

Supporting Information

Copies of HR-ESIMS for **1** and **1s/r**; LR-ESIMS for **1A**, **1B**, **1As/r**, **1A's/r**, and **1Bs/r**; and 1D and 2D NMR spectra for **1**, **1s/r**, **1A**, **1B**, **1As/r**, **1A's/r**, and **1Bs/r**; and **Figure S1**.

Table of Contents:

1. HR-ESIMS for compound 1	S4-S5
2. ¹ H (700 MHz) NMR spectrum of compound 1 in CD ₃ OD.....	S6-S8
3. ¹³ C (175 MHz) NMR spectrum of compound 1 in CD ₃ OD.....	S9-S13
4. ¹³ C (175 MHz) spectrum of compound 1 in CD ₃ OH	S14
5. Comparison of ¹³ C (175 MHz) NMR spectrum of compound 1 in CD ₃ OH with that in CD ₃ OD	S15
6. DEPT135 (175 MHz) spectrum of compound 1 in CD ₃ OD.....	S16-S20
7. ¹ H- ¹ H COSY (700 MHz) spectrum of compound 1 in CD ₃ OD	S21-S24
8. HSQC (700 MHz) spectrum of compound 1 in CD ₃ OD	S25-S28
9. HMBC (700 MHz) spectrum of compound 1 in CD ₃ OD	S29-S35
10. NOESY (700 MHz) spectrum of compound 1 in CD ₃ OD	S36-S41
11. 2D JRES (700 MHz) spectrum of compound 1 in CD ₃ OD.....	S42-S44
12. HETLOC (700 MHz) spectrum of compound 1 in CD ₃ OD.....	S45-S48
13. UV spectrum of compound 1	S49
14. LR-ESIMS for fragment 1A	S50-S51
15. ¹ H (600 MHz) NMR spectrum of the fragment 1A in CD ₃ OD.....	S52-S55
16. ¹ H- ¹ H COSY (600 MHz) spectrum of the fragment 1A in CD ₃ OD	S56-S59
17. LR-ESIMS for fragment 1B	S60-S61
18. ¹ H (600 MHz) NMR spectrum of the fragment 1B in CD ₃ OD.....	S62-S65
19. ¹ H- ¹ H COSY (600 MHz) spectrum of the fragment 1B in CD ₃ OD	S66-S69
20. HR-ESIMS for compound 1s	S70-S71
21. ¹ H (400 MHz) NMR spectrum of compound 1s in CDCl ₃	S72-S74
22. ¹ H- ¹ H COSY (400 MHz) spectrum of compound 1s in CDCl ₃	S75-S77

23. HR-ESIMS for compound 1r	S78-S79
24. ¹ H (400 MHz) NMR spectrum of compound 1r in CDCl ₃	S80-S82
25. ¹ H- ¹ H COSY (400 MHz) spectrum of compound 1r in CDCl ₃	S83-S86
26. LR-ESIMS for fragment 1As	S87
27. ¹ H (700 MHz) NMR spectrum of the fragment 1As in CD ₃ OD	S88-S90
28. ¹ H- ¹ H COSY (700 MHz) spectrum of the fragment 1As in CD ₃ OD	S91-S94
29. LR-ESIMS for fragment 1Ar	S95
30. ¹ H (700 MHz) NMR spectrum of the fragment 1Ar in CD ₃ OD	S96-S99
31. ¹ H- ¹ H COSY (700 MHz) spectrum of the fragment 1Ar in CD ₃ OD	S100-S103
32. LR-ESIMS for fragment 1A's	S104
33. ¹ H (700 MHz) NMR spectrum of the fragment 1A's in CD ₃ OD	S105-S107
34. ¹ H- ¹ H COSY (700 MHz) spectrum of the fragment 1A's in CD ₃ OD	S108-S111
35. LR-ESIMS for fragment 1A'r	S112
36. ¹ H (700 MHz) NMR spectrum of the fragment 1A'r in CD ₃ OD	S113-S116
37. ¹ H- ¹ H COSY (700 MHz) spectrum of the fragment 1A'r in CD ₃ OD	S117-S120
38. LR-ESIMS for fragment 1Bs	S121
39. ¹ H (600 MHz) NMR spectrum of the fragment 1Bs in CD ₃ OD	S122-S124
40. ¹ H- ¹ H COSY (600 MHz) spectrum of the fragment 1Bs in CD ₃ OD	S125-S128
41. LR-ESIMS for fragment 1Br	S129
42. ¹ H (600 MHz) NMR spectrum of the fragment 1Br in CD ₃ OD	S130-S132
43. ¹ H- ¹ H COSY (600 MHz) spectrum of the fragment 1Br in CD ₃ OD	S133-S136
44. Figure S1. Agonistic effects of chenodeoxycholic acid on hFXR in HepG2 cells	S137

HR-ESIMS for compound 1

Mass Spectrum SmartFormula Report

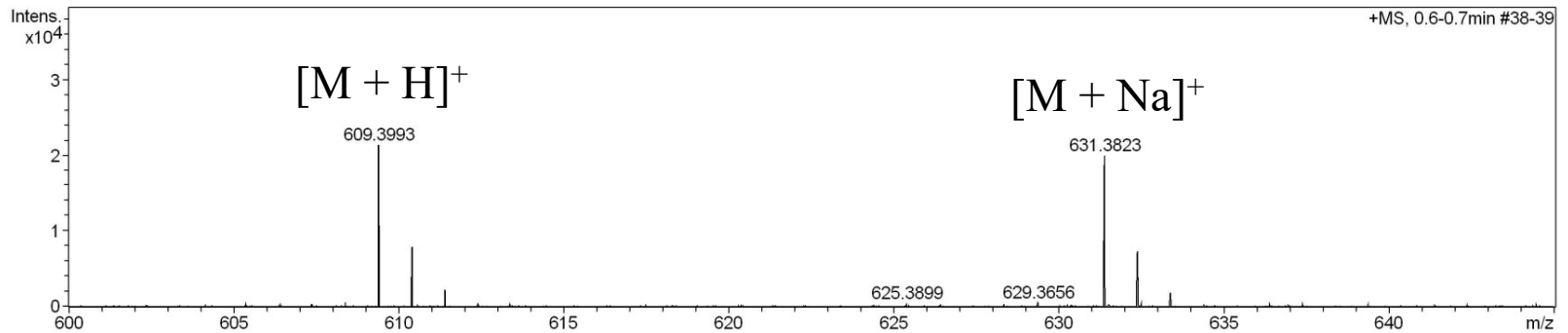
Analysis Info

Analysis Name D:\Data\MS\data\201905\liwanshan_2-37_pos_35_01_6636.d
Method LC_Direct Infusion_pos_70-500mz.m
Sample Name liwanshan_2-37_pos
Comment

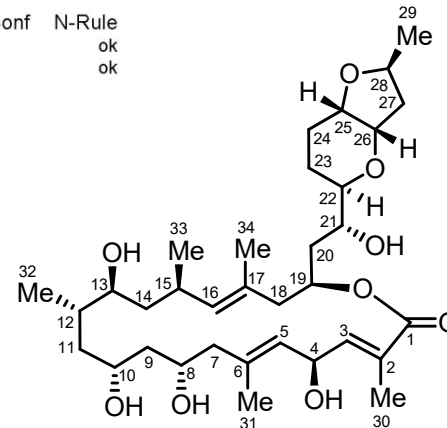
Acquisition Date 5/14/2019 4:36:58 PM
Operator SCSIO
Instrument maXis 255552.00029

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
609.3993	1	C34H57O9	100.00	609.3997	-0.6	-0.4	9.0	6.5	even	ok
631.3823	1	C34H56NaO9	100.00	631.3817	1.0	0.6	5.6	6.5	even	ok



HR-ESIMS for compound 1

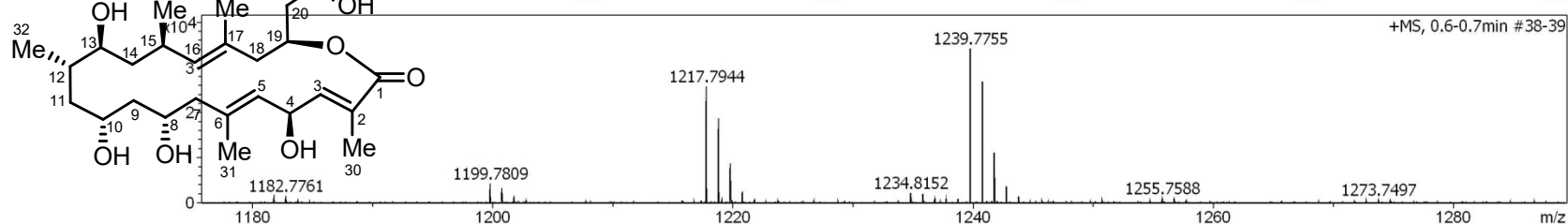
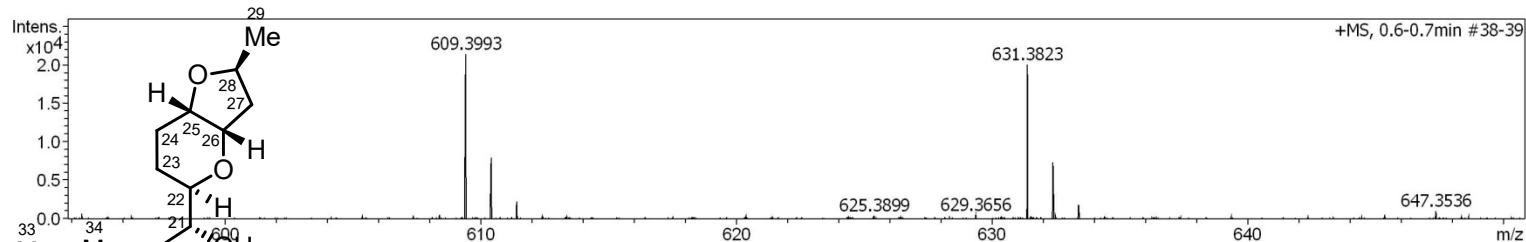
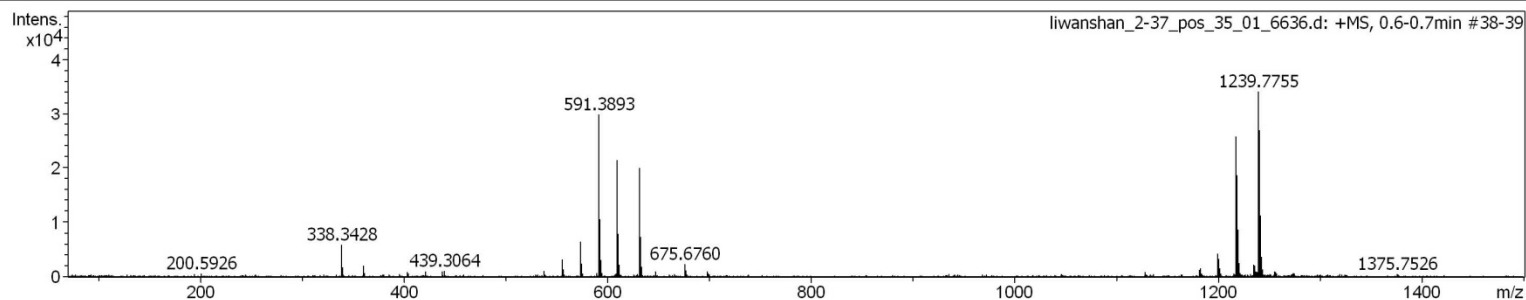
Generic Display Report

Analysis Info

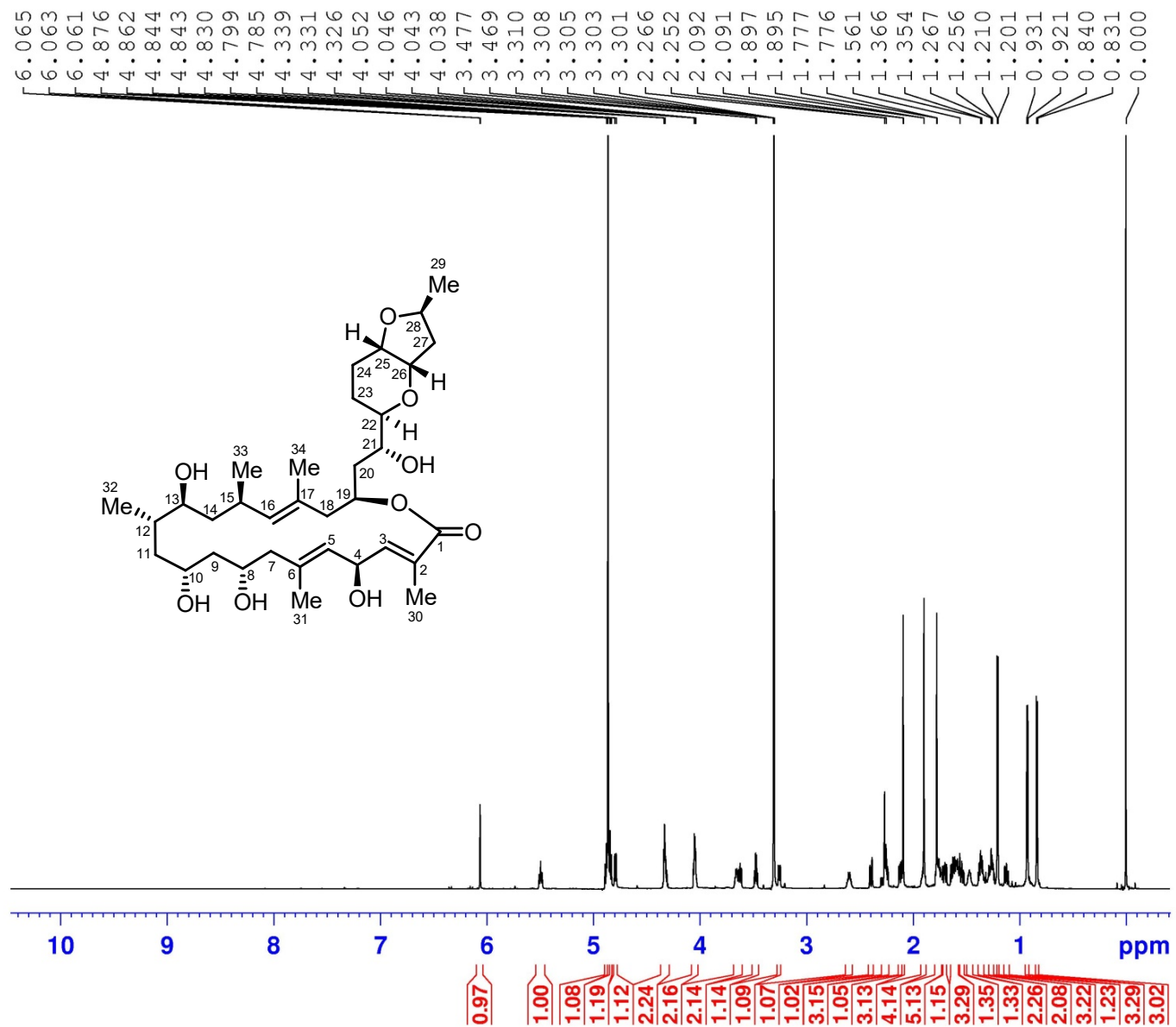
Analysis Name D:\Data\MS\data\201905\liwanshan_2-37_pos_35_01_6636.d
Method LC_Direct Infusion_pos_70-500mz.m
Sample Name liwanshan_2-37_pos
Comment

Acquisition Date 5/14/2019 4:36:58 PM

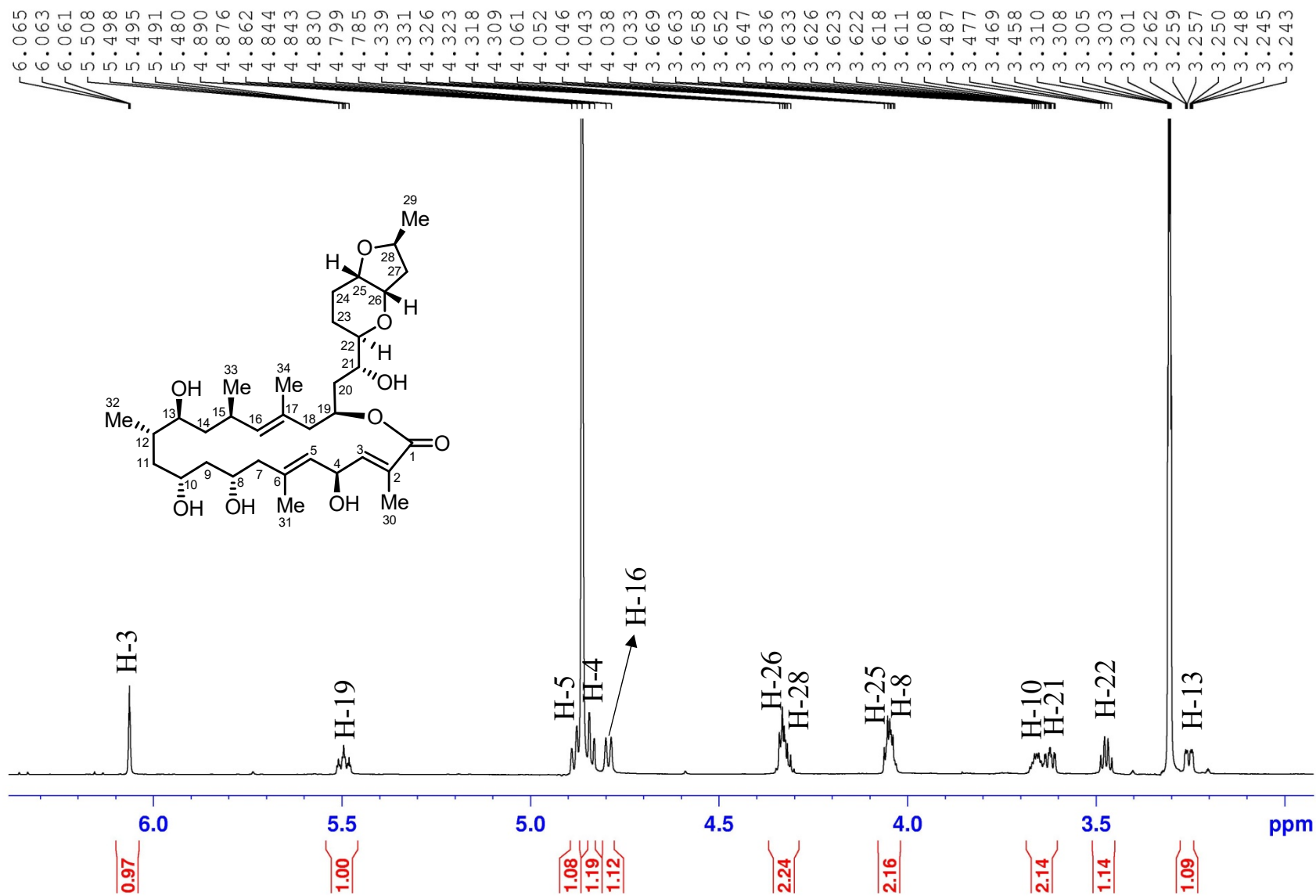
Operator SCSIO
Instrument maXis



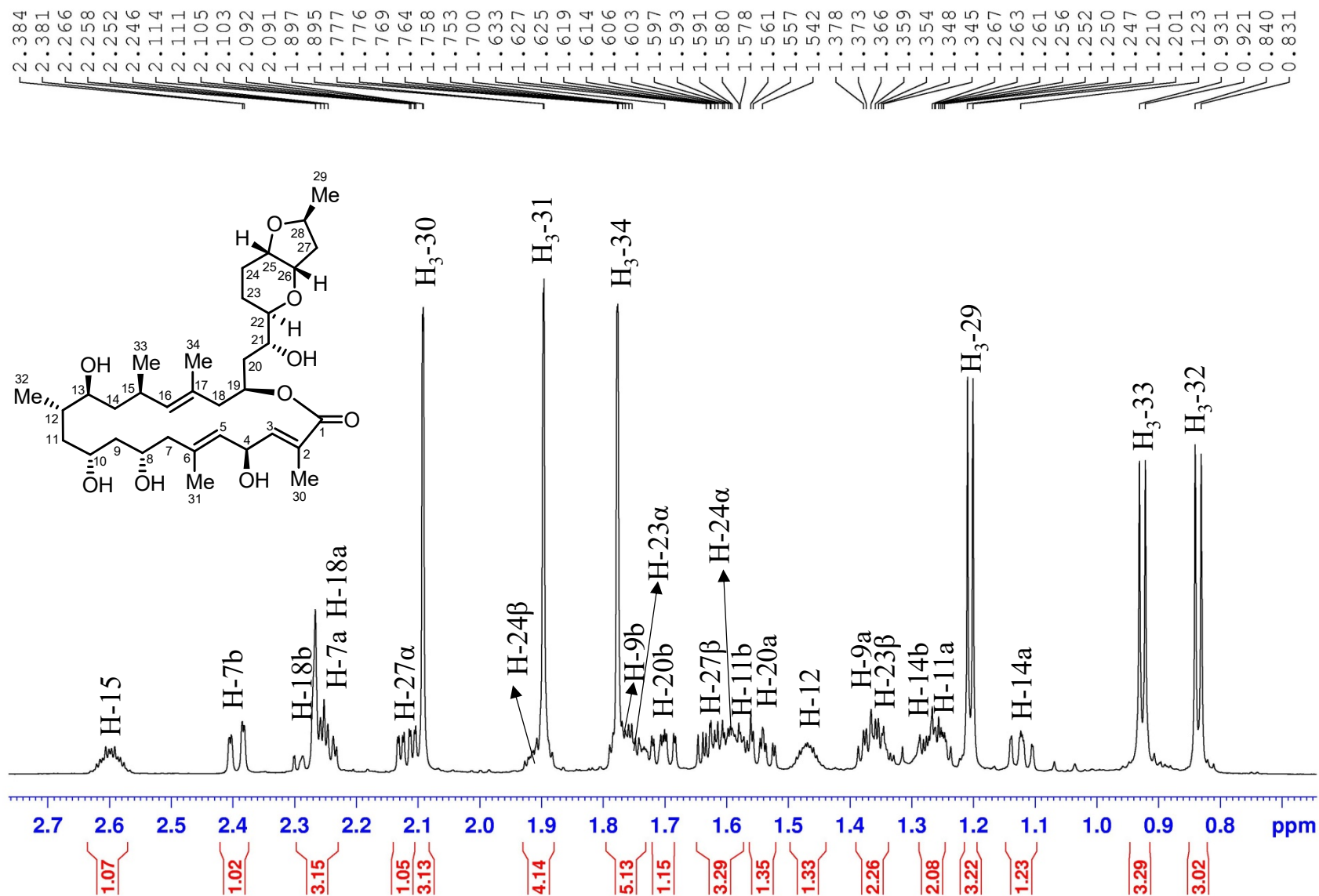
^1H (700 MHz) NMR spectrum of compound **1** in CD_3OD



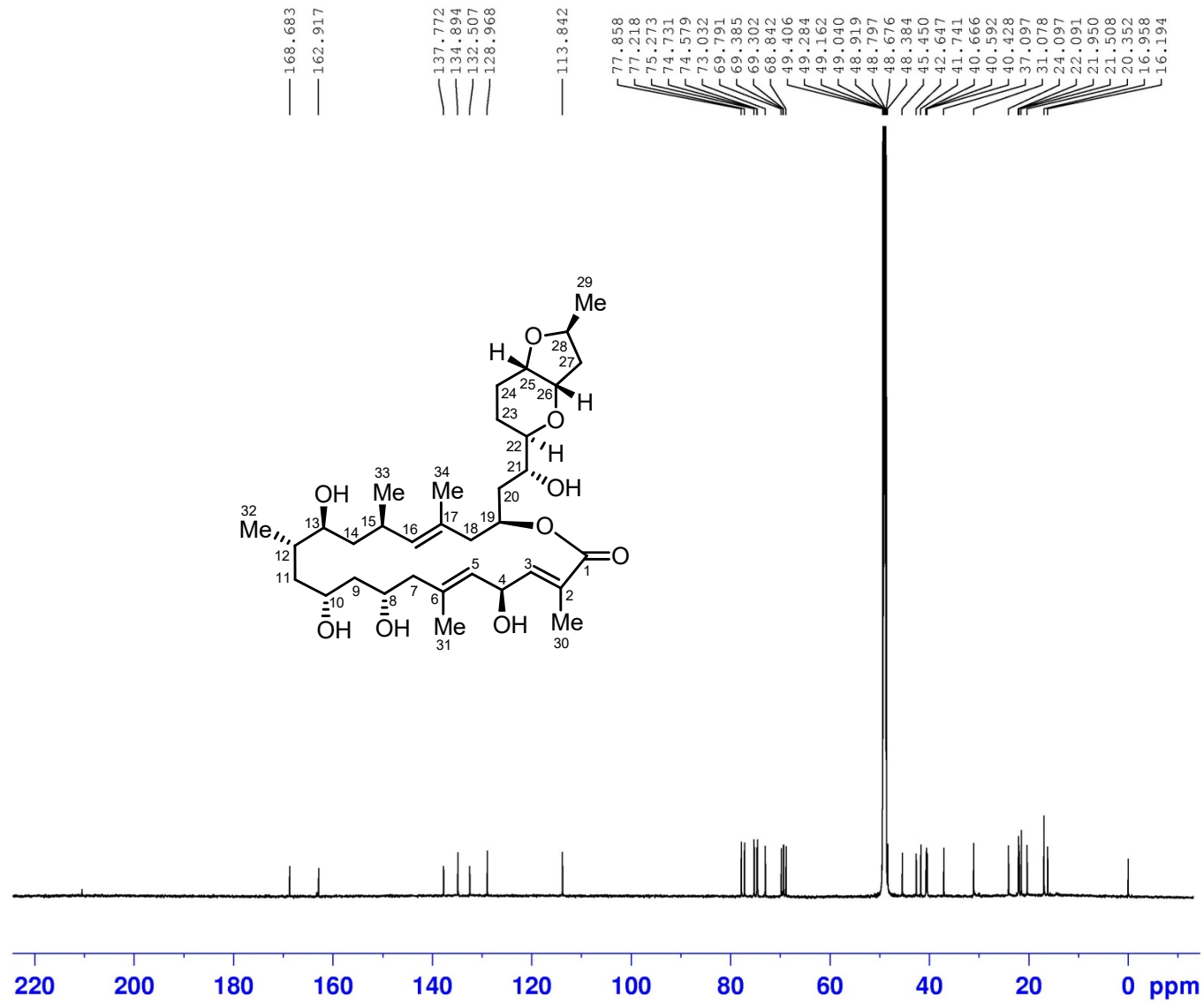
^1H (700 MHz) NMR spectrum of compound **1** in CD_3OD



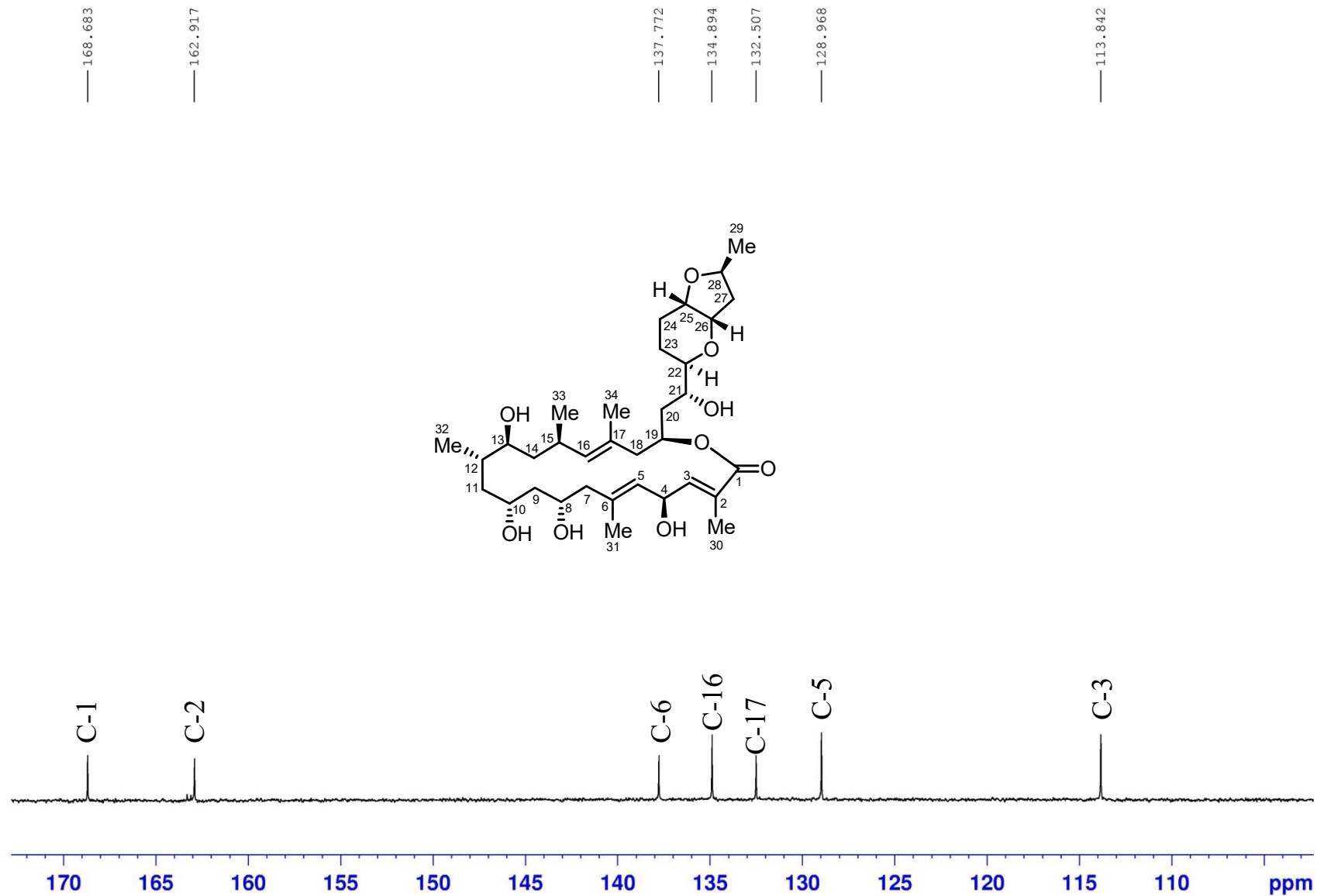
^1H (700 MHz) NMR spectrum of compound **1** in CD_3OD



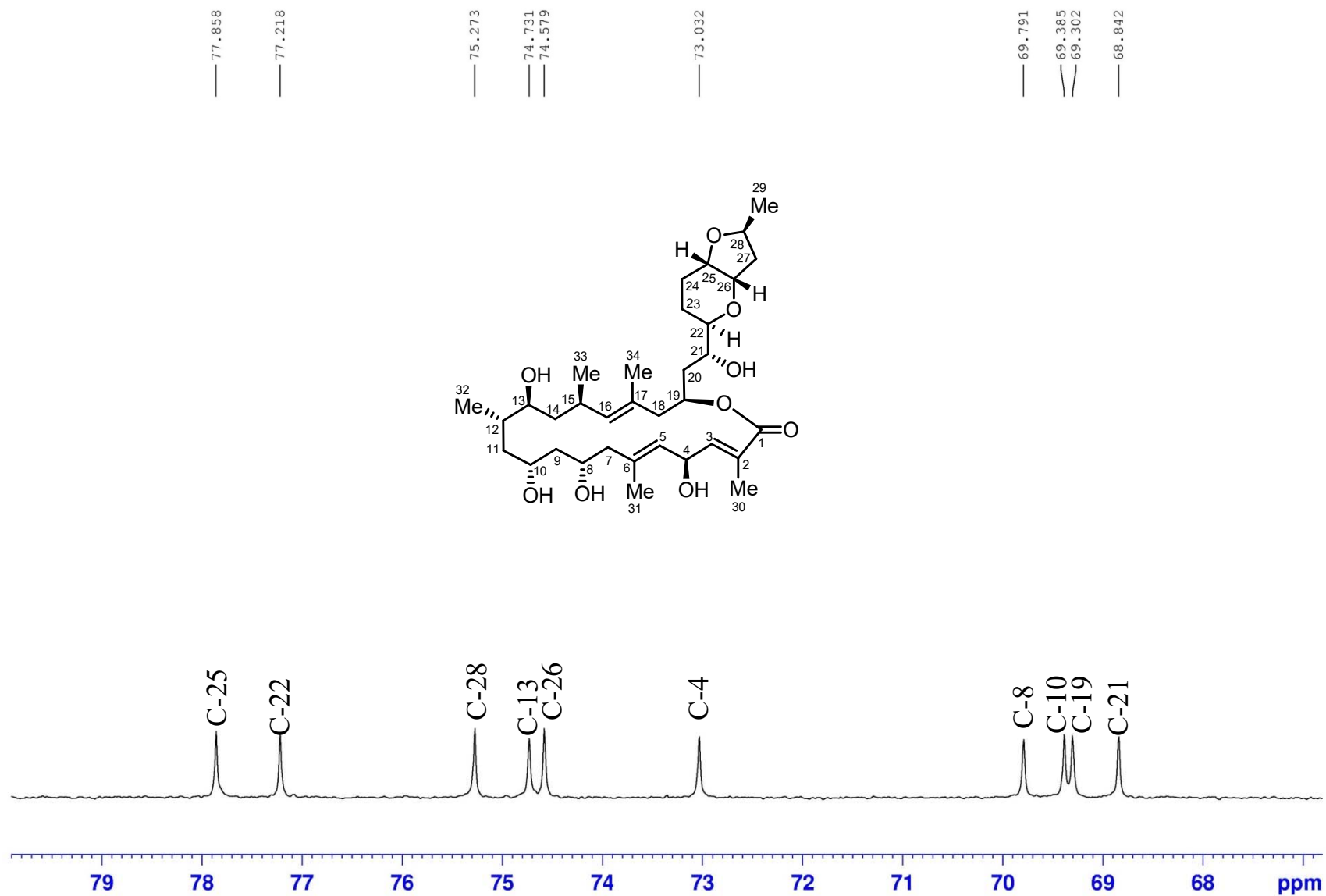
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



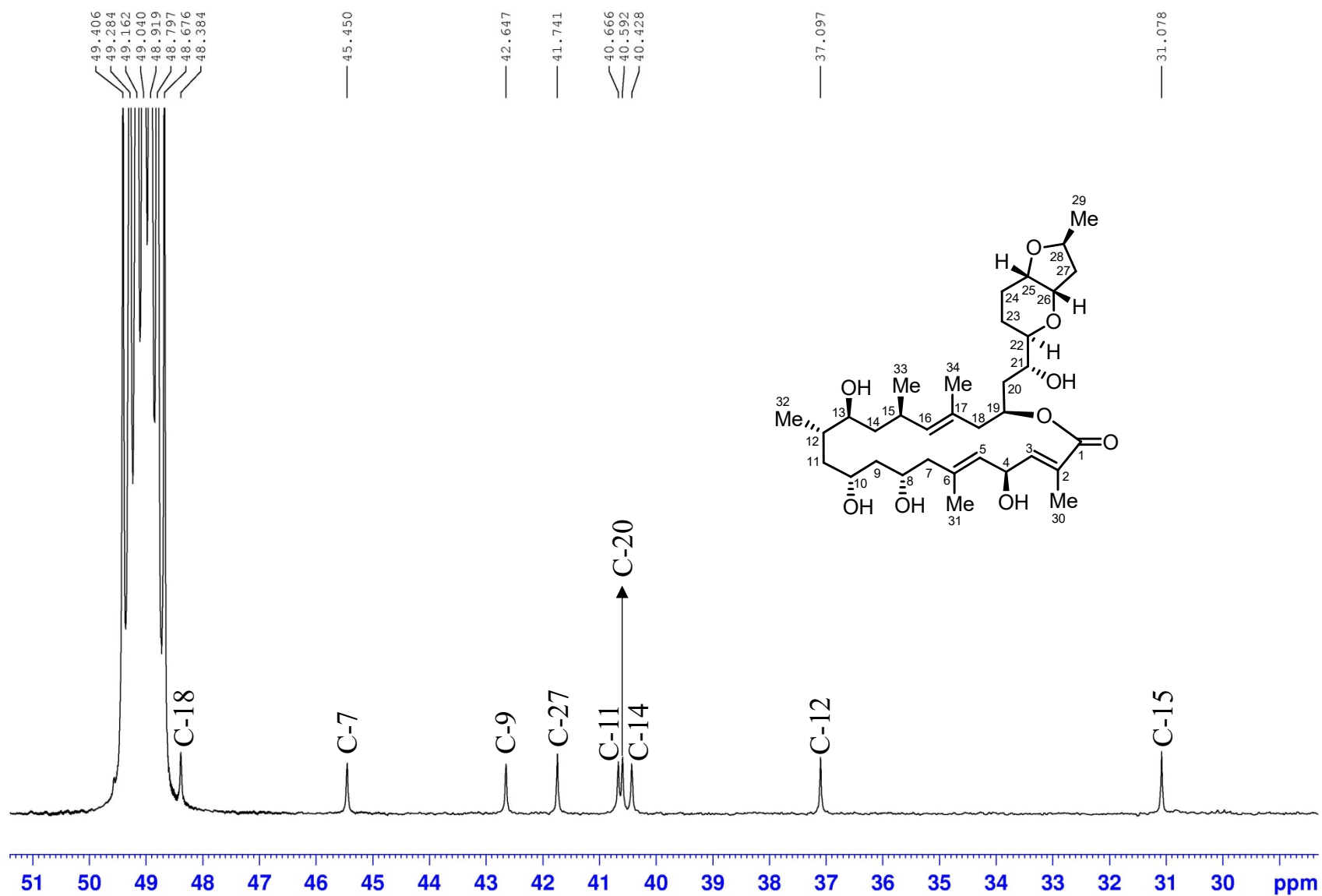
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



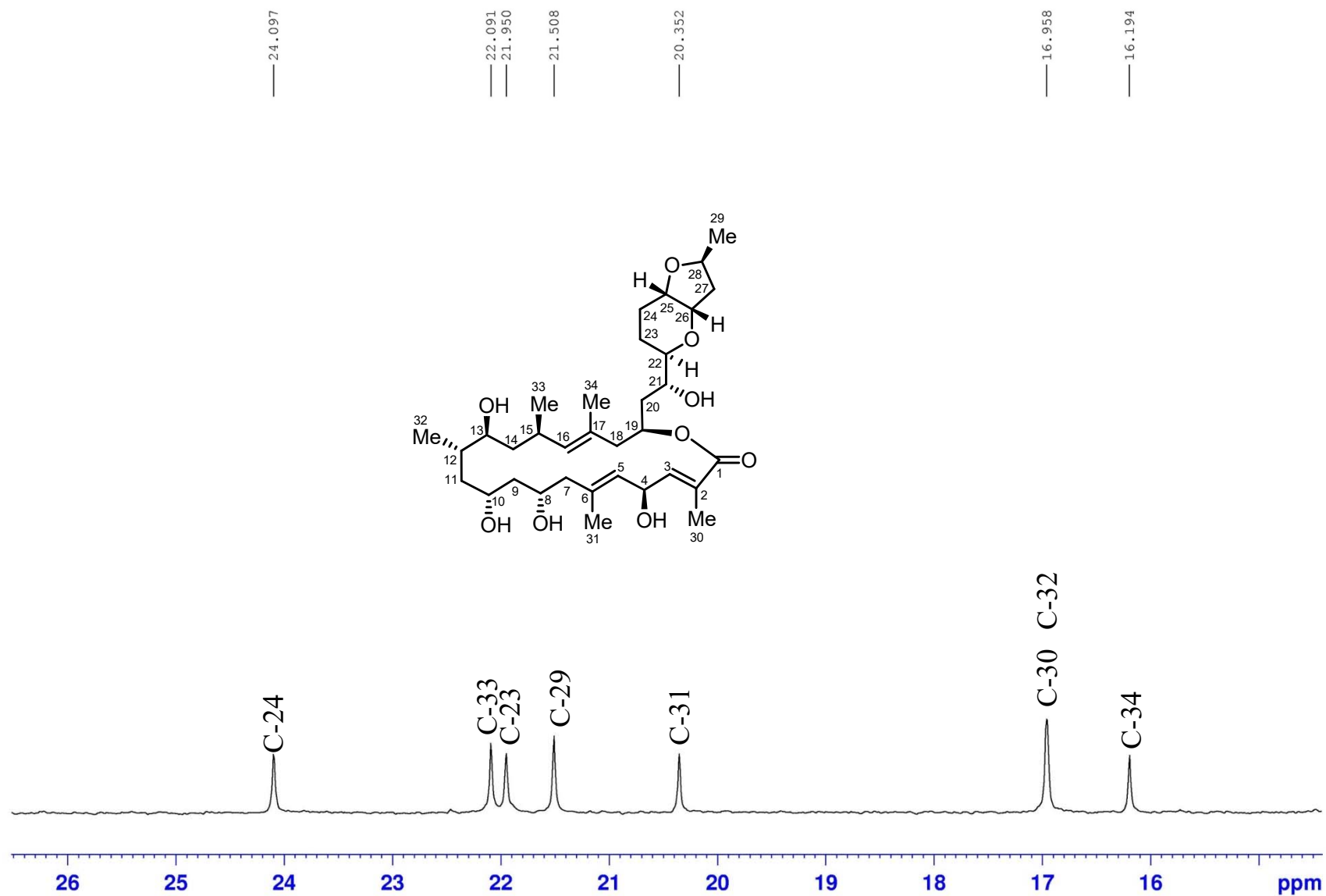
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



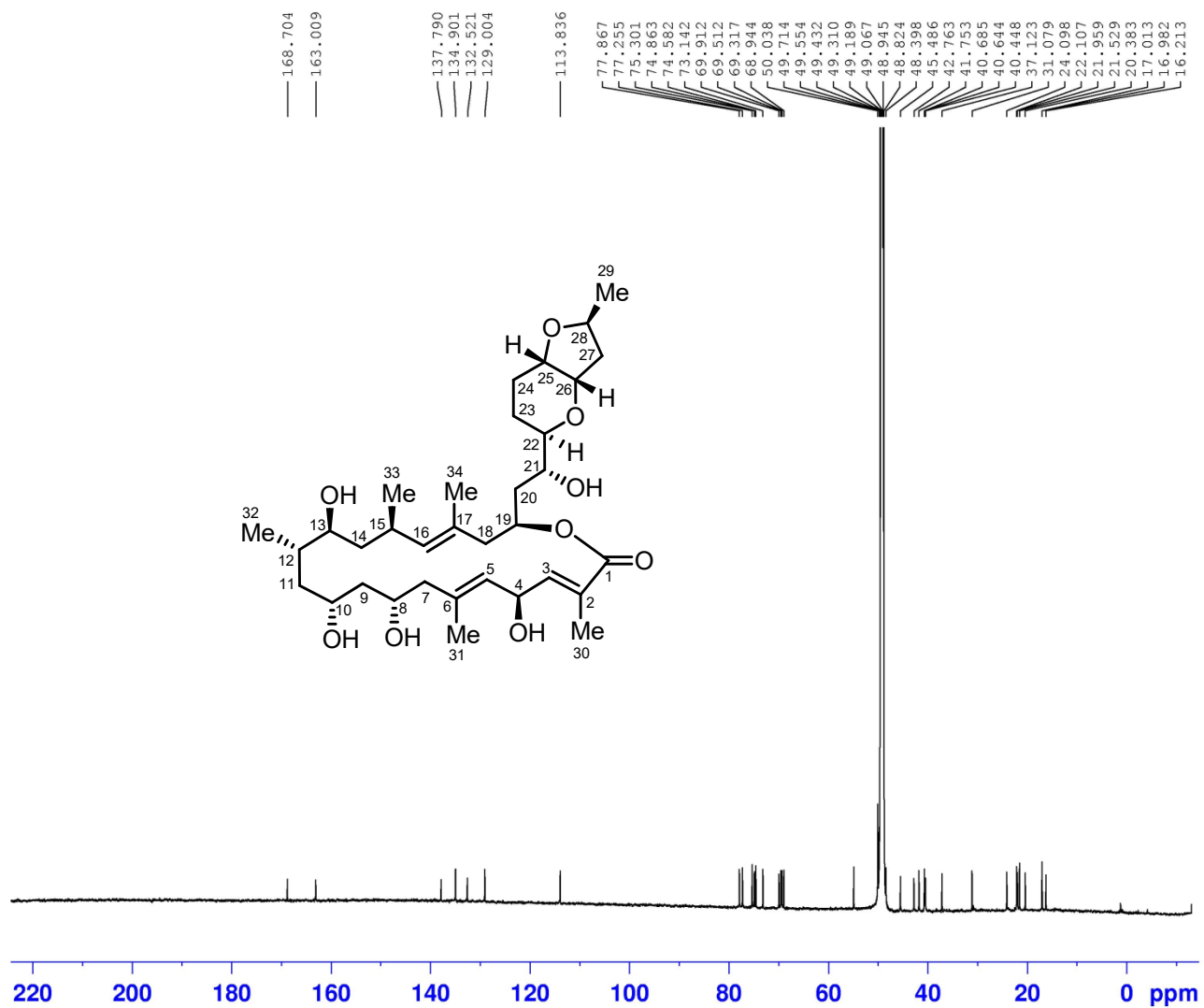
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



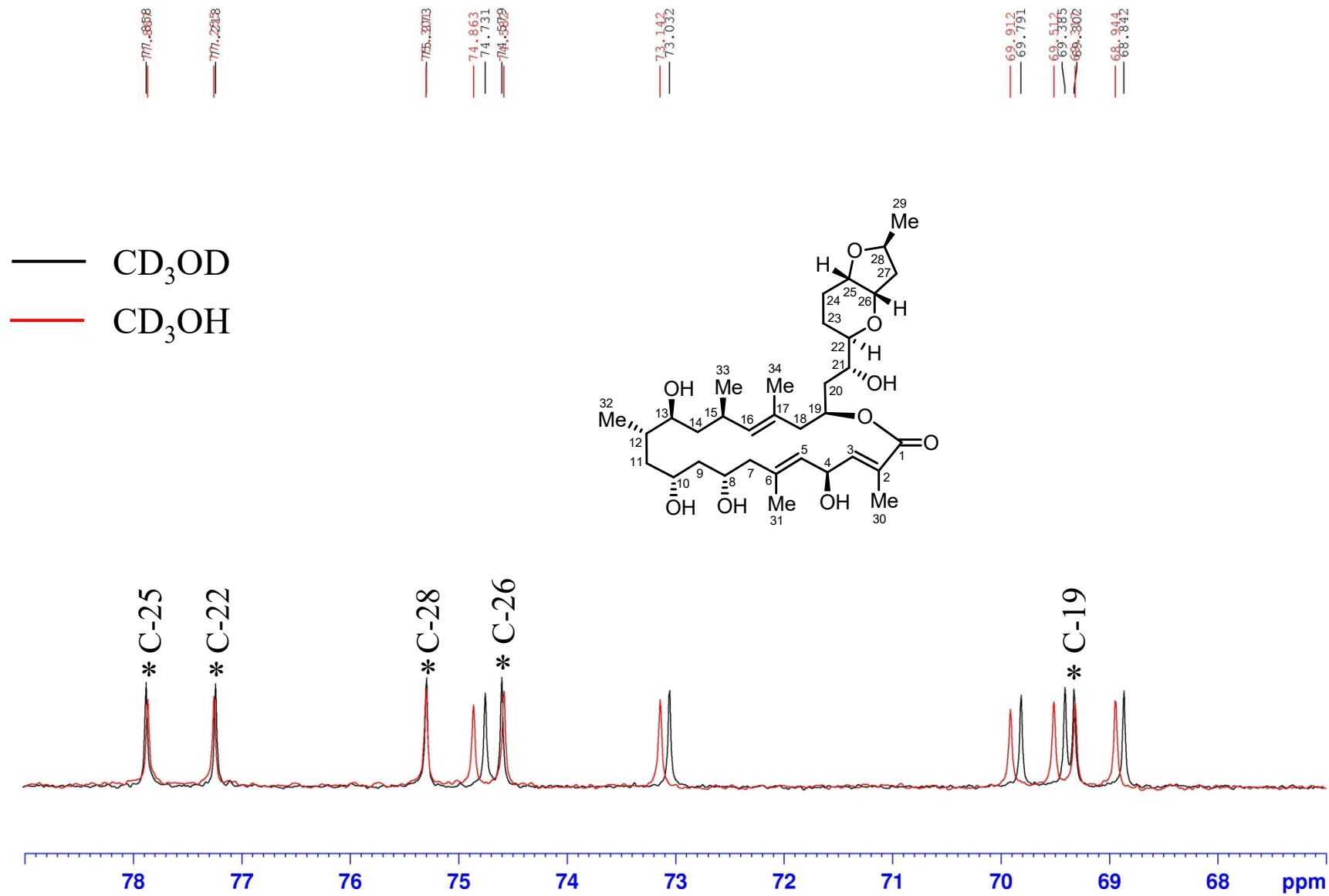
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



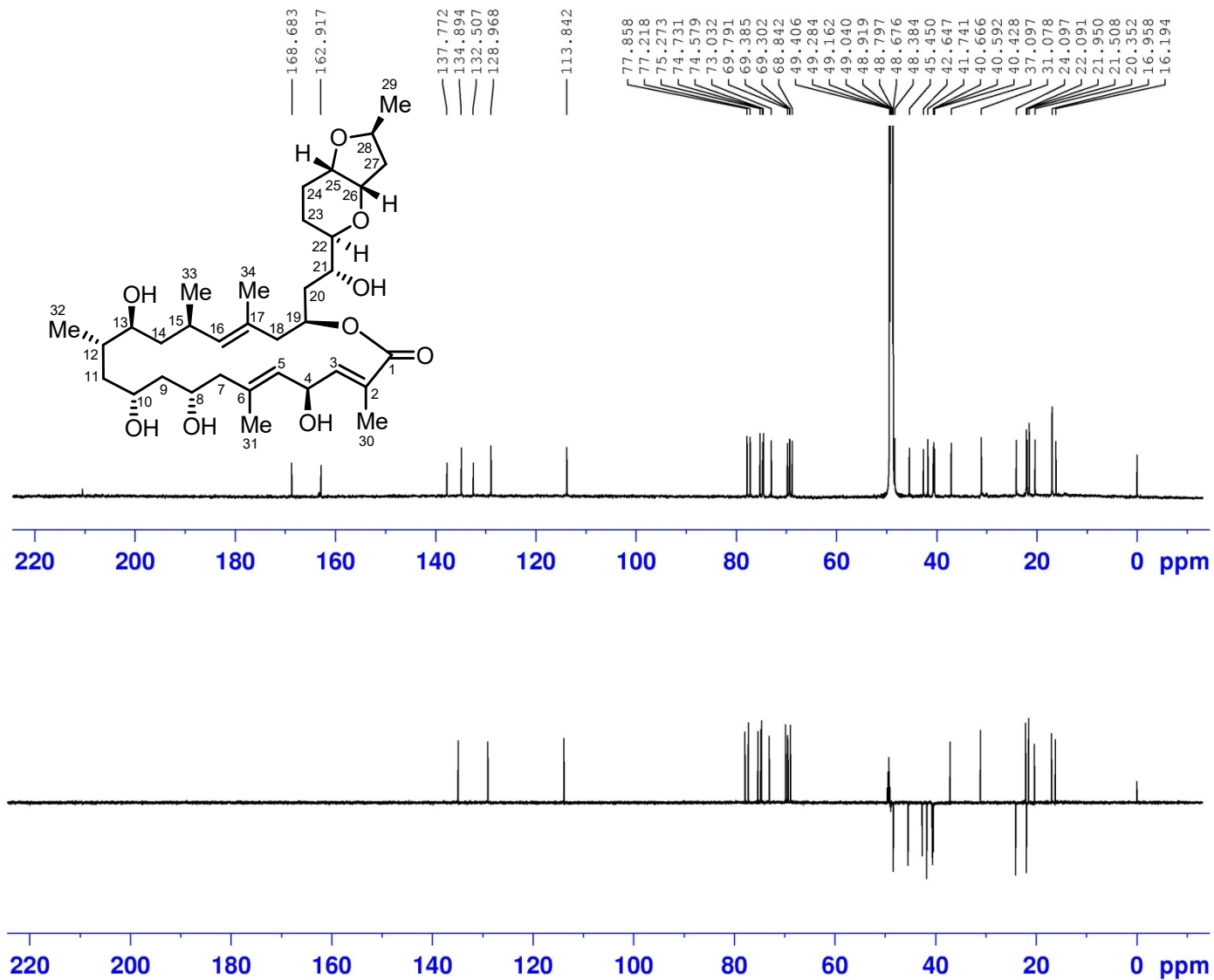
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OH



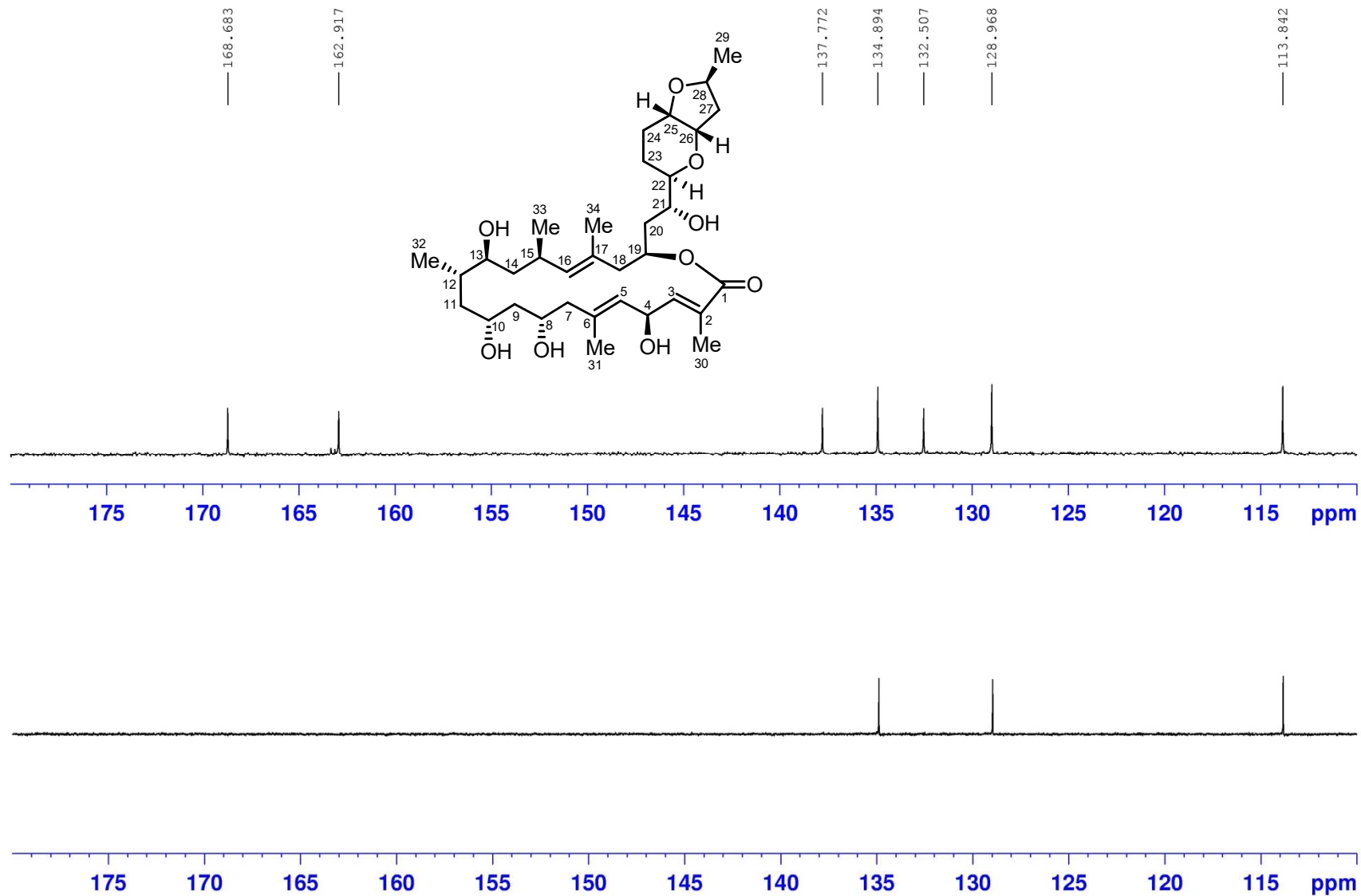
Comparison of ^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OH with that in CD_3OD



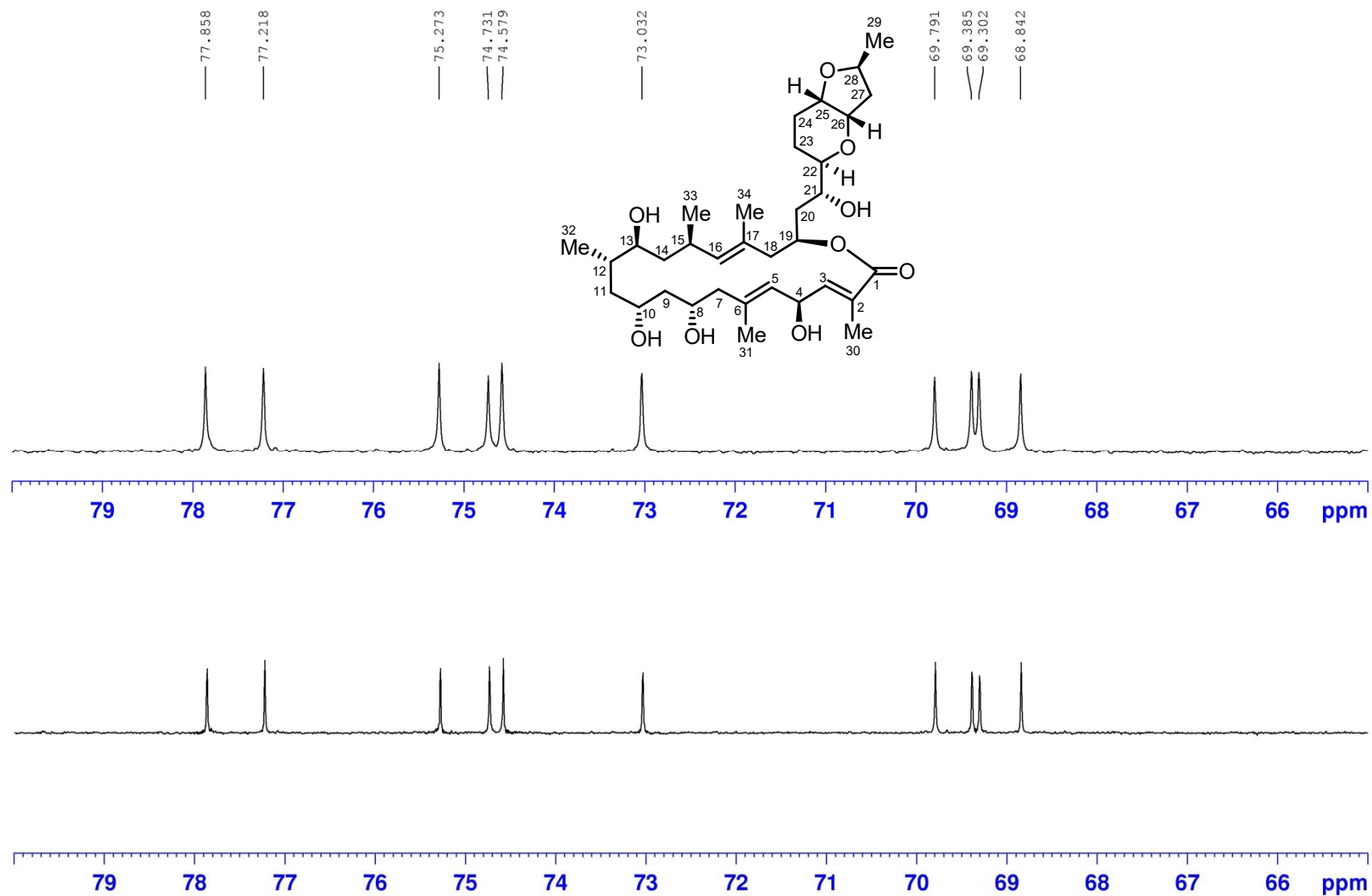
DEPT135 (175 MHz) spectrum of compound **1** in CD₃OD



