Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

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:

HR-ESIMS for compound **1**

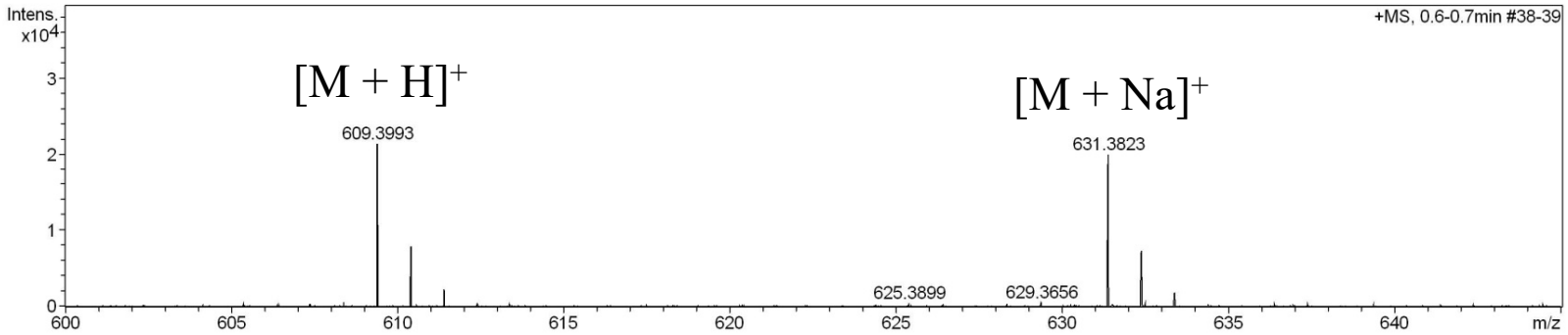
Mass Spectrum SmartFormula Report

Analysis Info

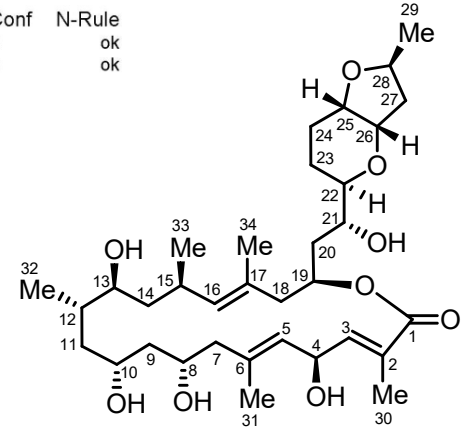
Analysis Name	D:\Data\MS\data\201905\liwanshan_2-37_pos_35_01_6636.d	Acquisition Date	5/14/2019 4:36:58 PM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	liwanshan_2-37_pos	Instrument	maXis 255552.00029
Comment			

Acquisition Parameter

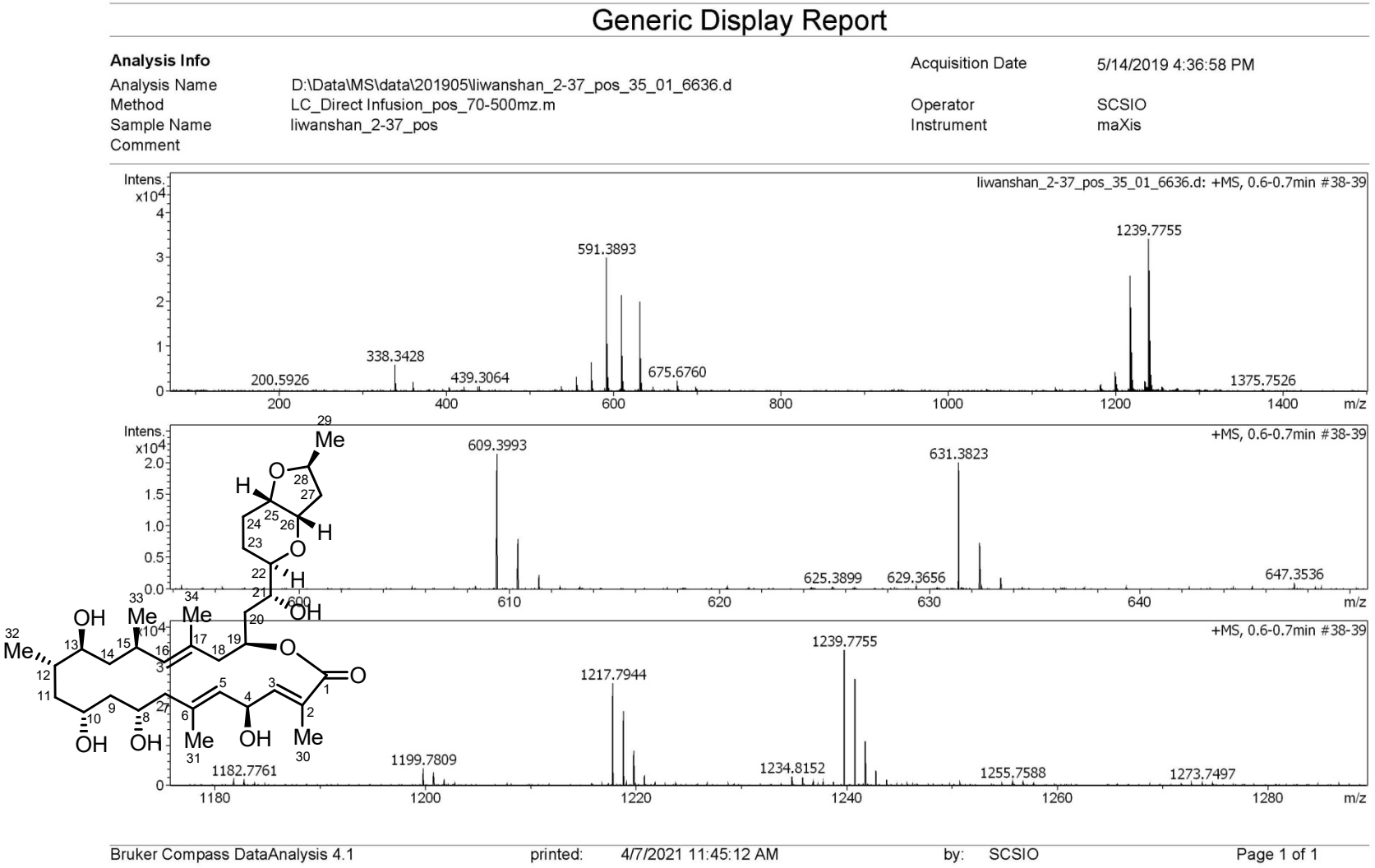
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	70 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



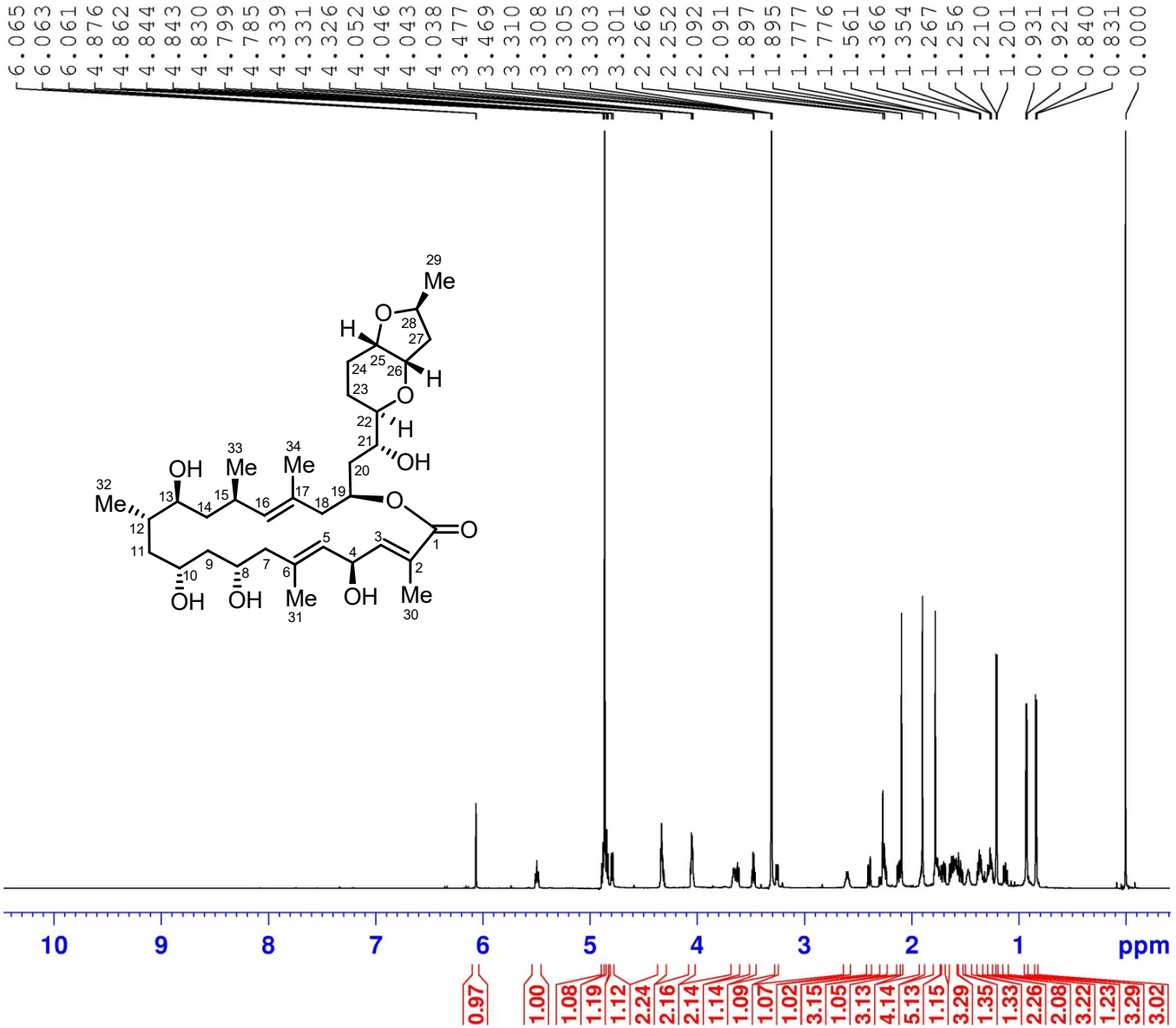
Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
609.3993	1	C34H57O9	100.00	609.3997	-0.6	-0.4	9.0	6.5	even	ok
631.3823	1	C34H56NaO9	100.00	631.3817	1.0	0.6	5.6	6.5	even	ok



HR-ESIMS for compound **1**



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



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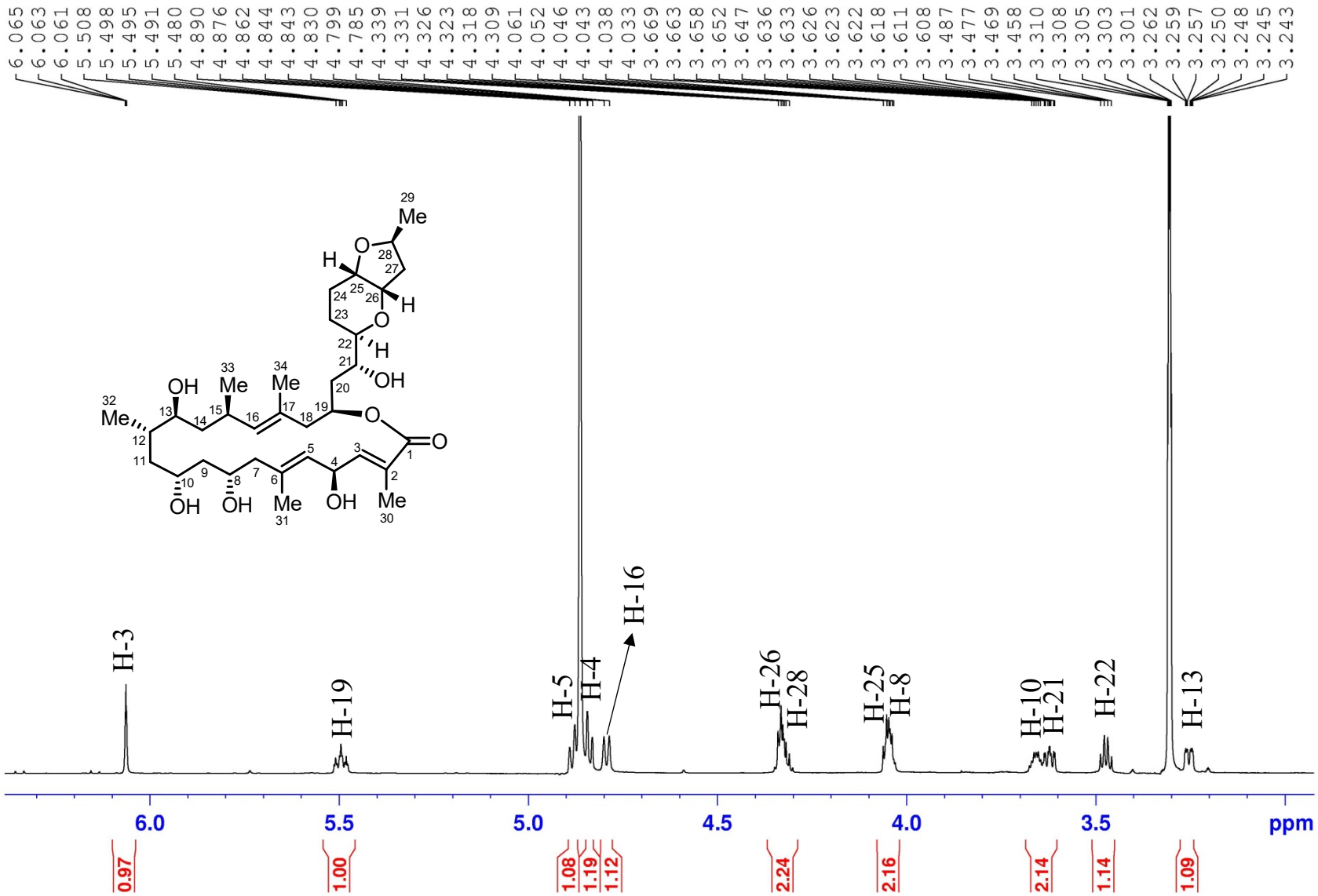

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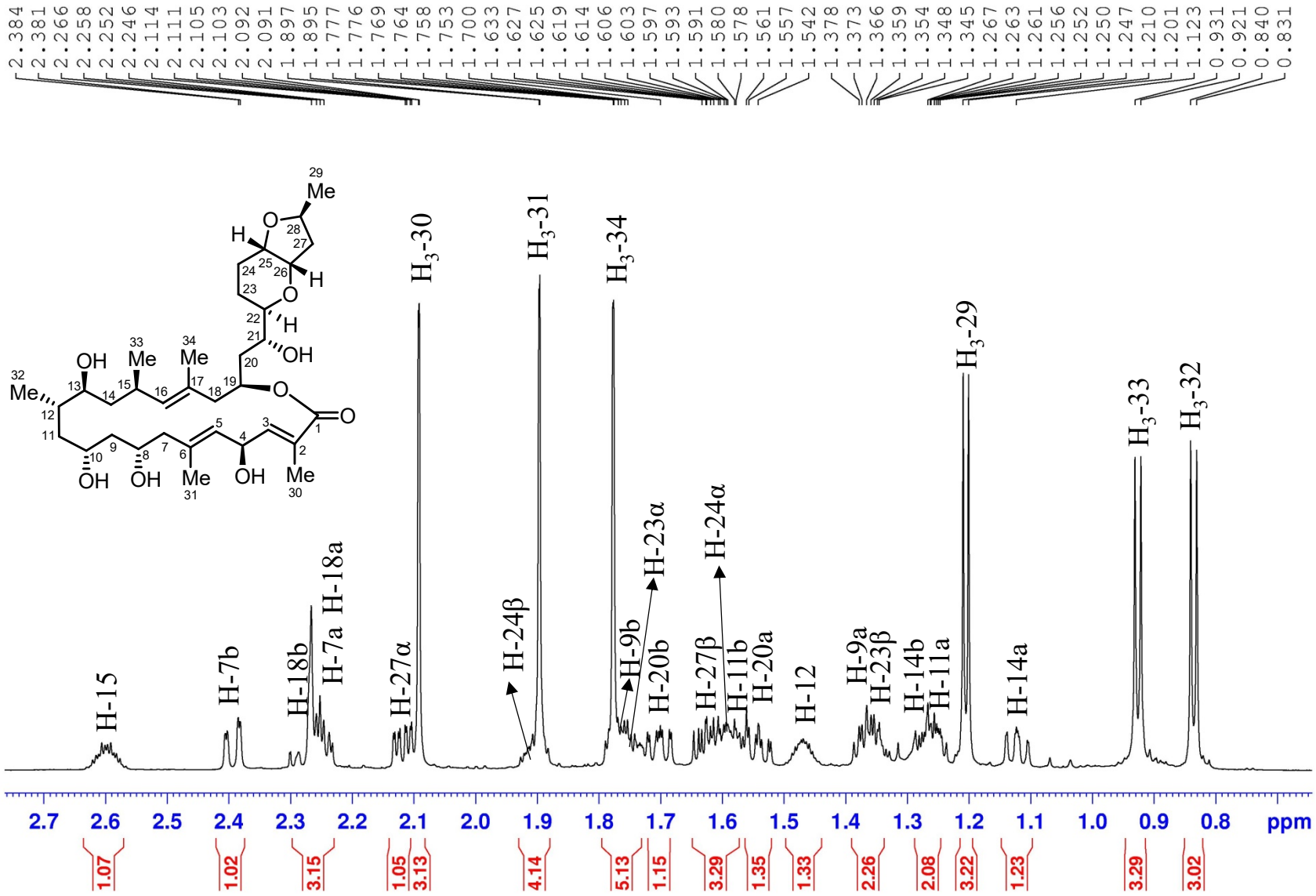
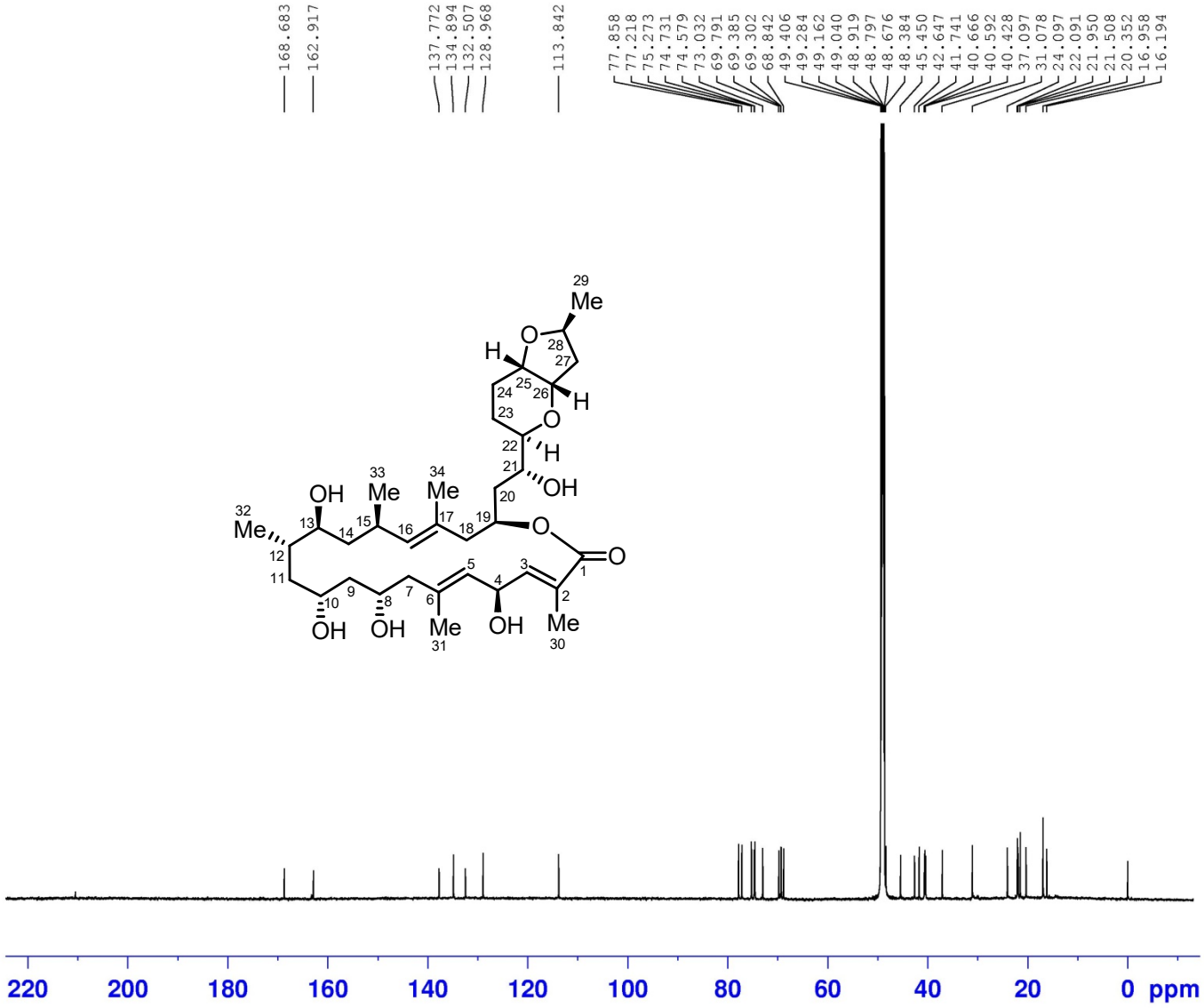
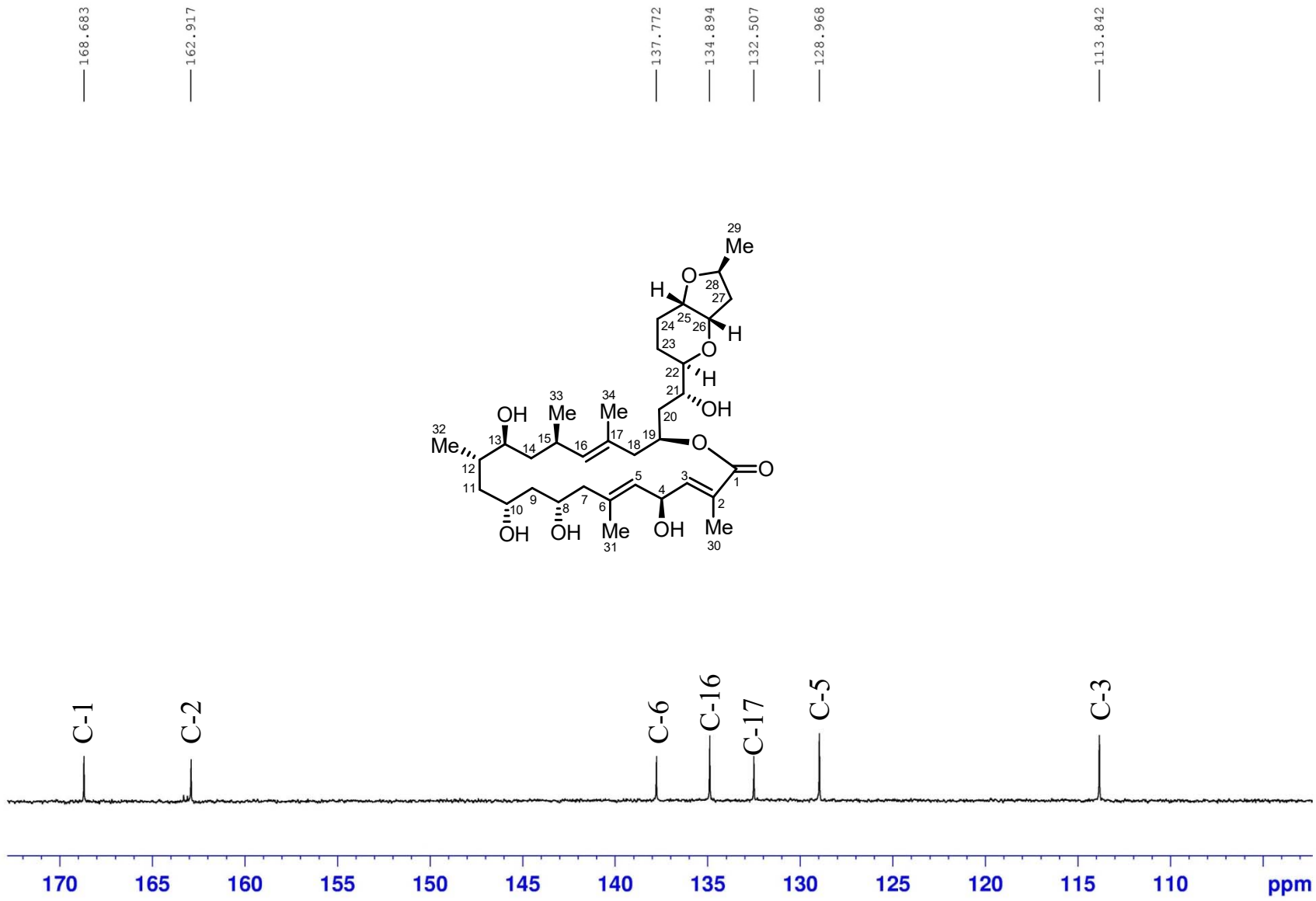


^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



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



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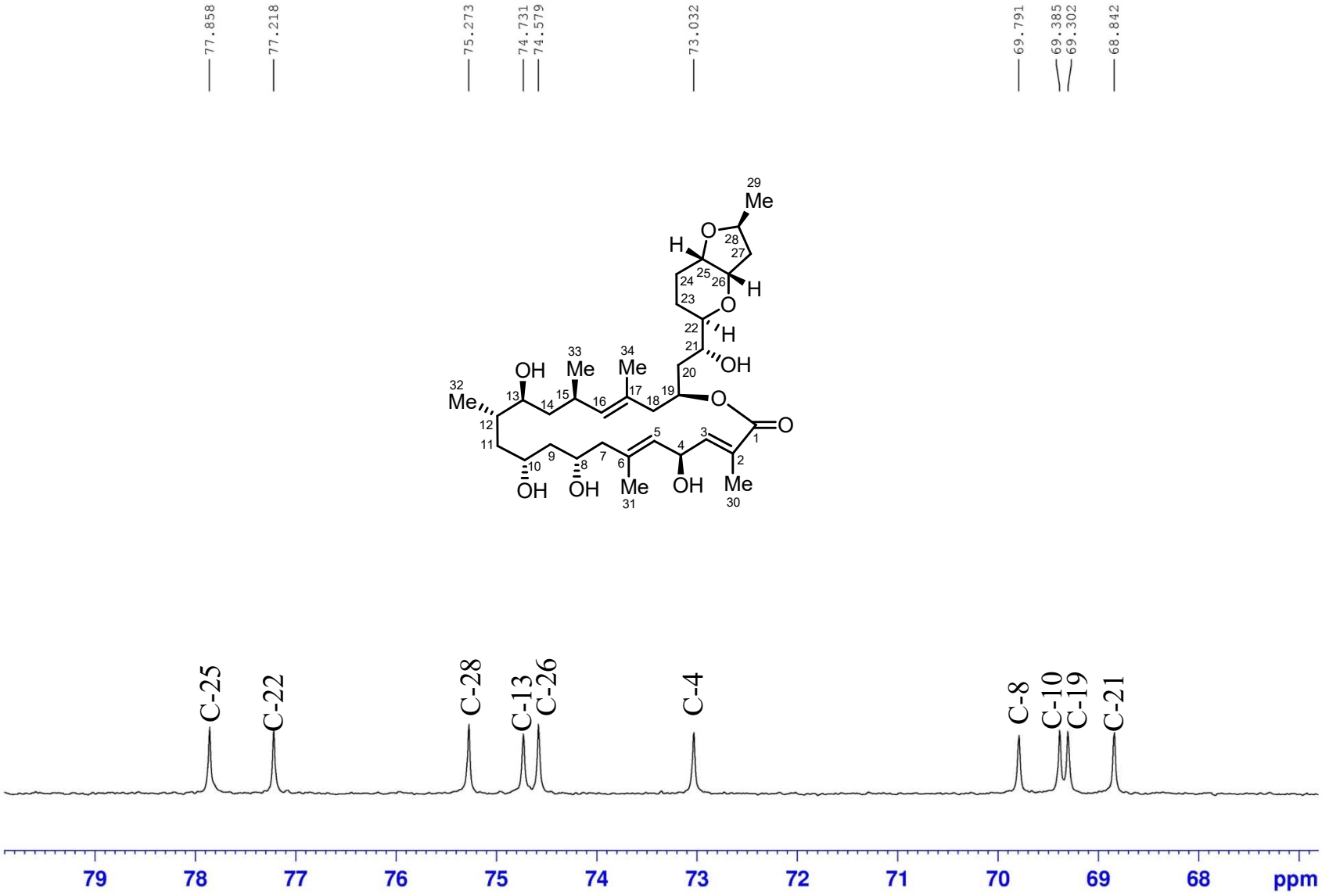
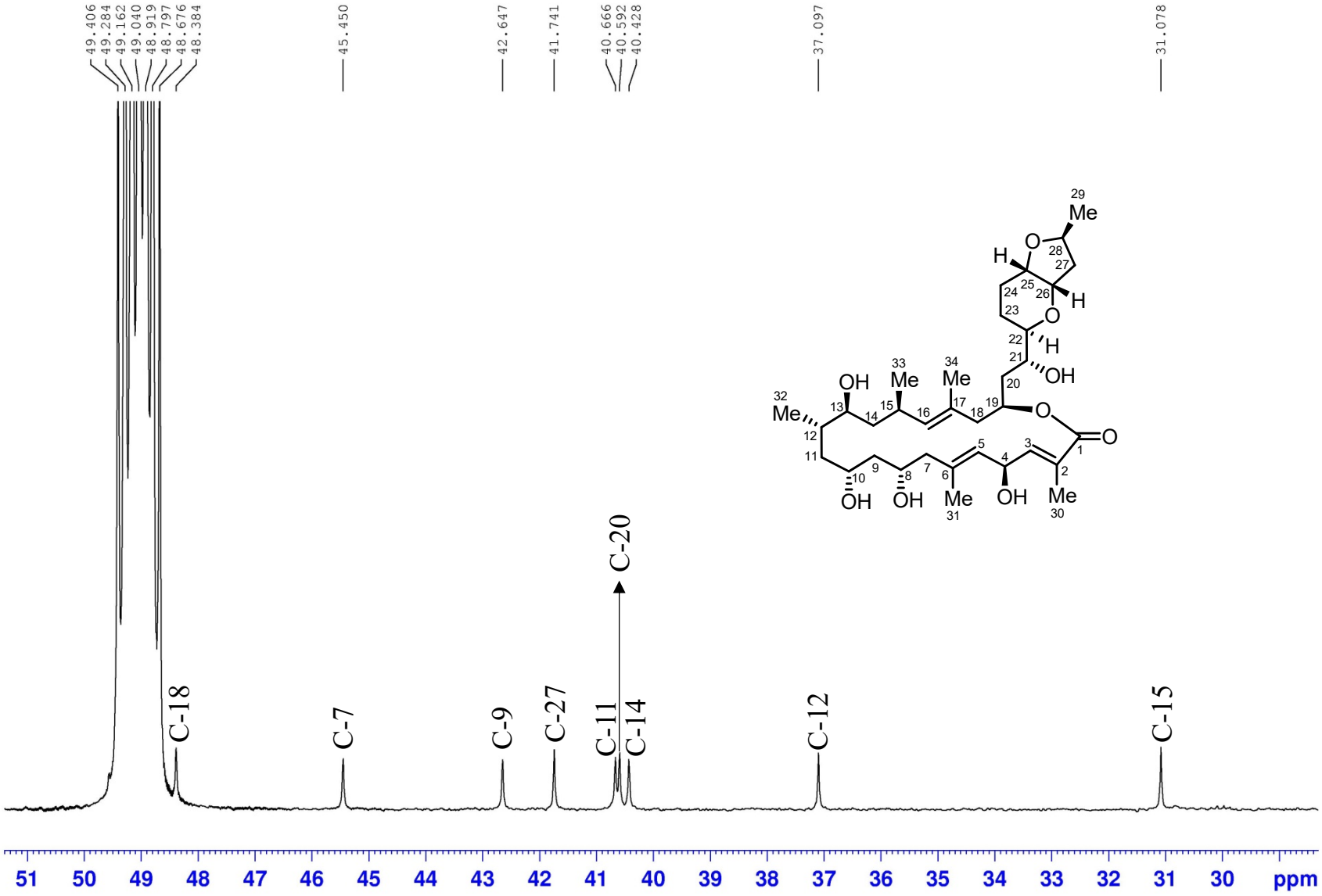
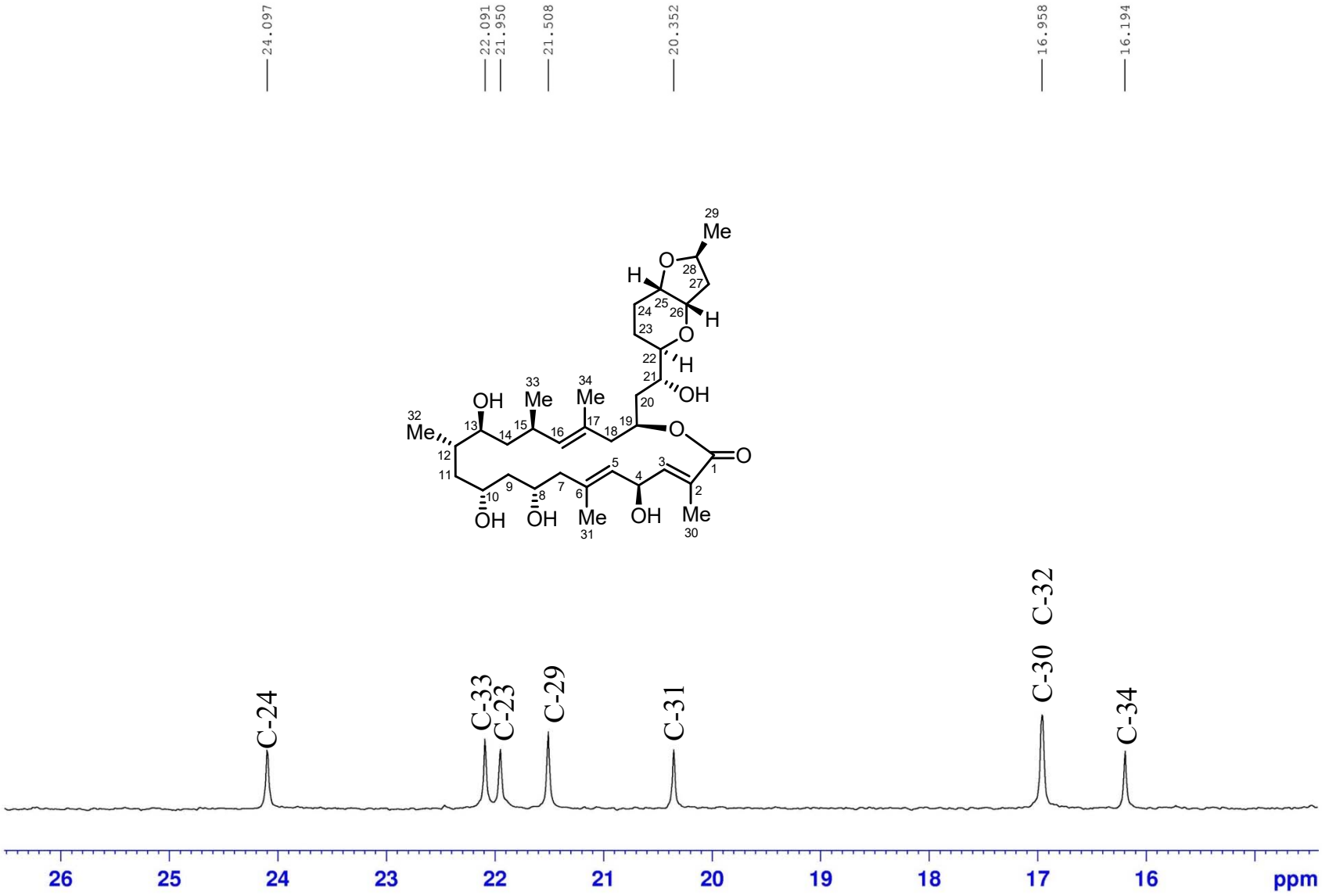


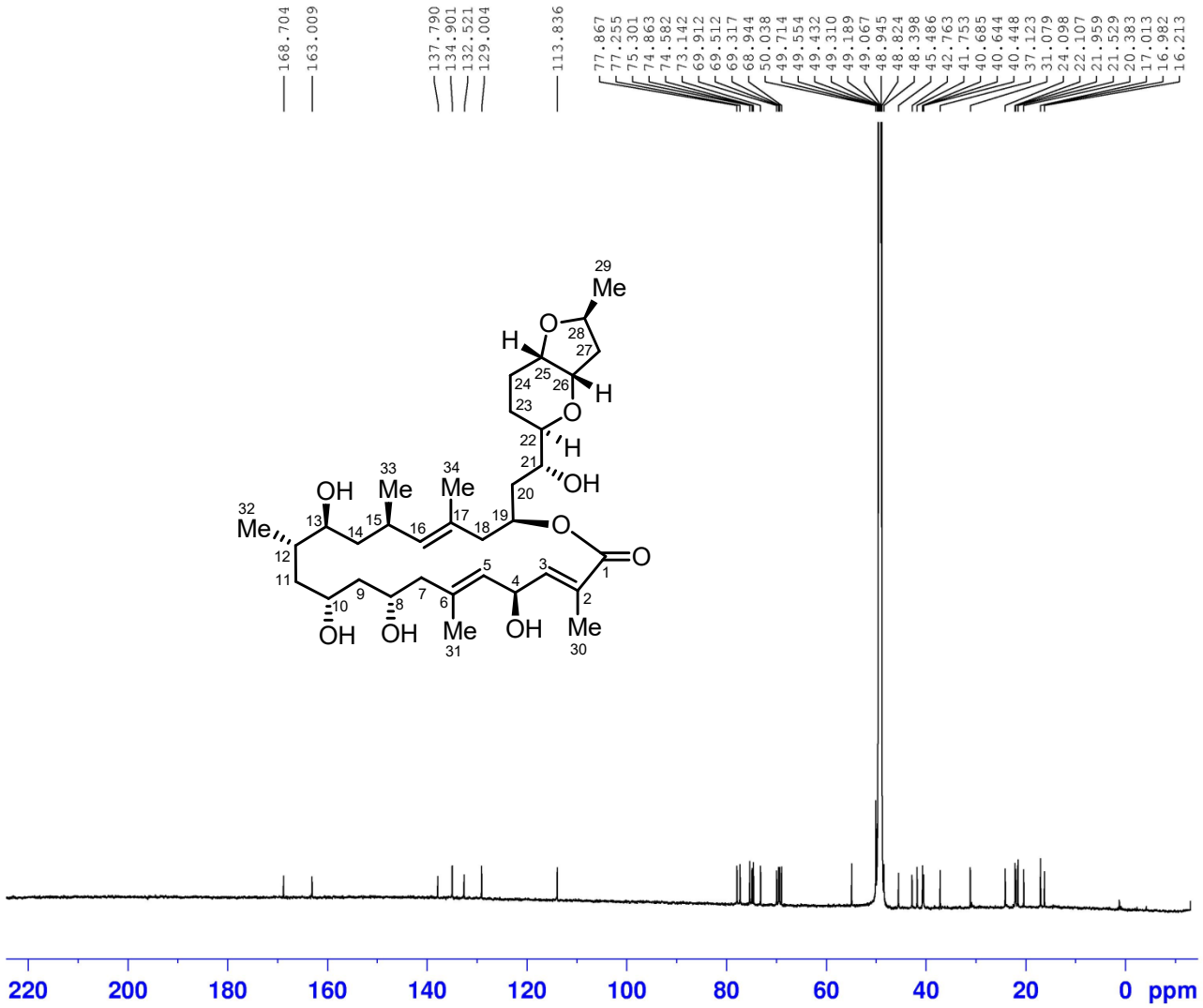
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



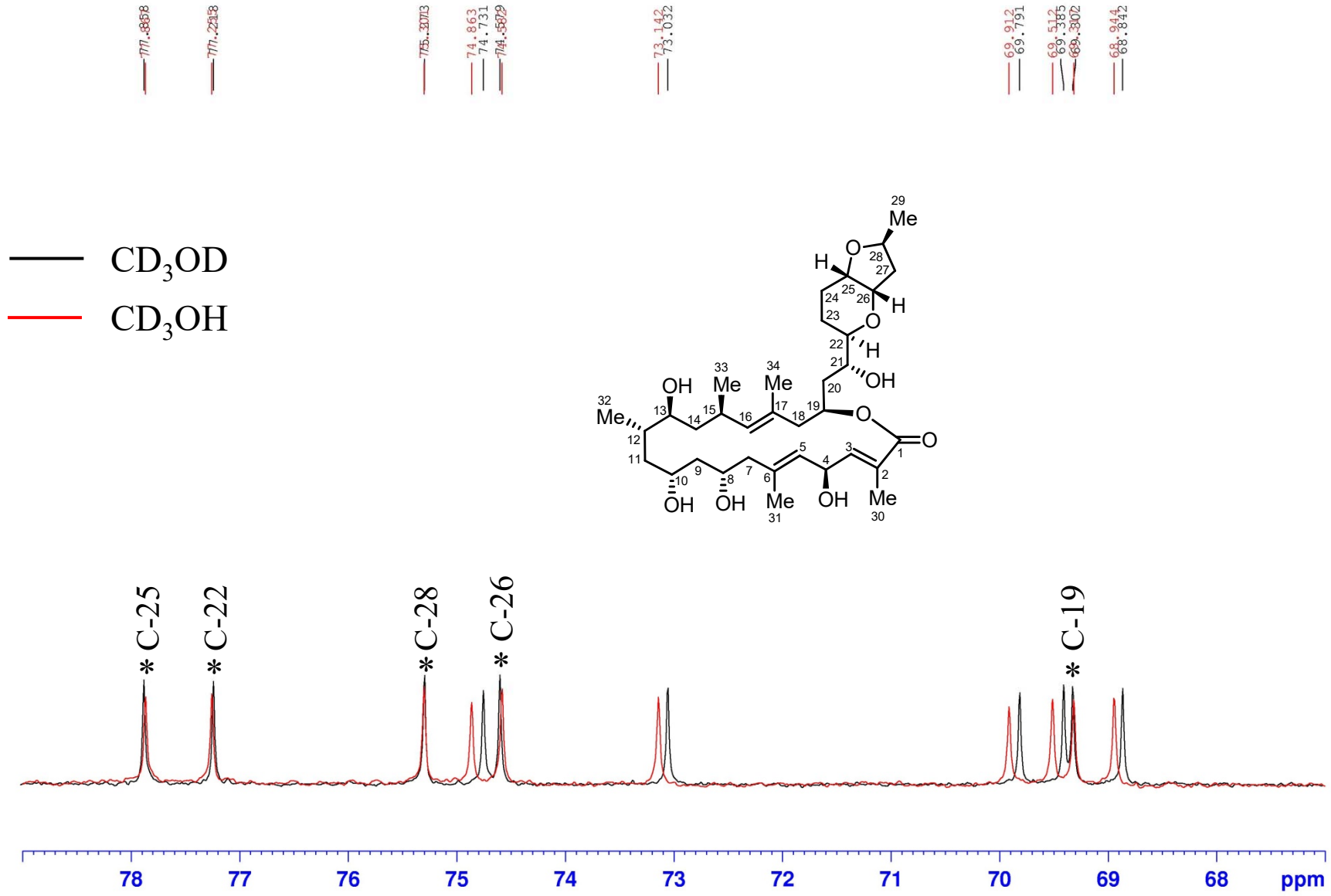
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



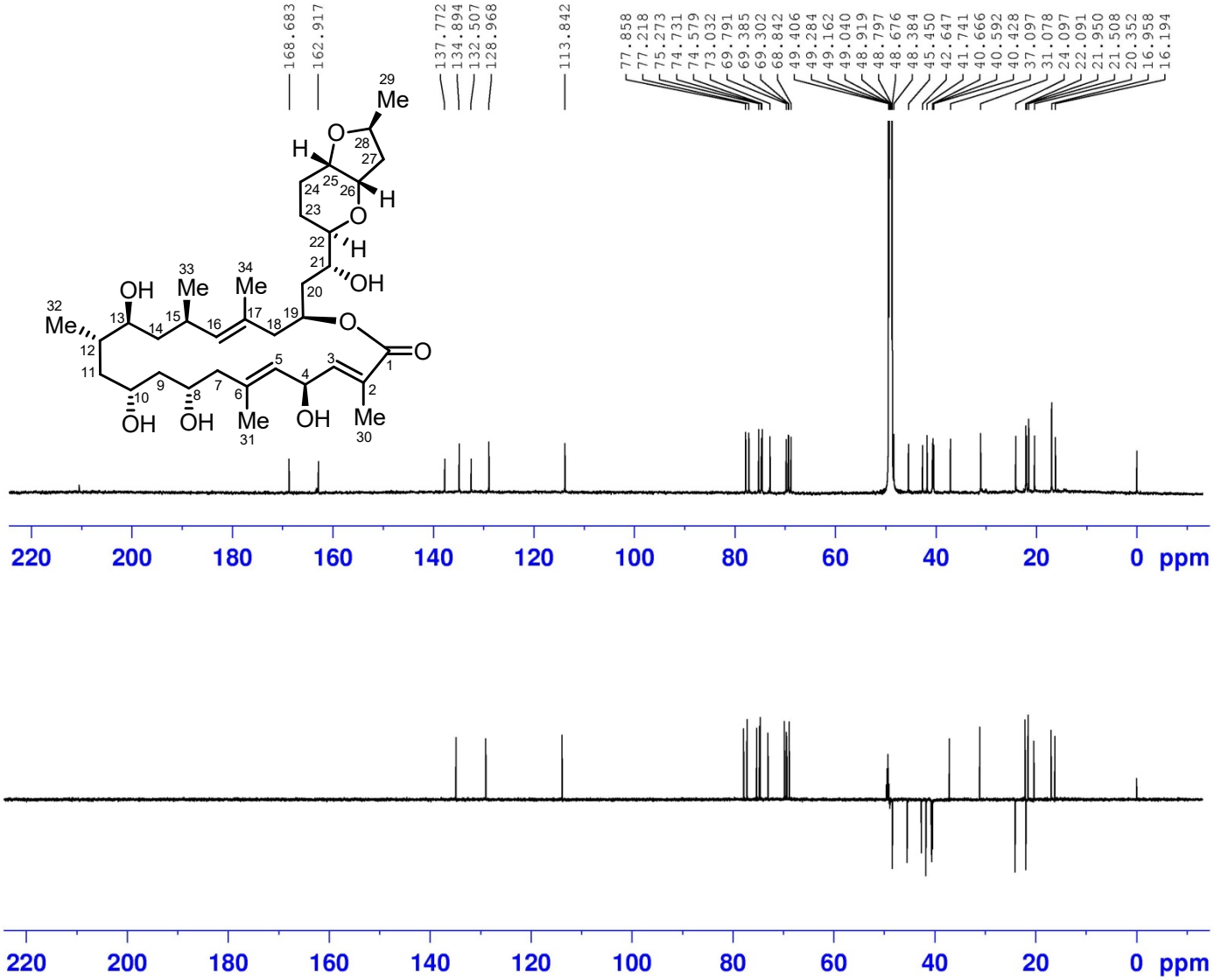
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OH



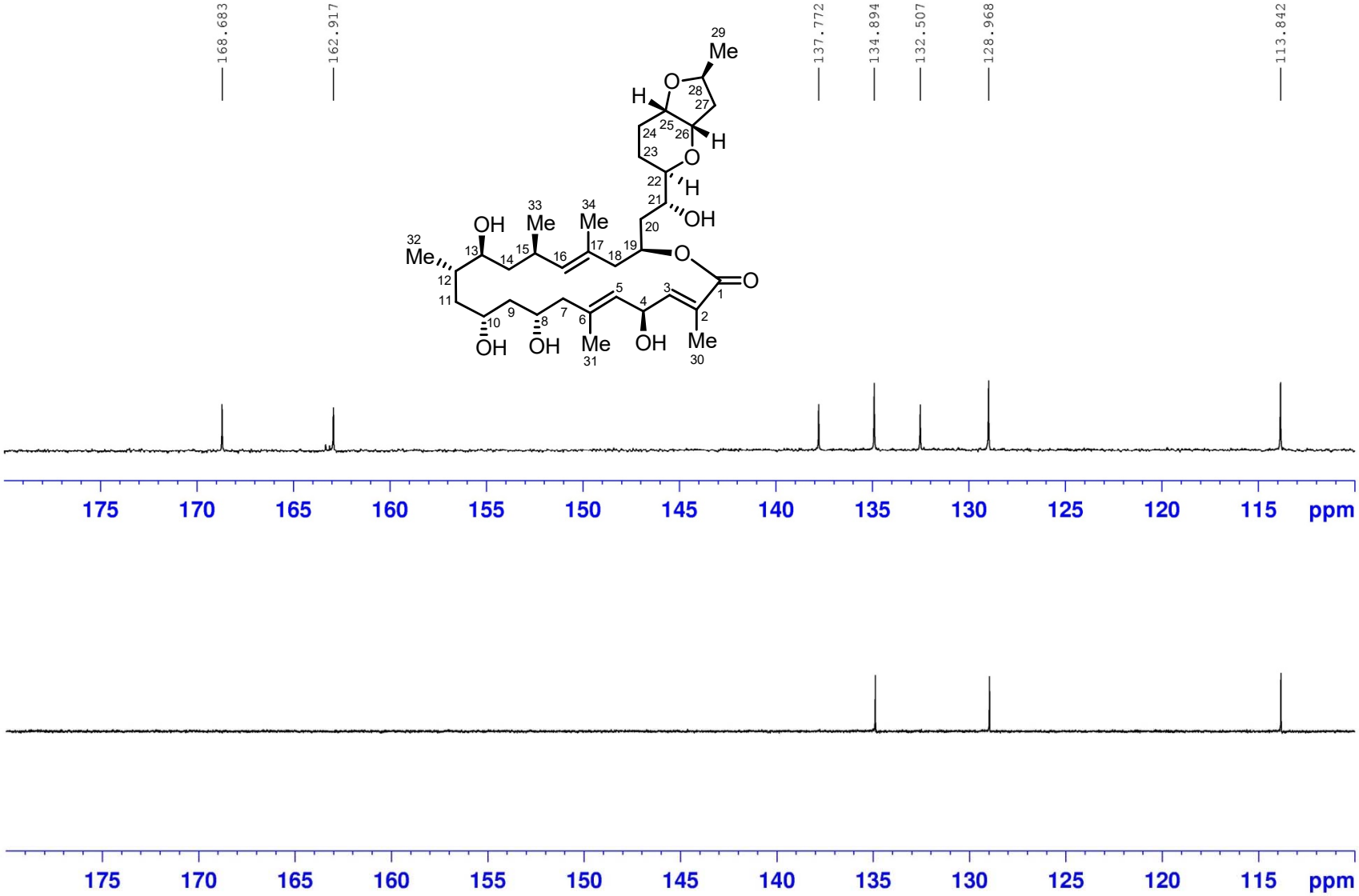
Comparison of ^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OH with that in CD_3OD



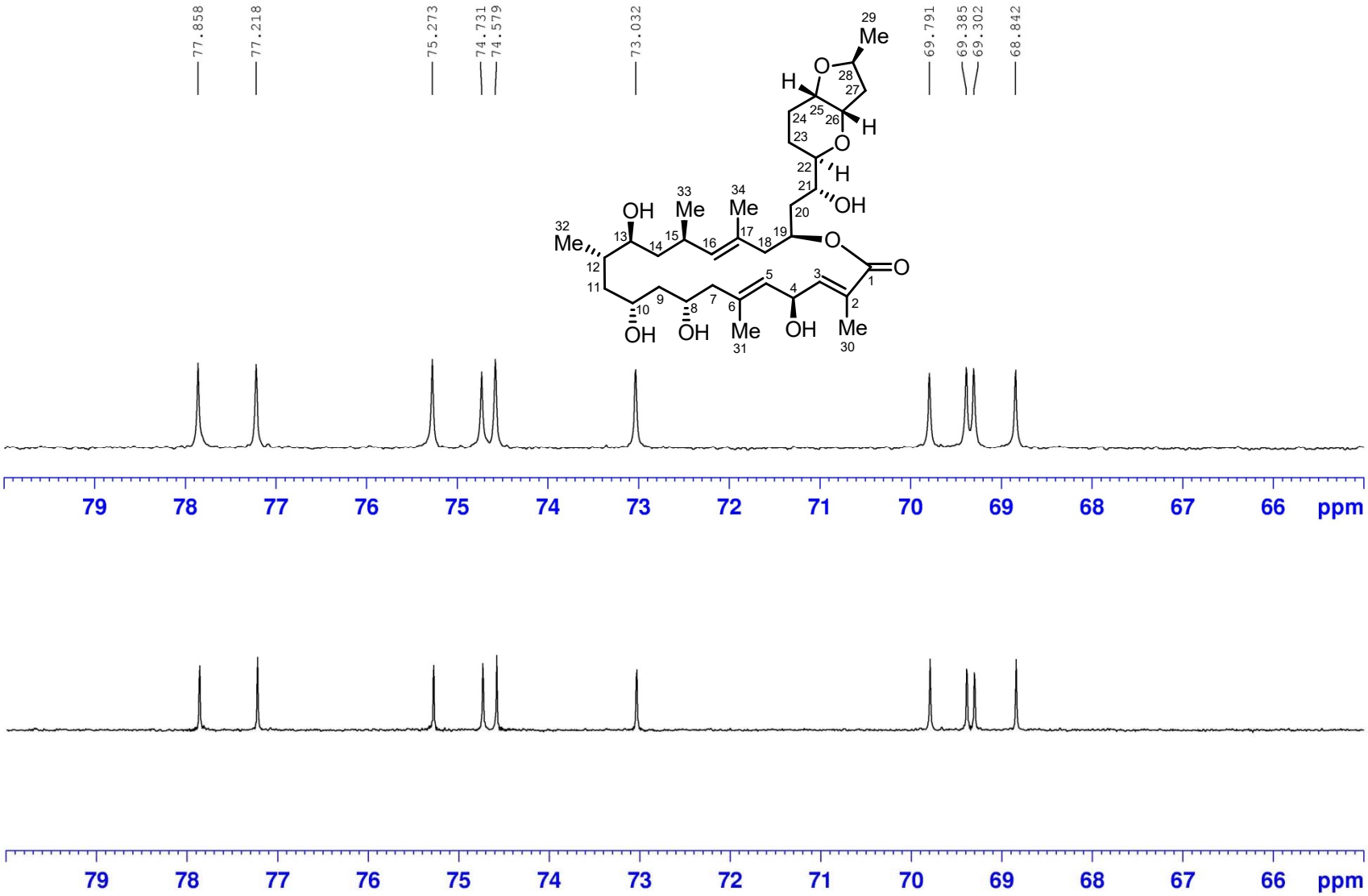
DEPT135 (175 MHz) spectrum of compound **1** in CD_3OD



DEPT135 (175 MHz) spectrum of compound **1** in CD_3OD



DEPT135 (175 MHz) spectrum of compound **1** in CD_3OD



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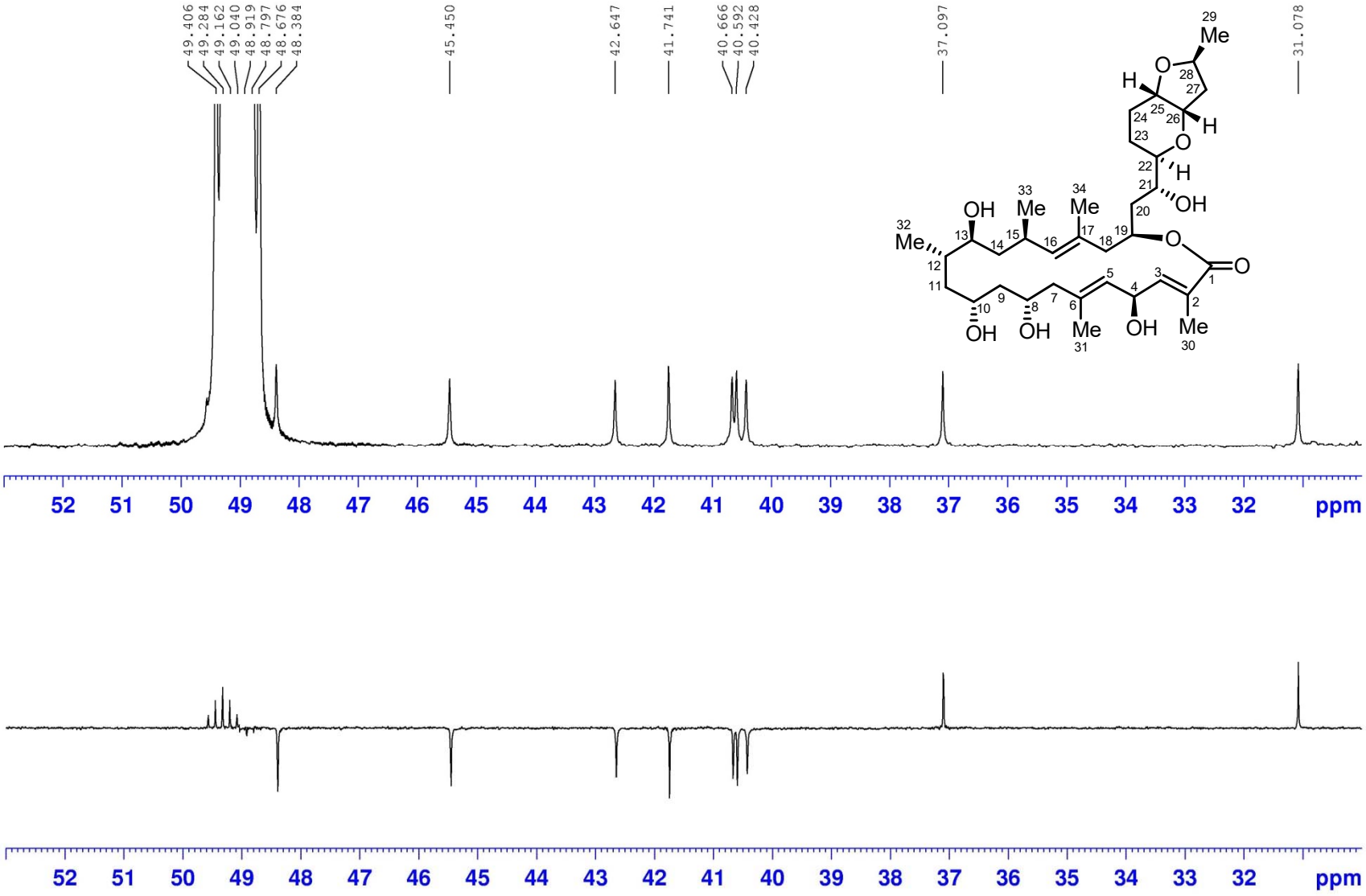

