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# Chemical Constituents of Flower Essential Oil of Ageratum conyzoides growing in Nigeria Usman, $L.A^{1,*}$ , Zubair, M.F<sup>1</sup> Olawore, N.O<sup>2</sup> Muhammad, N.O<sup>3</sup>, M'Civer, F.A<sup>4</sup> and Ismaeel, R.O<sup>1</sup>

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ABSTRACT

Hydrodistilled flowers (500g) of Ageratum convzoides yielded 0.25% v/w of essential oil. Characterization of the oil using GC, GC-MS revealed the predominance of demothoxyageratochromene. Other principal constituents were; β-caryophyllene (19.5%), βcubebene (5.2%), germacrene D (3.9%),  $\alpha$ -caryophyllene (2.9%) and trans- $\beta$ -farmesene (2.4%).

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### Keywords

Hydrodistillation, Demethoxyageratochromene, β-caryophyllene,  $\beta$ -cubebene, germarene D.

## Introduction

Ageratum conyzoides L. (family Asteraceae) is an annual herbaceous plant widely grown in several parts of the world. It is very common in Nigeria where it is known as "Imi esu" by the Yorubas and "Nri-ewu" by the Igbos<sup>[1]</sup>. Its application in herbal medicine varies by region. In central Africa, it is use for the treatments of pneumonia, and wounds caused by burns <sup>[2]</sup>. Traditional communities in Cameroon and Congo use the plant to treat; fever, rheumatism, headache, diabetics and colic  $^{[3,\bar{4},5]}$ .

In addition to its popular use for skin disease and wound healing in Nigeria, a decoction of the plant could be taken to treat diarrhea and relieve pain associated with navel in children

Pharmacological activities such as, antimicrobial <sup>[7, 8]</sup>, antiinflammatory [9], antispasmotic[10], antihyperglycemic[11], haematopoietic,[12] and analgesics,[13] of the plant extract justify its use in traditional medicine.

Phytochemical investigations of the plant revealed the presence of flavonoids, steroids, alkaloids, coumarins and tannins <sup>[14]</sup>. Analysis of the plant essential oils from different countries showed significant variations in the oil constituents. For instance, the oil obtained from Himalayan grown A. conyzoides in Indian was of agerato chromene chemotype<sup>[15]</sup>, while that of R'eunion grown A. conyzoides was characterized by the abundance of demethoxyageratochromene and  $\beta$ -caryophyllene respectively<sup>[16]</sup>. Characterization of leaf essential oil of Nigeria grown A. conyzoides revealed that 71% of the oil was dominated by eight different chromenes of which two of them were novel<sup>[17]</sup>. Meanwhile, there is no report on the flower essential oil of the Nigerian grown plant. It is on this basis that we investigate the oil.

## Experimental

Plant Materials: The fresh flowers of Ageratum conyzoides were obtained in Ilorin, Kwara State, North-Central, Nigeria. Identification was carried out at the herbarium of Forestry Research Institute of Nigeria (FRIN) Ibadan, where voucher specimens were deposited (Herbarium Voucher Number: FHI106480).

Oil Isolation: Pulverized leaves were hydrodistilled for 3h in a Clevenger-type apparatus, according to the British Pharmacopoea Specification<sup>[18]</sup>. The resulting oil was collected, preserved in a sealed sample tube and stored under refrigeration until analysis.

Gas Chromatography: GC analysis were performed on an orion micromat 412 double focusing gas chromatography system fitted with two capillary columns coated with CP-Sil 5 and CP-Sil 19 (fused silica,  $25m \times 0.25mm$ ,  $0.15\mu m$  film thickness) and flame ionization detector (FID). The volume injected was 0.2µL and the split ratio was 1:30. Oven temperature was programmed from 50-230 <sup>o</sup>C respectively. Qualitative data were obtained by electronic integration of FID area percents without the use of correction factors.

Gas Chromatography/Mass Spectrometry: A Hewlett Packard (HP 5890A) GC interfaced with a VG Analytical 70-250S double focusing mass spectrometer was used. Helium was the carrier gas at 1.2ml/min. The MS operating conditions were: ionization voltage 70ev, ion source temperature 230 °C. The GC was fitted with a 25m×0.25mm, fused silica capillary column coated with CP-Sil 5. The film thickness was 0.15µm the GC operating conditions were identical with those of GC analysis. The MS data were acquired and processed by online desktop computer equipped with disk memory. The percentage compositions of the oil were computed in each case from GC peak areas. The identification of the components was based on the retention indices (determined relative to the retention times of series of n-alkanes) and mass spectra with those of authentic samples and with data from Literature <sup>[19-21]</sup>.

