

Characterization of Herbal Cigarette Smoke by using HRLC-MS Technique

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Abstract: As we all know that smoking of tobacco cigarette is injurious to health, which significantly raises the risk of causing numerous cancers such as mouth, throat, lung mostly causes lung cancers and cancer almost anywhere on the body along with breathing problems, chronic respiratory conditions heart disease, stroke and blood circulation problems. Tobacco smoke consists of more than 4000 chemical compounds and approximately 60 known carcinogens. Herbal cigarettes are nicotine-free and tobacco-free alternatives formulated from different kinds of medicinal herbs Present research was undertaken to overcome these problems, in this study different medicinal plants viz., *Curcuma longa L.* (rhizome), *Zingiber officinale Roscoe* (Rhizome), and *Ocimum tenuiflorum L.* (leaf). Smoke of herbal cigarette screened by using HRLC-MS technique which revealed existence of various secondary metabolites viz., 2-Diethylaminoethanol, Daimuron, Pirimicarb, Artemisyl propionate, Oleandolide, (S)-Menthone 8-thioacetate, Valyl-Histidine, Naltrindole, Glutamyl-lysine, Eupatoroxin, Palmitic Acid and Stearic acid. Further study of these individual drugs is necessary which can be used in the treatment of different kinds of diseases

Keywords: Herbal cigarette, Smoke, phytochemical, HRLC-MS

I. INTRODUCTION

For many individuals nicotine addiction and habitual behaviors associated with smoking is a major cause of cancer. Despite widespread awareness about health risks, smoking cessation is remains a significant challenge for individual. Primarily due to the harmful effects of nicotine, tar, and other toxic chemicals present in tobacco products cigarette causes different kinds of cancer and other related saviour diseases and finally leads in to death. To overcome this problem, there has been growing interest to develop different alternatives for tobacco cigarette which is safer and free from nicotine and tobacco, herbal cigarette is one of the safer alternatives (Singh, *et al.*, 2010).

Plants are used in herbal medicine for their antimicrobial, anti-inflammatory, antiasthematic and respiratory-supportive effects. Herbal cigarettes prepared a blend of various medicinal plants in different combinations known for their therapeutic properties which reduced the exposure to harmful substances. *Glycyrrhiza glabra* (Licorice), *Mentha arvensis* (Mint), *Ocimum sanctum* (Tulsi), and *Syzygium aromaticum* (Clove) are commonly used herbs in cigarettes due to their immense medicinal values (Wankhade *et al.*, 2025).

Around 1800, British colonizers in India learned that people there smoked *Datura ferox*, sometimes mixed with tobacco, to treat asthma (Mark Jackson, 2010). During the late 19th and early 20th centuries, inhalation of fumes from burning preparations of stramonium, lobelia, tobacco, and potash became increasingly popular amongst asthmatics and their physicians throughout the world (Jay Grossman, 1994).

The aim of present study not only o develop herbal cigarette but also to provide safe alternative to conventional tobacco cigarette which can deliver mild therapeutic effects through inhalation (Wankhade *et al.*, 2025). In present study herbal cigarette using selected medicinal herbs evaluated for their potential phytochemical properties.



II. MATERIALS AND METHODS

For the present study highly medicinally important plants viz., *Curcuma longa* (rhizome), *Zingiber officinale* (Rhizome), *Ocimum tenuiflorum* (leaf) were selected and collected from surrounding agriculture field. These plants were identified by using authentic floristic literature (Sharma et al, 1996; Diwakar and Sharma, 2000; Singh, et al, 2001). Selected plant material was washed, chopped into fine pieces and shade dried for 5-6 days. By using combination of these plants cigarette was prepared. The smoke of medicinal cigarette were collected in the sample bottle and dissolved in ethyl alcohol. This smoke was sent to IIT Powai, Mumbai for the analysis of different secondary metabolites by using HRLC-MS technique (Jadhao et al., 2024).

HRLC- MS analysis

Instruments and chromatographic conditions

Equipment and conditions for identification of metabolites from an active sub-fraction of methanol extract was carried out at SAIF, IIT, Powai, Bombay. 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 (Jadhao and Bhuktar, 2019).

