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Chemo and Bioinformatics Resources For In Silico Drug Discovery from Acalypha Hispida beyond Their Traditional Use

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Abstract
There is a constant demand to develop new, effective and affordable drugs. The traditional medicine (TM) is a valuable and alternative resource for identifying novel drug agents. *In silicon* approaches have been widely recognized to be useful for drug discovery. Here, we consider the significance of available databases of medicinal plants and chemo and bioinformatics tools for *in silicon* drug discovery beyond the traditional use of folk medicines. In this study, we aim to identify the different compounds from plants through preliminary studies by using chemo and bioinformatics tools. We first predicted compounds from GCMS analysis and analyzed for the active compound. Similarity analysis revealed that 75% of the compounds are highly similar to the approved anti-cancer drugs. Based on the predicted compounds, we identified properties of plants by activity enrichment. The identified plant is *Acalypha hispida*, the chenille plant, is a flowering shrub which belongs to the family Euphorbiaceae, which broadens the scope of the drug screening. Finally, we constructed a network of predicted that the plant are approved based on the above results.

Keywords: Phytochemical, GCMS, Drug Discovery

1. Introduction

For ages nature has gifted us plenty of herbs and plants which form the main source of traditional medicines used to help in relief from illness and are still widely used all over the world. Herbs are safe, less toxic, economical and a reliable key natural resource of drugs all over the world[1]. It is estimated that about 7,500 plants are used in local health traditions in mostly, rural and tribal villages of India. Out of these, the real medicinal value of over 4,000 plants is either little known or unknown to the mainstream population[2]. A detailed investigation and documentation of plants used in local health traditions and pharmacological evaluation of these plants and their taxonomical relatives can lead to the development of invaluable plant drugs for many dreaded diseases. Random screening of plants has not proved economically effective[3]. Plant materials remain an important resource to combat serious diseases in the world[4].

Phytochemicals are naturally occurring and biologically active plant compounds that have potential disease inhibiting capabilities. It is believed that phyochemicals may be effective in combating or preventing disease[5]. Phytochemical works as antioxidant, hormonal actions, stimulation of enzymes, interference with DNA replication and anti-microbial effect, etc. Phytochemicals are non-nutritive plant chemicals that have protective or disease preventive properties. They are nonessential nutrients, meaning that they are not required by the human body for sustaining life[6].

According to world health organization (WHO), more than 80% of the world's population relies on traditional medicines for their primary health care needs. GC-MS studies have been increasingly applied for the analysis of medicinal plants as this technique has proved to be a valuable method for the analysis of non-polar components and volatile essential oil, fatty acids, lipids[7] and alkaloids[8]. It also plays a fundamental role as an analytical technique for quality control and standardization of phyto-therapeuticals[9]. Screening of active components from plants has direct to the development of new medicinal drugs which have efficient

protection and treatment role against various diseases[10]. Gas Chromatography Mass Spectroscopy, a hyphenated system which is a very compatible technique and the most commonly used technique for the identification and quantification purpose. The unknown organic compounds in a complex mixture can be determined by interpretation and also by matching the spectra with reference spectra[11].

Bioinformatics and systems biology approaches are becoming increasingly important along with the above-mentioned 60 chemo informatics methods to study the therapeutic potential of medicinal plants[12]. They are used to select targets for docking and to identify relationships between the revealed actions of phytochemicals on targets and the known therapeutic effects of medicinal plants. The various available databases of medicinal plants and *in silicon* tools for their utilization in new drug discovery based on expanding the use of folk medicinal plants through the exploration of phytochemical diversity. Computer-based methods have been employed in the prediction of ADMET properties of drug leads at early stages of drug discovery and such approaches are becoming increasingly popular [13, 14, and 15]. The rationale behind *in silicon* approaches are the relatively lower cost and the time factor involved, when compared to standard experimental approaches for ADMET profiling[16, 17]. As an example, it takes a minute in an *in silicon* model to screen 20,000 molecules, but takes 20 weeks in the "wet" laboratory to do the same exercise[18]. Due to the accumulated ADMET data in the late 1990s, many pharmaceutical companies are now using computational models that, in some cases, are replacing the "wet" screens[18].

Thus, the present study deals with the screening based on phytochemical tests, GCMA analysis and Drug discovery of the particular medicinal plant used which is *Acalypha hispida*, the chenille plant, is a flowering shrub which belongs to the family Euphorbiaceae. *Acalypha* is the fourth largest genus, this plant is also known as the Philippines Medusa, red hot cat's tail and fox tail in English. *Acalypha hispida* is cultivated as a house plant because of its attractiveness and brilliantly colored, furry flowers[19]. The Latin specific epithet *hispida* means "bristly", referring to the pendent flowers which vaguely resemble brushes.

2 Materials and methods

2.1 Collection of Plant Materials

The fresh plant leaves of *Acalypha hispida* were collected randomly from the Yercaurd, Salem District, Tamil Nadu. Plant materials were washed under running tap water, air dried and then homogenized to fine powder and stored in airtight bottles in refrigerator.

2.2 Preparation of Extract of *Acalypha Hispida*

Crude sample extract was prepared by Soxhlet extraction method. About 20gm of powdered material was uniformly packed into a thimble and extracted with 250ml of methanol separately. The process of extraction has to be continued for 24 hours or till the solvent in siphon tube of extractor become colorless. After that the extract was taken in a beaker and kept on hot plate and heated at 30-40ºC till all the solvent got evaporated. Dried extract was kept in refrigerator at 4ºC till future use.

2.3 Phytochemical Screening of *Acalypha Hispida*

Preliminary phytochemical analysis was carried out for methanol extracts of *Acalypha hispida* as per standard methods [20, 21].

2.3.1 Detection of alkaloids

Extracts were dissolved individually in dilute hydrochloric acid and filtered. The filtrate was used to test the presence of alkaloids.

Mayer's test: Filtrates were treated with Mayer's reagent. Formation of a yellow cream precipitate indicates the presence of alkaloids.

