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Profiling of bioactive chemical entities in *Barleria buxifolia* L. using GC-MS analysis – a significant ethno medicinal plant

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ABSTRACT

The present study was designed at to ascertain the plausible bioactive compounds of the aerial methanolic extract of *Barleria buxifolia* via GC-MS analysis which is used as a noteworthy ethnomedicinal plant for treating various diseases. The peaks perceived in the mass spectra were identified as compounds and were matched with the National Institute of Standards and Technology and Wiley library. Identified compounds were predicted for its activity using PASS software. Interestingly, about 30 compounds were scrutinized with their retention time, molecular formula, molecular weight, peak area (%). Based on structure, activities were predicted. The GC-MS analysis unveiled the different kinds of bioactive compounds such as alkaloids, terpenoids, triterpenoids, esters, aliphatic ketones, β-carotene etc. In bioinformatics approach, using the software, Prediction Activity Spectra for Substances (PASS), pharmacological effects and drug likeness were determined for all the compounds precisely which endorse the traditional usage of B. buxifolia for the treatment of various kinds of diseases such as anti-inflammatory, antiulcer, antihypertensive, antiviral, antiobesity, antidiabetic, caridioprotectant, vasoprotector, spasmolytic, respiratory analeptic, carminative etc. It is inferred that the putative hits obtained from *B. buxifolia* could potentially serve as a launching pad for a hit-to-lead a novel drug development. *Barleria buxifolia*, Acanthaceae, GC-MS analysis, PASS prediction, Drug likeness, Activity.

Keywords: *Barleria buxifolia*, Acanthaceae, GC-MS analysis, PASS prediction, Drug likeness, Biological activity.

INTRODUCTION

In recent decades, about 80% of people in developing countries rely on medicinal plants for the treatment of various kinds of diseases which is relatively safe and effective. Therefore, tremendous interest has been considerably increased in the field of phytochemistry to find out the natural vital substances especially from medicinal plants. Now a days, many modern methods are available for the standardization of crude drugs, of them Gas Chromatography Mass Spectrum (GC-MS) has become firmly established to identify the active principles in both plants and non-plant organisms [1].

Barleria buxifolia (Acanthaceae) is an annual or perennial herb, found in Peninsular India. This plant is used for curing various kinds of diseases by different ethnic communities. The root decoction of the plant is used for the treatment of gastrointestinal upset by the local cultural groups of Attock (Punjab) district of Northern Pakistan [2]. The rural people of Madukkarai hills, southern Western Ghats of Coimbatore district, Tamil Nadu, India prescribed the leaves and rootsfor the remedy of cough and inflammations [3]. The whole plant decocotion is used to reduce cold as well as malarial fevers by the local indigenous groups of Kirthar National Park, Dadu district, Sindh, Pakistan [4]. The aboriginals of Ada'ar district of the Afar Region, Ethiopia are prescribing the root part of this plant to cure blackleg diseases in cattle's with oral, nasal or auricular administration [5]. The local people in the region of Randa, Djibouti endorsed the fresh leaf decoction made by soaking crushed fresh leaves in boiled water and the water is take normally for reducing the back pain [6]. Roots and leaves of the plant part are used to alleviate the stomach ache and febrifuge by the local peoples of Muniandavar scared groves of Thiuvaiyaru, Thanjavur, Tamil Nadu, India [7]. A paste of the root (rose mullippoondu) is applied to heal inflammations and boils by the local ethnic groups of Pachaimalai hills, Trichy district, Tamil Nadu, India [8-10]. The leaf extract of *B. buxifolia* has exerted potent anxiolytic, antidepressant [11] and antihelmintic activities [12]. The leaf extract exhibits antimicrobial activity also against the food borne pathogens [13].

Despite this species has huge ethnomedicinal value, there is a lack of information regarding on its phytochemicals. To address this lacuna, an attempt was made to enlightening the knowledge of ethnopharmacological importance and to explore the vital phytocompounds of the study species, *B. buxifolia* by GC-MS analysis. Furthermore, the biological activity and drug likeness of the GC-MS identified compounds were predicted by the computer programme, Prediction Activity Spectra for Substances (PASS).

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MATERIALS AND METHODS

Collection and Extraction

The fresh leaf part of the study plant was collected at foot hills of Maruthamalai, the Western Ghats, Tamil Nadu, India. They were washed with running tap water to eliminate the dust particles on the surface and simultaneously dried under shade condition for further analysis.

Extract Preparation

The shade dried leaves were pulverized into course powder. About, 40 g of leaf powder were extracted with methanol (250 ml) in soxhlet apparatus. Further, the crude leaf extract was condensed to dryness under room temperature and the percentage of yield was calculated (10.23%). The air dried extract was subjected to GC-MS analysis.

GC-MS Analysis

GC-MS analysis was carried out on thermo GC - trace ultra ver: 5.0, thermo MS DSQ II, DB 35-MS capillary standard non-polar column (30 × 0.25mm ID; film thickness: 0.25μm), operating in electron impact mode at 70 eV. Pure helium (99.999%) was used as carrier gas at a constant flow of1 ml/min and an injection volume of 1 μL was employed (split ratio is 10:1). Mass transfer line and injector temperature were set at 230 and 250°C respectively. The oven temperature was programmed from 70 (isothermal for 3 min) to 260°C (isothermal for 9 min) at the rate of 6°C/min. Total GC running time was 37.51 min and the MS detection was completed within 35min.

Identification of Chemical Constituents

The bioactive compounds existing in the crude leaf extract were identified by appraisal of their retention indices and mass spectra fragmentation patterns with those stored on the computer library and also with the published literature. It also found out by National Institute of Standards and Technology library sources [14,15].

Prediction Activity Spectra for Substances (PASS)

This computer system can predict biological activity based on structural formula of a chemical compound. The PASS approach is based on the suggestion, Activity=Function (Structure). Thus, "comparing" structure of a new substance with that of the standard biologically active substances, it is possible to find out whether a new substance has a particular effect or not. PASS estimates the probabilities of a particular substances belonging to the active and inactive sub-sets from the SAR Base (Structure-Activity Relationships Base) [16,17].

External Files of Substances

PASS uses Sdfile (.sdf) or MOLfile (.mol) formats as an external source of structure and activity data to prepare both SAR Base and the set of substances to be predicted [13]. SD files can be exported either from ISIS/Base 2.0+ (MDL Information Systems, Inc.) or from another moleculaar editor which has the option of SD file's export. MOL files can be prepared by ISIS/Draw. Molecular properties and 3D structure of compound were determined by using .sdf format which is obtained from Pubchem database (NCBI) [14]. The .mol generates 3D images using ArgusLab [15].