Experimental Results:

In the present study we characterized chemical profile of smoke of medicinal cigarette prepared from *Curcuma longa* (rhizome), *Zingiber officinale* (Rhizome), *Ocimum tenuiflorum* (leaf) using HRMS spectra. The chromatogram showed relative concentrations of various compounds getting eluted as a function of retention time. The heights of peak indicate relative concentrations of components present in plantextract.

The mass spectrometer analyzes compounds eluted at different times to identify nature and structure of the compounds. The large compound fragments into small compounds giving rise to appearance of peaks at different m/z ratios. These mass spectra are fingerprint of that compound which can be identified from the data library. Compound prediction is based on Dr. Duke's Phytochemical and Ethnobotanical Databases.

Results revealed that presence of major abundant metabolites identified in herbal cigarette smoke extract fraction by ESI-QTOF-MS analysis were 2-Diethylaminoethanol, Daimuron, Pirimicarb, Artemisyl propionate, Oleandolide, (S)-Menthone 8-thioacetate, Valyl-Histidine, Naltrindole, Glutamyl-lysine, Eupatoroxin, Palmitic Acid and Stearic acid. The retention time, m/z value, mass, molecular formula and the DB difference (ppm) of the major 9 abundant metabolites are shown in table, the spectra showed counts versus mass to charge (m/z) ratio (Table 1).



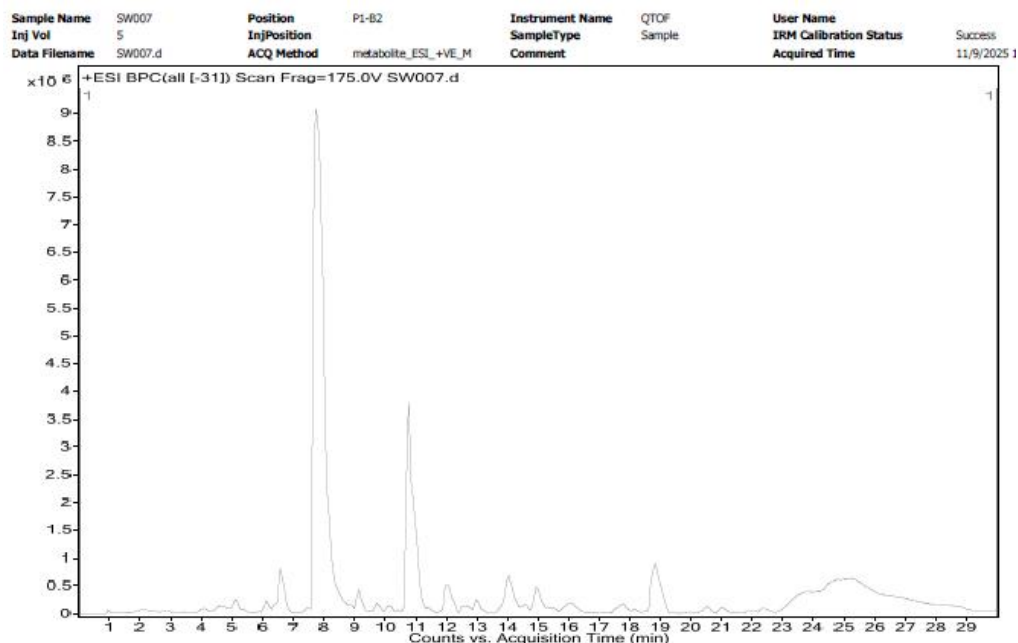


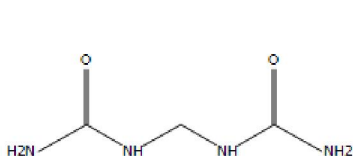
Fig. 1. HPLC-MS Chromatogram of medicinal cigarette smoke

