Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supplementary Information

Structurally Diverse Diterpenoids from *Isodon pharicus*

Zheng-Xi Hu,[a,b] Hou-Chao Xu,[a] Kun Hu,[a] Miao Liu,[a] Xiao-Nian Li,[a] Xing-Ren Li,[a] Xue Du,[a] Yong-Hui Zhang,*[,b] Pema-Tenzin Puno,*[,a] and Han-Dong Sun[a]

[a]*State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650201, China*

[b]*Hubei Key Laboratory of Natural Medicinal Chemistry and Resource Evaluation, School of Pharmacy, Tongji Medical College, Huazhong University of Science and Technology, Wuhan 430030, China*

* Corresponding author Tel.: (86) 871-65223616

E-mail: zhangyh@mails.tjmu.edu.cn; punopematenzin@mail.kib.ac.cn.

Contents of Supporting Information

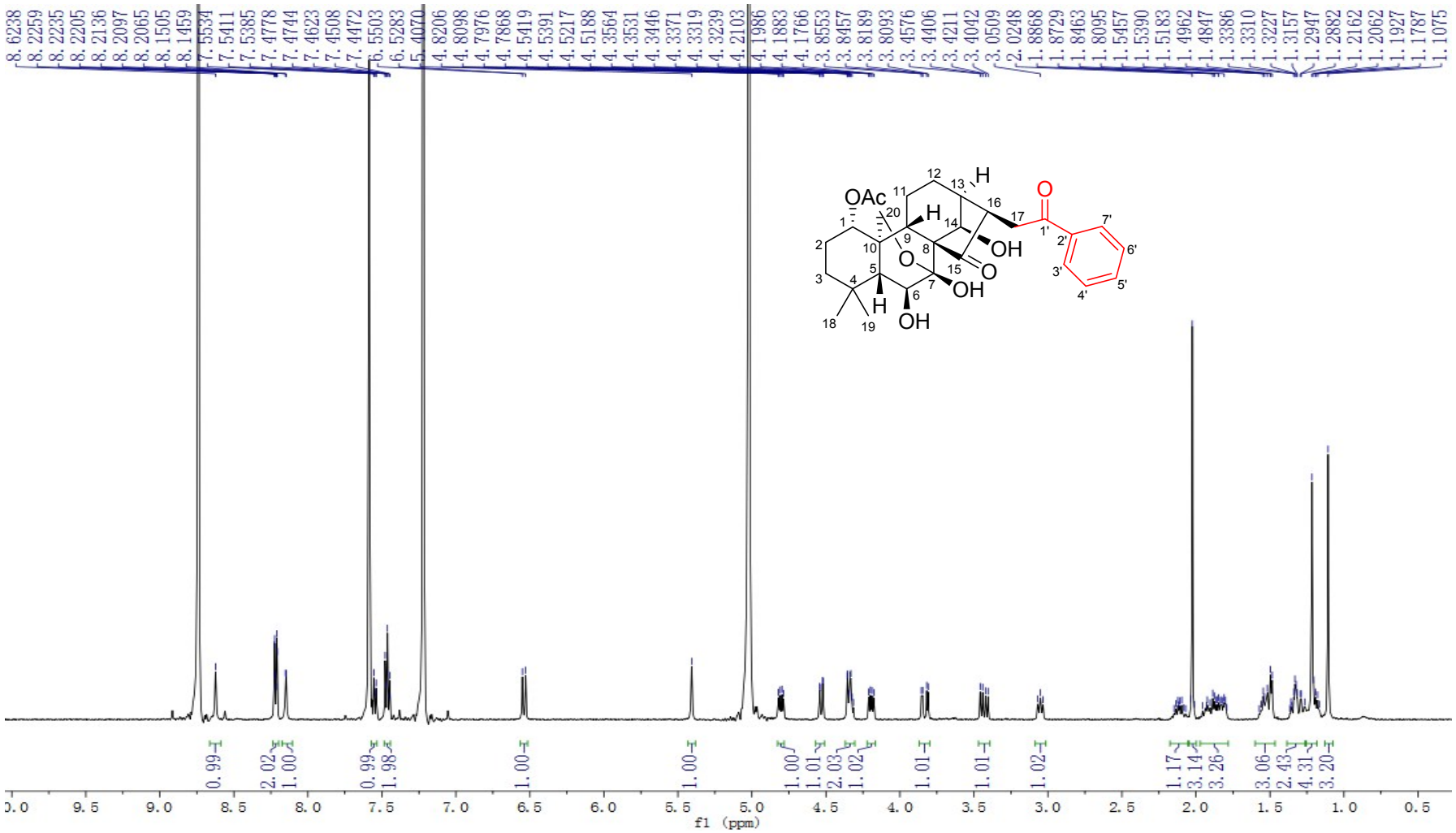


Figure S1. ^{1}H NMR spectrum of compound **1** (Recorded in pyridine-d_5)

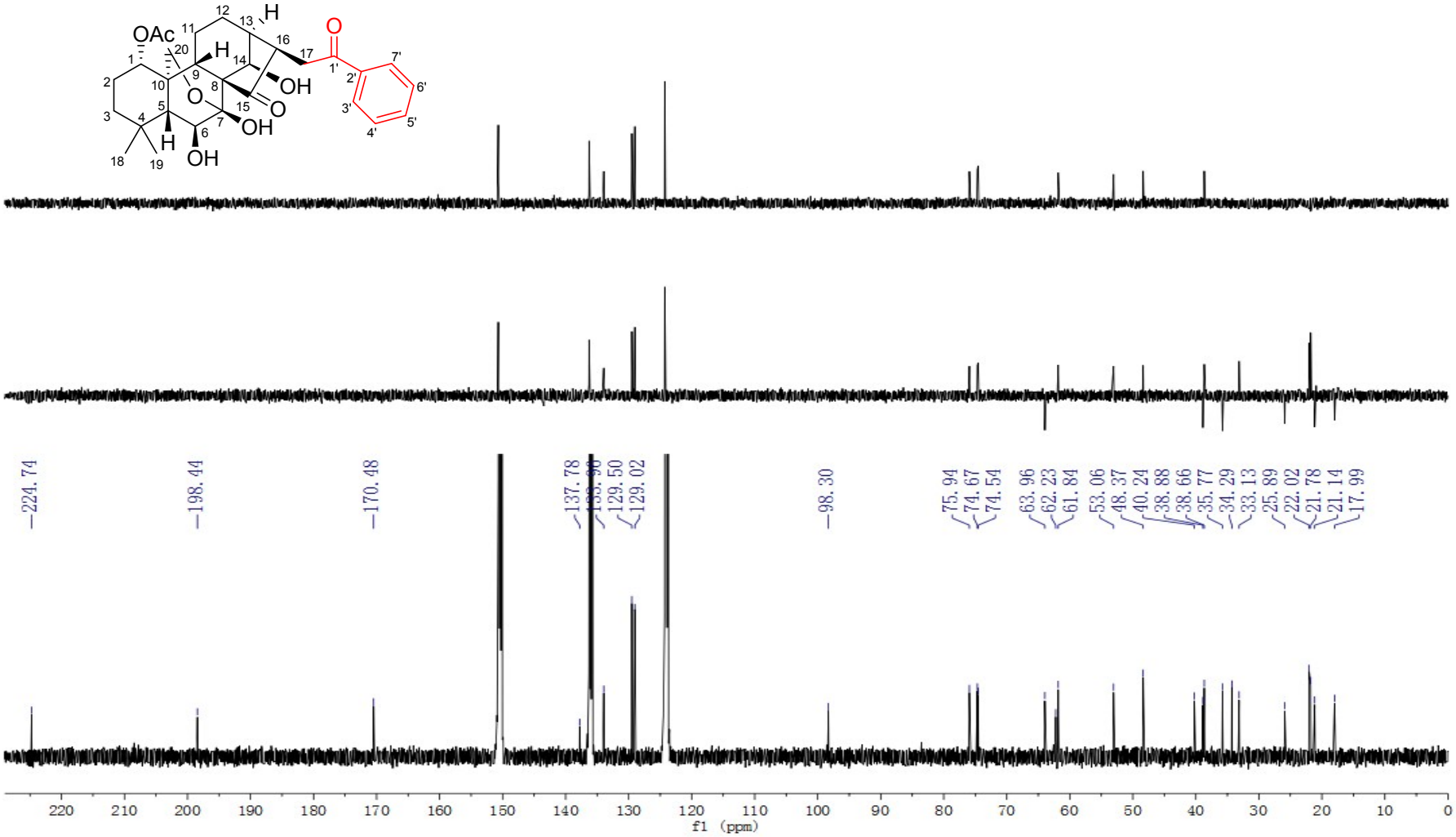


Figure S2. ^{13}C NMR spectrum of compound **1** (Recorded in pyridine-d_5)

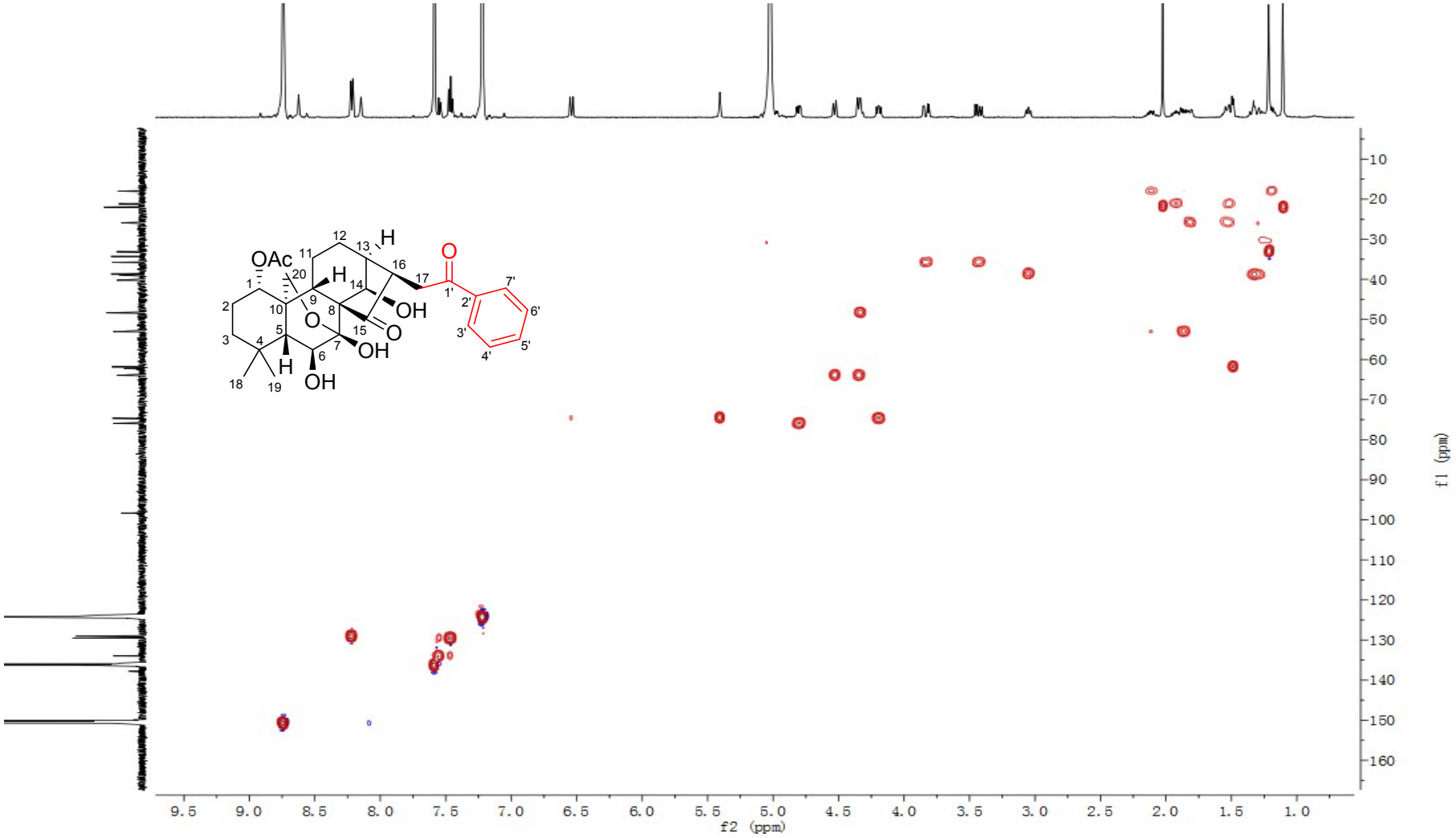


Figure S3. HSQC spectrum of compound **1** (Recorded in pyridine-d_5)

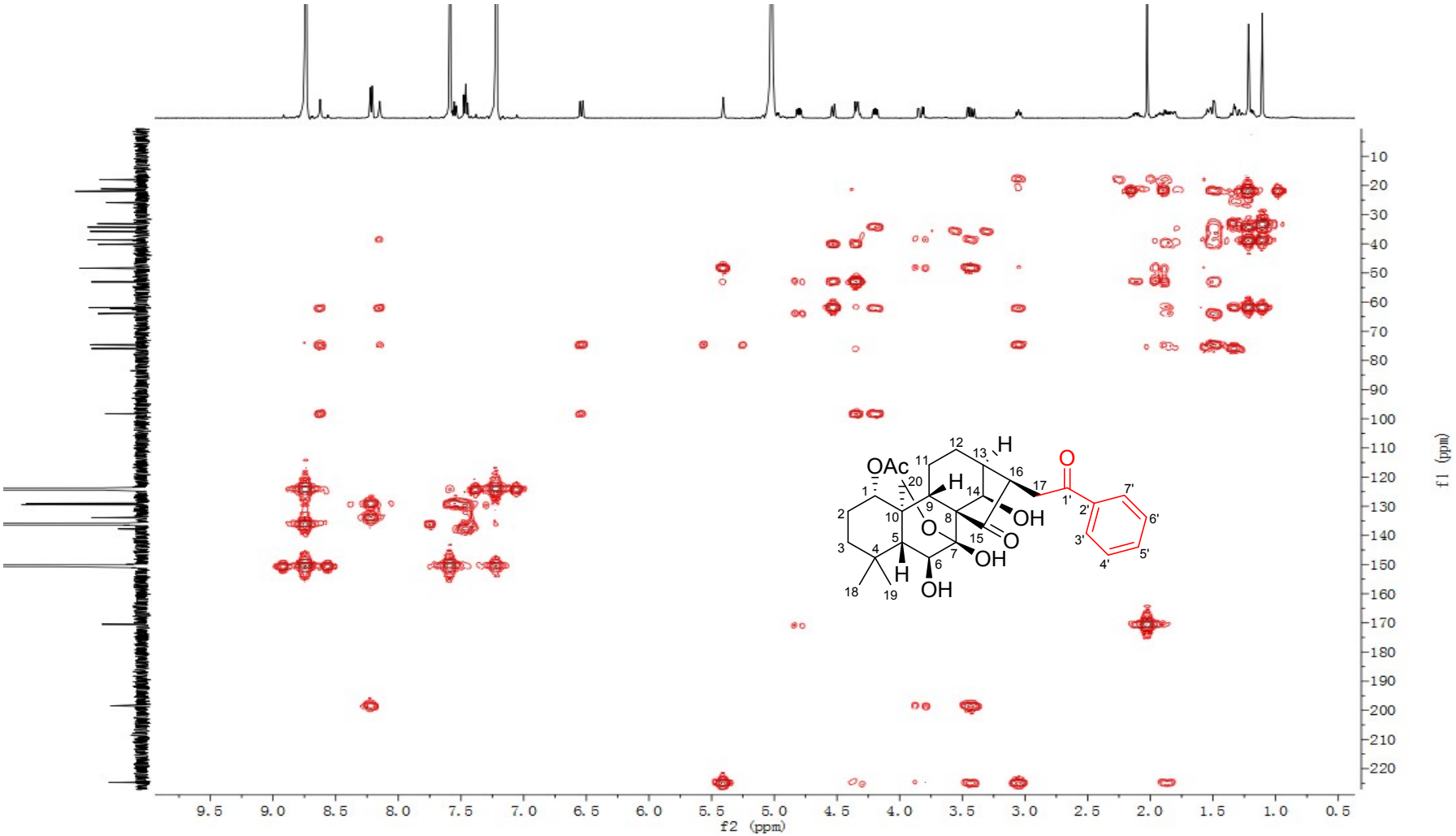


Figure S4. HMBC spectrum of compound **1** (Recorded in pyridine-d_5)

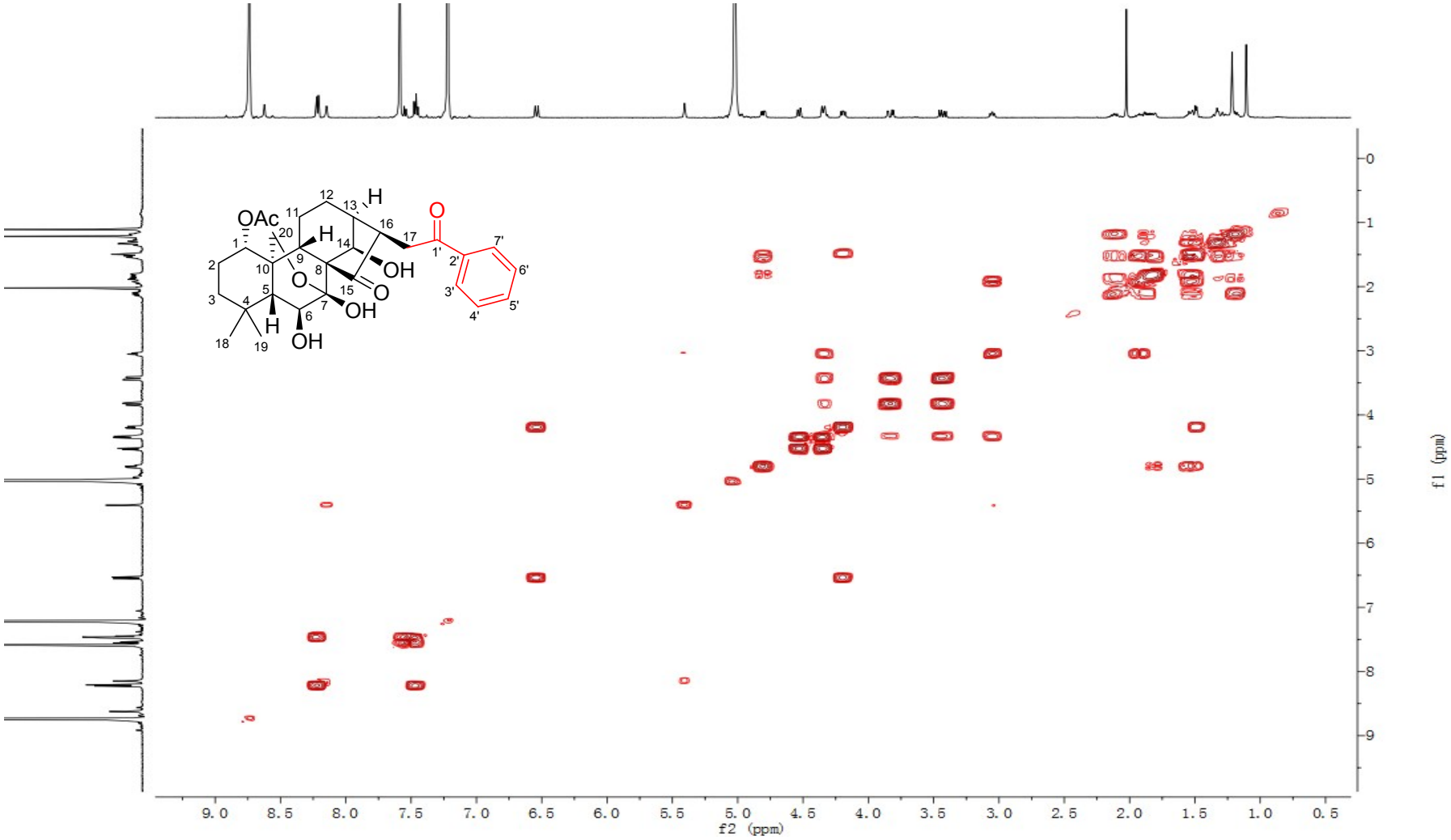


Figure S5. ^{1}H–^{1}H COSY spectrum of compound **1** (Recorded in pyridine-d_5)

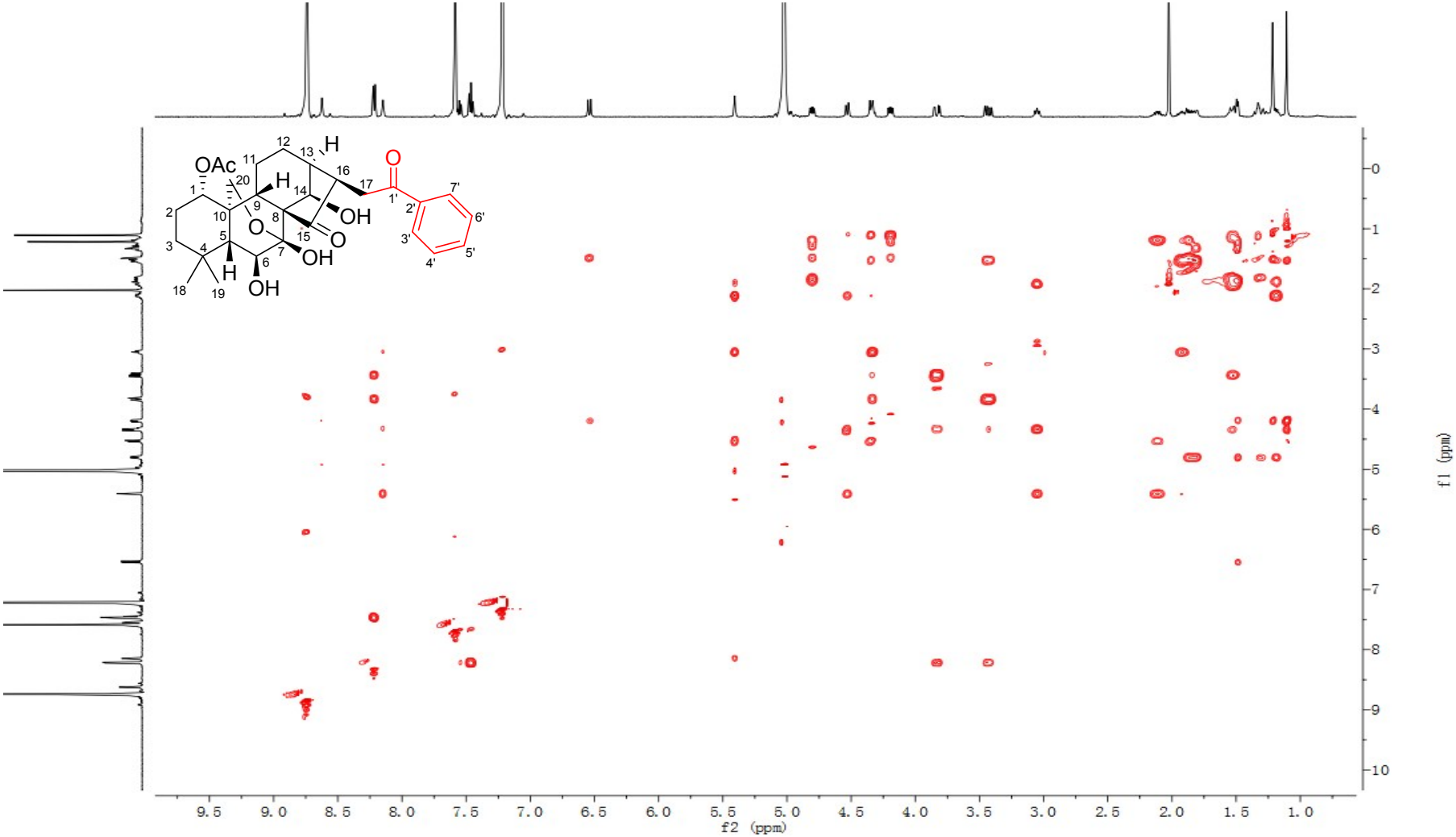


Figure S6. ROESY spectrum of compound **1** (Recorded in pyridine-d_5)

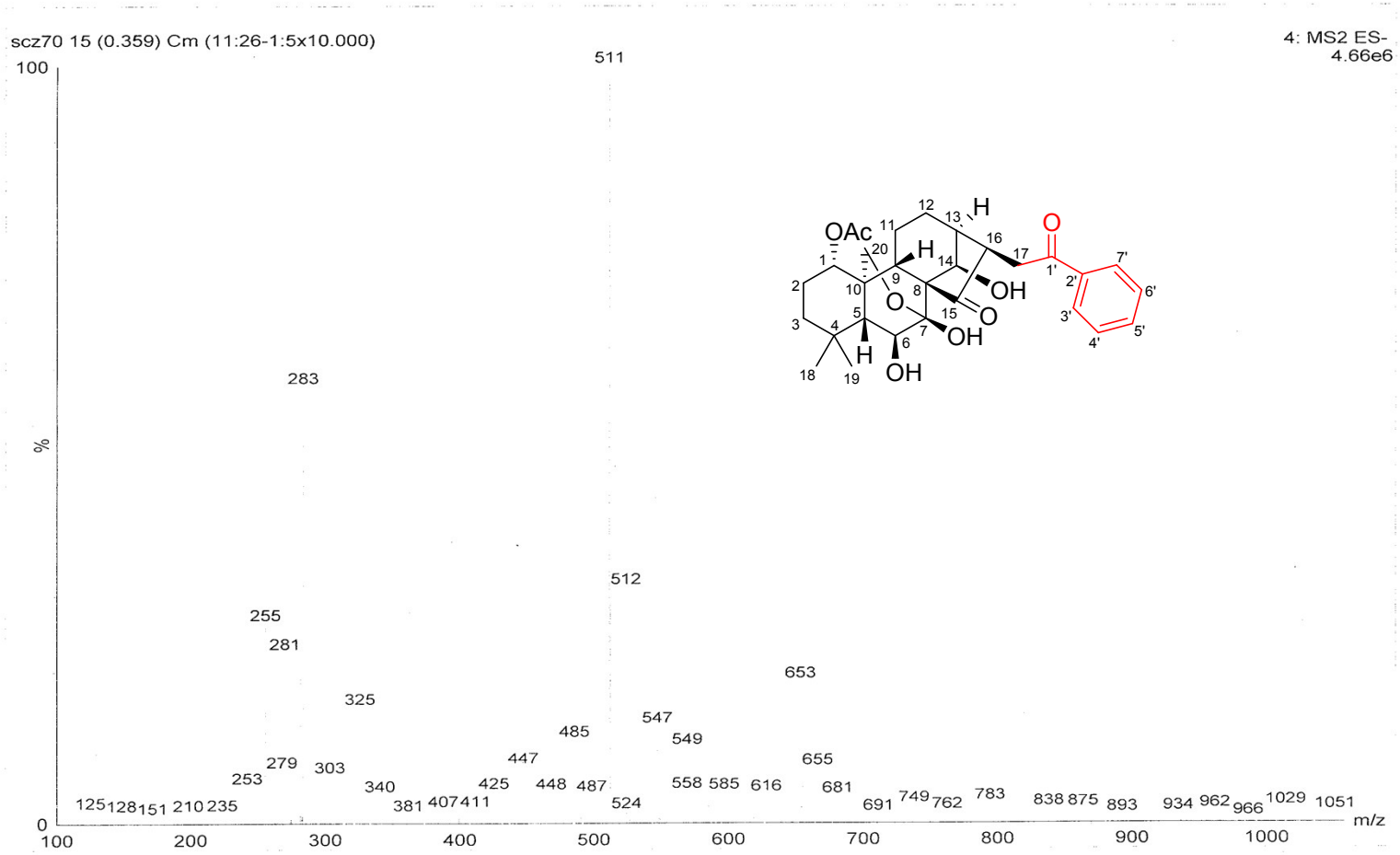


Figure S7. ESI spectrum of compound **1**

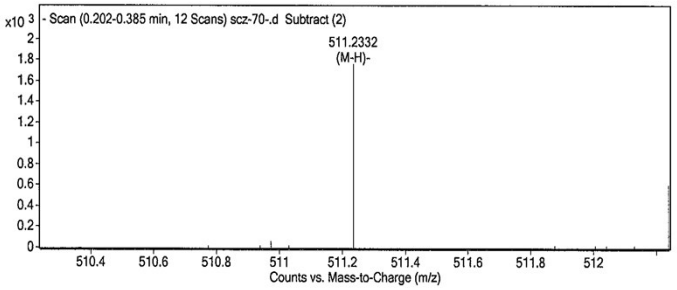
Qualitative Analysis Report

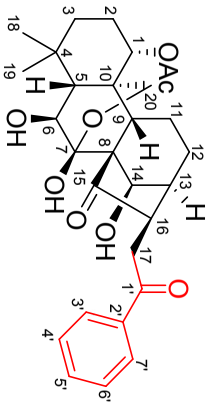
Data Filename	scz-70-.d	**Sample Name**	scz-70
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU-ESI-i.m	**Acquired Time**	11/10/2015 10:47:09 AM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

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

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI





Peak List

m/z	z	Abund	Formula	Ion
89.0245		1179.13		
253.2172		701.02		
255.233	1	4226.32		
256.2358	1	769.77		
283.2641	1	4038.11		
284.2676	1	846.9		
511.2332	1	1764.13	C29 H36 O8	(M-H)-
512.2369	1	606.14	C29 H36 O8	(M-H)-

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
C29 H36 O8	512.2410	511.2337	511.2332	0.5	0.9	12.0000

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Figure S8. HRESIMS spectrum of compound **1**

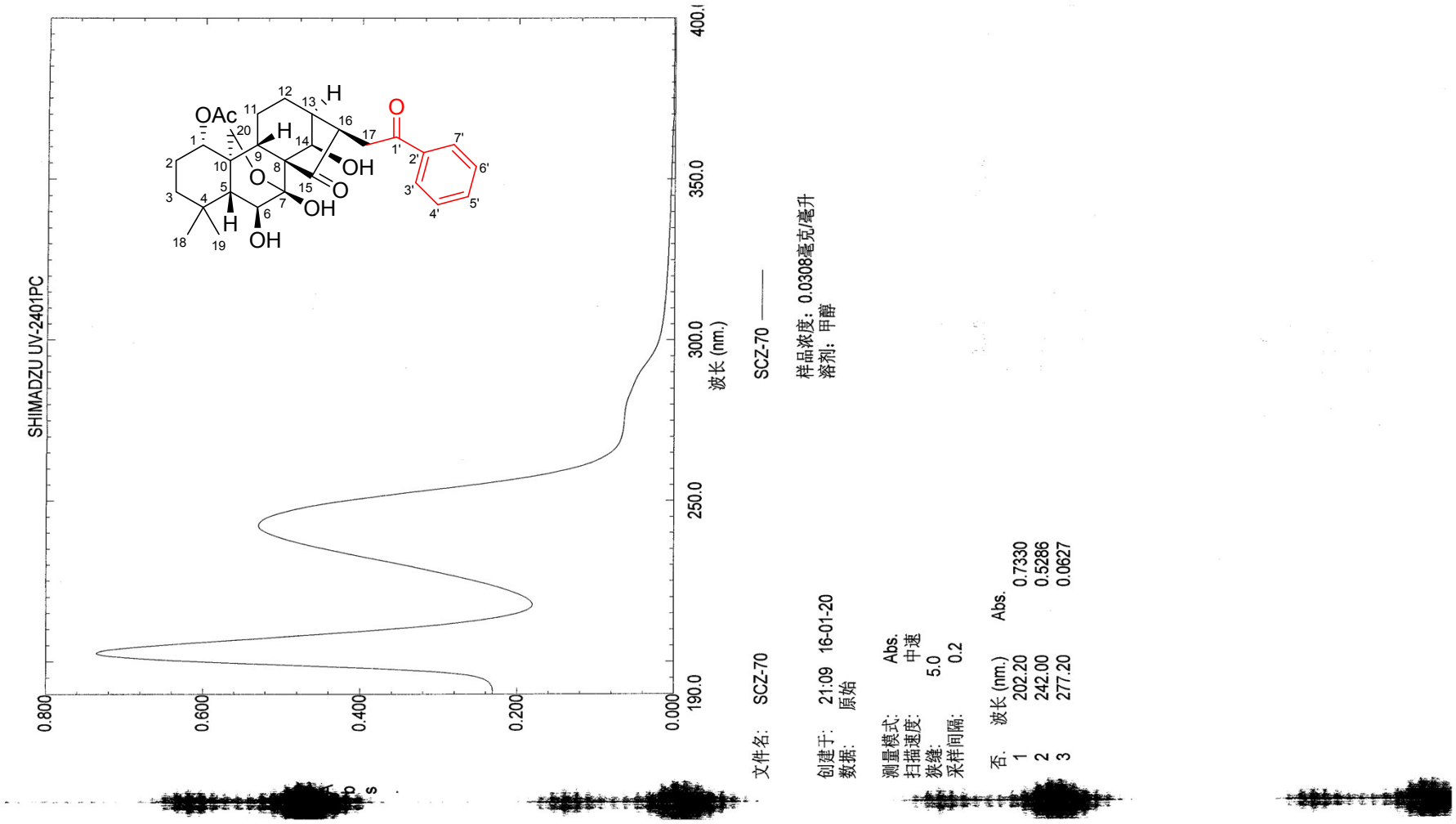
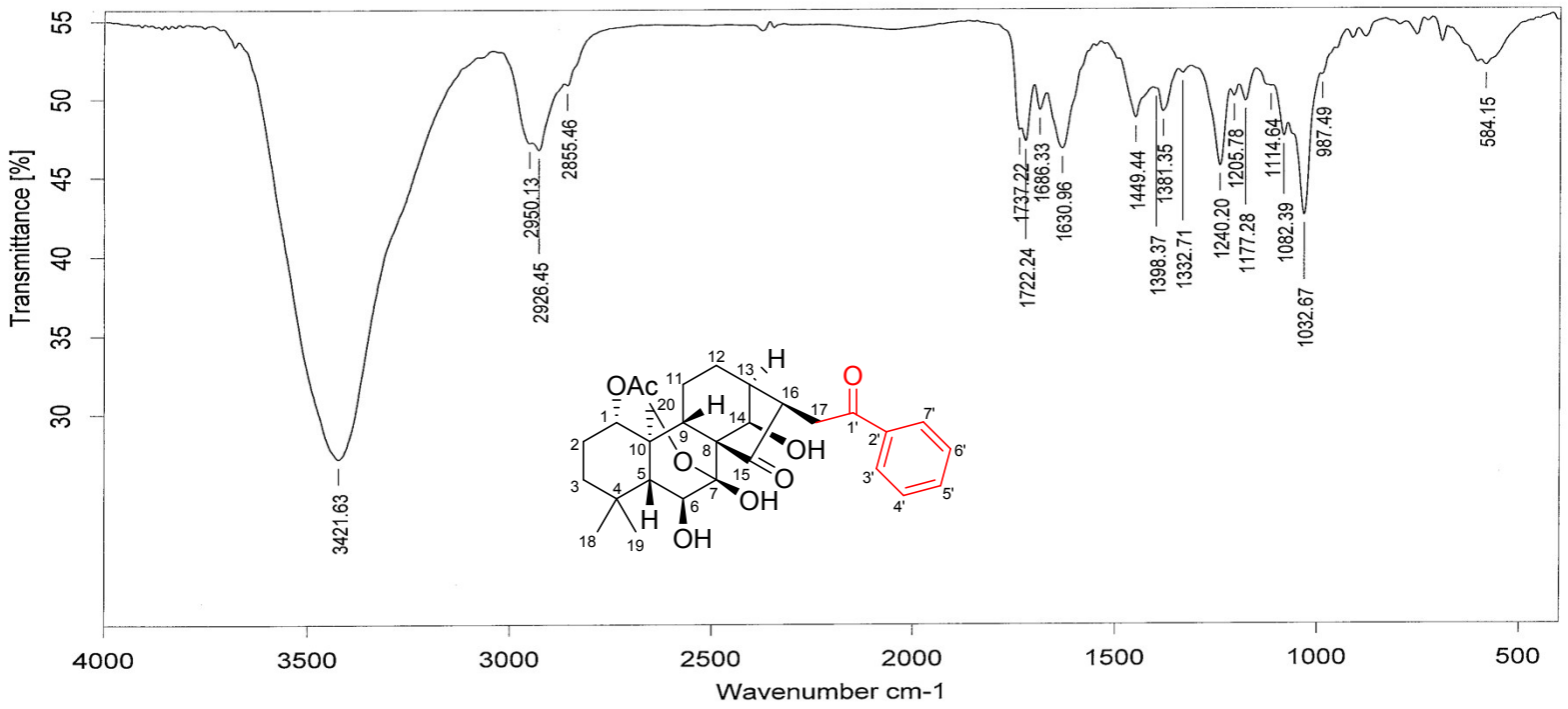


Figure S9. UV spectrum of compound **1**



Sample : scz-70	Frequency Range : 399.246 - 3996.32	Measured on : 21/01/2016	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 160121IR13	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S10. IR spectrum of compound **1**

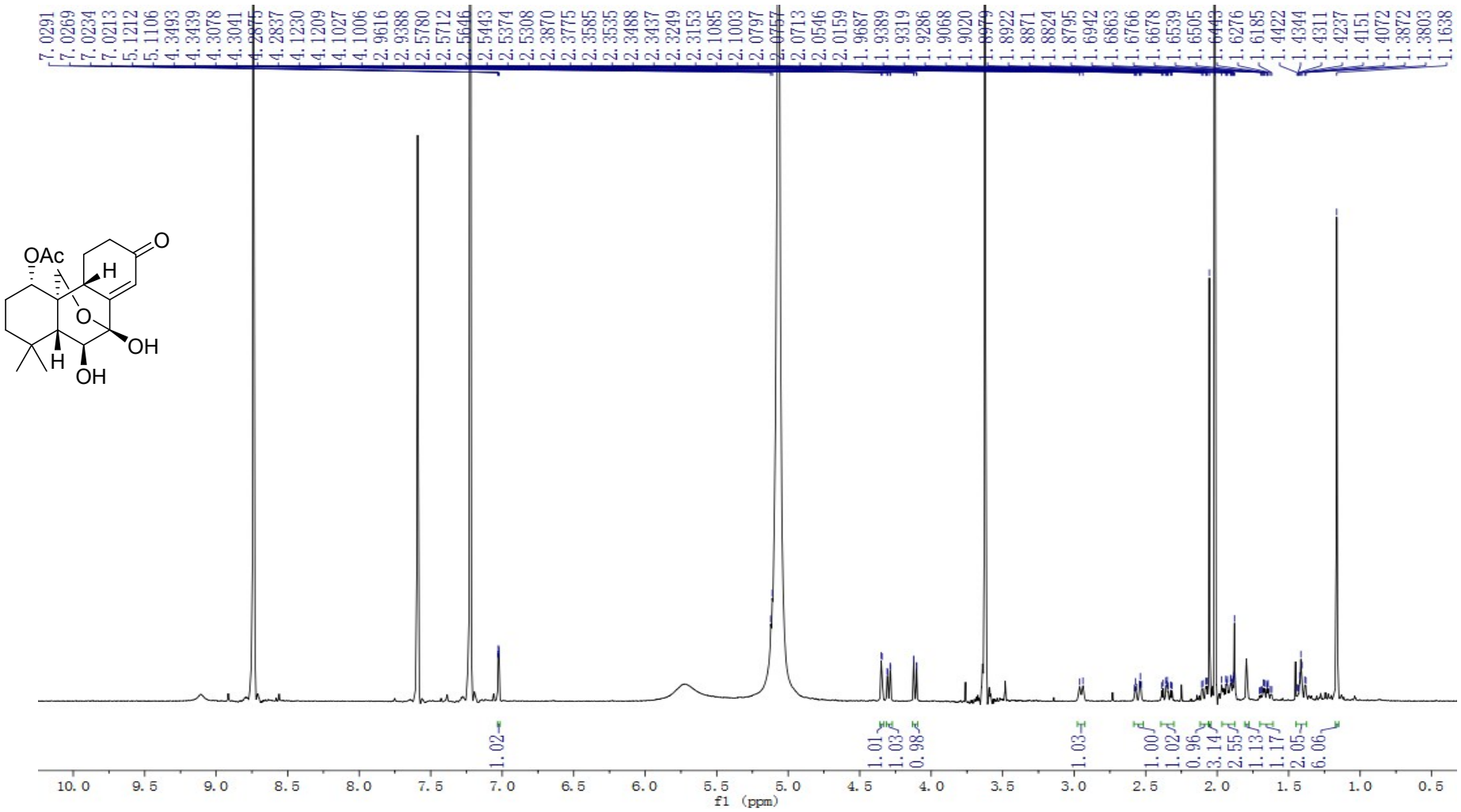


Figure S11. ^{1}H NMR spectrum of compound **2** (Recorded in pyridine-d_5)

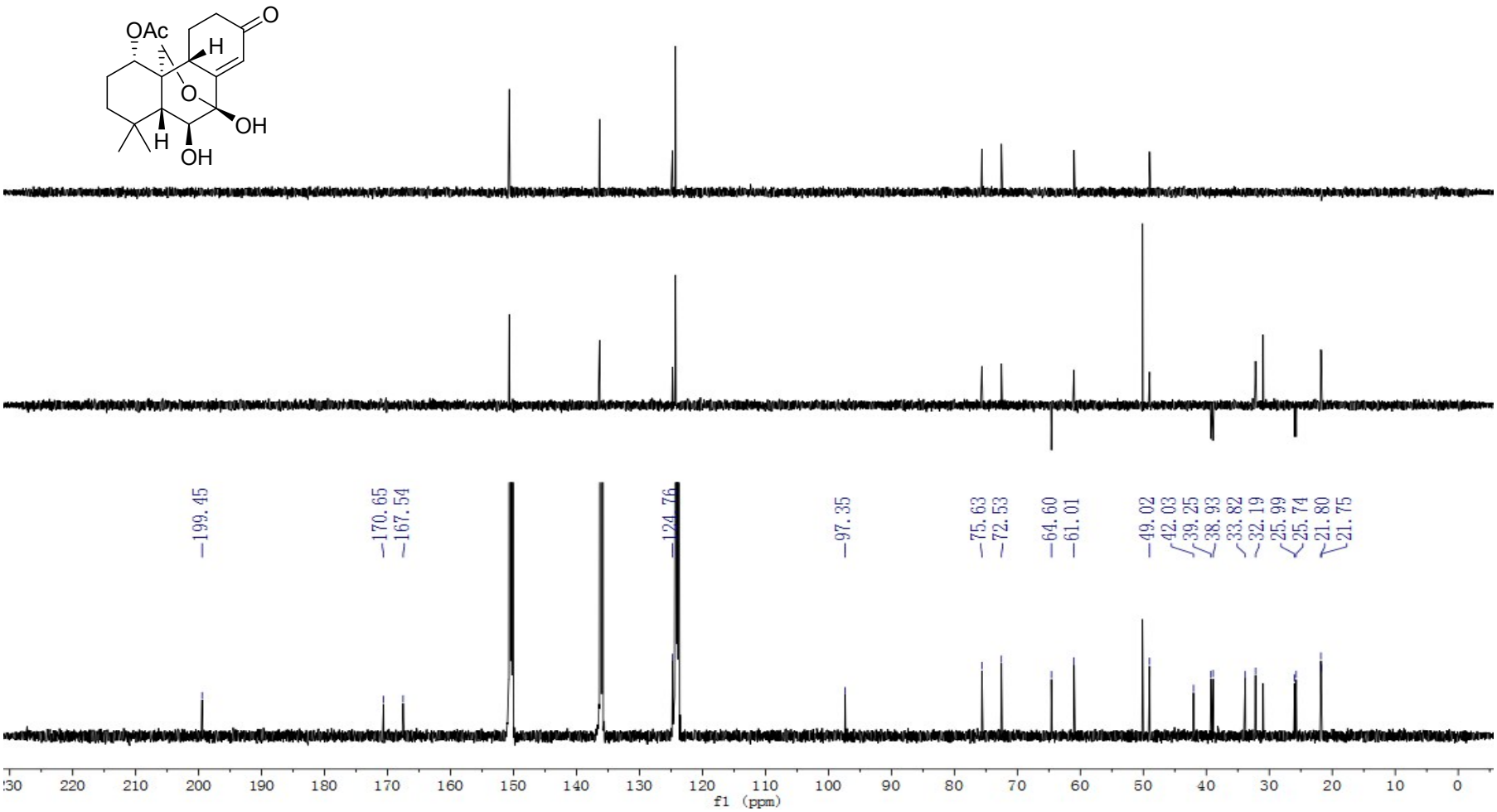


Figure S12. ^{13}C NMR spectrum of compound **2** (Recorded in pyridine-d_5)

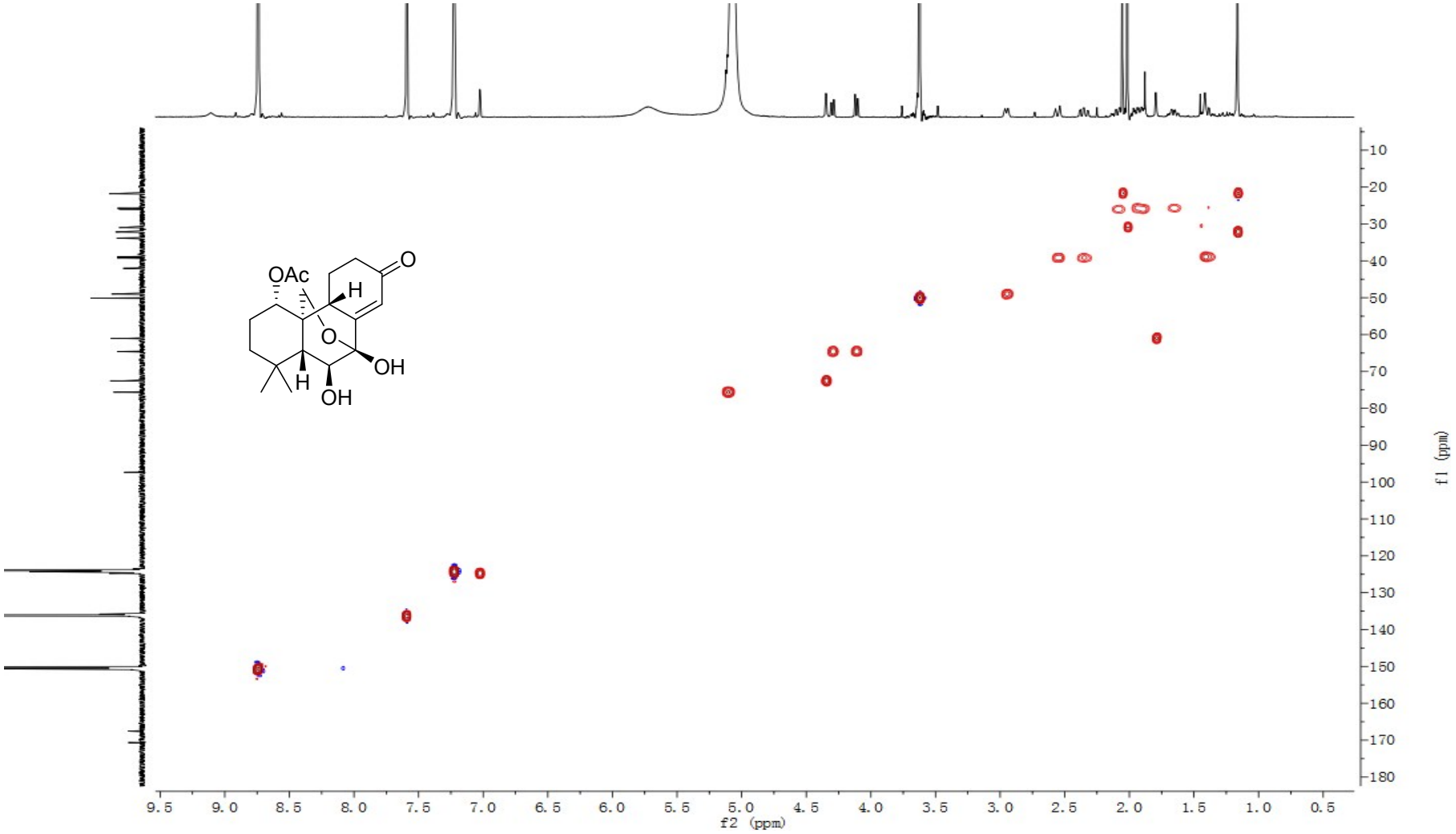


Figure S13. HSQC spectrum of compound **2** (Recorded in pyridine-d_5)