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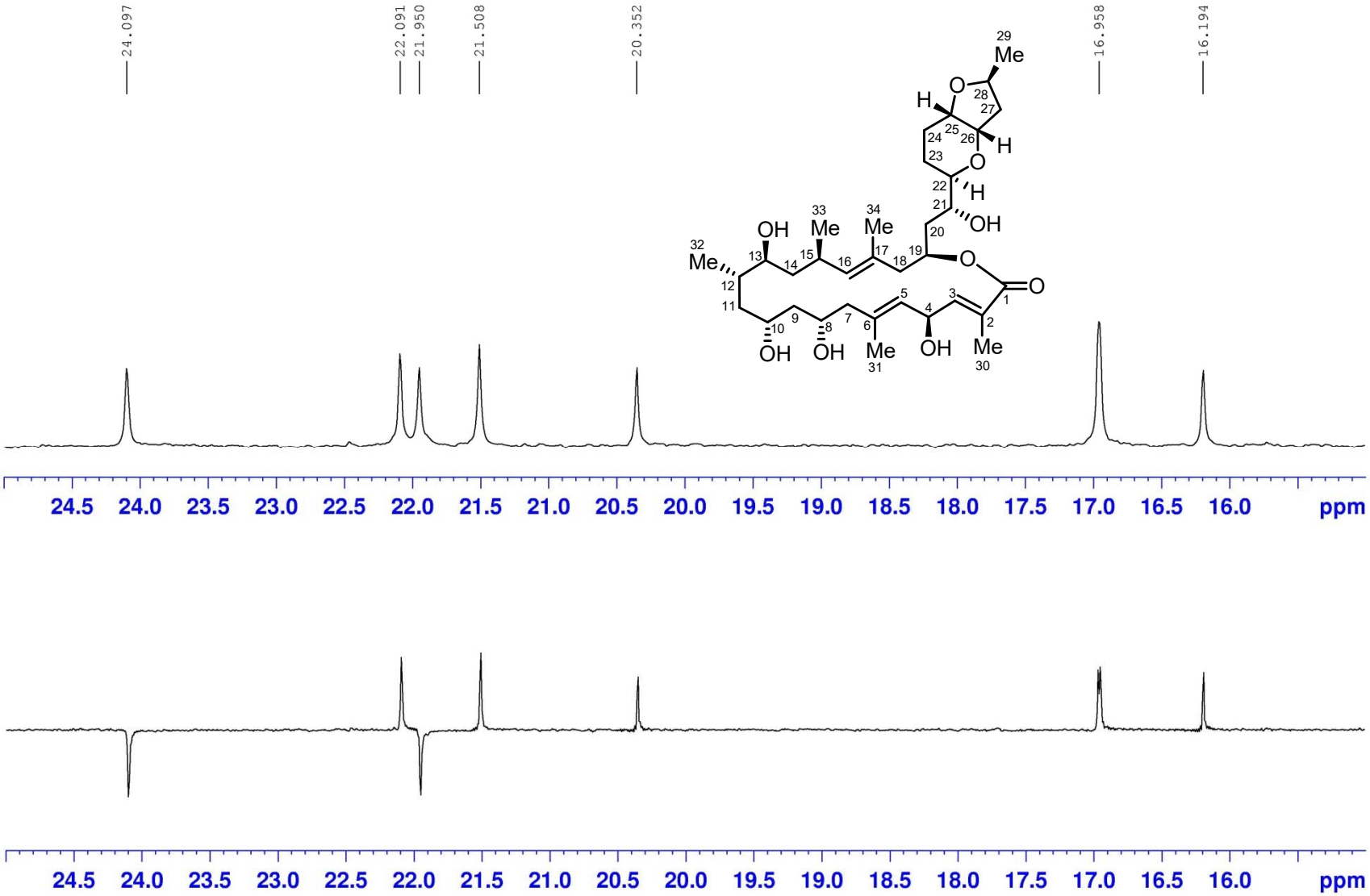
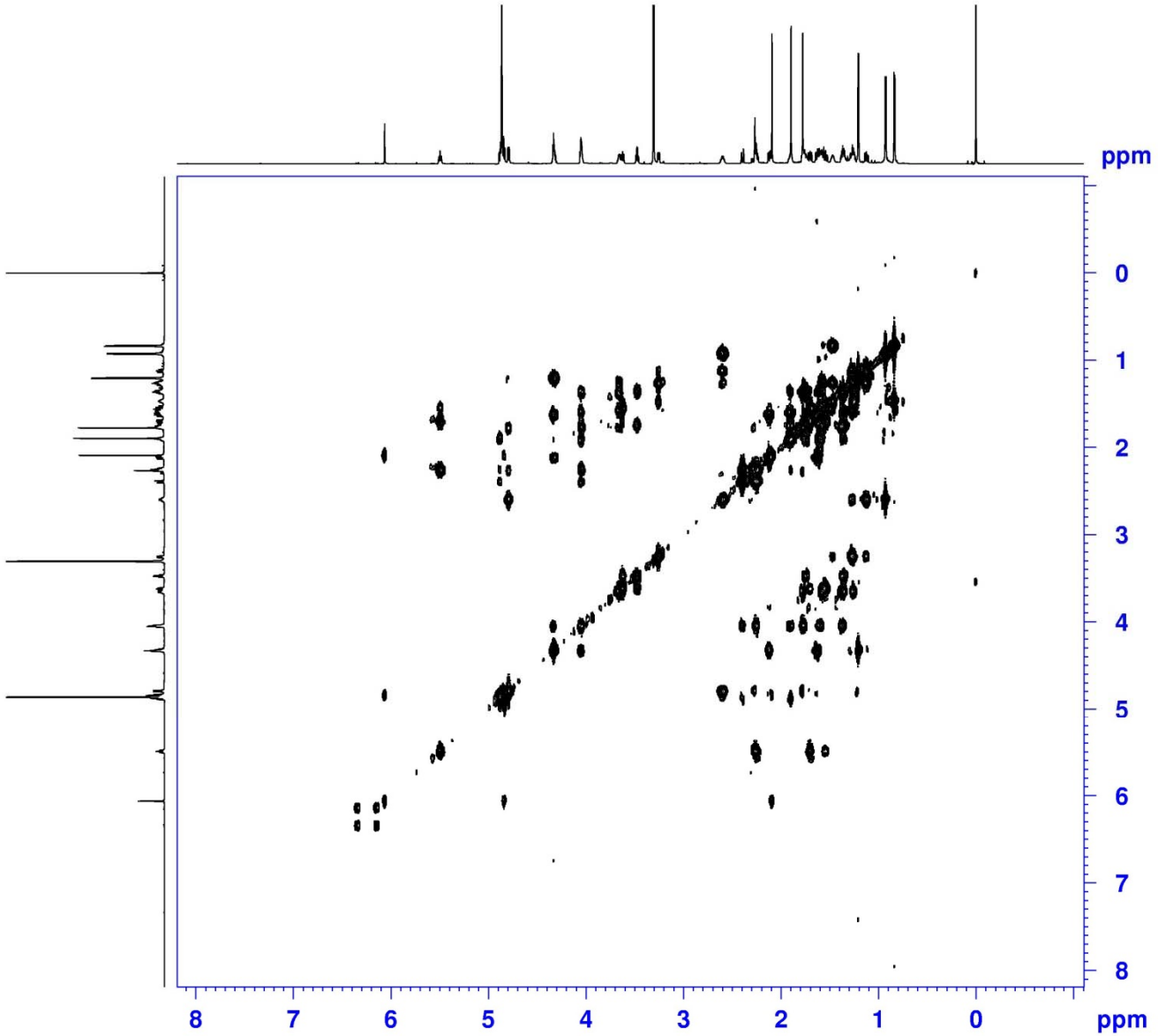
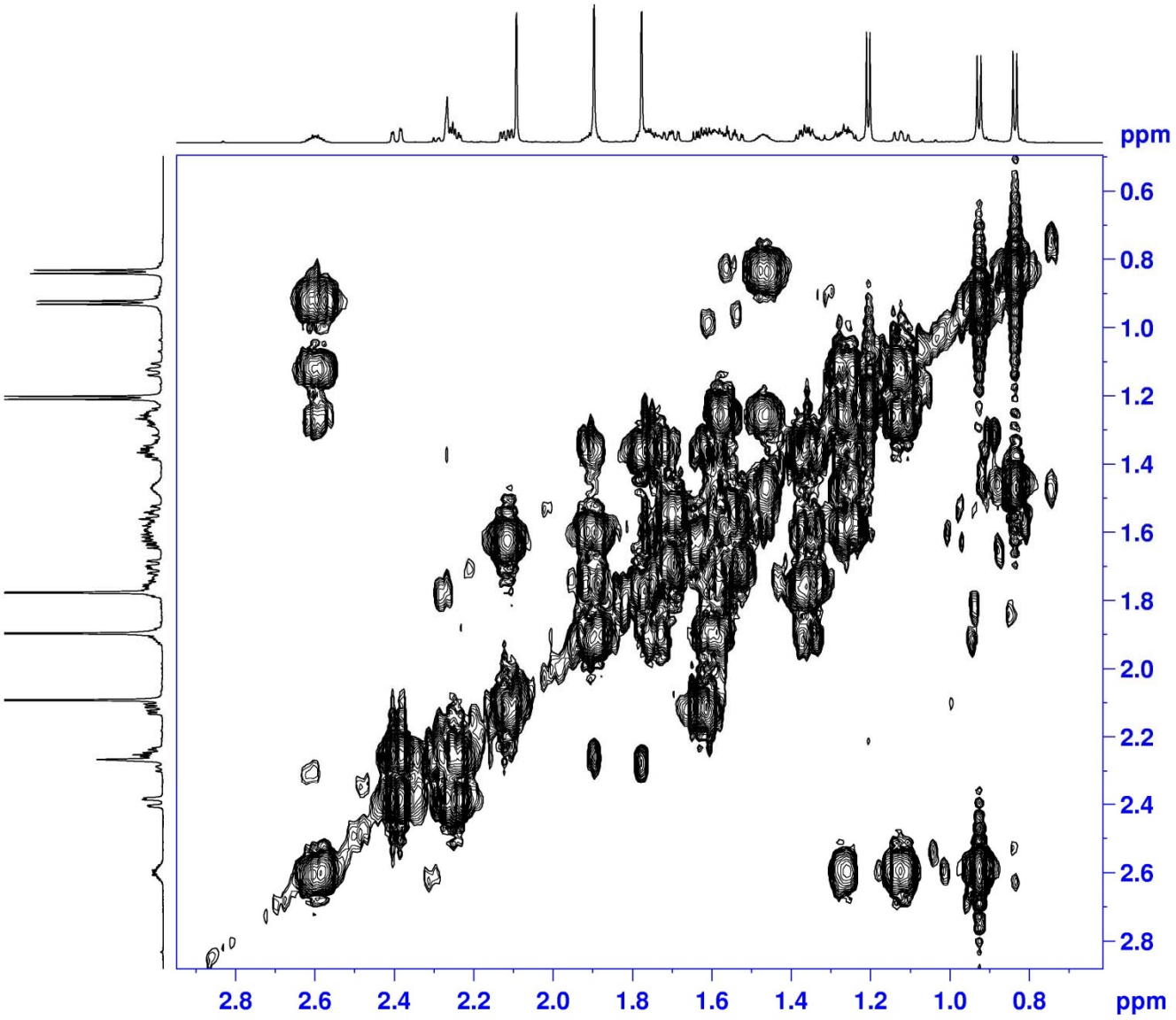


^{1}H–^{1}H COSY (700 MHz) spectrum of compound **1** in CD_3OD



$^{1}H–^{1}H$ COSY (700 MHz) spectrum of compound **1** in CD_3OD



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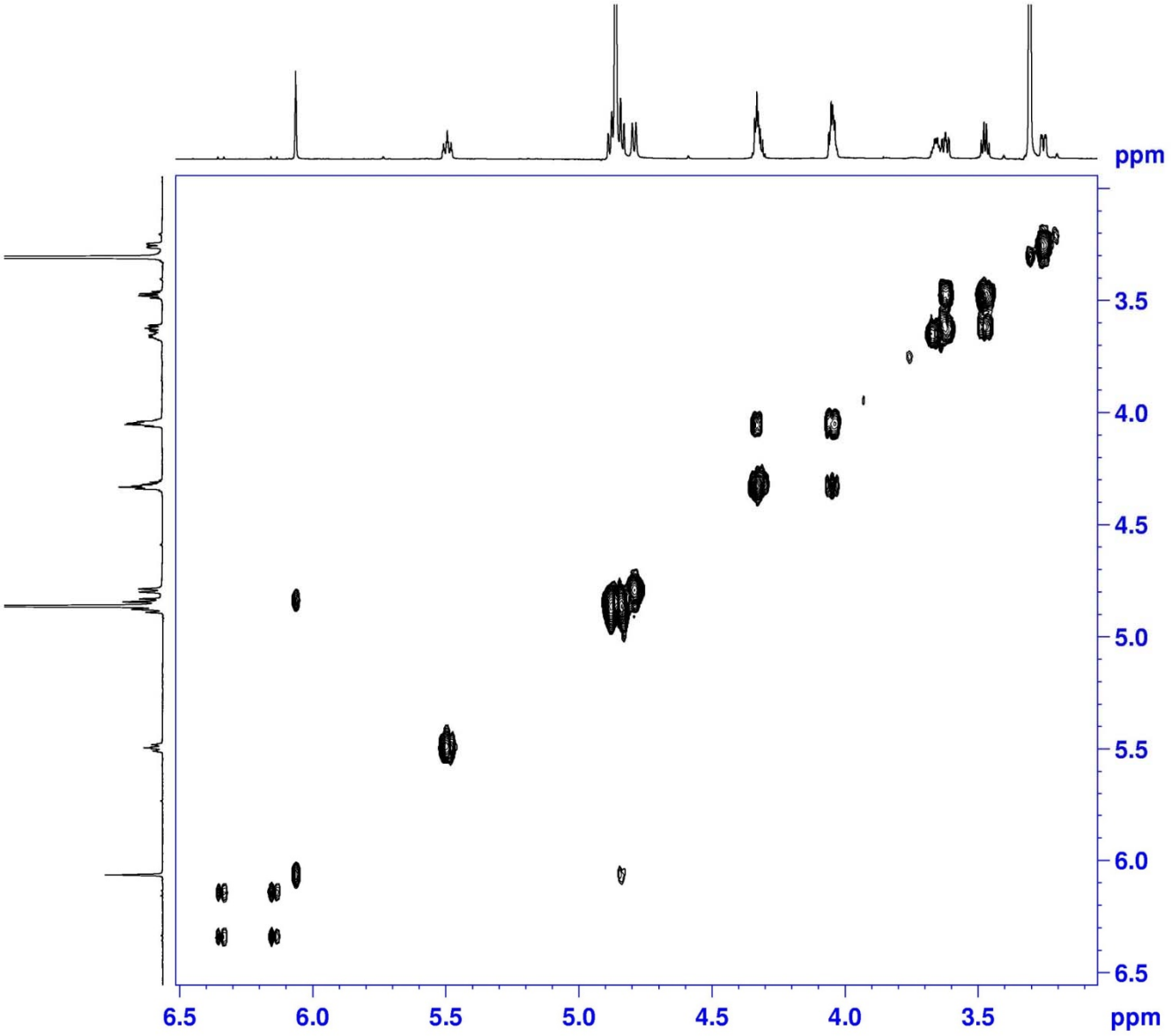
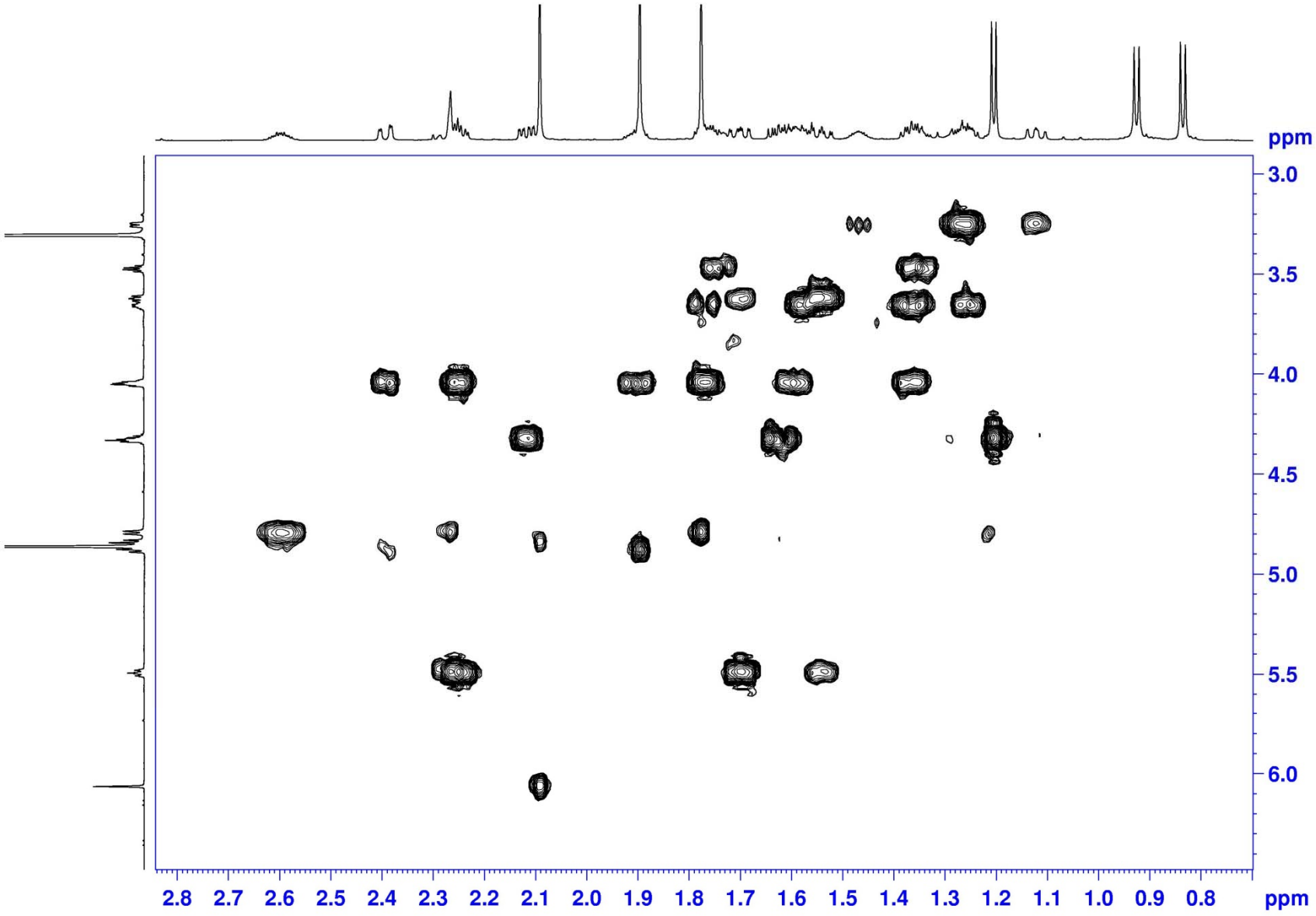
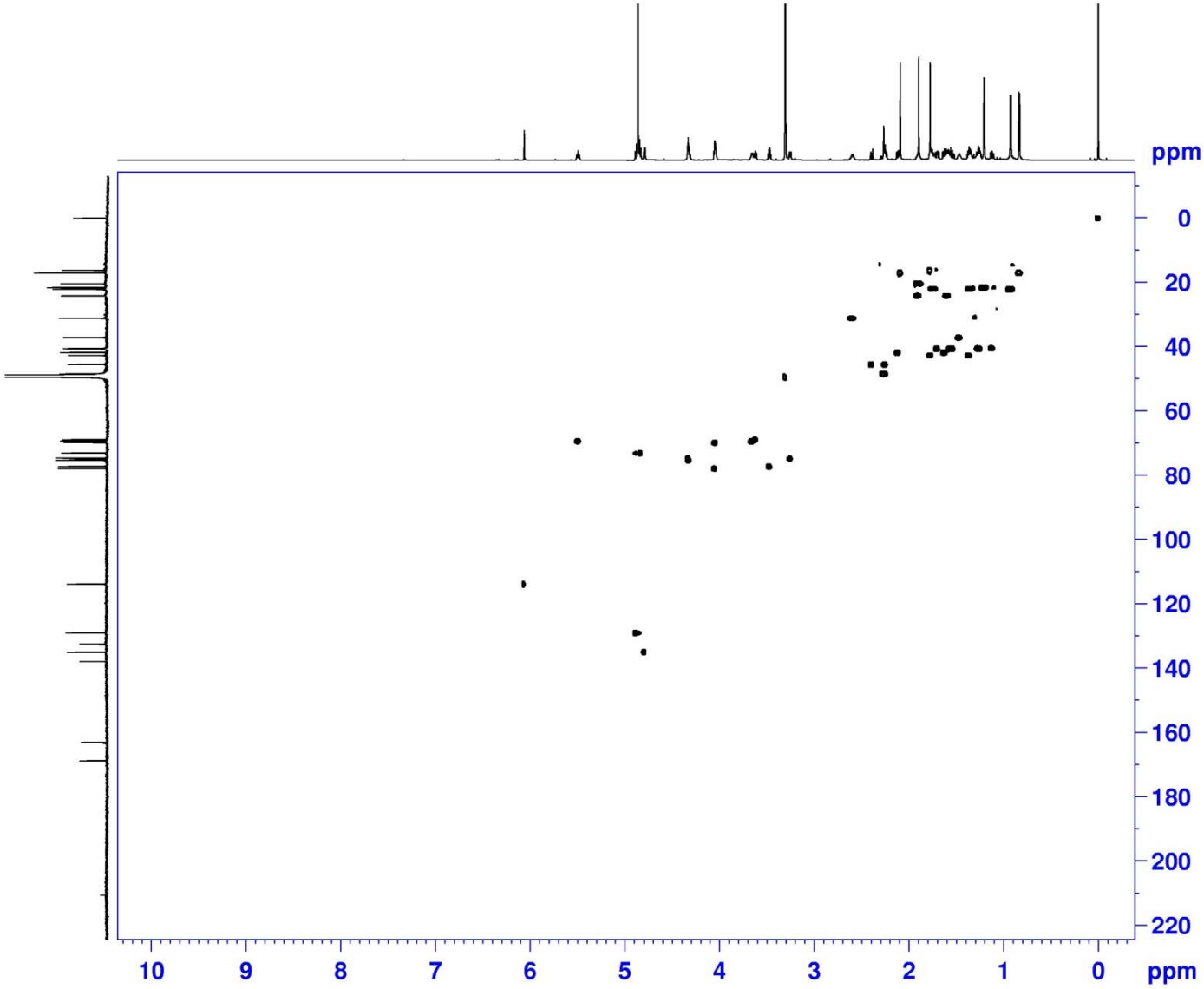


$^{1}H–^{1}H$ COSY (700 MHz) spectrum of compound **1** in CD_3OD



HSQC (700 MHz) spectrum of compound **1** in CD_3OD



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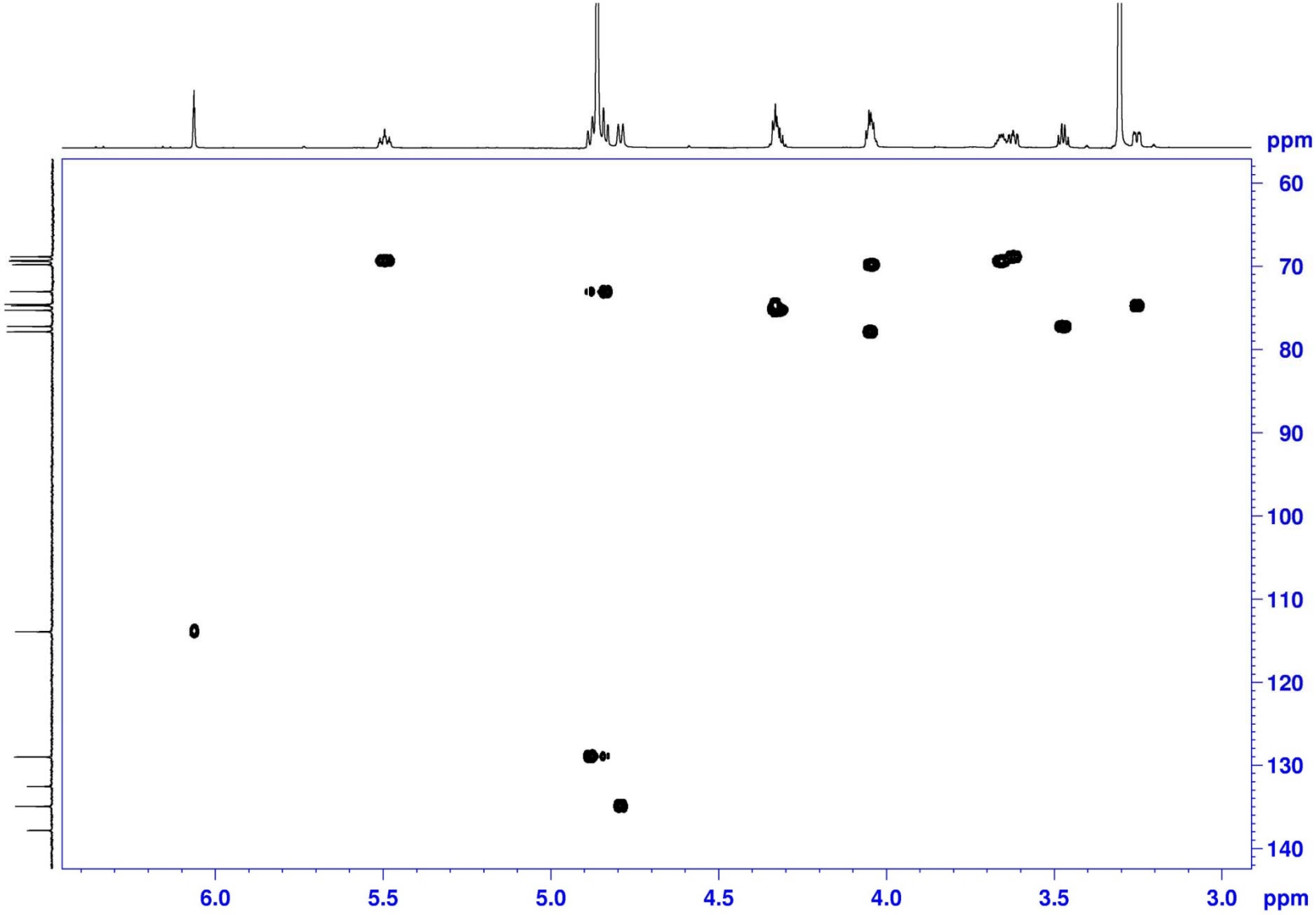

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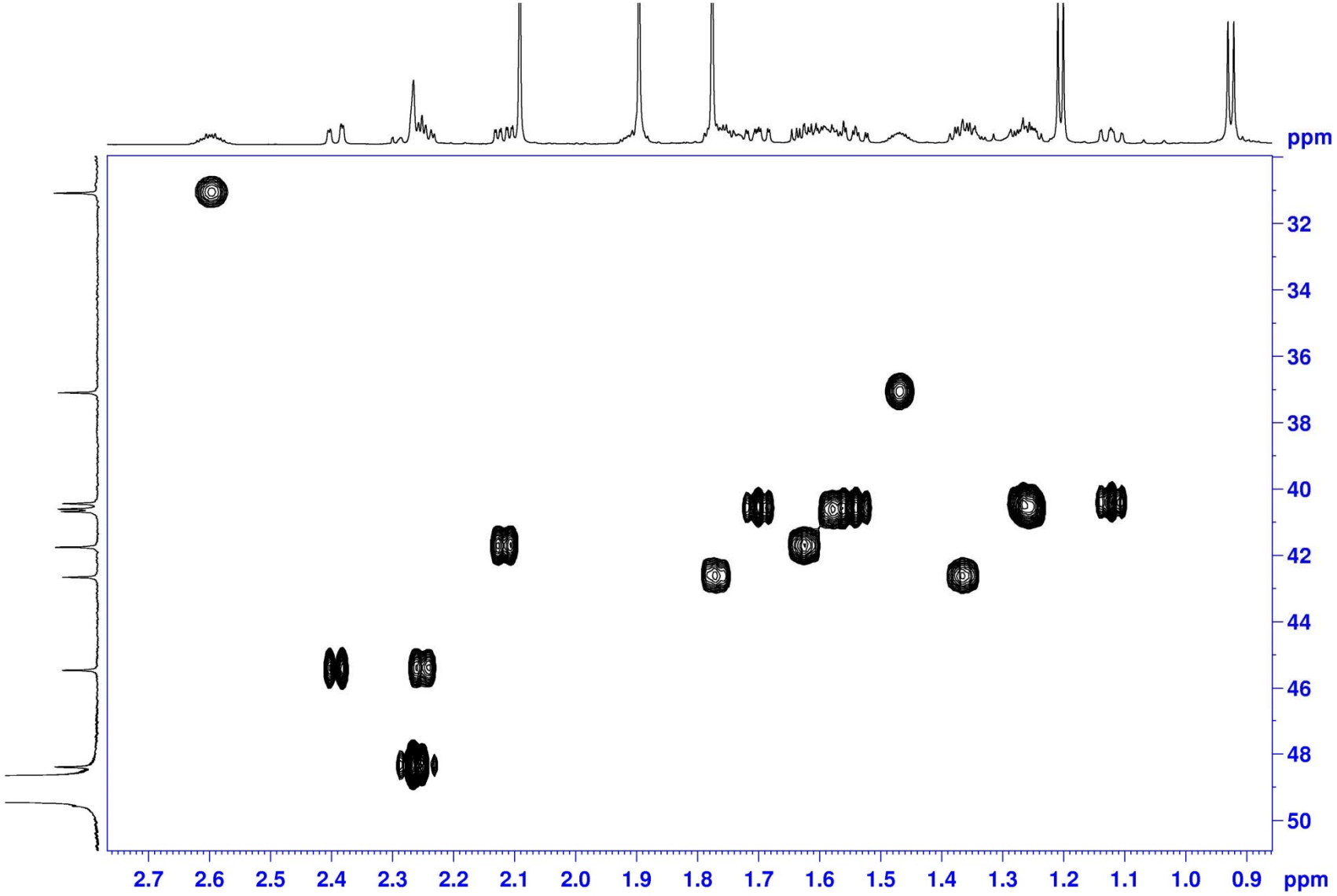

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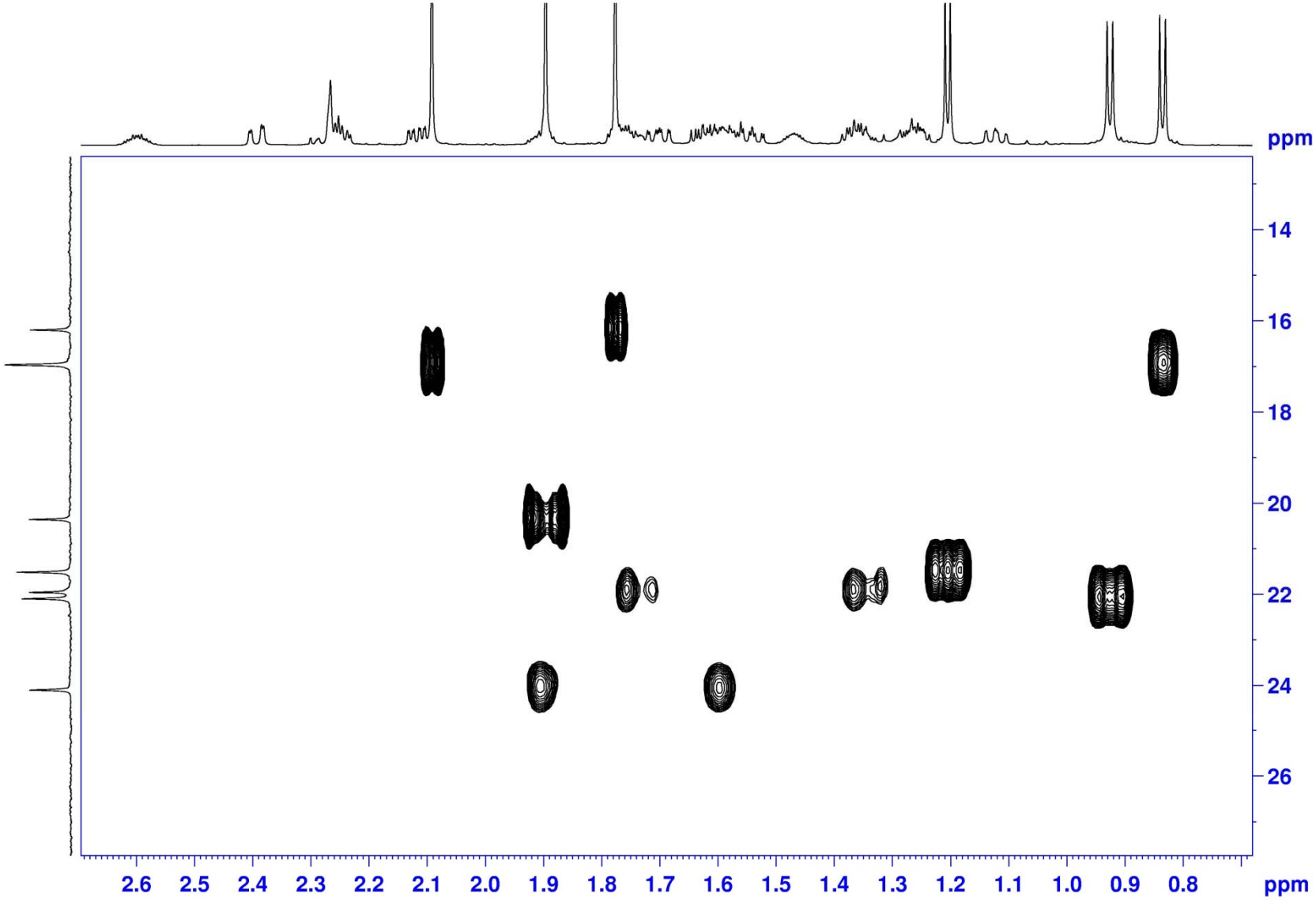
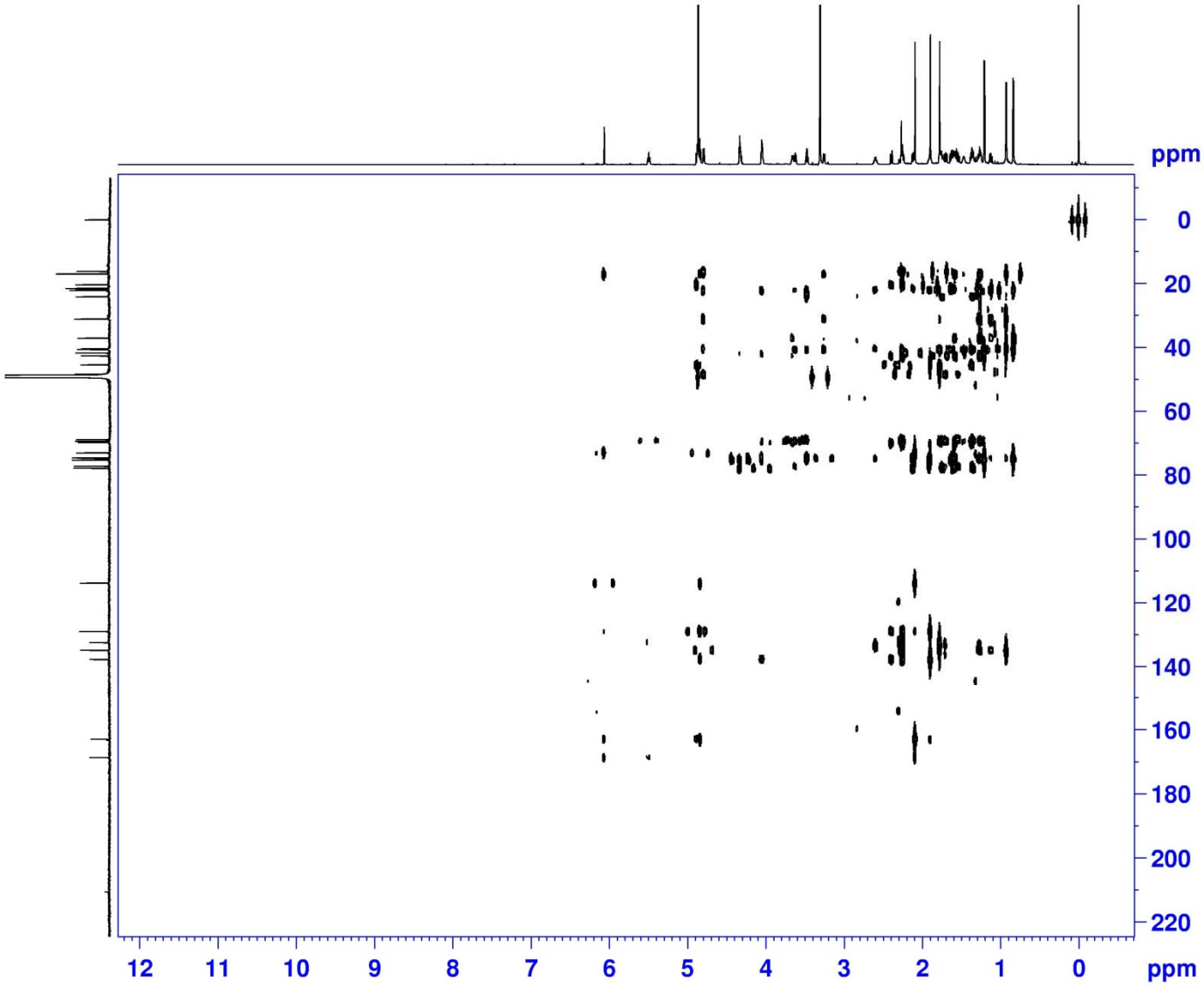
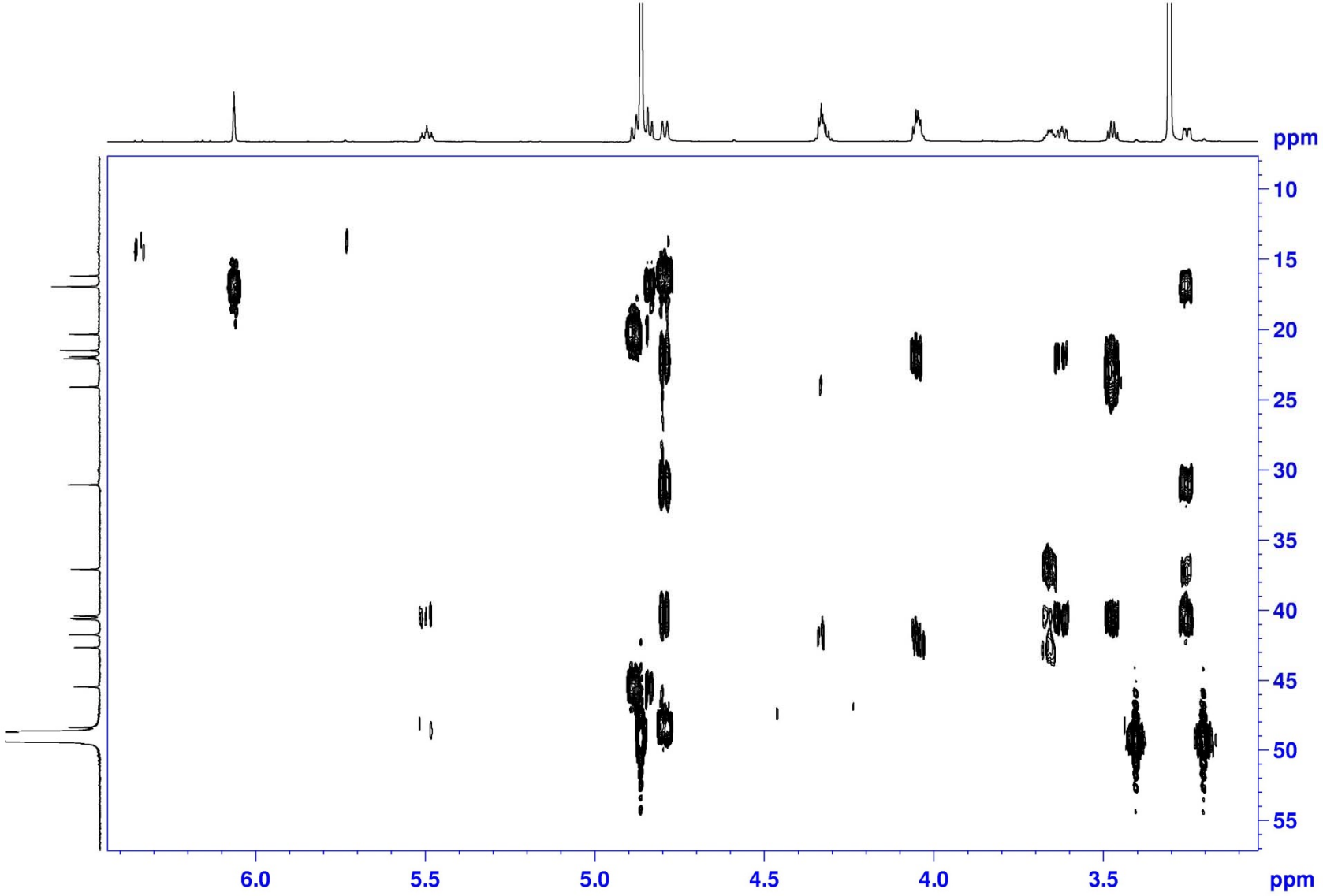


HMBC (700 MHz) spectrum of compound **1** in CD_3OD



HMBC (700 MHz) spectrum of compound **1** in CD_3OD



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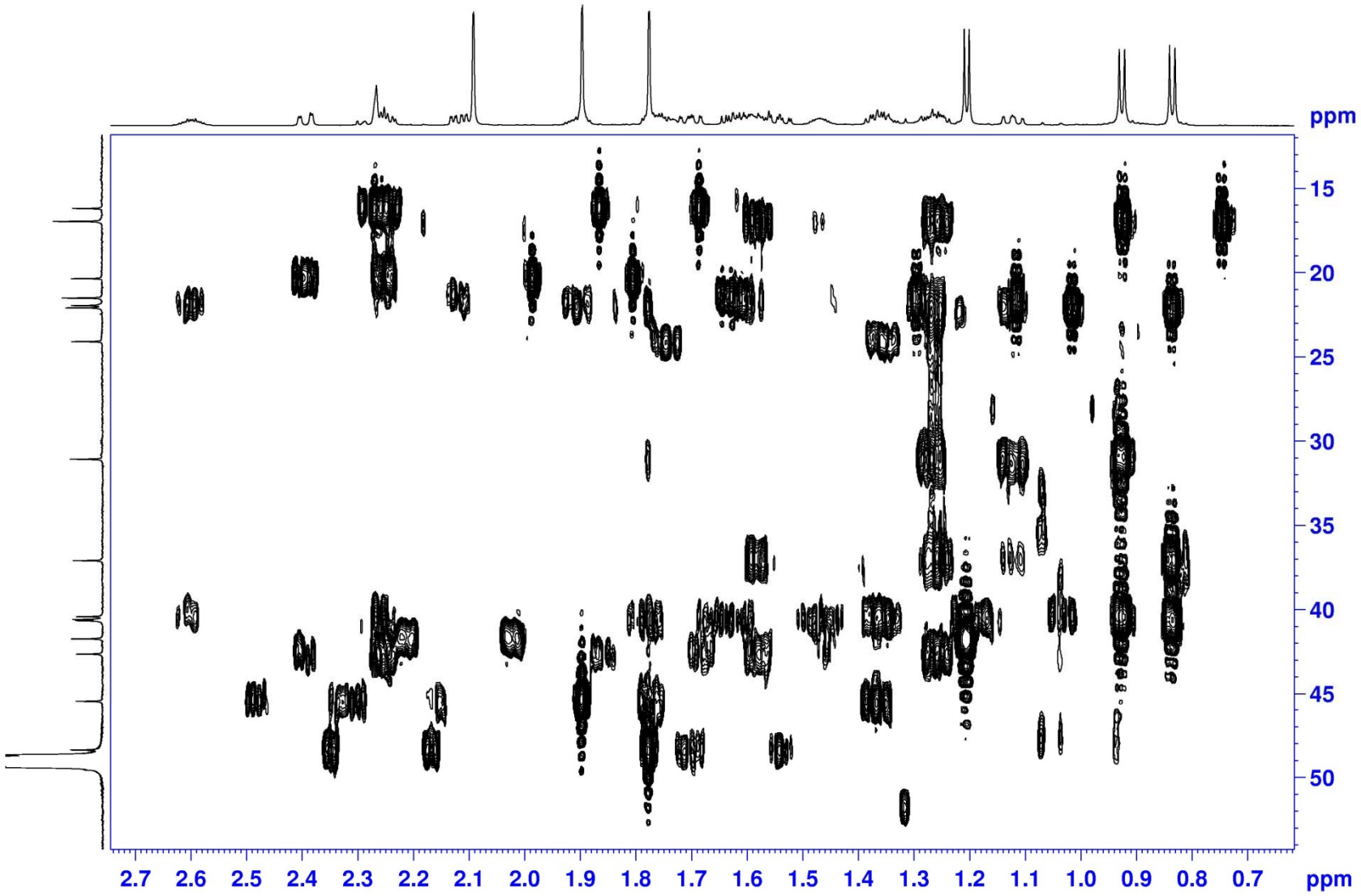

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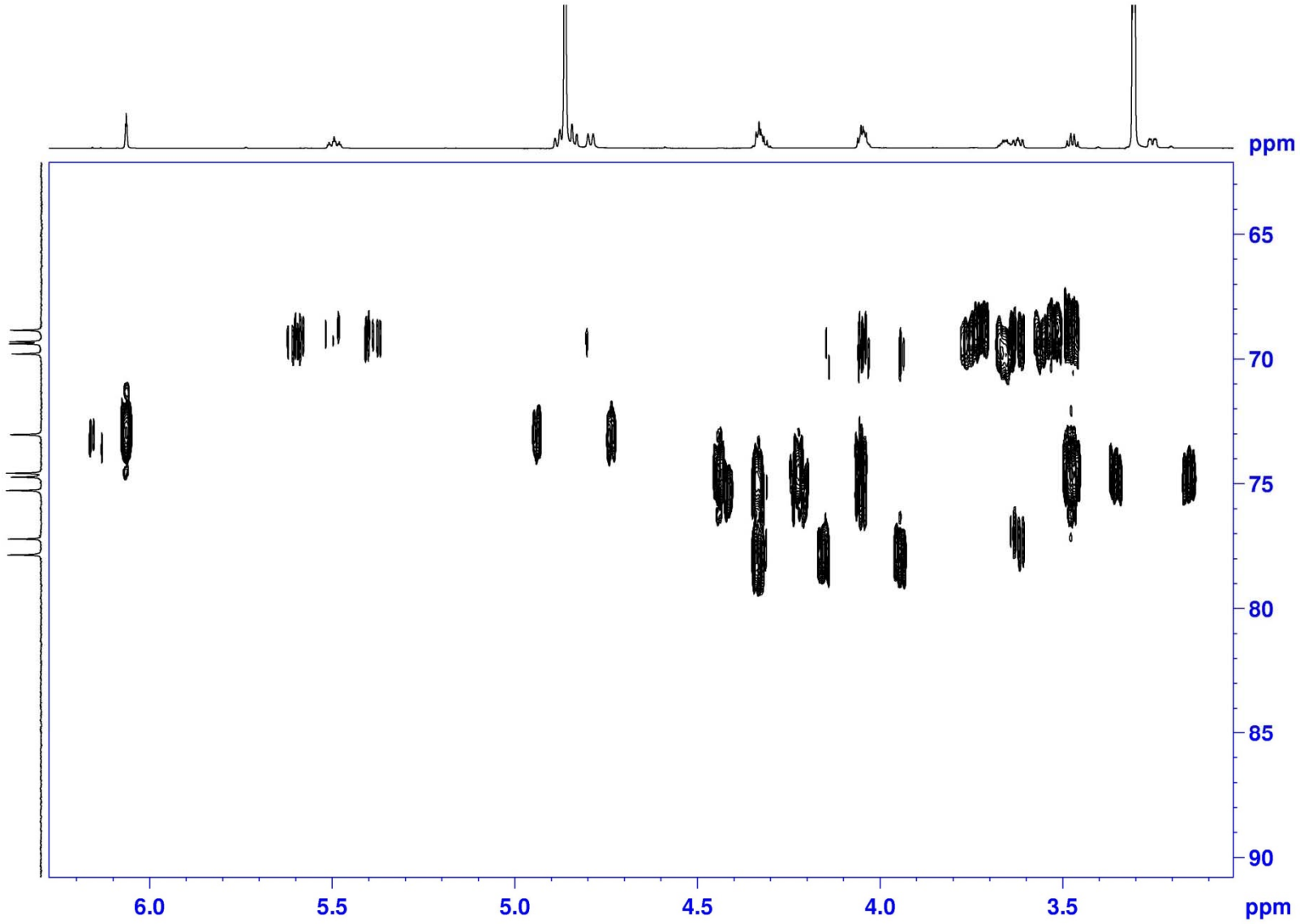

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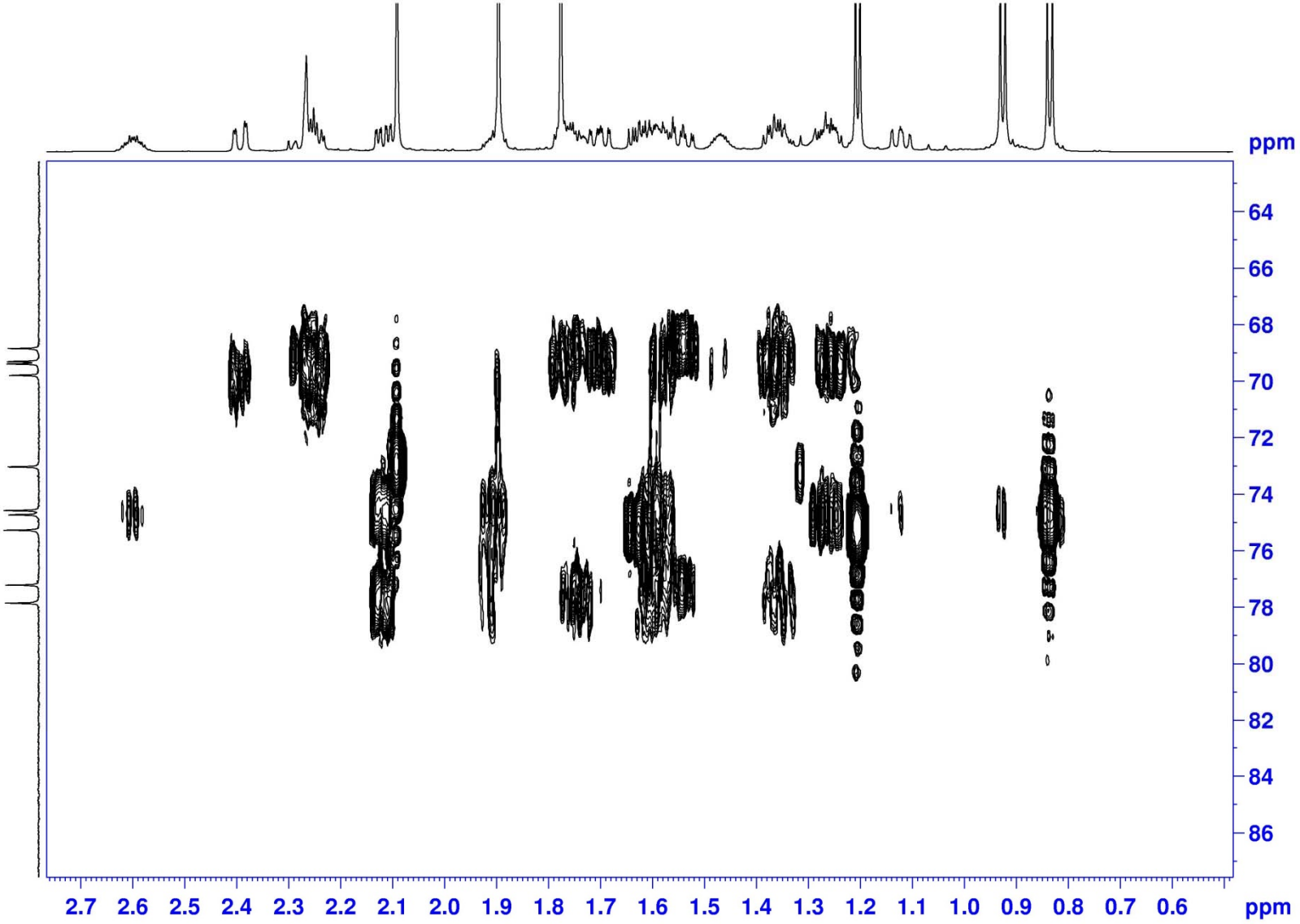

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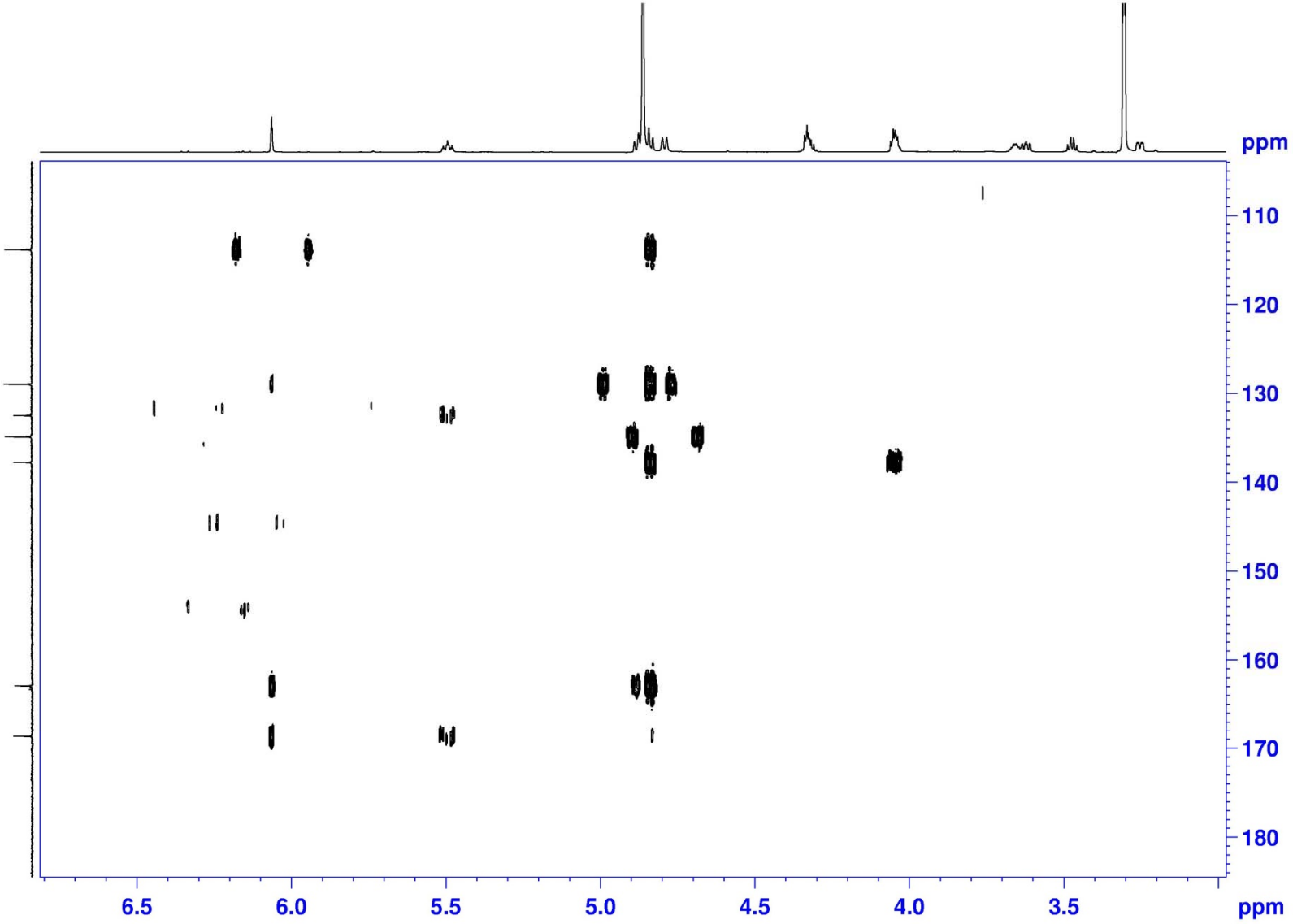

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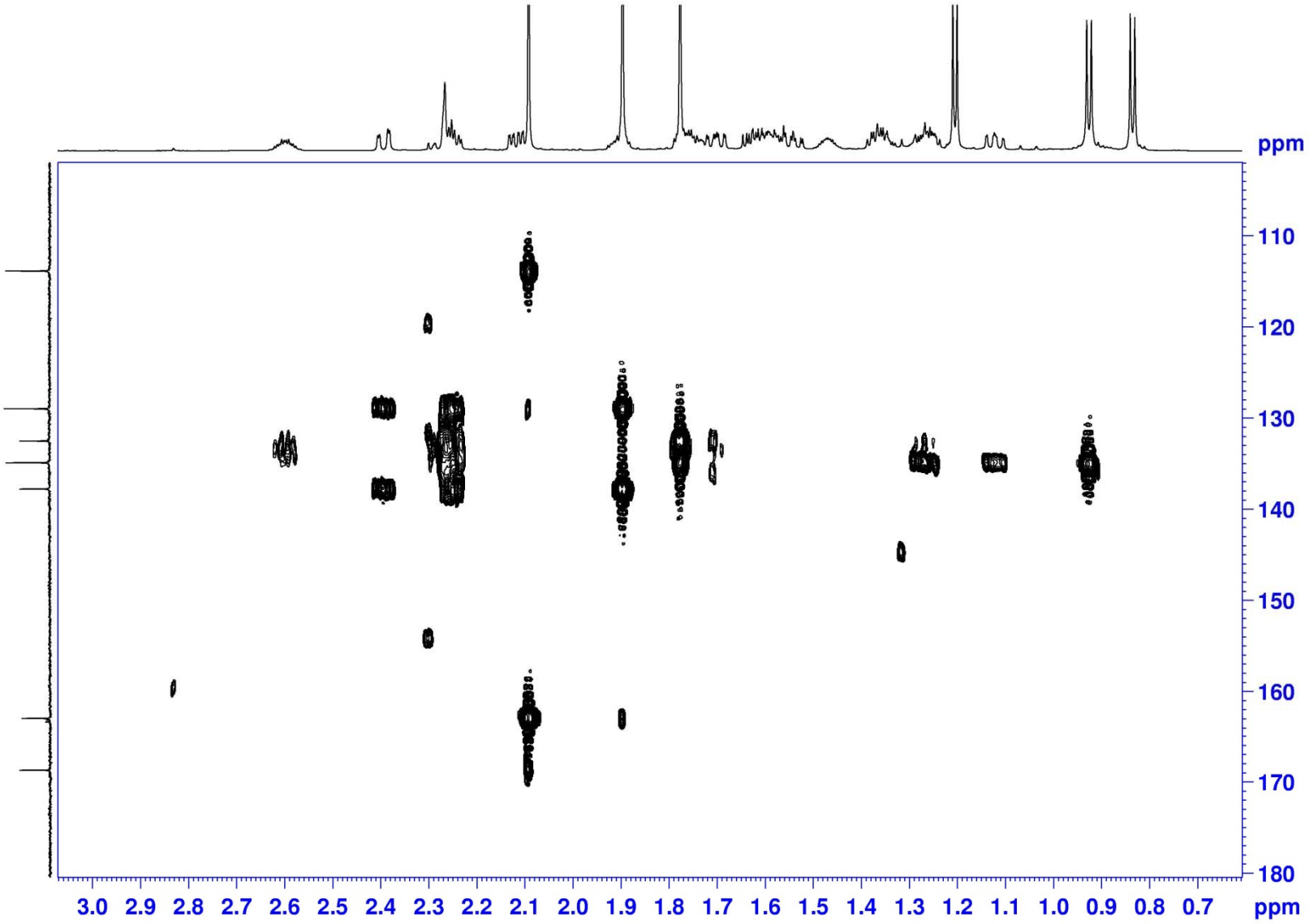
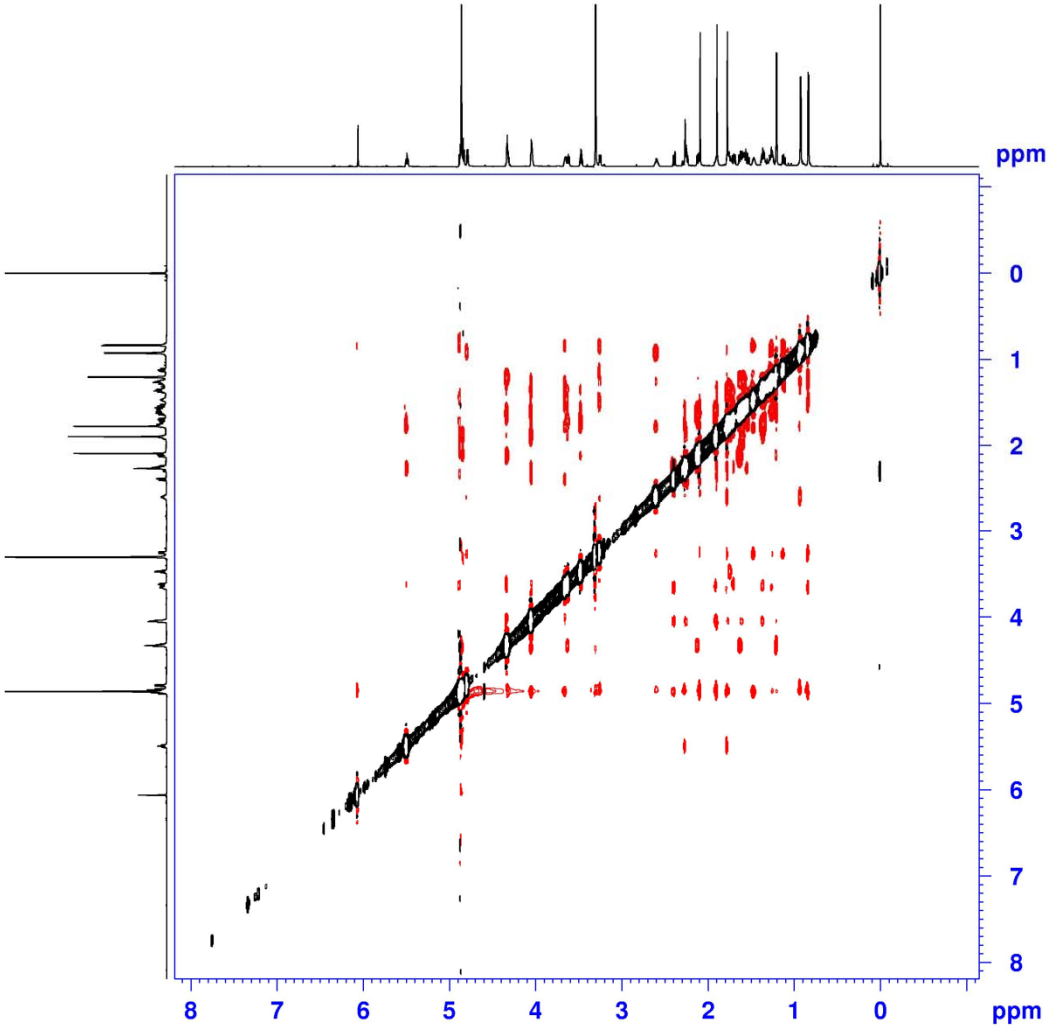


NOESY (700 MHz) spectrum of compound **1** in CD_3OD



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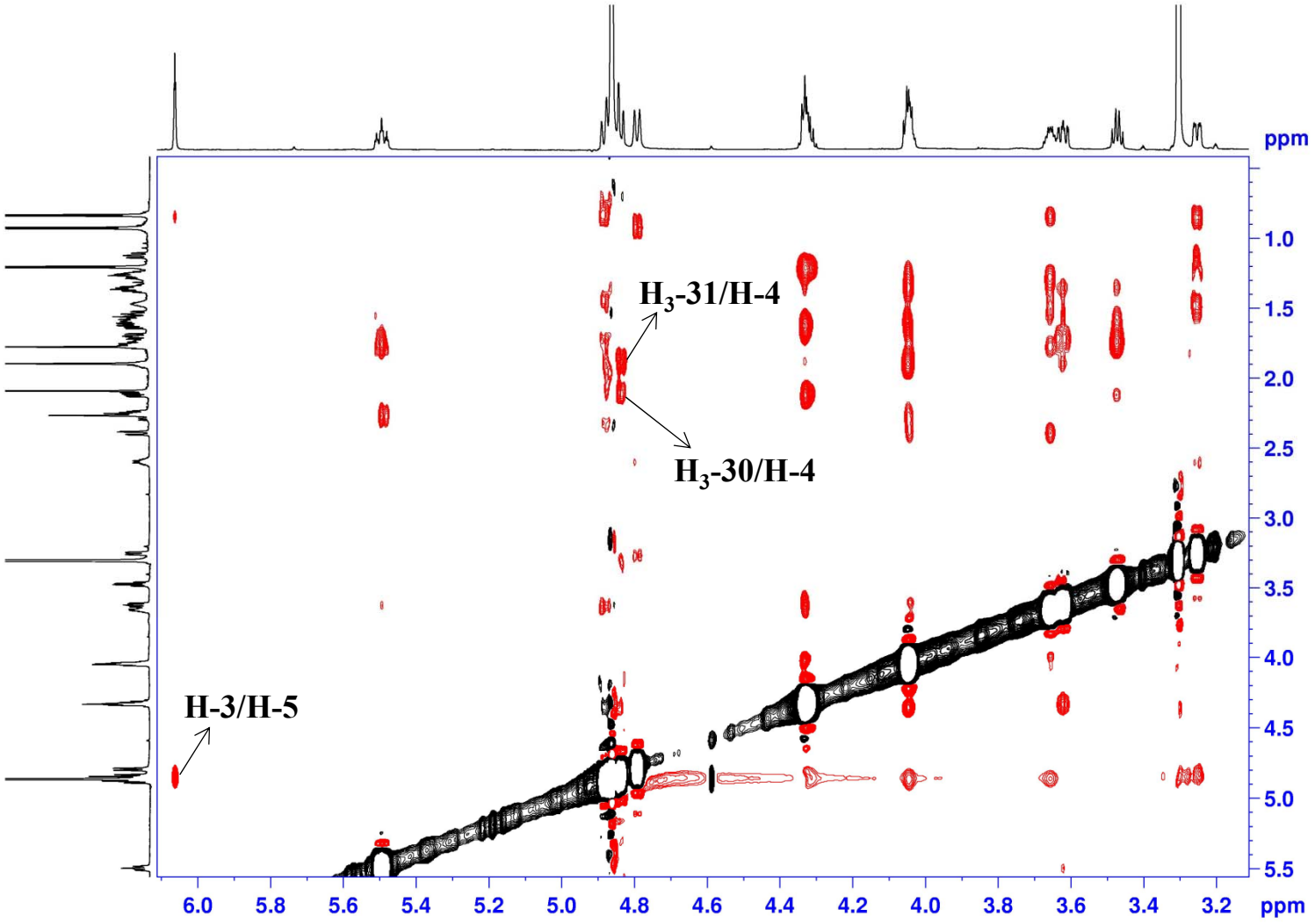

