

SUPPLEMENTARY MATERIAL

Structure-Based Molecular Networking for the Discovery of Anti-HBV compounds from *Saussurea lappa* *Saussurea lappa* (Decne.) C.B Clarke

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Table S1. The top ten square nodes.

Number	Degree	Smiles	Skeleton _types
45	27	<chem>C(C)(C)C1CC2C(C)(CC1)CCCC2C</chem>	Eudesmane
21	21	<chem>C(C)(C)C1CC2C(C)CCC2C(C)CC1</chem>	Guaiane
26	20	<chem>C(C)(C)C1C2C(C(C)CC1)CCC(C)C2</chem>	Cadinane
54	18	<chem>CC1CCCC(C)CCC(C(C)C)CC1</chem>	Germacane
40	16	<chem>C(CCCC(C)C1CCC(C)CC1)(C)C</chem>	Bisabolane
9	16	<chem>C(C)(C)C1CCC(CCCC)C(C)CC1</chem>	secoguaiane
27	15	<chem>C(C)(C)C1C2C(C(C)CC1)CC(C)CC2</chem>	Lasserane
17	15	<chem>C(C)(C)C1CC2C(C)(CCC2CC)CC1</chem>	Iphionane
87	14	<chem>CC(CC1)CC21CC(C(C)C)CCC2C</chem>	Spiroaxane
73	13	<chem>CC1C(C)CCC(C)C2C(C(C)CC2)C1</chem>	Dumortane

Table S2. Classification of medicinal plants.

No	Skeleton	Skeleton_SMILES	Sources_A	Sources_B	Sources_C	Sources_D	Sources_E
21	Guaiane	<chem>C(C)(C)C1CC2C(C)CC2C(C)CC1</chem>	<i>Saussurea</i> DC	<i>Artemisia</i> L.	<i>Mikania</i> Willd	<i>Glebionis</i> Cass.	<i>Anthemis</i> L.
54	Germacane	<chem>CC1CCCC(C)CCC(C(C)C)CC1</chem>	<i>Saussurea</i> DC	<i>Inula</i> L.	<i>Carpesium</i> L.	<i>Pseudelephantopus</i> Rohr.	<i>Helianthus</i> .
45	Eudesmane	<chem>C(C)(C)C1CC2C(C)(C1)CCCC2C</chem>	<i>Saussurea</i> DC	<i>Tugarinovia</i> Iljin	<i>Inula</i> L.	<i>Atractylodes</i>	<i>Tanacetum</i> L.
40	Bisabolane	<chem>C(CCCC(C)C1CCC(C)CC1)(C)C</chem>	<i>Ligusticum</i> L.	<i>Eupatorium</i> L.	<i>Cremanthodium</i> Benth	<i>Artemisia</i> L.	<i>Matricaria</i>
26	Cadinane	<chem>C(C)(C)C1C2C(C(C)C1)CCC(C)C2</chem>	<i>Pteridium</i>	<i>Pulicaria</i> Gaertn.	<i>Eupatorium</i> L.	<i>Artemisia</i> L.	<i>Cyperus</i> L.
22	Carotane	<chem>CC1(CCC2C(C)C)C2C(C)CC1</chem>	<i>Inula</i> L.	<i>Ageratum</i> L.	<i>Ferula</i> L.	<i>Sium</i> L.	<i>Daucus</i> L.
63	Caryophyllane	<chem>CC1(C)C2C(C(C)CCC(C)CC2)C1</chem>	<i>Dacrydium pierrei</i> Hickel	<i>Juniperus formosana</i> Hayata	<i>Sindora</i> Miq.	<i>Gossypium</i> L.	<i>Pulicaria</i> Gaertn.
44	Prezizaane	<chem>CC(CC1)C2(CC3)C1C(C)(C)C(C)C3C2</chem>	<i>Juniperus</i> L.	<i>Neocallitropsis</i>	<i>Vetiveria</i>	<i>Illicium</i> L.	<i>Streptomyces</i>
119	Patchoulane	<chem>CC1CCC(C2(C)C)C3(C)C1CC2CC3</chem>	<i>Pogostemon helferi</i>	<i>Cyperus</i> L.	<i>Croton crassifolius</i> .	<i>Daphne</i> L.	<i>Agastache</i> Clayt. in Gronov
50	Eremophila ne	<chem>C(C)(C)C1CC2(C)C(C)CCCC2CC1</chem>	<i>Senecio</i> L.	<i>Solidago</i> L. .	<i>Ligularia</i> Cass.	<i>Litsea</i>	<i>Pedicularis</i> L.

Table S3. Classification of *Saussurea* DC

NAME	Number of documents	Skeleton_number	Skeleton_types
<i>Saussurea cauloptera</i>	1	2	Eudesmane、Serpentine
<i>Saussurea deltoidei</i>	1	2	Guaiane、elemane
<i>Saussurea laniceps</i>	2	2	Guaiane、Germacrane
<i>Saussurea lappa</i>	4	3	Eudesmane、Guaiane、Germacrane
<i>Saussurea macrota</i>	1	2	Guaiane、Germacrane
<i>Saussurea medusa</i>	2	2	Eudesmane、Cadinene)
<i>Saussurea medusa Maxim</i>	1	2	Eudesmane、Amyrane
<i>Saussurea pulchella</i>	1	2	Guaiane、Germacrane
<i>Saussureae Radix</i>	1	2	Eudesmane、Guaian

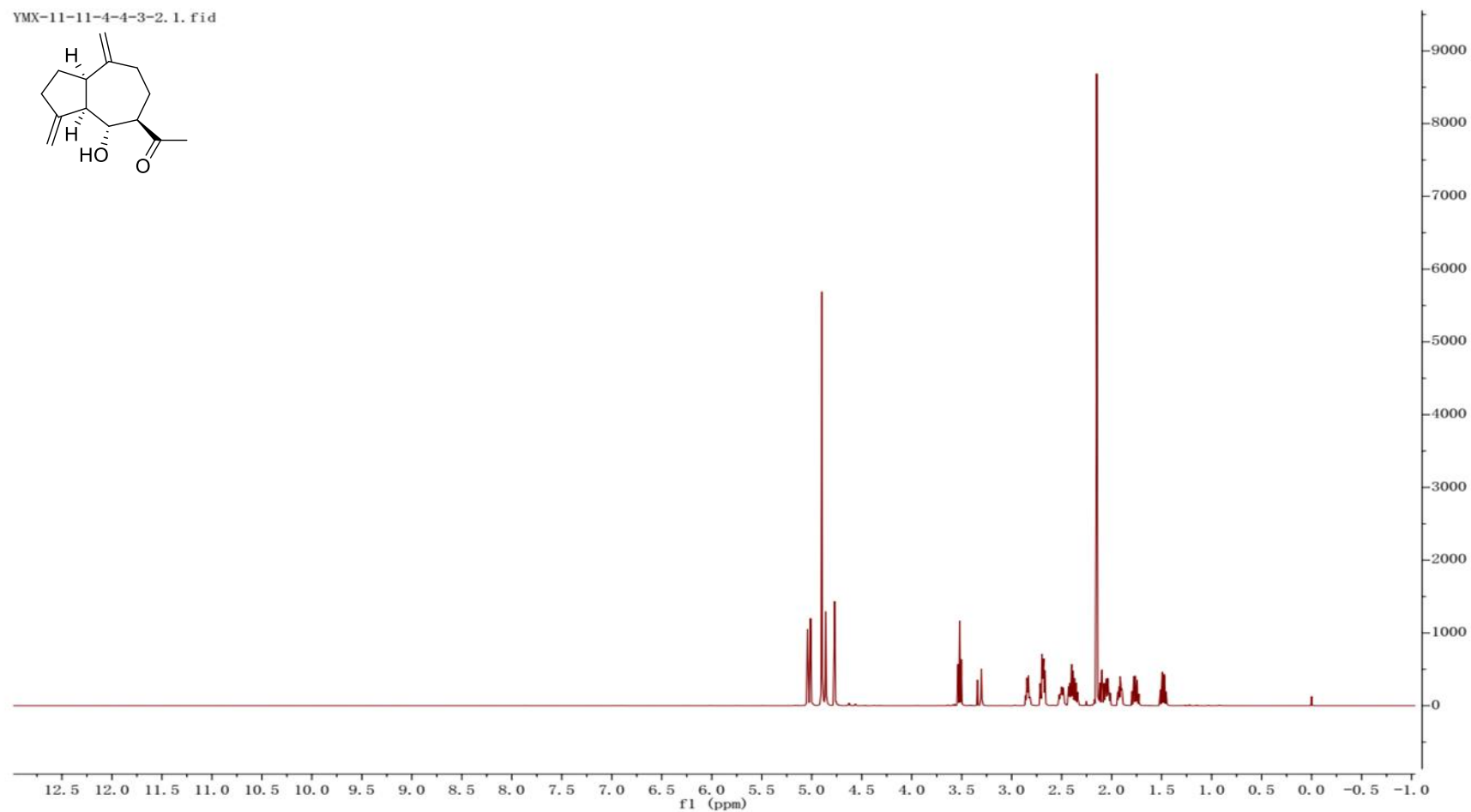


Figure S1. ^1H NMR spectrum of compound **1** (CD_3OD , 600 MHz)

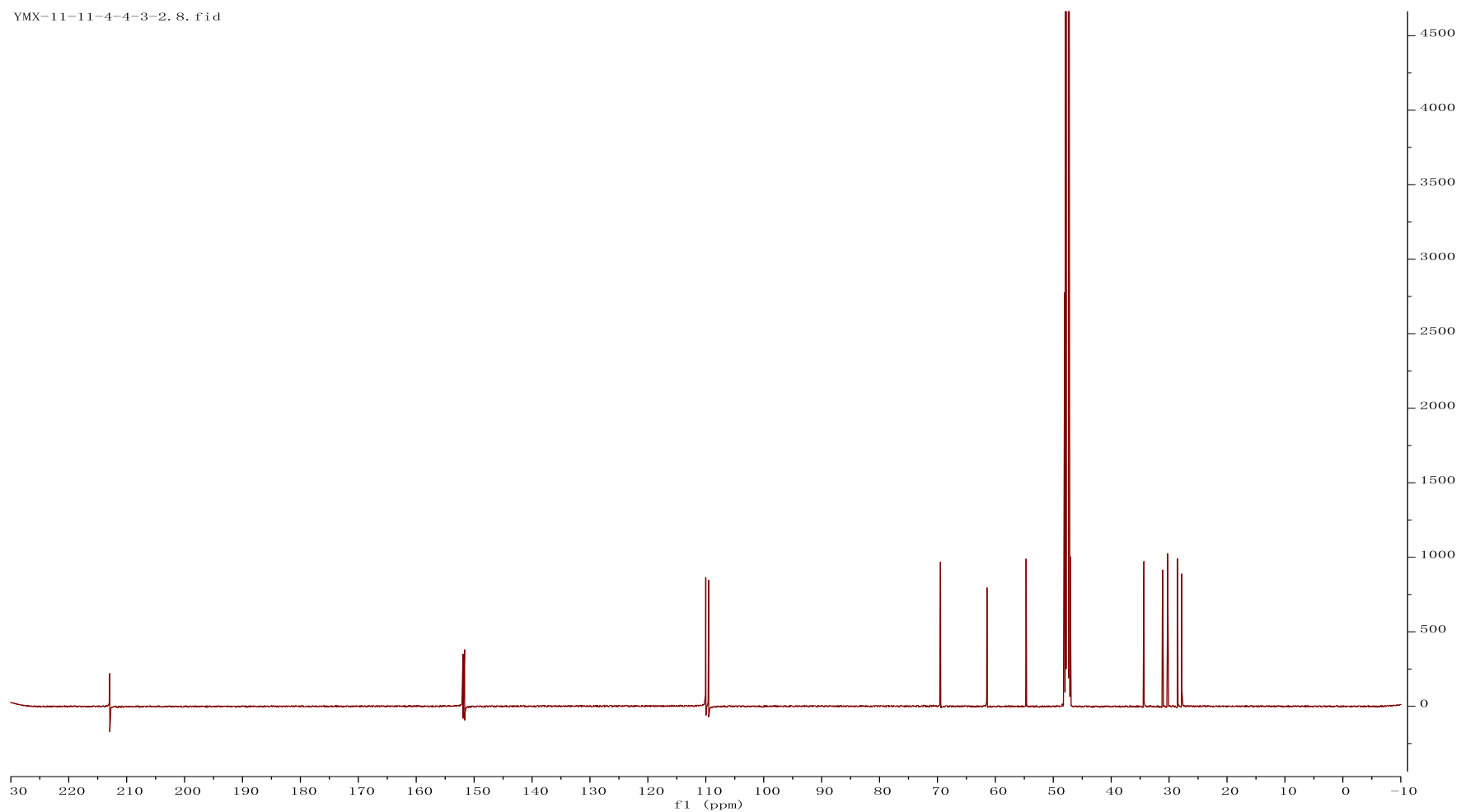


Figure S2. ^{13}C NMR spectrum of compound **1** (CD_3OD , 150 MHz)

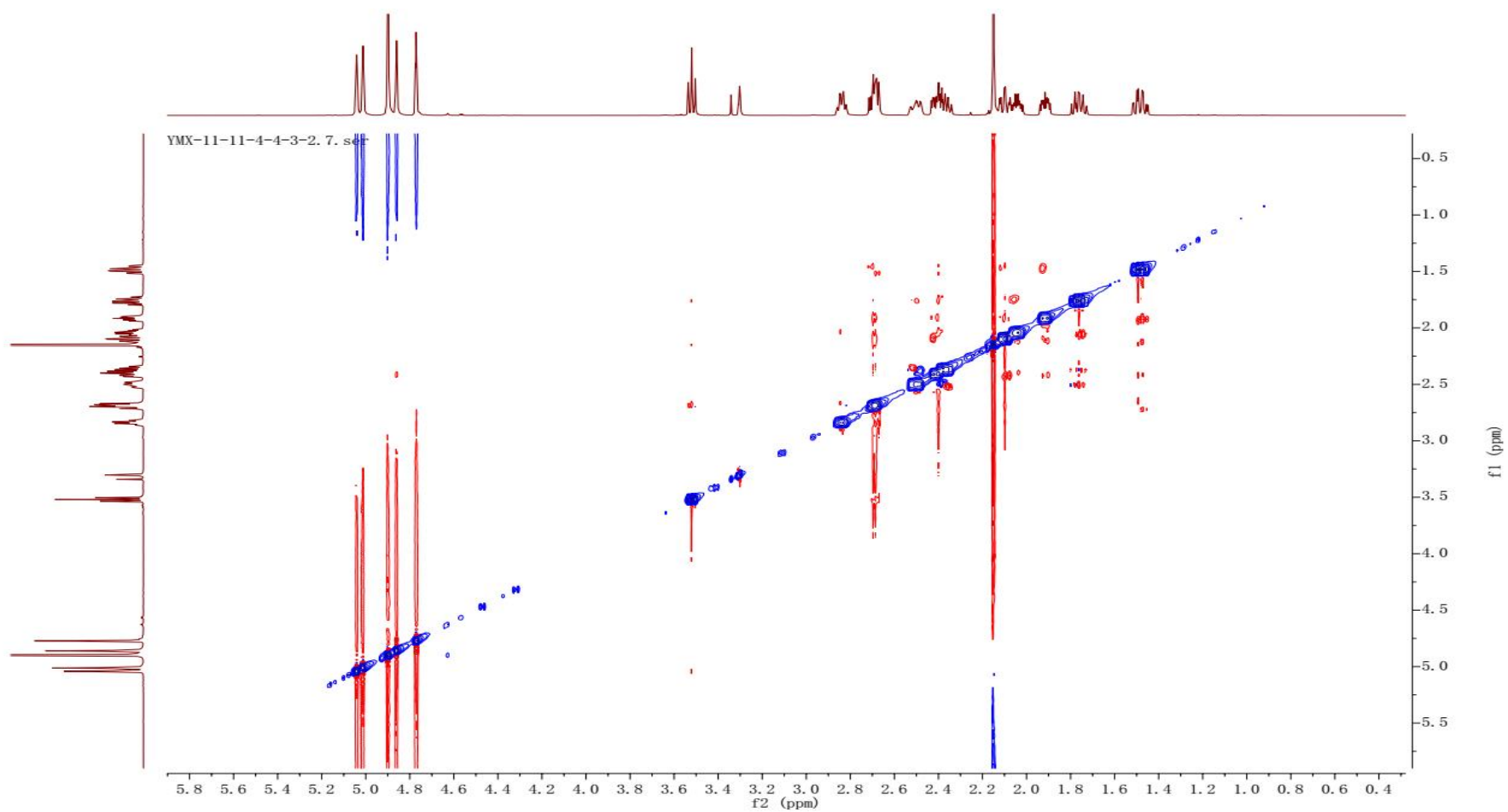


Figure S3. ROESY spectrum of compound **1** (CD₃OD, 600 MHz)

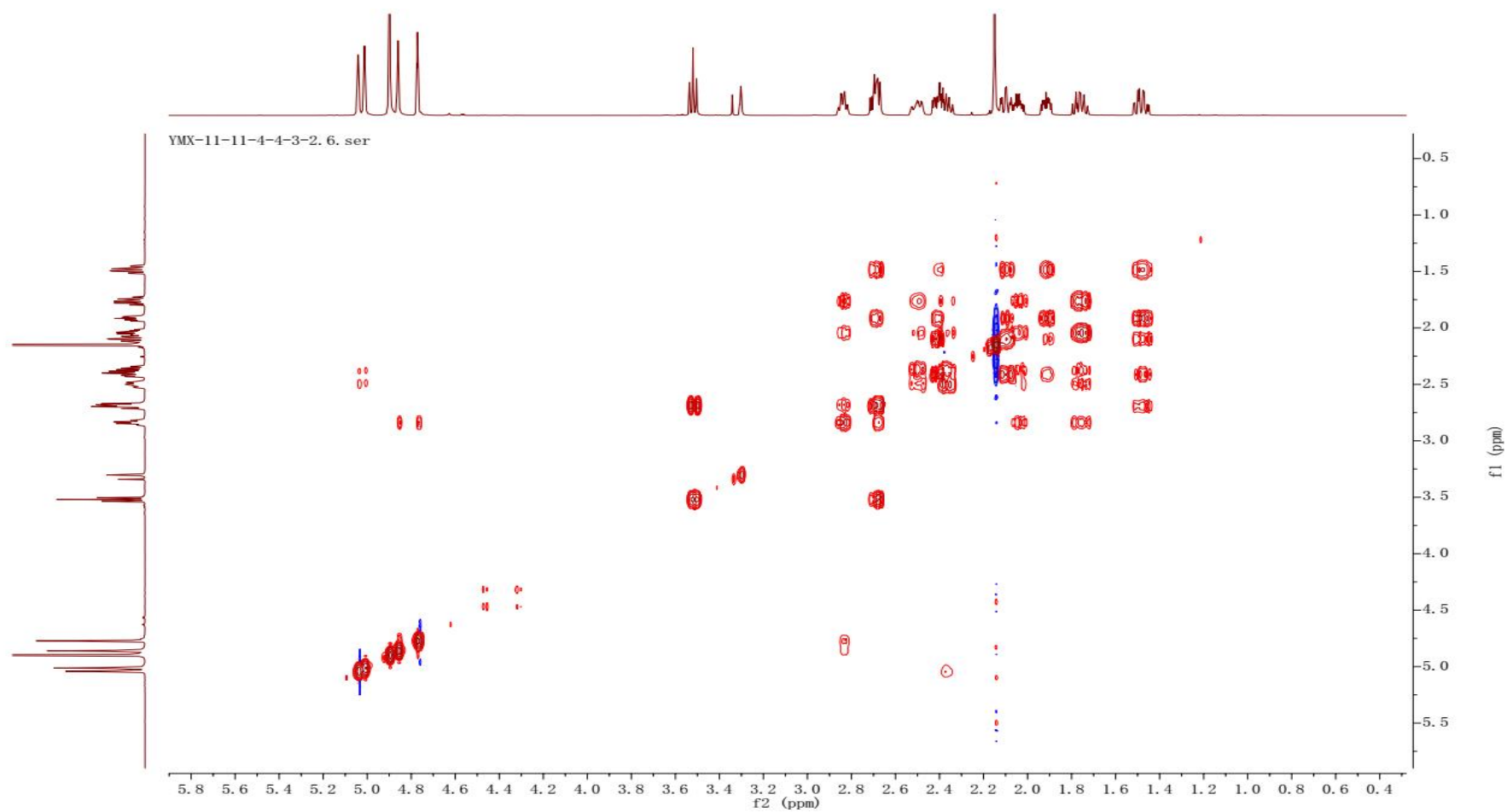


Figure S4. ^1H - ^1H COSY spectrum of compound **1** (CD_3OD , 600 MHz)

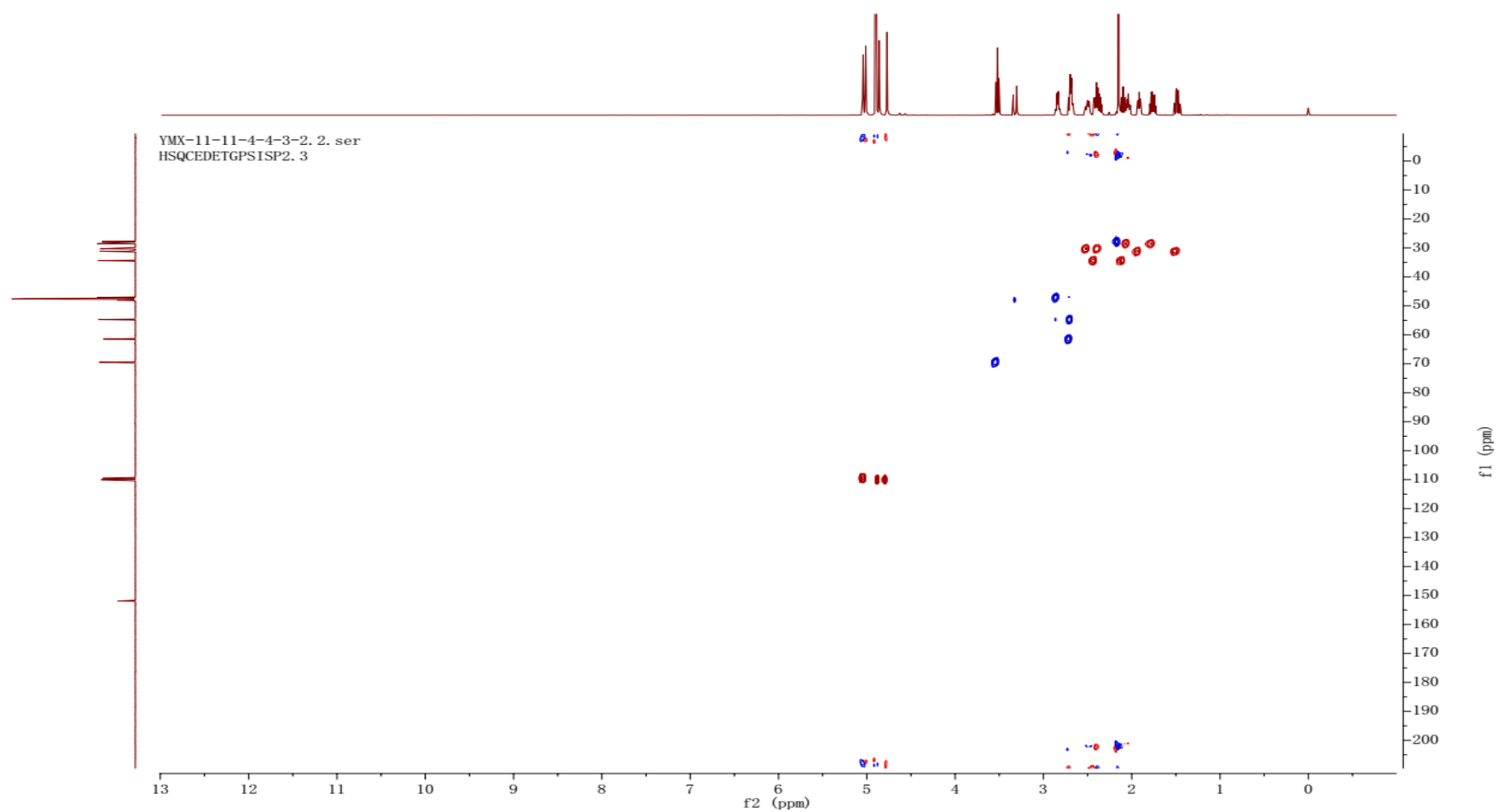


Figure S5. HSQC spectrum of compound **1** (CD₃OD, 600 MHz)

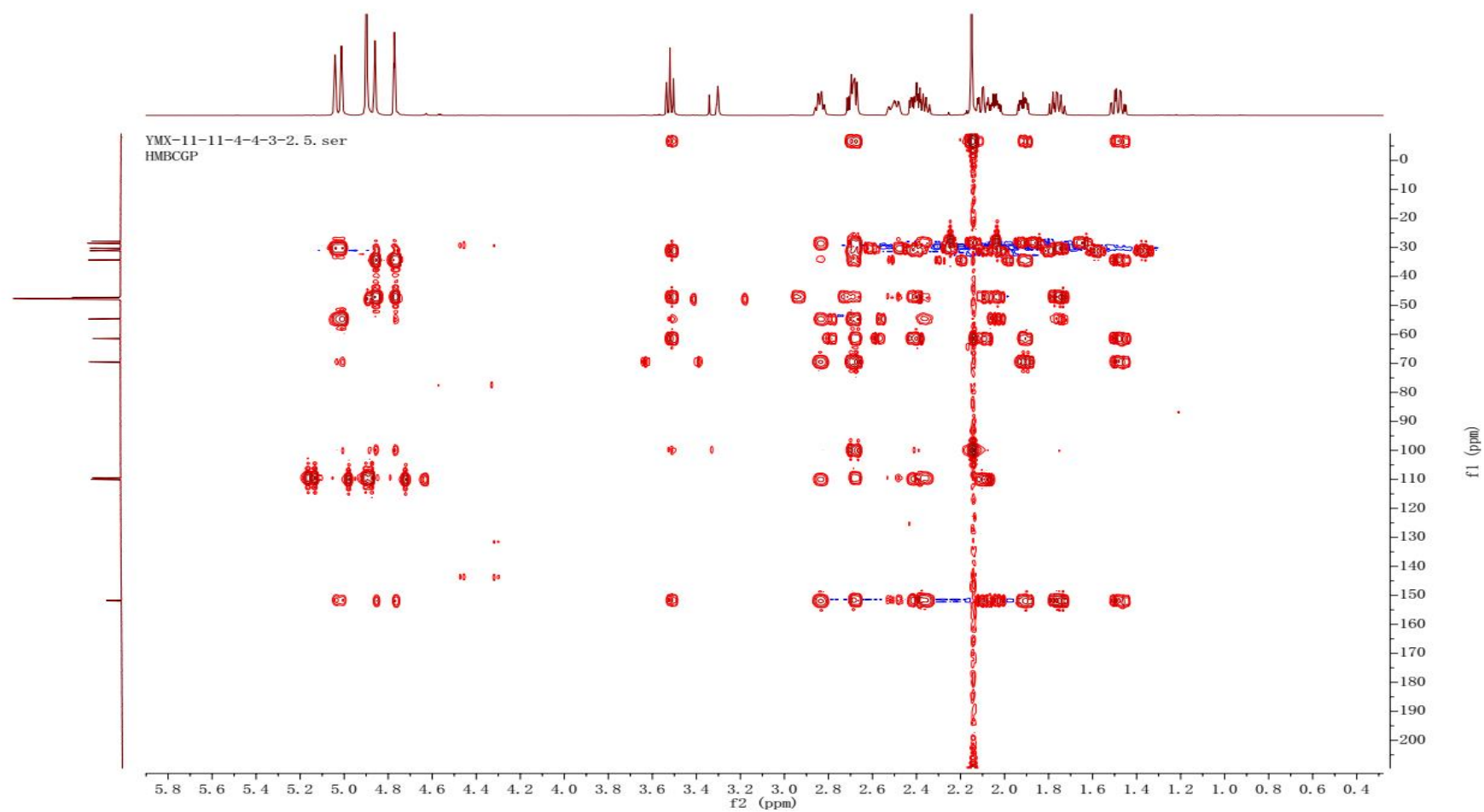
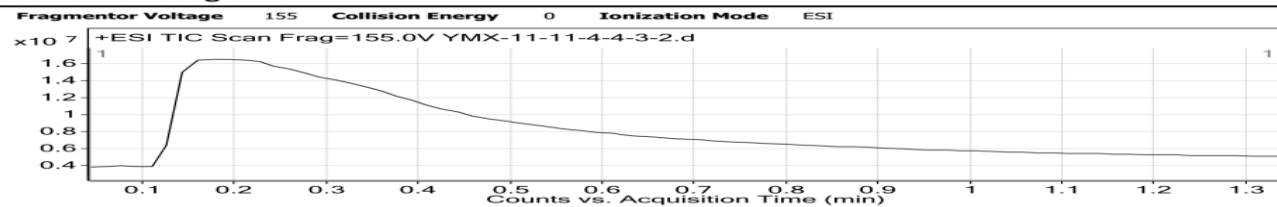


Figure S6. HMBC spectrum of compound **1** (CD₃OD, 600 MHz)

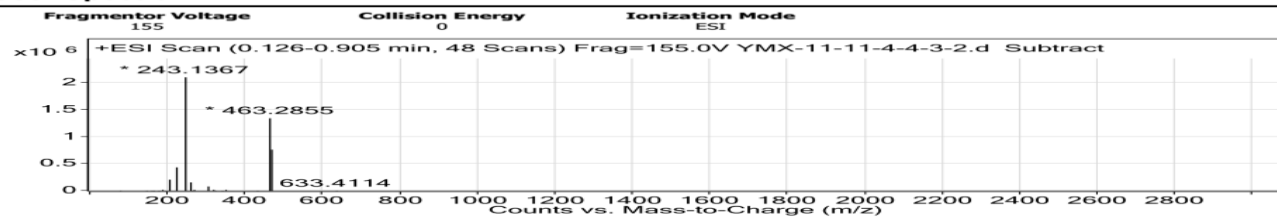
Qualitative Analysis Report

Data Filename	YMX-11-11-4-4-3-2.d	Sample Name	YMX-11-11-4-4-3-2
Sample Type	Sample	Position	p1b2
Instrument Name	Instrument 1	User Name	Q-TOF-HP\Q-TOF
Acq Method	default20190111-ms.m	Acquired Time	1/12/2020 12:37:26 AM
IRM Calibration Status	Success	DA Method	1.m
Comment			
Sample Group	6200 series TOF/6500 series	Info.	
Acquisition SW	Q-TOF B.05.01 (B5125.3)		
Version			

User Chromatograms



User Spectra

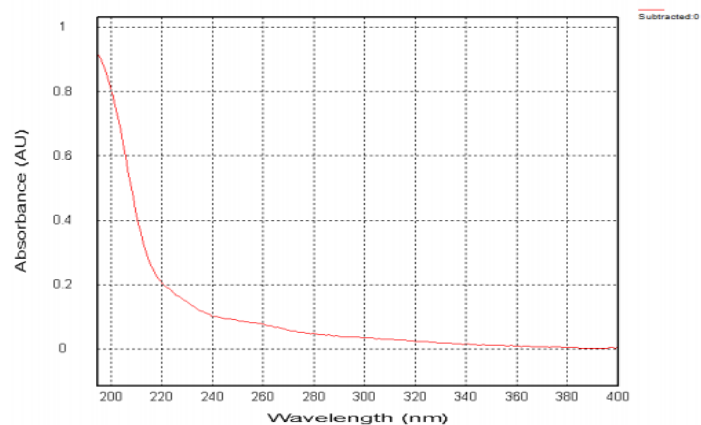
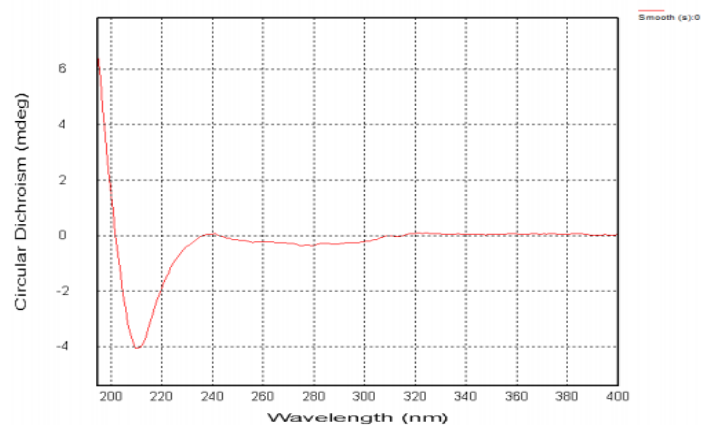


Peak List

m/z	z	Abund
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221.1527	1	446446.97
243.1367	1	2108812
243.2699	1	151521.28
244.1382	1	518419.28
259.1082	1	160975.52
463.2855	1	1355956.25
463.464	1	123497.32

Figure S7. HRESI spectrum of compound 1

YMX-11-11-4-4-3-2



File: YMX-11-11-4-4-3-2 (195-400 nm) 20112718.dsx

ProBinaryX

Attributes :

- Time Stamp : Fri Nov 27 19:51:12 2020

- File ID : {A8234499-FCB9-4b69-BBF6-E4E19927A8D4}

- Is CFR Compliant : false

- Original data has not been modified.

