

PYROLYSIS MOLECULE OF *CLERODENDRUM TRICHOTOMUM* FOR POTENTIAL BIOMEDICINE

by

**Xiaofan ZHANG^a, Shuaiwei DONG^b, Zhiyong SUN^b, Yaoming WANG^c,
Xuefeng LUO^b, Bo CHEN^b, Guanzhong YAO^b, Yang GAO^b, Chunxia LV^b,
Dongfang ZHENG^a, Yong ZHAO^a, Ting WANG^a, Shuangxi YAN^a,
and Wanxi PENG^{a*}**

^a School of Forestry, Henan Agricultural University, Zhengzhou, China

^b Scientific Research Institution, Henan Xiaoqinling National Nature Reserve Administration Bureau,
Sanmenxia, China

^c Science and Technology Department, Luanchuan Laojunshan Forest Farm, Luoyang, China

Original scientific paper
<https://doi.org/10.2298/TSCI190701030Z>

In this experiment, Fourier transform infrared technology, gas chromatography-mass spectrometry and liquid chromatography-mass spectrometry were used to detect and analyze the extract of Clerodendrum trichotomum root. The results showed that the extract of Clerodendrum trichotomum root contained a large amount of biologically active ingredients and active ingredients. Clerodendrum trichotomum is rich in essential ingredients and has broad application prospects in biopharmaceuticals and fragrances. This study is of great significance for the development of the medicinal potential of Clerodendrum trichotomum and the identification of its value for further development in modern medicine.

Key words: *Clerodendrum trichotomum*, biological activity, analysis, experiment, medical

Introduction

Clerodendrum trichotomum is a low shrub of Verbenaceae Daqing genus, also known as Stinky Hibiscus, Stinky Indus, etc. These nicknames all point out its *stink*, but this shortcoming does not prevent *Clerodendrum trichotomum* from becoming a famous ornamental plant, because it is really beautiful! *Clerodendrum trichotomum* has lush plants, thick green leaves, large inflorescences, beautiful flowers and fruits, especially in early autumn, fruits have formed one after another. The inflorescence of Changshan Mountain in Haizhou is very large [1, 2]. Many large umbrellas stand on the branches, forming the *mountains* of high and low flowers. Perhaps it is also named for this.

Clerodendrum trichotomum prefers sunshine, shade, moist and fertile loam, which is more drought-resistant, adaptable and cold-resistant. It avoids low-lying stagnant water and has strong salt and alkali resistance [3].

Clerodendrum trichotomum has a certain medicinal value. Its roots, stems, leaves and flowers can be used as medicines. It has useful ingredients of anti-cell proliferation, lowering serum cholesterol, antimicrobial and sedative effects. In addition, *Clerodendrum tri-*

* Corresponding author, e-mail: pengwanxi@163.com

chotomum has clinical effects on hypertension, rheumatoid arthritis, hemorrhoids, dermatitis, cervical spondylosis, ulcerative malaria and other diseases. Various studies have shown that *Clerodendrum trichotomum* has a very high level. Pharmacological research value [4]. Further isolation and screening of active ingredients such as blood pressure lowering, arthritis curing and tumors from leaves and stem bark of Changshan Mountain in Haizhou, and large-scale development of non-toxic, safe and natural medicines with health care effects have important theoretical and practical effects on modern refractory diseases, giving full play to their medicinal functions and benefiting the people [5, 6].

Materials and methods

Experimental materials

Samples of *Clerodendrum trichotomum* were obtained from the Luanchuan Forest District, Henan Province. Samples from roots are processed into powder. They were extracted with reagents: ethanol, phenylethanol (1:1), ethanol water, methanol, 100 °C distilled water, and 40 °C distilled water.

Experimental methods

The FT-IR Analysis

The 200 mg pure KBr was ground uniformly and placed in the mould. The transparent thin sheet was pressed by (5~10)10⁷ Pa pressure on the hydraulic press. Two drops of sample were dried on the thin sheet. The sample could be used for determination after drying. Samples and KBr should be dried and ground to a particle size less than 2 microns in order to avoid the influence of scattering light. The FT-IR spectra of the samples were obtained by FT-IR spectrophotometer (IR100). [7-10].

The GC-MS analysis

GC: Column HP-5MS (30 m × 250 μm × 0.25 μm). Elastic quartz capillary column, the carrier gas used for high purity helium, flow rate of 1 mL/min [11-14]. The split ratio is 50:1. The temperature program of the GC starts at 50 °C, rises to 250 °C at a rate of 10 °C/min, and then rises to 280 °C at a rate of 5 °C/min. MS conditions: program scan mass range of 30 amu-600 amu, ionization voltage of 70 eV, ionization current of 150 μA electron ionization (EI). The ion source and the quadrupole temperature were set at 230 °C and 150 °C, respectively [15, 16].

