SUPPLEMENTARY MATERIAL

Chemical characterisation of essential oils of leaves of two Solanaceae: *Solanum rugosum* and *Solanum erianthum* from Côte d'Ivoire.

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Abstract: This study made it possible to characterise by GC (in combination with retention indices), GC-MS and ^{13}C NMR, the chemical composition of the essential oils from *Solanum rugosum* and *Solanum erianthum*, two Solanaceae of the Ivorian flora. The two essential oils were characterised by a very high proportion of sesquiterpenes. Specifically, the essential oil of *S. rugosum* was dominated by (E)-β-caryophyllene (33.7%), β-elemol (19.8%) and germacrene D (14.4%), while that of *S. erianthum* was mainly composed of α-humulene (38.6%), β-elemol (17.8%) and (E)-β-caryophyllene (16.7%). The chemical composition of *Solanum rugosum* is described here for the first time**.**

Keywords: Essential oil composition; *Solanum rugosum; Solanum erianthum*; hydrodistillation; GC-MS; ^{13}C NMR

Experimental

Plant material

Leaves of *S. rugosum* and *S. erianthum* were harvested in the Abidjan district respectively at Abobo and Adjamé in the period from July to September 2017 and then dried under permanent cooling at a temperature of 18°C for three days. The identification was made by the botanists of Université Nangui Abrogoua and CNF (Centre National de Floristique) of Université Félix Houphouët-Boigny with references LAA 10504 and LAA 10503.

Hydrodistillation

The extraction of the essential oils was made from a Clevenger type apparatus during 4 hours. Each oil was dried over anhydrous $MgSO_4$ and then conserved in refrigerator (4°C).

Gas chromatography (GC) analyses

The extracted essential oils were analysed by means of a gas chromatograph (Perkin-Elmer type Clarus 500), equipped with a divider injector, with two columns of apolar and polar silica of 50 x 0.22 mm. internal diameter, 0.25 µm thick of the film, respectively lined with polydimethylsiloxane (C_2H_6OSi) n and polyethylene glycol, and two flame ionization detectors. The operating conditions are as follows: the carrier gas is hydrogen; the pressure at the top of the column is 20 psi; the temperature of the injector and detectors is 250 ° C. The temperature programming is 60 ° up to 220 ° C at a rate of 2 ° C / min, with a bearing of 20 min at 220 ° C; the injection was done by divider mode with a 1/60 ratio. The quantity of sample injected is 0.5 µL from a solution containing 50 µl of HE in 350 µl of $CDCl_3$.

Gas chromatography coopled with mass spectroscopy (GC-MS)

The analyses were carried out using a Perkin Elmer autosystem XL chromatograph, equipped with an automatic injector and an apolar column (Rtx-1) (internal diameter: 60 mx 0.22 mm, film thickness 0, 25 µm), coupled to a Perkin Elmer TurboMass mass detector. The carrier gas is hydrogen (1 mL / min) and exerts a column pressure at 25 psi. The temperature of the injector is 250 ° C and that of the detector 280 ° C. The programming of the temperature consists of an elevation of 60 ° C to 230 ° C, at 2 ° C / min, then a 45-minute plateau at 230 ° C. The injection was done by split mode with a division ratio of 1/50. The quantity of sample injected is 0.2 µL. The mass spectra are obtained by means of a quadrupole filter detector and the ionization is made by electronic impact by an electron beam of 70 eV.

Nuclear Magnetic Resonance (NMR) analyses

The NMR spectra were carried out using a Bruker 400 AVANCE spectrometer operating at 100.623 MHz for the ^{13}C. The spectra were recorded with a 5 mm probe. The solvent is $CDCl_3$ supplemented with tetramethylsilane (TMS). The chemical shifts are given in ppm (δ) with respect to the TMS taken as internal reference.

Identification of individual constituents

Component identification was based on: (a) comparison of their GC retention indices (RI) on polar and apolar columns determined relative to the retention times of a series of *n*-alkanes (C7-C28) with linear interpolation (Target Compounds software from Perkin Elmer) with those of authentic compounds or literature data (König et al. 2001), (b) on computer matching with a laboratory-made and commercial mass spectral libraries and comparison of spectra with literature data (McLafferty and Stauffer 1994; Adams 2001), (c) on comparison of the signals in the ^{13}C NMR spectra of essential oils with those of reference spectra compiled in the laboratory spectral library with the help of laboratory-developed software (Tomi et al. 1995; Rezzi et al. 2002; Ouattara et al. 2014). In the investigated samples, individual components were identified by ^{13}C-NMR at contents as low as 0.4 - 0.5%.

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Table S1. Chemical composition of *S. rugosum* and *S. erianthum* leaf essential oil

N°	Compounds	RIa	RIp	%^{a} *S.rugosum*	%^{a} *S.erianthum*	Identification
1	Hexanal	771	1088	-	0.3	RI, MS
2	(Z)-Hex-3-en-1-ol	833	1386	-	0.3	RI, MS
3	Linalool	1083	1549	2.0	-	RI, MS, ^{13}C NMR
4	*α*-Terpineol	1171	1698	0.3	-	RI, MS
5	Safranal	1173	1648	0.2	-	RI, MS
6	Geraniol	1233	1849	0.4	-	RI, MS
7	(E)- *β* -Damascenone	1361	1823	0.4	-	RI, MS
8	*β*-Elemene	1386	1592	1.3	1.1	RI, MS, ^{13}C NMR
9	(E)-*β*- Caryophyllene	1417	1599	33.7	16.7	RI, MS, ^{13}C NMR
10	*α*-Humulene	1448	1669	2.5	38.6	RI, MS, ^{13}C NMR
11	*β*-Ionone	1462	1939	0.8	0.5	RI, MS, ^{13}C NMR
12	Germacrene D	1474	1710	14.4	3.1	RI, MS, ^{13}C NMR
13	Bicyclogermacrene	1488	1733	1.7	0.2	RI, MS, ^{13}C NMR
14	*γ*-Cadinene	1504	1746	0.2	-	RI, MS
15	*δ*-Cadinene	1512	1757	0.5	0.9	RI, MS, ^{13}C NMR
16	*β*-Elemol	1534	2081	19.8	17.8	RI, MS, ^{13}C NMR
17	Caryophyllene oxide	1567	1980	0.7	0.4	RI, MS, ^{13}C NMR
18	Guaiol	1583	2089	4.4	4.4	RI, MS, ^{13}C NMR
19	Humulene oxide II	1592	2037	-	1.0	RI, MS, ^{13}C NMR
20	*γ*-Eudesmol	1616	2167	2.2	2.3	RI, MS, ^{13}C NMR
21	*τ*-Cadinol	1623	2158	-	0.3	RI, MS
22	*β*-Eudesmol	1632	2219	1.9	1.7	RI, MS, ^{13}C NMR
23	*α*-Eudesmol	1637	2228	2.4	2.2	RI, MS, ^{13}C NMR
24	*α*-Cadinol	1639	2230	0.3	-	RI, MS
25	Bulnesol	1650	2201	0.9	1.0	RI, MS, ^{13}C NMR
26	(E)-Phytol	2098	2612	2.5	1.0	RI, MS, ^{13}C NMR
	Total			93.5	93.8	
Oxygenated monoterpenes				2.9	-	
Sesquiterpenes hydrocarbons				54.3	60.6	
Oxygenated sesquiterpenes				32.6	31.1	
Diterpenes				2.5	1.0	
Other				1.2	1.1	

The order of elution and the percentages are given on apolar column (BP-1)

RIa and RIp: retention indices measured on apolar (BP-1) and polar (BP-20) columns, respectively.