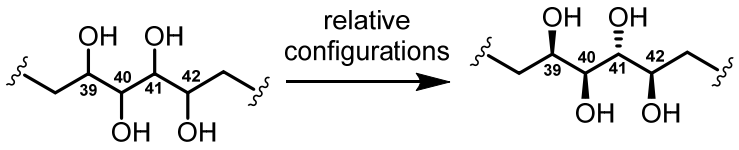
Supporting Information-I

Table of Contents:

Table S1. $^{3}J_{H,H}$ (Hz) of the 1,2,3,4-tetraol moiety in **1c** (CD_3OD).[1]



	1c	Kishi's universal NMR database							
		SSS	AAA	ASA	SAS	**SAA**	AAS	SSA	ASS
$^{3}J_{H\text{-}39,H\text{-}40}$	1.8	4.4	5.1	8.7	1.8	**2.0**	4.4	4.7	8.1
$^{3}J_{H\text{-}40,H\text{-}41}$	8.1	4.8	6.7	1.0	9.2	**8.5**	8.5	2.3	2.3
$^{3}J_{H\text{-}41,H\text{-}42}$	4.9	4.0	5.8	8.9	1.4	**4.4**	2.0	8.1	4.7
Σ|ΔHz|	N/A	6.8	5.6	18.0	4.6	**1.1**	5.9	11.9	12.3

A: *anti*; S: *syn*

Reference

[1]. Seike, I. Ghoshi, Y. Kishi, Attempts to assemble a universal NMR database without synthesis of NMR database compounds. *Org*. *Lett*. **2006**, *8*, 3861-3864.

Table S2. ^{1}H (700 MHz) and ^{13}C (175 MHz) NMR data for the fragment **1a** in CD_3OD (δ in ppm and J in Hz).

No.	δ_H	δ_C
1a	3.41 dd (11.2, 6.3)	67.4 CH_2
1b	3.46 dd (11.2, 4.2)	
2	3.54 m	73.5 CH
3a	1.39 m	31.8 CH_2
3b	1.51 m	
4a	1.32 m	34.8 CH_2
4b	1.36 m	
5	1.69 m	30.3 CH
6a	1.17 m	46.2 CH_2
6b	1.43 m	
7	3.76 m	68.1 CH
8a	1.28 m	43.2 CH_2
8b	1.48 m	
9	1.78 m	33.7 CH
10a	3.38 dd (10.5, 6.3)	68.0 CH_2
10b	3.44 dd (10.5, 5.6)	
71	0.91 d (7.0)	19.5 CH_3
72	0.94 d (7.0)	18.0 CH_3

Table S3. ^{1}H (700 Hz) and ^{13}C (175 Hz) NMR data for the fragment **1b** in CD_3OD (δ in ppm, J in Hz).

No.	δ_H	δ_C
13	3.74 m	68.6 CH
13'	3.73 m	68.9 CH
14a/14b	1.48 m/1.65 m	36.5 CH_2
14a'/14b'		36.7 CH_2
15a/15b	1.46 m/1.66 m	29.9 CH_2
15a'/15b'	1.38 m/1.73 m	30.2 CH_2
16	3.41 m	76.3 CH
16'	3.40 m	76.5 CH
17	3.69 m	72.8 CH
18a	1.50 m	41.3 CH_2
18b	1.67 m	
19	4.10 m	66.5 CH
20a	1.58 m	46.9 CH_2
20b	1.58 m	
21	4.11 m	66.44 CH
22a	1.58 m	46.9 CH_2
22b	1.58 m	

23	4.11 m	66.36 CH
24a 24b	1.55 m 1.80 m	41.5 CH_2
25	3.89 ddd (9.8, 6.3, 2.1)	70.7 CH
26	3.37 t (6.3)	78.7 CH
27	3.85 ddd (9.1, 6.3, 2.8)	73.3 CH
28a 28b	1.58 m 1.86 m	40.4 CH_2
29	3.97 m	69.9 CH
30a 30b	1.32 m 1.56 m	42.6 CH_2
31	1.81 m	33.4 CH
32a 32b	3.39 dd (10.5, 6.3) 3.47 dd (10.5, 5.6)	68.0 CH_2
74 74'	1.16 d (6.3)	23.58 CH_3 23.63 CH_3
75	0.96 d (6.3)	18.2 CH_3

Table S4. ^{1}H (700 MHz) and ^{13}C (175 MHz) NMR data for the fragment **1c** in CD_3OD (δ in ppm, J in Hz).

No.	δ_H	δ_C
33 33'	3.75 m	68.49 CH 68.54 CH
34a/34b	1.50 m/1.61 m	36.5 CH_2
34a'/34b'	1.49 m/1.63 m	36.7 CH_2
35a/35b	1.58 m/1.60 m	30.2 CH_2
35a'/35b'	1.47 m/1.68 m	30.4 CH_2
36	3.44 m	75.4 CH
37	3.68 m	73.6 CH
38a 38b	1.78 m 1.82 m	37.3 CH_2
39	4.13 ddd (9.2, 5.3, 1.8)	70.3 CH
40	3.45 dd (8.1, 1.8)	74.6 CH
41	3.69 dd (8.1, 4.9)	75.6 CH
42	4.04 ddd (10.5, 4.9, 2.1)	70.0 CH
43a 43b	1.77 m 1.98 m	34.8 CH_2
44	3.67 m	70.9 CH
45	3.03 t (8.4)	77.6 CH
46	3.74 m	70.3 CH
47a 47b	1.70 m 1.88 m	37.6 CH_2
48	3.93 m	73.1 CH

49a 49b	1.38 m 1.92 m	32.4 CH_2
50a 50b	1.52 m	23.3 CH_2
51a 51b	1.52 m 1.75 m	32.7 CH_2
52	3.41 m	76.4 CH
53	3.14 t (7.7)	75.2 CH
54	3.72 t (7.7)	75.1 CH
55	3.78 dd (7.7, 4.9)	73.8 CH
56	3.60 dd (9.1, 4.9)	75.7 CH
57	4.40 m	67.7 CH
58a 58b	1.52 m 1.86 m	42.0 CH_2
59	4.10 m	67.1 CH
60a 60b	1.67 m 1.84 m	42.6 CH_2
61	4.09 m	69.7 CH
62	3.25 dd (7.7, 1.4)	77.1 CH
63	3.83 ddd (9.8, 7.7, 2.8)	71.8 CH
64a 64b	1.63 m 1.94 m	42.5 CH_2
65	4.11 m	68.8 CH
66a 66b	1.55 m 1.59 m	41.7 CH_2
67	3.87 m	70.1 CH
68a 68b	3.46 dd (11.2, 6.3) 3.49 dd (11.2, 4.2)	67.9 CH_2
76 76'	1.17 d (6.3)	23.6 CH_3 23.5 CH_3

Table S5. ^{1}H (400 MHz) NMR data for **1as** and **1ar** in CD_3OD (δ in ppm, J in Hz).

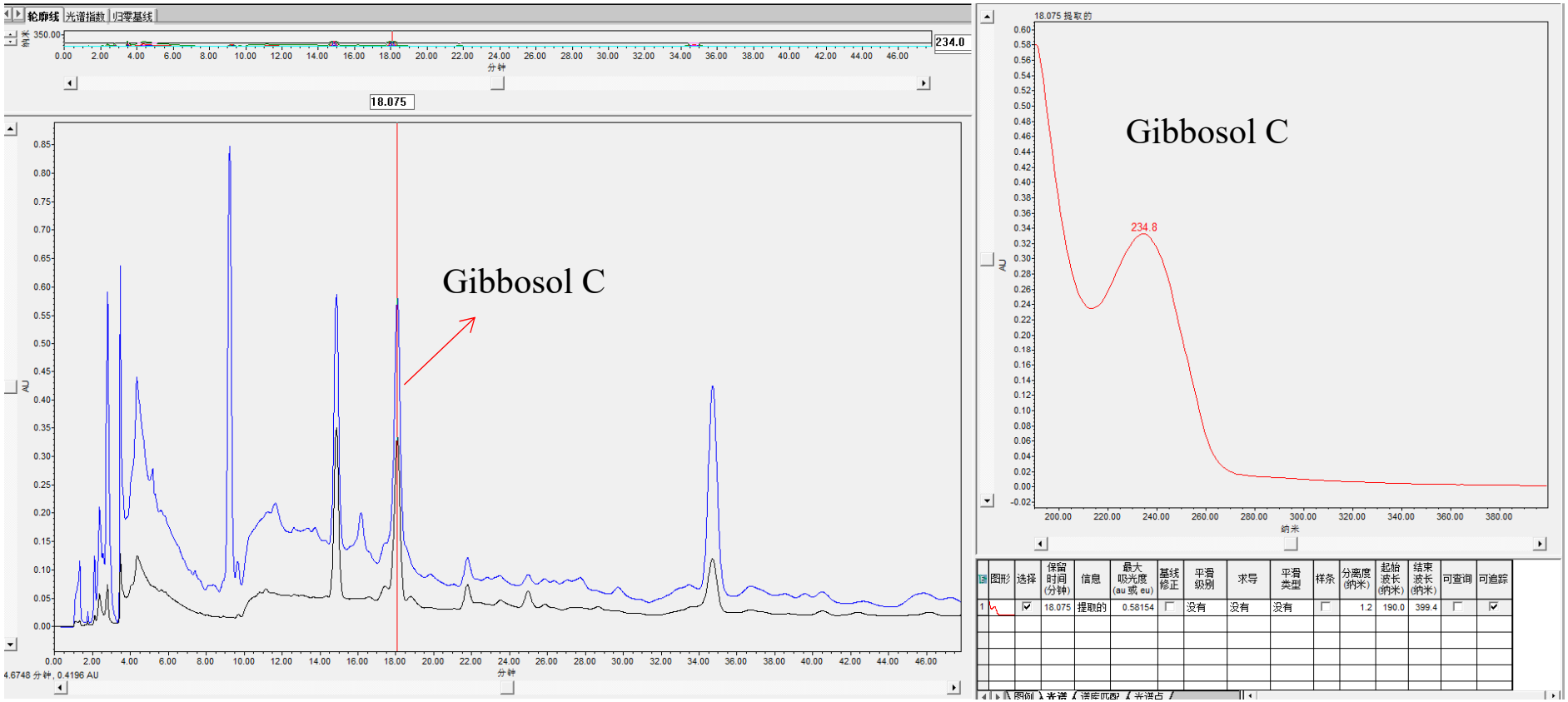
No.	**1as**	**1ar**
1a	4.34 dd (12.8, 6.0)	4.22 dd (12.4, 4.4)
1b	4.71 dd (12.8, 2.4)	4.55 dd (12.4, 2.4)
2	5.26 m	5.19 m
3a	1.49 m	1.50 m
3b	1.49 m	1.50 m
4a	0.95 m	1.05 m
4b	1.09 m	1.10 m
5	1.24 m	1.06 m
6a	1.11 m	1.10 m
6b	1.46 m	1.43 m
7	5.16 m	5.19 m
8a	1.48 m	1.56 m
8b	1.48 m	1.56 m
9	1.69 m	1.84 m
10a	4.13 dd (10.8, 4.8)	4.18 dd (10.8, 6.0)
10b	4.18 dd (10.8, 5.6)	4.29 dd (10.8, 5.2)
71	0.74 d (6.4)	0.73 d (5.2)
72	0.86 d (6.4)	0.96 d (6.8)

Supporting Information-II

Copies of High Performance Liquid Chromatogram, the UV spectrum, HR-ESI-MS for **1**; LR-ESI-MS for **1a–1c**, **1as**, and **1ar**; and 1D and 2D NMR spectra for **1**, **1a–1c**, **1as**, and **1ar**.

Table of Contents:

High Performance Liquid Chromatogram and the UV spectrum for compound **1**



Mobile Phase: MeCN/H_2O, 21:79; Flow Rate: 1.0 mL/min

HR-ESI-MS for compound **1**

Mass Spectrum SmartFormula Report

Analysis Info

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Comment			

Acquisition Parameter

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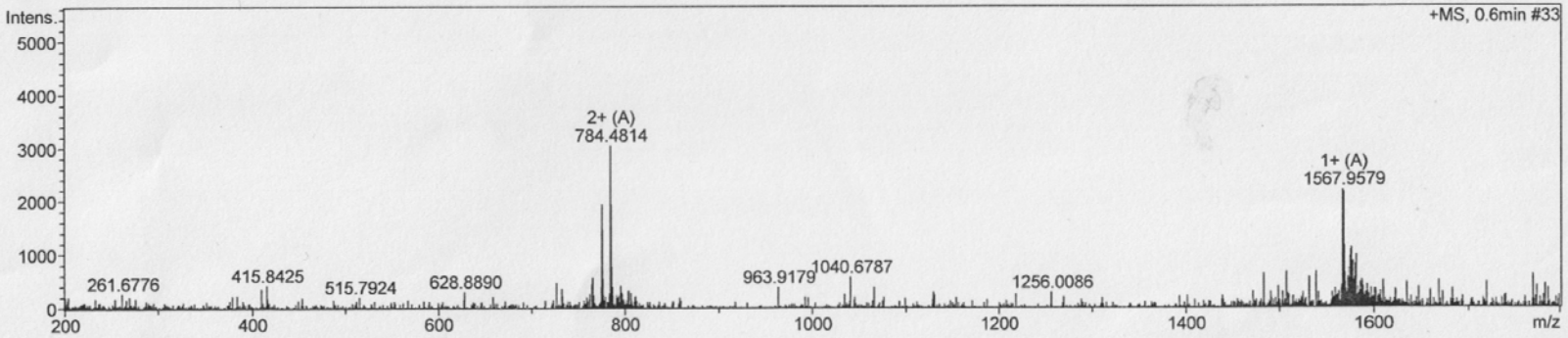
Scan End	3500 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



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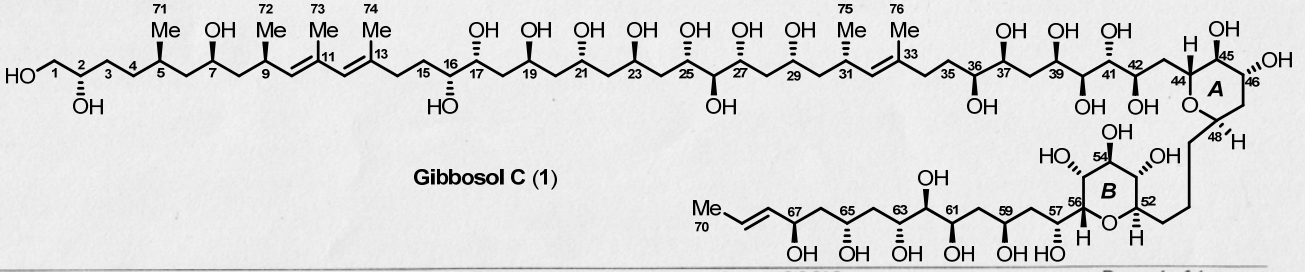
1567.9579	1	C76H143O32	100.00	1567.9557	1.4	2.2	79.1	5.5	even	ok



Gibbosol C (1)

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HR-ESI-MS for compound **1**

Generic Display Report

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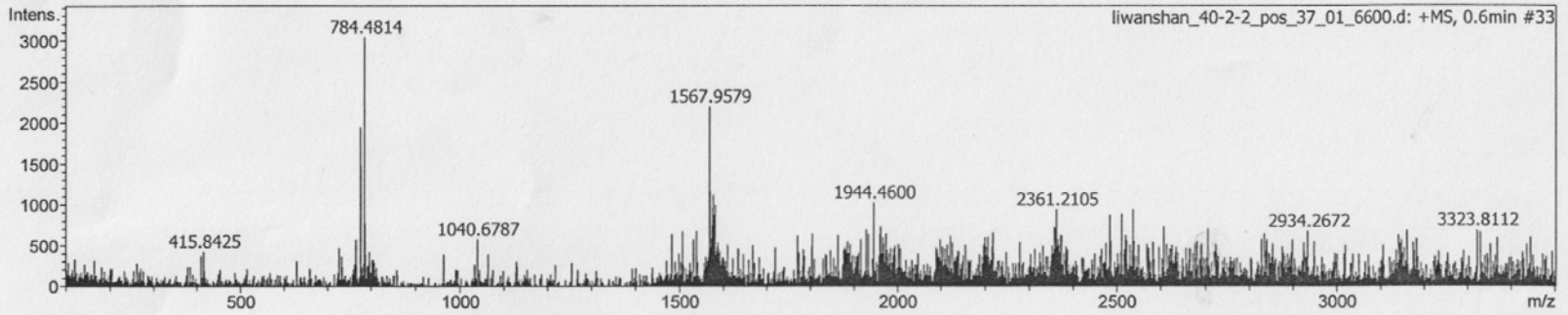
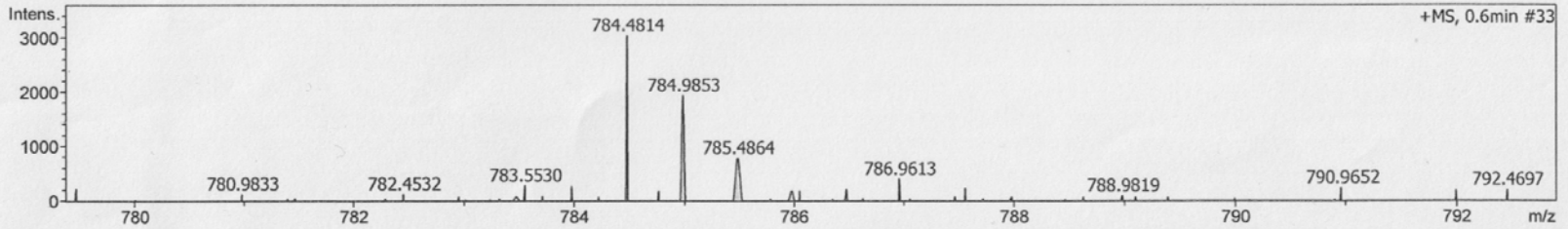
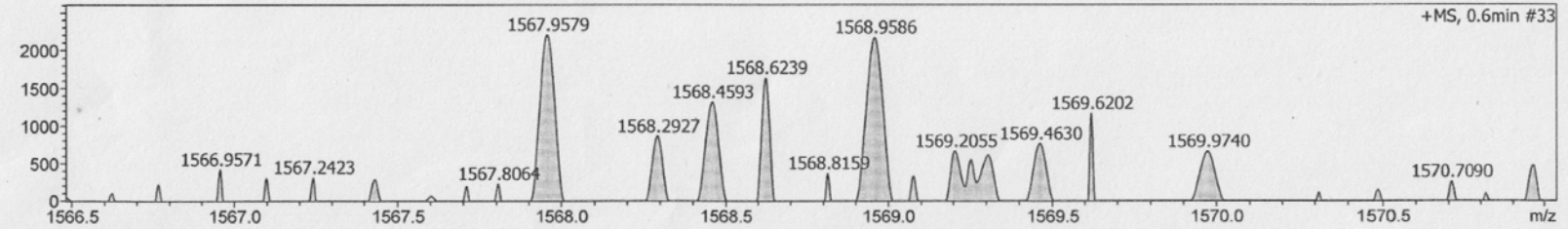
Comment			







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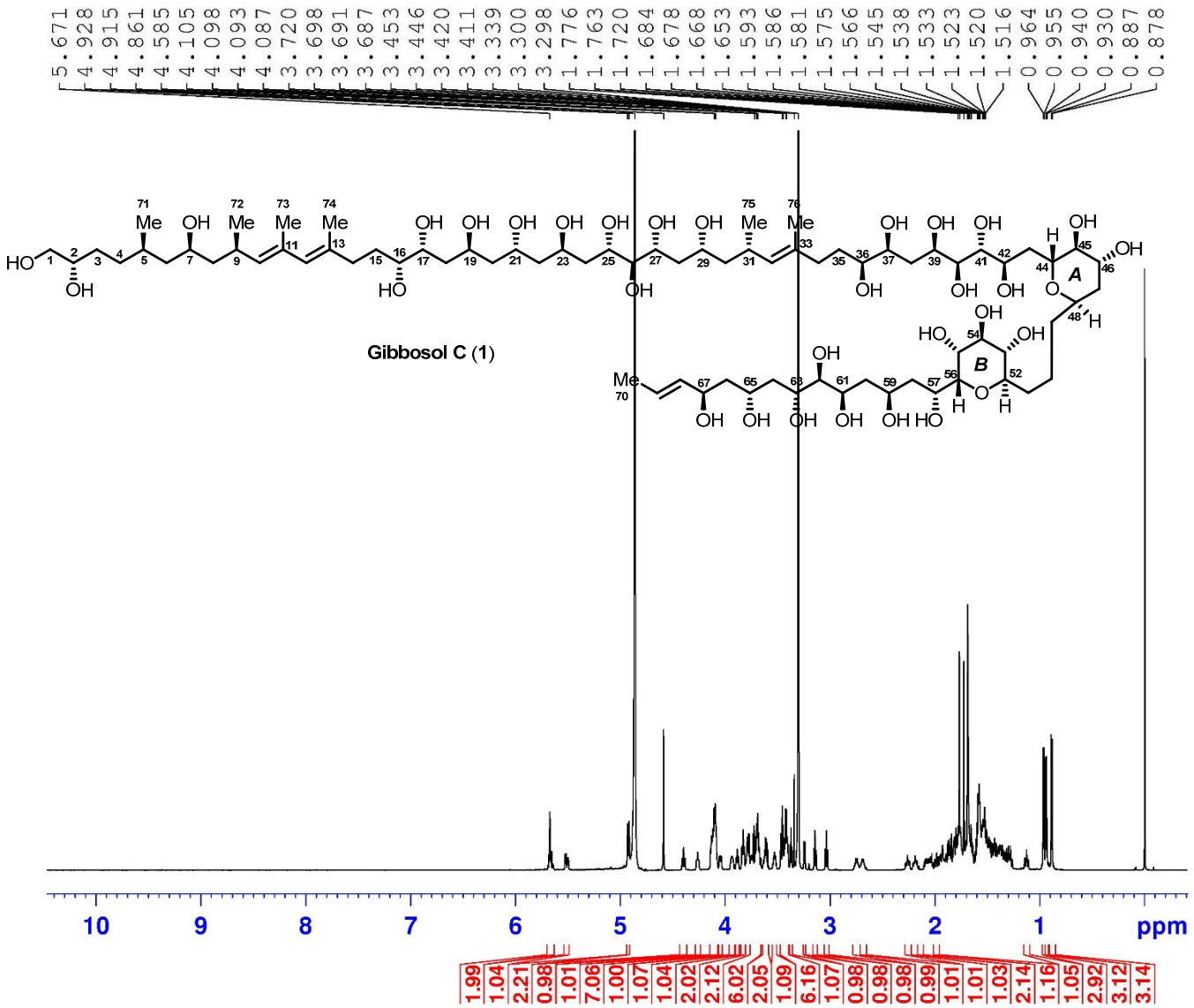
^{1}H (700 MHz) NMR spectrum of compound **1** in CD_3OD



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TE	298.0 K
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TD0	1
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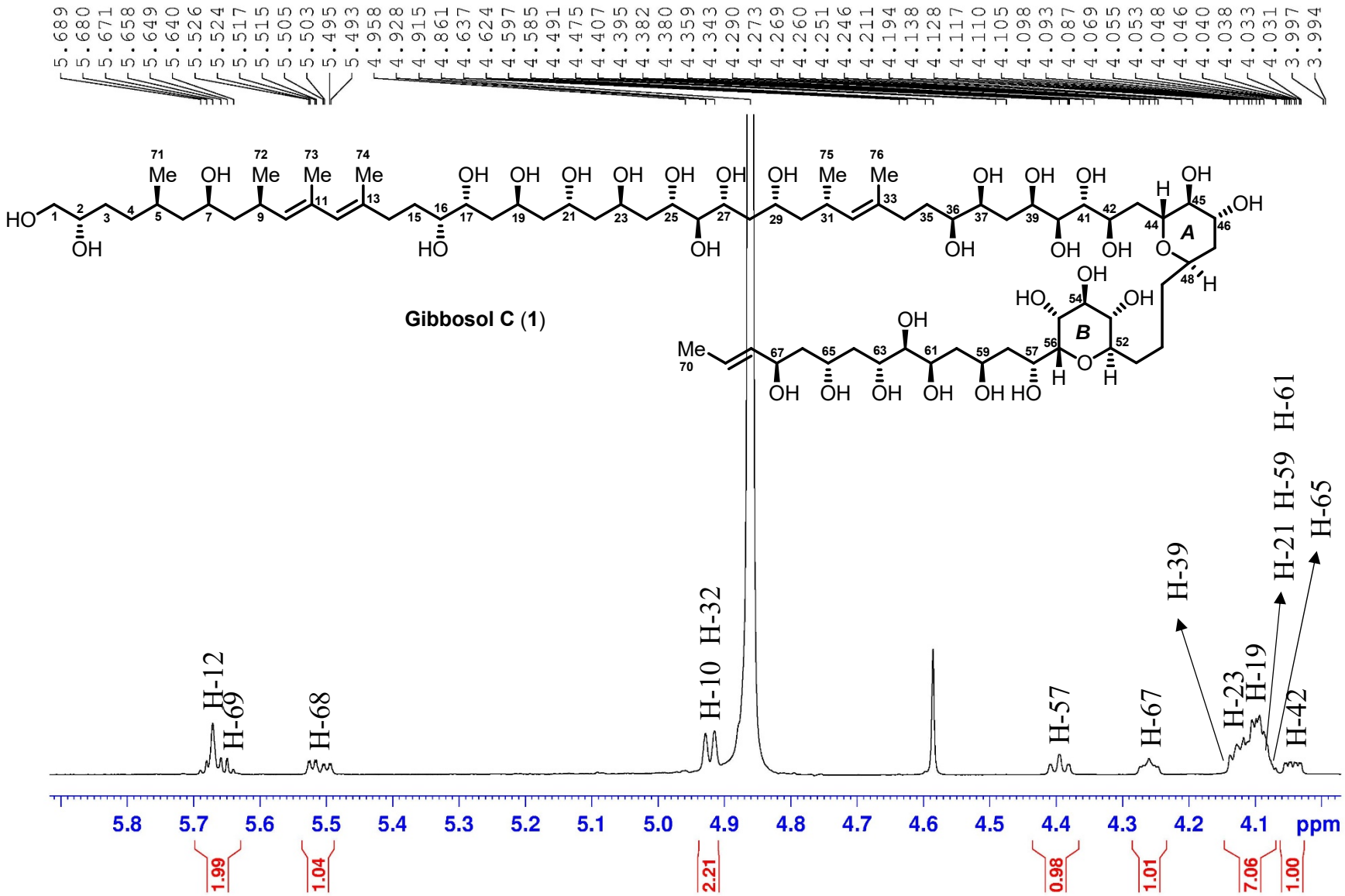
^{1}H (700 MHz) NMR spectrum of compound **1** in CD_3OD



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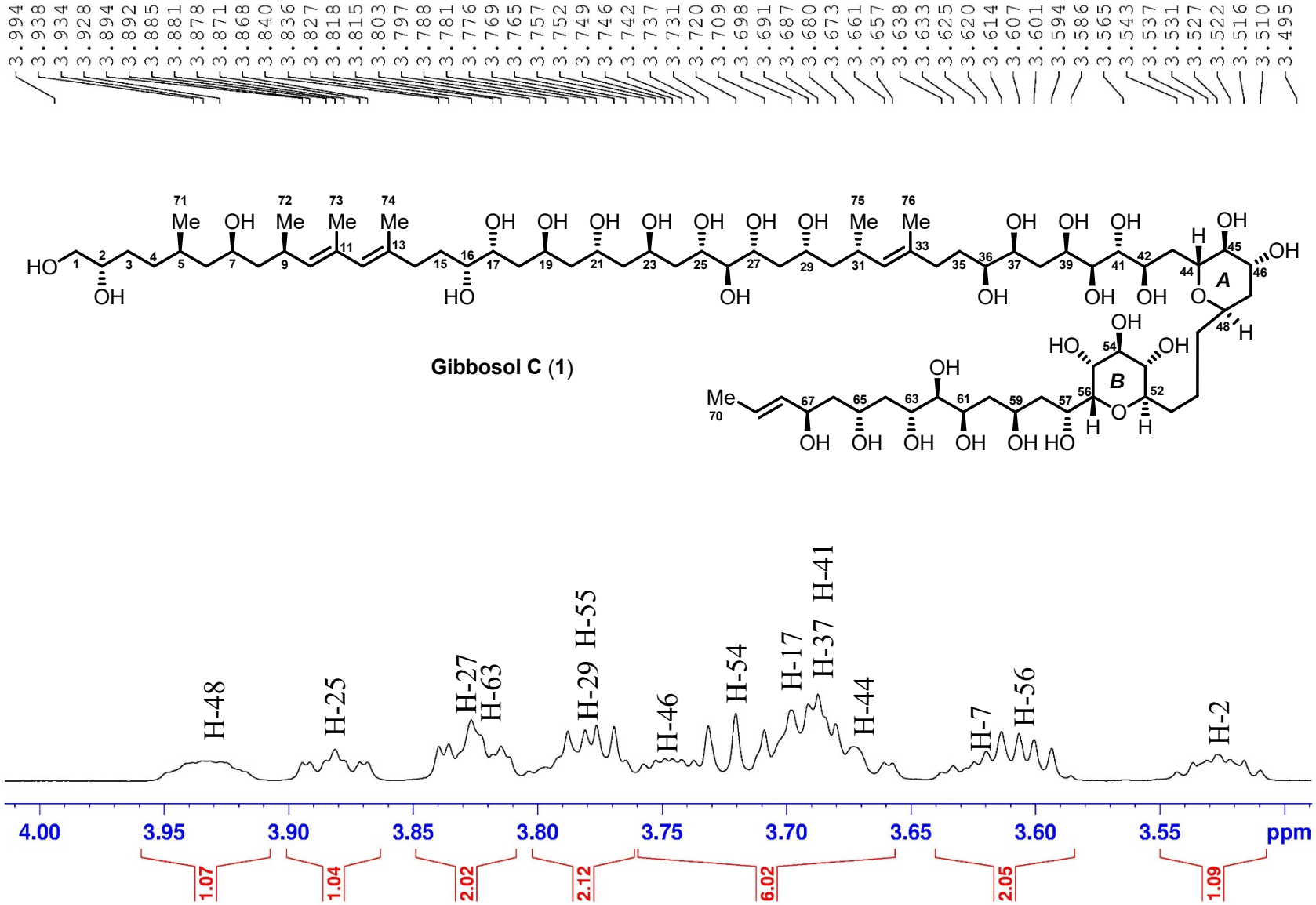

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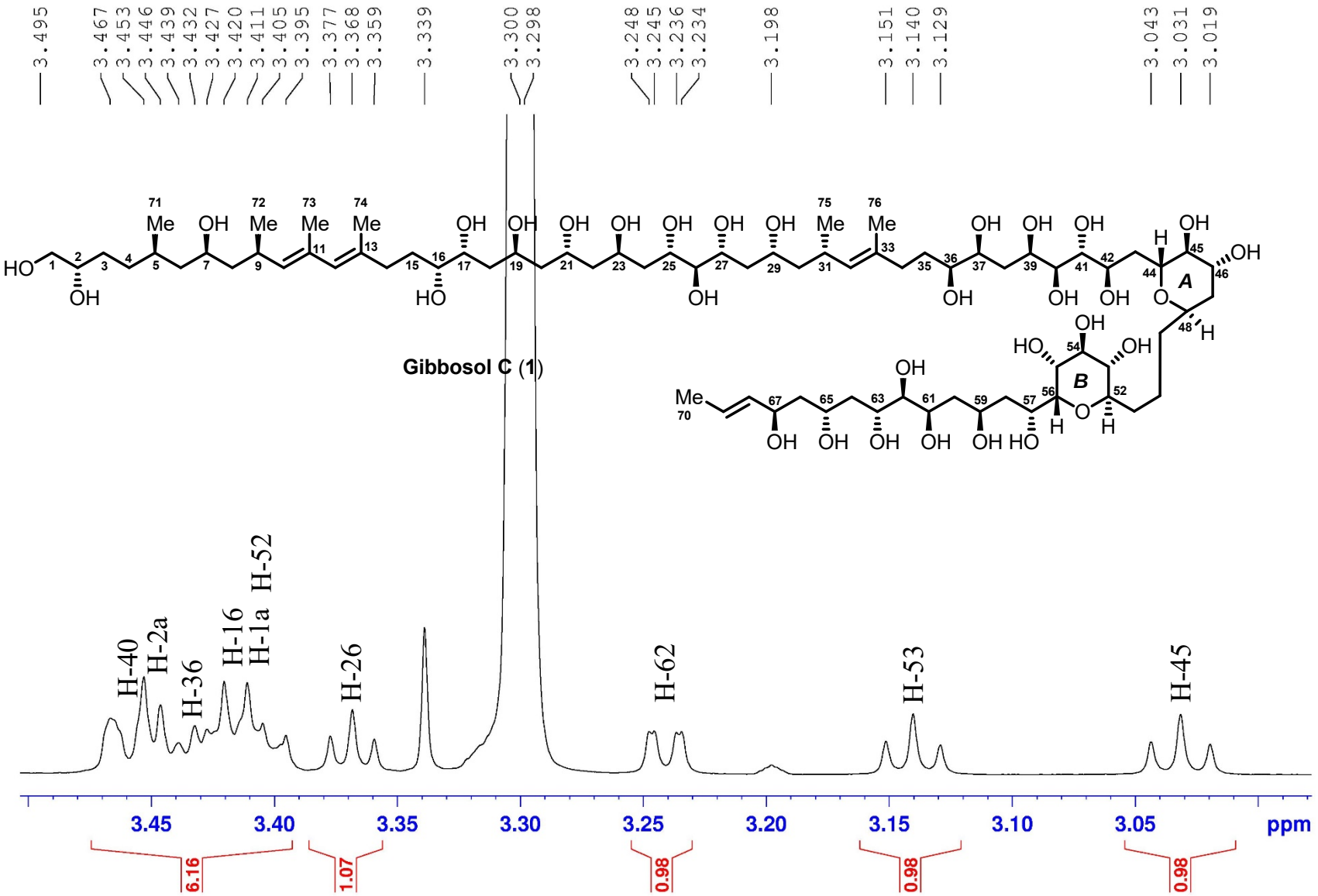

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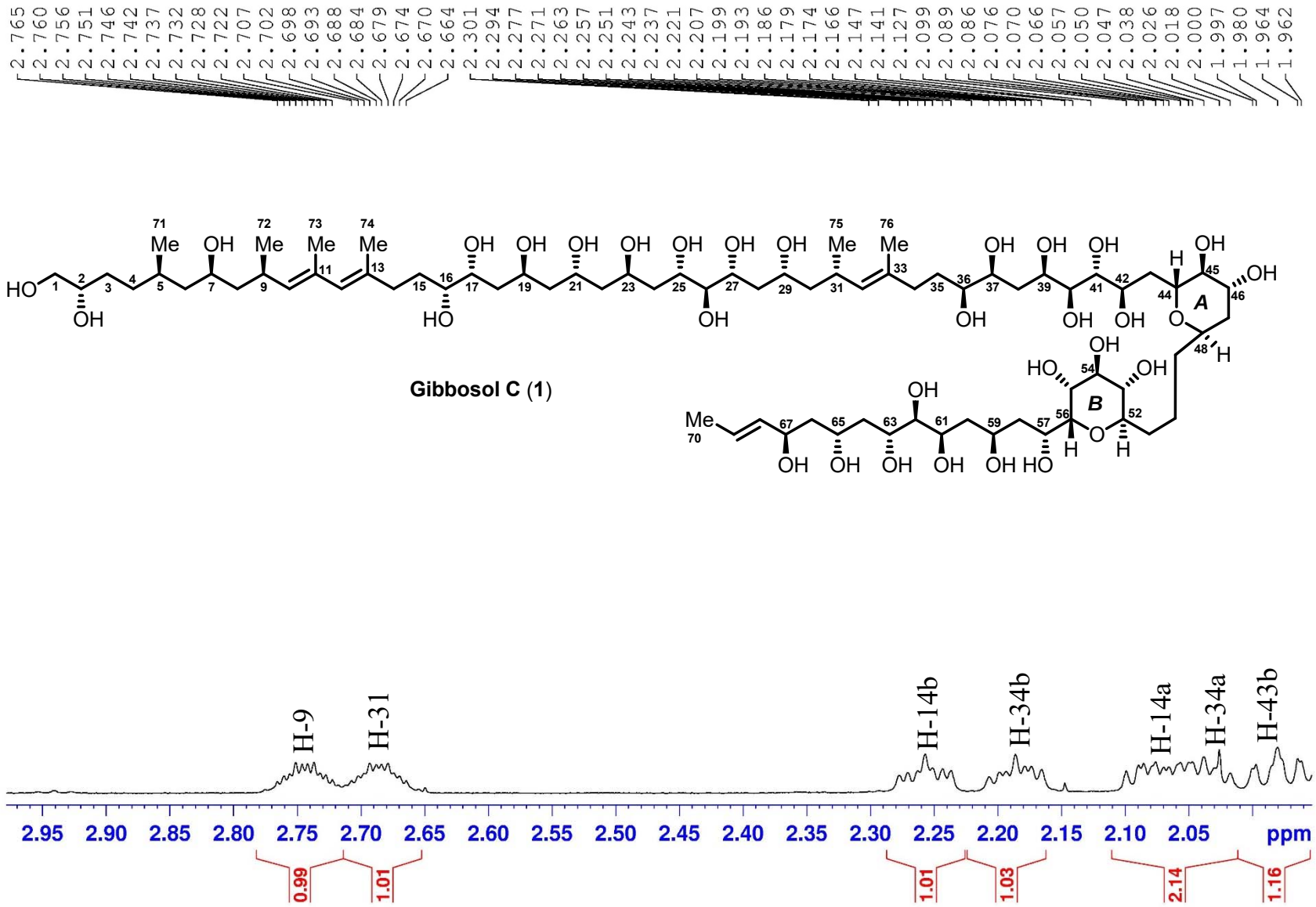

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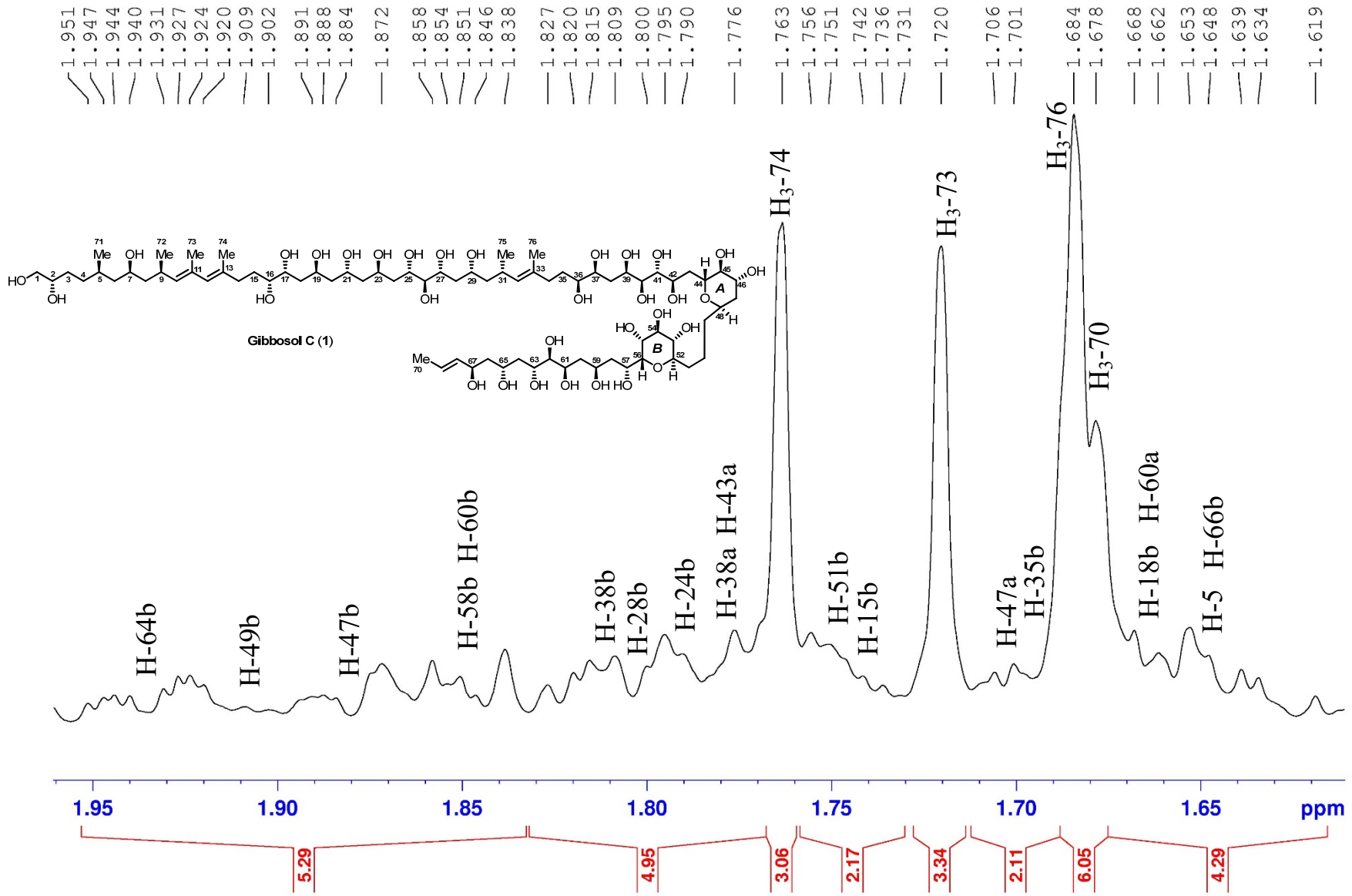

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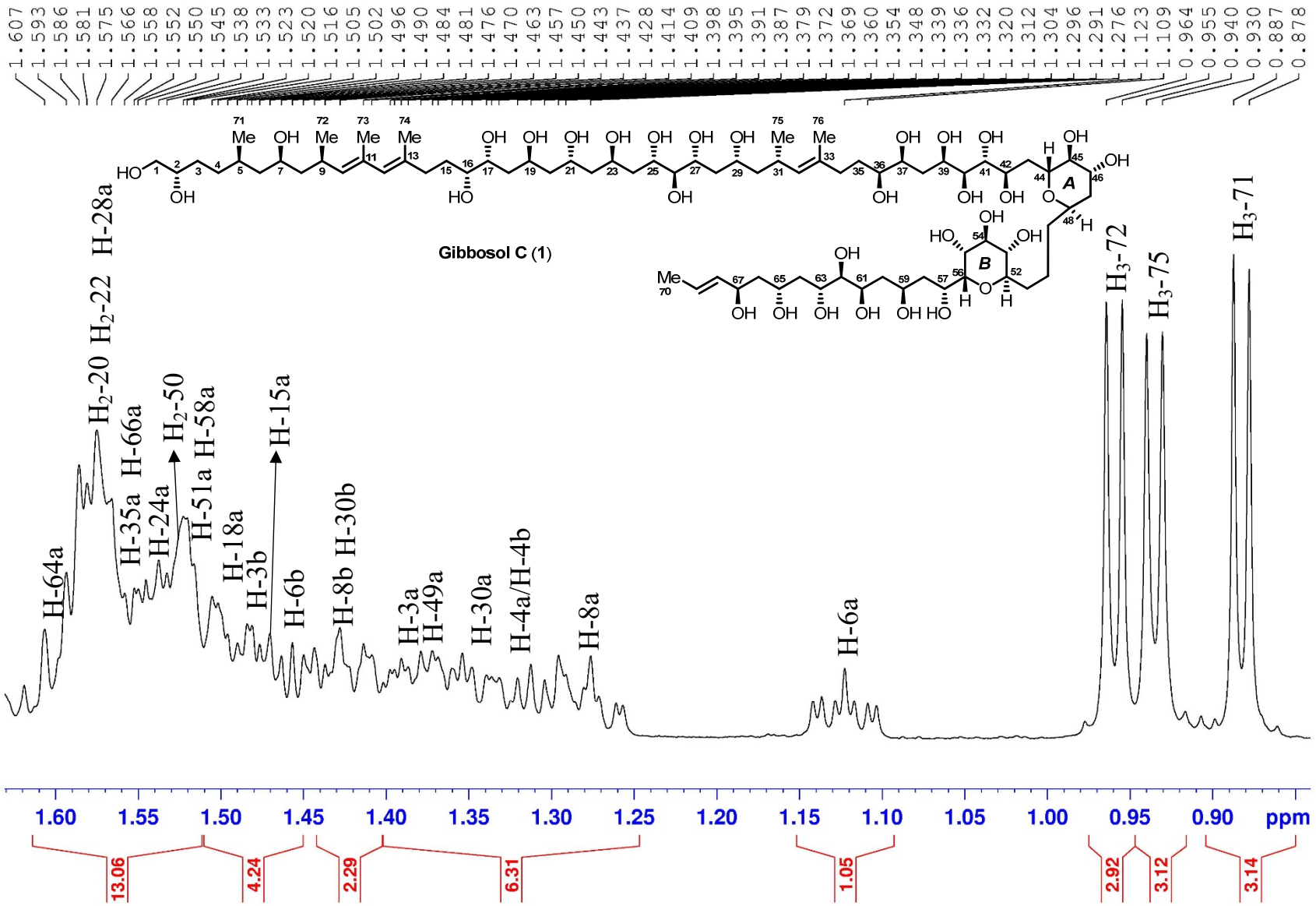
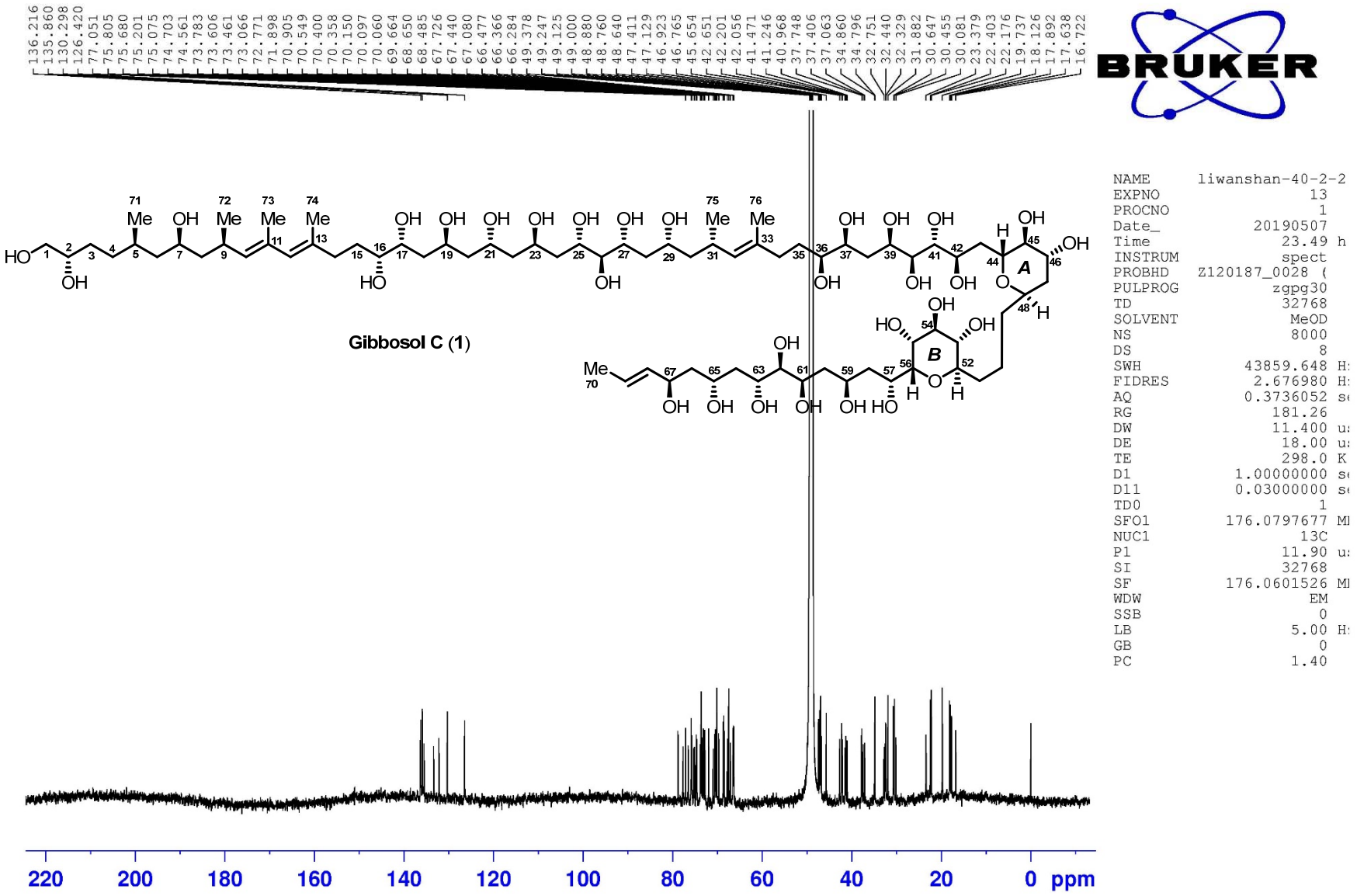


^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



BRUKER

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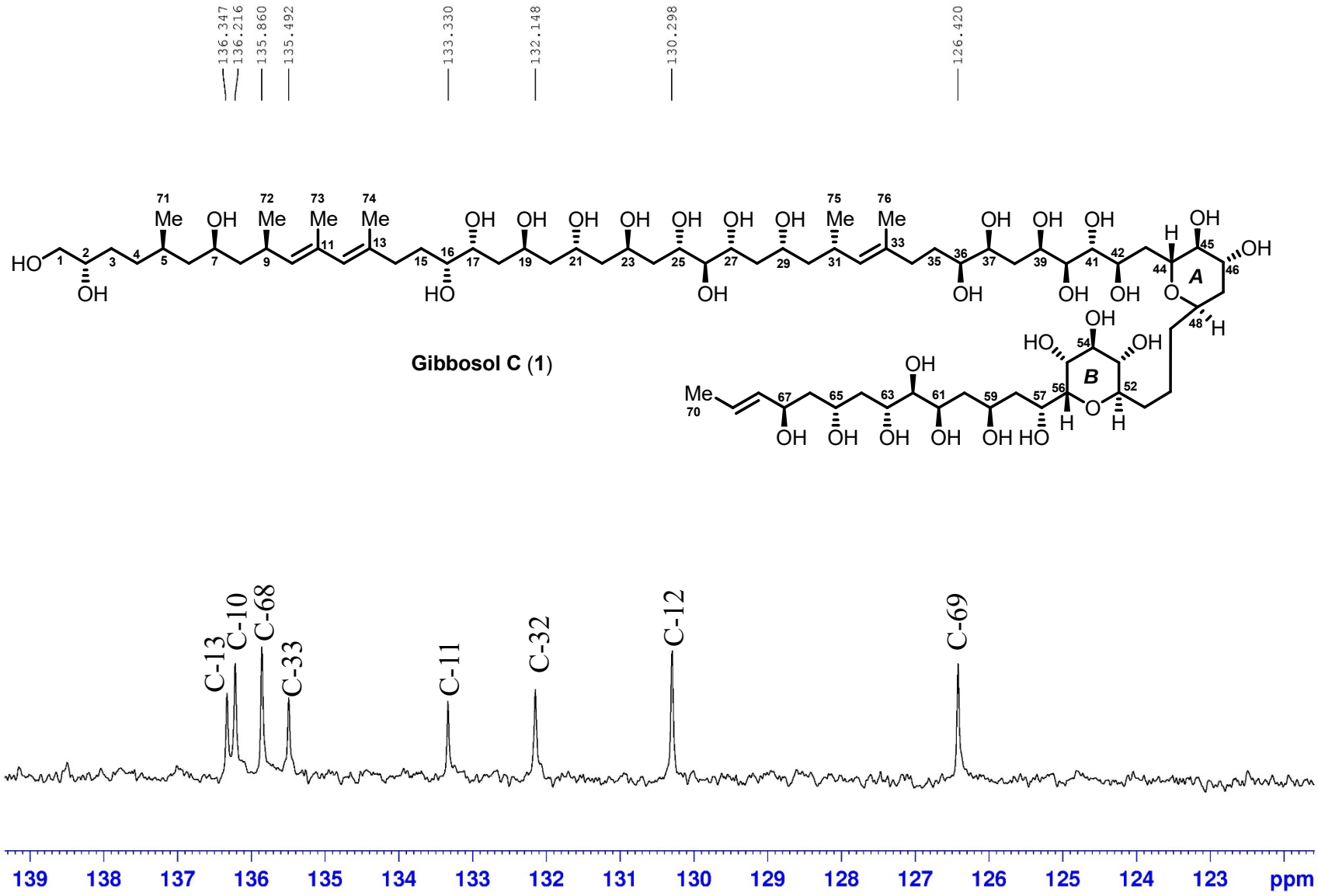
^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OD