Remarks:

- User: CD

- Date: 2020/11/27

- Instrument: 0547

- DetectorType: LAAPD

- DichOS Calibration Correction Curve: 0547/2

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.1680mg/mL MeOH

- Pathlength: 1 mm

- Temperature: 20°C

Settings:

- Time-per-point: 1s (25us x 40000)

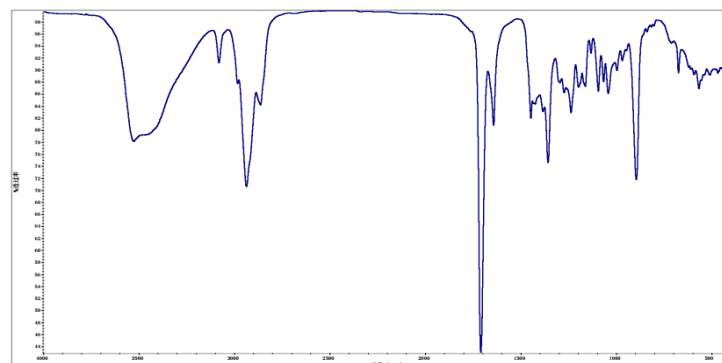
- SE

- Wavelength: 195nm - 400nm

- Step Size: 1nm

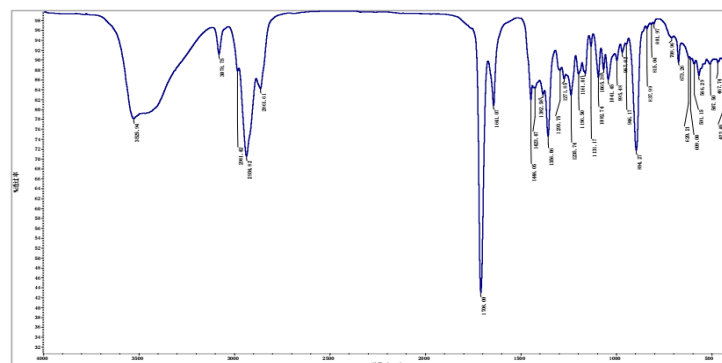
- Bandwidth: 1nm

Figure S8. CD and UV spectrum of compound **1**



Sample Name: YMX-11-11-4-4-3-2
KBr压片
采集时间: 星期三 10月 28 16:21:54 2020 (GMT+08:00)
仪器型号: NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00



Sample Name: YMX-11-11-4-4-3-2
KBr压片
采集时间: 星期三 10月 28 16:21:54 2020 (GMT+08:00)
仪器型号: NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00

星期三 10月 28 16:28:45 2020 (GMT+08:00)

标峰:

谱图: YMX-11-11-4-4-3-2
范围: 4000.00 400.00
(绝对) 阈值: 97.507
灵敏度: 99

峰表:

峰位置:	410.06	强度:	91.307
峰位置:	420.72	强度:	91.303
峰位置:	435.26	强度:	90.300
峰位置:	444.53	强度:	90.177
峰位置:	467.74	强度:	89.349
峰位置:	507.50	强度:	89.121
峰位置:	566.29	强度:	86.817
峰位置:	591.15	强度:	89.154
峰位置:	609.00	强度:	90.052
峰位置:	620.21	强度:	90.420
峰位置:	673.26	强度:	89.510
峰位置:	709.96	强度:	94.430
峰位置:	801.97	强度:	97.265
峰位置:	815.04	强度:	97.097
峰位置:	837.99	强度:	96.283
峰位置:	894.27	强度:	71.654
峰位置:	946.17	强度:	93.158
峰位置:	967.82	强度:	91.498
峰位置:	995.48	强度:	89.847
峰位置:	1041.45	强度:	86.025
峰位置:	1065.38	强度:	88.027
峰位置:	1092.74	强度:	86.427
峰位置:	1131.17	强度:	92.740
峰位置:	1161.01	强度:	87.220
峰位置:	1196.50	强度:	87.110
峰位置:	1235.74	强度:	82.836
峰位置:	1271.85	强度:	86.159
峰位置:	1293.75	强度:	87.843
峰位置:	1356.06	强度:	74.534
峰位置:	1382.58	强度:	83.024
峰位置:	1423.47	强度:	84.289
峰位置:	1446.05	强度:	81.823
峰位置:	1641.07	强度:	80.757
峰位置:	1708.00	强度:	42.918
峰位置:	2861.61	强度:	84.143
峰位置:	2934.82	强度:	70.524
峰位置:	2981.42	强度:	87.694
峰位置:	3078.75	强度:	91.125
峰位置:	3525.94	强度:	78.053

Figure S9. IR spectrum of compound 1

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 26-NOV-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>
5	-30.07	0.12	-0.39	-29.90	-30.20

<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>
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2	YMX-11-11-4-4-3	02:35:56 PM	-30.13	SR	-0.0904	589	100.00	0.300	23.1
3	YMX-11-11-4-4-3	02:36:04 PM	-30.10	SR	-0.0903	589	100.00	0.300	23.1
4	YMX-11-11-4-4-3	02:36:12 PM	-29.90	SR	-0.0897	589	100.00	0.300	23.1
5	YMX-11-11-4-4-3	02:36:20 PM	-30.00	SR	-0.0900	589	100.00	0.300	23.1

Figure S10. $[\alpha]^{25}_D$ of compound 1

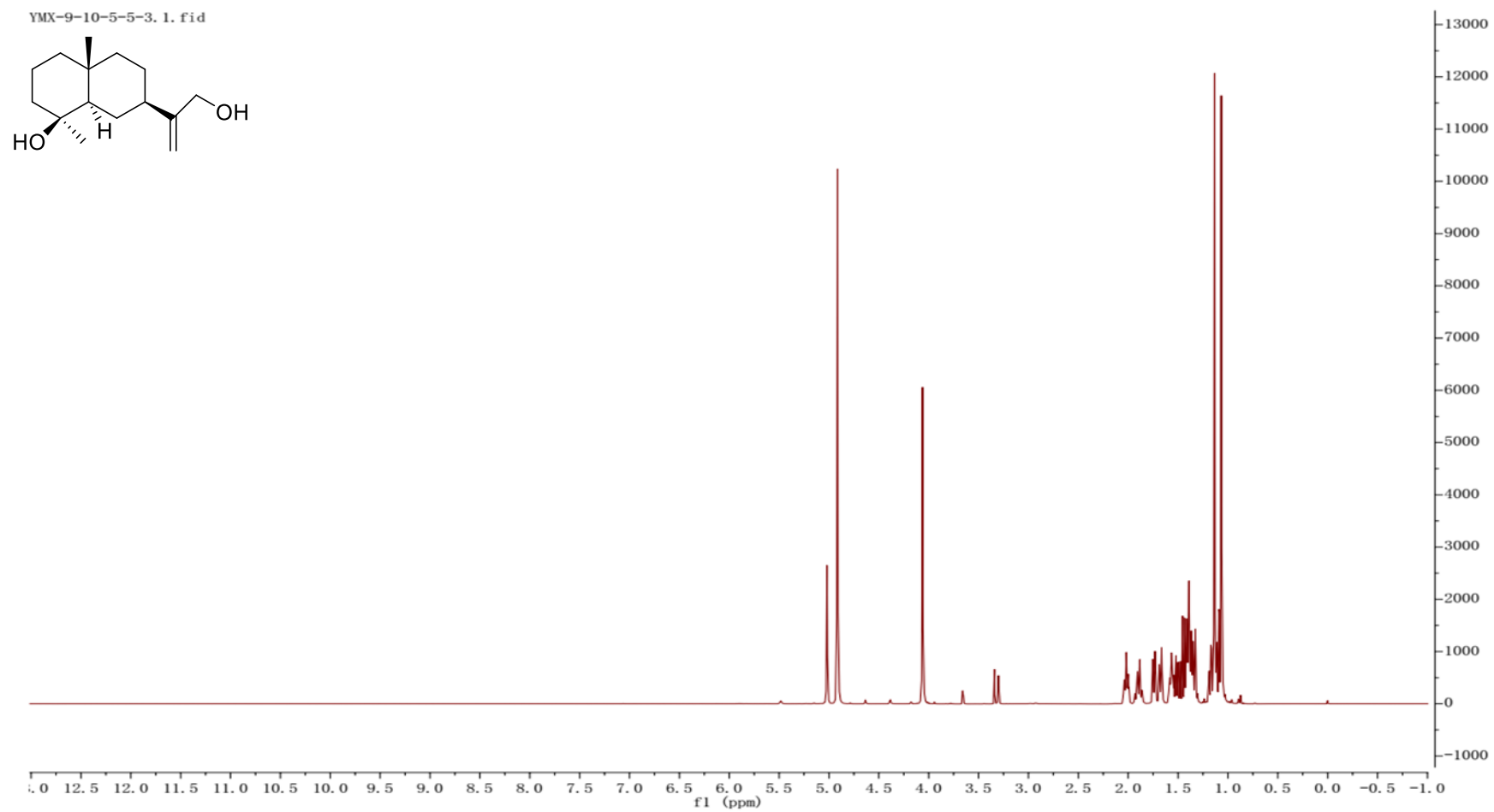


Figure S11. ^1H NMR spectrum of compound **2** (CD_3OD , 600 MHz)

YMX-9-10-5-5-3. 3. fid

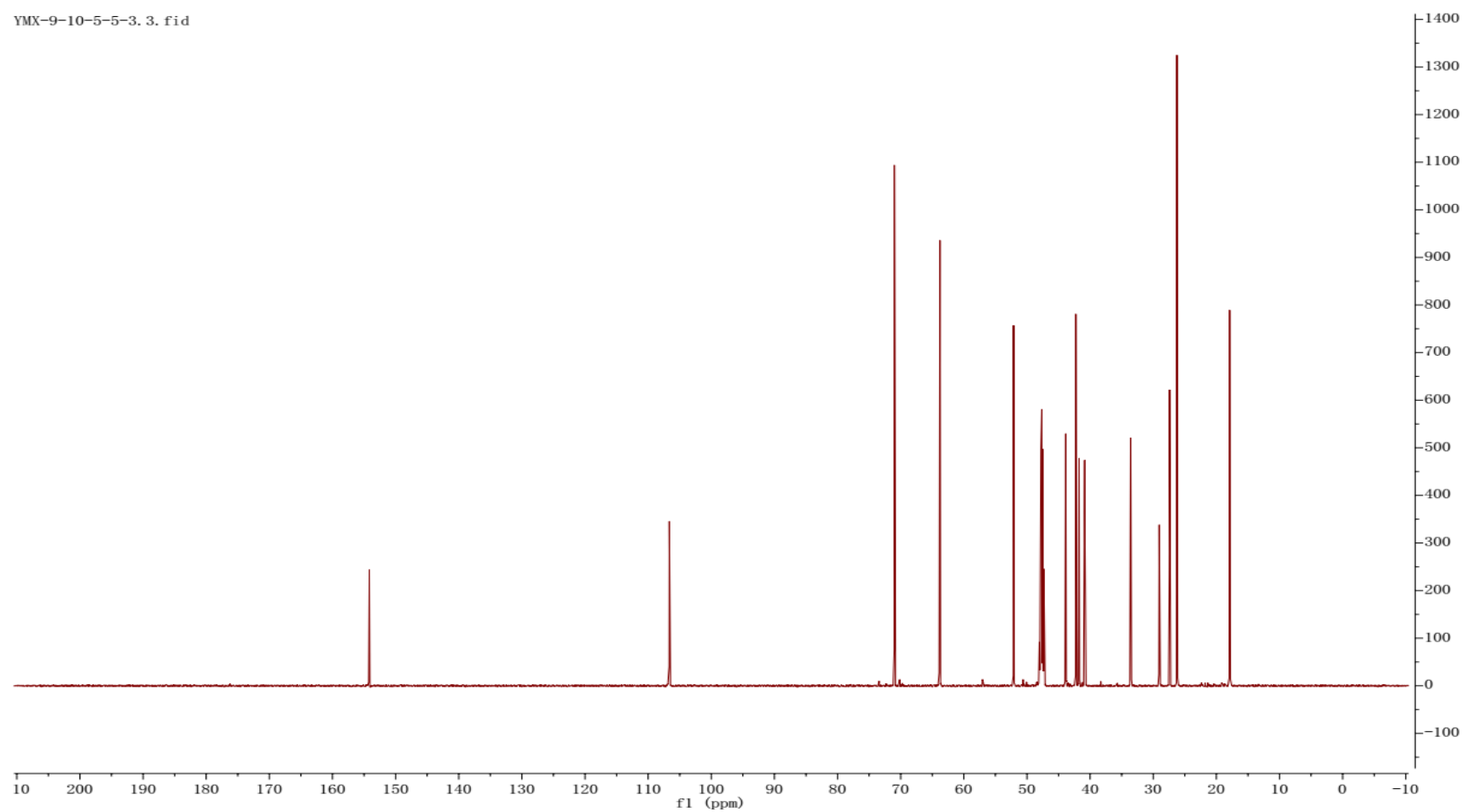


Figure S12. ^{13}C NMR spectrum of compound **2** (CD_3OD , 150 MHz)

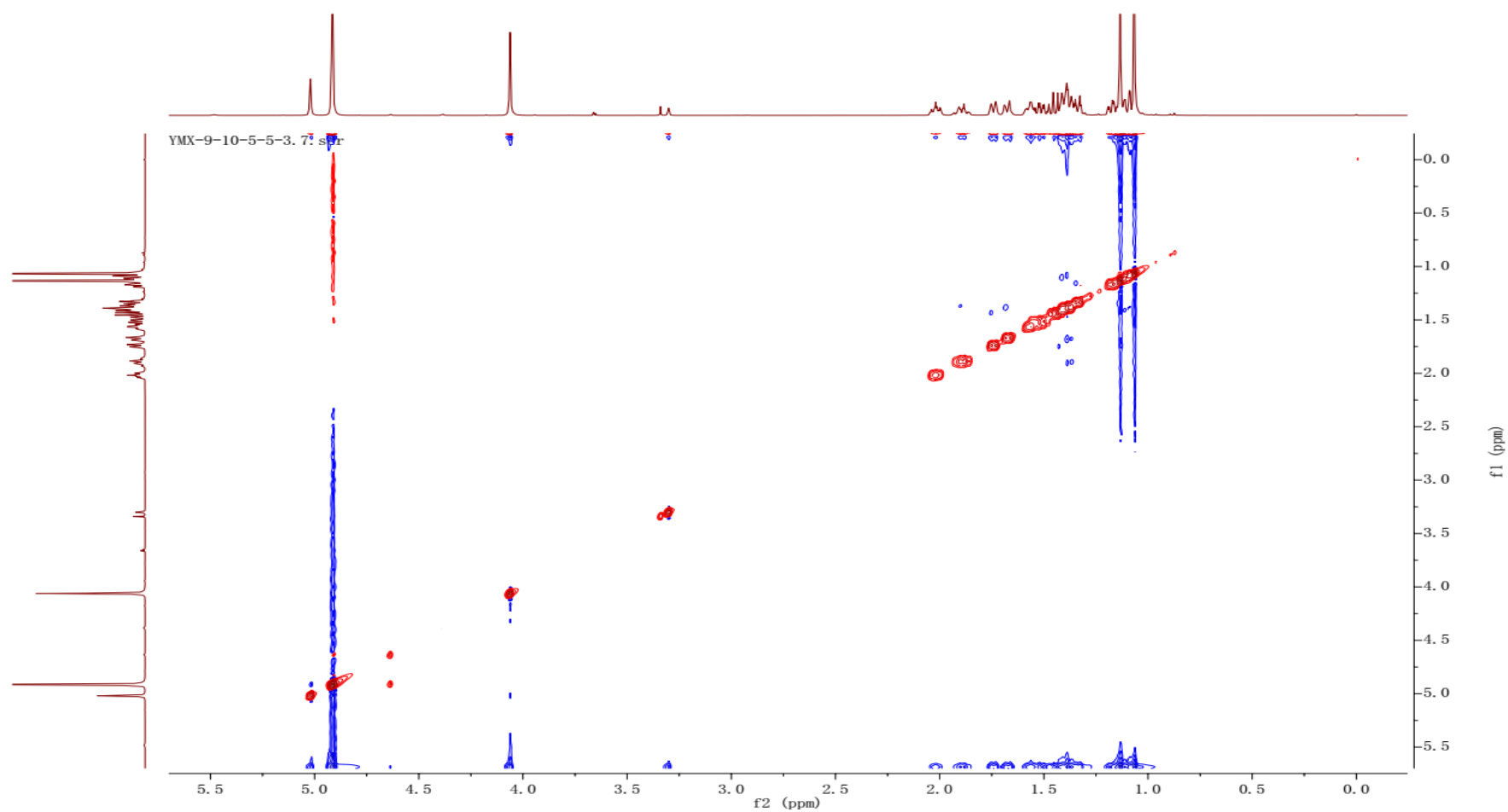


Figure S13. ROESY spectrum of compound **2** (CD₃OD, 600 MHz)

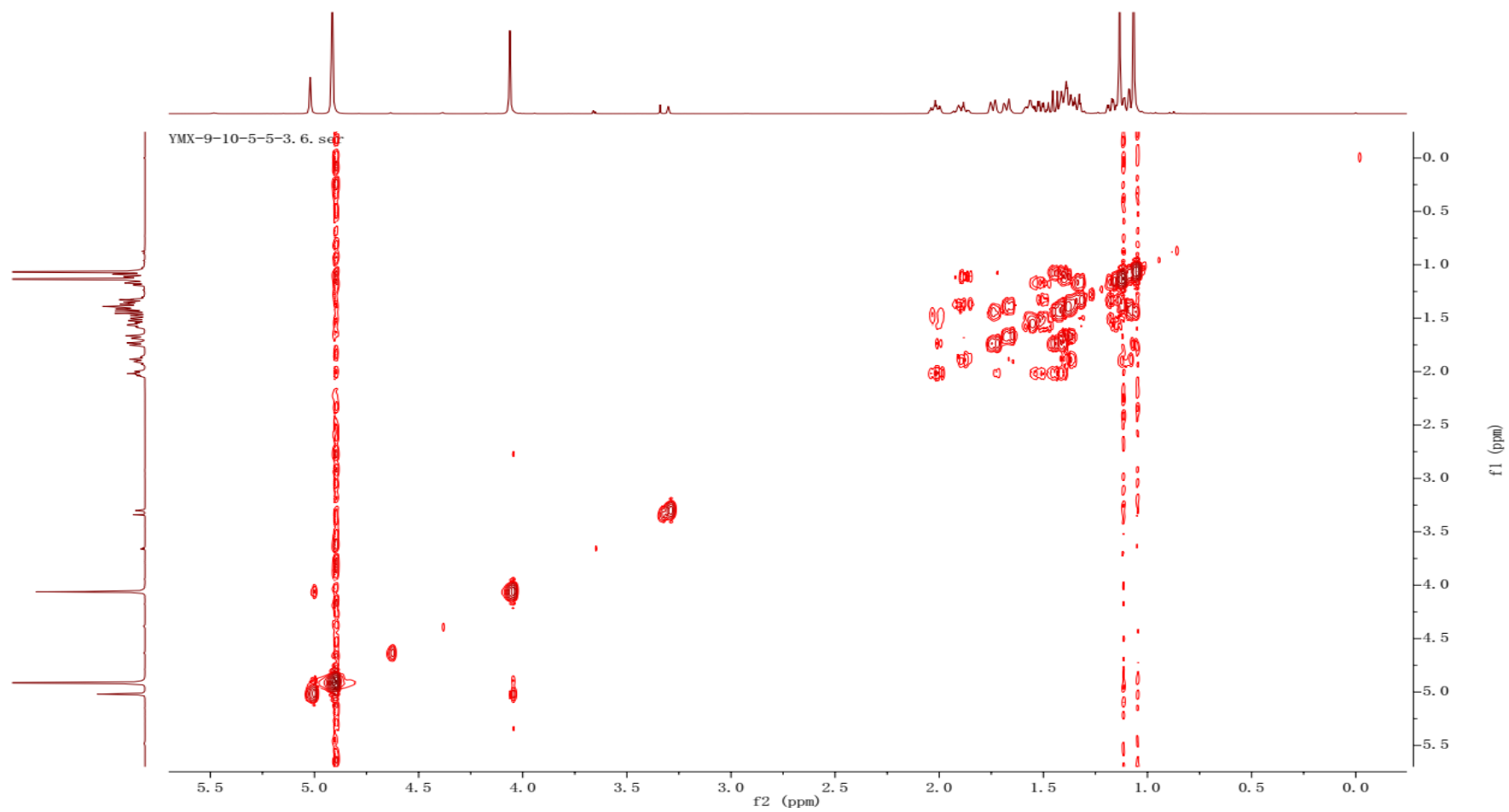


Figure S14. ^1H - ^1H COSY spectrum of compound **2** (CD_3OD , 600 MHz)

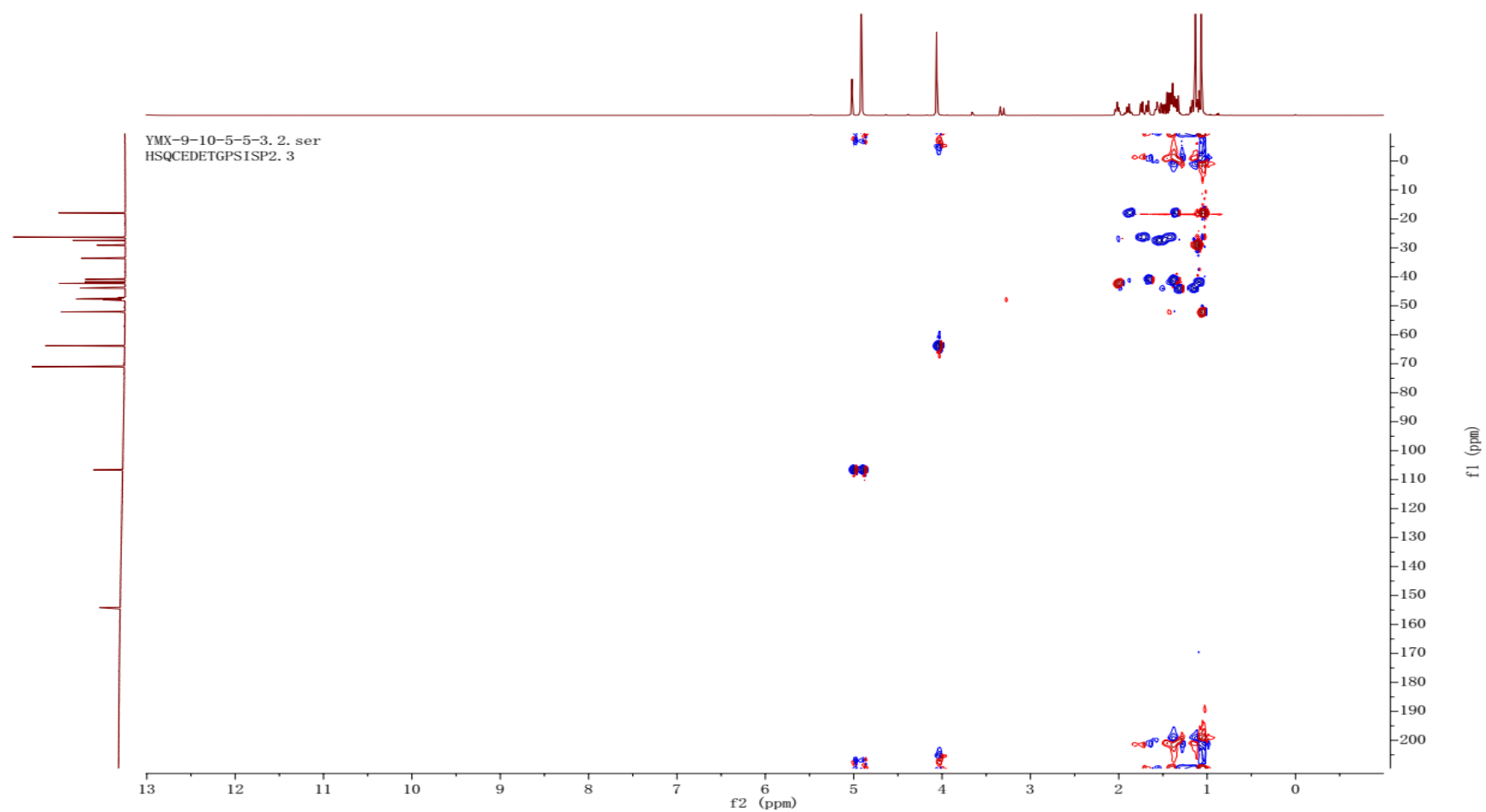


Figure S15. HSQC spectrum of compound **2** (CD₃OD, 600 MHz)

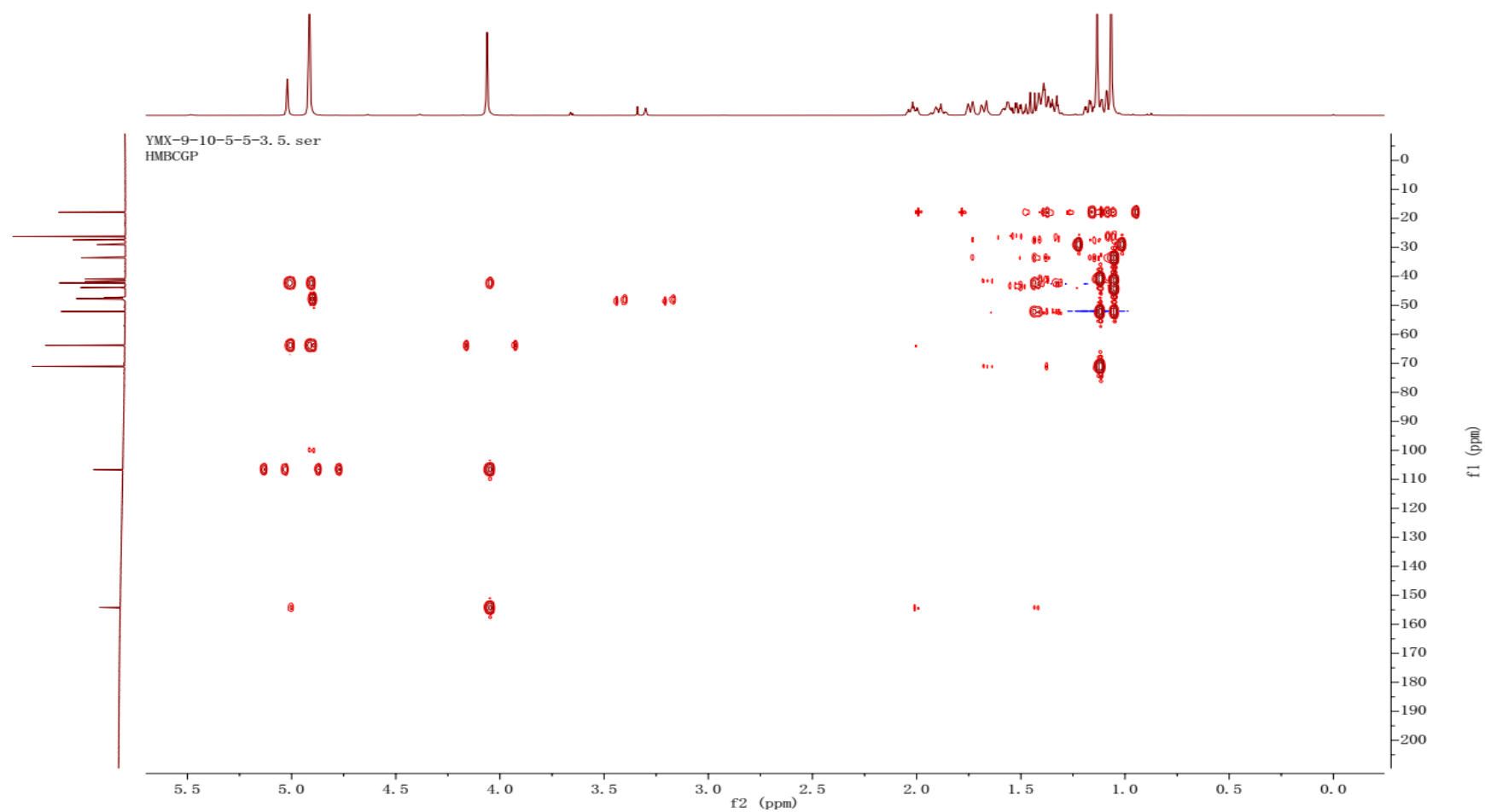


Figure S16. HMBC spectrum of compound **2** (CD₃OD, 600 MHz)

Data File: E:\DATA\2021\0901\YMX-9-10-5-5-3.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	5	150	O	2	0	30	P	3	0	0	Se	2	0	0	H
2H	1	0	0	F	1	0	0	S	2	0	0	Br	1	0	0	Na
B	3	0	0	Na	1	0	0	Cl	1	0	0	Pd	2	0	0	
C	4	5	100	Mg	2	0	0	Co	2	0	0	Ag	1	0	0	
N	3	0	10	Si	4	0	0	Cu	2	0	0	I	3	0	0	

Error Margin (ppm): 5

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: not fixed

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: OR

Electron Ions: both

Use MSn Info: yes

Isotope Res: 10000

Max Results: 20

Event#: 1 MS(E+) Ret. Time : 0.280 -> 1.000 Scan#: 43 -> 151

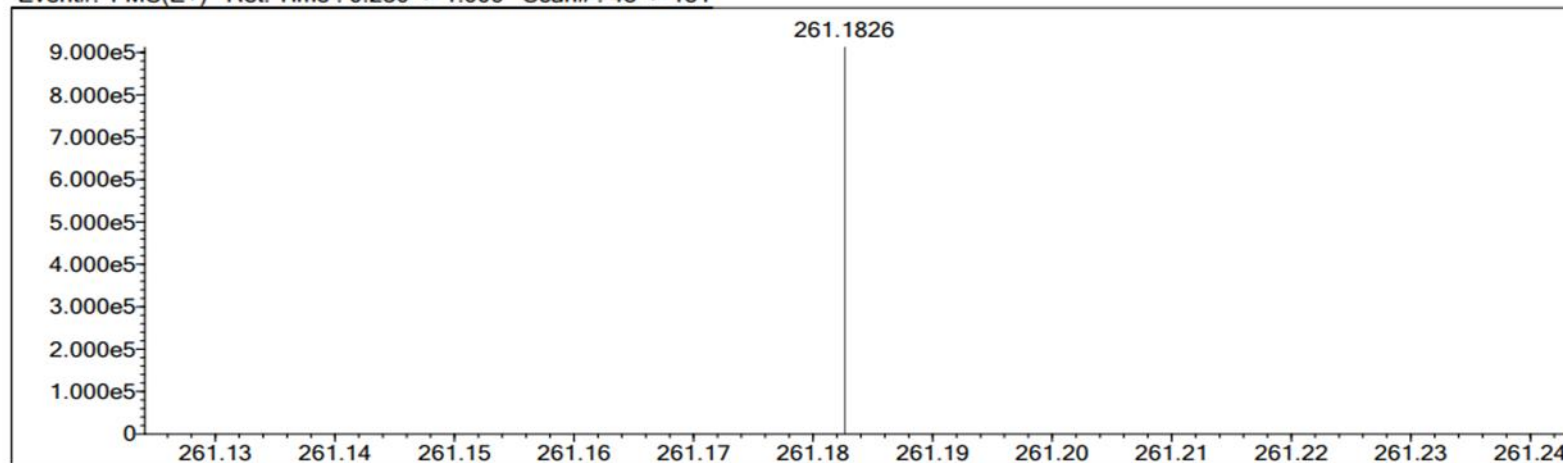
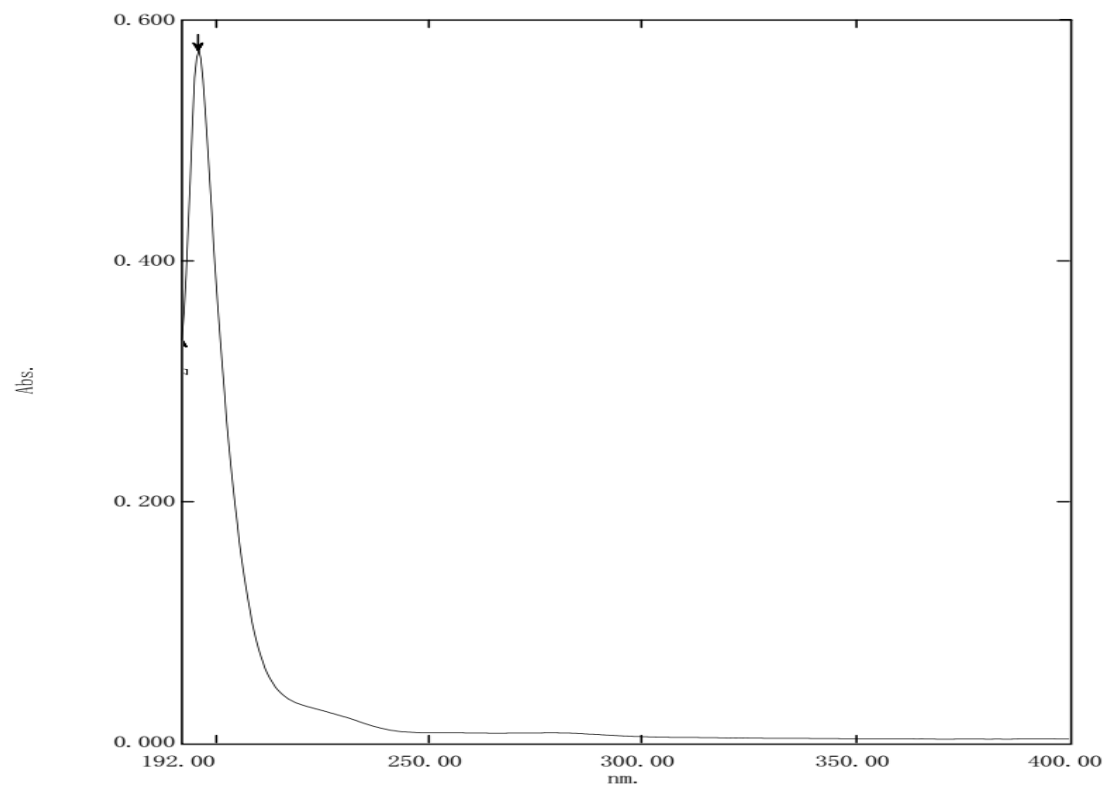


