Supporting Information

Structurally Diverse Diterpenoids from *Isodon scoparius* and Their Bioactivity

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Contents of Supporting Information

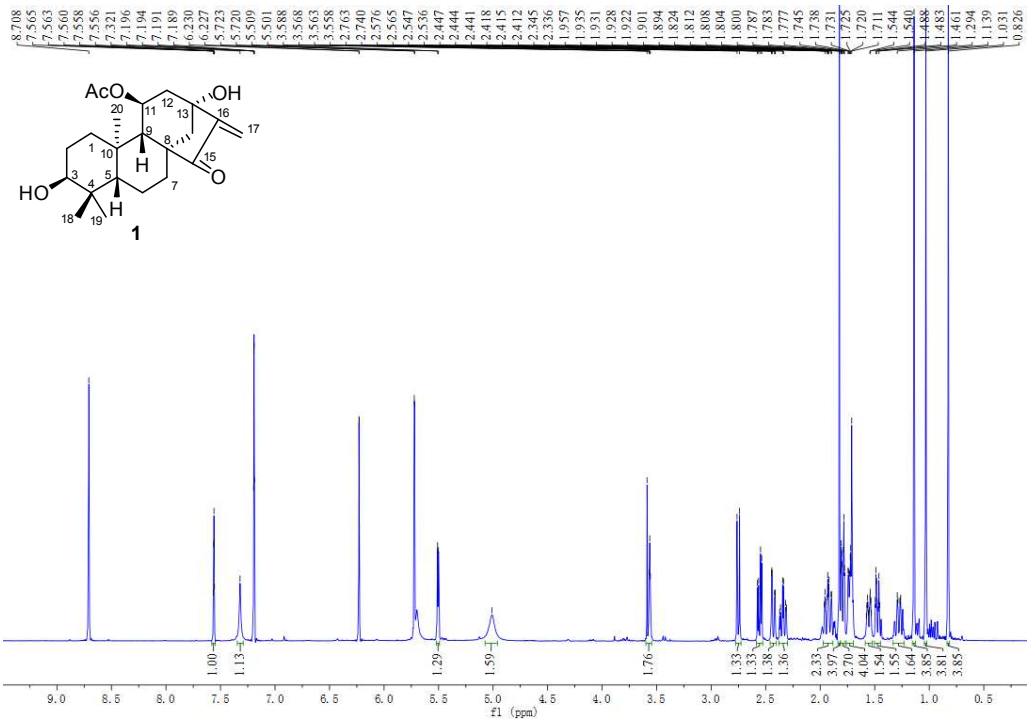


Figure 1: ^{1}H NMR spectrum of 3-epi-isodopharicin A (**1**) recorded in C_5D_5N at 400 MHz

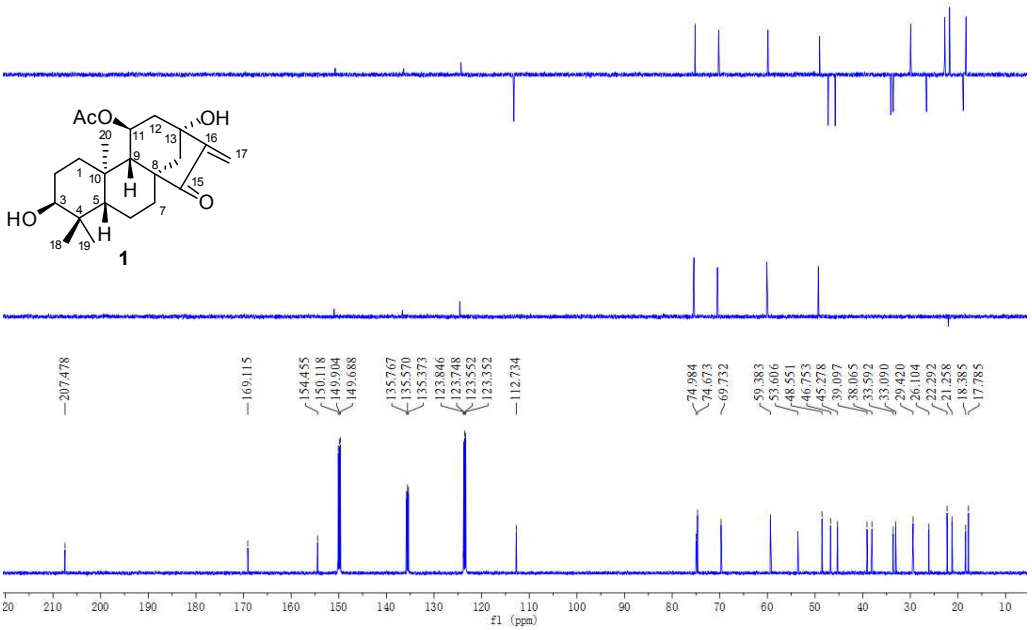


Figure 2: ^{13}C NMR spectrum of 3-epi-isodopharicin A (**1**) recorded in C_5D_5N at 125 MHz

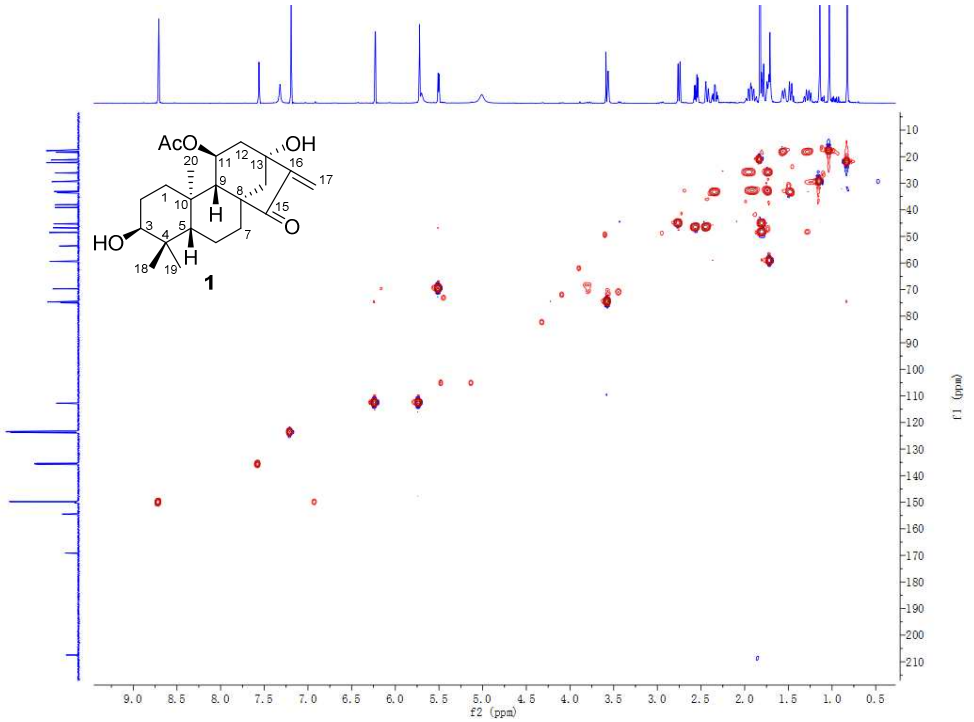


Figure 3: HSQC spectrum of 3-epi-isodopharicin A (**1**) recorded in C_5D_5N

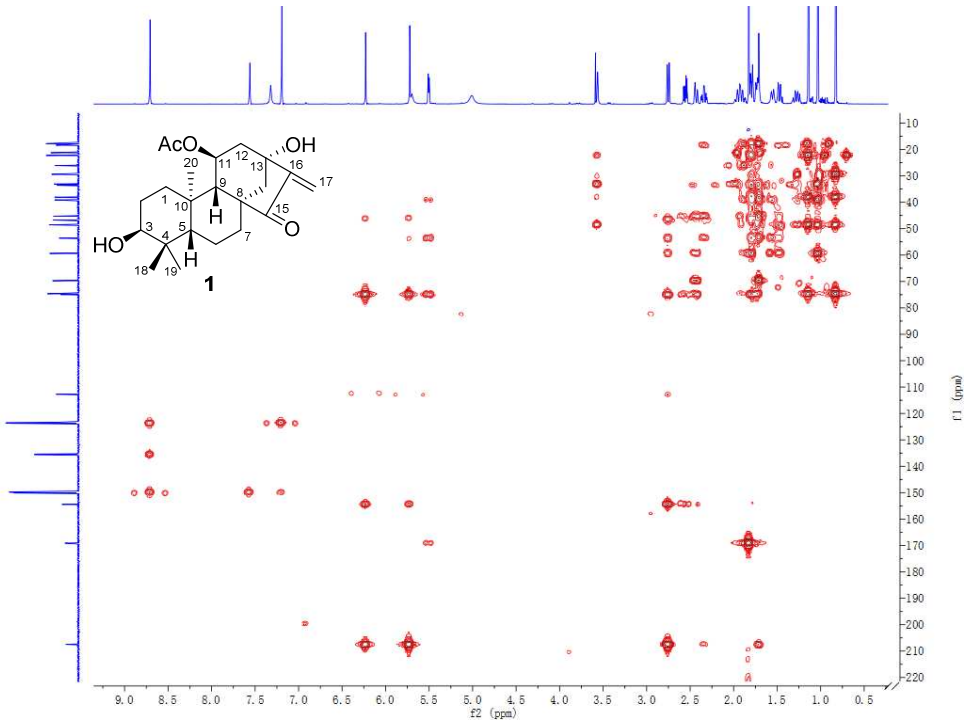


Figure 4: HMBC spectrum of 3-epi-isodopharicin A (**1**) recorded in C_5D_5N

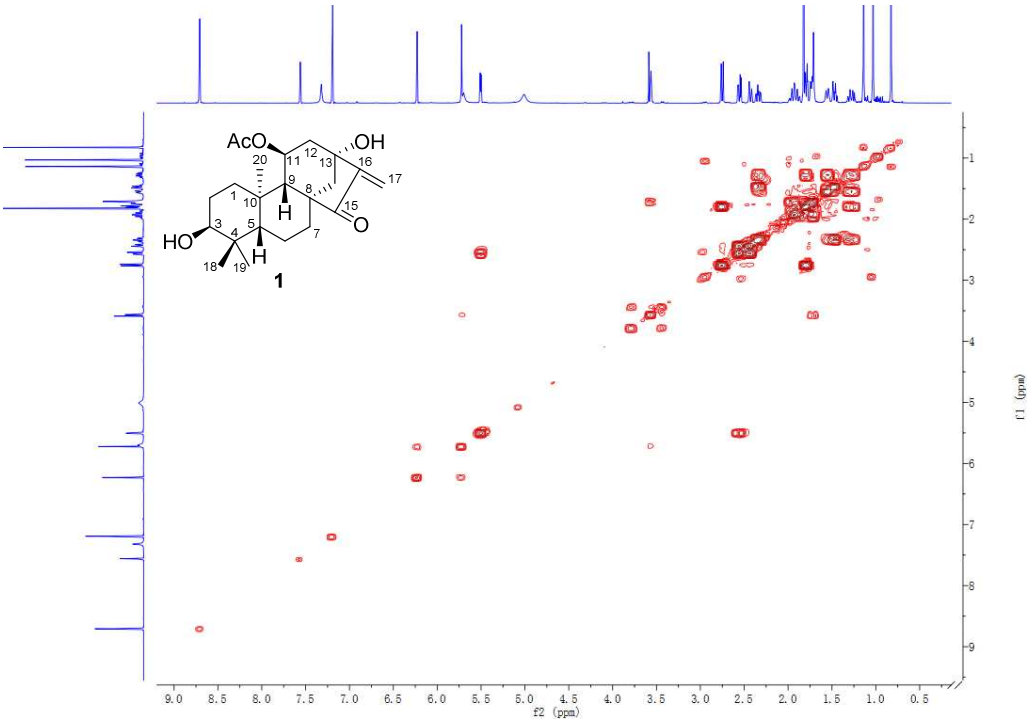


Figure 5: ^{1}H-^{1}H COSY spectrum of 3-epi-isodopharicin A (**1**) recorded in C_5D_5N

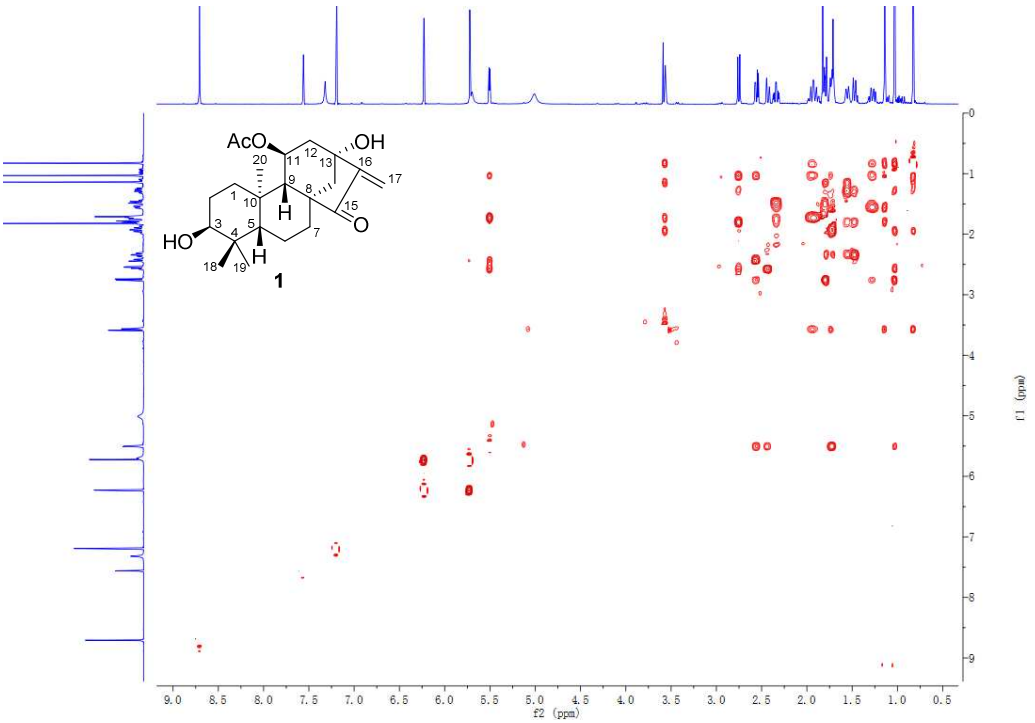
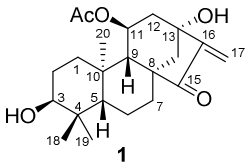


Figure 6: ROESY spectrum of 3-epi-isodopharicin A (**1**) recorded in C_5D_5N

Qualitative Analysis Report

Data Filename	SISJ75.d	**Sample Name**	SISJ75
Sample Type	Sample	**Position**	P1-A5
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/23/2016 9:35:48 AM
IRM Calibration Status	Success	**DA Method**	FSI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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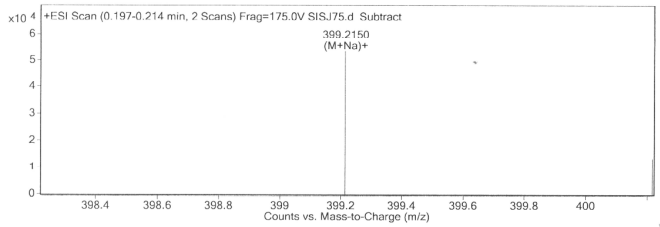

Peak List

m/z	z	Abund	Formula	Ion
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394.2598	1	12845.37		
399.215	1	53509.84	C22 H32 O5	(M+Na)+
400.2177	1	13248.24	C22 H32 O5	(M+Na)+
431.2408	1	15540.98		
497.2125	1	9535.59		
775.44	1	13851.42		
776.4437	1	6723.95		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C22 H32 O5	376.2250	399.2142	399.2150	-0.7	-1.8	7.0000

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Agilent Technologies Page 1 of 1 Printed at: 9:37 AM on: 9/23/2016

Figure 7: HRESIMS spectrum of 3-epi-isodopharicin A (**1**)

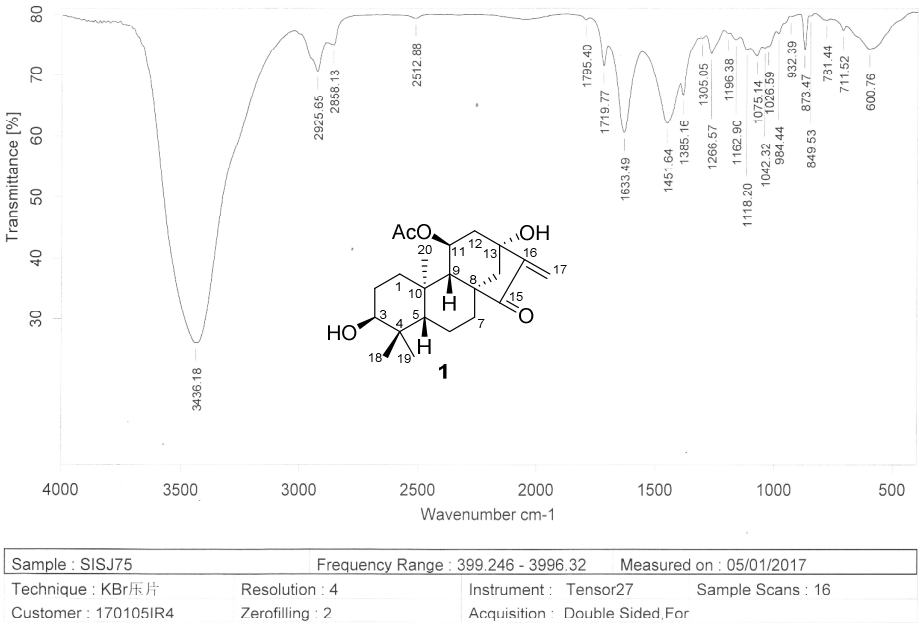

Figure 8: IR spectrum of 3-epi-isodopharicin A (**1**)

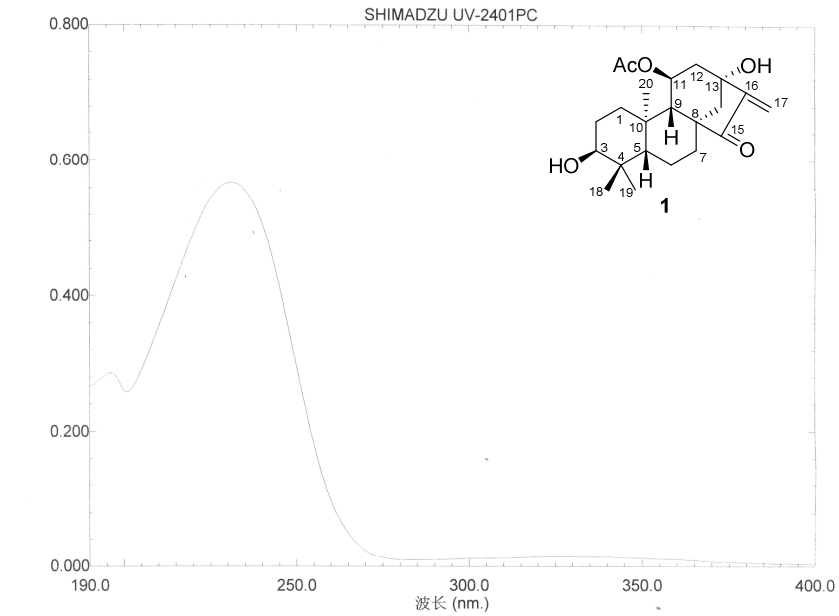

Figure 9: UV spectrum of 3-epi-isodopharicin A (**1**)

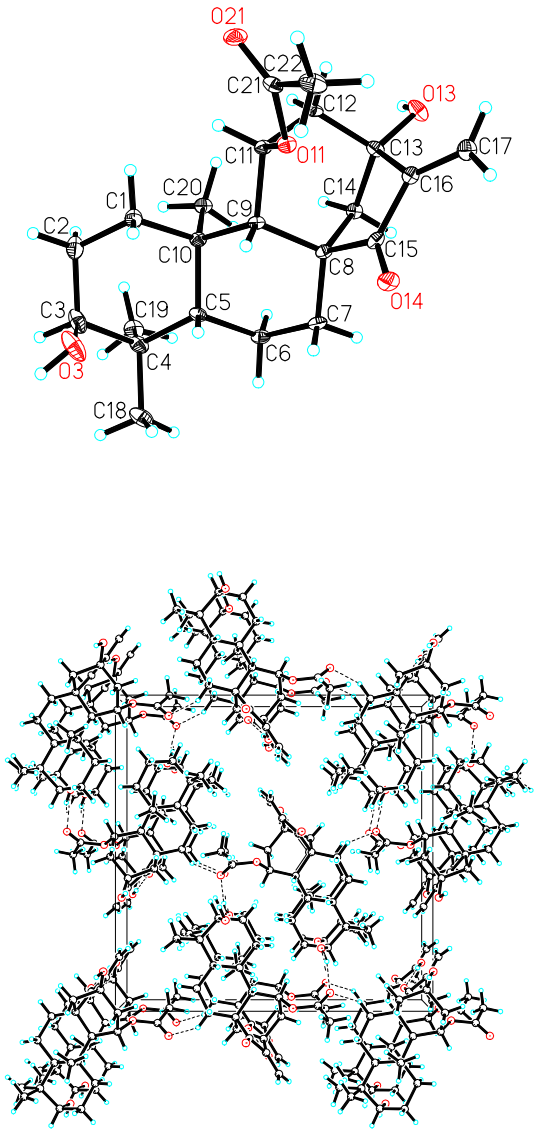

Figure 10: X-ray structure of 3-epi-isodopharicin A (**1**)

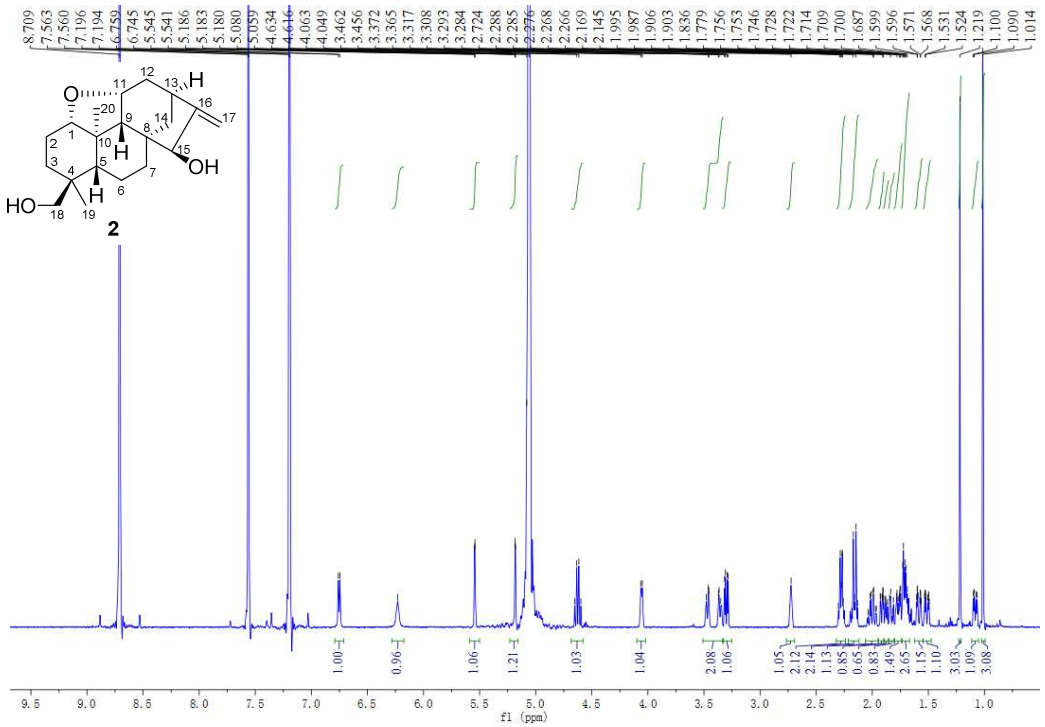

Figure 11: ^{1}H NMR spectrum of scopariusol A (**2**) recorded in C_5D_5N at 500 MHz

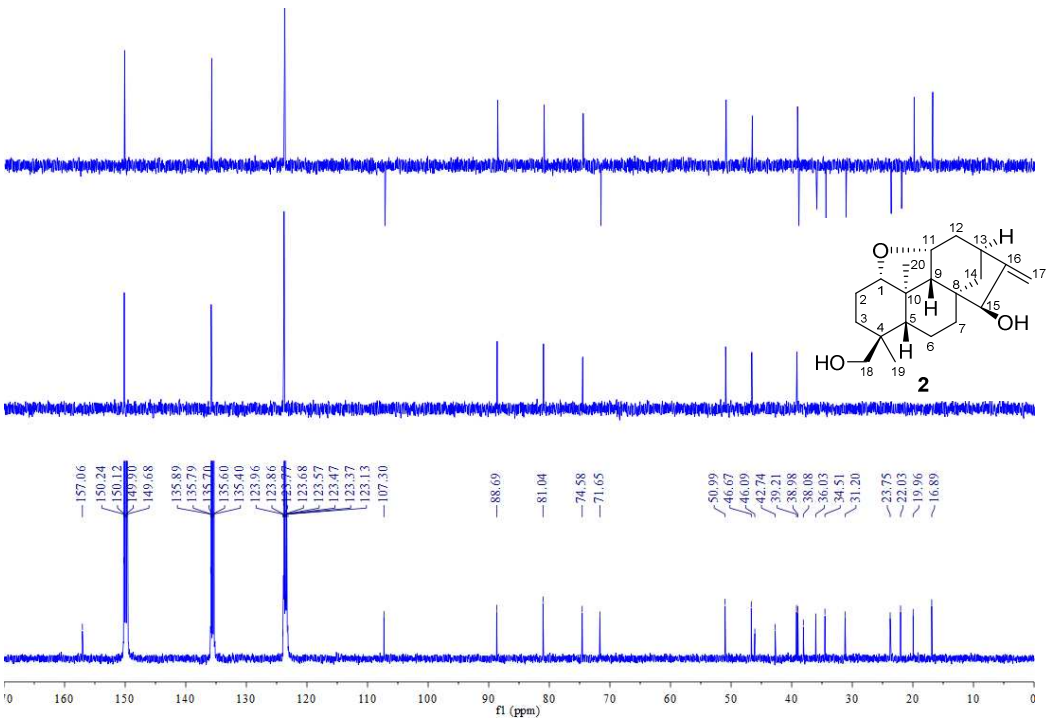

Figure 12: ^{13}C NMR spectrum of scopariusol A (**2**) recorded in C_5D_5N at 125 MHz

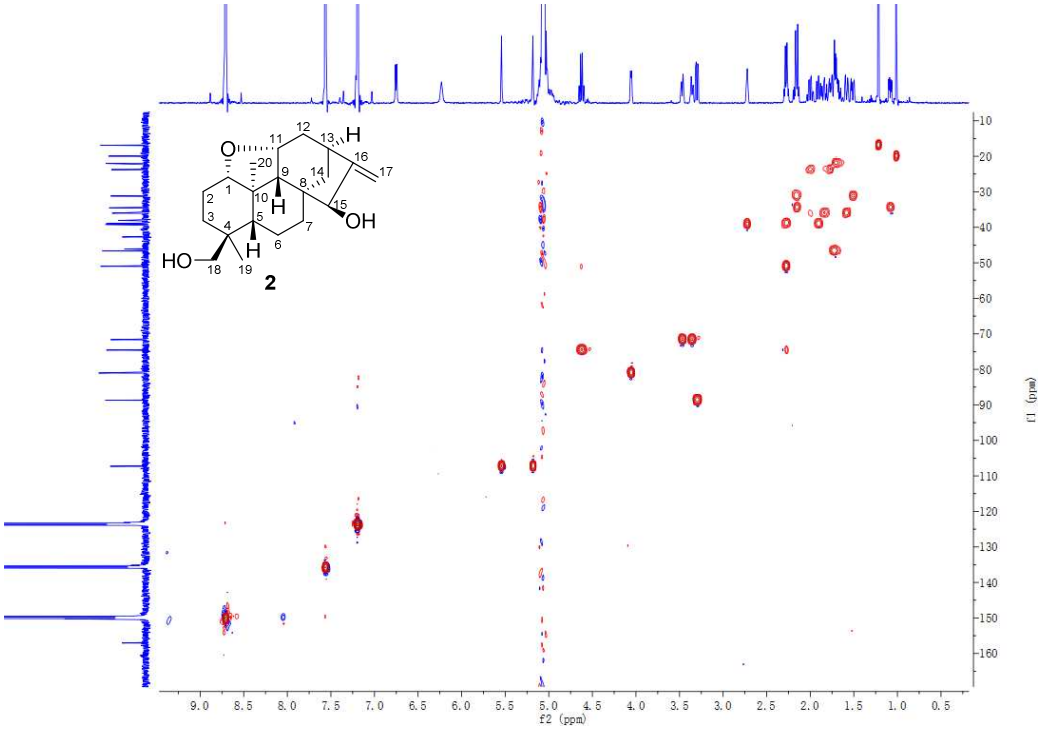

Figure 13: HSQC spectrum of scopariusol A (**2**) recorded in C_5D_5N

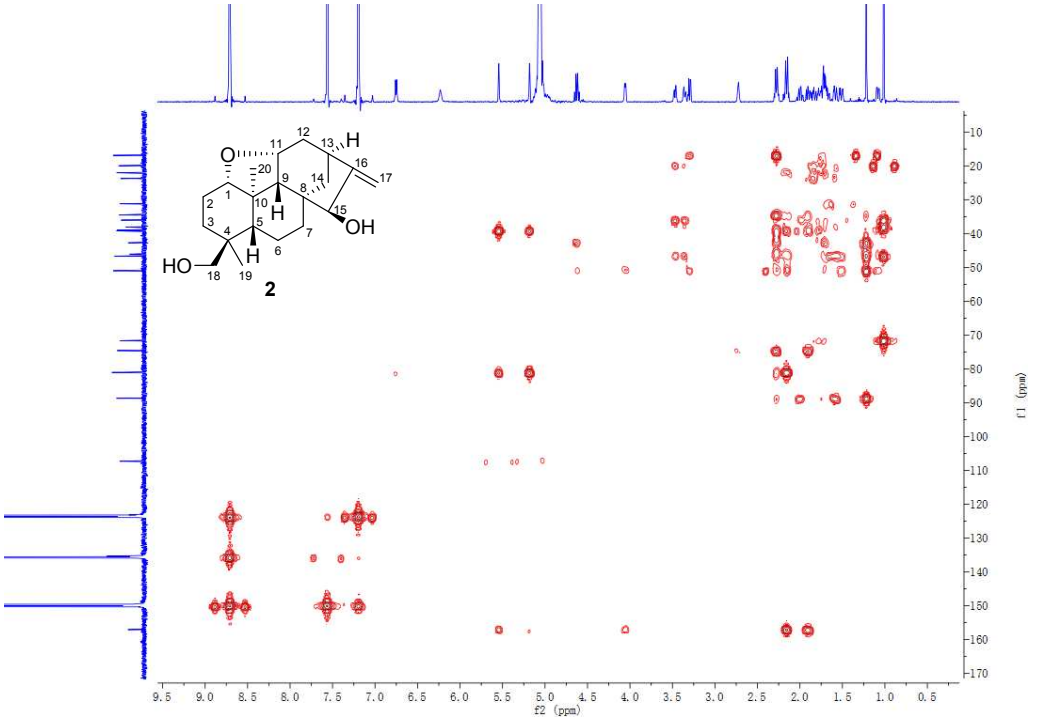

Figure 14: HMBC spectrum of scopariusol A (**2**) recorded in C_5D_5N

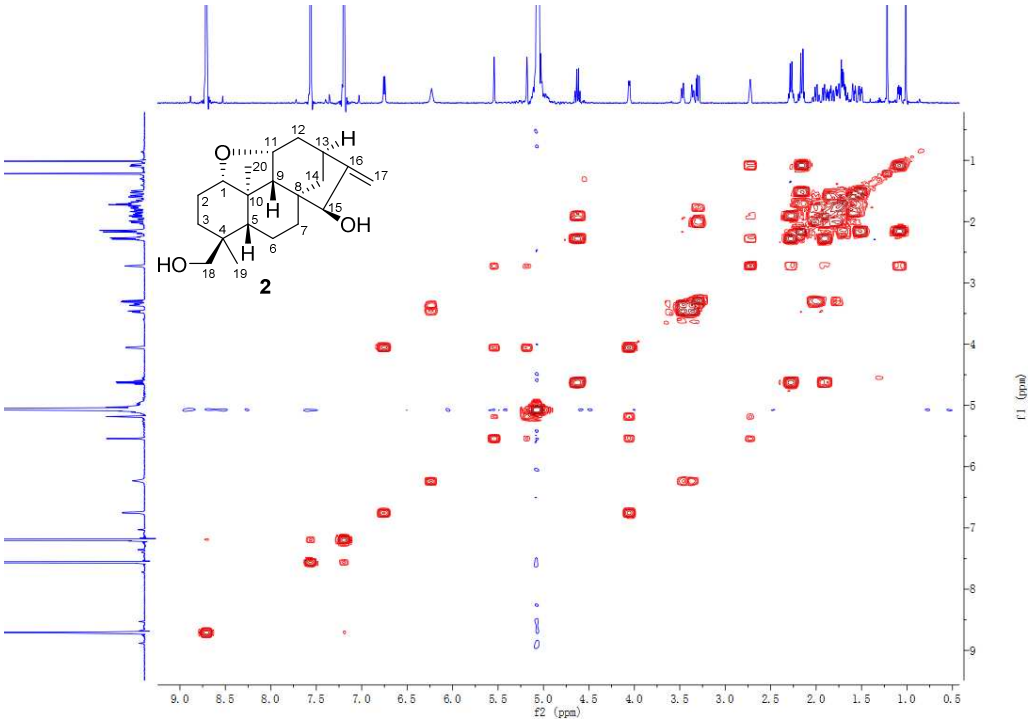

Figure 15: ^{1}H-^{1}H COSY spectrum of scopariusol A (**2**) recorded in C_5D_5N

