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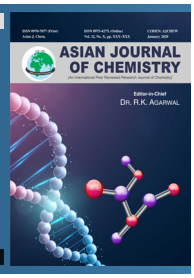

Chemical Composition of the Essential Oil Extracted from *Baeckea frutescens* L. Harvested in Hai Duong Province, Vietnam using GC-MS

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Baeckea frutescens is a tropical plant with great medicinal potential. The oil of *B. frutescens* has high inhibitory, antibacterial and anti-fungal properties, especially against *Staphylococcus aureus* strains. The oil of *B. frutescens* has a spicy, bitter and warm properties that can cure aches and pains. In this study, the essential oils were obtained by hydrodistillation and the chemical analysis of *B. frutescens* essential oils was carried out using GC-MS. It was revealed that main components of leaf oil *B. frutescens* included 26 compounds such as tasmanone (21.46%), β-pinene (15.64%), 1,8-cineole (11.32%), α-thujene (8.74%), α-pinene (7.18%), linalool (7.44%), terpinen-4-ol (5.11%), α-terpineol (4.46%), γ-terpinene (3.37%), *o*-cymene (2.72%). The results open new directions in the application of compounds in *B. frutescens* essential oils to expand research and development of pharmaceutical, cosmetic and food industries.

Keywords: *Baeckea frutescens* L., Essential oils, Hydrodistillation, Chemical composition analysis, GC-MS.

INTRODUCTION

Essential oils, often defined as mixtures of natural volatile aromatic compounds, are substances conventionally extracted from various parts of fragrant plants and shrub species. The composition of essential oils often varies depending the materials from which the oil is extracted and generally consists of mono-terpenes, sesquiterpenes, aliphatic and aromatic compounds [1-5]. Essential oils play an important role in many industries such as pharmaceutical, cosmetic and food industries, in modern and in traditional medicine. *Baeckea frutescens* L., belonging to the Myrtaceae family, is an medicinal plant species whose essential oils have been widely exploited as a traditional ingredient in folk medicine in South East Asian countries. The family Myrtaceae consists of about 100 genera and about 300 species worldwide and is geographically distributed in tropical regions and Australia. The *Baeckea frutescens* shrub is 0.5-2 m high, branching right from the root, stems and small branches. Leaves are needle-shaped, stalkless, smooth, about 1cm long and releases an aromatic fragrance when crushed. The flowers are white, small, single-grown or in pairs in leaf axils [6].

Several studies have identified ingredients isolated from *B. frutescens* extracts such as flavonoids, chromones, sterols [7] and flavonol glycoside [8]. *B. frutescens* is also recognized as having anti-inflammatory, antioxidant [9], antipyretic, antidysentery, antibacterial activities as well as cytotoxicity [10,11]. In terms of composition, a vast array of studies reporting on the essential oils of *B. frutescens* grown in different regions revealed that essential oil yield and composition of the plant may vary drastically depending on parts, age of plants, habitat and extraction methods [12-14]. In addition, major constituents found in *B. frutescens* essential oils were α-pinene, β-pinene, γ-terpinene, ρ-cymene, β-caryophyllene, α-thujene, α-humulene, 1,8-cineole and linalool [15]. In this study, essential

oil from leaves of *B. frutescens* will be obtained by hydrodistillation. The essential oil after distillation was analyzed to determine the volatile composition by GC-MS method. It was found that the oil yield of essential oils extracted from the aerial parts of the plant is quite high (0.7-0.8% of fresh weight and 1.1-1.2% of dry weight), suggesting that *B. frutescens* is a medicinal plant containing essential oils that deserve attention. Moreover, since the essential oil content of the *B. frutescens* invariantly changes throughout the seasons, the supply for *B. frutescens* essential oil could be maintained all year round. The result is expected to contribute to comprehensive data on essential oil and *Baeckea frutescens*, which could extend the economic value of the plant in the industry and medicinal applications.

EXPERIMENTAL

Plant material: The twigs and leaves of *Baeckea frutescens* (Myrtaceae) were collected from January 2019 in the south of Con Son mountain in Chi Linh district of Hai Duong province, Vietnam (21º102′03″N, 106º252′03″E). The collected materials were dried at ambient temperature in the laboratory until its weight become stable and then the leaf was separated from the stem. To ensure the uniformity of sample, collected materials were uniform in quality, fresh and free from pests and diseases and were collected in dry conditions.

Extraction of *Baeckea frutescens* essential oil: The extraction of essential oils from the leaves of *B. frutescens* was performed by hydrodistillation in a Clevenger-type apparatus. The distillation process was carried out by boiling 158 g of fresh ingredients at a ratio of 1:2 raw materials/distilled water. The extraction time was about 3 h in average. The extraction time was started when the first drop of condensed essential oil dropped into the oil extraction system. After distillation, the essential oil was removed from water with anhydrous Na_2SO_4 and then stored in a dark bottle until analyzed with gas chromatography (GC).