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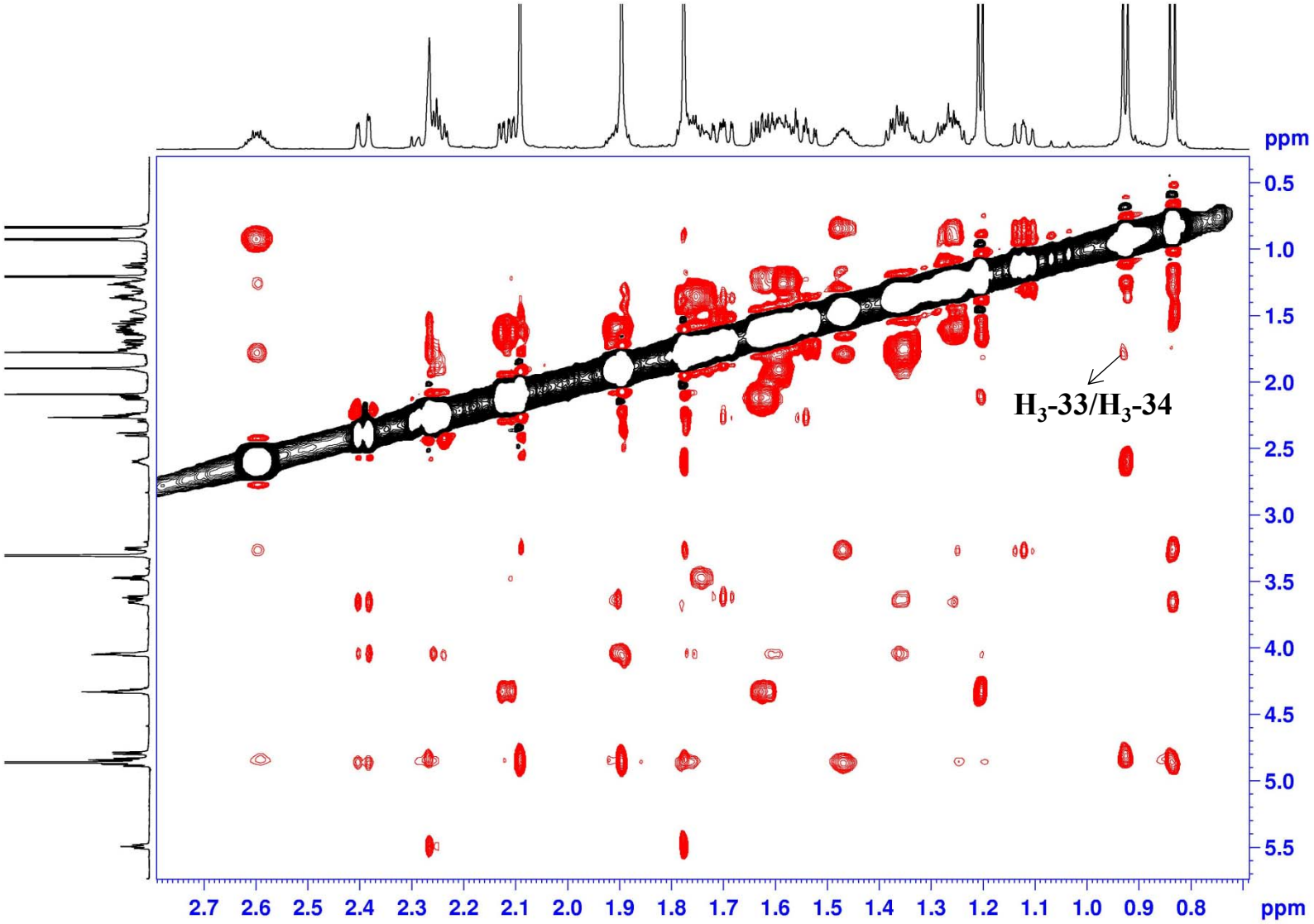

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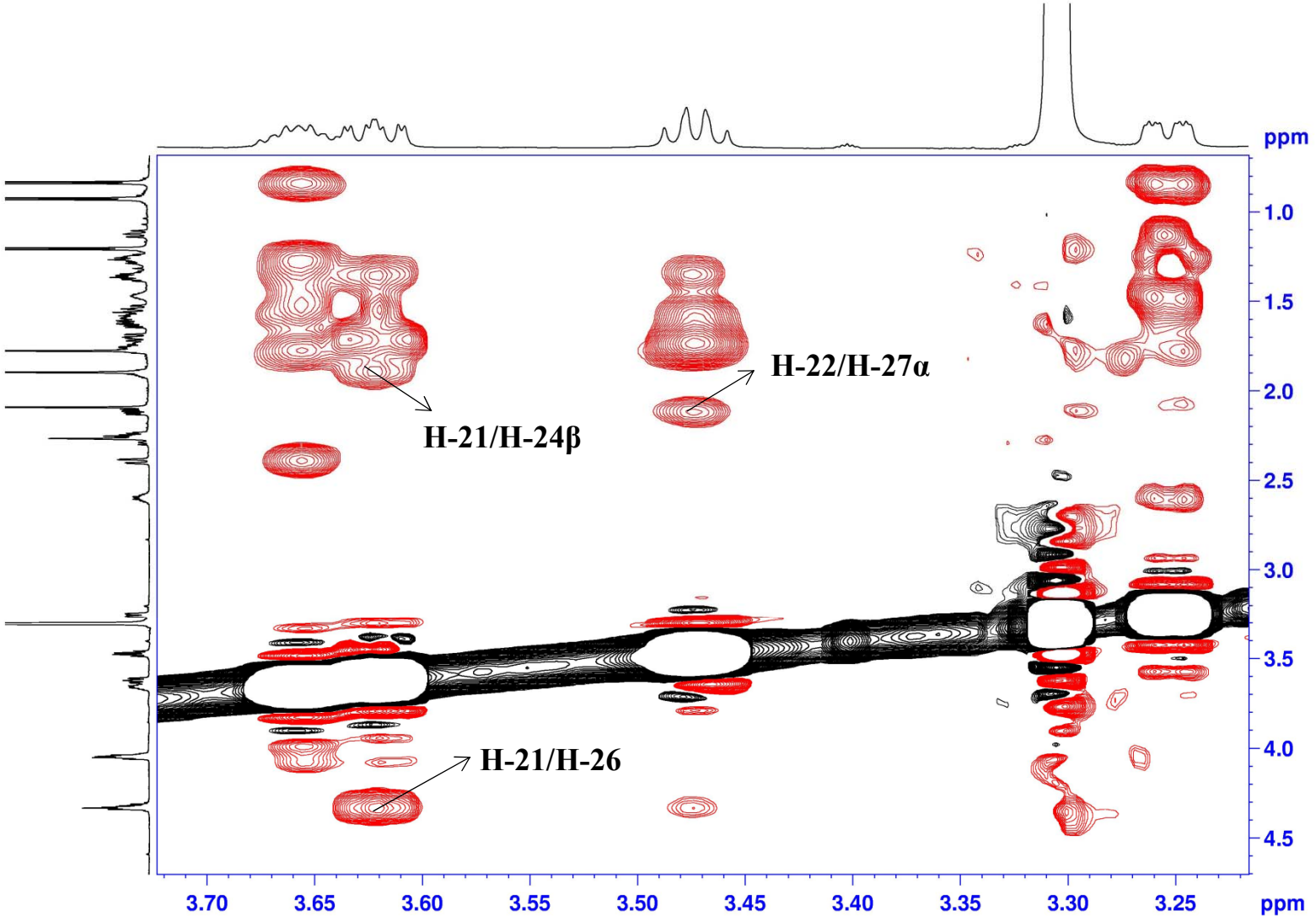

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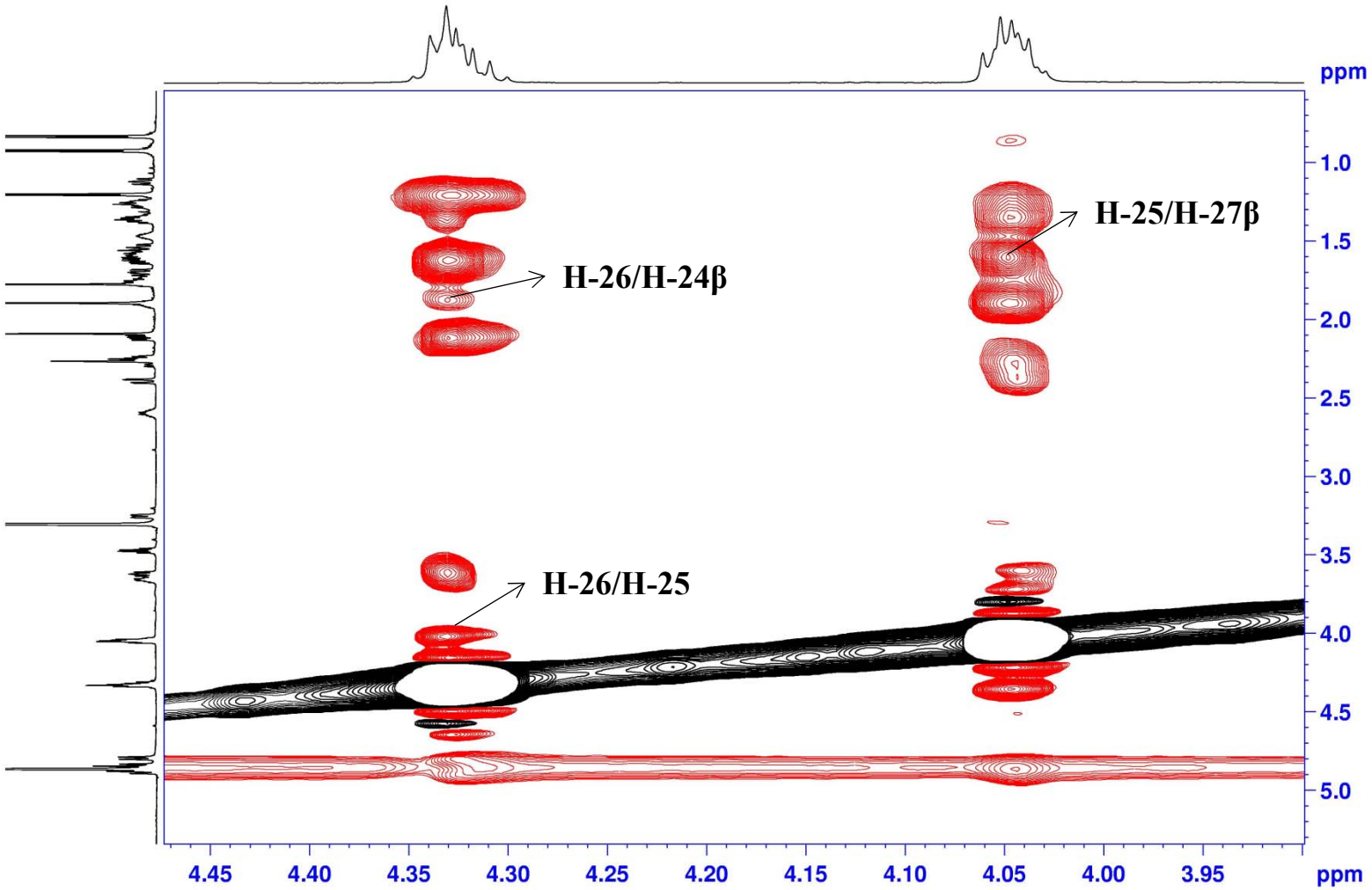

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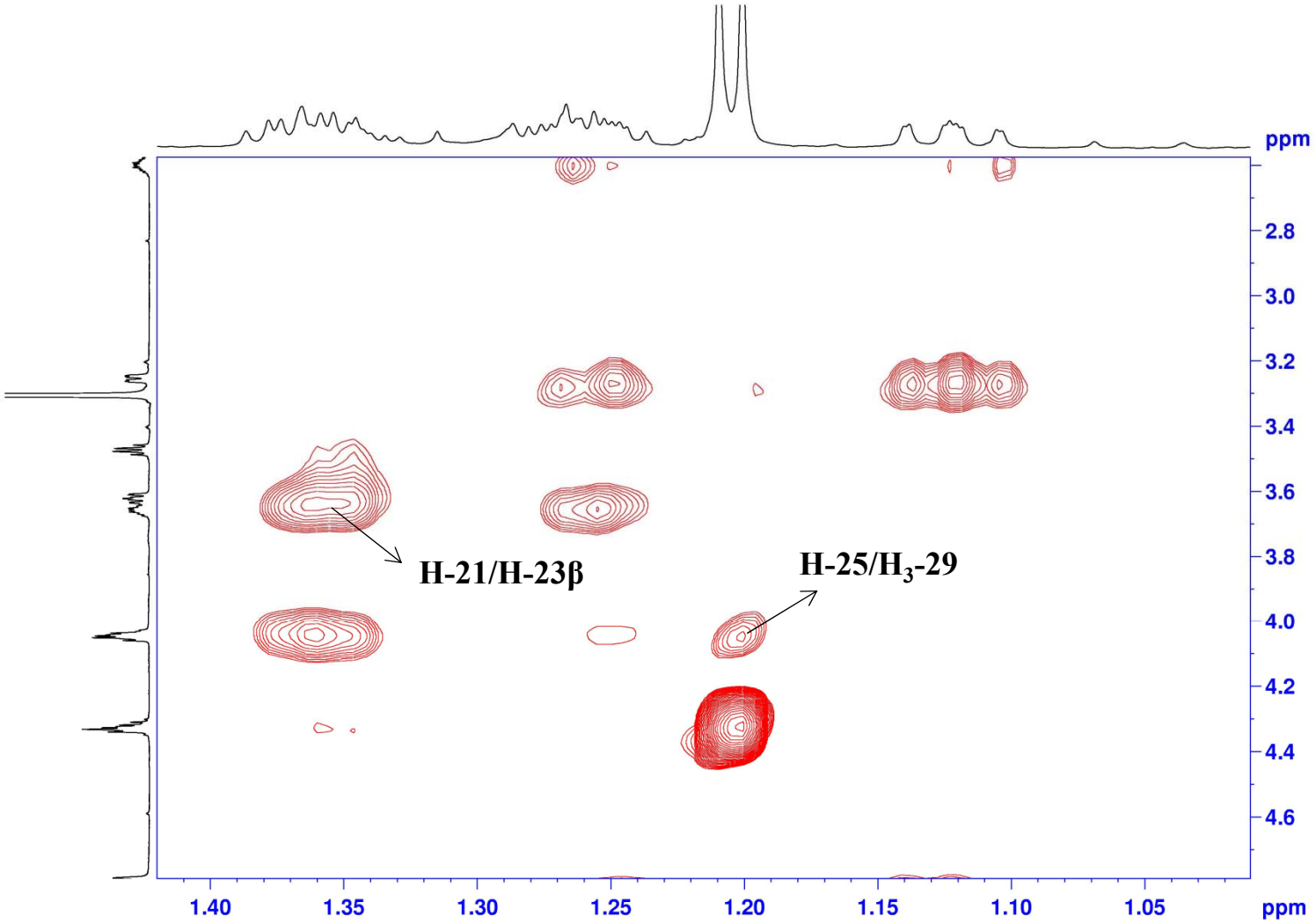
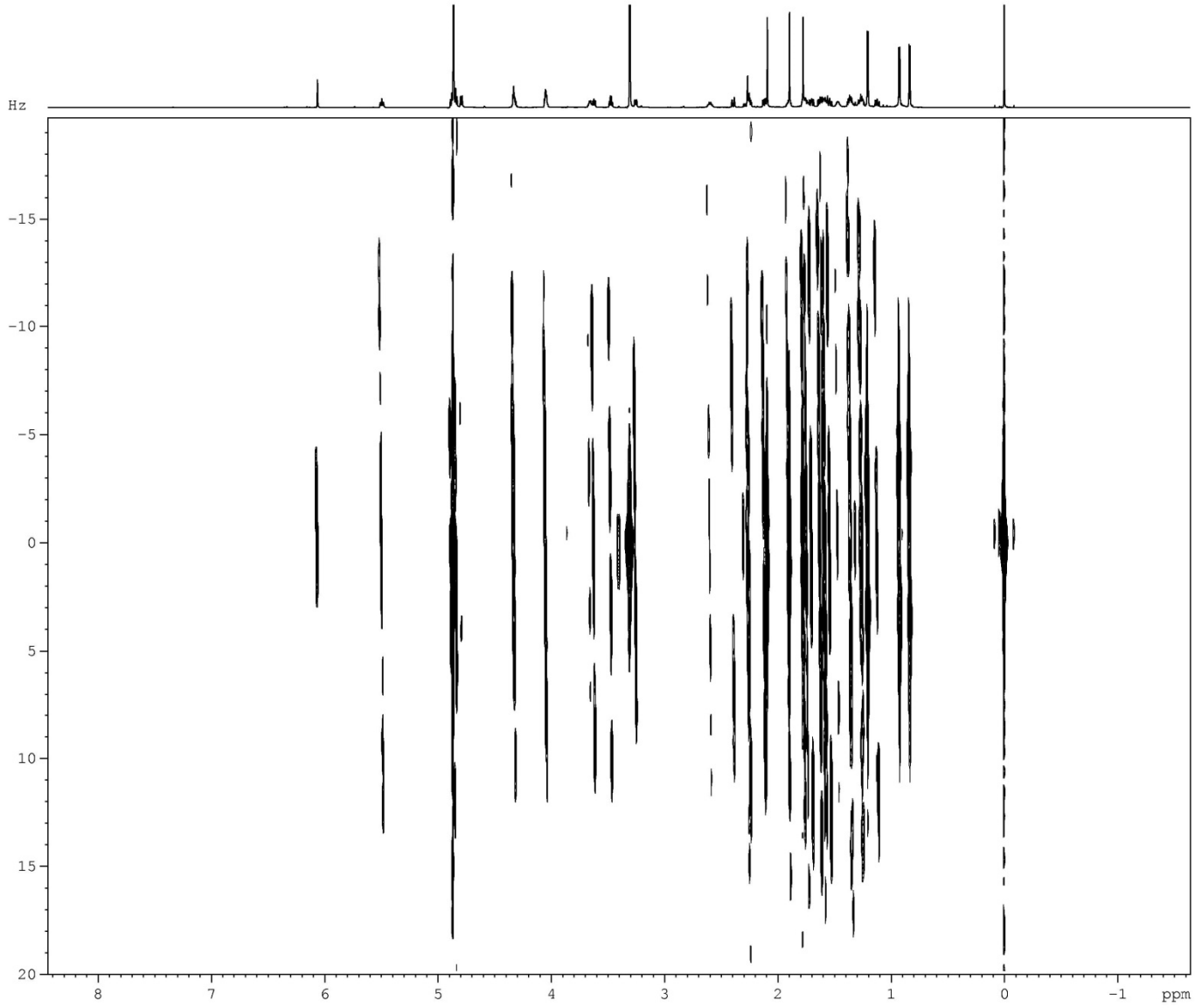
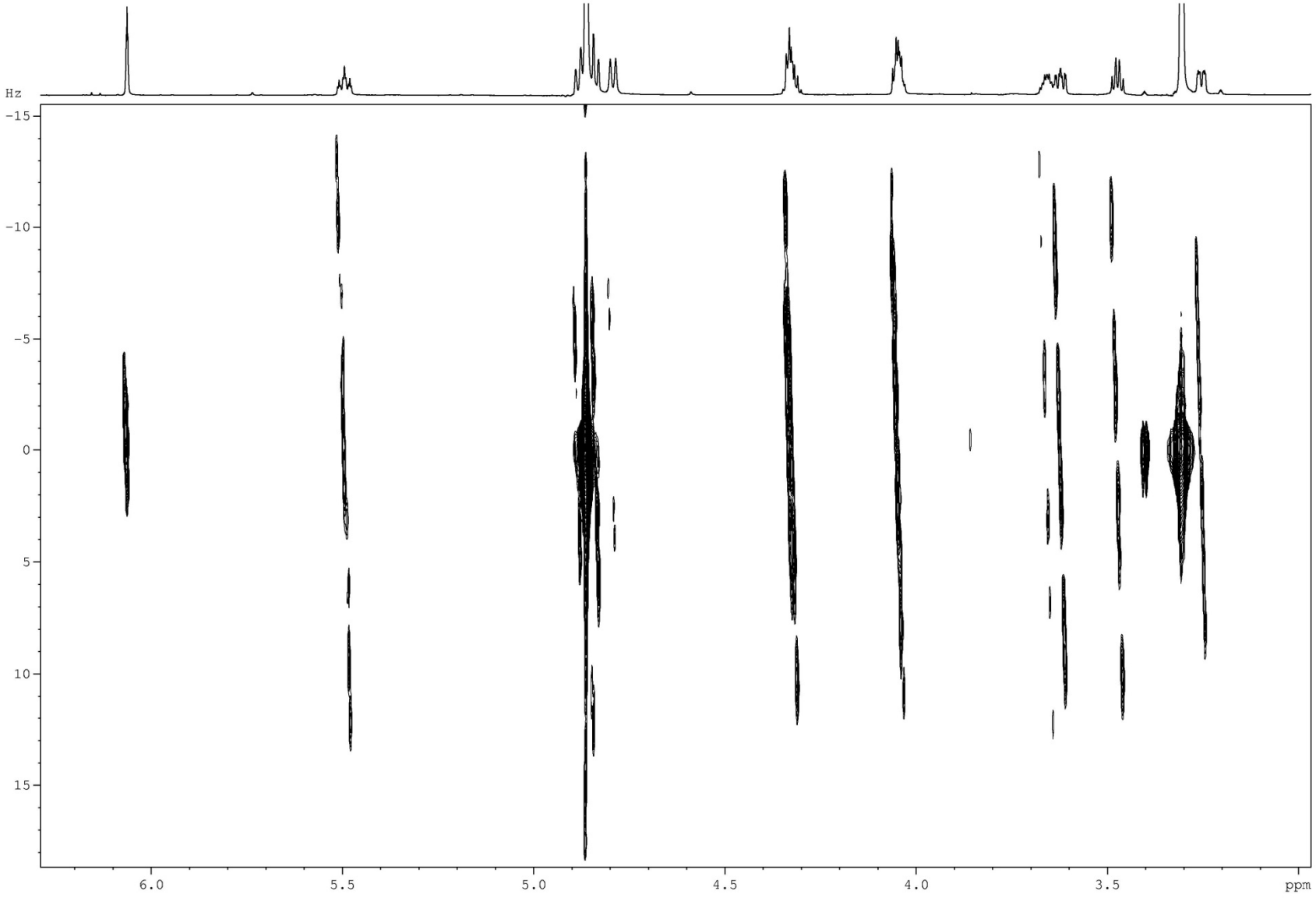


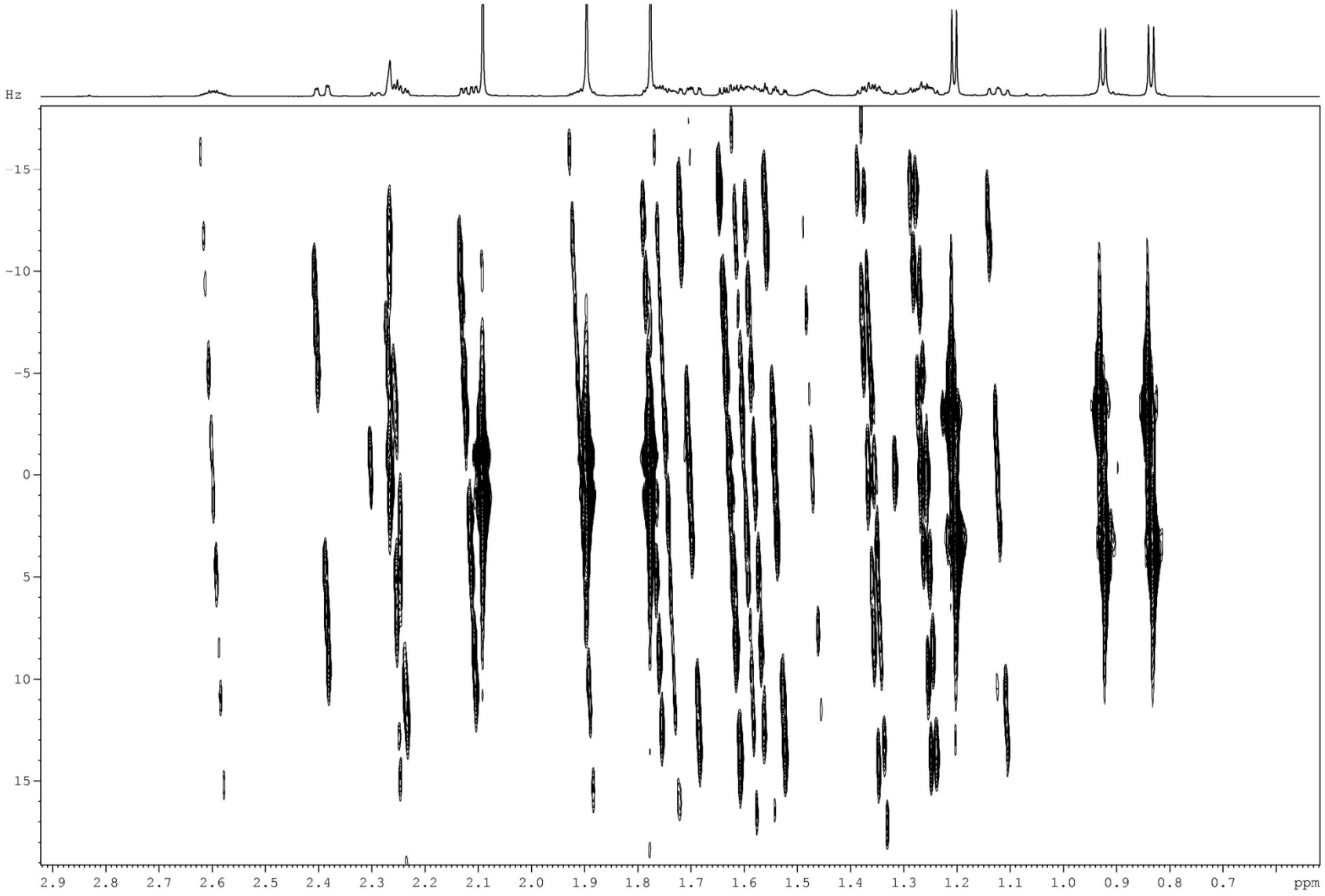
2D *J*RES (700 MHz) spectrum of compound **1** in CD_3OD



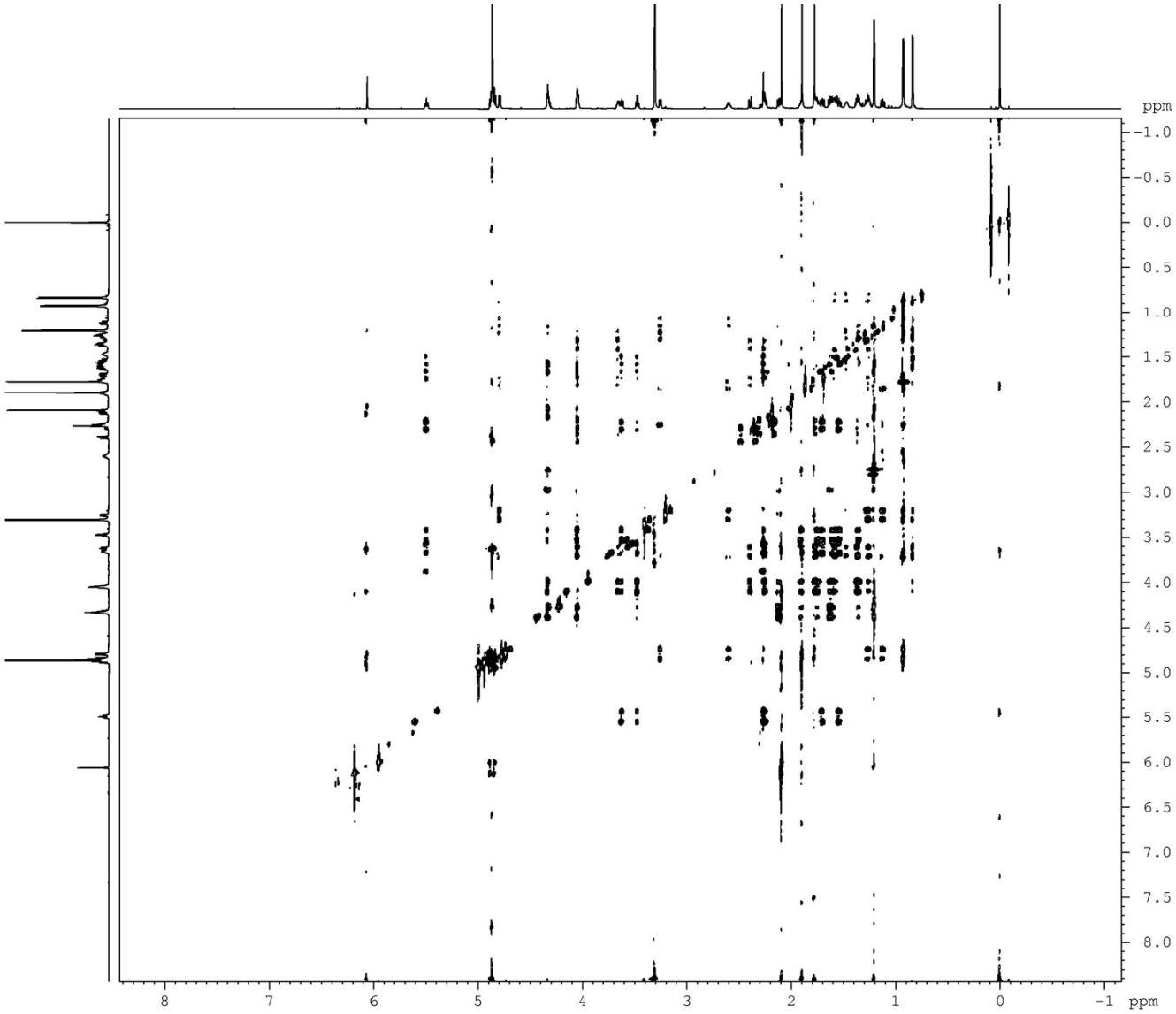
2D *J*RES (700 MHz) spectrum of compound **1** in CD_3OD



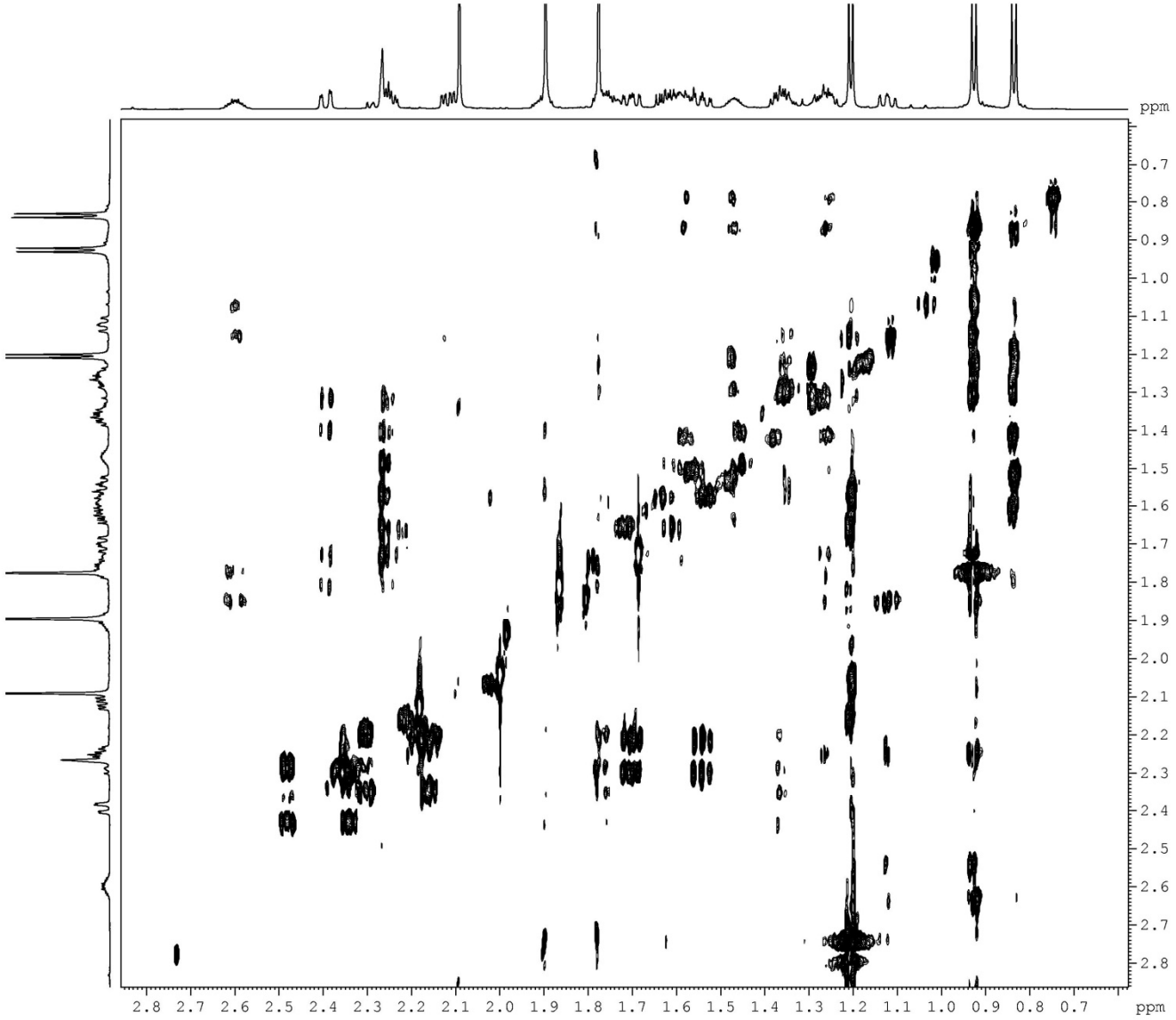
2D *J*RES (700 MHz) spectrum of compound **1** in CD_3OD



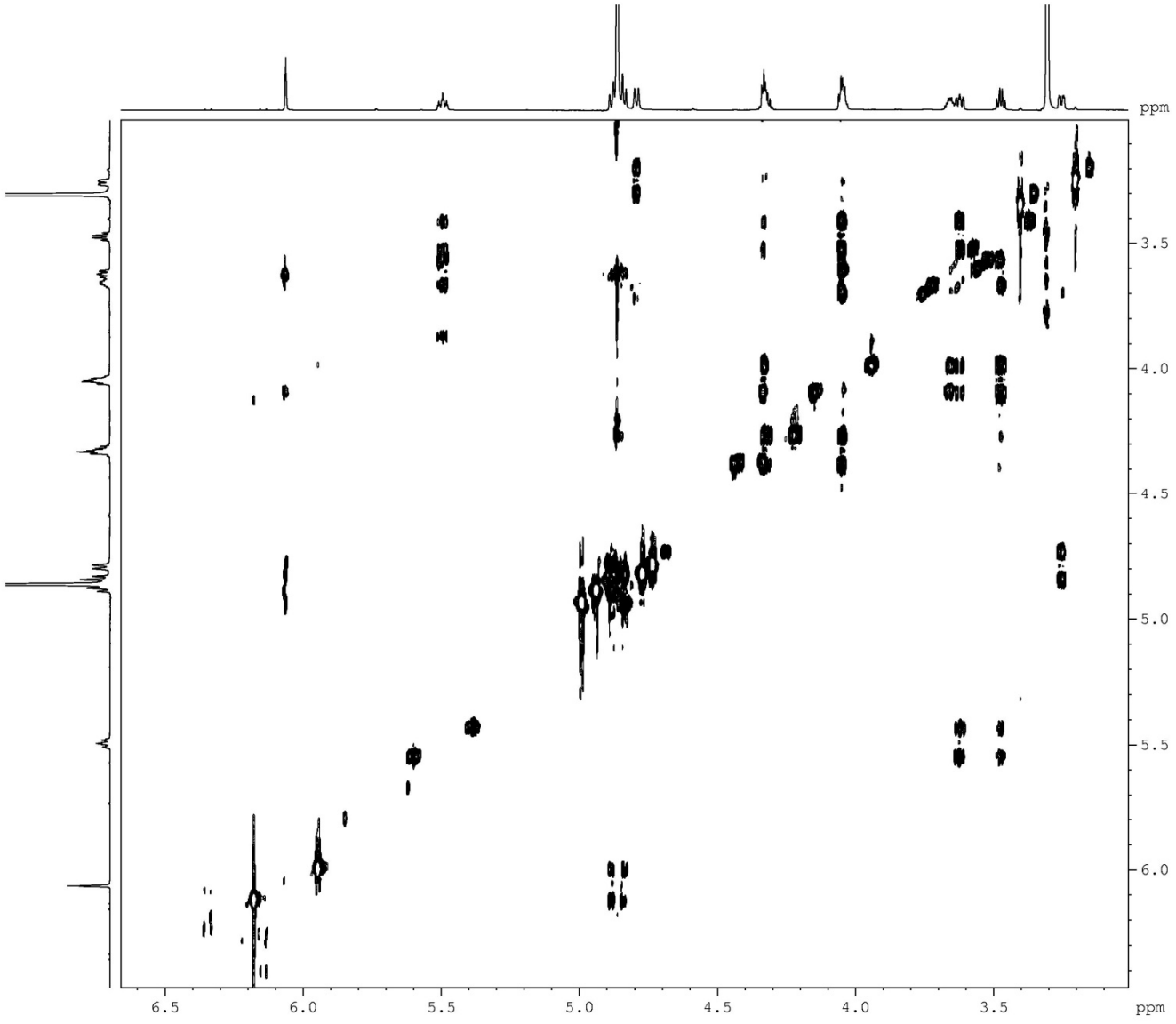
HETLOC (700 MHz) spectrum of compound **1** in CD_3OD



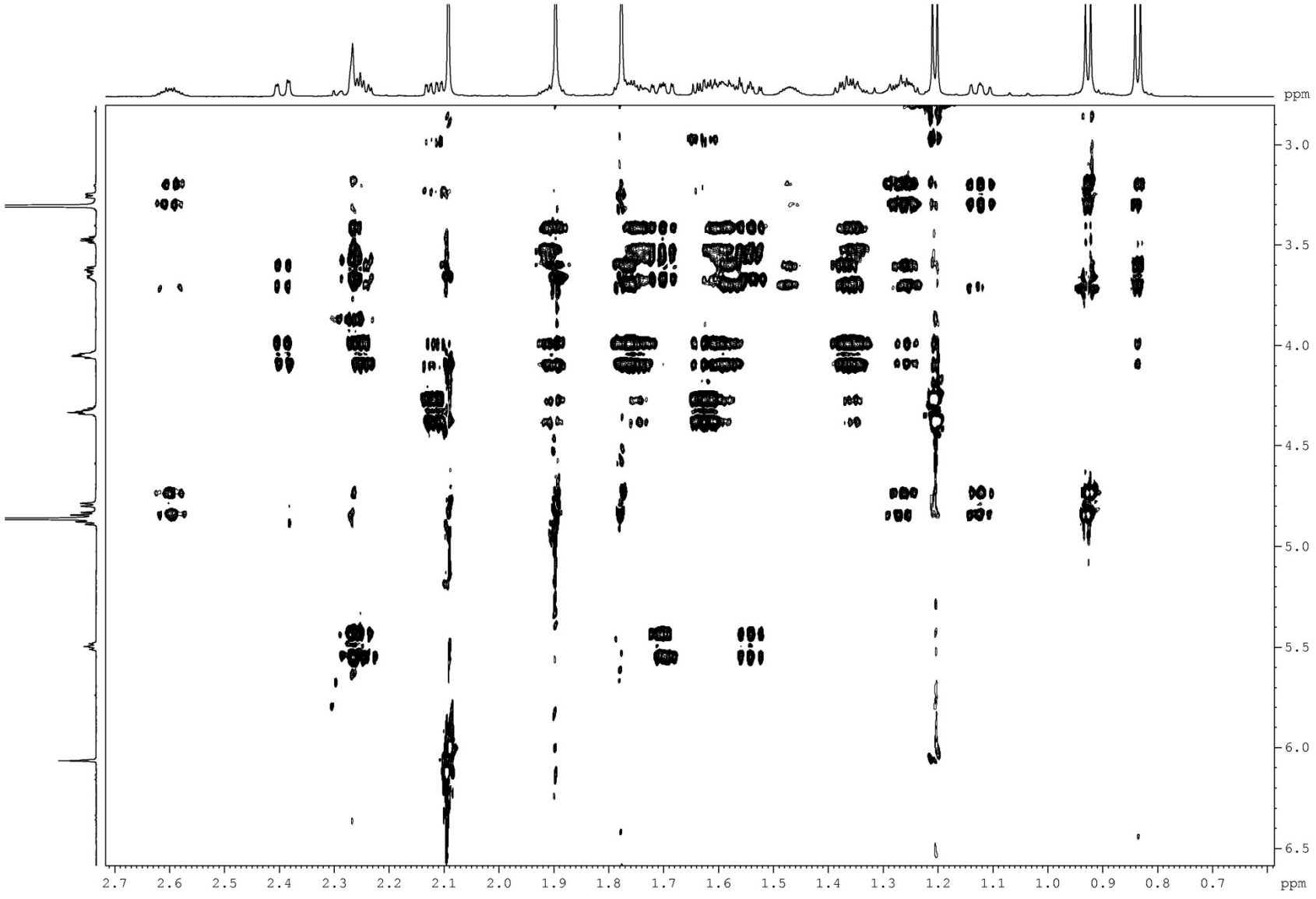
HETLOC (700 MHz) spectrum of compound **1** in CD_3OD



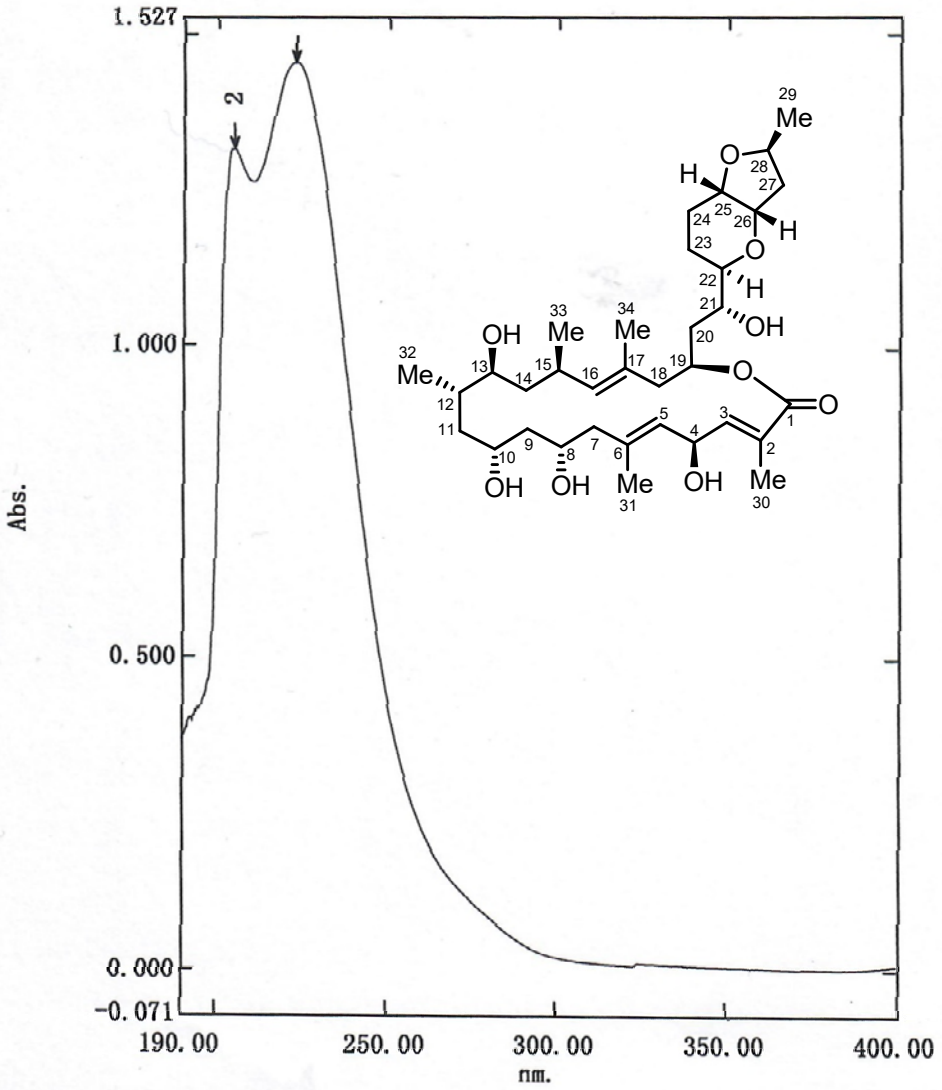
HETLOC (700 MHz) spectrum of compound **1** in CD_3OD



HETLOC (700 MHz) spectrum of compound **1** in CD_3OD

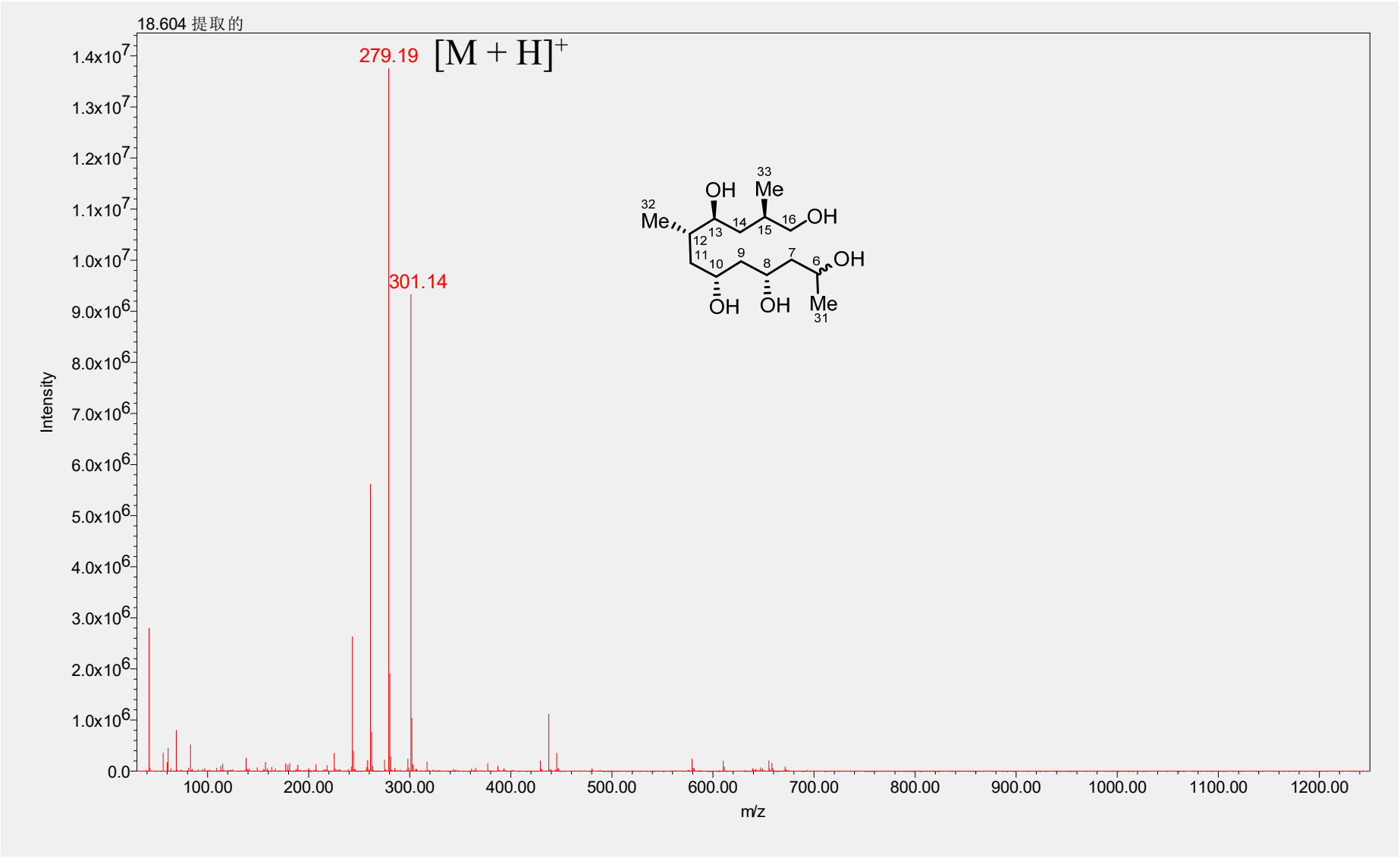


UV spectrum of compound **1**

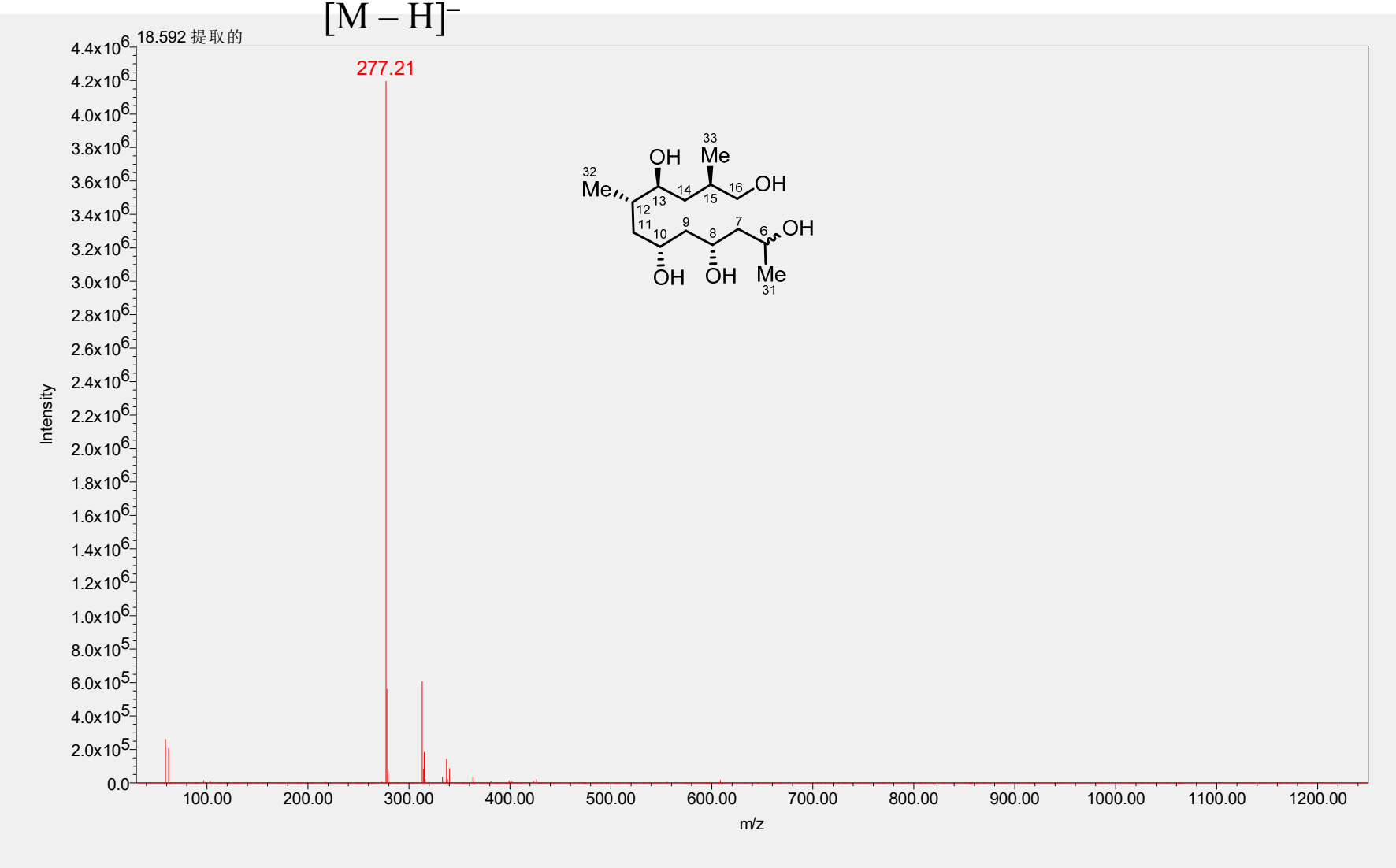


No.	P/V	(nm)	
1		223.20	1.455
2		204.80	1.312

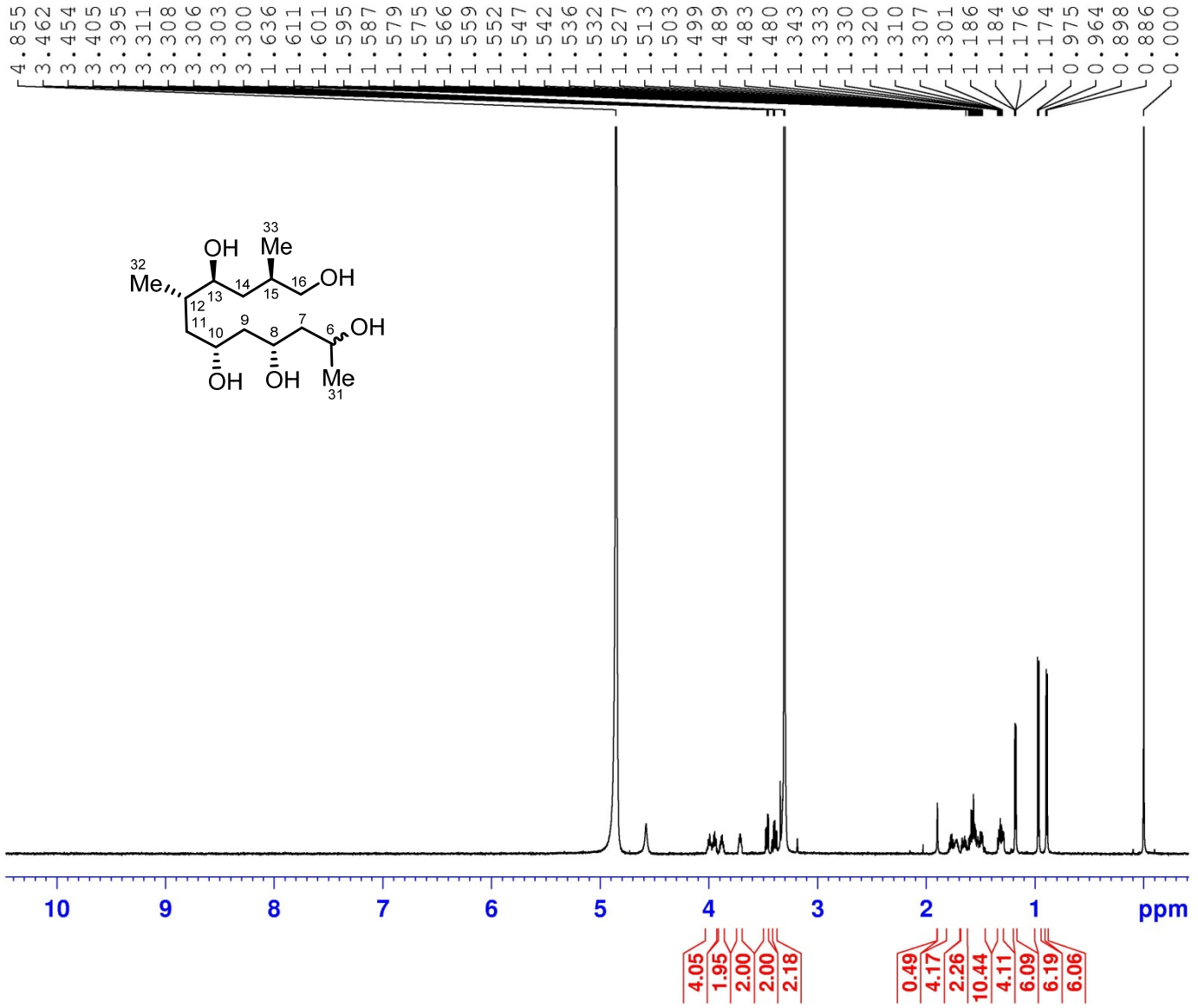
LR-ESIMS for the fragment **1A**



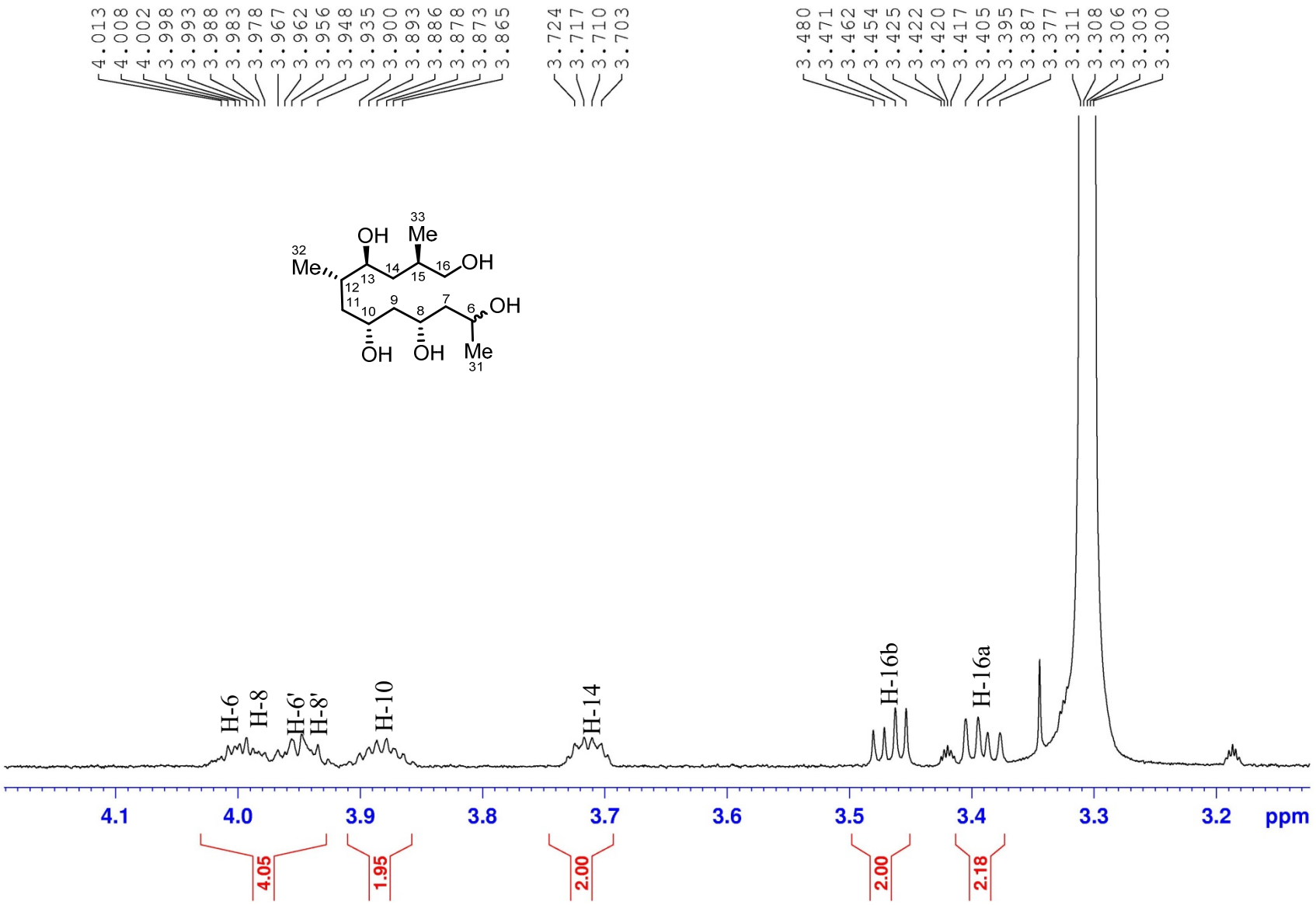
LR-ESIMS for the fragment **1A**



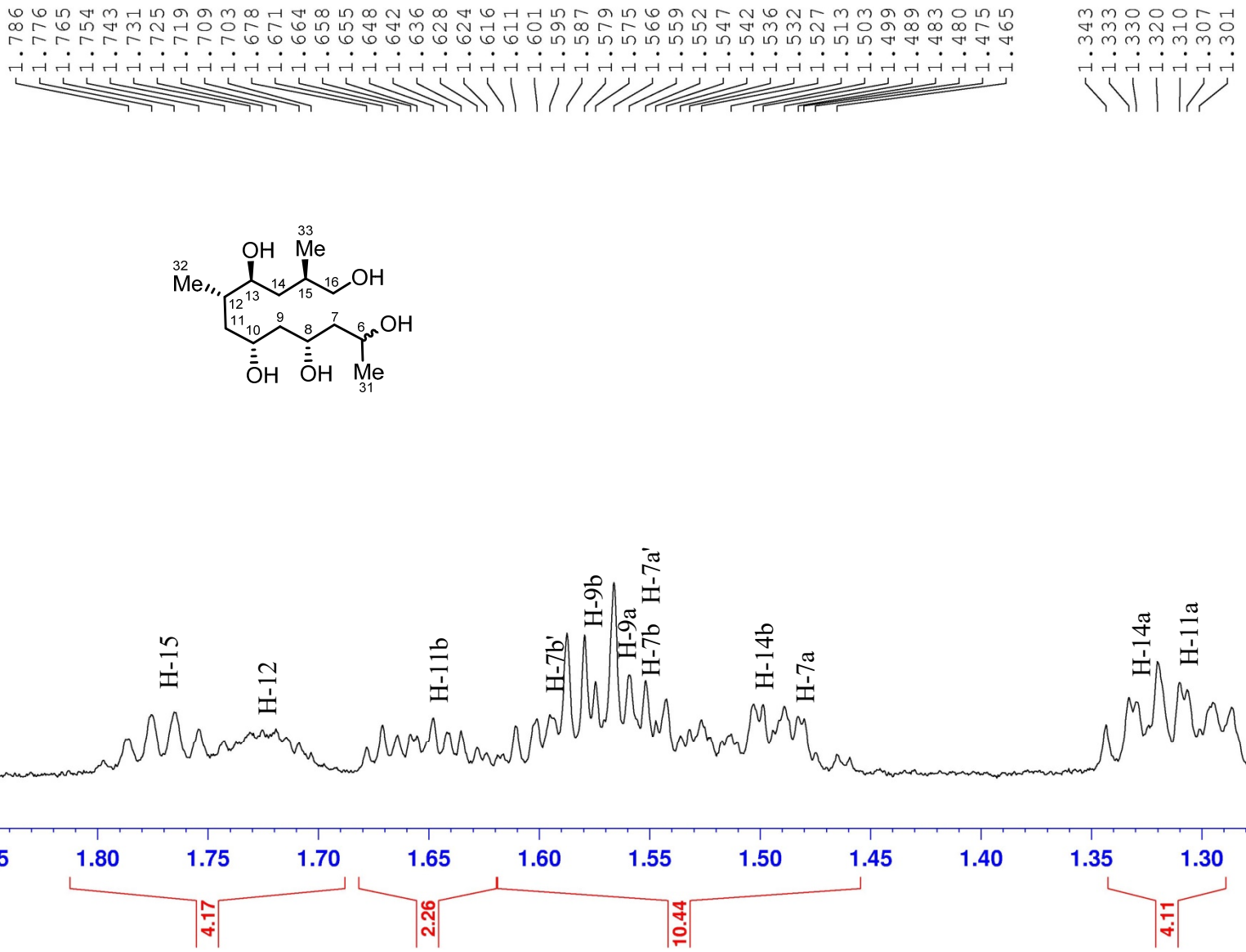
^{1}H (600 MHz) NMR spectrum of the fragment **1A** in CD_3OD



