

Supporting Information

UPLC-MS-guided isolated single ether linkage dimeric 2-(2-phenylethyl)chromones from *Aquilaria sinensis*

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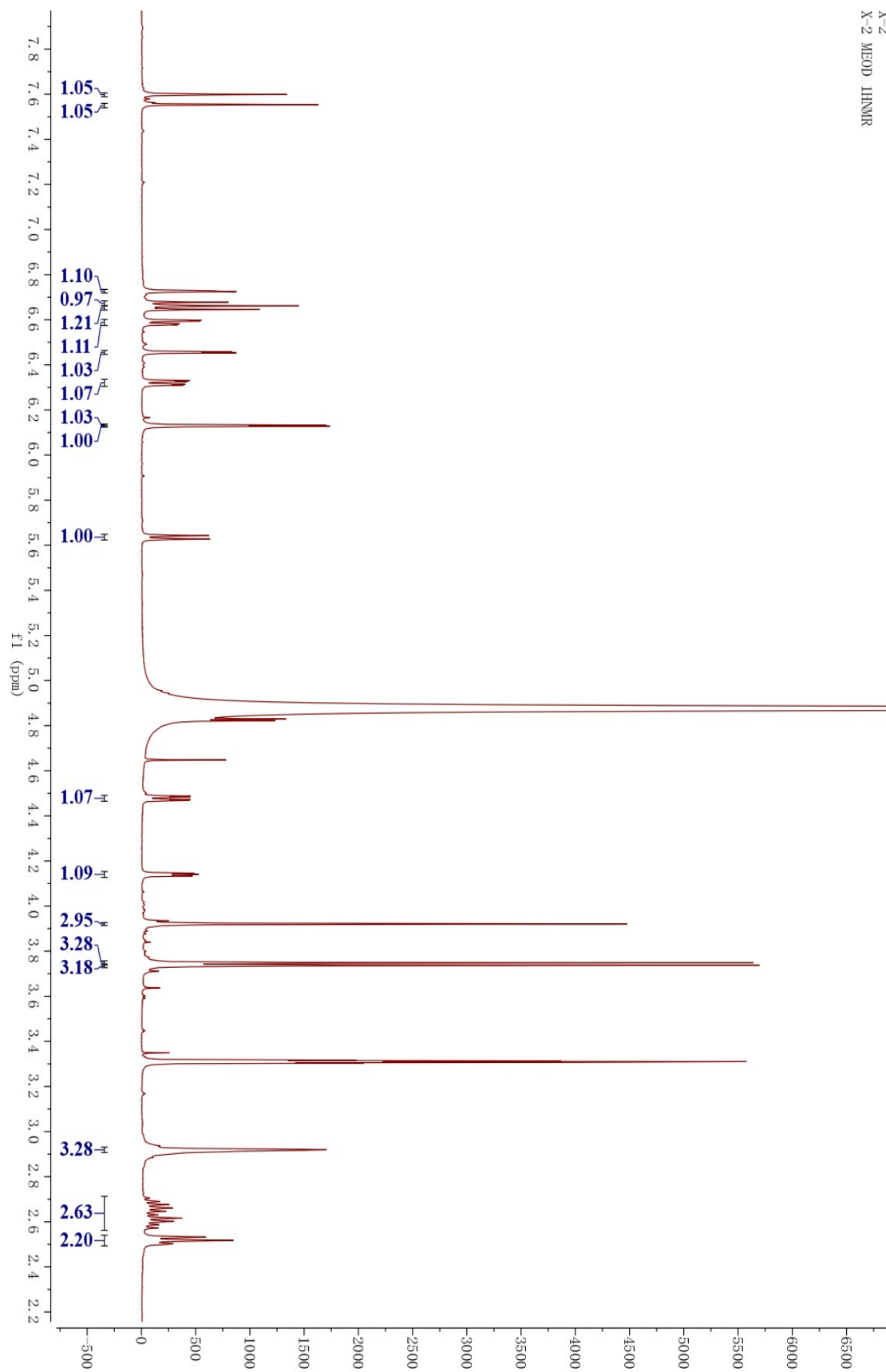


Figure S1. ¹H NMR spectrum (500 MHz) of compound 1 in CD₃OD.

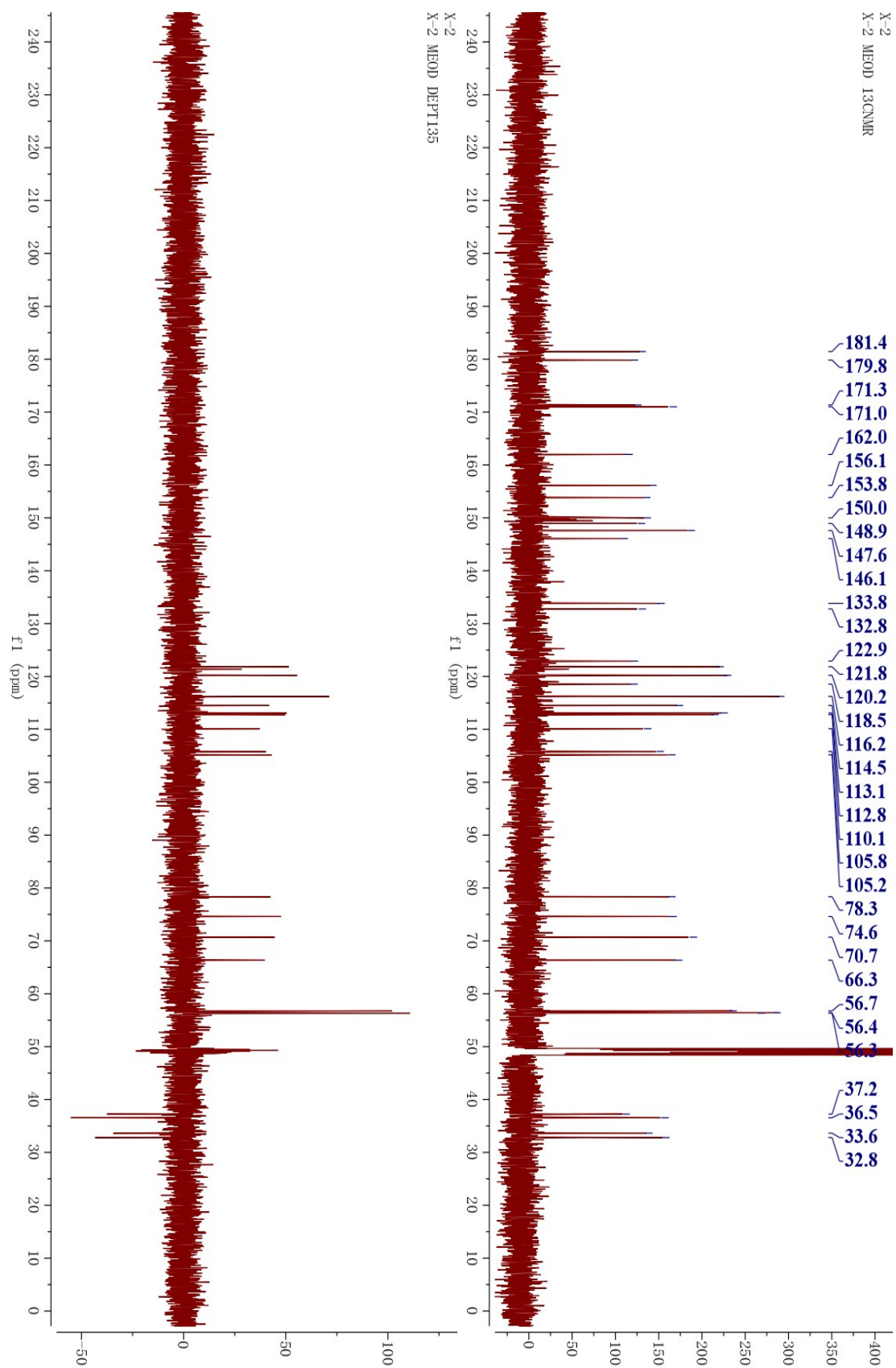


Figure S2. ^{13}C NMR spectrum (125 MHz) of compound **1** in CD_3OD .

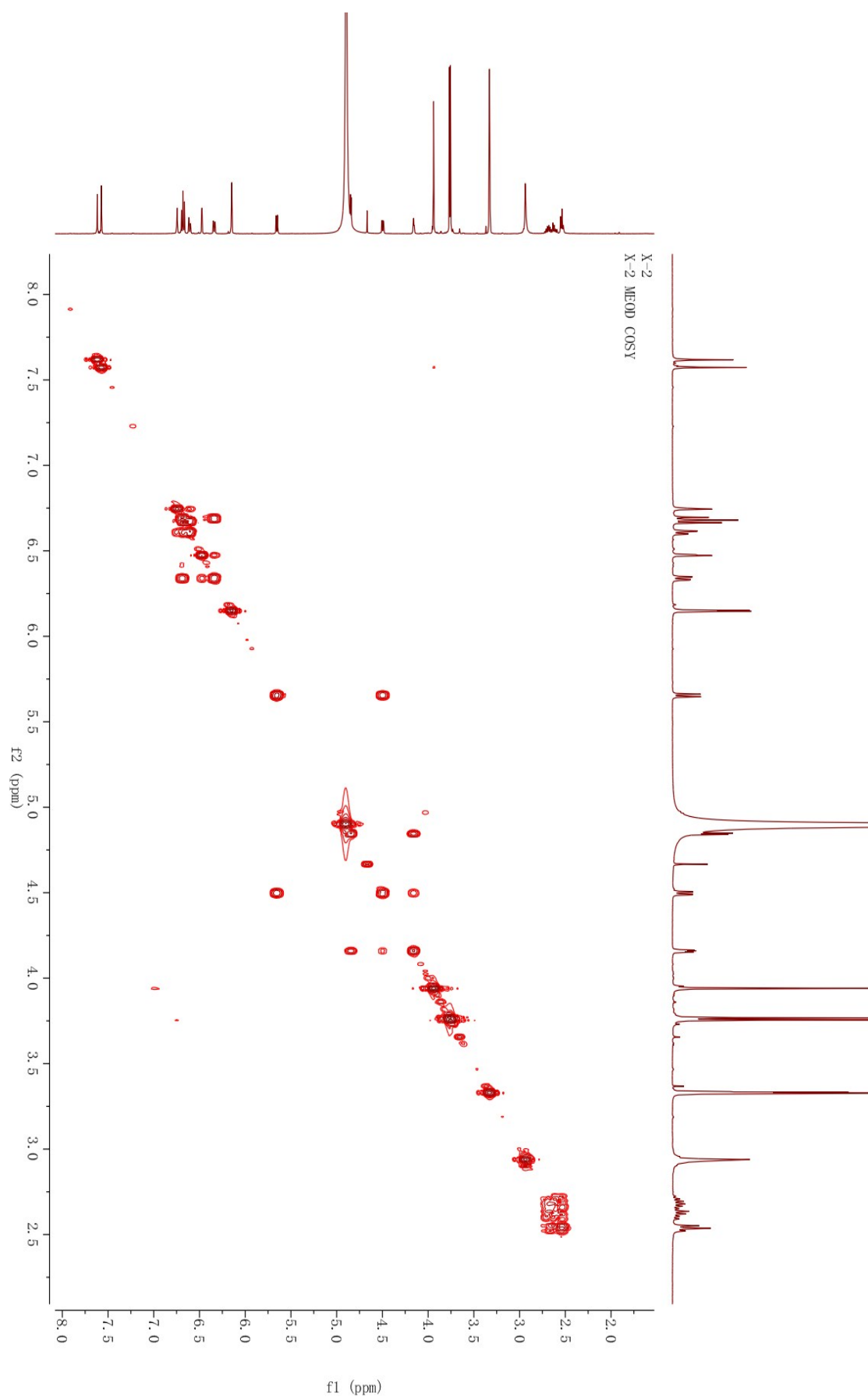


Figure S3. ^1H - ^1H COSY spectrum of compound **1** in CD_3OD .

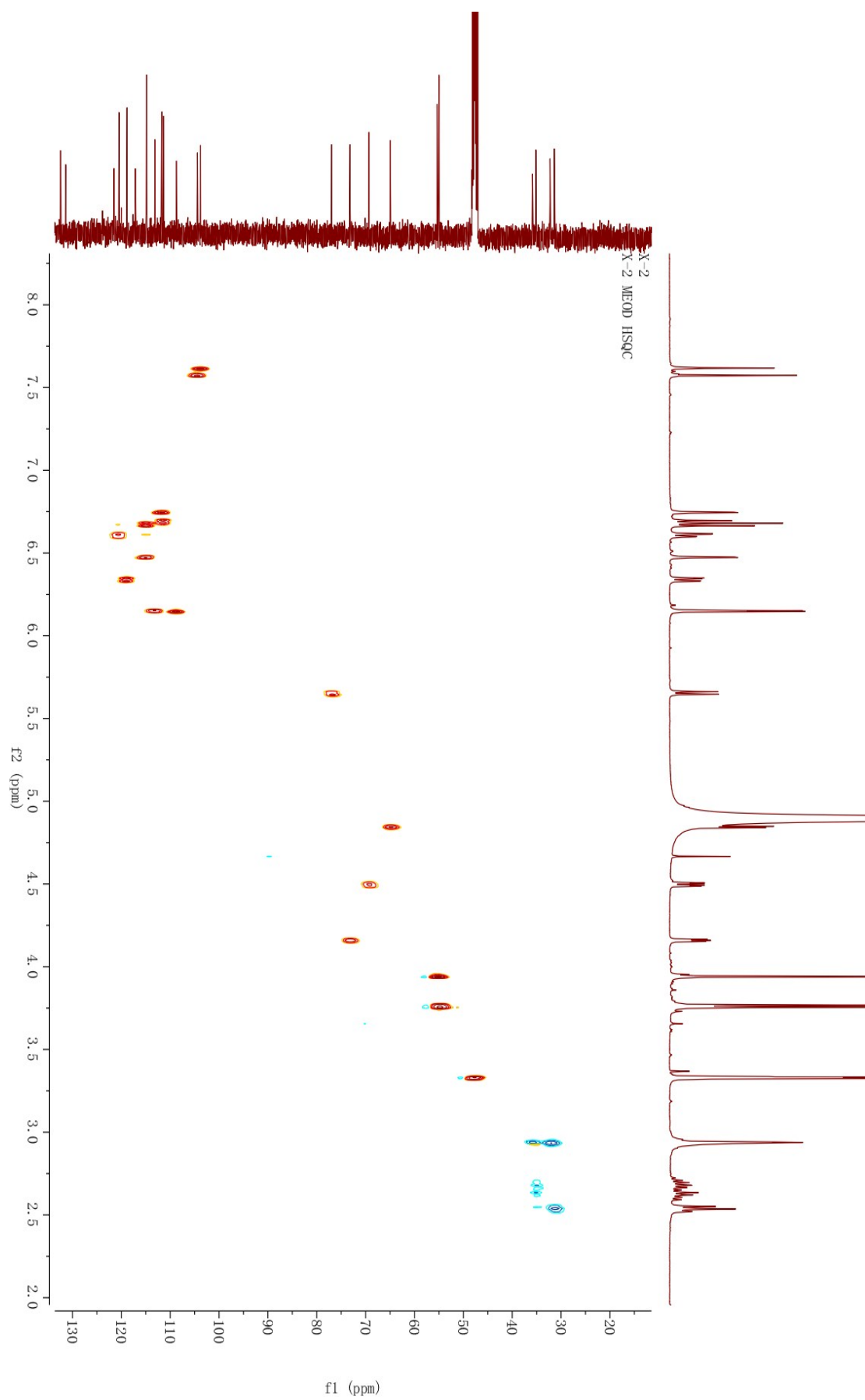


Figure S4. HSQC spectrum of compound **1** in CD₃OD.

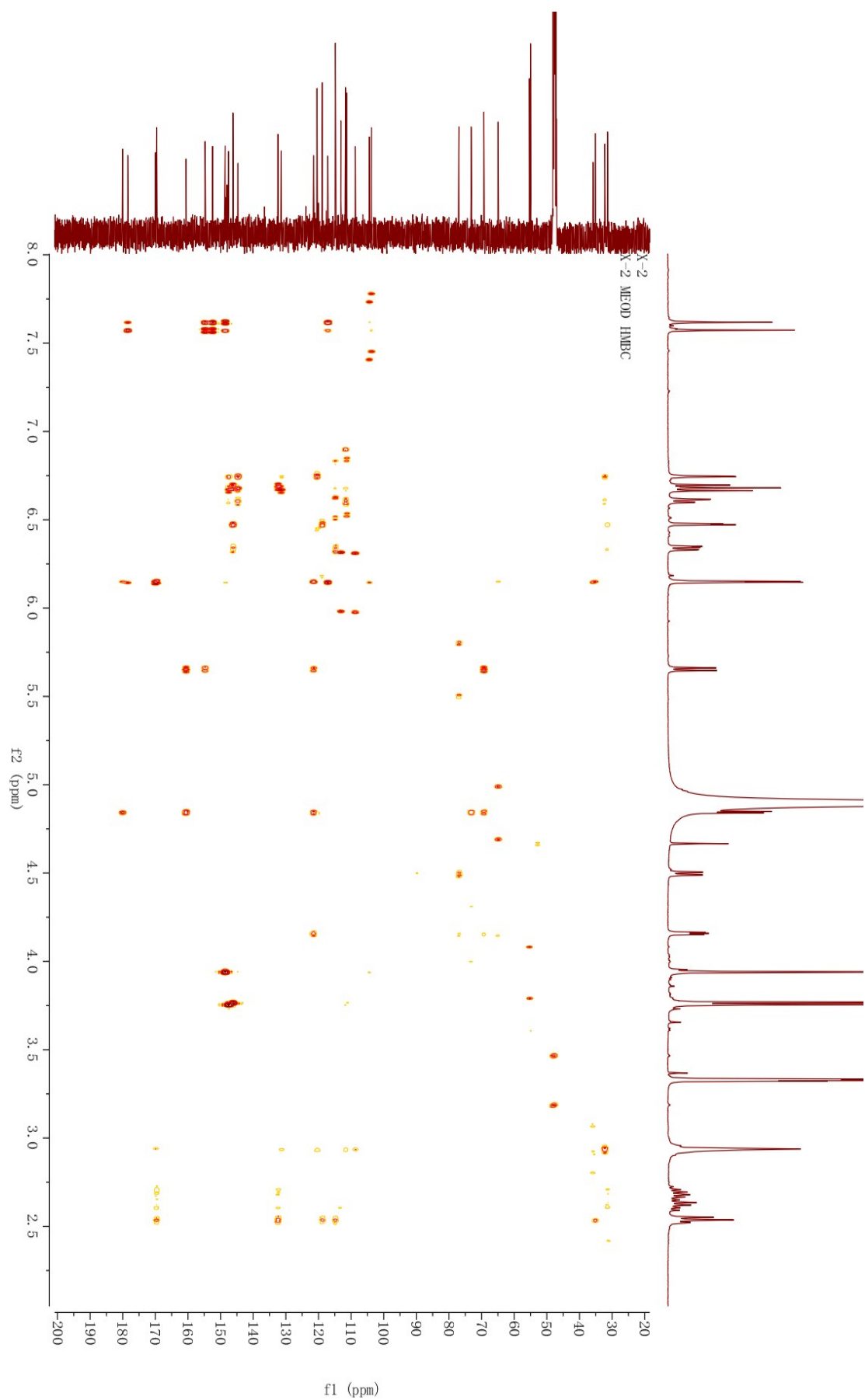


Figure S5. HMBC spectrum of compound **1** in CD₃OD.

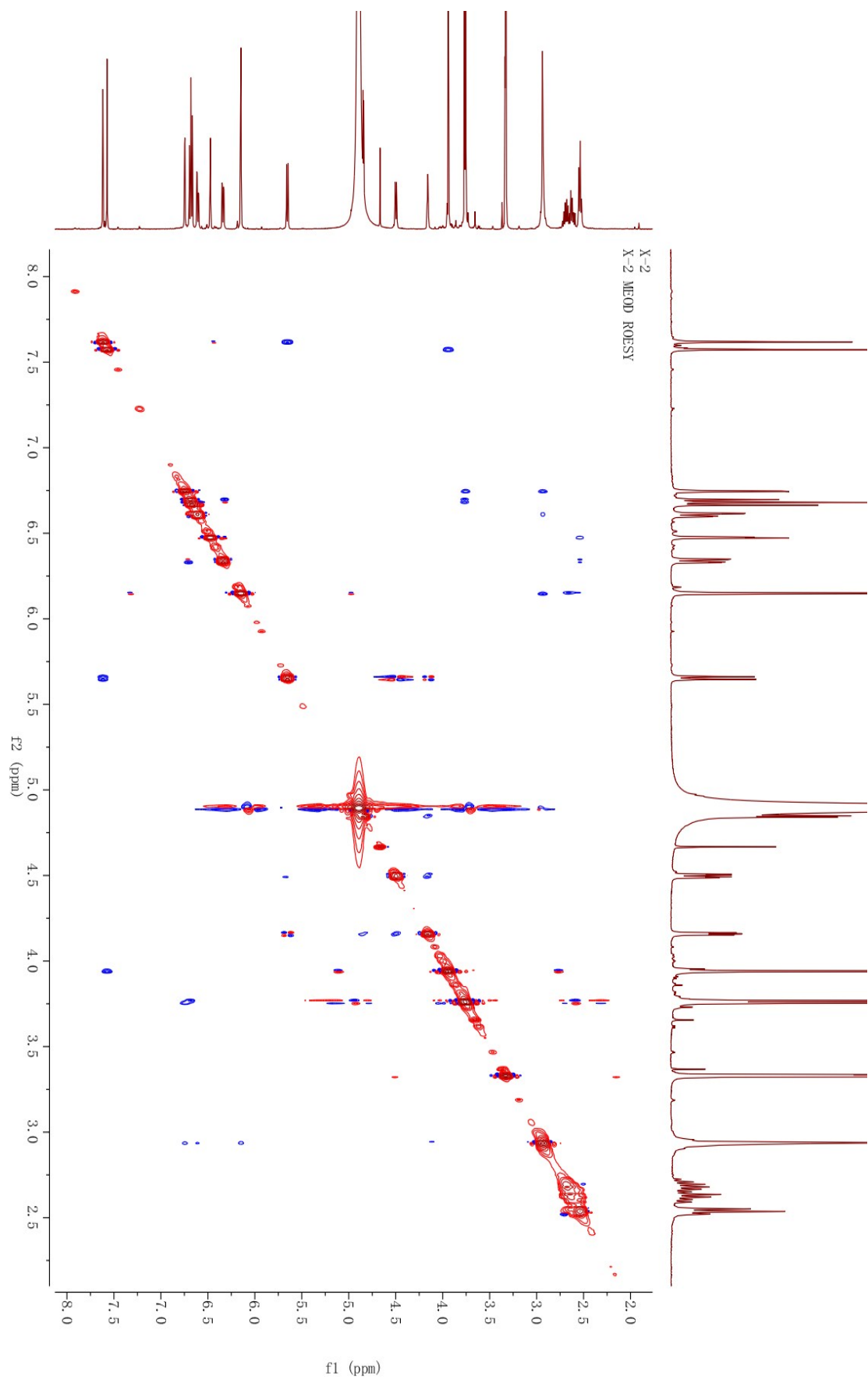


Figure S6. ROESY spectrum of compound **1** in CD₃OD.

Compound Spectrum SmartFormula Report

Analysis Info

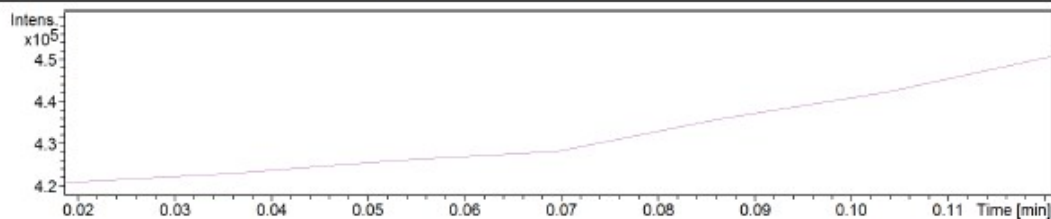
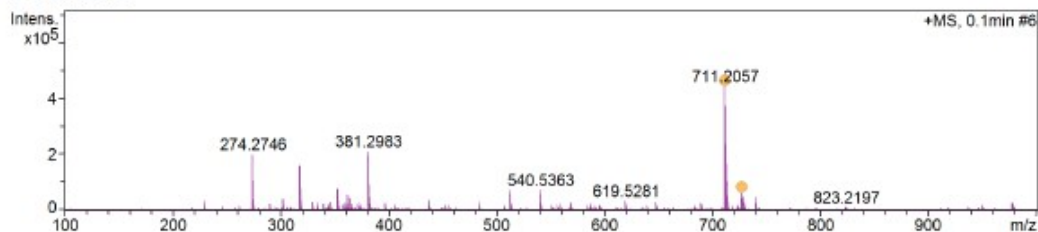
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 Method DirectInfusion - MS - positive.m
 Sample Name kfd-8-25
 Comment

Acquisition Date 2017-12-15 17:27:07

Operator Demo User
 Instrument compact 8255754.20156

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C


+MS, 0.1min #6


#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
1	C37H23N14O3	711.2072	1.5	2.1	244.3	34.0	even	ok
1	C39H28N8NaO5	711.2075	1.8	2.5	242.4	30.0	even	ok
1	C36H32KN8O6	711.2078	1.9	2.7	211.7	25.0	even	ok
1	C39H23N10O6	727.1797	-1.1	-1.6	248.8	34.0	even	ok
1	C38H20N14NaO2	727.1788	-2.2	-3.0	249.0	36.0	even	ok
1	C39H28KN8O5	727.1814	0.6	0.9	202.2	30.0	even	ok
2	C39H35O13	711.2072	1.5	2.1	250.9	23.0	even	ok
2	C38H32N4NaO9	711.2061	0.5	0.6	252.4	25.0	even	ok
2	C35H36KN4O10	711.2063	0.6	0.9	221.3	20.0	even	ok
2	C36H15N20	727.1783	-2.5	-3.4	251.1	40.0	even	ok
2	C38H32KN4O9	727.1801	-0.7	-1.0	211.1	25.0	even	ok
3	C36H27N10O7	711.2059	0.2	0.3	254.2	29.0	even	ok
3	C35H24N14NaO3	711.2048	-0.9	-1.3	255.8	31.0	even	ok
3	C38H27N6O10	727.1783	-2.5	-3.4	255.8	29.0	even	ok
3	C35H24KN14O3	727.1787	-2.1	-2.8	214.3	31.0	even	ok
4	C35H31N6O11	711.2045	-1.2	-1.6	264.1	24.0	even	ok
4	C37H36NaO13	711.2048	-0.9	-1.2	262.4	20.0	even	ok
4	C37H36KO13	727.1787	-2.0	-2.8	220.1	20.0	even	ok

+MS, 0.1min #5

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by: demo

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Figure S7. HRESIMS spectrum of compound 1.

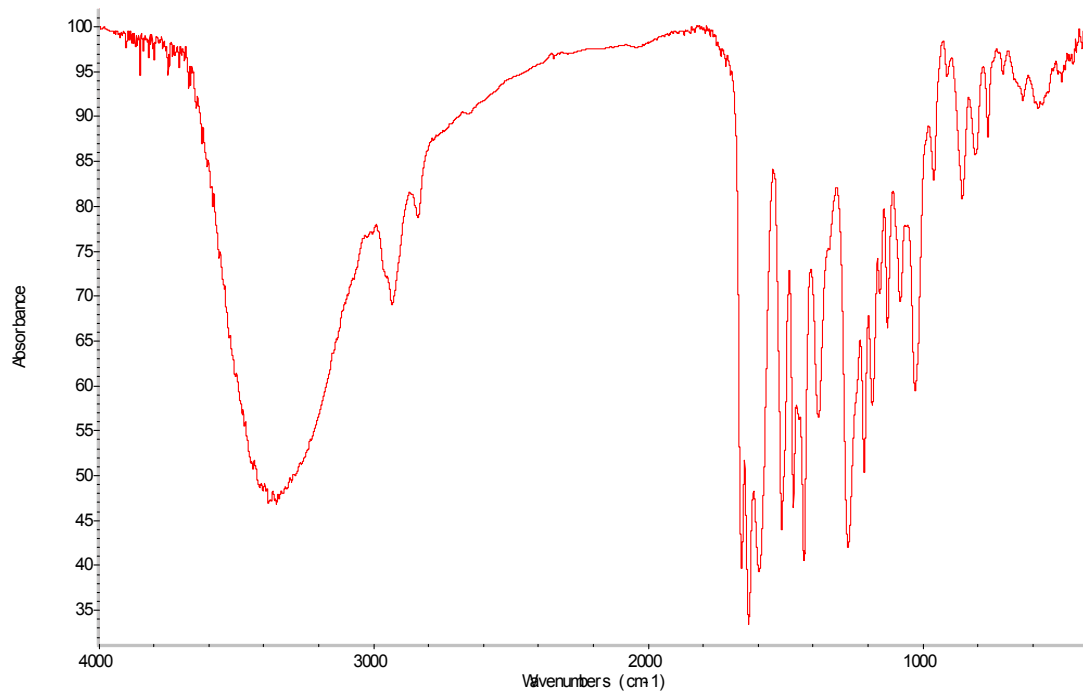


Figure S8. IR spectrum of compound 1.

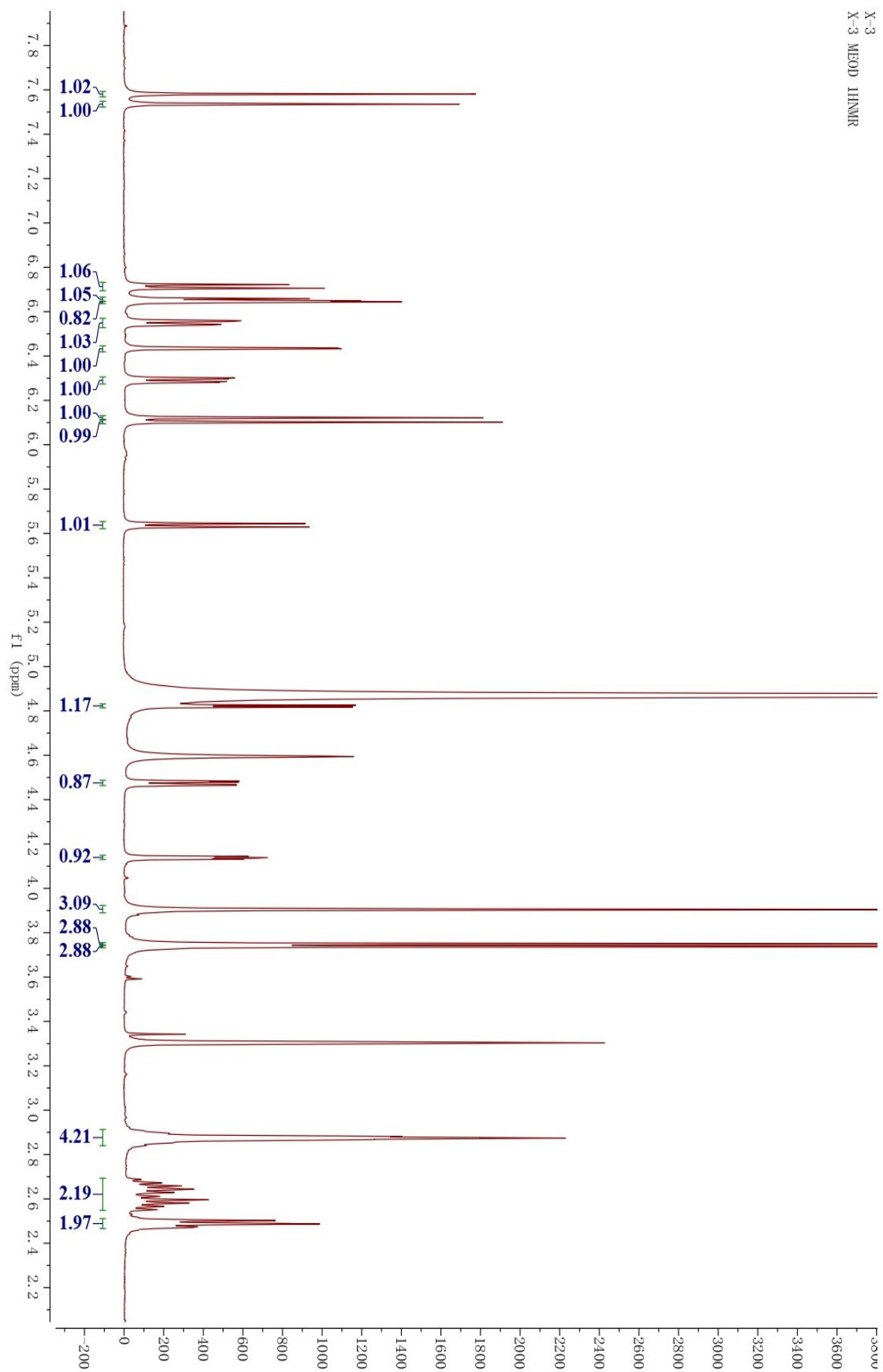


Figure S9. ¹H NMR spectrum (500 MHz) of compound **2** in CD₃OD.

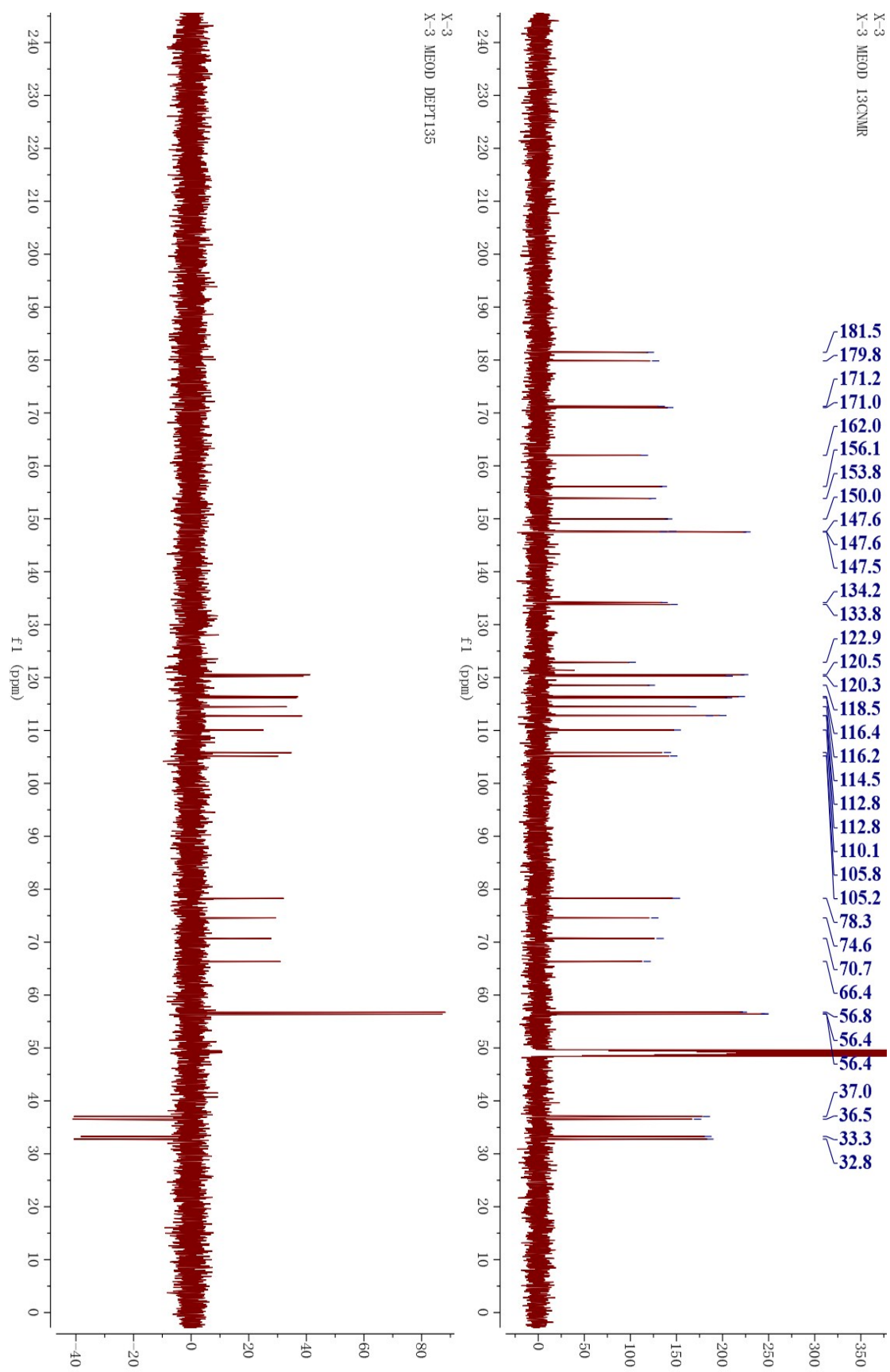


Figure S10. ^{13}C NMR spectrum (125 MHz) of compound **2** in CD_3OD .

