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# Volatile components of the aerial parts of *Prunella vulgaris* L. (Lamiaceae)

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**Abstract**
*Prunella vulgaris* ("heal-all") is found throughout the northern hemisphere and has been used as a traditional medicine in many cultures. In this work, the aerial parts of *P. vulgaris*, growing wild in north Alabama, were collected and hydro distilled to give the essential oil, which was analyzed by gas chromatography – mass spectrometry. The major components in the essential oil were germacrene D (49.7%), β-barbatene (9.0%), hexanal (5.1%), (3*Z*)-hexenol (4.6%), and cuparene (4.5%). The essential oil of *P. vulgaris* was screened for antifungal activity against *Aspergillus niger*, *Candida albicans*, and *Cryptococcus neoformans*, but showed negligible activity (MIC = 625, 1250, and 156 μg/mL, respectively).

**Keywords:** Essential oil composition, germacrene, barbatene

## 1. Introduction
*Prunella vulgaris* L., "heal-all" or "self-heal" (Lamiaceae), is a perennial Holarctic herb and can be found throughout North America [1, 2]. The plant serves as a traditional herbal medicine in several cultures. For example, it has been used in Chinese traditional medicine for "heat clearing" effects [3, 4], in Kashmir, the plant is used in Unani medicine as a "brain tonic" and to treat symptoms of colds [5], and in Europe, the herb has been used externally to treat wounds and internally as a tonic and as a gargle for sore throat and mouth sores [1, 6]. Native Americans have also used *P. vulgaris* as a traditional medicine. The Blackfoot used an infusion of the plant on sores, the Cherokee used an infusion on burns, and the Iroquois took an infusion internally as a tonic and to treat backache [7].
Phytochemical studies of *P. vulgaris* have shown the plant to be rich in triterpenoids and phenolics [8]. As part of our ongoing interest in essential oils from Cherokee aromatic medicinal plants [8-14], we have examined the essential oil composition from the aerial parts of *P. vulgaris* collected in north Alabama.

## 2. Materials and methods
### 2.1 Plant material
The aerial parts of *P. vulgaris* were collected on 15September 2018 near the community of Gurley in north Alabama (34°39′19.2″N, 86°24′47.4″W, elev. 215 m). The plant was identified by S.K. Lawson; a voucher specimen (20190401-000952) has been deposited in the University of Alabama in Huntsville herbarium. The fresh plant material (22.47 g) was hydrodistilled using a Likens-Nickerson apparatus, with continuous extraction with $CH_2Cl_2$, for 3 h to give a pale-yellow essential oil (5.0 mg).
### 2.2 Gas Chromatographic – mass spectral analysis
The essential oil of *P. vulgaris* was analyzed by GC-MS, as described previously [15, 16], using a Shimadzu GC-MS-QP2010 Ultra fitted with a Phenomenex ZB-5ms column. Identification of the essential oil components was determined by comparison of their retention indices and their mass spectral fragmentation patters with those in the essential oil databases [17-20].
### 2.3 Antifungal screening
The *C. coelestinum* essential oil was screened for antifungal activity against *Aspergillus niger* (ATCC 16888), *Candida albicans* (ATCC 18804), and *Cryptococcus neoformans* (ATCC 24607) using the micro broth dilution method as previously described [21]. Amphotericin B was used as the positive control and RPMI medium was used as the negative control.

## 3. Results and discussion
The aerial parts of *P. vulgaris* were collected from wild-growing plants in north Alabama and

hydrodistilled to give a pale-yellow essential oil in 0.022% yield. Twenty-seven compounds representing 99.2% of the composition were identified in the essential oil (see Table 1). The sesquiterpene germacrene D (49.7%) dominated the essential oil with lesser concentrations of β-barbatene (9.0%), hexanal (5.1%), (3*Z*)-hexenol (4.6%), and cuparene (4.5%).