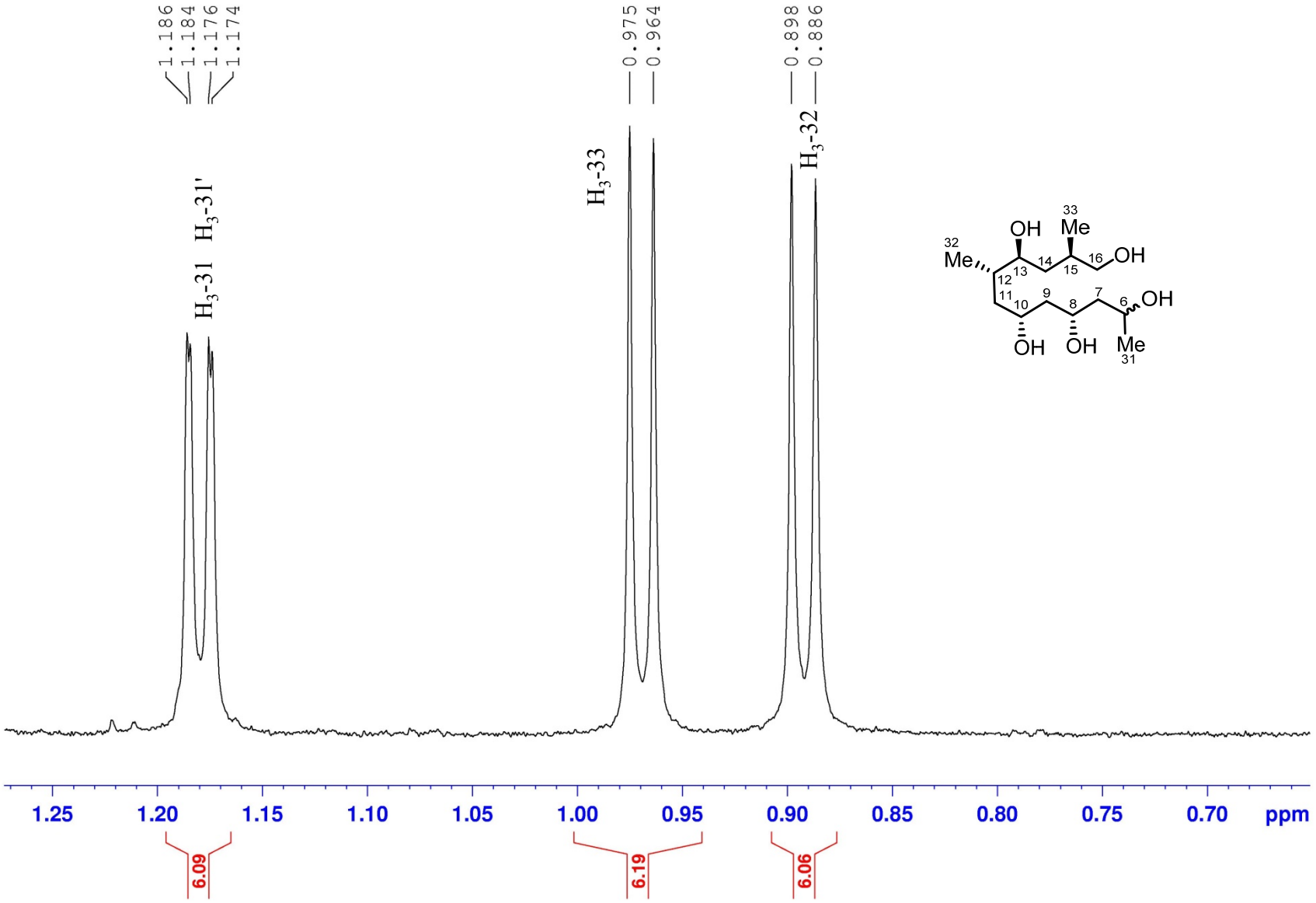
^{1}H (600 MHz) NMR spectrum of the fragment **1A** in CD_3OD



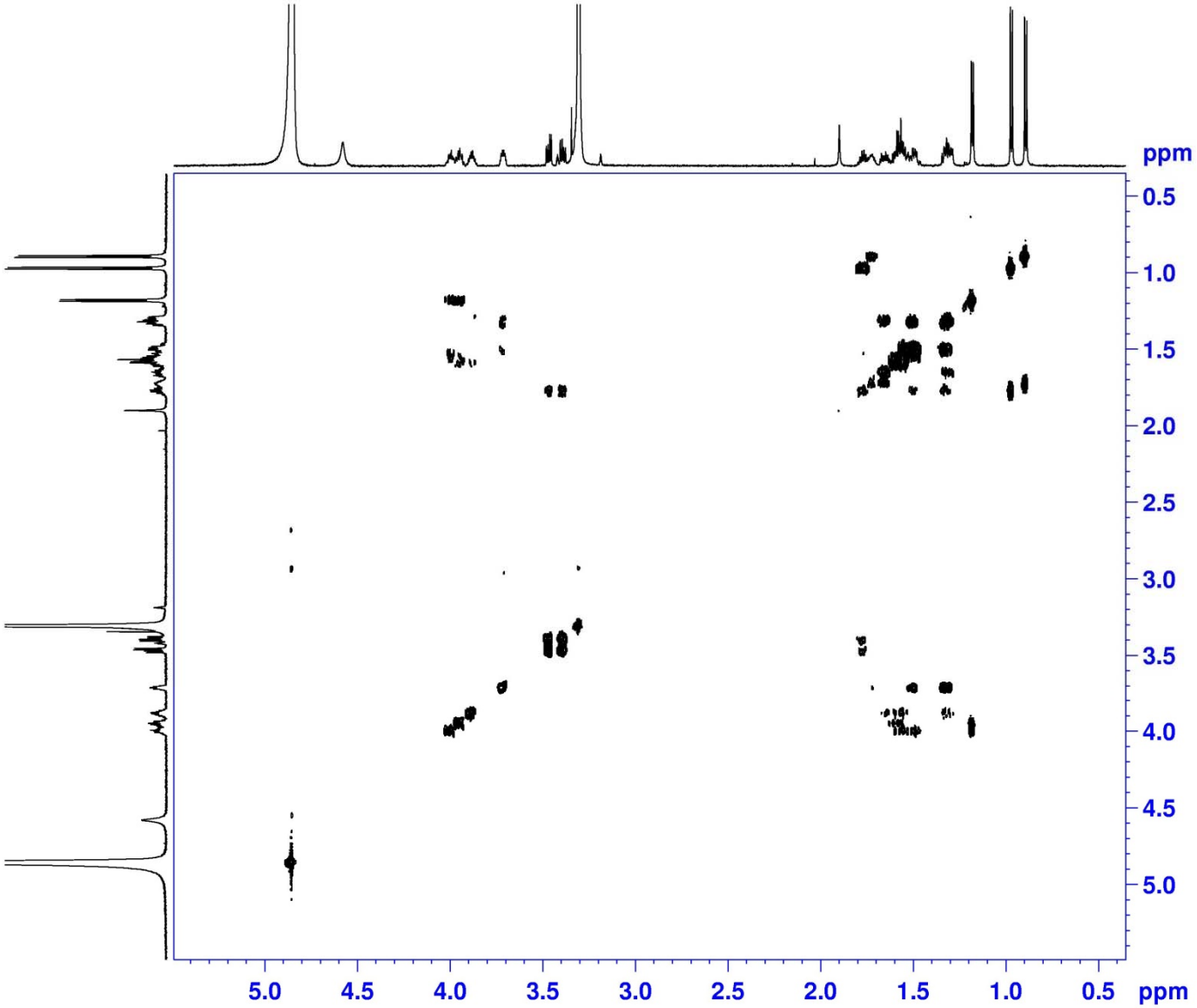
^{1}H (600 MHz) NMR spectrum of the fragment **1A** in CD_3OD



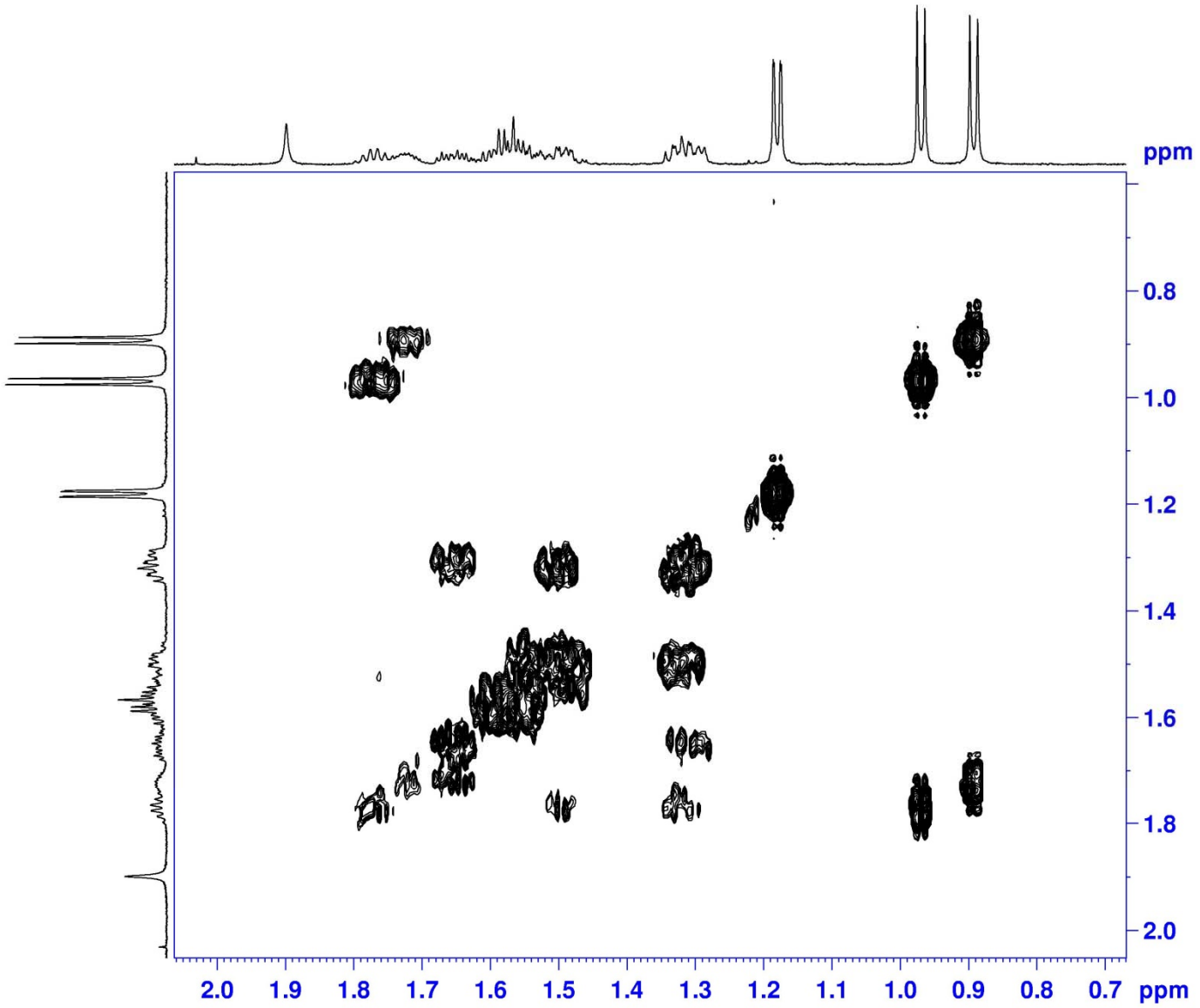
^{1}H (600 MHz) NMR spectrum of the fragment **1A** in CD_3OD



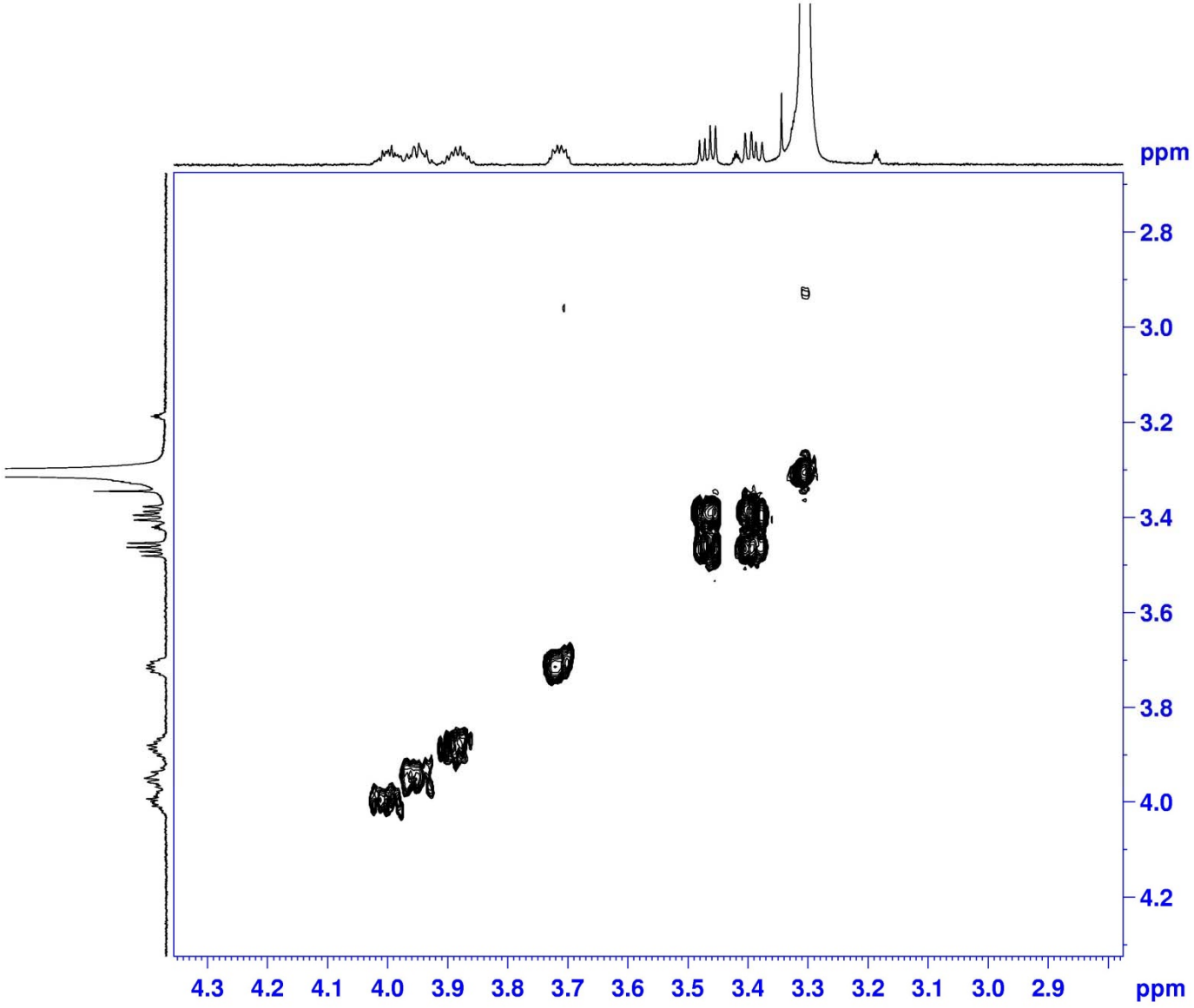
^{1}H–^{1}H COSY (600 MHz) spectrum of the fragment **1A** in CD_3OD



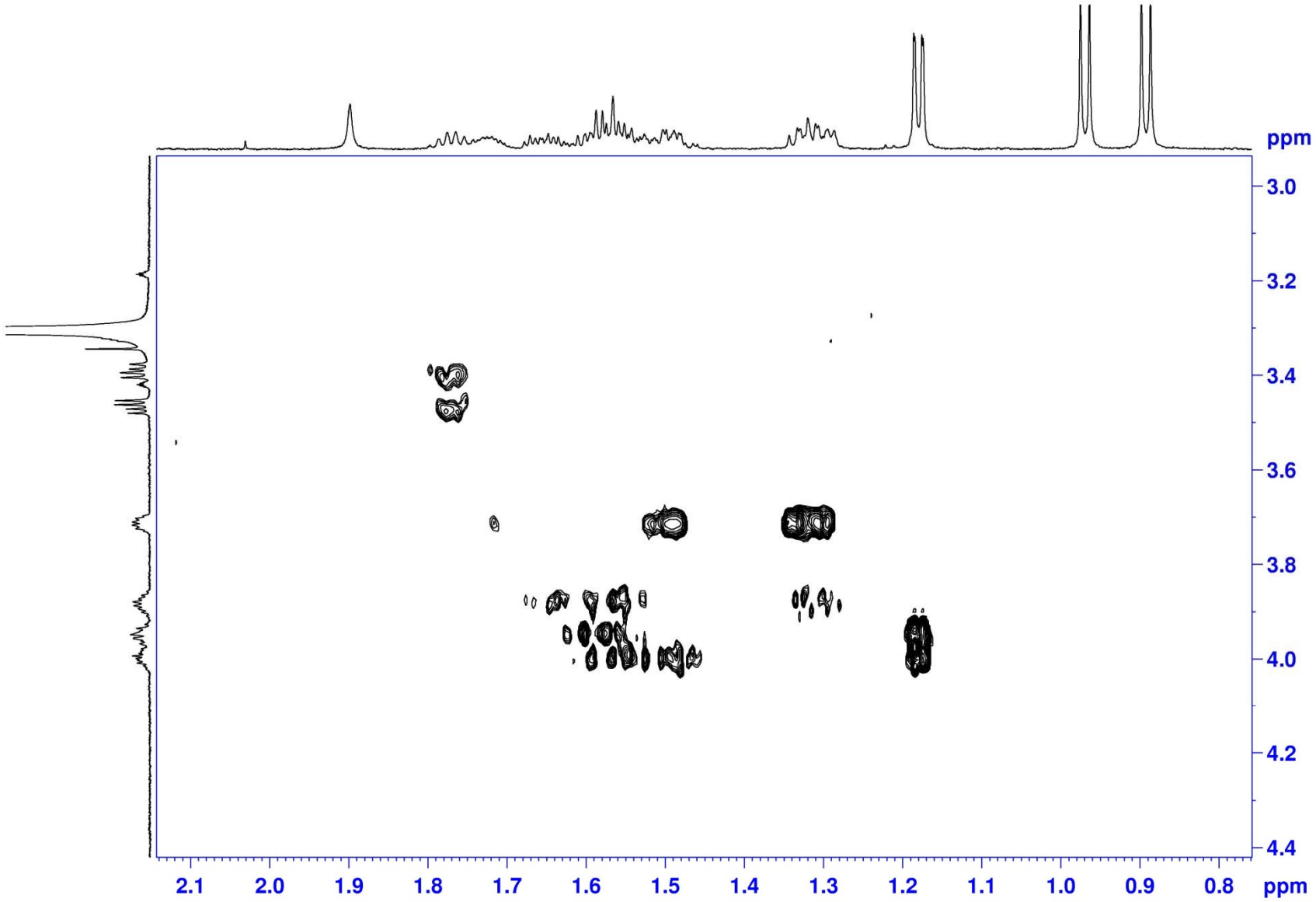
^{1}H–^{1}H COSY (600 MHz) spectrum of the fragment **1A** in CD_3OD



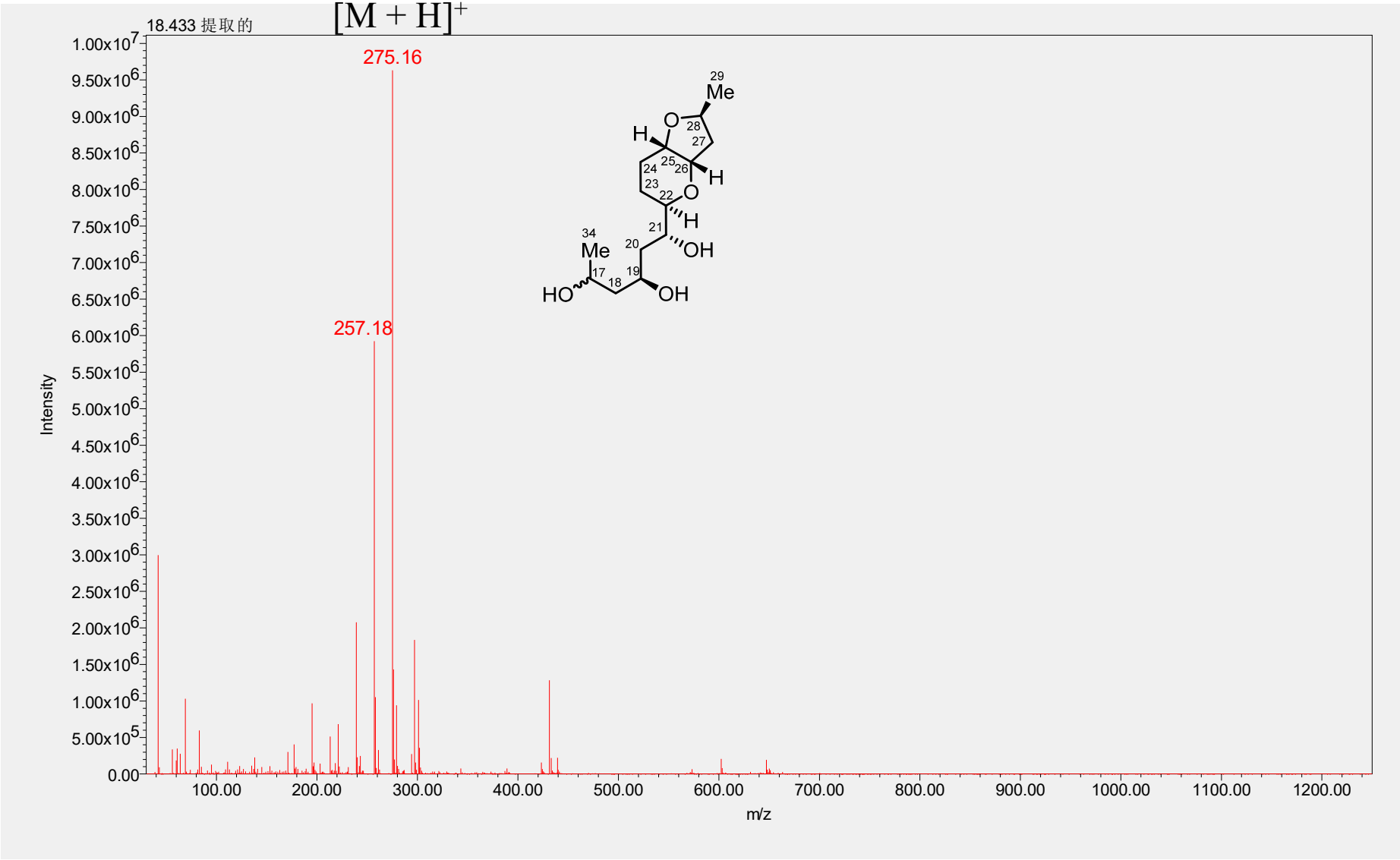
$^{1}H–^{1}H$ COSY (600 MHz) spectrum of the fragment **1A** in CD_3OD



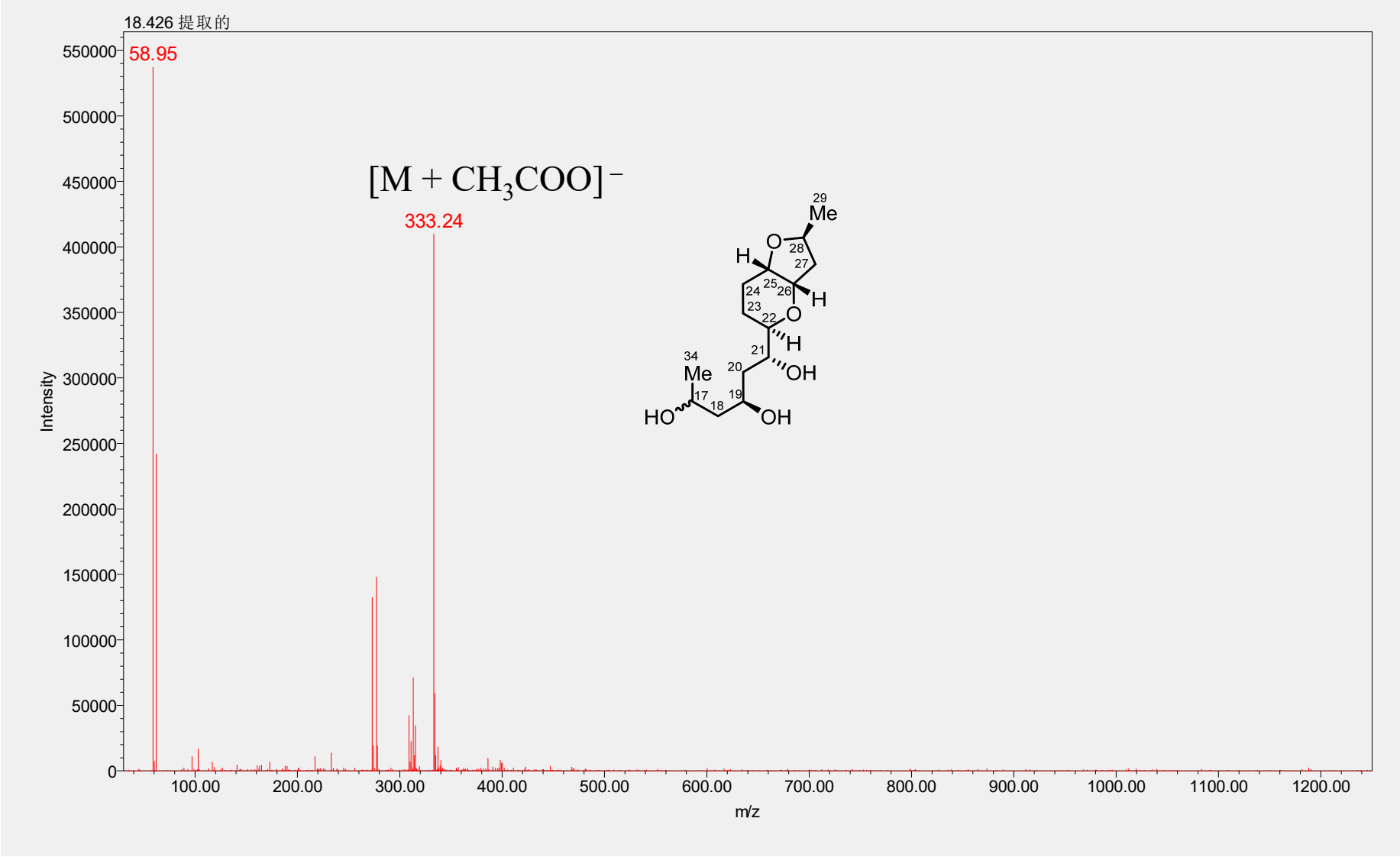
$^{1}H–^{1}H$ COSY (600 MHz) spectrum of the fragment **1A** in CD_3OD



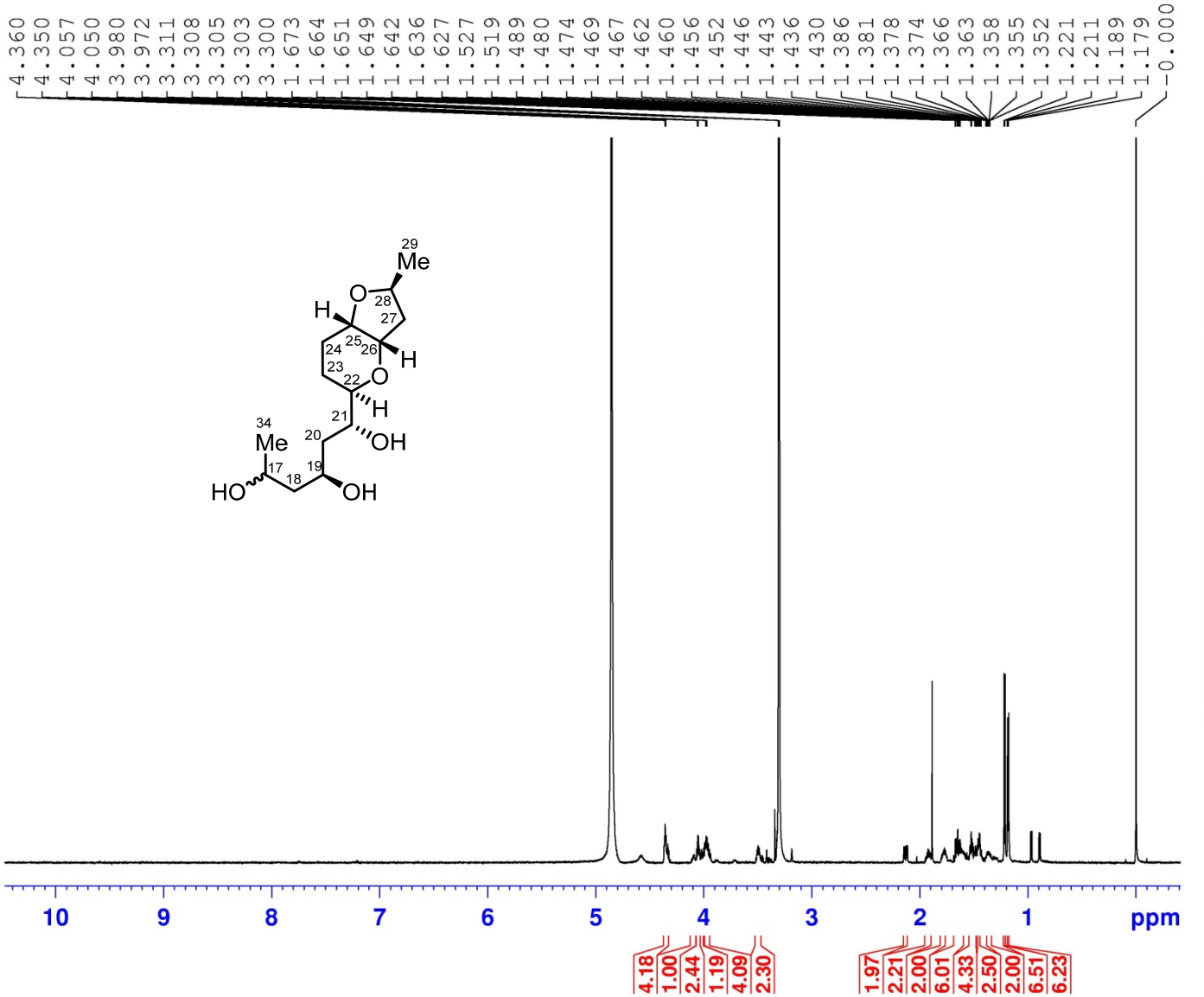
LR-ESIMS for the fragment **1B**



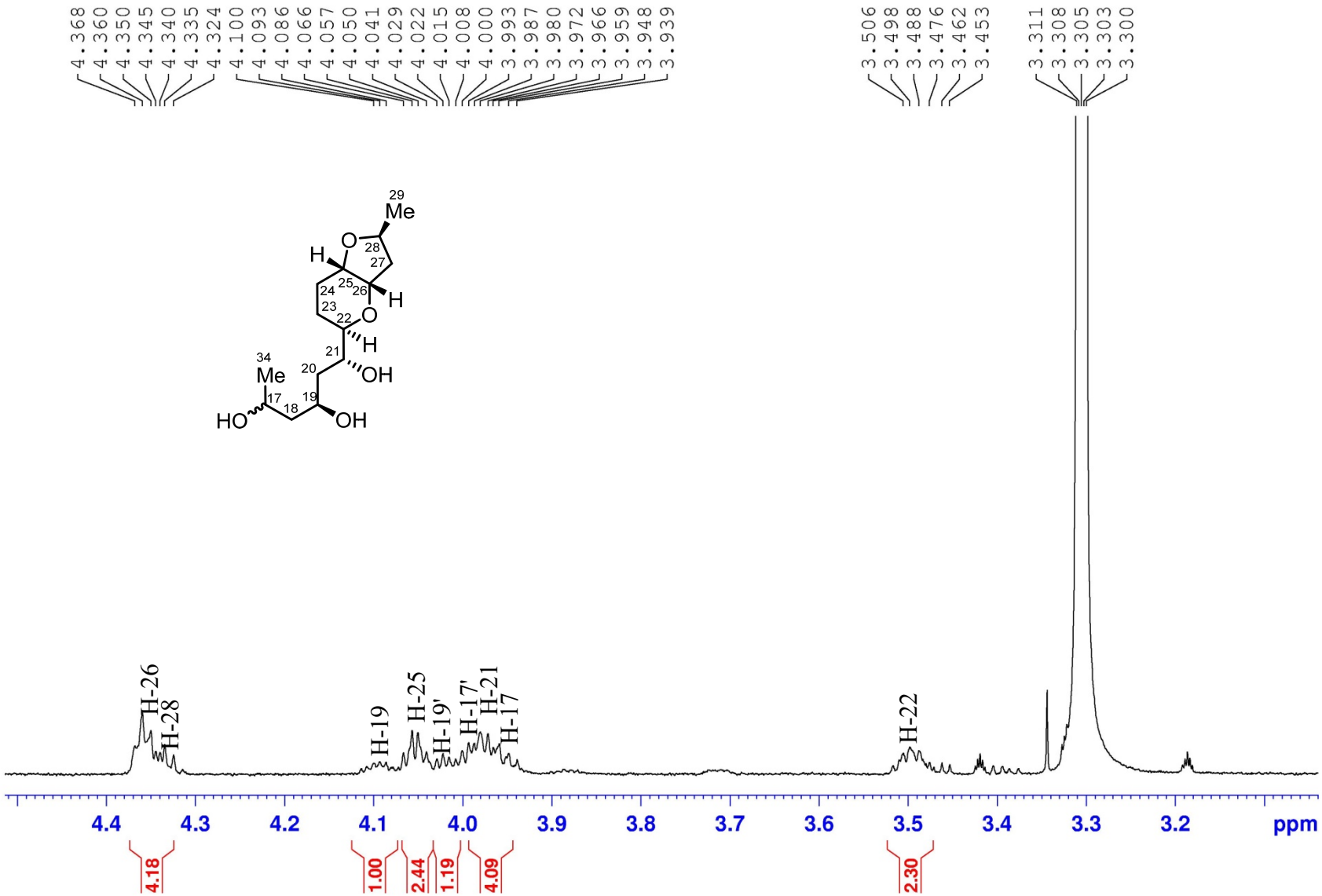
LR-ESIMS for the fragment **1B**



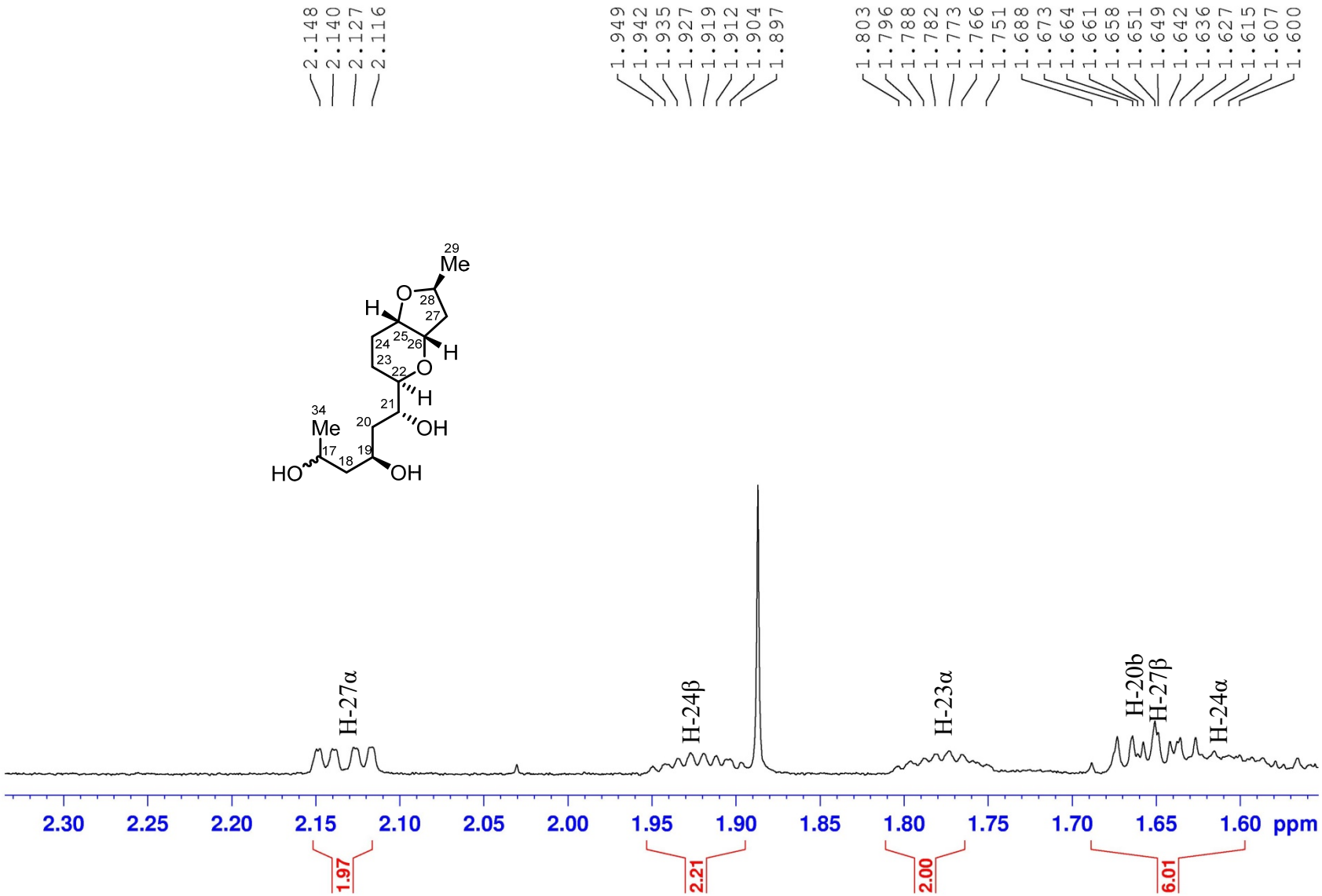
^{1}H (600 MHz) NMR spectrum of the fragment **1B** in CD_3OD



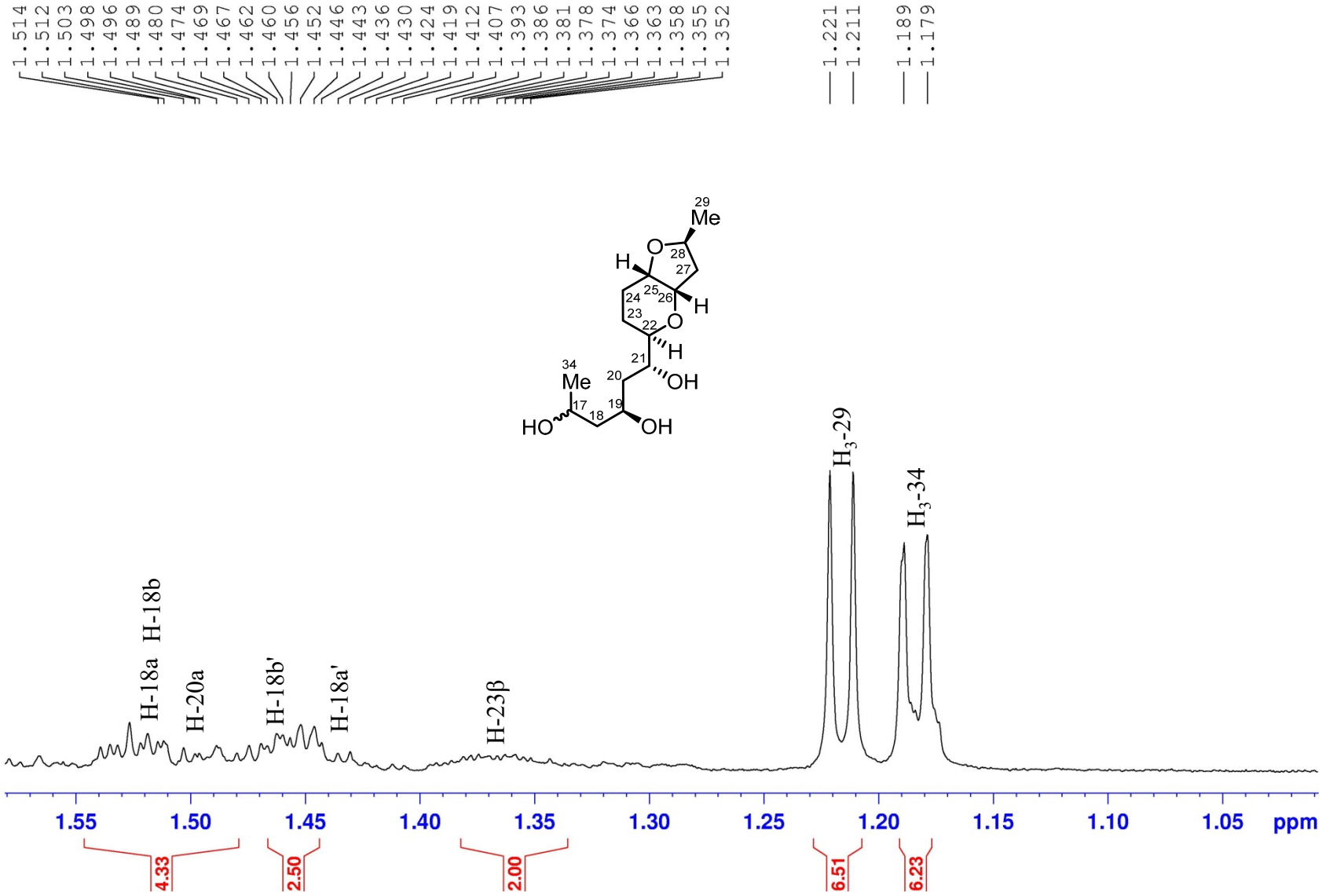
^{1}H (600 MHz) NMR spectrum of the fragment **1B** in CD_3OD



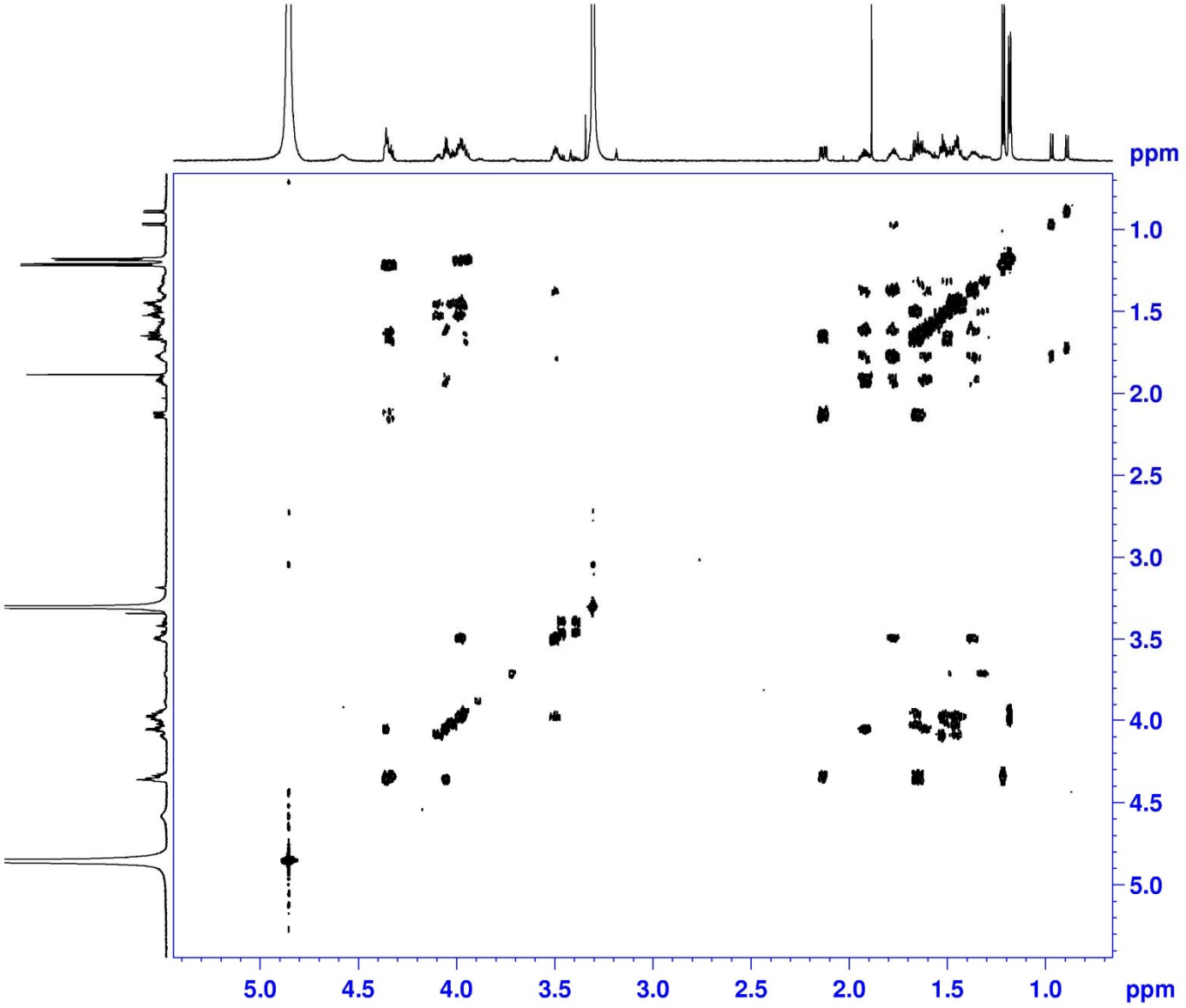
^{1}H (600 MHz) NMR spectrum of the fragment **1B** in CD_3OD



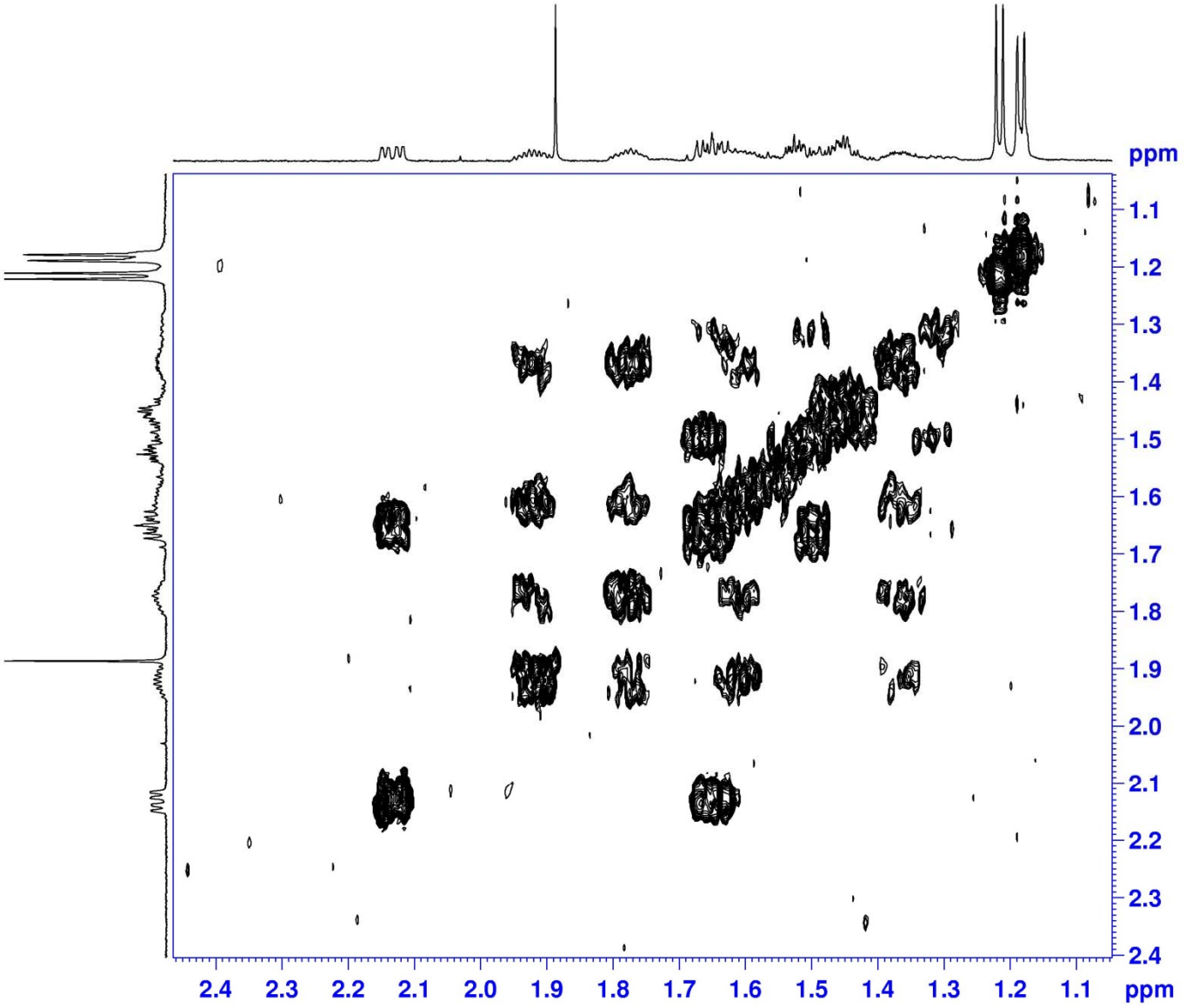
^{1}H (600 MHz) NMR spectrum of the fragment **1B** in CD_3OD



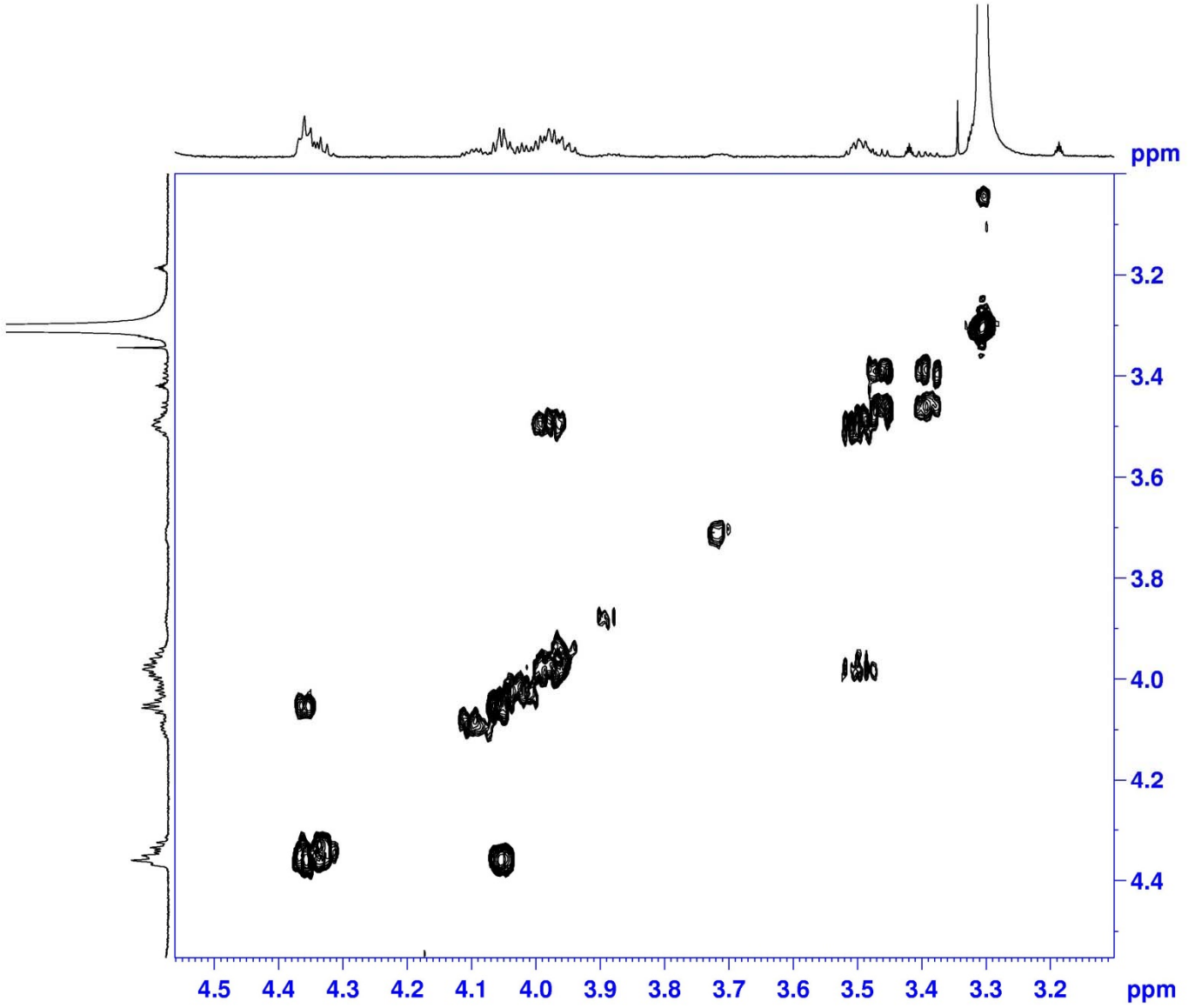
$^{1}H–^{1}H$ COSY (600 MHz) spectrum of the fragment **1B** in CD_3OD



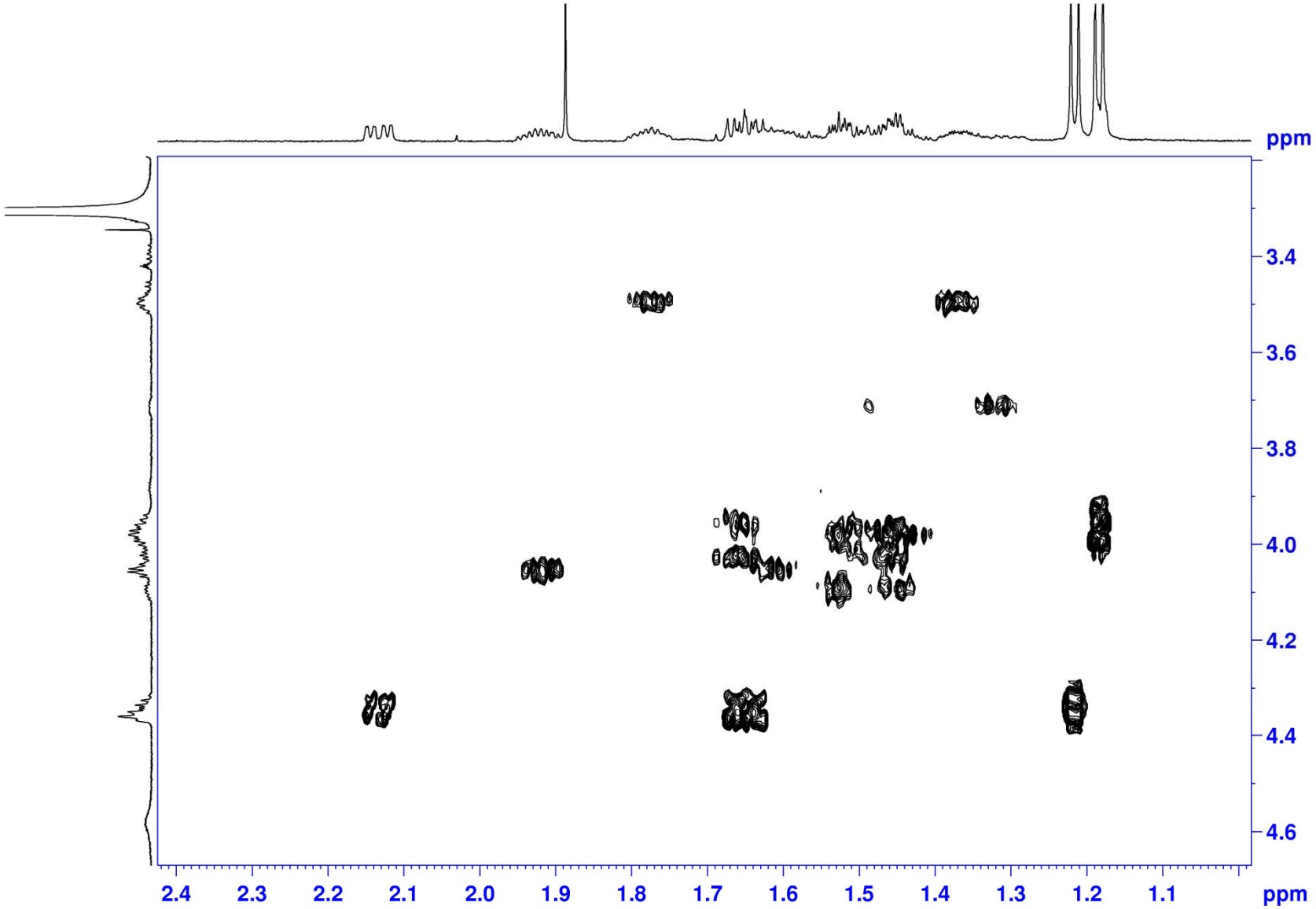
$^{1}H–^{1}H$ COSY (600 MHz) spectrum of the fragment **1B** in CD_3OD



$^{1}H–^{1}H$ COSY (600 MHz) spectrum of the fragment **1B** in CD_3OD



$^{1}H–^{1}H$ COSY (600 MHz) spectrum of the fragment **1B** in CD_3OD



HR-ESIMS for compound **1s**

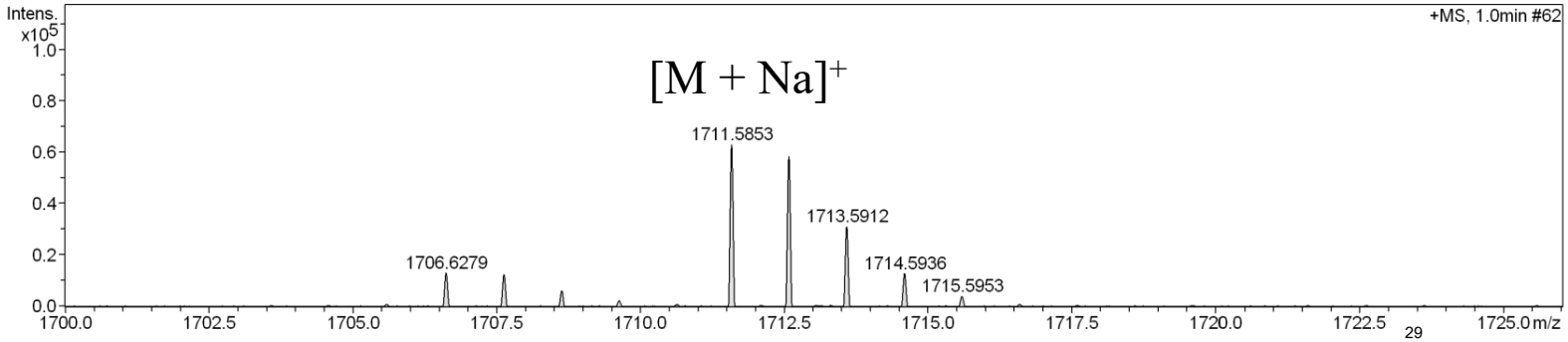
Mass Spectrum SmartFormula Report

Analysis Info

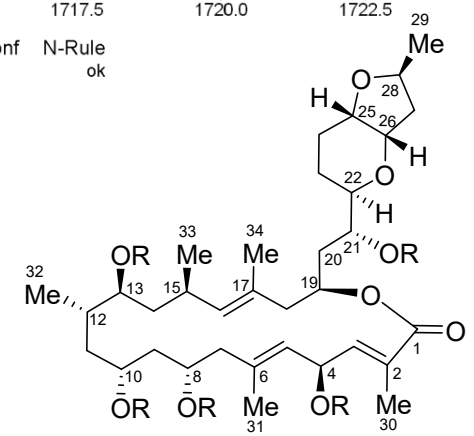
Analysis Name	D:\Data\MS\data\202011\jiangzhongping_37-1-R_pos_3_01_9232.d	Acquisition Date	11/16/2020 4:13:55 PM
Method	LC_Direct Infusion_pos_100-3000mz.m	Operator	SCSIO
Sample Name	jiangzhongping_37-1-R_pos	Instrument	maXis 255552.00029
Comment			

