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A comparative investigation of bioactive compounds present in *Datura stramonium* L. leaves extract in various solvents (ethanol, aqua, and ether) using TLC, IR, and GC-MS analytical techniques

Vijayavilas Sathyan Sangeetha[1*] and Christina Ruby Stella[2]

[1]PG & Research Department of Chemistry, Dhanalakshmi Srinivasan College of Arts and Science for Women (Autonomous), Perambalur, Tamil Nadu, India. [2]PG & Research Department of Chemistry, Holy Cross College (Autonomous), Tiruchirapalli, Tamilnadu, India. *Author for correspondence. E-mail: sangeethavasanth23@gmail.com

ABSTRACT. The present study is an experimental comparative investigation of the biomolecules present in ethanol, aqua and ether extract of *Datura stramonium* L. leaves. The purpose of the study is to monitor the phytochemical constituents in the plant leaves by thin layer chromatography (TLC), Gas Chromatography-Mass Spectrometry (GC-MS), and infrared spectroscopy analytical techniques. The *Datura Stramonium* L. leaves were collected, dried and was extracted with ethanol, water and ether at room temperature. A comparative investigation of bioactive compounds have been carried out using TLC, GC-MS, and IR Analytical techniques. Preliminary phytochemical analysis revealed the presence of protein, alkaloid, phenol and tannins, flavanoid, glycoside, sterols, saponin, resins, anthocyanin, and carboxylic acid. More number of bio active phytochemicals were identified, and the chromatograph showed peaks of individual compounds. The result of this study offers a platform for understanding the Phytochemical present in ethanol, aqua and ether extract of studied plant leaves and to identify them as herbal alternative for various diseases and it can be used as functional pharmaceutical when once it extracted and treated carefully.

Keywords: UAE; ET; Etem; S/M ratio; Phytochemical screening; TLC; GC-MS.

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Introduction

Medicinal Plants have taken part in a major role in the treatment of human contusion and diseases all over the world. The need for traditional medicinal plant is increasing day by day in both developed and developing countries due to growing identification of natural products in plants.

Datura stramonium L. is an annual plant and it belonging to Solanaceae family. It is an undomesticated flowering plant and is a local source for tropane alkaloids. And this plant often specified as thorn apple even though considered as one of the deadliest plant species for its super toxic components. And this is observed as boot strapper of medicinal components if purified properly (Oseni, Olarinoye, & Amoo, 2011). The therapeutic impact of the plant is due to the presence of alkaloids, tannins, saponins and cardiac glycosides. It is normally germinating in the tropical parts of India and the temperate regions of the Himalayas and is also found growing wildly in fertile calcareous soil of North America, Uganda, Kenya, Mexico, North Africa, Tanzania, and Bangladesh.Employment of any plant part may result in an awful medicament reaction that may cause to high toxicity and sometime lead to diagnostic difficulties. Many incidents of fortuitous poisoning have been noted when these plants were accidentally eaten (Devi, Bawari, Paul, & Sharma, 2011).

Leaves extract is consumed orally for the treatment of asthma and sinus infections, and stripped bark are applied externally to treat swellings, burns and ulcers (Soni, Siddiqu, Dwivedi, & Soni, 2012). In a study of the secondary metabolites identified in the plant materials showed its antimicrobial activity. This plants consist of sixty-four various types of tropane alkaloids (Srivastava & Srivastava, 2020). Using bioinformatic tools and applications it was analyzed gene divergence of tropane alkaloids (TAs), terpene synthases (TPSs) and other members of Solanaceae Family (Velazquez-Marquez, de-la-Cruz, Tapia-Lopez, & Nunez-Farfan, 2021).

Common names

This plant have different label in different part of the world which include Jimsonweed,Jamestown weed, Purple thorn-apple, Hell's bell, Devil's snare, Stinkweed, Mad apple, Moonflower, Stink wort, Devil's-apple , Devil's cucumber, faulty castor-oil, Stramonium jimsonweed, Devil's horn, Prickly burr, and Devil's weed. In India it is commonly termed as Dhuttura Kanaka or Kanakahvya in Sanskrit, Sada Dhatura in Hindi, Ummetta in Telugu, Ummattangani in Tamil and Dhattura in Bengali, Maraummam in Malayalam.

Scientific classification

This plant belonging to Kingdom - Plantae, Division - Magnoliophyta, Class - Magnoliopsida, Order - Solanales, Family - Solanaceae, and Genus - Datura.

Plant appearance

It is an annual plant (Figure 1). It has non woody, branched and sparingly hairy stem. The plant reaches a height of one meter by growing. The branching stems are widen, leafy, rotund, flush and pale green in color, branching repeatedly in a branched manner. Leaves are fuzzy, big, zig-zag, 4-6 inch long, pale green and carry funnel shaped, white or purple toned flowers, with 5 stamens and upper level ovary.The average length of floret is about 3 inches.It have a lengthy, tubiform and somewhat a bulge below and very sharply five angled surounted by five sharp teeth calyx. Corolla is channel shaped. Stem stalk greenish white. It has black, kidney shape and flat seeds and is called as thorn apple because of the presence of thorny fruits. It is a strong narcotic plant and on action on the human it is valuable as medicines. Entire parts of the plant are fatal and the seeds are the most agile.The poisoning symptoms included dehydration of the mouth and extreme thirst, drouth of the skin, diminish vision, urinary detention,speedy heartbeat, puzzlement, nervousness, hallucinations, and loss of responsiveness (Das, Kumar, & Basu, 2012).The phytochemicals present in the studied plant were included in many psycopharmacologies because of their different anticholinergic activities(Shagal, Modibbo, & Liman, 2012). Pharmacological activities of the extracts in different solvents and phyto compounds have diverse activity like antitumor, antiinflammation, antioxidant, antimicrobial, antispasmodic, anticoagulant, analgesic, hypoglycemic and xanthine oxidase inhibitory and as well as the effects on central nervous system and immune system (Lian et al., 2022). At a therapeutic dose of 0.05 to 0.1 g of plant extract have anticancer effect against human epidermal carcinoma. However, care should be taken when making use of this plant as an anticancer agent because of its adverse anticholinergic effects (Kadam, Chavhan, Shinde, &Sapkal, 2018).

Figure 1. *Datura stramonium* plant (Source: Prepared by the author).

Toxicity

The *Datura stramonium* L. plant is very toxic in nature and hence the possibility of poisoning is very high during criminal investigations. The toxic phyto components present in all parts like leaves, seeds, stem and flowers of the plant. Scopolamine/Hyoscine, atropine are the main toxic components present in the plant 50/100 seeds contain an approximate of 3-6 mg of atropine and each seed contains 0.1mg of atropine (Yadav, Singla, Srivastava, & Gupta, 2021). Usual indicator of poisoning are constituted by flushing, sinus tachycardia, dry skin and mucosa, mydriasis, hyperpyrexia, decreased bowel activity, urinary retention, and neurological disorders with ataxia, disorientation, confusion, impaired short-term memory, hallucinations (visual and audio), psychosis, agitated delirium, seizures, and coma (Tranca, Szabo, & Cocis, 2017). It is very important for individuals to be aware of the toxic nature and potential risks related with the use of this plant (Gaire &

Subedi, 2013). Some studies on this plant have reported on potential pharmacological effects but information about the toxicity stay almost uncertain. Furthermore the frequent abuse of the plant for recreational purposes has produced toxic syndromes (Sharma, Dhaliwal, Rana, Delta, & Kaushik, 2021).

Material and methods

Collection of plant material

The leaves of the studied plant leaves were collected from the local field of Perambalur, Tamilnadu, India. Leaves were shade dried, coarsely powdered with an electrical blender, dried leaves were ground into powder and used for further studies.