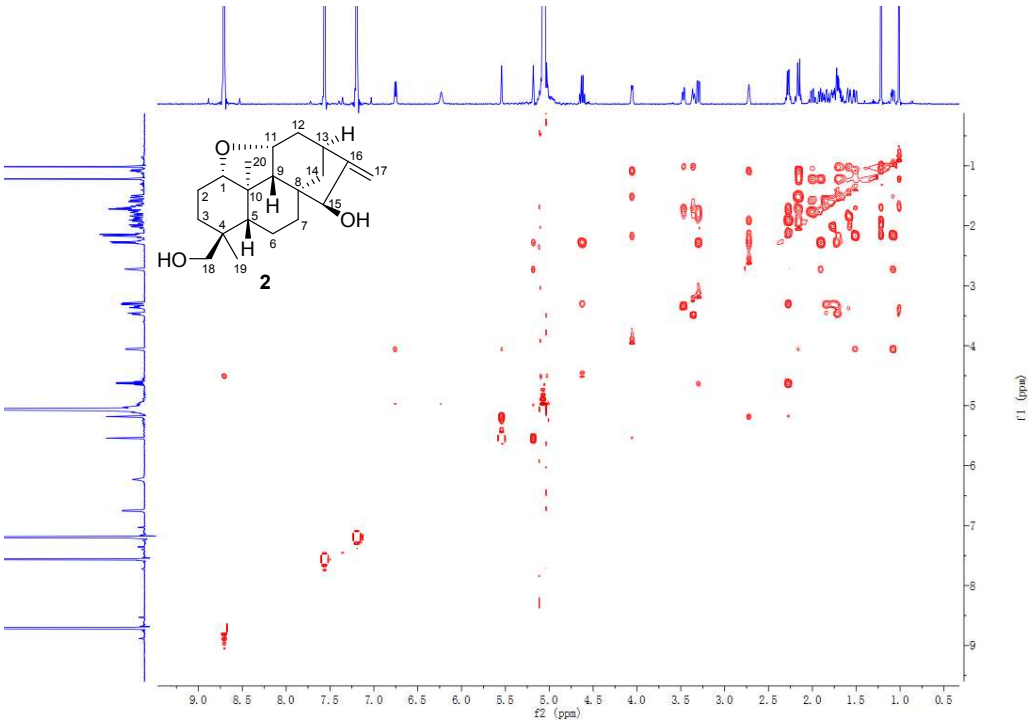

Figure 16: ROESY spectrum of scopariusol A (**2**) recorded in C_5D_5N

Qualitative Analysis Report

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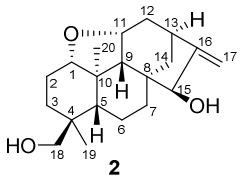
Sample Type	Sample	**Position**	P1-A6
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/20/2016 2:11:45 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)



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User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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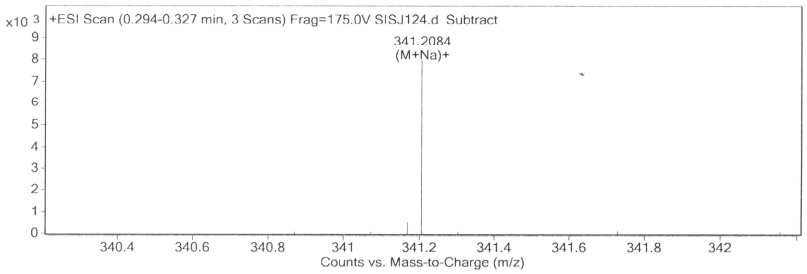

Peak List

m/z	z	Abund	Formula	Ion
274.2751	1	5787.56		
283.2062	1	3035.44		
301.2161	1	2802.45		
318.302	1	2950.65		
341.2084	1	7926.41	C20 H30 O3	(M+Na)+
417.2788	1	3005.92		
419.2956	1	12158.45		
420.2976	1	2945.45		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H30 O3	318.2195	341.2087	341.2084	0.1	0.2	6.0000

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Figure 17: HRESIMS spectrum of scopariusol A (**2**)

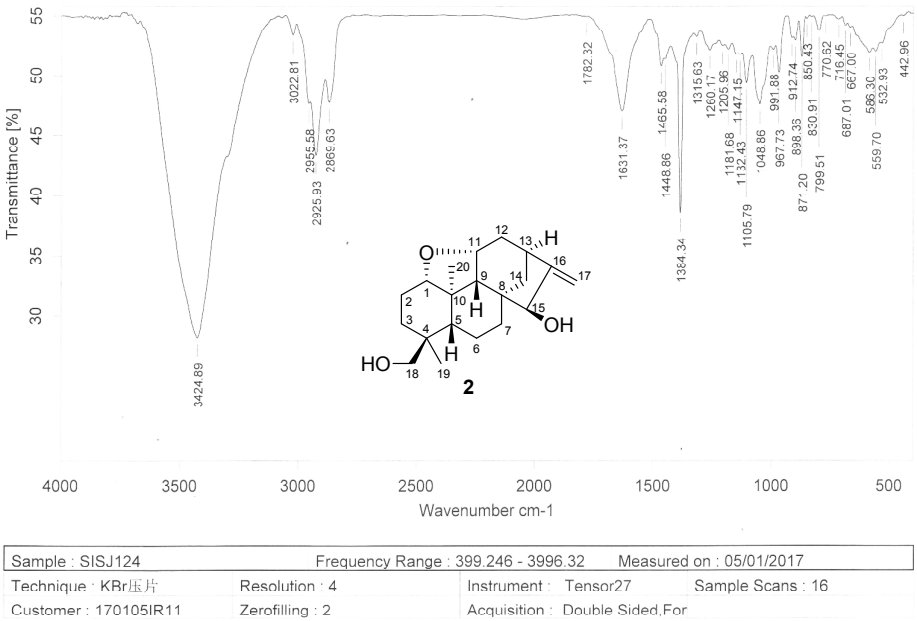


Figure 18: IR spectrum of scopariusol A (**2**)

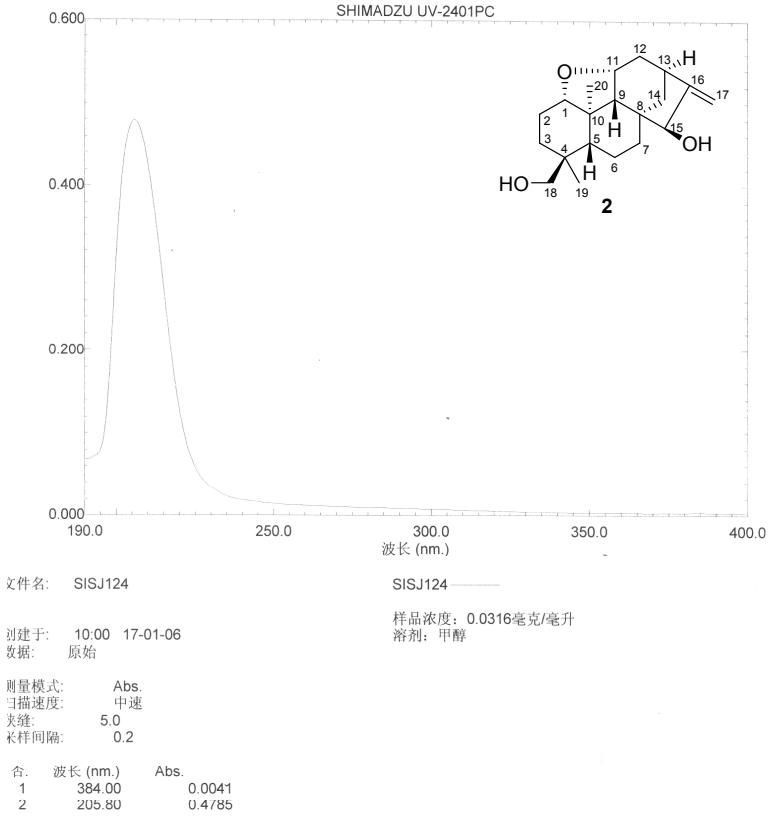


Figure 19: UV spectrum of scopariusol A (**2**)

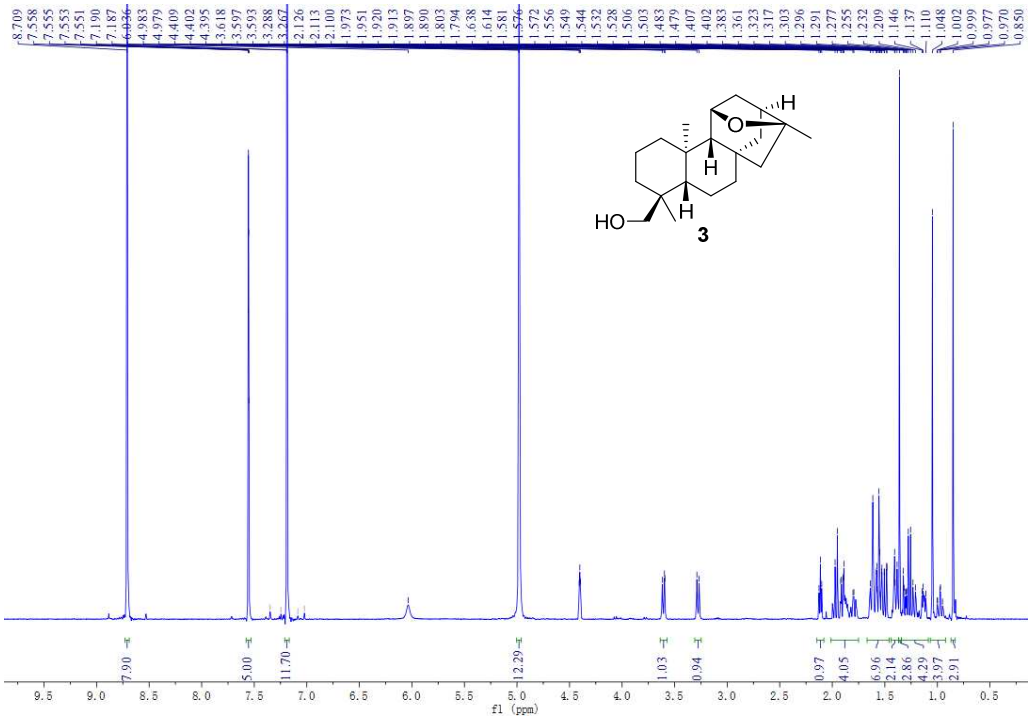


Figure 20: ^{1}H NMR spectrum of scopariusol B (**3**) recorded in C_5D_5N at 500 MHz

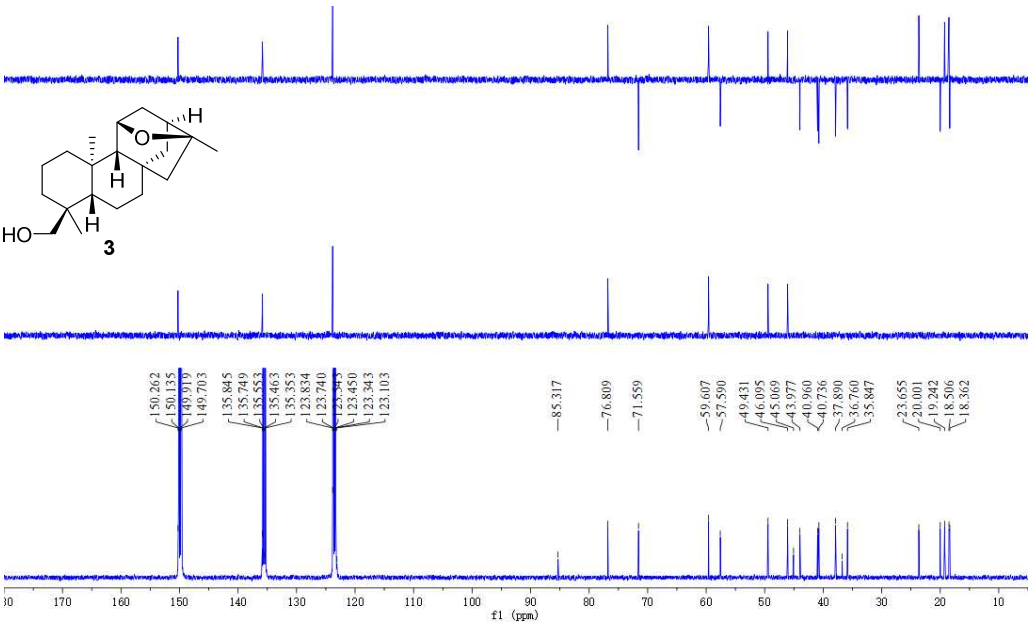


Figure 21: ^{13}C NMR spectrum of scopariusol B (**3**) recorded in C_5D_5N at 125 MHz

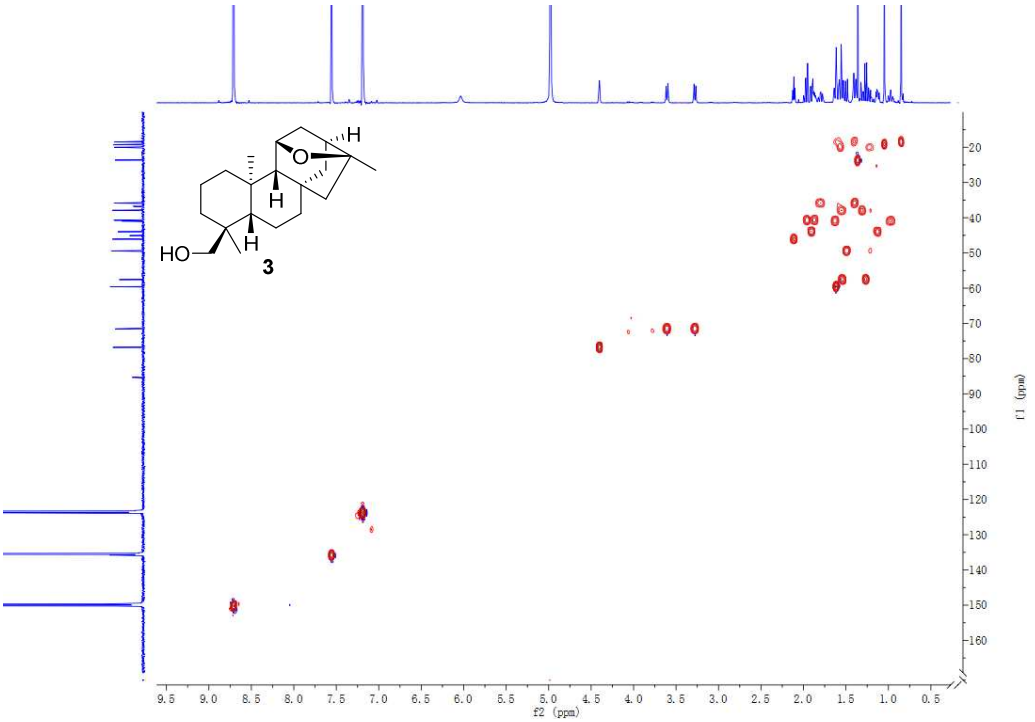


Figure 22: HSQC spectrum of scopariusol B (**3**) recorded in C_5D_5N

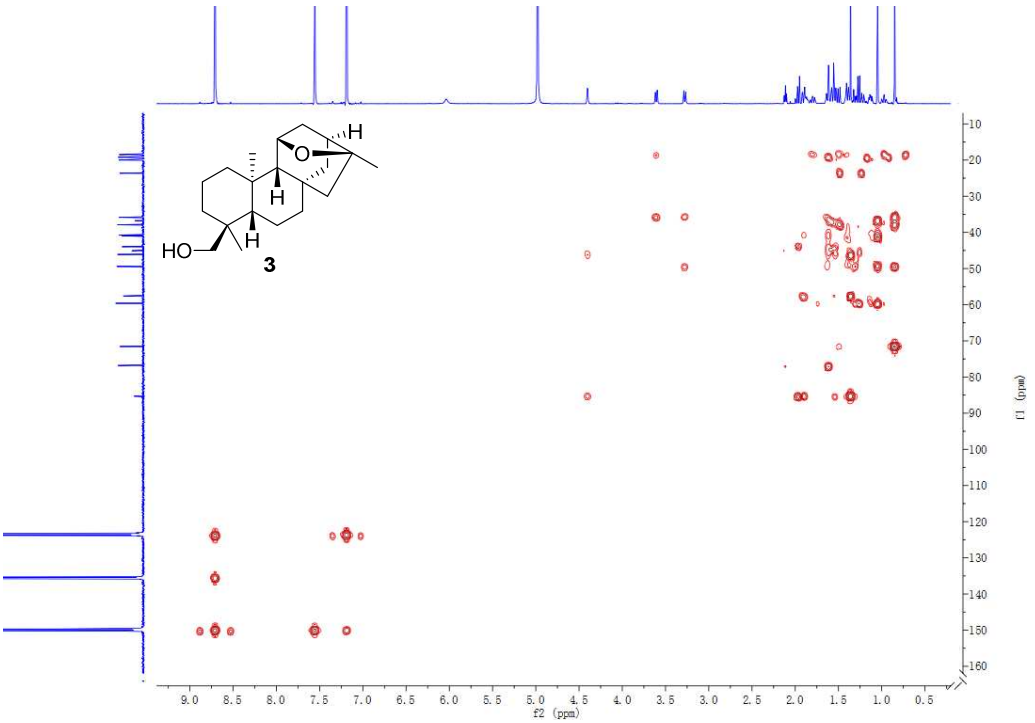


Figure 23: HMBC spectrum of scopariusol B (**3**) recorded in C_5D_5N

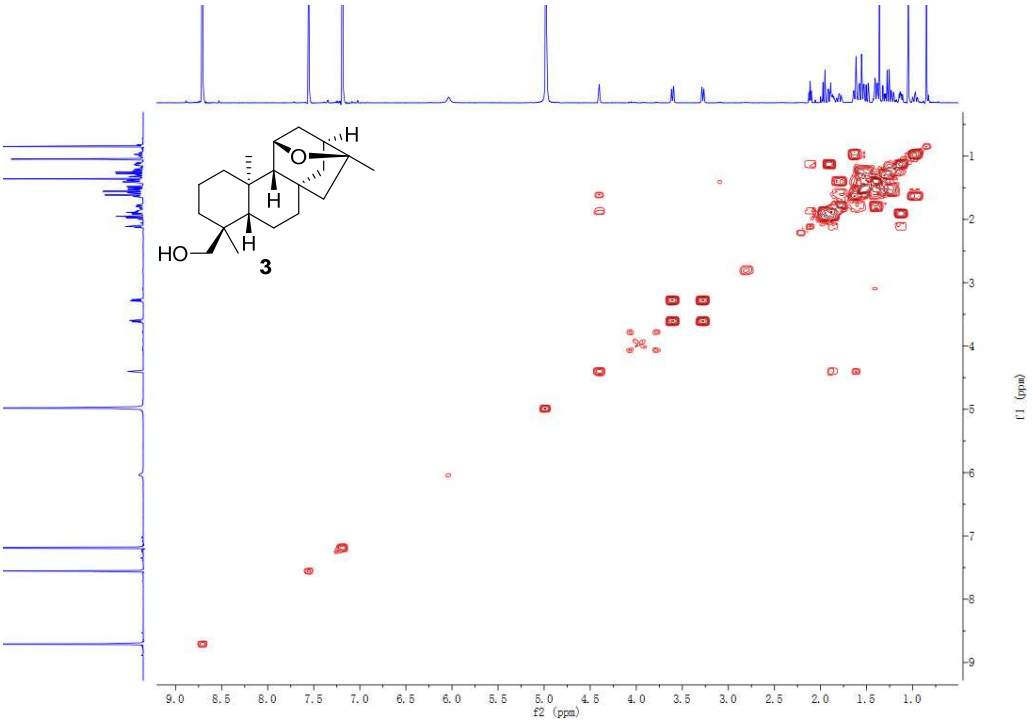


Figure 24: ^{1}H-^{1}H COSY spectrum of scopariusol B (**3**) recorded in C_5D_5N

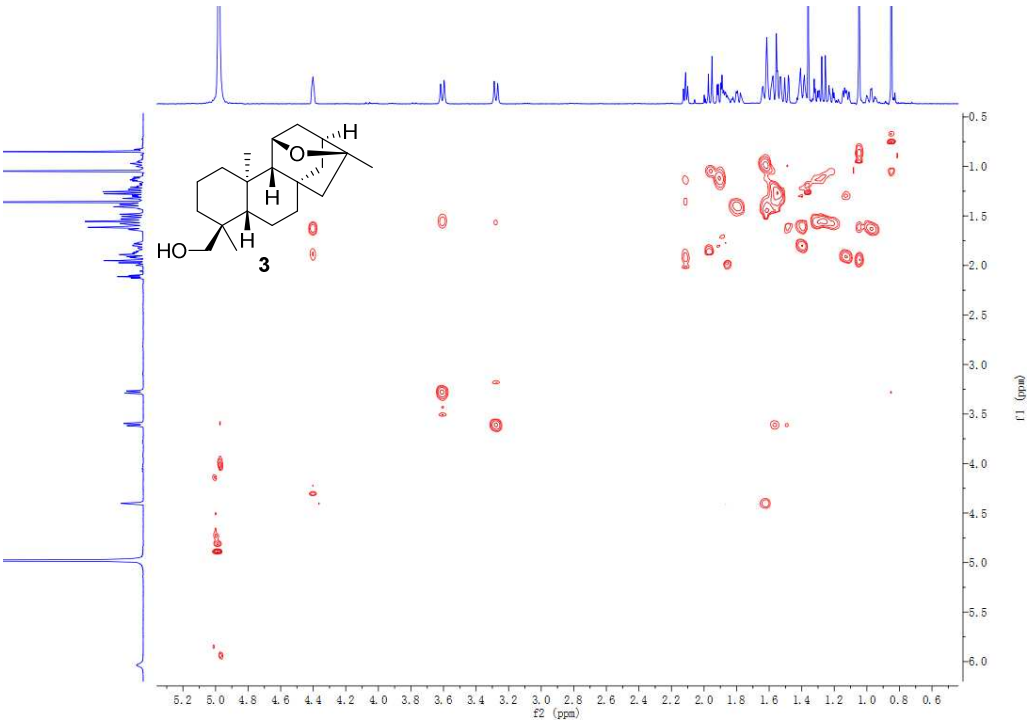


Figure 25: ROESY spectrum of scopariusol B (**3**) recorded in C_5D_5N

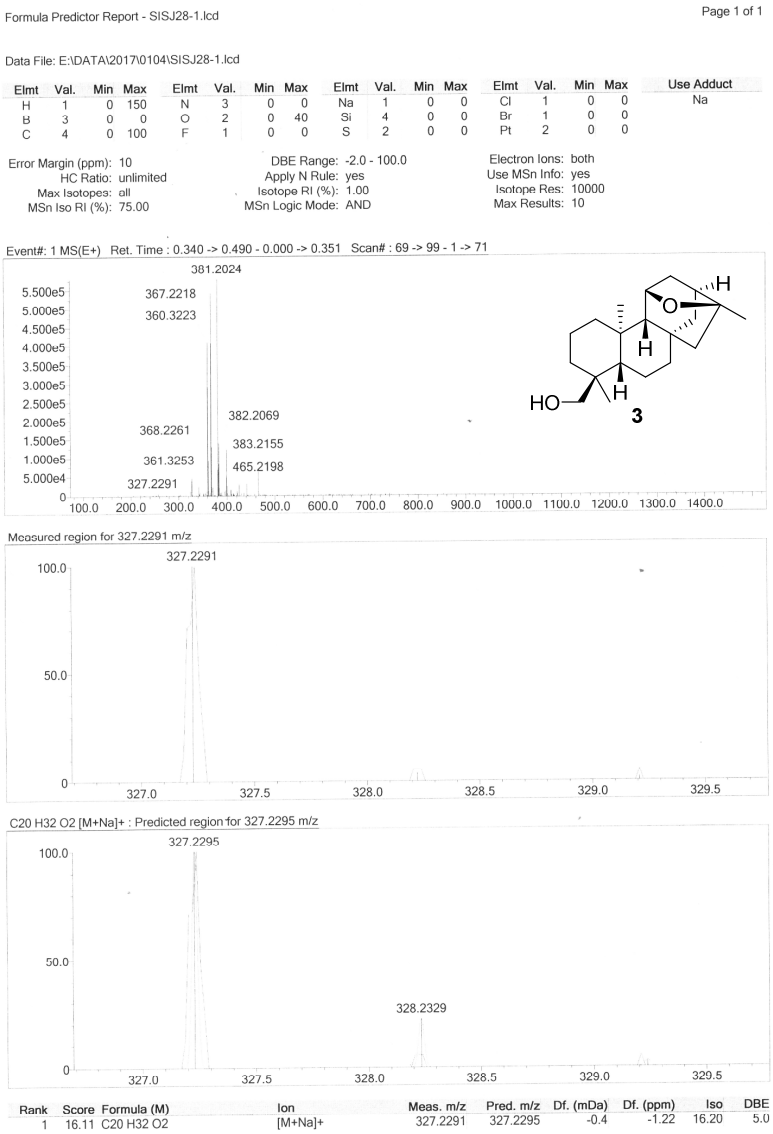
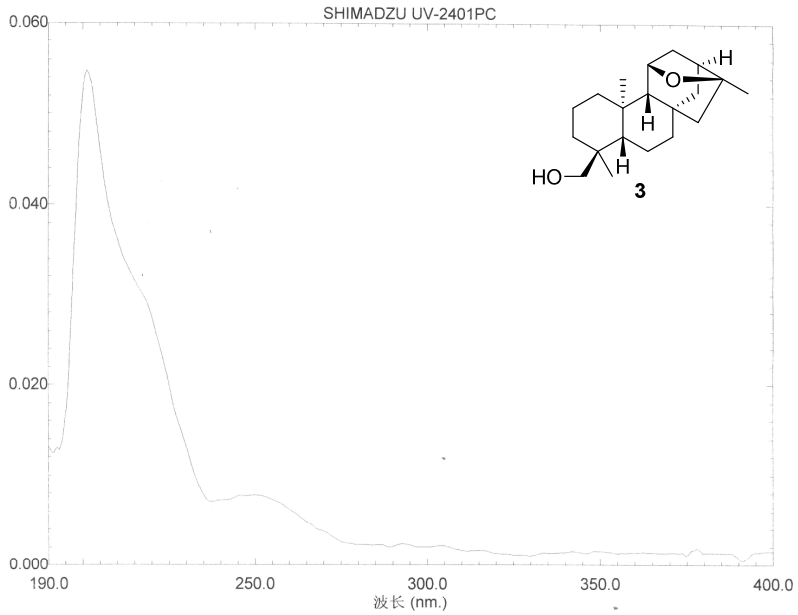


Figure 26: HRESIMS spectrum of scopariusol B (**3**)



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采样间隔: 0.2

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2	213.60	0.0326
3	249.40	0.0078

Figure 27: UV spectrum of scopariusol B (**3**)

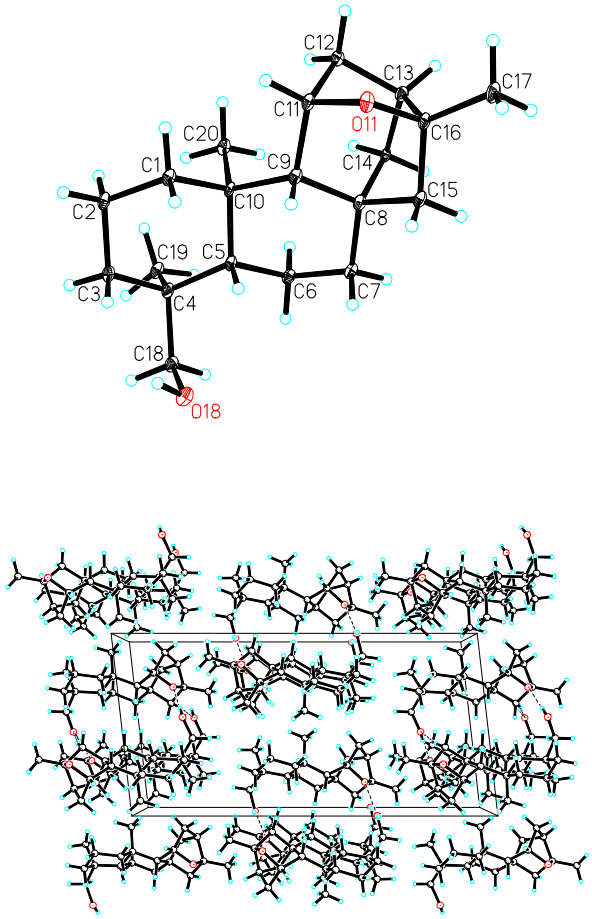

Figure 28: X-ray structure of scopariusol B (**3**)

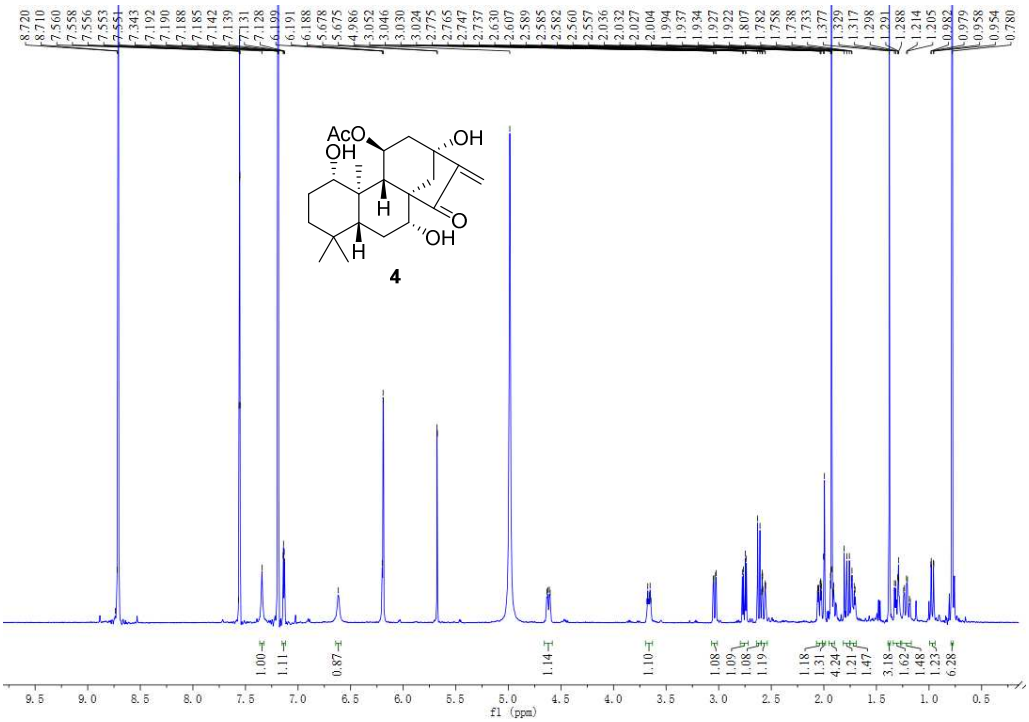

Figure 29: ^{1}H NMR spectrum of scopariusol C (**4**) recorded in C_5D_5N at 500 MHz

