SUPPLEMENTARY MATERIAL

Nine sesquiterpenes from *Solanum torvum*

Pulong Yuan, Fujiang Guo, Kaikai Zheng, Kaixian Chen, Qi Jia* and Yiming Li*

*Department of TCM Chemistry, School of Pharmacy, Shanghai University of Traditional Chinese Medicine, Shanghai 201203, PR China

Correspondence to: Qi Jia, School of Pharmacy, Shanghai University of Traditional Chinese Medicine, 1200 Cailun Road, Shanghai 201203, China.

E-mail: q_jia@126.com

Correspondence to: Yiming Li, School of Pharmacy, Shanghai University of Traditional Chinese Medicine, 1200 Cailun Road, Shanghai 201203, China.

E-mail: ymlius@163.com
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**Abstract:** Three new sesquiterpenes, namely, 3\(\beta\),11-dihydroxy-4,14-oxideenantioeudesmane (1), 1\(\beta\),10\(\beta\),12,14-tetrahydroxy-*allo*-aromadendrane (2), and 1\(\beta\),10\(\beta\),13,14-tetrahydroxy-*allo*-aromadendrane (3), along with six known sesquiterpenes (4–9), were isolated from the roots of *Solanum torvum*. Compound 4 and 5 are epimers, their main difference lies in the C-11 configuration. Normally, epimers do not make a huge difference in CNMR spectra, but in this kind of structure of A, B, C rings, and C ring is sterically strained structure, stericall effects influence strongly the \(^{13}\)C NMR chemical shifts, when C-11 configuration changed, it makes a huge difference in the three-ring of structure, such as C-6, C-7, C-11. New compound 2 and 3 are epimers and similar to compound 4 and 5, their just increase a hydroxy in C-1 and have a same regular pattern in CNMR spectra, otherwise, compound 5 was firstly confirmed by single-crystal X-ray diffraction.

**Key word:** *Solanum torvum*; \(^{13}\)C NMR; sesquiterpenes; epimers
Supporting information

**Figure S1.** Key HMBC, COSY and NOESY correlations of compound 1.

**Figure S2.** Key HMBC, COSY and NOESY correlations of compound 2.

**Figure S3.** Key HMBC, COSY and NOESY correlations of compound 3.

**Figure S4.** X-ray crystallographic structure of compound 5

**Table S1.** $^{13}$C-NMR data of 1-3 (at 100 MHz, $\delta$ in ppm, CH$_n$ fragment from DEPT)

**Table S2.** $^1$H-NMR data of 1-3 (at 400 MHz; $\delta$ in ppm, $J$ in Hz)

**Table S3.** X-ray data of compound 5.

**Figure S5.** Original spectra of compound 1. (H NMR, C NMR, DEPT, HSQC, HMBC, COSY, NOESY)

**Figure S6.** Original spectra of compound 2. (H NMR, C NMR, DEPT, HSQC, HMBC, COSY, NOESY)

**Figure S7.** Original spectra of compound 3. (H NMR, C NMR, DEPT, HSQC, HMBC, COSY, NOESY)
Figure S1. Key HMBC (from H to C), COSY and NOESY correlations of compound 1.

Figure S2. Key HMBC (from H to C), COSY and NOESY correlations of compound 2.

Figure S3. Key HMBC (from H to C), COSY and NOESY correlations of compound 3.
Figure S4. X-ray crystallographic structure of compound 5.

