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# 石家庄野生荆条败花精油的化学成分

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**摘 要**:用水蒸馏法提取并用气相色谱-质谱法分析石家庄野生荆条败花精油的化学成分。共鉴定出 21 种成分,占精油总量的 94.8%。精油的主要成分为 β-丁香烯(42.2%)、香桧烯(12.2%)和 1,8-桉叶素(5.5%),并可作为 β-丁香烯的良好来源。

**关键词**:荆条;马鞭草科;精油;气相色谱-质谱;β-丁香烯;香桧烯

**中图分类号**:R284.1 **文献标识码**:A

# Chemical Composition of the Aborted Flower Essential Oil of *Vitex negundo* var. *heterophylla* Growing Wild in Shijiazhuang

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**Abstract**: The essential oil of the aborted flowers of *Vitex negundo* var. *heterophylla* growing wild in Shijiazhuang was extracted by hydrodistillation and analyzed by gas chromatography-mass spectrometry (GC-MS). Twenty one constituents accounting for 94.8% of the total oil were identified. The oil consisted mainly of β-caryophyllene (42.2%), sabinene (12.2%) and 1,8-cineole (5.5%), and can serve as a good source of β-caryophyllene.

**Key words**: *Vitex negundo* var. *heterophylla*; Verbenaceae; essential oil; gas chromatography-mass spectrometry; β-caryophyllene; sabinene

## Introduction

The genus *Vitex* (family: Verbenaceae) consists of about 250 species and is represented in the flora of China by 14 species, 7 varieties and 3 forms. *Vitex negundo* L. var. *heterophylla* (Franch.) Rehd. is a shrubby wild plant distributed in China and Japan and used in traditional medicine. The stems and leaves of this plant have been used for diarrhea, the fruits as sedatives and analgesic, and the roots as anthelmintic [1]. The leaf essential oil has been used for chronic tracheitis, and can significantly enhance the phagocytosis of peritoneal macrophages in mice [2]. The chemical components of the essential oils from the leaves [3-6], stems [5,6], leaves-inflorescences [7] and fruits [8] of *V. negundo* var. *heterophylla* have been analyzed. However, the chemical constituents of the aborted flower essential oil of *V. negundo* var. *heterophylla* have not been reported. The objective of this study was to analyze the chemical constituents of the aborted flower essential oil of *V. negundo* var. *heterophylla* growing wild in Shijiazhuang, China.

## Materials and Methods

### Plant material

The aborted flowers (consist mostly of indeciduous calyces) of *V. negundo* var. *heterophylla* growing wild in Shijiazhuang were collected during fruiting period in November 2010. The plant was identified and authenticated by one of the authors (ZHANG Shu-feng). A voucher specimen was deposited in the Herbarium of the Department of Pharmacy, Bethune Medical Noncommissioned Officer Academy.

### Extraction of the essential oil

The essential oil of the dried aborted flowers was ex-

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tracted by hydrodistillation in an essential oil determination apparatus for 5 h [9]. The oil was dried over anhydrous sodium sulphate and stored at 4 °C.

**Gas chromatography - mass spectrometry (GC - MS) analysis**

The oil was analyzed by GC-MS using a Thermo Fisher DSQII GC-MS system equipped with a Thermo TR-5MS GC column (30 m × 0.25 mm i. d. and 0.25 μm film thikness). Temperature program: from 40 °C (1 min) to 200 °C (5 min) at 8 °C/min, and then to 250 °C (2 min) at 10 °C/min. Injection temperature: 250 °C. Carrier gas: He, flow rate: 1.0 mL/min. Injection mode: split (1∶30). MS mode: EI; ionization voltage: 70 eV; ion source temperature: 250 °C; mass range: 50 - 400 amu.

**Identification of the components**

Identification of the essential oil components was based on a comparison of their mass spectra and retention time with those of the authentic compounds and by computer matching with NIST library.

## Results and Discussion

Hydrodistillation of the dried aborted flowers of *V. negundo* var. *heterophylla* yielded 0.6% (v/w) essential oil. The total ion chromatogram of the aborted flower essential oil of *V. negundo* var. *heterophylla* are shown in Fig. 1. Twenty one compounds representing 94.8% of the oil were identified and listed in Table 1. Monoterpenes (80.2%) constituted the major fraction of the oil, while sesquiterpenes accounted to 11.6% of the oil. The major components of the oil were β-caryophyllene (42.2%), sabinene (12.2%) and 1,8-cineole (5.5%).

