Nat. Volatiles & Essent. Oils, 2021; 8(2): 37-41
DOI: 10.37929/nveo.817562

NVEO
Natural Volatiles & Essential Oils

RESEARCH ARTICLE

Spathulenol as the most abundant component of essential oil of *Moluccella aucheri* (Boiss.) Scheen

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Submitted: 01.11.2020; Accepted: 17.03.2021

Abstract

The genus *Moluccella* (Lamiaceae) encompasses eight species among which *Moluccella aucheri* (Boiss.) Scheen and *M. laevis* L. are available in Iran. The aim of this study is characterizing the essential oil of dried aerial parts of *M. aucheri* collected from the South of Iran. The essential oil was hydrodistilled and then analysed by GC-MS. Twenty-one compounds were identified in the oil of *M. aucheri*. The most abundant components of the oil were an aromadendrane sesquiterpene; spathulenol (63.3%) together with a diterpenoid; phytol (3.5%) and a linear sesquiterpene, *E*-nerolidol (3.1%).

Keywords: Essential oil, *Moluccella aucheri,* spathulenol, Lamiaceae

Introduction

Moluccella aucheri (Boiss.) Scheen *(syn. Otostegia aucheri* Boiss.) belongs to *Moluccella* genus and is native to Iran and Pakistan (Scheen & Albert, 2007, 2009). This genus encompasses eight species which are widely distributed in South-Western Asia and the Mediterranean (http://wcsp.science.kew.org/). There are only two species of *Moluccella* genus reported from Iran; *M. aucheri* and *M. laevis* L. of which the earlier is growing wild in the South of the country (Mozaffarian, 2013).

M. aucheri is described previously as *Otostegia aucheri* Boiss. and is a shrub of perennial, growing 30 to 60 cm or rarely up to 80 cm, with leaves of slightly fleshy, pale green, narrow, spinose-apiculate (pungent) flowering branches, multiple flower cycles, funnel-shaped calyx and white flowers (Jamzad, 2012). *M. aucheri* is used as a hair tonic and herbal medicine to prevent hair lost, also it is used for strengthening gums and dental cleanings in Iranian traditional medicine (Sadeghi et al., 2014).

Based on the molecular analysing investigations, *M. aucheri* is suggested as a sister of the two species *M. laevis* L. and *M. spinosa* L. (Scheen & Albert, 2009). Recent GC-MS analysis of the essential oil (EO) of the flowers of *M. laevis* exhibited α-pinene, chrysanthenyl acetate, and isobornyl acetate as the major constituents, while isobornyl acetate, 2-methyl-4-butanolide, 1-heptene oxide and methyl benzoate were detected in the oil of the plants' leaves (Hamed et al., 2020). In another attempt, the EOs' constituents of *M. laevis* were characterized by GC-MS as α-pinene, pinocarvone, methyl chavicol and β-caryophyllene (Shehata, 2001). The EO of *M. spinosa* was analysed by GC-MS and α-pinene, caryophyllene oxide, β-caryophyllene were reported as its major components (Casiglia et al., 2015).

To the best of our knowledge, this is the first phytochemical report on *M. aucheri*.

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Materials and Methods

Plant material

Moluccella aucheri (Boiss.) Sheen was collected during its flowering stage in May 2017, from Hormozgan (Geno mountain, near Bandar Abbas, N 27˚ 23', E 56˚ 14'). Mr. Mehdi Zare identified the plant material as *O. aucheri* syn. *M. aucheri* and deposited voucher specimens (PC-96-3-23-3.1) in the Herbarium of Medicinal and Natural Products Chemistry Research Center, Shiraz University of Medical Sciences (MNCRC), Shiraz, Iran (Jamzad 2012).

Extraction of the essential oil

The aerial parts of *M. aucheri* was dried in the shade (100 g) and was subjected to hydrodistillation for extraction of the EO using a British Pharmacopoeia (BP) apparatus for 3 h. A yellow EO (100 mg, 0.1 % w/w) was obtained and dried over anhydrous Na_2SO_4 and stored at -20 °C until further GC-MS analyses (Jassbi et al., 2018).

