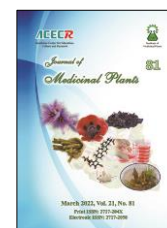




Institute of  
Medicinal Plants

## Journal of Medicinal Plants

Journal homepage: [www.jmp.ir](http://www.jmp.ir)



### Research Article

## Chemical composition of the essential oils and aromatic waters of some native *Scutellaria* species from Iran

Mostafa Pirali Hamedani<sup>1</sup>, Hediye Yousefi<sup>1</sup>, Fateme Tajabadi<sup>2</sup>, Zahra Tofighi<sup>1,3</sup>, Abbas Hadjiakhoondi<sup>1,3</sup>, Saied Goodarzi<sup>3,\*</sup>

<sup>1</sup> Department of Pharmacognosy, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran

<sup>2</sup> Medicinal Plants Research Center, Institute of Medicinal Plants, ACECR, Karaj, Iran

<sup>3</sup> Medicinal Plants Research Center, Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran

### ARTICLE INFO

#### Keywords:

*Scutellaria*

Essential oil

Aromatic water

Linalool

Caryophyllene

Germacrene D

### ABSTRACT

**Background:** Plants of the genus *Scutellaria*, commonly known as skullcap, belong to the Lamiaceae family. There are 22 species of *Scutellaria* in Iran, 10 species of which are native to Iran. Plants of this genus have several effects including neuroprotective, hepatoprotective, anti-cancer, antimicrobial, antiviral, and antioxidant. They are also effective in insomnia and dementia conditions. **Objective:** The aim of this study was to investigate the composition of essential oils and aromatic waters of some native *Scutellaria* species from Iran. **Methods:** Aerial parts of *Scutellaria pinnatifida* with different subspecies such as *mucida*, *viridis*, and *alpina*, *Scutellaria tournefortii*, and *Scutellaria tomentosa* were collected from different regions of Iran. The essential oils and hexane extracts of aromatic waters of selected plants in this genus were obtained by hydrodistillation with clevenger type apparatus and analyzed by GC-MS. **Results:** The results of this study showed that germacrene D, caryophyllene derivatives and linalool are found in abundance in the essential oils of these plants. The main terpenoids in the aromatic waters of these plants were linalool and 1-octen-3-ol. **Conclusion:** The analysis of the essential oils and aromatic waters of *Scutellaria* species demonstrated that different geographical factors such as altitude and the season of plant collection can be effective on the production of plant secondary metabolites.

### 1. Introduction

*Scutellaria* genus is known as “Kolah-khoudi”, “Qashoqak” and “Boshqabi” in Persian name and also known as “Skullcap” in the world. *Scutellaria* is a member of Lamiaceae (Labiatae) family and the geographical distribution of the

species of this annual or perennial genus is almost all around the world [1]. Worldwide, there are about 350 species of *Scutellaria* which among them, about 22 species exist in Iran. The important point is that 10 species of *Scutellaria* are native to Iran [1, 2]. Species of *Scutellaria*

**Abbreviations:** Sc, *Scutellaria*; GC-MS, Gas Chromatography-Mass Spectrometry; KI, Kovats Index; Subsp., Subspecies

\*Corresponding author: [goodarzi\\_s@tums.ac.ir](mailto:goodarzi_s@tums.ac.ir)

doi: 10.52547/jmp.21.81.12

Received 20 September 2021; Received in revised form 13 December 2021; Accepted 19 December 2021

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genus usually grow in meadows and forests [3]. Various species of *Scutellaria* are used as neuroprotective, anti-diarrhea, blood pressure control, anticancer, liver protection, antimicrobial, and prevent bleeding and insomnia, in traditional medicine of different countries [4]. The aim of present study is investigation of compositions of essential oils and hexane fraction of aromatic waters of different species of some *Scutellaria* genus. In order to achieve and introduce the valuable species of *Scutellaria* genus in Iran, comparison

of the major compounds of each essential oil and aromatic water were done.

## 2. Materials and Methods

### 2.1. Plant material

Aerial parts of different species of *Scutellaria* were collected from several regions of Iran. All voucher specimens of these species of *Scutellaria* were deposited at the Herbarium of Faculty of Pharmacy, Tehran University of Medical Sciences, Tehran, Iran (Table 1).

