

Supplementary Information

MS Formula Results: + Scan (6.330 min) Sub (2017030601.d)

m/z	Ion	Formula	Abundance
571.2156	(M+Na) ⁺	C28 H36 Na O11	16594.6

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DRE
1	C28 H36 O11	C28 H36 Na O11	98.98		548.2264	548.2258	571.215	-1.11	1.11	99.96	98.44	97.64	11
2	C29 H32 N4 O7	C29 H32 N4 Na O7	98.56		548.2264	548.2271	571.2163	1.31	1.31	99.94	97.1	97.52	16
3	C25 H40 O11 S	C25 H40 Na O11 S	98.09		548.2264	548.2291	571.2184	5.02	5.02	99.19	99.12	94.65	6
4	C20 H40 N2 O13 S	C20 H40 N2 Na O13 S	97.6		548.2264	548.2251	571.2143	-2.33	2.33	99.83	96.76	94.15	2
5	C32 H36 O6 S	C32 H36 Na O6 S	97.5		548.2264	548.2233	571.2125	-5.69	5.69	98.96	96.97	95.23	15
6	C33 H32 N4 O2 S	C33 H32 N4 Na O2 S	97.29		548.2264	548.2245	571.2138	-3.26	3.26	99.66	95.14	95.12	20
7	C29 H40 O6 S2	C29 H40 Na O6 S2	97.19		548.2264	548.2266	571.2159	0.45	0.45	99.99	95.61	93.49	10
8	C30 H36 N4 O2 S2	C30 H36 N4 Na O2 S2	96.89		548.2264	548.229	571.2172	2.89	2.89	99.73	95.04	93.37	15
9	C38 H32 N2 S	C38 H32 N2 Na S	95.95		548.2264	548.2286	571.2178	4.08	4.08	99.46	90.38	95.62	24
10	C41 H28 N2	C41 H28 N2 Na	95.28		548.2264	548.2252	571.2145	-2.06	2.06	99.86	85.43	97.94	29

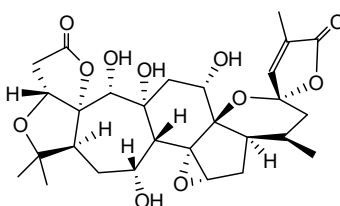
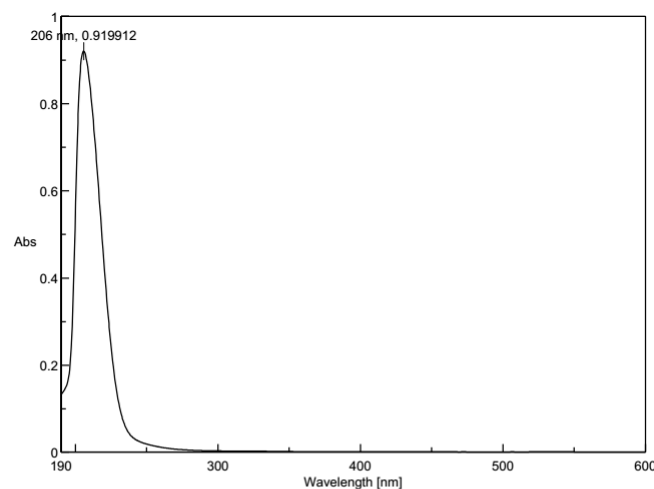


Figure S1. HRESIMS spectrum of 19(*R*)-hydroxyl-wuweizidilactone H (1)



[Comment]
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Comment 0.05
User
Division UV
Measurement Information
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Model Name V-650
Serial No. A034461150

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Accessory S/N A001761114
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Temperature 19.93 C
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Monitor Sensor Holder
Start Mode Start immediately

Photometric Mode Abs
Measurement range 600 - 190 nm
Data pitch 0.2 nm
Band width(UV/Vis) 2.0 nm
Response Medium
Scanning speed 200 nm/min
Source Change 340 nm
Light Source D2/VI
Filter Exchange Step
Correction Baseline

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Vertical Abs
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End 190 nm
Data pitch 0.2 nm
Data points 2051

Memory-4

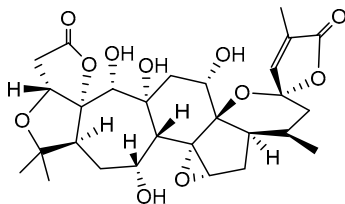


Figure S2. UV spectrum of 19(R)-hydroxyl-wuweizidilactone H (1)