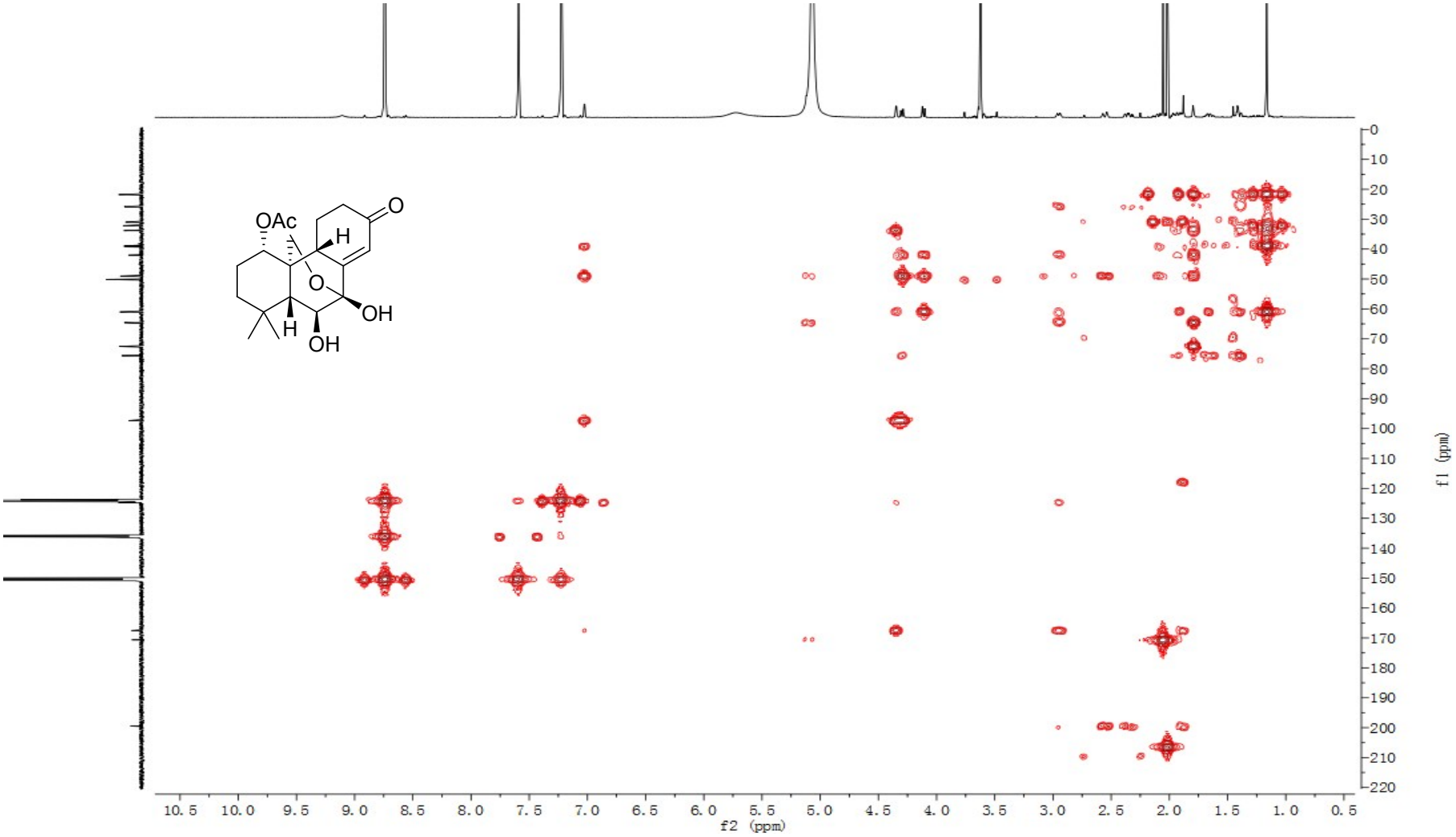


Figure S14. HMBC spectrum of compound **2** (Recorded in pyridine-d_5)

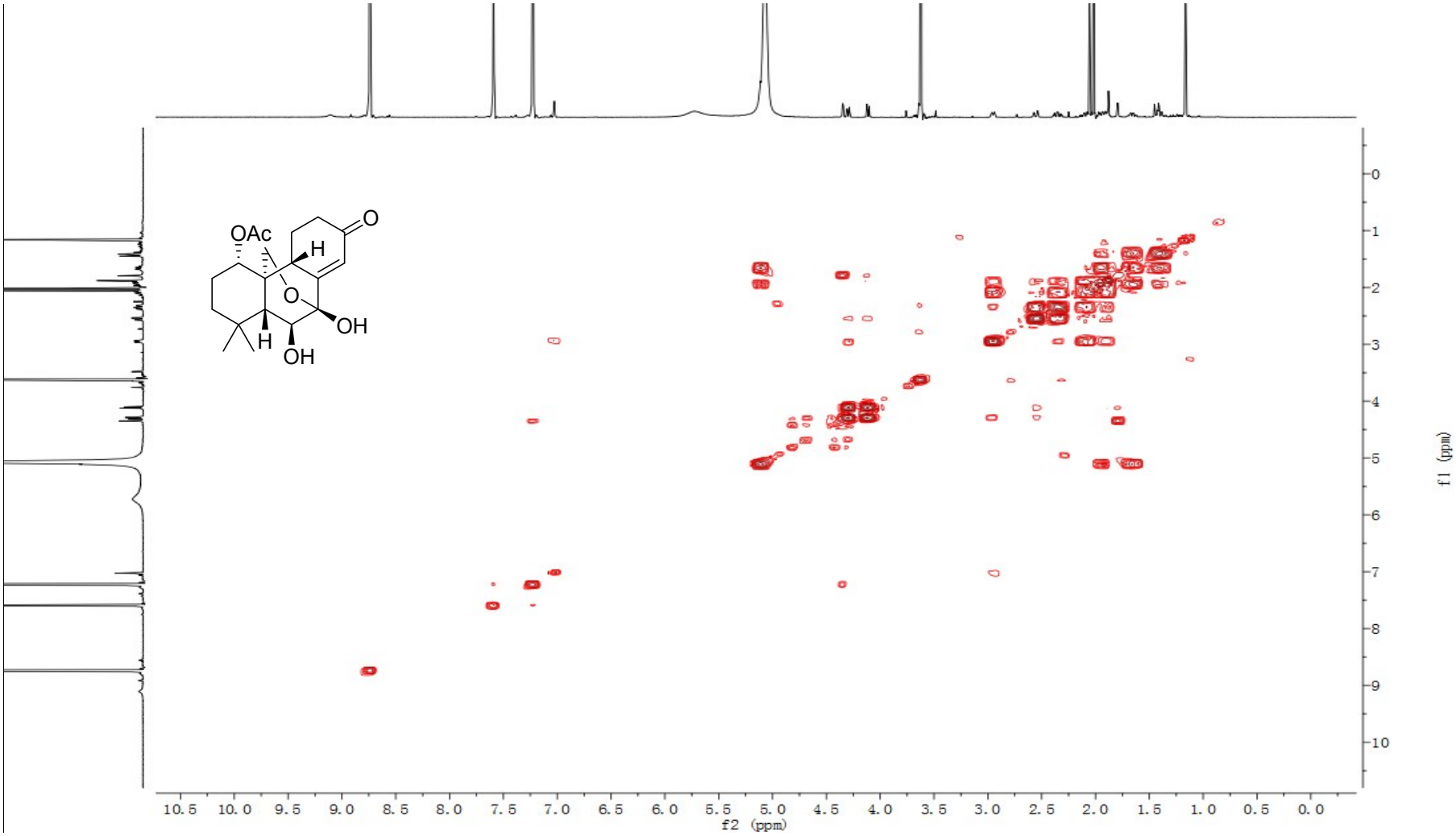


Figure S15. ^{1}H–^{1}H COSY spectrum of compound **2** (Recorded in pyridine-d_5)

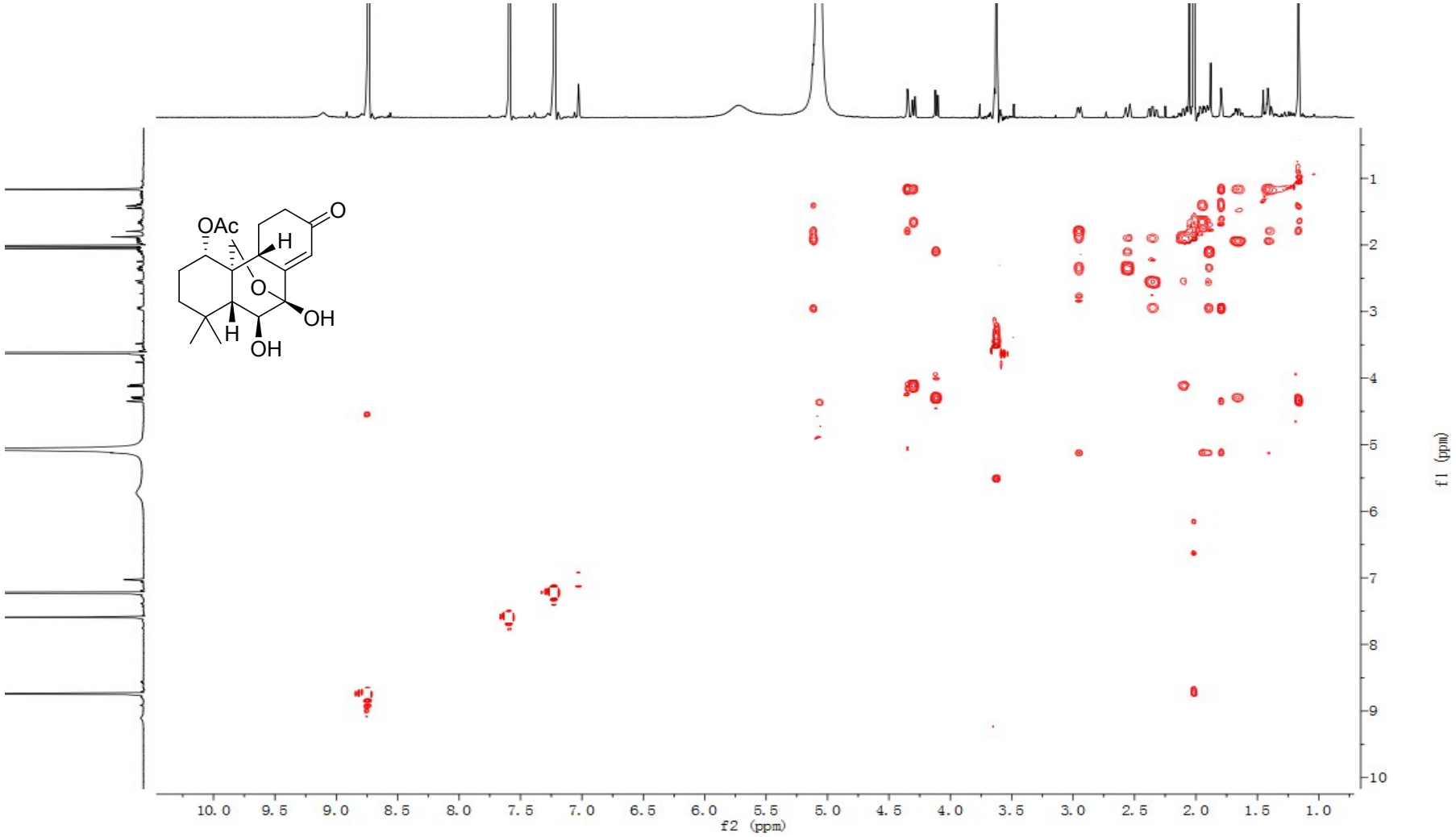
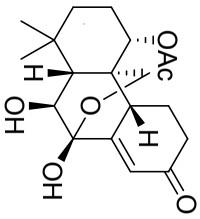


Figure S16. ROESY spectrum of compound **2** (Recorded in pyridine-d_5)

Qualitative Analysis Report

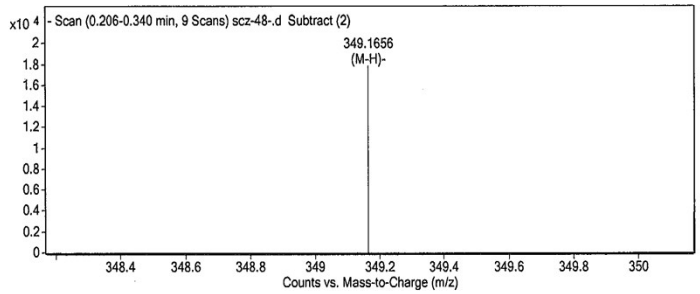
Data Filename	scz-48-.d	**Sample Name**	scz-48
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU-ESI-i.m	**Acquired Time**	9/15/2015 12:46:56 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

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



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
89.0242	1	4382.46		
349.1656	1	17904.79	C19 H26 O6	(M-H)-
385.1421	1	5158.69		
395.1712	1	19465.19		
396.1743	1	4077.37		
403.3067	1	4511.75		
463.1588	1	26735.3		
464.1617	1	6607.97		

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
C19 H26 O6	350.1729	349.1657	349.1656	0.1	0.3	7.0000

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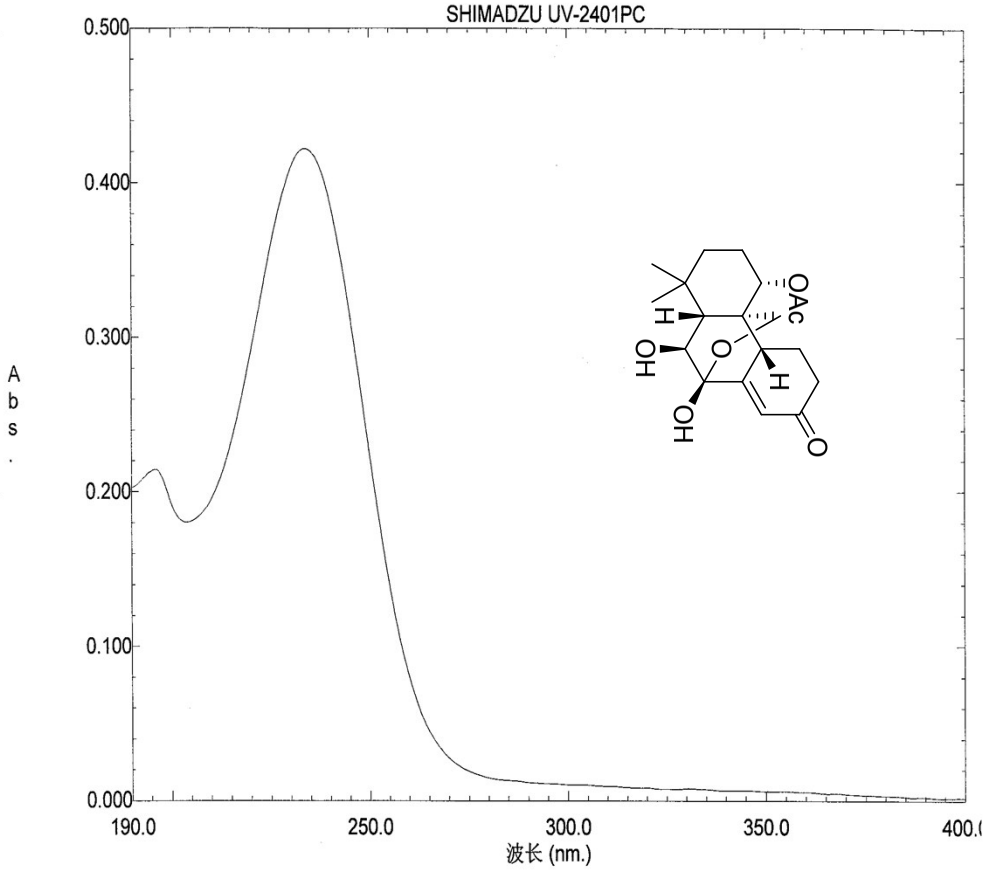
Figure S17. HRESIMS spectrum of compound **2**



文件名: SCZ-48

SCZ-48 ———

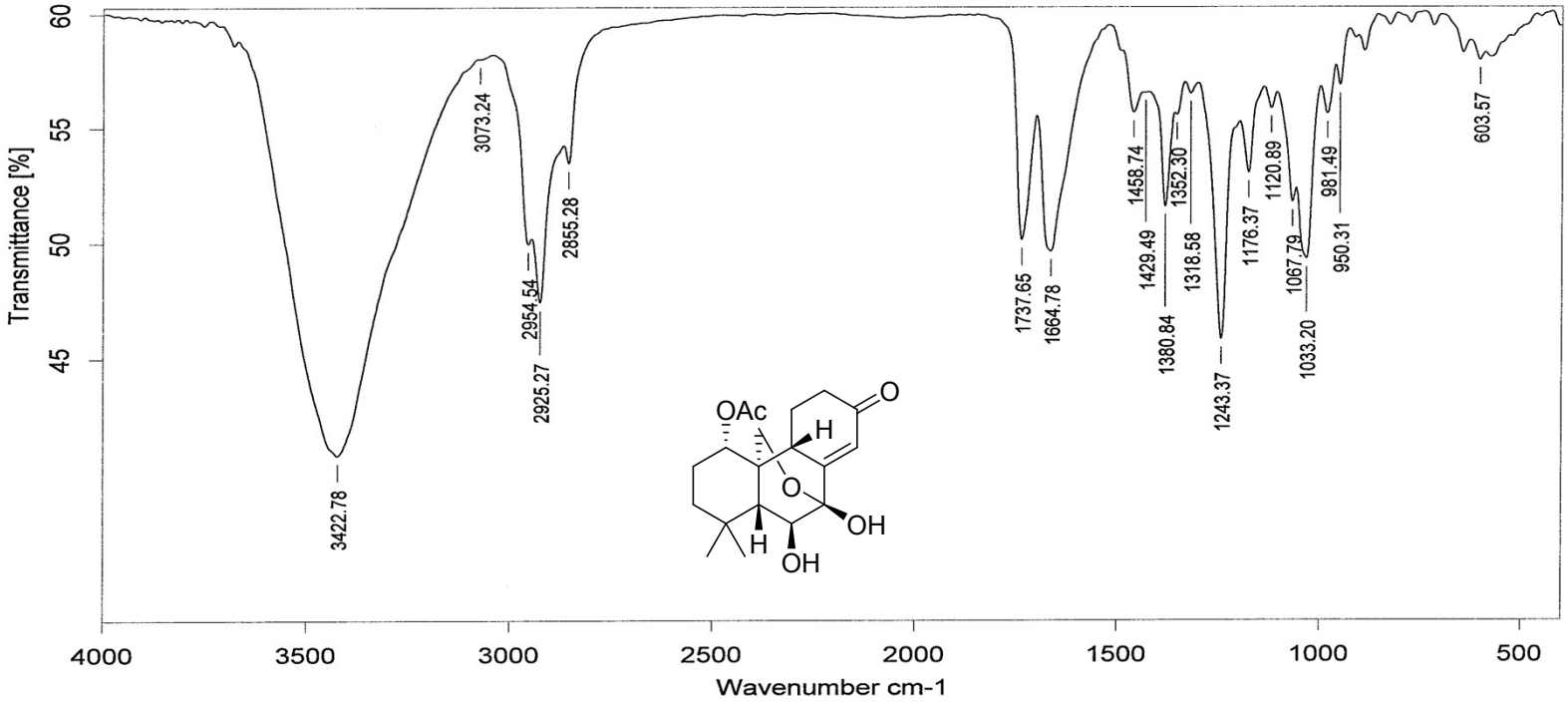
样品浓度：0.0090毫克/毫升
溶剂：甲醇

创建于: 16:26 15-09-19
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	233.80	0.4218
2	196.20	0.2143

Figure S18. UV spectrum of compound **2**



Sample : scz-48	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150925IR4	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S19. IR spectrum of compound **2**

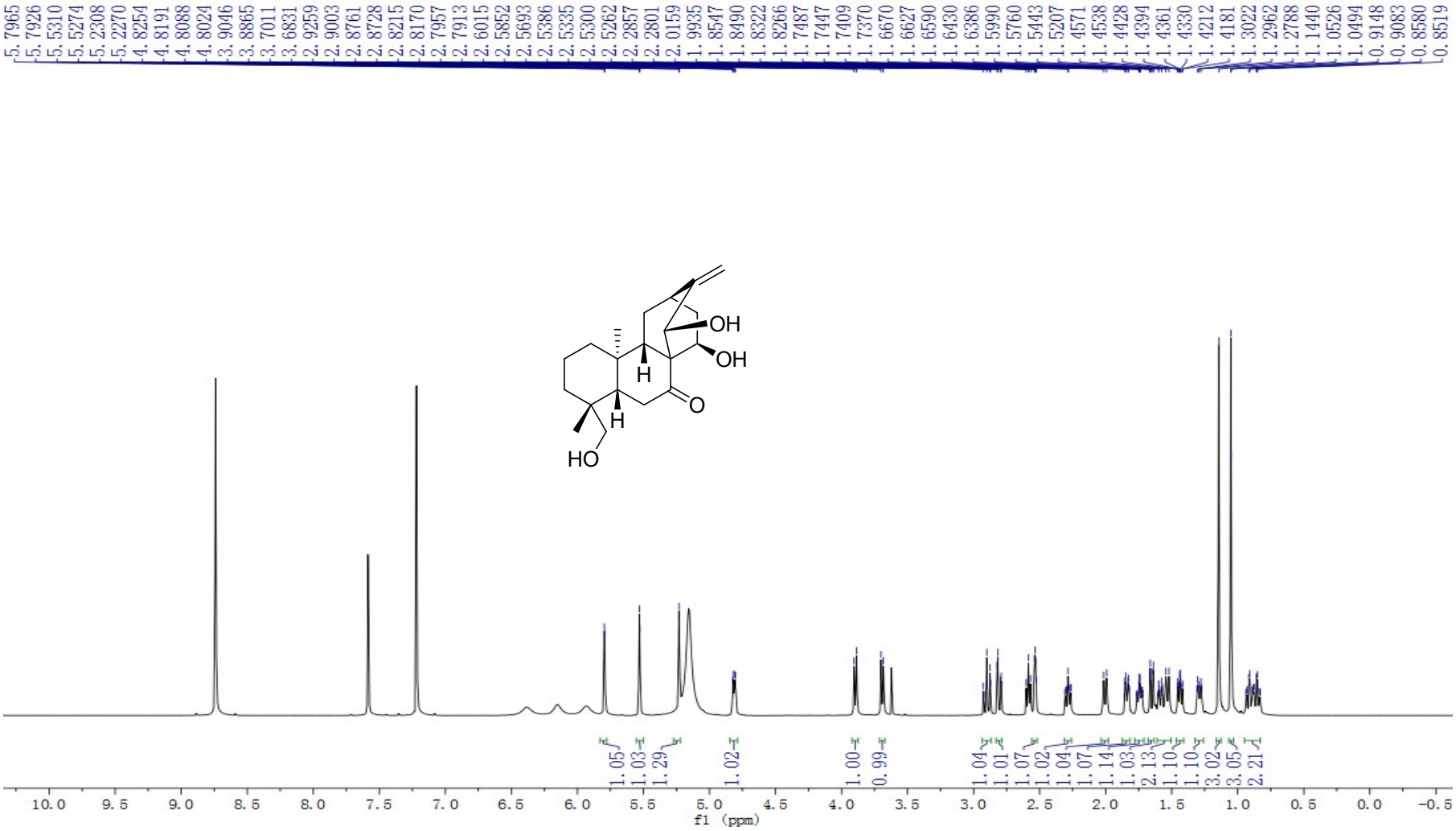


Figure S20. ^{1}H NMR spectrum of compound **3** (Recorded in pyridine-d_5)

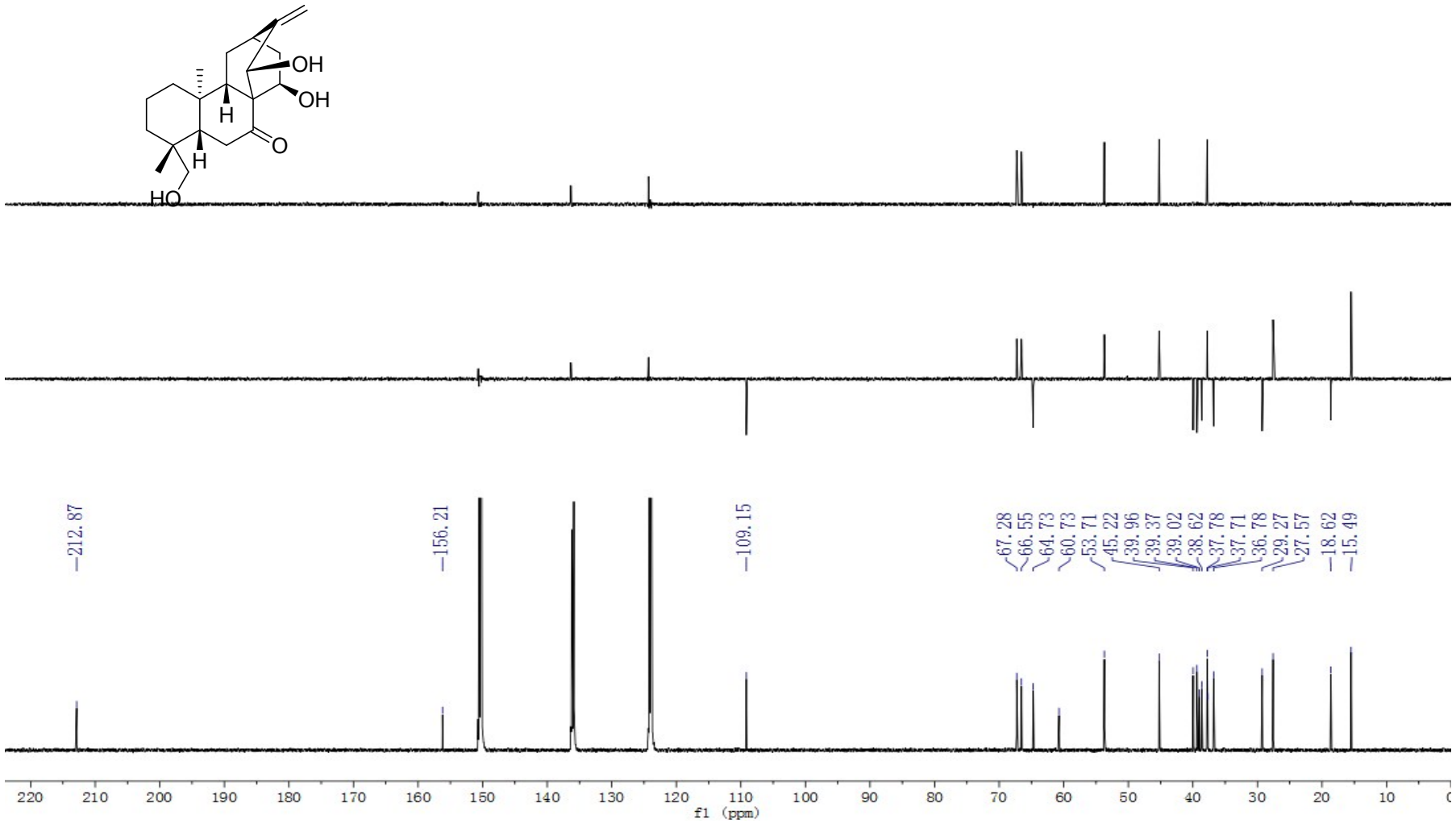


Figure S21. ^{13}C NMR spectrum of compound **3** (Recorded in pyridine-d_5)

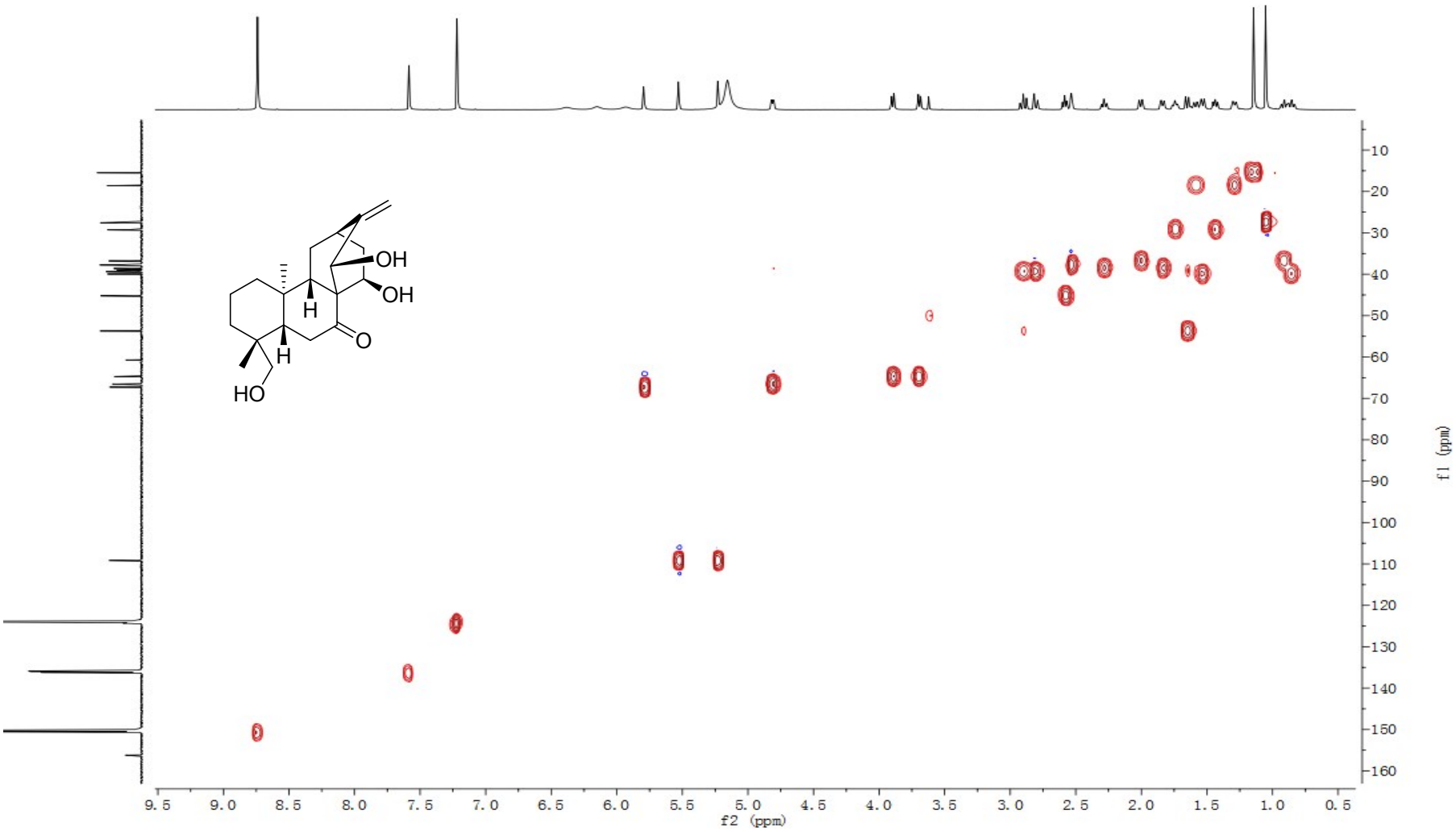


Figure S22. HSQC spectrum of compound **3** (Recorded in pyridine-d_5)

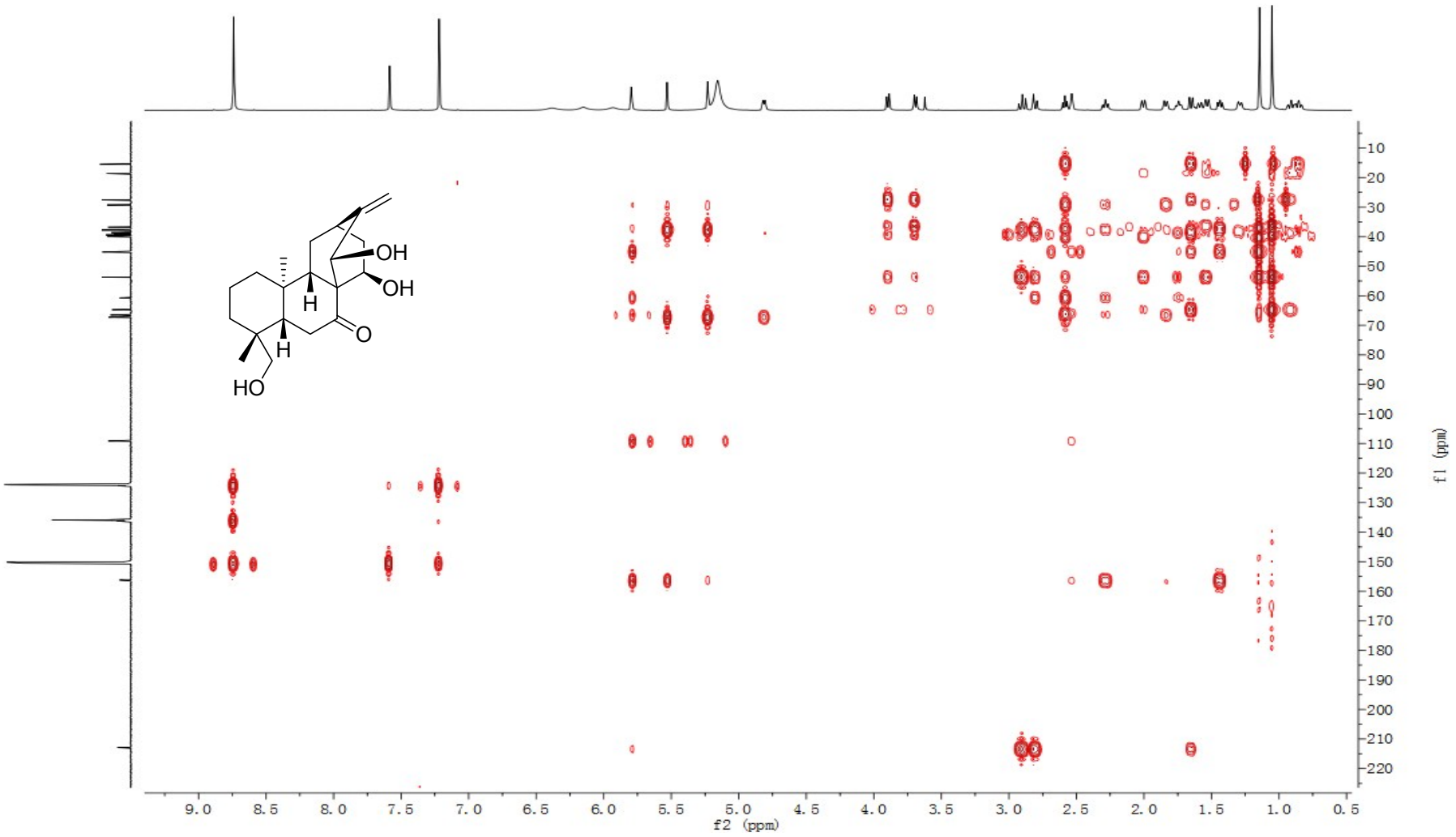


Figure S23. HMBC spectrum of compound **3** (Recorded in pyridine-d_5)

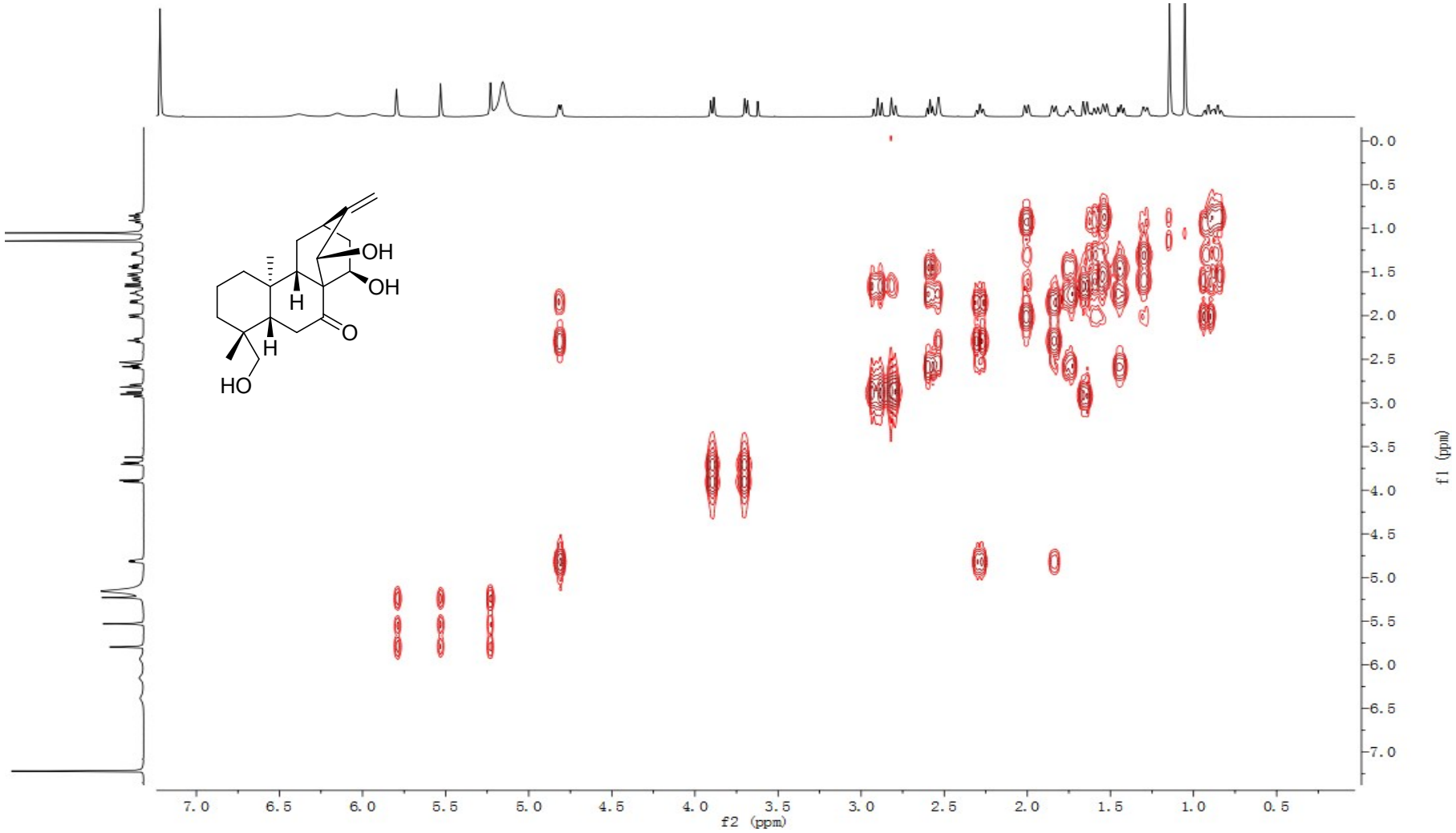


Figure S24. ^{1}H–^{1}H COSY spectrum of compound **3** (Recorded in pyridine-d_5)

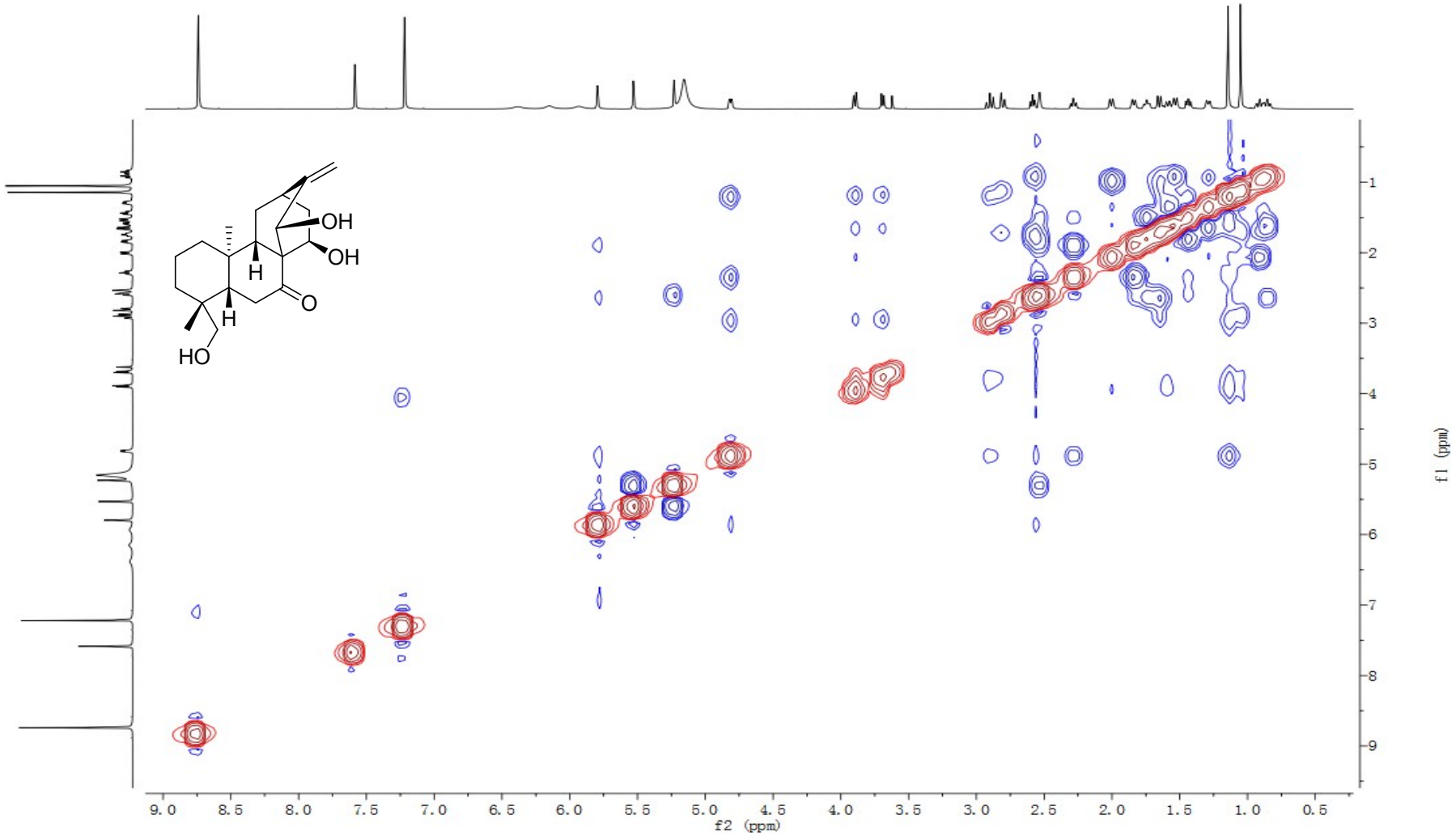


Figure S25. ROESY spectrum of compound **3** (Recorded in pyridine-d_5)

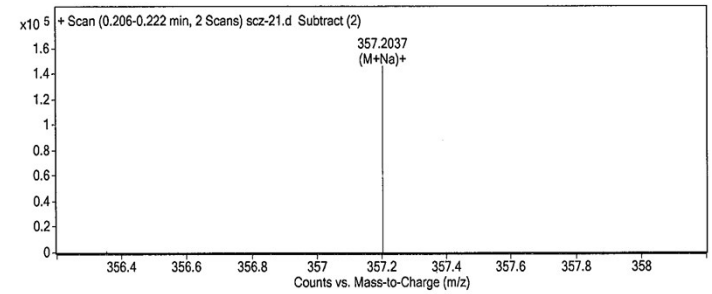
Qualitative Analysis Report

Data Filename	scz-21.d	**Sample Name**	scz-21
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/14/2015 4:08:19 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)

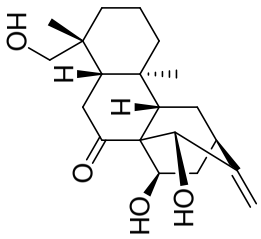
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
274.2742	1	41270.93		
317.2111	1	68488.55		
357.2037	1	146508.53	C20 H30 O4	(M+Na)+
358.2069	1	29956.74	C20 H30 O4	(M+Na)+
373.1774	1	82975.21		
691.4182	1	288209.78		
692.4213	1	115937.5		
693.4249	1	28164.4		



Formula Calculator Element Limits

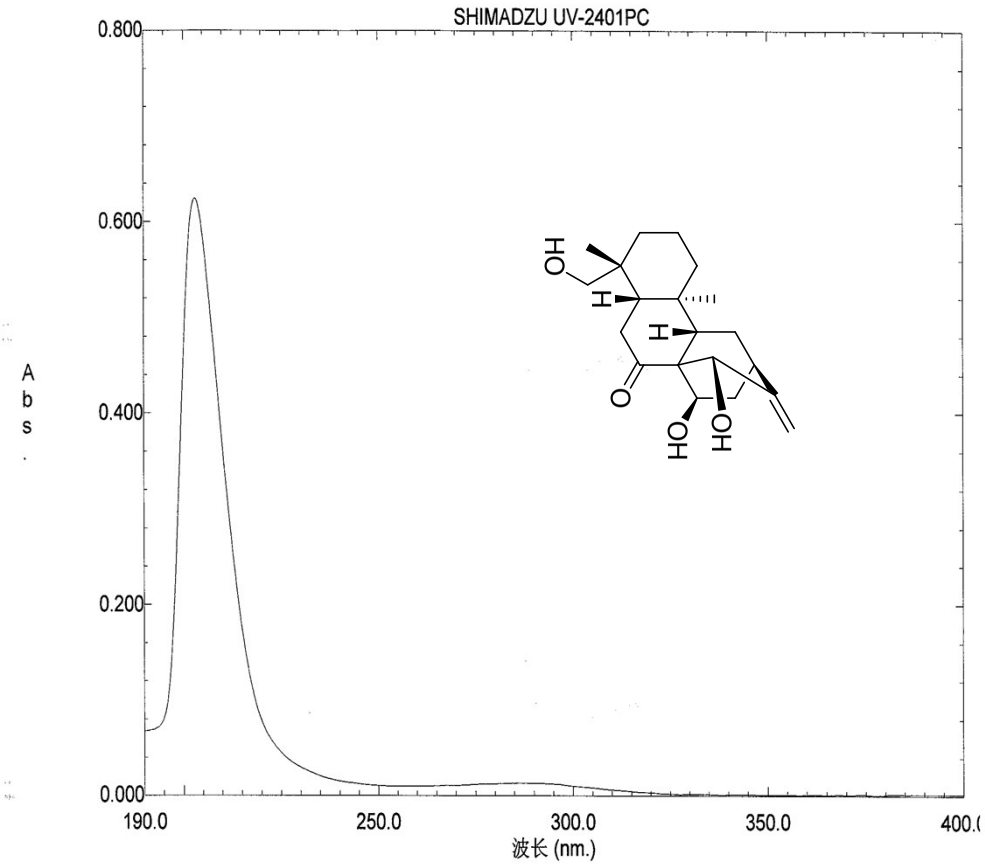
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H30 O4	334.2144	357.2036	357.2037	0.0	0.0	6.0000

