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Chemical compositions of the essential oils from aerial, seed and root parts of nigerian *Asystasia gangetica* (L)

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Abstract

Volatile oils from aerial, seed and root parts of *Asystasia gangetica* (L) were analyzed for their constituents by means of gas chromatography and gas chromatography coupled with mass spectrometry. Fifty-four compounds were identified in aerial, twenty-one in seed, fifteen in root, respectively which are responsible for 96.80%, 65.11% and78.50% of oil in each. Aerial is dominated by phthalates (39.00%), cycloalkanes (28.23%) and aromatics (17.14%); the most abundant compounds are toluene (9.12%), methylcyclohexane (9.02%) and bis-isodecyloctylphthalate (6.05%). Others in aerial are branched (6.13%) and straight chain alkanes (3.24%), esters (1.71%), alcohol (0.72%), acid (0.36%), heterocompound (0.27%), ketone (0.18%) and terpenoid (0.09%). Phthalates (24.67%), alcohols (16.28%) and straight chain alkanes (8.56%) are the largest groups in seed oil, with dinonylphthalate (9.40%), 1-octenol (8.05%) and methylcyclohexane (6.04%) as most important. Also it contain cycloalkanes (6.04%), aromatics (5.03%), terpenoid (4.03%), ester (3.02%), acid (1.01%), amide (1.01%) and branched alkane (0.50%). Root oil have alcohols (27.32%), straight chain alkanes (23.61%) and aldehydes (15.91%) as the most noticeable, while its dominant compounds are abietal (11.67%), n-tetracosane (10.08%) and palustrol (9.02%). It also have phthalate (5.83%), aromatics (5.83%) and cycloalkane (4.24%). Derivatives of phthalate are obvious in the three oils. There are no aldehyde in aerial; no ketone and aldehyde in seed; no terpenoid, ester, ketone, acid and hetero compounds in root. Notable is the low amount of ubiquitous terpenoids in aerial and seed essential oils, which is absent in root. Unsaturated compound and ether are not in the oils. Chemical composition of *Asystasia gangetica* (L) is reported for the first time in literature.

Keywords

Asystasia gangetica; Acanthaceae; Phthalates; Alcohols.

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INTRODUCTION

Asystasia gangetica (L) [Chinese violet], an annual perennial semi-woody herb belongs to the family Acanthaceae occurs throughout the tropics, it grows up to 1 m high[1]. It is occasionally cultivated as an ornamental plant and is commonly known as Chinese violet, creeping foxglove[2,3]. It is a local traditional vegetable not requiring cultivation. The plant is referred to in Nigeria by different ethnic names such as lobiri[*YORUBA*], èbóghògíró[*EDO*](Ross), ékèrè *Agukwu*[*IGBO*](Millson)[1]. It is called Isihobo in Zulu[4]. *Asystasia gangetica* occurs throughout tropical Africa where it is locally used as a potherb and leafy vegetable, mainly in times of scarcity of other vegetable.

The plant has many medicinal, nutritional and local values. In Nigeria the leaves are used to treat, combat and manage asthma[5]. In Kenya and Uganda it is utilized as a popular vegetable, mixed with beans and groundnut or sesame paste. It is also often prepared in a mix with other leafy vegetables. *Asystasia gangetica* is sometimes promoted as a cover plant in orchards because it checks erosion and prevents infestation by noxious weeds; it also attracts bees to the orchard. Because of its ability to grow under shade and its high nutritive value, *Asystasia gangetica* is used as forage for cattle, goats and sheep in Southeast Asia; it is either grazed or cut for stall feeding. Excessive consumption by sheep can result in bloat[4-6]. In Africa infusion of the plant is used to ease pain during childbirth, the sap is applied to cure sores, wounds and piles, and in embrocating to treat stiff neck and enlarged spleen in children. Powdered roots are considered analgesic, also used in treating stomach-ache and snakebites[1,6,7]. Leaf decoction is used as analgesic and to treat epilepsy and urethral discharge. In India the sap is applied to swellings and also used as a vermifuge and to treat rheumatism. In Moluccas (Indonesia) the juice, together with lime and onion juice, is recommended for dry coughs with an irritated throat and discomfort in the chest. In Philippines the leaves and flowers are used as an intestinal astringent[1,6-8]. In Tanzania plants are pounded with water to make a wash against fleas for young animals. The edible leafy vegetable not requiring cultivation has been recommended for commercial cultivation[9].