RESULTS AND DISCUSSION

The results pertaining to GC-MS analysis lead to profile of the bioactive chemical entities from the GC fractions of the methanolic aerial extract of *B. buxifolia.* The compound prediction is based on Dr. Dukes Phytochemical and Ethnobotanical Databases by Dr. Jim Duke of the Agricultural Research Service/USDA. The identified compounds and their rention time, molecular formula, molecular weight, peak aera (%), structure, nature of the compound and their activities retlated with medicinal uses are tabulated in Table 1. GC-MS analysis of the study plant revealed the existence of thirty compounds were perceived with differenct peak area percentage (Fig. 1). Apparently, the most prevailing major vital compounds in the methanolic extract of aerial part of *B. buxifolia* were, 5-hydroxy-6-methyl-12,13-dioxa-tricyclo[7.3.1.0(1,6)]tri decane-10-carboxylic acid, methyl ester (18.70%) (Fig. 2a), 9-Carbomethoxy-6,11-dichloroxy-5-oxoxantho[3,2-g]tetralin (10.49%) (Fig. 2b), 4-(4-Methoxy-6-methyl-5,6,7,8-tetrahydro-[1,3]dioxolo[4,5-g]isoquinolin-5-yl)-5-methyl-2,4-dihydro-pyrazol-3-one (7.47%) (Fig. 2c), 1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester (CAS) (7.28%) (Fig. 2d), 2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl- (CAS) (6.14%) (Fig. 2e), and 2-(4-(4-chlorophenyl) – 1 – oxo – 2(1H)-phthalazinyl) – N-(2, 2, 6,6tetramethyl – 4-piperidinyl) acetamide (5.99%) (Fig. 2f). The compound, 2,6,10,14,18,22-tetracosahexaene, 2,6,10,15,19,23-hexamethyl- (CAS) (peak area 6.14%) is suggested to be an triterpene which plays an important role in the synthesis of cholesterol, steroid hormone, and vitamin D in the human body and also used in cosmetic and pharmaceutical recipient. Another compound 2-(4-(4-chlorophenyl)-1-oxo-2(1H)-phthalazinyl)-N-(2,2,6,6tetramethyl-4-piperidinyl) acetamide (peak area 5.99%) is an alkaloid (organic heteromonocyclic compound, piperidine) employed in the treatment of asthma and cold. It is also supported hair dye, hallucinogen, helicicide, hemagglutinator, hematonic, hematopoietic, hemorrhagic, hepatocarcinogenic, hepatoprotective, hepatotonic, herbicide, HIV RV inhibitor, homeostatic, hyperglycemic, hypertensive, hyperthyroid, hyperlipidemic and hypertensive.

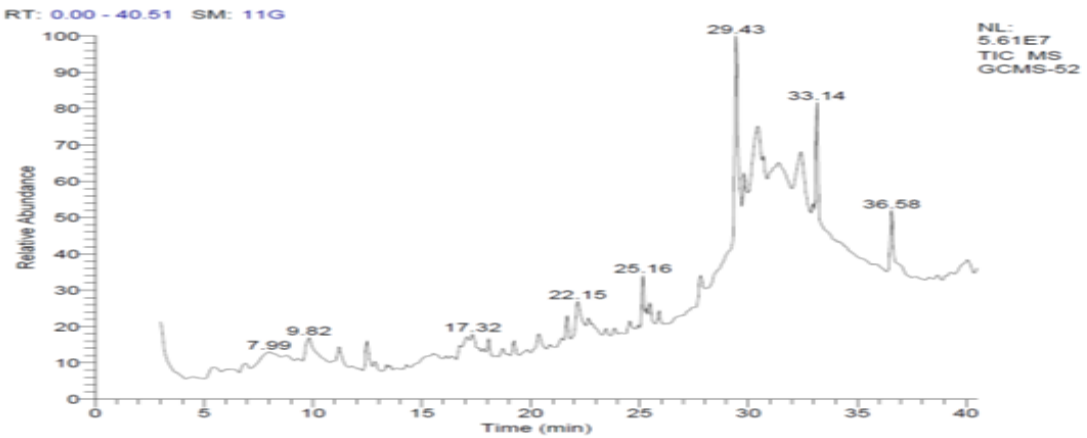


Figure 1: GC-MS chromatogram of methanolic aerial part extract of *B. buxifolia*

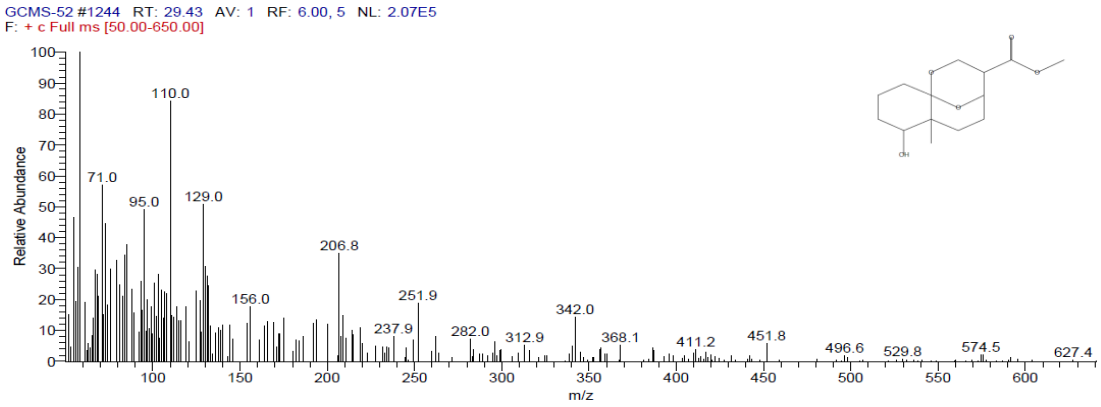


Figure 2a: Mass spectrum of 5-hydroxy-6-methyl-12,13-dioxa-tricyclo[7.3.1.0(1,6)]tri decane-10-carboxylic acid, methyl ester

