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Nine new tropane alkaloids from *Datura stramonium* L. identified by GC/MS

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ABSTRACT

Sixty seven tropane alkaloids were identified in the organs of *Datura stramonium* L. by GC/MS. Nine new tropane alkaloids, 3,7-dihydroxy-6-propionyloxytropane, 6,7-dehydro-3-tigloyloxytropane, 3-tigloyloxy-6,7-epoxytropane, 3,7-dihydroxy-6-(2′-methylbutyryloxy)tropane, 6,7-dehydroapoatropine, 3-(3′-methoxytropoyloxy)tropane, 3-tigloyloxy-6-isobutyryloxy-7-hydroxytropane, 3-tropoyloxy-6-isobutyryloxytropane, 3β-tropoyloxy-6β-isovaleroyloxytropane were tentatively identified. The alkaloids cyclotropine, dihydroaposcopolamine, 6,7-dehydrohyoscyamine and 4′-hydroxylittorine are reported for the first time for the genus *Datura* and 6,7-dehydrotropine for the family Solanaceae. Hyoscyamine and scopolamine figure as the major tropane alkaloids in the plant organs.

1. Introduction

Datura stramonium L. (Solanaceae) is a plant species distributed throughout most parts of temperate regions of the world [1] and is a noxious weed of cultivated cereal crops [2]. This herbaceous annual is an erect plant, with dark green leaves, white flowers and spiny capsule which are filled with numerous black, kidney-shaped seeds [3].

This plant, called in Morocco "*Chdek ej-jmel*", is used traditionally in medicine. The leaves and flowers are indicated in the treatment of Asthma. On the other hand, *D. stramonium* L. is used as a hallucinogenic and sedative product smoked alone or mixed with cannabis or even consumed by young people [4].

D. stramonium L. is a rich source of tropane alkaloids [1,5,7]. These alkaloids are used in the chemotaxonomy of Solanaceae family [2]. Knowledge of the complete alkaloid pattern is of interest not only phytochemically, but also in relation to aspects of alkaloid biogenesis and metabolism. Recent investigations of the genus *Datura* with GC-MS demonstrate that tropane alkaloid-containing plants generally have a large number of alkaloids which are not detected by other methods [1,5,7,10].

In this study we report the tropane alkaloid spectra of different organ plants from *D. stramonium* L. cultivated in Morocco (with subtropical climate).

2. Materials and methods

2.1. Plant material

D. stramonium L. was collected at the stage of opening of the first capsule in north-west of Morocco, in the locality of Temara, situated near the sea, in April 2009. Vouchers specimens were deposited in the toxicology department of the laboratory (LARATES). Roots, stems, leaves, flowers and seeds of the plant were air dried in the shade for several days at room temperature and powdered.

2.2. Alkaloid extraction and gas chromatography/mass spectra (GC/MS)

Alkaloid extraction was performed essentially as described in Ref. [9]. The GC/MS analysis was carried out on Agilent 6890/MSD5975B instrument operating in electron impact (EI) ionisation mode at 70 eV, with MS transfer line

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Table 1
Tropane alkaloids identified in *Datura stramonium* L. plant parts presented as a percentage of total ion current.

