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CHEMICAL PROFILING AND ADME PREDICTION OF SARACA ASOCA (ROXB) WILDE

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ABSTRACT

The dried powdered bark of *Saraca asoca* was extracted using ethyl acetate, acetone, ethanol and distilled water by a three-step sequential extraction procedure. Among all extracts, ethanolic extract showed highest phenol (438.78±0.86 mg/g gallic acid equivalent), proanthocyanidins (0.8±0.05) and coumarin **(**1.192±0.2 mg/g) content while highest flavonoid (179.5±0.47 mg/g rutin equivalent) were detected in ethyl acetate extract. Highest DPPH free radical quenching activity was observed in ethanolic extract of *Saraca asoca* (IC_{50} value 48.43) which was significantly comparable with ascorbic acid (IC_{50} value 14.12). The UV-visible and FTIR spectrum confirmed the presence of alcohols, phenols, alkanes, alkyl halides, aldehydes, carboxylic acids, aromatics, nitro compounds and amines in ethanolic extract. The FTIR, GC-MS spectrum profile along with the (ADME)-Toxicity analysis unveiled that the medicinally important plant *Saraca asoca* bark extract having various bioactive compounds and can be used as therapeutic agents.

KEYWORDS: ADMET, FTIR, GC-MS, *Saraca asoca*.

1. INTRODUCTION

Saraca asoca a component of several ayurvedic and traditional ethnomedical preparations belongs to the family *Caesalpinaceae* which is commonly known as ashoka meaning that "without sorrow" or which that gives no grief. In India, Ashoka is used in many pharmacological activities like anti-cancer, anti menorrhagic, anti oxytoxic, anti –microbial activity and have extend uses in ayurveda, unani and homeopathy [1]. It has many uses in treatment of skin infections, CNS function and genitor-urinary functions. It's bark mostly beneficial in uterine inertia, uterine pain, urinary calculus, dysurea, Leucorrhoea and urinary stone [2]. Some of the most important bioactive phytochemical constituents such as glycosides, alkaloids, flavonoids, tannins, steroids, terpenoids, essential oils and phenolic compounds are found in *Saraca asoca*[3]. Phenolics and flavonoids are polyphenols, an important class of secondary plant metabolites possessing an impressive array of pharmacological activity which include free radical scavenging, inhibition of hydrolytic and oxidative enzymes and anti-inflammatory action etc [4]. Oxidation reaction can produce free radicals, which can damage cells and tissues. Recently, there has been an upsurge of interest in the therapeutic potential of medicinal plants as antioxidants in reducing such free radical-induced tissue injury. As a result, profiling of medicinal plant by some platform technology such as gas chromatography-mass spectrometer (GC-MS), liquid chromatography-mass spectrometer as well as it's holistic overview of all metabolites present in extracts became crucial and valuable. Spectroscopic (UV-Vis, FTIR) methods together or separate can be used because of its simplicity, cost-effective and rapid test for detecting phytocomponents. Hence the present study is designed to evaluate the phytochemical profile of *Saraca asoca*, with the aid of GC-MS, UV-VIS and FTIR Techniques, to ascertain the rationale for its use in traditional medicine.

2. MATERIALS AND METHODS

2.1 Drugs

Saraca asoca barks were procured from Yogesh pharma Pvt. Ltd., Nanded (MS), India. It was identified and authenticated at Department of Botany, Babasaheb Ambedkar Marathwada University Aurangabad, India. The barks were washed thoroughly with water to remove dust and dried under the shade at room temperature for 5 days. The dried barks were ground using blender to obtain the course powder and kept in an air tight container

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till further use. Powdered plant material (150g) were successively extracted using Soxhlet apparatus using the solvents in order of increasing polarity viz., C), ethyl acetate, acetone, ethanol and distilled water. Each time the marc was dried and later extracted with other solvents. All the extracts were concentrated by distilling the solvent in a rotary vacuum evaporator.

2.2 Phytochemical Screening of Bark Extract

The four extracts obtained from the powdered bark of *Saraca asoca* were subjected to phytochemical tests to investigate the presence or absence of active secondary metabolites using standard procedures [5].

2.3 Qntitative Estimation of Total Phenols

Folin-Ciocalteu reagent was used to determine the total phenolic content (TPC) of the various organic crude extracts with slight modification [6]. 1.5 ml Folin-Ciocalteu reagent (diluted 1:10 with de-ionized water) was added to the 0.5 mL of the plant extract sample, and was vortexed for 5 min, followed by addition of 3 mL of sodium carbonate solution (7.5%). This reaction mixture was incubated for 30 min at room temperature in dark. The absorbance of the resulting blue colour was measured by using double beam UV-Vis spectrophotometer (UV Shimadzu- 1800) at fixed wavelength of 760 nm. The calibration curve was prepared by employing gallic acid at concentrations of 10 to100 µg/ml. The TPCs were determined using linear regression equation obtained from the standard plot of gallic acid. The content of total phenolic compounds was calculated as mean±SD (n=3) and expressed as mg/g gallic acid equivalent (GAE) of dry extract.

2.4 Quantitative Estimation of Total Flavonoid

Aluminum chloride colorimetric method was used for flavonoids determination as described by Madaan *et al.*[7]. 0.5 mL of each plant extract was mixed with 1.5 mL of ethanol, 0.1 mL of 10% aluminum chloride, 0.1 mL of 1 M potassium acetate and 2.8 mL of distilled water. The reaction mixture was allowed to stand at room temperature for 30 min and the absorbance of the reaction mixture was measured at 415 nm. The calibration curve was prepared by using rutin at concentrations of 10 to100 µg/ml in ethanol. The amount of flavonoid was calculated from linear regression equation obtained from the rutin calibration curve. The flavonoid content was calculated as mean±SD (n=3) and expressed as mg/g of rutin equivalent (RE) of dry extract.

2.5 Quantitative Estimation of total Proanthocyanidins

The total proanthocyanidin content were estimated using the procedure reported by Sun *et al*[8].A volume of 0.5 mL of 0.1 mg/mL of extract solution was mixed with 3.0 mL of 4% vanillin-methanol solution and 1.5 mL hydrochloric acid, the mixture was allowed to stand for 15 min at room temperature, the absorbance was measured at 500 nm. The proanthocyanidins content was calculated as mean±SD (n=3) and expressed as mg/g of catechin equivalent of dry extract.

2.6 Quantitative Estimation of total Coumarin

Coumarin content was estimated with slight modification in procedure reported by Bruna Medeiros-Neves *et al*[9].A volume of 0.5 mL of the extract was mixed with 2 ml of distilled water and 0.5 mL of lead acetate solution. The sample was shaken and then 7 ml of distilled water were added before transferring 2mL of this solution to a new test tube and added 8 mL of hydrochloric acid solution. The sample was incubated at room temperature for 30 minutes and the absorbance was measured at 500 nm. The coumarin content was calculated as mean±SD (n=3) and expressed as mg/g of coumarin equivalent of dry extract.

2.7 Free Radical Scavenging Activity by DPPH Assay Method

The capacity of the extracts and ascorbic acid to scavenge the stable 1, 1-diphenyl-2-picrylhydrazyl (DPPH) free radical was measured as per stated method [10]. 0.1 mL of extracts and ascorbic acid of different concentrations (10to200 µg/ml) was mixed with 2.9 mL of 0.1mM DPPH solution. The solution was rapidly mixed and allowed to stand in dark at room temperature for 30 min. The blank was prepared in a similar way without extract or ascorbic acid. The decrease in absorbance of each solution was measured at 517 nm using UV-Vis spectrophotometer. Negative control was prepared by mixing 0.1 mL of ethanol with 2.9 mL of DPPH solution. The percentage of radical scavenging activity of tested extracts and positive control ascorbic acid was calculated by using the following formula:

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Free radical scavenging activity (%) = $\frac{[Ac- As]}{Ac} \times 100$

Where Ac=Absorbance of control and As=Absorbance of sampleat 517 nm.