GC-MS analyses

GC-MS analysis was carried out on an Agilent 7890N chromatograph apparatus, equipped with HP-5 capillary column (30 m × 0.25 mm× 0.25 µm film thickness). The GC was coupled to an Agilent 5975C mass spectrometer (Agilent Technologies, USA). The injection volume was 1 µL and the flow rate of the carrier gas (helium) was 1 mL/min. The oven temperature increased from 60 °C to 250 °C with the temperature rate of 5 °C/min and 10 min remained at the final temperature. The ionization was taken in an EI mode at 70 eV followed by scanning the fragments ions in the octapole-quadropole analyser with 0.5 s/scan. The split ratio was 1: 10 (Asadollahi et al., 2019).

Identification of the oil's compositions

The relative retention index (RRI) was calculated for each of the GC-MS peaks in the chromatogram, relative to a series of n-alkane (C8-C20), with the Van den Dool formula (Van Den Dool & Kratz, 1963). Identification of the compounds was performed with the comparison of their mass spectra and calculated RRI with those of authentic samples presented in the literature (Adams, 2007).

Results and Discussion

The aerial parts of *M. aucheri* were subjected to hydrodistillation extraction to afford a yellow oil with 0.1 w/w yield. The GC-MS analysis of the EO resulted in characterization of 21 compounds (Table 1). The major constituents of the oil were an aromadendrane sesquiterpene; spathulenol (63.3%) together with bicyclogermacrene (3.7%), two diterpenoids; phytol (3.5%), sclareol (3.5%) and a linear sesquiterpene; *E*-nerolidol (3.1%). The monoterpenoids constituted only a small fraction of the oil (3.3%), while the sesquiterpenoids (63.3%) and diterpenoids (8.2%) were the most abundant constituents of the oil, respectively (Table 1)

Table 1: The GC-MS area% of the essential oil of *M. aucheri*

	Compounds	**Area *%***	**RRI_{exp}**	**RRI_{lit}**
1	1-octen-3-ol	t	998	974
2	linalool	0.9	1116	1095
3	bornyl acetate	0.8	1289	1287
4	*δ*-elemene	t	1333	1335

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	Compounds	**Area %**	**RRI_{exp}**	**RRI_{lit}**
5	*α*-cubebene	tr	1346	1345
6	*α*-terpinol acetate	1.6	1354	1346
7	dodecanal	0.1	1418	1408
8	β-caryophyllene	1.6	1422	1417
9	*α*-humulene	1.1	1458	1452
10	germacrene D	1.1	1484	1484
11	bicyclogermacrene	3.7	1500	1500
12	*E*-nerolidol	3.1	1582	1561
13	spathulenol	63.3	1606	1577
14	humulene epoxide II	2.1	1621	1608
15	2-pentadecanone-6,10,14-trimethyl	1.1	1849	1846*
16	farnesyl acetone C	tr	1919	1860
17	sclareol oxide	0.4	1988	1906*
18	manool oxide	0.2	2008	1987
19	*E, E*-geranyl linalool	0.6	2037	2026
20	phytol	3.5	2130	1942, 2135*
21	sclareol	3.5	2253	2222
	monoterpenes	3.3		
	sesquiterpene	76.0		
	diterpenes	8.2		
	other compounds	1.2		
	Total	88.7		

RRI_{exp}: Experimental Relative retention indices calculated using the retention times of a series of (C_8- C_{40}) *n*-alkanes, RRI_{lit}: RRI reported from a nonpolar GC column in the literature (Adams, 2007), or *National Institute of Standard and Technology, NIST Chemistry Web book (https://webbook.nist.gov/chemistry/name-ser/), tr= trace (<0.05%).

In a recent study, caryophyllene oxide (20.7 %), spathulenol (14.9 %), (*E*)-nerolidol (8.0 %), and phytol (9.2 %) were reported as major compounds of essential oil from *Stevia rebaudiana* Bertoni leaf. These compounds showed insecticidal effects against aphids; *Metopolophium dirhodum* (Walker, 1849), one of the main pests of cereals. Finally, phytol, (*E*)-nerolidol and spathulenol were introduced as environmentally-friendly insecticides against aphids (Benelli et al., 2020). Given in our study, these three compounds represent 69.9% of total EOs of *M. aucheri,* so the oil is suggested for further investigation for the production of green insecticides against aphids.