Wagner's test: Filtrates were treated with Wagner's reagent. Formation of brown/ reddish brown precipitate indicates the presence of alkaloids.

2.3.2 Detection of Flavonoids

Lead acetate test: Extracts were treated with few drops of lead acetate solution. Formation of yellow color precipitate indicates the presence of flavonoids.

H_2SO_4 test: Extracts were treated with few drops of H_2SO_4. Formation of orange colour indicates the presence of flavonoids.

2.3.3 Detection of Steroids

Liebermann- Burchard test: 2ml of acetic anhydride was added to 0.5g of the extracts, each with 2ml of H_2SO_4. The color changed from violet to blue or green in some samples indicate the presence of steroids.

2.3.4 Detection of Terpenoids

Salkowski's test: 0.2g of the extract of the whole sample was mixed with 2ml of chloroform and concentrated H_2SO_4 (3ml) was carefully added to form a layer. A reddish brown coloration of the inner face was indicates the presence of terpenoids.

2.3.5 Detection of Anthroquinones

Borntrager's test: About 0.2g of the extract was boiled with 10% HCl for few minutes in a water bath. It was filtered and allowed to cool. Equal volume of $CHCl_3$ was added to the filtrate. Few drops of 10% NH_3 were added to the mixture and heated. Formation of pink colour indicates the presence anthraquinones.

2.3.6 Detection of Phenols

Ferric chloride test: Extracts were treated with few drops of 5% ferric chloride solution. Formation of bluish black color indicates the presence of phenol.

Lead acetate test: Extract was treated with few drops of lead acetate solution. Formation of yellow color precipitate indicates the presence of phenol.

2.3.7 Detection of Saponins

Froth test: About 0.2g of the extract was shaken with 5ml of distilled water. Formation of frothing (appearance of creamy stable persistent of small bubbles) shows the presence of saponins.

2.3.8 Detection of Tannins

Ferric chloride test: A small quantity of extract was mixed with water and heated on water bath. The mixture was filtered and 0.1% ferric chloride was added to the filtrate. A dark green colour formation indicates the presence of tannins.

2.3.9 Detection of Carbohydrates

Fehling's test: 0.2gm filtrate is boiled on water bath with 0.2ml each of Fehling solutions A and B. A red precipitate indicates the presence of sugar.

2.3.10 Detection of Oils and Resins

Spot test: Test solution was applied on filter paper. It develops a transparent appearance on the filter paper. It indicates the presence of oils and resins.

2.4 GCMS Analysis of *Acalypha hispida*

GC-MS analysis was carried out on a Perkin Elmer Turbo Mass Spectrophotometer (Norwalk, CTO6859, and USA) which includes a Perkin Elmer Auto sampler XLGC. The column used was Perkin Elmer Elite - 5 capillary column measuring 30m × 0.25mm with a film thickness of 0.25mm composed of 95% Dimethyl polysiloxane. The carrier gas used was Helium at a flow rate of 0.5ml/min. 1µl sample injection volume was utilized. The inlet temperature was maintained as 250°C. The oven temperature was programmed initially at 110°C for 4 min, then an increase to 240°C. And then programmed to increase to 280°C at a rate of 20°C ending with a 5 min. Total run time was 90 min. The MS transfer line was maintained at a temperature of 200°C. The source temperature was maintained at 180°C. GCMS was analyzed using electron impact ionization at 70eV and data was evaluated using total ion count (TIC) for compound identification and quantification. The spectrums of the components were compared with the database of spectrum of known components stored in the GC-MS library. Measurement of peak areas and data processing were carried out by Turbo-Mass OCPTVS-Demo SPL software.

2.5 Initial Treatment of Chemical Structures and Calculation of ADMET-Related Descriptors

The 3,179 low energy 3D chemical structures in the Con Med NP library were saved in.mol2 format and initially treated with Lig Prep [22]. This implementation was carried out with the graphical user interface (GUI) of the Maestro software package[22], using the Optimized Potentials for Liquid Simulations (OPLS) force field [23, 24, 25]. Protonation states at biologically relevant pH were correctly assigned (group I metals in simple salts were dis-connected, strong acids were deprotonated, strong bases protonated, while topological duplicates and explicit hydrogen's were added). All molecular modelling was carried out on a Linux workstation with a 3.5 GHz Intel Core2 Duo processor. A set of ADMET-related proper-ties (a total of 46 molecular descriptors) were calculated by using the Qik Prop program[22] running in normal mode.

Qik Prop generates physically relevant descriptors, and uses them to perform ADMET predictions. An overall ADME-compliance score drug-likeness parameter (indicated by #stars), was used to assess the pharmacokinetic profiles of the compounds within the Con Med NP library. The #stars parameter indicates the number of property descriptors computed by Qik Prop that fall outside the optimum range of values for 95% of known drugs. Some of the computed ADMET descriptors, along with their recommended ranges for 95% of known drugs.

3 Results & Discussion

3.1 Yield Obtained

Yield from the plant material of *Acalypha hispida* were obtained from the methanol solvent. The yield obtained in the methanol extract was 26%. Extraction is the crucial first step in the analysis of medicinal plants, because it is necessary to extract the desired chemical components from the plant materials for further separation and characterization.

The basic operation included steps, such as pre-washing, drying of plant materials or freeze drying, grinding to obtain a homogenous sample and often improving the kinetics of analytic extraction and also increasing the contact of sample surface with the solvent system. Proper actions must be taken to assure that potential active constituents are not lost, distorted or destroyed during the preparation of the extract from plant samples. If the plant was selected on the basis of traditional uses[26] then it is needed to prepare the extract as described by the traditional healer in order to mimic as closely as possible for the traditional 'herbal' drug.

