirachtin	ADAM 17	ADAM17
Azadirachtin	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM

Azadirachtin	Phosphatidylinositol 3-kinase regulatory subunit alpha	PIK3R1
Azadirachtin	Glycogen phosphorylase, liver form	PYGL
Azadirachtin	Growth factor receptor-bound protein 2	GRB2
Azadirachtin	Proto-oncogene tyrosine-protein kinase ABL1	ABL1
Azadirachtin	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
Azadirachtin	Interleukin-2	IL2
Azadirachtin	Mast/stem cell growth factor receptor	KIT
Azadirachtin	Bcl-2-like protein 1	BCL2L1
Azadirachtin	Peptidyl-prolyl cis-trans isomerase FKBP1B	FKBP1B
Azadirachtin	3-hydroxy-3-methylglutaryl-coenzyme A reductase	HMGCR
Azadirachtin	Vitamin D3 receptor	VDR
Azadirachtin	Transforming growth factor beta-2	TGFB2
Azadirachtin	Caspase-1	CASP1
Azadirachtin	FK506-binding protein 3	FKBP3
Azadiradione	Bone morphogenetic protein 2	BMP2
Azadiradione	Serum albumin	ALB
Azadiradione	Integrin alpha-L	ITGAL
Azadiradione	Apolipoprotein A-II	APOA2
Azadiradione	Steryl-sulfatase	STS
Azadiradione	Complement factor B	CFB
Azadiradione	Kinesin-like protein KIF11	KIF11
Azadiradione	Carbonic anhydrase 2	CAH2
Azadiradione	Aldo-keto reductase family 1 member C2	AKR1C2
Azadiradione	Vitamin D-binding protein	GC
Azadiradione	Androgen receptor	AR
Azadiradione	Sex hormone-binding globulin	SHBG
Azadiradione	Annexin A5	ANXA5
Azadiradione	Mitogen-activated protein kinase 14	MAPK14
Azadiradione	Complement factor D	CFD
Azadiradione	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Azadiradione	Calmodulin	CALM
Azadiradione	Histone deacetylase 8	HDAC8
Azadiradione	SEC14-like protein 2	SEC14L2
Azadiradione	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
Azadiradione	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Azadiradione	Cell division protein kinase 2	CDK2
Azadiradione	Alcohol dehydrogenase 1C	ADH1C
Azadiradione	Aldo-keto reductase family 1 member C3	AKR1C3
Azadiradione	Aldo-keto reductase family 1 member C1	AKR1C1
Azadiradione	Alpha-tocopherol transfer protein	TTPA
Azadiradione	Alcohol dehydrogenase class-3	ADH5
Azadiradione	Trafficking protein particle complex subunit 3	TRAPPC3
Azadiradione	Glutathione S-transferase P	GSTP1
Azadiradione	Glycogen synthase kinase-3 beta	GSK3B
Azadiradione	Dipeptidyl peptidase 4	DPP4
Azadiradione	Glutathione S-transferase A1	GSTA1
Azadiradione	Hepatocyte growth factor receptor	MET
Azadiradione	Cytochrome P450 2C8	CYP2C8
Azadiradione	Retinol-binding protein 4	RBP4
Azadiradione	Peroxisome proliferator-activated receptor alpha	PPARA
Azadiradione	Sulfotransferase family cytosolic 2B member 1	SULT2B1
Azadiradione	Nuclear receptor subfamily 1 group I member 3	NR1I3
Azadiradione	Interleukin-2	IL2
Azadiradione	Leukocyte elastase	ELANE
Azadiradione	Fatty acid-binding protein, brain	FABP7
Azadiradione	Gastrotropin	FABP6
Azadiradione	Hepatocyte nuclear factor 4-gamma	HNF4G
Azadiradione	Estrogen sulfotransferase	SULT1E1

Azadiradione	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Azadiradione	Retinoic acid receptor gamma	RARG
Azadiradione	Glucocorticoid receptor	GCR
Azadiradione	Retinoic acid receptor beta	RARB
Azadiradione	Proto-oncogene tyrosine-protein kinase ABL1	ABL1
Azadiradione	Ferrochelatase, mitochondrial	FECH
Azadiradione	Vitamin D3 receptor	VDR
Azadiradione	Angiopoietin-1 receptor	TEK
Azadiradione	Leukotriene A-4 hydrolase	LTA4H
Azadiradione	Retinoic acid receptor RXR-beta	RXRB
Azadiradione	Growth factor receptor-bound protein 2	GRB2
Azadiradione	Eukaryotic translation initiation factor 4E	EIF4E
Azadiradione	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
Azadiradione	Phosphatidylcholine transfer protein	PCTP
Azadiradione	Endothelial protein C receptor	PROCR
Azadirone	Aldo-keto reductase family 1 member C2	AKR1C2
Azadirone	Carbonic anhydrase 2	CAH2
Azadirone	Progesterone receptor	PGR
Azadirone	Vitamin D-binding protein	GC
Azadirone	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Azadirone	ADAM 17	ADAM17
Azadirone	Estrogen-related receptor gamma	ESRRG
Azadirone	Bile salt sulfotransferase	SULT2A1
Azadirone	Proto-oncogene tyrosine-protein kinase Src	SRC
Azadirone	3-phosphoinositide-dependent protein kinase 1	PDPK1
Azadirone	Serine/threonine-protein phosphatase 5	PPP5C
Azadirone	Serine/threonine-protein kinase 6	O14965
Azadirone	Androgen receptor	AR
Azadirone	Complement factor D	CFD
Azadirone	Heat shock cognate 71 kDa protein	HSPA8
Azadirone	Mineralocorticoid receptor	MCR
Azadirone	Ig lambda chain V-II region MGC	P01709
Azadirone	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Azadirone	Cell division protein kinase 2	CDK2
Azadirone	Alcohol dehydrogenase 1C	ADH1C
Azadirone	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
Azadirone	Glutathione S-transferase P	GSTP1
Azadirone	Sulfotransferase family cytosolic 2B member 1	SULT2B1
Azadirone	Alcohol dehydrogenase class-3	ADH5
Azadirone	Placenta growth factor	PGF
Azadirone	Glutathione S-transferase A1	GSTA1
Azadirone	Adenosine kinase	ADK
Azadirone	Hepatocyte growth factor receptor	MET
Azadirone	Trafficking protein particle complex subunit 3	TRAPPC3
Azadirone	Nuclear receptor subfamily 1 group I member 3	NR1I3
Azadirone	Fatty acid-binding protein, brain	FABP7
Azadirone	Gastrotropin	FABP6
Azadirone	Retinol-binding protein 4	RBP4
Azadirone	Hepatocyte nuclear factor 4-gamma	HNF4G
Azadirone	Insulin-like growth factor IA	IGF1
Azadirone	cGMP-specific 3,5-cyclic phosphodiesterase	PDE5A
Azadirone	Nuclear receptor subfamily 1 group I member 2	NR1I2
Azadirone	Ferrochelatase, mitochondrial	FECH
Azadirone	Basic fibroblast growth factor receptor 1	FGFR1
Azadirone	Glucocorticoid receptor	GCR
Azadirone	Interleukin-2	IL2
Azadirone	Retinoic acid receptor RXR-alpha	RXRA
Azadirone	Protein-glutamine gamma-glutamyltransferase E	TGM3

Azadirone	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Azadirone	Retinoic acid receptor gamma	RARG
Azadirone	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM
Azadirone	Cellular retinoic acid-binding protein 2	CRABP2
Azadirone	Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1
Azadirone	Retinoic acid receptor beta	RARB
Azadirone	Retinoic acid receptor RXR-beta	RXRB
Azadirone	S-adenosylmethionine decarboxylase proenzyme	AMD1
Azadirone	Phosphatidylcholine transfer protein	PCTP
Azadirone	Branched-chain-amino-acid aminotransferase, mitochondrial	BCAT2
Azadirone	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
Azadirone	Endothelial protein C receptor	PROCR
β-SitoSterol	Vitamin D-binding protein	GC
β-SitoSterol	Mineralocorticoid receptor	MCR
β-SitoSterol	Collagenase 3	MMP13
β-SitoSterol	ADAM 17	ADAM17
β-SitoSterol	Nuclear receptor ROR-alpha	RORA
β-SitoSterol	Estrogen-related receptor gamma	ESRRG
β-SitoSterol	SEC14-like protein 2	SEC14L2
β-SitoSterol	Calmodulin	CALM
β-SitoSterol	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
β-SitoSterol	Vascular endothelial growth factor receptor 2	KDR
β-SitoSterol	cAMP-dependent protein kinase catalytic subunit alpha	PRKACA
β-SitoSterol	Methionine aminopeptidase 2	METAP2
β-SitoSterol	Sex hormone-binding globulin	SHBG
β-SitoSterol	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
β-SitoSterol	Dipeptidyl peptidase 4	DPP4
β-SitoSterol	Prothrombin	THRB
β-SitoSterol	Wiskott-Aldrich syndrome protein	WAS
β-SitoSterol	Trafficking protein particle complex subunit 3	TRAPPC3
β-SitoSterol	Bile acid receptor	NR1H4
β-SitoSterol	Histone deacetylase 8	HDAC8
β-SitoSterol	Aldo-keto reductase family 1 member C1	AKR1C1
β-SitoSterol	Glutathione-requiring prostaglandin D synthase	HPGDS
β-SitoSterol	E3 ubiquitin-protein ligase Mdm2	MDM2
β-SitoSterol	Alcohol dehydrogenase class-3	ADH5
β-SitoSterol	Nuclear receptor subfamily 1 group I member 3	NR1I3
β-SitoSterol	Cellular retinoic acid-binding protein 2	CRABP2
β-SitoSterol	Glutathione S-transferase A1	GSTA1
β-SitoSterol	Oxysterols receptor LXR-alpha	NR1H3
β-SitoSterol	Adenosine kinase	ADK
β-SitoSterol	Hepatocyte nuclear factor 4-gamma	HNF4G
β-SitoSterol	Flavin reductase	BLVRB
β-SitoSterol	Mitogen-activated protein kinase 10	MAPK10
β-SitoSterol	Oxysterols receptor LXR-beta	NR1H2
β-SitoSterol	Tyrosine-protein kinase SYK	SYK
β-SitoSterol	Cytochrome P450 2C8	CYP2C8
β-SitoSterol	Sulfotransferase family cytosolic 2B member 1	SULT2B1
β-SitoSterol	Receptor tyrosine-protein kinase erbB-4	ERBB4
β-SitoSterol	Retinol-binding protein 4	RBP4
β-SitoSterol	Insulin-like growth factor IA	IGF1
β-SitoSterol	Fatty acid-binding protein, brain	FABP7
β-SitoSterol	Lanosterol synthase	LSS
β-SitoSterol	Poly [ADP-ribose] polymerase 1	PARP1
β-SitoSterol	cGMP-specific 3,5-cyclic phosphodiesterase	PDE5A
β-SitoSterol	Thyroid hormone receptor alpha	THRA
β-SitoSterol	Glucocorticoid receptor	GCR
β-SitoSterol	72 kDa type IV collagenase	MMP2