Alkaloids	Tr[min]	M^+/ base ion (*m/z*)	Roots	Stems	Leaves	flowers	Seeds	MS Ref.
Hygrine (1)	09.04	141/84	0.3	<0.1	<0.1	–	–	[10]
6,7-Dehydrotropine (2) [c]	10.51	139/94	<0.1	<0.1	–	–	<0.1	[11]
Cyclotropine (3) [b]	11.39	139/68	<0.1	<0.1	0.1	–	<0.1	[13]
Tropinone (4)	12.28	139/82	<0.1	<0.1	<0.1	–	<0.1	[13]
Tropine (5)	12.54	141/82	1.1	0.6	3.2	4.6	0.3	[10]
Pseudotropine (6)	13.14	141/82	0.3	<0.1	–	–	<0.1	[10]
Scopoline (7)	15.56	155/96	<0.1	<0.1	0.4	1.8	0.2	[16]
Scopine (8)	16.76	155/42	<0.1	<0.1	0.5	1.4	<0.1	[16]
3-Acetoxytropane (9)	16.91	183/124	<0.1	–	–	–	–	[10]
3,6-Dihydroxytropane (10)	19.61	157/113	0.7	–	–	–	–	[17]
Methylecgonine (11)	22.26	199/82	0.3	<0.1	–	–	–	[18]
3-(Hydroxyacetoxy)tropane (12)	22.50	199/124	<0.1	–	–	–	–	[17]
3-Acetoxy-6-hydroxytropane (13)	23.07	199/94	<0.1	–	–	–	–	[16]
3-Hydroxy-6-acetoxytropane (14)	23.34	199/113	<0.1	–	–	–	–	[19]
3-Methylbutyryloxytropane (15)	24.03	225/124	<0.1	–	–	–	–	[10]
3,7-Dihydroxy-6-propionyloxytropane (16) [a]	24.67	229/113	0.1	–	–	–	–	–
6,7-Dehydro-3-tigloyloxytropane (17) [a]	25.46	221/94	<0.1	–	–	–	–	–
3,6-Diacetoxytropane (18)	25.62	241/94	<0.1	–	–	–	–	[19]
3α-Tigloyloxytropane (19)	27.01	223/124	0.6	–	–	–	0.4	[10]
3-Hydroxy-6-isobutyryloxytropane (20)	27.17	227/113	0.1	<0.1	–	–	–	[20]
3β-Tigloyloxytropane (21)	27.33	223/124	0.2	–	–	–	<0.1	[10]
3-Isovaleroyloxy-6-hydroxytropane or 3-(2′-methylbutyryloxy)-6-hydroxytropane (22)	29.44	241/94	<0.1	–	–	–	–	[8]
3-Hydroxy-6-(2′-methylbutyryloxy)tropane (23)	29.62	241/113	0.2	–	–	–	–	[10]
3-Hydroxy-6-methylbutyryloxytropane (24)	29.83	241/113	<0.1	–	–	–	–	[10]
3-Tigloyloxy-6,7-epoxytropane (25) [a]	30.02	237/94	<0.1	–	–	–	–	–
3-Tigloyloxy-6-hydroxytropane (26)	32.20	239/94	2.3	–	–	–	–	[10]
3α-Hydroxy-6β-tigloyloxytropane (27)	32.25	239/113	0.7	<0.1	<0.1	–	0.1	[10]
3β-Hydroxy-6β-tigloyloxytropane (28)	32.50	239/113	–	–	0.5	–	–	[10]
3-Tigloyloxy-6-acetoxytropane (29)	33.70	281/94	<0.1	–	–	–	–	[10]
3,7-Dihydroxy-6-(2′-methylbutyryloxy)tropane (30) [a]	34.08	257/113	0.1	–	–	–	–	–
3-Tigloyloxy-6-propionyloxy-7-hydroxytropane (31)	34.50	311/94	0.1	–	–	–	–	[18]
3-Phenylacetoxytropane (32)	34.89	259/124	0.2	0.8	0.6	0.3	0.4	[9]
3-(2′-Phenylpropionyloxy)tropane (33)	35.32	273/124	–	–	–	<0.1	–	[21]
3-Tigloyloxy-6-propionyloxytropane (34)	35.66	295/94	0.1	–	–	–	–	[10]