Figure S17. HRESI spectrum of compound 2

数据集: YMX-9-10-5-5-3 - RawData



[测定属性]
 波长范围(nm): 190.00 到 600.00
 扫描速度: 中速
 采样间隔: 0.5
 自动采样间隔: 停用
 扫描模式: 单个

[仪器属性]
 仪器类型: UV-2700 系列
 测定方式: 吸收值
 狭缝宽: 5.0 nm
 积分时间: 0.1 秒
 光源转换波长: 323.0 nm
 检测器单元: 直接
 S/R 转换: 标准
 阶梯校正: OFF

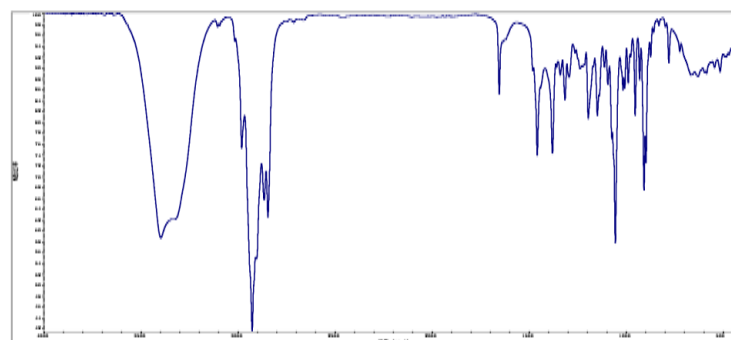
[附件属性]
 附件: 无

[数据处理参数]
 阈值: 0.0010000
 点: 4
 内插: 停用
 平均: 停用

[样品准备属性]
 重量:
 体积:
 稀释:
 光程长: 10mm
 附加信息: 样品浓度: 0.0300毫克/毫升
 溶剂: 甲醇

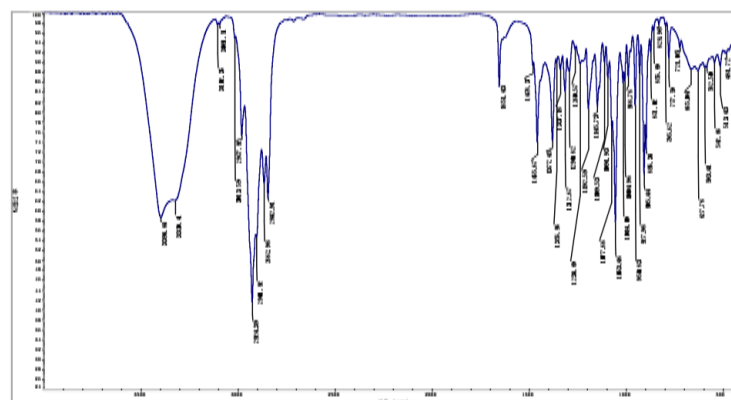
No.	P/V	波长 (nm)	Abs.	描述
1	⬆	196.00	0.575	
2	⬇	192.00	0.334	

Figure S18. CD and UV spectrum of compound 2



Sample Name: YMX-9-10-5-5-3
KBr压片
采集时间: 星期四 11月 19 10:11:27 2020 (GMT+08:00)
仪器型号: NICOLET IS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
功能速度: 0.4747
光阑: 80.00



Sample Name: YMX-9-10-5-5-3
KBr压片
采集时间: 星期四 11月 19 10:11:27 2020 (GMT+08:00)
仪器型号: NICOLET IS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
功能速度: 0.4747
光阑: 80.00

星期四 11月 19 10:21:41 2020 (GMT+08:00)

标峰:
谱图: YMX-9-10-5-5-3
范围: 4000.00 400.00
(绝对) 阈值: 98.492
灵敏度: 99

峰位置:	402.81	强度:	94.327
峰位置:	413.95	强度:	93.904
峰位置:	438.18	强度:	93.018
峰位置:	450.90	强度:	93.137
峰位置:	467.24	强度:	92.399
峰位置:	481.72	强度:	91.910
峰位置:	513.43	强度:	89.238
峰位置:	542.68	强度:	89.996
峰位置:	582.50	强度:	88.953
峰位置:	593.41	强度:	89.100
峰位置:	627.78	强度:	88.386
峰位置:	665.04	强度:	88.640
峰位置:	721.05	强度:	92.924
峰位置:	777.59	强度:	90.905
峰位置:	795.62	强度:	97.539
峰位置:	828.98	强度:	97.784
峰位置:	855.89	强度:	96.464
峰位置:	871.02	强度:	92.053
峰位置:	895.34	强度:	72.446
峰位置:	905.44	强度:	67.441
峰位置:	927.98	强度:	87.806
峰位置:	950.83	强度:	81.284
峰位置:	974.22	强度:	92.030
峰位置:	986.76	强度:	87.135
峰位置:	1004.96	强度:	86.176
峰位置:	1014.09	强度:	85.855
峰位置:	1053.46	强度:	57.686
峰位置:	1071.52	强度:	76.920
峰位置:	1091.93	强度:	86.914
峰位置:	1109.53	强度:	90.065
峰位置:	1145.73	强度:	81.207
峰位置:	1192.59	强度:	80.634
峰位置:	1236.25	强度:	89.819
峰位置:	1260.57	强度:	92.719
峰位置:	1290.82	强度:	88.204
峰位置:	1312.67	强度:	84.129
峰位置:	1337.18	强度:	88.586
峰位置:	1355.98	强度:	89.997
峰位置:	1377.45	强度:	74.205
峰位置:	1455.67	强度:	73.854
峰位置:	1478.37	强度:	89.459
峰位置:	1651.43	强度:	85.112
峰位置:	2710.46	强度:	98.337
峰位置:	2842.91	强度:	62.505
峰位置:	2862.98	强度:	65.579
峰位置:	2901.92	强度:	54.765
峰位置:	2924.39	强度:	41.457
峰位置:	2977.92	强度:	75.158
峰位置:	3013.59	强度:	94.910
峰位置:	3091.51	强度:	97.722
峰位置:	3102.35	强度:	97.548
峰位置:	3394.64	强度:	58.607

Figure S19. IR spectrum of compound 2

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 26-NOV-2020

Set Temperature : OFF

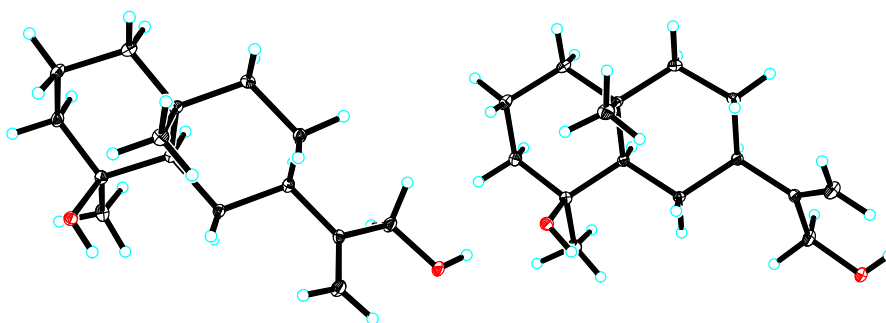
Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>					
5	-12.20	0.31	-2.54	-11.87	-12.67					
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>	
1	YMX-9-10-5-5-3	03:30:04 PM	-12.67	SR	-0.0190	589	100.00	0.150	23.2	
2	YMX-9-10-5-5-3	03:30:13 PM	-12.33	SR	-0.0185	589	100.00	0.150	23.2	
3	YMX-9-10-5-5-3	03:30:21 PM	-12.07	SR	-0.0181	589	100.00	0.150	23.2	
4	YMX-9-10-5-5-3	03:30:29 PM	-11.87	SR	-0.0178	589	100.00	0.150	23.2	
5	YMX-9-10-5-5-3	03:30:37 PM	-12.07	SR	-0.0181	589	100.00	0.150	23.2	

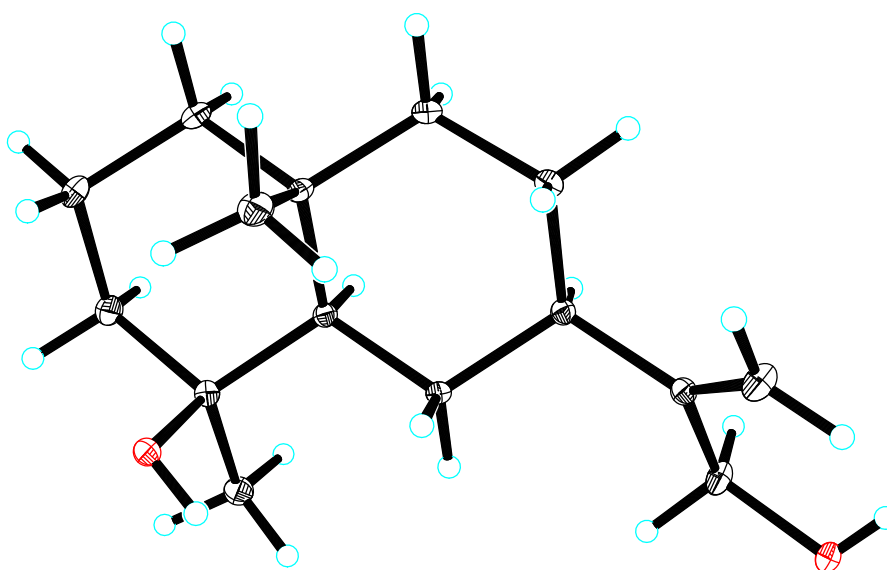
Figure S20. $[\alpha]^{25}_D$ of compound 2

Crystal data for xm7: $C_{15}H_{26}O_2$, $M = 238.36$, $a = 12.1080(3) \text{ \AA}$, $b = 6.30390(10) \text{ \AA}$, $c = 18.5396(4) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 94.6690(10)^\circ$, $\gamma = 90^\circ$, $V = 1410.39(5) \text{ \AA}^3$, $T = 100.(2) \text{ K}$, space group $P1211$, $Z = 4$, $\mu(\text{Cu K}\alpha) = 0.560 \text{ mm}^{-1}$, 30099 reflections measured, 5508 independent reflections ($R_{int} = 0.0467$). The final R_I values were 0.0312 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0785 ($I > 2\sigma(I)$). The final R_I values were 0.0320 (all data). The final $wR(F^2)$ values were 0.0792 (all data). The goodness of fit on F^2 was 1.078. Flack parameter = 0.03(5).



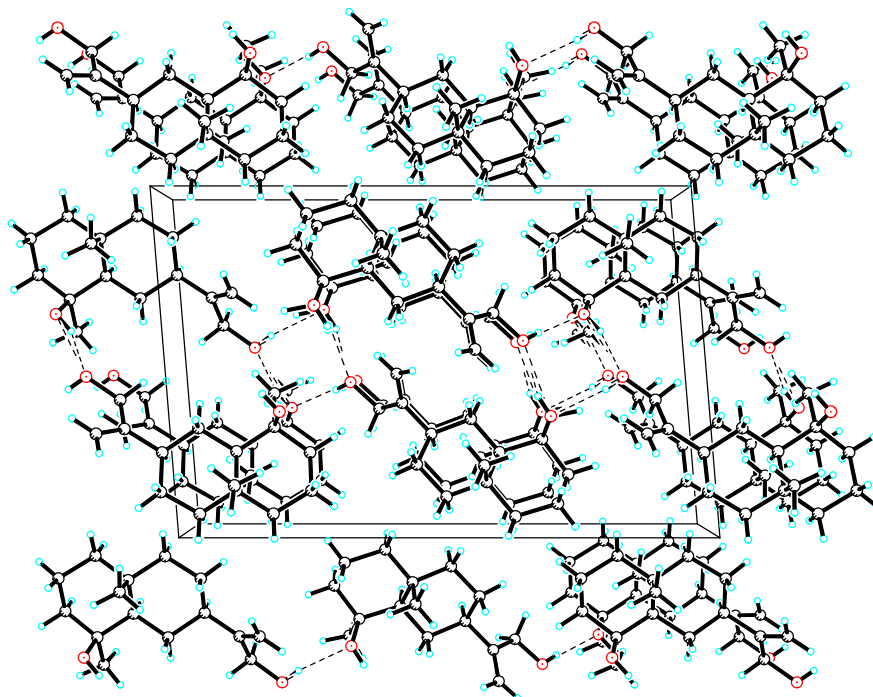
View of the molecules in an asymmetric unit.

Displacement ellipsoids are drawn at the 30% probability level.



View of a molecule of xm7 with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of xm7.

Hydrogen-bonds are shown as dashed lines.

Table 1. Crystal data and structure refinement for xm7_0m.

Identification code	global	
Empirical formula	C ₁₅ H ₂₆ O ₂	
Formula weight	238.36	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P 1 21 1	
Unit cell dimensions	a = 12.1080(3) Å	= 90°.
	b = 6.30390(10) Å	= 94.6690(10)°.
	c = 18.5396(4) Å	= 90°.
Volume	1410.39(5) Å ³	
Z	4	
Density (calculated)	1.123 Mg/m ³	
Absorption coefficient	0.560 mm ⁻¹	

F(000)	528
Crystal size	0.580 x 0.200 x 0.100 mm ³
Theta range for data collection	2.39 to 72.47°.
Index ranges	-14<= <i>h</i> <=14, -7<= <i>k</i> <=7, -22<= <i>l</i> <=22
Reflections collected	30099
Independent reflections	5508 [R(int) = 0.0467]
Completeness to theta = 72.47°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.95 and 0.76
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	5508 / 1 / 318
Goodness-of-fit on F ²	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0785
R indices (all data)	R1 = 0.0320, wR2 = 0.0792
Absolute structure parameter	0.03(5)
Largest diff. peak and hole	0.192 and -0.280 e.Å ⁻³

Figure S21. X-ray crystallographic analysis for compound **2**

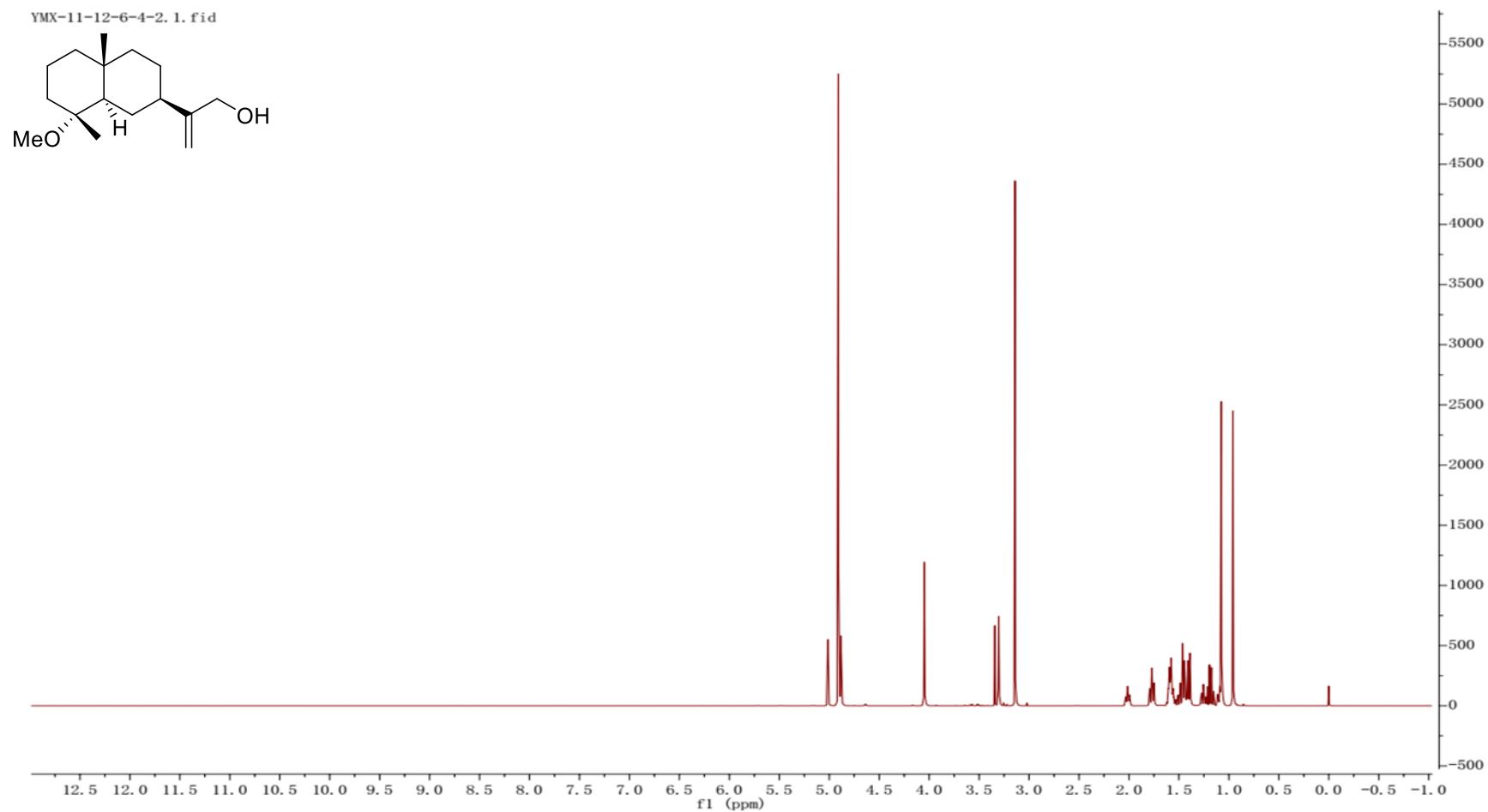


Figure S22. ^1H NMR spectrum of compound **3** (CD₃OD, 600 MHz)

YMX-11-12-6-4-2. 3. fid

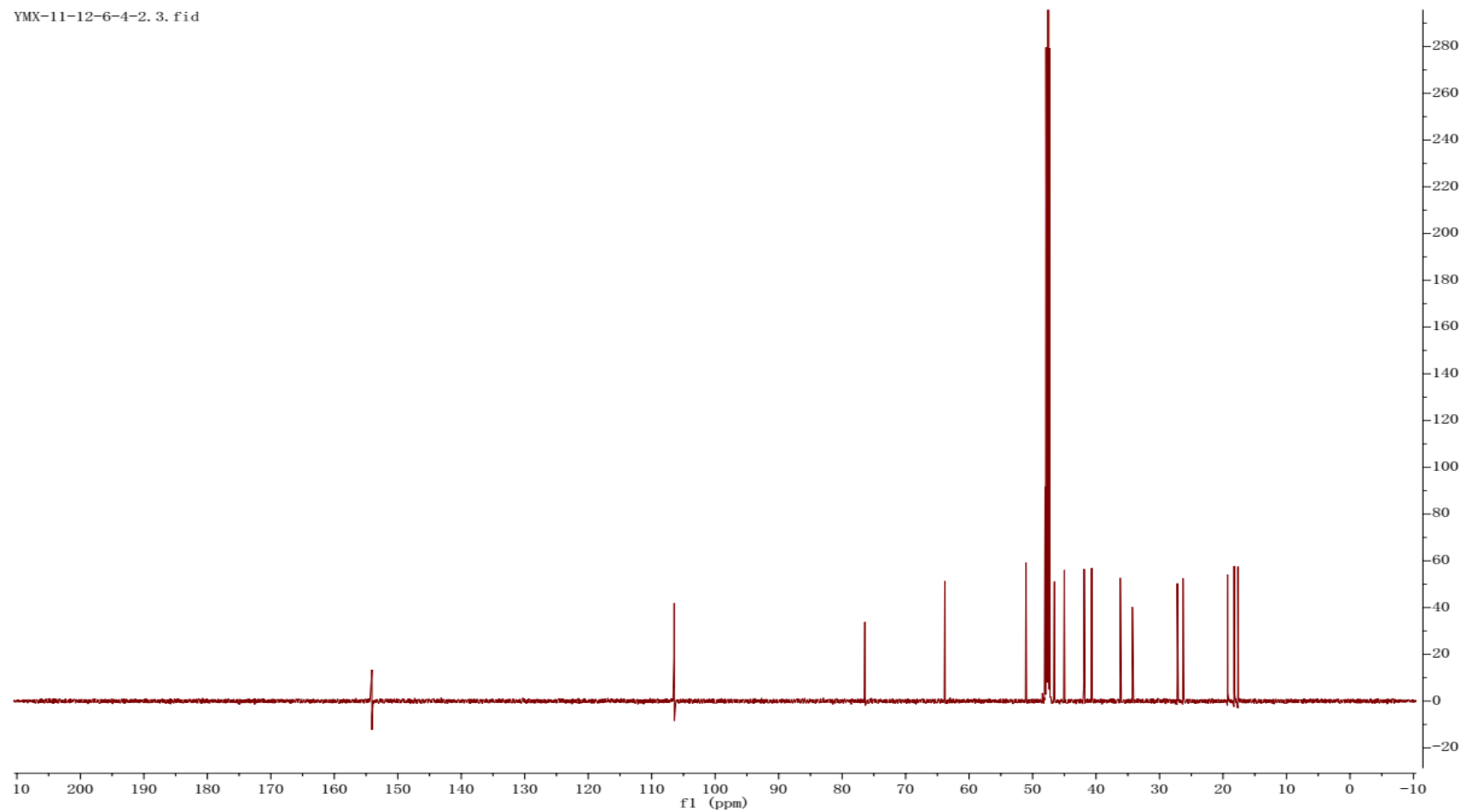


Figure S23. ^{13}C NMR spectrum of compound **3** (CD_3OD , 150 MHz)

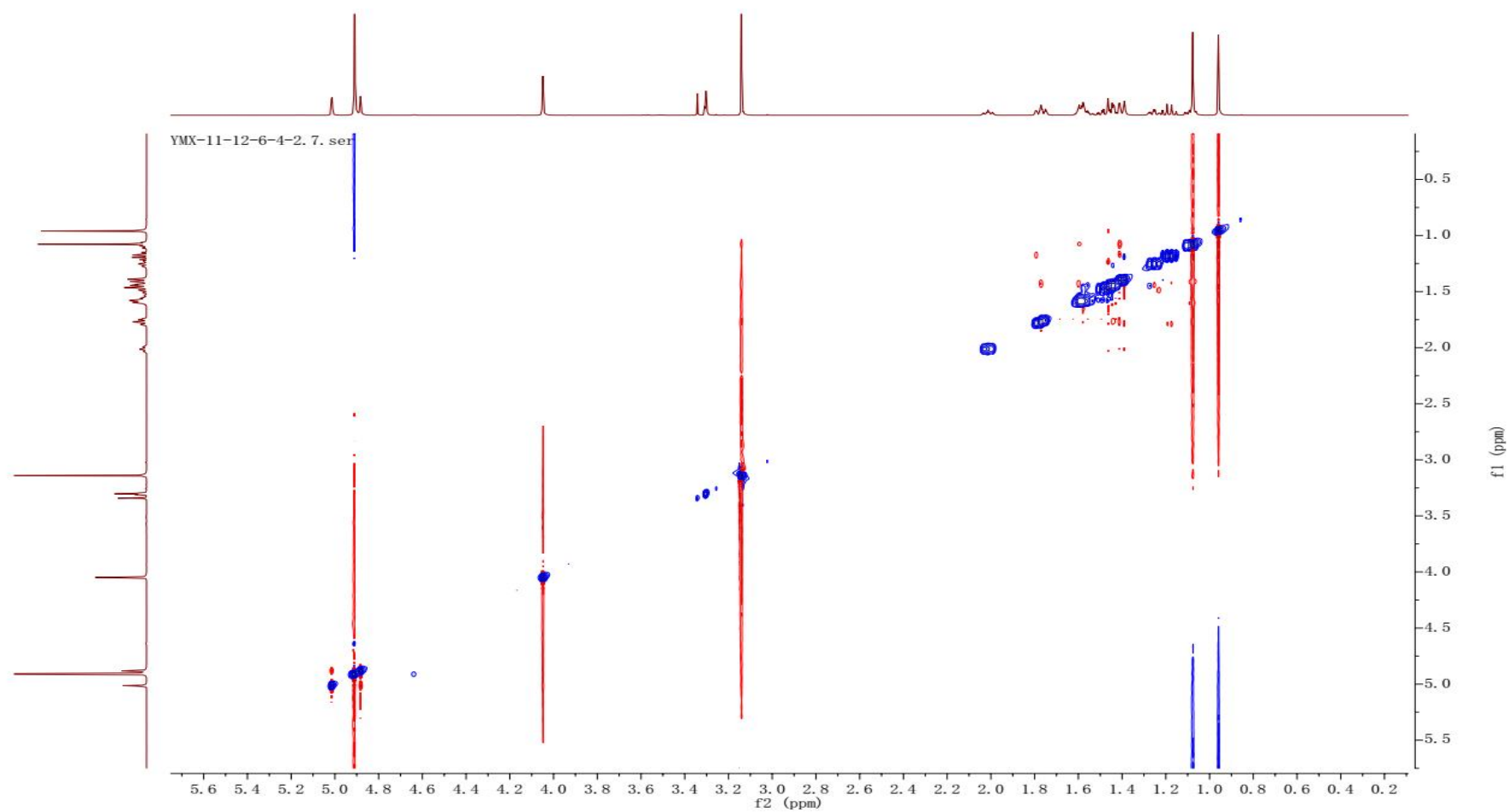


Figure S24. ROESY spectrum of compound **3** (CD₃OD, 600 MHz)

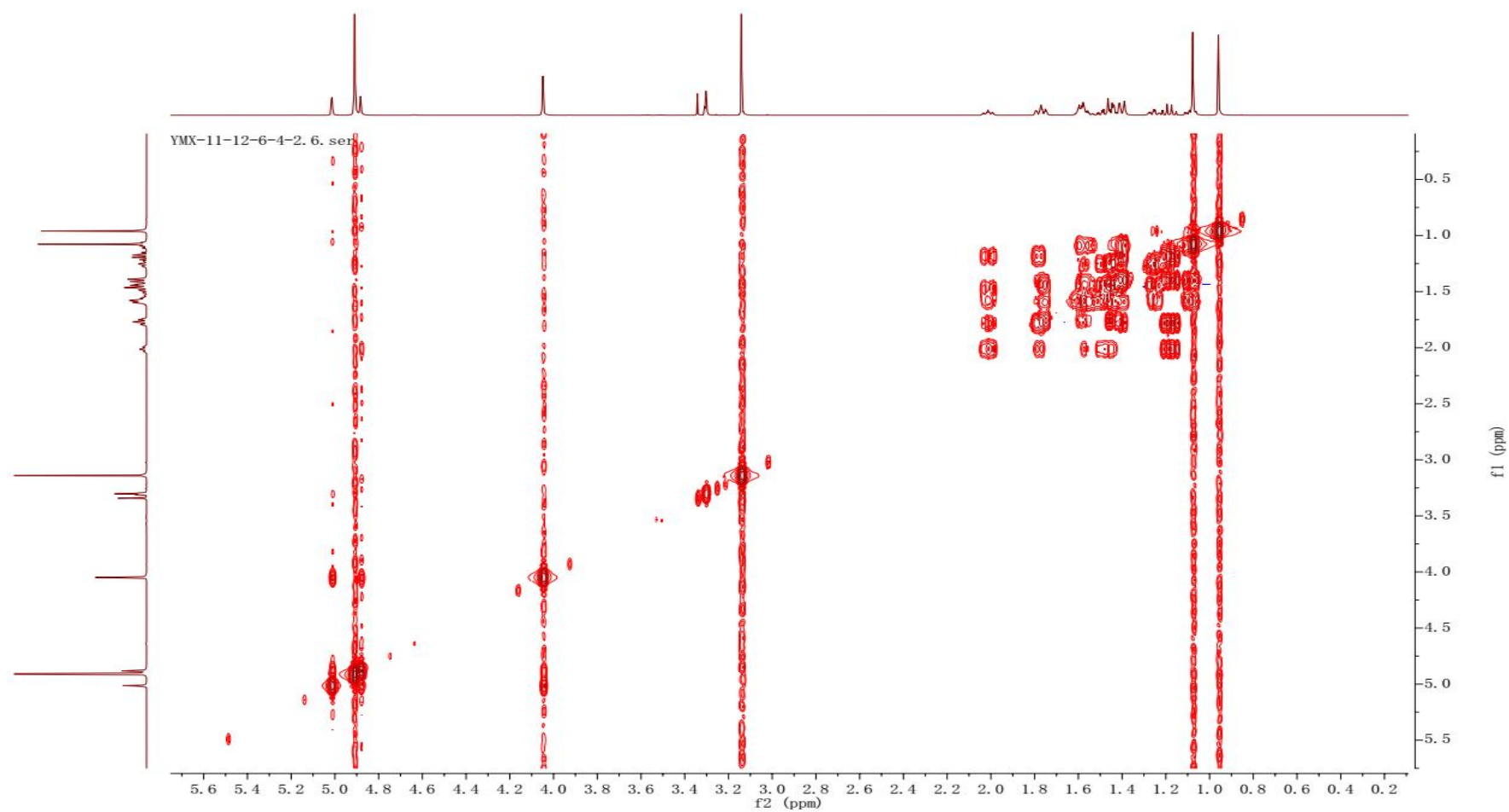


Figure S25. ^1H - ^1H COSY spectrum of compound **3** (CD_3OD , 600 MHz)

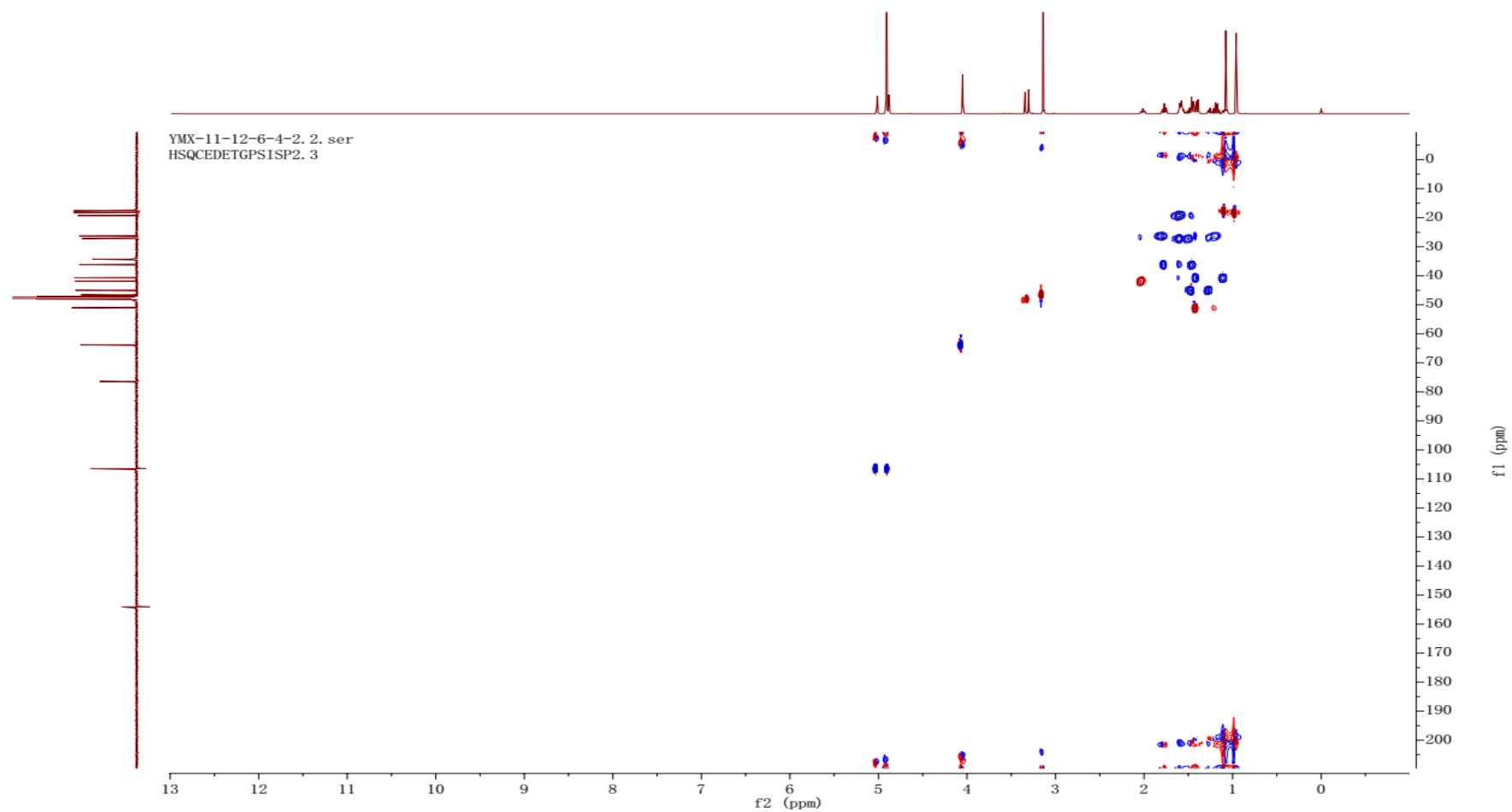


Figure S26. HSQC spectrum of compound **3** (CD₃OD, 600 MHz)