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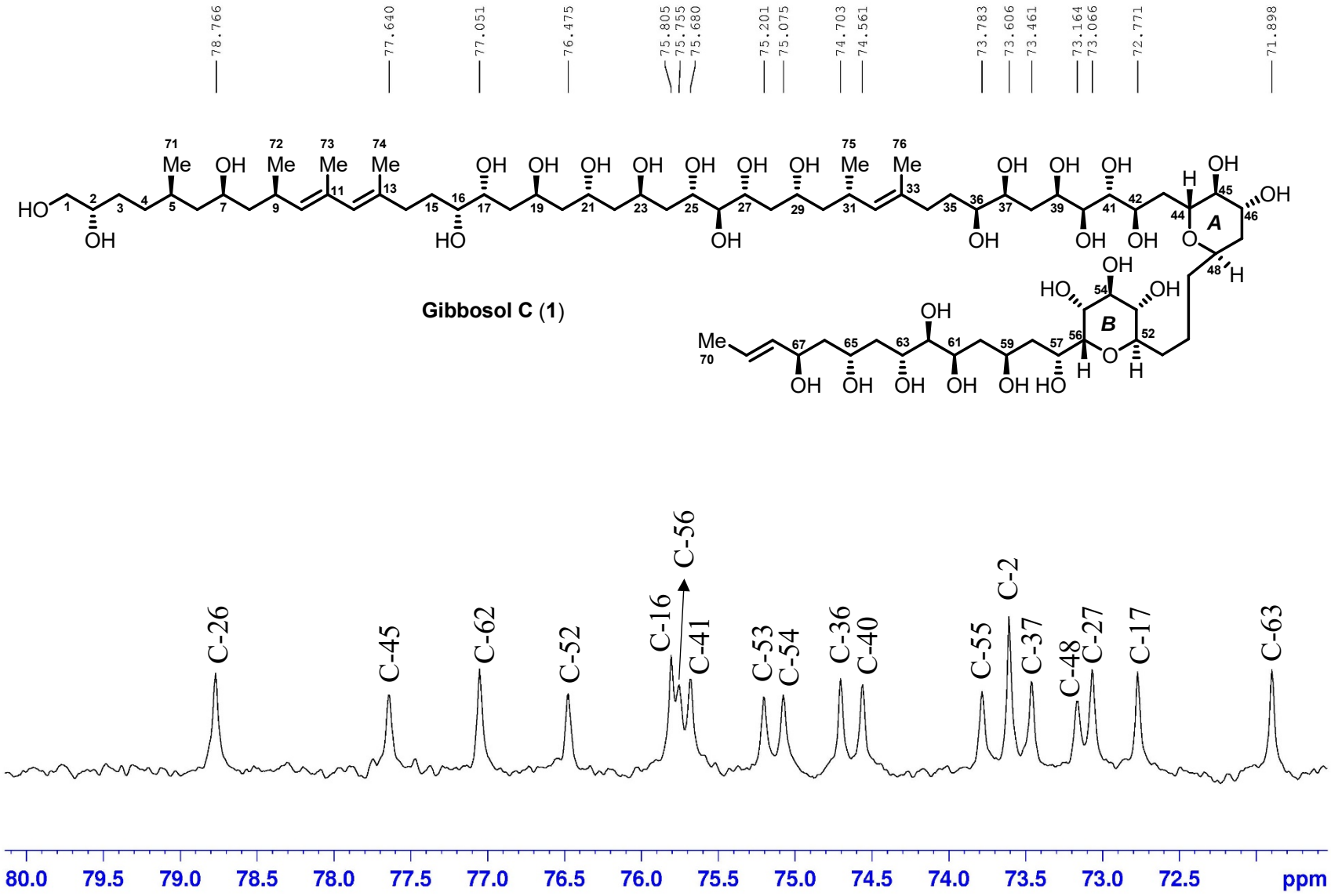

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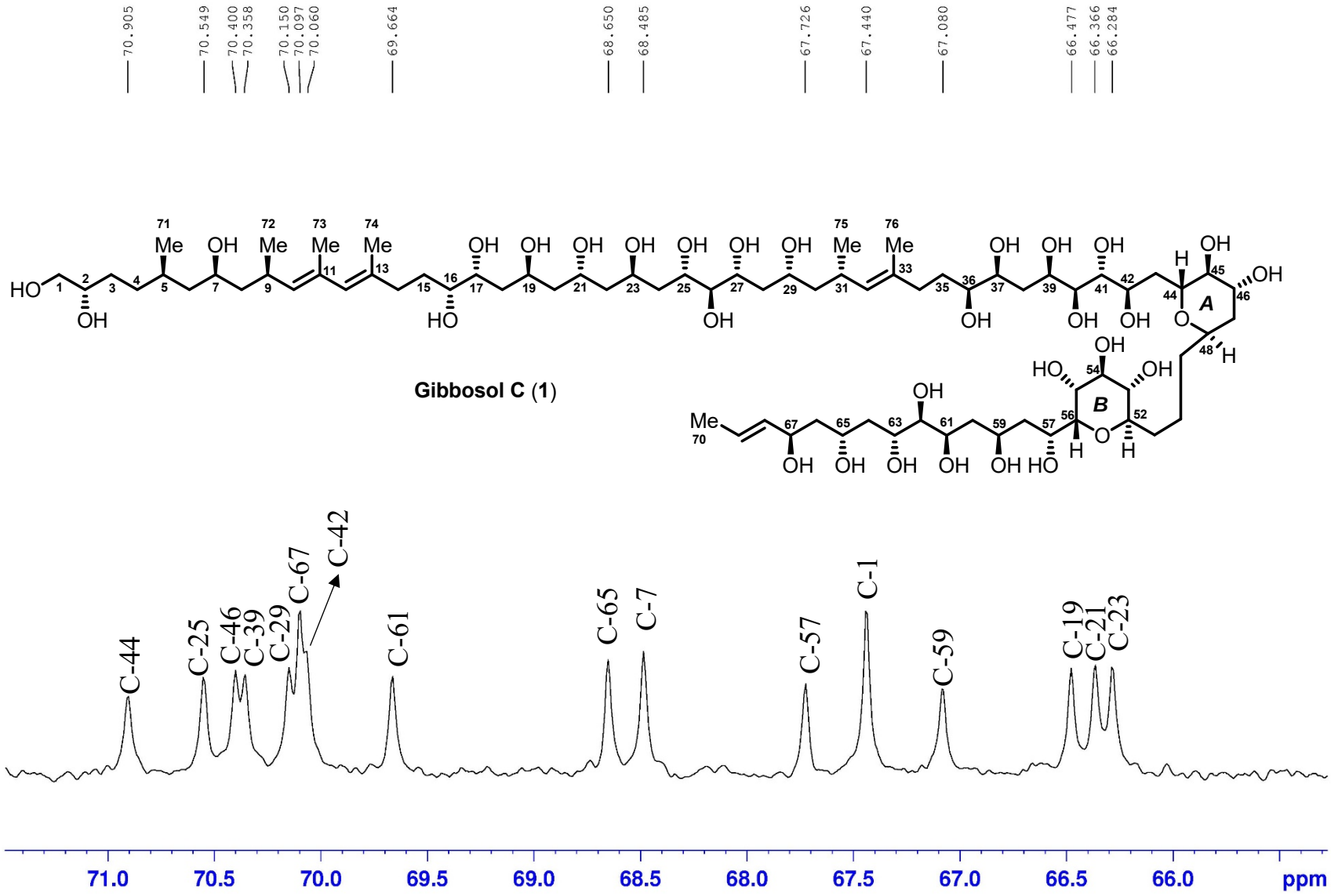

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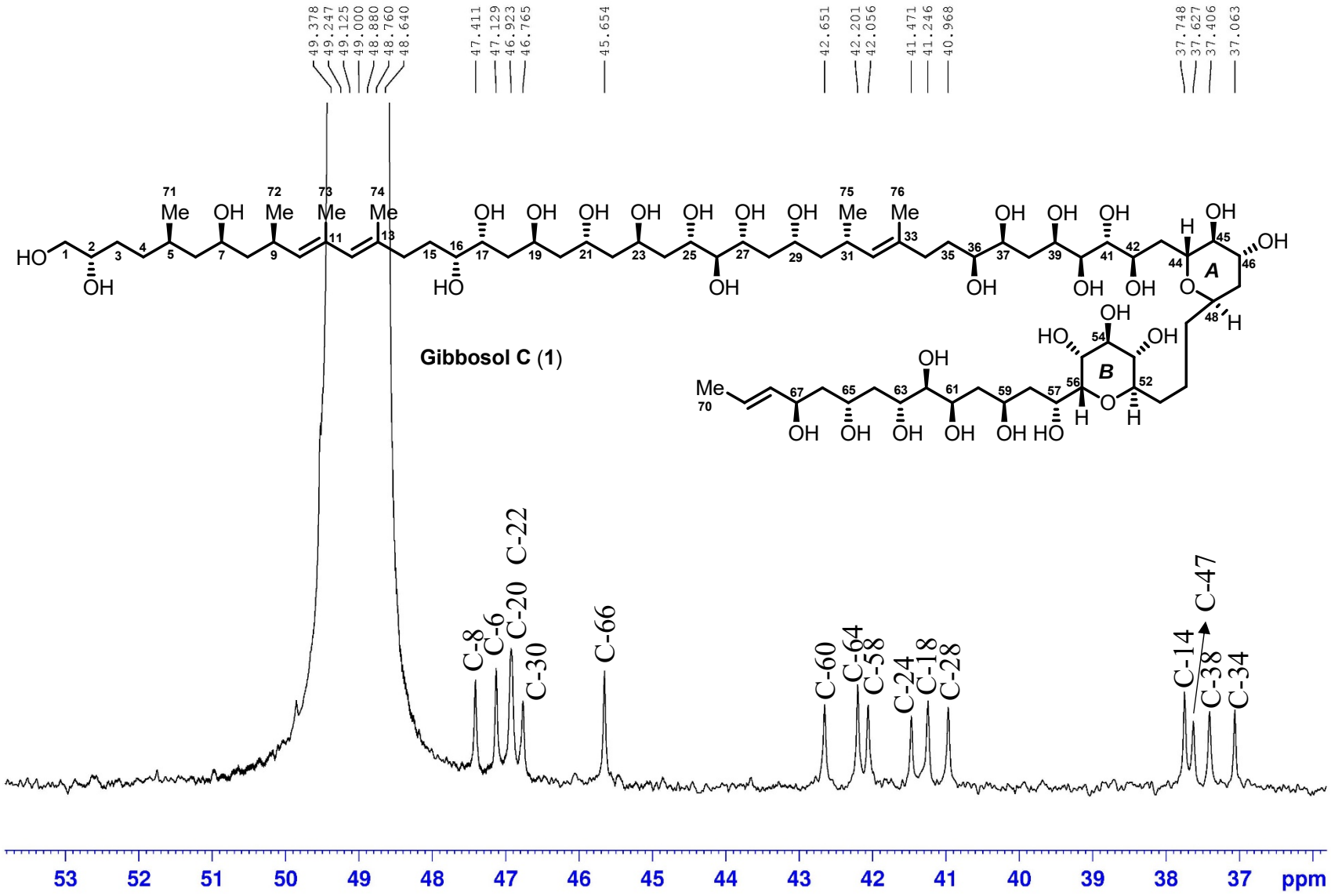

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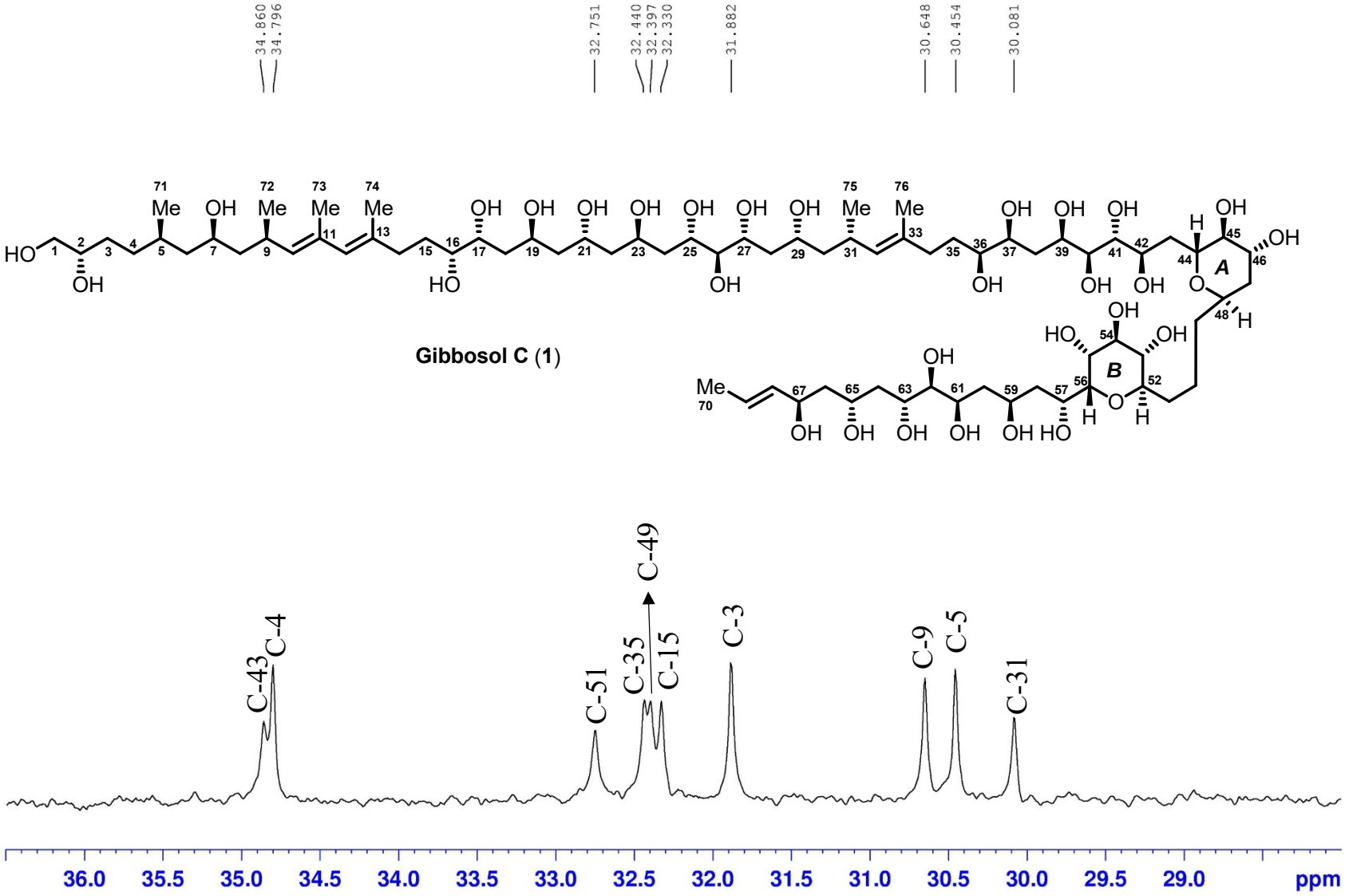

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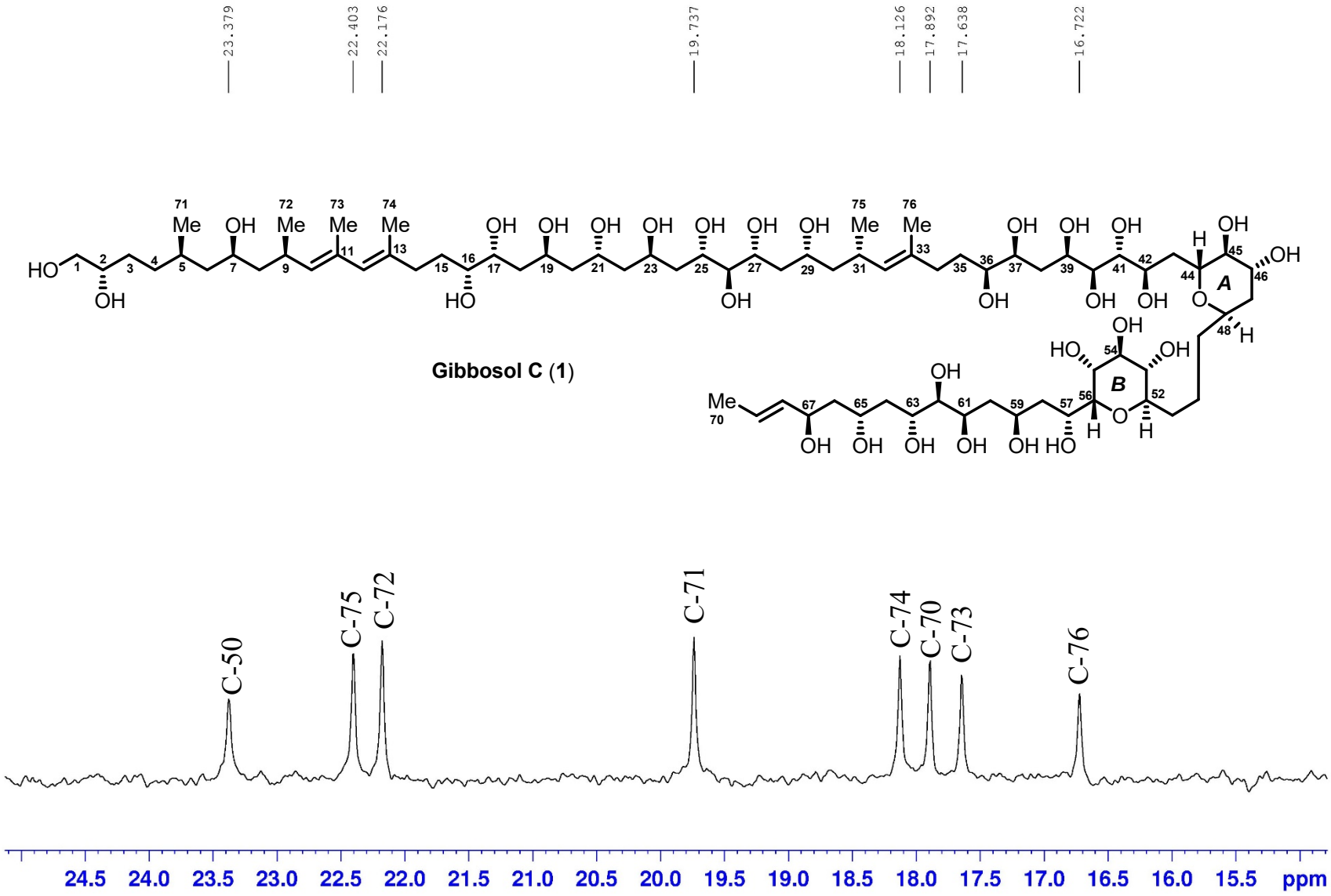

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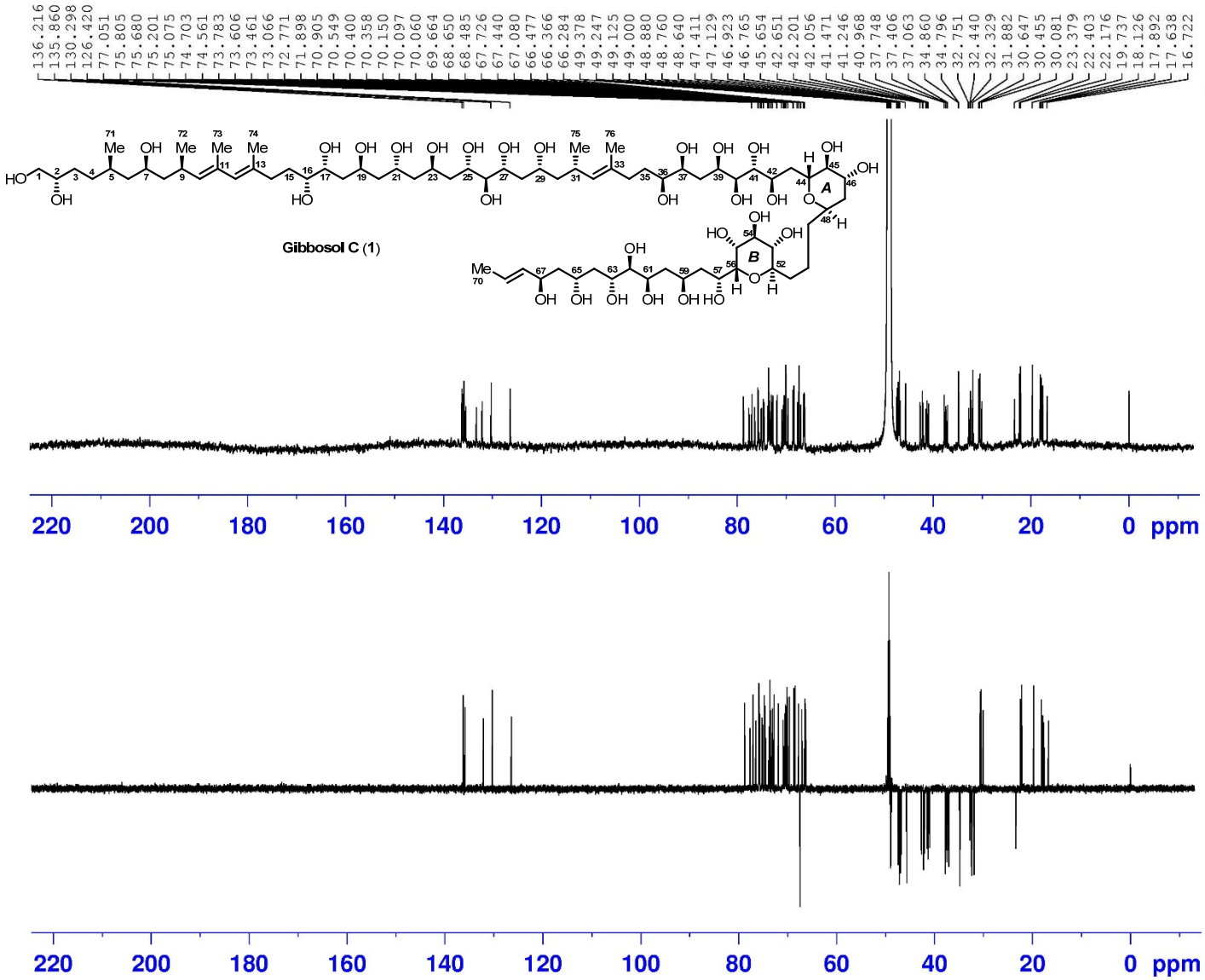

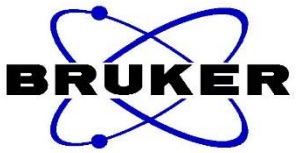

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FIDRES	2.676980 H
AQ	0.3736052 s
RG	181.26
DW	11.400 u
DE	18.00 u
TE	298.0 K
CNST2	145.0000000
D1	1.00000000 s
D2	0.00344828 s
D12	0.00002000 s
TD0	1
SFO1	176.0797677 M
NUC1	13C
P1	11.90 u
P13	2000.00 u
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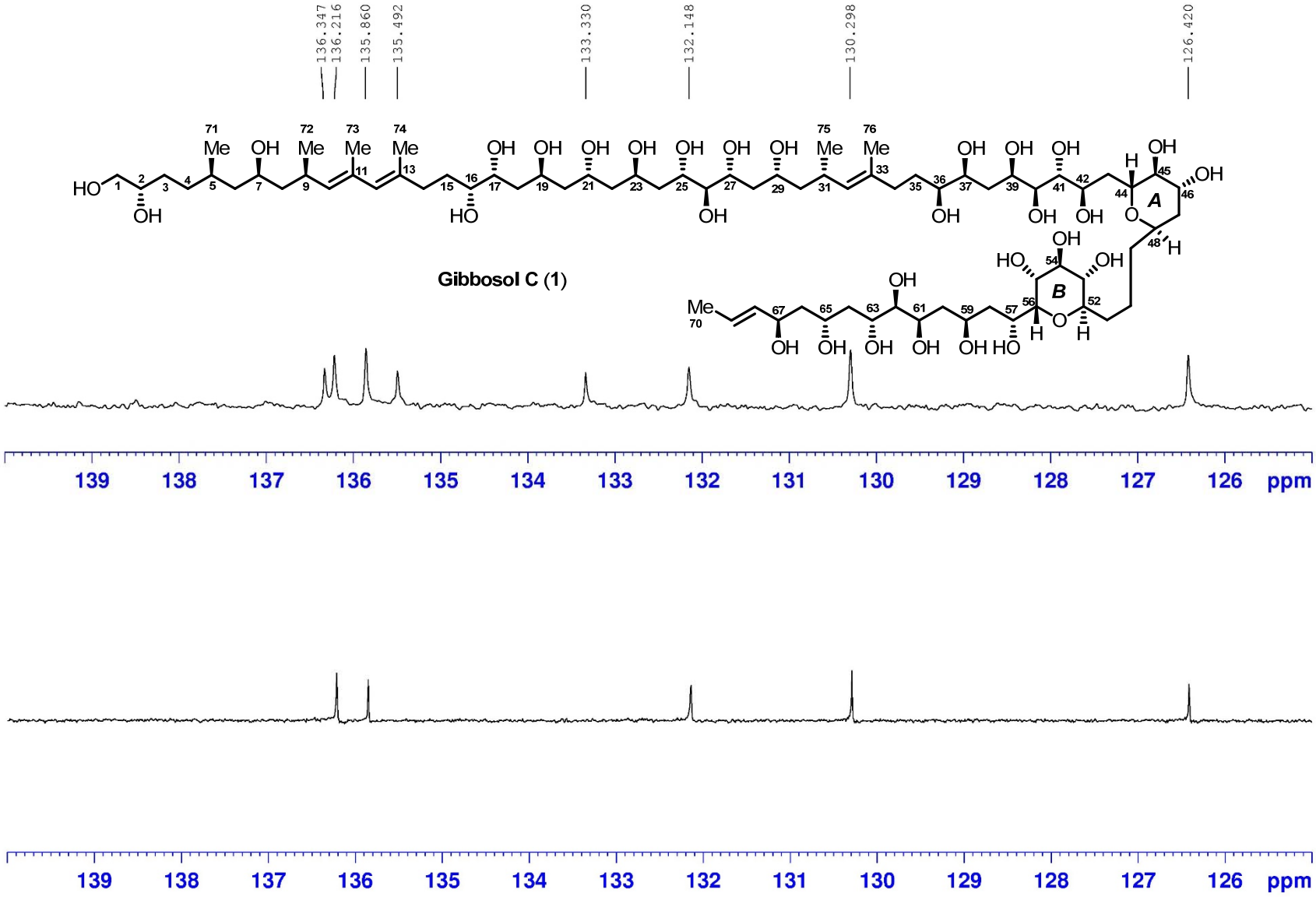

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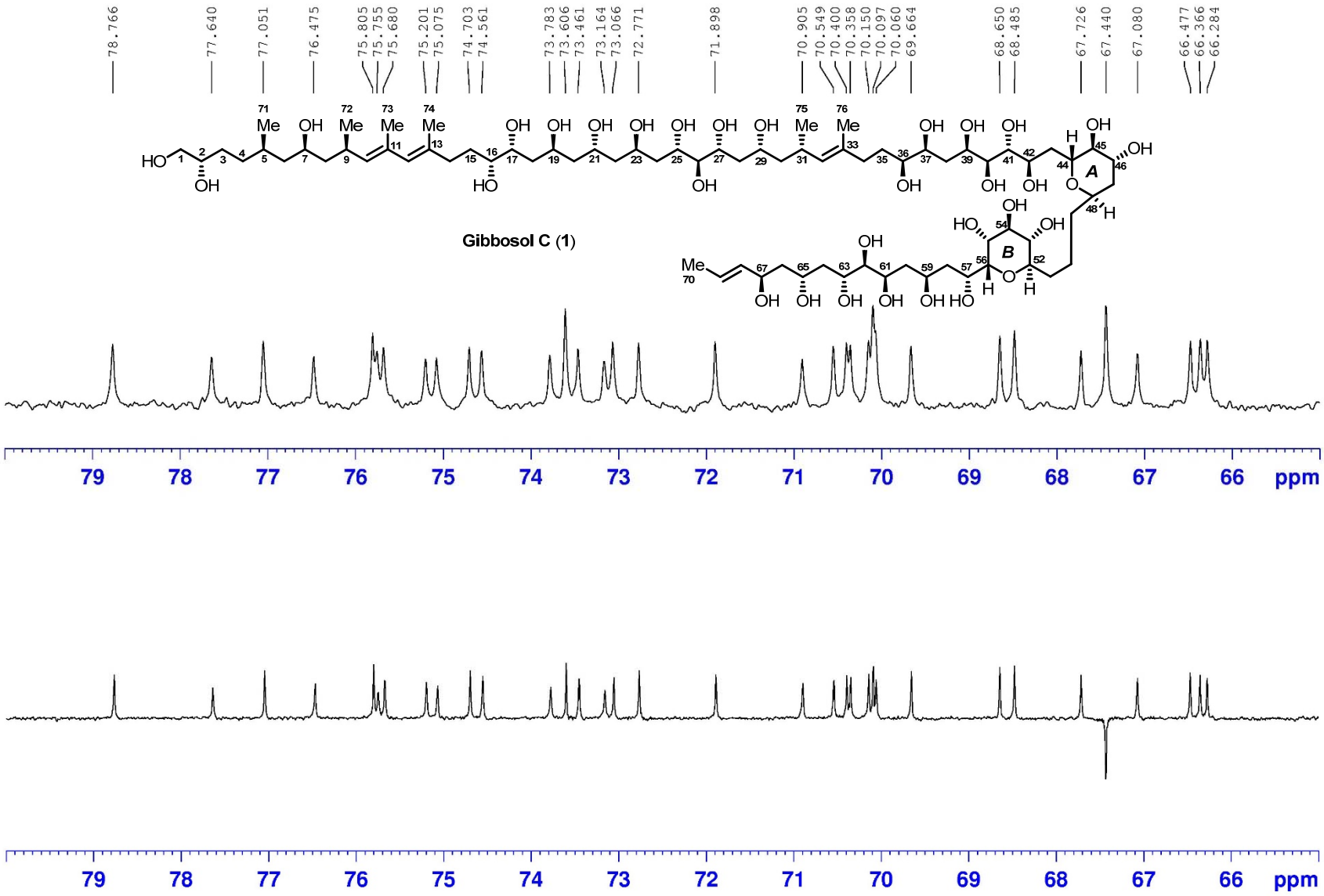

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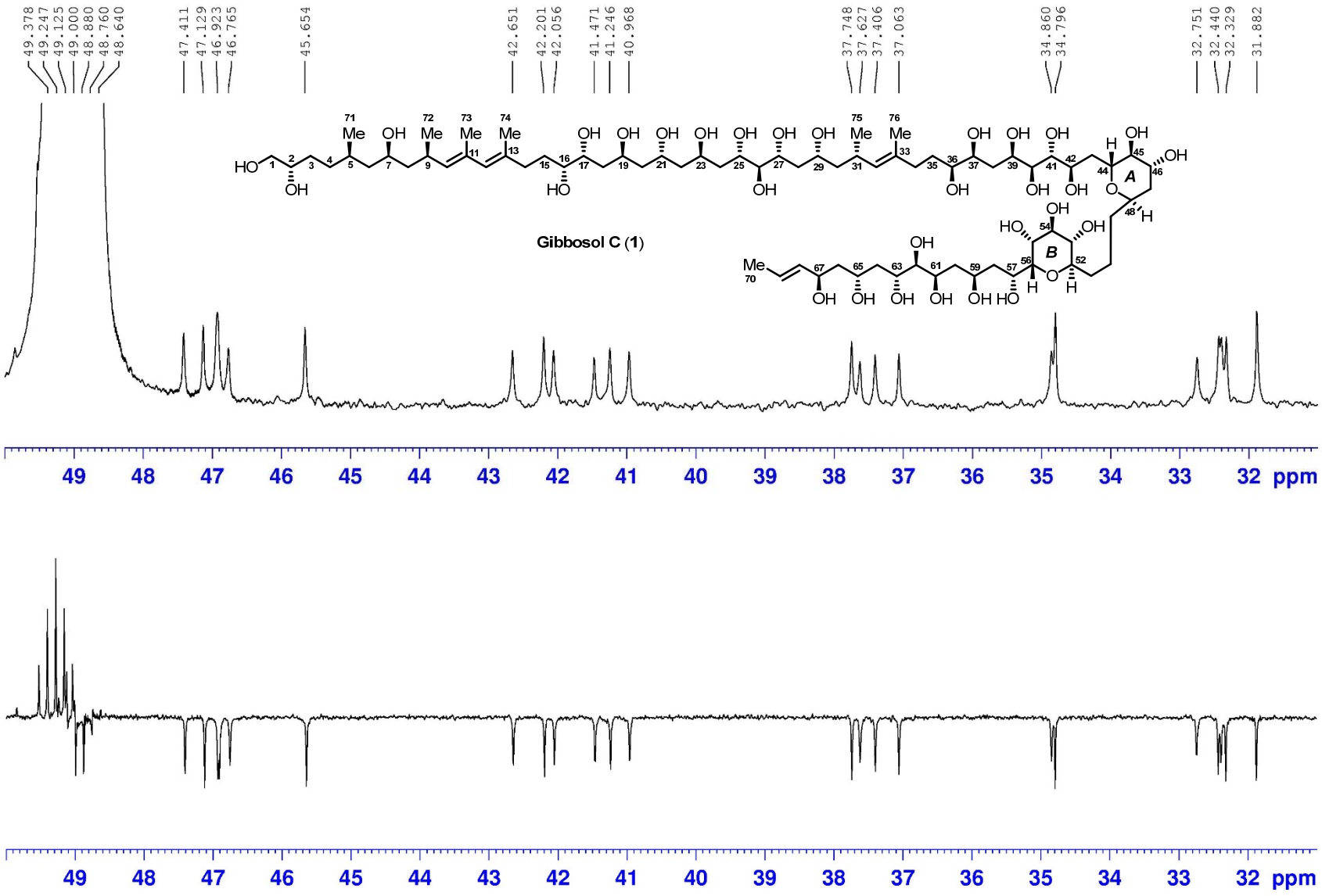
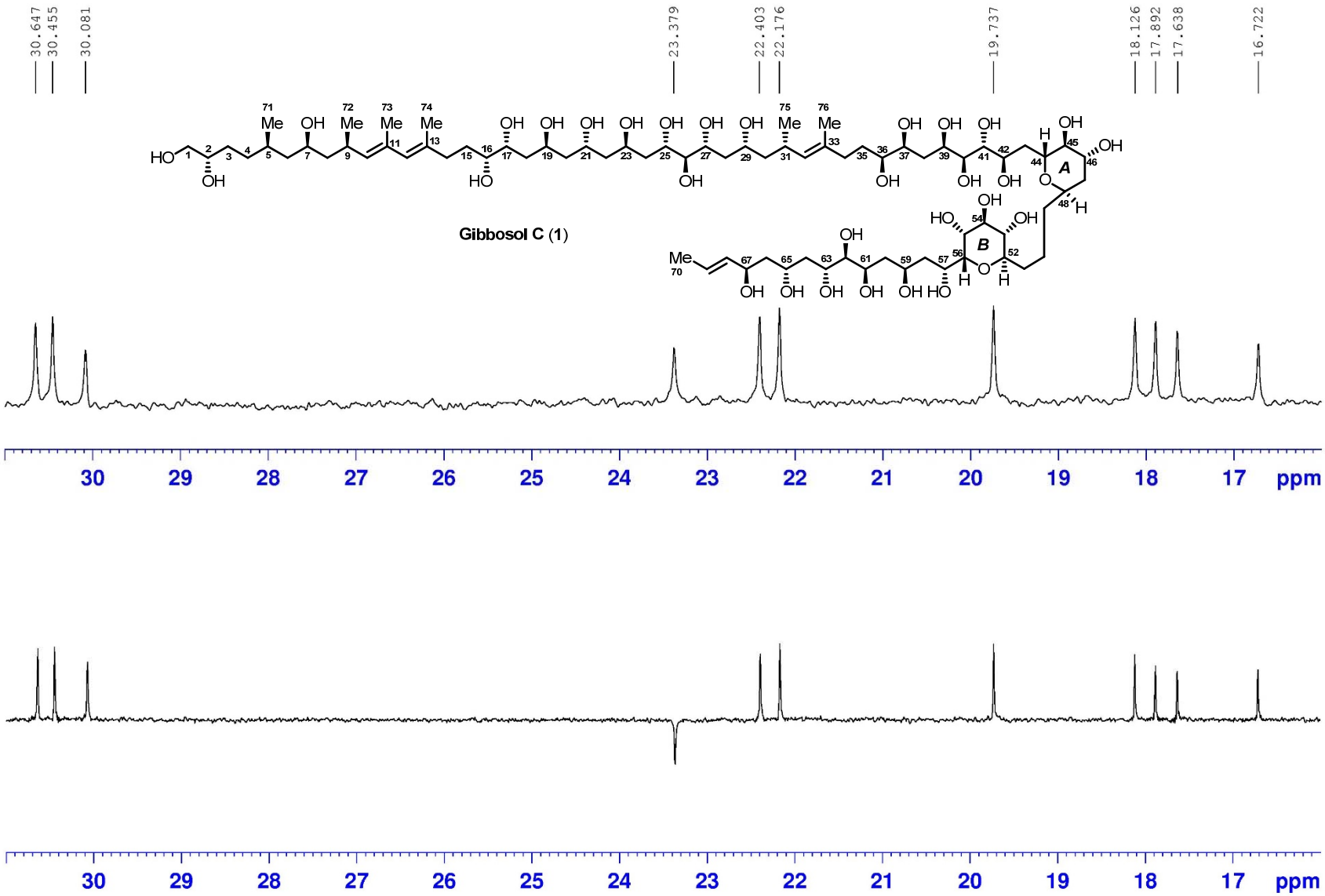
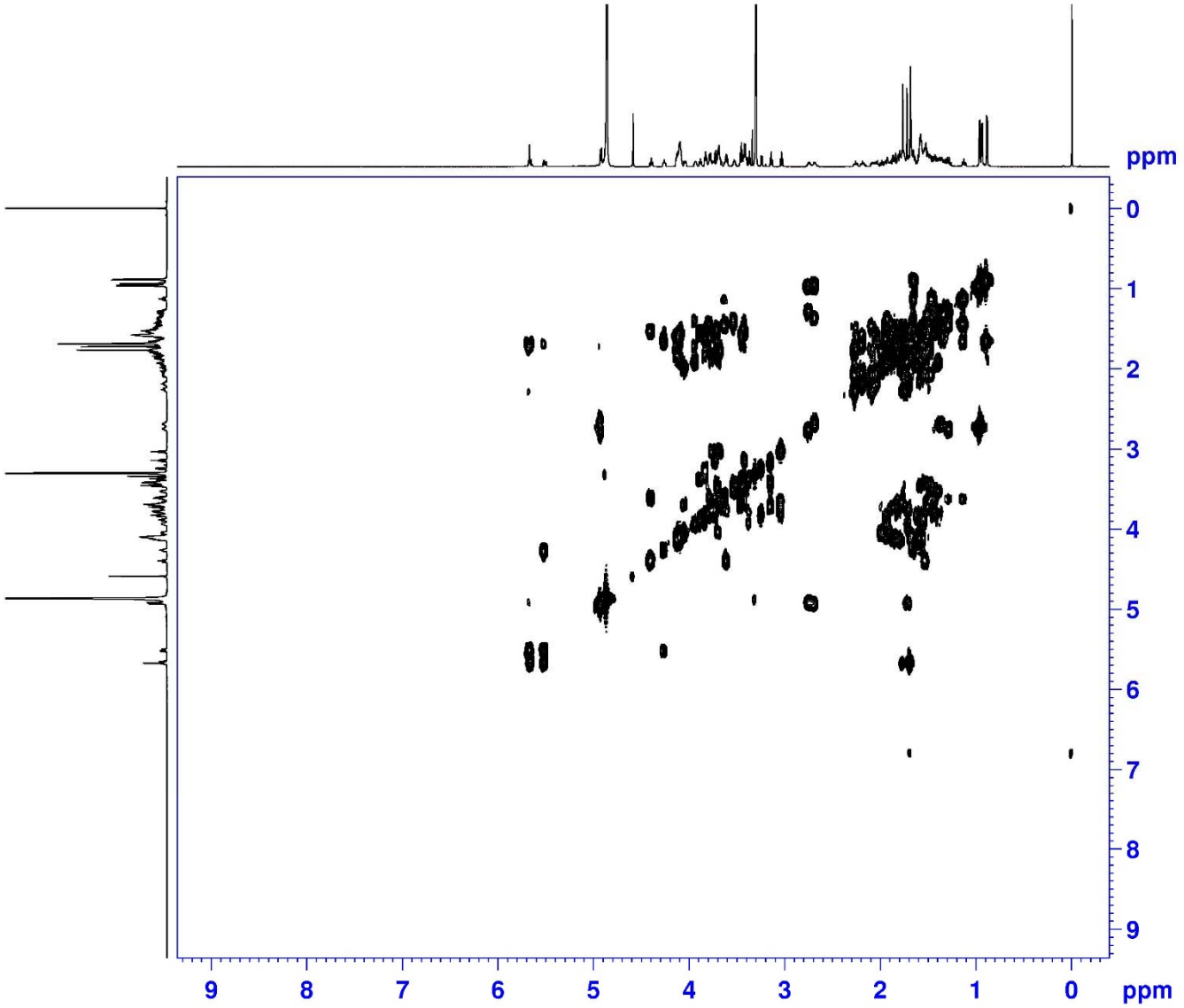