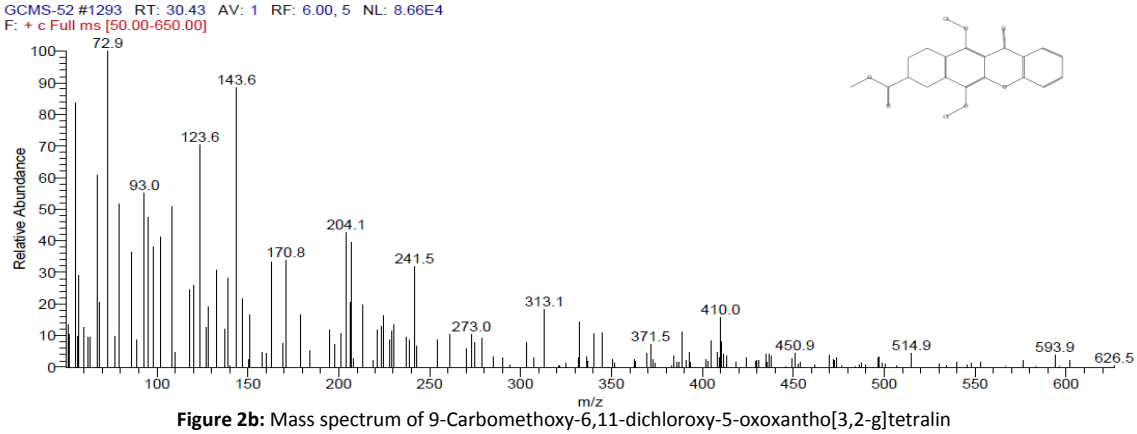


Figure 2b: Mass spectrum of 9-Carbomethoxy-6,11-dichloroxy-5-oxoxantho[3,2-g]tetralin

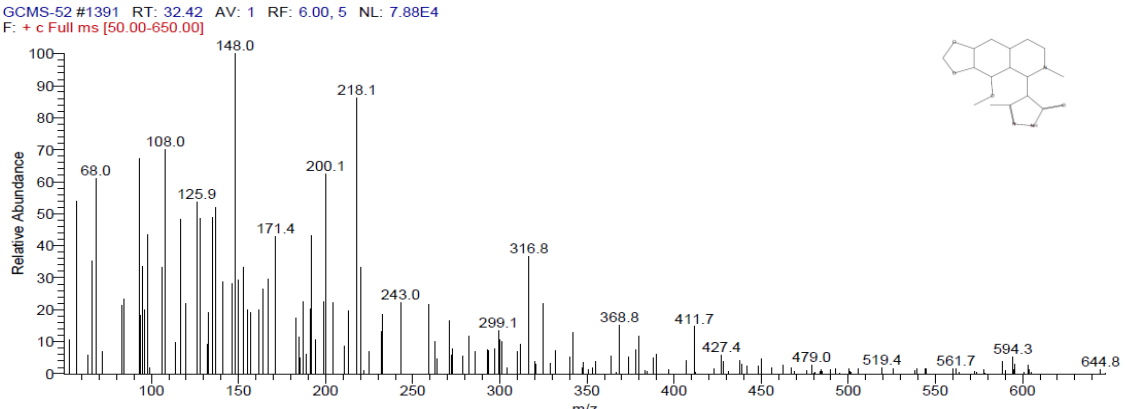


Figure 2c: Mass spectrum of 4-(4-Methoxy-6-methyl-5,6,7,8-tetrahydro-[1,3]dioxolo[4,5-g]isoquinolin-5-yl)-5-methyl-2,4-dihydro-pyrazol-3-one

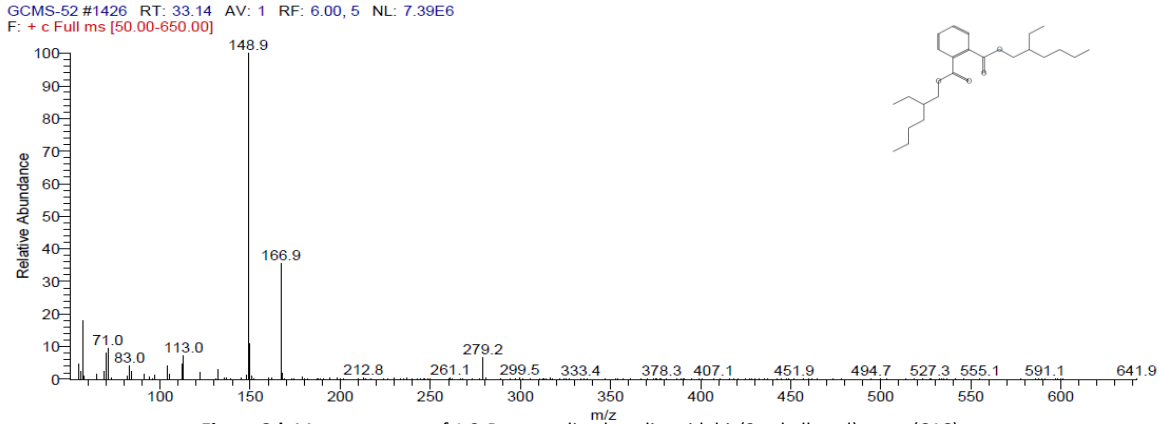


Figure 2d: Mass spectrum of 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester (CAS)

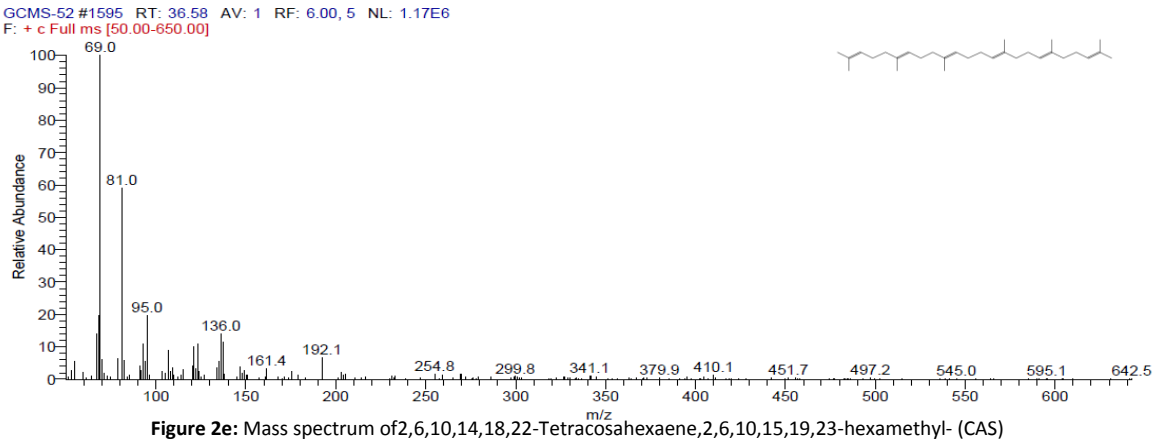


Figure 2e: Mass spectrum of2,6,10,14,18,22-Tetracosahexaene,2,6,10,15,19,23-hexamethyl- (CAS)

