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Evaluation of Antioxidant activity of *Andira inermis* (*W. Wright) H.B.K.* Leaves extracts by DPPH free radical method and *In-silico* Characterization of its isoflavones as potential pharmacophores

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A B S T R A C T

Homoeopathic floras have been a valuable and immense source of therapeutic drugs for eras and still numerous of currently used drugs are plant-derived natural products or their derivatives. A well accepted scientific consensus emanating from several scientific investigations is that different plant extracts contains high levels of antioxidants polyphenols including isoflavones. This work had two objectives: the first, to evaluate the Antioxidant activity of *Andira inermis* leaf extracts by DPPH free radical method and second, to assess for drug likeness properties, bioactivity score, ADME/T profiles, and health effects of its six isolated isoflavones by using bioinformatics tools. The dose dependent scavenging was observed at concentrations 20, 40, 60, 80 and 100 µg/ml, which were compared to ascorbic acid. The result shows that ethyl acetate extract having good antioxidant activity when compared to methanol extract and ascorbic acid. The six isolated compounds were tested for pharmacokinetic profiles and biological activities using various improved generation chemoinformatics and bioinformatics tools and the result shows that all the compounds were obeying Lipinski's RO5 and having good pharmacokinetics profile with many pharmacological activities, thus this work findings provide evidence that the crude ethyl acetate extract of *Andira inermis* is a potential source of natural antioxidants, and the isolated compounds were potential pharmacophres thus, combination of computational approach and experimental analysis provides efficient, cost effective and time saving pathway for Drug discovery.

Keywords: *Andira inermis*, Antioxidants, DPPH scavenging assay, Isoflavones, ADMET, pharmacokinetics, drug discovery.

A R T I C L E I N F O

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1. Introduction

Oxygen is one of the most essential element for survival but under certain abnormal physiological conditions oxygen, react with free radicals to become radicals themselves, also referred to as reactive oxygen species (ROS) (Jamkhande *et al., 2014*). The ROS include superoxide anions (O^{+2}), hydrogen peroxide (H_2O_2) and hydroxyl radicals (^{+}OH) generally these are formed under normal conditions but become fatal when not being eliminated by the endogenous systems (Choi *et al.,* 2002). The clinical and experimental evidences revealed that free radicals and reactive oxygen species (ROS) are the source of primary catalyst which helps in oxidation which in turn creates the oxidative stress which damages nucleic acids, proteins, lipids and carbohydrates etc., (Prakash and Gupta, 2009) this results in numerous diseases and disorders disorders such as arthritis, connective tissue disorders, liver disorders, neurodegenerative disorders, diabetes, chronic inflammation, cancer and in the process of ageing (Katiyar *et al*., 2013).

Medicinal Plants are the natural and important sources antioxidants (chanda and Dave, 2009), Antioxidants is any substance that directly scavenges Reactive Oxygen Species (ROS) orindirectly acts to up-regulate antioxidant defences or inhibit ROS production. Ethnobotanical sources constitute an important source of bioactive components which differ widely in terms of structures, phrmacological activities and mechanisms of actions. Various phytochemical components, especially polyphenols (such as isoflavones, flavonoids, phenyl propanoids, phenolic acids, tannins, etc) are known to be responsible for the free radical scavenging and antioxidant activities of plants (Sateesh, 2009; Sangeetha and Vijayalakshmi, 2011; Naik et al., 2014).

Andira inermis (W. Wright) H.B.K. (Fabaceae) is commomly known as cabbage tree, river almond, cabbage bark, cabbage angelin, brown heart. *Andira inermis* is a deciduous tree up to 15(-35) m tall, bole usually short, straight and cylindrical, up to 50(-100) cm in diameter. This is a deciduous tree which continually replaces its foliage throughout the year especially before flowering. As a febrifuge, the bark is boiled in milk, sweetened water or performed in pills. It is also used as a purgative, vermifuge, or for dermal irritations. The bark is used as a vermifuge, seeds are purgative and have narcotic properties (Orwa *et al*., 2009). Krafts *et al* reported six isoflavones from *Andirainermis*(table 1) in which Calycosin and genistein possess in vitro activity against the chloroquine-sensitive strain poW and the chloroquine-resistant clone Dd2 of *Plasmodium falciparum* .The present investigation aimed to evaluate the antioxidant potential of *Andira inermis* leaves extract by DPPH free radical scavenging assay and to assess the pharmacokinetics profiles and biological activities of the isolated phytocompounds by *in silico* methods with the help of advanced chemoinformatics and bioinformatics tools, keeping in mind to provide novel and thereupatic drugs.

