Volatile constituents of *Thalassia testudinum* Banks ex König Leaves

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Abstract

The volatile constituents from the sea grass *Thalassia testudinum* was analyzed by GC and GC/MS. One-hundred-forty-two constituents were identified which constituted more than 95% of the oil composition, all of them reported for the first time in this species. The most prominent volatile compound was ethyl (Z)-1-propenyl disulfide (31% of the total composition).

Key Word Index

Turtle grass, *Thalassia testudinum*, Hydrocharitaceae, essential oil composition, ethyl (Z)-1-propenyl disulfide.

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Table I. Volatile compounds in Thalassia testudinum leaves

| Compound | RI | % | Compound | RI | % |
|---------------------------------|------|----------|------------------------------|------|----------|
| 3-methylbutanal | 653 | 0.3 | linalool | 1097 | 0.7 |
| 2-methylbutanal | 665 | 0.4 | nonanal | 1101 | 0.3 |
| 1-penten-3-ol | 683 | 1.1 | isophorone | 1121 | 0.1 |
| 1-penten-3-one | 686 | 0.4 | trans-pinocarveol | 1139 | 0.1 |
| pentanal | 705 | 0.5 | camphor | 1145 | 1.4 |
| 2-ethylfuran | 707 | 0.6 | (Z)-2-nonenal | 1149 | t |
| acetoin | 720 | t | 4-ethylbenzaldehyde | 1164 | 0.4 |
| acetal | 730 | 0.1 | borneol | 1169 | 0.4 |
| sopentanol | 741 | 0.1 | ethyl benzoate | 1172 | 0.2 |
| E)-3-penten-2-one | 745 | 0.2 | 2,5-dimethylbenzaldehyde | 1175 | 0.3 |
| dimethyl disulfide | 753 | 0.2 | terpinen-4-ol | 1175 | 0.5 |
| E)-2-pentenal | 754 | 0.1 | α-terpineol | 1189 | 0.6 |
| 1H)-pyrrole | 762 | 0.1 | | 1192 | 0.0 t |
| Z)-2-pentenol | 774 | 1.1 | methyl salicylate | | 0.2 |
| 3-hexanone | 784 | t | safranal | 1197 | |
| 2-hexanone | 792 | t | dodecane | 1200 | 0.1 |
| | | ر 3.4 | decanal | 1203 | 0.1 |
| nexanal | 802 | | β-cyclocitral | 1223 | 0.7 |
| ethyl (Z)-1-propenyl disulfide | 813 | 31.0 | dimethyl tetrasulfide | 1232 | 0.1 |
| 2-methylpyridine | 816 | t | geraniol | 1253 | t |
| 2-furfural | 835 | t | linalyl acetate | 1258 | t |
| E)-2-hexenal | 855 | 1.7 | bornyl acetate | 1289 | 0.1 |
| Z)-3-hexenol | 859 | 0.5 | 2-undecanone | 1294 | 0.1 |
| sovaleric acid | 885 | t | (1H)-indole | 1296 | 0.1 |
| o-xylene | 865 | 0.2 | tridecane | 1300 | t |
| 2,6-dimethypyridine | 884 | t | trans-carvyl acetate | 1340 | t |
| 3-heptanone | 887 | t | α-terpinyl acetate | 1349 | 2.2 |
| nexanol | 890 | 0.4 | eugenol | 1359 | 1.4 |
| 2-heptanone | 892 | 0.5 | α-ylangene | 1375 | t |
| Z)-4-heptenal | 901 | 0.3 | α-copaene | 1377 | 0.1 |
| neptanal | 903 | 0.8 | β-maaliene | 1382 | 0.1 |
| aleric acid | 909 | t | β-elemene | 1390 | 0.6 |
| E,E)-2,4-hexadienal | 910 | 0.2 | 2-dodecanone | 1396 | t |
| nethyl (Z)-1-propenyl disulfide | 922 | 2.8 | tetradecane | 1400 | 0.1 |
| X-pinene | 939 | 0.2 | methyl eugenol | 1400 | 0.1 |
| l-decanol | 946 | 0.1 | dedecanal | 1404 | 0.9 t |
| camphene | 954 | t | - | | |
| nethyl (E)-1-propenyl disulfide | 956 | 2.6 | β-caryophyllene | 1418 | 1.9 |
| | 959 | 2.0 t | methyl undecanoate | 1427 | t |
| 3-ethylpyridine | 961 | 0.4 | (E)-α-ionone | 1430 | 0.1 |
| oenzaldehyde | | | α- <i>trans</i> -bergamotene | 1435 | t |
| dimethyl trisulfide | 970 | 0.2 | dihydro-β-ionone | 1436 | 0.2 |
| neptanol | 971 | 0.1 | (E)-cinnamyl acetate | 1446 | t |
| sabinene | 975 | 0.1 | geranylacetone | 1455 | 0.4 |
| 3-pinene | 979 | 0.2 | α -humulene | 1455 | 0.3 |
| I-octen-3-ol | 980 | 0.1 | ethyl (E)-cinnamate | 1467 | 0.1 |
| 3-octanone | 984 | 0.1 | germacrene D | 1486 | 0.2 |
| S-methyl-5-hepten-2-one | 986 | 0.1 | (E)-β-ionone | 1489 | 7.2 |
| 2-pentylfuran | 991 | 1.1 | pentadecane | 1500 | 2.5 |
| e-octanone | 993 | t | tridecanal | 1510 | 0.3 |
| octanal | 998 | t | δ -cadinene | 1522 | t |
| lecane | 1000 | t | dihydroactinidiolide | 1533 | 0.5 |
| λ-phellandrene | 1002 | t | β-calacorene | 1545 | 0.1 |
| E,E)-2,4-heptadienal | 1011 | 0.2 | elemicin | 1557 | t |
| x-terpinene | 1015 | 0.1 | (E)-nerolidol | 1564 | t |
| iexanoic acid | 1019 | 0.1 | (E)-2-tridecenal | 1569 | 0.2 |
| o-cymene | 1025 | 0.3 | spathulenol | 1578 | 0.2 |
| monene | 1029 | 0.5 | • | 1589 | 1.1 |
| ,8-cineole | 1023 | 3.1 | caryophyllene oxide | 1600 | 0.3 |
| 2,2,6-trimethylcyclohexanone | 1034 | 0.4 | hexadecane | | |
| | 1034 | 0.4 | teradecanal | 1614 | 0.5 |
| 5-ethyl-2(5H)-furanone | | | benzophenone | 1628 | t |
| penzyl alcohol | 1037 | t | β-eudesmol | 1653 | 0.1 |
| /-terpinene | 1060 | 0.3 | selin-11-en-4-α-ol | 1660 | 0.2 |
| acetophenone | 1065 | 0.3 | tetradecanol | 1673 | 0.8 |
| p-tolualdehyde | 1068 | t | heptadecane | 1700 | 1.2 |
| octanol | 1069 | t | pentadecanal | 1713 | 1.9 |
| 2-pyrrolidinone | 1076 | 0.1 | pentadecanol | 1773 | 0.3 |
| 2-nonanone | 1090 | 0.1 | hexahydrofarnesyl acetone | 1846 | 1.7 |

