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Essential Oil Profile of Areal Part of *Datura stramonium* L. and *D. innoxia* from Iran

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ABSTRACT

The chemical constituents of essential oils of *Datura stramonium* L. and *D. innoxia* (family Solanaceae) are being reported. In this study, the collected seeds of Ardabil and Urmia were planted in grow bags and placed for three months in a greenhouse of the College of Agriculture, Tarbiat Modares University in Tehran. Under greenhouse conditions, the average air temperature was 25 °C. Air-dried areal parts of *D. stramonium* and *D. innoxia* were prepared and their essential oils (EOs) were isolated by hydrodistillation for 3 h in a Clevenger-type apparatus. EOs content and composition were examined with gas chromatography techniques. The EOs yield of *D. stramonium* and *D. innoxia* were 0.03% and 0.02% (v/w), respectively. The major compounds in the *D. stramonium* EOs were Camphor (29.9%), Selin-11-en-4alpha-ol (13.0%), and Borneol (10.4%). Those in the *D. innoxia* were mostly fatty alkanes, including *n*-Decane (19.99%), 7-Pentadecyne (11.78%), and Linoleic acid (6.13%). The other important components identified in the EOs of *Datura* were Dihydrocitronellol, *n*-Dodecane, Isobornyl acetate, Germacrene D, and *n*-Tetradecane. Generally, the EOs of the areal parts in *D. stramonium* showed oxygenated monoterpenes.

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1. Introduction

Traditionally, plants are used to treat various diseases. According to World Health Organization, medicinal plants are the best source for obtaining a variety of drugs (Jaber *et al.*, 2019). The use of medicinal and aromatic plants as traditional sources of medicinal drugs has a long history (Nazir *et al.*, 2021). Volatile compounds of medicinal plants have different ethnopharmacological applications and are also used in food flavoring and perfume industries (Memarzadeh *et al.*, 2020). In fact, herbal products are natural and have healthy properties (Hosseini *et al.*, 2018). The genus *Datura*, family Solanaceae, is consisted of 13 species, originating from America and found as invasive plants in most subtropical regions of the world (Papagrigoriou *et al.*, 2019). All Datura plants contain atropane alkaloids such as scopolamine, hyoscyamine and atropine, primarily in their seeds and flowers (Cinelli and Jones, 2021). *Datura* species have a lot of variability in the morphology, i.e., leaf shape, flower and stem color, and seed morphology (Partap *et al.*, 2019). *Datura stramonium* and *Datura innoxia* are important species of *Datura* genus with several uses in folk medicine (Al-Zharani *et al.*, 2021; Batool *et al.*, 2020). *D. stramonium* commonly known as Jimson is an annual plant. Its height is 60-120 cm, leaves are hairy, ovate and pale green while the stem is herbaceous, branched, glabrous, and lightly hairy (Sharma *et al.*, 2021). It has traditional medicinal applications (Nasir *et al.*, 2022), such as anti-inflammatory, analgesic, anti-diarrheal, larvicidal, pesticidal toxicity, antifungal, and anticonvulsant (Kadam *et al.*, 2018). It is also used in the treatment of epilepsy and asthma (Mohammed *et al.*, 2021). *D. stramonium* contains different types of alkaloids, including atropine, hyoscyamine and scopolamine,

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tigloidin, aposcopolamine, apoatropine and N-oxide (Batool *et al.*, 2020). *D. innoxia* is an annual plant and its stem and leaves are vegetal, big and pale green (Chamani *et al.*, 2020). *D. innoxia* is present as both cultivated as a medicinal plant and as a wild population (Benabderrahim *et al.*, 2019). *D. innoxia* is used in folk medicine to treat skin eruptions, colds, and nervous disorders (Al-Zharani *et al.*, 2021). Also, several curative purposes for *D. innoxia* have been reported, such as pacifying, antispasmodic, pain relief, and treating respiratory ailments (Gajendran *et al.*, 2019). Saponins, tannins, steroids, alkaloids, flavonoids, phenols and glycosides have been identified as major and important components of both *D. stramonium* and *D. innoxia* (Al-Zharani *et al.*, 2021; Avila *et al.*, 2023). The phytochemical components isolated from *D. stramonium* such as daturaolone, daturadiol, stigmasterol and sitosterol were shown to possess considerable immunostimulatory activity (Gupta *et al.*, 2016).