2. Materials and Methods

Collection of plant materials and Preparation of leaf extracts: The leaves of *Andira inermis* were collected from Lalbagh Botanical garden, Bangalore. The leaves were washed with distilled water and shade-dried for 15 days and finally milled to a coarse powder using electric grinder. 20 gm of powdered material was soxhlet extracted with different solventsviz., methanol and ethylacetate (Sherikar and Mahanthesh, 2015).After extraction the extracts was concentrated by means of a rotary evaporator and then, the obtained concentrated samples were stored in sterile capped bottles under refrigeration condition (4 °C) until used.

DPPH radical scavenging assay

The ability of the extracts toscavenge DPPH radical was determined according to the method described by (chanda and Dave, 2009). The DPPH is a stable free radical and is widely used to assess the radical scavenging activity of antioxidant compounds. This method is based on the reduction of DPPH in methanol solution in the presence of a hydrogen–donating antioxidant due to the formation of the non radical form DPPH-H (Blois, 1958). 4.3 mg of DPPH (1, 1-Diphenyl –2-picrylhydrazyl) dissolved in 3.3 ml methanol and itis protected from exposure of light by covering the test tubes with aluminum foil. 150 µl DPPH solutions were added to 3ml methanol and absorbance was taken immediately at 517nm for control reading. Each of the extract samples with different concentration i.e., 20, 40, 60, 80, 100µg/ml, is taken and made up to 3ml using methanol and to each 150 µl DPPH will be added. Absorbances were taken after 15 minutes of incubation in dark chamber at 517nm using methanol as blank on UV-visible spectrometer. The DPPH free radical scavenging activity were calculated using the following formula: Inhibition (%) = (A0 – A1 / A0) × 100, Where; A0 is the absorbance of control and A1 is the absorbance of test. The antioxidant activity of the sample was expressed as IC50 value, was defined as concentration (in µg/ml) of sample that inhibits the formation of DPPH radicals by 50% (Argolo *et al*., 2004; Jamkhande *et al., 2014*).

***In silico* analysis of *pharmacokinetics* profiles**

Preparation of ligands-isoflavones

The six isoflavones isolated from *Andira inermis* (Kraft *et al*., 2000*) viz*.**,** **"**Biochanin A, calycosin, formononetin, genistein, pratensein, and prunetin" were tested for their pharmacokinetics i.e., ADMET analysis, pharmacological Potential and biological activity for use as promising phytopharmaceuticals. The 2D and 3D structures of these isolated compounds were retrieved from online server; PubChem (http://pubchem.ncbi.nlm.nih.gov/) and each chemical compound was constructed using ACD/ Chem

sketch software and saved in the '.mol' format (Mathew *et al*., 2016; Riju *et al*., 2009).

Computation of pharmacokinetics profiles and biological activity: All the six compounds were tested individually for their pharmaocological potential and biological activities. The "drug-likeness" properties of the compounds were carried out with Lipinski's "Rule of Five", ro5 (Lipinski, 2004) using Mol Soft online tool, and the pharmacokinetic profiles such as Absorption, Distribution, Metabolism, Excretion and the Toxicity of the phytochemicals is evaluated using admet SAR (http:// www.admetexp.org) online server which provides the latest and most comprehensive manually curated data for diverse chemicals associated with known ADMET profiles (Paramashivam *et al*., 2015; Polachi *et al*., 2015). Using Molinspiration online server bioactivity scores for the most important pharmacophoredrug targets such as GPCR ligand, Ion channel modulator , Kinase inhibitor, Nuclear receptor ligand, Protease inhibitor, Protease inhibitor and Enzyme inhibitor were predicted (Balasundaram *et al., 2016* ; Polachi *et al*., 2015). The lethal dose$_{50}$ (LD_{50}) in mouse and rat by intra peritoneal, oral, intravenous, subcutaneous and the probability of toxic health effects were checked in blood, cardiovascular system, gastro intestinal system, kidney, liver, and lung tissues using ACD/I labs which is a free online server which consists of a set of molecular and ADMET descriptors. PASS (Prediction of activity spectra for substances) is a online computational server employed for prediction of pharmacological activities and mechanism of actions based on structural activity relationship (SAR).