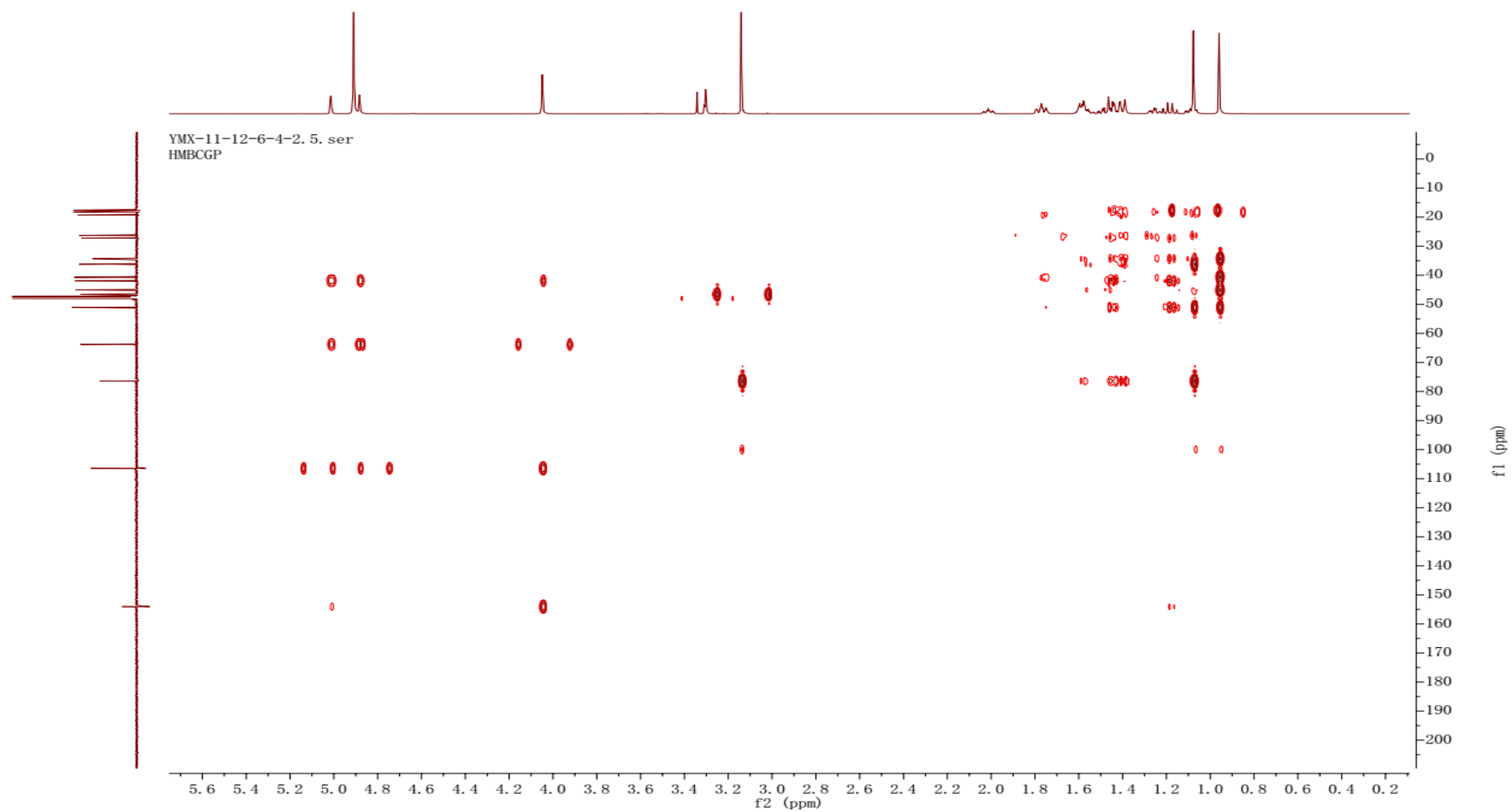
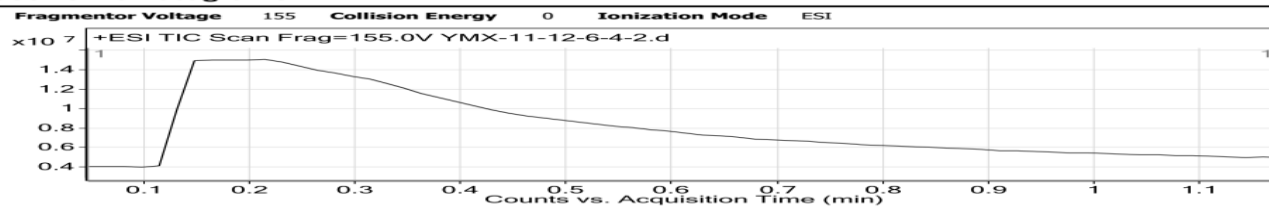


Figure S27. HMBC spectrum of compound **3** (CD₃OD, 600 MHz)

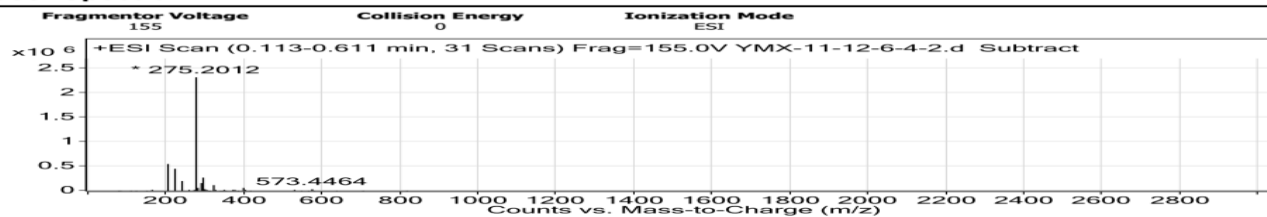
Qualitative Analysis Report

Data Filename	YMX-11-12-6-4-2.d	Sample Name	YMX-11-12-6-4-2
Sample Type	Sample	Position	p1b6
Instrument Name	Instrument 1	User Name	Q-TOF-HP\Q-TOF
Acq Method	default20190111-ms.m	Acquired Time	1/12/2020 3:53:15 PM
IRM Calibration Status	Success	DA Method	1.m
Comment			
Sample Group	Info.		
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.3)		

User Chromatograms



User Spectra

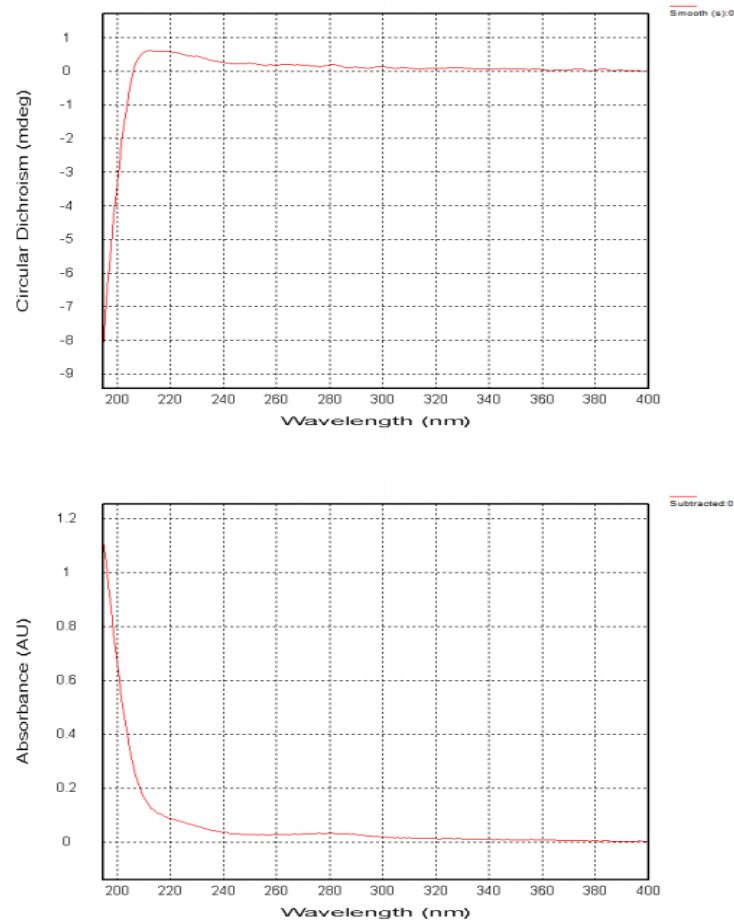


Peak List

m/z	z	Abund
203.1784	1	562934.5
221.1888	1	456599.94
238.2153	1	203270.44
275.2012	1	2326498.25
275.3404	1	322283.94
275.3859	1	111786.8
276.2007	1	1035205.25
289.1761	1	170995.88

Figure S28. HRESI spectrum of compound 3

YMX-11-12-6-4-2



File: YMX-11-12-6-4-2 (195-400 nm) 20112716.dsx

ProBinaryX

Attributes :

- Time Stamp : Fri Nov 27 19:17:31 2020

- File ID : {D6821013-5B01-4cf8-96AB-CEAAAE56FBC2}

- Is CFR Compliant : false

- Original data has not been modified.

Remarks:

- User: CD

- Date: 2020/11/27

- Instrument: 0547

- DetectorType: LAAPD

- DichOS Calibration Correction Curve: 0547/2

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.2700mg/mL MeOH

- Pathlength: 1 mm

- Temperature: 20°C

Settings:

- Time-per-point: 1s (25us x 40000)

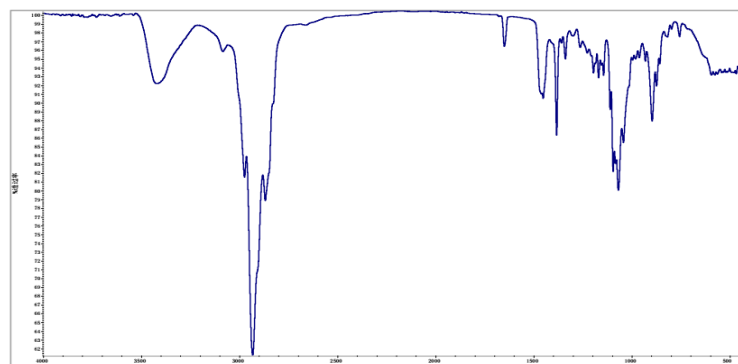
- SE

- Wavelength: 195nm - 400nm

- Step Size: 1nm

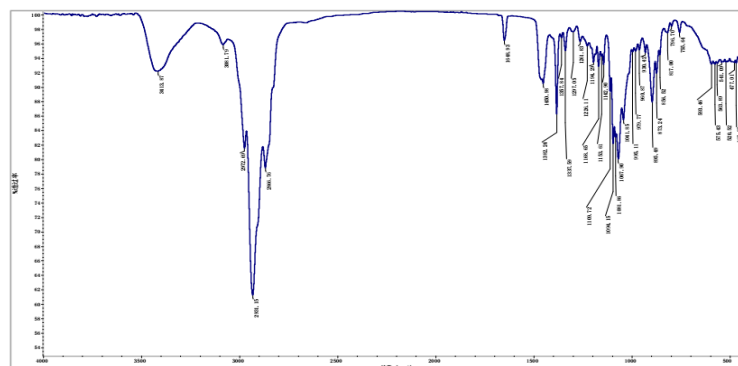
- Bandwidth: 1nm

Figure S29. CD and UV spectrum of compound **3**



Sample Name: YMX-11-12-6-4-2
KBr压片
采集时间: 星期三 10月 28 15:29:57 2020 (GMT+08:00)
仪器型号: NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00



Sample Name: YMX-11-12-6-4-2
KBr压片
采集时间: 星期三 10月 28 15:29:57 2020 (GMT+08:00)
仪器型号: NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00

星期三 10月 28 16:13:13 2020 (GMT+08:00)

标峰:

谱图: YMX-11-12-6-4-2
范围: 4000.00 400.00
(绝对) 阈值: 98.415
灵敏度: 99

峰表:

峰位置:	428.22	强度:	93.097
峰位置:	437.88	强度:	93.255
峰位置:	467.07	强度:	93.302
峰位置:	477.01	强度:	93.434
峰位置:	513.07	强度:	93.463
峰位置:	520.52	强度:	93.458
峰位置:	541.09	强度:	93.419
峰位置:	563.89	强度:	93.272
峰位置:	575.43	强度:	93.131
峰位置:	593.46	强度:	93.158
峰位置:	755.64	强度:	97.530
峰位置:	796.70	强度:	98.393
峰位置:	817.00	强度:	97.493
峰位置:	856.52	强度:	94.444
峰位置:	873.24	强度:	91.889
峰位置:	895.49	强度:	87.903
峰位置:	930.42	强度:	94.749
峰位置:	960.87	强度:	95.122
峰位置:	979.77	强度:	94.978
峰位置:	995.11	强度:	94.864
峰位置:	1041.85	强度:	85.458
峰位置:	1067.90	强度:	80.034
峰位置:	1081.86	强度:	83.002
峰位置:	1094.15	强度:	82.123
峰位置:	1109.72	强度:	89.205
峰位置:	1142.90	强度:	93.105
峰位置:	1153.61	强度:	94.253
峰位置:	1168.65	强度:	92.833
峰位置:	1194.29	强度:	93.392
峰位置:	1226.11	强度:	95.664
峰位置:	1261.83	强度:	96.304
峰位置:	1297.05	强度:	97.606
峰位置:	1337.59	强度:	94.985
峰位置:	1357.84	强度:	96.782
峰位置:	1382.24	强度:	86.283
峰位置:	1450.98	强度:	90.491
峰位置:	1648.93	强度:	96.434
峰位置:	2866.76	强度:	78.823
峰位置:	2931.15	强度:	61.206
峰位置:	2972.69	强度:	81.513
峰位置:	3081.79	强度:	95.841
峰位置:	3413.87	强度:	92.189

Figure S30. IR spectrum of compound 3

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Monday, 23-NOV-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>					
5	-58.40	0.10	-0.17	-58.33	-58.53					
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>	
1	YMX-11-12-6-4-2	09:21:22 PM	-58.53	SR	-0.0878	589	100.00	0.150	22.2	
2	YMX-11-12-6-4-2	09:21:30 PM	-58.33	SR	-0.0875	589	100.00	0.150	22.3	
3	YMX-11-12-6-4-2	09:21:38 PM	-58.33	SR	-0.0875	589	100.00	0.150	22.3	
4	YMX-11-12-6-4-2	09:21:46 PM	-58.33	SR	-0.0875	589	100.00	0.150	22.3	
5	YMX-11-12-6-4-2	09:21:54 PM	-58.47	SR	-0.0877	589	100.00	0.150	22.3	

Figure S31. $[\alpha]^{25}_D$ of compound **3**

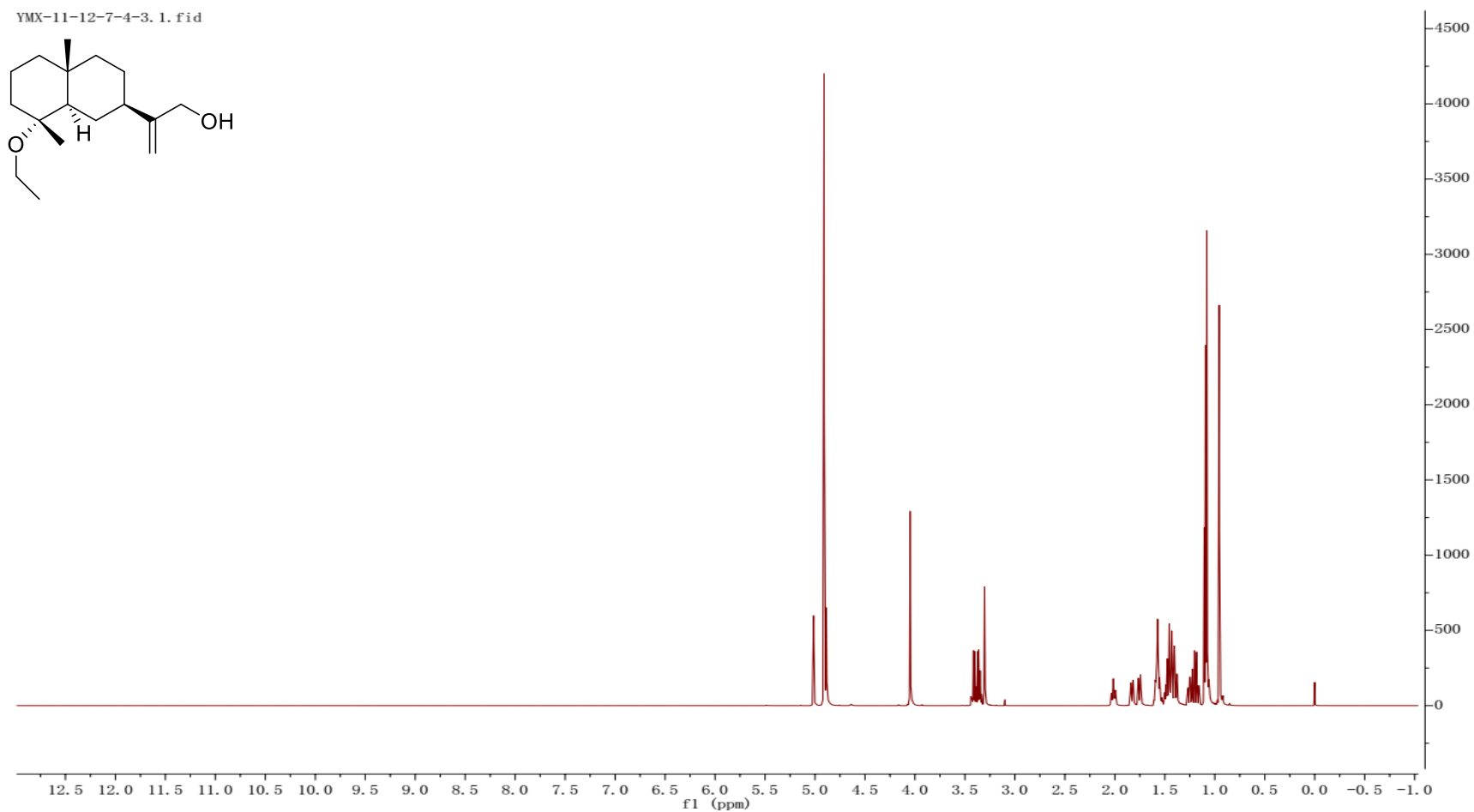


Figure S32. ¹H NMR spectrum of compound **4** (CD₃OD, 600 MHz)

YMX-11-12-7-4-3. 3. fid

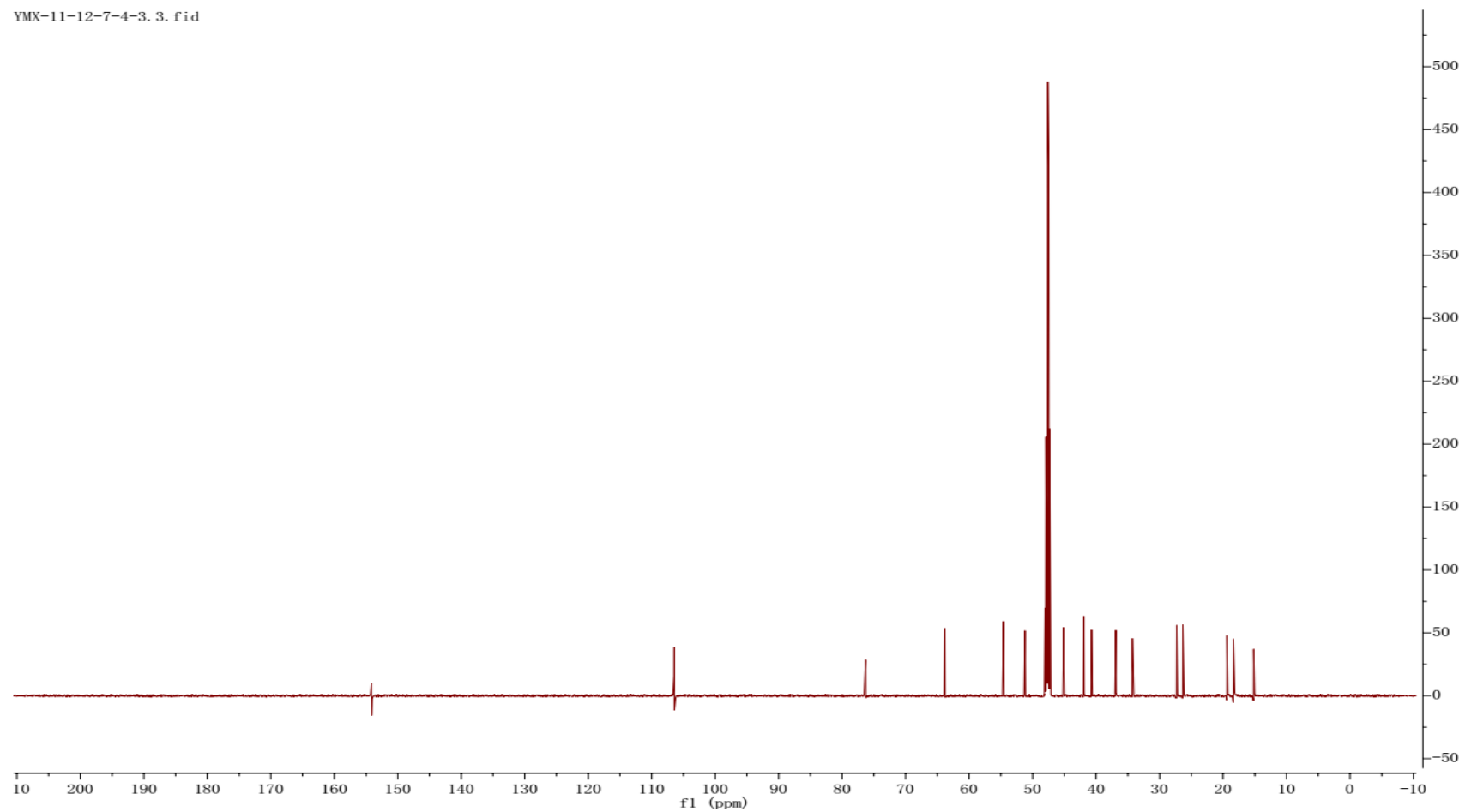


Figure S33. ^{13}C NMR spectrum of compound **4** (CD_3OD , 150 MHz)

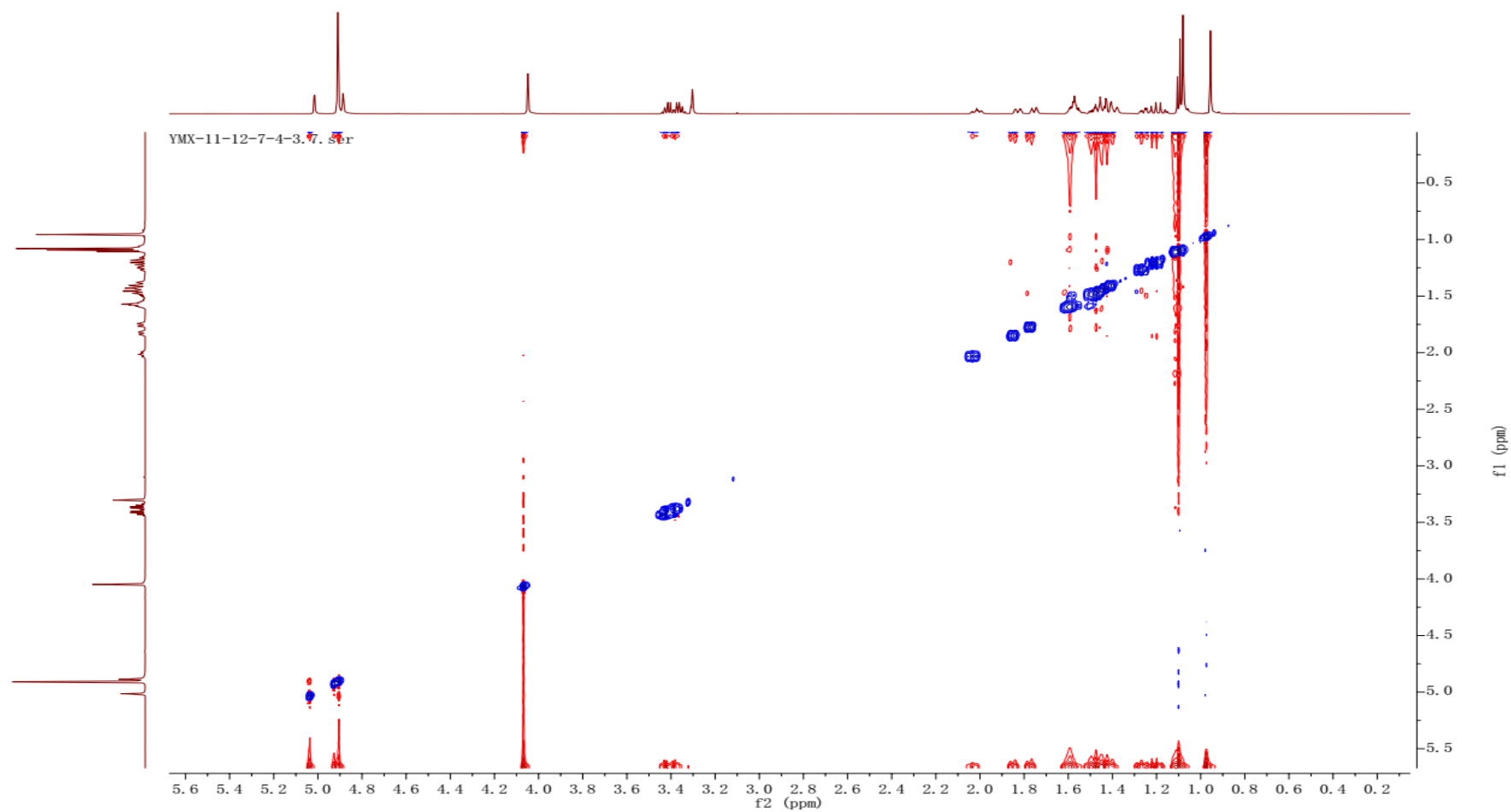


Figure S34. ROESY spectrum of compound **4** (CD₃OD, 600 MHz)

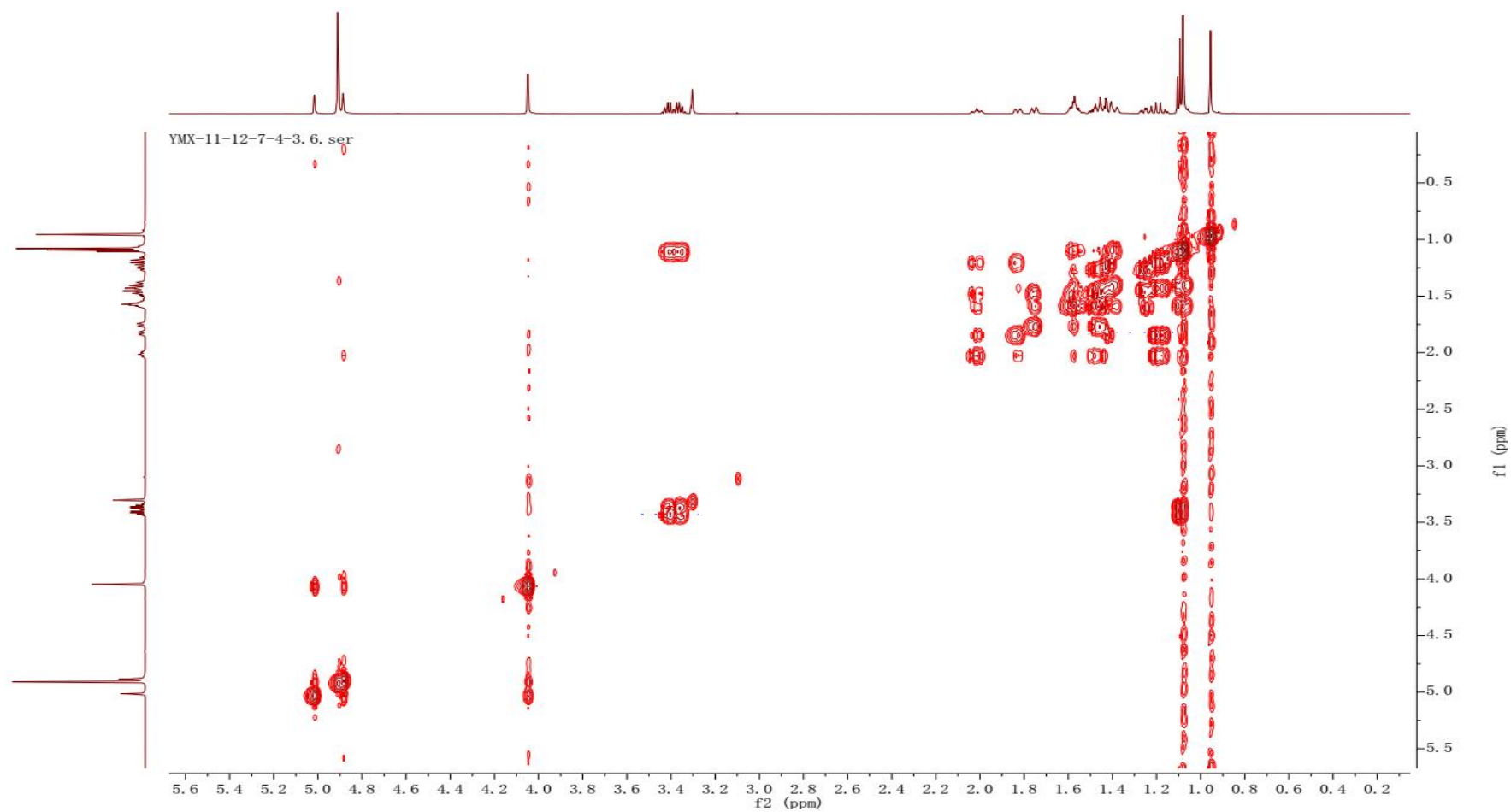


Figure S35. ^1H - ^1H COSY spectrum of compound **4** (CD_3OD , 600 MHz)