--- End Of Report ---

Figure S26. HRESIMS spectrum of compound **3**



文件名: SCZ-21

SCZ-21 ———

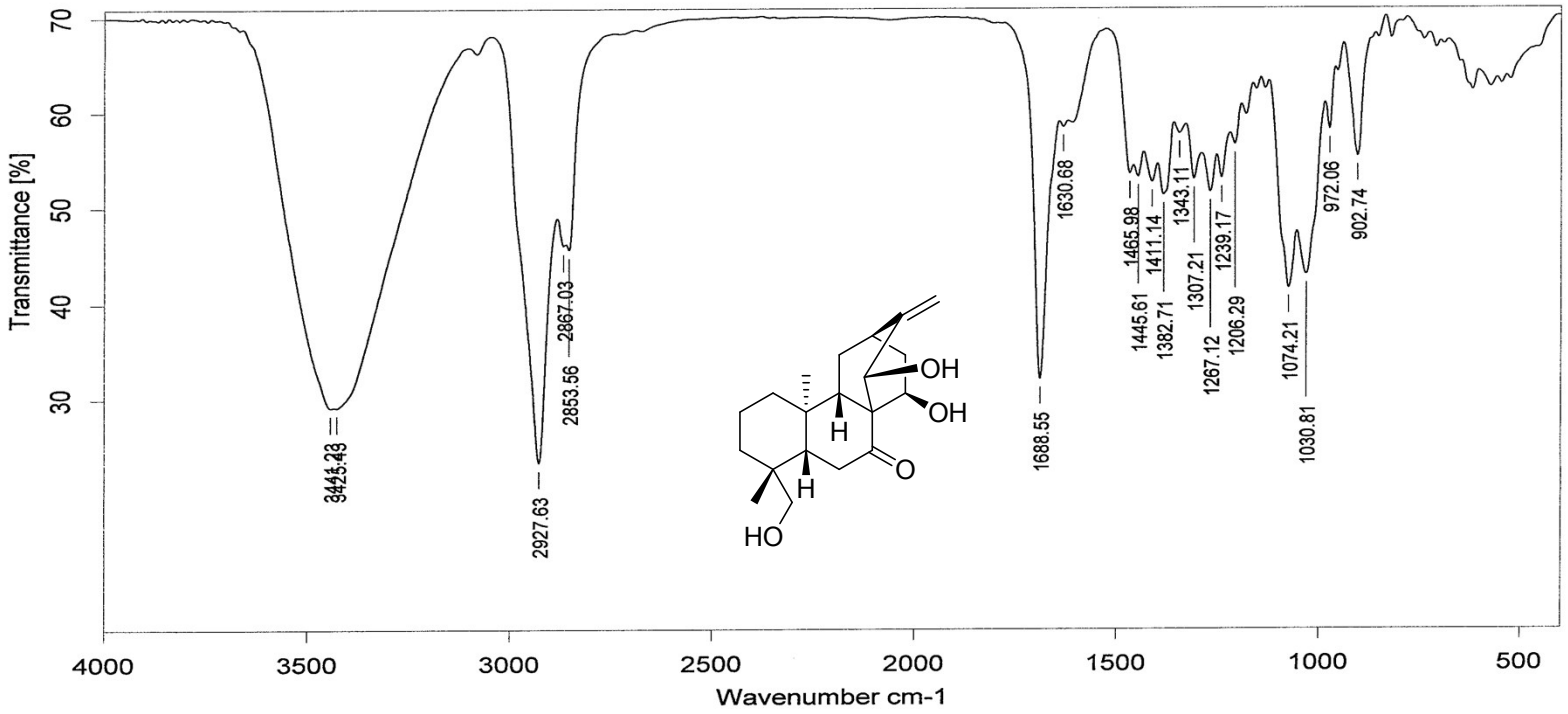
样品浓度：0.0313毫克/毫升
溶剂：甲醇

创建于: 15:29 15-09-19
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	286.60	0.0131
2	203.00	0.6244

Figure S27. UV spectrum of compound **3**



Sample : scz-21	Frequency Range : 399.246 - 3996.32	Measured on : 24/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150924IR5	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S28. IR spectrum of compound **3**

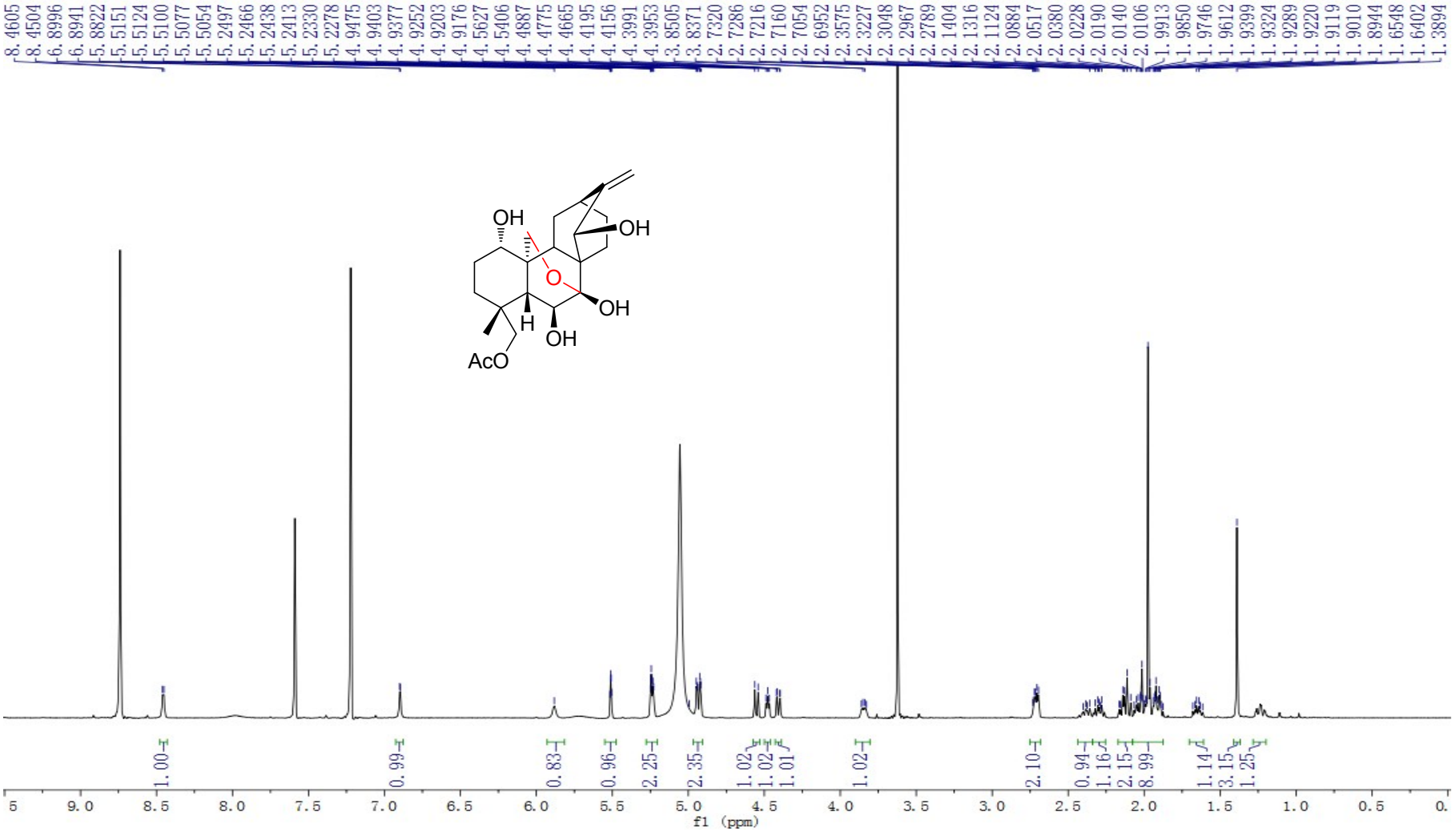


Figure S29. ^{1}H NMR spectrum of compound **4** (Recorded in pyridine-d_5)

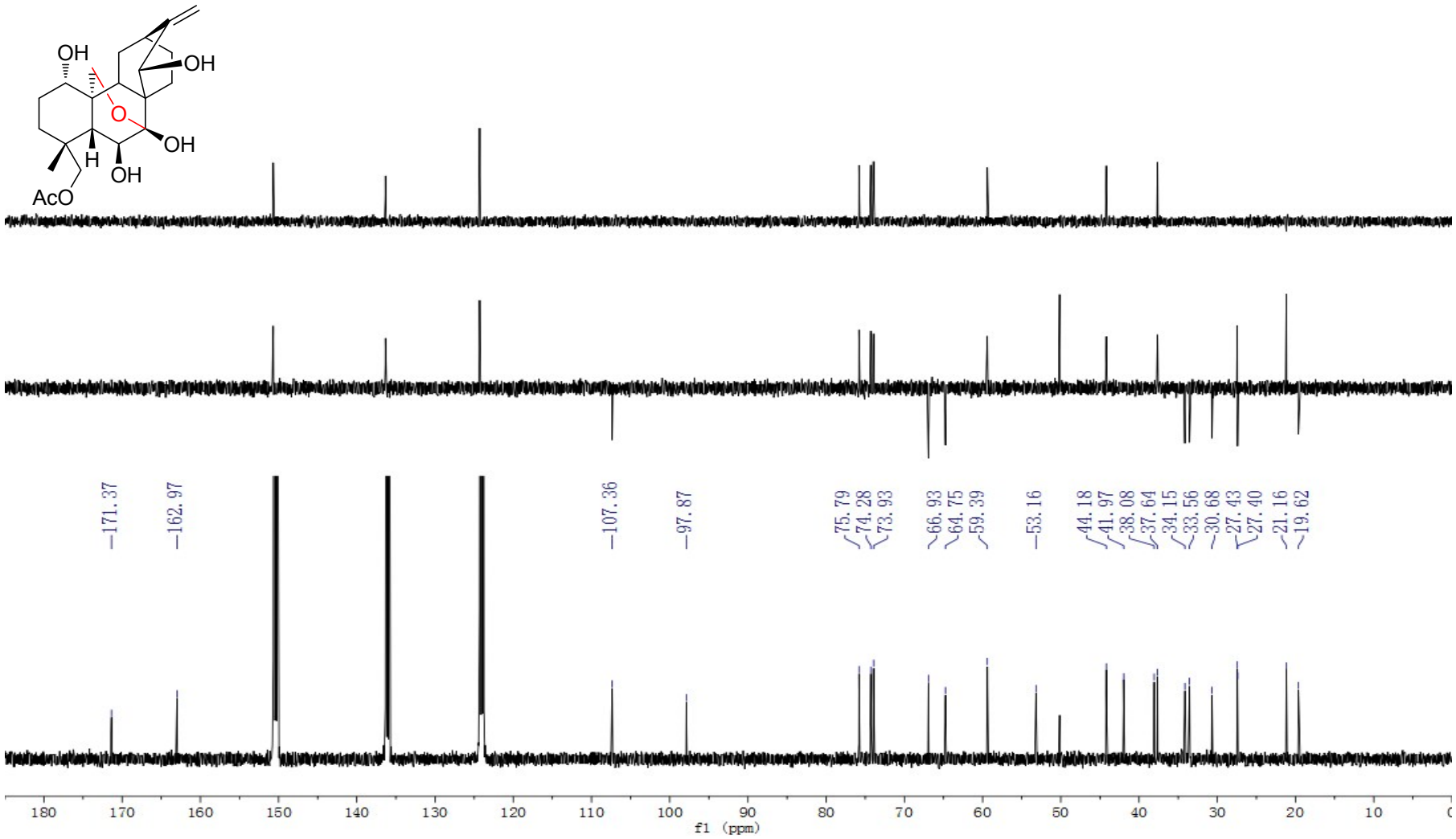


Figure S30. ^{13}C NMR spectrum of compound **4** (Recorded in pyridine-d_5)

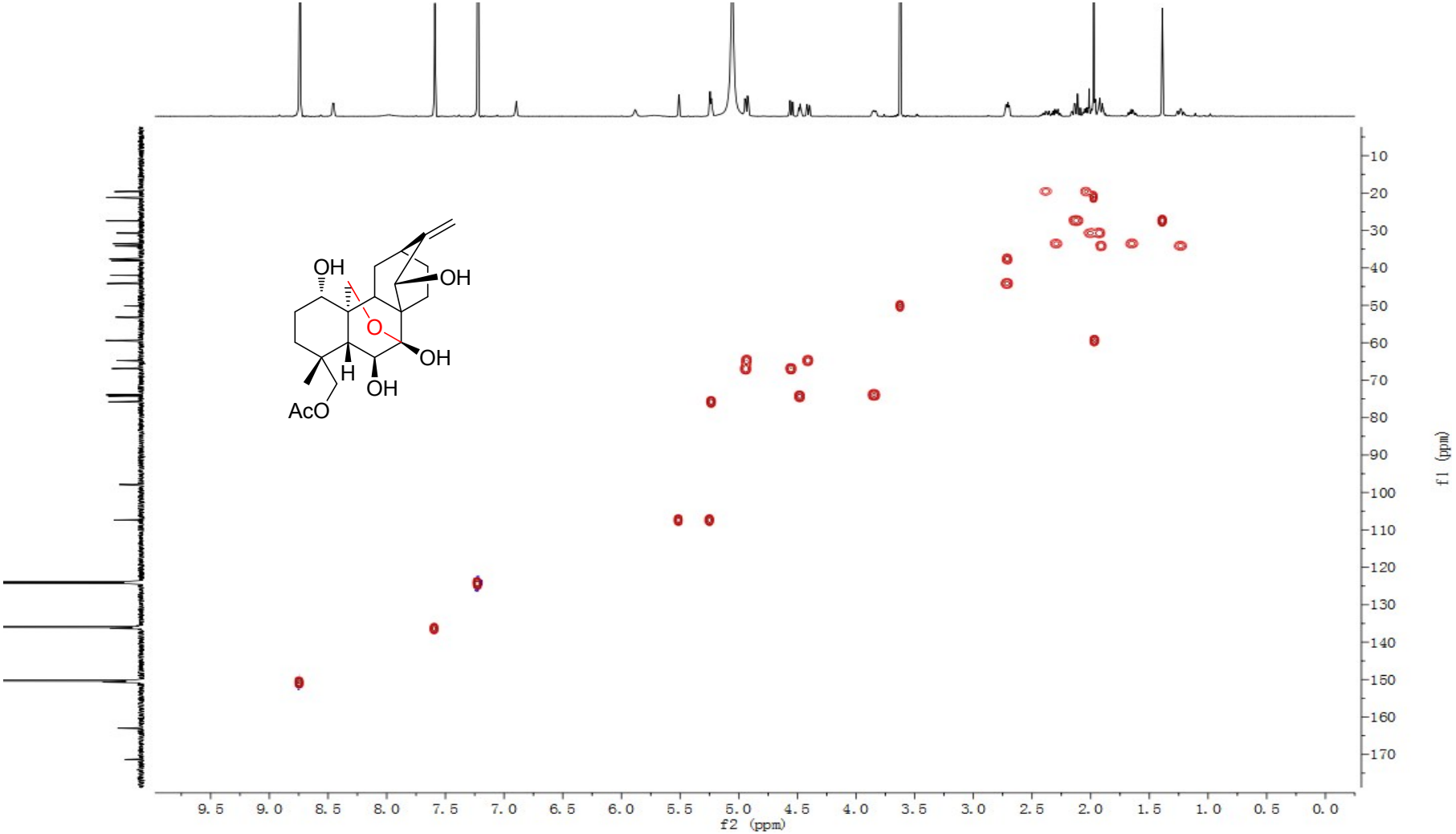


Figure S31. HSQC spectrum of compound **4** (Recorded in pyridine-d_5)

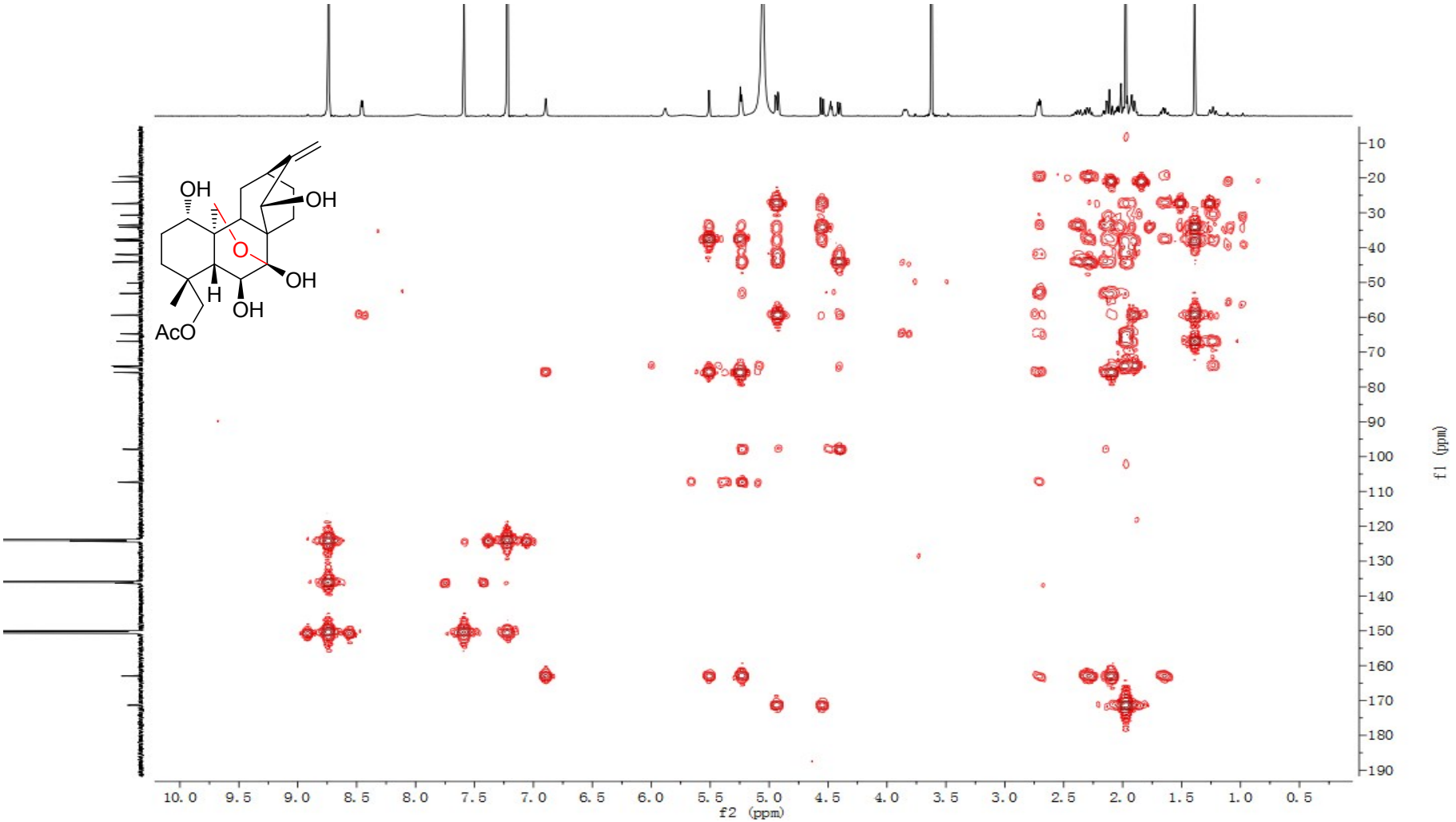


Figure S32. HMBC spectrum of compound **4** (Recorded in pyridine-d_5)

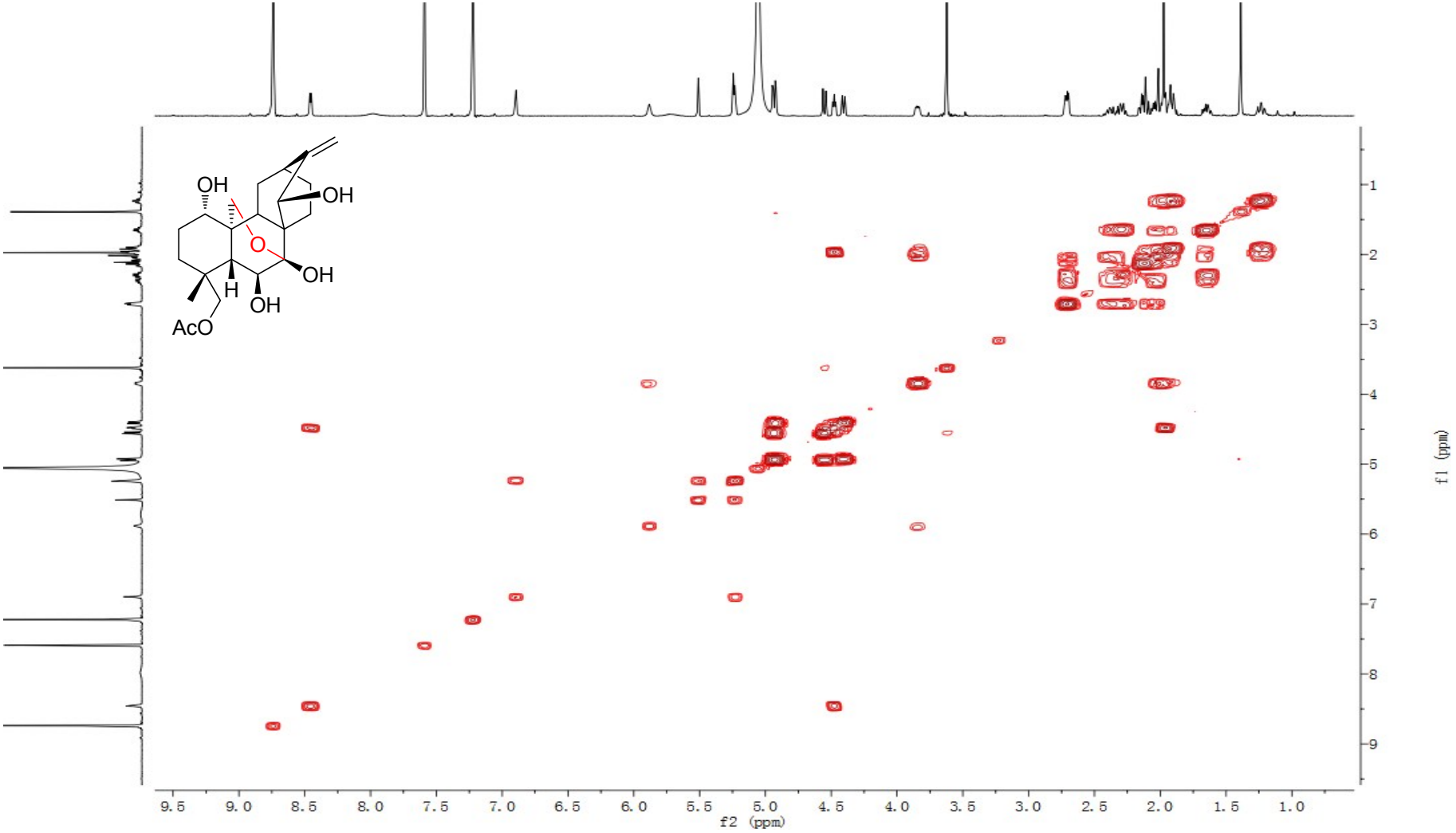


Figure S33. ^{1}H–^{1}H COSY spectrum of compound **4** (Recorded in pyridine-d_5)

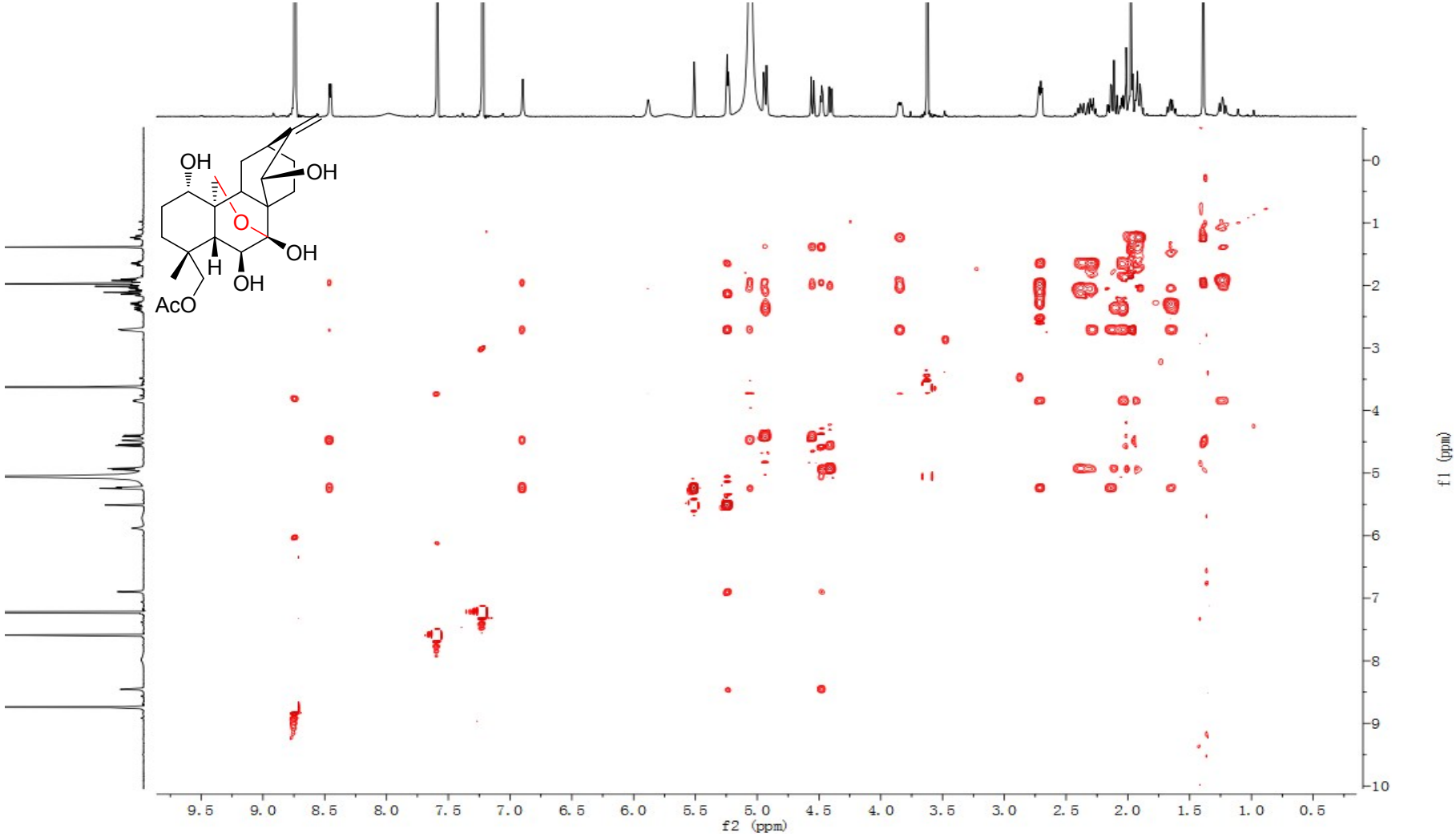
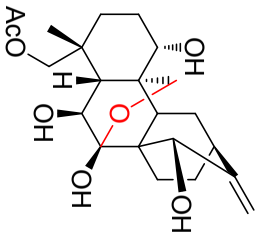


Figure S34. ROESY spectrum of compound **4** (Recorded in pyridine-d_5)

Qualitative Analysis Report

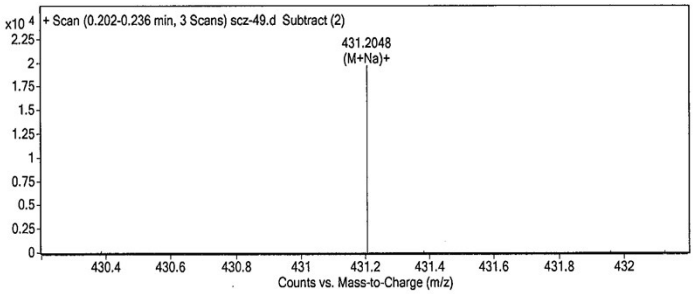
Data Filename	scz-49.d	**Sample Name**	scz-49
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/14/2015 4:21:49 PM
IRM Calibration Status	[redacted]	**DA Method**	ESI+.m
Comment			



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
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
274.2744	1	76448.73		
275.2775	1	13531.5		
302.3054	1	17854.88		
318.3004	1	44331.48		
426.2485	1	14575.13		
431.2048	1	19771.15	C22 H32 O7	(M+Na)+
437.1935	1	18764.11		
453.1673	1	42367.11		

Formula Calculator Element Limits

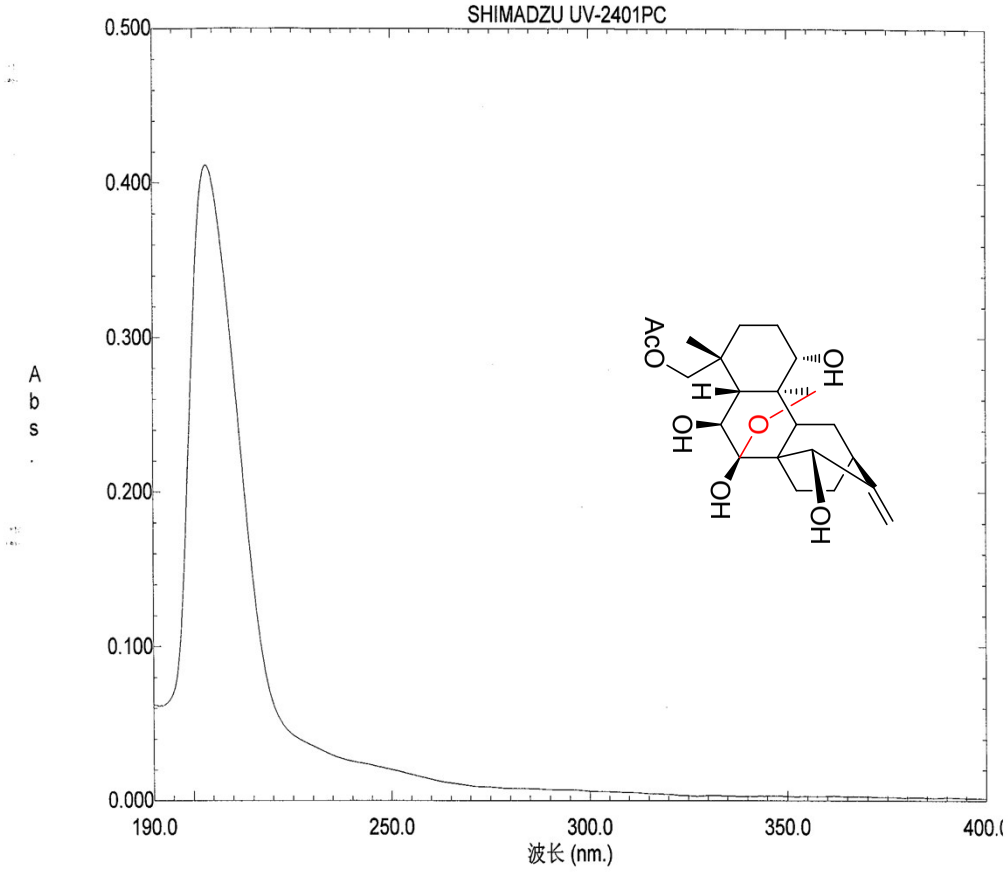
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C22 H32 O7	408.2148	431.2040	431.2048	-0.7	-1.7	7.0000

--- End Of Report ---

Figure S35. HRESIMS spectrum of compound **4**



文件名: SCZ-49

SCZ-49 ———

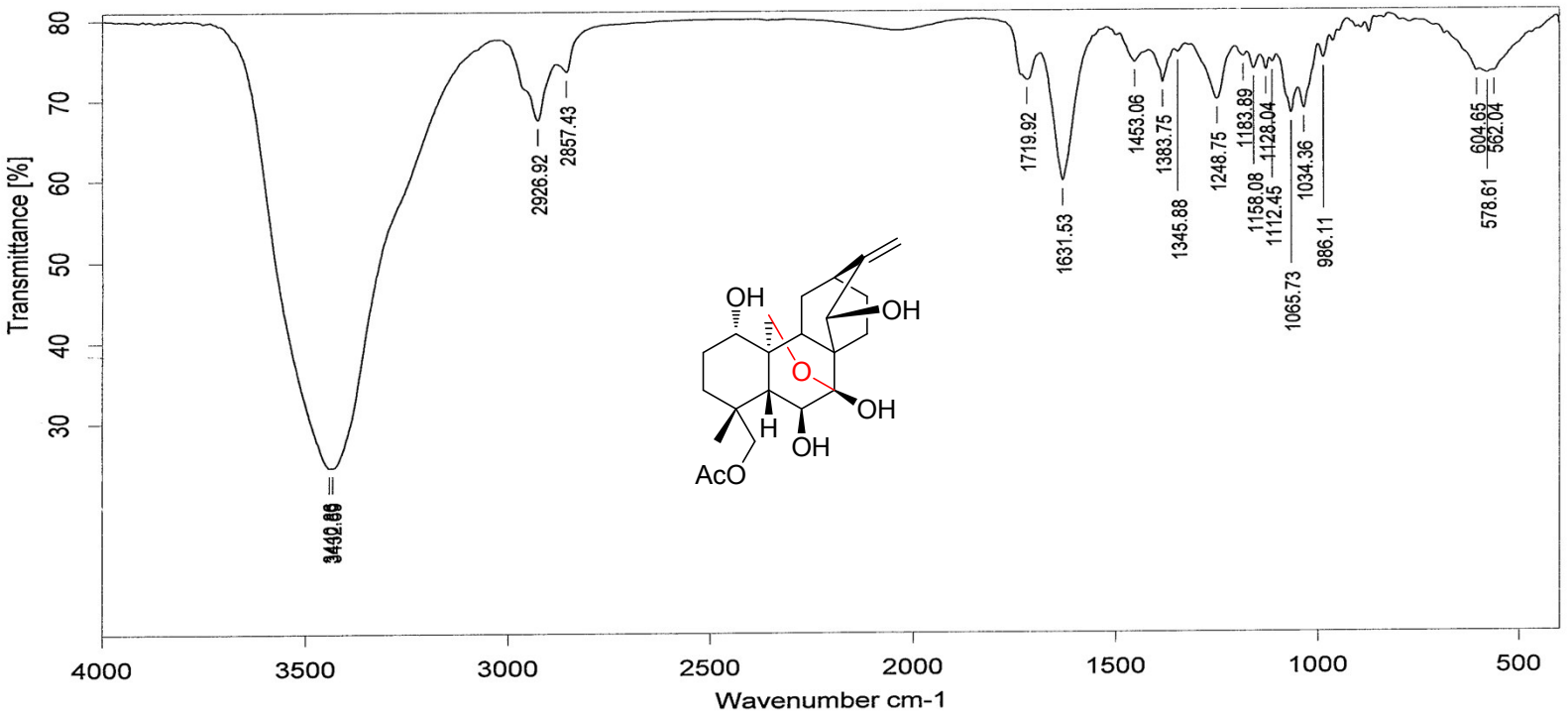
样品浓度：0.0315毫克/毫升
溶剂：甲醇

创建于: 16:39 15-09-19
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	203.40	0.4115

Figure S36. UV spectrum of compound **4**



Sample : scz-49	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150925IR5	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S37. IR spectrum of compound **4**

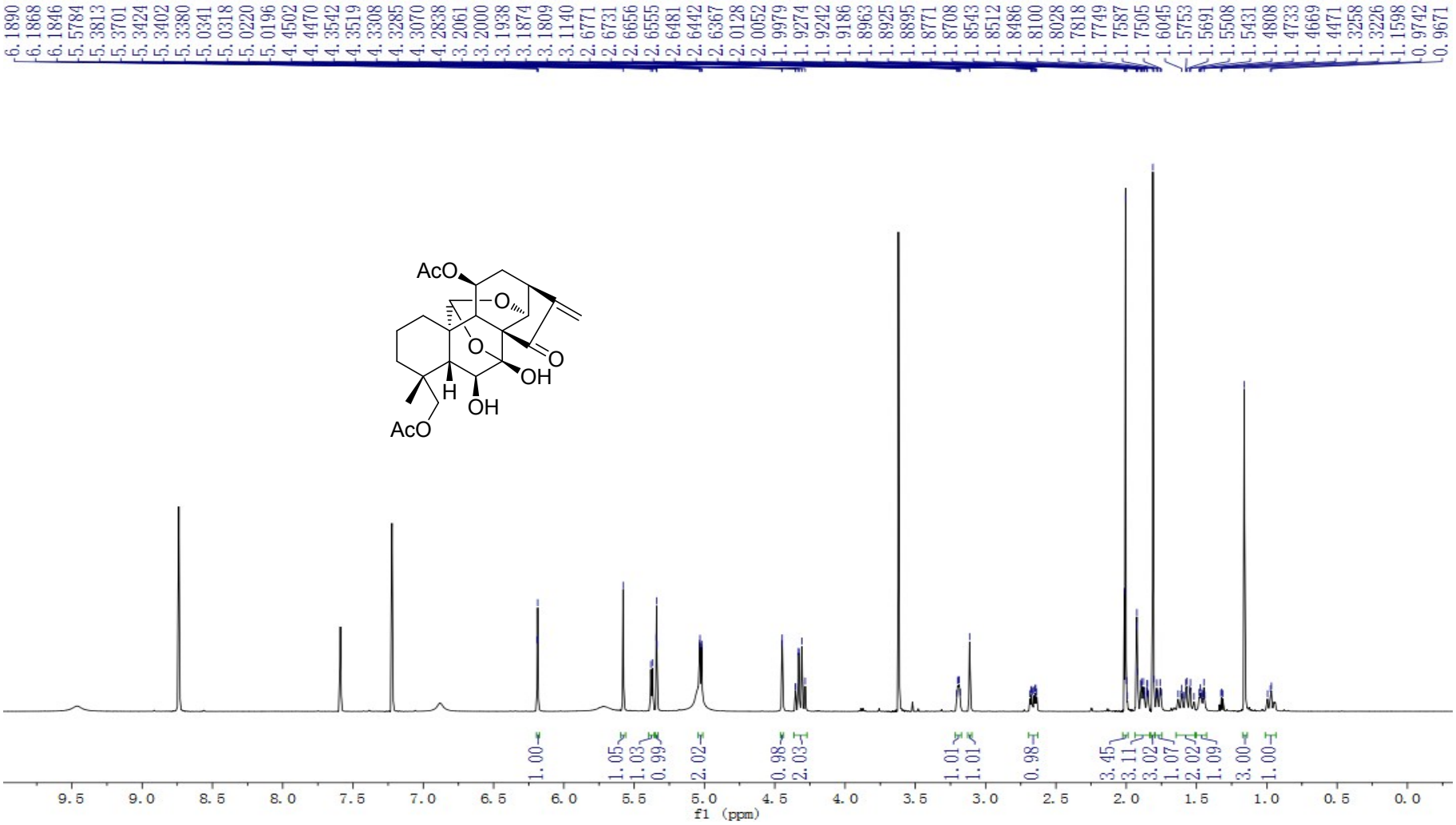


Figure S38. ^{1}H NMR spectrum of compound **5** (Recorded in pyridine-d_5)

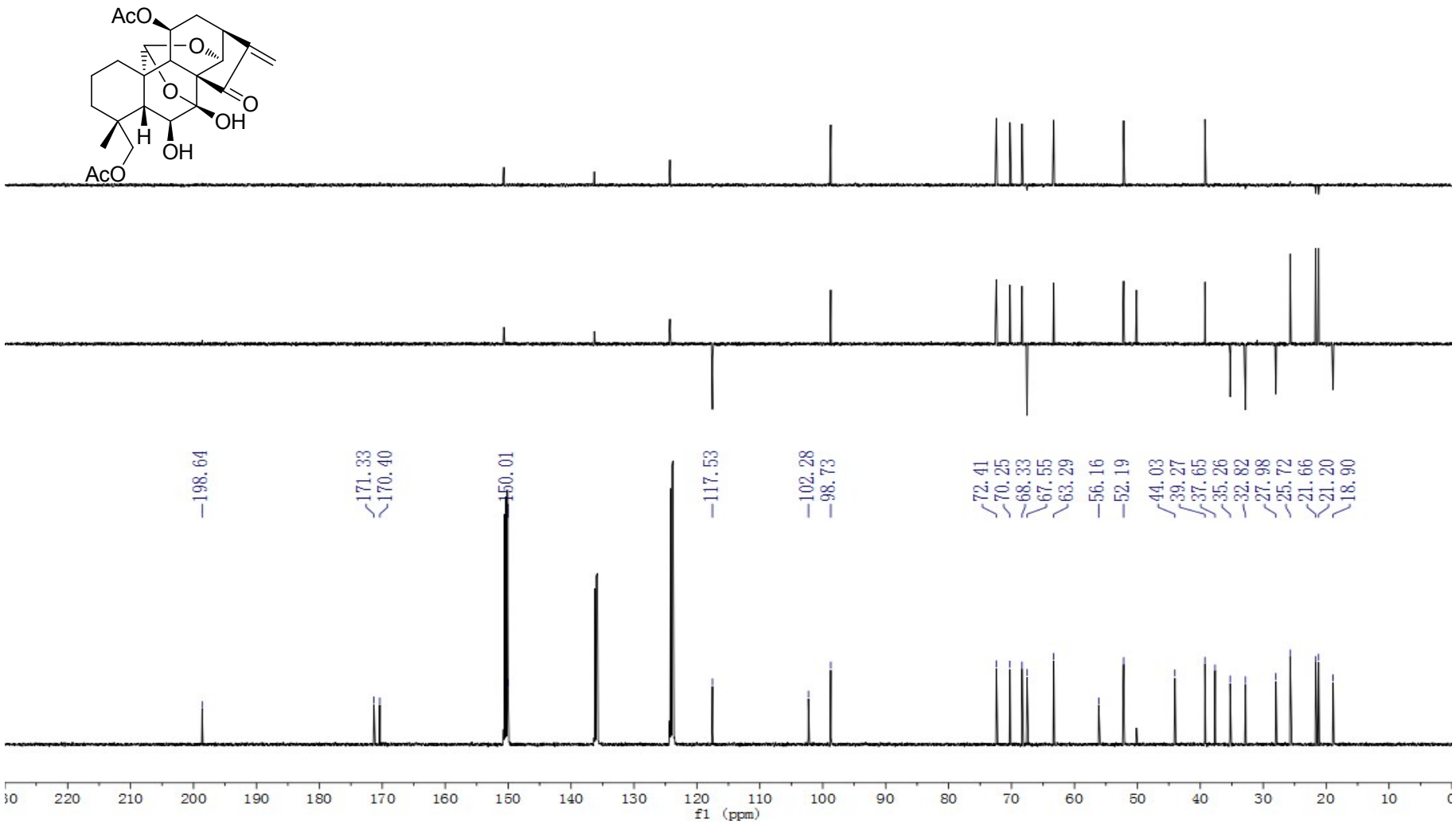


Figure S39. ^{13}C NMR spectrum of compound **5** (Recorded in pyridine-d_5)

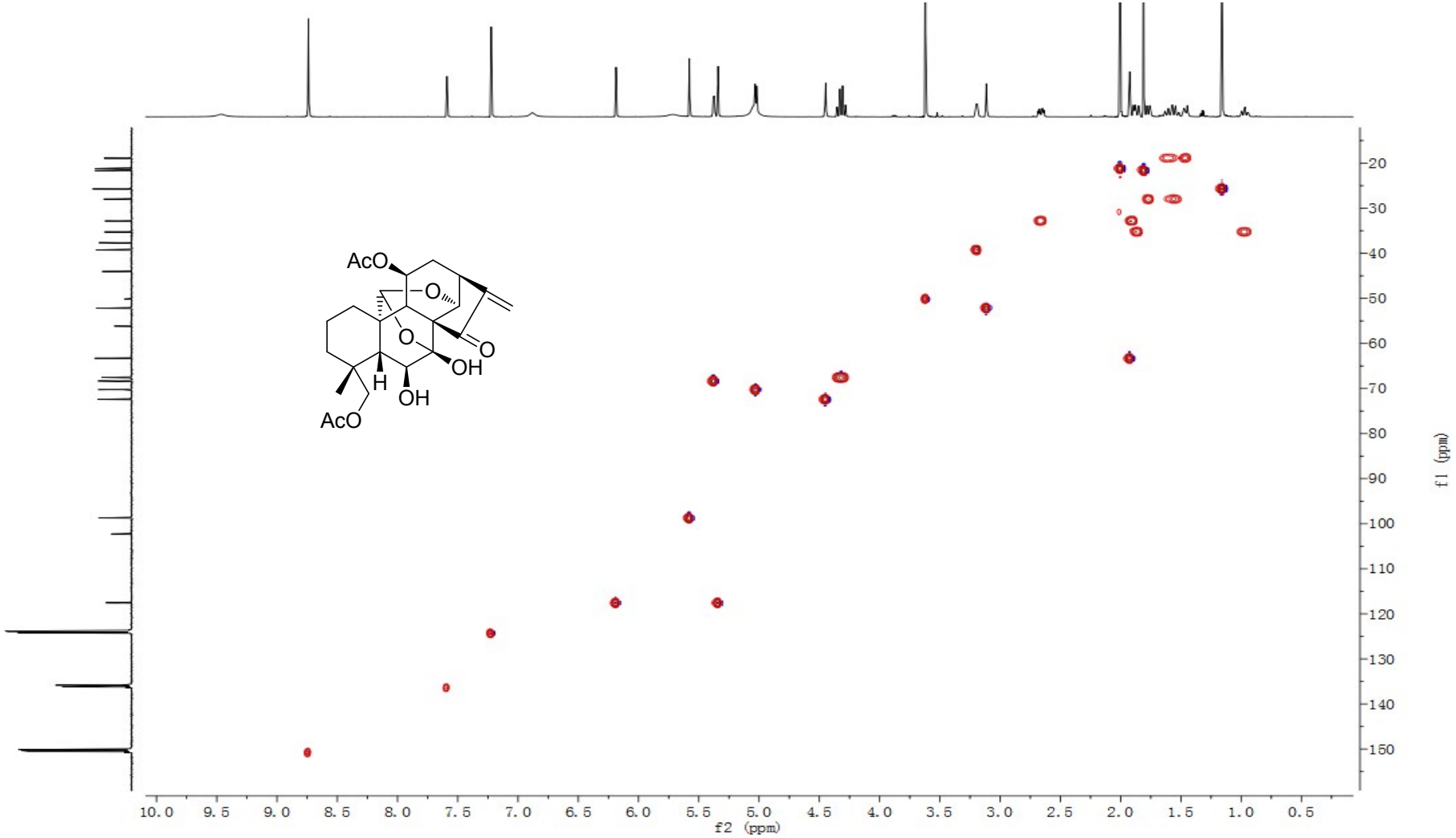


Figure S40. HSQC spectrum of compound **5** (Recorded in pyridine-d_5)

