# SUPPLEMENTARY MATERIAL

**A new cycloartane triterpene bisdesmoside from the rhizomes of *Actaea vaginata***

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A new cycloartane triterpene bisdesmoside, soulieoside T (**1**), and one known compound, oleanolic acid (**2**), were isolated from the ethanolic extract of the rhizomes of *Actaea vaginata*. Their structures were elucidated by spectroscopic methods and by comparison with data reported in the literature. Compound **1** 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 **1** (600 and 150 MHz, pyridine-$d_5$).

| No. | $\delta_H$ ($J$ in Hz) | $\delta_C$, type | No. | $\delta_H$ ($J$ in Hz) | $\delta_C$, type |
|---|---|---|---|---|---|
| **1** | 1.21, m; 1.52, m | 32.8, $CH_2$ | **23** | 2.15, m; 2.58 m | 29.0, $CH_2$ |
| **2** | 1.90, m; 2.25 m | 30.4, $CH_2$ | **24** | | 111.1, C |
| **3** | 3.40, dd (11.4, 4.2) | 88.7, CH | **25** | | 72.4, C |
| **4** | | 41.7, C | **26** | 1.64, s | 25.9, $CH_3$ |
| **5** | 1.28, m | 47.9, CH | **27** | 1.47, s | 25.6, $CH_3$ |
| **6** | 0.64, q (12.0); 1.52, m | 21.4, $CH_2$ | **28** | 1.38, s | 25.1, $CH_3$ |
| **7** | 1.00, m; 1.98, m | 26.8, $CH_2$ | **29** | 1.07, s | 15.8, $CH_3$ |
| **8** | 1.66, dd (12.6, 4.2) | 48.2, CH | **30** | 1.04, s | 14.1, $CH_3$ |
| **9** | | 20.0, C | **CO$\underline{CH_3}$-15** | 2.08, s | 21.9, $CH_3$ |
| **10** | | 26.5, C | **$\underline{CO}CH_3$-15** | | 170.6, C |
| **11** | 1.02, m; 1.08, m | 26.4, $CH_2$ | **Xyl-1′** | 4.76, d (7.2) | 107.6, CH |
| **12** | 1.67 m | 33.5, $CH_2$ | **2′** | 3.97, t (8.4) | 75.6, CH |
| **13** | | 47.0, C | **3′** | 4.19, t (8.4) | 77.0, CH |
| **14** | | 50.3, C | **4′** | 4.34, m | 78.3, CH |
| **15** | 5.67, d (2.4) | 86.6, CH | **5′** | 3.66, t (10.8), 4.42, dd (10.8, 4.8) | 65.1, $CH_2$ |
| **16** | 4.47, dd (6.6, 2.4) | 80.3, CH | **Glc-1″** | 5.00, d (7.8) | 104.7, CH |
| **17** | 1.81, d (6.6) | 51.6, CH | **2″** | 4.56, d (7.8) | 72.0, CH |
| **18** | 1.58, s | 22.0, $CH_3$ | **3″** | 4.16, m | 75.5, CH |
| **19** | 0.26, d (3.6); 0.48, d (3.6) | 31.0, $CH_2$ | **4″** | 4.54, m | 70.6, CH |
| **20** | | 82.8, C | **5″** | 4.12, m | 77.9, CH |
| **21** | 1.29, s | 26.1, $CH_3$ | **6″** | 4.47, br d (10.8), 4.41, dd (10.8, 4.8) | 62.7, $CH_2$ |
| **22** | 1.68, m; 1.89 m | 40.5, $CH_2$ | | | |

**Table S2.** Cytotoxicity of compound **1** against three human cancer cell lines.

| **Compounds** | $IC_{50}$ (μM) | | |
|---|---|---|---|
| | HepG2 | A549 | MDA-MB231 |
| **1** | 67.9 ± 2.7 | 81.5 ± 3.1 | 47.6 ± 1.9 |
| 5-FU[a] | 62.8 ± 3.7 | 79.8 ± 5.2 | 45.7 ± 4.6 |

Values present mean ± SD of triplicate experiments.