The concentration of sample required to scavenge 50% of DPPH free radical (IC_{50}) was determined from the curve of percent inhibitions plotted against the respective concentration.

2.8 UV-VIS and FTIR Spectroscopic analysis

The ethanolic extract was examined under visible and UV light for proximate analysis. For UV-VIS and FTIR spectrophotometer analysis, the extract was centrifuged at 5000 rpm for 15 min and filtered through Whatman No. 1 filter paper. The sample is diluted to 1:10 with the same solvent. The extract was scanned in the wavelength ranging from 200-1100 nm using UV-1800 Shimadzu UV Spectrophotometer and the characteristic peaks were detected. FTIR analysis was performed using Thermofisher Scientific, model-Nicolet 6700 FT-IR system in a scan range of 400 -4000 $cm^{-1}$and characteristic peaks and their functional groups were detected.

2.9 Gas Chromatography-Mass Spectrometry Analysis

The GC-MS analysis of the ethanolic extract was carried out using a Agilent 7890 A gas chromatogram equipped and coupled to a mass detector 5975 MSD spectrometer with DB 5 MS and 30m × 0.25 µm DF of capillary column. Ultra-high purity helium (99.99%) was used as carrier gas at a constant flow rate of 1.0 mL/min. The injection, transfer line and ion source temperatures were all 290 °C. The ionizing energy was 70 eV. Electron multiplier voltage was obtained from autotune. The oven temperature was programmed from 60 °C (hold for 2 min) to 320 °C at a rate of 3 °C/min. The crude ethanolic extract of *Saraca asoca* was diluted with appropriate solvent (1/10, V/V) and filtered. The particle-free diluted crude extracts (1 µL) were taken in a syringe and injected into injector with a split ratio 30:1. All data were obtained by collecting the full-scan mass spectra within the scan range 30-600 amu. The percentage composition of the crude extract constituents was expressed as a percentage by peak area. The identification and characterization of chemical compounds in ethanolic crude extract was based on GC retention time. AMDIS and NIST Version-Year 2011 was used MS data library and comparing the spectrum obtained through GC-MS compounds present in the plants sample was identified.

2.10ADMET predictions

ADMET (Absorption, Distribution, Metabolism, Excretion and Toxicity) analyses constitutes the pharmacokinetics of a drug molecule [11]. In this study, prediction and significant descriptors of drug likeness such as mutagenicity, toxicological dosage level and pharmacologically relevant properties of the compounds were predicted using Swissadme (http://www.swissadme.ch) and admetSAR (lmmd.ecust.edu.cn:8000) servers.

2.11Data Analysis

The results are expressed as mean ± SD. Student's *t*-test and one way ANOVA were applicable and used to analyze level of statistical significance between groups. $P<0.05$ were considered statistically significant. Linear regression analysis was used to calculate the IC_{50} values.

3 RESULTS AND DISCUSSION

3.1 Preliminary Phytochemical Screening

Preliminary phytochemical analysis showed the presence of major classes of secondary metabolites such as tannins, saponins, flavonoids, cardiac glycosides, *etc*. in extracts [Table I]. Alkoids were found to be absent in all the extracts.

3.2 Quantitative Estimation of phytoconstituents

The present study revealed relatively good amount of phenols, flavonoids, coumarin and proanthocyanidins contents in *Saraca asoca* extracts as shown in (Table II). The correlation coefficient of total phenols, total flavonoids, coumarin and total proanthocyanidins were (r =0.993, 0.984, 0.992 and 0.970) respectively (Fig. 1).

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3.3 Estimation of Free Radical Scavenging Activity

The antioxidant activity of *Saraca asoca* was evaluated using the DPPH free radical scavenging method. Ascorbic acid was used as standard compound. The *Saraca asoca* exhibited strong antioxidant activity in the DPPH inhibition assay as evidenced by the low IC_{50}values and were compared with standard antioxidant, ascorbic acid. All the extracts showed a dose dependent scavenging activity of DPPH comparable to standard antioxidant (Fig. 2). The IC_{50} value (in µg/mL) of the extracts was found in the order of distilled water>acetone>ethyl acetate>ethanol extract (Table III). IC_{50} value of ascorbic acid (14.12µg/mL) was less than the ethanol extract (18.4µg/mL).Higher phenol and flavonoid content in the plant tissue can also lead to increase in antioxidant activity [12].

3.4 Spectrophotometric analysis

The UV-VIS profile of *Saraca asoca* extract was selected at the wavelength of 200 to 400 nm and the spectrum profile showed the peaks at 344 and 232 nm with the absorption 3.600 and 1.256 respectively (Fig.3; Table IV). Occurrence of peaks at 234-676 nm reveals the presents of phenolic and alkaloids.The FTIR spectrum was used to identify the functional group of the active components based on the peak value in the region of infrared radiation. The results of FTIR peak values and functional groups were represented in (Fig. 4; Table V). FTIR spectrum confirmed the presence of alcohols, phenols, alkanes, alkynes, alkyl halides, aldehydes, carboxylic acids, aromatics, nitro compounds and amines in ethanol extract. On comparison of the spectra of bark shows that the extract has some similar alkaloid, phenolics and glycosides compounds[13]. Hence, UV and FTIR spectroscopy is reliable and sensitive method for detection of bioactive constituents.

3.5 Chemical Composition of Extracts by GC-MS Analysis

GC-MS chromatogram of the ethanolic extract of *S.asoca* (Fig. 5) showed 14 peaks indicating the presence of 14 phytochemical constituents. All the constituents were characterized and identified by comparison of the mass spectra of the constituents with the AMDIS and NIST Version-Year 2011library. The active principles with their retention time (RT), molecular formula, molecular weight (MW) and concentration (%) are presented in (Table VI). The prevailing compounds were à-D-(+)-Talopyranose, pentakis(trimethylsilyl) ether (68%) followed by Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-(61%), D-Pinitol, pentakis(trimethylsilyl) ether (57%) ,Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, L- (56%), Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl) (55%), , >Arabinopyranose, tetrakis-O-(trimethylsilyl)-, à-D- (47%) and Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, D-(37%). The biological activities listed (Table VII) are based on Dr.Duke's Phytochemical and Ethnobotanical Databases by Dr. Duke of the Agricultural Research Service/USDA [14]. The presence of various bioactive compounds in *Saraca asoca* justifies the use of the bark for various ailments by traditional practitioners.

3.6 ADMET Predictions

The potential ADME profiles of the compounds as predicted using admetSAR server, while the distribution profile of the compounds as obtained from admetSAR server is shown in (Table VIII). Computational study for the prediction of the relevant properties influencing bioactivity of the lead compounds was performed. The ADME properties of the compounds were evaluated and the selected properties are linked to metabolism, cell permeation.

4 CONCLUSIONS

The importance of the study is due to the biological activity and ADMET study of these compounds determined by GC-MS Analysis. The prevailing compounds are Arabinopyranose, Myo-Inositol, D-Pinitol, Sorbopyranose, Talopyranose. The UV- VIS profile showed the peaks at 344.09 nm and 232.50 nm respectively. The results of FTIR analysis confirmed the presence of phenol, alkanes, aldehyde, secondary alcohol, amino acid and aromatic amines. The results of this study offer a platform of using *Saraca asoca*bark as herbal alternative for various diseases including diabetic, cardiovascular, cancer, gout, urolithiasis, urinary tract infection etc. However isolation of individual phytochemical constituents and subjecting it to biological activity will definitely give fruitful results.

