

## In Silico drug activity prediction of chemical components of *Acalypha Indica*

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### ABSTRACT

*Acalypha indica* distributed in the southern part of India, particularly in Tamilnadu has potential medicinal properties and used as diuretic, anthelmintic and for respiratory problems such as bronchitis, asthma and pneumonia.

*Acalypha indica* plant contains alkaloids, tannins, steroids, saponins, terpenoids, flavanoids, cardiac glycosides and phenolic compounds. Some chemical components were selected to theoretically evaluate their drug likeness score using some drug designing softwares.. Their molecular properties were calculated using the software Molinspiration., Prediction of biological activities and pharmacological activities were done using PASS online. Calculation of binding energy was done using Gaussian.

**Keywords:** *Acalypha indica*, Gaussian, Molinspiration and PASS online.

### INTRODUCTION

*Acalypha indica* is a common annual herb, found mostly in the backyards of houses and waste places throughout the plains of India. Plants are used as emetic, expectorant, laxative, diuretic, bronchitis, pneumonia, asthma and pulmonary tuberculosis<sup>[1]</sup>. Leaves are laxative and antiparasiticide; ground with common salt or quicklime or lime juice applied externally in scabies. Leaf paste with lime juice is prescribed for ringworm; leaf juice is emetic for children. A decoction of the leaves is given in earache. Powder of the dry leaves is given to children to expell worms; also given in the form of decoction with little garlic. In homoeopathy, the plant is used in severe cough associated with bleeding from lungs, haemoptysis and incipient phthisis. The plant contains kaempferol, a cyanogenetic glucoside, a base, triacetoneamine and an alkaloid, acalyphine. It also contains the amide, acalyphamide and some other amides, 2-methylantraquinone,

tri-O-methyl ellagic acid and  $\gamma$ -sitosterol,  $\beta$ -sitosterol glucoside, stigmasterol, n-octacosanol, quinine, tannin, resin and essential oil [2,3]. The plant is traditionally used as an expectorant against asthma and pneumonia, and also as an emetic, emmenagogue and anthelmintic [4]. *Acalypha indica* contains acalyphine which is used in the treatment of sore gums [5]. The plant is reported to have a post-coital antifertility effect, anti-venom properties [6], wound healing effects [7], antioxidant activities [8], anti-inflammatory effects [9], acaricidal effects [10], diuretic effects [11] and anti bacterial activities [12].

Drug design, sometimes referred to as rational drug design or simply rational design, is the inventive process of finding new medications based on the knowledge of a biological target. The drug is most commonly an organic small molecule that activates or inhibits the function of a biomolecule such as a protein, which in turn results in a therapeutic benefit to the patient. In the most basic sense, drug design involves the design of molecules that are complementary in shape and charge to the biomolecular target with which they interact and therefore will bind to it. Drug design frequently but not necessarily relies

on computer modeling techniques. This type of modeling is often referred to as computer-aided drug design. Drug design that relies on the knowledge of the three-dimensional structure of the biomolecular target is known as structure-based drug design. In addition to small molecules, biopharmaceuticals and especially therapeutic antibodies are an increasingly important class of drugs and computational methods for improving the affinity, selectivity, and stability of this protein-based therapeutics have also been developed. The phrase "drug design" is to some extent a misnomer. A more accurate term is ligand design (i.e., design of a molecule that will bind tightly to its target). [13].

Identification of a lead compound plays a major role in drug designing. Some of the chemical components of *Acalypha Indica* were selected to evaluate their drug likeness character, using softwares Gaussian, Molinspiration and PASS

## EXPERIMENTAL METHOD

### SOFTWARE'S USE

Using the softwares (Gaussian, Molinspiration and PASS online) the calculation of physical properties and

prediction of biological activity has been done for some of the chemical components of *Acalypha Indica* listed below.

1. Compound 1 - 2,5-Di-tert butylphenol
2. Compound 2 - 2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane
3. Compound 3 - Trimethyl[4-(1,1,3,3,-tetramethylbutyl)phenoxy]silane
4. Compound 4 - Triacetoneamine
5. Compound 5 - Kaempferol
6. Compound 6 - Acalyphin
7. Compound 7 - Aurantiamide
8. Compound 8 - Flindersin
9. Compound 9 - Octacosanol
10. Compound 10 - Quebrachitol
11. Compound 11 -  $\beta$ -Sitosterol
12. Compound 12 - Nicotiflorin
13. Compound 13 - Clitorin
14. Compound 14 - Succinimide
15. Compound 15 - 4-Ethyl-5-octyl-2,2-bis (trifluoromethyl)-1,3-dioxolane<sup>[14, 15]</sup>.

bond<sup>[16]</sup>.

## RESULT AND DISCUSSION

### SOFTWARE STUDIES

Gaussian was used to calculate the binding energy.

In general, binding energy represents the mechanical work that must be done against the forces which hold an object together, disassembling the object into component parts separated by sufficient distance that further separation requires negligible additional work. At the atomic level the atomic binding energy of the atom derives from electromagnetic interaction and is the energy required to disassemble an atom into free electrons and a nucleus. Electron binding energy is a measure of the energy required to free electrons from their atomic orbits. This is more commonly known as ionization energy. At the molecular level, bond energy and bond-dissociation energy are measures of the binding energy between the atoms in a chemical



S.NO	Components	STO-3G	3-21G	6-31G
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## **Gaussian**

Binding energy of the 15 compounds was calculated using Gaussian software. Hartree-Fock and DFT energies were calculated using the basic sets STO-3G, 3-21G, 6-31G. The calculated energies are given in the Table-1 and Table-2.

