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Screening of bioactive components of the flower *Datura metel* using the GC-MS technology

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Abstract : The investigation was carried out to determine the possible bioactive components of the flower of *Datura metel* using GC-MS. The chemical compositions of the methanol extract of the flower *Datura metel* were investigated using Perkin-Elmer Gas chromatography – Mass spectrometry, while the mass spectra of the compounds found in the extract was matched with the National Institute of Standards and Technology (NIST) library. Four different components were identified from the flower of *Datura metel*.
Keywords: *Datura metel,* flower, GC-MS analysis, bioactive compounds.

INTRODUCTION

Medicinal plants used as sources for extracts or pure products for therapeutic use represent a rapidly expanding area of health science[1]. Higher plants, as sources of medicinal compounds have continued to play a dominant role in the maintenance of human health since ancient times. It is reported that over 50% of all modern clinical drugs are of natural product origin and natural products play an important role in drug development programs in the Pharmaceutical industry.[2]

Datura metel (Linn) (Thorn-apple, Devil trumpet) belong to the family Solanaceae is a Nigerian medicinal plant widely used in phytomedicine to cure diseases such as asthma, cough, convulsion and insanity. The leaves and seeds are widely used in herbal medicine as anesthetic, antispasmodic, bronchodilator and as hallucinogenic.[3&4] It is popular all over the world for its medicinal uses like its use in fever with catarrh, cerebral complications, diarrhea, skin diseases, antiseptic, animal bites, anti helmenthic and in herpetic diseases, and also has healing potential on burn wounds.[5&6] It is also known for its antibacterial activity against burn pathogens[7] and antifungal activity against phytopathogens.[8] A variety of phytochemicals have been found to occur in *Datura metel* and the phytoconstituents comprises alkaloids, flavonoids, phenols, tannins, saponins and sterols.[9&10] The phytoconstituents of *Datura* were analysed from various parts of the plant like the leaf,[11-13] root,[14] and shoot.[15-17]

The literature study showed a lacuna in the phytochemical study of the flowers of the *Datura* and hence the present investigation was carried out to determine the possible chemical components of *Datura metel* flowers using GC-MS.

MATERIAL AND METHODS

Plant material

Required quantities of the *Datura metel* flowers were collected from the nearly villages of Thoothukudi town of Tamilnadu. The botanical

identification of the plant was confirmed using Gamble Volume[18].

Plant sample extraction

20gm powdered flower material was soaked in 50ml of methanol overnight and then filtered through whatmann filter paper No.41 along with 2gm of sodium sulfate to remove the sediments and traces of water in the filtrate. Before filtering the filter paper along with sodium sulphate was wetted with methanol. The filtrate was then concentrated by bubbling nitrogen gas into the solution and reduced to the volume of 1ml. The extract contains both polar and non-polar phytocomponents of the plant material. The final extract was used for GC-MS analysis.

GC-MS Analysis

GC-MS was performed using the GC Clarus 500 Perkin Elmer equipment. Compounds were separated on Elite 5MS (5% Diphenyl /95% Dimethyl polysiloxane), 30X0.25mmX0.25µmdf capillary column. Samples were injected with a split ratio of 10:1 with a flow rate of helium 1ml/min (carrier gas). Mass detector used was Turbo mass gold Perkin Elmer. Software used was Turbomass 5.2. 2 µl of sample was injected. Other conditions monitored was as oven temperature up to 110°C – 2min hold; upto 200°C at the rate of 10°C/min-no hold; upto 280°C at the rate of 5°C/min – 9 min hold. Injector temperature was maintained at 250°C. The total GC running time was 36 minutes. The constituents were identified after comparison with those available in the computer library (NIST version 2005) attached to the GC – MS instrument and documented.

Identification of Components

Interpretation of mass spectrum GC-MS was conducted using the database of National Institute Standard and Technology (NIST) having more than 62,000 patterns. The spectrum of the unknown component was compared with the spectrum of the known components stored in the NIST library. The name, molecular weight and structure of the components of the test materials were ascertained.