Asystasia gangetica is one of the specially active eight out of 16 plants that demonstrated ACE inhibition activity. It has potential ACE inhibitor activity in herbal preparations to inhibit angiotensin- converting enzyme [ACE inhibitors]. This was presented during the Experimental Biology 2007 conference attended by 12,000 scientific researchers[10]. Phytochemical screening showed the presence of carbohydrates, proteins, alkaloids, tannins, steroidal aglycones, saponins, flavonoids, reducing sugars, and triterpenoids in the plant[5,11]. Asystoside an aliphatic alcohol glycoside and 3'-*O*-β-D-glucopyranosyl-catalpol an iridoid diglucoside were isolated from the aerial part of *Asystasia intrusa* along with benzyl β-D-glucopyranoside, zizybeoside I, (6*S*,9*R*)-roseoside, verbascoside, ehrenoside, 6β-hydroxyantirrhide, angeloside, catalpol, ajugol, 6-deoxycatalpol, and scutellarioside II[12]. There are about 50 species of *Asystasia* distributed in the tropics of the Old World, with about 30 species in tropical Africa[1,6-8].

This paper present chemical compositions of the essential oils from three parts [aerial, seed and root] of the locally useful *Asystasia gangetica* (L) which is scarce in literature. The results can also be of great industrial value.

EXPERIMENTAL

Plant collection

The plant material was collected fresh in January 2008 from the mini campus, Olabisi Onabanjo University, Ago-Iwoye. It was authenticated by staff of the herbarium, Department of Botany and Microbiology, University of Ibadan.

Collection of the essential oils

Fresh sample of *Asystasia gangetica* (L) were separated into leafy aerial, seed and root parts. Each separated part [aerial (1250g), seed (210g), root (190g)] was crushed and hydrodistilled for 2 to 3 hours in an all glass Clevenger-type apparatus designed to British Pharmacoepia specifications, with a small quantity of distilled *n*-hexane (0.3 ml), which was removed afterwards. The essential oils were procured in 0.10%, 0.56% and 0.51% yields respectively.

Gas chromatography (GC)

The three essential oils were subjected to GC analyses on an agilent model 6890 gas chromatograph fitted with a flame ionization detector (FID) and DB-5 (30x0.25mm, 0.25μm film thickness). Helium was used as carrier gas at a flow rate of 1ml/min. The GC oven temperature was programmed at 60°C (held for 2mins), heated to 250°C at 4°C/min, with final hold time of 20min. Injector and detector temperatures were fixed at 200°C and 250°C respectively.

Gas chromatography-Mass spectrometry (GC-MS)

The GC-MS analyses were performed on an Agilent model 6890 GC-MSD system with split/splitless automated injection interfaced to a 5973 mass selective detector operated at 70eV with a mass range of m/z 50-500. Same operations and temperature programming were used as for GC. Relative percentage amounts of the separated compounds were calculated from FID chromatograms as seen in TABLES 1, 2 and 3.

Identification of components

Identification of the essential oil components were based on their retention indices[RI] (determined with a reference to a homologous series of n-alkanes), and by comparison of their mass spectral fragmentation patterns in computer matching against in-built data

which gave qualitative correlation of not less than 98%; and commercials such as NIST database/ Chemstation data system, Wiley GC-MS Library[13], Adams Library[14], Mass Finder 3.1 Library[15] and in-house "Ba°er Library of Essential Oil Constituents" built up by genuine compounds and components of known oils.