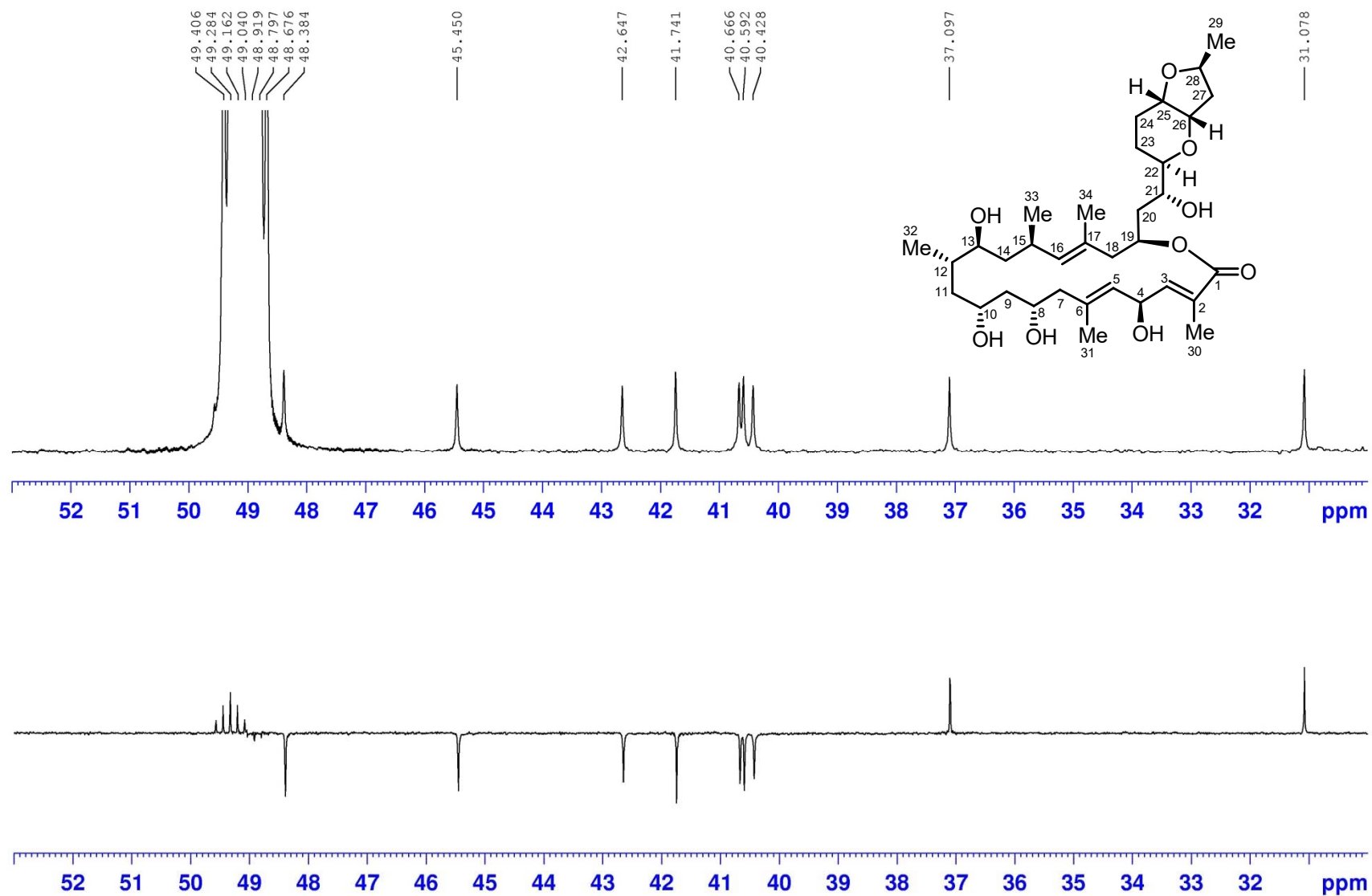
DEPT135 (175 MHz) spectrum of compound **1** in CD₃OD



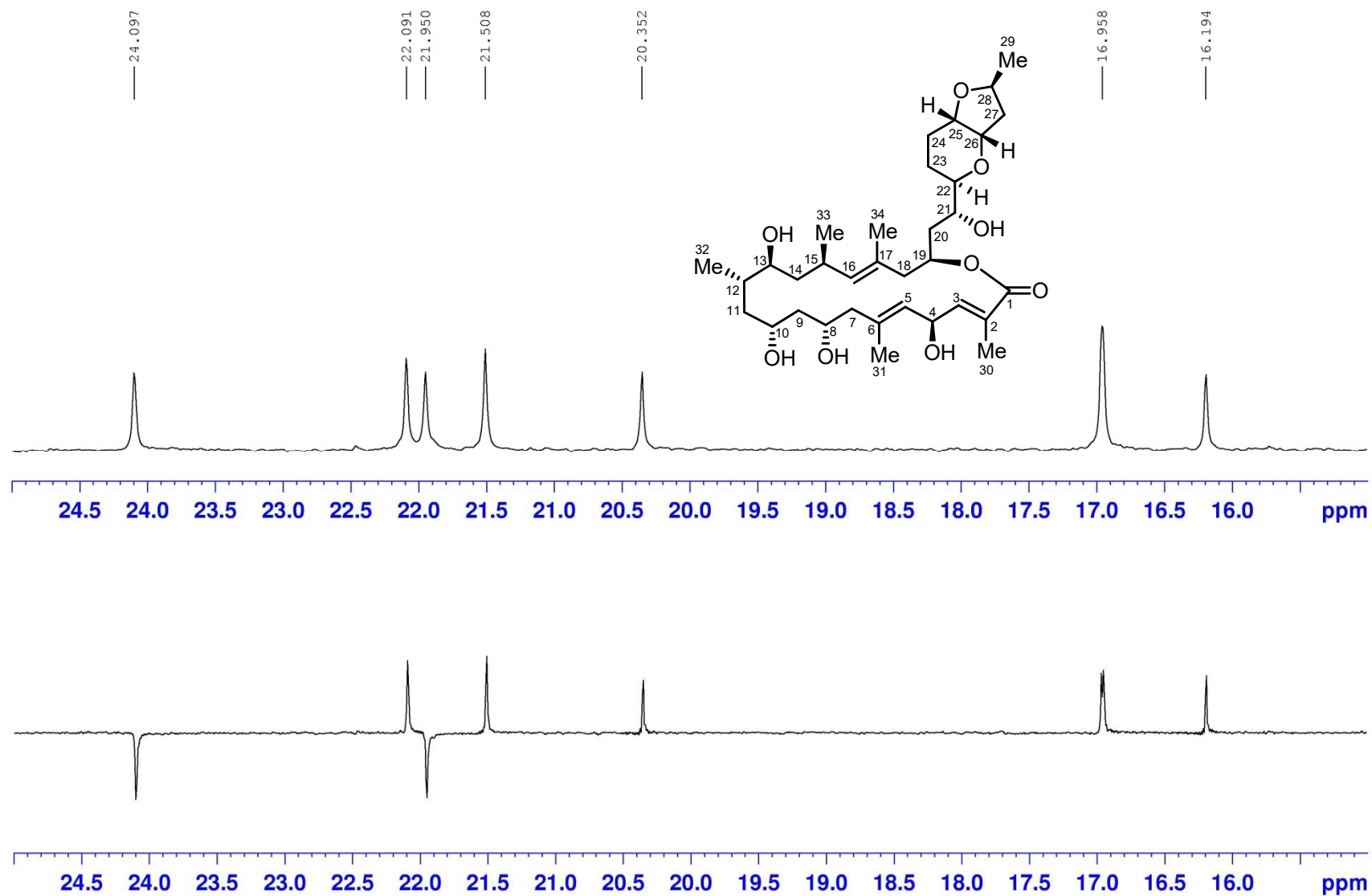
DEPT135 (175 MHz) spectrum of compound **1** in CD₃OD



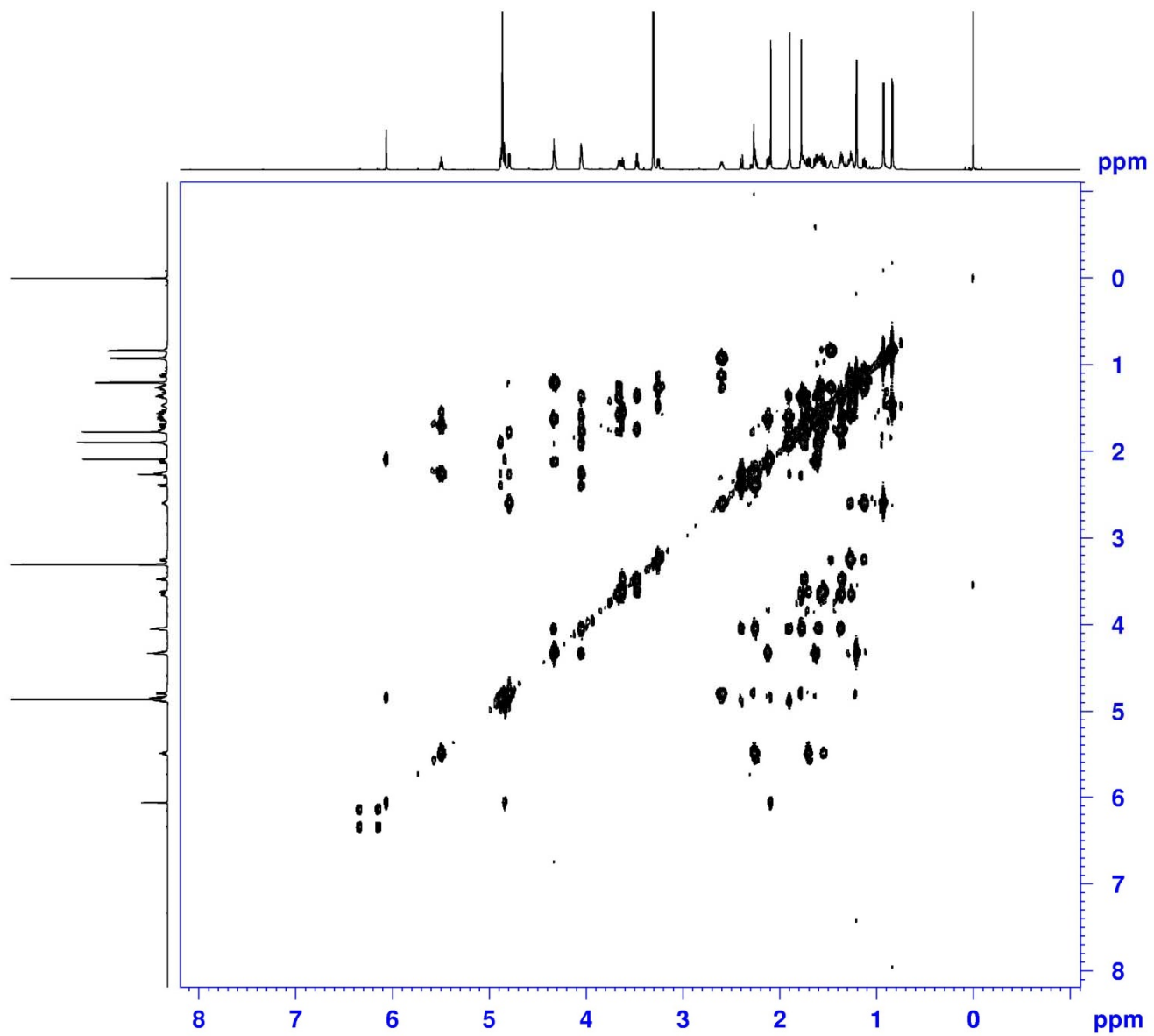
DEPT135 (175 MHz) spectrum of compound **1** in CD₃OD



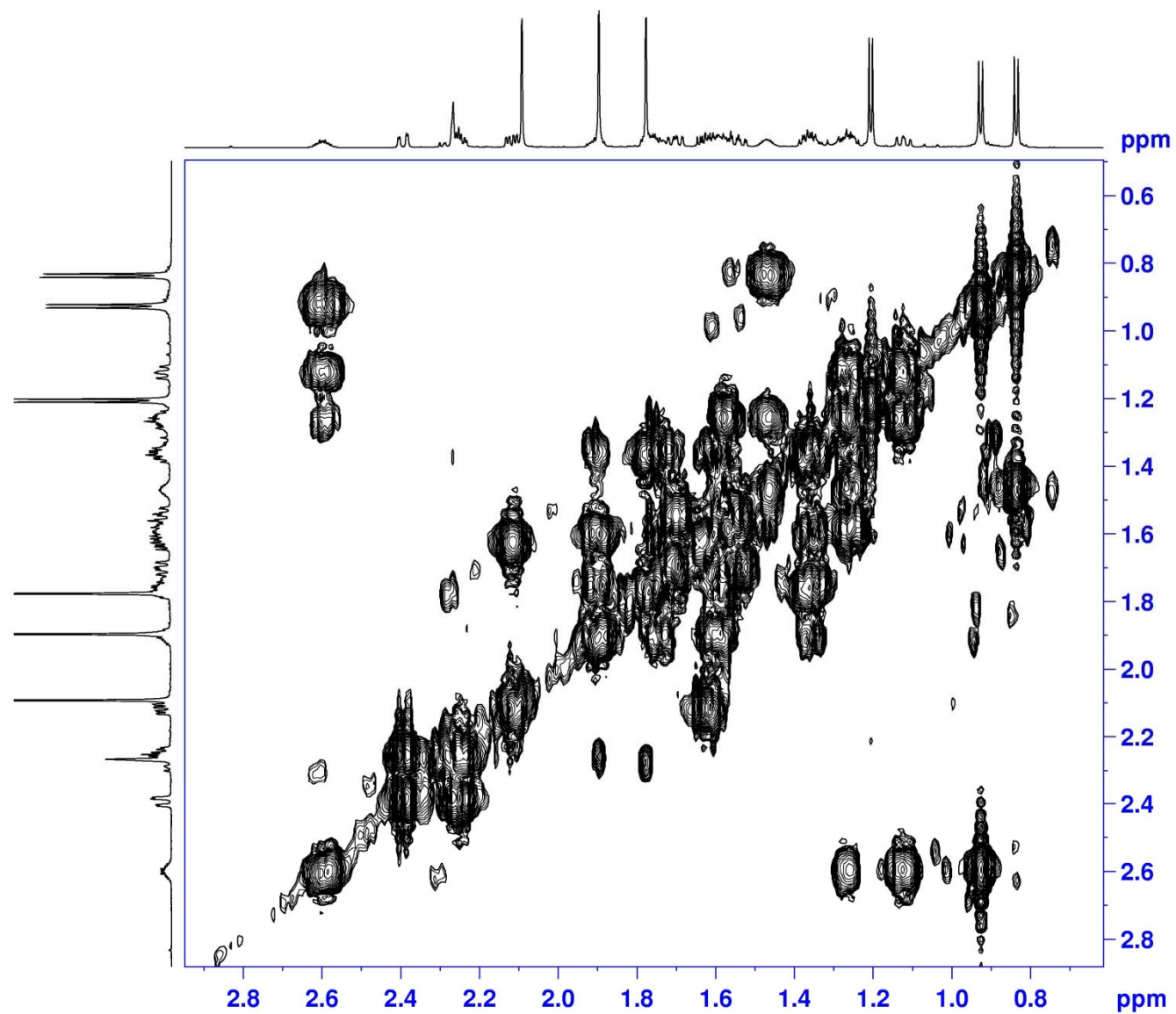
DEPT135 (175 MHz) spectrum of compound **1** in CD₃OD



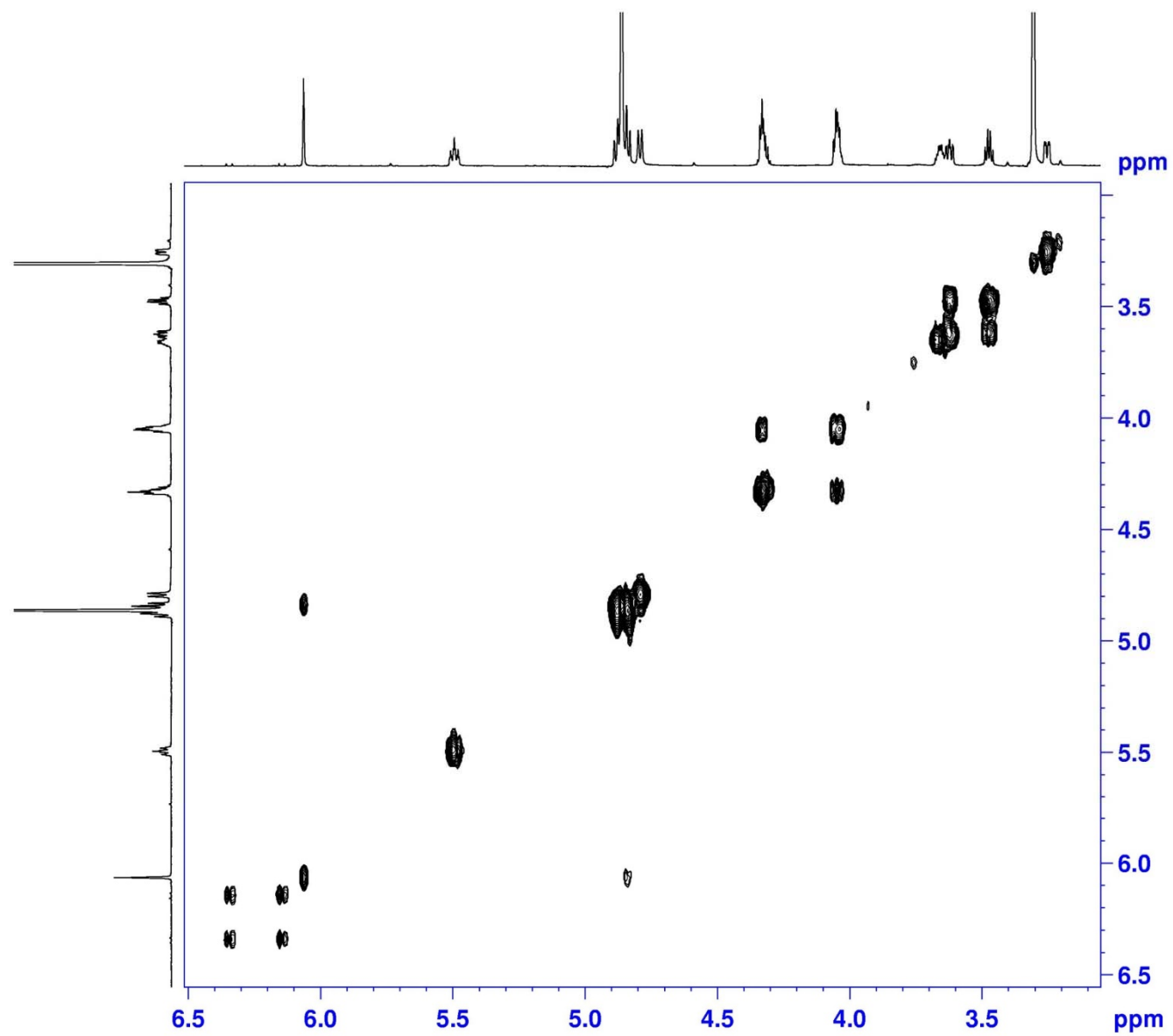
^1H - ^1H COSY (700 MHz) spectrum of compound **1** in CD_3OD



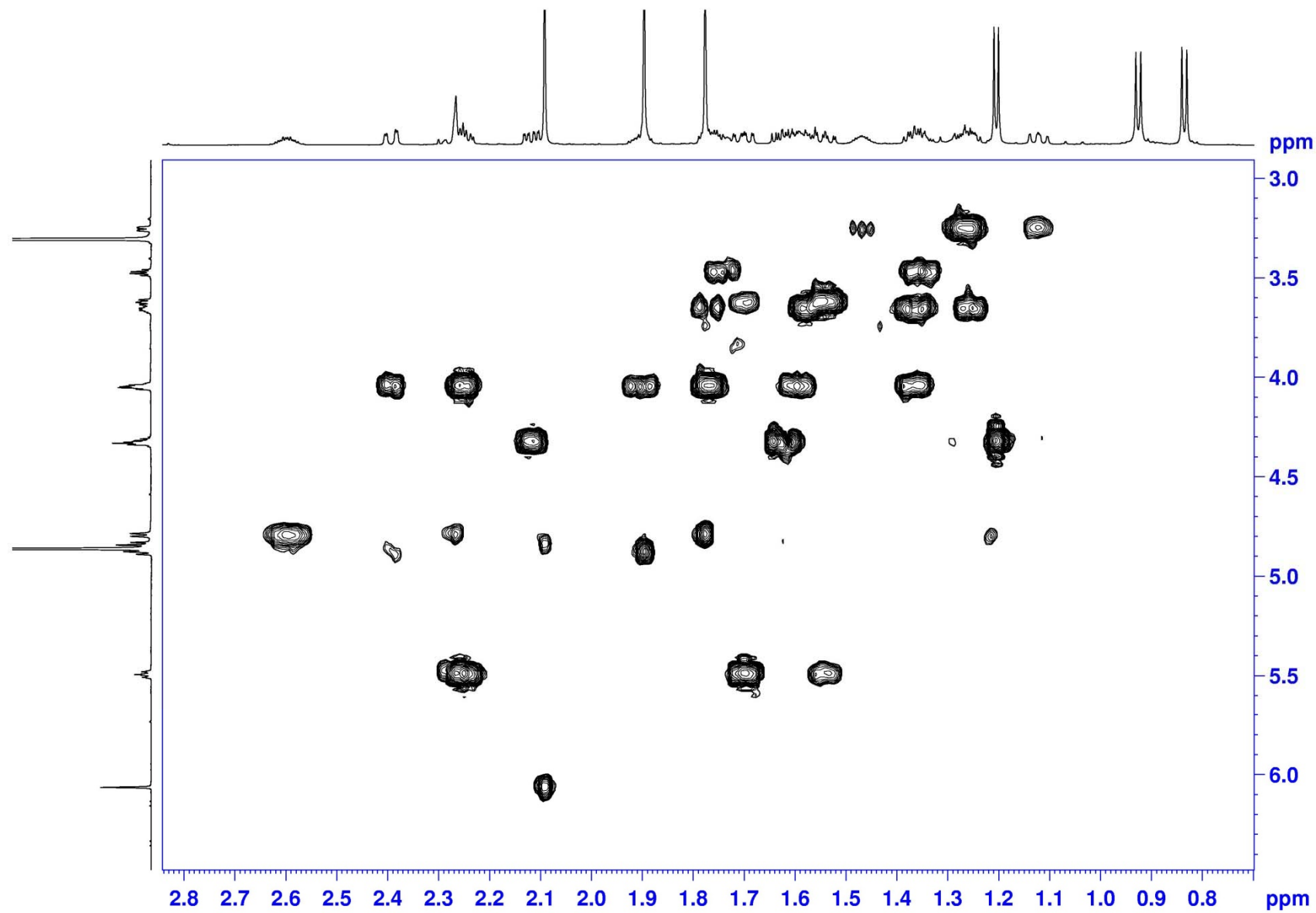
^1H - ^1H COSY (700 MHz) spectrum of compound **1** in CD_3OD



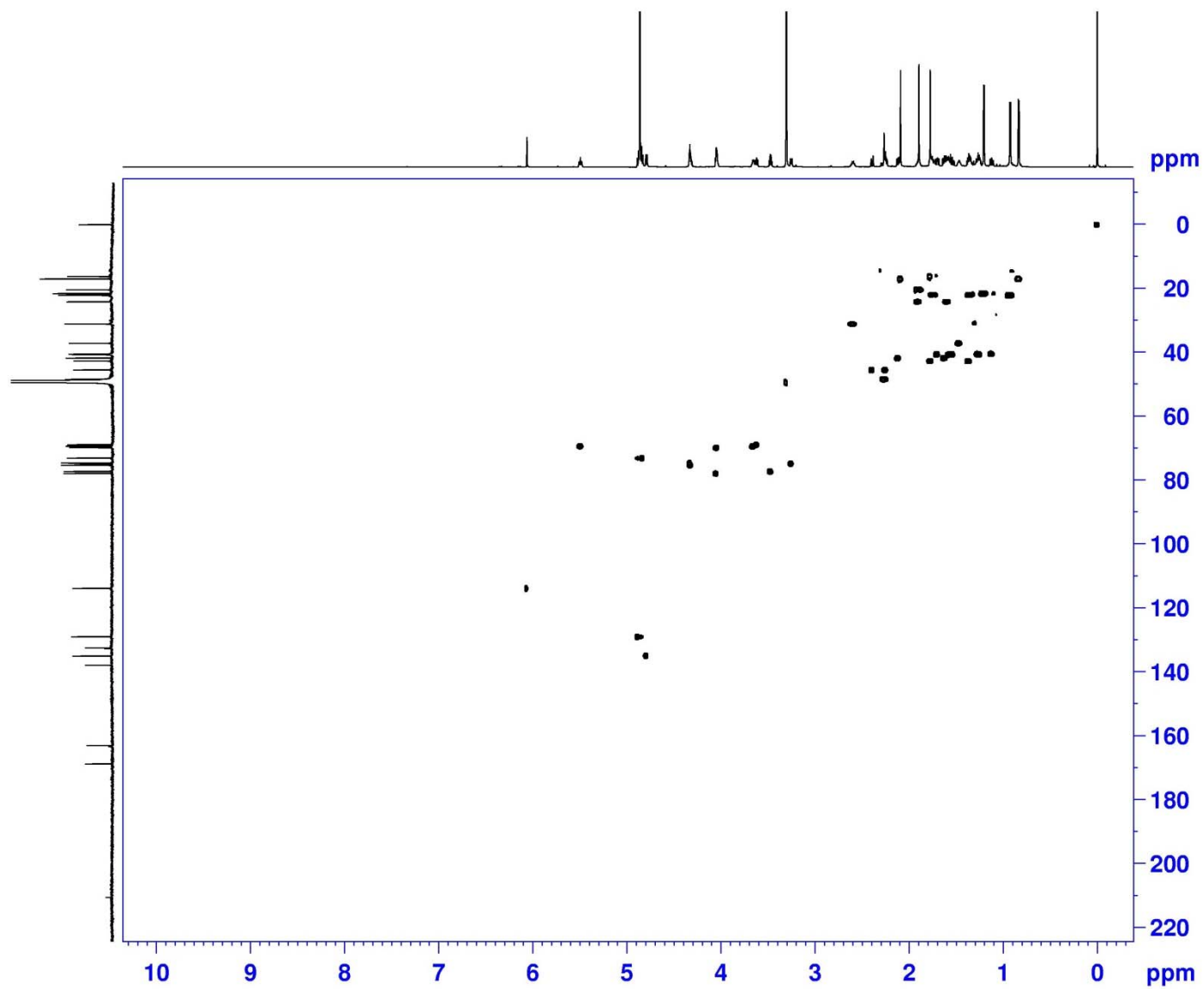
^1H - ^1H COSY (700 MHz) spectrum of compound **1** in CD_3OD



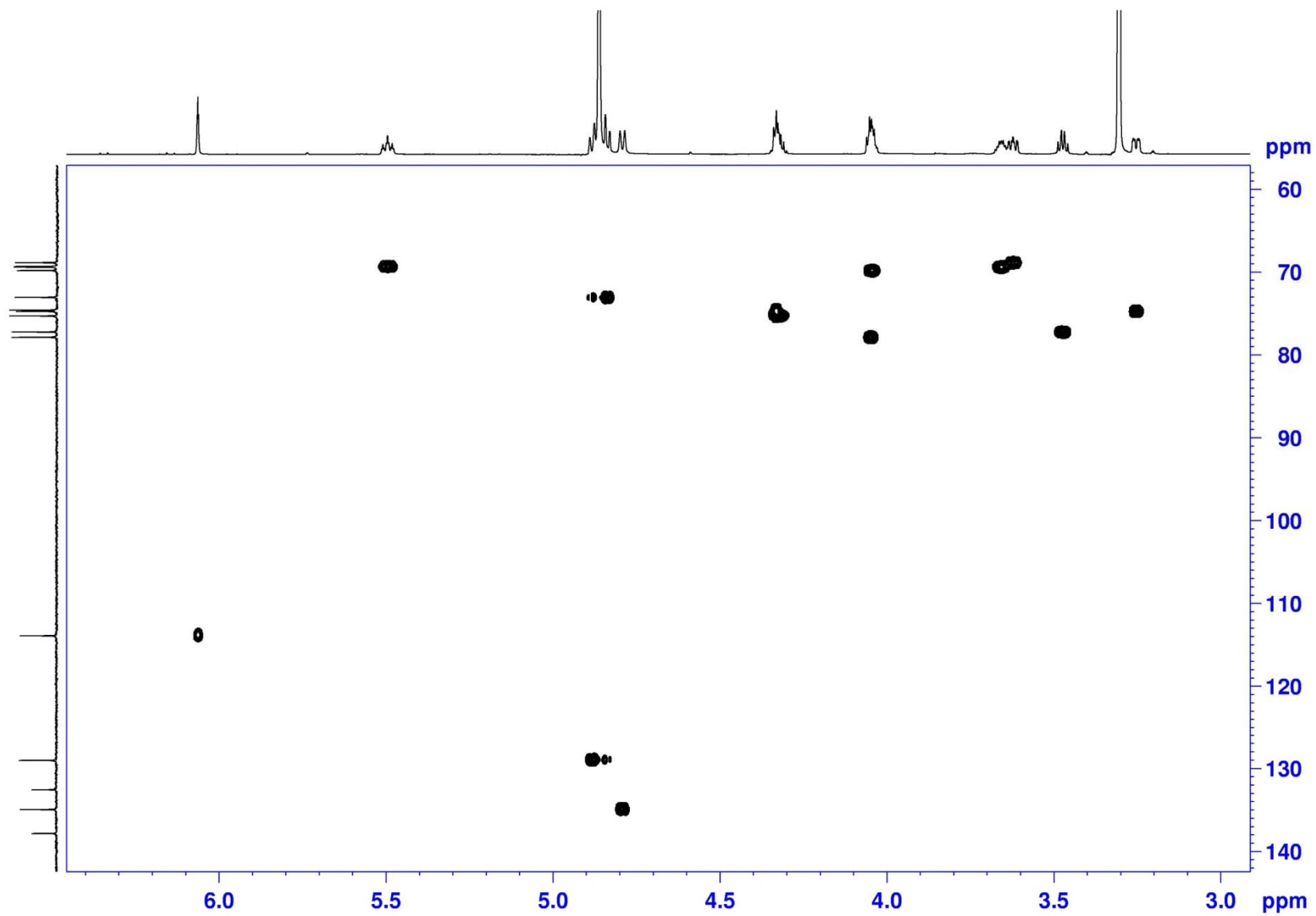
^1H - ^1H COSY (700 MHz) spectrum of compound **1** in CD_3OD



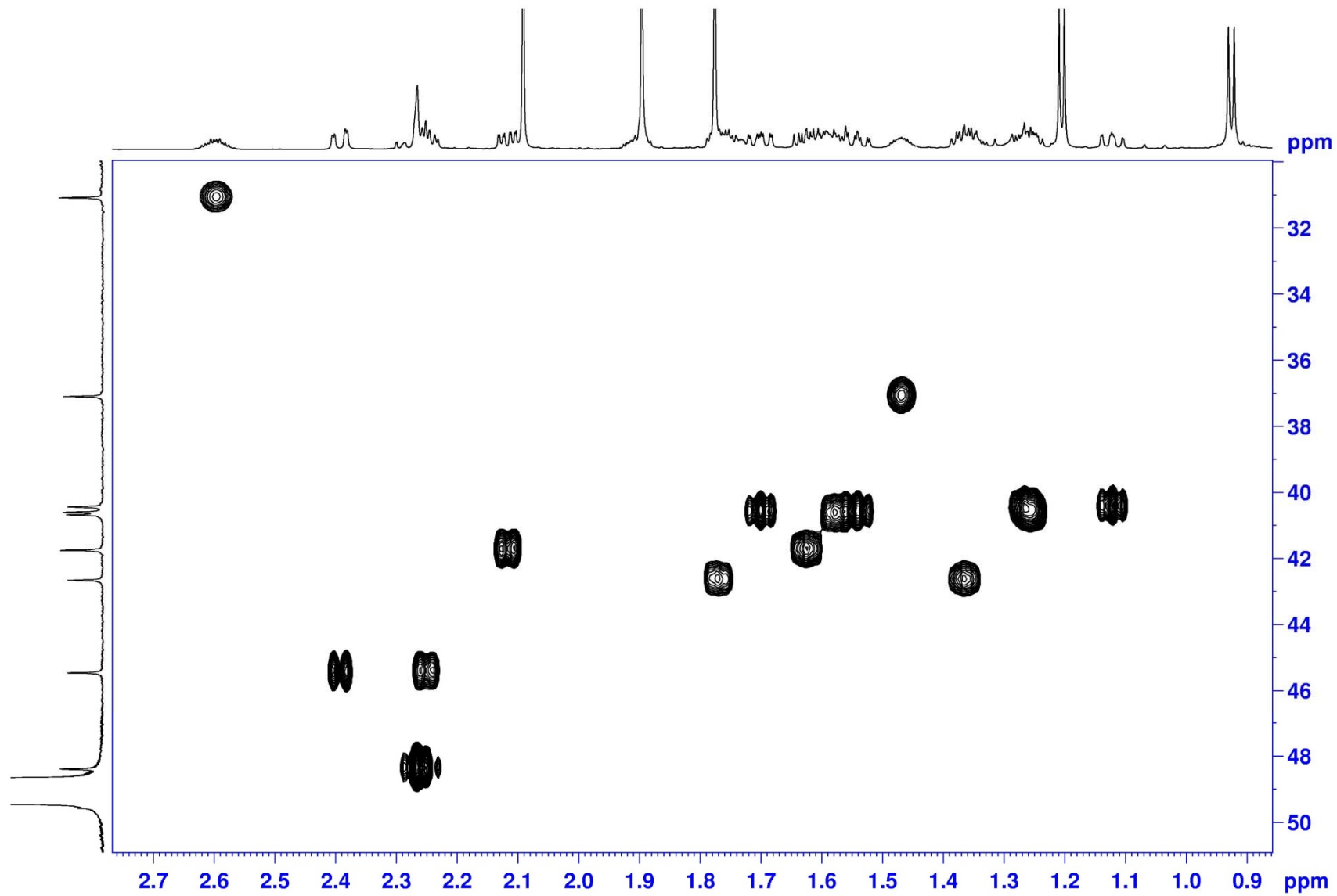
HSQC (700 MHz) spectrum of compound **1** in CD₃OD



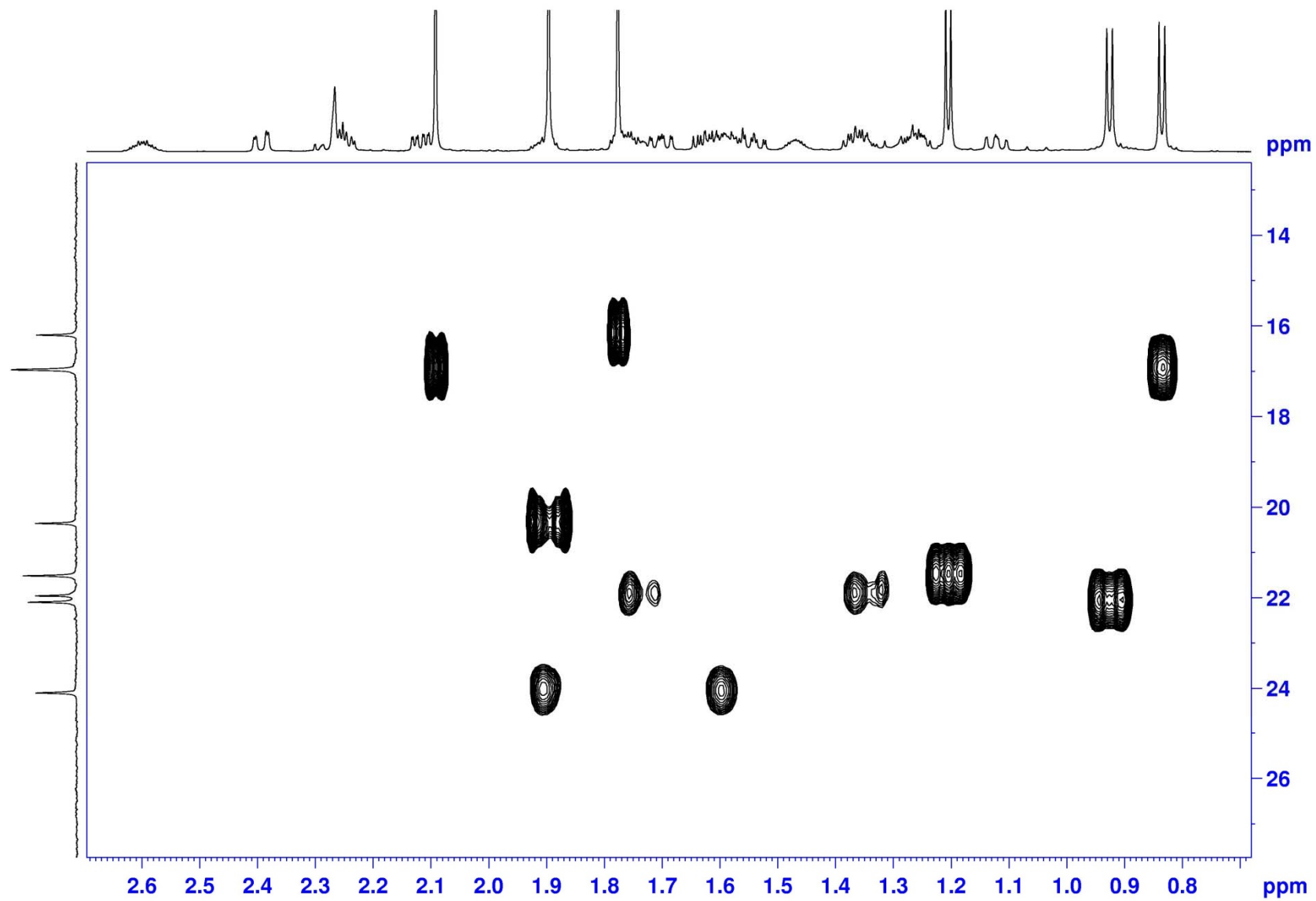
HSQC (700 MHz) spectrum of compound **1** in CD₃OD



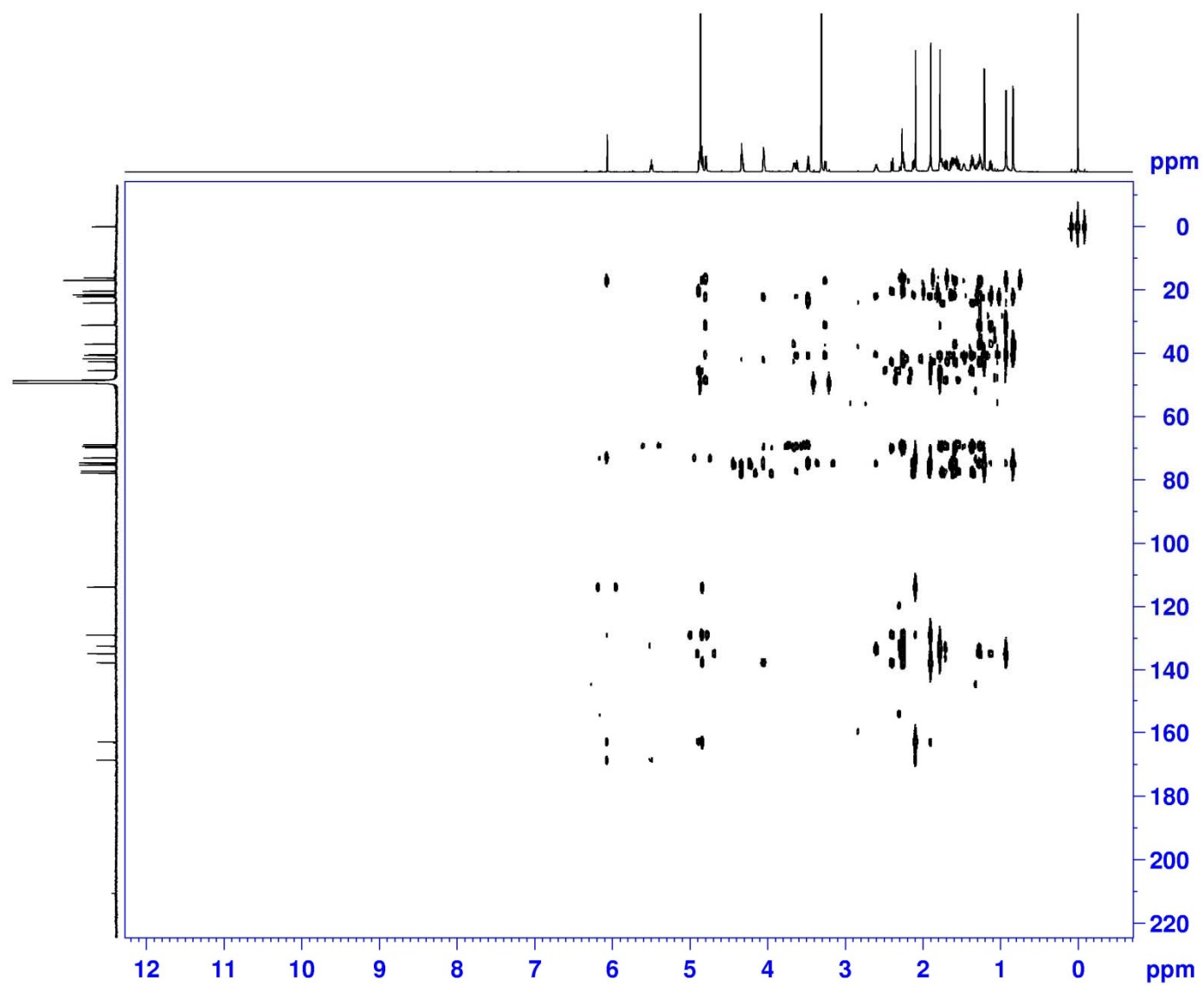
HSQC (700 MHz) spectrum of compound **1** in CD₃OD



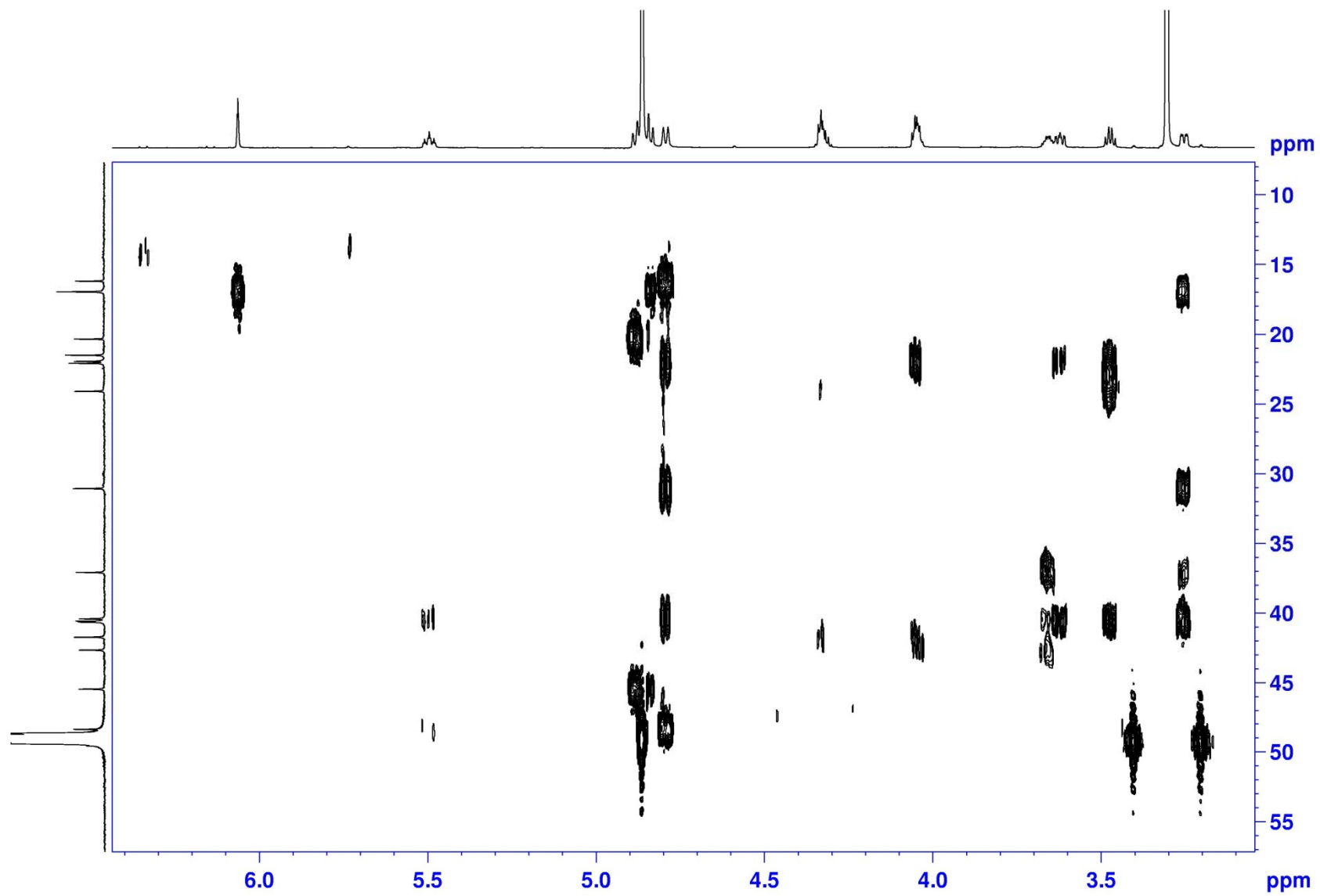
HSQC (700 MHz) spectrum of compound **1** in CD₃OD



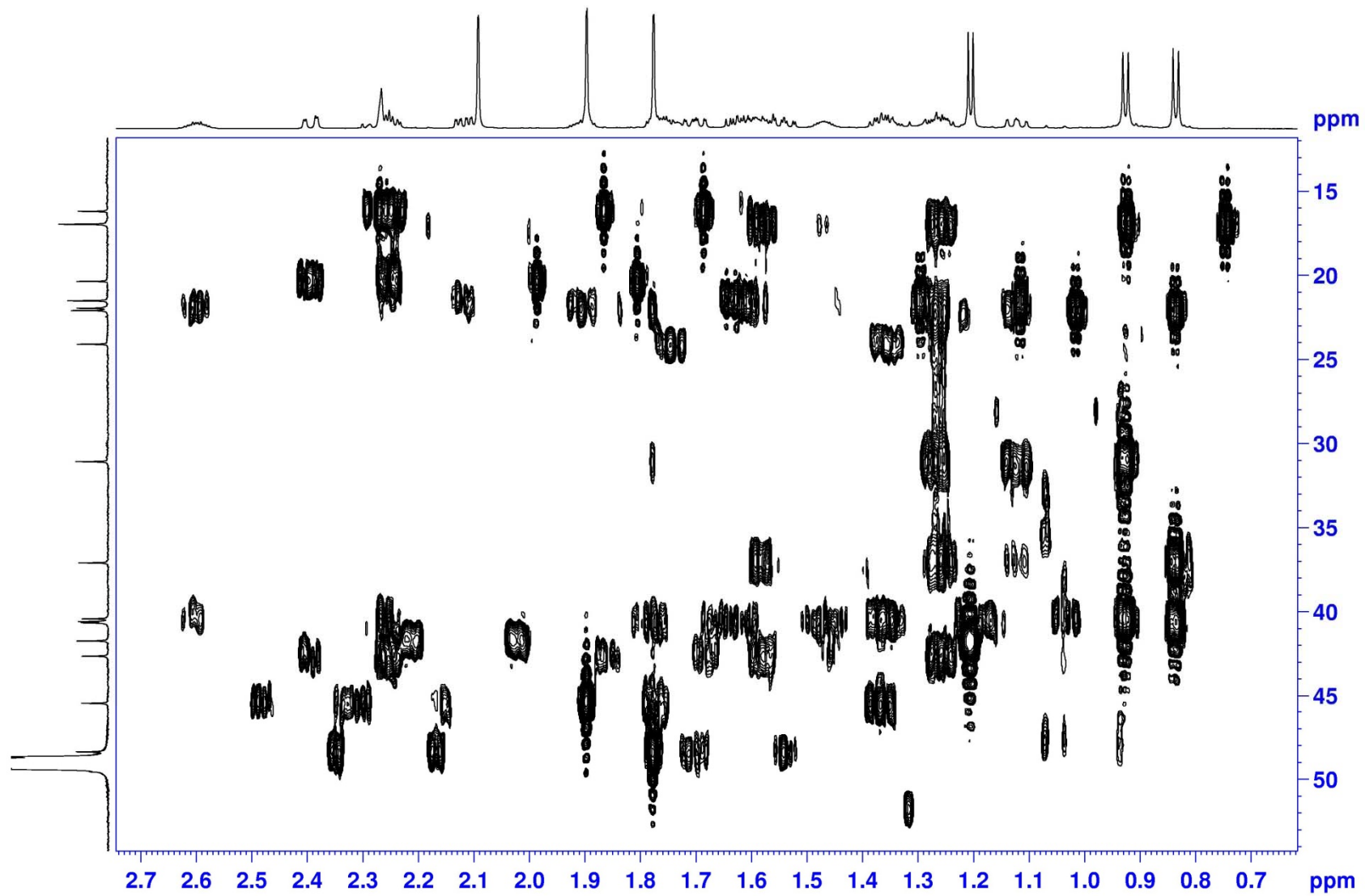
HMBC (700 MHz) spectrum of compound **1** in CD₃OD



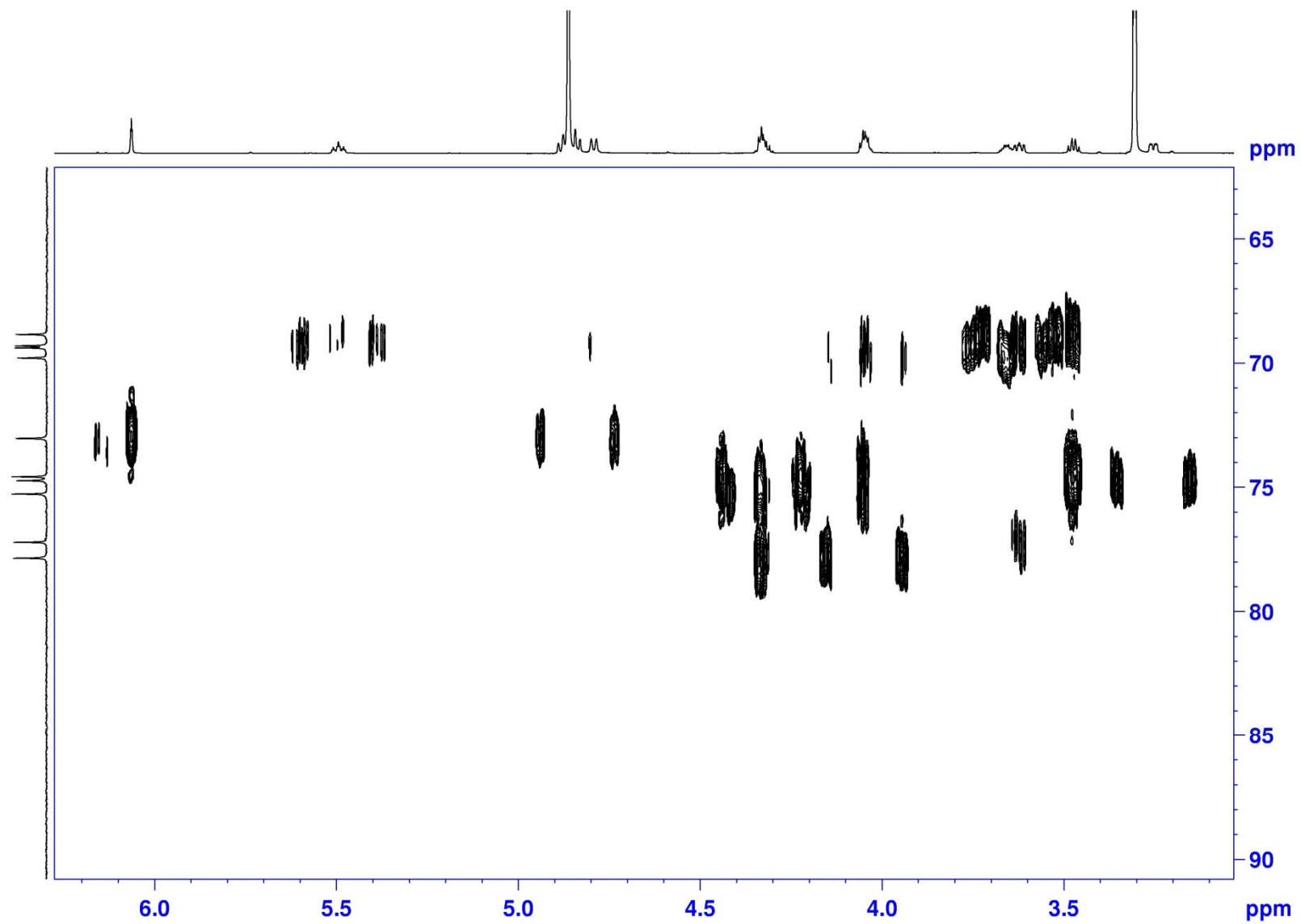
HMBC (700 MHz) spectrum of compound **1** in CD₃OD



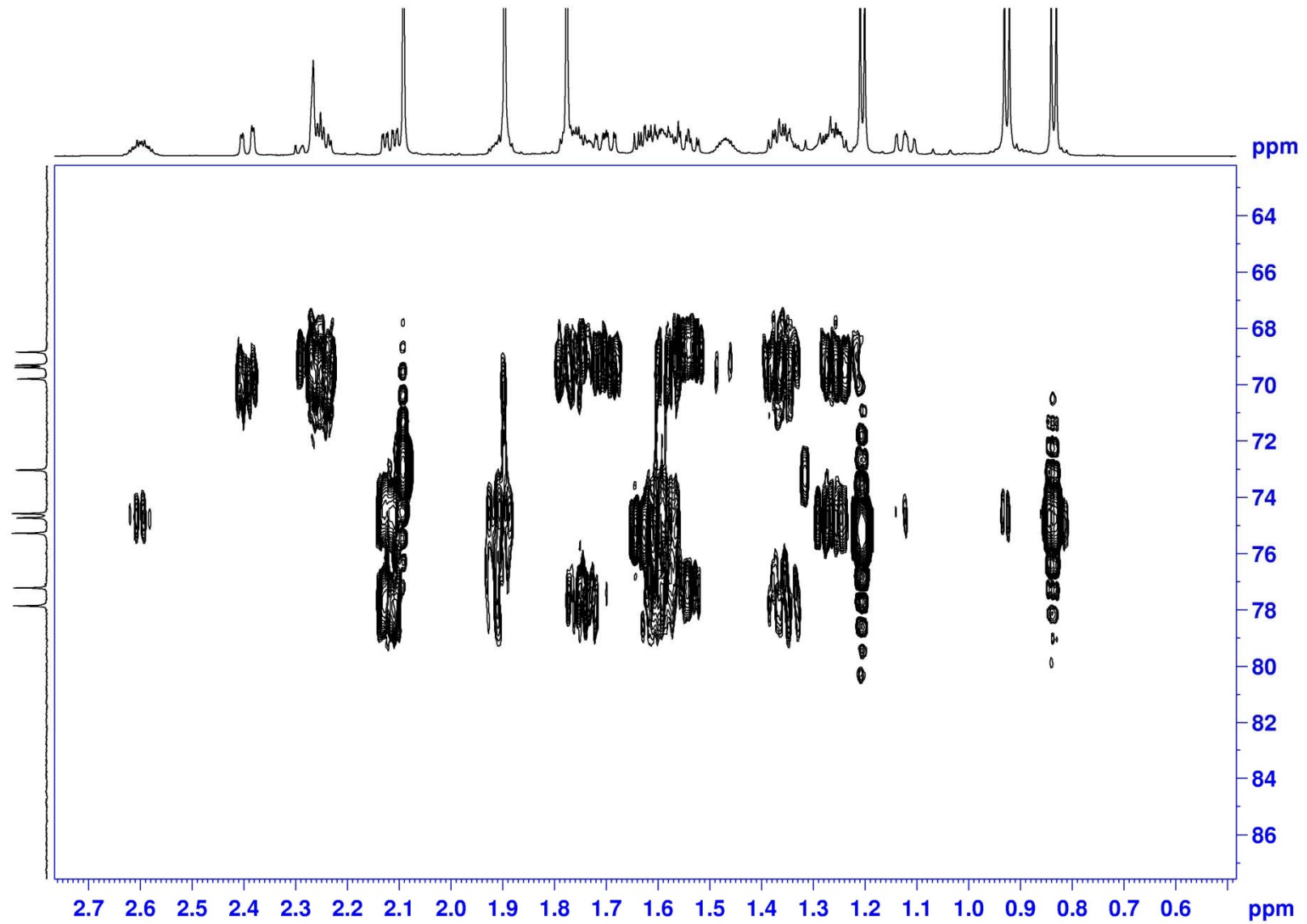
HMBC (700 MHz) spectrum of compound **1** in CD₃OD



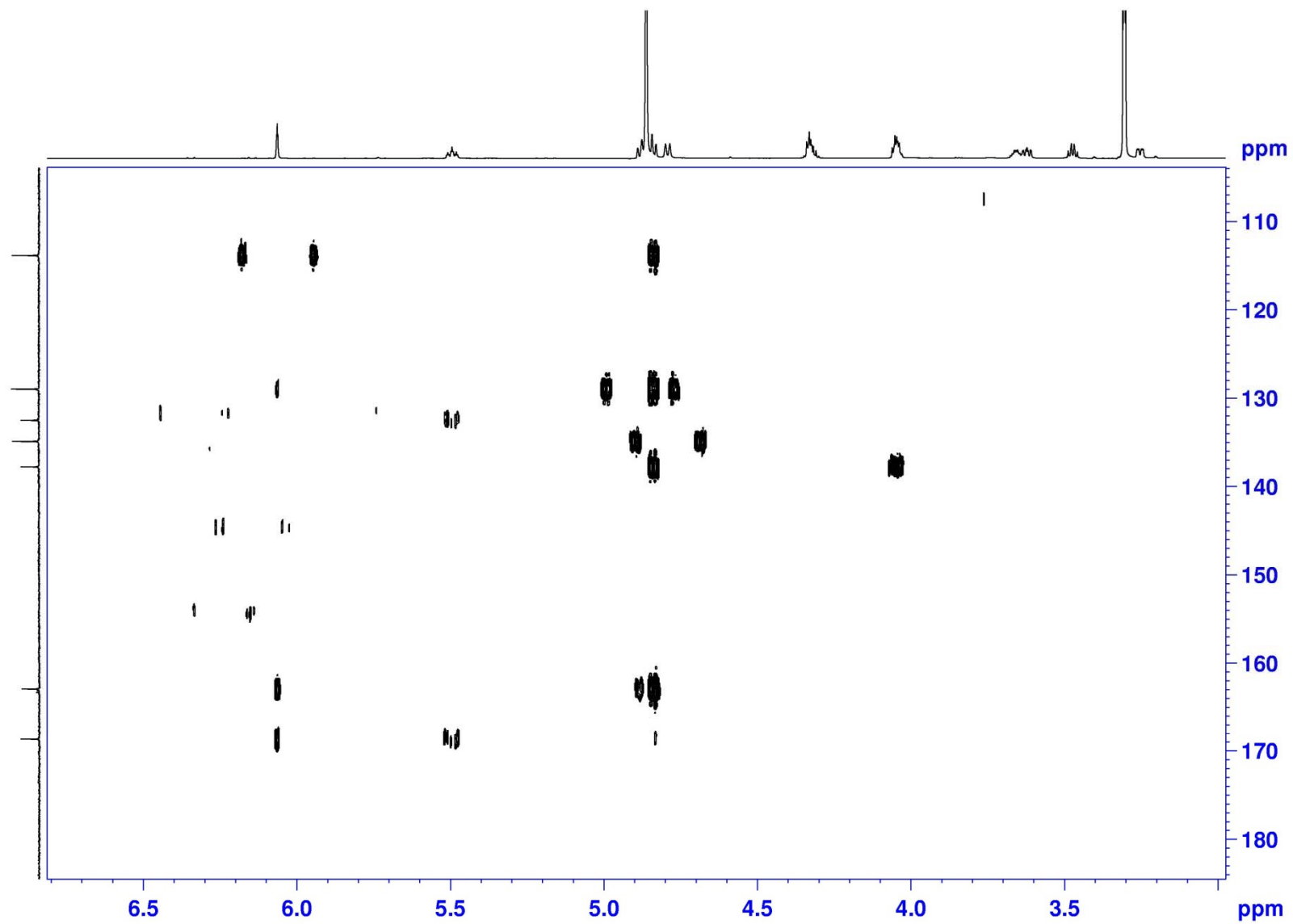
HMBC (700 MHz) spectrum of compound **1** in CD₃OD



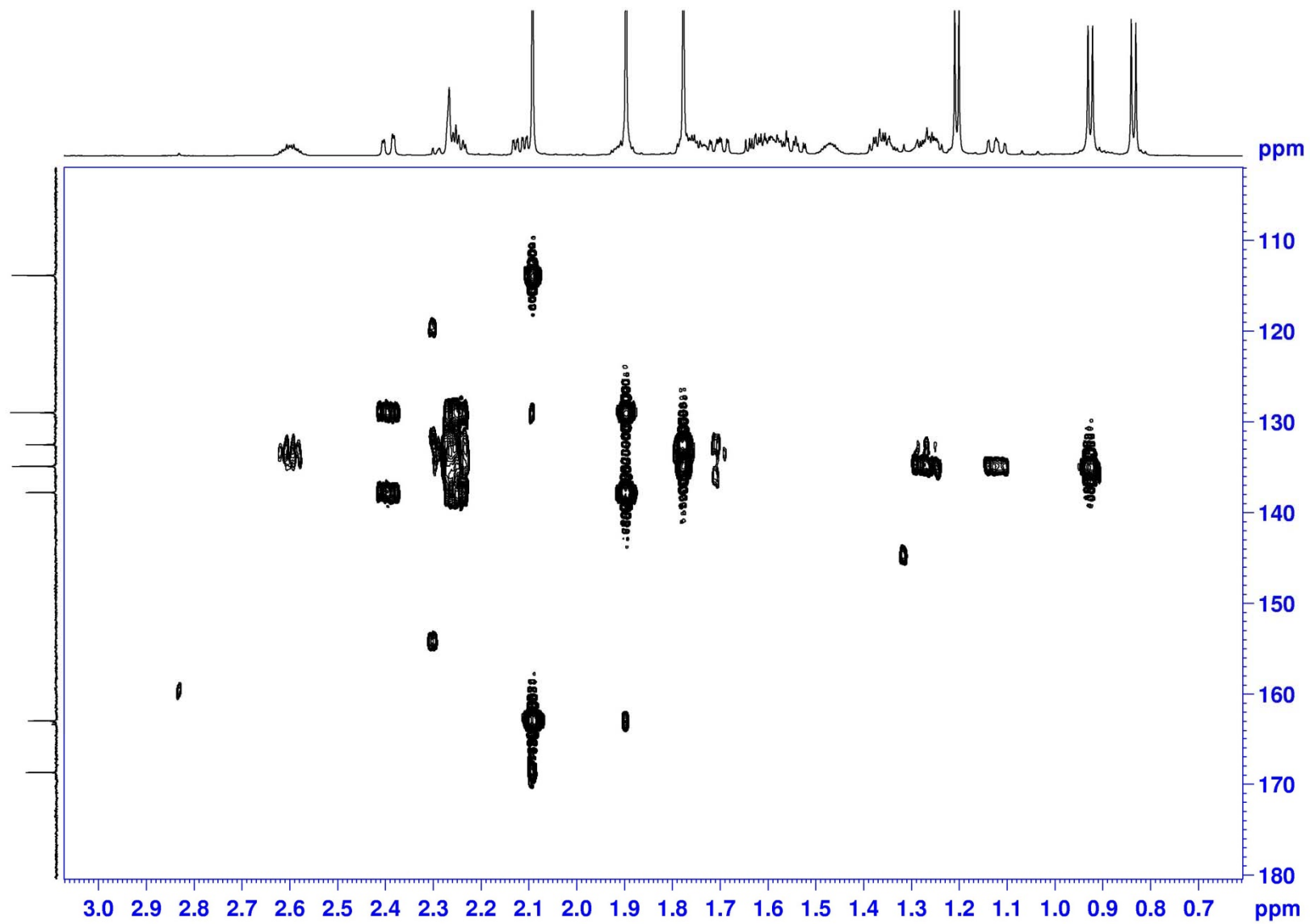
HMBC (700 MHz) spectrum of compound **1** in CD₃OD



