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Salvisertin A, a New Hexacyclic Triterpenoid, and Other Bioactive Terpenes from *Salvia deserta* Root

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Abstract

Using various chromatographic methods, a new hexacyclic triterpenoid, 2β , 3β , 24β -trihydroxy-12, 13-cyclo-taraxer-14-en-28oic acid (**1**), together with ten known compounds, 2α , 3α , 23-trihydroxyurs-12, 20(30)-dien-28oic acid (**2**), 6, 7-dehydroroleanone (**3**), horminone (**4**), 7-*O*-methylhorminone (**5**), sugiol (**6**), demethylcryptojaponol (**7**), 14-deoxycoleon U (**8**), 5, 6-didehydro-7-hydroxy-taxodone (**9**), ferruginol (**10**) and dichroanone (**11**), were isolated from the roots of *Salvia deserta*. Their structures were identified on the basis of spectroscopic analysis and comparison with the reported data. The individual compounds (**1**, **3–8**) were screened for cytotoxic activity, using the sulforhodamine B bioassay (SRB) method. As the results, Compounds **3**, **5** and **8** showed cytotoxic potency against A549, MDA-MB-231, KB, KB-VIN, and MCF7 cell lines with IC_{50} values ranging from 6.5 to 10.2 μ M.

Graphical abstract

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Supplementary Material

Supporting information for this article is available on the WWW under <http://dx.doi.org/10.1002/MS-number>.

Author Contribution Statement

L. S. M. Li and X. F. Huang contributed in the collection of plant material. Y. R. Wang, X. F. Huang designed the experiments and wrote the initial draft. Y. R. Wang, Y. Yu, W. Liu and X. F. Huang participated in the acquisition and interpretation of the data. K. H. Lee., M. Goto, and S. L. Morris-Natschke conducted the biological assays and refined the manuscript. All authors approved the final version for publication.

Keywords

Salvia deserta; Terpenes; Structure elucidation; Cytotoxicity

Introduction

Salvia deserta (Xin Jiang Shu Wei Cao) (family Lamiaceae) is a perennial herb widely distributed in northern Xinjiang Uygur Autonomous Region, China. All of the plant parts are used in Chinese folk medicines with antifebrile, detoxification, detumescent, lump-dissipation, antitussive and expectorant effects [1]. *Salvia* species are rich sources of structurally diverse terpenoids, which are likely responsible to a large extent for the therapeutic properties [2]. However, very few studies have been reported on the chemical constituents of the species *S. deserta*, and only on the isolation of several salvianolic acids. The objective of this current work was the investigation of the roots to identify bioactive terpenoids. The ethanolic extract was fractionated and a new triterpene, salvisertin A (**1**), was isolated. NOESY correlations allowed us to define the relative configuration of **1**. Compounds **1**, **2** and **5** were isolated from the genus *Salvia* for the first time, and **1**, **2**, **5–11** were firstly isolated from this species. The individual compounds (**1**, **3–8**) were screened for *in vitro* antiproliferative activity against A549, MDA-MB-231, MCF7, KB, and multidrug-resistant KB subline KB-VIN cell lines. The sulforhodamine B bioassay (SRB) method was used to determine cytotoxic activity.

Results and Discussion

Phytochemical investigation of an ethanol extract of *S. deserta* using various chromatographic methods led to the isolation of eleven compounds (Figure 1). Compound **1** was obtained as white powder with a molecular formula $C_{30}H_{45}O_5$, deduced from the deprotonated molecular ion peak $[M-H]^-$ at m/z 485.3289 (calc. for $C_{30}H_{44}O_5^-$: 485.3273), showing eight degrees of unsaturation. The 1H -NMR spectrum (Table 1) of **1** showed the presence of five tertiary methyl groups at $\delta(H)$ 0.97 (*s*, Me(29)), 1.04 (*s*, Me(25)), 1.08 (*s*, Me(30)), 1.17 (*s*, Me(26)), 1.63 (*s*, Me(23)). In the 1H - and ^{13}C -NMR spectra, H-atoms at $\delta(H)$ 5.87 (1H, *dd*, $J = 7.3, 3.7$) and carbons at $\delta(C)$ 157.0 and $\delta(C)$ 118.8 suggested a double bond in the molecule. H-atoms at $\delta(H)$ 3.82 (1H, *d*, $J = 10.9$), 4.11 (1H, *d*, $J = 10.9$) and their corresponding carbons at $\delta(C)$ 65.7 indicated the presence of a $-CH_2OH$ group. H-atoms at $\delta(H)$ 4.45 (1H, *dt*, $J = 11.0, 3.1$), 4.57 (1H, *d*, $J = 2.3$) and the