D. stramonium oil exhibited in vitro scavenging potential of free radicals by DPPH and ABTS assays (IC_{50} values 71.3 µg/ml and 61.0 µg/ml, respectively. Also, the treatment of human lymphocytes by *D. stramonium* oil enhanced their ability to kill colon cancer cells (Chandan *et al.*, 2020). There are only a few reports about the volatile constitutions of *D. stramonium* growing in Iran. Few studies have been carried out on the chemical composition of *D. stramonium* essential oils mostly of the leaves and seeds (Papagrigoriou *et al.*, 2019). Studies of volatile oils from *D. stramonium* leaves and have already been reported (Chandan *et al.*, 2020). The major constituents of the leaves oil of *D. stramonium*, collected from Solan (India) were phytol acetate (10.76%), β-damascenone (9.67%), and β-eudesmol (7.2%) (Chandan *et al.*, 2020). Citral (26.5%), 4,8-dimethyl-3,8-dien-2-one (11.2%), sesquirosefuran (11.1%), and geraniol (10.5%) were the major components in the essential oil of seeds (Aboluwodi *et al.*, 2017). A previous study on essential oils of *D. stramonium* from China showed 5.alpha.-Ergosta-7,22-dien-3.beta.-ol (16.53%), 3-Hydroxycholestan-5-yl, acetate (14.97%), and 26,26-Dimethyl-5,24(28)-ergostadien-3.beta.-ol (10.39%) (You and Wang, 2011). Despite *D. stramonium*, there are no reports about the volatile components of the *D. innoxia*. The study on essential oils of *Datura metel* has been reported the main components of leaves were ketone (18.84%) and phytol (18.71%). Ketone (39.45%) and phytol (31.32%) were the major components of petioles. Palmitic acid (30.60%) and ethyl linoleate (21.56%) were the major components of seeds. The major ingredient of roots was palmitic acid (52.61%). The main ingredients of the stems were palmitic acid (38.38%) and ethyl linoleate (17.38%) (Xue *et al.*, 2016). In fact, it is the first time that a study is conducted on *D. innoxia* essential oil. The phytochemicals of medicinal plants depend on various factors such as climatic conditions, genetic variations, collection period and others which increase the study of available plants in different growing sites, countries and geographical zones (Norani *et al.*, 2023). The aim of the present study was to report the chemical constituents identified in the essential oils of the areal part of *D. stramonium* from Ardabil and *D. innoxia* from Urmia as well as comparison of components identified in two species from different regions.

2. Materials and methods

2.1. Seed collection site

Mature seeds were collected during the late November of 2021, from plants of *Datura stramonium* growing in Ardabil (38º 22′ 08″ N, 48º 15′ 49″ E) and *D. innoxia* growing in Urmia (37º 42′ 18″ N, 45º 04′ 13″ E) of Iran (Table 1).

Table 1. Locality characteristics of *D. stramonium* and *D. innoxia*

Specie	Local Collection locations	Longitude (E)	Latitude (N)	Altitude (m a.s.l.)*
Datura stramonium	Ardabil, Iran	48°15'49"	38°22'07"	1332
Datura innoxia	Urmia, Iran	45°04'13"	37°42'18"	1800

* Meters above sea level

2.2. Plant materials

For this study, the collected seeds were planted in grow bags with 10 kg soil (sandy loam) and placed for three months in the Greenhouse of the Agricultural Faculty of Tarbiat Modares University, Tehran, Iran. Under greenhouse conditions, the average air temperature was 25°C. The areal parts of *D. stramonium* and *D. innoxia* were collected and dried for the next step.