**Table 1.** Specification of studied Iranian *Scutellaria* species

| Scientific name                                                       | Voucher number | Location                                           | Longitude (N) | Latitude (E) |
|-----------------------------------------------------------------------|----------------|----------------------------------------------------|---------------|--------------|
| <i>Scutellaria pinnatifida</i> subsp. <i>mucida</i> (Stapf) Rech.f.   | 7043-TEH       | Barajin protected area, Qazvin Province            | 36°21'9"      | 50°4'5"      |
| <i>Scutellaria pinnatifida</i> subsp. <i>viridis</i> (Bornm.) Rech.f. | 7039-TEH       | Kamard industrial area, Pardis, Tehran Province    | 35°44'50"     | 51°43'43"    |
| <i>Scutellaria pinnatifida</i> subsp. <i>alpina</i> (Boiss.) Rech.f.  | 7117-TEH       | Qatri mountain, Shahroud, Semnan province          | 36°45'37"     | 55°08'40"    |
| <i>Scutellaria tournefortii</i> Benth.                                | 7037-TEH       | Teymour Darreh forest, Galikesh, Golestan Province | 37°14'4"      | 55°32'29"    |
| <i>Scutellaria tournefortii</i> Benth.                                | 7046-TEH       | Jannat-Roudbar road, Ramsar, Mazandaran Province   | 36°49'38"     | 50°41'48"    |
| <i>Scutellaria tomentosa</i> Bertol.                                  | 7116-TEH       | Shikh Bahaei dam, Kashan, Isfahan Province         | 33°43'4"      | 51°27'49"    |

### 2.2. Essential oil

The essential oils of dried aerial parts of *Scutellaria* species were obtained by clevenger type apparatus by hydro-distillation method for 4 hrs. Yellow colored upper layer was separated as essential oil. Anhydrous sodium sulfate as a drying agent was added to essential oils to remove excess water of essential oils. Then, they were refrigerated for GC-MS analysis.

### 2.3. Aromatic water

In Clevenger type apparatus, the distilled water contain two layers, upper layer defined as

essential oil and lower layer defined as aromatic water that not mixed with each other due to different polarities of them. After removal of the upper layer as essential oil, the lower layer existing in Clevenger type apparatus was separated as aromatic water, then it was extracted with hexane (analytical grade). Then, anhydrous sodium sulfate was added to the organic phase of hexane extract of aromatic water (hydrolate). Hexane extract of aromatic waters were refrigerated for GC-MS analysis.

## 2.4. GC-MS analysis

The analysis of essential oils and hexane extracts of aromatic waters were performed by Agilent 6890 GC equipped with silica column BPX5, 30m length, 250µm diameter, 0.25 µm thickness that was connected to Agilent 5973N MS. The conditions of GC system: oven temperature from 50 °C to 300 °C (50-240 °C increasing rate 3 °C/min, and 240-300 °C increasing rate 15°C/min), injector temperature was 250°C. Flow rate of Helium as carrier gas

was 0.5 ml/min with 1/35 split ratio. Ionization energy of MS was taken at 70eV. Scan time was 1 s and mass range was 40-500 AMU [5].

## 3. Results

### 3.1. GC-MS analysis of essential oils

The chemical compositions of the essential oils and hexane extracts of aromatic waters of different species of *Scutellaria* genus were shown in Table 2 and Table 3.

**Table 2.** Chemical composition of the hexane extract of aromatic waters of different species of *Scutellaria* genus

| No.       | KI*         | Components           | Aromatic Waters |             |             |             |             |             |
|-----------|-------------|----------------------|-----------------|-------------|-------------|-------------|-------------|-------------|
|           |             |                      | (1)             | (2)         | (3)         | (4)         | (5)         | (6)         |
| 1         | 700         | Heptane              | 8.1             | 13.6        | 21.0        | -           | 22.5        | -           |
| 2         | 726         | Cyclohexylmethane    | 0.8             | 1.6         | 2.2         | -           | 2.5         | -           |
| 3         | 750         | Isopentyl alcohol    | 0.2             | 1.5         | -           | -           | -           | -           |
| 4         | 783         | 1-Pentanol           | -               | 0.3         | -           | -           | -           | -           |
| 5         | 819         | Hexanal              | -               | 0.5         | -           | -           | -           | 16.4        |
| 6         | 855         | Furfural             | -               | -           | -           | -           | -           | 0.4         |
| 7         | 870         | cis-3-Hexen-1-ol     | 7.4             | 17.3        | -           | 11.5        | 3.1         | -           |
| 8         | 881         | trans-2-Hexen-1-Ol   | 4.8             | 4.0         | 1.9         | 1.8         | 0.6         | 1.0         |
| 9         | 885         | 1-Hexanol            | 7.2             | 6.5         | 4.0         | 4.8         | 1.9         | 3.0         |
| 10        | 987         | Benzaldehyde         | -               | 0.6         | -           | 4.7         | 1.6         | 6.8         |
| <b>11</b> | <b>998</b>  | <b>1-Octen-3-ol</b>  | <b>11.1</b>     | <b>10.1</b> | <b>14.1</b> | <b>25.1</b> | <b>28.5</b> | <b>28.7</b> |
| 12        | 1013        | 3-Octanol            | 0.6             | 0.5         | 0.24        | 0.9         | 0.6         | 1.3         |
| 13        | 1035        | 2,4-Heptadien-1-al   | -               | -           | -           | -           | 0.1         | -           |
| 14        | 1049        | Eucalyptol           | 0.7             | -           | -           | -           | -           | -           |
| 15        | 1069        | Benzeneacetaldehyde  | 0.7             | 1.4         | -           | 0.5         | -           | 1.3         |
| 16        | 1088        | cis-Linalool oxide   | 0.3             | 0.5         | -           | -           | -           | -           |
| 17        | 1090        | 1-Octanol            | 0.2             | -           | -           | -           | -           | -           |
| 18        | 1091        | Acetophenone         | 6.2             | 9.3         | 12.0        | 31.8        | 7.0         | 13.7        |
| 19        | 1102        | trans-Linalool oxide | -               | 0.2         | -           | -           | -           | -           |
| 20        | 1111        | Guaiacol             | 4.8             | 1.1         | -           | 0.3         | -           | -           |
| <b>21</b> | <b>1117</b> | <b>Linalool</b>      | <b>20.4</b>     | <b>14.6</b> | <b>11.7</b> | <b>5.2</b>  | <b>24.0</b> | <b>6.5</b>  |
| 22        | 1121        | Borneol              | -               | -           | 0.7         | -           | -           | -           |
| 23        | 1186        | Menthone             | -               | -           | -           | 0.3         | -           | -           |
| 24        | 1196        | Terpinen-4-ol        | 1.9             | -           | 0.8         | -           | -           | -           |
| 25        | 1189        | 1-Nonanol            | -               | -           | -           | -           | -           | -           |
| 26        | 1221        | α-Terpineol          | 3.9             | 4.8         | 2.5         | 2           | 1.9         | 0.7         |
| 27        | 1222        | cis-Dihydrocarvone   | -               | -           | -           | -           | -           | 0.7         |
| 28        | 1229        | trans-Dihydrocarvone | -               | -           | -           | -           | -           | 1.0         |