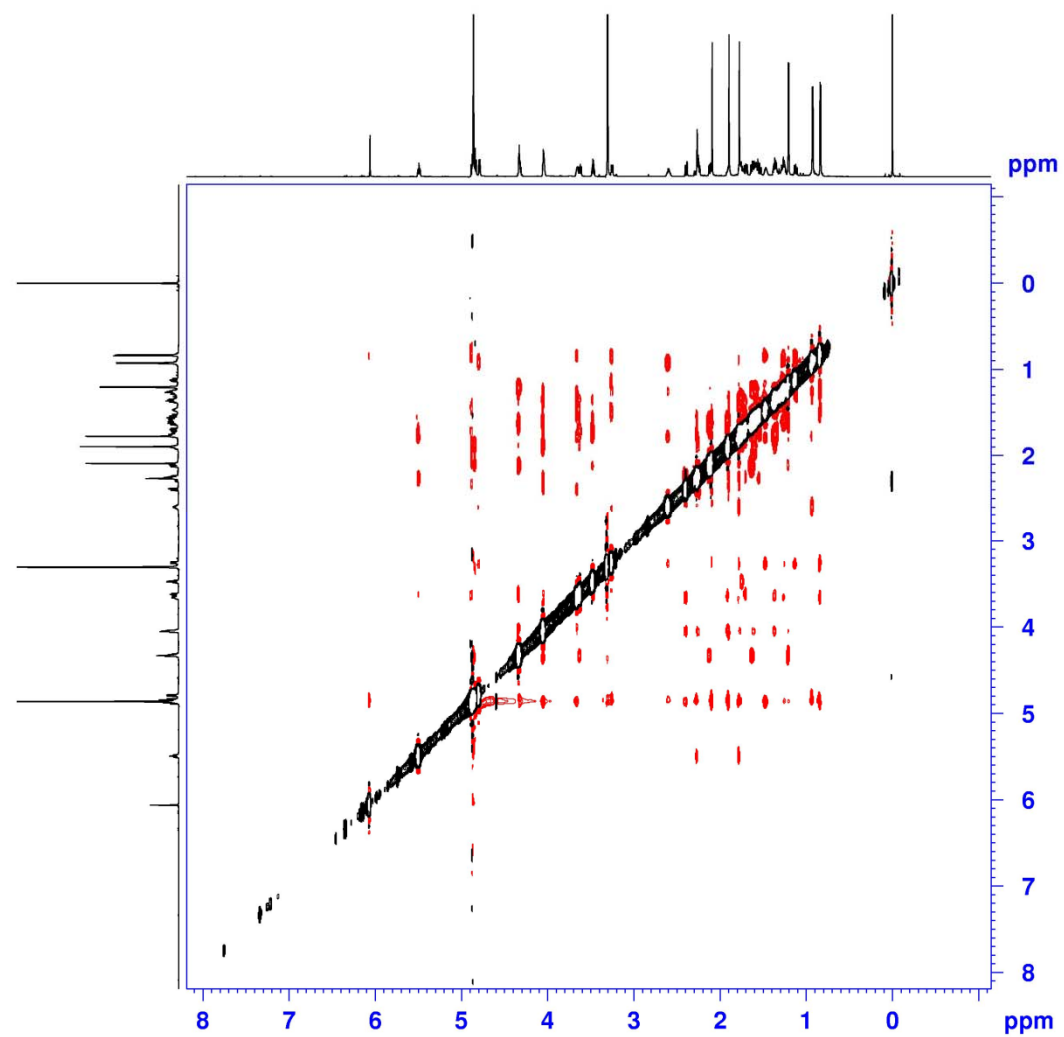
HMBC (700 MHz) spectrum of compound **1** in CD₃OD



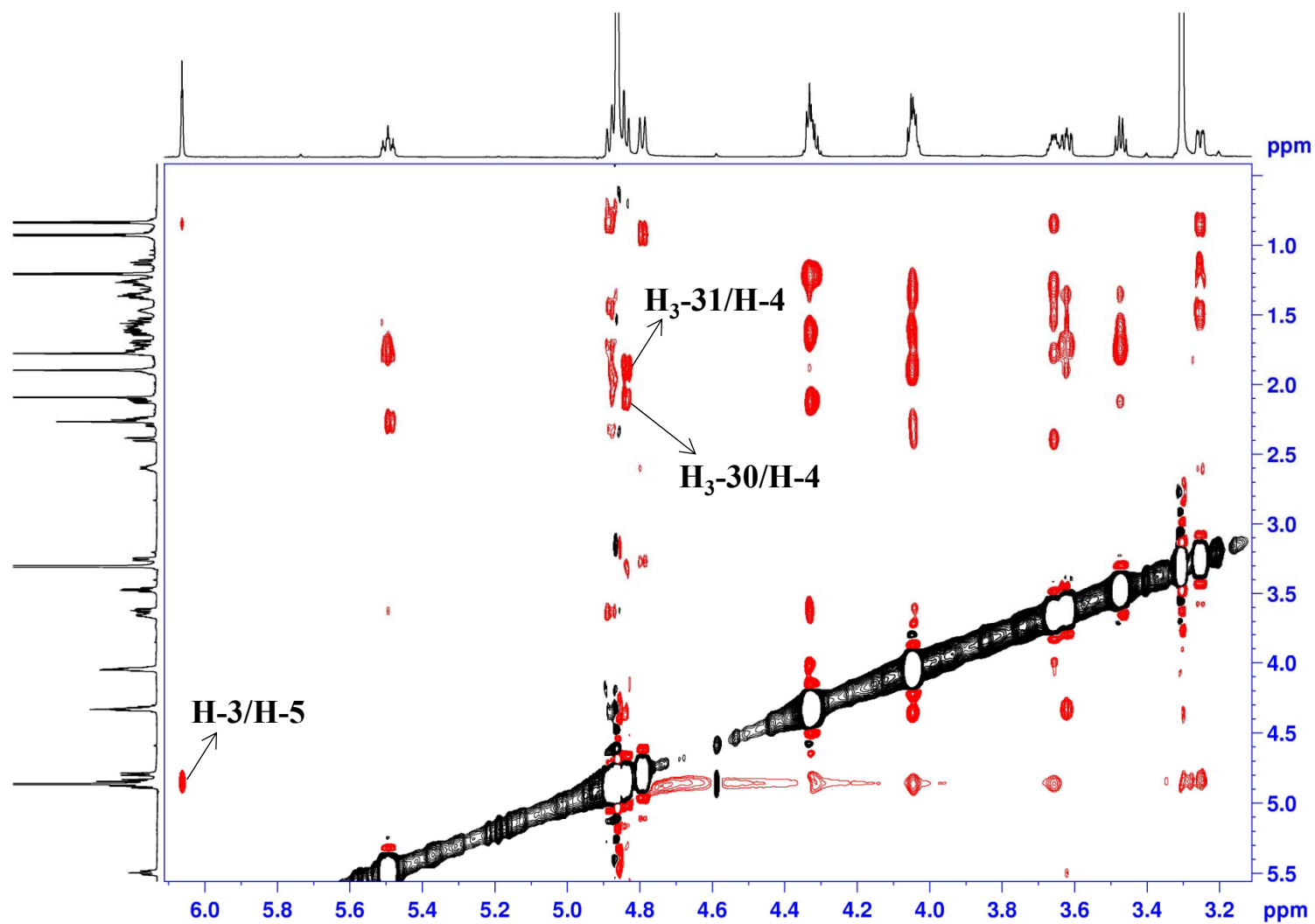
HMBC (700 MHz) spectrum of compound **1** in CD₃OD



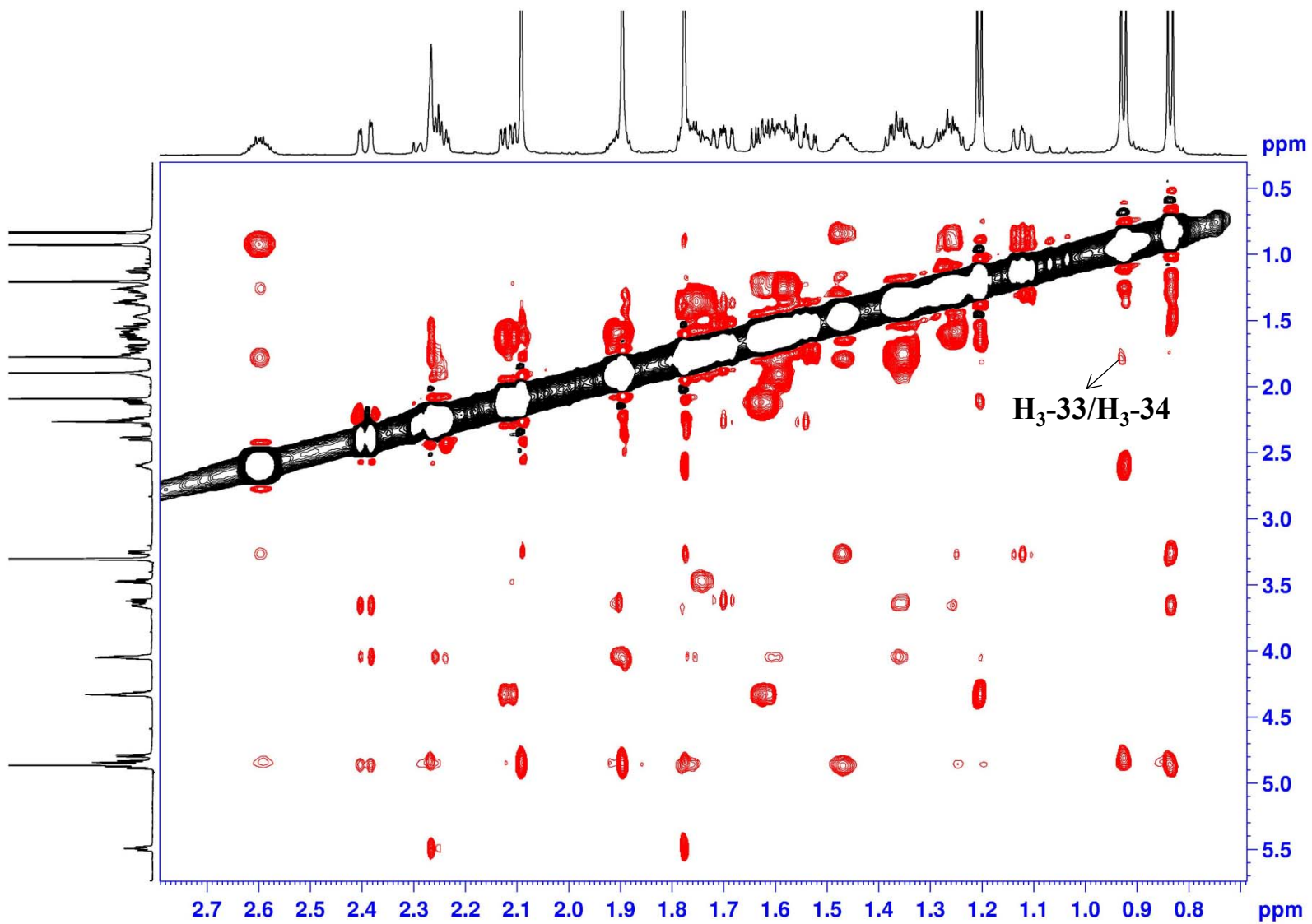
NOESY (700 MHz) spectrum of compound **1** in CD₃OD



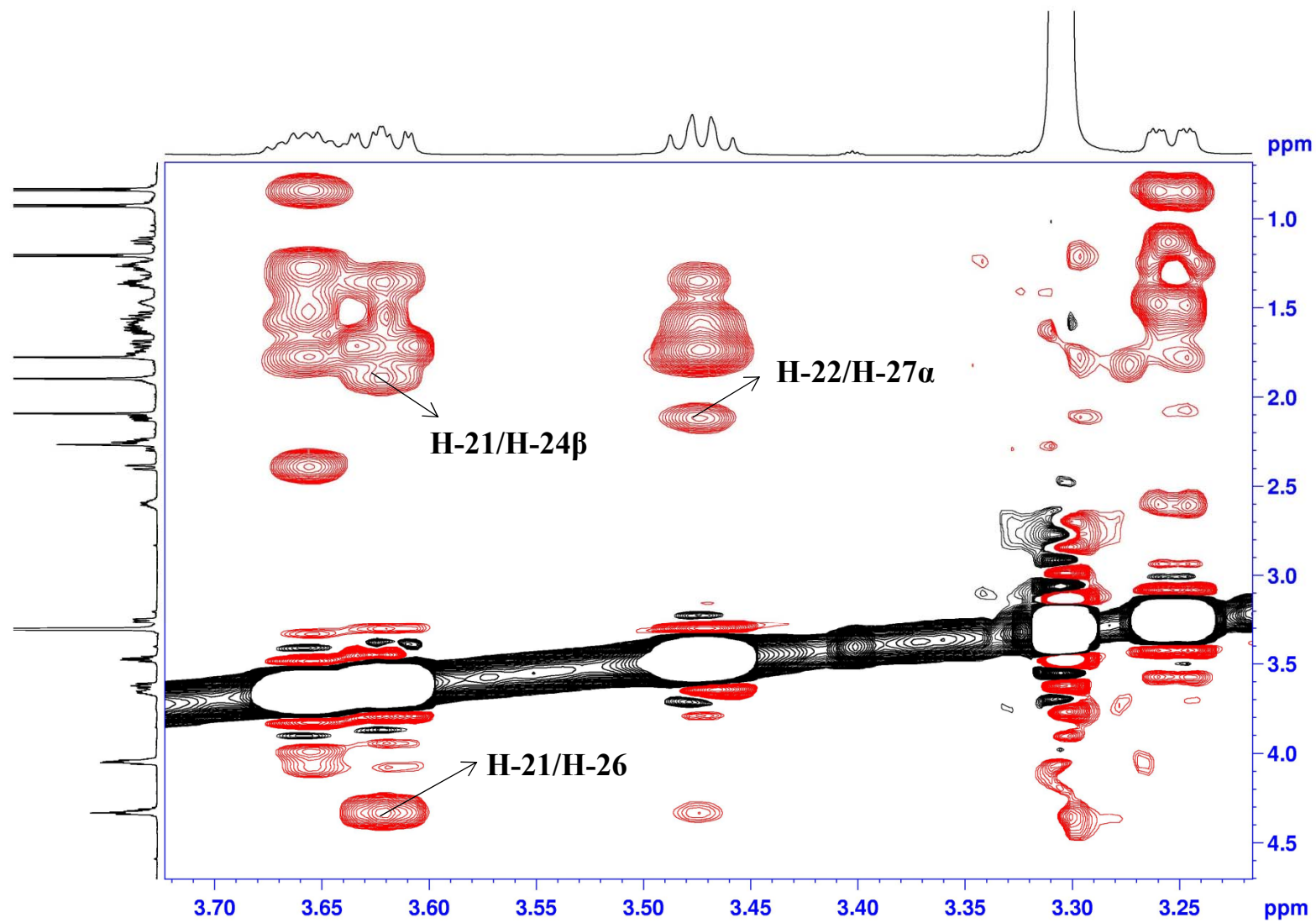
NOESY (700 MHz) spectrum of compound **1** in CD₃OD



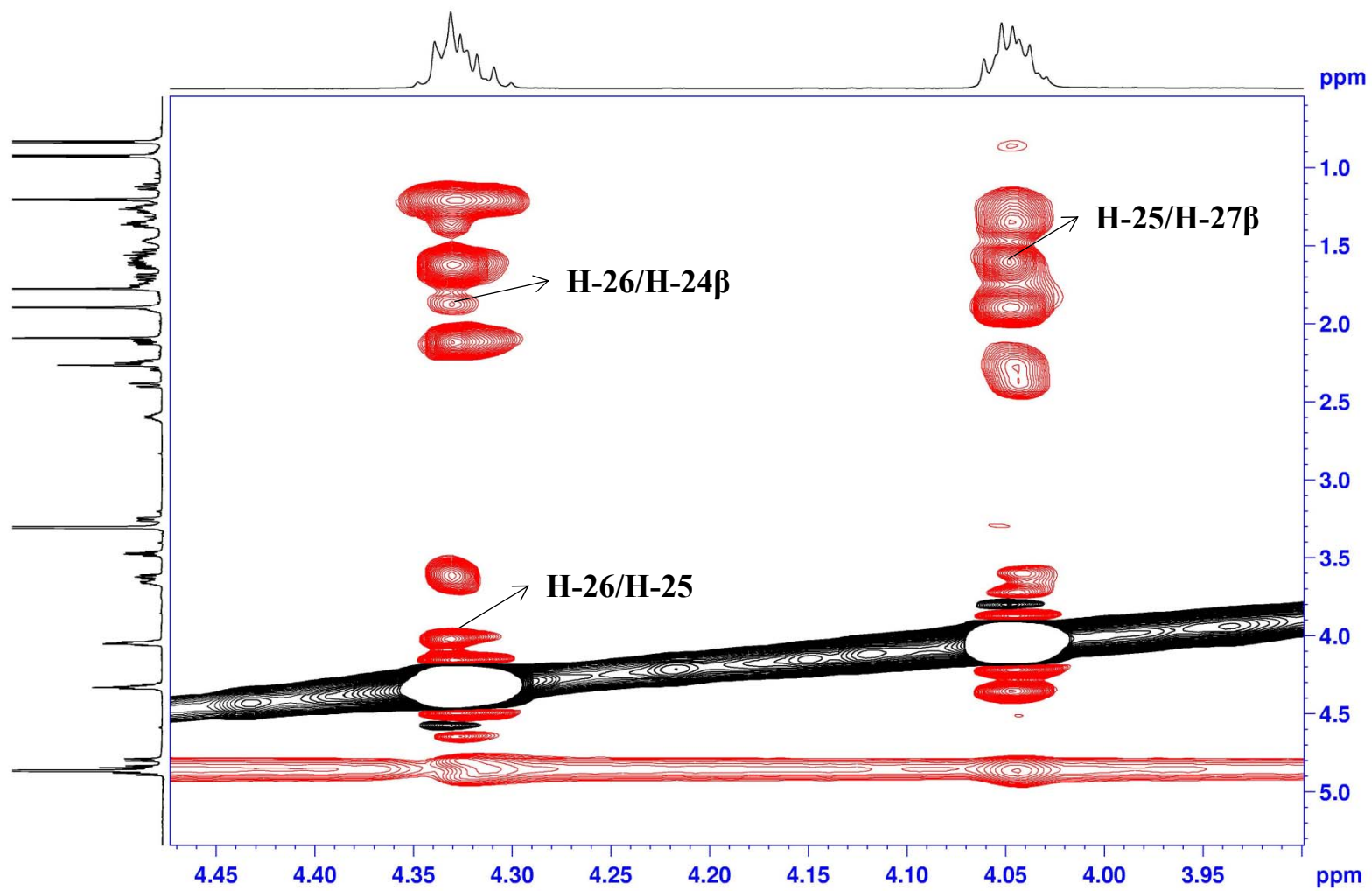
NOESY (700 MHz) spectrum of compound **1** in CD₃OD



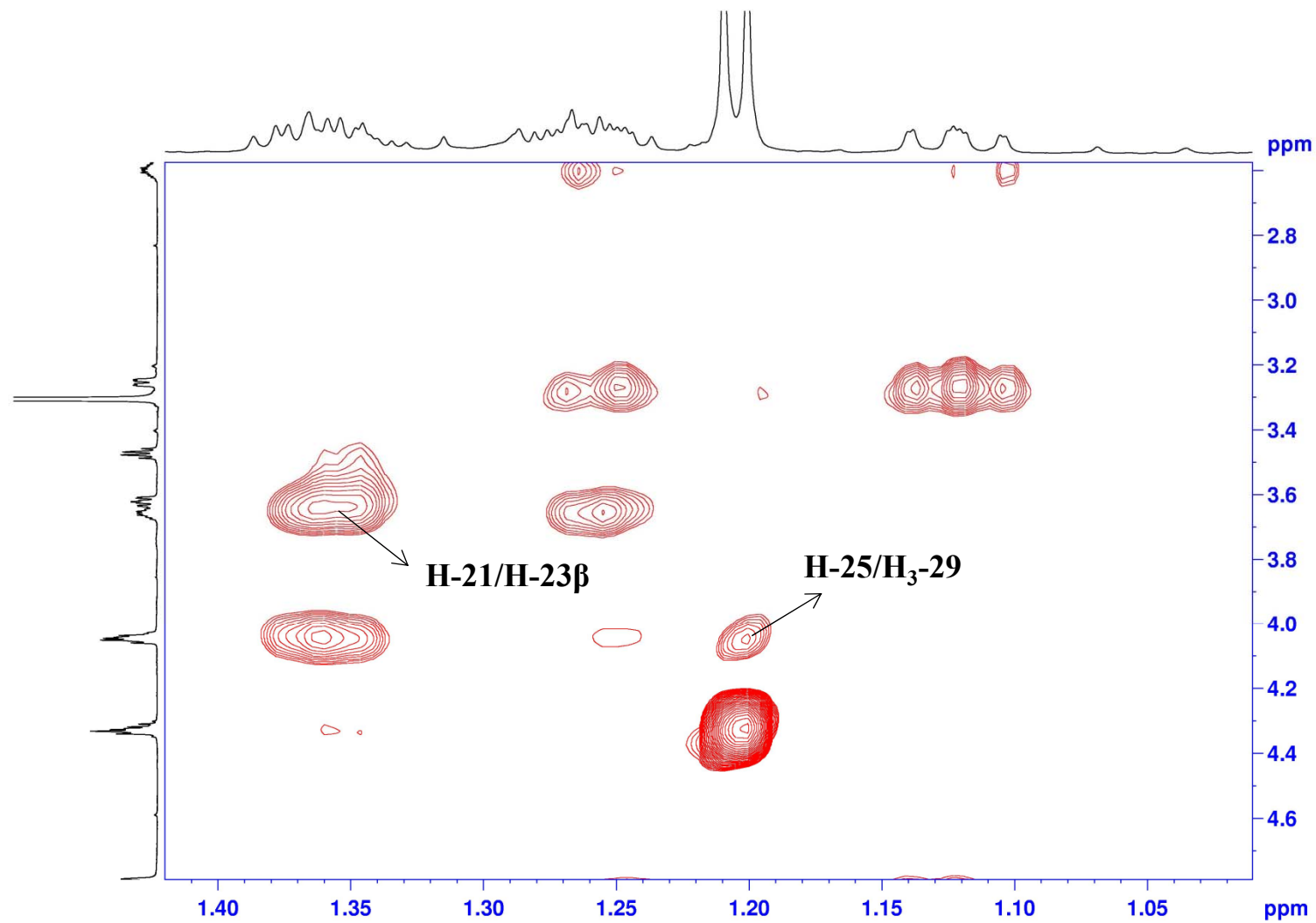
NOESY (700 MHz) spectrum of compound **1** in CD₃OD



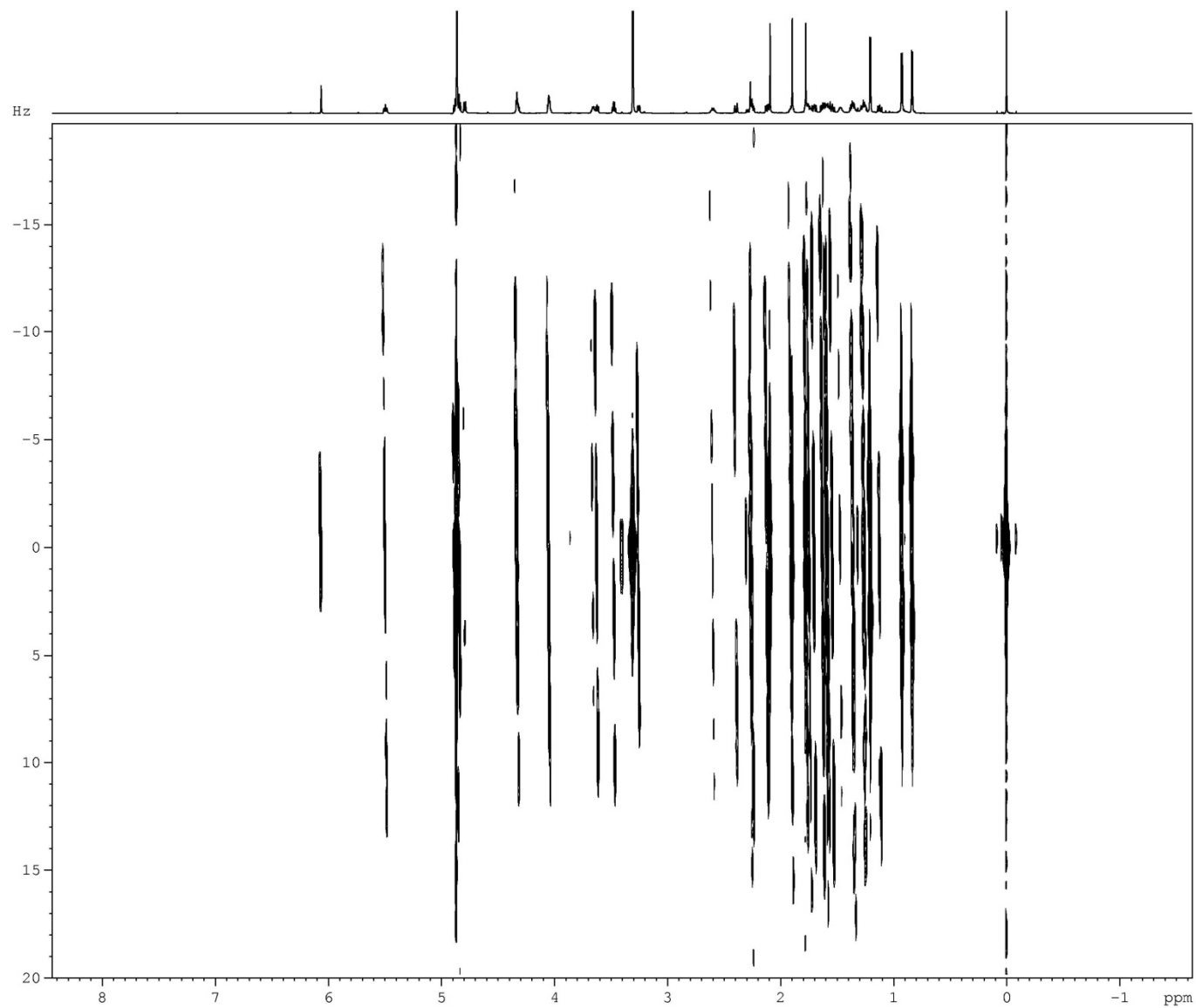
NOESY (700 MHz) spectrum of compound **1** in CD₃OD



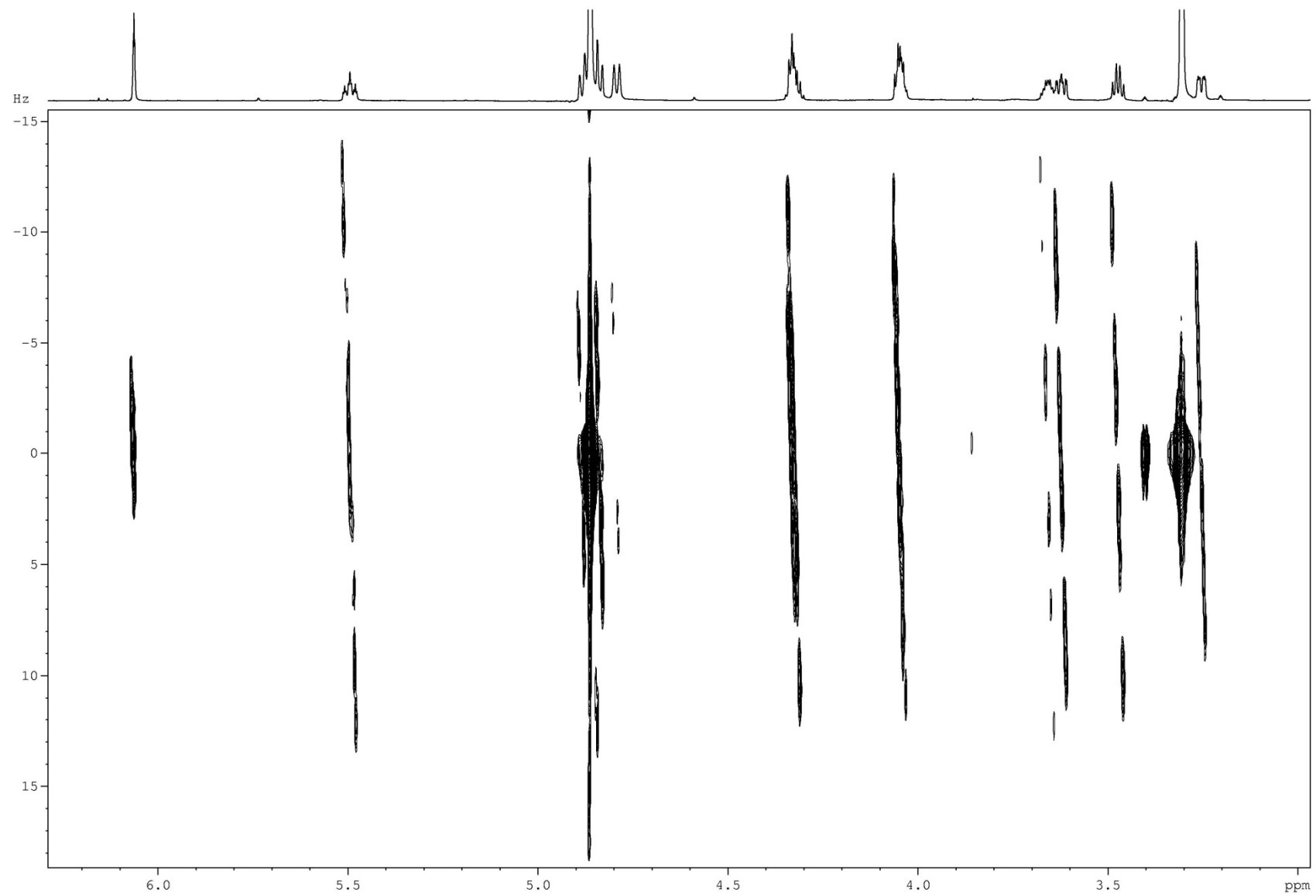
NOESY (700 MHz) spectrum of compound **1** in CD₃OD



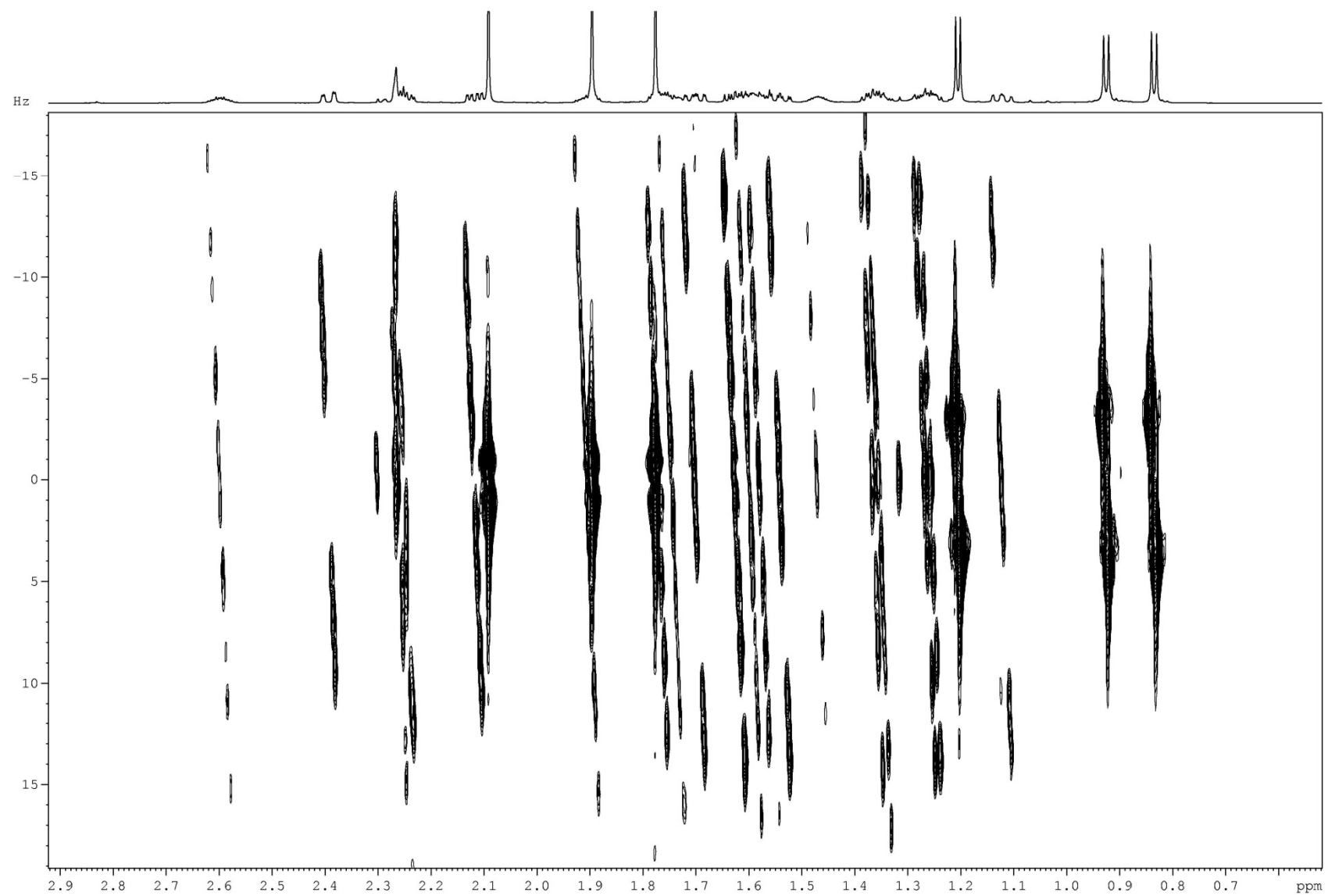
2D JRES (700 MHz) spectrum of compound **1** in CD₃OD



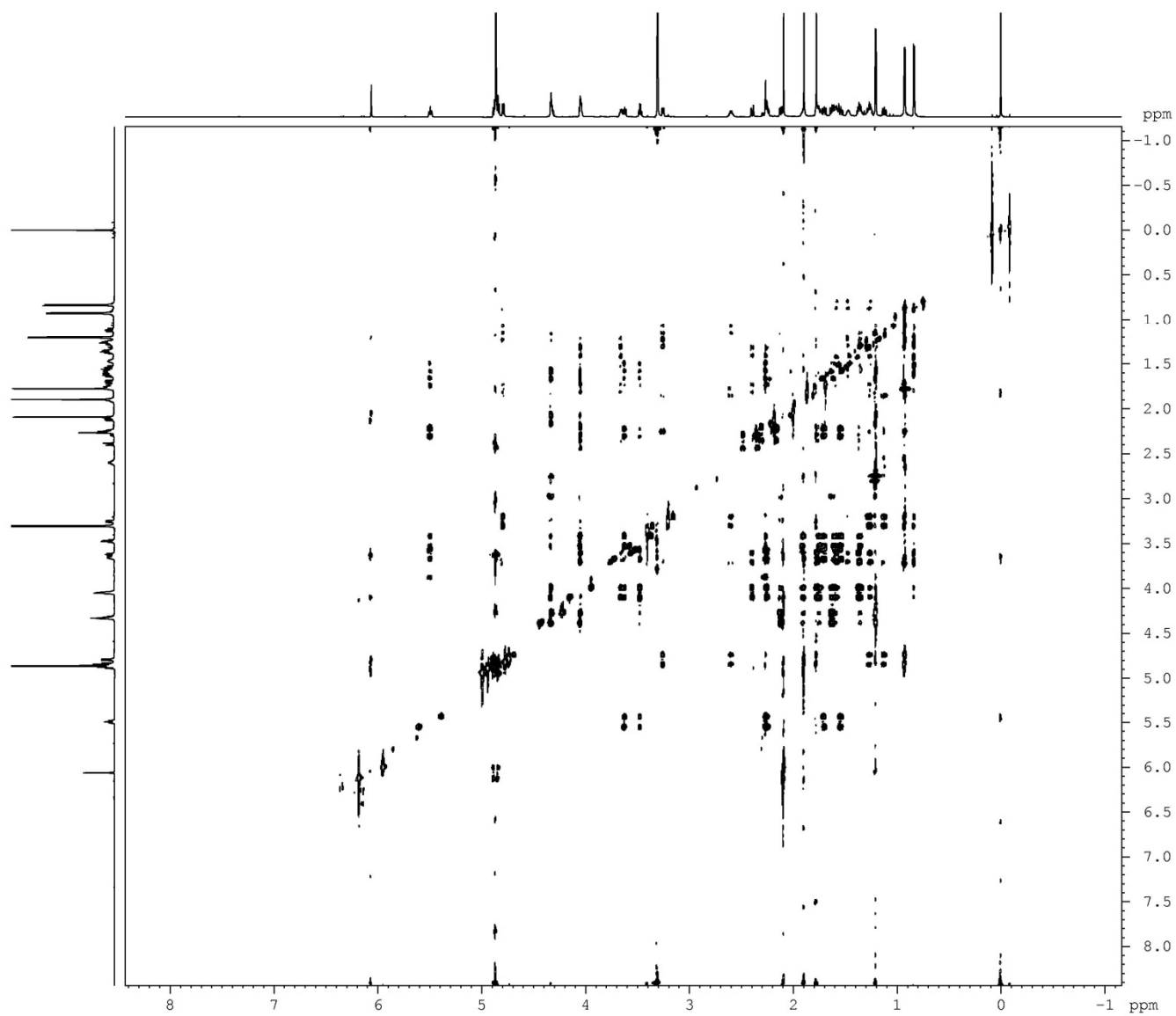
2D JRES (700 MHz) spectrum of compound **1** in CD₃OD



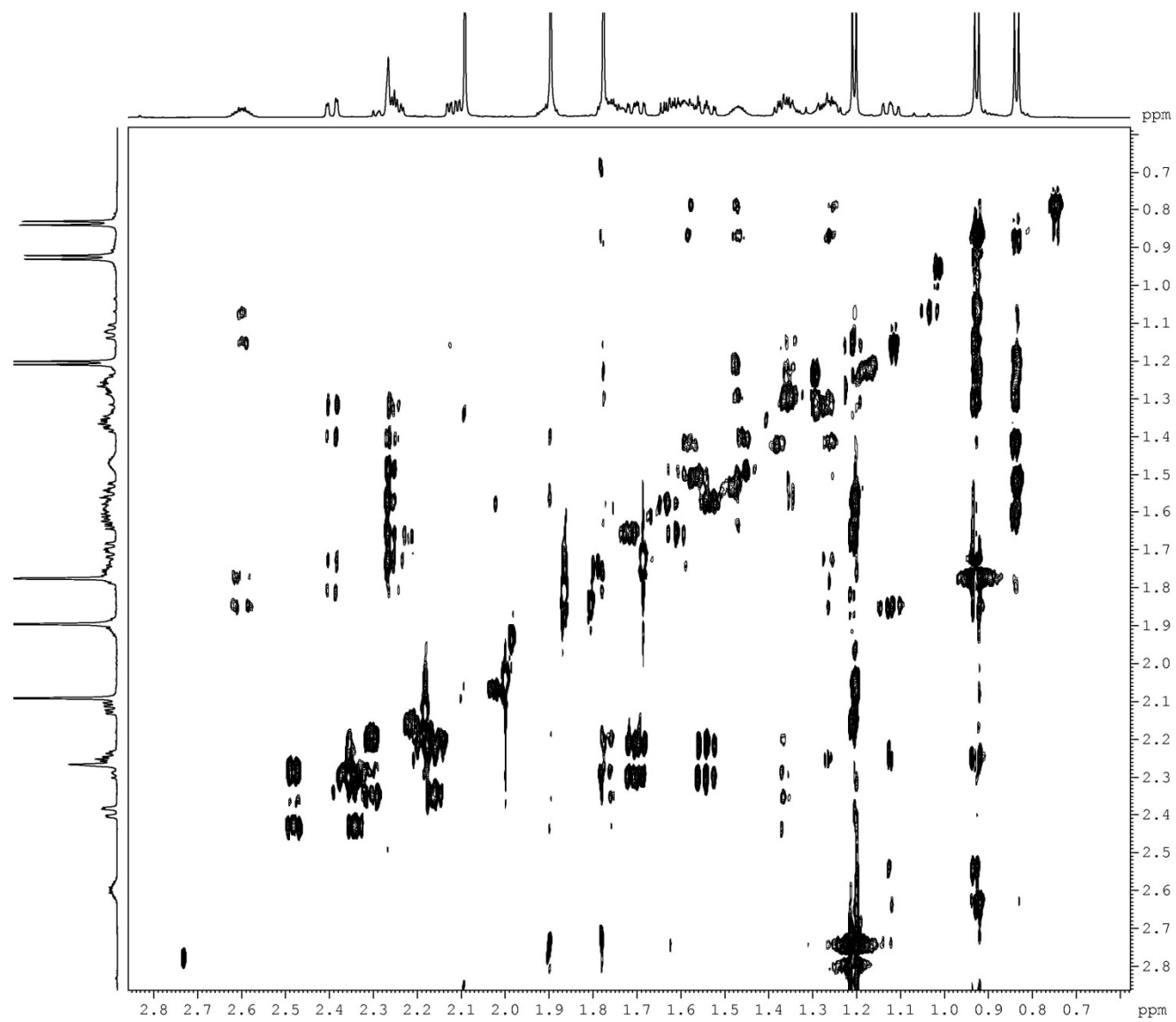
2D JRES (700 MHz) spectrum of compound **1** in CD₃OD



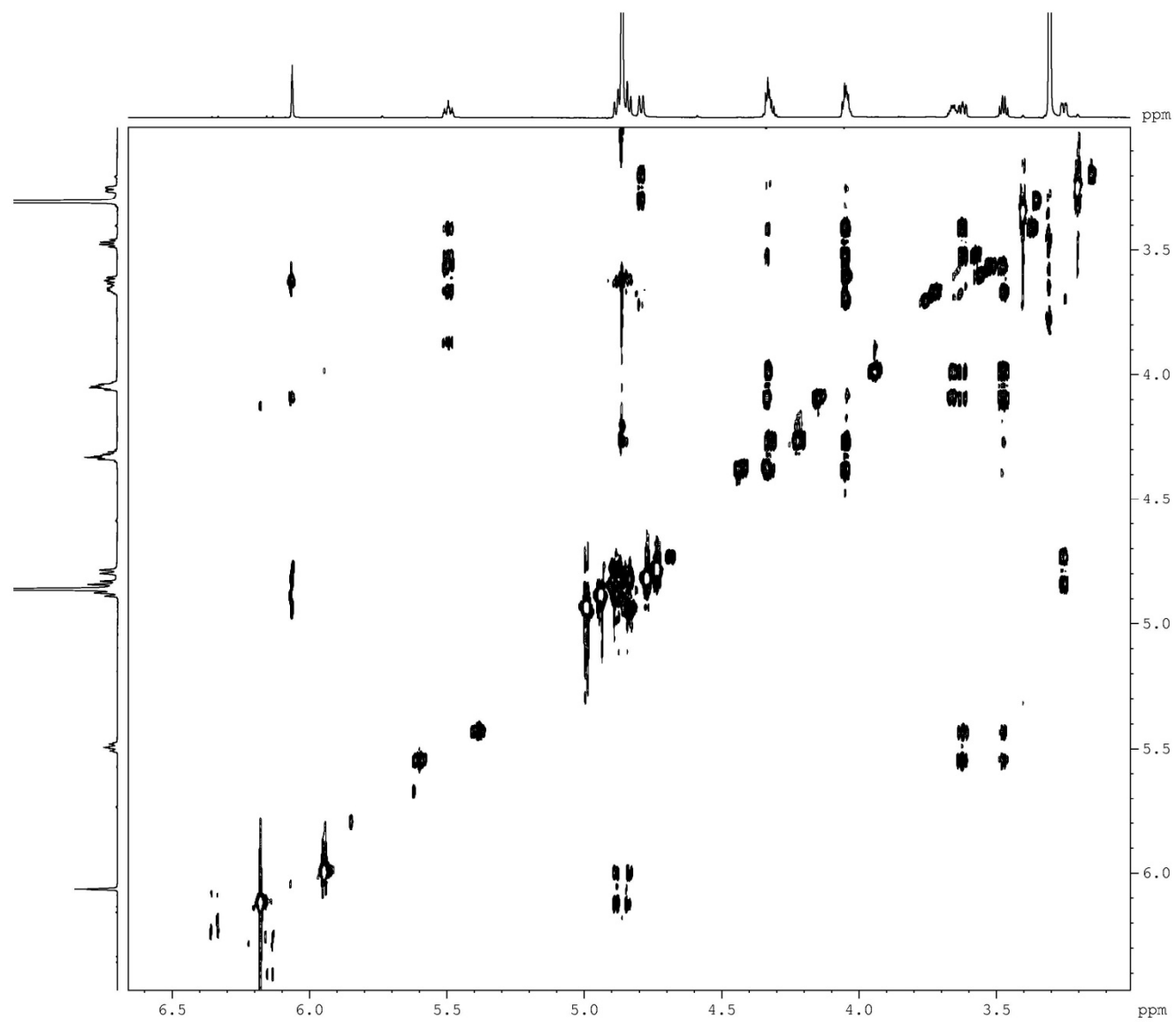
HETLOC (700 MHz) spectrum of compound **1** in CD₃OD



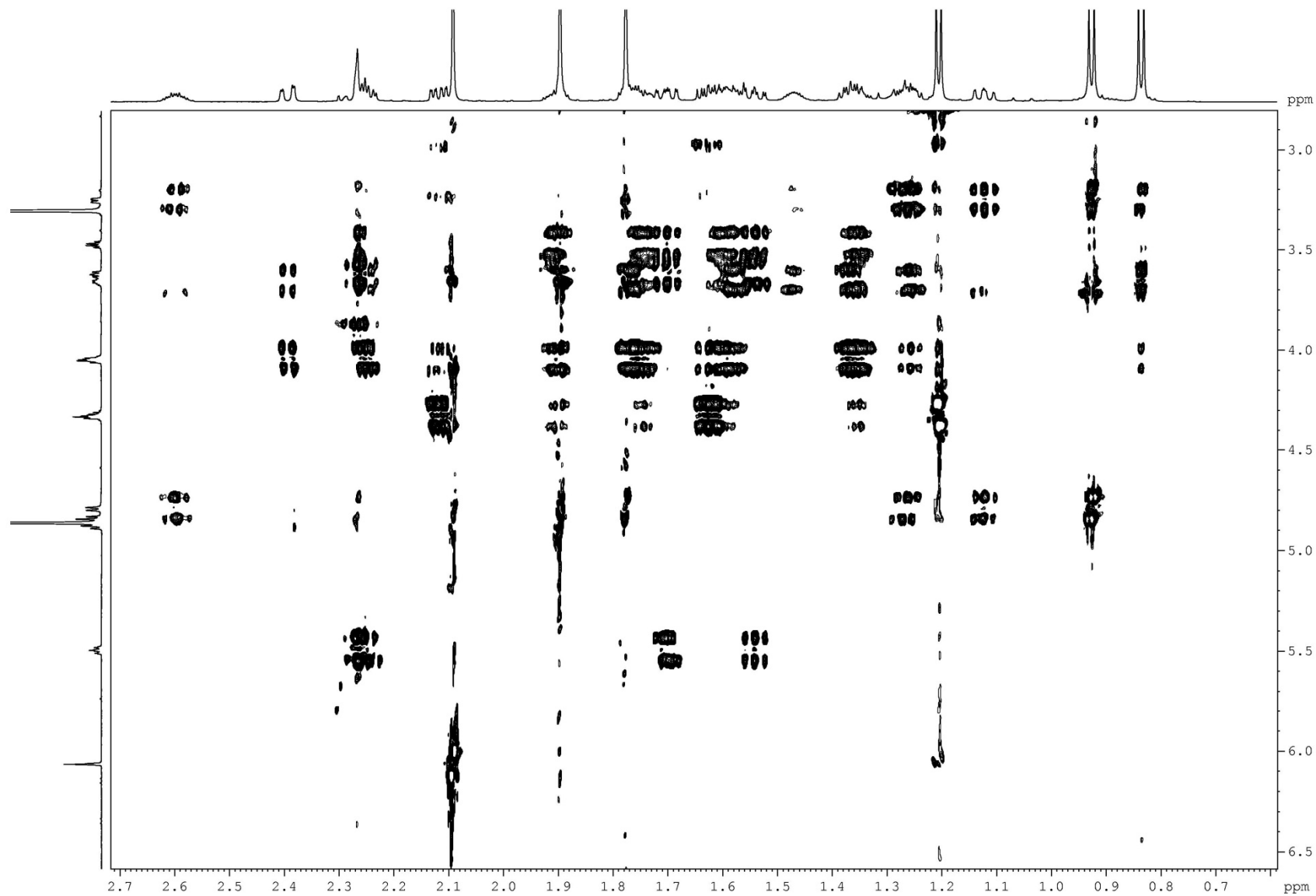
HETLOC (700 MHz) spectrum of compound **1** in CD₃OD



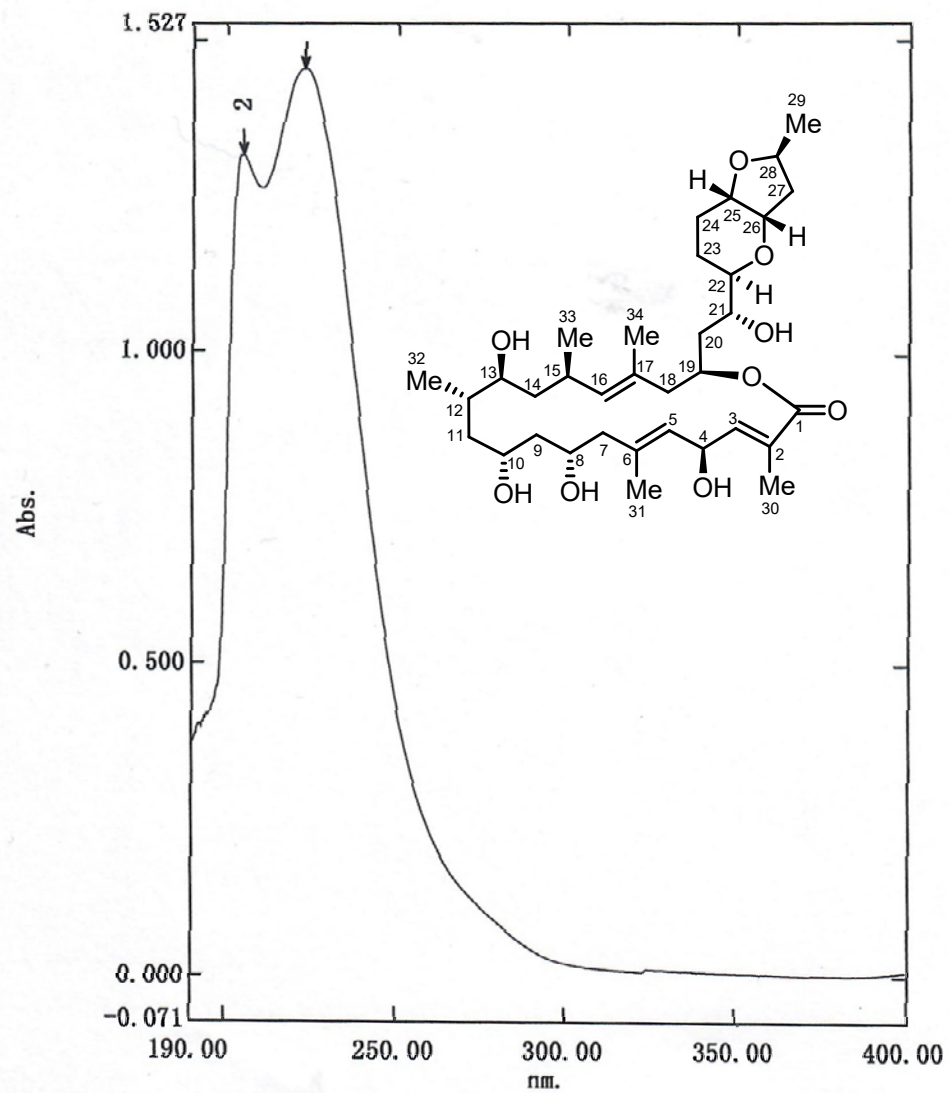
HETLOC (700 MHz) spectrum of compound **1** in CD₃OD