2.3. Extraction and analysis of essential oil

About 50 grams air-dried of areal part of *D. stramonium* and *D. innoxia* including leaves, stems, and seeds were prepared in three replications to grind into powders for each sample. All samples immersed in 500 mL of distilled water and the essential oils (EOs) was isolated by hydrodistillation for 3 h in a Clevenger-type apparatus. The EOs were separated from the water and dried over anhydrous sodium sulfate and stored at 4 °C until analysis. Gas chromatography (GC) analysis was performed, using an Agilent Technologies 7890B (Santa Clara, CA, USA) with a flame ionization detector. The instrument was equipped with an HP-5 fused silica column (length 30 m, inner diameter 0.32 mm and film thickness 0.25 µm) and helium was used as the carrier gas at a flow rate of 1.0 mL/minute. The qualification of individual peaks was carried out by injecting the oil into Thermoquest-Finnigan gas chromatography, coupled with a trace mass spectrometer (GC/MS) with the same parameter for fused silica column (except for the inner diameter of 0.25 mm), oven temperature, injector temperature, carrier gas, and flow rate. The ionization voltage was 70 eV. Ion source and interface temperatures were 200°C and 250°C, respectively. Identification was confirmed by comparison of each component's mass spectra with those of the internal mass spectra library of the main library, Wiley 7.0 and Adams and further identification was based on the comparison of peak retention indices by using a homologous series (C8 to C24) recorded under the same operating conditions and the published data (Adams, 2007). Identification was confirmed by comparison of each component's mass spectra with those of the internal mass spectra library of the main library, Wiley 7.0 and Adams and further identification was based on a comparison of peak retention indices by using a homologous series (C8 to C24) recorded under the same operating conditions and the published data.

3. Results and discussion

The yield of areal parts essential oil in *D. stramonium* and *D. innoxia* was 0.03% and 0.02 (v/w), respectively, which are in agreement with the previous report of Aboluwodi et al. (2017). Forty-one compounds comprising 95.06% of the oil were identified in the areal parts of *D. stramonium* (Table 2, Figure 1-A). Camphor, Selin-11-en-4alpha-ol and borneol were the major compounds in oil with amounts of 29.9%, 13.0%, and 10.4%, respectively. The other important components identified in the EO of *D. stramonium* were Dihydrocitronellol (2.9%), *n*-Dodecane (2.7%), Isobornyl acetate (7.8%), Germacrene D (2.6%), and *n*-Tetradecane (2.6%).

Table 2. Chemical composition (%) of areal parts essential oils of *Datura stramonium*