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

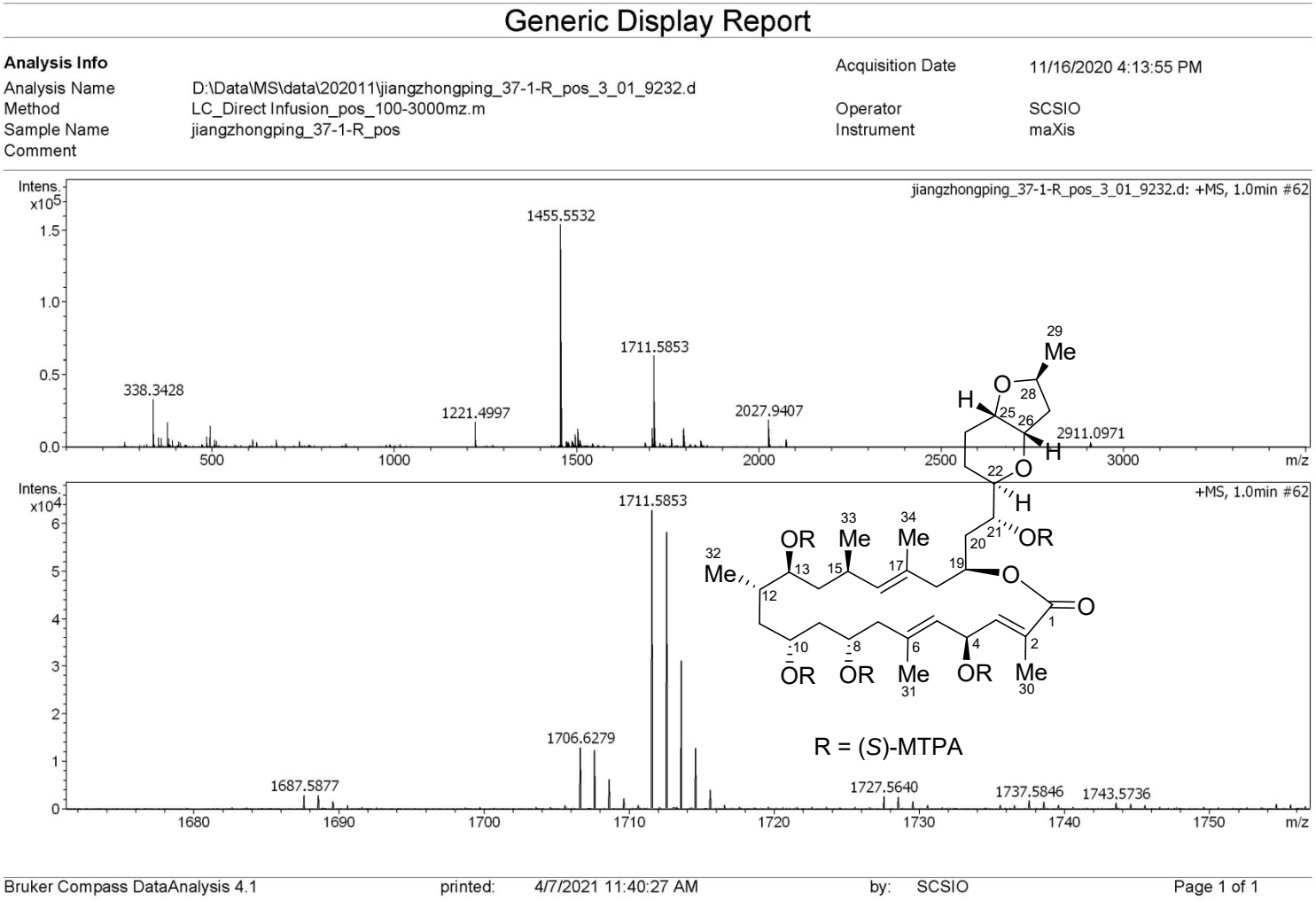


Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
1711.5853	1	C84H91F15NaO19	100.00	1711.5807	-2.7	-4.6	22.5	31.5	even	ok

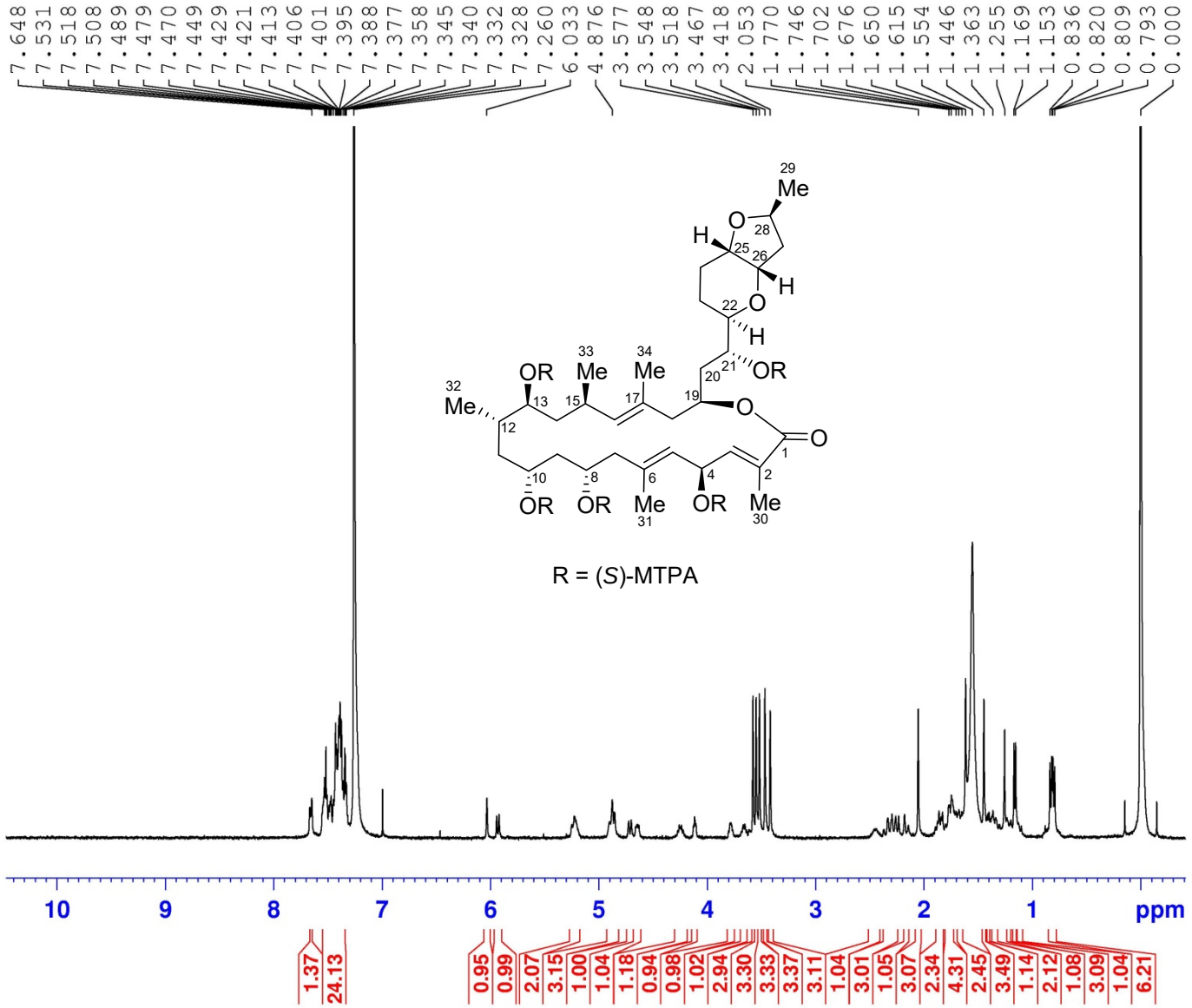


R = (*S*)-MTPA

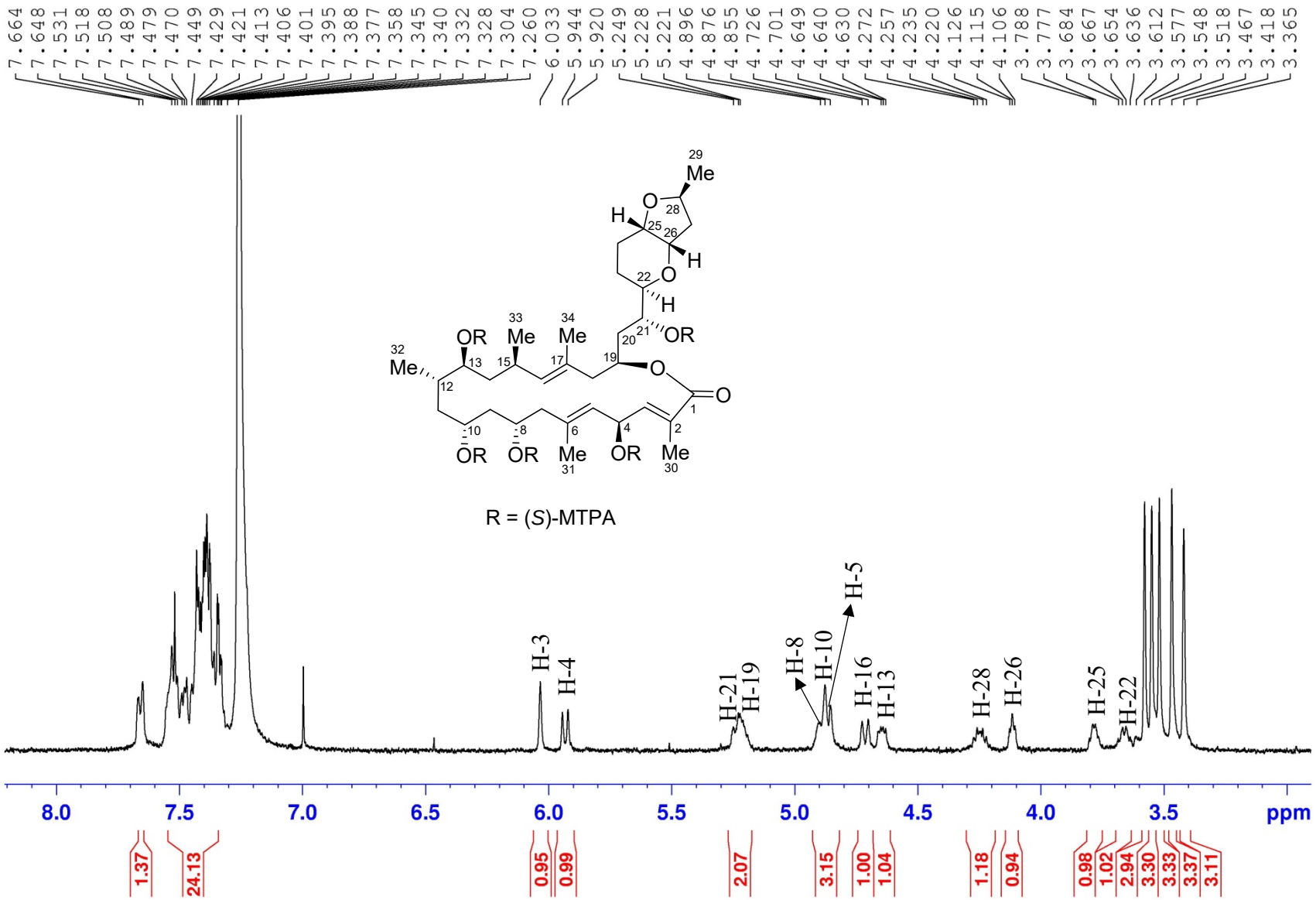
HR-ESIMS for compound **1s**



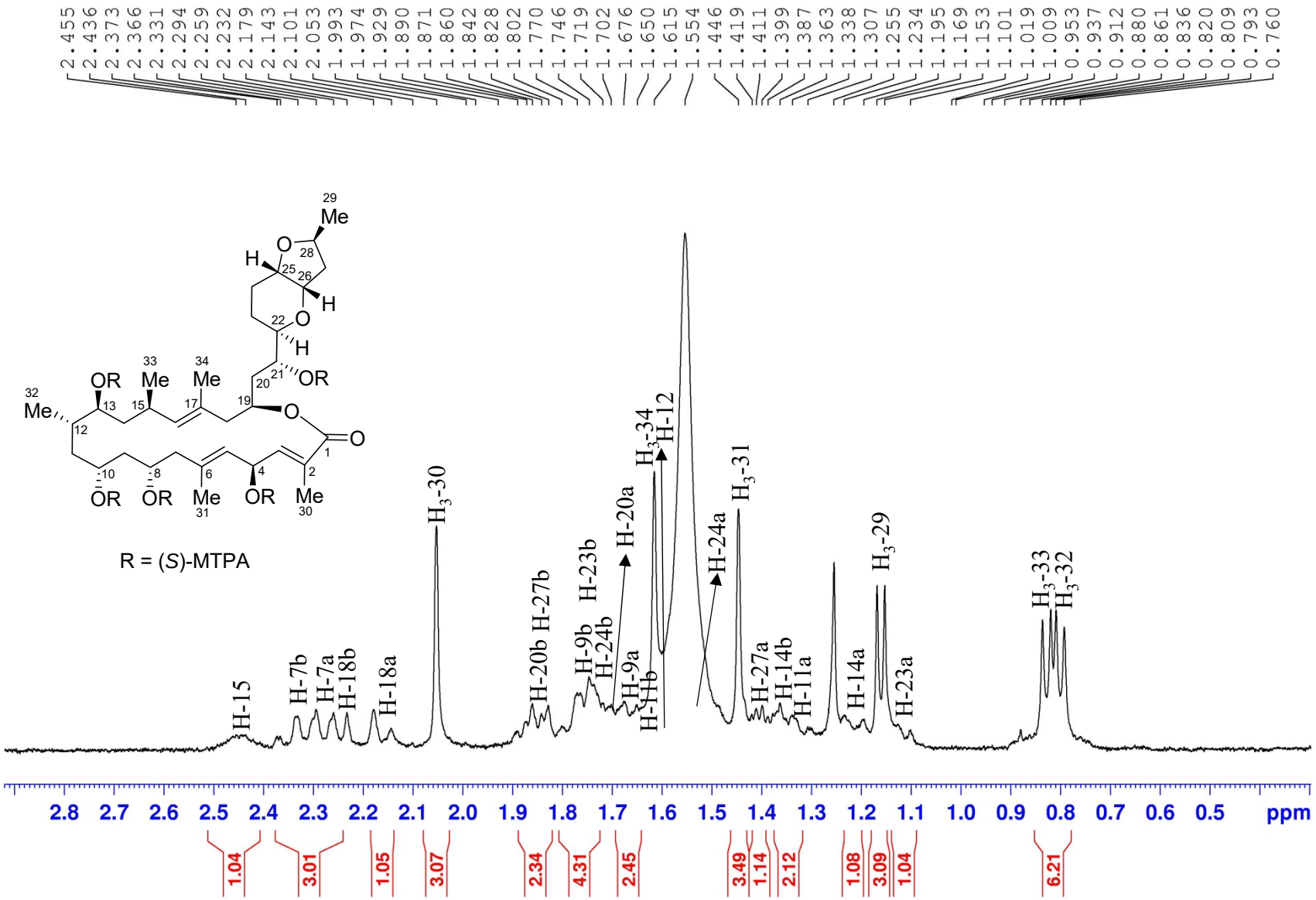
^{1}H (400 MHz) NMR spectrum of compound **1s** in $CDCl_3$



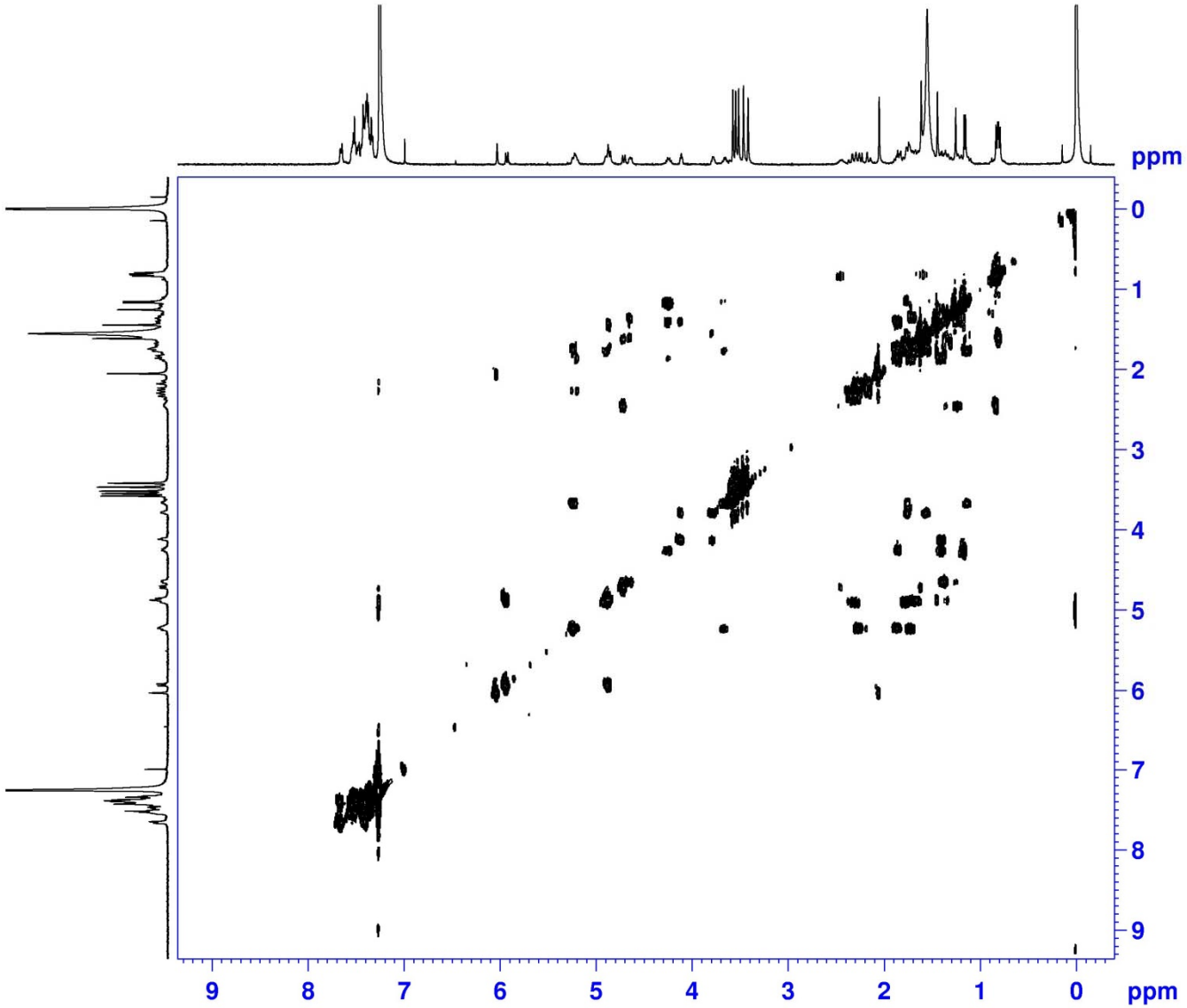
^{1}H (400 MHz) NMR spectrum of compound **1s** in $CDCl_3$



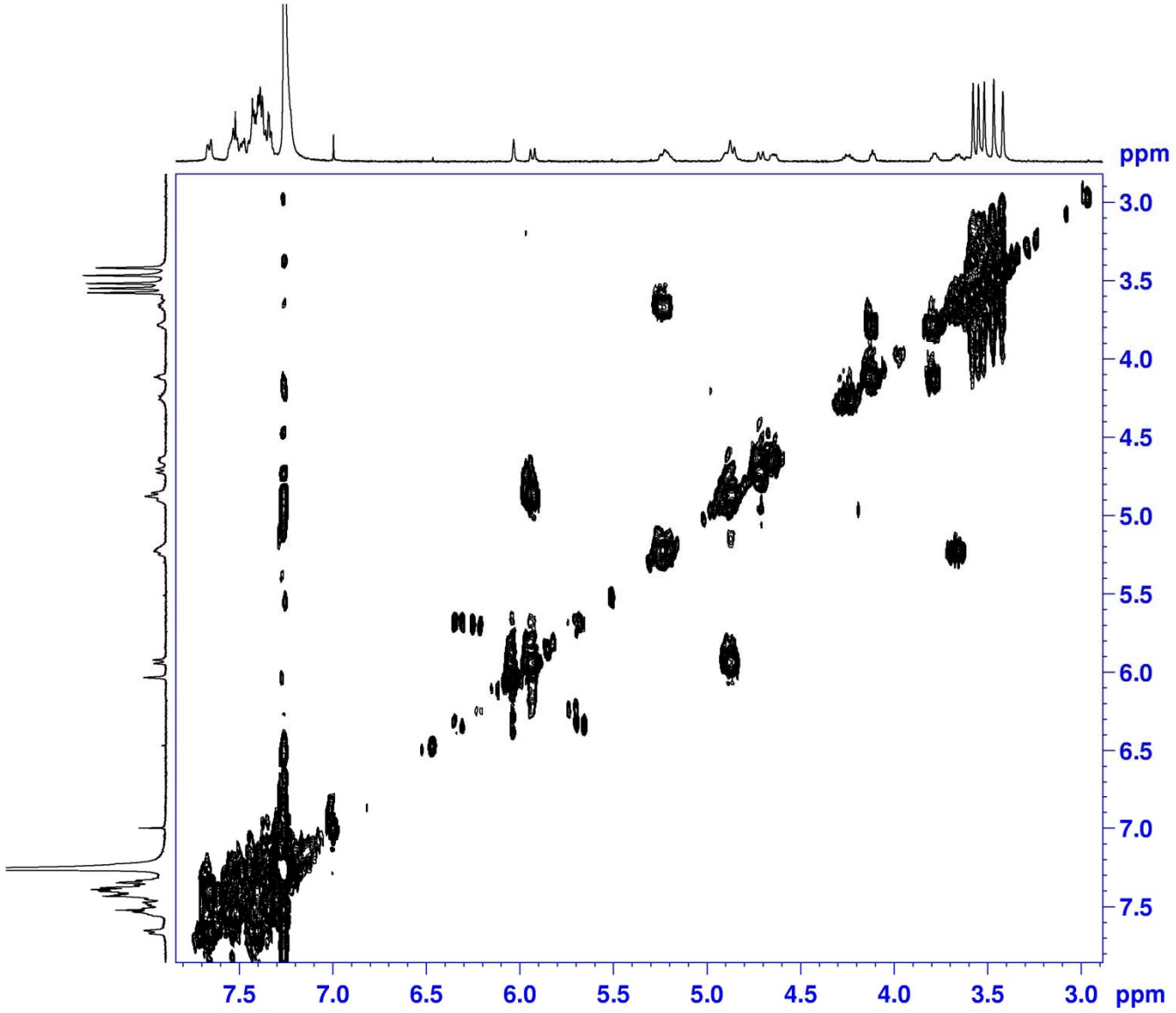
^{1}H (400 MHz) NMR spectrum of compound **1s** in $CDCl_3$



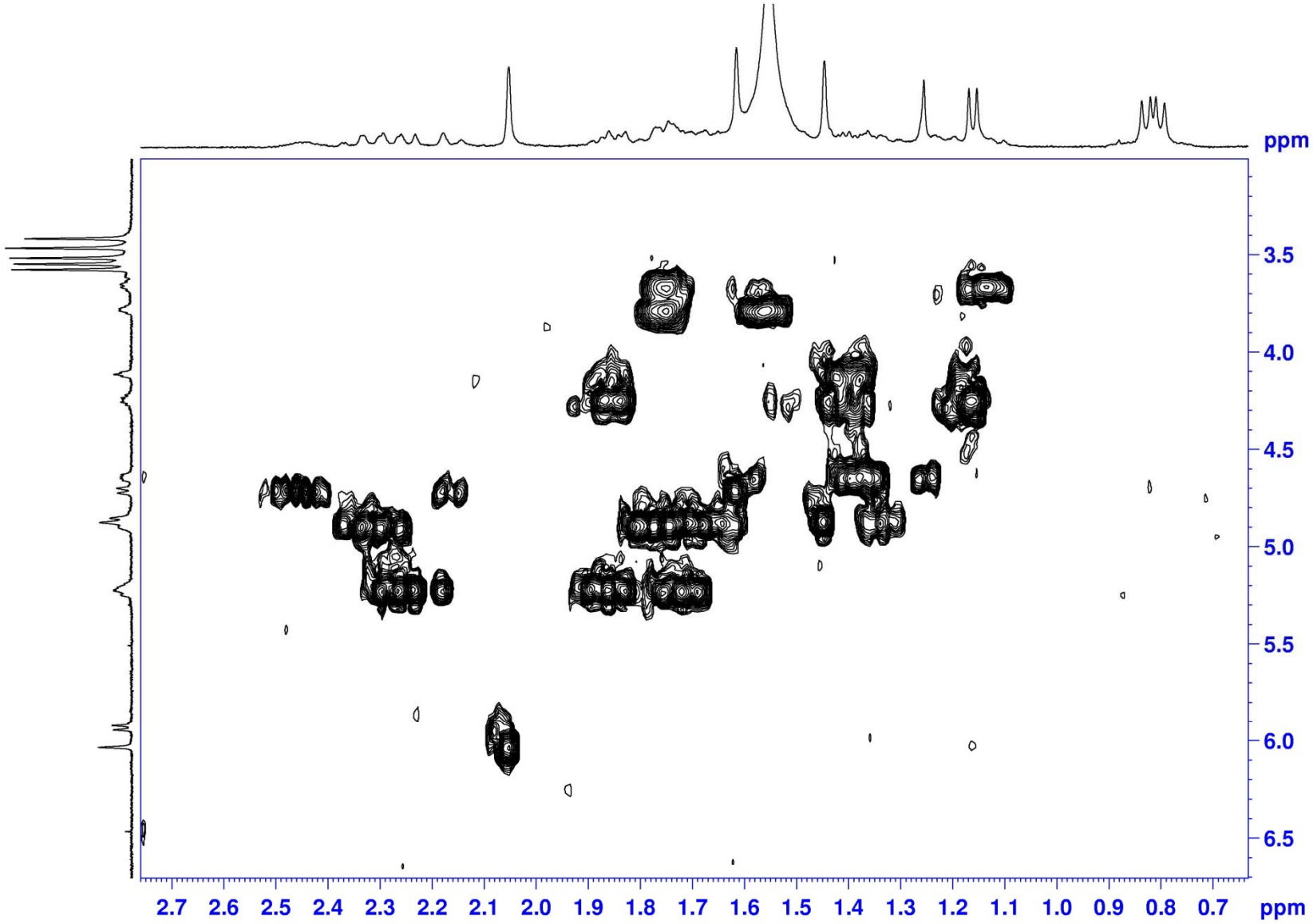
^{1}H–^{1}H COSY (400 MHz) spectrum of compound **1s** in $CDCl_3$



^{1}H–^{1}H COSY (400 MHz) spectrum of compound **1s** in $CDCl_3$



^{1}H–^{1}H COSY (400 MHz) spectrum of compound **1s** in $CDCl_3$



HR-ESIMS for compound **1r**

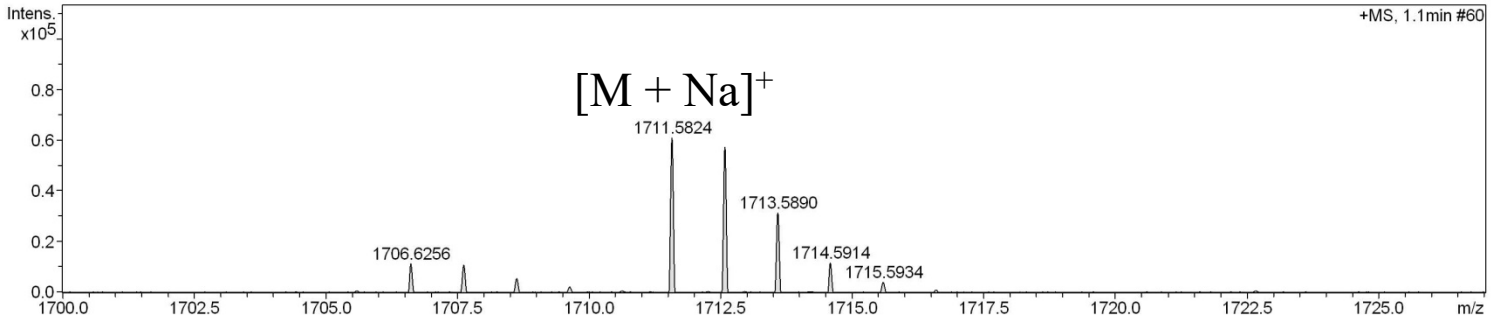
Mass Spectrum SmartFormula Report

Analysis Info

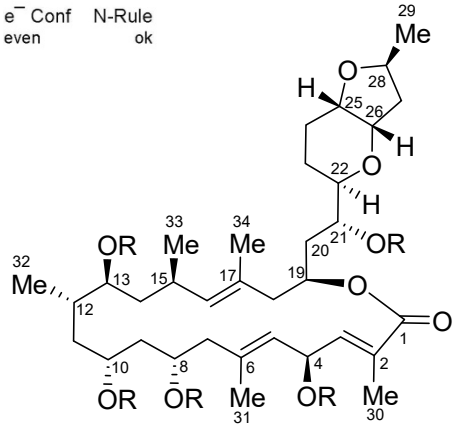
Analysis Name	D:\Data\MS\data\202011\jiangzhongping_37-1-S_pos_4_01_9233.d	Acquisition Date	11/16/2020 4:17:22 PM
Method	LC_Direct Infusion_pos_100-3000mz.m	Operator	SCSIO
Sample Name	jiangzhongping_37-1-S_pos	Instrument	maXis 255552.00029
Comment			

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

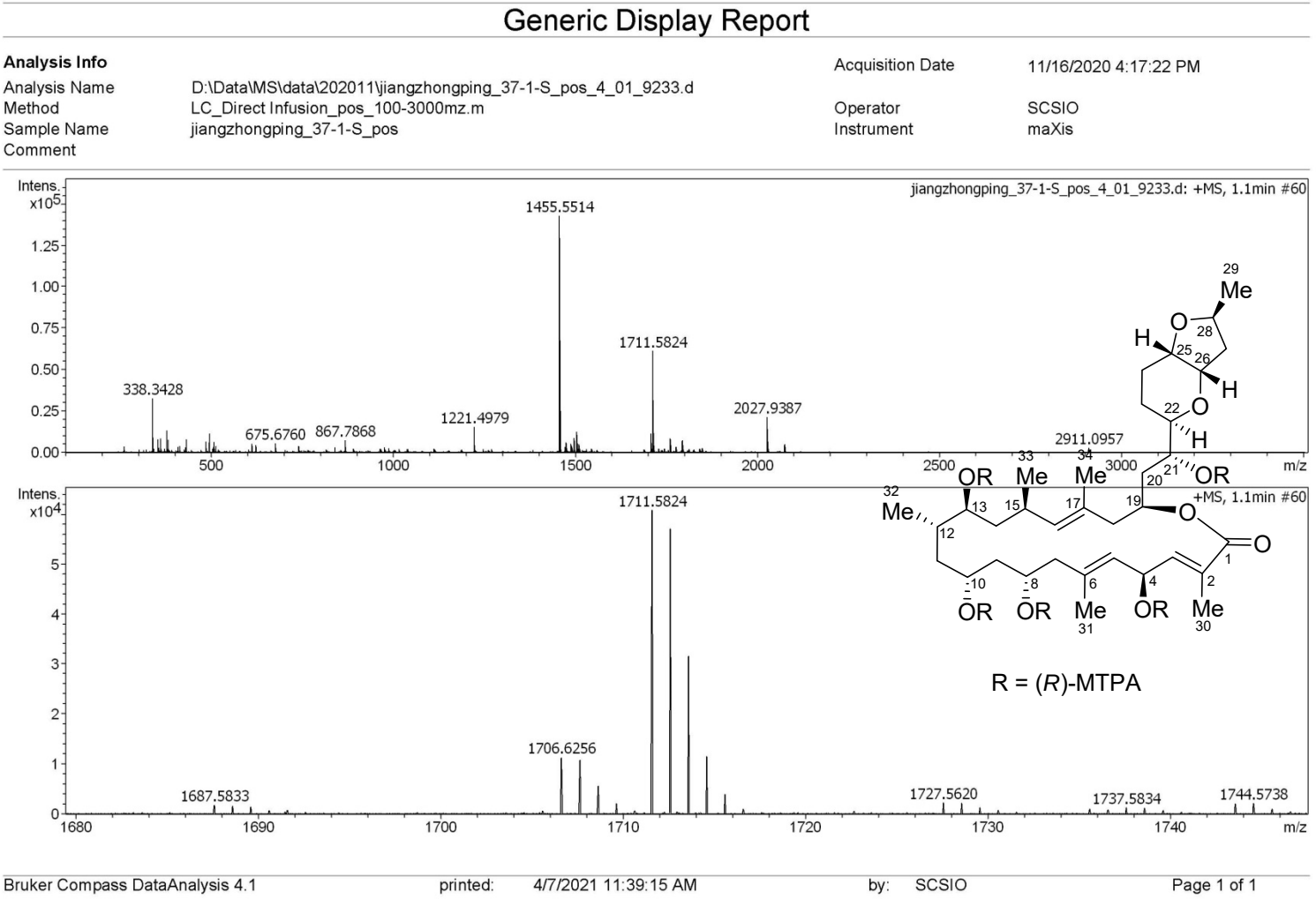


Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
1711.5824	1	C84H91F15NaO19	100.00	1711.5807	-1.0	-1.7	26.8	31.5	even	ok

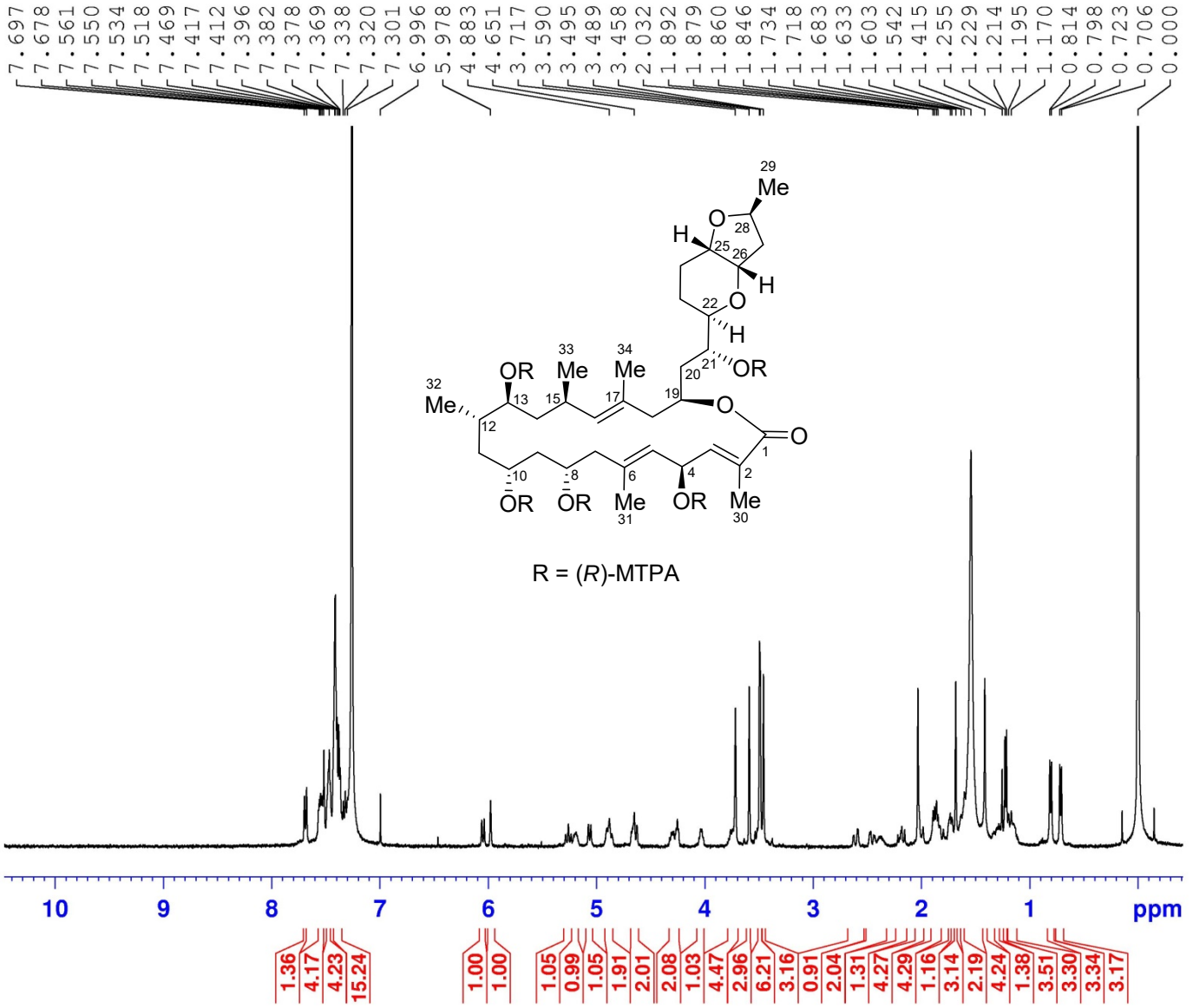


R = (*R*)-MTPA

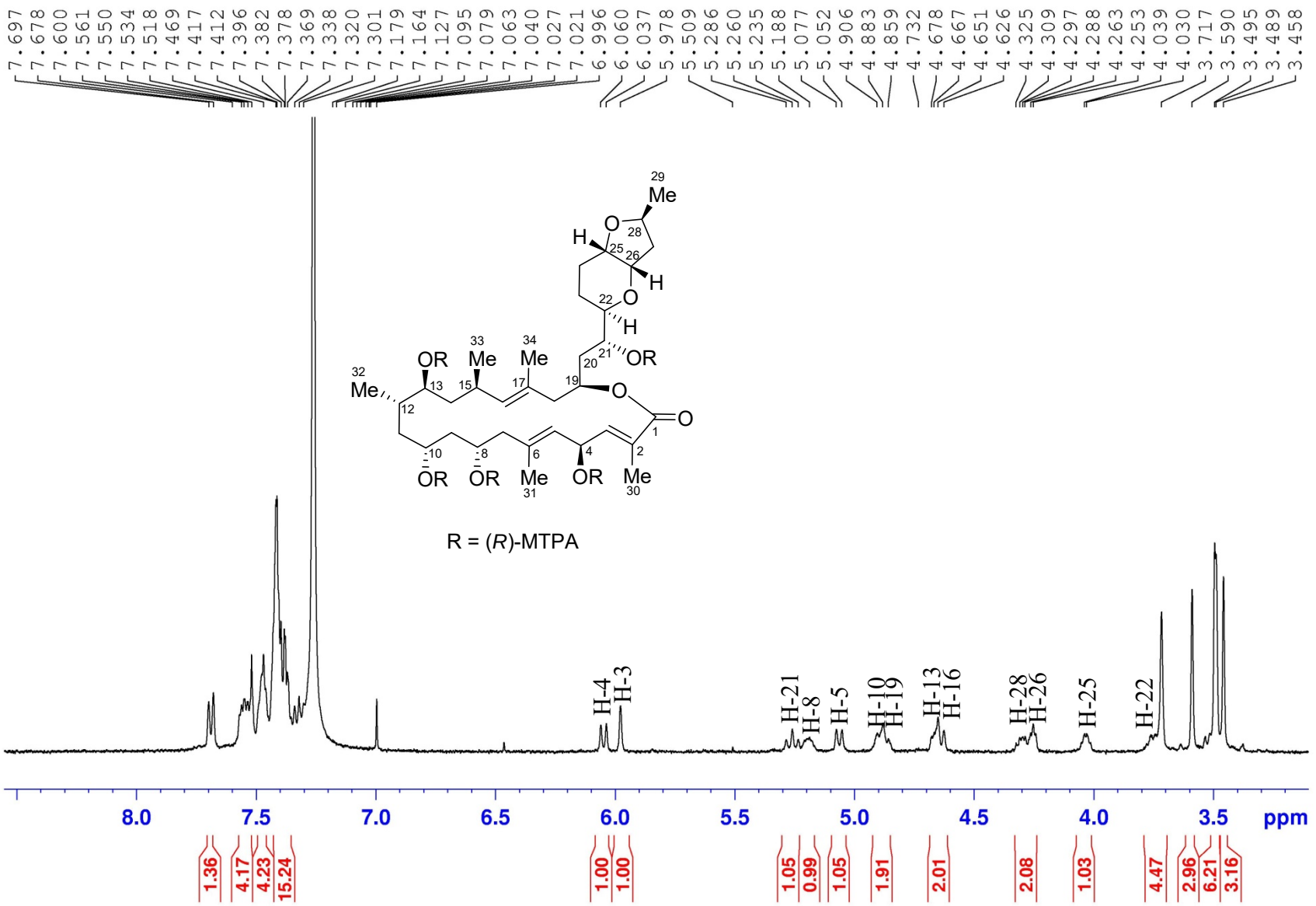
HR-ESIMS for compound **1r**



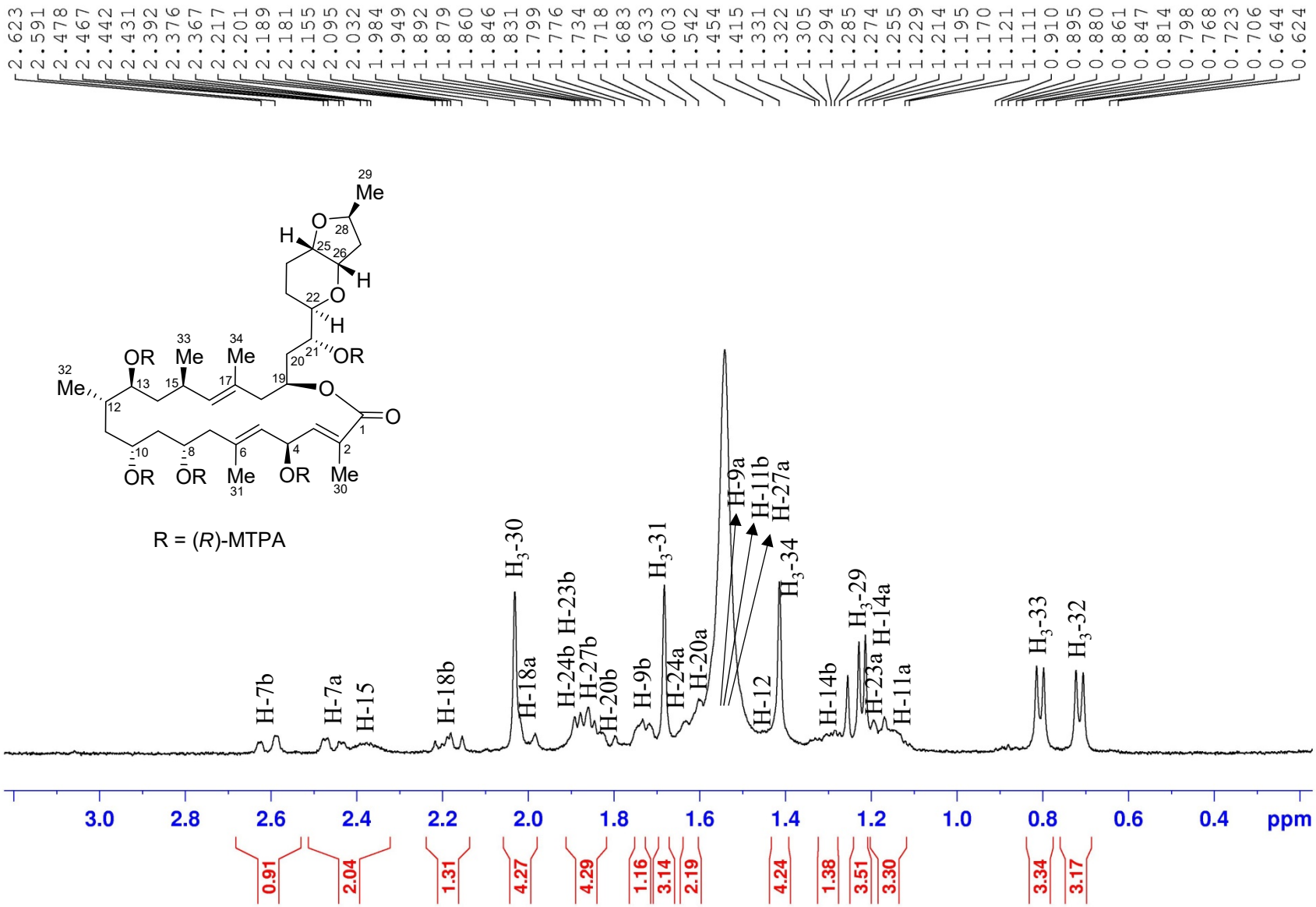
^{1}H (400 MHz) NMR spectrum of compound **1r** in $CDCl_3$



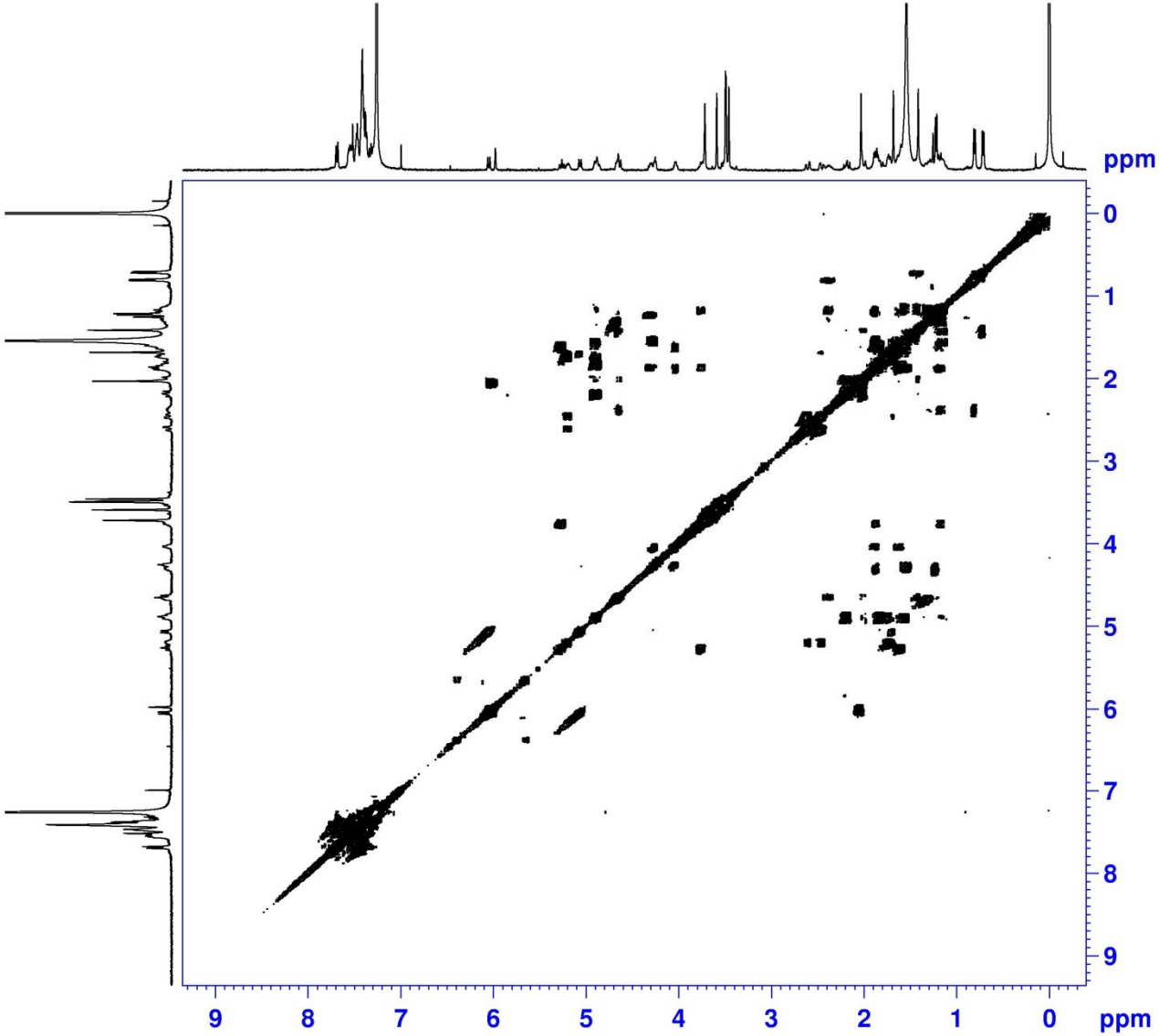
^{1}H (400 MHz) NMR spectrum of compound **1r** in $CDCl_3$



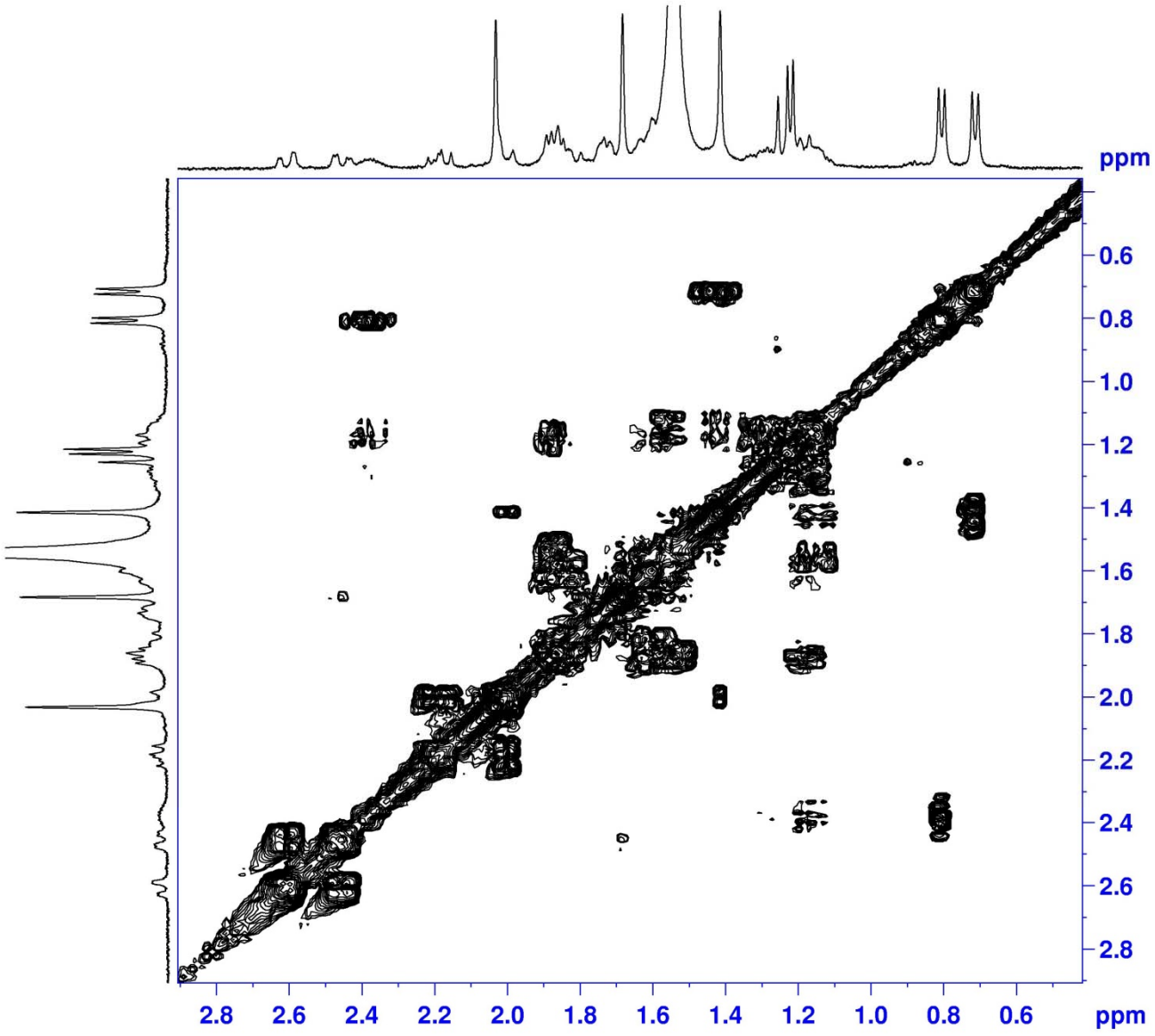
^{1}H (400 MHz) NMR spectrum of compound **1r** in $CDCl_3$



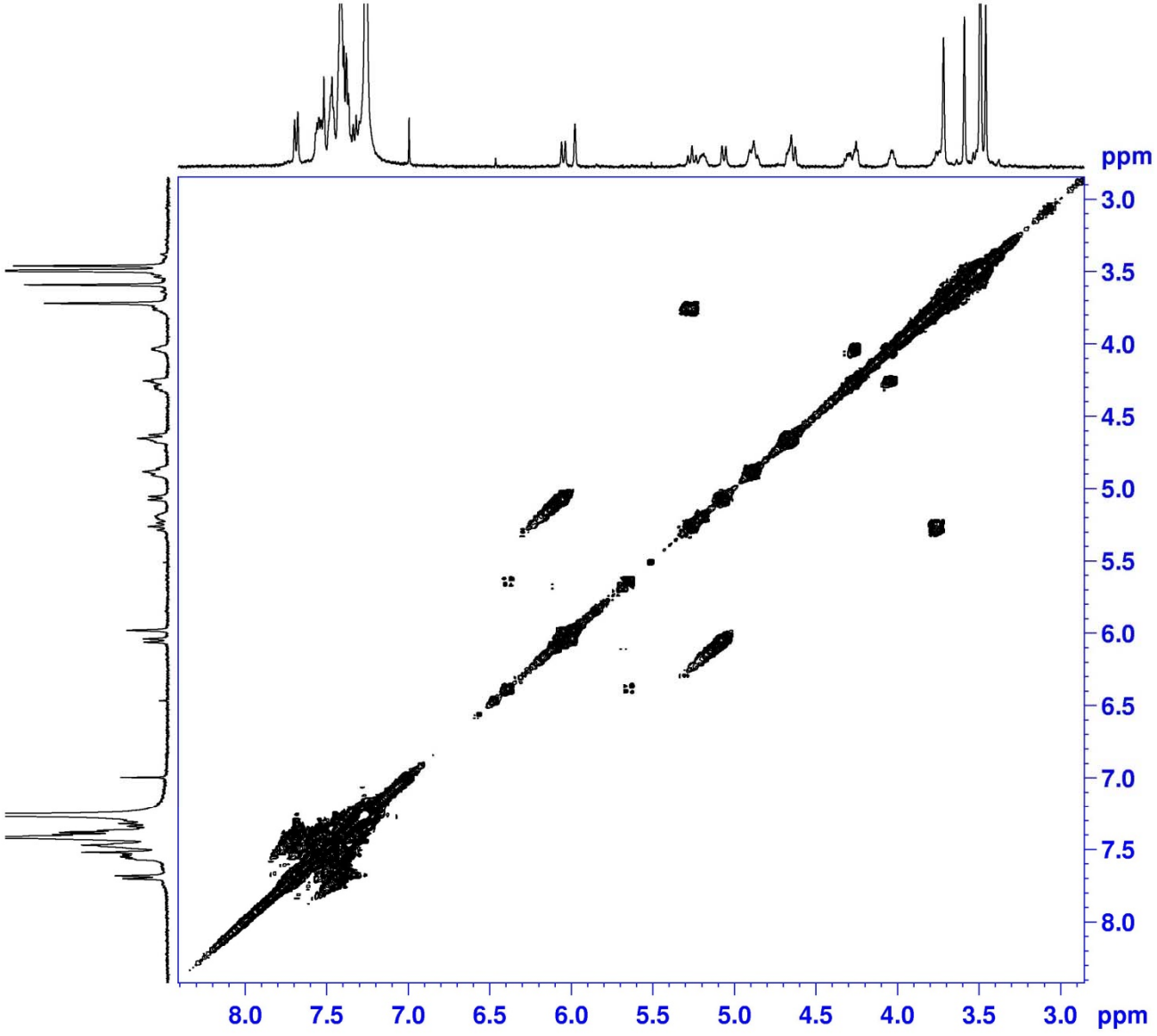
^{1}H–^{1}H COSY (400 MHz) spectrum of compound **1r** in $CDCl_3$



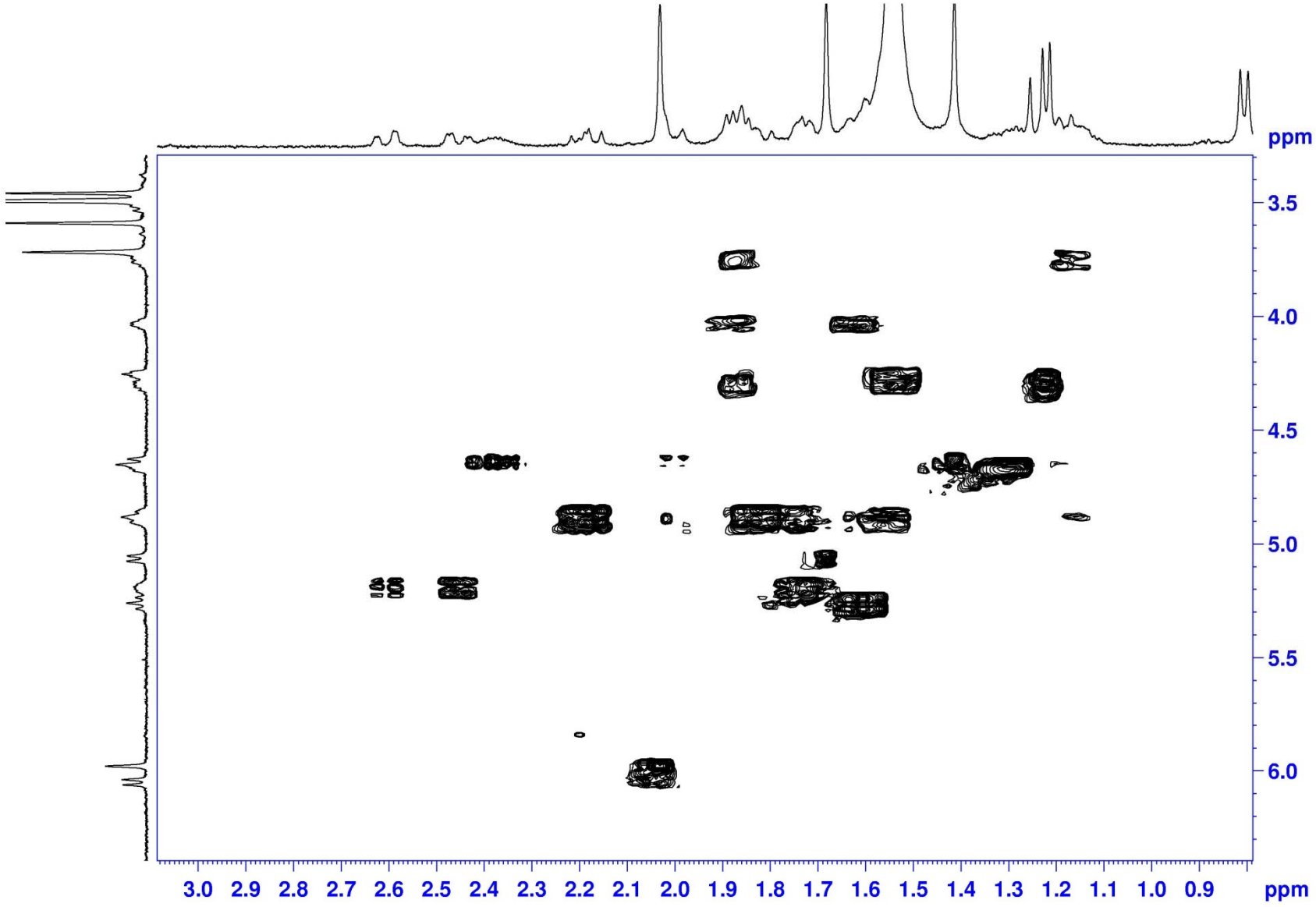
^{1}H–^{1}H COSY (400 MHz) spectrum of compound **1r** in $CDCl_3$