The QTOF-GC-MS analysis

LC: The column was Agilent Eclipse Plus C18 (2.1 x 100 mm, 1.8 μm). Mobile phase-cationic mode: 0.10% (v/v) formic acid (A), acetonitrile and 0.10% (v/v) formic acid (B). Negative ion mode: 1 mM ammonium fluoride (or ammonium formate) (A), acetonitrile (B). Flow rate: 0.30 mL/min. Column temperature: 40 °C. Release time: 5 minutes. Gradient elution: [time (minutes), B (%)] is [0, 5], [2, 5], [20, 100], [25, 100]. MS: Ion source: AJS ESI. Detection mode: positive ion mode/negative ion mode. Dry gas flow rate [Lmin⁻¹]: 15 L/min (QTOF6550)/7 L/min (QTOF6530/6545) [17, 18]. Drying gas temperature: 200 °C (QTOF6550)/325 °C (QTOF6530/6545). Nebulizer airflow: 35 psig. Sheath gas velocity: 11 L/min. Sheath gas temperature: 350 °C. Capillary voltage: 3.5 kV (positive ion mode)/3.0 kV (negative ion mode). Fragment voltage: 0 kV (positive ion mode)/1.5 kV (negative ion mode). Scan quality range program: 50-1200 m/z. Reference ions: 121.0509 (64.0158), 922.0098 (positive ion mode); 112.9855 (68.9958), 1033.9881 (negative ion mode) [19, 20].

Experimental analysis

The FT-IR analysis

Figure 1 shows the infrared contrast spectra of three extracts from *Clerodendrum trichotomum*. The absorption peaks of the three extract samples were mainly concentrated at 3385 cm^{-1} , 2930 cm^{-1} , 1921 cm^{-1} , 1806 cm^{-1} , 1725 cm^{-1} , 1676 cm^{-1} , 1595 cm^{-1} , 1496 cm^{-1} , and 1268 cm^{-1} . The absorption peak at 3385 cm^{-1} and 2930 cm^{-1} is an unsaturated carbon C-H stretching vibration absorption, and the substance contained therein may be an olefin, an alkyne, an aromatic compound or an aldehyde ketone compound, respectively [21]. The absorption peak at 1921 cm^{-1} and 1496 cm^{-1} may be caused by the stretching vibration of $\text{C}\equiv\text{C}$, and may include a cumulative conjugated compound and an aromatic hydrocarbon. The absorption peak at 1806 cm^{-1} , 1725 cm^{-1} , 1676 cm^{-1} , 1595 cm^{-1} is caused by the stretching vibration of $\text{C}=\text{O}$, and the compounds contained are aryl, aroyl peroxide, and α -chlorinated A cyclic ketone, an α , β -unsaturated ketone or an aryl ketone and a carboxyl anion. The absorption peak at 1268 cm^{-1} is caused by stretching of Ar-O, and the substance may be an ether compound [22, 23]. Through infrared spectroscopy, the main chemical components can be identified as olefins, phenols, organic acids, amides, aldehydes, aroyl peroxides and aromatic compounds.

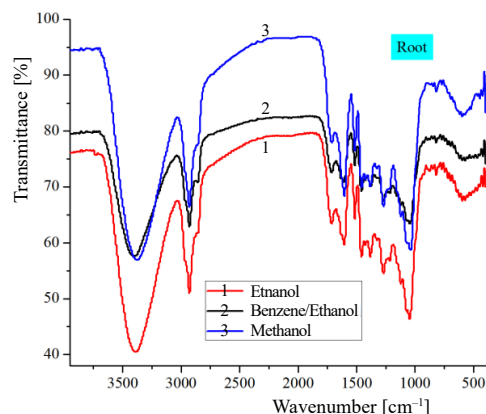


Figure 1. The FT-IR analysis of different extracts from *Clerodendrum trichotomum*

The GC-MS analysis

Based on the results of the GC-MS analysis, 28 peaks were detected and 21 chemical constituents were identified in fig. 2, 17 peaks were detected and 14 chemical constituents were identified in fig. 3, 27 peaks were detected and 25 chemical constituents were identified in fig. 4. The effects of the contained substances are: D-Galactose is used in organic synthesis, in medicine to determine liver function and nutritional drugs [24, 25]; d-Mannose is used as biochemical reagent for cell culture and molecular biology [26]; L-Sorbose is used as intermediate of vitamin C [27, 28]; Stigmasterol stigmasterol is mainly used as raw material for the synthesis of steroids, but also as raw material for the production of vitamin D3. For biochemical