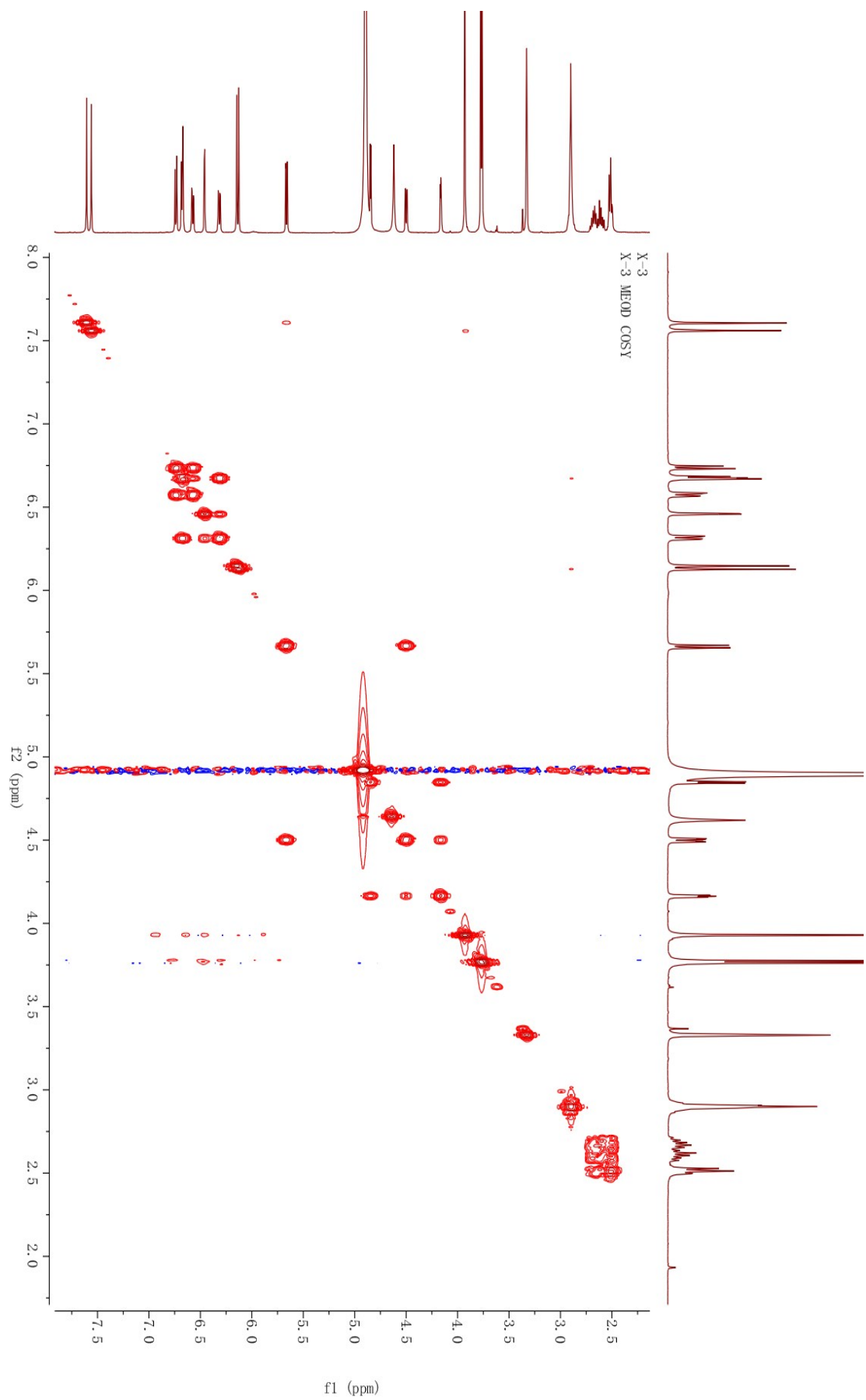


Figure S11. ^1H - ^1H COSY spectrum of compound **2** in CD_3OD .

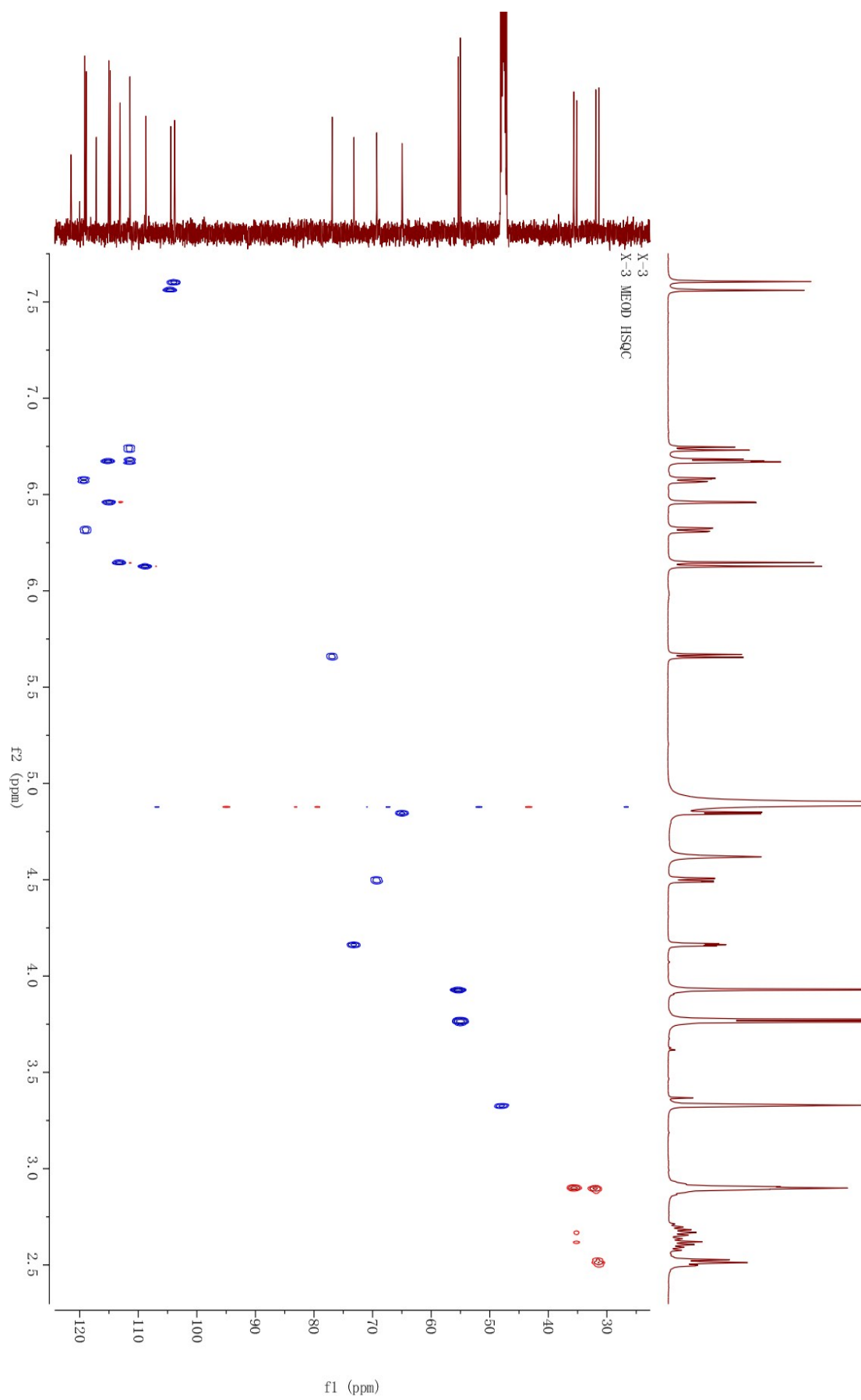


Figure S12. HSQC spectrum of compound **2** in CD₃OD.

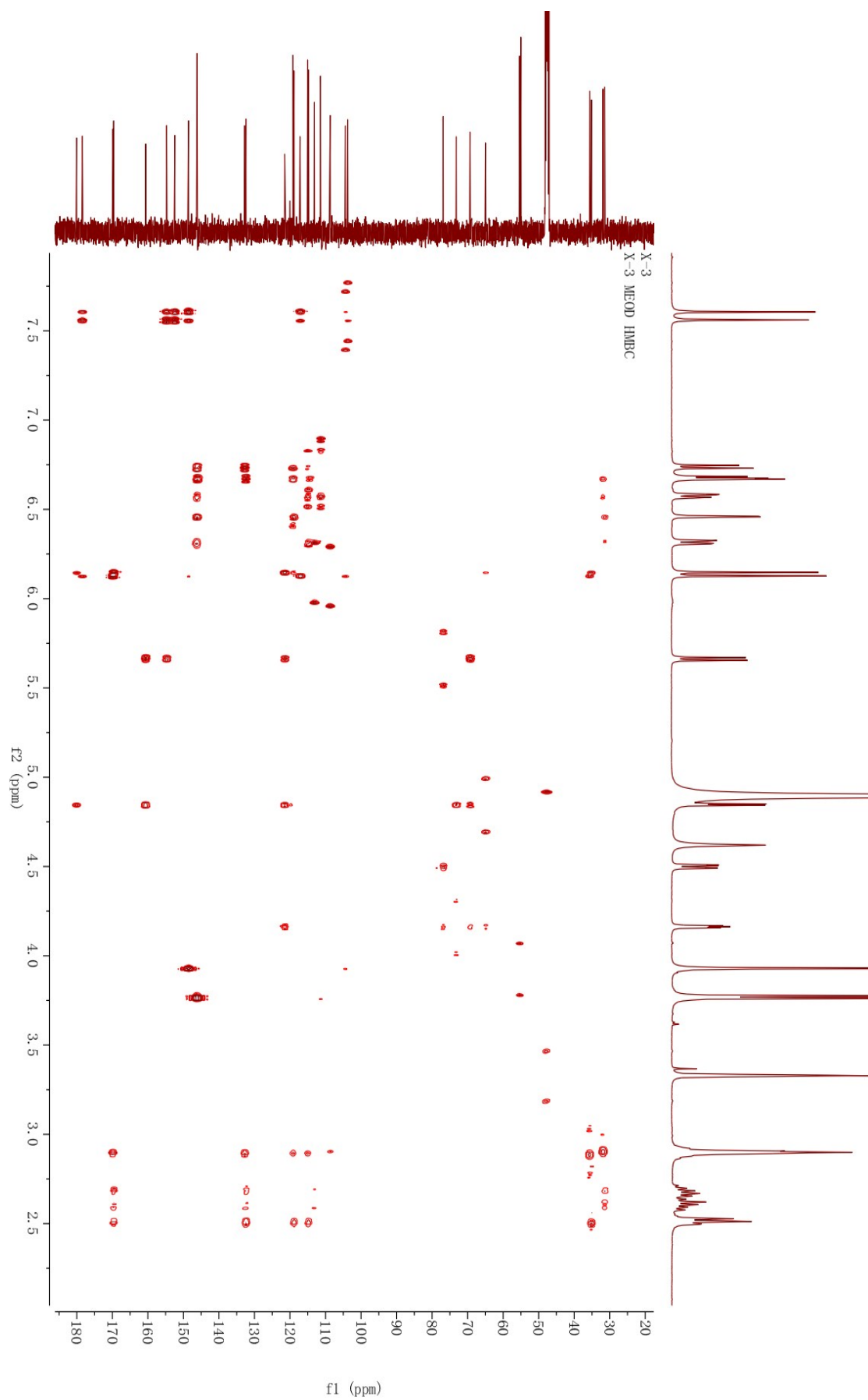


Figure S13. HMBC spectrum of compound **2** in CD₃OD.

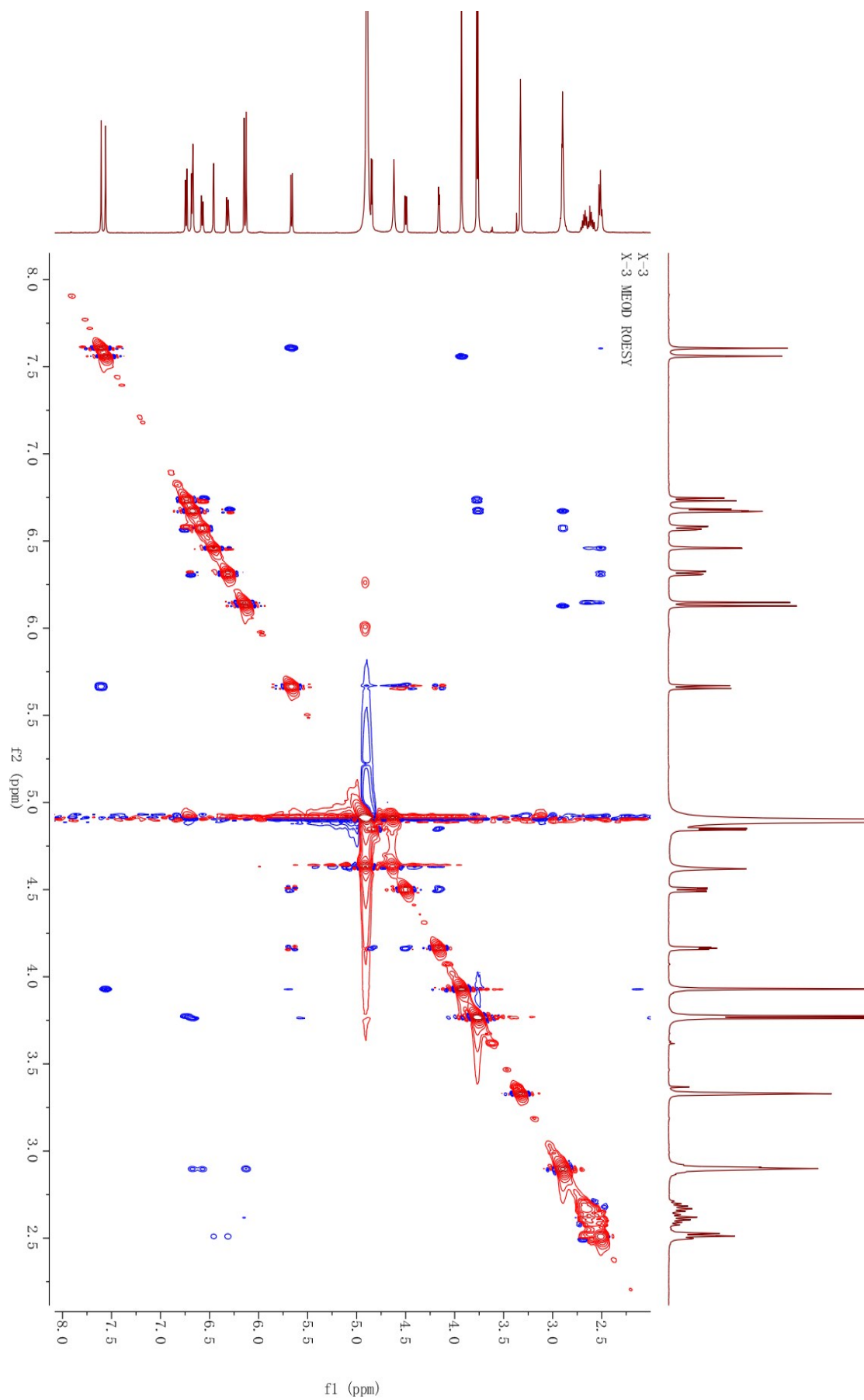


Figure S14. ROESY spectrum of compound **2** in CD₃OD.

Compound Spectrum SmartFormula Report

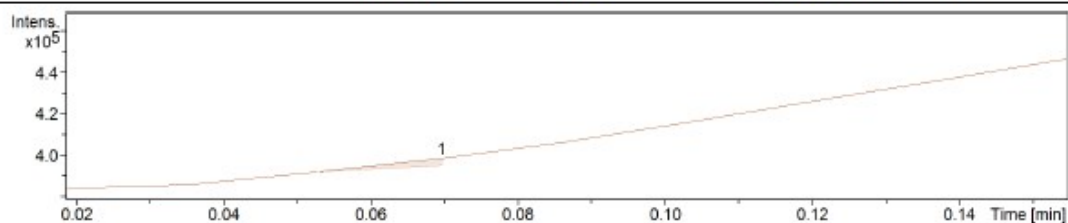
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 Sample Name kfd-8-25
 Comment

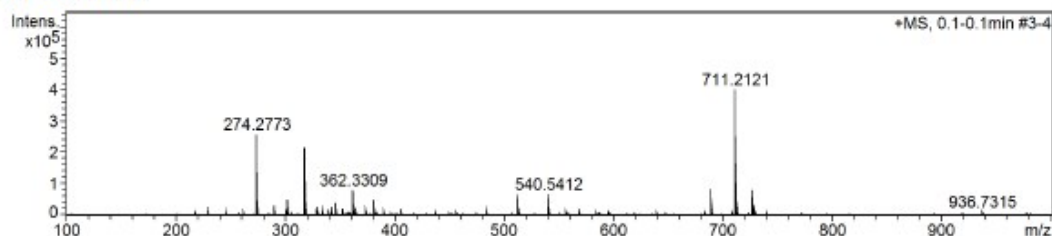
Acquisition Date 2017-12-15 17:59:24
 Operator Demo User
 Instrument compact 8255754.20158

Acquisition Parameter

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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
1	0.1	3404.9	Manual	398690	1.3	BPC +All MS	711.2121	0.0

Cmpd 1, 0.1 min


#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
1	C35H70NaO	529.5319	1.0	1.8	46.9	1.0	even	ok
1	C37H33N8O8	689.2354	4.9	7.1	5.3	25.0	even	ok
1	C36H30N10NaO4	689.2344	3.8	5.5	8.6	27.0	even	ok
1	C38H38KN2O8	689.2260	-4.6	-6.6	32.4	21.0	even	ok
1	C37H36NaO13	711.2048	-7.2	-10.2	4.9	20.0	even	ok
1	C38H72N4NaO14	831.4937	-0.0	-0.0	118.9	5.0	even	ok
1	C36H31N4O13	727.1882	1.2	1.6	32.5	24.0	even	ok
1	C39H75O18	831.4948	1.1	1.3	115.4	3.0	even	ok
1	C39H32N2NaO11	727.1898	2.8	3.8	33.7	25.0	even	ok
1	C36H36KN2O12	727.1900	2.9	4.0	4.8	20.0	even	ok
1	C36H72KN8O11	831.4952	1.5	1.8	81.3	5.0	even	ok
2	C36H37N2O12	689.2341	3.5	5.1	7.7	20.0	even	ok
2	C39H34KN8O4	689.2273	-3.2	-4.7	35.7	26.0	even	ok
2	C37H32N8NaO8	711.2174	5.3	7.5	5.1	25.0	even	ok
2	C37H32KN8O8	727.1913	4.3	5.9	12.4	25.0	even	ok
2	C39H68N8NaO10	831.4951	1.3	1.6	119.2	10.0	even	ok
2	C37H27N8O9	727.1896	2.5	3.4	35.5	29.0	even	ok
2	C36H24N12NaO5	727.1885	1.4	2.0	39.6	31.0	even	ok
2	C36H67N10O12	831.4934	-0.3	-0.3	121.0	9.0	even	ok

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Figure S15. HRESIMS spectrum of compound 2.

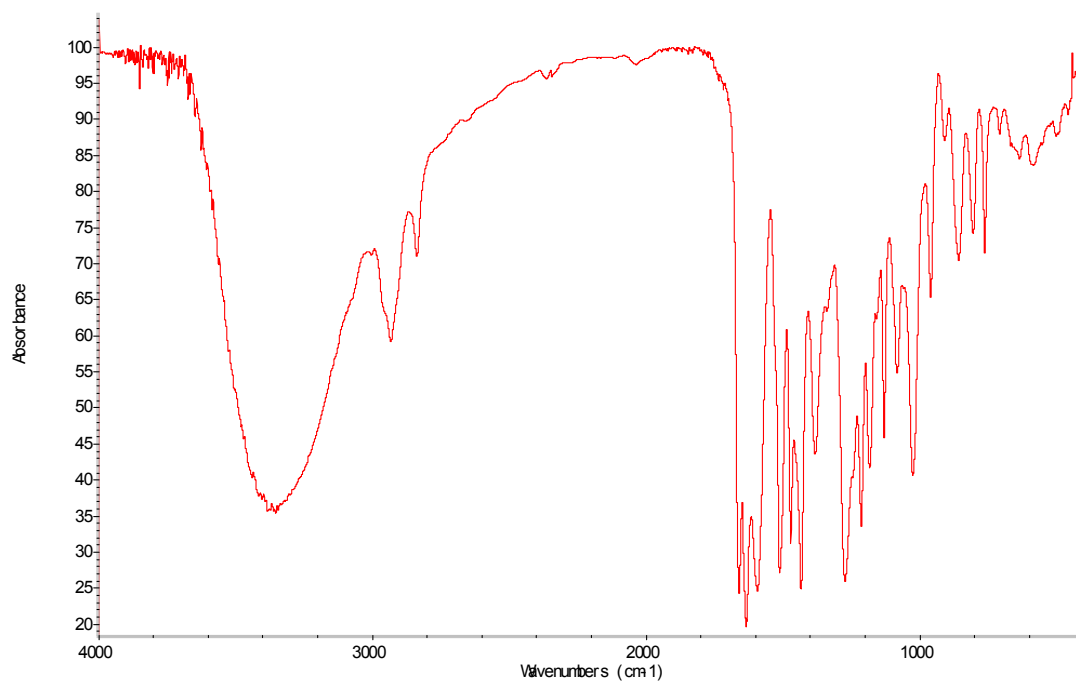


Figure S16. IR spectrum of compound 2.

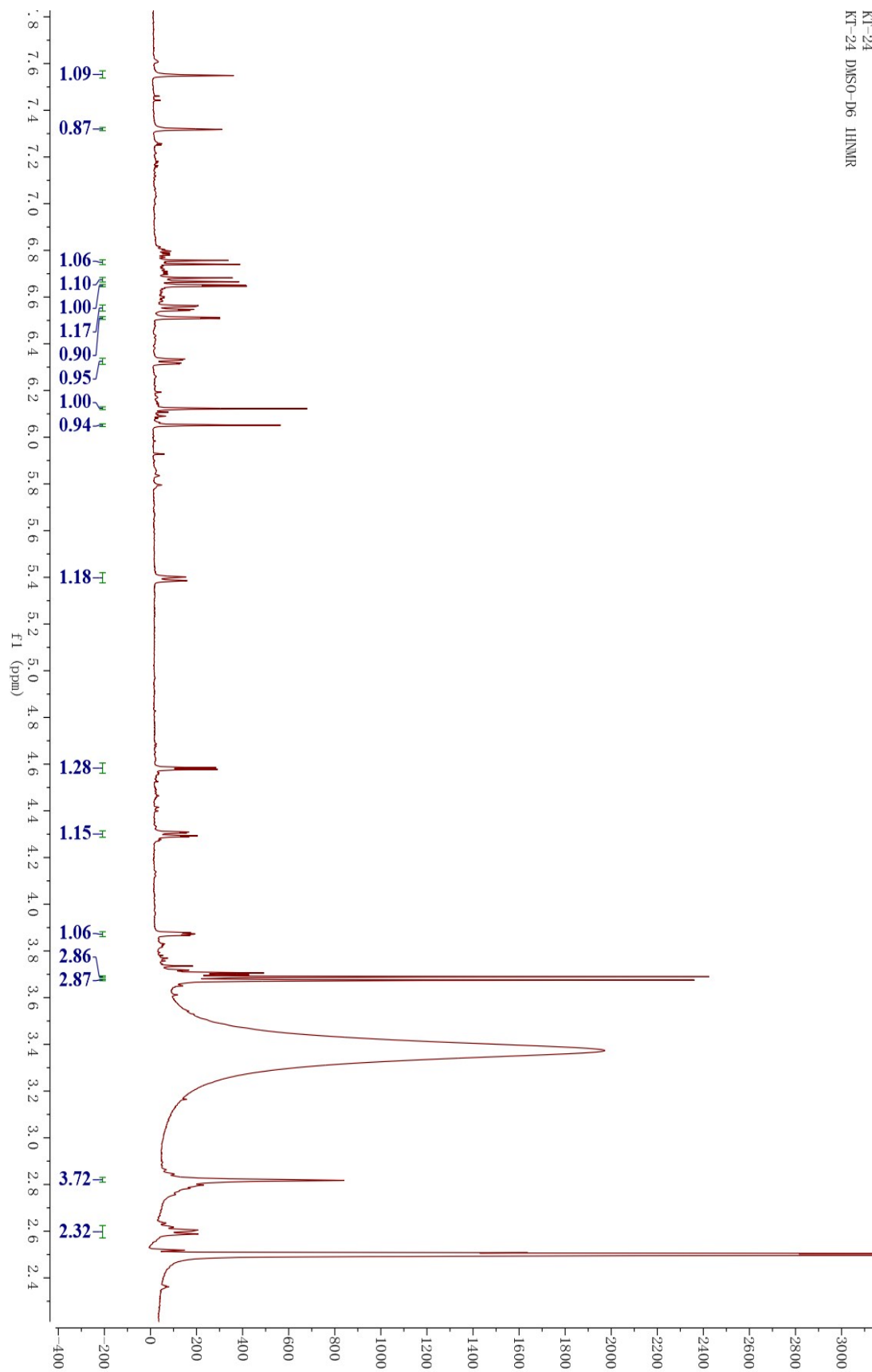


Figure S17. ¹H NMR spectrum (500 MHz) of compound **3** in DMSO-*d*₆.

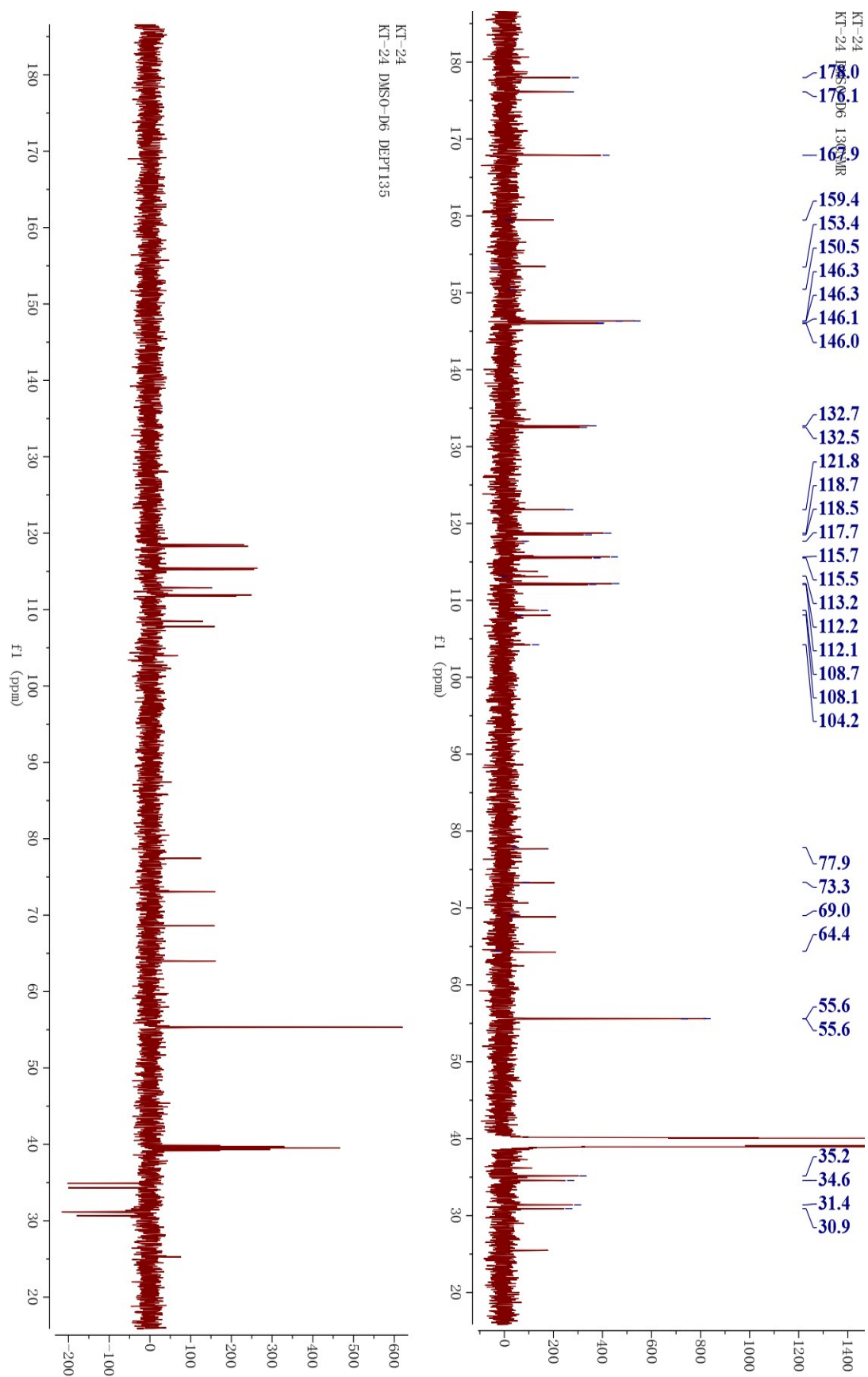


Figure S18. ^{13}C NMR spectrum (125 MHz) of compound **3** in $\text{DMSO-}d_6$.

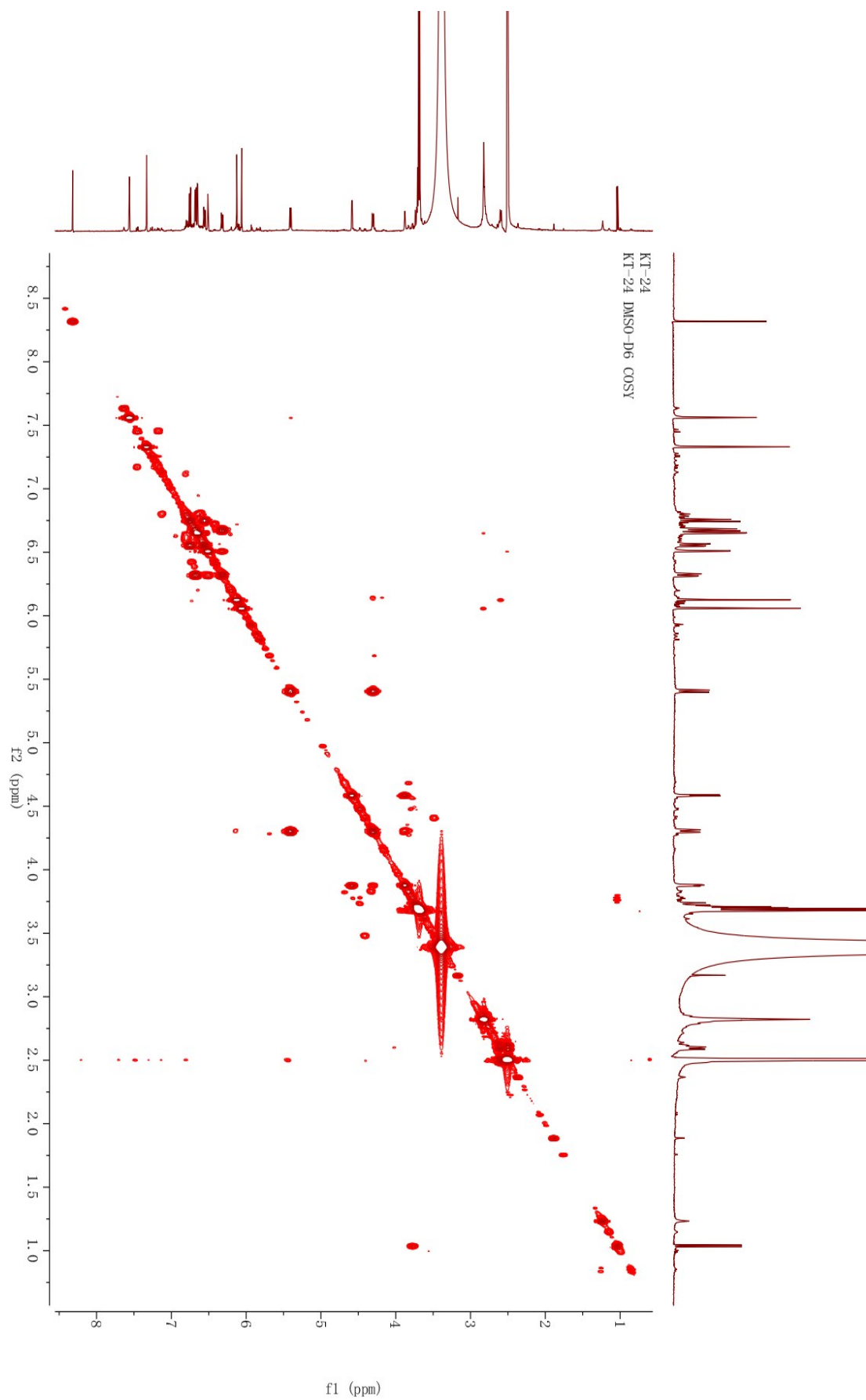


Figure S19. ^1H - ^1H COSY spectrum of compound **3** in $\text{DMSO-}d_6$.

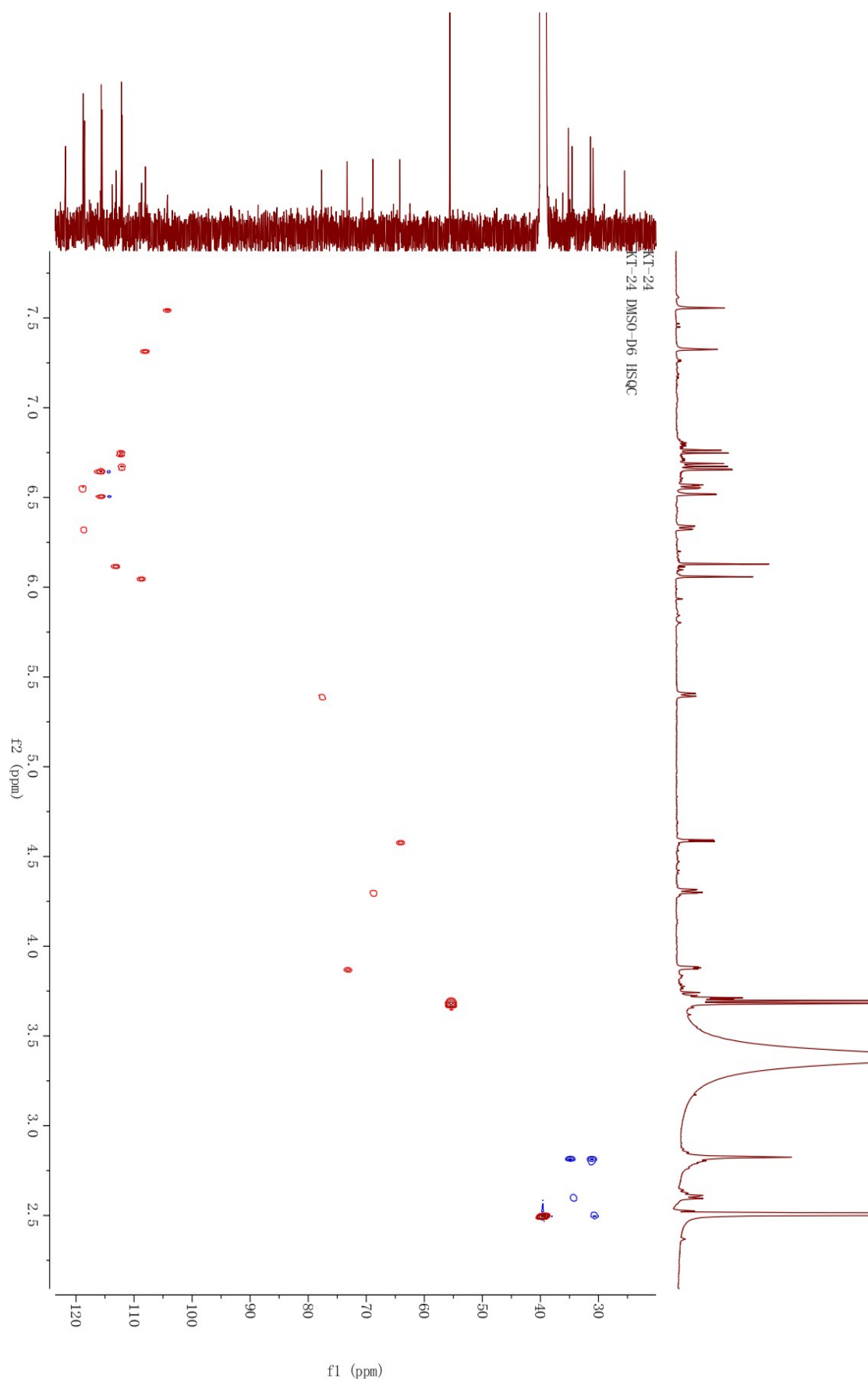


Figure S20. HSQC spectrum of compound **3** in DMSO- d_6 .

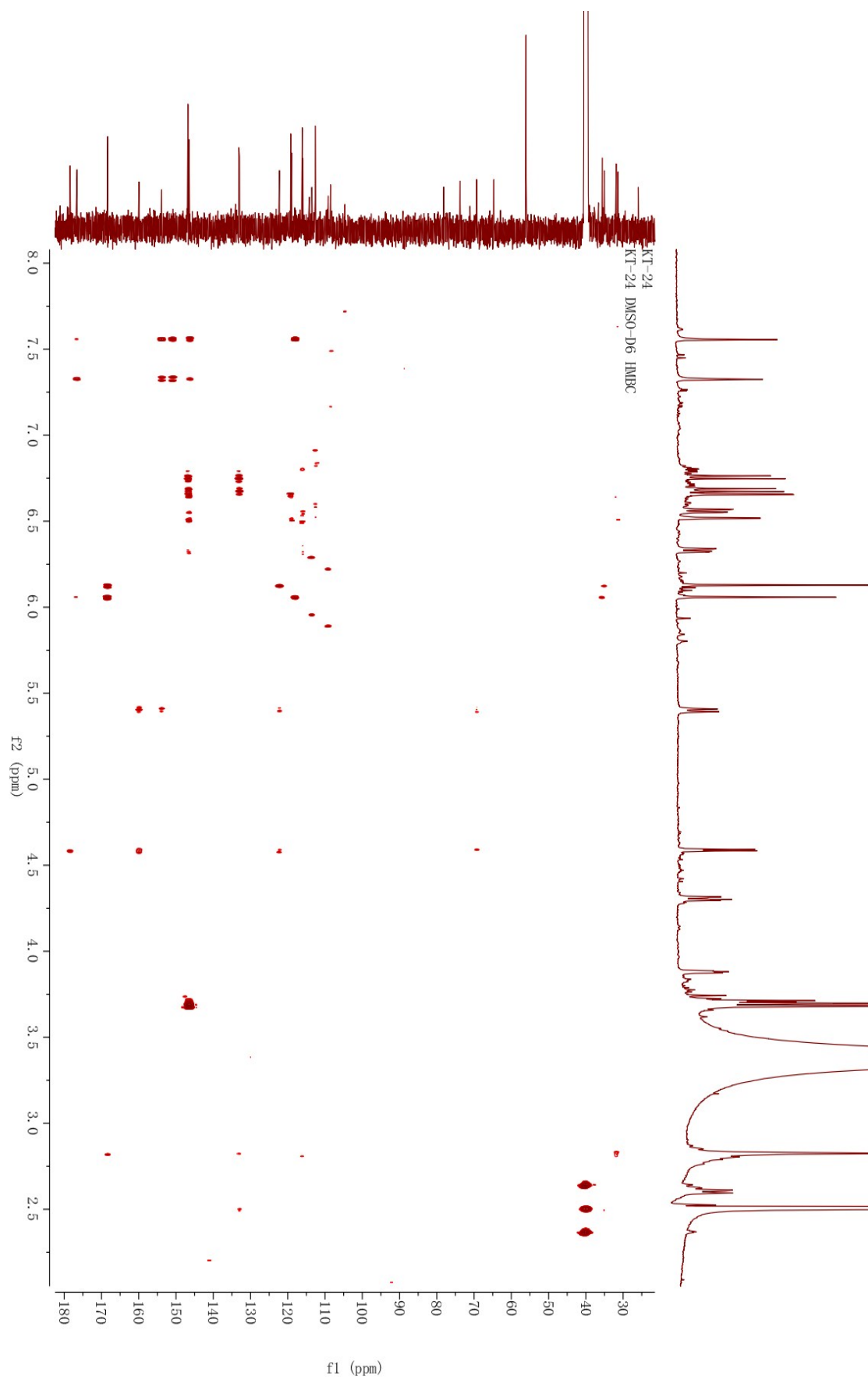


Figure S21. HMBC spectrum of compound **3** in DMSO-*d*₆.

