SUPPLEMENTARY MATERIAL

Nine sesquiterpenes from *Solanum torvum*

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Abstract: Three new sesquiterpenes, namely, 3 β ,11-dihydroxy-4,14-oxideenantioeudesmane (1), 1 β ,10 β ,12,14-tetrahydroxy-*allo*-aromadendrane (2), and 1 β ,10 β ,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, sterically effects influence strongly the ¹³C 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, they 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*; ¹³C 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, δ in ppm, CH_n fragment from DEPT)

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

Table S3. X-ray datas 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, δ in ppm, CH_n fragment from DEPT)

NO.	1* (CDCl_3)	2* (CD_3OD)	3* (CD_3OD)	4 (CD_3OD)	5 (CD_3OD)
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)

14	72.8 (CH ₂)	69.7 (CH ₂)	69.6 (CH ₂)	71.5 (CH ₂)	71.5 (CH ₂)
15	16.2 (CH ₃)	16.4 (CH ₃)	16.2 (CH ₃)	16.9 (CH ₃)	16.7 (CH ₃)

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

NO.	1 (CDCl ₃)	2 (CD ₃ OD)	3 (CD ₃ OD)
1	1.49 (d, 6.4) 1.32 (m)		
2	2.07 (m) 1.53 (m)	1.97 (m) 1.51 (m)	1.97 (m) 1.55 (m)
3	3.38 (dd, 5.9, 10.4)	1.90 (m) 1.34 (m)	1.93 (m) 1.34 (m)
4		2.68 (m)	2.68 (m)
5	1.30 (m)	1.71 (m)	1.74 (m)
6	1.76 (ddd, 2.5, 5.0, 12.7) 1.03 (dd, 2.4, 24.8)	0.20 (t, 9.5)	0.21 (t, 9.5)
7	1.26 (t, 2.5)	0.82 (ddd, 6.3, 9.5, 15.8)	0.89 (m)
8	1.68 (ddd, 2.2, 4.4, 12.5) 1.13 (dd, 3.9, 12.9)	1.75 (m) 1.63 (dd, 2.1, 13.6)	1.65 (m) 1.53 (m)
9	1.62 (m) 1.35 (m)	1.84 (dd, 6.9, 14.0) 1.54 (m)	1.83 (dd, 6.4, 12.4) 1.57 (m)
10			
11			
12	1.18 (s)	3.65 (d, 11.4) 3.58 (d, 11.4)	1.07 (s)
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 systetm	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 (Å ³)	2866.96(7)
Calc. density (g/cm ³)	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 ¹H-NMR spectrum of compound **1**

The ¹³C-NMR spectrum of compound **1**

The DEPT spectrum of compound 1

The HSQC spectrum of compound 1

The HMBC spectrum of compound **1**

The ^1H - ^1H COSY spectrum of compound **1**

The NOESY spectrum of compound **1**

Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
55.05615 *	71860	3.39	0.48	-1.4	1.5	C4.H7
57.03403 *	28561	1.35	0.19	0.0	1.5	C3.H5.O
59.04970 *	162052	7.64	1.09	0.0	0.5	C3.H7.O
67.05591 *	70543	3.32	0.47	-1.1	2.5	C5.H7
69.07066 *	75556	3.56	0.51	-0.2	1.5	C5.H9
71.04934 *	50033	2.36	0.34	0.4	1.5	C4.H7.O
77.03826 *	46033	2.17	0.31	0.9	4.5	C6.H5
79.05445 *	90597	4.27	0.61	0.3	3.5	C6.H7
81.06844 *	64517	3.04	0.43	2.0	2.5	C6.H9
83.04744 *	22687	1.07	0.15	2.2	2.5	C5.H7.O
90.05580 *	28308	1.33	0.19			
91.05390 *	112069	5.28	0.75	0.9	4.5	C7.H7
92.06078 *	20155	0.95	0.14	1.8	4.0	C7.H8
93.07048 *	122248	5.76	0.82	-0.1	3.5	C7.H9
95.04982 *	94699	4.46	0.64	-0.1	3.5	C6.H7.O
95.08529 *	45222	2.13	0.30	0.8	2.5	C7.H11
96.05605 *	54591	2.57	0.37	1.5	3.0	C6.H8.O
97.06499 *	24257	1.14	0.16	0.4	2.5	C6.H9.O
105.0684 *	77278	3.64	0.52	2.0	4.5	C8.H9
107.0839 *	73227	3.45	0.49	2.2	3.5	C8.H11
109.0629 *	48514	2.29	0.33	2.4	3.5	C7.H9.O
109.0996 *	21421	1.01	0.14	2.1	2.5	C8.H13
110.0708 *	24510	1.15	0.16	2.4	3.0	C7.H10.O
117.0692 *	33068	1.56	0.22	1.3	5.5	C9.H9
119.0864 *	79557	3.75	0.53	-0.3	4.5	C9.H11
120.0924 *	21421	1.01	0.14	1.5	4.0	C9.H12
121.0660 *	137744	6.49	0.92	-0.6	4.5	C8.H9.O
121.1016 *	29321	1.38	0.20	0.1	3.5	C9.H13
123.0823 *	31752	1.50	0.21	-1.3	3.5	C8.H11.O
131.0860 *	24358	1.15	0.16	0.1	5.5	C10.H11
133.0660 *	22383	1.05	0.15	-0.7	5.5	C9.H9.O
133.1026 *	71505	3.37	0.48	-0.9	4.5	C10.H13
135.0812 *	261410	12.32	1.75	-0.2	4.5	C9.H11.O
135.1175 *	65691	3.09	0.44	-0.1	3.5	C10.H15
136.0865 *	38031	1.79	0.26	2.3	4.0	C9.H12.O
137.0959 *	41424	1.95	0.28	0.8	3.5	C9.H13.O
145.1025 *	30739	1.45	0.21	-0.8	5.5	C11.H13
147.1172 *	26485	1.25	0.18	0.1	4.5	C11.H15
149.1333 *	25320	1.19	0.17	-0.3	3.5	C11.H17
159.1171 *	51147	2.41	0.34	0.3	5.5	C12.H15
161.1326 *	23497	1.11	0.16	0.4	4.5	C12.H17
175.1489 *	26333	1.24	0.18	-0.2	4.5	C13.H19
177.1282 *	1937083	91.27	12.99	-0.3	4.5	C12.H17.O
178.1314 *	236140	11.13	1.58			
179.1068 *	20509	0.97	0.14	0.4	4.5	C11.H15.O2
179.1368 *	21218	1.00	0.14			
195.1394 *	2122430	100.00	14.23	-0.8	3.5	C12.H19.O2
196.1413 *	269918	12.72	1.81			
197.1420 *	18990	0.89	0.13			
221.1544 *	73126	3.45	0.49	-0.2	4.5	C14.H21.O2
236.1778 *	20053	0.94	0.13	-0.2	4.0	C15.H24.O2
254.1873 *	166964	7.87	1.12	0.9	3.0	C15.H26.O3
255.1908 *	27346	1.29	0.18			