Gas chromatography (GC) analysis: To perform GC-MS analysis of the essential oils, an Agilent Technologies HP7890A GC was utilized. The instrument was equipped with a mass spectrum detector (MSD) Agilent Technologies HP5975C and a DB-XLB column (60 m × 0.25 mm, film thickness 0.25 µm, Agilent Technologies). The temperature of injector and detector was set at 250 ºC and 280 ºC, respectively. The thermal progress of the column was set from 40 ºC to 140 ºC at 20 ºC/min, followed by an increase at 4 ºC/min to 270 ºC. The carrier gas was helium at a flow rate of 1 mL/min. Essential oil samples were injected by splitting with the ratio of 100:1 and the volume of 1 µL. Conditions of the mass spectrum detector included ionization voltage of 70 eV, emission current of 40 mA, acquisitions scan mass range of 35-450 amu under full scan. For each component, its retention time indices were identified with respect to those of a homologous *n*-alkane series obtained using the identical GC conditions. Contents of constituent were calculated based on the GC peak area (MSD response) without correction.

RESULTS AND DISCUSSION

The average yield of essential oils extracted from *B. frutescens* by the hydrodistillation method of about 0.75-0.82%. The essential oil of *B. frutescens* was light yellow, a light scent similar to eucalyptus oil and lighter than water. The extraction performance in this study was relatively lower in comparison with results from the same species studied by

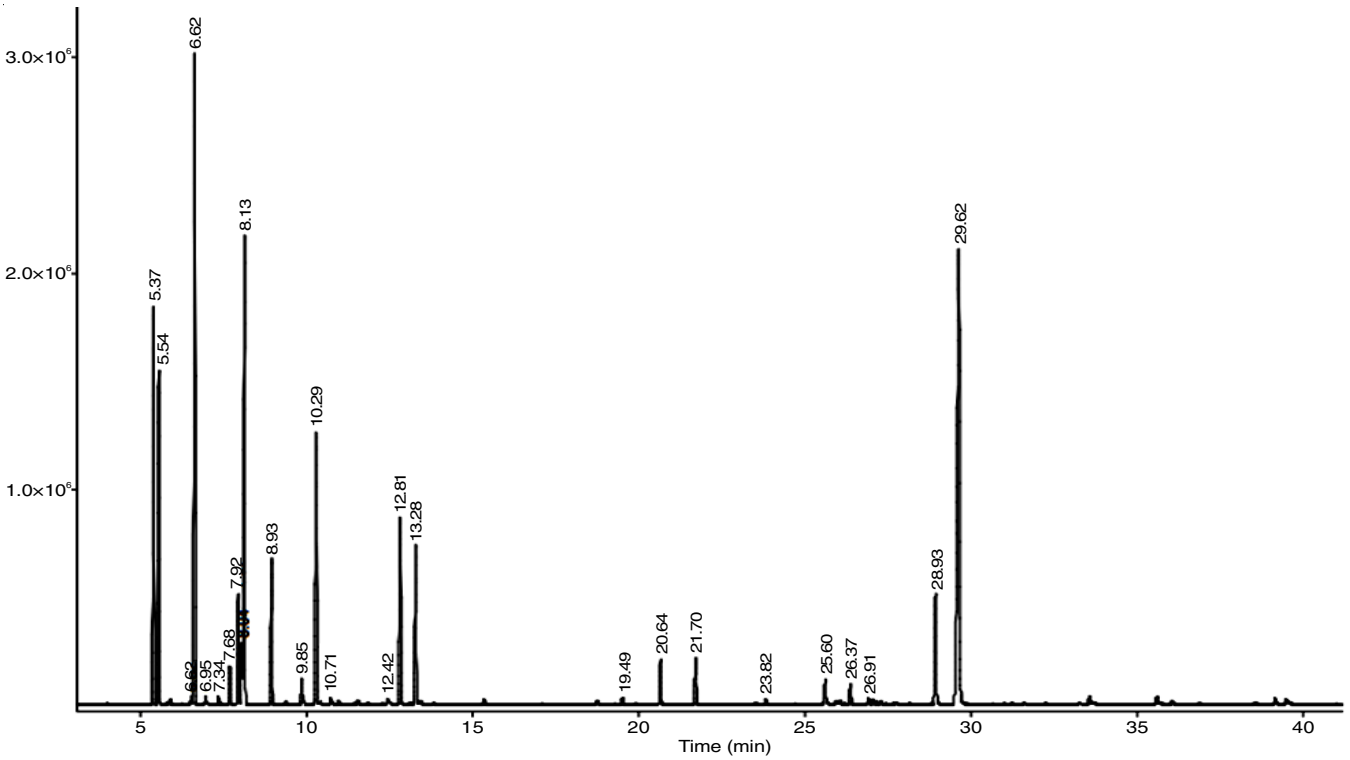

Fig. 1. Chromatogram showing the chemical composition of essential oils extracted from *B. frutescens* leaves analyzed by GC

Jantan *et al*. [16] in Malaysia with a content of about 1.8-2.3%. In contrast, in the report of Jemi *et al*. [17], the percentage of yield obtained from hydrodistillation of *B. frutescens* (0.071%) leaves was lower in this study.