(1): *S. tomentosa* (Kashan), (2): *S. pinnatifida* subsp. *viridis* (Tehran) (3): *S. pinnatifida* subsp. *mucida* (Qazvin),

(4): *S. pinnatifida* subsp. *alpina* (Shahroud), (5): *S. tournefortii* (Gorgan), (6): *S. tournefortii* (Ramsar)

\* Kovats indices were reported based on NIST and Wiley libraries

**Table 2.** Chemical composition of the hexane extract of aromatic waters of different species of *Scutellaria* genus (Continued)

| No. | KI*  | Components                 | Aromatic Waters |      |      |      |      |      |
|-----|------|----------------------------|-----------------|------|------|------|------|------|
|     |      |                            | (1)             | (2)  | (3)  | (4)  | (5)  | (6)  |
| 29  | 1243 | <i>trans</i> -Carveol      | -               | -    | -    | -    | -    | 0.9  |
| 30  | 1263 | Pulegon                    | 0.42            | -    | -    | 2.6  | -    | -    |
| 31  | 1271 | Carvone                    | -               | -    | -    | -    | -    | 12.9 |
| 32  | 1339 | 4-Hydroxy-3-methoxystyrene | -               | 0.15 | -    | -    | -    | -    |
| 33  | 1342 | 4-Ethenyl-2-methoxyphenol  | 0.4             | -    | -    | -    | -    | -    |
| 34  | 1382 | Eugenol                    | 7.6             | 5.6  | 3.3  | -    | -    | -    |
| 35  | 1506 | Germacrene D               | 0.3             | -    | -    | -    | -    | -    |
| 36  | 1609 | Spathulenol                | 1.2             | -    | -    | 0.3  | -    | -    |
| 37  | 1615 | Caryophyllene oxide        | -               | -    | -    | 0.3  | -    | -    |
| 38  | 1689 | $\alpha$ -Cadinol          | 0.8             | -    | -    | -    | -    | -    |
|     |      | Oxygenated Monoterpenes    | 27.6            | 20.1 | 15.7 | 10.1 | 25.9 | 22.7 |
|     |      | Sesquiterpene Hydrocarbons | 0.3             | 0    | 0    | 0    | 0    | 0    |
|     |      | Oxygenated Sesquiterpenes  | 2.0             | 0    | 0    | 0.6  | 0    | 0    |
|     |      | Other                      | 60.1            | 74.1 | 76.0 | 81.4 | 68.4 | 72.6 |
|     |      | Total Identified           | 90.0            | 94.1 | 91.7 | 92.1 | 94.3 | 95.3 |
|     |      | Unknown                    | 10.0            | 5.9  | 8.3  | 7.9  | 5.7  | 4.7  |

(1): *S. tomentosa* (Kashan), (2): *S. pinnatifida* subsp. *viridis* (Tehran) (3): *S. pinnatifida* subsp. *mucida* (Qazvin), (4): *S. pinnatifida* subsp. *alpina* (Shahrud), (5): *S. tournefortii* (Gorgan), (6): *S. tournefortii* (Ramsar)

