

Baiseitova A.M.<sup>1</sup>, Aisa H.<sup>2,3</sup>, Jenis J.<sup>1\*</sup><sup>1</sup>Faculty of Chemistry and Chemical Technology, Al-Farabi Kazakh National University, Almaty, Kazakhstan<sup>2</sup>Xinjiang Technical Institutes of Physics and Chemistry, Central Asian of Drug Discovery and Development,<sup>3</sup>Xinjiang Key Laboratory of Plant Resources and Natural Product Chemistry, XTIPC CAS, R. P. China.

\*e-mail: aizhabaiseitova@gmail.com

### Chemical constituents of *Dracocephalum nutans*

**Abstract.** In this study we investigate the chemical constituent in aerial parts of *Dracocephalum nutans*. The moisture content (6.13%), total ash (2.18%), extractives (35.25%) and quantitative and qualitative analysis of biologically active constituents of aerial parts of *Dracocephalum nutans* were determined. In The Institute of Combustion Problems using the method of multi-element atomic emission spectral analysis in the ash of *Dracocephalum nutans* were found 11 macro-micro elements, main of them was K(794.5750 µg/ml), Ca (440.63 µg/ml), Fe (4.5005 µg/ml), Zn (1.6911 µg/ml). The volatile oil constitutes were extracted from the aerial parts of *Dracocephalum nutans* by water steam distillation were analyzed by GC-MS method. More than forty compounds were separated. Their relative contents were determined by area normalization in which 45 volatiles were identified. The major volatile oils of 1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene (14.23%), Caryophyllene oxide (11.30%), 1,6-Octadien-3-ol, 3,7-dimethyl (7.69%), (-)-myrtenyl acetate (5.67%), Naphthalene, 1,2,3,4,4A,5,6,8A-octahydro-7-methyl-4-methylene (5.29%), (-)-spathulenol (4.76%), Benzene, 1-methoxy-4-(1-propenyl) (4.73%), 4-ah-cycloprop[e]azulen-4A-ol, decahydro-1,1,4,7-tetra[ethenyl] (4.65%), Germacrene D (4.42%), (E)-3(10)-caren-4-ol (4.23%), Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methulene (3.67%),  $\alpha$ -Caryophyllene (3.60%), 12-oxabicyclo[9.1.0]dodeca-3,7-diene, 1,5,5,8-tetramethyl (2.13%).

**Key words:** *Dracocephalum nutans*; chemical constituent, Altay region; quantitative and qualitative analysis, Volatile oils; GC-MS

### Introduction

*Dracocephalum L.* (dragonhead) is a genus of about 60 to 70 species of flowering plants in the family Lamiaceae, native to temperate regions of the Northern Hemisphere distributed in alpine and steppe regions of Asia [1–2]. The main distribution centre is assumedly the alpine steppes of the Pamir Altai and Tian-Shan [2]. The genus *Dracocephalum L.* is represented by 45 species in Eurasia, 22 species grow in mountains of Kazakhstan. Among them *D. goloskokovii*, *D. pavlovii*, *D. karataviense* are endemic rare in the Kazakhstan [3]. *Dracocephalum L.* extracts and oil are used in the pharmaceutical, cosmetic, food and flavouring industries. *Dracocephalum L.* essential oil extracts has antibacterial, antimicrobial, and antioxidant activities [4].

Essential elements are not only present in the body, playing important roles in the processes of the organism, but can be derived from the outside world, can then be used to insufficient life processes in organs and cells. Due to the rich presence of certain elements in the various medicinal plants, such plants are widely

used in traditional medicine as herbs and drugs [5].

Essential oils are volatile compounds derived from primarily from non-wood plant parts such as leaves, flowers and fruit. Essential oils have a pleasant aroma, because of what is used in cosmetics, detergent and food products [6]. Plants use essential oils for protection against insects, because of which the extracted essential oils have been used in agriculture as pesticides [7]. The important characteristic of the essential oils is their healing ability, so their pharmacology and medicine used for the treatment and prevention of various, both internal and external diseases and deficiencies.

In this study has been made the investigation the chemical constituents from Kazakh traditional medicinal plant of *Dracocephalum nutans* [8] grown in Altay region of Kazakhstan for the first time.

