THE CHEMICAL CONSTITUENTS' OF THE LEAVE ESSENTIAL OIL OF ALTERNANTHERA PUNGENS (KUNTH)

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ABSTRACT

Alternanthera pungens Kunth commonly called khaki weed is from the family Amaranthaceae. It is a herbaceous perennial plant that has stems prostrate, rarely rising and about 10-50 cm long. The work was carried out due to the scarcity of information on the volatile constituents from the plant leaves despite works on the flower and other parts. The extraction of the essential oils from the dried leaves was carried out by the hydro distillation method using an all-glass Clevenger apparatus. The extracted oils were then analyzed using gas chromatography-mass spectrometry (GC-MS). A total of twelve constituents' representing 93.39% of *A. Pungens* oil with a yield of 0.4% (v/w) was obtained. The analysis of the GC-MS results of the leaf oil showed that it was dominated by *β*-ionone (42.18%) and hexahydrofarnesyl acetone (15.53%), others in trace amounts include; methyl palmitate (6.13%), 1-octadecyne (4.72%), undecane (3.73%), para-mentha-1, 3, 8-triene (3.65%), isophytol (3.21%), ɗ-cadinene (3.06%), 1, 2-dimethyl cyclooctene (3.05%), para-cymene (2.96%), phytol (2.67%) and neophytadiene (2.50%). The common classes of compounds present in the leaves oil are aceto monocyclic monoterpenoid (42.18%), sesquiterpenoids (18.59%), hydrocarbons (11.50%), diterpenoids (8.38%), monoterpenes (6.61%) and fatty acids (6.13%).The constituents and the compositional pattern of essential oil identified from the leaves of *Alternanthera pungens* grown in Nigeria differ quantitatively and qualitatively from previously reported member of the genus and the presence of sesquiterpenoid as one of the major components of the oils justify the traditional use of the plants in treating pains, headaches and inflammations.

Keywords: *Alternanthera pungens*, Essential oil, *β*-iononeand Hexahydrofarnesyl acetone.

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INTRODUCTION

The genus Alternanthera contains medicinal plants that possess volatile constituents, essential amino acids, flavonoids, glycosides and steroids (Khatun *et al.* 2012). *Alternanthera pungens* Kunth commonly known as khaki weed in English and 'dágunró 'in Yoruba Southwest Nigeria, belongs to the Amaranthaceae family. It grows widely in tropical and subtropical regions throughout the world (Burkill, 1985). It is an herbaceous perennial plant that has stems prostrate, rarely rising and about 10-50 cm long (Marchant *et al.,* 1987; Naidu, 2012; Hossain *et al.,* 2018). *Alternanthera pungens* is reported to be used traditionally for the treatment of naso-pharyngeal infections, diarrhea, dysentery, vermifuges, dropsy, swellings, oedema, gout and venereal diseases (Zongo *et al.,* 2011; Hundiwale *et al.,* 2012). It is also use as a painkiller, for treating stomachache, swelling and for lactation stimulus in veterinary (Burkill, 1985; Mourya *et al.,* 2018).

The plant has been shown to exhibit antioxidant, antimicrobial, antidiabetic, antidiarrhea, spasmogenic, diuretic, and anti-HIV properties (Petrusand Seetharaman, 2005). The analgesic potential of *Alternanthera pungens* ethanolic extract leaves investigated revealed an improved analgesic effect compared to the standard used. The analgesic effect was attributed to the presence of phytochemicals like flavonoids, tannins and phenolic compounds (Hossain *et al.,* 2018). Furthermore, phytochemicals such as; saponins, alkaloids, steroids, triterpenoids, leucoanthocyanidins, *β*-spinasterol, saponin sheteroside of oleanolic acid, glycosides, flavonoid stannins, carbohydrate, *β*-carotene, lutein, violaxanthin, zeaxanthin and choline has been previously described from this plant extracts (Gupta and Saxena, 1987; Mourya *et al.,* 2018).