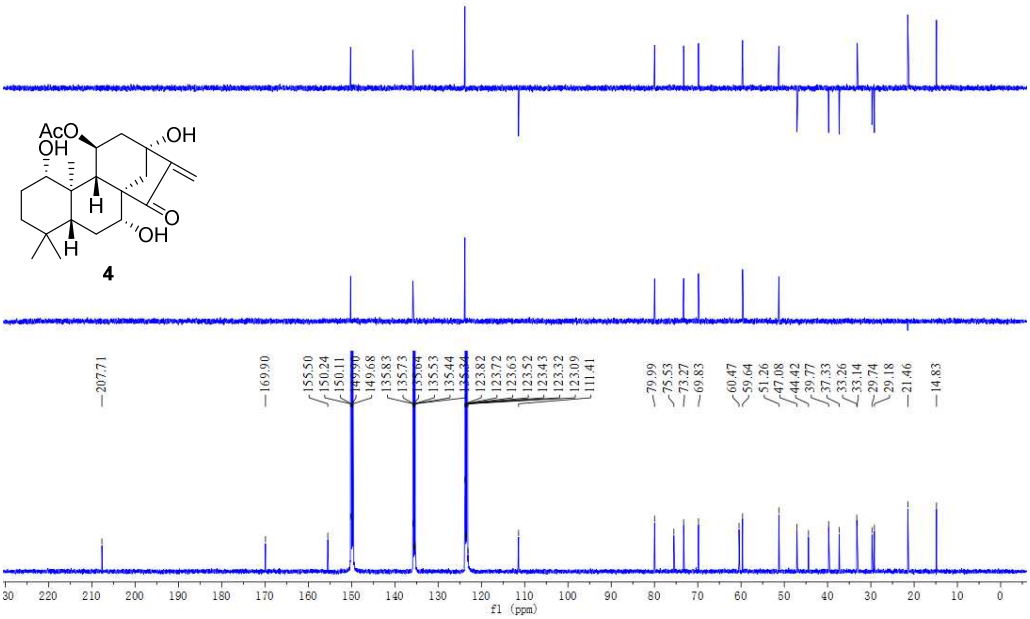

Figure 30: ^{13}C NMR spectrum of scopariusol C (**4**) recorded in C_5D_5N at 125 MHz

Qualitative Analysis Report

Data Filename	SISJ78.d	**Sample Name**	SISJ78
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/23/2016 9:25:16 AM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
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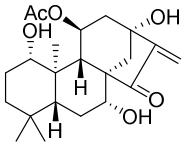

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User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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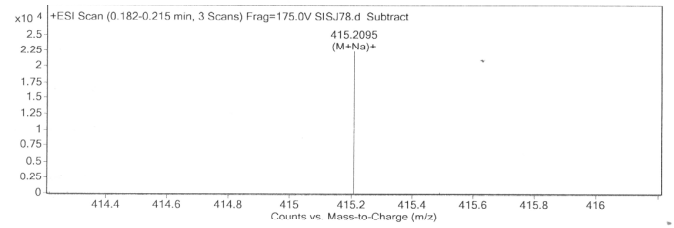

Peak List

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416.2133	1	5749.34	C22 H32 O6	(M+Na)+
548.3367	1	5631.74		
553.2934	1	46707.39		
554.2967	1	17705.56		
807.4326	1	8704.18		
945.5128	1	8919		
1083.5965	1	7057.73		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C22 H32 O6	392.2199	415.2091	415.2095	-1.1	-2.7	7.0000

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Figure 31: HRESIMS spectrum of scopariusol C (**4**)

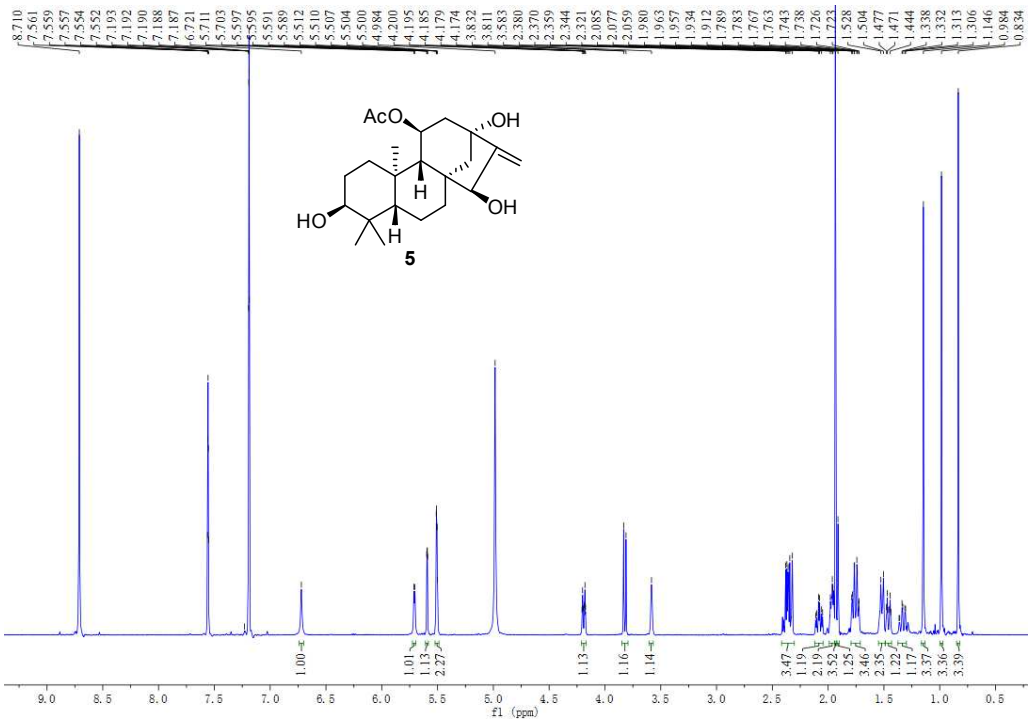

Figure 32: ^{1}H NMR spectrum of scopariusol D (**5**) recorded in C_5D_5N at 500 MHz

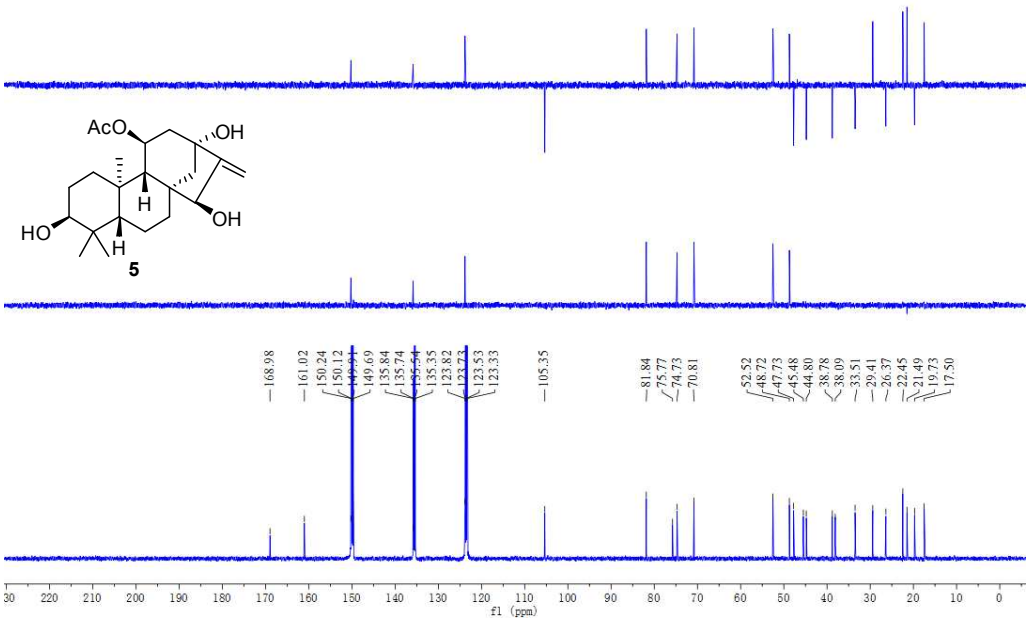

Figure 33: ^{13}C NMR spectrum of scopariusol D (**5**) recorded in C_5D_5N at 125 MHz

Qualitative Analysis Report

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Sample Type	Sample	**Position**	P1-F6
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Comment			
Sample Group		**Info.**	
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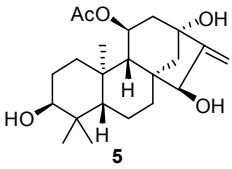

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User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
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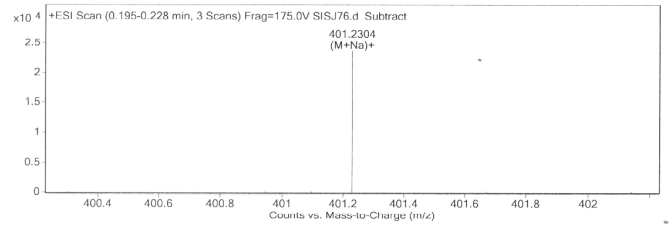

Peak List

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110.0086	1	10956.63		
259.1669	1	5066.7		
274.274	1	6094.22		
318.3012	1	4403.56		
401.2304	1	23772.11	C22 H34 O5	(M+Na)+
402.2322	1	5532.96	C22 H34 O5	(M+Na)+
779.472	1	5562.38		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C22 H34 O5	378.2406	401.2298	401.2304	-0.2	-0.5	6.0000

--- End Of Report ---

Figure 34: HRESIMS spectrum of scopariusol D (**5**)

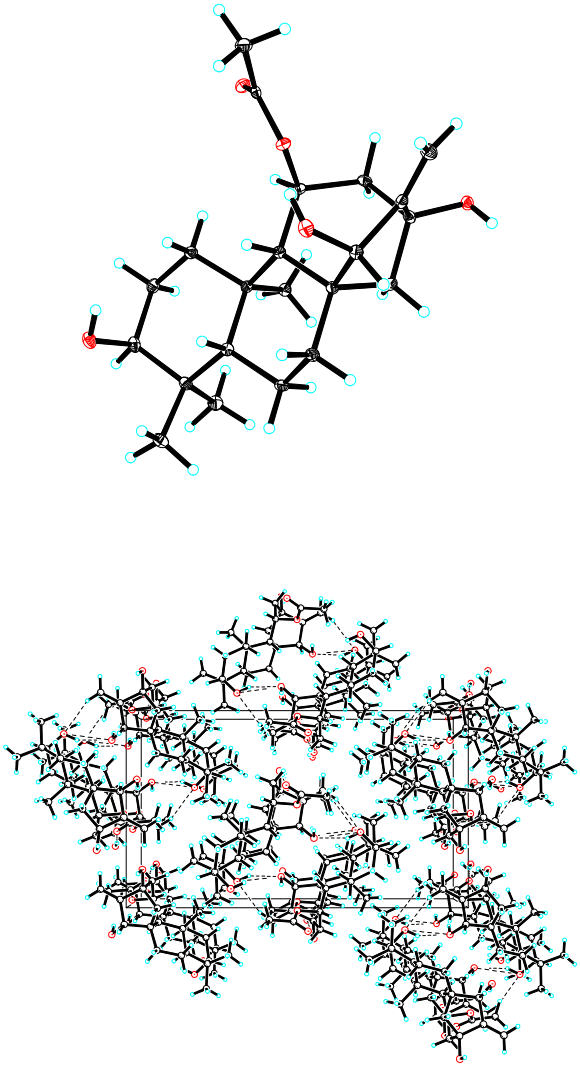


Figure 35: X-ray structure of scopariusol D (**5**)

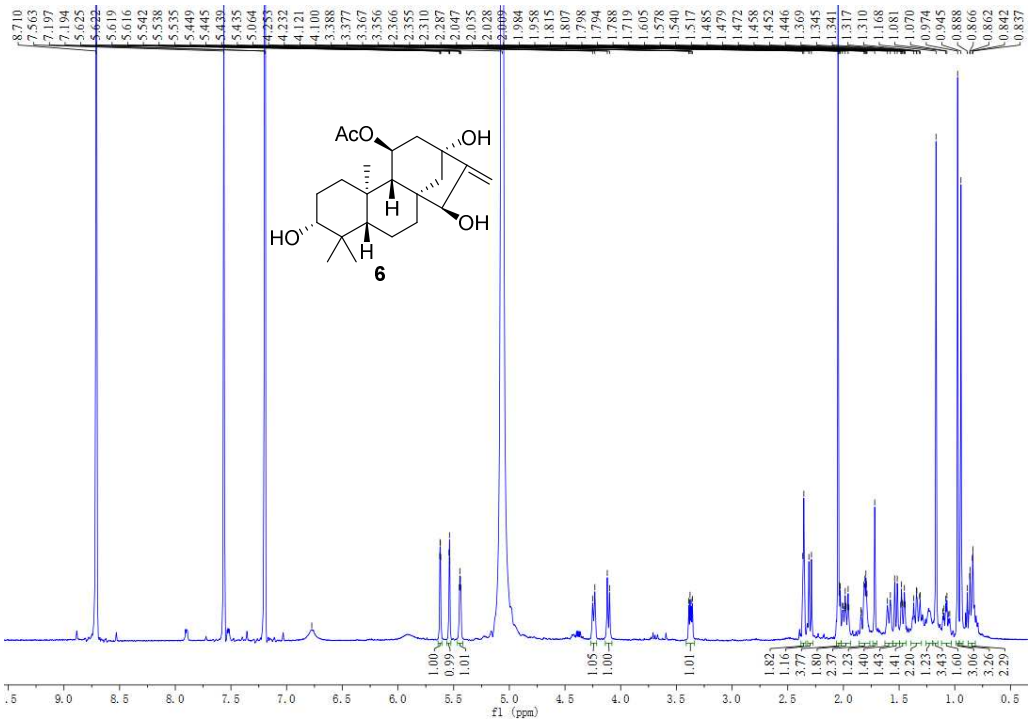


Figure 36: ^{1}H NMR spectrum of 3-episcopariusol D (**6**) recorded in C_5D_5N at 500 MHz

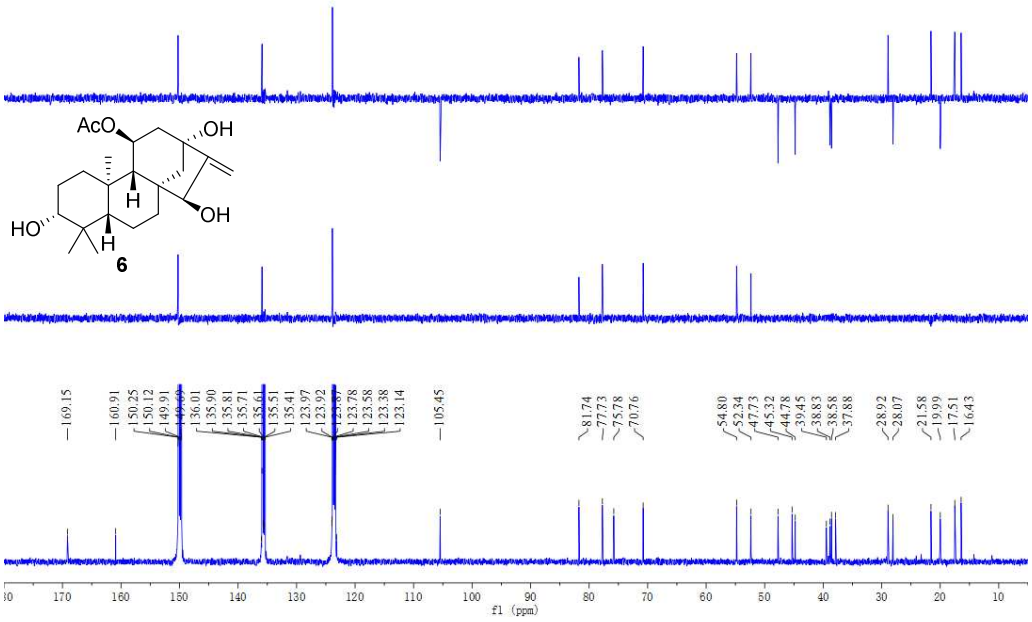
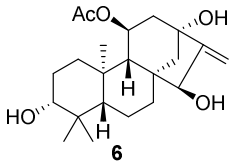


Figure 37: ^{13}C NMR spectrum of 3-episcopariusol D (**6**) recorded in C_5D_5N at 125 MHz

Qualitative Analysis Report

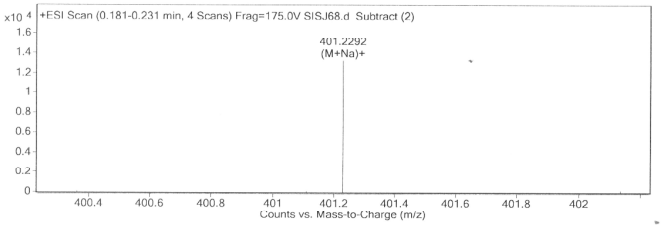
Data Filename	SISJ68.d	**Sample Name**	SISJ68
Sample Type	Sample	**Position**	P1-F7
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/14/2016 3:14:45 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		



6

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
267.157		4913.72		
283.2058	1	19745.82		
301.2163	1	23566.87		
302.2196	1	5129.9		
329.1213	1	14288.69		
401.2292	1	13265.25	C22 H34 O5	(M+Na)+
417.1996	1	4871.52		
463.2007	1	4455.94		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C22 H34 O5	378.2406	401.2298	401.2292	1.5	3.8	6.0000

--- End Of Report ---

Figure 38: HRESIMS spectrum of 3-episcopariusol D (**6**)

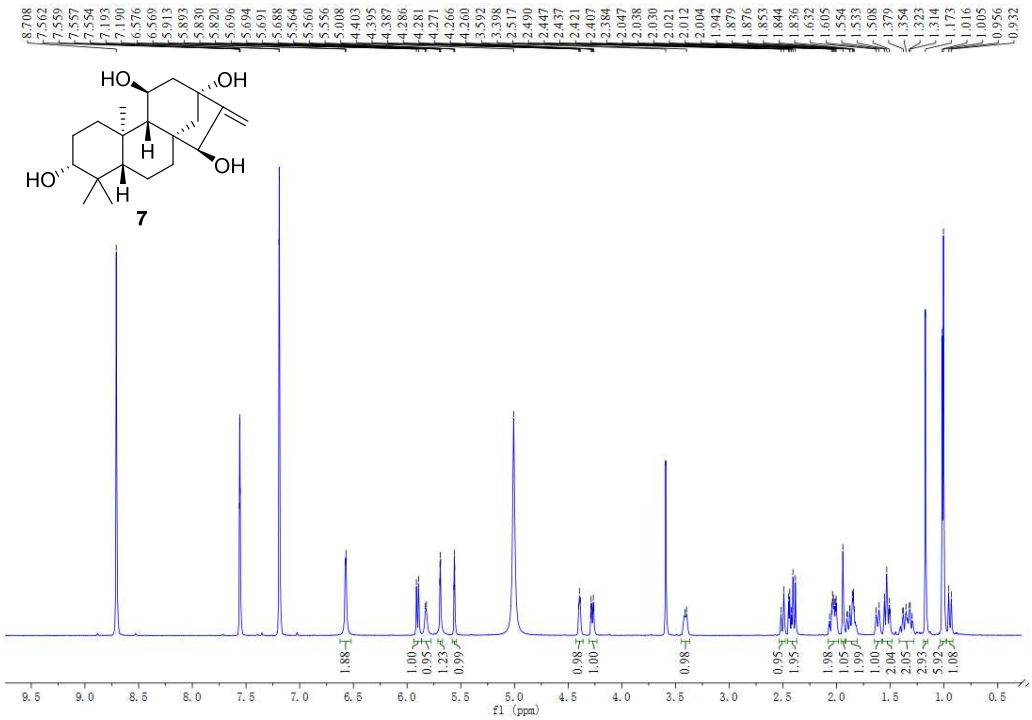


Figure 39: ^{1}H NMR spectrum of scopariusol E (**7**) recorded in C_5D_5N at 500 MHz

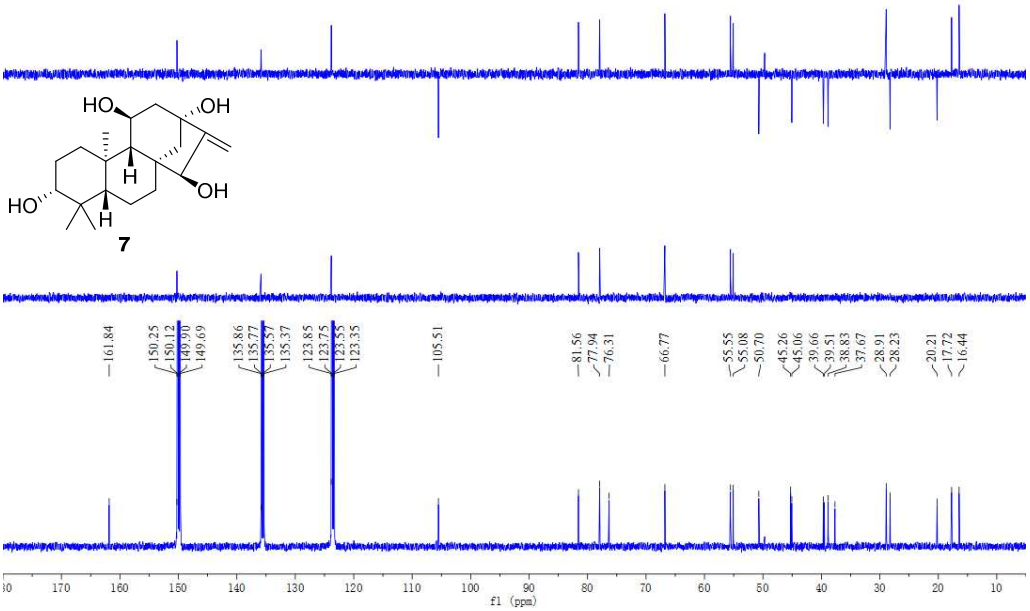
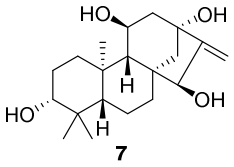


Figure 40: ^{13}C NMR spectrum of scopariusol E (**7**) recorded in C_5D_5N at 125 MHz

Qualitative Analysis Report

Data Filename	SISJ133.d	**Sample Name**	SISJ133
Sample Type	Sample	**Position**	P1-F5
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/10/2016 4:44:12 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

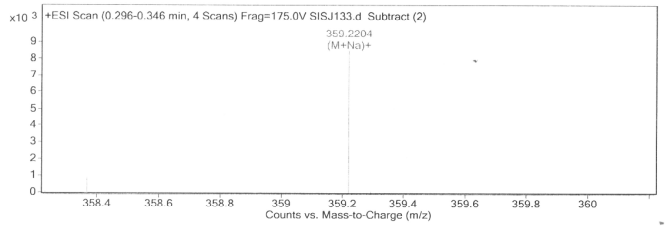
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)



7

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
84.9598		14910.82		
98.9618	1	11572.06		
259.1676	1	9555.97		
359.2204	1	8509.81	C20 H32 O4	(M+Na)+
610.1857	1	13974.67		
611.1851	1	7813.28		
619.5292	1	8246.52		
684.2033	1	11637.79		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H32 O4	336.2301	359.2193	359.2204	-0.1	-0.3	5.0000

--- End Of Report ---

Figure 41: HRESIMS spectrum of scopariusol E (**7**)

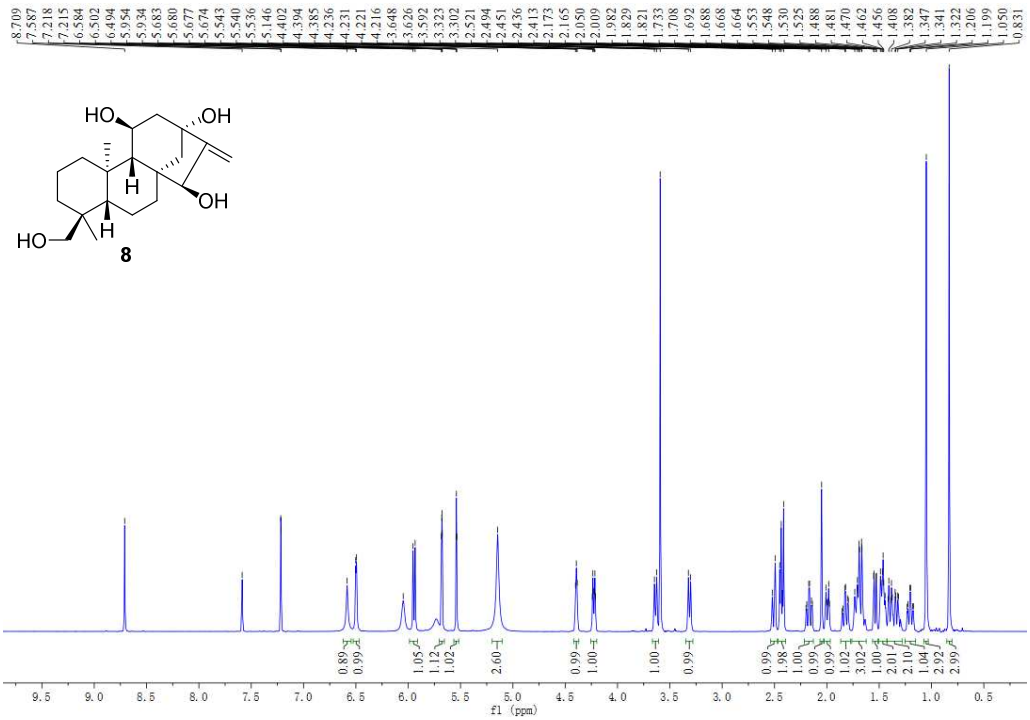


Figure 42: ^{1}H NMR spectrum of scopariusol F (**8**) recorded in C_5D_5N at 500 MHz

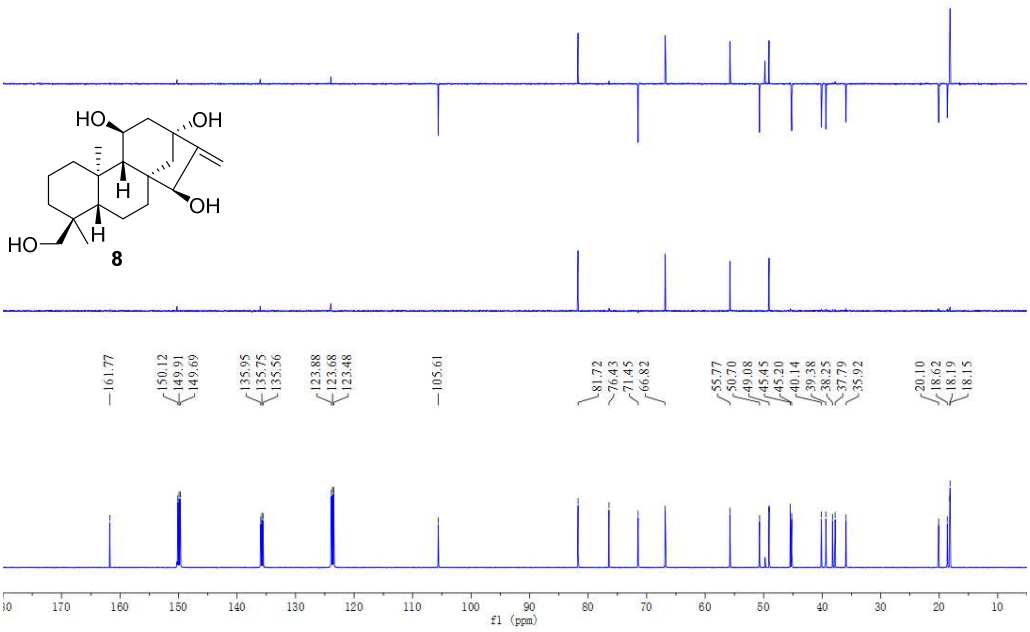
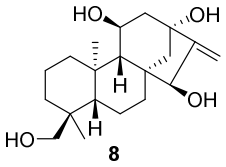


Figure 43: ^{13}C NMR spectrum of scopariusol F (**8**) recorded in C_5D_5N at 125 MHz

Qualitative Analysis Report

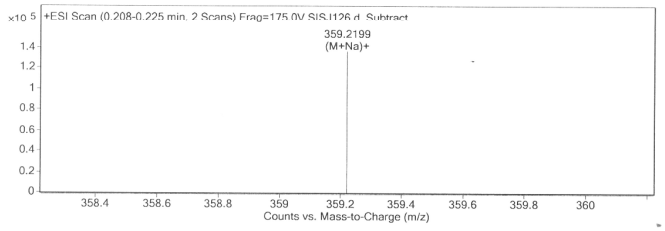
Data Filename	SISJ126.d	**Sample Name**	SISJ126
Sample Type	Sample	**Position**	P1-A1
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/14/2016 4:40:31 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		



8

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
301.2169	1	279723.44		
359.2199	1	137194.17	C20 H32 O4	(M+Na)+
521.3276	2	81578.87		
524.829	2	55899.09		
673.47	1	578126.56		
674.4739	1	234479.33		
695.4523	1	425864.47		
696.4559	1	183268.92		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H32 O4	336.2301	359.2193	359.2199	-0.6	-1.6	5.0000

--- End Of Report ---

Figure 44: HRESIMS spectrum of scopariusol F (**8**)

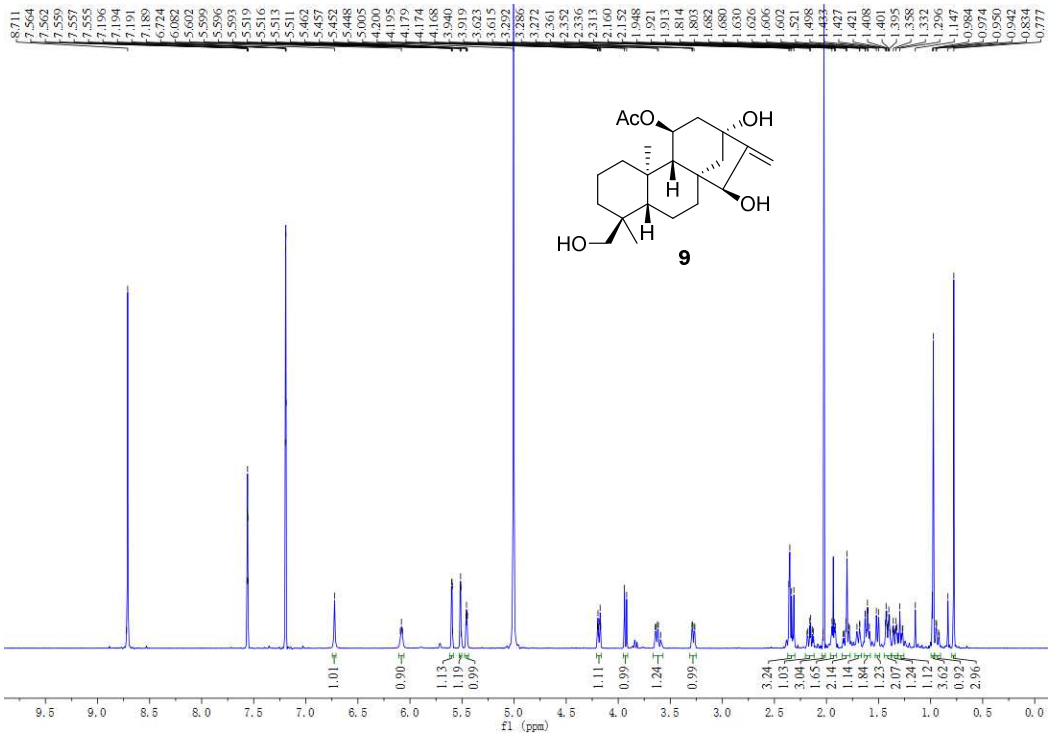


Figure 45: ^{1}H NMR spectrum of 11-*O*-acetyl-scopariusol F (**9**) recorded in C_5D_5N at 500 MHz