3.2 Phytochemical Analysis

The qualitative phytochemical analysis of *Acalypha hispida* was done for the methanol extract solvent. The qualitative phytochemical analysis of *Acalypha hispida* had shown the presence of Alkaloids, flavonoids, steroids, phenols, saponins, tannins and carbohydrates and absence of terpenoids, arthroquinone and oils and resins in the methanol extract. The presence of these constitute gives an indication of the medicinal value of *Acalypha hispida* for example, flavonoids have been found to have antioxidant properties, antibacterial and antimicrobial properties.

The medicinal value of these secondary metabolites is due to the presence of chemical substances that produce a definite physiological action on human body. The most important of these include: alkaloids, glycosides, steroids, flavonoids, fatty oils, resins, mucilages, tannins, gums, phosphorus and calcium for cell growth, replacement, and body building[27].

3.3. GCMS analysis

The results pertaining to GC-MS analysis of the methanol extract of *Acalypha hispida* lead to the identification of a number of compounds. These compounds were identified through mass spectrometry attached with GC. The GC-MS spectrum confirmed the presence of various components with different retention times. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library[28].

The results pertaining to GC-MS analysis led to the identification of number of compounds from the GC fractions of the methanol extract of *Acalypha hispida*. These compounds were identified through mass spectrometry attached with GC. The results of the present study were tabulated in Table. The gas chromatogram shows the relative concentrations of various compounds getting eluted as a function of retention time. The heights of the peak indicate the relative concentrations of the components present in the plant.

From the GCMS results it is observed that Xylitol, 4H-pyran-4-one, 2-3-dihydro-3, 5- dihydroxy-6- methyl-, 5-Hydroxymethylfurfural, Beta-Amyrin, 3- Deoxy-d-mannoic-d-arabitol, Decanoic acid and 5, 12-Naphthacenequinone is present in the *Acalypha hispida.* Molecular Formula and molecular weight are presented in table. Structure for the present compounds is also presented in table.

This report is the first of its kind to analyze the chemical constituents of *Acalypha hispida* using GC-MS. In addition to this, the results of the GC-MS profile can be used as pharmacognostical tool for the identification of the plant compounds with different chemical structures[29].

3.4 Bioinformatics studies (Drug Discovery) for compound Beta-Amyrin

3.4.1 Physico Chemical Determination

The physioco chemical determination of the compound Beta Amyrin was carried out for molecular refractory, molecular volume, index of refraction, surface tension, Density and Polari ability. The molecular weight of Beta Amyrin is 426.72 and its molecular formula is $C_{30}H_{50}O$. It is derived from the elemental analysis.

3.4.2 Absorption studies

The absorption study for the compound Beta Ampyrin was carried out. In the absorption study, the physico – chemical determinants, maximum passive absorption and permeability were reported. In the compound the maximum passive absorption is 100% reliable. The similar structures for the particular compound were Vitamin D2, D3 and Lynostrenol.

3.4.3 AMES Test

Ames test was carried out to determine the mutagenic activity of chemicals by absorption whether they cause mutation in particular sample. The probability of the Ames test shows 0.01 and its reliability is moderate (0.57) for the compound Beta Amyrin. Similar structures for the compound are cholesterol, beat – silosterol, Vitamin D3, L-Borneol, Vitamin D3, L- Borneol and Geosmin.

3.4.4 Bioavailability study

Bio availability refers to the relative amount of drug from an administered dosage from which enters the systemic circulation and the rate at which the drug appears in the systemic circulation.

The oral Bio availability study was screened for the compound which lies between 30% and 70%. The similar structures are Lynestrenol, Testosterone and Medroxprogesterone. From the oral bioavailability test the probability that compound has % F (Oral) > 30% is 0.811 and that of %F (oral) > 70% is 0.205. The results of dbp test predict that RI is 0.47 and LogKa HSA is 5.86.

3.4.5 Drug predominantly bind study

Drug Binding to Plasma Proteins: Many drugs bind reversibly to plasma proteins such as albumin (which binds primarily to acidic drugs) and $alpha_1$-acid glycoprotein (which binds primarily to basic drugs). Although analogous to binding to receptors, no pharmacological response is triggered when a drug attaches to a protein binding sites. Reversible binding to plasma proteins generally obeys the law of mass action, with the degree of binding being dependent on the concentration of protein, the concentration of drug, and the association and dissociation rate constants.

The extent of drug binding depends on the mechanisms of bioactivation of the drug, the reactivity of the resulting metabolite, and the cellular mechanism of defense. Because of their capability to participate in many different biotransformation reactions, CYP isozymes are usually involved in reactions leading to covalent binding. In this reliability is in border line. The similar structures were Dihydrotachysterol, Ergocalciferol, cholecalciferol, pregrenolone and Lynestrenol.

3.4.6 Health Effects Study

Health effects were screened for blood, cardio vascular, Gastro intestinal, kidney, Liver and Lungs. Higher probability is found in Gastro intestinal system. The similar structure for blood are cholesterol, Ergocalciferol, Androst-4-en-3-one, 17-beta-hydroxy-17-methyl, Estr -4-en- 3-one, 17- beta- hydroxyl- 17- alpha- methyl and cholestan- 3-alpha- ol.

Toxicity is a measure of any undesirable or adverse effect of chemicals. Specific types of these adverse effects are called toxicity endpoints, such as carcinogenicity or genotoxicity, and can be quantitative (e.g., LD_{50}: lethal dose to 50% of tested individuals) Rowe, 2010 or qualitative, such as binary (e.g., toxic or non-toxic) or ordinary (e.g., low, moderate, or high toxicity). Toxicity tests aim to identify harmful effects caused by substances on humans, animals, plants, or the environment through acute-exposure (single dose) or multiple-exposure (multiple doses). Several factors determine the toxicity of chemicals, such as route of exposure (e.g., oral, dermal, inhalation), dose (amount of the chemical), frequency of exposure (e.g., single versus multiple exposure), duration of exposure (e.g., 96 h), ADME properties (absorption, distribution, metabolism, and excretion/elimination), biological properties (e.g., age, gender), and chemical properties [30].