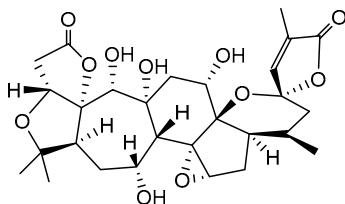
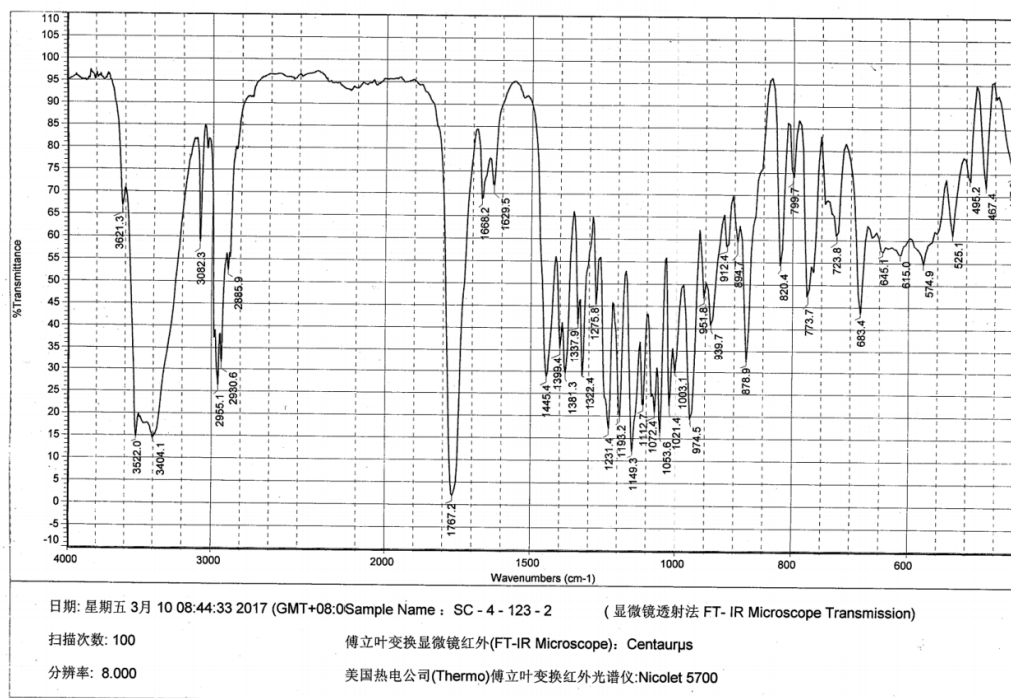


Figure S3. IR spectrum of 19(R)-hydroxyl-wuweizidilactone H (1)

