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# VOLATILE CONSTITUENTS OF *Ainsliaea pertyoides* OILS

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*Ainsliaea pertyoides* Franch. var. *albomentosa* Beauverd, a member of the *Ainsliaea* genus of the Asteraceae (Compositae) family, is an herbaceous wild plant, and grows spontaneously at an altitude of 1900–2700 m mostly in the southwest part of China [1]. It is significantly different from all other species of the genus *Ainsliaea*. For instance, in this genus, *A. pertyoides* is the only species that has the branches from the main stem [2].

*A. pertyoides* is a Chinese native species known as "Ye-xia-hua" in the regions where it grows. Since ancient times, the whole plant of *A. pertyoides* has been one of the most important Chinese herbal medicines in orthopedics [3–5], especially for treatment of ankylosing spondylitis [6]. And it also possesses antimicrobial activity and emmenagogue effect [7].

As already touched upon, *A. pertyoides* has not been the subject of phytochemical research up to now. Further, there are no studies on the volatiles of *A. pertyoides*, and very few studies on the volatiles of other species in the genus *Ainsliaea*. As part of a program of chemical investigation on the essential oil of Chinese aromatic plants, the chemical constituents of the essential oils from the whole plant of *A. pertyoides* are reported for the first time.

The yields of essential oils obtained from fresh and dried materials were 0.13% and 0.21% (v/w) respectively. Table 1 shows the composition of the essential oils obtained from fresh and dried *A. pertyoides*. Compounds are listed in order of their elution from a DB-5 non-polar column. Fifty-four compounds of oils were identified. As can be seen, no great qualitative variations were observed in the composition of essential oils of the fresh and dried materials; however, there are considerable quantitative variations in the percentages of some components of these two oils. The major components of the oils of the fresh and dried materials were $\beta$-caryophyllene (24.48% and 4.25%), $\beta$-elemene (16.34% and 17.75%), germacrene B (10.46% and 1.04%), $\alpha$-guaiene (7.17% and 3.15%), and *trans*-$\beta$-nerolidol (6.33% and 1.13%) (Table 1). Sesquiterpenes (79.37% and 65.57%) were the major components of the fresh and dried plant materials, followed by aliphatics (8.68% and 12.41%) and monoterpenes (0.92% and 0.26%). It should be noted that a large number of these volatile constituents are azulene derivatives (23.44% and 15.12%).

The fresh and dried materials of *A. pertyoides* were collected from Yunnan province (southwest China). The plant was identified at the Botany Department of Southwest Forestry University, and a voucher specimen (No. 2 116) was deposited at the Herbarium of Southwest Forestry University, Kunming Yunnan, China.

Plants were crushed and extracted for 6 hours using simultaneous distillation-extraction (SDE) [8]. Plant materials were added to sample vials containing 1000 mL distilled water, and 250 mL dichloromethane (AR) was placed in the collecting vial. The samples and the extracting solvent were heated to 100°C and 40°C respectively, and the hydrodistilled volatiles were extracted by organic solvent in both the liquid and the gas phase at the same time. Then the essential oil was dried over anhydrous sodium sulfate and stored in sealed vials at 4°C until analysis.

The oils were analyzed by GC/MS using a Shimadzu GC-MS QP5050A system. A DB-5 column (30 m × 0.25 mm i.d., 0.5 mm film thickness) was used with helium as a carrier gas. The GC oven temperature was kept at 60°C and programmed to 260°C at a rate of 5°C/min, and then kept constant at 260°C for 40 min. Split flow was adjusted at 50 mL/min. The injector temperature was at 250°C. MS were taken at 70 eV. Mass range was between *m/z* 30 to 425. A library search was carried out using the Wiley GC-MS Library and the in-house TBAM Library of Essential Oil Constituents. The MS were also compared with those of reference compounds and confirmed with the aid of retention indices from published sources.