Table S1. $^{13}$C-NMR data of 1-3 (at 100 MHz, $\delta$ in ppm, CH$_n$ fragment from DEPT)

| NO. | 1* (CDCl$_3$) | 2* (CD$_3$OD) | 3* (CD$_3$OD) | 4 (CD$_3$OD) | 5 (CD$_3$OD) |
|-----|---------------|---------------|---------------|--------------|--------------|
| 1   | 37.9 (CH$_2$) | 89.5 (C)      | 89.4 (C)      | 54.3 (CH)    | 54.2 (CH)    |
| 2   | 30.4 (CH$_2$) | 32.3 (CH$_2$) | 32.6 (CH$_2$) | 25.3 (CH$_2$)| 25.5 (CH$_2$)|
| 3   | 75.6 (CH$_2$) | 29.4 (CH$_2$) | 29.6 (CH$_2$) | 30.1 (CH$_2$)| 30.2 (CH$_2$)|
| 4   | 87.4 (C)      | 35.5 (CH)     | 35.7 (CH)     | 39.5 (CH)    | 39.7 (CH)    |
| 5   | 50.1 (CH)     | 48.2 (CH)     | 47.6 (CH)     | 40.8 (CH)    | 40.3 (CH)    |
| 6   | 24.9 (CH$_2$) | 25.4 (CH)     | 20.7 (CH)     | 30.4 (CH)    | 20.1 (CH)    |
| 7   | 47.9 (CH)     | 31.0 (CH)     | 27.8 (CH)     | 24.8 (CH)    | 27.2 (CH)    |
| 8   | 23.0 (CH$_2$) | 18.4 (CH$_2$) | 18.3 (CH$_2$) | 19.2 (CH$_2$)| 19.1 (CH$_2$)|
| 9   | 30.9 (CH$_2$) | 34.0 (CH$_2$) | 33.7 (CH$_2$) | 32.9 (CH$_2$)| 32.7 (CH$_2$)|
| 10  | 42.4 (C)      | 78.3 (C)      | 78.3 (C)      | 77.2 (C)     | 77.2 (C)     |
| 11  | 72.7 (C)      | 25.9 (C)      | 27.0 (C)      | 25.4 (C)     | 26.6 (C)     |
| 12  | 27.3 (CH$_3$) | 64.0 (CH$_2$) | 12.2 (CH$_3$) | 64.0 (CH$_2$)| 12.2 (CH$_3$)|
| 13  | 26.8 (CH$_3$) | 24.2 (CH$_3$) | 72.7 (CH$_2$) | 24.4 (CH$_3$)| 73.3 (CH$_2$)|
| NO. | 1 (CDCl₃) | 2 (CD₃OD) | 3 (CD₃OD) |
|-----|-----------|-----------|-----------|
| 1   | 1.49 (d, 6.4) | 1.97 (m) | 1.97 (m) |
|     | 1.32 (m) | 1.51 (m) | 1.55 (m) |
| 2   | 2.07 (m) | 1.90 (m) | 1.93 (m) |
|     | 1.53 (m) | 1.34 (m) | 1.34 (m) |
| 3   | 3.38 (dd, 5.9, 10.4) | 1.76 (dd, 2.5, 5.0,12.7) | 0.20 (t, 9.5) |
|     | 1.90 (m) | 0.21 (t, 9.5) | 1.03 (dd, 2.4, 24.8) |
| 4   | 2.68 (m) | 2.68 (m) |           |
| 5   | 1.30 (m) | 1.71 (m) | 1.74 (m) |
| 6   | 1.76 (dd, 2.5, 5.0,12.7) | 0.20 (t, 9.5) | 0.21 (t, 9.5) |
|     | 0.82 (ddd, 6.3, 9.5, 15.8) | 1.03 (dd, 2.4, 24.8) |           |
| 7   | 1.26 (t,2.5) | 1.13 (dd, 3.9, 12.9) | 1.53 (m) |
| 8   | 1.68 (ddd, 2.2, 4.4, 12.5) | 1.75 (m) | 1.65 (m) |
|     | 1.13 (dd, 3.9, 12.9) | 1.63 (dd, 2.1, 13.6) | 1.53 (m) |
| 9   | 1.62 (m) | 1.84 (dd, 6.9, 14.0) | 1.83 (dd, 6.4, 12.4) |
|     | 1.35 (m) | 1.54 (m) | 1.57 (m) |
| 10  |           |           |           |
| 11  |           |           |           |
| 12  | 1.18 (s) | 3.65 (d,11.4) | 1.07 (s) |
|     |           | 3.58 (d,11.4) |           |
| 13  | 1.19 (s) | 1.12 (s) | 3.03 (d, 11.4) |
|     |           |           | 3.57 (d, 11.4) |
| 14  | 3.89 (dd, 1.7, 8.0) | 3.68 (d, 10.9) | 3.40 (d, 10.9) |
| 3.51 (d, 8.0) | 3.39 (d, 10.9) | 3.69 (d, 10.9) |
|---------------|---------------|---------------|
| 15  1.22 (s)  | 0.99 (d, 7.0) | 0.94 (d, 7.0) |