#### **Result and Discussion**

Pulverized flower (500g) of Ageratum conyzoides yielded 0.25% (v/w) of essential oil. The yield compared favourably with the yield from flower of Fijian grown A. conyzoides<sup>[22]</sup>.

Table 1 shows the percentage composition, retention indices and identities of the constituents of the oil. Seventeen compounds that represent 98.5% of the oil were identified from their retention indices. The oil was characterized by the abundance of chromene specifically demethoxyageratochromene (57.2%). Sesquiterpenes constituted 39.2% of the oil, while the percentage composition of hydrocarbon and oxygenated monoterpenes were 1.6 and 1.2 % respectively.

 Table 1: Chemical Composition (%) of Flower Essential Oil of Ageratum conyzoides

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Compound <sup>a</sup>	RI <sup>b</sup>	% Composition
Camphene	953	0.7
Car-4-ene	1001	0.8
Limonene	1027	0.1
Borneol	1165	0.4
Isobonyl formate	1233	0.3
Isobonylacetate	1285	0.4
α-cubebene	1349	1.6
Eugenol	1354	0.4
β-cubebene	1389	5.2
β-elemene	1391	0.8
β-cary op hy llene	1418	18.5
α-cary op hy llene	1454	2.9
Cis-β-farnesene	1456	1.5
Demethoxy ageratochromene	1460	57.2
Germacrene D	1479	3.9
Trans-β-farnesene	1523	2.4
Germacrene B	1556	1.4
TOTAL		98.5%

<sup>a</sup>Compound are listed in order of elution from silica capillary column coated in Cp-sil 5; <sup>b</sup>retention indicies on fused silica capillary coloumn coated with Cp-sil 5.

β-caryophyllene (18.5%), β-cubebene (5.2%), germacrene D (3.9%), α-caryopyllene (2.9%) and trans-β-farnesene (2.4%) were the predominant sesquiterpenes in the oil. Germacrene B (1.4%), cis-β-fernesene (1.5%) and α-cubebene (1.6%) were also detected in appreciable quantities. The only aromatic compound eugenol (0.4%) existed as minor constituent. Car-4-ene (0.8%) and camphene (0.7%) were the abundant hydrocarbon monoterpenes in the oil. Limonene (0.1%) was detected as minor constituent. The predominant oxygenated monoterpenes were borneol (0.4%) and Iso bonylacetate (0.4%). But they were found in low proportions.

Qualitatively, the oil and the leaf essential oil of Nigerian and Ivorian grown A. conyzoides were of chromene chemotypes. However, demethoxy ageratochromene was the only chromenes in the oil, while eight different chromenes were detected in the leaf essential oil Nigerian grown A. conyzoides <sup>[17]</sup>. On the other hand, demethoxy ageratochromene was the only chromene found in the leaf essential oil of Ivorian grown A. conyzoides<sup>[23]</sup>. But the chromene, is of greater abundance in the leaf essential oil than the flower essential oil of Nigerian grown A. conyzoides<sup>[23]</sup>.

 $\beta$ -caryophyllene found in significant proportion in the oil compared favourably with  $\beta$ -caryophyllene reported in the leaf essential oil of Ivorian grown A. conyzoides <sup>[23]</sup>. Germacrene D that was detected in significant amount in the oil existed as minor constituent of leaf essential oil of Ivorian grown A. conyzoides<sup>[23]</sup>. Variations in composition pattern of the oil and

the leaf essential oils of A. conyzoides, is attributable to different roles of essential oil in the parts of the plant.

Furthermore, the composition patterns of the oil and flower essential oil of Fijian grown A. conyzoides were similar with respect to the abundance of sesquiterpenes and chromenes<sup>[22]</sup>. But ageratochromene that was found in flower essential oil of Fijian grown A. conyzoides was not identified in the oil. Absence of the chromene in the oil may be due to agro climatic and geographical conditions.

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