[a] Positive control substance

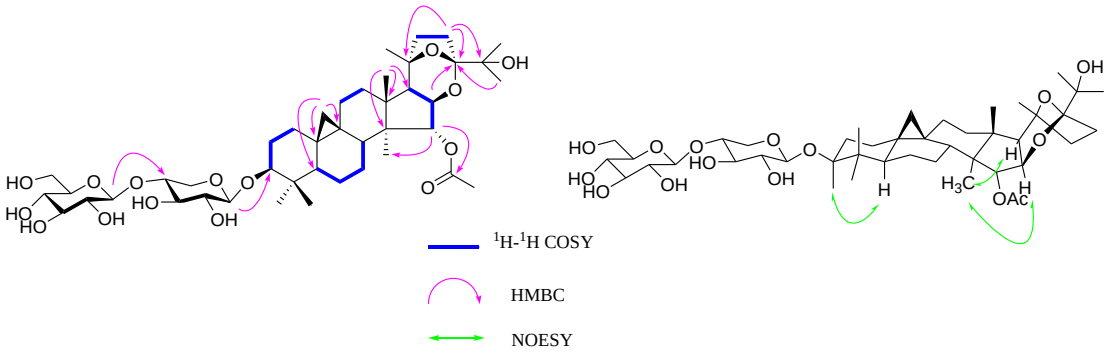


**Figure S1.** Key HMBC, $^{1}$H–$^{1}$H COSY and NOESY correlations of **1**.

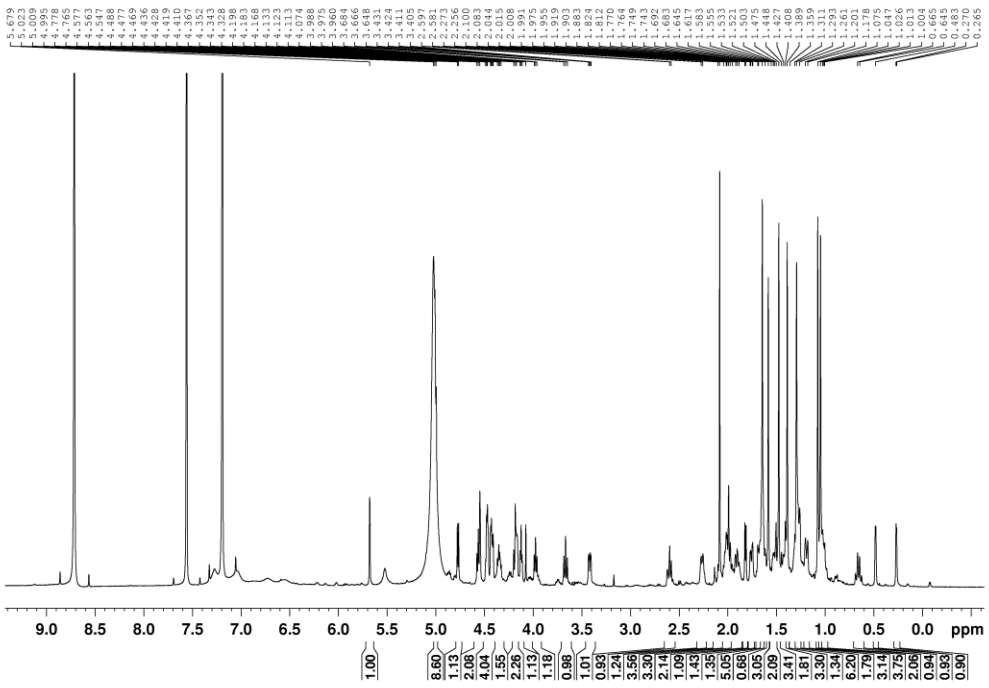