3. Results and Discussions

Radical scavenging activity (RSA) of *Andira inermis* plant extracts. (DPPH assay): The antioxidant potential of *Andira inermis* extracts was determined against ascorbic acid as percent inhibition of DPPH free radicals. The capacity for scavenging free radicals was evaluated for the methanol and ethyl acetate extracts and the results are shown in Fig. 1.From the dose dependent response value of DPPH radical scavenging activity of different plant extracts of *Andirainermis*, it was observed that the ethyl acetate extract had higher radical scavenging activity than methanol extract and standard ascorbic acid. At a concentration of 40µg/ml, the scavenging activity of ethyl acetate extract reached 57%, which was comparable to that of standard. The IC_{50} values were found to be 47, 55 and 90 µg/ml for ethylacetate, methanol and ascorbic acid respectively, thus Theethyl acetate plant extract of *Andira inermis* showed excellent antioxidant and free radical scavenging activity.

Evaluation of Drug-Likeness parameters

The drug-likness properties of the compounds was predicted using molsoft online server based on the 'rule-of-five' given by Lipinski, the rule states that most "druglike" molecules must have log P≤ 5(partition coefficient) , molecular weight ≤ 500, number of hydrogen bond acceptors(HBA) ≤ 10, and number of hydrogen bond donors(HBD) ≤ 5. Molecules violating more than one of these rules may have problems with oral bioavailability (Sateesh *et al* 2016). By investigation it was pleasant to see that all the six isoflavones significantly following the Lipinski's RO5 and having good oral bioavailability (table 2) with good Drug-likeness model score (fig.2-fig.7) which shows that these compounds are potential pharmocophores.

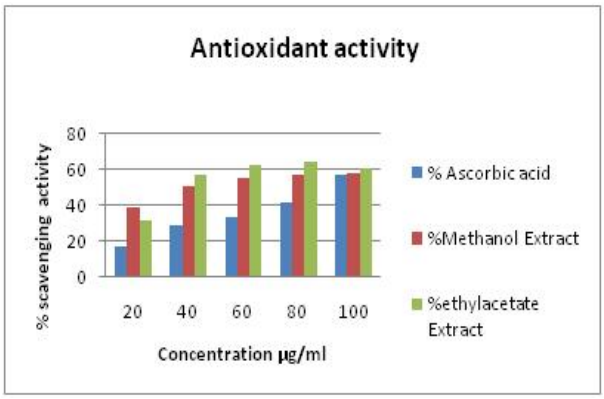


Figure 1: Shows DPPH free radical scavenging activity of *Andirainermis.*

Prediction of bioactivity score

The bioactivity scores was predicted using molinspiration tool (www.molinspiration.com) for the most important drug targets (GPCR ligands, kinase inhibitors, ion channel modulators, enzymes and nuclear receptors) and the Drug likeliness property of six compounds against these targets were depicted in table 3 .The compound having bioactivity score more than 0.00 is likely to possess considerable biological activities, values -0.50 to 0.00 are expected to be moderately active and if score is less than -0.50, it is presumed to be inactive (Paramashivam *et al*., 2015). Hence from the evaluated scores one can say that all the compounds having bioactivity score in acceptable ranges.

ADME/T analysis:

The knowledge of pharmacokinetics and pharmaco dynamics of compounds is very essential in order to provide safe and effective drug therapy. Since most of the drug like compounds just fails to enter the market as they have poor of pharmacokinetics profiles and high range of toxicity (Ntie-Kang, 2013). In view of these, computer-based methods like ADMET tool plays a vital role in the studies of molecular descriptors and drug-likeness properties (Polachi*et al*., 2015; Lombardo *et al*., 2003).The various parameters such as blood brain barrier , Caco-2 cell permeability, Human intestinal absorption, P-gp substrate, P-gp inhibitor, Ames mutagenecity and carcinogenicity were analyzed through computational methods by employing Admet SAR tool,this database is having 22 qualitative classification and 5 quantitative regression models with highly predictive accuracy, used to estimate mammalian ADMET properties for novel compounds (Balakin *et al*., 2005). The predicted values of ADMET parameters were reported in table 4 and It was fortunate to see that all the compounds predicted to be having very good ADMET profiles with neither toxic nor mutagenic in nature.