β-SitoSterol	Retinoic acid receptor gamma	RARG
β-SitoSterol	Retinoic acid receptor alpha	RARA
β-SitoSterol	Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1
β-SitoSterol	Basic fibroblast growth factor receptor 1	FGFR1
β-SitoSterol	Vitamin D3 receptor	VDR
β-SitoSterol	Proto-oncogene tyrosine-protein kinase ABL1	ABL1
β-SitoSterol	Mast/stem cell growth factor receptor	KIT
β-SitoSterol	Endothelial protein C receptor	PROCR
Catechin	Estrogen-related receptor gamma	ESRRG
Catechin	Glutathione reductase, mitochondrial	GSR
Catechin	Proto-oncogene serine/threonine-protein kinase Pim-1	PIM1
Catechin	Mitogen-activated protein kinase 14	MAPK14
Catechin	Estrogen receptor beta	Esr2
Catechin	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Catechin	Sorbitol dehydrogenase	SORD
Catechin	Collagenase 3	MMP13
Catechin	Ephrin type-B receptor 4	EPHB4
Catechin	Vascular endothelial growth factor receptor 2	KDR
Catechin	Complement factor D	CFD
Catechin	Neutrophil collagenase	MMP8
Catechin	Aldo-keto reductase family 1 member C3	AKR1C3
Catechin	Proto-oncogene tyrosine-protein kinase Src	SRC
Catechin	Kinesin-like protein KIF11	KIF11
Catechin	Mineralocorticoid receptor	MCR
Catechin	Aldo-keto reductase family 1 member C1	AKR1C1
Catechin	Catenin alpha-1	CTNNA1
Catechin	Cell division protein kinase 6	CDK6
Catechin	Coagulation factor X	F10
Catechin	Heat shock protein HSP 90-alpha	HSP90AA1
Catechin	Prothrombin	THRB
Catechin	Carbonyl reductase [NADPH] 1	CBR1
Catechin	Histone deacetylase 8	HDAC8
Catechin	Coagulation factor VII	F7
Catechin	Macrophage metalloelastase	MMP12
Catechin	Tyrosine-protein kinase JAK3	JAK3
Catechin	Proto-oncogene tyrosine-protein kinase LCK	LCK
Catechin	Histo-blood group ABO system transferase	ABO
Catechin	Bile acid receptor	NR1H4
Catechin	Oxysterols receptor LXR-beta	NR1H2
Catechin	B transferase	ABO
Catechin	Cytochrome P450 2C9	CYP2C9
Catechin	Oxysterols receptor LXR-alpha	NR1H3
Catechin	Ras-related protein Rab-11A	RAB11A
Catechin	Glycogen synthase kinase-3 beta	GSK3B
Catechin	Alpha-1-antitrypsin	SERPINA1
Catechin	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
Catechin	T-cell surface glycoprotein CD1a	CD1A
Catechin	Tyrosine-protein kinase ZAP-70	ZAP70
Catechin	Tyrosine-protein kinase JAK2	JAK2
Catechin	Nicotinamide mononucleotide adenylyltransferase 1	NMNAT1
Catechin	Serine/threonine-protein kinase 6	O14965
Catechin	Ferrochelatase, mitochondrial	FECH
Catechin	cAMP-dependent protein kinase, alpha-catalytic subunit	PRKACA
Catechin	Neprilysin	NEP
Catechin	Glucose-6-phosphate isomerase	GPI
Catechin	Thymidine kinase, cytosolic	TK1
Catechin	Dual specificity protein kinase CLK1	CLK1
Catechin	Baculoviral IAP repeat-containing protein 4	XIAP

Catechin	Betaine--homocysteine S-methyltransferase 1	BHMT
Catechin	Glucocorticoid receptor	GCR
Catechin	Proto-oncogene tyrosine-protein kinase ABL1	ABL1
Catechin	Eukaryotic translation initiation factor 4E	EIF4E
Catechin	Vitamin D3 receptor	VDR
Catechin	Glycolipid transfer protein	GLTP
Catechin	Glutathione S-transferase Mu 1	GSTM1
Catechin	Trifunctional purine biosynthetic protein adenosine-3	GART
Catechin	Caspase-3	CASP3
Epicatechin	Estrogen-related receptor gamma	ESRRG
Epicatechin	Glutathione reductase, mitochondrial	GSR
Epicatechin	Proto-oncogene serine/threonine-protein kinase Pim-1	PIM1
Epicatechin	Mitogen-activated protein kinase 14	MAPK14
Epicatechin	Estrogen receptor beta	Esr2
Epicatechin	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Epicatechin	Sorbitol dehydrogenase	SORD
Epicatechin	Collagenase 3	MMP13
Epicatechin	Ephrin type-B receptor 4	EPHB4
Epicatechin	Vascular endothelial growth factor receptor 2	KDR
Epicatechin	Complement factor D	CFD
Epicatechin	Neutrophil collagenase	MMP8
Epicatechin	Aldo-keto reductase family 1 member C3	AKR1C3
Epicatechin	Proto-oncogene tyrosine-protein kinase Src	SRC
Epicatechin	Kinesin-like protein KIF11	KIF11
Epicatechin	Mineralocorticoid receptor	MCR
Epicatechin	Aldo-keto reductase family 1 member C1	AKR1C1
Epicatechin	Catenin alpha-1	CTNNA1
Epicatechin	Cell division protein kinase 6	CDK6
Epicatechin	Coagulation factor X	F10
Epicatechin	Heat shock protein HSP 90-alpha	HSP90AA1
Epicatechin	Prothrombin	THRB
Epicatechin	Carbonyl reductase [NADPH] 1	CBR1
Epicatechin	Histone deacetylase 8	HDAC8
Epicatechin	Coagulation factor VII	F7
Epicatechin	Macrophage metalloelastase	MMP12
Epicatechin	Tyrosine-protein kinase JAK3	JAK3
Epicatechin	Proto-oncogene tyrosine-protein kinase LCK	LCK
Epicatechin	Histo-blood group ABO system transferase	ABO
Epicatechin	Bile acid receptor	NR1H4
Epicatechin	Oxysterols receptor LXR-beta	NR1H2
Epicatechin	B transferase	ABO
Epicatechin	Cytochrome P450 2C9	CYP2C9
Epicatechin	Oxysterols receptor LXR-alpha	NR1H3
Epicatechin	Ras-related protein Rab-11A	RAB11A
Epicatechin	Glycogen synthase kinase-3 beta	GSK3B
Epicatechin	Alpha-1-antitrypsin	SERPINA1
Epicatechin	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
Epicatechin	T-cell surface glycoprotein CD1a	CD1A
Epicatechin	Tyrosine-protein kinase ZAP-70	ZAP70
Epicatechin	Tyrosine-protein kinase JAK2	JAK2
Epicatechin	Nicotinamide mononucleotide adenylyltransferase 1	NMNAT1
Epicatechin	Serine/threonine-protein kinase 6	O14965
Epicatechin	Ferrochelatase, mitochondrial	FECH
Epicatechin	cAMP-dependent protein kinase, alpha-catalytic subunit	PRKACA
Epicatechin	Neprilysin	NEP
Epicatechin	Glucose-6-phosphate isomerase	GPI
Epicatechin	Thymidine kinase, cytosolic	TK1
Epicatechin	Dual specificity protein kinase CLK1	CLK1

Epicatechin	Baculoviral IAP repeat-containing protein 4	XIAP
Epicatechin	Betaine--homocysteine S-methyltransferase 1	BHMT
Epicatechin	Glucocorticoid receptor	GCR
Epicatechin	Proto-oncogene tyrosine-protein kinase ABL1	ABL1
Epicatechin	Eukaryotic translation initiation factor 4E	EIF4E
Epicatechin	Vitamin D3 receptor	VDR
Epicatechin	Glycolipid transfer protein	GLTP
Epicatechin	Glutathione S-transferase Mu 1	GSTM1
Epicatechin	Trifunctional purine biosynthetic protein adenosine-3	GART
Epicatechin	Caspase-3	CASP3
Epoxyazadiradione	Carbonic anhydrase 2	CAH2
Epoxyazadiradione	Bone morphogenetic protein 2	BMP2
Epoxyazadiradione	Peptidyl-prolyl cis-trans isomerase A	PPIA
Epoxyazadiradione	Steryl-sulfatase	STS
Epoxyazadiradione	Ephrin type-B receptor 4	EPHB4
Epoxyazadiradione	Serum albumin	ALB
Epoxyazadiradione	Complement factor B	CFB
Epoxyazadiradione	Liver carboxylesterase 1	EST1
Epoxyazadiradione	Vitamin D-binding protein	GC
Epoxyazadiradione	Mineralocorticoid receptor	MCR
Epoxyazadiradione	Chitotriosidase-1	CHIT1
Epoxyazadiradione	NONE	NONE
Epoxyazadiradione	Collagenase 3	MMP13
Epoxyazadiradione	cAMP-specific 3,5-cyclic phosphodiesterase 4D	PDE4D
Epoxyazadiradione	Amine oxidase [flavin-containing] B	AOFB
Epoxyazadiradione	Proto-oncogene tyrosine-protein kinase Src	SRC
Epoxyazadiradione	Epidermal growth factor receptor	EGFR
Epoxyazadiradione	Glutathione S-transferase P	GSTP1
Epoxyazadiradione	Sorbitol dehydrogenase	SORD
Epoxyazadiradione	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Epoxyazadiradione	Catenin alpha-1	CTNNA1
Epoxyazadiradione	Alcohol dehydrogenase 1C	ADH1C
Epoxyazadiradione	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
Epoxyazadiradione	Aldo-keto reductase family 1 member C1	AKR1C1
Epoxyazadiradione	Dipeptidyl peptidase 4	DPP4
Epoxyazadiradione	Lanosterol synthase	LSS
Epoxyazadiradione	E3 ubiquitin-protein ligase Mdm2	MDM2
Epoxyazadiradione	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Epoxyazadiradione	Neutrophil collagenase	MMP8
Epoxyazadiradione	Urokinase-type plasminogen activator	PLAU
Epoxyazadiradione	Coagulation factor X	F10
Epoxyazadiradione	Cytochrome P450 2C9	CYP2C9
Epoxyazadiradione	Gastrotropin	FABP6
Epoxyazadiradione	Leukocyte elastase	ELANE
Epoxyazadiradione	Hepatocyte growth factor receptor	MET
Epoxyazadiradione	Fatty acid-binding protein, brain	FABP7
Epoxyazadiradione	Estrogen sulfotransferase	SULT1E1
Epoxyazadiradione	Fatty acid-binding protein, heart	FABP3
Epoxyazadiradione	C-1-tetrahydrofolate synthase, cytoplasmic	MTHFD1
Epoxyazadiradione	Basic fibroblast growth factor receptor 1	FGFR1
Epoxyazadiradione	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Epoxyazadiradione	Protein-glutamine gamma-glutamyltransferase E	TGM3
Epoxyazadiradione	Neutrophil gelatinase-associated lipocalin	LCN2
Epoxyazadiradione	Glucocorticoid receptor	GCR
Epoxyazadiradione	Medium-chain specific acyl-CoA dehydrogenase	ACADM
Epoxyazadiradione	ADP-ribosyl cyclase 2	BST1
Epoxyazadiradione	Thymidylate kinase	DTYMK
Epoxyazadiradione	Baculoviral IAP repeat-containing protein 4	XIAP