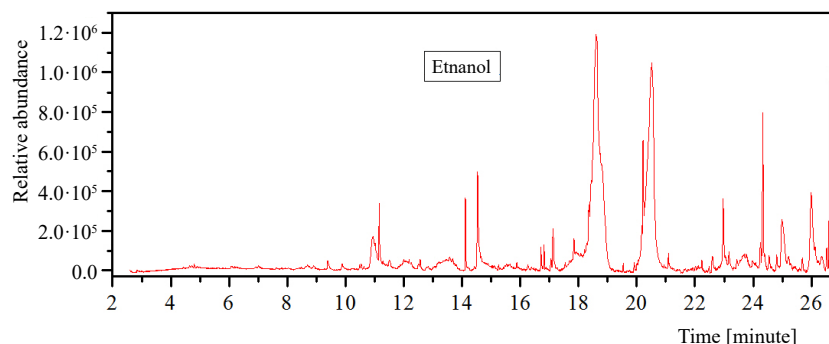


Figure 2. Total ion chromatograms of *Clerodendrum trichotomum* root ethanol extractives

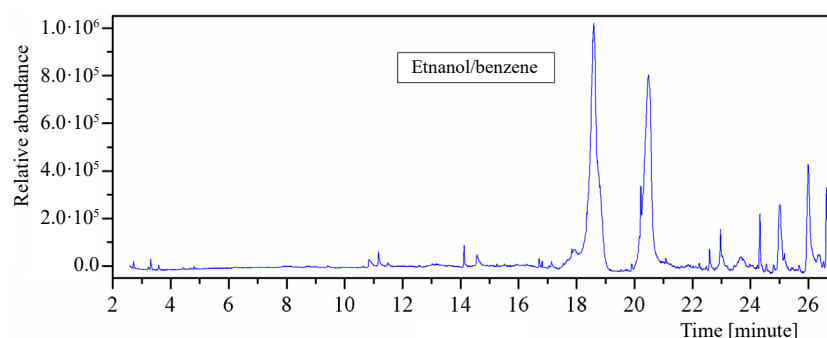


Figure 3. Total ion chromatograms of *Clerodendrum trichotomum* root ethanol/benzene extractives

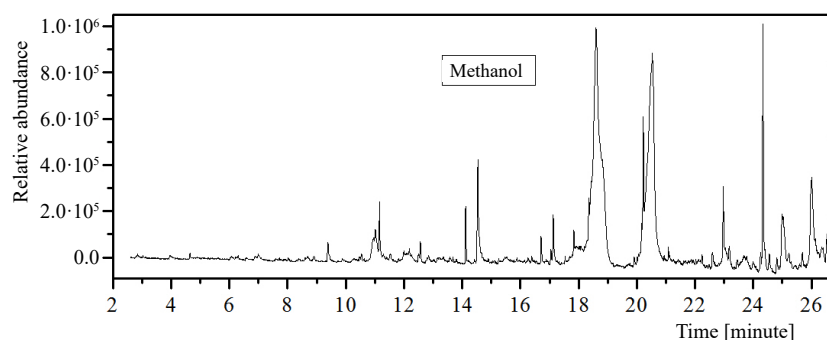


Figure 4. Total ion chromatograms of *Clerodendrum trichotomum* root methanol extractives

research and progesterone, it is also a raw material for progesterone production in medicine. Phenol, 2-methyl-5- (1-methylethyl) are used as flavoring agents, fungicides and disinfectants [29-31]. They are used as flavors in toothpaste, soap and other daily necessities, and are also used as food flavors.

The QTOF-GC-MS analysis

Based on the results of the QTOF-LCMS analysis, 74 peaks were detected and 72 chemical constituents were identified in fig. 5, 27 peaks were detected and 27 chemical constituents were identified in fig. 6, 25 peaks were detected and 25 chemical constituents were identified in fig. 7. The effects of the contained substances are: 2, 3, 5-Trimethylpyrazine is mainly used to prepare cocoa, chocolate and fried nuts. 2-Amino-benzoic acid is used as an intermediate in chemical dyes, medicines, pesticides and perfumes. Arrhythmia drugs often porphyrin, vitamin L, non-steroidal anti-inflammatory analgesics mefenamic acid, inflammatory pain, non-barbital hypnotics hypnotics, strong tranquilizer Terden [32]; Chenodeoxycholic acid used to dissolve gallstone Drugs for the prevention and treatment of cholesterol gallstones and hyperlipidemia, for stones caused by high cholesterol, biliary tract and cholecystitis [33]; Crocetin has anti-tumor, anti-atherosclerosis, antihypertensive and therapeutic bleeding Sexual shock, anti-oxidation, liver and gallbladder effects [34, 35]; Bruceine A has the effect of treating malignant tumors, anti-malarial and anti-inflammatory; Phenyl isothiocyanate is used in the pharmaceutical industry and organic synthesis, is a chromatographic derivatization reagent.