The similar compounds for cardiovascular system are Ergocalciferol, Urs- 12- ene- 27, 28- dioic acid, 3- beta-hydroxyl. The similar compounds for Gastrointestinal system are Ergocalciferol, Androst – 4-en- 3- one, 7-beta, 17 alpha – dimethyl- 17- beta – hydroxy – 9,10 – secocholesta, 5,7,10 (19)- trien- 3- beta –ol and Urs- 12-ene – 27, 28 –dioic acid, 3- beta – hydroxy.

The similar structures for Liver are Androsta-1, 4-dien-3-one, 17-beta-hydroxy -17- alpha- methyl, Androst 4- en- 3-one, 17- beta – hydroxyl – 17 methyl, Cholestan – 3- alpha-ol, Androst – 5- en -17 – one, 3- beta- hydroxyl and 19 – Nor -17 –alpha- pregn – 5(10) –en- 20 –yn-3- one, 17 hydroxy.

The similar structures for Lungs are Testosterone, Urs- 12-ene – 27, 28 –dioic acid, 3- beta – hydroxyl, pregn-4-ene-3, 20-dione, 17-hydroxy- 6-alpha – methy, 5-beta-Pregnane-3-alpha, 20- alpha –diol and 9,10-Secocolesta,5,7,1019-triene-1,3-diol,1-alpha, 3-beta.5Z.7E.

3.4.7 Low Dosage 50 Percentage

Animal models have been used for a long time for toxicity testing. However, *in vitro* toxicity tests became plausible due to the advances in high throughput screening. *In silico* toxicology (computational toxicology) is one type of toxicity assessment that uses computational resources (i.e., methods, algorithms, software, data, etc.) to organize,

analyze, model, simulate, visualize, or predict toxicity of chemicals. It is intertwined with *in silico* pharmacology, which uses information from computational tools to analyze beneficial or adverse effects of drugs for therapeutic purposes.

Low dosage level (LD_{50}) percentage is higher in oral in rat and intravenous in mouse. Similar structures for Mouse/Intraperitioneal are Olean- 12 –en- 28-oic acid, 3-hydroxyl, (3- beta) and Olean- 12 –en- 28-oic acid, 3- beta – hydroxyl, 2- (dimethylamino) ethyl ester, hydrochloride.

LD_{50} value and their reliability for Mouse/ Intra-peritoneal are 280 and 0.53 and that of Mouse/ oral are 530 and 0.4. Mouse/ Intravenous exhibited a result of 11 and 0.42. Mouse/ sub-cultaneous, Rat / Insta-peritonea and Rat / oral are 47, 24 and 5.9 with RI values of 0.25, 0.29 and 0. Molar refractivity is 131.92 ± 0.4 cm^3, Molar volume is 420.8 ± 5. 0 cm^3, Parachor is Molar refractivity is 1054.8 ± 6.0cm^3, Index of refraction is 1.539 ± 0.33. Surface tension 39.5 is 39.48 ± 5.0.

Table 1: Qualitative phytochemical analysis of *Acalypha hispida*

Phytochemicals	Observations	Methanol extract
Alkaloids Mayer's test Wagner's test	Cream color Reddish brown solution/ precipitate	+ +
Flavonoids Lead acetate test H_2SO_4 test	Yellow orange Reddish brown / Orange color precipitate	+ +
Steroids Liebermann-Burchard test	Violet to blue or Green color formation	+
Terpenoids Salkowski test	Reddish brown precipitate	-
Arthroquinone Borntrager's test	Pink color	-
Phenols Ferric chloride test Lead acetate test	Deep blue to Black color formation White precipitate	+ +
Saponin	Stable persistent	+
Tannin	Brownish green / Blue black	+
Carbohydrates	Yellow / brownish / blue / green color	+
Oils & Resins	Filter paper method	-

Table 2: GCMS Analysis for *Acalypha hispida* of methanol extract

S.No	RT	Name of the compound	M.F.	M.W.	Area	Activity
1.	5.32	Xylitol	$C_5H_{12}O_5$	152.15	8.46	Antimicrobial activity
2.	8.06	4H- pyran-4-one, 2-3-dihydro-3,5-dihydroxy-6- methyl-	$C_6H_8O_4$	144.12	4.19	Antimicrobial activity
3.	9.45	5- Hydroxymethylfurfural	$C_6H_6O_3$	126.11	7.11	Toxic Comp, antimicrobial, anticancer, anti - inflammatory
4.	12.02	Beta-Amyrin	$C_{30}H_{50}O$	426.729	0.89	Antitumor, anticancer, antidote, antimicrobial, anti – viral activity
5.	15.17	3-Deoxy-d-annoic-d-arabitol	$C_6H_{10}O_5$	162.14	35.69	Antioxidant, antimicrobial, bactericide, antipyretic, anti – inflammatory activity
6.	20.25	Decanoic acid	$C_{10}H_{20}O_2$	172.26	49.407	Flavoring agent, perfumes, ice cream
7.	22.52	5,12-Naphthacenequinone	$C_{18}H_{10}O_2$	258.27	3.928	Antimicrobial activity Anti – inflammatory, diver tic, Anti – tuberculosis agent