**Table-1: The binding energy calculated using Gaussian 5.0.9 by Hartree fock method**

1	2,5-Di-tert butylphenol	-597.8666	-602.2505	-605.3799
2	2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane	-645.3738	-650.5287	-653.9455
3	Trimethyl[4-(1,1,3,3-tetramethylbutyl)phenoxy]silane	-1005.7359	-1013.6752	-1018.9577
4	Triacetoneamine	-468.8778	-472.8209	-475.3268
5	Kaempferol	-1009.4746	-1016.9197	-1022.1855
6	Acalyphin	-1224.7244	-1234.2845	-1240.6281
7	Aurantiamide	-1462.2571	-1472.7643	-1480.4527
8	Flindersin	-655.4508	-660.1618	-663.5961
9	Octacosanol	-962.2058	-968.3470	-973.3229
10	Quebrachitol	-669.7477	-675.2082	-678.7033
11	$\beta$ -Sitosterol	-942.8205	-950.1457	-955.2184
12	Nicotiflorin	-2085.1480	-2101.1778	-2112.0208
13	Clitorin	-2642.4677	-2662.5828	-2676.2840
14	Succinimide	-353.7822	-356.3855	-358.2312
15	4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane	-1294.8175	-1307.6186	-1314.2902

**Table-2 Binding energy calculated using Gaussian 5.0.9 by DFT method**



S.No	Compounds	STO-3G	3-21 G	6-31 G
1	2,5-Di-tert butylphenol	-602.9108	-606.2868	-609.4820
2	2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane	-650.4494	-65.5946	-659.0896
3	Trimethyl[4-(1,1,3,3-tetramethylbutyl)phenoxy]silane	-1011.8269	-1019.9048	-1025.2843
4	Triacetoneamine	-472.2890	-476.3420	-478.8966
5	Kaempferol	-1015.1921	-1022.9400	-1028.3117
6	Acalyphin	-1231.8052	-1241.6906	-1248.1752
7	Aurantiamide	-1471.4516	-1482.2821	-1490.1015
8	Flindersin	-659.4792	-664.3406	-667.8365
9	Octacosanol	-968.7508	-975.2533	-980.3188
10	Quebrachitol	-673.4554	-679.0381	-682.6062
11	$\beta$ -Sitosterol	-949.5986	-957.0718	-962.2094
12	Nicotiflorin	-2096.6675	-2113.2244	-2124.8671
13	Clitorin	-2657.3995	-2678.2365	-2692.2383
14	Succinimide	-355.7964	-358.5142	-360.3960
15	4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane	-1302.2825	-1315.5779	-1322.3995



If the value of binding energy is negative the drug may be more active and it is more stable. All the compounds have negative binding energy value. All the compounds can act as drug.

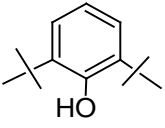
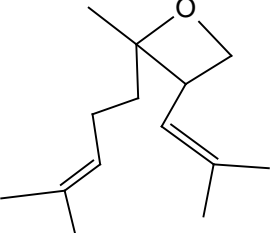
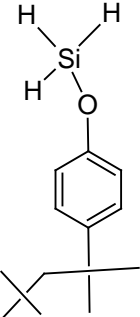
## **Molinspiration**

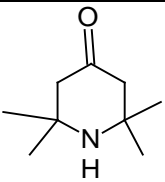
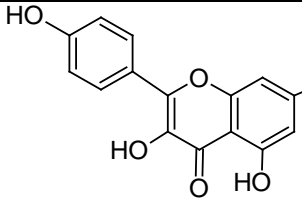
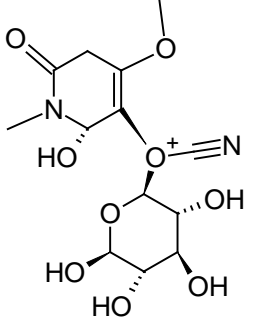
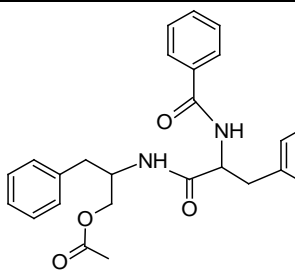
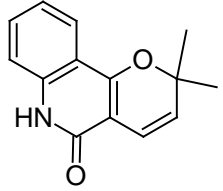
Molinspiration was used to predict the molecular properties and bioactivity score of the 15 compounds. Their structure in molinspiration window, the calculated molecular properties and bioactivity scores compared with the standard values are summarized in Tables 3&4