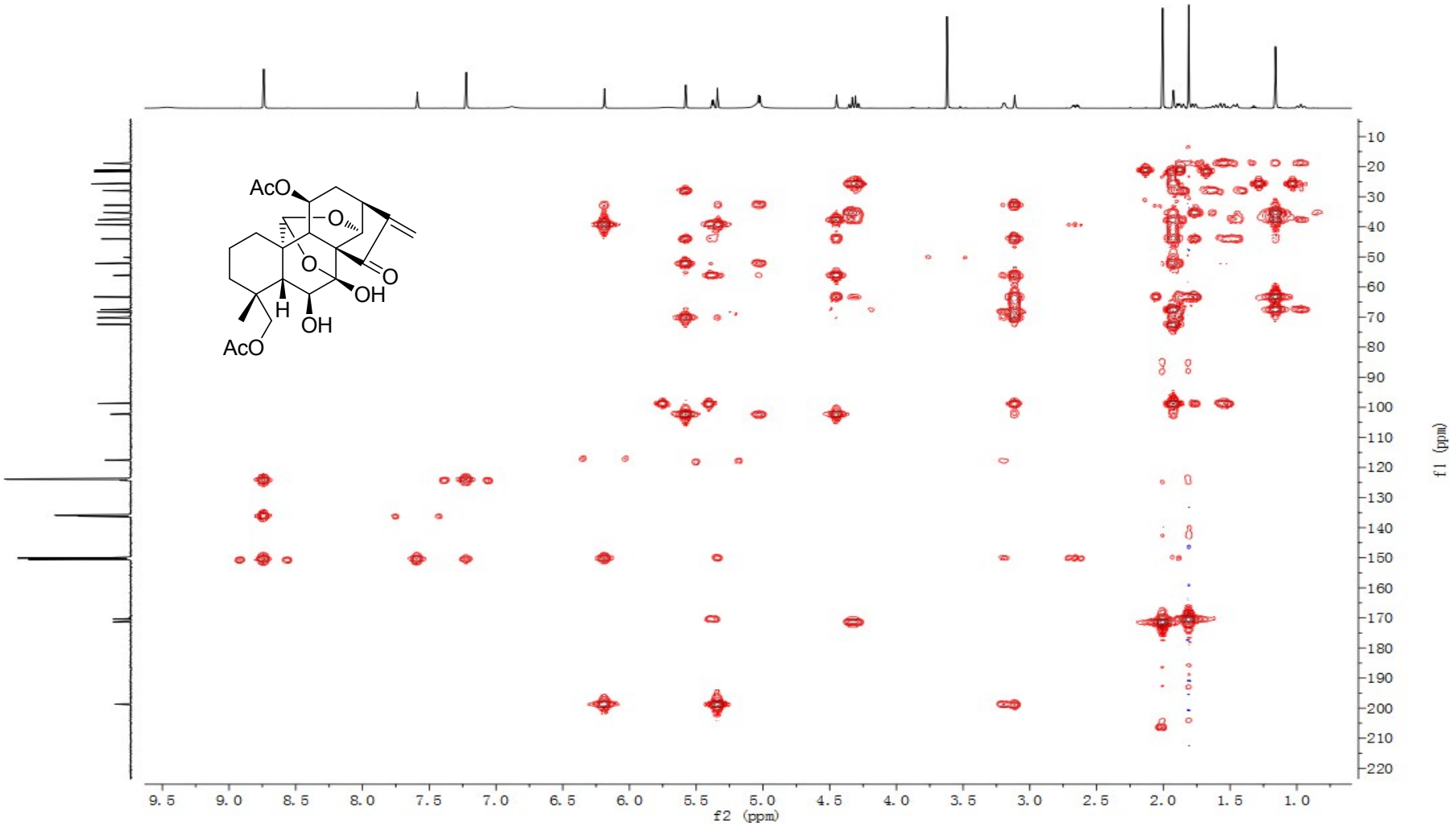


Figure S41. HMBC spectrum of compound **5** (Recorded in pyridine-d_5)

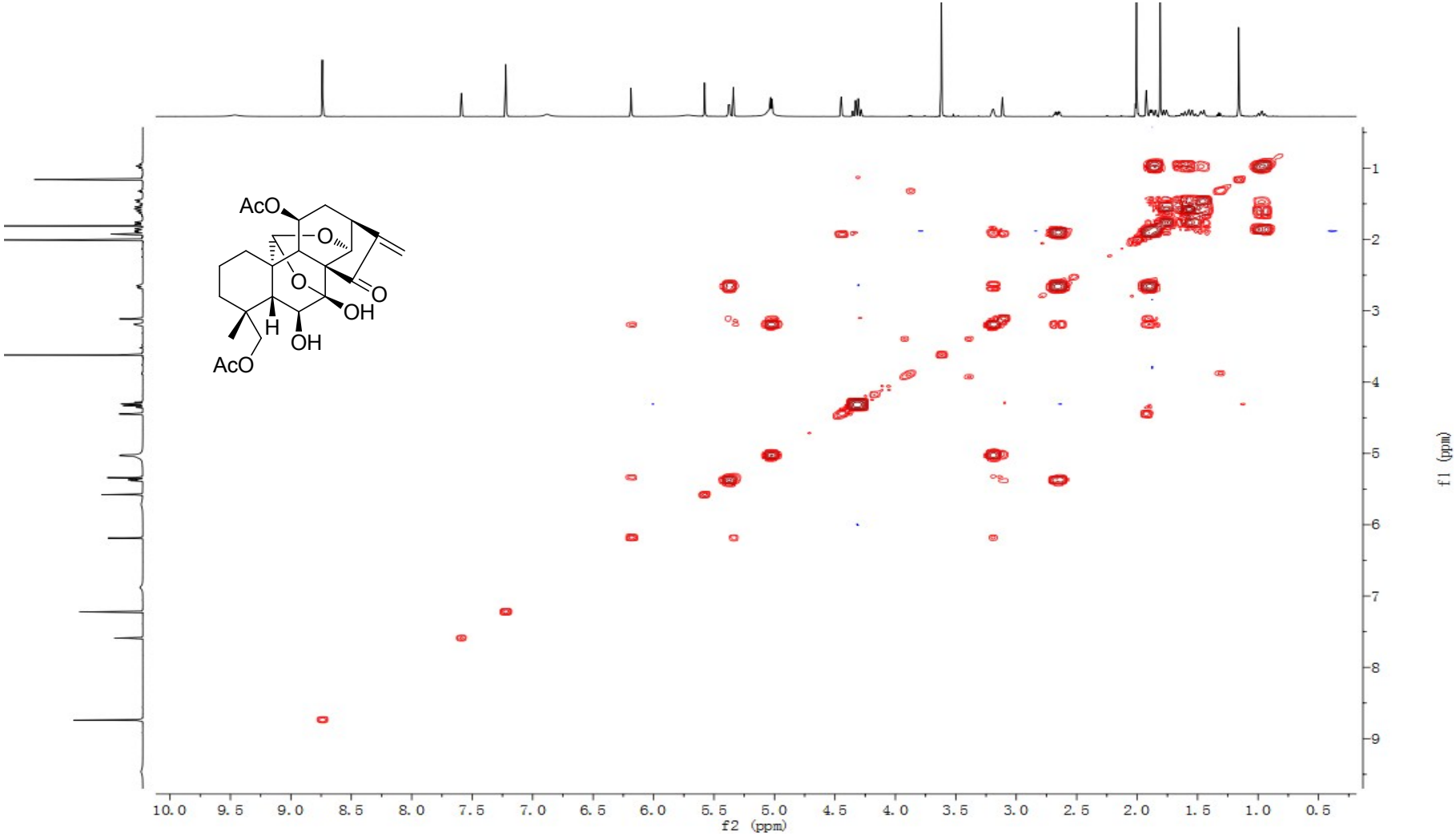


Figure S42. ^{1}H–^{1}H COSY spectrum of compound **5** (Recorded in pyridine-d_5)

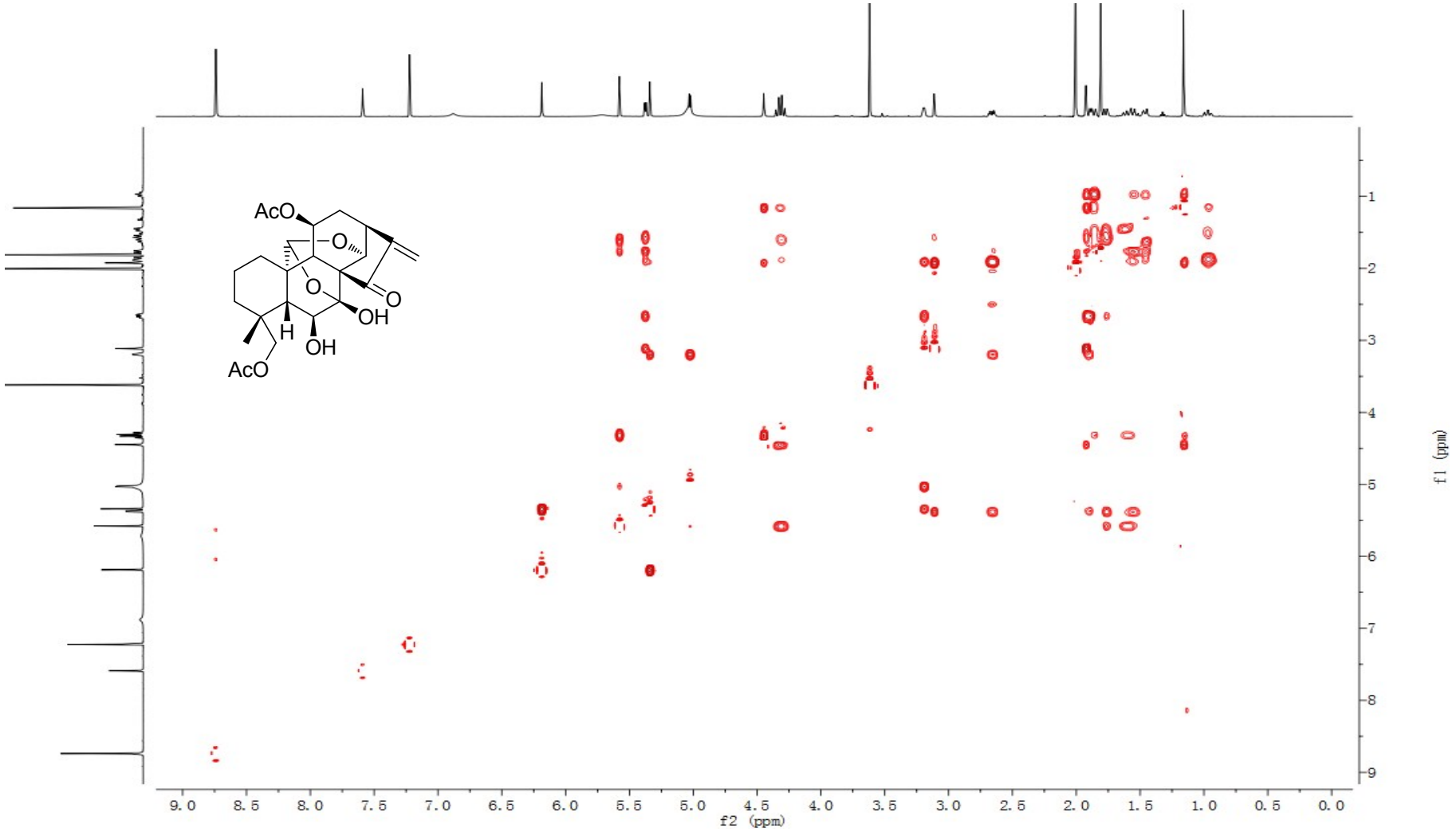


Figure S43. ROESY spectrum of compound **5** (Recorded in pyridine-d_5)

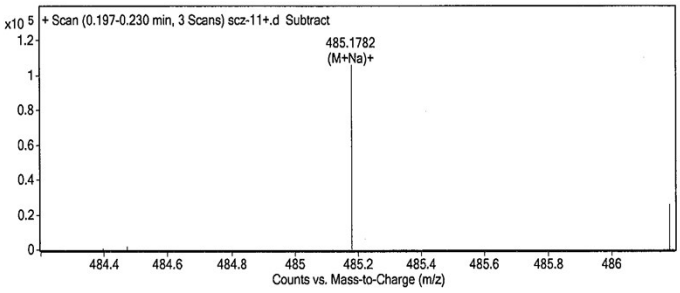
Qualitative Analysis Report

Data Filename	scz-11+.d	**Sample Name**	scz-11
Sample Type	Sample	**Position**	P1-B1
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/15/2015 10:38:39 AM
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)

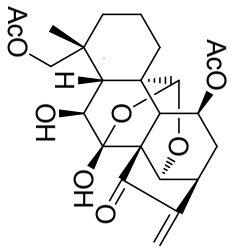
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
274.2746	1	147807.8		
302.3057	1	44620.69		
318.3005	1	120294.45		
346.3318	1	42375.7		
485.1782	1	106108.09	C24 H30 O9	(M+Na)+
947.3671	1	83594.93		
948.3703	1	42660.61		
969.3487	1	40381.38		



Formula Calculator Element Limits

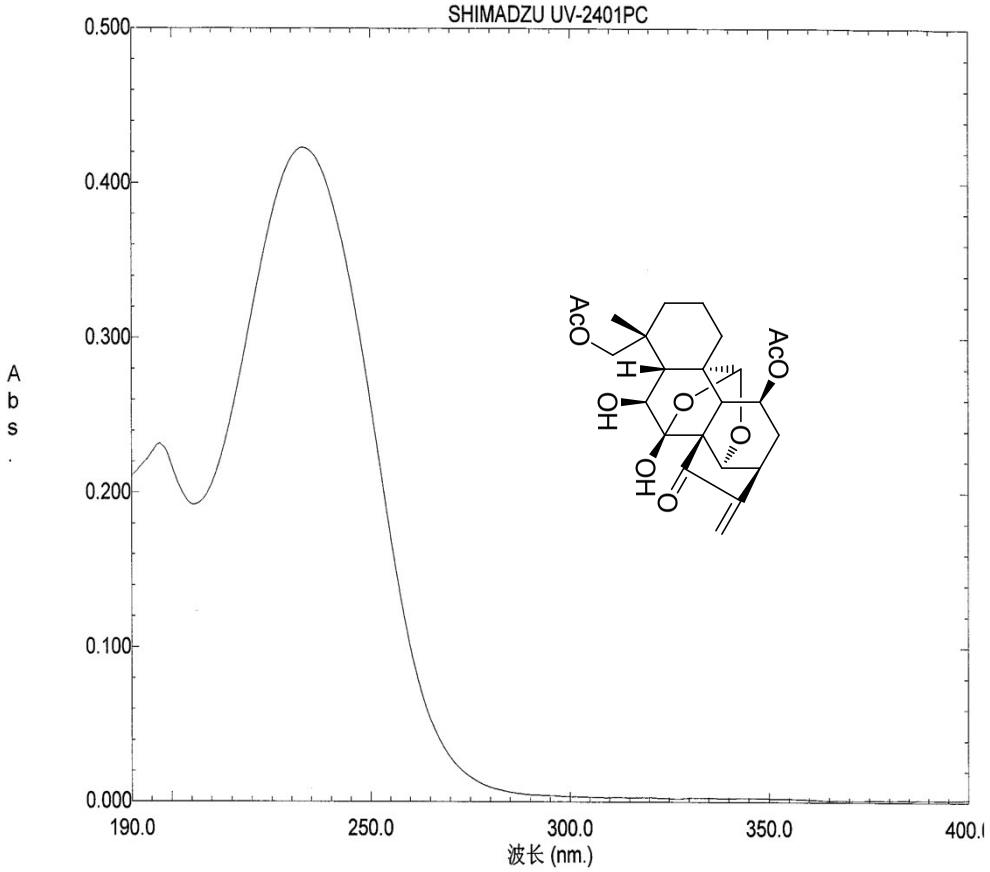
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C24 H30 O9	462.1890	485.1782	485.1782	0.0	-0.1	10.0000

--- End Of Report ---

Figure S44. HRESIMS spectrum of compound **5**



文件名: SCZ-11

SCZ-11 ———

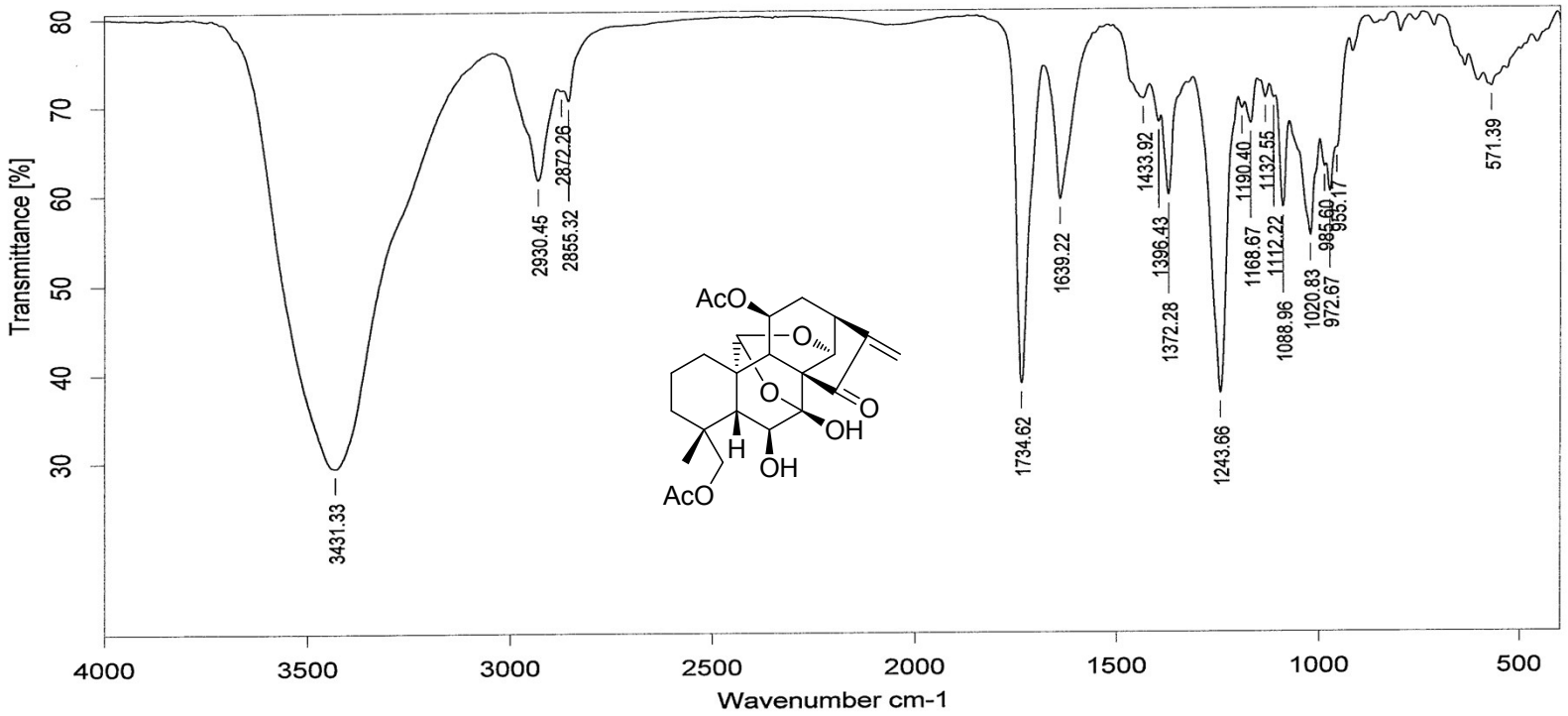
样品浓度：0.0318毫克/毫升
溶剂：甲醇

创建于: 15:15 15-09-19
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	233.20	0.4227
2	197.20	0.2314

Figure S45. UV spectrum of compound **5**



Sample : scz-11	Frequency Range : 399.246 - 3996.32	Measured on : 24/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150924IR3	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S46. IR spectrum of compound **5**

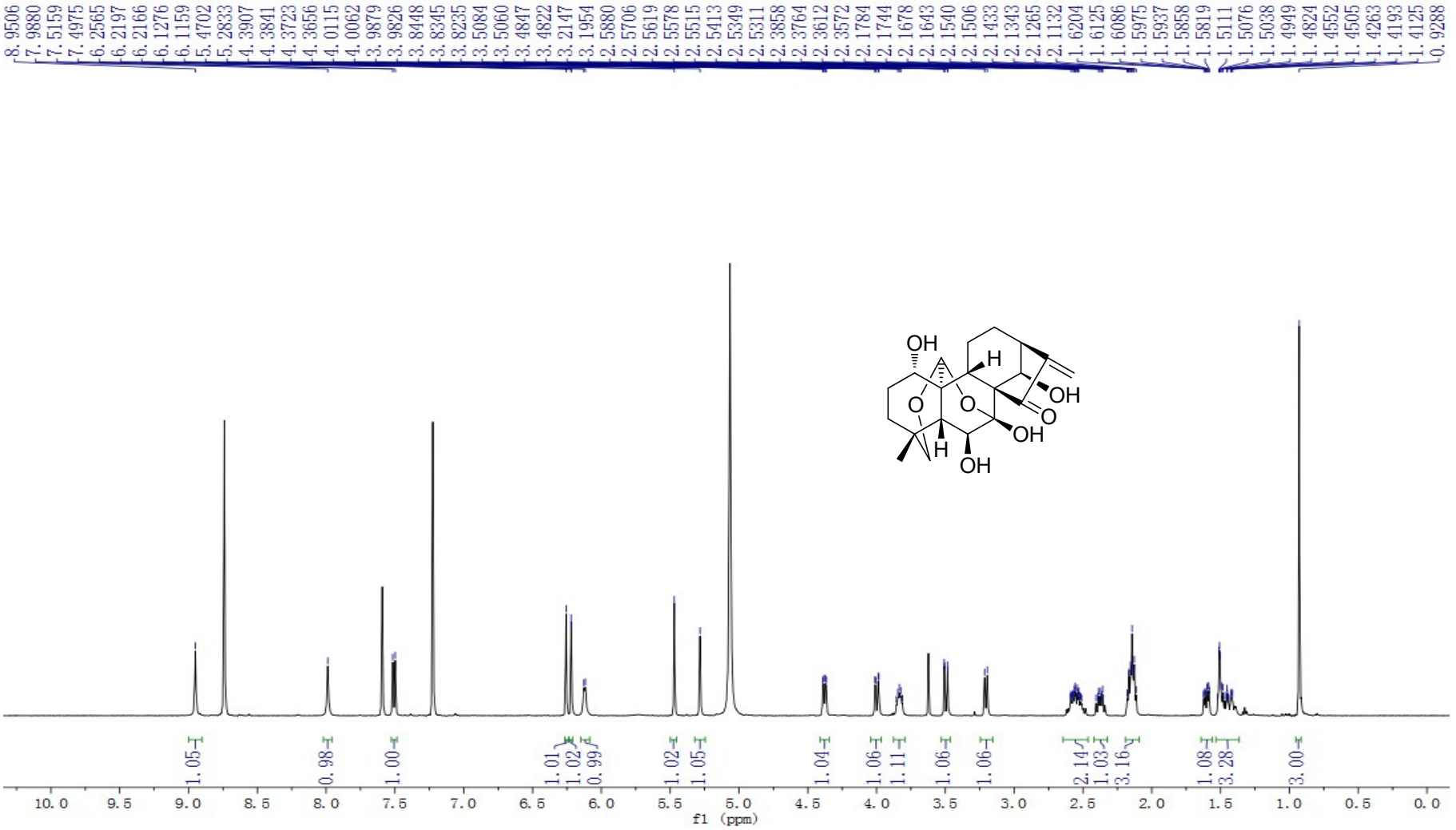


Figure S47. ^{1}H NMR spectrum of compound **6** (Recorded in pyridine-d_5)

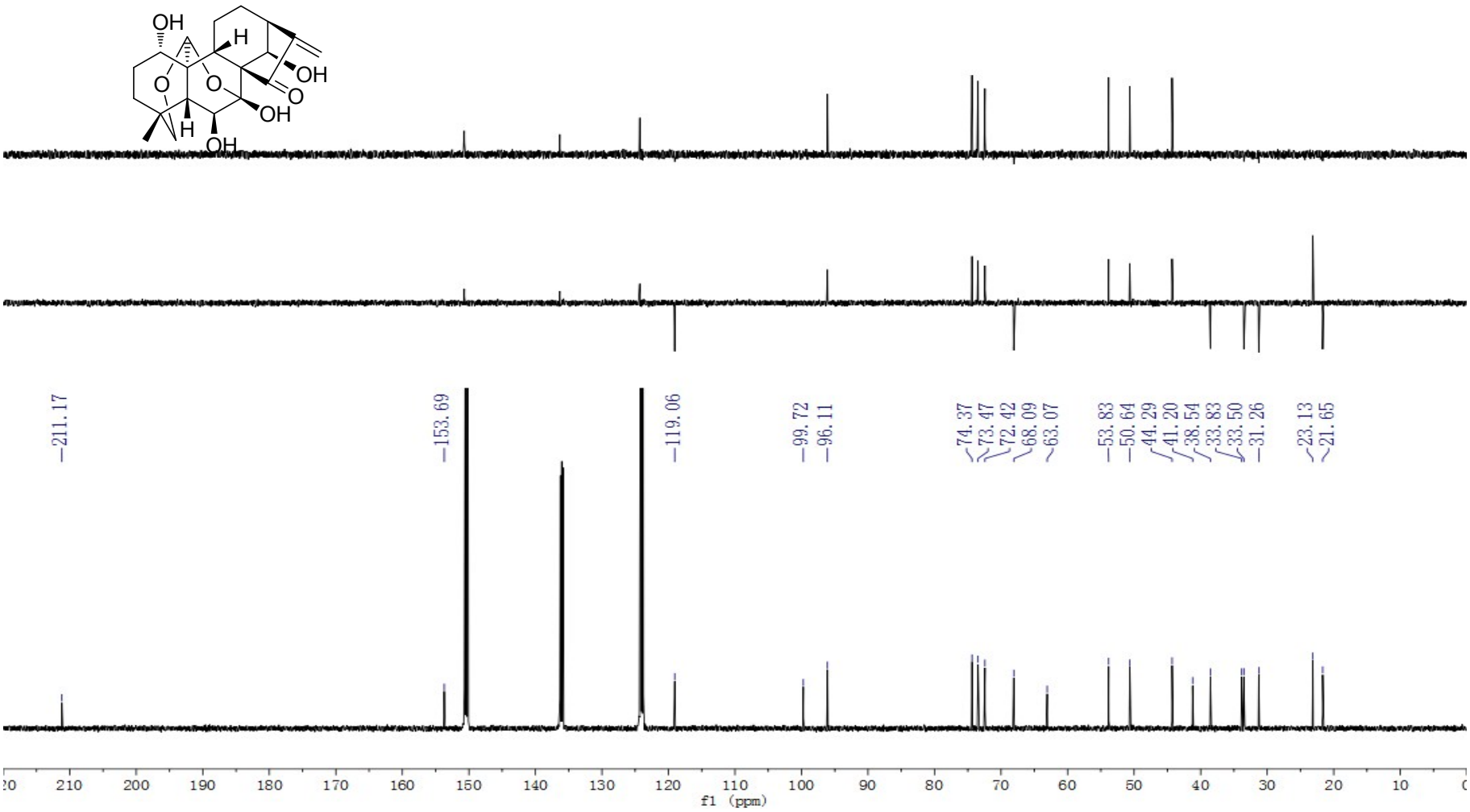


Figure S48. ^{13}C NMR spectrum of compound **6** (Recorded in pyridine-d_5)

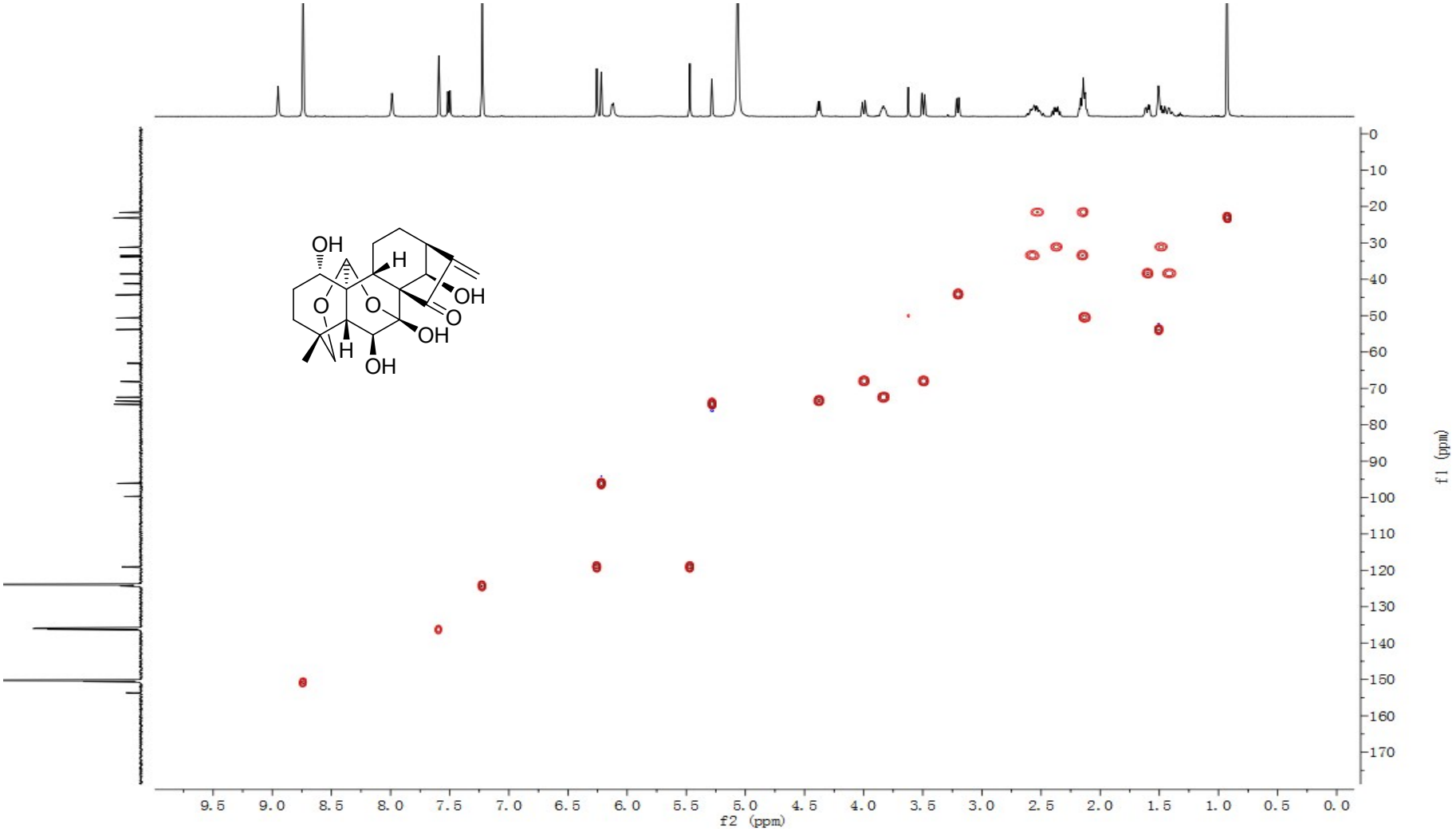


Figure S49. HSQC spectrum of compound **6** (Recorded in pyridine-d_5)

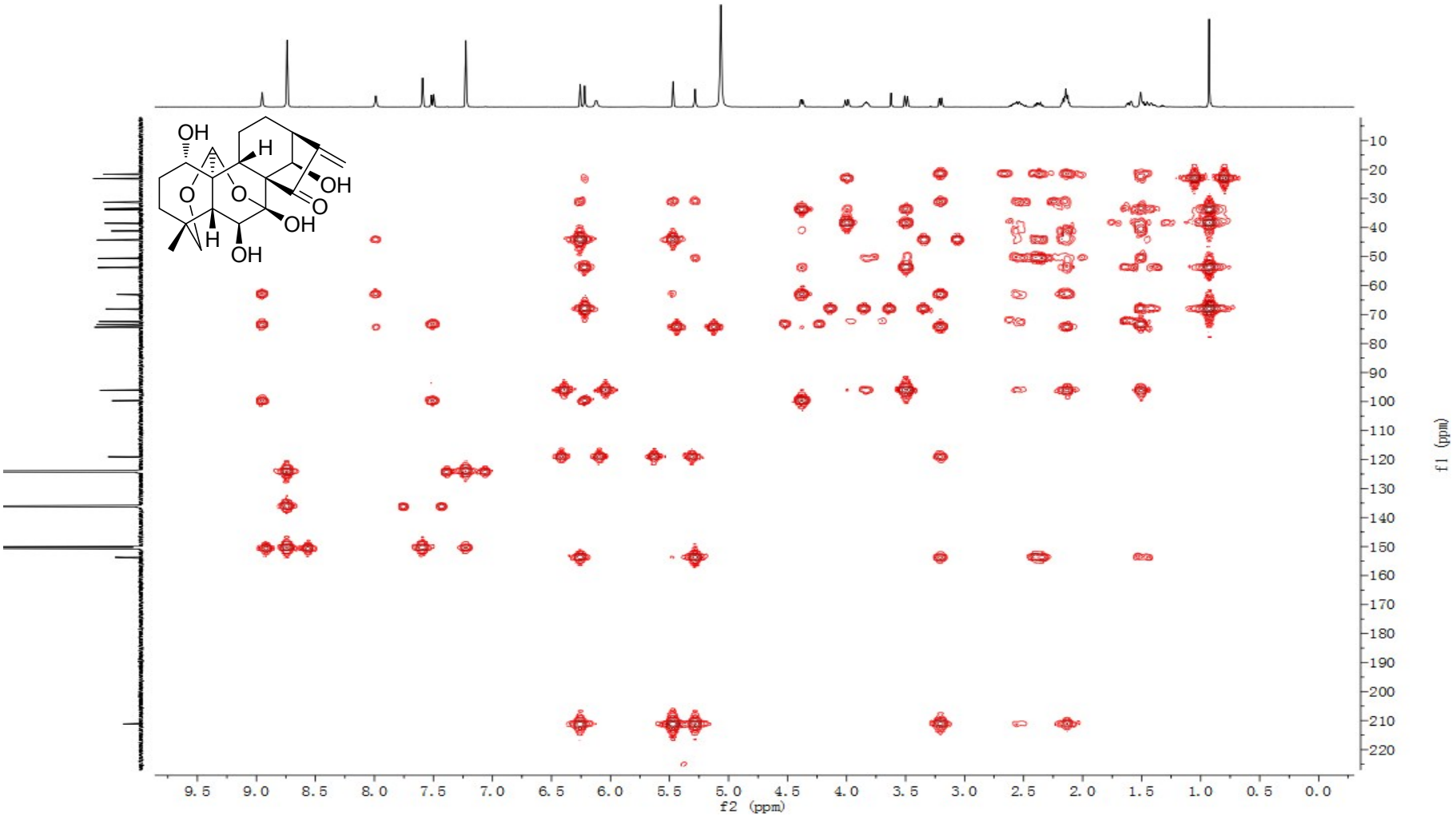


Figure S50. HMBC spectrum of compound **6** (Recorded in pyridine-d_5)

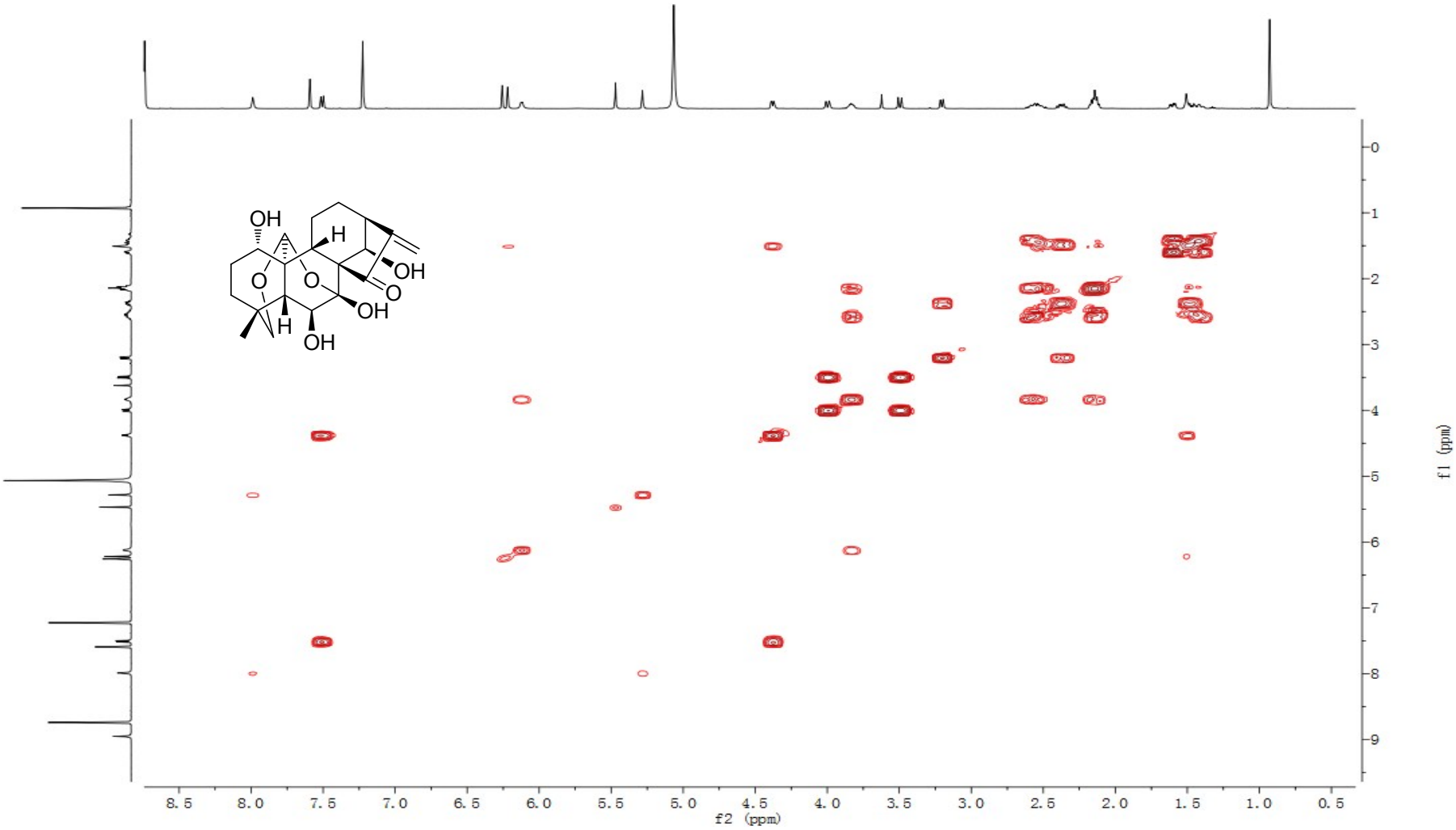


Figure S51. ^{1}H–^{1}H COSY spectrum of compound **6** (Recorded in pyridine-d_5)

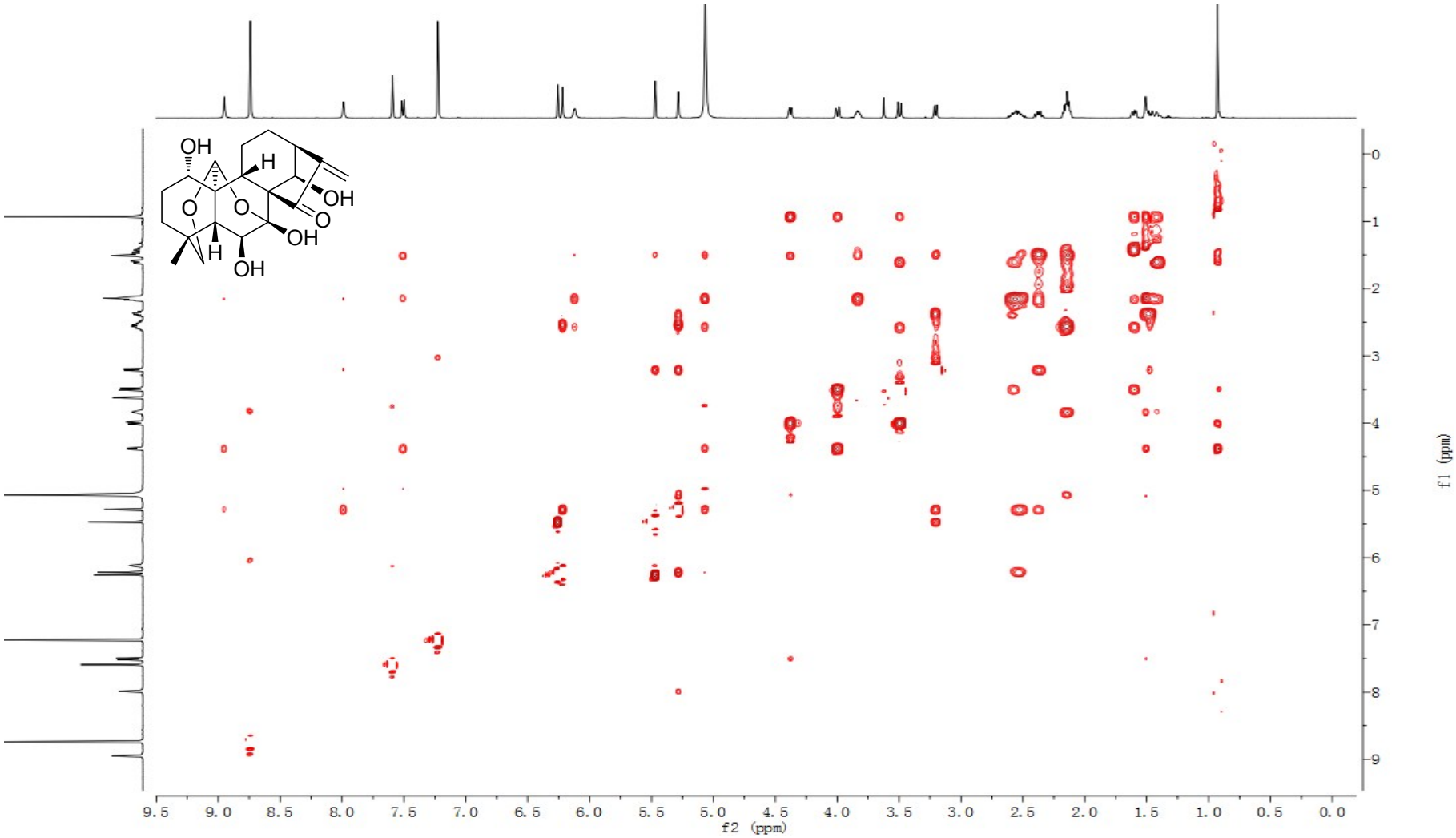


Figure S52. ROESY spectrum of compound **6** (Recorded in pyridine-d_5)

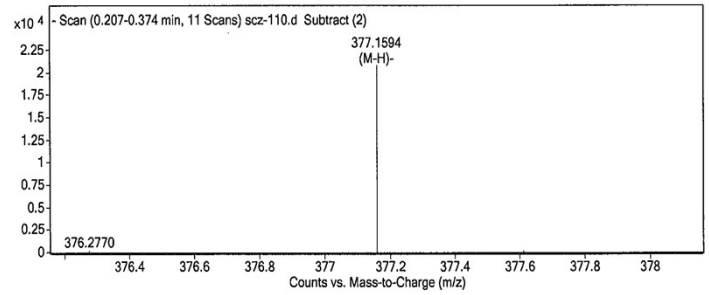
Qualitative Analysis Report

Data Filename	scz-110.d	**Sample Name**	scz-110
Sample Type	Sample	**Position**	P1-C6
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU-ESI-i.m	**Acquired Time**	1/18/2016 10:13:42 AM
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)

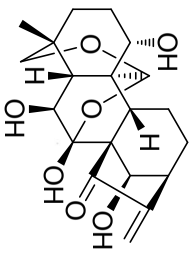
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
89.0247	1	1453.03		
359.1493	1	3614.41		
360.154	1	674.91		
377.1594	1	20838.25	C20 H26 O7	(M-H)-
378.163	1	4720.65	C20 H26 O7	(M-H)-
379.1656	1	864.03	C20 H26 O7	(M-H)-
413.1375	1	1980.77		
423.163	1	2480.15		



Formula Calculator Element Limits

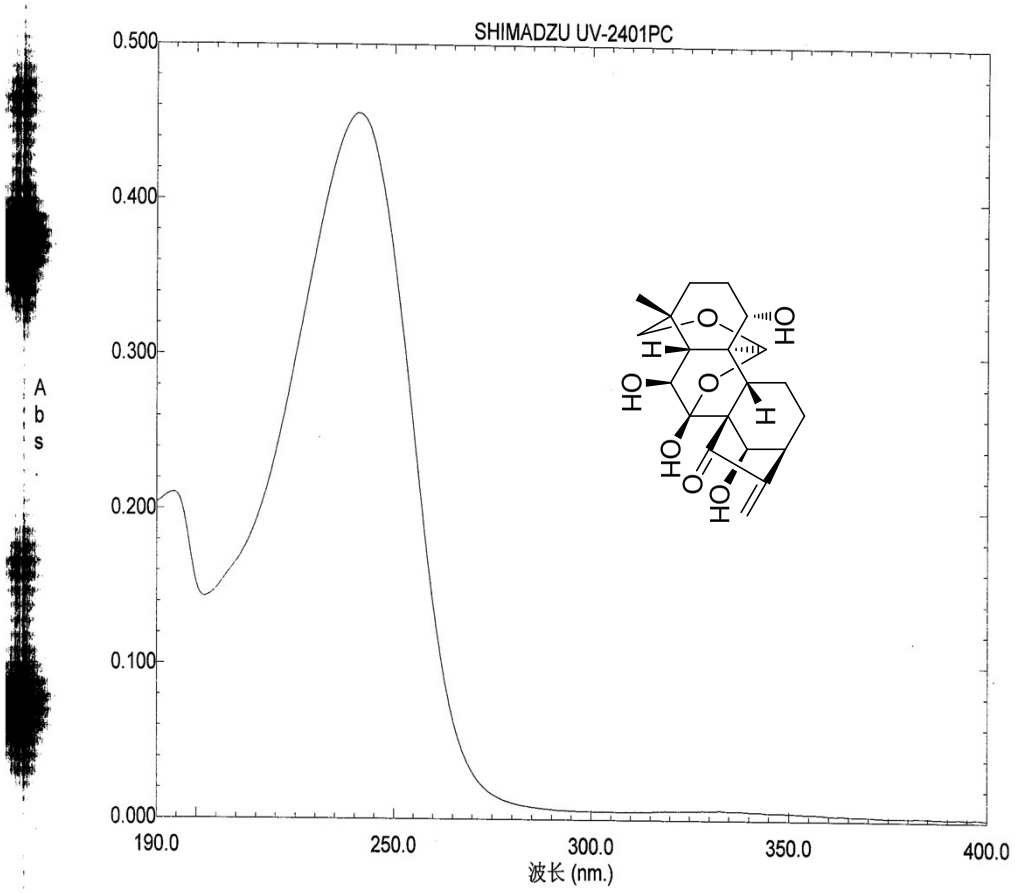
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H26 O7	378.1679	377.1606	377.1594	1.1	3.0	8.0000