\* Kovats indices were reported based on NIST and Wiley libraries

**Table 3.** Chemical composition of the essential oils of different species of *Scutellaria* genus

| No. | KI*  | Components                 | Essential Oils |      |     |     |     |     |
|-----|------|----------------------------|----------------|------|-----|-----|-----|-----|
|     |      |                            | (1)            | (2)  | (3) | (4) | (5) | (6) |
| 1   | 750  | Isopentyl alcohol          | -              | 0.3  | 0.6 | -   | -   | -   |
| 2   | 870  | <i>cis</i> -3-Hexen-1-ol   | 0.3            | 1.3  | 1.4 | -   | -   | -   |
| 3   | 881  | <i>trans</i> -2-Hexen-1-ol | -              | 0.4  | 0.3 | -   | -   | -   |
| 4   | 885  | 1-Hexanol                  | 0.3            | 0.9  | 0.6 | -   | -   | -   |
| 5   | 976  | <i>o</i> -Ethyltoluene     | -              | 0.3  | 0.4 | -   | -   | -   |
| 6   | 985  | Mesitylene                 | -              | 0.3  | -   | -   | 0.3 | 0.2 |
| 7   | 987  | Benzaldehyde               | -              | -    | -   | -   | -   | -   |
| 8   | 998  | 1-Octen-3-ol               | 1.0            | 4.8  | 4.3 | 1.7 | 5.3 | 4.3 |
| 9   | 1011 | Pseudocumol                | -              | 0.7  | 0.7 | -   | 0.4 | 0.3 |
| 10  | 1013 | 3-Octanol                  | -              | 0.7  | 0.9 | -   | 0.8 | 0.6 |
| 11  | 1035 | 2,4-Heptadien-1-al         | -              | -    | -   | -   | -   | -   |
| 12  | 1044 | Limonene                   | -              | -    | -   | 0.6 | -   | 1.3 |
| 13  | 1049 | Eucalyptol                 | 0.2            | -    | -   | -   | -   | -   |
| 14  | 1090 | 1-Octanol                  | -              | 0.3  | 0.2 | -   | -   | -   |
| 15  | 1091 | Acetophenone               | -              | 0.6  | 0.7 | 0.5 | -   | -   |
| 16  | 1117 | Linalool                   | 5.5            | 19.8 | 7.8 | 4.9 | 5.2 | 6.1 |

(1): *S. tomentosa* (Kashan), (2): *S. pinnatifida* subsp. *viridis* (Tehran) (3): *S. pinnatifida* subsp. *mucida* (Qazvin), (4): *S. pinnatifida* subsp. *alpina* (Shahrud), (5): *S. tournefortii* (Gorgan), (6): *S. tournefortii* (Ramsar)

\* Kovats indices were reported based on NIST and Wiley libraries

**Table 3.** Chemical composition of the essential oils of different species of *Scutellaria* genus (Continued)

| No. | KI*  | Components                                    | Essential Oils |      |      |      |     |     |
|-----|------|-----------------------------------------------|----------------|------|------|------|-----|-----|
|     |      |                                               | (1)            | (2)  | (3)  | (4)  | (5) | (6) |
| 17  | 1121 | Borneol                                       | -              | -    | 0.2  | -    | -   | -   |
| 18  | 1196 | Terpinen-4-ol                                 | 0.2            | 0.2  | 0.2  | -    | -   | -   |
| 19  | 1189 | 1-Nonanol                                     | -              | 0.2  | -    | -    | -   | -   |
| 20  | 1221 | $\alpha$ -Terpineol                           | 3.3            | 3.3  | 4.7  | 0.3  |     | 0.2 |
| 21  | 1222 | <i>cis</i> -Dihydrocarvone                    | -              | -    | -    | -    | 0.3 | 0.4 |
| 22  | 1229 | <i>trans</i> -Dihydrocarvone                  | -              | -    | -    | -    | 0.5 | 0.6 |
| 23  | 1243 | <i>trans</i> -Carveol                         | -              | -    | -    | -    | 0.2 | 0.2 |
| 24  | 1263 | Pulegon                                       | -              | -    | -    | 1.2  | -   | -   |