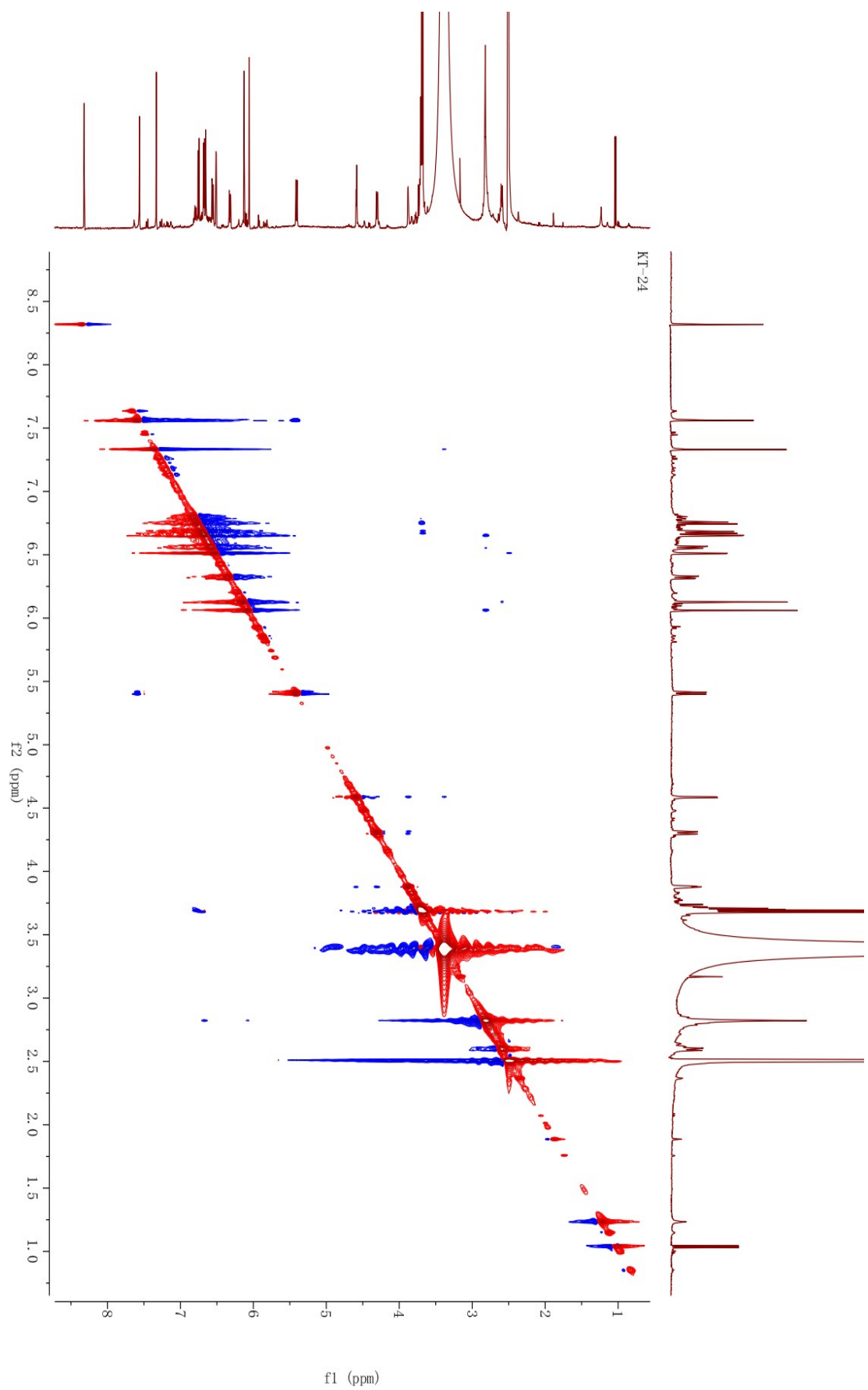
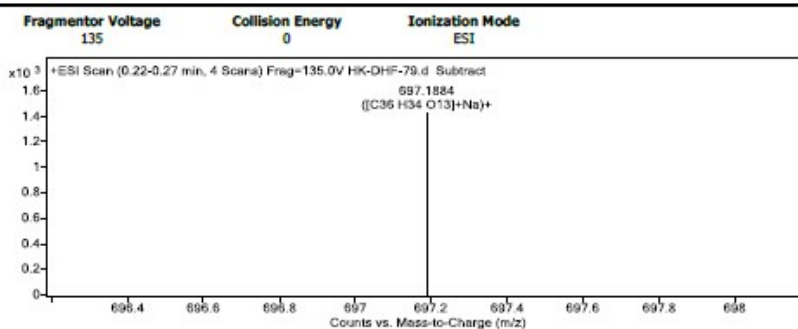


Figure S22. ROESY spectrum of compound **3** in DMSO-*d*₆.

Qualitative Analysis Report

Data Filename	HK-DHF-79.d	Sample Name	HK-DHF-79
Sample Type	Sample	Position	P1-D7
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IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund
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96.0432	2	5143.66
104.0324	2	14708.21
107.0405	1	65952.41
138.0683	2	6437.37
146.0583	2	11968.7
274.274	1	6651.35
318.2998	1	4804.76

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
C36 H34 O13	674.1999	697.1892	697.1884	0.80	1.15	20.0000

--- End Of Report ---

Figure S23. HRESIMS spectrum of compound 3.

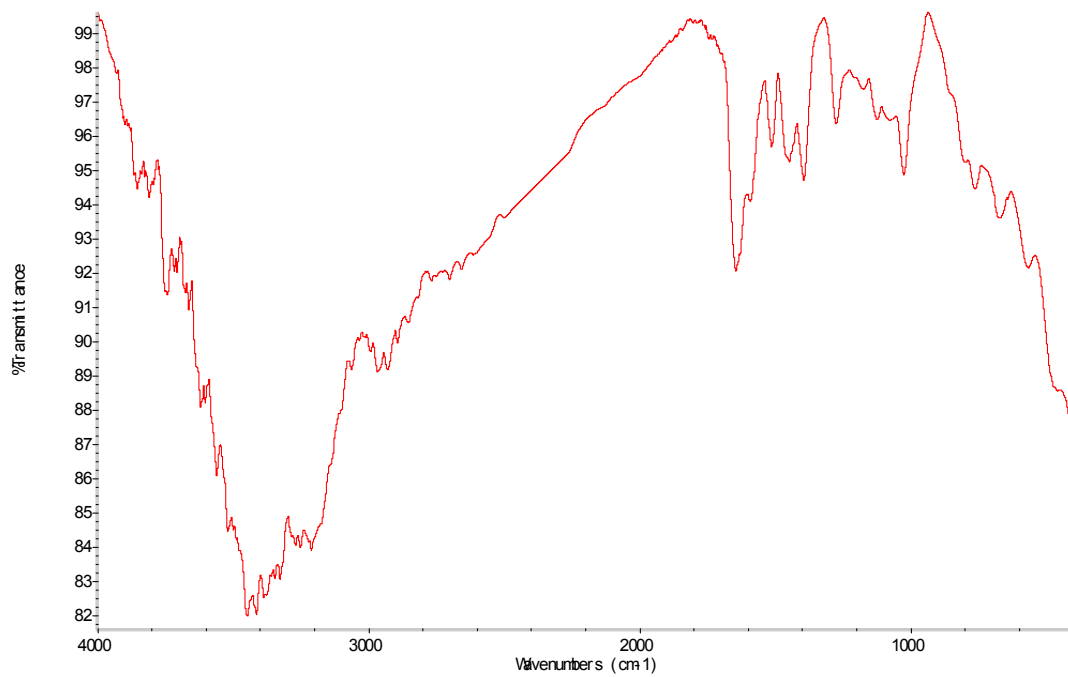


Figure S24. IR spectrum of compound **3**.

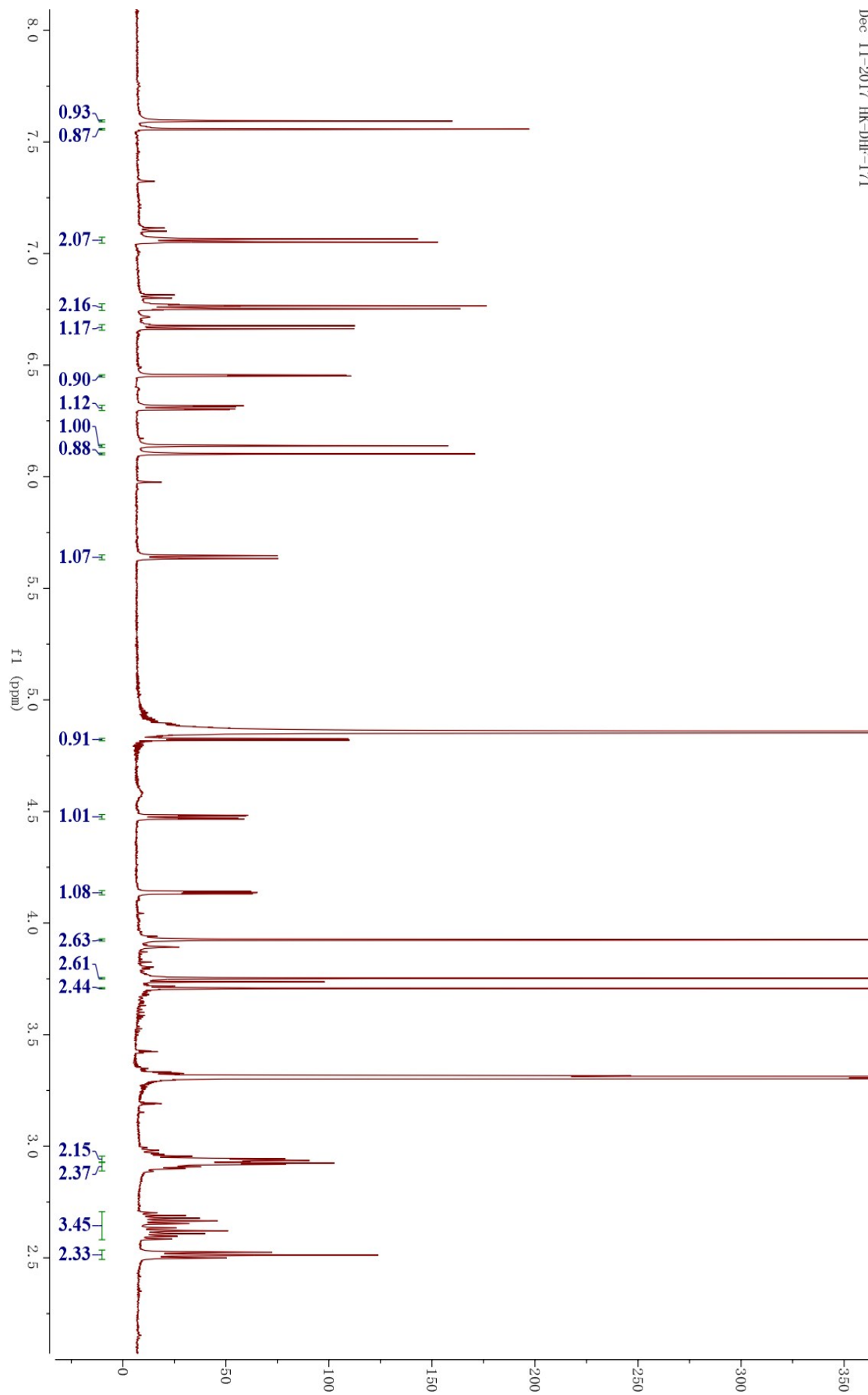


Figure S25. ^1H NMR spectrum (600 MHz) of compound **4** in CD_3OD .

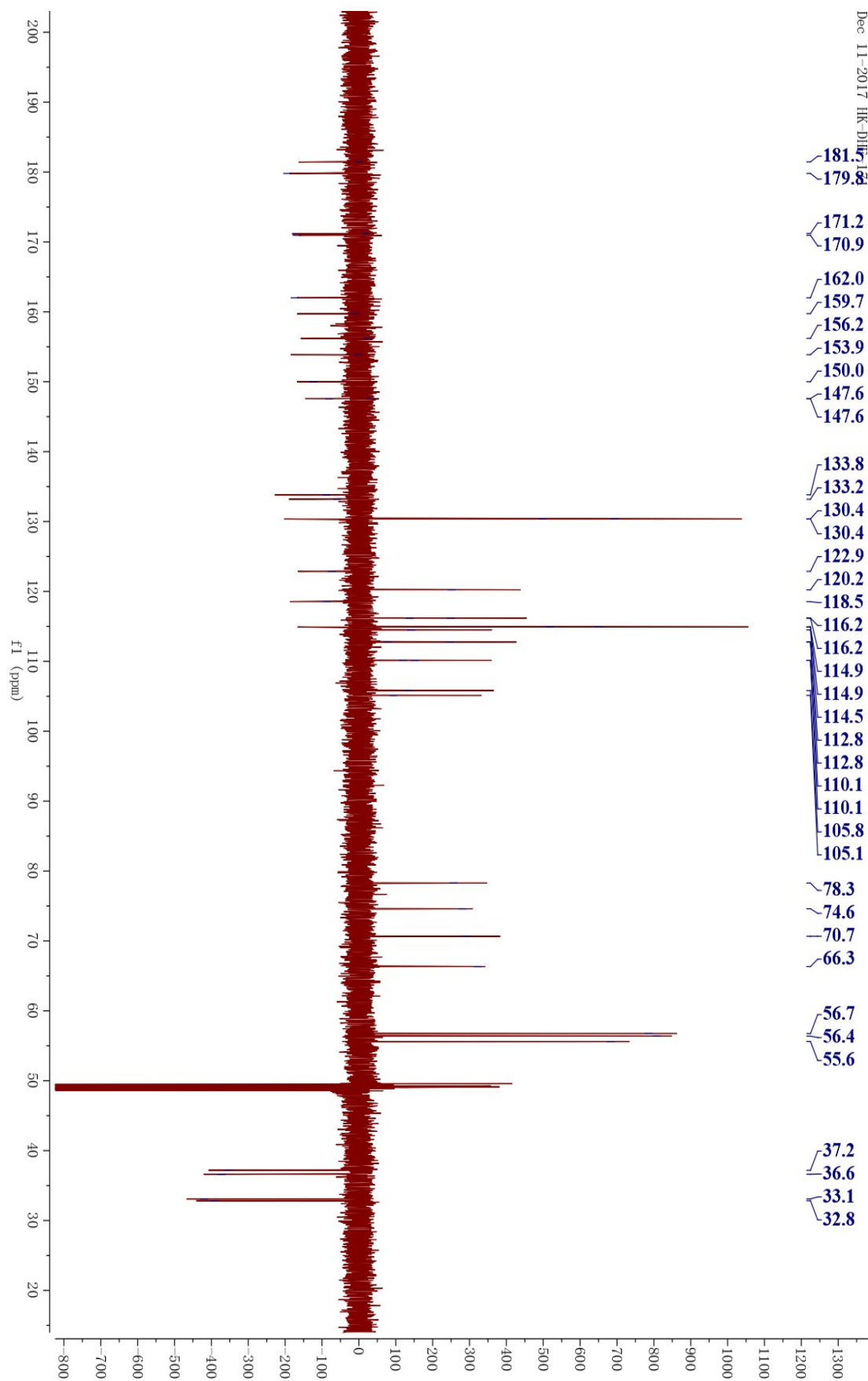


Figure S26. DEPTQ spectrum (150 MHz) of compound **4** in CD₃OD.

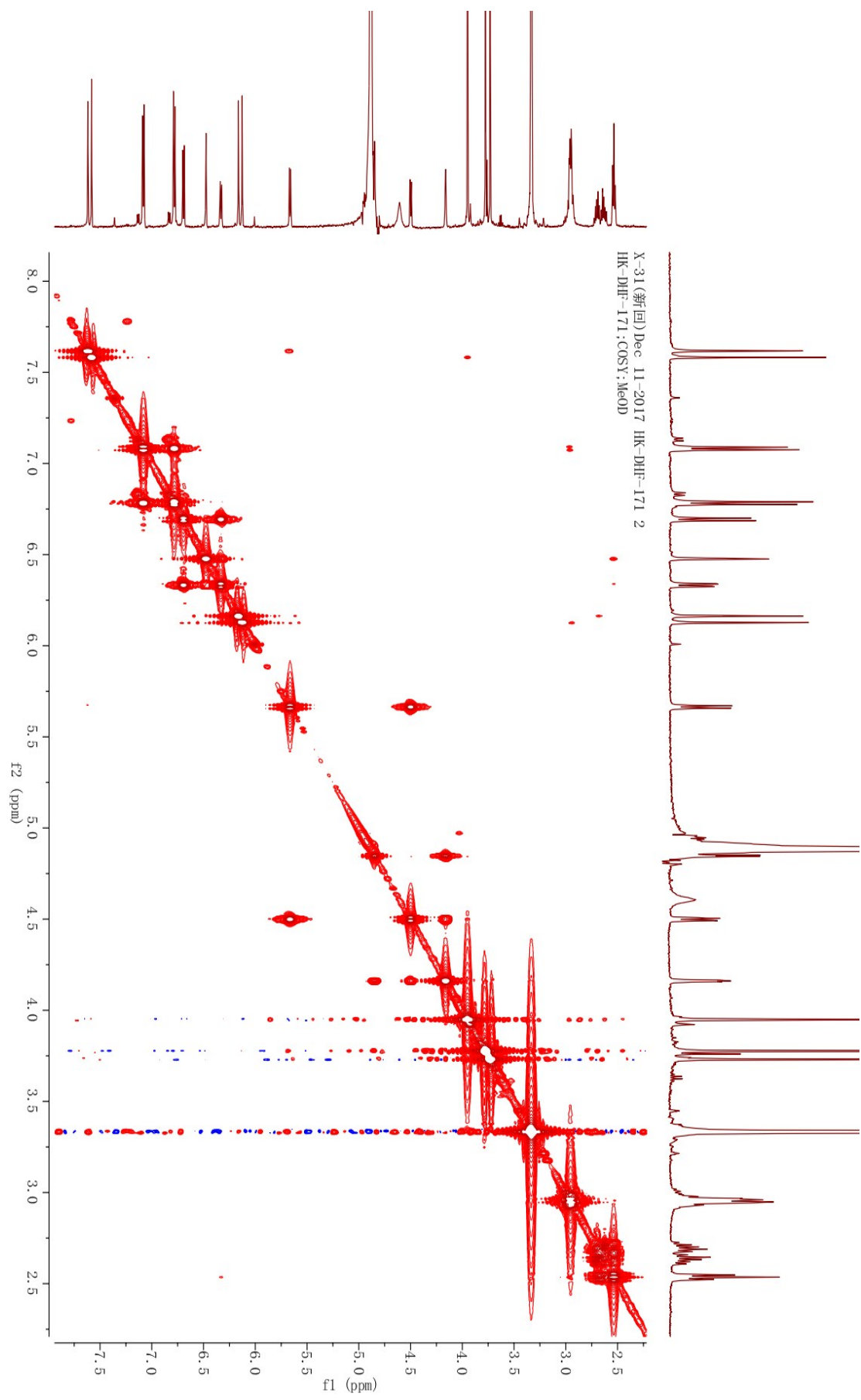


Figure S27. ^1H - ^1H COSY spectrum of compound **4** in CD_3OD .

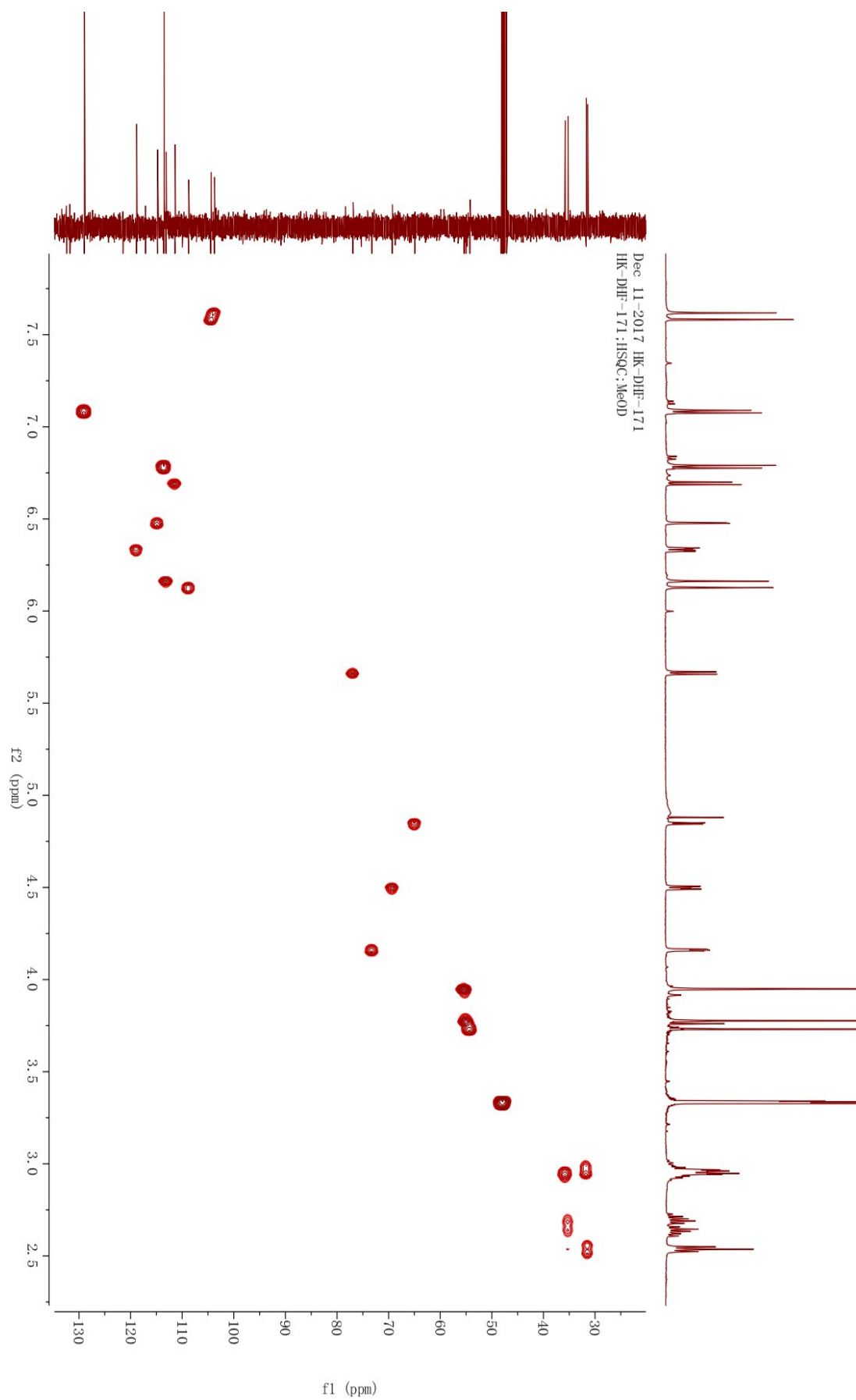


Figure S28. HSQC spectrum of compound **4** in CD_3OD .

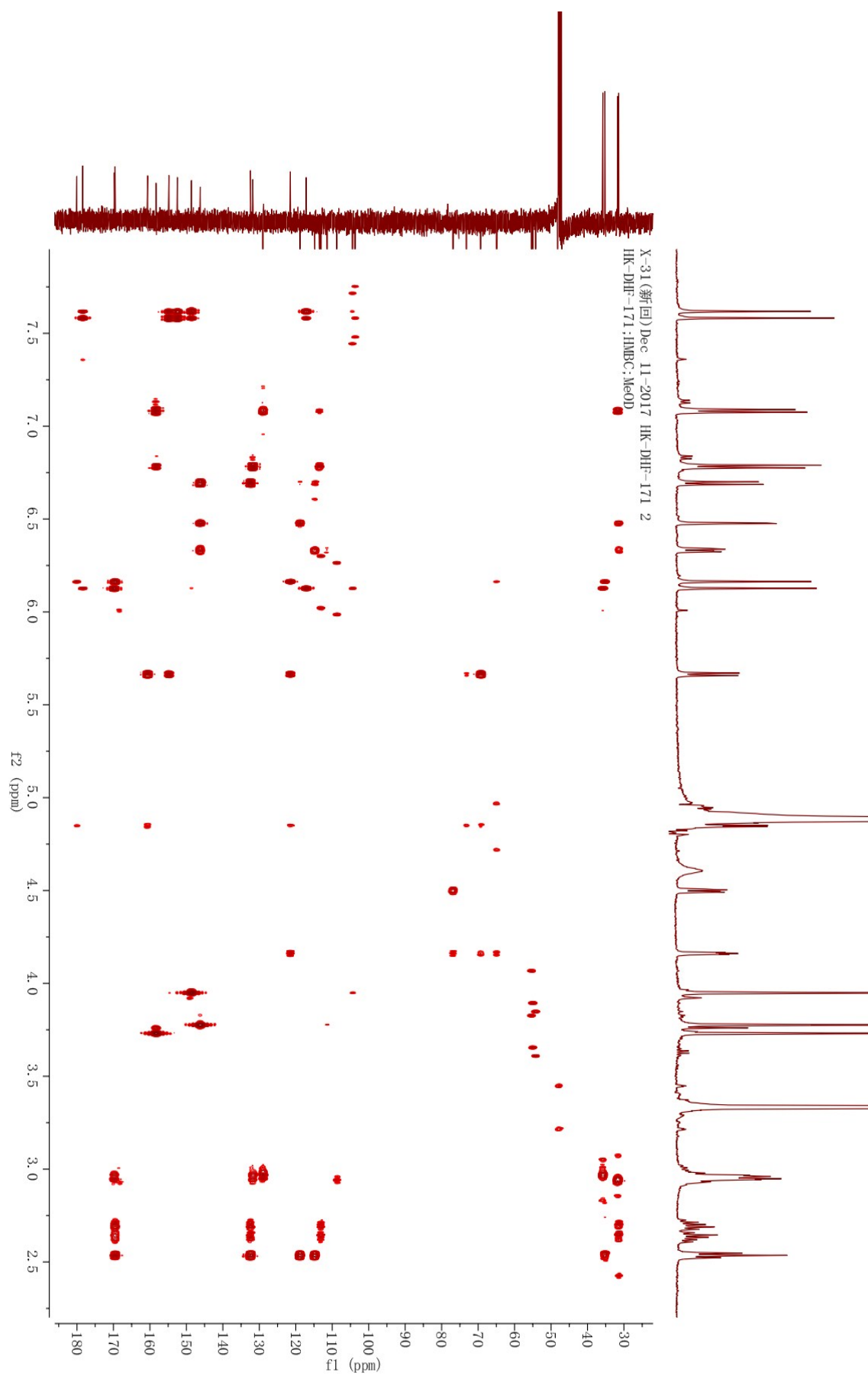


Figure S29. HMBC spectrum of compound **4** in CD₃OD.

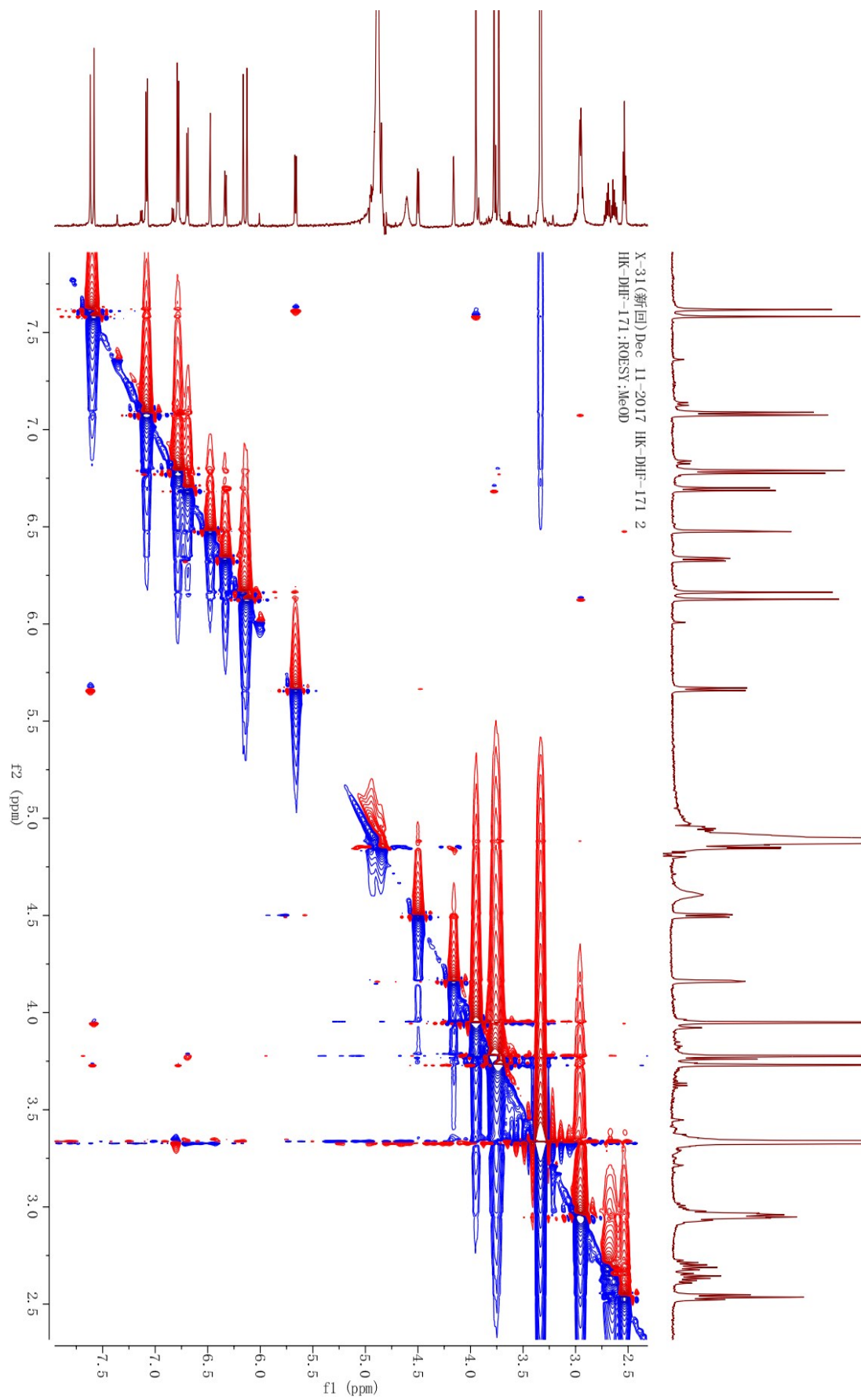


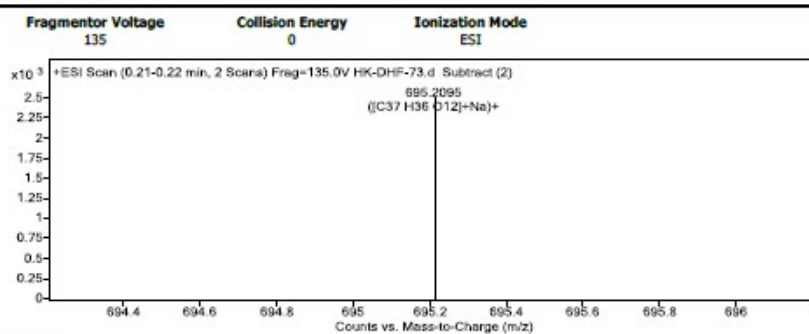
Figure S30. ROESY spectrum of compound **4** in CD₃OD.

Qualitative Analysis Report

Data Filename	HK-DHF-73.d	Sample Name	HK-DHF-73
Sample Type	Sample	Position	P1-D1
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	2/1/2018 2:35:03 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (85125.2)	

User Spectra



Peak List

m/z	z	Abund
407.7925	2	6024.41
418.7835	2	5888.34
475.3261	2	5912.81
701.4931	1	18174.44
702.4971	1	7817.4
814.5776	1	16452.2
815.5804	1	7787.79
927.661	1	4873.8

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
C37 H36 O12	672.2207	695.2099	695.2095	0.40	0.58	20.0000

--- End Of Report ---

Figure S31. HRESIMS spectrum of compound 4.

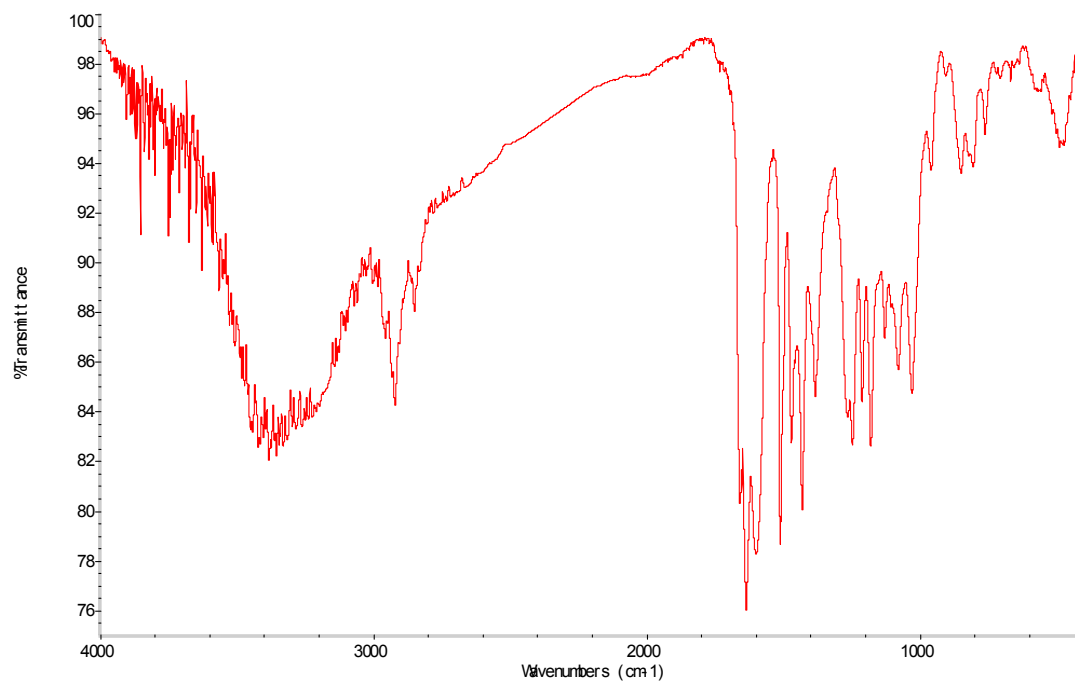


Figure S32. IR spectrum of compound 4.

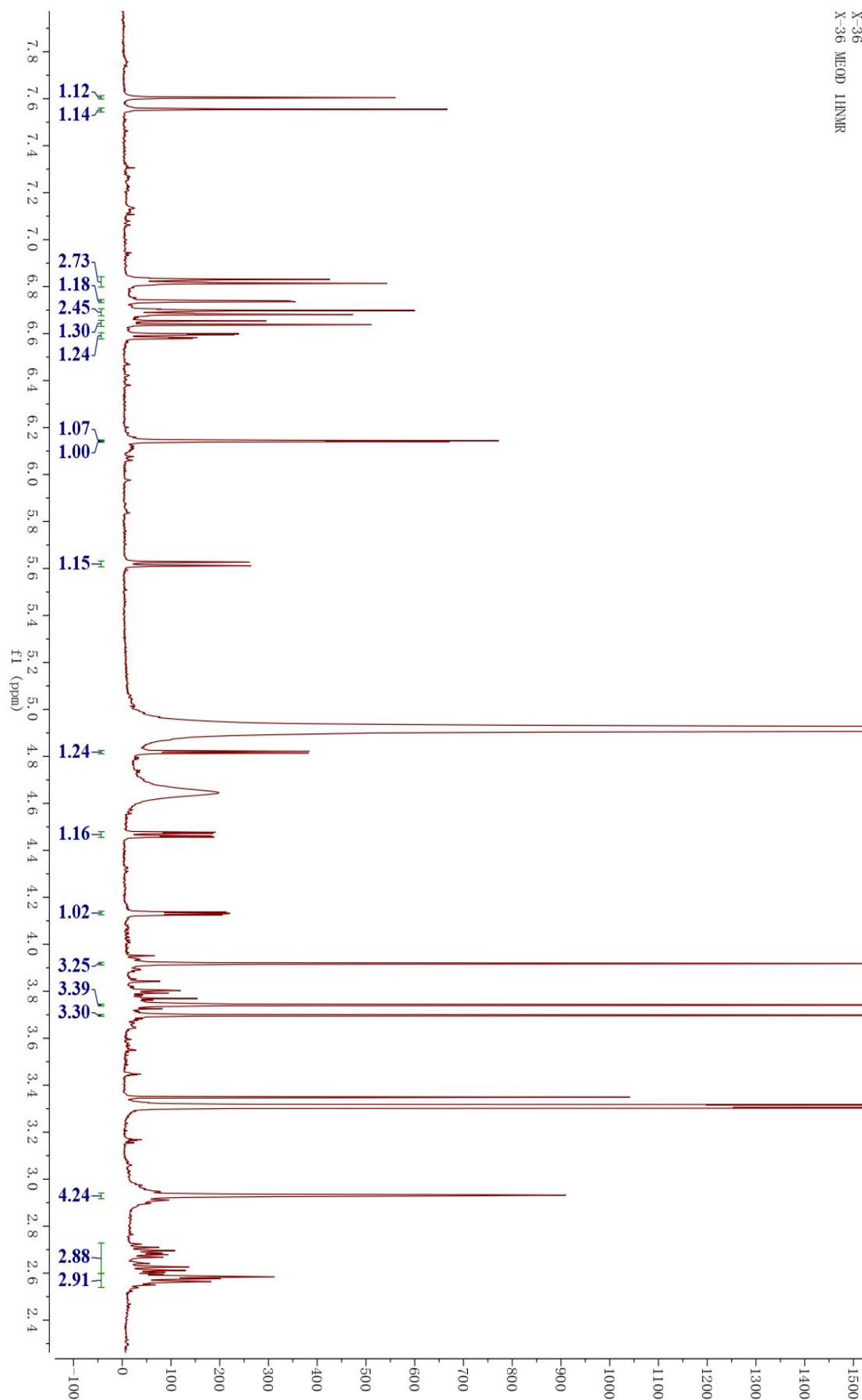


Figure S33. ¹H NMR spectrum (500 MHz) of compound 5 in CD₃OD.

