# 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 ${ }^{1} \mathrm{H},{ }^{13} \mathrm{C}$ 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 $\mathbf{1}$ ( Scheme ) from the $80 \% \mathrm{EtOH}$ 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 $\mathrm{H}_{2} \mathrm{O}$ and stilled for 24 h . The deposit was fractionated by silica gel column chromatography to afford compound $\mathbf{l} . \mathbf{1}$ was isolated as red-purple needle crystals, $\mathrm{mp} 188-189^{\circ} \mathrm{C}$. UV $\lambda_{\max }(\mathrm{MeOH}) \mathrm{nm}: 225,289$. FAB-MS $m / z: 556\left(\mathrm{M}^{+}\right), 579\left(\mathrm{M}^{+}+\mathrm{Na}\right), 595\left(\mathrm{M}^{+}+\mathrm{K}\right)$, EI-MS $m / z: 278\left[\mathrm{M}^{+} / 2\right]$. According to the data of the NMR spectra, the molecular formula was deduced to be $\mathrm{C}_{36} \mathrm{H}_{28} \mathrm{O}_{6}$. Its IR spectrum showed the presence of carbonyl groups $\left(1665 \mathrm{~cm}^{-1}\right)$. In the ${ }^{1} \mathrm{H}-\mathrm{NMR}$ spectrum of $\mathbf{1}$, the signals at $\delta 7.78(\mathrm{~d}, 1 \mathrm{H}, \mathrm{J}=7.9 \mathrm{~Hz}), 7.45(\mathrm{~d}, 1 \mathrm{H}, \mathrm{J}=7.9 \mathrm{~Hz}), 7.42(\mathrm{~d}, 1 \mathrm{H}$, $\mathrm{J}=7.9 \mathrm{~Hz}), 7.33(\mathrm{~d}, 1 \mathrm{H}, \mathrm{J}=7.9 \mathrm{~Hz})$ indicated that there were two pairs of $o$-aromatic protons. While the signals at $\delta 7.20(\mathrm{~d}, 1 \mathrm{H}, \mathrm{J}=1.2 \mathrm{~Hz}), 7.18(\mathrm{~d}, 1 \mathrm{H}, \mathrm{J}=1.2 \mathrm{~Hz}), \delta 6.00(\mathrm{~m}$, $1 \mathrm{H}), 5.50(\mathrm{~s}, 1 \mathrm{H}), 5.00(\mathrm{~s}, 1 \mathrm{H})$ indicated that there were four double bonds at least.

The ${ }^{13} \mathrm{C}-\mathrm{NMR}$ spectrum gave thirty-six carbon signals. The DEPT spectrum

[^0]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 $\mathbf{1}$ should be composed of two tanshinone II-A without cycle A. The detailed data of NMR spectrum see Table 1.

