NOTE

GC-MS Analysis of Chemical Composition of the Essential Oil of *Toona sinensis* (A. Juss.) Roem Roots

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The essential oil of *Toonasinensis* (A. Juss.) Roem roots, a traditional herbal medicine in China, was extracted by hydrodistillation and analyzed by gas chromatography coupled to mass spectrometry (GC-MS). Twenty compounds were identified. The essential oil yield and the percentage of identified compounds were 1.62 and 91.23 %, respectively. The major components were tridecane (15.54 %), tetradecane (7.00 %), 9-octadecenoic acid, methyl ester (6.19 %), 13-docosenoic acid, methyl ester (5.13 %), (Z,Z)-9,12-octadecadienoic acid (4.53 %), 1-hexadecyne (3.79 %), and α -cubebene (3.07 %). The study can provide quality control evidence and further exploitation of *Toonasinensis* (A. Juss.) Roem.

Keywords: *Toonasinensis* (A. Juss.) Roem, Essential oil, Hydrodistillation, Chemical composition.

For more than a decade, there has been a considerable interest in screening plant essential oils for medical use all over the world¹. Essential oils are valuable natural products used as raw materials in many fields, such as perfumes, cosmetics, aromatherapy, spices, and nutrition²⁻⁴. Moreover, plant essential oils and their components have multiple and varied biological activities such as antitumor, antimicrobial, and antioxidant properties⁵⁻⁷.

Toona sinensis (A. Juss.) Roem is a species of *Toona* native to eastern and south eastern Asia, from North Korea south through most of eastern, central and south western China to Nepal, north eastern India, Myanmar, Thailand, Malaysia, and western Indonesia⁸. It is a deciduous tree growing to 25 m tall with a trunk up to 70 cm diameter. The leaves of *T. sinensis* (A. Juss.) Roem are a vegetable that has been very popular with vegetarians in China⁹. The tender leaves and stem have been used as a carminative and to treat enteritis, dysentery and itch in oriental medicine¹⁰. Also, its roots have been proved to inhibit tumor growth *via* induction of cancer cell apoptosis¹¹. Previous phytochemical studies on *T. sinensis* (A. Juss.) Roem resulted in the identification of retinoid, vitamins B and C, *o*-coumaric acid, kaempferol, megallate, quercetin, afzelin, quercitrin, isoquercitrin and rutin¹². Studies have also reported the chemical composition of the essential oils extracted from

its tender leaves and seeds¹³⁻¹⁶. However, the composition of the essential oil of its roots remain unclear. In present work, the essential oil of *T. sinensis* (A. Juss.) Roem roots was extracted by hydrodistillation, and was analyzed by gas chromatography-mass spectrometry (GC-MS).

Fresh samples of *T. sinensis* (A. Juss.) Roem were collected from Bijie, Guizhou Province in China, in August 2011. Prof. Qingde Long, Department of Medicine, Guiyang Medical University, identified the plant material. A voucher specimen was deposited at Guiyang Medical University, Guiyang, China.

Extraction of essential oil: About 250 g of dried roots of *T. sinensis* (A. Juss.) Roem were cut into pieces, followed by hydrodistillation using a Clevenger-type apparatus for 5 h. The essential oil was collected over water, dried over anhydrous sodium sulphate and stored at 4 °C until analyzed. The oil yield was about 1.62 %.

Gas chromatography-mass spectroscopy (GC-MS) analysis: A gas chromatographic-mass spectral analysis was performed on essential oil of *T. sinensis* (A. Juss.) Roem roots using an Agilent 6890 GC with Agilent 5973 mass selective detector (EI-MS, electron energy = 70 eV, scan range = 10-550 amu), and a fused silica capillary column (HP-5 ms, 30 m $\times$ 0.25 mm) coated with 5 % phenyl methyl siloxane (0.25 μ m

phase thickness). The carrier gas was helium (99.999 %) with a flow rate of 1 mL/min. The injector temperature was 250 °C, and the oven temperature was programmed to initially hold for 2 min at 50 °C, then ramp to 290 °C at 5 °C/min for 2 min. The interface temperature was 280 °C. A 1 % (w/v) solution of each sample in dichloromethane was prepared, and 1 µL was injected using a split injection technique with split ratio 20:1. The components were identified by comparison of their mass spectra with those of the NIST 5 mass spectra library.