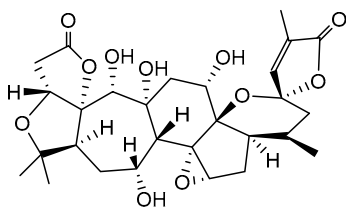
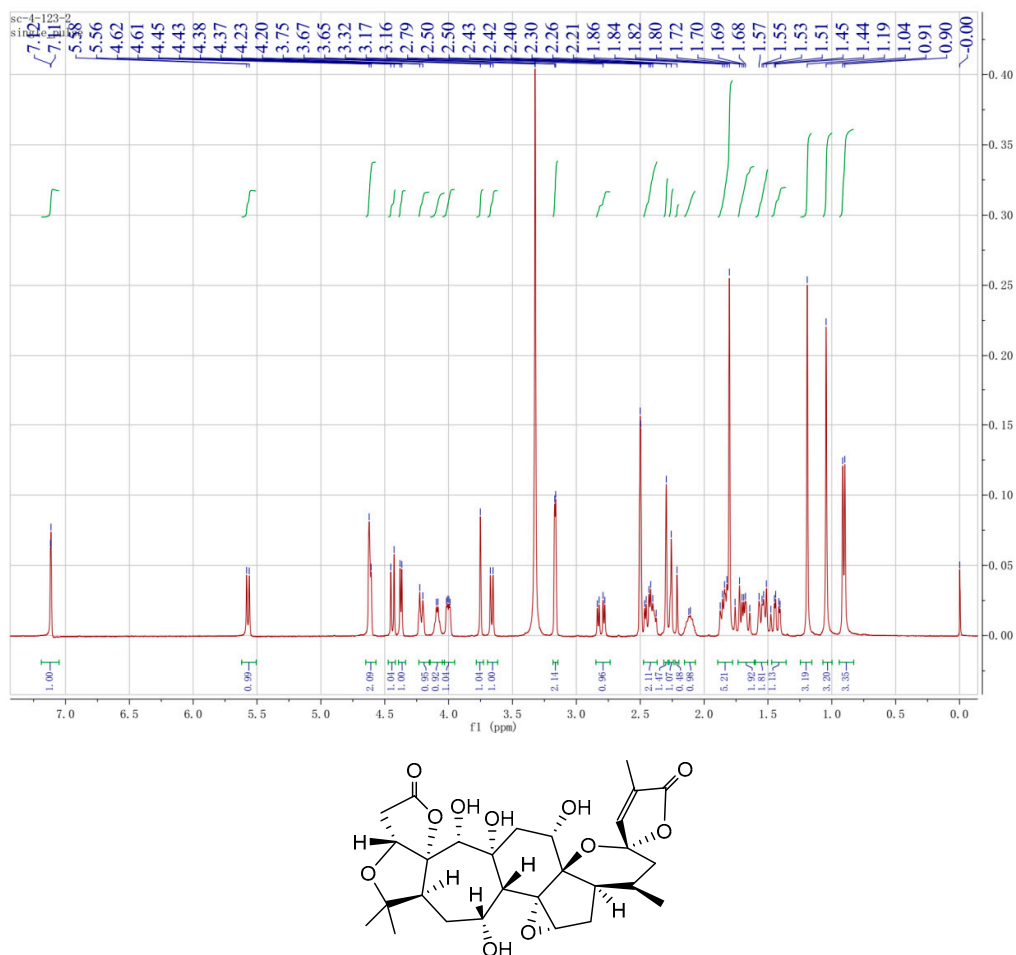
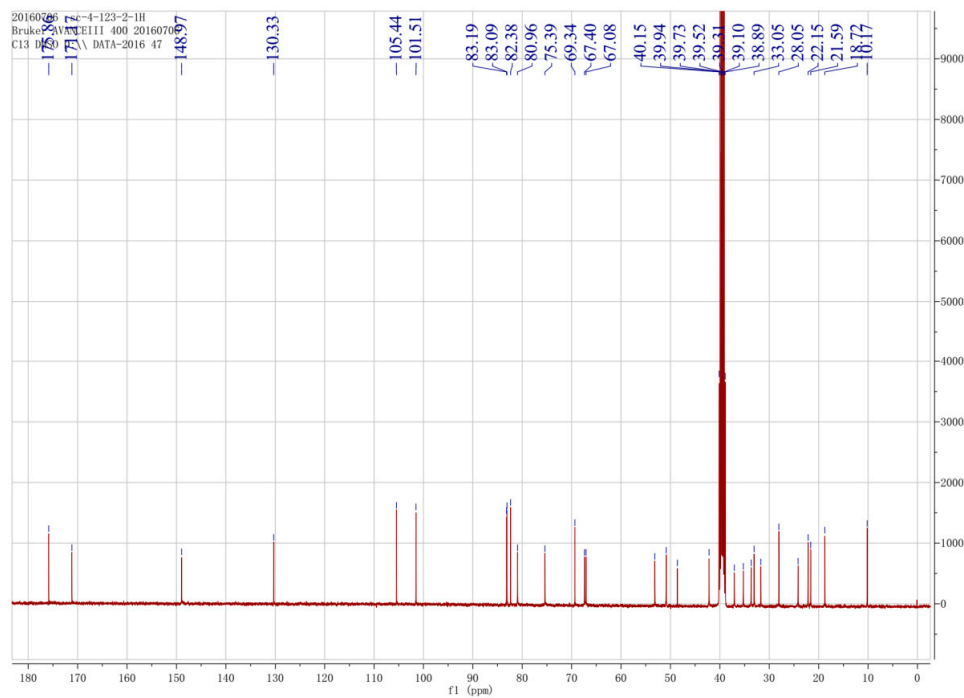


Figure S4. ¹H NMR spectrum of 19(R)-hydroxyl-wuweizidilactone H (1; 600 MHz, DMSO-*d*₆)



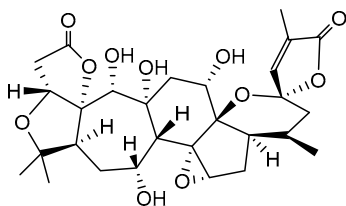


Figure S5. ^{13}C NMR spectrum of 19(*R*)-hydroxyl-wuweizidilactone H (1; 150 MHz, $\text{DMSO}-d_6$)

