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# 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 [1]. 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 homoepathy, 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, triacetonamine and an alkaloid, acalyphine. It also contains the amide, acalyphamide and some other amides, 2-methylanthraquinone,

tri-O-methyl ellagic acid and γ-sitosterol, ß-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 anthelminthic [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 drugdesign. 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 likness 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 - β-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 [14, 15].

bond [16].

## 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 |
|---|---|---|---|---|

## Gaussian

Binding energy of the 15 compounds was calculated using Gaussian software. Hartree-Fock and DFT energies were calculaed 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 Hartee 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 | β-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**

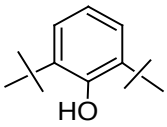
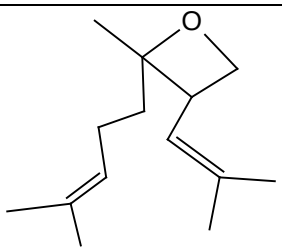
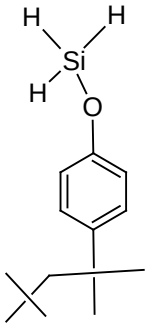
| S.No | Compounds | STO-3G | 3-21 G | 6-31 G |
|---|---|---|---|---|
| 1 | 2,5-Di-tert butylphenol | -602.9108 | -606.2868 | -609.4820 |
| 2 | 2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane | -650.4494 | -65.5946 | -659.0896 |
| 3 | Trimethyl[4-(1,1,3,3,-tetramethylbutyl)phenoxy]silane | -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 | β-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 |

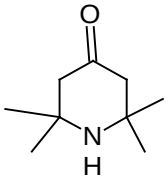
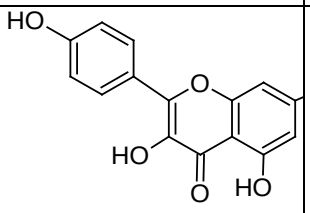
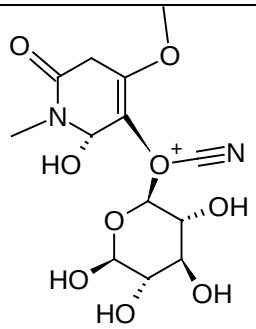
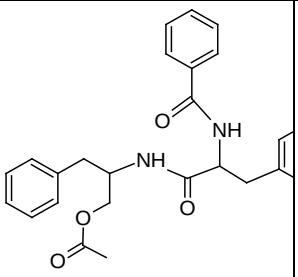
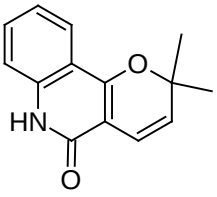
If the value of binding energy is negative the drug may be more active and it is more stable. All the compounds have negative binding energy value. All the compounds can act as drug.

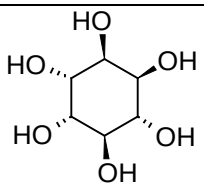
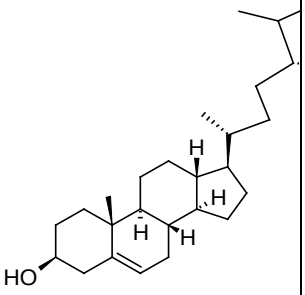
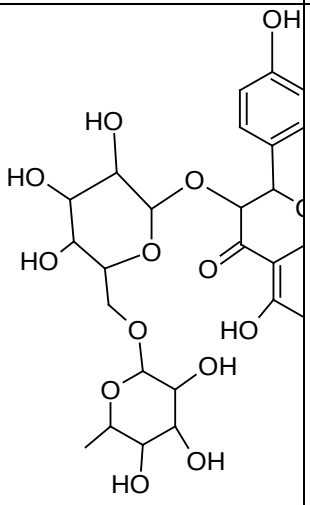
## Molinspiration