No.	RT	Components	Molecular formulae	%	RI*
1	7.7	Dihydrocitronellol	$C_{10}H_{20}O$	2.9	930
2	8.7	α-Pinene	$C_{10}H_{16}$	1.44	932
3	9.6	1,8-Cineole	$C_{10}H_{18}O$	1.95	1026
4	11.6	*n*-Undecane	$C_{11}H_{24}$	1.29	1100
5	13.1	Camphor	$C_{10}H_{16}O$	29.9	1141
6	13.7	Borneol	$C_{10}H_{18}O$	10.4	1175
7	13.9	2-Nonen-4-one	$C_9H_{16}O$	0.48	-
8	14.2	*n*-Dodecane	$C_{12}H_{26}$	2.7	1200
9	14.7	4,8-Dimethylnona-3,8-dien-2-one	$C_{11}H_{18}O$	0.26	1240
10	15.0	Citral	$C_{10}H_{16}O$	0.11	1249
11	16.8	Isobornyl acetate	$C_{12}H_{20}O$	7.8	1283
12	16.9	*n*-Tridecane	$C_{13}H_{28}$	0.87	1300
13	18.0	Nonanoic acid	$C_9H_{18}O_2$	0.45	1308
14	18.7	α-Copaene	$C_{15}H_{24}$	0.49	1374
15	18.8	Geranyl acetate	$C_{12}H_{20}O_2$	0.47	1387
16	19.0	2,3,3,4,5-pentaethyl 1,2,5-Oxadiborolane	$C_{10}H_{20}$	0.73	-
17	19.5	*n*-Tetradecane	$C_{14}H_{30}$	2.56	1400
18	19.8	Isobornyl isobutanoate	$C_{14}H_{24}O_2$	0.62	1410
19	20.1	(*E*)- Caryophyllene	$C_{15}H_{24}$	0.77	1441
20	20.4	(*E*)-β-Farnesene	$C_{15}H_{24}$	0.26	1454
21	21.7	Germacrene D	$C_{15}H_{24}$	2.56	1484
22	21.8	β-selinene	$C_{15}H_{24}$	1.23	1489
23	22.0	Bicyclogermacrene	$C_{15}H_{24}$	0.57	1500
24	22.2	Isobornyl isovalerate	$C_{15}H_{26}O_2$	0.87	1521
25	22.4	Isobornyl 2-methyl butanoate	$C_{15}H_{26}O_2$	2.15	1523
26	23.3	Spathulenol	$C_{15}H_{24}O$	0.25	1577
27	24.0	Caryophyllene oxide	$C_{15}H_{24}O$	0.67	1582
28	24.2	*n*-Hexadecane	$C_{16}H_{34}$	2.6	1600
29	24.5	α-Muurolol	$C_{15}H_{26}O$	0.71	1644
30	25.0	β-Eudesmol	$C_{15}H_{26}O$	0.12	1649
31	25.8	Selin-11-en-4alpha-ol	$C_{15}H_{26}O$	13.0	1660
32	26.1	Valeranone	$C_{15}H_{26}O$	1.22	1674
33	28.4	Octadecene	$C_{18}H_{36}$	1.13	1789
34	29.6	6,10,14-Trimethylpentadecan-2-one	$C_{18}H_{36}O$	0.7	1842
35	30.0	2-Pentadecanone, 6,10,14-trimethyl	$C_{18}H_{36}O$	0.25	1847
36	30.2	(*E*)-En-yn-dicycloether	$C_{13}H_{12}O_2$	1.15	1902
37	30.6	*m*-Camphorene	$C_{20}H_{32}$	0.13	1960
38	31.6	Hexadecanoic acid	$C_{16}H_{32}O$	0.53	1961
39	32.3	*n*-Eicosane	$C_{20}H_{42}$	0.51	2000
40	35.0	(*E*)-Phytyl acetate	$C_{22}H_{42}O_2$	0.97	2218
41	35.8	Docosane	$C_{22}H_{46}$	0.12	2200
		Total compounds		95.06	-

* RI: retention indices according to the normal alkanes between C8-C24

In areal parts of *D. innoxia*, about 28 components, containing 78.9% of oil were obtained (Table 3, Figure

1-B). The number of compounds identified in the essential oil of *D. stramonium* was significantly lower than that of the essential oil of *D. innoxia*. The important components identified in the EO of *D. innoxia* were mostly fatty alkanes, including *n*-Decane (19.99%), 7-Pentadecyne (11.78%), and Linoleic acid (6.13%). This is the first report about volatile compounds in *D. innoxia*.