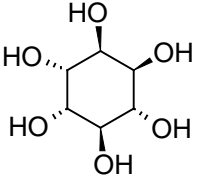
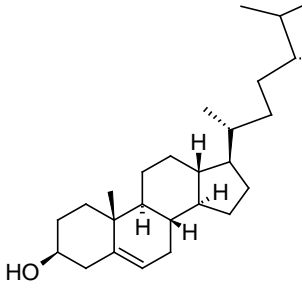
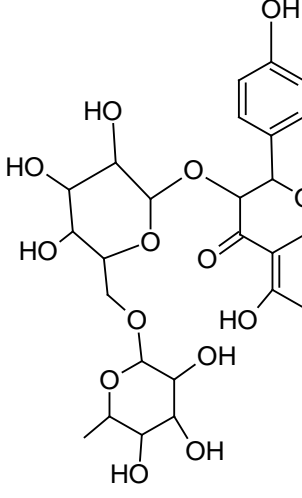


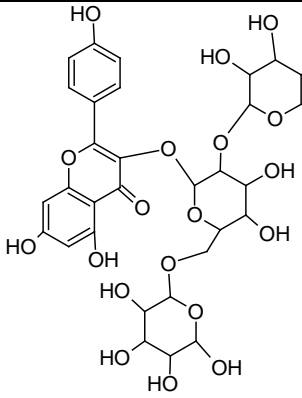
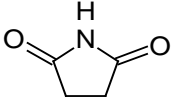
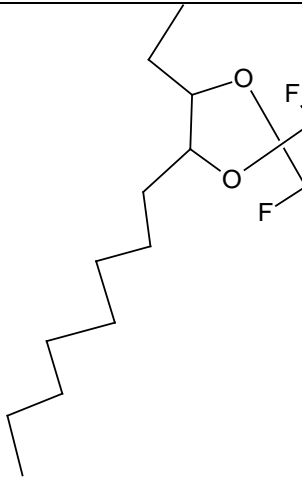


**Table 3: Comparison of calculated molecular properties with standard values**

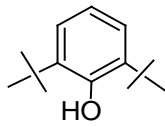
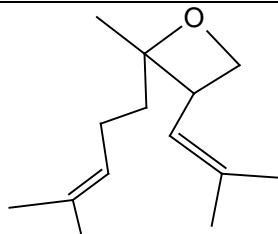
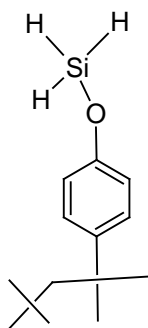
Component NO	Structure of Components	Mi Log P	TPSA	N atoms	mW	nON	nOHNH	Nviolations	Nrotb	Volume
1	 <p><b>2,5-Di-tert butylphenol</b></p>	5.04	20.23	15	206.33	1	1	1	2	224.44
2	 <p><b>2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane</b></p>	5.36	9.23	16	222.37	1	0	1	5	248.96
3	 <p><b>Trimethyl[4-(1,1,3,3-tetramethylbutyl)phenoxy]silane</b></p>	7.41	9.23	19	278.51	1	0	1	5	304.87

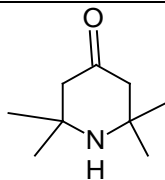
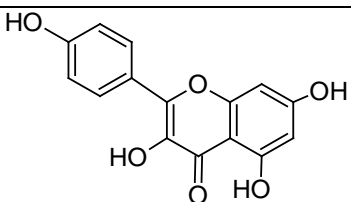
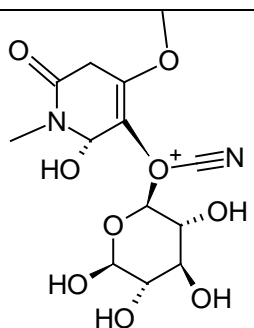
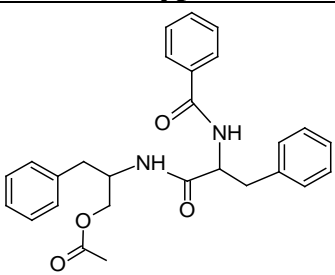
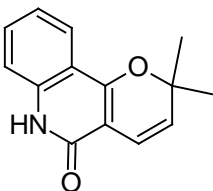
4	 <p><b>Triacetoneamine</b></p>	1.29	29.1 0	11	155.2 4	2	1	0	0	166.0 3
5	 <p><b>Kaempferol</b></p>	2.17	111.1 12	21	286.2 4	6	4	0	1	232.0 7
6	 <p><b>Acalyphin</b></p>	- 4.11	172. 94	25	360.3 2	11	5	1	4	301.4 3
7	 <p><b>Aurantiamide</b></p>	3.89	84.5 0	33	444.5 3	6	2	0	11	418.2 2
8	 <p><b>Flindersin</b></p>	2.59	42.1 0	17	227.2 6	3	1	0	0	207.1 9