6,7-Dehydro-3-apotropoyloxytropane (35) [a]	35.87	269/94	–	<0.1	<0.1	–	<0.1	–
3-Tigloyloxy-6-isobutyryloxytropne (36)	36.38	309/94	0.5	–	–	–	–	[10]
3-Tigloyloxy-6,7-dihydroxytropane (37)	36.55	255/94	3.7	–	–	–	–	[10]
Apoatropine (38)	36.99	271/124	2.2	12.9	7.5	1.8	7.5	[9]
3,7-Dihydroxy-6-tigloyloxytropane (39)	37.12	255/113	0.5	–	–	–	–	[22]
3-Phenylacetoxy-6,7-epoxytropane (40)	37.63	273/94	0.1	0.6	0.5	1.1	0.1	[14]
Dihydroaposcopolamine (41) [b]	38.07	287/94	–	–	–	<0.1	–	[25]
3-Tigloyloxy-6-(2′-methylbutyryloxy)tropane (42)	38.34	323/94	0.2	–	–	–	–	[10]
3-Tigloyloxy-6-methylbutyryloxytropane (43)	38.62	323/94	<0.1	–	–	–	–	[10]
6,7-Dehydrohyoscyamine (44) [b]	39.10	287/94	0.1	<0.1	0.2	<0.1	<0.1	[11]
3-(3′-Methoxytropoyloxy)tropane (45) [a]	39.24	303/124	–	0.4	<0.1	–	<0.1	–
3-Phenylacetoxy-6-hydroxytropane (46)	39.34	275/94	0.3	–	–	–	–	[17]
Aponorscopolamine (47)	39.35	271/122	–	<0.1	–	–	<0.1	[23]
Aposcopolamine (48)	39.49	285/94	0.6	5.2	4.2	1.7	3.1	[10]
3-Tigloyloxy-6-isobutyryloxy-7-hydroxytropane (49) [a]	39.72	325/94	5.9	–	–	–	–	–
Littorine (50)	40.31	289/124	<0.1	–	–	–	–	[17]
Hyoscyamine (Atropine) (51)	40.59	289/124	29.5	57.0	55.0	50.6	65.7	[9]
3,6-Ditigloyloxytropane (52)	41.15	321/94	0.4	–	–	–	–	[10]
6-Hydroxyapoatropine (53)	41.25	287/94	0.7	0.5	0.8	–	0.4	[10]
3α-Tigloyloxy-6-isovaleroyloxy-7-hydroxytropane (54)	41.52	339/94	7.3	–	–	–	–	[24]
3β-Tigloyloxy-6-isovaleroyloxy-7-hydroxytropane (55)	41.83	339/94	2.2	–	–	–	–	[6]
Methylscopolamine (56)	42.10	317/94	–	<0.1	–	–	–	[16]
3-(3′-Acetoxytropoyloxy)tropane (57)	42.33	331/124	0.2	–	–	–	–	[5]
Scopolamine (58)	43.21	303/94	4.7	20.1	23.9	36.3	20.3	[10]
4′-Hydroxylittorine (59) [b]	43.69	305/124	0.1	–	–	–	–	[15]
3,6-Ditigloyloxy-7-hydroxytropane (60)	44.32	337/94	23.4	–	–	–	–	[10]
7-Hydroxyhyoscyamine (61)	44.50	305/94	1.7	0.5	1.0	<0.1	0.4	[16]
6-Hydroxyhyoscyamine (62)	44.79	305/94	2.2	0.5	1.1	<0.1	0.5	[16]
3-Tropoyloxy-6-acetoxytropane (63)	45.49	347/94	<0.1	–	–	–	–	[18]
3-Tropoyloxy-6-isobutyryloxytropane (64) [a]	47.58	375/94	<0.1	–	–	–	–	–
3α-Tropoyloxy-6β-isovaleroyloxytropane (65)	49.23	389/94	0.1	–	–	–	–	[16]
3β-Tropoyloxy-6β-isovaleroyloxytropane (66) [a]	49.47	389/94	<0.1	–	–	–	–	[16]
3-Tropoyloxy-6-tigloyloxytropane (67)	51.51	387/94	0.1	–	–	–	–	[10]