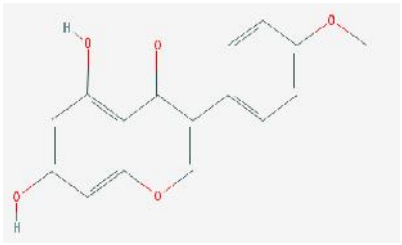
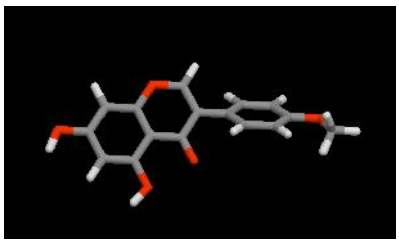
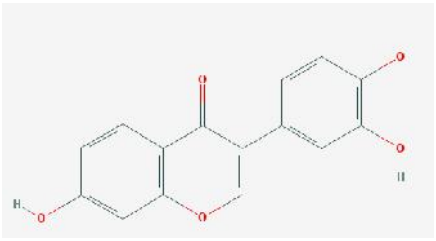
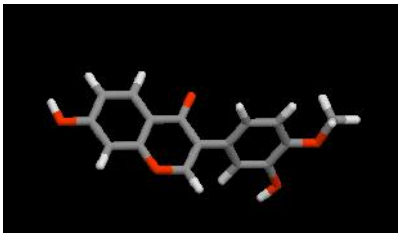
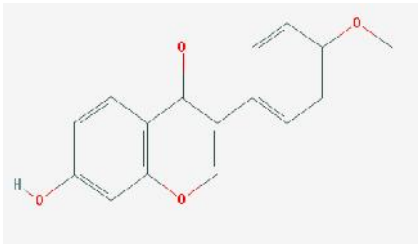
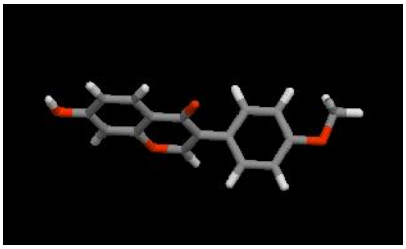
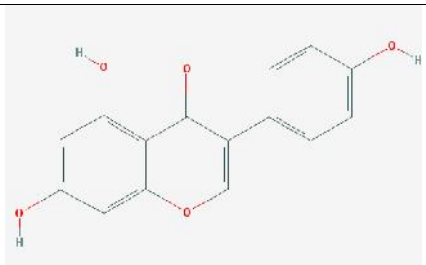
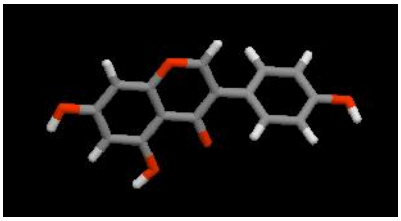
Prediction of Lethal dose 50 values and probability of health effects: The LD50 values and probability of health

effects was computed using ACD/I-Lab (https:/ /ilab.acdlabs.com/). The lethal dose values of compounds were predicted by the cumulative potential of acute toxicity that has administered through oral, intraperitoneal, intravenous and subcutaneous on mouse and rat models and the adverse effects of compounds were tested with different organs and their systems viz., blood, cardiovascular system, gastrointestinal system, kidneys, liver, and lungs were represented in table 5. The overall results suggested that all compounds had less toxic effect on internal tissues and no side-effect were observed in the tested dosages.

Prediction of pharmacological potential:

The biological activities of the six compounds was predicted with the help of PASS (Prediction of activity spectra for substances) computer program (http://www.way2drug.com/ PASS online/) (Jamkhande *et al.*, 2014) and the various probable biological activities such as Antialcoholic, antiallergic, anticarcinogenic, antimutagenic, antiseborrheic, apoptosis agonist, anticarcinogenic, anti-Helicobacter pylori, anti-inflammatory, Antimycobacterial, antialcoholic, etc., shown by these compounds were reported in table 6. The program Prediction of this spectrum by PASS is based on structural activity relationship (SAR) analysis of the training set containing more than 205,000 compounds exhibiting more than 3750 kinds of biological activities. The predicted activity spectrum of a compound is estimates as probable activity (Pa) and probable inactivity (Pi) the values of Pa and Pi vary between 0.000 and 1.000. Only activities with Pa > Pi are considered as possible for a particular compound. If Pa > 0.7, the probability of experimental pharmacological action is high and if 0.5 < Pa < 0.7, probability of experimental pharmacological action is less (Goel *et al*., 2011; sateesh *et al*., 2016).