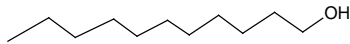
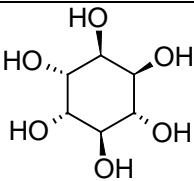
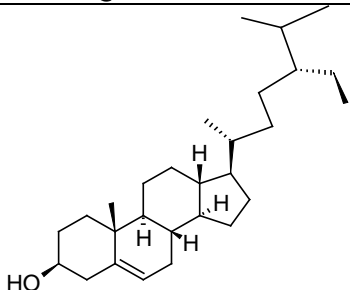
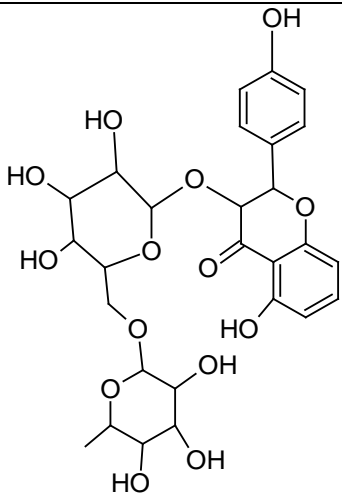
9	 <b>Octacosanol</b>	9.83	20.2 3	29	410.7 7	1	1	1	26	490.8 6
10	 <b>Quebrachitol</b>	- 1.99	110. 37	13	194.1 8	6	5	0	1	168.3 9
11	 <b>β-Sitosterol</b>	8.62	20.2 3	30	414.7 2	1	1	1	6	456.5 2
12	 <b>Nicotiflorin</b>	- 0.57	249. 20	42	594.5 2	15	9	3	6	488.0 5

13	 <p><b>Clitorin</b></p>	- 1.27	308. 12	52	740.6 6	19	11	3	8	611.9 1
14	 <p><b>Succinimide</b></p>	- 0.86	46.1 7	7	99.09	3	1	0	0	85.77
15	 <p><b>4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane</b></p>	6.86	18.4 7	23	3550. 34	2	0	1	10	300.0 5
	Standard	-	20.2	60	220.5	1	1	0	2	240.9

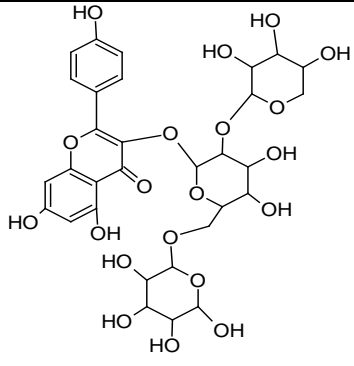
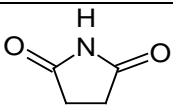
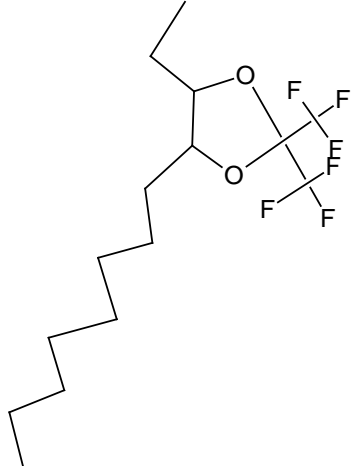
**Table 4: Comparison of calculated bioactivity scores with standard values.**

Components NO	Structure of components	GPSR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
1	 <b>2,5-Di-tert butylphenol</b>	-0.37	0.05	-0.51	-0.07	-0.64	-0.07
2	 <b>Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane</b>	-0.24	0.30	-0.52	0.00	-0.26	0.13
3	 <b>Trimethyl[4-(1,1,3,3-tetramethylbutyl)phenoxy]silane</b>	0.44	0.40	-0.13	0.07	0.27	0.80

4	 <p><b>Triacetoneamine</b></p>	-1.10	-0.41	-1.46	-1.43	-0.96	-0.67
5	 <p><b>Kaempferol</b></p>	0.10	-0.21	0.221	0.32	-0.27	0.26
6	 <p><b>Acalyphin</b></p>	0.11	0.04	-0.07	-0.16	0.27	0.41
7	 <p><b>Aurantiamide</b></p>	0.26	0.09	0.12	-0.13	0.42	0.15
8		0.07	0.02	0.01	0.10	0.08	0.08

	<b>Flindersin</b>						
9	 <p><b>Octacosanol</b></p>	-0.54	-0.08	-0.69	-0.55	-0.51	-0.05
10	 <p><b>Quebrachitol</b></p>	0.14	0.05	-0.51	0.73	0.07	0.51
11	 <p><b>Octacosanol</b></p>	-0.01	-0.43	-0.09	-0.17	-0.04	0.18
12	 <p><b>Nicotiflorin</b></p>	-0.88	-1.90	-1.36	-1.49	-0.60	-0.99



13	 <p><b>Clitorin</b></p>	-4.37	-4.26	-5.17	-4.42	-4.19	-4.17
14	 <p><b>Succinimide</b></p>	-0.10	-0.03	-0.28	0.23	0.00	0.08
15	 <p><b>4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane</b></p>	-0.34	0.00	-0.48	-0.08	-0.57	-0.07
	Standard	-0.34	0.00	-0.48	-0.08	-0.57	-0.07

If  $\text{mlogp}$  of any compound is below 5 then the compound has good permeability across cell membrane. TPSA below 160,  $\text{nvio} = 1 < 0$  means the compound can easily bind to receptor. Molecular mass  $< 500$ ,  $\text{nrotb} < 5$ , number of hydrogen bond donors  $\leq 5$  (The sum of OHs

and NHs), number of hydrogen bond acceptors  $\leq 10$  are desirable properties for any molecule to show drug like behaviour. Comparisons with standard values show that many of the compounds show good drug likeness score.

**Pass**

Pass is online software. Using PASS, the Pharmacological activity of the 15 compounds have been evaluated. The values are given in the Tables (5-19).

