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Identification Of Phytochemical Compounds And Their Associated Medicinal Properties In Solanum Nigrum Fruit Extract Using Gas Chromatography-Mass Spectrometry

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ABSTRACT

Solanum nigrum, commonly known as black nightshade, is a plant species renowned for its diverse pharmacological properties due to the presence of various bioactive compounds. In this study, a comprehensive phytochemical analysis of *Solanum nigrum* fruit extract was conducted using Gas Chromatography-Mass Spectrometry (GC-MS) analysis. The extraction process was optimized to maximize the recovery of bioactive constituents. The GC-MS analysis revealed the presence of twenty-two major phytochemicals. The identified compounds were characterized based on their retention times and mass spectra. The findings of this study provide valuable insights into the chemical composition of *Solanum nigrum* fruit extract, which could serve as a foundation for further pharmacological investigations and the development of novel therapeutic agents.

KEYWORDS

Solanum nigrum, phytochemicals, GCMS analysis**,**

1. INTRODUCTION

Since the dawn of civilization on Earth, humanity has relied on plants as medicinal agents. Over 80% of the population in developing nations depends on plants as therapeutic remedies (Uddin et al, 2018, Huq et al, 2016).

Numerous studies indicate that approximately 20% of synthetic medicines prescribed globally are derived from plant origins. In the contemporary world, there is a growing demand for therapeutics sourced from plants as drug developers seek to minimize side effects, toxicity, and abuse associated with established synthetic medications (Das et al, 2019; Rates, 2001).

Solanum nigrum (Black nightshade/ blackberry nightshade) is a member of the Solanaceae family, which includes various genera renowned for their medicinal properties. (Sivaraj et al, 2020; Acharya and Pokhrel, 2006; Ge˛barowska et al, 2022).

The fruit and flower of *S. nigrum* are as remedies for diuretic issues, bronchitis, and pulmonary tuberculosis (Zahara et al, 2019); hydrophobia, convulsions, ophthalmopathy, and as an antidiarrheal agent (Hameed et al, 2018). Furthermore, it has been shown to be effective in reducing the risk of heart disease, particularly in treating cardiopathy, nephropathy, leprosy, dropsy, hemorrhoids, ophthalmopathy, and general debility (Mehmood et al, 2021; Kunwar et al, 2021; Campisi et al, 2019; Zakaria et al, 2006).

Solanum nigrum contains a rich array of natural compounds with diverse structural patterns and beneficial properties. Researchers have identified approximately 188 phytochemical compounds within this plant species. These compounds include steroids, alkaloids, organic acids, flavonoids, phenylpropanoids, their glycosides, and various other bioactive substances. (Chen 2022**,** Jain et al, 2011, Gogoi et al, 2012)

The vast array of natural products, including plant extracts available in pure form or standardized extracts, offers immense potential for discovering new drugs due to their unparalleled chemical diversity. However, determining the therapeutic effects of herbs or herbal extracts requires identifying their active ingredients or cofactors (**Prasath** et al, **2016)**

Gas chromatography mass spectrometry (GC-MS) has been extensively developed and acknowledged as a crucial technique for systematically profiling metabolites from plants (Mutale et al, 2020; Sivaraj et al, 2020). Its application is significant in conducting chemotaxonomic studies and phytochemical analyses of medicinal plants containing biologically active components (Shaheen and Ahmed, 2020).

In the present investigation, the GC-MS technique was employed to analyze and identify the phytoconstituents present in the fruit extracts of Solanum nigrum, with the aim of isolating potentially effective components.

2. Materials and Methods

2.1 Collection and Preparation of plant material

The fruits of *Solanum nigrum* were collected from Jabalpur district, central India (Figure 1). Collected Solanum *nigrum* fruits were washed, shade dried and powdered using mechanical blender. the powder was stored in air tight plastic container for the future evaluation with proper labelling.

2.2 Preparation of plant extract

The organic solvent extract of the plant was prepared following the method proposed by Ladd Jr. and Jacobson. Methanol was chosen as the polar solvent for extraction. Dry powders of the plant's fruits were weighed (10 g) and placed in a Soxhlet extractor by making thimble. A ratio of 75/75 mL methanol/water was added to each, and the extraction was conducted for 48 hours at 80°C. This process was repeated several times to obtain the required quantity for the experiment. To estimate GC-MS, the prepared extract was filtered and centrifuged twice for 10 minutes at 10,000 rpm. After the second filtration, 3 mL of the filtered extract was transferred into a GC-MS analysis vial.