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FIGURES

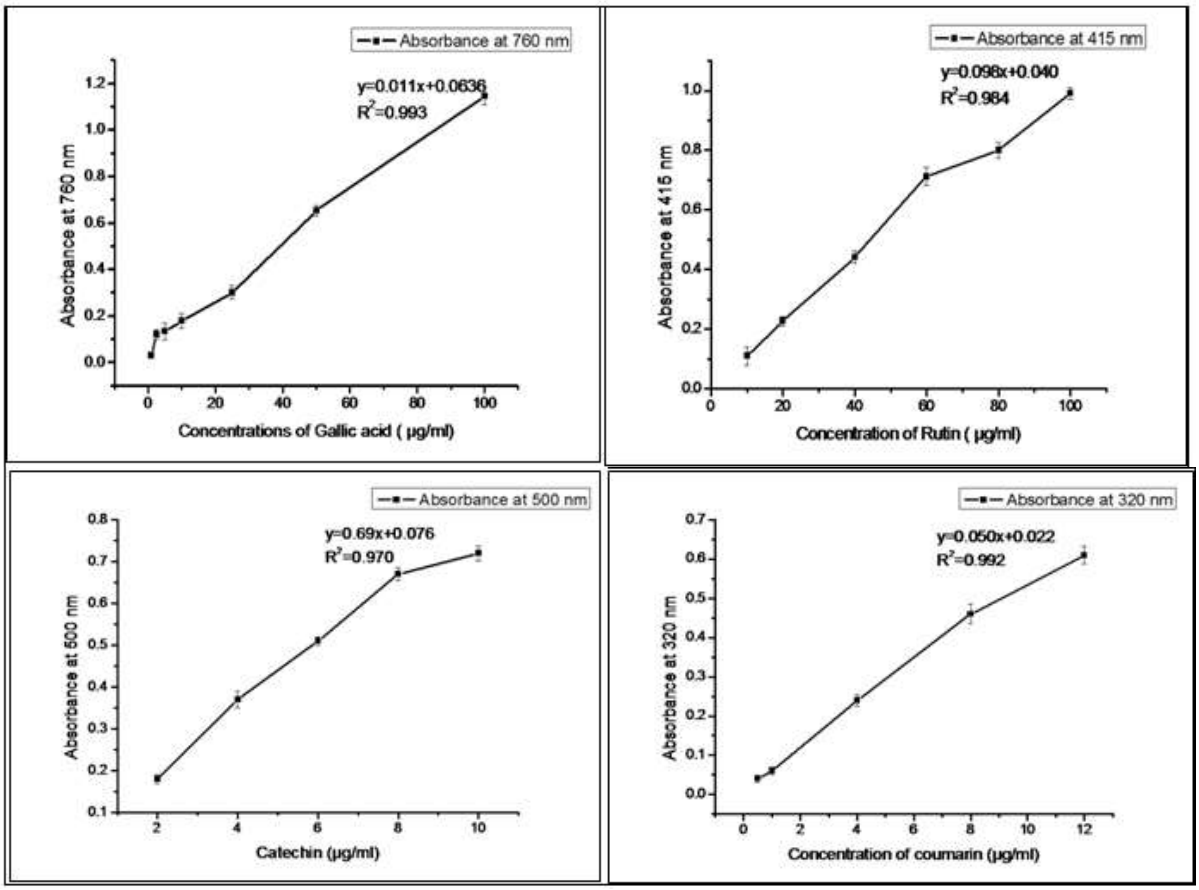

Fig.1: Standard calibration curve for total phenolic content for standard gallic acid , total flavonoids content for standard rutin , total proanthocyanidins content for standard catechin and total coumarin content for standard coumarin

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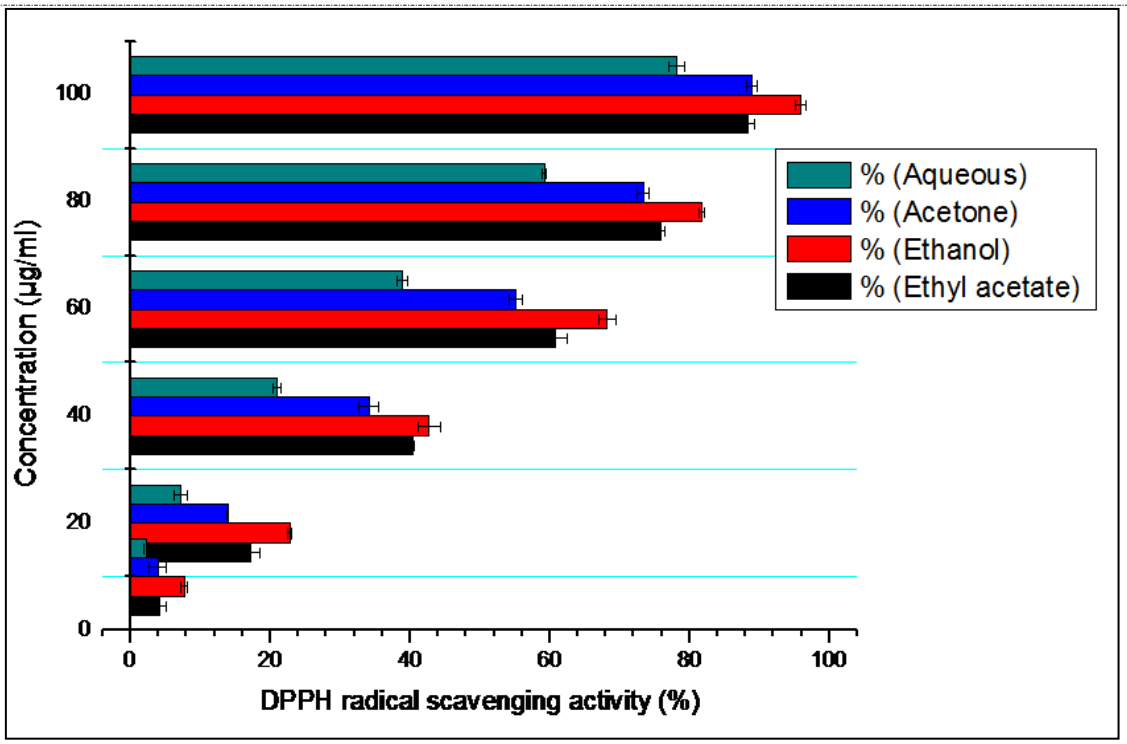

Fig. 2: Percentage inhibition of DPPH free radical by crude extracts of Saraca asoca