RESULTS

TABLE 1 : Essential oil composition of aerial parts of *Asystasia gangetica* (L)

Peak No[a]	Identified Compound[b]	%TIC[c]	RI[d]	RT [mins][e]	Peak No[a]	Identified Compound[b]	%TIC[c]	RI[d]	RT [mins][e]
1	2,2,3,3-tetramethylbutane	0.54	313	3.28	28	propylcyclohexane	0.45	751	8.62
2	Methylcyclohexane	9.02	319	3.38	29	2,6-dimethyloctane	0.27	754	8.73
3	ethylcyclopentane	3.61	326	3.49	30	2-methyl,4-heptanone	0.18	761	8.99
4	1α,2β,4α-trimethylcyclopentane	2.80	330	3.56	31	cis-pinane	0.09	769	9.26
5	1α,2α,3β-trimethylcyclopentane	2.62	337	3.66	32	methylarsonic acid	0.36	779	9.62
6	2-methylheptane	1.71	352	3.89	33	4-methylnonane	0.27	784	9.79
7	toluene	9.12	360	4.03	34	1-ethyl,2-methylbenzene	0.81	788	9.91
8	1,3-dimethylcyclohexane	3.61	371	4.19	35	1,3,5-trimethylbenzene	0.63	796	10.21
9	1,1-dimethylcyclohexane	0.81	381	4.35	36	1-octen-3-ol	0.72	1063	10.72
10	1-ethyl,2-methylcyclopentane	0.45	386	4.43	37	1,2,3-trimethylbenzene	1.26	1074	11.19
11	2,4-dimethylheptane	2.17	448	4.54	38	n-decane	1.44	1078	11.32
12	ethylpentanoate	1.44	449	4.55	39	4-methyldecane	0.36	1099	12.21
13	1,2-dimethylcyclohexane	1.44	450	4.59	40	1,2,4-trimethylbenzene	0.45	1102	12.34
14	1,4-dimethylcyclohexane	0.54	457	4.75	41	o-cymene	0.09	1473	14.83
15	3,7-dimethylundecane	0.36	476	5.25	42	undecane	0.36	1483	15.27
16	ethylcyclohexane	0.99	484	5.47	43	bis-2-ethylhexylphthalate	1.53	4938	50.49
17	1,1,3-trimethylcyclohexane	0.99	487	5.56	44	bis-7-methyloctylphthalate	0.99	4940	50.55
18	chlorobenzene	0.27	501	5.91	45	bis-butyldecylphthalate	2.26	4977	51.66
19	1α,2β,4β- trimethylcyclohexane	0.45	504	6.00	46	bis-diheptylphthalate	3.61	5193	51.96
20	isopropylbutyrate	0.27	507	6.06	47	bis-heptyloctylphthalate	2.35	5221	52.76
21	ethylbenzene	0.72	517	6.33	48	bis-decylhexylphthalate	4.15	5229	53.00
22	2,5-dimethylheptane	0.45	525	6.54	49	bis-isodecylhexylphthalate	4.06	5239	53.30
23	o-xylene	2.62	527	6.61	50	bis-decyloctylphthalate	5.69	5264	54.03
24	1-ethyl,4-methylcyclohexane	0.45	709	7.13	51	bis-isodecyloctylphthalate	6.05	5271	54.24
25	p-xylene	0.72	716	7.40	52	bis-didecylphthalate	2.62	5276	54.41
26	nonane	1.44	719	7.49	53	bis-diundecylphthalate	5.69	5280	54.50
27	cis-octahydro-1H-indene	0.45	740	8.25	54	4-methoxy-3-(8-quinolinyloxymethyl) benzaldehyde	tr[f]	5488	54.90

[a]According to the pattern of elution from the GC [Figure 1 Asy.gan AERIAL]; [b] see identification of components [c] % composition from total ion concentration [TIC] on chromatograph; [d] Retention Index; [e] Retention time in minutes; [f] In trace amount less than 0.01%.