Occasionally, other genus like *A. sessilis*, *A. philoxeroides*, *A. bettizicikiana* and *A. brasiliana* (flowers, leaves, stems and roots extracts) have been reported to contain similar or related, but not necessarily the same chemical constituents in different percentages. Some of them includes; phaeophytina, *β*-sitosterol, 3*β*-hydroxystigmast -5-en-7-one, 24-methylene cycloartanol, cycloeucalenol, phytol, *β*-carotene, *α*-spinasterol, campesterol, triterpenoids, phytosterols, glycosides, alkaloids, flavonoids, steroids, phenolic compounds, carbohydrate, amino acids, proteins, ionone derivatives, saponins, lipids and tannins (De Sooza *et al.,* 1998; Ragasa *et al.,*2002; Fang *et al.,* 2006; Aguirre *et al.,* 2013; Walter *et al.,* 2014; Vidhya *et al.,* 2015; Devi *et al.,* 2015; Pulipati *et al.,* 2016). The chemical compositions of essential oils (oxygenated sesquiterpenes, diterpenes, ketones, fatty acid and esters) extracted from the flower and leaf of *Alternanthera sessilis* by hydro distillation showed remarkable difference in constituents and percentage composition as well as difference in the antioxidant effect on 1-diphenyl-2-picrylhydrazyl (DPPH) radical scavenging capacities. The major chemical composition of leaves oil are; 1, 1, 1, 5, 5, 5-hexamethyl-3, 3-bis [(trimethylsilyl) oxy] trisiloxane (15.43%) which is an oxygenated diterpenes followed by S, S-dioxide trans-2-methyl-4-*N*-pentylthiane (11.27%), didodecylphthalate (10.62%) and tetrahydro-2, 5-dimethoxy furan (10.01%) while the prominent ones from flower oil are; 1, 1, 1, 5, 5, 5-hexamethyl-3, 3-bis [(trimethylsilyl) oxy] trisiloxane (17.76%), trans-4-ethyl-5-octyl-2, 2-bis (trifluromethyl)-1, 3-dioxolane (11.12%) and tetrahydro-2, 5-dimethoxy furan (9.10%). (Khan *et al.,*2016). Similarly, *A. triandra* seed oil reported a moderate source of ricinoleic acid (22.1%), myristic acid (3.9%), palmitc acid (16.9%), stearic acid (5.90%), oleic acid (26.0%) and linoleic acid (25.2%) (Hosamani *et al.,*2004). Although, the essential oil of *Alternanthera pungens* flower has been analyzed with the following phytochemicals identified; *α*-pinene (7.40%), *β*-pinene (6.42%), camphene (4.21%), myrecene (3.61%), p-cymene (4.29%) limonene (3.52%), *β*-ocimene (2.35%), 1,8-cineole (6.28%), *α*-thujone (3.62%), *α*-borneol (4.46%), *α*-curcumene (2.36%), camphor (5.52%), linalool (6.29%), geraniol (7.42%), *α*-terpineol (3.82%), elemol acetate (6.14%), eudesmol (5.38%), azulene (3.16%) and three unidentified compounds (Gupta and Saxena, 1987). However, there is paucity of information on the essential oil of the leaves. This research is therefore focused on the extraction and determination of the volatile constituents from the leaves of *Alternanthera pungens.*

Materials and Methods

Plant materials

Fresh leaves of *Alternanthera pungens* were obtained from a farm land within Olabisi Onabanjo University, Ago Iwoye, Ogun State, Nigeria. The sample was identified and authenticated at the herbarium of the Forestry Research Institute of Nigeria (FRIN) Ibadan by Mr. A. O. Adeyemo and a voucher specimen with herbarium number FHI-110461 was deposited. The leaves were air dried at room temperature and pulverised before further study.

Extraction of the leaf oil

The air-dried pulverised leaves of *Alternanthera pungens* (500g) was subjected to hydro distillation in a Clevenger-type glass apparatus for 3 h in accordance with established procedure (Ogundajo et al., 2016). The oils collected in hexane was preserved in anamber bottle and stored ina refrigerator for further analysis.

Gas Chromatography-Mass Spectrometry (GC/MS) of the leaf oil.

The GC-MS analysis of the essential oil was carried out on an Agilent model 7890 A gas chromatograph equipped with a FID and fitted with a fused silica capillary HP-5MS column (30 m x 0.32 mm id, film thickness 0.25 µm). The oven temperature was programmed from 80-240oC at the rate of 8oC/min. The ion source was put at 240oC while electron ionisation was set at 70eV. Helium was used as the carrier gas at a flow rate of 2mL/ min. Scanning range was 35-425 amu. Diluted oil in n-hexane (1.0 µL) was injected into the GC/MS.

Identification of the Leaf Essential Oil

The identification of the constituents was performed on the basis of retention indices (RI) determined by co-injection with reference to a homologous series of n-alkanes, under identical experimental conditions. Further identification of the components was done by comparison of their

mass spectra with those from NIST (Data base 69) and Wiley 9th Version and the home-made MS library composed of pure substances and components of known essential oils, as well as by comparing their retention indices with literature values (Adams, 2007; Aboaba *et al.,* 2010).