**Table 5: PASS Predicted List of Pharmacological activity of 2, 5-Di-tert butylphenol**

S.No	Pa	Pi	Activity
1	0,922	0,005	Aspulvinone dimethylallyltransferase inhibitor
2	0,917	0,004	Ubiquinol-cytochrome-c reductase inhibitor
3	0,910	0,004	Alkenylglycerophosphocholine hydrolase inhibitor
4	0,881	0,004	Dehydro-L-gulonate decarboxylase inhibitor
5	0,880	0,009	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
6	0,874	0,004	Linoleate diol synthase inhibitor
7	0,869	0,001	SULT1A2 substrate
8	0,880	0,017	CYP2C12 substrate
9	0,860	0,004	Dextranase inhibitor
10	0,857	0,004	Glutathione thiolesterase inhibitor

The pass prediction of 2,5-Di-tert butylphenol shows Aspulvinone dimethylallyltransferase inhibitor, Ubiquinol-cytochrome-c reductase inhibitor, Alkenylglycerophosphocholine hydrolase inhibitor activity with Pa value greater than 90% .It also posses Dehydro-L-gulonate decarboxylase inhibitor, Testosterone 17beta-dehydrogenase

(NADP+) inhibitor, Linoleate diol synthase inhibitor, SULT1A2 substrate, CYP2C12 substrate, Dextranase inhibitor and Glutathione thiolesterase inhibitor property with Pa value greater than 85%.

**Table 6: PASS Predicted List of Pharmacological activity of 2-Methyl-3-**

**(3-methyl-but-2-enyl)-2-(4-methyl pent-3-enyl)-oxetane**

S.No	Pa	Pi	Activity
1	0,868	0,016	CDP-glycerol glycerophosphotransferase inhibitor
2	0,838	0,005	Antiarthritic
3	0,819	0,005	Antiallergic
4	0,757	0,010	Apoptosis agonist
5	0,736	0,002	Myc inhibitor
6	0,742	0,005	Prenyl-diphosphatase inhibitor
7	0746	0,036	Mucomembranous protector
8	0,736	0,052	Aspulvinone dimethylallyltransferase inhibitor
9	0,722	0,060	Ubiquinol-cytochrome-c reductase inhibitor
10	0,668	0,008	Undecaprenyl-phosphate mannosyltransferase inhibitor

The pass prediction of 2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl pent-3-enyl)-oxetane shows CDP-glycerol glycerophosphotransferase inhibitor, Antiarthritic, Antiallergic properties with Pa value greater than 80%. Apoptosis agonist, Myc inhibitor, Prenyl-diphosphatase inhibitor, Mucomembranous protector, Aspulvinone dimethylallyltransferase

inhibitor, Ubiquinol-cytochrome-c reductase inhibitor properties have Pa value greater than 70%. Undecaprenyl-phosphate mannosyltransferase inhibitor has Pa value greater than 65%.

**Table 7: PASS Predicted List of Pharmacological activity of Trimethyl[4-(1,1,3,3, tetramethylbutyl)phenoxy] silane**

S.No	Pa	Pi	Activity
1	0,970	0,001	Glyceryl-ether monooxygenase inhibitor
2	0,963	0,001	Undecaprenyl-phosphate mannosyltransferase inhibitor
3	0,910	0,004	Alkenylglycerophosphocholine hydrolase inhibitor

4	0,895	0,006	Ubiquinol-cytochrome-c reductase inhibitor
5	0,889	0,001	Retinol dehydrogenase inhibitor
6	0,861	0,002	Long-chain-aldehyde dehydrogenase inhibitor
7	0,859	0,008	Sphinganine kinase inhibitor
8	0,853	0,004	N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
9	0,846	0,001	CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor
10	0,847	0,005	Apoptosis agonist

The pass prediction of Trimethyl[4-(1,1,3,3, tetramethylbutyl)phenoxy] silane shows Glyceryl-ether monooxygenase inhibitor, Undecaprenyl-phosphate mannosyltransferase inhibitor, Alkenylglycerophosphocholine hydrolase inhibitor activities. Pa value of these activities is greater than 90%. Ubiquinol-cytochrome-c reductase inhibitor, Retinol dehydrogenase inhibitor, Long-chain-aldehyde dehydrogenase inhibitor, Sphinganine kinase inhibitor, N-acetylneuraminate 7-O (or 9-O)-acetyltransferase inhibitor activities have Pa value greater than 85%. CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor and Apoptosis agonist have the Pa value greater than 80%.

**Table 8: PASS Predicted List of Pharmacological activity of Triacetoneamin**

S.No	Pa	Pi	Activity
1	0,894	0,007	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
2	0,838	0,003	Thioredoxin inhibitor
3	0,842	0,012	CYP2J substrate
4	0,820	0,004	Pterin deaminase inhibitor
5	0,811	0,003	General pump inhibitor
6	0,812	0,011	CYP2J2 substrate
7	0,801	0,011	Nicotinic alpha6beta3beta4alpha5 receptor antagonist
8	0,815	0,028	Ubiquinol-cytochrome-c reductase inhibitor
9	0,800	0,014	5 Hydroxytryptamine release stimulant

10	0,805	0,035	CYP2C12 substrate
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The pass prediction of triacetoneamine shows Testosterone 17beta-dehydrogenase (NADP+) inhibitor activity. Pa value of this is greater than 85%. Thioredoxin inhibitor, CYP2J substrate, Pterin deaminase inhibitor, General pump inhibitor, CYP2J2 substrate, nicotinic alpha6beta3beta4alpha5 receptor antagonist, Ubiquinol-cytochrome-c reductase inhibitor, 5 Hydroxytryptamine release stimulant and CYP2C12 substrate activities have Pa value greater than 80%.

