A New Compound from the Root of Salvia przewalskii Maxim

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Abstract: Neo-przewaquinone A was isolated from the root of *Salvia przewalskii* Maxim. The structure elucidation and ¹H, ¹³C NMR assignments were achieved by spectroscopic method.

Keywords: Salvia przewalskii Maxim., neo-przewaquinone A.

We report here the isolation and structural elucidation of neo-przewaquinone A **1** (**Scheme**) from the 80% EtOH extract of the root of *Salvia przewalskii* Maxim.

Scheme The HMBC correlation of compound 1



The 80% EtOH extract of the root of *S. przewalskii* was concentrated in vacuum to yield extract (SPE). The SPE was suspended in H₂O and stilled for 24 h. The deposit was fractionated by silica gel column chromatography to afford compound **l**. **1** was isolated as red-purple needle crystals, mp 188-189°C. UV λ_{max} (MeOH) nm: 225, 289. FAB-MS m/z: 556 (M⁺), 579(M⁺+Na), 595(M⁺+K), EI-MS m/z: 278[M⁺/2]. According to the data of the NMR spectra, the molecular formula was deduced to be C₃₆H₂₈O₆. Its IR spectrum showed the presence of carbonyl groups (1665 cm⁻¹). In the ¹H-NMR

spectrum of **1**, the signals at δ 7.78 (d, 1H, J=7.9 Hz), 7.45 (d, 1H, J=7.9Hz), 7.42 (d, 1H, J=7.9 Hz), 7.33 (d, 1H, J=7.9 Hz) indicated that there were two pairs of *o*-aromatic protons. While the signals at δ 7.20(d, 1H, J=1.2 Hz), 7.18(d, 1H, J=1.2 Hz), δ 6.00 (m, 1H), 5.50(s, 1H), 5.00(s, 1H) indicated that there were four double bonds at least.

The ¹³C-NMR spectrum gave thirty-six carbon signals. The DEPT spectrum

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revealed twenty quaternary carbons, seven tertiary carbons, six secondary carbons and three primary carbons.

Compared with NMR spectra of tanshinone $II-A^1$, it was found that **1** should be composed of two tanshinone II-A without cycle A. The detailed data of NMR spectrum see **Table 1**.

No.	$\delta_{\rm H} \text{ppm}$	\boldsymbol{J}_{Hz}	$\delta_{\rm C} ppm$	No.	$\delta_{\rm H} ppm$	\boldsymbol{J}_{Hz}	$\delta_{\rm C}$ ppm
2	7.18(d)	1.2	141.6d	2'	7.20(d)	1.2	141.2d
3			120.7s	3'			120.1s
4			121.3s	4'			121.2s
5			176.2s	5'			175.5s
6			184.2s	6'			183.3s
7			126.5s	7'			126.2s
8			144.4s	8'			144.6s
9			139.0s	9'			138.5s
10	7.33(d)	7.9	128.2d	10'	7.42(d)	7.9	130.8d
11	7.45 (d)	7.9	120.7d	11'	7.78(d)	7.9	120.3d
12			127.3s	12'			129.0s
13			161.6s	13'			161.3s
14	2.20(s)		8.8q	14'	2.20(s)		8.8q
15			131.0s				
16	6.00(m)		128.6d				
17	2.22(m)		22.5t				
18	3.28(t)	7.9	24.9t				
19			143.3s				
20	2.47(t)	6.4	32.1t				
21	1.85(m)		23.3t				
22	3.21(t)	6.4	29.4t				
23	$5.50(s, \alpha), 5.00(s, \beta)$		110.5t				
24	2.00(d)	1.6	19.8q				

Table 1NMR spectra data of 1 (CDCl₃)

In the $^1\text{H-}{}^{13}\text{C}$ COSY spectrum, signal at $\delta_C110.5$ was correlated with the signal at δ_H 5.50 and 5.00, $\delta_C128.6$ with δ_H 6.00. In the $^1\text{H-}{}^1\text{H}$ COSY spectrum, correlation among the signal at $_H1.85$ and $_H3.21,\ 2.47,$ the signal at δ_H 2.22 and $\delta_H6.00,\ 3.28$ indicated that there should be the -CH_2CH_2CH_2- moiety, and \searrow C=CHCH_2CH_2- moiety.

In the HMBC spectrum, the signal at $\delta_H 1.85$ was correlated with $\delta_C 143.3$ and 144.4, $\delta_H 2.00$ with $\delta_C 128.6$ and 139.0, $\delta_H 6.00$ with $\delta_C 19.8$, 24.9 and 139., $\delta_H 5.50$ and 5.00 with $\delta_C 32.1$ and 138.5. The NOESY spectrum showed that the signal of $\delta_H 2.00$ was correlated with the signal at $\delta_H 7.33$, $\delta_H 5.50$ with 7.78. Above data mentioned suggested further that a cycle composed of twelve carbons existed. It was the ring that combined the two moieties of tanshinone II-A without cycle A.

From these evidences, 1 is identified as neo-przewaquinone A.

References

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