DISCUSSION

Procured volatile oils from the aerial, seed and root parts of *Asystasia gangetica* (L) [Chinese violet] had characteristic odours: the aerial had leafy odour, seed with fairly peppery fruity odour, and the root had characteristic dry paper woody-like odour. They were obtained in the following yields: 0.10% (aerial), 0.56% (seed) and 0.51% (root). GC and GC-MS analyses of the essential oils showed that not less than fifty-four compounds are in the aerial oil which make-up 96.80% of it, thirty-one in the seed is responsible for 100% of it and twenty-two in the root part make up 99.97% of it. Identified compounds are fifty-four in the aerial (96.80%), twenty-one in seed (65.11%), and fifteen in root (78.50%).

Aerial essential oil is dominated by phthalates (39.00%), cycloalkanes (28.23%) and aromatics (17.14%); the most abundant compounds are toluene (9.12%), methylcyclohexane (9.02%), bis-isodecyloctylphthalate (6.05%), bis-decyloctylphthalate (5.69%) and bis-diundecylphthalate (5.69%). Other groups in the aerial essential oil are branched (6.13%) and straight chain alkanes (3.24%), esters (1.71%), alcohol (0.72%), acid (0.36%), heterocompound (0.27%), ketone (0.18%) and terpenoid (0.09%) [TABLE 1].

Phthalates (24.67%), alcohols (16.28%) and straight chain alkanes (8.56%) are the largest group of compounds in the seed oil, with dinonylphthalate (9.40%), 1-octenol (8.05%), methylcyclohexane (6.04%), heptyloctylphthalate (5.03%) and n-tetracosane (4.70%) as most important compounds. It also have cycloalkanes (6.04%), aromatics (5.03%), terpenoid (4.03%), ester (3.02%), acid (1.01%), amide (1.01%) and branched alkane (0.50%) [TABLE 2].

Root oil have alcohols (27.32%), straight chain alkanes (23.61%) and aldehydes (15.91%) as the most noticeable groups, while its dominant compounds are abietal (11.67%), n-tetracosane (10.08%), palustrol (9.02%), abietol (8.49%) and tricosane (7.43%). Also present are phthalate (5.83%), aromatics (5.83%) and cycloalkane (4.24%) [TABLE 3].

Generally components in the three essential oils can be grouped into about fourteen important classes of compounds with varied percentage compositions [TABLE 4]. Derivatives of phthalate are obvious in the three essential oils of *Asystasia gangetica*. Identified compounds do not contain aldehyde in the aerial volatile oil; ketone and aldehyde, are not in seed oil; no terpenoid, ester, ketone, acid and hetero compounds in root oil.

TABLE 2 : Essential oil composition of the seed of *Asystasia gangetica* (L)

Peak No[a]	Identified Compound[b]	%TIC[c]	RI[d]	RT [mins][e]	Peak No[a]	Identified Compound[b]	%TIC[c]	RI[d]	RT [mins][e]
1	methylcyclohexane	6.04	319	3.37	17	n-tricosane	1.68	5587	57.70
2	toluene	1.51	365	4.10	18	Didodecylphthalate	3.19	5792	58.30
3	2,5-dimethylheptane	0.50	523	6.50	19	Bis-(7-methyloctyl)phthalate	3.69	5799	58.49
4	1-octen-2-ol	8.05	1063	10.72	20	Palustrol	4.03	5817	59.00
5	1,2,3-trimethylbenzene	1.17	1075	11.20	21	n-tetracosane	4.70	5826	59.25
6	n-docosane	1.17	4963	51.35	22	ui[g]	4.03	5854	60.00
7	Phenyl-3-deoxy-β-d-ribo-hexapyranoside	1.34	5225	52.90	23	ui[g]	3.52	5861	60.20
8	11-phenoxy-undecanoic acid	1.01	5236	53.23	24	ui	5.03	5876	60.62
9	2-butyl-2-hydroxy-N-(pyridyl)-hexanamide	1.01	5250	53.62	25	ui	4.70	5885	60.86
10	Heptyloctylphthalate	5.03	5274	54.33	26	ui	3.86	5904	61.38
11	Manool	2.52	5292	54.87	27	ui	3.52	5913	61.64
12	octadecanol	1.68	5499	55.20	28	ui	2.85	5934	62.20
13	Methyl 2-methyl hexacosanoate	3.02	5513	55.61	29	ui	2.18	5941	62.40
14	diisooctylphthalate	3.36	5531	56.10	30	ui	3.52	5968	63.14
15	Dinonylphthalate	9.40	5542	56.42	31	ui	1.68	5977	63.40
16	n-heneicosane	1.01	5569	57.20					

[a] According to the pattern of elution from the GC [Figure 2 Asy.gan SEED]; [b]see identification of components [c] % composition from total ion concentration [TIC] on chromatograph; [d]Retention Index; [e]Retention time in minutes; [g]unidentified compound.

