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ORIGINAL ARTICLE

Chemical profile of *Datura stramonium* L. by using HRLC-MS spectra.

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ABSTRACT

The chemical profile of *Datura stramonium* L. was characterized by using HRLC-MS spectra. The relative concentrations of various compounds getting eluted as a function of retention time gives in chromatogram. The relative concentration of the bioactive compounds present in the plants was indicated by the height of peak. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. These mass spectra are fingerprint of that compound which can be identified from the data library. This report is the first of its kind to analyze the bioactive compounds of *Datura stramonium* L. using HRLC-MS. The results are relevant to HRLC-MS analysis of methanolic leaf extract of *Datura stramonium* L. spectrum profile (fig. 1) gives presence of 100 compounds. Out of that 25 major compounds confirmed on the basis of their retention time, molecular formula and mass. The phytochemical study of *Datura stramonium* L. using HRLC-MS indicates the presence of fatty acids, organic compounds, phenolics, alkaloids, phytoharmone, coenzyme, aminopyrimidines, dipeptide and tripeptides like important metabolites in these leaves. These results suggested to do further investigations which may lead to the development of drug formulation.

Keywords: *Datura stramonium,* Phytochemical, aminopyrimidines, HR-LCMS, phytoharmone and methanol.

INTRODUCTION

Datura is a wild weed belonging to family Solanaceae, its name derived from Sanskrit word "Dhutra" (divine inebriation) is used for its healing properties. Various species of *Datura* are known and widely employed for their medicinal and toxic properties that are based upon more than 30 alkaloids. *Datura* is known as a medicinal plant and plant hallucinogen all over the world.

Datura has a very special place in Ayurveda since all parts of the plant namely leaves, flowers, seeds, roots, have been used for a wide range of medication such as treatment of leprosy, rabies, insanity, etc. The extract of *Datura*, however, is a potent poison and its indiscriminate use may lead to delirium and acute poisoning that may lead to death. The active constituents in *Datura* include scopolamine, atropine, hyoscyamine, with anolides (lactones) and other tropanes [1]. All parts of the plant shows anti-inflammatory property [2] stimulation of the central nervous system (CNS) [3]; [3], respiratory decongestion [5], treatment of dental and skin infections [6]; [7]; [8]and also in the treatment of toothache [9] and alopecia [6].

Recently plant-derived substances became great interest to know their various applications. These compounds were varying from plant to plant, some produce large and some produce in small quantity. Recently plant-derived substances became great interest to know their various applications [10]. In number of plants, Phytochemicals are existing in their biologically active forms in healthy plants, but others occur as inactive precursors and were activated in response to tissue damage or pathogen attack Osbourne, 1996. Phytochemicals are naturally present in the plants and play significant role to defend themselves against various pathogenic microbes by showing the antimicrobial activity by inhibition or killing mechanisms. Ethno pharmacologists, botanists, microbiologists, and natural-product chemists are searching the earth for phytochemicals which could be developed for the treatment of infectious diseases [11] especially in drug-resistant microorganisms and to produce more effective antimicrobial agents. Many workers were studied that in some plants there are many components such as peptides, aldehydes, alkaloidal constituents, some essential oils, phenols and water, ethanol, chloroform, methanol and butanol soluble compounds 12, 13 . Such compounds being biodegradable and selective in their toxicity are considered valuable for controlling some plant diseases.

Aderotimi Banso and Samuel Adeyemo 14 studied phytochemical screening and antimicrobial assessment of *Abutilon mauritianum, Bacopa monnifera* and *Datura stramonium*. Berkov *et al*. [15] observed that *D. stramonium* contains Sixty-four tropane alkaloids. Two new tropane alkaloids, 3- phenylacetoxy-6, 7-epoxynortropane and 7- hydroxyapoatropine were tentatively identified. The alkaloids scopoline, 3-(hydroxyacetoxy) tropane, 3-hydroxy-6-(2-methyl-butyryloxy) tropane, 3a-tigloyloxy-6-hydroxytropane, 3,7- dihydroxy-6-tigloyloxytropane, 3-tigloyloxy-6-propionyloxytropane, 3-phenylacetoxy-6,7- epoxytropane, 3-phenylacetoxy-6-hydroxytropane, aponorscopolamine, 3a,6a-ditigloyloxytropane and 7-hydroxyhyoscyamine are reported for the first time for this species. Maibam *et al*. [16] reviewed neurotoxic and medicinal properties of *Datura stramonium* L. Sixty-four tropane alkaloids have been detected from D. stramonium. Das *et al*. [17] studied phytoconstituents and therapeutic potentials of D*atura stramonium* Linn. *Datura stromonium* has been scientifically proved to have alkaloids, tannins, carbohydrates, proteins. This study highlights the pharmacological activities of *Datura stramonium*, which may be due to the presence of its scientifically proven chemical constituents. Keeping this in view, Chemical profile of *Datura stramonium* L. were carried out by using HRLC-MS spectra.