### Materials and methods

Plant material: *Dracocephalum nutans* was collected in Altay region of east Kazakhstan, in 2014 and identified by Prof. Shen Guan Min from the Xin-

jiang Institute of Ecology and Geography, Chinese Academy of Sciences.

The moisture content, total ash, extractives and quantitative and qualitative contents of biologically

active constituents of aerial parts of *Dracocephalum nutans* were determined according to methods reported in the State Pharmacopeia XI edition techniques.

**Table 1** – Qualitative and quantitative screening of the powdered aerial parts of *Dracocephalum nutans*

Contents, %						
Moisture contents	Total ash	Extractives (80% C <sub>2</sub> H <sub>5</sub> OH)	Organic acids	Flavonoids	Saponins	Polysaccharides
6.13	2.18	35.25	0.39	0.11	2.29	1.17

In The Institute of Combustion Problems using the method of multielement atomic emission spectral

analysis in the ash of *Dracocephalum nutans* were analyzed elemental constituents.

**Table 2** – Compozition of macro–micro elements

Element	Cu	Zn	Cd	Pb	Fe	Ni	Mn	K	Na	Mg	Ca
µg/ml	0.6098	1.6911	0.0374	0.4522	4.5005	0.0149	1.3556	794.5750	4.5919	107.73	440.63

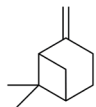
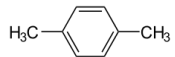
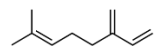
The oils were isolated by water–distillation for 4 hrs and then dried over anhydrous sodium sulphate.

GC–MS analysis: the aerial part of *Dracocephalum nutans* were analyzed by Electron Impact Ionization (EI) method on Perkin–Elemer Autosystem XL – TurboMass (Gas Chromatograph coupled to Mass Spectrometer) fused silica capillary column (30m x 2.5mm; 0.25 µm film thickness), coated with PE–5 ms were utilized. The carrier gas was helium (99.999%). The column temperature was programmed from 60°C (held for 5 min) at 2°C/min to 180°C at 3.5°C/min to 290°C.


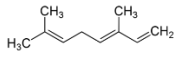
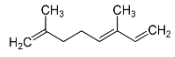
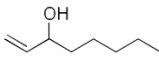
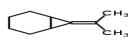
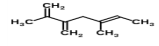
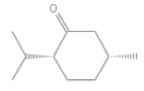

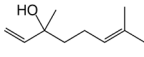
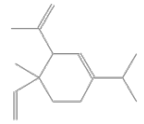
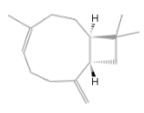
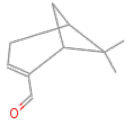
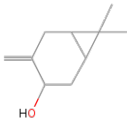
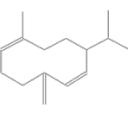
The latter temperature maintained for 40 min (acquisition parameters full scan; scan range 40–350 amu). The injector temperature was 310°C. Injection with a 0.1 µl detector ion source (EI–70eV). Samples were injected by splitting with the split ratio 1:60.

Identification of the compounds: Identification of compounds was done by comparing the NIST and Wiley library data of the peaks and mass spectra of the peaks with those reported in literature. Percentage composition was computed from GC peak areas on PE–5 ms column without applying correction factors.

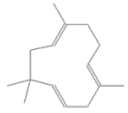
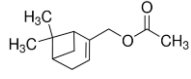
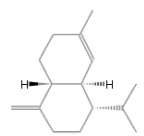
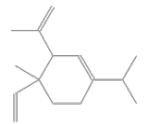
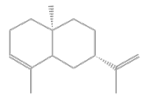
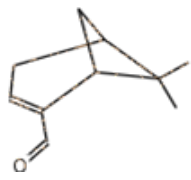
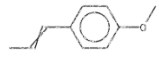
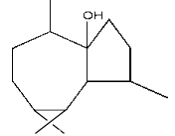
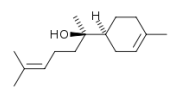
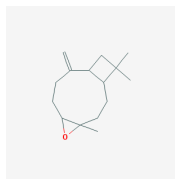
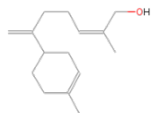
**Table 3** – The volatile constituents of aerial parts of *Dracocephalum nutans*