^{1}H–^{1}H COSY (400 MHz) spectrum of compound **1r** in $CDCl_3$



^{1}H–^{1}H COSY (400 MHz) spectrum of compound **1r** in $CDCl_3$

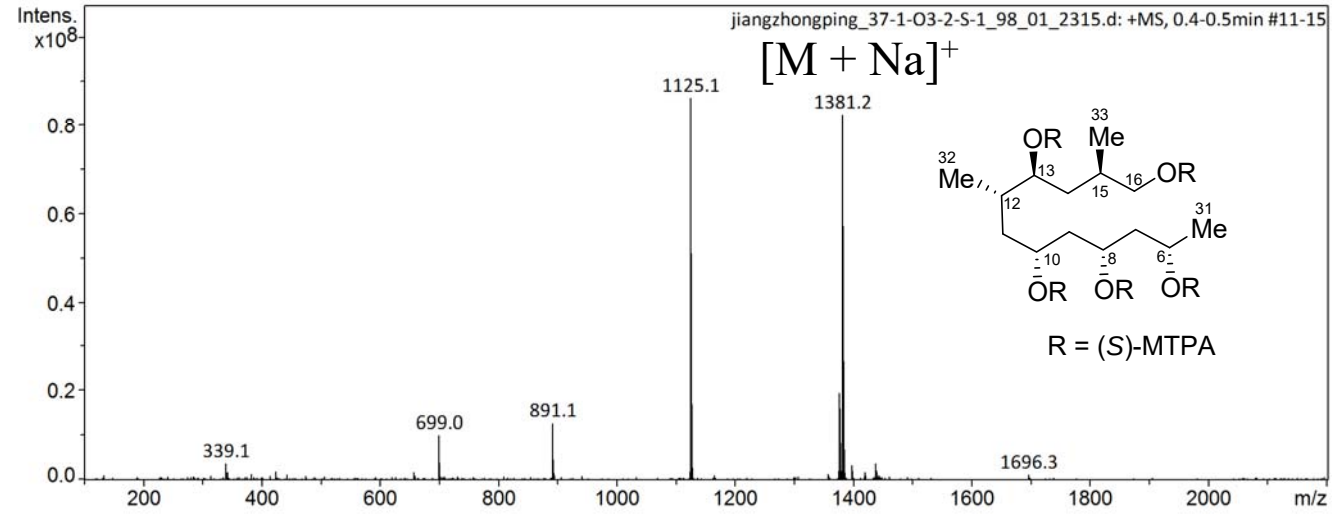


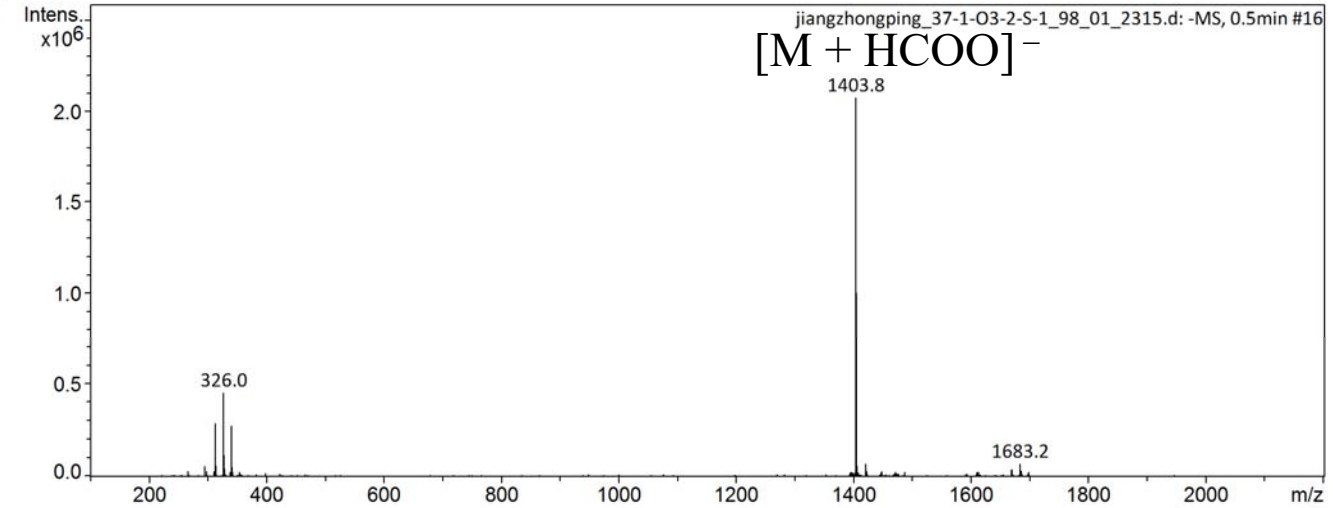
LR-ESIMS for the fragment **1As**

Generic Display Report

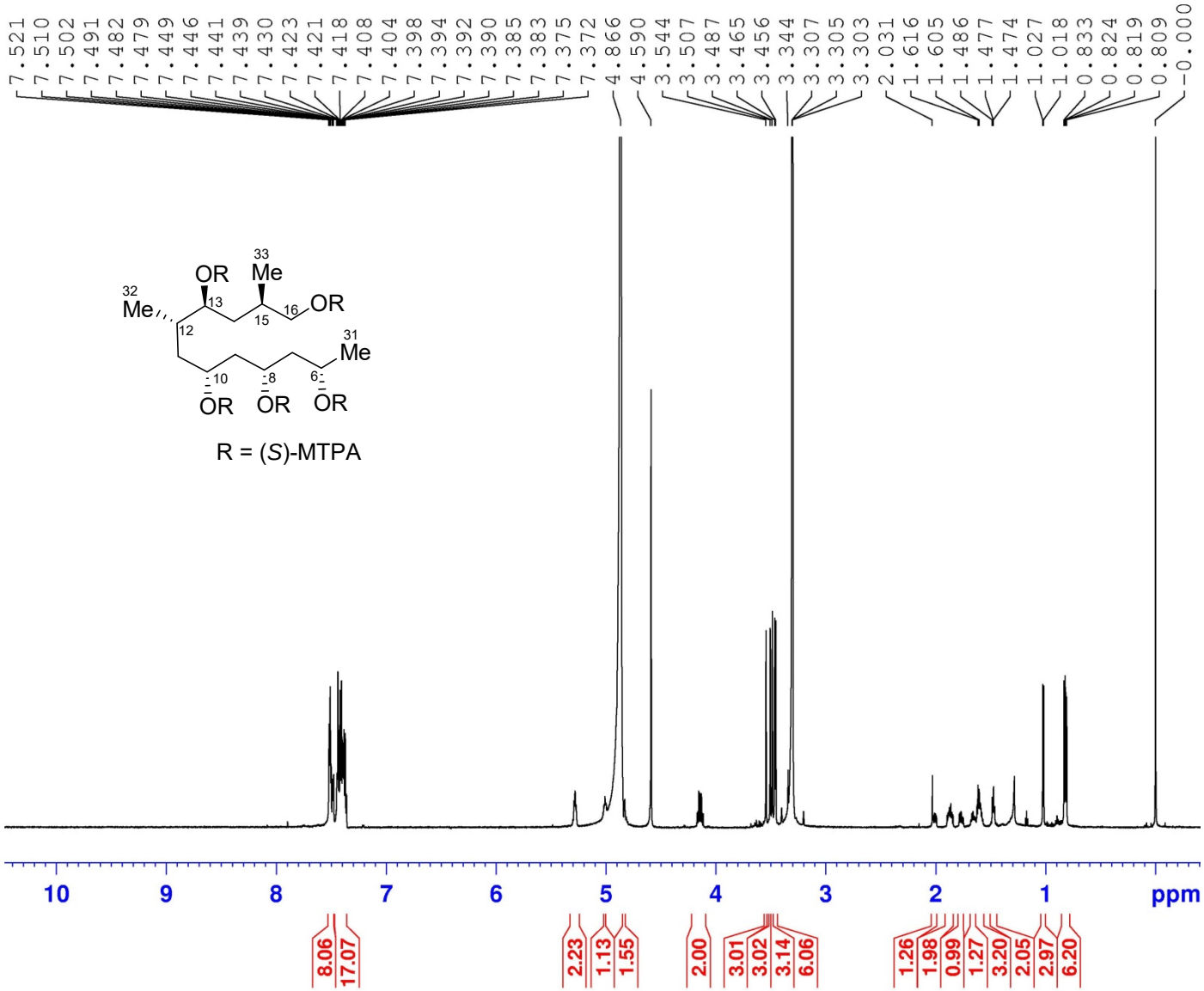
Analysis Info

Acquisition Date	2020-11-09 15:57:29		
Analysis Name	D:\Data\amaZon SL\MS\data\202011\jiangzhongping_37-1-O3-2-S-1_98_01_2315.d		
Method	2315.m	Operator	bruker
Sample Name	jiangzhongping_37-1-O3-2-S-1	Instrument	amaZon SL
Comment			

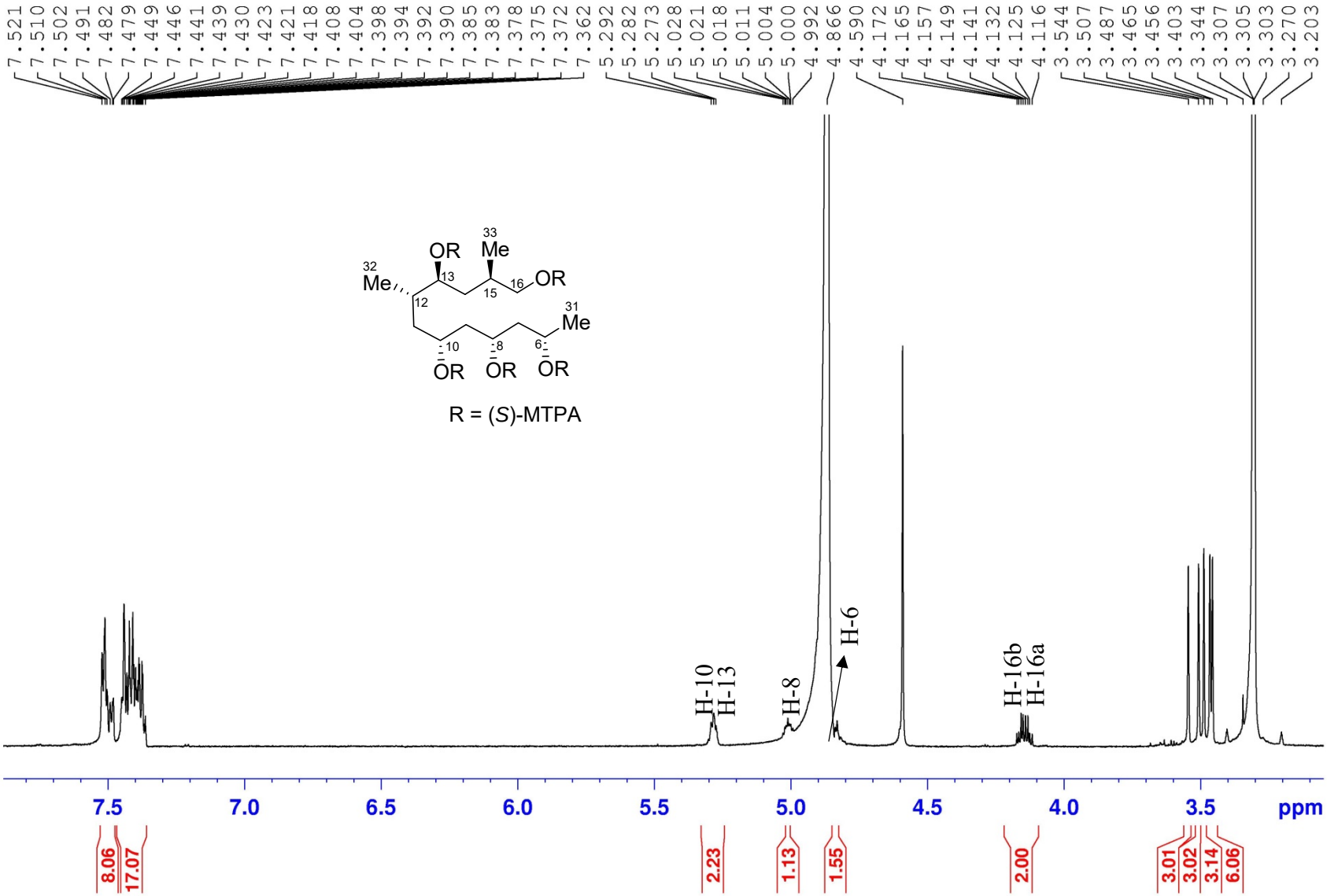




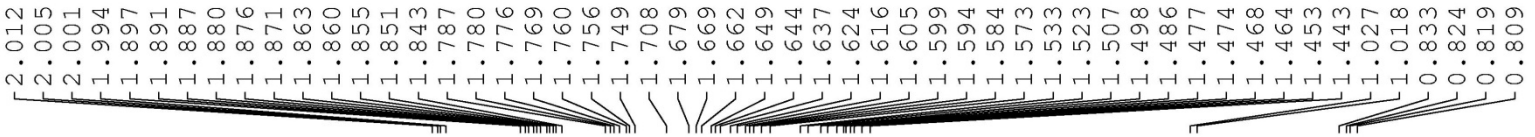
^{1}H (700 MHz) NMR spectrum of the fragment **1As** in CD_3OD

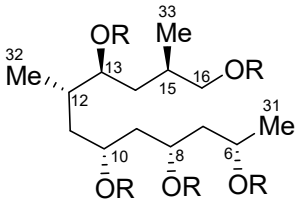


^{1}H (700 MHz) NMR spectrum of the fragment **1As** in CD_3OD

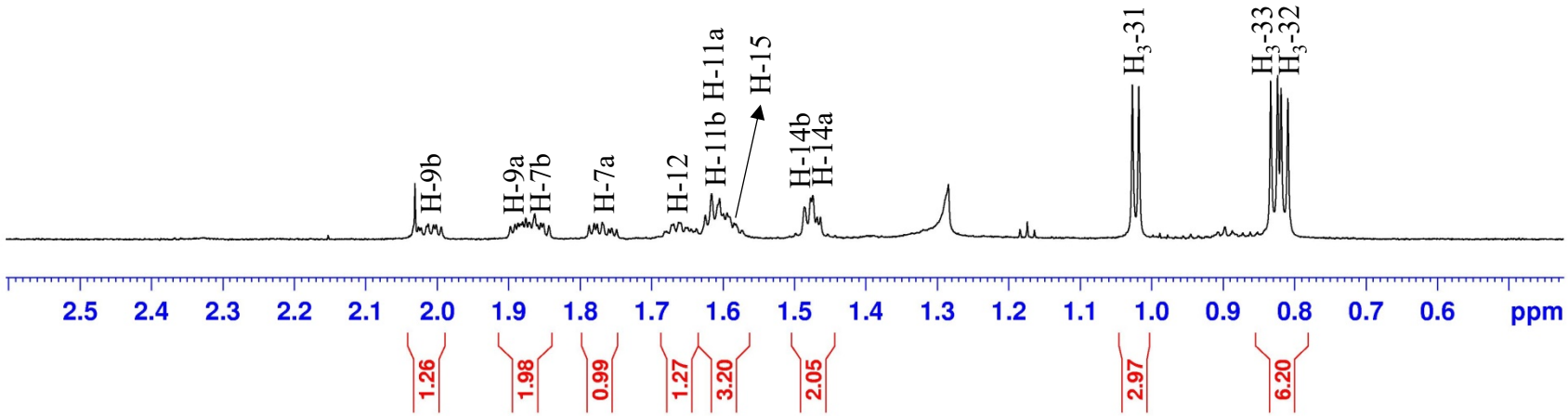


^{1}H (700 MHz) NMR spectrum of the fragment **1As** in CD_3OD

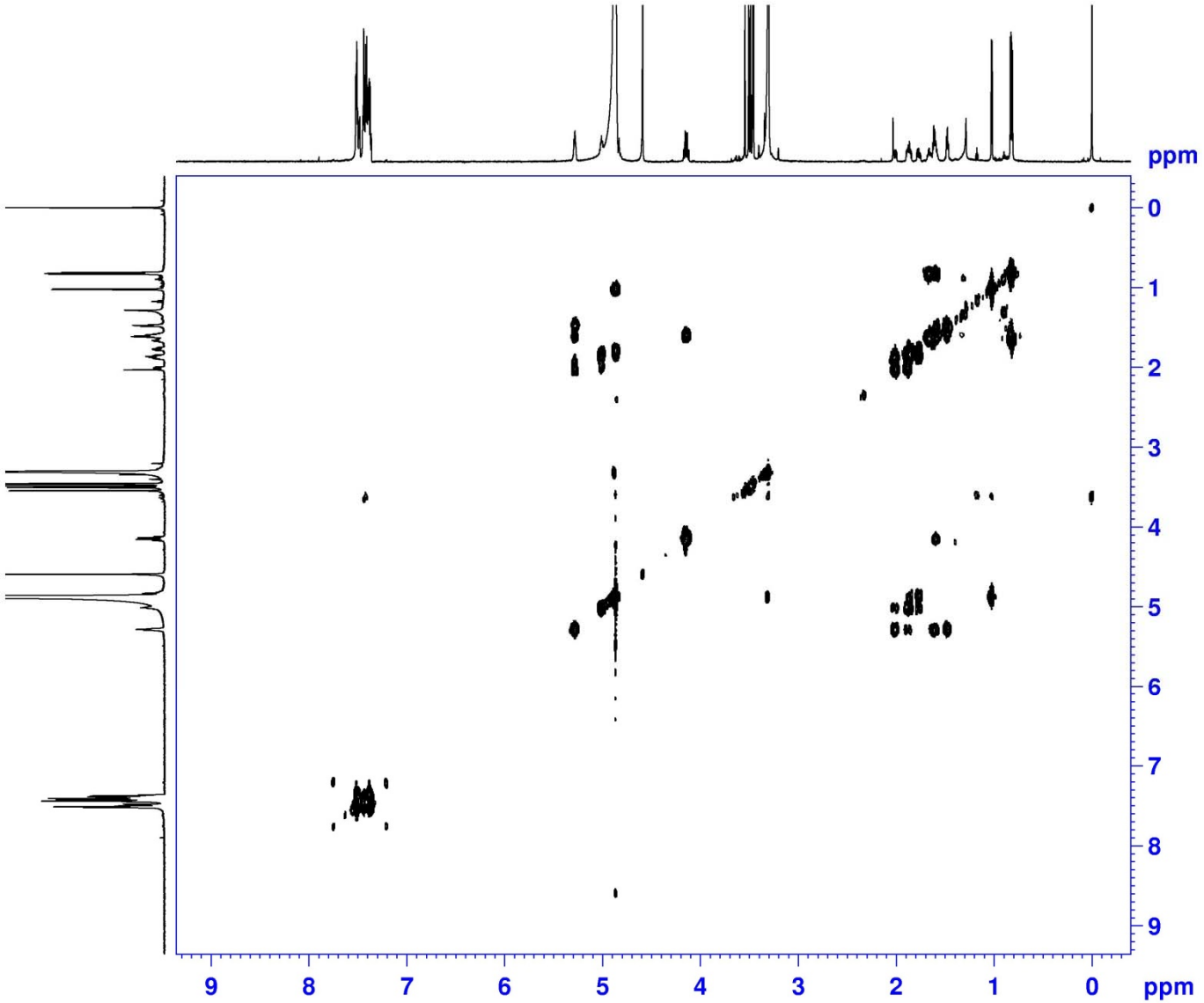




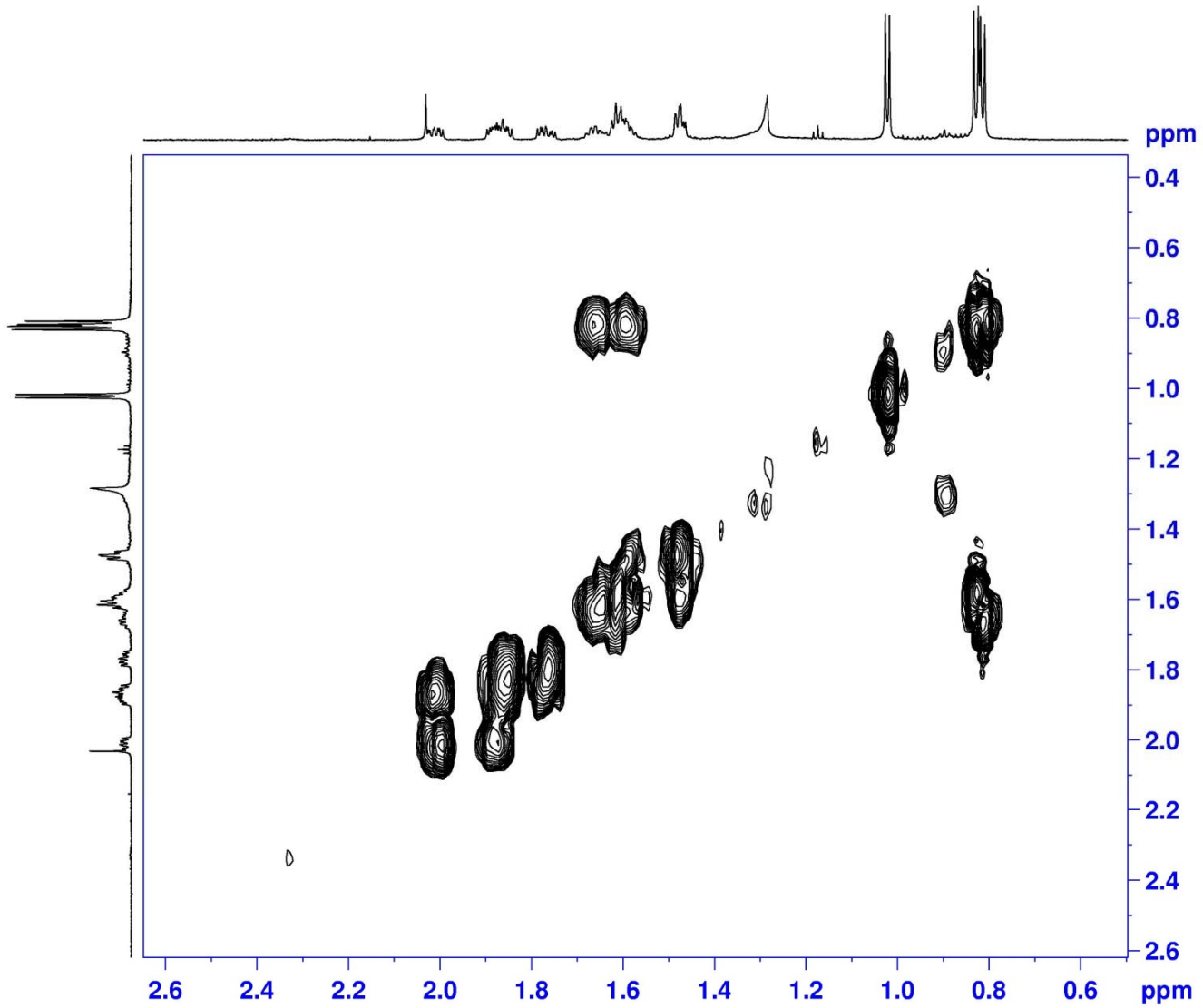
R = (*S*)-MTPA



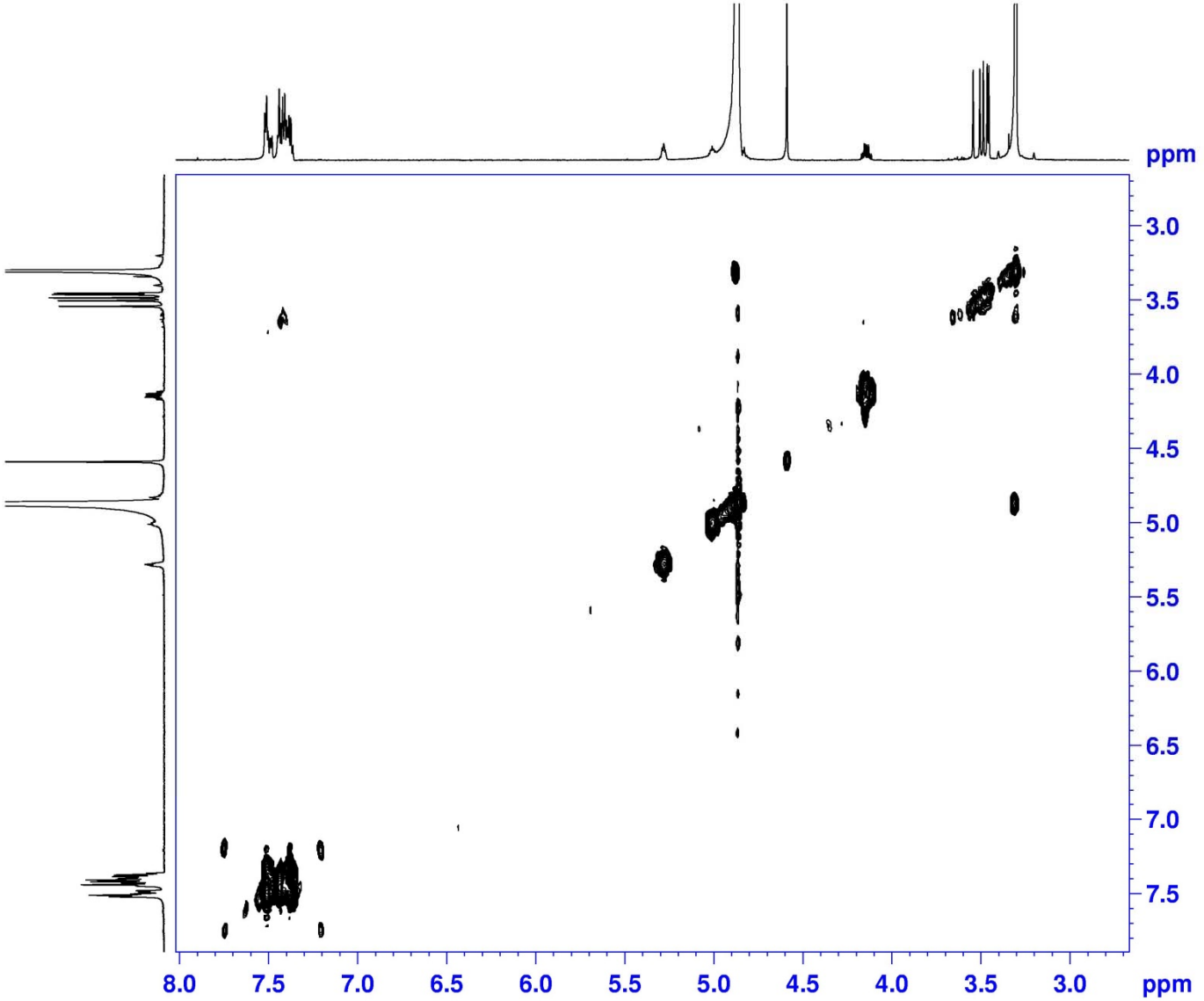
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1As** in CD_3OD



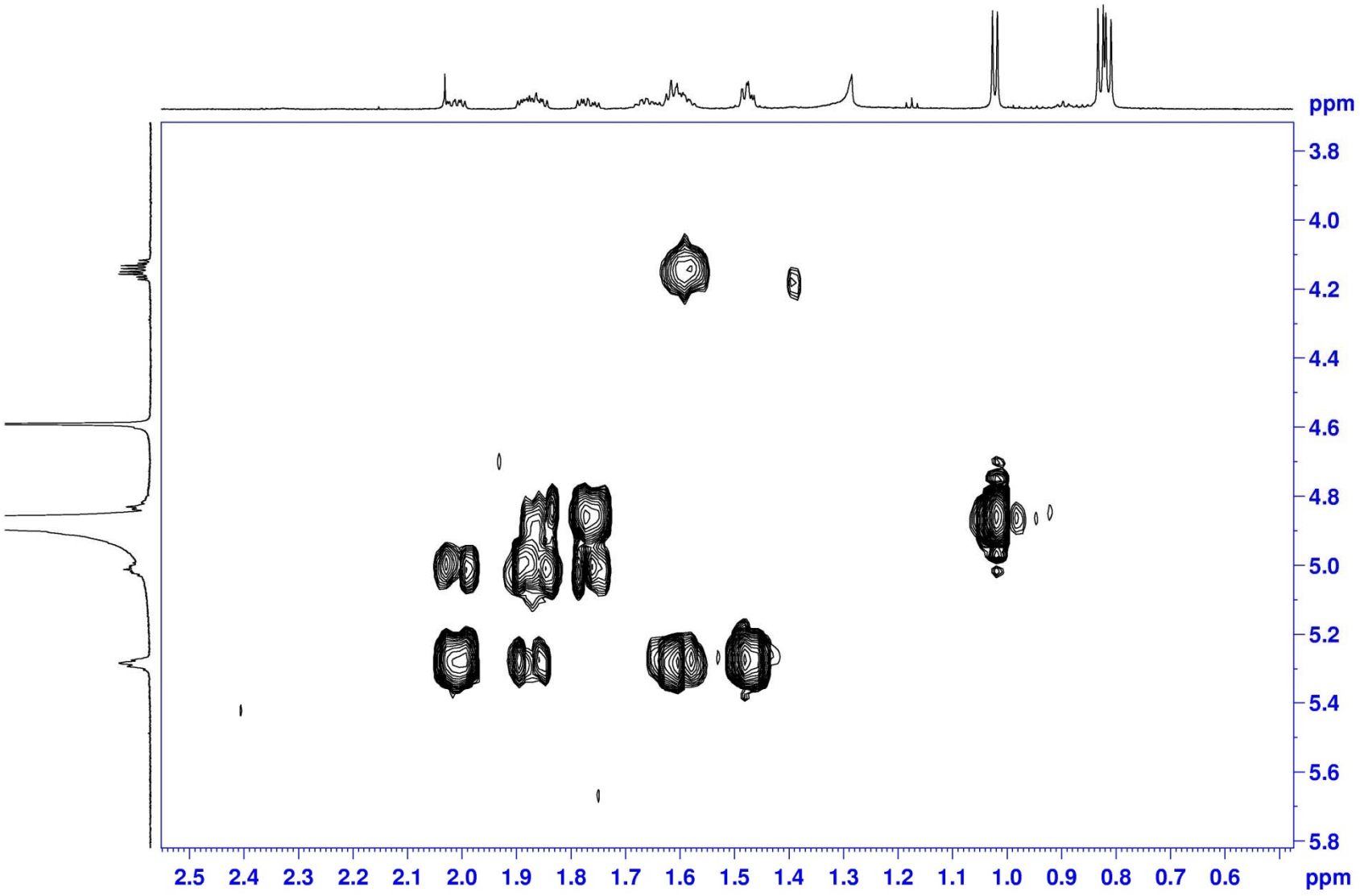
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1As** in CD_3OD



$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1As** in CD_3OD



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

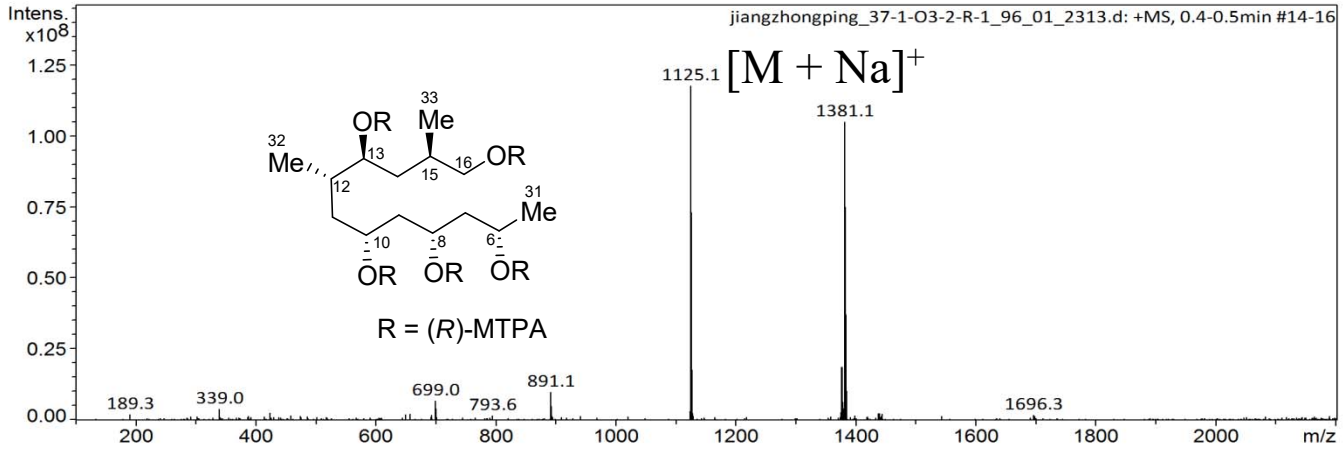


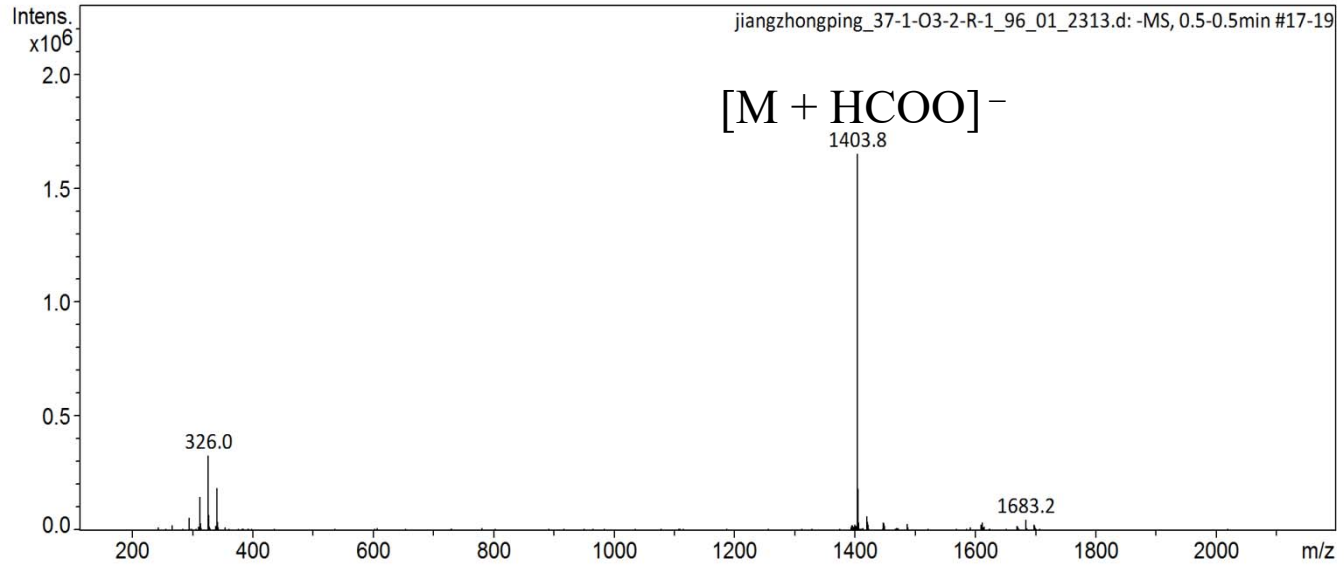
LR-ESIMS for the fragment **1Ar**

Generic Display Report

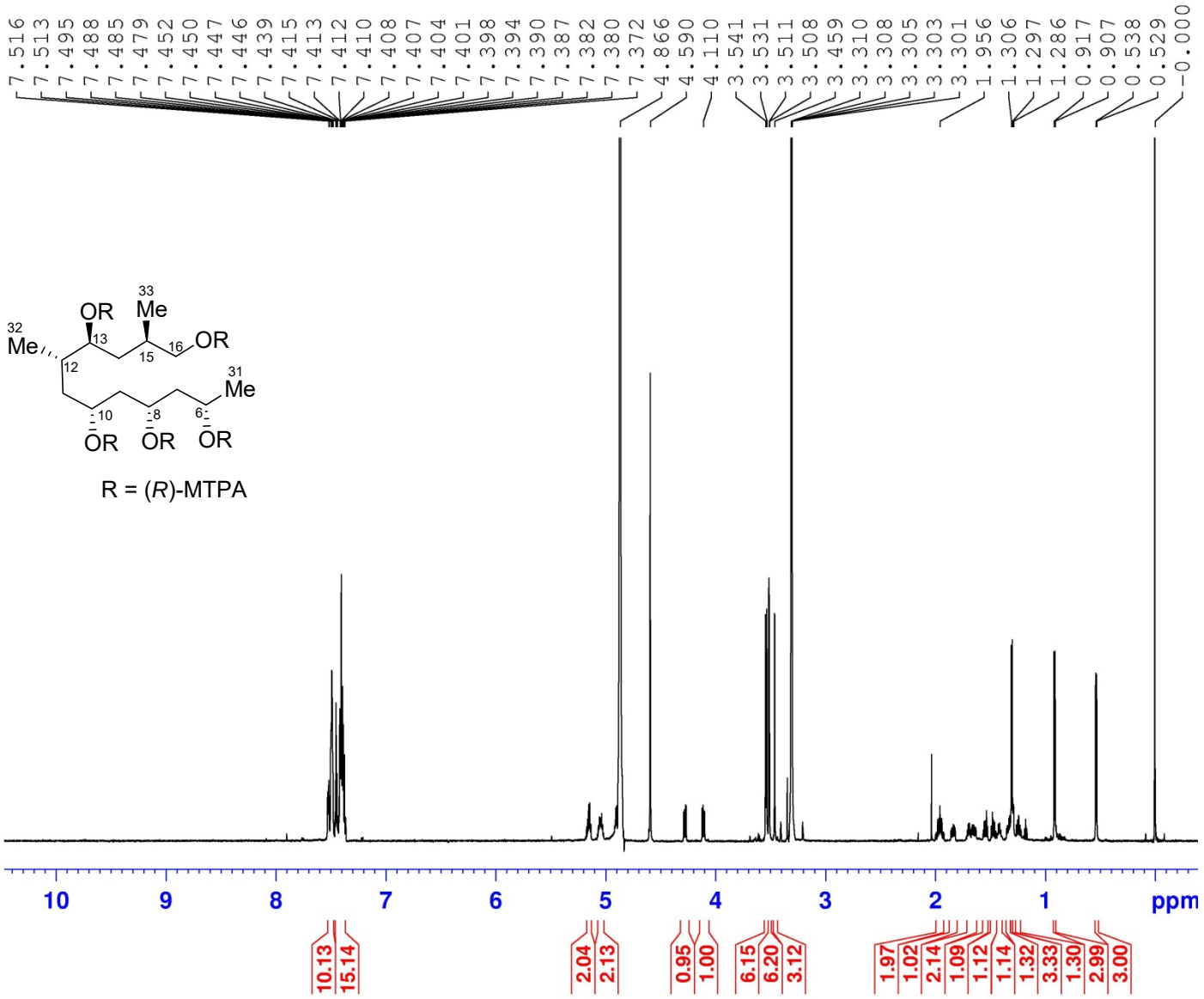
Analysis Info

Acquisition Date	2020-11-09 15:52:38		
Analysis Name	D:\Data\amaZon SL\MS\data\202011\jiangzhongping_37-1-O3-2-R-1_96_01_2313.d		
Method	2313.m	Operator	bruker
Sample Name	jiangzhongping_37-1-O3-2-R-1	Instrument	amaZon SL
Comment			

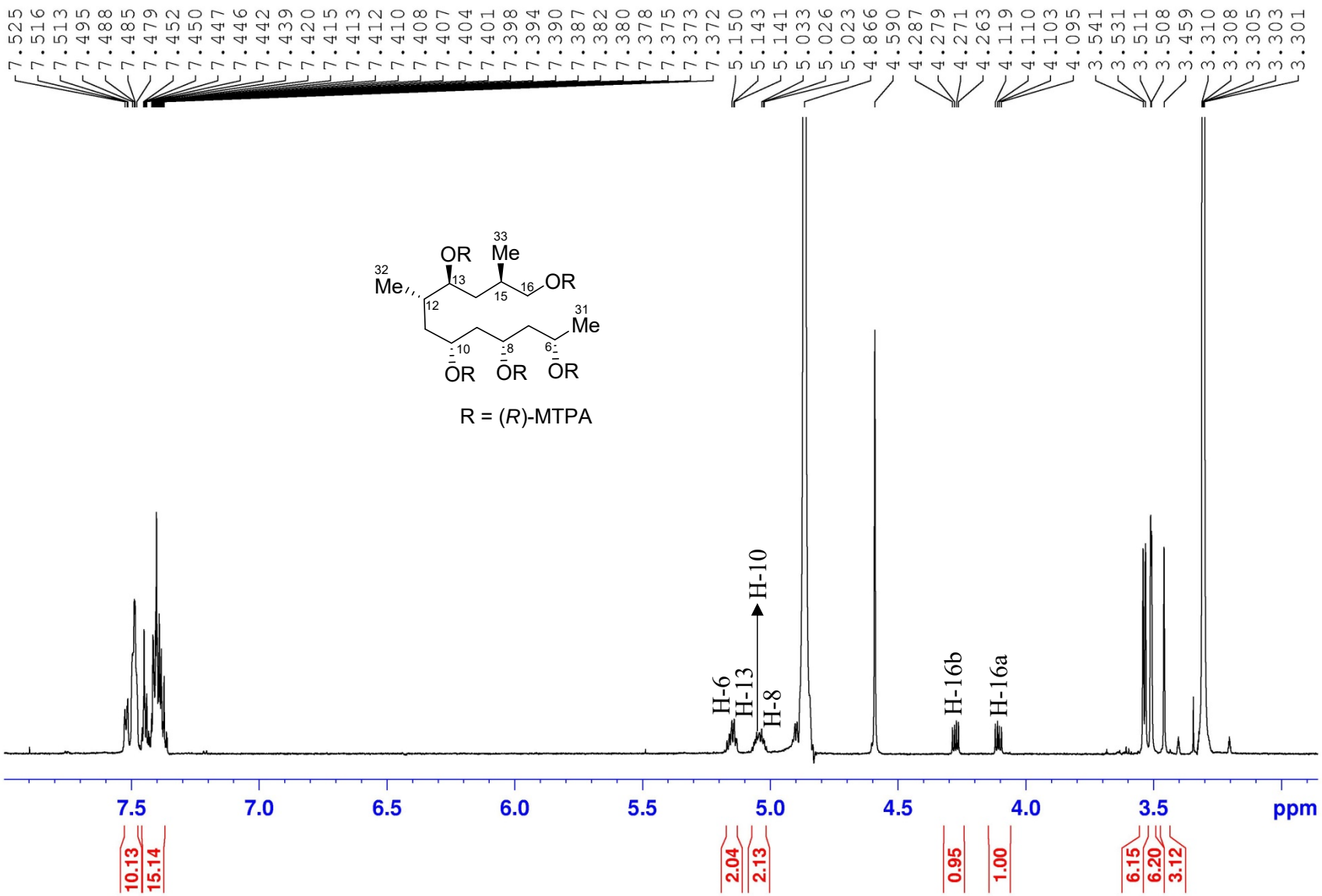




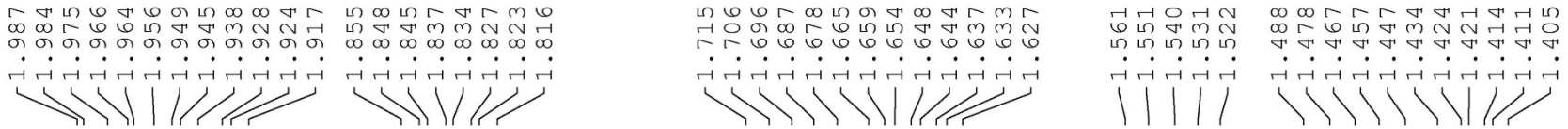
^{1}H (700 MHz) NMR spectrum of the fragment **1Ar** in CD_3OD

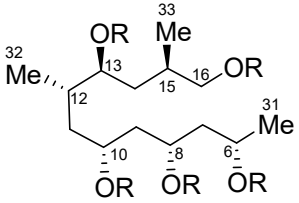


^{1}H (700 MHz) NMR spectrum of the fragment **1Ar** in CD_3OD



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





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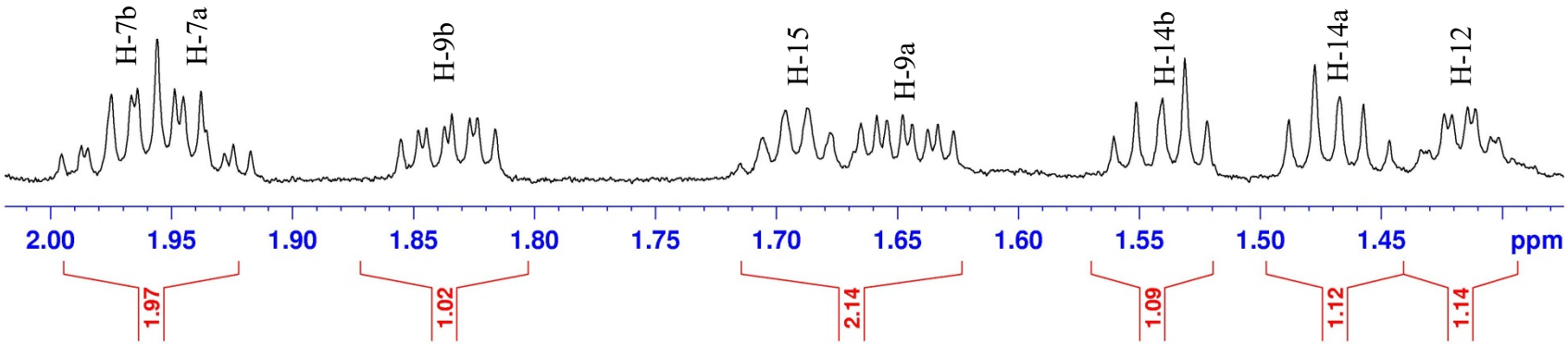
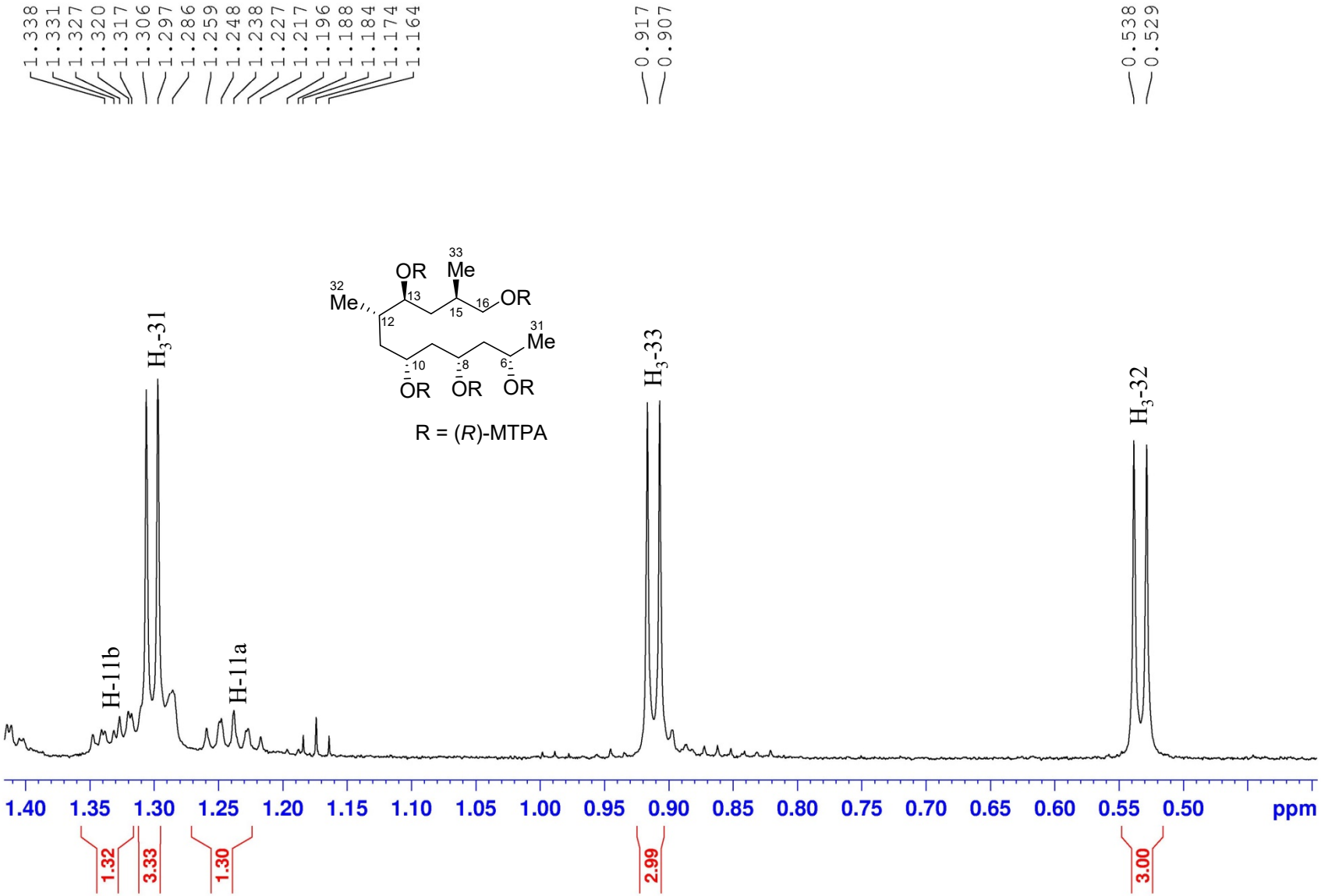
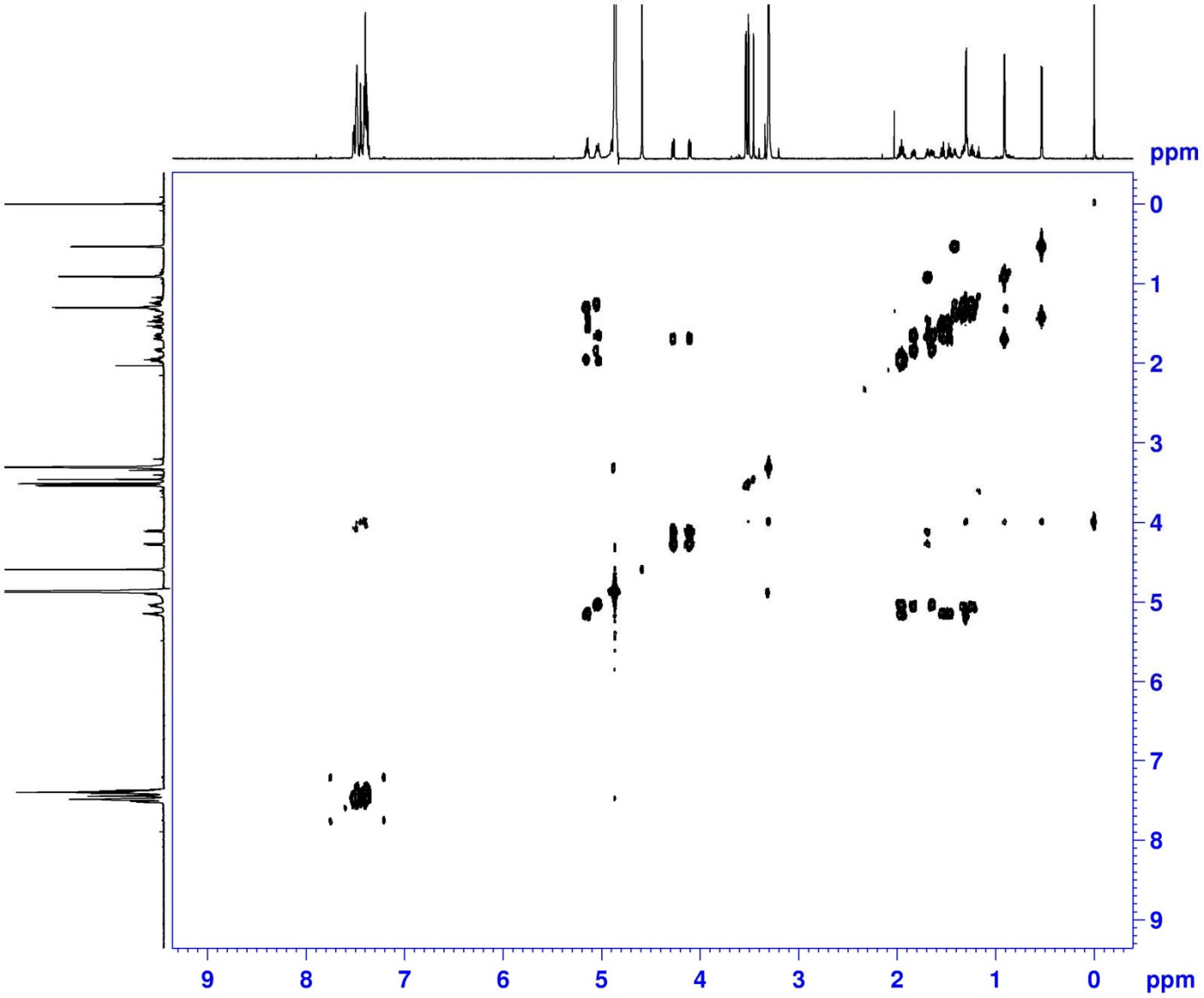


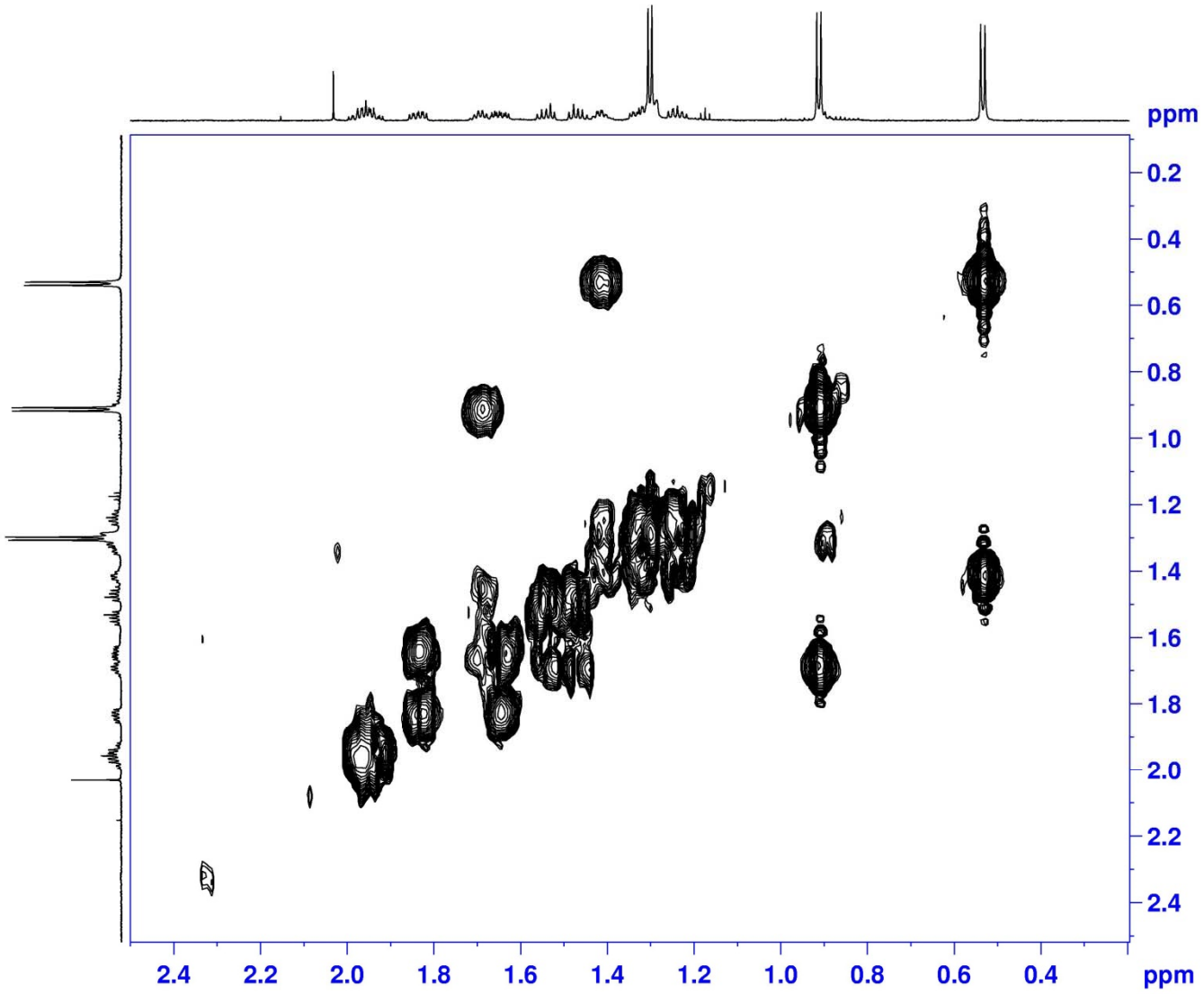
[1]H (700 MHz) NMR spectrum of the fragment **1Ar** in CD_3OD



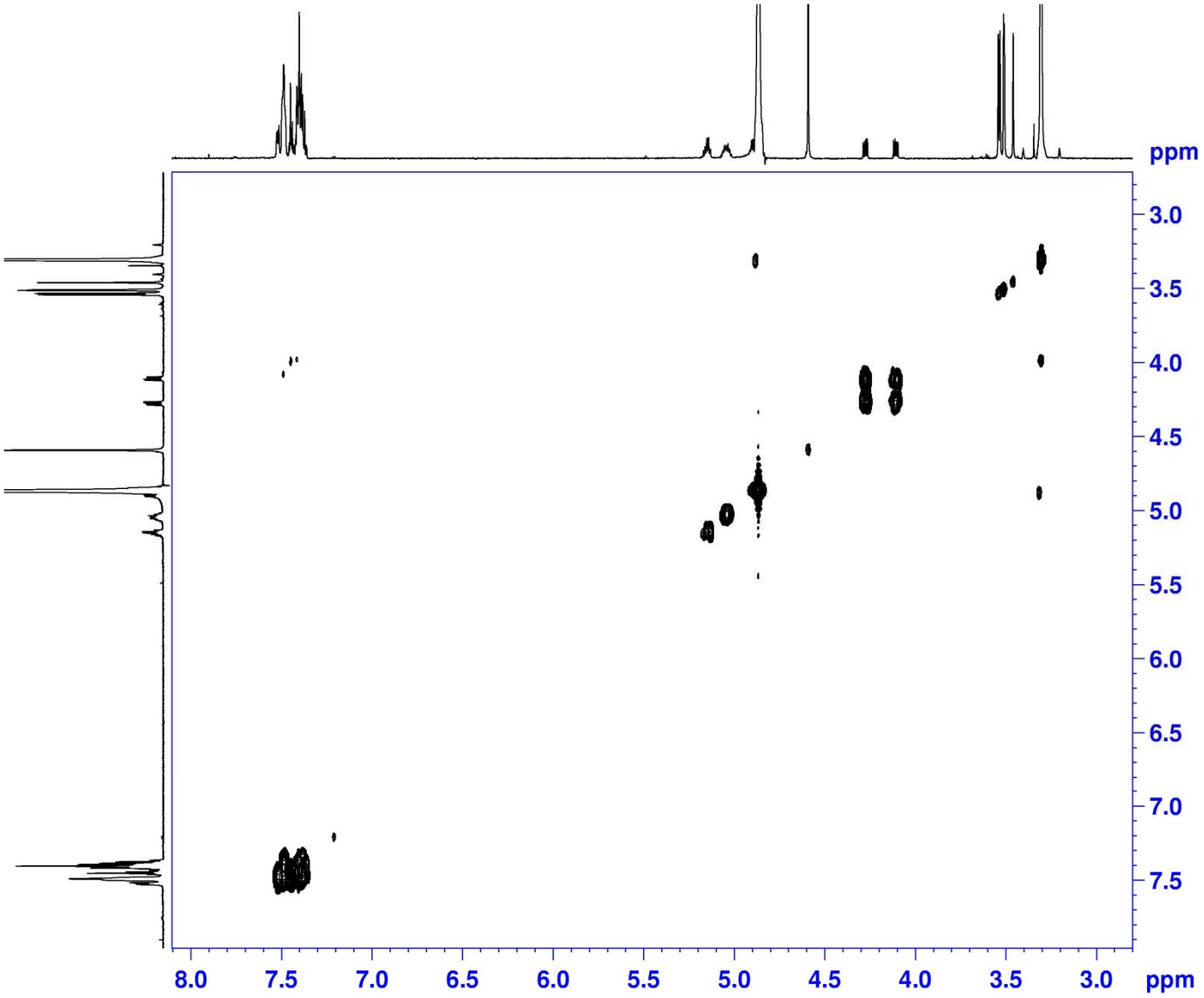
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1Ar** in CD_3OD



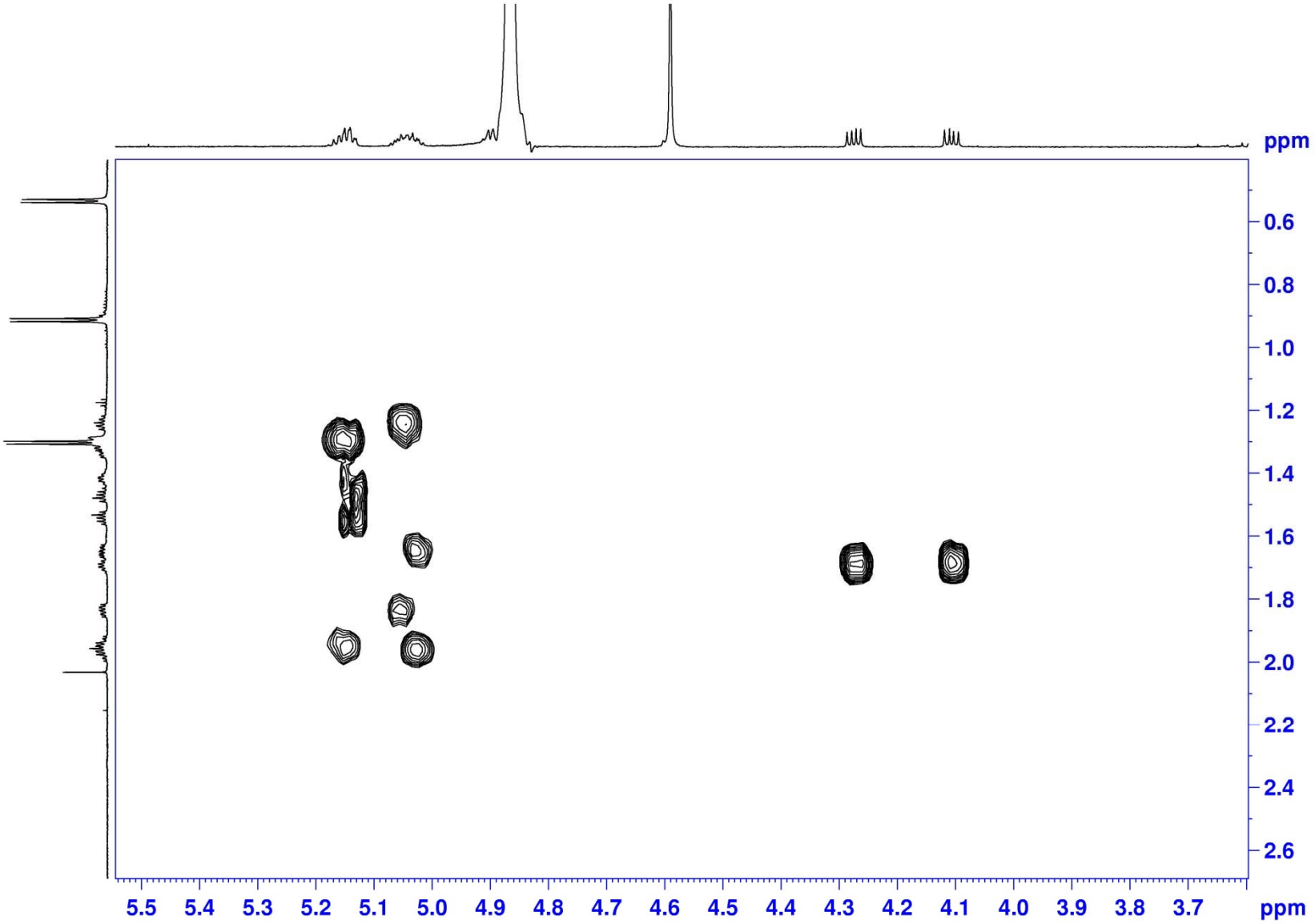
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1Ar** in CD_3OD