The HR-EI-MS of compound **1**

Rudolph Research Analytical

Monday, 09/15/2014

This sample was measured on an Autopol VI, serial number 90079, manufactured by Rudolph Research Analytical, Hackettstown, NJ.

LotID : sqg33

Set Temperature : OFF

Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	6.167	0.2582	6.500	6.000

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	sqg33	03:32:25 PM	6.000	SR	0.012	589	100.00	0.200	23.8
2	sqg33	03:32:31 PM	6.000	SR	0.012	589	100.00	0.200	23.8
3	sqg33	03:32:38 PM	6.500	SR	0.013	589	100.00	0.200	23.8
4	sqg33	03:32:44 PM	6.000	SR	0.012	589	100.00	0.200	23.8
5	sqg33	03:32:51 PM	6.000	SR	0.012	589	100.00	0.200	23.8
6	sqg33	03:32:57 PM	6.500	SR	0.013	589	100.00	0.200	23.8

The specific rotation of compound 1

The IR spectrum of compound 1

Figure S5. Original spectra of compound 1.

The ¹H-NMR spectrum of compound 2

The ¹³C-NMR spectrum of compound 2

The DEPT spectrum of compound 2

The HSQC spectrum of compound 2

The HMBC spectrum of compound **2**

The ^1H - ^1H COSY spectrum of compound **2**

The NOESY spectrum of compound **2**

The HR-ESI-MS of compound **2**

LotID : sqg46
Set Temperature : OFF
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-3.167	0.2582	-3.000	-3.500

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	589	100.00	0.200	24.5
2	sqg46	03:41:00 PM	-3.500	SR	-0.007	589	100.00	0.200	24.5
3	sqg46	03:41:07 PM	-3.500	SR	-0.007	589	100.00	0.200	24.5
4	sqg46	03:41:13 PM	-3.000	SR	-0.006	589	100.00	0.200	24.5
5	sqg46	03:41:19 PM	-3.000	SR	-0.006	589	100.00	0.200	24.5
6	sqg46	03:41:26 PM	-3.000	SR	-0.006	589	100.00	0.200	24.5

The specific rotation of compound **2**

The IR spectrum of comopund **2**
Figure S6. Original spectra of compound **2**.

The ¹H-NMR spectrum of compound **3**

The ¹³C-NMR spectrum of compound **3**

The DEPT spectrum of compound **3**

The HSQC spectrum of compound **3**

The HMBC spectrum of compound **3**

The ^1H - ^1H COSY spectrum of compound **3**

The NOESY spectrum of compound **3**

The HR-ESI-MS of compound **3**

LotID : sqg77
Set Temperature : OFF
Temp Corr : OFF

n	Average	Std.Dev.	Maximum	Minimum
6	-7.250	0.2739	-7.000	-7.500

S.No	Sample ID	Time	Result	Scale	OR °Arc	WLG	Lg.mm	Conc.	Temp.
1	sqg77	03:47:01 PM	-7.500	SR	-0.015	589	100.00	0.200	25.0
2	sqg77	03:47:08 PM	-7.500	SR	-0.015	589	100.00	0.200	25.0
3	sqg77	03:47:13 PM	-7.000	SR	-0.014	589	100.00	0.200	25.0
4	sqg77	03:47:20 PM	-7.000	SR	-0.014	589	100.00	0.200	25.0
5	sqg77	03:47:26 PM	-7.000	SR	-0.014	589	100.00	0.200	25.0
6	sqg77	03:47:33 PM	-7.500	SR	-0.015	589	100.00	0.200	25.0

The specific rotation of compound **3**

The IR spectrum of comopund **3**
Figure S7. Original spectra of compound **3**.