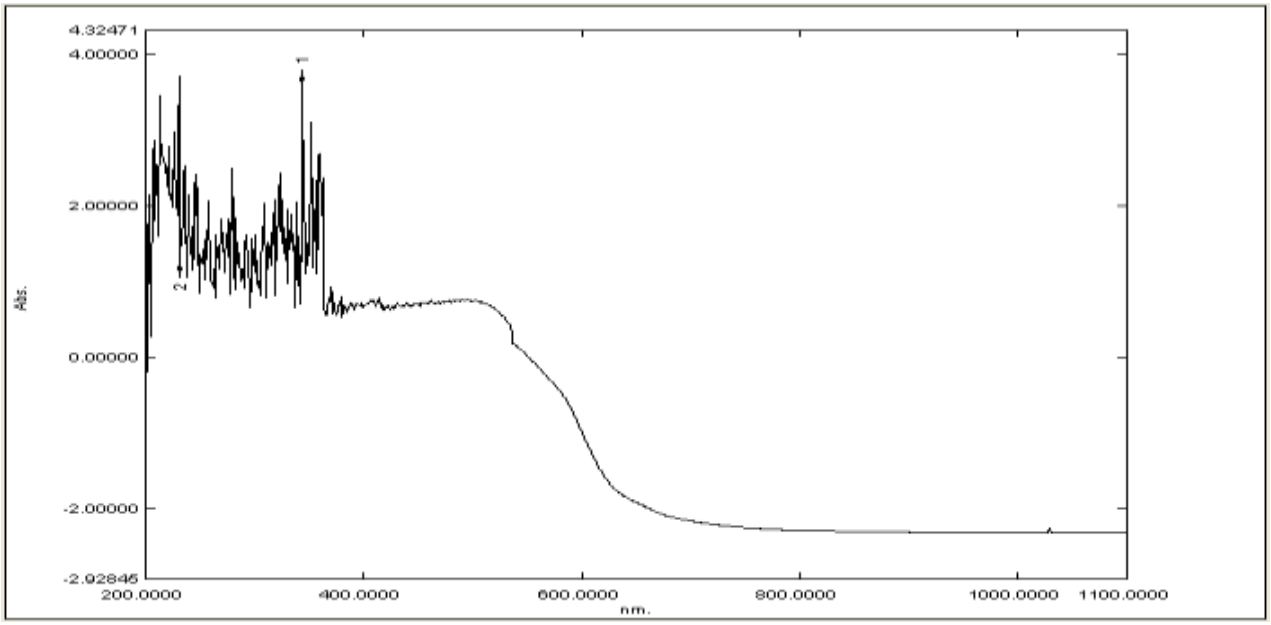

Fig. 3: UV-Visible spectrum of ethanolic extract of S.asoca.

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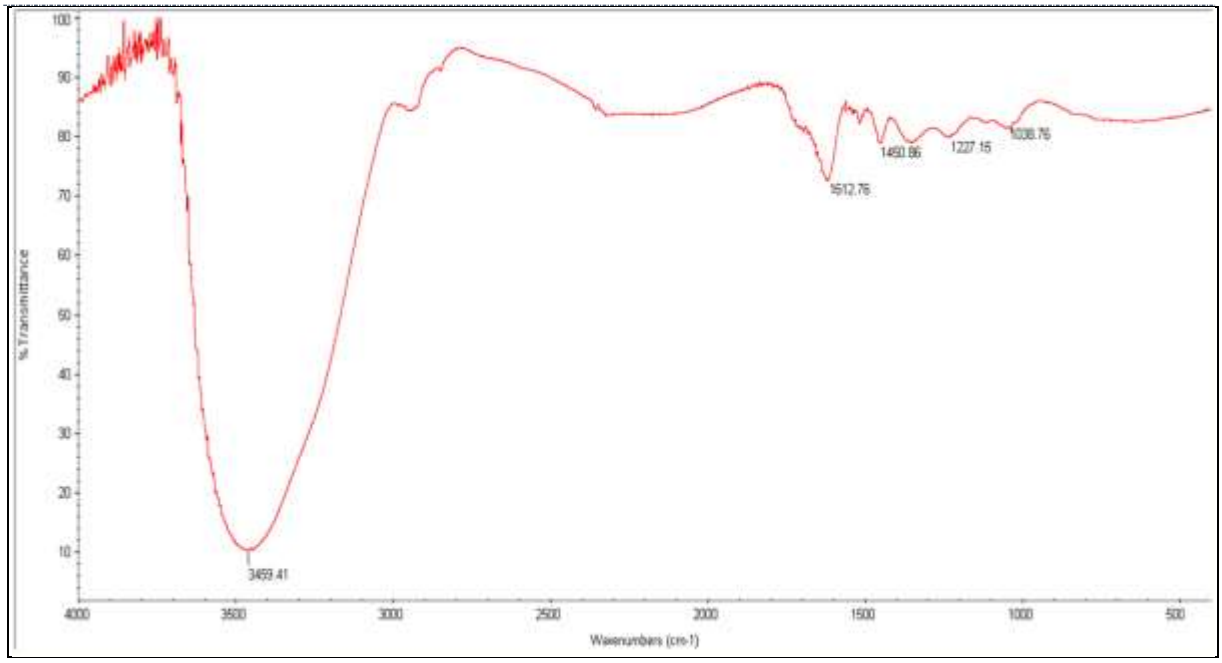

Fig. 4: FTIR spectrum of ethanolic extract of Saraca asoca

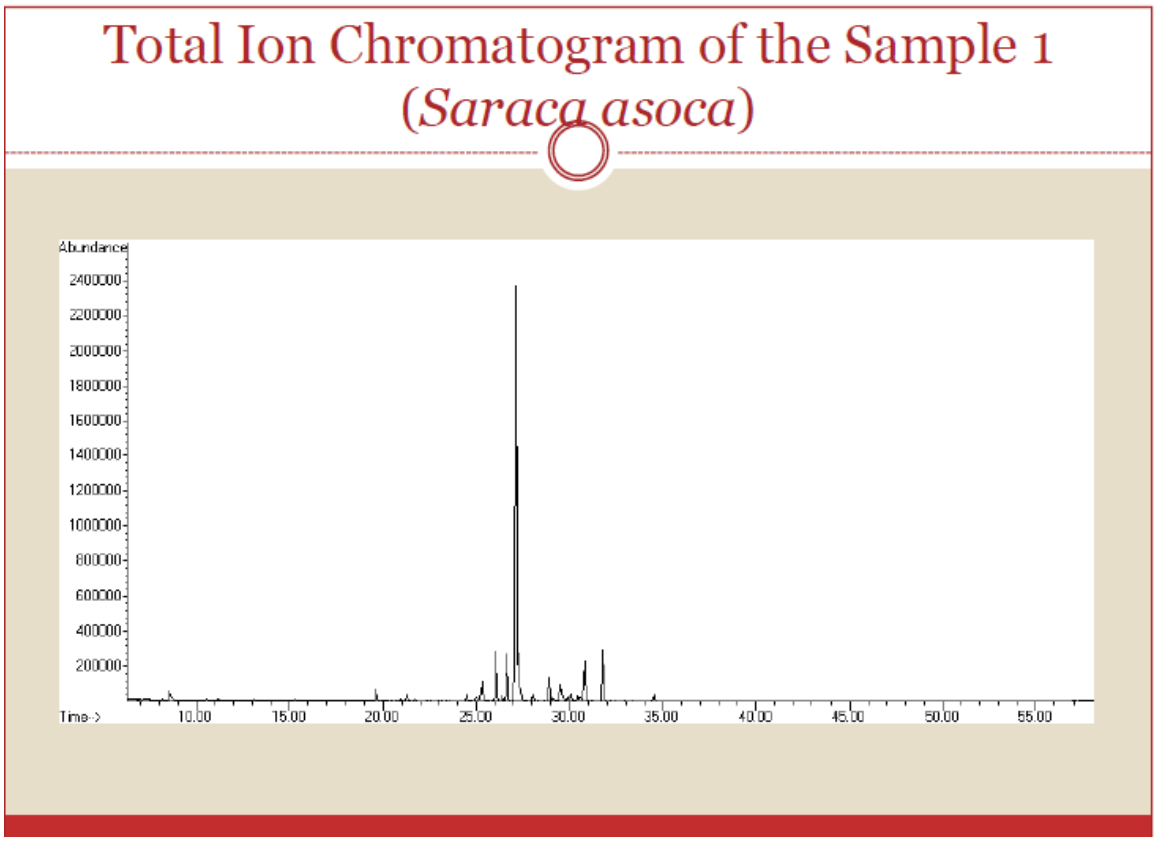

Fig. 5: GC-MS chromatogram of Saraca asoca ethanolic extract

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TABLES

Table I: Preliminary phytochemical screening of Saraca asoca (bark)