Epoxyazadiradione	Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1
Epoxyazadiradione	Retinoic acid receptor RXR-beta	RXRB
Epoxyazadiradione	Glutathione S-transferase Mu 2	GSTM2
Epoxyazadiradione	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
Epoxyazadiradione	Endothelial protein C receptor	PROCR
Epoxyazadiradione	Amine oxidase [flavin-containing] A	MAOA
Gedunin	Bone morphogenetic protein 2	BMP2
Gedunin	Proto-oncogene serine/threonine-protein kinase Pim-1	PIM1
Gedunin	Carbonic anhydrase 2	CA2
Gedunin	Transthyretin	TTR
Gedunin	Peptidyl-prolyl cis-trans isomerase A	PPIA
Gedunin	Collagenase 3	MMP13
Gedunin	Progesterone receptor	PGR
Gedunin	Androgen receptor	AR
Gedunin	3-phosphoinositide-dependent protein kinase 1	PDPK1
Gedunin	Complement factor D	CFD
Gedunin	Proto-oncogene tyrosine-protein kinase Src	SRC
Gedunin	Glycogen synthase kinase-3 beta	GSK3B
Gedunin	Heat shock cognate 71 kDa protein	HSPA8
Gedunin	cGMP-specific 3,5-cyclic phosphodiesterase	PDE5A
Gedunin	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Gedunin	Catenin alpha-1	CTNNA1
Gedunin	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Gedunin	Bile salt sulfotransferase	SULT2A1
Gedunin	Sex hormone-binding globulin	SHBG
Gedunin	Sorbitol dehydrogenase	SORD
Gedunin	Cytochrome P450 2C9	CYP2C9
Gedunin	Cell division protein kinase 6	CDK6
Gedunin	Hepatocyte growth factor receptor	MET
Gedunin	Tyrosine-protein kinase JAK3	JAK3
Gedunin	Aldo-keto reductase family 1 member C3	AKR1C3
Gedunin	Cyclin-T1	CCNT1
Gedunin	Sulfotransferase family cytosolic 2B member 1	SULT2B1
Gedunin	Adenosine kinase	ADK
Gedunin	Leukocyte elastase	ELANE
Gedunin	Tyrosine-protein kinase ITK/TSK	ITK
Gedunin	Trafficking protein particle complex subunit 3	TRAPPC3
Gedunin	Protein kinase C theta type	PRKCQ
Gedunin	Fatty acid-binding protein, brain	FABP7
Gedunin	Histo-blood group ABO system transferase	ABO
Gedunin	Tyrosine-protein kinase HCK	HCK
Gedunin	Tyrosine-protein kinase ZAP-70	ZAP70
Gedunin	Gastrotropin	FABP6
Gedunin	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Gedunin	Protein-glutamine gamma-glutamyltransferase E	TGM3
Gedunin	Glucocorticoid receptor	GCR
Gedunin	Nuclear receptor subfamily 1 group I member 2	NR1I2
Gedunin	Fatty acid-binding protein, heart	FABP3
Gedunin	Endoplasmic reticulum mannosyl-oligosaccharide 1,2- alpha-mannosidase	Q9UKM7
Gedunin	Retinoic acid receptor gamma	RARG
Gedunin	Dipeptidase 1	DPEP1
Gedunin	Matrix metalloproteinase-9	MMP9
Gedunin	Ornithine aminotransferase, mitochondrial	OAT
Gedunin	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM
Gedunin	Retinoic acid receptor alpha	RARA
Gedunin	Glutathione S-transferase A3	GSTA3
Gedunin	Caspase-1	CASP1
Gedunin	Hydroxyacyl-coenzyme A dehydrogenase, mitochondrial	Q16836

Isomargolonone	Apolipoprotein A-II	APOA2
Isomargolonone	Steryl-sulfatase	STS
Isomargolonone	Bone morphogenetic protein 2	BMP2
Isomargolonone	Prothrombin	THRB
Isomargolonone	Carbonic anhydrase 2	CAH2
Isomargolonone	Peptidyl-prolyl cis-trans isomerase A	PPIA
Isomargolonone	Beta-secretase 1	BACE1
Isomargolonone	Transthyretin	TTR
Isomargolonone	Kinesin-like protein KIF11	KIF11
Isomargolonone	ADAM 17	ADAM17
Isomargolonone	Androgen receptor	AR
Isomargolonone	Progesterone receptor	PGR
Isomargolonone	Serine/threonine-protein kinase Chk1	CHEK1
Isomargolonone	3-phosphoinositide-dependent protein kinase 1	PDPK1
Isomargolonone	Peroxisome proliferator-activated receptor gamma	PPARG
Isomargolonone	Macrophage migration inhibitory factor	MIF
Isomargolonone	Dual specificity protein phosphatase 6	DUSP6
Isomargolonone	Glycogen synthase kinase-3 beta	GSK3B
Isomargolonone	Alcohol dehydrogenase 1C	ADH1C
Isomargolonone	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Isomargolonone	cAMP-dependent protein kinase catalytic subunit alpha	PRKACA
Isomargolonone	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Isomargolonone	Methionine aminopeptidase 2	METAP2
Isomargolonone	Sex hormone-binding globulin	SHBG
Isomargolonone	Dipeptidyl peptidase 4	DPP4
Isomargolonone	Receptor tyrosine-protein kinase erbB-4	ERBB4
Isomargolonone	Coagulation factor X	F10
Isomargolonone	Glutathione S-transferase P	GSTP1
Isomargolonone	Fatty acid-binding protein, heart	FABP3
Isomargolonone	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM
Isomargolonone	Glucocorticoid receptor	GCR
Isomargolonone	Protein S100-A9	S100A9
Isomargolonone	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Isomargolonone	Glucokinase	GCK
Isomargolonone	Angiopoietin-1 receptor	TEK
Isomargolonone	Histo-blood group ABO system transferase	ABO
Isomargolonone	S-adenosylmethionine decarboxylase proenzyme	AMD1
Isomargolonone	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
Isomargolonone	Peptidyl-prolyl cis-trans isomerase FKBP1B	FKBP1B
Isomargolonone	Caspase-3	CASP3
Isomargolonone	Scavenger mRNA-decapping enzyme DcpS	DCPS
Isomargolonone	FK506-binding protein 3	FKBP3
Mahmoodin	Apolipoprotein A-II	APOA2
Mahmoodin	Steryl-sulfatase	STS
Mahmoodin	Serum albumin	ALB
Mahmoodin	Aldo-keto reductase family 1 member C2	AKR1C2
Mahmoodin	Integrin alpha-L	ITGAL
Mahmoodin	Triggering receptor expressed on myeloid cells 1	TREM1
Mahmoodin	Vitamin D-binding protein	GC
Mahmoodin	Mitogen-activated protein kinase 8	MAPK8
Mahmoodin	Progesterone receptor	PGR
Mahmoodin	Annexin A5	ANXA5
Mahmoodin	S-methyl-5-thioadenosine phosphorylase	MTAP
Mahmoodin	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Mahmoodin	Sex hormone-binding globulin	SHBG
Mahmoodin	cAMP-specific 3,5-cyclic phosphodiesterase 4D	PDE4D
Mahmoodin	Mitogen-activated protein kinase 14	MAPK14
Mahmoodin	Serine/threonine-protein kinase Chk1	CHEK1

Mahmoodin	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
Mahmoodin	Sorbitol dehydrogenase	SORD
Mahmoodin	Mineralocorticoid receptor	MCR
Mahmoodin	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
Mahmoodin	Dihydroorotate dehydrogenase, mitochondrial	PYRD
Mahmoodin	Alpha-tocopherol transfer protein	TTPA
Mahmoodin	Ribosyldihydronicotinamide dehydrogenase [quinone]	NQO2
Mahmoodin	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Mahmoodin	Aldo-keto reductase family 1 member C3	AKR1C3
Mahmoodin	Lanosterol synthase	LSS
Mahmoodin	Carbonyl reductase [NADPH] 1	CBR1
Mahmoodin	Tyrosine-protein kinase SYK	SYK
Mahmoodin	Glycogen synthase kinase-3 beta	GSK3B
Mahmoodin	Superoxide dismutase [Mn], mitochondrial	SOD2
Mahmoodin	Adenosine kinase	ADK
Mahmoodin	Cytochrome P450 2C9	CYP2C9
Mahmoodin	Serine/threonine-protein kinase 6	O14965
Mahmoodin	Gastrotropin	FABP6
Mahmoodin	Basic fibroblast growth factor receptor 1	FGFR1
Mahmoodin	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Mahmoodin	Stromelysin-1	MMP3
Mahmoodin	Fatty acid-binding protein, heart	FABP3
Mahmoodin	Estrogen sulfotransferase	SULT1E1
Mahmoodin	Oxysterols receptor LXR-alpha	NR1H3
Mahmoodin	Thyroid hormone receptor alpha	THRA
Mahmoodin	Cellular retinoic acid-binding protein 2	CRABP2
Mahmoodin	L-serine dehydratase	SDS
Mahmoodin	Histo-blood group ABO system transferase	ABO
Mahmoodin	Interleukin-2	IL2
Mahmoodin	Glucocorticoid receptor	GCR
Mahmoodin	Glutathione S-transferase A1	GSTA1
Mahmoodin	Protein-glutamine gamma-glutamyltransferase E	TGM3
Mahmoodin	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM
Mahmoodin	72 kDa type IV collagenase	MMP2
Mahmoodin	Retinoic acid receptor beta	RARB
Mahmoodin	Baculoviral IAP repeat-containing protein 4	XIAP
Mahmoodin	Vitamin D3 receptor	VDR
Mahmoodin	Leukotriene A-4 hydrolase	LTA4H
Mahmoodin	Baculoviral IAP repeat-containing protein 7	BIRC7
Mahmoodin	Retinoic acid receptor RXR-beta	RXRB
Mahmoodin	Tryptophanyl-tRNA synthetase, cytoplasmic	WARS1
Margolonone	Bone morphogenetic protein 2	BMP2
Margolonone	Carbonic anhydrase 2	CAH2
Margolonone	Transthyretin	TTR
Margolonone	Vascular endothelial growth factor receptor 2	KDR
Margolonone	Mitogen-activated protein kinase 10	MAPK10
Margolonone	Peptidyl-prolyl cis-trans isomerase A	PPIA
Margolonone	Oxysterols receptor LXR-beta	NR1H2
Margolonone	Mitogen-activated protein kinase 8	MAPK8
Margolonone	B-Raf proto-oncogene serine/threonine-protein kinase	BRAF1
Margolonone	Mitogen-activated protein kinase 14	MAPK14
Margolonone	Methionine aminopeptidase 2	METAP2
Margolonone	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Margolonone	Peroxisome proliferator-activated receptor gamma	PPARG
Margolonone	Sorbitol dehydrogenase	SORD
Margolonone	Dual specificity protein phosphatase 6	DUSP6
Margolonone	Ephrin type-B receptor 4	EPHB4
Margolonone	Sex hormone-binding globulin	SHBG

Margolonone	Mineralocorticoid receptor	MCR
Margolonone	Cell division protein kinase 2	CDK2
Margolonone	Coagulation factor X	F10
Margolonone	Macrophage metalloelastase	MMP12
Margolonone	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
Margolonone	Fibroblast growth factor receptor 2	FGFR2
Margolonone	Glycogen synthase kinase-3 beta	GSK3B
Margolonone	Placenta growth factor	PGF
Margolonone	Aldo-keto reductase family 1 member C3	AKR1C3
Margolonone	Nuclear receptor subfamily 1 group I member 2	NR1I2
Margolonone	Insulin-like growth factor 1 receptor	IGF1R
Margolonone	Histone deacetylase 8	HDAC8
Margolonone	Cytochrome P450 2C9	CYP2C9
Margolonone	Glutathione S-transferase A1	GSTA1
Margolonone	Leukocyte elastase	ELANE
Margolonone	Peroxisome proliferator-activated receptor alpha	PPARA
Margolonone	Tyrosine-protein kinase JAK2	JAK2
Margolonone	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Margolonone	Fatty acid-binding protein, adipocyte	FABP4
Margolonone	Fatty acid-binding protein, heart	FABP3
Margolonone	Baculoviral IAP repeat-containing protein 4	XIAP
Margolonone	Tyrosine-protein kinase HCK	HCK
Margolonone	Dipeptidase 1	DPEP1
Margolonone	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM
Margolonone	Glucocorticoid receptor	GCR
Margolonone	Retinoic acid receptor gamma	RARG
Margolonone	Eukaryotic translation initiation factor 4E	EIF4E
Margolonone	Bcl-2-like protein 1	BCL2L1
Margolonone	Scavenger mRNA-decapping enzyme DcpS	DCPS
Margolonone	FK506-binding protein 3	FKBP3
Meliantriol	Steryl-sulfatase	STS
Meliantriol	Serum albumin	ALB
Meliantriol	Integrin alpha-L	ITGAL
Meliantriol	Glutathione S-transferase P	GSTP1
Meliantriol	Aldo-keto reductase family 1 member C2	AKR1C2
Meliantriol	Vitamin D-binding protein	GC
Meliantriol	Estrogen receptor	ESR1
Meliantriol	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Meliantriol	Collagenase 3	MMP13
Meliantriol	Mineralocorticoid receptor	MCR
Meliantriol	Progesterone receptor	PGR
Meliantriol	Androgen receptor	AR
Meliantriol	Beta-secretase 1	BACE1
Meliantriol	Dihydrofolate reductase	DYR
Meliantriol	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
Meliantriol	SEC14-like protein 2	SEC14L2
Meliantriol	Sex hormone-binding globulin	SHBG
Meliantriol	Coagulation factor X	F10
Meliantriol	Bile salt sulfotransferase	SULT2A1
Meliantriol	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Meliantriol	Cell division protein kinase 2	CDK2
Meliantriol	Glycogen synthase kinase-3 beta	GSK3B
Meliantriol	Aldo-keto reductase family 1 member C1	AKR1C1
Meliantriol	Alpha-tocopherol transfer protein	TTPA
Meliantriol	Lanosterol synthase	LSS
Meliantriol	Adenosine kinase	ADK
Meliantriol	Alcohol dehydrogenase 1C	ADH1C
Meliantriol	Alcohol dehydrogenase class-3	ADH5