corresponding carbons at $\delta(C)$ 66.8 and $\delta(C)$ 74.6 indicated the presence of two -CHOH groups. The ^{13}C -NMR spectrum showed five signals for methyl, ten methylene, seven methine and eight quaternary carbons, including one carboxyl group ($\delta(C)$ 180.3). The total of 30 carbon resonances indicated a triterpenoid structure. The ^1H - and ^{13}C -NMR spectra were completely assigned by detailed 2D-NMR experiments. In the HMBC spectrum (Figure 2), correlations between $\delta(H)$ 0.01 (1H, t , $J = 4.8$) and $\delta(C)$ 15.5 (C(12)), 20.1 (C(11)), 24.3 (C(13)), 157.0 (C(14)), $\delta(H)$ 1.00 (1H, dd , $J = 9.3, 4.8$) and $\delta(C)$ 20.1 (C(11)), 24.3 (C(13)), 35.4 (C(18)), 157.0 (C(14)) confirmed the presence of a cyclopropane ring.

The ^1H - and ^{13}C -NMR data were quite similar to those reported for methyl(12*R*, 13*S*)-2*α*, 3*α*, 24-trihydroxy-12, 13-cyclo-taraxer-14-en-28-oate [3] previously isolated from *Prunella vulgaris* var. *lilacina* Nakai, except that the ^1H and ^{13}C -NMR spectra of **1** lacking a signal for methyl ester group. However, while the structure of **1** resembled that of (12*R*, 13*S*)-2*α*, 3*α*, 24-trihydroxy-12,13-cyclo-taraxer-14-en-28oic acid [3], which was reported with incomplete spectroscopic data and determination of relative configuration, the A ring proton and carbon signals of **1** did not match completely. Therefore, a ^1H , ^1H -NOESY experiment (Figure 3) was performed and the relative configuration of the stereogenic centers were deduced. The presence of NOE correlations between H-C(27) and H-C(9), H-C(9) and H_a-C(1) confirmed H-C(27) was α -oriented. The configuration of the cyclopropane ring was concluded to be *cis* to H-C(9). NOESY correlations between H-C(3) and H-C(5), H-C(3) and H_a-C(1), without H-C(3) and H_b-C(1), confirmed H-C(3) was α -oriented and OH-C(3) was β -oriented. The observed coupling constant value for the H-C(2) and H-C(3) ($J_{\text{H-C(2)-H-C(3)}} = 2.3$ Hz), together with H-C(3) proton in an axial configuration, was compatible only with a spatial arrangement in which the H-C(2) proton was equatorial substituent [4][5]. Hence OH-C(2) was β -oriented. A NOESY correlation between H-C(24) and H-C(25), without H-C(23) and H-C(25), confirmed H-C(24) was β -oriented. In addition, if the H-C(24) is α -oriented, the chemical shift of the Me(23) group is generally lower than 18 ppm and C(24) is present at about $\delta(C)$ 68 ppm; while if H-C(24) is β -oriented, the chemical shift of the Me(23) group is usually higher than 20 ppm and C(24) is present at around $\delta(C)$ 64 ppm. These differences occur because the equatorial hydroxymethylene is less shielded than its axial counterpart [6][7]. The chemical shifts of the C(23) and C(24) in **1** were 24.2 ppm and 65.7 ppm, respectively, indicating that H-C(23) was α -oriented, whereby H-C(24) was β -oriented. Thus, the structure of **1** was characterized as 2*β*, 3*β*, 24*β*-trihydroxy-12, 13-cyclo-taraxer-14-en-28oic acid. To our knowledge, it is a rare triterpenoid type in nature.