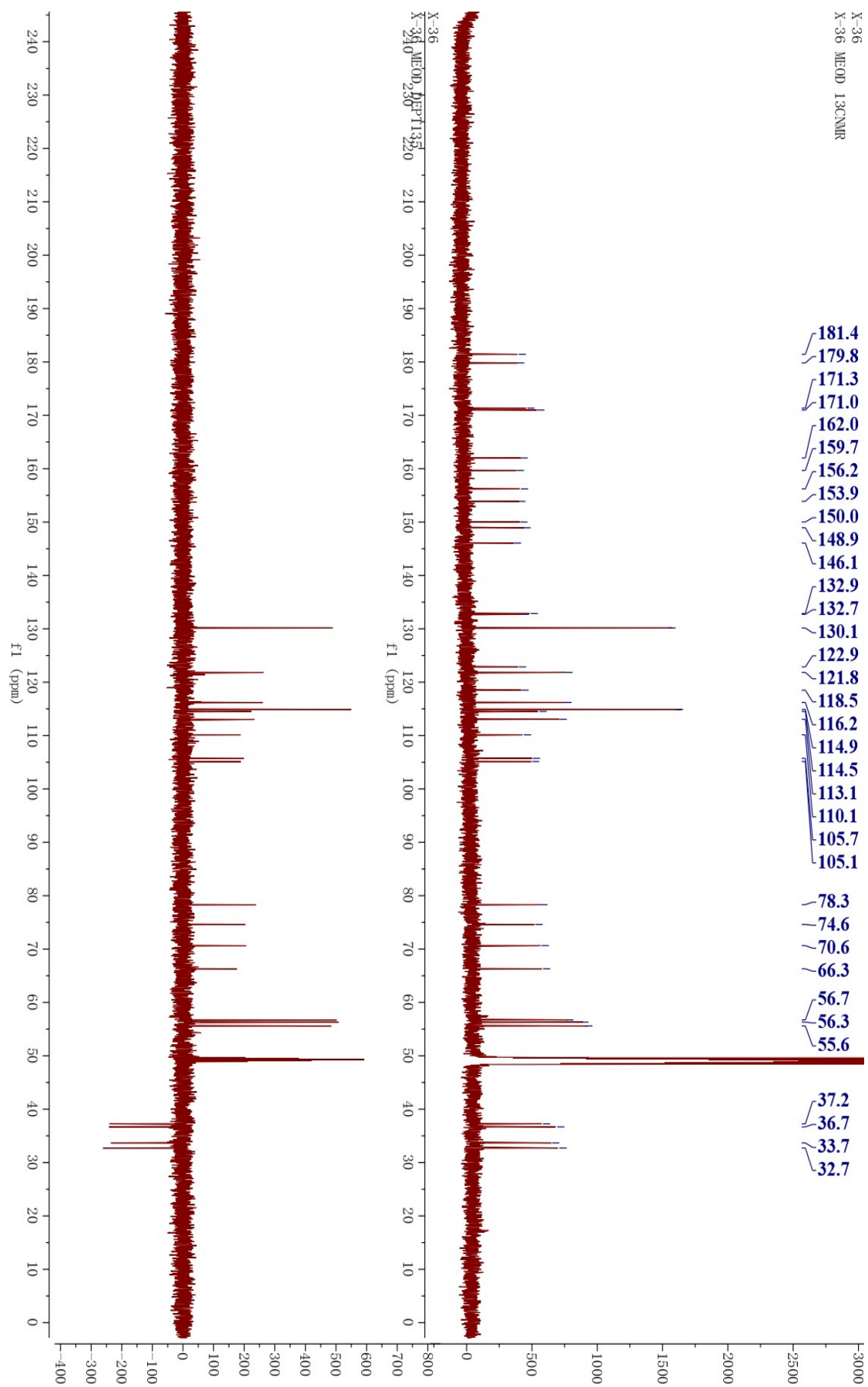


Figure S34. ^{13}C NMR spectrum (125 MHz) of compound **5** in CD_3OD .

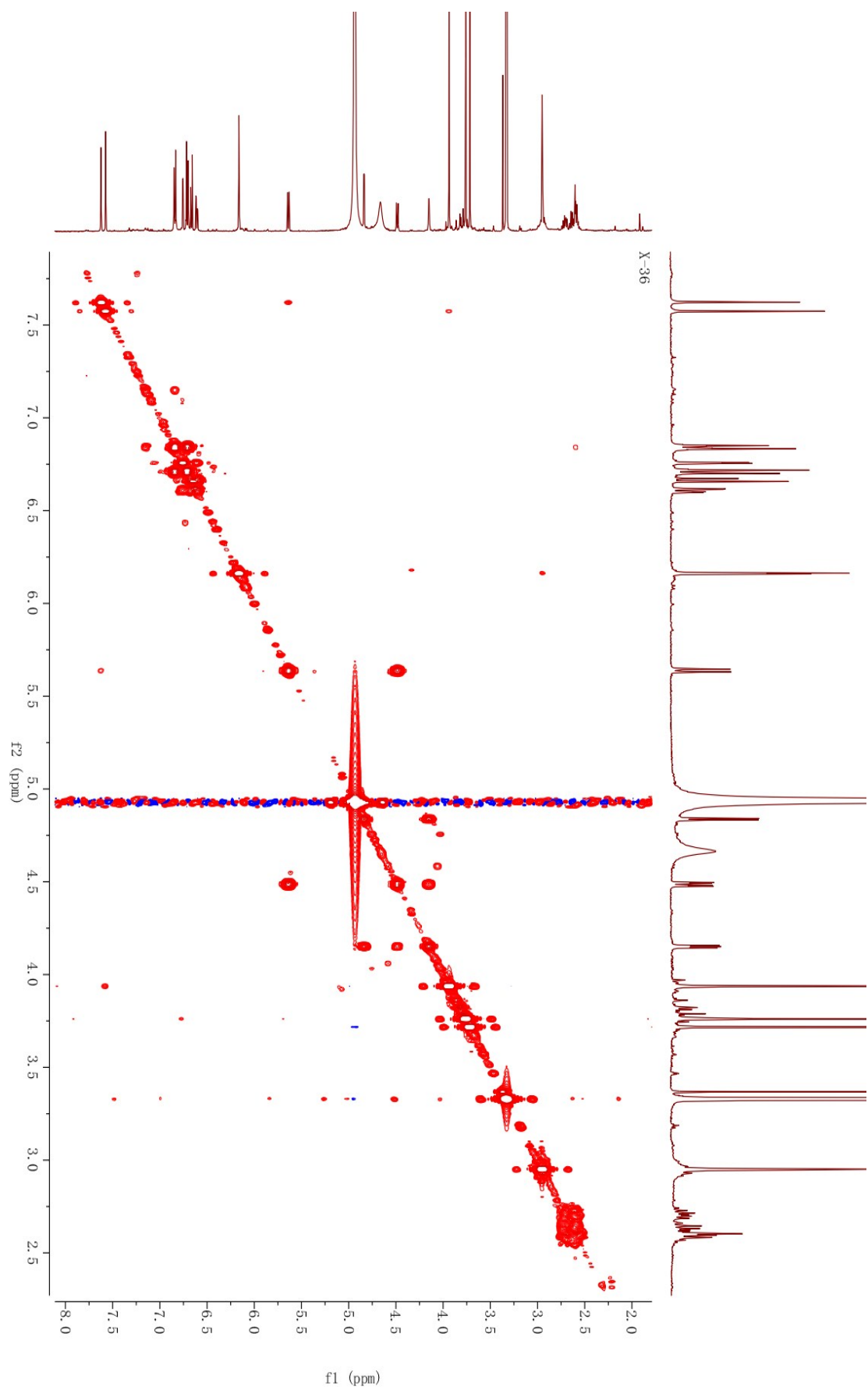


Figure S35. ^1H - ^1H COSY spectrum of compound **5** in CD_3OD .

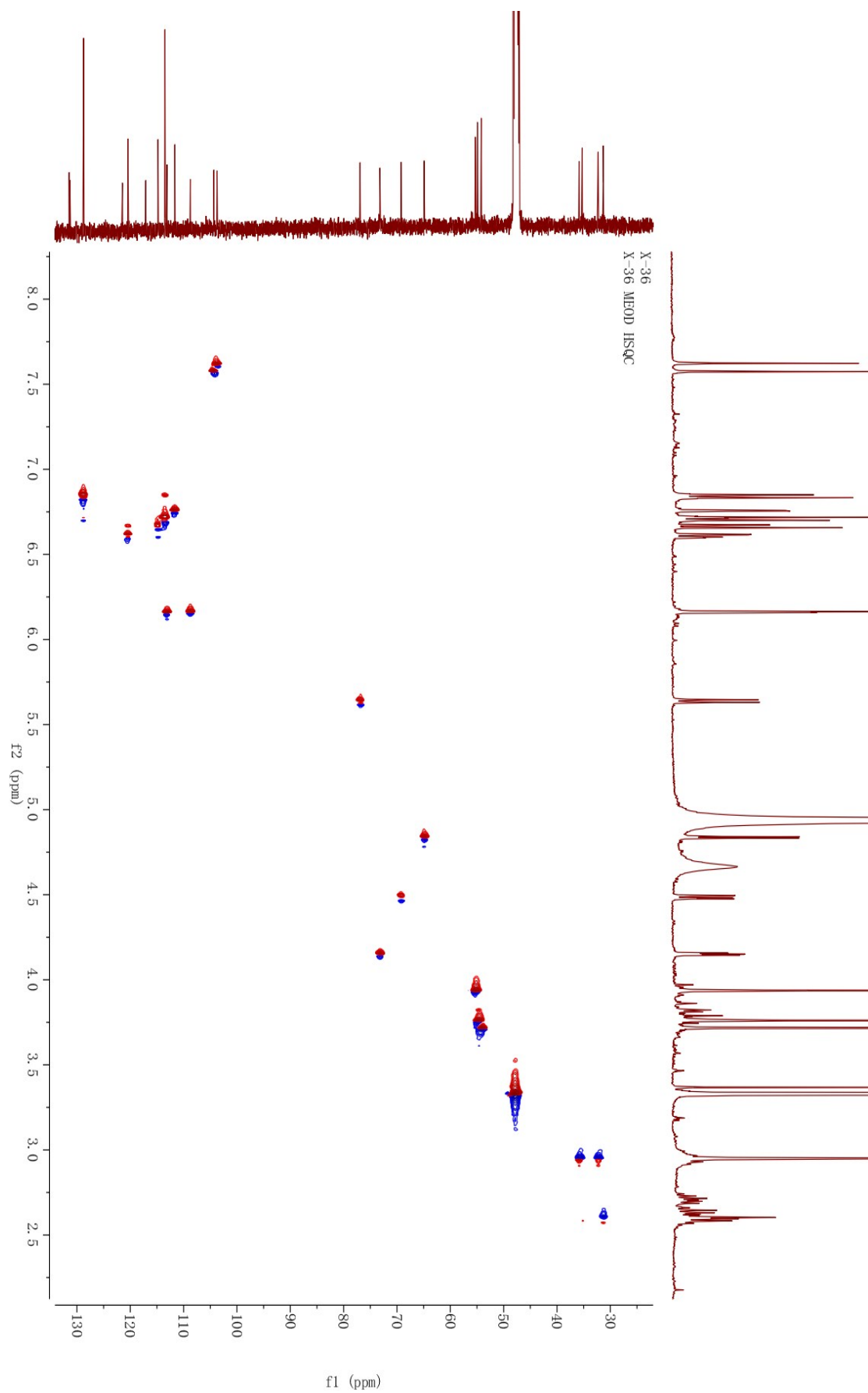


Figure S36. HSQC spectrum of compound **5** in CD₃OD.

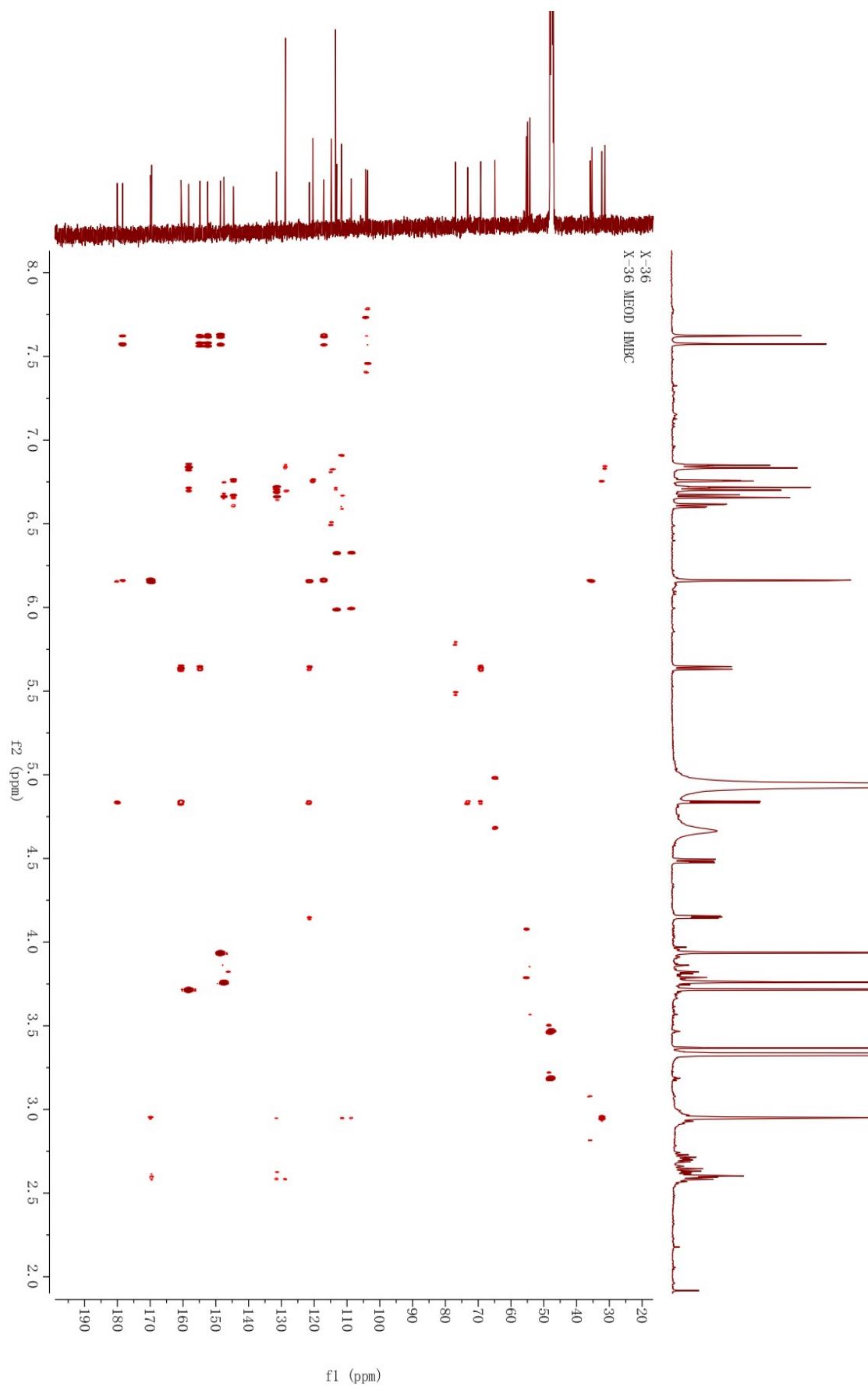


Figure S37. HMBC spectrum of compound **5** in CD₃OD.

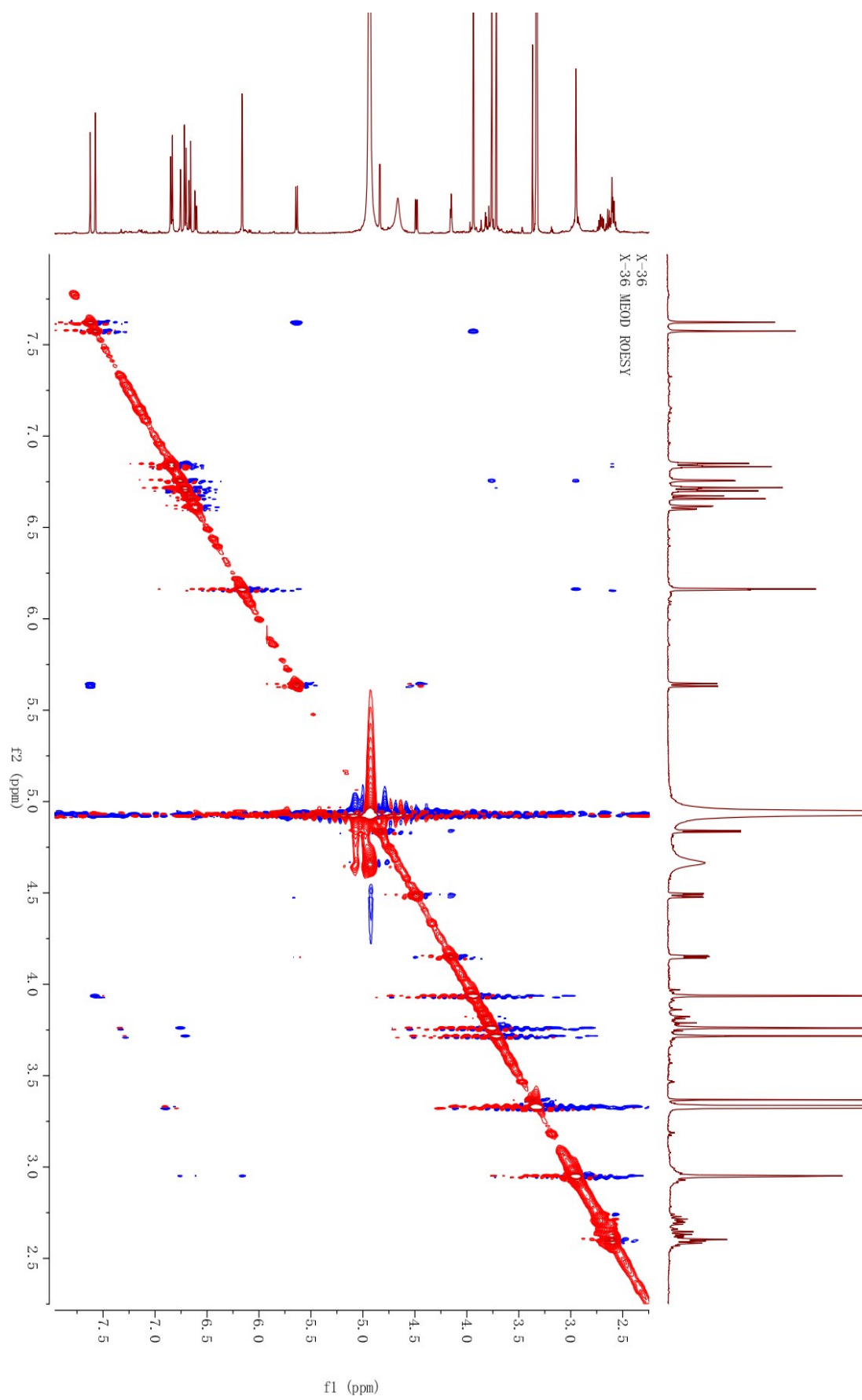
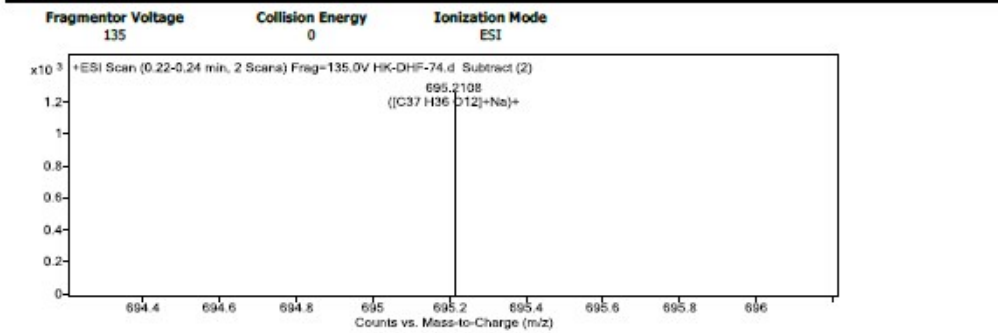


Figure S38. ROESY spectrum of compound **5** in CD₃OD.

Qualitative Analysis Report

Data Filename	HK-DHF-74.d	Sample Name	HK-DHF-74
Sample Type	Sample	Position	P1-D2
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	2/1/2018 2:36:25 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Acquisition SW	6200 series TOF/6500 series		
Version	Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund
212.116	1	3340.93
246.2423		2541.65
274.2739	1	21890.75
275.2766	1	3753.26
302.3051	1	3578.05
318.3004	1	10426.92
507.2717	1	2470.15
523.2463	1	4448.28

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C37 H36 O12	672.2207	695.2099	695.2108	-0.90	-1.29	20.0000

--- End Of Report ---

Figure S39. HRESIMS spectrum of compound **5**.

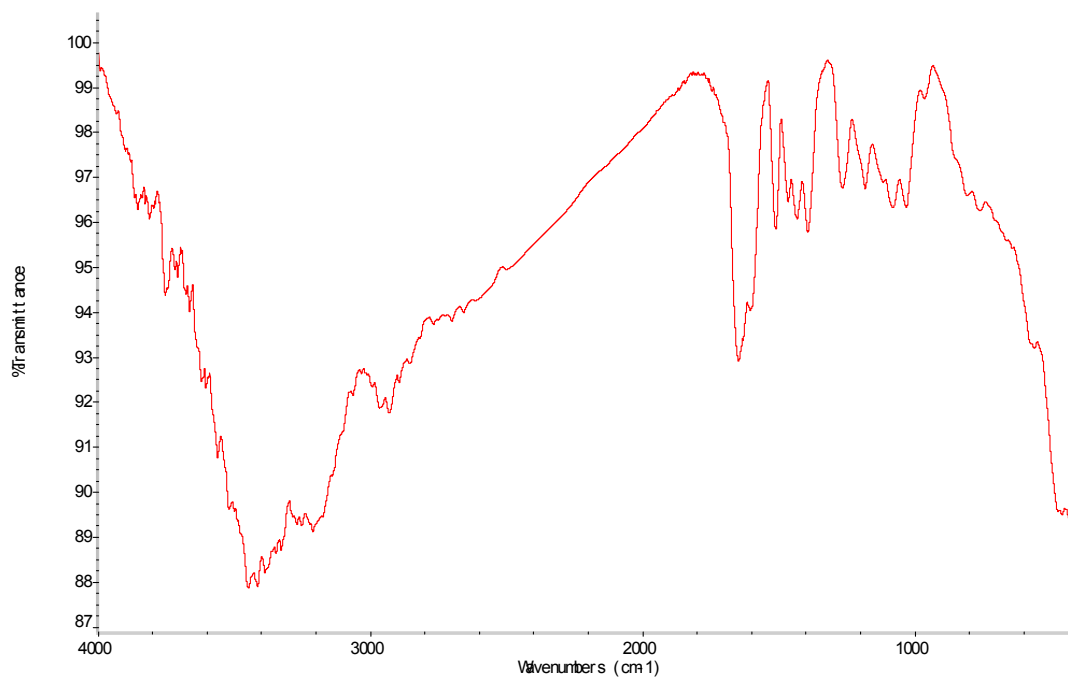


Figure S40. IR spectrum of compound **5**.

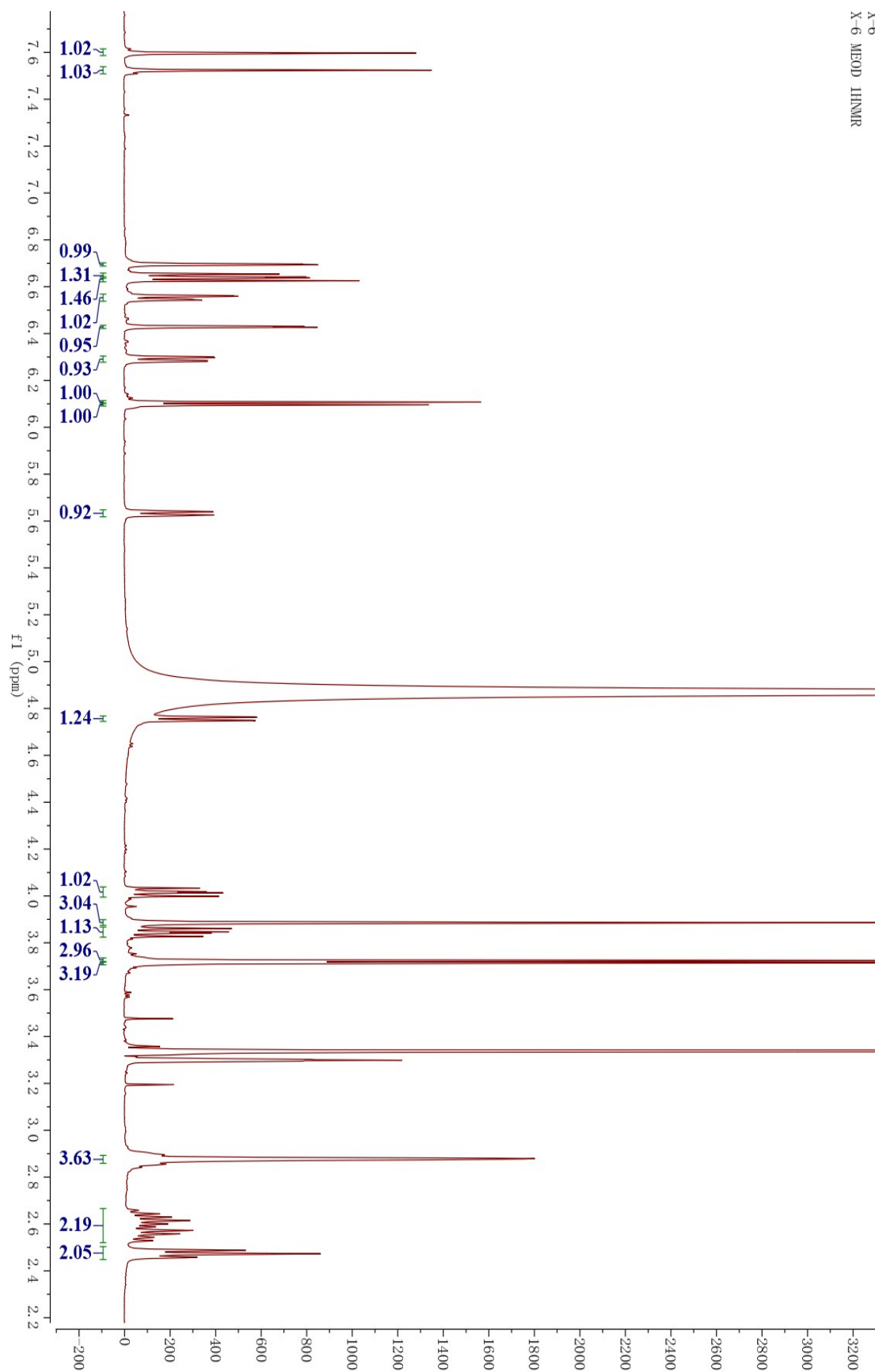


Figure S41. ¹H NMR spectrum (500 MHz) of compound 6 in CD₃OD.

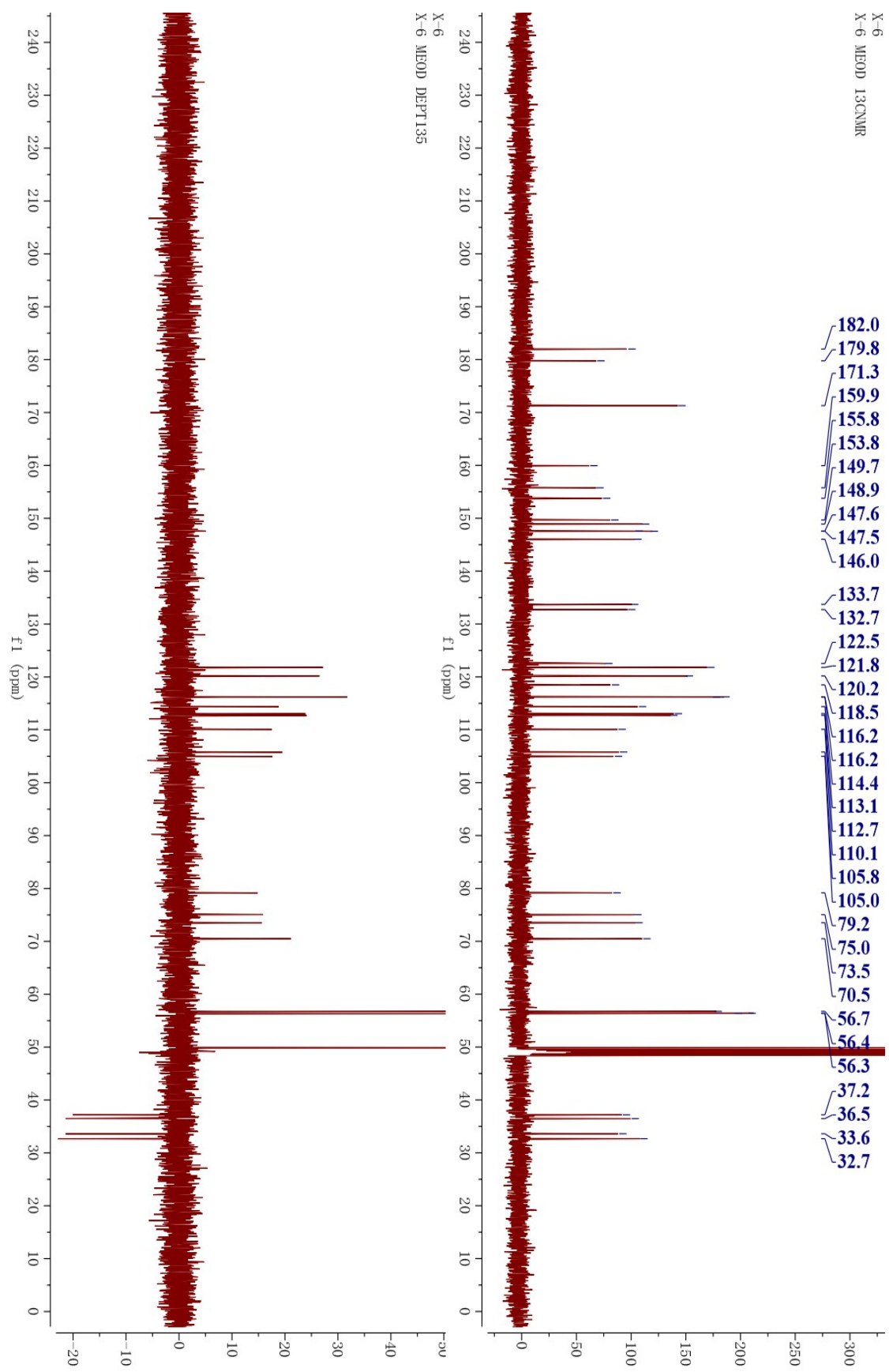


Figure S42. ^{13}C NMR spectrum (125 MHz) of compound **6** in CD_3OD .

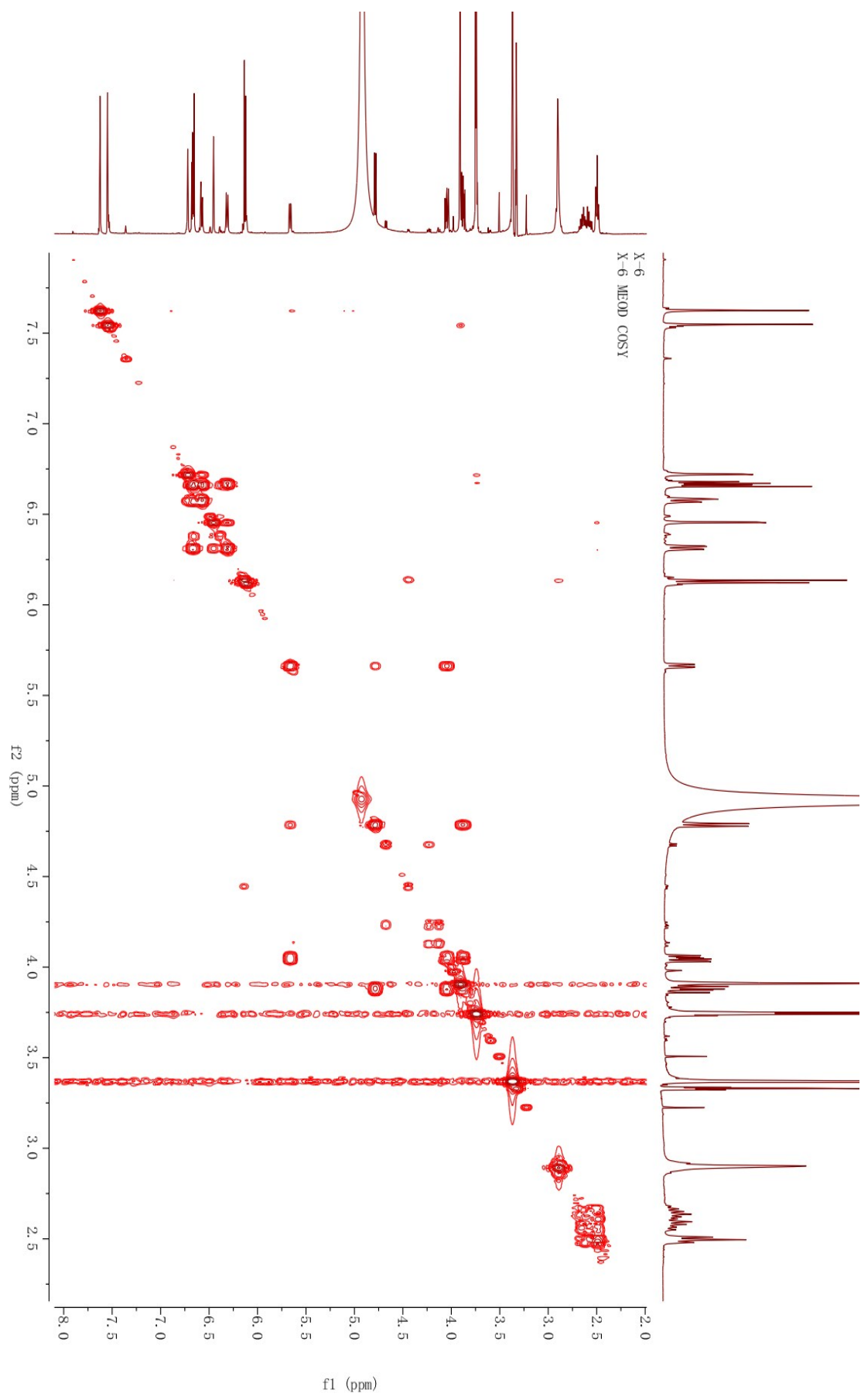


Figure S43. ^1H - ^1H COSY spectrum of compound **6** in CD_3OD .

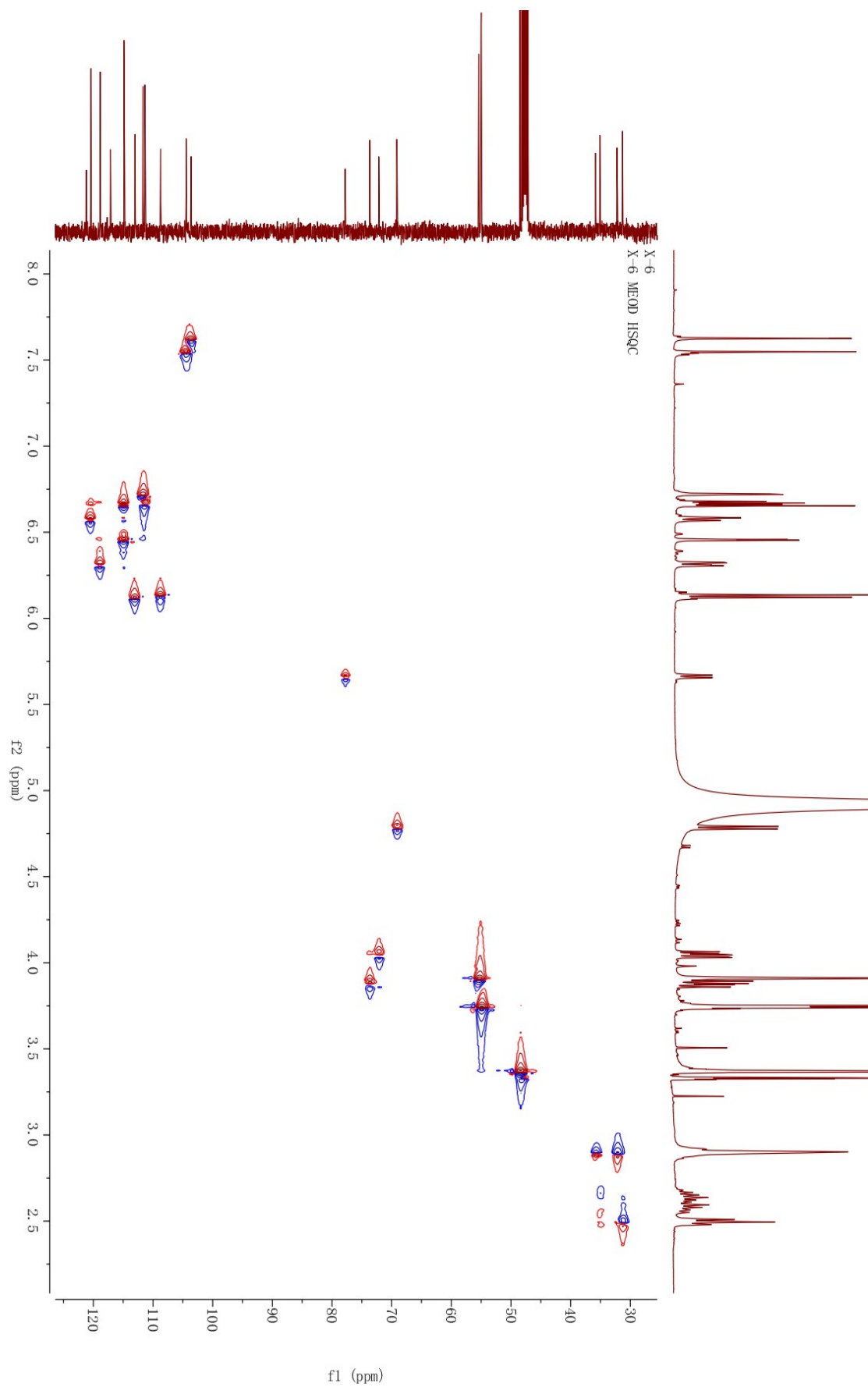


Figure S44. HSQC spectrum of compound **6** in CD₃OD.