Meliantriol	Trafficking protein particle complex subunit 3	TRAPPC3
Meliantriol	Histo-blood group ABO system transferase	ABO
Meliantriol	Glutathione S-transferase A1	GSTA1
Meliantriol	C-1-tetrahydrofolate synthase, cytoplasmic	MTHFD1
Meliantriol	Gastrotropin	FABP6
Meliantriol	Glutathione-requiring prostaglandin D synthase	HPGDS
Meliantriol	Hepatocyte growth factor receptor	MET
Meliantriol	Peroxisome proliferator-activated receptor alpha	PPARA
Meliantriol	Fatty acid-binding protein, brain	FABP7
Meliantriol	Estrogen sulfotransferase	SULT1E1
Meliantriol	Cellular retinoic acid-binding protein 2	CRABP2
Meliantriol	Retinoic acid receptor RXR-alpha	RXRA
Meliantriol	Retinol-binding protein 4	RBP4
Meliantriol	Interleukin-2	IL2
Meliantriol	Retinoic acid receptor gamma	RARG
Meliantriol	Cytochrome P450 2C8	CYP2C8
Meliantriol	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Meliantriol	Nuclear receptor subfamily 1 group I member 2	NR1I2
Meliantriol	Protein S100-A9	S100A9
Meliantriol	Ferrochelatase, mitochondrial	FECH
Meliantriol	72 kDa type IV collagenase	MMP2
Meliantriol	Phospholipase A2, membrane associated	PLA2G2A
Meliantriol	Protein-glutamine gamma-glutamyltransferase E	TGM3
Meliantriol	S-adenosylmethionine decarboxylase proenzyme	AMD1
Meliantriol	Vitamin D3 receptor	VDR
Meliantriol	Retinoic acid receptor beta	RARB
Meliantriol	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
Meliantriol	NAD-dependent malic enzyme, mitochondrial	ME2
Meliantriol	Endothelial protein C receptor	PROCR
Nimbin	Aldo-keto reductase family 1 member C2	AKR1C2
Nimbin	Serum albumin	ALB
Nimbin	Proto-oncogene serine/threonine-protein kinase Pim-1	PIM1
Nimbin	Carbonic anhydrase 2	CAH2
Nimbin	Chymase	CMA1
Nimbin	Progesterone receptor	PGR
Nimbin	Vitamin D-binding protein	GC
Nimbin	Annexin A5	ANXA5
Nimbin	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Nimbin	3-phosphoinositide-dependent protein kinase 1	PDPK1
Nimbin	Mitogen-activated protein kinase 14	MAPK14
Nimbin	Complement factor D	CFD
Nimbin	Epidermal growth factor receptor	EGFR
Nimbin	Alcohol dehydrogenase 1C	ADH1C
Nimbin	Glycogen synthase kinase-3 beta	GSK3B
Nimbin	Sex hormone-binding globulin	SHBG
Nimbin	Aldo-keto reductase family 1 member C3	AKR1C3
Nimbin	Androgen receptor	AR
Nimbin	Serine/threonine-protein kinase Chk1	CHEK1
Nimbin	Macrophage metalloelastase	MMP12
Nimbin	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
Nimbin	NONE	NONE
Nimbin	Sorbitol dehydrogenase	SORD
Nimbin	Phospholipase A2, membrane associated	PLA2G2A
Nimbin	Calmodulin	CALM
Nimbin	Hepatocyte growth factor receptor	MET
Nimbin	Epoxide hydrolase 2	EPHX2
Nimbin	Carbonyl reductase [NADPH] 1	CBR1
Nimbin	Stromelysin-1	MMP3

Nimbin	Fatty acid-binding protein, heart	FABP3
Nimbin	Dihydroorotate dehydrogenase, mitochondrial	PYRD
Nimbin	Collagenase 3	MMP13
Nimbin	Heat shock protein HSP 90-alpha	HSP90AA1
Nimbin	Adenosine kinase	ADK
Nimbin	Gastrotropin	FABP6
Nimbin	Tyrosine-protein kinase ITK/TSK	ITK
Nimbin	Glutathione S-transferase A1	GSTA1
Nimbin	Nuclear receptor subfamily 1 group I member 3	NR1I3
Nimbin	Histone deacetylase 8	HDAC8
Nimbin	cAMP-specific 3,5-cyclic phosphodiesterase 4D	PDE4D
Nimbin	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Nimbin	Thyroid hormone receptor alpha	THRA
Nimbin	Peroxisome proliferator-activated receptor delta	PPARD
Nimbin	Ganglioside GM2 activator	GM2A
Nimbin	Hepatocyte nuclear factor 4-gamma	HNF4G
Nimbin	B-Raf proto-oncogene serine/threonine-protein kinase	BRAF1
Nimbin	Glucocorticoid receptor	GCR
Nimbin	Interleukin-2	IL2
Nimbin	Tyrosine-protein kinase JAK2	JAK2
Nimbin	Glucokinase	GCK
Nimbin	ADP-ribosyl cyclase 2	BST1
Nimbin	Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1
Nimbin	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM
Nimbin	Baculoviral IAP repeat-containing protein 7	BIRC7
Nimbin	Cathepsin S	CATS
Nimbin	Growth factor receptor-bound protein 2	GRB2
Nimbin	Beta-secretase 1	BACE1
Nimbin	Ornithine aminotransferase, mitochondrial	OAT
Nimbin	Caspase-1	CASP1
Nimbiene	Serum albumin	ALB
Nimbiene	Steryl-sulfatase	STS
Nimbiene	Glutathione S-transferase P	GSTP1
Nimbiene	TGF-beta receptor type-1	TGFBR1
Nimbiene	Vitamin D-binding protein	GC
Nimbiene	Aldose reductase	ALDR
Nimbiene	Proto-oncogene tyrosine-protein kinase Src	SRC
Nimbiene	3-phosphoinositide-dependent protein kinase 1	PDPK1
Nimbiene	Calmodulin	CALM
Nimbiene	SEC14-like protein 2	SEC14L2
Nimbiene	Catenin alpha-1	CTNNA1
Nimbiene	Histone deacetylase 8	HDAC8
Nimbiene	Alpha-tocopherol transfer protein	TTPA
Nimbiene	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
Nimbiene	Complement factor D	CFD
Nimbiene	NONE	NONE
Nimbiene	Alcohol dehydrogenase 1C	ADH1C
Nimbiene	Mitogen-activated protein kinase 14	MAPK14
Nimbiene	Glycogen synthase kinase-3 beta	GSK3B
Nimbiene	Cell division protein kinase 2	CDK2
Nimbiene	Cytochrome P450 2C9	CYP2C9
Nimbiene	Adenosine kinase	ADK
Nimbiene	Alcohol dehydrogenase class-3	ADH5
Nimbiene	Trafficking protein particle complex subunit 3	TRAPPC3
Nimbiene	Prostatic acid phosphatase	PPAP
Nimbiene	[Pyruvate dehydrogenase [lipoamide]] kinase isozyme 2, mitochondrial	PDK2
Nimbiene	Retinol-binding protein 4	RBP4
Nimbiene	ADP-ribosyl cyclase 2	BST1

Nimbiene	Cytochrome P450 2C8	CYP2C8
Nimbiene	Fatty acid-binding protein, heart	FABP3
Nimbiene	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Nimbiene	Gastrotropin	FABP6
Nimbiene	Dual specificity mitogen-activated protein kinase	MAP2K1
	kinase 1	
Nimbiene	Glucosamine-6-phosphate isomerase	GNPDA1
Nimbiene	Tyrosine-protein kinase JAK2	JAK2
Nimbiene	Retinoic acid receptor gamma	RARG
Nimbiene	Retinoic acid receptor RXR-alpha	RXRA
Nimbiene	Ferrochelatase, mitochondrial	FECH
Nimbiene	Glucocorticoid receptor	GCR
Nimbiene	B-Raf proto-oncogene serine/threonine-protein kinase	BRAF1
Nimbiene	Deoxycytidine kinase	DCK
Nimbiene	Vitamin D3 receptor	VDR
Nimbiene	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM
Nimbiene	S-adenosylmethionine decarboxylase proenzyme	AMD1
Nimbiene	Angiopoietin-1 receptor	TEK
Nimbiene	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
Nimbiene	Coagulation factor XI	F11
Nimbiene	Heme oxygenase 1	HMOX1
Nimbiene	Eukaryotic translation initiation factor 4E	EIF4E
Nimbiene	Histone acetyltransferase PCAF	KAT2B
Nimbolide	Serum albumin	ALB
Nimbolide	Aldo-keto reductase family 1 member C2	AKR1C2
Nimbolide	Ribosyldihydronicotinamide dehydrogenase [quinone]	NQO2
Nimbolide	Aldose reductase	ALDR
Nimbolide	Annexin A5	ANXA5
Nimbolide	ADAM 17	ADAM17
Nimbolide	Peroxisome proliferator-activated receptor gamma	PPARG
Nimbolide	cAMP-specific 3,5-cyclic phosphodiesterase 4B	PDE4B
Nimbolide	cAMP-specific 3,5-cyclic phosphodiesterase 4D	PDE4D
Nimbolide	Heat shock protein HSP 90-alpha	HSP90AA1
Nimbolide	Sorbitol dehydrogenase	SORD
Nimbolide	Prothrombin	THRB
Nimbolide	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Nimbolide	Glycogen synthase kinase-3 beta	GSK3B
Nimbolide	Calmodulin	CALM
Nimbolide	Alpha-tocopherol transfer protein	TTPA
Nimbolide	NAD(P)H dehydrogenase [quinone] 1	NQO1
Nimbolide	Cell division protein kinase 6	CDK6
Nimbolide	Macrophage metalloelastase	MMP12
Nimbolide	Catenin alpha-1	CTNNA1
Nimbolide	Tyrosine-protein phosphatase non-receptor type 1	PTPN1
Nimbolide	Glutathione-requiring prostaglandin D synthase	HPGDS
Nimbolide	Alcohol dehydrogenase 1C	ADH1C
Nimbolide	Hepatocyte nuclear factor 4-gamma	HNF4G
Nimbolide	Stromelysin-1	MMP3
Nimbolide	Sulfotransferase family cytosolic 2B member 1	SULT2B1
Nimbolide	Adenosine kinase	ADK
Nimbolide	Fatty acid-binding protein, heart	FABP3
Nimbolide	Nuclear receptor subfamily 1 group I member 3	NR1I3
Nimbolide	Tyrosine-protein kinase JAK3	JAK3
Nimbolide	Cytochrome P450 2C9	CYP2C9
Nimbolide	Coagulation factor X	F10
Nimbolide	Renin	RENI
Nimbolide	Histone-lysine N-methyltransferase SETD7	SETD7
Nimbolide	ADP-ribosyl cyclase 2	BST1