Phytoconstituents	Test/Reagents	Ethyl acetate extract	Acetone extract	Ethanolic extract	Aqueous extract
Alkoids	Dragendorff's Test	+	-	-	-
	Hager's Test	+	-	-	-
	Wagner's Test	+	-	-	-
Proteins	Biuret Test	-	+	+	-
	Ninhydrin's Test	-	+	+	-
	Millon's Test	-	+	+	-
Tannins	Lead acetate	+	+	+	+
	Ferric chloride	+	+	+	+
Steroids	Salkowski test	+	+	+	+
Carbohydrate	Fehling's Test	+	+	+	+
	Benedict's Test	+	+	+	+
Flavonoids	Shinoda test	+	+	+	-
	Lead Acetate Test	+	+	+	-
	Sodium Hydroxide Test	+	+	+	-
Glycoside	Keller-killani Test	+	+	+	-
Saponins	Foam Test	+	-	-	-

(+): Detected; (-): Not Detected

Table II: Quantitative estimation of total phenolics, flavonoids, proanthocyanidins and coumarin (n=3)

Plants	Extracts	Total phenolics (GAE mg/g)	Total flavonoids (RE mg/g)	Total Proanthocyanidins (Catechin mg/g)	Total coumarin (coumarin mg/g)
Saraca asoca	**Ethanolic**	438.78±0.86	80.16±0.29	0.8±0.05	1.192±0.2
	Acetone	322.66±0.57	55.07±0.47	0.58±0.01	1.147±0.3
	Ethyl acetate	255.8±0.23	179.5±0.47	0.35±0.08	ND
	Aqueous	20.9±0.22	ND	0.05	0.45±0.01

Values are expressed in mean±SD ; $P<0.05$.

Table III: IC_{50} value of free radical scavenging activity by DPPH method

Plants	IC_{50} of DPPH inhibition in µg/ml			
	Ethanolic extract	Acetone extract	Ethyl acetate extract	Aqueous extract
Saraca asoca	48.43±0.19	57±0.43	54.58±1.24	69.81±0.76
Ascorbic acid (Control)	14.82 ± 0.27			

Values are expressed in mean±SD ; $P<0.05$.

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Table IV: UV-VIS peak values of ethanolic extracts of Saraca asoca.

Wavelength (nm)	Abs.
344	3.600
232	1.256

Table V: FTIR peak values and functional groups of Saraca asoca (ethanolic extract)

Peak values	Functional group
3459.41	Alcohol
1612.76	Non acid carbonyl, Alkenes, Primary amines
1450.86	Aromatics
1227.15	Alcohols
1038.76	Aliphatic amines

Table VI: Phytocomponents identified in the ethanolic extract of S.asoca using GC-MS.

CAS Registration Number	Name of Compounds	RT	Purity (%)	Molecular formula	Molecular weight
19127152	Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, L-	21.2876	56%	$C_{18}H_{44}O_5Si_4$	452.88
20585619	Arabinopyranose, tetrakis-O-(trimethylsilyl)-, à-D-	21.7509	47%	$C_{17}H_{42}O_5Si_4$	438.85
30645024	Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-	26.6452	53%	$C_{21}H_{52}O_6Si_5$	541.06
EPA-380134	D-Pinitol, pentakis(trimethylsilyl) ether	27.134	67%	$C_{22}H_{54}O_6Si_5$	555.08
30645024	Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-	28.0439	61%	$C_{21}H_{52}O_6Si_5$	541.06
6736998	Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, D-	28.9004	57%	$C_{21}H_{52}O_6Si_5$	541.06
18623228	D-Xylose, tetrakis(trimethylsilyl)-	29.5126	54%	$C_{18}H_{45}NO_5Si_4$	467.89
14199805	Trimethylsilyl ether of glucitol	30.4657	46%	$C_{24}H_{62}O_6Si_6$	615.25
EPA-380134	D-Pinitol, pentakis(trimethylsilyl) ether	30.8015	57%	$C_{22}H_{54}O_6Si_5$	555.08
6736976	D-Glucose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-	31.7746	59%	$C_{21}H_{52}O_6Si_5$	541.06
EPA-380170	à-D-(+)-Talopyranose, pentakis(trimethylsilyl) ether	31.7913	68%	$C_{21}H_{52}O_6Si_5$	541.06
6736998	Mannose, 2,3,4,5,6-	31.9226	37%	$C_{21}H_{52}O_6Si_5$	541.06

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	pentakis-O-(trimethylsilyl)-, D-				
2582798	Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-	34.5206	55%	$C_{24}H_{60}O_6Si_6$	613.24

Table VII : Bioactivity of phytocomponents identified in the ethanolic extract of Saraca asoca.

Name of the compound	Biological Activity**
Arabinopyranose, tetrakis-O-(trimethylsilyl)-, à-D-	Antitumor, Decrease oxalate excretion, Inhibit production of uric acid, NADH-oxidase inhibitor, Xanthine oxidase inhibitor,Decrease Lactate/pyruvate ratio, Decalcifier, diuretic,Provide Vitamin D.
Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-	Antidepression, liver problems, panic disorders, and diabetes.
D-Pinitol, pentakis(trimethylsilyl) ether	Smart drug, Anticancer, CNS-depressant, Decalcifier, Decongestant, coronary dialator, Decrease oxalate excretion, Decrease Lactate/pyruvate ratio, Dehydrogenase inhibitor, diuretic, provide vitamin D.
Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)-, L-	Low oxalate, Anti-LDL, Anticancer, Antitumor, Decrease Lactate/pyruvate ratio, laxative, litholytic, decrease oxalate excretion, and inhibit production of uric acid, xo inhibitor.
Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-	Larvicidal, Lactation, Anticancer, Laxative, Anti-leukemia, Litholytic, Lymphatic diseases, oxidase inhibitor.
Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, D-	Diabetes, Disinfectant, Diuretic, Digestive diseases, Dropsy, Lymphatic diseases, skin diseases, Oncolytic,
à-D-(+)-Talopyranose, pentakis(trimethylsilyl) ether	Down regulation of nuclear and cytosol androgen, inhibit destruction of glycosaminoglycans, inhibit production of tumor necrosis factor and inhibit production of uric acid.

(**Activity source: Dr. Duke's Phytochemical and Ethnobotanical Database)

Table VIII: ADME profiles of the compounds

Compound 1: Arabinopyranose, tetrakis-O-(trimethylsilyl)-, à-D-

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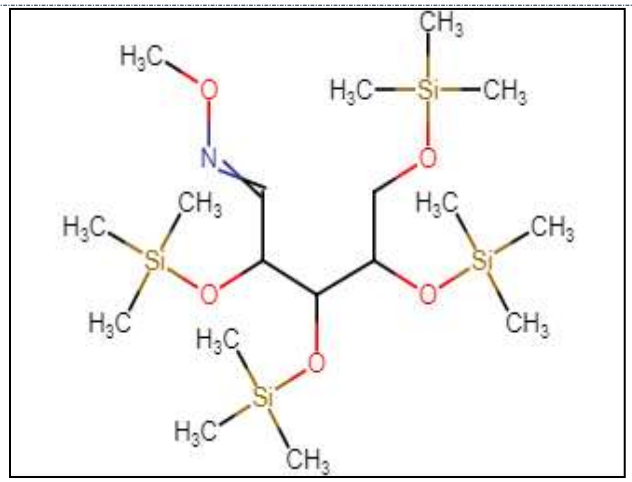