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: Comparision of calculated molecular properties with standard values**

| Components NO | Structure of Components | MiLogP | TPSA | Natoms | mW | nON | nOHNH | Nviolations | Nrotb | Volume |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 |  **2,5-Di-tert butylphenol** | 5.04 | 20.23 | 15 | 206.33 | 1 | 1 | 1 | 2 | 224.44 |
| 2 |  2-**Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane** | 5.36 | 9.23 | 16 | 222.37 | 1 | 0 | 1 | 5 | 248.96 |
| 3 |  **Trimethyl[4-(1,1,3,3,-tetramethylbutyl)phenoxy]silane** | 7.41 | 9.23 | 19 | 278.51 | 1 | 0 | 1 | 5 | 304.87 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 |  **Triacetoneamine** | 1.29 | 29.10 | 11 | 155.24 | 2 | 1 | 0 | 0 | 166.03 |
| 5 |  **Kaempferol** | 2.17 | 111.12 | 21 | 286.24 | 6 | 4 | 0 | 1 | 232.07 |
| 6 |  **Acalyphin** | -4.11 | 172.94 | 25 | 360.32 | 11 | 5 | 1 | 4 | 301.43 |
| 7 |  **Aurantiamide** | 3.89 | 84.50 | 33 | 444.53 | 6 | 2 | 0 | 11 | 418.22 |
| 8 |  **Flindersin** | 2.59 | 42.10 | 17 | 227.26 | 3 | 1 | 0 | 0 | 207.19 |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 |  **Octacosanol** | 9.83 | 20.23 | 29 | 410.77 | 1 | 1 | 1 | 26 | 490.86 |
| 10 |  **Quebrachitol** | -1.99 | 110.37 | 13 | 194.18 | 6 | 5 | 0 | 1 | 168.39 |
| 11 |  **β-Sitosterol** | 8.62 | 20.23 | 30 | 414.72 | 1 | 1 | 1 | 6 | 456.52 |
| 12 |  **Nicotiflorin** | -0.57 | 249.20 | 42 | 594.52 | 15 | 9 | 3 | 6 | 488.05 |