HETLOC (700 MHz) spectrum of compound **1** in CD₃OD

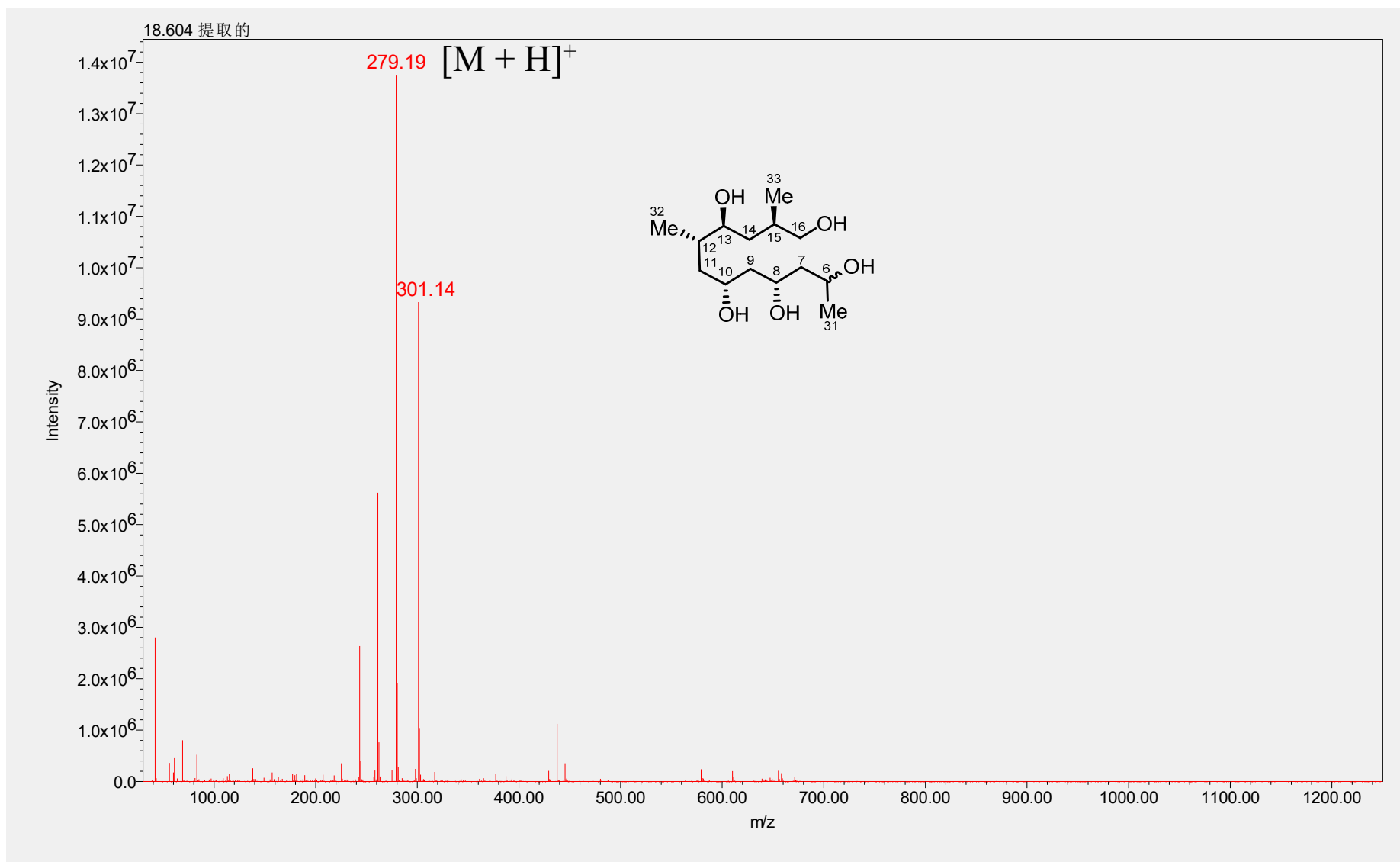


UV spectrum of compound 1

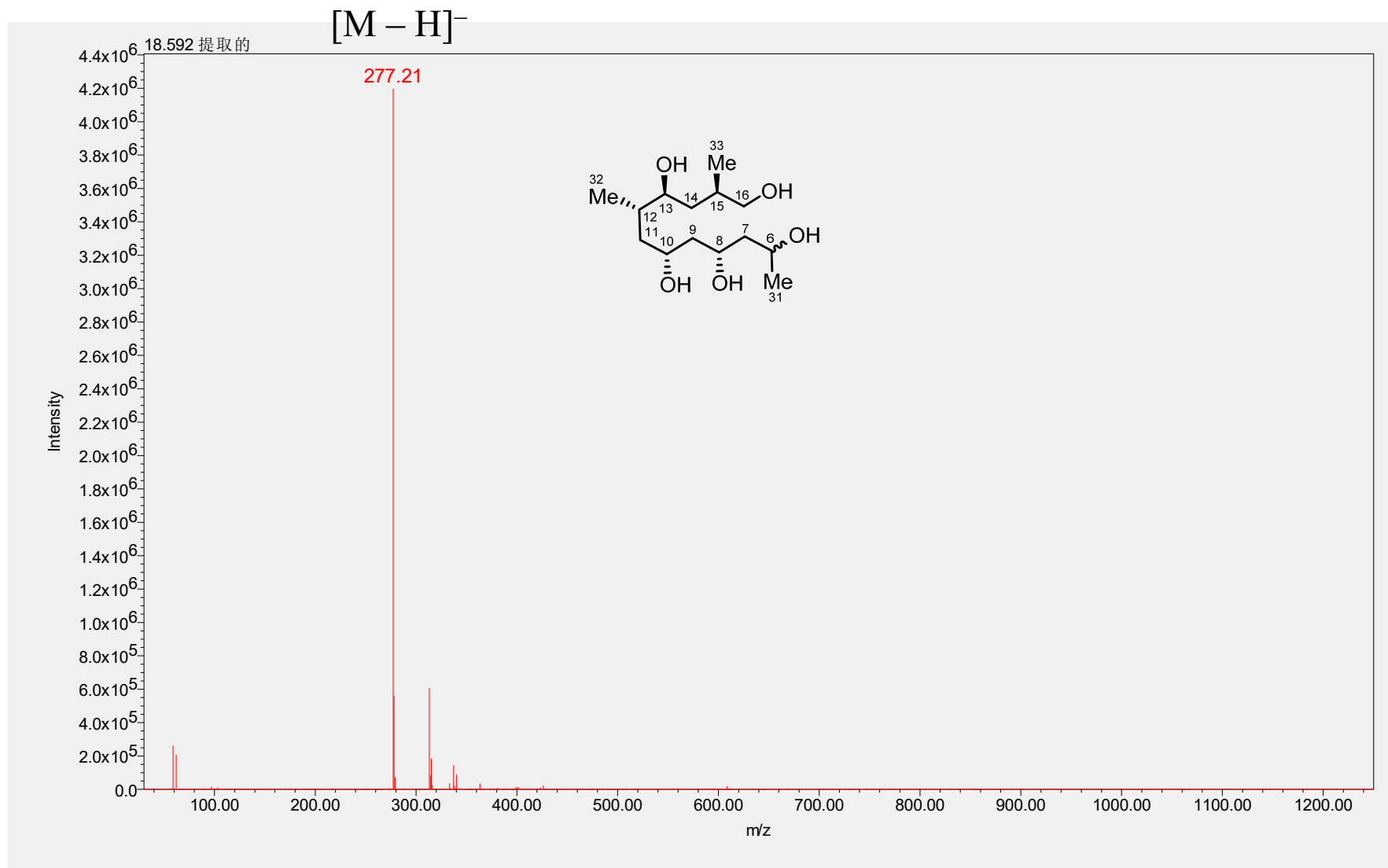


No.	P/V	(nm)	
1	Ⓢ	223.20	1.455
2	Ⓢ	204.80	1.312

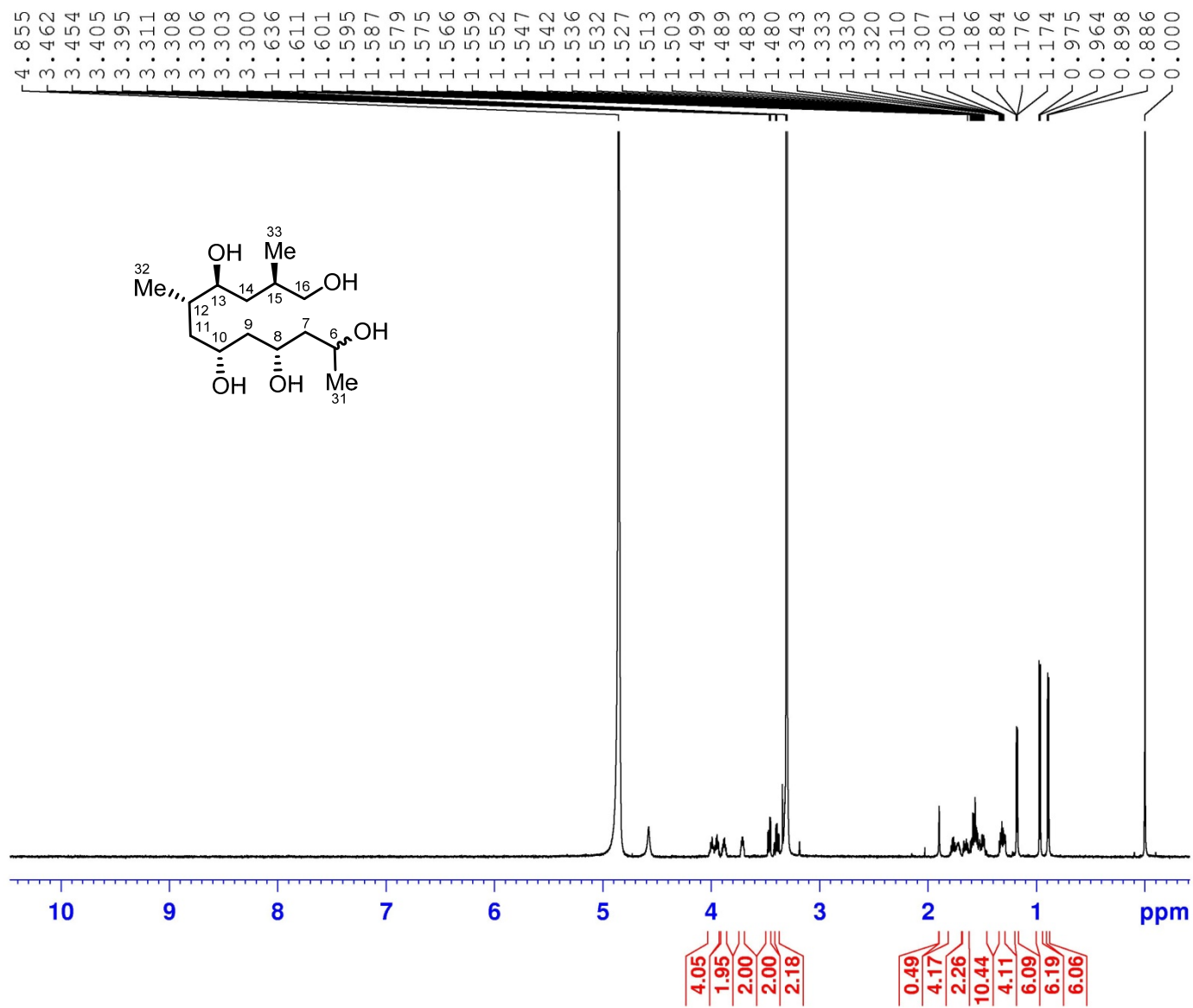
LR-ESIMS for the fragment 1A



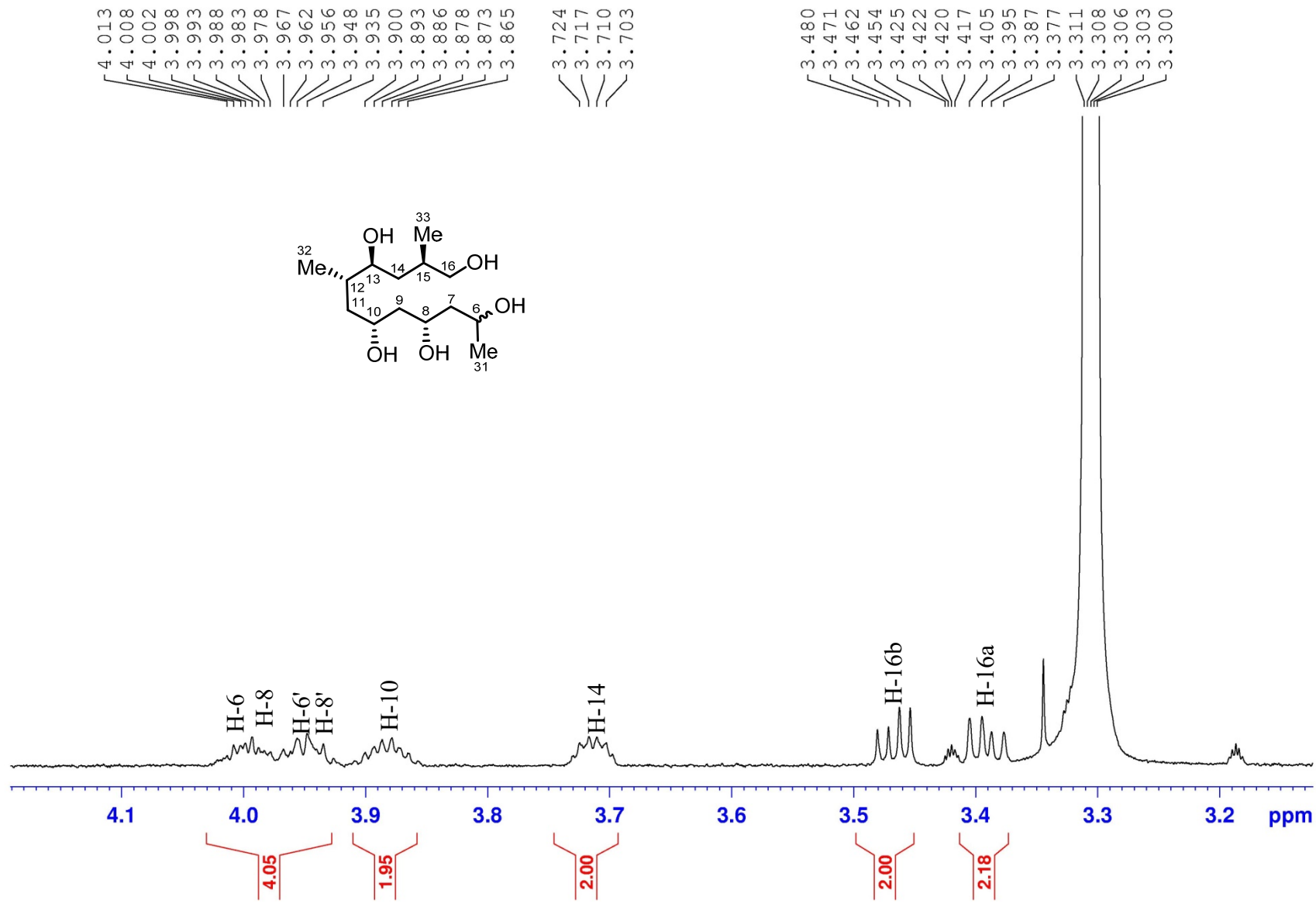
LR-ESIMS for the fragment 1A



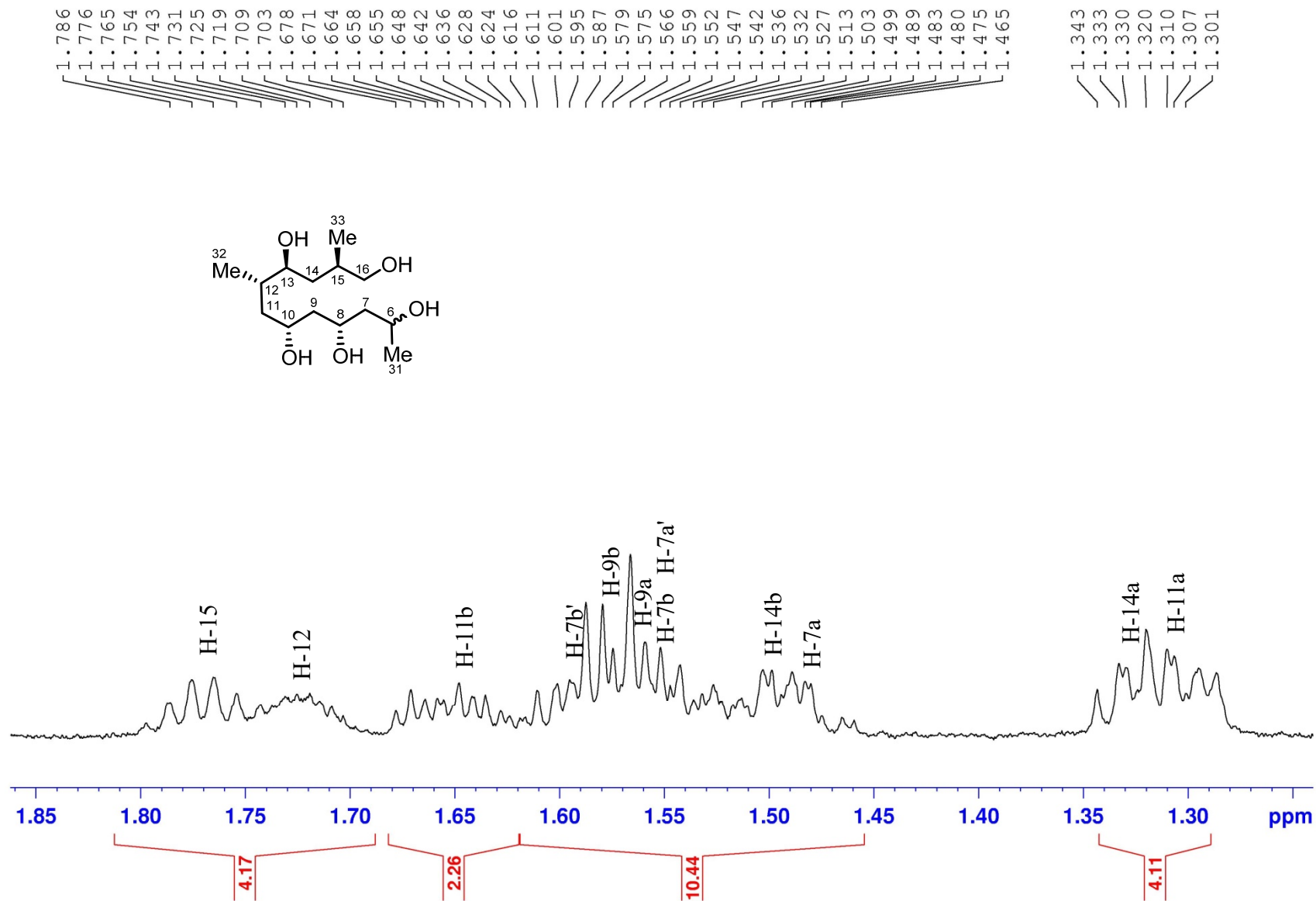
^1H (600 MHz) NMR spectrum of the fragment **1A** in CD_3OD



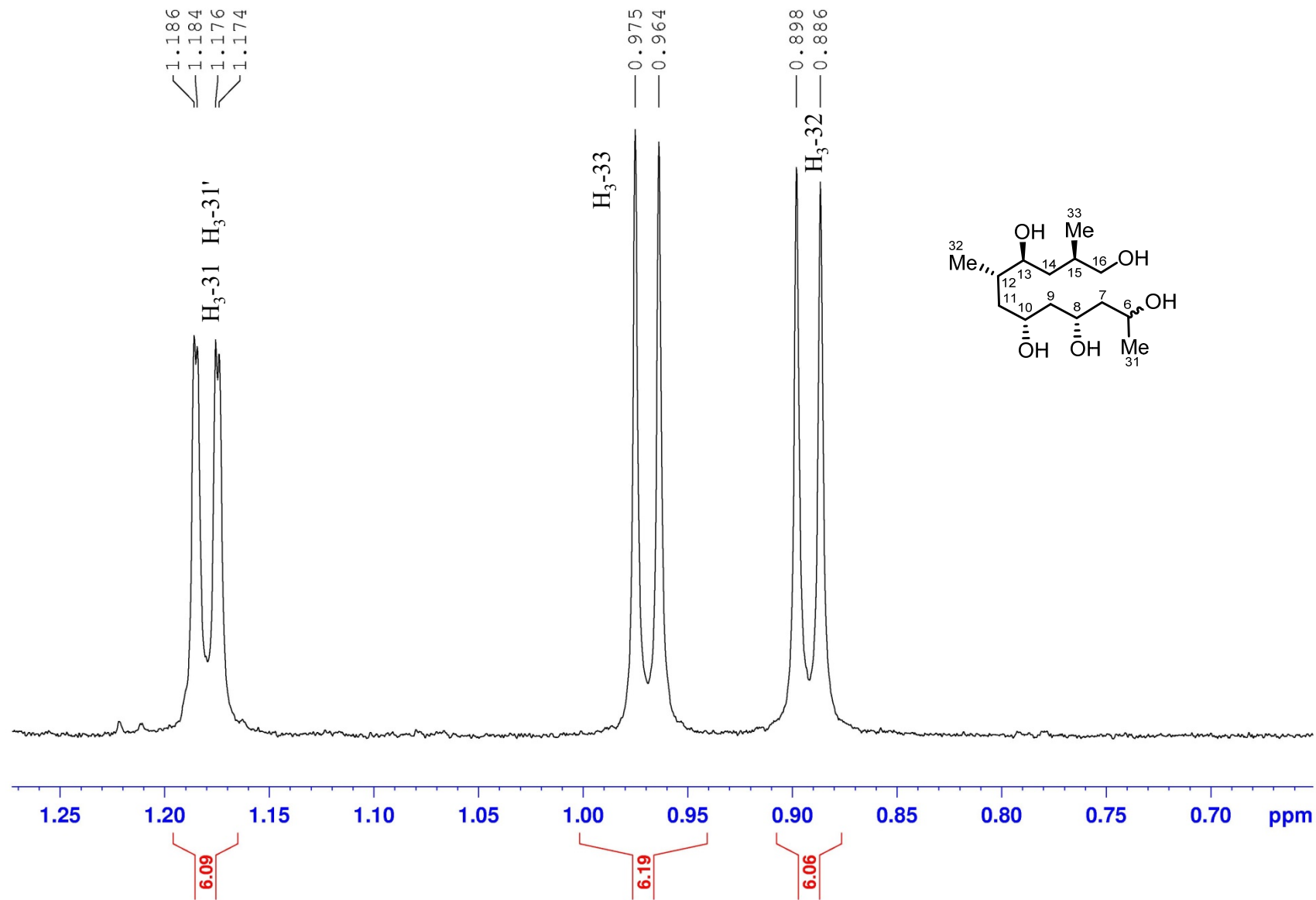
^1H (600 MHz) NMR spectrum of the fragment **1A** in CD_3OD



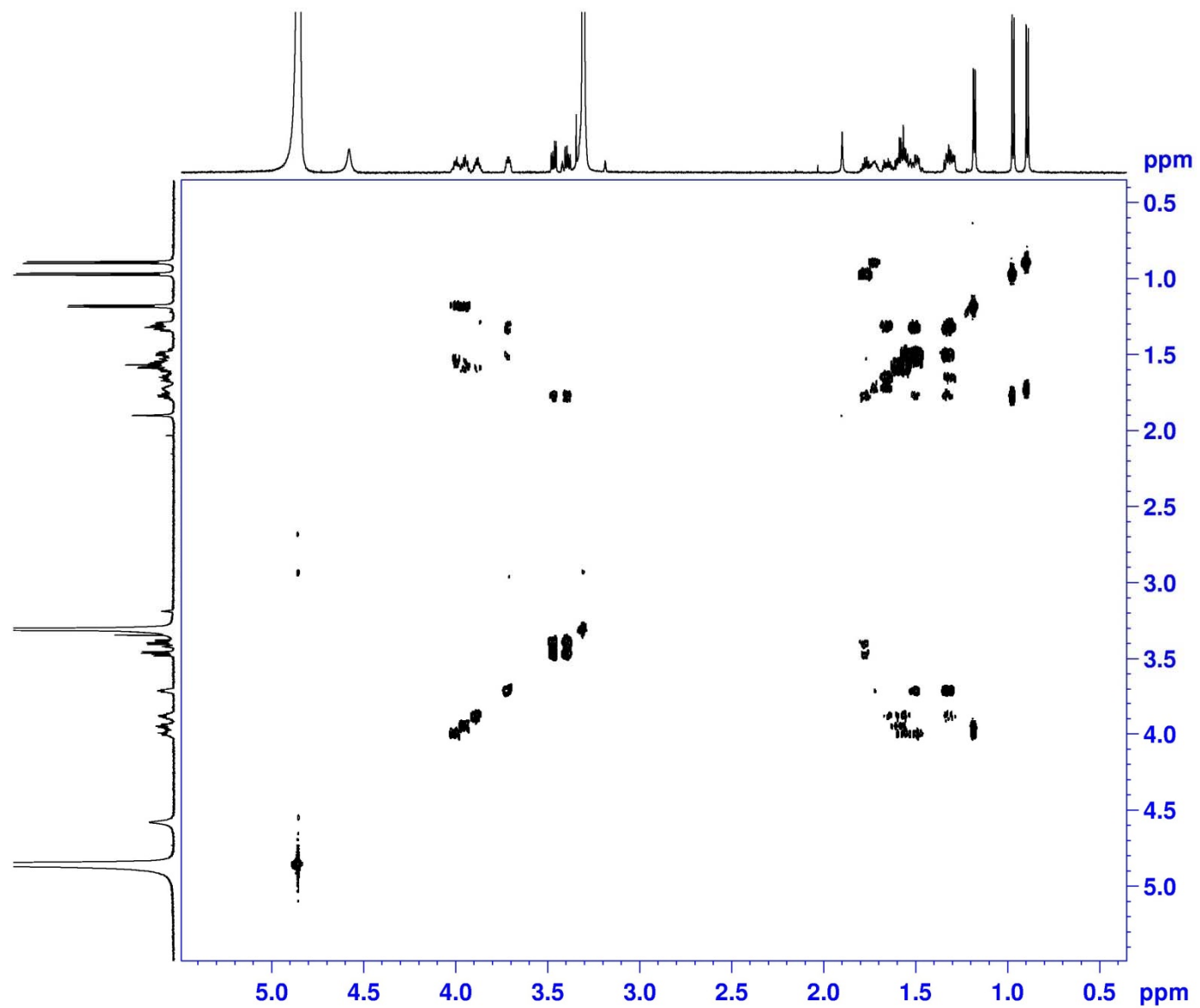
^1H (600 MHz) NMR spectrum of the fragment **1A** in CD_3OD



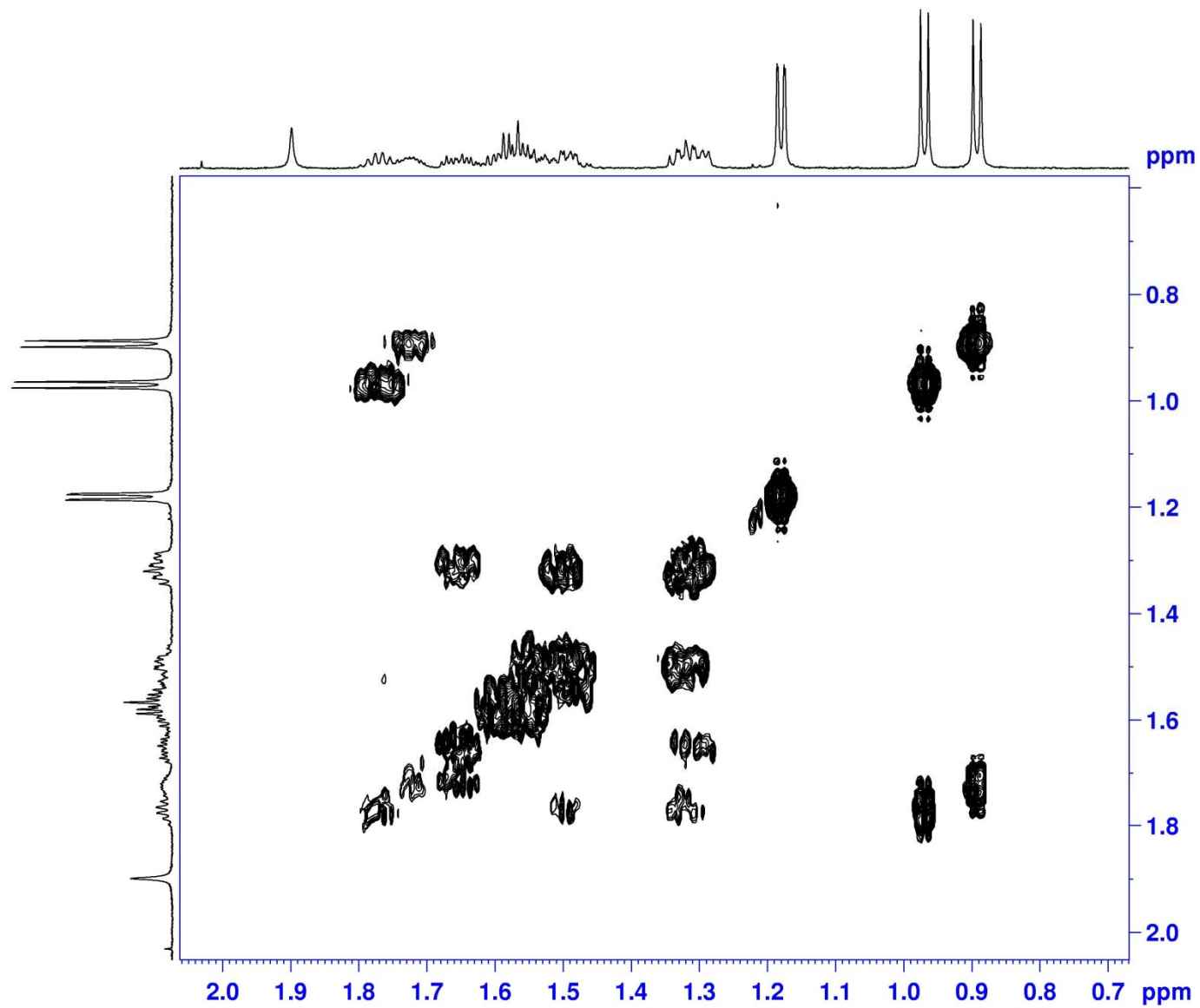
^1H (600 MHz) NMR spectrum of the fragment **1A** in CD_3OD



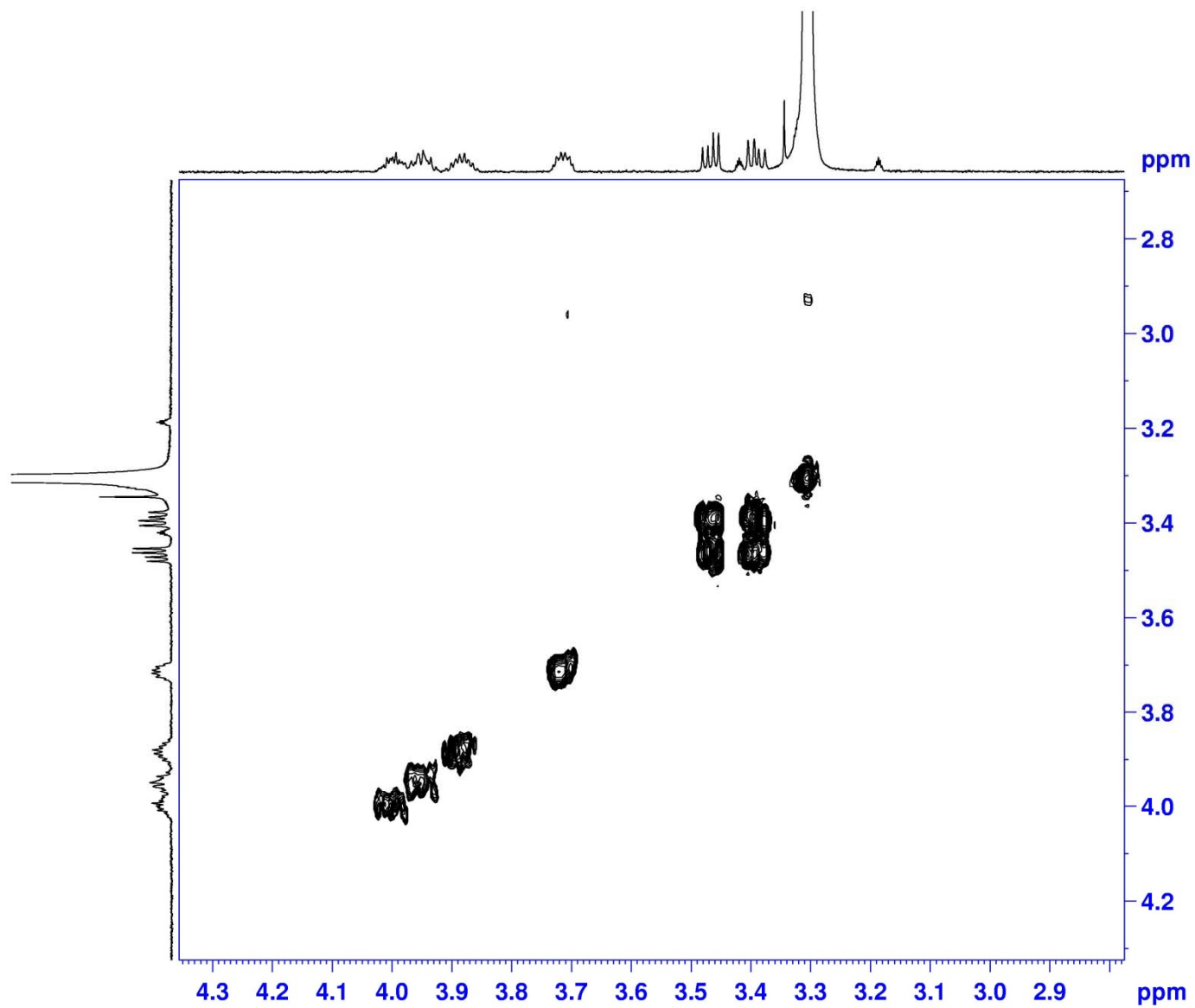
^1H - ^1H COSY (600 MHz) spectrum of the fragment **1A** in CD_3OD



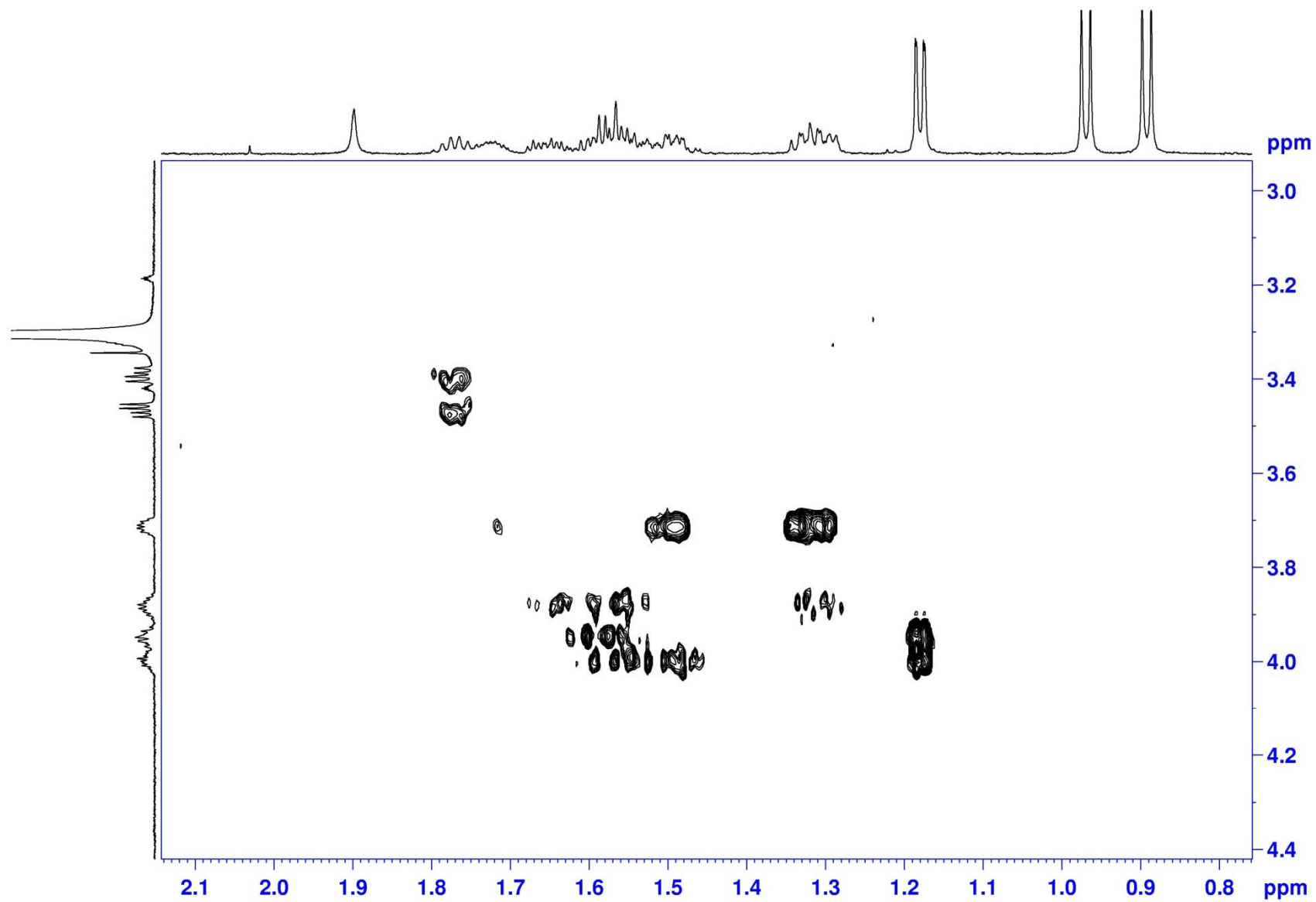
^1H - ^1H COSY (600 MHz) spectrum of the fragment **1A** in CD_3OD



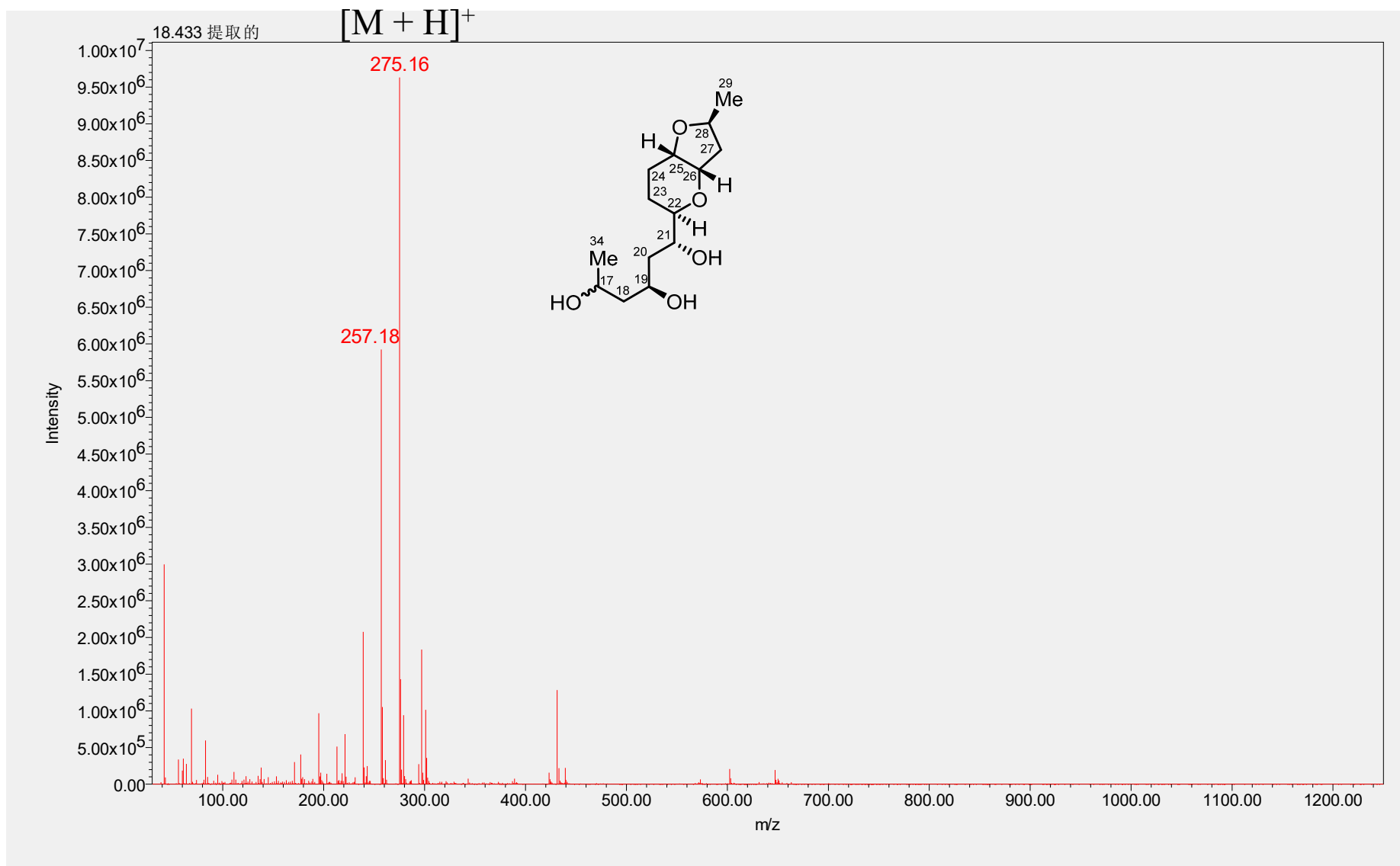
^1H - ^1H COSY (600 MHz) spectrum of the fragment **1A** in CD_3OD



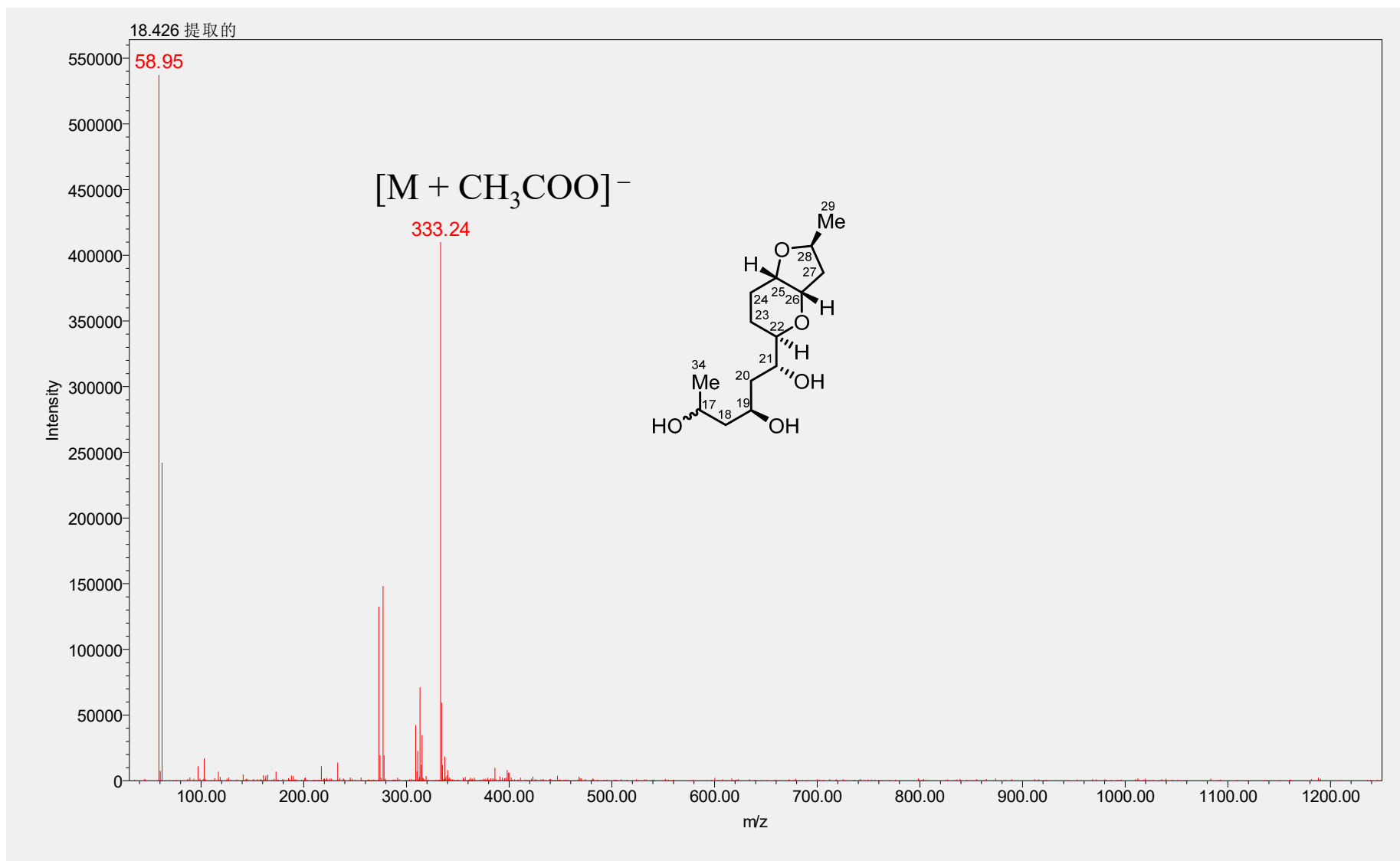
^1H - ^1H COSY (600 MHz) spectrum of the fragment **1A** in CD_3OD



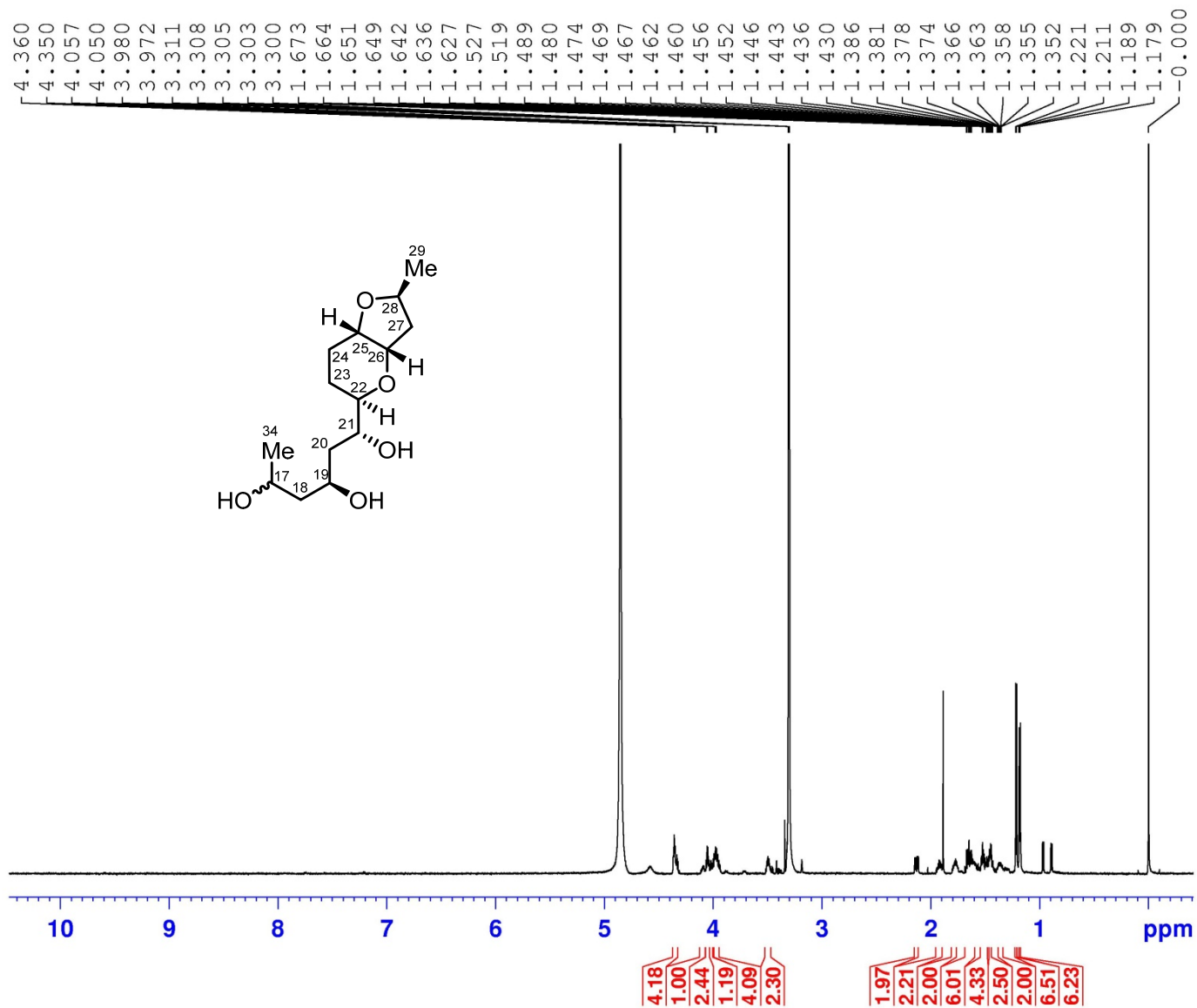
LR-ESIMS for the fragment 1B



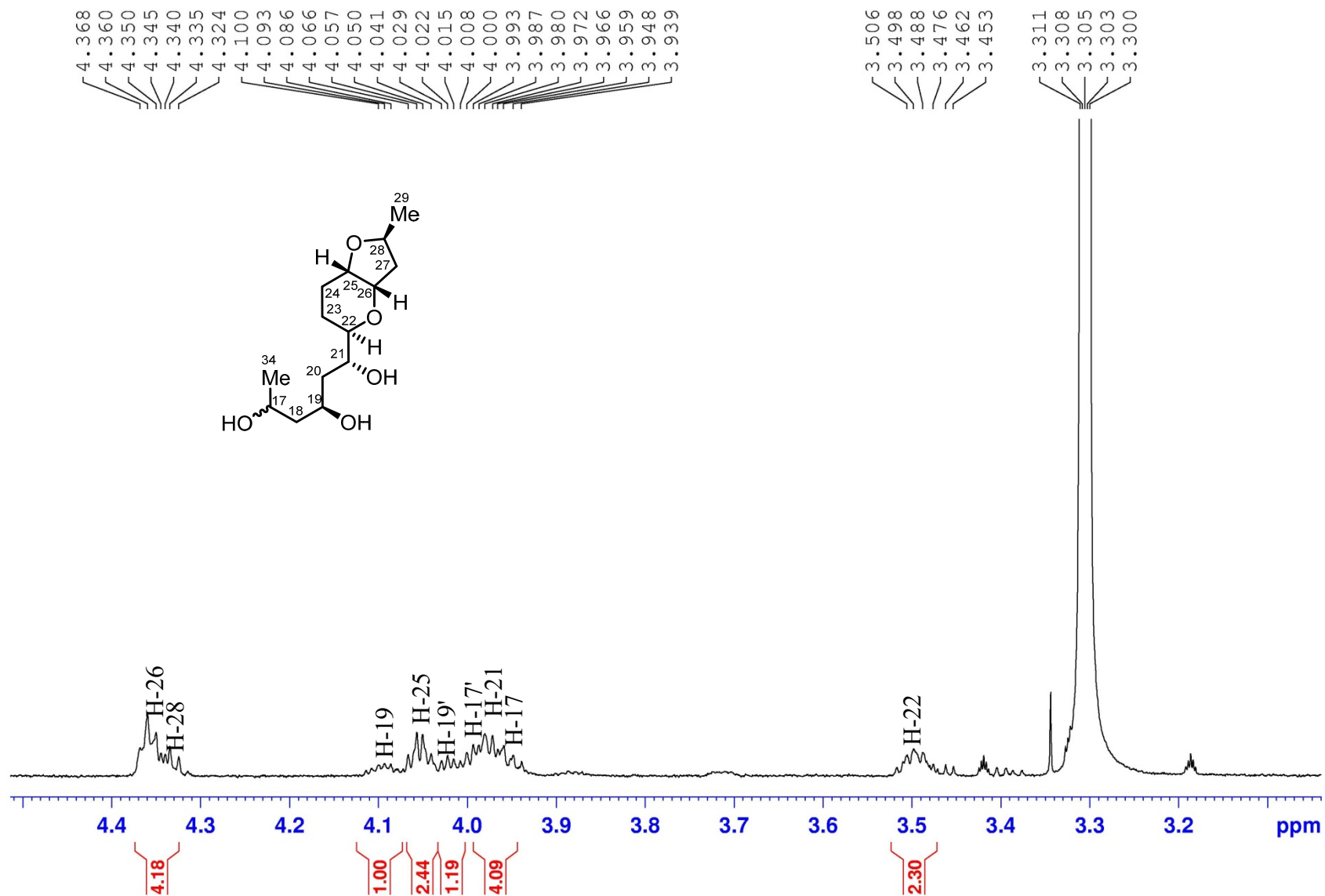
LR-ESIMS for the fragment **1B**



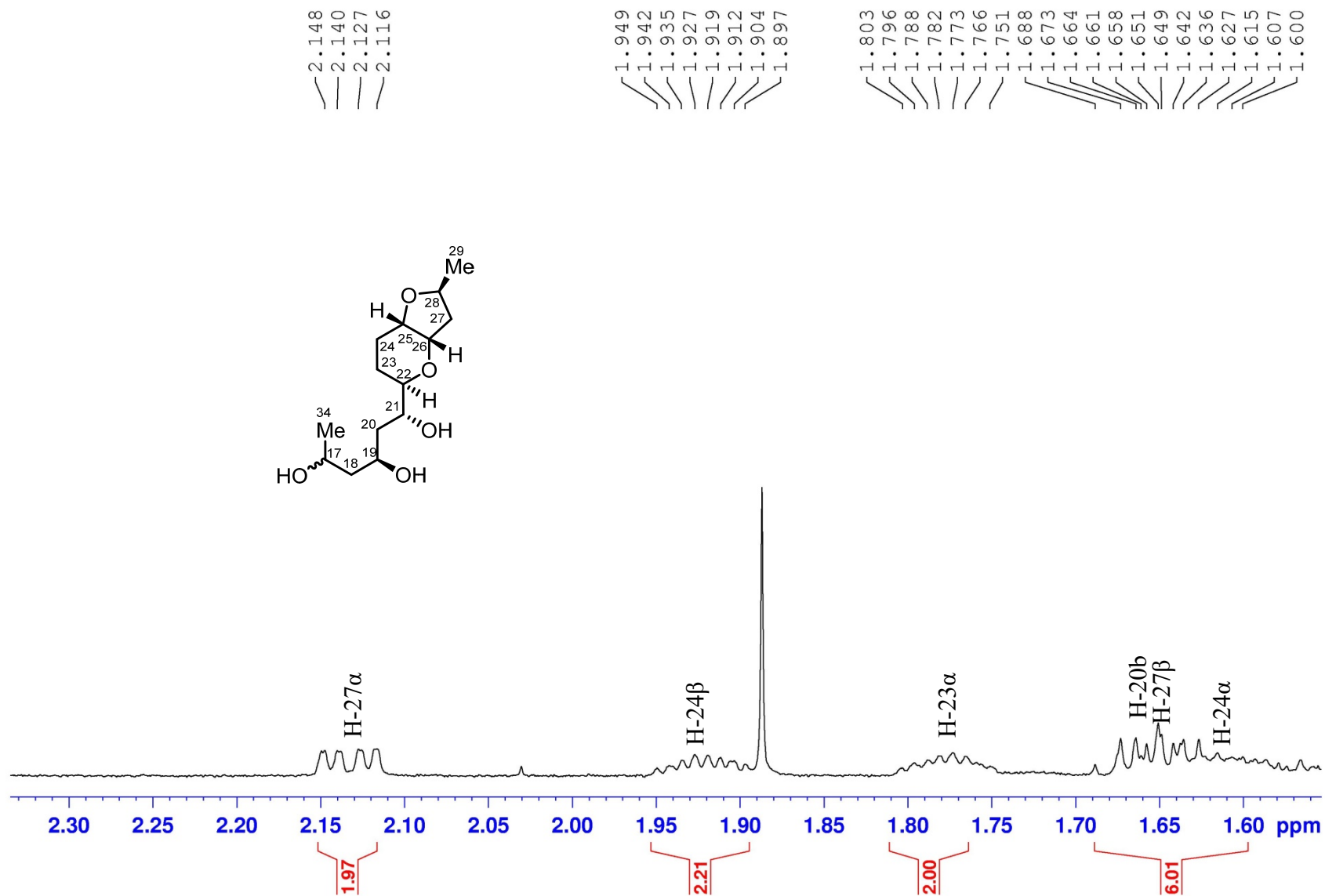
^1H (600 MHz) NMR spectrum of the fragment **1B** in CD_3OD



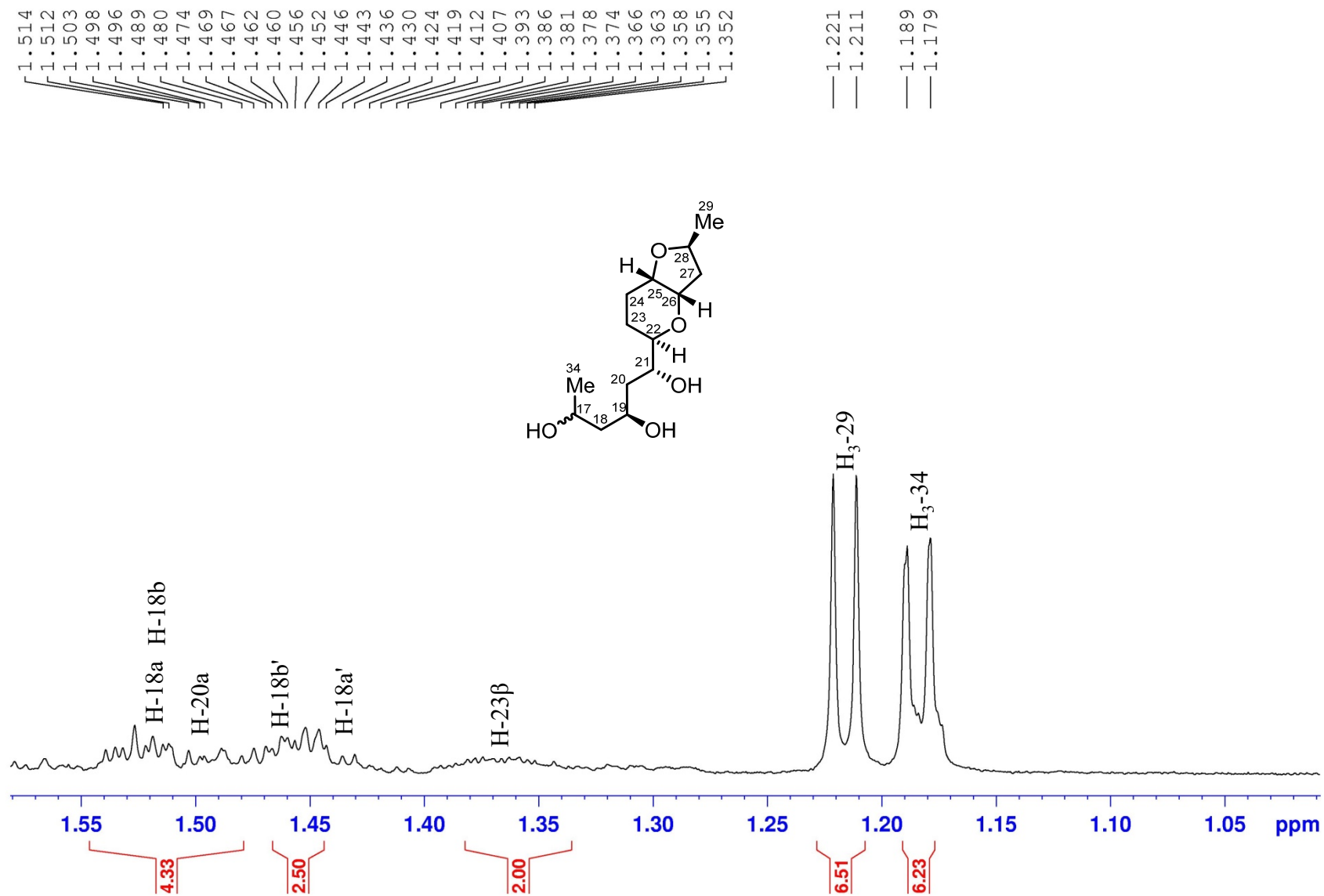
^1H (600 MHz) NMR spectrum of the fragment **1B** in CD_3OD



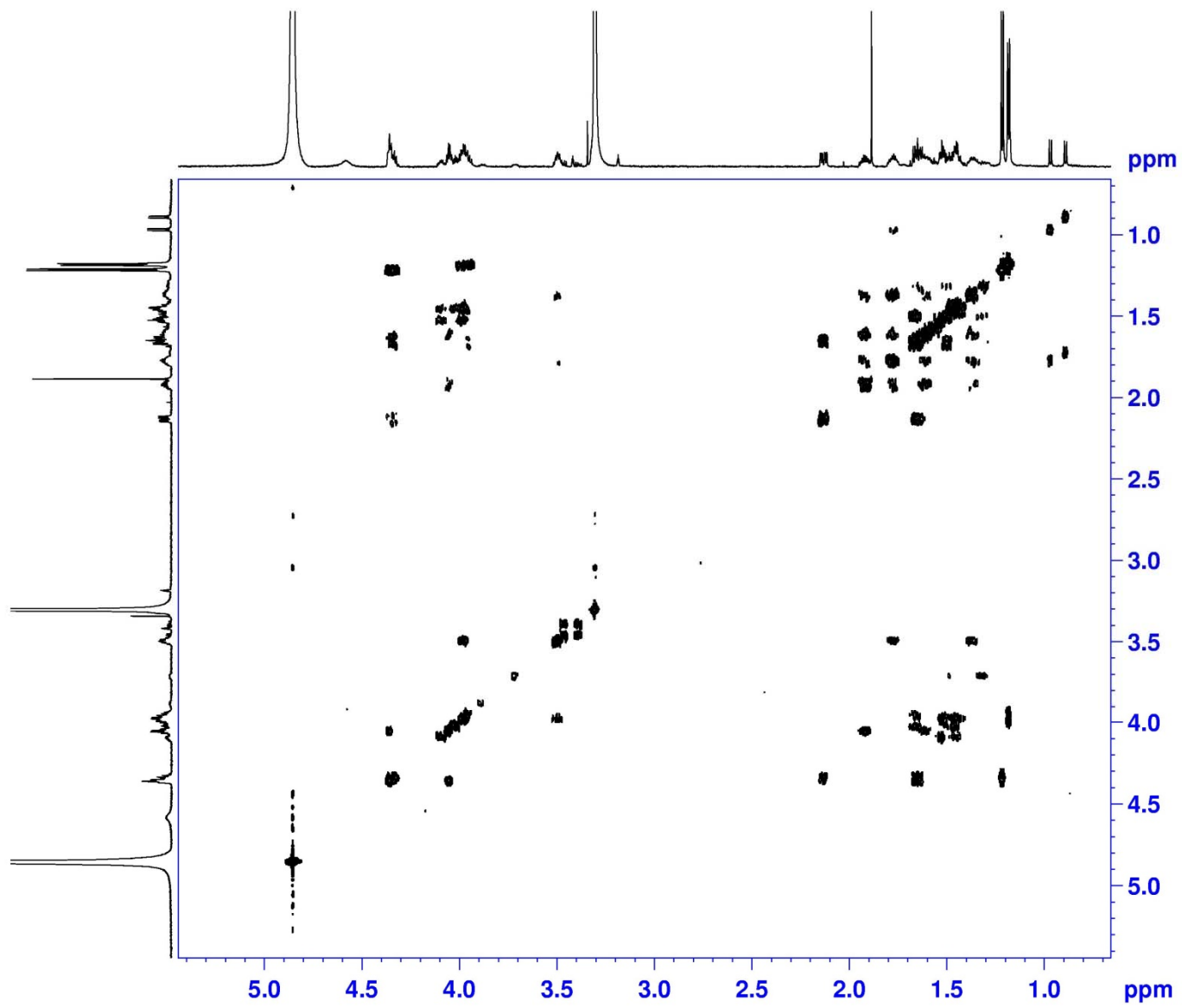
^1H (600 MHz) NMR spectrum of the fragment **1B** in CD_3OD



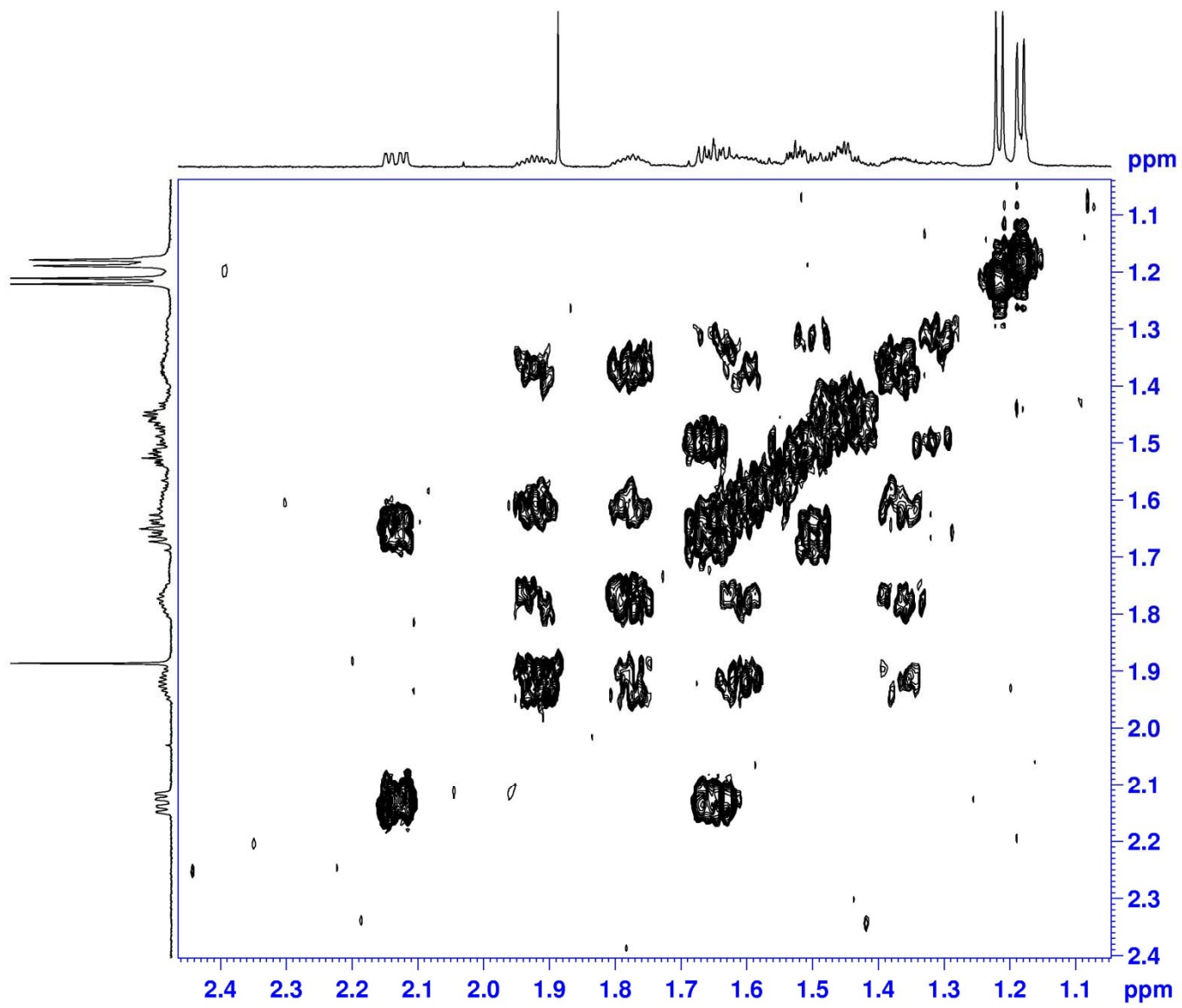
^1H (600 MHz) NMR spectrum of the fragment **1B** in CD_3OD



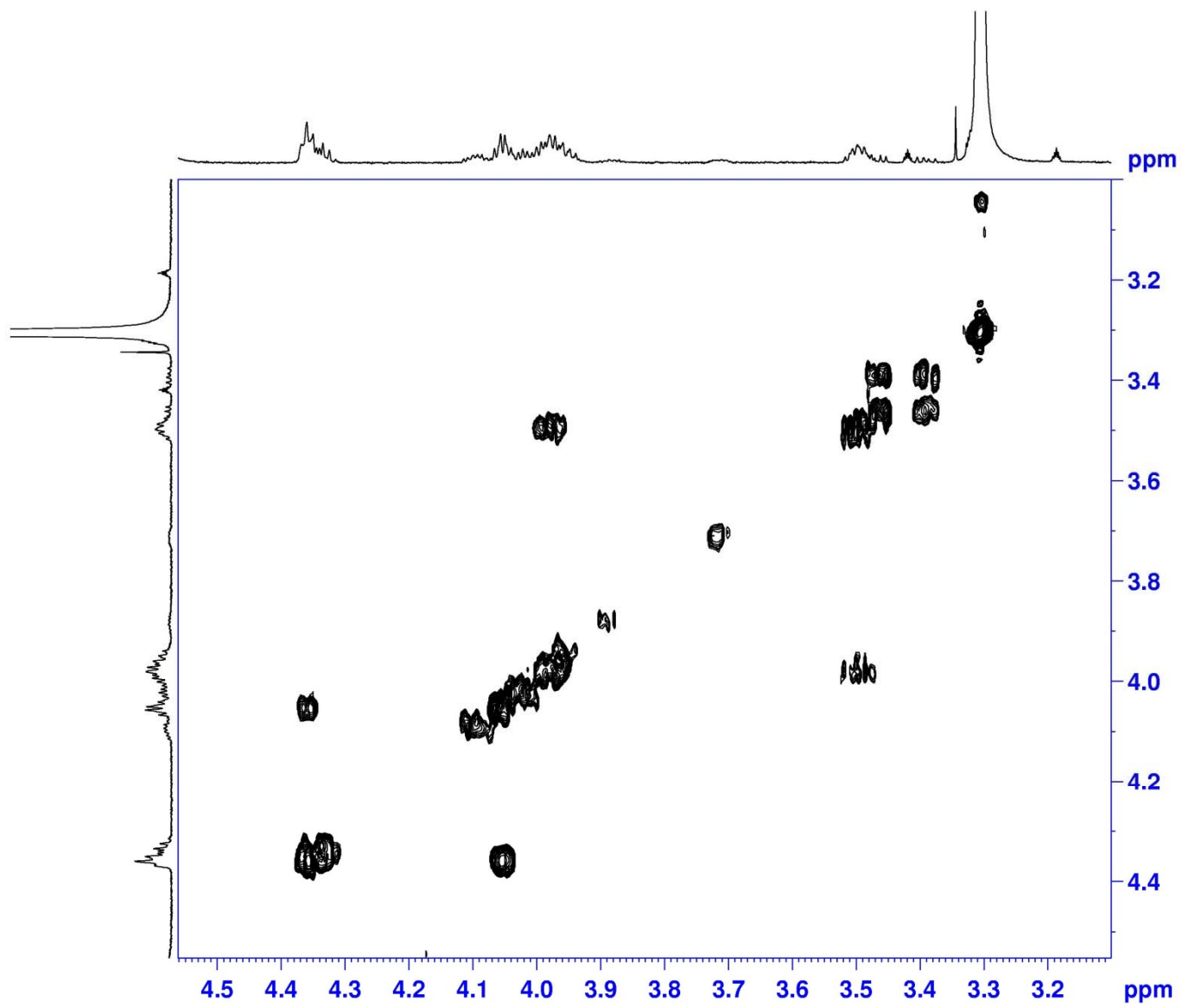
^1H - ^1H COSY (600 MHz) spectrum of the fragment **1B** in CD_3OD