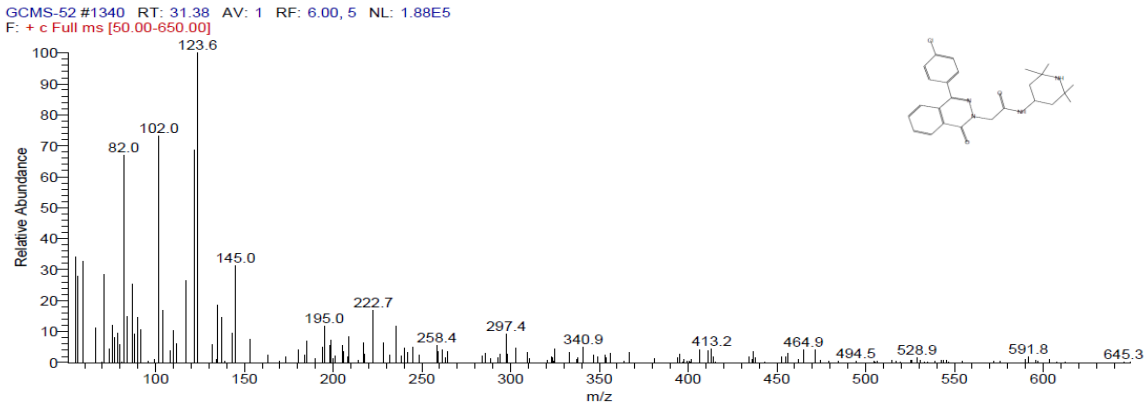


Figure 2f: Mass spectrum of 2-(4-(4-chlorophenyl)-1-oxo-2(1H)-phthalazinyl)-N-(2,2,6,6 tetramethyl-4-piperidinyl) acetamide

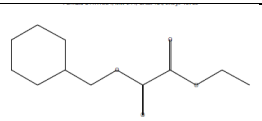
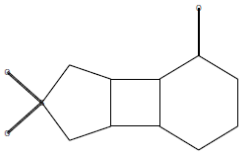
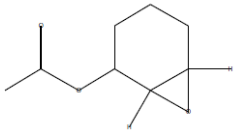
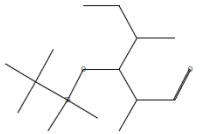
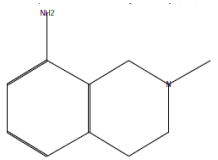
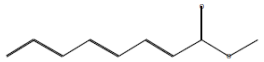
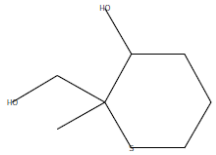
The pharmacological property and drug likeness of GC-MS identified compounds was predicted by PASS was presented in Table 2. It is found that the drug likeness of ten compounds *viz.*,Methyl 6-(vinylidene)penta-2,4-dien-1-oate], 2-(4-(4-chlorophenyl)-1-oxo-2(1H)-phthala zinyl)-N-(2,2,6,6 tetramethyl-4-piperidinyl) acetamide, 2,4,4-Trimethylcyclopenten-3-one, 1,3-D5-hexan-2-one 2,4 dinitrophenylhydrazone, anti-2,23-Dithia[3.3](1,4)triphenylenophane, 12-Tridecynoic acid, methyl ester (CAS), (2R,3R,4S)-3-dimethyl-t-butylsiloxy-2,4-dimethylhexanal, Hexadecanoic acid, methyl ester (CAS), Megastigmatrienone, 4,4,5,8-tetramethylchroman-2-ol, 4,14-Dibromo(2.2)metacyclophane and are 2.03, 1.83, 1.48, 1.38, 1.36, 1.35, 1.31, 1.28, 1.09, 1.02 and 1.04 respectively, which reveals more than 90% probability of being a drug.

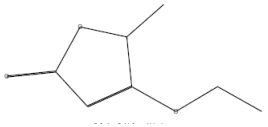
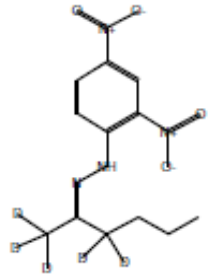
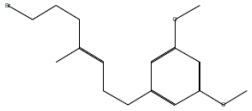
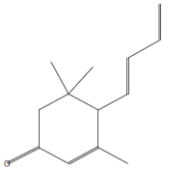
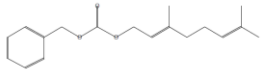
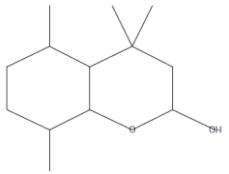
In order to find out the structure and specific activity of these compounds it is under gone for prediction of activity by using PASS software. The high drug likeness for the compounds such as 2-(4-(4-chlorophenyl)-1-oxo-2(1H)-phthala zinyl)-N-(2,2,6,6 tetramethyl-4-piperidinyl) acetamide (1.83), 9-Carbomethoxy-6,11-dichloroxy-5-oxoxantho[3,2-g]tetralin (0.85) and (+-)-4-ethoxy-5-methyl-2,5-dihydrofuran-2-one (0.70) proved the probability of being a drug. The antihypertensive (0.913 Pa), antiobesity (0.822 Pa) and antidiabetic (0.813 Pa) activity was shown by the compounds such as(2S,3S)-2-(hydroxymethyl)-2-methyltetrahydro-2H-thiopyran-3-ol. Diabetes mellitus is a chronic metabolic disorder caused by an absolute or relative lack of insulin and/or reduced insulin activity which results in hyperglycermia and abnormalities in carbohydrate, fat and protein metabolism [18,19]. Seemingly, apoptosis agonist activity was noticed in Methyl 6-(vinylidene)penta-2,4-dien-1-oate](0.922 Pa), 2,4,4-Trimethylcyclopenten-3-one(0.809 Pa),9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-(CAS)(0.703 Pa) and 2,6,10,14,18,22-Tetracosahexaene,2,6,10,15,19,23-hexamethyl- (CAS)(0.853 Pa).Furthermore, Benzyl geranyl carbonate, Hexadecanoic acid, methyl ester (CAS), 2,4,4-Trimethylcyclopenten-3-one, 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-(CAS) exerted anti-inflammatory activity with 0.785, 0.758 and 0.803 Pa value respectively. Likewise, antiulcer activity was perceived by the compoundsBenzyl geranyl carbonate(0.728 Pa), 2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-,[R-[R*,R*-(E)]]- (CAS)(0.736 Pa)and 9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-(CAS)(0.710 Pa). Interestingly cardiovascular property was seen in the compounds (+-)-4-ethoxy-5-methyl-2,5-dihydrofuran-2-one(0.703 Pa), 2,4,4-Trimethylcyclopenten-3-one(0.707 Pa)and 2,6,10,14,18,22-Tetracosahexaene,2,6,10,15,19,23-hexamethyl- (CAS)(0.723 Pa).