Nimbolide	L-serine dehydratase	SDS
Nimbolide	Retinoic acid receptor gamma	RARG
Nimbolide	Glutathione S-transferase A1	GSTA1
Nimbolide	Betaine--homocysteine S-methyltransferase 1	BHMT
Nimbolide	Ferrochelatase, mitochondrial	FECH
Nimbolide	Tyrosine-protein kinase ZAP-70	ZAP70
Nimbolide	Cellular retinoic acid-binding protein 2	CRABP2
Nimbolide	Protein kinase C theta type	PRKCQ
Nimbolide	Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1
Nimbolide	Glucokinase	GCK
Nimbolide	Protein S100-A9	S100A9
Nimbolide	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Nimbolide	Thymidylate kinase	DTYMK
Nimbolide	cGMP-specific 3,5-cyclic phosphodiesterase	PDE5A
Nimbolide	Retinoic acid receptor RXR-beta	RXRB
Nimbolide	Coagulation factor XI	F11
Nimbolide	S-adenosylmethionine decarboxylase proenzyme	AMD1
Nimbolide	Bcl-2-like protein 1	BCL2L1
Nimbolide	Eukaryotic translation initiation factor 4E	EIF4E
Nimbolide	Insulin receptor	INSR
Nimbolin A	Vitamin D-binding protein	GC
Nimbolin A	Cyclin-A2	CCNA2
Nimbolin A	Estrogen-related receptor gamma	ESRRG
Nimbolin A	Estrogen receptor	ESR1
Nimbolin A	Nuclear receptor ROR-alpha	RORA
Nimbolin A	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Nimbolin A	TGF-beta receptor type-1	TGFBR1
Nimbolin A	Sex hormone-binding globulin	SHBG
Nimbolin A	Calmodulin	CALM
Nimbolin A	Bile salt sulfotransferase	SULT2A1
Nimbolin A	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
Nimbolin A	SEC14-like protein 2	SEC14L2
Nimbolin A	Glycogen synthase kinase-3 beta	GSK3B
Nimbolin A	Alpha-tocopherol transfer protein	TTPA
Nimbolin A	Sorbitol dehydrogenase	SORD
Nimbolin A	Cathepsin K	CATK
Nimbolin A	cGMP-specific 3,5-cyclic phosphodiesterase	PDE5A
Nimbolin A	Catenin alpha-1	CTNNA1
Nimbolin A	Superoxide dismutase [Mn], mitochondrial	SOD2
Nimbolin A	Oxysterols receptor LXR-alpha	NR1H3
Nimbolin A	3-phosphoinositide-dependent protein kinase 1	PDPK1
Nimbolin A	Histone deacetylase 8	HDAC8
Nimbolin A	3-hydroxy-3-methylglutaryl-coenzyme A reductase	HMGCR
Nimbolin A	Carbonyl reductase [NADPH] 1	CBR1
Nimbolin A	Fatty acid-binding protein, heart	FABP3
Nimbolin A	Alcohol dehydrogenase class-3	ADH5
Nimbolin A	Nuclear receptor subfamily 1 group I member 2	NR1I2
Nimbolin A	Adenosine kinase	ADK
Nimbolin A	Cytochrome P450 2C9	CYP2C9
Nimbolin A	Trafficking protein particle complex subunit 3	TRAPPC3
Nimbolin A	Tyrosine-protein kinase ITK/TSK	ITK
Nimbolin A	Gastrotropin	FABP6
Nimbolin A	Ferrochelatase, mitochondrial	FECH
Nimbolin A	Sulfotransferase family cytosolic 2B member 1	SULT2B1
Nimbolin A	Serine hydroxymethyltransferase, cytosolic	GLYC
Nimbolin A	Flavin reductase	BLVRB
Nimbolin A	Neutrophil gelatinase-associated lipocalin	LCN2
Nimbolin A	Dipeptidase 1	DPEP1

Nimbolin A	Insulin-like growth factor IA	IGF1
Nimbolin A	Proactivator polypeptide	PSAP
Nimbolin A	Retinoic acid receptor gamma	RARG
Nimbolin A	Histo-blood group ABO system transferase	ABO
Nimbolin A	Glucocorticoid receptor	GCR
Nimbolin A	Cytochrome P450 2C8	CYP2C8
Nimbolin A	Protein-glutamine gamma-glutamyltransferase E	TGM3
Nimbolin A	Interleukin-2	IL2
Nimbolin A	Dual specificity protein kinase CLK1	CLK1
Nimbolin A	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Nimbolin A	Histamine N-methyltransferase	HNMT
Nimbolin A	Retinoic acid receptor alpha	RARA
Nimbolin A	Retinoic acid receptor beta	RARB
Nimbolin A	Retinoic acid receptor RXR-beta	RXRB
Nimbolin A	Leukotriene A-4 hydrolase	LTA4H
Nimbolin A	Signal transducer and activator of transcription 1-alpha/beta	STAT1
Nimbolin A	Vitamin D3 receptor	VDR
Nimbolin A	Bcl-2-like protein 1	BCL2L1
Nimbolin A	Histone acetyltransferase PCAF	KAT2B
Nimbolin A	Caspase-1	CASP1
Nimbolin A	Endothelial protein C receptor	PROCR
Nimocinol	Aldo-keto reductase family 1 member C2	AKR1C2
Nimocinol	Progesterone receptor	PGR
Nimocinol	Mitogen-activated protein kinase 10	MAPK10
Nimocinol	Vascular endothelial growth factor receptor 2	KDR
Nimocinol	Mitogen-activated protein kinase 14	MAPK14
Nimocinol	Carbonic anhydrase 2	CAH2
Nimocinol	Prothrombin	THRB
Nimocinol	Estrogen-related receptor gamma	ESRRG
Nimocinol	Sex hormone-binding globulin	SHBG
Nimocinol	Proto-oncogene tyrosine-protein kinase Src	SRC
Nimocinol	Complement factor D	CFD
Nimocinol	Heat shock cognate 71 kDa protein	HSPA8
Nimocinol	Nitric oxide synthase, endothelial	NOS3
Nimocinol	Bile salt sulfotransferase	SULT2A1
Nimocinol	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Nimocinol	Glycogen synthase kinase-3 beta	GSK3B
Nimocinol	Alcohol dehydrogenase 1C	ADH1C
Nimocinol	Sorbitol dehydrogenase	SORD
Nimocinol	Cell division protein kinase 2	CDK2
Nimocinol	Mineralocorticoid receptor	MCR
Nimocinol	Glutathione S-transferase P	GSTP1
Nimocinol	Hepatocyte growth factor receptor	MET
Nimocinol	Placenta growth factor	PGF
Nimocinol	Macrophage metalloelastase	MMP12
Nimocinol	Thyroid hormone receptor beta	THRB
Nimocinol	Tyrosyl-tRNA synthetase, cytoplasmic	YARS1
Nimocinol	Glutathione S-transferase A1	GSTA1
Nimocinol	Adenosine kinase	ADK
Nimocinol	Oxysterols receptor LXR-beta	NR1H2
Nimocinol	Cytochrome P450 2C9	CYP2C9
Nimocinol	Insulin-like growth factor IA	IGF1
Nimocinol	Gastrotropin	FABP6
Nimocinol	Angiotensin-converting enzyme	ACE
Nimocinol	C-1-tetrahydrofolate synthase, cytoplasmic	MTHFD1
Nimocinol	Histo-blood group ABO system transferase	ABO
Nimocinol	Fatty acid-binding protein, heart	FABP3
Nimocinol	Sulfotransferase family cytosolic 2B member 1	SULT2B1

Nimocinol	Fatty acid-binding protein, adipocyte	FABP4
Nimocinol	Ferrochelatase, mitochondrial	FECH
Nimocinol	Nuclear receptor subfamily 1 group I member 2	NR1I2
Nimocinol	Glucocorticoid receptor	GCR
Nimocinol	Thyroid hormone receptor alpha	THRA
Nimocinol	Protein-glutamine gamma-glutamyltransferase E	TGM3
Nimocinol	cGMP-specific 3,5-cyclic phosphodiesterase	PDE5A
Nimocinol	Basic fibroblast growth factor receptor 1	FGFR1
Nimocinol	Retinoic acid receptor gamma	RARG
Nimocinol	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Nimocinol	Heme oxygenase 1	HMOX1
Nimocinol	Vitamin D3 receptor	VDR
Nimocinol	Retinoic acid receptor beta	RARB
Nimocinol	Retinoic acid receptor RXR-beta	RXRB
Nimocinol	Glutathione S-transferase Mu 1	GSTM1
Nimocinol	Glutathione S-transferase A3	GSTA3
Nimocinol	Coagulation factor XI	F11
Nimocinol	Phosphatidylcholine transfer protein	PCTP
Nimocinol	Serine/threonine-protein phosphatase PP1-gamma catalytic subunit	PPP1CC
Nimocinol	Caspase-1	CASP1
Nimocinol	Endothelial protein C receptor	PROCR
Quercetein	Carbonic anhydrase 2	CAH2
Quercetein	Cell division protein kinase 6	CDK6
Quercetein	Cell division protein kinase 2	CDK2
Quercetein	Estrogen receptor beta	Esr2
Quercetein	Glutathione reductase, mitochondrial	GSR
Quercetein	Proto-oncogene tyrosine-protein kinase Src	SRC
Quercetein	Estradiol 17-beta-dehydrogenase 1	HSD17B1
Quercetein	3-phosphoinositide-dependent protein kinase 1	PDPK1
Quercetein	Carbonyl reductase [NADPH] 1	CBR1
Quercetein	Cyclin-A2	CCNA2
Quercetein	Sorbitol dehydrogenase	SORD
Quercetein	cAMP-specific 3,5-cyclic phosphodiesterase 4D	PDE4D
Quercetein	Deoxycytidine kinase	DCK
Quercetein	Hexokinase-1	HXK1
Quercetein	Phosphoenolpyruvate carboxykinase, cytosolic [GTP]	PCK1
Quercetein	B transferase	ABO
Quercetein	Beta-hexosaminidase subunit beta	HEXB
Quercetein	Vascular endothelial growth factor receptor 2	KDR
Quercetein	Triosephosphate isomerase	TPI1
Quercetein	Uridine 5-monophosphate synthase	UMPS
Quercetein	Basic fibroblast growth factor receptor 1	FGFR1
Quercetein	Alcohol dehydrogenase class-3	ADH5
Quercetein	Serine hydroxymethyltransferase, cytosolic	GLYC
Quercetein	Proto-oncogene tyrosine-protein kinase LCK	LCK
Quercetein	Rho GTPase-activating protein 1	ARHGAP1
Quercetein	cGMP-specific 3,5-cyclic phosphodiesterase	PDE5A
Quercetein	Uridine-cytidine kinase 2	UCK2
Quercetein	Ras-related protein Rab-5A	RAB5A
Quercetein	Nicotinamide mononucleotide adenylyltransferase 1	NMNAT1
Quercetein	Tyrosine-protein kinase JAK2	JAK2
Quercetein	ADP-ribosyl cyclase 2	BST1
Quercetein	Glutathione S-transferase theta-2	GSTT2
Quercetein	Histo-blood group ABO system transferase	ABO
Quercetein	Adenine phosphoribosyltransferase	APRT
Quercetein	GTPase HRas	RASH
Quercetein	Glutathione S-transferase A3	GSTA3
Quercetein	Ephrin type-A receptor 2	EPHA2