Ultrasonic-assisted extraction (UAE)

Ethanol, ether and aqueous extract of studied plant were obtained by ultrasonic extraction method. Ultrasonic-assisted extraction (UAE) is used to extract the bioactive components since it is a fast and efficient extraction technique that uses ultrasound to cause speedy movement of solvents, resulting in a higher mass transfer as well as acceleration of extraction (AE) is more monetary, ecological, and convenient by the reduction of time utilization, higher oil quality and cost reduction contrast to other advanced extraction techniques. Other parameters involved in the extraction are extraction time (ET), extraction temperature (ETem), solvent to material ratio (S/M Ratio), and type of solvent used. Extraction solvent (like Ethanol, ether, and aqua) are added to the sample placed in ultrasonic extraction vessel. Sonotrode were placed in contact with sample. Extraction occurs then the sample get ready for further studies. Ultrasound-assisted extraction (UAE) can also use for extracting alkaloids and phenolic compounds (Mokhtarpour, Naserian, Valizadeh, Danesh Mesgaran, & Pourmollae, 2014). The other methods used for isolation of volatile compounds such as terpenes and phenylpropanoids from leaves, flowers, stems, barks, roots, fruits and seeds of plants are by conventional techniques like solvent extraction, hydrodistillation, steam distillation and advanced microwave extraction, supercritical fluid extraction, subcritical liquid extraction methods (Aziz et al., 2018; Fitsiou & Pappa, 2019; Mohamed et al., 2020; Antonelo, Rodrigues, Wagner Júnior, & Montanher, 2022).

Qualitative phytochemical analysis

Phytochemical analysis was carried out for identification of tannins, terpenoids, flavonoid, alkaloid, phenol, phytosterol, Quinones and saponins according to standard methods like color reactions (Pant, Pant, Saru, Yadav, & Khanal, 2017).

Carbohydrates

One milliliter of extract and 1 mL of Barfoeds reagent were mixed in a test-tube and it heated in a water bath for 2 min. Presence of red precipitate indicate the the presence of carbohydrates.

Proteins

About 0.5 mg of extract in desired solvent and freshly prepared 0.2% ninhydrin reagent reagent were heated in a test tube.The presence of pink or purple colour confirm the presence of proteins.

Alkaloids

About 2 mL of extracts were measured in test tubes to which picric acid solution was added and mixed well. An orange coloration formed which indicate the presence of alkaloids.

Phenol

To 1 mL of plant leaf extract in the desired solvent few drops of alcohol and ferric chloride solution was added and allowed to stand for few minutes. Formation of yellow coloration represent the presence of phenol.

Tannins

A small portion of the extract was diluted with water and 3-4 drops of 10% ferric chloride solution was added and mixed well. Presence of blue colour indicate presence of Gallic tannins and green colour indicated the presence of catecholic tannins.

Flavonoids

One milliliter of 10% NaOH solution was added to 5 mL of different plant extract. Along the sides of the beaker 2 drops of concentrated HCl was added. Turning of yellow color solution to colorless is indicate the presence of flavonoids.

Glycosides

Two and a half milliliters of dil. sulphuric acid was added to 5 mL of plant leaf extract taken in a test tube and boiled for few minutes. Then cooled and neutralized with 10% NaOH, then 5 mL of Fehling solution was added. Presence of brick red precipitate indicates the presence of glycosides.

Saponins

Ten milliliter of sterile distilled water was added to 1 g of the sample taken in a conical flask and boiled for 5 minutes. After heating the mixture was filtered and 2.5 mL of the filtrate was added to 10 mL of sterile distilled water in a test tube and is shaken vigorously for about 30 seconds. It was then allowed to stand for half an hour. Honeycomb froth indicated the presence of saponins.

Anthraquinone

One milliliter of the extract was treated with 2 mL of 5% KOH and then the solution was filtered. Change in color was observed. Presence of mild Pink color represent the presence of anthraquinones.

Steroids

The desired plant leaf extract powder was dissolved in two mL of chloroform in a dry test tube. 10 drops of acetic anhydride and two drops of concentrated sulphuric acid were added. The appearance of red color initially and then turns to blue and finely bluish color indicated the presence of steroids.

Resin

One milliliter of various solvent extract were treated with few drops of acetic anhydride solution followed by 1 mL of concentrated H_2SO_4. Presence of orange or yellow color indicate presence of resin.

Anthocyanin

Two milliliter of the leaf extract mixed with 2 mL of 2N hydrochloric acid. The appearance of a pink red colour changed to purplish blue after addition of ammonia indicate presence of anthocyanin.

Carboxylic acid

One milliliter of plant extract were treated with sodium bicarbonate solution. Effervescence produced is an indication of presence of carboxylic acid.

Qualitative spectroscopic analysis

Thin layer chromatography (TLC)

Thin layer chromatography (TLC) technique is employed to separate mixtures. It was carry out on aluminium foil which was coated with a thin layer of adsorbent. After the sample has been spotted on the plate, a solvent or solvent mixture was drawn up the plate via capillary action. Separation is achieved since different Components have different rate of adsorption (Sangeetha, Christina Ruby Stella, Nivetha, Shanmugapriya, & Tikku, 2022).

Infrared spectroscopy

Infrared spectroscopy of the extracts in different solvents were done with IR spectrometer. The characteristic peaks were recorded and then it was analysed for their corresponding functional groups.

Gas chromatography-mass spectrometry (GC-MS)

The Gas chromatography/mass spectrometry (GC/MS) instrument separates chemical mixtures and identifies the components at a molecular level. It is one of the most accurate techniques for analysing unknown samples. This is works on the principle that a mixture will separate into individual substances when

heated. The fragmentation patterns of mass spectra were compared with those stored in the spectrometer database using National Institute of Standards and Technology Mass Spectral database (NIST-MS).

Results and discussion

Qualitative phytochemical analysis

The preliminary phytochemical analysis was carried out for different extracts of studied plant. It revealed the presence of protein, alkaloid, phenol and tannins, flavonoid, glycoside, sterols, saponin, sterol, resins, anthocyanin, and carboxylic acid, whereas carbohydrates and quinones were absent (Table 1). The ether extract of this plant contains more bioactive components when compared to other solvents. The Ether extract showed of the presence of protein, alkaloid, phenol, tannins, flavonoid, glycoside, sterols, saponin, sterol, resins, anthocyanin, and carboxylic acid and were confirmed in suitable chemical tests. The aqueous extract contain protein, phenol, tannins, flavonoid, sterols, saponin, sterol, and carboxylic acid (Table 1). The ether extract showed of the presence of alkaloid, phenol, tannins, flavonoids, sterol, resins, and anthocyanin. Moreover, the highest yield was also observed in ethanol extract. (Table 1). Presence of glycosides and other highly complexed bioactive poisonous components give toxicity to the plant through phytochemical study (Pillay & Sasidharan, 2019).

Table 1. Phytochemical screening of ethanol, ether and water extract of *Datura stramonium* L.

Test	Water extract	Ethanol extract	Ether extract
Carbohydrate	-	-	-
Protein	+	+	-
Alkaloid	-	+	+
Phenol and tannins	+	+	+
Flavonoids	+	+	+
Glycoside	-	+	-
Saponins	+	+	-
Quinones	-	-	-
Sterols	+	+	+
Resin	-	-	+
Anthocyanin	-	-	+
Carboxylic acid	+	+	-

+Present; -Absent.

Thin layer chromatography

Ethanolic extract of plant leaves gives three fractions at Rf value 0.47, 0.92, and 0.98. Ether extract gives four spots at Rf values 0.47, 0.49, 0.92, and 0.98 (Table 2). Water extract of plant leaves gives two spots at 0.49 and 0.90. Picric acid reagent was used for visualization of alkaloids on the plate and Rf values were calculated. These spots indicate presence of alkaloids, phenols, tannins, flavonoids, saponins, sterols.

Table 2. Rf values of different fractions.

Fraction	Ethanol extract	PE extract	Water extract
1	0.47	0.47	0.49
2	0.92	0.49	0.90
3	0.98	0.92	-
4	-	0.98	-

Infrared spectroscopy

When the extract was passed into the IR, the functional groups of the components were separated based on its peaks ratio. The results of IR analysis confirmed the presence of N-H, O-H, C=C, C-H, C-O, and CH_3 functional groups (Figures 2 to 4). IR spectroscopy is proved to be a reliable and sensitive method for detection of bio molecular composition (Pakkirisamy, Kalakandan, & Ravichandran, 2017)

Figure 2 shows the broad band at 3401.04 cm^{-1} correspond to O-H stretching vibrations of alcohol or phenol. The peak at 2926.63 cm^{-1} represents -C–H stretch of alkane. The peak at 2901.42 cm^{-1} corresponds to C-H, CH_2, CH_3 stretching vibrations of aliphatic groups. The band at 3070.36 cm^{-1} indicates = C-H stretch vibrations and it corresponds to the presence of aromatic compound.