Table no 1: List of secondary metabolites present in medicinal cigarette smoke

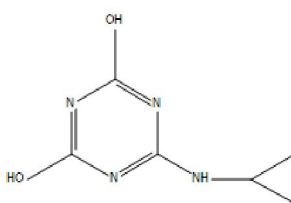
Sr. no.	Compound name	Mol. formula	RT	M/Z
1	Methylenediurea	C ₃ H ₈ N ₄ O ₂	2.279	133.0722
2	N-Cyclopropylammelide	C ₆ H ₈ N ₄ O ₂	4.493	169.0717
3	2-Diethylaminoethanol	C ₆ H ₁₅ N O	5.468	140.1033
4	10,11-Epoxy-3,7,11-trimethyl-2E,6E-tridecadienoic acid	C ₁₆ H ₂₆ O ₃	5.916	267.199
5	Deoxyguanidinoproclavaminic acid	C ₉ H ₁₆ N ₄ O ₃	6.213	229.1276
6	Seriny-Serine	C ₆ H ₁₂ N ₂ O ₅	6.374	193.0809
7	Daimuron	C ₁₇ H ₂₀ N ₂ O	6.674	269.1673
8	Pirimicarb	C ₁₁ H ₁₈ N ₄ O ₂	7.623	239.1472
9	Etonogestrel	C ₂₂ H ₂₈ O ₂	7.670	325.2204
10	3-Mercaptohexyl hexanoate	C ₁₂ H ₂₄ O ₂ S	7.711	233.1587
11	Artemisyl propionate	C ₁₃ H ₂₂ O ₂	8.574	233.1525
12	Altretamine	C ₉ H ₁₈ N ₆	8.887	233.1482
13	Oleandolide	C ₂₀ H ₃₄ O ₇	9.687	387.2338
14	Octadecanoic acid trichloroethyl ester	C ₂₀ H ₃₇ Cl ₃ O ₂	10.102	437.171
15	(S)-Menthone 8-thioacetate	C ₁₂ H ₂₀ O ₂ S	10.494	229.1268
16	(-)-Ormosanine	C ₂₀ H ₃₅ N ₃	10.899	318.2922
17	Valyl-Histidine	C ₁₁ H ₁₈ N ₄ O ₃	11.830	277.1254
18	Naltrindole	C ₂₆ H ₂₆ N ₂ O ₃	11.877	415.2018
19	Dimethindene	C ₂₀ H ₂₄ N ₂	13.452	293.2024
20	Valyl-Valine	C ₁₀ H ₂₀ N ₂ O ₃	13.769	217.1528



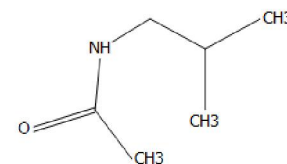
21	Glutamyl-lysine	$C_{11} H_{21} N_3 O_5$	14.412	298.1358
22	Gibberellin A39	$C_{20} H_{26} O_8$	17.237	417.1488
23	Eupatoroxin	$C_{20} H_{24} O_8$	17.528	415.1339
24	Saccharin	$C_7 H_5 N O_3 S$	2.979	181.9922
25	5-Methyl-2,5-di-1-pyrrolidinyl cyclopenten-1-one	$C_{14} H_{22} N_2 O$	9.341	233.1668
26	Antirhine	$C_{19} H_{24} N_2 O$	9.378	295.1835
27	Sodium Tetradecyl Sulfate	$C_{14} H_{30} O_4 S$	20.94	293.1806
28	Palmitic Acid	$C_{16} H_{32} O_2$	22.792	255.2347
29	Stearic acid	$C_{18} H_{36} O_2$	24.759	283.2653