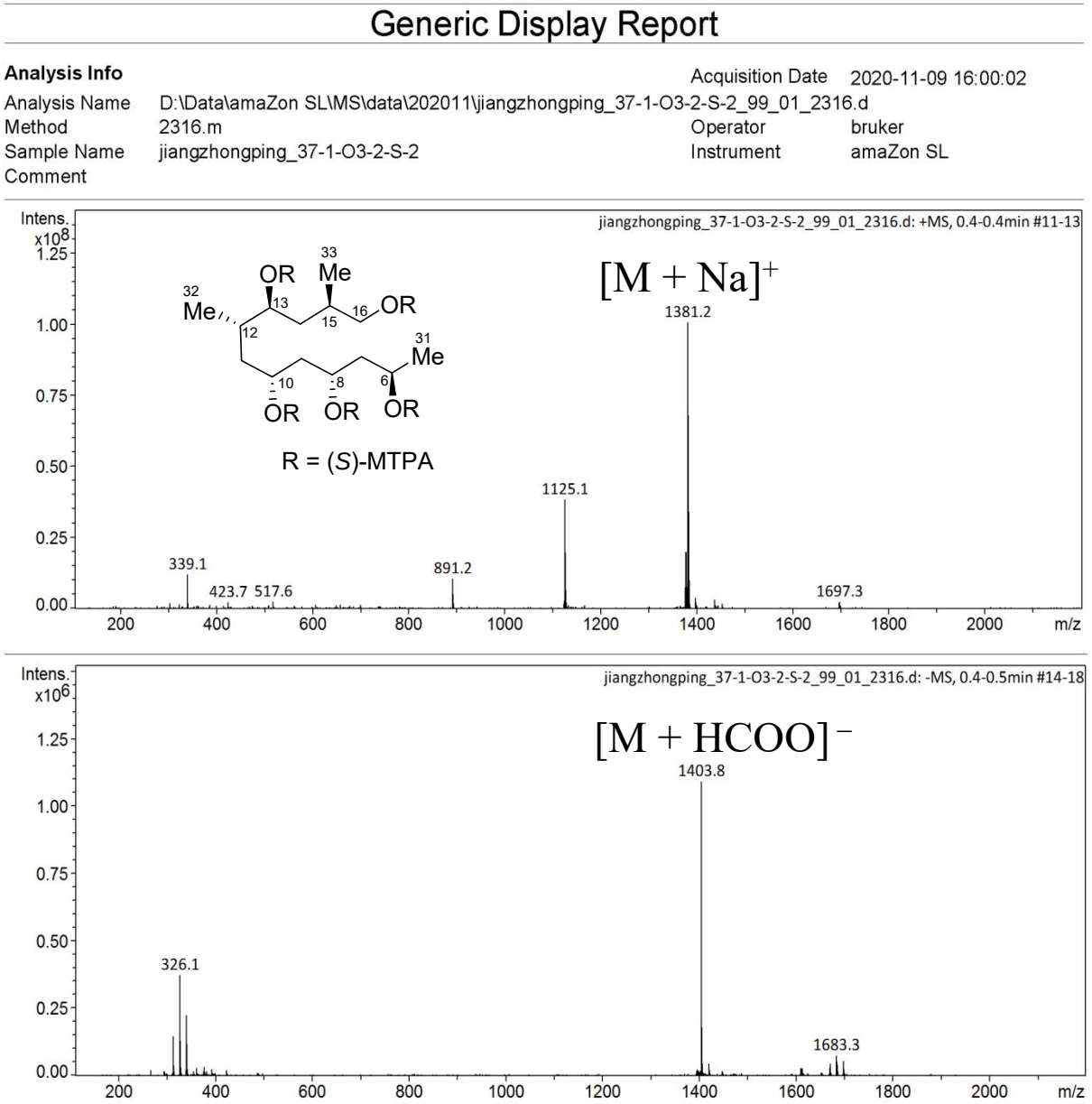
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1Ar** in CD_3OD



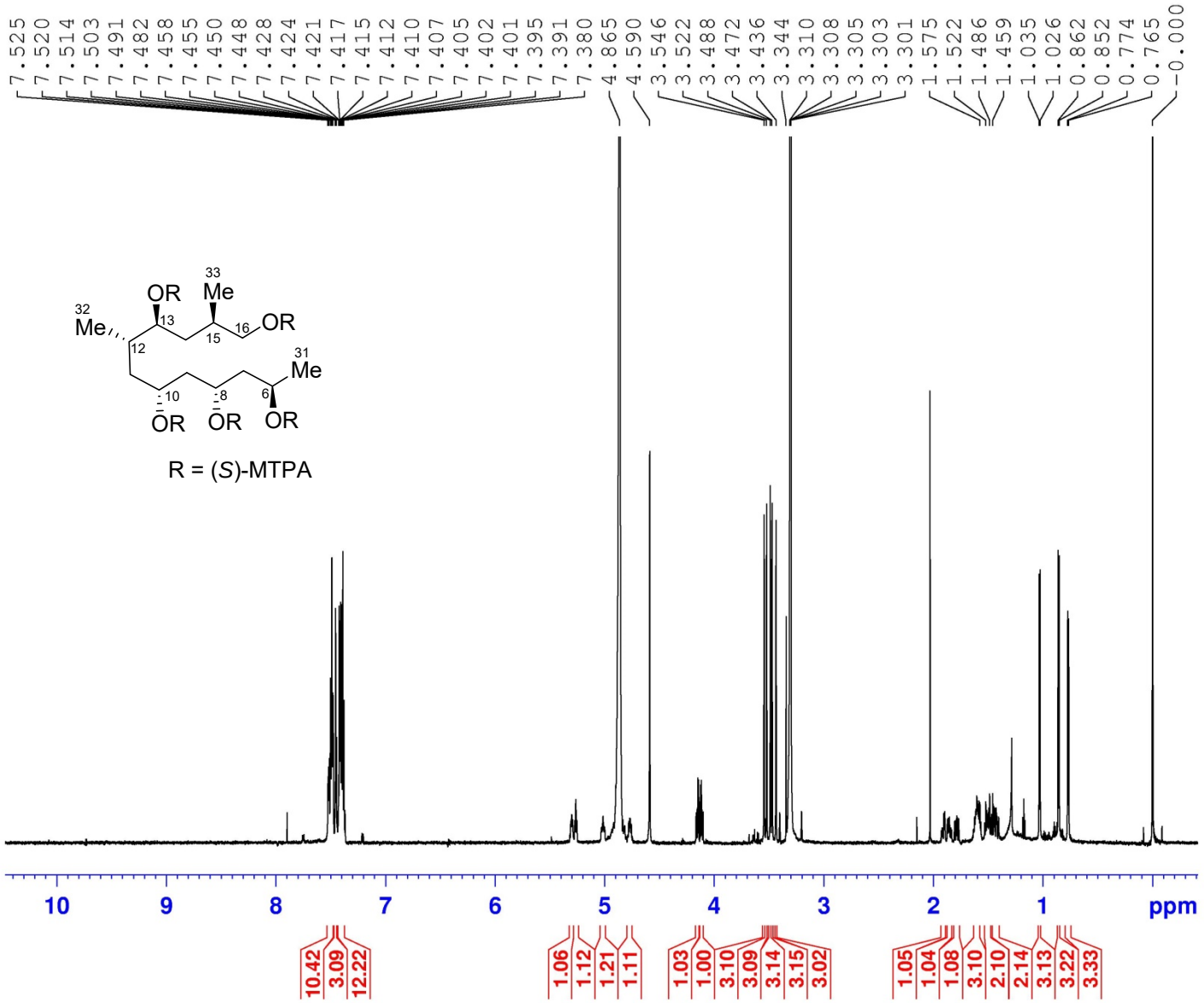
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1Ar** in CD_3OD



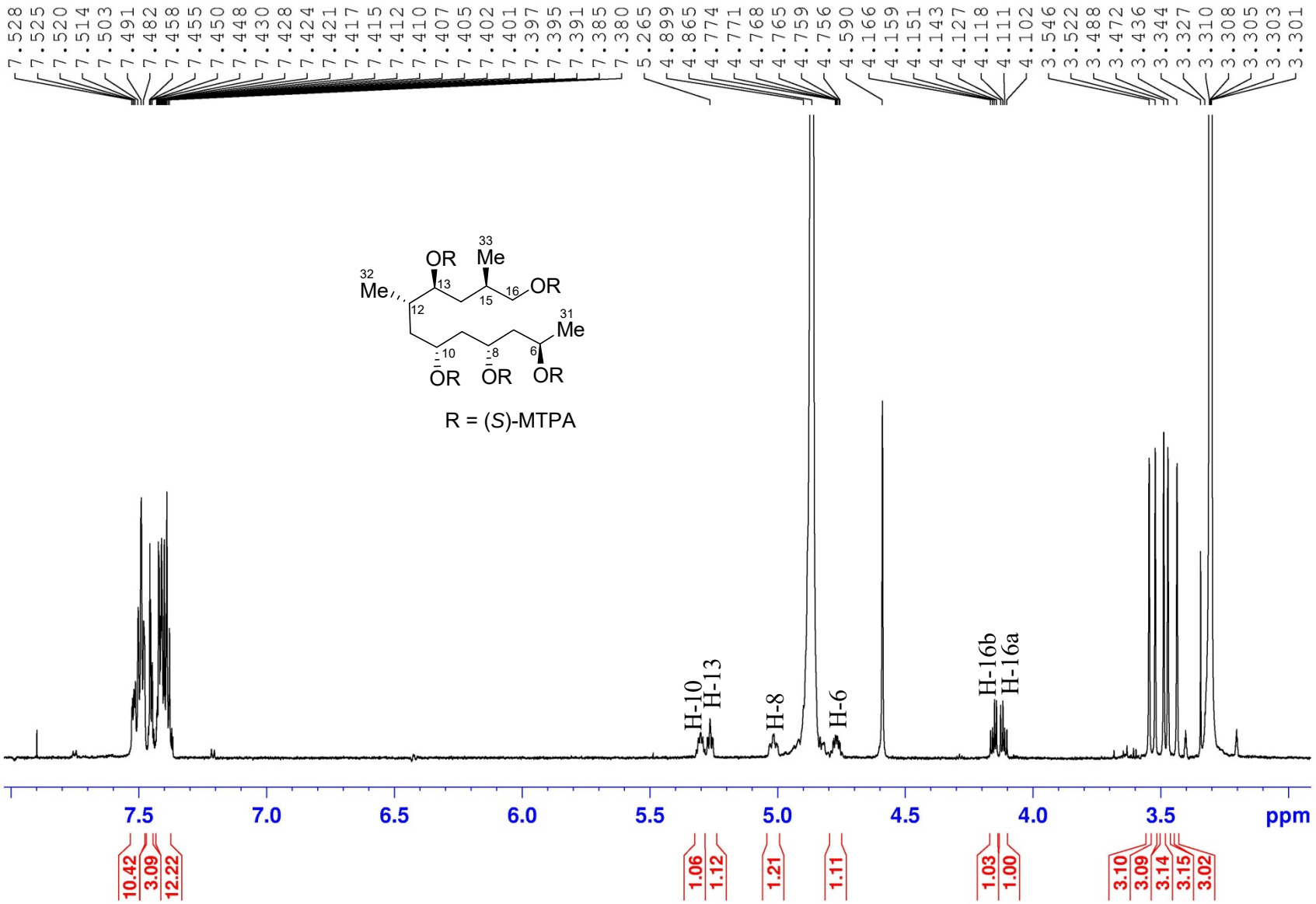
LR-ESIMS for the fragment **1A's**



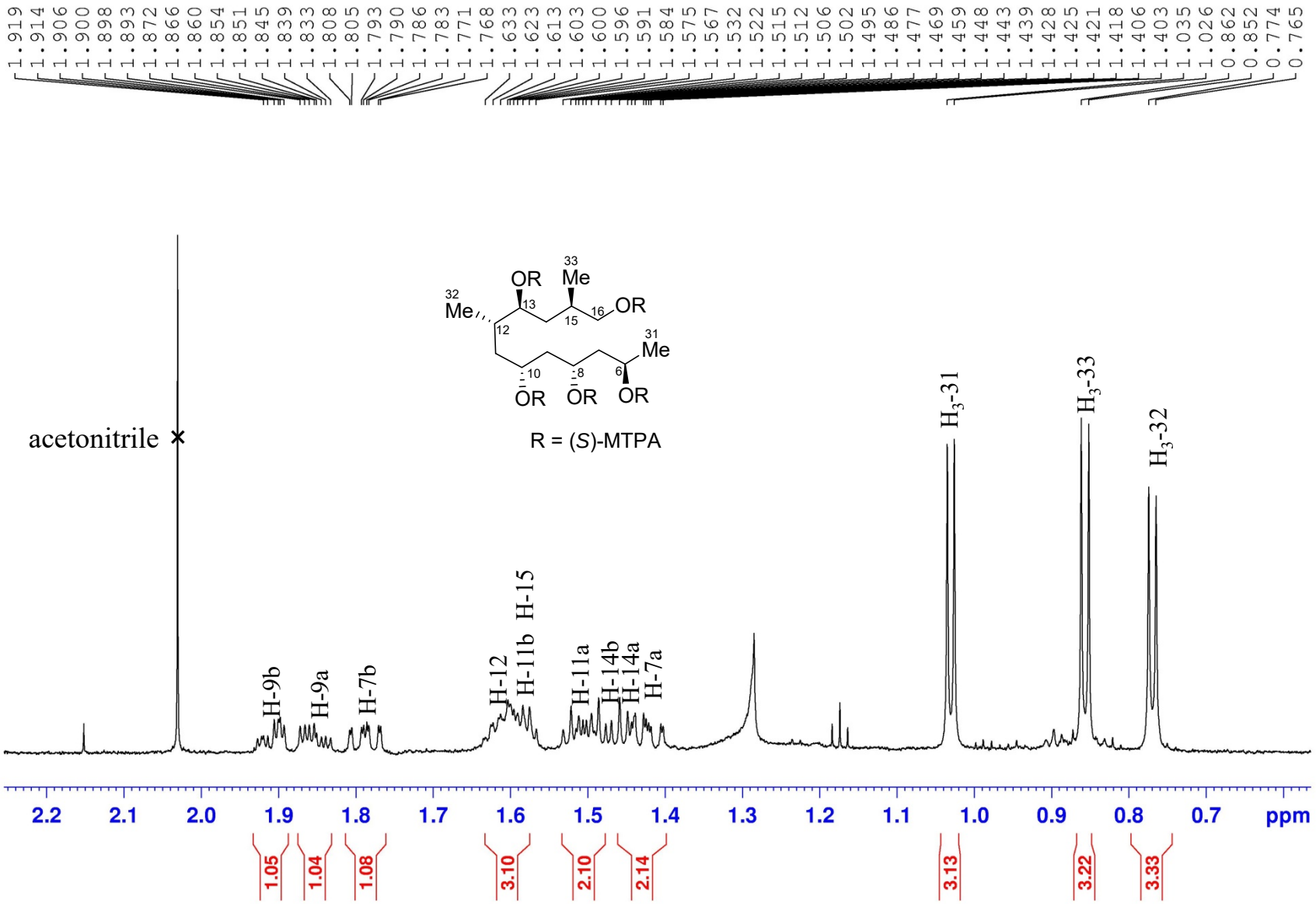
^{1}H (700 MHz) NMR spectrum of the fragment **1A's** in CD_3OD



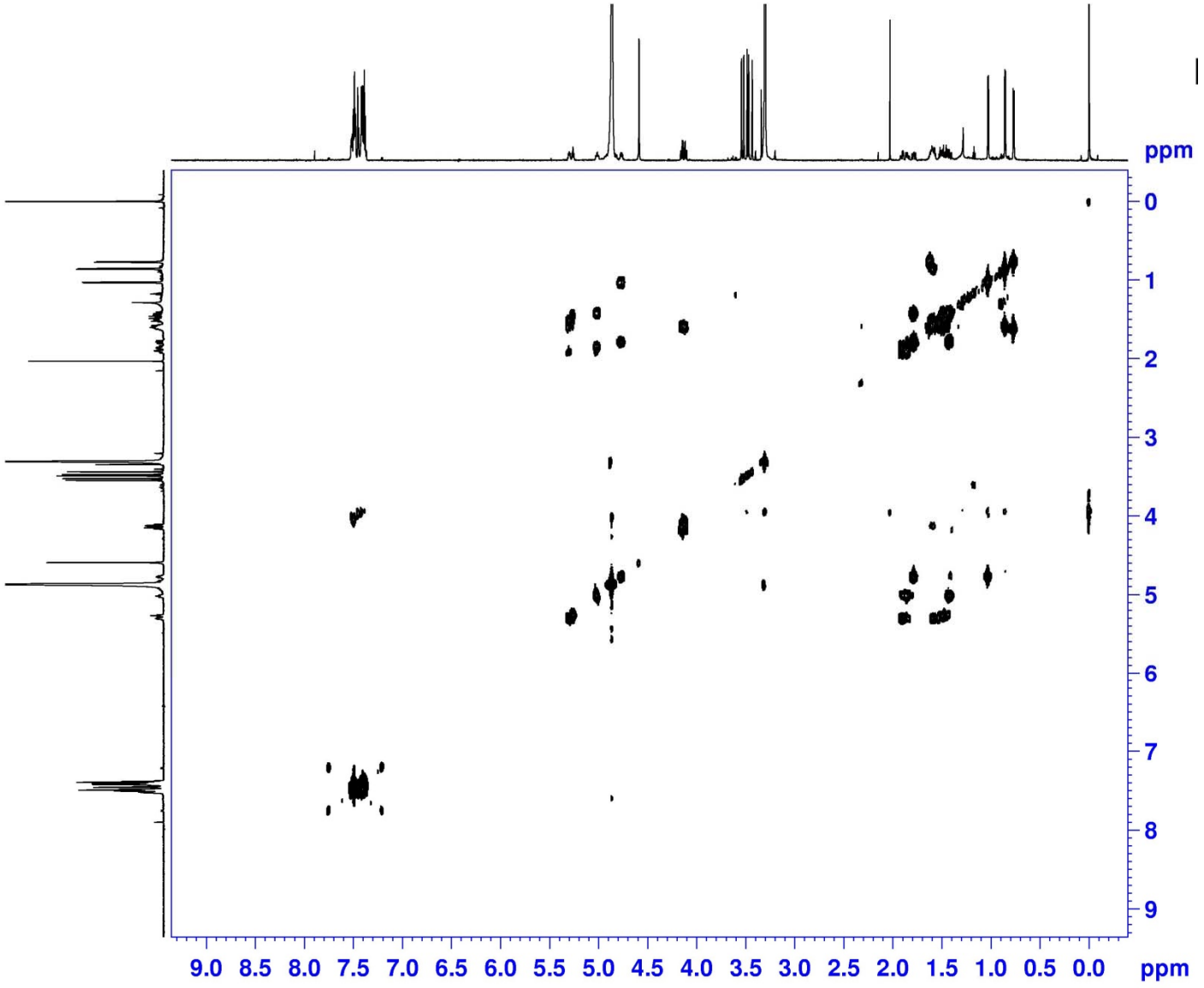
^{1}H (700 MHz) NMR spectrum of the fragment **1A's** in CD_3OD



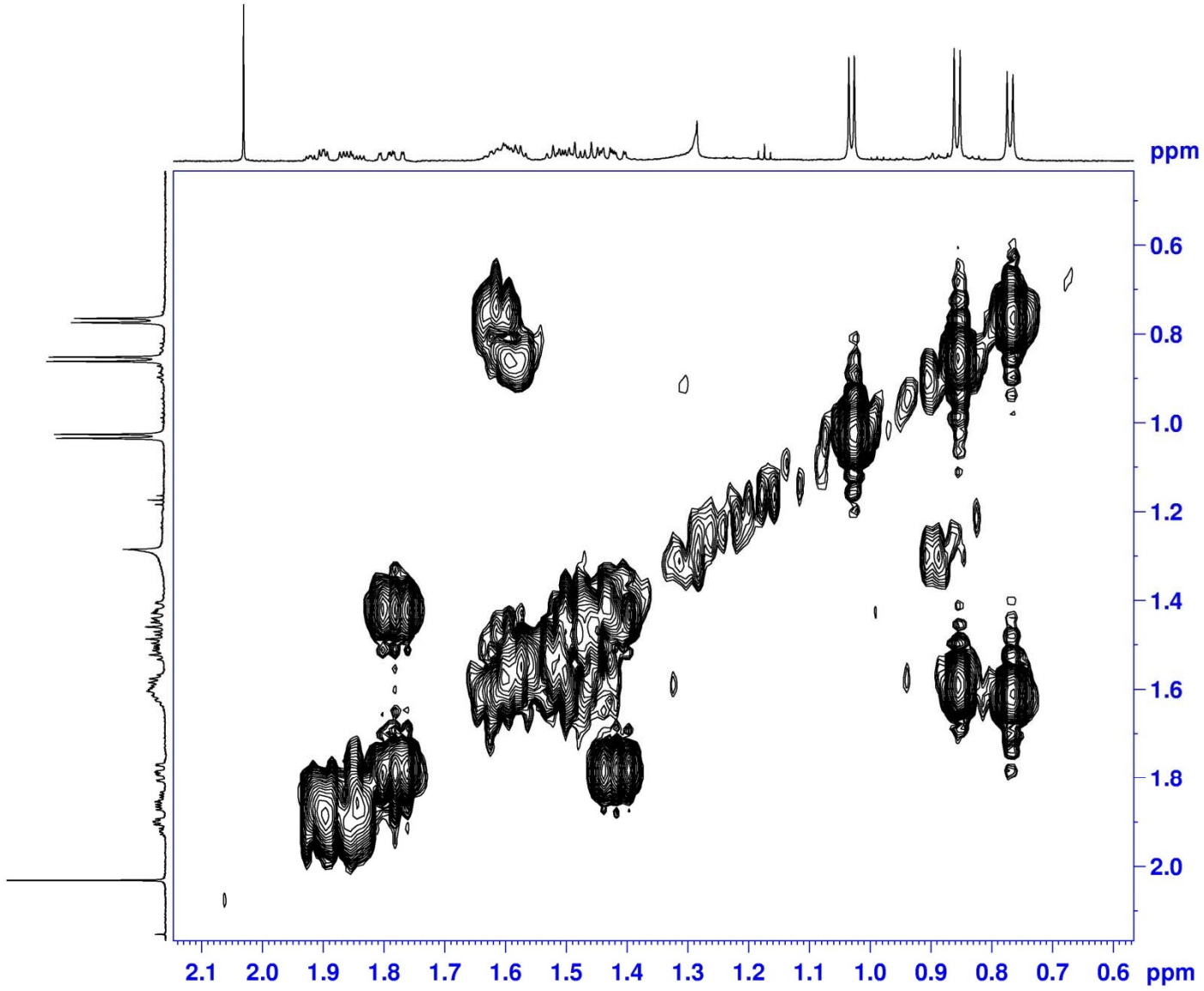
^{1}H (700 MHz) NMR spectrum of the fragment **1A's** in CD_3OD



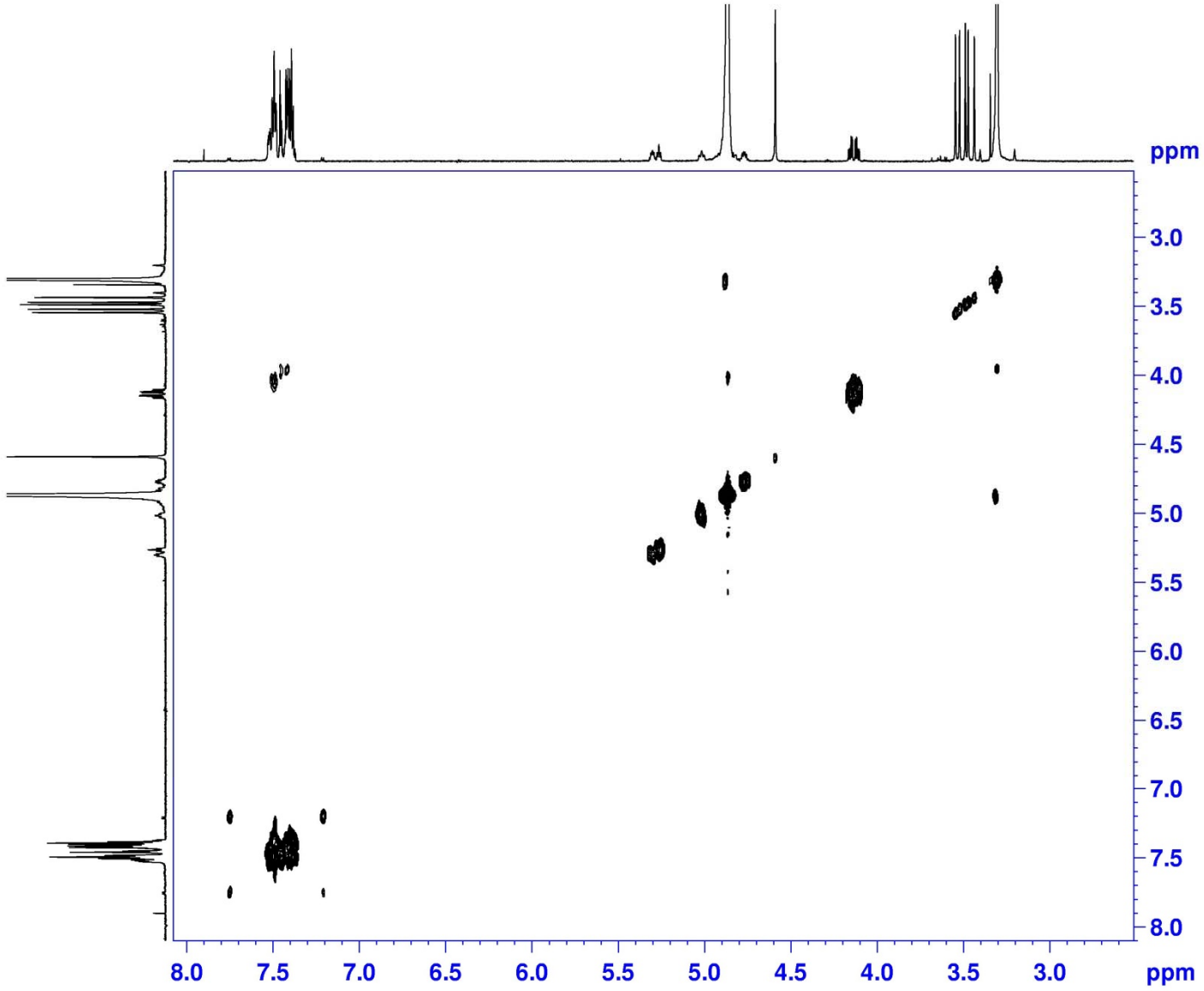
^{1}H–^{1}H COSY (700 MHz) spectrum of the fragment **1A's** in CD_3OD



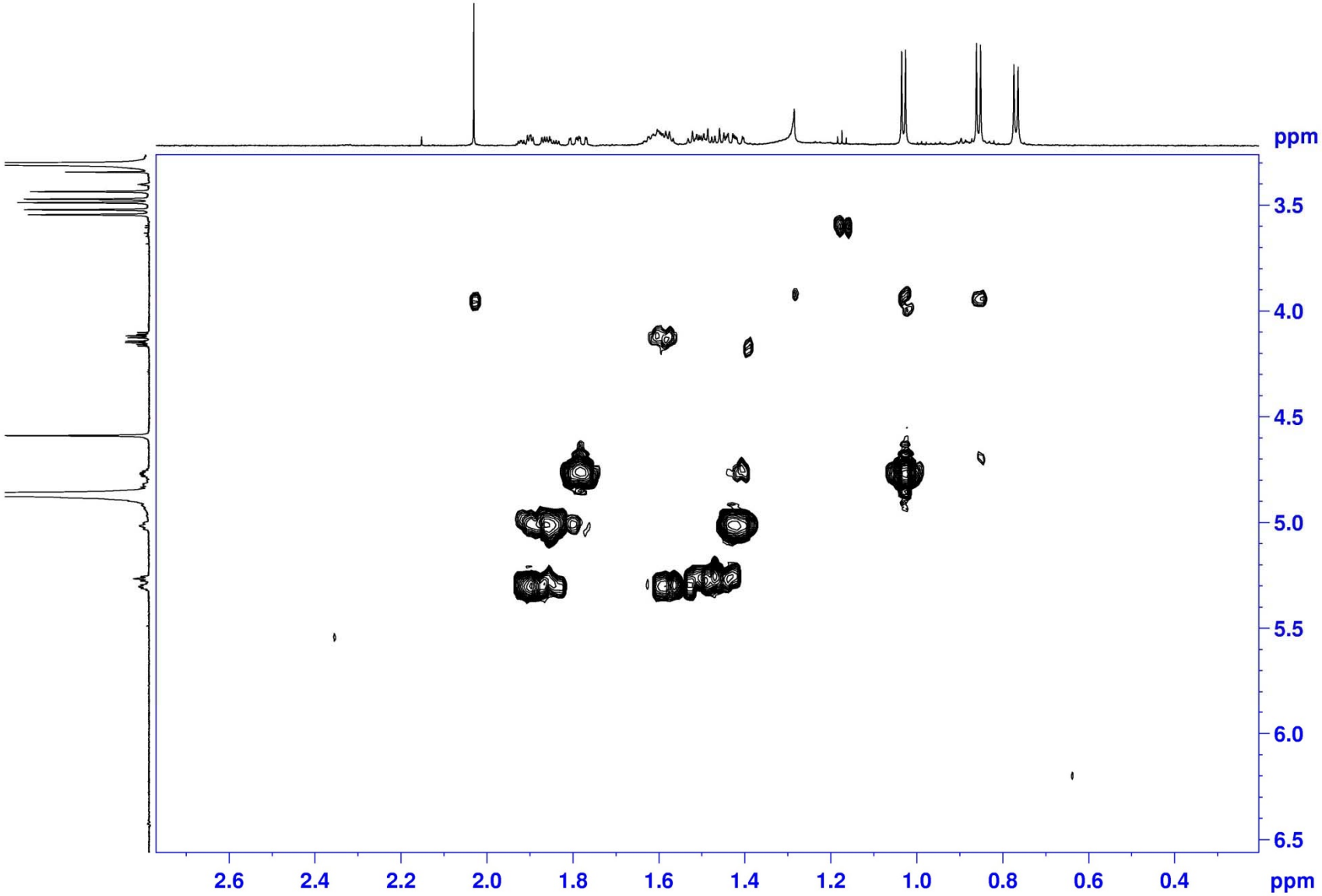
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1A's** in CD_3OD



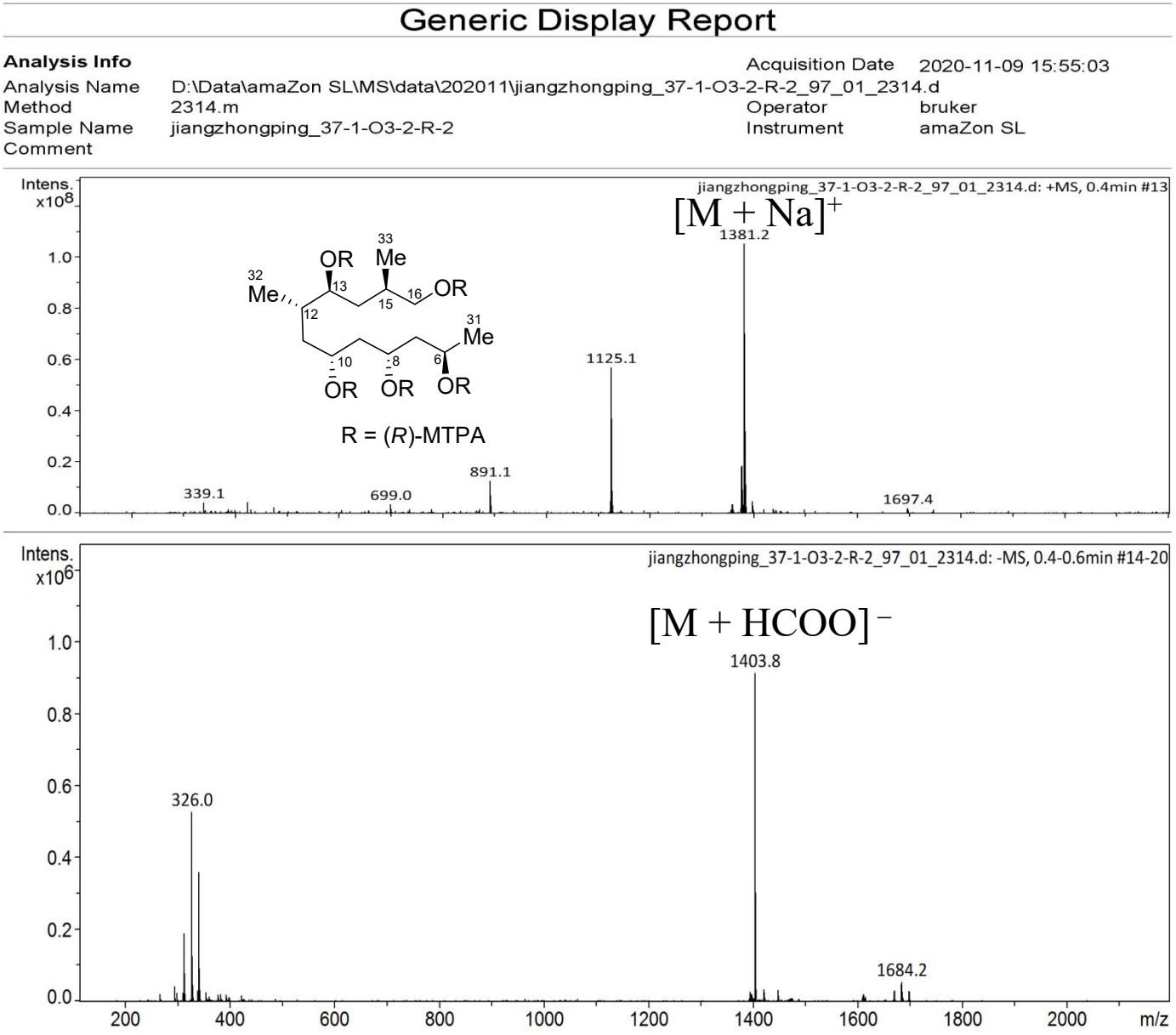
^{1}H–^{1}H COSY (700 MHz) spectrum of the fragment **1A's** in CD_3OD



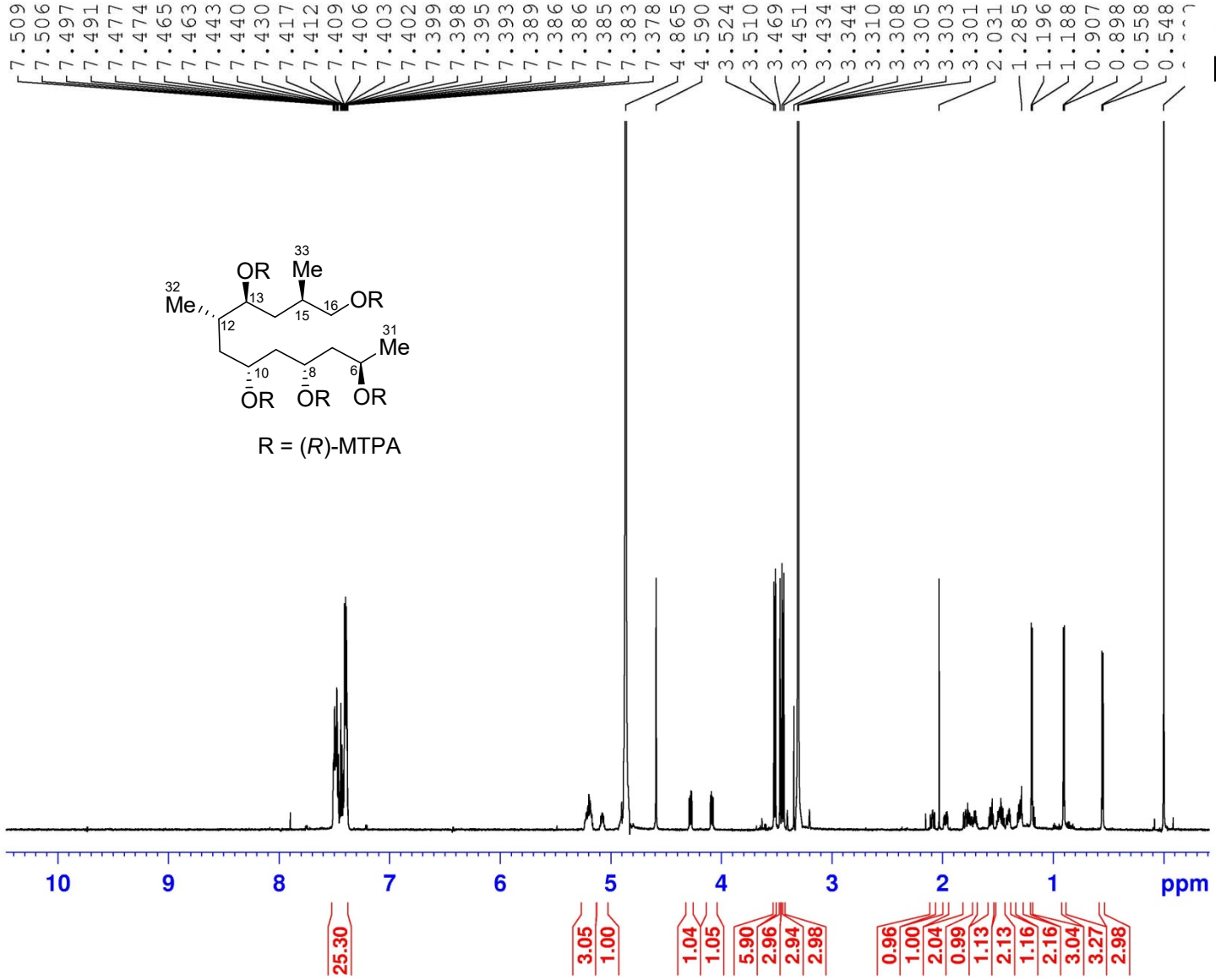
^{1}H–^{1}H COSY (700 MHz) spectrum of the fragment **1A's** in CD_3OD



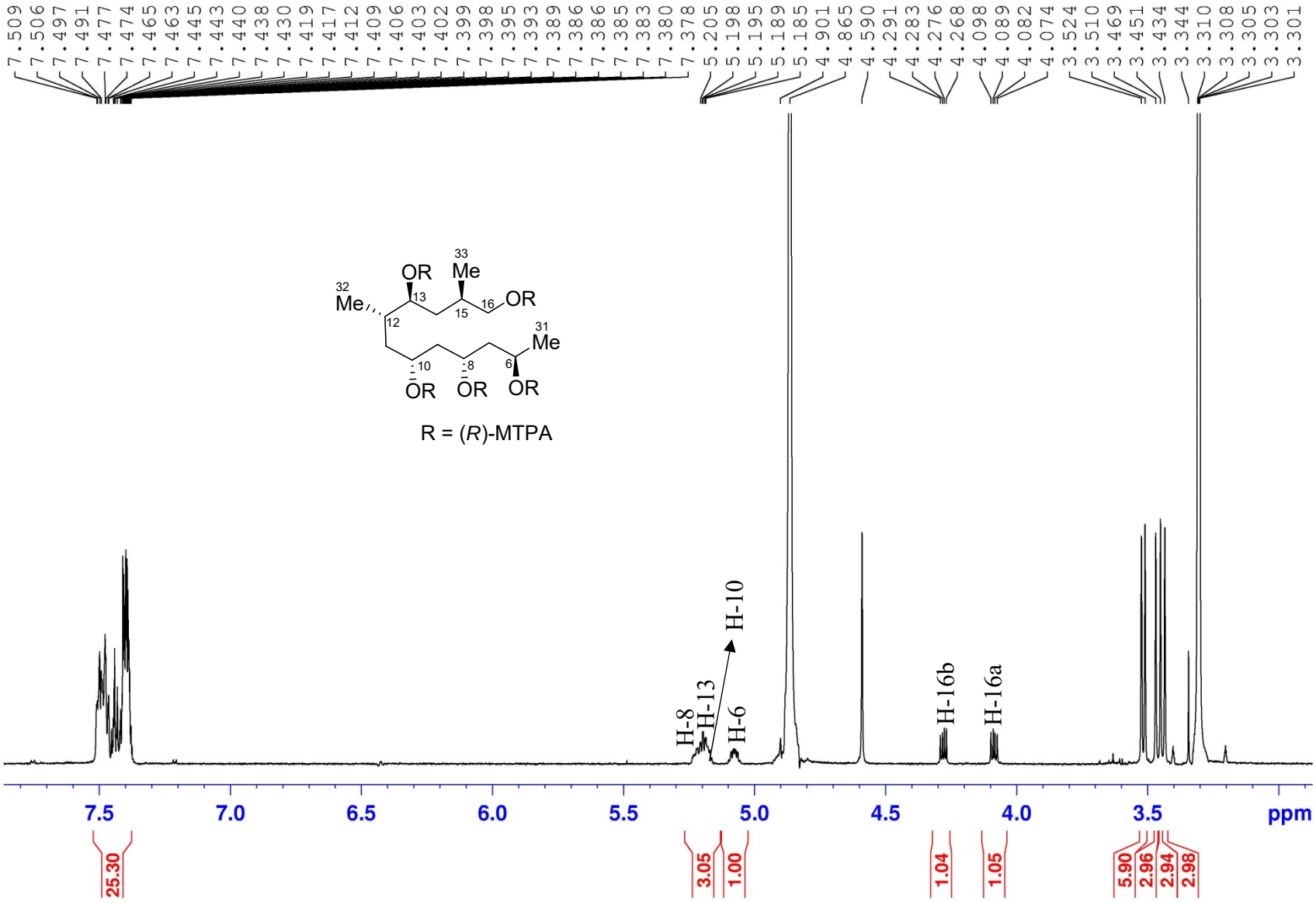
LR-ESIMS for the fragment **1A'r**



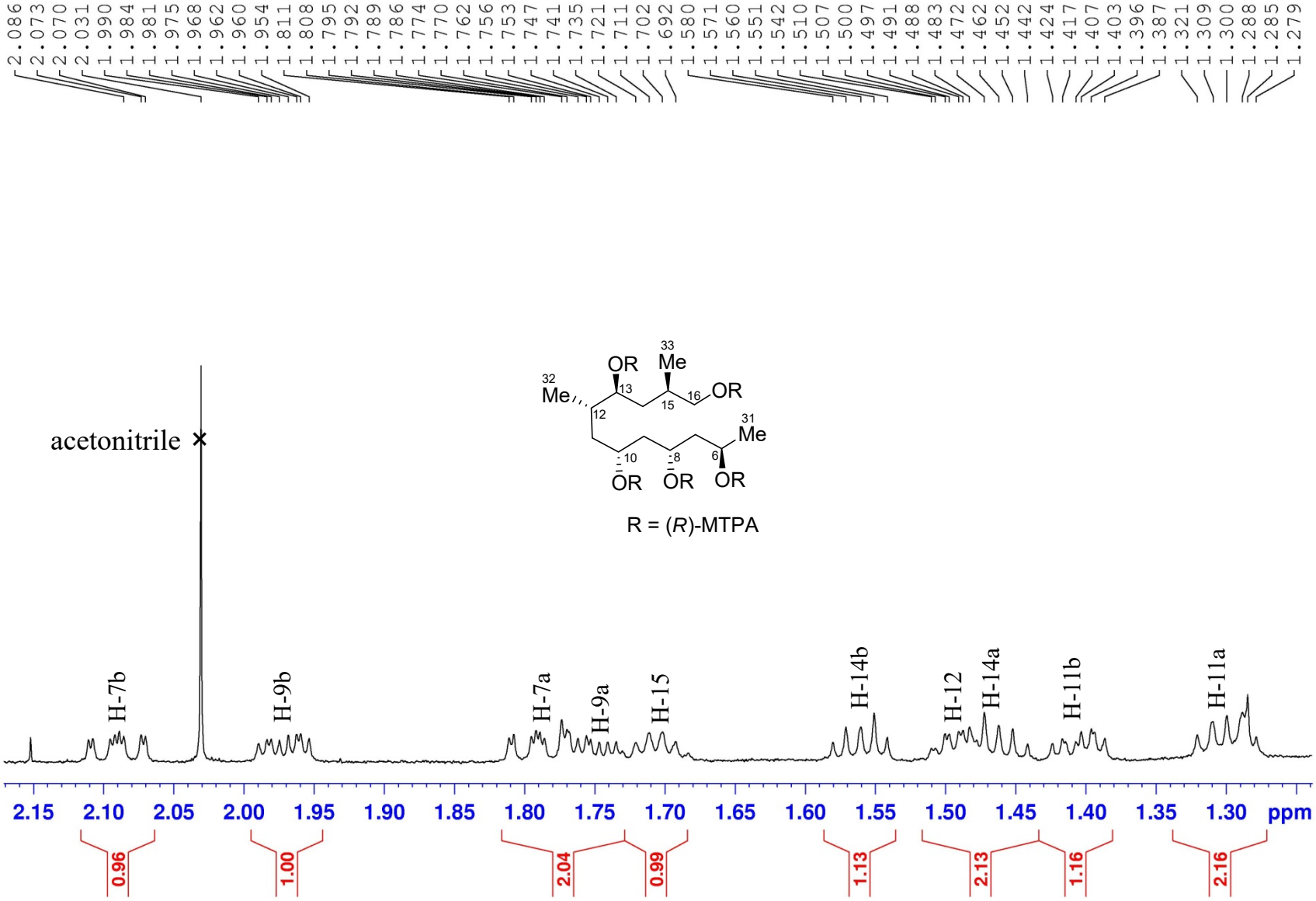
^{1}H (700 MHz) NMR spectrum of the fragment **1A'r** in CD_3OD



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



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



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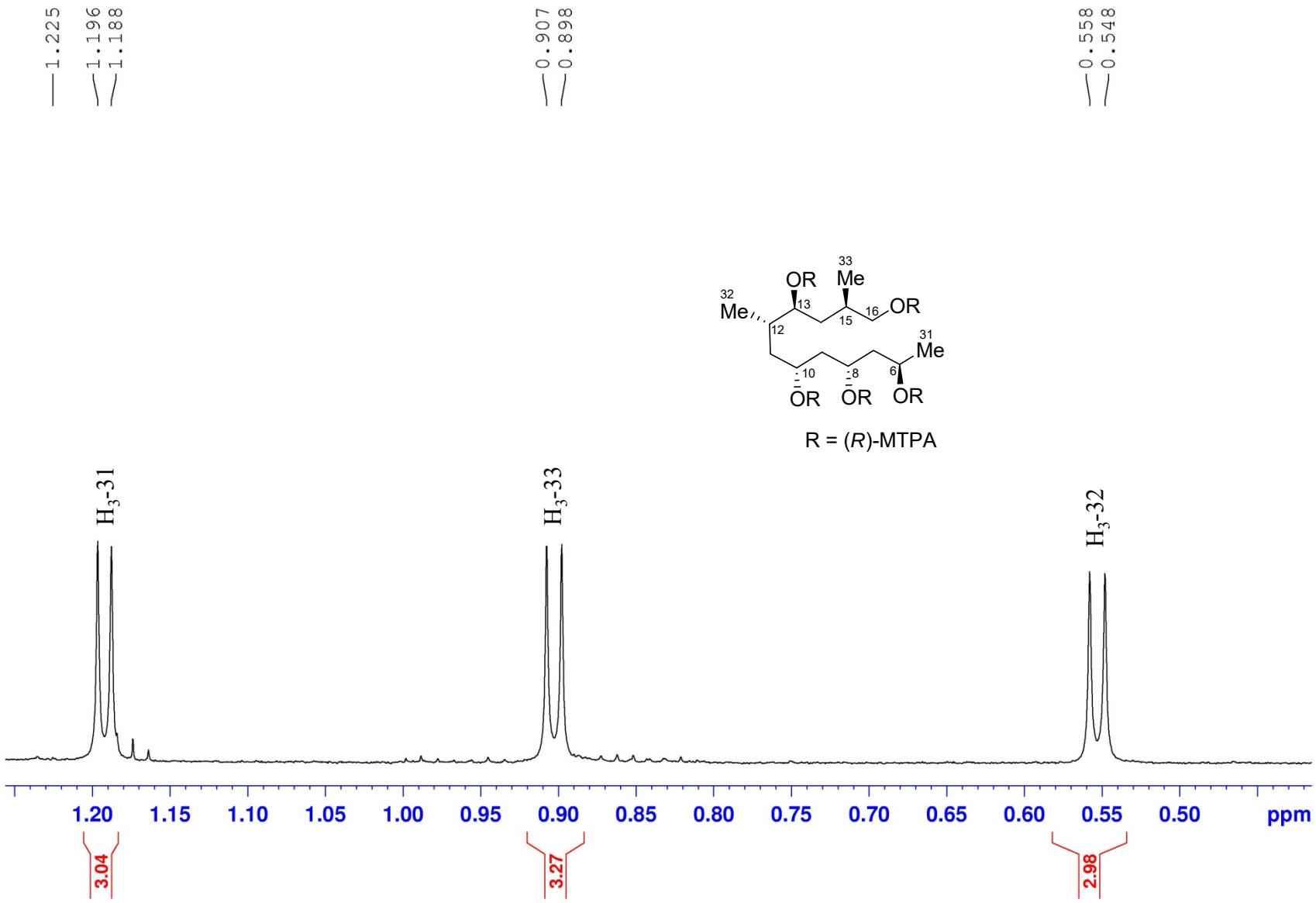
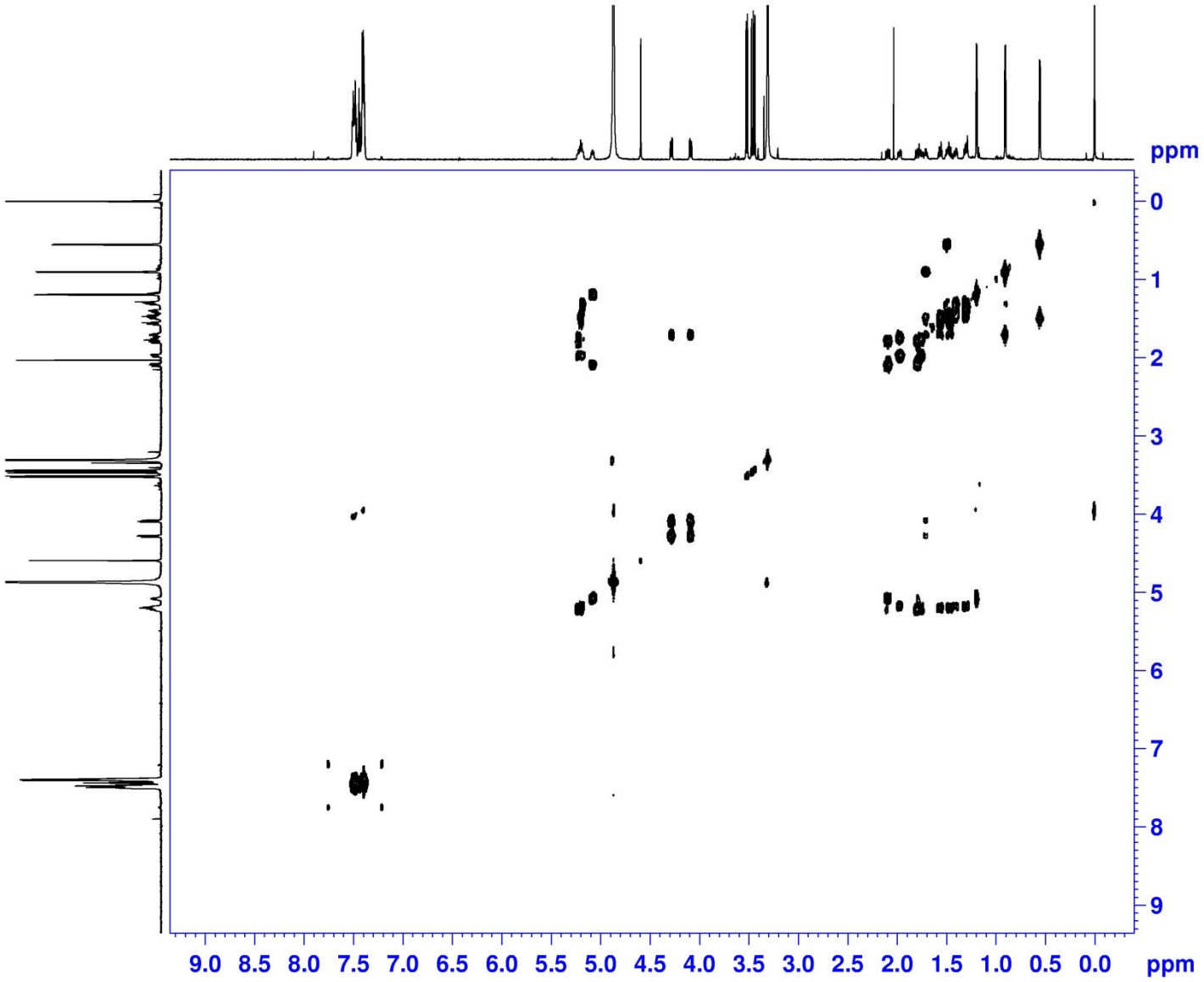
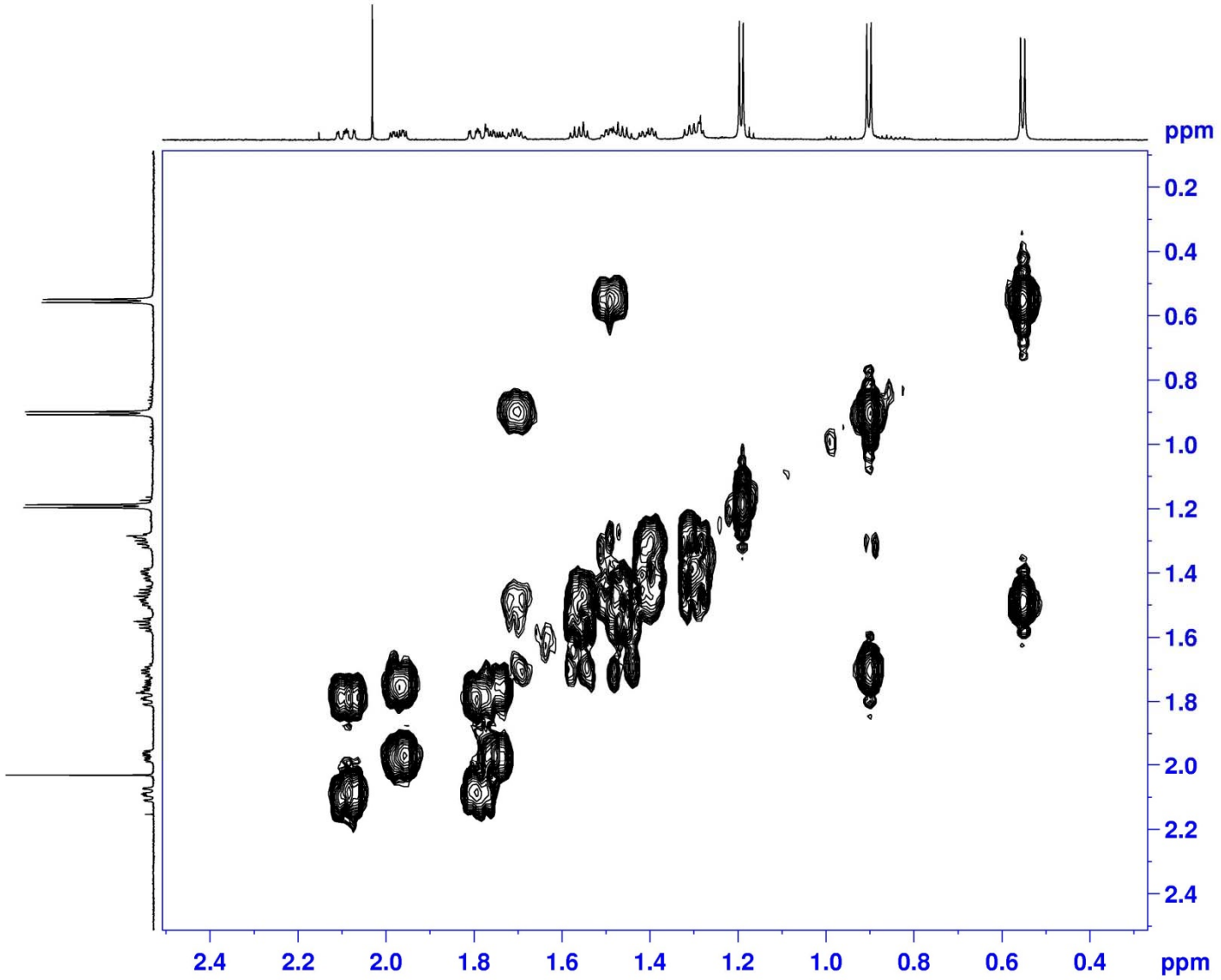


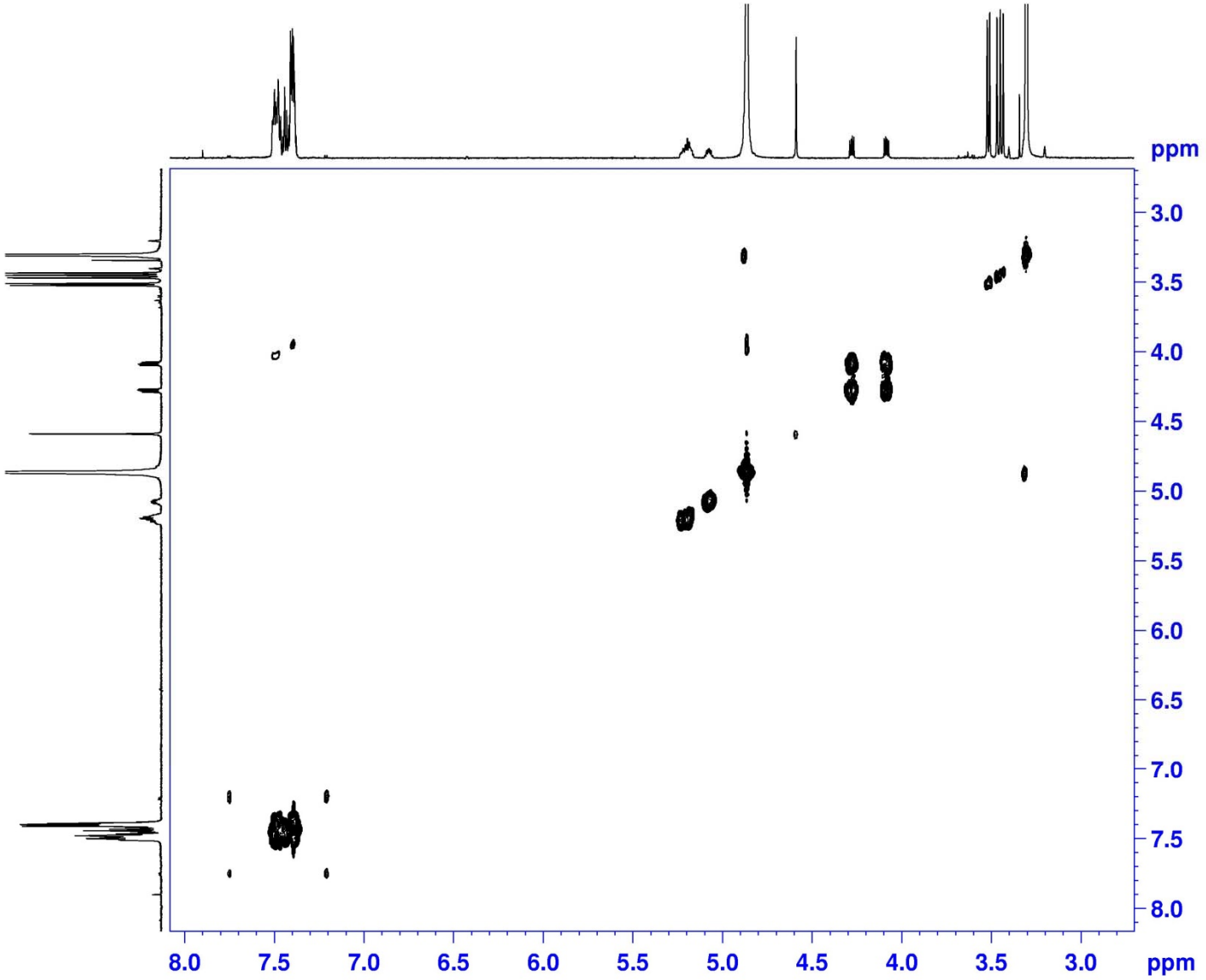
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1A'r** in CD_3OD



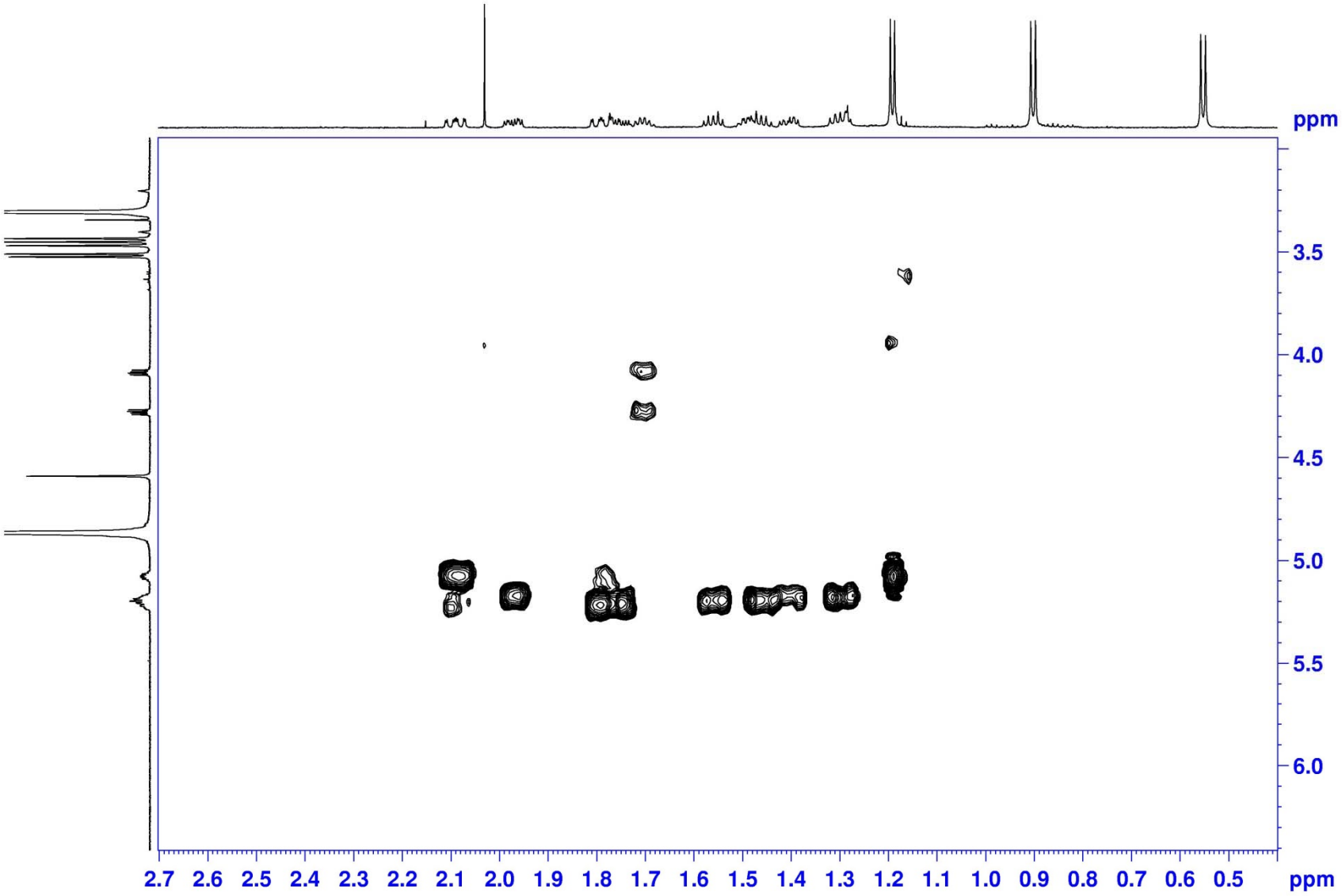
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1A'r** in CD_3OD