The band at 2131.08 cm^{-1} correspond to C≡C/C≡N stretching vibrations of alkyne and nitriles. The peak at 1923.32cm^{-1} represents C=C=CH_2 stretching of alkenes. The peak at 1647.09 cm^{-1} corresponds to C=C- stretching vibrations of alkene. The band at 1454.40 cm^{-1} indicates CH_2 stretch vibrations and it corresponds to the presence of CH_2 group. The bands at 1381.02 cm^{-1}, 1393.81 cm^{-1}, and 1407.14 cm^{-1} indicate presence of CH_3 groups. Peaks at 1273.69 cm^{-1} corresponds to N-H stretching of secondary amines. Bands at 1336.87 cm^{-1} represent presence of NO_2 group. And have a peak at 1086.55 cm^{-1} indicate the presence of C-O-C, C-O-H stretch of ether. Band at 880.38 cm^{-1} correspond to ring C=C bond. Peaks at 662.15 cm^{-1} indicate presence of halogen substituted biomolecule.

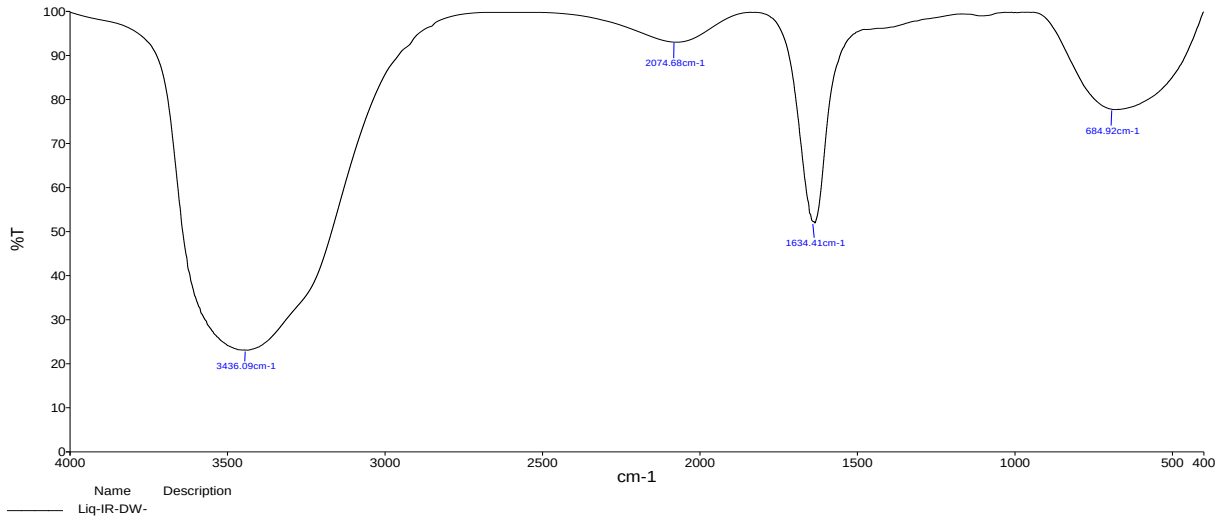

Figure 2. IR spectra of ethanol fraction of *Datura stramonium*. The figure shows peaks developed in IR region for ethanolic extract of *Datura Stramonium* L. functional groups corresponding to each peaks illustrated above (Prepared by the author).

Figure 3 shows the band at 3436.09 cm^{-1} correspond to N-H stretching vibrations of amine. The peak at 2074.68 cm^{-1} represents N=C=S Stretch of isothiocyanate. The peak at 1634.41 cm^{-1} correspond to C=C vibration of alkene. The band at 684.52 cm^{-1} indicate presence of C=C of benzene derivative.

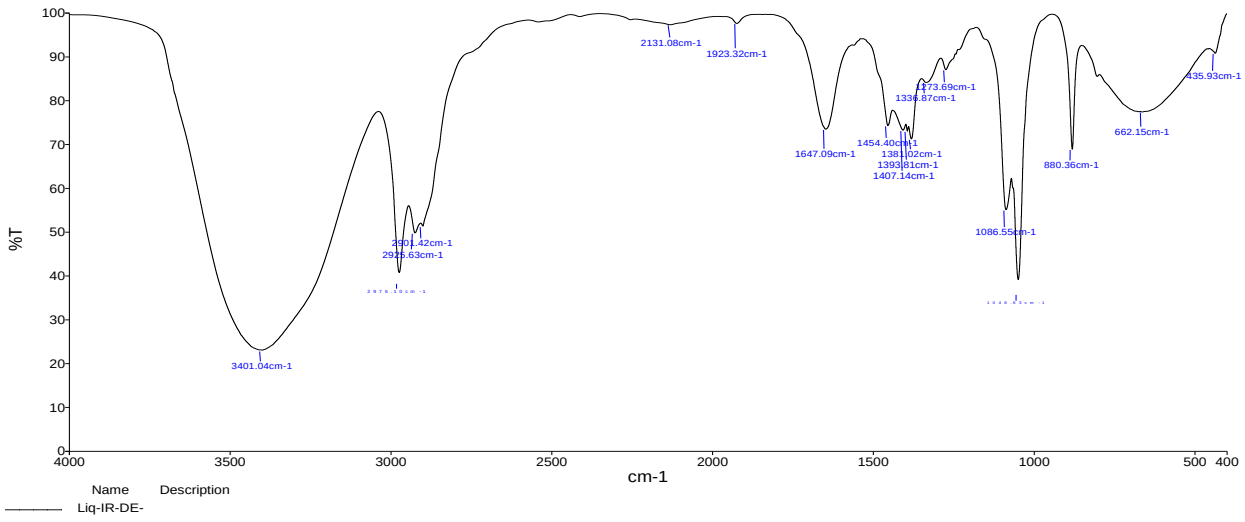

Figure 3. IR spectra of aqua fraction of *Datura stramonium*. The figure shows peaks developed in IR region for aqua extract of *Datura Stramonium* L. functional groups corresponding to each peaks illustrated above (Prepared by the author).

Figure 4 shows the broad band at 3422.10 cm^{-1} correspond to N–H/C-H/O-H stretching vibrations of alcohol or phenol, amine or amide. The peak at 2964.33 cm^{-1} represents O-H stretch of carboxylic acid. The peak at 2931.12 cm^{-1} and 2878.03 cm^{-1} corresponds to C-H stretching vibrations of alkane. The band at 1642.97 cm^{-1} indicates C=O stretch vibrations and it corresponds to the presence of amide carbonyl.

The band at 1464.75 cm^{-1} correspond to C-C stretching vibrations of aromatic carbon. The peak at 1379.03 cm^{-1} represents N-O stretching of NO_2 group. The peak at 1062.51 cm^{-1} corresponds to C-O - stretching vibrations of primary alcohol. The band at 885.61 cm^{-1} indicates aromatic hydrocarbon. The Band at 724.25 cm^{-1} indicate presence of N-H Wag vibration of primary, secondary amines groups.

Infrared spectral analysis of fraction of *Datura stramonium* L. was carried out with plant leaf extract in different solvent to identify the possible biomolecules. This spectrum shows lot of absorption bands indicates the presence of active functional groups in the plant**.** Peaks give the indication of presence of alcohol, phenols, carboxylic acid and also shows bands for amide, primary and secondary amine.