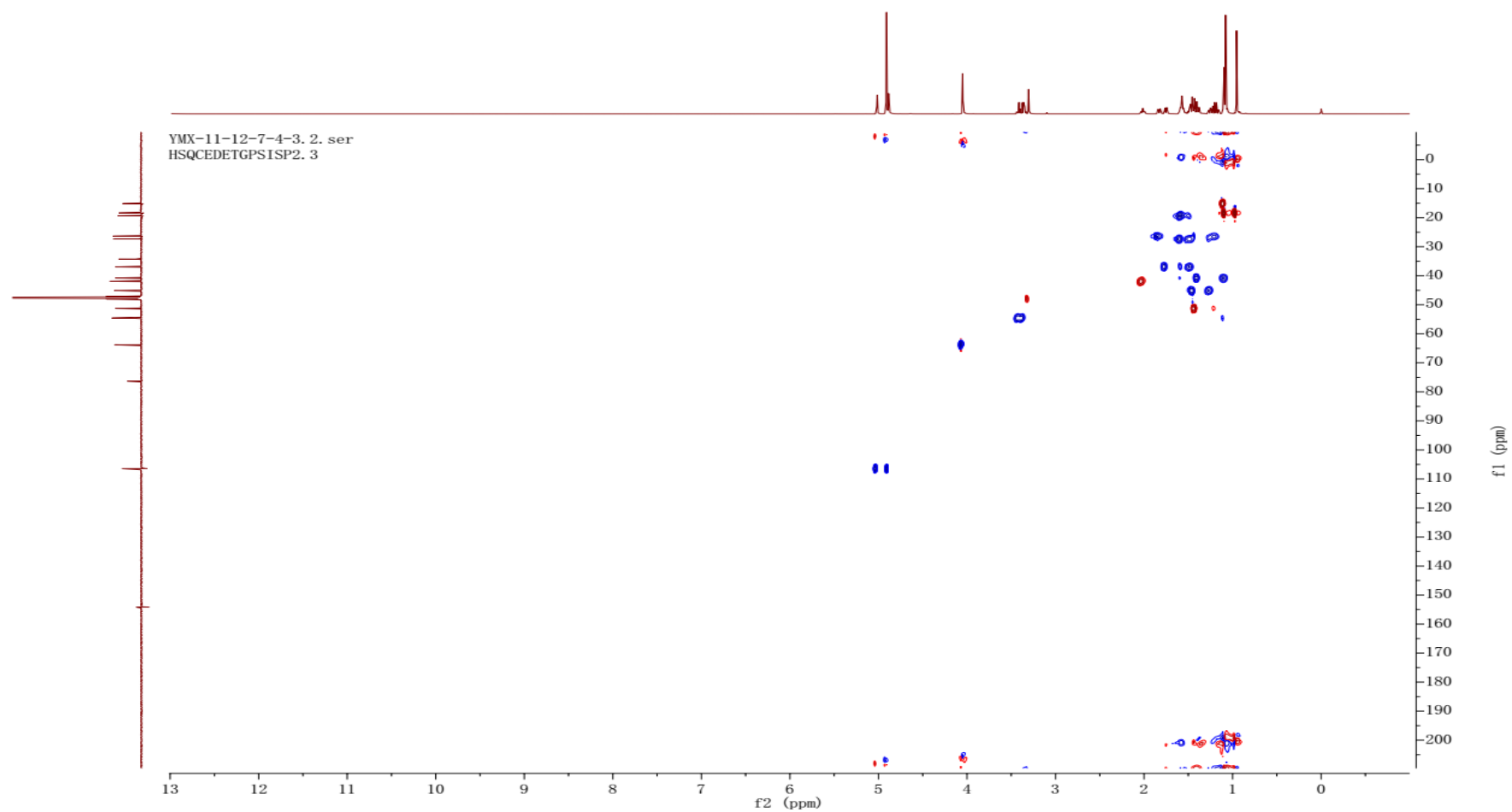


Figure S36. HSQC spectrum of compound **4** (CD₃OD, 600 MHz)

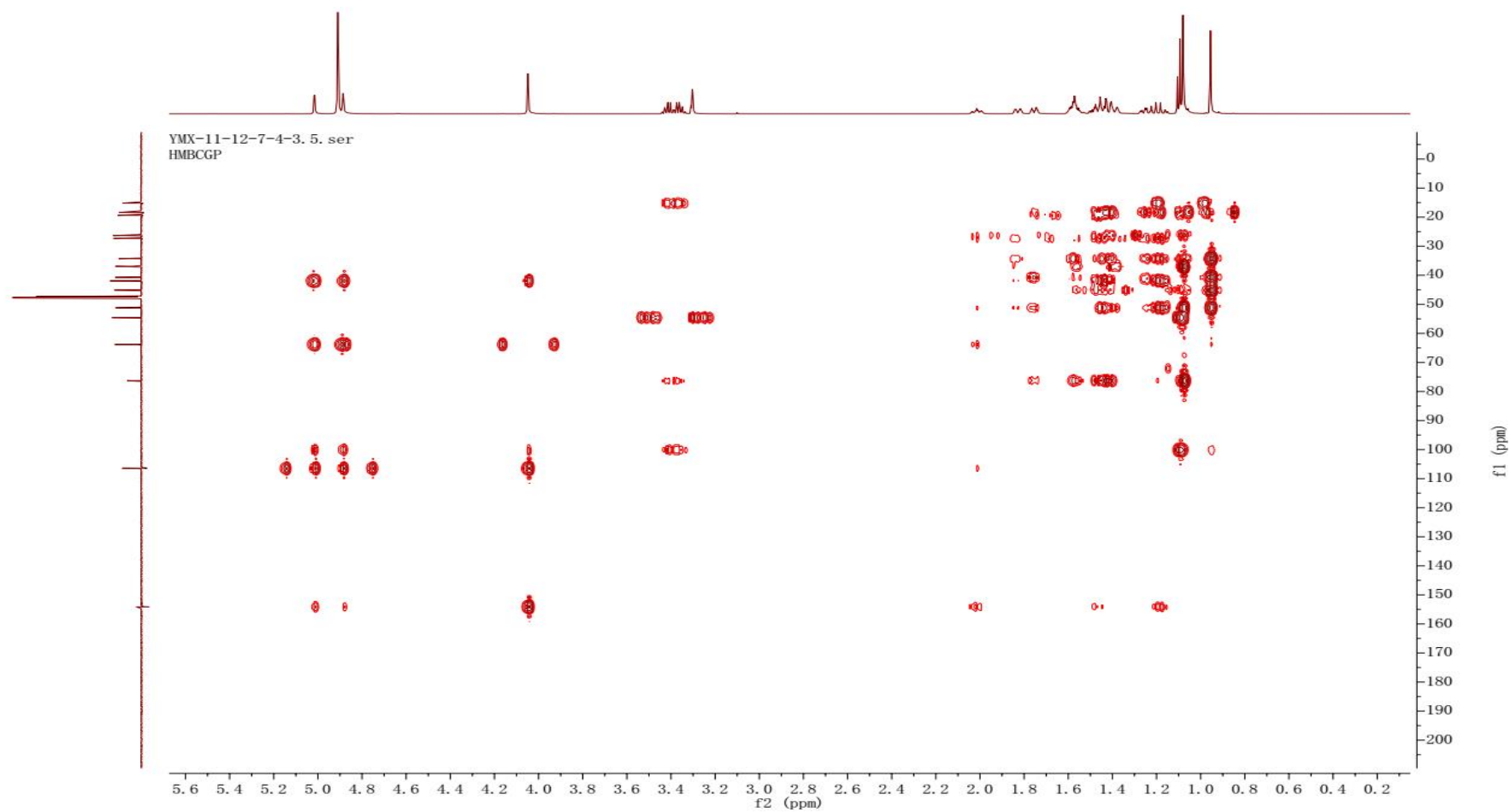
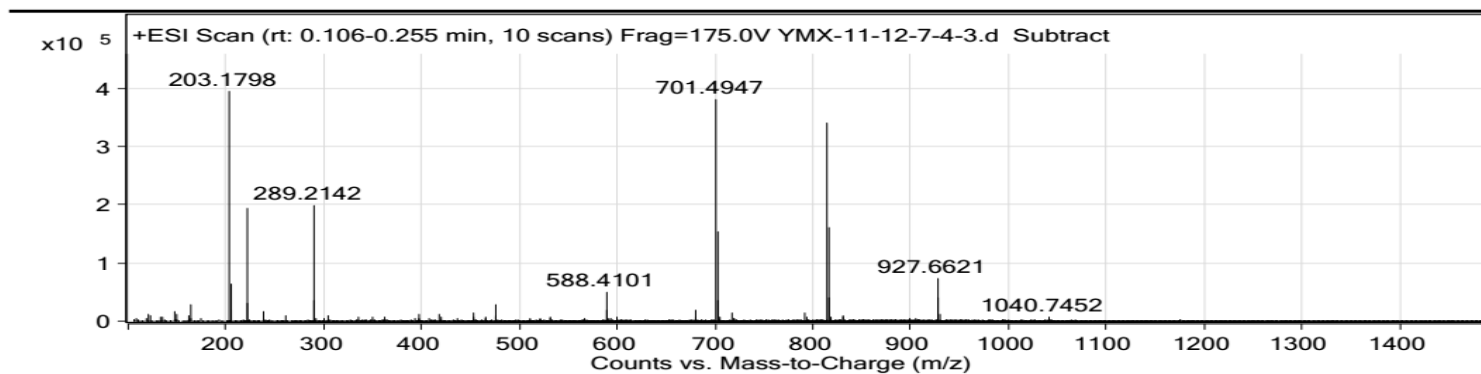


Figure S37. HMBC spectrum of compound **4** (CD₃OD, 600 MHz)

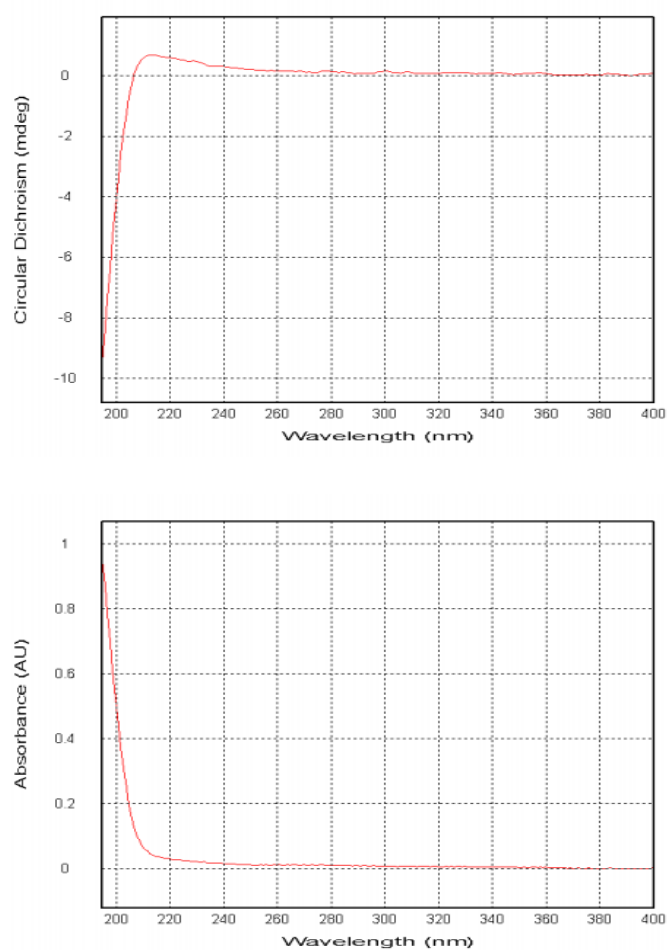
Qualitative Analysis Report



Peak List

m/z	z	Abund
163.1479	1	29645.47
203.1798	1	395609.72
204.1828	1	62958.54
205.1934	1	17911.16
221.1902	1	195222.67
222.1935	1	30062.8
289.2142	1	198920.55
290.2176	1	35569.34
475.3259	2	29273.89
588.4101	1	50941.28
589.413	1	17897.13
679.5111	1	18046.72
701.4947	1	380123.91
702.4978	1	153495.44
703.5	1	35624.95
814.5788	1	339993.13
815.5817	1	162160.91
816.5844	1	41294.73
927.6621	1	72421.57
928.6646	1	40550.8

Figure S38. HRESI spectrum of compound 4



File: YMX-11-12-7-4-3 (195-400 nm) 20112719.dsx

ProBinaryX

Attributes :

- Time Stamp : Fri Nov 27 20:15:48 2020

- File ID : {E8796B06-0EF0-4e14-9505-25E7F76C5594}

- Is CFR Compliant : false

- Original data has not been modified.

Remarks:

- User: CD

- Date: 2020/11/27

- Instrument: 0547

- DetectorType: LAAPD

- DichOS Calibration Correction Curve: 0547/2

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.6500mg/mL MeOH

- Pathlength: 1 mm

- Temperature: 20°C

Settings:

- Time-per-point: 1s (25us x 40000)

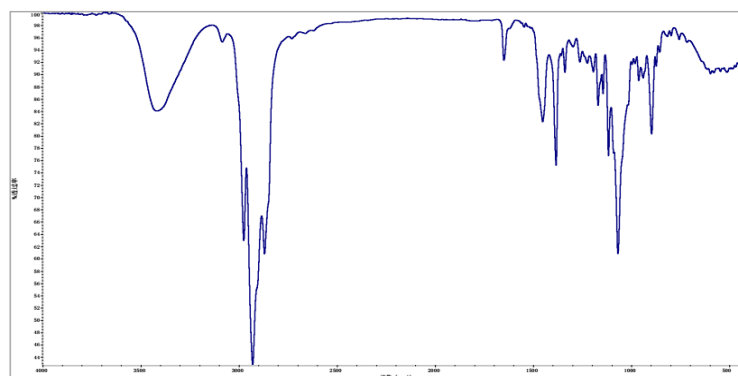
- SE

- Wavelength: 195nm - 400nm

- Step Size: 1nm

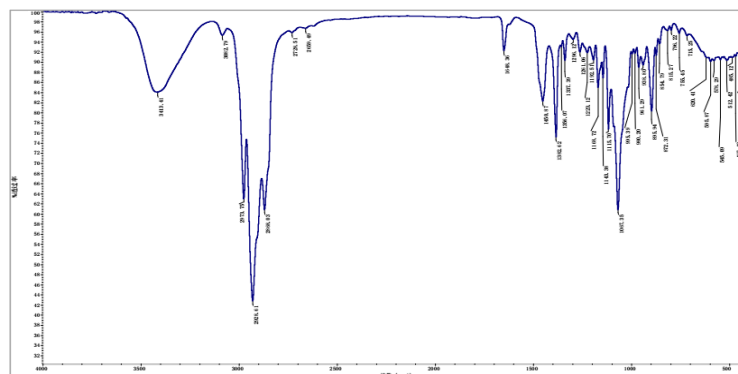
- Bandwidth: 1nm

Figure S39. CD and UV spectrum of compound 4



Sample Name: YMX-11-12-7-4-3
KBr压片
采集时间: 星期四 10月 29 10:22:16 2020 (GMT+08:00)
仪器型号: NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00



Sample Name: YMX-11-12-7-4-3
KBr压片
采集时间: 星期四 10月 29 10:22:16 2020 (GMT+08:00)
仪器型号: NICOLET iS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00

星期四 10月 29 10:52:47 2020 (GMT+08:00)

标峰:

谱图: YMX-11-12-7-4-3
范围: 4000.00 400.00
(绝对) 阈值: 97.382
灵敏度: 99

峰表:

峰位置:	411.53	强度:	92.625
峰位置:	432.24	强度:	91.099
峰位置:	453.24	强度:	91.639
峰位置:	467.43	强度:	91.155
峰位置:	485.12	强度:	90.882
峰位置:	512.42	强度:	90.304
峰位置:	545.09	强度:	90.458
峰位置:	578.29	强度:	90.285
峰位置:	595.87	强度:	90.092
峰位置:	715.25	强度:	95.228
峰位置:	755.45	强度:	95.663
峰位置:	796.22	强度:	96.297
峰位置:	815.27	强度:	96.160
峰位置:	854.79	强度:	93.601
峰位置:	872.31	强度:	91.325
峰位置:	895.94	强度:	80.277
峰位置:	938.80	强度:	89.396
峰位置:	961.29	强度:	88.930
峰位置:	980.20	强度:	91.718
峰位置:	995.39	强度:	91.590
峰位置:	1067.35	强度:	60.756
峰位置:	1115.70	强度:	76.698
峰位置:	1143.38	强度:	86.808
峰位置:	1168.72	强度:	84.945
峰位置:	1192.51	强度:	90.372
峰位置:	1223.12	强度:	91.797
峰位置:	1261.06	强度:	91.989
峰位置:	1296.12	强度:	94.483
峰位置:	1337.39	强度:	90.320
峰位置:	1356.07	强度:	93.043
峰位置:	1382.62	强度:	75.159
峰位置:	1450.87	强度:	82.245
峰位置:	1648.36	强度:	92.241
峰位置:	2659.49	强度:	96.667
峰位置:	2728.51	强度:	95.803
峰位置:	2868.03	强度:	60.744
峰位置:	2928.61	强度:	42.689
峰位置:	2973.75	强度:	62.895
峰位置:	3082.79	强度:	95.265
峰位置:	3413.41	强度:	84.019

Figure S40. IR spectrum of compound 4

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 26-NOV-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>					
5	-24.66	0.07	-0.28	-24.56	-24.72					
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>	
1	YMX-11-12-7-4-3	02:54:20 PM	-24.72	SR	-0.0618	589	100.00	0.250	22.6	
2	YMX-11-12-7-4-3	02:54:29 PM	-24.68	SR	-0.0617	589	100.00	0.250	22.6	
3	YMX-11-12-7-4-3	02:54:37 PM	-24.72	SR	-0.0618	589	100.00	0.250	22.6	
4	YMX-11-12-7-4-3	02:54:45 PM	-24.64	SR	-0.0616	589	100.00	0.250	22.6	
5	YMX-11-12-7-4-3	02:54:53 PM	-24.56	SR	-0.0614	589	100.00	0.250	22.6	

Figure S41. $[\alpha]^{25}_D$ of compound 4

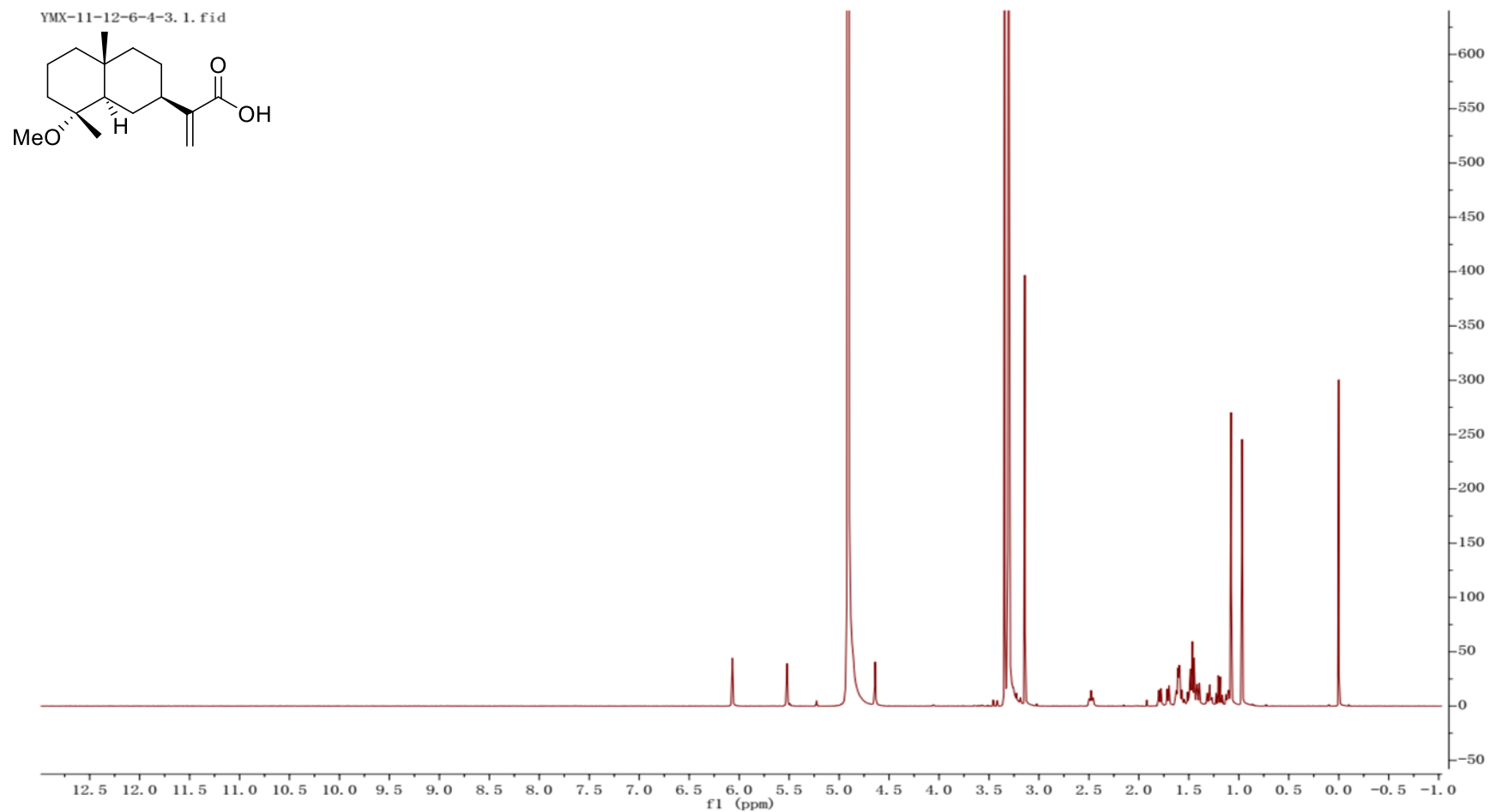


Figure S42. ¹H NMR spectrum of compound **5** (CD₃OD, 600 MHz)

YMX-11-12-6-4-3. 3. fid

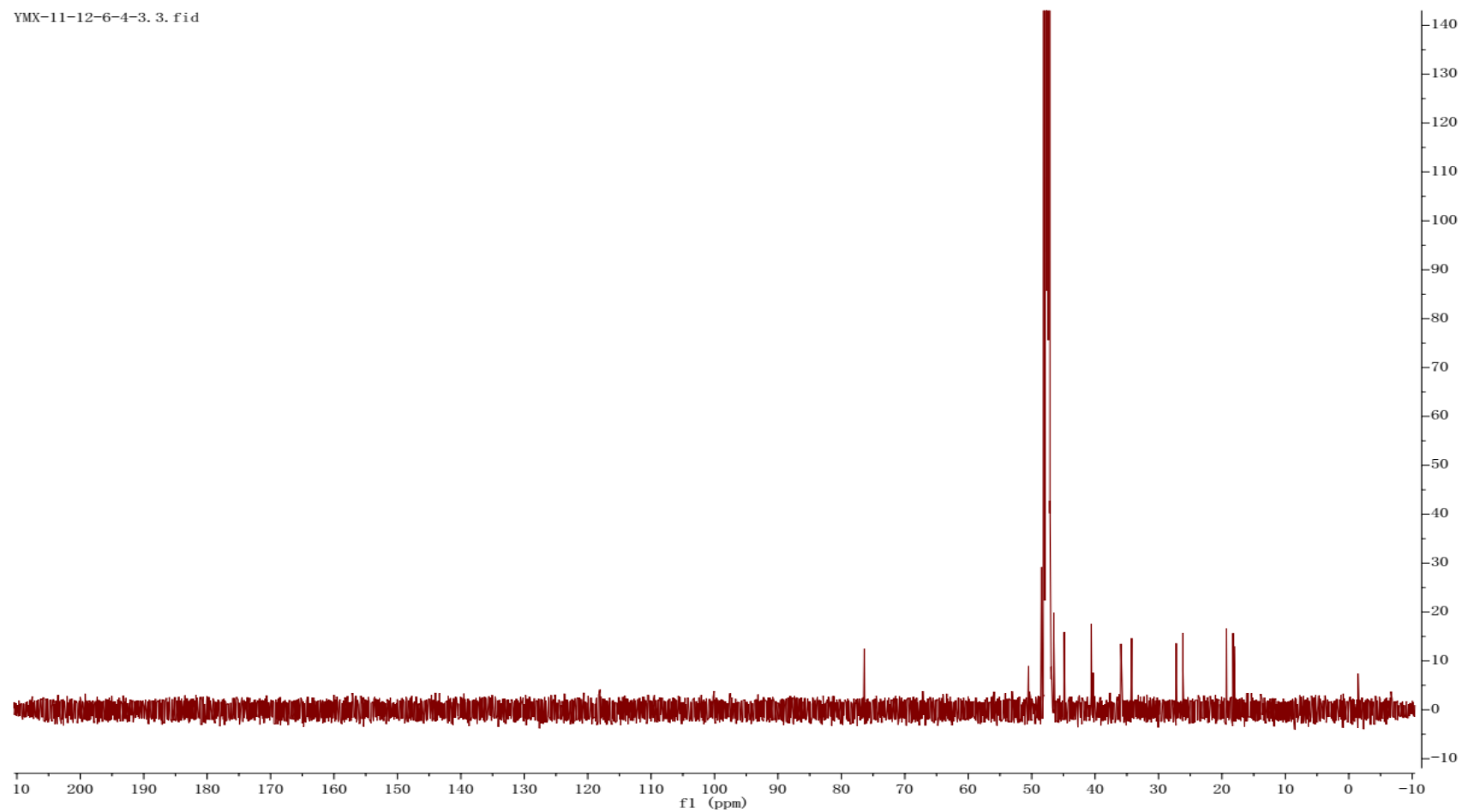


Figure S43. ^{13}C NMR spectrum of compound **5** (CD_3OD , 150 MHz)

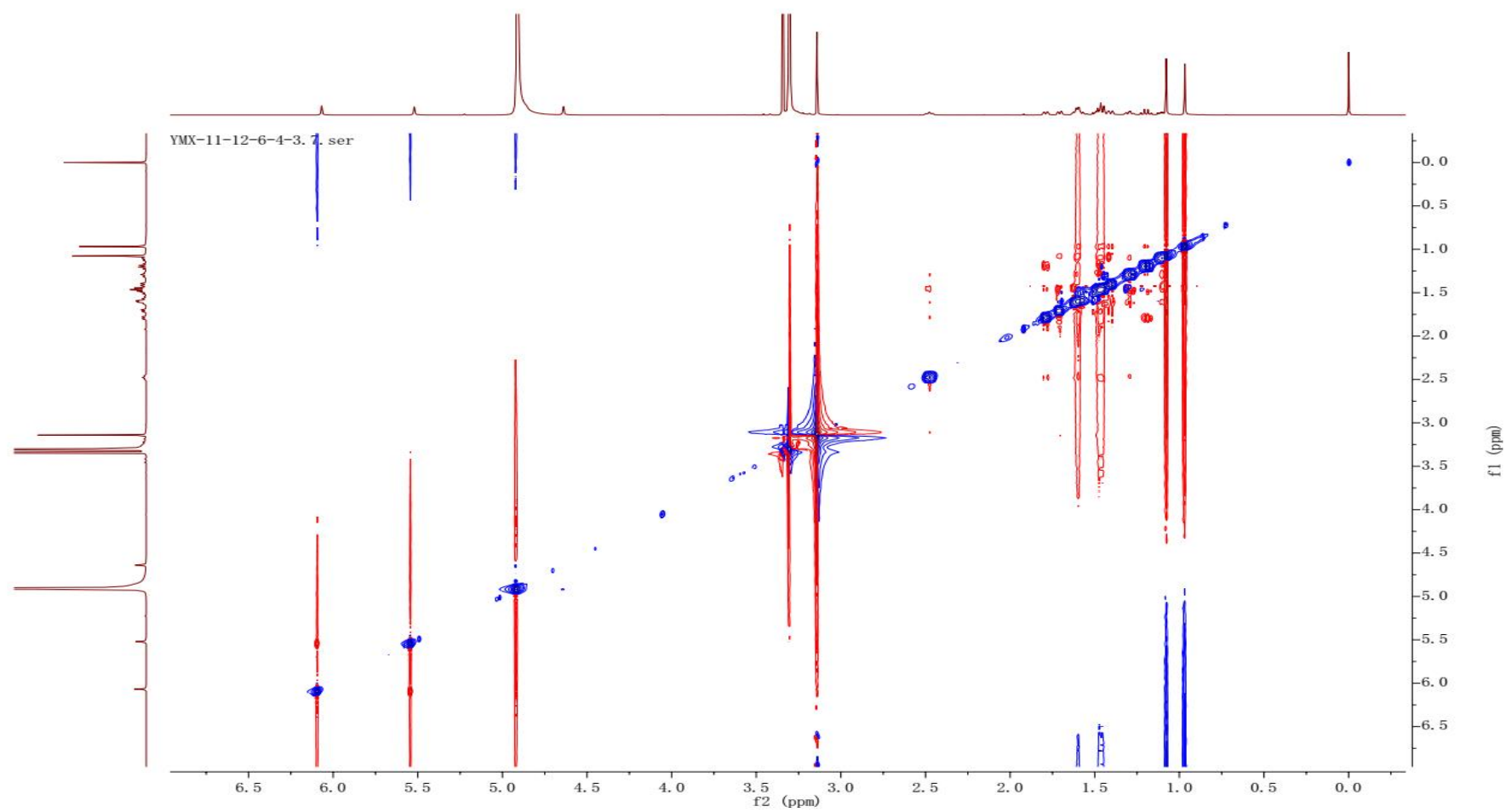


Figure S44. ROESY spectrum of compound **5** (CD₃OD, 600 MHz)

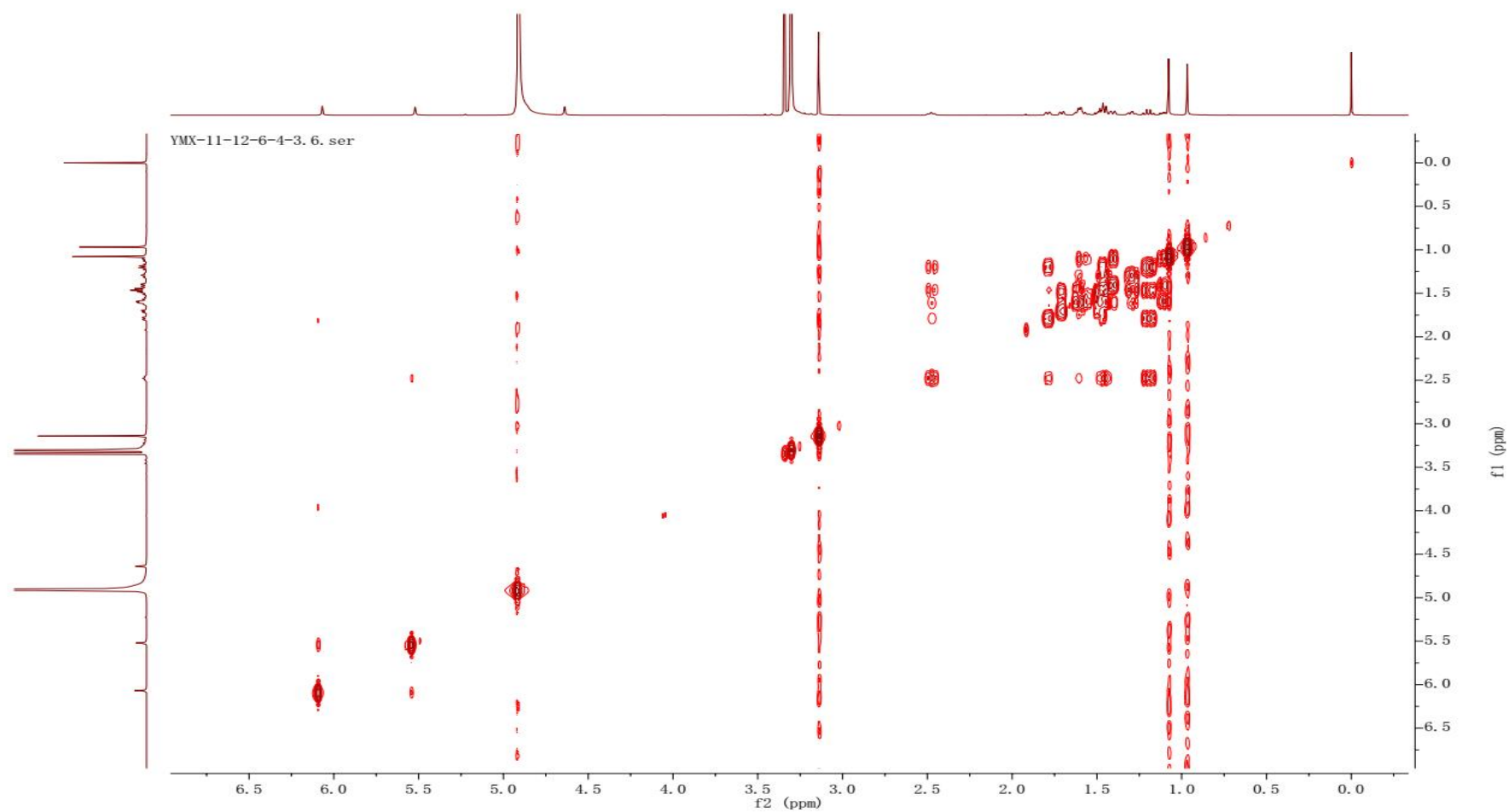


Figure S45. ^1H - ^1H COSY spectrum of compound **5** (CD_3OD , 600 MHz)