**Table 1:** Aerial parts essential oil composition of *Prunella vulgaris* L

| RI[a] | Compound | % | | RI[a] | Compound | % |
|---|---|---|---|---|---|---|
| 795 | 1-Methylhept-2-ene | 0.4 | | 1480 | Germacrene D | 49.7 |
| 800 | Octane | 0.8 | | 1494 | Bicyclogermacrene | 2.5 |
| 801 | Hexanal | 5.1 | | 1505 | α-Chamigrene | 0.6 |
| 810 | 2-Hexanol | 0.5 | | 1507 | Cuparene | 4.5 |
| 850 | (2*E*)-Hexenal | 1.9 | | 1517 | δ-Cadinene | 0.8 |
| 851 | (3*Z*)-Hexenol | 4.6 | | 1533 | γ-Cuprenene | 1.5 |
| 864 | 1-Hexanol | 1.5 | | 1576 | Spathulenol | 2.4 |
| 932 | α-Pinene | 0.5 | | 1654 | α-Cadinol | 0.6 |
| 1028 | Limonene | 1.0 | | 1829 | Unidentified sesquiterpenoid[b] | 0.8 |
| 1043 | Benzene acetaldehyde | 1.4 | | 1839 | Phytone | 1.4 |
| 1383 | β-Bourbonene | 1.3 | | | Monoterpene hydrocarbons | 1.5 |
| 1388 | β-Elemene | 2.9 | | | Sesquiterpene hydrocarbons | 76.6 |
| 1411 | 2,5-Dimethoxy-*p*-cymene | 0.5 | | | Oxygenated sesquiterpenoids | 3.0 |
| 1414 | α-Barbatene | 1.8 | | | Diterpenoids | 1.4 |
| 1417 | β-Ylangene | 0.9 | | | Benzenoids | 1.9 |
| 1429 | β-Copaene | 0.7 | | | Others | 14.8 |
| 1434 | *cis*-Thujopsene | 0.5 | | | Total Identified | 99.2 |
| 1448 | β-Barbatene | 9.0 | | | | |

[a] Retention Index determined with reference to a homologous series of *n*-alkanes on a ZB-5ms column
[b]207(6%), 191(100%), 163(40%), 151(71%), 146(37%), 131(43%), 123(74%), 107(67%), 105(61%), 95(60%), 93(77%), 91(71%), 83(95%), 81(76%), 79(57%), 77(54%), 69(61%), 67(53%), 55(52%), 43(28%), 41(47%)

The aerial parts essential oil of *P. vulgaris* from north Alabama showed a chemical composition markedly different from previous reports from Iran [22] and from China [23-24].

Chen and co-workers reported that the leaf essential oil of *P. vulgaris* collected from Anhui province, China, was composed mainly of aromadendrene (55.4%), cucumber alcohol (8.5%) and phytol (5.1%) [23]. This analysis is doubtful, however. The Kovats retention indices were not reported, but the retention time of "aromadendrene" was between those of limonene and linalool on a DB-5 column, and there are several other compounds listed that are out of order for elution from a DB-5 column. Yang and co-workers used headspace solid-phase micro extraction (HS-SPME) followed by GC-MS to analyze *P. vulgaris* aerial parts from Changchun, China, and found phytone (12.5%), α-santalene (11.2%), α-bourbonene (5.7%), geranyl acetone (5.7%), and caryophyllene oxide (5.1%) to be the major components [24]. The identification of geranyl acetone and α-santalene are in doubt, however; the reported RI values (1446 and 1453, respectively on a DB-5 column) are too different from those in the Adams database (1453 and 1416, respectively on a DB-5 column) [17].

The essential oil of *P. vulgaris* was screened for antifungal activity against *Aspergillus niger*, *Candida albicans*, and *Cryptococcus neoformans*, but showed negligible activity (MIC = 625, 1250, and 156 μg/mL, respectively).

## 4. Conclusions

The essential oil compositions from *P. vulgaris* from different geographical areas vary widely. The chemical differences are likely to have profound effects on the biological activities of this herbal medicine and should be considered. Since the essential oil compositions of *P. vulgaris* reported in the literature are in doubt, it would be useful for additional analysis of this herbal medicinal plant from other geographical areas to be carried out.

## 5. Acknowledgments

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## 6. Conflicts of Interest

The authors declare no conflicts of interest.

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