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TABLE 1. Percentage Composition of the Essential Oils of *A. pertyoides*

| Compound | RI* | Fresh | Dried | Compound | RI* | Fresh | Dried |
|---|---|---|---|---|---|---|---|
| Hexanal | 801 | 0.27 | – | *β*-Chamigrene | 1498 | 0.78 | Tr. |
| Acetic acid, pentyl ester | 883 | 0.35 | 0.92 | *α*-Zingiberene | 1500 | 1.02 | 2.14 |
| 3-Methyl-3,4-diethenyl-cyclohexene | 938 | 0.49 | – | (+)-Ledene | 1505 | 0.14 | 0.68 |
| *β*-Linalool | 1098 | 0.33 | 0.28 | *δ*-Guaiene | 1508 | 2.16 | 0.99 |
| *E*-Undec-5-en-3-yne | 1161 | 1.65 | – | *α*-Farnesene | 1509 | 2.42 | 0.24 |
| Thymoquinone | 1249 | 0.57 | 0.13 | l-*β*-Bisabolene | 1519 | 0.32 | 2.53 |
| [+]-Cyclosativene | 1369 | 1.03 | 0.80 | (+)-Nerolidol | 1554 | 0.51 | Tr. |
| Copaene | 1377 | 0.33 | Tr. | Germacrene B | 1561 | 10.46 | 1.04 |
| Patchoulene | 1383 | 0.52 | 1.00 | *trans*-*β*-Nerolidol | 1564 | 6.33 | 1.13 |
| *β*-Cubebene | 1392 | 0.67 | – | (+)-Ledol | 1565 | – | 1.18 |
| ***β*-Elemene** | 1393 | **16.34** | **17.75** | *E*-12-Methyl-1,5,9,11-tridecatetraene | 1568 | 1.23 | 8.35 |
| *β*-Patchoulene | 1395 | 1.86 | 0.71 | Cadinol | 1570 | 0.32 | – |
| 2,5,5-Trimethyl-1,3,4,5,6,7-hexahydro-2*H*-2,4a-ethanonaphthalene | 1398 | 0.31 | Tr. | (–)-Globulol | 1580 | Tr. | 0.84 |
| | | | | Spathulenol | 1585 | 0.25 | 1.97 |
| 2,3,4,5-Tetramethyl-tricyclo-[3.2.1.$0^{2,7}$]oct-3-ene | 1400 | 0.54 | 0.12 | Ledane | 1601 | 0.11 | 0.63 |
| | | | | (–)-Spathulenol | 1619 | 0.49 | 1.6 |
| *α*-Cedrene | 1404 | 0.91 | 2.55 | Isospathulenol | 1620 | Tr. | 1.73 |
| Isocaryophyllene | 1407 | 0.94 | 0.77 | *cis*-5,8,11,14,17-Eicosapentaenoic acid, methyl ester | 1639 | 0.34 | 3.14 |
| (–)-*α*-Gurjunene | 1415 | 1.84 | 0.67 | | | | |
| *β*-Caryophyllene | 1420 | 24.48 | 4.25 | 1,4a,7-Trimethyl-7-ethyl,6-hydroxy-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrenecarboxylic acid | 1645 | – | 0.32 |
| *α*-Bergamotene | 1435 | 0.29 | 2.44 | | | | |
| *α*-Guaiene | 1438 | 7.17 | 3.15 | | | | |
| Aromadendrene | 1440 | 0.91 | 5.82 | | | | |
| *β*-Farnesene | 1458 | 1.07 | 6.06 | 2-(7-Heptadecynyloxy)-tetrahydro-2*H*-pyran | 1654 | Tr. | 3.65 |
| Acoradiene | 1471 | 0.27 | 3.36 | | | | |
| (+)-*β*-Selinene | 1476 | 2.42 | 4.13 | Platambin | 1686 | – | 0.59 |
| Germacrene D | 1485 | 1.86 | Tr. | *α*-Bisabolol | 1697 | 0.39 | – |
| *α*-Curcumene | 1486 | Tr. | 1.85 | (+)-Aromadendrene | 1706 | 1.96 | Tr. |
| *α*-Selinene | 1490 | 0.29 | 2.92 | Isochamecynone | 1799 | – | 1.27 |
| Eremophilene | 1493 | 0.33 | 2.44 | Verrucarol | 1811 | Tr. | 1.08 |
| *β*-Himachalene | 1496 | 0.15 | 0.94 | | | | |

*Retention indices on a non-polar capillary column. Tr.: trace (< 0.1%).


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