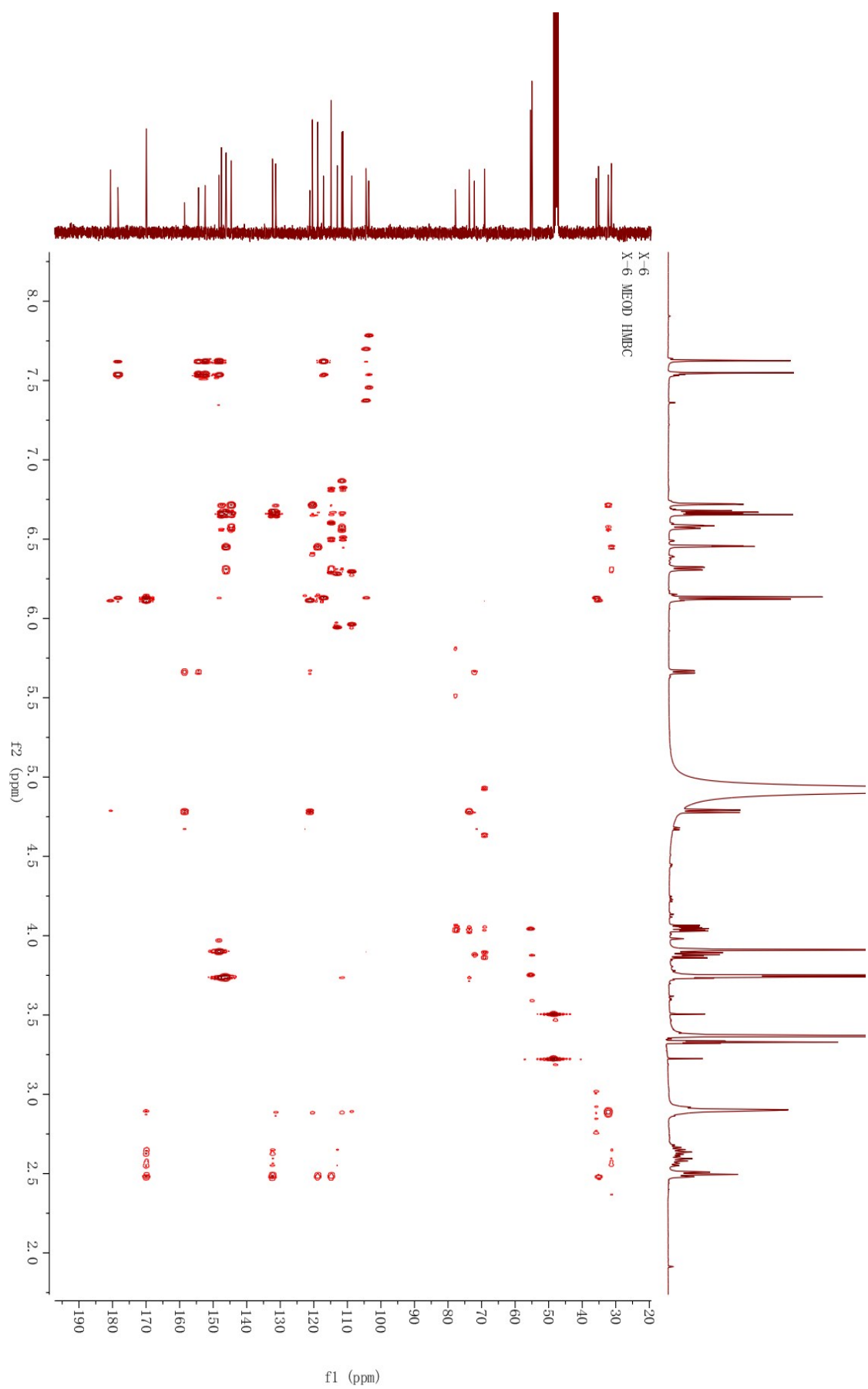


Figure S45. HMBC spectrum of compound **6** in CD₃OD.

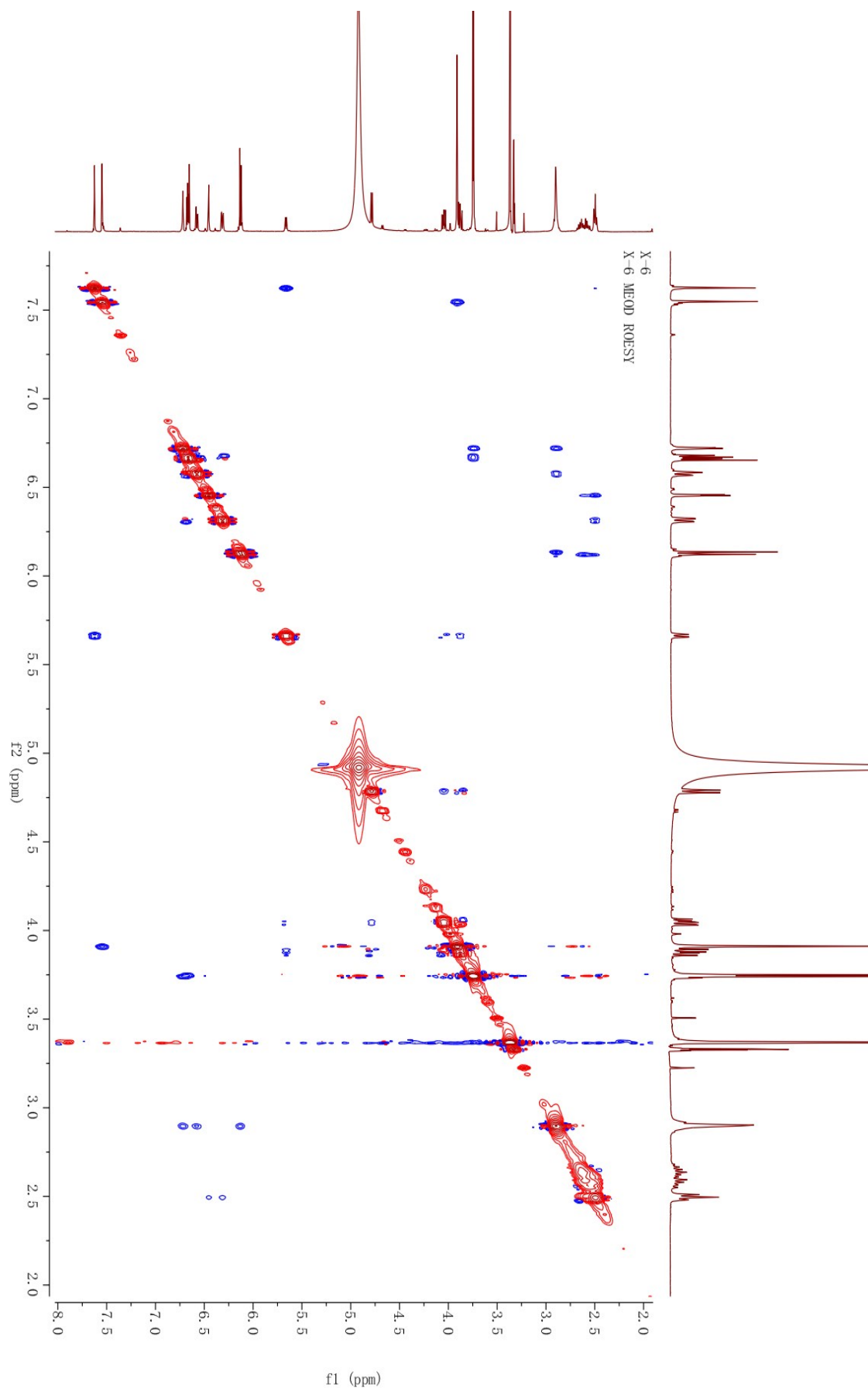
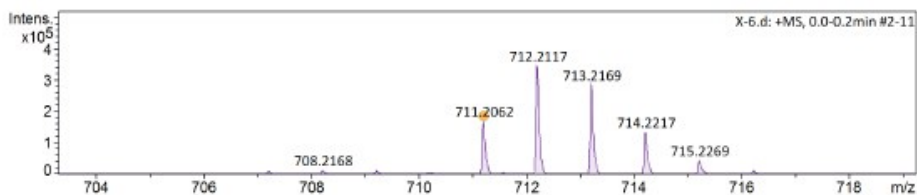
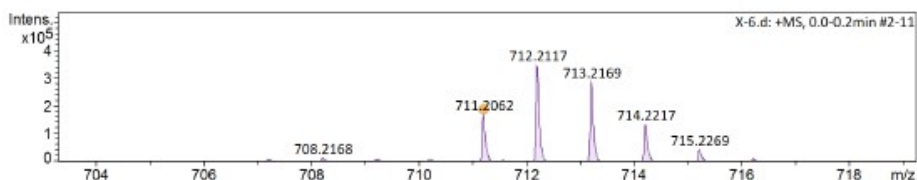
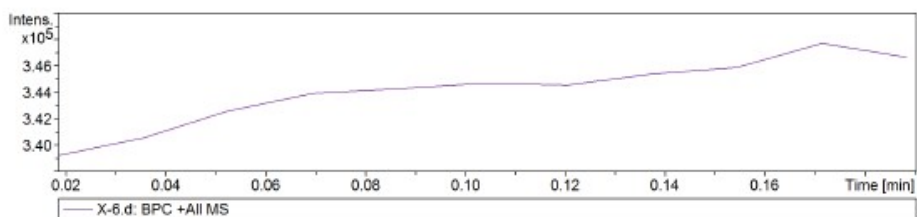


Figure S46. ROESY spectrum of compound **6** in CD₃OD.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	
Analysis Name	D:\Data\A501\Wanghui\X-6.d	2017-12-15 18:12:03	
Method	DirectInfusion - MS - positive.m	Operator	Demo User
Sample Name	kfd-6-25	Instrument	compact 8255754.20156
Comment			

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule	Adduct
1	C37H36NaO13	711.2048	-1.3	-1.9	559.8	20.0	even	ok	M+Na

X-6.d

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by: demo

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Figure S47. HRESIMS spectrum of compound 6.

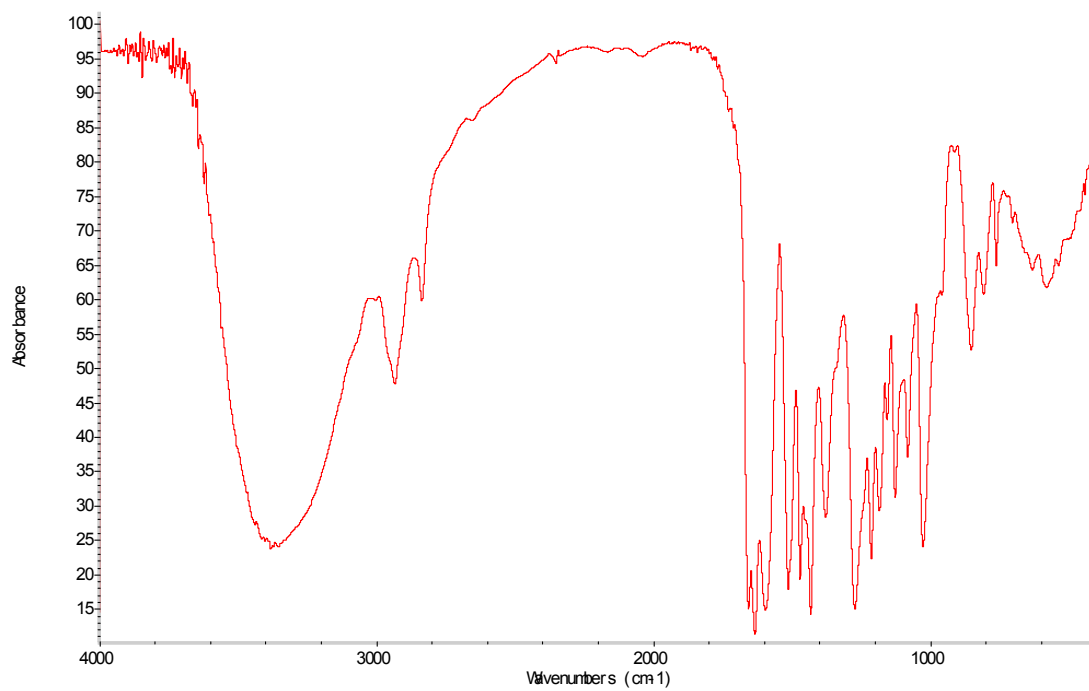


Figure S48. IR spectrum of compound 6.

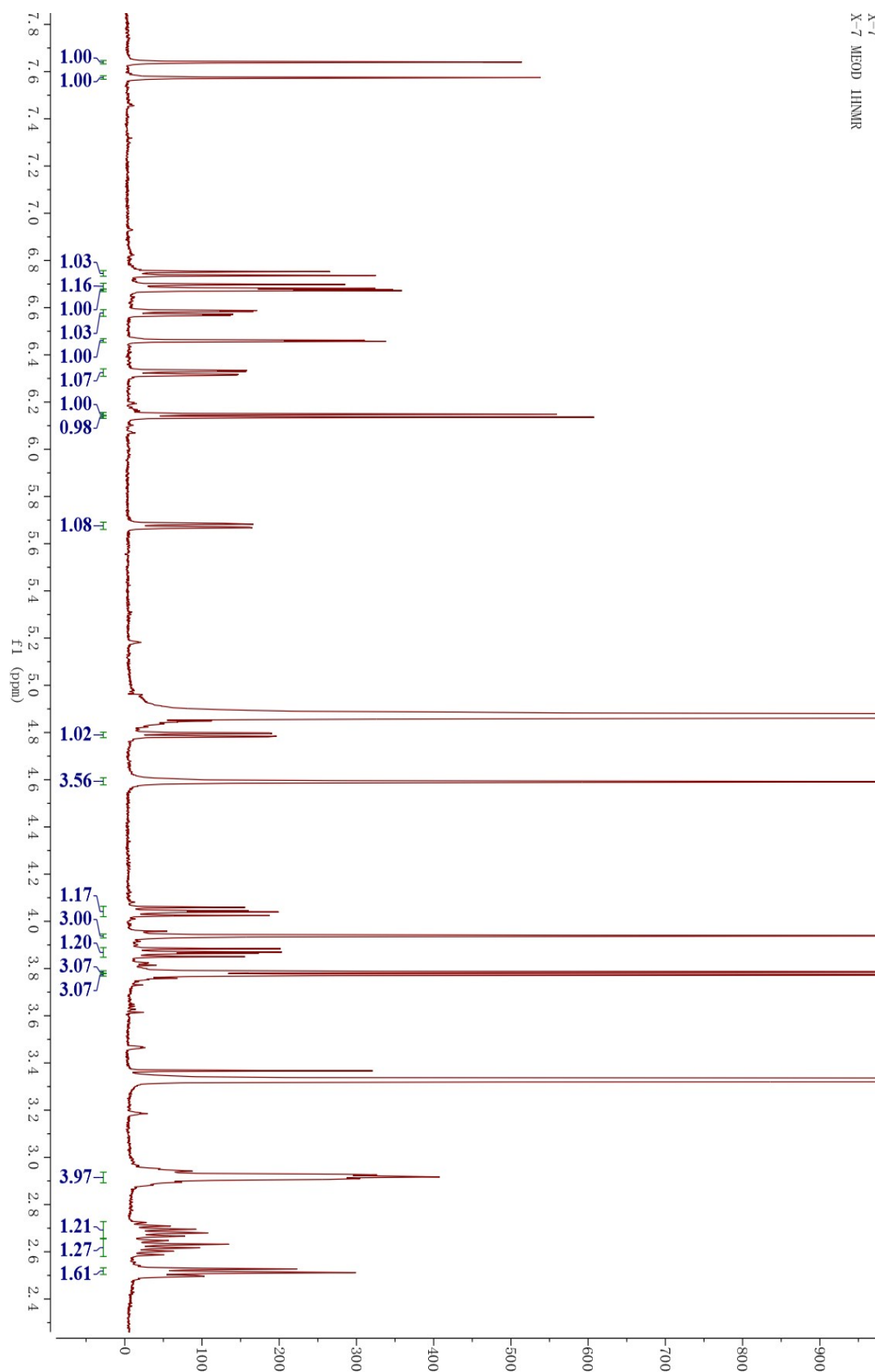


Figure S49. ¹H NMR spectrum (500 MHz) of compound 7 in CD₃OD.

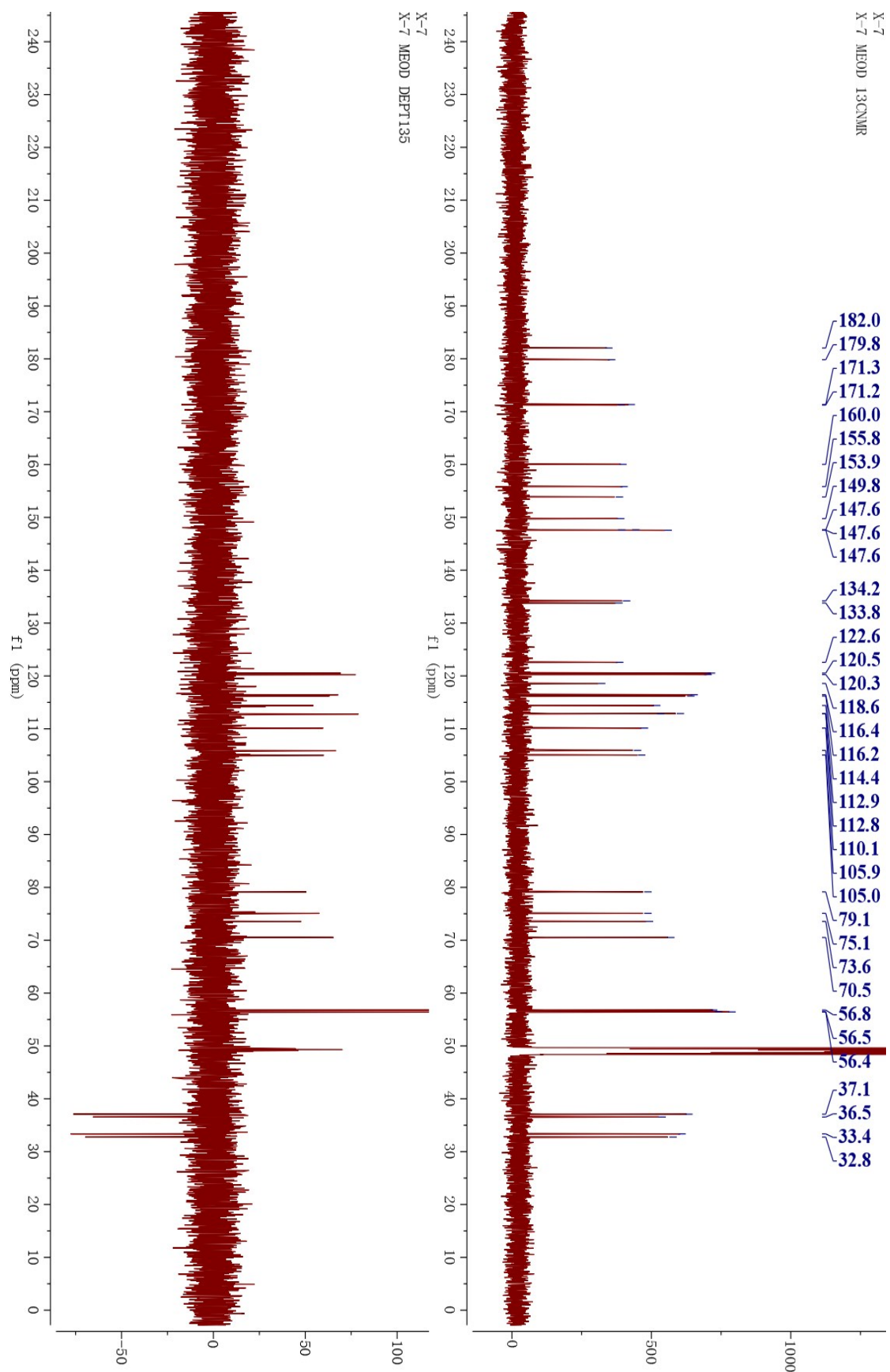


Figure S50. ^{13}C NMR spectrum (125 MHz) of compound **7** in CD_3OD .

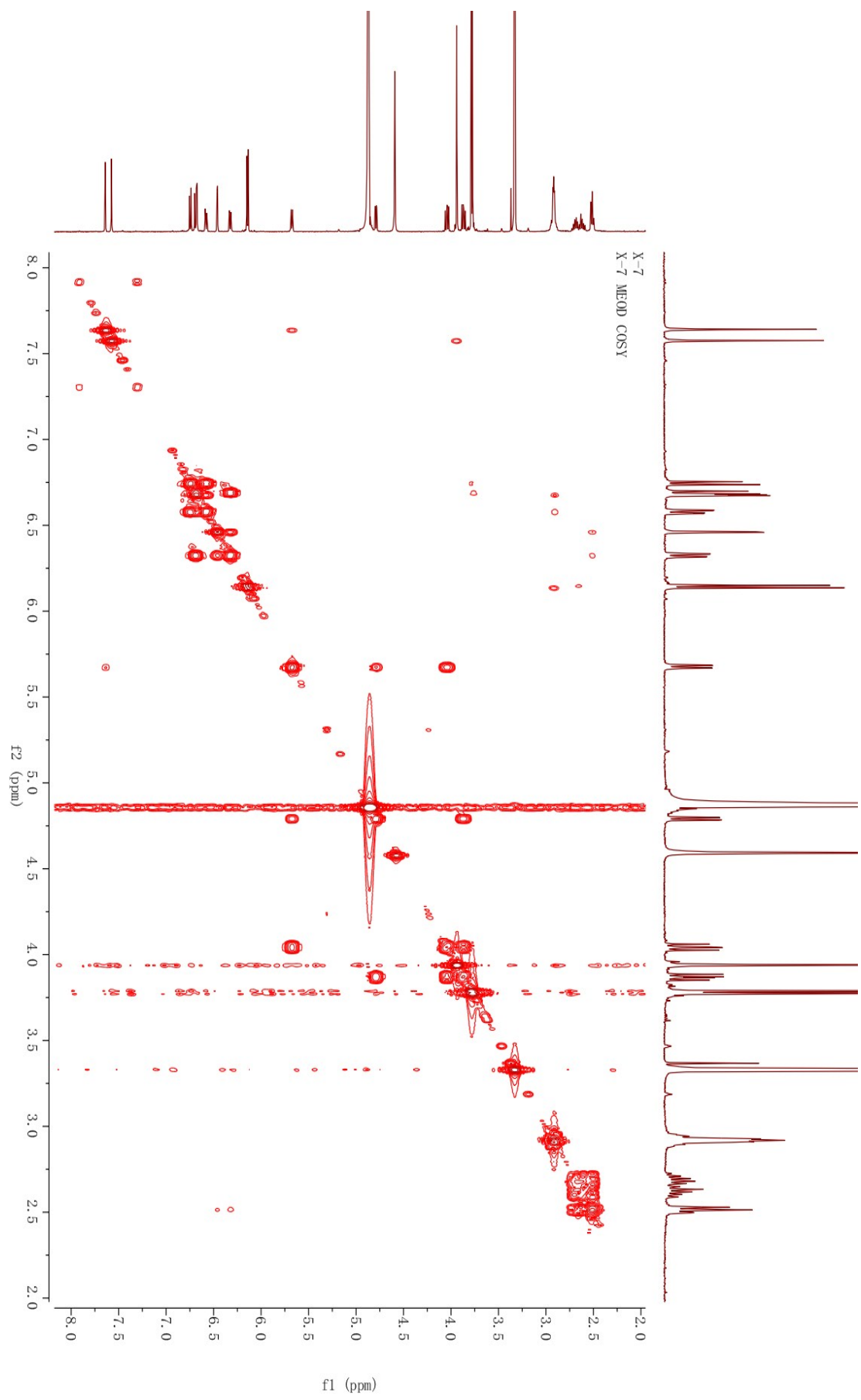


Figure S51. ^1H - ^1H COSY spectrum of compound **7** in CD_3OD .

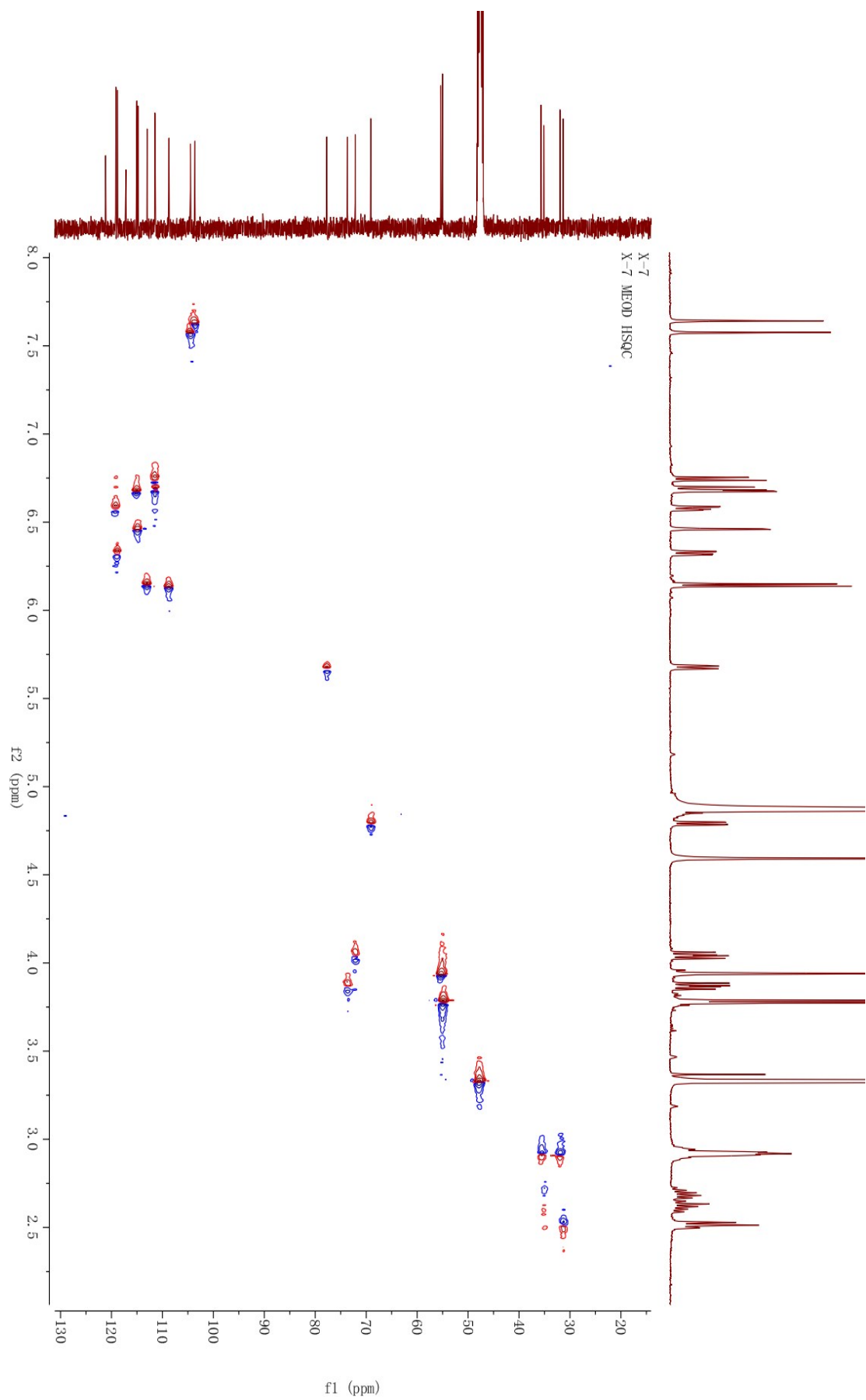


Figure S52. HSQC spectrum of compound **7** in CD_3OD .

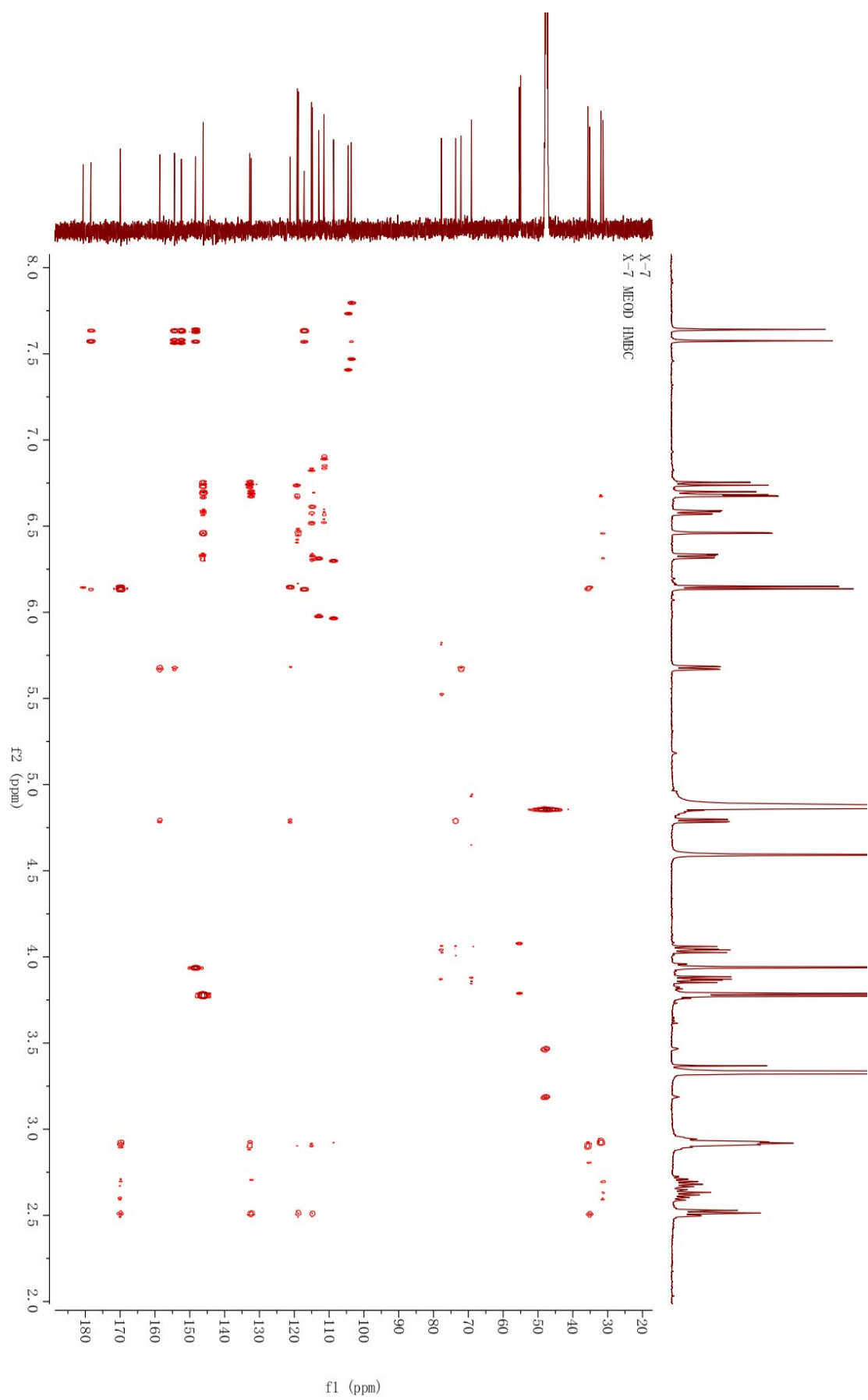


Figure S53. HMBC spectrum of compound **7** in CD₃OD.

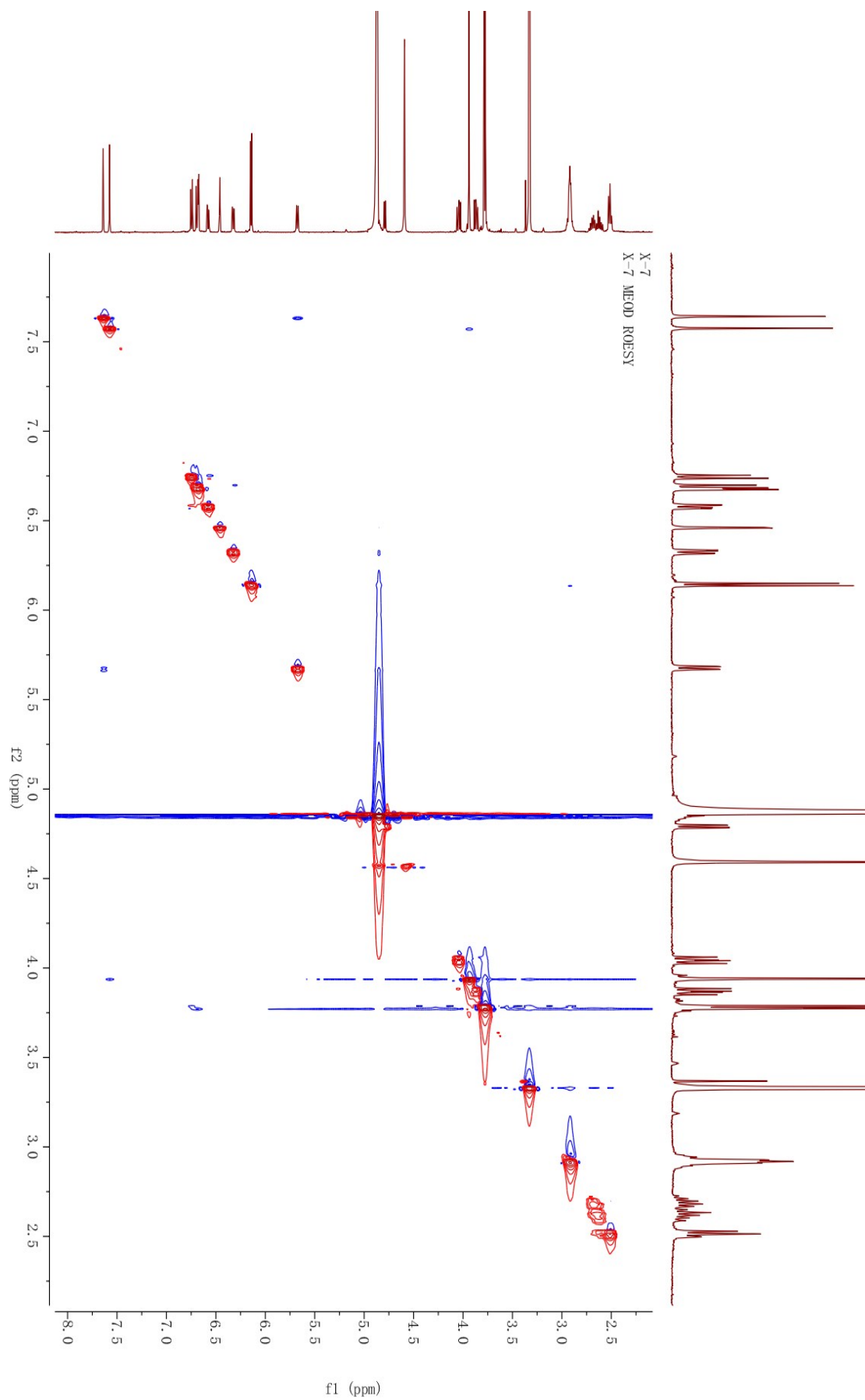
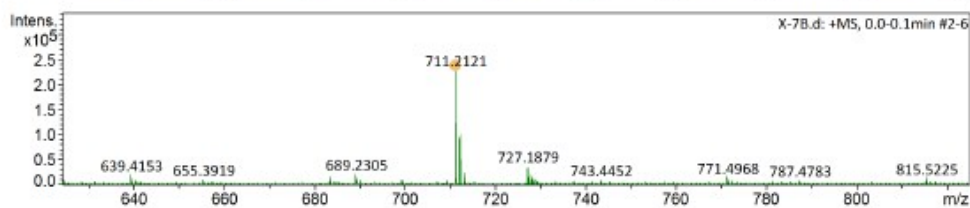
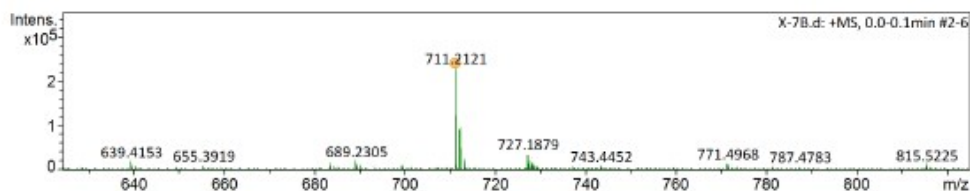
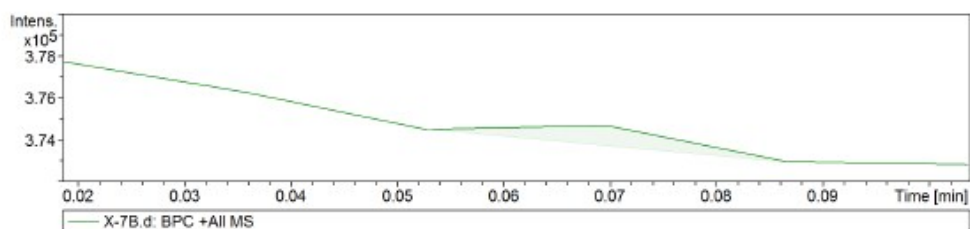


Figure S54. ROESY spectrum of compound **7** in CD₃OD.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date 2017-12-15 17:52:55			
Analysis Name	D:\Data\A501\Wanghui\X-7B.d	Operator	Demo User		
Method	DirectInfusion - MS - positive.m	Instrument	compact	8255754.20158	
Sample Name	kfd-8-25	Comment			
Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule	Adduct
1	C37H36NaO13	711.2048	-7.3	-10.3	3.0	20.0	even	ok	M+Na

X-7B.d

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by: demo

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Figure S55. HRESIMS spectrum of compound 7.