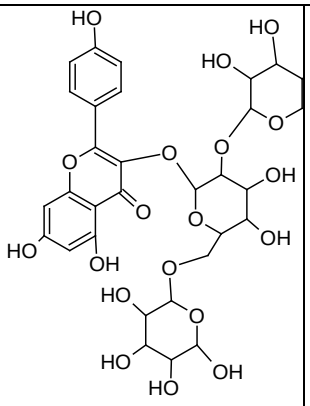
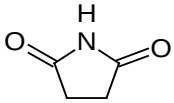
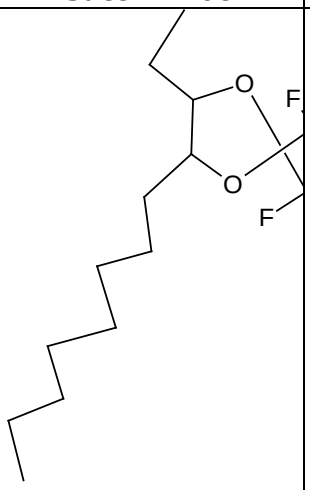
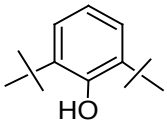
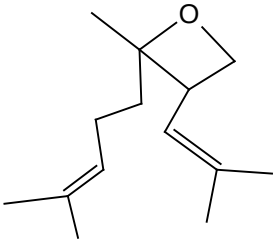
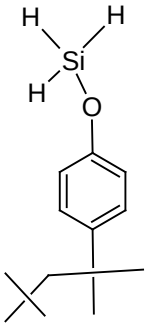
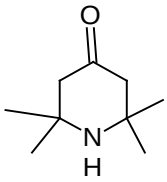
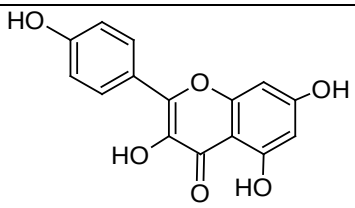
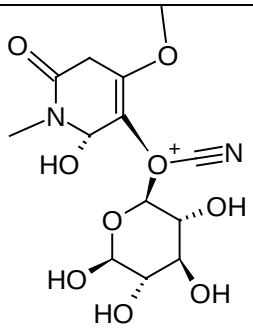
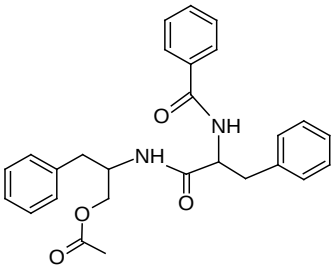
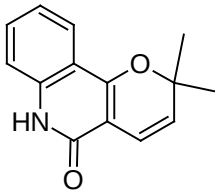
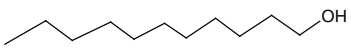
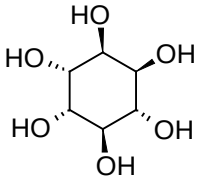
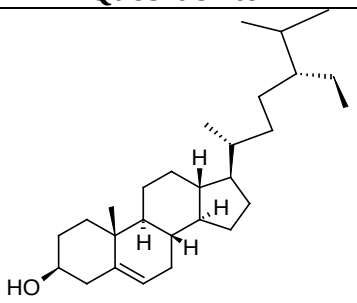
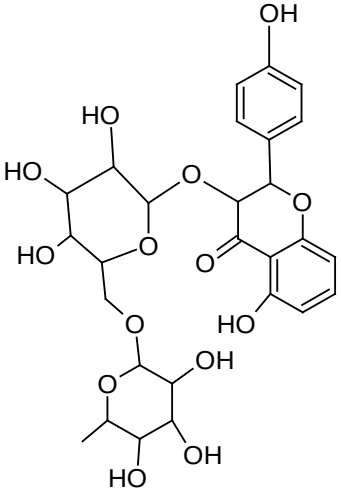
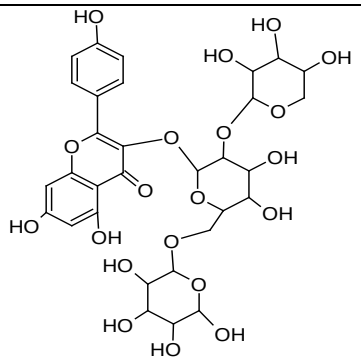
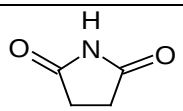
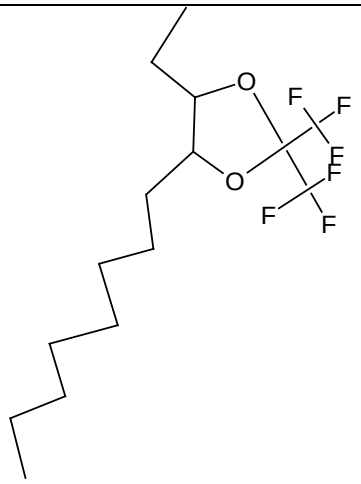
| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 |  **Clitorin** | -1.27 | 308.12 | 52 | 740.66 | 19 | 11 | 3 | 8 | 611.91 |
| 14 |  **Succinimide** | -0.86 | 46.17 | 7 | 99.09 | 3 | 1 | 0 | 0 | 85.77 |
| 15 |  **4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane** | 6.86 | 18.47 | 23 | 3550.34 | 2 | 0 | 1 | 10 | 300.05 |
| | Standard | - | 20.2 | 60 | 220.5 | 1 | 1 | 0 | 2 | 240.9 |