ADMET Predicted Profile --- Classification

Model	Result	Probability
Absorption		
Blood-Brain Barrier	BBB+	0.8827
Human Intestinal Absorption	HIA+	0.6426
Caco-2 Permeability	Caco2-	0.5405
P-glycoprotein Substrate	Non-substrate	0.6829
P-glycoprotein Inhibitor	Non-inhibitor	0.6470
	Non-inhibitor	0.8045
Renal Organic Cation Transporter	Non-inhibitor	0.8434
Distribution		
Subcellular localization	Mitochondria	0.7063
Metabolism		
CYP450 2C9 Substrate	Non-substrate	0.8123
CYP450 2D6 Substrate	Non-substrate	0.8160
CYP450 3A4 Substrate	Substrate	0.5652
CYP450 1A2 Inhibitor	Non-inhibitor	0.8670
CYP450 2C9 Inhibitor	Non-inhibitor	0.8627
CYP450 2D6 Inhibitor	Non-inhibitor	0.8911
CYP450 2C19 Inhibitor	Non-inhibitor	0.7965
CYP450 3A4 Inhibitor	Non-inhibitor	0.9008
CYP Inhibitory Promiscuity	Low CYP Inhibitory Promiscuity	0.9624
Excretion		
Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	Weak inhibitor	0.9649
	Non-inhibitor	0.8872
AMES Toxicity	Non AMES toxic	0.5000
Carcinogens	Carcinogens	0.6667
Fish Toxicity	Low FHMT	0.8148
Tetrahymena Pyriformis Toxicity	Low TPT	0.7104
Honey Bee Toxicity	High HBT	0.6987
Biodegradation	Not ready biodegradable	0.6385
Acute Oral Toxicity	III	0.5320

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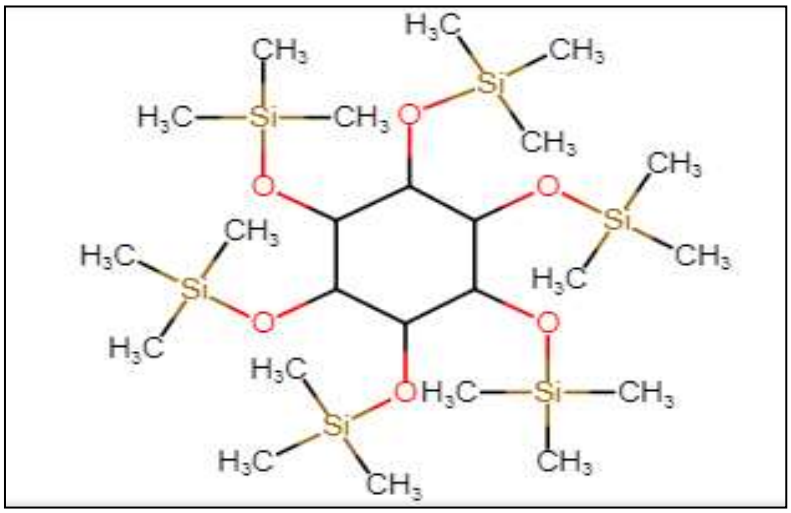
Carcinogenicity (Three-class)	Non-required	0.5694

ADMET Predicted Profile --- Regression

Model	Value	Unit
Absorption		
Aqueous solubility	-1.6569	LogS
Caco-2 Permeability	0.7028	LogPapp, cm/s
Distribution		
Metabolism		
Excretion		
Toxicity		
Rat Acute Toxicity	2.6942	LD50, mol/kg
Fish Toxicity	1.4991	pLC50, mg/L
Tetrahymena Pyriformis Toxicity	-0.2513	pIGC50, ug/L

Compound 2: Myo-Inositol, 1,2,3,4,5,6-hexakis-O-(trimethylsilyl)-



ADMET Predicted Profile --- Classification

Model	Result	Probability
Absorption		
Blood-Brain Barrier	BBB+	0.9112
Human Intestinal Absorption	HIA+	0.7965
Caco-2 Permeability	Caco2+	0.5800
P-glycoprotein Substrate	Non-substrate	0.6926
P-glycoprotein Inhibitor	Non-inhibitor	0.6467
	Non-inhibitor	0.9721
Renal Organic Cation Transporter	Non-inhibitor	0.9037
Distribution		
Subcellular localization	Mitochondria	0.7017
Metabolism		
CYP450 2C9 Substrate	Non-substrate	0.8327
CYP450 2D6 Substrate	Non-substrate	0.8141
CYP450 3A4 Substrate	Substrate	0.5518
CYP450 1A2 Inhibitor	Non-inhibitor	0.8293

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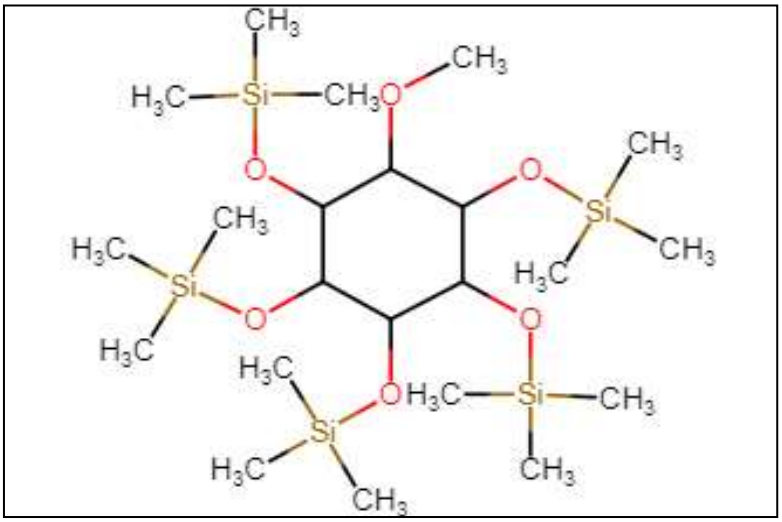
CYP450 2C9 Inhibitor	Non-inhibitor	0.8767
CYP450 2D6 Inhibitor	Non-inhibitor	0.9374
CYP450 2C19 Inhibitor	Non-inhibitor	0.6998
CYP450 3A4 Inhibitor	Non-inhibitor	0.9147
CYP Inhibitory Promiscuity	Low CYP Inhibitory Promiscuity	0.9436
Excretion		
Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	Weak inhibitor	0.9590
	Non-inhibitor	0.9482
AMES Toxicity	Non AMES toxic	0.7651
Carcinogens	Non-carcinogens	0.5987
Fish Toxicity	Low FHMT	0.7004
Tetrahymena Pyriformis Toxicity	Low TPT	0.9318
Honey Bee Toxicity	High HBT	0.8376
Biodegradation	Not ready biodegradable	0.7998
Acute Oral Toxicity	III	0.4080
Carcinogenicity (Three-class)	Non-required	0.6017

ADMET Predicted Profile --- Regression

Model	Value	Unit
Absorption		
Aqueous solubility	-2.4271	LogS
Caco-2 Permeability	1.0786	LogPapp, cm/s
Distribution		
Metabolism		
Excretion		
Toxicity		
Rat Acute Toxicity	2.2058	LD50, mol/kg
Fish Toxicity	2.0719	pLC50, mg/L
Tetrahymena Pyriformis Toxicity	-0.5608	pIGC50, ug/L

Compound 3: D-Pinotol, pentakis(trimethylsilyl) ether



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ADMET Predicted Profile --- Classification

Model	Result	Probability
Absorption		
Blood-Brain Barrier	BBB+	0.9112
Human Intestinal Absorption	HIA+	0.7965
Caco-2 Permeability	Caco2+	0.5800
P-glycoprotein Substrate	Non-substrate	0.6926
P-glycoprotein Inhibitor	Non-inhibitor	0.6467
	Non-inhibitor	0.9721
Renal Organic Cation Transporter	Non-inhibitor	0.9037
Distribution		
Subcellular localization	Mitochondria	0.7017
Metabolism		
CYP450 2C9 Substrate	Non-substrate	0.8327
CYP450 2D6 Substrate	Non-substrate	0.8141
CYP450 3A4 Substrate	Substrate	0.5518
CYP450 1A2 Inhibitor	Non-inhibitor	0.8293
CYP450 2C9 Inhibitor	Non-inhibitor	0.8767
CYP450 2D6 Inhibitor	Non-inhibitor	0.9374
CYP450 2C19 Inhibitor	Non-inhibitor	0.6998
CYP450 3A4 Inhibitor	Non-inhibitor	0.9147
CYP Inhibitory Promiscuity	Low CYP Inhibitory Promiscuity	0.9436
Excretion		
Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	Weak inhibitor	0.9590
	Non-inhibitor	0.9482
AMES Toxicity	Non AMES toxic	0.7651
Carcinogens	Non-carcinogens	0.5987
Fish Toxicity	Low FHMT	0.7004
Tetrahymena Pyriformis Toxicity	Low TPT	0.9318
Honey Bee Toxicity	High HBT	0.8376
Biodegradation	Not ready biodegradable	0.7998
Acute Oral Toxicity	III	0.4080
Carcinogenicity (Three-class)	Non-required	0.6017