Qucertein	Betaine--homocysteine S-methyltransferase 1	BHMT
Qucertein	Interstitial collagenase	MMP1
Qucertein	Retinoic acid receptor alpha	RARA
Qucertein	Peptidyl-prolyl cis-trans isomerase FKBP1A	FKBP1A
Qucertein	Proto-oncogene tyrosine-protein kinase ABL1	ABL1
Qucertein	Leukocyte elastase	ELANE
Qucertein	Histidine triad nucleotide-binding protein 1	HINT1
Qucertein	GMP reductase 1	GMPR
Qucertein	Coagulation factor XI	F11
Qucertein	Chitotriosidase-1	CHIT1
Qucertein	Eukaryotic translation initiation factor 4E	EIF4E
Qucertein	Hypoxanthine-guanine phosphoribosyltransferase	HPRT1
Qucertein	Ras-related protein Rab-9	RAB9A
Qucertein	Glutathione S-transferase Mu 2	GSTM2
Qucertein	ADP-ribosylation factor-like protein 5A	ARL5A
Qucertein	CD209 antigen	CD209
Qucertein	3 histone mRNA exonuclease 1	ERI1
Qucertein	Phenylethanolamine N-methyltransferase	PNMT
Qucertein	Riboflavin kinase	RFK
Salannol	Kinesin-like protein KIF11	KIF11
Salannol	Vitamin D-binding protein	GC
Salannol	Annexin A5	ANXA5
Salannol	Peroxisome proliferator-activated receptor gamma	PPARG
Salannol	Cell division protein kinase 2	CDK2
Salannol	Epidermal growth factor receptor	EGFR
Salannol	Estrogen receptor	ESR1
Salannol	Peroxisome proliferator-activated receptor delta	PPARD
Salannol	Nuclear receptor ROR-alpha	RORA
Salannol	TGF-beta receptor type-1	TGFBR1
Salannol	Wiskott-Aldrich syndrome protein	WAS
Salannol	Heat shock cognate 71 kDa protein	HSPA8
Salannol	Bile salt sulfotransferase	SULT2A1
Salannol	Catenin alpha-1	CTNNA1
Salannol	cAMP-specific 3,5-cyclic phosphodiesterase 4D	PDE4D
Salannol	Sex hormone-binding globulin	SHBG
Salannol	Mineralocorticoid receptor	MCR
Salannol	Proto-oncogene tyrosine-protein kinase Src	SRC
Salannol	Tyrosine-protein phosphatase non-receptor type 11	PTPN11
Salannol	Trafficking protein particle complex subunit 3	TRAPPC3
Salannol	Heat shock protein HSP 90-alpha	HSP90AA1
Salannol	Adenosine kinase	ADK
Salannol	Histone deacetylase 8	HDAC8
Salannol	Coagulation factor X	F10
Salannol	Tyrosine-protein kinase SYK	SYK
Salannol	Phospholipase A2, membrane associated	PLA2G2A
Salannol	Alpha-tocopherol transfer protein	TTPA
Salannol	Corticosteroid 11-beta-dehydrogenase isozyme 1	HSD11B1
Salannol	Poly [ADP-ribose] polymerase 1	PARP1
Salannol	cAMP-dependent protein kinase catalytic subunit alpha	PRKACA
Salannol	Glycogen synthase kinase-3 beta	GSK3B
Salannol	Hepatocyte growth factor receptor	MET
Salannol	Vascular endothelial growth factor receptor 2	KDR
Salannol	Carbonyl reductase [NADPH] 1	CBR1
Salannol	Aldo-keto reductase family 1 member C3	AKR1C3
Salannol	NAD(P)H dehydrogenase [quinone] 1	NQO1
Salannol	Glutathione S-transferase A1	GSTA1
Salannol	Nuclear receptor subfamily 1 group I member 3	NR1I3
Salannol	Tyrosine-protein kinase JAK3	JAK3

Salannol	Gastrotropin	FABP6
Salannol	Tyrosine-protein kinase ITK/TSK	ITK
Salannol	Fatty acid-binding protein, brain	FABP7
Salannol	Leukocyte elastase	ELANE
Salannol	Cytochrome P450 2C9	CYP2C9
Salannol	Interleukin-2	IL2
Salannol	Fatty acid-binding protein, heart	FABP3
Salannol	Cytochrome P450 2C8	CYP2C8
Salannol	Proactivator polypeptide	PSAP
Salannol	Ferrochelatase, mitochondrial	FECH
Salannol	Sulfotransferase family cytosolic 2B member 1	SULT2B1
Salannol	Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1
Salannol	Protein kinase C theta type	PRKCQ
Salannol	B transferase	ABO
Salannol	Ganglioside GM2 activator	GM2A
Salannol	Tyrosine-protein kinase ZAP-70	ZAP70
Salannol	Hepatocyte nuclear factor 4-gamma	HNF4G
Salannol	Nuclear receptor subfamily 1 group I member 2	NR1I2
Salannol	Retinoic acid receptor gamma	RARG
Salannol	Dipeptidase 1	DPEP1
Salannol	Insulin-like growth factor IA	IGF1
Salannol	Histamine N-methyltransferase	HNMT
Salannol	cAMP-dependent protein kinase, alpha-catalytic subunit	PRKACA
Salannol	Baculoviral IAP repeat-containing protein 4	XIAP
Salannol	Protein S100-A9	S100A9
Salannol	Cathepsin F	CTSF
Salannol	Medium-chain specific acyl-CoA dehydrogenase, mitochondrial	ACADM
Salannol	Retinoic acid receptor alpha	RARA
Salannol	Mast/stem cell growth factor receptor	KIT
Salannol	Vitamin D3 receptor	VDR
Salannol	Retinoic acid receptor RXR-beta	RXRB
Salannol	Growth factor receptor-bound protein 2	GRB2
Salannol	Phosphatidylinositol 3-kinase regulatory subunit alpha	PIK3R1
Salannol	Phosphatidylcholine transfer protein	PCTP
Salannol	Endothelial protein C receptor	PROCR

Table 4: Common genes obtained from Venny 2.1.0 database.

THRB	BMP2	CA2	GSTP1	ANXA5	PDE4D	HSPA8	SHBG	SRC	SULT2A1
AURKA	SDS	FABP6	MMP3	FABP4	GSTA1	PAK6	FABP7	PYGL	HNF4G
MTHFD1	ABO	NR1I2	IL2	DPEP1	TGM3	FECH	CRABP2	RARB	BHMT
RXRB	MIF	PDPK1	MMP12	MMP8	DPP4	LCK	FGFR1	ACE	HCK
MMP9	JAK2	RARG	RARA	SETD7	ACADM	VDR	HMOX1	INSR	PPARG
EGFR	GSK3B	MMP13	NR1I3	CLK1	DCK	GSTM1	RORA	APOA2	FNTA
CBR1	NR1H4	PDE3B	NR1H3	MMP2	CASP1	STS	ESR1	ADH1B	PDE5A
RXRA	DUT	ALDH2	PPARA	ERBB4	NR1H2	ZAP70	MMP16	GRB2	CCNA2
STAT1	JAK3	IGF1R	FKBP3	PNMT	EPHB4	CDK6	KIF11	HDAC8	CD209
CASP3	PIM1	RAB5A	XIAP	ADK	GSTT2	HINT1	NQO2	CCNT1	RTN4R
CMA1	TPH1	CCL5	C1S	NOS2	KIT	CSK	PADI4	TGFB2	GSTM2
NOS3	BACE1	CASP7	MDM2	PDK2	NQO1	FABP5	AKT2	ISG20	EPHA2
OAT	RAF1	GSTO1	CDC42	MET					

Table 5: Topology analysis data of drug-disease interaction gene (Degree > 10).

Name	Full Name	Degree	Uniprot ID	Protein Class
SRC	Proto-oncogene tyrosine-protein kinase Src	66	P12931	protein kinase superfamily
EGFR	Epidermal growth factor receptor	65	P00533	protein kinase superfamily
CASP3	Caspase-3	49	P42574	peptidase C14A family
ESR1	Estrogen receptor	49	P03372	nuclear hormone receptor family.
CCND1	G1/S-specific cyclin-D1	45	P24385	cyclin family

PPARG	Peroxisome proliferator-activated receptor gamma	42	P37231	nuclear hormone receptor family
CD4	T-cell surface glycoprotein	42	P01730	None
MMP9	Matrix metalloproteinase-9	42	P14780	peptidase M10A family.
CDC42	Cell division control protein 42 homolog	36	P60953	Rho family
GRB2	Growth factor receptor-bound protein 2	36	P62993	GRB2/sem-5/DRK family
ANXA5	Annexin A5	35	P08758	annexin family.
HGF	Hepatocyte growth factor	35	P14210	peptidase S1 family
IL2	Interleukin-2	34	P60568	IL-2 family
JAK2	Tyrosine-protein kinase	34	O60674	protein kinase superfamily
MDM2	E3 ubiquitin-protein ligase	32	Q00987	MDM2/MDM4 family.
MMP2	type IV collagenase	31	P08253	peptidase M10A family
STAT1	Signal transducer and activator of transcription 1-alpha/beta	30	P42224	transcription factor STAT family
GSK3B	Glycogen synthase kinase-3 beta	29	P49841	CMGC Ser/Thr protein kinase family
KIT	Mast/stem cell growth factor receptor	28	A0A0U2N547	CAMK Ser/Thr protein kinase family
PPARA	Peroxisome proliferator-activated receptor alpha	27	Q07869	nuclear hormone receptor family
HMOX1	Heme oxygenase	27	Q96DI8	heme oxygenase family
LCK	Tyrosine-protein kinase	26	P06239	Tyr protein kinase family
CCL5	C-C motif chemokine 5	26	A0A494C1Q1	None
AKT2	RAC-beta serine/threonine-protein kinase	25	P31751	AGC Ser/Thr protein kinase family
TIMP1	Metalloproteinase inhibitor 1	24	Q5H9B5	None
NOS3	Nitric oxide synthase	24	P29474	NOS family
RAF1	RAF proto-oncogene serine/threonine-protein kinase	24	P04049	TKL Ser/Thr protein kinase family
IGF1R	Insulin-like growth factor 1 receptor	24	P08069	Tyr protein kinase family
RXRA	Retinoic acid receptor RXR-alpha	23	P19793	nuclear hormone receptor family
XIAP	E3 ubiquitin-protein ligase XIAP	23	B1AKU2	None
CCNA2	Cyclin-A2	22	P20248	cyclin family
MET	Hepatocyte growth factor receptor	21	P08581	Tyr protein kinase family
CDK6	Cyclin-dependent kinase 6	20	Q00534	CMGC Ser/Thr protein kinase family
ACE	Angiotensin-converting enzyme	18	A0A0A0MSN4	peptidase M2 family.
MMP3	Matrix metalloproteinase 3	18	A5GZ70	None
INSR	Insulin receptor	17	P06213	Tyr protein kinase family
NOS2	Nitric oxide synthase	17	A0A2R8YDS4	NOS family
BMP2	Bone morphogenetic protein 2	17	C8C060	TGF-beta family
FGFR1	Fibroblast Growth factor 1	17	P11362	Tyr protein kinase family
VDR	Vitamin D3 receptor	16	P11473	nuclear hormone receptor family
TGFB2	Transforming growth factor beta-2 proprotein	16	P61812	TGF-beta family.
NQO1	NAD(P)H dehydrogenase [quinone] 1	15	H3BRK3	NAD(P)H dehydrogenase (quinone) family
CSK	Tyrosine-protein kinase CSK	15	P41240	Tyr protein kinase family
CASP1	Caspase-1	15	P29466	peptidase C14A family
AURKA	Aurora kinase	15	A3KFJ0	Ser/Thr protein kinase family
ERBB4	Receptor tyrosine-protein kinase	15	Q15303	Tyr protein kinase family.
HCK	Tyrosine-protein kinase	15	P08631	Tyr protein kinase family.
ZAP70	Tyrosine-protein kinase	15	P43403	Tyr protein kinase family.
RXRB	Retinoic acid receptor RXR-beta	15	E9PK75	None
GSTP1	Glutathione S-transferase P	14	P09211	Pi family
LCP2	Lymphocyte cytosolic protein 2	14	Q13094	None
RARA	Retinoic acid receptor alpha	14	P10276	nuclear hormone receptor family
DPP4	Dipeptidyl peptidase 4	13	P27487	peptidase S9B family
GSTA1	Glutathione S-transferase A1	12	P08263	Alpha family.
CASP7	Caspase-7	12	P55210	peptidase C14A family.
HSPA8	Heat shock cognate	12	P11142	heat shock protein 70 family
STUB1	E3 ubiquitin-protein ligase CHIP	12	Q9UNE7	None
IL2RB	Interleukin-2 receptor subunit beta	12	P14784	type I cytokine receptor family
JAK3	Tyrosine-protein kinase	12	P52333	Tyr protein kinase family.
FABP6	Gastrotropin	12	P51161	Fatty-acid binding protein (FABP) family
EPOR	Erythropoietin receptor	12	P19235	type I cytokine receptor family
NGFR	Tumor necrosis factor receptor superfamily member 16	11	P08138	None

EPHA2	Ephrin type-A receptor 2	11	P29317	Tyr protein kinase family
NR1H4	Bile acid receptor	11	Q96RI1	nuclear hormone receptor family
FABP4	Fatty acid-binding protein	10	P15090	. Fatty-acid binding protein (FABP) family
BACE1	Beta-secretase 1	10	P56817	peptidase A1 family
GSTM2	Glutathione S-transferase Mu 2	10	P28161	Mu family
GSTM1	Glutathione S-transferase Mu 1	10	P09488	Mu family
PDPK1	3-phosphoinositide-dependent protein kinase 1	10	O15530	AGC Ser/Thr protein kinase family
MCM5	DNA replication licensing factor	10	P33992	MCM family
MMP13	Collagenase 3	10	P45452	peptidase M10A family
SOS2	Son of sevenless homolog	10	Q07890	None
WASL	WAS/WASL-interacting protein family member 1	10	O43516	verprolin family.