| Compound | RI | % | Compound | RI | % |
|------------------------|------|-----|---------------------|------|-----|
| pentadecanoic acid | 1869 | t | hexadecanoic acid | 1983 | t |
| hexadecanol | 1876 | 0.6 | ethyl hexadecanoate | 1992 | t |
| nonadecane | 1900 | t | geranyl linalool | 2006 | t |
| (E,E)-farnesyl acetone | 1915 | 0.3 | heneicosane | 2100 | 0.2 |
| methyl hexadecanoate | 1922 | t | phytol | 2112 | 0.9 |

Plant Name, Source and Part

Thalassia testudinum Banks *ex* König (Hydrocharitaceae) plants were collected in March 2007 from "La Concha" Beach (22°05'45"N/82°27'15"W) and identified by Areces J.A., Ph.D., Instituto de Oceanología (La Habana). A voucher sample (No. IdO39) has been deposited in the Herbarium of the Cuban National Aquarium.

Leaves were washed with distilled water and air-dried for about three days. The oil was obtained from 100 g of leaves by simultaneous distillation-solvent extraction with 25 mL of diethyl ether for 3 h (previously distilled). The extract was dried over anhydrous sodium sulfate and concentrated with a Kuderna-Danish apparatus to 0.9 mL, and then to 0.2 mL with a gentle stream of nitrogen.

Introduction

Thalassia testudinum is a sea grass, commonly known as turtle grass (1), which plays an important role in marine ecosystems, supplying nursery grounds for many invertebrate and fish species, stabilizing the sediments of near shore coast, etc. (2). This plant is the largest and most robust sea grass in Florida and the Caribbean. The leaves are ribbon-like, are about 1.3 cm wide and up to 35 cm long, and grow in water up to 25 m and salinities as low as 20 ppt. It prefers shallower water up to 10 m and salinities between 25–40 ppt (3).

Previous studies have shown that luteolin 7- β -D-glucopyranosyl-2"-sulfate (thalassiolin A), isolated from *T. testudinum* (collected in the Bahamas coasts) has antibiotic activity against Zoosporic fungi (4). Moreover, a recent study demonstrated that thalassiolin A, chrysoeriol 7- β -D-glucopyranosyl-2"-sulfate (thalassiolin B) and apigenin 7- β -D-glucopyranosyl-2"-sulfate (thalassiolin C), represent a new series of HIV integrase inhibitors (5). A review of the literature reveals that the volatiles of this plant have not been the subject of previous studies.

Process

An HP 6890 GC with a FID, equipped with an HP-5MS fused silica column (30 m x 0.25 mm x 0.25 μ m) was used. The column temperature was programmed as follows: 70°C isothermal for 2 min, 70°C to 230°C at 4°C/min, then held for 10 min. Helium carrier gas was used at a flow rate of 0.9 mL/min. The injector and detector were maintained at 230°C. Sample

injection volume was $0.3 \ \mu$ l with a split ratio of 1:10. Linear retention indices were calculated using n-paraffin standards.

An HP 6890 Series II equipped with a mass selective detector HP-5973N was employed. A same capillary column and temperature program as in the GC-FID technique was used. Mass spectra were recorded in the electron-impact mode at 70 eV by 1.8 scans/s, and the mass range used was m/z 35–400; ion source and connecting parts temperature: 230°C.

Compounds were identified as far as possible from the best match to their mass spectrum in the NBS/Wiley and NIST libraries or in-house FLAVORLIB library, and confirmed in many compounds by their relative retention indices. Whenever possible, retention indices and mass spectra were also compared with those of authentic samples. Mass spectra from the literature were also compared (6). Quantitative analysis was made by the normalization method from the electronic integration of the FID peak areas without the use of correction factors.

The identified compounds in the leaf oil of *T. testudinum* are listed in Table I. One-hundred-forty-two constituents were identified which constitute more than 95% of the composition, all of them reported for the first time in this species. The most prominent volatile compound was ethyl (*Z*)-1-propenyl disulfide (31%).

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