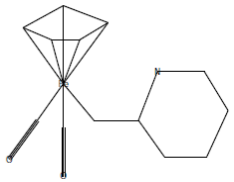
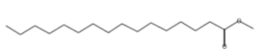
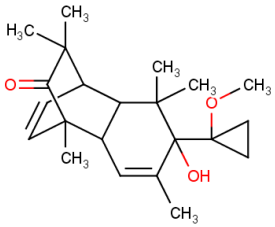
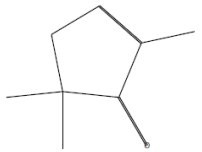
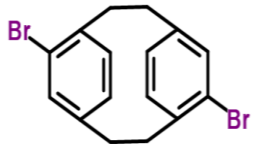
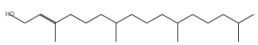
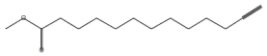
CONCLUSION

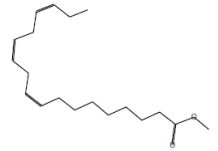
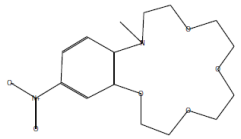
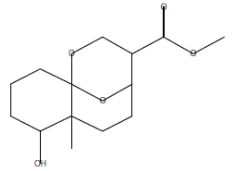
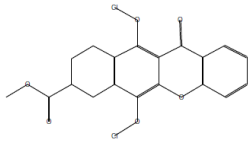
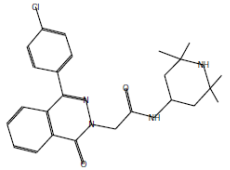
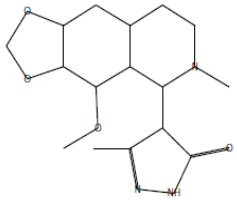
Our systematic investigation of th e crude plant extract unveils the potential of *B. buxifolia* aerial part as a good source of bioactive compounds such as alkaloids, terpenoids, triterpenoids, esters, aliphatic ketones, β-carotene etc. Prediction of biological activity of these compounds using the PASS software was fruitful to certain greatness. The manifestation of numerous bioactive compounds and their therapeutic confirmations rationalizes the use of this plant for curing various ailments by ethnopractitioners. Further, research interest in the study of these compounds might yield ecofriendly agents such as antioxidants, antibiotics etc.

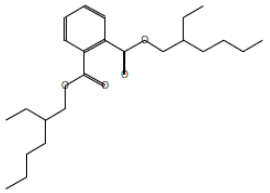
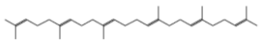
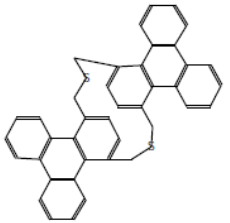
Table 1: Identification of bioactive vital compounds in methanolic aerial extract of *Barleria buxifolia*

S. No	Name of the compound	Retention Time	Molecular formula	Molecular weight	Peak area (%)	Nature of compound	Structure	Activity*
1.	Oxalic acid, cyclohexylmethyl ethyl ester	5.38	$C_{11}H_{18}O_4$	214	1.43	Fatty acid ester		-
2.	4-thiatricyclo[5.4.0.0(2,6)]undecan-8-one 4,4-dioxide	6.29	$C_{10}H_{14}O_3S$	214	0.70	Hetero Cyclic ketone		-
3.	3-(Acetyloxy)-cis-1,2-epoxycyclohexane	6.86	$C_8H_{12}O_3$	156	0.94	Essential oil		-
4.	(2R,3R,4S)-3-dimethyl-t-butylsiloxy-2,4-dimethylhexanal	7.95	$C_{14}H_{30}O_2Si$	258	2.15	Aliphatic aldehyde (or) Siloxy aldehyde		Free radical scavenging, RAN stimulant, Selective serotonin reuptake inhibitor, 5-Alph reductase inhibitor, Ant repellent, Anthocyanidin and anthocyanoside rich
5.	2-methyl-1,2,3,4-tetrahydroisochinolin-8-amin	9.82	$C_{10}H_{14}N_2$	162	3.08	Alkaloid		Increase aromatic amino acid decarboxylase activity, catechol-O-methyl-transferase-inhibitro, methyl donor, methyl guanidine inhibitor. Antithrombotic activity [20], Free radical scavenger and inhibitor of glutamate induced excitotoxicity [21], analgesic [22], antihypertensive [23] and antiviral [24]
6.	Methyl 6-(vinylidene)penta-2,4-dien-1-oate]	11.21	$C_9H_{10}O_2$	150	2.01	Aliphatic ester		-
7.	(2S,3S)-2-(hydroxymethyl)-2-methyltetrahydro-2H-thiop yran-3-ol	12.48	$C_7H_{14}O_2S$	162	2.68	Alcohol		Smart drug, adrenal support, adrenocortical stimulant, analgesic-synergist, ANS stimulant, anticancer (skin, stomatch), antidiabetic, antidote, antifeedant and antimetastatic (stomach).