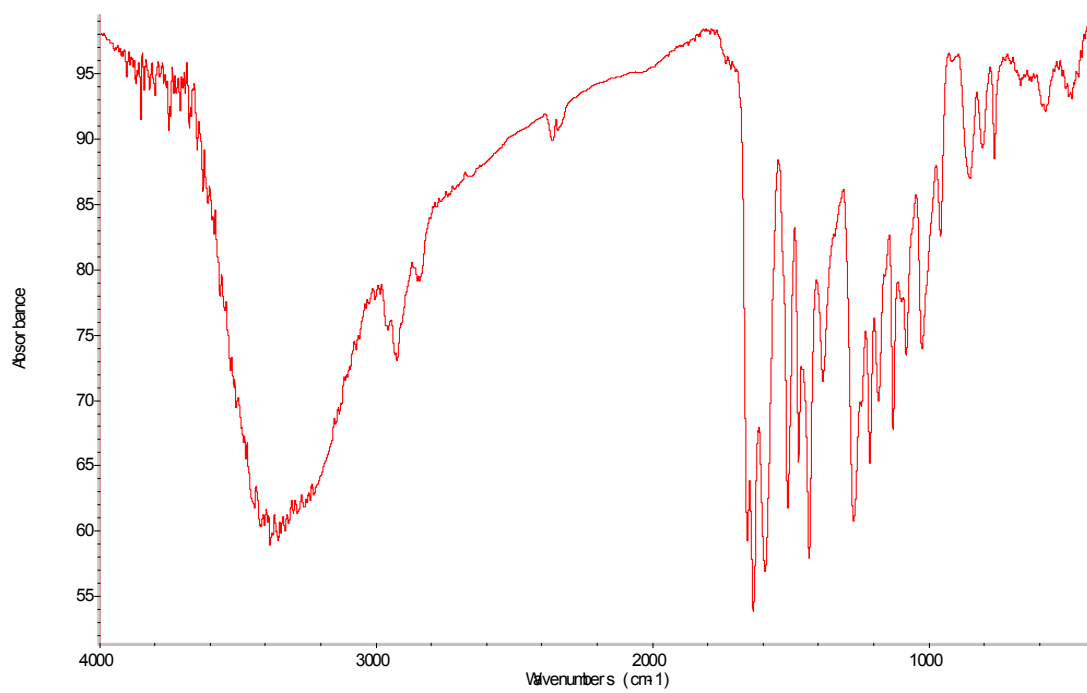


Figure S56. IR spectrum of compound 7.

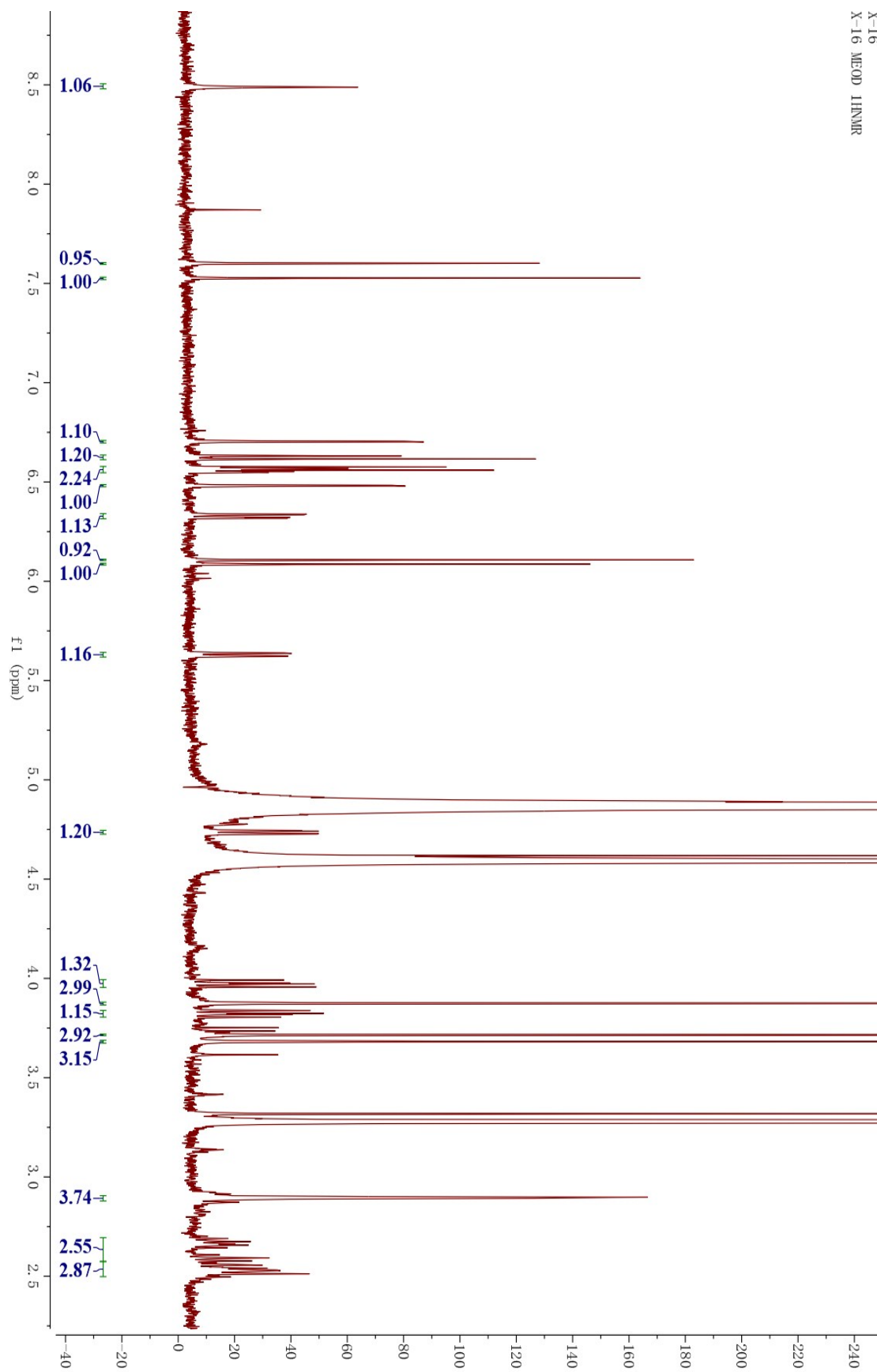


Figure S57. ¹H NMR spectrum (600 MHz) of compound **8** in CD₃OD.

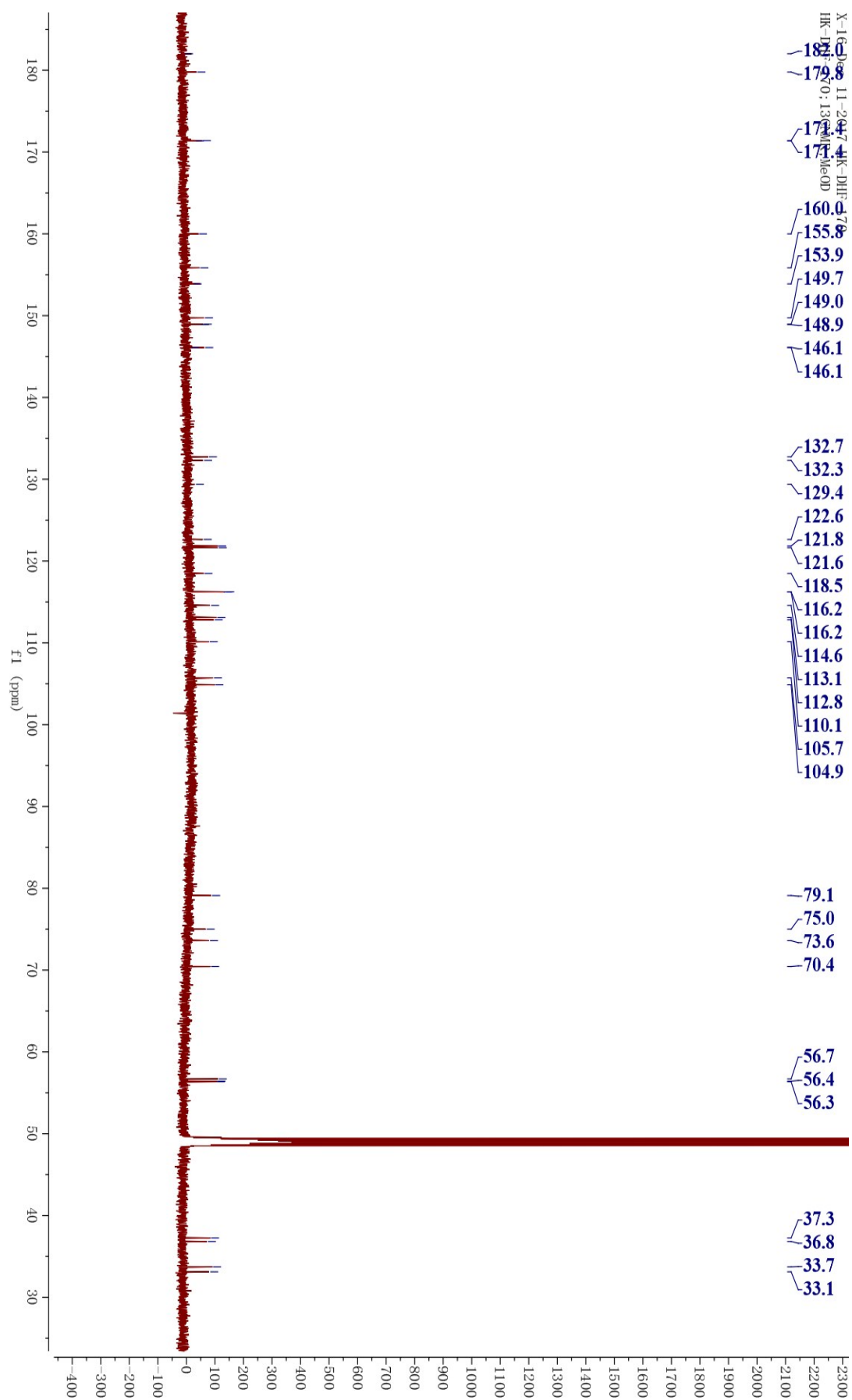


Figure S58. ^{13}C NMR spectrum (150 MHz) of compound **8** in CD_3OD .

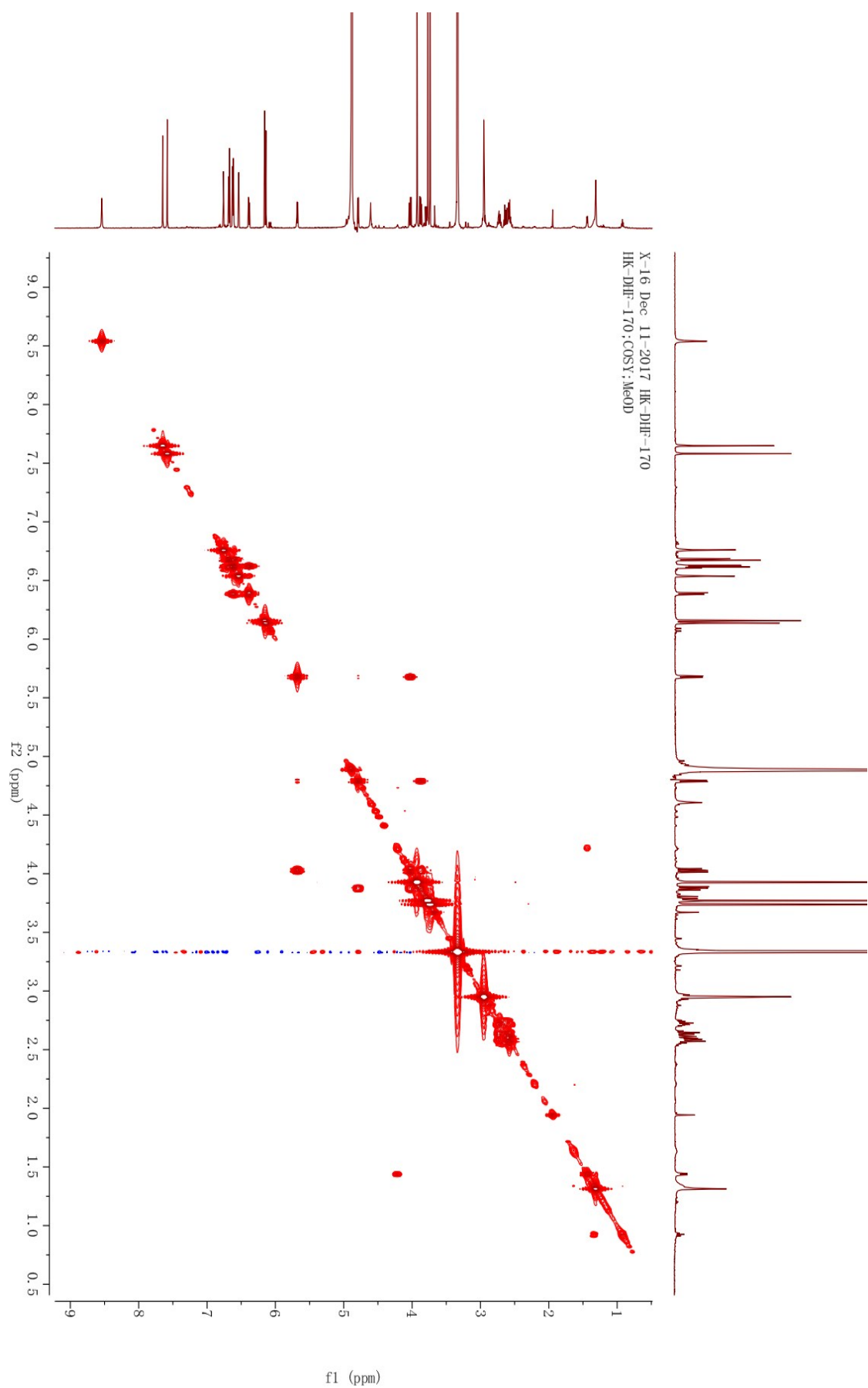


Figure S59. ^1H - ^1H COSY spectrum of compound **8** in CD_3OD .

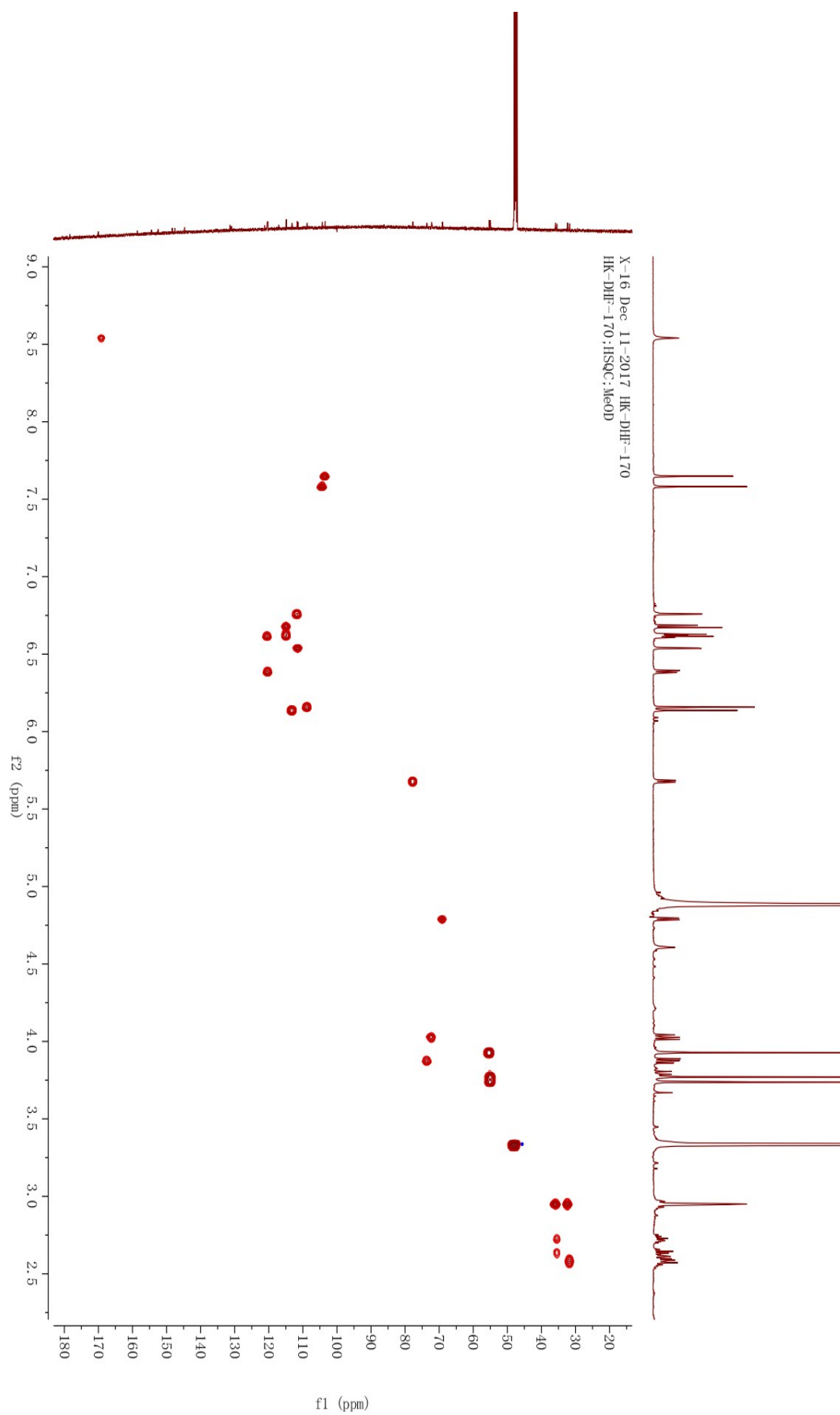


Figure S60. HSQC spectrum of compound **8** in CD_3OD .

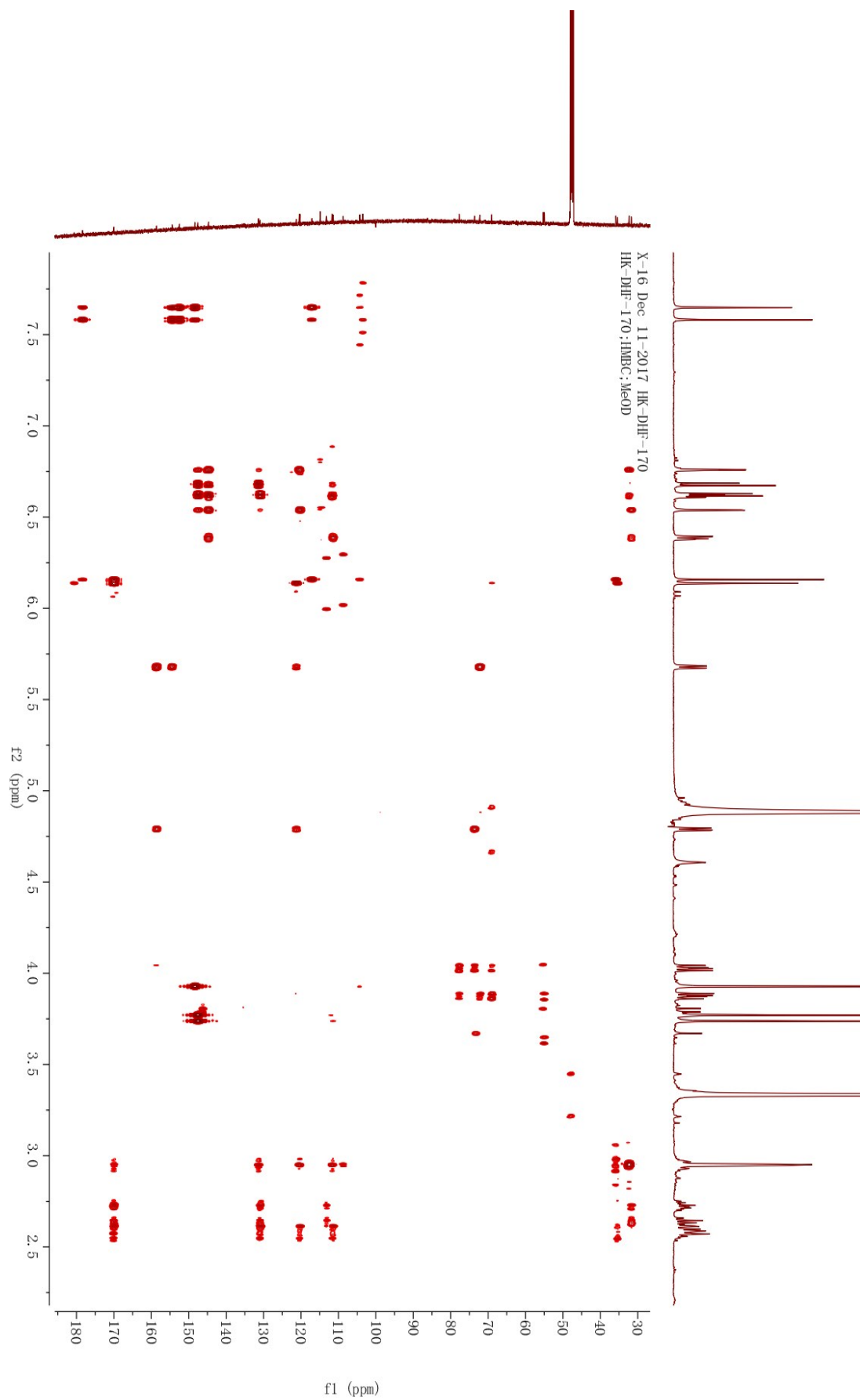


Figure S61. HMBC spectrum of compound **8** in CD₃OD.

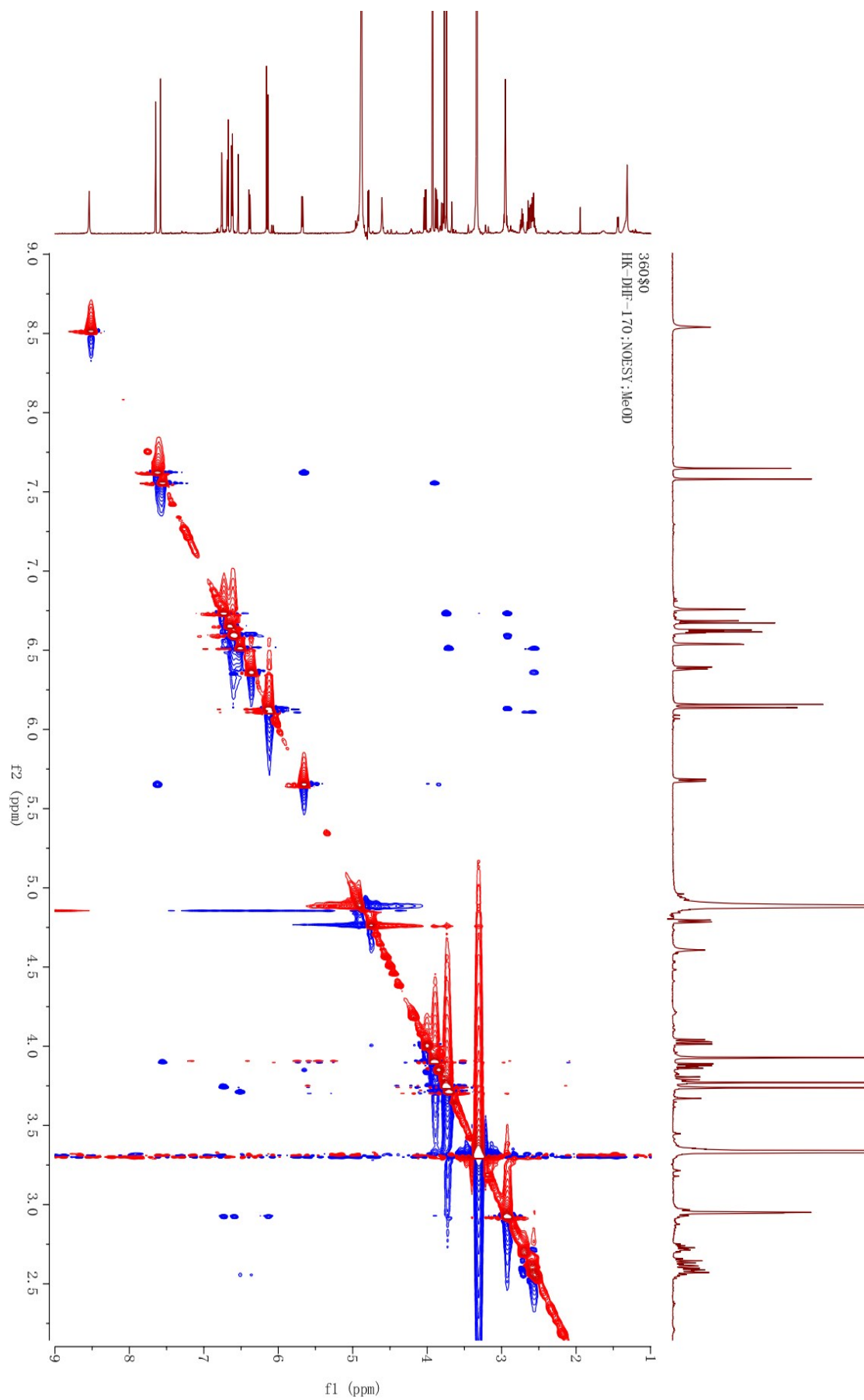
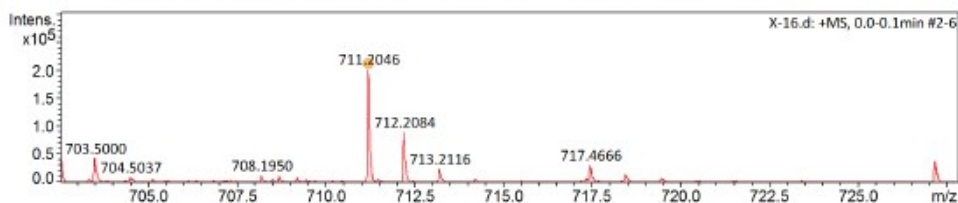
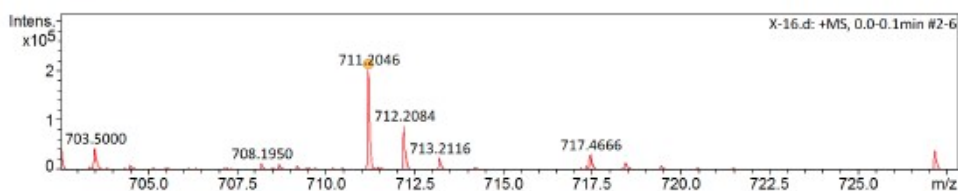
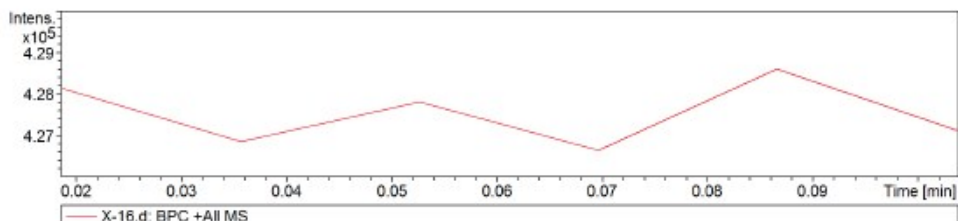


Figure S62. NOESY spectrum of compound **8** in CD₃OD.

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	2018-05-07 16:53:28	
Analysis Name	D:\Data\A5011\YZ\2018.05.07\X-16.d	Operator	Demo User	
Method	DirectInfusion - MS - positive.m	Instrument	compact	8255754.20158
Sample Name	X-16	Comment		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule	Adduct
711.2046	1	C ₃₇ H ₃₆ NaO ₁₃	711.2048	0.3	14.2	1	100.00	20.0	even	ok	M+Na

X-16.d

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by: demo

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Figure S63. HRESIMS spectrum of compound **8**.

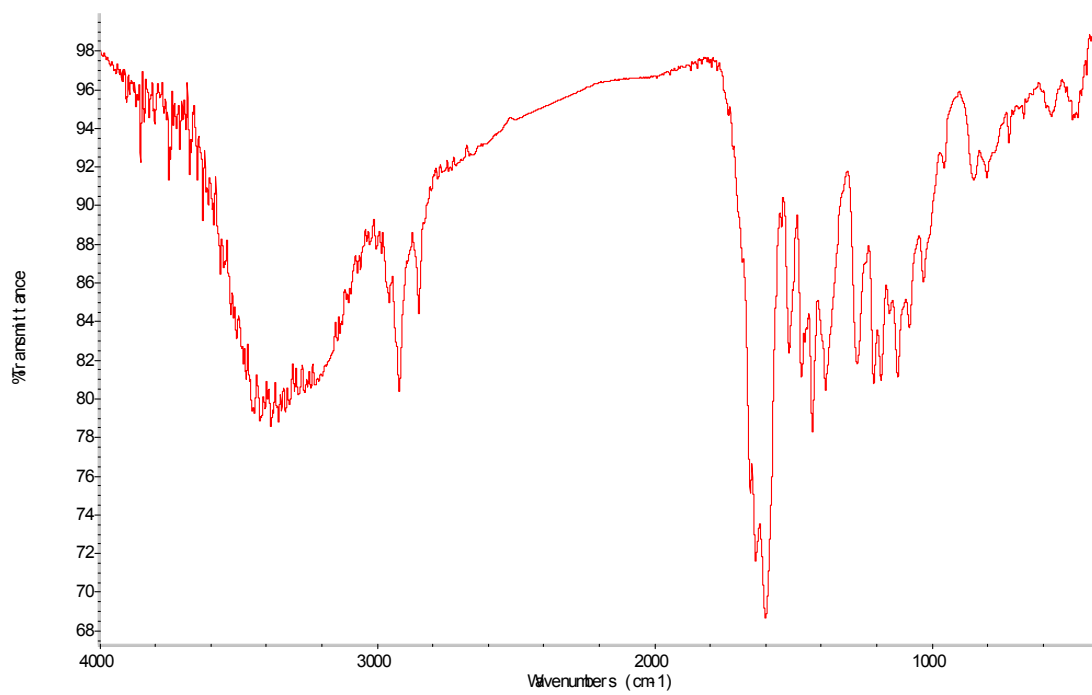


Figure S64. IR spectrum of compound **8**.

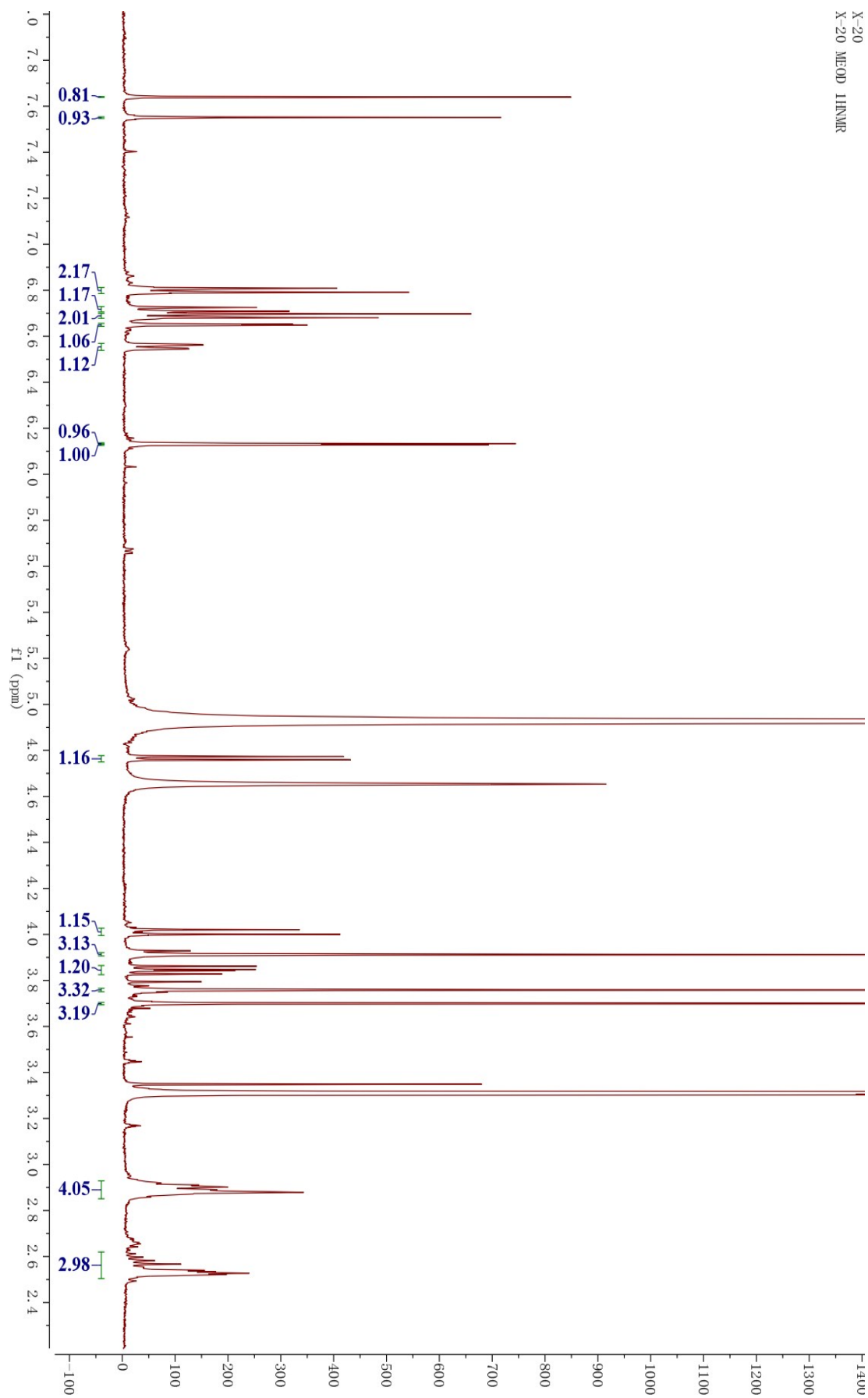


Figure S65. ¹H NMR spectrum (500 MHz) of compound 9 in CD₃OD.

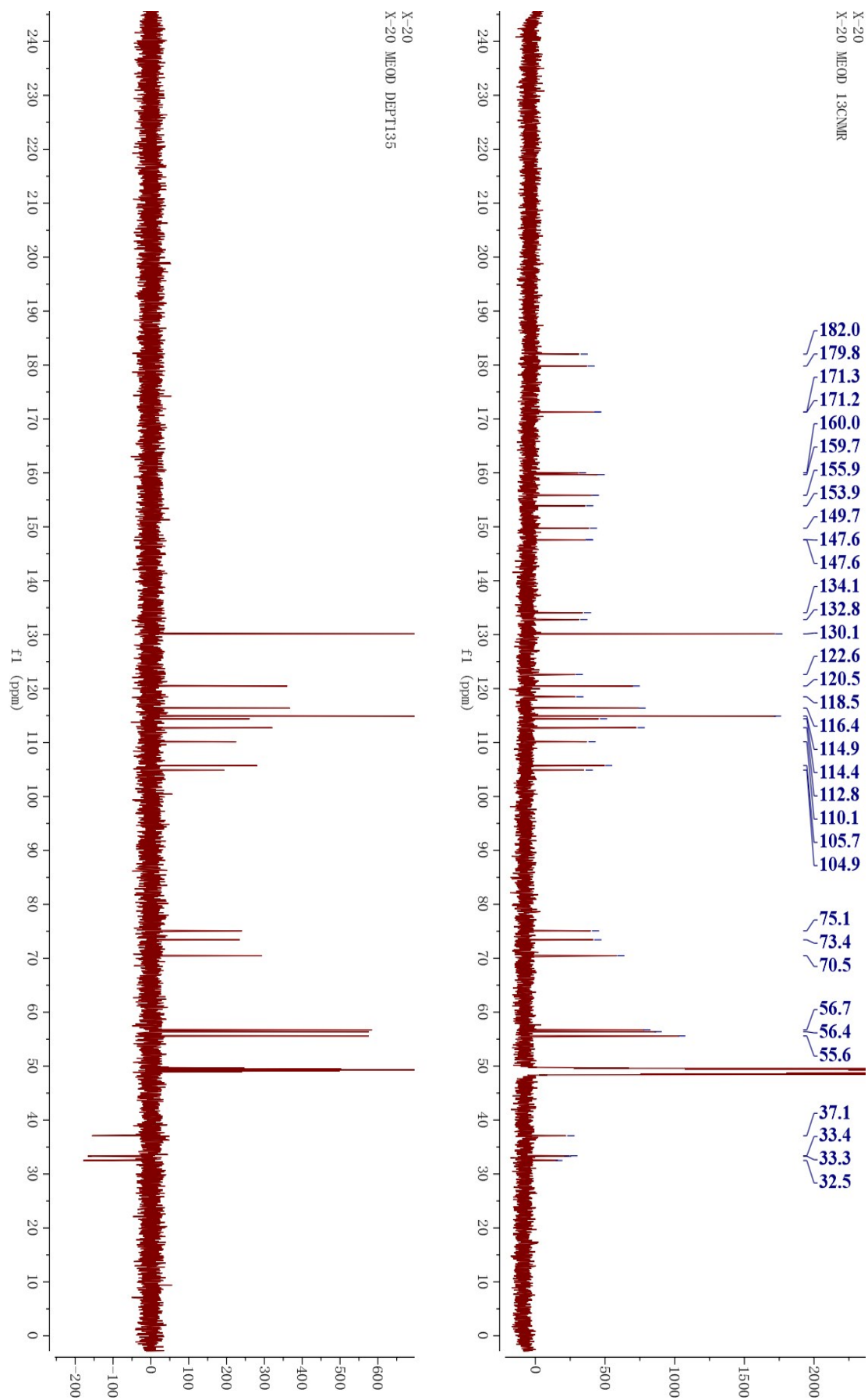


Figure S66. ^{13}C NMR spectrum (125 MHz) of compound **9** in CD_3OD .