--- End Of Report ---

Figure S53. HRESIMS spectrum of compound **6**



文件名: SCZ-110

SCZ-110———

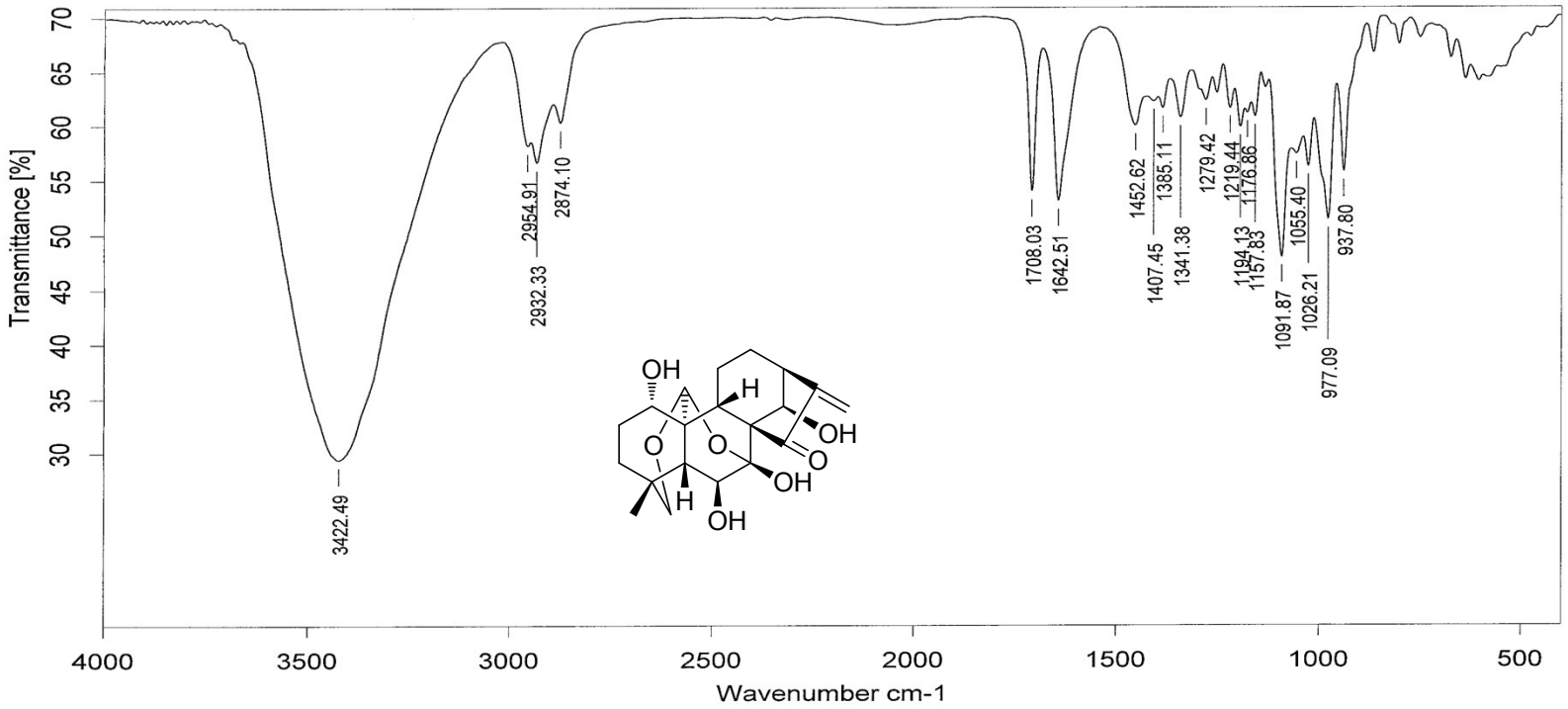
样品浓度：0.0304毫克/毫升
溶剂：甲醇

创建于: 10:04 16-01-27
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	241.00	0.4554
2	194.20	0.2106

Figure S54. UV spectrum of compound **6**



Sample : scz-110	Frequency Range : 399.246 - 3996.32	Measured on : 25/01/2016	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 160125IR6	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S55. IR spectrum of compound **6**

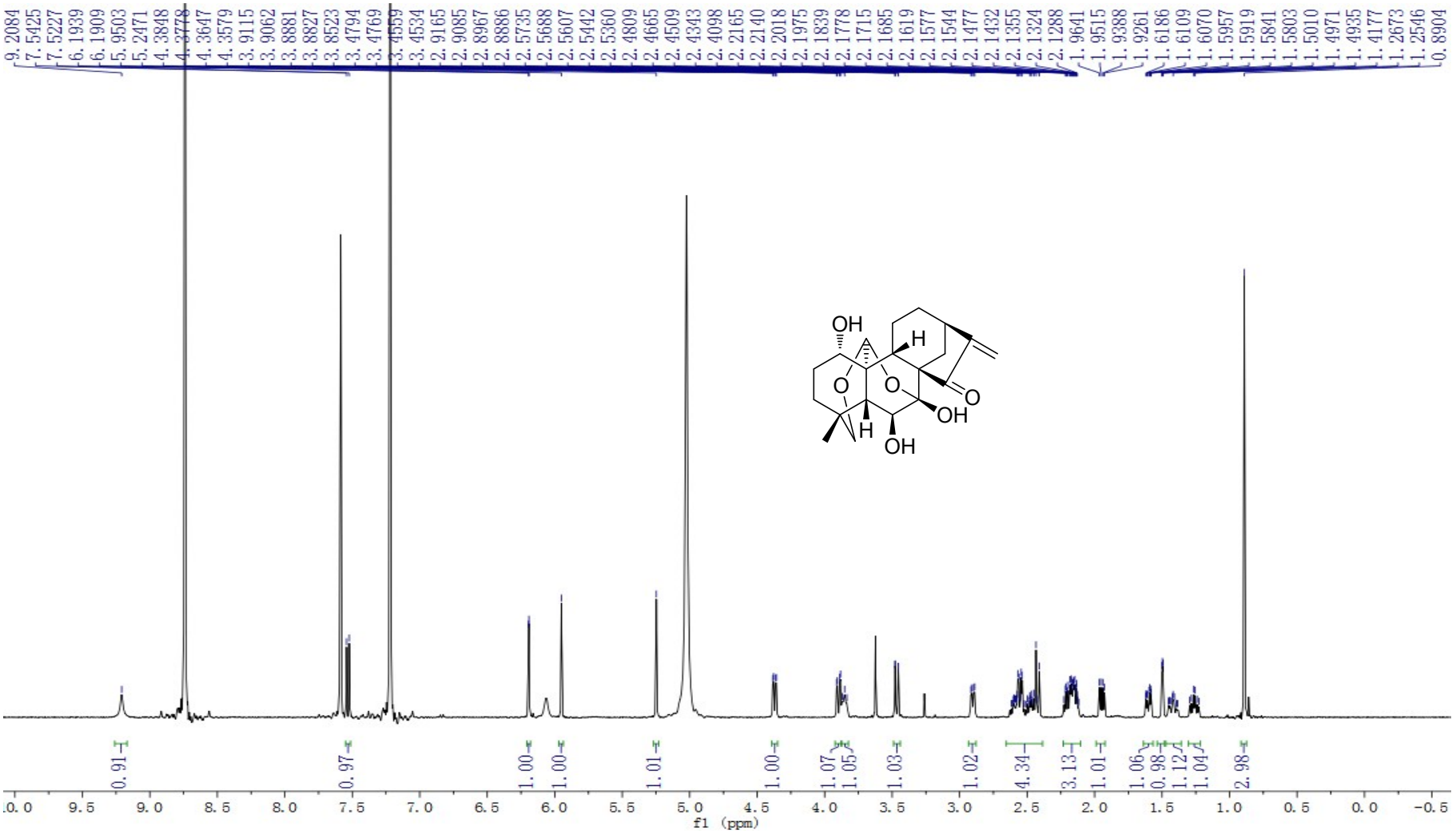


Figure S56. ^{1}H NMR spectrum of compound **7** (Recorded in pyridine-d_5)

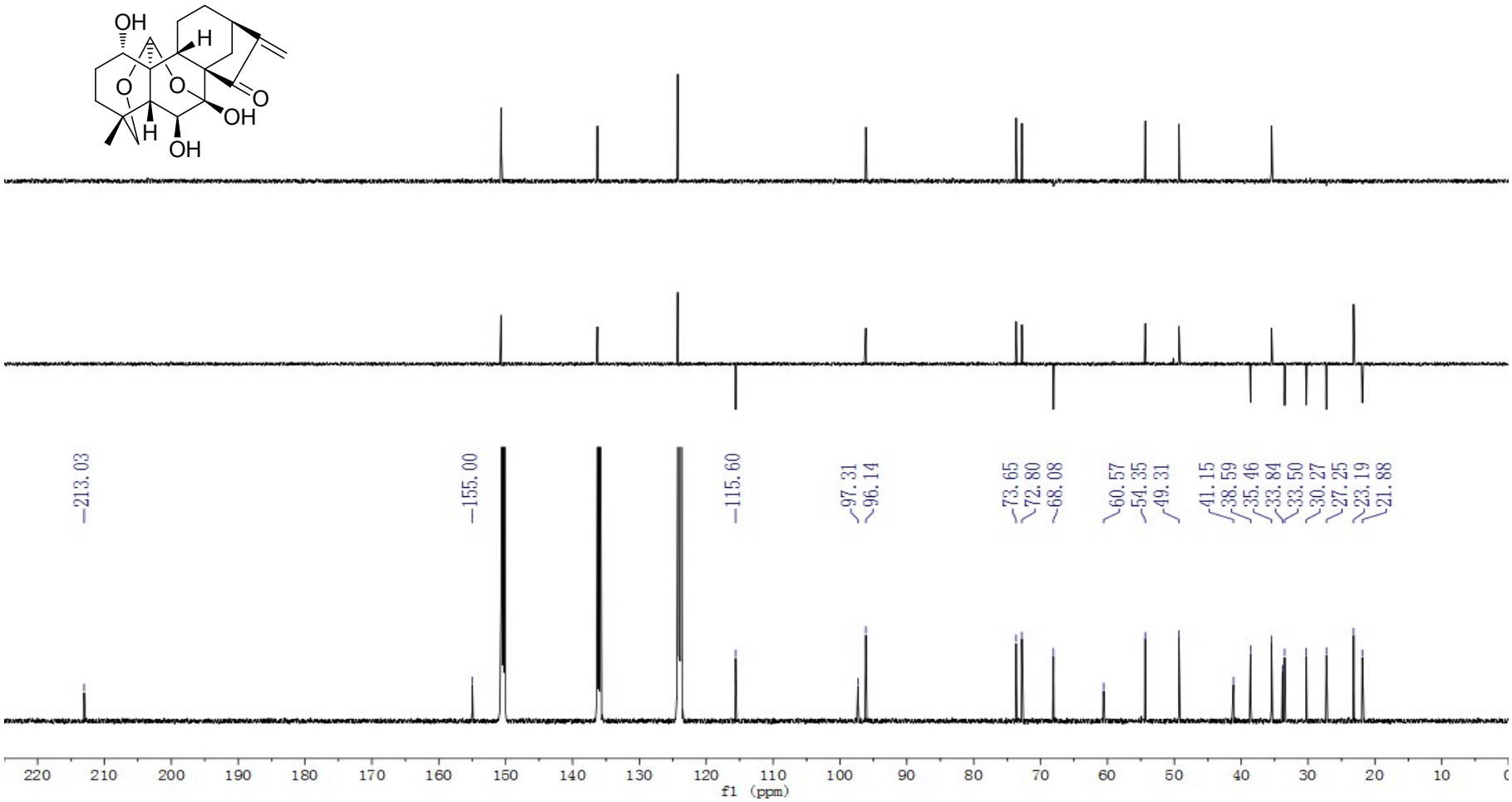


Figure S57. ^{13}C NMR spectrum of compound **7** (Recorded in pyridine-d_5)

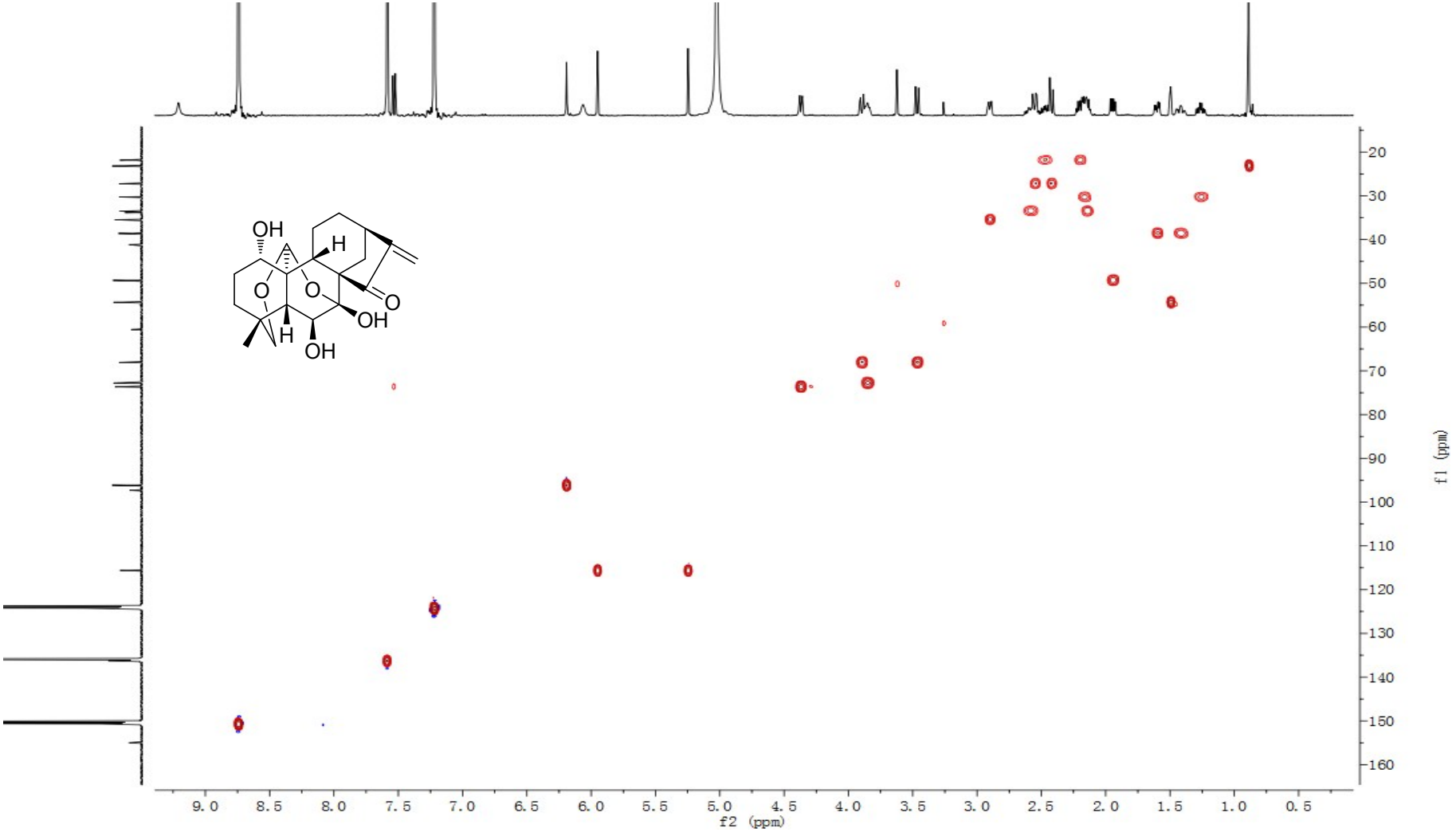


Figure S58. HSQC spectrum of compound **7** (Recorded in pyridine-d_5)

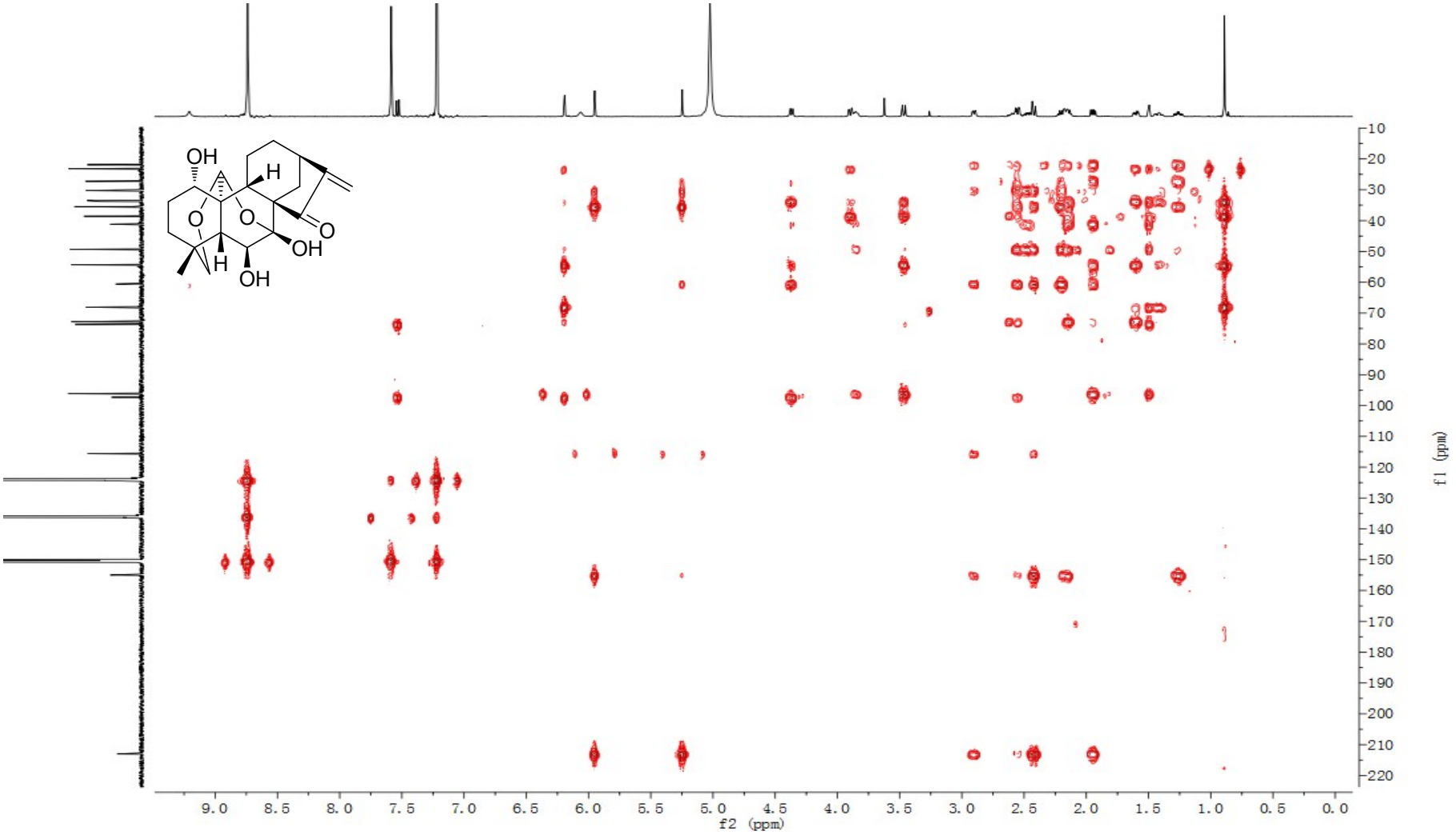


Figure S59. HMBC spectrum of compound **7** (Recorded in pyridine-d_5)

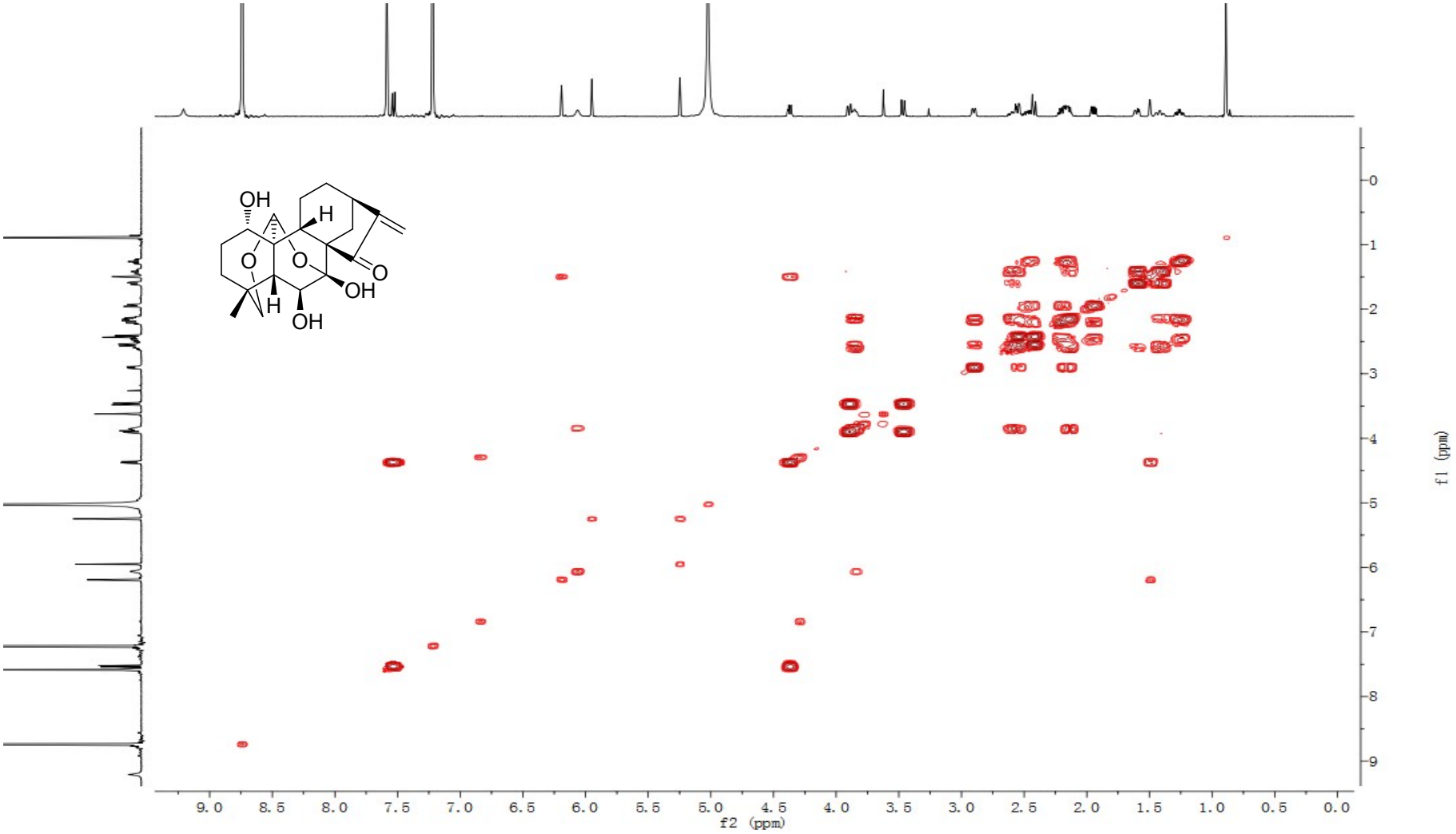


Figure S60. ^{1}H–^{1}H COSY spectrum of compound **7** (Recorded in pyridine-d_5)

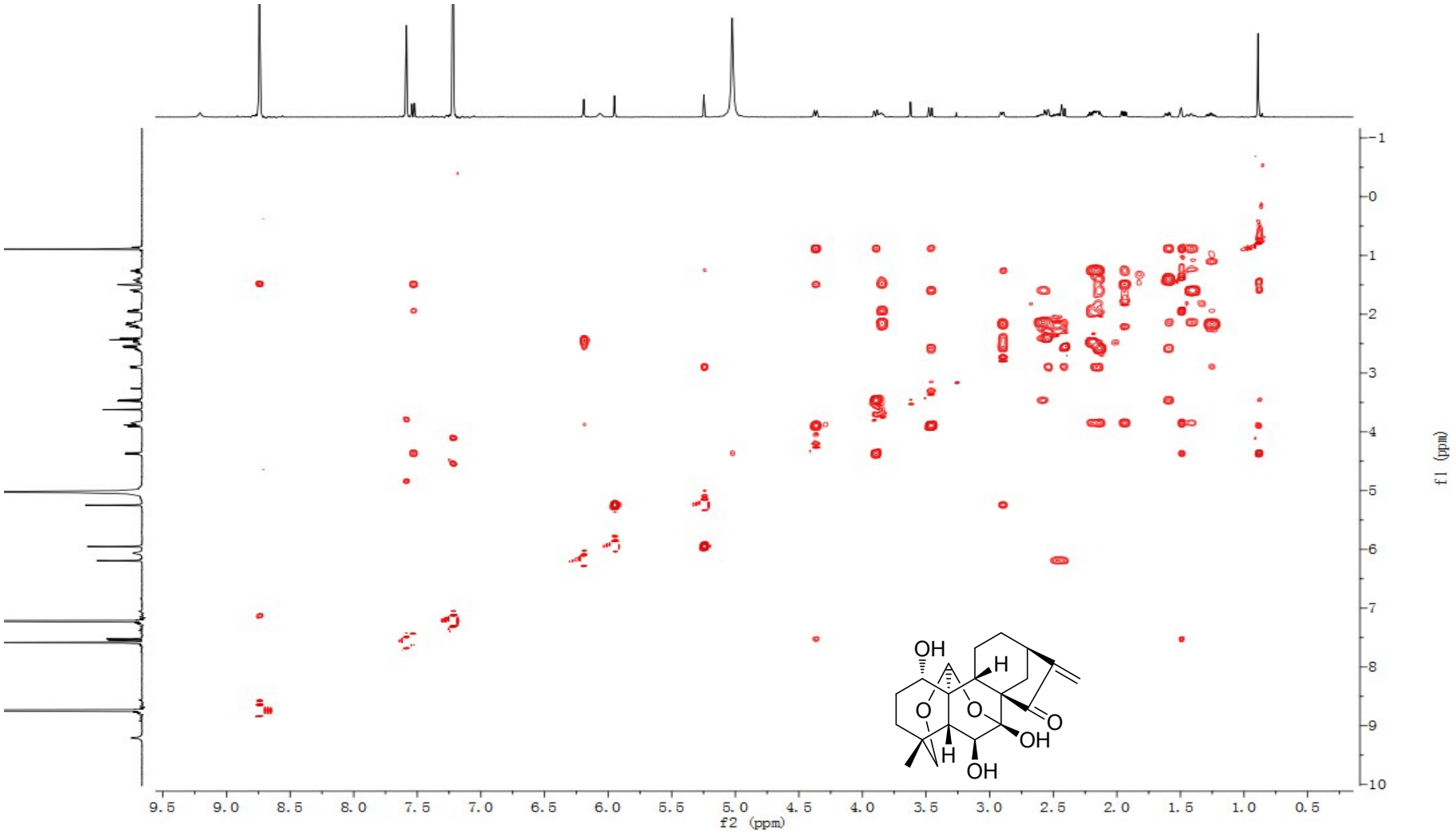


Figure S61. ROESY spectrum of compound **7** (Recorded in pyridine-d_5)

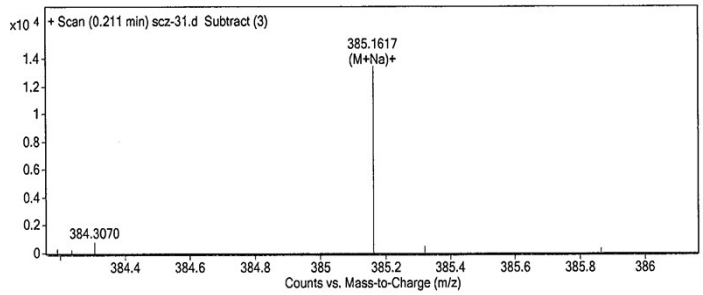
Qualitative Analysis Report

Data Filename	scz-31.d	**Sample Name**	scz-31
Sample Type	Sample	**Position**	P1-B5
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/14/2015 4:11:18 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)

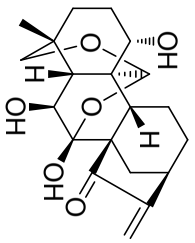
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
274.2742	1	36771.67		
302.3055	1	9222.46		
318.3	1	23783.22		
346.331		7649.91		
363.18	1	11071.24		
385.1617	1	13497.4	C20 H26 O6	(M+Na)+
401.1365	1	12031.1		
453.167	1	22502.33		



Formula Calculator Element Limits

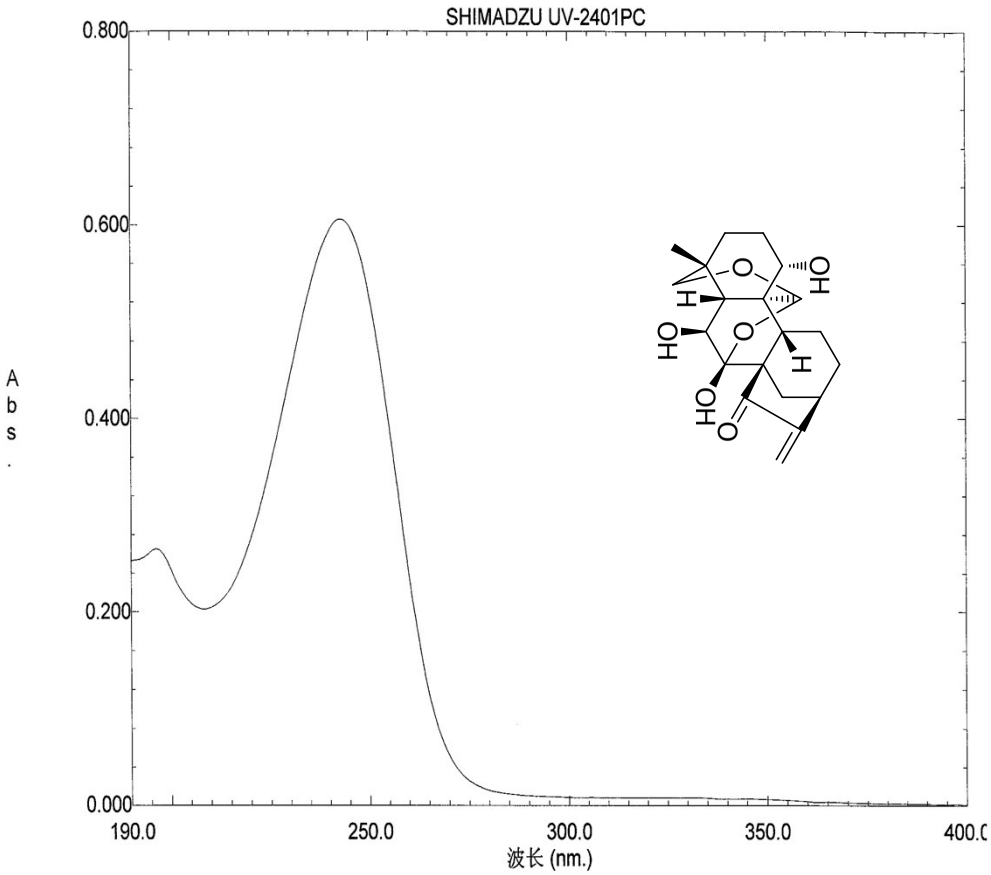
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H26 O6	362.1729	385.1622	385.1617	0.3	0.7	8.0000

--- End Of Report ---

Figure S62. HRESIMS spectrum of compound **7**



文件名: SCZ-31

SCZ-31 ———

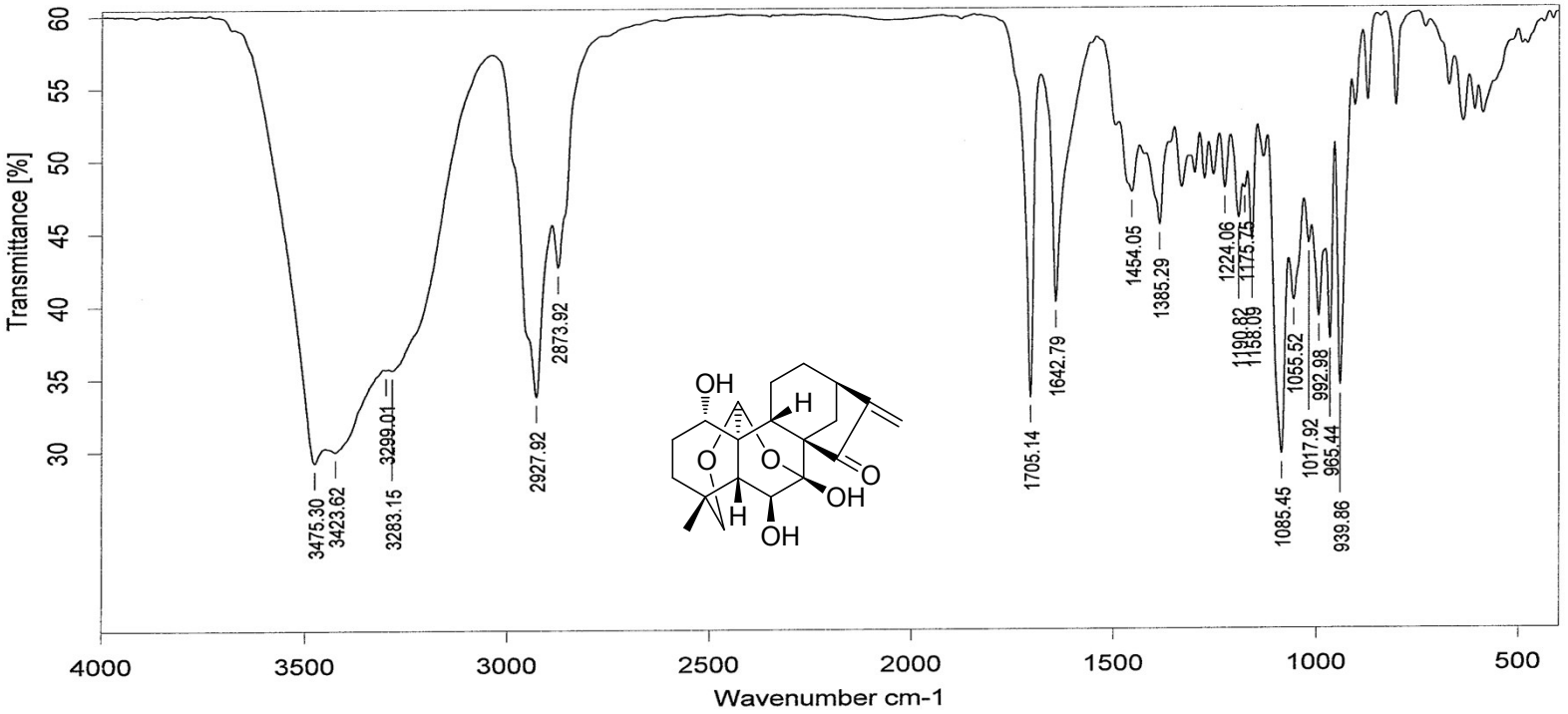
样品浓度：0.0319毫克/毫升
溶剂：甲醇

创建于: 15:40 15-09-19
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	345.80	0.0069
2	242.80	0.6055
3	196.40	0.2650

Figure S63. UV spectrum of compound **7**



Sample : scz-31	Frequency Range : 399.246 - 3996.32	Measured on : 24/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150924IR7	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S64. IR spectrum of compound **7**

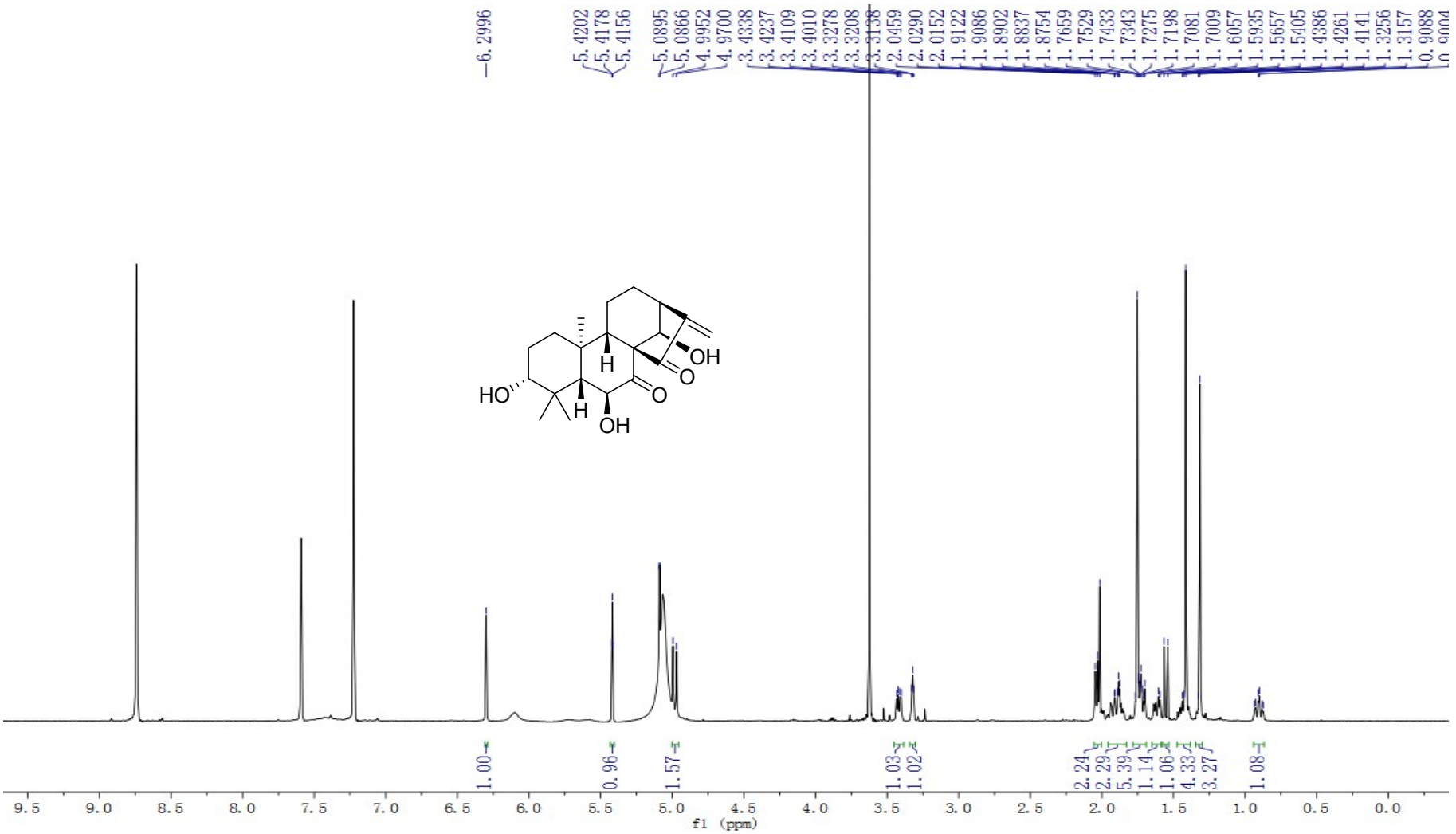


Figure S65. ^{1}H NMR spectrum of compound **8** (Recorded in pyridine-d_5)

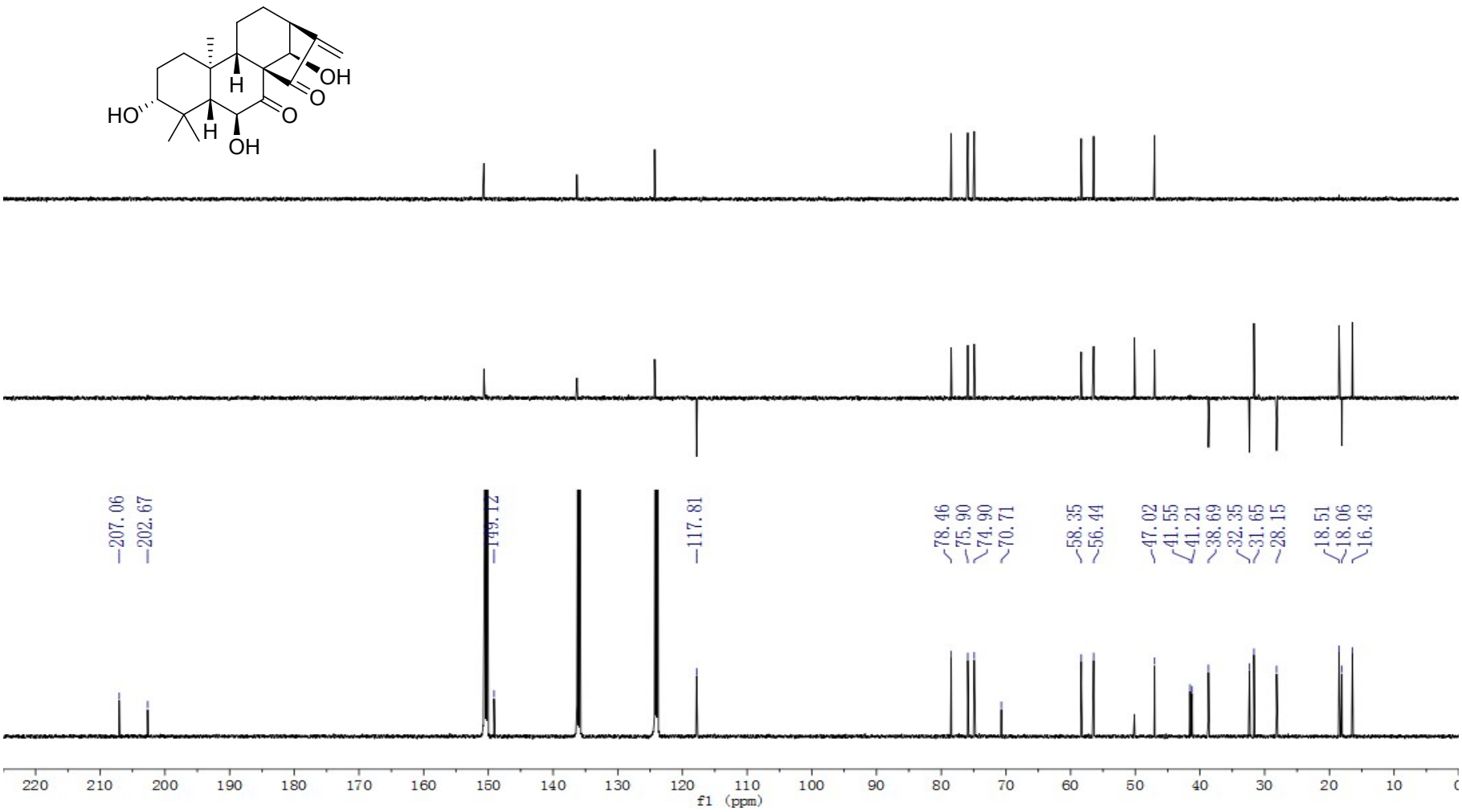


Figure S66. ^{13}C NMR spectrum of compound **8** (Recorded in pyridine-d_5)

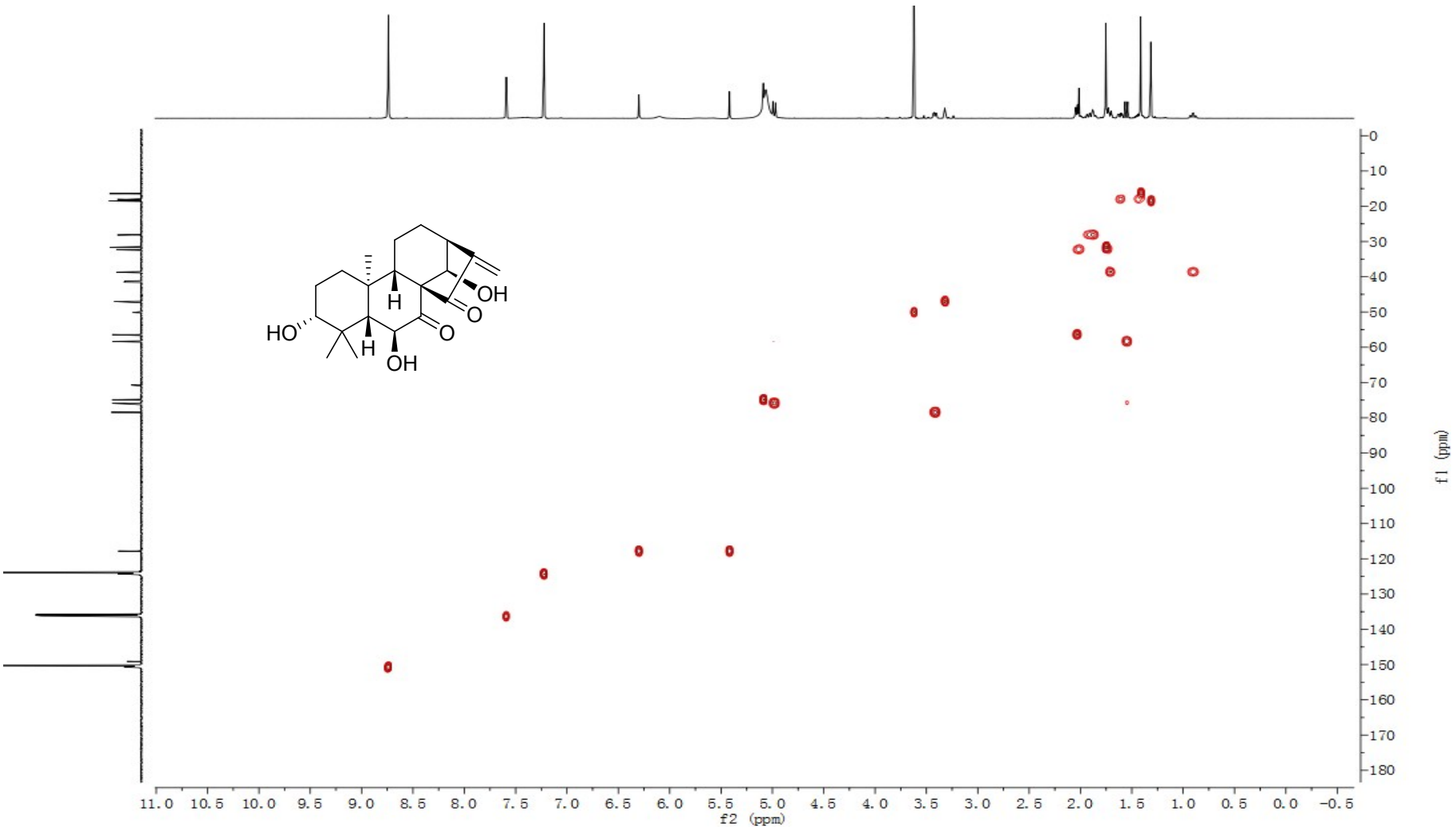


Figure S67. HSQC spectrum of compound **8** (Recorded in pyridine-d_5)

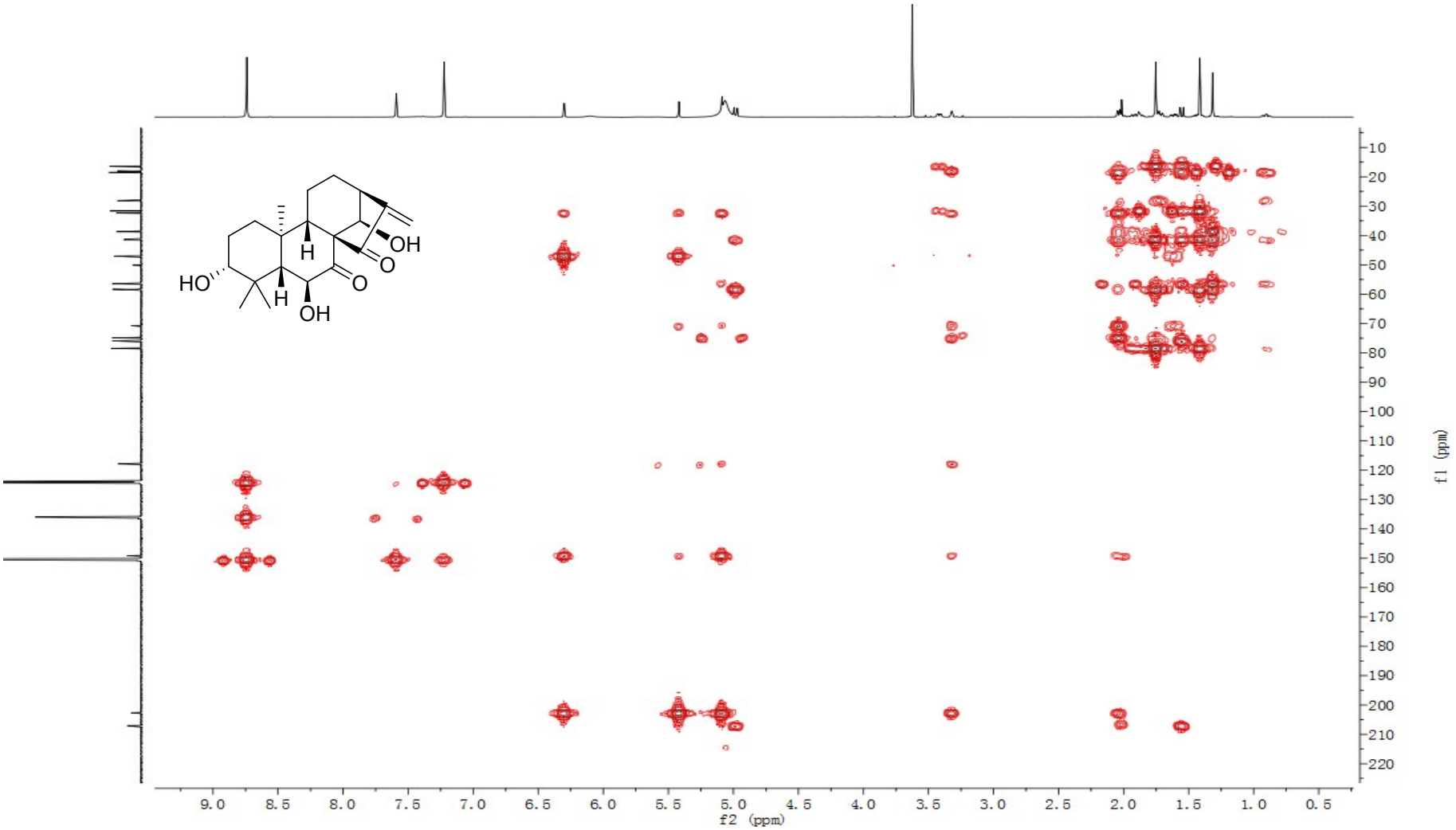


Figure S68. HMBC spectrum of compound **8** (Recorded in pyridine-d_5)