DEPT135 (175 MHz) spectrum of compound **1** in CD_3OD



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

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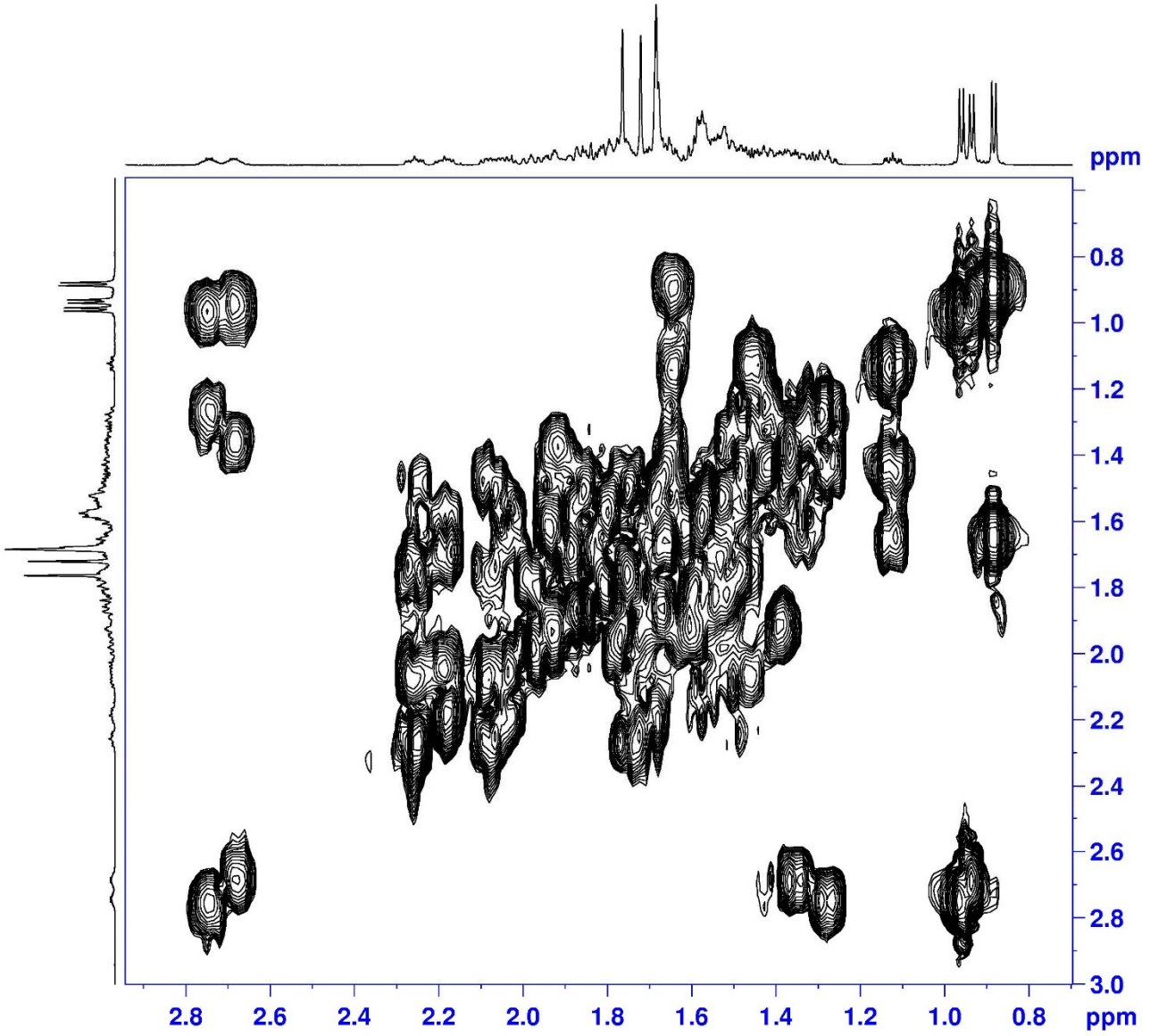
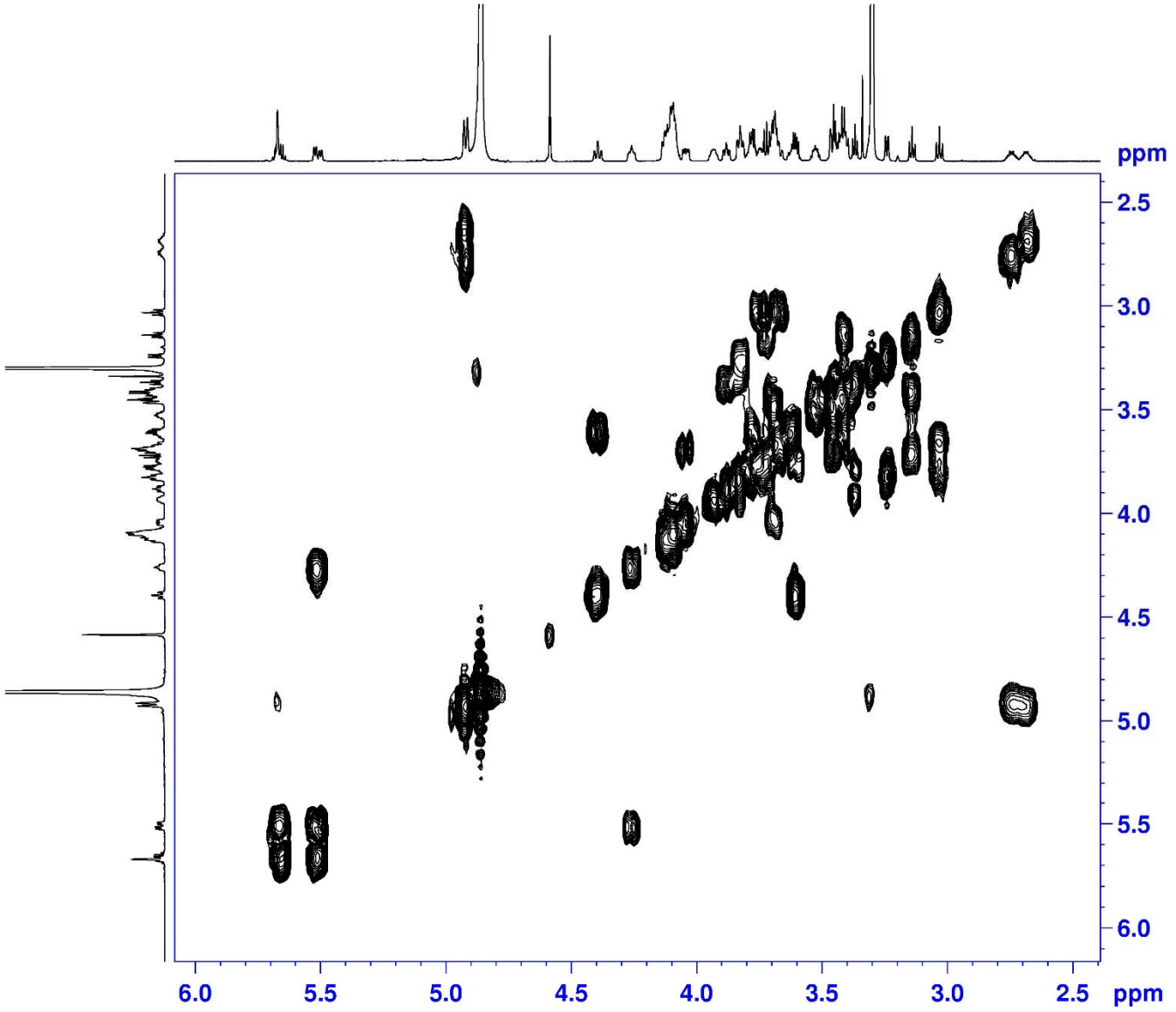
AQ                0.0961695 sec
RG                   181.26
DW                   46.933 usec
DE                   10.00 usec
TE                   298.0 K
D0                0.00000300 sec
D1                1.00000000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00009380 sec
ND0                       1
TD                      128
SFO1             700.1848 MHz
FIDRES           83.288910 Hz
SW                  15.226 ppm
FnMODE                  QF
SI                    1024
SF            700.1800160 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.40
SI                    1024
MC2                     QF
SF            700.1800140 MHz
WDW                   SINE
SSB                      0
LB                    0.00 Hz
GB                       0
```

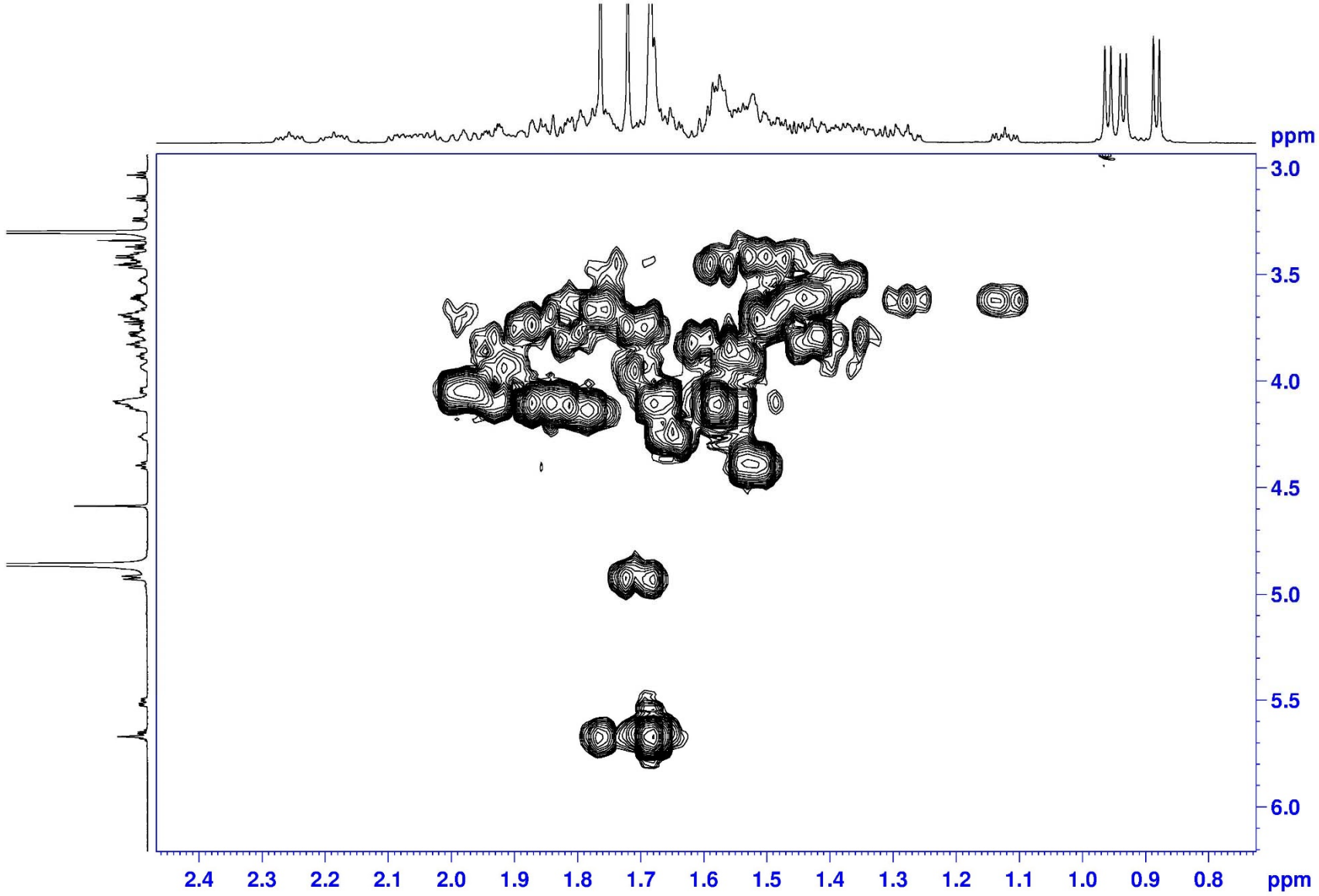
^{1}H–^{1}H COSY (700 MHz) spectrum of compound **1** in CD_3OD



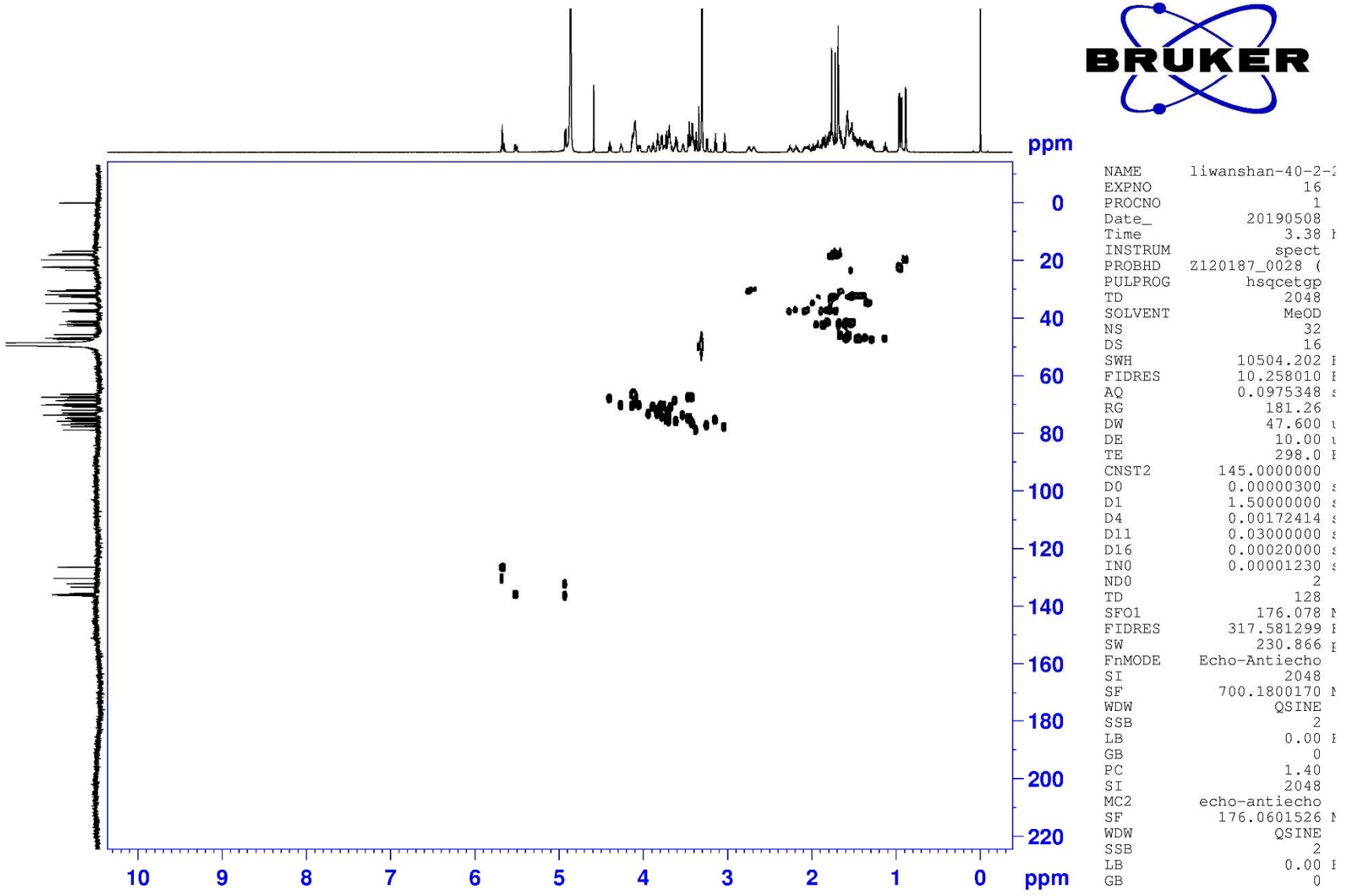
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of compound **1** in CD_3OD



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



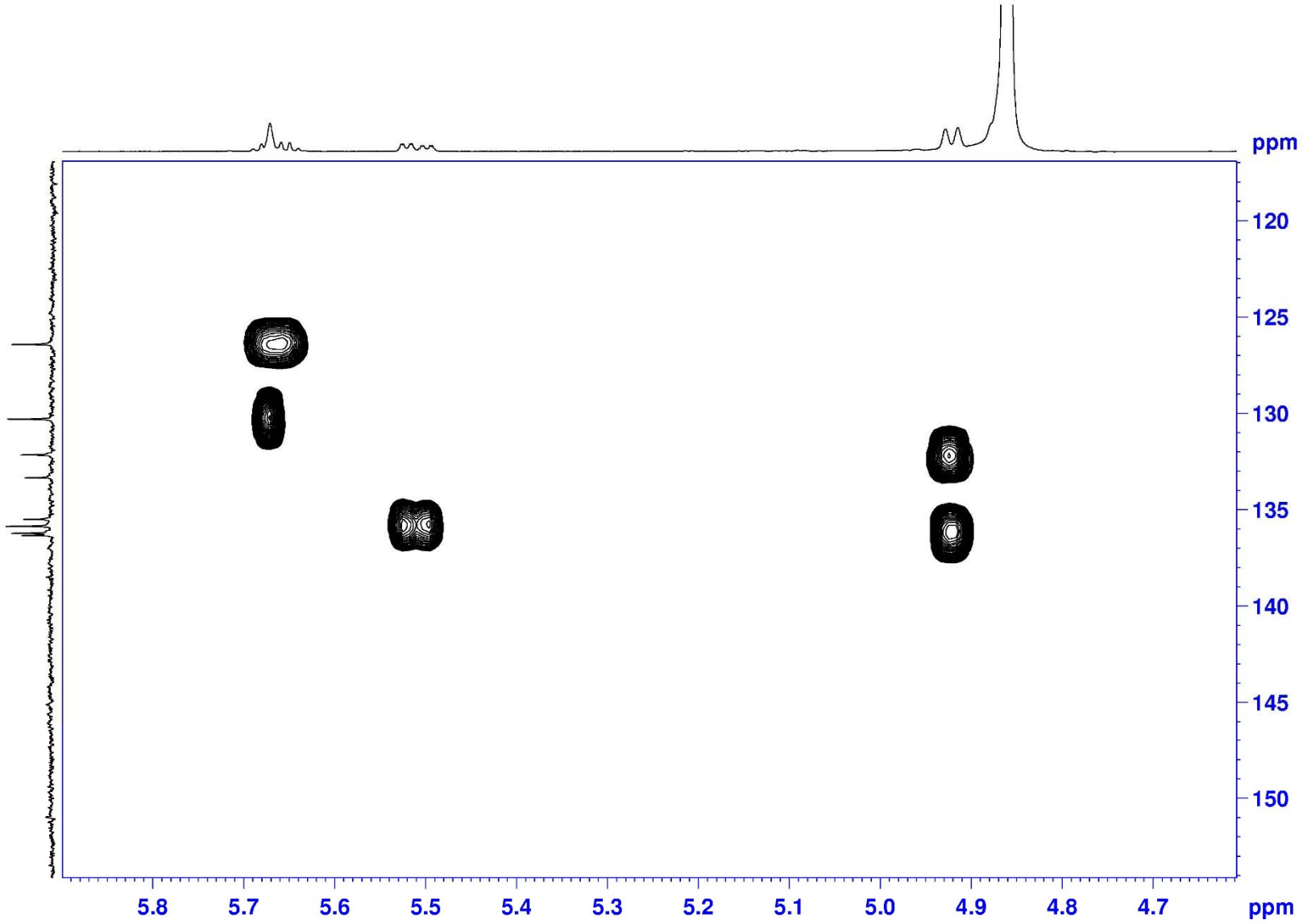
HSQC (700 MHz) spectrum of compound **1** in CD_3OD



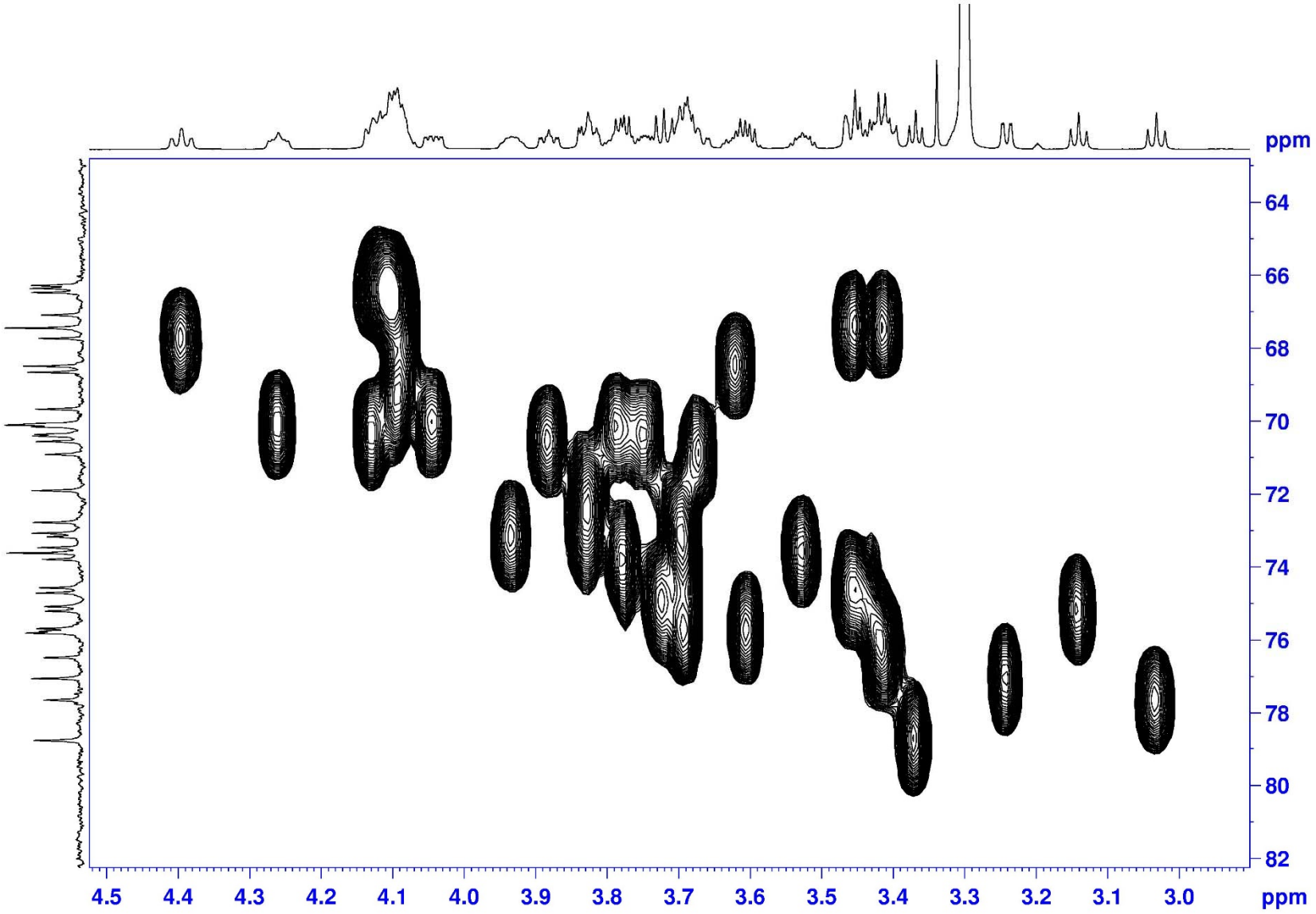
BRUKER

NAME	liwanshan-40-2-2
EXPNO	16
PROCNO	1
Date_	20190508
Time	3.38 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hsqcetgp
TD	2048
SOLVENT	MeOD
NS	32
DS	16
SWH	10504.202 H
FIDRES	10.258010 H
AQ	0.0975348 s
RG	181.26
DW	47.600 u
DE	10.00 u
TE	298.0 K
CNST2	145.0000000
D0	0.00000300 s
D1	1.50000000 s
D4	0.00172414 s
D11	0.03000000 s
D16	0.00020000 s
IN0	0.00001230 s
ND0	2
TD	128
SFO1	176.078 M
FIDRES	317.581299 H
SW	230.866 p
FnMODE	Echo-Antiecho
SI	2048
SF	700.1800170 M
WDW	QSINE
SSB	2
LB	0.00 H
GB	0
PC	1.40
SI	2048
MC2	echo-antiecho
SF	176.0601526 M
WDW	QSINE
SSB	2
LB	0.00 H
GB	0

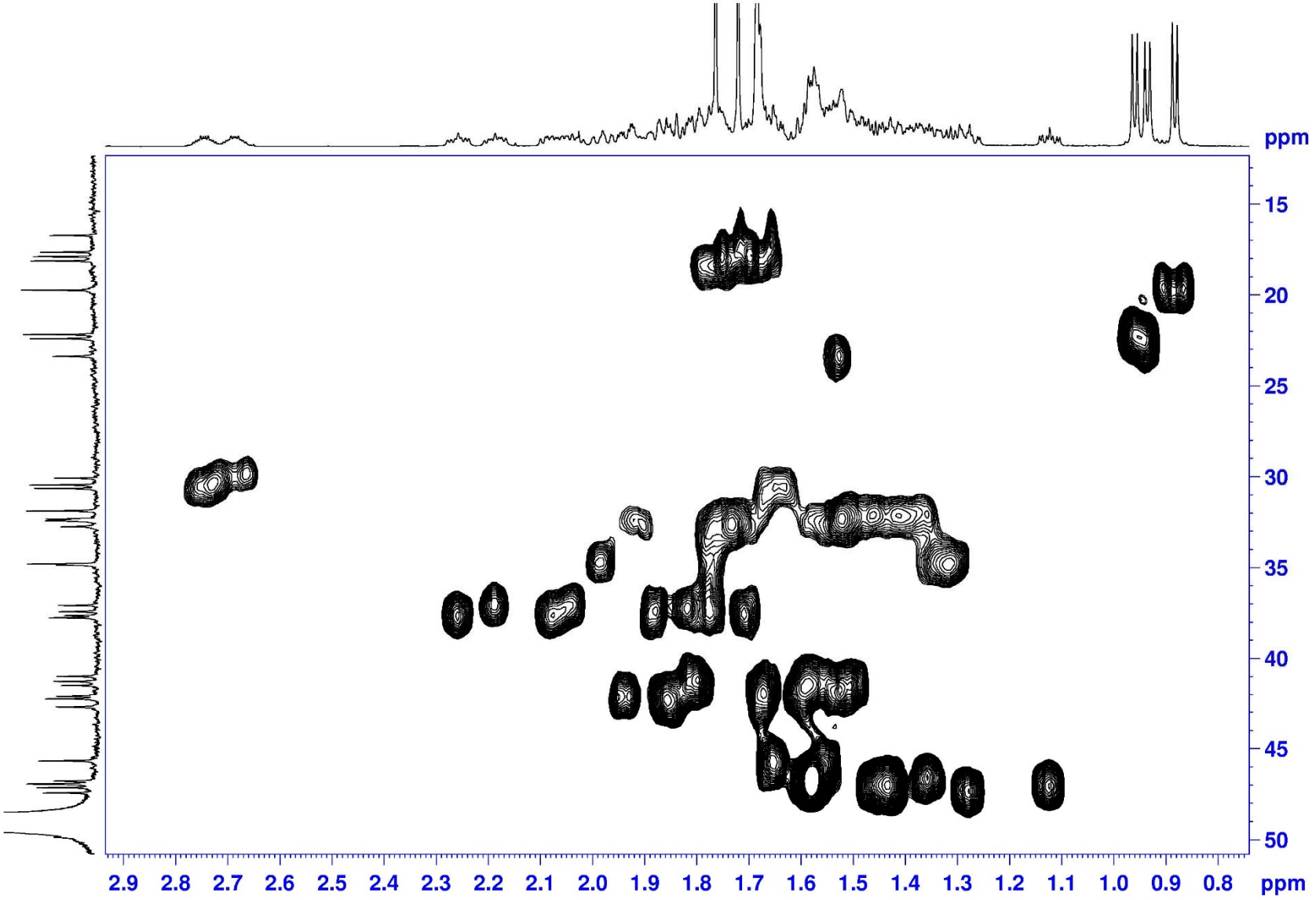
HSQC (700 MHz) spectrum of compound **1** in CD_3OD



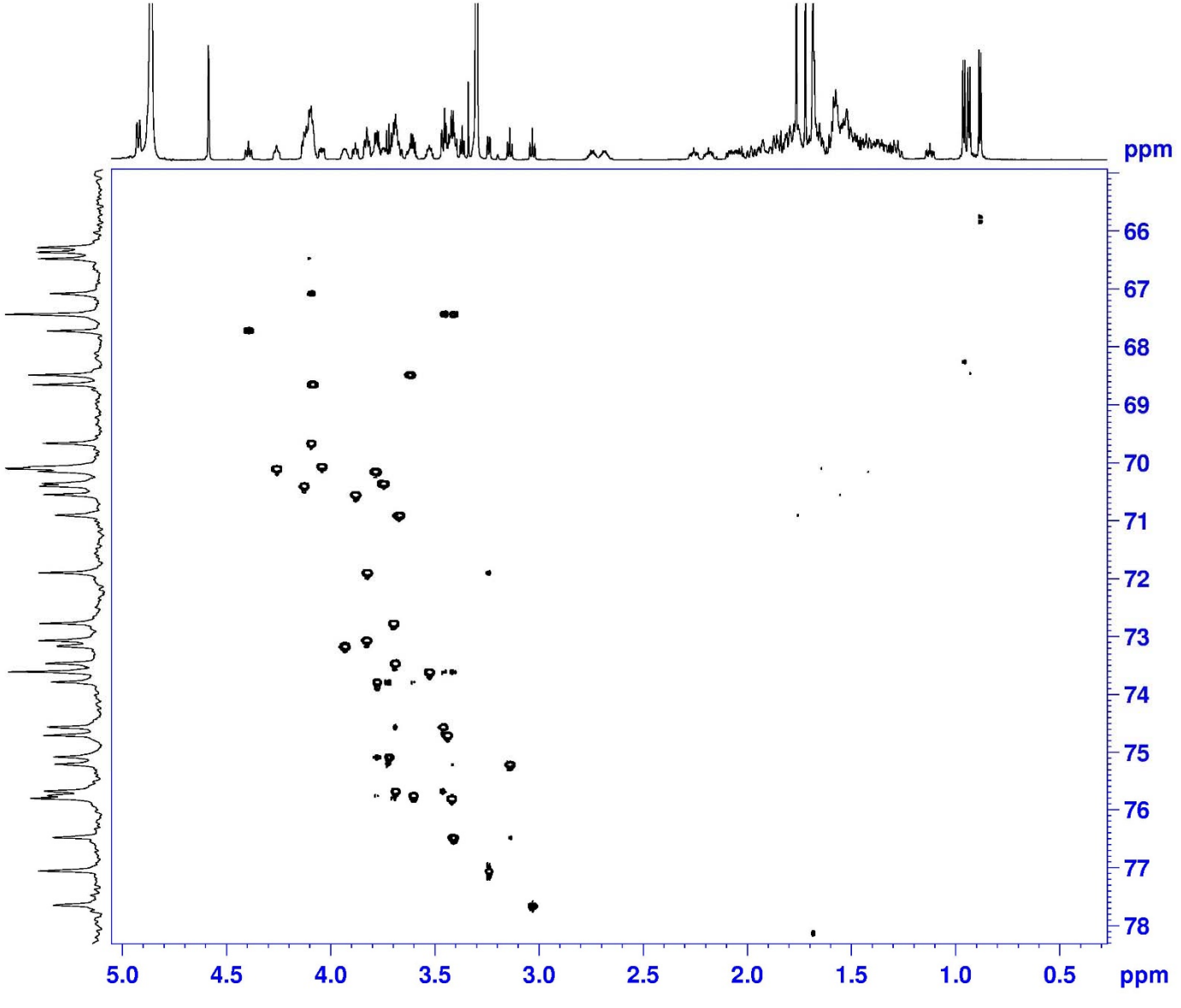
HSQC (700 MHz) spectrum of compound **1** in CD_3OD



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



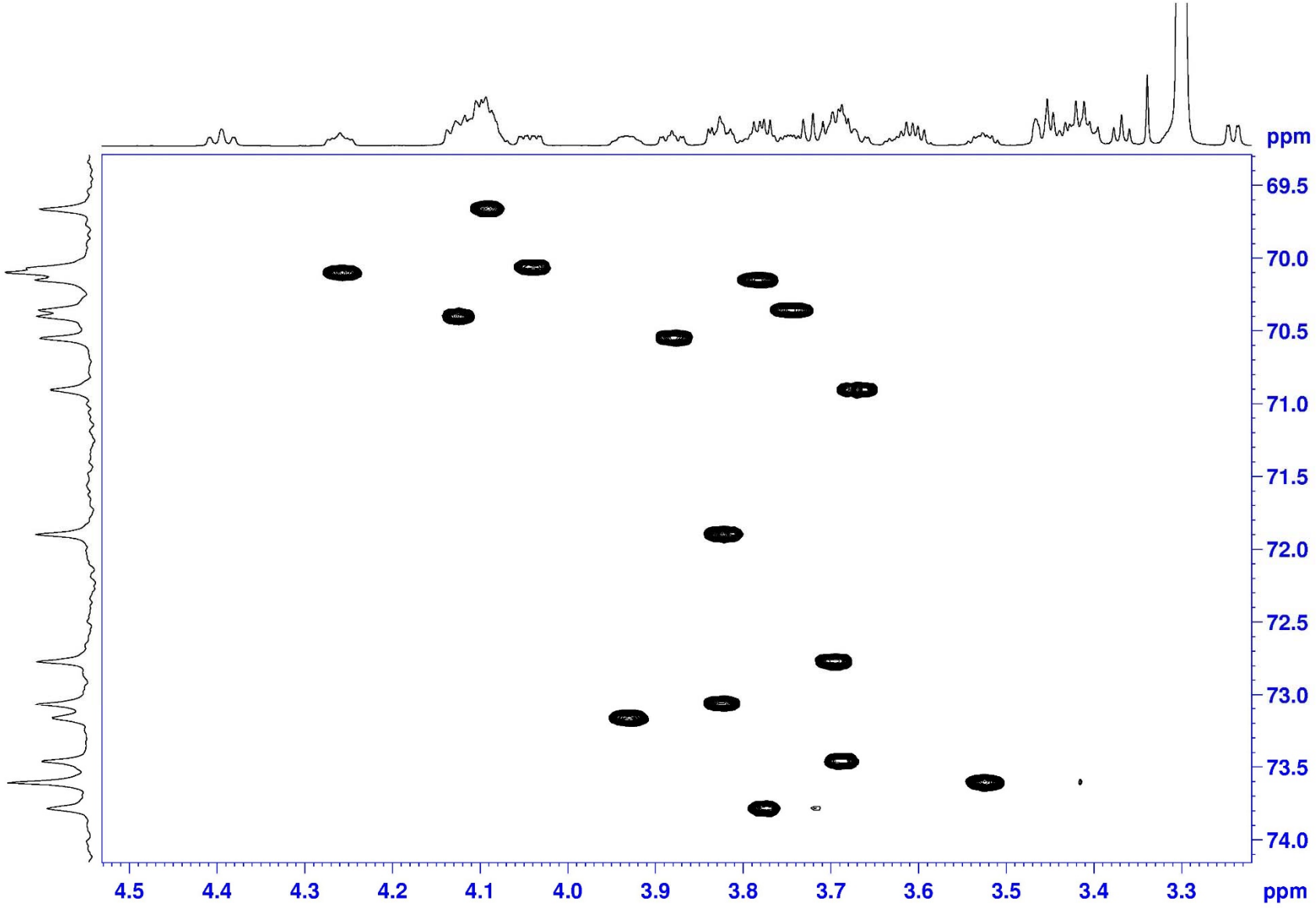
Selective-HSQC (700 MHz) spectrum of compound **1** in CD_3OD



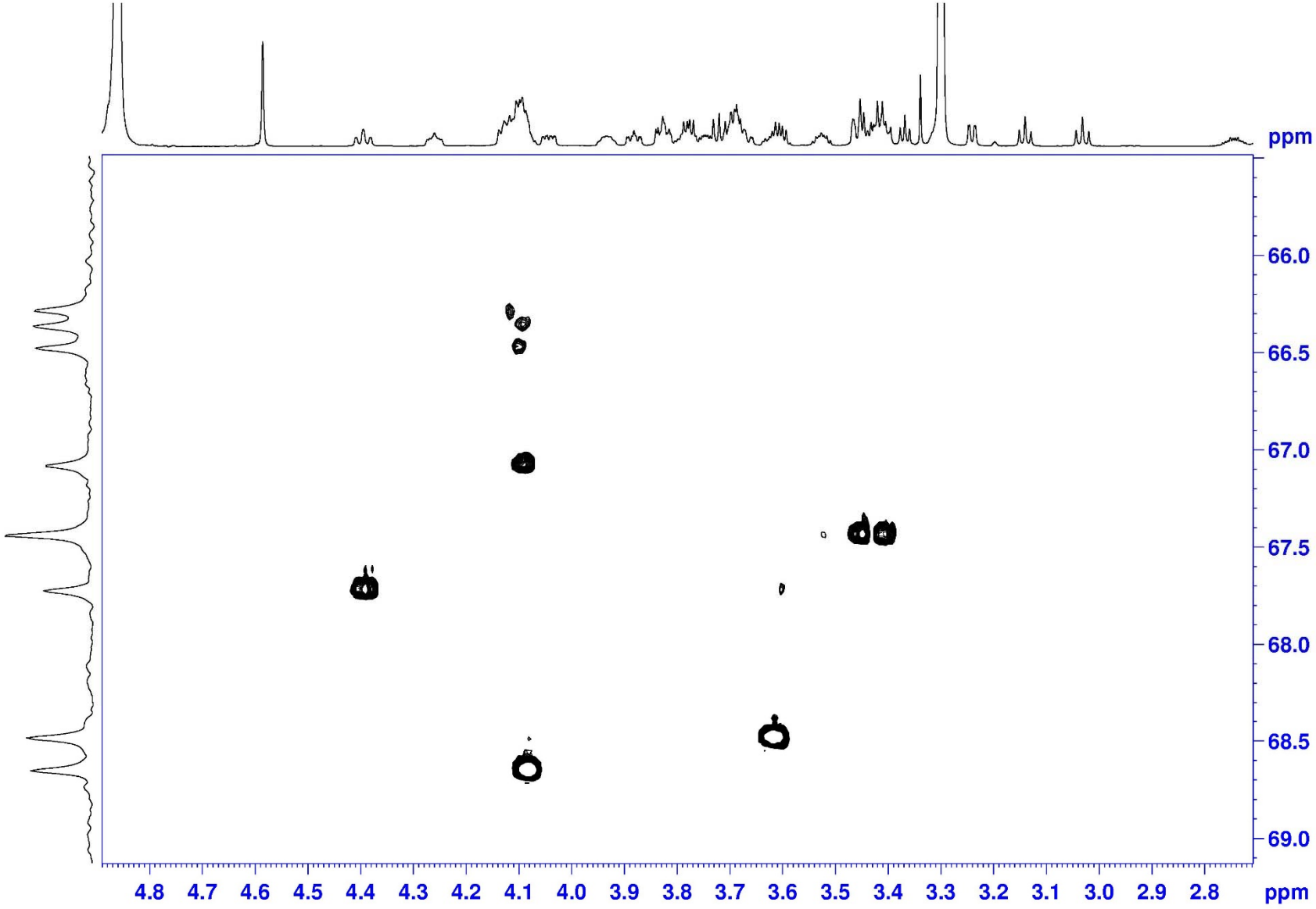
BRUKER

NAME	liwanshan-40-2-2
EXPNO	17
PROCNO	1
Date_	20190510
Time	15.49 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	shsqcetgpsisp2.2
TD	2048
SOLVENT	MeOD
NS	32
DS	16
SWH	4340.278 Hz
FIDRES	4.238553 Hz
AQ	0.2359796 se
RG	181.26
DW	115.200 us
DE	10.00 us
TE	298.0 K
CNST2	145.0000000
CNST17	-0.5000000
D0	0.00000300 se
D1	1.00000000 se
D4	0.00172414 se
D11	0.03000000 se
D16	0.00020000 se
D24	0.00089000 se
IN0	0.00018500 se
ND0	2
TD	256
SFO1	176.0729 MH
FIDRES	10.557432 Hz
SW	15.350 pp
FnMODE	Echo-Anticcho
SI	1024
SF	700.1800207 MH
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	176.0601526 MH
WDW	QSINE
SSB	2
LB	0.00 Hz

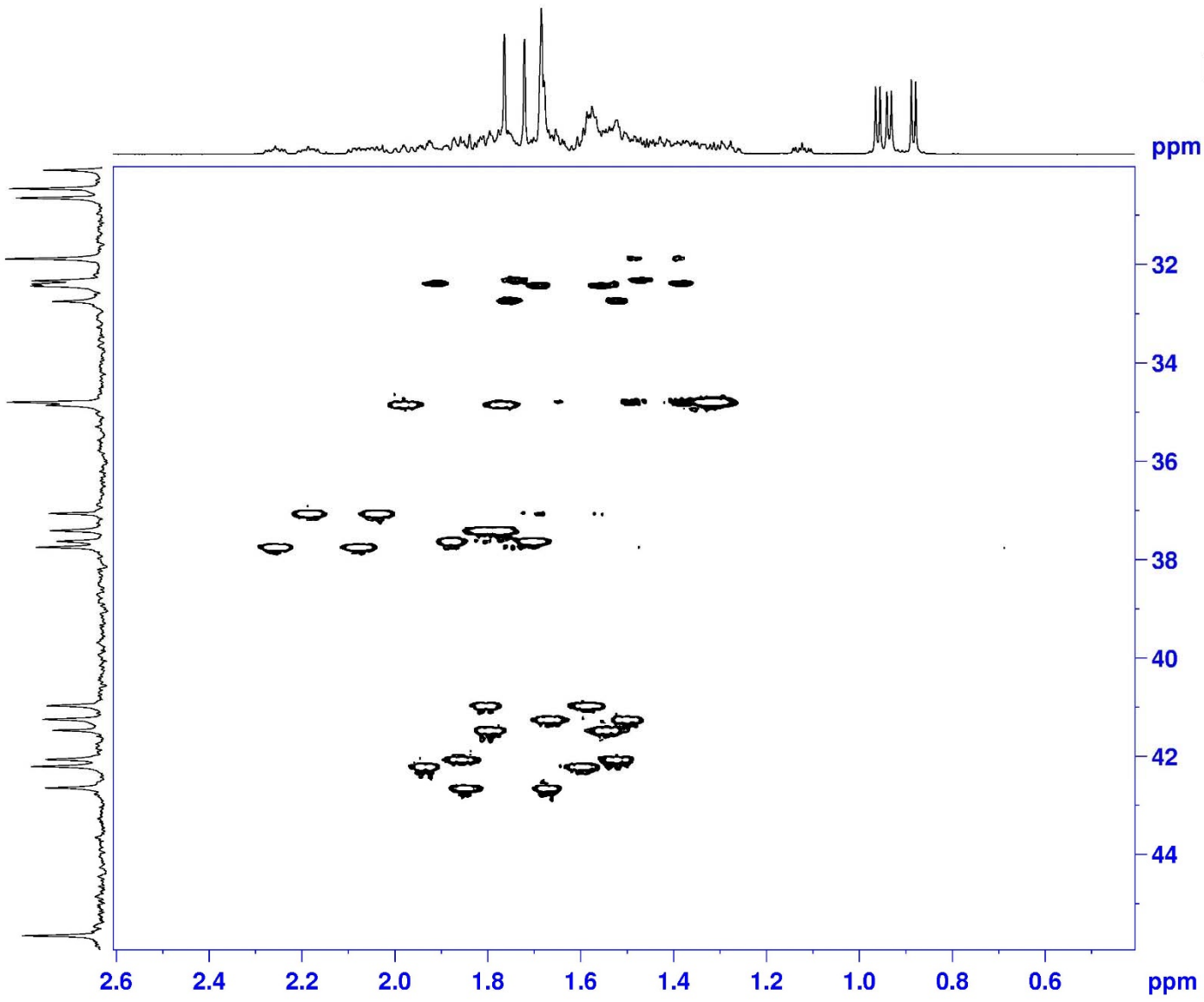
Selective-HSQC (700 MHz) spectrum of compound **1** in CD_3OD



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

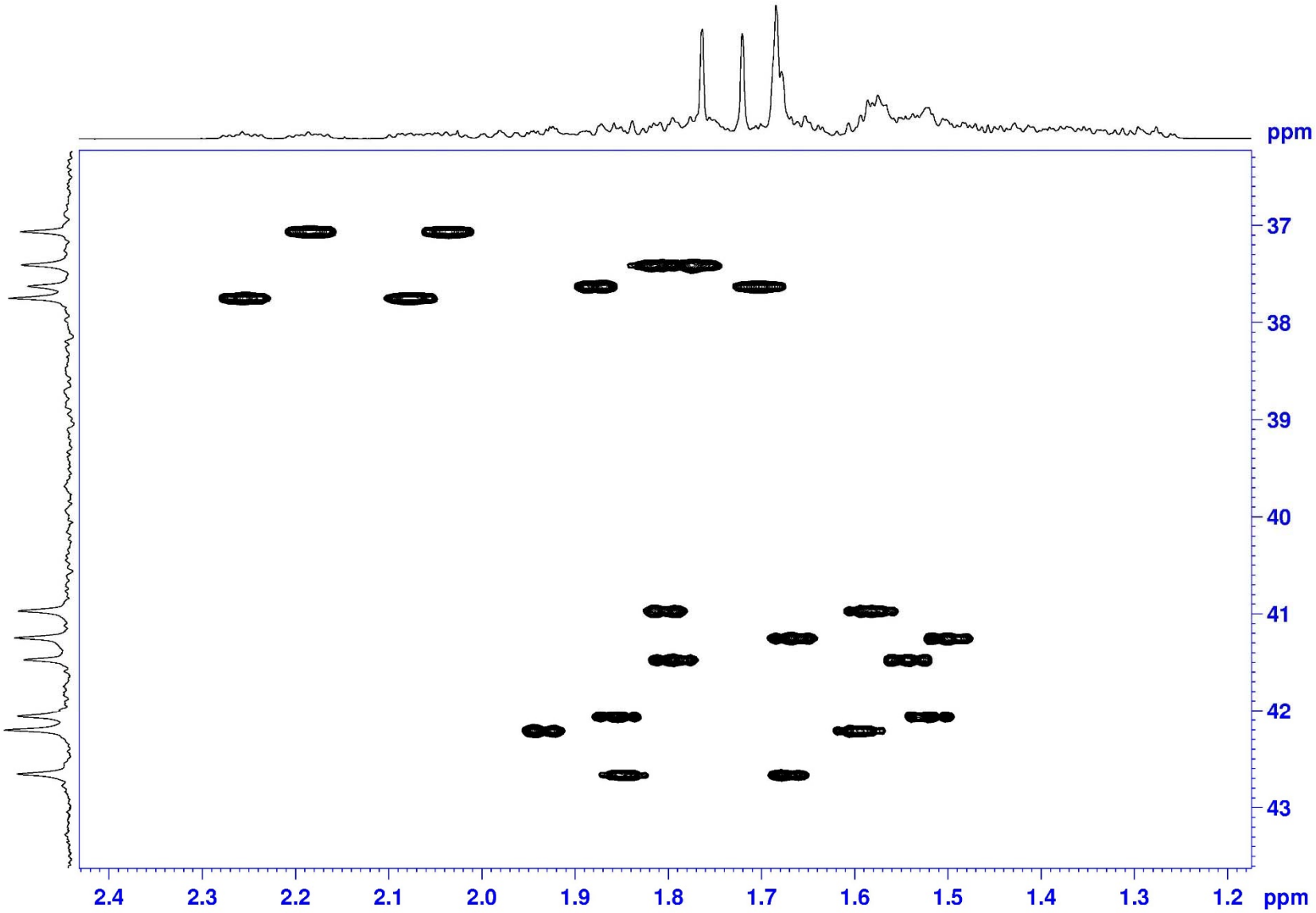


Selective-HSQC (700 MHz) spectrum of compound **1** in CD_3OD

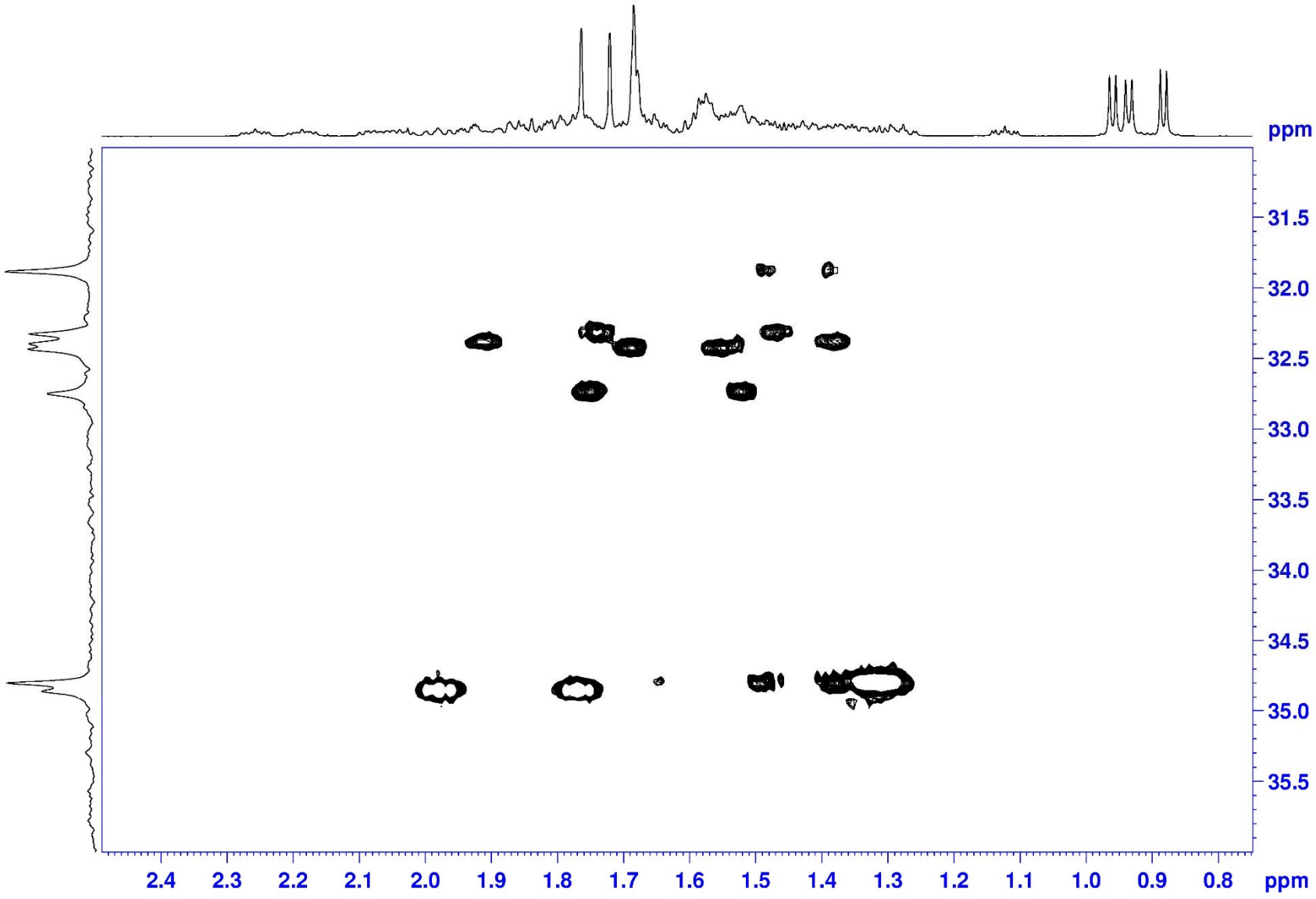



```
NAME      liwanshan-40-2-2
EXPNO                   18
PROCNO                   1
Date_             20190510
Time                18.45 h
INSTRUM              spect
PROBHD    Z120187_0028 (
PULPROG   shsqcetgpsisp2.2
TD                    2048
SOLVENT                MeOD
NS                       32
DS                       16
SWH               4340.278 H
FIDRES            4.238553 H
AQ                0.2359796 s
RG                   181.26
DW                   115.200 u
DE                    10.00 u
TE                    298.0 K
CNST2           145.0000000
CNST17           -0.5000000
D0                0.00000300 s
D1                1.00000000 s
D4                0.00172414 s
D11               0.03000000 s
D16               0.00020000 s
D24               0.00089000 s
IN0               0.00014230 s
ND0                       2
TD                      256
SFO1               176.0669 M
FIDRES            13.725404 H
SW                   19.957 p
FnMODE       Echo-Antiecho
SI                      1024
SF              700.1800207 M
WDW                   QSINE
SSB                       2
LB                     0.00 H
GB                        0
PC                     1.40
SI                      1024
MC2          echo-antiecho
SF               176.0601526 M
WDW                   QSINE
SSB                       2
LB                     0.00 H
GB                        0
```

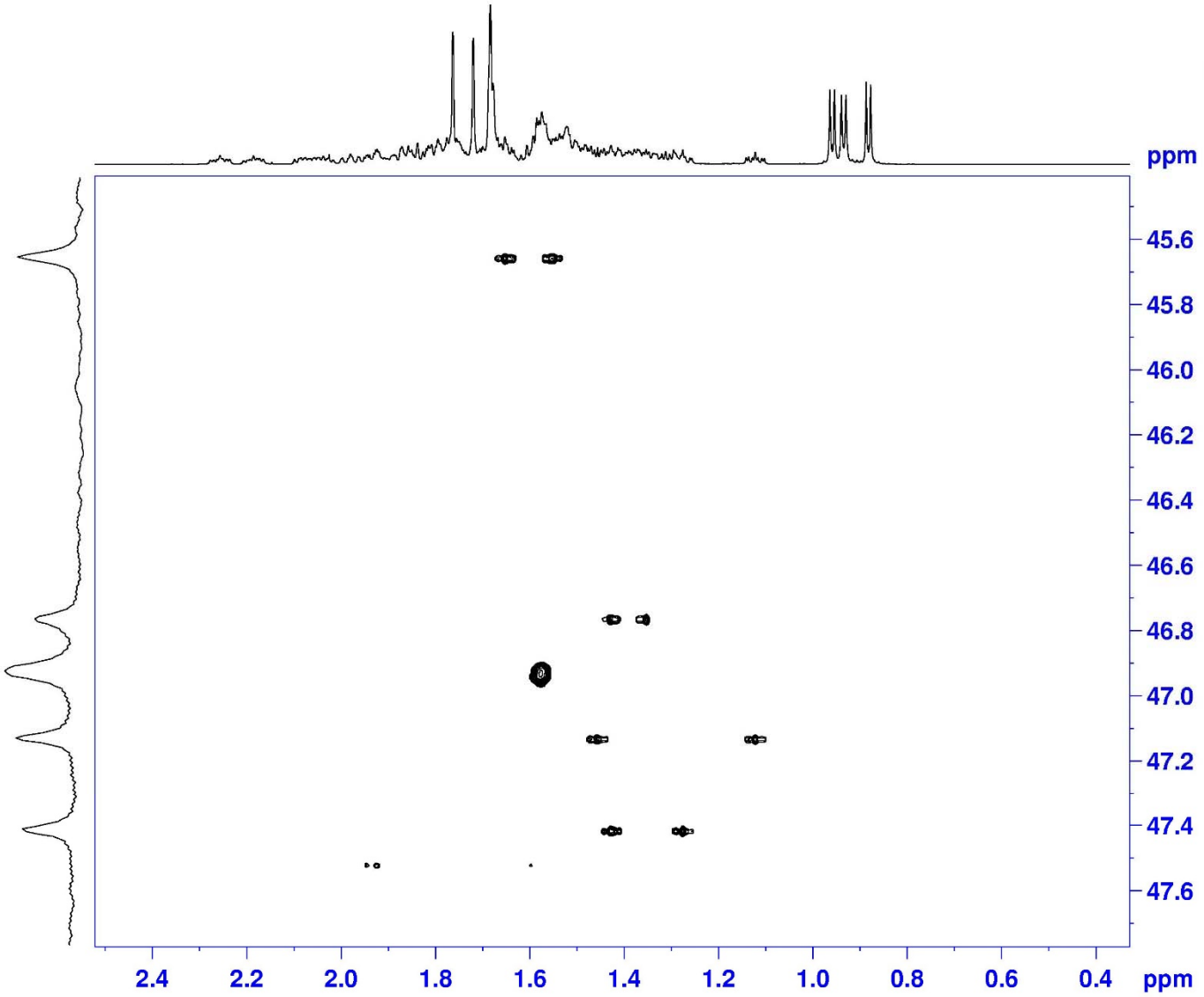
Selective-HSQC (700 MHz) spectrum of compound **1** in CD_3OD



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

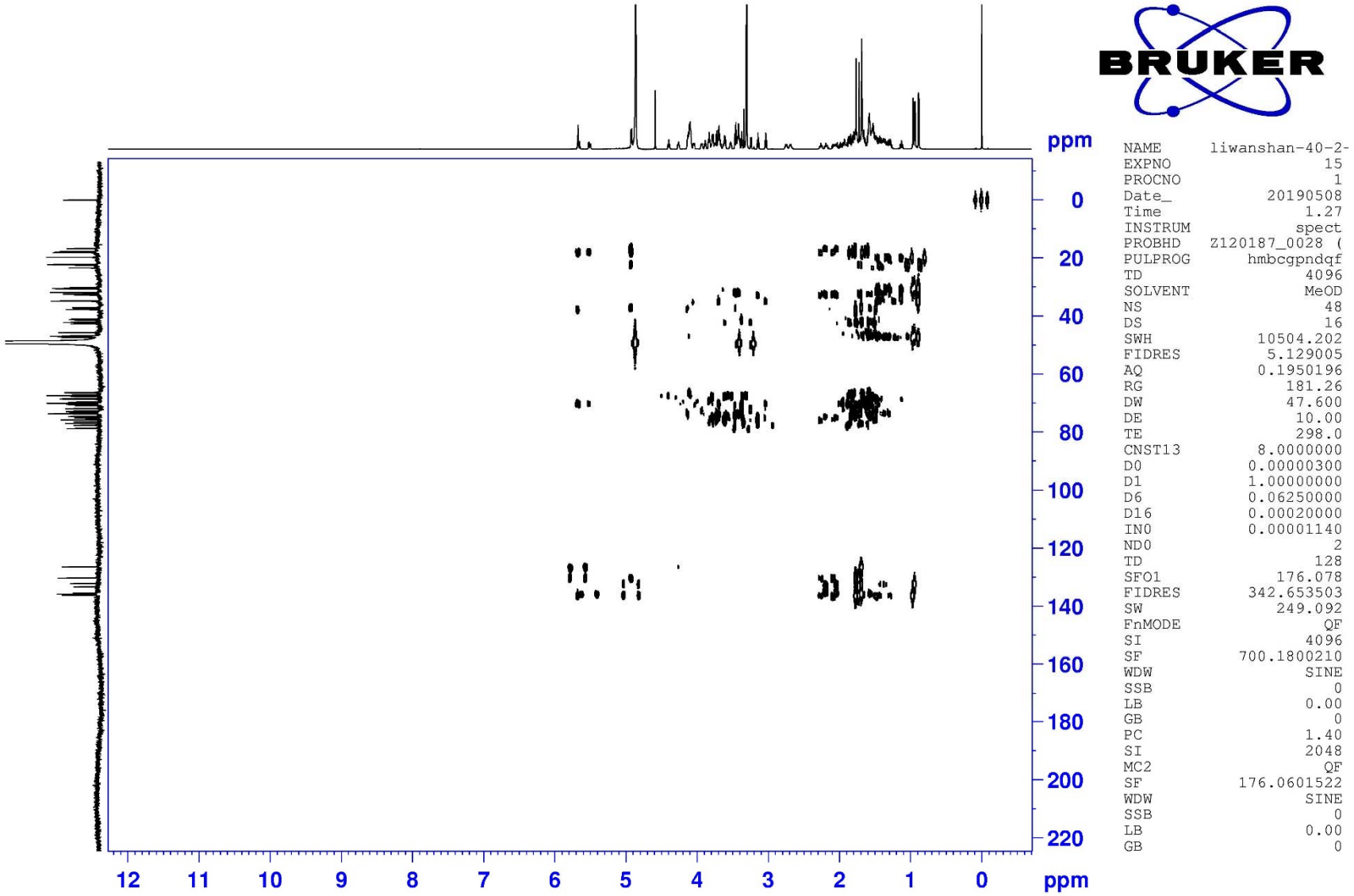


Selective-HSQC (700 MHz) spectrum of compound **1** in CD_3OD



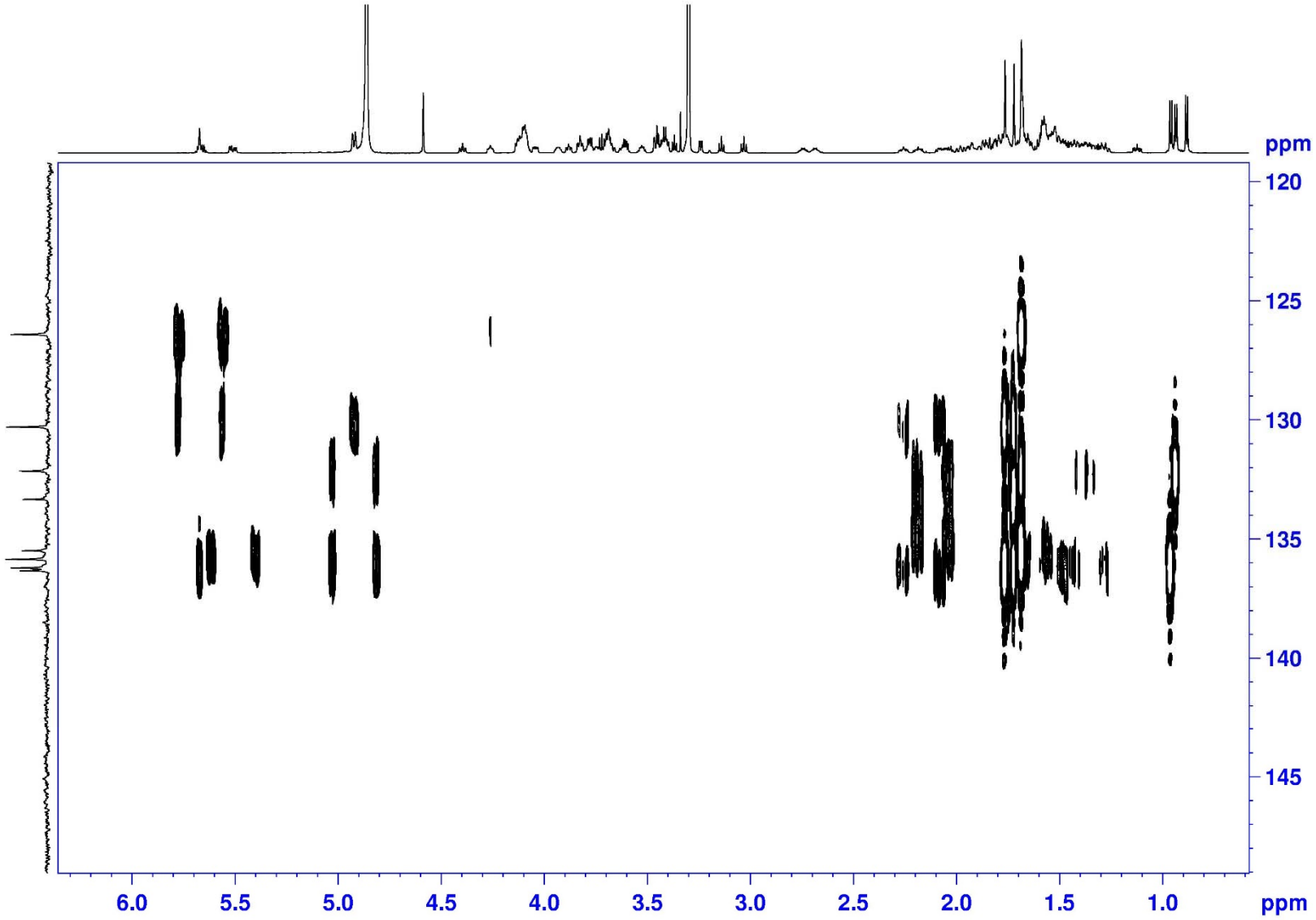