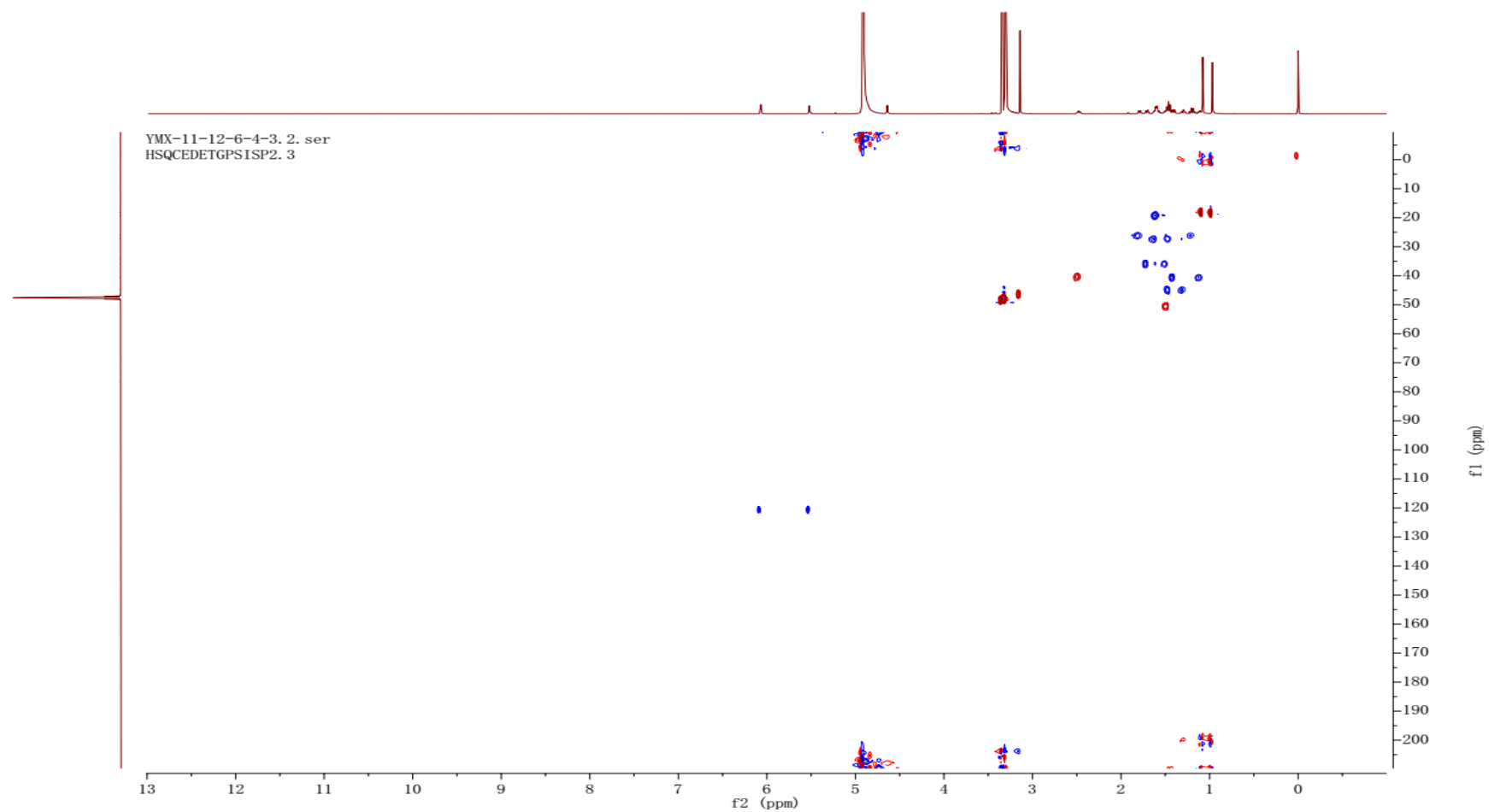


Figure S46. HSQC spectrum of compound **5** (CD₃OD, 600 MHz)

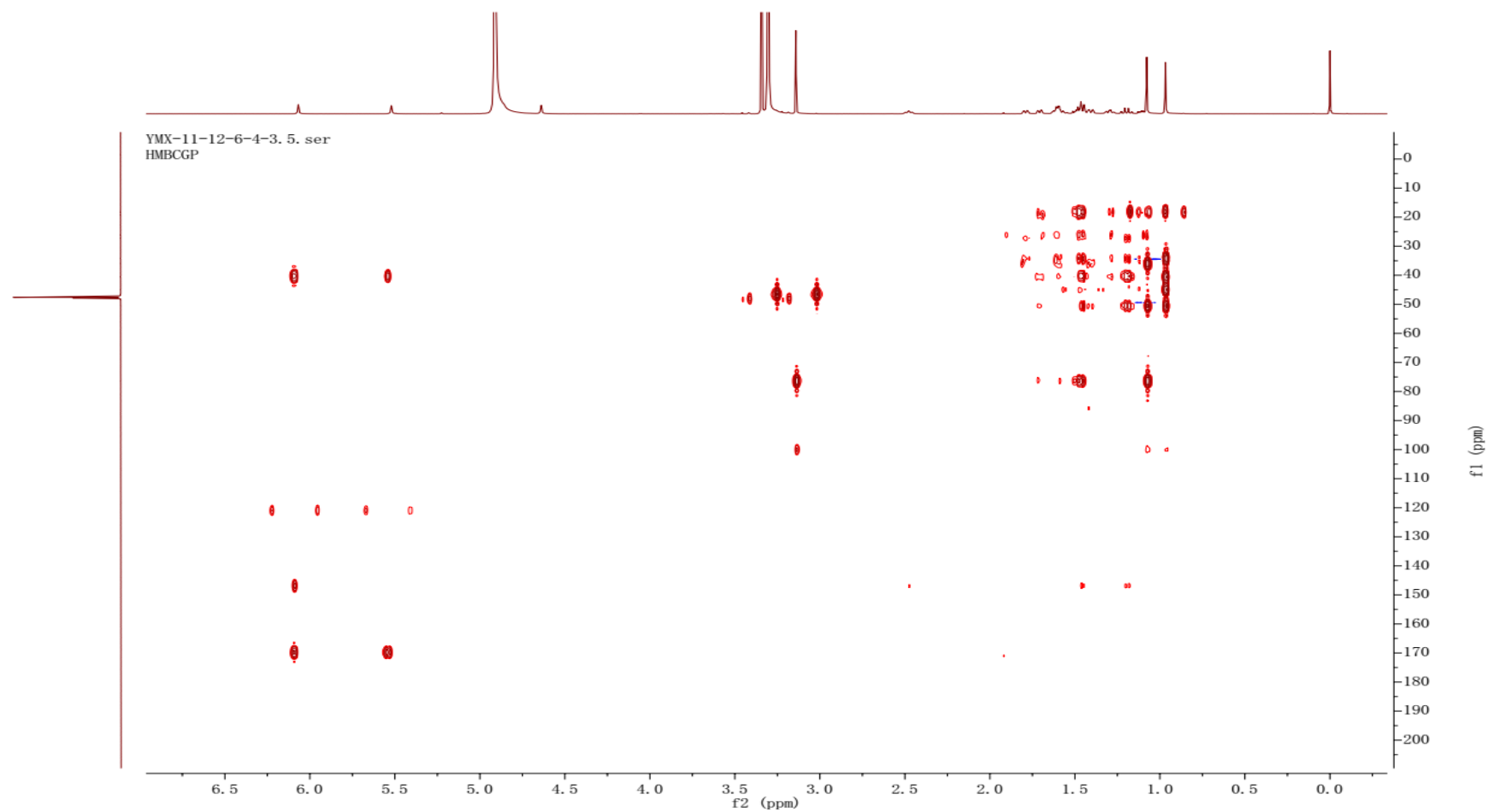
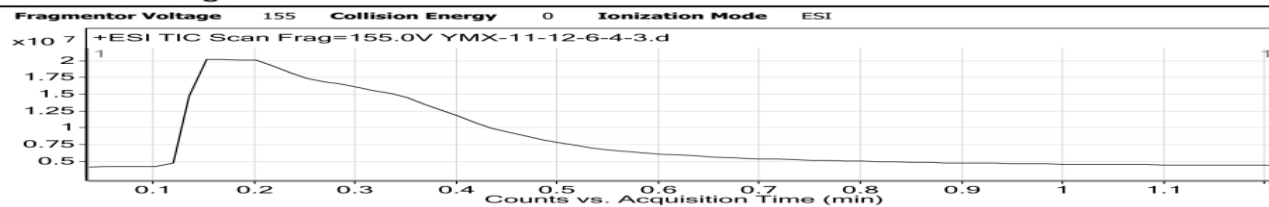


Figure S47. HMBC spectrum of compound **5** (CD₃OD, 600 MHz)

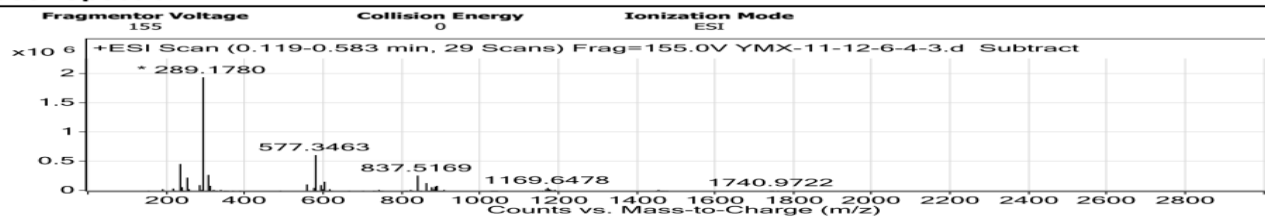
Qualitative Analysis Report

Data Filename	YMX-11-12-6-4-3.d	Sample Name	YMX-11-12-6-4-3
Sample Type	Sample	Position	p1b7
Instrument Name	Instrument 1	User Name	Q-TOF-HP\Q-TOF
Acq Method	default20190111-ms.m	Acquired Time	1/12/2020 3:56:11 PM
IRM Calibration Status	Success	DA Method	1.m
Comment			
Sample Group	6200 series TOF/6500 series	Info.	
Acquisition SW	Q-TOF B.05.01 (B5125.3)		
Version			

User Chromatograms



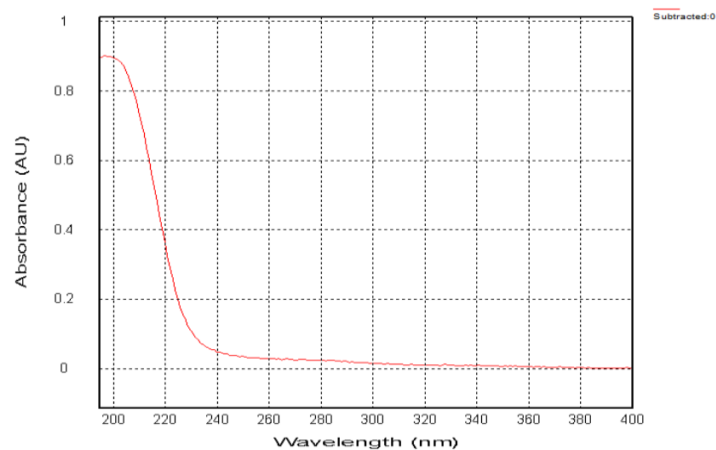
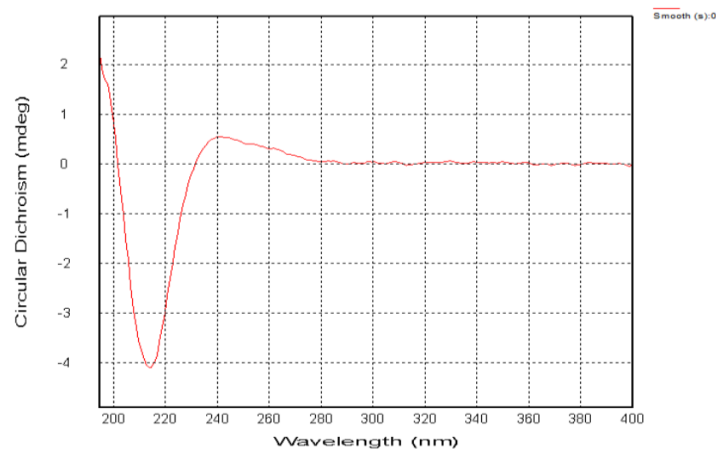
User Spectra



Peak List

m/z	z	Abund
235.1682	1	466617.69
252.1947	1	229973.59
289.178	1	1947617.25
290.1797	1	470698.53
305.1497	1	283320.63
577.3463	1	622858.25
578.3492	1	192049.98
599.3274	1	159994.36

Figure S48. HRESI spectrum of compound 5



File: YMX-11-12-6-4-3 (195-400 nm) 20112717.dsx

ProBinaryX

Attributes :

- Time Stamp :Fri Nov 27 19:34:36 2020

- File ID : {E3C61445-D6E4-4321-8A56-F058D491F92A}

- Is CFR Compliant : false

- Original data has not been modified.

Remarks:

- User: CD

- Date: 2020/11/27

- Instrument: 0547

- DetectorType: LAAPD

- DichOS Calibration Correction Curve: 0547/2

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.3300mg/mL MeOH

- Pathlength: 1 mm

- Temperature: 20°C

Settings:

- Time-per-point: 1s (25us x 40000)

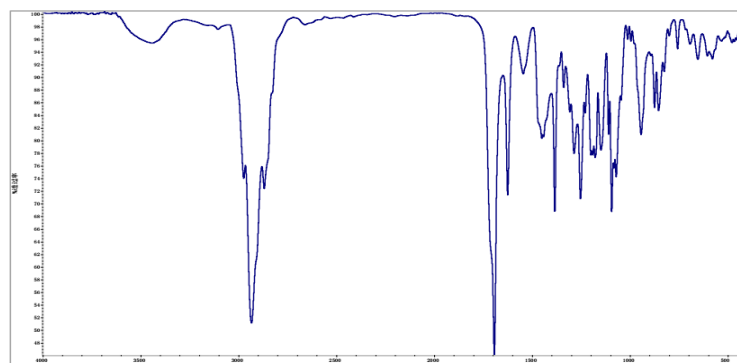
- SE

- Wavelength: 195nm - 400nm

- Step Size: 1nm

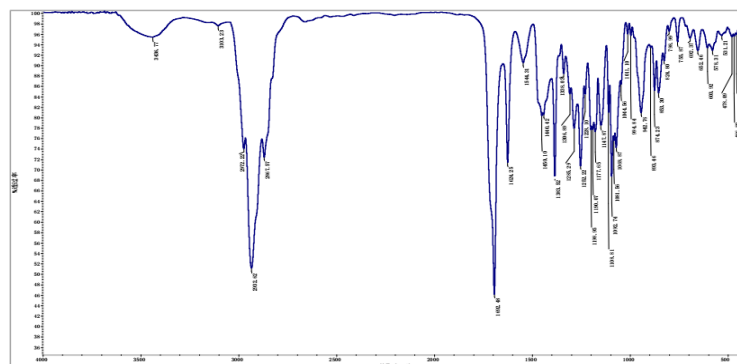
- Bandwidth: 1nm

Figure S49. CD and UV spectrum of compound **5**



Sample Name: YMX-11-12-6-4-3
KBr压片
采集时间: 星期三 10月 28 15:50:22 2020 (GMT+08:00)
仪器型号: NICOLET IS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00



Sample Name: YMX-11-12-6-4-3
KBr压片
采集时间: 星期三 10月 28 15:50:22 2020 (GMT+08:00)
仪器型号: NICOLET IS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00

星期三 10月 28 16:17:58 2020 (GMT+08:00)

标峰:

谱图: YMX-11-12-6-4-3
范围: 4000.00 400.00
(绝对) 阈值: 98.027
灵敏度: 99

峰表:

峰位置:	412.82	强度:	96.662
峰位置:	428.77	强度:	95.522
峰位置:	453.94	强度:	95.875
峰位置:	466.80	强度:	95.609
峰位置:	478.09	强度:	95.467
峰位置:	531.21	强度:	95.695
峰位置:	578.31	强度:	92.856
峰位置:	603.92	强度:	93.347
峰位置:	652.46	强度:	92.811
峰位置:	692.37	强度:	95.215
峰位置:	755.87	强度:	94.485
峰位置:	798.99	强度:	96.532
峰位置:	824.80	强度:	90.853
峰位置:	853.30	强度:	84.659
峰位置:	874.23	强度:	85.192
峰位置:	893.46	强度:	93.418
峰位置:	942.76	强度:	80.892
峰位置:	994.84	强度:	95.705
峰位置:	1011.10	强度:	95.968
峰位置:	1044.56	强度:	86.363
峰位置:	1069.87	强度:	74.184
峰位置:	1081.56	强度:	75.599
峰位置:	1092.74	强度:	68.662
峰位置:	1108.81	强度:	80.982
峰位置:	1147.87	强度:	78.456
峰位置:	1177.65	强度:	77.247
峰位置:	1190.07	强度:	77.700
峰位置:	1198.95	强度:	77.649
峰位置:	1228.10	强度:	84.290
峰位置:	1252.22	强度:	70.643
峰位置:	1285.29	强度:	77.882
峰位置:	1306.89	强度:	84.494
峰位置:	1338.03	强度:	88.230
峰位置:	1383.52	强度:	68.059
峰位置:	1440.42	强度:	80.577
峰位置:	1450.10	强度:	80.296
峰位置:	1544.31	强度:	90.498
峰位置:	1624.25	强度:	71.351
峰位置:	1692.48	强度:	46.060
峰位置:	2867.57	强度:	72.352
峰位置:	2932.62	强度:	51.049
峰位置:	2972.22	强度:	73.976
峰位置:	3103.23	强度:	97.566
峰位置:	3436.77	强度:	95.382

Figure S50. IR spectrum of compound 5

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 26-NOV-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>				
5	-29.43	0.11	-0.37	-29.33	-29.60				
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>
1	YMX-11-12-6-4-3	02:24:56 PM	-29.60	SR	-0.0444	589	100.00	0.150	22.8
2	YMX-11-12-6-4-3	02:25:04 PM	-29.33	SR	-0.0440	589	100.00	0.150	22.8
3	YMX-11-12-6-4-3	02:25:12 PM	-29.33	SR	-0.0440	589	100.00	0.150	22.8
4	YMX-11-12-6-4-3	02:25:20 PM	-29.47	SR	-0.0442	589	100.00	0.150	22.8
5	YMX-11-12-6-4-3	02:25:28 PM	-29.40	SR	-0.0441	589	100.00	0.150	22.9

Figure S51 $[\alpha]^{25}_D$ of compound 5

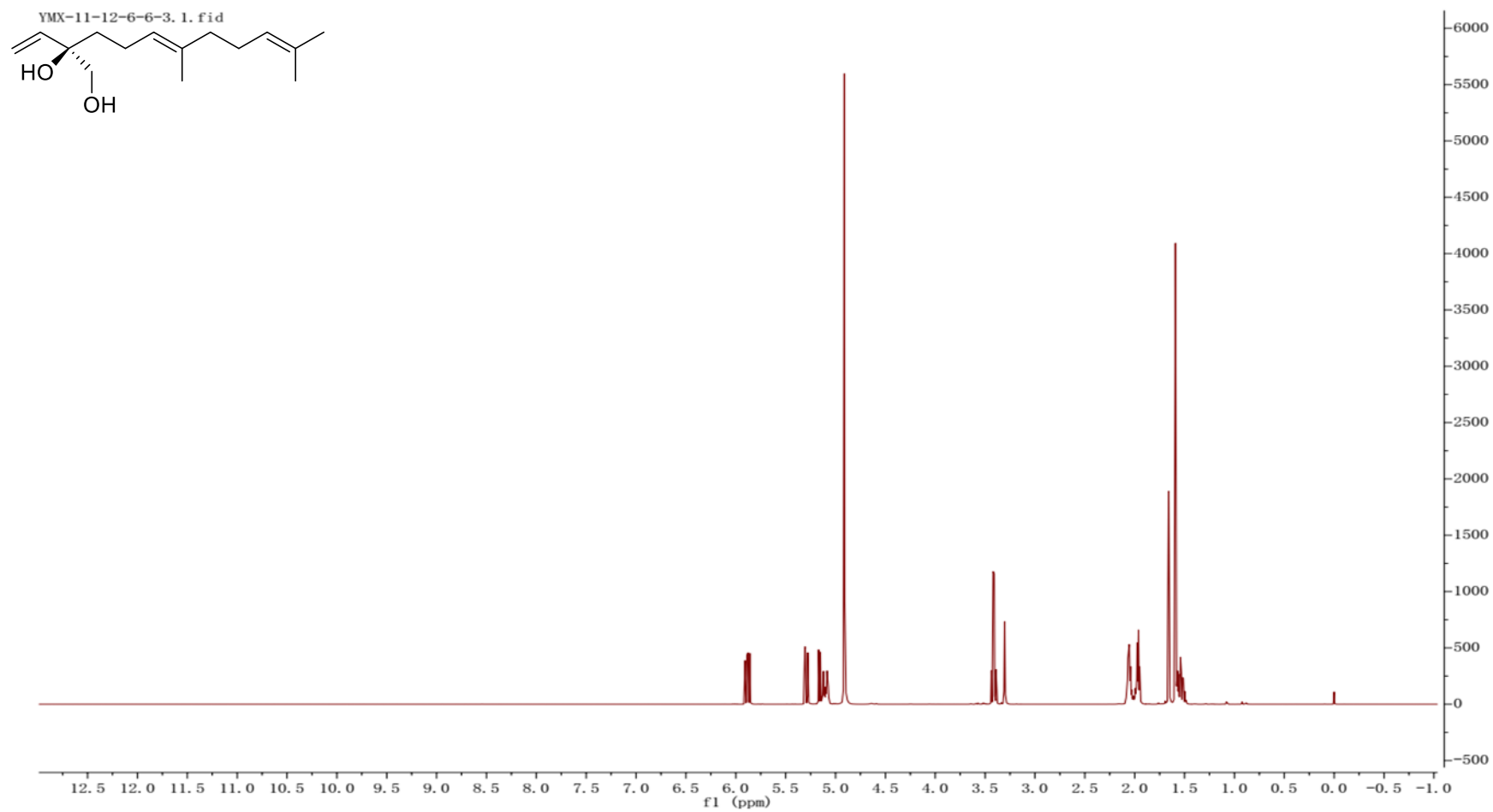


Figure S52. ^1H NMR spectrum of compound **6** (CD₃OD, 600 MHz)

YMX-11-12-6-6-3. 3. fid

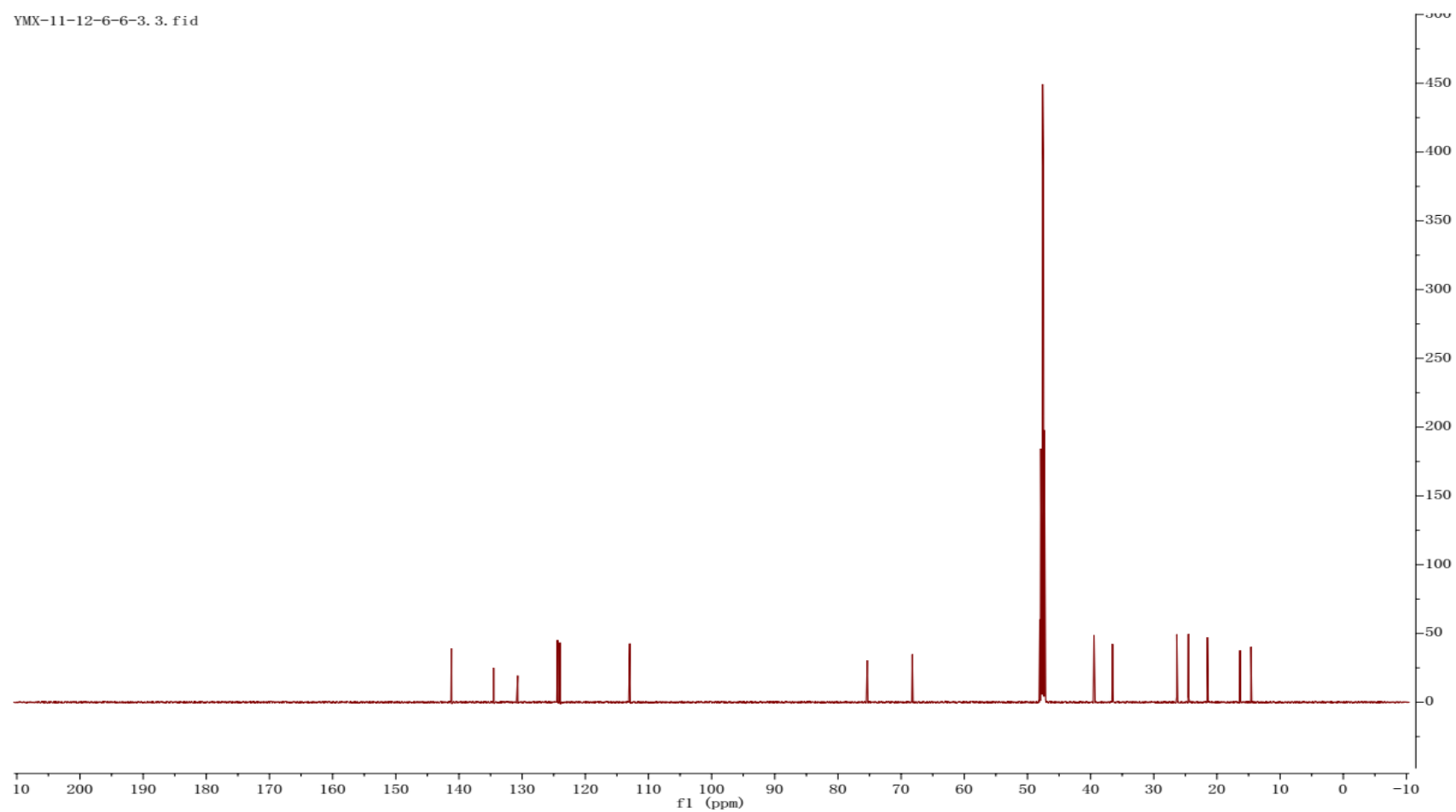


Figure S53. ^{13}C NMR spectrum of compound **6** (CD_3OD , 150 MHz)

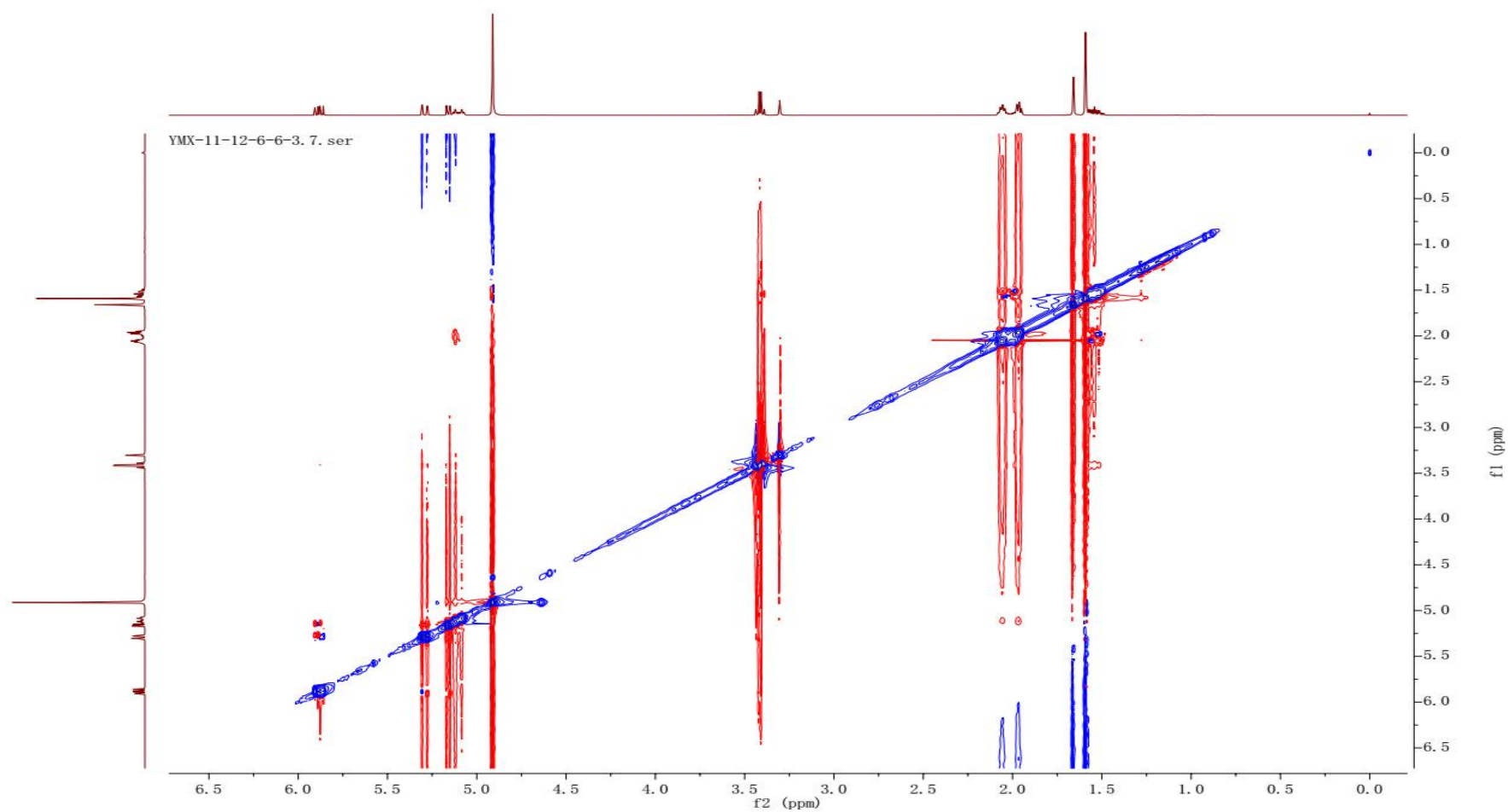


Figure S54. ROESY spectrum of compound **6** (CD₃OD, 600 MHz)

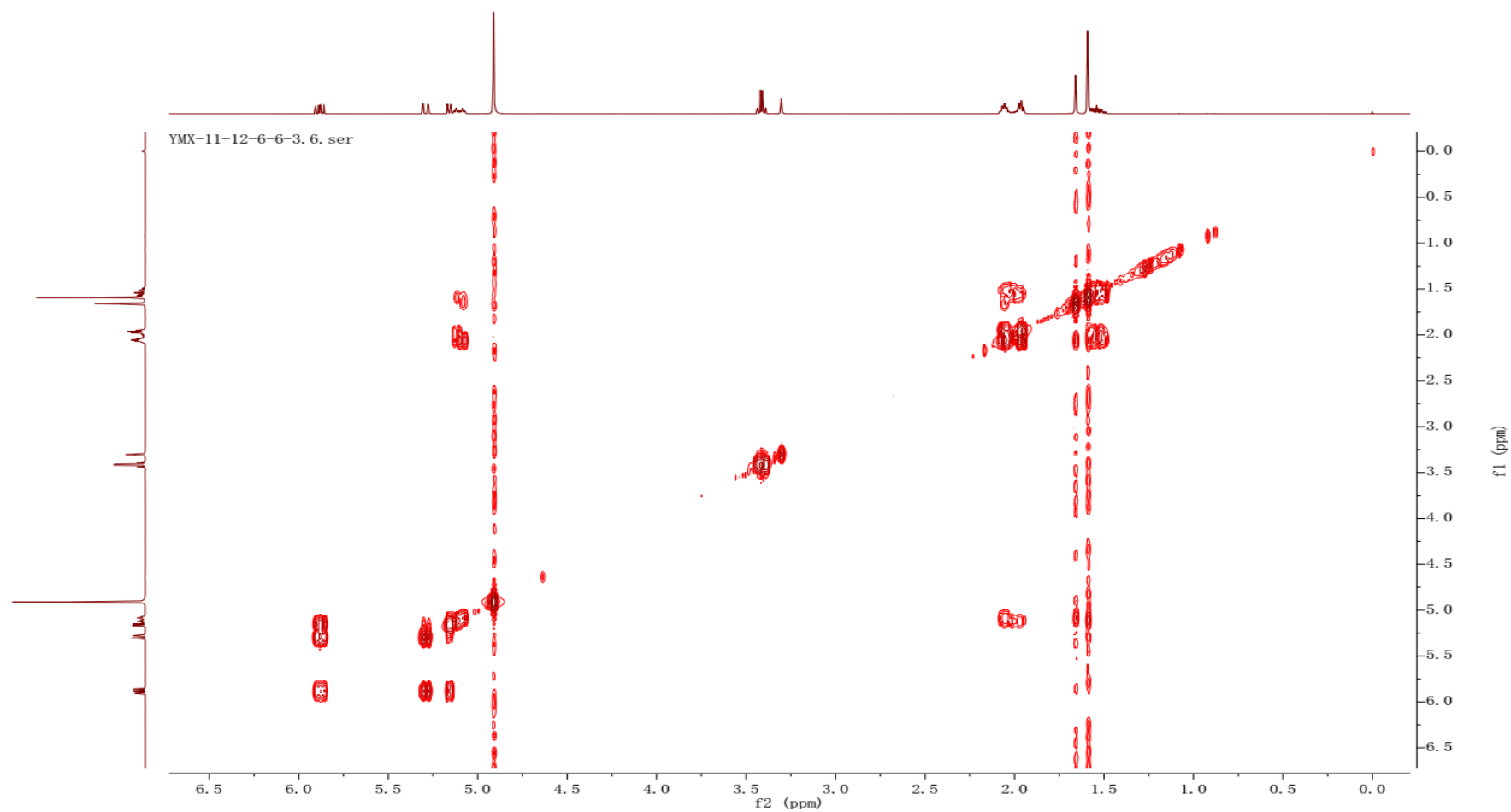


Figure S55. ^1H - ^1H COSY spectrum of compound **6** (CD_3OD , 600 MHz)