ADMET Predicted Profile --- Regression

Model	Value	Unit
Absorption		
Aqueous solubility	-2.4271	LogS
Caco-2 Permeability	1.0786	LogPapp, cm/s
Distribution		
Metabolism		

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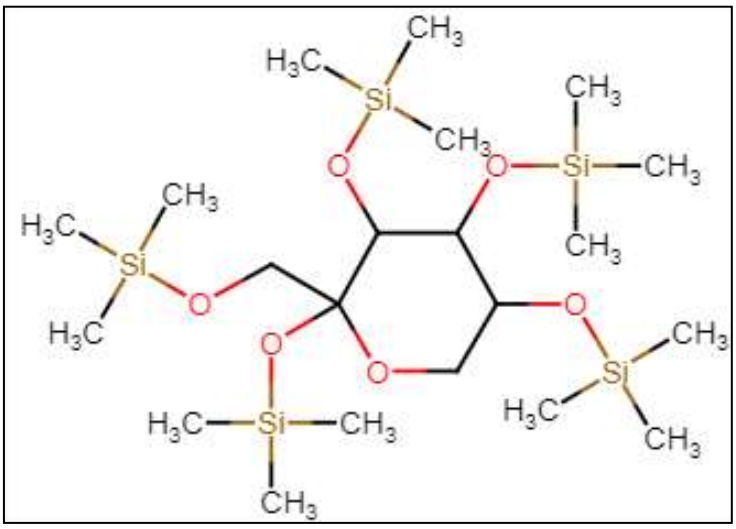
Excretion		
Toxicity		
Rat Acute Toxicity	2.2058	LD50, mol/kg
Fish Toxicity	2.0719	pLC50, mg/L
Tetrahymena Pyriformis Toxicity	-0.5608	pIGC50, ug/L

Compound 4:Sorbopyranose, 1,2,3,4,5-pentakis-O-(trimethylsilyl)-, L-



ADMET Predicted Profile --- Classification

Model	Result	Probability
Absorption		
Blood-Brain Barrier	BBB+	0.8947
Human Intestinal Absorption	HIA-	0.9220
Caco-2 Permeability	Caco2+	0.5163
P-glycoprotein Substrate	Substrate	0.5421
P-glycoprotein Inhibitor	Inhibitor	0.5955
	Non-inhibitor	0.9550
Renal Organic Cation Transporter	Non-inhibitor	0.8222
Distribution		
Subcellular localization	Mitochondria	0.6088
Metabolism		
CYP450 2C9 Substrate	Non-substrate	0.8525
CYP450 2D6 Substrate	Non-substrate	0.8204
CYP450 3A4 Substrate	Substrate	0.5929
CYP450 1A2 Inhibitor	Non-inhibitor	0.8638
CYP450 2C9 Inhibitor	Non-inhibitor	0.8690
CYP450 2D6 Inhibitor	Non-inhibitor	0.9072
CYP450 2C19 Inhibitor	Non-inhibitor	0.7558
CYP450 3A4 Inhibitor	Non-inhibitor	0.9481
CYP Inhibitory Promiscuity	Low CYP Inhibitory Promiscuity	0.9583

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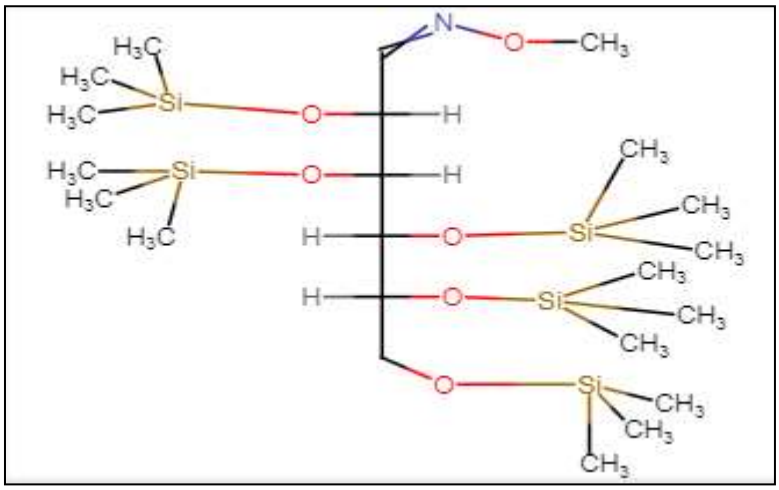
Excretion		
Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	Weak inhibitor	0.9242
	Non-inhibitor	0.8791
AMES Toxicity	Non AMES toxic	0.5000
Carcinogens	Non-carcinogens	0.7529
Fish Toxicity	Low FHMT	0.8427
Tetrahymena Pyriformis Toxicity	Low TPT	0.6449
Honey Bee Toxicity	High HBT	0.7305
Biodegradation	Not ready biodegradable	0.8833
Acute Oral Toxicity	III	0.5684
Carcinogenicity (Three-class)	Non-required	0.5874

ADMET Predicted Profile --- Regression

Model	**Value**	**Unit**
Absorption		
Aqueous solubility	-2.3267	LogS
Caco-2 Permeability	0.6844	LogPapp, cm/s
Distribution		
Metabolism		
Excretion		
Toxicity		
Rat Acute Toxicity	2.5394	LD50, mol/kg
Fish Toxicity	1.8088	pLC50, mg/L
Tetrahymena Pyriformis Toxicity	-0.1521	pIGC50, ug/L

Compound 5:Mannose, 2,3,4,5,6-pentakis-O-(trimethylsilyl)-, D-



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ADMET Predicted Profile --- Classification

Model	Result	Probability
Absorption		
Blood-Brain Barrier	BBB+	0.8827
Human Intestinal Absorption	HIA+	0.6426
Caco-2 Permeability	Caco2-	0.5405
P-glycoprotein Substrate	Non-substrate	0.6829
P-glycoprotein Inhibitor	Non-inhibitor	0.6470
	Non-inhibitor	0.8045
Renal Organic Cation Transporter	Non-inhibitor	0.8434
Distribution		
Subcellular localization	Mitochondria	0.7063
Metabolism		
CYP450 2C9 Substrate	Non-substrate	0.8123
CYP450 2D6 Substrate	Non-substrate	0.8160
CYP450 3A4 Substrate	Substrate	0.5652
CYP450 1A2 Inhibitor	Non-inhibitor	0.8670
CYP450 2C9 Inhibitor	Non-inhibitor	0.8627
CYP450 2D6 Inhibitor	Non-inhibitor	0.8911
CYP450 2C19 Inhibitor	Non-inhibitor	0.7965
CYP450 3A4 Inhibitor	Non-inhibitor	0.9008
CYP Inhibitory Promiscuity	Low CYP Inhibitory Promiscuity	0.9624
Excretion		
Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	Weak inhibitor	0.9649
	Non-inhibitor	0.8872
AMES Toxicity	Non AMES toxic	0.5000
Carcinogens	Carcinogens	0.6667
Fish Toxicity	Low FHMT	0.8148
Tetrahymena Pyriformis Toxicity	Low TPT	0.7104
Honey Bee Toxicity	High HBT	0.6987
Biodegradation	Not ready biodegradable	0.6385
Acute Oral Toxicity	III	0.5320
Carcinogenicity (Three-class)	Non-required	0.5694