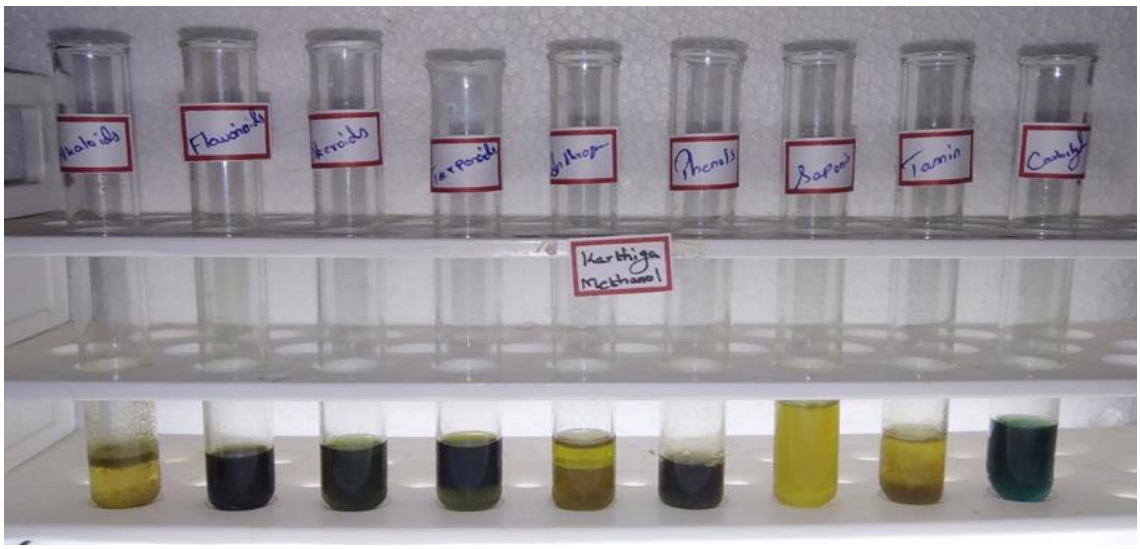


Fig. 1: Qualitative phytochemical analysis of *Acalypha hispida* in methanol extract

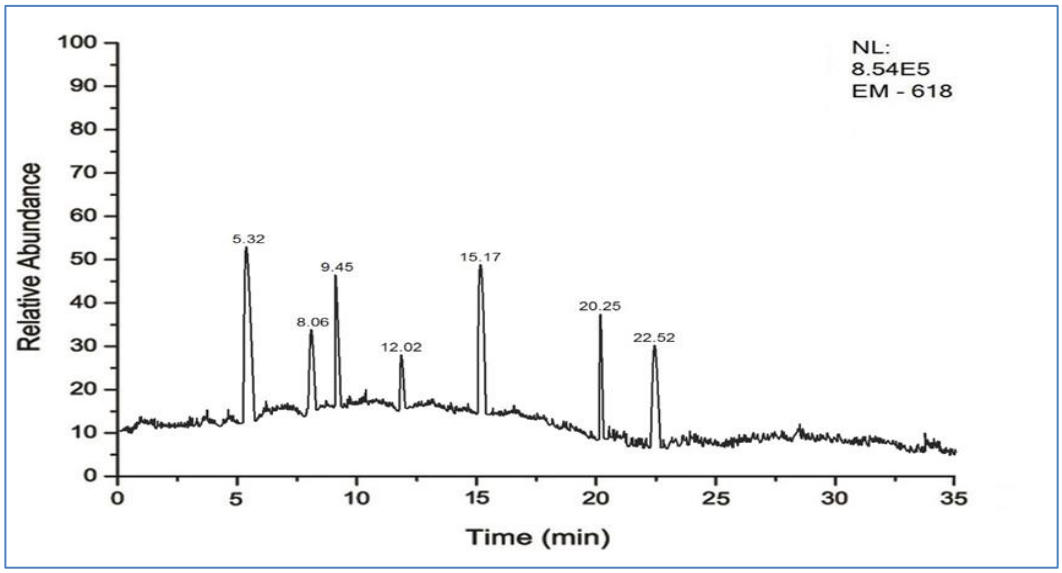


Fig. 2: GCMS Analysis for *Acalypha hispida* of methanol extract

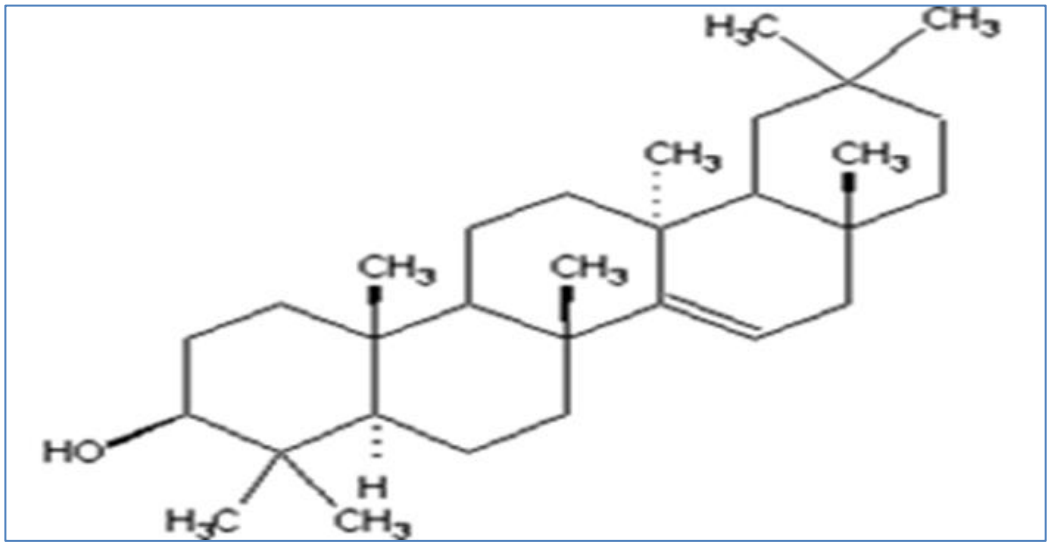
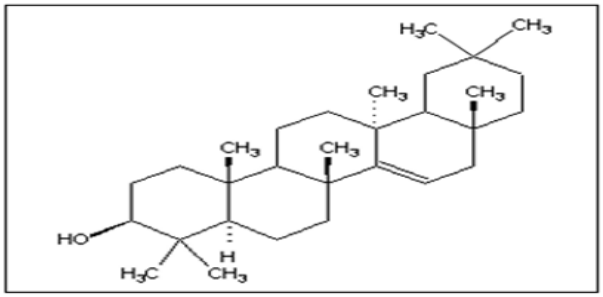