Table 6: Interaction network data of "*Azadirachta Indica* Leaves — compound class — active component — gene" (Degree > 20).

Name	Degree	Average Shortest Path Length	Betweenness Centrality	Closeness Centrality	Topological Coefficient
7-Deacetyl dedunin	121	1.206896552	0.679801647	0.828571429	0.196051423
β-Sitosterol	32	2.434482759	0.023222831	0.410764873	0.335069444
Gedunin	31	2.448275862	0.024449243	0.408450704	0.338709677
Nimbin	31	2.448275862	0.028490301	0.408450704	0.306451613
Mahmoodin	31	2.448275862	0.025644502	0.408450704	0.356630824
Salannol	31	2.448275862	0.026440886	0.408450704	0.370967742
Epoxyazadiradione	29	2.475862069	0.019935721	0.403899721	0.325670498
Nimbolin A	27	2.503448276	0.01483879	0.399449036	0.380658436
Meliantriol	26	2.517241379	0.040587337	0.397260274	0.305555556
Azadirone	24	2.544827586	0.013148547	0.39295393	0.409722222
Nimocinol	23	2.55862069	0.015053783	0.39083558	0.304347826
Nimbolide	22	2.572413793	0.011186023	0.388739946	0.315656566
Catechin	22	2.572413793	0.017749085	0.388739946	0.308080808
Nimbinene	22	2.572413793	0.014682385	0.388739946	0.353535354
Epicatechin.	21	2.586206897	0.010006844	0.386666667	0.293650794

Table 7: Target and genetic information of compounds with interaction network (Degree >20).

Compound	Receptor Proteins	Target Genes
Gedunin	Proto-oncogene tyrosine-protein kinase Src	SRC
Nimbin	Proto-oncogene tyrosine-protein kinase Src	SRC
Nimbin	Matrix metalloproteinase-9	MMP9
Nimbolide	Peroxisome proliferator-activated receptor gamma	PPARG
Nimbolide	Epidermal growth factor receptor	EGFR
Nimbolide	Matrix metalloproteinase-9	MMP9
Nimocinol	Estrogen receptor	ESR1
Nimocinol	Epidermal growth factor receptor	EGFR
Meliantriol	Peroxisome proliferator-activated receptor gamma	PPARG
Meliantriol	Estrogen receptor	ESR1
Meliantriol	Growth factor receptor-bound protein 2	GRB2
Nimbolin A	Estrogen receptor	ESR1
Margolonone	Peroxisome proliferator-activated receptor gamma	PPARG
Isomargolonone	Peroxisome proliferator-activated receptor gamma	PPARG
Catechin	Proto-oncogene tyrosine-protein kinase Src	SRC
Catechin	Epidermal growth factor receptor	EGFR
Catechin	Caspase-3	CASP3
Epicatechin.	Proto-oncogene tyrosine-protein kinase Src	SRC
Epicatechin.	Epidermal growth factor receptor	EGFR
Azadirone	Proto-oncogene tyrosine-protein kinase Src	SRC
Azadiradione	Estrogen receptor	ESR1
Epoxyazadiradione	Estrogen receptor	ESR1
Epoxyazadiradione	Proto-oncogene tyrosine-protein kinase Src	SRC
7-Deacetyl dedunin	Caspase-3	CASP3

7-Deacetyl dedunin	Peroxisome proliferator-activated receptor gamma	PPARG
7-Deacetyl dedunin	Estrogen receptor	ESR1
7-Deacetyl dedunin	Proto-oncogene tyrosine-protein kinase Src	SRC
7-Deacetyl dedunin	Epidermal growth factor receptor	EGFR
7-Deacetyl dedunin	Matrix metalloproteinase-9	MMP9
7-Deacetyl dedunin	Growth factor receptor-bound protein 2	GRB2
7-Deacetyl dedunin	Cell division control protein 42 homolog	CDC42
Salannol	Estrogen receptor	ESR1
Salannol	Epidermal growth factor receptor	EGFR
Nimbinene	Estrogen receptor	ESR1
Nimbinene	Matrix metalloproteinase-9	MMP9
β-Sitosterol	Epidermal growth factor receptor	EGFR

Table 8: GO enrichment analysis of the "*Azadirachta Indica* leaves -target gene" interaction gene.

GO ID	GO Description	p-Value	Corrected p-Value	Cluster Frequency
5901	Caveola (CC)	2.53E-09	4.38E-07	8/124 6.4%
5737	Cytoplasm (CC)	3.95E-09	4.38E-07	90/124 72.5%
44424	intracellular part (CC)	1.52E-08	8.91E-07	110/124 88.7%
45121	membrane raft (CC)	1.61E-08	8.91E-07	11/124 8.8%
5829	Cytosol (CC)	3.28E-08	1.46E-06	30/124 24.1%
5622	Intracellular (CC)	5.58E-08	2.06E-06	111/124 89.5%
30424	Axon (CC)	4.14E-04	1.15E-02	7/124 5.6%
44421	extracellular region part (CC)	4.37E-04	1.15E-02	18/124 14.5%
267	cell fraction (CC)	4.74E-04	1.15E-02	19/124 15.3%
5615	extracellular space (CC)	5.19E-04	1.15E-02	15/124 12.0%
3707	steroid hormone receptor activity (MF)	4.73E-24	2.37E-21	17/125 13.6%
4879	ligand-dependent nuclear receptor activity (MF)	1.57E-23	3.93E-21	17/125 13.6%
3824	catalytic activity (MF)	2.27E-21	3.80E-19	93/125 74.4%
4713	protein tyrosine kinase activity (MF)	1.09E-15	1.37E-13	17/125 13.6%
4672	protein kinase activity (MF)	6.53E-14	6.55E-12	27/125 21.6%
16740	transferase activity (MF)	1.65E-13	1.38E-11	44/125 35.2%
16773	phosphotransferase activity, alcohol group as acceptor (MF)	7.35E-13	5.27E-11	28/125 22.4%
16301	kinase activity (MF)	9.07E-13	5.69E-11	29/125 23.2%
16772	transferase activity, transferring phosphorus-containing groups (MF)	5.56E-11	3.10E-09	29/125 23.2%
1883	purine nucleoside binding(MF)	1.68E-10	8.41E-09	39/125 31.2%
3708	retinoic acid receptor activity(MF)	1.92E-10	8.43E-09	5/125 4.0%
8152	metabolic process (BP)	1.95E-21	4.48E-18	103/124 83.0%
42221	response to chemical stimulus (BP)	3.97E-21	4.57E-18	53/124 42.7%
10033	response to organic substance (BP)	4.99E-20	3.83E-17	41/124 33.0%
9719	response to endogenous stimulus (BP)	1.50E-18	8.61E-16	31/124 25.0%
42127	regulation of cell proliferation (BP)	9.30E-18	4.28E-15	38/124 30.6%
9725	response to hormone stimulus (BP)	7.01E-17	2.69E-14	28/124 22.5%
44238	primary metabolic process (BP)	6.30E-16	2.07E-13	90/124 72.5%
48545	response to steroid hormone stimulus (BP)	5.31E-15	1.53E-12	20/124 16.1%
48518	positive regulation of biological process (BP)	1.42E-14	3.64E-12	55/124 44.3%
6468	protein amino acid phosphorylation (BP)	3.44E-14	7.92E-12	30/124 24.1%
8284	positive regulation of cell proliferation (BP)	1.34E-13	2.81E-11	25/124 20.1%

Table 9: Results of KEGG enrichment analysis of "*Azadirachta Indica* leaves -target gene" interactive gene.

KEGG ID	GO Term	P-Value	Corr P-Value
hsa05200	Pathways in cancer	1.74e-39	3.87e-36
hsa05225	Hepatocellular carcinoma	1.07e-18	2.16e-16
hsa04151	PI3K-Akt signaling pathway	1.23e-17	1.82e-15
hsa05205	Proteoglycans in cancer	1.76e-17	2.31e-15

hsa01100	Metabolic pathways	2.55e-17	3.15e-15
hsa03320	PPAR signaling pathway	1.02e-16	1.14e-14
hsa05418	Fluid shear stress and atheros...	2.65e-15	2.46e-13
hsa01524	Platinum drug resistance	3.22e-15	2.87e-13
hsa05215	Prostate cancer	5.61e-14	4.17e-12
hsa04014	Ras signaling pathway	1.26e-12	7.02e-11

Table 10: The enrichment gene list of KEGG of "*Azadirachta Indica* leaves –breast cancer" interaction gene.

KEGG ID	Enriched genes in the KEGG pathway
hsa05200	TGFB2CASP3EGFRNOS2NQO1AKT2GSK3BRARARARBSTAT1JAK2 JAK3FGFR1IGF1RPIM1RXRARXRBGSTA1PPARGMDM2BMP2CASP 7GSTO1GSTT2ESR1GSTM1GSTM2HMOX1XIAPKITMETGSTP1GRB 2IL2CDK6MMP9MMP2CDC42
hsa05225	GSTP1IGF1RGSTO1GSTT2GSTM1GSTM2HMOX1GSTA1NQO1METAKT2GRB2CDK6E GFRGSK3BTGFB2
hsa04151	IGF1RNOS3EPHA2ERBB4IL2EGFRRXRAKITAKT2METINSRGRB2JAK2JAK3CDK6PDP K1MDM2GSK3BFGFR1
hsa05205	SRCIGF1RCASP3ERBB4ESR1EGFRTGFB2METAKT2GRB2MMP9PDPK1MDM2CDC42 MMP2FGFR1
hsa01100	VDRGSTA1NQO1OATACADMFECHDCKCBR1PDE3BPYGLPDE5AA DH1BNOS2NOS3ABOTPH1DUTADKBHMTGSTO1GSTT2MTHFD1S DSGSTM1GSTM2HMOX1ALDH2GSTP1PNMTCA2PDE4D
hsa03320	FABP7RXRARXRBFABP6PPARGFABP4FABP5PPARAPDPK1ACADMAPOA2NR1H3
hsa05418	GSTP1NOS3GSTT2SRCGSTM1GSTM2HMOX1GSTA1NQO1AKT2GSTO1MMP9MMP2
hsa01524	GSTP1GSTO1GSTT2GSTM1GSTM2GSTA1XIAPAKT2PDPK1MDM2CASP3
hsa05215	IGF1REGFRGSTP1GSK3BAKT2GRB2MMP9PDPK1MDM2MMP3FGFR1
hsa04014	IGF1RRAB5AEPHA2EGFRAKT2KITMETINSRGRB2ZAP70PAK6CDC42FGFR1

Table 11: Docking results of receptor proteins and ligand compounds.