Table 3. Chemical composition (%) of areal parts essential oils of *Datura innoxia*

No.	RT	Components	Molecular formulae	%	RI*
1	8.7	3,3-Dimethyl-2-pentanol	$C_7H_{16}O$	1.46	880
2	9.8	*n*-Nonane	C_9H_{20}	1.68	900
3	11.3	tetrahydro Citronellene	$C_{10}H_{22}O$	1.12	930
4	12.2	*n*-Decane	$C_{10}H_{22}$	19.99	1000
5	13.3	α-Terpineol	$C_{10}H_{18}O$	1.88	1189
6	14.3	*n*-Dodecane	$C_{12}H_{26}$	2.81	1200
7	16.7	2-nitrophenyl azide	$C_6H_4N_4O_2$	4.58	-
8	16.9	*n*-Tridecane	$C_{13}H_{28}$	0.98	1300
9	18.7	Cyclopropaneoctanal	$C_{11}H_{20}O$	1.84	-
10	18.8	2,3,3,4,5-pentaethyl 1,2,5-Oxadiborolane	$C_{10}H_{20}$	0.43	-
11	19.5	*n*-Tetradecane	$C_{14}H_{30}$	2.72	1400
12	21.6	9,17-Octadecadienal	$C_{18}H_{32}O$	1.22	-
13	21.7	1,19-Eicosadiene	$C_{20}H_{38}$	1.94	-
14	21.9	Heneicosyl formate	$C_{22}H_{44}O_2$	0.35	-
15	22.21	Linoleic acid	$C_{18}H_{32}O_2$	6.13	-
16	22.4	8-Tetradecen-1-ol	$C_{16}H_{32}O_3$	6.38	-
17	23.5	2,10-dimethyl-9-Undecenal	$C_{13}H_{24}O$	0.66	-
18	24.2	*n*-Hexadecane	$C_{16}H_{34}$	2.63	1600
19	25.5	3,5-Dihydroxybenzoic acid	$C_7H_6O_4$	2.14	1617
20	25.6	7-Pentadecyne	$C_{15}H_{30}$	11.78	-
21	27.4	Monoelaidin	$C_{21}H_{40}O_4$	0.34	-
22	28.4	*n*-Octadecane	$C_{18}H_{38}$	1.18	1800
23	29.3	6,10,14-Trimethy-2-pentadecanone	$C_{18}H_{36}O$	1.46	1847
24	29.9	(2*E*,6*E*)-Farnesyl acetate	$C_{17}H_{28}O_2$	0.93	1854
25	31.6	*m*-Camphorene	C_{20} H_{32}	1.6	1960
26	32.3	Oleic acid	$C_{18}H_{34}O_2$	0.53	2171
27	35.8	Octadecanoic acid	$C_{18}H_{36}O$	0.14	2179
-	-	Total compounds		78.9	-

* RI: retention indices according to the normal alkanes between C8-C24

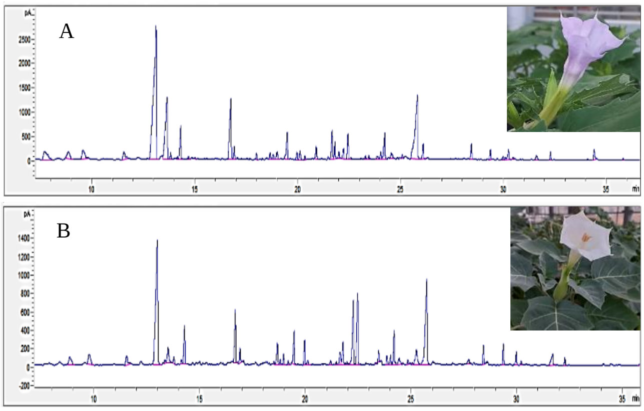

Figure 1. GC profile of essential oil from areal part of *D. stramonium* (A) and *D. innoxia* (B)