Spathulenol is a tricyclic sesquiterpene with 5,10-cycloaromadendrane skeleton. A literature survey indicated that spathulenol has important bioactivity such as anticholinesterase (Karakaya et al., 2020), anti-nociceptive, anti-hyperalgesic (Dos Santos et al., 2020), anti-mycobacterial (de Jesús Dzul-Beh et al., 2019; do Nascimento et al., 2018), antioxidant, anti-proliferative, anti-oedematogenic (do Nascimento et al., 2018), cytotoxicity (Mirzaei et al., 2017) and as chemotherapy adjuvant of MDR cancer (Martins et al., 2010). Since the EO of *M. aucheri* contains high levels of spathulenol, therefore, the above mentioned biological activities are expected for the oil, yet needs to be confirmed in the future.

In a recent study (Rosselli et al., 2019), *M. aucheri* was mistakenly synonymized to *Ballota aucheri* Boiss., a different, but taxonomically related plant of the Lamiaceae family (Jamzad 2012). To examine their similarity, we compared the EO composition of both species. The major constituents of *B. aucheri* oil were α-cadinol (21.0%), dehydroaromadendrane (11.8%), β-caryophyllene (8.1%), spathulenol (6.0%), carvone (6.4%) and

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linalool (4.8%) (Rustaiyan et al., 2006). Although, the two plants are rich in sesquiterpenoids, but some of their major constituents are different. The presence of cadinol, dehydroaromadendrane and carvone in *B. aucheri* and phytol and sclareol in *M. aucheri* can be distinctive.

Conclusion

This is the first phytochemical analytical report on the medicinal plant, *M. aucheri* from the Southern parts of Iran. The detected compounds, spathulenol, sclareol, phytol, and nerolidol are known as potent biological active agents which may confirm a part of medicinal properties of the plant. Therefore, due to the high levels noteworthy of spathulenol, it is suggested that the oil of *M. aucheri* could contribute to the production of environment-friendly insecticides against pests of cereals. Although, we found differences and similarities between *B. aucheri* and *M. aucheri*, still more chemical analyses are required to distinguish these species based on their phytochemicals.

ACKNOWLEDGMENT

We thank Mr. Rahman Asadpour for his efforts in collection and Mr. Mehdi Zare for the identification of the plant. This study was kindly supported by SUMS (Shiraz University of Medical Sciences, Shiraz, Iran) and Golestan University (Gorgan, Iran) and is a part of PhD dissertation of Mina Doorandishan for the fulfilment of her degree.

CONFLICTS OF INTEREST

The authors have no conflicts of interest to declare.

REFERENCES

Adams, R. P. (2007). *Identification of essential oil components by gas chromatography/mass spectrometry* (Vol. 456): Allured publishing corporation Carol Stream, IL.

Asadollahi, M., Firuzi, O., Heidary Jamebozorgi, F., Alizadeh, M., & Jassbi, A. R. (2019). Ethnopharmacological studies, chemical composition, antibacterial and cytotoxic activities of essential oils of eleven *Salvia* in Iran. *Journal of Herbal Medicine, 17*, 100250.

Benelli, G., Pavela, R., Drenaggi, E., Desneux, N., & Maggi, F. (2020). Phytol, (*E*)-nerolidol and spathulenol from *Stevia rebaudiana* leaf essential oil as effective and eco-friendly botanical insecticides against *Metopolophium dirhodum*. *Industrial Crops and Products, 155*, 112844.

Casiglia, S., Jemia, M. B., Riccobono, L., Bruno, M., Scandolera, E., & Senatore, F. (2015). Chemical composition of the essential oil of *Moluccella spinosa* L. (Lamiaceae) collected wild in Sicily and its activity on microorganisms affecting historical textiles. *Natural Product Research, 29*(13), 1201-1206.

de Jesús Dzul-Beh, A., García-Sosa, K., Uc-Cachón, A. H., Bórquez, J., Loyola, L. A., Barrios-García, H. B., Peña-Rodríguez, L. M., & Molina-Salinas, G. M. (2019). *In vitro* growth inhibition and bactericidal activity of spathulenol against drug-resistant clinical isolates of *Mycobacterium tuberculosis*. *Revista Brasileira de Farmacognosia, 29*(6), 798-800.

do Nascimento, K. F., Moreira, F. M. F., Santos, J. A., Kassuya, C. A. L., Croda, J. H. R., Cardoso, C. A. L., do Carmo Vieira, M., Ruiz, A. L. T. G., Foglio, M. A., & de Carvalho, J. E. (2018). Antioxidant, anti-inflammatory, antiproliferative and antimycobacterial activities of the essential oil of *Psidium guineense Sw.* and spathulenol. *Journal of Ethnopharmacology, 210*, 351-358.