**Table S3.** X-ray datas of compound 5.

|                          | 2014038 |
|--------------------------|---------|
| Project No.              | 038     |
| Formula                  | C15 H26 O3 |
| Crystal system           | Orthorhombic |
| Space group              | P212121 |
| Temperature (K)          | 296     |
| a (Å)                    | 7.40260(10) |
| b (Å)                    | 7.78380(10) |
| c (Å)                    | 49.7560(7)  |
| a (°)                    | 90.00   |
| β(°)                     | 90.00   |
| γ (°)                    | 90.00   |
| Cell volume (Å3)         | 2866.96(7) |
| Calc. density (g/cm3)    | 1.179   |
| Z                        | 8       |
| m (Cu-Ka)                | 1.54178 |
| Rint                     | 0.0514  |
| R1(I>2sigma(I))          | 0.0365  |
| wR2                      | 0.0977  |
| GOF                      | 1.101   |
The $^1$H-NMR spectrum of compound 1

The $^{13}$C-NMR spectrum of compound 1
The DEPT spectrum of compound 1

The HSQC spectrum of compound 1
The HMBC spectrum of compound 1

The $^1$H-$^1$H COSY spectrum of compound 1
The NOESY spectrum of compound 1

The HR-EI-MS of compound 1
The specific rotation of compound 1

The IR spectrum of compound 1

Figure S5. Original spectra of compound 1.
The $^1$H-NMR spectrum of compound 2

The $^{13}$C-NMR spectrum of compound 2
The DEPT spectrum of compound 2

The HSQC spectrum of compound 2
The HMBC spectrum of compound 2

The $^1$H-$^1$H COSY spectrum of compound 2
The NOESY spectrum of compound 2

The HR-ESI-MS of compound 2
The specific rotation of compound 2

| S.No | Sample ID | Time       | Result | Scale | OR °Arc | WLG | Lg.mm | Conc. | Temp. |
|------|-----------|------------|--------|-------|---------|-----|-------|-------|-------|
| 1    | sqg46     | 03:40:54 PM| -3.000 | SR    | -0.006  | 580 | 100.00| 0.200 | 24.5  |
| 2    | sqg46     | 03:41:00 PM| -3.500 | SR    | -0.007  | 580 | 100.00| 0.200 | 24.5  |
| 3    | sqg46     | 03:41:07 PM| -3.500 | SR    | -0.007  | 580 | 100.00| 0.200 | 24.5  |
| 4    | sqg46     | 03:41:13 PM| -3.000 | SR    | -0.006  | 580 | 100.00| 0.200 | 24.5  |
| 5    | sqg46     | 03:41:19 PM| -3.000 | SR    | -0.006  | 580 | 100.00| 0.200 | 24.5  |
| 6    | sqg46     | 03:41:26 PM| -3.000 | SR    | -0.006  | 580 | 100.00| 0.200 | 24.5  |

The IR spectrum of compound 2

**Figure S6.** Original spectra of compound 2.
The $^1$H-NMR spectrum of compound 3

The $^{13}$C-NMR spectrum of compound 3
The DEPT spectrum of compound 3

The HSQC spectrum of compound 3
The HMBC spectrum of compound 3

The $^1$H-$^1$H COSY spectrum of compound 3
The NOESY spectrum of compound 3

The HR-ESI-MS of compound 3
The specific rotation of compound 3

Figure S7. Original spectra of compound 3.