The result of this study showed there are significant differences between the compounds identified in the oil profiles of *D. stramonium* and *D. innoxia*. The reasons for these differences can be many factors such as genetic diversity, soils, position and time of sampling of seeds, insect and microorganism stress and other geological and environmental conditions (Heydari *et al*., 2022; Mirniyam *et al*., 2022; Yan *et al*., 2023). In previous study, GC-MS analysis of ethanolic extract for aerial parts of D. innoxia displayed that 3,5-Dihydroxybenzoic acid (16.53%), heneicosyl formate (14.14%), 2,3-dimethyl-3-pentanol (12.89%), 2-hydroxy-4-methyl pentanoic acid (5.19%) were the main phytoconstituents (Al-Zharani *et al*., 2021). Aboluwodi et al. (2017) reported that the main classes of compounds found in the leaf's oil of *D. stramonium* were diterpenes (74.8%) and oxygenated monoterpenes (10.4%). Also, oxygenated monoterpenes (41.4%), oxygenated sesquiterpenes (28.0%), and aliphatic ketones (13.9%) were the main classes of compounds present in the seed oil. Phytol (72.5%) was identified as the main component of the leaf's oil (Aboluwodi *et al*., 2017). However, in previous phytochemical studies on the Essential oils, sterols (Srivastava and Srivastava, 2020), aromatic compounds (Zhenguo *et al*., 2010), and fatty acids (Valiyeva *et al*., 2022) have been identified as the main dominant volatile compounds of *D. stramonium*. The seed oil of *D. stramonium* contained higher concentrations of phytate, tannin and oxalate (Batool *et al*., 2020). In a study on chemical constituents of the leaf, floral and fruit volatile oils of *Datura metel*, monoterpenoids were the dominant class of compounds in the leaf oil (100%), flower oil (81.4%) and fruit oils (58.8%), also α-phellandrene (38.3%), p-cymene (28.0%) and 1,8-cineole (12.4%) in the leaves; linalool (62.9%) and (E, E)-farnesol (11.1%) in the flowers; and p-cymene (31.4%), 1, 8-cineole (23.3%) and valerenal (9.4%) in the fruits were characterized as a main compounds (Essien *et al*., 2010). The essential oil and aqueous saturated solution of *D. stramonium* significantly inhibited the germination and growth of some plant such as *Amaranthus retroflexus* L., *Chenopodium album* L., and *Beta vulgaris* L. (Yorulmaz and Özkan, 2020). Monoterpenoid derivatives such as camphor and borneol have been extensively studied as therapeutic agents against the proliferation of cancer cells, for treating neurodegenerative disorders, and against virus replication and bacterial infections (Salakhutdinov *et al.*, 2017). In the previous study on camphor and borneol derivatives, were reported to be inhibitors of the influenza virus, filoviruses and orthopoxviruses (Sokolova *et al.*, 2021). Li et al. (2022) revealed that borneol applied a protective effect in PTZ-induced convulsions in mice. Camphor and borneol as a volatile component, was found to increase GABA concentration in PTZ induced convulsion animal model specially by affecting GABAA receptor (Karampour *et al.*, 2018). Phytochemical assessment is one of the substantial tools for quality evaluation which includes preliminary phytochemical screening and chemo profiling (Partap *et al.*, 2019). Generally, essential oils of *D. stramonium* have been mostly reported as oxygenated monoterpenes and diterpenes (Aboluwodi *et al.*, 2017). The comparison of volatile compounds of *D. stramonium* and *D. innoxia* showed that there is a significant difference in of phytochemical constituents.

4. Conclusion

In conclusion, *D. stramonium* and *D. innoxia* have relatively low yields of EO in areal plants. We have presented herein the first report on the volatile compounds of *D. stramonium* and *D. innoxia* growing in Ardabil and Urmia, Iran. In the aerial parts oil of *D. stramonium*, monoterpenes predominated over sesquiterpenes. The comparison of volatile compounds of *D. stramonium* and *D. innoxia* showed that there is a significant difference in phytochemical constituents.

Conflict of Interests

All authors have to declare their conflicts of interest.

Ethics approval and consent to participate

No human or animals were used in the present research.

Consent for publications

All authors read and approved the final manuscript for publication.

Availability of data and material

All the data are embedded in the manuscript.

Authors' contributions

All authors had an equal role in study design, work, statistical analysis and manuscript writing.

Informed Consent

The authors declare not to use any patients in this research.

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