| 25  | 1269 | Geraniol                                      | -              | 0.6  | 0.4  | -    | -   | -   |
| 26  | 1271 | Carvone                                       | -              | -    | -    | -    | 4.7 | 5.1 |
| 27  | 1319 | Thymol                                        | -              | -    | -    | -    | 0.1 | 0.2 |
| 28  | 1327 | Carvacrol                                     | -              | -    | -    | -    | 0.1 | 0.2 |
| 29  | 1350 | 1,5,5-Trimethyl-6-methylene-cyclohexene       | 0.5            | -    | -    | 0.3  | -   | -   |
| 30  | 1372 | $\alpha$ -Longipinene                         | 3              | -    | -    | 1.1  | -   | -   |
| 31  | 1382 | Eugenol                                       | 0.4            | 2.9  | 2.2  | -    | -   | -   |
| 32  | 1391 | Cyclosativene                                 | 0.7            | 0.4  | 0.3  | 2.3  | -   | -   |
| 33  | 1395 | $\alpha$ -Cubebene                            | -              | -    | -    | 4.7  | -   | -   |
| 34  | 1397 | $\alpha$ -Copaene                             | 3.3            | 1.6  | 1.2  | -    | -   | -   |
| 35  | 1405 | $\beta$ -Bourbonene                           | 1.5            | 2.1  | 3.2  | 1.4  | -   | -   |
| 36  | 1407 | $\beta$ -Cubebene                             | -              | -    | -    | 0.5  | -   | -   |
| 37  | 1424 | <b>Isocaryophyllene</b>                       | -              | 4.1  | 2.8  | -    | -   | -   |
| 38  | 1425 | Aromandendrene                                | 0.4            | -    | -    | -    | -   | -   |
| 39  | 1429 | $\alpha$ -Gurjunene                           | 0.7            | -    | -    | 0.9  | -   | -   |
| 40  | 1431 | $\beta$ -Caryophyllene                        | -              | -    | 0.2  | -    | -   | 2.3 |
| 41  | 1434 | <i>trans</i> - $\alpha$ -Bergamotene          | 1.2            | 0.7  | -    | 1.7  | -   | -   |
| 42  | 1445 | <b><math>\beta</math>-trans-Caryophyllene</b> | 14             | 2.7  | 6.7  | 17.4 | -   | -   |
| 43  | 1452 | $\alpha$ -Amorphene                           | -              | -    | -    | 1.5  | -   | -   |
| 44  | 1467 | <i>trans</i> -Geranylacetone                  | -              | 0.5  | -    | -    | -   | 0.2 |
| 45  | 1471 | $\beta$ -trans-Farnesene                      | 0.8            | -    | 0.4  | 0.7  | -   | -   |
| 46  | 1476 | $\alpha$ -Himachalene                         | 0.8            | -    | 0.4  | -    | -   | -   |
| 47  | 1481 | Humulene                                      | 1.5            | 0.6  | 1.3  | -    | -   | 0.7 |
| 48  | 1485 | Alloaromadendrene                             | 0.4            | -    | -    | -    | -   | -   |
| 49  | 1495 | 1-Dodecanol                                   | -              | -    | -    | -    | 1.2 | 0.6 |
| 50  | 1499 | $\gamma$ -Murolene                            | 0.7            | -    | -    | 0.5  | -   | -   |
| 51  | 1504 | $\beta$ -Ionone                               | -              | -    | -    | -    | -   | 0.7 |
| 52  | 1505 | <i>trans</i> - $\beta$ -Ionone                | -              | -    | -    | -    | 0.8 | -   |
| 53  | 1506 | <b>Germacrene D</b>                           | 23.5           | 11.3 | 13.1 | 25.5 | -   | -   |
| 54  | 1513 | Pentadecane                                   | -              | -    | -    | -    | 0.7 | 0.5 |
| 55  | 1522 | $\alpha$ -Farnesene                           | -              | -    | -    | -    | 0.4 | 0.4 |
| 56  | 1522 | Bicyclogermacrene                             | 5.8            | -    | 1.4  | 5    | -   | -   |