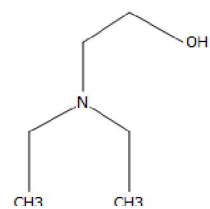
Methylenediurea



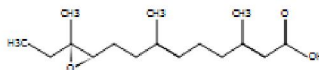
N-Cyclopropylammelide



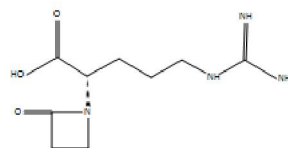
N-(2-Methylpropyl)acetamide



2-Diethylaminoethanol

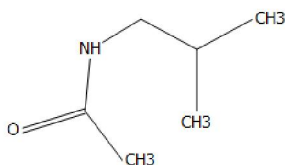


10,11-Epoxy-3,7,11-trimethyl-2E,6

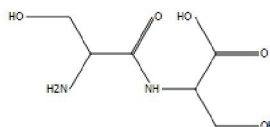


Deoxyguanidinoproclavaminic acid

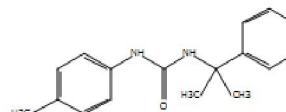
E-tridecadienoic acid



N-(2-Methylpropyl)acetamide

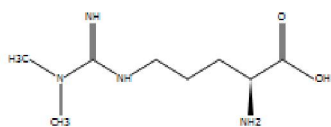


Serinyl-Serine

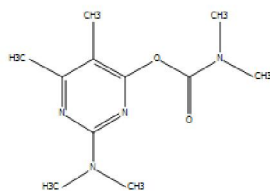


Daimuron

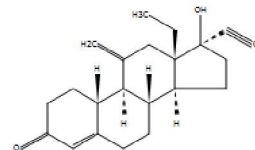




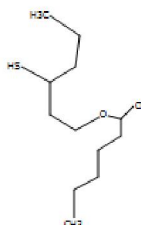
ADMA



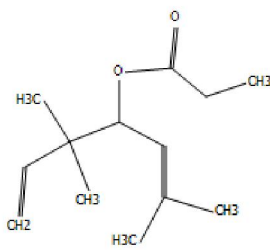
Pirimicarb



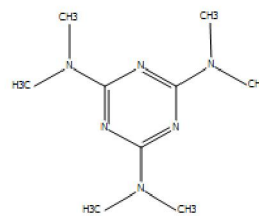
Etonogestrel



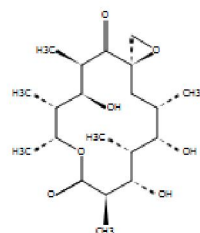
3-Mercaptohexyl hexanoate



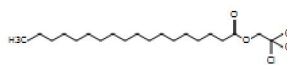
Artemisyl propionate



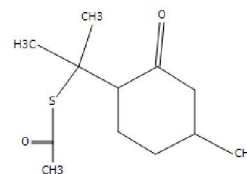
Altretamine



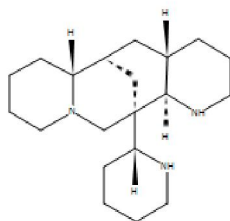
Oleandolide



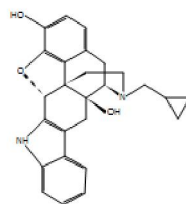
Octadecanoic acid trichloroethyl ester



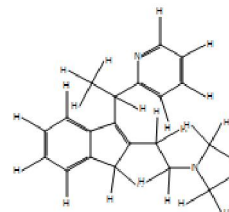
(S)-Menthone 8- thioacetate



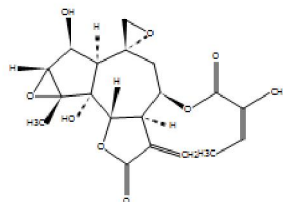
(-)-Ormosanine



Naltrindole



Dimethindene



Eupatoroxin



II. SUMMARY AND CONCLUSION

In the present study *Curcuma longa* (rhizome), *Zingiber officinale* (Rhizome), *Ocimum tenuiflorum* (leaf) used for preparation of herbal cigarette. Smoke of herbal cigarette screened by using HRLC-MS technique which revealed existence of various secondary metabolites viz., 2-Diethylaminoethanol, Daimuron, Pirimicarb, Artemisyl propionate, Oleandolide, (S)-Menthone 8-thioacetate, Valyl-Histidine, Naltrindole, Glutamyl-lysine, Eupatoroxin, Palmitic Acid and Stearic acid. Further study of these individual drugs is necessary which can be used in the treatment of different kinds of diseases.

III. ACKNOWLEDGEMENT

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