Peak No.	Constituents	t <sub>R</sub> (min)	Molecular Formula	Structure	MW	Content (%)
1	β–Pinene	21.14	C <sub>10</sub> H <sub>16</sub>		136	0.28
2	p–Xylene	23.51	C <sub>8</sub> H <sub>10</sub>		106	0.16
3	β– Myrcene	24.72	C <sub>10</sub> H <sub>16</sub>		136	0.35

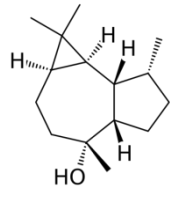
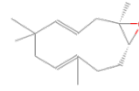
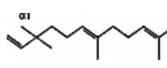
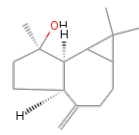
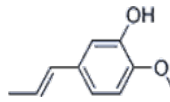
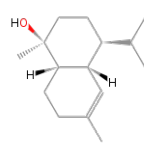
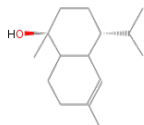
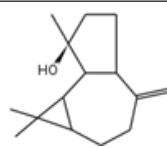
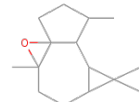
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Peak No.	Constituents	$t_R$ (min)	Molecular Formula	Structure	MW	Content (%)
4	Limonene	27.62	C <sub>10</sub> H <sub>16</sub>		136	0.30
5	1,3,6-Octatriene E,3,7-dimethyl -(E)-	30.25	C <sub>10</sub> H <sub>16</sub>		136	0.13
6	1,3,7-Octatriene,3,7-dimethyl-	31.75	C <sub>10</sub> H <sub>16</sub>		136	0.22
7	1-Octen-3-ol	48.95	C <sub>8</sub> H <sub>16</sub> O		128	0.48
8	Bicyclo[4.1.0]heptane,7-(1-methylethylidene)-	52.67	C <sub>10</sub> H <sub>16</sub>		136	0.35
9	1,5-Heptadiene, 2,5-dimethyl -3-methylene-	52.67	C <sub>10</sub> H <sub>16</sub>		136	0.35
10	Cyclonhexanone,5-methyl-2-(1-methylenhyl)-,cis	53.80	C <sub>10</sub> H <sub>18</sub> O		154	0.67
11	Cyclobutane[1,2,3,4] dicyclopentene, decahydro-32	56.52	C <sub>15</sub> H <sub>24</sub>		204	1.18
12	1,6-Octadien-3-ol,3,7-dimethyl-	58.12	C <sub>10</sub> H <sub>18</sub> O		154	7.69
13	Cyclohexane, 1-ethenyl-1-methyl-2,4-bis(1-methylethenyl)-,	63.21	C <sub>15</sub> H <sub>24</sub>		204	1.63
14	Bicyclo[7.2.0]undec-4-ene,4,11,11-trimethyl-8-methulene-	64.16	C <sub>15</sub> H <sub>24</sub>		204	3.67
15	Bicyclo[3.1.1]hept-2-ene-2carboxaldehyde, 6,6-dimethyl	66.08	C <sub>10</sub> H <sub>14</sub> O		150	0.87
16	(E)-3(10)-caren-4-ol	67.85	C <sub>10</sub> H <sub>16</sub> O		152	4.23
17	GermacreneD	67.42	C <sub>15</sub> H <sub>24</sub>		204	4.42