8.	(+-)-4-ethoxy-5-methyl-2,5-dihydrofuran-2-one	12.85	$C_7H_{10}O_3$	142	0.70	Aliphatic ketone		-
9.	1,3-D5-hexan-2-one 2,4 dinitrophenylhydrazone	15.18	$C_{12}H_{11}D_5N_4O_4$	280	0.95	Hetero cyclic ketone		Smart drug, anticancer (duodenum), antidote, antileukotriene-D4, circulatory-depressant, CNS depressant, coronary dilator, decalcifier, decarboxylase inhibitor, decongestant, debridement, decrease endothelial leukocyte and platelet adhesion.
10.	S-Methyl 2-pyridyldithiocarboxylate	15.53	C_7H_7NOS	153	0.88	Dithioester (or) Ester	-	Smart drug, adrenal support, adrenocortical stimulant, analgesic, ANS stimulant, antibehcet's, anticancer (skin, stomach), anticarcinomic, anticrohn's, antidiabetic, antidote and antifeedant.
11.	(E)-1-Bromo-7-(3,5-dimethoxyphenyl)-4-methyl-4-heptene	17.07	$C_{16}H_{23}BrO_2$	326	4.90	Aromatic hydro carbon		Anticancer (esophagu), antidote, antitennis, antitumor, emollient, emetic and endocrinactive
12.	Megastigmatrienone	18.07	$C_{13}H_{18}O$	190	0.94	Nor – isoprenoids (β-carotene)		Flavouring agent
13.	Benzyl geranyl carbonate	18.73	$C_{18}H_{24}O_3$	288	0.73	Benzylic carbonate		-
14.	4,4,5,8-tetramethylchroman-2-ol	19.23	$C_{13}H_{18}O_2$	206	1.02	Alkaloid		Oligospermy and oliguria. Oligosaccharide provider

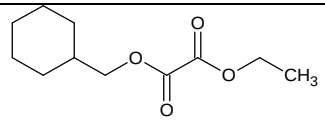
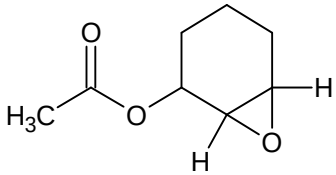
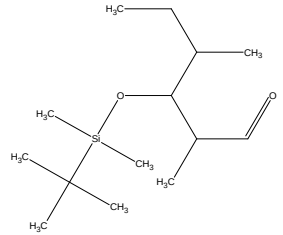
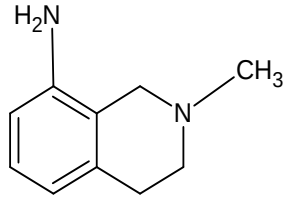
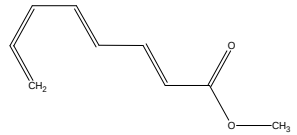
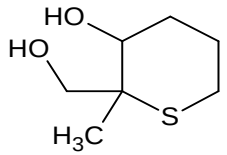
15.	Iron, dicarbonyl(ü5-2,4-cyclopentadien-1-yl)(2-pyridinylmethyl)- (CAS)	20.38	$C_{13}H_{11}FeNO_2$	269	2.02	Ferroeane complex		-
16.	Hexadecanoic acid, methyl ester (CAS)	21.68	$C_{17}H_{34}O_2$	270	2.22	Linoleic acidester		Anti-inflammatory, hypocholesterolemic, cancer preventive, hepatoprotective, nematicide, insectifuge, antihistaminic, antieczemic, antiacne, alpha reductase inhibitor, antiandrogenic, antiarthritic, anticoronary
17.	4-Hydroxy-4-(1'-methoxy-1'-cyclopropyl)-3,3,5,8,10,10-hexamethyltricyclo[6.2.2.0(2,7)]dodeca-5,11-diene-9-one	22.15	$C_{22}H_{32}O_3$	344	3.62	Cyclic ketone		Flavoring agent
18.	2,4,4-Trimethylcyclopenten-3-one	22.65	$C_8H_{12}O$	124	1.25	Terpenoid		-
19.	4,14-Dibromo(2.2)metacyclophane	24.55	$C_{16}H_{14}Br_2$	364	0.88	Alkaloid		-
20.	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]- (CAS)	25.16	$C_{20}H_{40}O$	296	3.87	Phytol (diterpene alcohol)		Antinociceptive and antioxidant [25]. Antiinflammatory [26]
21.	12-Tridecynoic acid, methyl ester (CAS)	25.48	$C_{14}H_{24}O_2$	224	1.27	Methyl isotetradecanoate		Acidifier, acidulant, arachidonic acid inhibitor, acidulant, acidifier, urinary acidulant and urine acidifier.

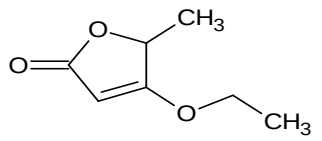
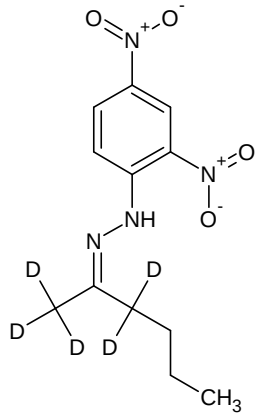
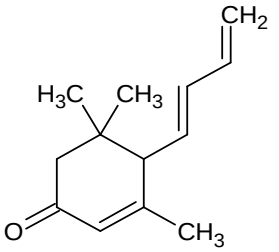
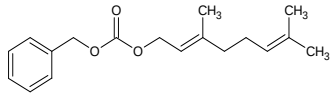
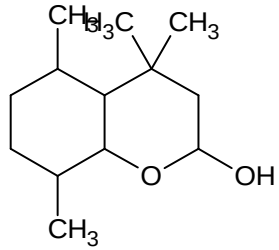
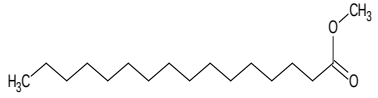
22.	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- (CAS)	25.90	$C_{19}H_{32}O_2$	292	0.78	Linoleic acid, methyl ester		Acidifier, acidulant, arachidonic acid inhibitor, inhibit production of uric acid, urine acidifier and urinary acidulant. Antiplasmodial [27]
23.	N-Methyl-4-nitrobenzo-13-aza-1,4,7,10-tetraoxa-15-crown-5	27.80	$C_{15}H_{22}N_2O_6$	326	2.44	Crown ether		Ache, antidote, anticancer, emission, lymphoma, nalaria, narcosis, narcotic, nausea, navel, neck, necrosis, nematicide.
24.	5-Hydroxy-6-methyl-12,13-dioxa-tricyclo[7.3.1.0(1,6)]tri decane-10-carboxylic acid, methyl ester	29.43	$C_{14}H_{22}O_5$	270	18.70	Ester		-
25.	9-Carbomethoxy-6,11-dichloroxy-5-oxoxantho[3,2-g]tetralin	30.4	$C_{19}H_{14}C_{l2}O_6$	408	10.49	-		-
26.	2-(4-(4-chlorophenyl)-1-oxo-2(1H)-phthala zinyl)-N-(2,2,6,6 tetramethyl-4-piperidinyl) acetamide	31.38	$C_{25}H_{29}C_lN_4O_2$	452	5.99	organic heteromonocyclic compound (piperidine)		Antidote, asthma, bite, cold, cosmetic, hair dye, hallucinogen, helicicide, hemagglutinator, hematonic, hematopoietic, hemorrhagic, hepatocarcinogenic, hepatoprotective, hepatotonic, herbicide, HIV RV inhibitor,homeostatic, hyperglycemic, hypertensive, hyperthyroid, hyperlipidemic, hypertensive
27.	4-(4-Methoxy-6-methyl-5,6,7,8-tetrahydro-[1,3]dioxolo[4 ,5-g]isoquinolin-5-yl)-5-methyl-2,4-dihydro-pyrazol-3-one	32.42	$C_{16}H_{19}N_3O_4$	317	7.47	Hetero cyclic ketone		-