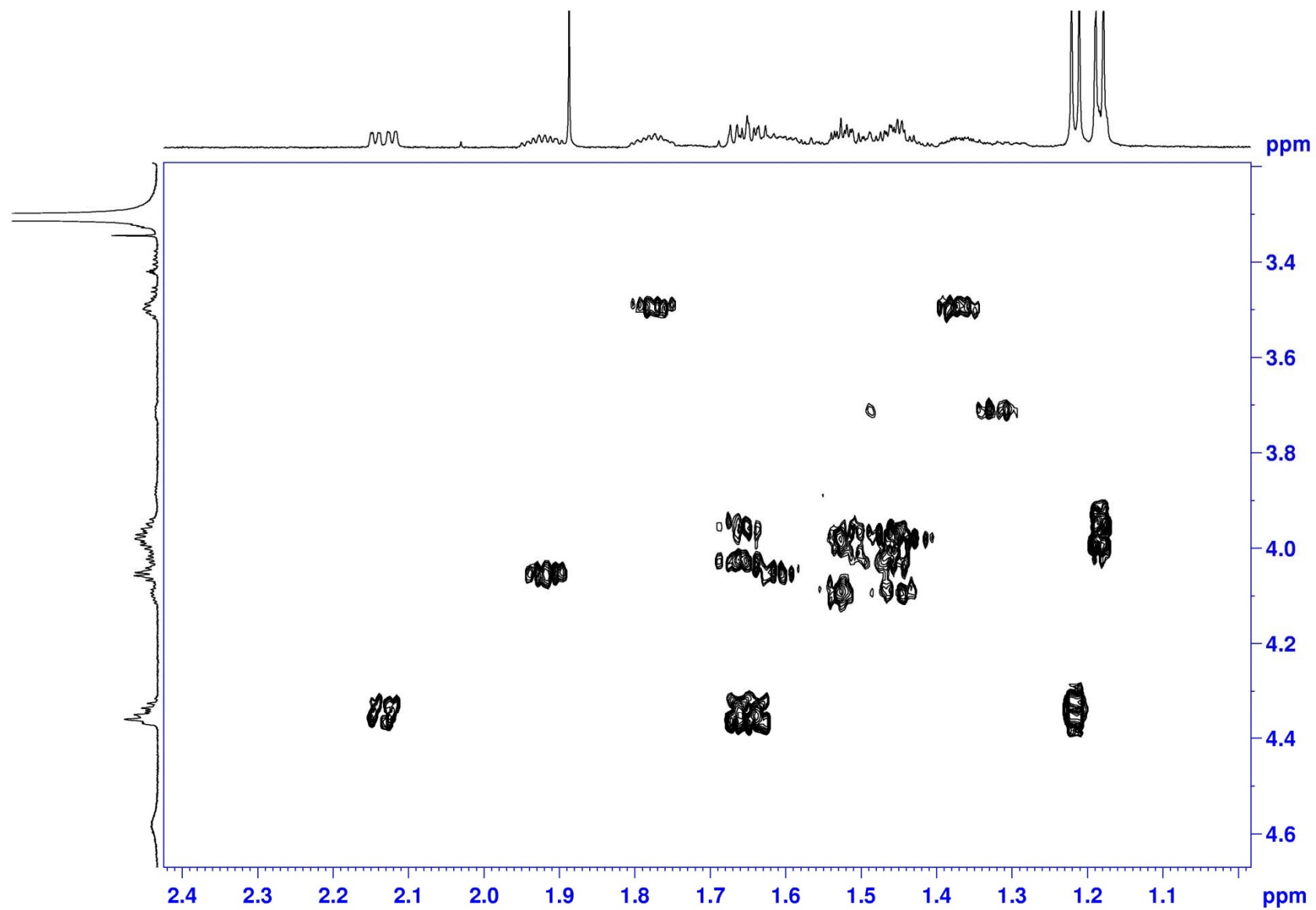
^1H - ^1H COSY (600 MHz) spectrum of the fragment **1B** in CD_3OD



^1H - ^1H COSY (600 MHz) spectrum of the fragment **1B** in CD_3OD



^1H - ^1H COSY (600 MHz) spectrum of the fragment **1B** in CD_3OD



HR-ESIMS for compound 1s

Mass Spectrum SmartFormula Report

Analysis Info

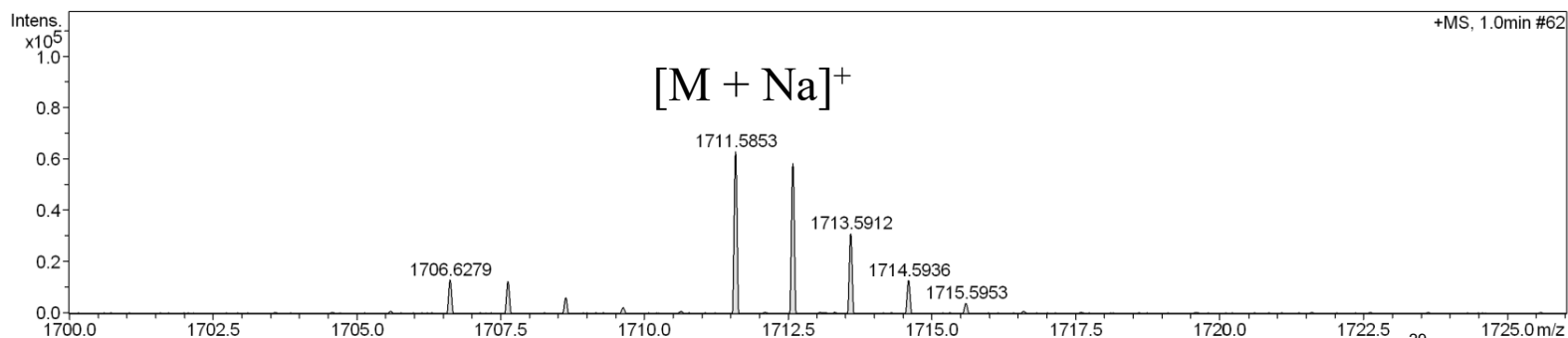
Analysis Name D:\Data\MS\data\202011\jiangzhongping_37-1-R_pos_3_01_9232.d
 Method LC_Direct Infusion_pos_100-3000mz.m
 Sample Name jiangzhongping_37-1-R_pos
 Comment

Acquisition Date 11/16/2020 4:13:55 PM

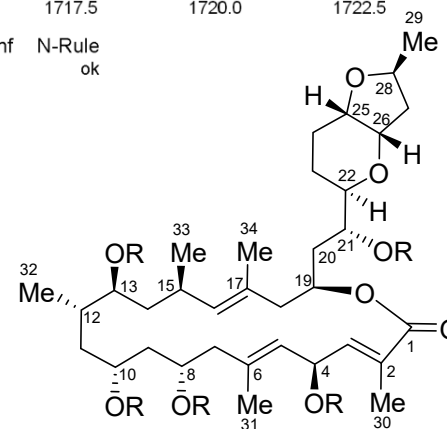
Operator SCSIO
 Instrument maXis 255552.00029

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	0 V	Set Dry Gas	4.0 l/min
Scan End	3500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
1711.5853	1	C84H91F15NaO19	100.00	1711.5807	-2.7	-4.6	22.5	31.5	even	ok



R = (S)-MTPA

S70

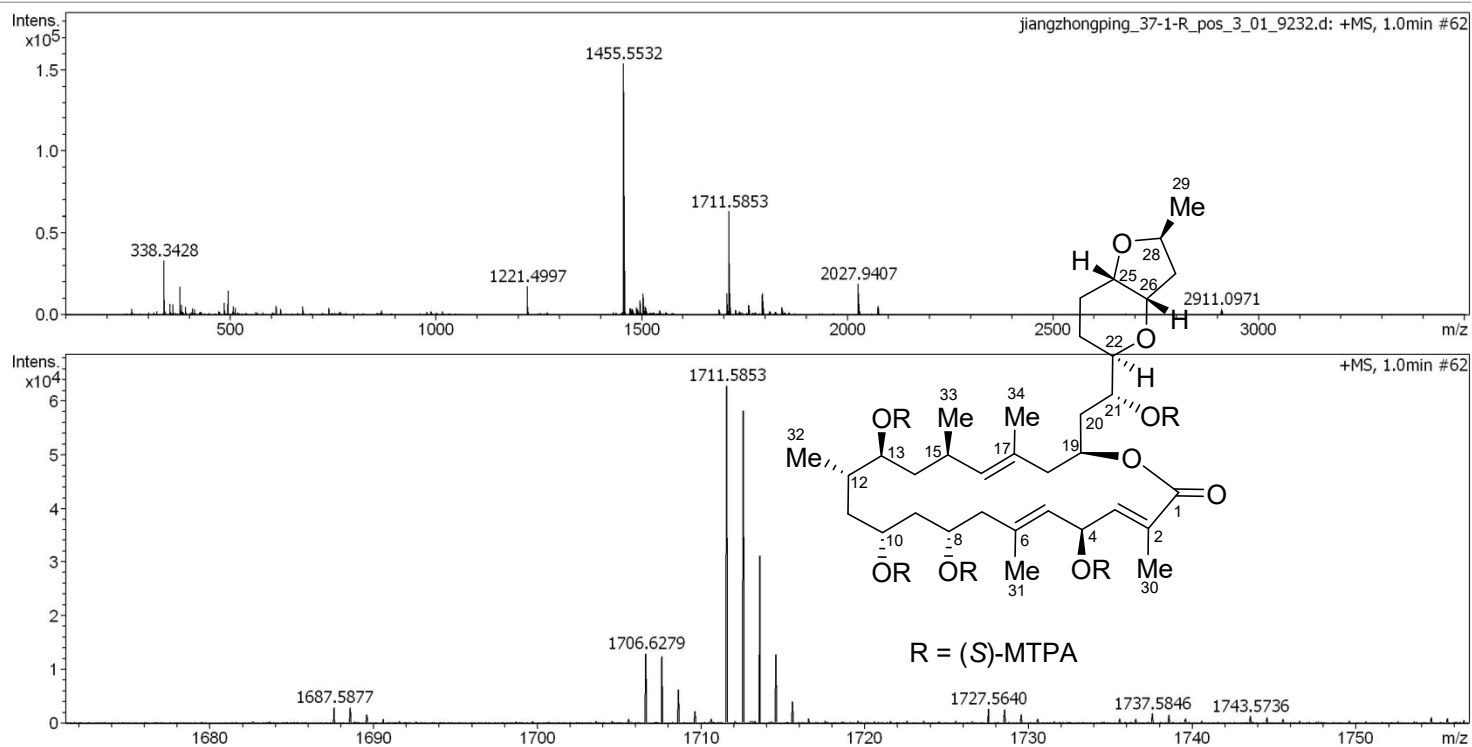
HR-ESIMS for compound 1s

Generic Display Report

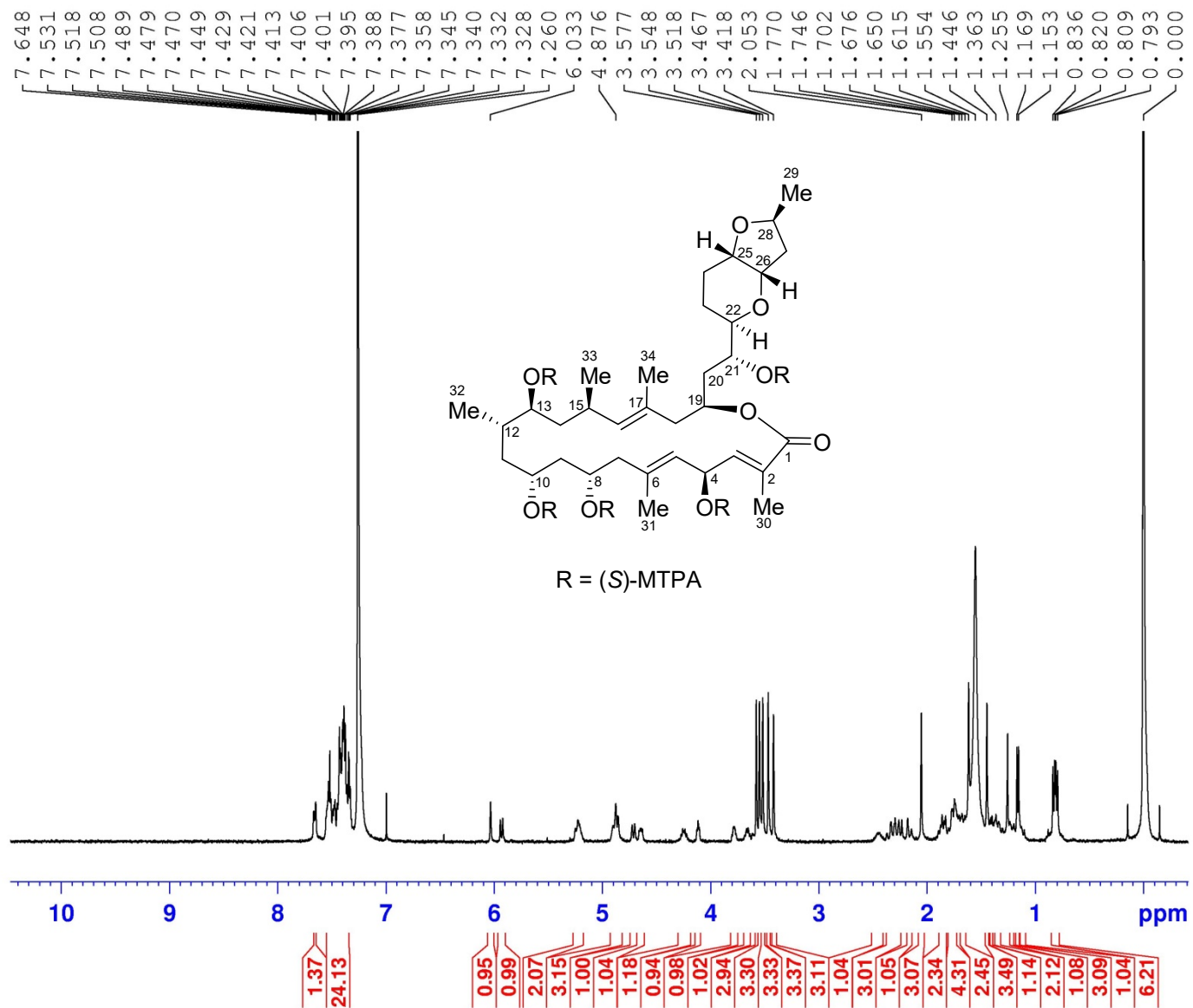
Analysis Info

Analysis Name D:\Data\MS\data\202011\jiangzhongping_37-1-R_pos_3_01_9232.d
Method LC_Direct Infusion_pos_100-3000mz.m
Sample Name jiangzhongping_37-1-R_pos
Comment

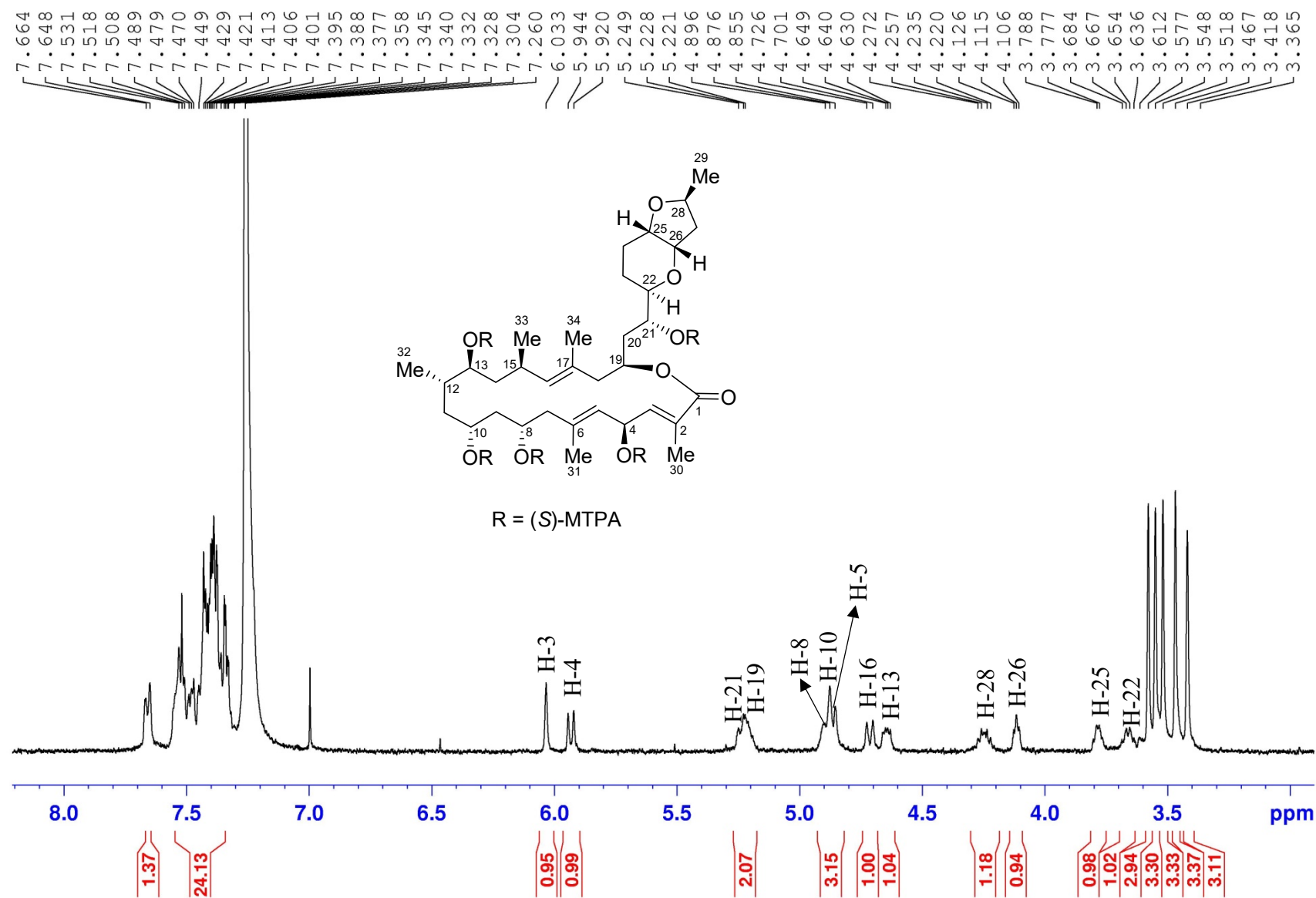
Acquisition Date 11/16/2020 4:13:55 PM
Operator SCSIO
Instrument maXis



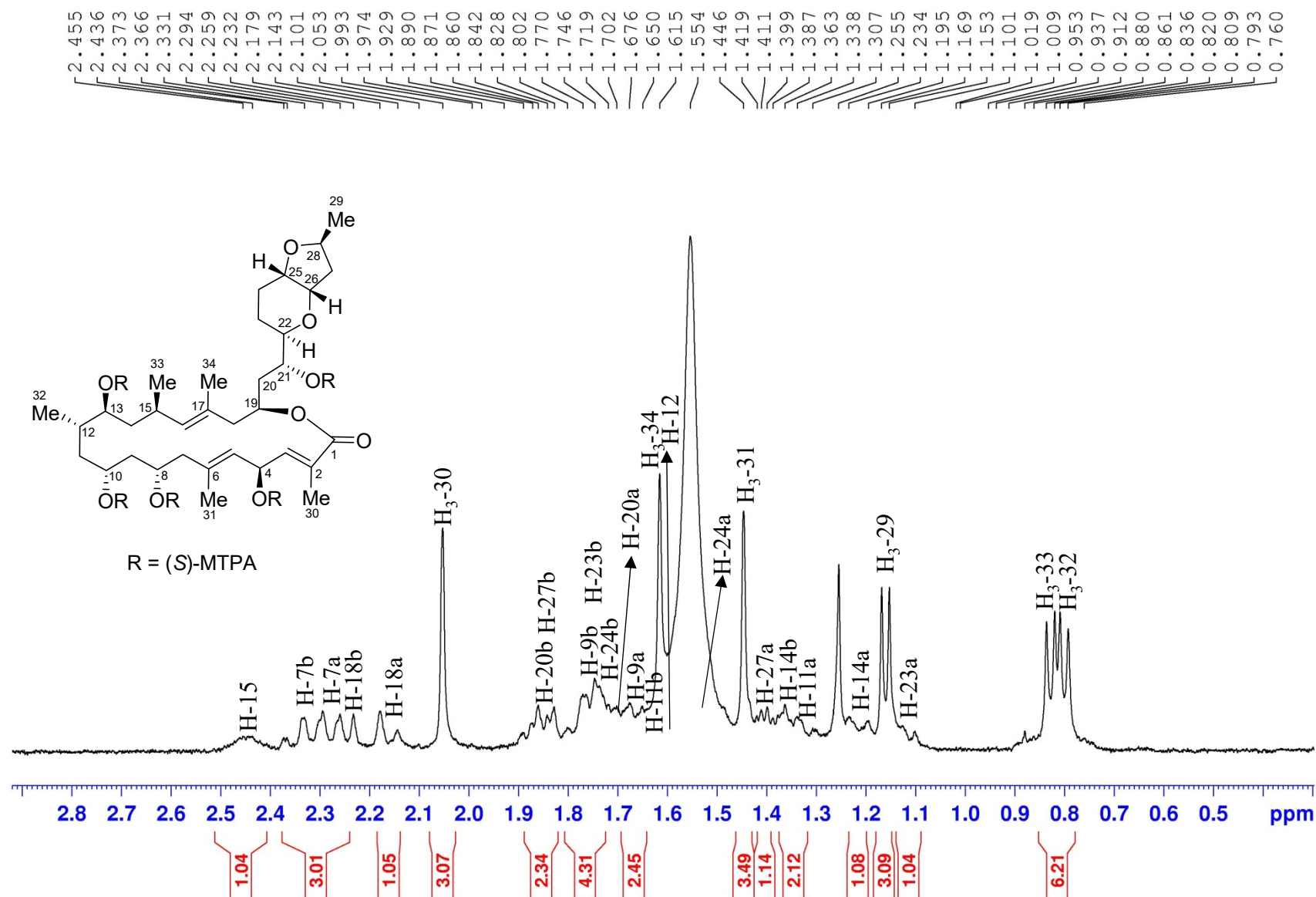
^1H (400 MHz) NMR spectrum of compound **1s** in CDCl_3



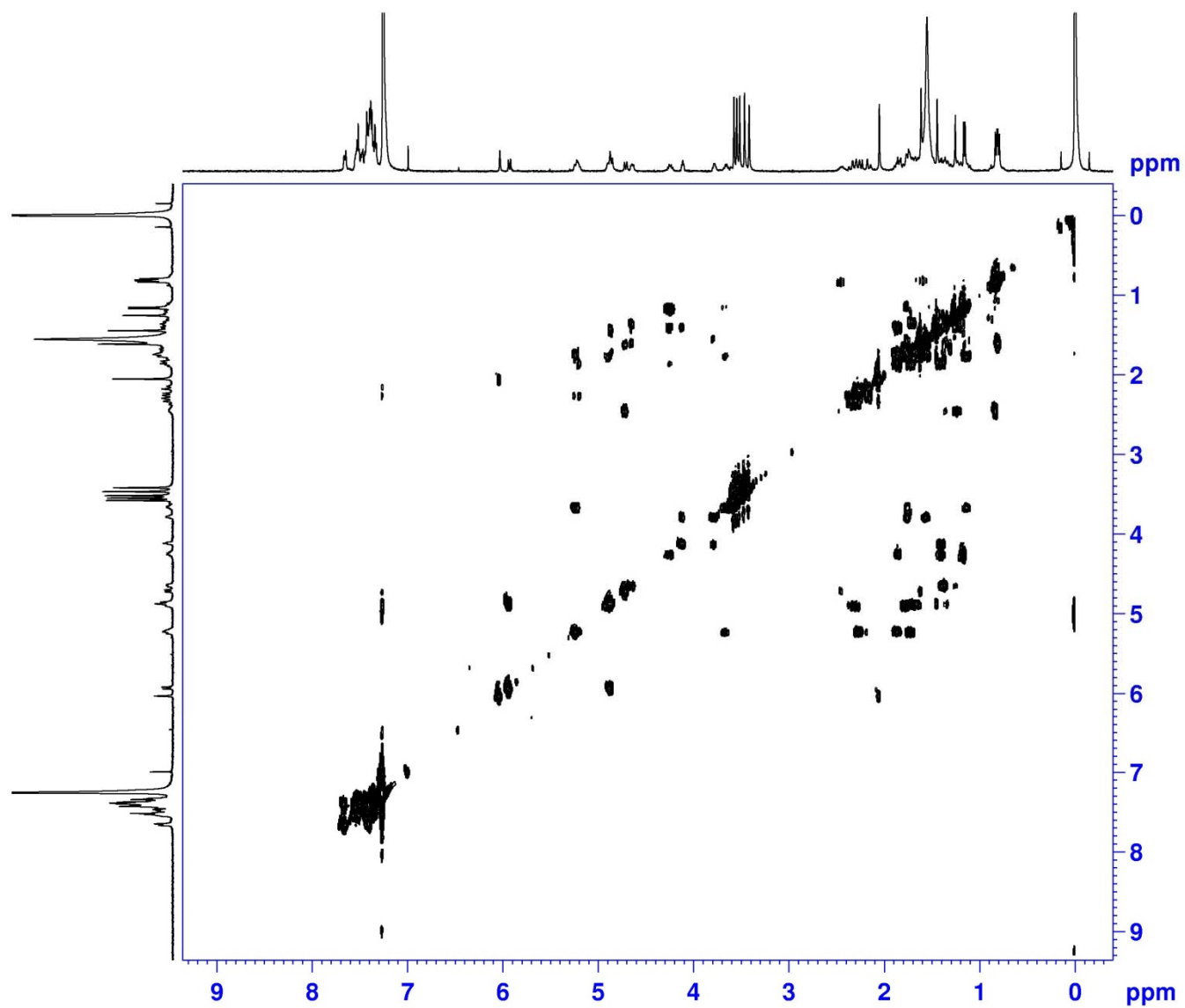
^1H (400 MHz) NMR spectrum of compound **1s** in CDCl_3



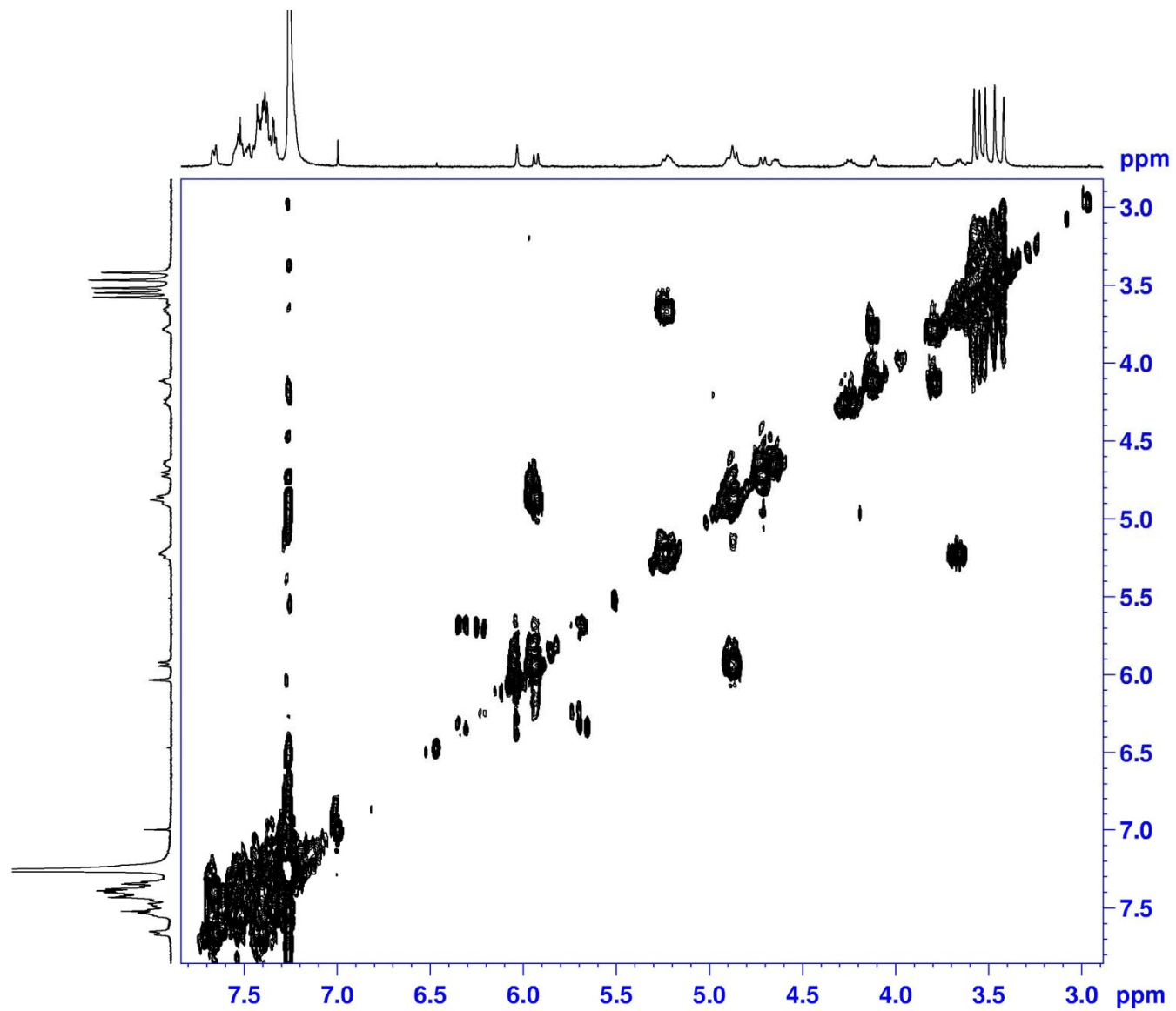
^1H (400 MHz) NMR spectrum of compound **1s** in CDCl_3



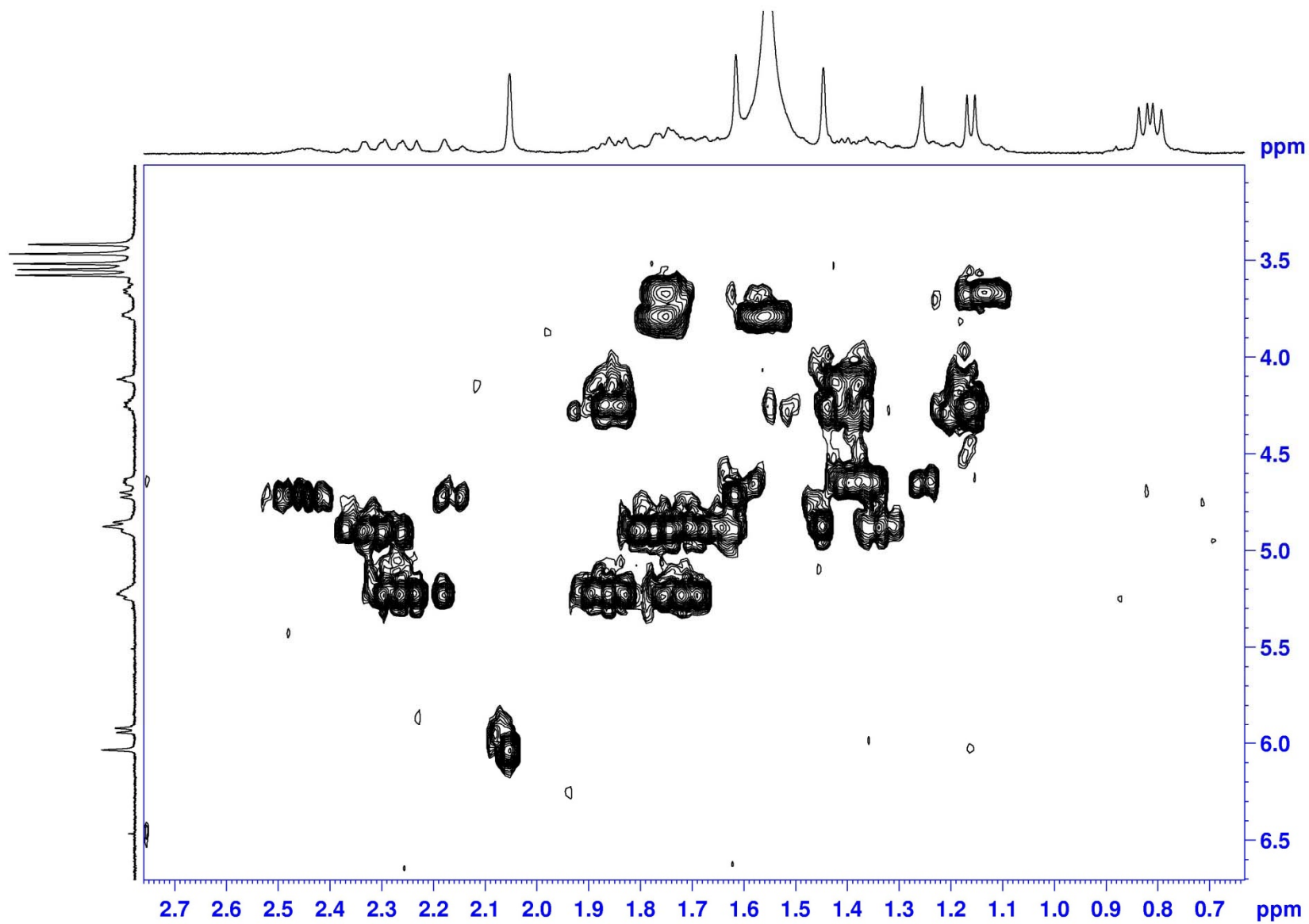
^1H - ^1H COSY (400 MHz) spectrum of compound **1s** in CDCl_3



^1H - ^1H COSY (400 MHz) spectrum of compound **1s** in CDCl_3



^1H - ^1H COSY (400 MHz) spectrum of compound **1s** in CDCl_3



HR-ESIMS for compound **1r**

Mass Spectrum SmartFormula Report

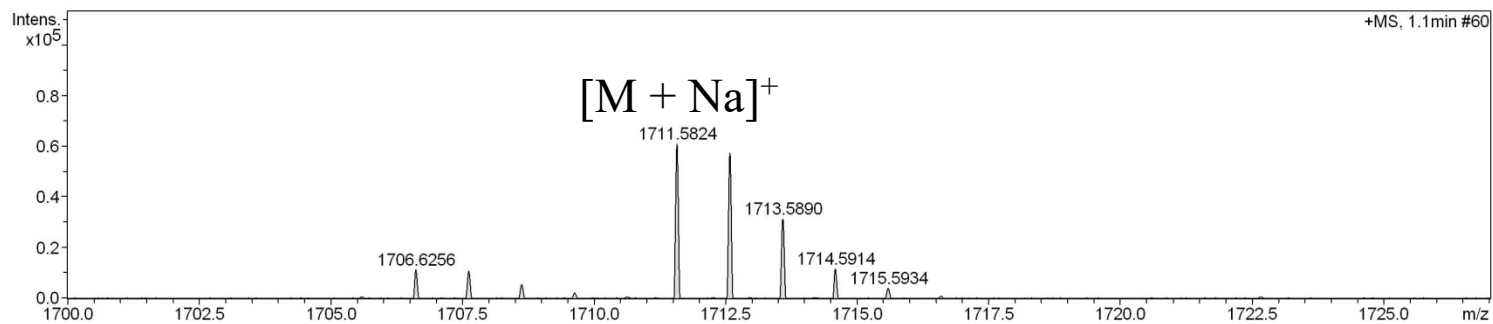
Analysis Info

Analysis Name D:\Data\MS\data\202011\jiangzhongping_37-1-S_pos_4_01_9233.d
 Method LC_Direct Infusion_pos_100-3000mz.m
 Sample Name jiangzhongping_37-1-S_pos
 Comment

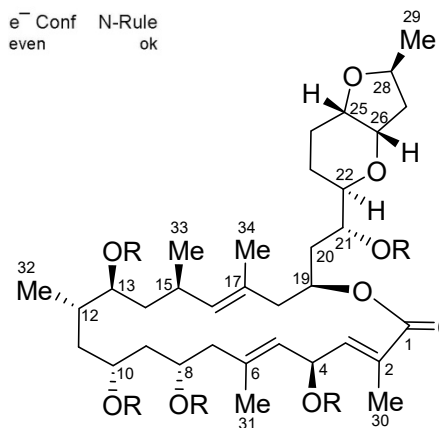
Acquisition Date 11/16/2020 4:17:22 PM
 Operator SCSIO
 Instrument maXis 255552.00029

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	0 V	Set Dry Gas	4.0 l/min
Scan End	3500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
1711.5824	1	C84H91F15NaO19	100.00	1711.5807	-1.0	-1.7	26.8	31.5	even	ok



R = (R)-MTPA

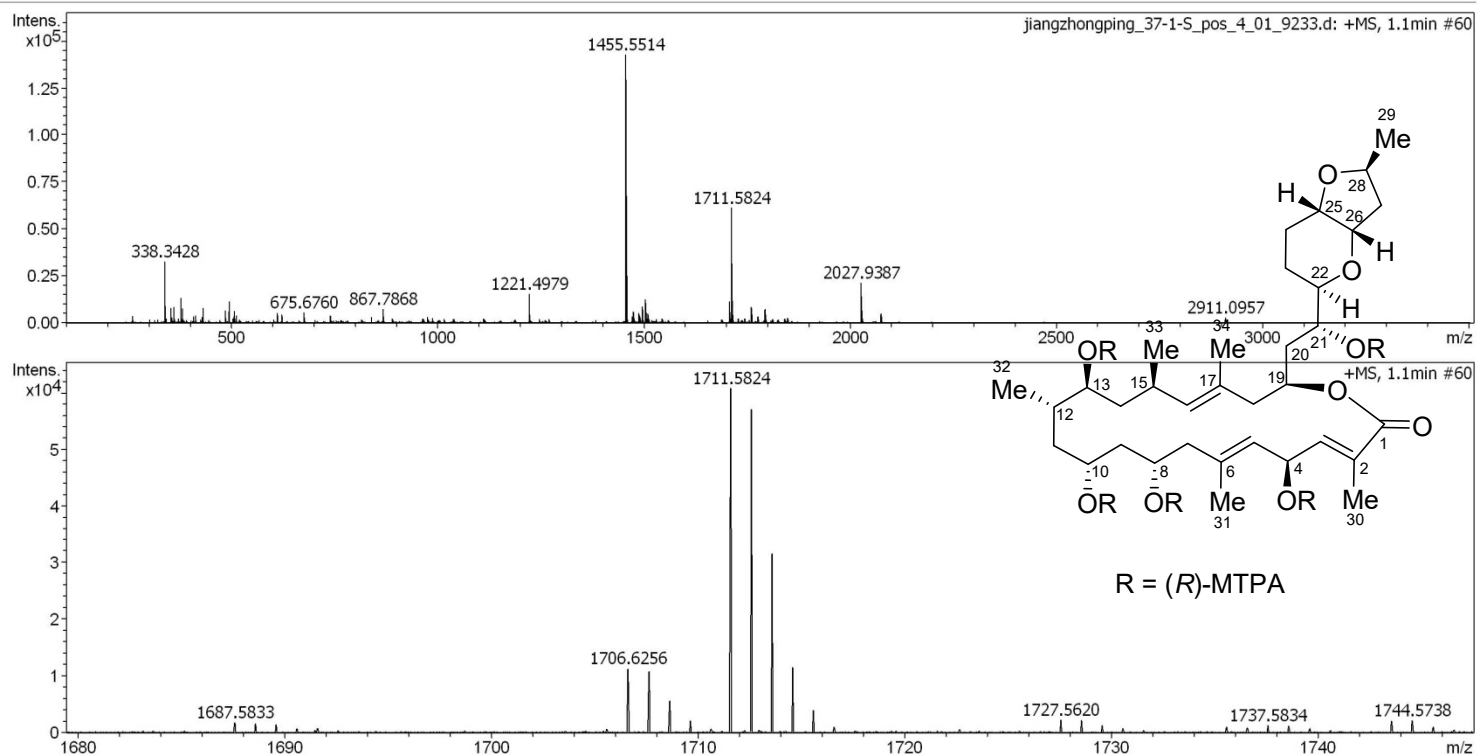
HR-ESIMS for compound 1r

Generic Display Report

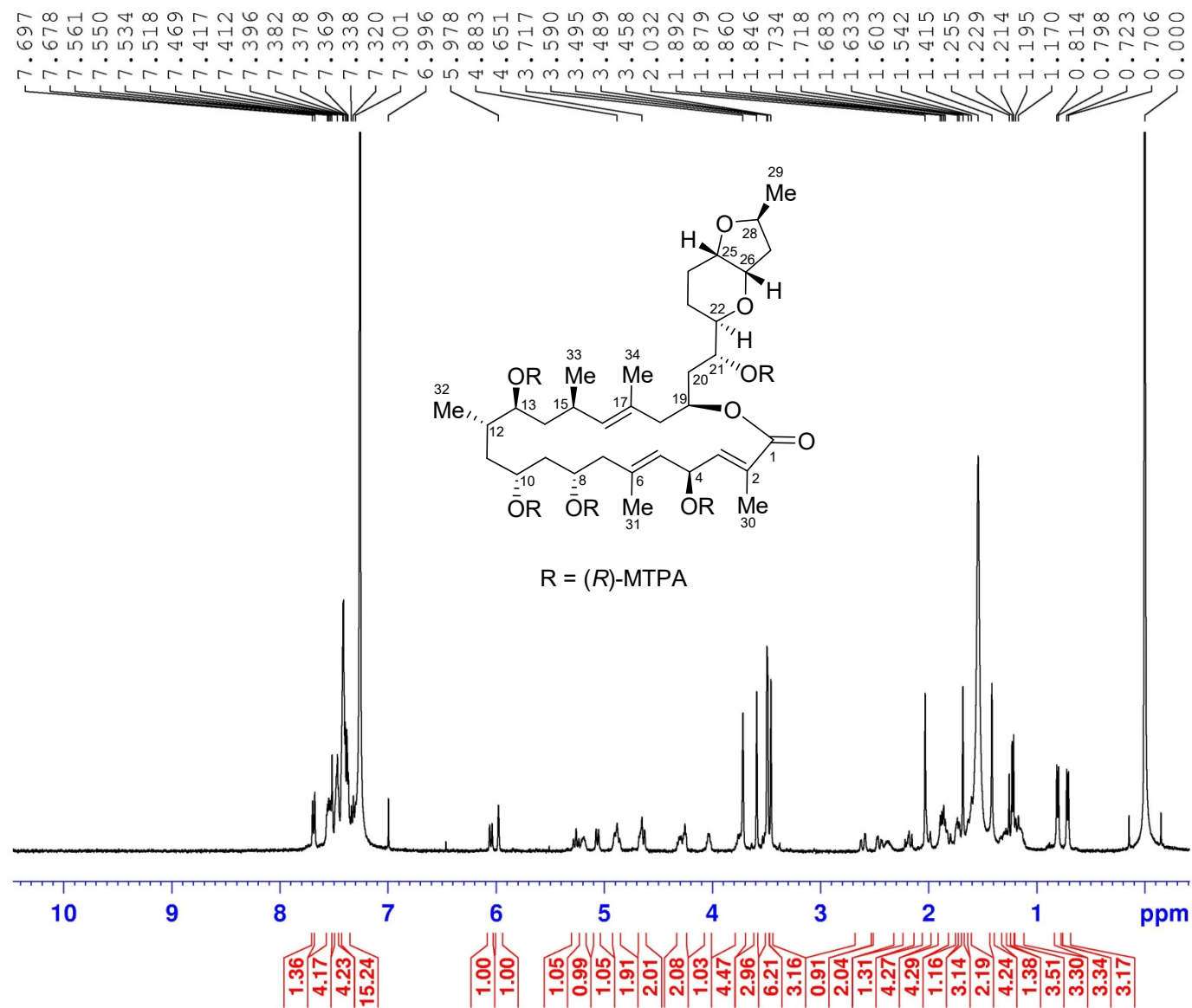
Analysis Info

Analysis Name D:\Data\MS\data\202011\jiangzhongping_37-1-S_pos_4_01_9233.d
Method LC_Direct Infusion_pos_100-3000mz.m
Sample Name jiangzhongping_37-1-S_pos
Comment

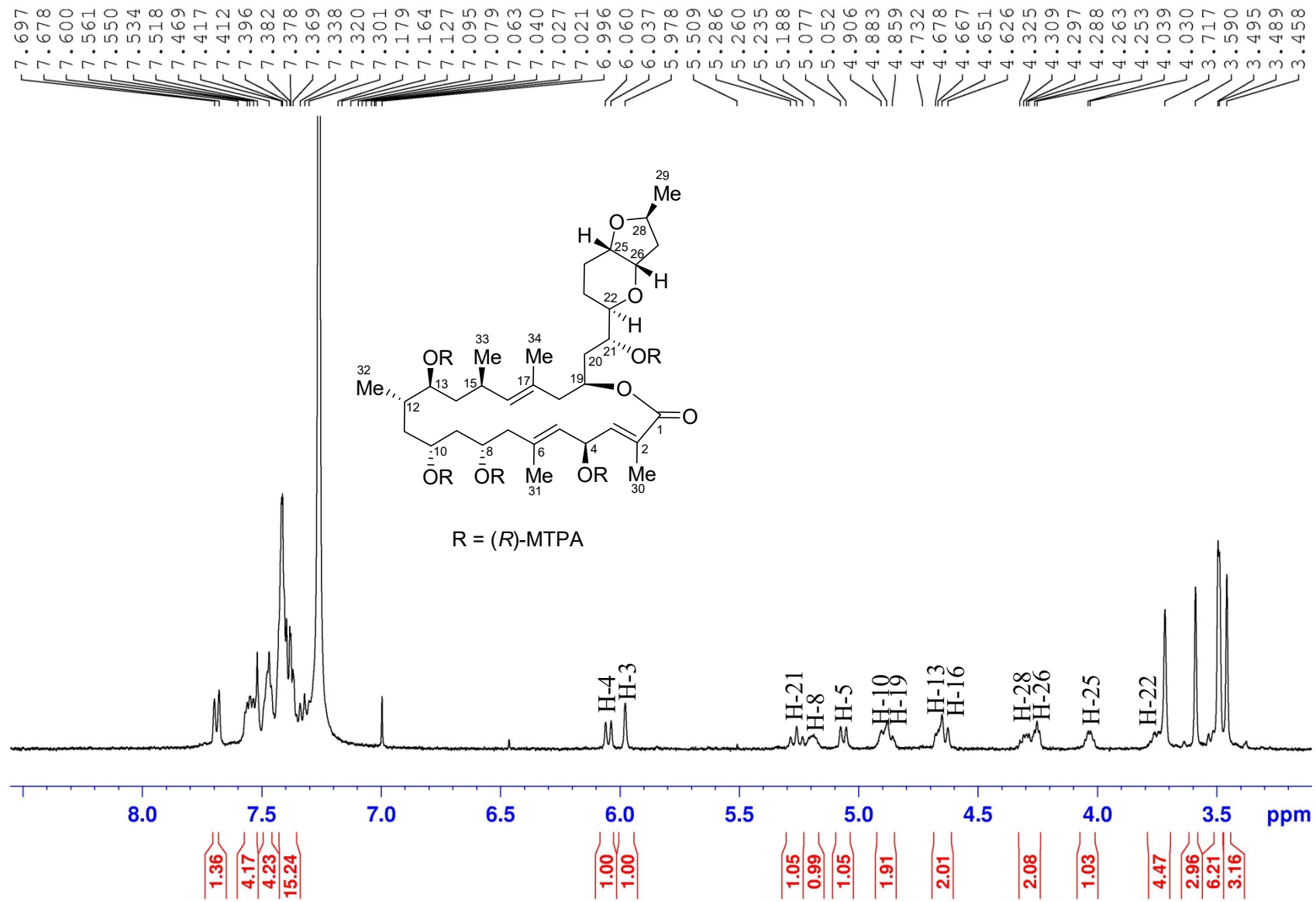
Acquisition Date 11/16/2020 4:17:22 PM
Operator SCSIO
Instrument maXis



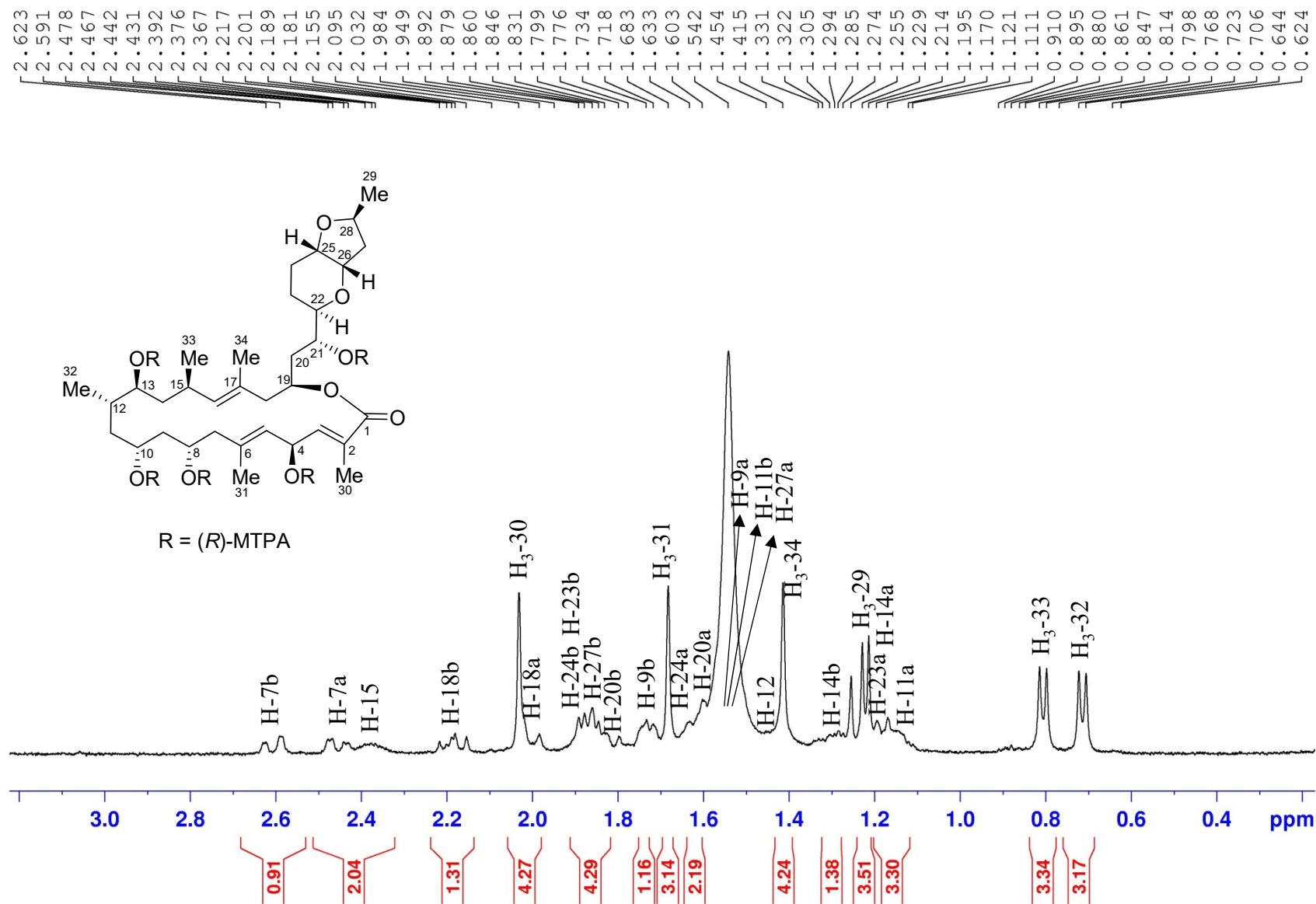
^1H (400 MHz) NMR spectrum of compound **1r** in CDCl_3



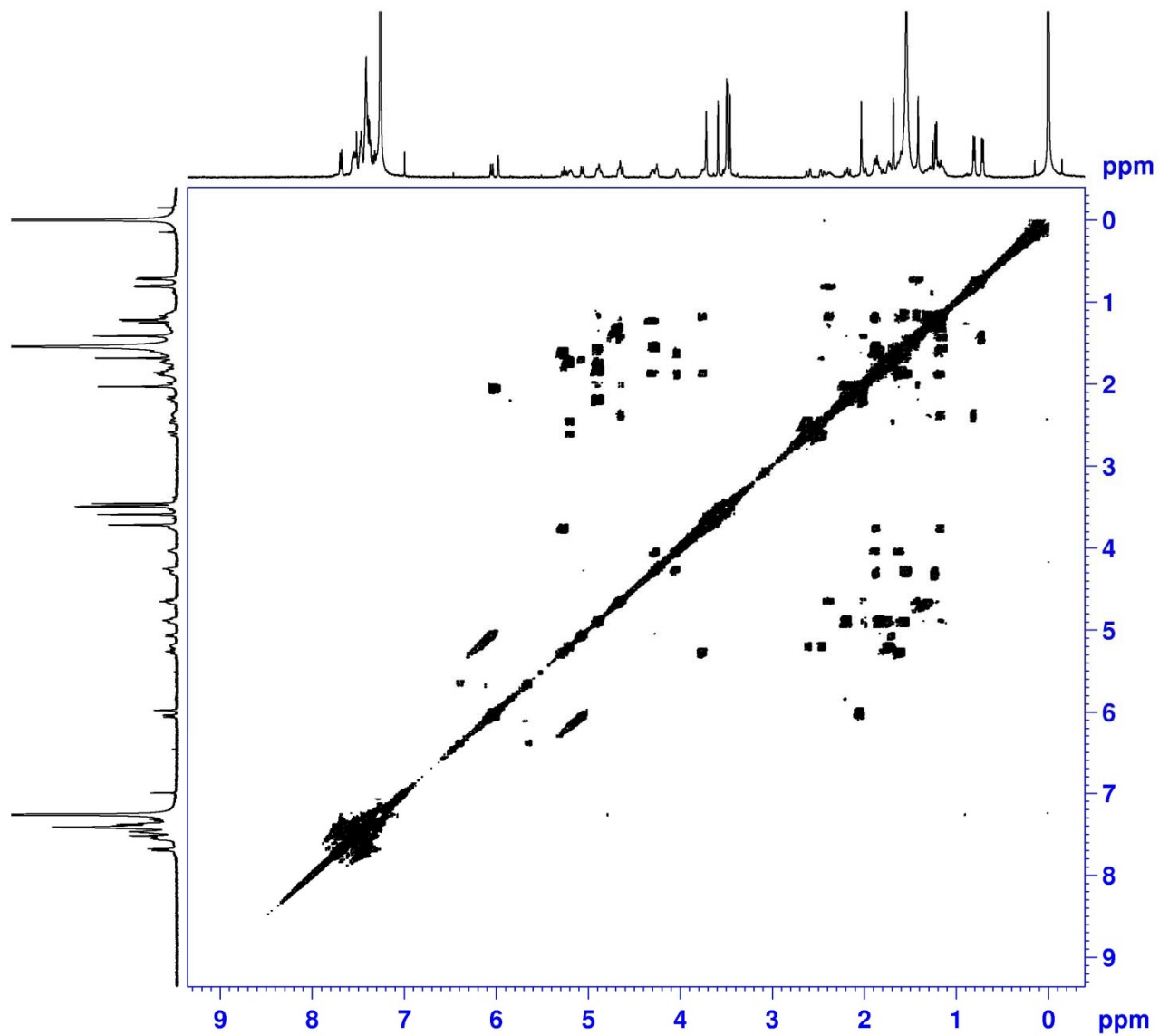
^1H (400 MHz) NMR spectrum of compound **1r** in CDCl_3



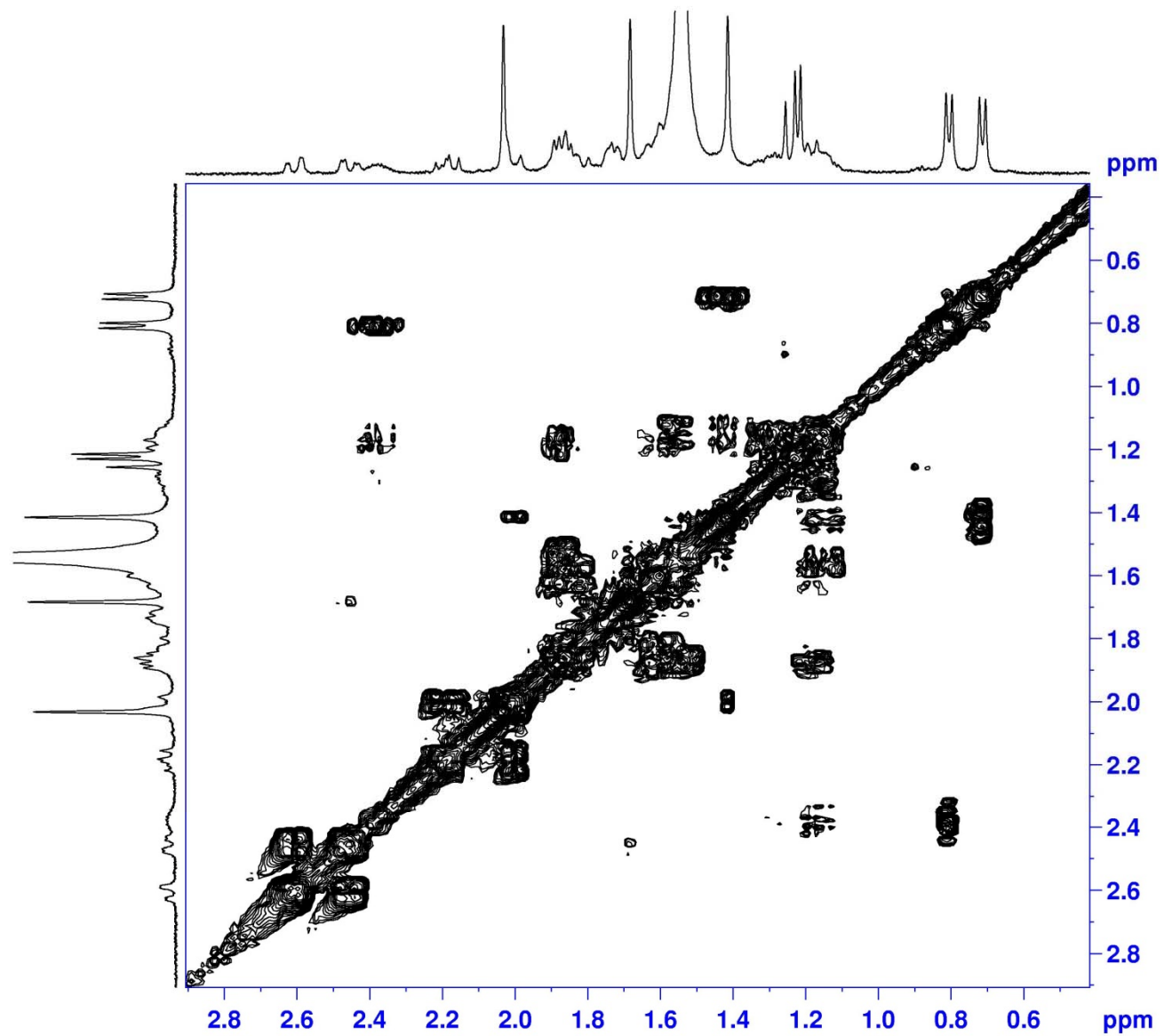
^1H (400 MHz) NMR spectrum of compound **1r** in CDCl_3



