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

Sims K Lawson, Layla G Sharp, Prabodh Satyal and William N Setzer

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%), (3Z)-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 Unami 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 [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 15 September 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 herbarium. The fresh plant material (22.47 g) was hydrodistilled using a Likens-Nickerson apparatus, with continuous extraction with CH$_2$Cl$_2$ 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...
The authors declare no conflicts of interest.

6. Confl icts of Interest

The essential oil compositions of 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.

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

<table>
<thead>
<tr>
<th>RI</th>
<th>Compound</th>
<th>%</th>
<th>RI</th>
<th>Compound</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>795</td>
<td>1-Methylhept-2-ene</td>
<td>0.4</td>
<td>1480</td>
<td>Germacrene D</td>
<td>49.7</td>
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<td>800</td>
<td>Octane</td>
<td>0.8</td>
<td>1494</td>
<td>Bicyclogermacrene</td>
<td>2.5</td>
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<tr>
<td>801</td>
<td>Hexanal</td>
<td>5.1</td>
<td>1505</td>
<td>α-Chamigrene</td>
<td>0.6</td>
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<tr>
<td>810</td>
<td>2-Hexanol</td>
<td>0.5</td>
<td>1507</td>
<td>Cuparene</td>
<td>4.5</td>
</tr>
<tr>
<td>850</td>
<td>(2E)-Hexenal</td>
<td>1.9</td>
<td>1517</td>
<td>δ-Cadinene</td>
<td>0.8</td>
</tr>
<tr>
<td>851</td>
<td>(3Z)-Hexenal</td>
<td>4.6</td>
<td>1533</td>
<td>γ-Cuparene</td>
<td>1.5</td>
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<td>864</td>
<td>1-Hexanol</td>
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<td>1576</td>
<td>Spathulenol</td>
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<tr>
<td>932</td>
<td>α-Pinene</td>
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<td>1654</td>
<td>α-Cadinol</td>
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</tr>
<tr>
<td>1028</td>
<td>Limonene</td>
<td>1.0</td>
<td>1829</td>
<td>Unidentified sesquiterpenoid</td>
<td>0.8</td>
</tr>
<tr>
<td>1043</td>
<td>Benzene acetaldehyde</td>
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<td>1839</td>
<td>Phytone</td>
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<tr>
<td>1383</td>
<td>β-Bourbonone</td>
<td>1.3</td>
<td>1415</td>
<td>Monoterpane hydrocarbons</td>
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<tr>
<td>1388</td>
<td>β-Elemene</td>
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<td>1416</td>
<td>Sesquiterpane hydrocarbons</td>
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<tr>
<td>1411</td>
<td>2,5-Dimethoxy-p-cymene</td>
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<td>1417</td>
<td>Oxygenated sesquiterpenoids</td>
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<tr>
<td>1414</td>
<td>α-Barbatene</td>
<td>1.8</td>
<td>1418</td>
<td>Diterpenoids</td>
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<tr>
<td>1417</td>
<td>β-Ylangene</td>
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<td>1420</td>
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<td>cis-Thujeopsene</td>
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<td>1421</td>
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<tr>
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<td>β-Barbatene</td>
<td>9.0</td>
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</table>

a Retention Index determined with reference to a homologous series of n-alkanes on a ZB-5ms column

b207(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 authors declare no conflicts of interest.

7. References

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