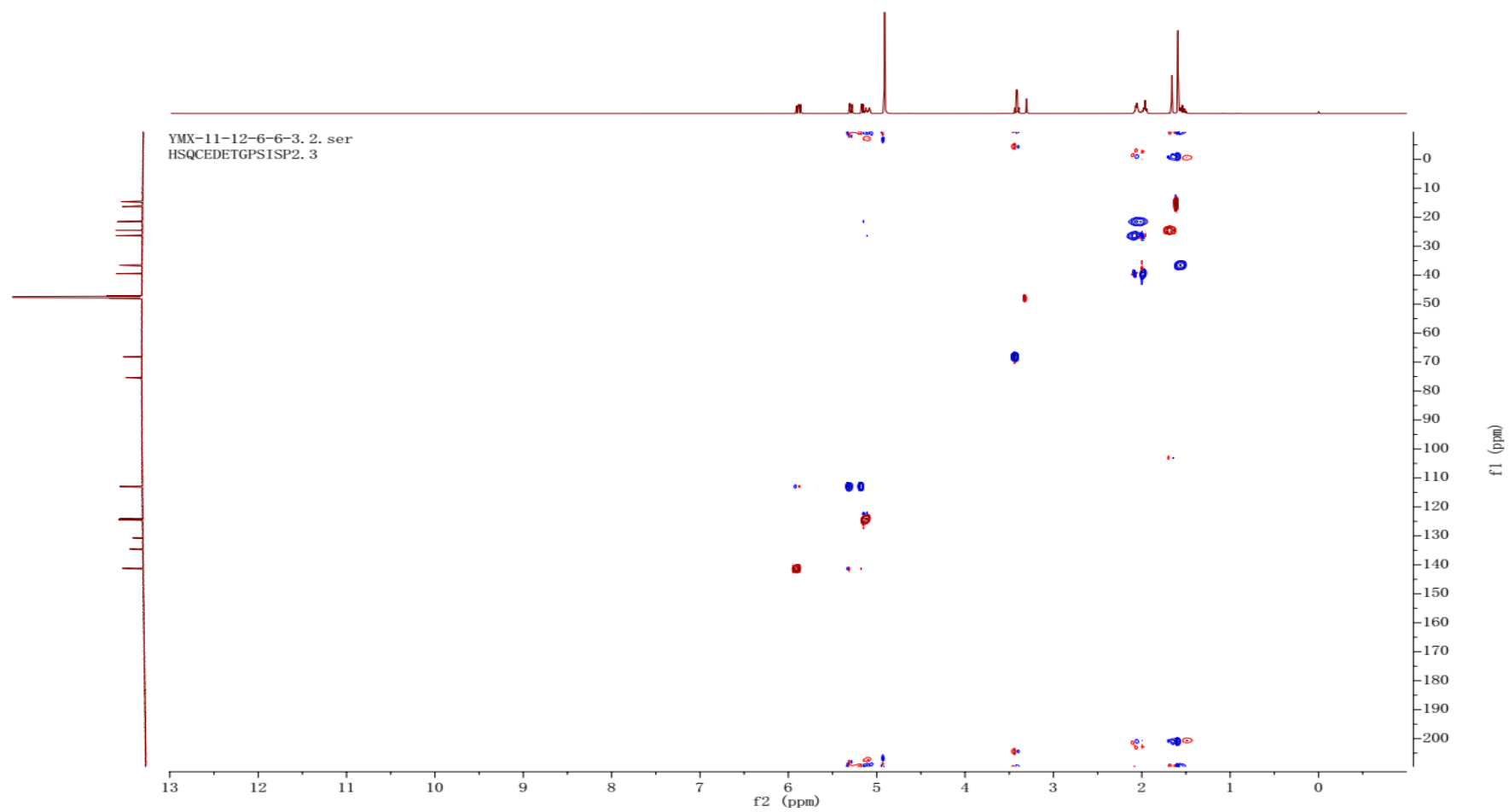


Figure S56. HSQC spectrum of compound **6** (CD₃OD, 600 MHz)

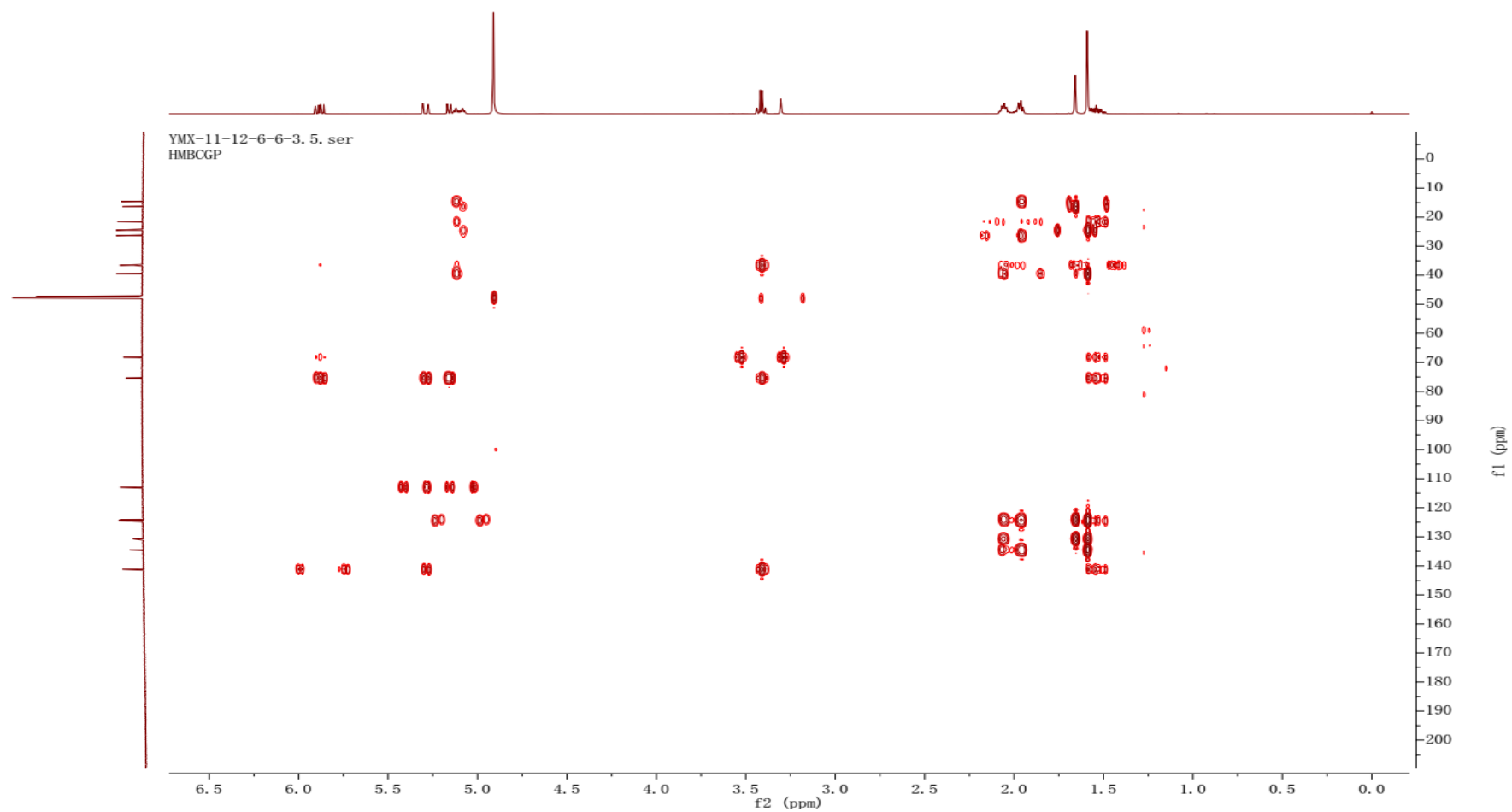


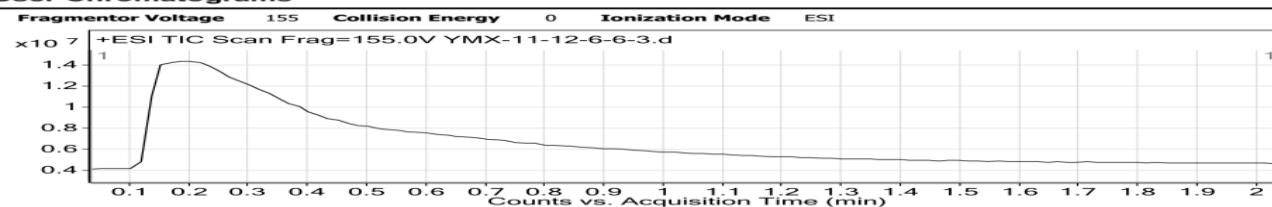
Figure S57. HMBC spectrum of compound **6** (CD₃OD, 600 MHz)

Qualitative Analysis Report

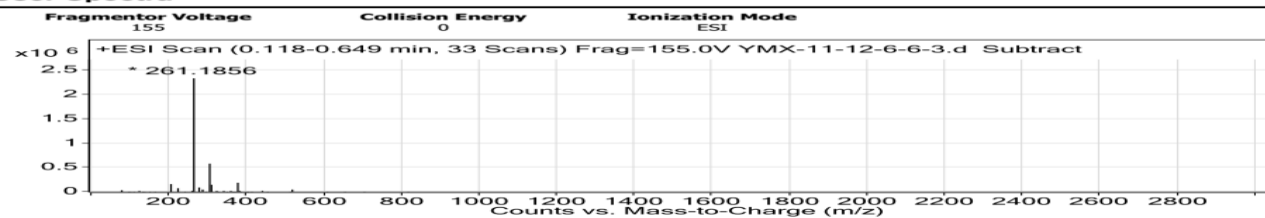
Data Filename Sample Type Instrument Name Acq Method IRM Calibration Status Comment Sample Group Acquisition SW Version	YMX-11-12-6-6-3.d Sample Instrument 1 default20190111-ms.m Success 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.3)	Sample Name Position User Name Acquired Time DA Method	YMX-11-12-6-6-3 p1c1 Q-TOF-HP\Q-TOF 1/12/2020 4:05:49 PM 1.m
--	--	---	--

Info.

User Chromatograms



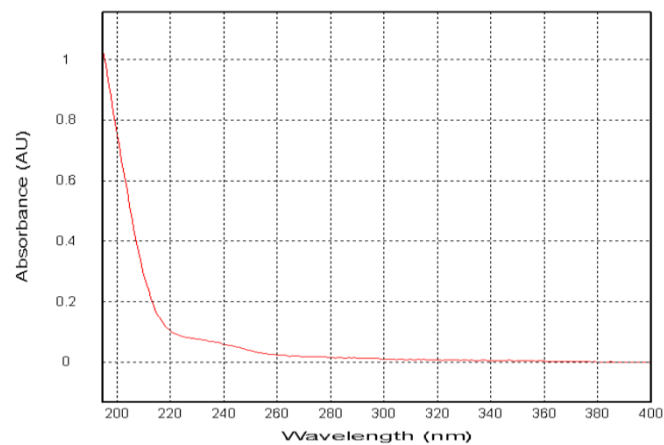
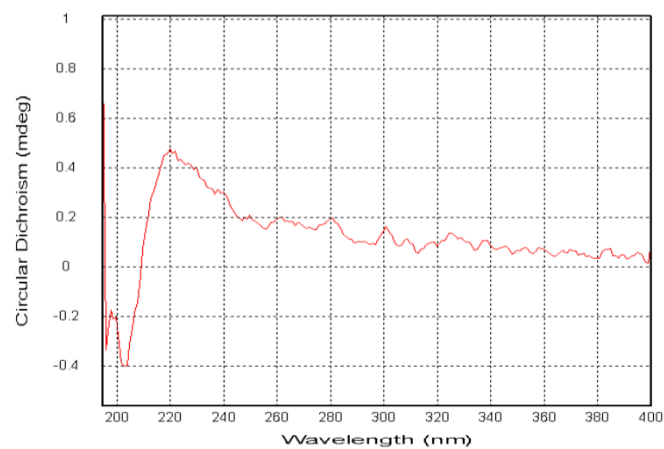
User Spectra



Peak List

m/z	z	Abund
203.1783	1	172827.08
261.1856	1	2338798.5
261.2774	1	96010.87
261.3213	1	342364
261.3655	1	121769.01
262.1851	1	1024942.81
277.1545	1	95900.87
303.1922	1	584750.81

Figure S58. HRESI spectrum of compound 6



File: YMX-11-12-6-6-3 (195-400 nm) 20112720.dsx

ProBinaryX

Attributes :

- Time Stamp :Fri Nov 27 20:42:05 2020

- File ID : {6F3D91B5-42E8-473d-B607-7EE2ACF6B1BD}

- Is CFR Compliant : false

- Original data has not been modified.

Remarks:

- User: CD

- Date: 2020/11/27

- Instrument: 0547

- DetectorType: LAAPD

- DichOS Calibration Correction Curve: 0547/2

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.1500mg/mL MeOH

- Pathlength: 1 mm

- Temperature: 20°C

Settings:

- Time-per-point: 1s (25us x 40000)

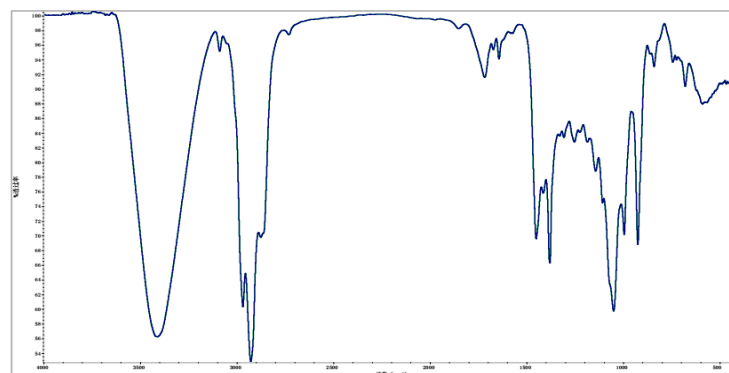
- SE

- Wavelength: 195nm - 400nm

- Step Size: 1nm

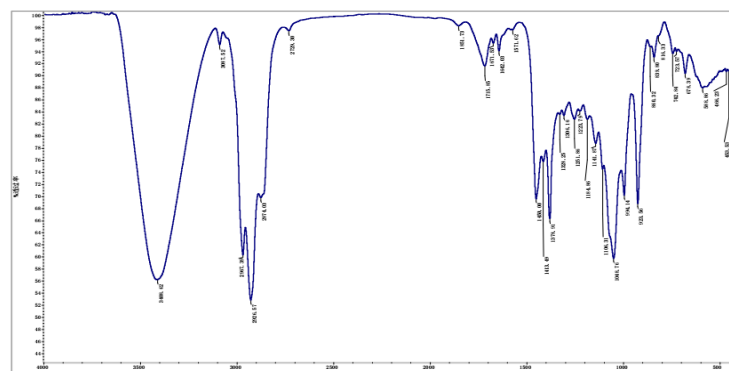
- Bandwidth: 1nm

Figure S59. CD and UV spectrum of compound **6**



Sample Name: YMX-11-12-6-6-3
KBr压片
采集时间: 星期四 10月 29 11:29:49 2020 (GMT+08:00)
仪器型号: NICOLET IS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00



Sample Name: YMX-11-12-6-6-3
KBr压片
采集时间: 星期四 10月 29 11:29:49 2020 (GMT+08:00)
仪器型号: NICOLET IS10
Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00

星期四 10月 29 13:55:28 2020 (GMT+08:00)

标峰:

谱图: YMX-11-12-6-6-3
范围: 4000.00 400.00
(绝对) 阈值: 99.389
灵敏度: 99

峰表:

峰位置:	强度:
410.39	93.079
421.03	92.003
437.63	91.084
453.53	90.767
466.23	90.657
488.75	90.640
497.17	90.619
588.86	87.915
678.39	90.326
723.57	93.959
742.84	93.655
839.80	93.032
860.32	94.743
923.56	68.766
994.14	70.116
1048.76	59.646
1106.31	74.437
1141.87	78.734
1184.86	82.714
1223.79	84.083
1251.86	82.717
1306.16	83.359
1328.25	83.547
1378.91	66.225
1413.49	75.733
1450.00	69.520
1571.62	97.551
1642.03	94.060
1671.53	95.362
1715.85	91.580
1851.73	98.214
2729.30	97.386
2874.03	69.723
2926.57	52.769
2967.39	60.236
3087.52	95.102
3408.62	56.161

Figure S60. IR spectrum of compound 6

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 26-NOV-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>					
5	0.32	0.19	59.37	0.53	0.13					
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>	
1	YMX-11-12-6-6-3	03:01:40 PM	0.13	SR	0.0002	589	100.00	0.150	22.5	
2	YMX-11-12-6-6-3	03:01:48 PM	0.47	SR	0.0007	589	100.00	0.150	22.5	
3	YMX-11-12-6-6-3	03:01:56 PM	0.13	SR	0.0002	589	100.00	0.150	22.5	
4	YMX-11-12-6-6-3	03:02:05 PM	0.33	SR	0.0005	589	100.00	0.150	22.5	
5	YMX-11-12-6-6-3	03:02:12 PM	0.53	SR	0.0008	589	100.00	0.150	22.5	

Figure S61. $[\alpha]^{25}_D$ of compound 6

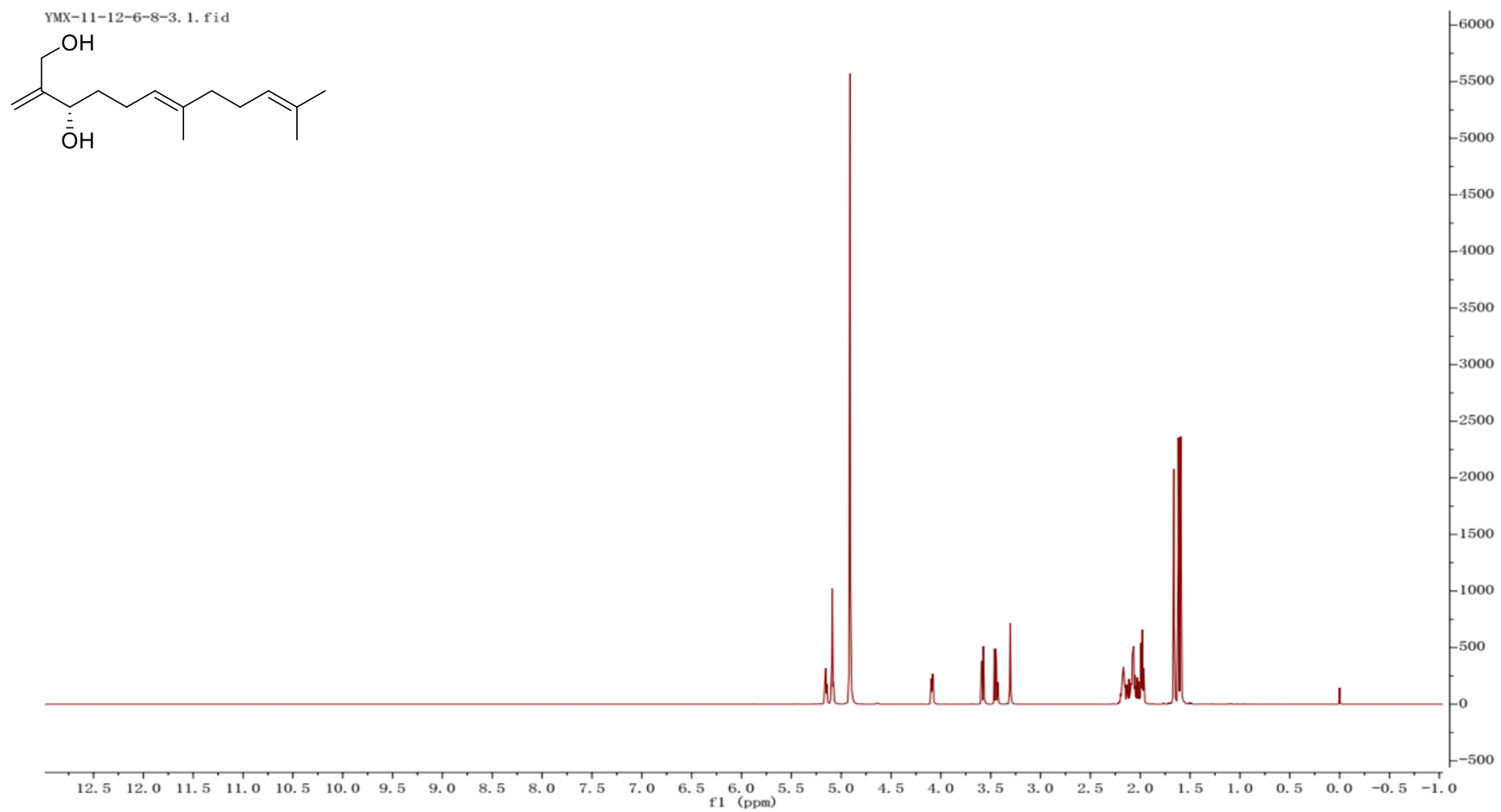


Figure S62. ^1H NMR spectrum of compound **7** (CD₃OD, 600 MHz)

YMX-11-12-6-8-3. 3. fid

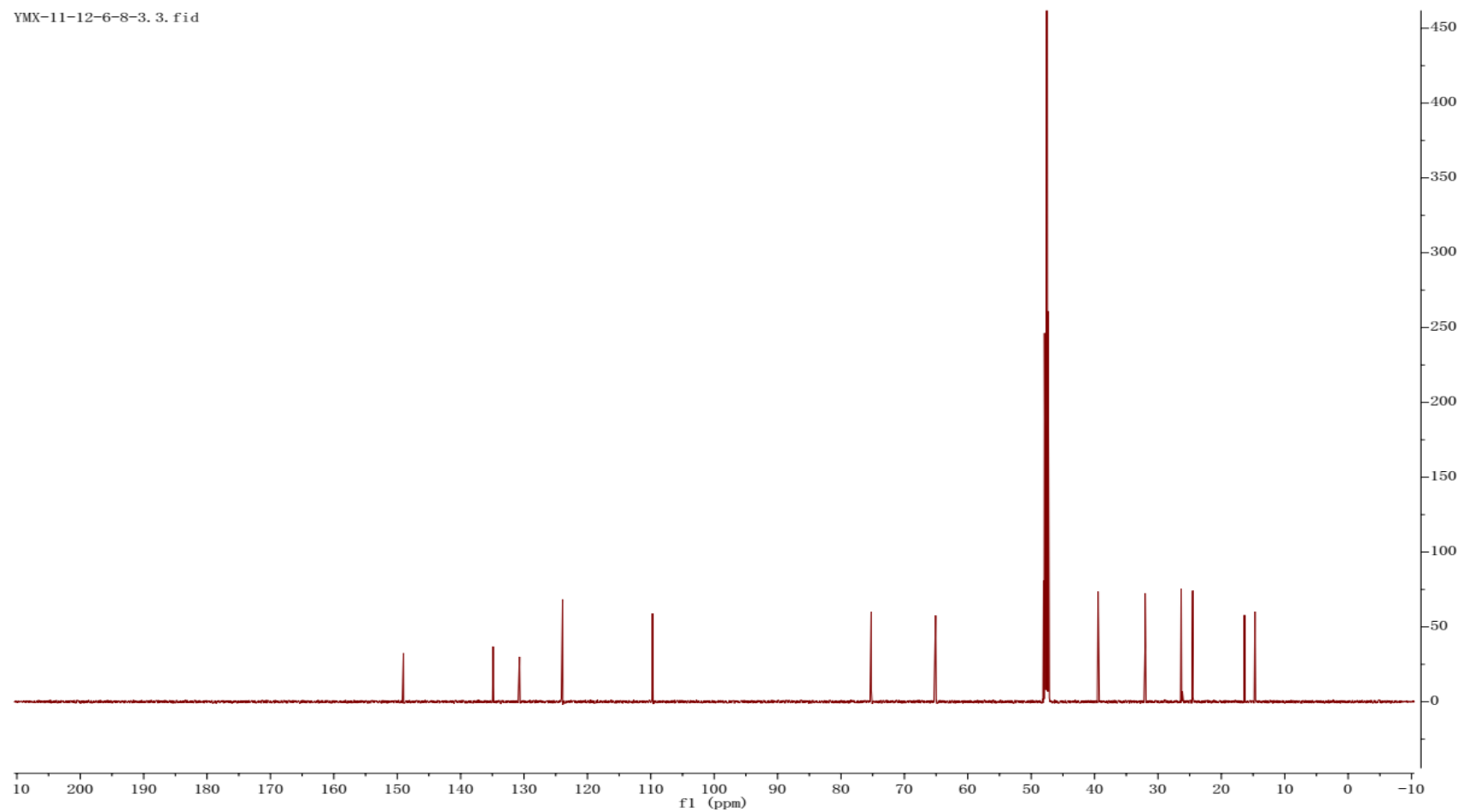


Figure S63. ^{13}C NMR spectrum of compound **7** (CD_3OD , 150 MHz)

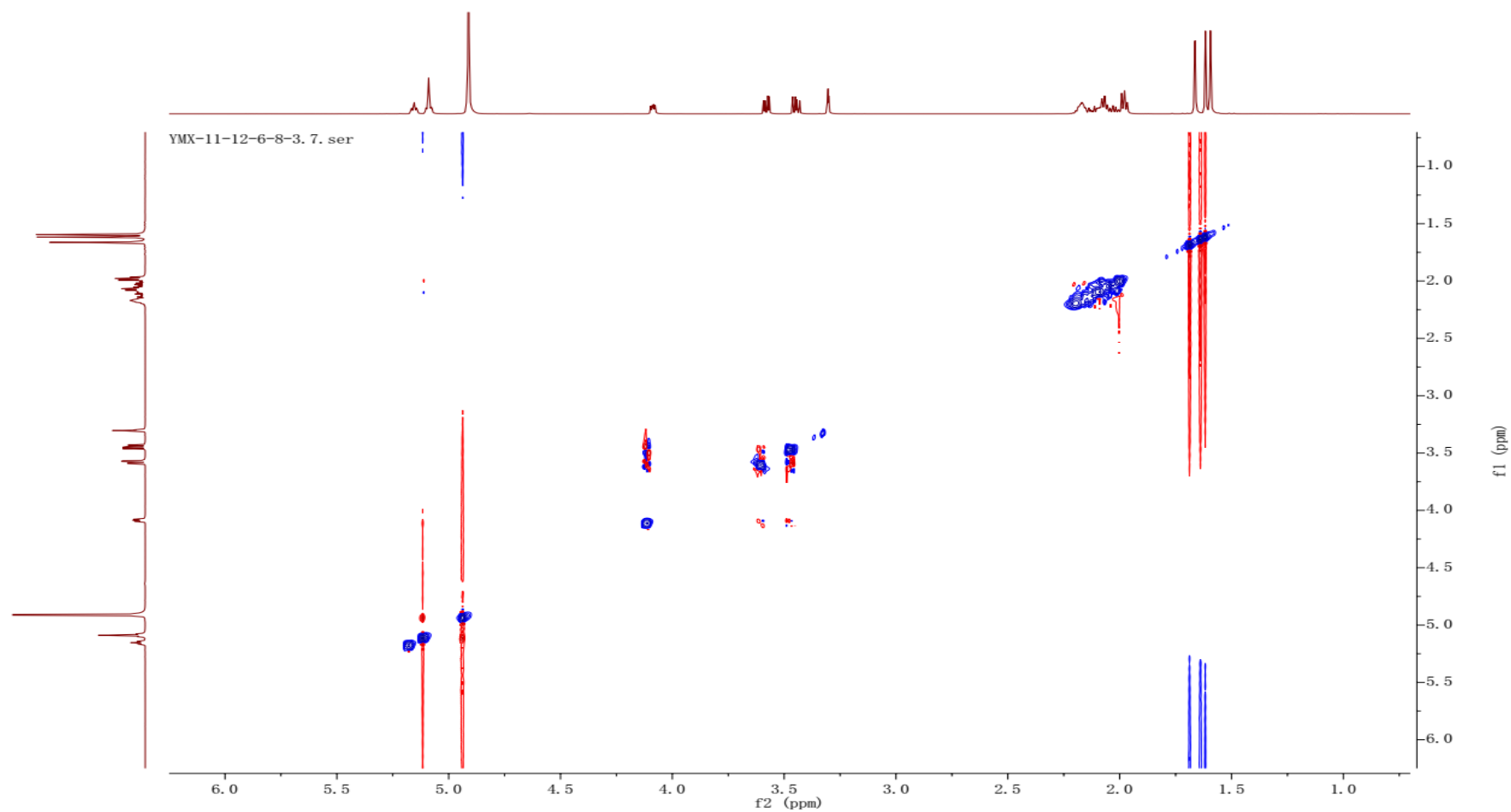


Figure S64. ROESY spectrum of compound **7** (CD₃OD, 600 MHz)

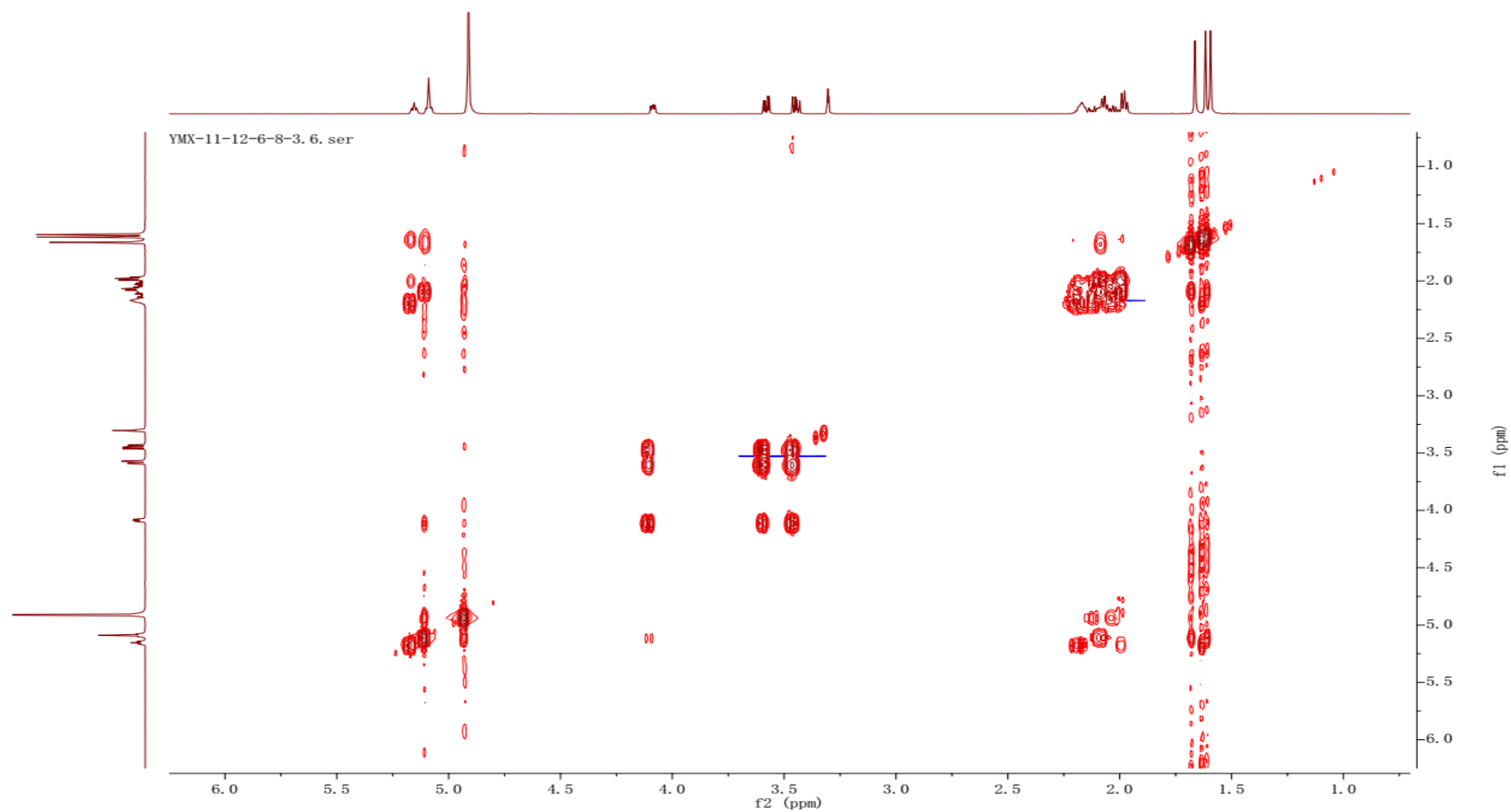


Figure S65. ^1H - ^1H COSY spectrum of compound **7** (CD_3OD , 600 MHz)