**Figure S2.** The $^{1}$H NMR (600 MHz, pyridine-$d_5$) spectrum of the new compound **1.**

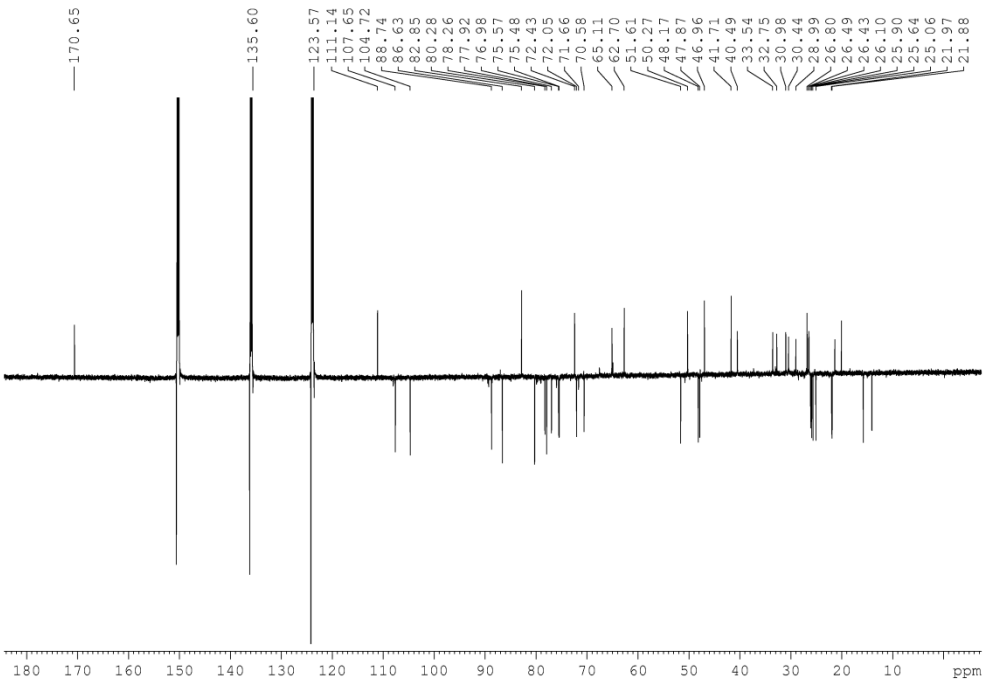


**Figure S3.** The $^{13}$C NMR (APT, 150 