2.3 GC-MS analysis:

GC-MS analysis of plant extracts was performed using Shimadzu GC-MS-QP 2020 Japan, a non-polar capillary column VF-5MS (30 m × 0.25 mm i.d., coating thickness 0.25 μm) and a polar capillary column CP-Wax 52 (30 m × 0.25 mm i.d., coating thickness 0.25 μm). Chromatographic conditions were as follows: helium was the carrier gas at 1 mL·min−1, injector temperature was 250ºC. Column temperature was programmed at 50ºC isothermal for 2 min, and then increased to 250ºC at a rate of 20 ºC min hold time 5 min and then increased to 300ºC at a rate of 20 ºC min held for 10 min. Total GC Running time was 32 min. The injected volume was 1 μL and the split ratio was 1:10. Mass spectrometry (MS) conditions were: ionization voltage 70 eV; ion source temperature 230ºC; interface temperature of 280°C; mass scan range: 45–450 mass units and solvent cut time is 3 min.

Figure 1: Medically important fruits of *Solanum nigrum*

3. Results and Discussions

In a current investigation bioactive compounds extracted from the fruit of *S. nigrum* were examined and identified using GC-MS (Gas Chromatography-Mass Spectrometry) analysis.

The GC-MS analysis reveiled the presence of 22 bioactive compounds in the extract fruit of S. nigrum and tabulated with the IUPAC names of compound, molecular formula and molecular weight (Table 1 and Figure 2).

Noteworthy compounds identified encompassed Amobarbital, Catechol, Campesterol, Carbromal, Dipentaerythritol, Digitoxigenin, dimethyl-Crotonic acid, Gitoxigenin, Heptanoic acid, hexadecyl- Maprotiline, Hydroquinone, Lupeol, Mequinol, Nordazepam, Octacosanol, Oleic Acid, Oxirane, Phloroglucitol, Pantolactone, Silanediol, 2TMS derivative, Scopoletin, and Uvaol in the in-fruit extract of *S. nigrum*.

The bioactive compounds Scopoletin and Oleic acid , identified in the present study were also reported from the *Solanum nigrum* extract in the investigations done by Zhao (2010), and Wang et al, (2007).

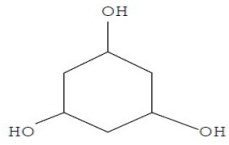
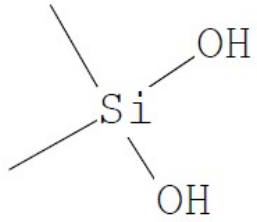
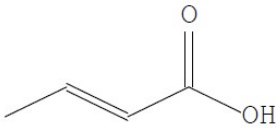
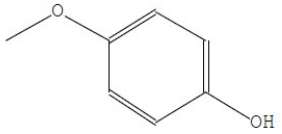
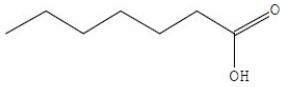
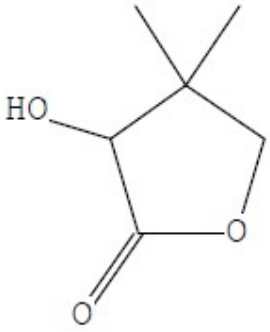
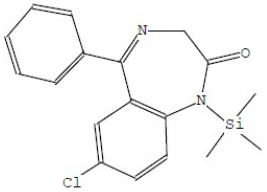
GC-MS analysis of ethanolic plant extract obtained from plants *Solanum nigrum* revealed major phytochemical compounds belong to different classes such as steroids, acid, phytosterols, alkaloids, ketones, ester including Oxetane, 3-(1methylethyl), 2 Hexadecen-1-ol,3,7,11,15-Tetramethyl, Vitamin E, hexadecanoic acid, ethyl ester, Ergost-5-EN-3-ol and 2-Acetyl-2-hydroxy, gamma-butyrol acetone (Revathi et al, 2014, Parveen et al, 2016).