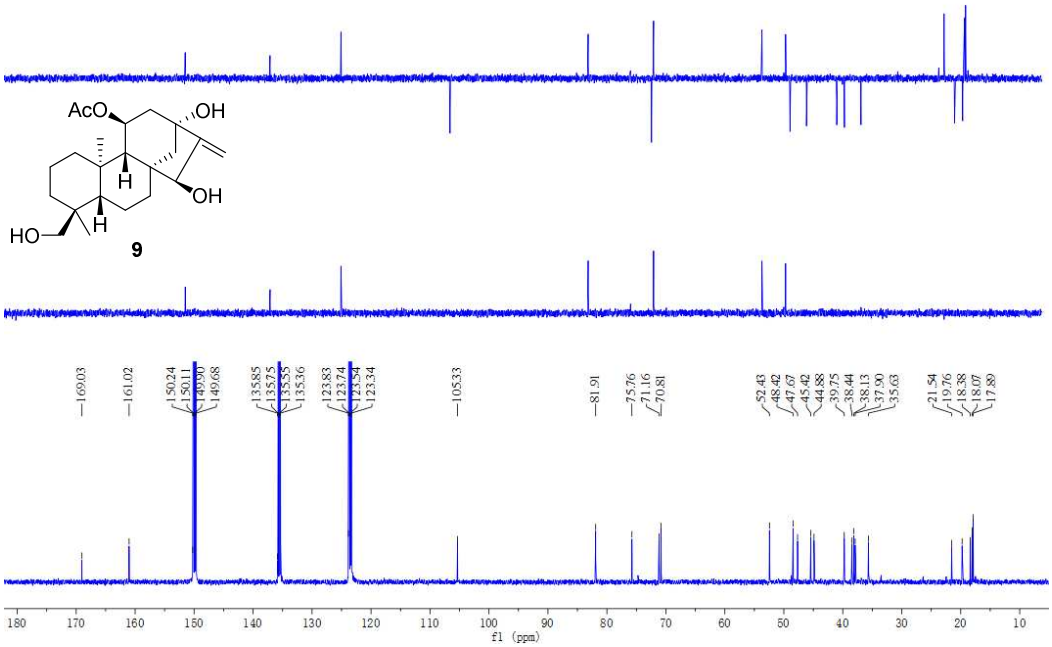
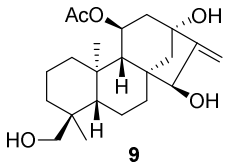


Figure 46: ^{13}C NMR spectrum of 11-*O*-acetyl-scopariusol F (**9**) recorded in C_5D_5N at 125 MHz

Qualitative Analysis Report

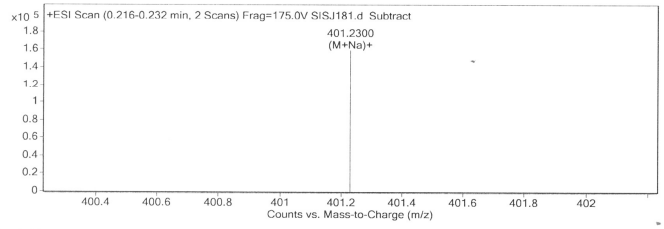
Data Filename	SISJ181.d	**Sample Name**	SISJ181
Sample Type	Sample	**Position**	P1-A4
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/14/2016 4:44:37 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		



9

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
283.206	1	104086.91		
301.2167	1	239113.5		
302.2198	1	45649.88		
319.2266	1	27196.22		
396.275	1	36469.65		
401.23	1	159748.8	C22 H34 O5	(M+Na)+
402.2329	1	35968.69	C22 H34 O5	(M+Na)+
417.2015	1	33318.89		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C22 H34 O5	378.2406	401.2298	401.2300	0.2	0.6	6.0000

--- End Of Report ---

Figure 47: HRESIMS spectrum of 11-*O*-acetyl-scopariusol F (**9**)

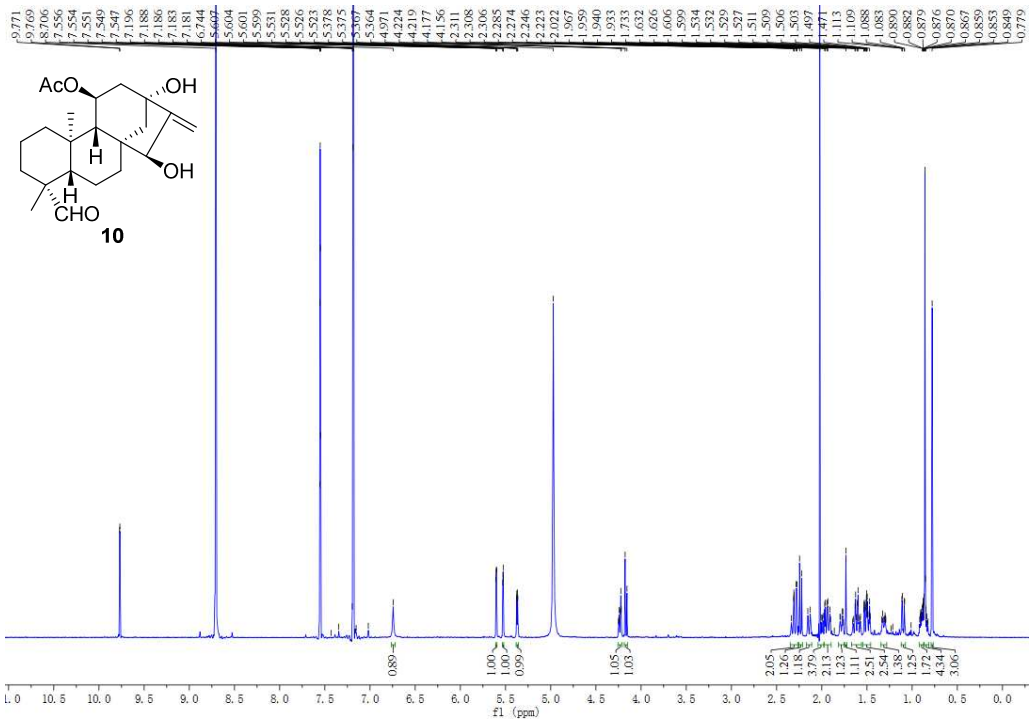


Figure 48: ^{1}H NMR spectrum of scopariusol G (**10**) recorded in C_5D_5N at 500 MHz

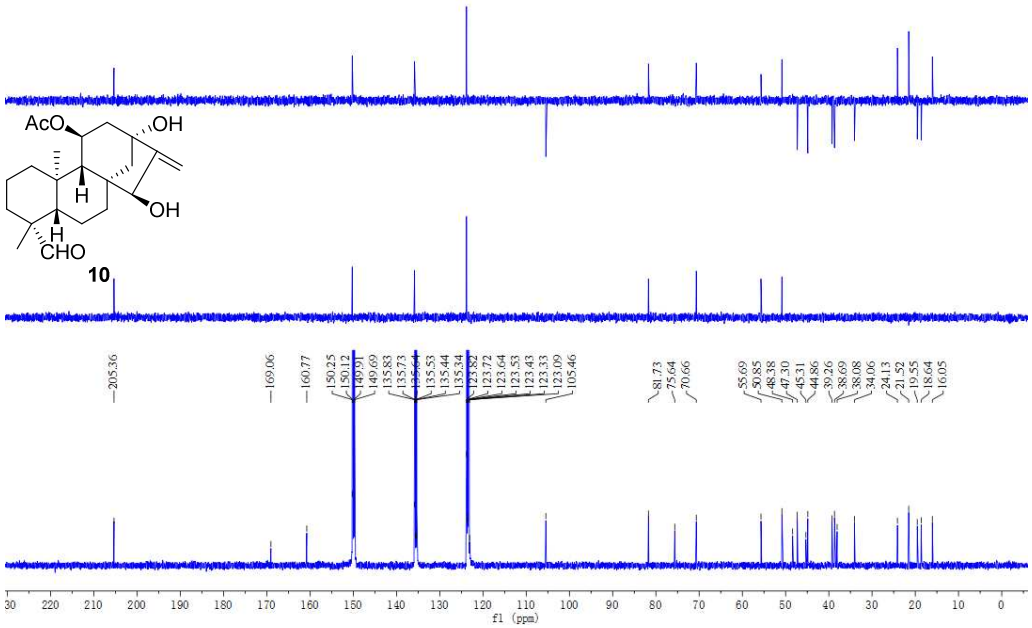
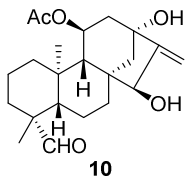


Figure 49: ^{13}C NMR spectrum of scopariusol G (**10**) recorded in C_5D_5N at 125 MHz

Qualitative Analysis Report

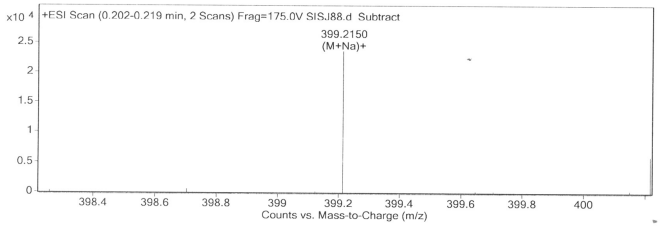
Data Filename	SISJ88.d	**Sample Name**	SISJ88
Sample Type	Sample	**Position**	P1-F5
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/14/2016 4:33:46 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		



10

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
101.0762		7506.39		
271.2064	1	7656.31		
281.1907	1	11538.85		
299.2012	1	37008.85		
300.2048	1	7553.37		
317.2111	1	13908.42		
399.215	1	23695.43	C22 H32 O5	(M+Na)+
475.2016	1	6623.28		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C22 H32 O5	376.2250	399.2142	399.2150	-0.5	-1.2	7.0000

--- End Of Report ---

Figure 50: HRESIMS spectrum of scopariusol G (**10**)

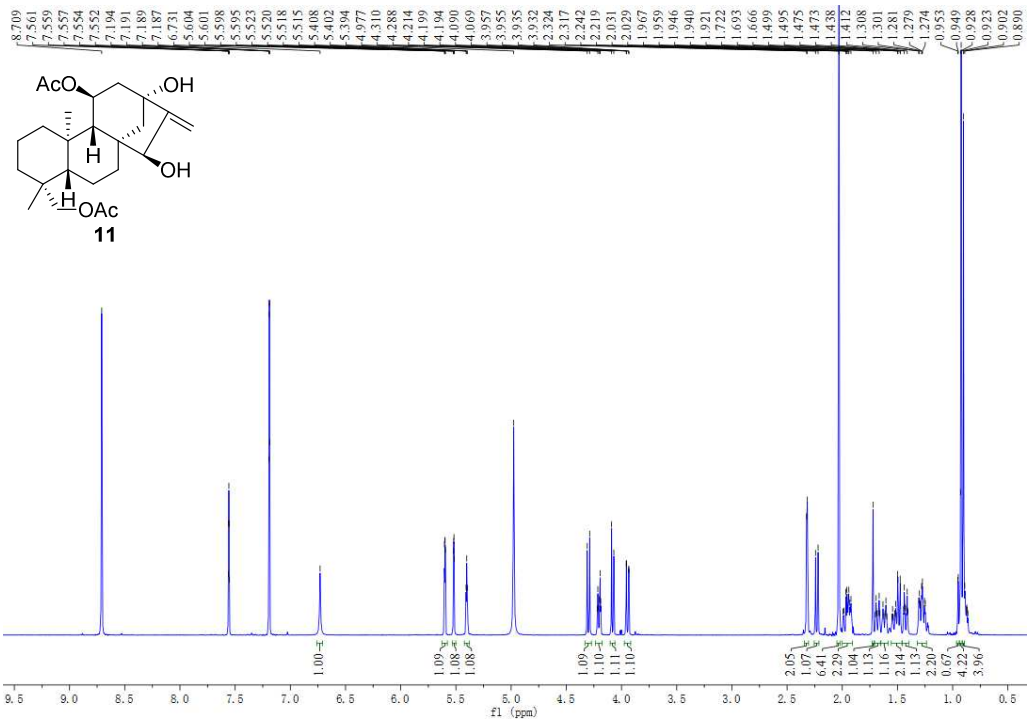


Figure 51: ^{1}H NMR spectrum of scopariusol H (**11**) recorded in C_5D_5N at 500 MHz

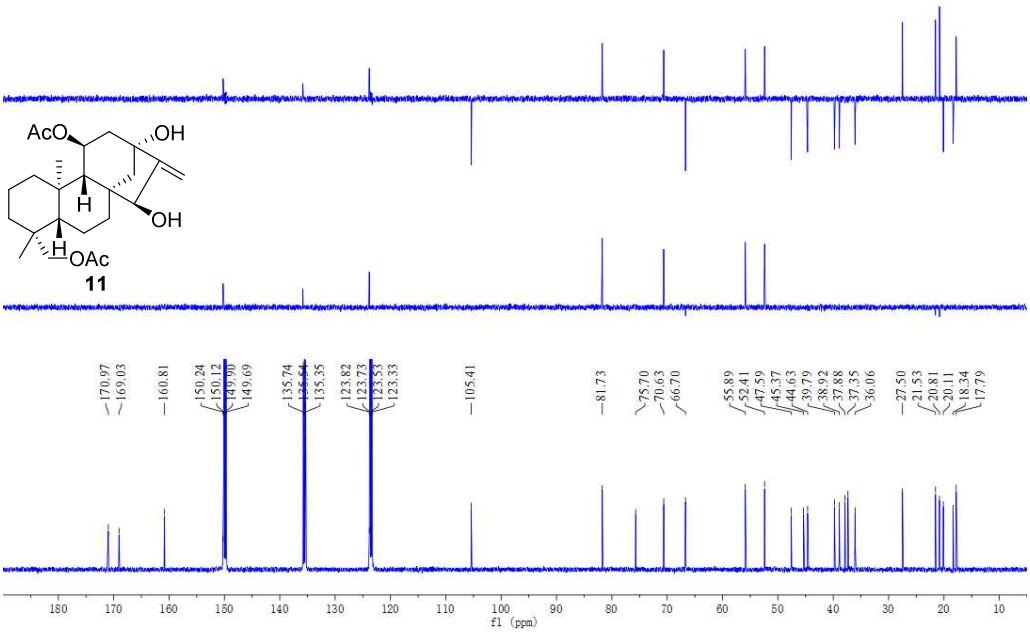
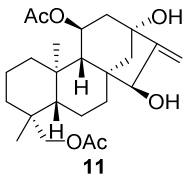


Figure 52: ^{13}C NMR spectrum of scopariusol H (**11**) recorded in C_5D_5N at 125 MHz

Qualitative Analysis Report

Data Filename	SISC71.d	**Sample Name**	SISC71
Sample Type	Sample	**Position**	P1-A2
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/14/2016 4:41:53 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

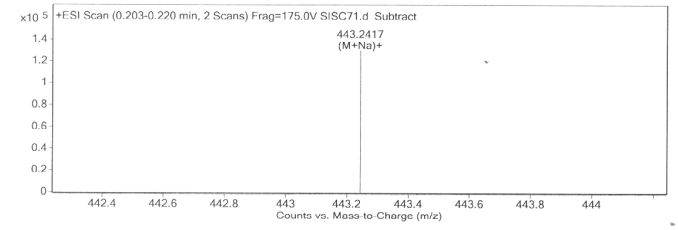
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)



11

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
283.2061	1	78212.65		
343.2277	1	60691.5		
361.2378	1	30162.19		
443.2417	1	129986.86	C24 H36 O6	(M+Na)+
444.2446	1	33641.28	C24 H36 O6	(M+Na)+
459.2129	1	22394.8		
650.3593	2	25072.34		
650.8608	2	21385.94		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C24 H36 O6	420.2512	443.2404	443.2417	-1.1	-2.6	7.0000

--- End Of Report ---

Figure 53: HRESIMS spectrum of scopariusol H (**11**)

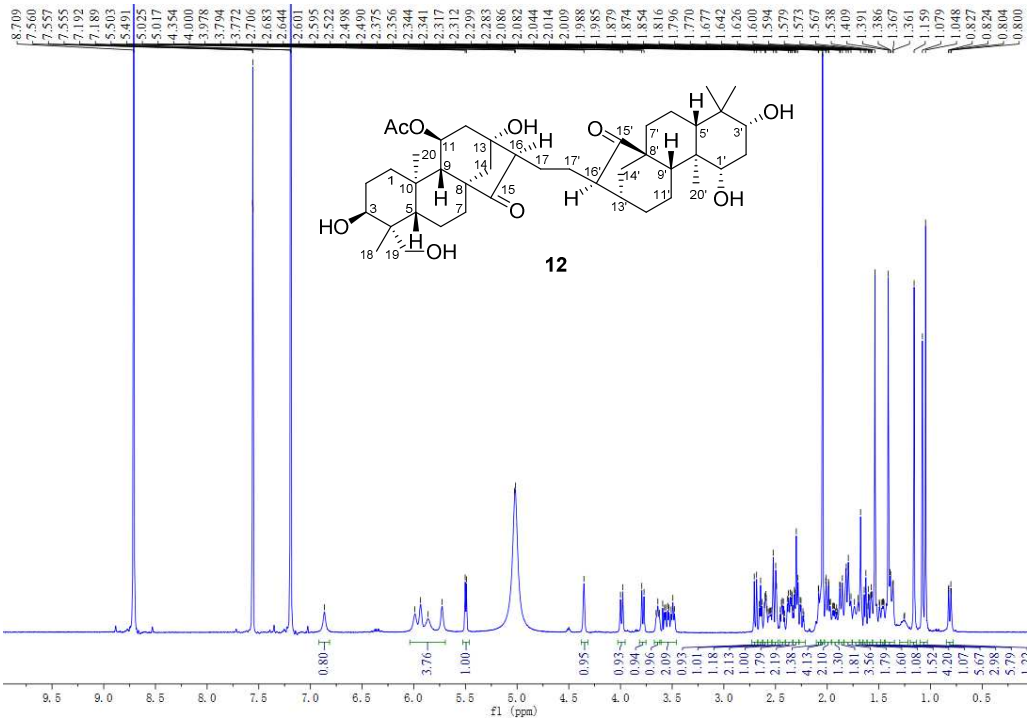


Figure 54: ^{1}H NMR spectrum of scopariusol I (**12**) recorded in C_5D_5N at 500 MHz

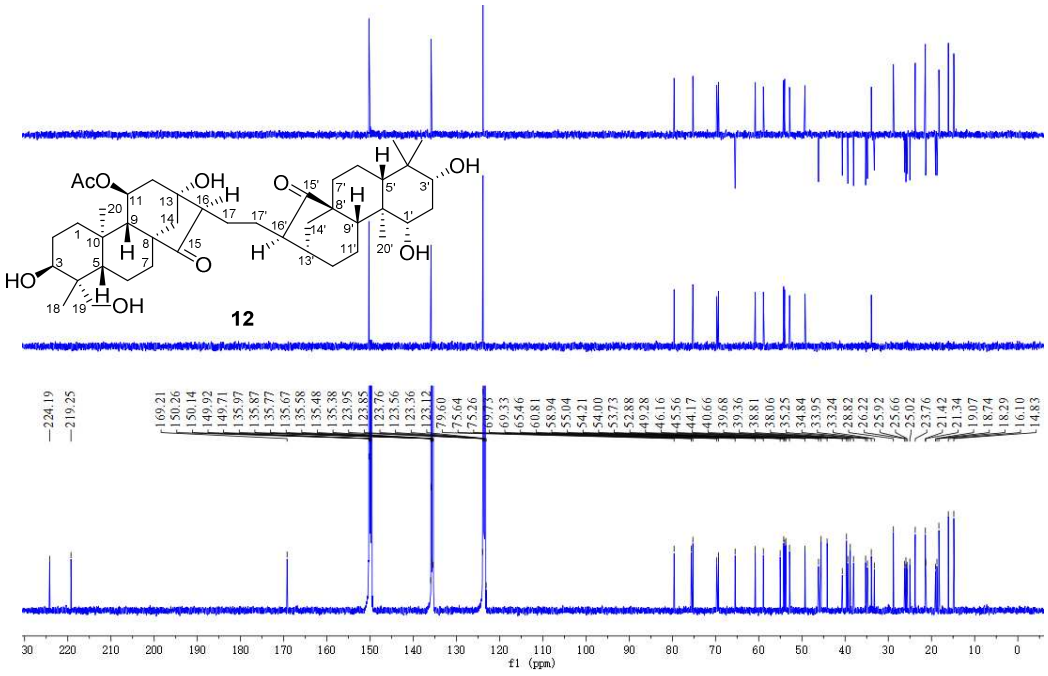


Figure 55: ^{13}C NMR spectrum of scopariusol I (**12**) recorded in C_5D_5N at 125 MHz

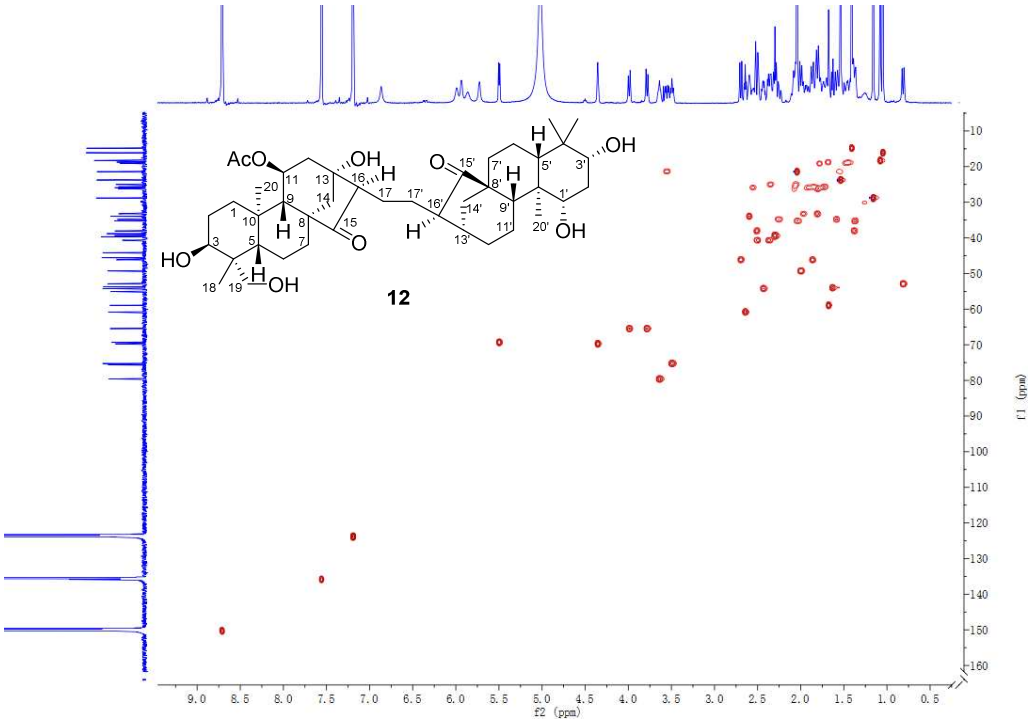


Figure 56: HSQC spectrum of scopariusol I (**12**) recorded in C_5D_5N

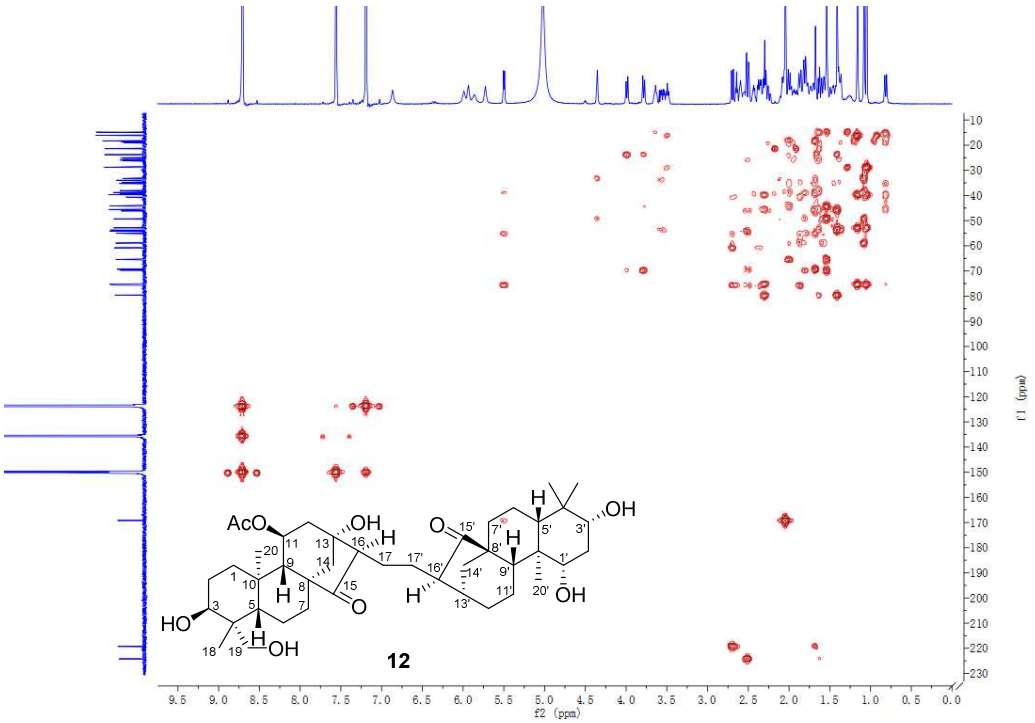


Figure 57: HMBC spectrum of scopariusol I (**12**) recorded in C_5D_5N

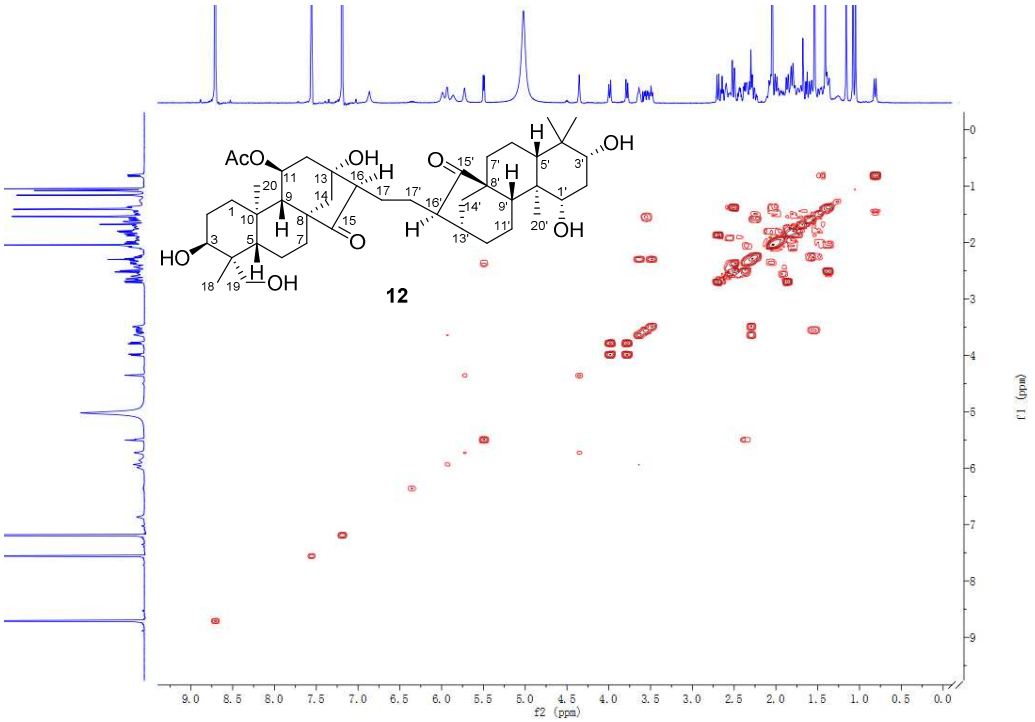


Figure 58: ^{1}H-^{1}H COSY spectrum of scopariusol I (**12**) recorded in C_5D_5N