```
NAME      liwanshan-40-2-2
EXPNO                   19
PROCNO                   1
Date_              20190518
Time                 19.20 h
INSTRUM              spect
PROBHD    Z120187_0028 (
PULPROG   shsqcetgpsisp2.2
TD                    2048
SOLVENT                MeOD
NS                       64
DS                       16
SWH               5013.369 H
FIDRES            4.895868 H
AQ                0.2043039 s
RG                   181.26
DW                   99.733 u
DE                   10.00 u
TE                   298.0 K
CNST2           145.0000000
CNST17           -0.5000000
D0                0.00000300 s
D1                1.00000000 s
D4                0.00172414 s
D11               0.03000000 s
D16               0.00020000 s
D24               0.00089000 s
IN0               0.00106830 s
ND0                      2
TD                     128
SFO1                176.0683 M
FIDRES            3.656510 H
SW                   2.658 p
FnMODE       Echo-Antiecho
SI                    1024
SF             700.1800207 M
WDW                  QSINE
SSB                      2
LB                    0.00 H
GB                       0
PC                    1.40
SI                    1024
MC2           echo-antiecho
SF              176.0601526 M
WDW                  QSINE
SSB                      2
LB                    0.00 H
GB                       0
```

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

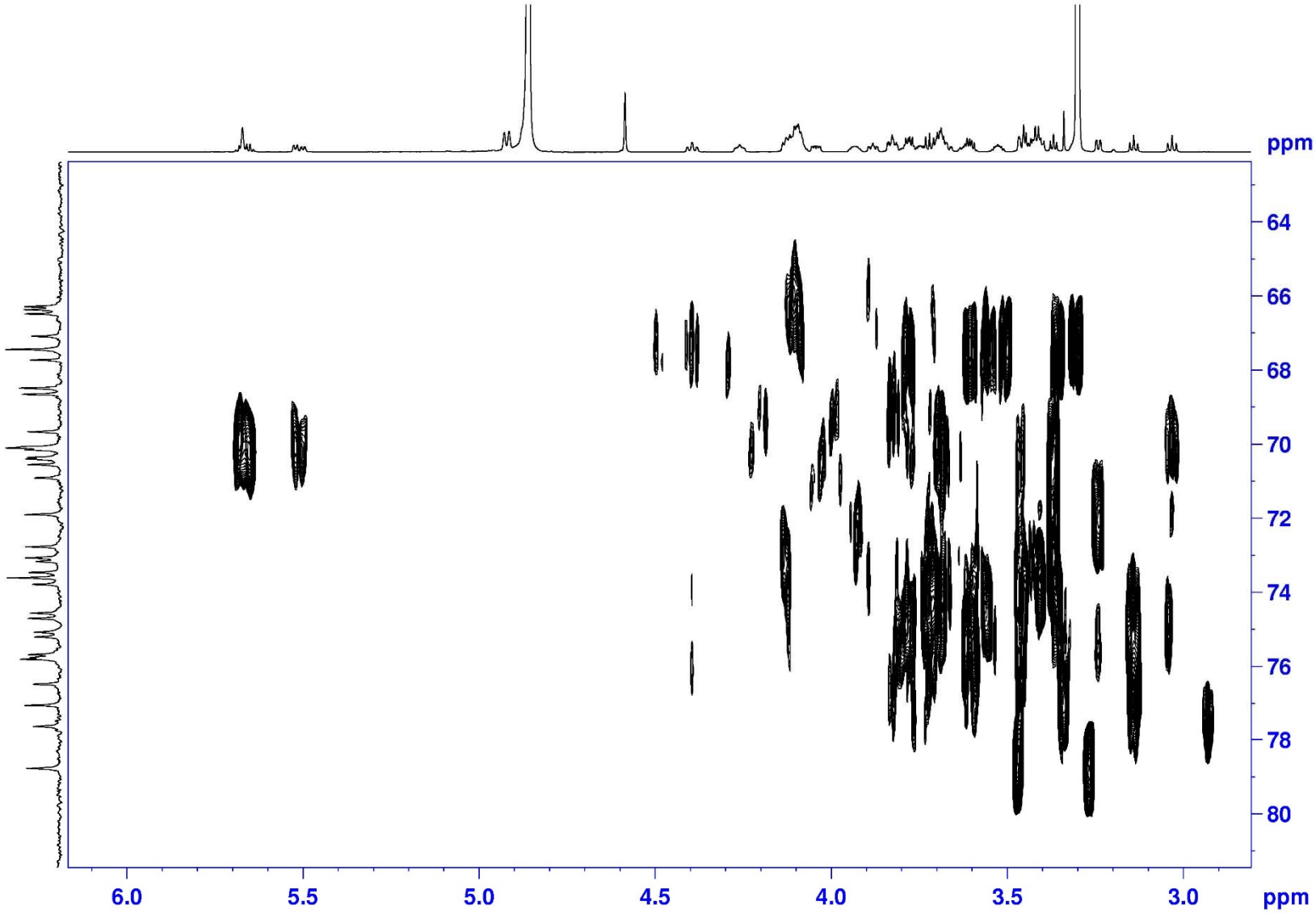


NAME	liwanshan-40-2-
EXPNO	15
PROCNO	1
Date_	20190508
Time	1.27
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hmbcgpndqf
TD	4096
SOLVENT	MeOD
NS	48
DS	16
SWH	10504.202
FIDRES	5.129005
AQ	0.1950196
RG	181.26
DW	47.600
DE	10.00
TE	298.0
CNST13	8.0000000
D0	0.00000300
D1	1.00000000
D6	0.06250000
D16	0.00020000
IN0	0.00001140
ND0	2
TD	128
SFO1	176.078
FIDRES	342.653503
SW	249.092
FnMODE	QF
SI	4096
SF	700.1800210
WDW	SINE
SSB	0
LB	0.00
GB	0
PC	1.40
SI	2048
MC2	QF
SF	176.0601522
WDW	SINE
SSB	0
LB	0.00
GB	0

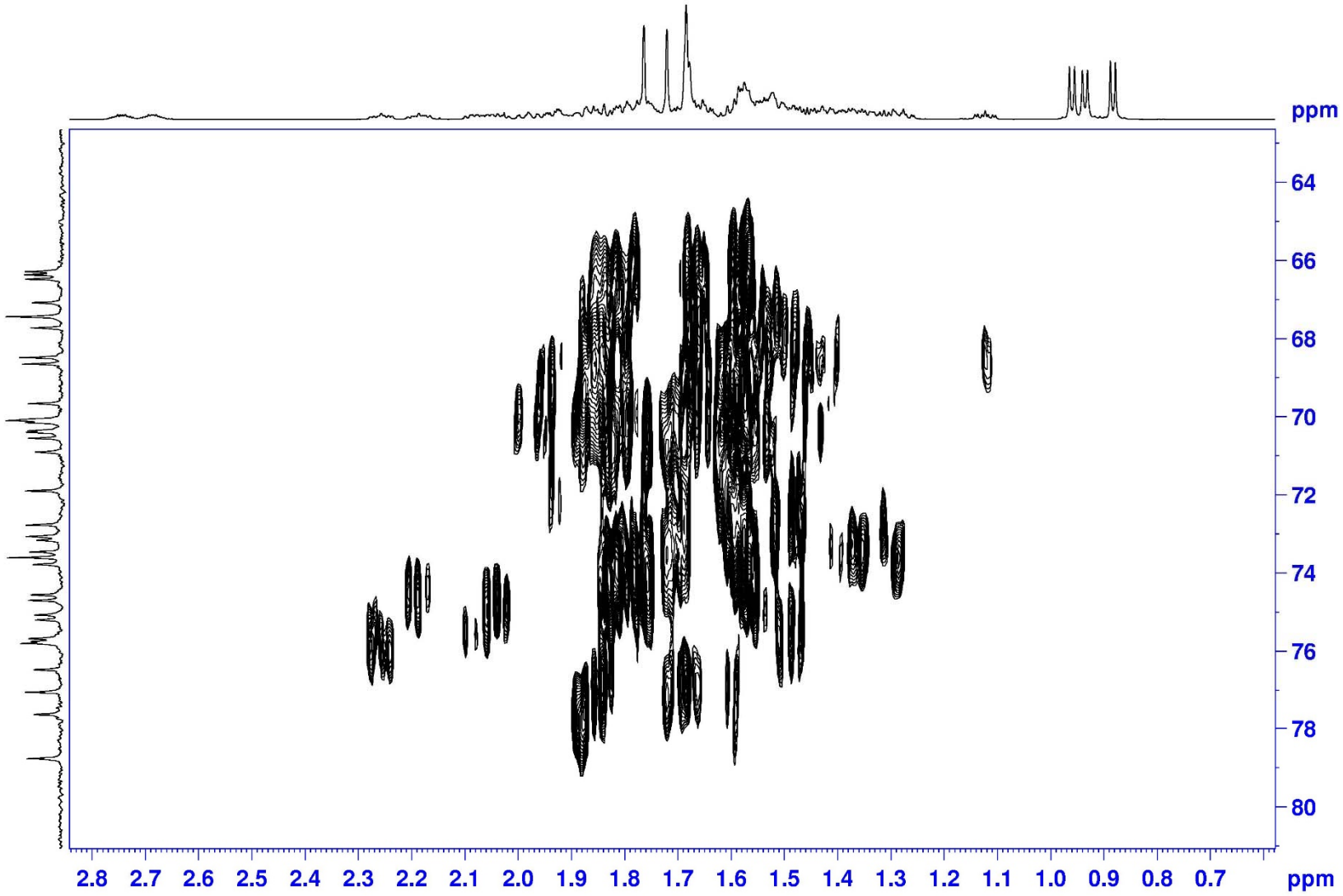
HMBC (700 MHz) spectrum of compound **1** in CD_3OD



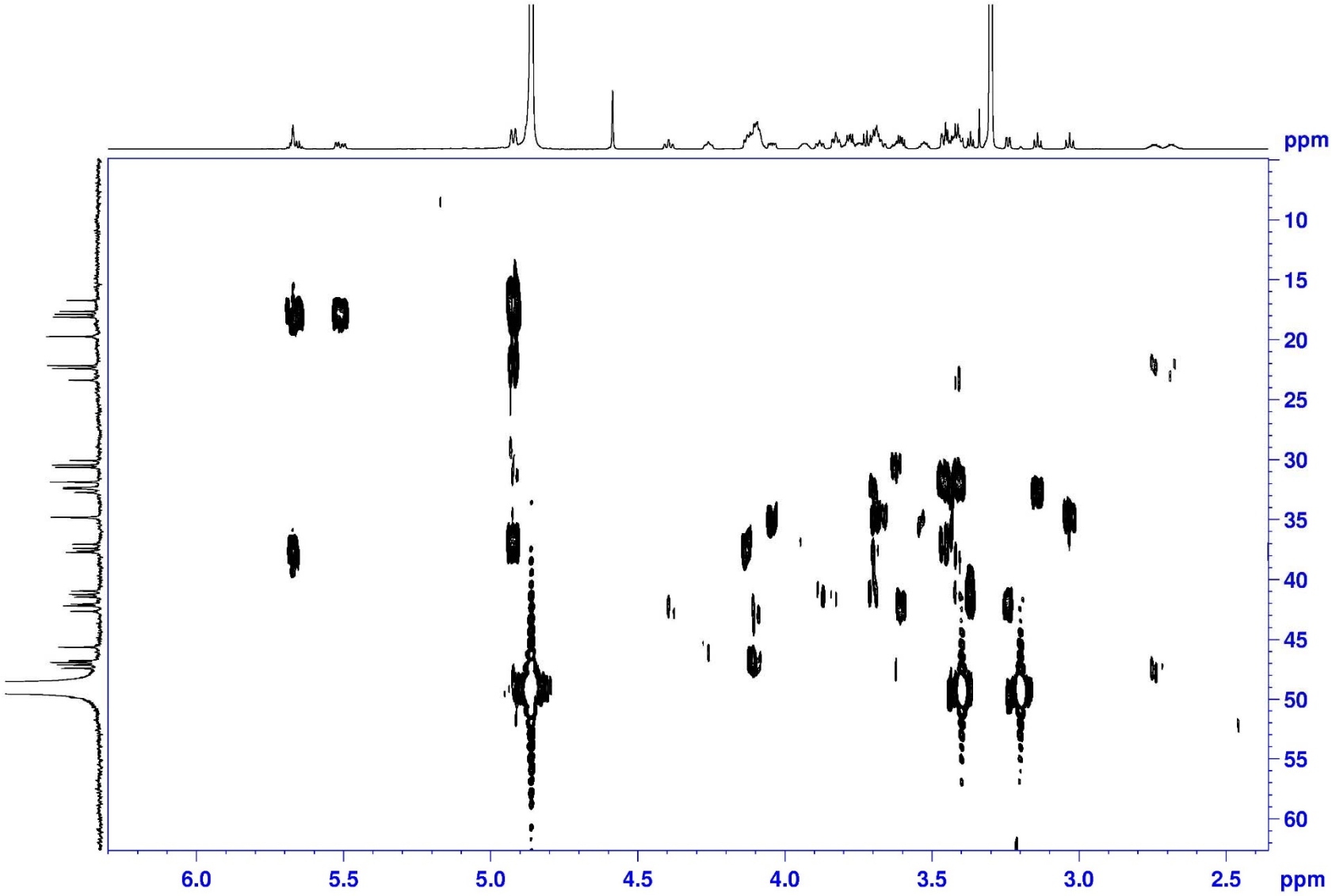
HMBC (700 MHz) spectrum of compound **1** in CD_3OD



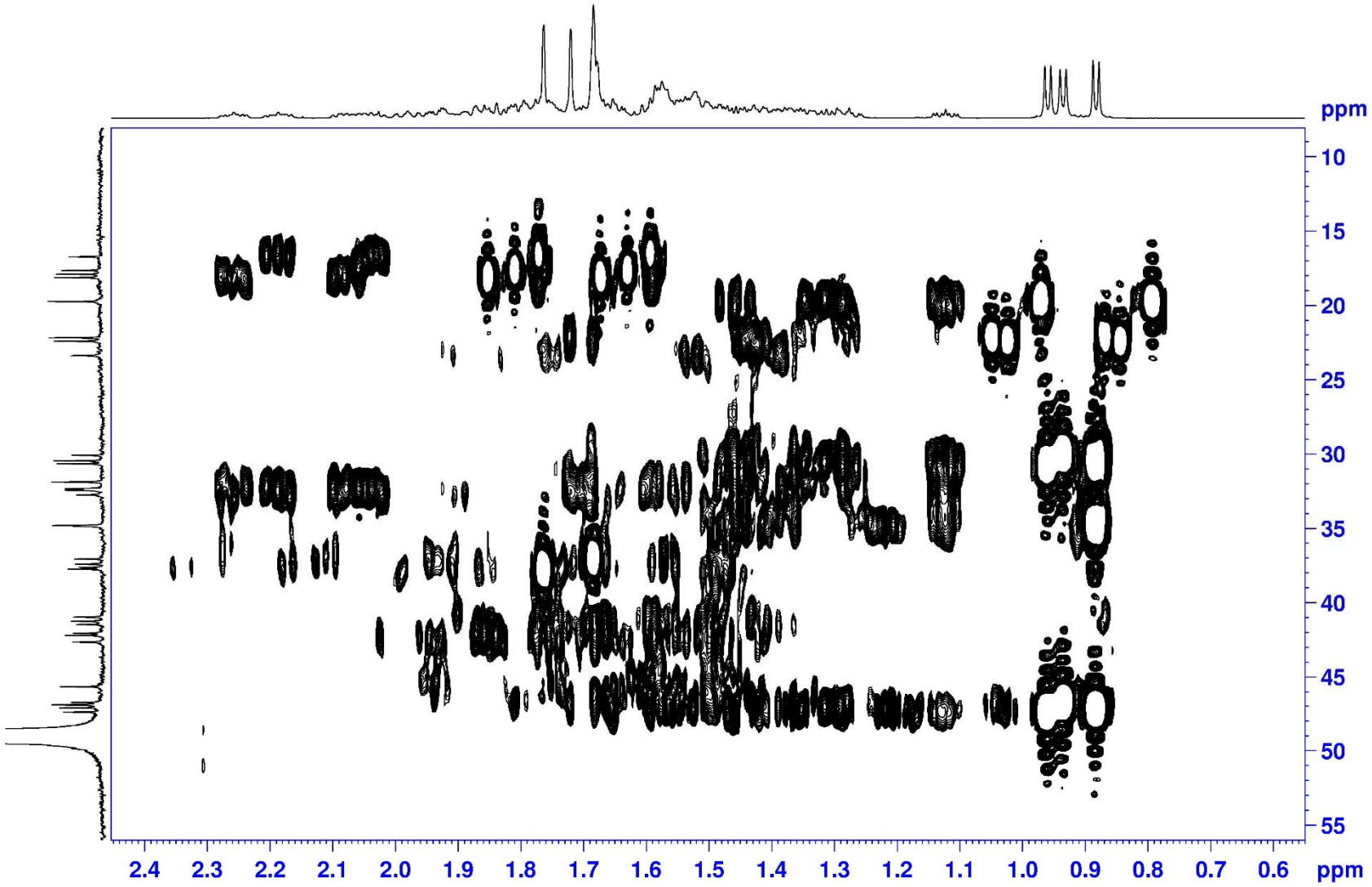
HMBC (700 MHz) spectrum of compound **1** in CD_3OD



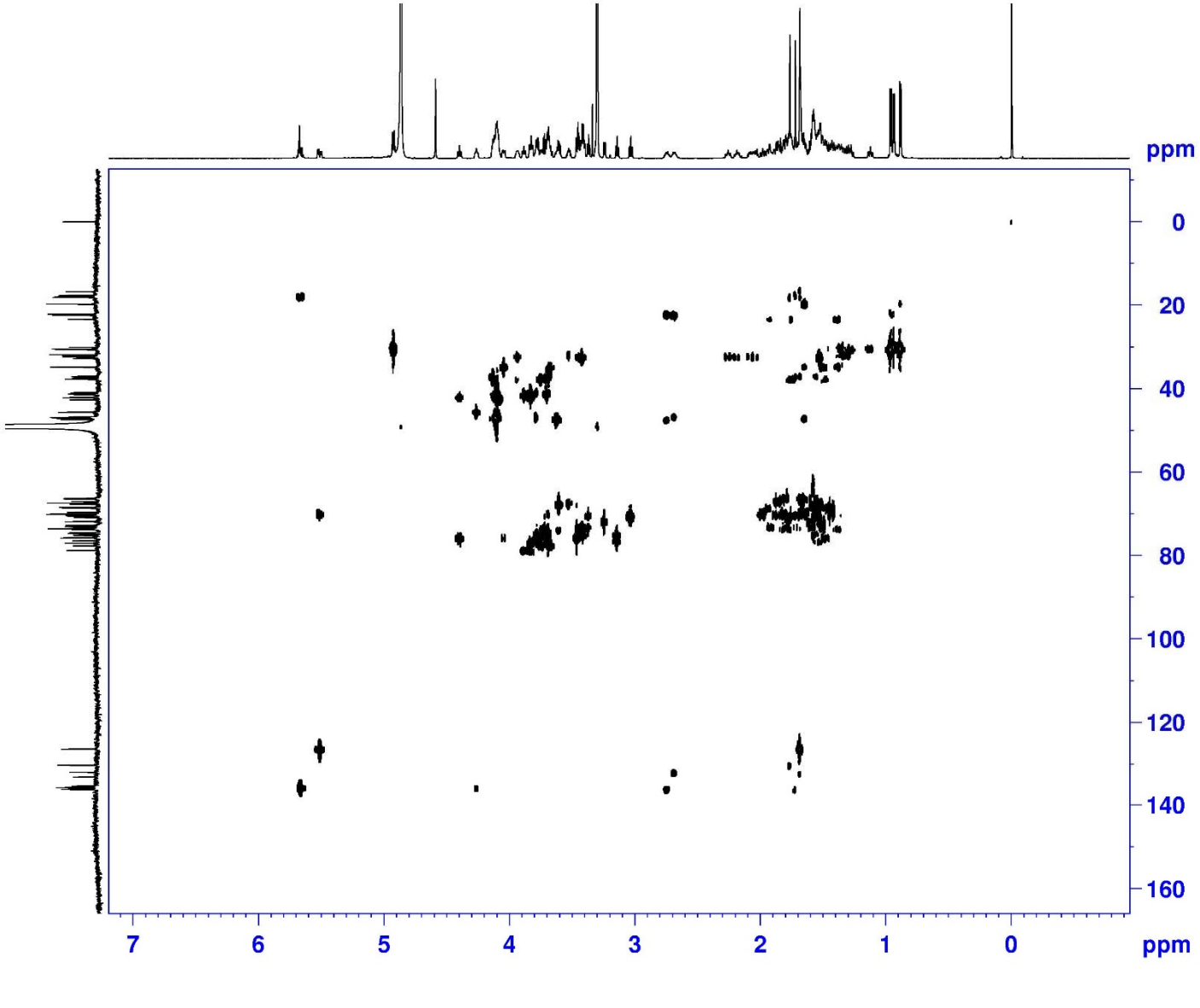
HMBC (700 MHz) spectrum of compound **1** in CD_3OD

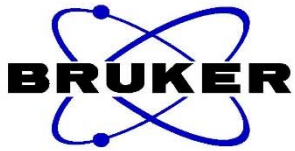


HMBC (700 MHz) spectrum of compound **1** in CD_3OD



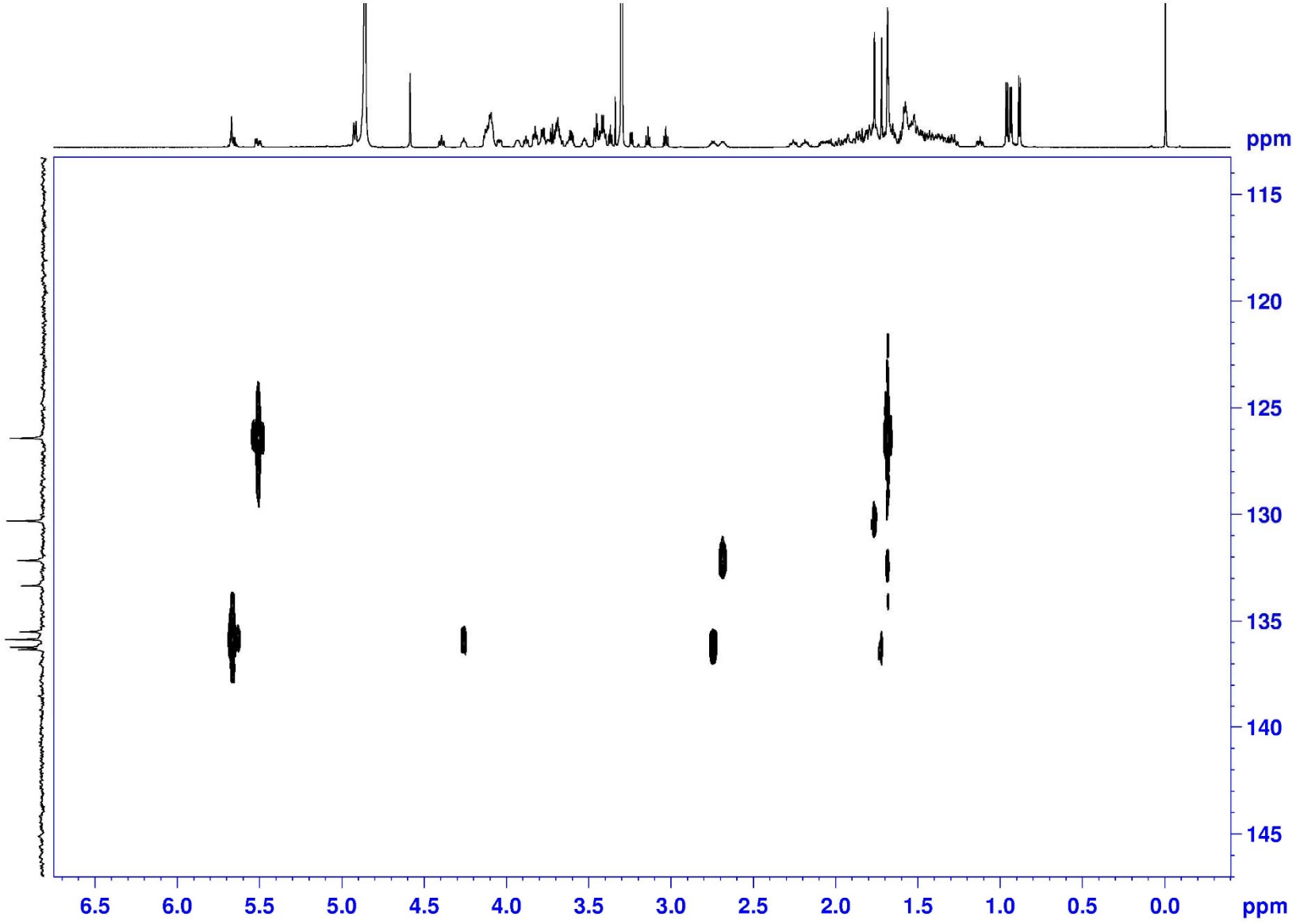
H2BC (700 MHz) spectrum of compound **1** in CD_3OD



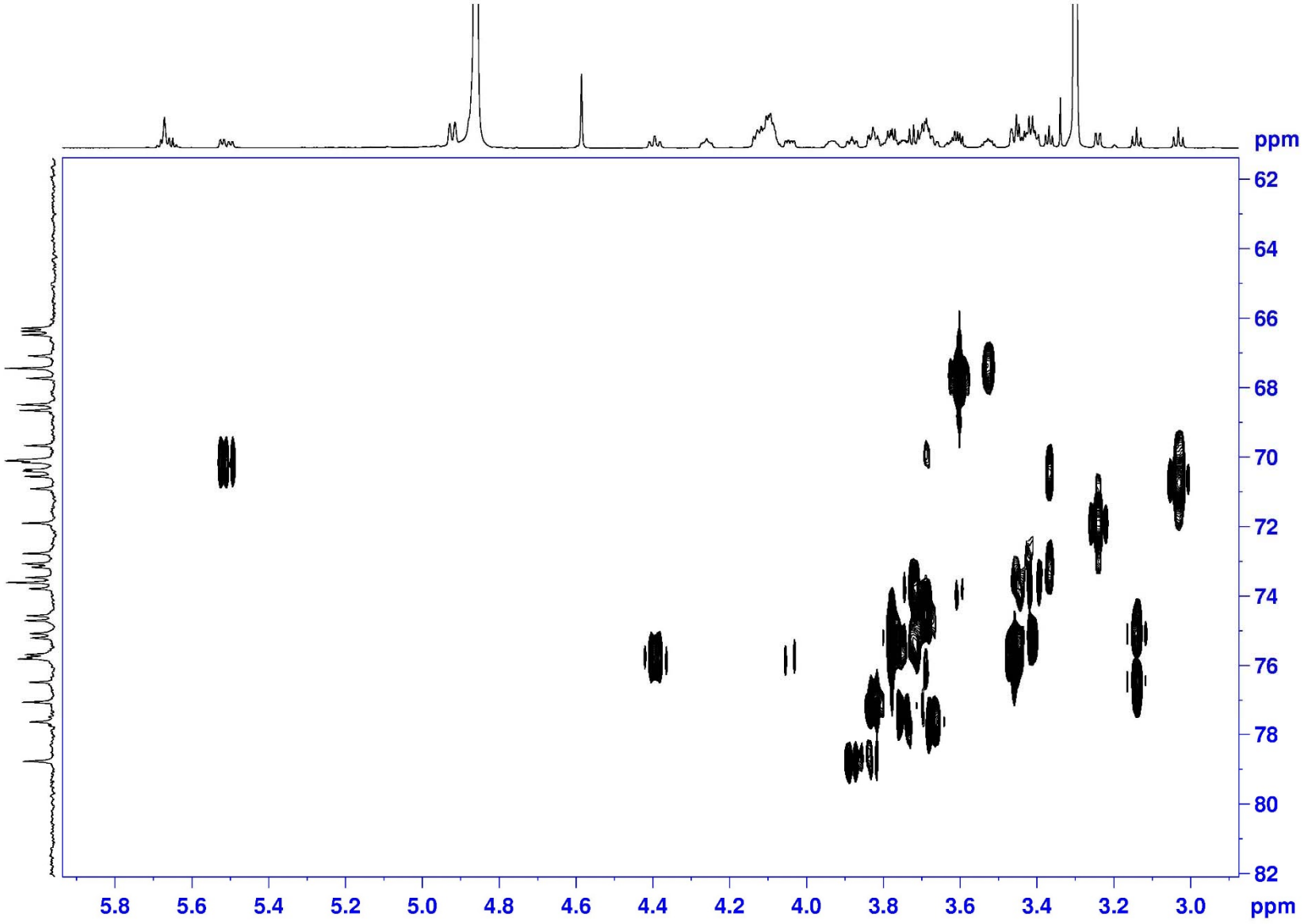


NAME	liwanshan-40-2-2
EXPNO	20
PROCNO	1
Date_	20190529
Time	11.06 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	h2bcetgpl3
TD	1024
SOLVENT	MeOD
NS	24
DS	16
SWH	5699.088 Hz
FIDRES	11.131032 Hz
AQ	0.0898889 se
RG	181.26
DW	87.733 us
DE	10.00 us
TE	298.0 K
CNST6	120.0000000
CNST7	170.0000000
D0	0.00000300 se
D1	1.50000000 se
D11	0.03000000 se
D16	0.00020000 se
D20	0.00211462 se
D21	0.02000000 se
D28	0.00653282 se
IN0	0.00001590 se
IN20	0.00001590 se
IN28	0.00001590 se
ND0	2
TD	256
SFO1	176.0739 MH
FIDRES	122.838051 Hz
SW	178.599 pp
FnMODE	Echo-Antiecho
SI	1024
SF	700.1800207 MH
WDW	SINE
SSB	4
LB	0.00 Hz
GB	0
PC	1.40
SI	8192
MC2	echo-antiecho
SF	176.0601526 MH
WDW	SINE
SSB	2

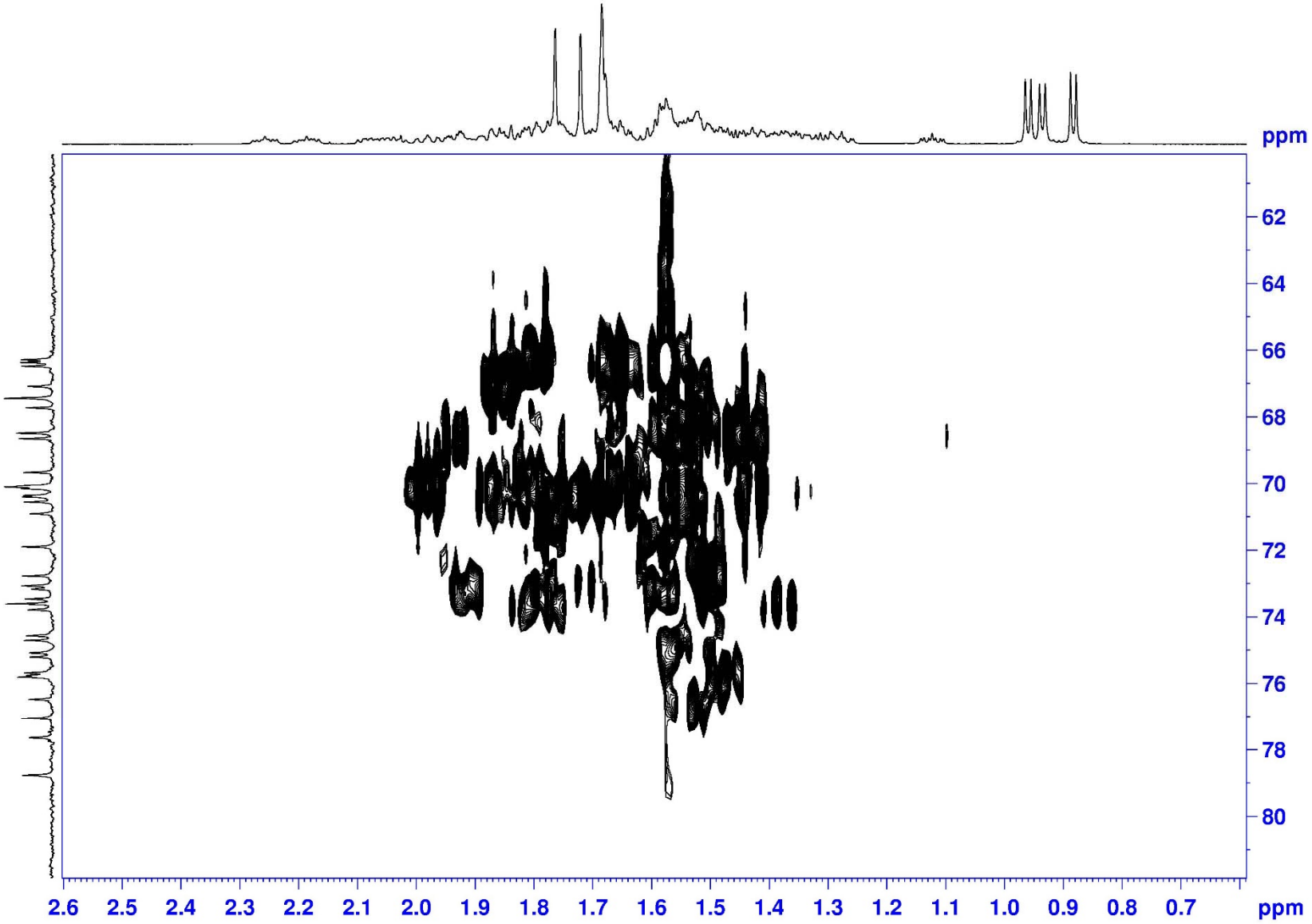
H2BC (700 MHz) spectrum of compound **1** in CD_3OD



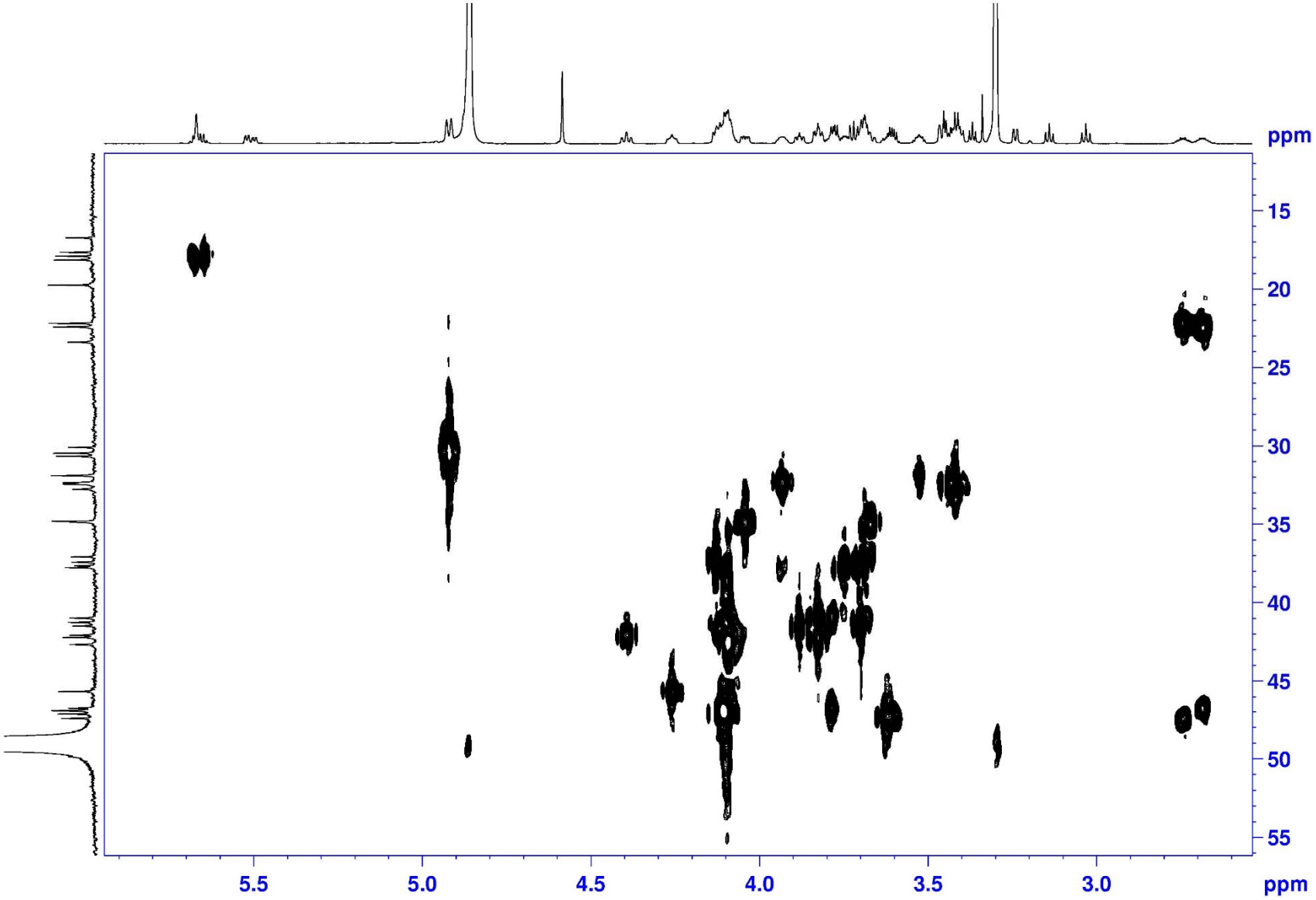
H2BC (700 MHz) spectrum of compound **1** in CD_3OD



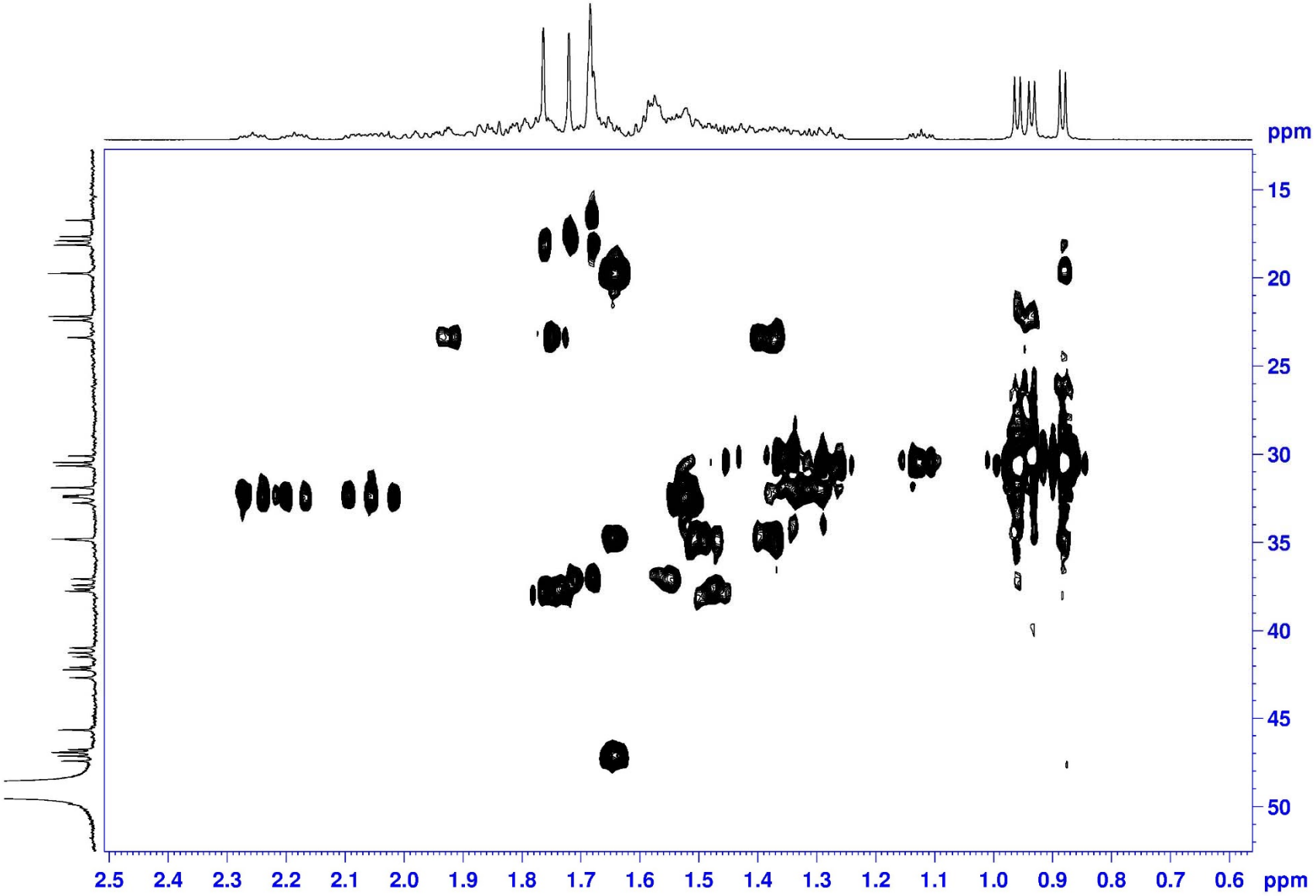
H2BC (700 MHz) spectrum of compound **1** in CD_3OD



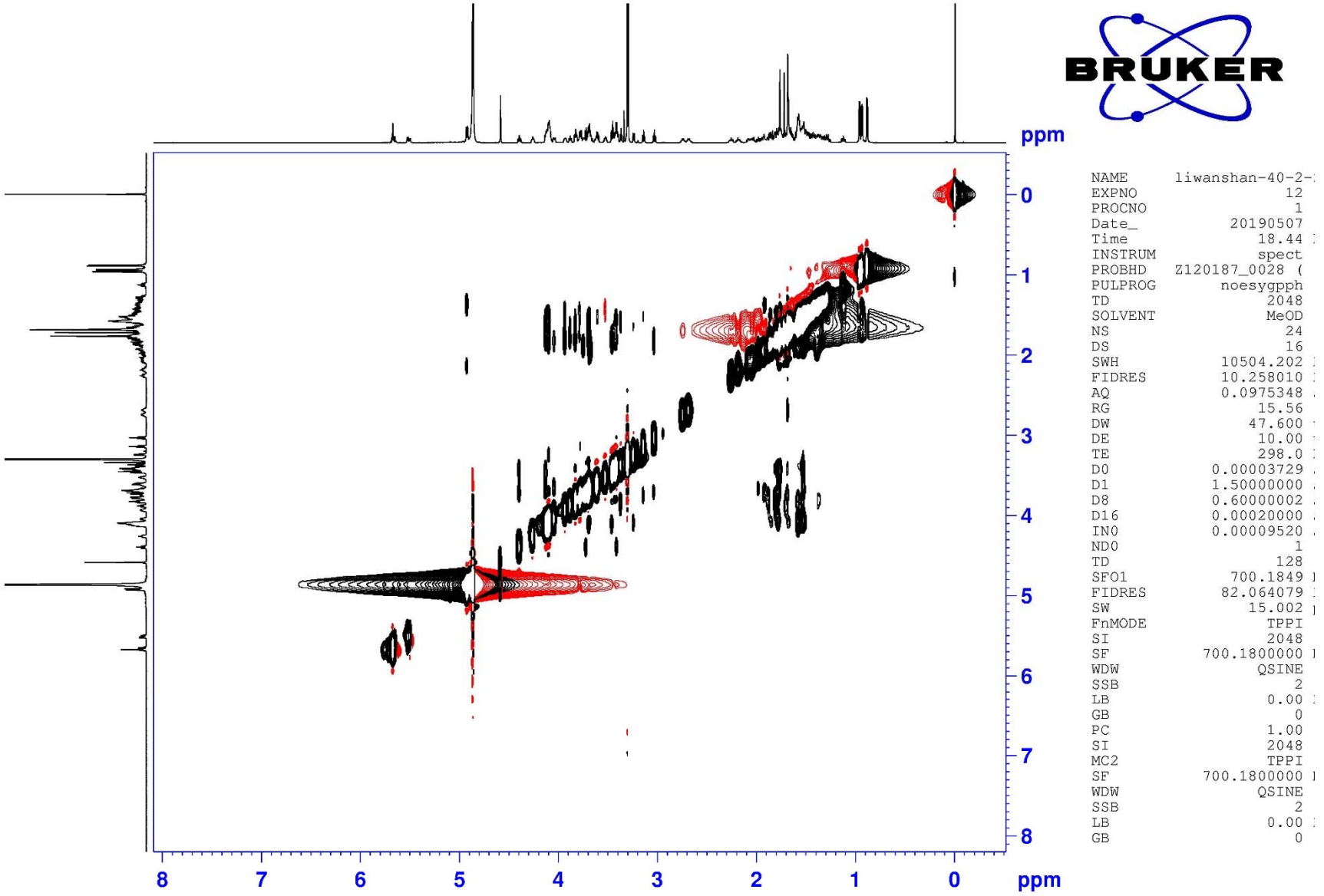
H2BC (700 MHz) spectrum of compound **1** in CD_3OD



H2BC (700 MHz) spectrum of compound **1** in CD_3OD

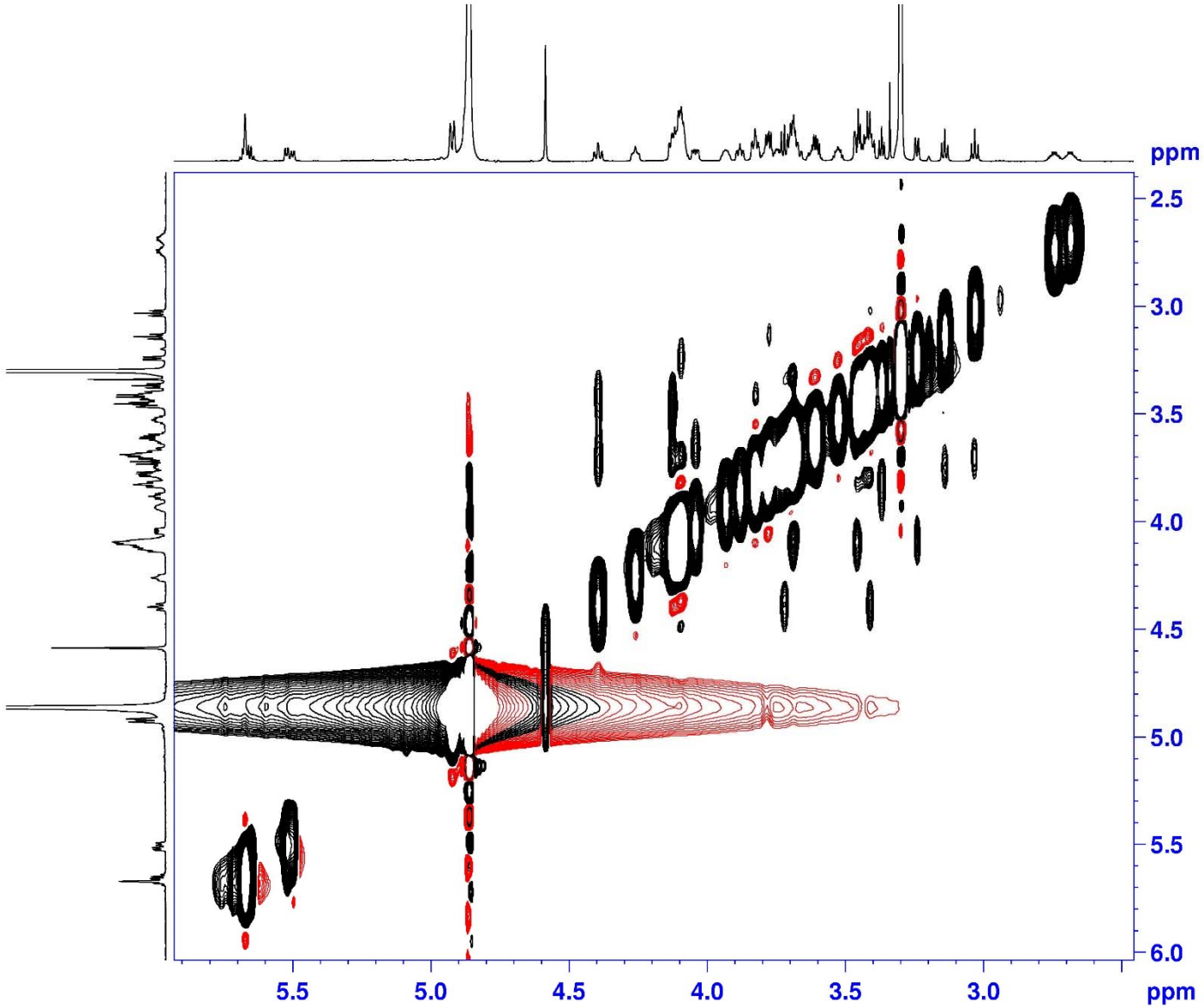


NOESY (700 MHz) spectrum of compound **1** in CD_3OD

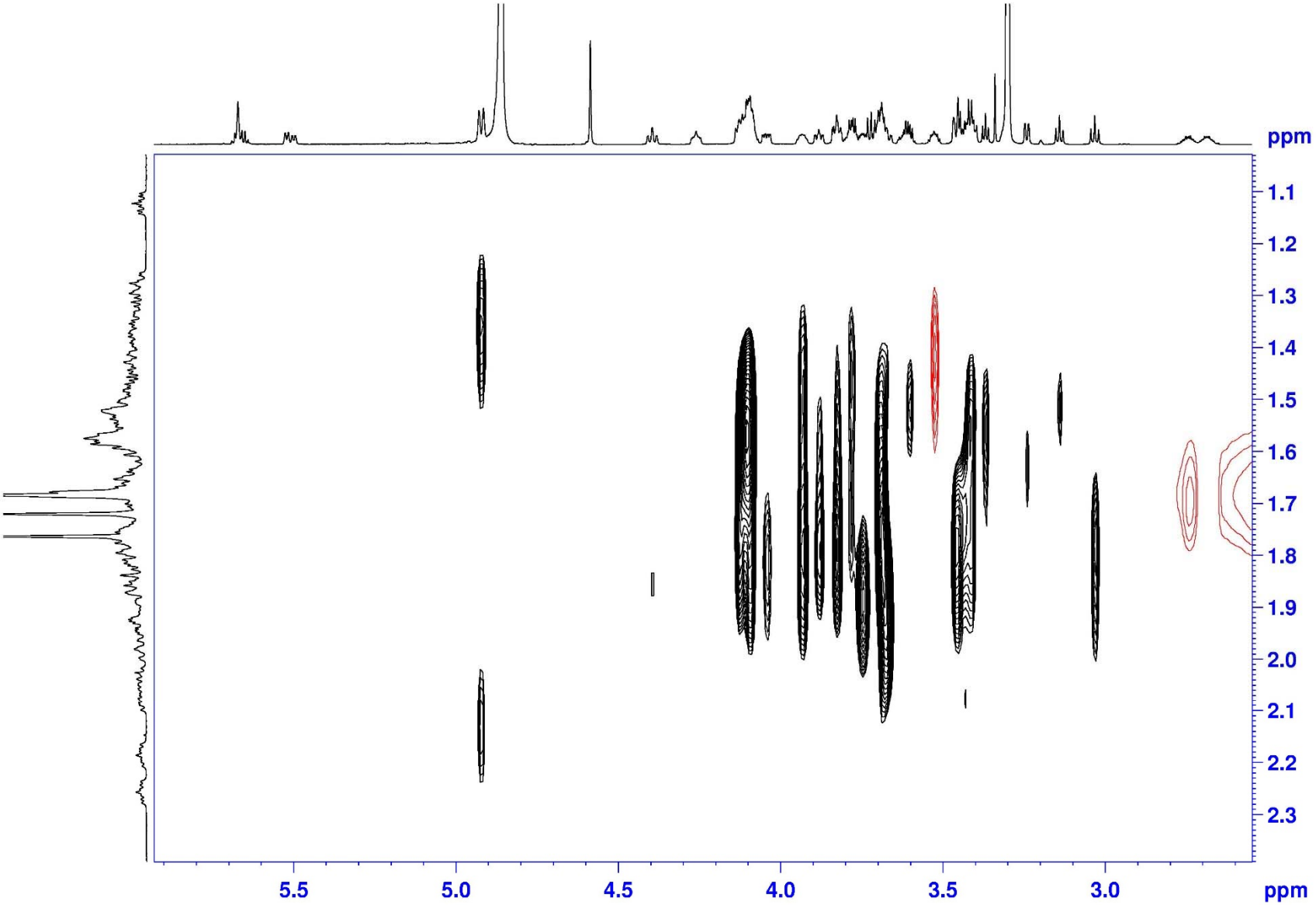


NAME	liwanshan-40-2-
EXPNO	12
PROCNO	1
Date_	20190507
Time	18.44
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	noesygpph
TD	2048
SOLVENT	MeOD
NS	24
DS	16
SWH	10504.202
FIDRES	10.258010
AQ	0.0975348
RG	15.56
DW	47.600
DE	10.00
TE	298.0
D0	0.00003729
D1	1.50000000
D8	0.60000002
D16	0.00020000
IN0	0.00009520
ND0	1
TD	128
SFO1	700.1849
FIDRES	82.064079
SW	15.002
FnMODE	TPPI
SI	2048
SF	700.1800000
WDW	QSINE
SSB	2
LB	0.00
GB	0
PC	1.00
SI	2048
MC2	TPPI
SF	700.1800000
WDW	QSINE
SSB	2
LB	0.00
GB	0

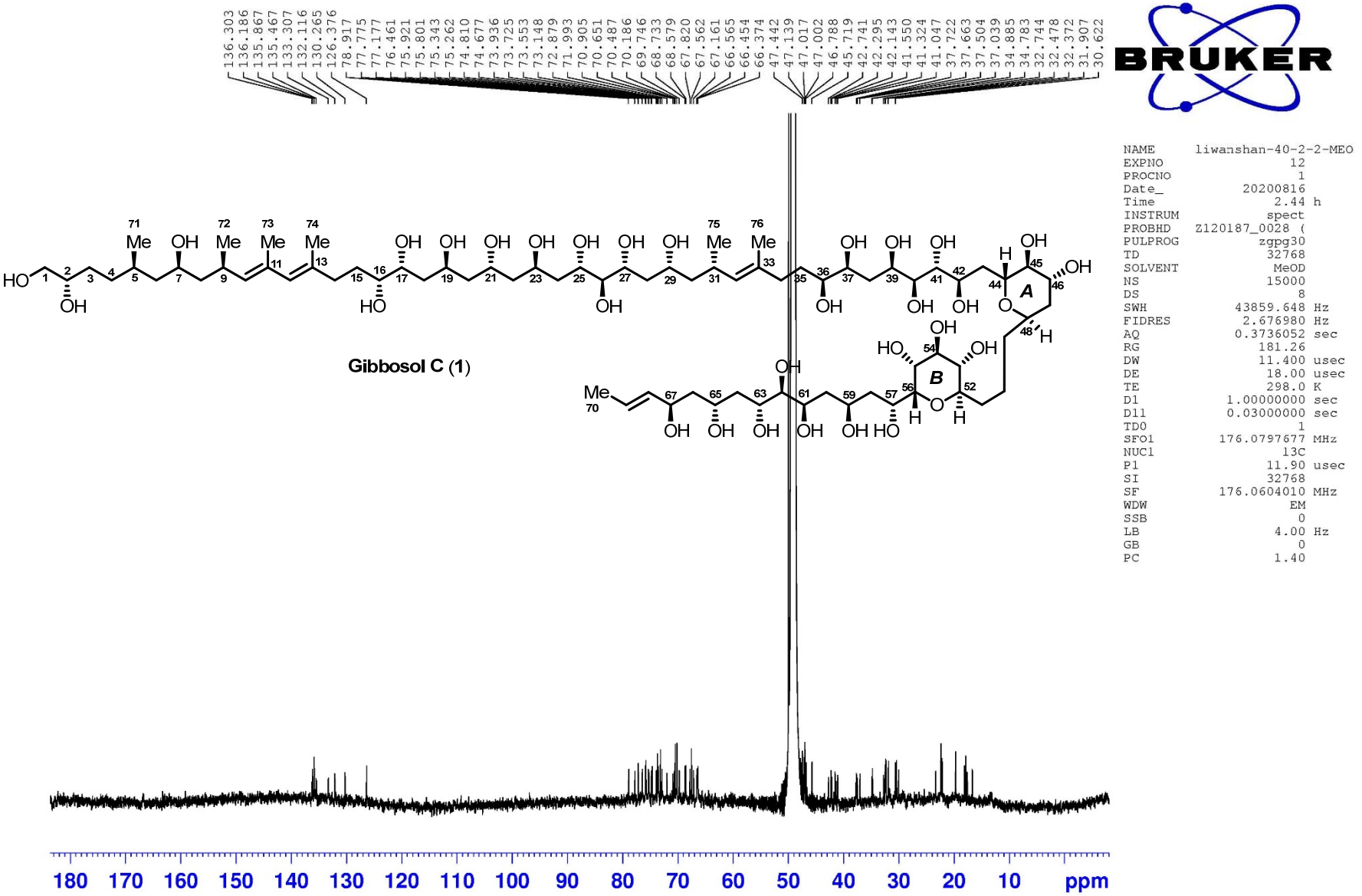
NOESY (700 MHz) spectrum of compound **1** in CD_3OD



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

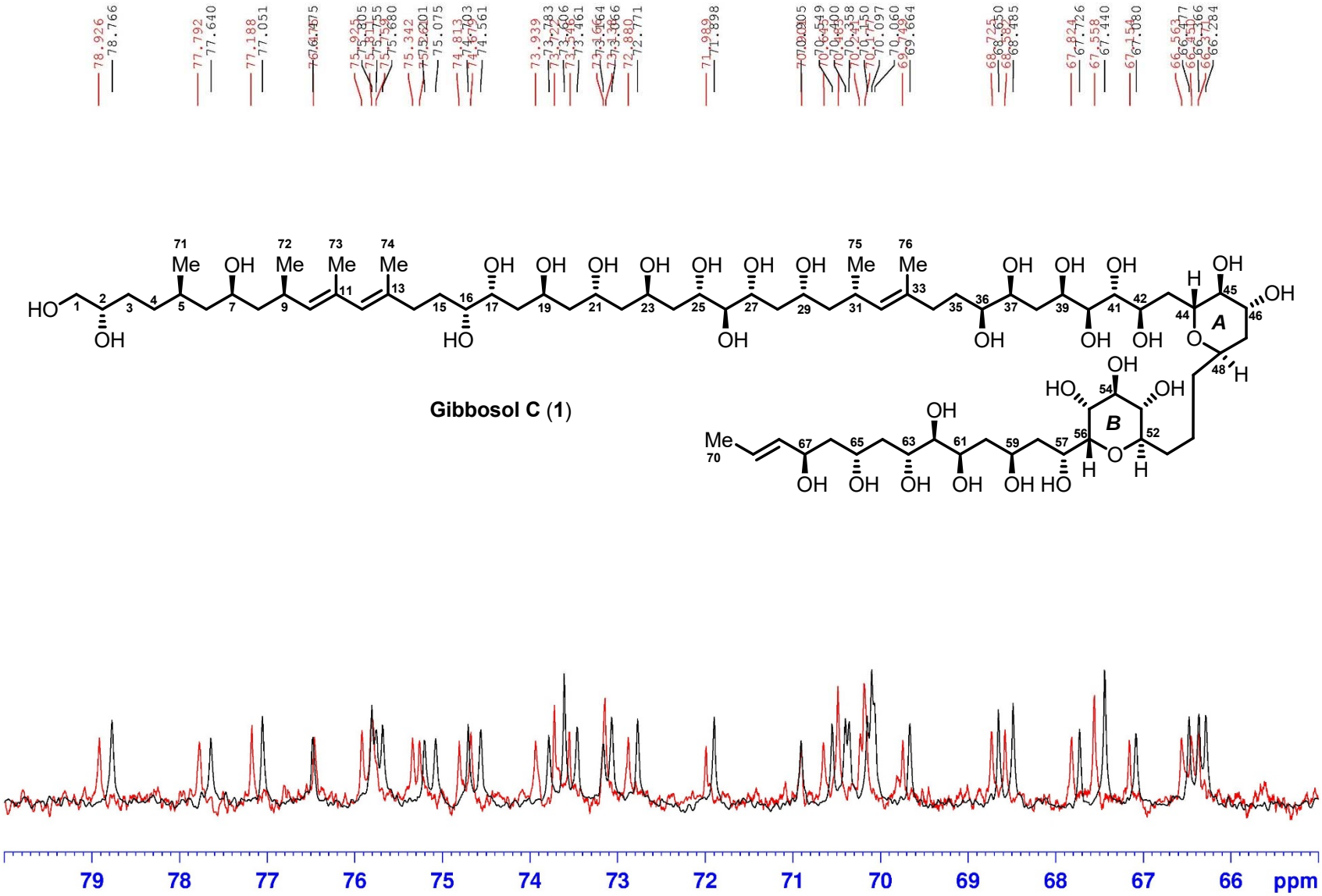


^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OH

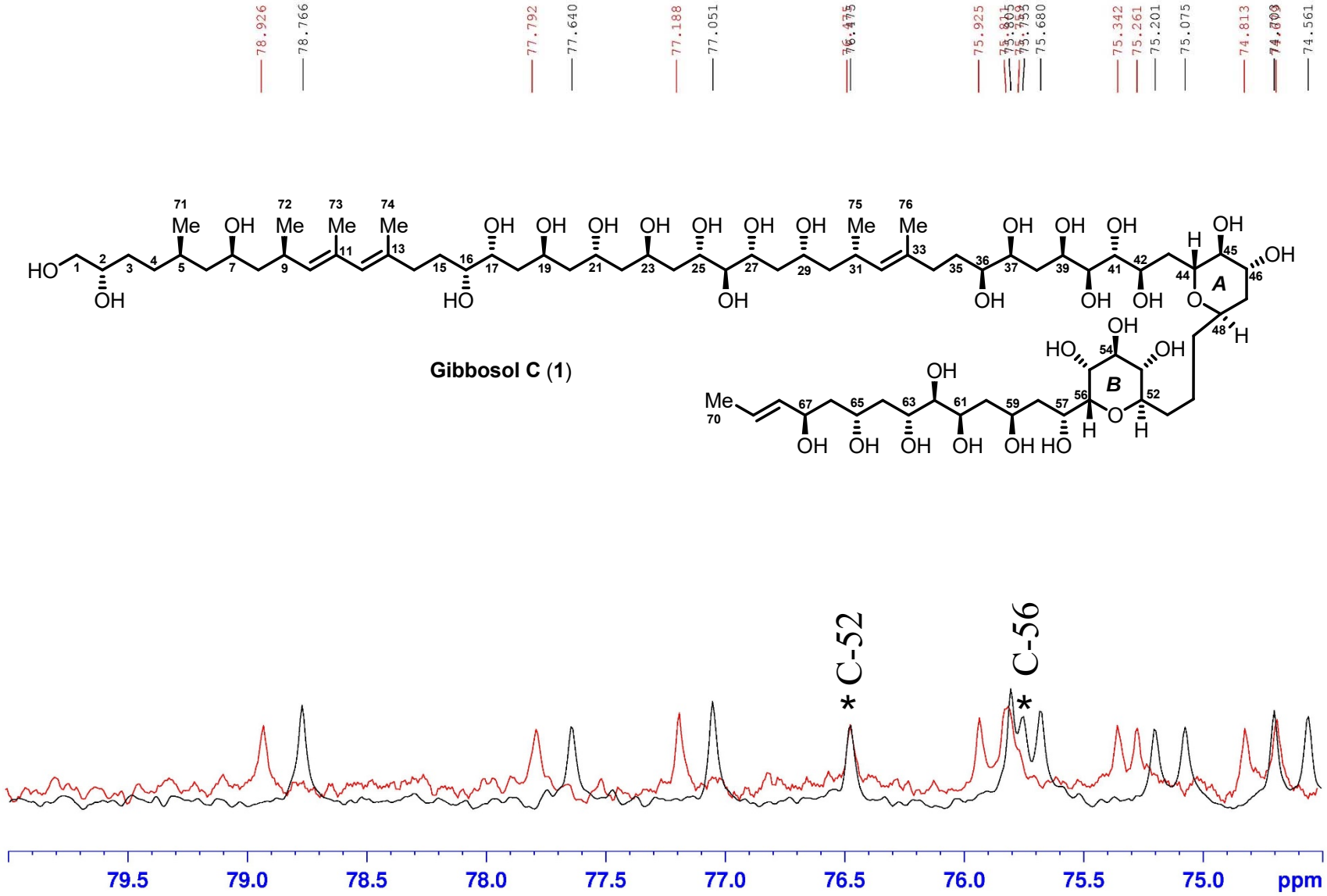


NAME	liwanshan-40-2-2-MEO
EXPNO	12
PROCNO	1
Date_	20200816
Time	2.44 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	zgpg30
TD	32768
SOLVENT	MeOD
NS	15000
DS	8
SWH	43859.648 Hz
FIDRES	2.676980 Hz
AQ	0.3736052 sec
RG	181.26
DW	11.400 usec
DE	18.00 usec
TE	298.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	176.0797677 MHz
NUC1	13C
P1	11.90 usec
SI	32768
SF	176.0604010 MHz
WDW	EM
SSB	0
LB	4.00 Hz
GB	0
PC	1.40

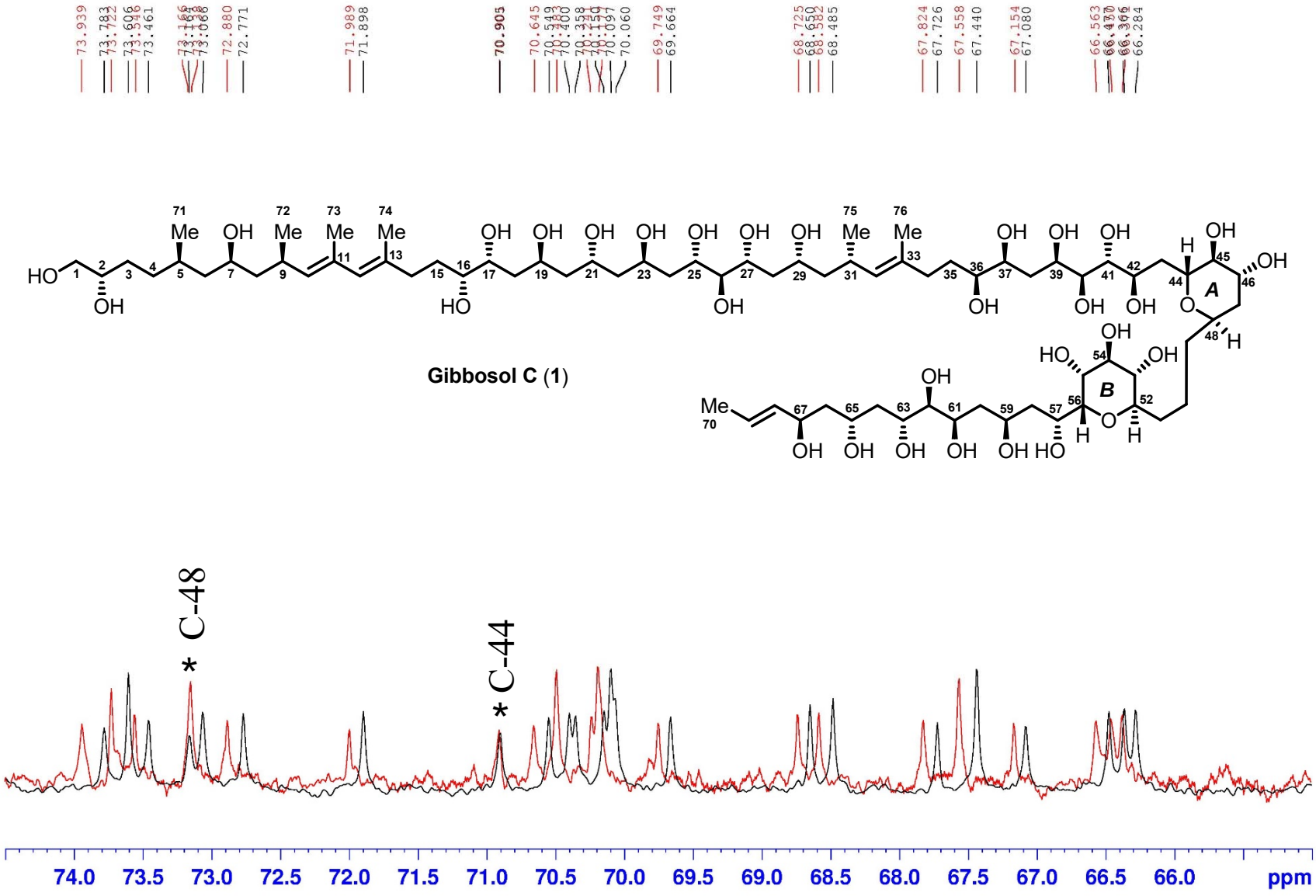
Comparison of ^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OH with that in CD_3OD



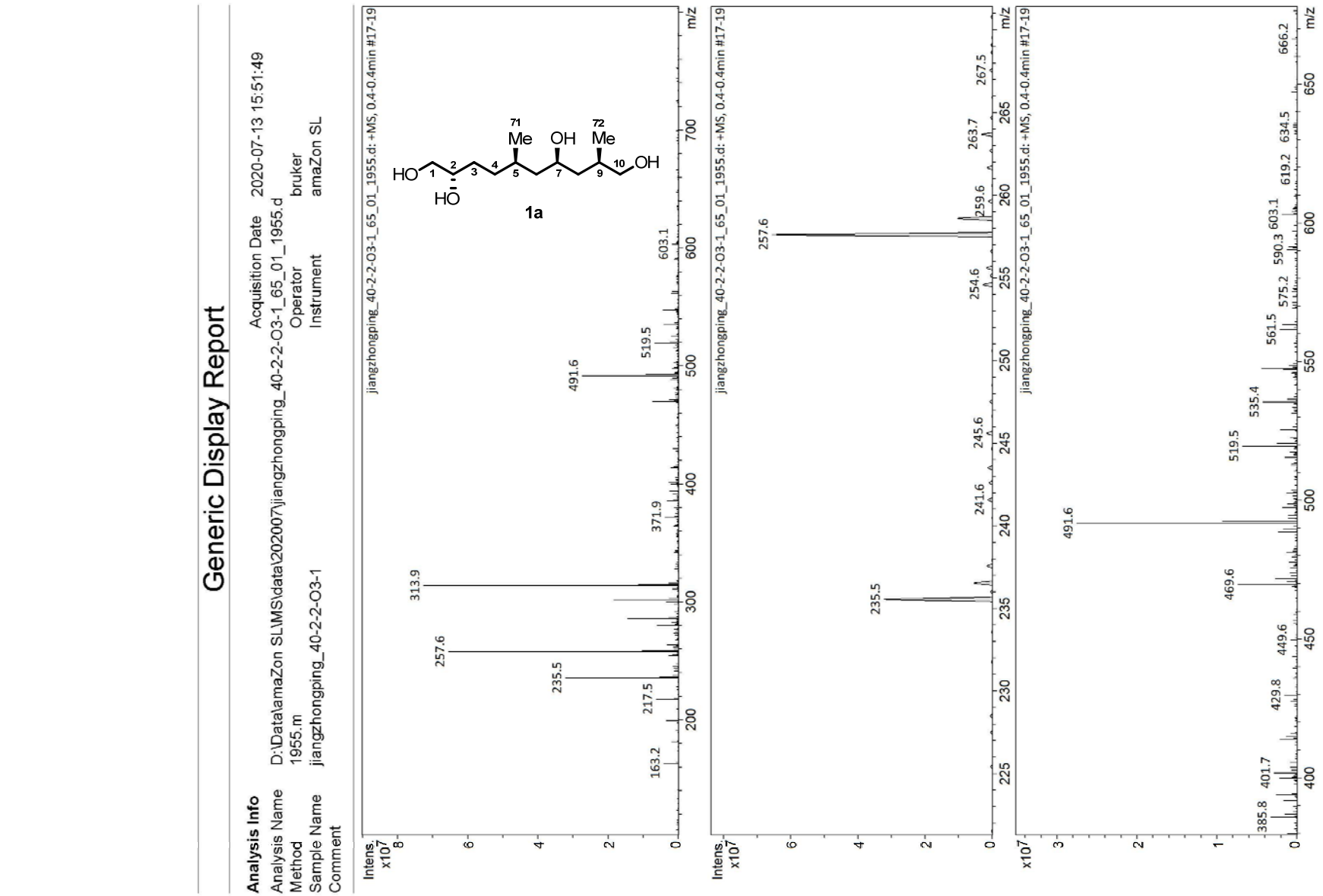
Comparison of ^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OH with that in CD_3OD



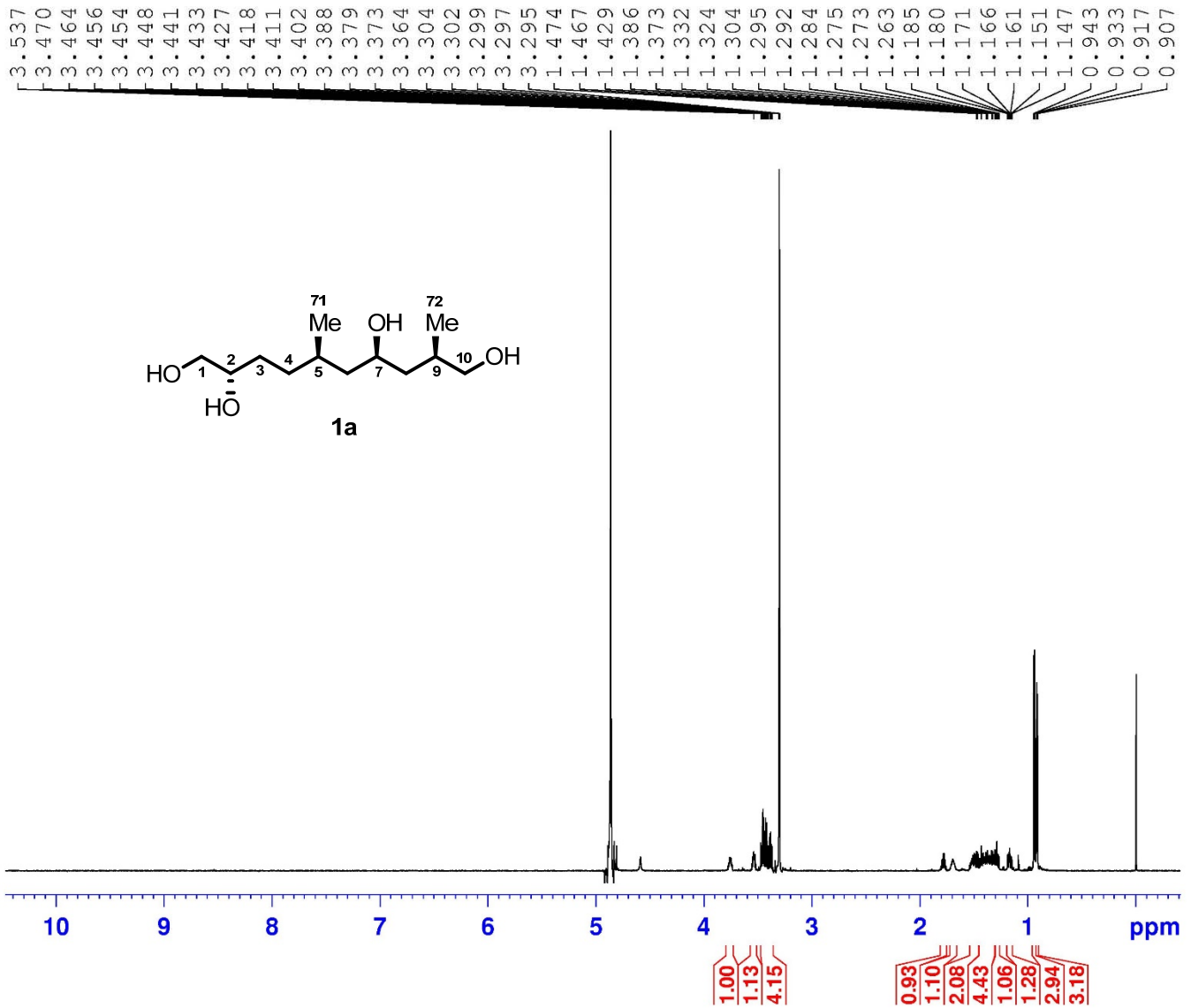
Comparison of ^{13}C (175 MHz) NMR spectrum of compound **1** in CD_3OH with that in CD_3OD

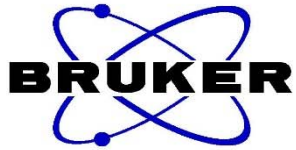