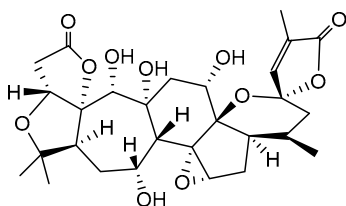
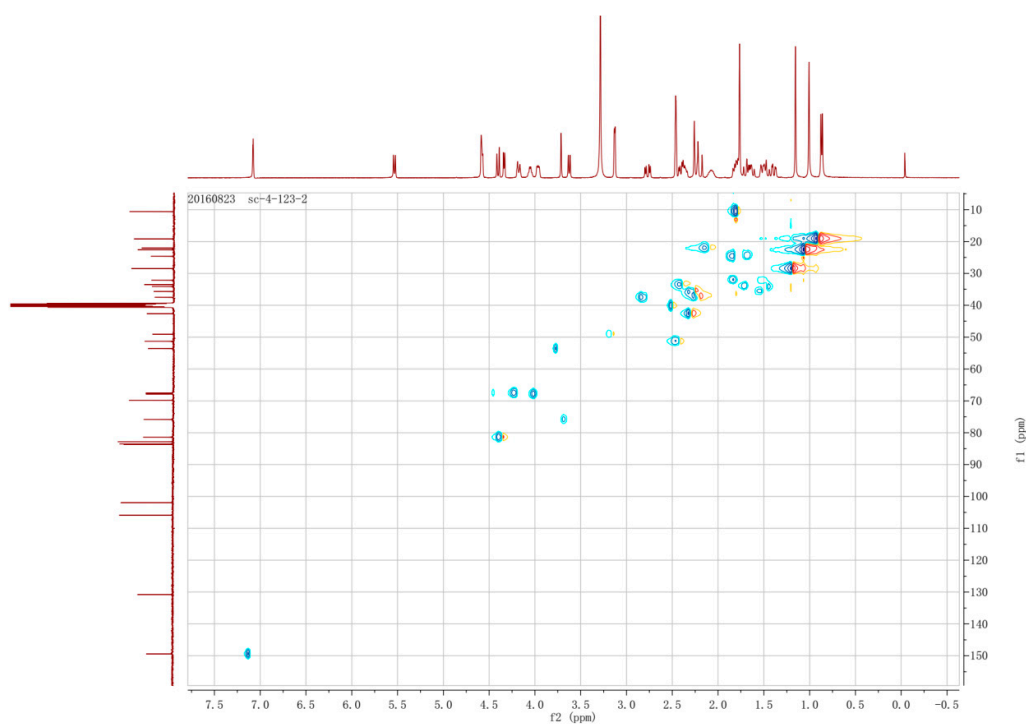


Figure S6. HSQC spectrum of 19(*R*)-hydroxyl-wuweizidilactone H (1; $\text{DMSO}-d_6$)

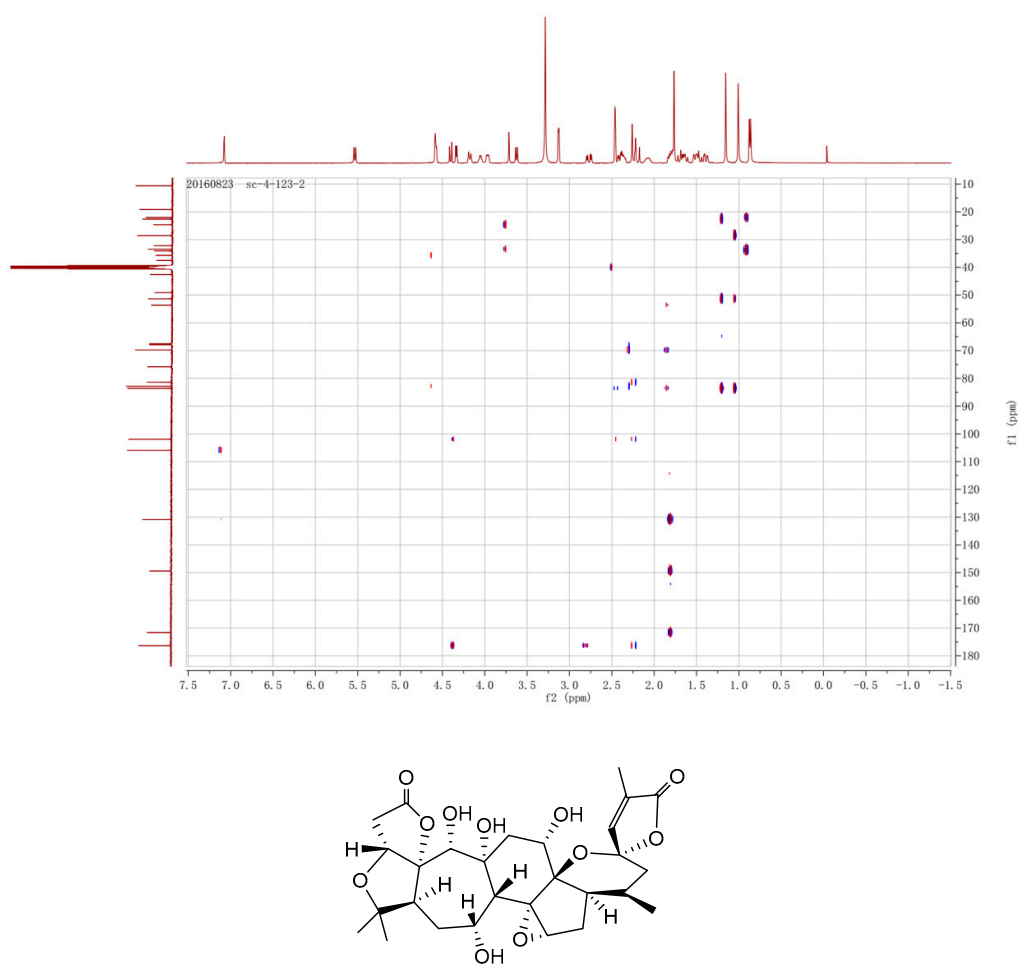
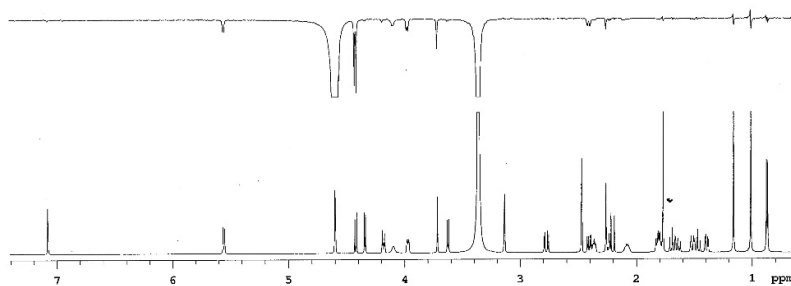