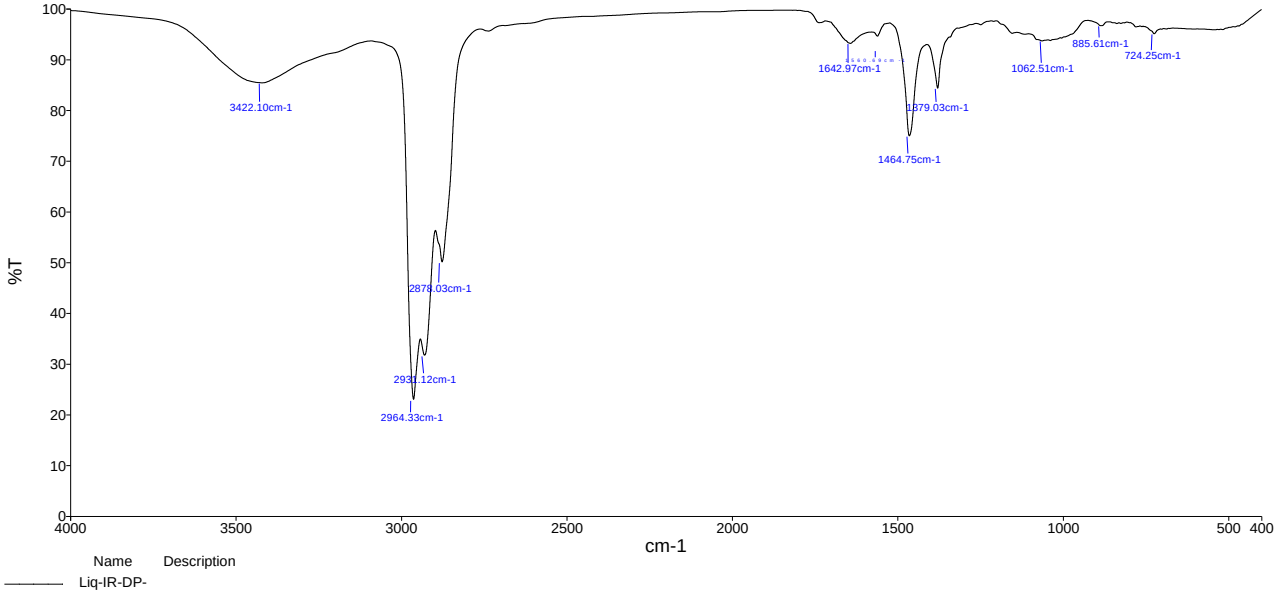

Figure 4. IR spectra of ether fraction of *Datura stramonium* L. The figure shows peaks developed in IR region for ether extract of Datura Stramonium. L. Functional groups corresponding to each peaks illustrated above (Prepared by the author).

Gas chromatography and mass spectroscopy

Gas chromatography and mass spectroscopy technique identified the major compounds present in ethanolic, aqua and ether fraction of *Datura stramonium* L. A comparative investigation of the three various extracts of plant leaves were carried out. This analysis revealed the presence of various components. Molecular formula (MF), molecular weight (MW) and compound name is tabulated in Tables 3, 4, and 5. The mass spectra of ethanolic extract of the plant shows in Figure 5. Figure 6 and Table 3 shows the presence of around fifteen bioactive phytochemical compounds in the ethanolic extract of studied plant. The mass spectra of aqua and ether extract of the plant shows in Figure 7 and 9 respectively. Figure 8 and Table 4 shows the presence of twenty-two bioactive phytochemical compounds in the aqua extract of *Datura stramonium* L leaves. And Figure 8 and Table 5 represent the presence of twenty-six bioactive phytochemical compounds in the ether extract of the plant.

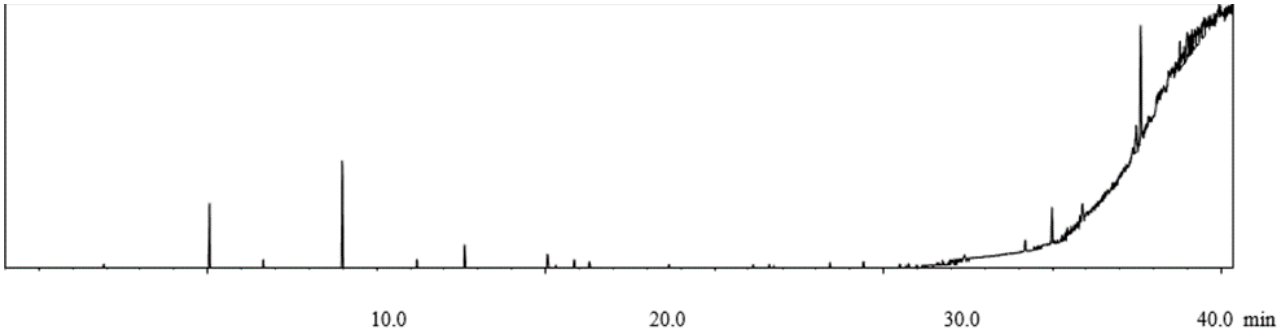

Figure 5. GC-MS chromatogram for ethanolic extract of *Datura stramonium* L.

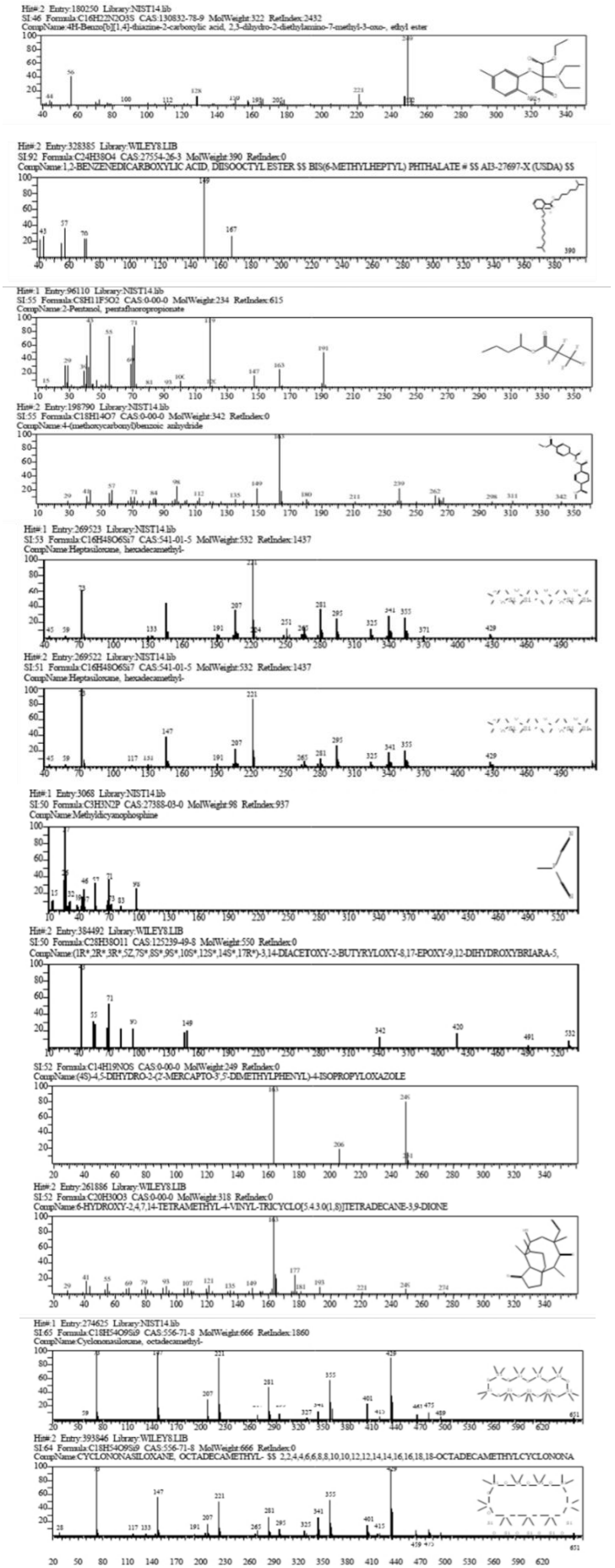

Figure 6 (cont.). Mass spectra of identified compounds from ethanolic extract of *Datura stramonium* L. leaves.