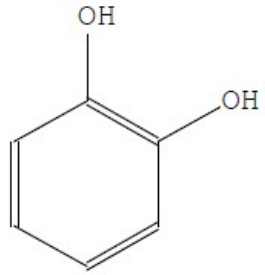
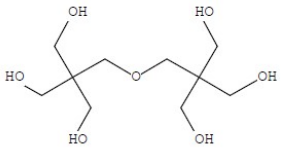
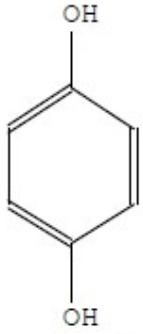
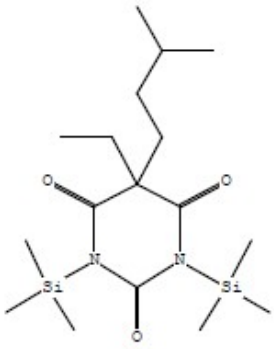
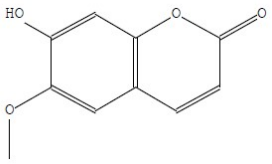
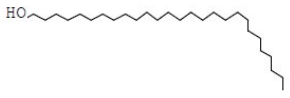
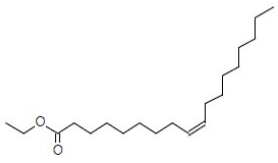
All the twenty-two Phyto-compounds identified in the GCMS analysis of *Solanum nigrum* fruit extract exhibits important medicinal Properties (Table 2). The majority of the compounds identified have been documented for their antibacterial,

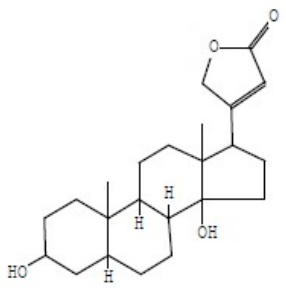
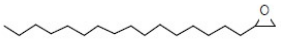
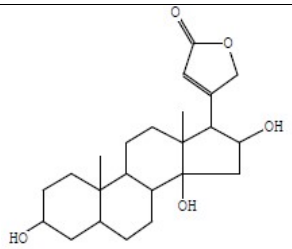
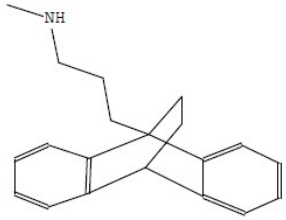
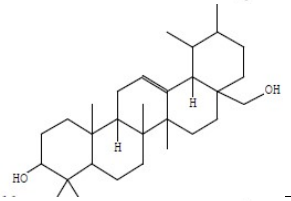
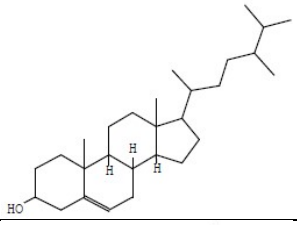
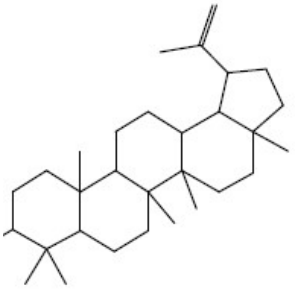
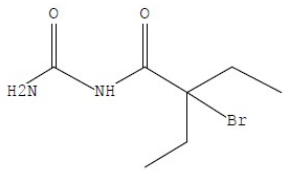
antifungal, antioxidant, and antiviral properties making them beneficial in treating skin infections (Jasmin et al, 2015; Meng et al, 2020; Santhanaraj et al, 2016; Rautela *et al* 2018; Soosairaj et al, 2016; Ertas et al, 2014).

Traditionally, *Solanum nigrum* plant extract has been utilized for treating liver cirrhosis and as an antidote for opium poisoning (Karuppasamy et al, 2016; Dhar et al, 1968). However, these berries are known for their effectiveness in combating heart diseases and have tonic, diuretic, and cathartic qualities (Gowdhami et al, 2014, Bhatia et al, 2011; Son et al, 2003).

Table 1: Phyto-compounds present in Methanolic extract of *Solanum nigrum* using GC-MS Profiling.

S. No	R. Time	F. Time	Compound Names	Molecular Weight	Structure
1	3.435	3.485	Phloroglucitol	132	
2	3.19	3.26	Silanediol, dimethyl-	92	
3	3.94	3.96	Crotonic acid	86	
4	4.995	5.02	Mequinol	124	
5	5.17	5.25	Heptanoic acid	130	
6	5.84	5.86	Pantolactone	130	
7	6.55	6.585	Nordazepam	342	

8	6.665	6.705	Catechol	110	
9	6.915	6.94	Dipentaerythritol	254	
10	7.535	7.565	Hydroquinone	110	
11	8.805	8.83	Amobarbital, 2TMS derivative	370	
12	12.3	12.335	Scopoletin	192	
13	12.355	12.375	Octacosanol	410	
14	13.25	13.325	Oleic Acid	310	

15	14.085	14.15	Digitoxigenin	374	
16	17.32	17.39	Oxirane, hexadecyl-	268	
17	19.655	19.69	Gitoxigenin	390	
18	20.305	20.335	Maprotiline	277	
19	21.825	22	Uvaol	442	
20	22.77	22.81	Campesterol	400	
21	26.875	26.97	Lupeol	426	
22	29.07	29.155	Carbromal	236	