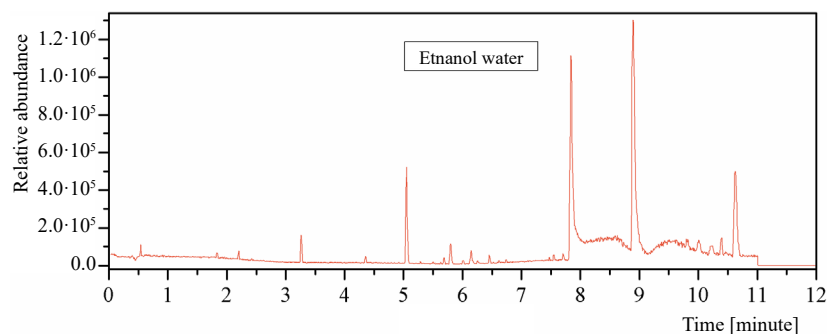


Figure 5. Total ion chromatograms of *Clerodendrum trichotomum* root ethanol water extractives

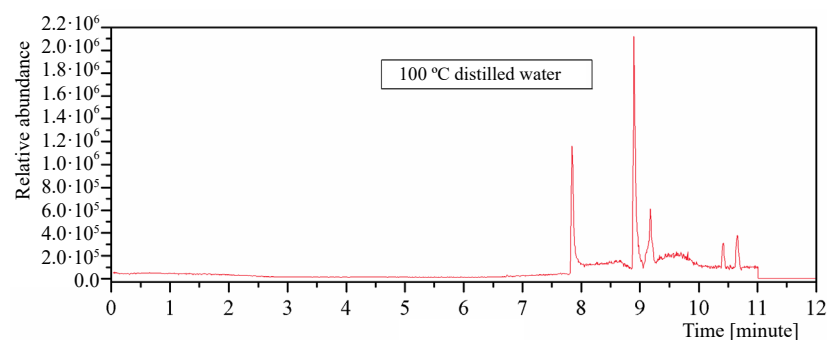


Figure 6. Total ion chromatograms of *Clerodendrum trichotomum* root 100 °C distilled water extractives

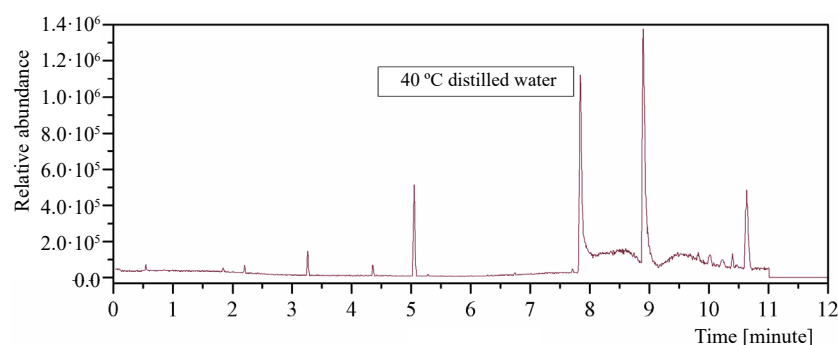


Figure 7. Total ion chromatograms of *Clerodendrum trichotomum* root 40 °C distilled water extractives

Conclusions

By analyzing the infrared spectrum of the *Clerodendrum trichotomum* root sample, it was found that the absorption peaks of the three extract samples were mainly concentrated at 3385 cm^{-1} , 2930 cm^{-1} , 1921 cm^{-1} , 1806 cm^{-1} , 1725 cm^{-1} , 1676 cm^{-1} , 1595 cm^{-1} , 1496 cm^{-1} and 1268 cm^{-1} . The main chemical components can be identified as olefins, phenols, organic acids, amides, aldehydes, aroyl peroxides and aromatic compounds.

Based on the results of GC-MS analysis, the *Clerodendrum trichotomum* root sample detected various chemical effects in the ethanol, benzene/ethanol and methanol extracts, such as various nutraceuticals, fungicides and disinfectants, and Biological chemical reagents.

Based on the results of the QTOF-LCMS analysis, the *Clerodendrum trichotomum* root sample was tested for chemical components rich in various biological activities in ethanol water, 100 °C distilled water, and 40 °C distilled water extract. These chemical ingredients act in many aspects in medicine and cosmetics. Analysis found that *Clerodendrum trichotomum* has a variety of biological activities, such as strong calming, lowering blood pressure, relaxing blood vessels, preventing atherosclerosis, inhibiting tumors, promoting blood circulation, anti-inflammatory, anti-malarial, anti-oxidation, prevention and treatment of cholesterol gallstones and hyperlipidemia.

Through the research and analysis of the extract of *Clerodendrum trichotomum* root, the organic chemical components contained in it can be clearly understood and found to have a wide range of potential industrial and medical uses, which can provide reference for the development of medicinal products and more comprehensive and broader value for *Clerodendrum trichotomum*.

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