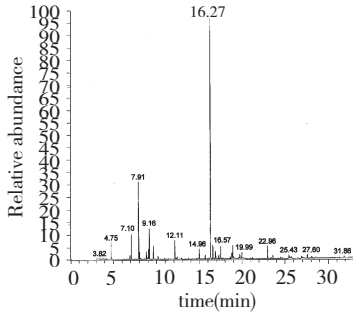


**Fig. 1 The total ion chromatogram of the aborted flower essential oil of *V. negundo* var. *heterophylla***

**Table 1 Chemical composition of the aborted flower essential oil of *V. negundo* var. *heterophylla***

| RT[a] (min) | Compound | Formula | Peak area (%) |
|---|---|---|---|
| 4.75 | Ethyl acetate | $C_4H_8O_2$ | 2.4 |
| 6.91 | Bicyclo[3.1.0]hexane,4-methyl-1-[1-methylethyl]didehydro derive | $C_{10}H_{16}$ | 0.6 |
| 7.10 | 1*R*-α-Pinene | $C_{10}H_{16}$ | 4.2 |
| 7.91 | Sabinene | $C_{10}H_{16}$ | 12.2 |
| 8.81 | α-Terpinene | $C_{10}H_{16}$ | 1.4 |
| 9.06 | *D*-Limonene | $C_{10}H_{16}$ | 1.7 |
| 9.16 | 1,8-Cineole | $C_{10}H_{18}O$ | 5.5 |
| 9.64 | *Γ*-Terpinene | $C_{10}H_{16}$ | 2.4 |
| 12.11 | Terpinen-4-ol | $C_{10}H_{18}O$ | 3.4 |
| 14.96 | Terpinyl acetate | $C_{12}H_{20}O$ | 1.7 |
| 15.67 | β-Elemene | $C_{15}H_{24}$ | 1.1 |
| 16.27 | β-Caryophyllene | $C_{15}H_{24}$ | 42.2 |
| 16.57 | β-Farnesene | $C_{15}H_{24}$ | 2.5 |
| 16.87 | α-Caryophyllene | $C_{15}H_{24}$ | 1.4 |
| 17.26 | β-Cubebene | $C_{15}H_{24}$ | 0.7 |
| 17.49 | *Γ*-Elemene | $C_{15}H_{24}$ | 2.2 |
| 18.81 | Spathulenol | $C_{15}H_{24}O$ | 1.3 |

| | | | |
|---|---|---|---|
| 18.91 | Caryophyllene oxide | $C_{15}H_{24}O$ | 2.9 |
| 19.73 | Agarospirol | $C_{15}H_{26}O$ | 0.8 |
| 19.99 | β-Eudesmol | $C_{15}H_{26}O$ | 1.2 |
| 22.96 | β-Iraldeine | $C_{14}H_{22}O$ | 3.0 |
| | Total identified | | 94.8 |

[a]RT: Retention time

Previous studies on the leaf, stem, leaf-inflorescence and fruit essential oils of *V. negundo* var. *heterophylla* showed various components (Table 2). β-Caryophyllene, sabinene and 1,8-cineole have been previously detected in the leaf or stem essential oils of *V. negundo* var. *heterophylla* from different regions of China, and the most dominant constituent of the leaf or stem essential oils of *V. negundo* var. *heterophylla* was β-caryophyllene [3-6]. However, the most dominant constituent of the fruit essential oil of *V. negundo* var. *heterophylla* was β-elemene [8]. The aborted flower essential oil of *V. negundo* var. *heterophylla* presently investigated shared similar composition pattern with respect to the major constituents in the leaf oil of *V. negundo* var. *heterophylla* grown in Beijing [3], and can be used as a good source of β-caryophyllene, which possesses anti-inflammatory, antibiotic, antioxidant, anticarcinogenic and local anaesthetic activities [10] and is commercially used in cosmetics and as a food additive [11] that potentially modulates inflammatory and other pathophysiological processes [12]. Consequently, further phytochemical and pharmacological studies of this oil should be addressed in future.

**Table 2 Major components of the essential oil of *V. negundo* var. *heterophylla* from different regions**

| Plant part | Major components (%) | Region |
|---|---|---|
| Leaves | β-Caryophyllene (37.6), sabinene (12.6), 1,8-cineole (7.1) [3] | Beijing, China |
| Leaves | β-Caryophyllene (48.7), β-farnesene (15.5) [4] | Henan, China |
| Leaves | β-Caryophyllene (38.8), sabinene (9.8), β-farnesene (5.7) [5] | Beijing, China |
| Leaves | β-Caryophyllene (44.2), β-methyl-ionone (14.2), β-farnesene (8.6) [6] | Beijing, China |
| Stems | β-Caryophyllene (31.8), β-farnesene (5.5), sabinene (5.1) [5] | Beijing, China |
| Stems | β-Caryophyllene (47.2), β-farnesene (10.6), β-methyl-ionone (8.7) [6] | Beijing, China |
| Leaves-inflorescences | α-Thujene, α-pinene, α-terpinene, 1,8-cineole, 4-terpinenol [7] | Beijing, China |
| Fruits | β-Elemene (28.0), linalool (12.4), kaurene (12.0), δ-elemene (10.5), isobornyl acetate (9.0) [8] | Shaanxi, China |

## Conclusions

In conclusion, the aborted flower essential oil of *V. negundo* var. *heterophylla* growing wild in Shijiazhuang, China is characterized by high content of β-caryophyllene, sabinene and 1,8-cineole, and can serve as a good source of β-caryophyllene for meeting the increasing demands of food, cosmetic and pharmaceutical industries.

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