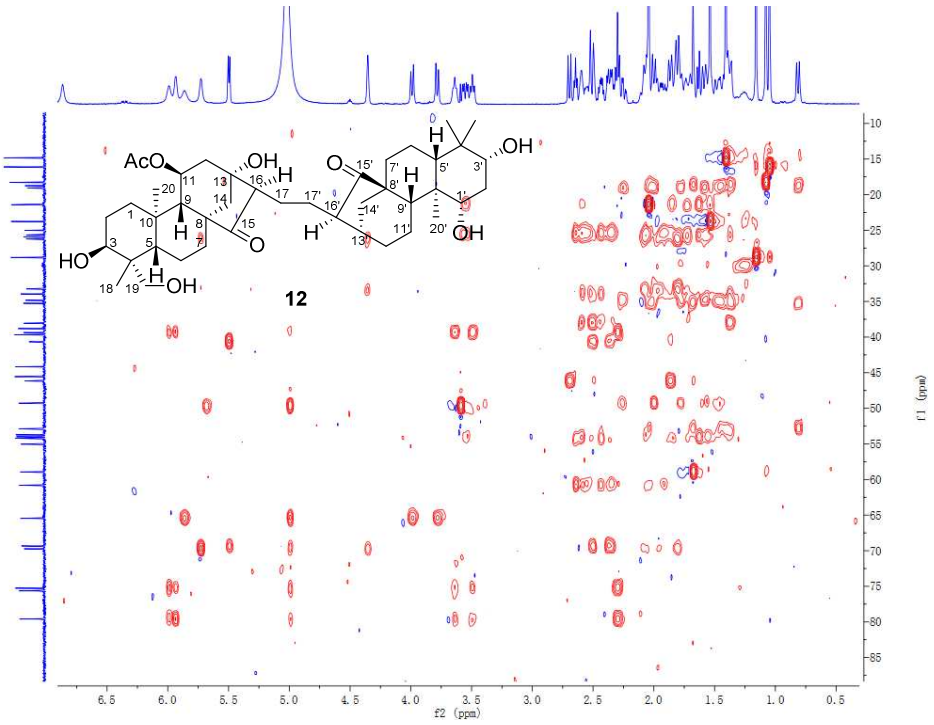


Figure 59: HSQC-TOCSY spectrum of scopariusol I (**12**) recorded in C_5D_5N

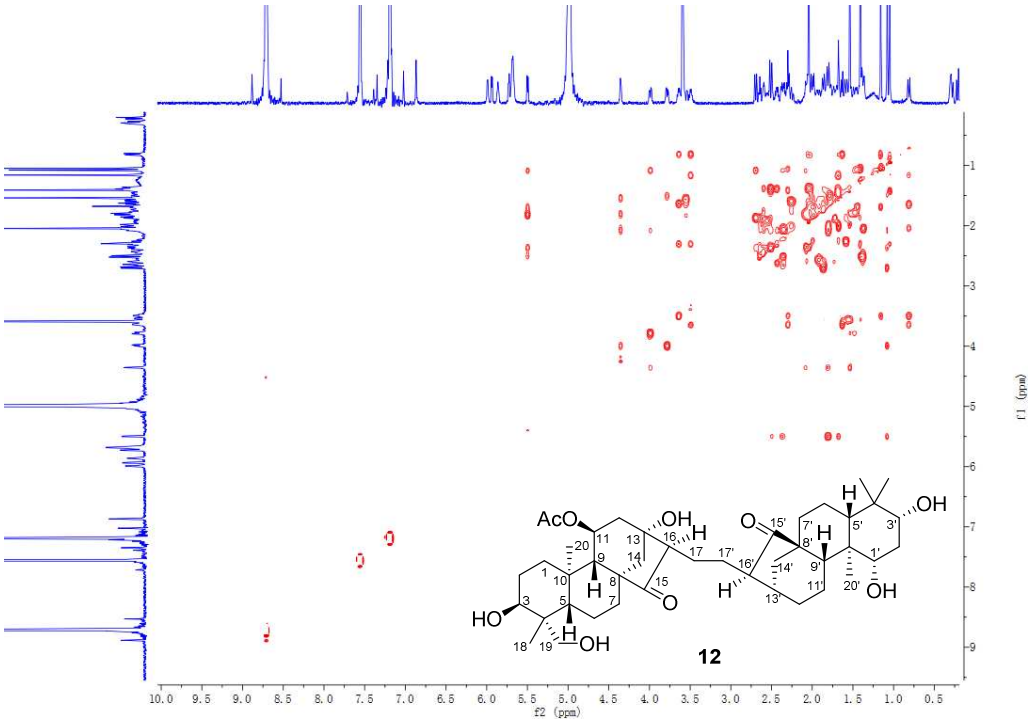


Figure 60: ROESY spectrum of scopariusol I (**12**) recorded in C_5D_5N

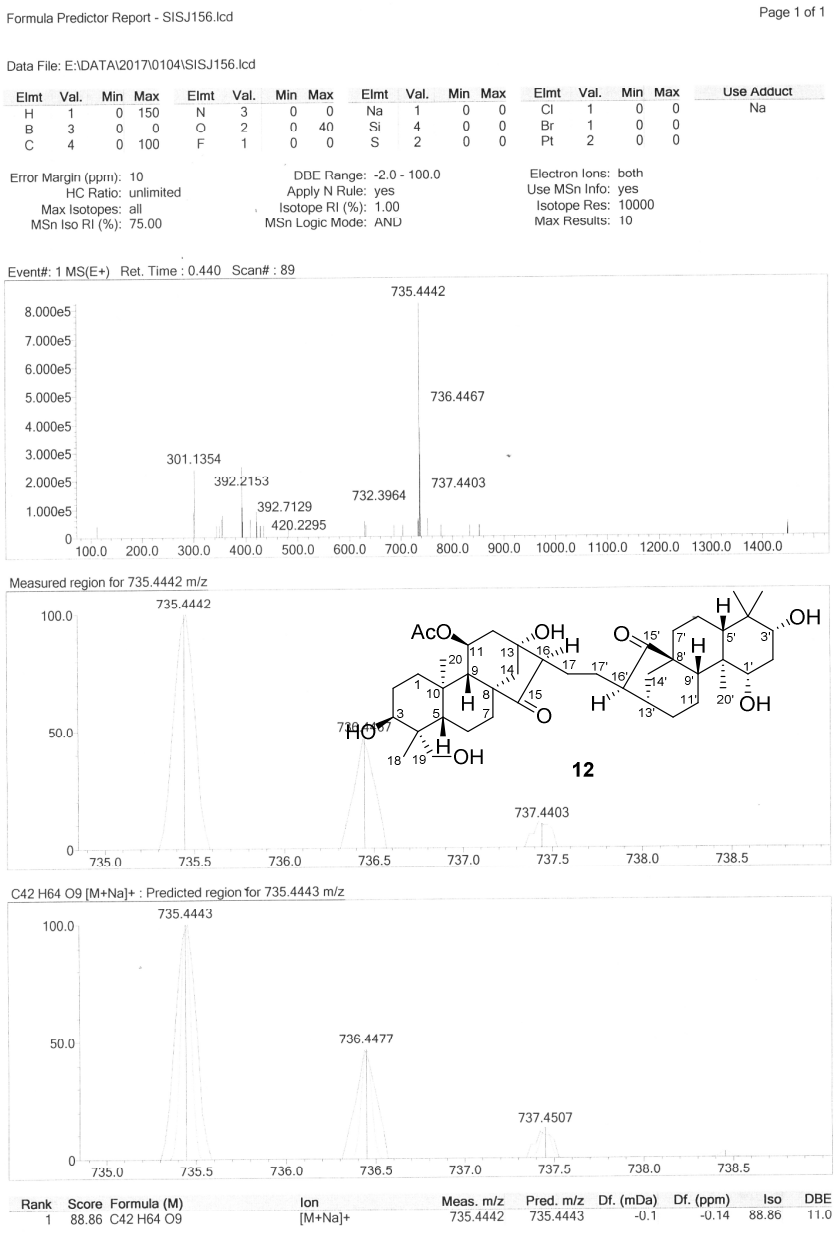


Figure 61: HRESIMS spectrum of scopariusol I (**12**)

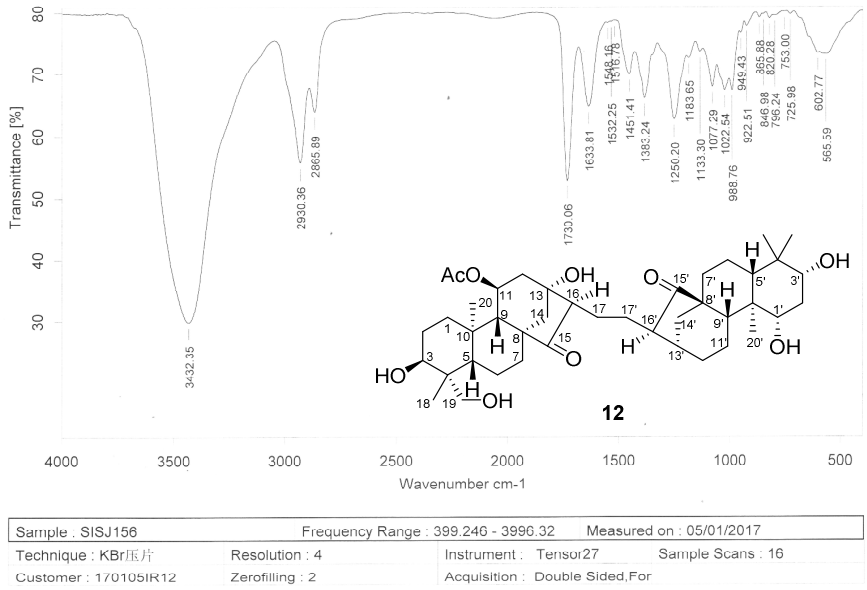


Figure 62: IR spectrum of scopariusol I (**12**)

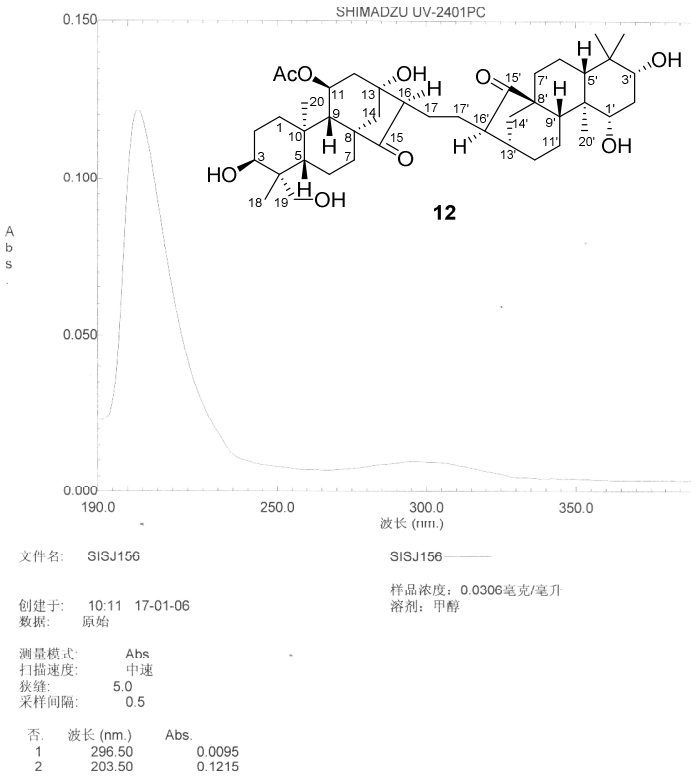


Figure 63: UV spectrum of scopariusol I (**12**)

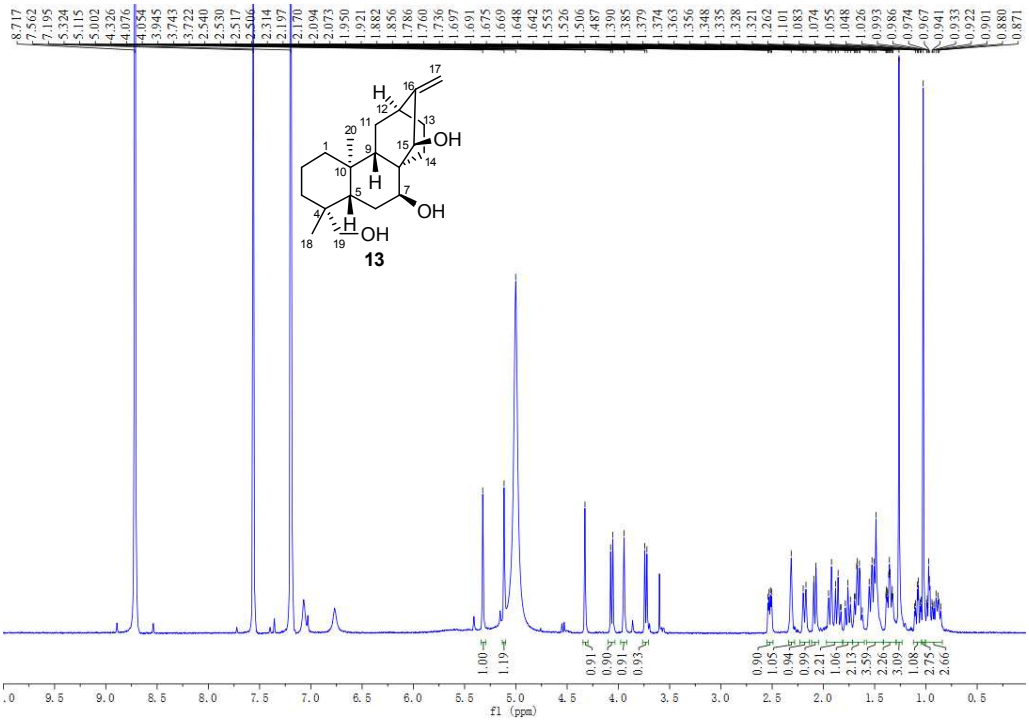


Figure 64: ^{1}H NMR spectrum of scopariusol J (**13**) recorded in C_5D_5N at 500 MHz

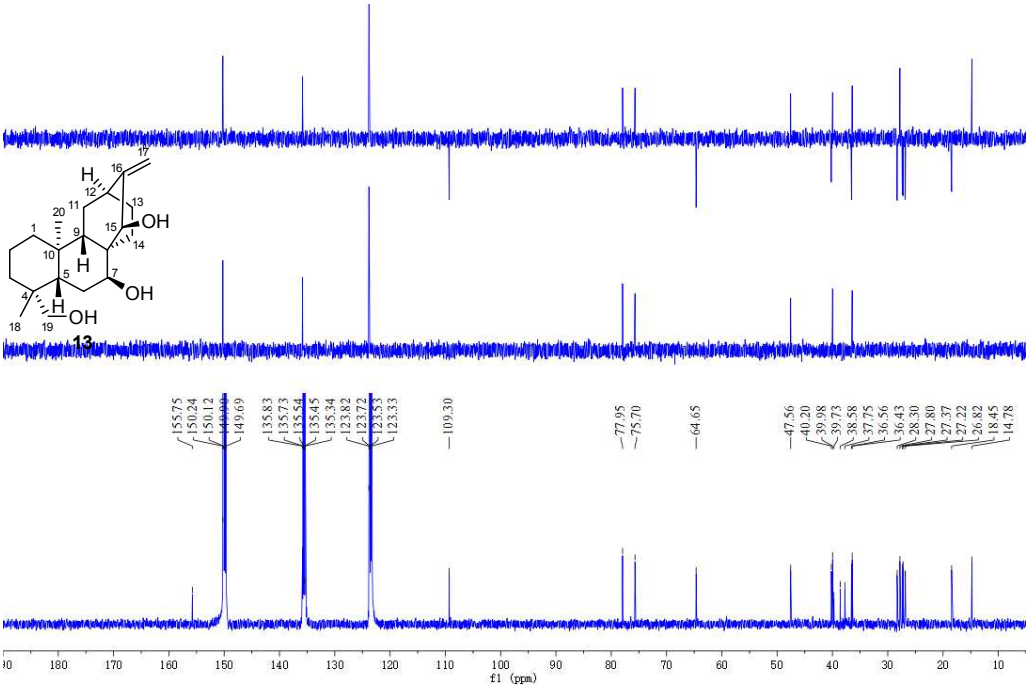


Figure 65: ^{13}C NMR spectrum of scopariusol J (**13**) recorded in C_5D_5N at 125 MHz

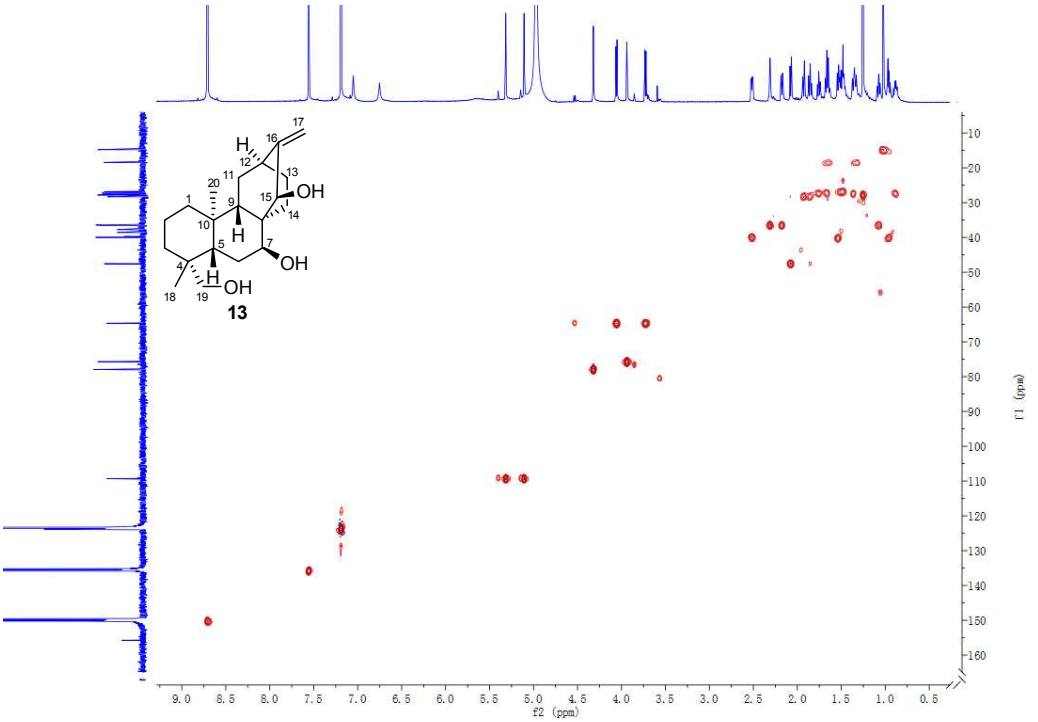


Figure 66: HSQC spectrum of scopariusol J (**13**) recorded in C_5D_5N

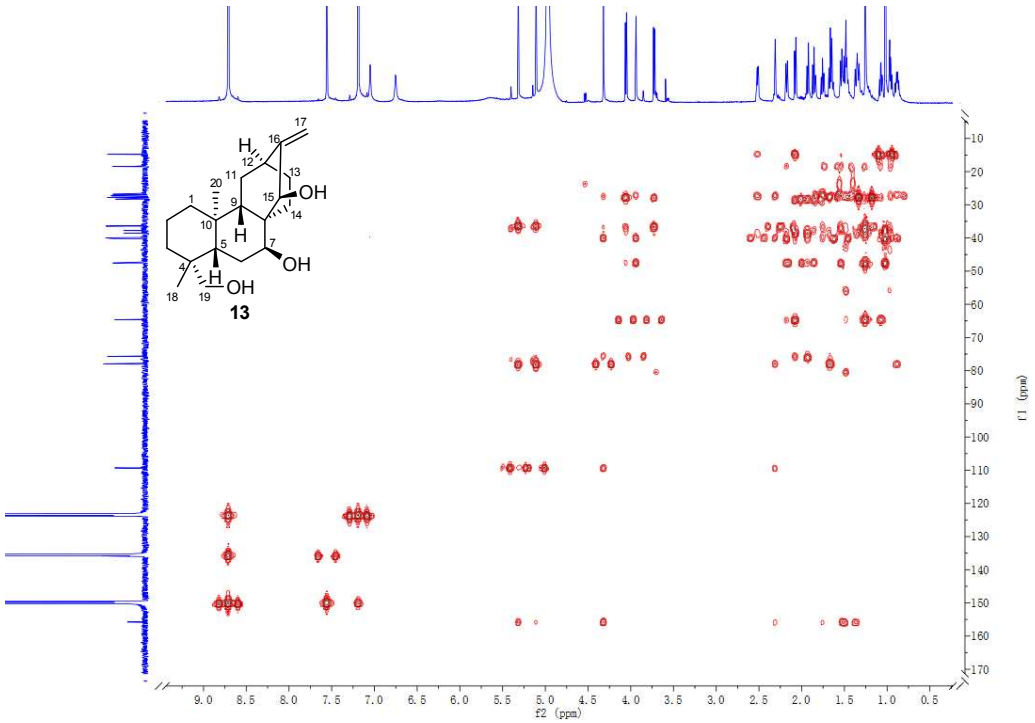


Figure 67: HMBC spectrum of scopariusol J (**13**) recorded in C_5D_5N

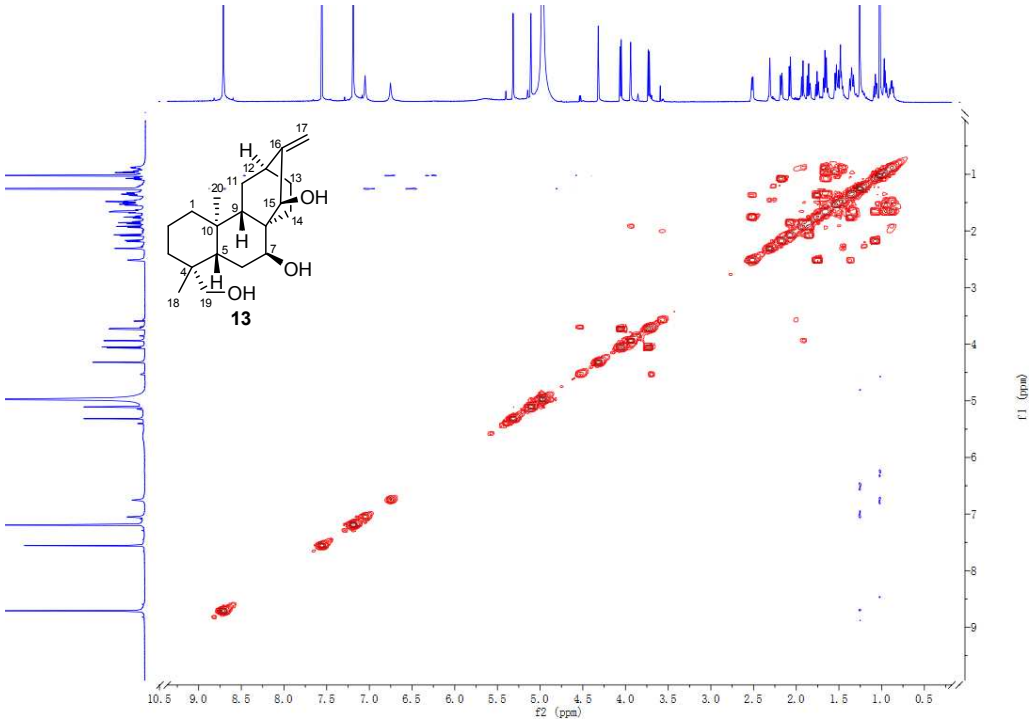


Figure 68: ^{1}H-^{1}H COSY spectrum of scopariusol J (**13**) recorded in C_5D_5N

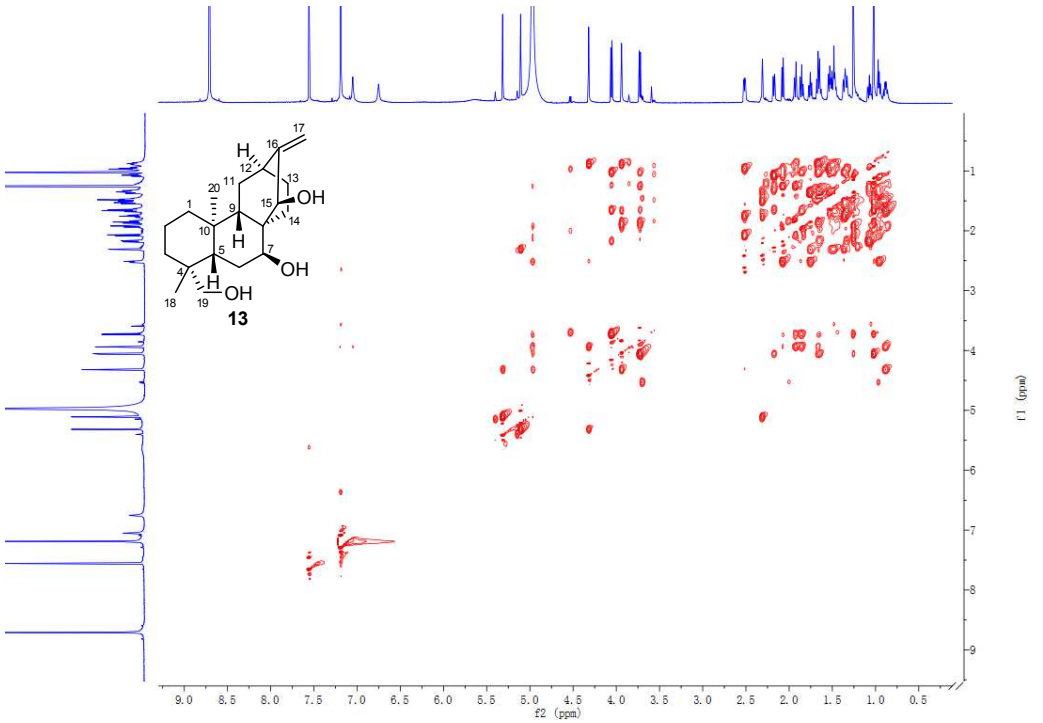
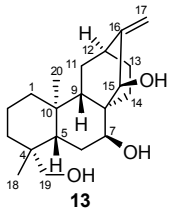


Figure 69: ROESY spectrum of scopariusol J (**13**) recorded in C_5D_5N

Qualitative Analysis Report

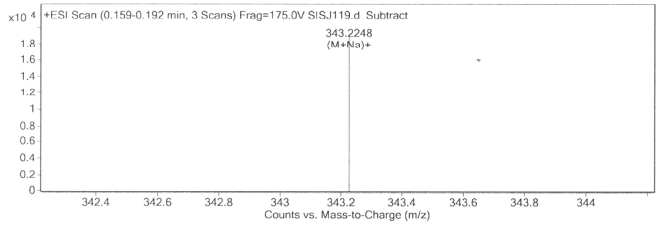
Data Filename	SISJ119.d	**Sample Name**	SISJ119
Sample Type	Sample	**Position**	Vial 2
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/14/2016 4:54:09 PM
IRM Calibration Status	Success	**DA Method**	FSI+.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		



13

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
267.2105	1	3461.66		
285.2218	1	10265.61		
303.2323	1	13011.88		
343.2248	1	19181.07	C20 H32 O3	(M+Na)+
344.2289	1	4367.81	C20 H32 O3	(M+Na)+
359.1989	1	5360.12		
663.4614	1	13171.2		
664.4642	1	6137		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H32 O3	320.2351	343.2244	343.2248	-0.6	-1.8	5.0000

End Of Report

Agilent Technologies Page 1 of 1 Printed at: 11:01 AM on: 10/18/2016

Figure 70: HRESIMS spectrum of scopariusol J (**13**)

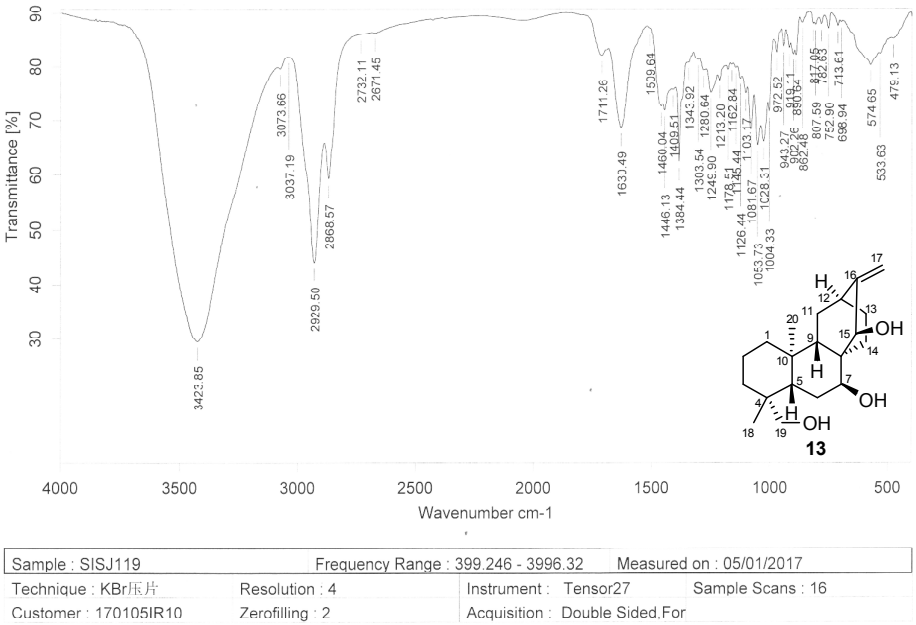


Figure 71: IR spectrum of scopariusol J (**13**)

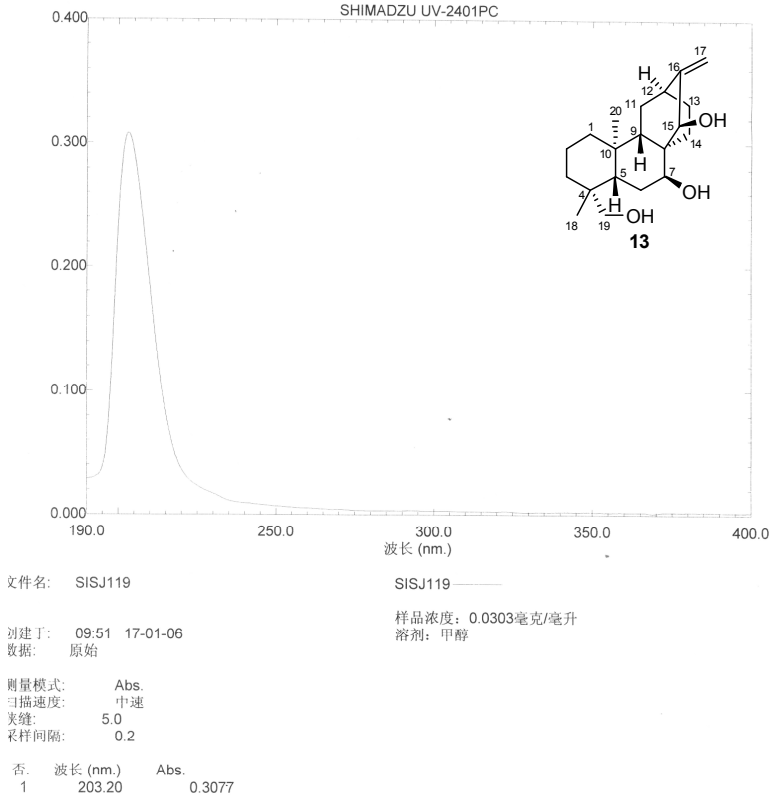


Figure 72: UV spectrum of scopariusol J (**13**)

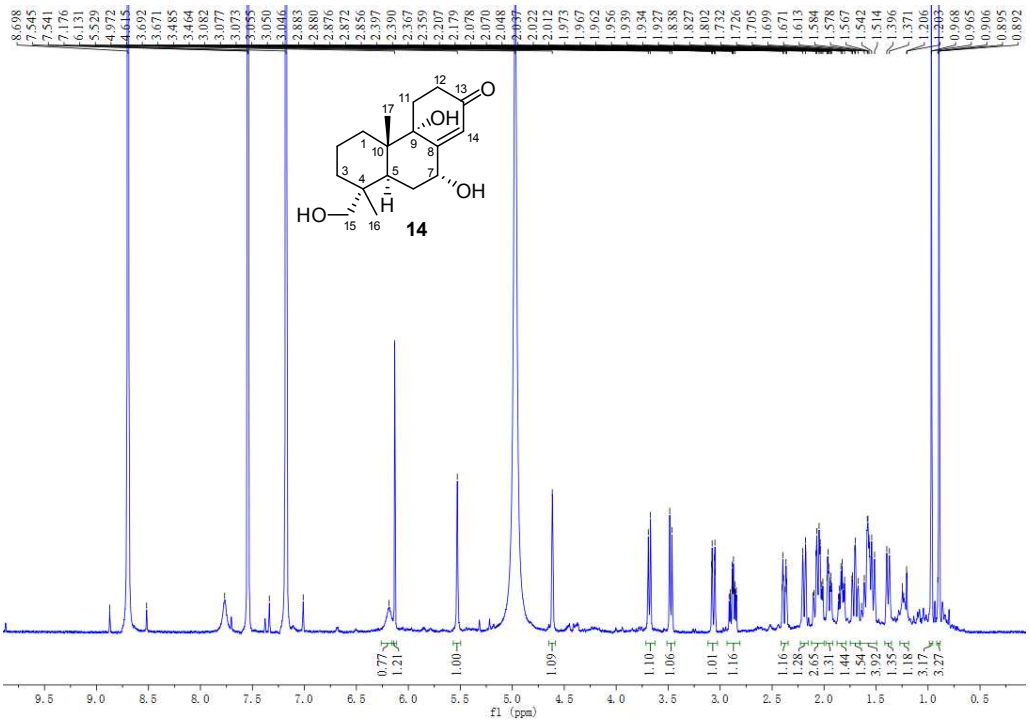


Figure 73: ^{1}H NMR spectrum of scopariusol K (**14**) recorded in C_5D_5N at 500 MHz

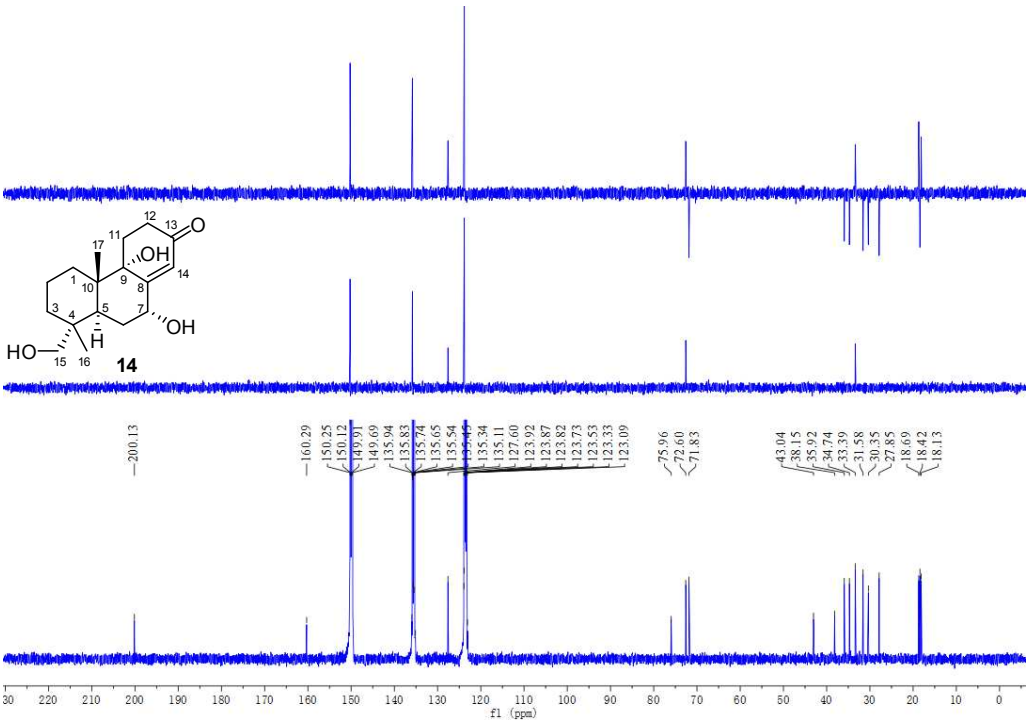


Figure 74: ^{13}C NMR spectrum of scopariusol K (**14**) recorded in C_5D_5N at 125 MHz