ADMET Predicted Profile --- Regression

Model	Value	Unit
Absorption		
Aqueous solubility	-1.6569	LogS
Caco-2 Permeability	0.7028	LogPapp, cm/s
Distribution		
Metabolism		
Excretion		
Toxicity		
Rat Acute Toxicity	2.6942	LD50, mol/kg
Fish Toxicity	1.4991	pLC50, mg/L
Tetrahymena Pyriformis Toxicity	-0.2513	pIGC50, ug/L

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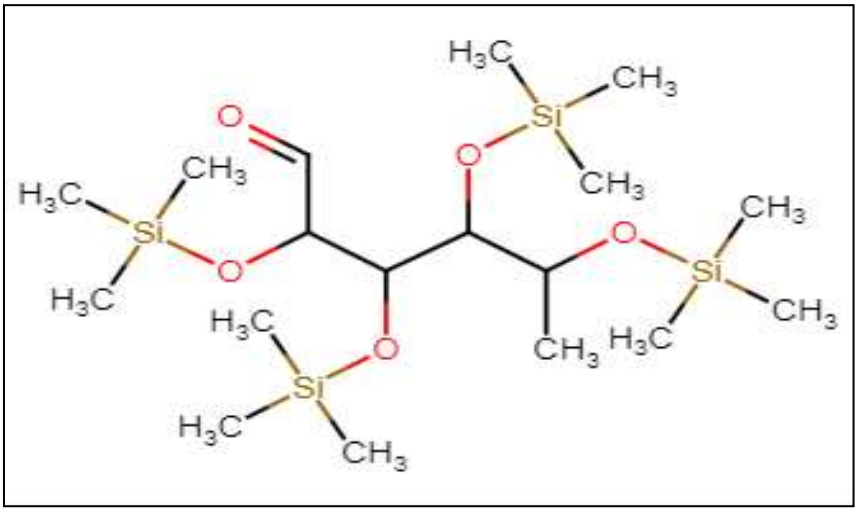
Compound 6: Mannose, 6-deoxy-2,3,4,5-tetrakis-O-(trimethylsilyl)



ADMET Predicted Profile --- Classification

Model	Result	Probability
Absorption		
Blood-Brain Barrier	BBB+	0.9473
Human Intestinal Absorption	HIA+	0.7642
Caco-2 Permeability	Caco2-	0.5238
P-glycoprotein Substrate	Non-substrate	0.7040
P-glycoprotein Inhibitor	Non-inhibitor	0.8254
	Non-inhibitor	0.9217
Renal Organic Cation Transporter	Non-inhibitor	0.9392
Distribution		
Subcellular localization	Mitochondria	0.7589
Metabolism		
CYP450 2C9 Substrate	Non-substrate	0.8449
CYP450 2D6 Substrate	Non-substrate	0.8613
CYP450 3A4 Substrate	Non-substrate	0.5215
CYP450 1A2 Inhibitor	Non-inhibitor	0.8736
CYP450 2C9 Inhibitor	Non-inhibitor	0.8713
CYP450 2D6 Inhibitor	Non-inhibitor	0.9349
CYP450 2C19 Inhibitor	Non-inhibitor	0.7864
CYP450 3A4 Inhibitor	Non-inhibitor	0.9446
CYP Inhibitory Promiscuity	Low CYP Inhibitory Promiscuity	0.9441
Excretion		
Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	Weak inhibitor	0.9871
	Non-inhibitor	0.9439
AMES Toxicity	Non AMES toxic	0.6867
Carcinogens	Carcinogens	0.7110
Fish Toxicity	Low FHMT	0.6785
Tetrahymena Pyriformis Toxicity	Low TPT	0.9571

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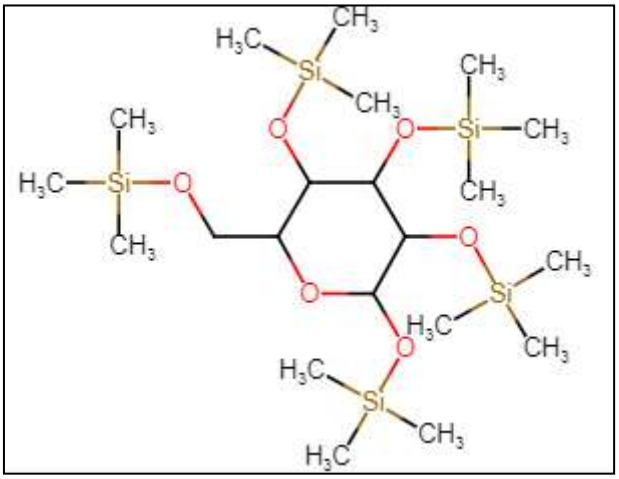
Honey Bee Toxicity	High HBT	0.8134
Biodegradation	Ready biodegradable	0.5187
Acute Oral Toxicity	III	0.4870
Carcinogenicity (Three-class)	Non-required	0.6385

ADMET Predicted Profile --- Regression

Model	Value	Unit
Absorption		
Aqueous solubility	-0.6165	LogS
Caco-2 Permeability	0.8255	LogPapp, cm/s
Distribution		
Metabolism		
Excretion		
Toxicity		
Rat Acute Toxicity	2.2175	LD50, mol/kg
Fish Toxicity	2.3096	pLC50, mg/L
Tetrahymena Pyriformis Toxicity	-1.0982	pIGC50, ug/L

Compound 7: à-D-(+)-Talopyranose, pentakis(trimethylsilyl) ether



ADMET Predicted Profile --- Classification

Model	Result	Probability
Absorption		
Blood-Brain Barrier	BBB+	0.8921
Human Intestinal Absorption	HIA-	0.8550
Caco-2 Permeability	Caco2+	0.5487
P-glycoprotein Substrate	Non-substrate	0.5765
P-glycoprotein Inhibitor	Inhibitor	0.5502
	Non-inhibitor	0.9673
Renal Organic Cation Transporter	Non-inhibitor	0.8459
Distribution		
Subcellular localization	Mitochondria	0.6510
Metabolism		
CYP450 2C9 Substrate	Non-substrate	0.8354

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CYP450 2D6 Substrate	Non-substrate	0.8224
CYP450 3A4 Substrate	Substrate	0.5799
CYP450 1A2 Inhibitor	Non-inhibitor	0.8483
CYP450 2C9 Inhibitor	Non-inhibitor	0.8869
CYP450 2D6 Inhibitor	Non-inhibitor	0.9098
CYP450 2C19 Inhibitor	Non-inhibitor	0.7904
CYP450 3A4 Inhibitor	Non-inhibitor	0.9682
CYP Inhibitory Promiscuity	Low CYP Inhibitory Promiscuity	0.9587
Excretion		
Toxicity		
Human Ether-a-go-go-Related Gene Inhibition	Weak inhibitor	0.9544
	Non-inhibitor	0.9550
AMES Toxicity	AMES toxic	0.5875
Carcinogens	Non-carcinogens	0.7804
Fish Toxicity	Low FHMT	0.9002
Tetrahymena Pyriformis Toxicity	Low TPT	0.5591
Honey Bee Toxicity	High HBT	0.7733
Biodegradation	Not ready biodegradable	0.6437
Acute Oral Toxicity	III	0.5012
Carcinogenicity (Three-class)	Non-required	0.6119

ADMET Predicted Profile --- Regression

Model	Value	Unit
Absorption		
Aqueous solubility	-1.9609	LogS
Caco-2 Permeability	0.7929	LogPapp, cm/s
Distribution		
Metabolism		
Excretion		
Toxicity		
Rat Acute Toxicity	2.5012	LD50, mol/kg
Fish Toxicity	1.4568	pLC50, mg/L
Tetrahymena Pyriformis Toxicity	-0.2406	pIGC50, ug/L