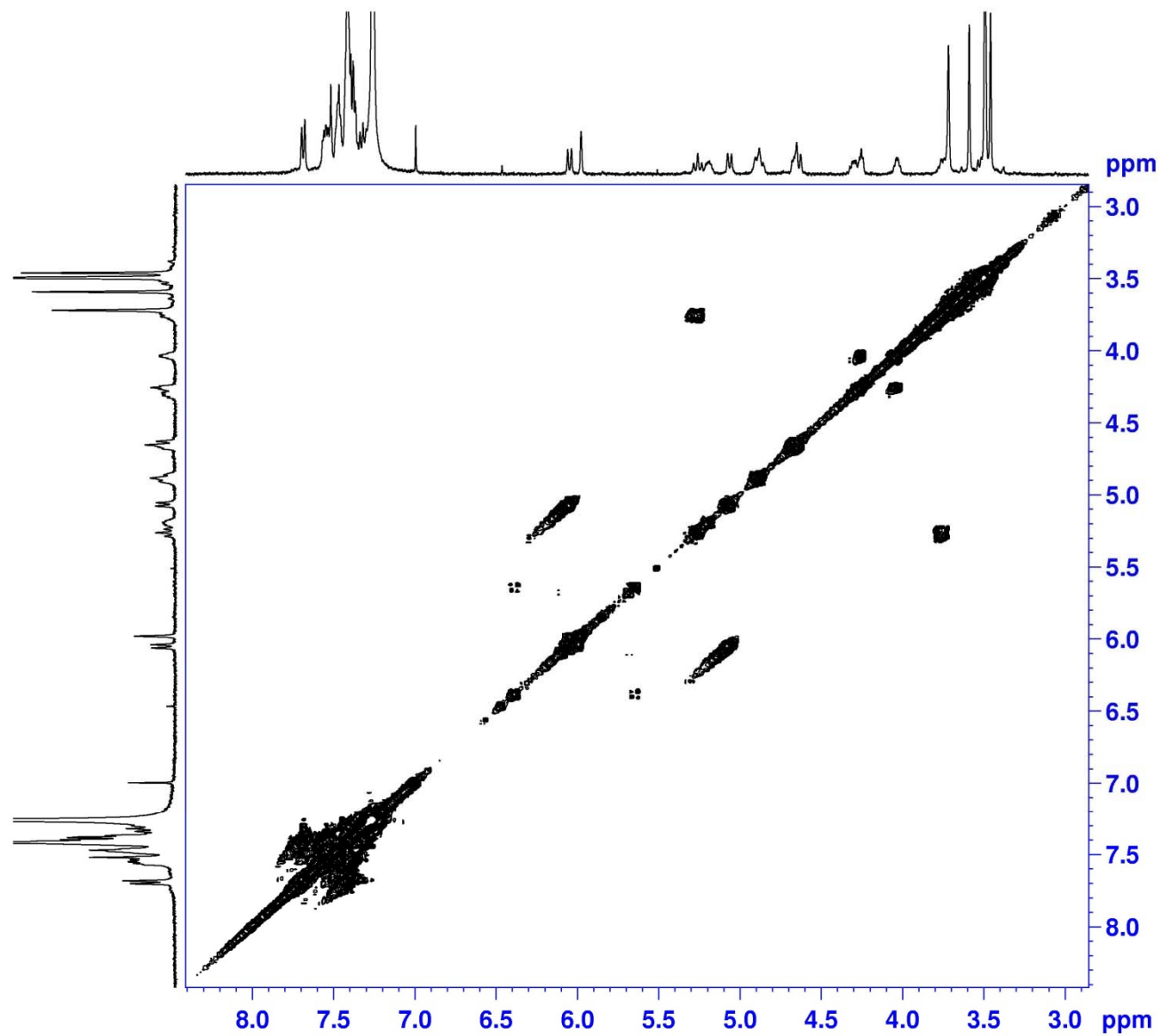
^1H - ^1H COSY (400 MHz) spectrum of compound **1r** in CDCl_3



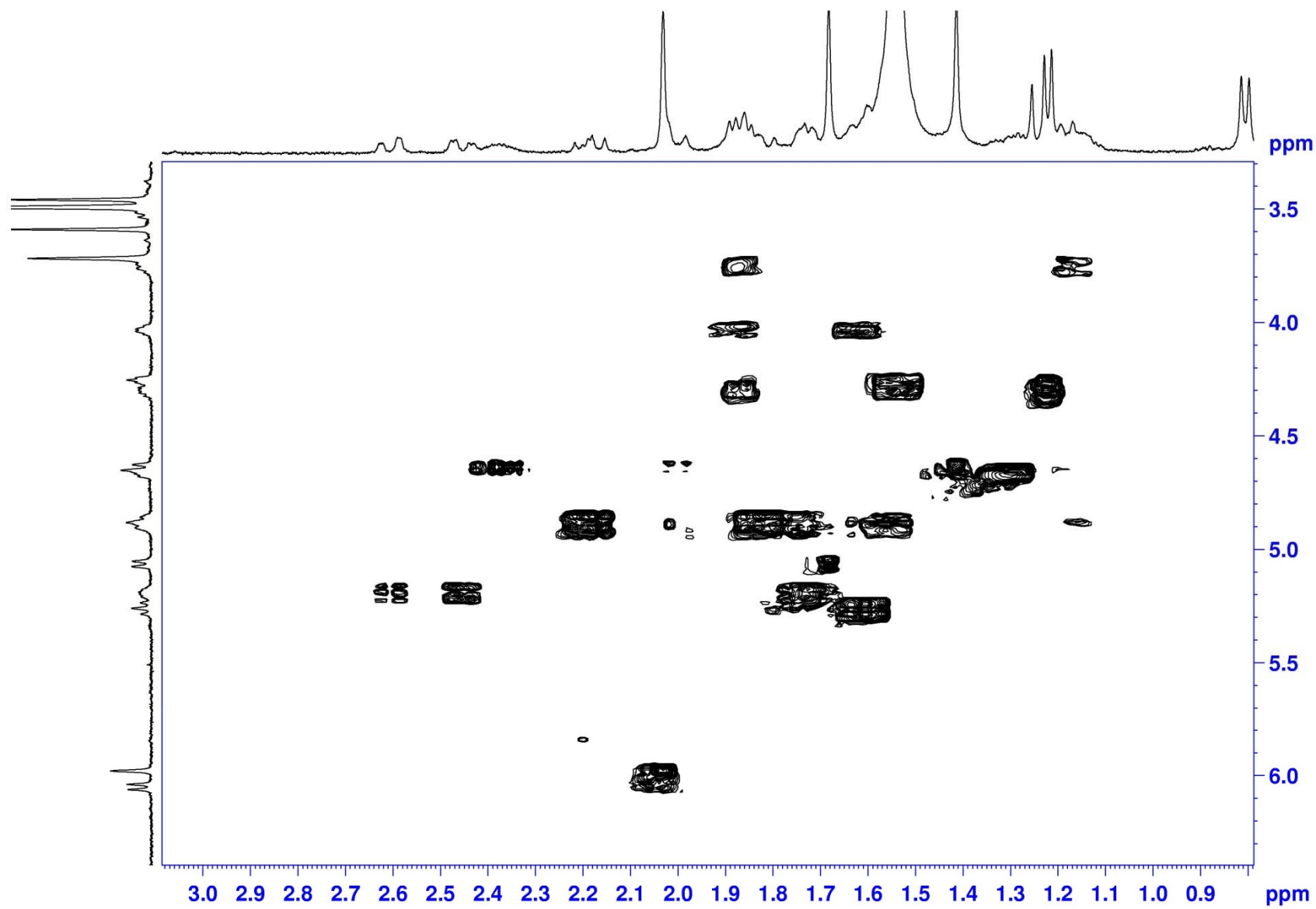
^1H - ^1H COSY (400 MHz) spectrum of compound **1r** in CDCl_3



^1H - ^1H COSY (400 MHz) spectrum of compound **1r** in CDCl_3



^1H - ^1H COSY (400 MHz) spectrum of compound **1r** in CDCl_3



LR-ESIMS for the fragment 1As

Generic Display Report

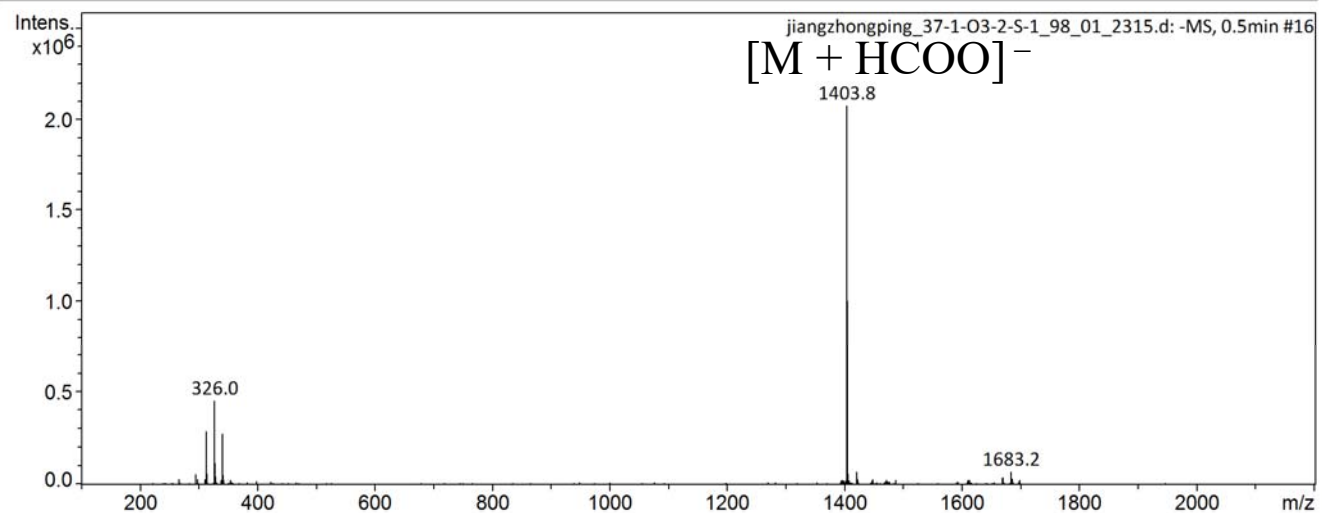
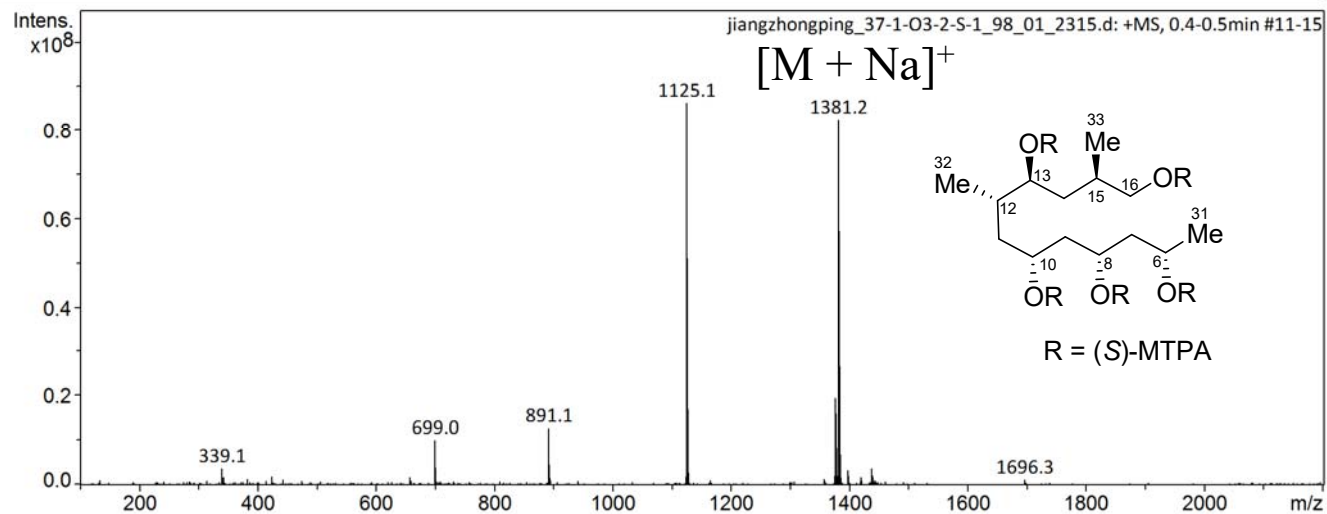
Analysis Info

Analysis Name D:\Data\amaZon SL\MS\data\202011\jiangzhongping_37-1-O3-2-S-1_98_01_2315.d
Method 2315.m
Sample Name jiangzhongping_37-1-O3-2-S-1
Comment

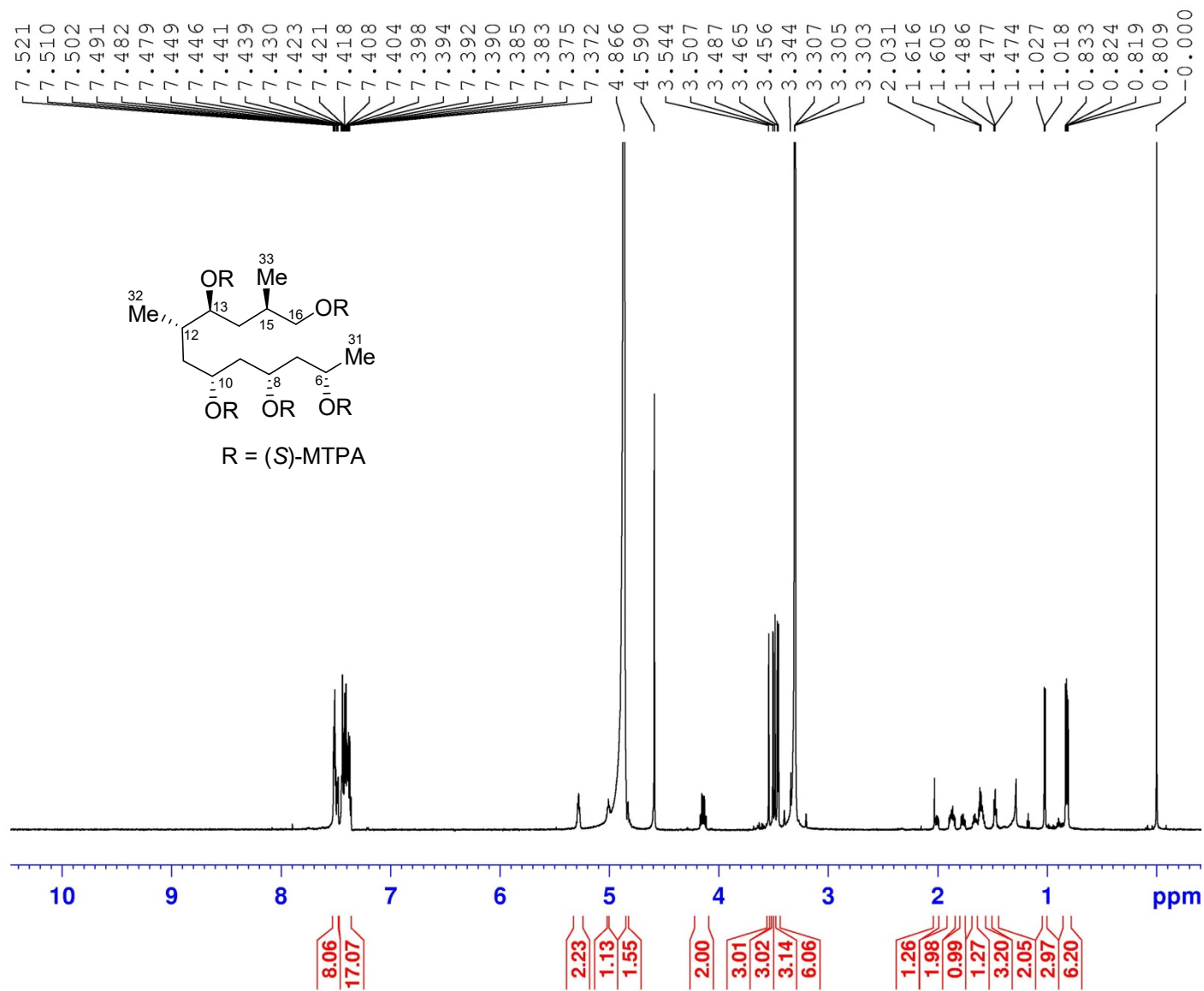
Acquisition Date 2020-11-09 15:57:29

Operator bruker

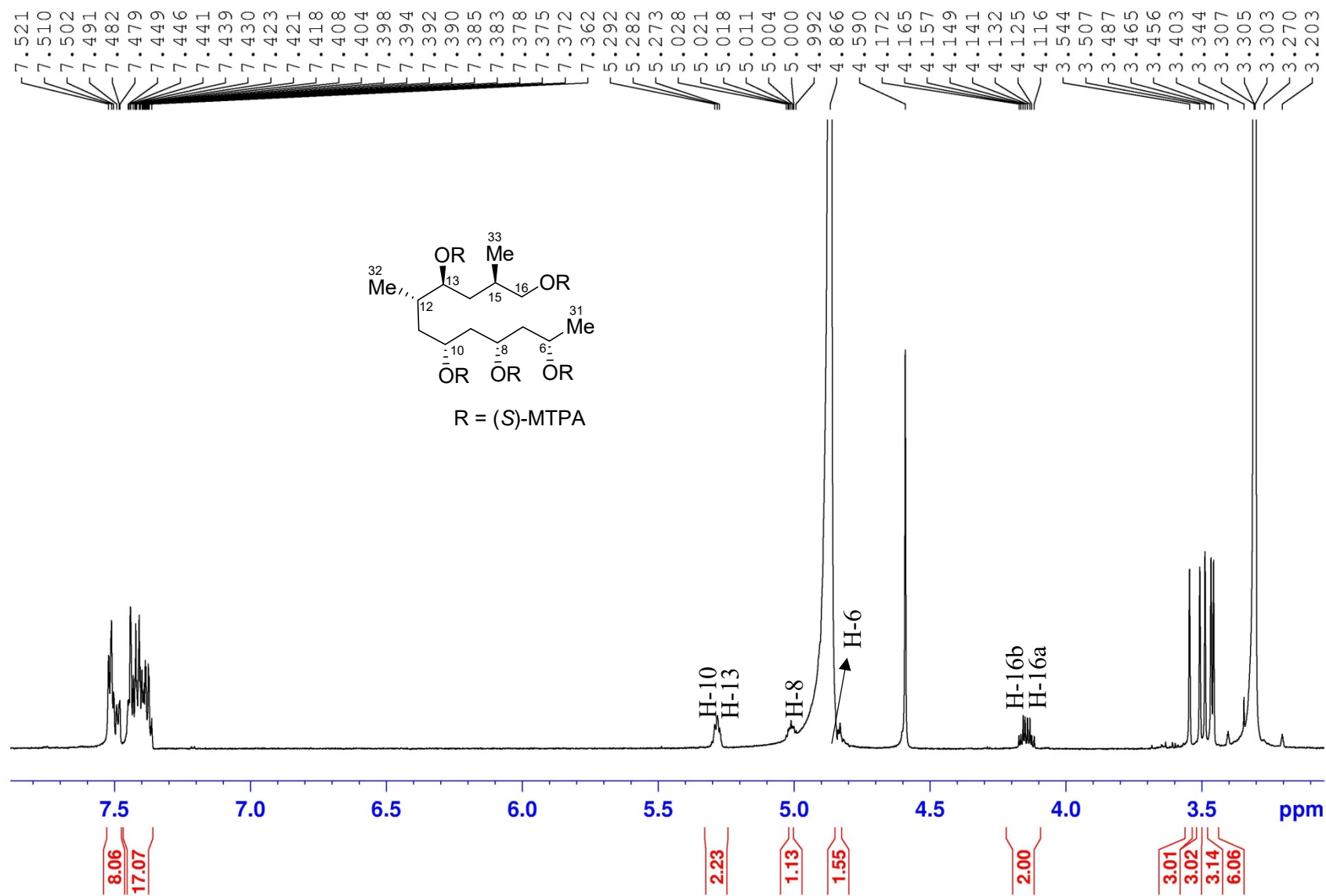
Instrument amaZon SL



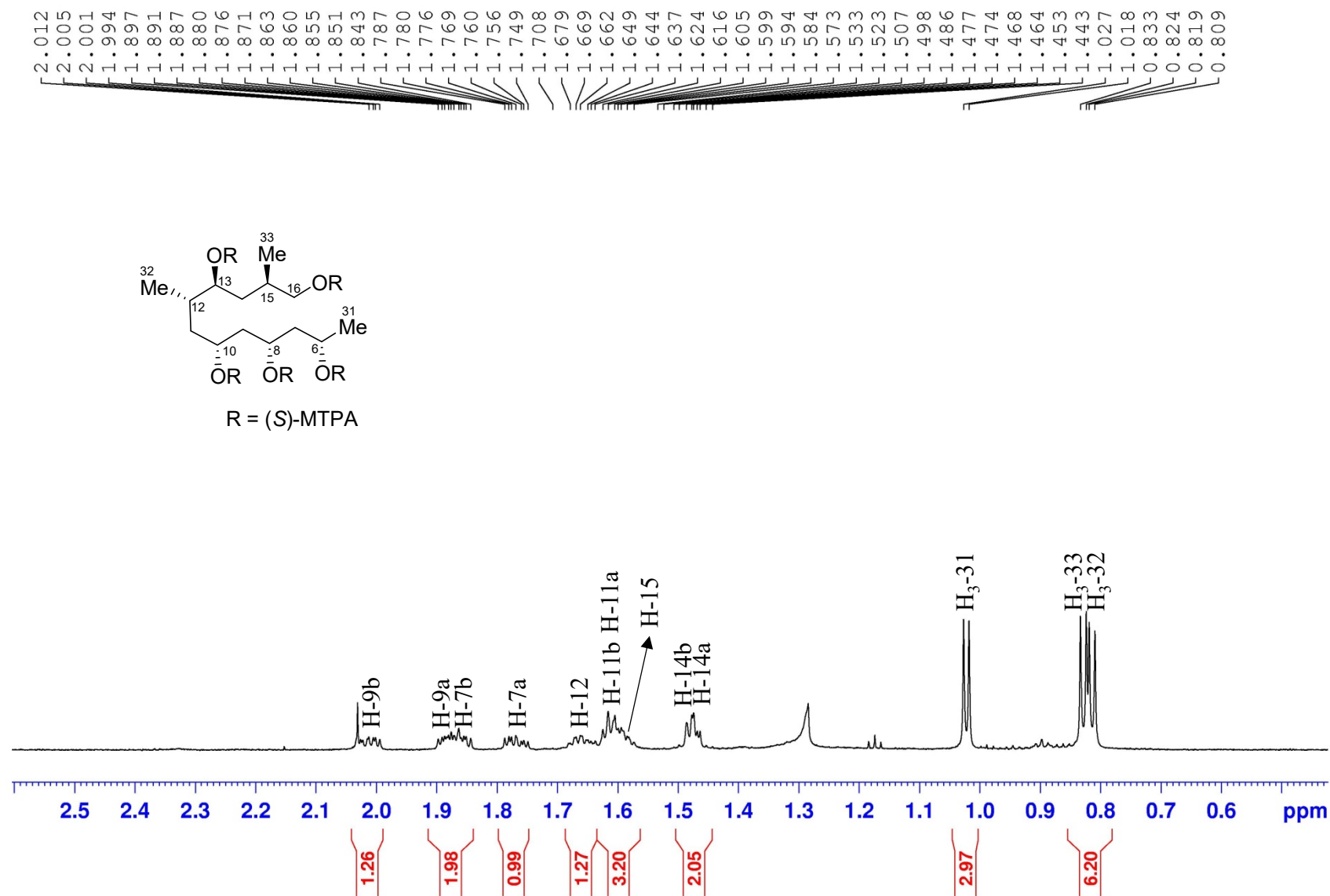
^1H (700 MHz) NMR spectrum of the fragment **1As** in CD_3OD



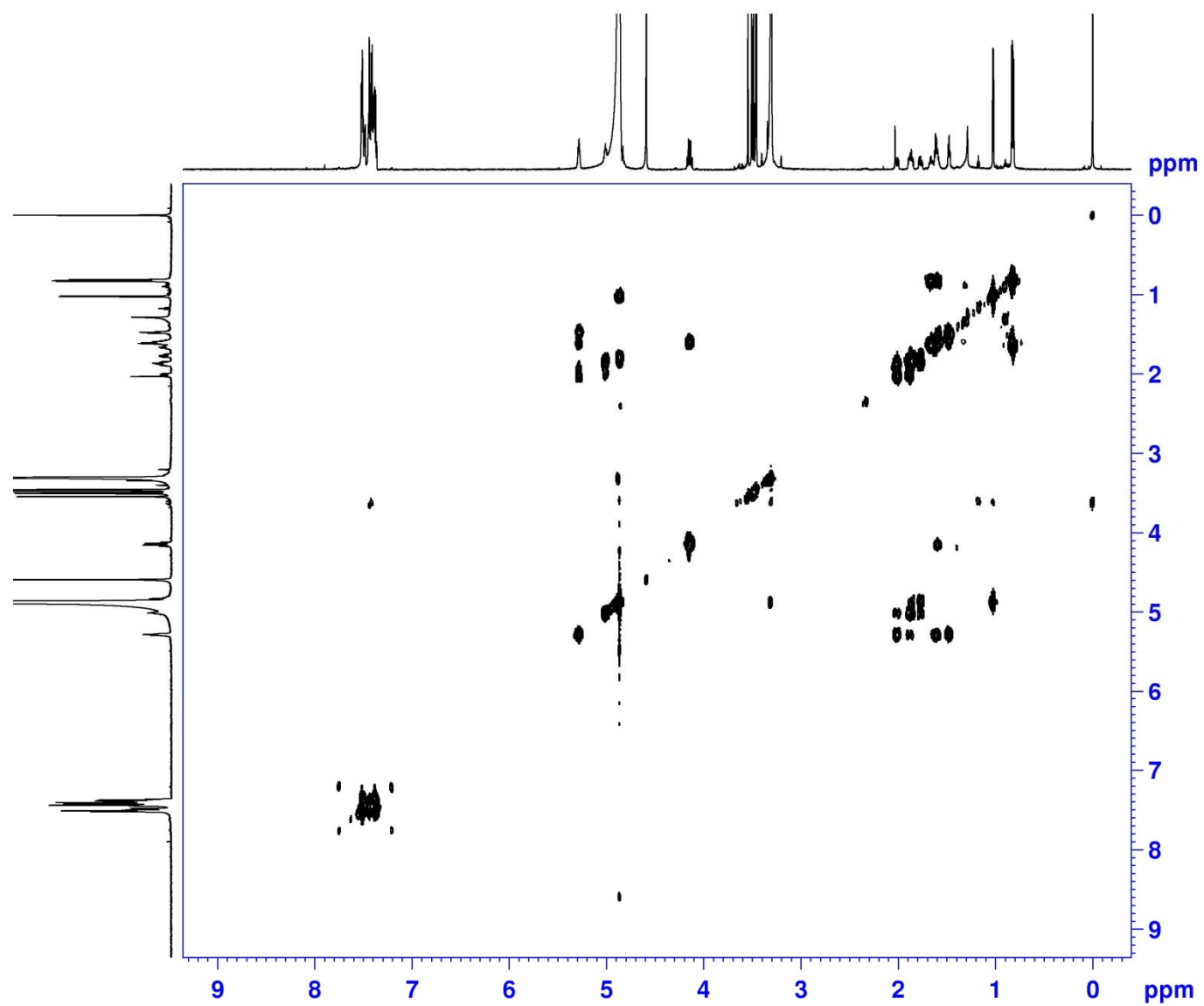
¹H (700 MHz) NMR spectrum of the fragment **1As** in CD₃OD



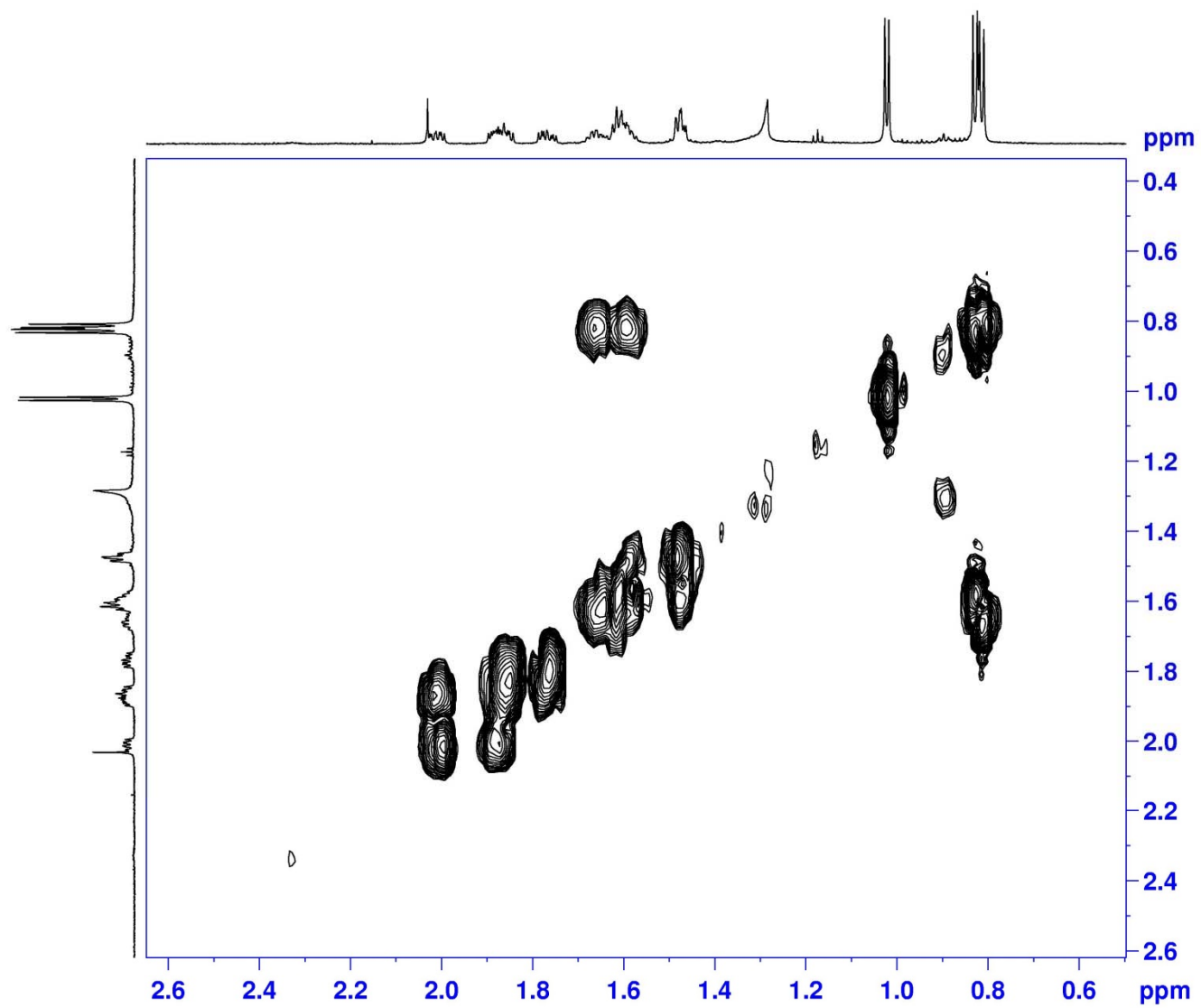
^1H (700 MHz) NMR spectrum of the fragment **1As** in CD_3OD



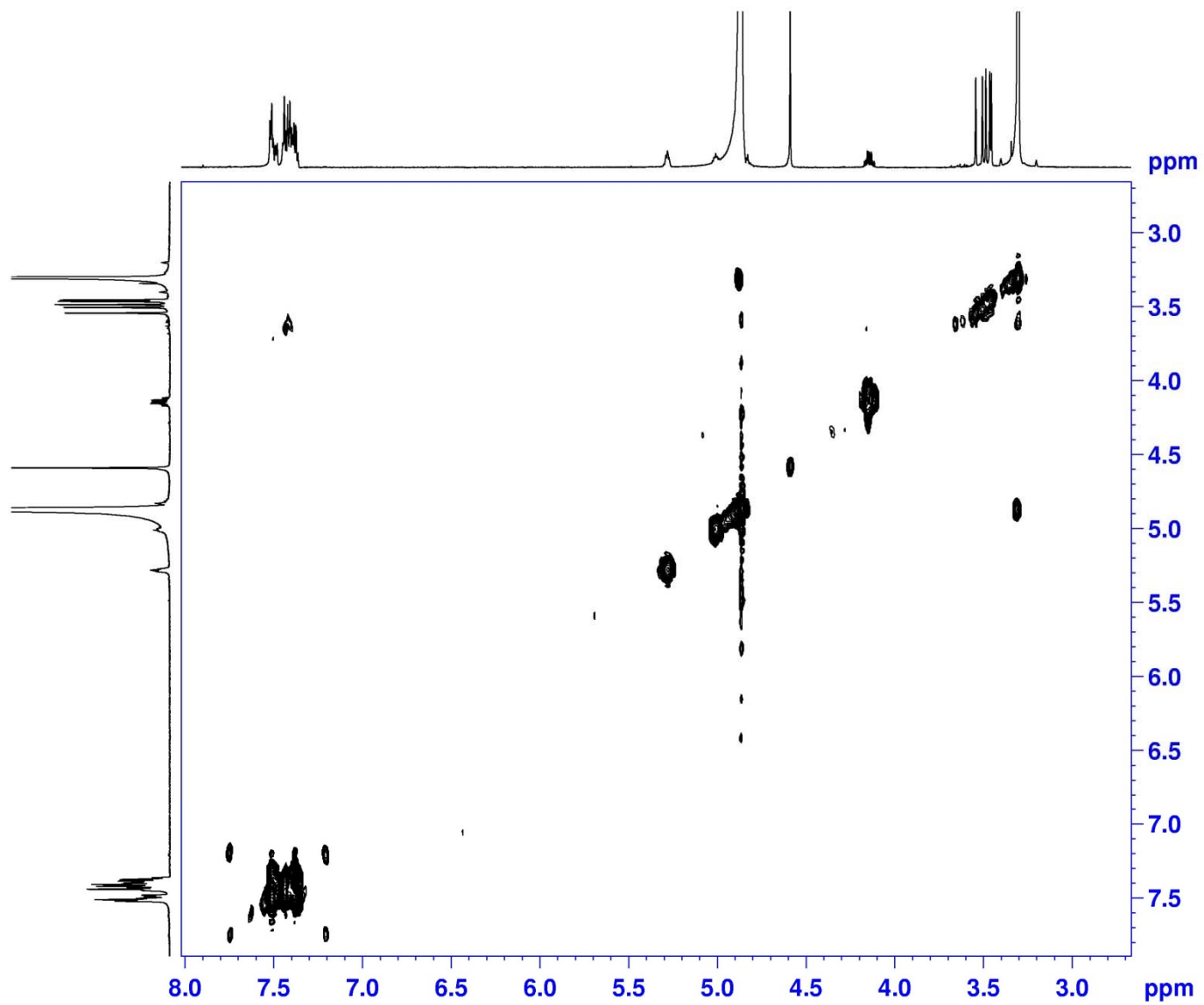
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1As** in CD_3OD



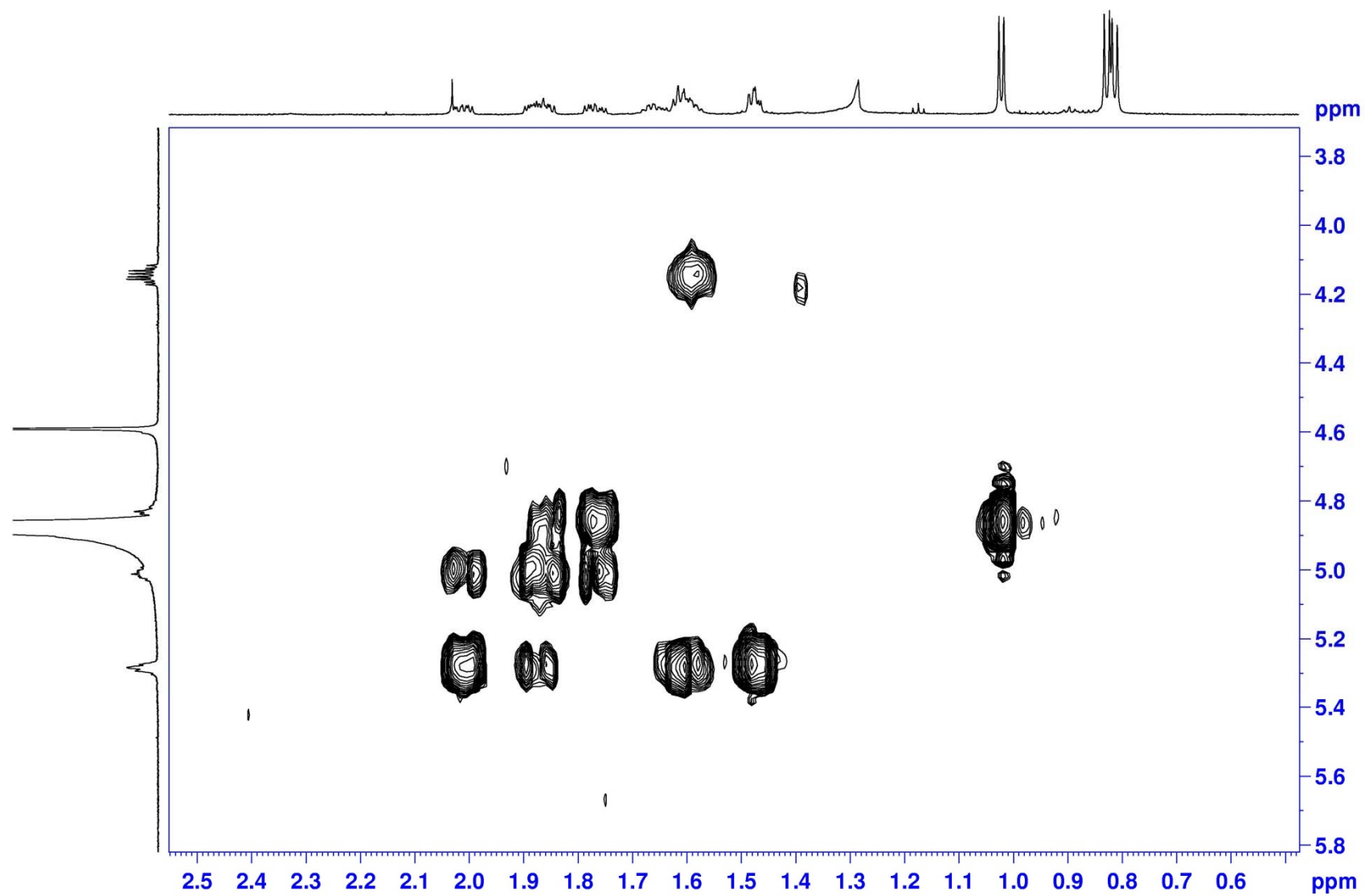
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1As** in CD_3OD



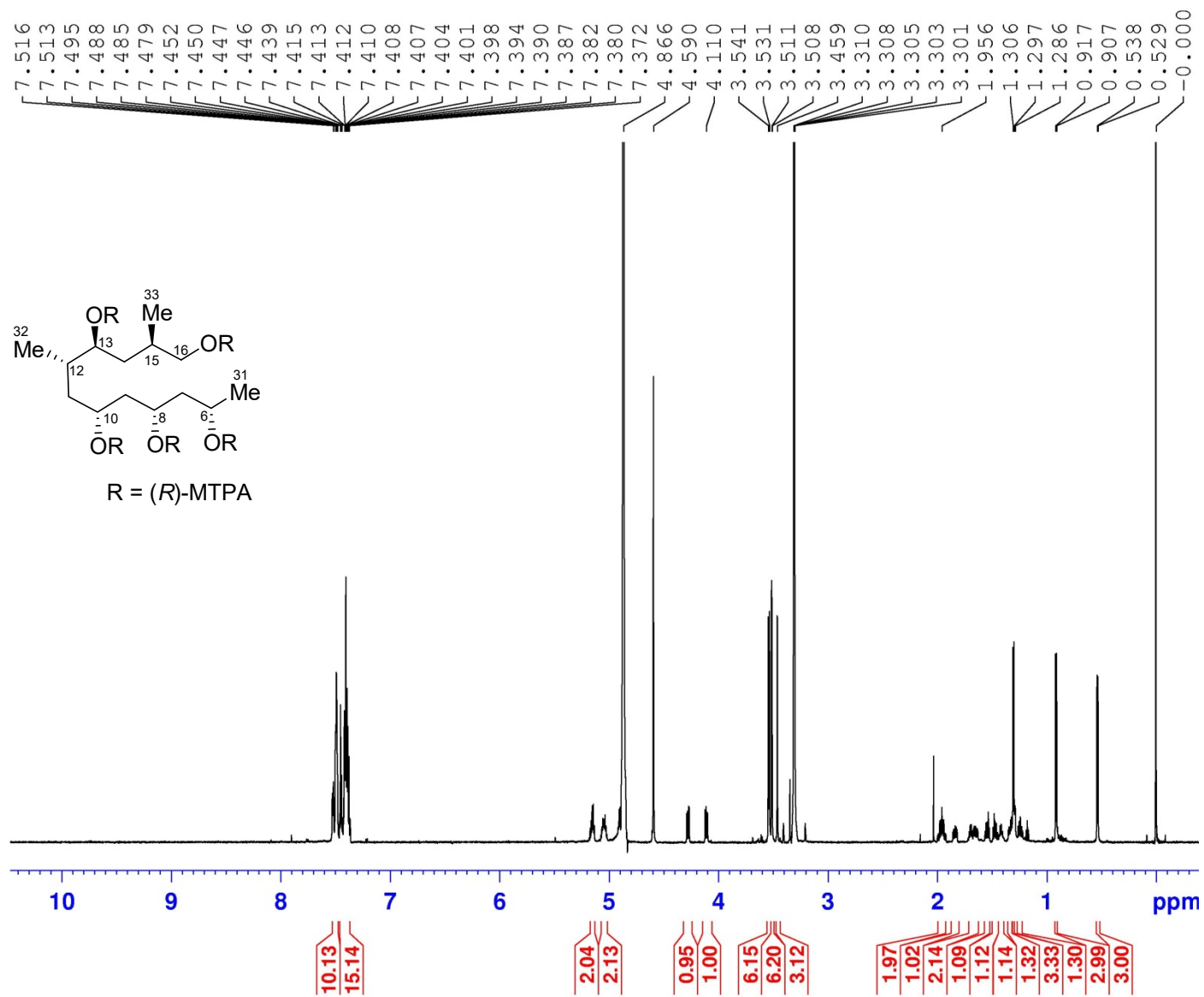
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1As** in CD_3OD



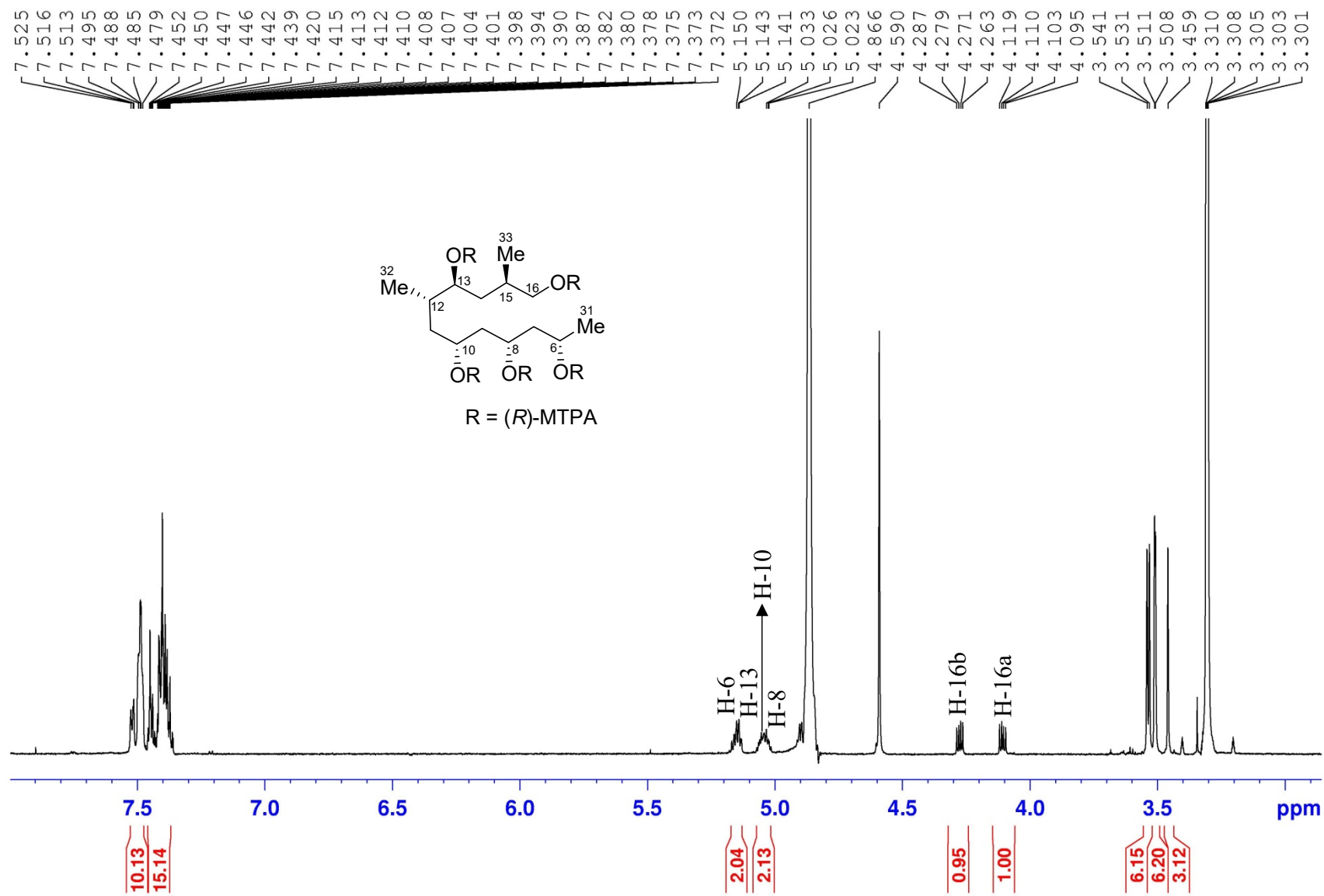
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1As** in CD_3OD



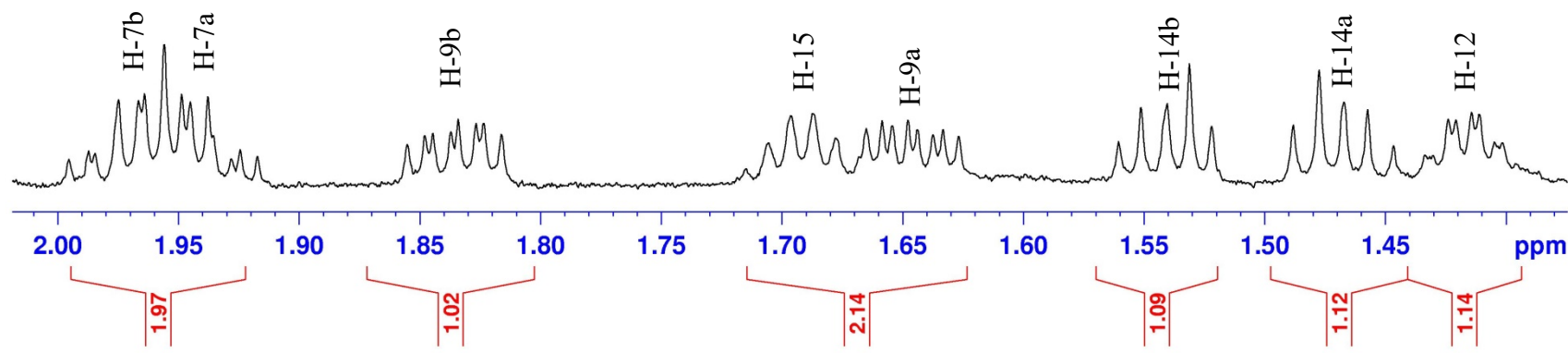
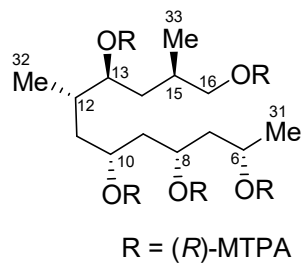
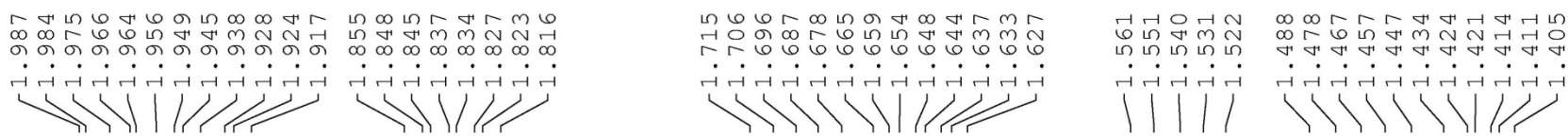
^1H (700 MHz) NMR spectrum of the fragment **1Ar** in CD_3OD



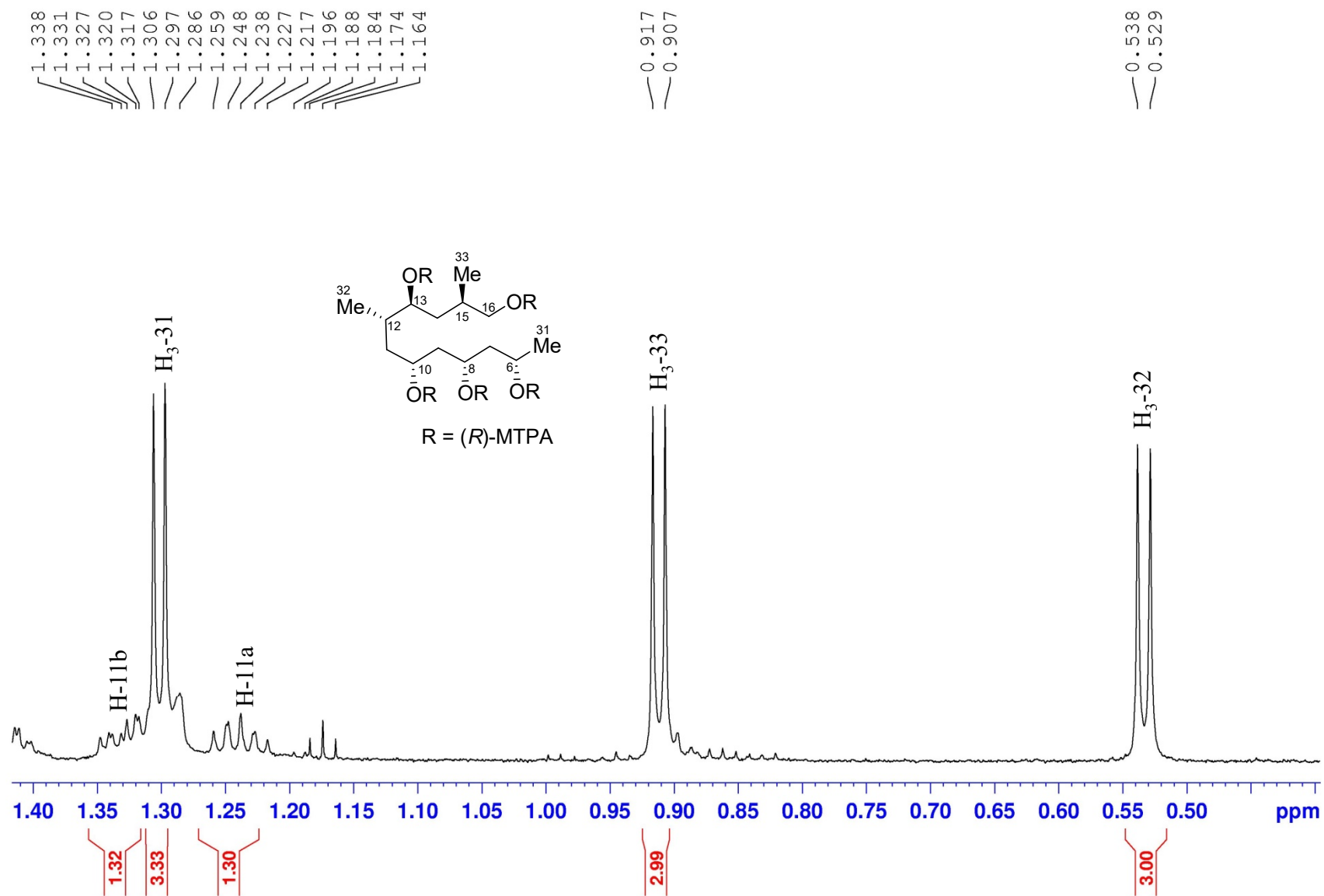
^1H (700 MHz) NMR spectrum of the fragment **1Ar** in CD_3OD



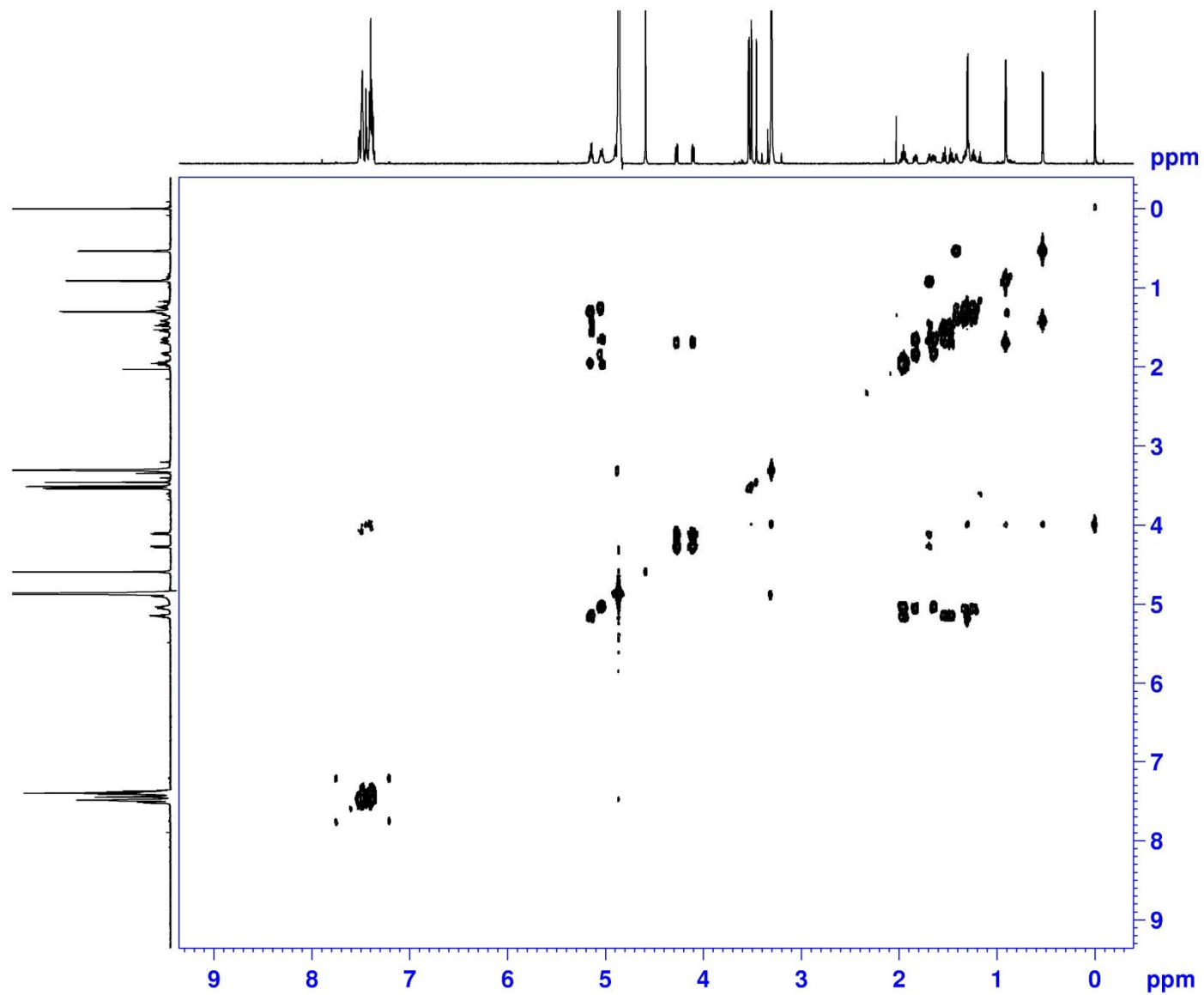
^1H (700 MHz) NMR spectrum of the fragment **1Ar** in CD_3OD



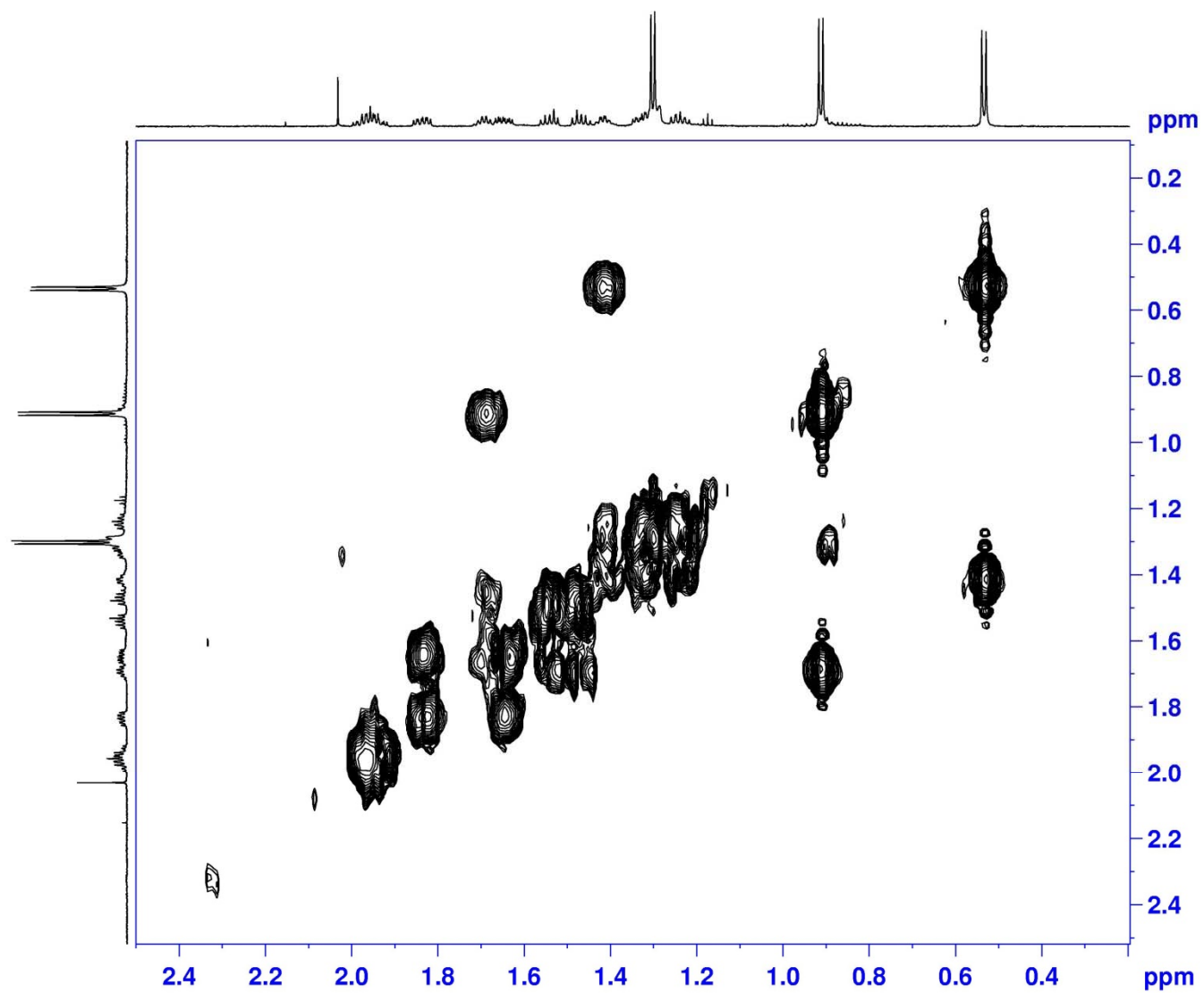
¹H (700 MHz) NMR spectrum of the fragment **1Ar** in CD₃OD



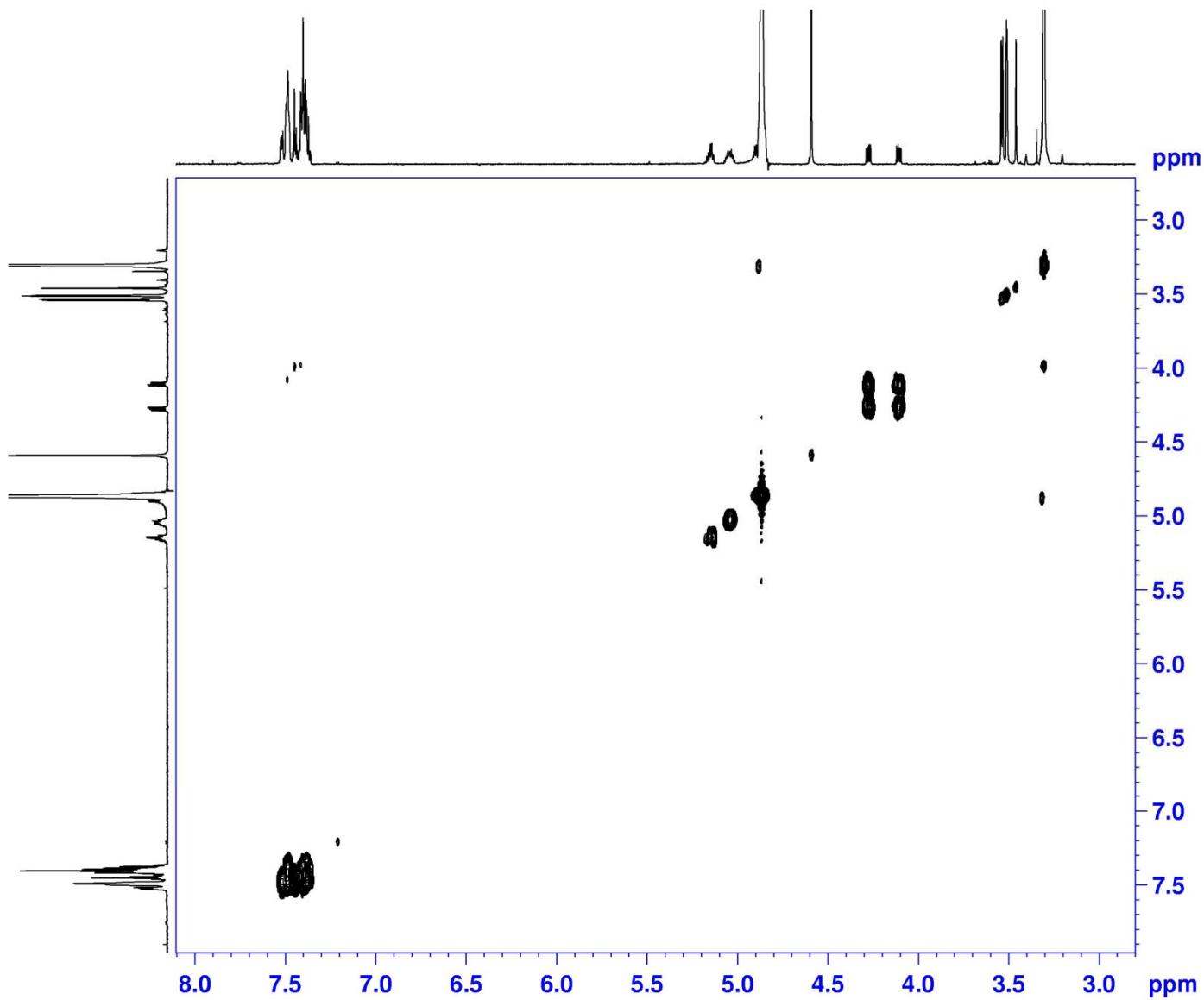
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1Ar** in CD_3OD