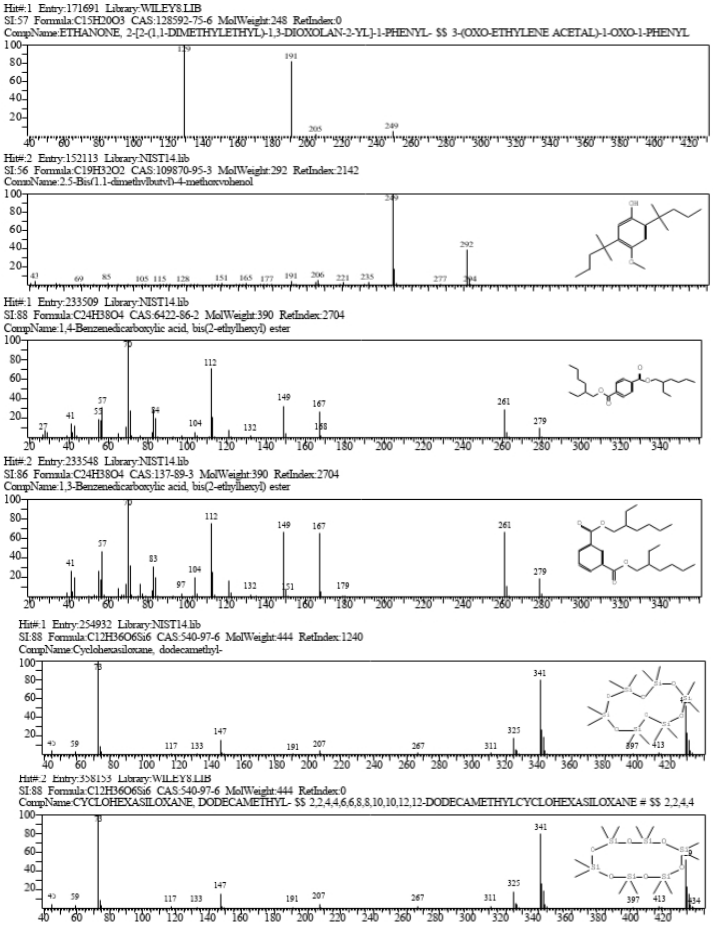

Figure 6. Mass spectra of identified compounds from ethanolic extract of *Datura stramonium* L. leaves.

Table 3. Data interpretation of the peaks obtained from GC-MS of ethanolic extract of *Datura stramonium* L. leaves.

S.NO	Molecular formula	Name of compound	Molecular weight
1	$C_{10}H_{30}O_5Si_5$	CYCLOPENTASILOXANE, DECAMETHYL	370
2	$C_{22}H_{30}OSi$	1,3-DIPHENYL-1-((TRIMETHYLSILYL)OXY)-1(Z)-HEPTENE	338
3	$C_{24}H_{38}O_4$	1,2-BENZENEDICARBOXYLIC ACID, DIOCTYL ESTER	390
4	$C_{18}H_{54}O_9Si_9$	CYCLONONASILOXANE, OCTADECAMETHYL	666
5	$C_{24}H_{38}O_4$	1,3-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	390
5	$C_{24}H_{38}O_4$	1,4-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	390
6	$C_{19}H_{18}O_6$	4H-1-BENZOPYRAN-4-ONE, 2-(2,6-DIMETHOXYPHENYL)-5,6-DIMETHOXY	342
7	$C_{15}H_{30}O_3Si_3$	1,3,5-BENZETRIOL, 3TMS DERIVATIVE	342
8	$C_{16}H_{48}O_6Si_7$	HEPTASILOXANE, HEXADECAMETHYL	532
9	$C_{19}H_{32}O_2$	2,5-BIS(1,1-DIMETHYLBUTYL)-4-METHOXYPHENOL	292
10	$C_8H_{11}F_5O_2$	PENTANOL, PENTAFLUOROPROPIONATE	234
11	$C_{18}H_{14}O_7$	4-(METHOXYCARBONYL)BENZOIC ANHYDRIDE	342
12	$C_{20}H_{30}O_3$	6-HYDROXY-2,4,7,14-TETRAMETHYL-4-VINYL-TRICYCLO [5.4.3.0(1,8)] TETRADECANE-3,9-DIONE	318
13	$C_{16}H_{22}N_2O_5S$	ETHYL 2-(DIETHYLAMINO)-7-METHYL-3-OXO-3,4-DIHYDRO-2H-1,4-BENZOTHIAZINE-2-CARBOXYLATE	322
14	$C_{32}H_{52}O_6Si$	18-O-FERULOYLOXYOCTADEC-9-ENOIC ACID, METHYL ESTER, TRIMETHYLSILYL ETHER	560
15	$C_{15}H_{28}$	4,7-DIMETHYL-1-ISOPROPYL-PERHYDRONAPHTHALENE	208

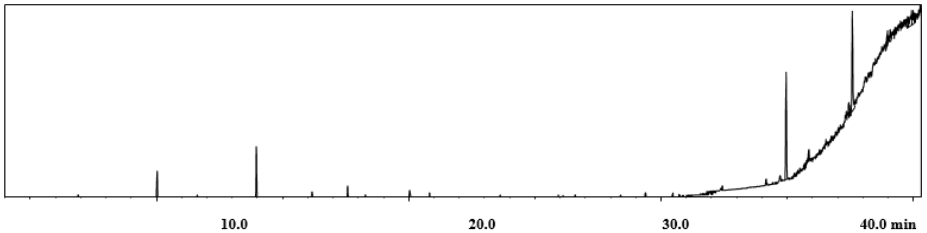

Figure 7. GC-MS chromatogram for aqua extract of *Datura stramonium* L.

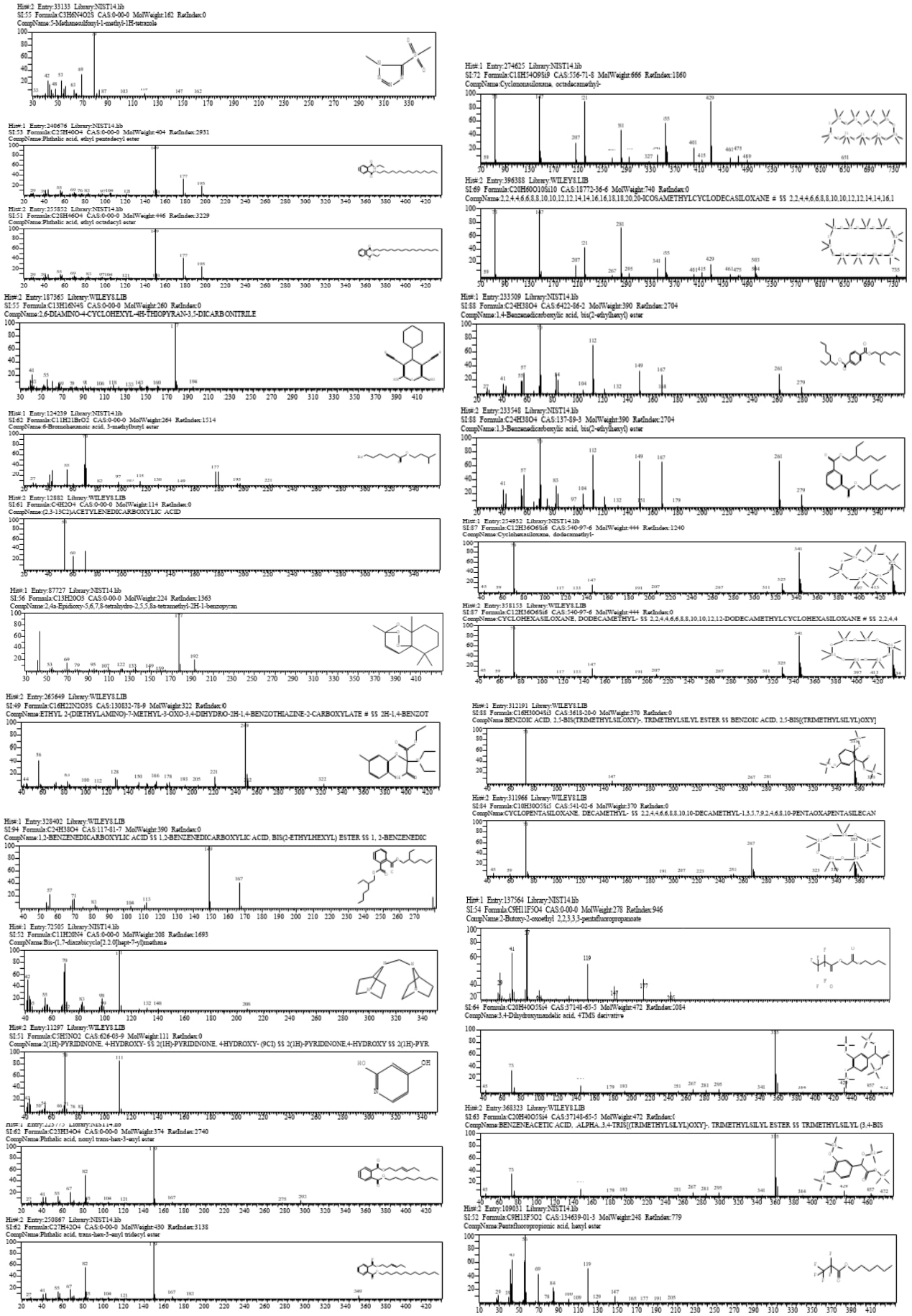

Figure 8 (cont.). Mass spectra of identified compounds from aqua extract of *Datura stramonium* L. leaves.