MHz, pyridine-$d_5$) spectrum of the new compound **1.**

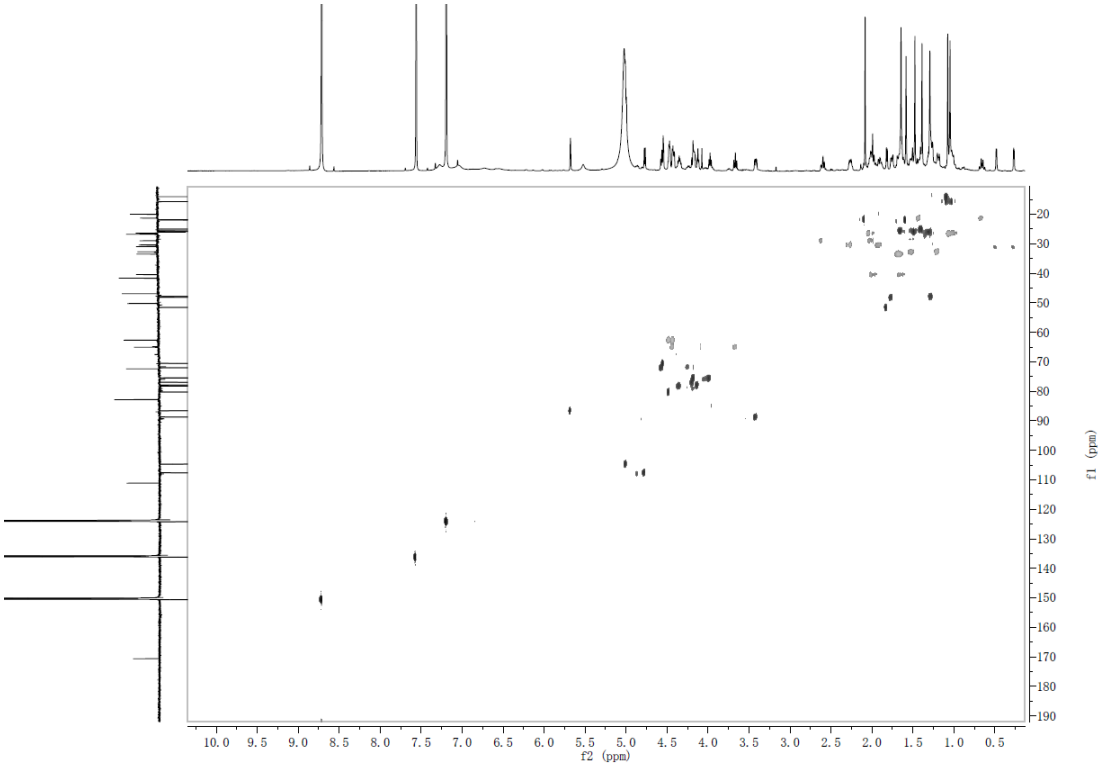


**Figure S4.** The HSQC spectrum of the new compound **1.**

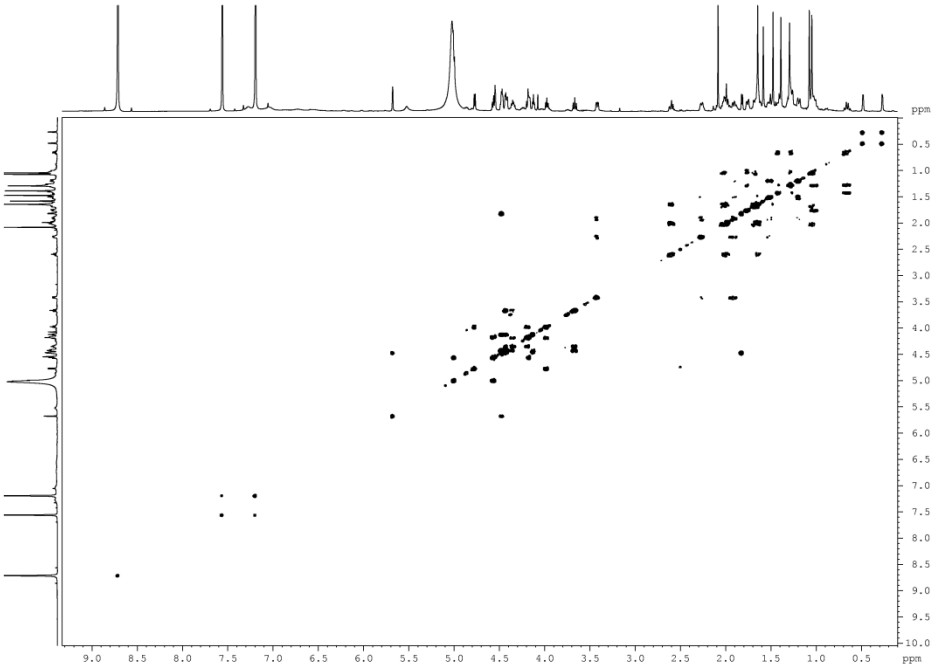