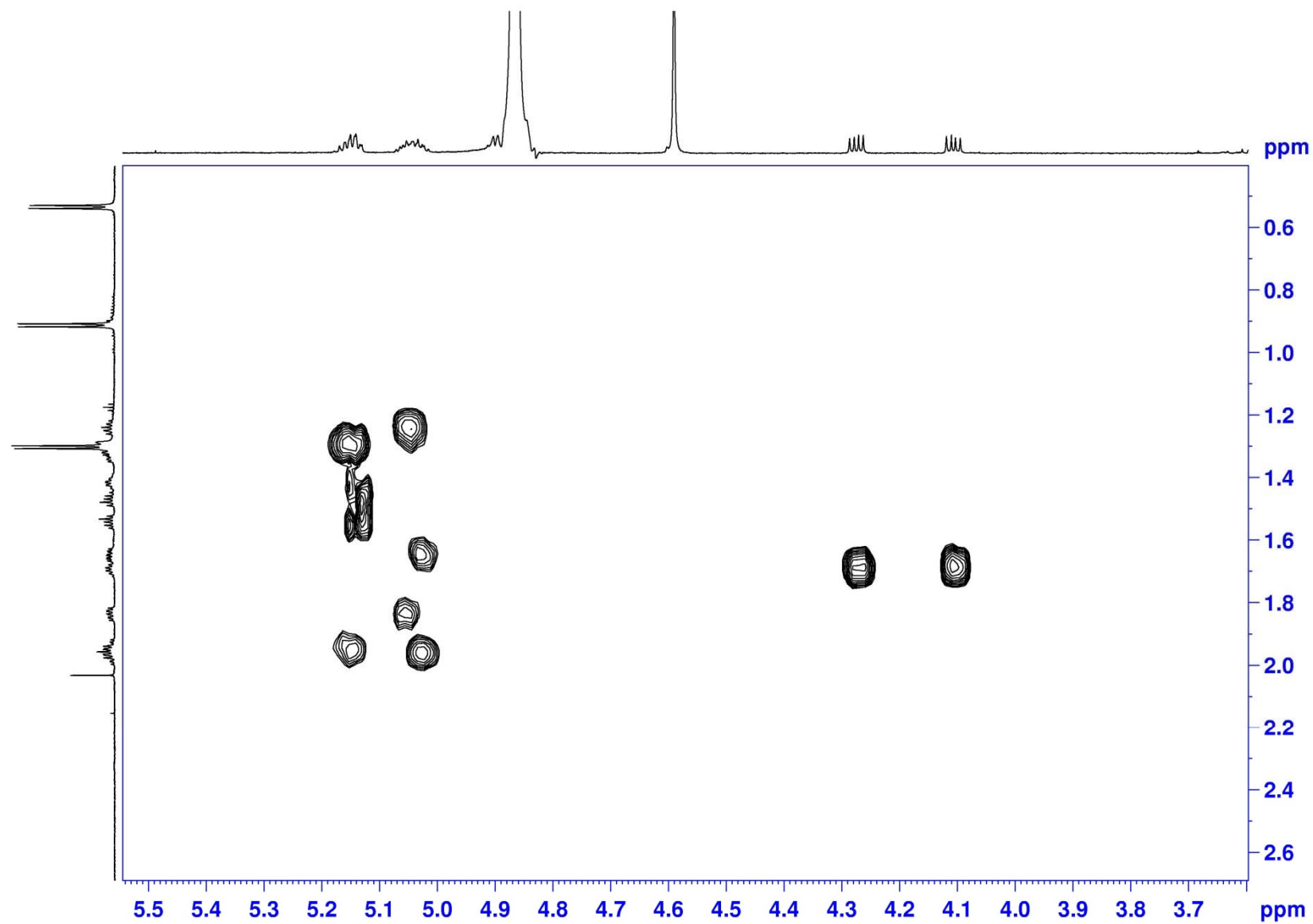
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1Ar** in CD_3OD



^1H - ^1H COSY (700 MHz) spectrum of the fragment **1Ar** in CD_3OD



^1H - ^1H COSY (700 MHz) spectrum of the fragment **1Ar** in CD_3OD

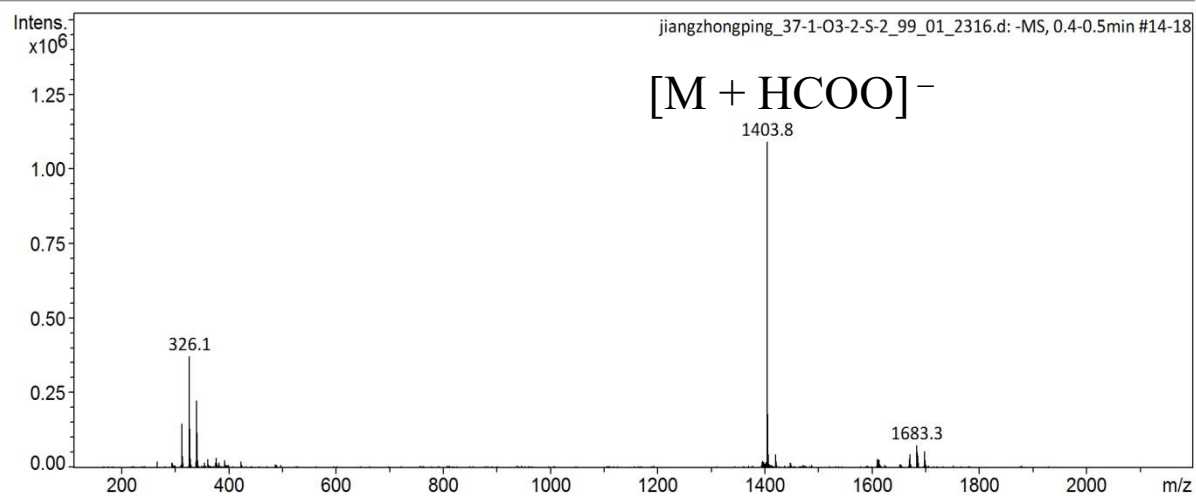
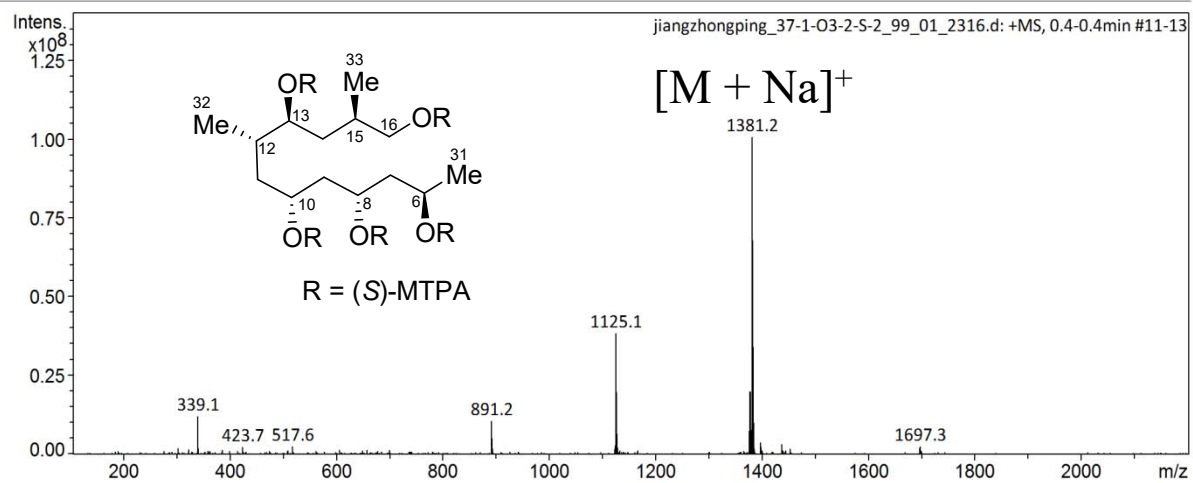


LR-ESIMS for the fragment 1A's

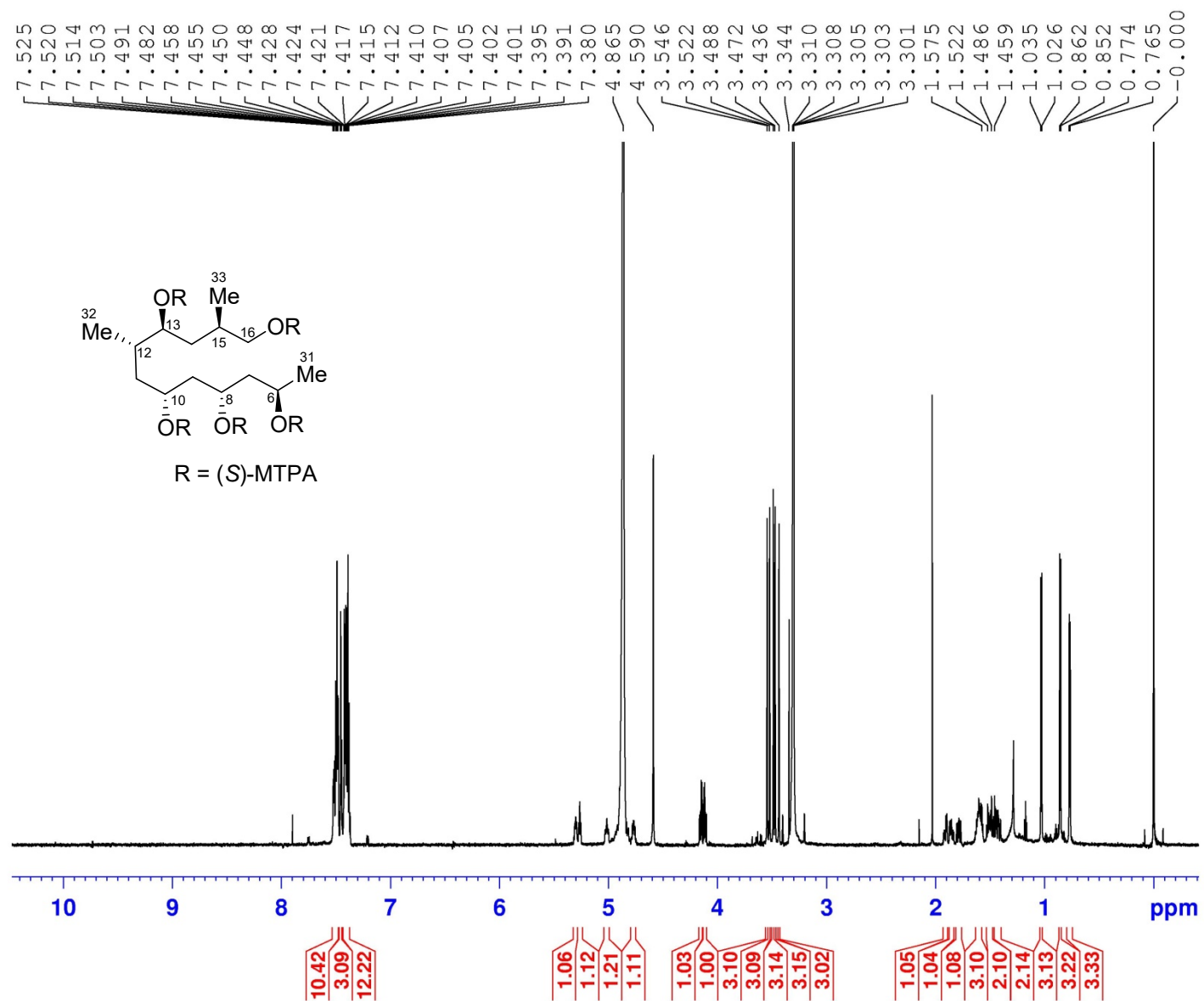
Generic Display Report

Analysis Info

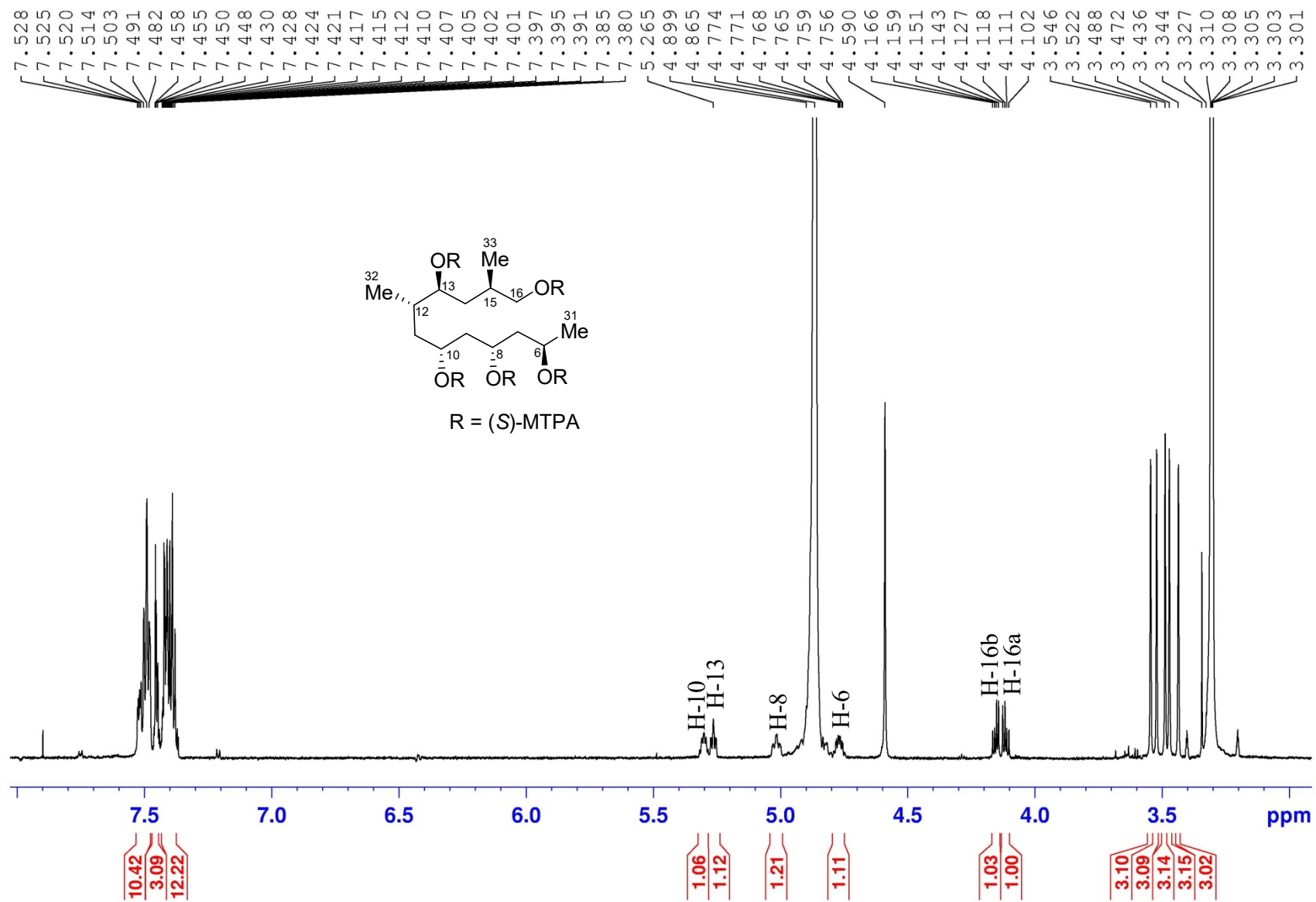
Analysis Name	D:\Data\amaZon SLIMS\data\202011\jiangzhongping_37-1-O3-2-S-2_99_01_2316.d	Acquisition Date	2020-11-09 16:00:02
Method	2316.m	Operator	bruker
Sample Name	jiangzhongping_37-1-O3-2-S-2	Instrument	amaZon SL
Comment			



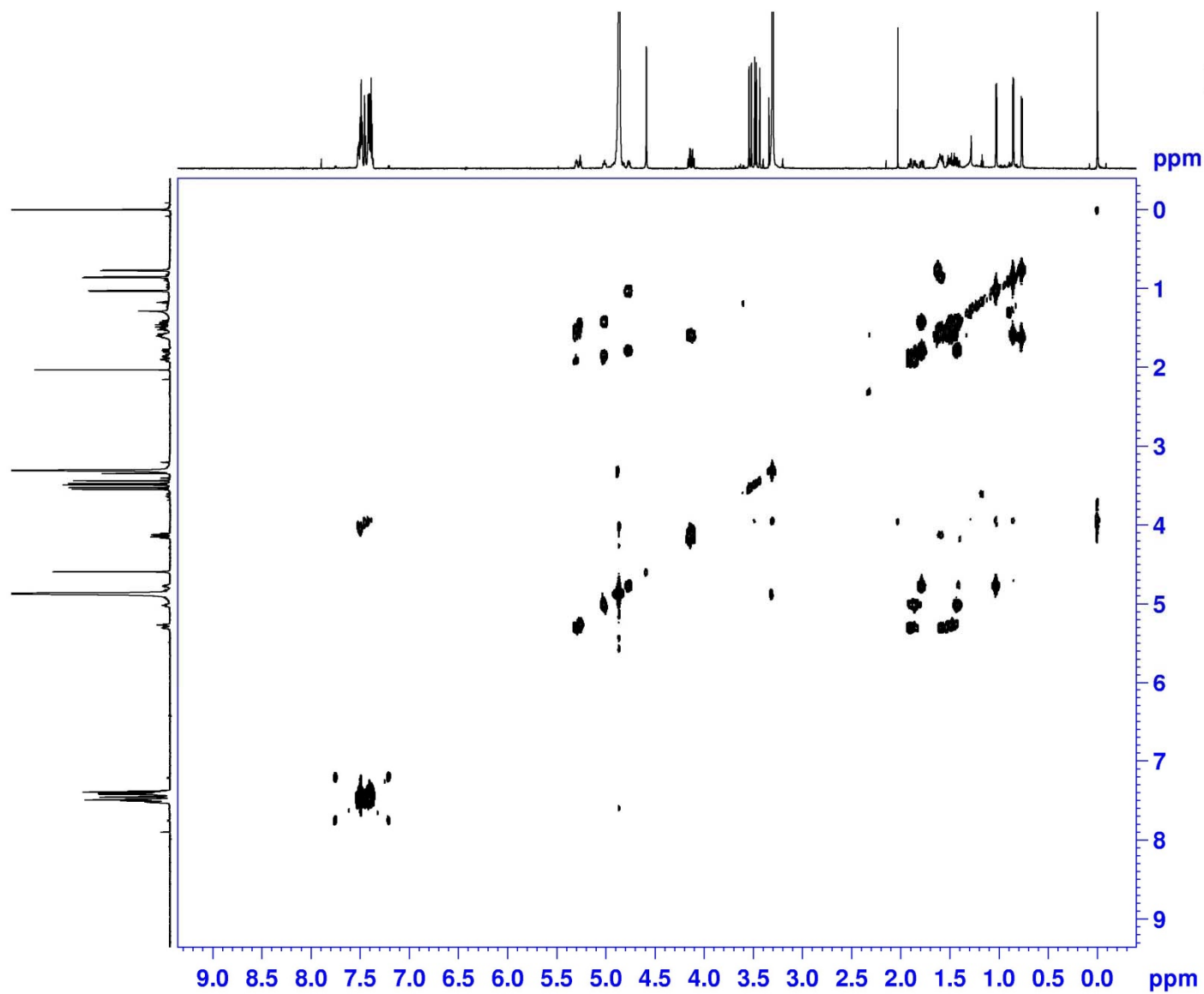
^1H (700 MHz) NMR spectrum of the fragment **1A's** in CD_3OD



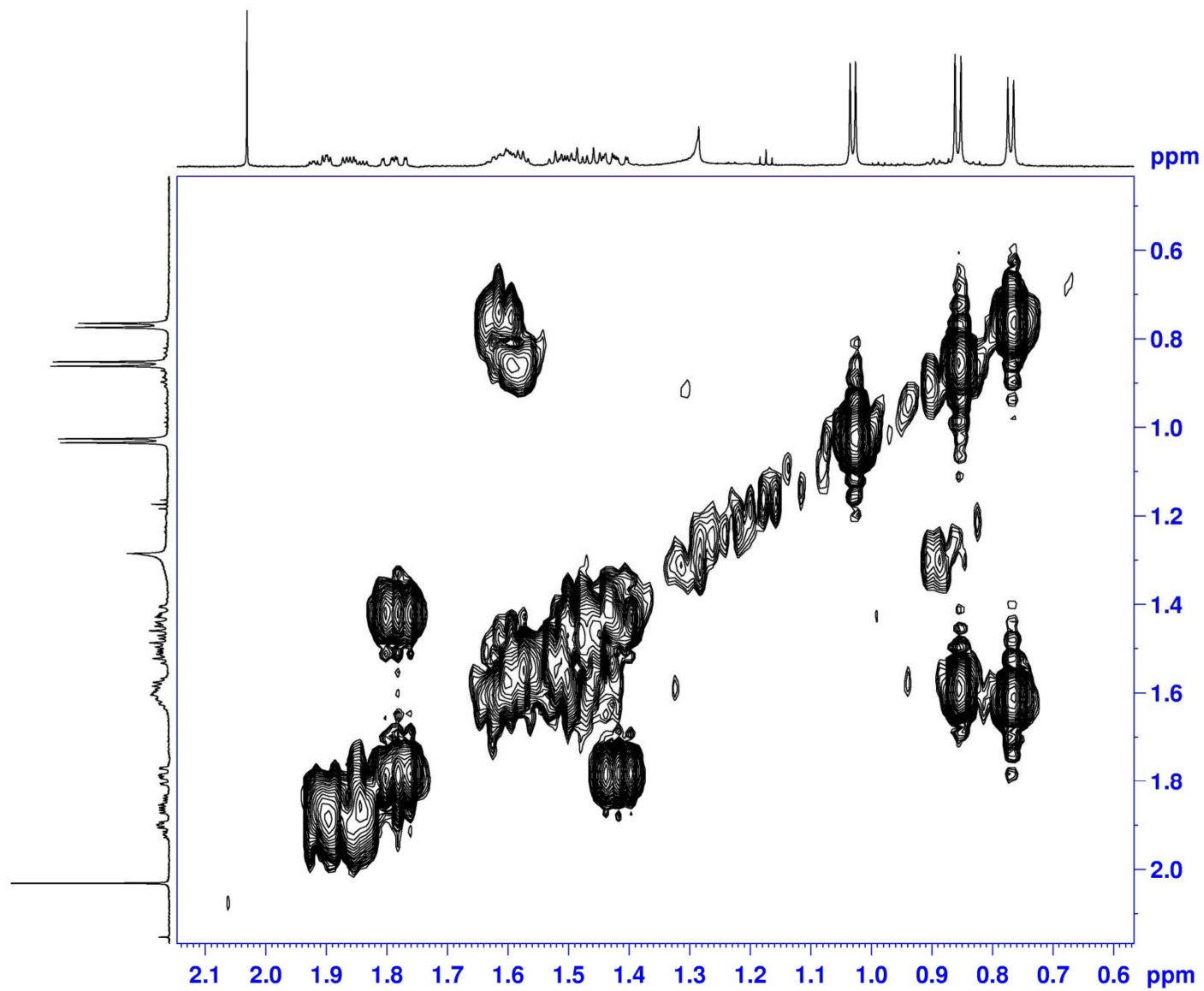
¹H (700 MHz) NMR spectrum of the fragment 1A's in CD₃OD



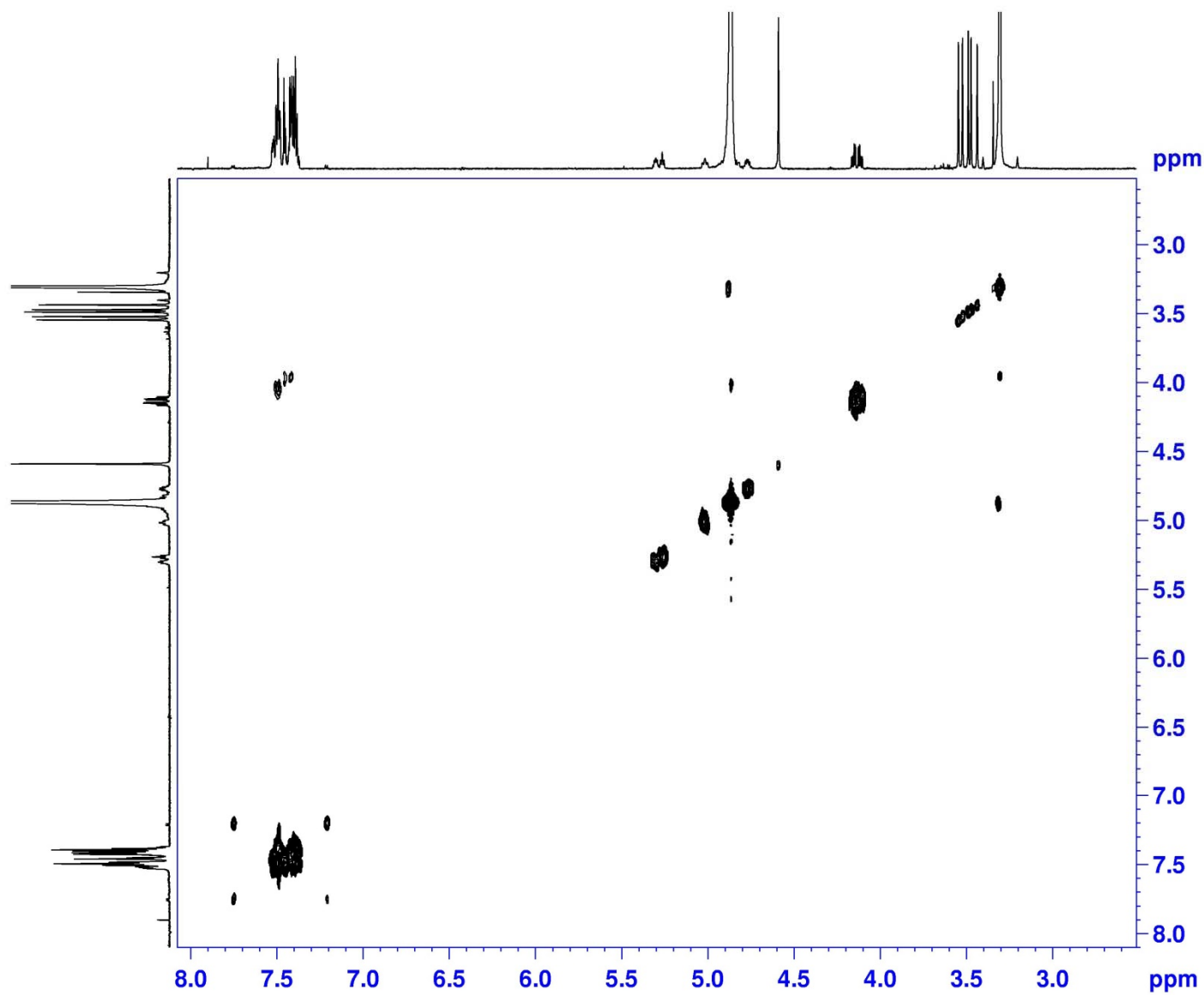
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1A**'s in CD_3OD



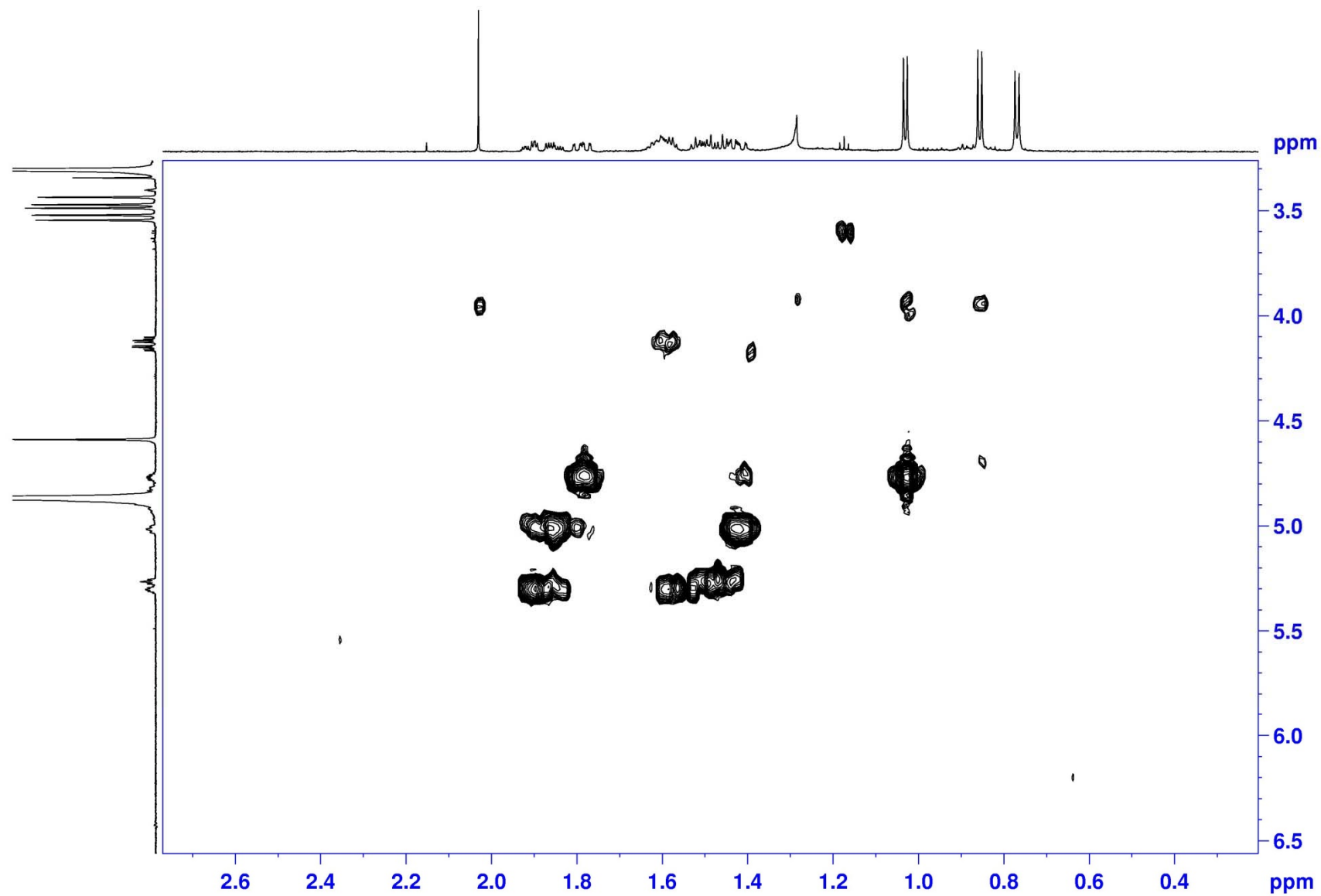
^1H - ^1H COSY (700 MHz) spectrum of the fragment 1A's in CD_3OD



^1H - ^1H COSY (700 MHz) spectrum of the fragment **1A**'s in CD_3OD



^1H - ^1H COSY (700 MHz) spectrum of the fragment 1A's in CD_3OD

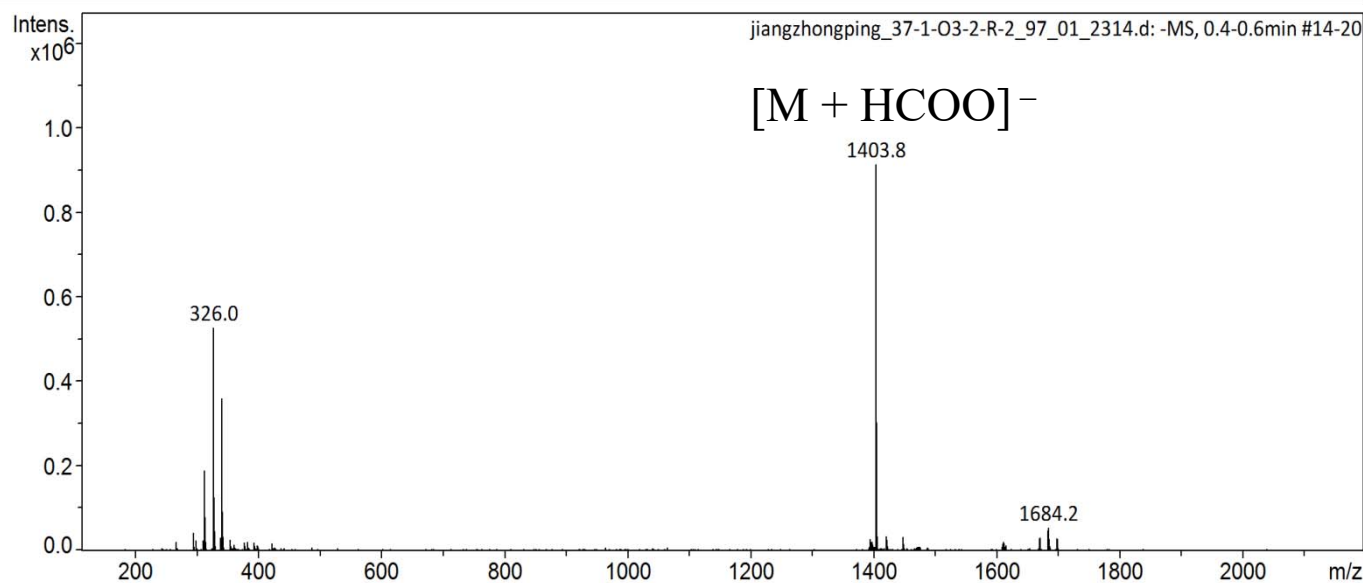
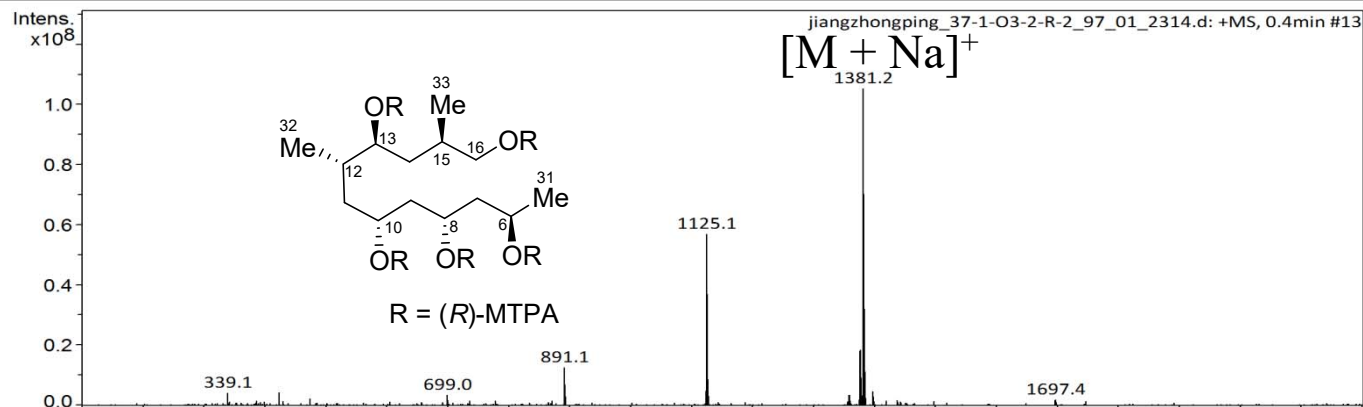


LR-ESIMS for the fragment 1A'r

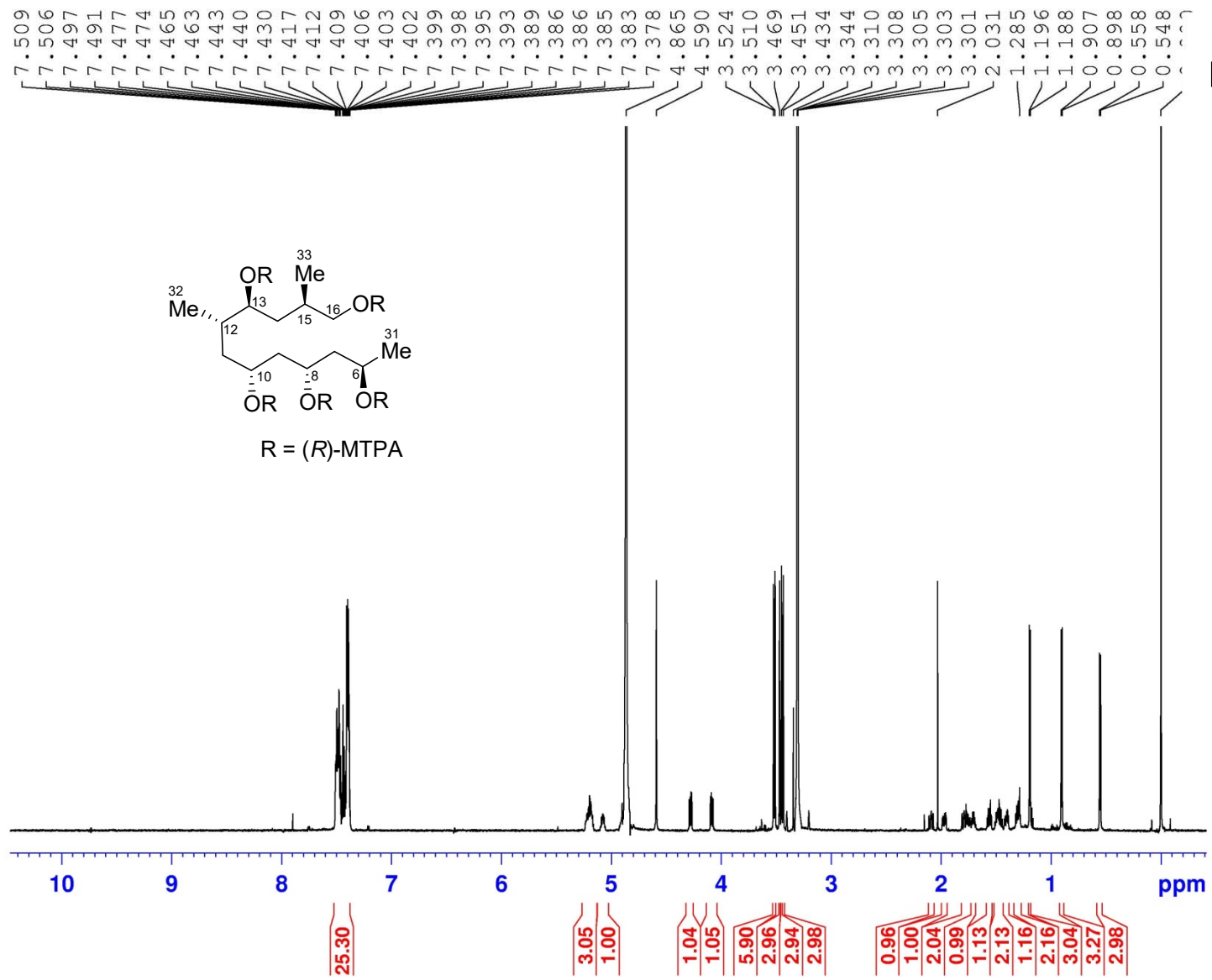
Generic Display Report

Analysis Info

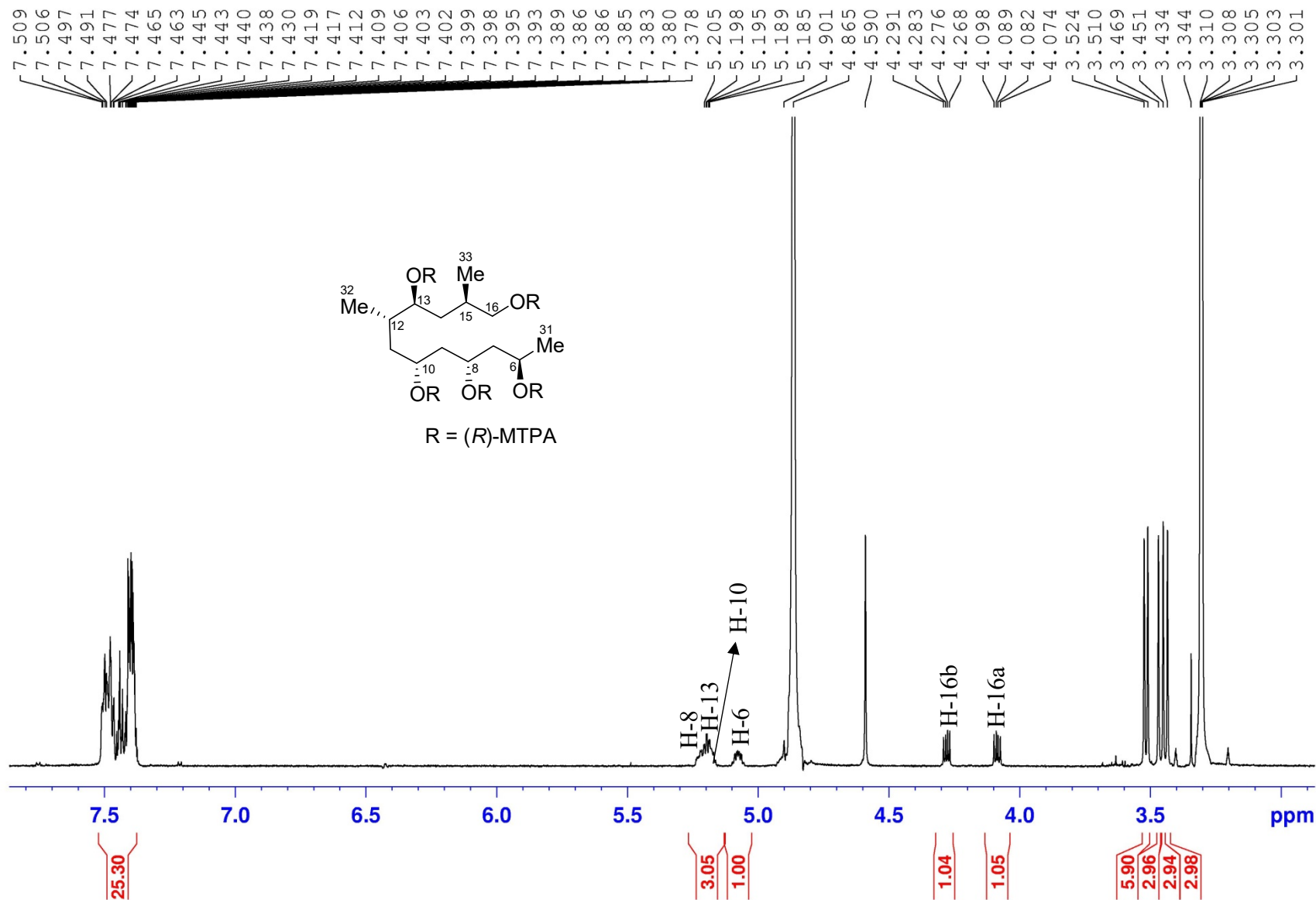
Analysis Name	D:\Data\amaZon SLIMS\data\202011\jiangzhongping_37-1-O3-2-R-2_97_01_2314.d	Acquisition Date	2020-11-09 15:55:03
Method	2314.m	Operator	bruker
Sample Name	jiangzhongping_37-1-O3-2-R-2	Instrument	amaZon SL
Comment			



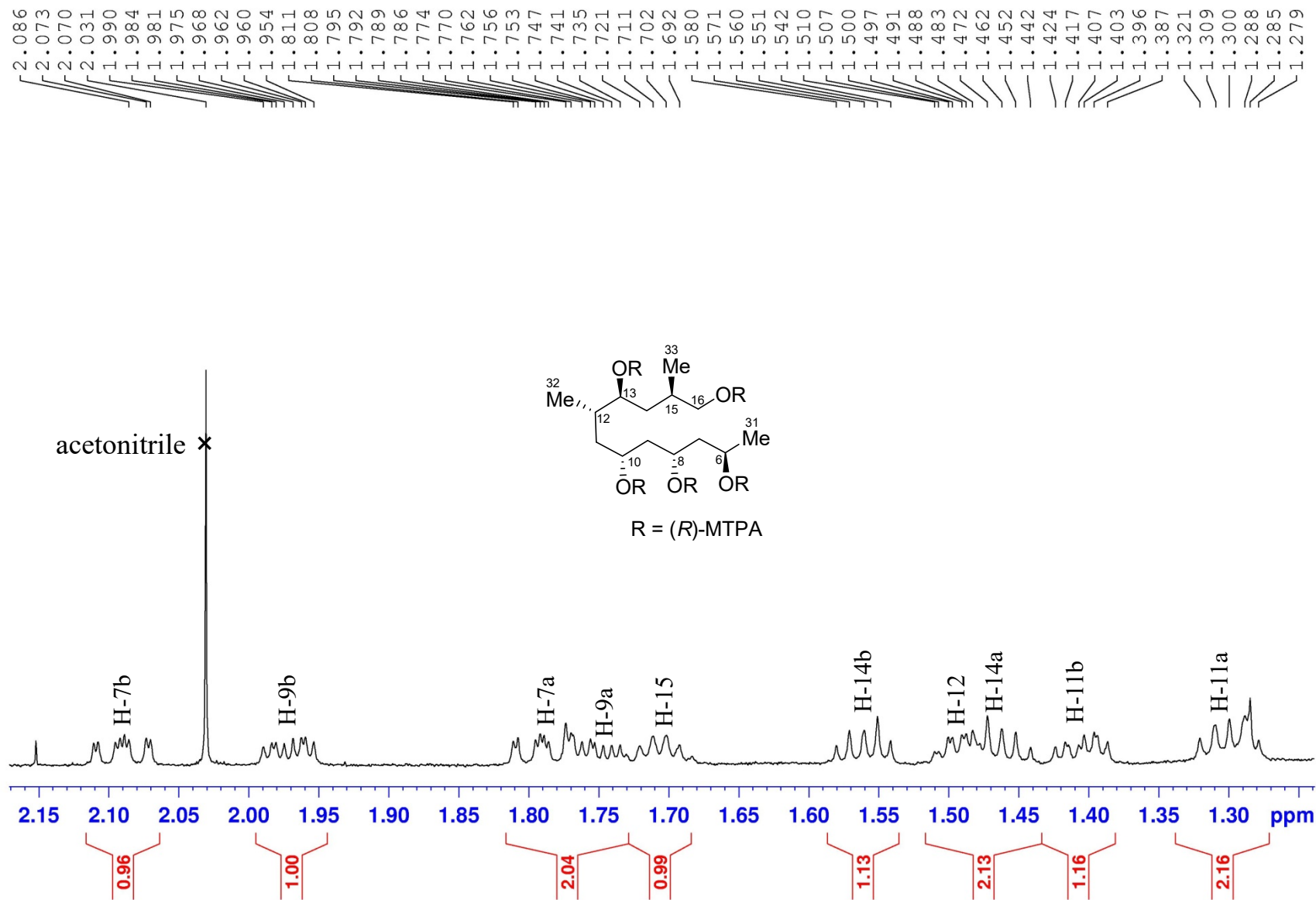
^1H (700 MHz) NMR spectrum of the fragment **1A'r** in CD_3OD



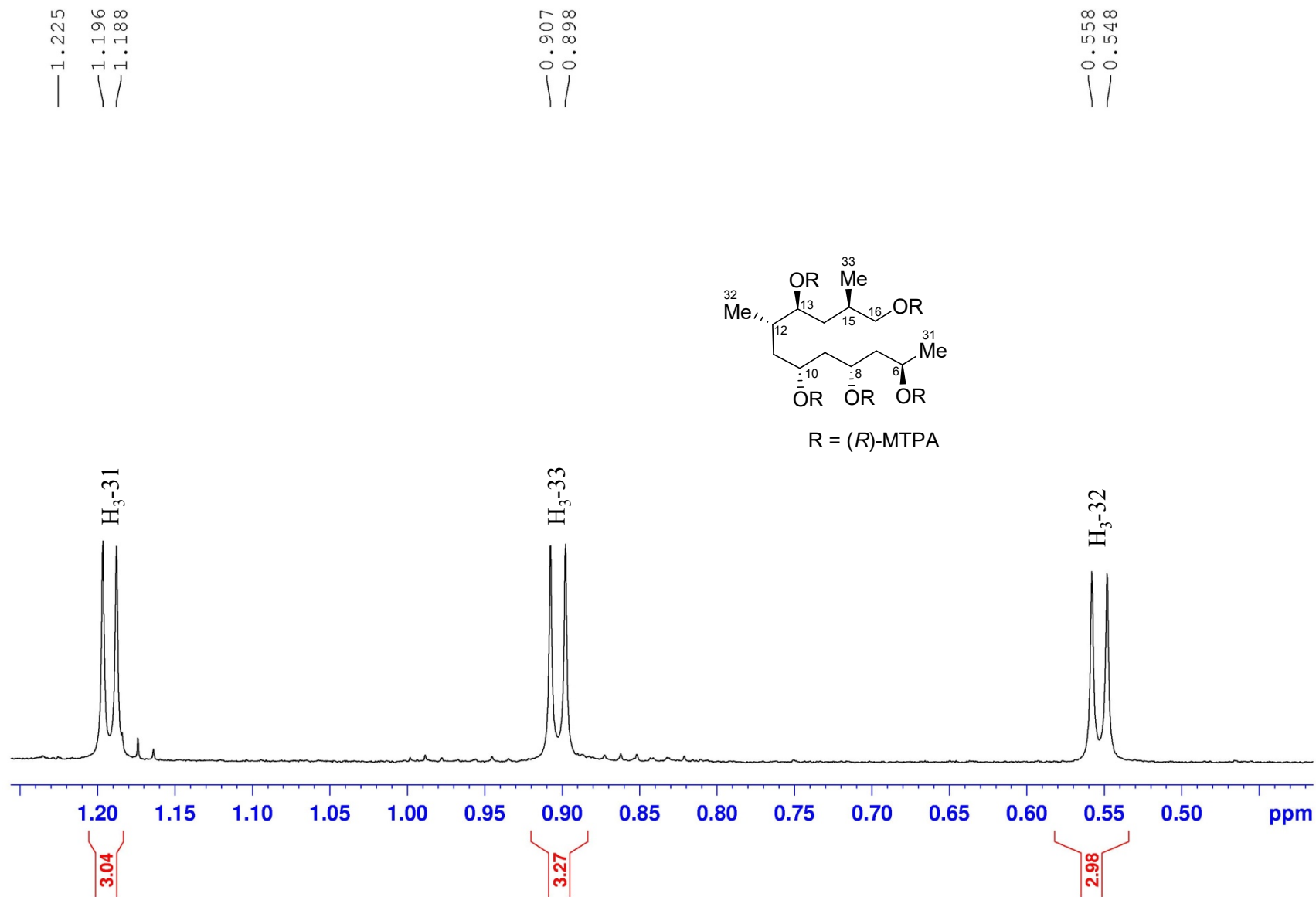
¹H (700 MHz) NMR spectrum of the fragment **1A'r** in CD₃OD



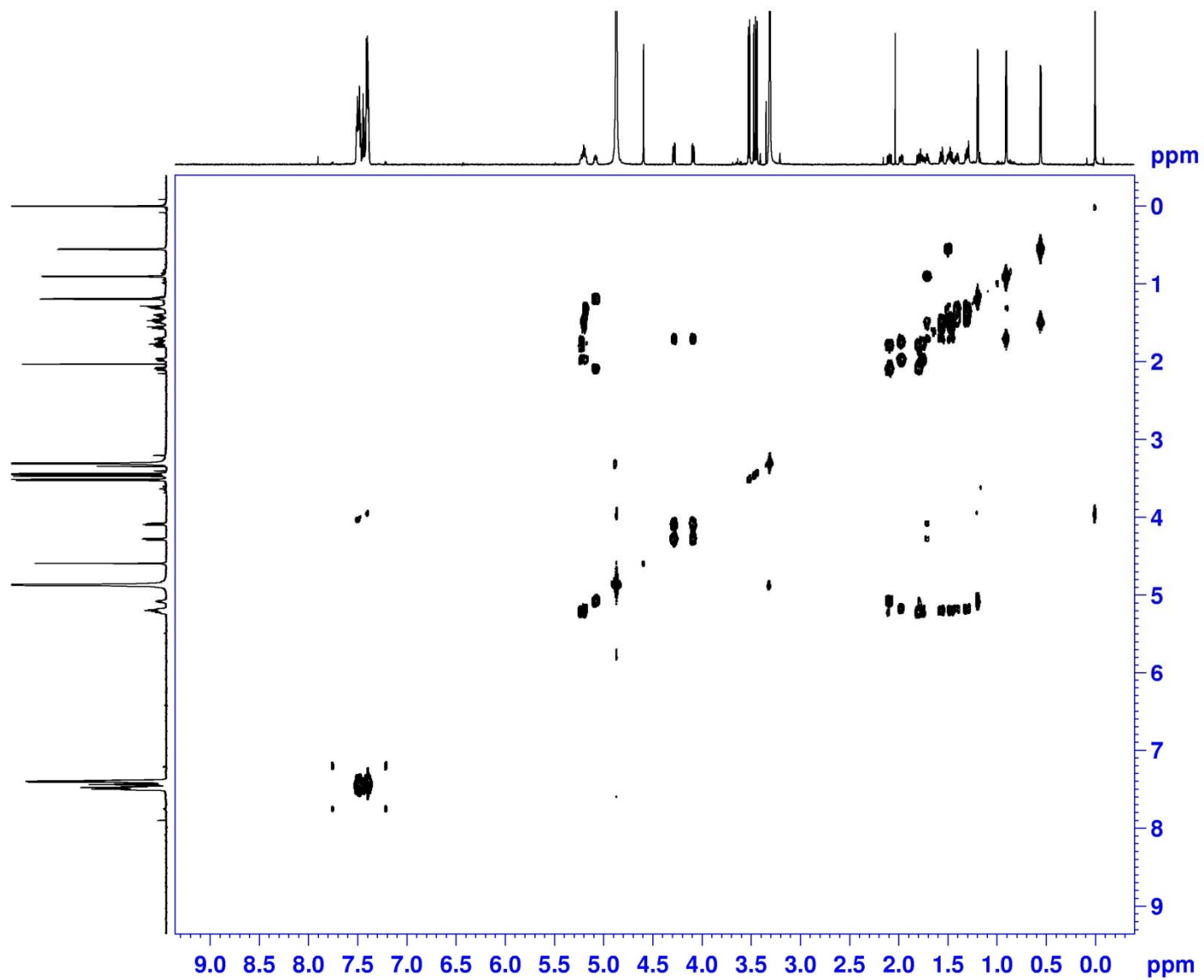
^1H (700 MHz) NMR spectrum of the fragment **1A'r** in CD_3OD



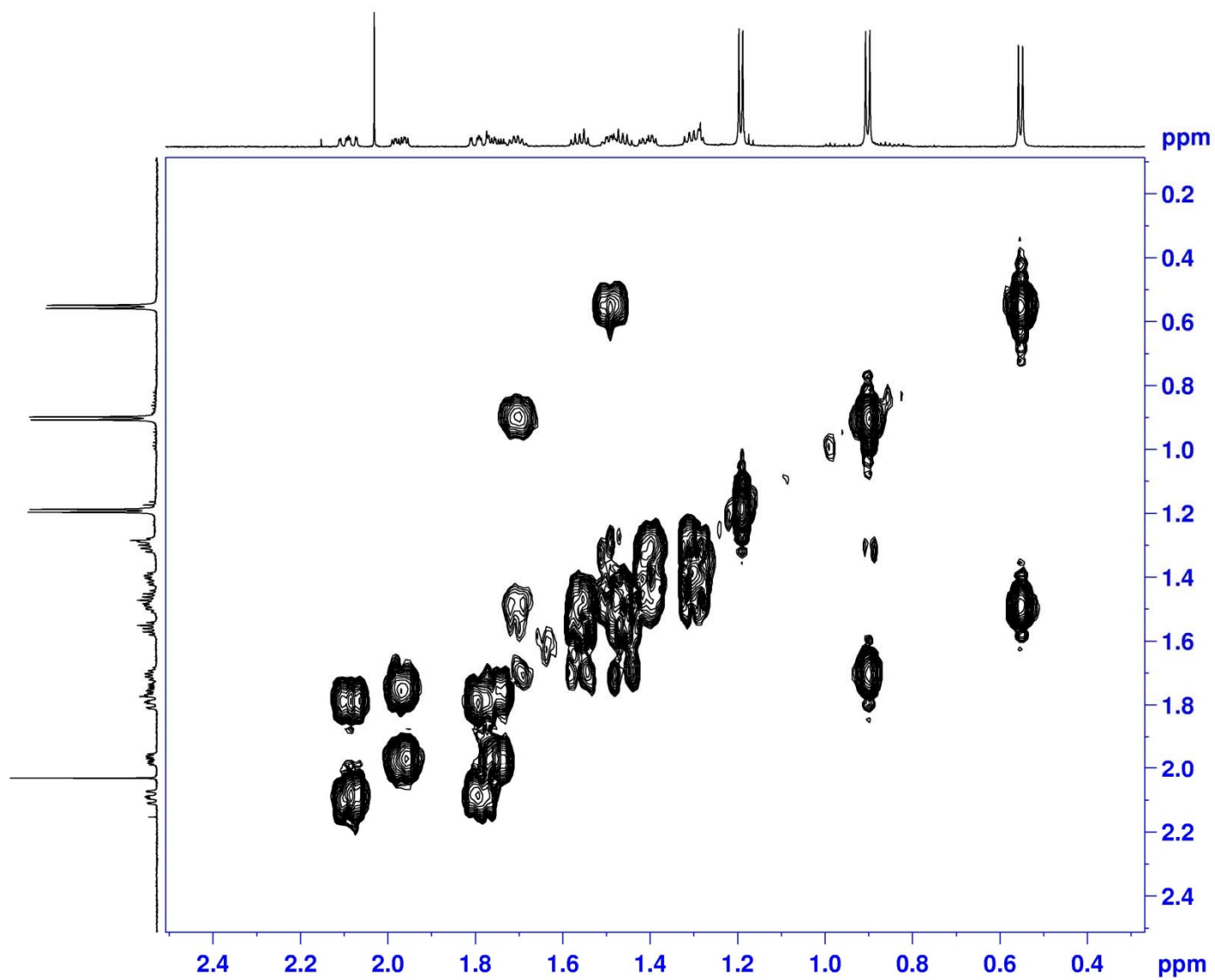
^1H (700 MHz) NMR spectrum of the fragment **1A'r** in CD_3OD



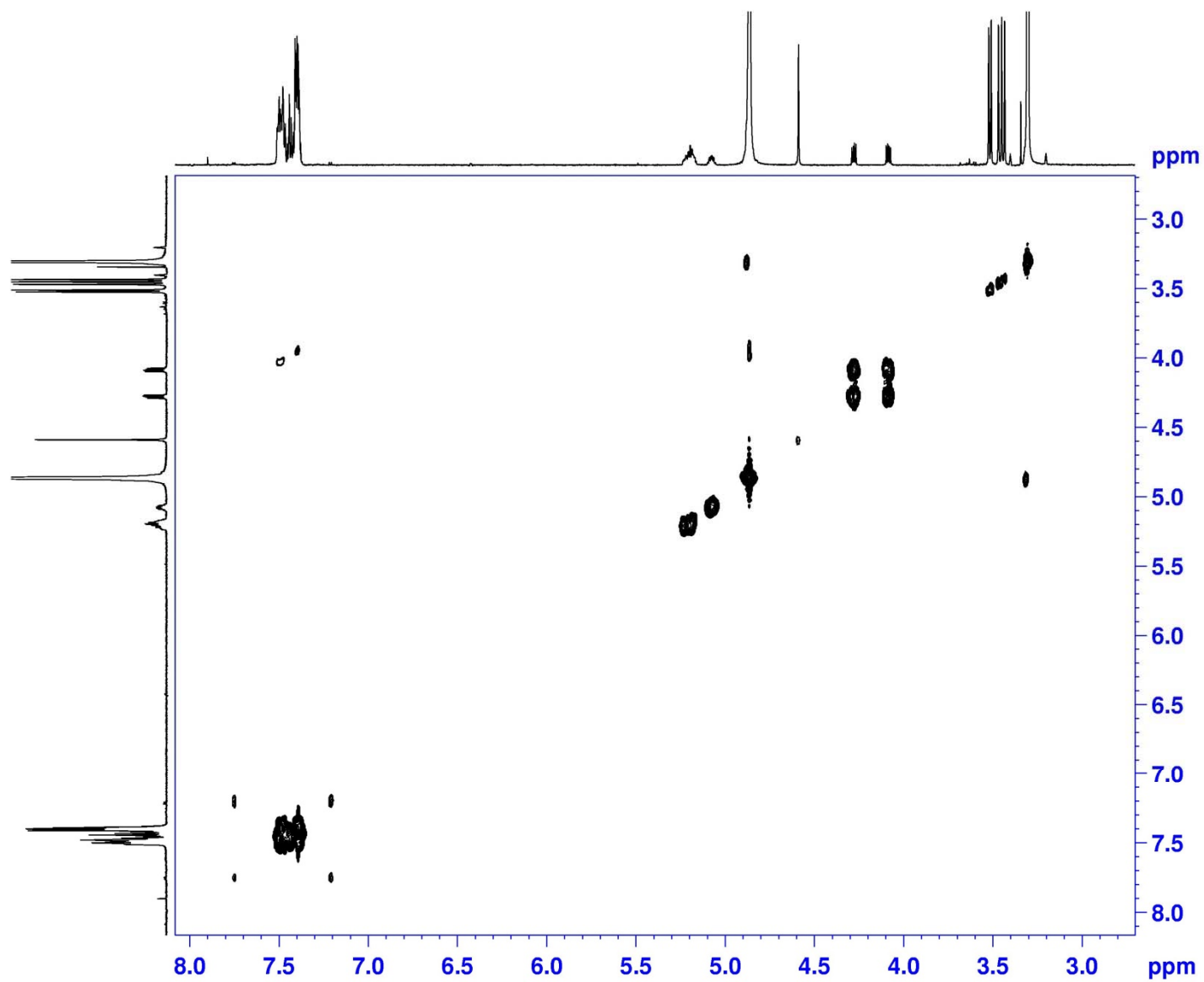
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1A'r** in CD_3OD