LR-ESI-MS for the fragment **1a**



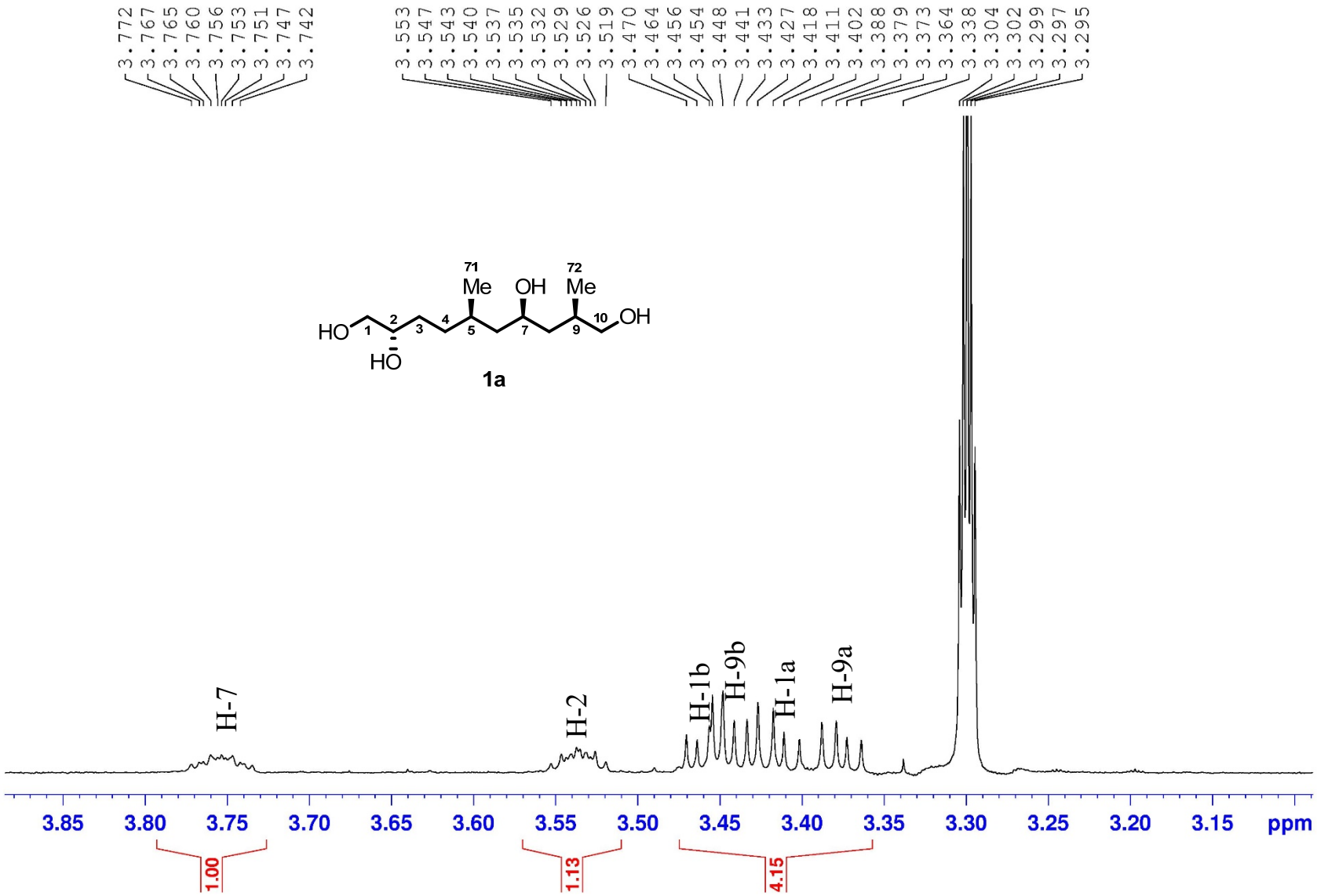
^{1}H (700 MHz) NMR spectrum of the fragment **1a** in CD_3OD



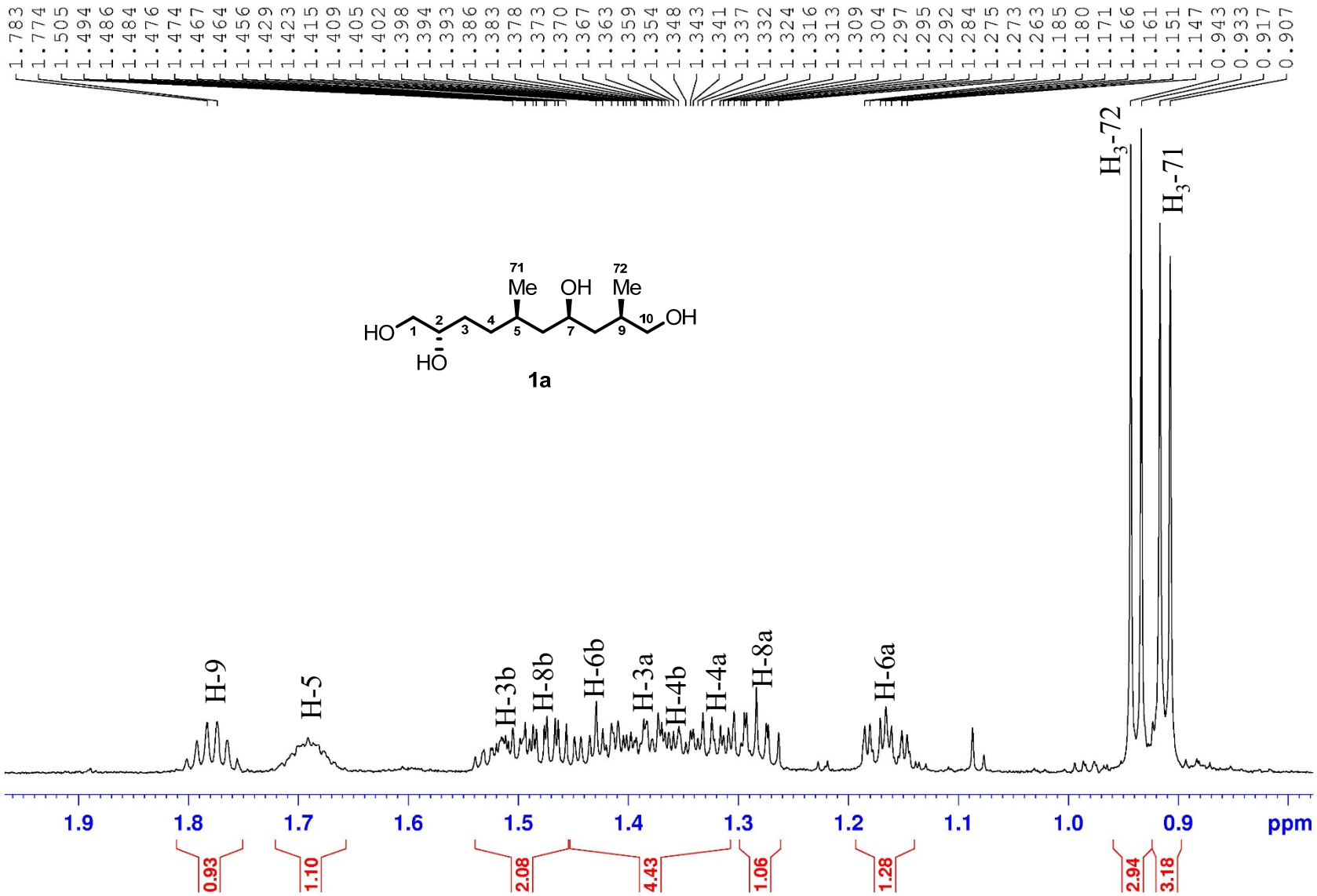


NAME	liwanshan-40-2-2-03-
EXPNO	12
PROCNO	1
Date_	20200306
Time	18.28 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	3
DS	2
SWH	14097.744 Hz
FIDRES	0.430229 Hz
AQ	2.3243935 sec
RG	3.96
DW	35.467 usec
DE	10.00 usec
TE	298.0 K
D1	1.50000000 sec
TD0	1
SFO1	700.1843236 MHz
NUC1	1H
P1	8.10 usec
SI	65536
SF	700.1800209 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

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



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

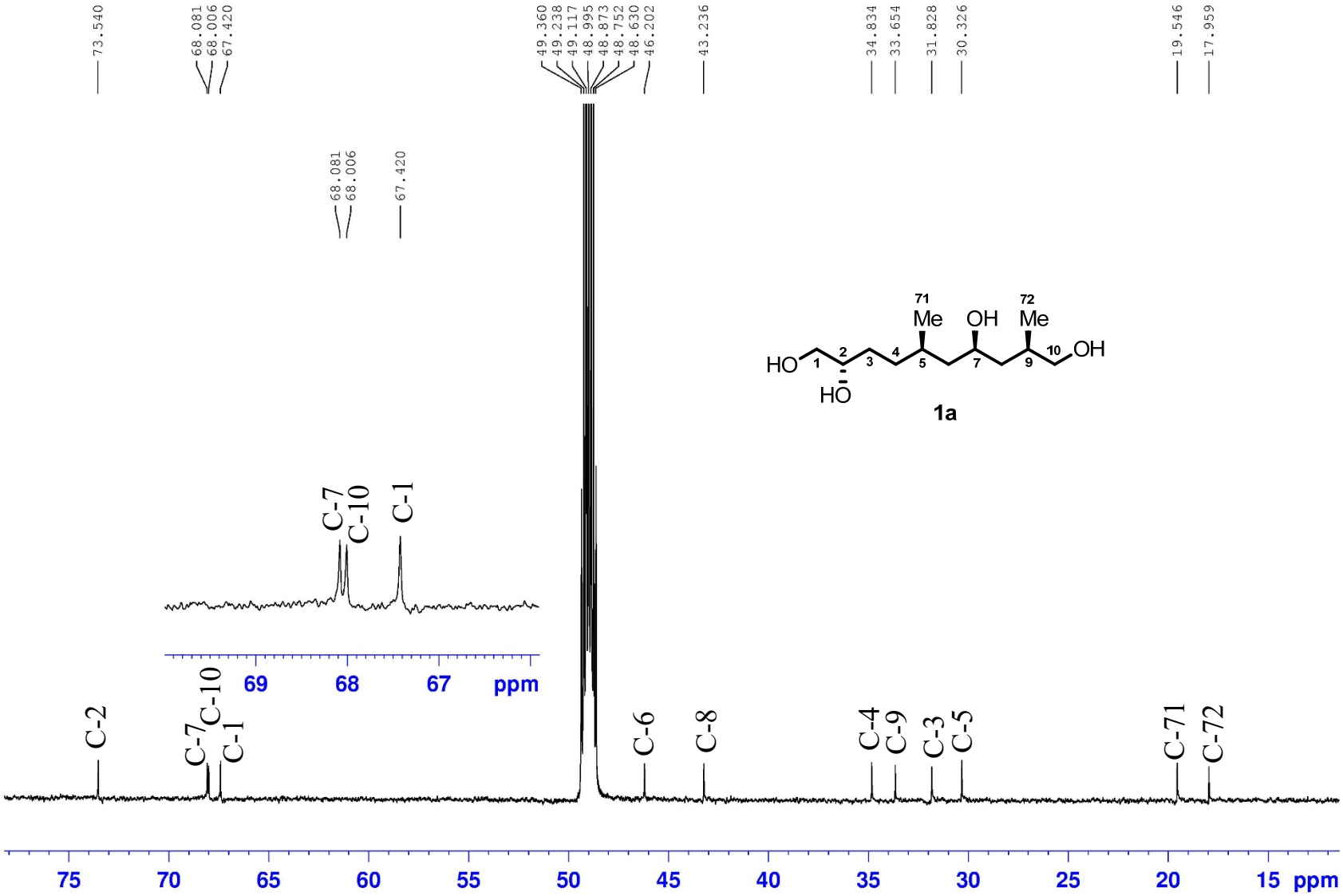


^{13}C (175 MHz) NMR spectrum of the fragment **1a** in CD_3OD

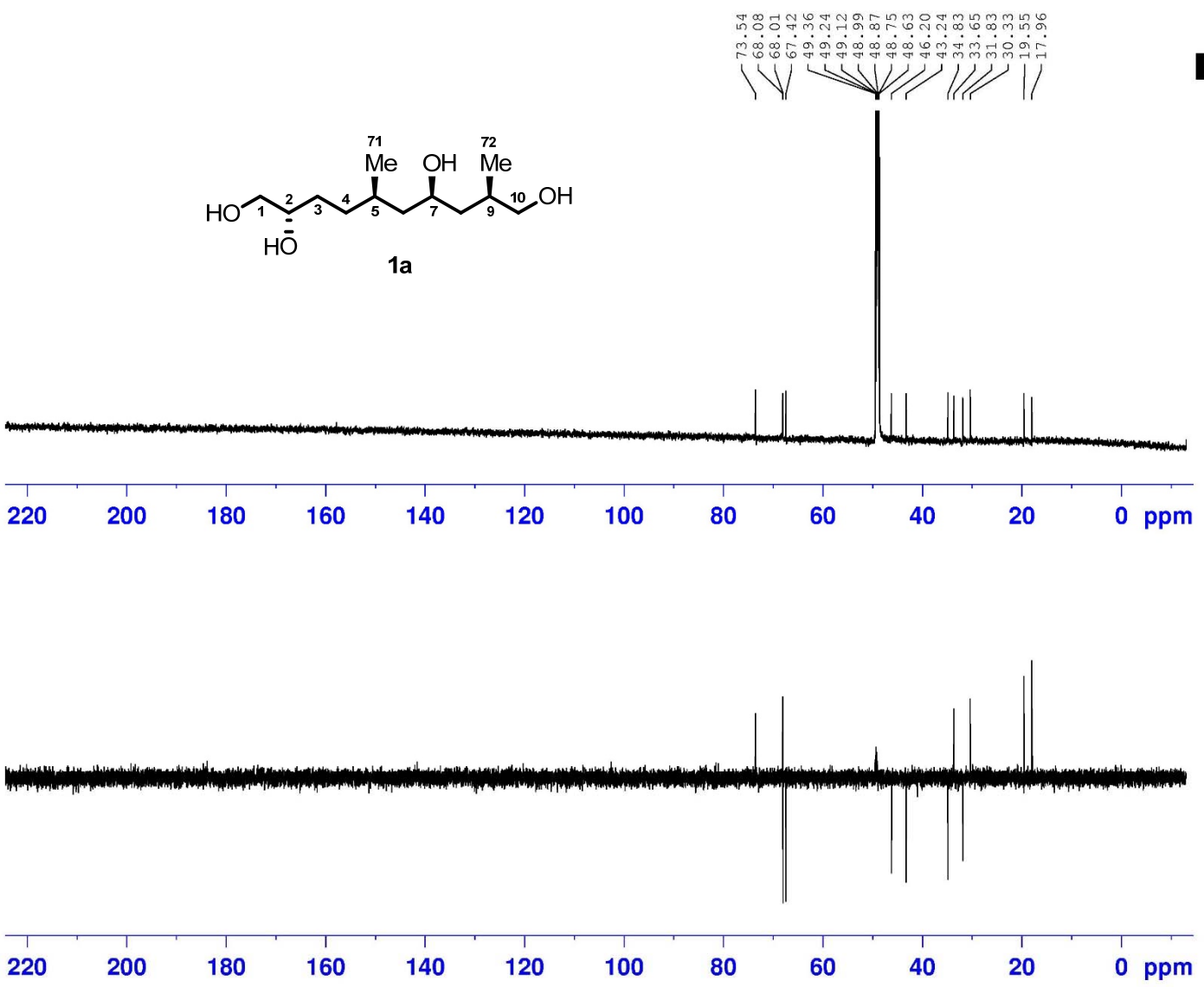
BRUKER

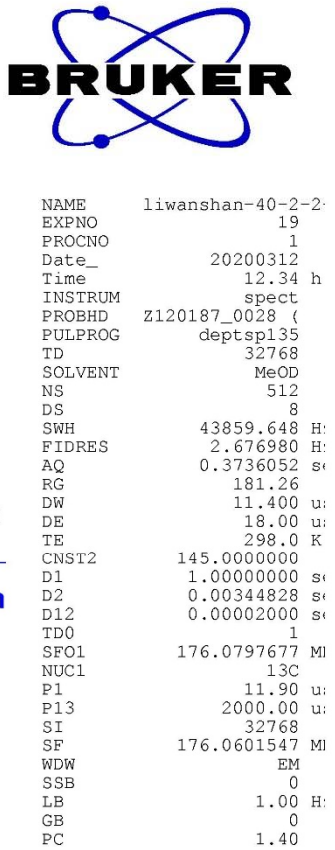
NAME	liwanshan-40-2-2-O
EXPNO	14
PROCNO	1
Date_	20200306
Time	22.40 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	zgpg30
TD	32768
SOLVENT	MeOD
NS	8000
DS	8
SWH	43859.648 Hz
FIDRES	2.676980 Hz
AQ	0.3736052 sec
RG	181.26
DW	11.400 use
DE	18.00 use
TE	298.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	176.0797677 MHz
NUC1	13C
P1	11.90 use
SI	32768
SF	176.0601541 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

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

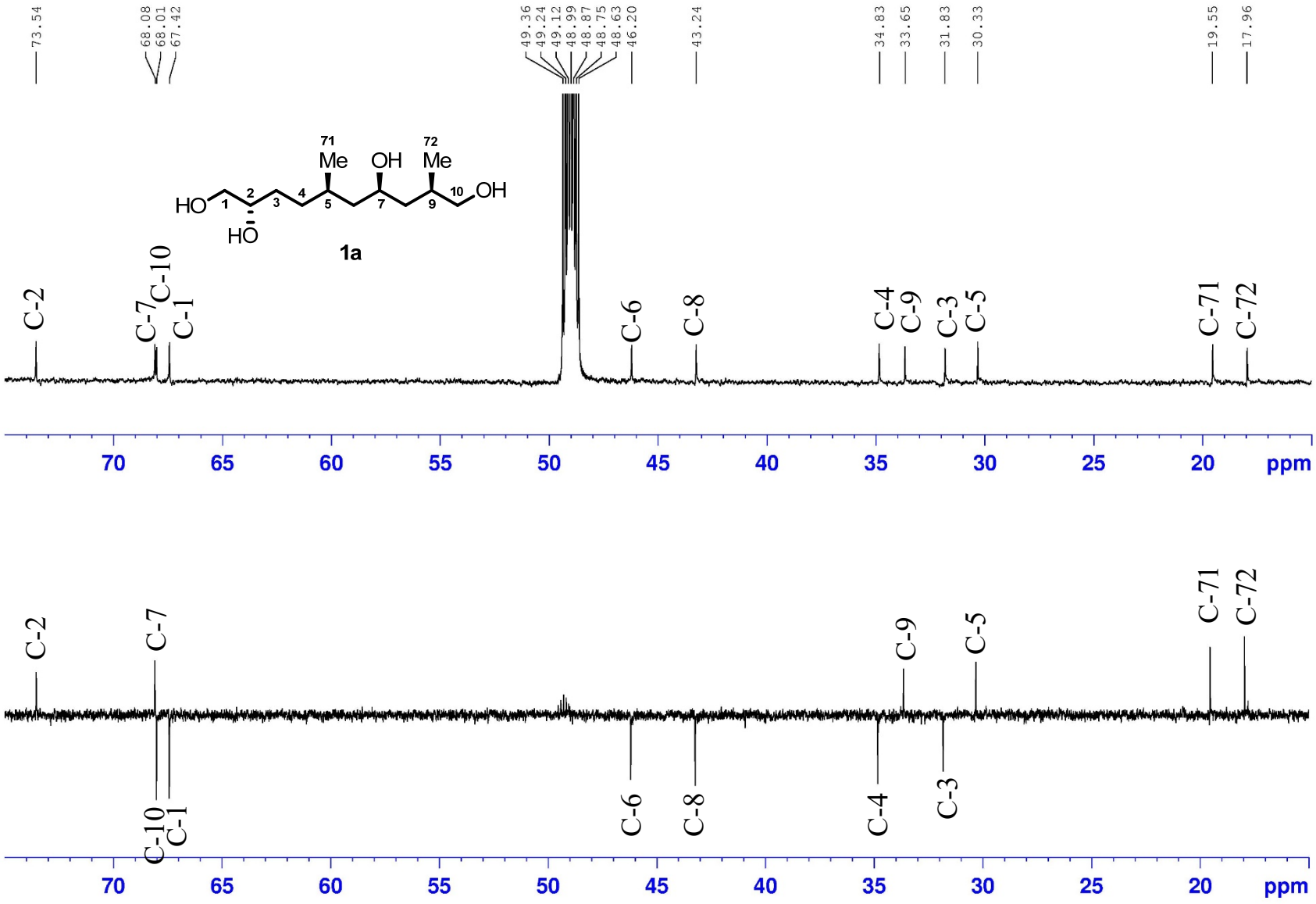


DEPT135 (175 MHz) spectrum of the fragment **1a** in CD_3OD

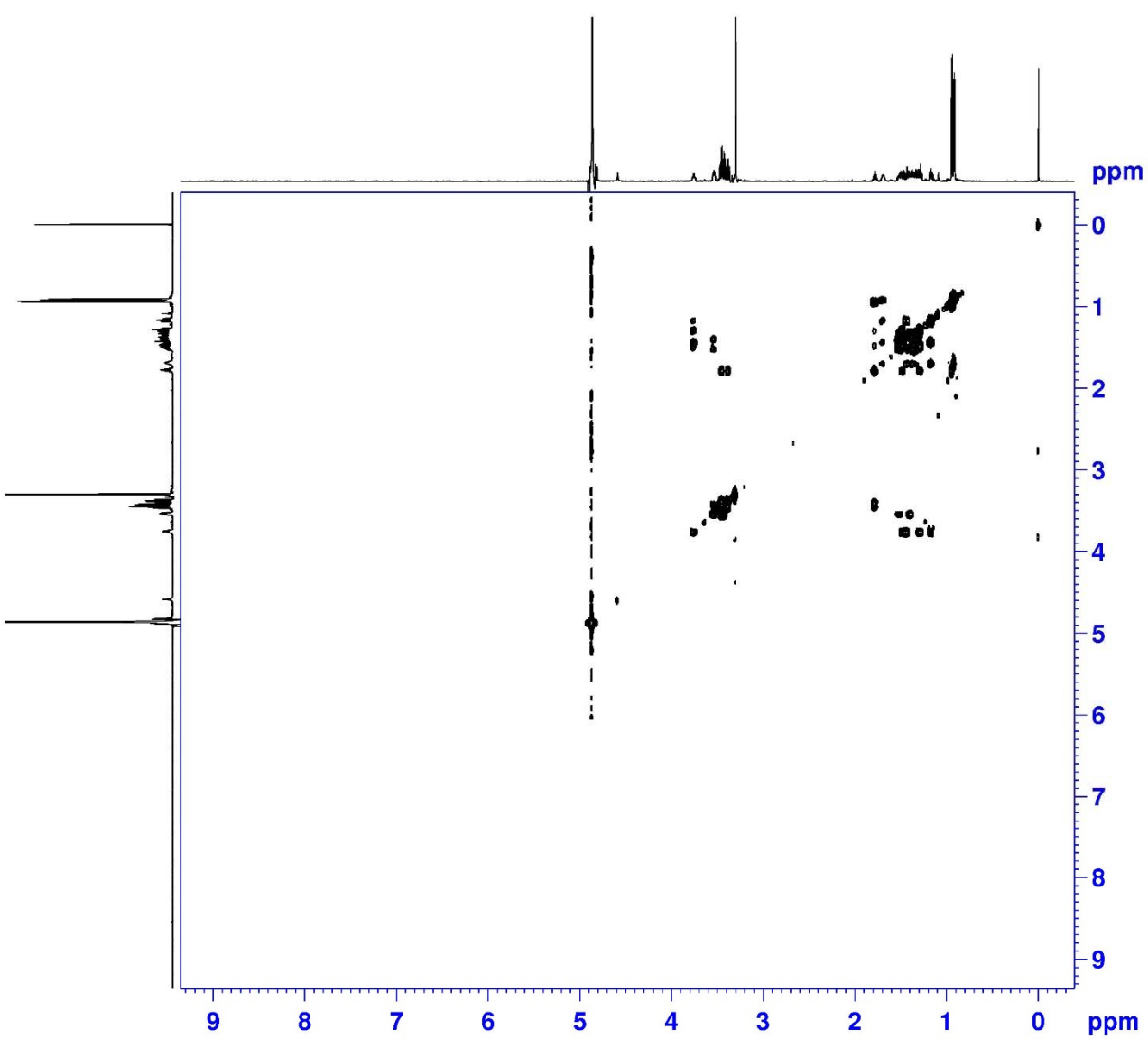


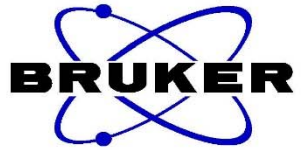


DEPT135 (175 MHz) spectrum of the fragment **1a** in CD_3OD



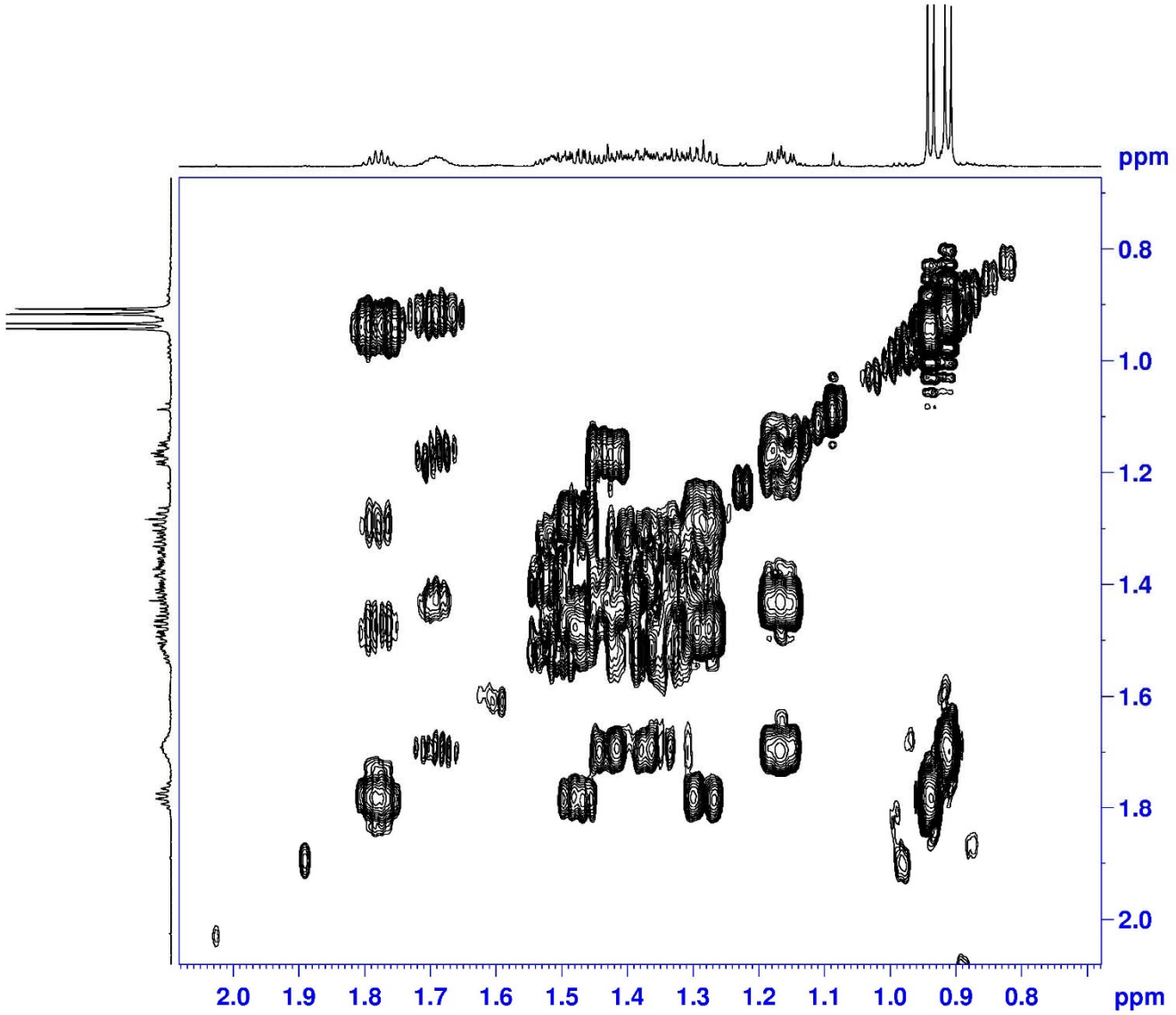
^{1}H–^{1}H COSY (700 MHz) spectrum of the fragment **1a** in CD_3OD



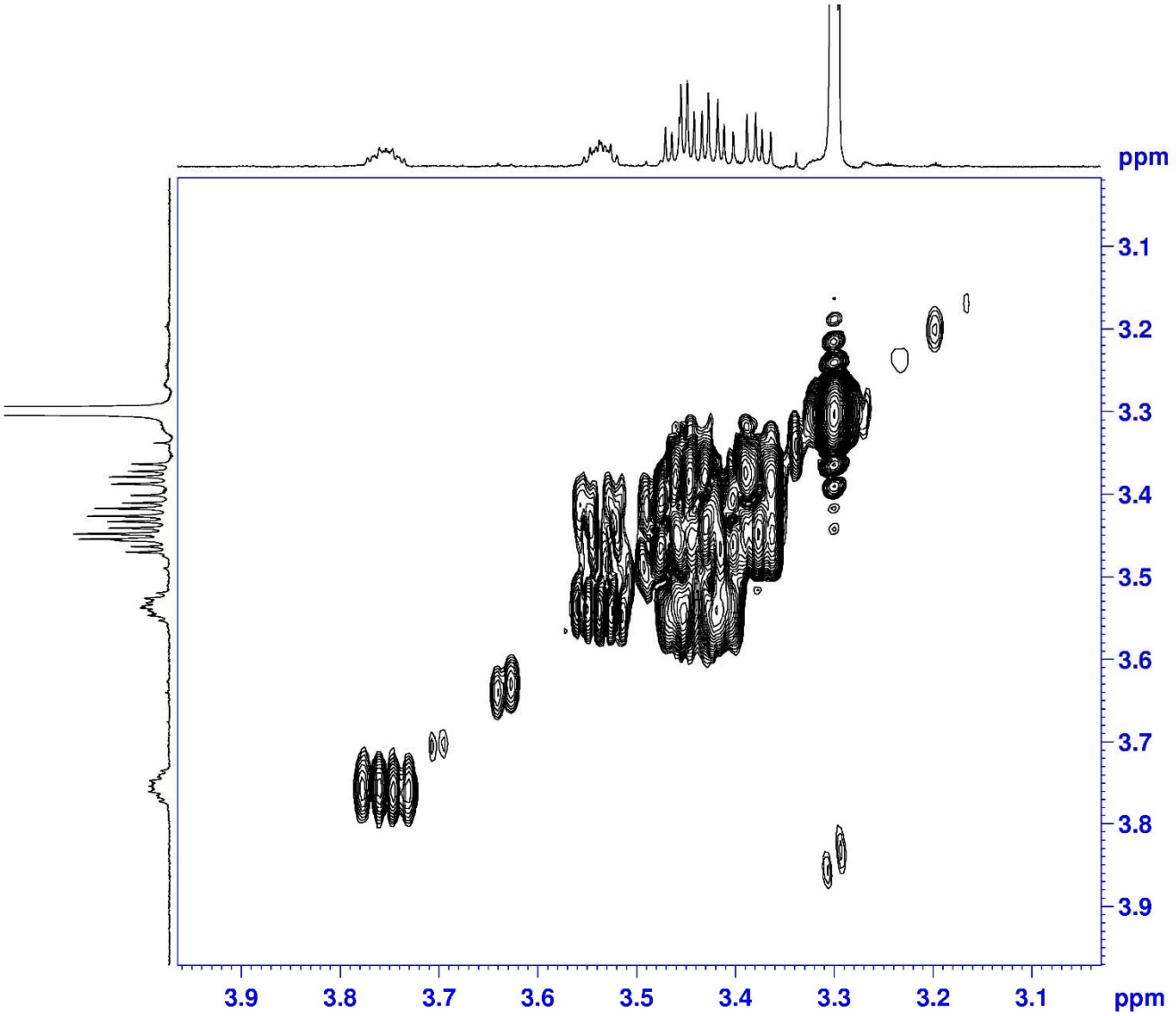


NAME	liwanshan-40-2-2-03-1	
EXPNO	16	
PROCNO	1	
Date_	20200312	
Time	8.54	h
INSTRUM	spect	
PROBHD	Z120187_0028 (	
PULPROG	cosygpppqf	
TD	2048	
SOLVENT	MeOD	
NS	24	
DS	16	
SWH	4606.879	Hz
FIDRES	4.498906	Hz
AQ	0.2223263	sec
RG	57.16	
DW	108.533	usec
DE	10.00	usec
TE	298.0	K
D0	0.00000300	sec
D1	1.00000000	sec
D11	0.03000000	sec
D12	0.00002000	sec
D13	0.00000400	sec
D16	0.00020000	sec
IN0	0.00021700	sec
ND0	1	
TD	128	
SFO1	700.182	MHz
FIDRES	36.002304	Hz
SW	6.582	ppm
FnMODE	QF	
SI	2048	
SF	700.1800190	MHz
WDW	QSINE	
SSB	0	
LB	0.00	Hz
GB	0	
PC	1.40	
SI	2048	
MC2	QF	
SF	700.1800180	MHz
WDW	QSINE	
SSB	0	
LB	0.00	Hz
GB	0	

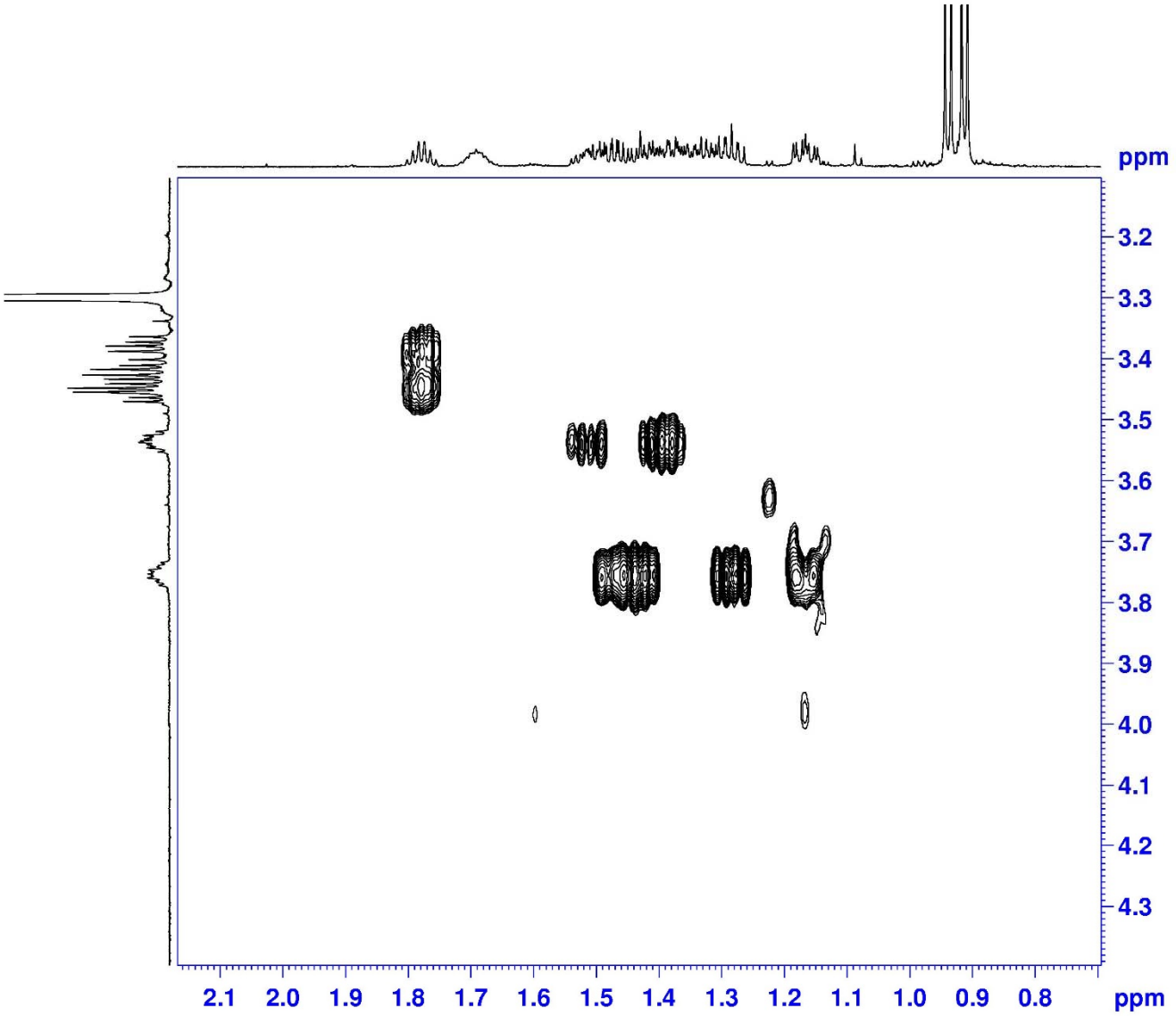
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1a** in CD_3OD



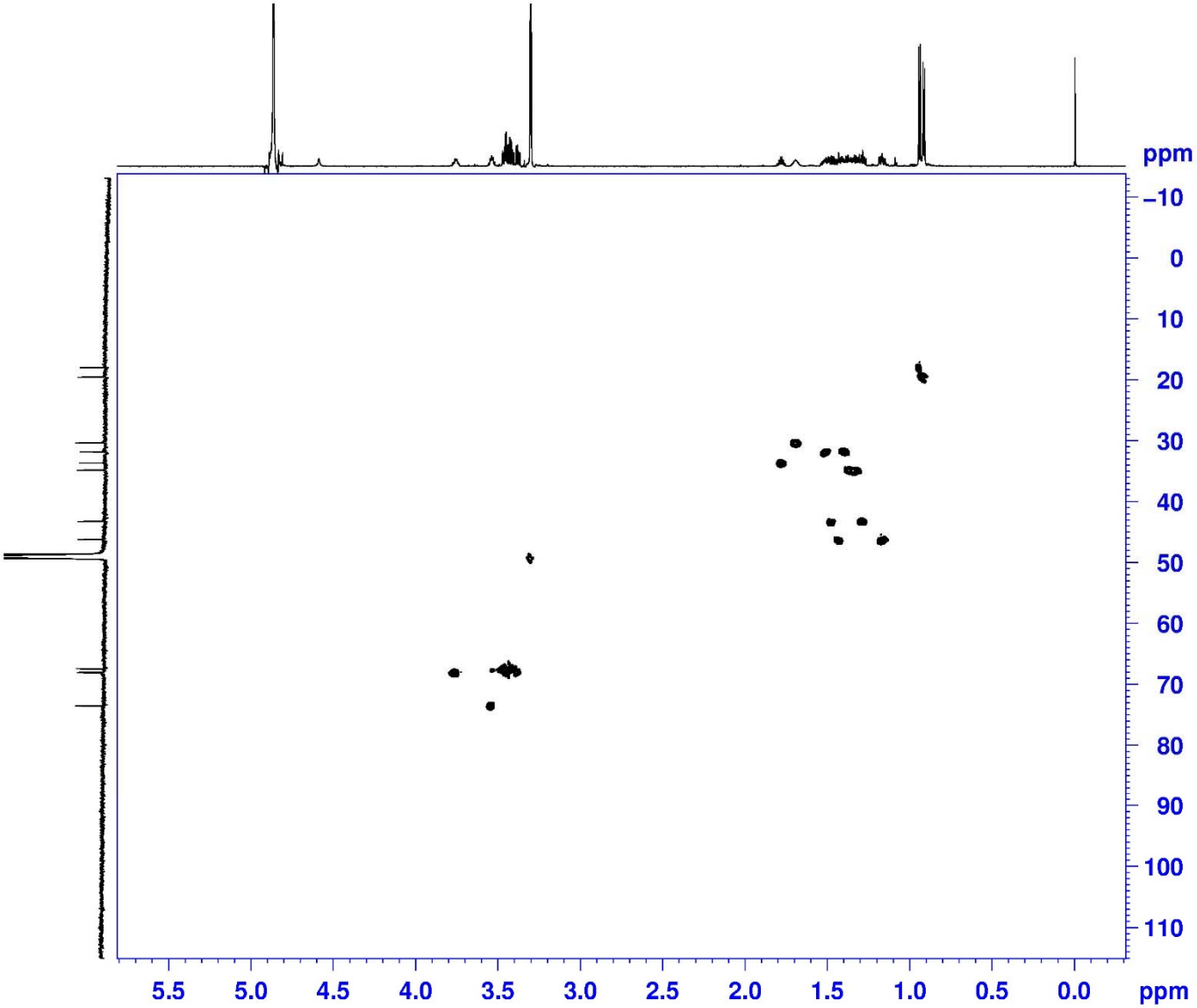
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1a** in CD_3OD



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



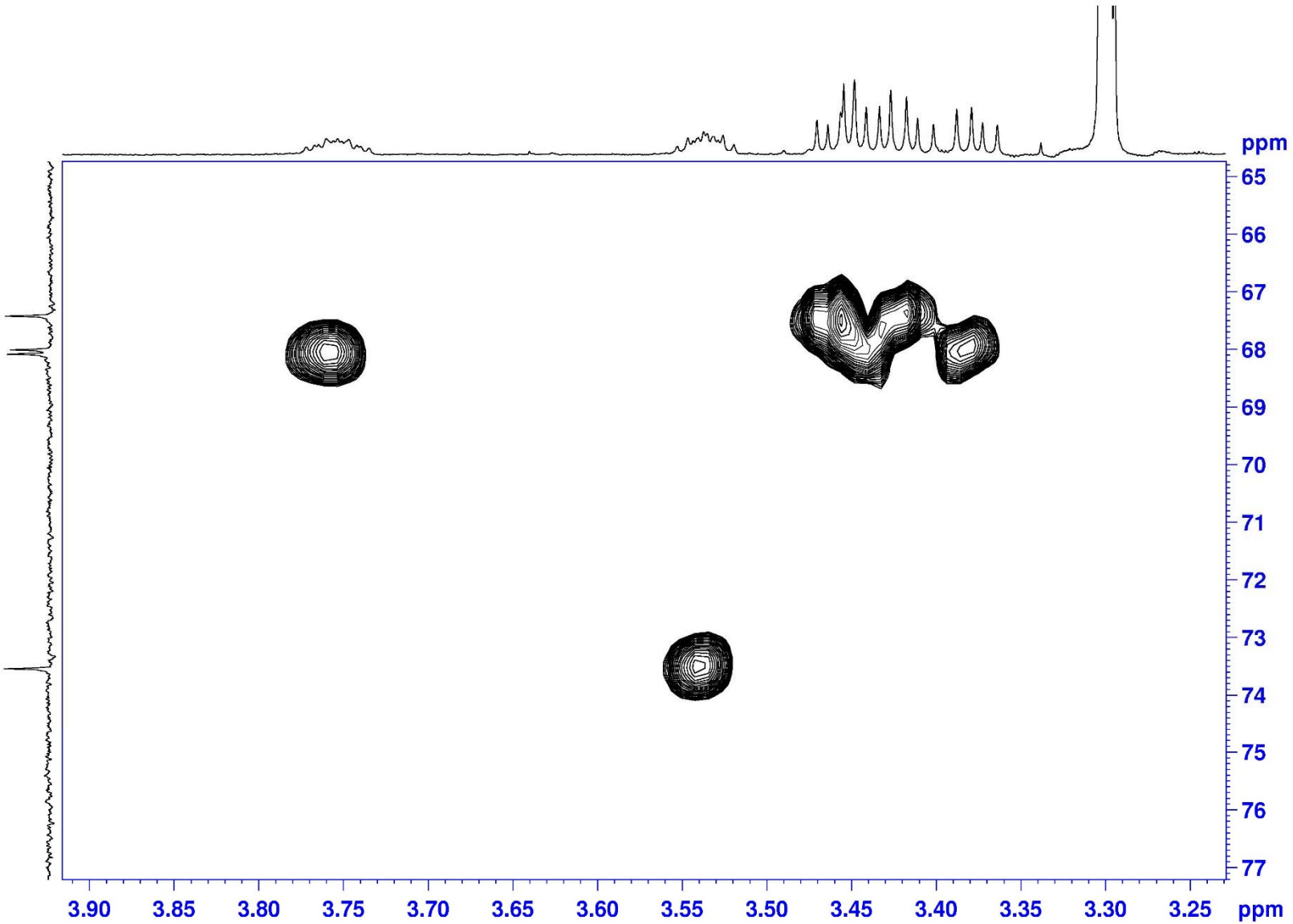
HSQC (700 MHz) spectrum of the fragment **1a** in CD_3OD



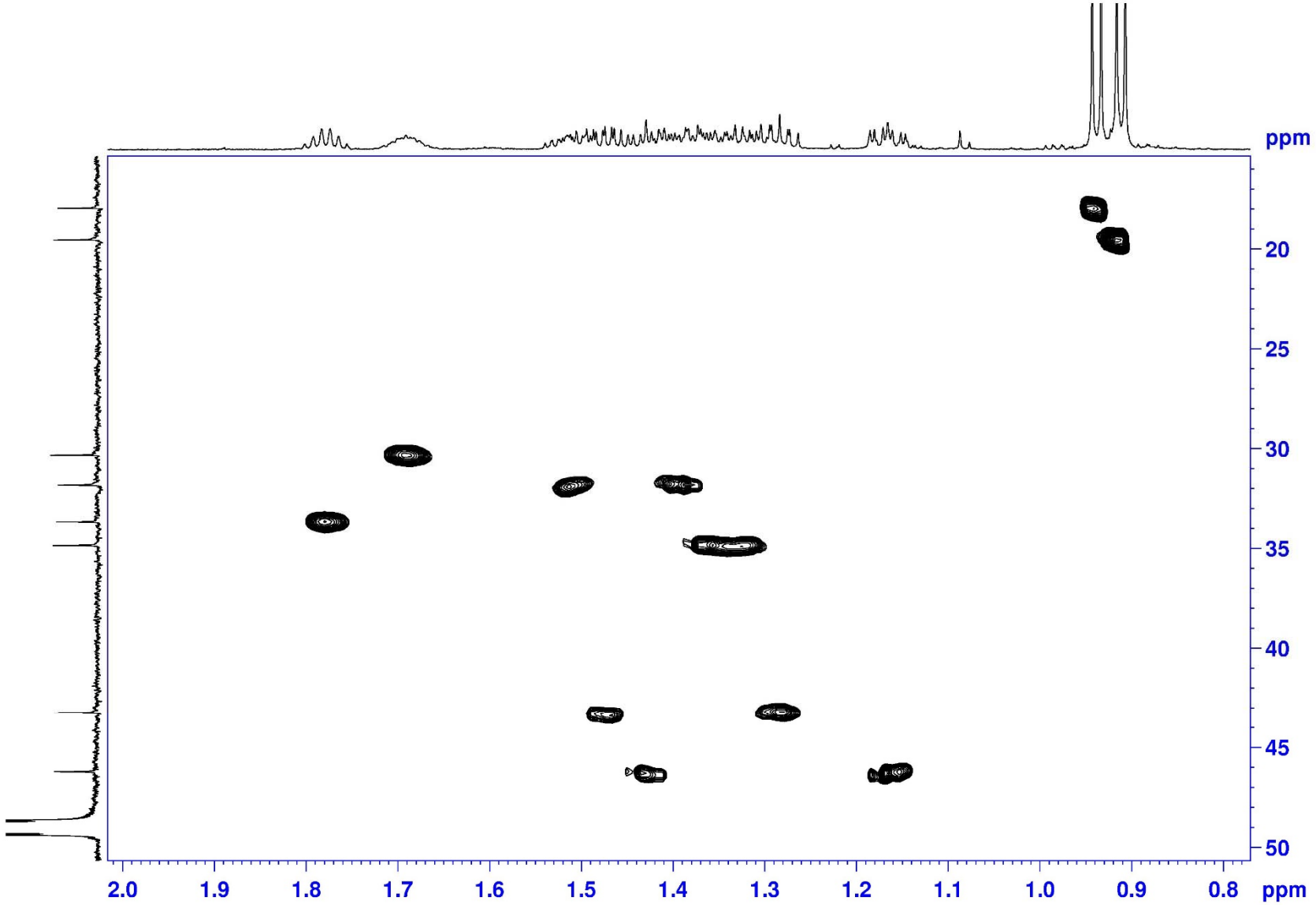
BRUKER

NAME	liwanshan-40-2-2-1
EXPNO	18
PROCNO	1
Date_	20200312
Time	11.21 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hsqcedetgp
TD	2048
SOLVENT	MeOD
NS	24
DS	16
SWH	5617.978 Hz
FIDRES	5.486306 Hz
AQ	0.1823220 se
RG	181.26
DW	89.000 us
DE	10.00 us
TE	298.0 K
CNST2	145.0000000
D0	0.00000300 se
D1	1.00000000 se
D4	0.00172414 se
D11	0.03000000 se
D13	0.00000400 se
D16	0.00020000 se
D21	0.00345000 se
IN0	0.00002870 se
ND0	2
TD	128
SFO1	176.0679 MH
FIDRES	136.106277 Hz
SW	98.948 pp
FnMODE	Echo-Antiecho
SI	1024
SF	700.1800160 MH
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	176.0601541 MH
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

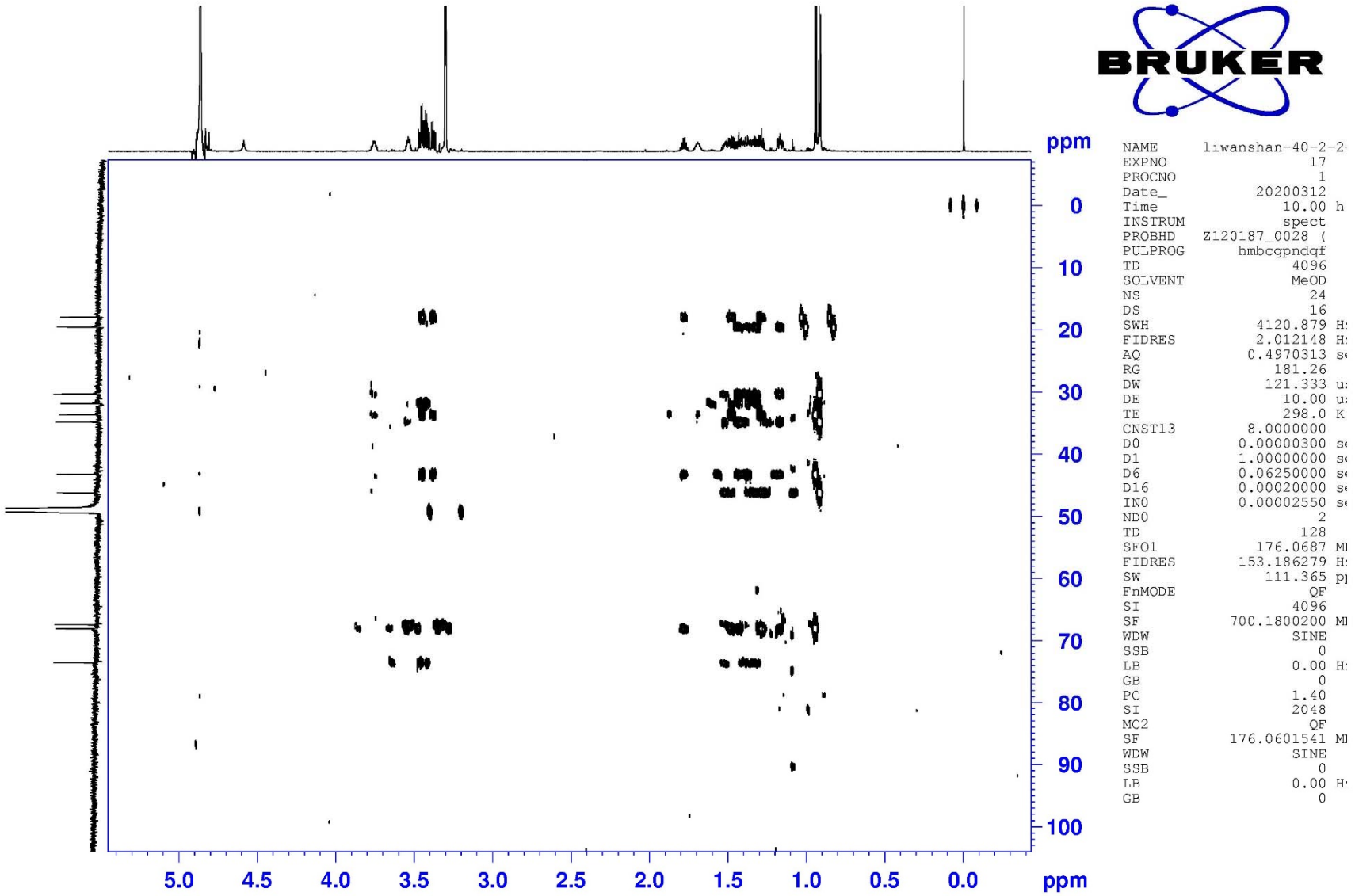
HSQC (700 MHz) spectrum of the fragment **1a** in CD_3OD



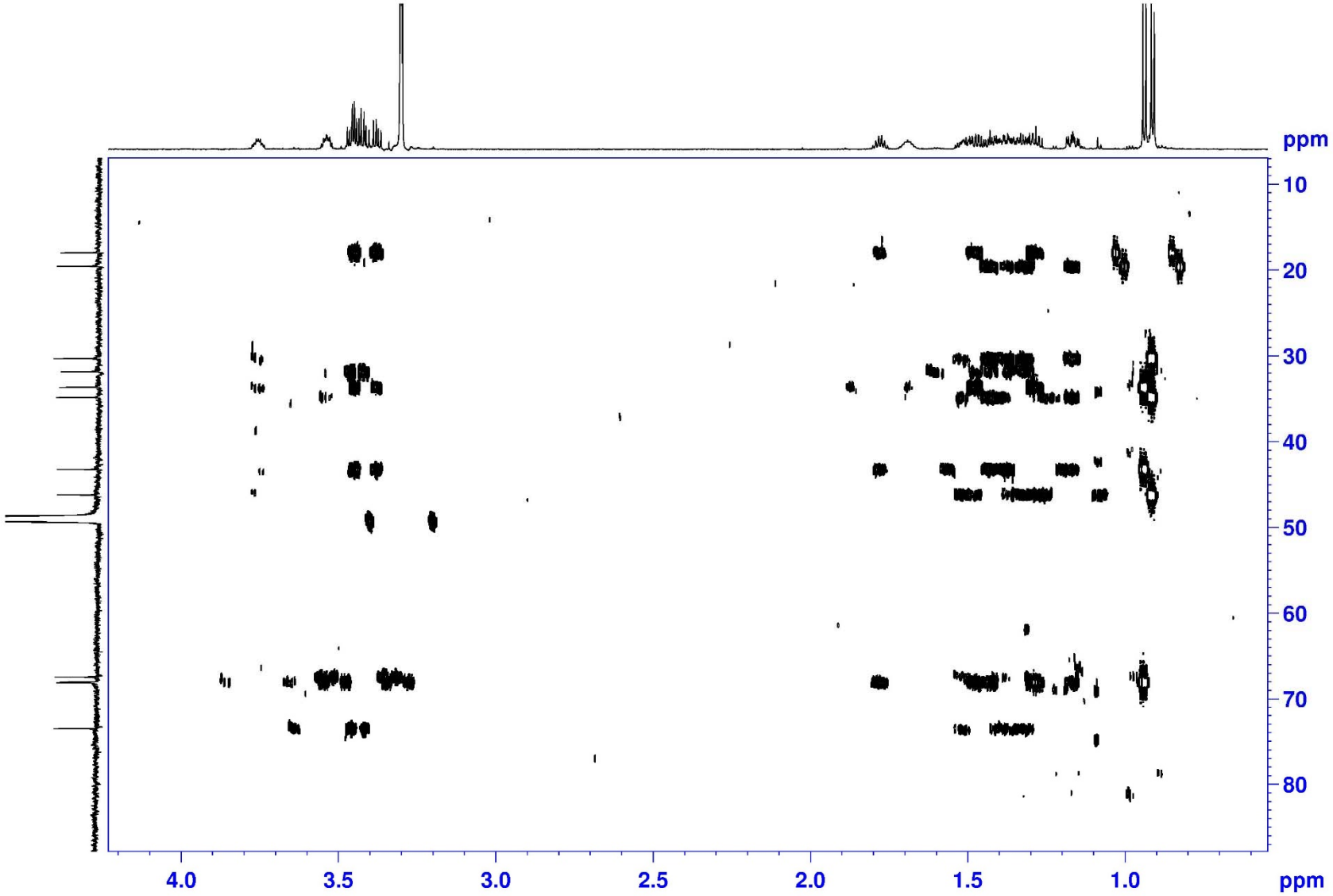
HSQC (700 MHz) spectrum of the fragment **1a** in CD_3OD



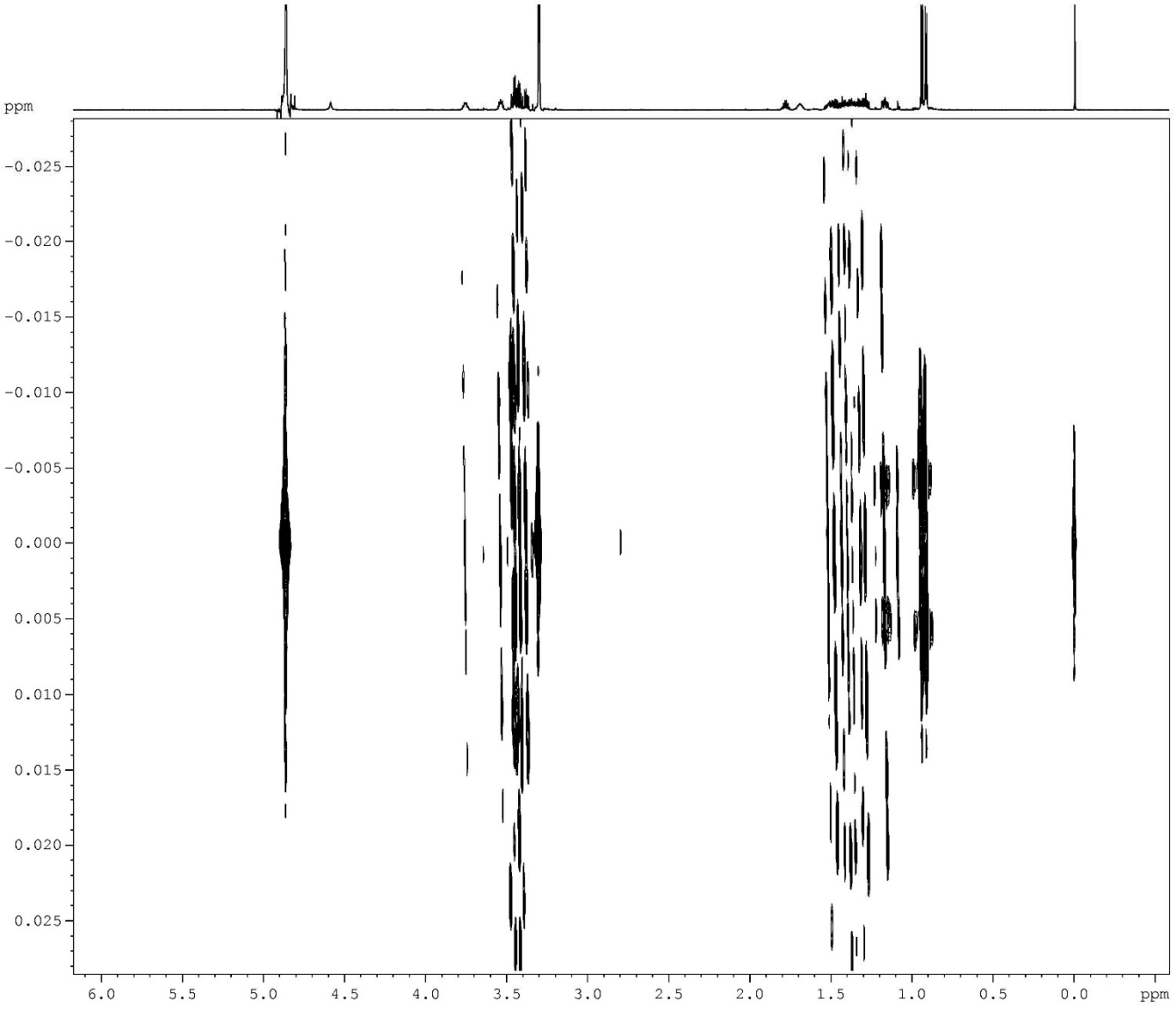
HMBC (700 MHz) spectrum of the fragment **1a** in CD_3OD



HMBC (700 MHz) spectrum of the fragment **1a** in CD_3OD



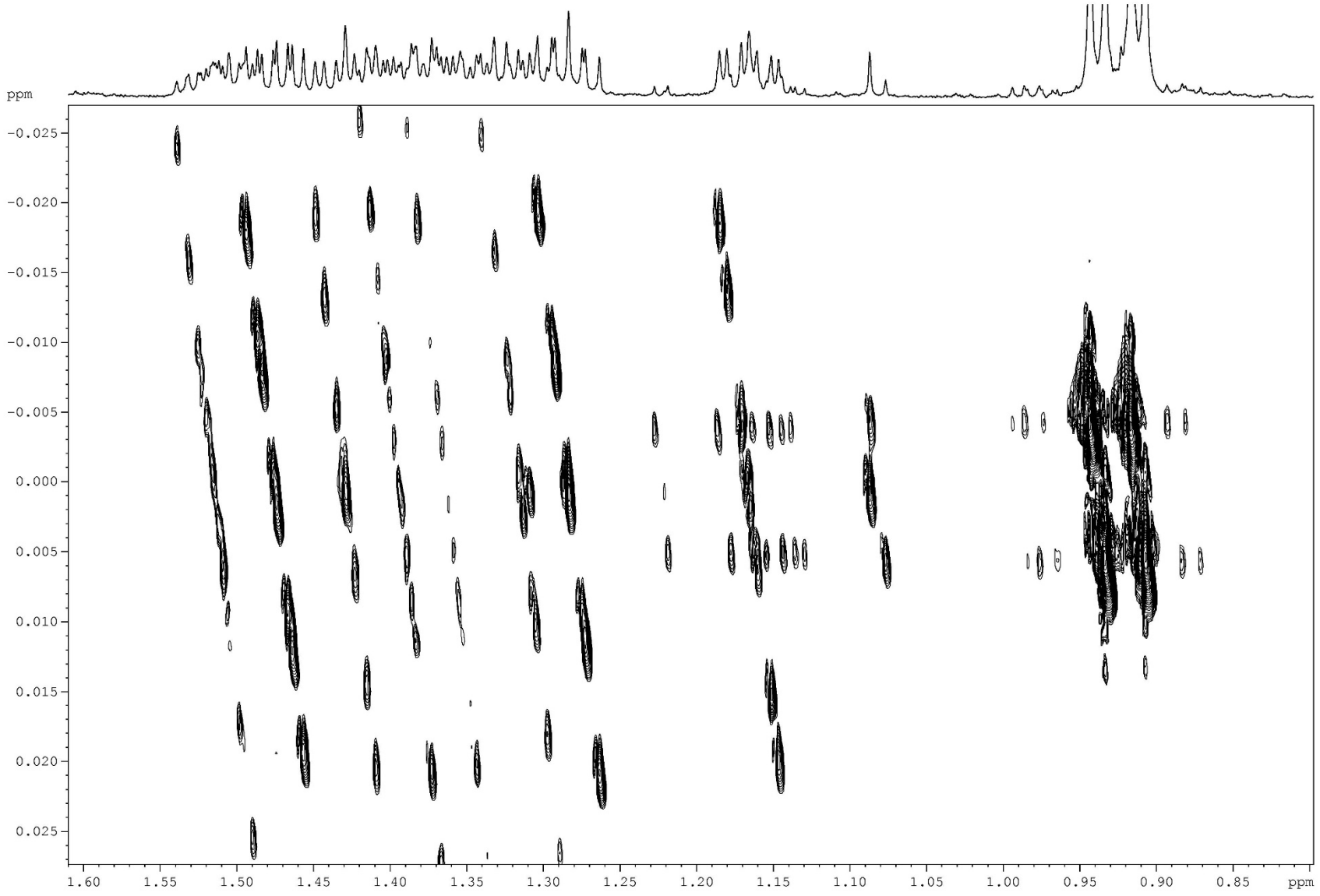
2D *J*RES (700 MHz) spectrum of the fragment **1a** in CD_3OD



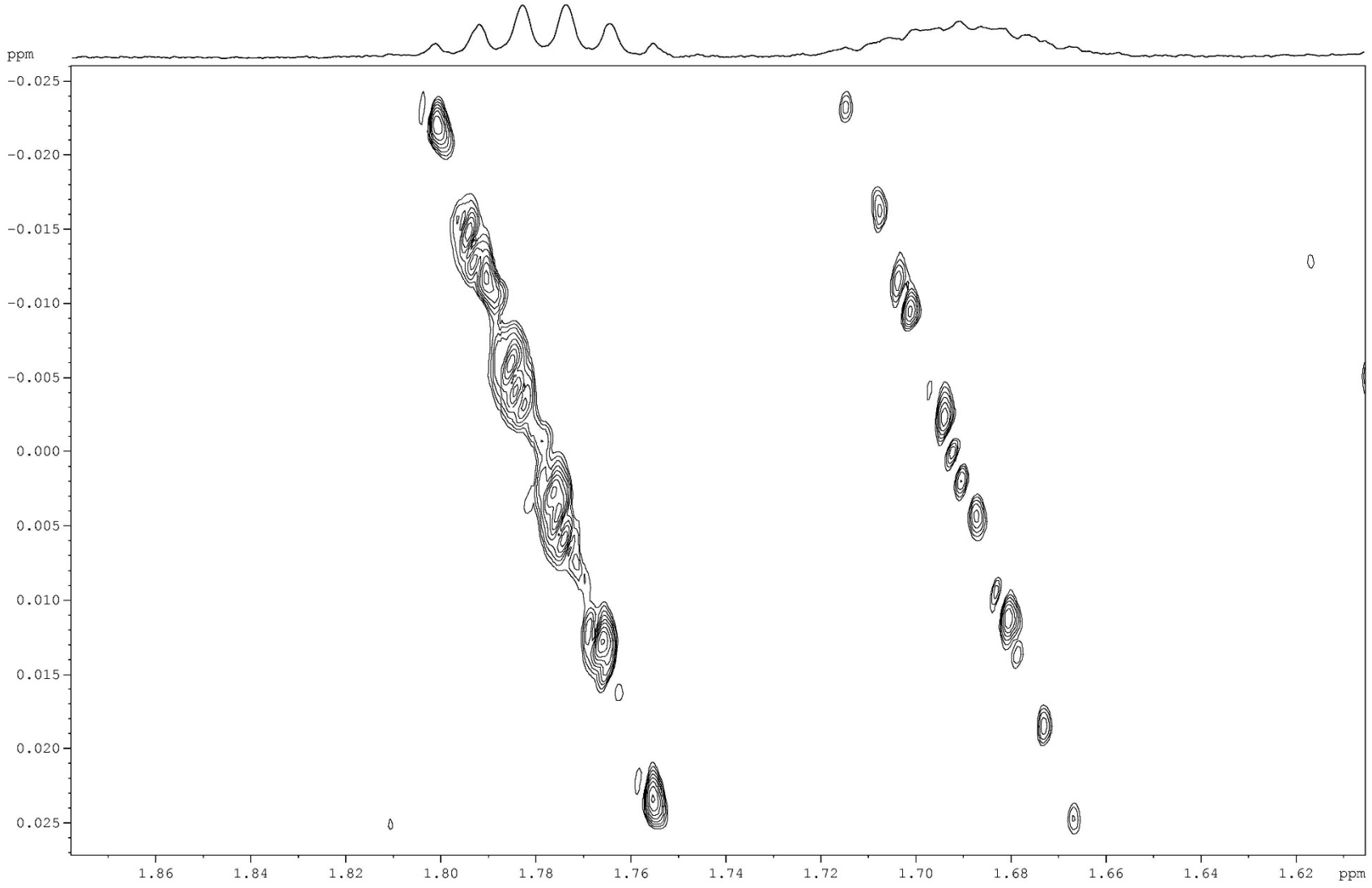
BRUKER

NAME	liwanshan-40-2-2-O3-1
EXPNO	20
PROCNO	1
Date_	20200403
Time	21.55 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	jresgpprqf
TD	8192
SOLVENT	MeOD
NS	128
DS	16
SWH	4734.849 Hz
FIDRES	1.155969 Hz
AQ	0.8651252 sec
RG	111.13
DW	105.600 usec
DE	10.00 usec
TE	298.0 K
D0	0.00000300 sec
D1	1.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
D16	0.00020000 sec
IN0	0.01250000 sec
ND0	2
TD	40
SFO1	700.182 MHz
FIDRES	1.000000 Hz
SW	0.057 ppm
FnMODE	QF
SI	16384
SF	700.1800192 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.00
SI	128
MC2	QF
SF	700.1819742 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

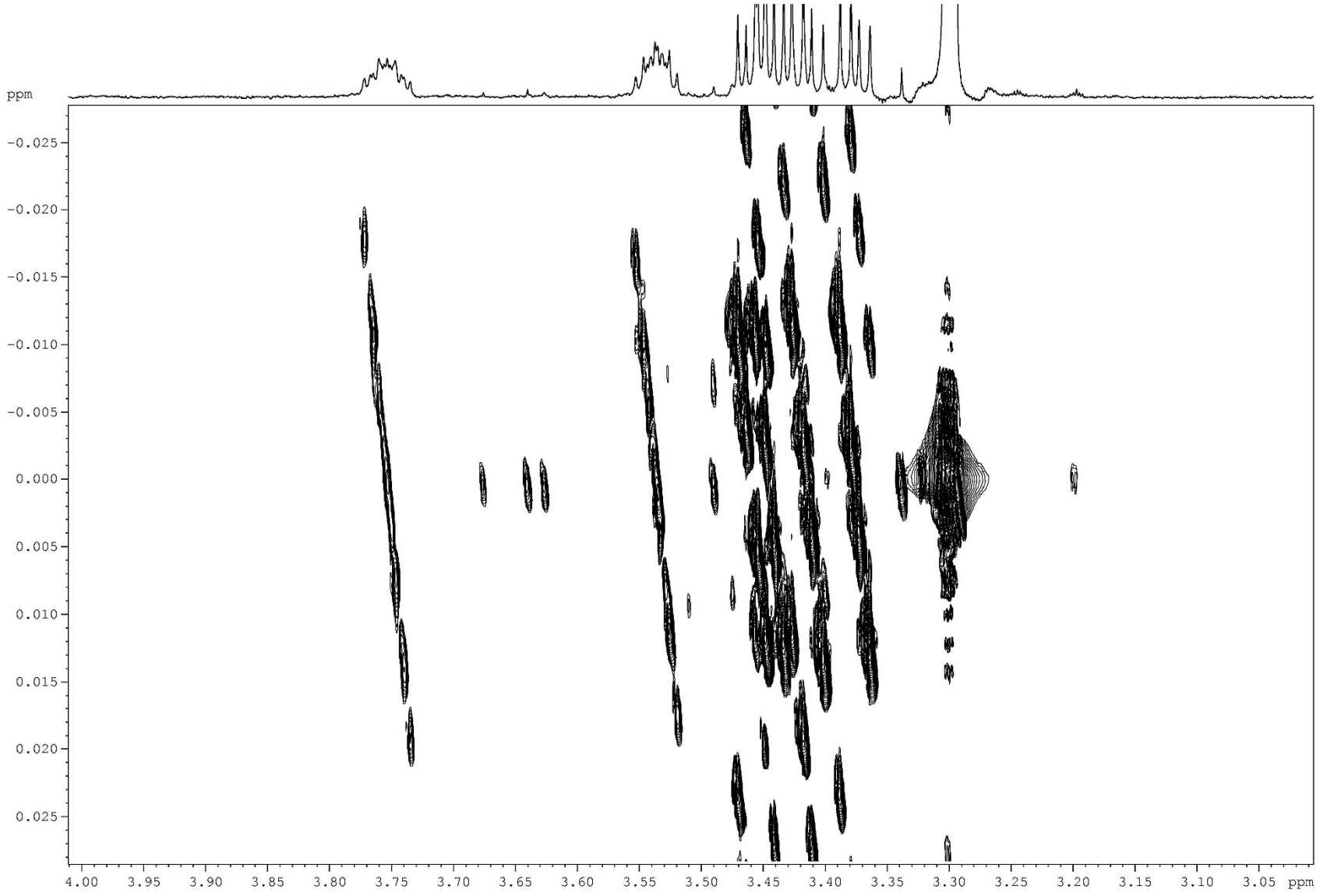
2D *J*RES (700 MHz) spectrum of the fragment **1a** in CD_3OD



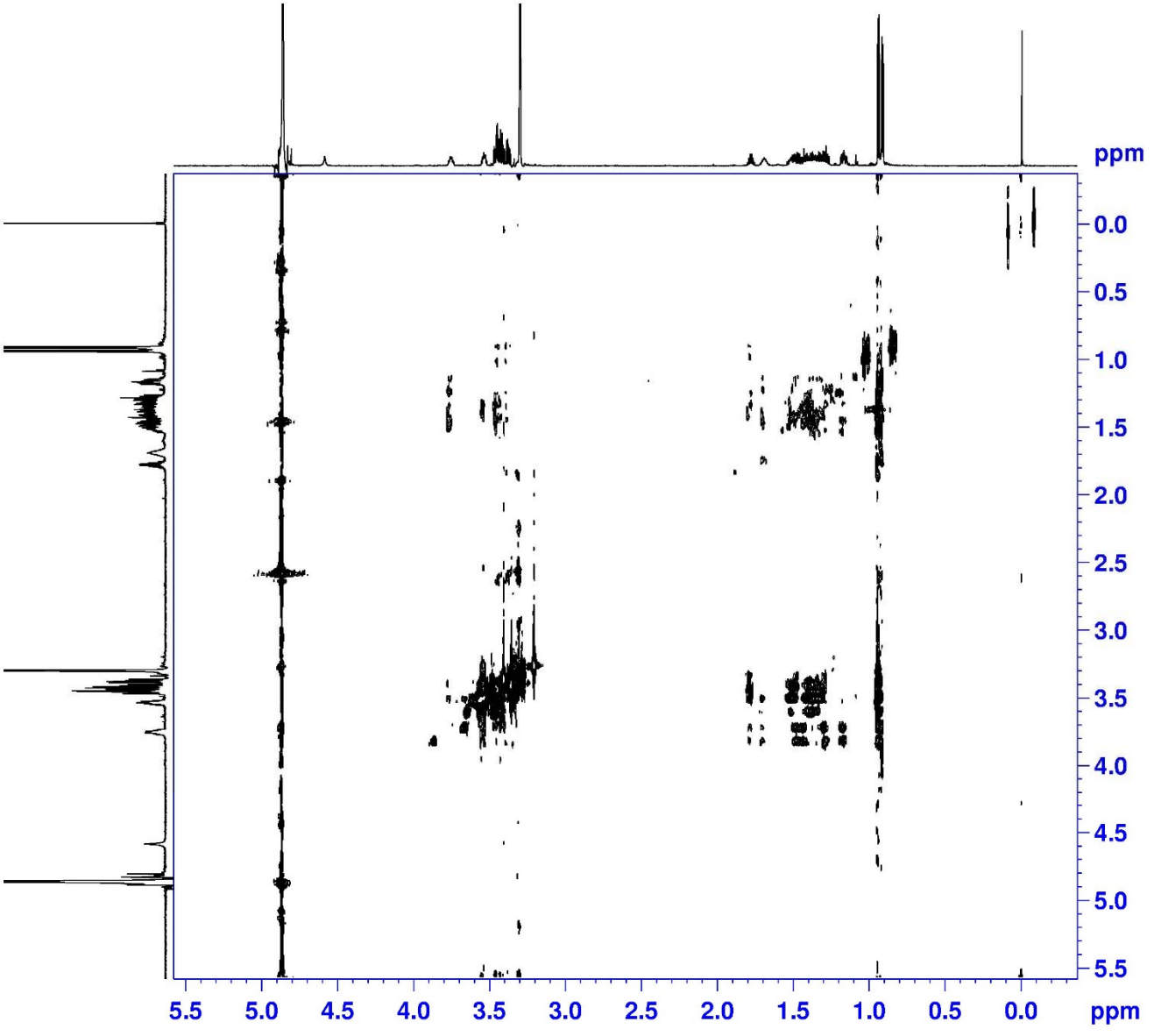
2D *J*RES (700 MHz) spectrum of the fragment **1a** in CD_3OD



2D *J*RES (700 MHz) spectrum of the fragment **1a** in CD_3OD

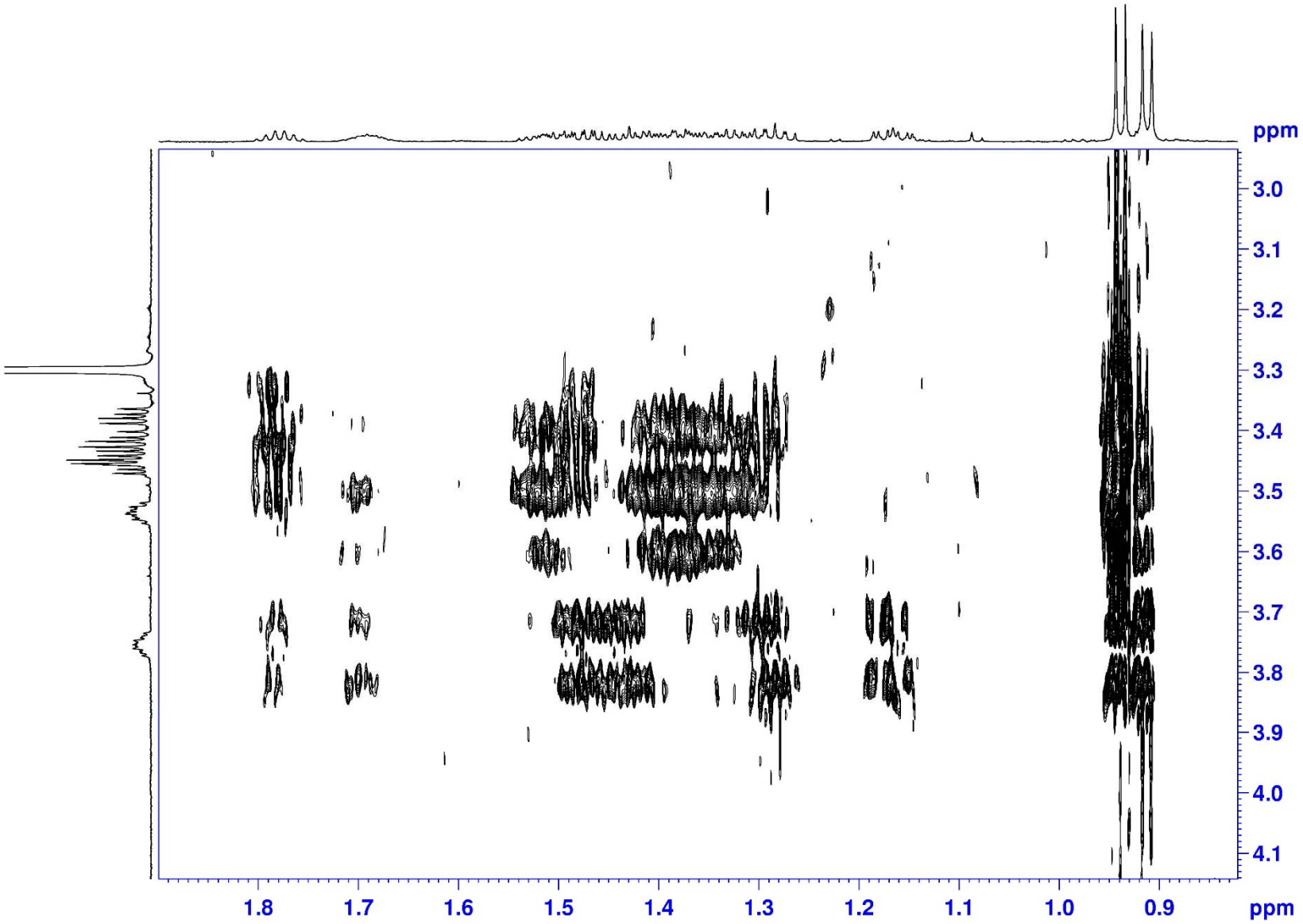


HETLOC (700 MHz) spectrum of the fragment **1a** in CD_3OD

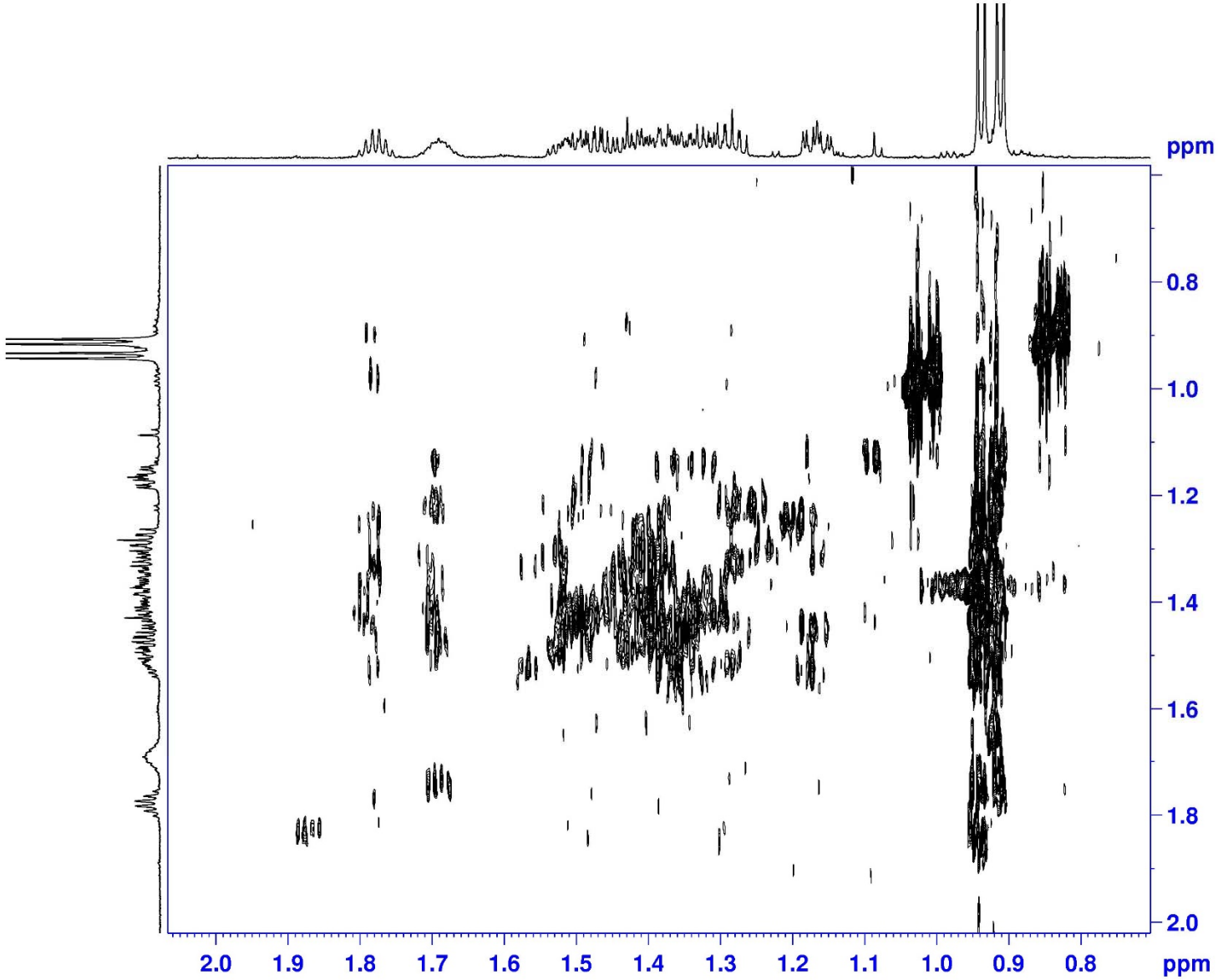


NAME	liwanshan-40-2-2-O3-1
EXPNO	21
PROCNO	1
Date_	20200404
Time	1.18 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	dipsi2etgpjcsix1
TD	4096
SOLVENT	MeOD
NS	64
DS	16
SWH	4166.667 Hz
FIDRES	2.034505 Hz
AQ	0.4915700 sec
RG	181.26
DW	120.000 usec
DE	10.00 usec
TE	298.0 K
CNST2	145.0000000
CNST16	0.5000000
D0	0.00000300 sec
D1	1.00000000 sec
D2	0.00344828 sec
D4	0.00172414 sec
D9	0.08000000 sec
D11	0.03000000 sec
D16	0.00020000 sec
D20	0.00000300 sec