The hydrodistillation of roots of *T. sinensis* (A. Juss.) Roem gave light yellowish oil with yield of 1.62 %. It is higher than reported for other plants industrially exploited as source of essential oils: lavender (0.8-1.8 %), mint (0.5-1 %), neroli (0.5-1 %), laurel (0.1-0.35 %) and *Lippiarotundifolia* (0.01 %)¹⁷. The identified constituents from the aerial parts of *T. sinensis* (A. Juss.) Roem, their retention data and chemical composition are presented in Table-1. All the compounds are arranged in order of their elution from the HP5-MS column. Twenty compounds have been identified representing around 91.23 % of the total oil. The major component was dodecane (27.95 %), other components present in appreciable contents being: tridecane (15.54 %), tetradecane (7 %), 9-octadecenoic acid, methyl ester (6.19 %), 13-docosenoic acid, methyl ester (5.13 %), (Z,Z)-9,12-octadecadienoic acid (4.53 %), 1-hexadecyne (3.79 %), and α -cubebene (3.07 %).

TABLE-1
CHEMICAL COMPONENTS OF ESSENTIAL
OIL OF *T. sinensis* (A. Juss.) ROEM ROOTS

No.	Compounds	Retention Time	Area (%)
1	Nonadecane	4.09	2.73
2	Dodecane	4.21	27.95
3	Tridecane	5.04	15.54
4	α -Cubebene	5.61	3.07
5	Tetradecane	5.89	7.00
6	(-)-Isolatedene	6.17	1.20
7	Pentadecane	6.72	1.54
8	β -Neoclovene	6.87	0.67
9	Calamenene	7.06	1.75
10	Pentadecanoic acid, 14-methyl-, methyl ester	9.78	1.45
11	Hexadecanoic acid, methyl ester	9.85	1.53
12	<i>n</i> -Hexadecanoic acid	10.05	1.16
13	(E,E)-9,12-Octadecadienoic acid, methyl ester	10.85	1.98
14	9-Octadecenoic acid, methyl ester	10.88	6.19
15	Octadecanoic acid, methyl ester	11.00	0.64
16	(Z,Z)-9,12-Octadecadienoic acid	11.05	4.53
17	11-Eicosenoic acid, methyl ester	11.91	0.84
18	1-Hexadecyne	12.20	3.79
19	13-Docosenoic acid, methyl ester	13.09	5.13
20	9,17-Octadecadienal	15.57	2.54

Intense studies on essential oil composition of its seeds and leaves have been already published. Chen *et al.*¹³ studied the composition of essential oil extracted from *T. sinensis* (A. Juss.) leaves by steam distillation, with caryophyllene (24.75 %), caryophyllene oxide (9.22 %), linalool (6.27 %), eudesma-4(14),11-diene (5.92 %), and palmitoleic acid (5.58 %) as the

main components. The essential oil of its seeds were also extracted, and its components were characterized by high percentages of *trans*-caryophyllene (11.45 %), γ -elemene (7.28 %), elemene (6.94 %), α -longipinene (6.46 %), and calarene (5.52 %)¹⁵. The essential oil composition determined in our study was different from that of the essential oil of *T. sinensis* (A. Juss.) Roem leaves and seeds. Aliphatic hydrocarbons were the dominant class of compounds, instead of sesquiterpenes. However, some terpenoids were also found in the essential oil of *T. sinensis* (A. Juss.) Roem roots, such as α -cubebene (3.07 %), (-)-isolodene (1.20 %), β -neoclovene (0.67 %), calamenene (1.75 %) and so on.

Conclusion

The aim of this study was to describe the chemical composition of essential oil of *T. sinensis* (A. Juss.) Roem roots. The essential oil, obtained from roots by hydrodistillation, was analyzed by gas chromatography-mass spectrometry (GC-MS). Twenty compounds were identified and the yield of essential oil was 1.62 %. The total identified compounds accounted for 91.23 % of the oil, with tridecane (15.54 %), tetradecane (7.00 %), 9-octadecenoic acid, methyl ester (6.19 %), 13-docosenoic acid, methyl ester (5.13 %), (Z,Z)-9,12-octadecadienoic acid (4.53 %), 1-hexadecyne (3.79 %), and α -cubebene (3.07 %), comprising the main portion of the oil.

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