**Table 9: PASS Predicted List of Pharmacological activity of Kaempferol**

S.No	Pa	Pi	Activity
1	0,983	0,001	Chlordecone reductase inhibitor
2	0,974	0,002	Membrane integrity agonist
3	0,969	0,002	HIF1A expression inhibitor
4	0,965	0,001	2-Dehydropantoate 2-reductase inhibitor
5	0,961	0,001	Aryl-alcohol dehydrogenase (NADP+) inhibitor
6	0,959	0,001	P-benzoquinone reductase (NADPH) inhibitor
7	0,959	0,001	Kinase inhibitor
8	0,957	0,002	Membrane permeability inhibitor
9	0,956	0,001	Peroxidase inhibitor
10	0,951	0,001	Quercetin 2,3-dioxygenase inhibitor

The pass prediction of kaempferol shows Chlordecone reductase inhibitor, Membrane integrity agonist, HIF1A expression inhibitor, 2-Dehydropantoate 2-reductase inhibitor, Aryl-alcohol dehydrogenase (NADP+) inhibitor, P-benzoquinone reductase (NADPH) inhibitor, Kinase inhibitor, Membrane permeability inhibitor, Peroxidase inhibitor and Quercetin 2,3-dioxygenase inhibitor activities. Pa values of these are greater than 95%.

**Table 10: PASS Predicted List of Pharmacological activity of Acalyphin**

S.No	Pa	Pi	Activity
1	0,917	0,007	CDP-glycerol glycerophosphotransferase inhibitor
2	0,853	0,010	Benzoate-CoA ligase inhibitor
3	0,828	0,009	Anaphylatoxin receptor antagonist
4	0,802	0,017	CYP2H substrate
5	0,760	0,004	Lactase inhibitor
6	0,753	0,010	UDP-N-acetylglucosamine 4-epimerase inhibitor
7	0,751	0,024	Sugar-phosphatase inhibitor
8	0,732	0,010	NAD(P)+-arginine ADP-ribosyltransferase inhibitor
9	0,726	0,004	Chitinase inhibitor
10	0,724	0,004	Mycothiol-S-conjugate amidase inhibitor

Pass prediction of acalyphin shows CDP-glycerol glycerophosphotransferase inhibitor activity. Pa values of these are greater than 90%. Benzoate-CoA ligase inhibitor, Anaphylatoxin receptor antagonist, and CYP2H substrate activities with Pa values are greater than 80%. Lactase inhibitor, UDP-N-acetylglucosamine 4-epimerase inhibitor, and Sugar-phosphatase inhibitor activities have Pa value greater than 75%. NAD (P) +-arginine ADP-ribosyltransferase inhibitors, Chitinase inhibitor and Mycothiol-S-conjugate amidase inhibitor activities have Pa values greater than 70%.

**Table 11: PASS Predicted List of Pharmacological activity of Aurantiamide**

S.No	Pa	Pi	Activity
1	0,887	0,002	Pin1 inhibitor
2	0,866	0,003	Peptide alpha-N-acetyltransferase inhibitor
3	0,852	0,012	Polyporopepsin inhibitor
4	0,813	0,029	Phobic disorders treatment
5	0,768	0,005	Hydrogen dehydrogenase inhibitor
6	0,783	0,021	Methylenetetrahydrofolate reductase (NADPH) inhibitor
7	0,740	0,004	Subtilisin inhibitor
8	0,763	0,029	Acrocyllindropepsin inhibitor
9	0,763	0,029	Chymosin inhibitor
10	0,763	0,029	Saccharopepsin inhibitor

Pass prediction of aurantiamide shows Pin1 inhibitor, Peptide alpha-N-acetyltransferase inhibitor and Polyporopepsin inhibitor activities. Pa value of these activities are greater than 80%. Hydrogen dehydrogenase inhibitor, Methylenetetrahydrofolate reductase (NADPH) inhibitor, Subtilisin inhibitor, Acrocyllindropepsin inhibitor, Chymosin inhibitor, and Saccharopepsin inhibitor activities have Pa values greater than 70%.

**Table 12: PASS Predicted List of Pharmacological activity of Flindersin**

S.No	Pa	Pi	Activity
			465

1	0,886	0,006	HIF1A expression inhibitor
2	0,759	0,045	Aspulvinone dimethylallyltransferase inhibitor
3	0,753	0,047	CYP2C12 substrate
4	0,674	0,013	Spasmolytic, urinary
5	0,667	0,011	(R)-6-hydroxynicotine oxidase inhibitor
6	0,680	0,048	Membrane permeability inhibitor
7	0,633	0,022	Thioredoxin inhibitor
8	0,646	0,044	Taurine dehydrogenase inhibitor
9	0,575	0,016	Polarisation stimulant
10	0,599	0,045	Antineoplastic

Pass prediction of flindersin shows HIF1A expression inhibitor activity .Pa value of this is greater than 85%. Aspulvinone dimethylallyltransferase inhibitors and CYP2C12 substrate activities have Pa value greater than 70%. Spasmolytic, urinary, R-6-hydroxynicotine oxidase inhibitors and Membrane permeability inhibitor activity have Pa value greater than 65%. Thioredoxin inhibitors, Taurine dehydrogenase inhibitor activities have Pa value greater than 60%. Polarisation stimulants and Antineoplastic activities have Pa value greater than 55%.