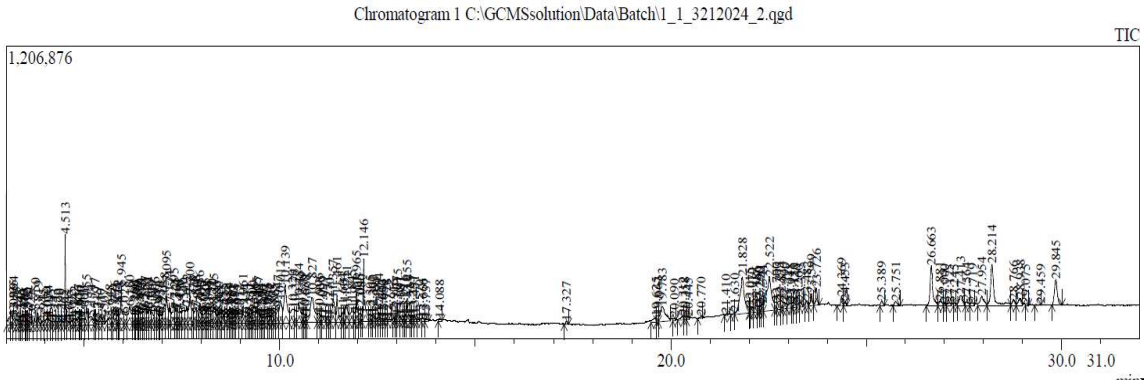


Figure 2: GC-MS Chromatogram of Methanolic leaf extract of selected Plant parts.

Table 2: Medicinal Properties of Phyto-compounds present in *Solanum nigrum*

S. No	R. Time	Compound Names	Medicinal properties
1	3.435	Phloroglucitol	Symptomatic treatment of painful manifestations in gastrointestinal tract, biliary tract, urinary tract, and uterine pain
2	3.19	Silanediol,	Bactericidal, Antimicrobial, HIV protease inhibitor,
3	3.94	Crotonic acid	Antimicrobial and antiscabies
4	4.995	Mequinol	Skin lesion and infections
5	5.17	Heptanoic acid	Anti-cholesterol agent
6	5.84	Pantolactone	Skin care
7	6.55	Nordazepam	anticonvulsant, anxiolytic, muscle relaxant and sedative properties
8	6.665	Catechol	Treatment of bradycardia and heart block
9	6.915	Dipentaerythritol	Hair care and Antioxidant
10	7.535	Hydroquinone	Dyschromia
11	8.805	Amobarbital, 2TMS derivative	Anxiety, Insomnia
12	12.3	Scopoletin	Cancer, liver disease, diabetes, neurodegenerative disease, and mental disorders
13	12.355	Octacosanol	anti-fatigue
14	13.25	Oleic Acid	Heart disease and reducing cholesterol
15	14.085	Digitoxigenin	Treating congestive heart failure and cardiac arrhythmias
16	17.32	Oxirane, hexadecyl-	Anticancer, Antimicrobial
17	19.655	Gitoxigenin	congestive heart failure and atrial arrhythmia
18	20.305	Maprotiline	depressive disorder, Mania
19	21.825	Uvaol	anti-inflammatory and antioxidant
20	22.77	Campesterol	Cholesterol lowering and Anticancer
21	26.875	Lupeol	Anti-inflammatory, antioxidant, anticancer, antimicrobial
22	29.07	Carbromal	Antianxiety and Insomnia

4. Conclusion

In conclusion, the phytochemical analysis of *Solanum nigrum* fruit extract using GC-MS analysis has revealed a rich diversity of 22 bioactive compounds with potential pharmacological significance. The presence of alkaloids, flavonoids, phenolic compounds, terpenoids, and fatty acids underscores the medicinal importance of this plant species. These compounds possess various biological activities, including antioxidant, anti-inflammatory, antimicrobial, and anticancer properties, which align with the traditional uses of *Solanum nigrum* in folk medicine. The identification and characterization of these phytochemicals provide a scientific basis for understanding the therapeutic potential of *Solanum nigrum* fruit extract and support its further exploration for the development of new pharmaceuticals and nutraceuticals. Moreover, the findings of this study contribute to the growing body of knowledge on natural products and their applications in medicine and healthcare. Further research aimed at elucidating the mechanisms of action and conducting preclinical and clinical studies are warranted to fully harness the therapeutic benefits of *Solanum nigrum* fruit extract.

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