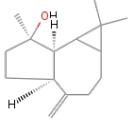
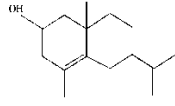
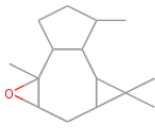
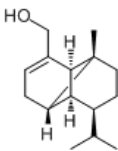
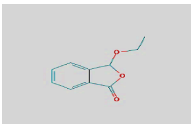
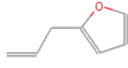
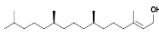
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Peak No.	Constituents	$t_R$ (min)	Molecular Formula	Structure	MW	Content (%)
18	$\alpha$ -Caryophyllene	69.99	C <sub>15</sub> H <sub>24</sub>		204	3.60
19	(-)-myrtenylacetate	71.00	C <sub>12</sub> H <sub>18</sub> O <sub>2</sub>		194	5.67
20	Naphthalene,1,2,3,4,4A,5,6,8A-octahydro-7-methyl-4-methylene	73.31	C <sub>15</sub> H <sub>24</sub>		204	5.29
21	Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethenyl)-1-(1-methylethyl)-	74.77	C <sub>15</sub> H <sub>24</sub>		204	0.56
22	Naphthalene,1,2,3,4,4A,5,6,8A-octahydro-7-methyl-4-methylene-1-methylethenyl)-(1- $\alpha$ .A. $\beta$ )	76.41	C <sub>15</sub> H <sub>24</sub>		204	0.40
23	Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	78.87	C <sub>10</sub> H <sub>16</sub> O		152	1.48
24	Benzene,1-methoxy-4-(1-propenyl)-	82.06	C <sub>10</sub> H <sub>12</sub> O		148	4.73
25	4H-cycloprop [e]azulen-4A-ol,decahydro-1,1,4,7-tetra-[ethenyl]-	90.30	C <sub>15</sub> H <sub>26</sub> O		222	4.65
26	$\alpha$ -Bisabolol	94.02	C <sub>15</sub> H <sub>26</sub> O		222	1.31
27	Caryophyllene oxide	95.03	C <sub>15</sub> H <sub>24</sub> O		220	11.30
28	Lanceol, cis	96.66	C <sub>27</sub> H <sub>42</sub> O <sub>3</sub>		414	0.41

Continuation of Table 3

Peak No.	Constituents	$t_R$ (min)	Molecular Formula	Structure	MW	Content (%)
29	Ledol	97.50	C <sub>15</sub> H <sub>26</sub> O		222	0.57
30	12-oxabicyclo [9.1.0]dodeca-3,7-diene,1,5,5,8-tetramethyl	98.75	C <sub>15</sub> H <sub>24</sub> O		220	2.13
31	1,6,10-dodecatrien -3-ol,3,7,11-trimethyl -	100.66	C <sub>15</sub> H <sub>26</sub> O		222	0.19
32	(-)-spathulenol	103.97	C <sub>15</sub> H <sub>24</sub> O		220	4.76
33	Phenol,2-methoxy-4-(1-propenyl)-	106.45	C <sub>10</sub> H <sub>12</sub> O <sub>2</sub>		164	0.71
34	Tau-Muurolol	107.88	C <sub>15</sub> H <sub>26</sub> O		222	0.36
35	α-Cadinol	111.05	C <sub>15</sub> H <sub>26</sub> O		222	0.81
36	1H-CYCLOPROP[E]AZULEN-7-OL, DECAHYDRO-1,1,7-TRIMETHYL-4-METHYLENE-	112.81	C <sub>15</sub> H <sub>24</sub> O		220	14.23
37	Ledene oxide - (II)	119.18	C <sub>15</sub> H <sub>24</sub> O		220	0.32

Continuation of Table 3

Peak No.	Constituents	t <sub>R</sub> (min)	Molecular Formula	Structure	MW	Content (%)
38	Spathulenol	119.86	C <sub>15</sub> H <sub>24</sub> O		220	0.43
39	6-isopropenyl -4,8A-dimethyl -1,2,3,5,6,7,8,8A-octahydro -naphthalen -2-ol	120.42	C <sub>15</sub> H <sub>24</sub> O		220	1.03
40	ISOAROMADENDRENE EPOXIDE	123.97	C <sub>15</sub> H <sub>24</sub> O		220	0.23
41	Tricyclo[4.4.0.02,7]dec-3-ene-3-methanol,1-methyl-8-(1-methylethyl)-	130.02	C <sub>15</sub> H <sub>24</sub> O		220	0.34
42	1(3H)-Isobenzofuranone,3-ethoxy	130.93	C <sub>10</sub> H <sub>10</sub> O <sub>3</sub>		178	1.72
43	Furan,2-(2-propenyl)-	132.08	C <sub>7</sub> H <sub>8</sub> O		108	0.37
44	Phytol	134.26	C <sub>20</sub> H <sub>40</sub> O		296	1.20

## Results and their discussion

The moisture content (6.13%), total ash (2.18%), extractives (35.25%) and quantitative and qualitative contents of biologically active constituents of aerial parts of *D. nutans* were determined. Total ash content is important in determining the mineral composition of the plant, due to the fact that they are basically the inorganic part of the plant. Moisture contents is also an important factor characterizing stability and also due to the fact that thanks to the water in the plant can be various microorganisms.