Table 1 NMR spectra data of $\mathbf{1}\left(\mathrm{CDCl}_{3}\right)$

| No. | $\delta_{\mathrm{H}} \mathrm{ppm}$ | $\mathrm{J}_{\mathrm{Hz}}$ | $\delta_{\mathrm{C}} \mathrm{ppm}$ | No. | $\delta_{\mathrm{H}} \mathrm{ppm}$ | $\mathrm{J}_{\mathrm{Hz}}$ | $\delta_{\mathrm{C}} \mathrm{ppm}$ |
| :---: | :---: | :---: | ---: | :---: | :---: | :---: | :---: |
| 2 | $7.18(\mathrm{~d})$ | 1.2 | 141.6 d | $2^{\prime}$ | $7.20(\mathrm{~d})$ | 1.2 | 141.2 d |
| 3 |  |  | 120.7 s | $3^{\prime}$ |  |  | 120.1 s |
| 4 |  |  | 121.3 s | $4^{\prime}$ |  | 121.2 s |  |
| 5 |  |  | 176.2 s | $5^{\prime}$ |  | 175.5 s |  |
| 6 |  |  | 184.2 s | $6^{\prime}$ |  | 183.3 s |  |
| 7 |  |  | 126.5 s | $7^{\prime}$ |  | 126.2 s |  |
| 8 |  |  | 144.4 s | $8^{\prime}$ |  | 144.6 s |  |
| 9 |  |  | 139.0 s | $9^{\prime}$ |  | 138.5 s |  |
| 10 | $7.33(\mathrm{~d})$ | 7.9 | 128.2 d | $10^{\prime}$ | $7.42(\mathrm{~d})$ | 7.9 | 130.8 d |
| 11 | $7.45(\mathrm{~d})$ | 7.9 | 120.7 d | $11^{\prime}$ | $7.78(\mathrm{~d})$ | 7.9 | 120.3 d |
| 12 |  |  | 127.3 s | $12^{\prime}$ |  | 129.0 s |  |
| 13 |  |  | 161.6 s | $13^{\prime}$ |  | 161.3 s |  |
| 14 | $2.20(\mathrm{~s})$ |  | 8.8 q | $14^{\prime}$ | $2.20(\mathrm{~s})$ |  | 8.8 q |
| 15 |  |  | 131.0 s |  |  |  |  |
| 16 | $6.00(\mathrm{~m})$ |  | 128.6 d |  |  |  |  |
| 17 | $2.22(\mathrm{~m})$ |  | 22.5 t |  |  |  |  |
| 18 | $3.28(\mathrm{t})$ | 7.9 | 24.9 t |  |  |  |  |
| 19 |  |  | 143.3 s |  |  |  |  |
| 20 | $2.47(\mathrm{t})$ | 6.4 | 32.1 t |  |  |  |  |
| 21 | $1.85(\mathrm{~m})$ |  | 23.3 t |  |  |  |  |
| 22 | $3.21(\mathrm{t})$ | 6.4 | 29.4 t |  |  |  |  |
| 23 | $5.50(\mathrm{~s}, \alpha), 5.00(\mathrm{~s}, \boldsymbol{\beta})$ |  | 110.5 t |  |  |  |  |
| 24 | $2.00(\mathrm{~d})$ | 1.6 | 19.8 q |  |  |  |  |

In the ${ }^{1} \mathrm{H}-{ }^{13} \mathrm{C}$ COSY spectrum, signal at $\delta_{\mathrm{C}} 110.5$ was correlated with the signal at $\delta_{\mathrm{H}} 5.50$ and $5.00, \delta_{\mathrm{C}} 128.6$ with $\delta_{\mathrm{H}} 6.00$. In the ${ }^{1} \mathrm{H}-{ }^{1} \mathrm{H}$ COSY spectrum, correlation among the signal at ${ }_{\mathrm{H}} 1.85$ and ${ }_{\mathrm{H}} 3.21,2.47$, the signal at $\delta_{\mathrm{H}} 2.22$ and $\delta_{\mathrm{H}} 6.00,3.28$ indicated that there should be the $-\mathrm{CH}_{2} \mathrm{CH}_{2} \mathrm{CH}_{2}$ - moiety, and $-\mathrm{C}=\mathrm{CHCH}_{2} \mathrm{CH}_{2}$ - moiety.

In the HMBC spectrum, the signal at $\delta_{\mathrm{H}} 1.85$ was correlated with $\delta_{\mathrm{C}} 143.3$ and $144.4, \delta_{\mathrm{H}} 2.00$ with $\delta_{\mathrm{C}} 128.6$ and $139.0, \delta_{\mathrm{H}} 6.00$ with $\delta_{\mathrm{C}} 19.8,24.9$ and $139 ., \delta_{\mathrm{H}} 5.50$ and 5.00 with $\delta_{\mathrm{C}} 32.1$ and 138.5 . The NOESY spectrum showed that the signal of $\delta_{\mathrm{H}} 2.00$ was correlated with the signal at $\delta_{\mathrm{H}} 7.33, \delta_{\mathrm{H}} 5.50$ 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, $\mathbf{1}$ is identified as neo-przewaquinone A.

## References

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