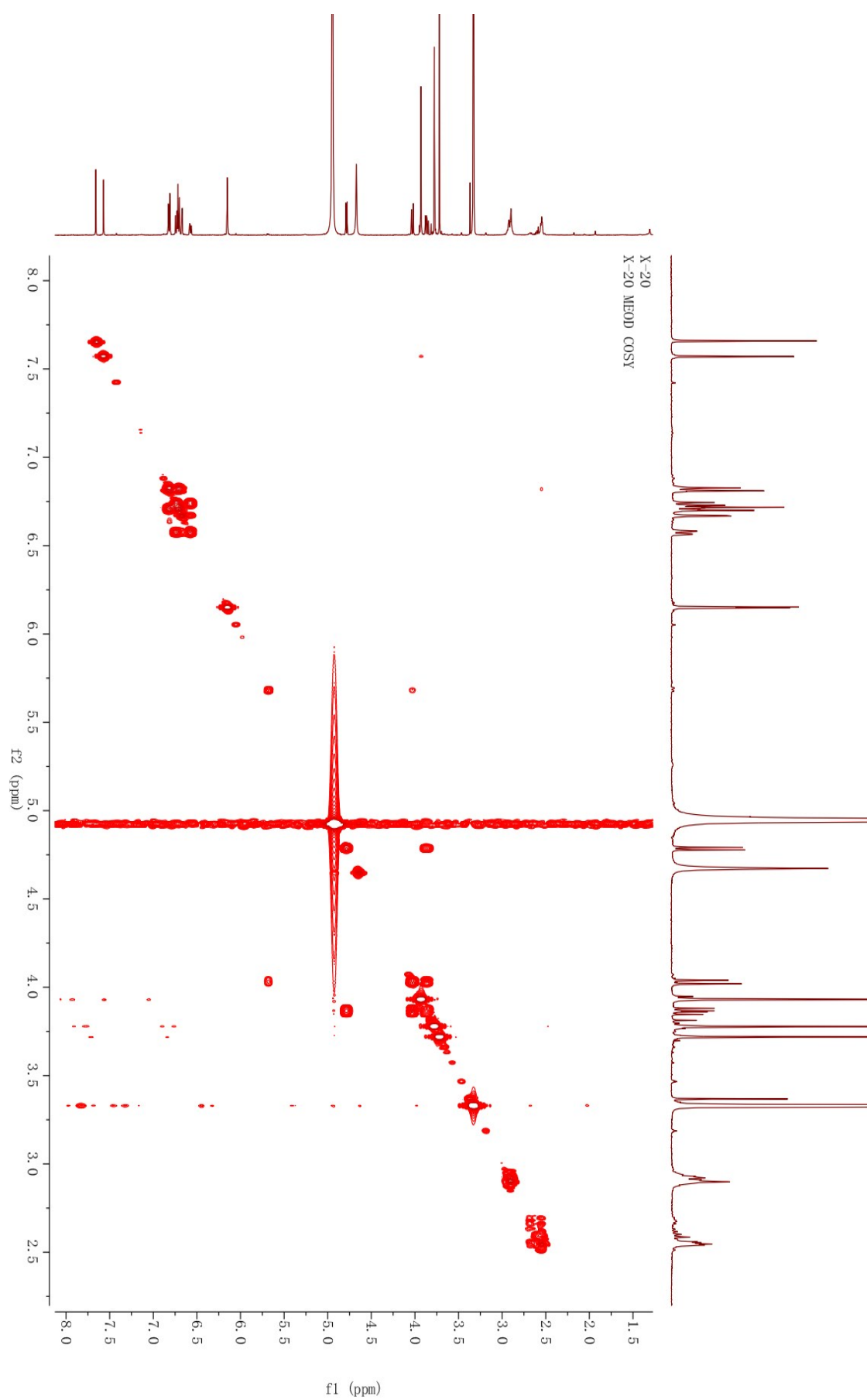


Figure S67. ^1H - ^1H COSY spectrum of compound **9** in CD_3OD .

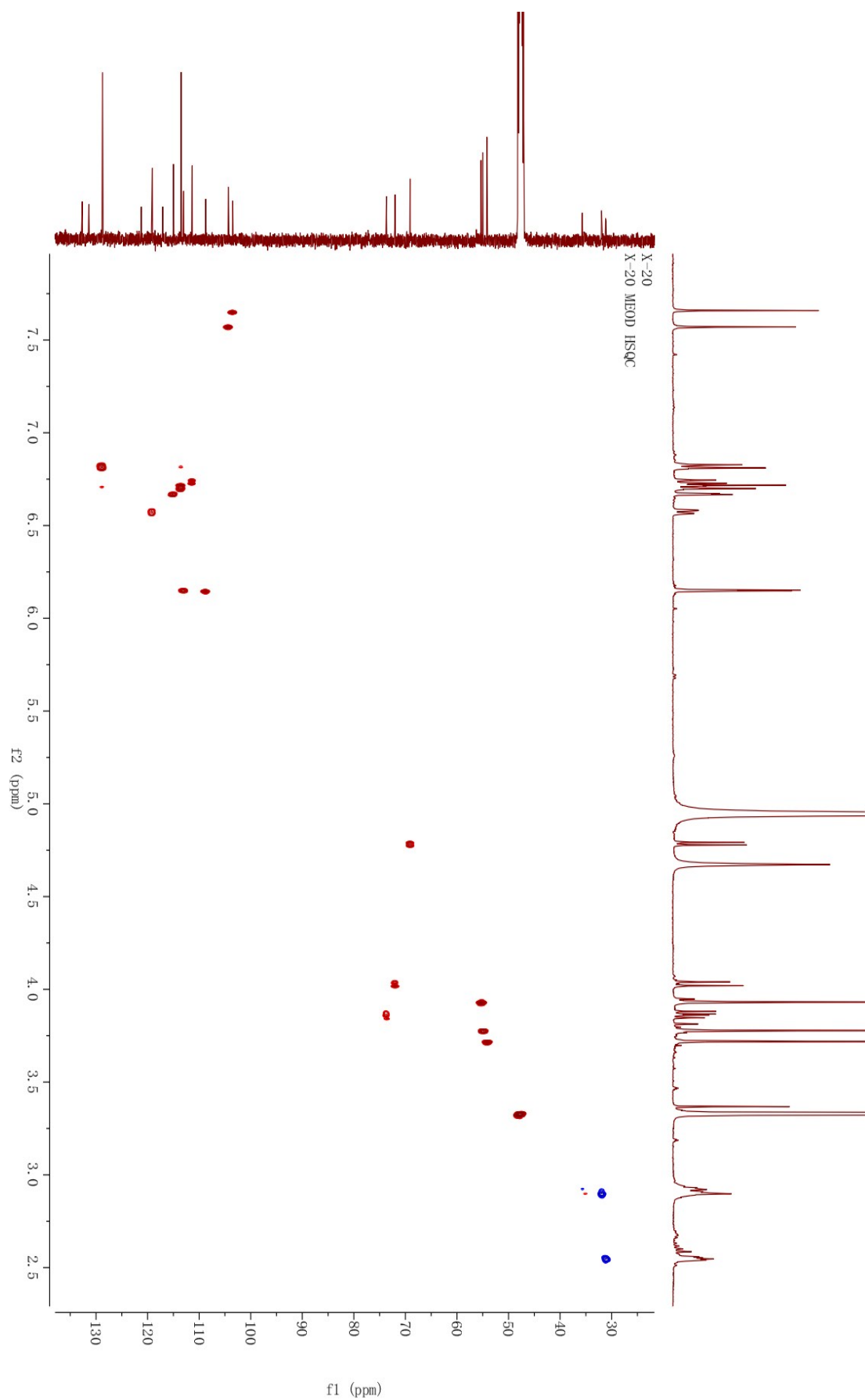


Figure S68. HSQC spectrum of compound **9** in CD₃OD.

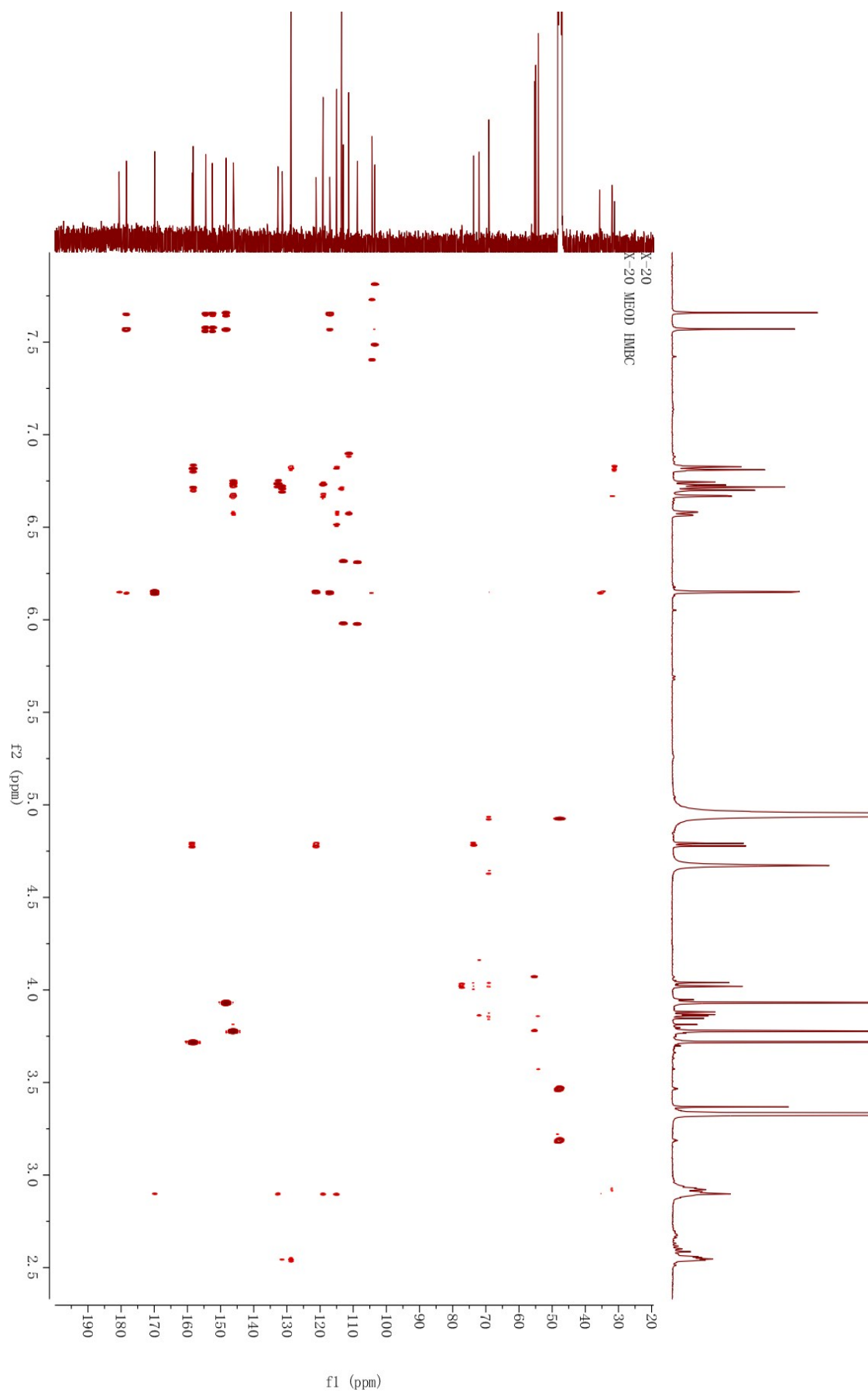


Figure S69. HMBC spectrum of compound **9** in CD₃OD.

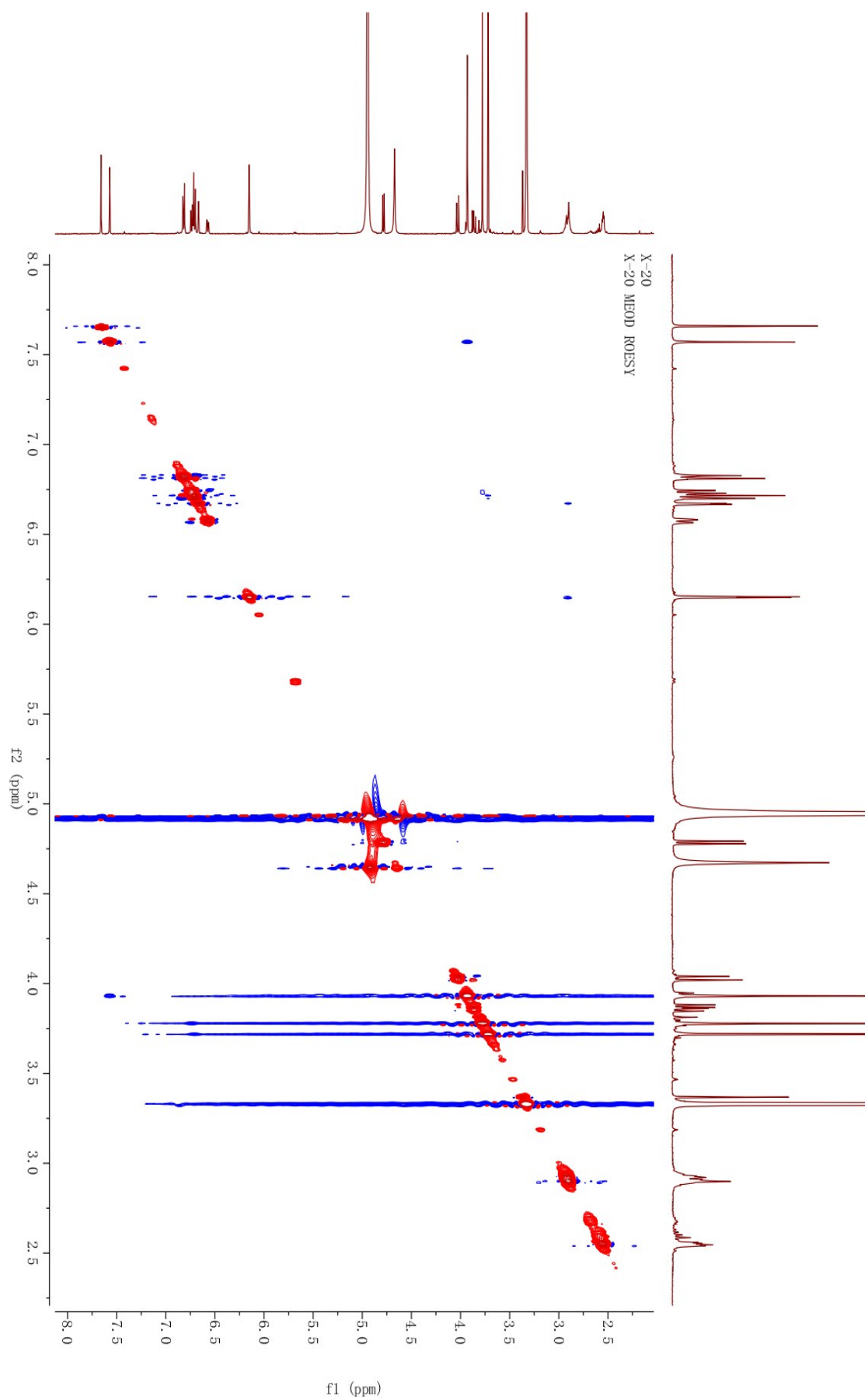


Figure S70. ROESY spectrum of compound **9** in CD₃OD.

Qualitative Analysis Report

Data Filename	HK-DHF-80-.d	Sample Name	HK-DHF-80
Sample Type	Sample	Position	P1-D8
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU-ESI-i.m	Acquired Time	2/5/2018 5:58:34 PM
IRM Calibration Status	Success	DA Method	Default.m

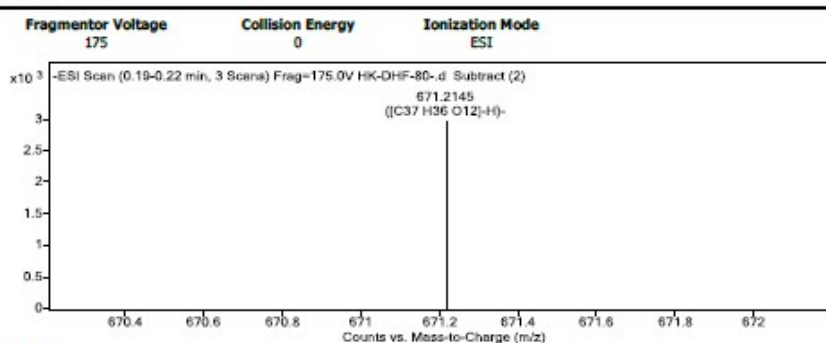
Comment

Sample Group Info.

Acquisition SW 6200 series TOF/6500 series

Version Q-TOF B.05.01 (B5125.2)

User Spectra



Peak List

m/z	z	Abund
339.2344	1	34566.72
340.2375	1	7758.13
341.1043	1	11185.37
369.2447	1	12446.29
713.4753	1	7309.66
740.494	1	16431.98
826.5586	1	6971.37
853.5782	1	11846.47

Formula Calculator Element Limits

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

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C37 H36 O12	672.2207	671.2134	671.2145	-1.10	-1.64	20.0000

--- End Of Report ---

Figure S71. HRESIMS spectrum of compound **9**.

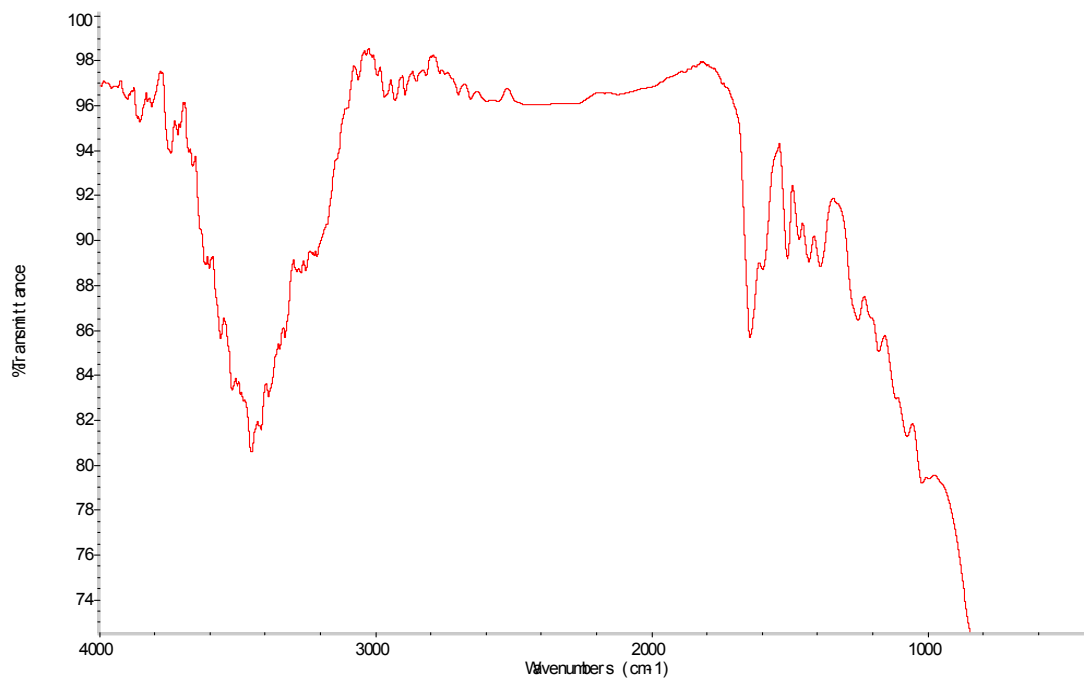


Figure S72. IR spectrum of compound **9**.

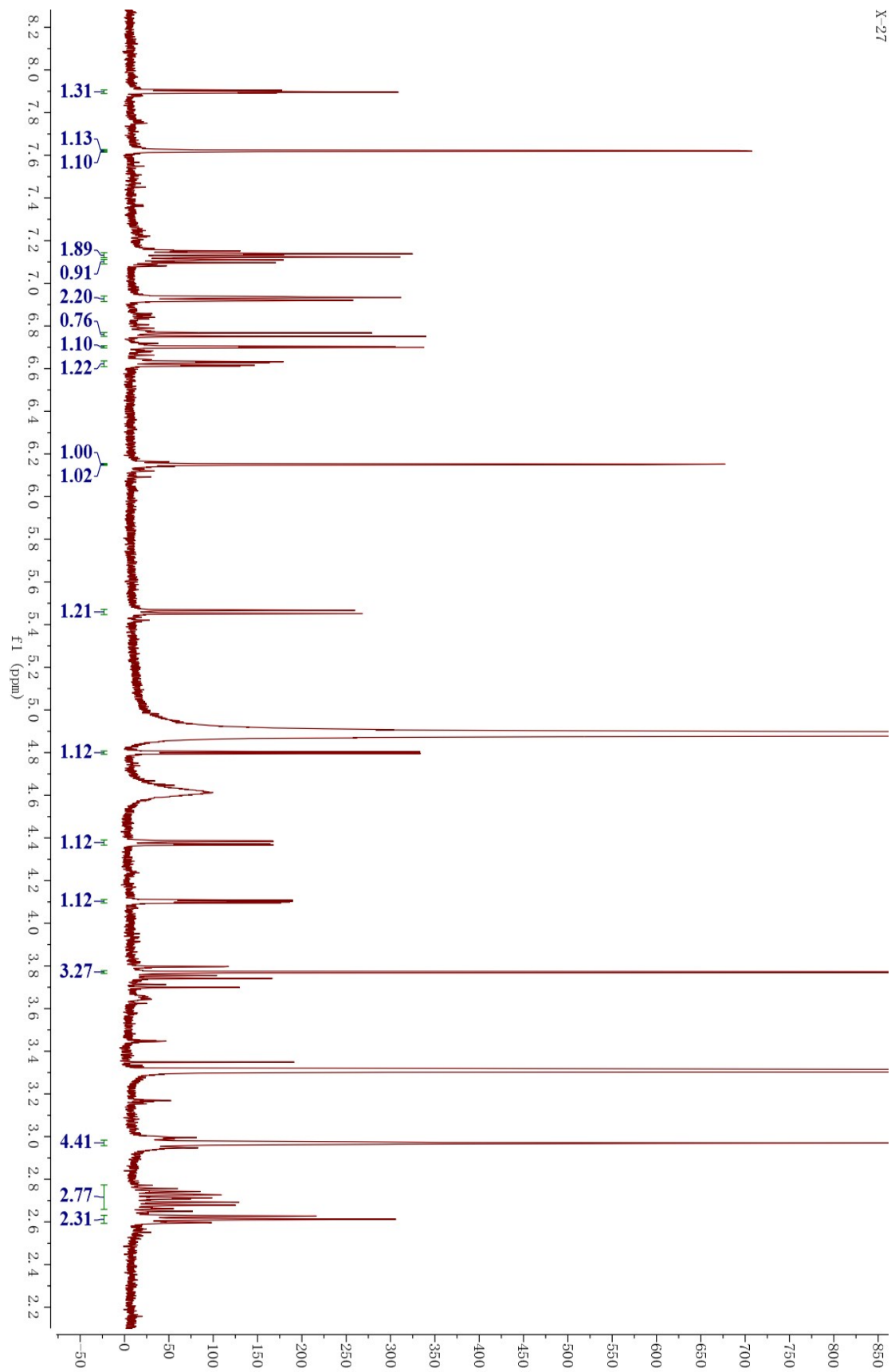


Figure S73. ^1H NMR spectrum (500 MHz) of compound **10** in CD_3OD .

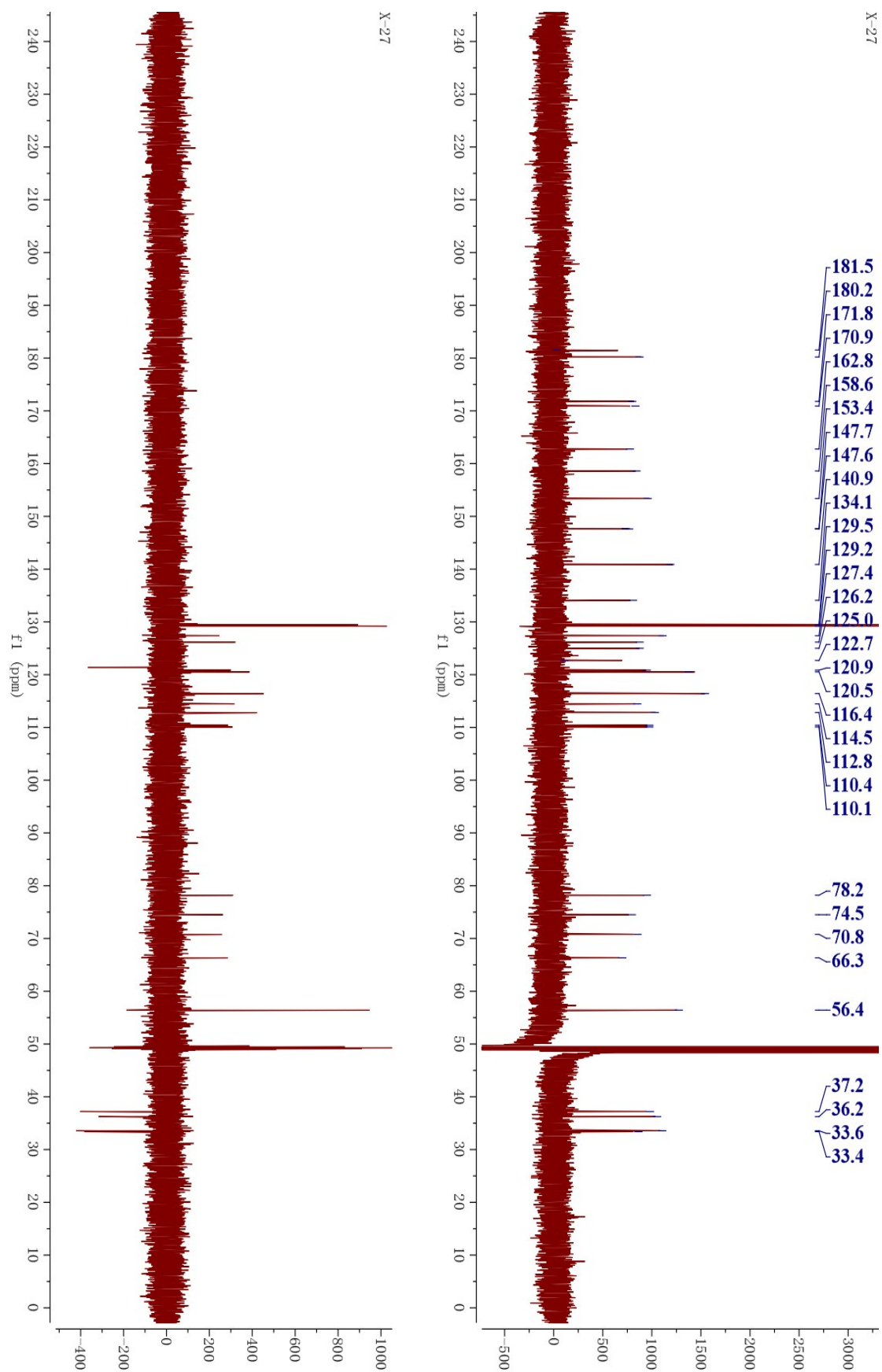


Figure S74. ¹³C NMR spectrum (125 MHz) of compound **10** in CD₃OD.

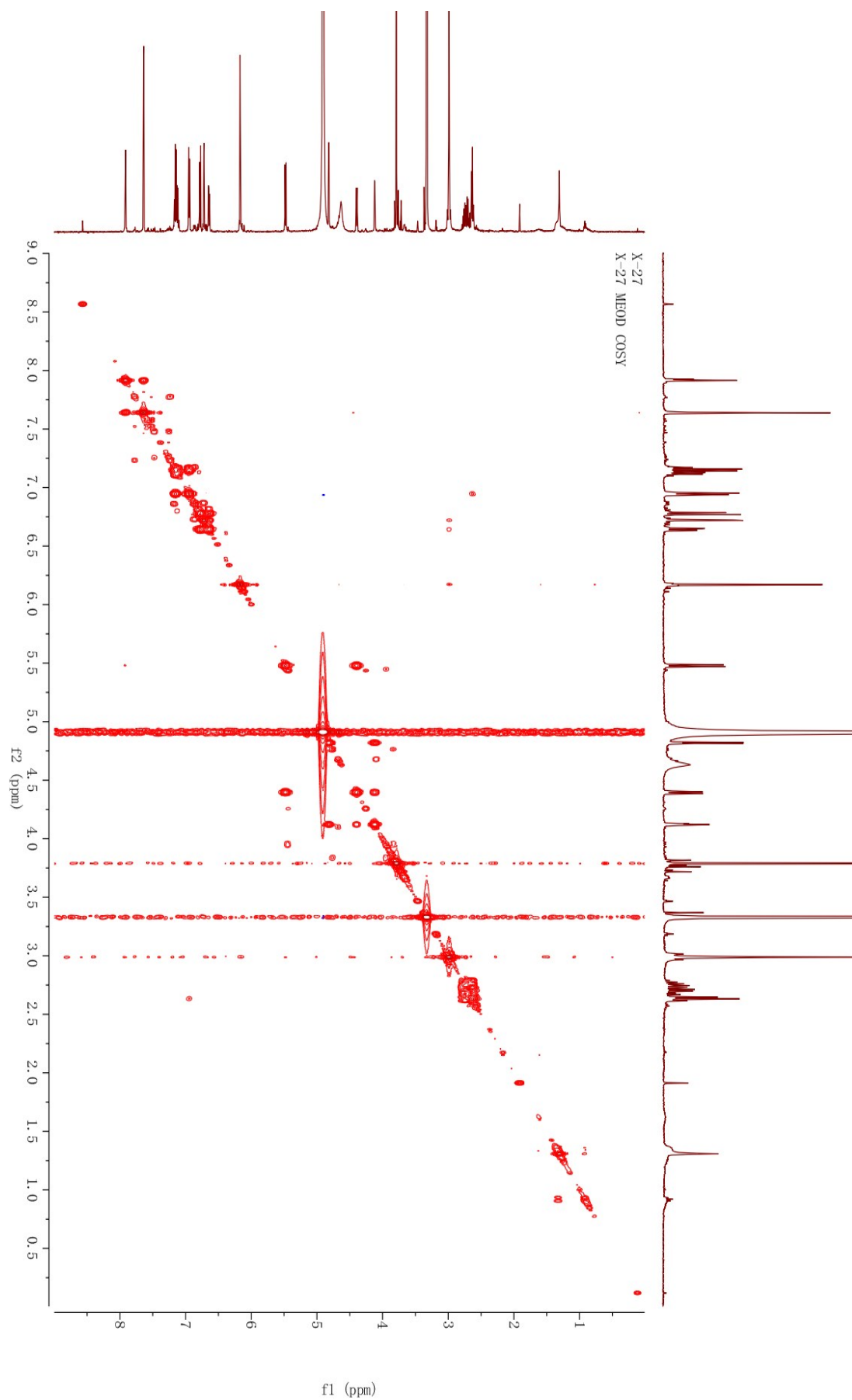


Figure S75. ^1H - ^1H COSY spectrum of compound **10** in CD_3OD .

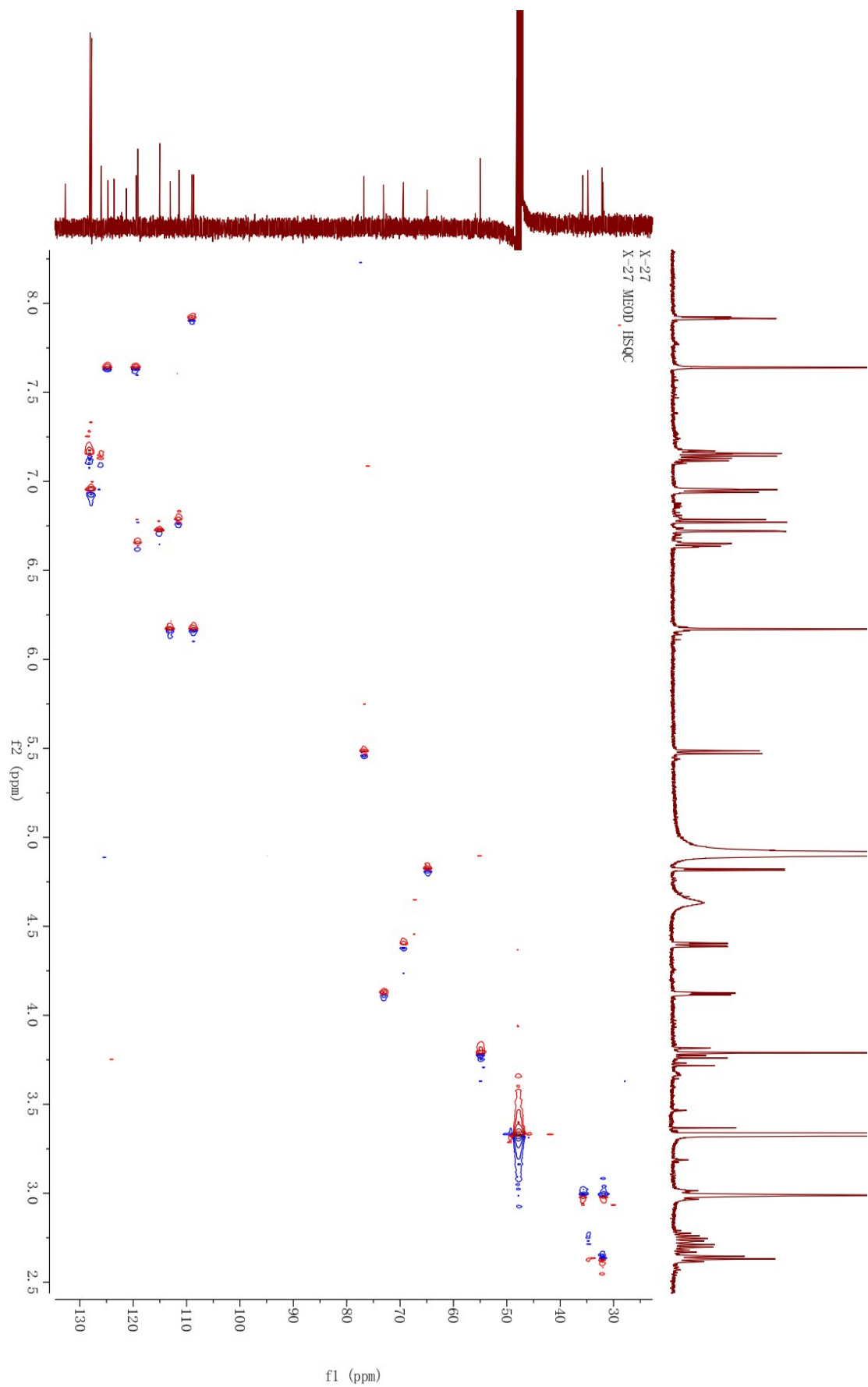


Figure S76. HSQC spectrum of compound **10** in CD₃OD.

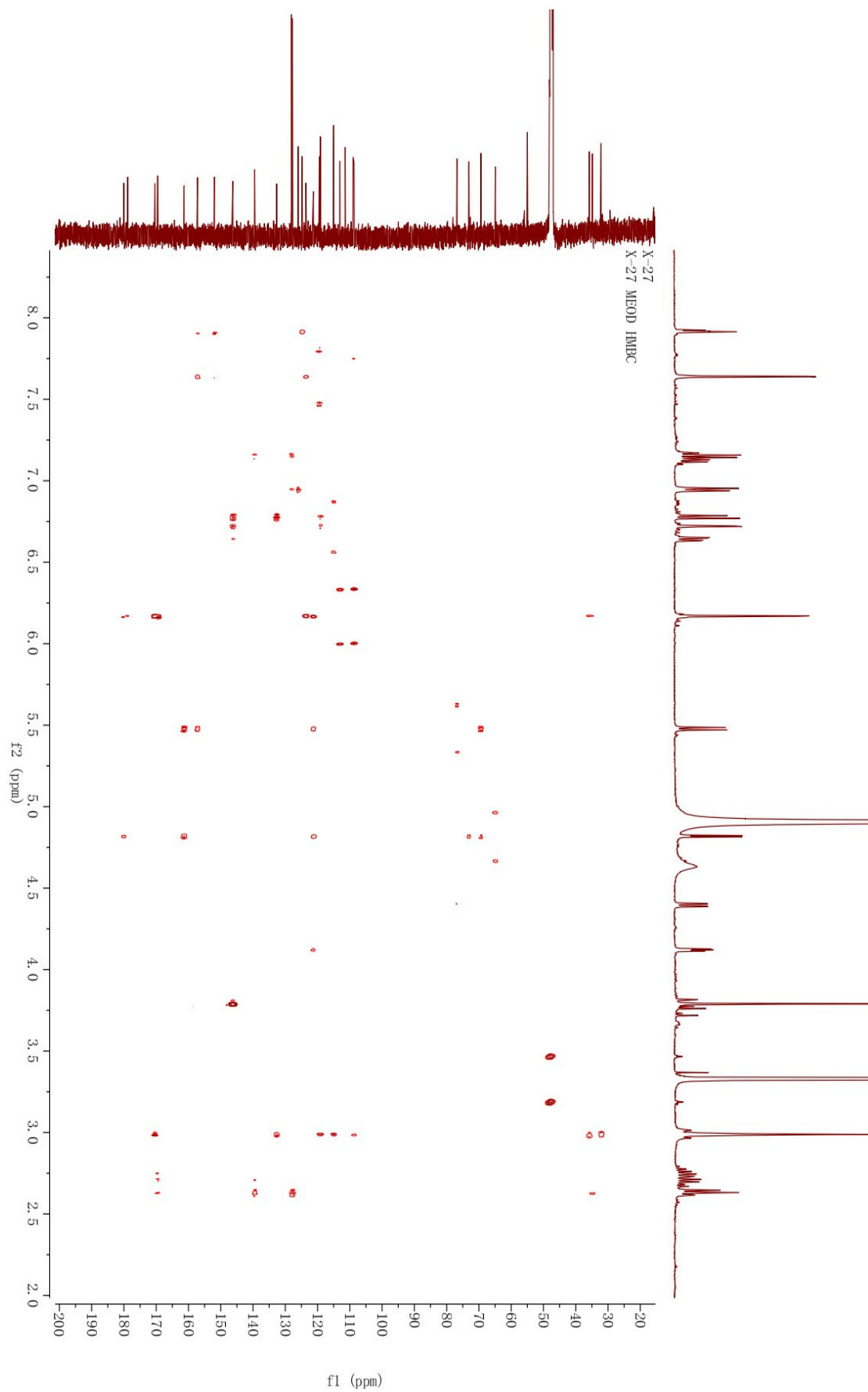


Figure S77. HMBC spectrum of compound **10** in CD₃OD.