Other 10 known compounds were identified as 2*α*, 3*α*, 24-trihydroxyurs-12, 20(30)-dien-28oic acid (**2**) [8], 6, 7-dehydroroleanone (**3**) [9], horminone (**4**) [10], 7-*O*-methylhorminone (**5**) [10], sugiol (**6**) [11], demethylcryptojaponol (**7**) [12], 14-deoxycoleon U (**8**) [13], 5, 6-didehydro-7-hydroxy-taxodone (**9**) [14], ferruginol (**10**) [15], and dichroanone (**11**) [16], by comparing their NMR data with those reported in the literature. Inside, compounds **1**, **2** and **5** were isolated from the genus *Salvia* for the first time, and **1**, **2**, **5–11** were firstly isolated from *S. deserta*.

The individual compounds (**1**, **3–8**) were evaluated for their cytotoxicity against A549, MDA-MB-231, KB, KB-VIN, and MCF7 cell lines, using the sulforhodamine B bioassay

(SRB) method, and paclitaxel was used as an experimental control (Table 2). As a result, compound **3** showed significant antiproliferative potency against A549, KB, KB-VIN cells, with IC_{50} values of 6.568, 8.916, 8.020 μ M, respectively. Compound **5** showed potent cytotoxicity against A549, MDA-MB-231, KB, KB-VIN cells, with IC_{50} values of 7.194, 8.450, 10.281, 7.303 μ M, respectively. Compound **8** also showed significant cytotoxicity against KB, KB-VIN, and MCF7 cells, with IC_{50} values of 7.689, 7.707, 8.695 μ M, respectively. In addition, compounds **4** and **7** exhibited moderate cytotoxic activity against A549, MDA-MB-231, KB, KB-VIN, and MCF7 cells, while the remaining two compounds showed weak activity. It is also worth noticing that, compounds **3** and **5** showed higher cytotoxicity against above cell lines than **4**, among which the difference between their structures was C ring, as also found in comparison compounds **7** with **8**. It is logical to assume that the activity of these molecules is due to the substituents associated with the C ring [10].

Conclusions

In conclusion, two triterpenoids (one oleanane- and one ursane-type), together with nine abietane-type diterpenoids were isolated from the roots of *S. deserta*. The investigation enriched the library of compounds isolated from this plant. Notably, the discovery of compound **1** and the determination of its relative configuration contributed to the chemical diversity of the oleanane-type triterpenoid family. These results might be helpful for explaining the use of *S. deserta* in traditional medicine.

Experimental Section

General

The HR-ESI-MS data were obtained on an *Agilent 6520B Q-TOF* spectrometer. The optical rotation was determined on a *JASCO P-1020* polarimeter. Analytical HPLC measurements were conducted on a *Shimadzu LC-20AT* pump with a *Shimadzu SPD-20A* UV-Vis detector, using a *ZORBAX SB-C18* column (250×4.6 mm, 5 μ m). Semi-preparative HPLC separation was performed on a *Shimadzu LC-6AD* pump with a *Shimadzu SPD-20A* UV-Vis detector, using a *ZORBAX SB-C18* column (250×9.4 mm, 5 μ m). NMR spectra were recorded on a *Bruker ACF* (300 and 500 MHz) spectrometer with deuterated solvent signals used as internal standards. Column chromatography was conducted on MCI gel (75–150 μ m; *Mitsubishi Chemical Corp.*, Tokyo, Japan), ODS (PrePAK-500/C18, *YMC*) and *Sephadex LH-20* (20–100 μ m, *Pharmacia*, U.S.A.) columns.

Plant materials

The dried roots of *S. deserta* were collected in 2015 from Urumqi County, Xinjiang Uygur Autonomous Region, China. The identity of the plant material was verified by Dr. *Wei Li* of Tasly R&D Institute, Tasly Pharmaceutical Co., Ltd., Tianjin, P. R. China and a voucher specimen (No. 20150916) was deposited at the Department of Natural Medicinal Chemistry, China Pharmaceutical University, Nanjing, China.

Extraction and isolation

The air-dried roots of *Salvia deserta* (4.0kg) were extracted four times with 75% ethanol under reflux (85°C). After filtration, the solvent was evaporated in vacuum to yield a crude ethanol extract (170.0g). All of the extract were suspended in water and successively partitioned with petroleum ether, EtOAc and BuOH to obtain PE fraction (10.0g), EtOAc fraction (25.0g), and BuOH fraction (20.0g), respectively. The EtOAc extract (25.0g) was separated by MCI gel column chromatography and eluted with a gradient of CH₃OH/H₂O (10:90, 30:70, 50:50, 70:30, 90:10, 100:0, v/v), to yield 10 fractions (*Fr.1*—*Fr.10*) based on TLC analysis.