Figure S7. HMBC spectrum of 19(R)-hydroxyl-wuweizidilactone H (1; DMSO-*d*₆)

VNU-600 NMR510 ao-4-123-2 IN dmsd Oct 11 2017



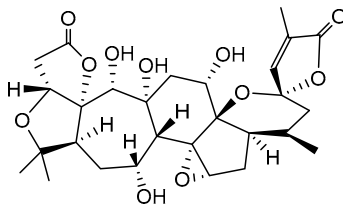


Figure S8. 1D NOSEY spectrum of 19(*R*)-hydroxyl-wuweizidilactone H (1; DMSO-*d*₆)

MS Formula Results: - Scan (8.364 min) Sub (2017031602.d)

m/z	Ion	Formula	Abundance
233.1542	(M-H) ⁻	C15 H21 O2	76161.7

Best	Formula (M)	Ion Formula	Score	Cross Sco	Mass	Calc Mass	Calc m/z	Diff (ppm)	Abs Diff (ppm)	Mass Match	Abund Match	Spacing Match	DBE
✓	C15 H22 O2	C15 H21 O2	99.77		234.1615	234.162	233.1547	2.16	2.16	99.86	99.49	99.93	5
✓	C10 H22 N2 O4	C10 H21 N2 O4	96.64		234.1615	234.158	233.1507	-15.02	15.02	93.58	98.95	100	1
✓	C12 H26 O2 S	C12 H25 O2 S	95.4		234.1615	234.1654	233.1581	16.55	16.55	92.26	97.09	99.64	0
✓	C9 H22 N4 O3	C9 H21 N4 O3	86.58		234.1615	234.1692	233.1619	32.94	32.94	72.69	98.61	99.93	-1
✓	C9 H22 N4 O S	C9 H21 N4 O S	78.98		234.1615	234.1514	233.1442	-42.9	42.9	58.22	96.54	99.42	1
✓	C14 H22 N2 O	C14 H21 N2 O	75.02		234.1615	234.1732	233.1659	50.13	50.13	47.78	99.63	99.99	5
✓	C12 H18 N4 O	C12 H17 N4 O	70.5		234.1615	234.1481	233.1408	-57.29	57.29	38.11	99.94	99.98	6

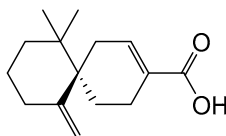
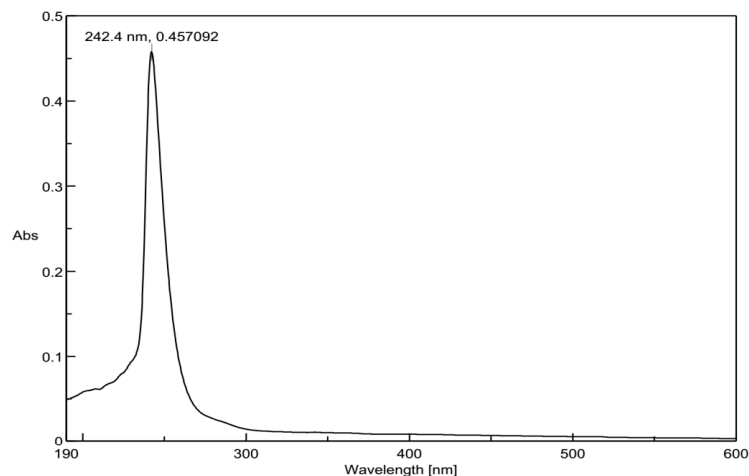