**Figure S5.** The $^{1}$H-$^{1}$H COSY spectrum of the new compound **1.**

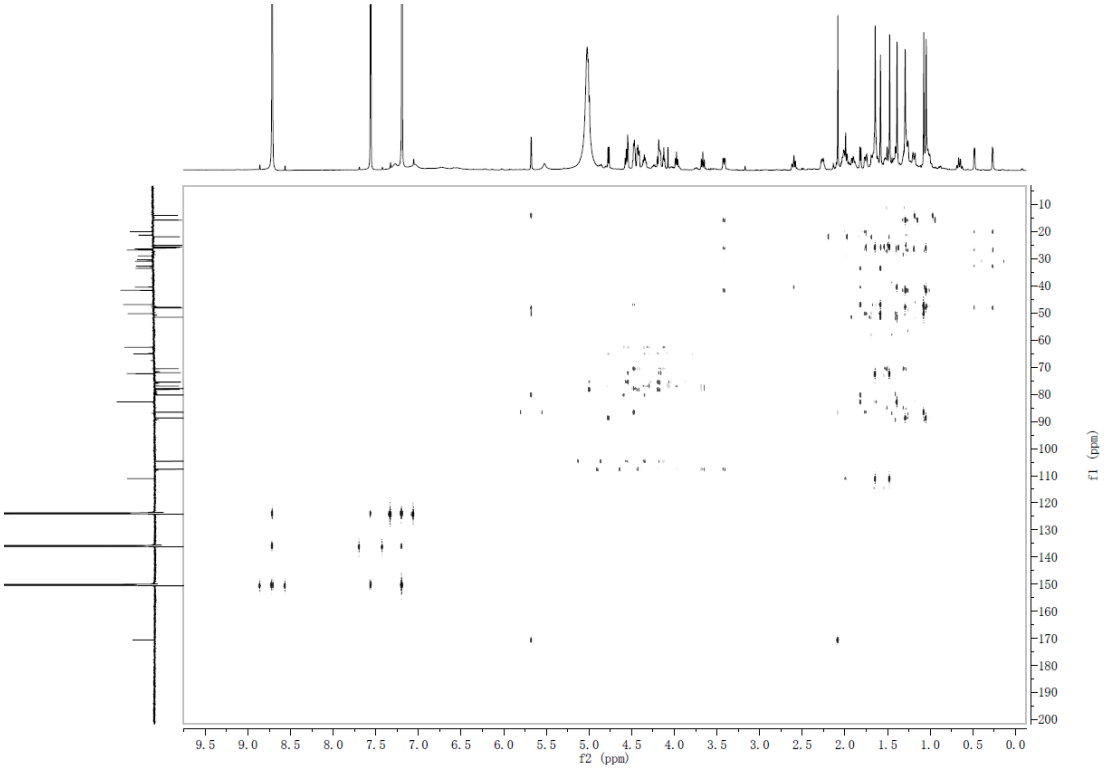


**Figure S6.** The HMBC spectrum of the new compound **1.**

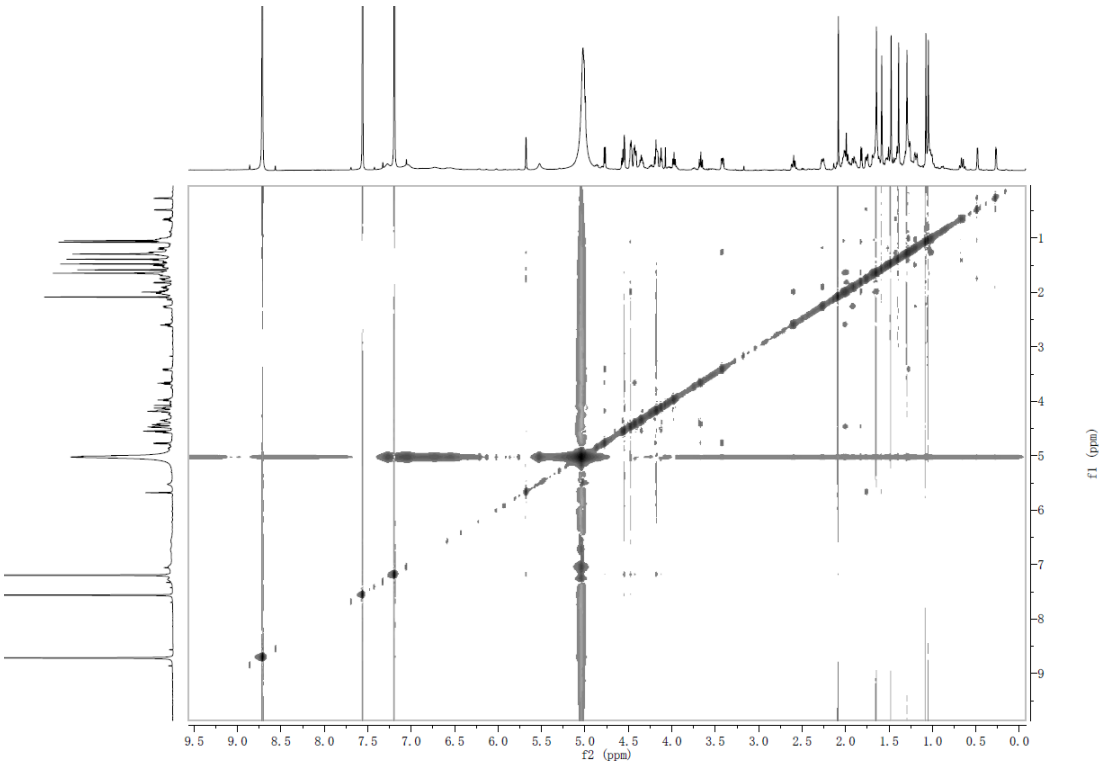