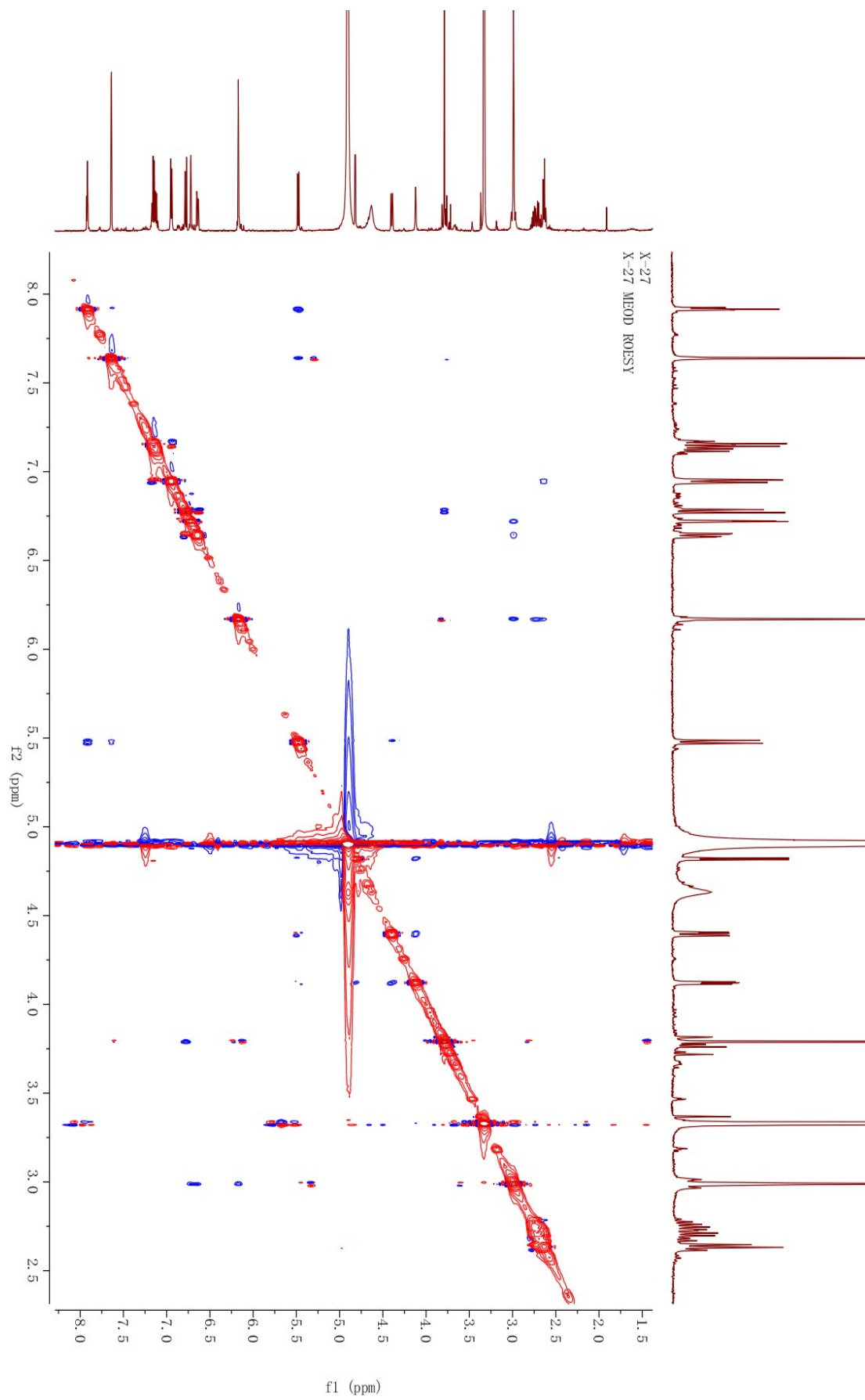


Figure S78. ROESY spectrum of compound **10** in CD₃OD.

Compound Spectrum SmartFormula Report

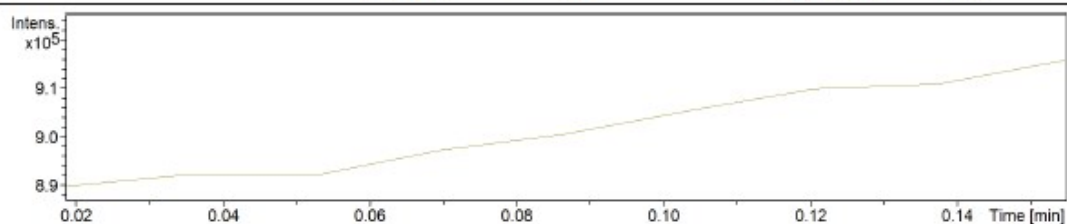
Analysis Info

Analysis Name D:\Data\A501\Wanghui\X-27.d
 Method DirectInfusion - MS - positive.m
 Sample Name kfd-8-25
 Comment

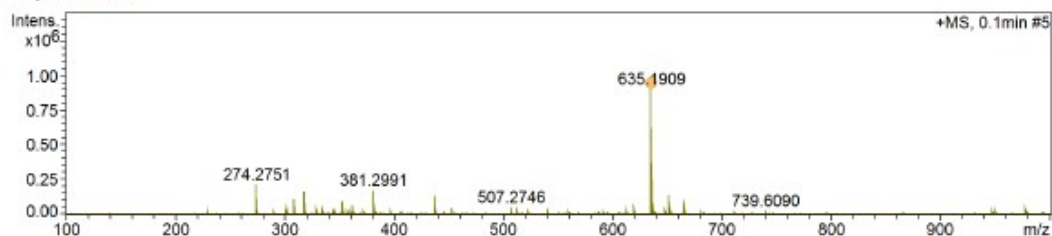
Acquisition Date 2017-12-15 18:23:29
 Operator Demo User
 Instrument compact 8255754.20158

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



+MS, 0.1min #5



#	Ion Formula	m/z	err [mDa]	err [ppm]	mSigma	rdB	e ⁻ Conf	N-Rule
1	C37H31O10	635.1912	0.3	0.4	1.6	23.0	even	ok
1	C36H28N4NaO6	635.1901	-0.8	-1.3	3.8	25.0	even	ok
1	C34H28KN8O3	635.1916	0.7	1.1	27.6	25.0	even	ok
2	C34H23N10O4	635.1898	-1.1	-1.7	6.0	29.0	even	ok
2	C33H20N14Na	635.1888	-2.2	-3.4	10.0	31.0	even	ok
2	C30H24KN14O	635.1889	-2.0	-3.2	28.4	26.0	even	ok
3	C38H27N4O6	635.1925	1.6	2.5	10.3	28.0	even	ok
3	C37H24N8NaO2	635.1914	0.5	0.8	11.6	30.0	even	ok
3	C33H32KN4O7	635.1903	-0.7	-1.0	30.5	20.0	even	ok
4	C35H19N14	635.1912	0.2	0.4	12.0	34.0	even	ok
4	C35H32NaO10	635.1888	-2.2	-3.4	12.9	20.0	even	ok
4	C32H36KO11	635.1889	-2.0	-3.1	36.6	15.0	even	ok
5	C33H27N6O8	635.1885	-2.4	-3.8	14.2	24.0	even	ok

X-27.d

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Figure S79. HRESIMS spectrum of compound **10**.

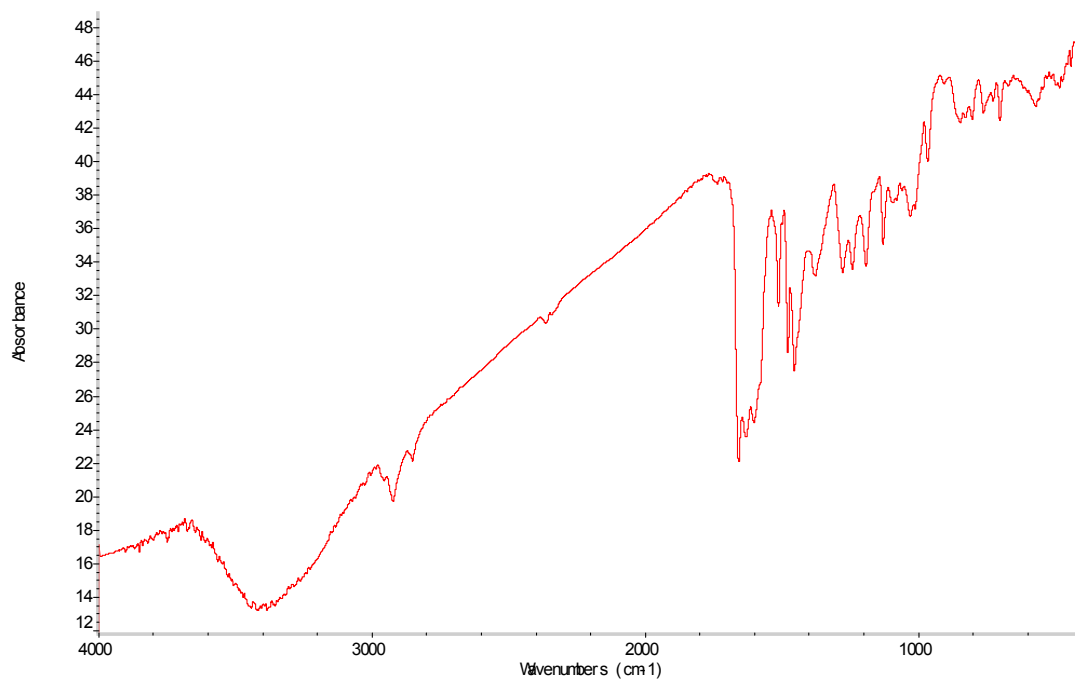


Figure S80. IR spectrum of compound **10**.

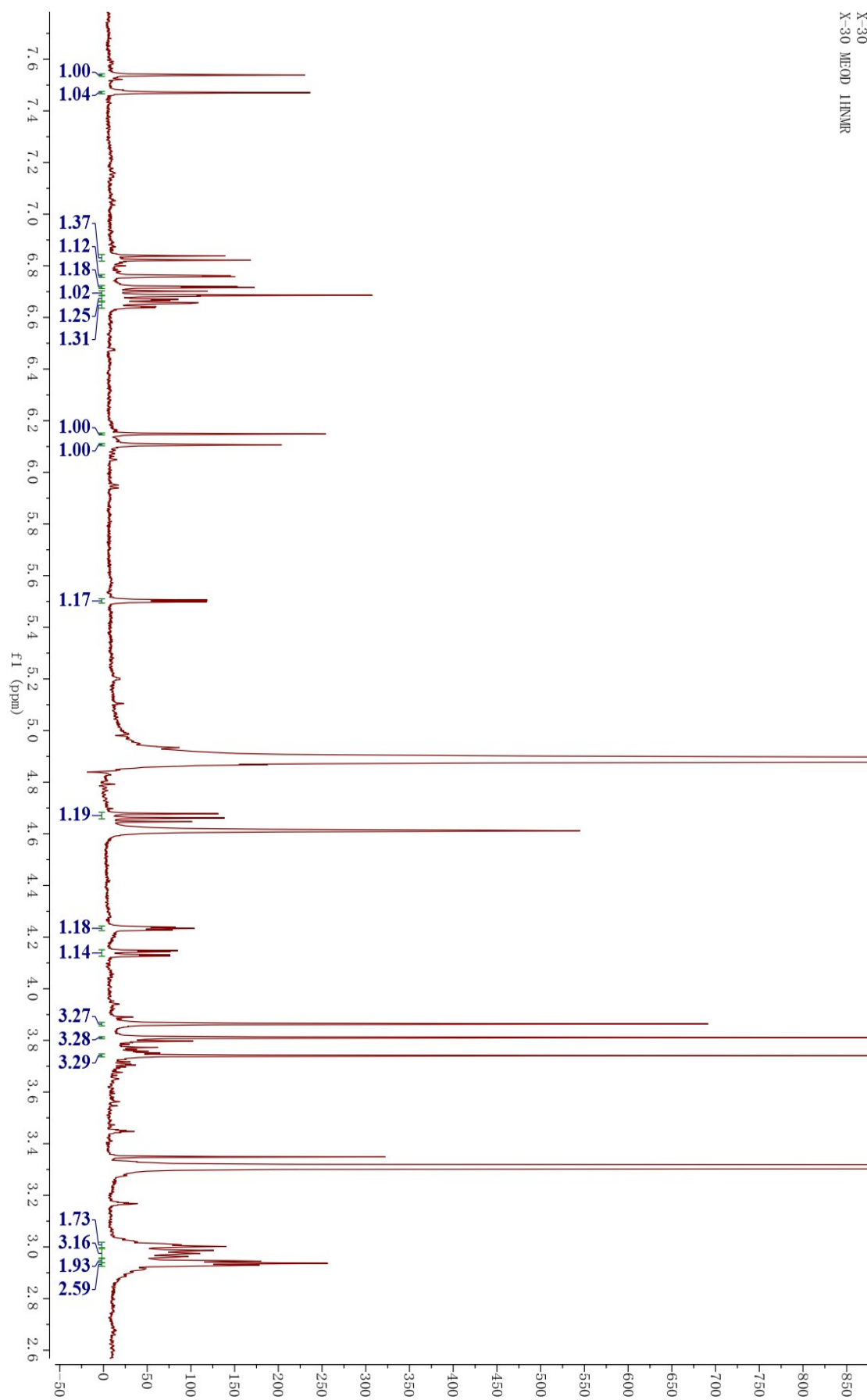


Figure S81. ¹H NMR spectrum (500 MHz) of compound 11 in CD₃OD.

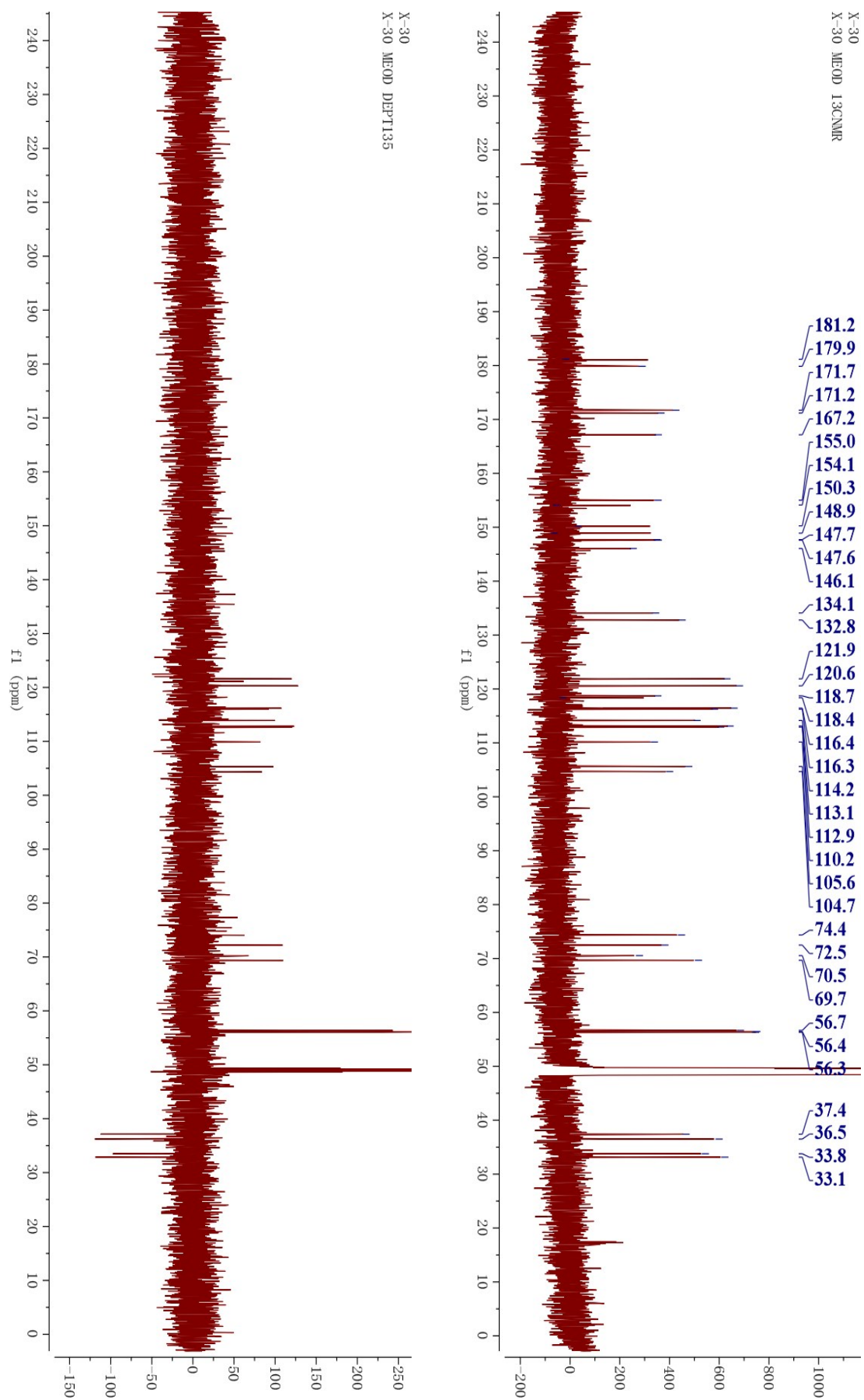


Figure S82. ^{13}C NMR spectrum (125 MHz) of compound **11** in CD_3OD .

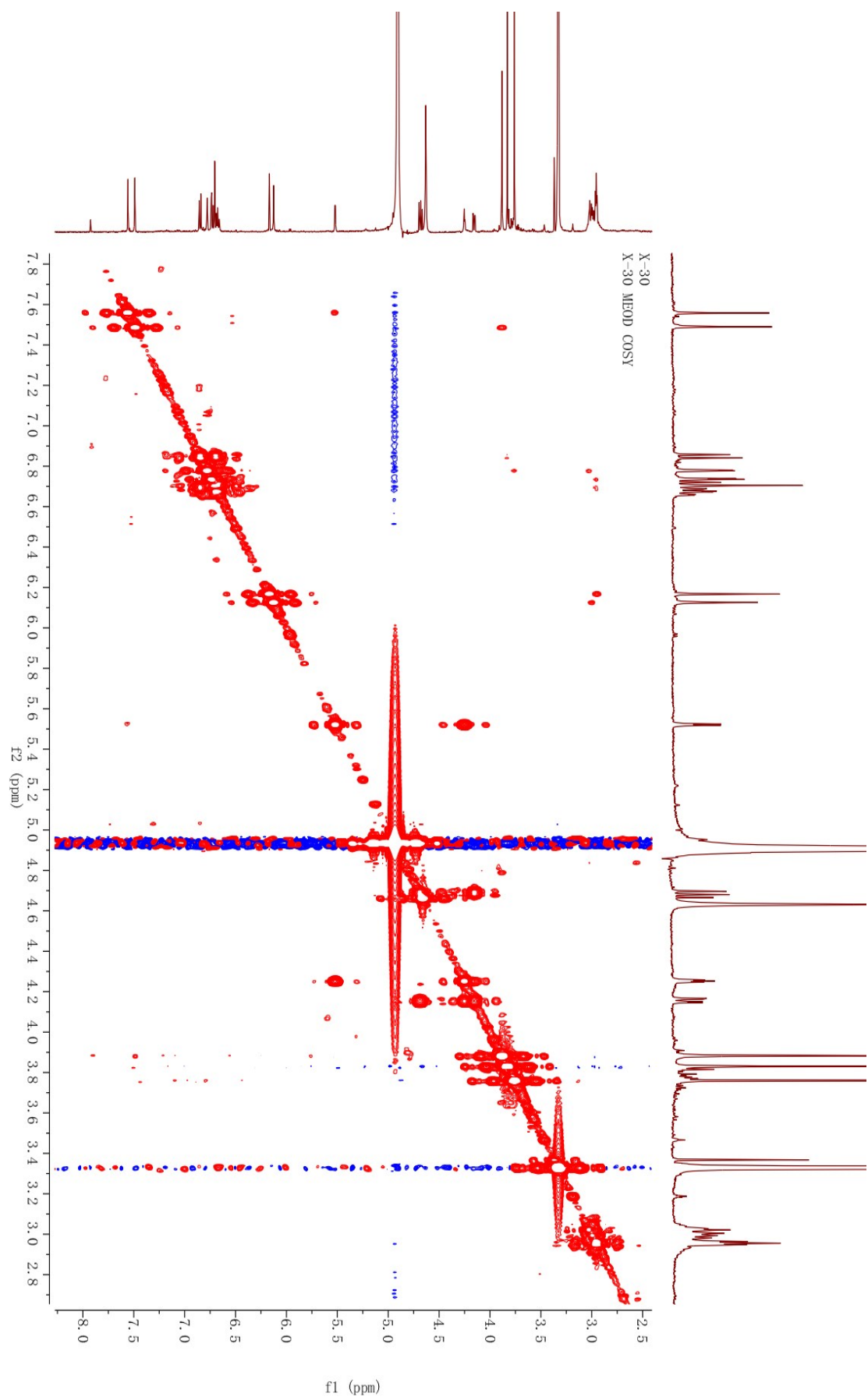


Figure S83. ^1H - ^1H COSY spectrum of compound **11** in CD_3OD .

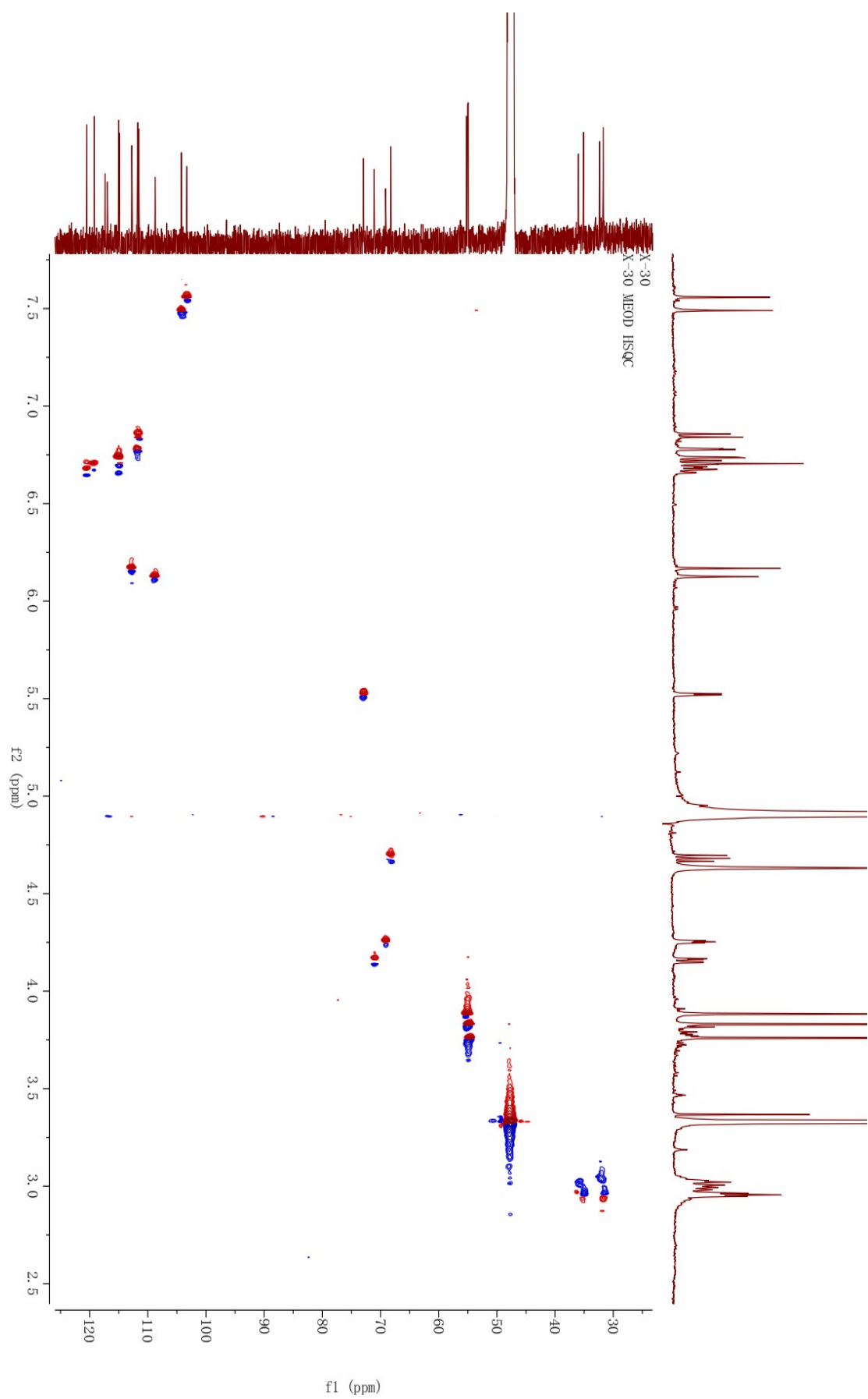


Figure S84. HSQC spectrum of compound **11** in CD₃OD.

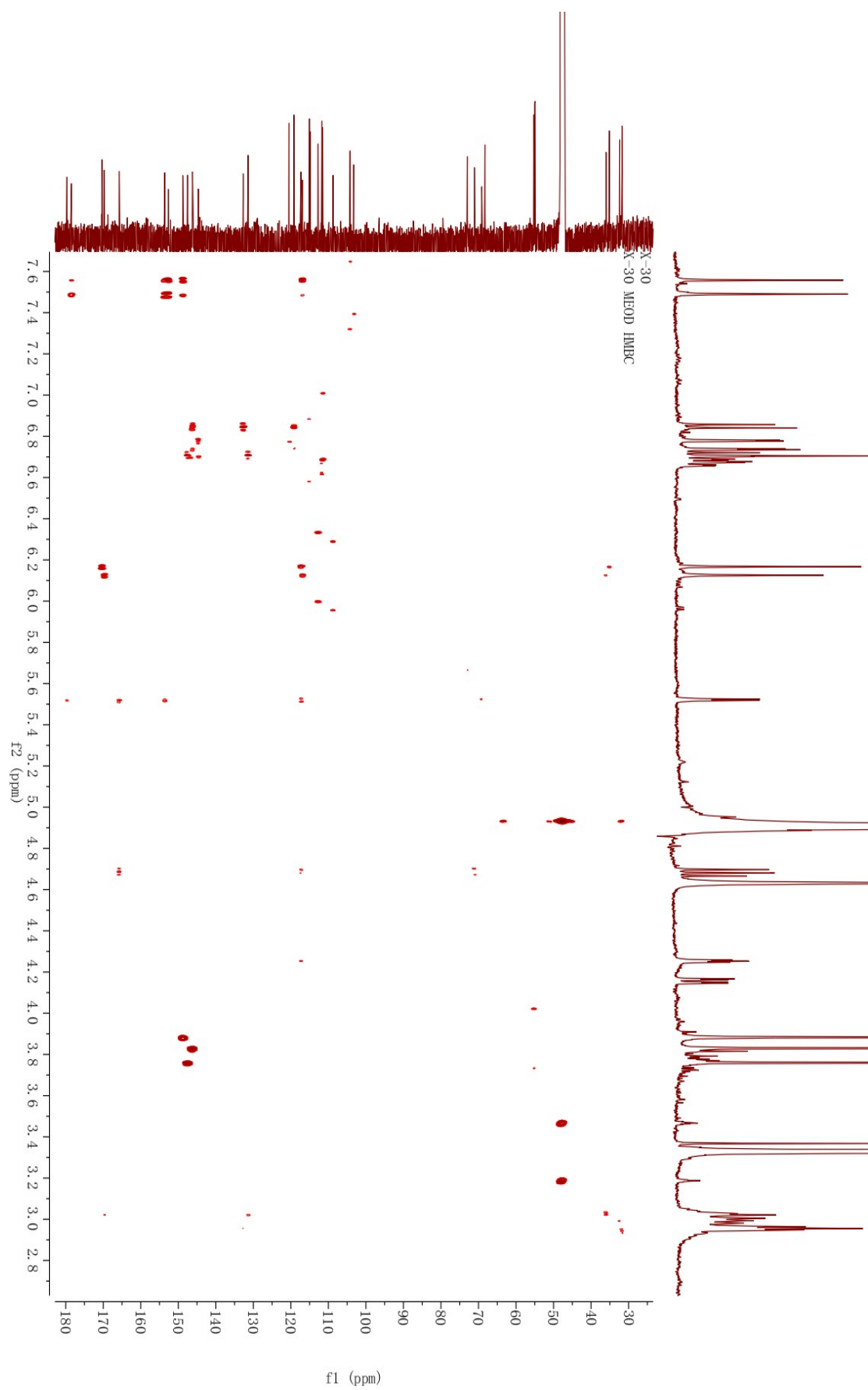


Figure S85. HMBC spectrum of compound **11** in CD₃OD.

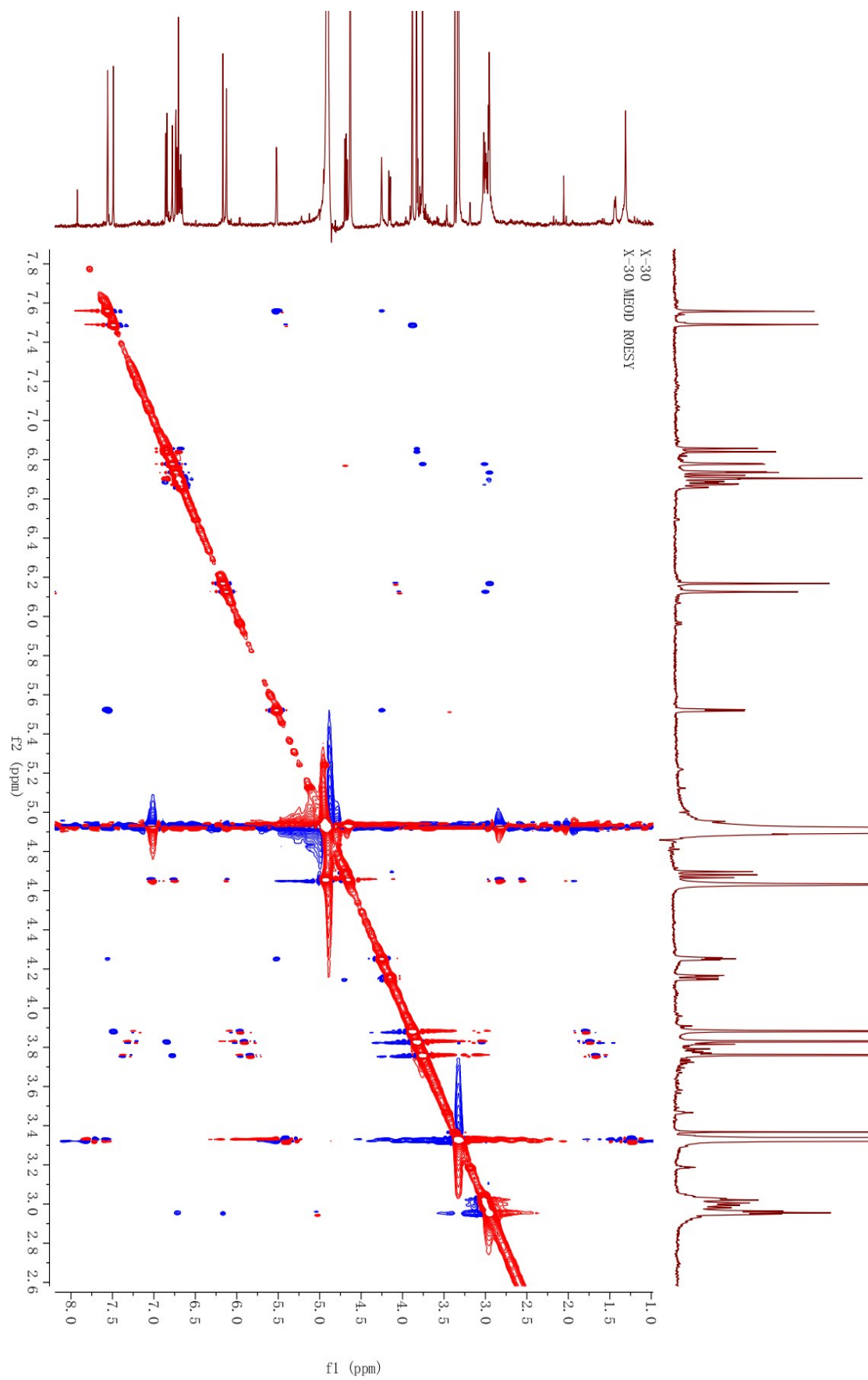


Figure S86. ROESY spectrum of compound 11 in CD₃OD.

Mass Spectrum SmartFormula Report

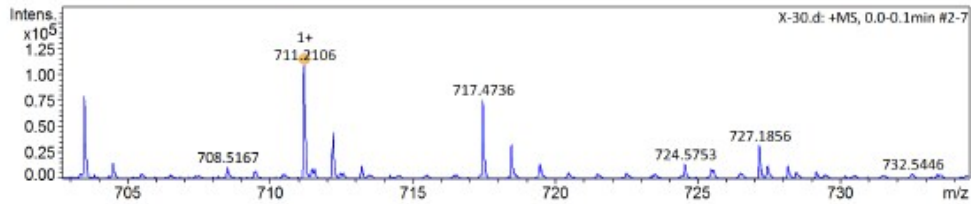
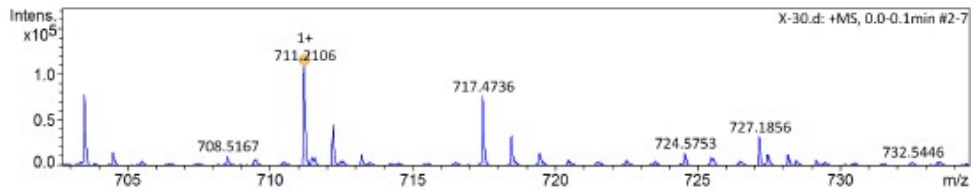
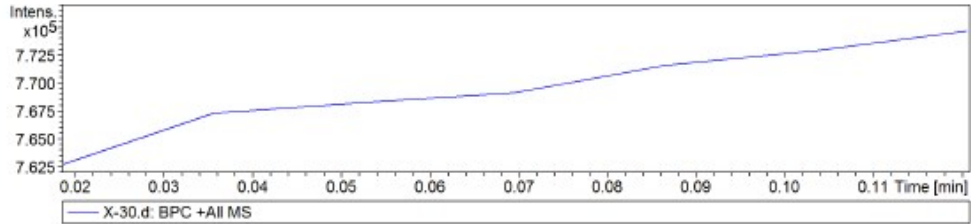
Analysis Info

Analysis Name D:\Data\A501\Wanghui\X-30.d
 Method DirectInfusion - MS - positive.m
 Sample Name kfd-6-25
 Comment

Acquisition Date 2017-12-15 18:27:54
 Operator Demo User
 Instrument compact 8255754.20158

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1300 m/z	Set Charging Voltage	2000 V	Set Divert Valve	Source
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	Adduct
711.210592	1	C37H38NaO13	100.00	711.204812	-5.8	-8.1	3.2	20.0	even	M+Na

X-30.d

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Figure S87. HRESIMS spectrum of compound **11**.

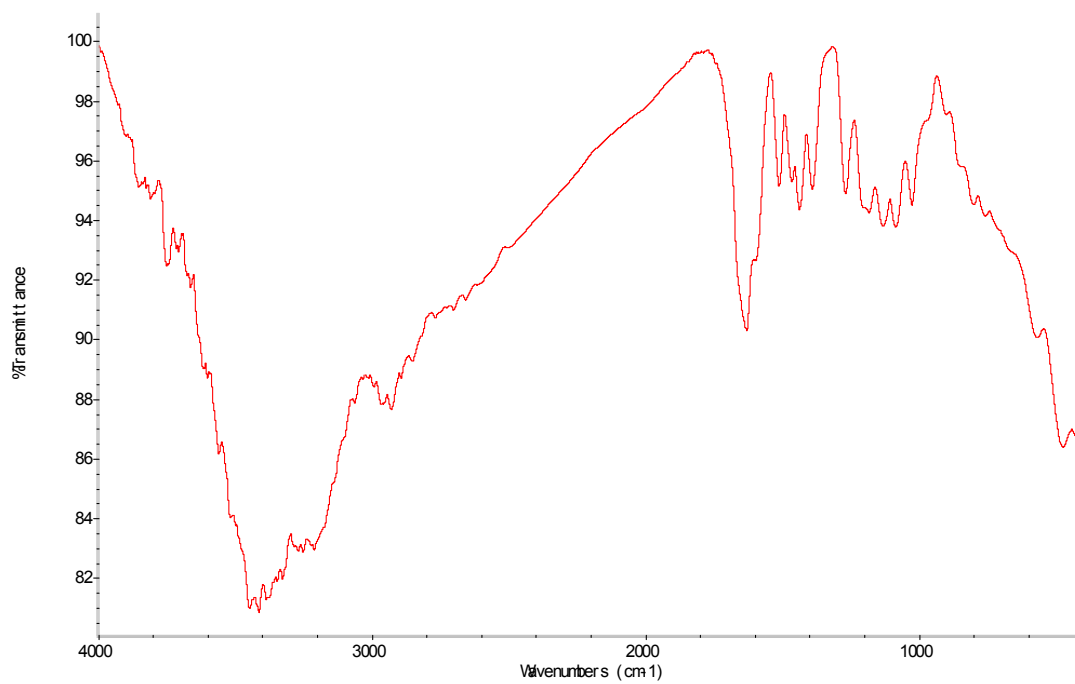


Figure S88. IR spectrum of compound **11**.