$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1A'r** in CD_3OD



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



LR-ESIMS for fragments **1Bs**

Generic Display Report

Analysis Info

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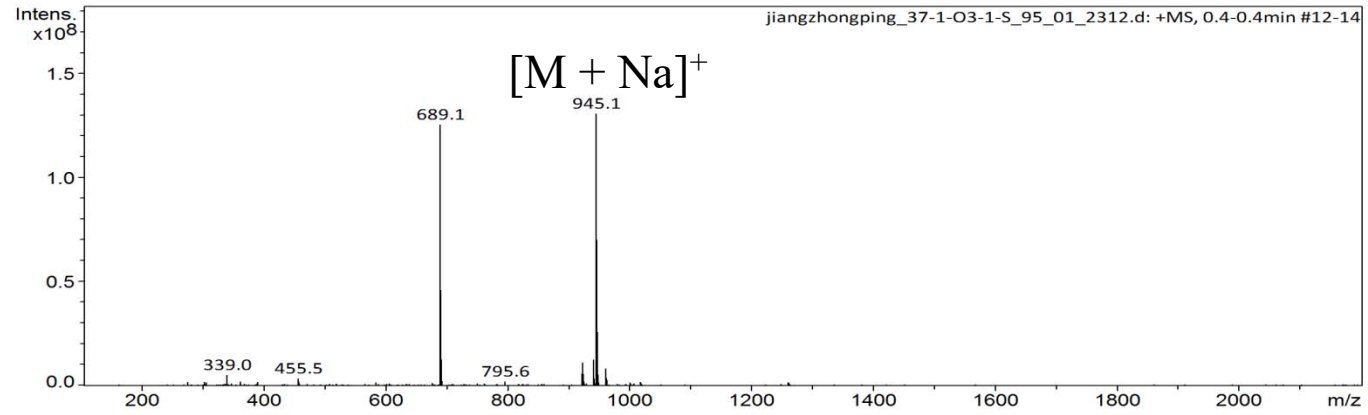
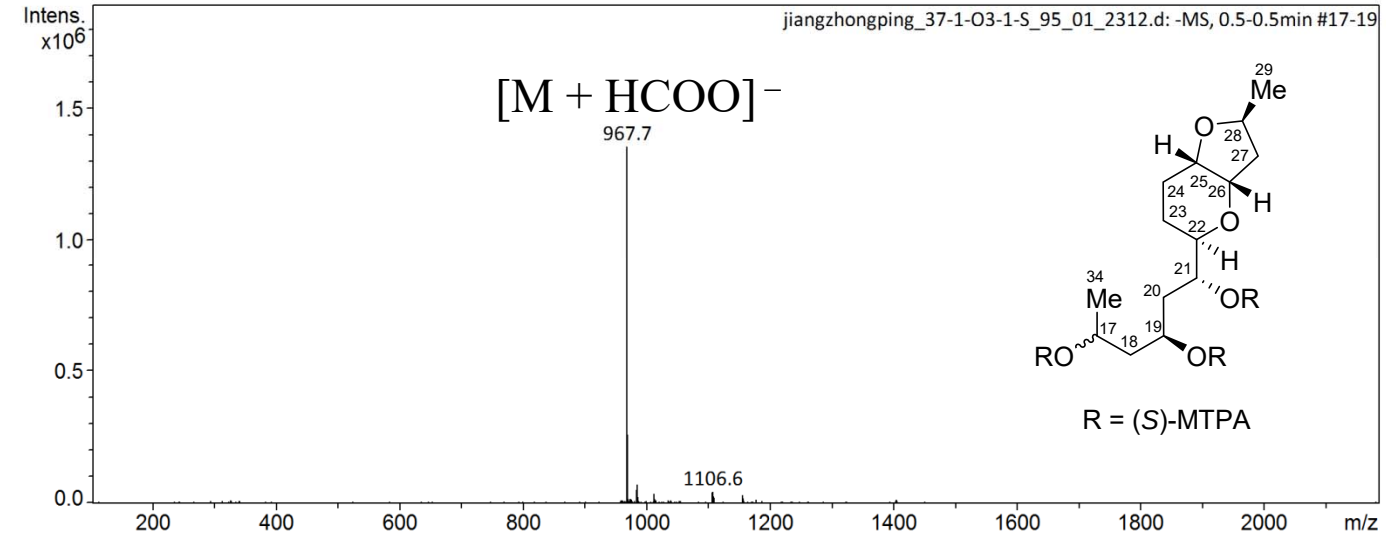
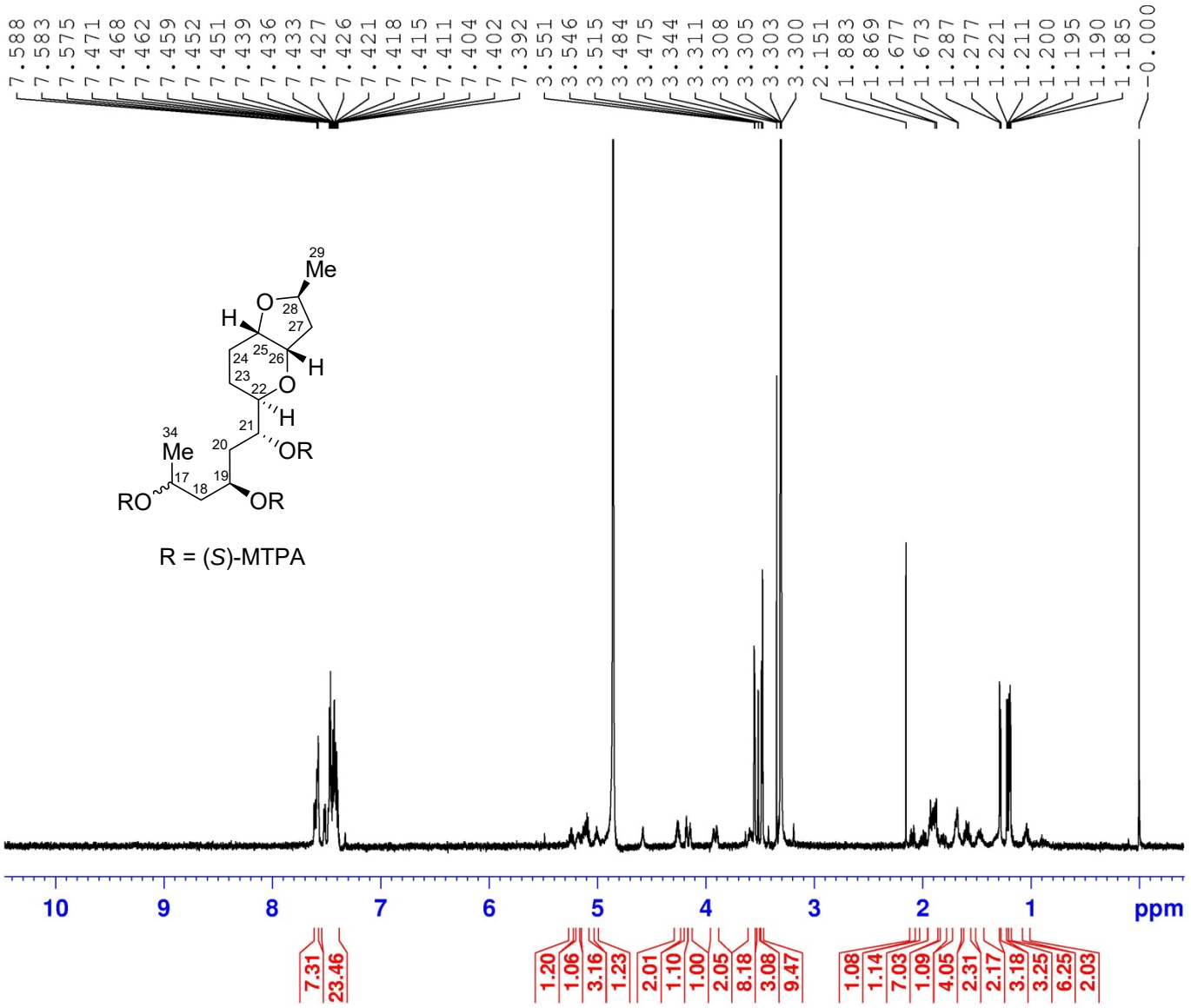




^{1}H (600 MHz) NMR spectrum of fragments **1Bs** in CD_3OD



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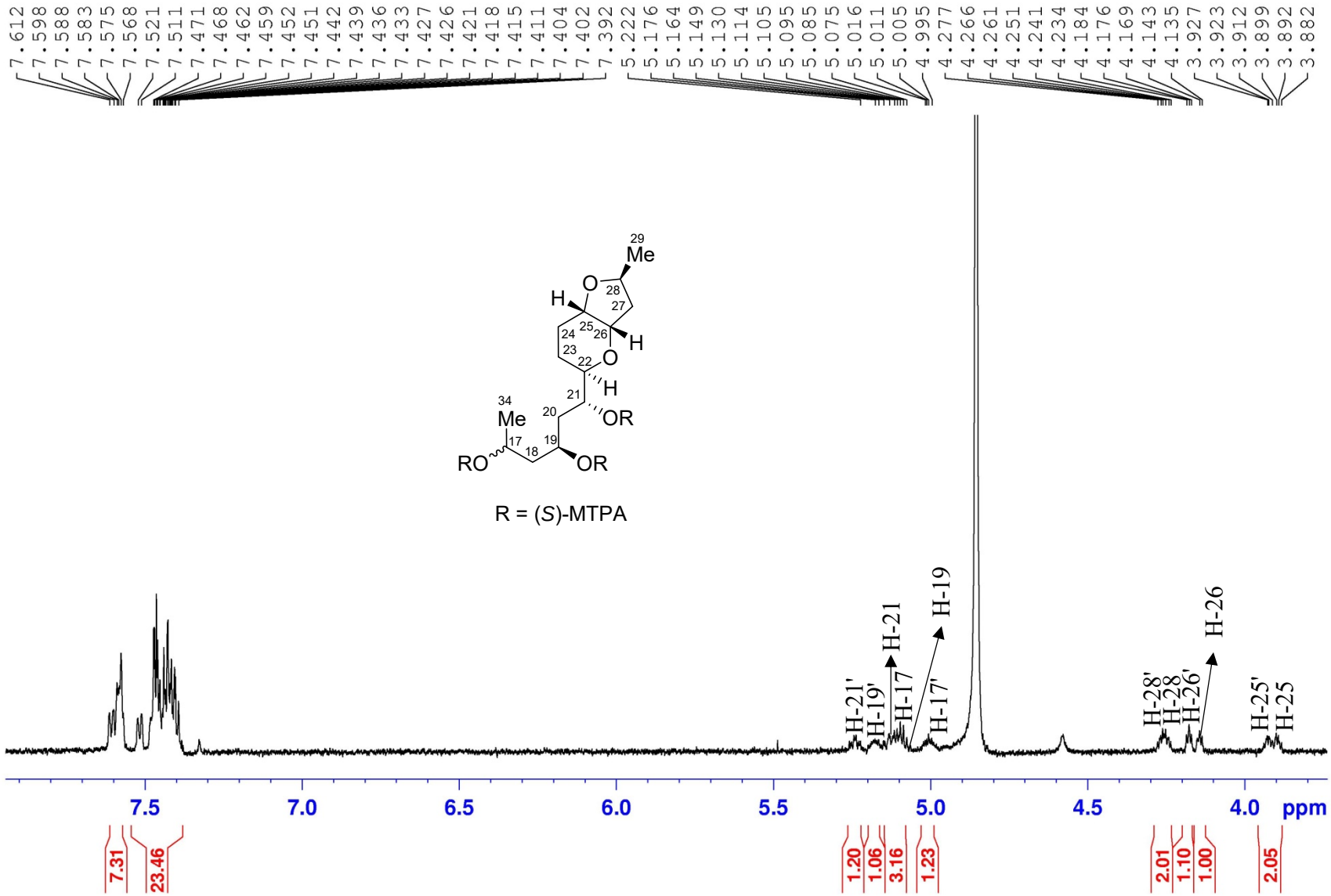

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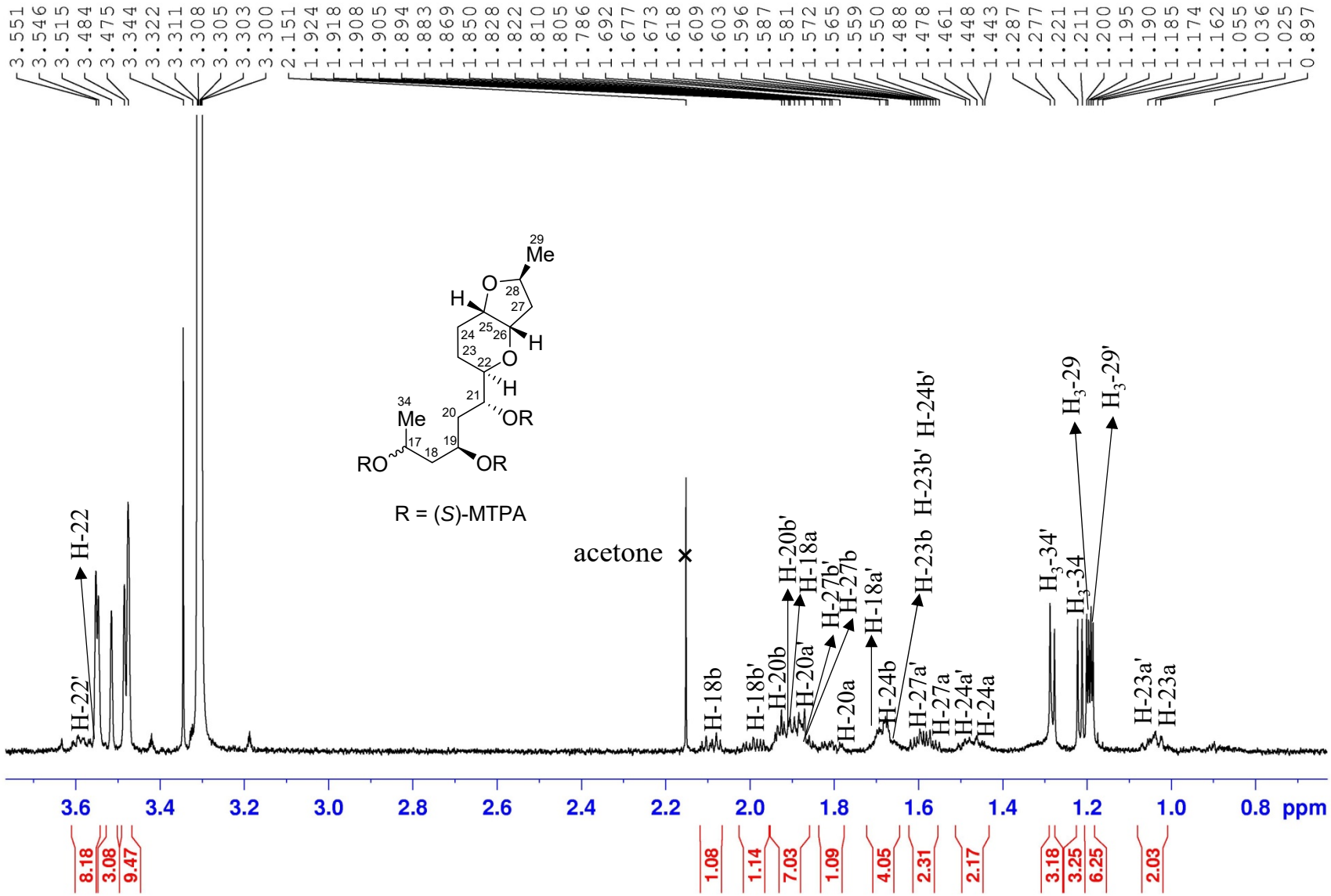
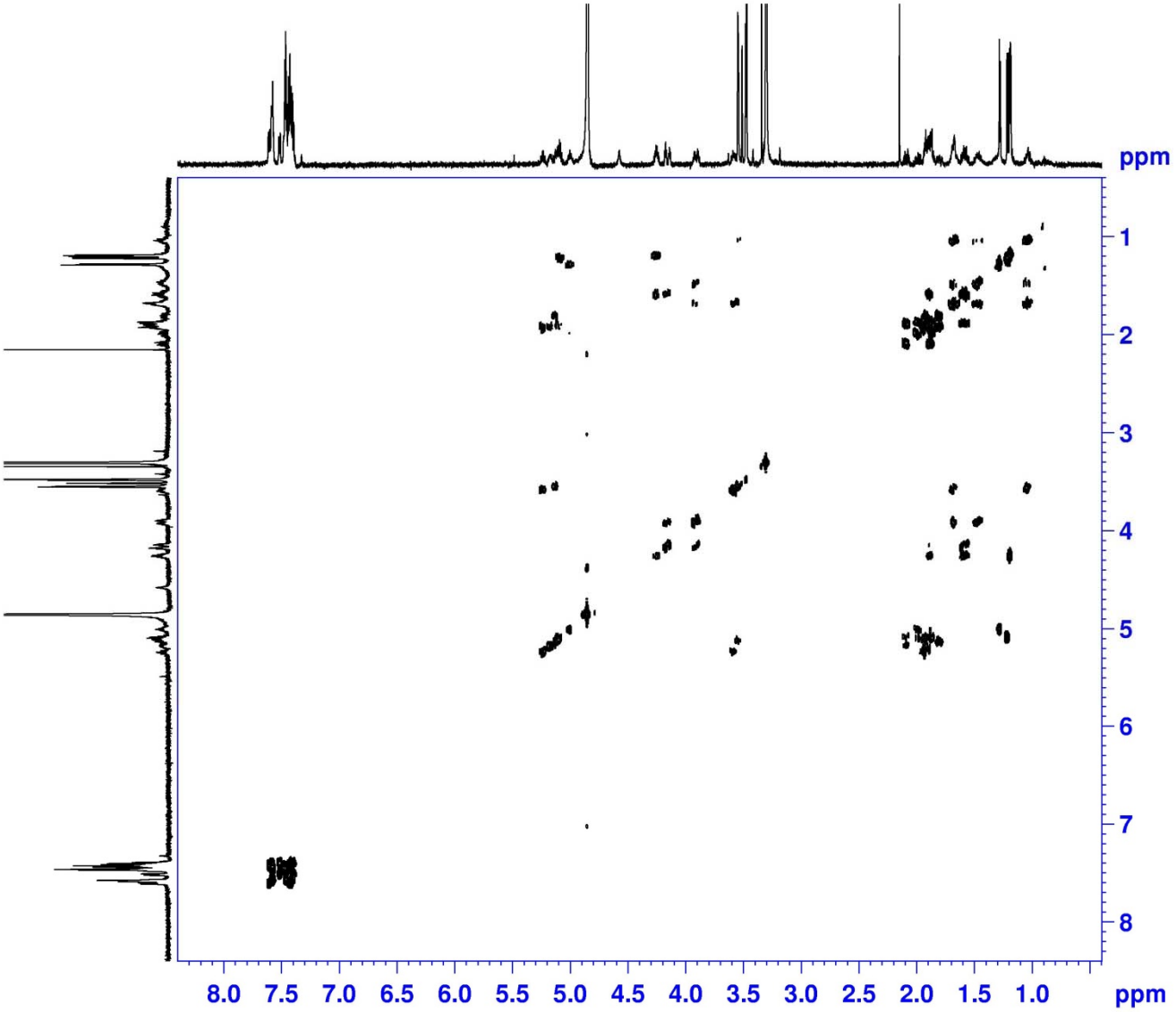
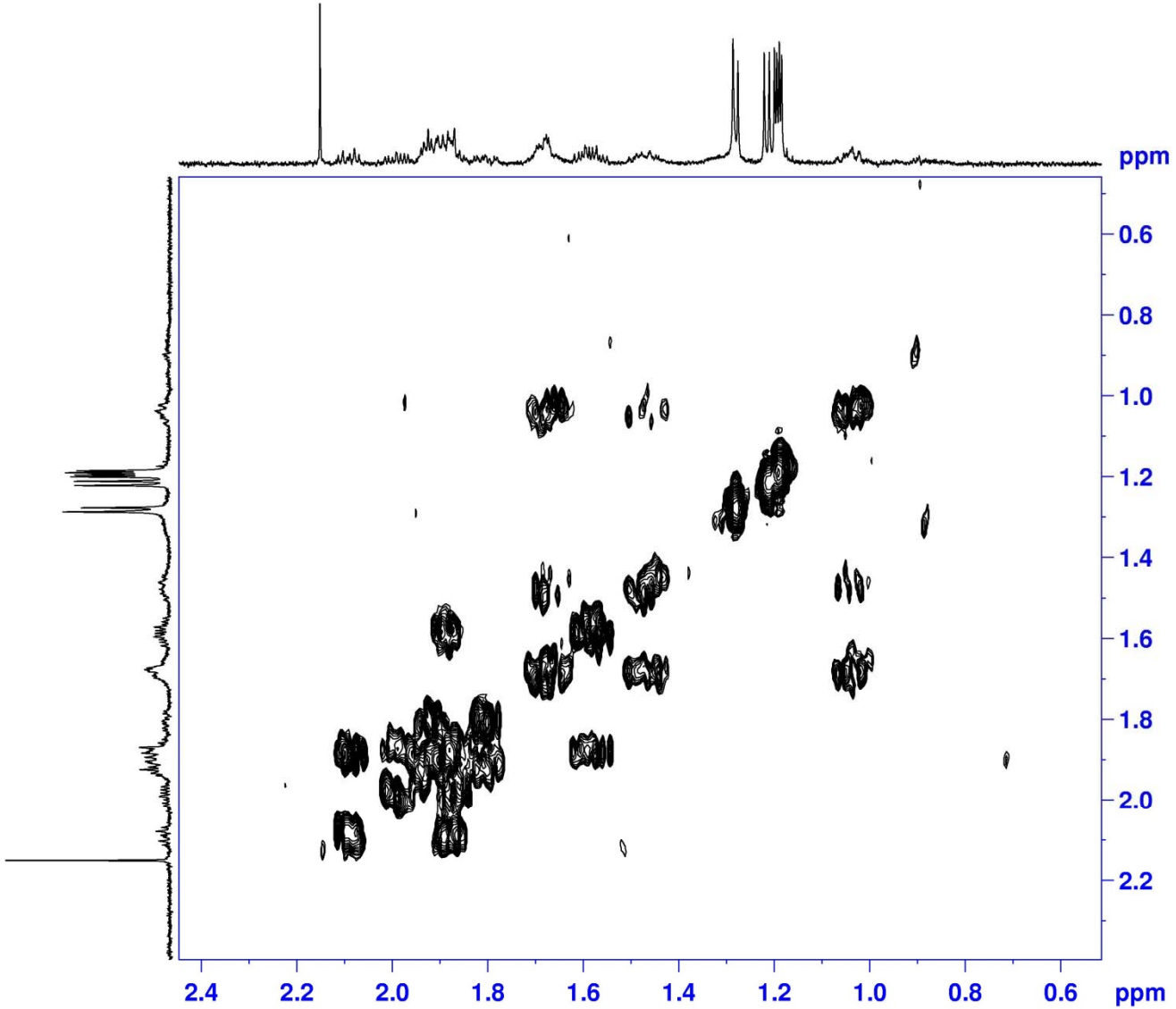


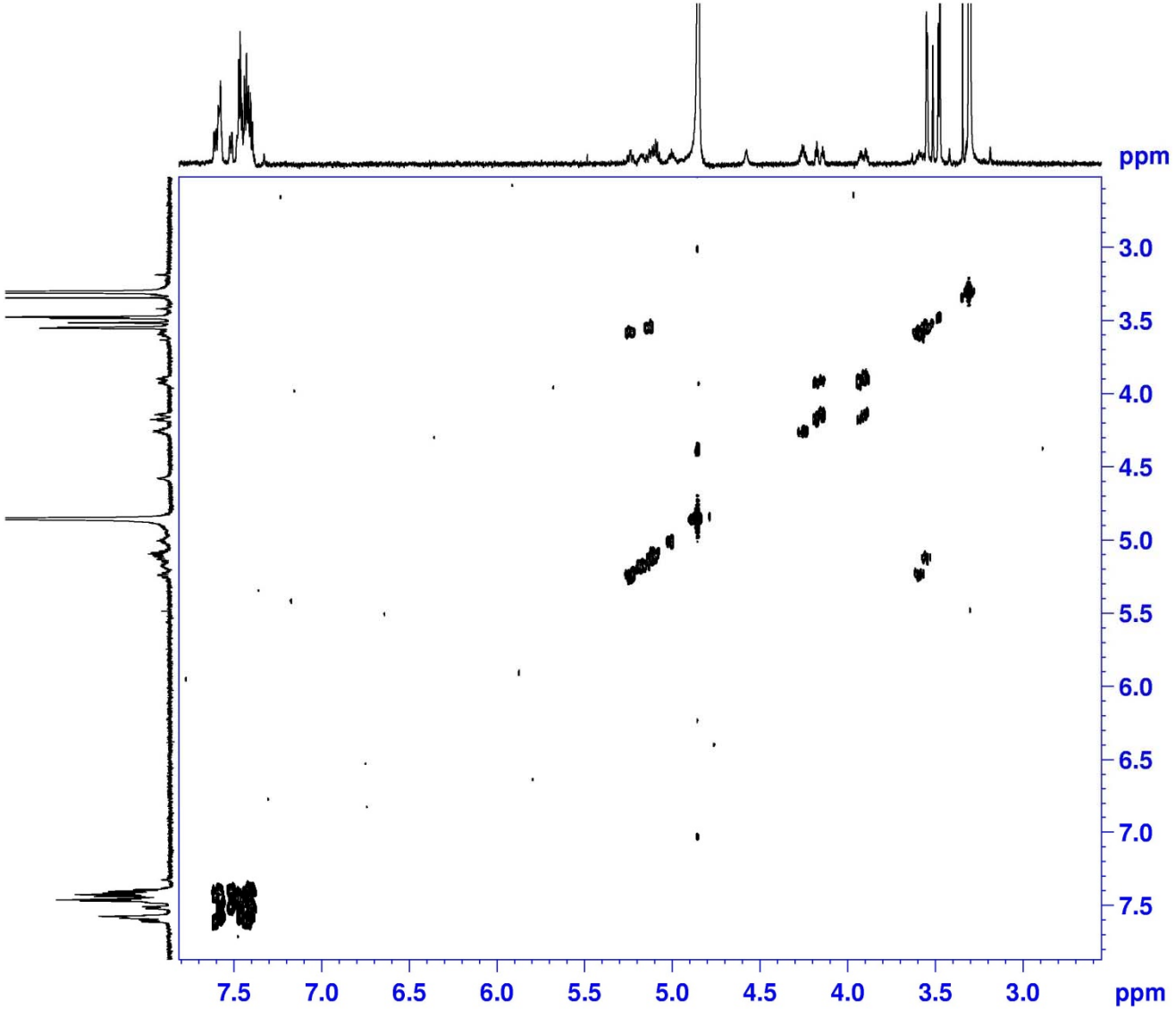
$^{1}H–^{1}H$ COSY (600 MHz) spectrum of fragments **1Bs** in CD_3OD



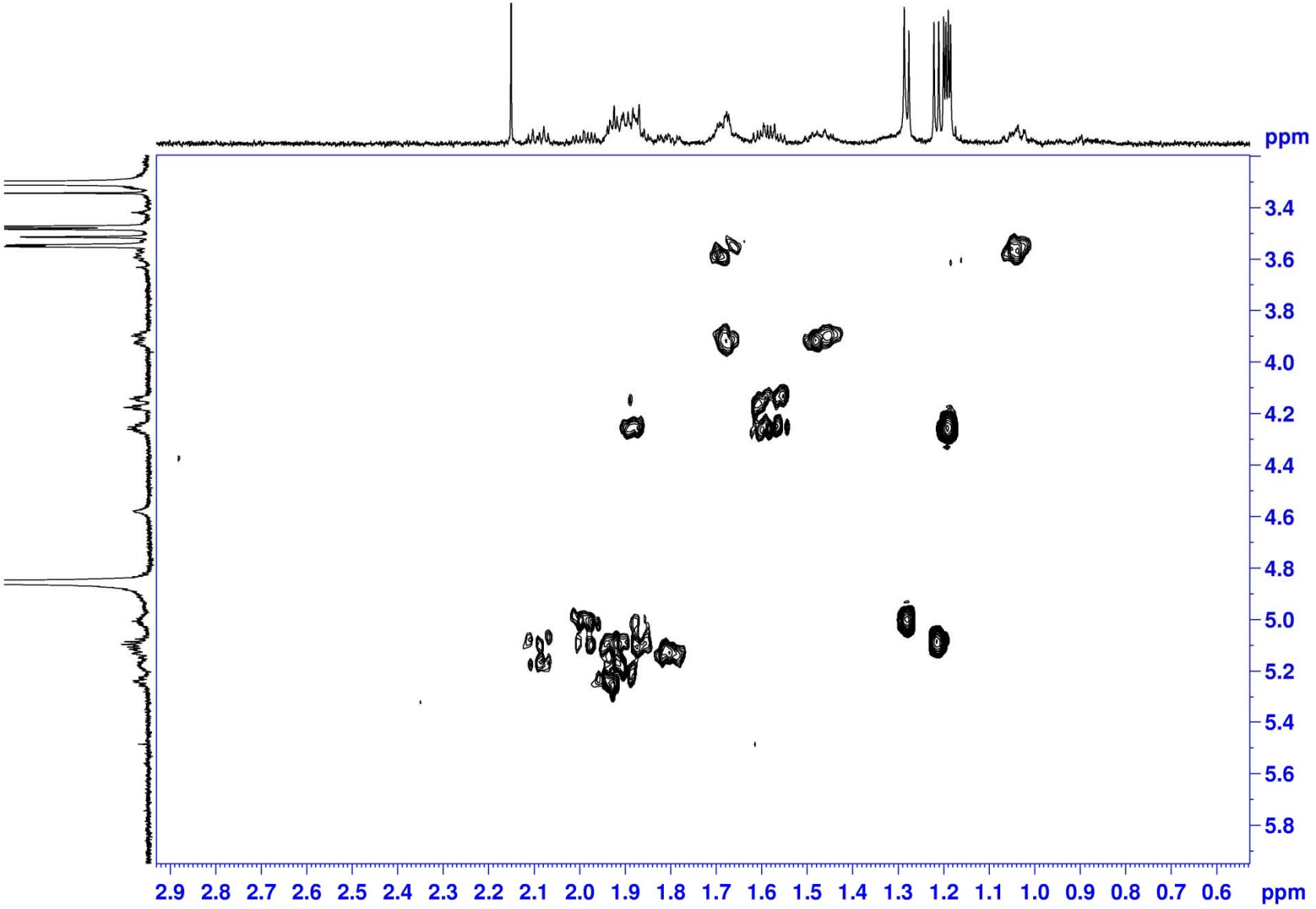
$^{1}H–^{1}H$ COSY (600 MHz) spectrum of fragments **1Bs** in CD_3OD



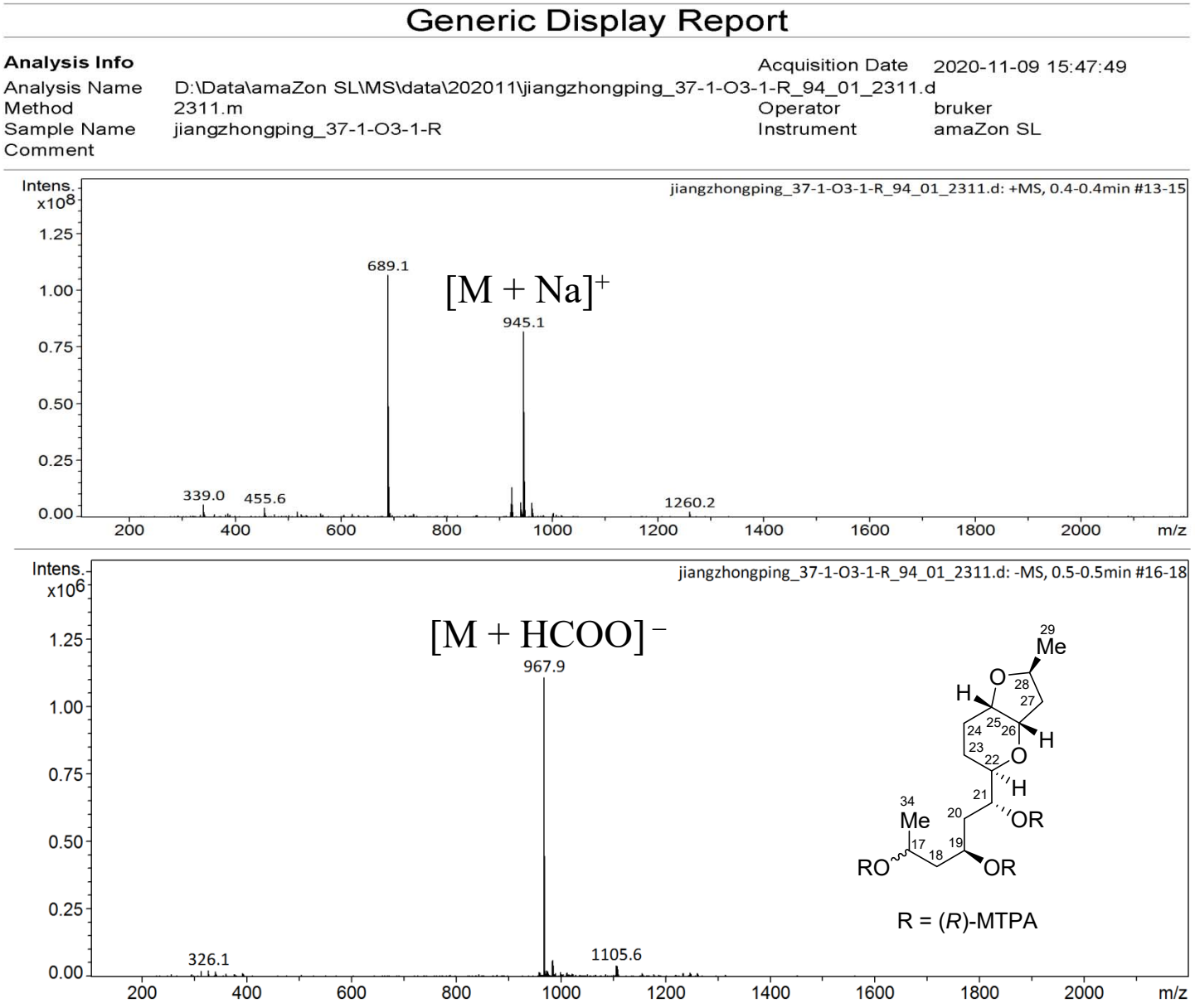
$^{1}H–^{1}H$ COSY (600 MHz) spectrum of fragments **1Bs** in CD_3OD



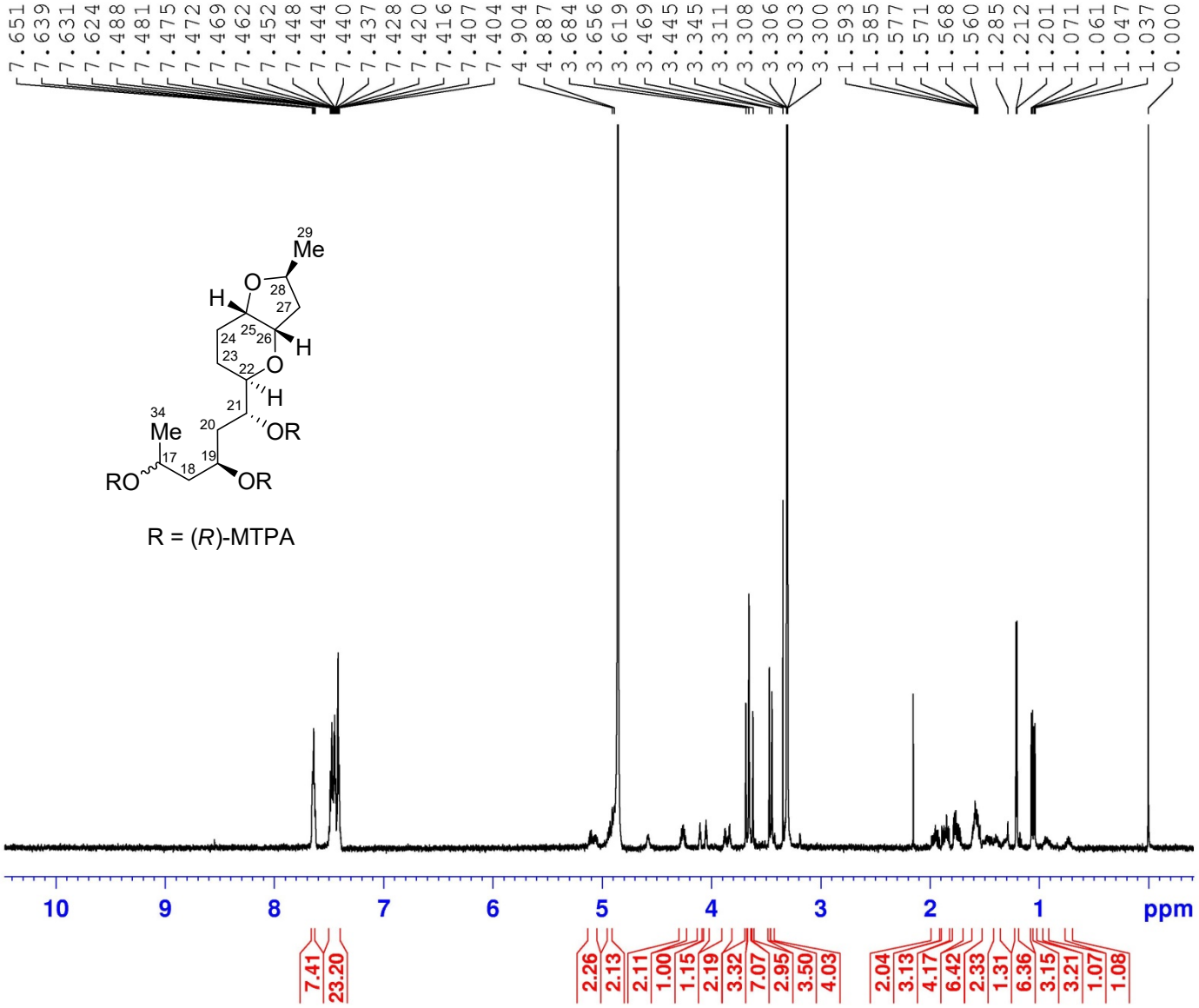
$^{1}H–^{1}H$ COSY (600 MHz) spectrum of fragments **1Bs** in CD_3OD



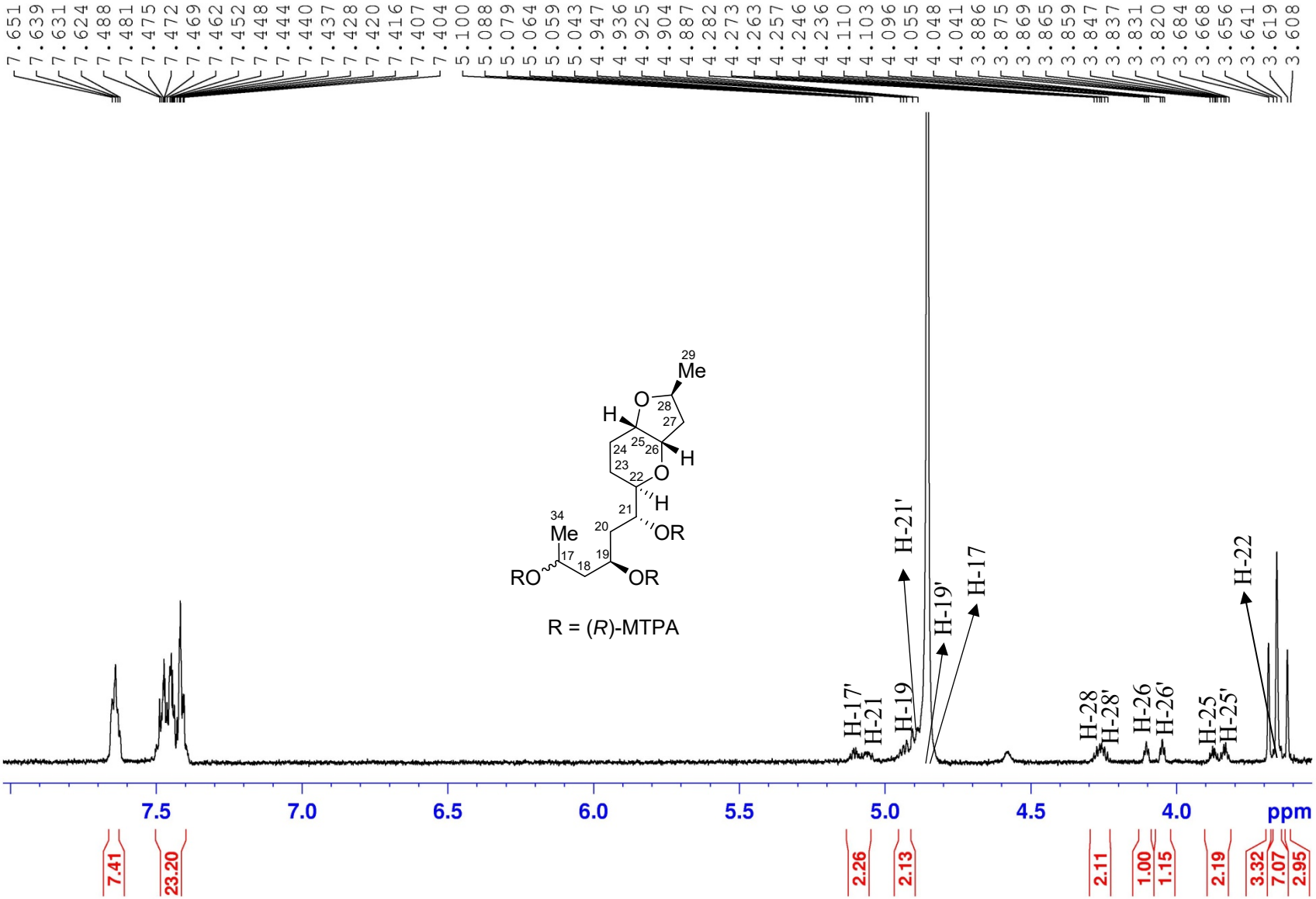
LR-ESIMS for fragments **1Br**



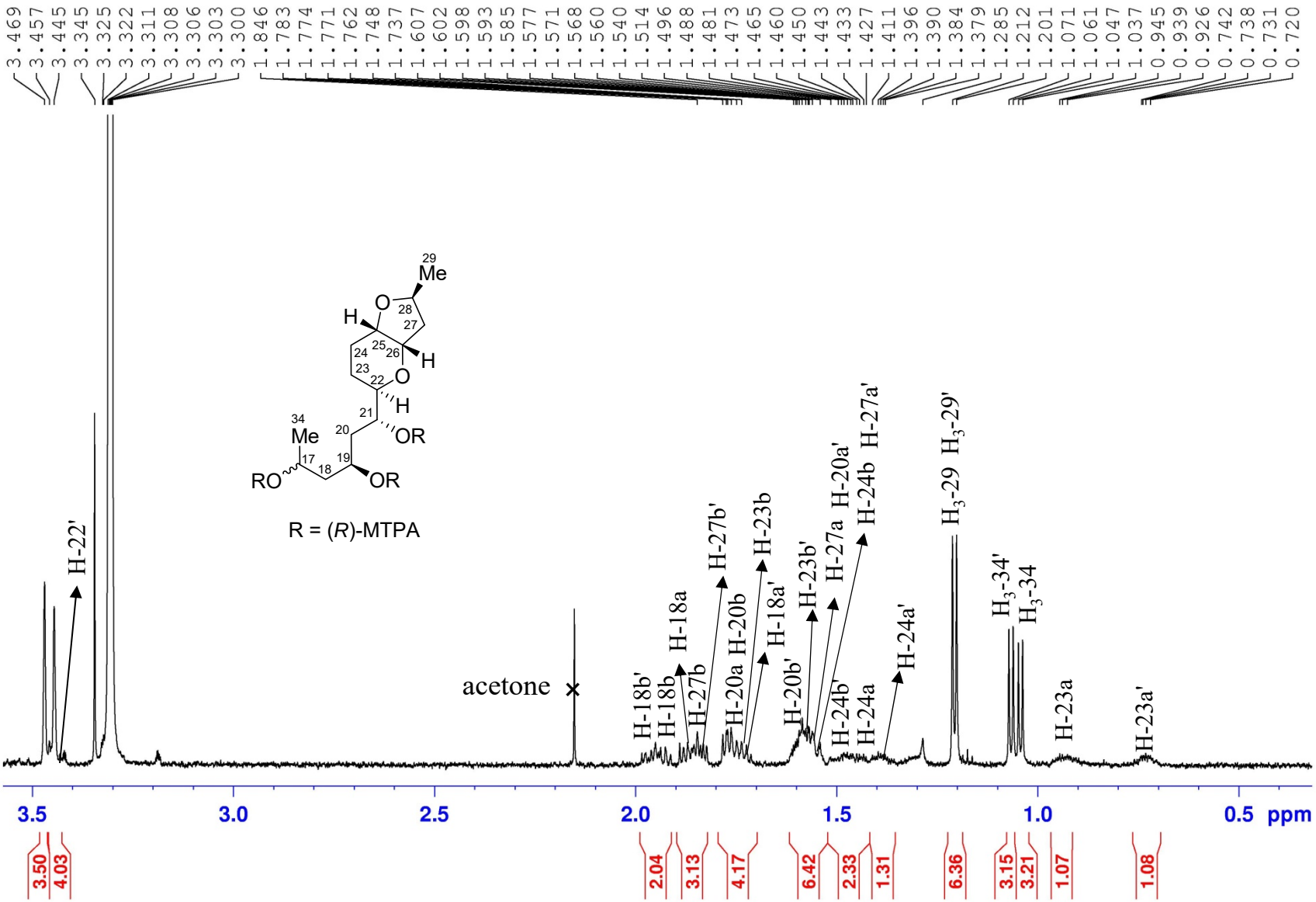
^{1}H (600 MHz) NMR spectrum of fragments **1Br** in CD_3OD



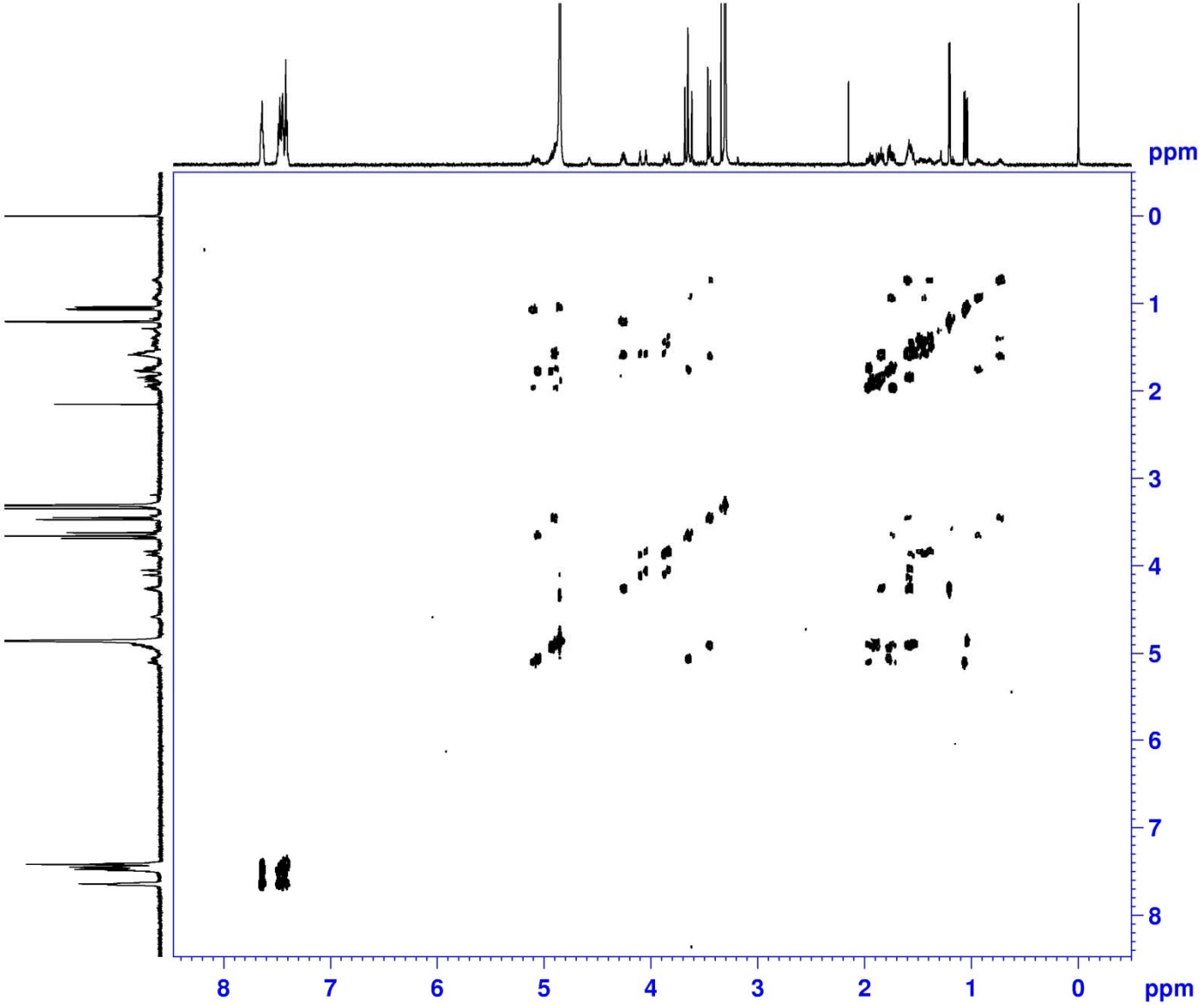
^{1}H (600 MHz) NMR spectrum of fragments **1Br** in CD_3OD



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



^{1}H–^{1}H COSY (600 MHz) spectrum of fragments **1Br** in CD_3OD



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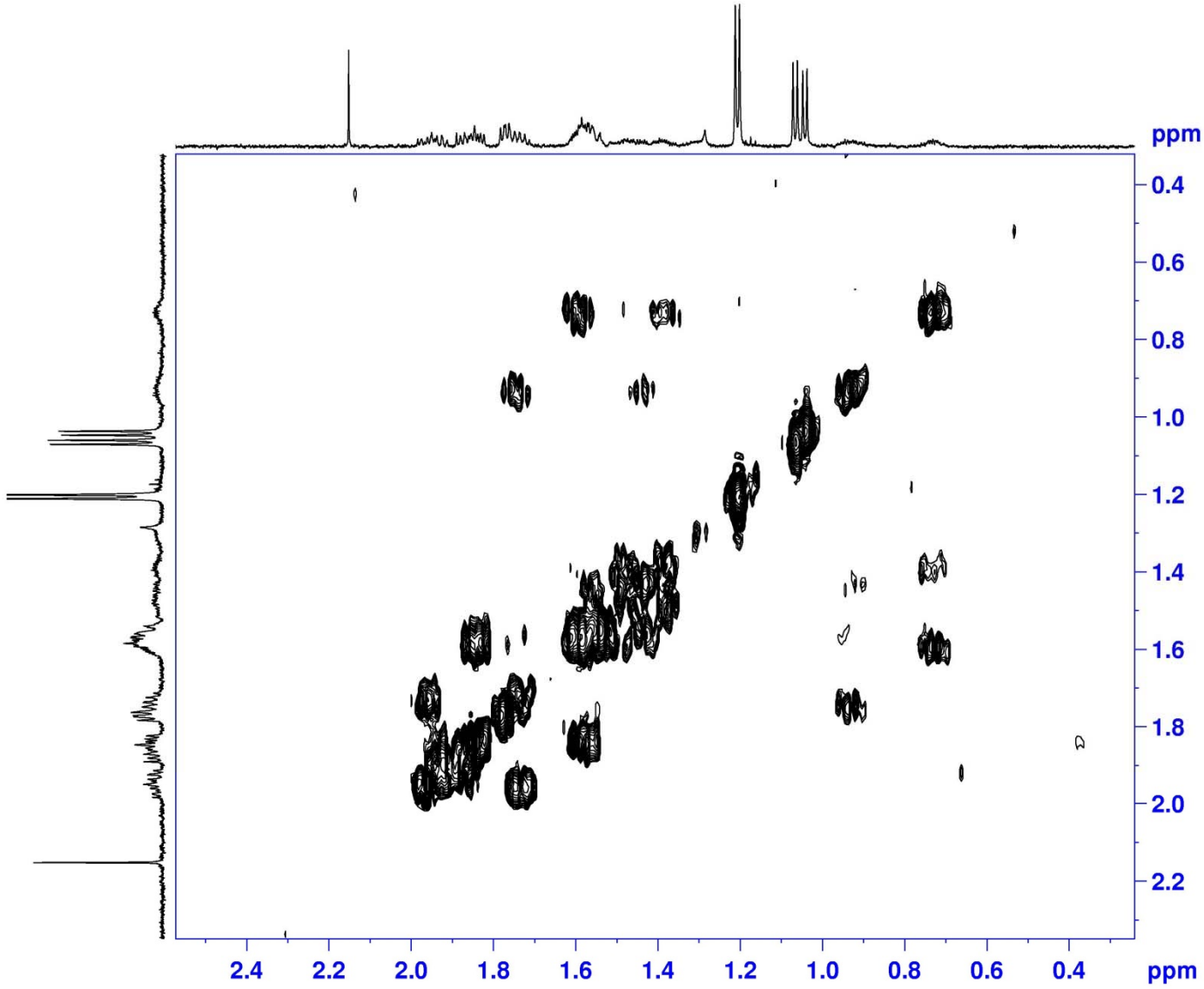
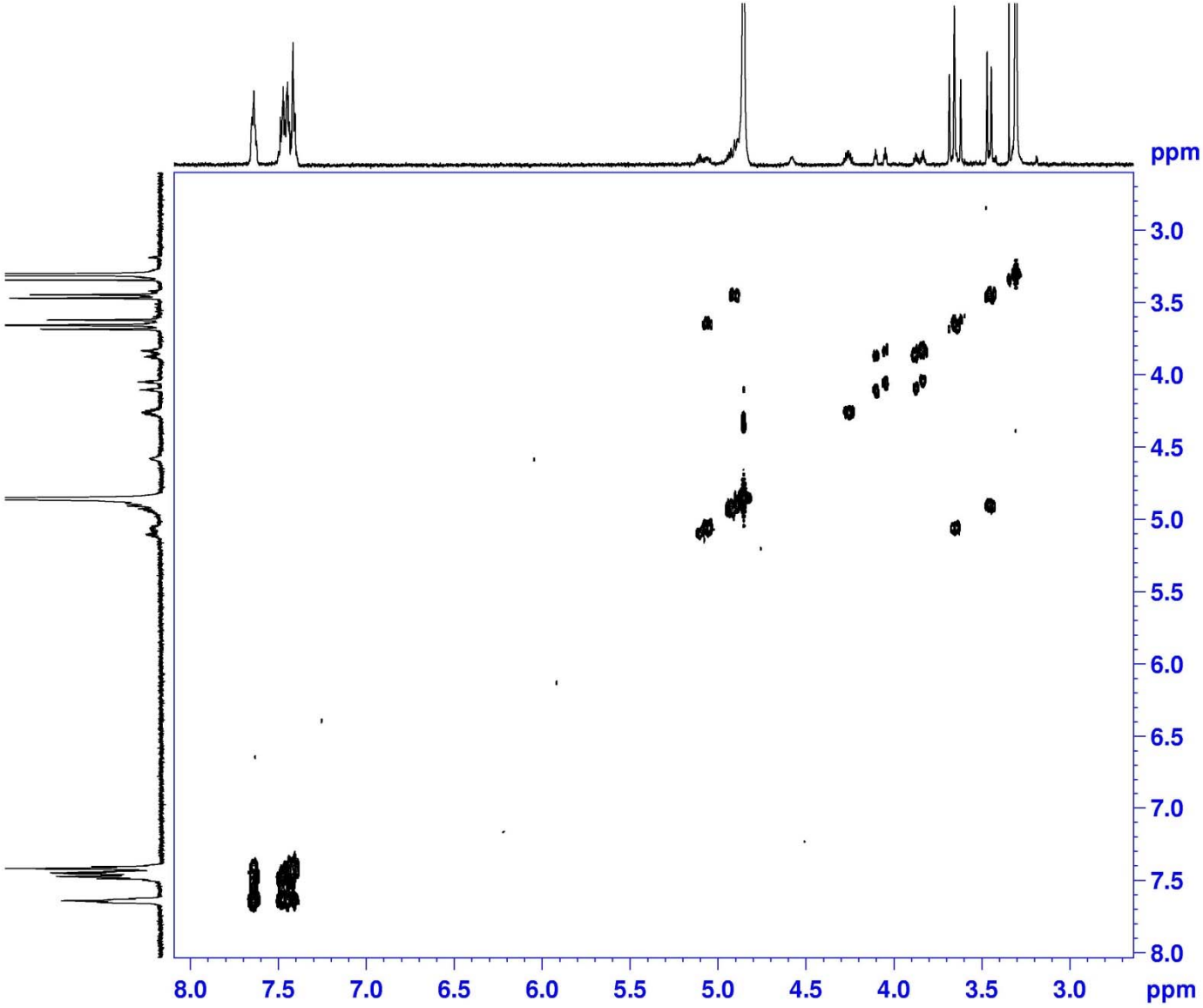
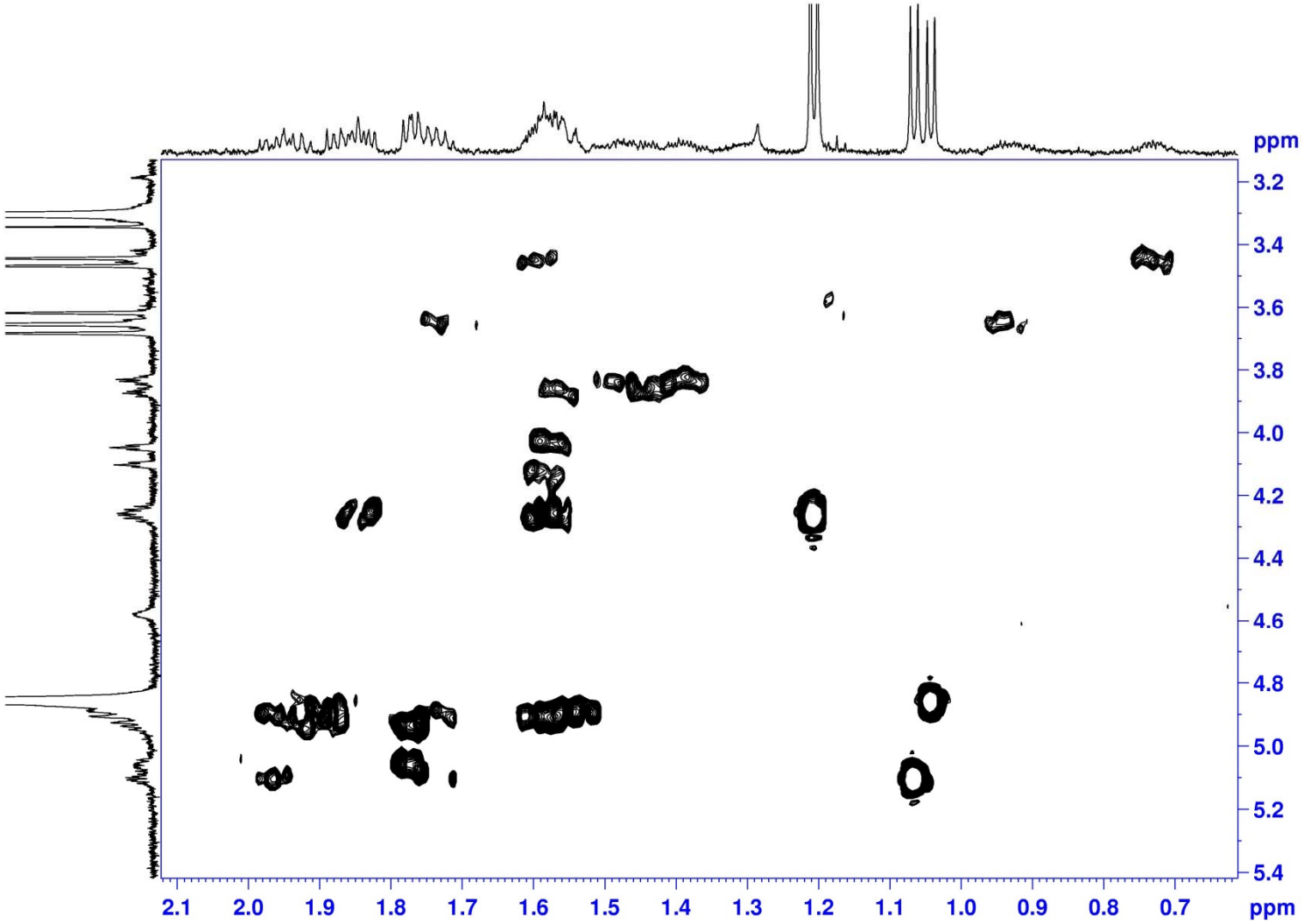


$^{1}H–^{1}H$ COSY (600 MHz) spectrum of fragments **1Br** in CD_3OD



^{1}H–^{1}H COSY (600 MHz) spectrum of fragments **1Br** in CD_3OD



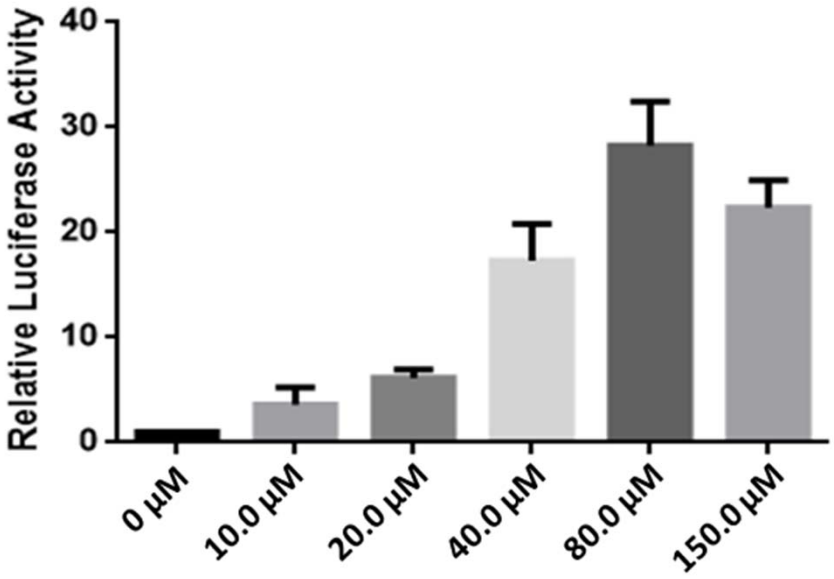


Figure S1. Agonistic effects of chenodeoxycholic acid (the positive control) on hFXR in HepG2 cells