D28	0.00000300 sec
IN0	0.00012000 sec
IN20	0.00006000 sec
IN28	0.00006000 sec
L1	28
ND0	2
TD	128
SFO1	700.1818 MHz
FIDRES	32.552082 Hz
SW	5.951 ppm
FnMODE	Echo-Antiecho
SI	8192
SF	700.1800174 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	700.1800076 MHz
WDW	QSINE
SSB	2

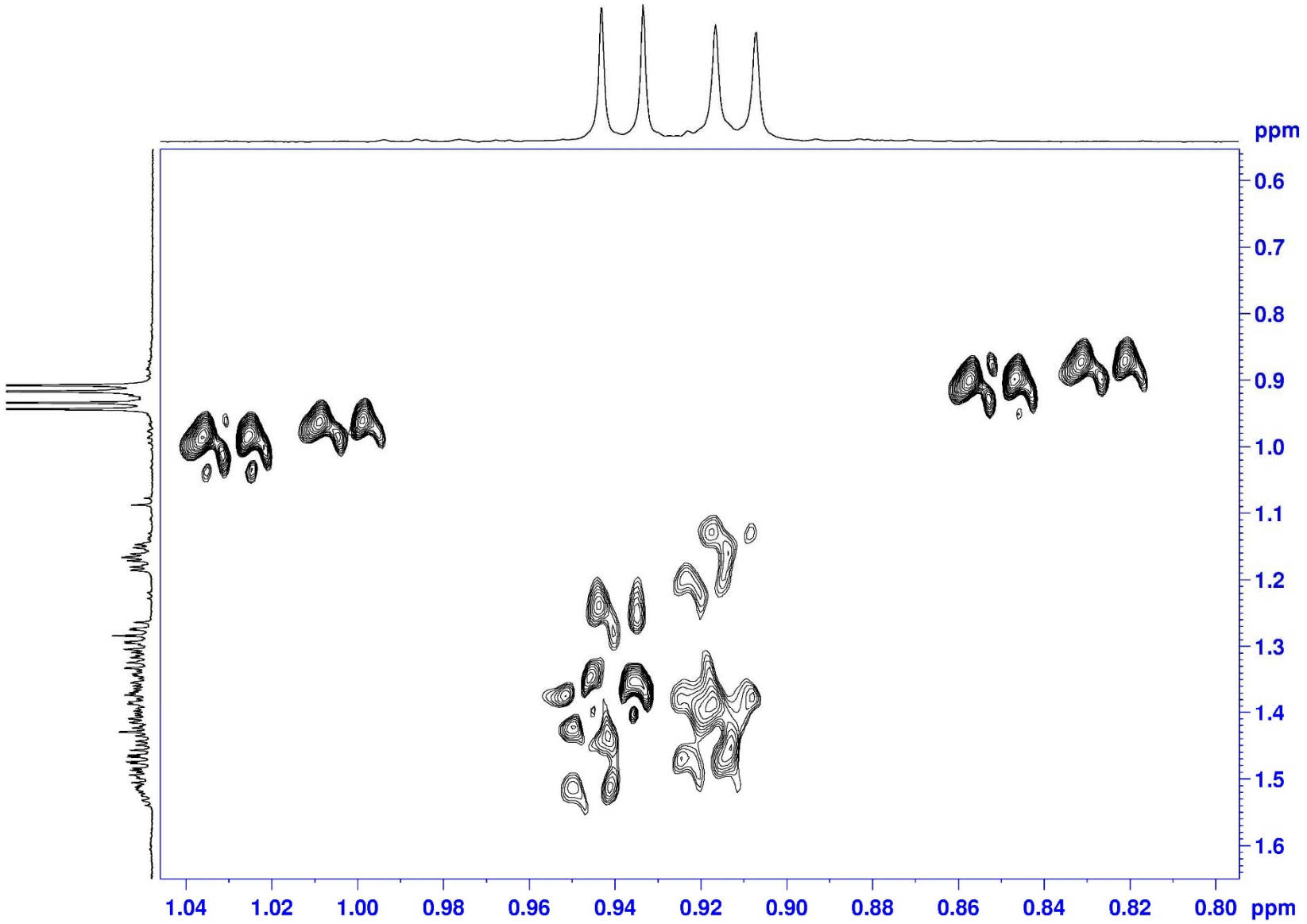
HETLOC (700 MHz) spectrum of the fragment **1a** in CD_3OD



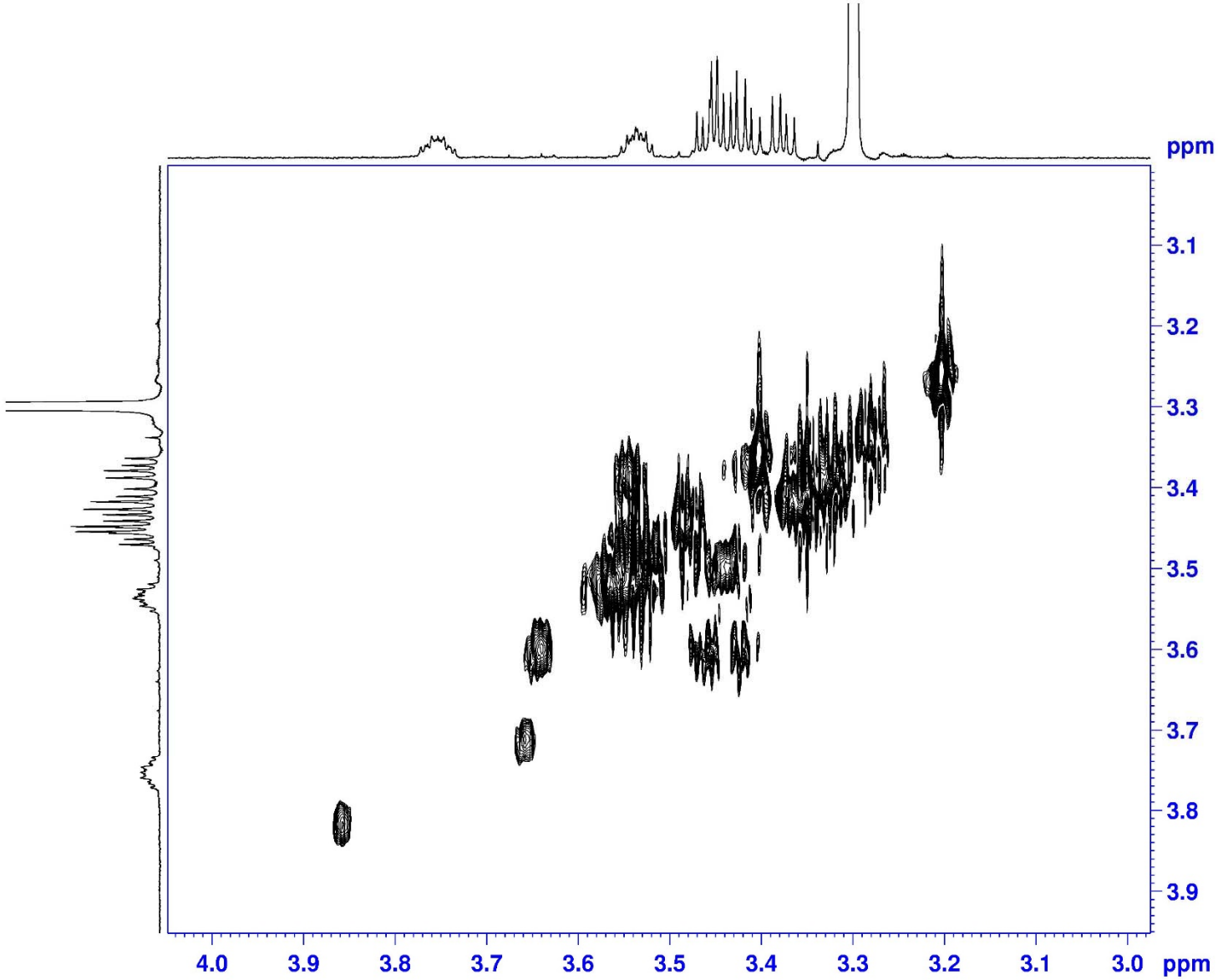
HETLOC (700 MHz) spectrum of the fragment **1a** in CD_3OD



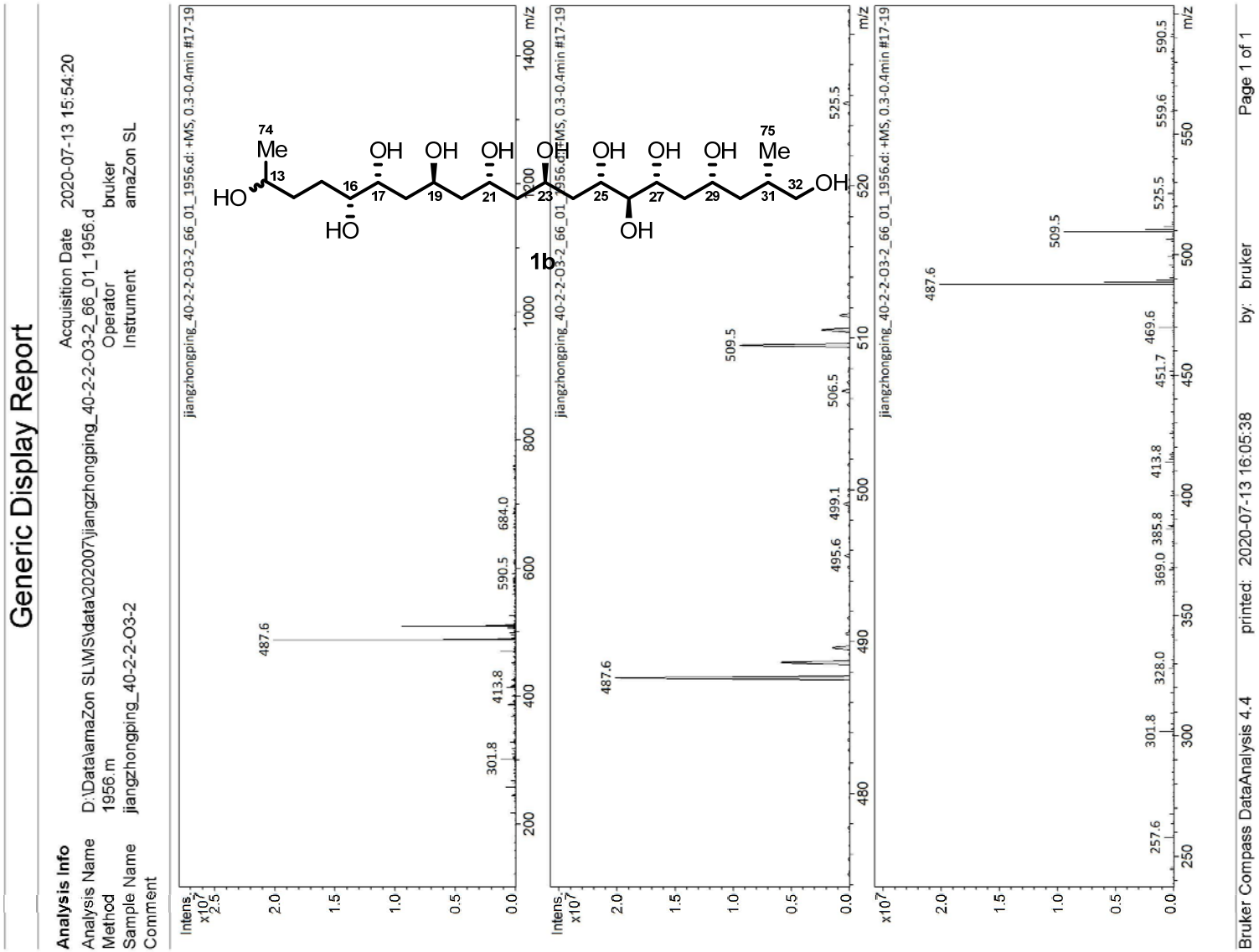
HETLOC (700 MHz) spectrum of the fragment **1a** in CD_3OD



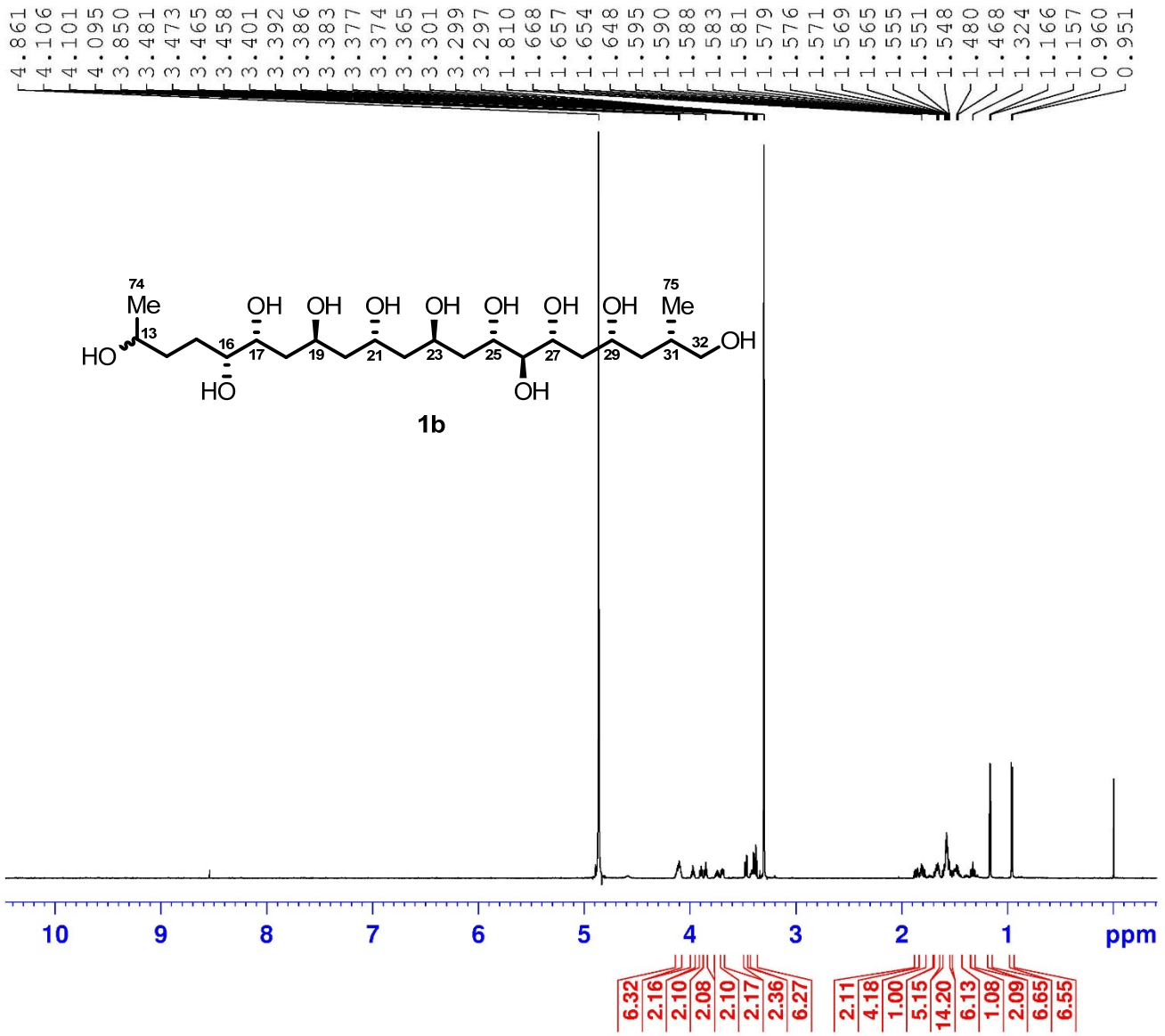
HETLOC (700 MHz) spectrum of the fragment **1a** in CD_3OD



LR-ESI-MS for the fragment **1b**



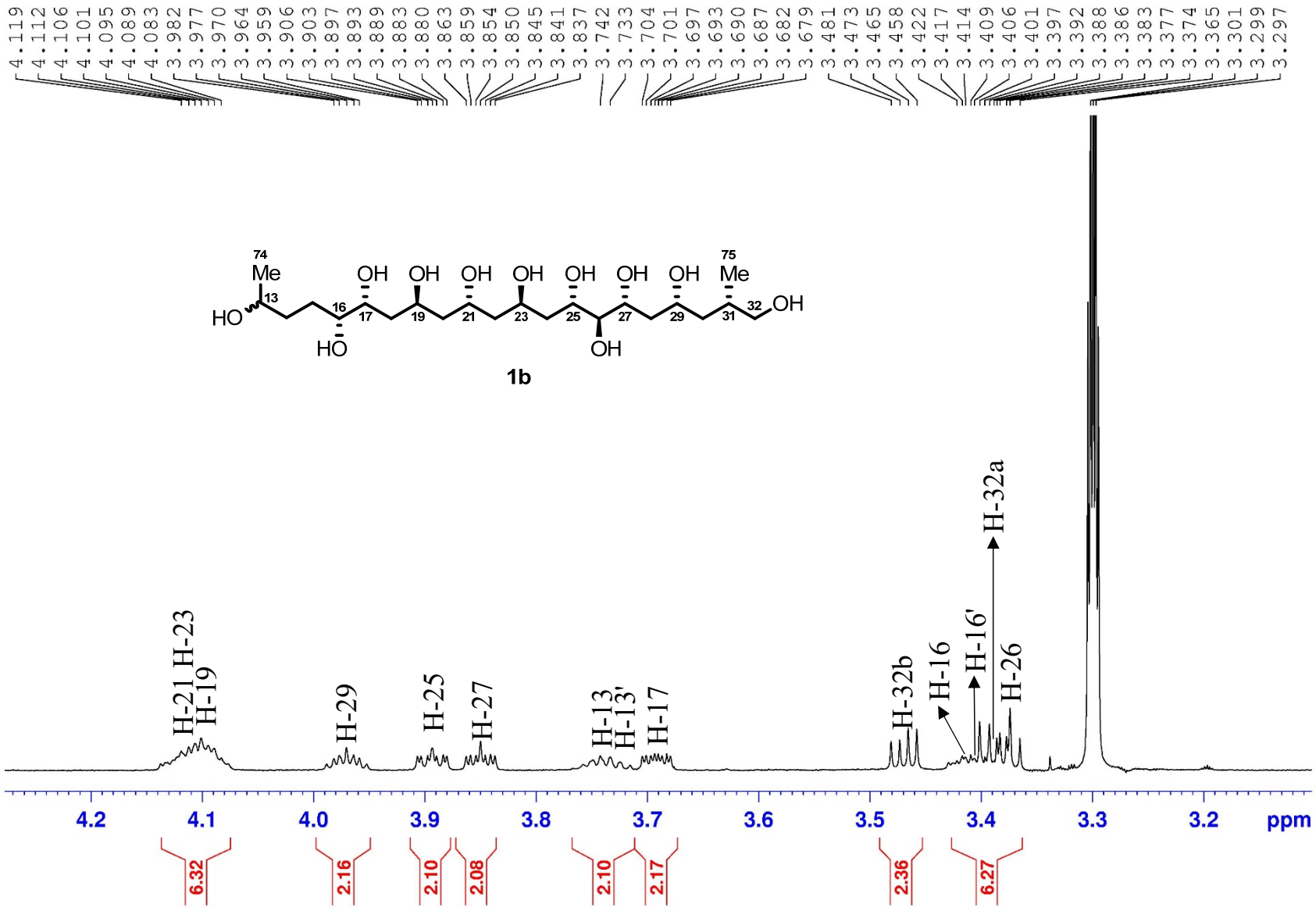
^{1}H (700 MHz) NMR spectrum of the fragment **1b** in CD_3OD



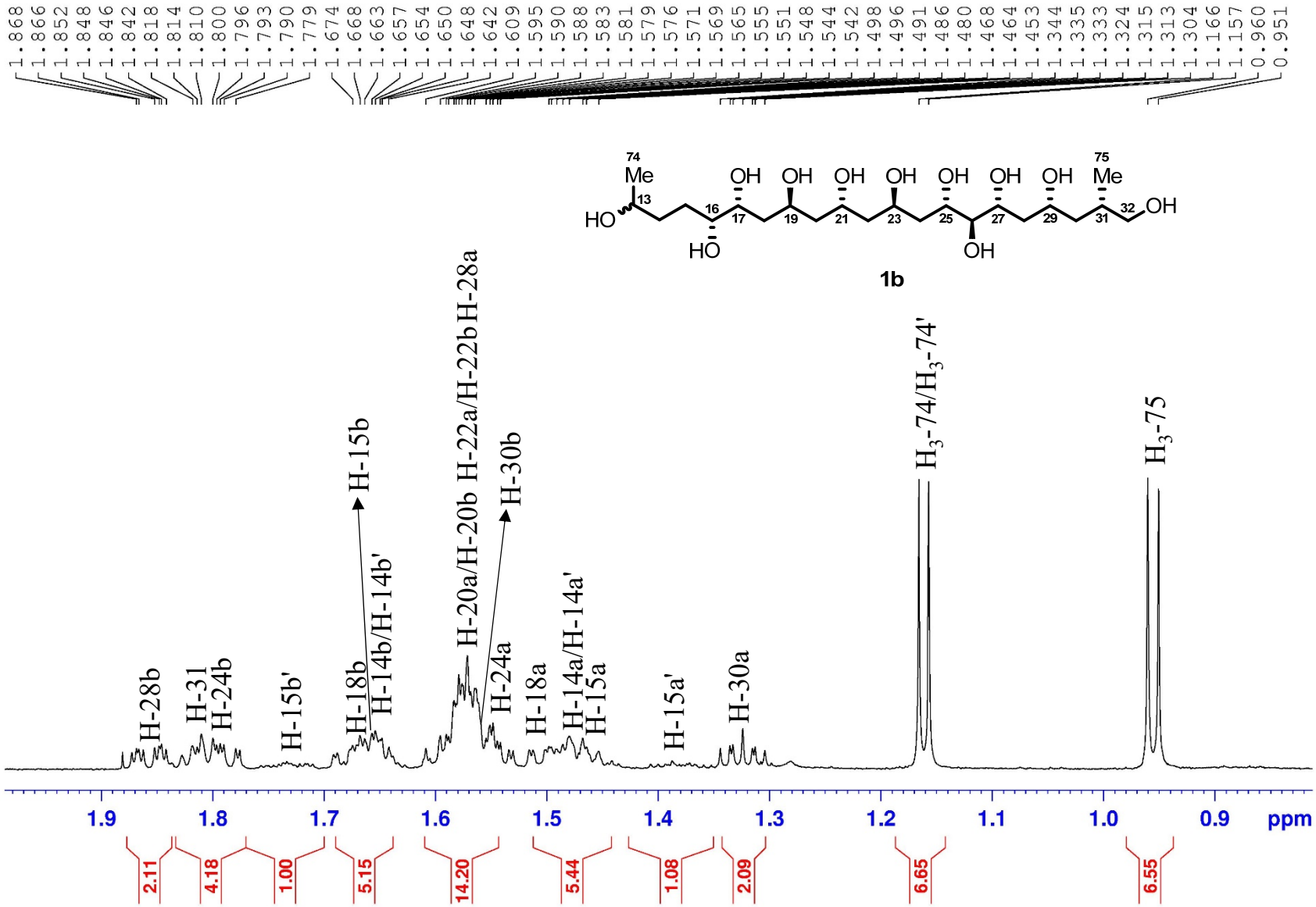
BRUKER

NAME	liwanshan-40-2-2-03-
EXPNO	12
PROCNO	1
Date_	20200307
Time	15.30 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	3
DS	2
SWH	14097.744 Hz
FIDRES	0.430229 Hz
AQ	2.3243935 sec
RG	3.96
DW	35.467 usec
DE	10.00 usec
TE	298.0 K
D1	1.50000000 sec
TD0	1
SFO1	700.1843236 MHz
NUC1	1H
P1	8.10 usec
SI	65536
SF	700.1800211 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

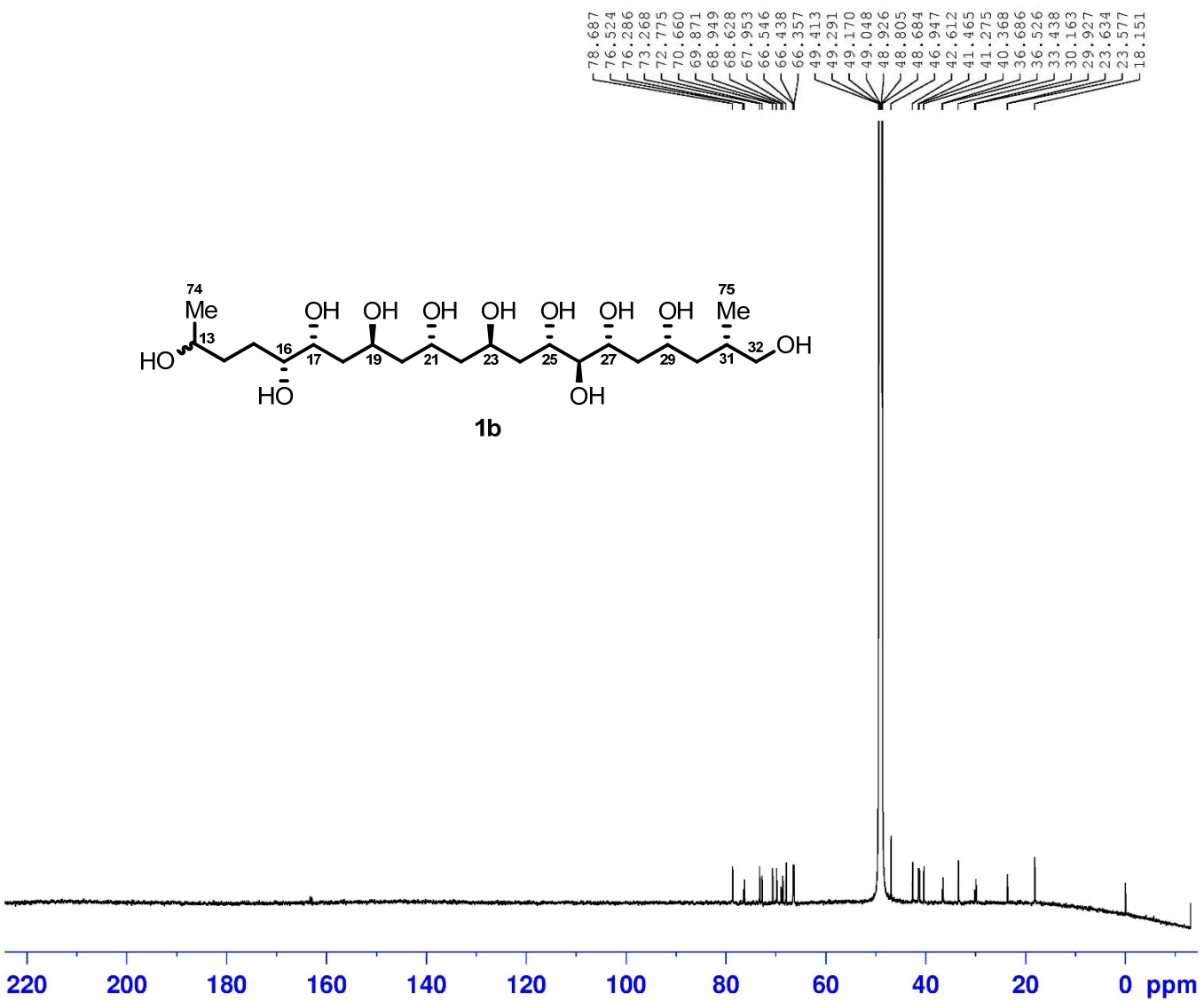
^{1}H (700 MHz) NMR spectrum of the fragment **1b** in CD_3OD



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



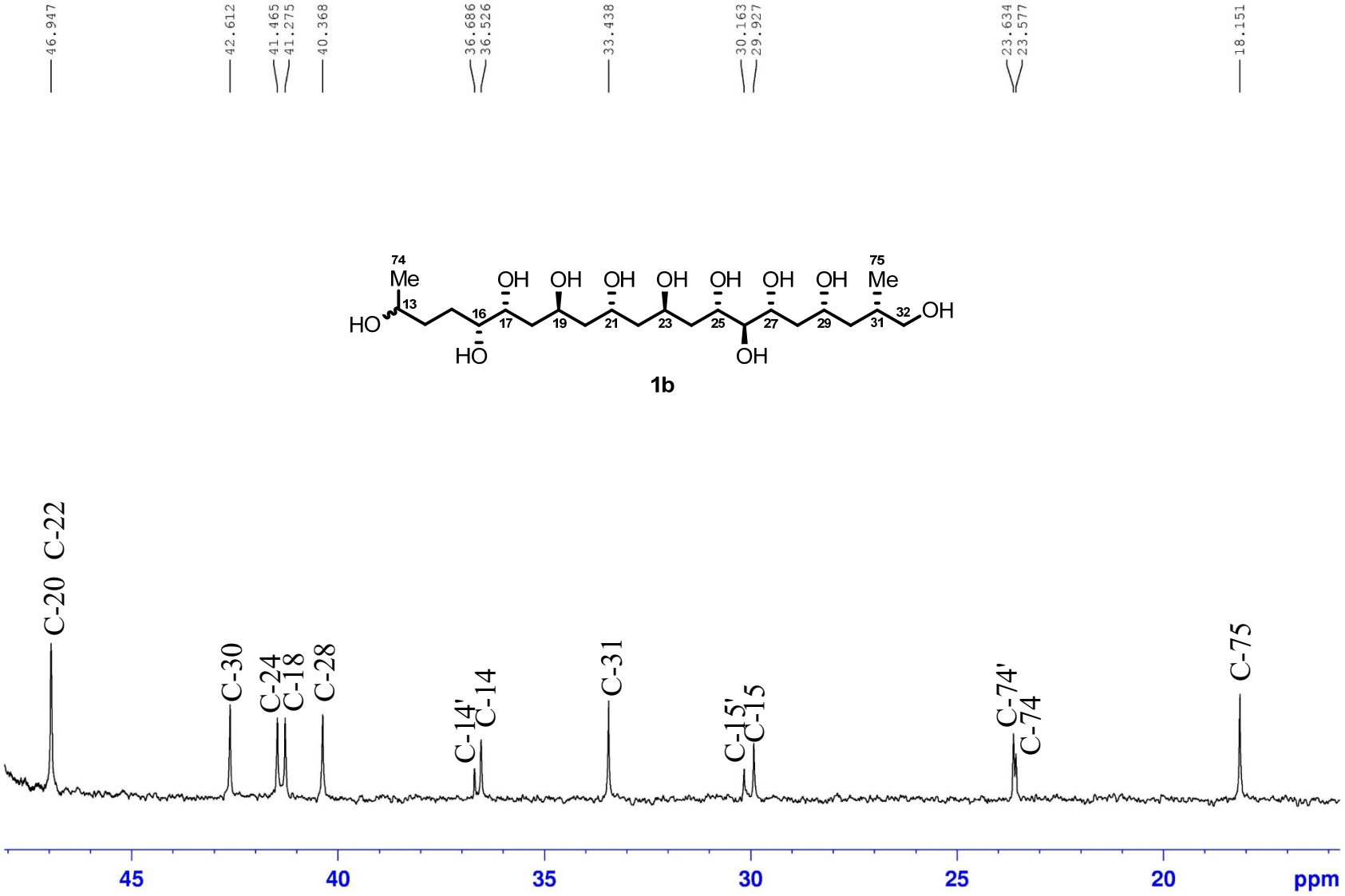
^{13}C (175 MHz) NMR spectrum of the fragment **1b** in CD_3OD



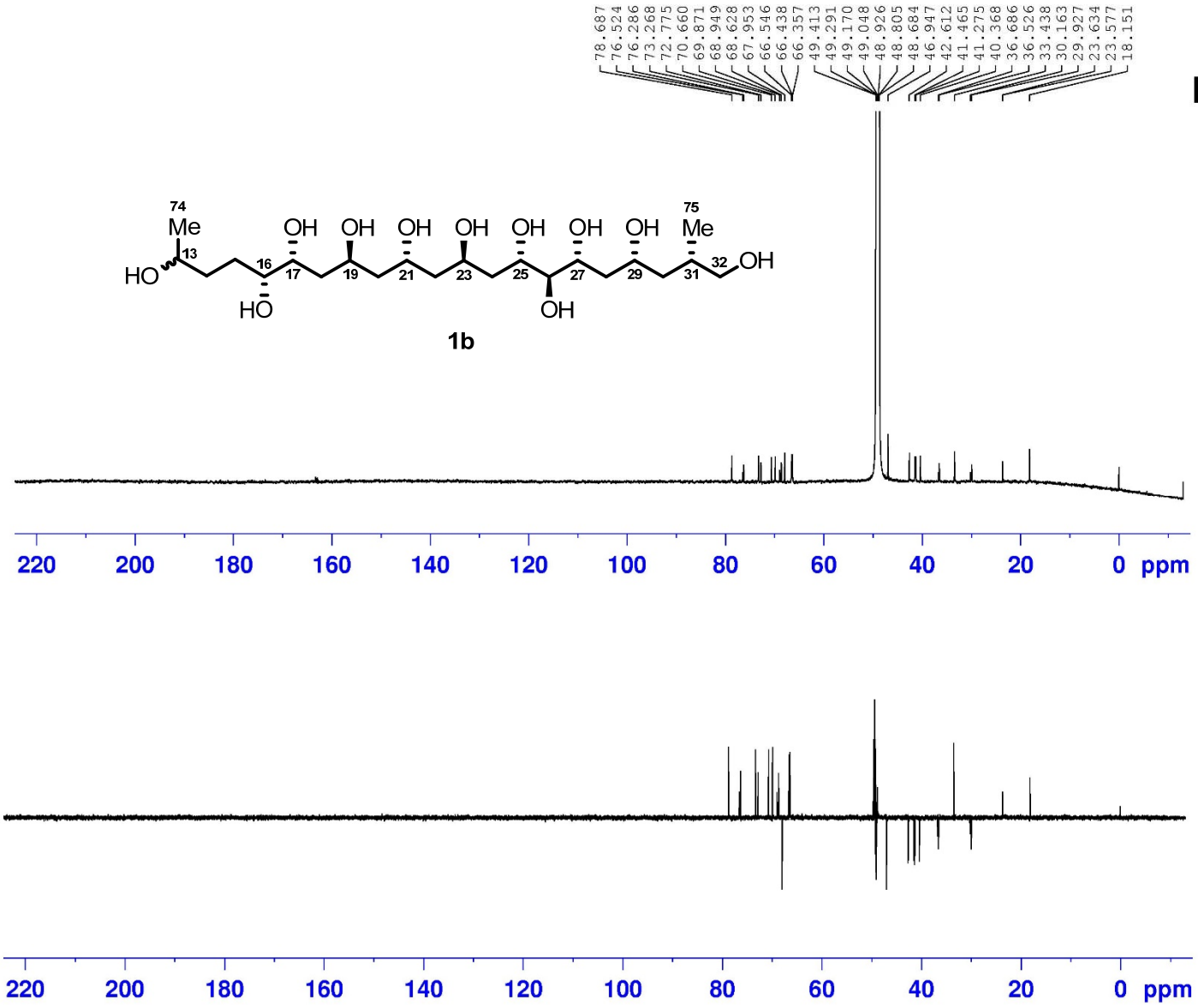
NAME	liwanshan-40-2-2-O
EXPNO	20
PROCNO	1
Date_	20200321
Time	5.36 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	zgpg30
TD	32768
SOLVENT	MeOD
NS	10000
DS	8
SWH	43859.648 Hz
FIDRES	2.676980 Hz
AQ	0.3736052 sec
RG	181.26
DW	11.400 use
DE	18.00 use
TE	298.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	176.0797677 MHz
NUC1	13C
P1	11.90 use
SI	32768
SF	176.0601446 MHz
WDW	EM
SSB	0
LB	5.00 Hz
GB	0
PC	1.40

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

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



DEPT135 (175 MHz) spectrum of the fragment **1b** in CD_3OD



1b

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NAME        liwanshan-40-2-2-
EXPNO                     21
PROCNO                     1
Date_               20200321
Time                    7.12 h
INSTRUM                 spect
PROBHD     Z120187_0028 (
PULPROG           deptsp135
TD                     32768
SOLVENT                 MeOD
NS                      4000
DS                         8
SWH                43859.648 Hz
FIDRES             2.676980 Hz
AQ                 0.3736052 se
RG                    181.26
DW                    11.400 us
DE                    18.00 us
TE                    298.0 K
CNST2             145.0000000
D1                  1.00000000 se
D2                  0.00344828 se
D12                 0.00002000 se
TD0                        1
SFO1              176.0797677 MH
NUC1                      13C
P1                    11.90 us
P13                 2000.00 us
SI                     32768
SF                176.0601437 MH
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```
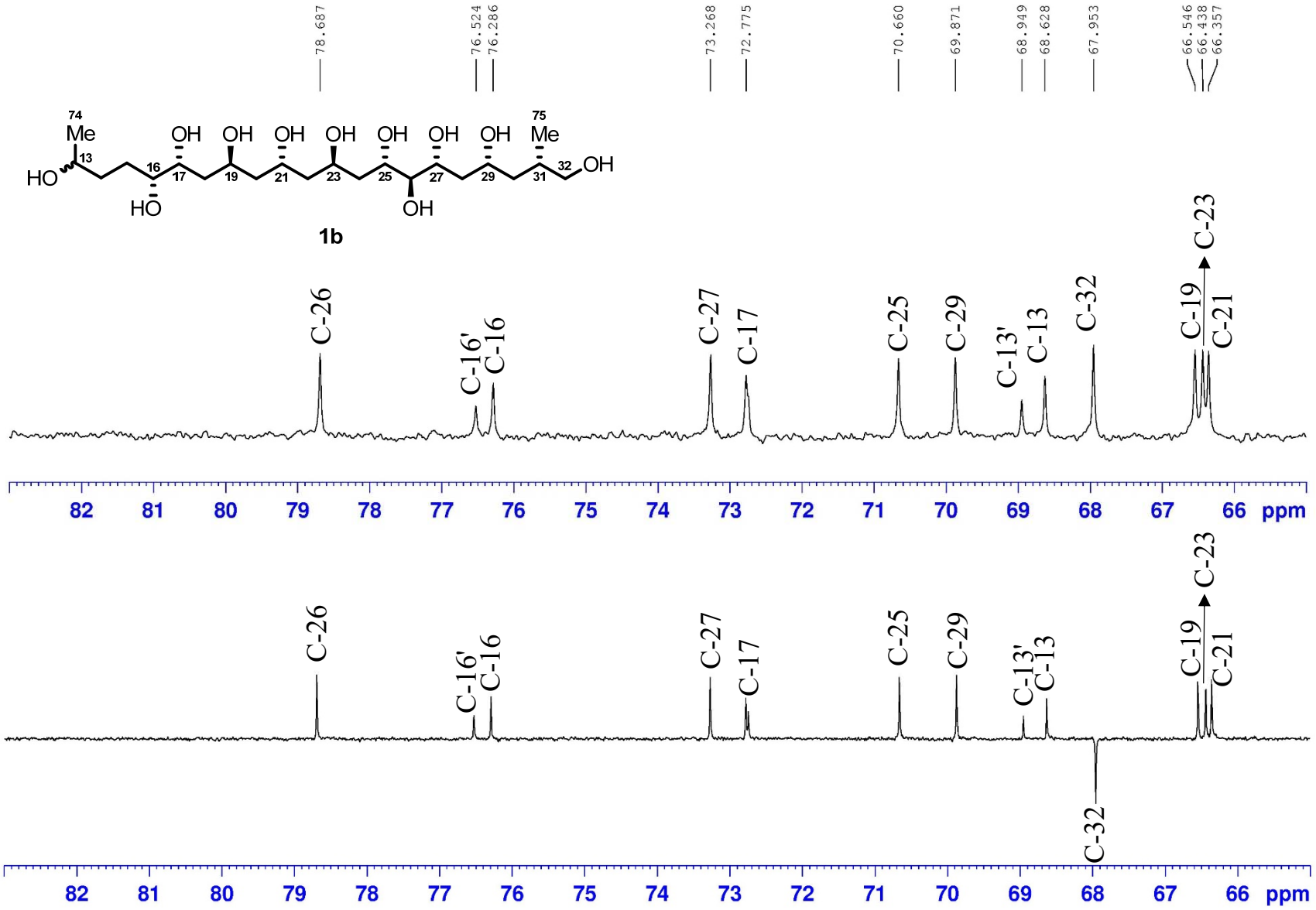
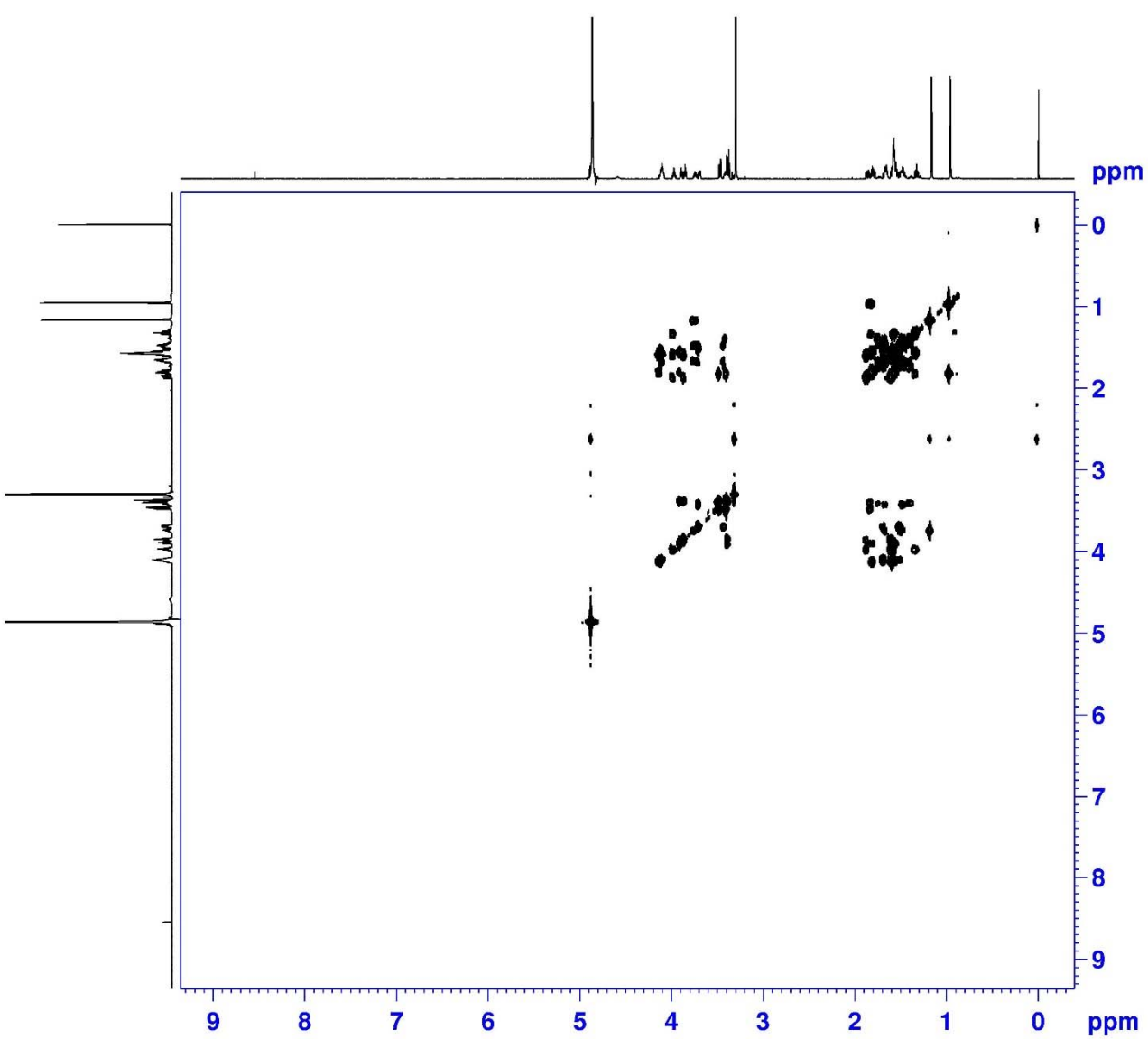

DEPT135 (175 MHz) spectrum of the fragment **1b** in CD_3OD



DEPT135 (175 MHz) spectrum of the fragment **1b** in CD_3OD

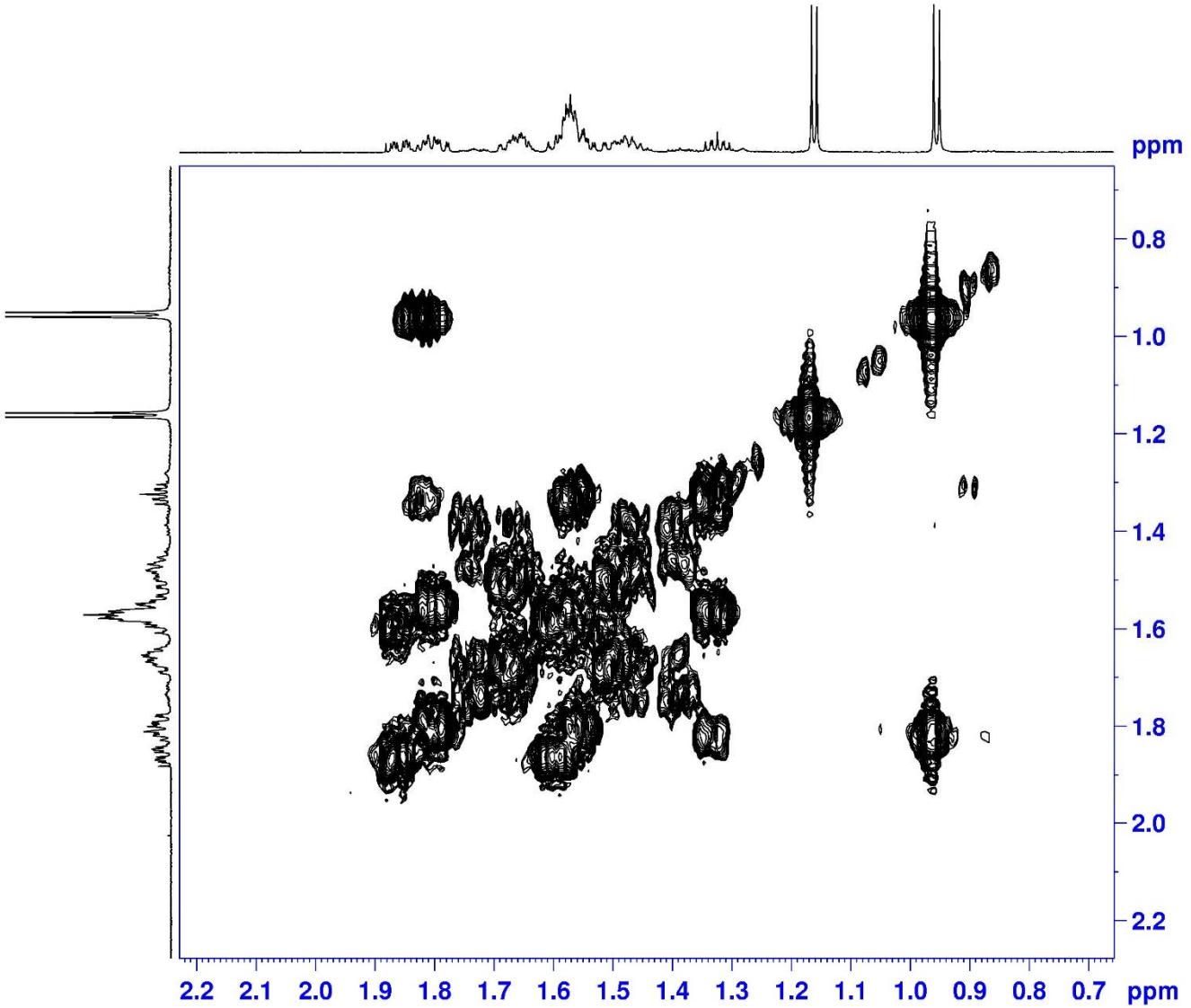
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1b** in CD_3OD



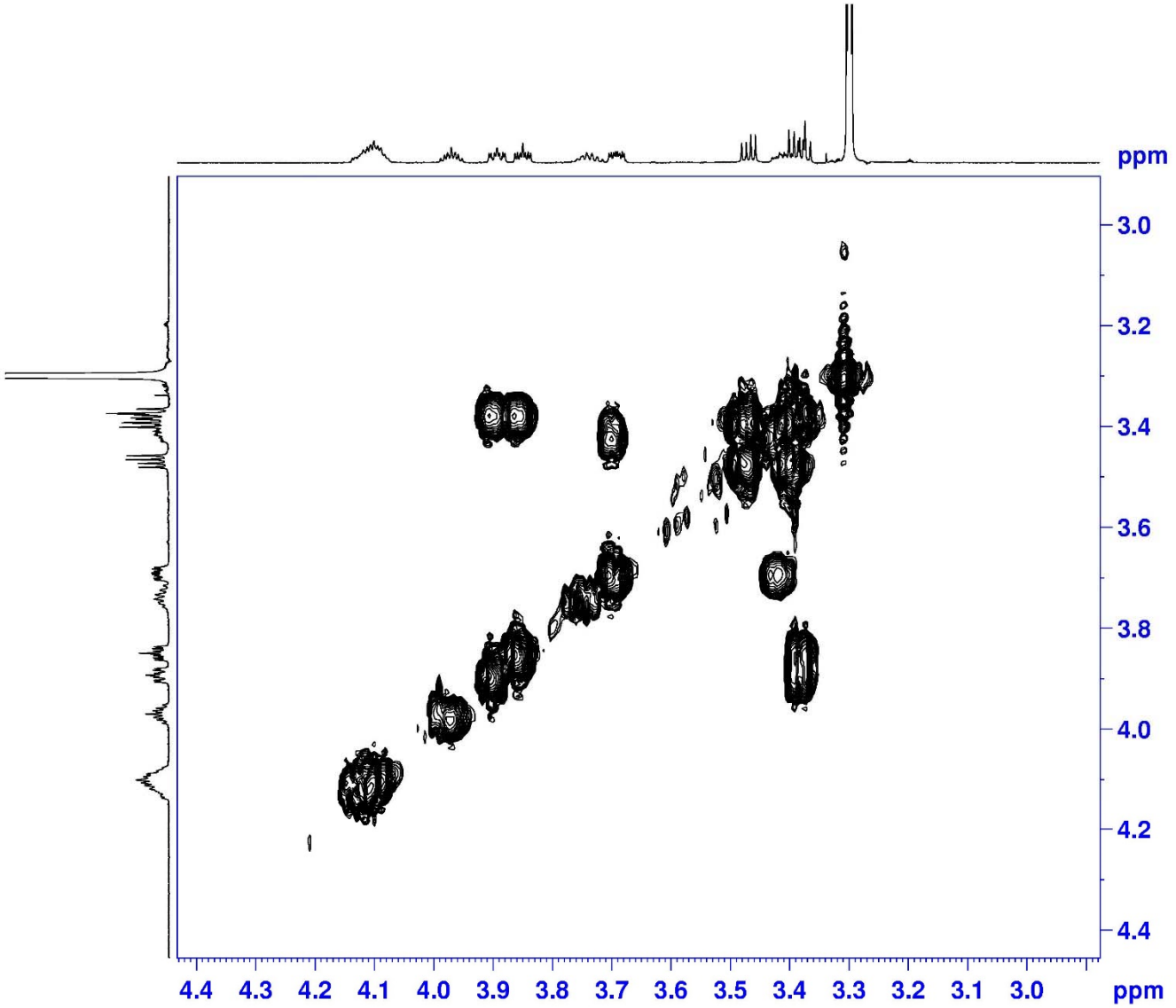
BRUKER

NAME	liwanshan-40-2-2-03-2
EXPNO	16
PROCNO	1
Date_	20200321
Time	7.14 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	cosygpmfqf
TD	2048
SOLVENT	MeOD
NS	32
DS	16
SWH	4347.826 Hz
FIDRES	4.245924 Hz
AQ	0.2355700 sec
RG	181.26
DW	115.000 usec
DE	10.00 usec
TE	298.0 K
D0	0.00000300 sec
D1	1.00000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00023000 sec
ND0	1
TD	128
SFO1	700.1819 MHz
FIDRES	33.967392 Hz
SW	6.210 ppm
FnMODE	QF
SI	1024
SF	700.1800165 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
ST	1024
MC2	QF
SF	700.1800165 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

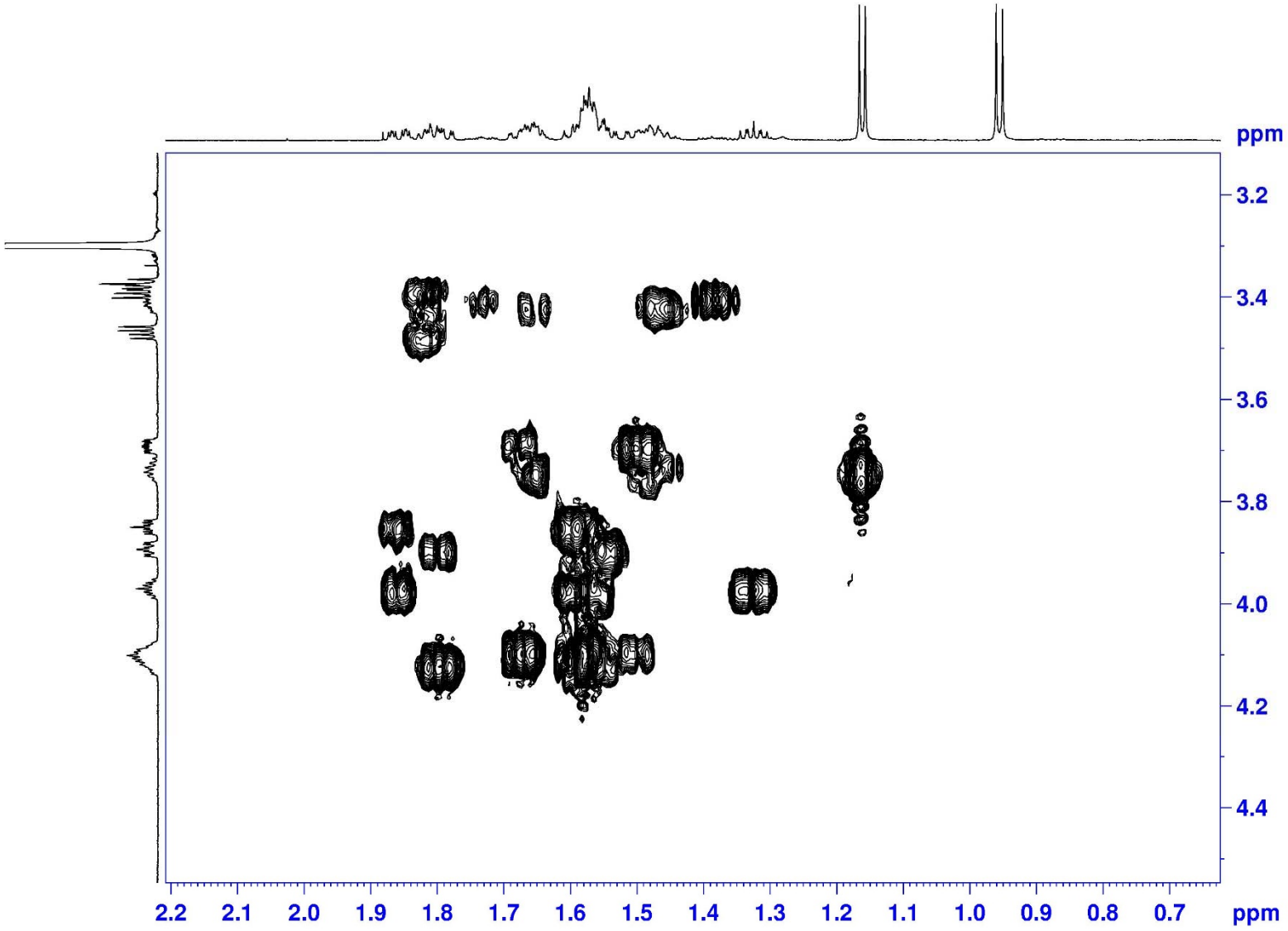
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1b** in CD_3OD



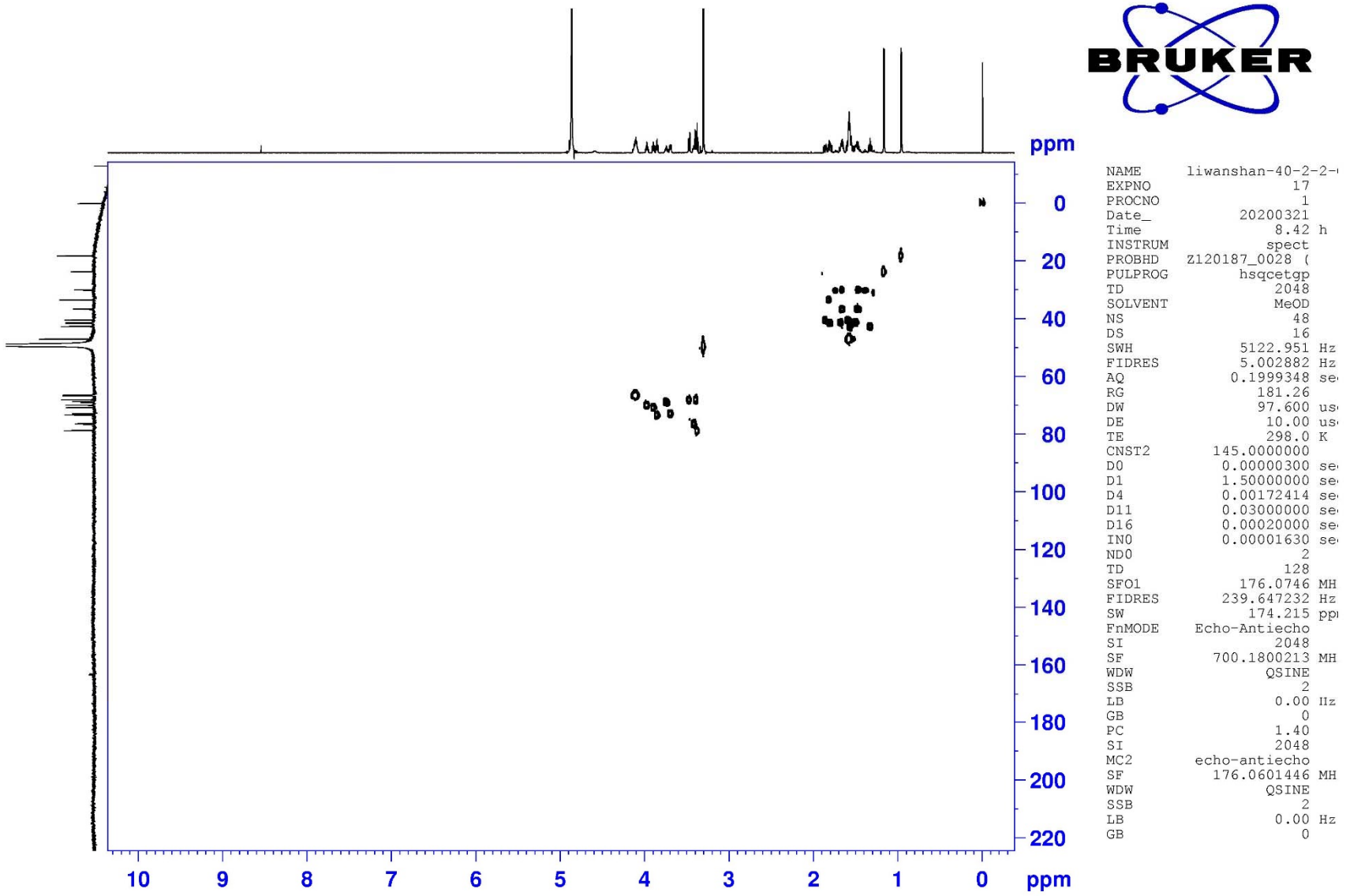
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1b** in CD_3OD



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

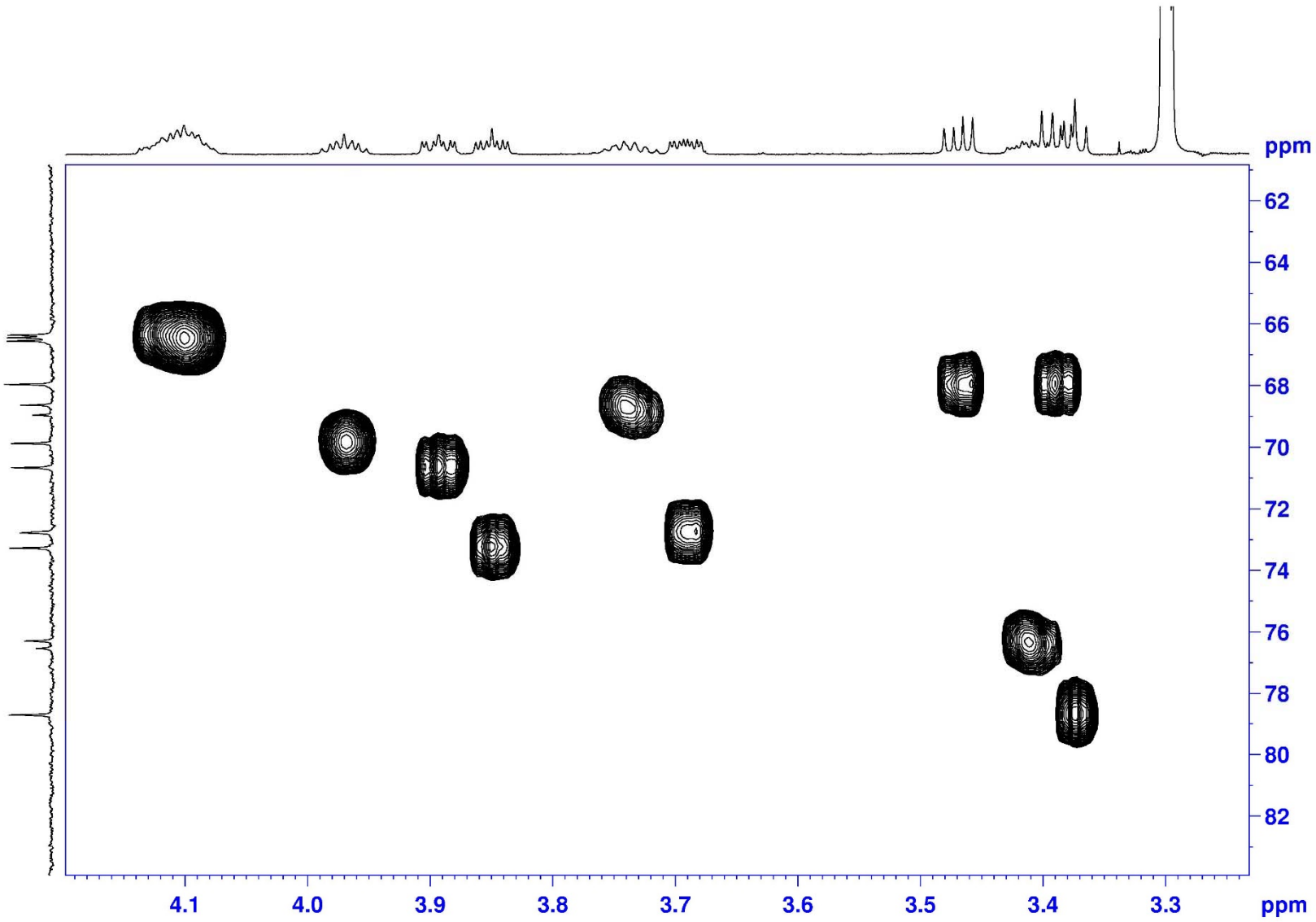


HSQC (700 MHz) spectrum of the fragment **1b** in CD_3OD

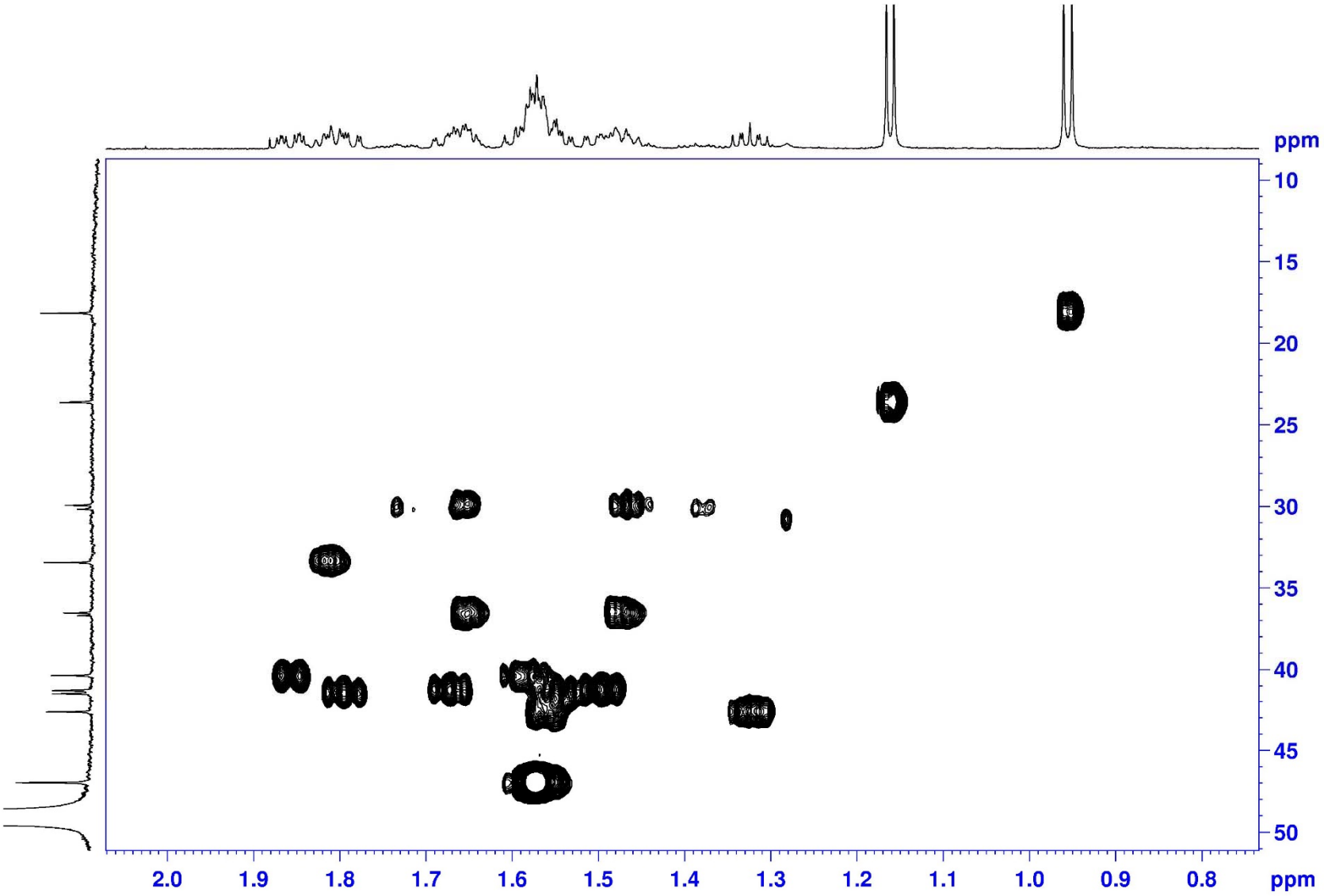


NAME	liwanshan-40-2-2-1
EXPNO	17
PROCNO	1
Date_	20200321
Time	8.42 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hsqcetgp
TD	2048
SOLVENT	MeOD
NS	48
DS	16
SWH	5122.951 Hz
FIDRES	5.002882 Hz
AQ	0.1999348 se
RG	181.26
DW	97.600 us
DE	10.00 us
TE	298.0 K
CNST2	145.0000000
D0	0.00000300 se
D1	1.50000000 se
D4	0.00172414 se
D11	0.03000000 se
D16	0.00020000 se
IN0	0.00001630 se
ND0	2
TD	128
SFO1	176.0746 MH
FIDRES	239.647232 Hz
SW	174.215 pp
FnMODE	Echo-Antiecho
SI	2048
SF	700.1800213 MH
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	2048
MC2	echo-antiecho
SF	176.0601446 MH
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

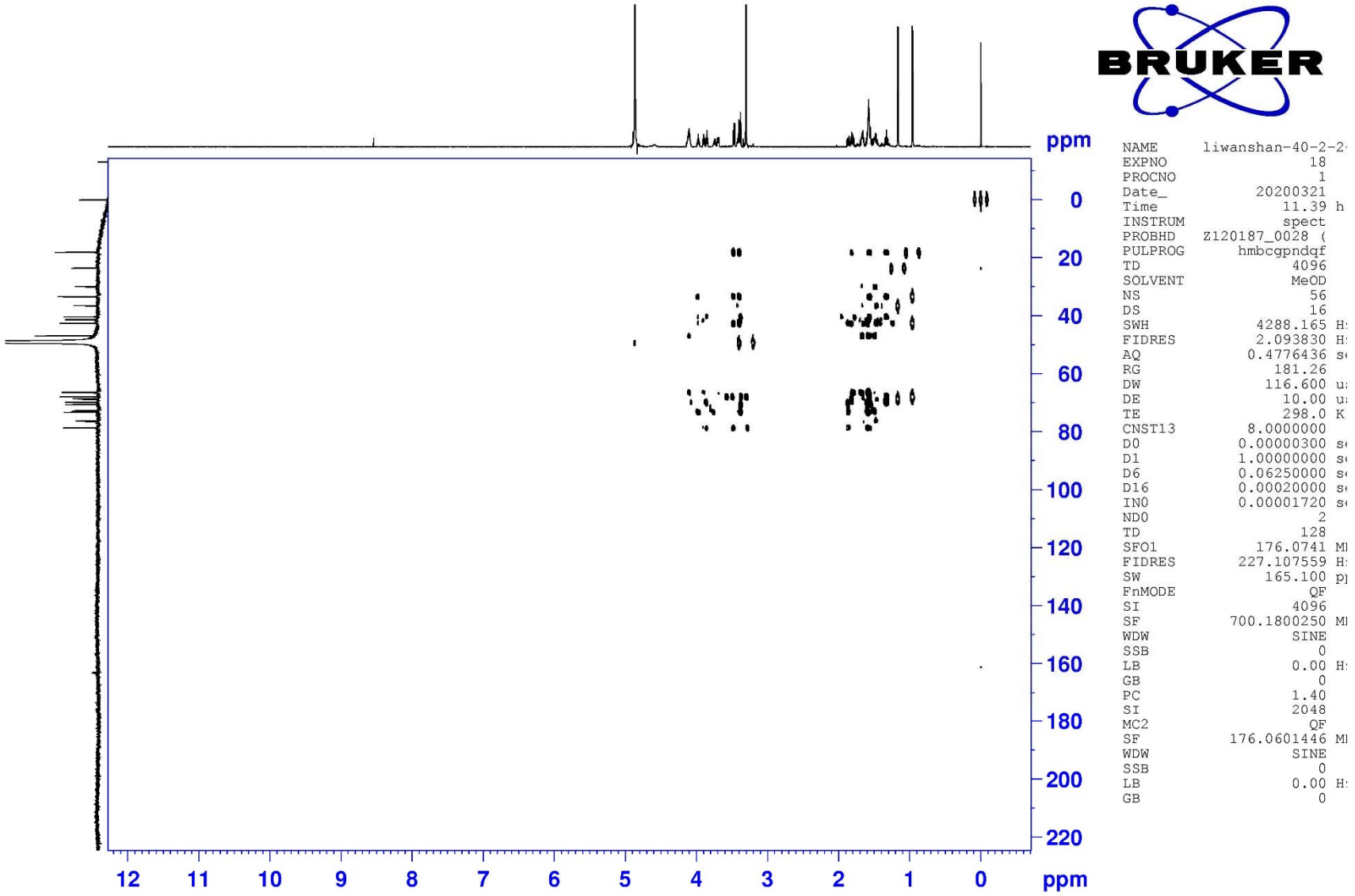
HSQC (700 MHz) spectrum of the fragment **1b** in CD_3OD



HSQC (700 MHz) spectrum of the fragment **1b** in CD_3OD

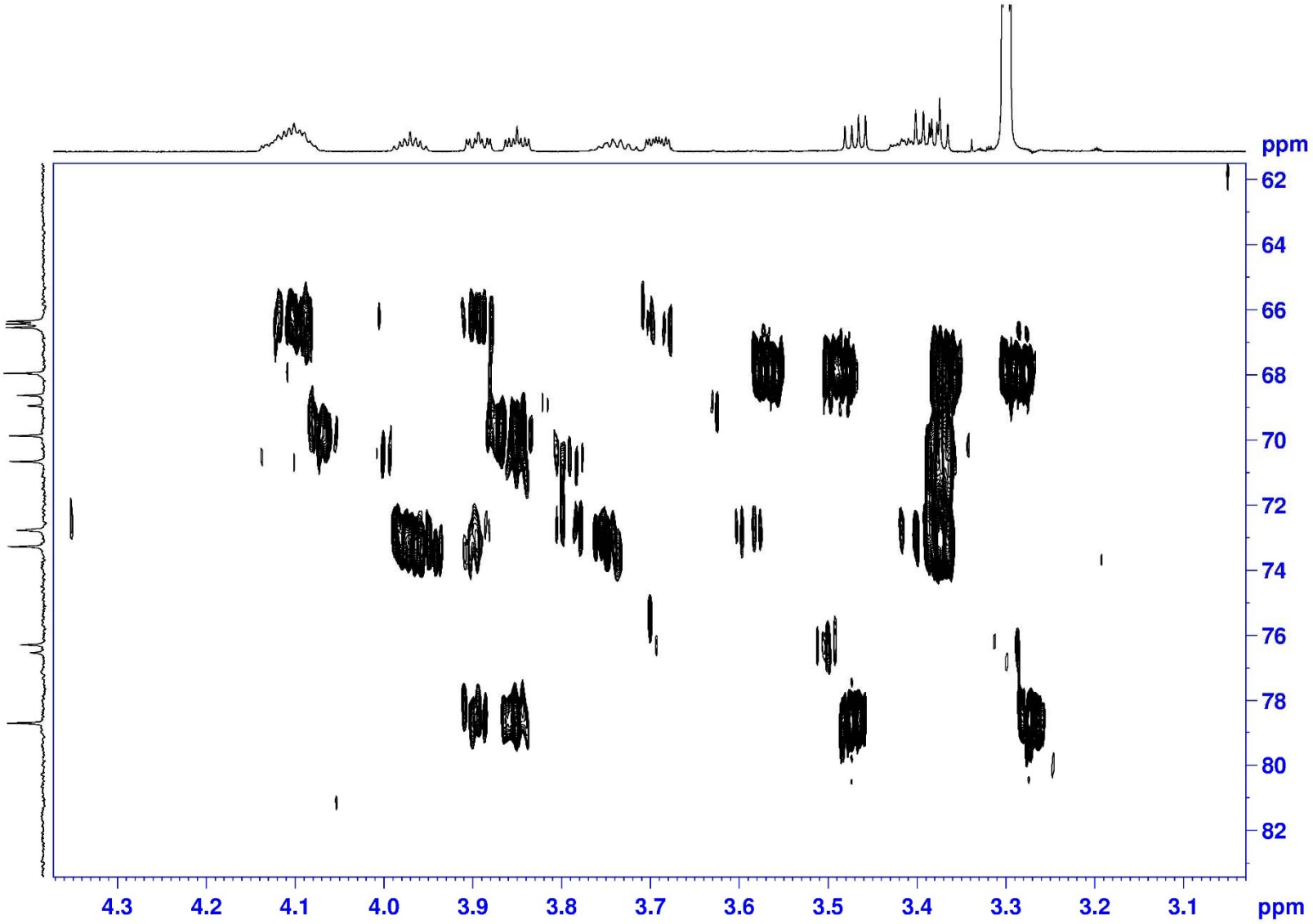


HMBC (700 MHz) spectrum of the fragment **1b** in CD_3OD

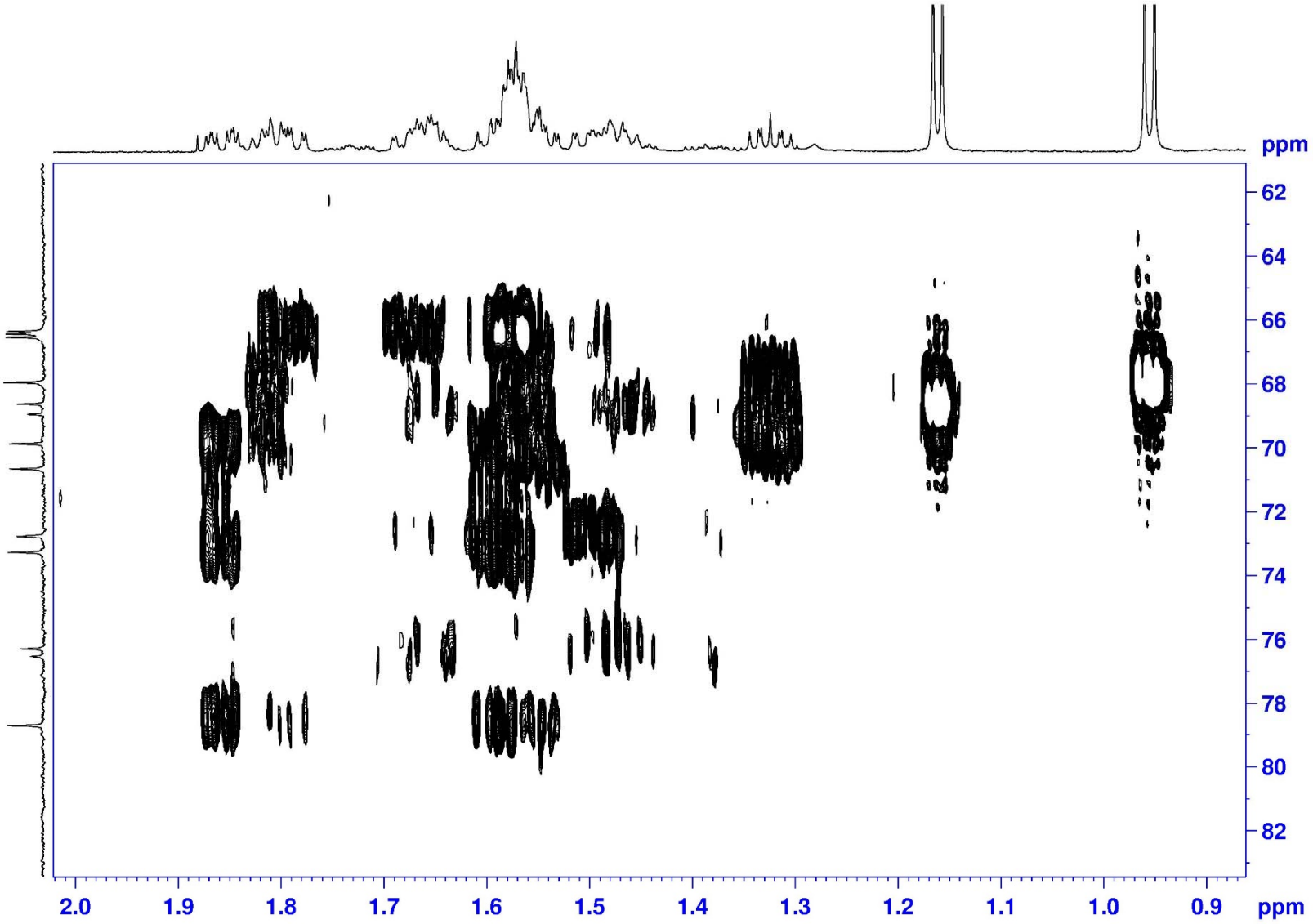