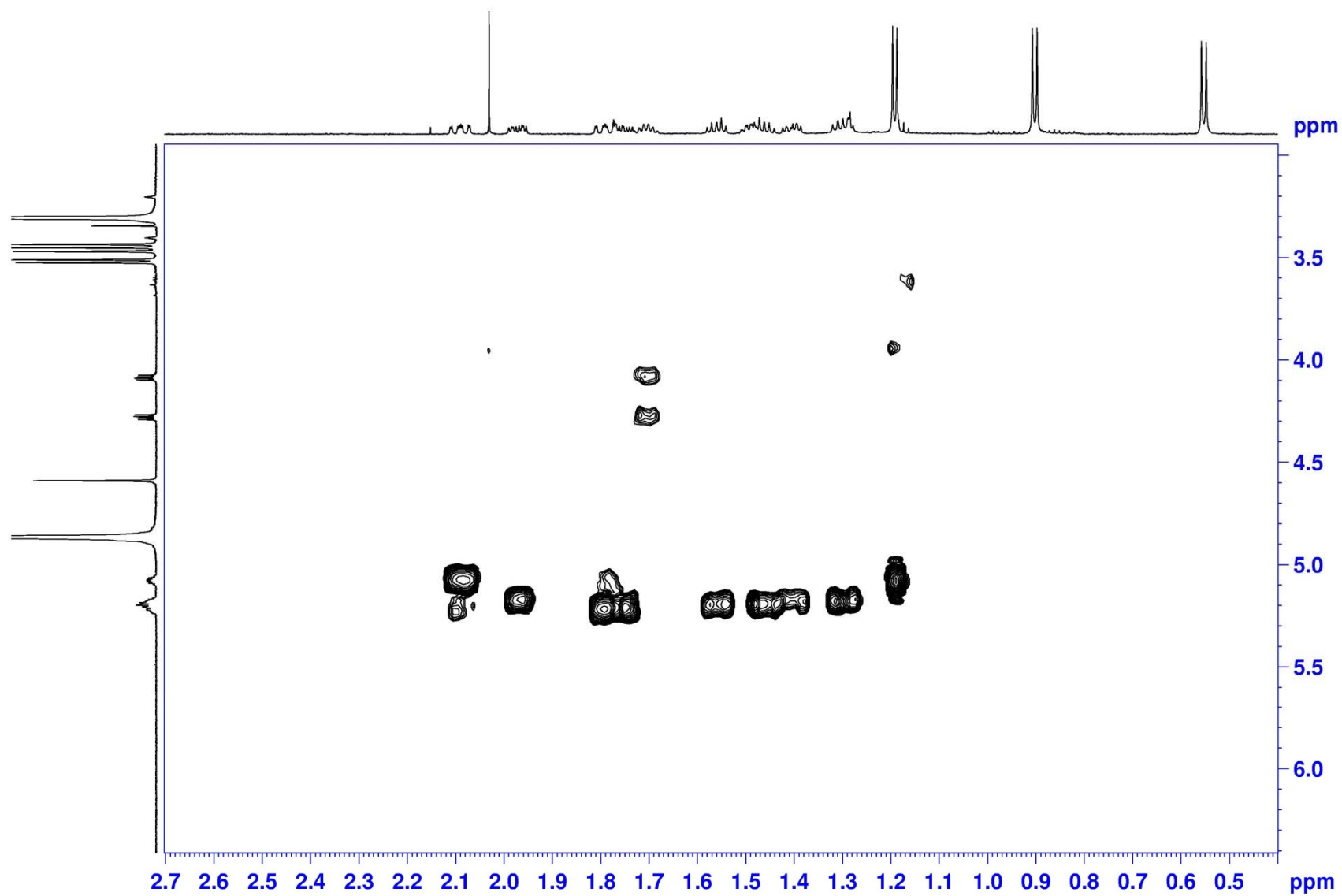
^1H - ^1H COSY (700 MHz) spectrum of the fragment **1A'r** in CD_3OD



^1H - ^1H COSY (700 MHz) spectrum of the fragment **1A'r** in CD_3OD



^1H - ^1H COSY (700 MHz) spectrum of the fragment **1A'r** in CD_3OD



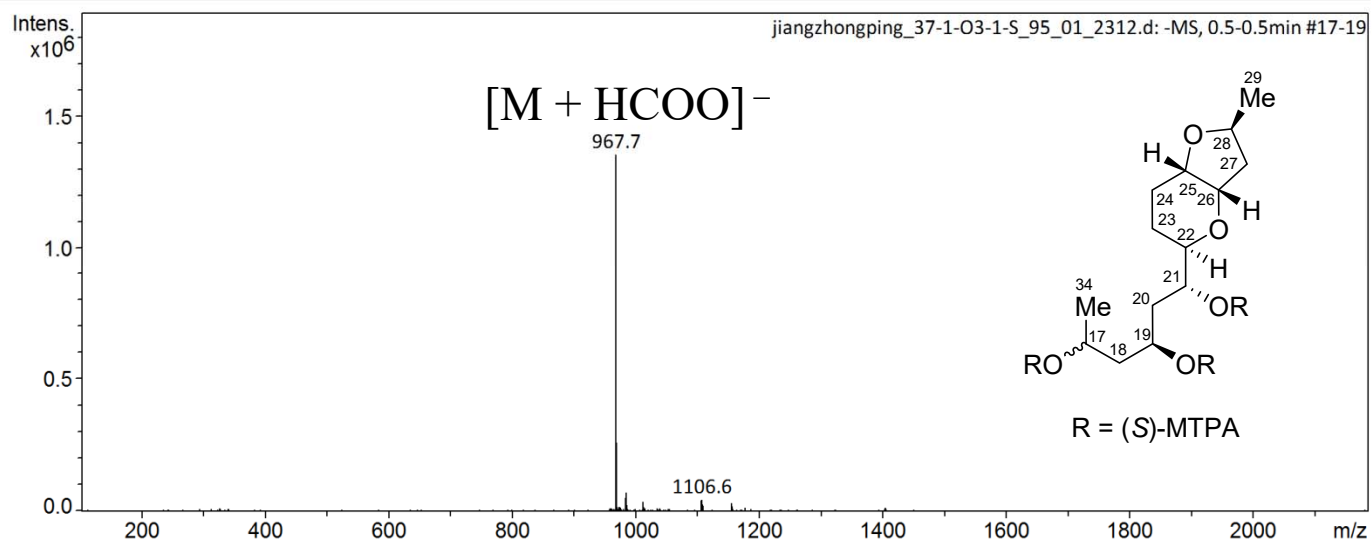
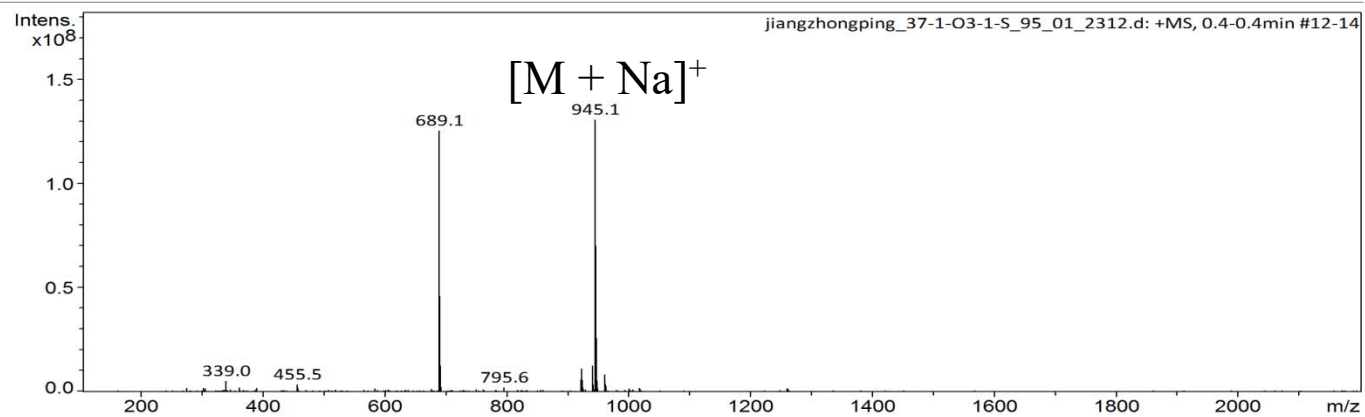
LR-ESIMS for fragments 1Bs

Generic Display Report

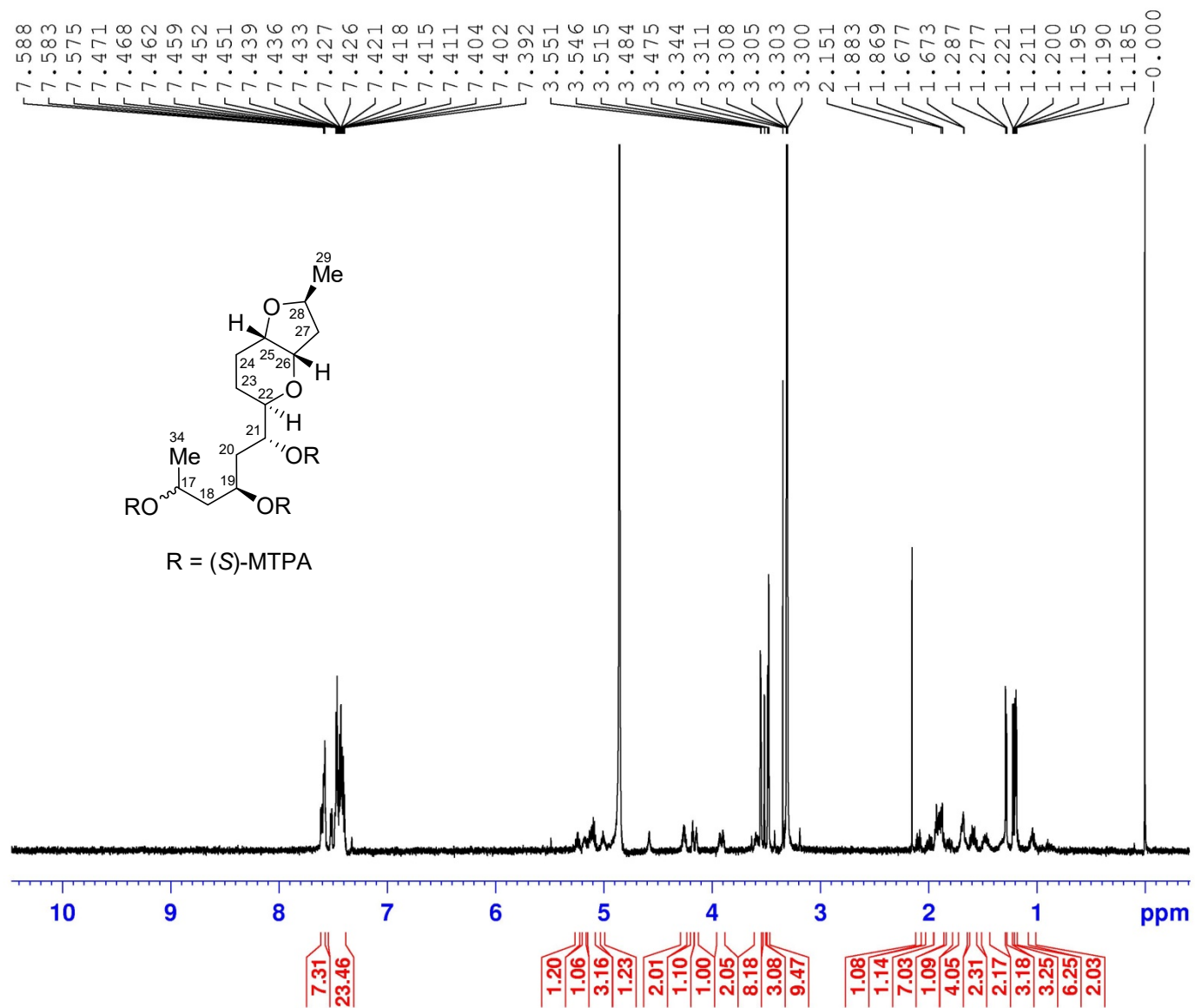
Analysis Info

Analysis Name D:\Data\amaZon SLIMS\data\202011\jiangzhongping_37-1-O3-1-S_95_01_2312.d
Method 2312.m
Sample Name jiangzhongping_37-1-O3-1-S
Comment

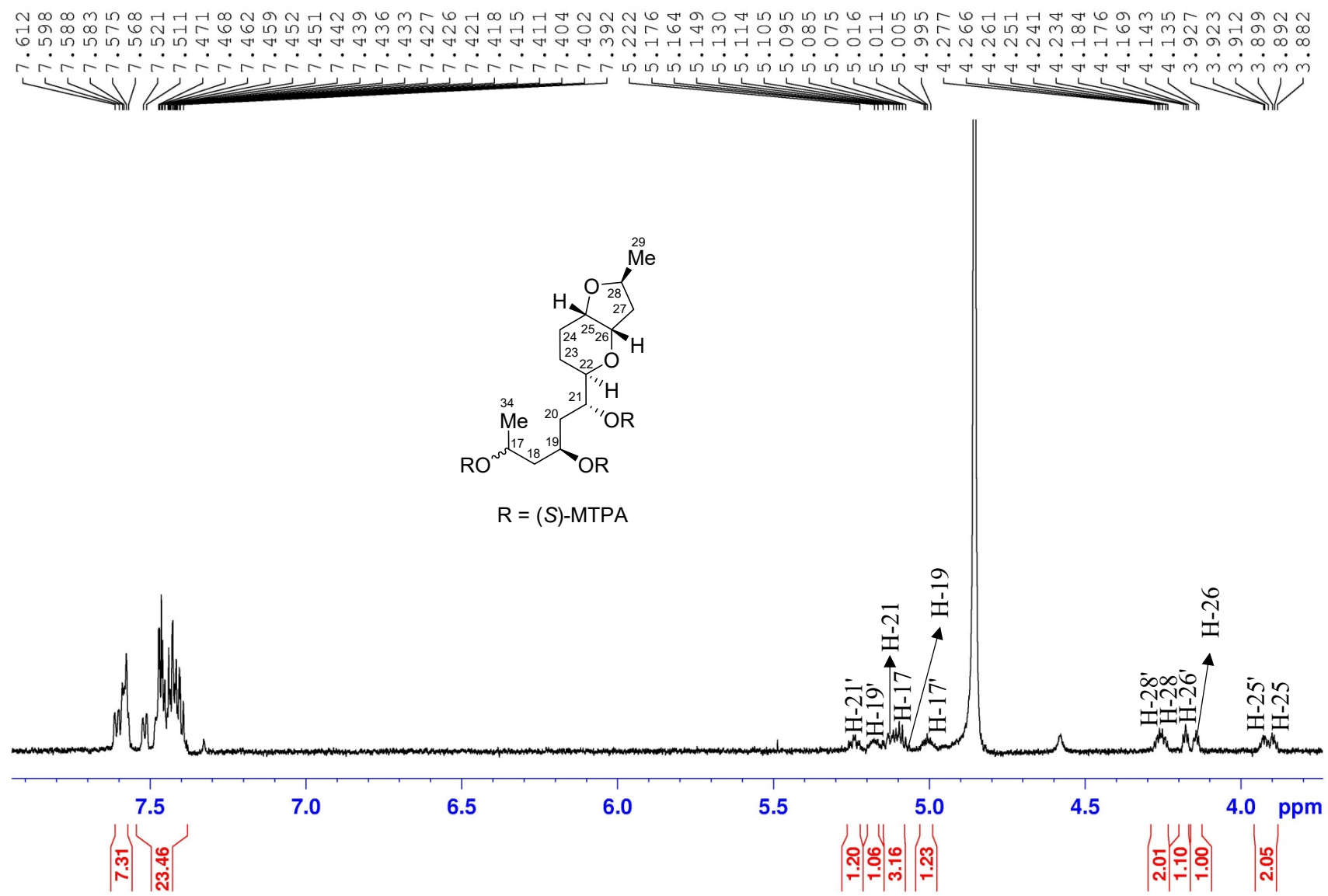
Acquisition Date 2020-11-09 15:50:13
Operator bruker
Instrument amaZon SL



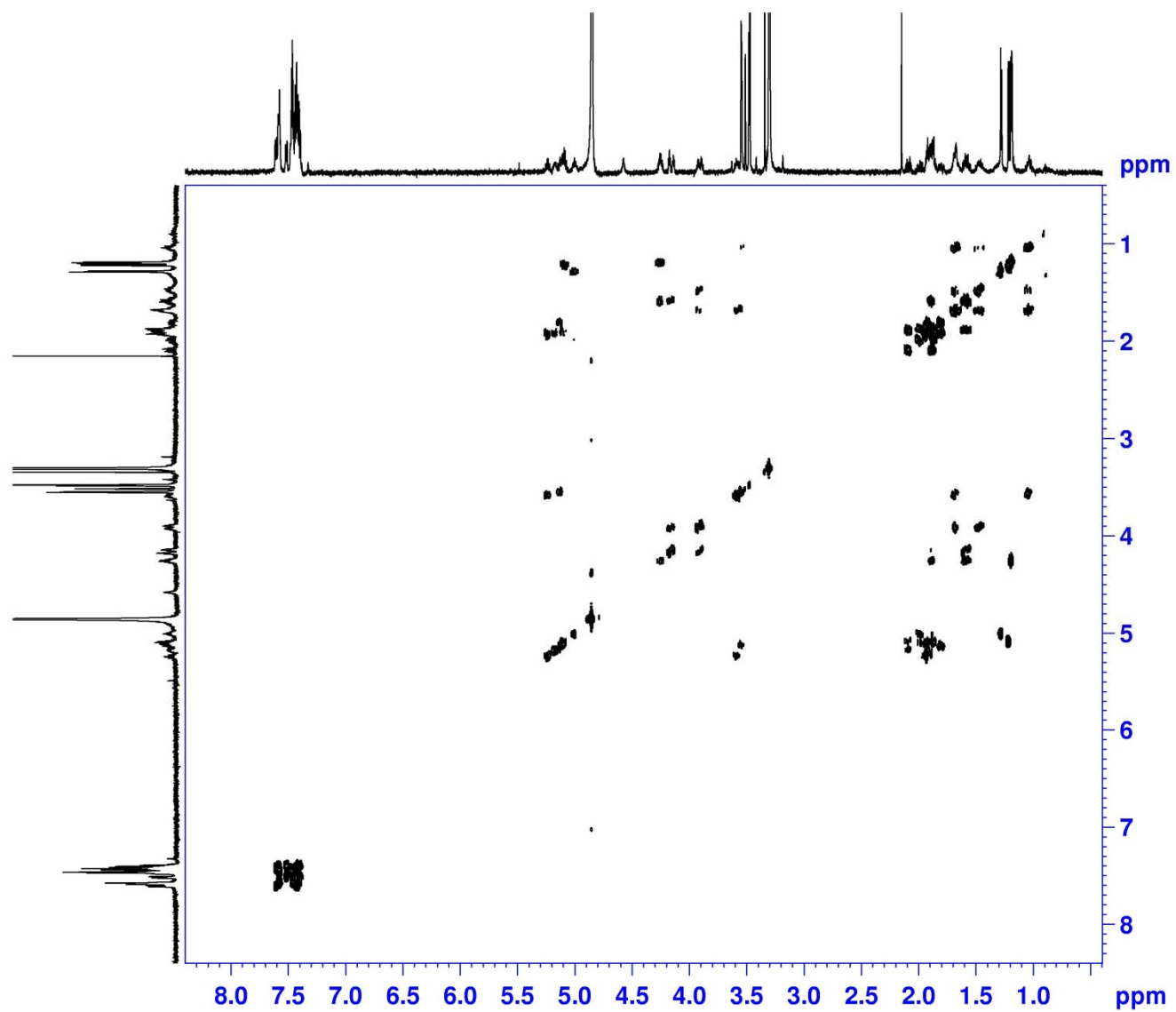
^1H (600 MHz) NMR spectrum of fragments **1Bs** in CD_3OD



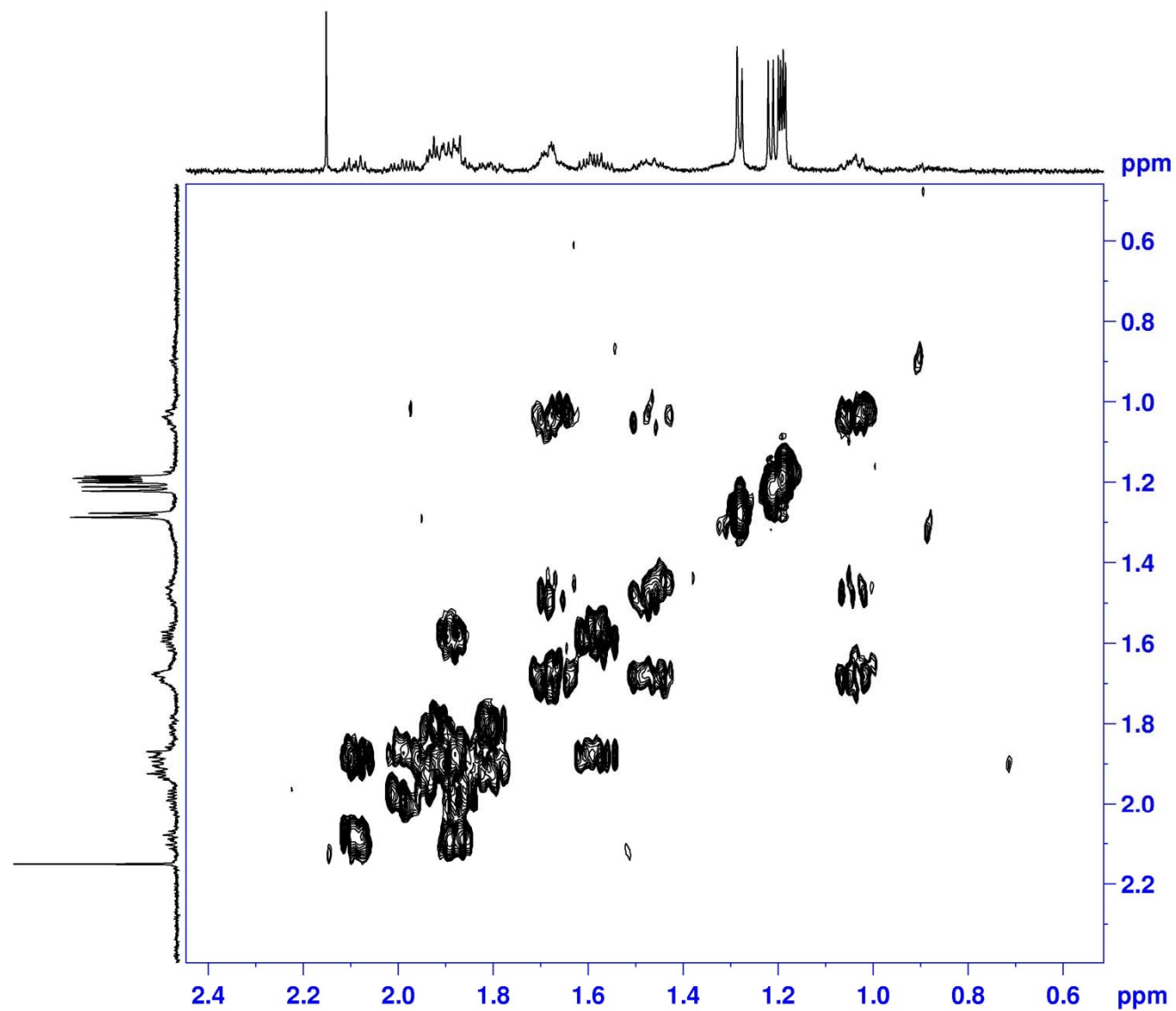
^1H (600 MHz) NMR spectrum of fragments **1Bs** in CD_3OD



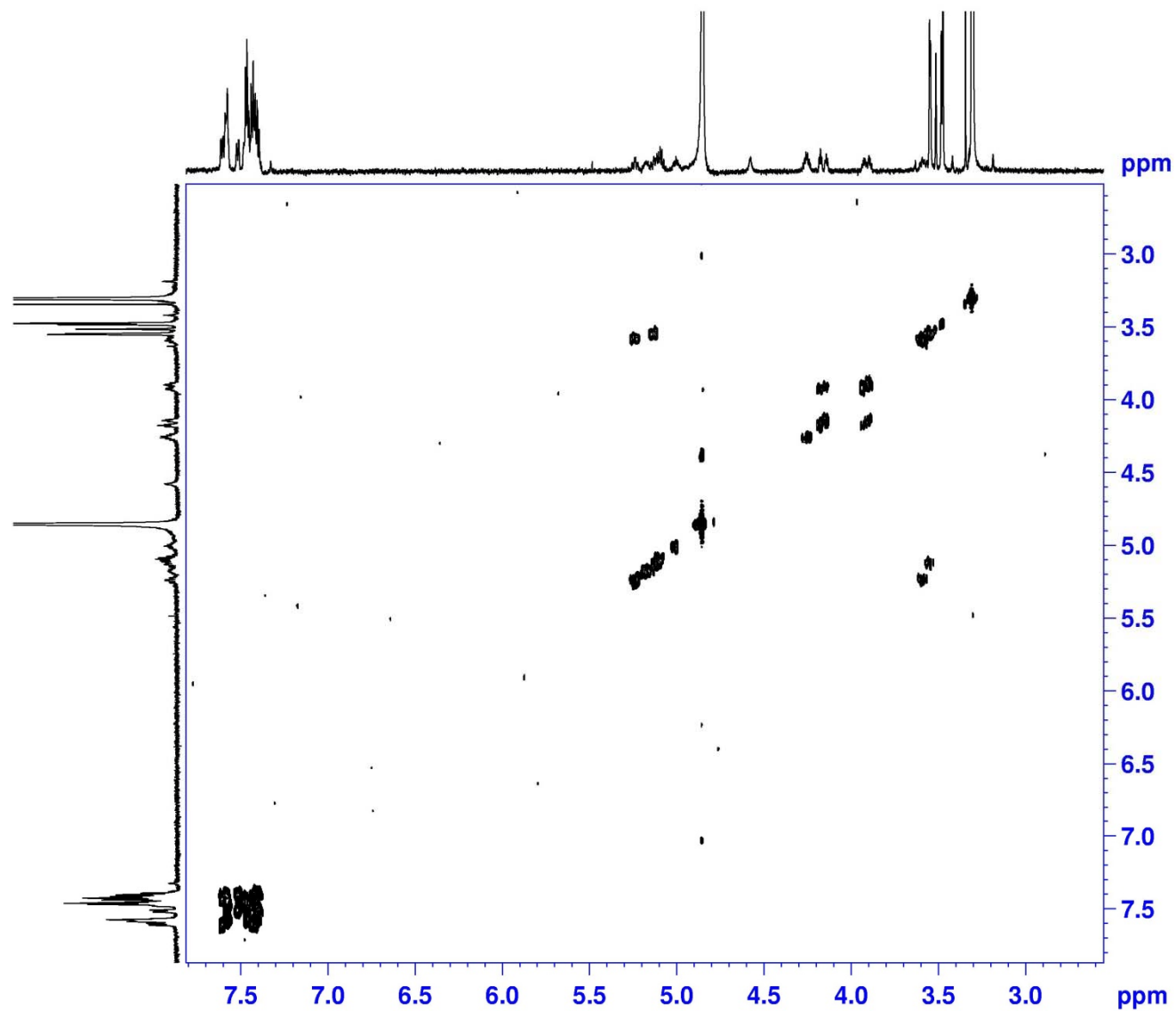
^1H - ^1H COSY (600 MHz) spectrum of fragments **1Bs** in CD_3OD



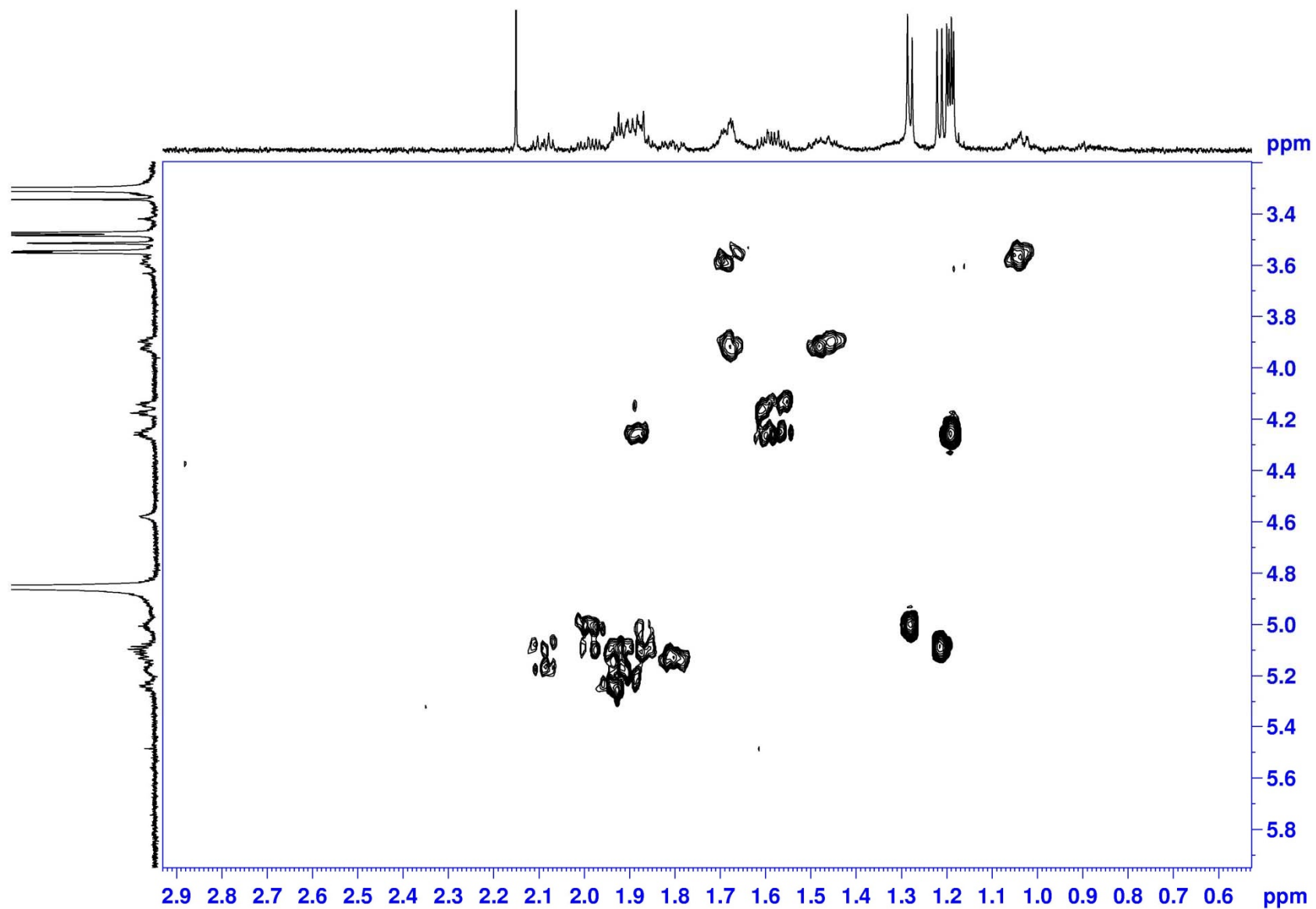
^1H - ^1H COSY (600 MHz) spectrum of fragments **1Bs** in CD_3OD



^1H - ^1H COSY (600 MHz) spectrum of fragments **1Bs** in CD_3OD



^1H - ^1H COSY (600 MHz) spectrum of fragments **1Bs** in CD_3OD

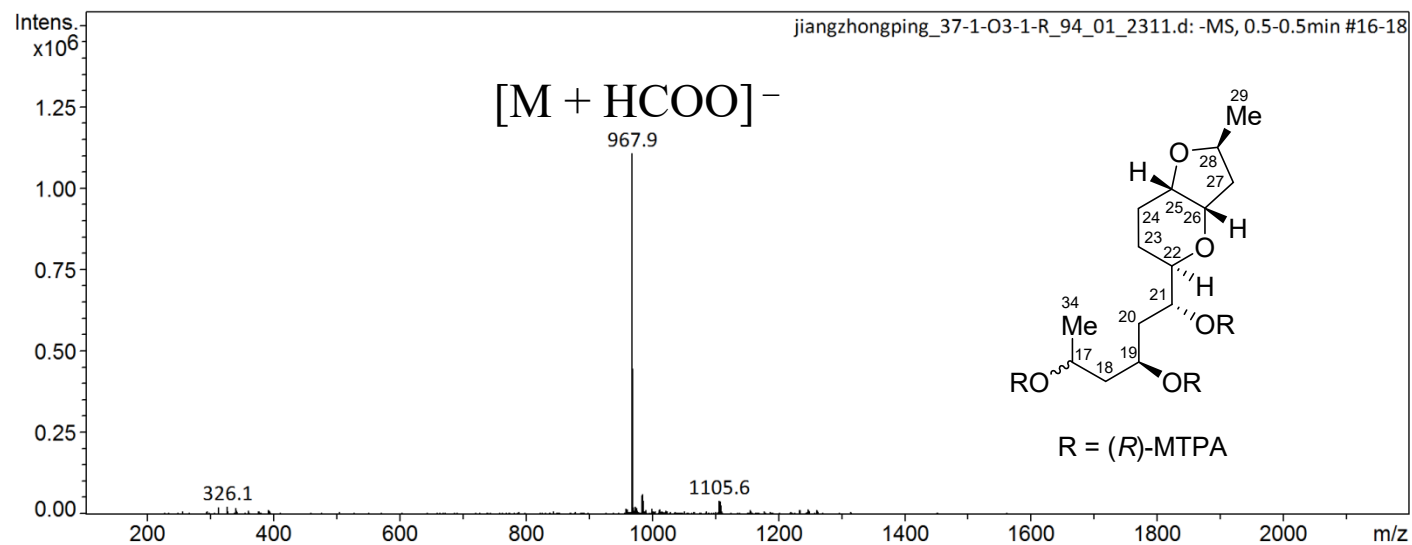
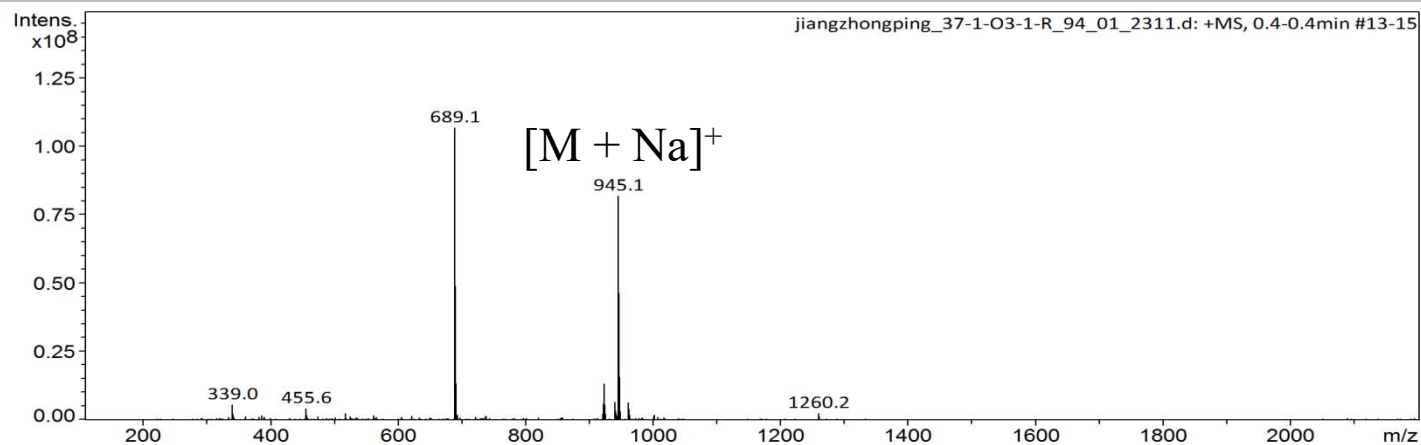


LR-ESIMS for fragments 1Br

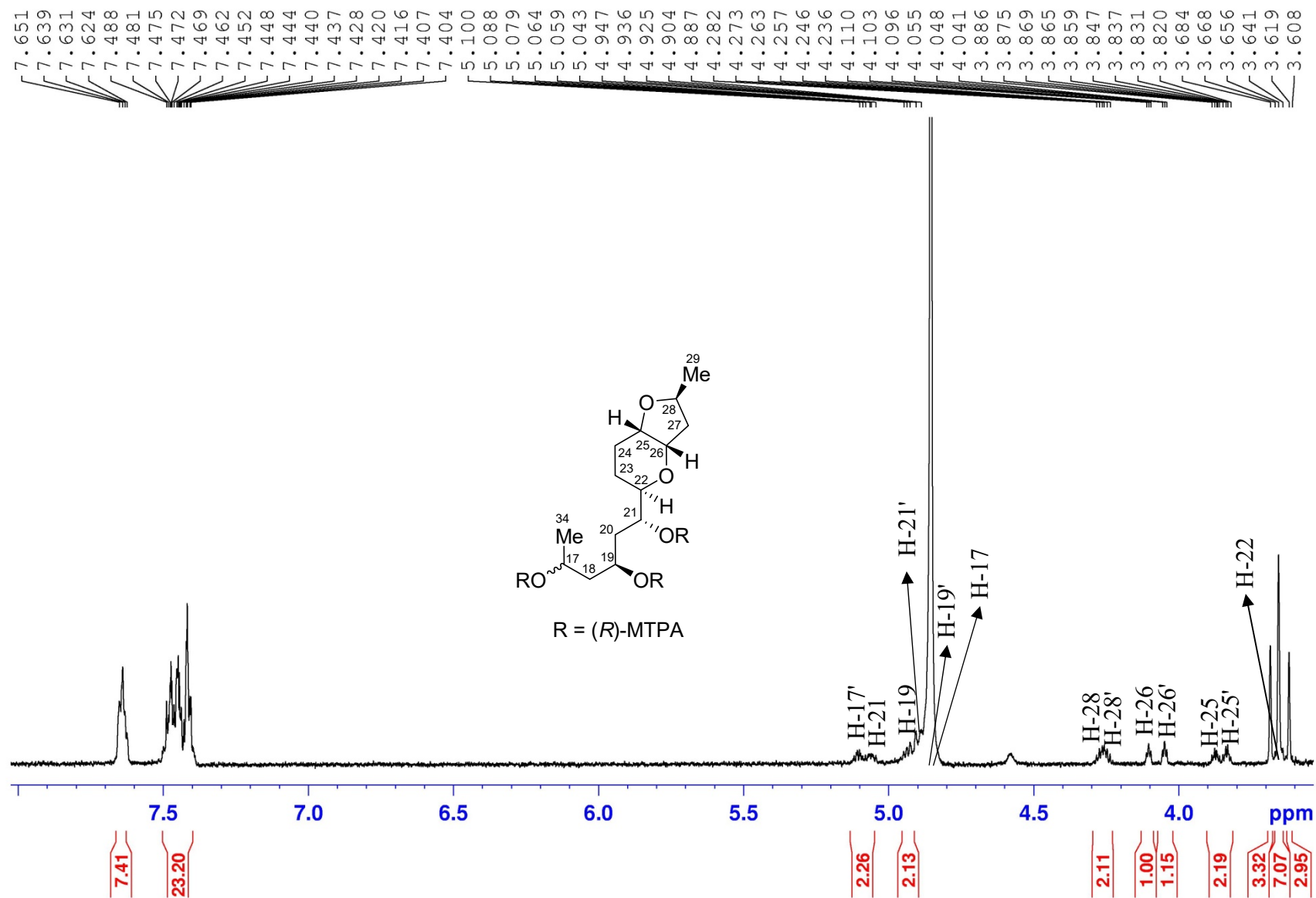
Generic Display Report

Analysis Info

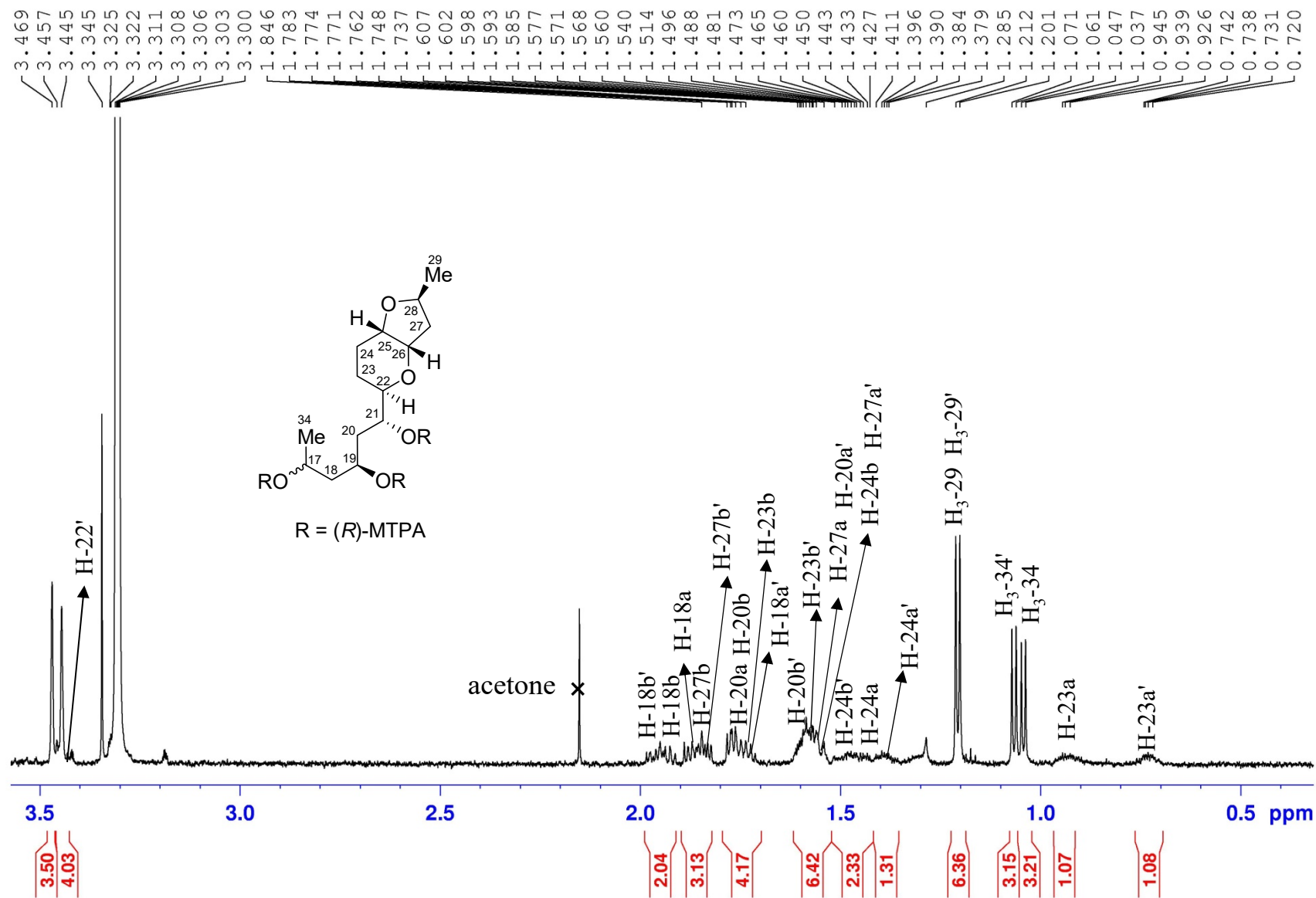
Analysis Name	D:\Data\amaZon SL\MS\data\202011\jiangzhongping_37-1-O3-1-R_94_01_2311.d	Acquisition Date	2020-11-09 15:47:49
Method	2311.m	Operator	bruker
Sample Name	jiangzhongping_37-1-O3-1-R	Instrument	amaZon SL
Comment			



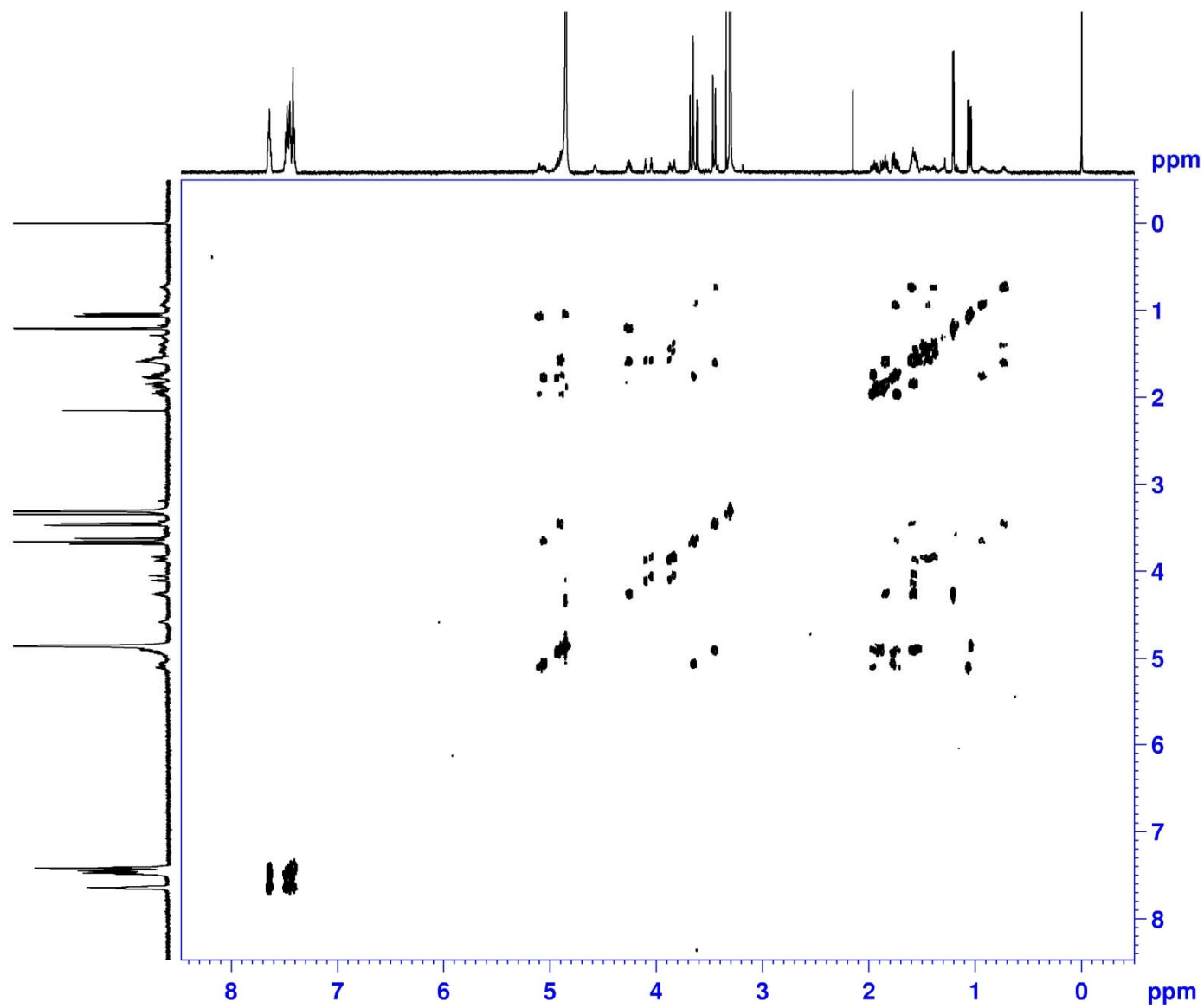
^1H (600 MHz) NMR spectrum of fragments **1Br** in CD_3OD



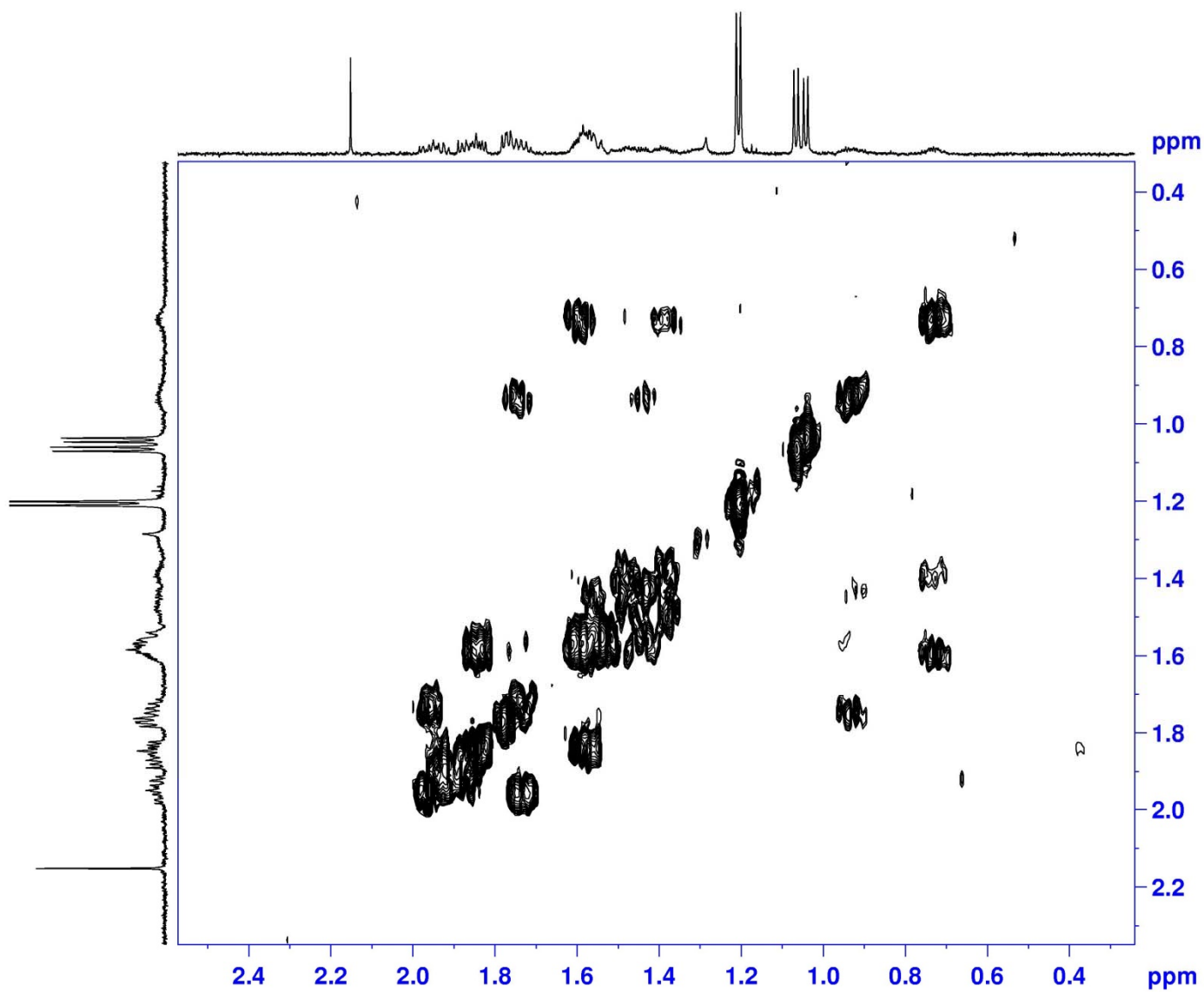
^1H (600 MHz) NMR spectrum of fragments **1Br** in CD_3OD



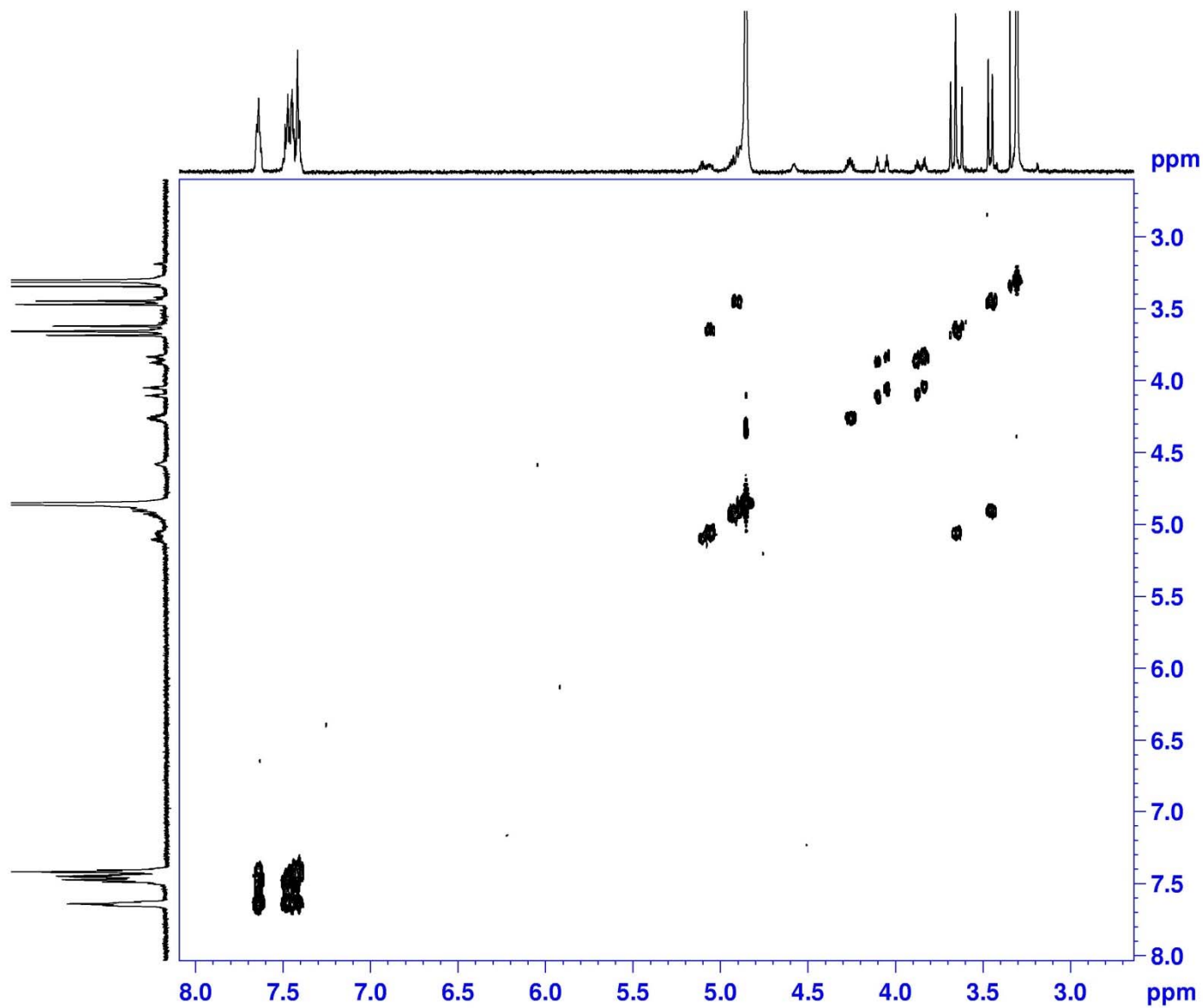
^1H - ^1H COSY (600 MHz) spectrum of fragments **1Br** in CD_3OD



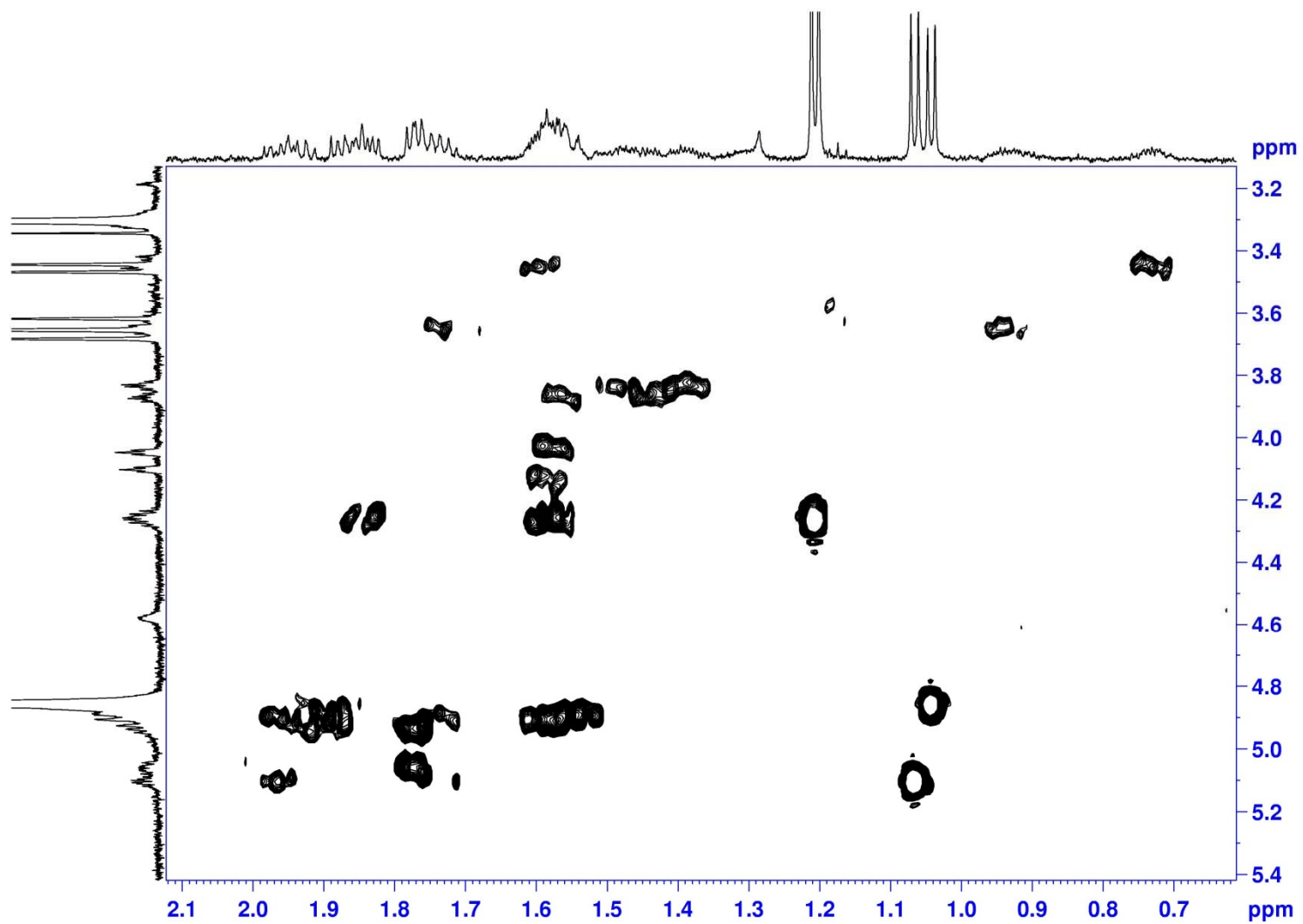
^1H - ^1H COSY (600 MHz) spectrum of fragments **1Br** in CD_3OD



^1H - ^1H COSY (600 MHz) spectrum of fragments **1Br** in CD_3OD



^1H - ^1H COSY (600 MHz) spectrum of fragments **1Br** in CD_3OD



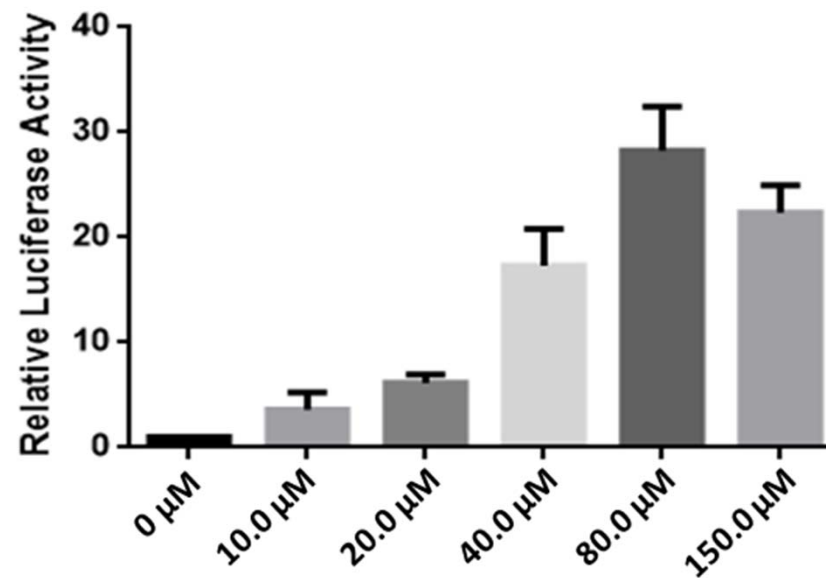


Figure S1. Agonistic effects of chenodeoxycholic acid (the positive control) on hFXR in HepG2 cells