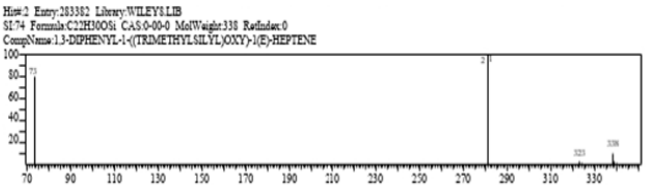

Figure 8. Mass spectra of identified compounds from aqua extract of *Datura stramonium* L. leaves.

Table 4. Data interpretation of the peaks obtained from GC-MS of aqua extract of *Datura stramonium* L. leaves.

S.NO	Molecular formula	Name of compound	Molecular weight
1	$C_{16}H_{30}O_4Si_3$	BENZOIC ACID, 2,5 BIS(TRIMETHYLSILOXY)-, TRIMETHYLSILYL ESTER	370
2	$C_{10}H_{30}O_5Si_5$	CYCLOPENTASILOXANE, DECAMETHYL	370
	$C_{12}H_{36}O_6Si_6$	CYCLOHEXASILOXANE, DODECAMETHYL	444
3	$C_{22}H_{30}OSi$	1,3-DIPHENYL-1-((TRIMETHYLSILYL)OXY)-1(Z)-HEPTENE	338
4	$C_{24}H_{38}O_4$	1,2-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	390
5	$C_{20}H_{40}O_5Si_4$	3,4-DIHYDROXYMANDELIC ACID, 4TMS DERIVATIVE	472
6	$C_{18}H_{54}O9Si_9$	CYCLONONASILOXANE, OCTADECAMETHYL	666
7	$C_{20}H_{60}O_{10}Si_{10}$	2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-ICOSAMETHYLCYCLODECASILOXANE	740
8	$C_{23}H_{34}O_4$	PHTHALIC ACID, NONYL TRANS-HEX-3-ENYL ESTER	374
9	$C_{27}H_{42}O_4$	PHTHALIC ACID, TRANS-HEX-3-ENYL TRIDECYL ESTER	430
10	$C_{24}H_{38}O_4$	1,4-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	390
11	$C_{24}H_{38}O_4$	1,3-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	390
12	$C_3H_6N_4O_2S$	1-METHYL-5-(METHYLSULFONYL)-1H-TETRAAZOLE	162
13	$C_{16}H_{22}N_2O_5S$	4H-BENZO[B] [1,4]-THIAZINE-2-CARBOXYLIC ACID, 2,3-DIHYDRO-2-DIETHYLAMINO-7-METHYL-3-OXO-, ETHYL ESTER	322
14	$C_9H_{11}F_5O_4$	2-BUTOXY-2-OXOETHYL 2,2,3,3,3-PENTAFLUOROPROPANOATE	278
15	$C_9H_{13}F_5O_2$	PENTAFLUOROPROPIONIC ACID, HEXYL ESTER	248
16	$C_{13}H_{20}O_3$	2,4A-EPIDIOXY-5,6,7,8-TETRAHYDRO-2,5,5,8A-TETRAMETHYL-2H-1-BENZOPYRAN	224
17	$C_{13}H_{16}N_4S$	2,6-DIAMINO-4-CYCLOHEXYL-4H-THIOPYRAN-3,5-DICARBONITRILE	260
18	$C_{25}H_{40}O_4$	PHTHALIC ACID ETHYL PENTADECYL ESTER	404
19	$C_{28}H_{46}O_4$	PHTHALIC ACID, ETHYL OCTADECYL ESTER	446
20	$C_{11}H_{20}N_4$	BIS-(1,7-DIAZABICYCLO [2.2.0] HEPT-7-YL) METHANE	208
21	$C_5H_5NO_2$	2(1H)-PYRIDINONE	111
22	$C_{11}H_{21}BrO_2$	6-BROMOHEXANOIC ACID ,3-METHYLBUTYL ESTER	262

Table 5. Data interpretation of the peaks obtained from GC-MS of ether extract of *Datura stramonium* L. leaves.

S.NO	Molecular formula	Name of compound	Molecular weight
1	$C_6H_{16}N_4$	1,2,4,5-TETRAZINE, 1,4-DIETHYLHEXAHYDRO	144
2	$C_6H_{16}N_4$	1,4-DIETHYL-1,2,4,5-TETRAAZIN	144
3	$C_6H_{11}Br_2P$	CYCLOHEXYLPHOSPHONOUS	272
4	$C_{16}H_{30}O_4Si_3$	BENZOIC ACID, 2,5-BIS(TRIMETHYLSILOXY)-, TRIMETHYLSILYL ESTER	370
5	$C_{10}H_{30}O_5Si_5$	2,2,4,4,6,6,8,8,10,10 DECAMETHYL-CYCLOPENTASILOXANE	370
6	$C_{12}H_{36}O_6Si_6$	CYCLOHEXASILOXANE, DODECAMETHYL	444
7	$C_{19}H_{54}O_7Si_7$	3-BUTOXY-1,1,1,7,7,7-HEXAMETHYL-3,5,5-TRIS(TRIMETHYLSILOXY)TETRASILOXANE	490
8	$C_{19}H_{54}O_7Si_7$	1-BUTOXY-3,3,3-TRIMETHYL-1-[(TRIMETHYLSILYL) OXY]DISILOXANYL TRIS(TRIMETHYLSILYL) ORTHOSILICATE	590
9	$C_{15}H_{32}$	PENTADECANE	212
10	$C_9H_9NOS_2$	2-(1,3-BENZOTHIAZOL-2-YLSULFANYL) ETHANOL	211
11	$C_{16}H_{32}O_2$	N-HEXADECANOIC ACID	256
12	$C_{20}H_{40}O$	[R-[R*, R*-(E)]]- 3,7,11,15-TETRAMETHYLHEXADEC-2-EN-1-OL	296
13	$C_5H_{11}Br$	BUTANE, 1-BROMO-2-METHYL- $$ (1)-1-BROMO-2-METHYLBUTANE $$ 1-BROMO-2-METHYKBUTANE $$ 1-BROMO-2-METHY	150
14	$C_{22}H_{42}O_4$	HEXANEDIOIC ACID, BIS(2-ETHYLHEXYL) ESTER $$ HEXANEDIOIC ACID, DIOCTYL ESTER $$ ADIPIC ACID BIS (2-ETHYLHE	370
15	$C_{22}H_{42}O_4$	HEXANEDIOIC ACID, DIOCTYL ESTER $$ ADIPIC ACID DIOCTYL ESTER $$ BIS(2-ETHYLHEXYL)	370

		HEXANEDIOATE $$ DIOCTY	
16	$C_{24}H_{38}O_4$	1,2-BENZENEDICARBOXYLIC ACID $$ 1,2-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER $$ 1, 2-BENZENEDIC	390
17	$C_{24}H_{38}O_4$	PHTHALIC ACID, DI(2-PROPYLPENTYL) ESTER	390
18	$C_{18}H_{54}O_9Si_9$	CYCLONONASILOXANE, OCTADECAMETHYL-	666
19	$C_{24}H_{38}O_4$	1,3-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	390
20	$C_{24}H_{38}O_4$	,4-BENZENEDICARBOXYLIC ACID, BIS(2-ETHYLHEXYL) ESTER	390
21	$C_{26}H_{42}O_4$	1,2-BENZENEDICARBOXYLIC ACID, DINONYL ESTER	418
22	$C26H_{42}O_4$	1,2-BENZENEDICARBOXYLIC ACID, BIS(7-METHYLOCTYL) ESTER $$ BIS(7-METHYLOCTYL) PHTHALATE	418
23	$C_{32}H_{54}O_4$	PHTHALIC ACID, NONYL PENTADECYL ESTER	502
24	$C_{16}H_{48}O_6Si_7$	HEPTASILOXANE, HEXADECAMETHYL	532
25	$C_{14}H_{42}O_5Si_6$	HEXASILOXANE, TETRADECAMETHYL	458