Figure S9. HRESIMS spectrum of (6*R*)-β-chamigrenic acid (2)



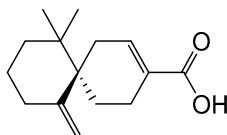
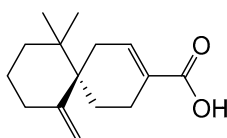
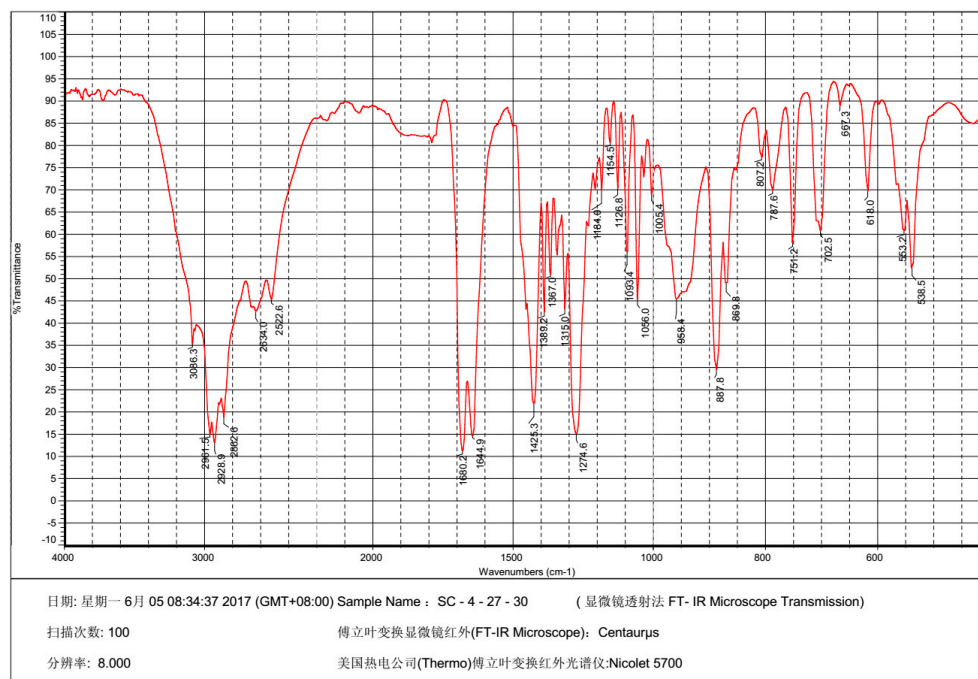
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 User
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 Instrument Name V-650
 Model Name V-650
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Accessory PSC-718
 Accessory S/N A001761114
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 Cell Length 10 mm
 Temperature 19.97 C
 Control Sensor Holder
 Monitor Sensor Holder
 Start Mode Start immediately

Photometric Mode Abs
 Measurement range 600 - 190 nm
 Data pitch 0.2 nm
 Band width(UV/Vis) 2.0 nm
 Response Medium
 Scanning speed 200 nm/min
 Source Change 340 nm
 Light Source D2/WI
 Filter Exchange Step
 Correction Baseline

[Data Information]
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 End 190 nm
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 Data points 2051

Memory-1

**Figure S10.** UV spectrum of (6*R*)- β -chamigrenic acid (2)**Figure S11.** IR spectrum of (6*R*)- β -chamigrenic acid (2)