**Table 4: Comparision 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 |  **2,5-Di-tert butylphenol** | -0.37 | 0.05 | -0.51 | -0.07 | -0.64 | -0.07 |
| 2 |  **Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane** | -0.24 | 0.30 | -0.52 | 0.00 | -0.26 | 0.13 |
| 3 |  **Trimethyl[4-(1,1,3,3,-tetramethylbutyl)phenoxy]silane** | 0.44 | 0.40 | -0.13 | 0.07 | 0.27 | 0.80 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 4 |  **Triacetoneamine** | -1.10 | -0.41 | -1.46 | -1.43 | -0.96 | -0.67 |
| 5 |  **Kaempferol** | 0.10 | -0.21 | 0.221 | 0.32 | -0.27 | 0.26 |
| 6 |  **Acalyphin** | 0.11 | 0.04 | -0.07 | -0.16 | 0.27 | 0.41 |
| 7 |  **Aurantiamide** | 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 |

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

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 13 |  **Clitorin** | -4.37 | -4.26 | -5.17 | -4.42 | -4.19 | -4.17 |
| 14 |  **Succinimide** | -0.10 | -0.03 | -0.28 | 0.23 | 0.00 | 0.08 |
| 15 |  **4-Ethyl-5-octyl-2,2-bis(trifluoromethyl)-1,3-dioxolane** | -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 mlogp of any compound is below 5 then the compound has good permeability across cell membrane. TPSA below 160, nviolations=1<0 means the compound can easily bind to receptor. Molecular mass<500, nrotb<5, number of hydrogen bond donors ≤5 (The sum of OHs and NHs), number of hydrogen bond acceptors ≤ 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 Aspulvinonedimethylallyltransferase 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 activites. Pa value of these acivities 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 activites have Pa value greater than 85%. CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitorand 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 |

The pass prediction of triacetoneamine shows Testosterone 17beta-dehydrogenase (NADP+) inhibitor acivity. 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 acivities 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 acivities. 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 acitivity. 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 acivities 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 | Acrocylindropepsin 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 acivities. Pa value of these acivities are greater than 80%. Hydrogen dehydrogenase inhibitor, Methylenetetrahydrofolate reductase (NADPH) inhibitor, Subtilisin inhibitor, Acrocylindropepsin inhibitor, Chymosin inhibitor, and Saccharopepsin inhibitor acivities have Pa values greater than 70%.

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

| S.No | Pa | Pi | Activity |
|---|---|---|---|

| | | | |
|---|---|---|---|
| 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 activites have Pa value greater than 60%. Polarisation stimulants and Antineopla activites 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 | Alkylacetylglycerophosphatase 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 | Fucosterol-epoxide lyase inhibitor |
| 9 | 0,940 | 0,002 | Pullulanase inhibitor |

| | | | |
|---|---|---|---|
| 10 | 0,939 | 0,001 | Gluconate 5-dehydrogenase inhibitor |

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 activites 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 activites 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 activites have Pa value greater than 85%.

**Table 15: PASS Predicted List of Pharmacological activity of β-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 | Alkylacetylglycerophosphatase 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 β-Sitosterol shows Antihypercholesterolemic, DELTA14-sterol reductase inhibitor, Prostaglandin-E2 9-reductase inhibitor, Cholesterol antagonist, CYP7 inhibitorA and lkenylglycerophosphocholine hydrolase inhibitor activities. Pa values of these are greater than 95%. Alkylacetylglycerophosphatase inhibitor, Hypolipemic, Acylcarnitine hydrolase inhibitor nad Testosterone 17beta-dehydrogenase (NADP+) inhibitor activites have Pa value greater than 90%.

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

| S.No | Pa | Pi | Activity |
|---|---|---|---|

| | | | |
|---|---|---|---|
| 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 activites.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 inhibito ractivites. Pa values of these are greater than 90%. Fibroblast growth factor agonist, Pyroglutamyl-peptidase II inhibitor, Mucositis treatment of these activites have Pa value greater than 80%. Fibroblast growth factors 1agonists 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 activites. 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 activites 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 | Acrocylindropepsin 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, Acrocylindropepsin inhibitor, Chymosin inhibitor and Saccharopepsin inhibitor activites. 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 likness 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 molinsperation 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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