**Table 13: PASS Predicted List of Pharmacological activity of Octacosanol**

S.No	Pa	Pi	Activity
1	0,965	0,002	Sugar-phosphatase inhibitor
2	0,958	0,002	Alkenylglycerophosphocholine hydrolase inhibitor
3	0,952	0,001	Carboxypeptidase Taq inhibitor
4	0,951	0,002	Alkylacetyl glycerophosphatase inhibitor
5	0,943	0,001	Alkylglycerone-phosphate synthase inhibitor
6	0,943	0,002	Dextranase inhibitor
7	0,942	0,001	Glucan 1,4-alpha-maltotriohydrolase inhibitor
8	0,940	0,002	Fucoesterol-epoxide lyase inhibitor
9	0,940	0,002	Pullulanase inhibitor



10	0,939	0,001	Gluconate 5-dehydrogenase inhibitor
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Pass prediction of octacosanol shows Sugar-phosphatase inhibitor, Alkenylglycerophosphocholine hydrolase inhibitor and Carboxypeptidase Taq inhibitor activity. Pa value of these are greater than 95%. Alkylglycerone-phosphate synthase inhibitor, Dextranase inhibitor, Glucan 1, 4-alpha-maltotriohydrolase inhibitor, Fucosterol-epoxide lyase inhibitor, Pullulanase inhibitor and Gluconate 5-dehydrogenase inhibitor activities have Pa value greater than 90%.

**Table 14: PASS Predicted List of Pharmacological activity of Quebrachitol**

S.No	Pa	Pi	Activity
1	0,966	0,002	CDP-glycerol glycerophosphotransferase inhibitor
2	0,928	0,003	Sugar-phosphatase inhibitor
3	0,927	0,004	Aspulvinone dimethylallyltransferase inhibitor
4	0,912	0,008	Membrane integrity agonist
5	0,900	0,005	Alkenylglycerophosphocholine hydrolase inhibitor
6	0,900	0,012	CYP2C12 substrate
7	0,895	0,007	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
8	0,884	0,004	Glucan endo-1,6-beta-glucosidase inhibitor
9	0,888	0,007	Ubiquinol-cytochrome-c reductase inhibitor
10	0,881	0,003	Ribulose-phosphate 3-epimerase inhibitor

Pass prediction of quebrachitol shows CDP-glycerol glycerophosphotransferase inhibitor activity. Pa values of this activity are greater than 95%. Sugar-phosphatase inhibitor, Aspulvinone dimethylallyltransferase inhibitor, Membrane integrity agonist, Alkenylglycerophosphocholine hydrolase inhibitor, CYP2C12 substrate activities have Pa value greater than 90%. Testosterone 17beta-dehydrogenase (NADP+) inhibitor, Glucan endo-1, 6-

beta-glucosidase inhibitor, Ubiquinol-cytochrome-c reductase inhibitor and Ribulose-phosphate 3-epimerase inhibitor activities have Pa value greater than 85%.

**Table 15: PASS Predicted List of Pharmacological activity of  $\beta$ -Sitosterol**

S.No	Pa	Pi	Activity
1	0,977	0,001	Antihypercholesterolemic
2	0,965	0,001	DELTA14-sterol reductase inhibitor
3	0,959	0,002	Prostaglandin-E2 9-reductase inhibitor
4	0,957	0,001	Cholesterol antagonist
5	0,952	0,000	CYP7 inhibitor
6	0,952	0,002	Alkenylglycerophosphocholine hydrolase inhibitor
7	0,945	0,002	Alkylacetyl glycerophosphatase inhibitor
8	0,933	0,003	Hypolipemic
9	0,928	0,003	Acylcarnitine hydrolase inhibitor
10	0,924	0,004	Testosterone 17beta-dehydrogenase (NADP+) inhibitor

Pass prediction of  $\beta$ -Sitosterol shows Antihypercholesterolemic, DELTA14-sterol reductase inhibitor, Prostaglandin-E2 9-reductase inhibitor, Cholesterol antagonist, CYP7 inhibitor and lkenylglycerophosphocholine hydrolase inhibitor activities. Pa values of these are greater than 95%. Alkylacetyl glycerophosphatase inhibitor, Hypolipemic, Acylcarnitine hydrolase inhibitor nad Testosterone 17beta-dehydrogenase (NADP+) inhibitor activities have Pa value greater than 90%.

**Table 16: PASS Predicted List of Pharmacological activity of Nicotiflorin**

S.No	Pa	Pi	Activity
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1	0,992	0,001	Hemostatic
2	0,989	0,000	Membrane permeability inhibitor
3	0,990	0,001	Cardioprotectant
4	0,984	0,001	Free radical scavenger
5	0,984	0,001	Membrane integrity agonist
6	0,979	0,001	CYP1A inducer
7	0,979	0,001	Vasoprotector
8	0,979	0,001	Lipid peroxidase inhibitor
9	0,978	0,001	Anticarcinogenic
10	0,971	0,000	Iodide peroxidase inhibitor

Pass prediction of nicotiflorin shows Hemostatic, Membrane permeability inhibitor, Cardioprotectant, Free radical scavenger, Membrane integrity agonist, CYP1A inducer, Vasoprotector, Lipid peroxidase inhibitor, Anticarcinogenic and Iodide peroxidase inhibitor activities. Pa value of these are greater than 95%.