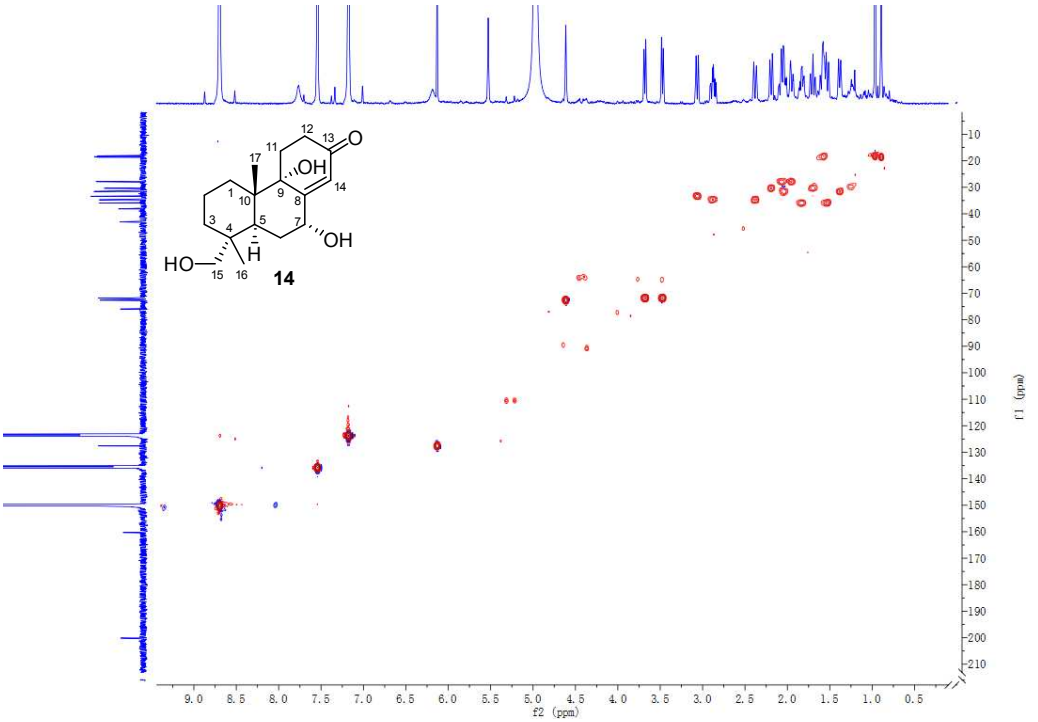


Figure 75: HSQC spectrum of scopariusol K (**14**) recorded in C_5D_5N

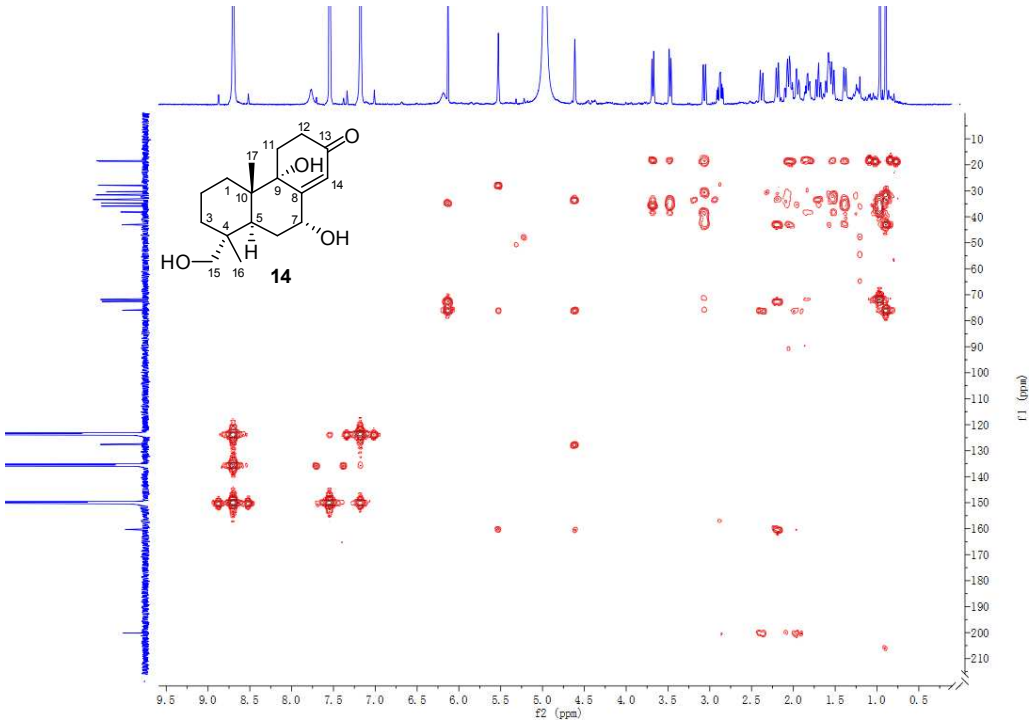


Figure 76: HMBC spectrum of scopariusol K (**14**) recorded in C_5D_5N

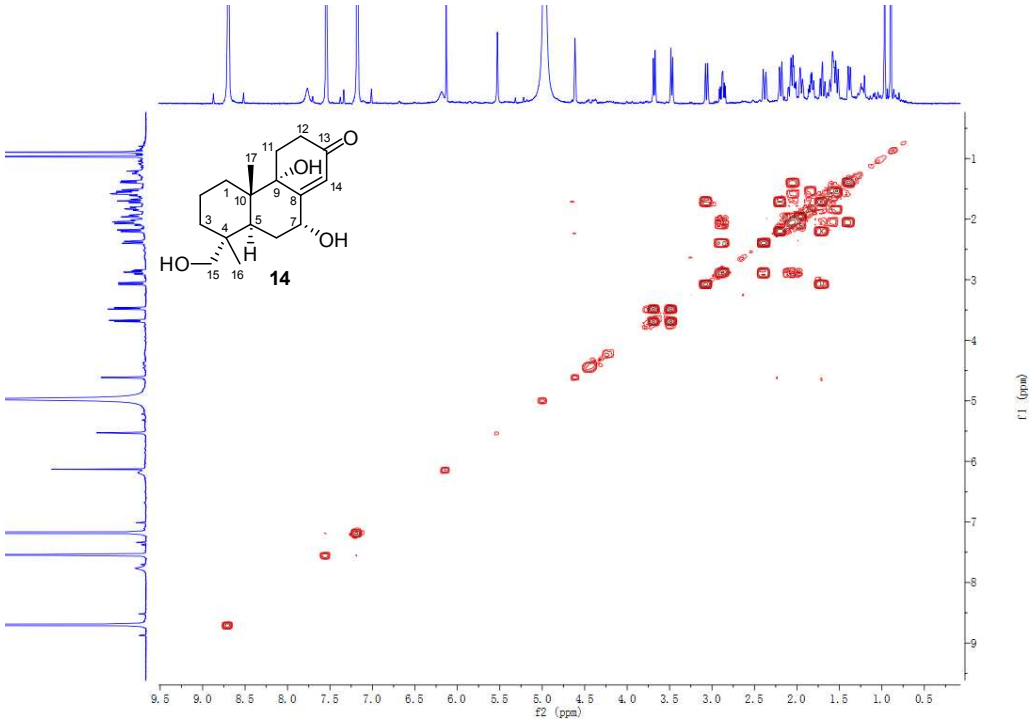


Figure 77: ^{1}H-^{1}H COSY spectrum of scopariusol K (**14**) recorded in C_5D_5N

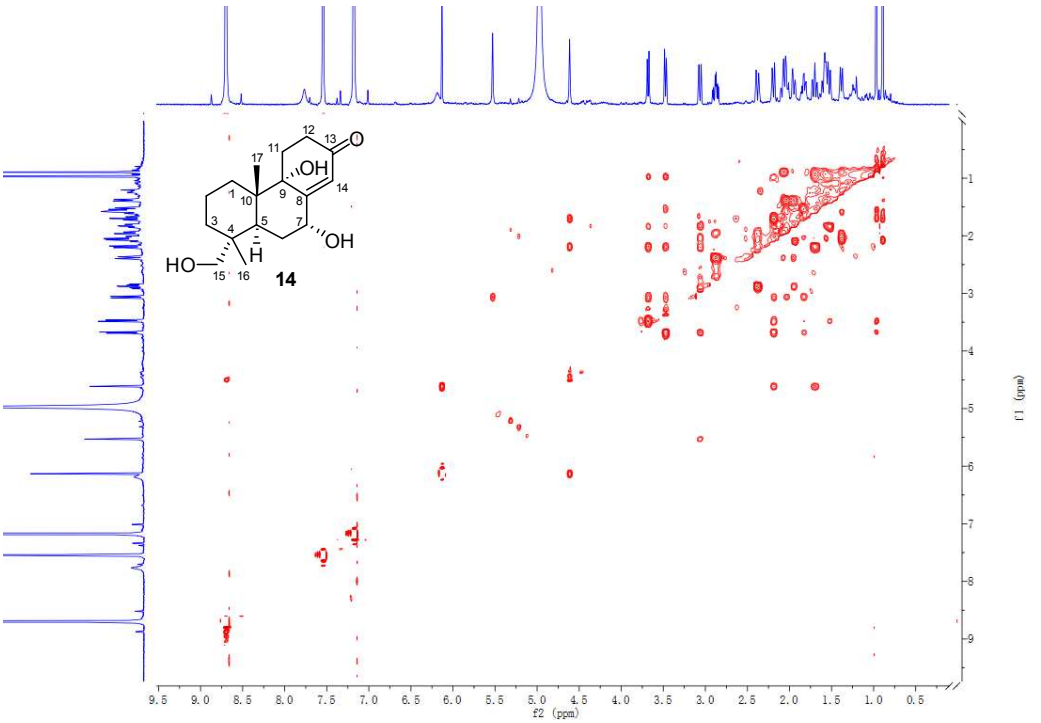
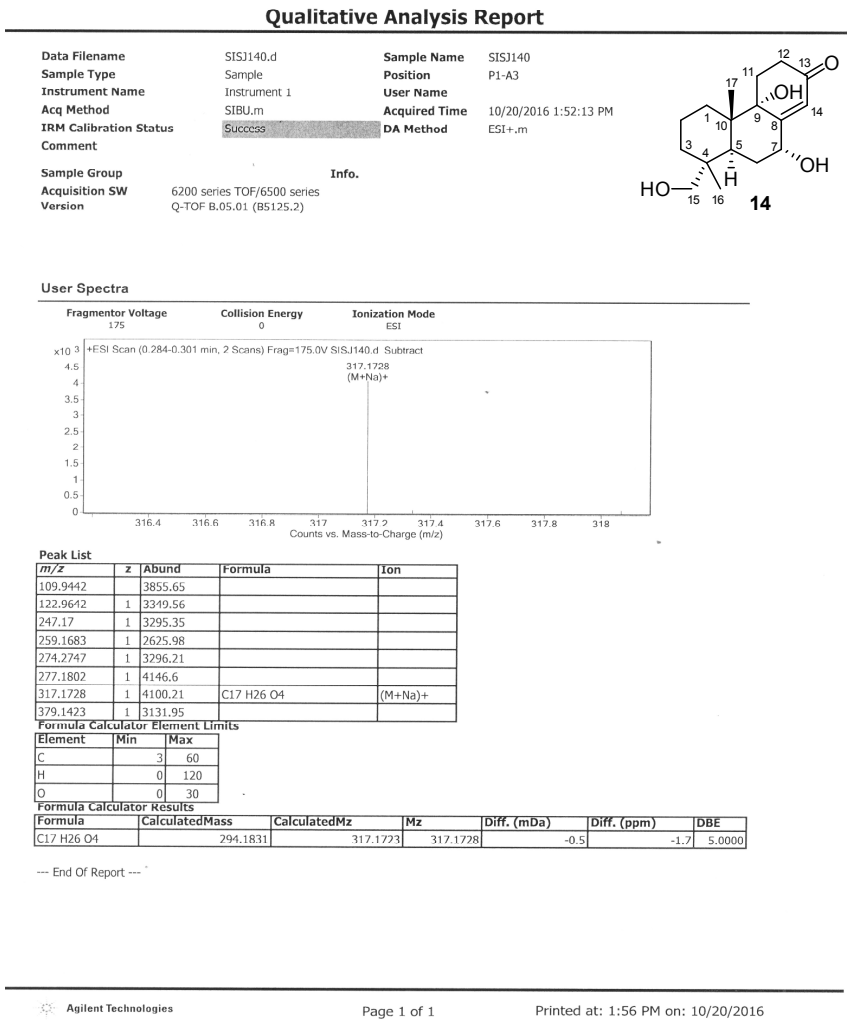


Figure 78: ROESY spectrum of scopariusol K (**14**) recorded in C_5D_5N



Qualitative Analysis Report

Data Filename	SISJ140.d	**Sample Name**	SISJ140
Sample Type	Sample	**Position**	P1-A3
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/20/2016 1:52:13 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			
Sample Group		**Info.**	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)		

14

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI

+ESI Scan (0.284-0.301 min, 2 Scans) Frag=175.0V SISJ140.d Subtract

317.1728
(M+Na)+

x10 3 4.5 4 3.5 3 2.5 2 1.5 1 0.5 0

316.4 316.6 316.8 317 317.2 317.4 317.6 317.8 318

Counts vs. Mass-to-Charge (m/z)

Peak List

m/z	z	Abund	Formula	Ion
109.9442		3855.65		
122.9642	1	3349.56		
247.17	1	3295.35		
259.1683	1	2625.98		
274.2747	1	3296.21		
277.1802	1	4146.6		
317.1728	1	4100.21	C17 H26 O4	(M+Na)+
379.1423	1	3131.95		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C17 H26 O4	294.1831	317.1723	317.1728	-0.5	-1.7	5.0000

--- End Of Report ---

Agilent Technologies Page 1 of 1 Printed at: 1:56 PM on: 10/20/2016

Figure 79: HRESIMS spectrum of scopariusol K (**14**)

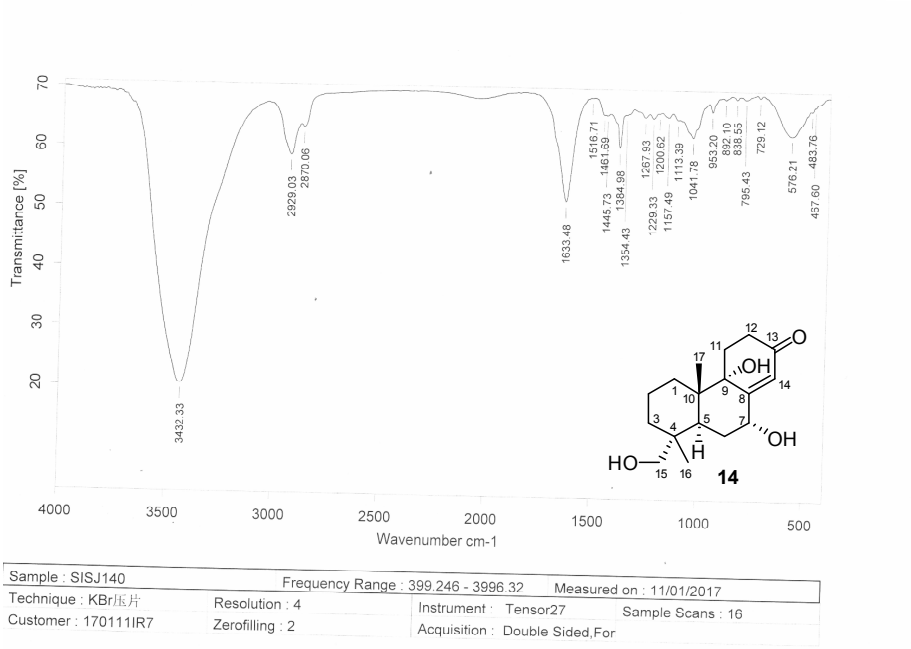


Figure 80: IR spectrum of scopariusol K (**14**)

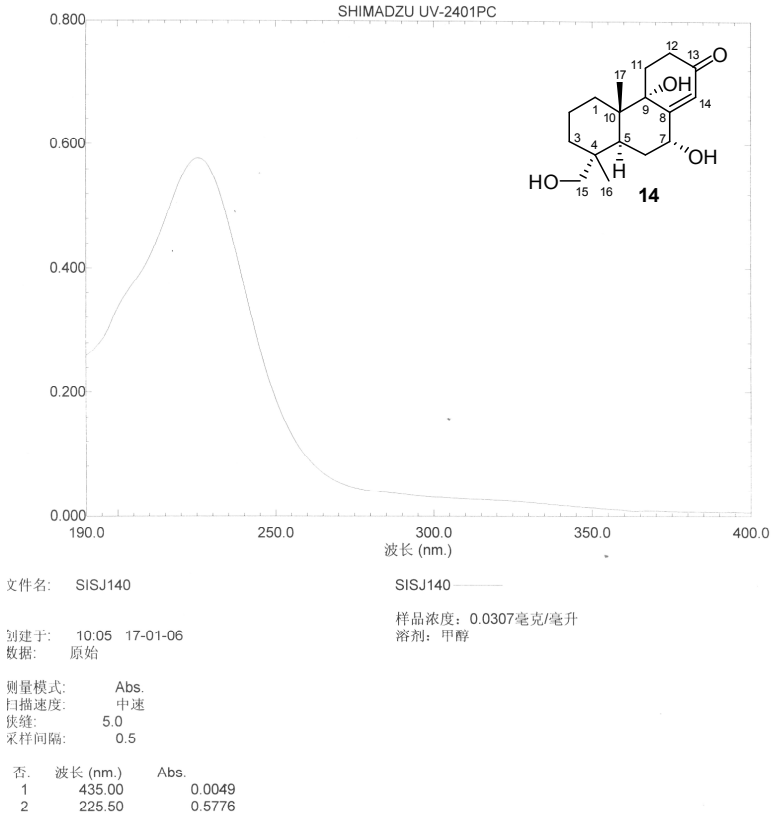


Figure 81: UV spectrum of scopariusol K (**14**)

SI-1: Computational details of scopariusol K (**14**) and *ent*-scopariusol K (*ent*-**14**)

The theoretical calculations of **14** and *ent*-**14** were carried out by using Gaussian 09 program package.[1] Conformational analysis was performed by using CONFLEX software[2] in MMFF94S force fields. The stable conformers were optimized by the density functional theory method at the B3LYP/6-31G(d) level. The optimized geometries were further checked by frequency calculation and resulted in no imaginary frequencies. The theoretical calculations of ECD were performed by using TDDFT at B3LYP/6-31G(d,p) level in the gas phase of the B3LYP/6-31G(d) optimized geometries. The calculated ECD curve was further generated by weighting the Boltzmann distribution rate of each geometric conformation in SpecDis 1.50 software[3] with σ=0.25 eV, and UV shift= -10nm.

The ECD spectra were simulated by overlapping Gaussian functions for each transition according to:

$$\Delta\varepsilon(E) = \frac{1}{2.297\times10^{-39}} \times \frac{1}{\sqrt{2\pi}\sigma} \sum_{i}^{A} \Delta E_i R_i e^{-\left[(E-E_i)/2\sigma\right]^2}$$

The σ represented the width of the band at 1/*e* height, and ΔE_i and R_i were the excitation energies and rotational strengths for transition *i*, respectively.

References:

(1) Frisch, M.-J.; Trucks, G.-W.; Schlegel, H.-B.; Scuseria, G.-E.; Robb, M.-A. Gaussian 09, revision C.O1; Gaussian, Inc.: Wallingford, CT, 2010.

(2) CONFLEX program, CONFLEX Corporation, AIOS Meguro 6F, 2-15-19, Kami-Osaki, Shinagawa-ku, Tokyo 141-0021, Japan; www.conflex.us.

(3) Bruhn, T.; Hemberger, Y.; Schaumloffel, A.; Bringmann, G. Spec Dis, version 1.50, University of Wurzburg, Germany, 2010.

Table 1: Input orientation of conformers of scopariusol K (**14**)

Conformer 1					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
1	6	0	2.219925	-2.43672	-0.40988
2	6	0	3.128162	-1.21273	-0.56526
3	6	0	2.72986	-0.03778	0.360198

4	6	0	1.207709	0.25478	0.170031
5	6	0	0.203735	-0.9452	0.191314
6	6	0	0.757365	-2.0814	-0.70448
7	6	0	0.686119	1.41234	1.039611
8	6	0	-0.62658	1.942834	0.463121
9	6	0	-1.6499	0.839597	0.279492
10	6	0	-1.1639	-0.41678	-0.45127
11	6	0	-2.9288	1.027346	0.648478
12	6	0	-4.02506	0.098929	0.283894
13	6	0	-3.64956	-0.95698	-0.73869
14	6	0	-2.24709	-1.51454	-0.46765
15	6	0	3.52791	1.231608	-0.07213
16	6	0	3.188137	-0.33025	1.804314
17	6	0	-0.0573	-1.47302	1.623488
18	1	0	1.165045	0.608581	-0.86365
19	8	0	-0.95528	-0.05363	-1.83089
20	8	0	3.033457	1.913288	-1.22563
21	8	0	-5.1556	0.238276	0.726133
22	8	0	-0.40278	2.507445	-0.85656
23	1	0	2.547999	-3.22736	-1.09661
24	1	0	2.319413	-2.8546	0.600566
25	1	0	4.17713	-1.48242	-0.38032
26	1	0	3.073693	-0.88251	-1.61555
27	1	0	0.13473	-2.97734	-0.59369
28	1	0	0.672831	-1.76459	-1.75039
29	1	0	1.400588	2.244021	1.078254
30	1	0	0.523999	1.101166	2.077547
31	1	0	-1.04176	2.729392	1.106702
32	1	0	-3.23249	1.931092	1.174309
33	1	0	-4.41082	-1.74246	-0.73707
34	1	0	-3.66132	-0.47793	-1.72749
35	1	0	-1.98056	-2.23959	-1.24228
36	1	0	-2.26258	-2.04725	0.487617
37	1	0	4.582337	0.948864	-0.21635
38	1	0	3.50714	1.981494	0.723981
39	1	0	2.773748	0.388592	2.519459
40	1	0	2.916526	-1.3333	2.142552
41	1	0	4.282322	-0.26095	1.869118
42	1	0	-0.71355	-0.81129	2.198685
43	1	0	0.868492	-1.58362	2.191618
44	1	0	-0.53369	-2.45812	1.601639
45	1	0	-0.76315	0.904863	-1.84969
46	1	0	3.146325	1.330139	-1.9927

47	1	0	0.544706	2.719833	-0.93818
Conformer 2					
1	6	0	-2.05085	2.605617	-0.16701
2	6	0	-3.0275	1.493556	-0.55461
3	6	0	-2.73094	0.133939	0.12754
4	6	0	-1.21289	-0.22784	-0.085
5	6	0	-0.15731	0.909416	0.184926
6	6	0	-0.61088	2.215324	-0.51431
7	6	0	-0.7735	-1.53523	0.601172
8	6	0	0.598589	-2.00468	0.10168
9	6	0	1.64948	-0.9075	0.150418
10	6	0	1.22805	0.442989	-0.43164
11	6	0	2.901332	-1.16016	0.579721
12	6	0	4.029461	-0.2193	0.422381
13	6	0	3.750859	0.97398	-0.47998
14	6	0	2.329512	1.514148	-0.2684
15	6	0	-3.62222	-0.90014	-0.62234
16	6	0	-3.21223	0.171889	1.594761
17	6	0	0.050455	1.170347	1.699401
18	1	0	-1.15586	-0.40639	-1.16619
19	8	0	0.986854	0.226663	-1.8564
20	8	0	-3.74039	-2.18699	-0.02543
21	8	0	5.124785	-0.42546	0.922549
22	8	0	0.525147	-2.51321	-1.2369
23	1	0	-2.31574	3.528613	-0.69823
24	1	0	-2.13783	2.836912	0.90268
25	1	0	-4.05866	1.795586	-0.32587
26	1	0	-2.98082	1.35826	-1.64616
27	1	0	0.064602	3.036565	-0.24548
28	1	0	-0.53255	2.081985	-1.59971
29	1	0	-1.49559	-2.32994	0.401002
30	1	0	-0.72983	-1.40503	1.690484
31	1	0	0.936755	-2.8523	0.706973
32	1	0	3.154369	-2.1271	1.010863
33	1	0	4.503848	1.745193	-0.29391
34	1	0	3.898839	0.640419	-1.51973
35	1	0	2.125392	2.330216	-0.96804
36	1	0	2.282891	1.938092	0.738443
37	1	0	-3.21734	-1.08238	-1.62344
38	1	0	-4.62271	-0.45415	-0.75045
39	1	0	-2.89554	-0.71176	2.157623
40	1	0	-2.85901	1.051917	2.137231
41	1	0	-4.31035	0.21505	1.624183

42	1	0	0.65967	0.395958	2.175487
43	1	0	-0.89709	1.208567	2.23573
44	1	0	0.549477	2.129424	1.871563
45	1	0	1.847482	0.032437	-2.26324
46	1	0	-4.2388	-2.08597	0.79956
47	1	0	0.416594	-1.73644	-1.81415
Conformer 3					
1	6	0	2.222162	-2.43257	-0.43742
2	6	0	3.128836	-1.20604	-0.58406
3	6	0	2.73079	-0.04566	0.359023
4	6	0	1.207903	0.249455	0.166699
5	6	0	0.203774	-0.95066	0.185576
6	6	0	0.756392	-2.07955	-0.72036
7	6	0	0.687535	1.405752	1.03904
8	6	0	-0.61907	1.941406	0.455479
9	6	0	-1.64678	0.841574	0.276527
10	6	0	-1.1672	-0.41956	-0.45048
11	6	0	-2.9244	1.03587	0.647158
12	6	0	-4.02489	0.110535	0.289003
13	6	0	-3.65501	-0.95344	-0.72724
14	6	0	-2.25389	-1.51412	-0.45543
15	6	0	3.525932	1.223017	-0.05103
16	6	0	3.18202	-0.35558	1.802525
17	6	0	-0.0548	-1.48612	1.615244
18	1	0	1.16964	0.595234	-0.86902
19	8	0	-0.97023	-0.06287	-1.83281
20	8	0	2.967007	1.826584	-1.22411
21	8	0	-5.15481	0.257912	0.730831
22	8	0	-0.38292	2.503106	-0.86386
23	1	0	2.547364	-3.21338	-1.13682
24	1	0	2.326629	-2.866	0.5664
25	1	0	4.176777	-1.48079	-0.39758
26	1	0	3.075646	-0.84551	-1.62031
27	1	0	0.13647	-2.97793	-0.6117
28	1	0	0.665467	-1.75477	-1.76286
29	1	0	1.404974	2.234809	1.083935
30	1	0	0.518459	1.091286	2.074925
31	1	0	-1.03328	2.733861	1.092217
32	1	0	-3.22354	1.943317	1.169369
33	1	0	-4.41921	-1.7361	-0.71899
34	1	0	-3.66682	-0.48078	-1.7191
35	1	0	-1.99164	-2.24595	-1.22516
36	1	0	-2.2691	-2.03943	0.503808

37	1	0	4.570462	0.929805	-0.23355
38	1	0	3.532189	1.949016	0.776207
39	1	0	2.764236	0.351977	2.527046
40	1	0	2.908708	-1.36372	2.12261
41	1	0	4.275977	-0.2887	1.873511
42	1	0	-0.71099	-0.82786	2.19487
43	1	0	0.871466	-1.59929	2.181785
44	1	0	-0.53026	-2.47155	1.588856
45	1	0	-0.76426	0.892275	-1.85842
46	1	0	3.619479	2.449018	-1.57825
47	1	0	0.576971	2.637476	-0.96568
Conformer 4					
1	6	0	2.126493	-2.42835	-0.17314
2	6	0	3.049793	-1.2562	-0.51018
3	6	0	2.670121	0.056802	0.221115
4	6	0	1.13937	0.346744	-0.00833
5	6	0	0.138482	-0.84632	0.206396
6	6	0	0.671902	-2.1002	-0.52609
7	6	0	0.62592	1.600855	0.726807
8	6	0	-0.76569	2.012275	0.254137
9	6	0	-1.75804	0.869274	0.200305
10	6	0	-1.25443	-0.42392	-0.44787
11	6	0	-3.03344	1.054419	0.588501
12	6	0	-4.11478	0.078293	0.317478
13	6	0	-3.73264	-1.05325	-0.61789
14	6	0	-2.3059	-1.54759	-0.34794
15	6	0	3.460191	1.206222	-0.45201
16	6	0	3.121712	-0.00785	1.697528
17	6	0	-0.08365	-1.16529	1.707283
18	1	0	1.083163	0.564521	-1.08243
19	8	0	-1.10154	-0.17598	-1.85998
20	8	0	4.851084	0.891565	-0.43091
21	8	0	-5.24198	0.234577	0.762897
22	8	0	-0.60666	2.52309	-1.09939
23	1	0	2.444641	-3.31715	-0.73301
24	1	0	2.212108	-2.69462	0.888825
25	1	0	4.093055	-1.50092	-0.28716
26	1	0	3.001126	-1.07908	-1.59514
27	1	0	0.033478	-2.9619	-0.29625
28	1	0	0.596153	-1.92832	-1.60661
29	1	0	1.285469	2.459983	0.569337
30	1	0	0.582406	1.428916	1.807675
31	1	0	-1.15551	2.817039	0.892244

32	1	0	-3.34579	1.979784	1.071912
33	1	0	-4.46879	-1.85689	-0.52373
34	1	0	-3.79084	-0.66561	-1.64451
35	1	0	-2.04179	-2.32196	-1.07334
36	1	0	-2.27501	-2.00584	0.644778
37	1	0	3.282972	2.155173	0.075876
38	1	0	3.107697	1.329821	-1.489
39	1	0	2.712676	0.817491	2.290942
40	1	0	2.838962	-0.94357	2.186503
41	1	0	4.212659	0.063711	1.736664
42	1	0	-0.72971	-0.43184	2.201618
43	1	0	0.855534	-1.19256	2.25998
44	1	0	-0.55513	-2.14489	1.834043
45	1	0	-0.78013	0.73971	-1.96037
46	1	0	5.330574	1.650606	-0.79389
47	1	0	-1.46979	2.876847	-1.37241
Conformer 5					
1	6	0	2.111165	-2.43438	-0.17494
2	6	0	3.040961	-1.26547	-0.50467
3	6	0	2.663332	0.047174	0.228597
4	6	0	1.133998	0.343061	-0.00174
5	6	0	0.127488	-0.84672	0.201372
6	6	0	0.660531	-2.0981	-0.53538
7	6	0	0.615719	1.589188	0.742976
8	6	0	-0.76396	2.021618	0.236784
9	6	0	-1.75994	0.881976	0.179627
10	6	0	-1.26072	-0.41555	-0.45956
11	6	0	-3.02998	1.0711	0.57603
12	6	0	-4.11279	0.090273	0.323867
13	6	0	-3.74144	-1.03629	-0.62085
14	6	0	-2.31628	-1.53663	-0.35524
15	6	0	3.460783	1.193782	-0.44066
16	6	0	3.110836	-0.02209	1.706036
17	6	0	-0.10204	-1.1729	1.699921
18	1	0	1.071955	0.567831	-1.07476
19	8	0	-1.09325	-0.177	-1.87106
20	8	0	4.84966	0.876546	-0.4132
21	8	0	-5.23168	0.240411	0.791107
22	8	0	-0.68463	2.502031	-1.13048
23	1	0	2.429139	-3.32289	-0.73528
24	1	0	2.190073	-2.70339	0.886875
25	1	0	4.082335	-1.5146	-0.27766
26	1	0	2.997344	-1.08554	-1.58939