RESULTS

The chemical constituents identified as revealed by GC-MS results as shows in (Fig. 1.0).Aceto monocyclic monoterpenoid (42.18%), sesquiterpenoids (18.59%), hydrocarbons (11.50%), diterpenoids (8.38%), monoterpenes (6.61%) and fatty acids (6.13%). However, sesterterpenes compounds were conspicuously absent in the essential oil. The yield of essential oil was 0.4% (v/w) calculated on a dry weight basis. The oil sample was cloudy white in colour with a strong herbal odour. A total of twelve constituents representing 93.39% of A. pungens oil were identified. In addition, out of the constituents identified, β-Ionone has the highest percentage (42.18%), followed by hexahy drofarnesyl acetone (15.53%), others include; methyl palmitate (6.13%), 1-octadecyne (4.72%), undecane (3.73%), para-mentha-1, 3, 8-triene (3.65%), isophytol (3.21%), □-cadinene (3.06%), 1, 2-dimethyl cyclooctene (3.05%), para-cymene (2.96%), phytol (2.67%) and neophytadiene (2.50%) with the lowest percentage (Table 1.0).

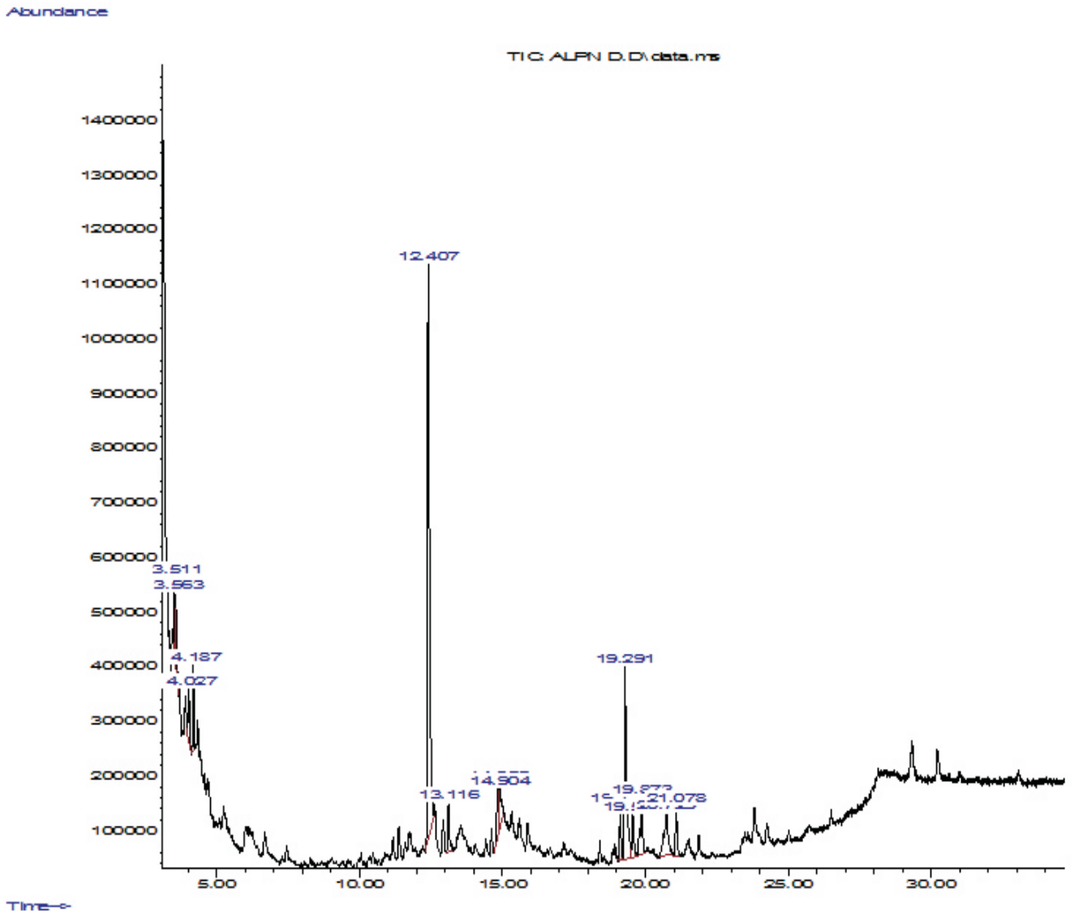

Fig. 1.0:Total Ion Chromatogram of leaf essential oil of *A. pungens*

Table 1.0: The chemical composition of the leaf essential oil of *A. pungens*

S/N	Compounds (common names)	Retention index cal	Retention index lit.	Retention time	% Composition	Molecular formulae
1	1, 2-Dimethyl cyclooctene	986	990	3.511	3.05	$C_{10}H_{18}$
2	*p*-Mentha-1,3,8-triene	1000	1110	3.562	3.65	$C_{10}H_{14}$
3	*p*-Cymene	1074	1073	4.025	2.96	$C_{10}H_{14}$
4	Undecane	1115	1100	4.186	3.73	$C_{11}H_{24}$
5	*β*-Ionone	1468	1461	12.408	42.18	$C_{13}H_{20}O$
6	*δ*-Cadinene	1374	1530	13.118	3.06	$C_{15}H_{24}$
7	Neophytadiene	1810	1827	19.126	2.50	$C_{20}H_{38}$
8	Hexahydrofarnesyl acetone	1954	1858	19.292	15.53	$C_{18}H_{36}O$
9	Phytol	2105	2111	19.566	2.67	$C_{20}H_{40}O$
10	1–Octadecyne	1920	1238	19.875	4.72	$C_{18}H_{34}$
11	Methyl palmitate	1942	1928	20.728	6.13	$C_{17}H_{34}O_2$
12	Isophytol	1899	1920	21.077	3.21	$C_{20}H_{40}O$

DISCUSSIONS AND CONCLUSION

The quantitative amount of *β*-ionone in this oil is noteworthy (42.18%), since it has not been previously reported to be a major compound of *A. pungens*. *β*-Ionone is one of essential constituents in most aromatic oils used in the production of perfumes due to its strong pleasant odour (Cseke *et al.,* 2007). Furthermore, *β*-ionone has been reported to be fragrance ingredient in perfumery, cosmetics, personal care products, household cleaners and detergents. It is also a flavouring agent in beverages, baked goods, and candies. *β*-ionone is of use, not only in perfumery, but also as a key intermediate in the synthesis of Vitamins A, E and K (Lalko *et al.,* 2007). Not surprisingly, the steam distillation of the flower essential oil (0.6%) of *A. pungens* has a very different composition compared to the leaf oils. These includes; *α*-pinene (7.40%), *β*-pinene (6.42%), camphene (4.21%), myrecene (3.61%), para-cymene (4.29%), limonene (3.52%), β-ocimene (2.35%), cineole (6.28%) among others (Gupta and Saxena, 1987). Previous report on essential oils of another specie; *A. sessilis* from Malaysia showed the major components of leaves as 1,1,1,5,5,5-hexamethyl-3, 3-bis [(trimethylsilyl) oxy] trisiloxane (15.43%), S, S - dioxide trans - 2 - methy l - 4 - *N* - penty l thiane (11.27%), didodecylphthalate (10.62%) and tetrahydro-2, 5-dimethoxy furan (10.01%), unlike the current work that was majorly dominated by *β*-ionone (42.18%) and hexahydrofarnesyl acetone (15.53%). The other characteristics compounds previously reported from *A. sessilis* were; octyl ester-2-propenoic acid (9.32%), 1-fluorododecane (6.60%), 1-chlorooctadecane (3.99%), methyl-2-*O*-methyl-*α*-*D*-xylofuranoside (3.13%), (*Z*)-7-tetradecene (3.12%), trimethyl (4-terbutylphenoxy) silane (2.98%), 1,1'-oxybis-heptane (2.41%), cis-4-penty l-5-propyl-2, 2-bis (trifluoromethyl)-1, 3-dioxane (2.29%) and 9-heptadecanone (2.06%) (Khan *et al.,* 2016).

The chemical compositions of essential oil from the leaves of *A. pungens* grown in Nigeria are being reported for the first time based on available information. The analysis of the extracted essential oil from *A. pungens* showed the presence of aceto monocyclic monoterpenoids (42.18%), sesquiterpenoids (21.41%) and hydrocarbons (11.50%) as the major predominant classes of compounds. Oxygenated diterpenes (11.27%) was reported as the most prominent from the leaf oil of *A. sessilis* (Khan *et al.,* 2016) as compared to aceto monocyclic monoterpenoids (42.18%) which is the major class in the present study. It was observed that constituents and the compositional pattern of

essential oil from the leaves of *Alternanthera pungens* grown in Nigeria differ quantitatively and qualitatively from previously reported member of the genus (Khan *et al.,* 2016). This may be attributable to factors such as the ecological and climatic conditions as well nature and age of the plant, period of collection, handling procedures and other related factors known to induce variation in essential oil composition extracted from plants (Gurusaravanan *et al.,* 2010; Verma *et al.,* 2013; Inikpi *et al.,* 2014; Rehman *et al.,* 2016; Ibanez and Blazquez, 2019). Conclusively, the chemical compositions of essential oil from the leaves of *A. pungens* grown in Nigeria are being reported for the first time based on available information. The presence of sesquiterpenoid as one of the major classes of compounds of the oils justifies the traditional use of the plants in treating pains, headaches and inflammations. Also, the identified chemical constituents of the plant are an addition to the chemical data base for the plant.

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