The main component of *B. frutescens* essential oil is determined based on the GC-MS analysis (Fig. 1) and the results are shown in Table-1, which corresponds to 26 essential constituents, accounts for 99.32% of *B. frutescens* leaf essential oil, of which an unidentified compound accounts for 3.44%. Major constituents in the essential oil of *B. frutescens* were tasmanone (21.46%), β-pinene (15.64%), 1,8-cineole (11.32%), α-thujene (8.74%), α-pinene (7.18%), linalool (7.44%), terpinen-4-ol (5.11%), α-terpineol (4.46%), γ-terpinene (3.37%), *o*-cymene (2.72%), and some other compounds with < 1% content.

Another report by Fokkens *et al*. [18] where *B. frutescens* essential oil of the material collected from Hue province, Vietnam identified seven main components. Of which, the compound with the highest contents consist of ρ-cymen (20.1%), followed by β-caryophyllene (13.7%), α-thujene (2.4%), α-pinene (5.5%) and baeekeol (10.1%).

Some compositional differences in the current results were also compared to results obtained previously from the essential oils of *B. frutescens* harvested from other regions. This discrepancy is possibly due to the environmental conditions, the season in which the plants are harvested, the care process, and the species. Additionally, dehydration process, the storage conditions that the plants are harvested until the extraction of essential oils, the method used to isolate the essential oils and the analytical conditions are among the factors affecting the determination of compounds of essential oil [19,20].

Tasmanone compound of *Baeckea frutescens* in the present study almost accounted for a relatively higher content than the tasmanone content in essential oils in the surrounding area material sources [14,21]. It was indicated by Tam *et al*. [14] that tasmonone is the equilibrium form of tautomers (Fig. 2). To be specific, as the intramolecular hydrogen bond is formed, connecting the hydrogen of hydroxyl group and the carbonyl group, a ring of six members could be formed at the origin.

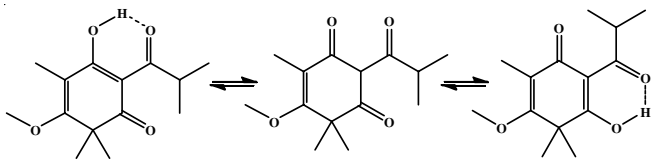

Fig. 2. Tasmanone tautomers

Conclusion

The optimized hydrodistillation of *Baeckea frutescens* achieves 0.75%-0.82% extraction efficiency. Chromatographic analysis of *B. frutescens* essential oil identified 29 different compounds, the most dominant being tasmanone (21.46%). Some other components were β-pinene (15.64%), 1,8-cineole (11.32%), α-thujene (8.74%), α-pinene (7.18%), linalool (7.44%), terpinen-4-ol (5.11%), α-terpineol (4.46%), γ-terpinene (3.37%), *o*-cymene (2.72%). *B. frutescens* oil has great economic

TABLE-1
RETENTION TIME (min) AND PEAK AREA (%) OF THE DIFFERENT COMPOUNDS FOUND IN *B. frutescens* ESSENTIAL OIL ANALYZED BY GC-MS

Peak	R.T.	RI	Hit (%)	Chemical name	Integral	%
1	5.37	927	93	α-Thujene	41331846	8.74
2	5.55	934	95	α-Pinene	33986497	7.18
3	6.52	975	93	Sabinene	836032	0.18
4	6.62	979	92	β-Pinene	73644826	15.64
5	6.95	992	98	Myrcene	786743	0.17
6	7.34	1007	80	α-Phellandrene	775002	0.17
7	7.68	1018	83	α-Terpinene	4051126	0.86
8	7.93	1026	93	*o*-Cymene	12715406	2.72
9	8.04	1030	89	Limonene	7643861	1.66
10	8.13	1033	71	1,8-Cineole	49440894	11.32
11	8.93	1060	91	γ-Terpinene	15889060	3.37
12	9.85	1090	88	Terpinolene	2654797	0.52
13	10.29	1104	79	Linalool	35076644	7.44
14	10.71	1117	51	*endo*-Fenchol	730862	0.13
15	12.42	1170	45	*endo*-Borneol	420882	0.22
16	12.81	1181	76	Terpinen-4-ol	24000782	5.11
17	13.28	1196	87	α-Terpineol	21086084	4.46
18	19.49	1386	56	Geranyl acetate	727329	0.16
19	20.64	1423	86	β-Caryophylene	5907078	1.25
20	21.70	1457	97	α-Humulene	6437486	1.37
21	23.82	1527	69	δ-Cadinene	650630	0.14
22	25.60	1588	55	Caryophyllene oxide	3523519	0.8
23	26.37	1615	63	Humulene Epoxide II	2851417	0.61
24	26.91	1634	38	1-*epi*-Cubenol	1789	0.2
25	28.93	1707	0	unknown (223, 238, RI 1707)	15802451	3.44
26	29.62	1732	100	Tasmanone	100979504	21.46
				Total		99.32

value as well as high use value. Since this species has not been fully exploited in Vietnam, this study is expected to contribute to future development in extending the use of *B. frutescens* oil to products used in daily life activities and in industrial applications.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

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