2. EXPERIMENTAL DETAILS

2.1 Preparation of sample:

Fresh and healthy leaves of *Datura stramonium* L. was collected from Shendra MIDC, Aurangabad (MS). The leaves were collected in sterile polythene bags and brought to the laboratory and washed with running tap water. These were dried in shade at room temperature till it gets constant weight. The dried material were crushed in mortar - pestle and then in mixture grinder to make fine powder.

2.2 Preparation of extracts:

The prepared powder samples were filtered through muslin cloth and 25 gm of fine powder were extracted with methanol as a solvent by using soxhlet extractor for 18 hours at 65^0C. These extracts were filtered through Whatman filter paper no. 42 and concentrated at 40^0C by using an evaporator and store in umber bottle at 4^0C. These extracts were sent for HR-LCMS (High Resolution Liquid Chromatography and Mass Spectroscopy) analysis to Sophisticated Analytical Instrumentation Facility, Indian Institute of Technology, Powai, Mumbai, India, for the detection of various phytochemicals.

Aderotimi Banso and Samuel Adeyemo 14 studied phytochen

2.3 HRLC-MS analysis:

At SAIF, IIT Powai, Mumbai, equipment and conditions Identification of metabolites from an active sub-fraction

of methanol extract was carried out. Samples were analyzed on a LC-ESI-Q-TOF-MS (Agilent Technologies 6550 i-Funnel) system equipped with a G4220B pump, G4226A auto sampler and G1316C, and a diode array detector (DAD). The elution solvent consisted of a gradient system of 0.1% formic acid in water (A) and acetonitrile (B) at a flow rate of 0.3 ml/min. The gradient system started with 95% A: 5% B reaching 5% A: 95% B in 50 min. then back to initial composition 95% A: 5% B in 10 min which was held at same composition for 5 min. The MS analysis was carried out by ESI positive ionization mode. MS source conditions were as follows: capillary voltage 3500 V, Gas temperature 250 C, drying gas flow 13 L/min, sheath Gas temp 300, sheath Gas Flow 11, nebulizing gas pressure 35 (psig), fragmentor 175 V, Skimmer 65 V, Octopole RF Peak 750 V, and mass range m/z 50–1000. The resolution was 40,000 FWHM. Metlin database was used to structure confirmation.

3. RESULTS AND DISCUSSION

The chemical profile of methanolic leaf extract of *Datura stramonium* L., by using HRLC-MS spectra (fig.1) gives presence of 100 compounds. Out of that 25 major compounds confirmed on the basis of their retention time, molecular formula and mass. These active compounds are presented in Table 1. The chemical profile of *Datura stramonium* L. was characterized by using HRLC-MS spectra. The relative concentrations of various compounds getting eluted as a function of retention time gives in chromatogram. The relative concentration of the bioactive compounds present in the plants was indicated by the height of peak. The mass spectrometer analyzes the compounds eluted at different times to identify the nature and structure of the compounds. These mass spectra are fingerprint of that compound which can be identified from the data library.