```
NAME        liwanshan-40-2-2
EXPNO               18
PROCNO              1
Date_           20200321
Time            11.39 h
INSTRUM         spect
PROBHD      Z120187_0028 (
PULPROG       hmbcgpndqf
TD                4096
SOLVENT           MeOD
NS                  56
DS                  16
SWH           4288.165 H
FIDRES        2.093830 H
AQ            0.4776436 s
RG              181.26
DW              116.600 u
DE               10.00 u
TE              298.0 K
CNST13         8.0000000
D0            0.00000300 s
D1            1.00000000 s
D6            0.06250000 s
D16           0.00020000 s
IN0           0.00001720 s
ND0                 2
TD                128
SFO1          176.0741 M
FIDRES        227.107559 H
SW              165.100 p
FnMODE              QF
SI                4096
SF          700.1800250 M
WDW               SINE
SSB                 0
LB                0.00 H
GB                  0
PC                1.40
SI                2048
MC2                 QF
SF          176.0601446 M
WDW               SINE
SSB                 0
LB                0.00 H
GB                  0
```

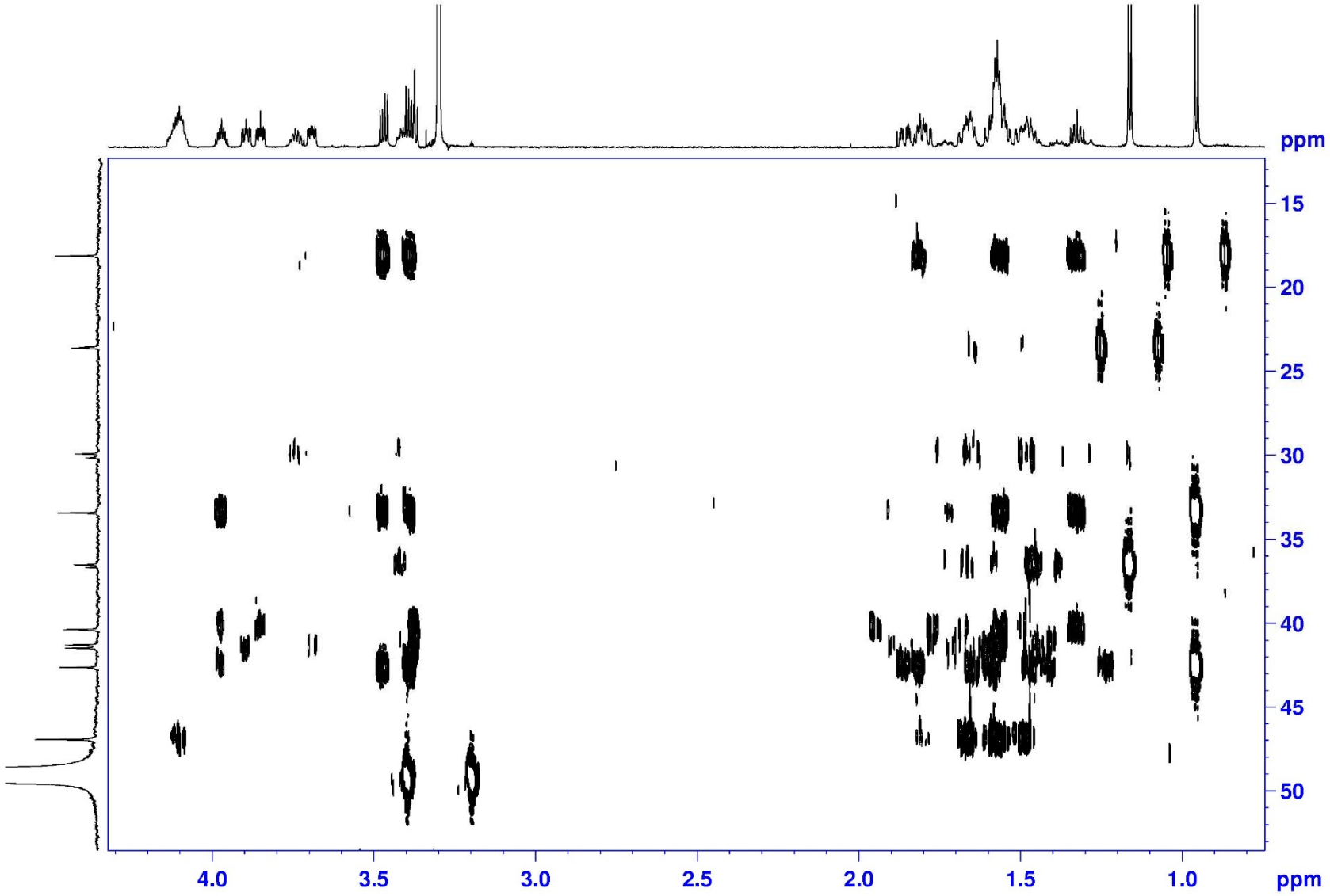
HMBC (700 MHz) spectrum of the fragment **1b** in CD_3OD



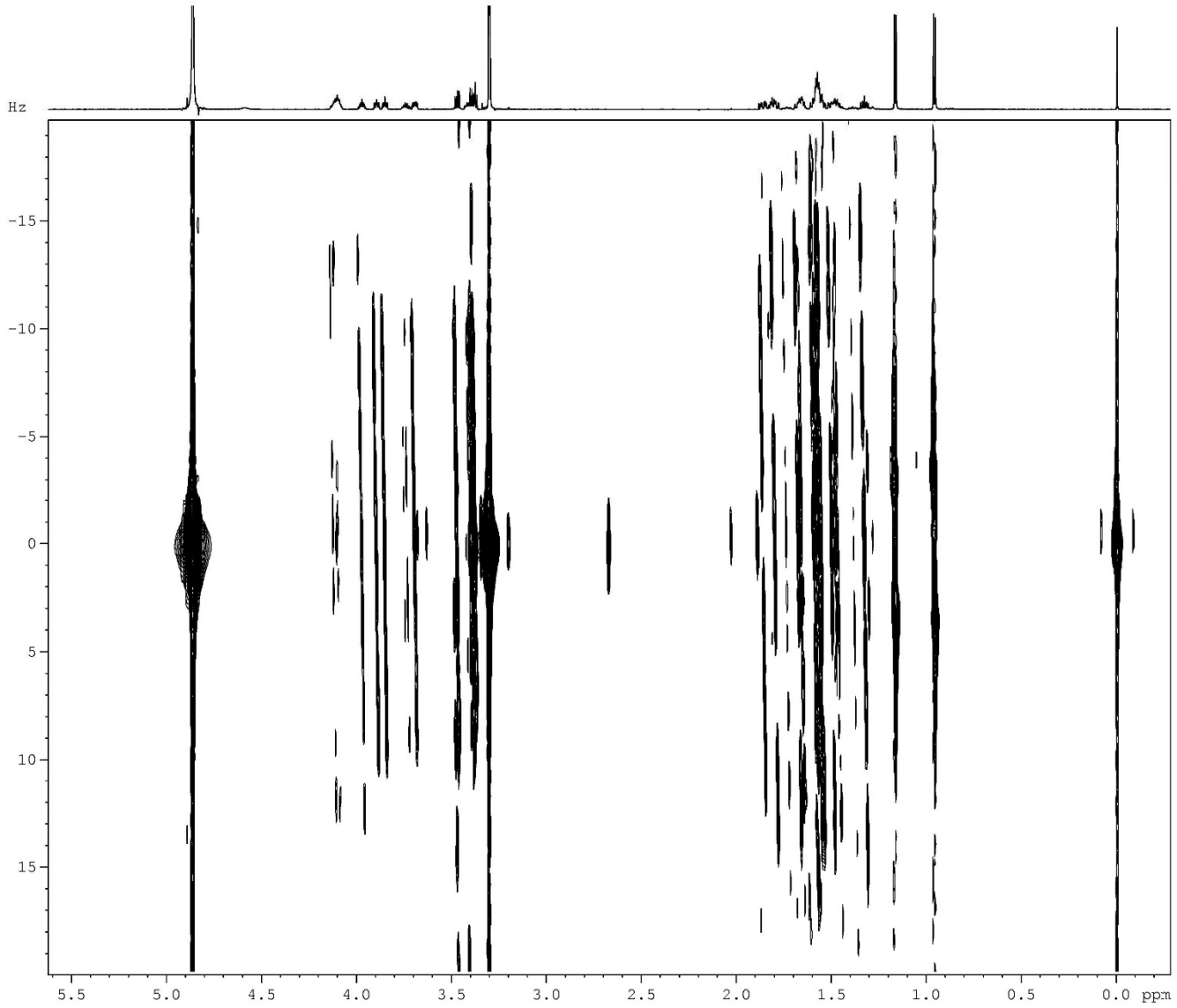
HMBC (700 MHz) spectrum of the fragment **1b** in CD_3OD



HMBC (700 MHz) spectrum of the fragment **1b** in CD_3OD

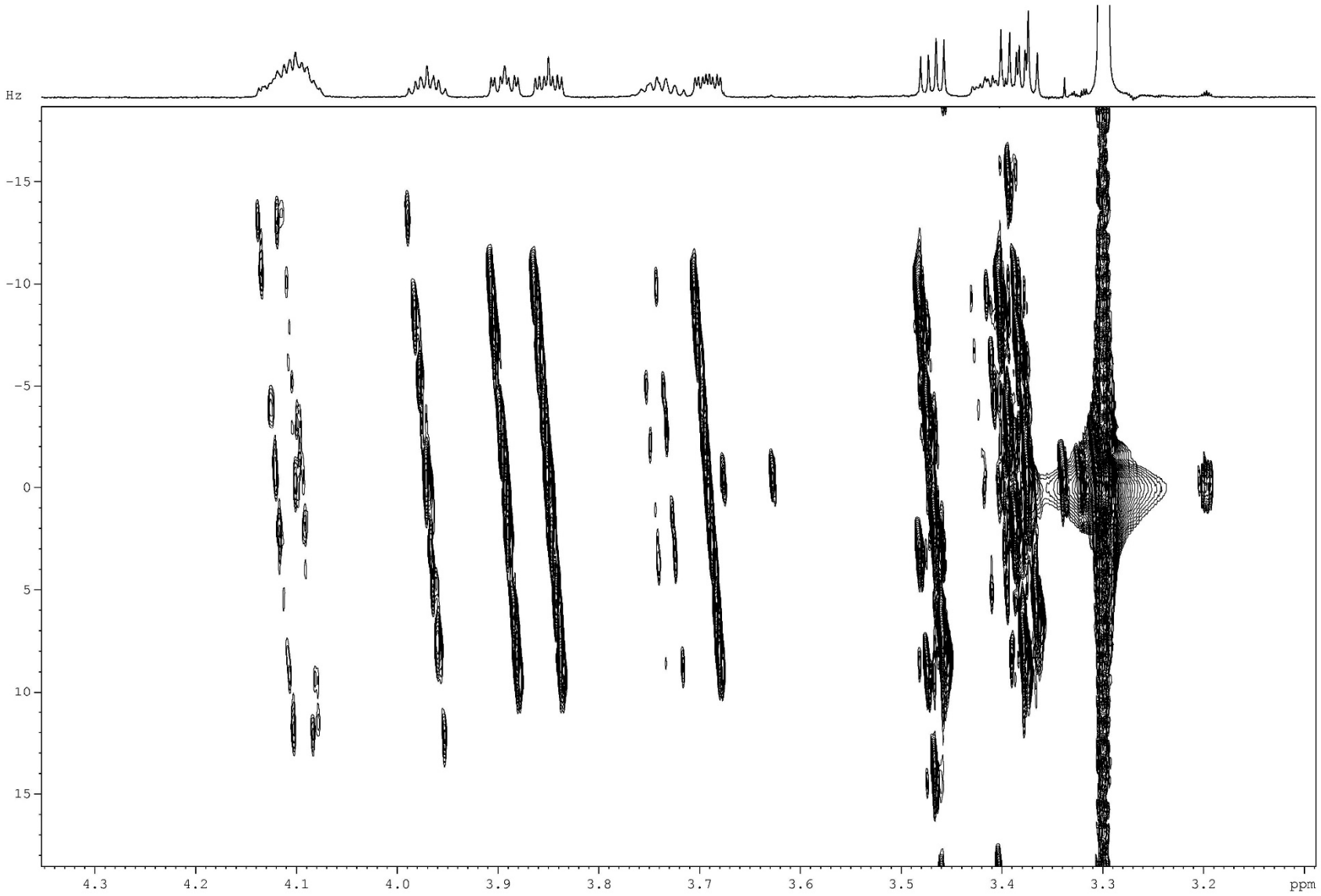


2D *J*RES (700 MHz) spectrum of the fragment **1b** in CD_3OD

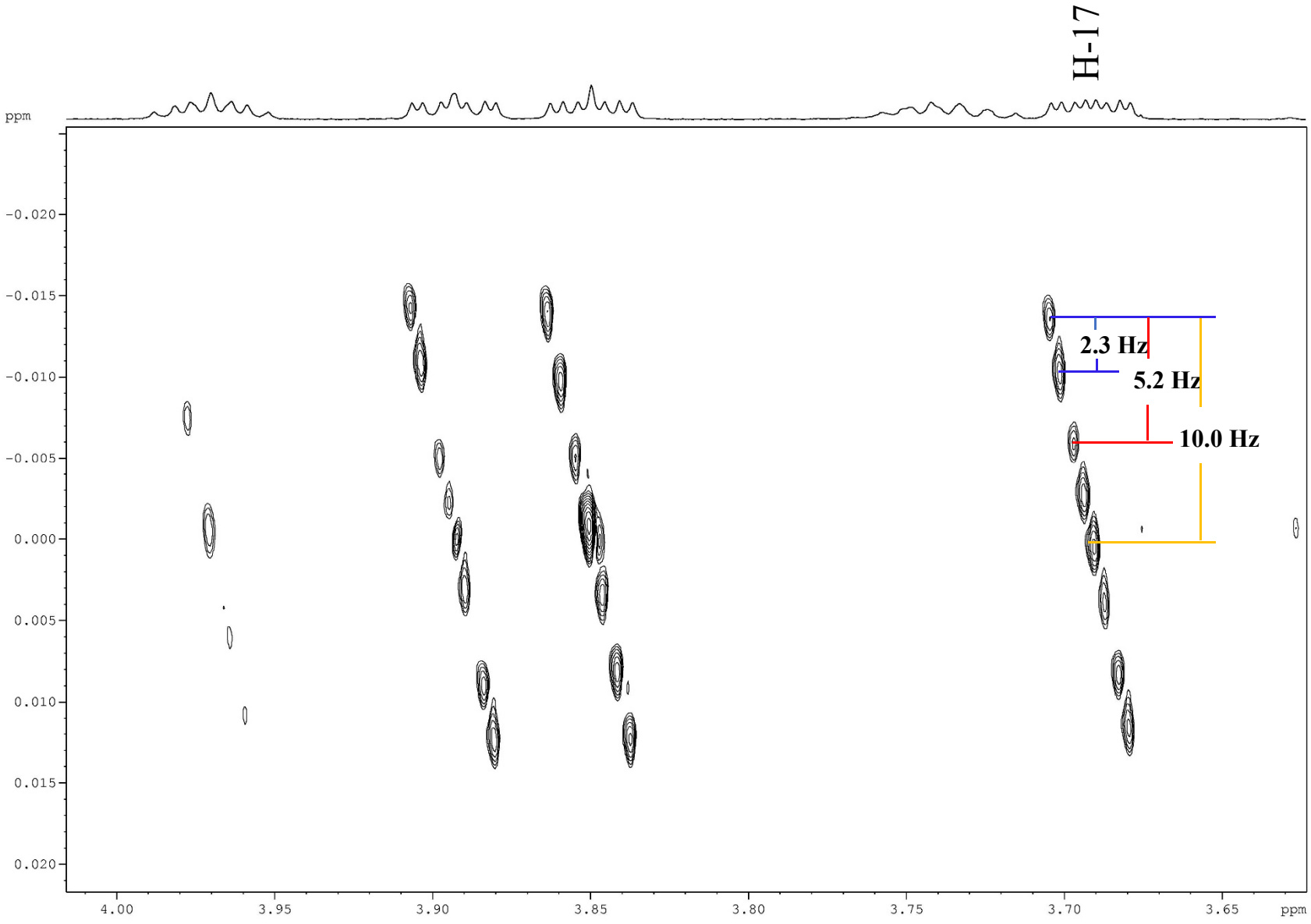