In The Institute of Combustion Problems using the method of multielement atomic emission spectral analysis in the ash of *D. nutans* were found 11 macro-micro elements, main of them was K (794.5750 µg/ml), Ca (440.63 µg/ml), Fe (4.5005 µg/ml), Zn (1.6911 µg/ml). Trace elements have a significant

role in the fight against various human diseases and diseases observed in the study of the elements in relation to the indigenous medicinal plants. At the same time, major and trace elements play an important role in the construction and restoration of health and disease conditions of the human body. Progress has occurred in the field of medical sciences during the last few years [9].

Volatile oils from the aerial parts of *D. nutans* were analyzed by GC-MS.

Forty four compounds were separated. Their relative contents were determined by area normalization. The yield from whole herbs of *D. nutans* was found to be 3.21%. Table 1 report the composition of the volatiles of the aerial parts of *D. nutans*. The components have been identified in the volatiles of *Dracocephalum nutans* which the major constituents are 1H - Cycloprop[e]azulen - 7 - ol, decahydro - 1, 1,

7 – trimethyl – 4 – methylene –, (14.23%), Caryophyllene oxide (11.30%), 1, 6 – Octadien – 3 – ol, 3, 7 – dimethyl – (7.69%), (–) – myrtenyl acetate (5.67%), Naphthalene, 1, 2, 3, 4, 4A, 5, 6, 8A – octahydro – 7 – methyl – 4 – methylene (5.29%), (–) – spathulenol (4.76%), Benzene, 1 – methoxy – 4 – (1 – propenyl) – (4.73%), 4 ah – cycloprop[e]azulen – 4A – ol, decahydro – 1, 1, 4, 7 – tetra – [ethenyl] – (4.65%), Germacrene D (4.42%), (E) – 3(10) – caren – 4 – ol (4.23%), Bicyclo [7.2.0] undec – 4 – ene, 4, 11, 11 – trimethyl – 8 – methylene – (3.67%),  $\alpha$  – Caryophyllene (3.60%), 12 – oxabicyclo [9.1.0] dodeca – 3, 7 – diene, 1, 5, 5, 8 – tetramethyl (2.13%).

According to the report 1H – Cycloprop[e]azulen – 7 – ol, decahydro – 1, 1, 7 – trimethyl – 4 – methylene (14.23%) is antifungal, insecticidal and larvicidal, agent [10]. And second major volatile constituent caryophyllene oxide (11.30%) showed analgesic and antiinflammatory activates [11]. 1,6 – Octadien – 3 – ol, 3, 7 – dimethyl – (7.69%) also called as linalool is used as a scent in 60–80% of perfumed hygiene products and cleaning agents including soaps, detergents, shampoos, and lotions [12–13].

Findings suggest that linalool reverses the histopathological hallmarks of AD and restores cognitive and emotional functions via an anti-inflammatory effect. Thus, linalool may be an AD prevention candidate for preclinical studies [14].

## Conclusion

The moisture content (6.13%), total ash (2.18%), extractives (35.25%) and quantitative and qualitative analysis of biologically active constituents of aerial parts of *D. nutans* were determined. In The Institute of Combustion Problems using the method of multi-element atomic emission spectral analysis in the ash of *D. nutans* were found 11 macro–micro elements, main of them was K(794.5750  $\mu\text{g/ml}$ ), Ca (440.63  $\mu\text{g/ml}$ ), Fe (4.5005  $\mu\text{g/ml}$ ), Zn (1.6911  $\mu\text{g/ml}$ ).

The volatile oils constitutes were extracted from the aerial parts of *Dracocephalum nutans* by water steam distillation which analyzed by GC–MS method. More than forty compounds were separated. Their relative contents were determined by area normalization in which 45 volatiles were identified. Active principles of the Kazakh traditional medicinal plant (*Dracocephalum nutans*) that responsible for the activity were determined. While the major volatile constituents are 1H – cycloprop[e]azulen – 7 – ol, decahydro – 1, 1, 7 – trimethyl – 4 – methylene (14.23%), caryophyllene oxide (11.30%), 1, 6 – octadien – 3 – ol, 3, 7 – dimethyl – (7.69%) which possessing an-

tifungal, insecticidal, larvicidal anti-inflammatory, and analgesic activities separately.

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