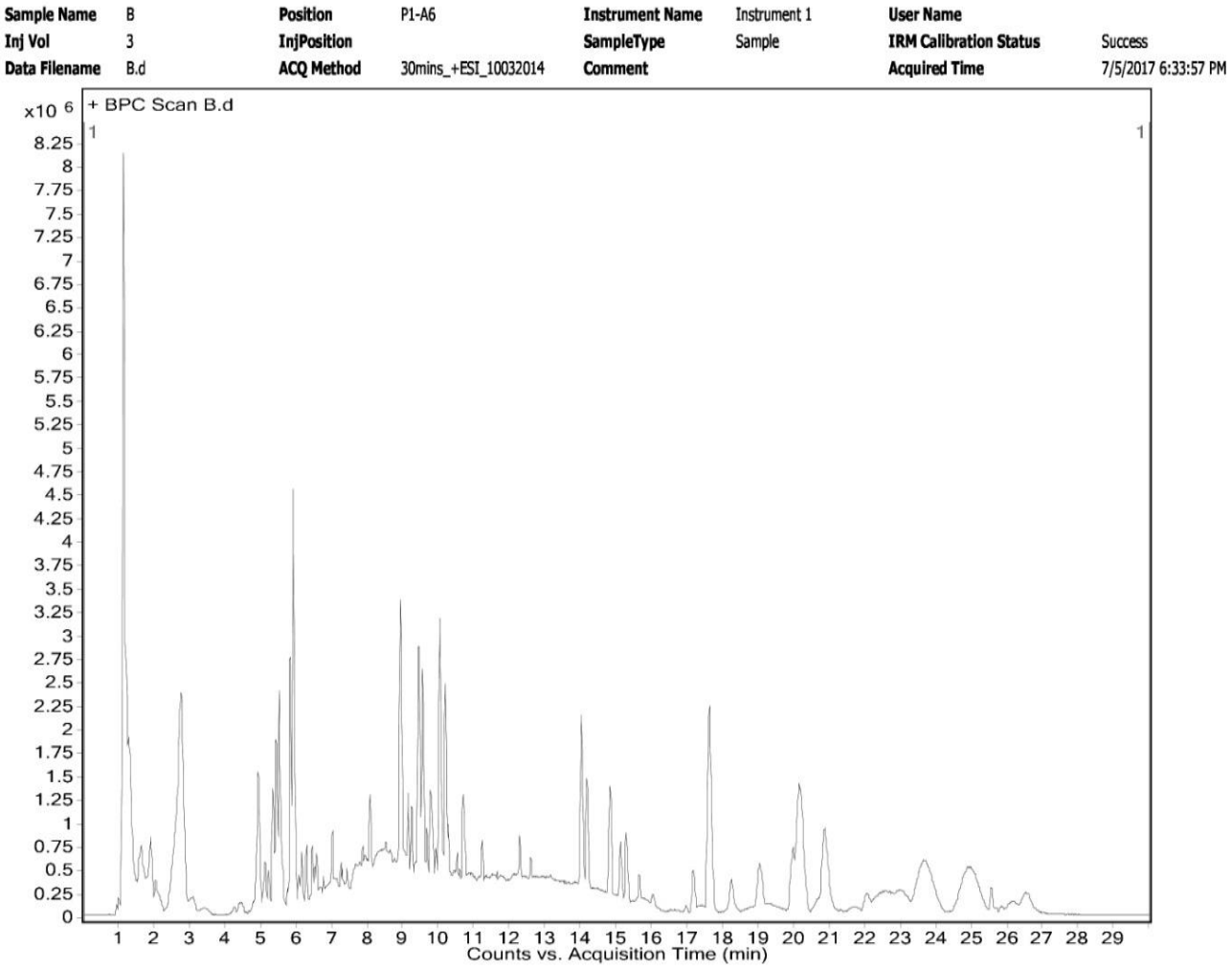

Fig.1: HRLC-MS Spectrogram of *Datura stramonium* L.