Table 1: 2D and 3D structures of isoflavones Isolated from *Andira inermis*

S.No	Compound	2D Structure	3D Structure
1	Biochanin A		
2	Calycosin		
3	Formonentin		
4	Genistein		

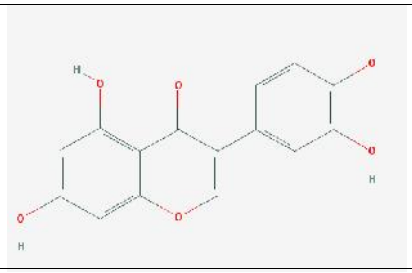
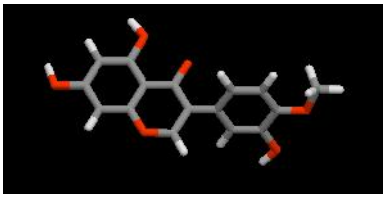
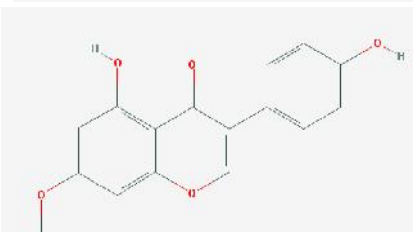
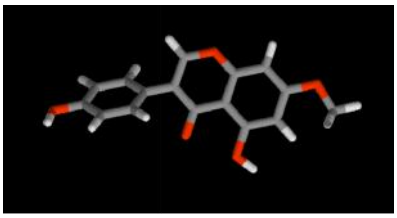
5	Pratensein		
6	Prunetin		

Table 2: Lipinski rule of five and Drug-likeness properties prediction using Molsoft.

Compound	Molecular Formula	Molecular Weight ≤ 500	Hydrogen Bond accepter (HBA) ≤ 10	Hydrogen Bond Donator (HBD)≤ 5	Mol LogP* P≤ 5	TPSA#	Drug-likeness model score
1	C16 H12 O5	284.07	5	2	3.07	79.90	0.35
2	C16 H12 O5	284.07	5	2	3.07	79.90	0.37
3	C16 H12 O4	268.07	4	1	3.45	59.67	0.70
4	C15 H10 O5	270.05	5	3	2.72	90.89	0.71
5	C16 H12 O6	300.06	6	3	2.69	100.13	0.25
6	C16 H12 O5	284.07	5	2	3.07	79.90	0.60

*LogP: Logarithm of the octanol/water partition coefficient, #TPSA: Topological polar surface area