(1): *S. tomentosa* (Kashan), (2): *S. pinnatifida* subsp. *viridis* (Tehran) (3): *S. pinnatifida* subsp. *mucida* (Qazvin), (4): *S. pinnatifida* subsp. *alpina* (Shahroud), (5): *S. tournefortii* (Gorgan), (6): *S. tournefortii* (Ramsar)

\* Kovats indices were reported based on NIST and Wiley libraries

**Table 3.** Chemical composition of the essential oils of different species of *Scutellaria* genus (Continued)

| No.       | KI*         | Components                                  | Essential Oils |             |             |             |      |      |
|-----------|-------------|---------------------------------------------|----------------|-------------|-------------|-------------|------|------|
|           |             |                                             | (1)            | (1)         | (1)         | (1)         | (1)  | (1)  |
| 57        | 1527        | $\beta$ -Himachalene                        | 2.4            | -           | -           | 0.8         | -    | -    |
| 58        | 1533        | Tridecanal                                  | -              | -           | -           | -           | 1.7  | -    |
| 59        | 1543        | $\delta$ -Cadinene                          | 2.4            | 0.8         | 0.7         | 2.2         | -    | -    |
| 60        | 1546        | Calamenene                                  | -              | 0.31        | -           | -           | -    | -    |
| 61        | 1583        | Nerolidol                                   | -              | -           | -           | -           | 0.7  | 2.6  |
| 62        | 1609        | Spathulenol                                 | 2.7            | 3.4         | 6.7         | 3.6         | -    | -    |
| 63        | 1613        | Hexadecane                                  | -              | -           | -           | -           | 1.5  | 0.7  |
| <b>64</b> | <b>1615</b> | <b>Caryophyllene oxide</b>                  | <b>15.3</b>    | <b>16.4</b> | <b>18.8</b> | <b>13.2</b> | -    | -    |
| 65        | 1637        | Tetradecanal                                | -              | -           | -           | -           | 2    | -    |
| 66        | 1668        | Caryophylla-4(12),8(13)-dien-5- $\beta$ -ol | -              | 0.4         | -           | -           | -    | -    |
| 67        | 1689        | $\alpha$ -Cadinol                           | 1.4            | 0.3         | 1.7         | 0.9         | -    | -    |
| 68        | 1715        | Heptadecane                                 | -              | -           | -           | -           | 5.2  | 4.7  |
| 69        | 1721        | 2-Pentadecanone                             | -              | -           | -           | -           | 1.3  | -    |
| 70        | 1740        | Pentadecanal                                | -              | -           | -           | -           | 3.6  | -    |
| 71        | 1742        | Fernesol                                    | -              | -           | -           | -           | 4.9  | 3.6  |
| 72        | 1765        | <i>trans</i> -Farnesal                      | -              | -           | -           | -           | 0.3  | 0.4  |
| 73        | 1796        | Tetradecanoic acid                          | -              | -           | 0.5         | -           | -    | -    |
| 74        | 1792        | Myristic acid                               | -              | 0.1         | -           | -           | -    | -    |
| 75        | 1810        | Benzyl Benzoate                             | -              | -           | -           | -           | 0.3  | 0.3  |
| 76        | 1814        | Octadecane                                  | -              | -           | -           | -           | 0.4  | 0.7  |
| 77        | 1863        | Hexahydrofarnesyl acetone                   | 0.5            | 0.9         | 0.8         | 0.3         | 0.4  | 0.6  |
| 78        | 1930        | Nonadecene                                  | -              | -           | -           | -           | 26.8 | 30.6 |
| 79        | 1936        | 2-Heptadecanone                             | -              | -           | -           | -           | 1.1  | -    |
| 80        | 1942        | Farnesyl acetone                            | -              | 0.3         | 0.2         | -           | -    | -    |
| 81        | 1959        | Palmitic acid, methyl ester                 | -              | 0.2         | -           | -           | -    | -    |
| 82        | 1961        | Octadecanal                                 | -              | -           | -           | -           | 1.7  | -    |
| 83        | 2011        | Palmitic acid                               | -              | 1.4         | -           | -           | -    | -    |
| 84        | 2020        | Eicosane                                    | -              | -           | -           | -           | 3.2  | 4.5  |
| 85        | 2067        | Linoleic acid, methyl ester                 | -              | -           | -           | -           | 0.4  | -    |
| 86        | 2068        | Heneicosane                                 | -              | -           | -           | -           | 13.3 | 14.5 |
| 87        | 2070        | Oleic acid, methyl ester                    | -              | -           | -           | -           | 0.8  | -    |
|           |             | Monoterpene Hydrocarbons                    | 0.5            | 0           | 0           | 0.9         | 0    | 1.3  |
|           |             | Oxygenated Monoterpenes                     | 9.2            | 24.4        | 13.3        | 5.2         | 11.9 | 13.2 |
|           |             | Sesquiterpene Hydrocarbons                  | 76             | 40.2        | 49.8        | 77.2        | 0.4  | 6    |
|           |             | Oxygenated Sesquiterpenes                   | 7              | 6.1         | 10.1        | 7           | 6.3  | 5.3  |
|           |             | Other                                       | 2              | 18.7        | 15.2        | 3.4         | 72   | 62.5 |
|           |             | Total Identified                            | 94.7           | 894         | 88.4        | 93.7        | 90.6 | 88.3 |
|           |             | Unknown                                     | 5.3            | 10.6        | 11.6        | 6.3         | 9.4  | 11.7 |

(1): *S. tomentosa* (Kashan), (2): *S. pinnatifida* subsp. *viridis* (Tehran) (3): *S. pinnatifida* subsp. *mucida* (Qazvin), (4): *S. pinnatifida* subsp. *alpina* (Shahroud), (5): *S. tournefortii* (Gorgan), (6): *S. tournefortii* (Ramsar)

\* Kovats indices were reported based on NIST and Wiley libraries

#### 4. Discussion

Plants of *Scutellaria* genus grow widespread in different regions and weathers [6]. This genus is located at sea level until 2500 m altitude in Iran [7]. In essential oils of *S. tournefortii* the percentage of monoterpene hydrocarbons was

more than other categories of terpenes. On the other hand, the percentage of sesquiterpene hydrocarbons in all subspecies of *S. pinnatifida* was higher than other classes of terpenes. Also, the percentages of sesquiterpene hydrocarbons were different in each subspecies (49.8 % in

*S. pinnatifida* subsp. *mucida*, 77.2 % in *S. pinnatifida* subsp. *alpina*, and 40.2 % in *S. pinnatifida* subsp. *viridis*). These differences could be related to various factors such as geographical region, climate, time of collection, temperature, and other factors [8].

The results of this study showed Germacrene D, Caryophyllene derivatives and Linalool were abundant compounds in the essential oils of *Scutellaria* species and the major terpenoids in their aromatic waters were linalool and 1-octen-3-ol. The previous studies on essential oil of *S. pinnatifida* demonstrated similarities in composition such as existence of germacrene D and caryophyllene as major compounds of essential oil. In another study, germacrene D (39.7 %) and caryophyllene (15 %) were abundant compounds of *S. pinnatifida* subsp. *alpina* [9]. Also germacrene D (39 %) and caryophyllene (23.2 %) were two top compounds in essential oil of *S. pinnatifida* [10]. Germacrene D (16.5 %) and caryophyllene (13.4 %) were abundant in essential oil of *S. orientalis* subsp. *virens* [11]. But, there were some differences in some species. Farnesene (20.3 %) in *S. litwinowii* [12], anethole (28.5 %) in *S. araxensis* [13], and cadinene (27 %) in *S. lateriflora* essential oils were known as major components in previous studies [14]. According to the other studies, linalool was another one of major compounds in essential oil of different species of *Scutellaria* genus.