**Table 17: PASS Predicted List of Pharmacological activity of Clitorin**

S.No	Pa	Pi	Activity
1	0,959	0,002	Pyroglutamyl-peptidase I inhibitor
2	0,913	0,005	Nootropic
3	0,900	0,004	Immunostimulant
4	0,815	0,004	Fibroblast growth factor agonist
5	0,812	0,003	Pyroglutamyl-peptidase II inhibitor
6	0,803	0,013	Mucositis treatment
7	0,757	0,003	Fibroblast growth factor 1 agonist
8	0,750	0,004	Metabolic disease treatment
9	0,696	0,003	Amyloid beta aggregation inhibitor
10	0,657	0,005	Wound healing agent

Pass prediction of clitorin shows Pyroglutamyl-peptidase I inhibitor and Nootropic, Immunostimulant inhibitor activities. Pa values of these are greater than 90%. Fibroblast growth factor agonist, Pyroglutamyl-peptidase II inhibitor, Mucositis treatment of these activities have Pa value greater than 80%. Fibroblast growth factors 1 agonists and metabolic disease treatment activities with of Pa value greater than 75%. Amyloid beta aggregation inhibitors and Wound healing agent activity have Pa value greater than 65%.

**Table 18: PASS Predicted List of Pharmacological activity of Succinimide**

S.No	Pa	Pi	Activity
1	0,923	0,002	Glucan endo-1,6-beta-glucosidase inhibitor
2	0,917	0,003	Pullulanase inhibitor
3	0,910	0,005	Testosterone 17beta-dehydrogenase (NADP+) inhibitor
4	0,902	0,002	Glucan 1,4-alpha-maltotriohydrolase inhibitor
5	0,898	0,003	Creatininase inhibitor
6	0,896	0,007	Methylenetetrahydrofolate reductase (NADPH) inhibitor
7	0,887	0,003	Ribulose-phosphate 3-epimerase inhibitor
8	0,879	0,004	N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor
9	0,884	0,011	Aspulvinone dimethylallyltransferase inhibitor
10	0,874	0,003	L-glutamate oxidase inhibitor

Pass prediction of succinimide shows Glucan endo-1,6-beta-glucosidase inhibitor, Pullulanase inhibitor, Testosterone 17beta-dehydrogenase (NADP+) inhibitor and Glucan 1,4-alpha-maltotriohydrolase inhibitor activities. Pa values of these are greater than 90%. Creatininase inhibitor, Methylenetetrahydrofolate reductase (NADPH) inhibitor, Ribulose-phosphate 3-epimerase inhibitor, N-acetylneuraminate 7-O (or 9-O)-acetyltransferase inhibitor, Aspulvinone dimethylallyltransferase inhibitor and L-glutamate oxidase inhibitor activities have Pa value greater than 85%.

**Table 19: PASS Predicted List of Pharmacological activity of 4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane**

S.No	Pa	Pi	Activity
1	0,862	0,009	CYP2H substrate
2	0,853	0,009	Sugar-phosphatase inhibitor
3	0,851	0,011	Acrocyllindropepsin inhibitor
4	0,851	0,011	Chymosin inhibitor
5	0,851	0,011	Saccharopepsin inhibitor
6	0,843	0,019	Ubiquinol-cytochrome-c reductase inhibitor
7	0,809	0,002	Angiogenesis stimulant
8	0,799	0,004	Glucan 1,4-alpha-maltotriohydrolase inhibitor
9	0,806	0,019	CYP2J substrate
10	0,801	0,020	Polyporopepsin inhibitor

Pass prediction of 4-Ethyl-5-octyl-2, 2-bis (trifluoromethyl)-1, 3-dioxolane shows CYP2H substrate, Sugar-phosphatase inhibitor, Acrocyllindropepsin inhibitor, Chymosin inhibitor and Saccharopepsin inhibitor activities. Pa values of these are greater than 85%. Ubiquinol-cytochrome-c reductase inhibitors, Angiogenesis stimulant, CYP2J substrate, and Polyporopepsin inhibitor activities have Pa value greater than 80%. Glucan 1, 4-alpha-maltotriohydrolase inhibitor activities have Pa value greater than 75%.

## Conclusion

Identification of a lead compound plays a major role in drug designing. Some of the chemical components of *Acalypha Indica* were selected to evaluate their drug likeness character. Using Gaussian software the binding energy of the fifteen compounds were calculated. If the value of binding energy is negative the drug may be more active and it is more stable. All the compounds have negative value of binding energy. All compounds can act as drug. Using molinspiration physical properties and bioactivity score were calculated for all the chosen compounds. Comparison of the properties of the compounds with standard values revealed that all the compounds have drug likeness character. Pharmacological activities of all compounds were predicted using PASS software and all of them were found to have a list of biological activities.

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