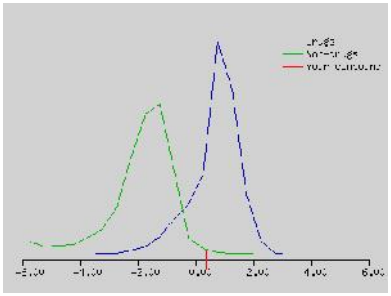


Fig2. Drug-likenessmodel score: **0.35**

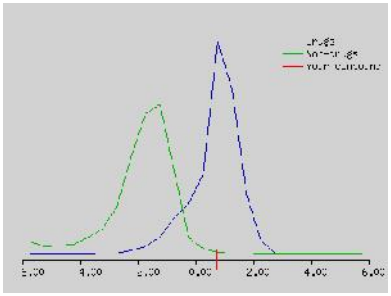


Fig3. Drug-likeness model score: **0.37**

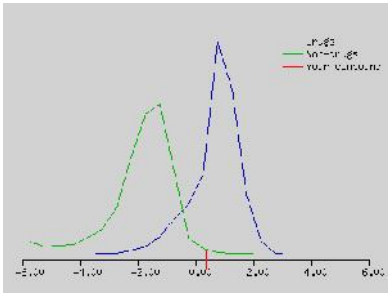


fig4. Drug-likeness model score:0.70

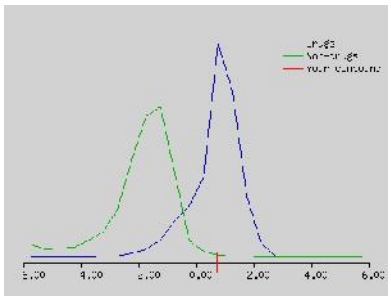


Fig5. Drug-likeness model score: 0.71

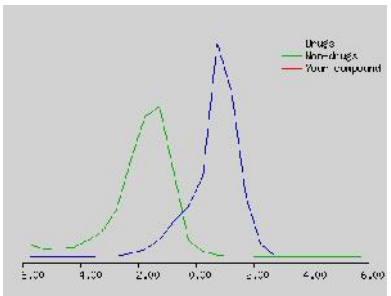


Fig 6. Drug-likeness model score: **0.25**

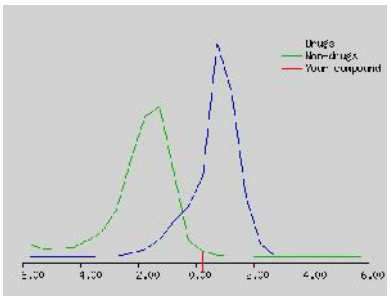


Fig7. Drug-likeness model score: **0.60**

Table 3: Bioactivity scores of Phytocompounds predicted by Molinspiration

Compond	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
1	-0.23	-0.59	-0.07	0.23	-0.66	0.07
2	-0.25	-0.65	-0.08	0.06	-0.78	0.01
3	-0.30	-0.69	-0.19	0.05	-0.80	-0.02
4	-0.22	-0.54	-0.06	0.23	-0.68	0.13
5	-0.19	-0.56	0.03	0.22	-0.65	0.09
6	-0.23	-0.59	-0.07	0.23	-0.66	0.07

Table 4: ADME/TOX and pharmacological parameter assessment of phytocompounds predicted using admet SAR toolbox.

Compond	PlogBB[a]	PCaco[b]	log_{HIA}[c]	logpGI (substrate)[d]	logpGI (non-inhibitor)[e]	PlogS[f]	AMES Toxicity	Carcin-ogens
1	0.5674	0.9526	0.9816	0.6232	0.8111	-3.1911	NT	NC
2	0.5447	0.8934	0.9898	0.6272	0.6246	-3.4244	NT	NC
3	0.7840	0.9438	0.9949	0.5366	0.5992	-3.4576	NT	NC
4	0.6785	0.7002	0.9877	0.5000	0.9288	-3.0925	NT	NC
5	0.6382	0.8866	0.9783	0.6384	0.7108	-3.2219	NT	NC
6	0.5230	0.9478	0.9913	0.6115	0.7490	-3.3828	NT	NC

[a]-Predicted blood/brain barrier partition coefficient (concern value is −3.0 to 1.0) , [b]-predicted Caco-2 cell permeability in nm/s (acceptable range: −1 is poor, 1 is great), [c]-predicted human intestinal absorption in nm/s (acceptable range: 0 poor, >1 great), [d]-predicted P-gp substrate in nm/s (acceptable range of −5 is poor, 1 is great), [e]-predicted P-glycoprotein inhibitor in nm/s (accepted range: 0-1), [f]-predicted aqueous solubility, (concern value is −6.5 to –0.5). P-gp: P-glycoprotein, HIA: Human intestinal absorption, ADME: Absorption, distribution, metabolism, excretion NT: Non Ames toxic, NC: non carcinogens.

Table 5: LD 50 and probability of health effects of Phytocompounds predicted using ACD/I-Lab.

ADME-TOX Parameters	1	2	3	4	5	6
LD_{50} mouse[1] (mg/kg, intraperitoneal)	250	70	53	320	530	390
LD_{50} mouse[1] (mg/kg, oral)	850	1400	1900	960	570	1200
LD_{50} mouse[1] (mg/kg, intravenous)	280	96	270	410	260	79
LD_{50} mouse[1] (mg/kg, subcutaneous)	340	220	1300	400	110	130
LD_{50} Rat[1] (mg/kg, intraperitoneal)	970	350	570	1300	710	430
LD_{50} Rat[1] (mg/kg, oral)	780	420	900	680	510	1500
Probability of blood effect[2]	0.41	0.41	0.43	0.46	0.4	0.41
Probability of cardiovascular system effect[2]	0.56	0.56	0.59	0.61	0.86	0.56
Probability of gastrointestinal system effect[2]	0.76	0.76	0.76	0.46	0.77	0.74
Probability of kidney effect[2]	0.61	0.52	0.59	0.59	0.8	0.61
Probability of liver effect[2]	0.49	0.41	0.22	0.51	0.41	0.49
Probability of lung effect[2]	0.25	0.25	0.27	0.25	0.26	0.3

[1]Estimates LD 50 value in mg/kg after intraperitoneal, oral, intravenous and subcutaneous administration to mice and rat, [2]Estimates probability of blood, gastrointestinalsystem, kidney, liver and lung effect at therapeutic dose range, 1-6 represents the phytocompounds and the drugs with moderate effect on reliability index (>0.5), the drugs with border line effect on reliability index (>0.3, <0.5), LD50: Lethal dose50.