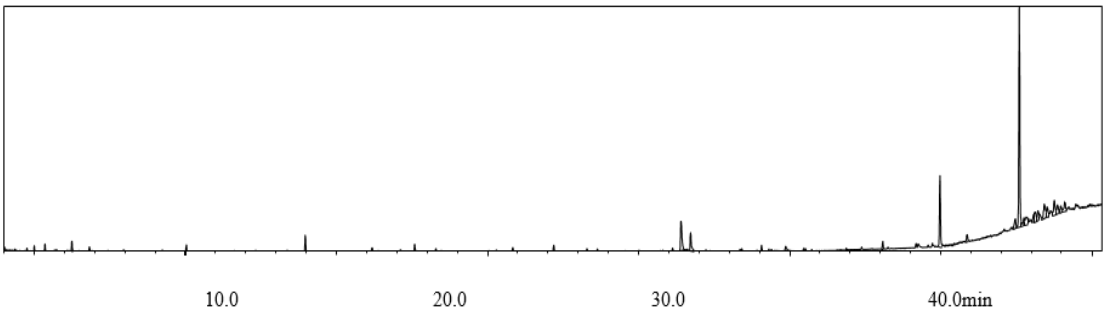

Figure 9. GC-MS chromatogram for ether extract of *Datura stramonium*.

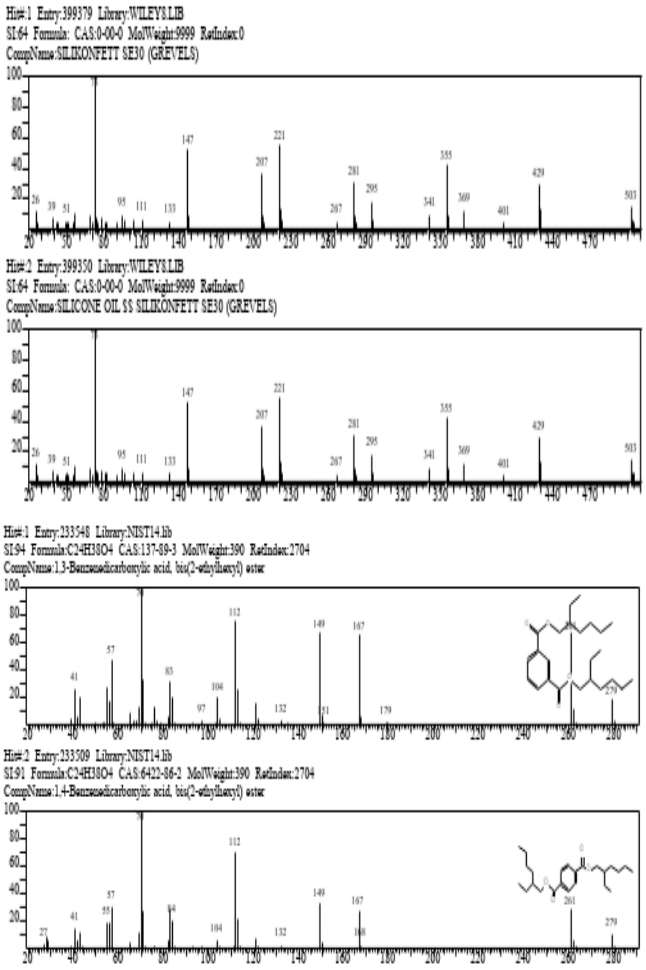

Figure 10 (cont.). Mass spectra of identified compounds from ether extract of *Datura stramonium* L. leaves.

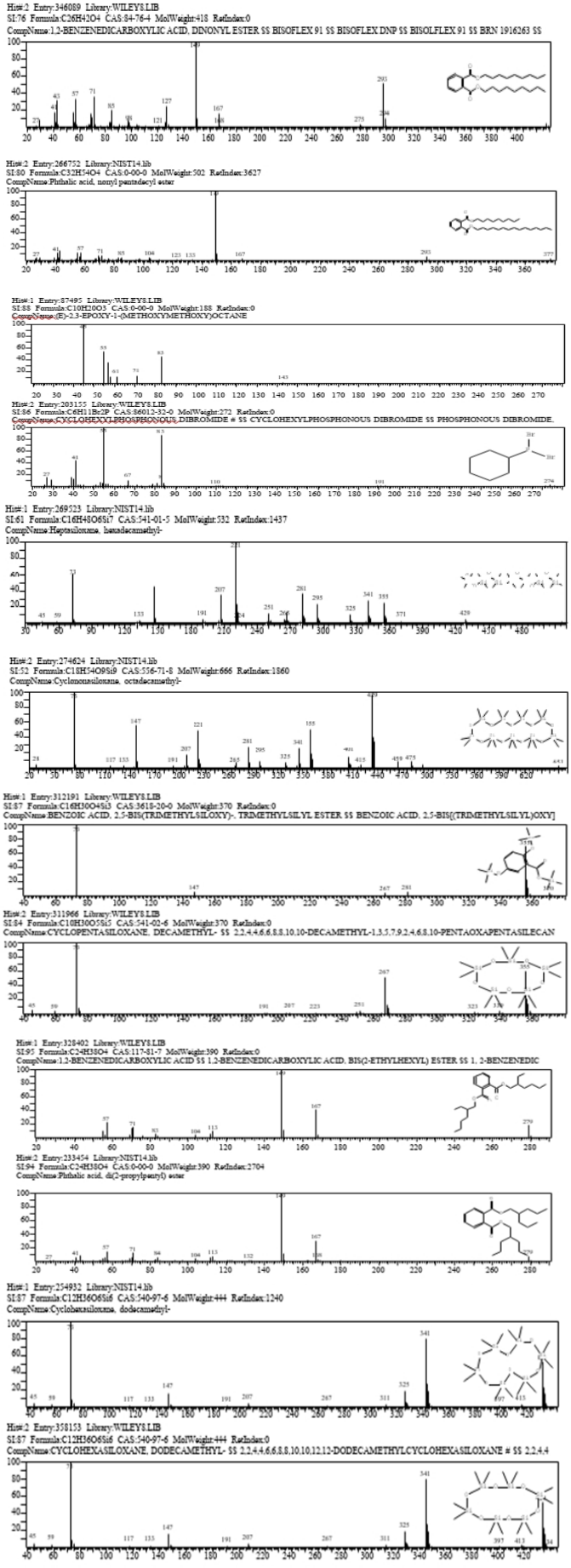

Figure 10 (cont.). Mass spectra of identified compounds from ether extract of *Datura stramonium* L. leaves.