Table 1. Components detected in *Datura metel* flower extract

S. NO	Room Temperature	Name of the compound	Molecular Formula	Molecular Weight	Peak Area %	Compound Nature
1.	17.08	1,4-Cyclohexadiene, 1-methyl-	C_7H_{10}	94	12.22	Alkene compound
2.	31.13	Acetic acid, trifluoro-, 2,2-dimethylpropyl ester	$C_7H_{11}F_3O_2$	184	31.97	Fluro compound
3.	31.66	4-Trifluoroacetoxyoctane	$C_{10}H_{17}F_3O_2$	226	19.28	Fluro compound
4.	32.98	cis-2-Nitro-4-t-butylcyclohexanone	$C_{10}H_{17}NO_3$	199	36.54	Nitrogen compound

Figure 1.GC-MS Chromatogram of methanol flower extract of *Datura metel*

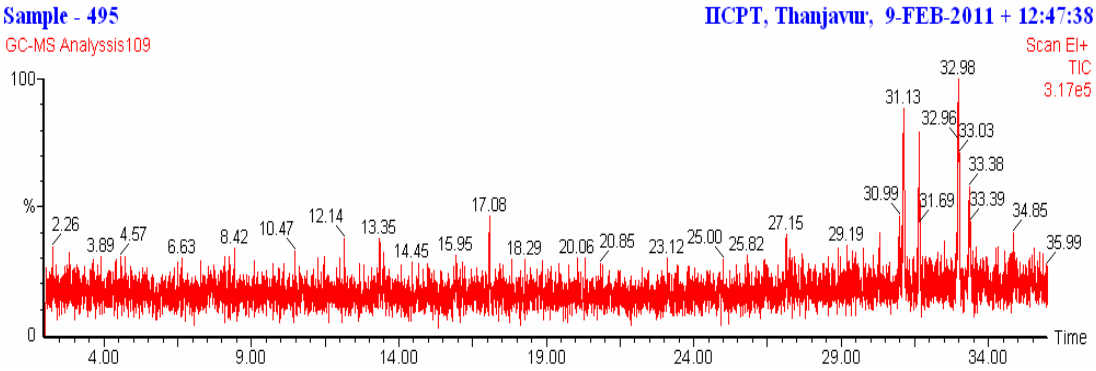
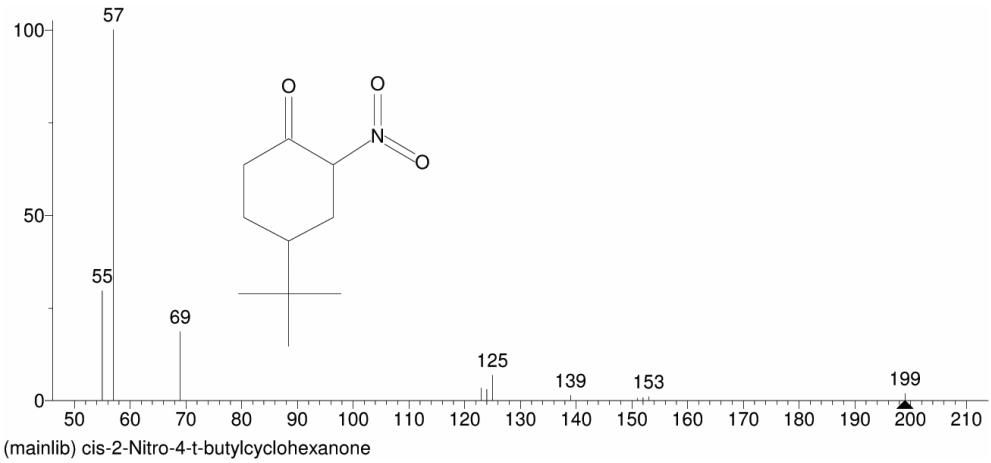


Figure 2. Mass spectrum of cis-2-Nitro-4-t-butylcyclohexanone (RT-36.54)



RESULT AND DISCUSSION

The results pertaining to the GC-MS analysis are given in Figure 1 and Table 1. Four compounds were detected in methanolic extracts of *Datura metel* flower. The active principles with their retention time (RT), molecular formula, molecular weight (MW) and concentration (%) are presented in Table 1 and Figure 1. The results revealed that the methanolic extract of *Datura metel* flower showed the presence of the compound such as cis-2-Nitro-4-t-butylcyclohexanone (36.54%) a followed by Acetic acid, trifluoro-, 2,2-dimethylpropyl ester (31.97%), 4-Trifluoroacetoxyoctane (19.28%) and 1,4-Cyclohexadiene, 1-methyl- (12.22%). Among the four compounds the cis-2-Nitro-4-t-butylcyclohexanone was represented in high percentage. According to Dr. Duke's[19] the components identified such as Acetic acid, trifluoro-, 2,2-dimethylpropyl ester, 4-Trifluoroacetoxyoctane and 1,4-Cyclohexadiene, 1-methyl- have the antimicrobial property where as the property of cis-2-Nitro-4-t-butylcyclohexanone is not known.

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