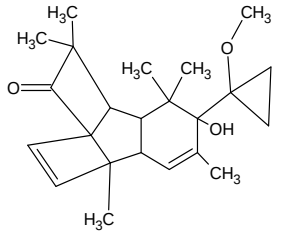
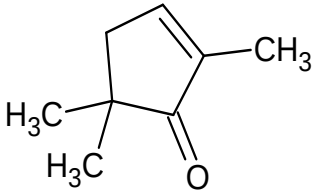
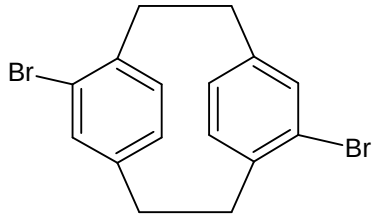
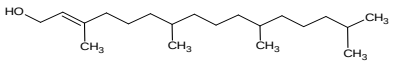
28.	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester(CAS)	33.14	$C_{24}H_{38}O_4$	390	7.28	Ester		-
29.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl- (CAS)	36.58	$C_{30}H_{50}$	410	6.14	Triterpene		Important role in the synthesis of cholesterol, steroid hormones, and vitamin D in the human body. Used in cosmetic and pharmaceutical excipient
30.	anti-2,23-Dithia[3.3](1,4)triphenylenophane	40.04	$C_{40}H_{28}S_2$	572	2.48	Hetero aromatic compound		-

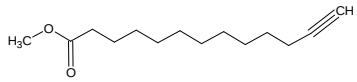
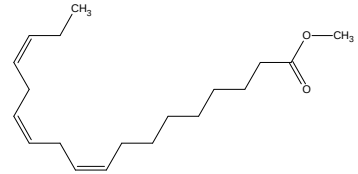
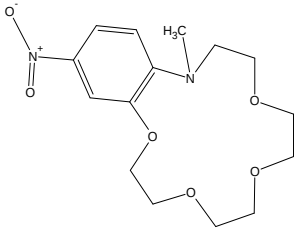
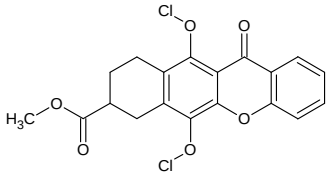
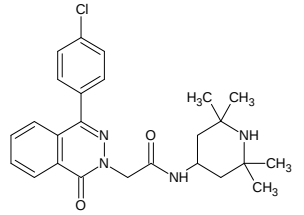
* Source: Dr. Dukes Phytochemical and Ethnobotanical Databases (Online database).

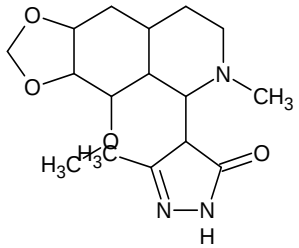
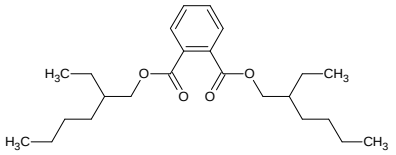
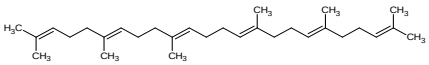
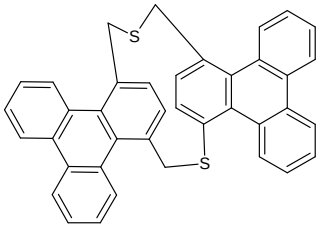
Table 2: Predicted activities and pa and pi values of compounds identified from GC-MS analysis in *Barleria buxifolia* using PASS.

S No	Name of the compound	Hydrogen bond Donor	Hydrogen bond acceptor	Drug likeness	Pa	Pi	Activity*	Structure
1.	Oxalic acid, cyclohexylmethyl ethyl ester	0	4	-0.50	0.903	0.005	Antieczematic	
					0.740	0.008	Cutinase inhibitor	
2..	3-(Acetyloxy)-cis-1,2-epoxycyclohexane	0	3	-0.96	0.879	0.006	Antieczematic	
					0.838	0.008	Antineoplastic	
					0.811	0.016	Mucomembranous protector	
					0.793	0.002	Beta glucuronidase inhibitor	
					0.785	0.009	Respiratory analeptic	
					0.783	0.022	Antiseborrheic	
					0.707	0.010	Analeptic	
3.	(2R,3R,4S)-3-dimethyl-t-butylsiloxy-2,4-dimethylhexanal	0	2	-1.31	0.848	0.004	Antiviral	
					0.785	0.003	Antiviral (HIV)	
					0.789	0.013	Antineoplastic	
					0.740	0.002	HIV-1 reverse transcriptase inhibitor	
					0.727	0.006	Antiinfective	
4.	2-methyl-1,2,3,4-tetrahydroisochinolin-8-amin	2	1	0.24	0.857	0.001	Octopamine antagonist	
					0.814	0.013	5 Hydroxytryptamine release stimulant	
					0.775	0.021	Antineurotic	
5.	Methyl 6-(vinylidene)penta-2,4-dien-1-oate]	0	2	-2.03	0.922	0.004	Apoptosis agonist	
					0.755	0.029	Antieczematic	
					0.721	0.020	GST A substrate	
					0.717	0.036	Polyporopepsin inhibitor	
6.	(2S,3S)-2-(hydroxymethyl)-2-methyltetrahydro-2H-thiopyran-3-ol	2	3	-0.94	0.913	0.004	Antihypertensive	
					0.852	0.009	Antieczematic	
					0.822	0.005	Antiobesity	
					0.813	0.005	Antidiabetic	
					0.742	0.022	Antiischemic. cerebral	