Compound	Receptor Proteins	PDB ID	Target Genes	CB DOCK
Gedunin	Proto-oncogene tyrosine-protein kinase Src	4U5J	SRC	-9.43
Nimbin	Proto-oncogene tyrosine-protein kinase Src	4U5J	SRC	-8.73
Nimbin	Matrix metalloproteinase-9	1HOV	MMP9	-6.04
Nimbolide	Peroxisome proliferator-activated receptor gamma	2PRG	PPARG	-7.62
Nimbolide	Epidermal growth factor receptor	4G5J	EGFR	-8.5
Nimbolide	Matrix metalloproteinase-9	1HOV	MMP9	-6.8
Nimocinol	Estrogen receptor	1UOM	ESR1	-7.4
Nimocinol	Epidermal growth factor receptor	4G5J	EGFR	-8.05
Meliantriol	Peroxisome proliferator-activated receptor gamma	2PRG	PPARG	-8.32
Meliantriol	Estrogen receptor	1UOM	ESR1	-7.13
Meliantriol	Growth factor receptor-bound protein 2	2DKZ	GRB2	-7.73
Nimbolin A	Estrogen receptor	1UOM	ESR1	-7.43
Margolonone	Peroxisome proliferator-activated receptor gamma	2PRG	PPARG	-8.34
Isomargolonone	Peroxisome proliferator-activated receptorgamma	2PRG	PPARG	-9.44
Catechin	Proto-oncogene tyrosine-protein kinase Src	4U5J	SRC	-7.84
Catechin	Epidermal growth factor receptor	4G5J	EGFR	-7.75
Catechin	Caspase-3	6DEU	CASP3	-7.15
Epicatechin.	Proto-oncogene tyrosine-protein kinase Src	4U5J	SRC	-8.14
Epicatechin.	Epidermal growth factor receptor	4G5J	EGFR	-7.75
Azadirone	Proto-oncogene tyrosine-protein kinase Src	4U5J	SRC	-8.63
Azadiradione	Estrogen receptor	1UOM	ESR1	-6.93
Epoxyazadiradione	Estrogen receptor	1UOM	ESR1	-7.73
Epoxyazadiradione	Proto-oncogene tyrosine-protein kinase Src	4U5J	SRC	-9.44
7-Deacetyl dedunin	Caspase-3	6DEU	CASP3	-7.7
7-Deacetyl dedunin	Peroxisome proliferator-activated receptor gamma	2PRG	PPARG	-9.02
7-Deacetyl dedunin	Estrogen receptor	1UOM	ESR1	-8.03
7-Deacetyl dedunin	Proto-oncogene tyrosine-protein kinase Src	4U5J	SRC	-9.62
7-Deacetyl dedunin	Epidermal growth factor receptor	4G5J	EGFR	-8.5

7-Deacetyl dedunin	Matrix metalloproteinase-9	1HOV	MMP9	-7.54
7-Deacetyl dedunin	Growth factor receptor-bound protein 2	2DKZ	GRB2	-7.53
7-Deacetyl dedunin	Cell division control protein 42 homolog	5C2J	CDC42	-10.23
Salannol	Estrogen receptor	1UOM	ESR1	-6.43
Salannol	Epidermal growth factor receptor	4G5J	EGFR	-7.5
Nimbinene	Estrogen receptor	1UOM	ESR1	-6.6
Nimbinene	Matrix metalloproteinase-9	1HOV	MMP9	-6.6
β-Sitosterol	Epidermal growth factor receptor	4G5J	EGFR	-8.7

CONCLUSION

Based on a network pharmacology analysis, we investigated the systematic mechanisms of *Azadirachta indica* leaves activity against breast cancer. On human breast Cancer cells, it elicited anticancer effects. Twenty-two chemical compounds were identified as potentially bioactive, with the potential to target 125 breast cancer-associated genes/proteins and exert therapeutic effects. The GO terms associated with the modulation of cellular processes, such as cell proliferation, cell cycle progression, and cell apoptosis, were enriched in the targets. Pathway enrichment analysis of the targets revealed that the targets were significantly enriched in a variety of pathways important for BC pathology, including the PI3K-Akt, MAPK, focal adhesion, FoxO, TNF, and estrogen signalling pathways. Our findings, based on a network perspective, provide detailed insights into the therapeutic properties of *Azadirachta indica* leaves in breast Cancer treatment in Future.

REFERENCES

1. Rahmani AH, Almatroudi A, Alrumaihi F, Khan AA. Pharmacological and therapeutic potential of neem (Azadirachta indica). phcogrev.com [Internet]. 2018 [cited 2022 Mar 17]; Available from: https://phcogrev.com/sites/default/files/PhcogRev_2018 _12_24 250.pdf
2. Dash S, Dixit S, Biochem SS-BA, 2017 undefined. Phytochemical and biochemical characterizations from leaf extracts from Azadirachta Indica: an important medicinal plant. researchgate.net [Internet]. 2017 [cited 2022 Mar 17]; 6: 323. Available from: https://www.researchgate.net/profile/Souvagyalaxmi-Sahoo/publication/318193124_
3. Paul R, Prasad M, Sah NK. Anticancer biology of Azadirachta indica L (neem): A mini review. Cancer Biol Ther., 2011 Sep 15; 12(6): 467–76.
4. Alternative MA-E-BC and, 2016 undefined. Therapeutics role of Azadirachta indica (Neem) and their active constituents in diseases prevention and treatment. hindawi.com [Internet]. [cited 2022 Mar 17]; Available from: https://www.hindawi.com/journals/ecam/2016/7382506/.
5. Sharma G, Dave R, … JS-J of advanced, 2010 undefined. Various types and management of breast cancer: an overview. ncbi.nlm.nih.gov [Internet]. [cited 2022 Mar 17]; Available from: https://www.ncbi.nlm.nih.gov/pmc/articles/pmc3255438/.
6. Chakraborty T, Sharma A, Gupta S, Sharma A, Pahari PK. Biomarkers: An Important Tool for Diagnosing and Treating Breast Cancer. researchgate.net [Internet]. 2020 [cited 2022 Mar 17]; 32(12): 46–54. Available from: https://www.researchgate.net/profile/Tulshi-Chakraborty/publication/343349978_.
7. Sharma G, Dave R, … JS-J of advanced, 2010 undefined. Various types and management of breast cancer: an overview. ncbi.nlm.nih.gov [Internet]. [cited 2022 Mar 17]; Available from: https://www.ncbi.nlm.nih.gov/pmc/articles/pmc3255438/.
8. Zhang X, Shen T, Zhou X, Tang X, Gao R, reports LX-S, et al. Network pharmacology based virtual screening of active constituents of Prunella vulgaris L. and the molecular mechanism against breast cancer. nature.com [Internet]. [cited 2022 Mar 17]; Available from: https://www.nature.com/articles/s41598-020-72797-8.
9. Morris GM, Lim-Wilby M. Molecular docking. In... - Google Scholar [Internet]. [cited 2022 Mar17]. Available from: https://scholar.google.com/scholar?hl=en&as_sdt=
10. 0%2C5&q=9.%09Morris+GM%2C+LimWilby+M.+Molecular+docking.+In+Molecular+modelling+of+ proteins+2008+%28pp.+365-382%29.+Humana+Press&btnG=.
11. Kim S, Thiessen PA, Bolton EE, Chen J, Fu G, Gindulyte A, et al. PubChem Substance and Compound databases. Nucleic Acids Res [Internet]. 2016 [cited 2022 Mar 17]; 44(D1): D1202–13. Available from: https://pubmed.ncbi.nlm.nih.gov/26400175/
12. Wang Y, Xiao J, Suzek TO, Zhang J, Wang J, Bryant SH. PubChem: a public information system for analyzing bioactivities of small molecules. Nucleic Acids Res [Internet]. 2009 [cited 2022 Feb 24]; 37(Web Server issue): W623. Available from: https://www.nature.com/articles/srep42717
13. Daina A, Michielin O, Zoete V. SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci Reports 2017 71 [Internet]. 2017 Mar 3 [cited 2022 Feb 25]; 7(1): 1–13. Available from: https://www.nature.com/articles/srep42717
14. Wang X, Shen Y, Wang S, Li S, Zhang W, Liu X, et al. PharmMapper 2017 update: a web server for potential drug target identification with a

comprehensive target pharmacophore database. Nucleic Acids Res [Internet]. 2017 Jul 3 [cited 2022 Feb 25]; 45(W1): W356–60. Available from: https://pubmed.ncbi.nlm.nih.gov/28472422/

15. Liu X, Ouyang S, Yu B, Liu Y, Huang K, Gong J, et al. PharmMapper server: a web server for potential drug target identification using pharmacophore mapping approach. Nucleic Acids Res [Internet]. 2010 Apr 29 [cited 2022 Feb 25]; 38(Web Server issue): W609. Available from: /pmc/articles/PMC2896160/
16. Rappaport N, Twik M, Plaschkes I, Nudel R, Stein TI, Levitt J, et al. MalaCards: an amalgamated human disease compendium with diverse clinical and genetic annotation and structured search. Nucleic Acids Res [Internet]. 2017 Jan 4 [cited 2022 Feb 25]; 45(D1): D877–87. Available from: https://academic.oup.com/nar/article/45/D1/D877/2572056
17. Athanasios A, Charalampos V, Vasileios T, Ashraf G. Protein-Protein Interaction (PPI) Network: Recent Advances in Drug Discovery. Curr Drug Metab [Internet]. 2017 Jan 24 [cited 2022 Feb 25]; 18(1): 5–10. Available from: https://pubmed.ncbi.nlm.nih.gov/28889796/
18. Hillenmeyer S, Davis LK, Gamazon ER, Cook EH, Cox NJ, Altman RB. Stams: STRING-assisted module search for genome-wide association studies and application to autism. Bioinformatics, 2016 Dec 15; 32(24): 3815–22.
19. Szklarczyk D, Morris JH, Cook H, Kuhn M, Wyder S, Simonovic M, et al. The STRING database in 2017: quality-controlled protein-protein association networks, made broadly accessible. Nucleic Acids Res [Internet]. 2017 [cited 2022 Feb 25]; 45(Database issue): D362. Available from: /pmc/articles/PMC5210637/
20. Shannon P, Markiel A, Ozier O, Baliga NS, Wang JT, Ramage D, et al. Cytoscape: a software environment for integrated models of biomolecular interaction networks. Genome Res [Internet]. 2003 Nov [cited 2022 Feb 25]; 13(11): 2498–504. Available from: https://pubmed.ncbi.nlm.nih.gov/14597658/
21. Ashburner M, Ball CA, Blake JA, Botstein D, Butler H, Cherry JM, et al. Gene Ontology: a tool for the unification of biology. Nat Genet 2000 251 [Internet]. 2000 May [cited 2022 Feb 26]; 25(1): 25–9. Available from: https://www.nature.com/articles/ng0500_25
22. The Kyoto Encyclopedia of Genes and Genomes—KEGG. Yeast, 2000 Jan 1; 1(1): 48–55.
23. Grosdidier A, Zoete V, Michielin O. SwissDock, a protein-small molecule docking web service based on EADock DSS. Nucleic Acids Res [Internet]. 2011 Jul 1 [cited 2022 Feb 26]; 39 (Web Server issue). Available from: https://pubmed.ncbi.nlm.nih.gov/21624888/
24. Liu Y, Grimm M, Dai WT, Hou MC, Xiao ZX, Cao Y. CB-Dock: a web server for cavity detection-guided protein-ligand blind docking. Acta Pharmacologica Sinica, 2020 Jan; 41(1): 138-44.
25. Cao Y, Li L. Improved protein-ligand binding affinity prediction by using a curvature-dependent surface-area model. Bioinformatics, 2014 Jun 15; 30(12): 1674- 80.