**Figure S7.** The NOESY spectrum of the new compound **1.**

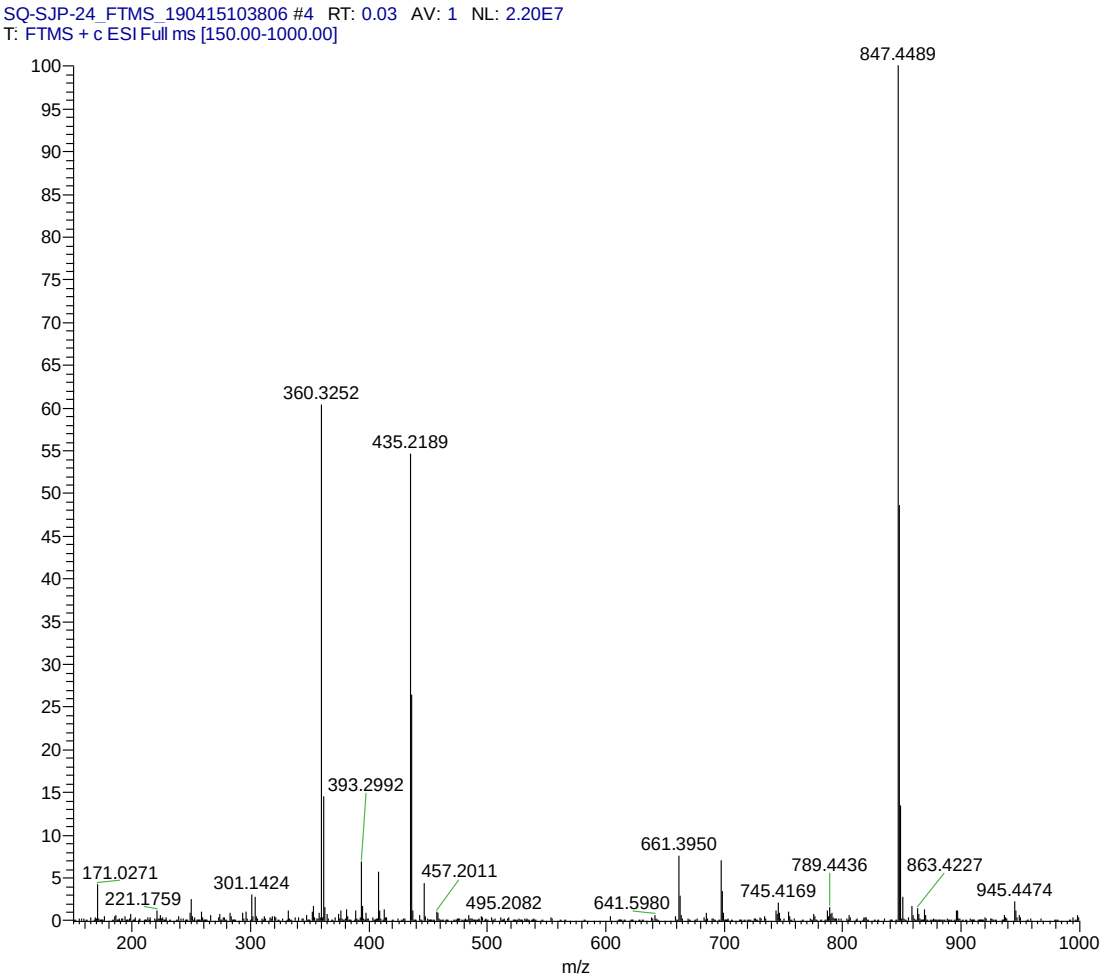


**Figure S8.** The HRESIMS spectrum of the new compound **1.**