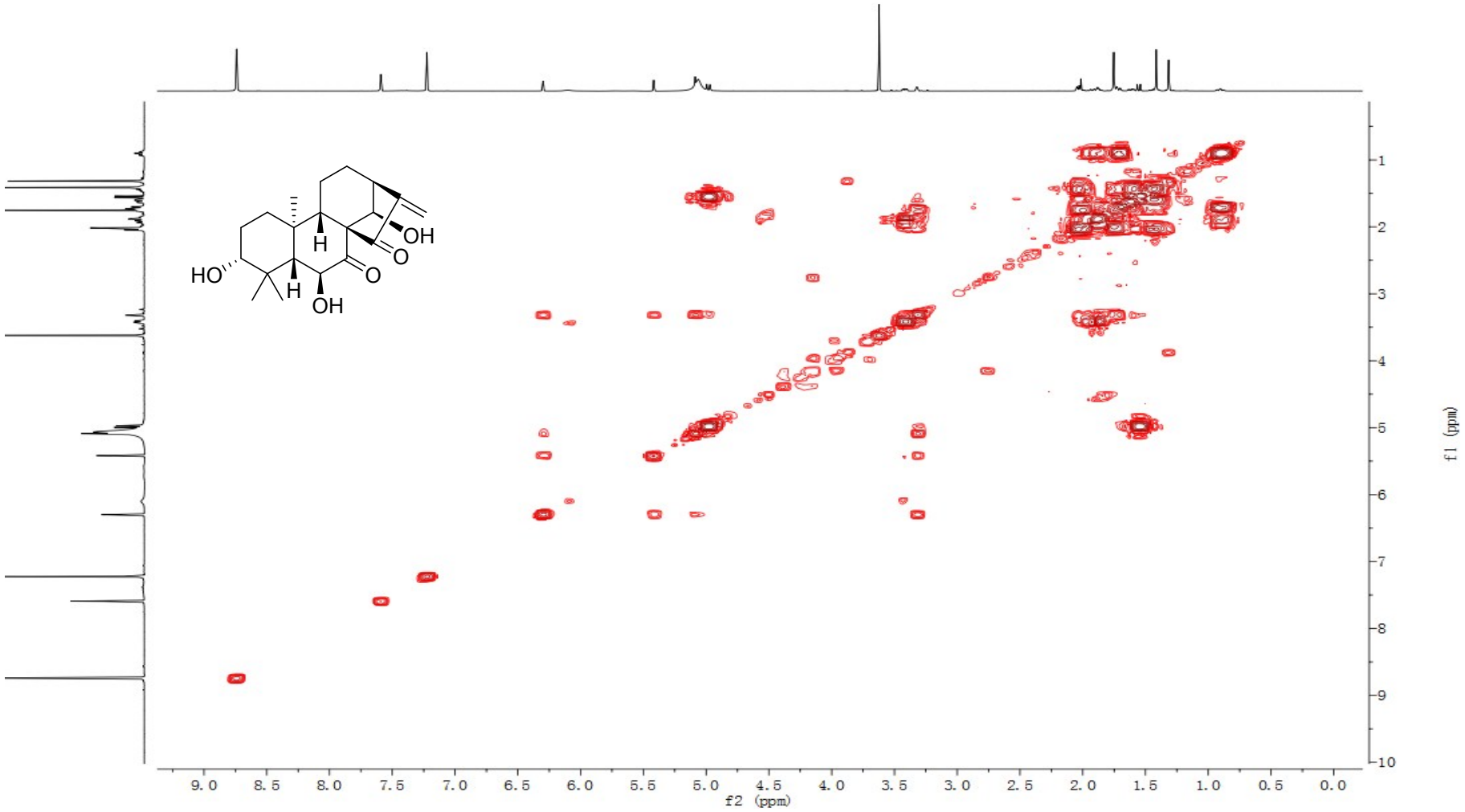


Figure S69. ^{1}H–^{1}H COSY spectrum of compound **8** (Recorded in pyridine-d_5)

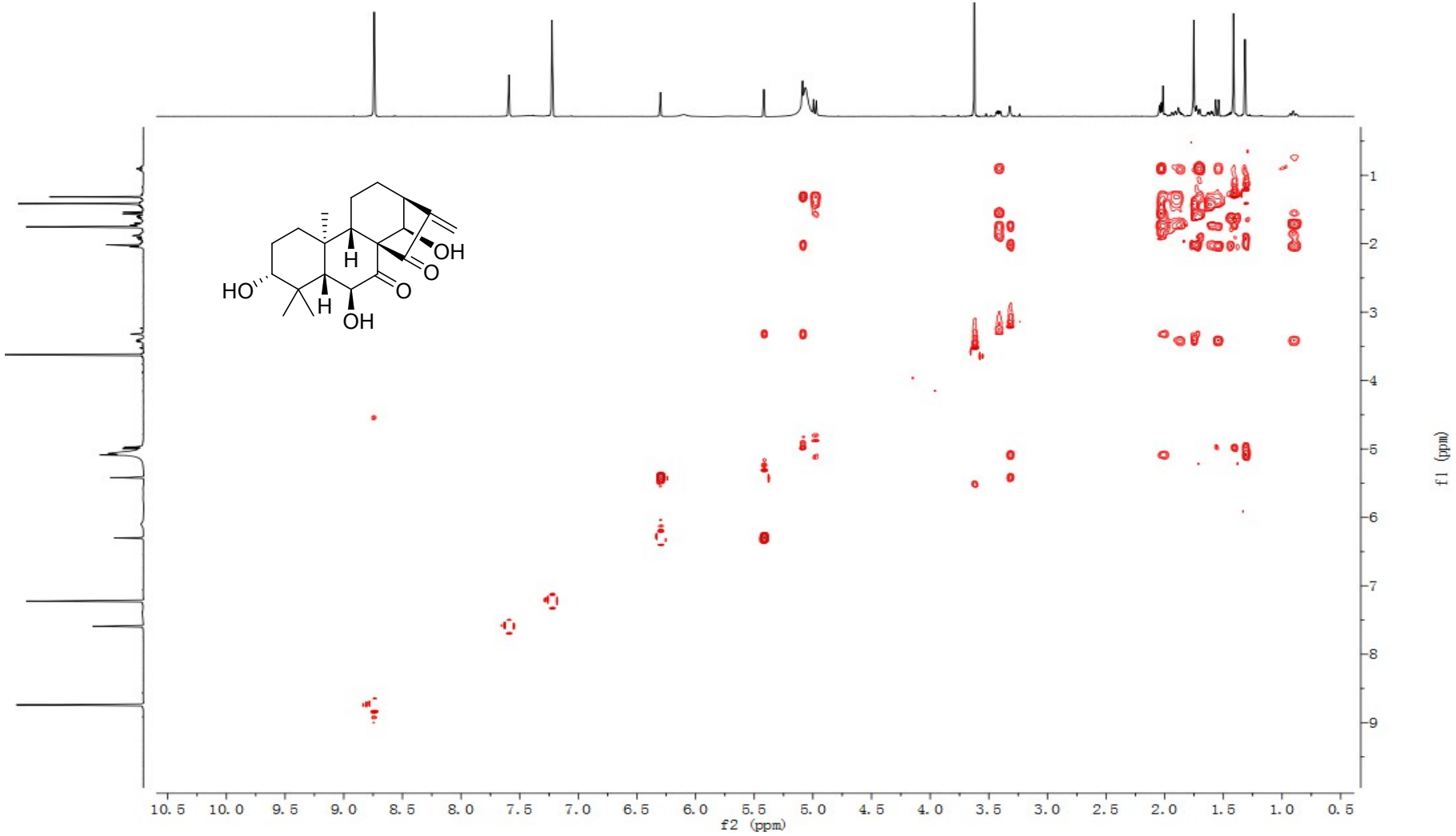


Figure S70. ROESY spectrum of compound **8** (Recorded in pyridine-d_5)

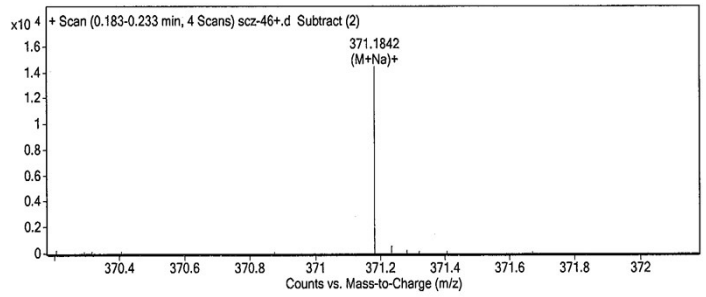
Qualitative Analysis Report

Data Filename	scz-46+.d	**Sample Name**	scz-46
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/15/2015 10:41:47 AM
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)

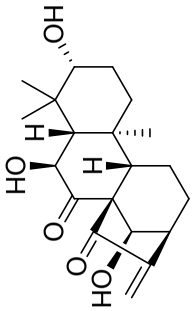
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund
274.2745	1	210409.84
290.2693	1	36682.04
302.3056	1	59554.64
318.3008	1	157119.78
330.3369	1	51515.18
346.3319	1	53366.46
362.3266	1	37519.59
374.363	1	42969.08



Formula Calculator Element Limits

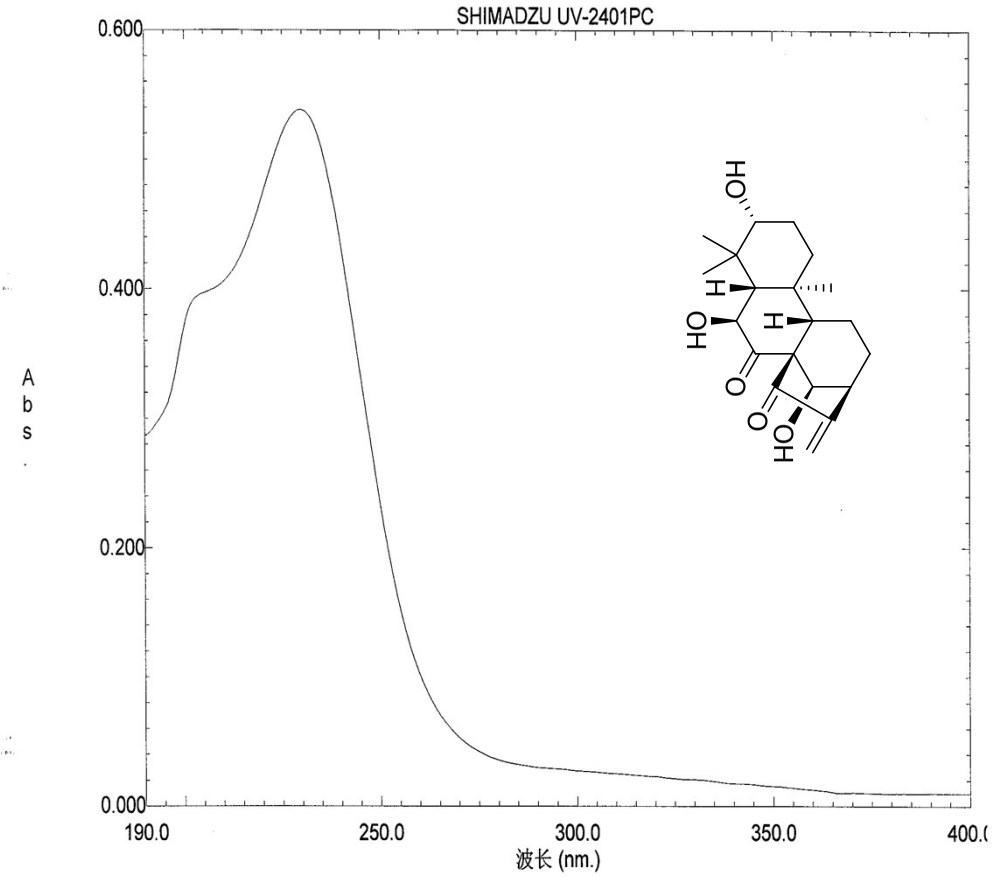
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H28 O5	348.1937	371.1829	371.1842	-1.3	-3.7	7.0000

--- End Of Report ---

Figure S71. HRESIMS spectrum of compound **8**



文件名: SCZ-46

SCZ-46 ———

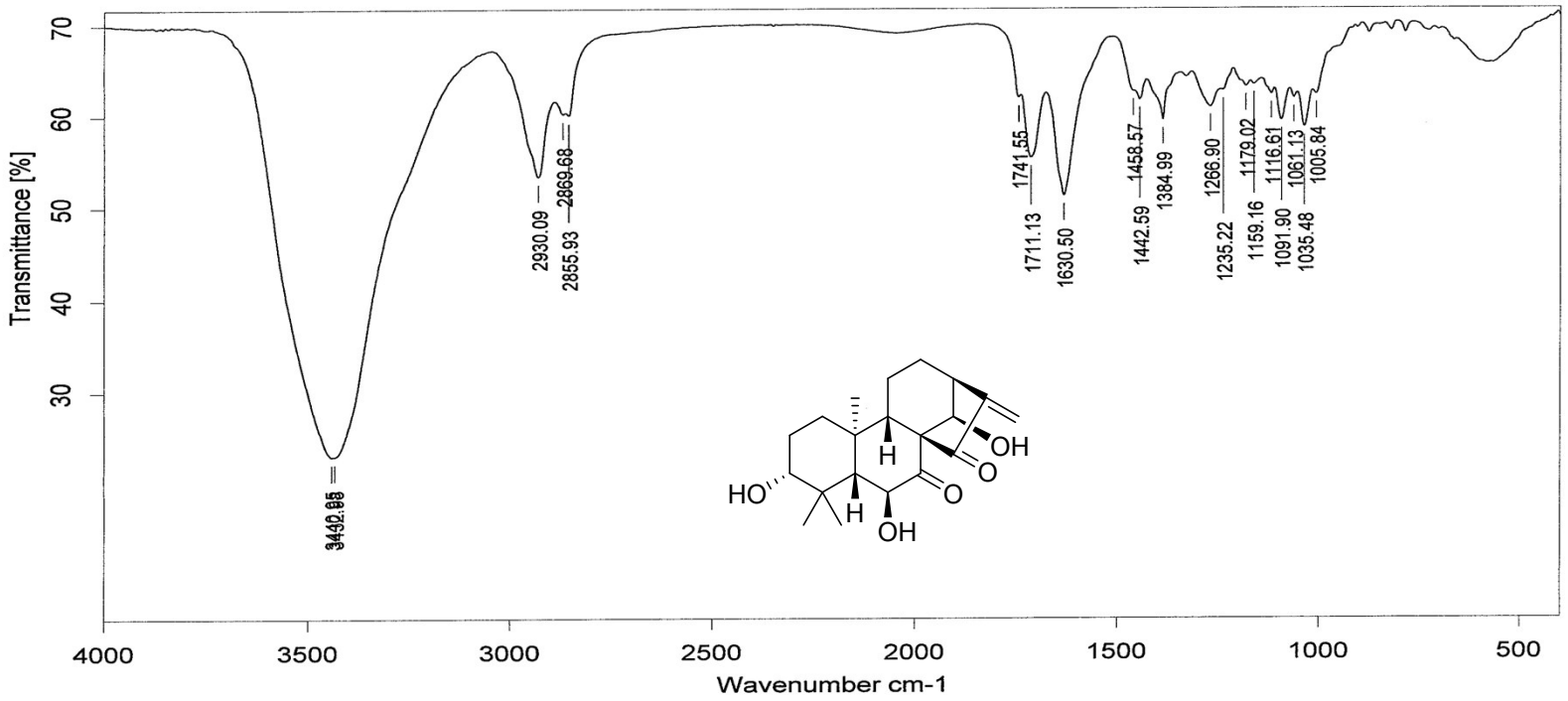
样品浓度：0.0310毫克/毫升
溶剂：甲醇

创建于: 16:34 15-09-19
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	204.80	0.3962
2	229.20	0.5379

Figure S72. UV spectrum of compound **8**



Sample : scz-46	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150925IR3	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S73. IR spectrum of compound **8**

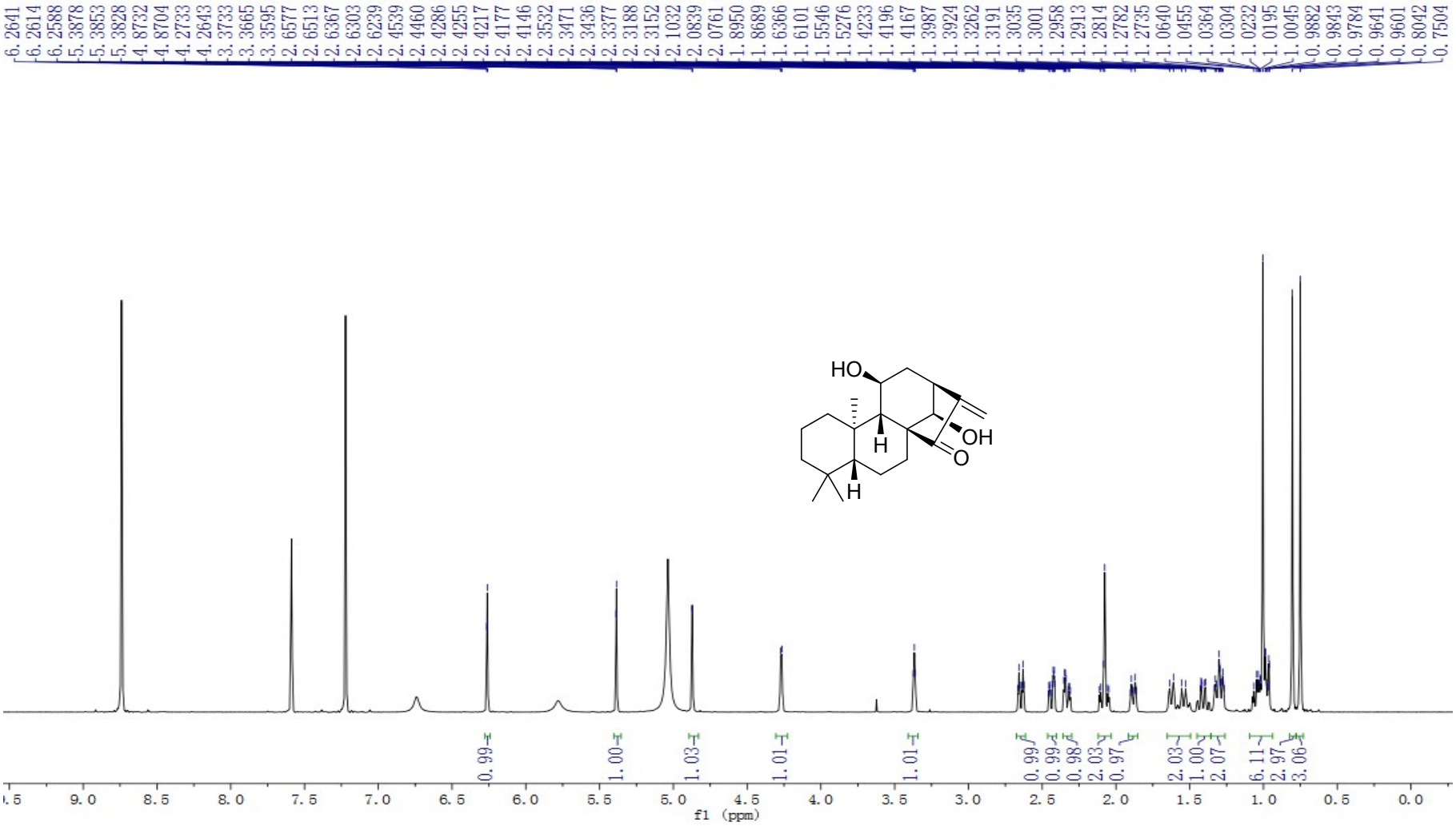


Figure S74. ^{1}H NMR spectrum of compound **9** (Recorded in pyridine-d_5)

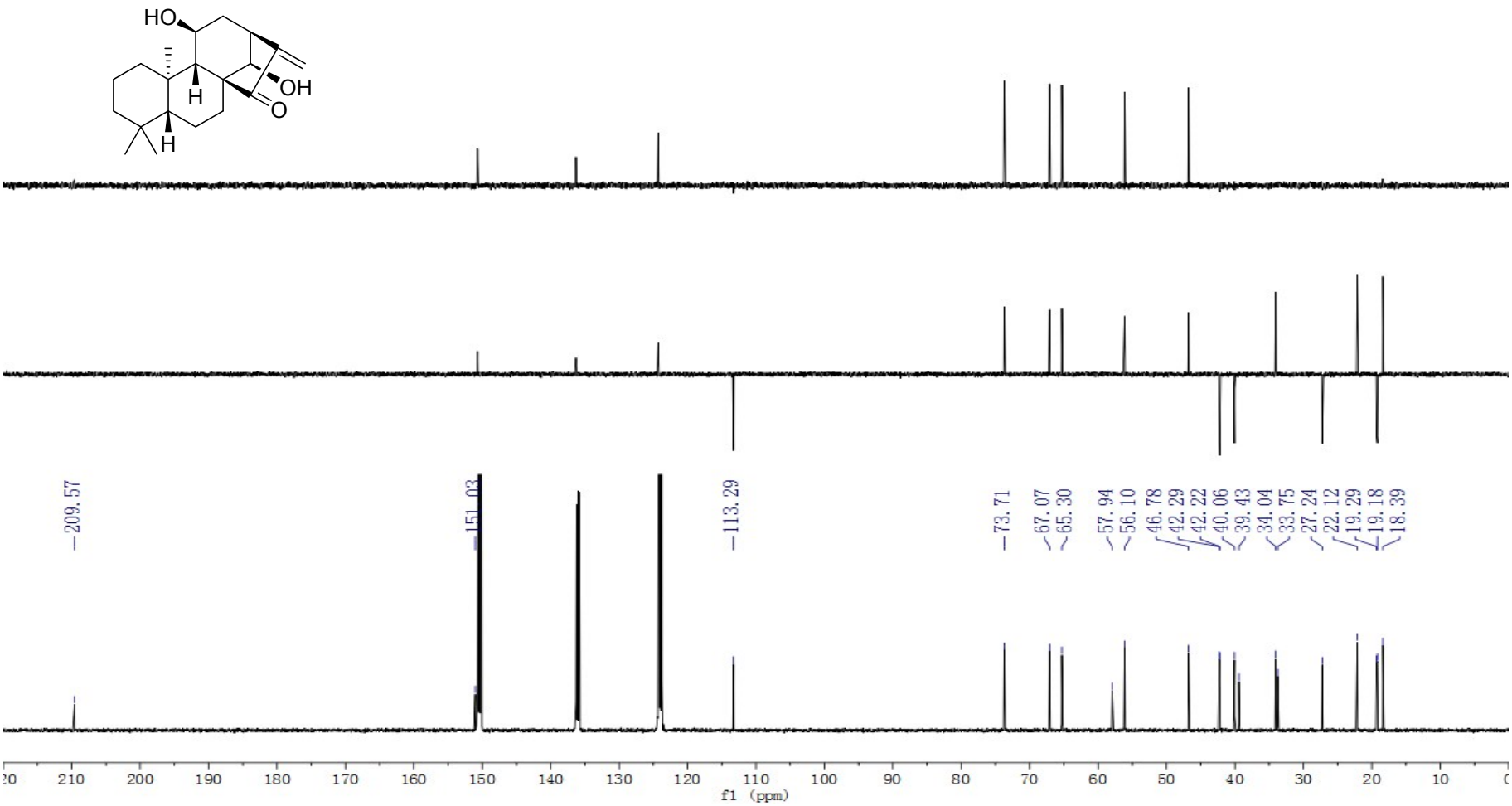


Figure S75. ^{13}C NMR spectrum of compound **9** (Recorded in pyridine-d_5)

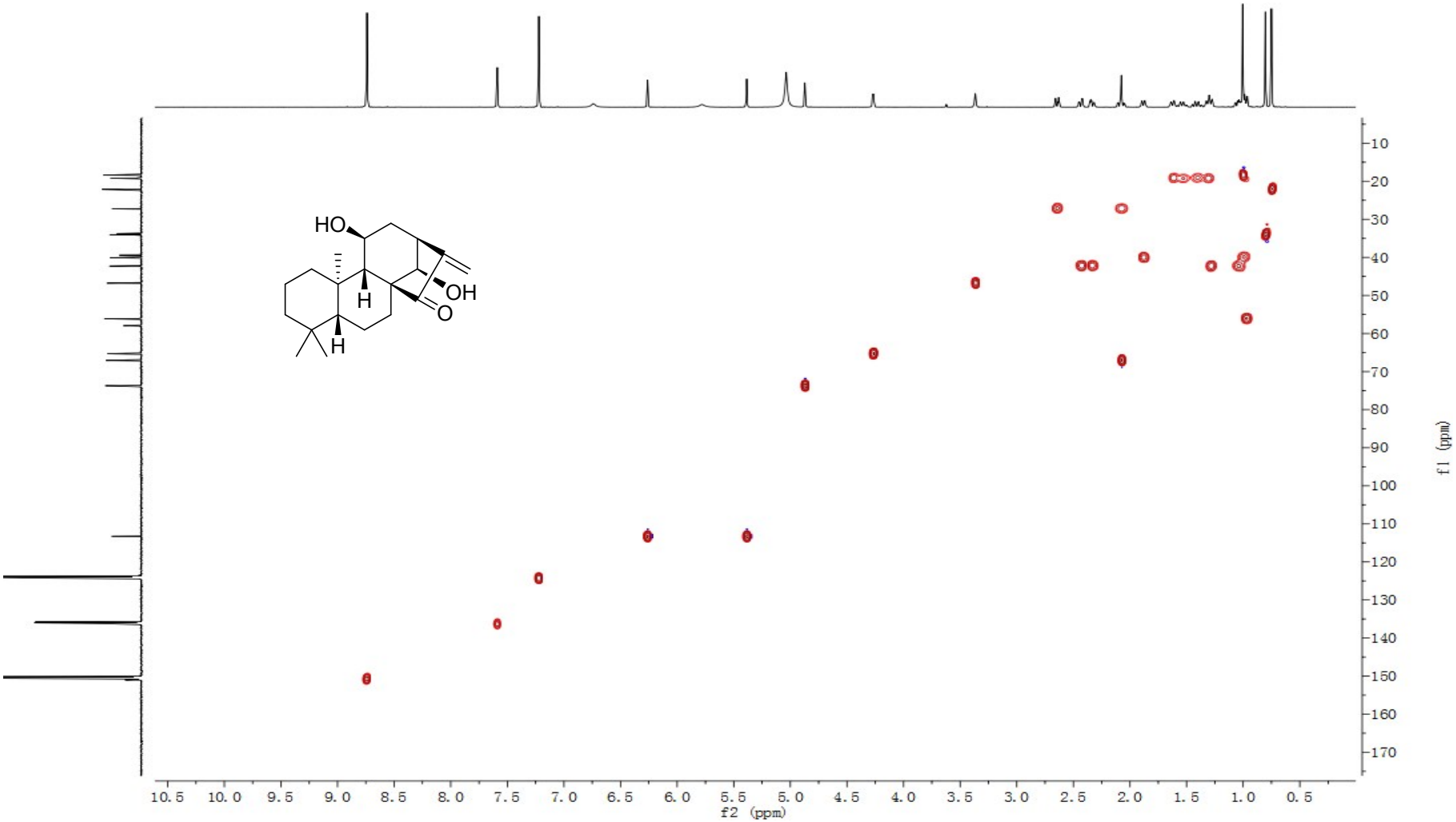


Figure S76. HSQC spectrum of compound **9** (Recorded in pyridine-d_5)

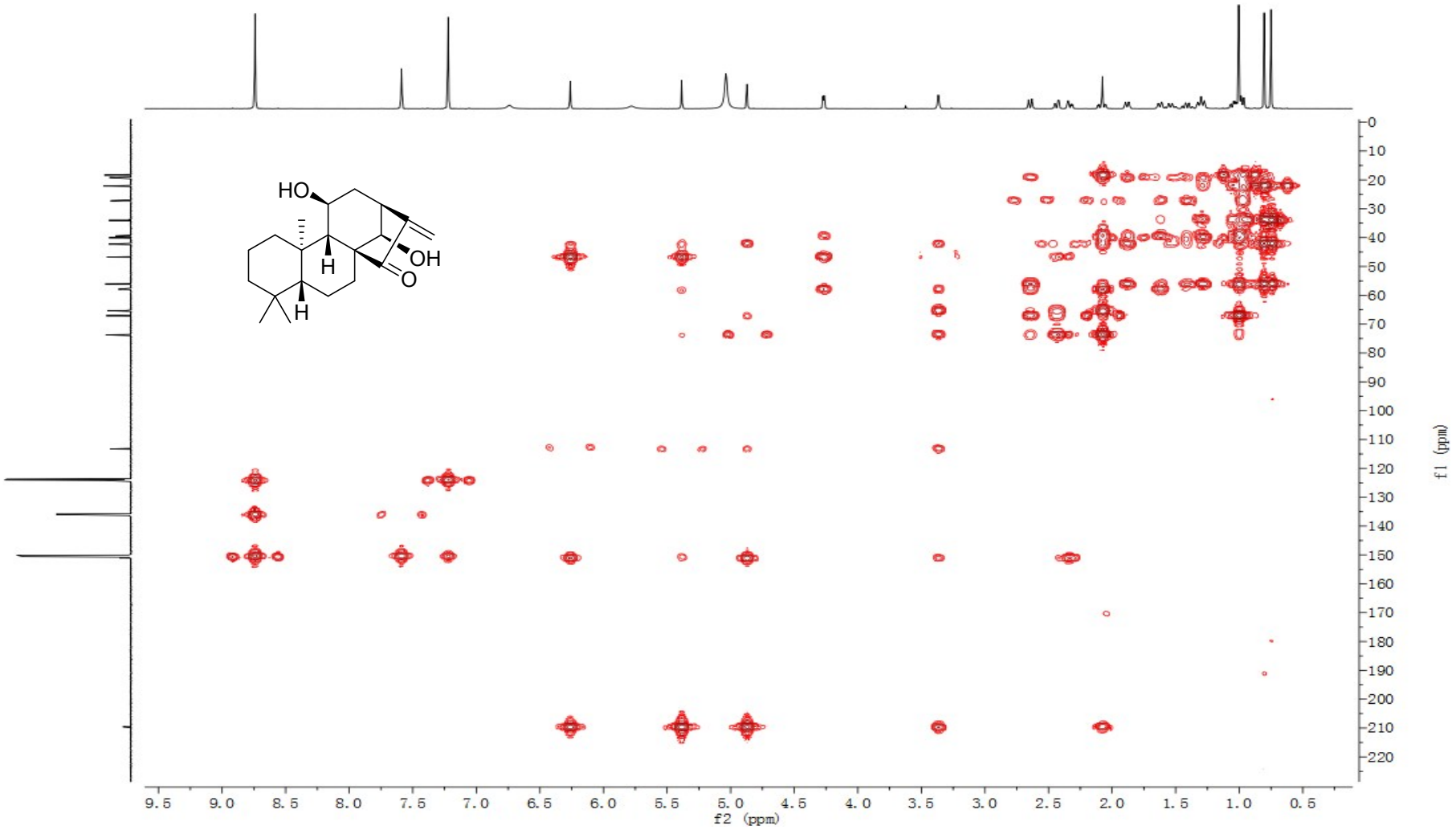


Figure S77. HMBC spectrum of compound **9** (Recorded in pyridine-d_5)

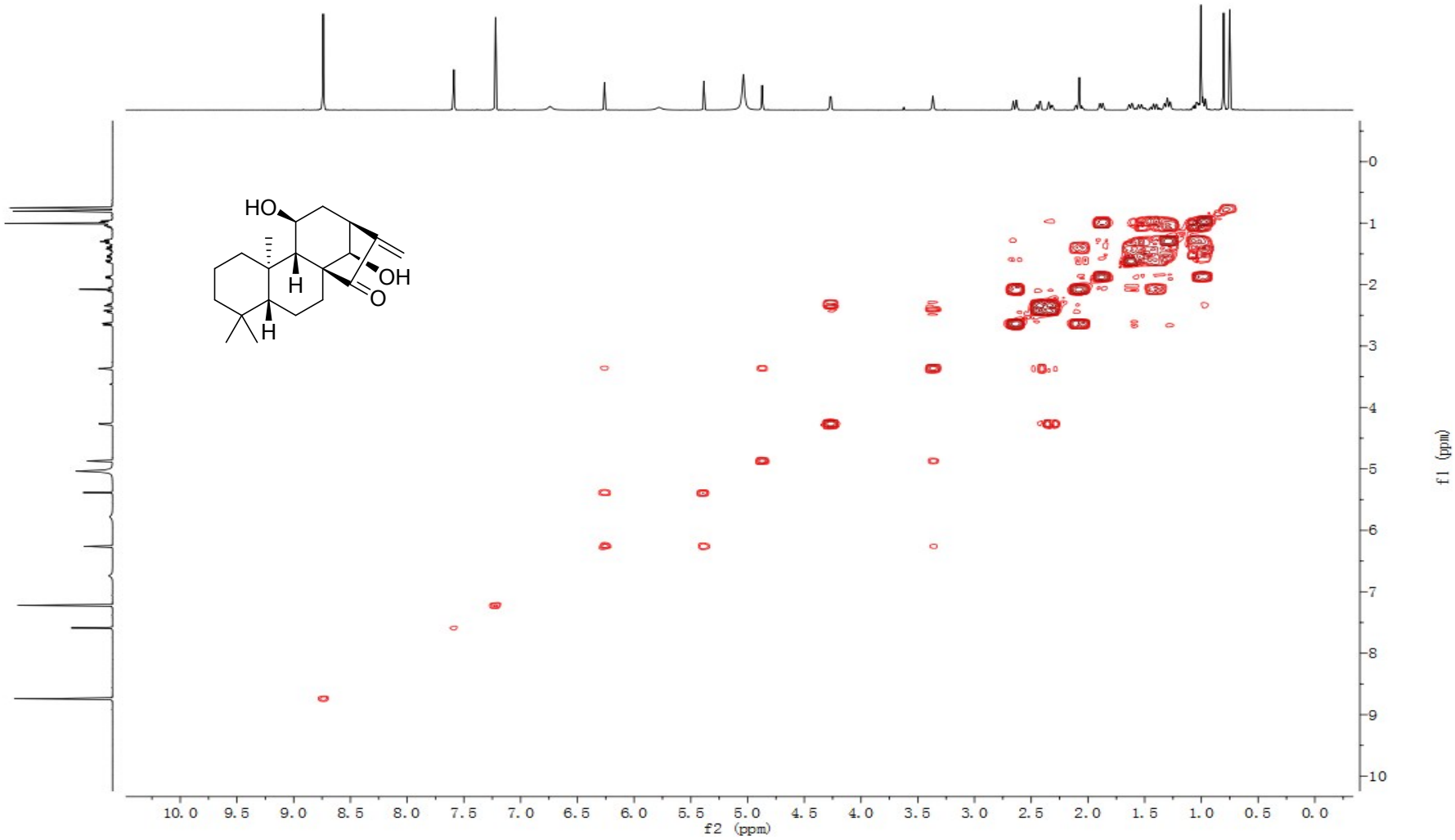


Figure S78. ^{1}H–^{1}H COSY spectrum of compound **9** (Recorded in pyridine-d_5)

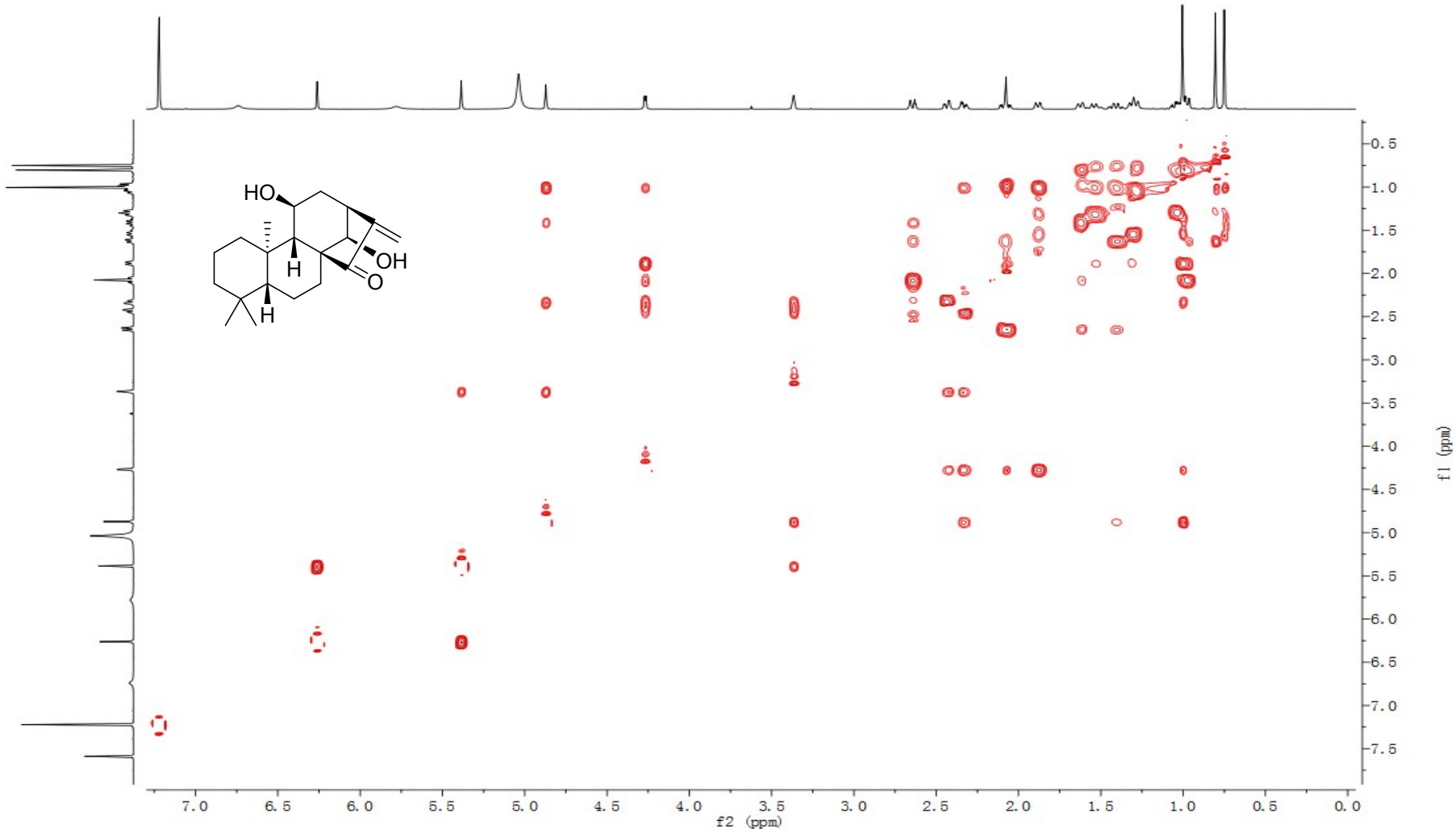


Figure S79. ROESY spectrum of compound **9** (Recorded in pyridine-d_5)

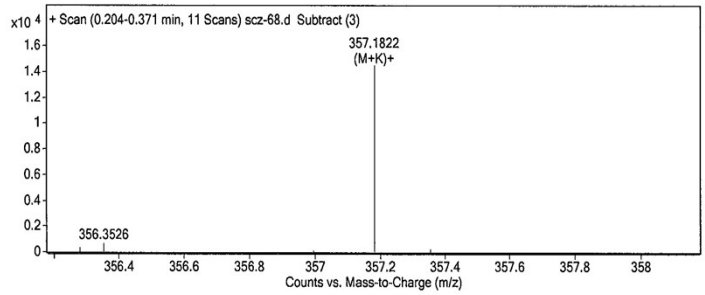
Qualitative Analysis Report

Data Filename	scz-68.d	**Sample Name**	scz-68
Sample Type	Sample	**Position**	P1-B3
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	11/9/2015 4:14:14 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)

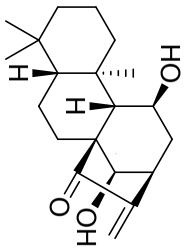
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
274.2738	1	40677.78		
275.2774	1	8276.29		
302.305	1	8791.02		
318.2999	1	28975.87		
341.2082	1	10715.98		
357.1822	1	14518.47	C20 H30 O3	(M+K)+
659.4282	1	15373.29		
675.4022	1	8896.3		



Formula Calculator Element Limits

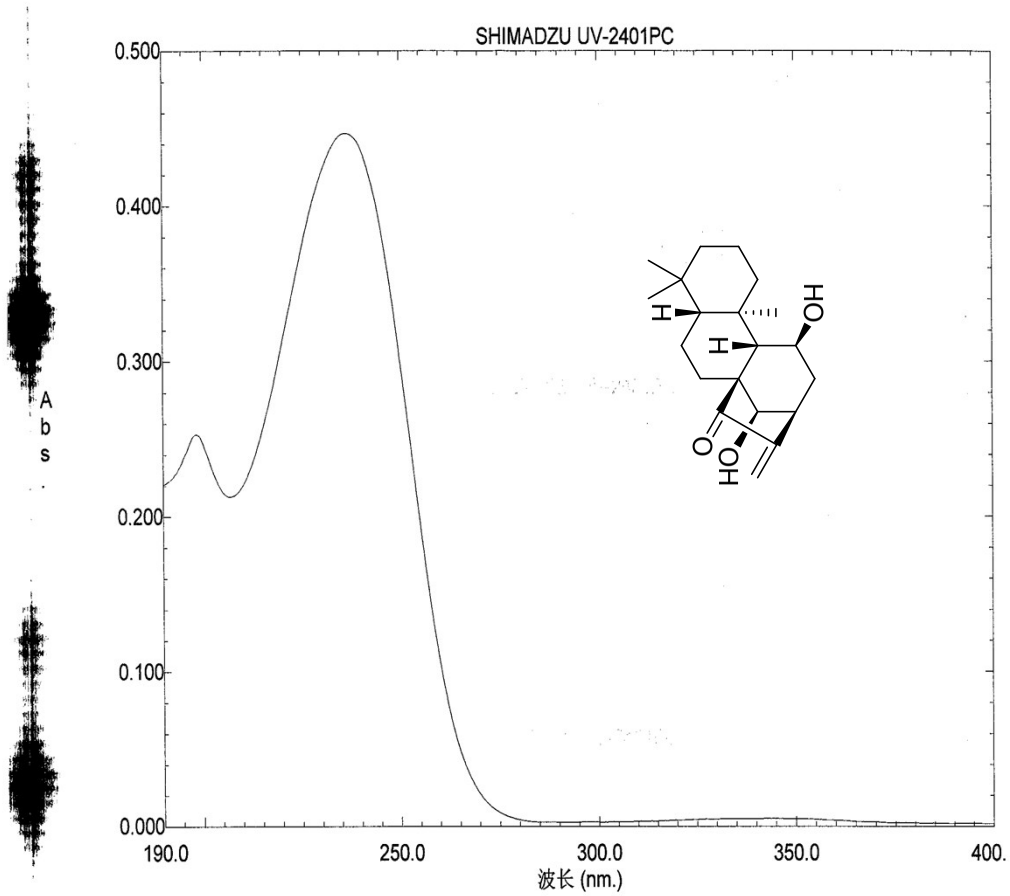
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H30 O3	318.2195	357.1827	357.1822	0.4	1.4	6.0000

--- End Of Report ---

Figure S80. HRESIMS spectrum of compound **9**



文件名: SCZ-68

SCZ-68 ———

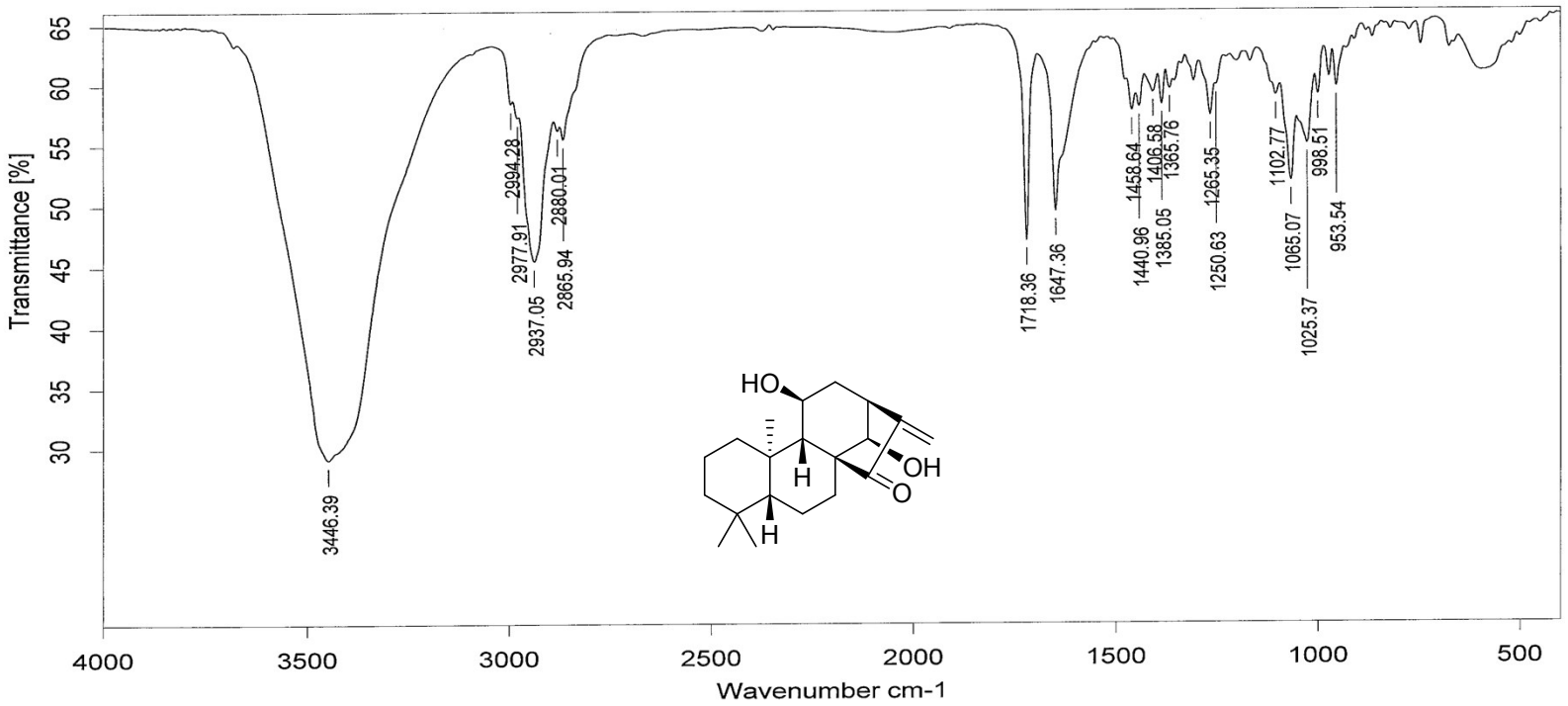
样品浓度：0.0308毫克/毫升
溶剂：甲醇

创建于: 20:51 16-01-20
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	236.40	0.4466
2	198.60	0.2530