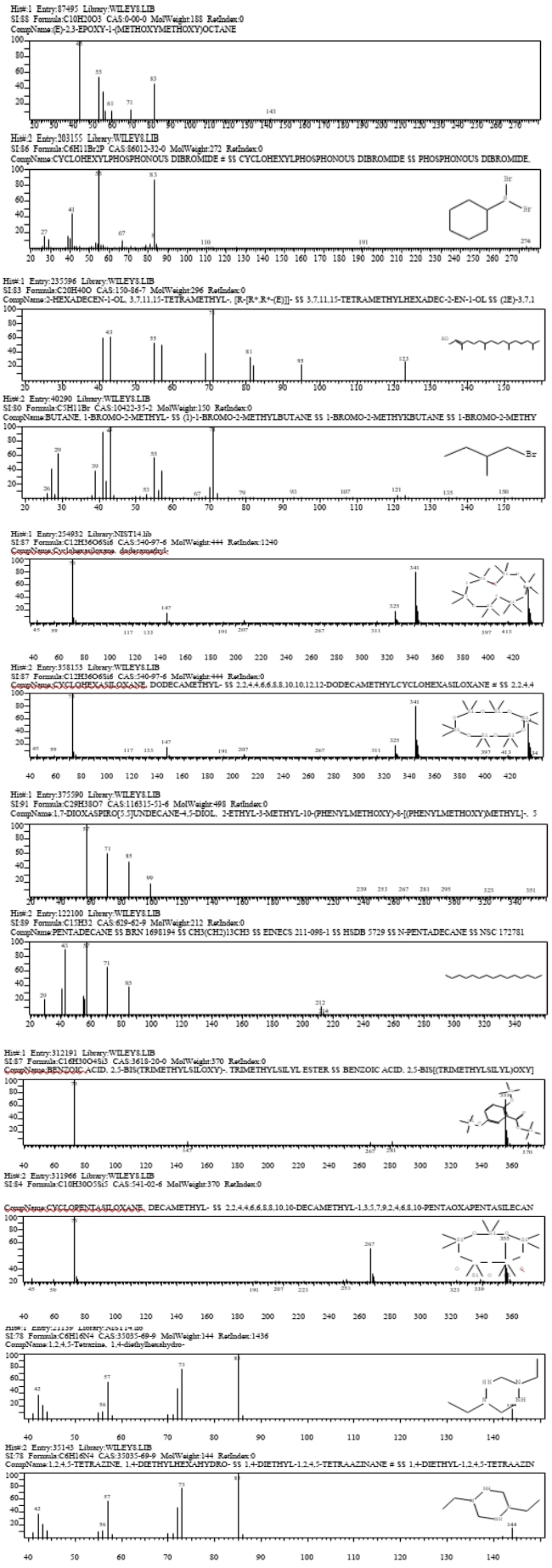

Figure 10 (cont.). Mass spectra of identified compounds from ether extract of *Datura stramonium* L. leaves.

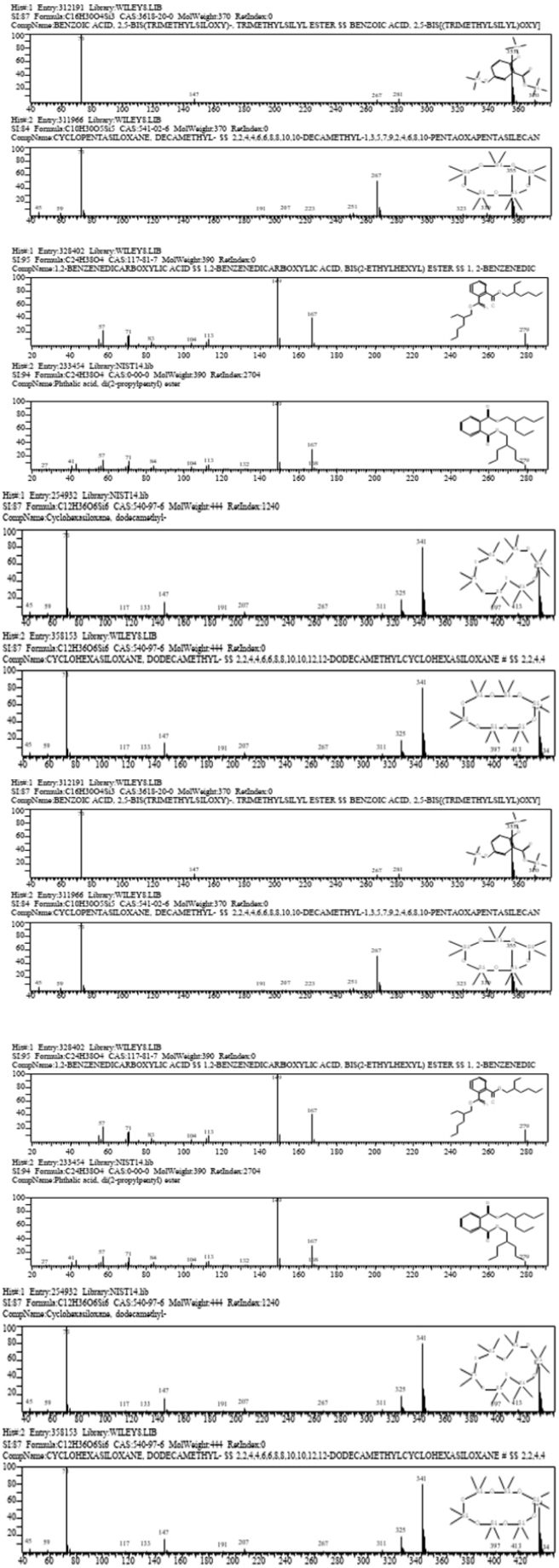

Figure 10 (cont.). Mass spectra of identified compounds from ether extract of *Datura stramonium* L. leaves.

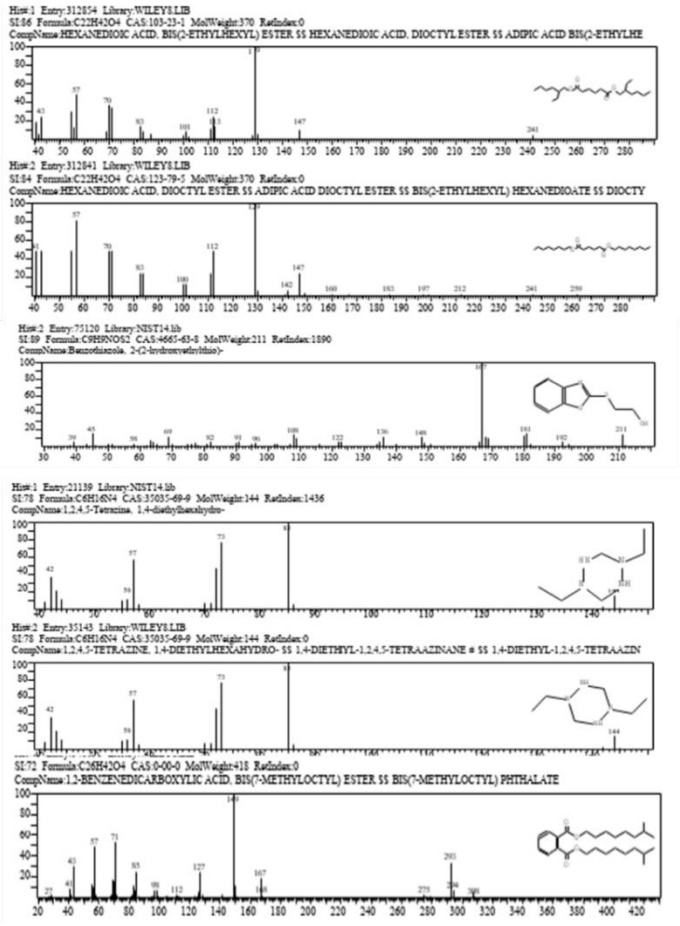

Figure 10. Mass spectra of identified compounds from ether extract of *Datura stramonium* L. leaves.

Conclusion

Medicinal plants have key role in traditional medicine. The studies reveal that *Datura stramonium* L is a potential source of new phytonutrients with therapeutic value. The comparative phytochemical screening of the plant leaves in ethanol, water and ether solvents showed the presence of alkaloids, phenols, tannins, flavonoids, saponins, sterols etc. and the corresponding spots were identified by thin layer chromatography. This study substantiate with the previous literature that the leaves of *Datura stramonium* L. is a hallucinogenic plant that causes serious poisoning (Sharma et al., 2021). The results of IR analysis of plant leaves extract in different solvents shows number of absorption bands which indicates the presence of N-H, O-H, C=C, C-H, C=O, and CH_3 functional groups. IR peaks give the indication of presence of alcohol, phenols, carboxylic acid and also shows the characteristic bands for amide, primary and secondary amine. Infrared spectral data provide evidence for bioactive molecule and hence *Datura stramonium* L. plant can be used for further application studies. Investigation of bioactive compounds was executed using Gas chromatography and Mass spectroscopy analysis. The fragmentation patterns confirmed the presence of different phytonutrients. And the studies reveal presence of fifteen phyto components in ether extract, twenty-two in aqua extract and twenty-six phytochemicals in ether extract of *Datura stramonium* L. leaves.

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