SUPPLEMENTARY MATERIAL

Soulieoside U, a new cycloartane triterpene glycoside from *Actaea vaginata*

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Abstract: One new cycloartane triterpene bisdesmoside, soulieoside U, was isolated from the rhizomes of Actaea vaginata. Its structure was elucidated by extensive analysis of the NMR and MS data. Soulieoside U was evaluated for cytotoxic activities against three human cancer cell lines.

Keywords: Actaea vaginata; cycloartane triterpene; cytotoxicity
List of Contents

Table S1. $^1$H and $^{13}$C NMR spectroscopic data of soulieoside U (600 and 150 MHz, pyridine-$d_5$).

Table S2. Cytotoxicity of soulieoside U against three human cancer cell lines.

Figure S1. The Key HMBC (---), NOESY (←→) and $^1$H-$^1$H COSY (—) correlations of soulieoside U.

Figure S2. The $^1$H NMR (600 MHz, pyridine-$d_5$) spectrum of soulieoside U.

Figure S3. The $^{13}$C NMR (APT, 150 MHz, pyridine-$d_5$) spectrum of soulieoside U.

Figure S4. The HSQC spectrum of soulieoside U.

Figure S5. The $^1$H-$^1$H COSY spectrum of soulieoside U.

Figure S6. The HMBC spectrum of soulieoside U.

Figure S7. The NOESY spectrum of soulieoside U.

Figure S8. The HRESIMS spectrum of soulieoside U.
Table S1. $^1$H and $^{13}$C NMR spectroscopic data of soulieside U (600 and 150 MHz, pyridine-$d_5$).

| No. | $\delta$ (J in Hz) | $\delta$, type | No. | $\delta$ (J in Hz) | $\delta$, type |
|-----|-------------------|----------------|-----|-------------------|----------------|
| 1   | 1.15, m; 1.50, m  | 32.4, CH$_2$   | 23  | 2.27, m; 2.90 m   | 31.7, CH$_2$   |
| 2   | 1.86, m; 2.35 m   | 30.4, CH$_2$   | 24  |                   | 114.1, C       |
| 3   | 3.47, dd (11.4, 3.6) | 88.6, CH | 25  |                   | 80.9, C       |
| 4   |                   | 41.7, C       | 26  | 1.77, s           | 23.0, CH$_3$ |
| 5   | 1.23, m           | 47.8, CH      | 27  | 1.76, s           | 24.5, CH$_3$ |
| 6   | 0.65, q-like (13.2); 1.43, m | 20.8, CH$_3$ | 28  | 1.32, s           | 26.1, CH$_3$ |
| 7   | 0.93, m; 1.18, m  | 26.9, CH$_3$  | 29  | 0.99, s           | 15.8, CH$_3$ |
| 8   | 1.28, m           | 47.2, CH      | 30  | 0.88, s           | 22.6, CH$_3$ |
| 9   |                   | 19.2, C       | 30  |                   | 21.8, CH$_3$ |
| 10  | 27.8, C           | COCH$_3$-16   |     |                   | 170.6, C     |
| 11  | 1.15, m; 1.89, m  | 26.9, CH$_2$  | Xyl-1' | 4.86, d (7.8) | 108.0, CH    |
| 12  | 1.45, m; 2.84, m  | 28.7, CH$_2$  | 2'  | 4.05, t (8.4)    | 76.0, CH     |
| 13  |                   | 44.7, C       | 3'  | 4.16, t (8.4)    | 79.1, CH     |
| 14  |                   | 53.0, C       | 4'  | 4.25, m           | 71.7, CH     |
| 15  | 1.34, m; 1.98, dd (10.8, 7.2) | 43.4, CH$_2$ | 5'  | 3.74, t (10.8); 4.35, m | 67.6, CH$_2$ |
| 16  | 5.61, m           | 73.5, CH      | Glc-1'' | 5.29, d (7.8) | 99.7, CH       |
| 17  | 2.60, d (10.2)    | 59.7, CH      | 2'' | 4.01, t (7.8)    | 76.0, CH     |
| 18  | 4.30, d (12.6); 4.48, d (12.6) | 67.0, CH$_2$ | 3'' | 3.96, m           | 78.6, CH     |
| 19  | 0.08, d (4.2); 0.39, d (4.2) | 31.3, CH$_2$ | 4'' | 4.22, m           | 72.2, CH     |
| 20  |                   | 87.7, C       | 5'' | 4.29, m           | 79.3, CH     |
| 21  | 1.36, s           | 33.0, CH$_2$  | 6'' | 4.37, m; 4.50, m  | 63.3, CH$_2$ |
| 22  | 1.85, m; 2.80, m  | 38.0, CH$_2$  |     |                   |               |
Table S2. Cytotoxicity of soulieoside U against three human cancer cell lines.

| Compounds | IC_{50} (μM) | A549  | HT-29  | MDA-MB231 |
|-----------|--------------|-------|--------|-----------|
| 1         |              | 45.7 ± 6.2 | 23.6 ± 4.3 | 18.6 ± 3.4 |
| 5-FU\(^a\) |              | 87.6 ± 4.3 | 56.9 ± 5.7 | 38.5 ± 6.2 |

Values present mean ± SD of triplicate experiments.

\(^a\) Positive control substance
**Figure S1.** Key HMBC, $^1$H–$^1$H COSY and NOESY correlations of soulieoside U.
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Figure S3. The $^{13}$C NMR (APT, 150 MHz, pyridine-$d_5$) spectrum of soulicoside U.
Figure S4. The HSQC spectrum of soulieoside U.
Figure S5. The $^{1}$H-$^{1}$H COSY spectrum of soulieoside U.
Figure S6. The HMBC spectrum of soulieoside U.
Figure S7. The NOESY spectrum of sulieoside U.
Figure S8. The HRESIMS spectrum of soulieoside U.