*S. tournefortii* was collected from north of Iran, from Hyrcanian forests about 500 m in elevation, Mazandaran and Golestan province. Analysis of essential oils and aromatic waters of *S. tournefortii* demonstrated that most compounds were other components without structure of terpene. Oxygenated monoterpenes

were the next class of components with high percentage in both essential oils and aromatic waters but it was interesting that despite the equal amounts of linalool in two samples, the dominance of linalool (24 %) in aromatic water of *S. tournefortii* of Golestan province was much more than linalool (6.5 %) in aromatic water of *S. tournefortii* of Mazandaran province. This difference was probably due to the collection or flowering season because *Scutellaria* from Mazandaran was collected in September and *Scutellaria* from Golestan was collected in July. Humidity and temperature in September is more than July in North of Iran. On the other side, this temperature and humidity may lead to the formation of other compounds.

*S. pinnatifida* with three subspecies were collected from three regions from southern foothills of the Alborz mountain range of Iran, Kamard industrial area of Tehran 1500 m in elevation, Barajin forest park of Qazvin 1600 m in elevation, and around Abr forest of Shahroud, 2300 m in elevation. Altitude is one of the effective factors on the amount of essential oil in plants [15]. By increase of height, the structural skeleton of essential oil components shifts to more complex structures such as sesquiterpenes. It was considerable the major compounds of *S. pinnatifida* essential oils was belong to sesquiterpene hydrocarbons class (40.2 % in *S. pinnatifida* subsp. *viridis*, 49.8 % in *S. pinnatifida* subsp. *mucida*, and 77.2 % in *S. pinnatifida* subsp. *alpina*). Therefore, this change resulted in the increase of major compounds percentages in essential oils of *S. pinnatifida* subspecies such as caryophyllene derivatives (23.6, 28.5, 30.6 %), and germacrene D (11.3, 13.1, 25.5 %) in *S. pinnatifida* subsp. *viridis*, *S. pinnatifida* subsp. *mucida*, and *S. pinnatifida*



subsp. *alpina*, respectively. Also, decrease the amount of monoterpenoids such as linalool (19.8, 7.8, 4.9 %) may depend on increase of height, too.

The compositions of essential oil of *S. tomentosa* that was collected from foothills of Zagros mountain range 2000 m in elevation, was as same as *S. pinnatifida*; germacrene D (23.5 %) and caryophyllene derivatives (29.3 %) were abundant compounds of essential oils belong to sesquiterpene hydrocarbons class.

Chemical analysis of *Scutellaria* aromatic waters demonstrated that the percentage of non-terpenoid compounds in aromatic water of all species was higher than other, and the second order belongs to oxygenated monoterpenes. In aromatic waters, 1-octen-3-ol was a common structure in all species of *Scutellaria*. The percentage of this compound was higher than other in *S. tournefortii* samples that were collected from Golestan and Mazandaran Provinces (28.5 and 28.7 %, respectively), and linalool as second major compounds is an oxygenated monoterpene with 24.0 and 6.5 %, respectively. The amount of Linalool in aromatic waters of *S. pinnatifida* subspecies *viridis*, *mucida*, and *alpina* were 14.6, 11.7, 5.2 %, respectively.

Caryophyllene and its derivatives were abundant in essential oils of *Scutellaria*. This sesquiterpene had strong affinity to bind to cannabinoid receptors type 2 [16]. These receptors were involved in some physiological process such as pain, inflammation, mood, arthrosclerosis, and etc. [17].

Germacrene D and caryophyllene played an important role in antibacterial activity of Verbenaceae family [18]. Also, studies have shown that germacrene D can attract insects to pollinate [19].

Linalool as a main compound of essential oils and aromatic water of *Scutellaria* species had some pharmacological effects such as antimicrobial [20], anticancer [21], anti-oxidant [22], anti-inflammatory [23], and sedative [24].

## 5. Conclusion

The Results of this study demonstrated essential oils and aromatic waters of various species of *Scutellaria* have different patterns of composition. These variations are related to agricultural differences in plant growth. However, three compounds (linalool, germacrene D, and caryophyllene) were known as major valuable terpenoids in the effectiveness of *Scutellaria* genus. Also, due to the presence of caryophyllene and its derivatives in essential oils and linalool in aromatic waters and their pharmacological effects, similar effects can be expected for the essential oil and aromatic water of *Scutellaria* species.

## Author contributions

S. G. was designed and was the supervisor of this study. M. P. H. was wrote this manuscript and also was accomplished the experiments with H. Y., Also, F. T. was analyzed the GC-MS results. Z. T. and A. H. were contributed to the interpretation of the results. All authors approved the manuscript.