27	1	0	0.016944	-2.95811	-0.3146
28	1	0	0.592396	-1.91917	-1.61515
29	1	0	1.29897	2.442555	0.631512
30	1	0	0.54756	1.403646	1.820622
31	1	0	-1.16246	2.826807	0.869527
32	1	0	-3.3399	2.005539	1.040876
33	1	0	-4.48056	-1.83755	-0.53008
34	1	0	-3.79819	-0.64028	-1.64427
35	1	0	-2.05675	-2.31061	-1.08271
36	1	0	-2.28561	-1.99693	0.636686
37	1	0	3.284232	2.144318	0.086453
38	1	0	3.113556	1.316166	-1.48044
39	1	0	2.704706	0.804521	2.299864
40	1	0	2.819914	-0.95675	2.191857
41	1	0	4.202073	0.042011	1.749396
42	1	0	-0.76231	-0.44936	2.190021
43	1	0	0.832492	-1.19014	2.261154
44	1	0	-0.56204	-2.15867	1.81982
45	1	0	-0.90316	0.772577	-1.99118
46	1	0	5.334694	1.631763	-0.77683
47	1	0	0.085745	3.089988	-1.19643
Conformer 6					
1	6	0	-2.05002	2.613866	-0.16633
2	6	0	-3.02474	1.500232	-0.55358
3	6	0	-2.72752	0.138911	0.126782
4	6	0	-1.20412	-0.21046	-0.05293
5	6	0	-0.15189	0.927958	0.201422
6	6	0	-0.61063	2.220996	-0.51229
7	6	0	-0.76583	-1.49613	0.675734
8	6	0	0.599031	-1.98027	0.18063
9	6	0	1.651012	-0.89023	0.169413
10	6	0	1.22674	0.44617	-0.44495
11	6	0	2.903217	-1.1479	0.584328
12	6	0	4.035541	-0.21426	0.376081
13	6	0	3.735815	0.950589	-0.54758
14	6	0	2.331744	1.512424	-0.29379
15	6	0	-3.59441	-0.89101	-0.65256
16	6	0	-3.23204	0.16326	1.585996
17	6	0	0.062658	1.209176	1.710942
18	1	0	-1.12113	-0.41456	-1.12821
19	8	0	1.072433	0.249557	-1.86407
20	8	0	-3.65489	-2.21281	-0.11729
21	8	0	5.137595	-0.42722	0.859022

22	8	0	0.512803	-2.41986	-1.20061
23	1	0	-2.31797	3.534345	-0.70042
24	1	0	-2.13884	2.847751	0.902911
25	1	0	-4.05773	1.798156	-0.32727
26	1	0	-2.97426	1.36684	-1.64507
27	1	0	0.06512	3.046057	-0.25727
28	1	0	-0.53061	2.067642	-1.59526
29	1	0	-1.50319	-2.29186	0.523889
30	1	0	-0.70623	-1.33503	1.758822
31	1	0	0.948206	-2.82159	0.795247
32	1	0	3.159305	-2.10756	1.03023
33	1	0	4.510736	1.712866	-0.42484
34	1	0	3.791976	0.576284	-1.57912
35	1	0	2.122924	2.316648	-1.00498
36	1	0	2.305282	1.9482	0.709417
37	1	0	-3.19985	-1.01077	-1.66745
38	1	0	-4.61308	-0.48065	-0.74604
39	1	0	-2.94458	-0.73552	2.141999
40	1	0	-2.86227	1.024606	2.146961
41	1	0	-4.32885	0.230755	1.600143
42	1	0	0.676389	0.443055	2.195726
43	1	0	-0.88062	1.259808	2.256917
44	1	0	0.56712	2.168412	1.863629
45	1	0	0.844726	-0.6893	-2.00739
46	1	0	-4.14883	-2.17162	0.715877
47	1	0	-0.31471	-2.92018	-1.29876
Conformer 7					
1	6	0	-2.11323	2.431709	-0.16687
2	6	0	-3.0441	1.259375	-0.48431
3	6	0	-2.66007	-0.05542	0.240768
4	6	0	-1.13278	-0.34434	0.002713
5	6	0	-0.12763	0.846008	0.20344
6	6	0	-0.665	2.094352	-0.5349
7	6	0	-0.61274	-1.592	0.742883
8	6	0	0.765484	-2.02204	0.230643
9	6	0	1.760519	-0.88126	0.176218
10	6	0	1.260113	0.417501	-0.45963
11	6	0	3.030914	-1.06967	0.571727
12	6	0	4.112587	-0.08675	0.322089
13	6	0	3.740189	1.041312	-0.62048
14	6	0	2.314553	1.539478	-0.35358
15	6	0	-3.45946	-1.20907	-0.43485
16	6	0	-3.11051	0.007172	1.716014

17	6	0	0.100439	1.173615	1.70161
18	1	0	-1.07398	-0.56849	-1.07098
19	8	0	1.089377	0.182587	-1.87129
20	8	0	-4.86898	-1.02099	-0.42738
21	8	0	5.231344	-0.23622	0.789526
22	8	0	0.682743	-2.49575	-1.13834
23	1	0	-2.43653	3.318463	-0.7267
24	1	0	-2.18727	2.699838	0.895068
25	1	0	-4.07892	1.523966	-0.23
26	1	0	-3.01502	1.087353	-1.57277
27	1	0	-0.02302	2.956767	-0.3198
28	1	0	-0.60136	1.912658	-1.61448
29	1	0	-1.29634	-2.44469	0.631256
30	1	0	-0.54083	-1.40889	1.82068
31	1	0	1.165929	-2.82958	0.858968
32	1	0	3.342099	-2.00495	1.033943
33	1	0	4.478307	1.84325	-0.52794
34	1	0	3.797503	0.647539	-1.64472
35	1	0	2.054215	2.314692	-1.07956
36	1	0	2.283736	1.997781	0.639326
37	1	0	-3.30737	-2.15024	0.102202
38	1	0	-3.09348	-1.34926	-1.46599
39	1	0	-2.69251	-0.81285	2.309991
40	1	0	-2.83986	0.946427	2.205628
41	1	0	-4.20108	-0.08116	1.754062
42	1	0	0.765232	0.453501	2.190451
43	1	0	-0.83419	1.183698	2.263325
44	1	0	0.554432	2.162098	1.822471
45	1	0	0.902935	-0.76761	-1.99376
46	1	0	-5.07031	-0.27845	-1.01682
47	1	0	-0.08395	-3.08859	-1.205

Table 2: Input orientation of conformers of *ent*-scopariusol K (*ent*-**14**)

Conformer 1					
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
1	6	0	-2.21985	-2.43673	-0.40987
2	6	0	-3.12822	-1.21282	-0.56509
3	6	0	-2.72985	-0.03781	0.360278
4	6	0	-1.2077	0.254819	0.170047
5	6	0	-0.2037	-0.94514	0.191237
6	6	0	-0.75734	-2.08131	-0.70458

7	6	0	-0.6861	1.412467	1.039524
8	6	0	0.626644	1.942909	0.463027
9	6	0	1.649926	0.839652	0.27947
10	6	0	1.163921	-0.41669	-0.45136
11	6	0	2.928815	1.027352	0.64852
12	6	0	4.025069	0.098968	0.28389
13	6	0	3.649595	-0.95694	-0.73872
14	6	0	2.247083	-1.51447	-0.46775
15	6	0	-3.52803	1.231537	-0.07194
16	6	0	-3.18803	-0.33026	1.804424
17	6	0	0.057368	-1.47307	1.623329
18	1	0	-1.16514	0.608625	-0.86364
19	8	0	0.955264	-0.05349	-1.83096
20	8	0	-3.03396	1.913159	-1.22563
21	8	0	5.1555	0.238044	0.726469
22	8	0	0.40301	2.507367	-0.85673
23	1	0	-2.3192	-2.85467	0.600562
24	1	0	-2.54792	-3.22735	-1.09662
25	1	0	-4.17713	-1.48262	-0.37994
26	1	0	-3.07401	-0.88266	-1.6154
27	1	0	-0.13465	-2.97723	-0.5939
28	1	0	-0.67291	-1.76444	-1.75048
29	1	0	-1.40056	2.244149	1.078131
30	1	0	-0.52399	1.101337	2.077474
31	1	0	1.041804	2.729482	1.106597
32	1	0	3.232529	1.931058	1.17441
33	1	0	3.661469	-0.4779	-1.72752
34	1	0	4.410834	-1.74245	-0.73702
35	1	0	1.980592	-2.23949	-1.24243
36	1	0	2.262496	-2.04721	0.487505
37	1	0	-3.50708	1.981467	0.724125
38	1	0	-4.58249	0.948759	-0.2159
39	1	0	-2.77356	0.388535	2.519562
40	1	0	-2.91649	-1.33337	2.14261
41	1	0	-4.28221	-0.2609	1.869268
42	1	0	-0.86839	-1.5835	2.191558
43	1	0	0.533499	-2.4583	1.601357
44	1	0	0.713884	-0.81155	2.198472
45	1	0	0.762888	0.904962	-1.84983
46	1	0	-3.14609	1.329545	-1.99247
47	1	0	-0.54435	2.720338	-0.93826
Conformer 2					
1	6	0	2.046605	2.615818	-0.15883

2	6	0	3.025943	1.505596	-0.5417
3	6	0	2.731345	0.140129	0.135918
4	6	0	1.206584	-0.21199	-0.04316
5	6	0	0.15254	0.928407	0.200223
6	6	0	0.611914	2.218691	-0.51695
7	6	0	0.765164	-1.48697	0.702839
8	6	0	-0.59883	-1.97577	0.210754
9	6	0	-1.65139	-0.88725	0.179106
10	6	0	-1.22319	0.44193	-0.4477
11	6	0	-2.90636	-1.14086	0.588267
12	6	0	-4.03735	-0.21028	0.361965
13	6	0	-3.73105	0.946682	-0.5696
14	6	0	-2.3282	1.510241	-0.31284
15	6	0	3.596135	-0.87372	-0.65124
16	6	0	3.238089	0.15782	1.593711
17	6	0	-0.06889	1.218944	1.707375
18	1	0	1.123273	-0.4273	-1.1163
19	8	0	-1.06316	0.229618	-1.86445
20	8	0	3.604052	-2.16616	-0.04031
21	8	0	-5.14358	-0.41978	0.837074
22	8	0	-0.50608	-2.43558	-1.16503
23	1	0	2.126823	2.847321	0.911364
24	1	0	2.316601	3.537712	-0.68956
25	1	0	4.056184	1.805645	-0.30677
26	1	0	2.981256	1.376803	-1.63409
27	1	0	-0.06861	3.042743	-0.27159
28	1	0	0.542118	2.060112	-1.60001
29	1	0	1.498568	-2.2885	0.567206
30	1	0	0.705949	-1.30973	1.78286
31	1	0	-0.95053	-2.80929	0.834389
32	1	0	-3.16483	-2.09535	1.043799
33	1	0	-3.78129	0.563493	-1.59821
34	1	0	-4.50644	1.710254	-0.45819
35	1	0	-2.1152	2.307772	-1.03029
36	1	0	-2.3068	1.955276	0.686455
37	1	0	4.622564	-0.47681	-0.69583
38	1	0	3.224591	-0.9415	-1.68692
39	1	0	2.99597	-0.76644	2.123825
40	1	0	2.836999	0.998243	2.165666
41	1	0	4.330618	0.258017	1.601553
42	1	0	0.871922	1.269262	2.257235
43	1	0	-0.57154	2.18059	1.851267
44	1	0	-0.68723	0.457699	2.19386

45	1	0	-0.83633	-0.71124	-1.99507
46	1	0	4.315517	-2.68108	-0.44926
47	1	0	0.335571	-2.91307	-1.25452
Conformer 3					
1	6	0	-2.22216	-2.43257	-0.43742
2	6	0	-3.12884	-1.20604	-0.58406
3	6	0	-2.73079	-0.04566	0.359023
4	6	0	-1.2079	0.249455	0.166699
5	6	0	-0.20377	-0.95066	0.185576
6	6	0	-0.75639	-2.07955	-0.72036
7	6	0	-0.68754	1.405752	1.03904
8	6	0	0.619074	1.941406	0.455479
9	6	0	1.646783	0.841574	0.276527
10	6	0	1.167199	-0.41956	-0.45048
11	6	0	2.924399	1.03587	0.647158
12	6	0	4.024887	0.110535	0.289003
13	6	0	3.655011	-0.95344	-0.72724
14	6	0	2.253893	-1.51412	-0.45543
15	6	0	-3.52593	1.223017	-0.05103
16	6	0	-3.18202	-0.35558	1.802525
17	6	0	0.054803	-1.48612	1.615244
18	1	0	-1.16964	0.595234	-0.86902
19	8	0	0.970226	-0.06287	-1.83281
20	8	0	-2.96701	1.826584	-1.22411
21	8	0	5.154812	0.257912	0.730831
22	8	0	0.382917	2.503106	-0.86386
23	1	0	-2.32663	-2.866	0.5664
24	1	0	-2.54736	-3.21338	-1.13682
25	1	0	-4.17678	-1.48079	-0.39758
26	1	0	-3.07565	-0.84551	-1.62031
27	1	0	-0.13647	-2.97793	-0.6117
28	1	0	-0.66547	-1.75477	-1.76286
29	1	0	-1.40497	2.234809	1.083935
30	1	0	-0.51846	1.091287	2.074925
31	1	0	1.033276	2.733861	1.092217
32	1	0	3.223543	1.943317	1.169369
33	1	0	3.66682	-0.48078	-1.7191
34	1	0	4.419208	-1.7361	-0.71899
35	1	0	1.991641	-2.24595	-1.22516
36	1	0	2.269102	-2.03943	0.503808
37	1	0	-3.53219	1.949016	0.776207
38	1	0	-4.57046	0.929805	-0.23355
39	1	0	-2.76424	0.351977	2.527046

40	1	0	-2.90871	-1.36372	2.12261
41	1	0	-4.27598	-0.2887	1.873511
42	1	0	-0.87147	-1.59929	2.181785
43	1	0	0.530262	-2.47155	1.588856
44	1	0	0.710993	-0.82786	2.19487
45	1	0	0.764259	0.892275	-1.85842
46	1	0	-3.61948	2.449018	-1.57825
47	1	0	-0.57697	2.637476	-0.96568
Conformer 4					
1	6	0	2.126541	2.428421	-0.17287
2	6	0	3.049762	1.256265	-0.51011
3	6	0	2.670084	-0.0568	0.221049
4	6	0	1.139312	-0.34678	-0.0083
5	6	0	0.138421	0.846297	0.206524
6	6	0	0.671929	2.100308	-0.52573
7	6	0	0.625962	-1.60087	0.726985
8	6	0	-0.76563	-2.01231	0.254217
9	6	0	-1.75801	-0.86931	0.200292
10	6	0	-1.2544	0.423976	-0.44783
11	6	0	-3.03341	-1.05441	0.588404
12	6	0	-4.11475	-0.07832	0.317374
13	6	0	-3.73266	1.053282	-0.61795
14	6	0	-2.30585	1.54762	-0.34807
15	6	0	3.460097	-1.2061	-0.45231
16	6	0	3.121675	0.007581	1.697461
17	6	0	-0.08389	1.165062	1.707381
18	1	0	1.083001	-0.56459	-1.08239
19	8	0	-1.10157	0.175976	-1.85999
20	8	0	4.851031	-0.8914	-0.43111
21	8	0	-5.24197	-0.23472	0.762674
22	8	0	-0.60635	-2.52299	-1.0993
23	1	0	2.212297	2.694579	0.889119
24	1	0	2.444647	3.317256	-0.7327
25	1	0	4.09306	1.500902	-0.28713
26	1	0	3.000987	1.079312	-1.59509
27	1	0	0.033543	2.962	-0.29572
28	1	0	0.596122	1.928656	-1.6063
29	1	0	1.285559	-2.45995	0.569527
30	1	0	0.582486	-1.42883	1.80783
31	1	0	-1.15568	-2.81711	0.892146
32	1	0	-3.34586	-1.97978	1.071796
33	1	0	-3.79088	0.665644	-1.64457
34	1	0	-4.46872	1.85699	-0.52374

35	1	0	-2.0418	2.321869	-1.07362
36	1	0	-2.27505	2.006047	0.644581
37	1	0	3.10769	-1.32938	-1.48936
38	1	0	3.282998	-2.15522	0.075281
39	1	0	2.712749	-0.81803	2.290599
40	1	0	2.838616	0.943045	2.186715
41	1	0	4.212621	-0.06383	1.73659
42	1	0	0.855378	1.193052	2.259908
43	1	0	-0.55606	2.144317	1.834201
44	1	0	-0.72934	0.431171	2.201822
45	1	0	-0.77961	-0.73953	-1.96037
46	1	0	5.33053	-1.65054	-0.79387
47	1	0	-1.4695	-2.87649	-1.37261
Conformer 5					
1	6	0	2.111243	2.434353	-0.1749
2	6	0	3.040959	1.265431	-0.50476
3	6	0	2.663355	-0.04722	0.228522
4	6	0	1.134005	-0.34304	-0.00173
5	6	0	0.127534	0.846757	0.201449
6	6	0	0.660567	2.098161	-0.53528
7	6	0	0.615713	-1.58911	0.743031
8	6	0	-0.76397	-2.02153	0.236931
9	6	0	-1.75994	-0.8819	0.179724
10	6	0	-1.26073	0.415598	-0.45944
11	6	0	-3.03001	-1.07106	0.576081
12	6	0	-4.11286	-0.09032	0.323734
13	6	0	-3.74142	1.036426	-0.62071
14	6	0	-2.31627	1.53669	-0.35508
15	6	0	3.460746	-1.19387	-0.44076
16	6	0	3.110935	0.022047	1.705936
17	6	0	-0.10192	1.172864	1.700021
18	1	0	1.071875	-0.56779	-1.07475
19	8	0	-1.09324	0.177083	-1.87096
20	8	0	4.849653	-0.87671	-0.4134
21	8	0	-5.23189	-0.24074	0.790549
22	8	0	-0.68468	-2.50194	-1.13037
23	1	0	2.190212	2.703274	0.886932
24	1	0	2.429236	3.322893	-0.73519
25	1	0	4.082361	1.514526	-0.27785
26	1	0	2.997214	1.085503	-1.58948
27	1	0	0.017038	2.95819	-0.3144
28	1	0	0.592353	1.919294	-1.61506
29	1	0	1.298955	-2.4425	0.631569

30	1	0	0.547617	-1.40355	1.820687
31	1	0	-1.16245	-2.82673	0.869674
32	1	0	-3.33992	-2.00549	1.040926
33	1	0	-3.7983	0.640594	-1.6442
34	1	0	-4.48053	1.837685	-0.52979
35	1	0	-2.05671	2.310719	-1.08249
36	1	0	-2.28557	1.996948	0.636874
37	1	0	3.113478	-1.31629	-1.48052
38	1	0	3.28421	-2.14439	0.086399
39	1	0	2.704895	-0.80461	2.299765
40	1	0	2.820008	0.956684	2.191806
41	1	0	4.202179	-0.04199	1.749243
42	1	0	0.832631	1.190118	2.261226
43	1	0	-0.56197	2.158599	1.820022
44	1	0	-0.76211	0.449251	2.190129
45	1	0	-0.90356	-0.77258	-1.99116
46	1	0	5.334612	-1.63189	-0.77722
47	1	0	0.085778	-3.08979	-1.19639
Conformer 6					
1	6	0	2.049951	2.613835	-0.16628
2	6	0	3.024772	1.500261	-0.5534
3	6	0	2.727555	0.138905	0.126854
4	6	0	1.204092	-0.21044	-0.05267
5	6	0	0.151841	0.928021	0.201456
6	6	0	0.610659	2.220894	-0.51245
7	6	0	0.765769	-1.49608	0.676075
8	6	0	-0.59907	-1.98025	0.180902
9	6	0	-1.651	-0.89018	0.169668
10	6	0	-1.22671	0.446102	-0.44499
11	6	0	-2.90323	-1.14778	0.584534
12	6	0	-4.03555	-0.21422	0.375988
13	6	0	-3.73579	0.95037	-0.54804
14	6	0	-2.33177	1.512352	-0.29417
15	6	0	3.594409	-0.89095	-0.65267
16	6	0	3.232288	0.163194	1.586004
17	6	0	-0.06277	1.209539	1.710913
18	1	0	1.121092	-0.41465	-1.12792
19	8	0	-1.07219	0.249045	-1.86404
20	8	0	3.65449	-2.21292	-0.11779
21	8	0	-5.13758	-0.42696	0.859069
22	8	0	-0.51286	-2.41975	-1.20037
23	1	0	2.13861	2.847739	0.902969
24	1	0	2.317901	3.534317	-0.70038

25	1	0	4.057739	1.798204	-0.32698
26	1	0	2.974421	1.366903	-1.64489
27	1	0	-0.06515	3.045978	-0.25763
28	1	0	0.530847	2.067347	-1.5954
29	1	0	1.503139	-2.29182	0.52444
30	1	0	0.706008	-1.33484	1.759131
31	1	0	-0.94832	-2.82154	0.79551
32	1	0	-3.15931	-2.10734	1.030652
33	1	0	-3.7917	0.575749	-1.57947
34	1	0	-4.51075	1.712665	-0.4257
35	1	0	-2.12296	2.316434	-1.00551
36	1	0	-2.3054	1.948328	0.708962
37	1	0	4.613171	-0.48076	-0.74587
38	1	0	3.200039	-1.01037	-1.66767
39	1	0	2.944802	-0.73553	2.142043
40	1	0	2.8628	1.024664	2.146976
41	1	0	4.329117	0.230557	1.599937
42	1	0	0.880451	1.259854	2.257009
43	1	0	-0.56687	2.169012	1.863337
44	1	0	-0.67693	0.443755	2.195696
45	1	0	-0.84438	-0.68984	-2.00702
46	1	0	4.148941	-2.17227	0.715097
47	1	0	0.315049	-2.91937	-1.2987
Conformer 7					
1	6	0	2.113142	2.431765	-0.16683
2	6	0	3.044046	1.25946	-0.48434
3	6	0	2.660065	-0.05536	0.24074
4	6	0	1.132794	-0.34438	0.002595
5	6	0	0.127583	0.845945	0.203347
6	6	0	0.664932	2.094359	-0.5349
7	6	0	0.612808	-1.59208	0.742724
8	6	0	-0.76546	-2.0221	0.230596
9	6	0	-1.7605	-0.88131	0.176159
10	6	0	-1.2601	0.417432	-0.45976
11	6	0	-3.03087	-1.06966	0.571758
12	6	0	-4.11253	-0.08673	0.322181
13	6	0	-3.74019	1.041251	-0.62052
14	6	0	-2.31452	1.539418	-0.35375
15	6	0	3.459566	-1.20904	-0.43474
16	6	0	3.110372	0.007402	1.716011
17	6	0	-0.10063	1.173491	1.701495
18	1	0	1.074052	-0.56852	-1.07109
19	8	0	-1.08929	0.182471	-1.87143

20	8	0	4.869095	-1.0211	-0.42711
21	8	0	-5.23116	-0.23598	0.789959
22	8	0	-0.68287	-2.4958	-1.13837
23	1	0	2.187179	2.699828	0.895118
24	1	0	2.436415	3.318555	-0.72663
25	1	0	4.078863	1.524167	-0.23006
26	1	0	3.01494	1.087469	-1.5728
27	1	0	0.022902	2.956728	-0.31975
28	1	0	0.601325	1.912739	-1.6145
29	1	0	1.296414	-2.44474	0.63101
30	1	0	0.540918	-1.40902	1.82054
31	1	0	-1.16585	-2.82962	0.858991
32	1	0	-3.34203	-2.00489	1.034091
33	1	0	-3.7975	0.647388	-1.64473
34	1	0	-4.47825	1.843247	-0.52805
35	1	0	-2.05425	2.314557	-1.07984
36	1	0	-2.2836	1.99784	0.639124
37	1	0	3.093727	-1.34925	-1.46593
38	1	0	3.307401	-2.15019	0.102321
39	1	0	2.692147	-0.81241	2.310117
40	1	0	2.839847	0.946824	2.20538
41	1	0	4.200919	-0.08116	1.754188
42	1	0	0.833963	1.183709	2.263252
43	1	0	-0.55483	2.16189	1.822322
44	1	0	-0.76533	0.453252	2.19028
45	1	0	-0.90265	-0.76769	-1.9939
46	1	0	5.070477	-0.27766	-1.01542
47	1	0	0.083471	-3.08913	-1.20499

Table 3: Important thermodynamic parameters of optimized 14 at B3LYP/6-31G(d) level in gas phase.

Species	*E*	*E'*	*H*	*G*
Conformer 1	-963.908728	-963.889237	-963.888293	-963.95353
Conformer 2	-963.902914	-963.882997	-963.882053	-963.948309
Conformer 3	-963.907258	-963.88765	-963.886706	-963.952229
Conformer 4	-963.90639	-963.886427	-963.885483	-963.951881
Conformer 5	-963.904046	-963.883983	-963.883039	-963.949604
Conformer 6	-963.90695	-963.88717	-963.886226	-963.952206
Conformer 7	-963.905623	-963.885757	-963.884812	-963.95093

E, *E'*, *H*, *G*: total energy, total energy with zero point energy (ZPE), enthalpy, and Gibbs free energy.

Table 4: Conformational analysis of **14** at B3LYP/6-31+G(d) level in gas phase.

Species	ΔE	P_E%	$\Delta E'$	$P_{E'}$%	ΔG	P_G%
Conformer 1	0.00	66.9625	0.00	72.49291	0.00	56.95487
Conformer 2	3.64	0.141733	3.91	0.097719	3.27	0.225914
Conformer 3	0.92	14.11405	0.99	13.49887	0.81	14.35783
Conformer 4	1.46	5.628384	1.76	3.696018	1.03	9.931468
Conformer 5	2.93	0.470084	3.29	0.277669	2.46	0.890481
Conformer 6	1.11	10.18535	1.29	8.119025	0.83	14.01229
Conformer 7	1.94	2.497895	2.18	1.817788	1.63	3.627158

ΔE, $\Delta E'$, ΔG: Relative energy, relative energy with ZPE, and relative Gibbs free energy in kcal/mol. P_E%, $P_{E'}$%, P_G%: Conformational distribution calculated by using the respective parameters in Table S2.

Table 5: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for 3-epi-isodopharicin A (**1**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(21)	1557(3)	704(1)	11708(1)	28(1)
O(11)	369(3)	275(1)	10557(1)	19(1)
O(3)	-1023(4)	2980(1)	8529(1)	44(1)
O(13)	4865(3)	-1400(1)	9815(1)	27(1)
O(14)	-1808(3)	-678(1)	9154(1)	24(1)
C(21)	307(4)	355(1)	11329(1)	20(1)
C(11)	2200(4)	540(1)	10147(1)	17(1)
C(9)	1430(4)	720(1)	9316(1)	16(1)
C(10)	2421(4)	1452(1)	8925(1)	18(1)
C(5)	1253(4)	1560(1)	8142(1)	18(1)
C(4)	1525(4)	2348(1)	7711(1)	24(1)
C(3)	1073(5)	3008(2)	8297(2)	33(1)
C(6)	1503(4)	841(1)	7625(1)	21(1)
C(7)	528(4)	133(1)	8012(1)	20(1)
C(8)	1388(3)	-39(1)	8811(1)	16(1)
C(15)	23(4)	-626(1)	9242(1)	18(1)
C(16)	1313(4)	-1120(1)	9748(1)	18(1)
C(17)	712(4)	-1746(2)	10140(2)	25(1)
C(13)	3442(4)	-801(1)	9668(1)	18(1)
C(12)	3792(3)	-105(1)	10216(1)	19(1)

C(22)	-1512(4)	-49(2)	11659(2)	29(1)
C(20)	4741(4)	1380(1)	8837(1)	22(1)
C(1)	1940(5)	2161(1)	9441(1)	26(1)
C(2)	2335(5)	2939(2)	9031(2)	33(1)
C(14)	3413(3)	-489(1)	8830(1)	17(1)
C(19)	3639(5)	2475(2)	7350(2)	28(1)
C(18)	-30(5)	2408(2)	7049(2)	34(1)

Table 6: Bond lengths [Å] and angles [º] for 3-epi-isodopharicin A (**1**).

O(21)-C(21)	1.209(3)
O(11)-C(21)	1.337(3)
O(11)-C(11)	1.471(3)
O(3)-C(3)	1.439(4)
O(3)-H(3)	0.8400
O(13)-C(13)	1.414(3)
O(13)-H(13)	0.8400
O(14)-C(15)	1.220(3)
C(21)-C(22)	1.498(4)
C(11)-C(12)	1.530(3)
C(11)-C(9)	1.549(3)
C(11)-H(11)	1.0000
C(9)-C(8)	1.565(3)
C(9)-C(10)	1.568(3)
C(9)-H(9)	1.0000
C(10)-C(1)	1.539(3)
C(10)-C(20)	1.543(3)
C(10)-C(5)	1.564(3)
C(5)-C(6)	1.530(3)
C(5)-C(4)	1.551(3)
C(5)-H(5)	1.0000
C(4)-C(18)	1.537(4)
C(4)-C(19)	1.542(4)
C(4)-C(3)	1.545(4)
C(3)-C(2)	1.518(4)
C(3)-H(3A)	1.0000
C(6)-C(7)	1.526(3)

C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.517(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(15)	1.540(3)
C(8)-C(14)	1.542(3)
C(15)-C(16)	1.484(3)
C(16)-C(17)	1.328(4)
C(16)-C(13)	1.513(3)
C(17)-H(17A)	0.9500
C(17)-H(17B)	0.9500
C(13)-C(12)	1.538(3)
C(13)-C(14)	1.540(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(1)-C(2)	1.532(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(21)-O(11)-C(11)	118.13(19)
C(3)-O(3)-H(3)	109.5
C(13)-O(13)-H(13)	109.5

O(21)-C(21)-O(11)	124.5(2)
O(21)-C(21)-C(22)	124.7(2)
O(11)-C(21)-C(22)	110.8(2)
O(11)-C(11)-C(12)	107.59(18)
O(11)-C(11)-C(9)	103.64(18)
C(12)-C(11)-C(9)	116.14(18)
O(11)-C(11)-H(11)	109.7
C(12)-C(11)-H(11)	109.7
C(9)-C(11)-H(11)	109.7
C(11)-C(9)-C(8)	110.76(18)
C(11)-C(9)-C(10)	114.81(18)
C(8)-C(9)-C(10)	115.70(17)
C(11)-C(9)-H(9)	104.7
C(8)-C(9)-H(9)	104.7
C(10)-C(9)-H(9)	104.7
C(1)-C(10)-C(20)	108.9(2)
C(1)-C(10)-C(5)	107.68(19)
C(20)-C(10)-C(5)	114.42(19)
C(1)-C(10)-C(9)	107.31(18)
C(20)-C(10)-C(9)	113.0(2)
C(5)-C(10)-C(9)	105.11(18)
C(6)-C(5)-C(4)	114.29(18)
C(6)-C(5)-C(10)	110.66(18)
C(4)-C(5)-C(10)	117.28(19)
C(6)-C(5)-H(5)	104.3
C(4)-C(5)-H(5)	104.3
C(10)-C(5)-H(5)	104.3
C(18)-C(4)-C(19)	107.1(2)
C(18)-C(4)-C(3)	107.8(2)
C(19)-C(4)-C(3)	109.5(2)
C(18)-C(4)-C(5)	109.6(2)
C(19)-C(4)-C(5)	114.9(2)
C(3)-C(4)-C(5)	107.65(19)
O(3)-C(3)-C(2)	107.0(2)
O(3)-C(3)-C(4)	110.0(3)
C(2)-C(3)-C(4)	112.4(2)
O(3)-C(3)-H(3A)	109.1
C(2)-C(3)-H(3A)	109.1

C(4)-C(3)-H(3A)	109.1
C(7)-C(6)-C(5)	109.97(18)
C(7)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6A)	109.7
C(7)-C(6)-H(6B)	109.7
C(5)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
C(8)-C(7)-C(6)	113.16(19)
C(8)-C(7)-H(7A)	108.9
C(6)-C(7)-H(7A)	108.9
C(8)-C(7)-H(7B)	108.9
C(6)-C(7)-H(7B)	108.9
H(7A)-C(7)-H(7B)	107.8
C(7)-C(8)-C(15)	110.22(18)
C(7)-C(8)-C(14)	116.10(19)
C(15)-C(8)-C(14)	99.75(17)
C(7)-C(8)-C(9)	110.44(18)
C(15)-C(8)-C(9)	106.55(17)
C(14)-C(8)-C(9)	112.86(18)
O(14)-C(15)-C(16)	126.7(2)
O(14)-C(15)-C(8)	124.5(2)
C(16)-C(15)-C(8)	108.71(19)
C(17)-C(16)-C(15)	126.1(2)
C(17)-C(16)-C(13)	128.0(2)
C(15)-C(16)-C(13)	105.79(18)
C(16)-C(17)-H(17A)	120.0
C(16)-C(17)-H(17B)	120.0
H(17A)-C(17)-H(17B)	120.0
O(13)-C(13)-C(16)	109.69(18)
O(13)-C(13)-C(12)	110.74(19)
C(16)-C(13)-C(12)	111.34(19)
O(13)-C(13)-C(14)	115.36(19)
C(16)-C(13)-C(14)	101.49(19)
C(12)-C(13)-C(14)	107.91(18)
C(11)-C(12)-C(13)	114.23(18)
C(11)-C(12)-H(12A)	108.7
C(13)-C(12)-H(12A)	108.7
C(11)-C(12)-H(12B)	108.7

C(13)-C(12)-H(12B)	108.7
H(12A)-C(12)-H(12B)	107.6
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(10)-C(20)-H(20A)	109.5
C(10)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(10)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(2)-C(1)-C(10)	112.7(2)
C(2)-C(1)-H(1A)	109.1
C(10)-C(1)-H(1A)	109.1
C(2)-C(1)-H(1B)	109.1
C(10)-C(1)-H(1B)	109.1
H(1A)-C(1)-H(1B)	107.8
C(3)-C(2)-C(1)	111.0(2)
C(3)-C(2)-H(2A)	109.4
C(1)-C(2)-H(2A)	109.4
C(3)-C(2)-H(2B)	109.4
C(1)-C(2)-H(2B)	109.4
H(2A)-C(2)-H(2B)	108.0
C(13)-C(14)-C(8)	101.79(17)
C(13)-C(14)-H(14A)	111.4
C(8)-C(14)-H(14A)	111.4
C(13)-C(14)-H(14B)	111.4
C(8)-C(14)-H(14B)	111.4
H(14A)-C(14)-H(14B)	109.3
C(4)-C(19)-H(19A)	109.5
C(4)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(4)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5

C(4)-C(18)-H(18A)	109.5
C(4)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(4)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5

Symmetry transformations used to generate equivalent atoms.