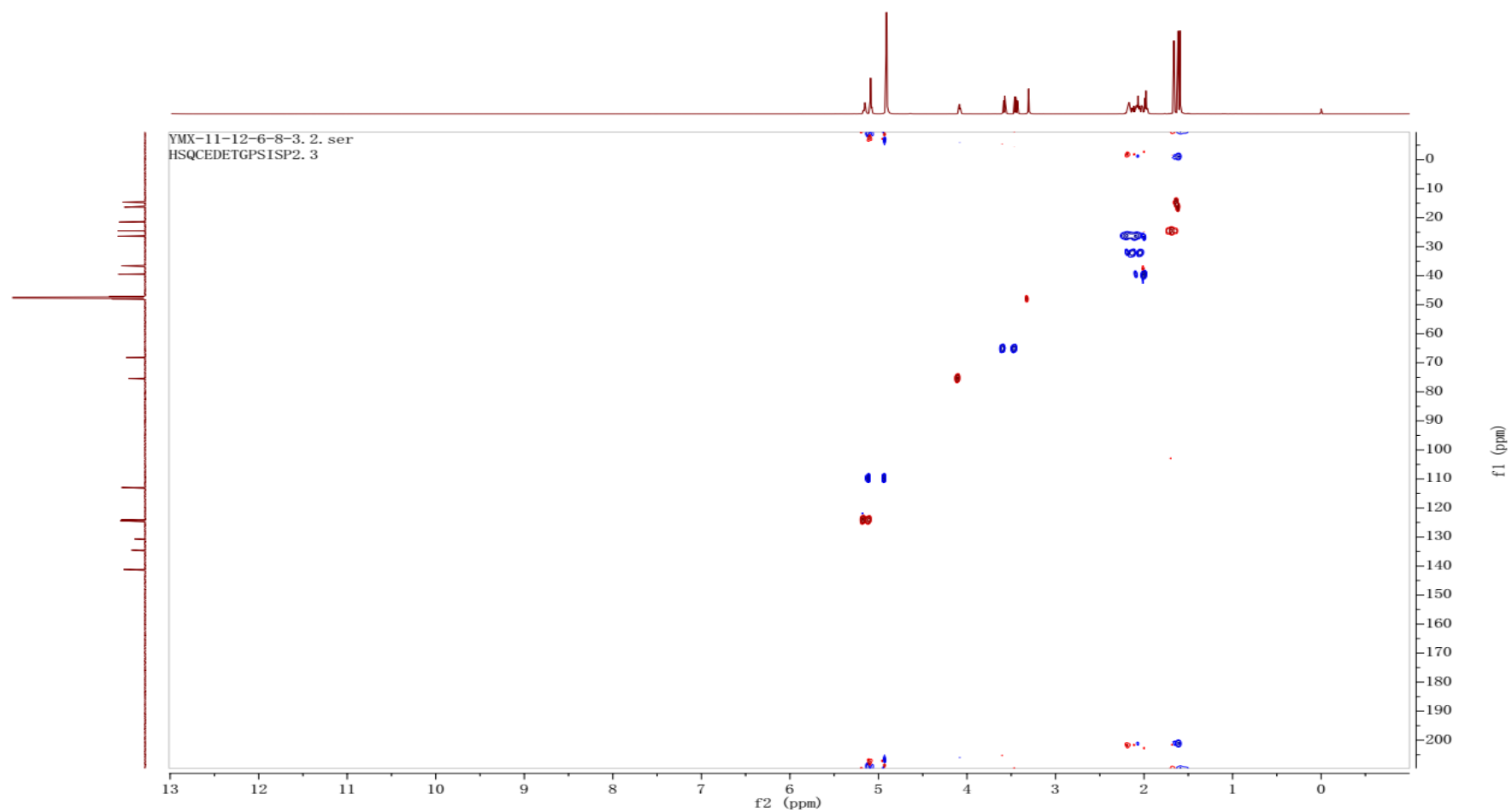


Figure S66. HSQC spectrum of compound **7** (CD₃OD, 600 MHz)

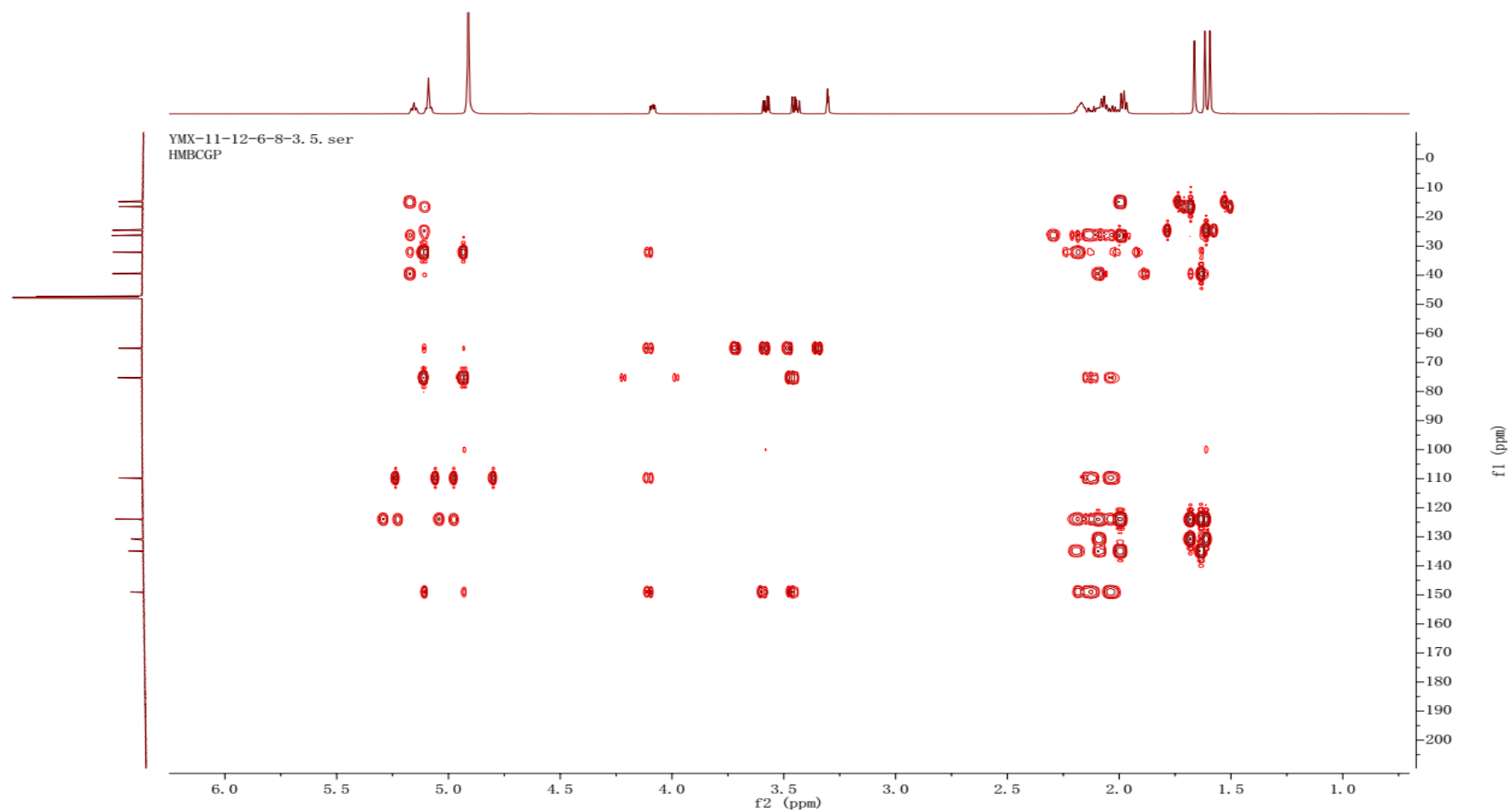


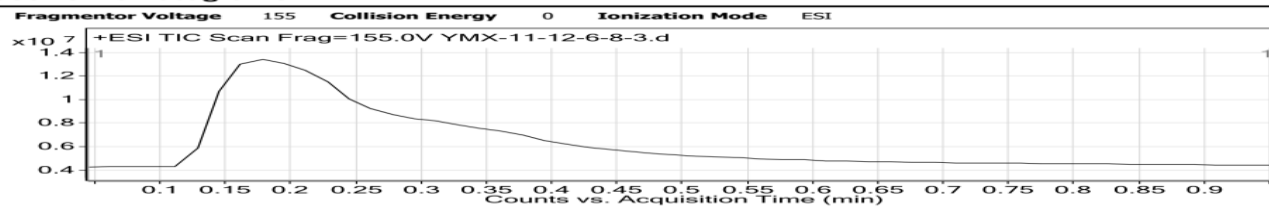
Figure S67. HMBC spectrum of compound **7** (CD₃OD, 600 MHz)

Qualitative Analysis Report

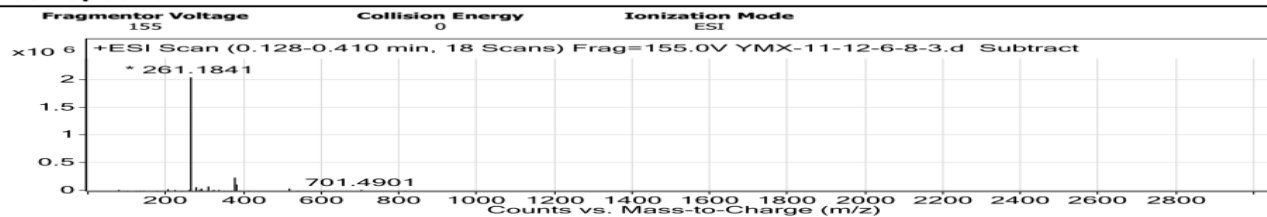
Data Filename Sample Type Instrument Name Acq Method IRM Calibration Status Comment Sample Group Acquisition SW Version	YMX-11-12-6-8-3.d Sample Instrument 1 default20190111-ms.m Success 6200 series TOF/6500 series Q-TOF B.05.01 (B5125.3)	Sample Name Position User Name Acquired Time DA Method
		YMX-11-12-6-8-3 p1c2 Q-TOF-HP\Q-TOF 1/12/2020 4:11:00 PM 1.m

Info.

User Chromatograms



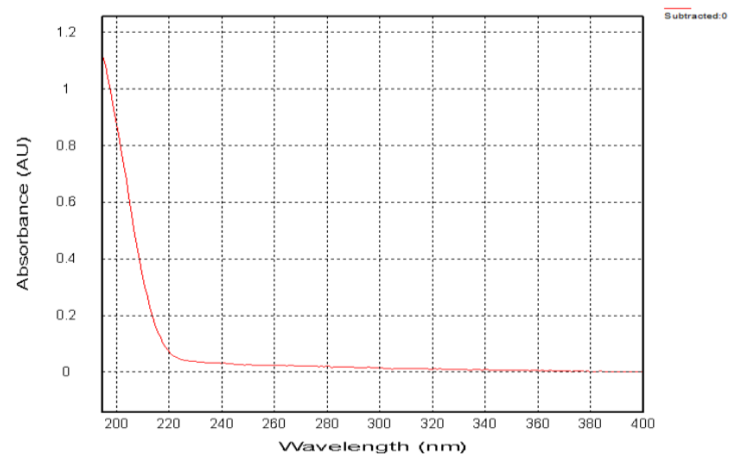
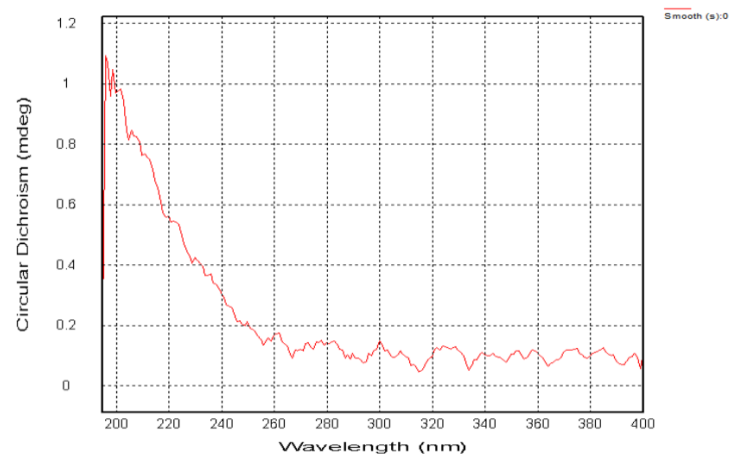
User Spectra



Peak List

m/z	z	Abund
261.1841	1	2048351.13
261.3211	1	247079.53
261.3652		79286.84
262.1848	1	765918.75
263.1873	1	64784.36
277.154	1	69289
287.1966	1	53615.05
305.2071	1	83044.34

Figure S68. HRESI spectrum of compound 7



File: YMX-11-12-6-8-3 (195-400 nm) 20112721.dsx

ProBinaryX

Attributes :

- Time Stamp :Fri Nov 27 21:06:34 2020

- File ID : {B308C0DA-C265-4041-837A-C29D563B6A3C}

- Is CFR Compliant : false

- Original data has not been modified.

Remarks:

- User: CD

- Date: 2020/11/27

- Instrument: 0547

- DetectorType: LAAPD

- DichOS Calibration Correction Curve: 0547/2

- HV (CDDC channel): 0 v

- Time per point: 1 s

- Description: Sample 1

- Concentration: 0.0300mg/mL MeOH

- Pathlength: 1 mm

- Temperature: 20°C

Settings:

- Time-per-point: 1 s (25us x 40000)

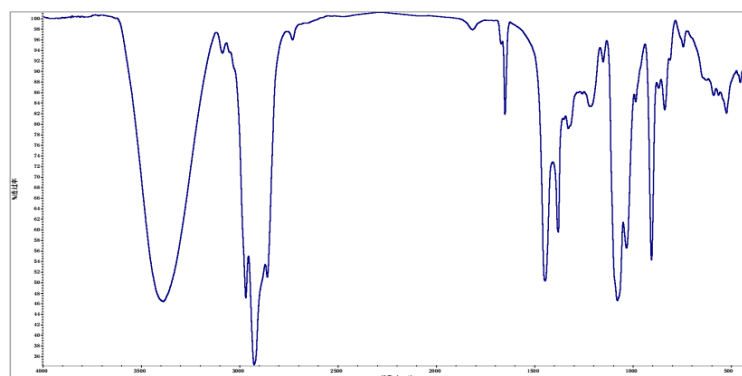
- SE

- Wavelength: 195nm - 400nm

- Step Size: 1nm

- Bandwidth: 1nm

Figure S69. CD and UV spectrum of compound 7



Sample Name: YMX-11-12-6-8-3

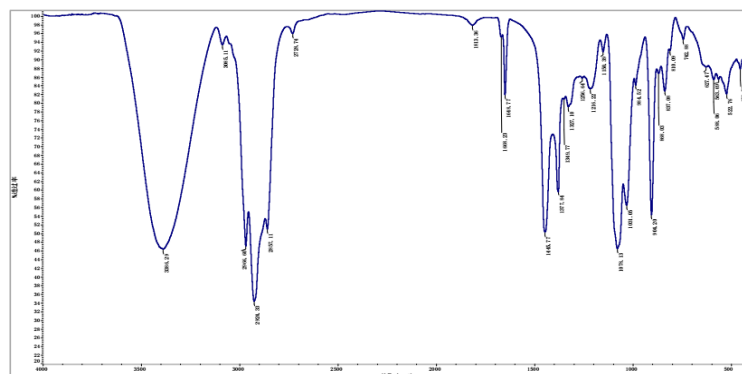
KBr压片

采集时间: 星期四 10月 29 13:59:18 2020 (GMT+08:00)

仪器型号: NICOLET IS10

Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00



Sample Name: YMX-11-12-6-8-3

KBr压片

采集时间: 星期四 10月 29 13:59:18 2020 (GMT+08:00)

仪器型号: NICOLET IS10

Software version: OMNIC 9.8.372

样品扫描次数: 16
背景扫描次数: 16
分辨率: 4.000
采样增益: 1.0
扫描速度: 0.4747
光阑: 80.00

星期四 10月 29 14:08:54 2020 (GMT+08:00)

标峰:

谱图: YMX-11-12-6-8-3

范围: 4000.00 400.00

(绝对) 阈值: 99.048

灵敏度: 99

峰表:

峰位置:	419.85	强度:	91.589
峰位置:	453.50	强度:	87.820
峰位置:	522.76	强度:	82.009
峰位置:	563.69	强度:	85.413
峰位置:	588.06	强度:	85.353
峰位置:	627.47	强度:	88.267
峰位置:	742.88	强度:	94.593
峰位置:	810.09	强度:	92.055
峰位置:	837.08	强度:	82.668
峰位置:	868.03	强度:	86.752
峰位置:	904.20	强度:	54.157
峰位置:	984.52	强度:	84.050
峰位置:	1031.05	强度:	56.415
峰位置:	1078.13	强度:	46.430
峰位置:	1150.39	强度:	91.709
峰位置:	1216.22	强度:	83.269
峰位置:	1256.64	强度:	85.690
峰位置:	1327.10	强度:	79.070
峰位置:	1349.77	强度:	80.820
峰位置:	1377.84	强度:	59.485
峰位置:	1445.77	强度:	50.201
峰位置:	1648.77	强度:	81.777
峰位置:	1668.23	强度:	95.109
峰位置:	1813.36	强度:	97.836
峰位置:	2728.74	强度:	95.955
峰位置:	2857.11	强度:	50.853
峰位置:	2924.33	强度:	34.298
峰位置:	2966.60	强度:	46.976
峰位置:	3085.11	强度:	93.374
峰位置:	3386.29	强度:	46.275

Figure S70. IR spectrum of compound 7

Rudolph Research Analytical

This sample was measured on an Autopol VI, Serial #91058
Manufactured by Rudolph Research Analytical, Hackettstown, NJ, USA.

Measurement Date : Thursday, 26-NOV-2020

Set Temperature : OFF

Time Delay : Disabled

Delay between Measurement : Disabled

<u>n</u>	<u>Average</u>	<u>Std.Dev.</u>	<u>% RSD</u>	<u>Maximum</u>	<u>Minimum</u>					
5	3.18	0.09	2.83	3.28	3.04					
<u>S.No</u>	<u>Sample ID</u>	<u>Time</u>	<u>Result</u>	<u>Scale</u>	<u>OR °Arc</u>	<u>WLG.nm</u>	<u>Lg.mm</u>	<u>Conc.g/100ml</u>	<u>Temp.</u>	
1	YMX-11-6-8-3	03:24:21 PM	3.20	SR	0.0080	589	100.00	0.250	23.4	
2	YMX-11-6-8-3	03:24:30 PM	3.16	SR	0.0079	589	100.00	0.250	23.4	
3	YMX-11-6-8-3	03:24:38 PM	3.28	SR	0.0082	589	100.00	0.250	23.4	
4	YMX-11-6-8-3	03:24:46 PM	3.20	SR	0.0080	589	100.00	0.250	23.4	
5	YMX-11-6-8-3	03:24:54 PM	3.04	SR	0.0076	589	100.00	0.250	23.4	

Figure S71. $[\alpha]^{25}_D$ of compound 7

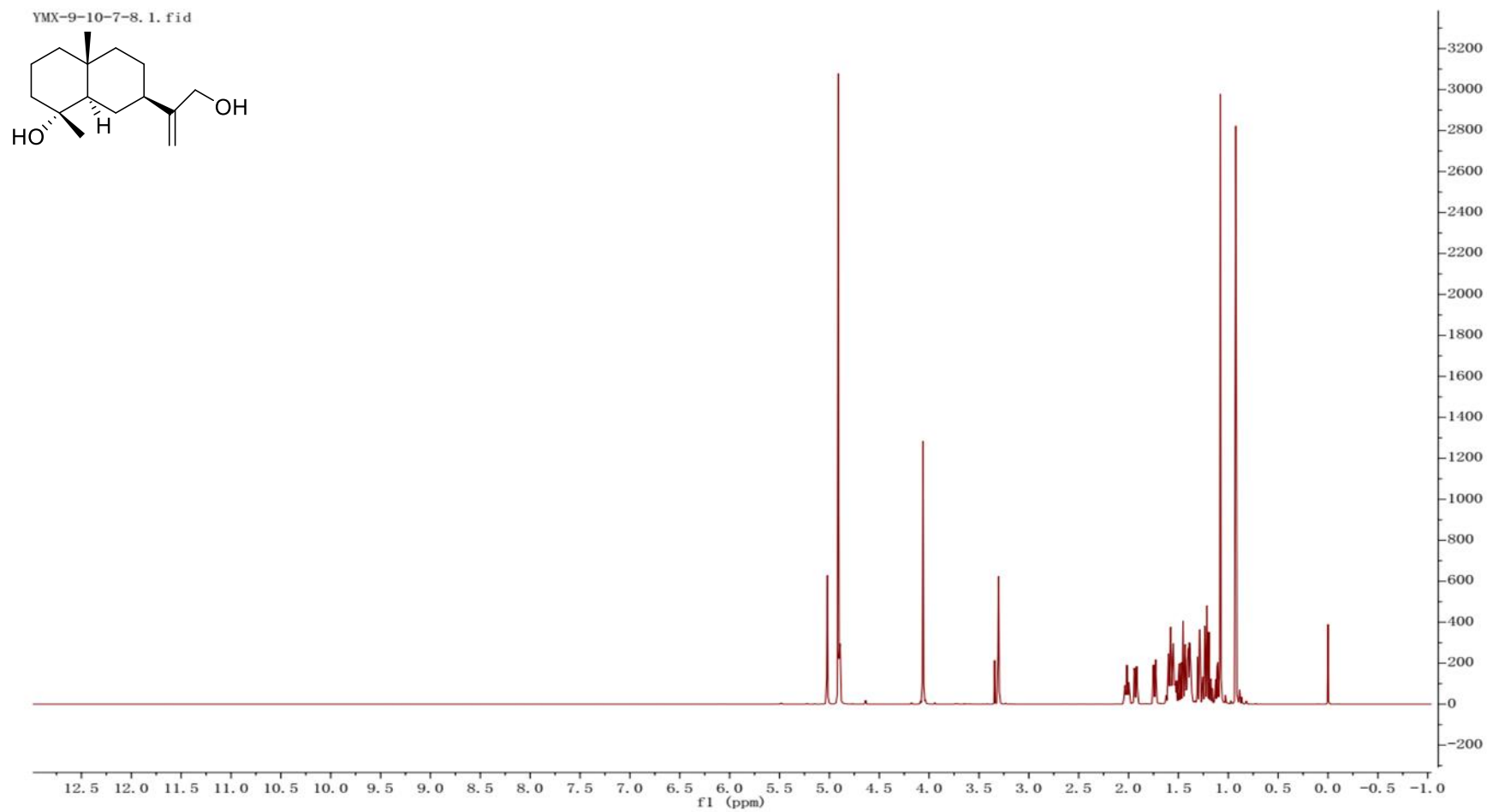


Figure S72. ¹H NMR spectrum of compound **10** (CD₃OD, 600 MHz)

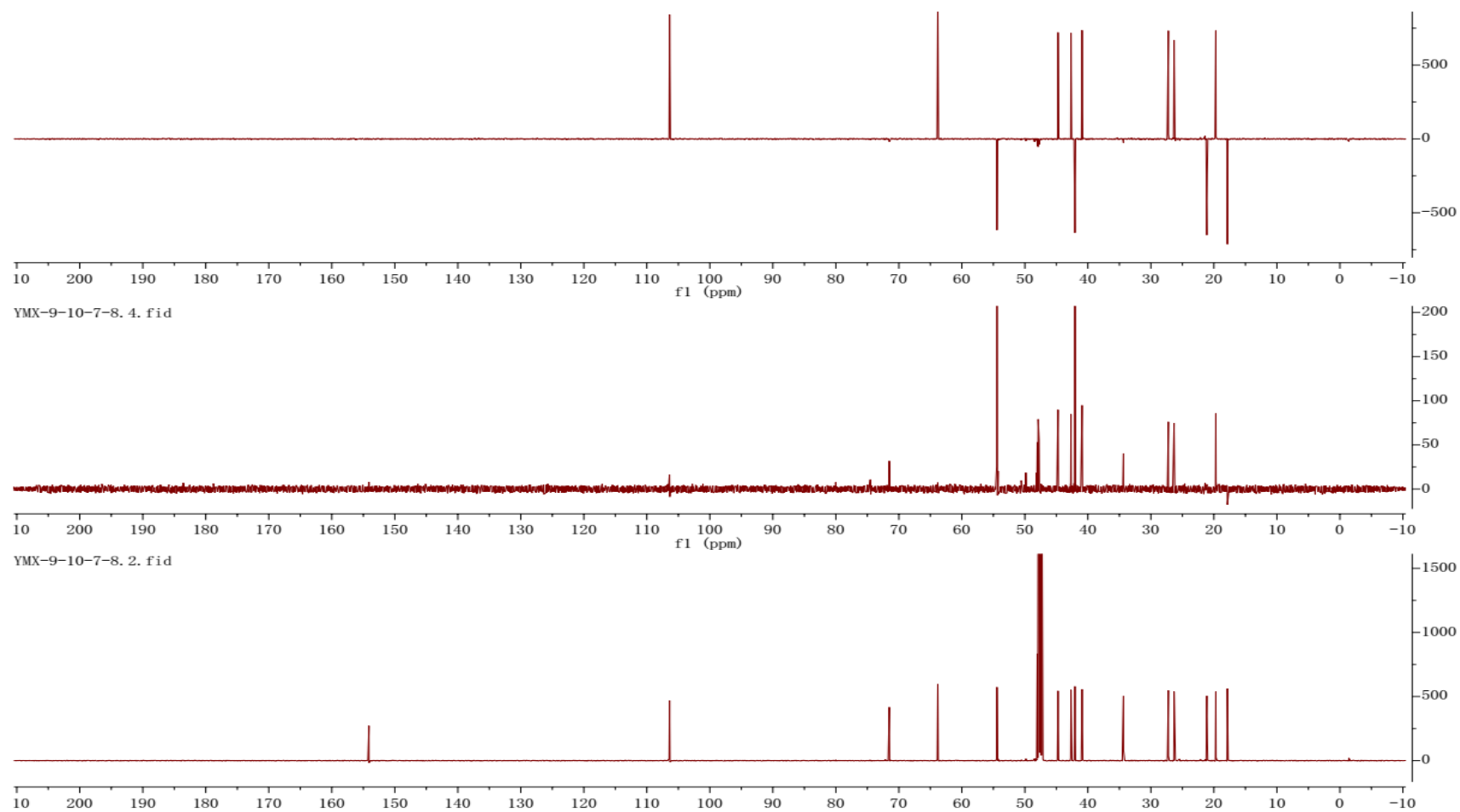


Figure S73. ¹³C NMR and DEPT spectrum of compound **6** (CD₃OD, 150 MHz)

Sample Name	YMX-9-10-7-8	Position	P1-B9	Instrument Name	Instrument 1	User Name	
Inj Vol	1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	YMX-9-10-7-8-.d	ACQ Method	s-.m	Comment		Acquired Time	10/25/2019 2:35:31 PM

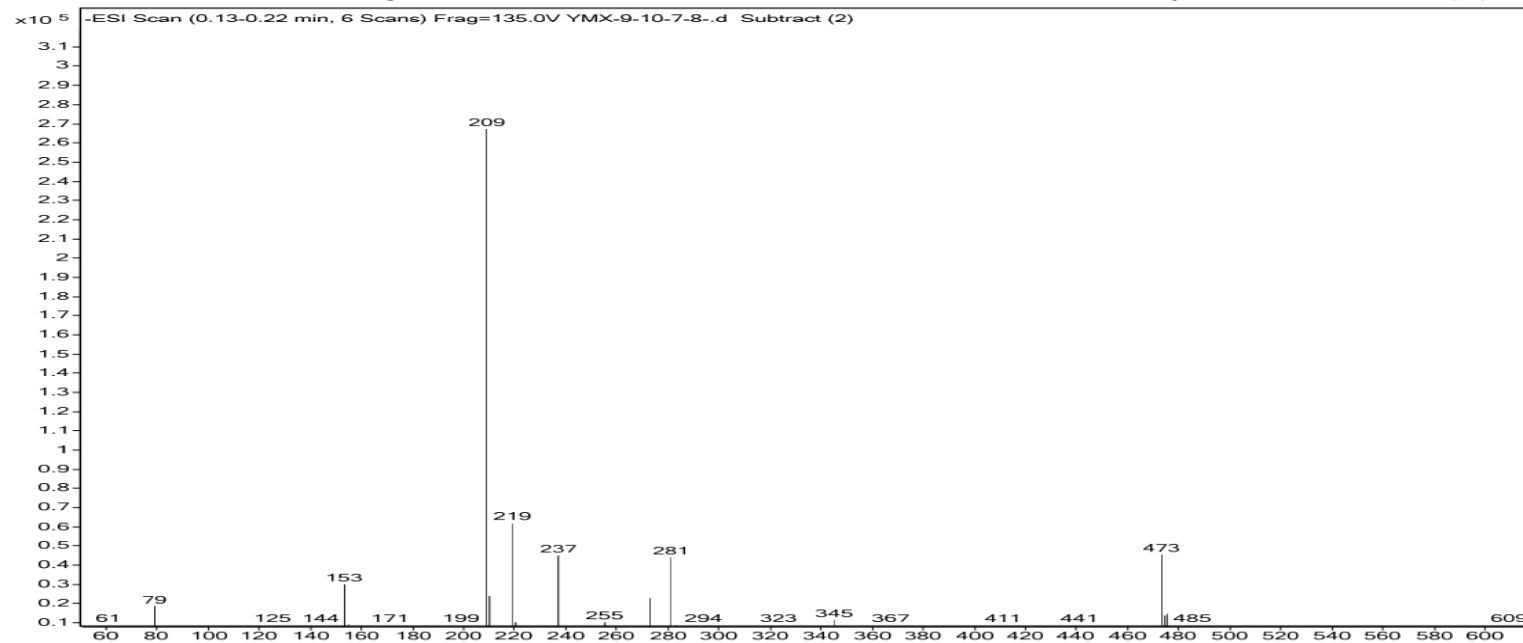
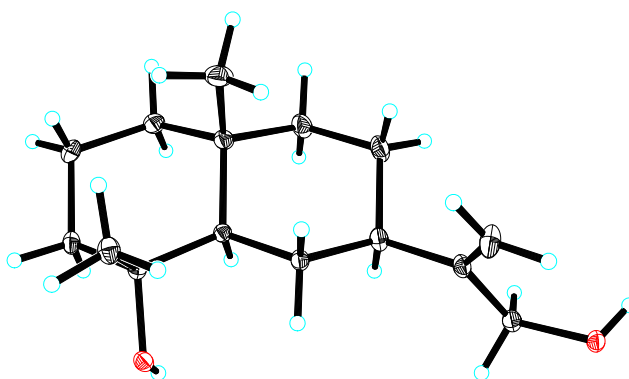


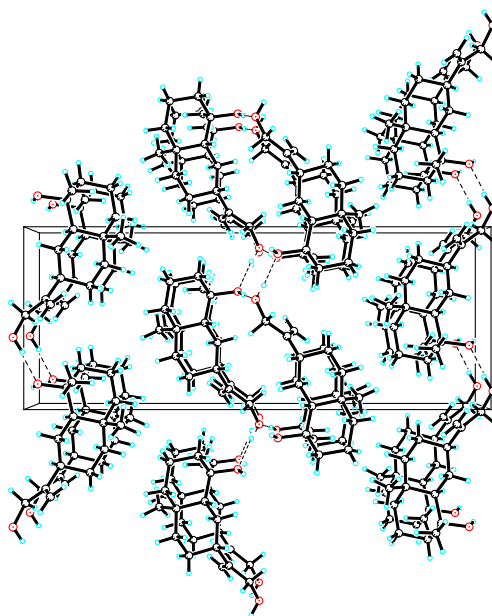
Figure S74. ESI+ spectrum of compound **10**

Crystal data for ymx-9-10-7-8: $C_{15}H_{26}O_2$, $M = 238.36$, $a = 6.36380(10)$ Å, $b = 9.3648(2)$ Å, $c = 23.8658(4)$ Å, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 1422.30(4)$ Å³, $T = 100.(2)$ K, space group $P212121$, $Z = 4$, $\mu(\text{Cu K}\alpha) = 0.555$ mm⁻¹, 11628 reflections measured, 2807 independent reflections ($R_{int} = 0.0377$). The final R_I values were 0.0292 ($I > 2\sigma(I)$). The final $wR(F^2)$ values were 0.0730 ($I > 2\sigma(I)$). The final R_I values were 0.0304 (all data). The final $wR(F^2)$ values were 0.0741 (all data). The goodness of fit on F^2 was 1.059. Flack parameter = -0.01(7).



View of a molecule of ymx-9-10-7-8 with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of ymx-9-10-7-8.

Hydrogen-bonds are shown as dashed lines.

Table 1. Crystal data and structure refinement for ymx-9-10-7-8.

Identification code	global	
Empirical formula	C ₁₅ H ₂₆ O ₂	
Formula weight	238.36	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2 ₁ 2 ₁ 2 ₁	
Unit cell dimensions	a = 6.36380(10) Å	= 90°.
	b = 9.3648(2) Å	= 90°.
	c = 23.8658(4) Å	= 90°.
Volume	1422.30(4) Å ³	
Z	4	
Density (calculated)	1.113 Mg/m ³	
Absorption coefficient	0.555 mm ⁻¹	
F(000)	528	
Crystal size	0.230 x 0.180 x 0.140 mm ³	
Theta range for data collection	3.70 to 72.17°.	
Index ranges	-6<=h<=7, -11<=k<=11, -29<=l<=29	
Reflections collected	11628	

Independent reflections	2807 [R(int) = 0.0377]
Completeness to $\theta = 72.17^\circ$	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.93 and 0.77
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2807 / 0 / 160
Goodness-of-fit on F^2	1.059
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0292, wR2 = 0.0730
R indices (all data)	R1 = 0.0304, wR2 = 0.0741
Absolute structure parameter	-0.01(7)
Largest diff. peak and hole	0.188 and -0.168 e. \AA^{-3}

Figure S75. X-ray crystallographic analysis for compound **10**