Figure S81. UV spectrum of compound **9**



Sample : scz-68	Frequency Range : 399.246 - 3996.32	Measured on : 21/01/2016	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 160121IR1	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S82. IR spectrum of compound **9**

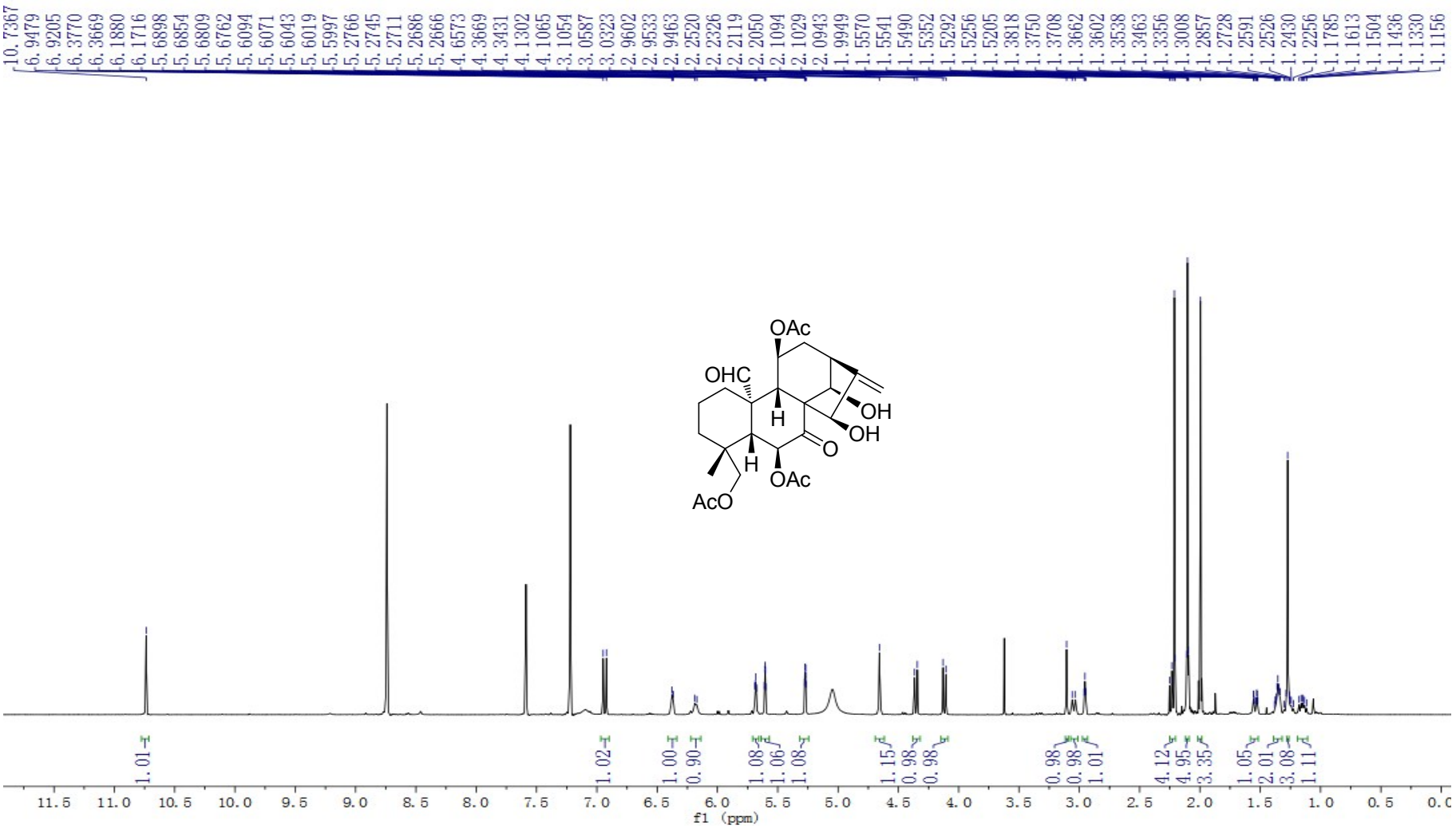


Figure S83. ^{1}H NMR spectrum of compound **10** (Recorded in pyridine-d_5)

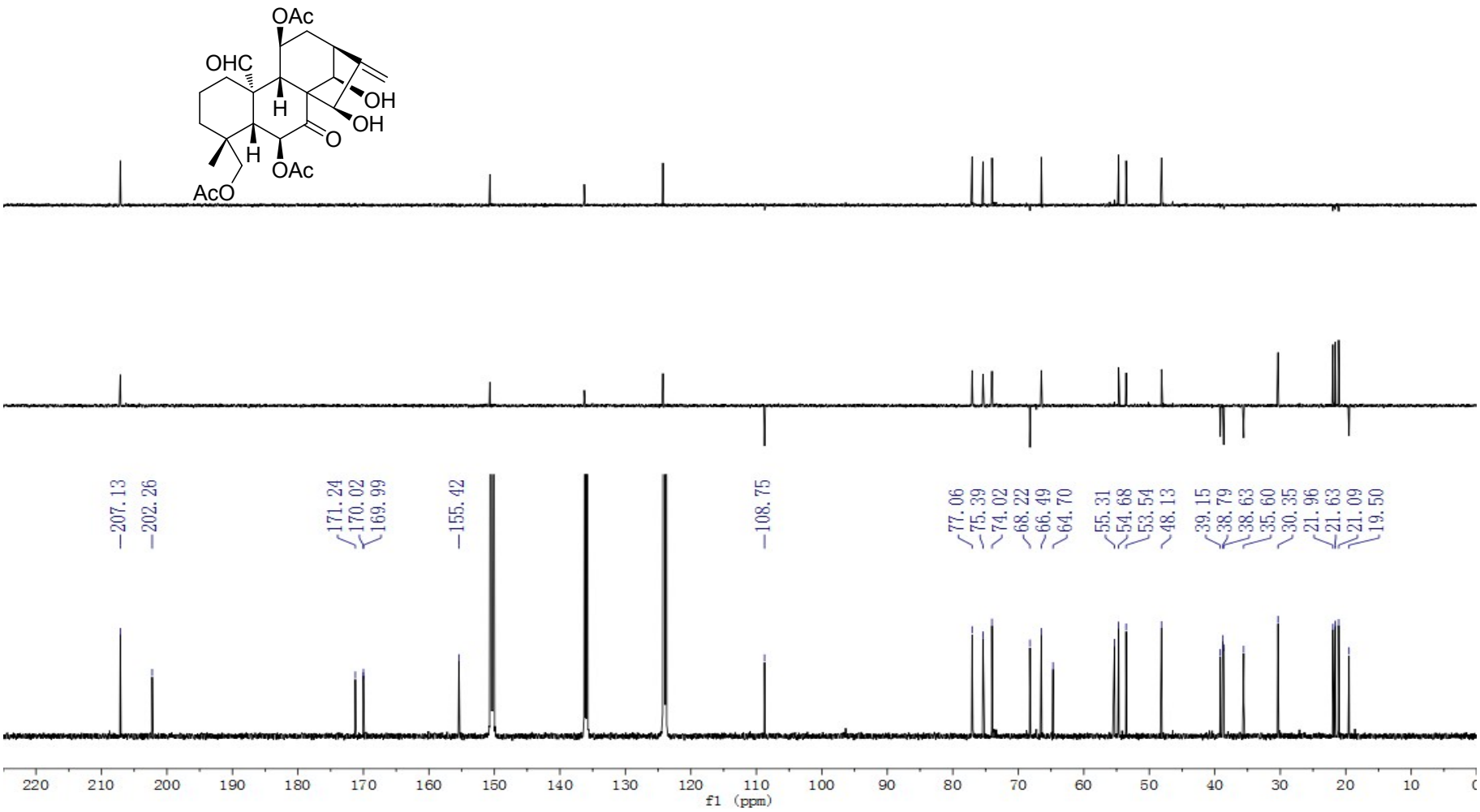


Figure S84. ^{13}C NMR spectrum of compound **10** (Recorded in pyridine-d_5)

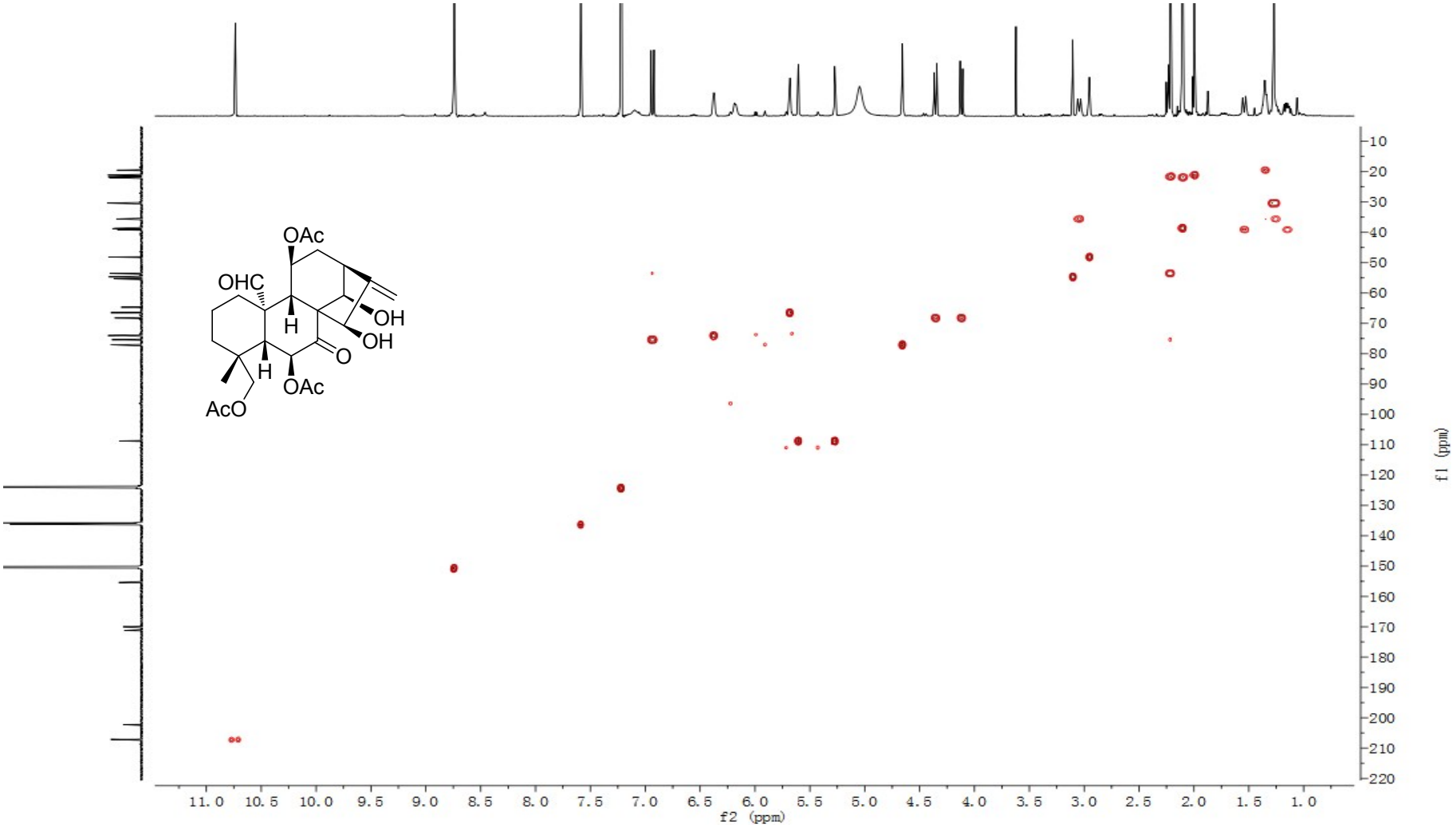


Figure S85. HSQC spectrum of compound **10** (Recorded in pyridine-d_5)

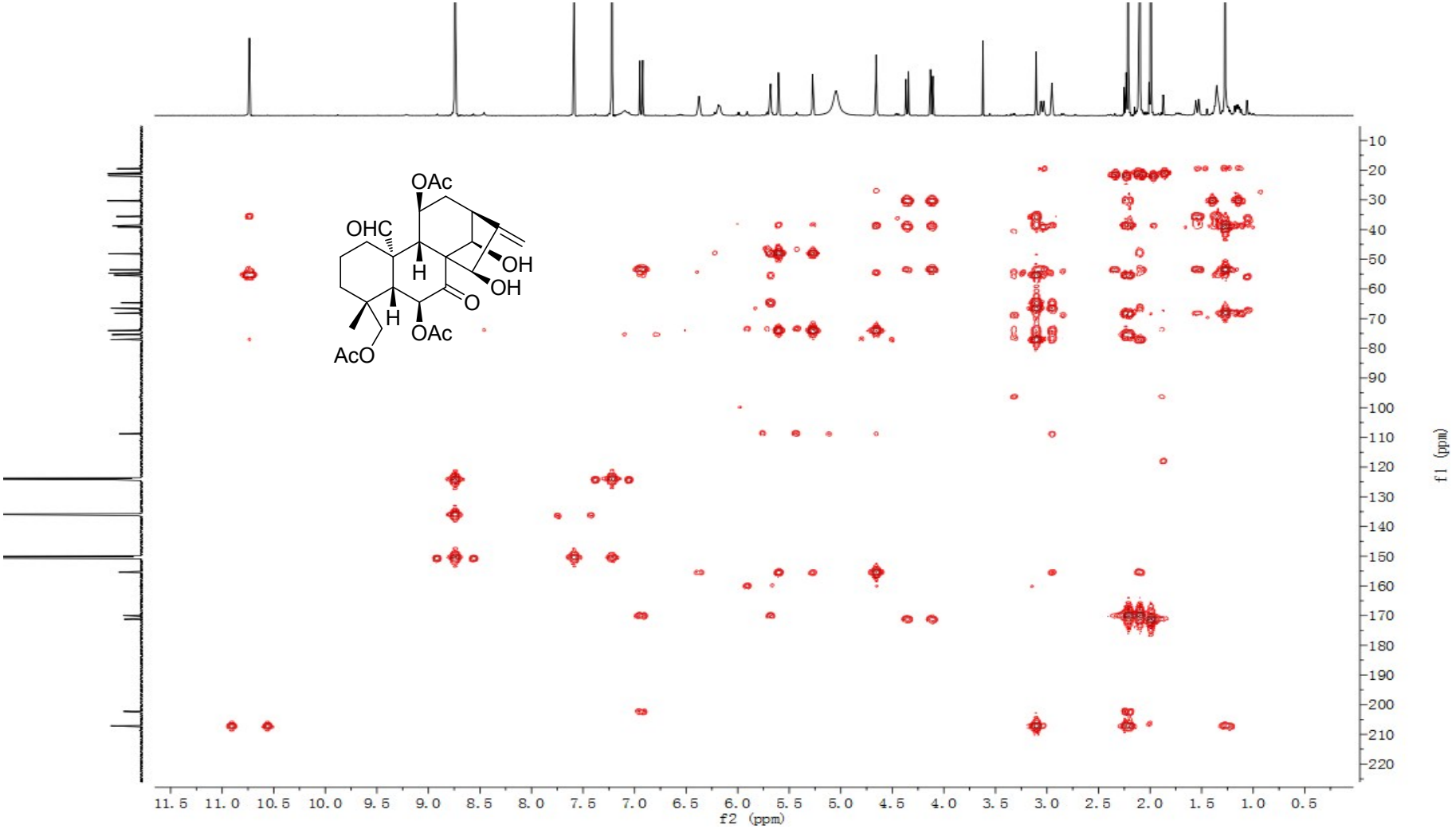


Figure S86. HMBC spectrum of compound **10** (Recorded in pyridine-d_5)

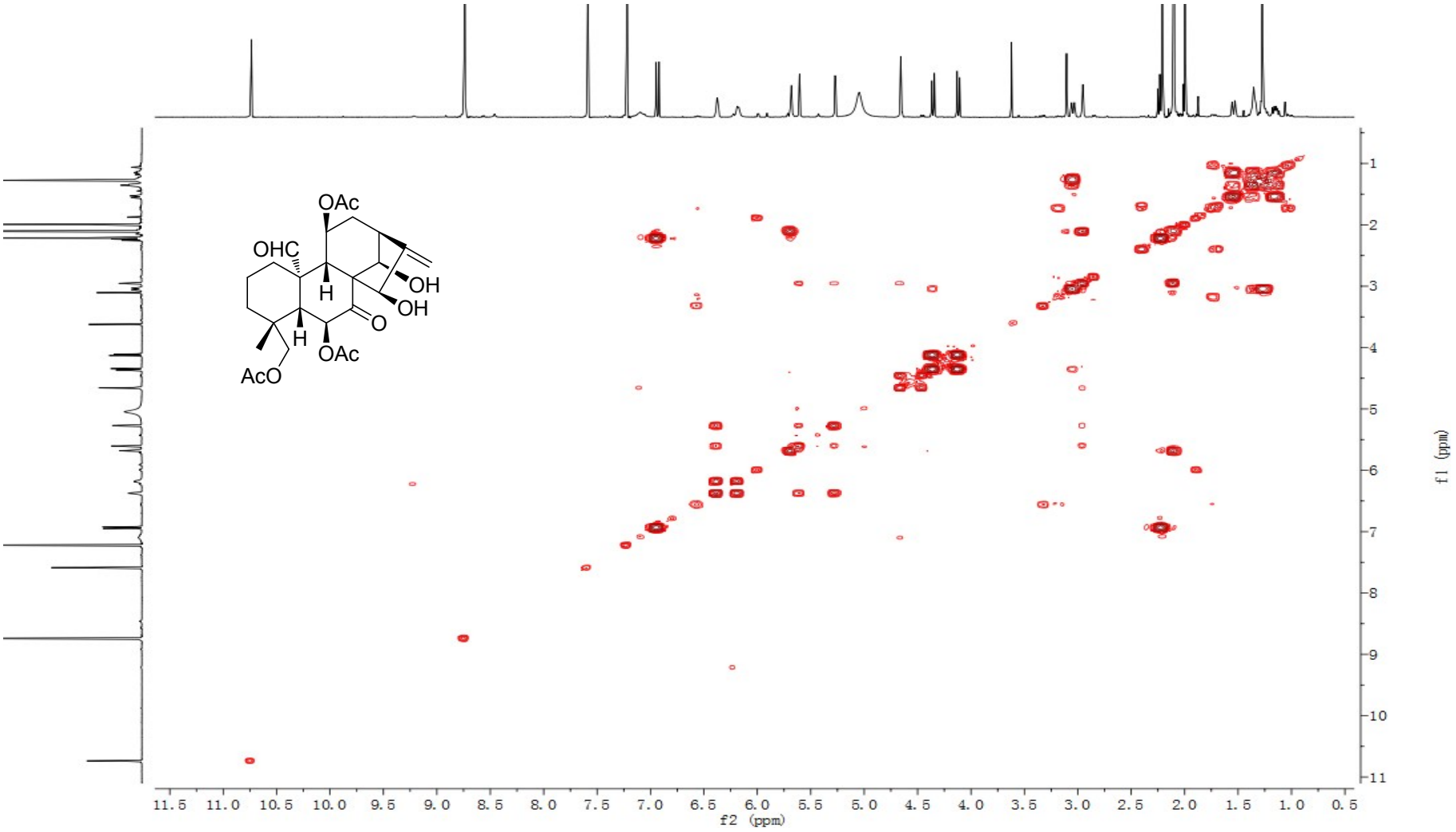


Figure S87. ^{1}H–^{1}H COSY spectrum of compound **10** (Recorded in pyridine-d_5)

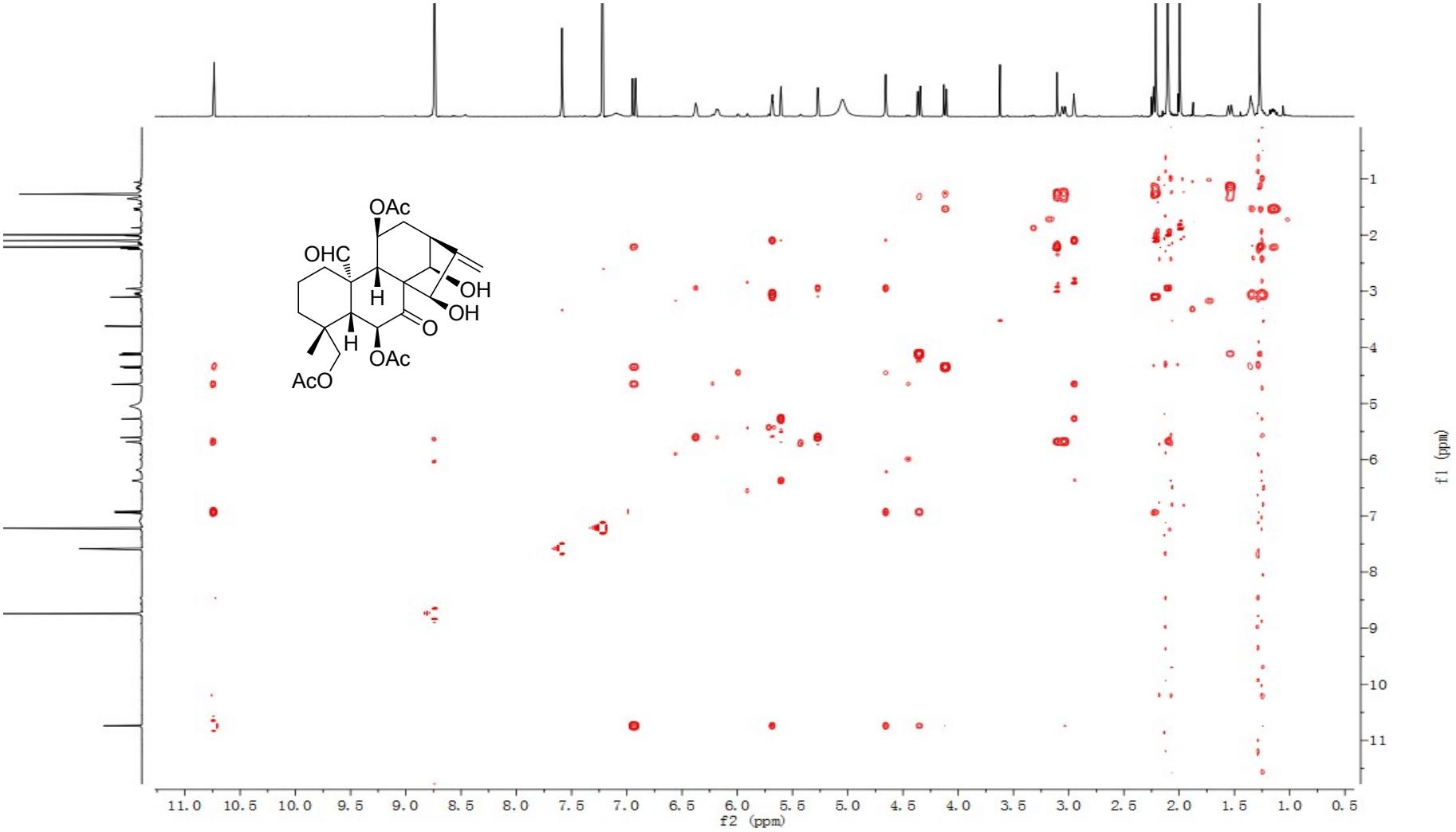


Figure S88. ROESY spectrum of compound **10** (Recorded in pyridine-d_5)

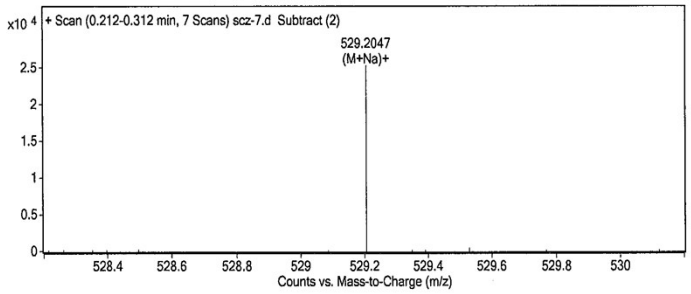
Qualitative Analysis Report

Data Filename	scz-7.d	**Sample Name**	scz-7
Sample Type	Sample	**Position**	P1-F1
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	3/27/2015 1:31:38 PM
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

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

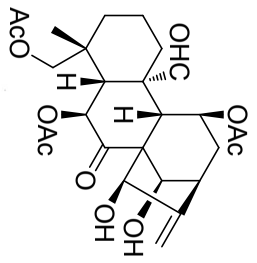
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund
488.358	1	83069.14
493.3135	1	53281.49
532.3843	1	144221.34
553.3135	1	72772.22
576.4105	1	137719.19
577.414	1	47604.04
597.34	1	83024.52
620.4368	1	109169.55
641.3661	1	63046.77
664.4631	1	67774.63



Formula Calculator Element Limits

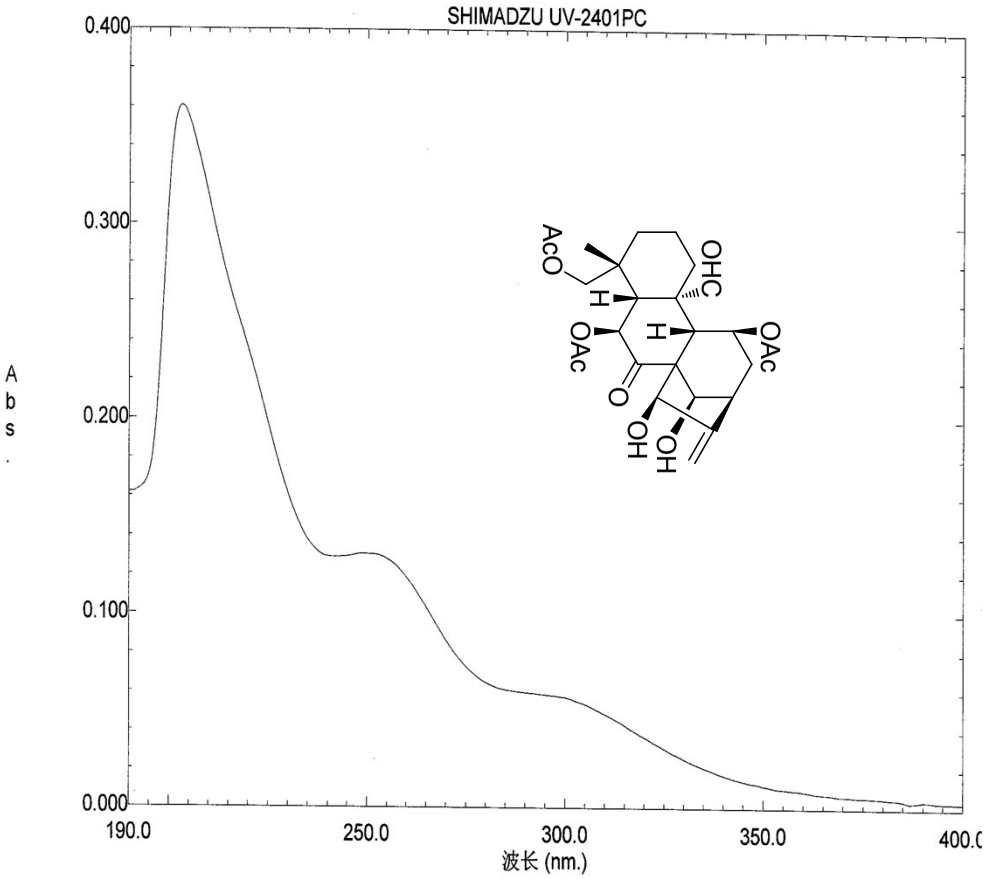
Element	Min	Max
C	3	30
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C26 H34 O10	506.2152	529.2044	529.2047	0.0	0.1	10.0000

--- End Of Report ---

Figure S89. HRESIMS spectrum of compound **10**



文件名: SCZ-7

SCZ-7 ———

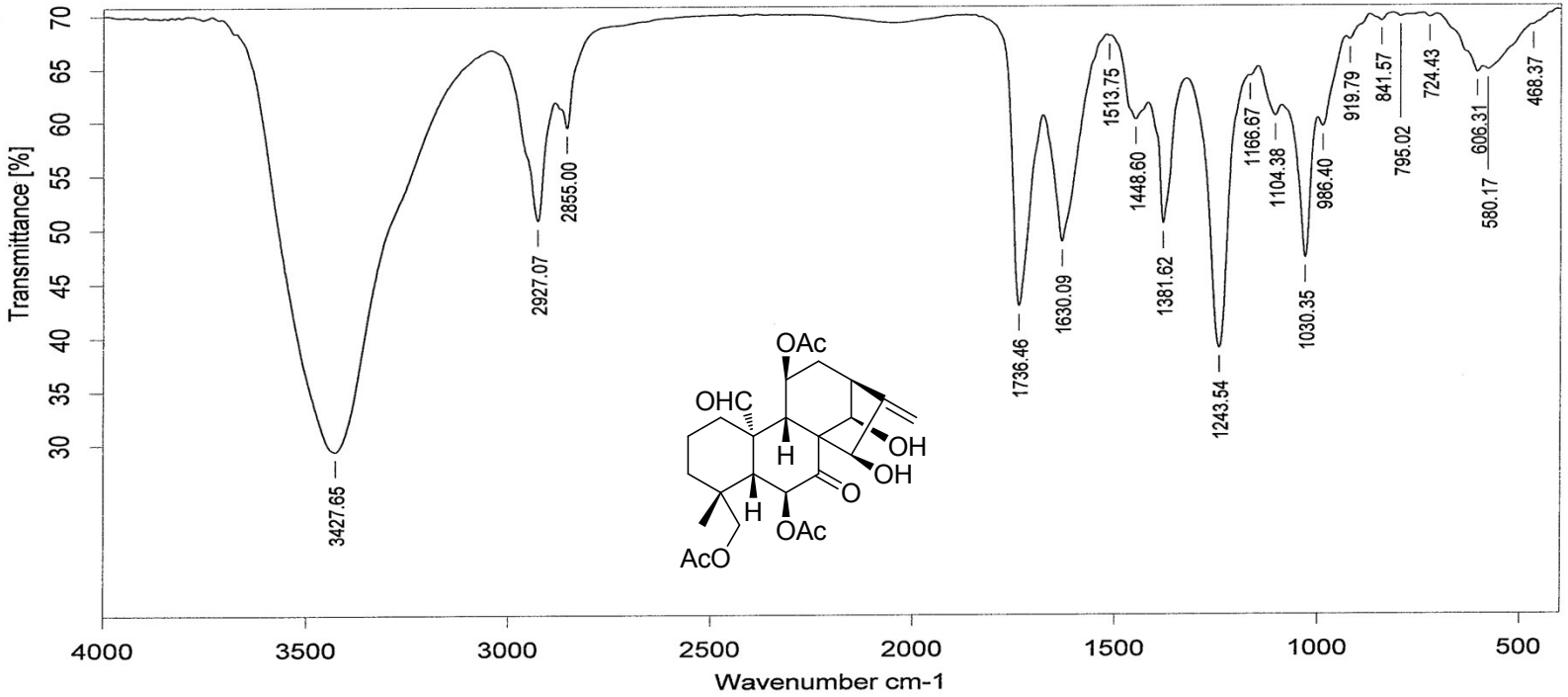
样品浓度：0.0320毫克/毫升
溶剂：甲醇

创建于: 18:36 15-09-17
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	202.80	0.3602
2	248.80	0.1305
3	295.40	0.0583

Figure S90. UV spectrum of compound **10**



Sample : scz-7	Frequency Range : 399.246 - 3996.32	Measured on : 24/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150924IR0	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S91. IR spectrum of compound **10**

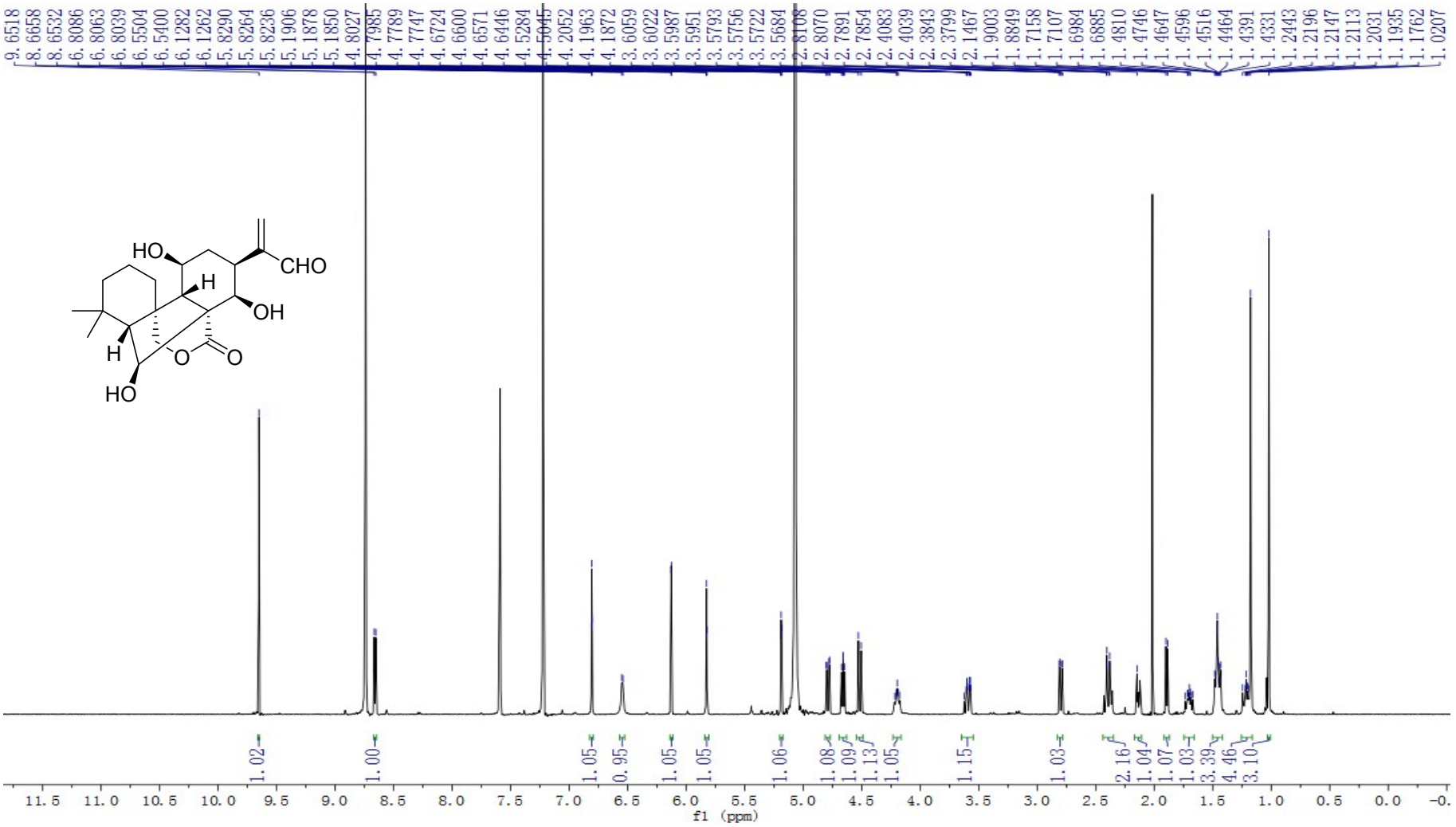


Figure S92. ^{1}H NMR spectrum of compound **11** (Recorded in pyridine-d_5)

Figure S93. ^{13}C NMR spectrum of compound **11** (Recorded in pyridine-d_5)

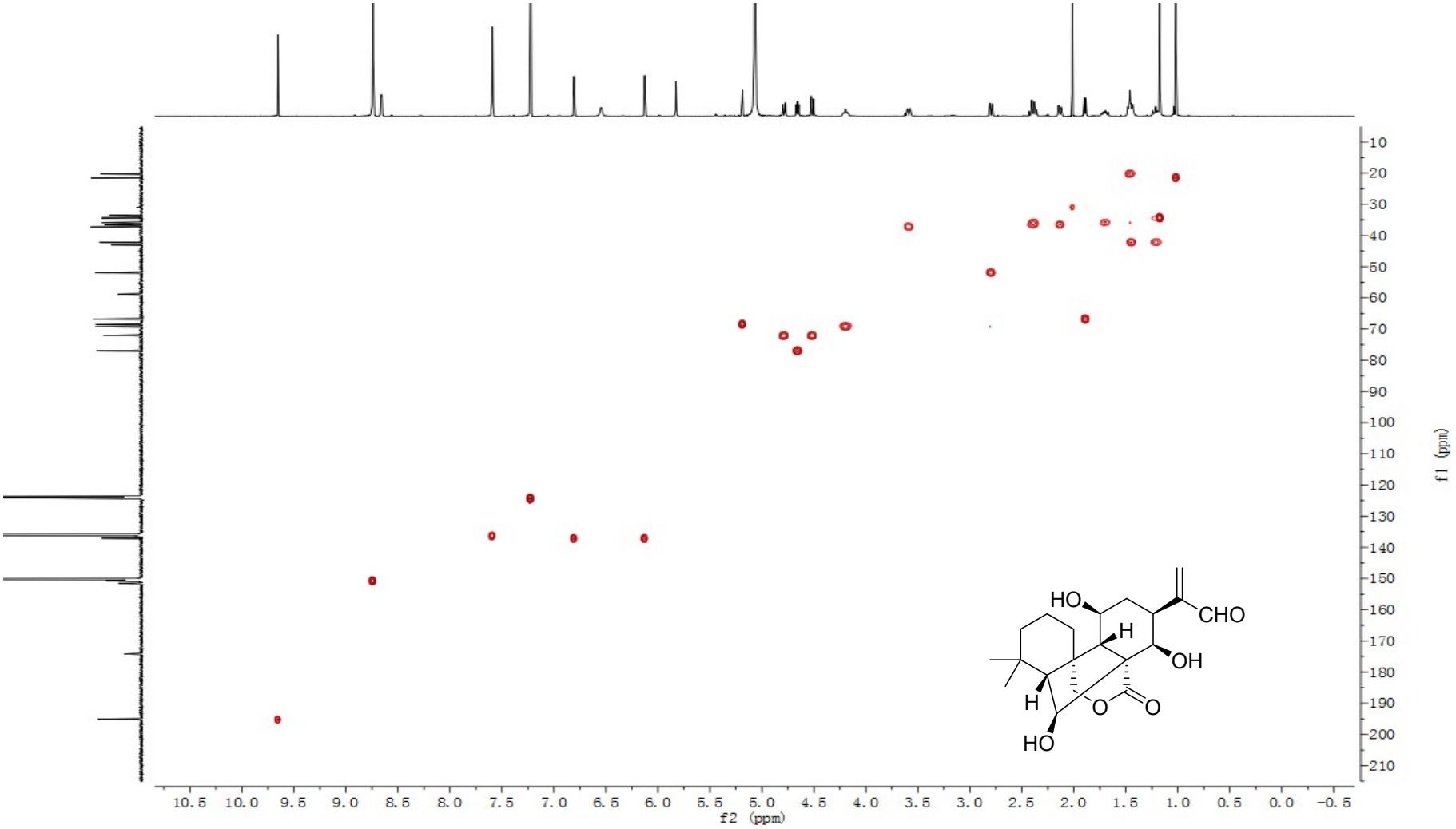


Figure S94. HSQC spectrum of compound **11** (Recorded in pyridine-d_5)

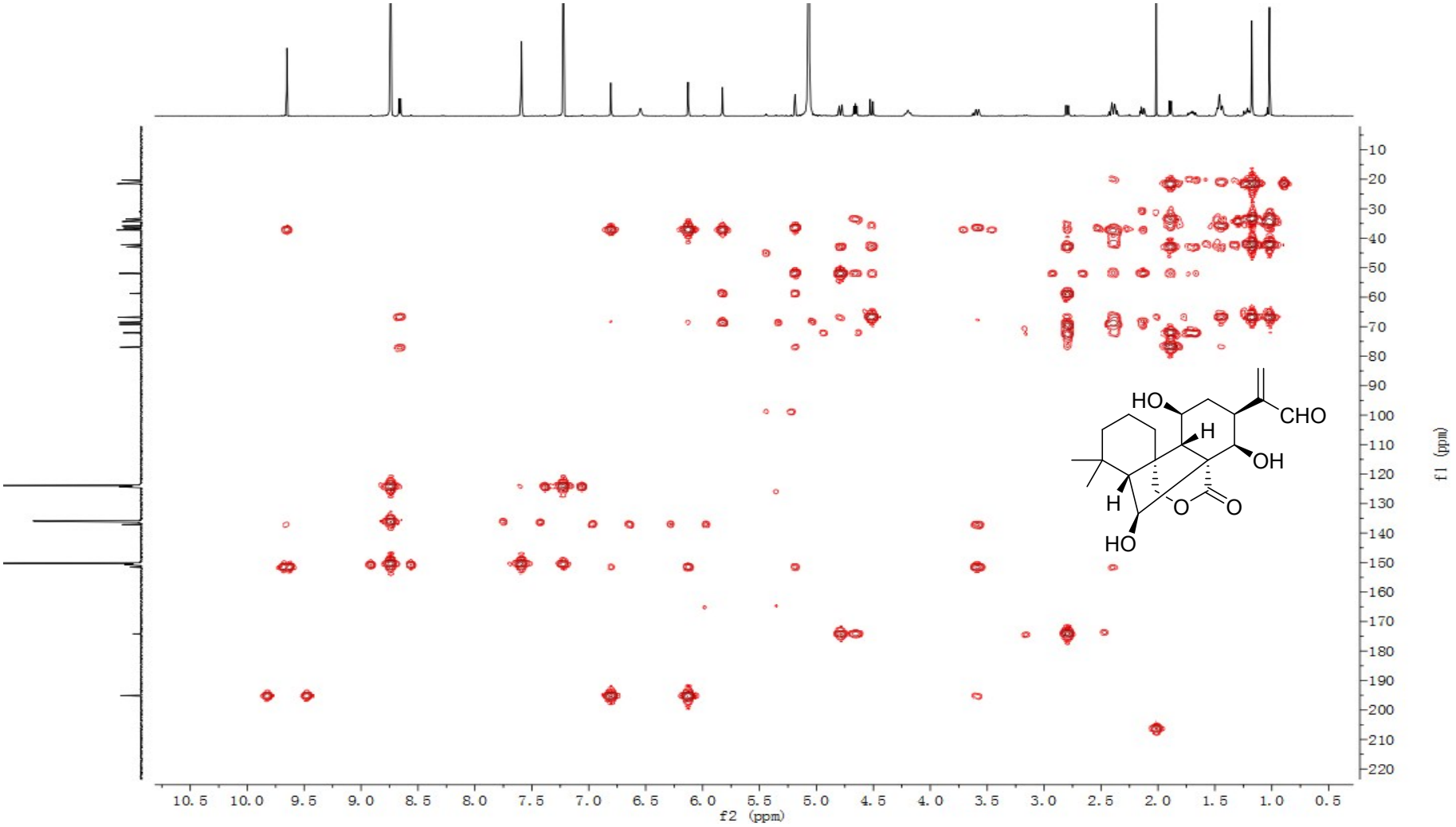


Figure S95. HMBC spectrum of compound **11** (Recorded in pyridine-d_5)

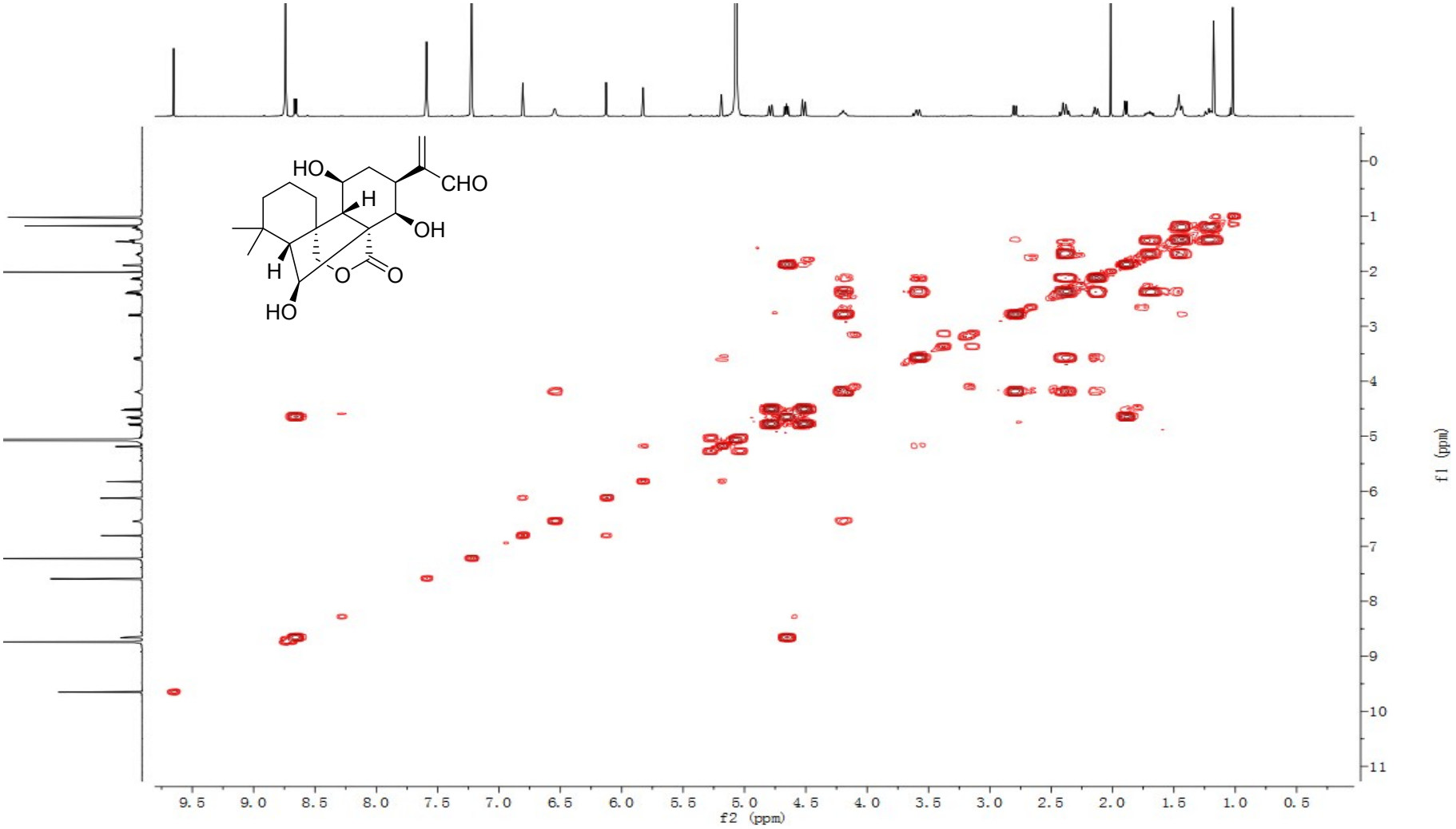


Figure S96. ^{1}H–^{1}H COSY spectrum of compound **11** (Recorded in pyridine-d_5)