Table 1:Major phytochemicals from leaves of *Datura stramonium* L. by HRLC-MS

Sr. No	Name	RT	Mass	Formula	m/z
1	Ethosuximide M5	1.121	155.05	$C_7H_9O_3$	138.05
2	Carnitine	1.151	162.11	$C_7H_{16}NO_3$	144.10
3	Methyl N-(amethyl butyryl) glycine	1.163	173.10	$C_8H_{15}NO_3$	156.10
4	Northiadene	1.918	281.12	$C_{18}H_{19}NS$	282.13
5	4-Hydroxy phenyl ethanol	2.760	138.06	$C_8H_{10}O_2$	121.06
6	a-[1-(ethylamino)ethyl]-p-hydroxy-Benzyl alcohol	2.763	195.12	$C_{11}H_{17}NO_2$	178.12
7	Diacetolo	4.89	308.17	$C_{16}H_{24}N_2O_4$	291.16
8	4-Hydroxyoxprenolol	5.366	281.16	$C_{15}H_{23}NO4$	304.15
9	9-acetyl pelargonic acid	5.423	200.13	$C_{11}H_{20}O_3$	183.13
10	Anisodamine	5.454	305.16	$C_{17}H_{23}NO_4$	306.17
11	Perindoprilat lactam A	5.461	322.18	$C_{17}H_{26}N_2O_4$	305.18
12	4-Hydroxypropranolo	5.847	275.15	$C_{16}H_{21}NO_3$	276.15
13	4-Trimethylammoniobutanal	8.071	130.12	$C_7H_{16}NO$	130.12
14	3-O-Methylisoetharine	9.126	253.16	$C_{14}H_{23}NO_3$	236.16
15	Deoxycholic acid 3- glucuronide	9.153	568.31	$C_{30}H_{48}O_{10}$	569.32
16	3 β -Hydroxydeoxo dihydrodeoxygedunin	9.271	470.26	$C_{28}H_{38}O_6$	453.26
17	Dihydro deoxy streptomycin	9.573	567.29	$C_{21}H_{41}N_7O_{11}$	568.29
18	1 α -hydroxy-24- methylsulfonyl-25,26,27- trinor vitamin D3	9.807	436.26	$C_{25}H_{40}O_4S$	419.25
19	3-methyl-decanoic acid	12.30	186.16	$C_{11}H_{22}O_2$	191.14
20	1 α,25- dihydroxy-22-thia-20- epichole calciferol	14.04	434.28	$C_{26}H_{42}O_3S$	457.27
21	Ipecac (Methylpsychotrine)	14.2	478.27	$C_{29}H_{38}N_2O_4$	483.25
22	Lactone of PGF-MUM	14.82	296.16	$C_{16}H_{24}O_5$	301.14
23	Hydrocortisone cypionate	15.14	486.29	$C_{29}H_{42}O_6$	469.29
24	Ramipril glucuronide	17.64	592.26	$C_{29}H_{40}N_2O_{11}$	593.27
25	3-β,6α,7α Trihydroxy-5beta-cholan-24-oiic Acid	20.88	408.28	$C_{24}H_{40}O_5$	413.26

This report is the first of its kind to analyze the bioactive compounds of *Datura stramonium* L**.** using HRLC-MS.

This study also helped to identify the formula and structure of biomolecules which can be used as natural fungicides. The phytochemical study of *Datura stramonium* L. using HRLC-MS indicates the presence of fatty acids, organic compounds, phenolics, alkaloids, phytoharmone, coenzyme, aminopyrimidines, dipeptide and tripeptides like important metabolites in these leaves. These results suggested to do further investigations which may lead to the development of drug formulation. The retention time, m/z value, mass, and molecular formula of the 25 major metabolites are shown in Table 1. The spectrum shows counts versus mass to charge (m/z) ratio (Fig. 1).

This result was confirmed by many authors. Priyanka *et al*. [18] detected Sixty-four tropane alkaloids from *D. stramonium*. Two new tropane alkaloids, 3-phenylacetoxy-6, 7-epoxynortropane and 7-hydroxyapoatropine were tentatively identified. The phytochemical analysis of the plant revealed that *D. stramonium* contained saponins, tannins, alkaloids and glycosides. Langonjam and Okram 19) overviewed phytochemistry and pharmacognosy of *Datura stramonium.* Aqib Sayyed and Mohib Shah [20] reviewed phytochemistry, pharmacological and traditional uses of *Datura stramonium* L. and revealed that *Datura stramonium* contains biologically active substances like alkaloids, atropine, scopolamine, tannin, carbohydrate and proteins. Kumar *et al*. [21] observed the preliminary phytochemical analysis of crude extracts of leaves, fruits and stem of *Datura stramonium* using aqueous, benzene

chloroform as solvents. Three different extracts of leaves, stem and fruits of *D. stramonium* were found to contain various secondary metabolites like triterpenoids, steroids, glycosides, saponins, alkaloids, flavonoids and tannins. Sepide Miraj [22] updated review of *Datura stramonium*.

4. CONCLUSION

The phytochemical study of the leaves of *Datura stramonium* L. using HRLC-MS indicates the presence of fatty acids, organic compounds, phenolics, alkaloids, phytoharmone, coenzyme, aminopyrimidines, dipeptide and tripeptides like important bioactive compounds. It may be contributing natural antimicrobial, antioxident, anti-inflammentary activity and further investigations which may lead to the development of drug formulation.

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