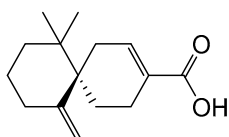
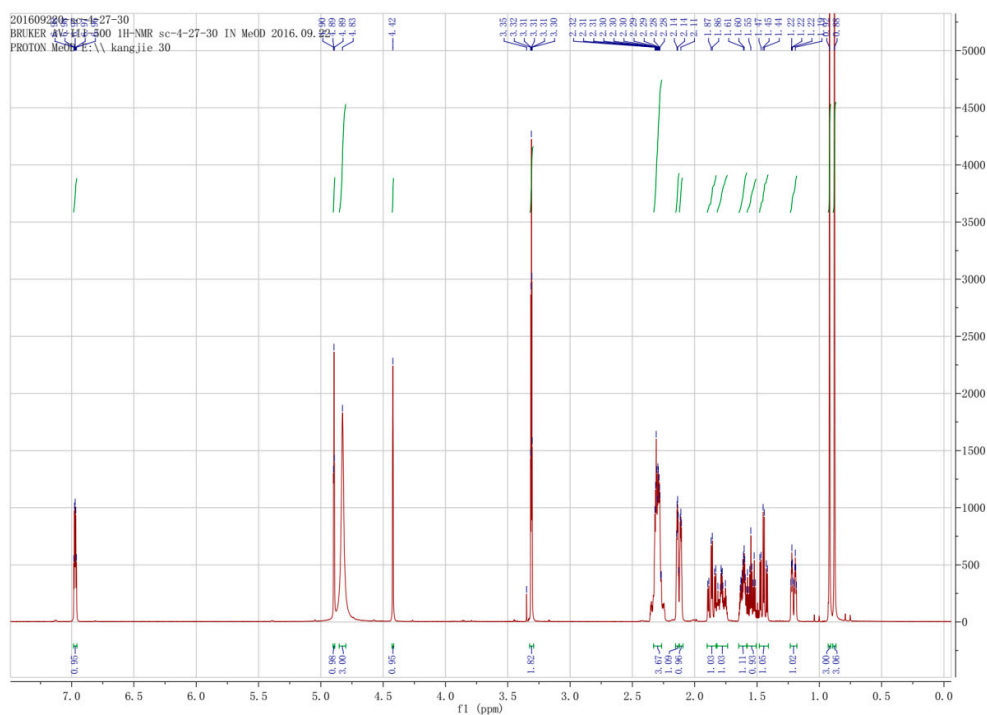
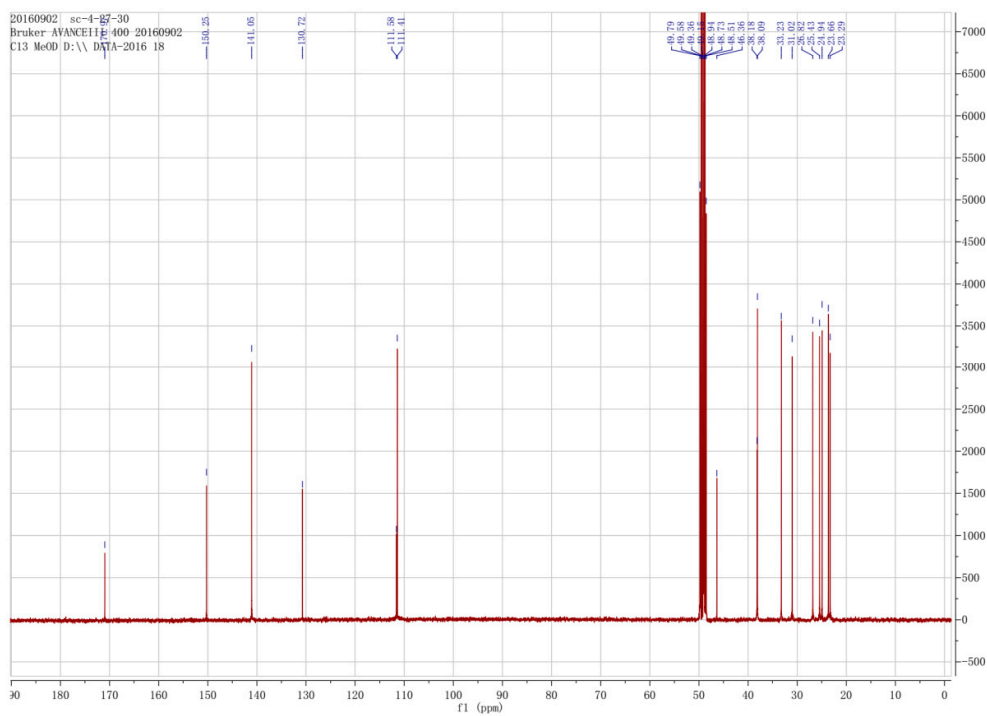


Figure S12. ^1H NMR spectrum of (6*R*)- β -chamigrenic acid (2; 600 MHz, CD_3OD)



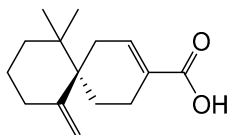


Figure S13. ^{13}C NMR spectrum of (6*R*)- β -chamigrenic acid (2; 150 MHz, CD_3OD)