Table 6: Predicted biological activities with Pa and Pi values of phytocompounds using PASS.

Compound	pa	pi	Predicted biological activity	pa	pi	Predicted biological activity
Biochanin A	0,869	0,003	Antimutagenic	0,574	0,015	Antiinfective
	0,823	0,007	Apoptosis agonist	0,602	0,031	Antiinflammatory
	0,803	0,018	Antiseborrheic	0,475	0,023	Antimycobacterial
	0,784	0,004	Cardioprotectant	0,577	0,012	Antineoplastic (breast cancer)

	0,776	0,006	Vasoprotector	0,449	0,004	Antineoplastic (uterine cancer)
	0,749	0,007	Antiprotozoal (Leishmania)	0,561	0,011	Antiosteoporotic
	0,735	0,007	Anticarcinogenic	0,678	0,004	Antioxidant
	0,737	0,020	Antineoplastic	0,454	0,016	Antiseptic
	0,584	0,004	Anti-Helicobacter pylori	0,447	0,015	Antitussive
	0,489	0,032	Antifungal	0,693	0,007	Chemopreventive
	0,411	0,038	Antihelmintic (Nematodes)	0,638	0,004	Chemoprotective
	0,584	0,004	Anti-Helicobacter pylori	0,776	0,006	Vasoprotector
	0,783	0,005	Antihypercholesterolemic			
Calycosin	0,864	0,003	Antimutagenic	0,686	0,009	Antihypercholesterolemic
	0,778	0,009	Apoptosis agonist	0,567	0,016	Antiinfective
	0,772	0,004	Cardioprotectant	0,565	0,039	Antiinflammatory
	0,720	0,009	Vasoprotector	0,426	0,022	Antileukemic
	0,717	0,007	Insulysin inhibitor	0,432	0,032	Antimycobacterial
	0,713	0,008	Anticarcinogenic	0,564	0,013	Antineoplastic (breast cancer)
	0,712	0,012	Kinase inhibitor	0,479	0,004	Antineoplastic (uterine cancer)
	0,705	0,009	Antiprotozoal (Leishmania)	0,418	0,095	Antinociceptive
	0,720	0,034	Antiseborrheic	0,498	0,015	Antiosteoporotic
	0,710	0,024	Antineoplastic	0,617	0,004	Antioxidant
	0,514	0,045	Alopecia treatment	0,489	0,021	Antiprotozoal (Trypanosoma)
Formonentin	0,539	0,004	Anti-Helicobacter pylori	0,426	0,071	Antipruritic, allergic
	0,415	0,017	Antialcoholic	0,491	0,013	Antiseptic
	0,407	0,050	Antiallergic	0,484	0,012	Antitussive
	0,713	0,008	Anticarcinogenic			
	0,831	0,003	Antimutagenic	0,647	0,036	Antineoplastic
	0,807	0,018	Antiseborrheic	0,480	0,004	Antineoplastic (uterine cancer)
	0,730	0,012	Apoptosis agonist	0,403	0,107	Antinociceptive
	0,525	0,004	Anti-Helicobacter pylori	0,545	0,012	Antiosteoporotic
	0,444	0,011	Antialcoholic	0,568	0,005	Antioxidant
	0,656	0,010	Anticarcinogenic	0,687	0,010	Antiprotozoal (Leishmania)
	0,400	0,050	Antifungal	0,479	0,022	Antiprotozoal (Trypanosoma)
	0,696	0,008	Antihypercholesterolemic	0,450	0,061	Antipruritic, allergic
	0,585	0,014	Antiinfective	0,443	0,017	Antiseptic
	0,534	0,047	Antiinflammatory	0,420	0,017	Antitussive
	0,432	0,032	Antimycobacterial	0,639	0,015	Vasoprotector
Genistein	0,874	0,003	Antimutagenic	0,431	0,014	Antialcoholic
	0,846	0,005	Apoptosis agonist	0,502	0,030	Antifungal
	0,844	0,004	Kinase inhibitor	0,480	0,020	Antihelmintic (Nematodes)
	0,832	0,013	Antiseborrheic	0,452	0,004	Antihemorrhagic
	0,822	0,004	Vasoprotector	0,648	0,010	Antiinfective
	0,792	0,004	Cardioprotectant	0,648	0,023	Antiinflammatory
	0,781	0,004	Antioxidant	0,471	0,024	Antimycobacterial
	0,777	0,005	Antihypercholesterolemic	0,571	0,013	Antineoplastic (breast cancer)
	0,753	0,018	Antineoplastic	0,437	0,030	Antiprotozoal (Trypanosoma)
	0,723	0,008	Anticarcinogenic	0,477	0,014	Antiseptic
	0,723	0,008	Antiprotozoal (Leishmania)	0,430	0,024	Antiviral (Herpes)
Pratensein	0,896	0,002	Antimutagenic	0,450	0,004	Antineoplastic (uterine cancer)
	0,849	0,003	Cardioprotectant	0,503	0,013	Antiseptic
	0,844	0,005	Apoptosis agonist	0,508	0,010	Antitussive
	0,822	0,004	Vasoprotector	0,413	0,030	Antiviral (Herpes)
	0,781	0,006	Anticarcinogenic	0,646	0,004	Chemoprotective
	0,772	0,005	Antihypercholesterolemic	0,459	0,012	Choleretic
	0,775	0,015	Antineoplastic	0,560	0,045	Cytoprotectant
	0,761	0,006	Antiprotozoal (Leishmania)	0,668	0,011	Cytostatic