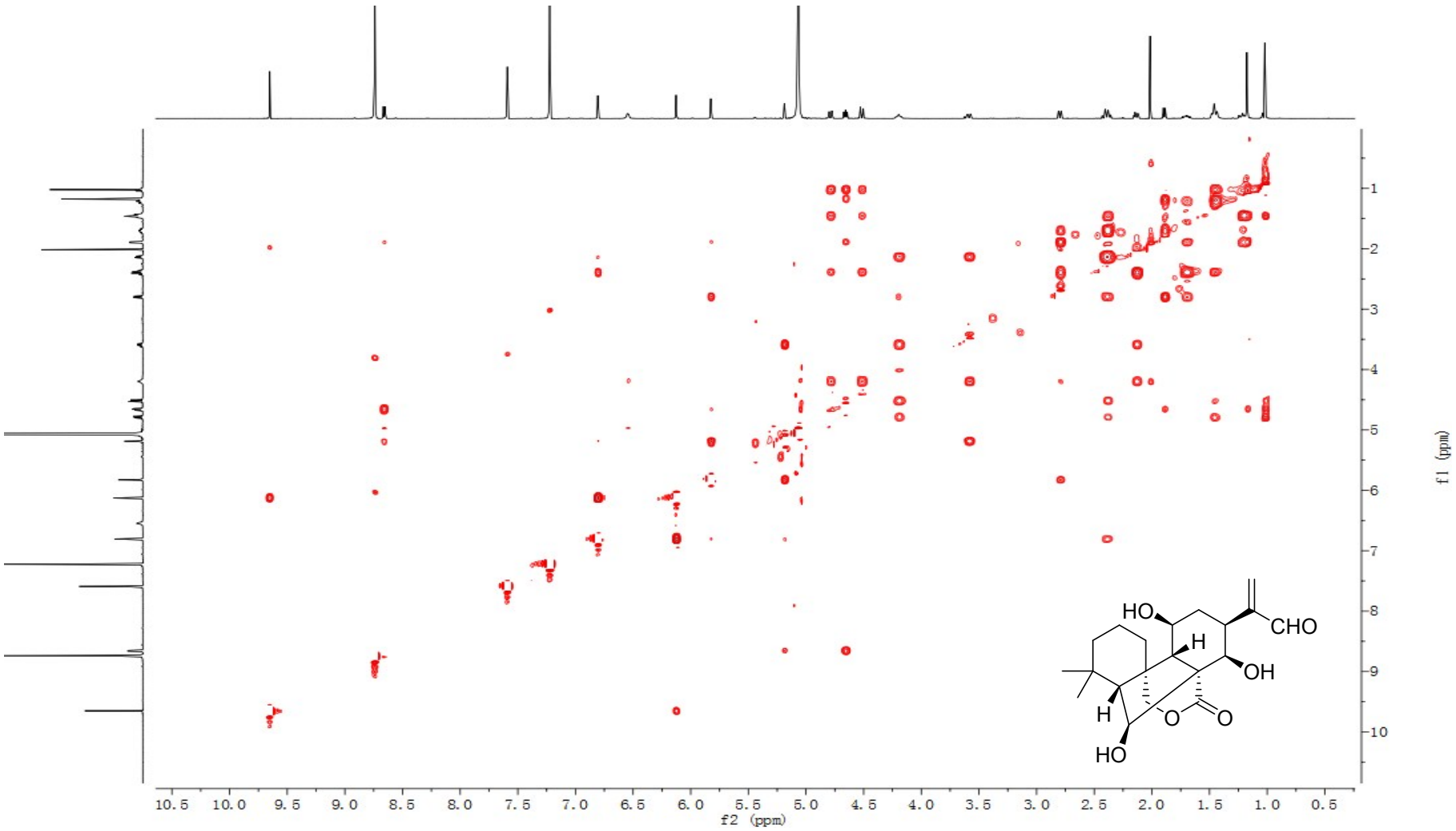


Figure S97. ROESY spectrum of compound **11** (Recorded in pyridine-d_5)

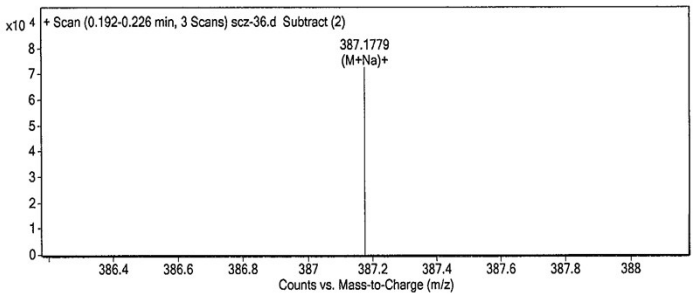
Qualitative Analysis Report

Data Filename	scz-36.d	**Sample Name**	scz-36
Sample Type	Sample	**Position**	P1-B7
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/14/2015 4:14:22 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)

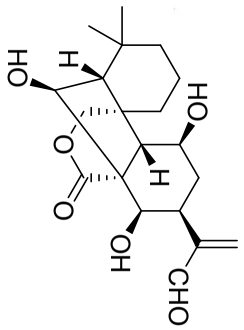
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
274.2743	1	29522.98		
318.3004	1	18011.42		
387.1779	1	72832.29	C20 H28 O6	(M+Na)+
388.1814	1	15061.83	C20 H28 O6	(M+Na)+
403.1516	1	58711.01		
751.3665	1	78392.84		
752.3699	1	35027.96		
767.3404	1	31548.97		



Formula Calculator Element Limits

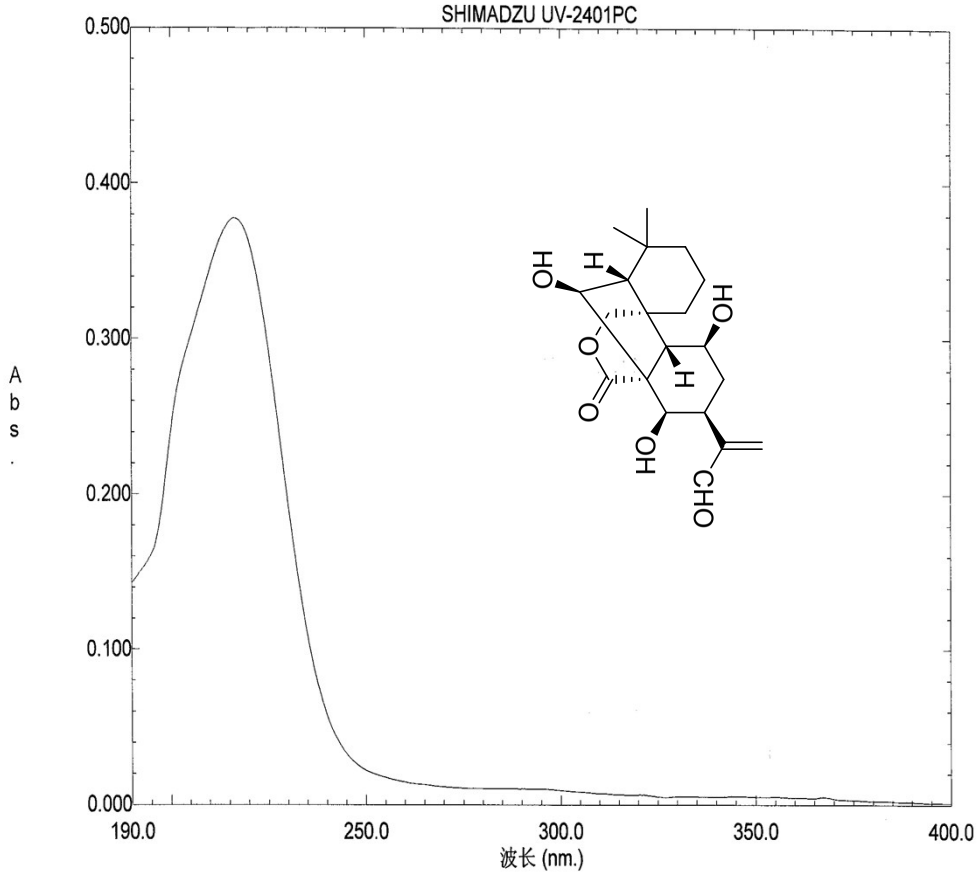
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H28 O6	364.1886	387.1778	387.1779	-0.1	-0.2	7.0000

--- End Of Report ---

Figure S98. HRESIMS spectrum of compound **11**



文件名: SCZ-36

SCZ-36 ———

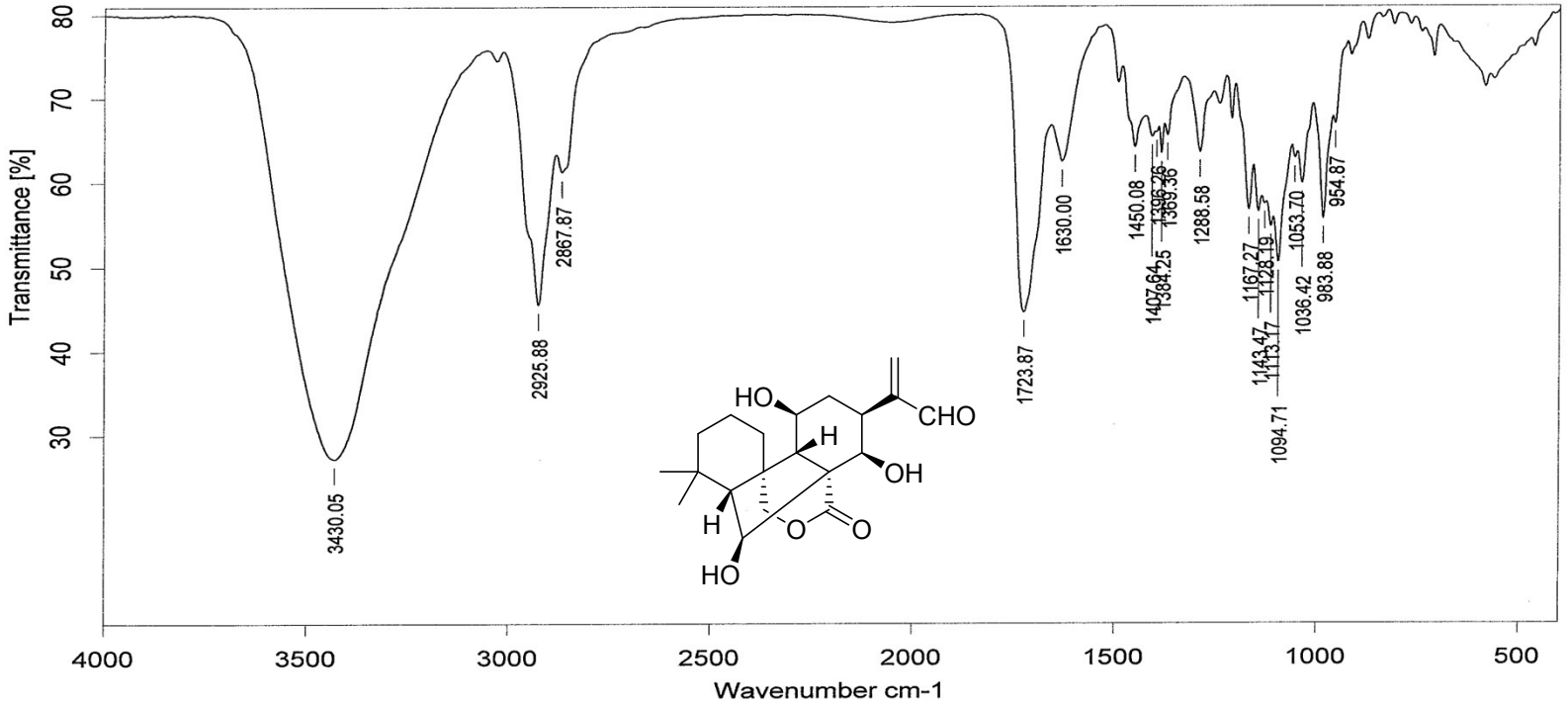
样品浓度：0.0315毫克/毫升
溶剂：甲醇

创建于: 15:51 15-09-19
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	367.40	0.0051
2	216.60	0.3774

Figure S99. UV spectrum of compound **11**



Sample : scz-36	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150925IR0	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S100. IR spectrum of compound **11**

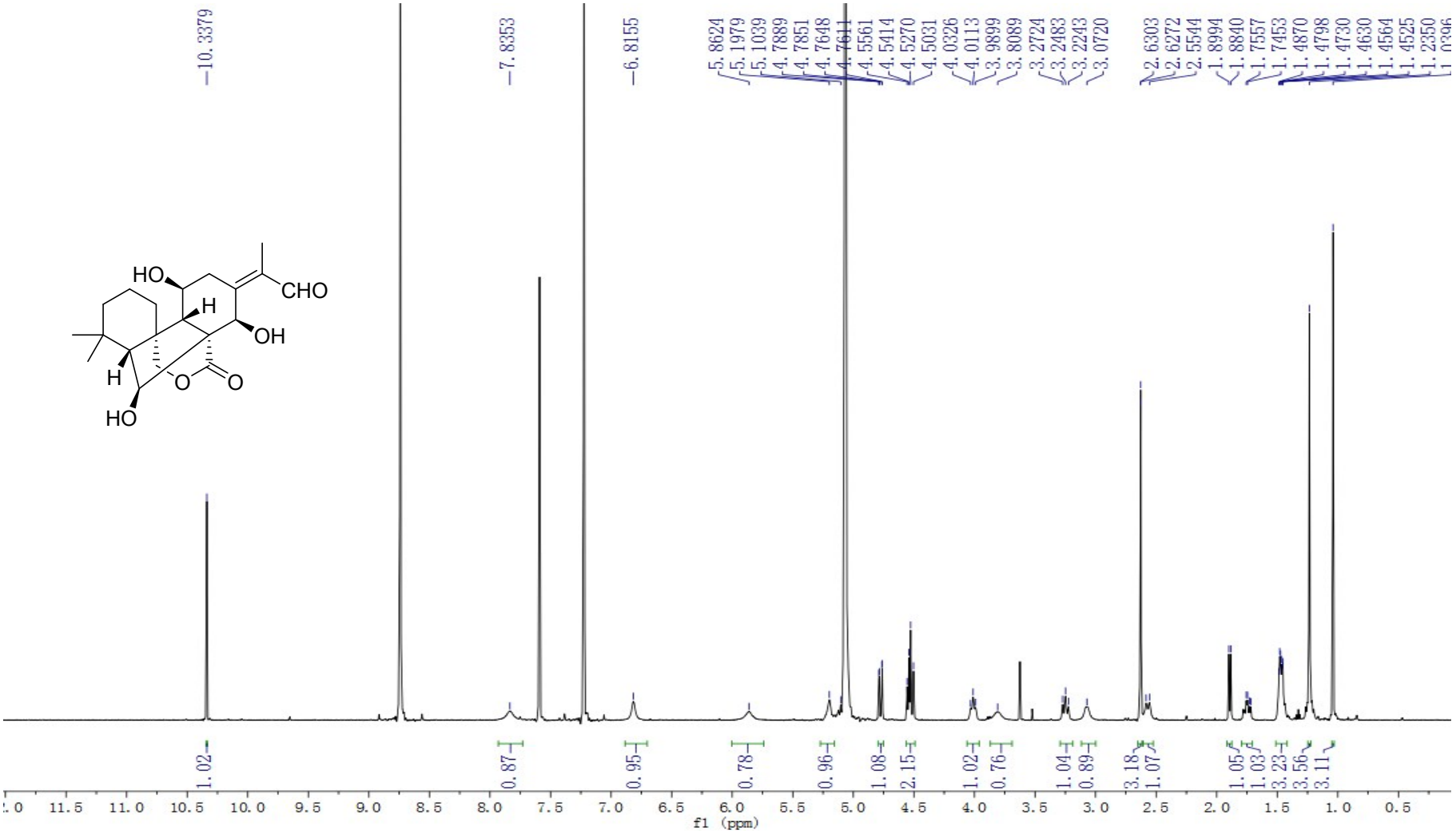


Figure S101. ^{1}H NMR spectrum of compound **12** (Recorded in pyridine-d_5)

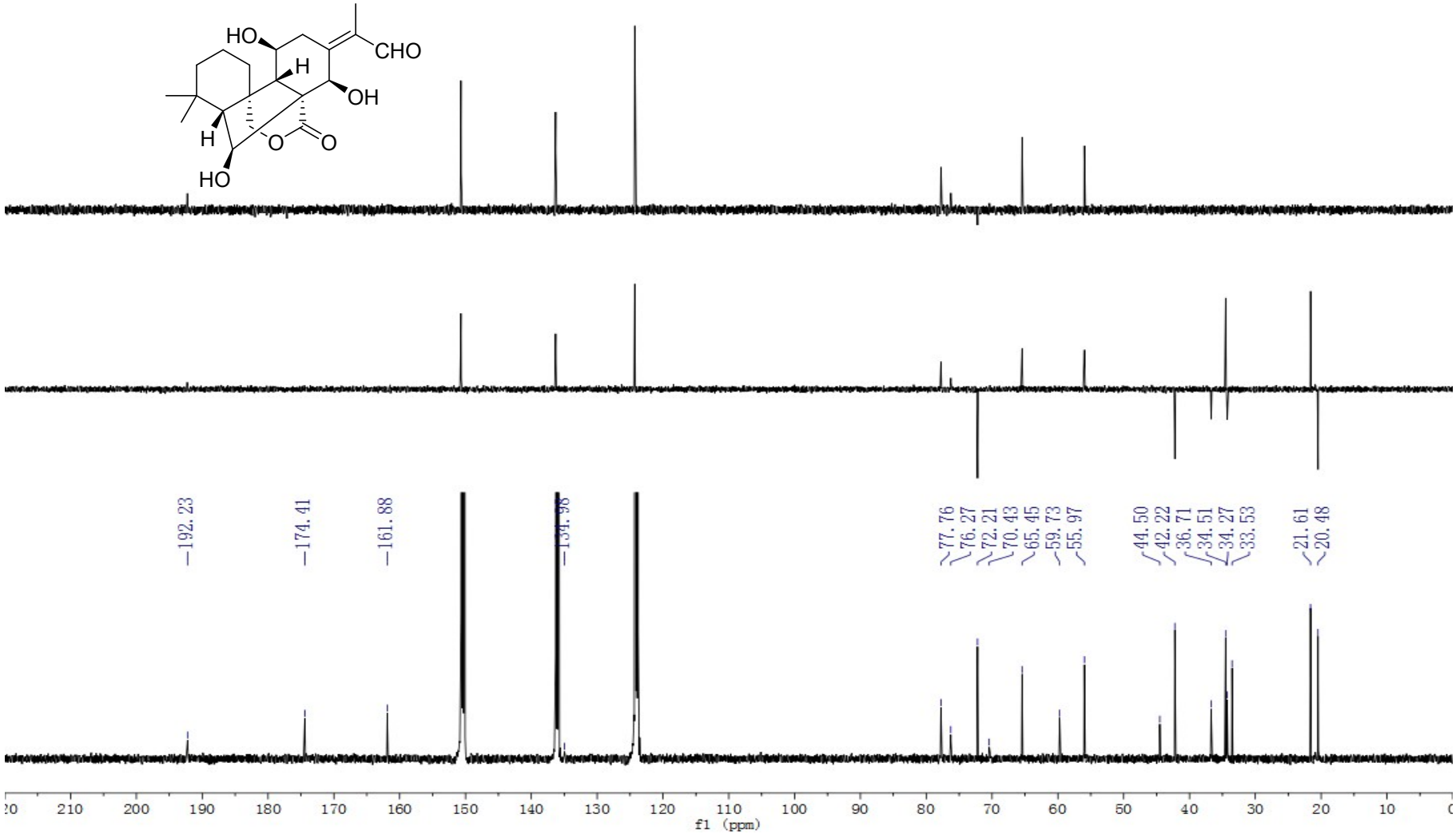


Figure S102. ^{13}C NMR spectrum of compound **12** (Recorded in pyridine-d_5)

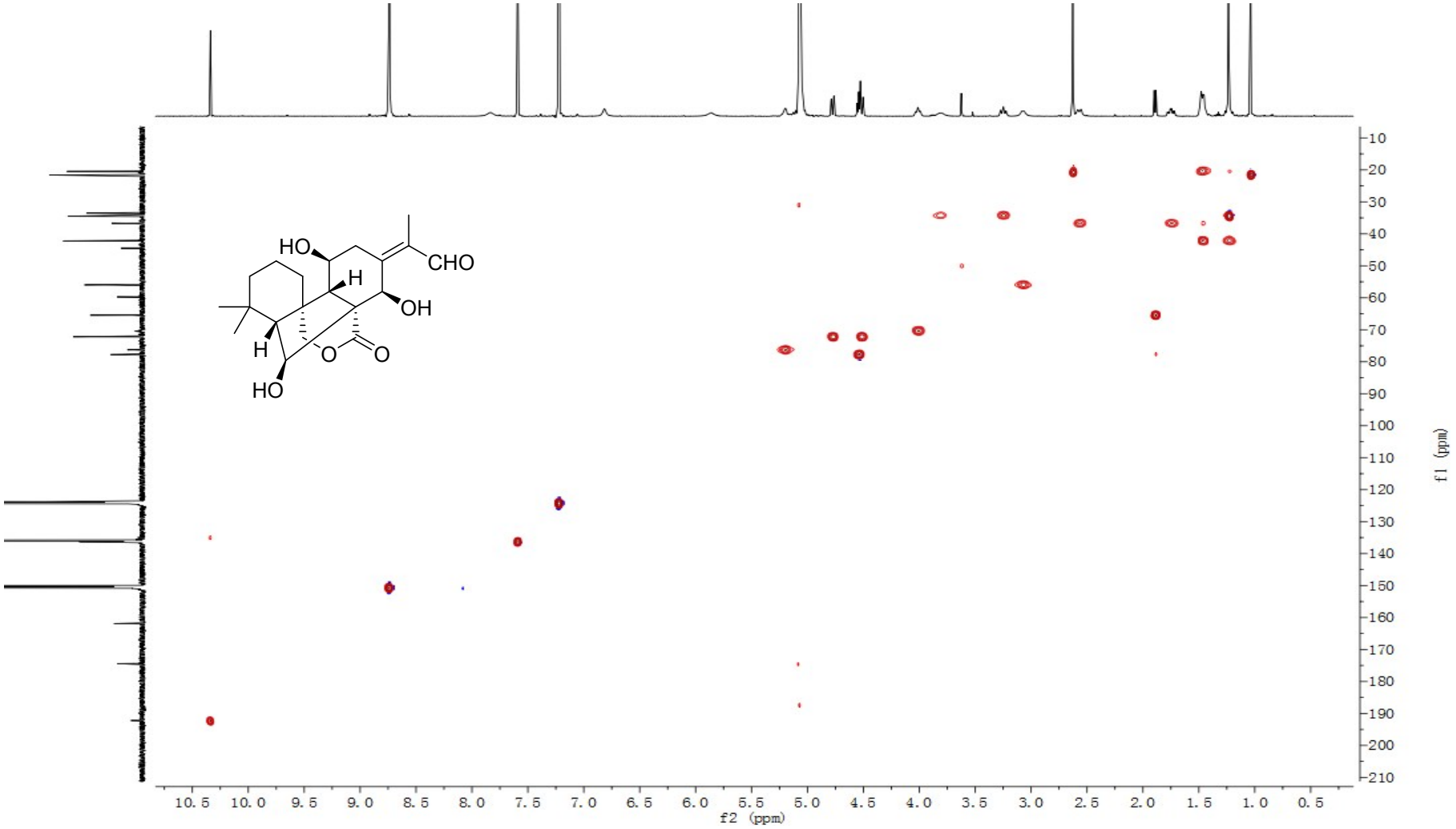


Figure S103. HSQC spectrum of compound **12** (Recorded in pyridine-d_5)

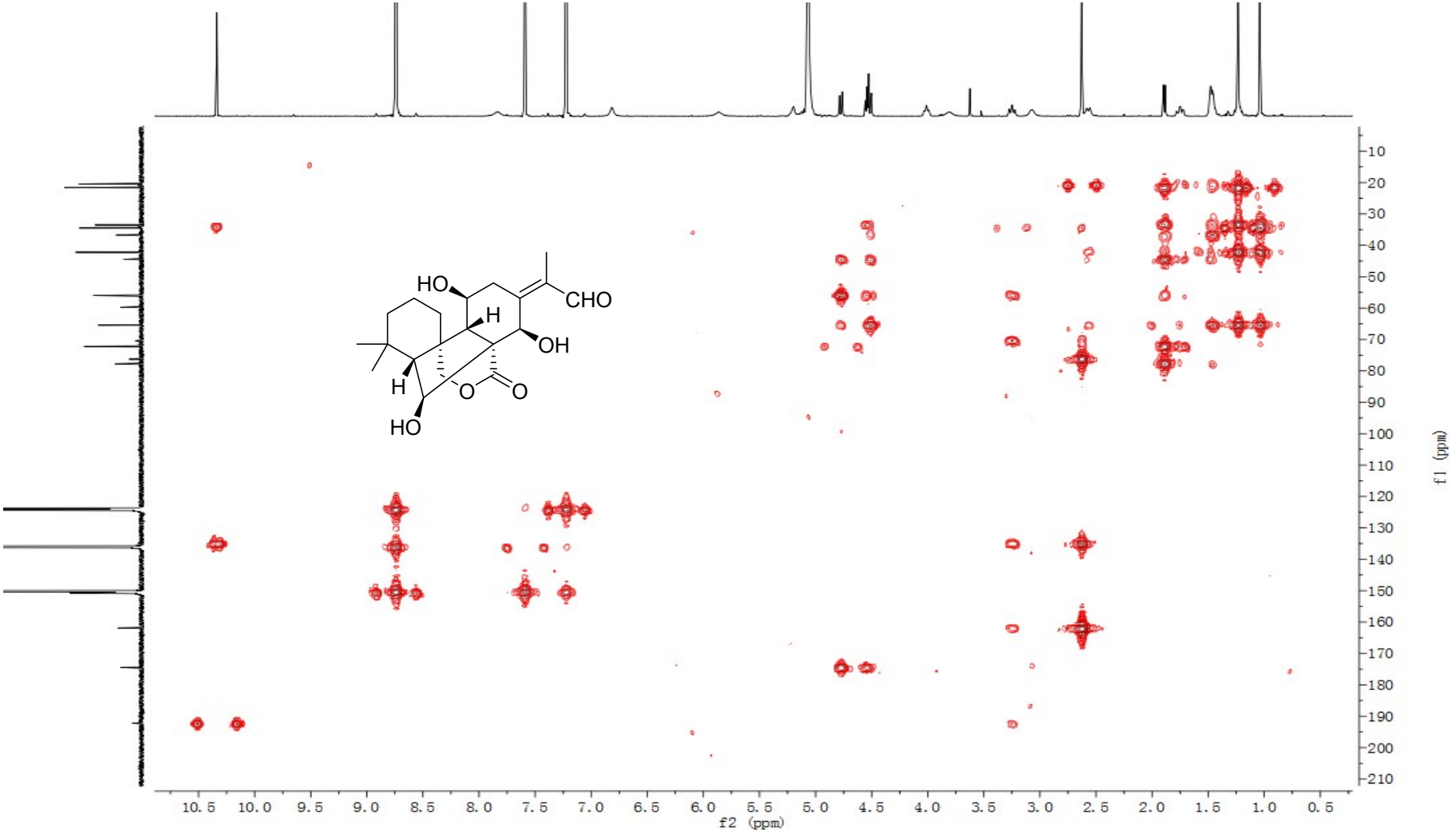


Figure S104. HMBC spectrum of compound **12** (Recorded in pyridine-d_5)

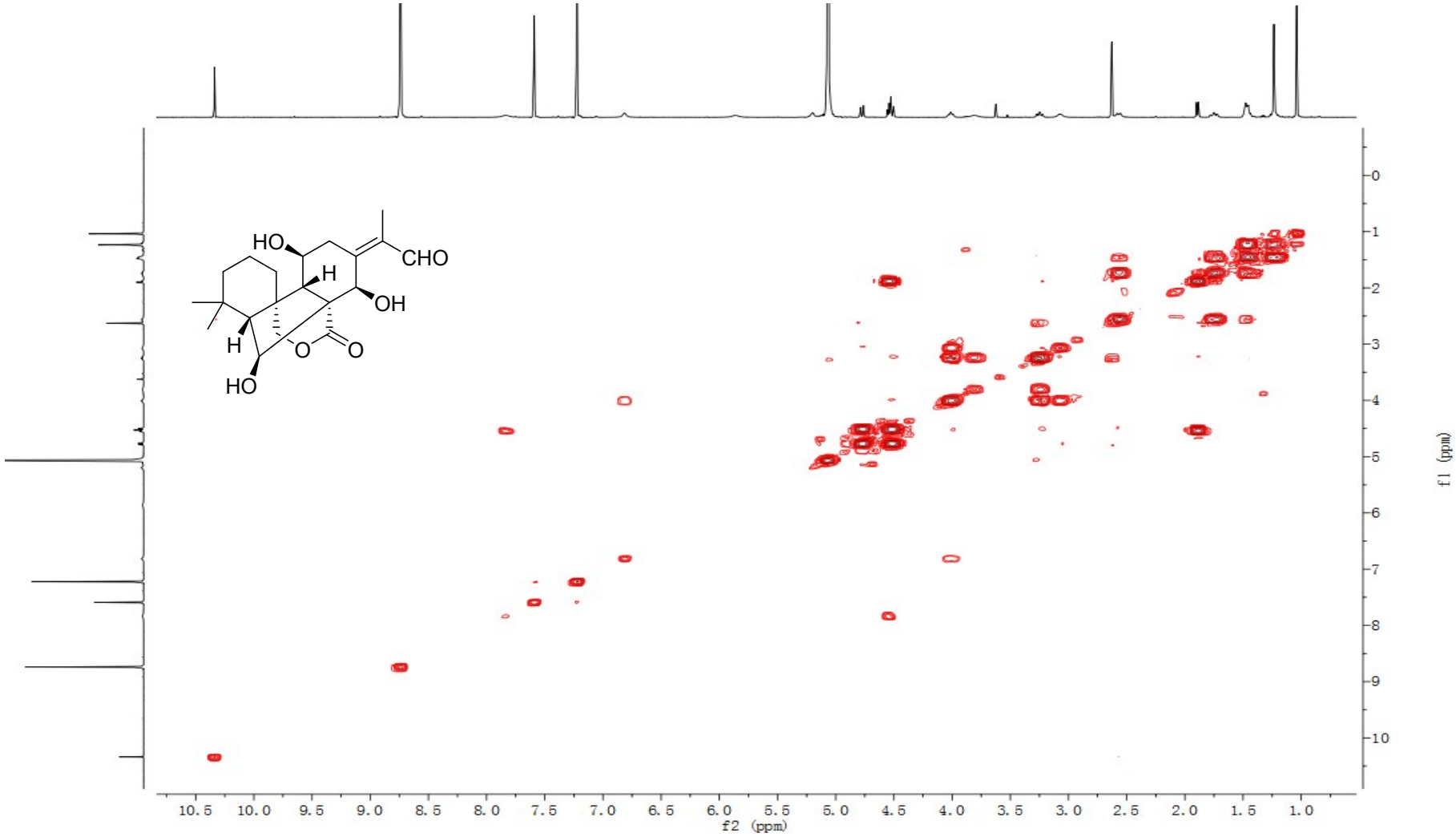


Figure S105. ^{1}H–^{1}H COSY spectrum of compound **12** (Recorded in pyridine-d_5)

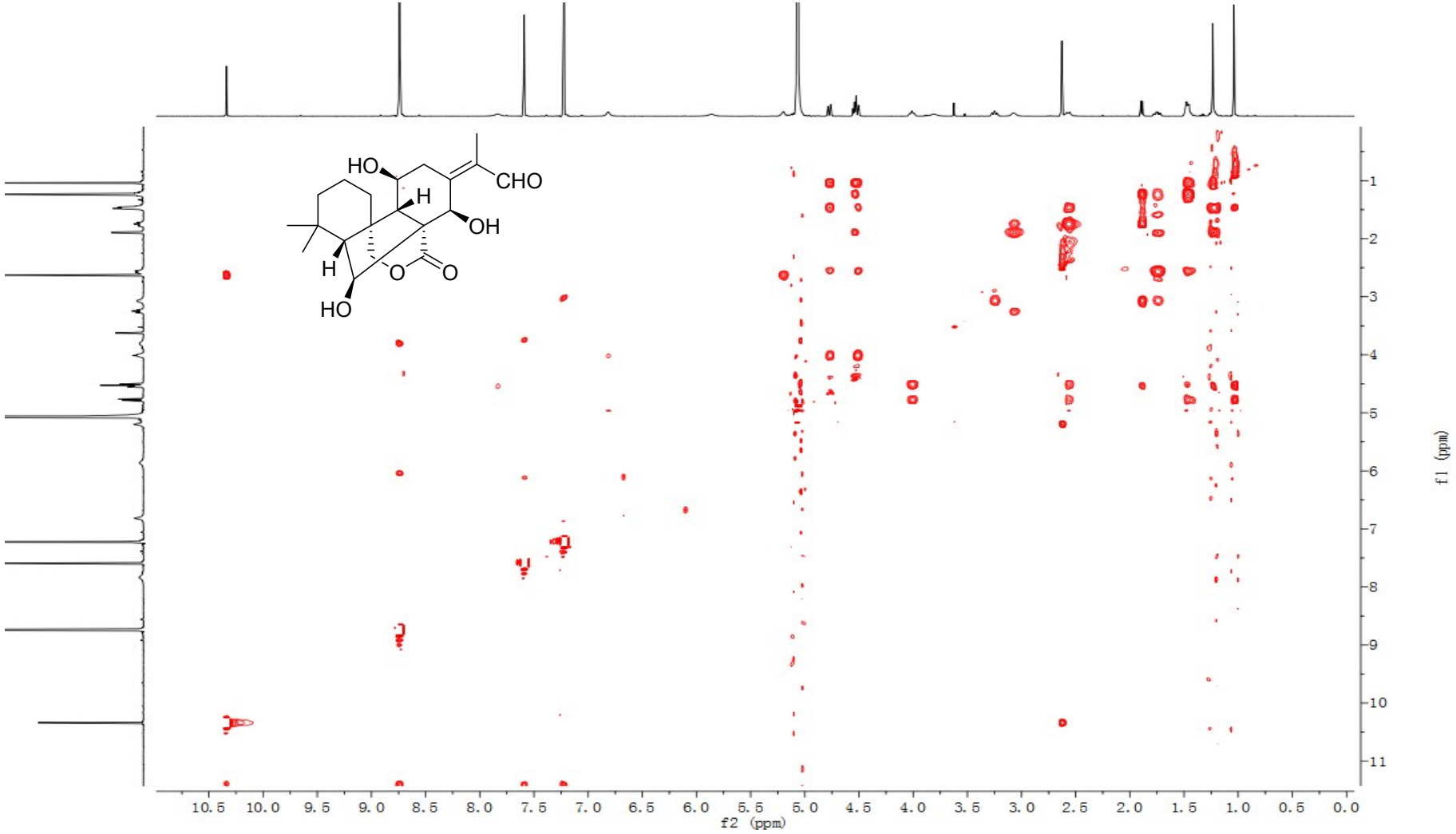


Figure S106. ROESY spectrum of compound **12** (Recorded in pyridine-d_5)

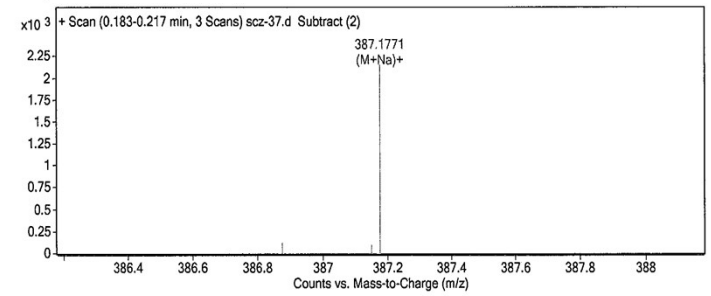
Qualitative Analysis Report

Data Filename	scz-37.d	**Sample Name**	scz-37
Sample Type	Sample	**Position**	P1-B8
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	9/14/2015 4:15:52 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)

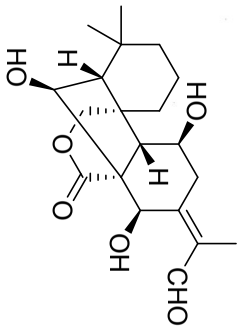
User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund
274.2744	1	28114.84
275.2776	1	4923.05
290.2698	1	5409.84
302.3059	1	5876.47
318.3007	1	17033.77
346.3317	1	4765.49
437.1934	1	6159.32
453.1675	1	16878.92



Formula Calculator Element Limits

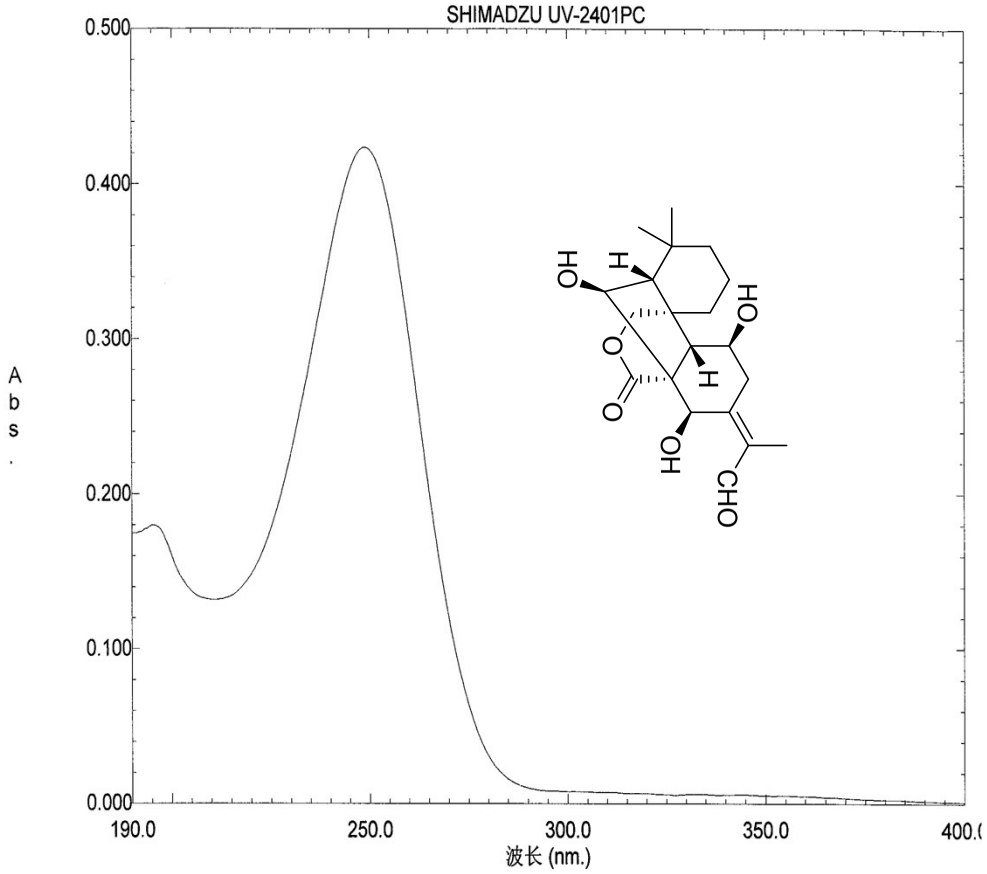
Element	Min	Max
C	3	60
H	0	120
O	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H28 O6	364.1886	387.1778	387.1771	-1.1	-3.1	7.0000

--- End Of Report ---

Figure S107. HRESIMS spectrum of compound **12**



文件名: SCZ-37

SCZ-37 ———

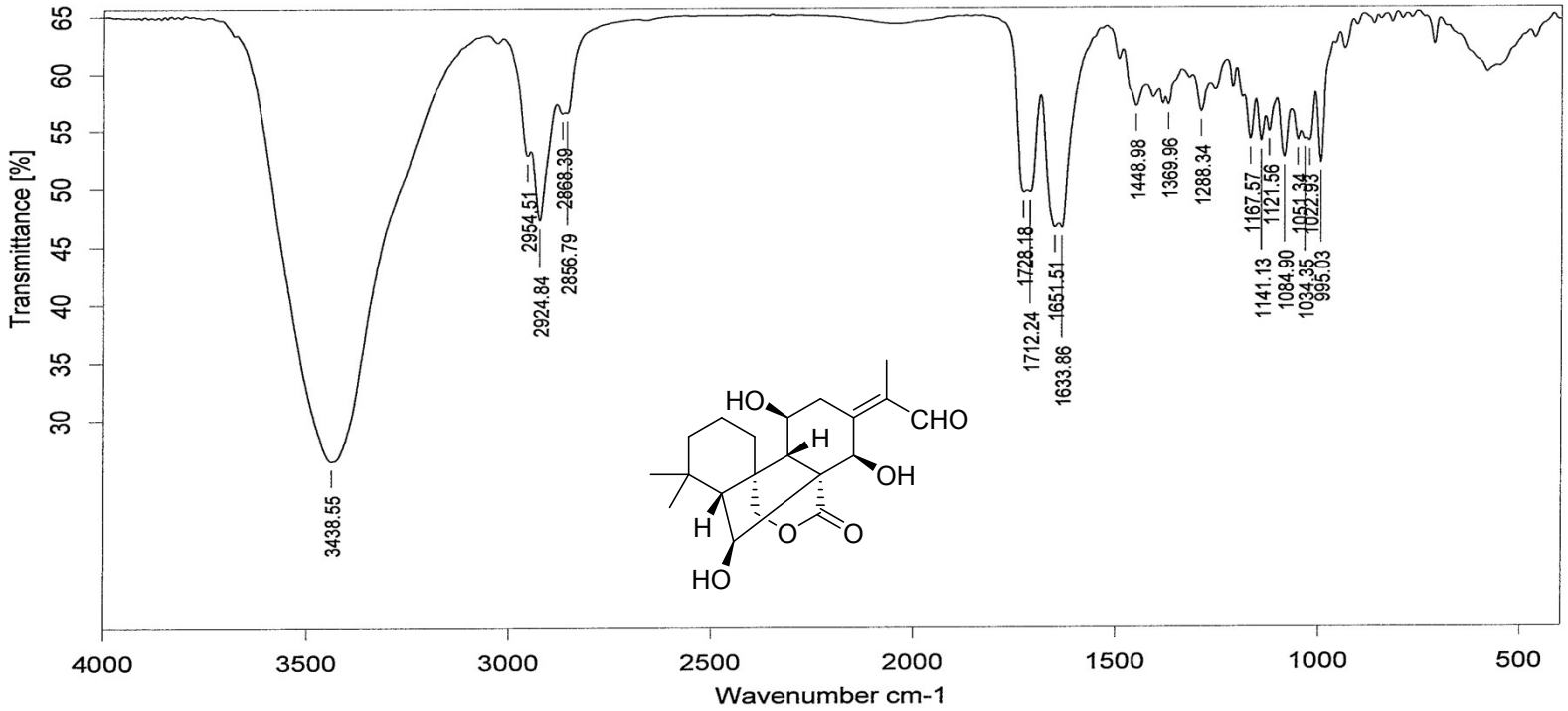
样品浓度：0.0158毫克/毫升
溶剂：甲醇

创建于: 16:03 15-09-19
数据: 原始

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.2

否.	波长 (nm.)	Abs.
1	248.80	0.4235
2	195.60	0.1797

Figure S108. UV spectrum of compound **12**



Sample : scz-37	Frequency Range : 399.246 - 3996.32	Measured on : 25/09/2015	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27	Sample Scans : 16
Customer : 150925IR1	Zerofilling : 2	Acquisition : Double Sided,For	

Figure S109. IR spectrum of compound **12**

Computational section

Conformational analysis of (1*S*,5*R*,6*S*,7*S*,9*S*,10*S*)-**2** was initially performed in Spartan'16 (Wavenfunction, Irvine, CA, USA, 2016) using the Monte Carlo algorithm and Merck molecular force field (MMFF) with standard parameters and convergence criteria. Only one conformer was found for (1*S*,5*R*,6*S*,7*S*,9*S*,10*S*)-**2** within an energy window of 5 kcal/mol. It was optimized with DFT calculations at M062x/def2svp level of theory with D3 correction (EmpiricalDispersion = GD3) using Gaussian 09 program,[1] and frequency analysis was run at the same level of theory to ensure that no imaginary frequencies exist. Optical rotatory dispersion (ORD) of (1*S*,5*R*,6*S*,7*S*,9*S*,10*S*)-**2** was calculated using the optimized conformer at three levels of theories: PBE1PBE/def2SVPD, PBE1PBE/6-31++G(d,p), B3LYP/6-31++G(d,p) levels with IEFPCM solvent model in methanol, resulting in the calculated ORD values of –66.88, –70.08, –69.12, respectively. The calculated results were in good consistence with the experimental value of –105.6. Thus, the absolute structure of **2** was established.

Reference: 1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, et al. Gaussian 09: Gaussian, Inc., Wallingford CT, 2010.

Table S1. Optimized Z-matrixes of (1*S*,5*R*,6*S*,7*S*,9*S*,10*S*)-2 in the gas phase (Å) at the M062x/def2svp level.

C	2.729172	1.278250	0.034680	C	0.061879	4.668020	1.022915
C	3.337112	0.076277	-0.680103	H	2.886508	1.211158	1.122494
C	2.668853	-1.256464	-0.299157	H	3.209568	2.209334	-0.300383
C	1.151689	-1.100176	-0.568490	H	4.417082	0.020328	-0.470048
C	0.445030	0.128899	0.071483	H	3.236640	0.218638	-1.770084
C	1.234131	1.398474	-0.235013	H	1.084047	1.663267	-1.294772
C	0.315535	-2.366785	-0.295120	H	0.924340	-3.141072	0.203424
C	-0.788944	-2.020370	0.704256	H	1.160017	0.092878	2.159790
C	-1.730232	-1.003380	0.081839	H	-0.520493	0.619241	1.954326
C	-0.980738	0.145319	-0.553040	H	-1.981014	-2.987568	1.847653
C	0.244363	-0.084190	1.583011	H	2.778613	-3.337984	-0.977958
O	-1.393392	-3.190728	1.107981	H	4.293765	-2.424348	-1.151366

H	1.075197	-0.945017	-1.657435	H	2.942164	-2.140325	-2.280235
C	3.198489	-2.353525	-1.231591	H	2.923702	-0.803586	1.848143
C	3.028181	-1.638384	1.144870	H	2.403158	-2.459678	1.521417
O	-0.220891	-2.839231	-1.503596	H	4.078435	-1.964457	1.184927
C	-3.064836	-1.072563	0.156409	H	-0.817793	-3.568658	-1.289790
C	-3.922996	0.016600	-0.373238	H	-3.579813	-1.921658	0.611840
C	-3.199901	1.169635	-1.050577	H	-3.110633	0.898788	-2.117778
C	-1.806436	1.429652	-0.476806	H	-3.853474	2.050108	-0.996635
O	-5.126869	-0.022256	-0.281396	H	-1.316706	2.235124	-1.044496
H	-0.866151	-0.110884	-1.623082	H	-1.884358	1.764648	0.570166
O	-0.164679	-1.421209	1.825418	H	0.188428	5.685886	0.642629
O	0.698448	2.450754	0.577355	H	-1.008406	4.435768	1.118094
O	1.104575	3.958269	-1.029157	H	0.514788	4.560891	2.016513
C	0.687123	3.693776	0.063643				