Fig. 3: Structure of Beta Ampyrin

Compound structure



Physical properties

- Molar Refractivity: 131.92 ± 0.4 cm^3
- Molar Volume: 420.8 ± 5.0 cm^3
- Parachor: 1054.8 ± 6.0 cm^3
- Index of Refraction: 1.539 ± 0.03
- Surface Tension: 39.4 ± 5.0 dyne/cm
- Density: 1.01 ± 0.1 g/cm^3
- Error: Cannot calculate Dielectric Constant.
- Polarizability: 52.29 ± 0.5 $10^{-24}cm^3$

Lipinski-type properties

- Molecular Weight: 426.72
- No. of Hydrogen Bond Donors: 1
- No. of Hydrogen Bond Acceptors: 1
- TPSA: 20.23
- No. of Rotatable Bonds: 0

Mass Spectroscopy related properties

- Monoisotopic Mass: 426.386166 Da
- Nominal Mass: 426 Da
- Average Mass: 426.7174 Da
- M+: 426.385618 Da
- M-: 426.386715 Da
- [M+H]+: 427.393443 Da
- [M+H]-: 427.39454 Da
- [M-H]+: 425.377793 Da
- [M-H]-: 425.37889 Da

Fig. 4: Physico Chemical Determination

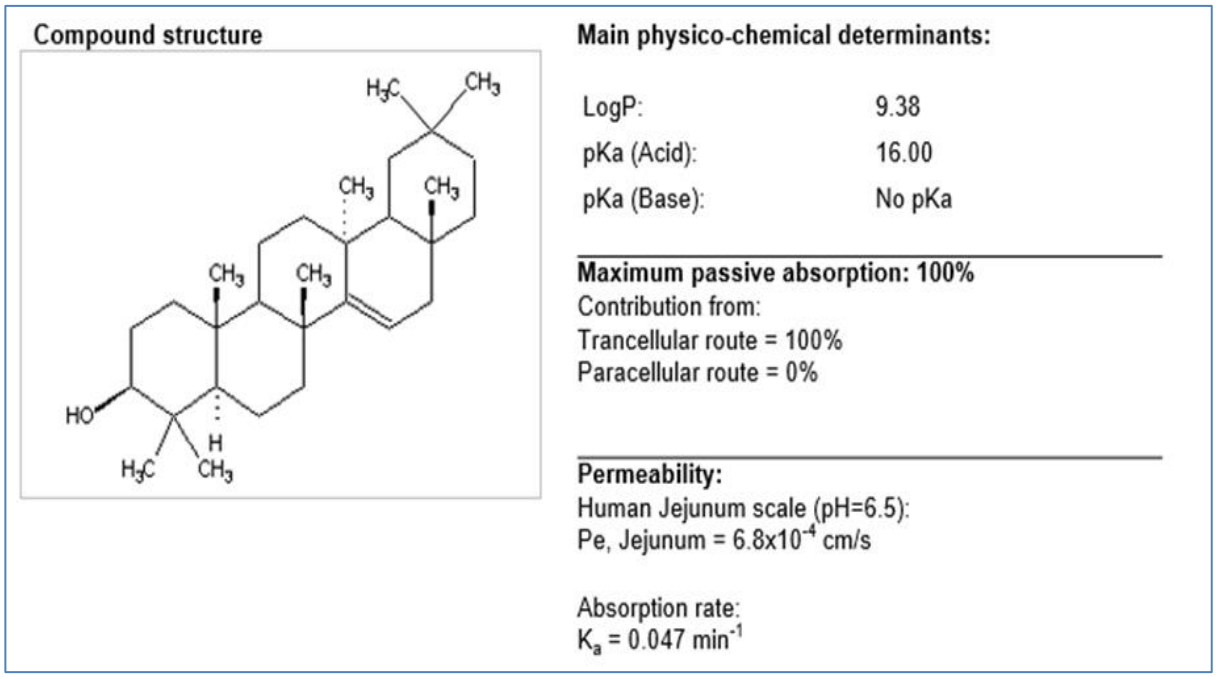


Fig. 5: Absorption studies

