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# A New Abietane Diterpenoid from *Orthosiphon wulfenioides*

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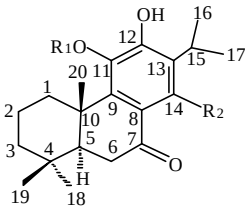
**Abstract:** A new abietane diterpenoid, orthosiphonol (11-methoxy-12, 14-dihydroxy-8, 11, 13-abieta trien-7-one) (**1**) together with known 11-hydroxysugiol (**2**) were isolated from *Orthosiphon wulfenioides*. Their structures were determined on the basis of spectroscopic evidence.

**Keywords:** *Orthosiphon wulfenioides*, abietane diterpenoid, orthosiphonol.

*Orthosiphon wulfenioides*, a medicinal plant grown in Southwest of China, is used for treating fracture, dyspepsy, arthritic, vascular inflammation, edema, and biliary lithiasis[1-3]. The phytochemical study of the plant led to the isolation of a new compound, named orthosiphonol (**1**), together with a known compound, 11-hydroxysugiol (**2**)[4,5]. This is the first instance of abietane diterpenoid from the *Orthosiphon* genus.




**1**: $R_1$ = Me $R_2$ = OH

**2**: $R_1$ = H $R_2$ = H

Orthosiphonol (**1**), yellow powder, $[\alpha]_D^{26}$ +26.5 (*c* = 0.40, $CHCl_3$), was established to have a molecular formula of $C_{21}H_{30}O_4$ by EIMS ($[M^+]$ *m/z* 346) and $^{13}C$ NMR data including DEPT technique. The NMR spectra of **1** indicated the presence of one methoxy group, five methyl groups, four methylenes, two methines and nine quaternary carbons (including one ketonic carbon and six aromatic carbons). Comparing NMR spectral data of **1** with those of **2** revealed the presence of a methoxyl group and an additional hydroxyl group at the aromatic ring of **1**. The chemical shift at δ13.30 indicated that there was a phenolic hydroxyl group at C-14, which could form hydrogen bond with carbonyl at C-7. The cross peaks of the proton of $OCH_3$ (δ 3.75) with H-1β (δ 2.94) and H-20 (δ 1.36) in the NOESY spectrum of **1** indicated the $OCH_3$ was located at C-11. The HMBC experiment

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(shown in **Figure 2**) confirmed the positions of all substituents in **1**. Therefore, **1** was established as 11-methoxy-12, 14-dihydroxy-8, 11, 13-abietatrien-7-one and named orthosiphonol.

**Figure 1** Key NOESY correlations of **1**

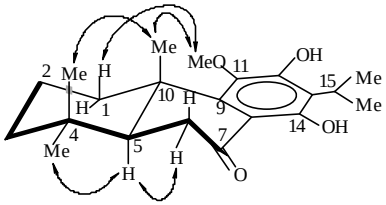


**Figure 2** Key HMBC correlations of **1**

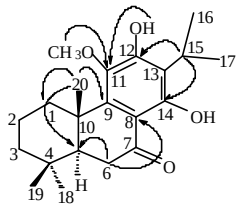


**Table 1** $^{13}$C NMR (500MHz) spectral data of **1** and **2** in $CDCl_3$ ( in ppm)

| Position | **1** | **2** | Position | **1** | **2** |
|---|---|---|---|---|---|
| 1 | 37.45 (t) | 35.39 (t) | 11 | 137.25 (s) | 141.73 (s) |
| 2 | 19.14 (t) | 18.92 (t) | 12 | 155.70 (s) | 147.62 (s) |
| 3 | 40.95 (t) | 41.05 (t) | 13 | 119.86 (s) | 132.62 (s) |
| 4 | 33.53 (s) | 33.35 (s) | 14 | 161.87 (s) | 118.14 (d) |
| 5 | 49.18 (d) | 50.25 (d) | 15 | 24.21 (d) | 26.93 (d) |
| 6 | 35.60 (t) | 36.45 (t) | 16 | 20.07 (q) | 22.37 (q) |
| 7 | 204.44 (s) | 200.94 (s) | 17 | 20.16 (q) | 22.59 (q) |
| 8 | 108.85 (s) | 124.63 (s) | 18 | 33.00 (q) | 32.98 (q) |
| 9 | 144.00 (s) | 139.21 (s) | 19 | 21.69 (q) | 21.43 (q) |
| 10 | 40.38 (s) | 40.03 (s) | 20 | 21.23 (q) | 18.26 (q) |
| | | | $OCH_3$ | 61.80 (q) | |

**Table 2** $^{1}$H NMR (500MHz) spectral data of **1** and **2** in $CDCl_3$ ( in ppm, J in Hz)

| Position | **1** | **2** | Position | **1** | **2** |
|---|---|---|---|---|---|
| 1 | 1.65 (m) | 1.60 (m) | 15 | 3.16 (h, 7.1) | 3.16 (h, 7.1) |
| 1 | 2.94 (m) | 2.61 (m) | 16 | 1.34 (d, 7.1) | 1.22 (d, 7.1) |
| 2 | 1.65 (m) | 1.73 (m) | 17 | 1.35 (d, 7.1) | 1.20 (d, 7.1) |
| 2 | 1.66 (m) | 1.74 (m) | 18 | 0.96 (s) | 0.89 (s) |
| 3a | 1.34 (m) | 1.38 (m) | 19 | 1.00 (s) | 0.94 (s) |
| 3b | 1.50 (m) | 1.55 (m) | 20 | 1.36 (s) | 1.38 (s) |
| 5 | 1.82 (dd, 3.7, 11.5) | 1.84 (dd, 4.0, 11.9) | $OCH_3$ | 3.75 (s) | |
| 6 | 2.65 (m) | 2.56 (m) | OH-12 | 6.46 (brs) | |
| 14 | | 7.61 (s) | OH-14 | 13.30 (brs) | |

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