Table 7: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for scopariusol B (**3**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(18)	10002(4)	-267(6)	6709(2)	20(1)
O(11)	8227(4)	2022(6)	3488(2)	16(1)
O(18')	4583(4)	4806(7)	8317(2)	19(1)
O(11')	7130(4)	7051(6)	11418(2)	16(1)
C(18)	8783(6)	-916(10)	6805(3)	17(1)
C(4)	7698(6)	-13(9)	6357(3)	15(1)
C(5)	7968(6)	-238(9)	5651(3)	12(1)
C(6)	7981(6)	-2177(9)	5414(3)	15(1)
C(7)	8732(6)	-2294(9)	4831(3)	14(1)
C(8)	8164(6)	-1078(9)	4286(3)	12(1)
C(15)	9082(6)	-890(9)	3770(3)	14(1)
C(16)	8253(6)	182(9)	3253(3)	13(1)
C(17)	8697(6)	203(10)	2599(3)	21(2)
C(3)	7696(6)	1972(10)	6539(3)	15(1)
C(2)	6899(6)	3175(9)	6060(3)	15(1)
C(1)	7304(6)	2929(9)	5387(3)	14(1)
C(10)	7182(6)	1001(9)	5142(3)	11(1)
C(20)	5772(6)	492(9)	5036(3)	14(1)
C(9)	7860(6)	857(10)	4520(3)	14(1)
C(14)	7042(6)	-1919(9)	3856(3)	11(1)
C(13)	6877(6)	-540(9)	3299(3)	15(1)
C(11)	7291(6)	1981(10)	3937(3)	14(1)
C(12)	6194(6)	1099(9)	3520(3)	13(1)
C(19)	6470(6)	-914(10)	6514(3)	16(1)
C(18')	5741(6)	4111(10)	8133(3)	15(1)
C(4')	6912(6)	4982(9)	8509(3)	14(1)
C(5')	6847(6)	4762(8)	9235(3)	11(1)
C(6')	6872(6)	2821(9)	9472(3)	14(1)
C(7')	6334(6)	2710(9)	10113(3)	14(1)
C(8')	7017(6)	3931(9)	10622(3)	11(1)
C(15')	6247(6)	4137(9)	11198(3)	15(1)
C(16')	7169(6)	5228(10)	11660(3)	16(1)
C(17')	6905(7)	5257(10)	12350(3)	20(2)
C(11')	7933(6)	7009(9)	10905(3)	13(1)

C(9')	7241(6)	5861(9)	10361(3)	14(1)
C(10')	7761(6)	5962(9)	9692(3)	12(1)
C(20')	9147(6)	5384(10)	9706(3)	15(1)
C(1')	7640(6)	7909(9)	9456(3)	14(1)
C(2')	7828(6)	8130(9)	8751(3)	16(2)
C(3')	6887(6)	6971(10)	8330(3)	16(1)
C(12')	9111(6)	6154(9)	11265(3)	15(1)
C(13')	8516(7)	4510(9)	11531(3)	16(2)
C(14')	8225(6)	3136(9)	10992(3)	14(1)
C(19')	8049(7)	4065(10)	8254(3)	20(2)

Table 8: Bond lengths [Å] and angles [º] for scopariusol B (**3**).

O(18)-C(18)	1.415(8)
O(18)-H(18)	0.8400
O(11)-C(11)	1.448(7)
O(11)-C(16)	1.456(8)
O(18')-C(18')	1.426(7)
O(18')-H(18')	0.8400
O(11')-C(16')	1.447(9)
O(11')-C(11')	1.449(7)
C(18)-C(4)	1.557(9)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(4)-C(3)	1.525(10)
C(4)-C(19)	1.533(9)
C(4)-C(5)	1.556(8)
C(5)-C(6)	1.526(9)
C(5)-C(10)	1.578(9)
C(5)-H(5)	1.0000
C(6)-C(7)	1.541(8)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.532(9)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(14)	1.544(9)
C(8)-C(15)	1.545(8)

C(8)-C(9)	1.567(10)
C(15)-C(16)	1.543(9)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.506(8)
C(16)-C(13)	1.568(9)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(3)-C(2)	1.531(9)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(2)-C(1)	1.539(8)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(1)-C(10)	1.524(10)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(10)-C(20)	1.534(8)
C(10)-C(9)	1.569(8)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(9)-C(11)	1.551(9)
C(9)-H(9)	1.0000
C(14)-C(13)	1.554(8)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(13)-C(12)	1.518(9)
C(13)-H(13)	1.0000
C(11)-C(12)	1.525(9)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(18')-C(4')	1.539(9)

C(18')-H(18C)	0.9900
C(18')-H(18D)	0.9900
C(4')-C(3')	1.525(10)
C(4')-C(19')	1.534(9)
C(4')-C(5')	1.550(8)
C(5')-C(6')	1.526(9)
C(5')-C(10')	1.566(9)
C(5')-H(5')	1.0000
C(6')-C(7')	1.527(8)
C(6')-H(6'1)	0.9900
C(6')-H(6'2)	0.9900
C(7')-C(8')	1.525(9)
C(7')-H(7'1)	0.9900
C(7')-H(7'2)	0.9900
C(8')-C(14')	1.541(9)
C(8')-C(15')	1.544(8)
C(8')-C(9')	1.564(9)
C(15')-C(16')	1.533(9)
C(15')-H(15C)	0.9900
C(15')-H(15D)	0.9900
C(16')-C(17')	1.513(8)
C(16')-C(13')	1.576(9)
C(17')-H(17D)	0.9800
C(17')-H(17E)	0.9800
C(17')-H(17F)	0.9800
C(11')-C(12')	1.525(9)
C(11')-C(9')	1.546(9)
C(11')-H(11')	1.0000
C(9')-C(10')	1.574(8)
C(9')-H(9')	1.0000
C(10')-C(20')	1.528(8)
C(10')-C(1')	1.531(10)
C(20')-H(20D)	0.9800
C(20')-H(20E)	0.9800
C(20')-H(20F)	0.9800
C(1')-C(2')	1.532(8)
C(1')-H(1'1)	0.9900
C(1')-H(1'2)	0.9900

C(2')-C(3')	1.525(9)
C(2')-H(2'1)	0.9900
C(2')-H(2'2)	0.9900
C(3')-H(3'1)	0.9900
C(3')-H(3'2)	0.9900
C(12')-C(13')	1.512(9)
C(12')-H(12C)	0.9900
C(12')-H(12D)	0.9900
C(13')-C(14')	1.534(9)
C(13')-H(13')	1.0000
C(14')-H(14C)	0.9900
C(14')-H(14D)	0.9900
C(19')-H(19D)	0.9800
C(19')-H(19E)	0.9800
C(19')-H(19F)	0.9800

C(18)-O(18)-H(18)	109.5
C(11)-O(11)-C(16)	104.1(4)
C(18')-O(18')-H(18')	109.5
C(16')-O(11')-C(11')	104.3(5)
O(18)-C(18)-C(4)	113.0(5)
O(18)-C(18)-H(18A)	109.0
C(4)-C(18)-H(18A)	109.0
O(18)-C(18)-H(18B)	109.0
C(4)-C(18)-H(18B)	109.0
H(18A)-C(18)-H(18B)	107.8
C(3)-C(4)-C(19)	110.1(5)
C(3)-C(4)-C(5)	110.5(5)
C(19)-C(4)-C(5)	114.3(5)
C(3)-C(4)-C(18)	106.6(5)
C(19)-C(4)-C(18)	105.5(5)
C(5)-C(4)-C(18)	109.3(5)
C(6)-C(5)-C(4)	115.1(5)
C(6)-C(5)-C(10)	110.7(5)
C(4)-C(5)-C(10)	116.5(5)
C(6)-C(5)-H(5)	104.3
C(4)-C(5)-H(5)	104.3
C(10)-C(5)-H(5)	104.3

C(5)-C(6)-C(7)	109.8(5)
C(5)-C(6)-H(6A)	109.7
C(7)-C(6)-H(6A)	109.7
C(5)-C(6)-H(6B)	109.7
C(7)-C(6)-H(6B)	109.7
H(6A)-C(6)-H(6B)	108.2
C(8)-C(7)-C(6)	111.8(5)
C(8)-C(7)-H(7A)	109.3
C(6)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7B)	109.3
C(6)-C(7)-H(7B)	109.3
H(7A)-C(7)-H(7B)	107.9
C(7)-C(8)-C(14)	114.4(5)
C(7)-C(8)-C(15)	110.8(5)
C(14)-C(8)-C(15)	97.4(5)
C(7)-C(8)-C(9)	112.5(5)
C(14)-C(8)-C(9)	112.7(5)
C(15)-C(8)-C(9)	107.9(5)
C(16)-C(15)-C(8)	101.0(5)
C(16)-C(15)-H(15A)	111.6
C(8)-C(15)-H(15A)	111.6
C(16)-C(15)-H(15B)	111.6
C(8)-C(15)-H(15B)	111.6
H(15A)-C(15)-H(15B)	109.4
O(11)-C(16)-C(17)	108.7(5)
O(11)-C(16)-C(15)	106.1(5)
C(17)-C(16)-C(15)	116.1(5)
O(11)-C(16)-C(13)	104.4(5)
C(17)-C(16)-C(13)	116.7(5)
C(15)-C(16)-C(13)	103.9(5)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(4)-C(3)-C(2)	114.5(5)
C(4)-C(3)-H(3A)	108.6

C(2)-C(3)-H(3A)	108.6
C(4)-C(3)-H(3B)	108.6
C(2)-C(3)-H(3B)	108.6
H(3A)-C(3)-H(3B)	107.6
C(3)-C(2)-C(1)	110.4(5)
C(3)-C(2)-H(2A)	109.6
C(1)-C(2)-H(2A)	109.6
C(3)-C(2)-H(2B)	109.6
C(1)-C(2)-H(2B)	109.6
H(2A)-C(2)-H(2B)	108.1
C(10)-C(1)-C(2)	113.7(5)
C(10)-C(1)-H(1A)	108.8
C(2)-C(1)-H(1A)	108.8
C(10)-C(1)-H(1B)	108.8
C(2)-C(1)-H(1B)	108.8
H(1A)-C(1)-H(1B)	107.7
C(1)-C(10)-C(20)	109.0(5)
C(1)-C(10)-C(9)	108.5(5)
C(20)-C(10)-C(9)	113.1(5)
C(1)-C(10)-C(5)	107.6(5)
C(20)-C(10)-C(5)	112.7(5)
C(9)-C(10)-C(5)	105.7(5)
C(10)-C(20)-H(20A)	109.5
C(10)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(10)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(11)-C(9)-C(8)	108.7(5)
C(11)-C(9)-C(10)	116.8(5)
C(8)-C(9)-C(10)	117.1(5)
C(11)-C(9)-H(9)	104.1
C(8)-C(9)-H(9)	104.1
C(10)-C(9)-H(9)	104.1
C(8)-C(14)-C(13)	101.0(5)
C(8)-C(14)-H(14A)	111.6
C(13)-C(14)-H(14A)	111.6
C(8)-C(14)-H(14B)	111.6

C(13)-C(14)-H(14B)	111.6
H(14A)-C(14)-H(14B)	109.4
C(12)-C(13)-C(14)	108.3(5)
C(12)-C(13)-C(16)	102.9(5)
C(14)-C(13)-C(16)	104.2(5)
C(12)-C(13)-H(13)	113.5
C(14)-C(13)-H(13)	113.5
C(16)-C(13)-H(13)	113.5
O(11)-C(11)-C(12)	99.6(5)
O(11)-C(11)-C(9)	107.2(5)
C(12)-C(11)-C(9)	115.4(6)
O(11)-C(11)-H(11)	111.3
C(12)-C(11)-H(11)	111.3
C(9)-C(11)-H(11)	111.3
C(13)-C(12)-C(11)	99.4(5)
C(13)-C(12)-H(12A)	111.9
C(11)-C(12)-H(12A)	111.9
C(13)-C(12)-H(12B)	111.9
C(11)-C(12)-H(12B)	111.9
H(12A)-C(12)-H(12B)	109.6
C(4)-C(19)-H(19A)	109.5
C(4)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(4)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(18')-C(18')-C(4')	112.1(5)
O(18')-C(18')-H(18C)	109.2
C(4')-C(18')-H(18C)	109.2
O(18')-C(18')-H(18D)	109.2
C(4')-C(18')-H(18D)	109.2
H(18C)-C(18')-H(18D)	107.9
C(3')-C(4')-C(19')	109.7(5)
C(3')-C(4')-C(18')	106.9(5)
C(19')-C(4')-C(18')	104.7(5)
C(3')-C(4')-C(5')	110.1(5)
C(19')-C(4')-C(5')	115.1(5)
C(18')-C(4')-C(5')	109.9(5)

C(6')-C(5')-C(4')	115.0(5)
C(6')-C(5')-C(10')	110.5(5)
C(4')-C(5')-C(10')	117.0(5)
C(6')-C(5')-H(5')	104.2
C(4')-C(5')-H(5')	104.2
C(10')-C(5')-H(5')	104.2
C(5')-C(6')-C(7')	110.2(5)
C(5')-C(6')-H(6'1)	109.6
C(7')-C(6')-H(6'1)	109.6
C(5')-C(6')-H(6'2)	109.6
C(7')-C(6')-H(6'2)	109.6
H(6'1)-C(6')-H(6'2)	108.1
C(8')-C(7')-C(6')	113.3(5)
C(8')-C(7')-H(7'1)	108.9
C(6')-C(7')-H(7'1)	108.9
C(8')-C(7')-H(7'2)	108.9
C(6')-C(7')-H(7'2)	108.9
H(7'1)-C(7')-H(7'2)	107.7
C(7')-C(8')-C(14')	115.4(5)
C(7')-C(8')-C(15')	111.2(5)
C(14')-C(8')-C(15')	97.1(5)
C(7')-C(8')-C(9')	112.2(5)
C(14')-C(8')-C(9')	112.3(5)
C(15')-C(8')-C(9')	107.5(5)
C(16')-C(15')-C(8')	101.3(5)
C(16')-C(15')-H(15C)	111.5
C(8')-C(15')-H(15C)	111.5
C(16')-C(15')-H(15D)	111.5
C(8')-C(15')-H(15D)	111.5
H(15C)-C(15')-H(15D)	109.3
O(11')-C(16')-C(17')	109.0(5)
O(11')-C(16')-C(15')	106.3(5)
C(17')-C(16')-C(15')	116.4(6)
O(11')-C(16')-C(13')	104.3(5)
C(17')-C(16')-C(13')	116.1(5)
C(15')-C(16')-C(13')	103.7(5)
C(16')-C(17')-H(17D)	109.5
C(16')-C(17')-H(17E)	109.5

H(17D)-C(17')-H(17E)	109.5
C(16')-C(17')-H(17F)	109.5
H(17D)-C(17')-H(17F)	109.5
H(17E)-C(17')-H(17F)	109.5
O(11')-C(11')-C(12')	98.9(5)
O(11')-C(11')-C(9')	107.2(5)
C(12')-C(11')-C(9')	115.6(6)
O(11')-C(11')-H(11')	111.5
C(12')-C(11')-H(11')	111.5
C(9')-C(11')-H(11')	111.5
C(11')-C(9')-C(8')	108.9(5)
C(11')-C(9')-C(10')	116.9(5)
C(8')-C(9')-C(10')	116.2(5)
C(11')-C(9')-H(9')	104.4
C(8')-C(9')-H(9')	104.4
C(10')-C(9')-H(9')	104.4
C(20')-C(10')-C(1')	108.5(5)
C(20')-C(10')-C(5')	112.3(5)
C(1')-C(10')-C(5')	108.4(5)
C(20')-C(10')-C(9')	113.7(5)
C(1')-C(10')-C(9')	108.1(5)
C(5')-C(10')-C(9')	105.6(5)
C(10')-C(20')-H(20D)	109.5
C(10')-C(20')-H(20E)	109.5
H(20D)-C(20')-H(20E)	109.5
C(10')-C(20')-H(20F)	109.5
H(20D)-C(20')-H(20F)	109.5
H(20E)-C(20')-H(20F)	109.5
C(10')-C(1')-C(2')	113.6(5)
C(10')-C(1')-H(1'1)	108.8
C(2')-C(1')-H(1'1)	108.8
C(10')-C(1')-H(1'2)	108.8
C(2')-C(1')-H(1'2)	108.8
H(1'1)-C(1')-H(1'2)	107.7
C(3')-C(2')-C(1')	110.8(5)
C(3')-C(2')-H(2'1)	109.5
C(1')-C(2')-H(2'1)	109.5
C(3')-C(2')-H(2'2)	109.5

C(1')-C(2')-H(2'2)	109.5
H(2'1)-C(2')-H(2'2)	108.1
C(2')-C(3')-C(4')	114.4(5)
C(2')-C(3')-H(3'1)	108.7
C(4')-C(3')-H(3'1)	108.7
C(2')-C(3')-H(3'2)	108.7
C(4')-C(3')-H(3'2)	108.7
H(3'1)-C(3')-H(3'2)	107.6
C(13')-C(12')-C(11')	99.7(5)
C(13')-C(12')-H(12C)	111.8
C(11')-C(12')-H(12C)	111.8
C(13')-C(12')-H(12D)	111.8
C(11')-C(12')-H(12D)	111.8
H(12C)-C(12')-H(12D)	109.6
C(12')-C(13')-C(14')	108.7(5)
C(12')-C(13')-C(16')	102.4(6)
C(14')-C(13')-C(16')	104.1(5)
C(12')-C(13')-H(13')	113.6
C(14')-C(13')-H(13')	113.6
C(16')-C(13')-H(13')	113.6
C(13')-C(14')-C(8')	101.8(5)
C(13')-C(14')-H(14C)	111.4
C(8')-C(14')-H(14C)	111.4
C(13')-C(14')-H(14D)	111.4
C(8')-C(14')-H(14D)	111.4
H(14C)-C(14')-H(14D)	109.3
C(4')-C(19')-H(19D)	109.5
C(4')-C(19')-H(19E)	109.5
H(19D)-C(19')-H(19E)	109.5
C(4')-C(19')-H(19F)	109.5
H(19D)-C(19')-H(19F)	109.5
H(19E)-C(19')-H(19F)	109.5

Symmetry transformations used to generate equivalent atoms.

Table 9: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for scopariusol D (**5**). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	1371(2)	5224(1)	9992(1)	14(1)
O(2)	-388(2)	1164(1)	8157(1)	20(1)
O(3)	5921(2)	6958(1)	9481(1)	15(1)
O(4)	-906(2)	6141(1)	9688(1)	19(1)
O(5)	3709(2)	3549(1)	10483(1)	17(1)
C(1)	-541(3)	5594(2)	10811(1)	21(1)
C(2)	-88(2)	5704(2)	10108(1)	15(1)
C(3)	2014(2)	5318(2)	9323(1)	12(1)
C(4)	2666(2)	4127(1)	9145(1)	12(1)
C(5)	2131(2)	3768(2)	8437(1)	12(1)
C(6)	248(2)	3686(2)	8426(1)	15(1)
C(7)	-416(2)	3131(2)	7805(1)	17(1)
C(8)	279(3)	1951(2)	7699(1)	17(1)
C(9)	4962(2)	5961(1)	9508(1)	14(1)
C(10)	3236(2)	6297(2)	9308(1)	14(1)
C(11)	2678(2)	4642(2)	7921(1)	15(1)
C(12)	2817(2)	2550(2)	8317(1)	13(1)
C(13)	4673(2)	2537(2)	8396(1)	16(1)
C(14)	5136(2)	2834(1)	9095(1)	15(1)
C(15)	4508(2)	3990(2)	9313(1)	13(1)
C(16)	4811(2)	4135(2)	10063(1)	14(1)
C(17)	4919(2)	5405(2)	10177(1)	14(1)
C(18)	4943(2)	5932(2)	10744(1)	19(1)
C(19)	5529(2)	4993(1)	9065(1)	13(1)
C(20)	2164(2)	1932(2)	7697(1)	15(1)
C(21)	2787(3)	2422(2)	7049(1)	20(1)
C(22)	2713(3)	685(2)	7714(1)	20(1)

Table 10: Bond lengths [Å] and angles [º] for scopariusol D (**5**).

O(1)-C(2)	1.344(2)
O(1)-C(3)	1.473(2)

O(2)-C(8)	1.429(2)
O(2)-H(2)	0.85(3)
O(3)-C(9)	1.417(2)
O(3)-H(3)	0.79(3)
O(4)-C(2)	1.207(2)
O(5)-C(16)	1.427(2)
O(5)-H(9)	0.86(3)
C(1)-C(2)	1.494(3)
C(1)-H(1)	0.9800
C(1)-H(5)	0.9800
C(1)-H(4)	0.9800
C(3)-C(10)	1.530(3)
C(3)-C(4)	1.548(2)
C(3)-H(32)	1.0000
C(4)-C(15)	1.556(2)
C(4)-C(5)	1.575(2)
C(4)-H(31)	1.0000
C(5)-C(6)	1.545(3)
C(5)-C(11)	1.546(2)
C(5)-C(12)	1.564(2)
C(6)-C(7)	1.532(3)
C(6)-H(20)	0.9900
C(6)-H(19)	0.9900
C(7)-C(8)	1.521(3)
C(7)-H(21)	0.9900
C(7)-H(22)	0.9900
C(8)-C(20)	1.544(3)
C(8)-H(23)	1.0000
C(9)-C(17)	1.521(2)
C(9)-C(10)	1.524(3)
C(9)-C(19)	1.533(2)
C(10)-H(34)	0.9900
C(10)-H(33)	0.9900
C(11)-H(7)	0.9800
C(11)-H(8)	0.9800
C(11)-H(6)	0.9800
C(12)-C(13)	1.529(3)
C(12)-C(20)	1.560(2)

C(12)-H(30)	1.0000
C(13)-C(14)	1.525(3)
C(13)-H(17)	0.9900
C(13)-H(18)	0.9900
C(14)-C(15)	1.526(2)
C(14)-H(16)	0.9900
C(14)-H(15)	0.9900
C(15)-C(19)	1.536(2)
C(15)-C(16)	1.567(2)
C(16)-C(17)	1.521(2)
C(16)-H(12)	1.0000
C(17)-C(18)	1.320(3)
C(18)-H(11)	0.9500
C(18)-H(10)	0.9500
C(19)-H(13)	0.9900
C(19)-H(14)	0.9900
C(20)-C(21)	1.538(3)
C(20)-C(22)	1.540(3)
C(21)-H(24)	0.9800
C(21)-H(26)	0.9800
C(21)-H(25)	0.9800
C(22)-H(29)	0.9800
C(22)-H(27)	0.9800
C(22)-H(28)	0.9800
C(2)-O(1)-C(3)	116.88(14)
C(8)-O(2)-H(2)	111.6(18)
C(9)-O(3)-H(3)	106.7(19)
C(16)-O(5)-H(9)	105.5(17)
C(2)-C(1)-H(1)	109.5
C(2)-C(1)-H(5)	109.5
H(1)-C(1)-H(5)	109.5
C(2)-C(1)-H(4)	109.5
H(1)-C(1)-H(4)	109.5
H(5)-C(1)-H(4)	109.5
O(4)-C(2)-O(1)	123.19(17)
O(4)-C(2)-C(1)	125.98(18)
O(1)-C(2)-C(1)	110.82(16)
O(1)-C(3)-C(10)	108.02(14)

O(1)-C(3)-C(4)	105.96(13)
C(10)-C(3)-C(4)	117.17(15)
O(1)-C(3)-H(32)	108.5
C(10)-C(3)-H(32)	108.5
C(4)-C(3)-H(32)	108.5
C(3)-C(4)-C(15)	112.09(15)
C(3)-C(4)-C(5)	111.47(14)
C(15)-C(4)-C(5)	116.49(15)
C(3)-C(4)-H(31)	105.2
C(15)-C(4)-H(31)	105.2
C(5)-C(4)-H(31)	105.2
C(6)-C(5)-C(11)	108.68(15)
C(6)-C(5)-C(12)	107.39(15)
C(11)-C(5)-C(12)	113.70(15)
C(6)-C(5)-C(4)	108.01(15)
C(11)-C(5)-C(4)	111.77(14)
C(12)-C(5)-C(4)	107.06(14)
C(7)-C(6)-C(5)	113.23(16)
C(7)-C(6)-H(20)	108.9
C(5)-C(6)-H(20)	108.9
C(7)-C(6)-H(19)	108.9
C(5)-C(6)-H(19)	108.9
H(20)-C(6)-H(19)	107.7
C(8)-C(7)-C(6)	112.24(15)
C(8)-C(7)-H(21)	109.2
C(6)-C(7)-H(21)	109.2
C(8)-C(7)-H(22)	109.2
C(6)-C(7)-H(22)	109.2
H(21)-C(7)-H(22)	107.9
O(2)-C(8)-C(7)	111.00(16)
O(2)-C(8)-C(20)	111.94(16)
C(7)-C(8)-C(20)	112.86(15)
O(2)-C(8)-H(23)	106.9
C(7)-C(8)-H(23)	106.9
C(20)-C(8)-H(23)	106.9
O(3)-C(9)-C(17)	114.09(15)
O(3)-C(9)-C(10)	106.66(14)
C(17)-C(9)-C(10)	109.53(15)

O(3)-C(9)-C(19)	115.36(15)
C(17)-C(9)-C(19)	102.66(14)
C(10)-C(9)-C(19)	108.37(15)
C(9)-C(10)-C(3)	113.86(15)
C(9)-C(10)-H(34)	108.8
C(3)-C(10)-H(34)	108.8
C(9)-C(10)-H(33)	108.8
C(3)-C(10)-H(33)	108.8
H(34)-C(10)-H(33)	107.7
C(5)-C(11)-H(7)	109.5
C(5)-C(11)-H(8)	109.5
H(7)-C(11)-H(8)	109.5
C(5)-C(11)-H(6)	109.5
H(7)-C(11)-H(6)	109.5
H(8)-C(11)-H(6)	109.5
C(13)-C(12)-C(20)	114.98(16)
C(13)-C(12)-C(5)	110.50(15)
C(20)-C(12)-C(5)	115.88(15)
C(13)-C(12)-H(30)	104.7
C(20)-C(12)-H(30)	104.7
C(5)-C(12)-H(30)	104.7
C(14)-C(13)-C(12)	110.13(15)
C(14)-C(13)-H(17)	109.6
C(12)-C(13)-H(17)	109.6
C(14)-C(13)-H(18)	109.6
C(12)-C(13)-H(18)	109.6
H(17)-C(13)-H(18)	108.1
C(13)-C(14)-C(15)	113.44(14)
C(13)-C(14)-H(16)	108.9
C(15)-C(14)-H(16)	108.9
C(13)-C(14)-H(15)	108.9
C(15)-C(14)-H(15)	108.9
H(16)-C(14)-H(15)	107.7
C(14)-C(15)-C(19)	114.17(15)
C(14)-C(15)-C(4)	110.77(15)
C(19)-C(15)-C(4)	112.01(14)
C(14)-C(15)-C(16)	109.38(14)
C(19)-C(15)-C(16)	98.88(14)

C(4)-C(15)-C(16)	111.06(15)
O(5)-C(16)-C(17)	114.98(15)
O(5)-C(16)-C(15)	116.11(15)
C(17)-C(16)-C(15)	105.55(14)
O(5)-C(16)-H(12)	106.5
C(17)-C(16)-H(12)	106.5
C(15)-C(16)-H(12)	106.5
C(18)-C(17)-C(16)	127.00(17)
C(18)-C(17)-C(9)	126.22(16)
C(16)-C(17)-C(9)	106.77(14)
C(17)-C(18)-H(11)	120.0
C(17)-C(18)-H(10)	120.0
H(11)-C(18)-H(10)	120.0
C(9)-C(19)-C(15)	102.35(14)
C(9)-C(19)-H(13)	111.3
C(15)-C(19)-H(13)	111.3
C(9)-C(19)-H(14)	111.3
C(15)-C(19)-H(14)	111.3
H(13)-C(19)-H(14)	109.2
C(21)-C(20)-C(22)	106.36(15)
C(21)-C(20)-C(8)	109.15(16)
C(22)-C(20)-C(8)	107.84(16)
C(21)-C(20)-C(12)	114.45(15)
C(22)-C(20)-C(12)	109.28(15)
C(8)-C(20)-C(12)	109.53(15)
C(20)-C(21)-H(24)	109.5
C(20)-C(21)-H(26)	109.5
H(24)-C(21)-H(26)	109.5
C(20)-C(21)-H(25)	109.5
H(24)-C(21)-H(25)	109.5
H(26)-C(21)-H(25)	109.5
C(20)-C(22)-H(29)	109.5
C(20)-C(22)-H(27)	109.5
H(29)-C(22)-H(27)	109.5
C(20)-C(22)-H(28)	109.5
H(29)-C(22)-H(28)	109.5
H(27)-C(22)-H(28)	109.5

Symmetry transformations used to generate equivalent atoms.