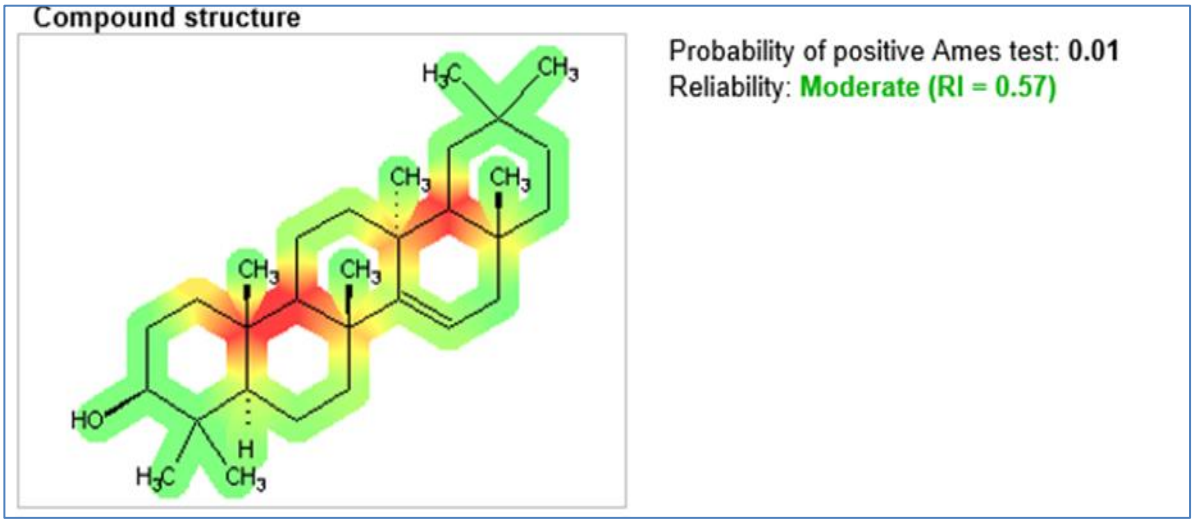


Fig. 6: Ames test

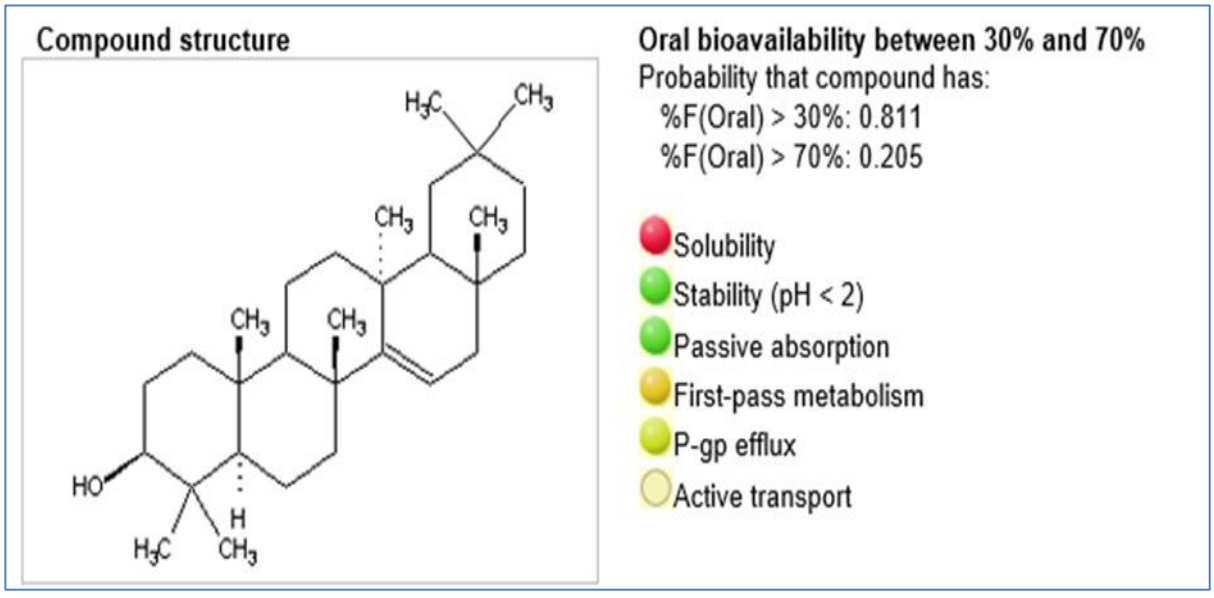


Fig. 7: Bioavailability study

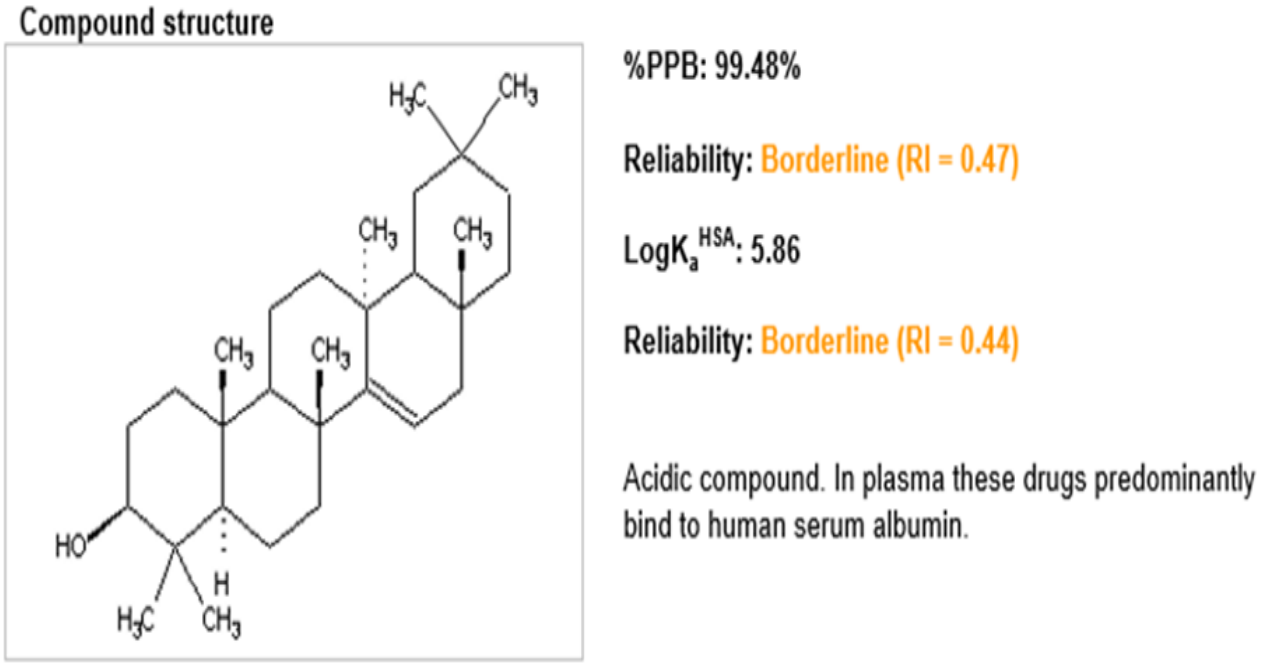


Fig. 8: Drug predominantly bind study

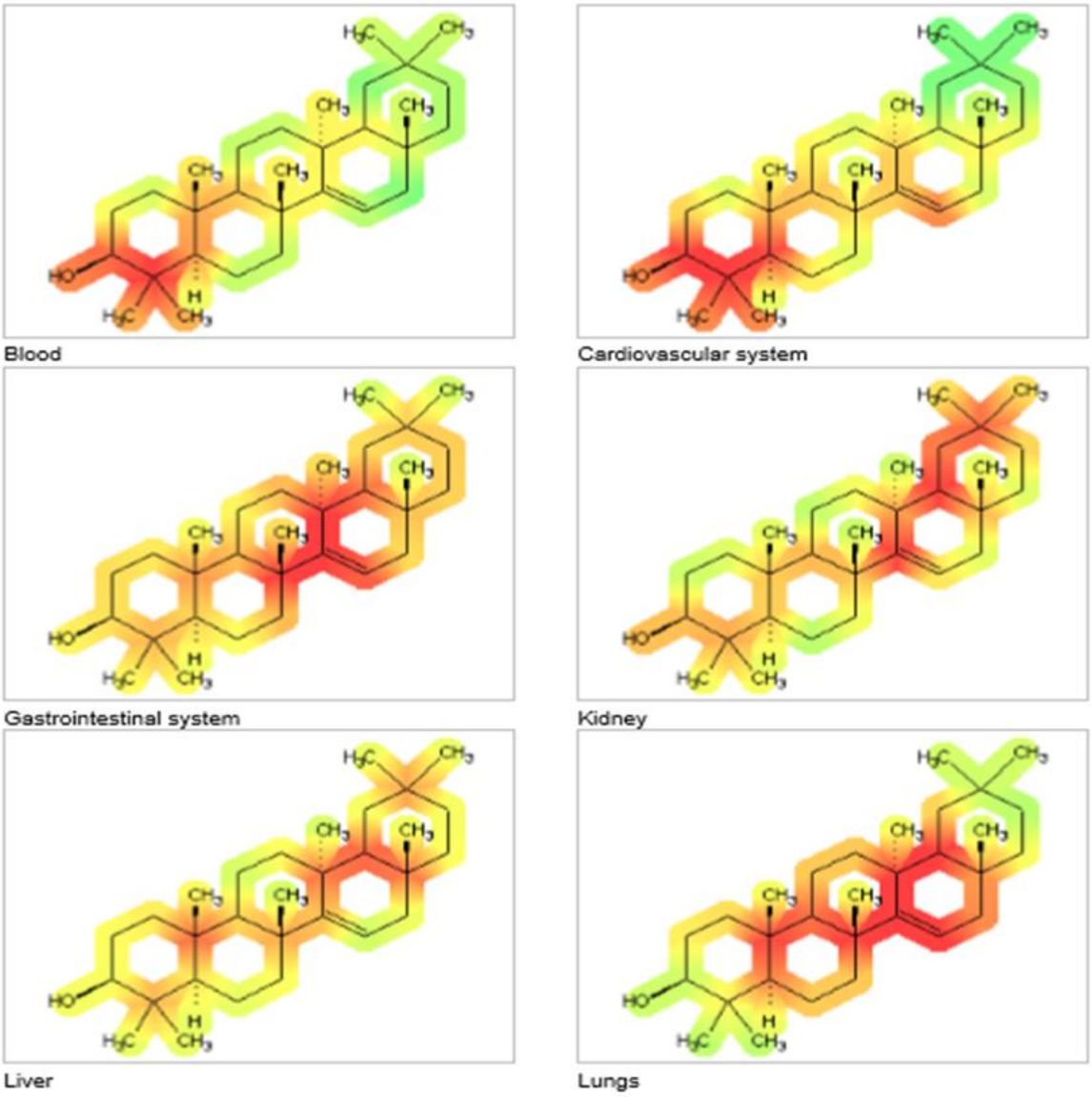
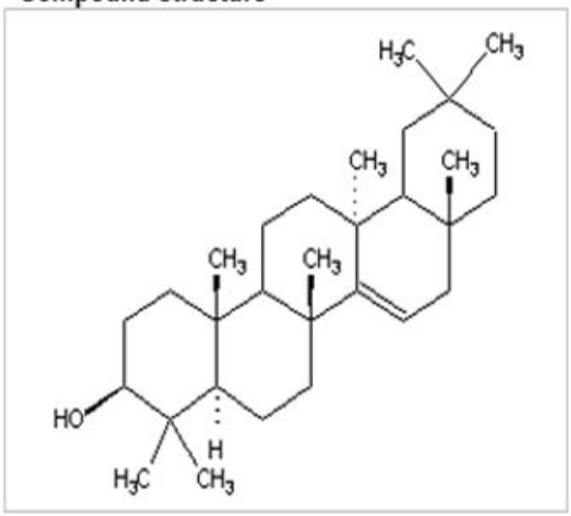


Fig. 9: Health Effects Study

Compound structure



Species/Administration route	LD50 (mg/kg)	Reliability (RI)
Mouse/Intraperitoneal	280	Moderate(0.53)
Mouse/Oral	530	Borderline(0.4)
Mouse/Intravenous	11	Borderline(0.42)
Mouse/Subcutaneous	47	Not Reliable(0.25)
Rat/Intraperitoneal	24	Not Reliable(0.29)
Rat/Oral	5.9	Not Reliable(0)

Fig. 10: Low Dosage 50 Percentage

Conclusions

The phytochemical, GC-MS and Bioinformatics analyses of *Acalypha hispida* were conducted in this study. The yield of the methanol extracts of *Acalypha hispida* was measured. Since the yield in the methanol fraction was far higher. Qualitative phytochemical analysis was done in methanol extracts of *Acalypha hispida* and it was found that alkaloids, flavonoids, saponins, tannins and carbohydrates were present in the methanol extract. In the quantitative analysis of the phytochemicals, alkaloids and flavonoids were estimated and it was noted that alkaloids were present in higher amount.

The methanol extract of *Acalypha hispida* was subjected to GC-MS and drug discovery study. From the GC-MS analysis, several compounds with medicinal values were found to be present in the methanol extract. From the above results obtained in this study, it can be concluded that the methanol extract of *Acalypha hispida* has potent medicinal properties against various diseases. The presence of many compounds in the extract showed that these compounds can be isolated and used as lead compound in drug discovery.

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