7.	(+-)-4-ethoxy-5-methyl-2,5-dihydrofuran-2-one	0	3	0.70	0.819 0.782 0.730 0.703	0.004 0.023 0.005 0.007	Vasoprotector Antieczematic Anesthetic general Cardiovascular analeptic	
8.	1,3-D5-hexan-2-one 2,4 dinitrophenylhydrazone	3	5	-1.38	0.811	0.005	Cutinase inhibitor	
9.	Megastigmatrienone	0	1	-1.09	0.814 0.784 0.784	0.004 0.014 0.022	Carminative Antineoplastic Antieczematic	
10.	Benzyl geranyl carbonate	0	3	-0.98	0.785 0.728	0.008 0.005	Antiinflammatory Antiulcerative	
11.	4,4,5,8-tetramethylchroman-2-ol	2	1	-1.22	0.731	0.012	Antidyskinetic	
12.	Hexadecanoic acid, methyl ester (CAS)	0	2	-1.28	0.885 0.854 0.807	0.003 0.009 0.004	Cutinase inhibitor Antieczematic Eye irritation. inactive	

					0.805	0.009	Membrane permeability inhibitor	
					0.794	0.005	Macrophage colony stimulating factor agonist	
					0.758	0.002	Antiinflammatory. intestinal	
					0.777	0.023	Antiseborrheic	
					0.744	0.005	Anesthetic general	
					0.738	0.010	Superoxide dismutase inhibitor	
					0.719	0.002	Oxidizing agent	
					0.708	0.005	Oxygen scavenger	
					0.701	0.005	Cytoprotectant	
					0.688	0.002	Vanilloid agonist	
					0.653	0.034	Antineoplastic	
					0.604	0.024	Spasmolytic. urinary	
13.	4-Hydroxy-4-(1'-methoxy-1'-cyclopropyl)-3,3,5,8,10,10-hexamethyltricyclo[6.2.2.0(2,7)]dodeca-5,11-diene-9-one	1	3	-0.86	0.568	0.002	Thromboxane synthase stimulant	
					0.524	0.012	Menopausal disorders treatment	
					0.520	0.011	Dementia treatment	
					0.855	0.003	Carminative	
					0.846	0.005	Antiinflammatory	
					0.809	0.008	Apoptosis agonist	
14.	2,4,4-Trimethylcyclopenten-3-one	0	1	-1.48	0.768	0.003	Nitric oxide antagonist	
					0.775	0.024	Antiseborrheic	
					0.749	0.010	Antidyskinetic	
					0.707	0.007	Cardiovascular analeptic	
					0.780	0.020	Antineurotic	
					0.721	0.007	Kidney function stimulant	
15.	4,14-Dibromo(2.2)metacyclophane	0	0	-1.04	0.708	0.017	Glutathione thiolesterase inhibitor	
					0.725	0.035	Chlordecone reductase inhibitor	
					0.707	0.036	Antiseborrheic	
					0.736	0.005	Antiulcerative	
16.	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]- (CAS)	1	1	-0.87	0.724	0.011	Macrophage colony stimulating factor agonist	
					0.721	0.010	Peroxidase inhibitor	
					0.710	0.003	Antiviral (Rhinovirus)	

17.	12-Tridecynoic acid, methyl ester (CAS)	0	2	-1.35	0.751	0.030	Antieczematic	
					0.949	0.003	Antieczematic	
					0.803	0.006	Antiinflammatory	
					0.796	0.005	Macrophage colony stimulating factor agonist	
					0.741	0.008	Cutinase inhibitor	
					0.739	0.007	Antisecretoric	
18.	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)- (CAS)	0	2	-0.94	0.734	0.007	Vasodilator. peripheral	
					0.727	0.001	Cyclooxygenase 1 substrate	
					0.725	0.007	Antihypercholesterolemic	
					0.722	0.007	Antithrombotic	
					0.713	0.004	Gastrin inhibitor	
					0.710	0.005	Antiulcerative	
					0.703	0.005	Eye irritation. inactive	
					0.703	0.014	Apoptosis agonist	
19.	N-Methyl-4-nitrobenzo-13-aza-1,4,7,10-tetraoxa-15-crown-5	1	6	-0.91	0.720	0.031	Membrane permeability inhibitor	
					0.882	0.016	Membrane integrity agonist	
20.	9-Carbomethoxy-6,11-dichloroxy-5-oxoxantho[3,2-g]tetralin	0	6	0.85	0.849	0.010	CYP2H substrate	
					0.811	0.008	Membrane permeability inhibitor	
					0.749	0.020	Antiischemic. cerebral	
21.	2-(4-(4-chlorophenyl)-1-oxo-2(1H)-phthala zinyl)-N-(2,2,6,6 tetramethyl-4-piperidinyl) acetamide	2	4	1.83	0.702	0.009	Anticonvulsant	

22.	4-(4-Methoxy-6-methyl-5,6,7,8-tetrahydro-[1,3]dioxolo[4,5-g]isoquinolin-5-yl)-5-methyl-2,4-dihydro-pyrazol-3-one	1	6	0.01	0.460	0.005	Antineoplastic (brain cancer)	
23.	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester(CAS)	0	4	0.26	0.973	0.002	Eye irritation. inactive	
					0.949	0.003	Skin irritation. inactive	
					0.927	0.002	Cutinase inhibitor	
					0.819	0.015	Antiseborrheic	
					0.771	0.005	Anesthetic general	
					0.727	0.010	Macrophage colony stimulating factor agonist	
					0.853	0.005	Apoptosis agonist	
					0.817	0.001	Antiviral (Rhinovirus)	
					0.801	0.003	Ecdysone 20-monooxygenase inhibitor	
					0.801	0.012	Antineoplastic	
24.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10,15,19,23-hexamethyl- (CAS)	0	0	-0.85	0.793	0.005	Macrophage colony stimulating factor agonist	
					0.803	0.018	Antieczematic	
					e0.739	0.007	Antisecretoric	
					0.737	0.005	Antineoplastic (breast cancer)	
					0.737	0.008	Cutinase inhibitor	
					0.723	0.006	Cardiovascular analeptic	
					0.714	0.006	Carminative	
					0.704	0.006	Antineoplastic (lung cancer)	
25.	anti-2,23-Dithia[3.3](1,4)triphenylenophane	0	2	-1.36	0.978	0.000	Neurotransmitter uptake inhibitor	

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