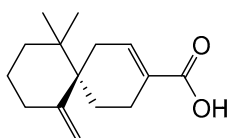
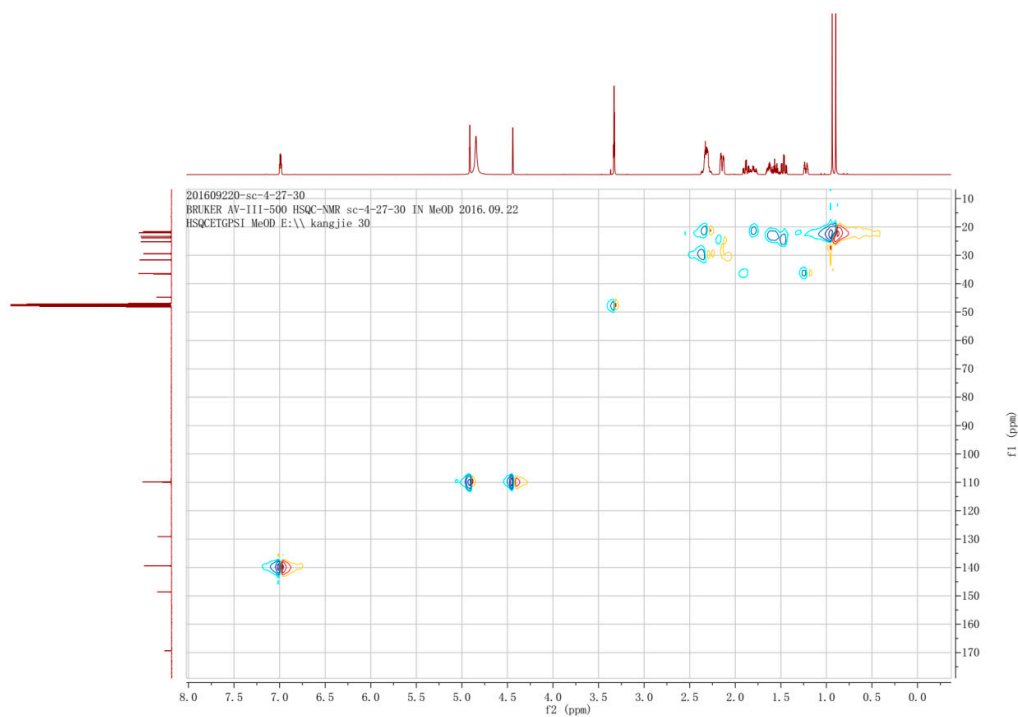


Figure S14. HSQC spectrum of (6*R*)- β -chamigrenic acid (2; CD_3OD)

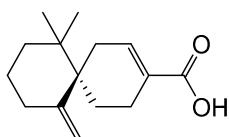
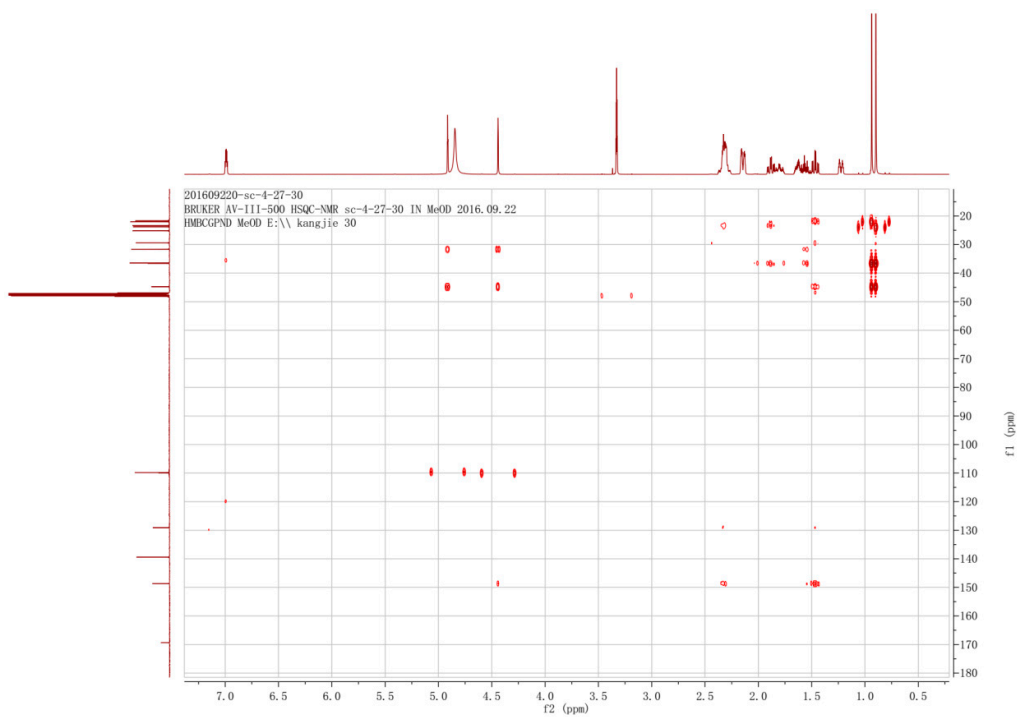


Figure S15. HMBC spectrum of (6*R*)-β-chamigrenic acid (2; CD₃OD)