## Conflicts of interest

The authors declare that there are no conflicts of interest.

## Acknowledgments

This research was supported by a grant of Medicinal Plants Research Center, Tehran University of Medical Sciences, Tehran, Iran (No. 50948).

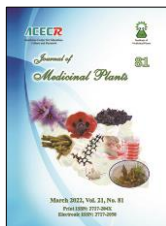


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How to cite this article: Pirali Hamedani M, Yousefi H, Tajabadi F, Tofighi Z, Hadjiakhoondi A, Goodarzi S. Chemical composition of essential oils and aromatic waters of some native *Scutellaria* species from Iran. *Journal of Medicinal Plants* 2022; 21(81): 12-21. doi: 10.52547/jmp.21.81.12



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مقاله تحقیقاتی

## ترکیبات شیمیایی اسانس و عرق برخی گونه‌های گیاه بشقابی بومی ایران

مصطفی پیرعلی همدانی<sup>۱</sup>، هدیه یوسفی<sup>۱</sup>، فاطمه تاج‌آبادی<sup>۲</sup>، زهرا توفیقی<sup>۱،۳</sup>، عباس حاجی‌آخوندی<sup>۱،۳</sup>، سعید گودرزی<sup>۱،۳\*</sup><sup>۱</sup> گروه فارماکونگوزی، دانشکده داروسازی، دانشگاه علوم پزشکی تهران، تهران، ایران<sup>۲</sup> مرکز تحقیقات گیاهان دارویی، پژوهشکده گیاهان دارویی جهاد دانشگاهی، کرج، ایران<sup>۳</sup> مرکز تحقیقات گیاهان دارویی، دانشکده داروسازی، دانشگاه علوم پزشکی تهران، تهران، ایران

| اطلاعات مقاله | چکیده                                                                                                            |
|---------------|------------------------------------------------------------------------------------------------------------------|
| گل‌واژگان:    | مقدمه: گیاهان جنس <i>Scutellaria</i> با نام عمومی skullcap و با نام فارسی بشقابی شناخته می‌شوند. این گیاهان      |
| بشقابی        | متعلق به خانواده Lamiaceae یا نعنائیان هستند. در ایران ۲۲ گونه از جنس بشقابی وجود دارد که ۱۰ گونه از آنها        |
| اسانس         | بومی ایران است. گیاهان این جنس دارای اثرات متعددی از جمله محافظت‌کننده عصبی، محافظت‌کننده کبد،                   |
| عرق           | ضدسرطان، ضد میکروبی، ضد ویروسی و آنتی‌اکسیدانی هستند. همچنین در شرایط بی‌خوابی و زوال عقل موثر هستند.            |
| لینالول       | هدف: هدف از این مطالعه بررسی ترکیب اسانس‌ها و عرق‌های برخی از گونه‌های بومی بشقابی ایران بود. روش                |
| کاربوفیلن     | بررسی: قسمت‌های هوایی گیاه بشقابی سنبله‌ای ( <i>Scutellaria pinnatifida</i> ) با زیرگونه‌های مختلف <i>mucida</i> |
| جرماکرن-د     | <i>viridis</i> و <i>alpine</i> و گونه‌های بشقابی جنگلی ( <i>Scutellaria tournefortii</i> ) و بشقابی نم‌دین       |
|               | ( <i>Scutellaria tomentosa</i> ) از مناطق مختلف ایران جمع‌آوری شدند. اسانس و عصاره هگزانی عرق‌های گیاهان         |
|               | منتخب در این جنس به روش تقطیر با آب و توسط دستگاه کلونجر به دست آمد و سپس توسط دستگاه GC-MS                      |
|               | مورد تجزیه و تحلیل قرار گرفت. نتایج: نتایج این مطالعه نشان داد که ترکیبات جرم‌اکرن-د، مشتقات کاربوفیلن و         |
|               | لینالول در اسانس این گیاهان به وفور یافت می‌شود. ترپنوئیدهای اصلی موجود در عرق این گیاهان، لینالول و ترکیب       |
|               | ۱-اُکتِن-۳-اُل بود. نتیجه‌گیری: نتایج حاصل از آنالیز اسانس‌ها و عرق‌های گونه‌های مختلف بشقابی نشان داد که        |
|               | عوامل جغرافیایی مانند ارتفاع، فصل جمع‌آوری گیاهان و ... می‌تواند بر تولید متابولیت‌های ثانویه گیاهی موثر باشد.   |

مخفف‌ها: Sc، بشقابی؛ GC-MS، کروماتوگرافی گازی متصل به طیف‌سنج جرمی؛ KI، اندیس کوآتس؛ Subsp.، زیرگونه

\* نویسنده مسؤول: [goodarzi\\_s@tums.ac.ir](mailto:goodarzi_s@tums.ac.ir)

تاریخ دریافت: ۲۹ شهریور ۱۴۰۰؛ تاریخ دریافت اصلاحات: ۲۲ آذر ۱۴۰۰؛ تاریخ پذیرش: ۲۸ آذر ۱۴۰۰

doi: 10.52547/jmp.21.81.12

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