TABLE 3 : Essential oil composition of the root part of *Asystasia gangetica* (L)

Peak No[a]	Identified Compound[b]	%TIC[c]	RI[d]	RT[mins][e]	Peak No[a]	Identified Compound[b]	%TIC[c]	RI[d]	RT[mins][e]
1	methylcyclohexane	4.24	321	3.4	12	abietal	11.67	5538	56.31
2	toluene	1.06	359	4.0	13	ui	4.24	5794	58.36
3	o-xylene	0.53	527	6.6	14	tricosane	7.43	5799	58.49
4	1-octenol	2.65	1062	10.7	15	palustrol	9.02	5814	58.92
5	n-decane	0.53	1077	11.3	16	abietol	8.49	5818	59.05
6	ui[g]	0.26	2356	24.4	17	decylhexylphthalate	5.83	5830	59.34
7	ui[g]	1.33	3907	39.6	18	tetracosane	10.08	5834	59.47
8	ui	0.53	3984	42.3	19	ui	9.81	5845	59.77
9	ui	1.59	4962	44.5	20	neoabietol	7.16	5851	59.92
10	n-docosane	1.86	4966	51.35	21	n-pentacosane	3.71	5862	60.24
11	dehydroabietal	4.24	5273	54.32	22	ui	3.71	5870	60.45

[a] According to the pattern of elution from the GC [Figure 3 Asy.gan ROOT]; [b]see identification of components [c] % composition from total ion concentration [TIC] on chromatograph; [d]Retention Index; [e]Retention time in minutes; [g]unidentified compound.

TABLE 4 : Important classes of compounds in the three essential oils [AERIAL, SEED and ROOT] of *Asystasia gangetica* (L)

Part of plant	n-Alkane	Branched alkane	Cyclo alkane	Aromatics	Terpenoids	Esters	Ketones	Acids	Aldehydes	Alcohols	Phthalates	Hetero compounds	Others
AERIAL %	3.24	6.13	28.23	17.14	0.09	1.71	0.18	0.36	-	0.72	39.00	0.27	-
SEED %	8.56	0.50	6.04	5.03	4.03	3.02	-	1.01	-	16.28	24.67	-	1.01
ROOT %	23.51	-	4.24	5.83	-	-	-	-	15.91	27.32	5.83	-	-
TOTAL %	35.31	6.63	38.51	28.00	4.12	4.73	0.18	1.37	15.91	44.32	69.50	0.27	1.01

Notable also is the low amount of ubiquitous terpenoids in aerial and seed essential oils, which is absent in root of *Asystasia gangetica* (L) [Chinese violet], unsaturated compound and ether are not in all the three. There is presence of isomers of cycloalkanes and aromatic compounds. Chemical composition of *Asystasia gangetica* (L) is being reported for the first time in literature.

CONCLUSION

Essential oils of aerial, seed and root parts of *Asystasia gangetica* (L) [Chinese violet] were procured by hydro distillation under iced water in 0.10%, 0.56% and 0.51% yields respectively and each had characteristic odours. Identified compounds from GC and GC-MS analyses were fifty-four in the aerial (96.80%), twenty-one in seed (65.11%), and fifteen in root (78.50%). Derivatives of phthalate are obvious in the three essential oils of *Asystasia gangetica* (L), where the three volatile oils differ in composition. There are isomers of cycloalkanes and aromatic compounds with low amount of ubiquitous terpenoids in the chemical compositions of *Asystasia gangetica* (L) which is reported for the first time in literature.

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