Fr.6 (1000.0mg) was applied to *ODS* column with CH₃OH/H₂O (30:70, 50:50, 70:30, 100:0, v/v) as the eluent to give eight subfractions *Fr.6.1*—*Fr.6.5*. *Fr.6.1* was further subjected to semi-preparative HPLC eluting with CH₃CN/H₂O/CF₃COOH (60:40:0.02, v/v/v) to give compounds **5** (9.6mg) and **6** (4.1mg), *Fr.6.2* eluting with CH₃CN/H₂O/CF₃COOH (65:35:0.02, v/v/v) to give compound **4** (8.6mg), *Fr.6.4* eluting with CH₃CN/H₂O/CF₃COOH (50:50:0.02, v/v/v) to give compounds **7** (32.4mg) and **8** (69.6mg).

Fr.7 (1270.0mg) was subjected to silica gel column chromatography and gradiently eluted with the solvent of CH₂Cl₂/MeOH (50:1, 20:1, 8:1, 5:1, v/v/v) to give twelve subfractions *Fr.7.1*—*Fr.7.12*. *Fr.7.6* was subjected to *Sephadex LH-20* column eluting with CH₂Cl₂/CH₃OH (1:1, v/v) to produce compound **2** (5.9mg). *Fr.7.10* was recrystallized with methanol to afford compound **1** (10.3mg).

Fr.8 (1540.0mg) was subjected to silica gel column chromatography and gradiently eluted with the solvent of CH₂Cl₂/MeOH (100:1, 70:1, 50:1, 20:1, 5:1, v/v/v) to give seven subfractions *Fr.8.1*—*Fr.8.7*. *Fr.8.1* was subjected to semi-preparative HPLC using CH₃CN/H₂O/CF₃COOH (67:33:0.02, v/v/v) as the mobile phase to provide compounds **10** (10.2mg) and **11** (6.9mg), *Fr.8.4* using CH₃CN/H₂O/CF₃COOH (60:40:0.02, v/v/v) to provide compound **9** (4.9mg). *Fr.9* (500.0mg) was recrystallized with methanol to afford compound **3** (153.2mg).

2 β , 3 β , 24 β -trihydroxy-12, 13-cyclo-taraxer-14-en-28oic acid (1)—White powder. $[\alpha]_D^{25} = +58.6$ ($c = 0.10$, MeOH). ¹H- and ¹³C-NMR: see Table 1. HR-ESI-MS: 485.3289 ($[M - H]^-$, C₃₀H₄₄O₅⁻; calc. 485.3273).

Bioassays

Human lung carcinoma (A549), originally isolated as epidermoid carcinoma of the nasopharynx (KB), P-glycoprotein-overexpressing multidrug-resistant KB subline (KB-VIN), and triple-negative or hormone-responsible breast cancer (MDA-MB-231 or MCF7, respectively) cell lines were obtained from ATCC or UNC Lineberger Comprehensive Cancer Center. All cell lines were maintained in RPMI-1640 medium containing 25 mM HEPES and 2 mM L-glutamine (Gibco, Invitrogen Corporation, NY) supplemented with 10% fetal bovine serum (Gibco, Invitrogen Corporation, NY), in a humidified environment with 5% CO₂ at 37 °C.

Cytotoxic activity was determined by the sulforhodamine B (SRB) colorimetric assay as previously described [17]. In brief, the cells ($4-11 \times 10^3$ cells/well) were seeded in 96-well plates filled with culture medium containing various concentrations of samples, and incubated for 72 h. At the end of the exposure period, the attached cells were fixed in cold 10% trichloroacetic acid for 30 min followed by staining with 0.04% SRB (Sigma Chemical Co.) for 30 min. The bound SRB was solubilized in 10 mM Tris-base and the absorbance was measured at 515 nm on a Microplate Reader ELx800 (Bio-Tek Instruments, Winooski, VT) with a Gen5 software. All results were representative of three or more experiments.

The inhibition was calculated with the formula: Inhibition % = $(ODc - ODt)/ODc \times 100\%$

where ODc is the absorbance of negative control, and ODt is the absorbance of tested drug.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

Acknowledgments

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Figure 1.
The structures of compounds **1** – **11** isolated from the EtOH extract of *S. deserta* root.