Dos Santos, E., Radai, J. A. S., do Nascimento, K. F., Formagio, A. S. N., de Matos Balsalobre, N., Ziff, E. B., Castelon Konkiewitz, E., & Kassuya, C. A. L. (2020). Contribution of spathulenol to the anti-nociceptive effects of *Psidium guineense*. *Nutritional Neuroscience*, 1-11.

Hamed, A., Ahmed, N., Attia, E., & Desoukey, S. (2020). Phytochemical investigation of saponifiable matter & volatile oils and antibacterial activity of *Moluccella laevis* L., family Lamiaceae (Labiatae). *Journal of advanced Biomedical and Pharmaceutical Sciences, 3*(4), 213-220.

Jamzad, Z. (2012). *Flora of Iran, no. 76, Lamiaceae*: Ministry of Jihad-e-Agriculture, Research Institute of Forests & Rangelands Press, Iran.

Jassbi, A. R., Mirzaie, Y., Firuzi, O., & Asadollahi, M. (2018). Composition and cytotoxic activity of the essential oils of *Mentha mozaffarianii* Jamzad at different phenological stages. *Current Bioactive Compounds, 14*(2), 191-196.

Karakaya, S., Yilmaz, S. V., Özdemir, Ö., Koca, M., Pınar, N. M., Demirci, B., Yıldırım, K., Sytar, O., Turkez, H., & Baser, K. H. C. (2020). A caryophyllene oxide and other potential anticholinesterase and anticancer agent in *Salvia verticillata* subsp. *amasiaca* (Freyn & Bornm.) Bornm. (Lamiaceae). *Journal of Essential Oil Research, 32*(6), 512-525.

Martins, A., Hajdú, Z., Vasas, A., Csupor-Löffler, B., Molnár, J., & Hohmann, J. (2010). Spathulenol inhibit the human ABCB1 efflux pump. *Planta Medica, 76*(12), P608.

Mirzaei, H. H., Firuzi, O., Baldwin, I. T., & Jassbi, A. R. (2017). Cytotoxic activities of different Iranian solanaceae and lamiaceae plants and bioassay-guided study of an active extract from *Salvia lachnocalyx*. *Natural Product Communications, 12*(10), 1563-1566.

Mozaffarian, V. (2013). *Identification of Medicinal and Aromatic Plants of Iran. Tehran*: Farhang Moaser Press.

Rosselli, S., Fontana, G., & Bruno, M. (2019). A review of the phytochemistry, traditional uses, and biological activities of the Genus *Ballota* and *Otostegia*. *Planta Medica, 85*(11-12), 869-910.

Rustaiyan, A., Masoudi, S., Ameri, N., Samiee, K., & Monfared, A. (2006). Volatile constituents of *Ballota aucheri* Boiss., *Stachys benthamiana* Boiss. and Perovskia abrotanoides Karel. growing wild in Iran. *Journal of Essential Oil Research, 18*(2), 218-221.

Sadeghi, Z., Kuhestani, K., Abdollahi, V., & Mahmood, A. (2014). Ethnopharmacological studies of indigenous medicinal plants of Saravan region, Baluchistan, Iran. *Journal of Ethnopharmacology, 153*(1), 111-118.

Scheen, A. C., & Albert, V. A. (2007). Nomenclatural and taxonomic changes within the *Leucas clade* (Lamioideae; Lamiaceae). *Systematics and Geography of Plants, 77*, 229-238.

Scheen, A. C., & Albert, V. A. (2009). Molecular phylogenetics of the *Leucas* group (Lamioideae; Lamiaceae). *Systematic Botany, 34*(1), 173-181.

Shehata, I. (2001). A pharmacognostical study of *Moluccella laevis* L. *Bull Facult Pharm (Cairo University), 39*, 239-251.

Van Den Dool, H., & Kratz, P. (1963). A generalization of the retention index system including linear temperature programmed gas-liquid partition chromatography. *Journal of Chromatography, 11*, 463-471.