	0,743	0,005	Chemopreventive	0,475	0,024	Vasodilator
	0,731	0,004	Antioxidant	0,420	0,047	Vasodilator, coronary
	0,713	0,035	Antiseborrheic	0,822	0,004	Vasoprotector
Prunetin	0,869	0,003	Antimutagenic	0,577	0,012	Antineoplastic (breast cancer)
	0,811	0,005	Kinase inhibitor	0,449	0,004	Antineoplastic (uterine cancer)
	0,803	0,018	Antiseborrheic	0,561	0,011	Antiosteoporotic
	0,784	0,004	Cardioprotectant	0,678	0,004	Antioxidant
	0,783	0,005	Antihypercholesterolemic	0,454	0,016	Antiseptic
	0,749	0,007	Antiprotozoal (Leishmania)	0,447	0,015	Antitussive
	0,735	0,007	Anticarcinogenic	0,410	0,031	Antiviral (Herpes)
	0,737	0,020	Antineoplastic	0,784	0,004	Cardioprotectant
	0,584	0,004	Anti-Helicobacter pylori	0,444	0,023	Carminative
	0,411	0,038	Antihelmintic (Nematodes)	0,693	0,007	Chemopreventive
	0,574	0,015	Antiinfective	0,638	0,004	Chemoprotective
	0,602	0,031	Antiinflammatory	0,518	0,009	Free radical scavenger
	0,475	0,023	Antimycobacterial	0,776	0,006	Vasoprotector

4. Conclusion

The use of ethnobotanicals to treat diseases is almost universal among non-industrialized societies and is more affordable than purchasing expensive modern pharmaceutical.From past decades, many people in developed countries are turning to alternative or ethnomedicinal therapies, due to side effect raised by conventional synthetic or semi synthetic drugs. In the present study, *in vitro* analysis of antioxidant potential of leaf extracts of *Andirainermis*by DPPH scavenging assay showed a good correlation with its reductive potentials specially the ethylacetate extract. From the computational PASS analysis it was revealed that all the six isolated isoflavones were having potential antioxidant activity moreover Genistein and Pratenseinwere having high pa value i.e. 0,781 and 0,731 respectively which shows that Genistein and Pratensein are majorly responsible antioxidant activity. The pharmacophore properties of the six compounds where found to be obeying the Lipinski rule of five parameters significantly and The ADMET prediction using admet SAR and ACD/i-lab revealed that all the compounds were in the acceptable range having no or less toxic effects with many biological activities. Overall our results concluded that all the compounds had significant phyto pharmaceutical potential. This information may be useful in drug design and clinical use of antioxidants. Moreover, such screening of plants can provide novel sources of new bioactive compounds with functional properties beneficial to restore health.

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