Figure 2.
Main $^1\text{H}, ^1\text{H}$ -COSY correlations and HMBCs in the spectra of **1**.

Figure 3.
Key NOE correlations of **1** in the NOESY spectrum.

Table 1
¹H-NMR (500MHz) and ¹³C-NMR (126 MHz) spectroscopic data in pyridine-*d*₅ (δ in ppm, *J* in Hz).
 Atom numbering as indicated in the text.

Position	δ (H)	δ (C)	Position	δ (H)	δ (C)
1 α	1.74 (<i>m</i>)	43.6	17		53.3
1 β	2.05 (<i>m</i>)		18	3.12 (<i>dd</i> , <i>J</i> = 13.7, 3.5)	35.4
2	4.45 (<i>dt</i> , <i>J</i> = 11.0, 3.1)	66.8	19 α	1.05 (<i>m</i>)	36.2
3	4.57 (<i>d</i> , <i>J</i> = 2.3)	74.6	19 β	0.79 (<i>dd</i> , <i>J</i> = 12.9, 3.5)	
4		45.6	20		29.5
5	1.77 (<i>m</i>)	50.0	21 α	1.32 (<i>dt</i> , <i>J</i> = 13.8, 3.8)	34.8
6 α	1.71 (<i>m</i>)	19.4	21 β	1.44 (<i>m</i>)	
6 β	1.48 (<i>m</i>)		22 α	1.60 (<i>m</i>)	31.6
7 α	1.52 (<i>m</i>)	39.9	22 β	2.08 (<i>m</i>)	
7 β	1.92 (<i>m</i>)		23	1.63 (<i>s</i>)	24.2
8		38.0	24	4.11 (<i>d</i> , <i>J</i> = 10.9)	65.7
9	1.13 (<i>dd</i> , <i>J</i> = 13.1, 4.2)	48.7		3.82 (<i>d</i> , <i>J</i> = 10.9)	
10		39.1	25	1.04 (<i>s</i>)	18.4
11 α	1.97 (<i>dd</i> , <i>J</i> = 13.1, 3.5)	20.1	26	1.17 (<i>s</i>)	23.2
11 β	1.86 (<i>m</i>)		27	0.01 (<i>t</i> , <i>J</i> = 4.8)	12.1
12	1.17 (<i>m</i>)	15.5		1.00 (<i>dd</i> , <i>J</i> = 9.3, 4.8)	
13		24.3	28		180.3
14		157.0	29	0.97 (<i>s</i>)	33.0
15	5.87 (<i>dd</i> , <i>J</i> = 7.3, 3.7)	118.8	30	1.08 (<i>s</i>)	30.0
16 α	2.12 (<i>m</i>)	33.5			
16 β	2.83 (<i>dd</i> , <i>J</i> = 13.0, 7.3)				

Table 2

Cytotoxicity data of compounds isolated from the roots of *S. deserti*.

Compound	Cytotoxic activity ^a , IC ₅₀ (μM)					
	A549	MDA-MB-231	KB	KB-VIN	MCF-7	
1 2β, 3β, 24β - trihydroxy - 12, 13 - cyclo - taraxer-14-en-28oic acid	>40	>40	>40	>40	>40	>40
3 6, 7-dehydroroyleanone	6.568±0.176	13.320±1.473	8.916±1.186	8.020±0.258	20.779±1.257	20.779±1.257
4 horminone	19.354±0.342	23.624±1.812	29.581±1.117	24.455±0.459	34.833±0.922	34.833±0.922
5 7- <i>O</i> -methylhorminone	7.194±0.260	8.450±0.174	10.281±0.648	7.303±0.285	13.716±0.654	13.716±0.654
6 sugiol	>40	>40	>40	>40	>40	>40
7 demethylcryptojaponol	23.187±0.996	26.243±0.140	23.501±0.960	21.804±0.525	28.590±0.336	28.590±0.336
8 14-deoxycoleon U	12.249±0.719	18.062±0.008	7.689±0.416	7.707±0.187	8.695±0.975	8.695±0.975
Paclitaxel (nM) ^b	4.191±0.493	5.497±0.240	3.529±0.398	2345.602±35.469	11.941±1.305	11.941±1.305

^a IC₅₀ values based on triplicate five points, presented as the mean ± S.D.^b Experimental control.