```
NAME      liwanshan-40-2-2-03-2
EXPNO                    24
PROCNO                    1
Date_              20200326
Time                  22.32 h
INSTRUM                spect
PROBHD    Z120187_0028 (
PULPROG          jresgpprqf
TD                     8192
SOLVENT                MeOD
NS                      128
DS                       16
SWH                4139.073 Hz
FIDRES             1.010516 Hz
AQ                 0.9896436 sec
RG                    124.11
DW                   120.800 usec
DE                    10.00 usec
TE                    298.0 K
D0                0.00000300 sec
D1                1.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
D16               0.00020000 sec
IN0               0.01250000 sec
ND0                      2
TD                      40
SFO1               700.1819 MHz
FIDRES             1.000000 Hz
SW                    0.057 ppm
FnMODE                   QF
SI                    16384
SF              700.1800224 MHz
WDW                    SINE
SSB                       0
LB                    0.00 Hz
GB                        0
PC                     1.00
SI                      128
MC2                      QF
SF              700.1818905 MHz
WDW                    SINE
SSB                       0
LB                    0.00 Hz
GB                        0
```

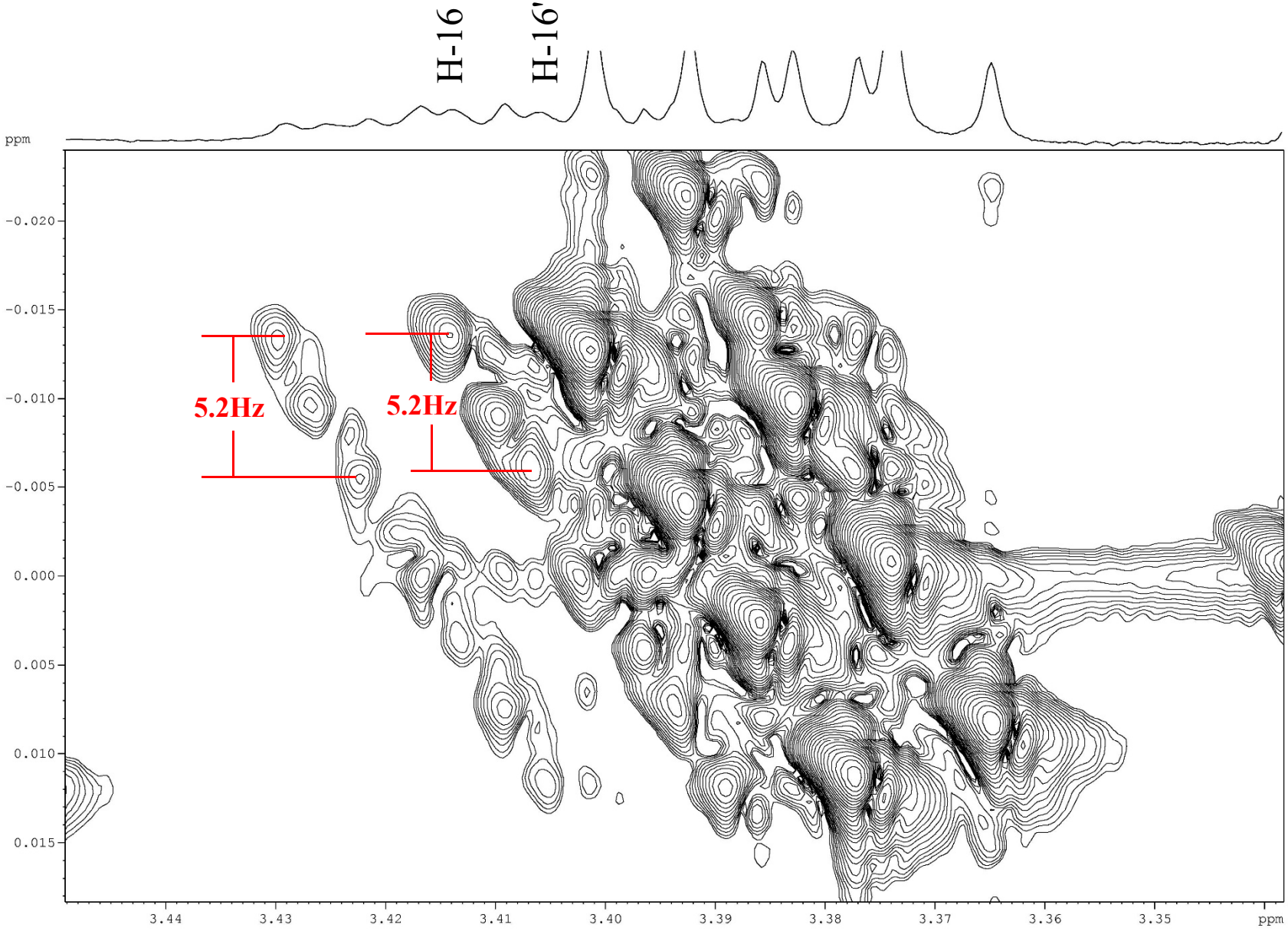
2D *J*RES (700 MHz) spectrum of the fragment **1b** in CD_3OD



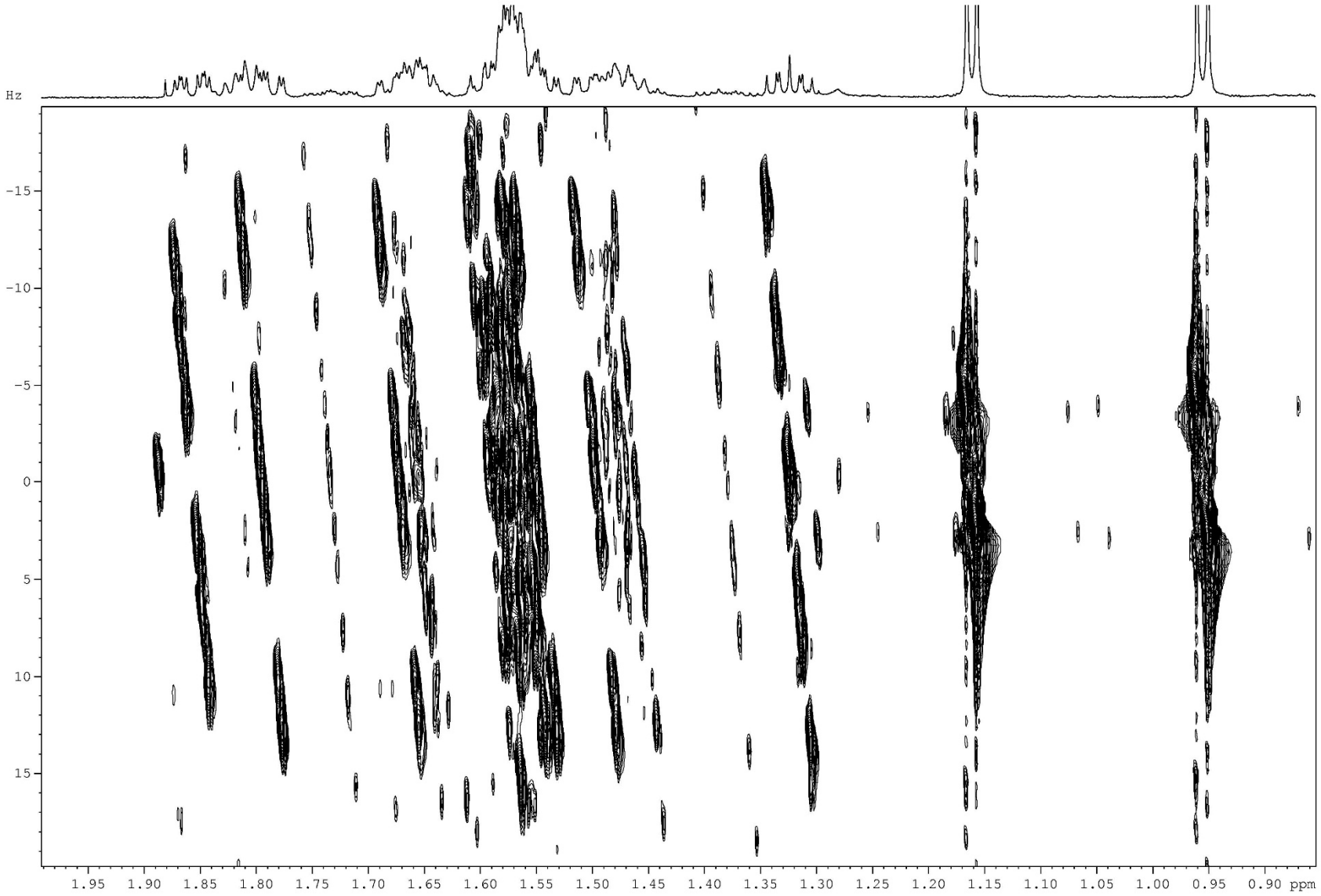
2D *J*RES (700 MHz) spectrum of the fragment **1b** in CD_3OD



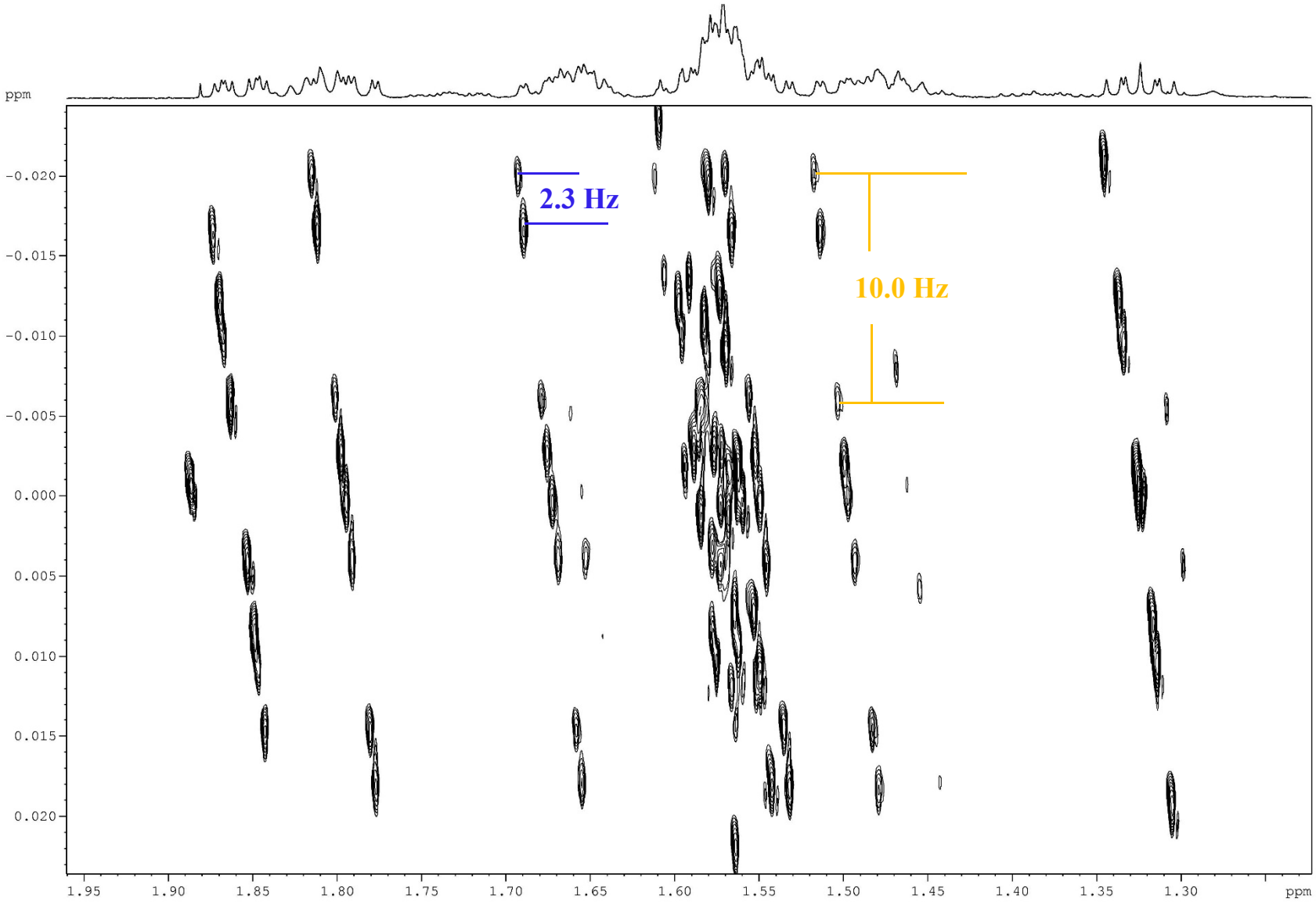
2D *J*RES (700 MHz) spectrum of the fragment **1b** in CD_3OD



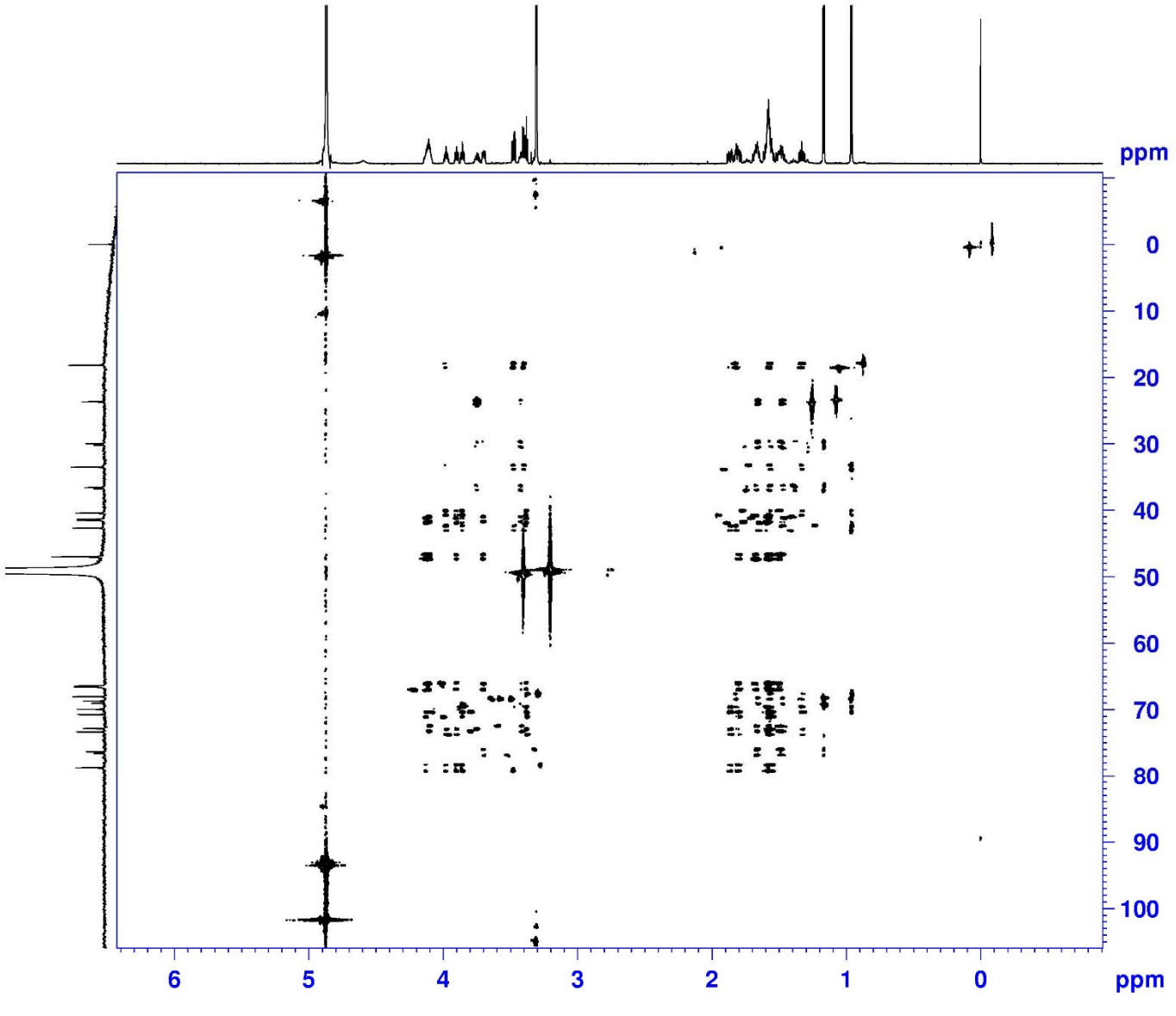
2D *J*RES (700 MHz) spectrum of the fragment **1b** in CD_3OD

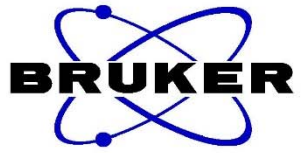


2D *J*RES (700 MHz) spectrum of the fragment **1b** in CD_3OD



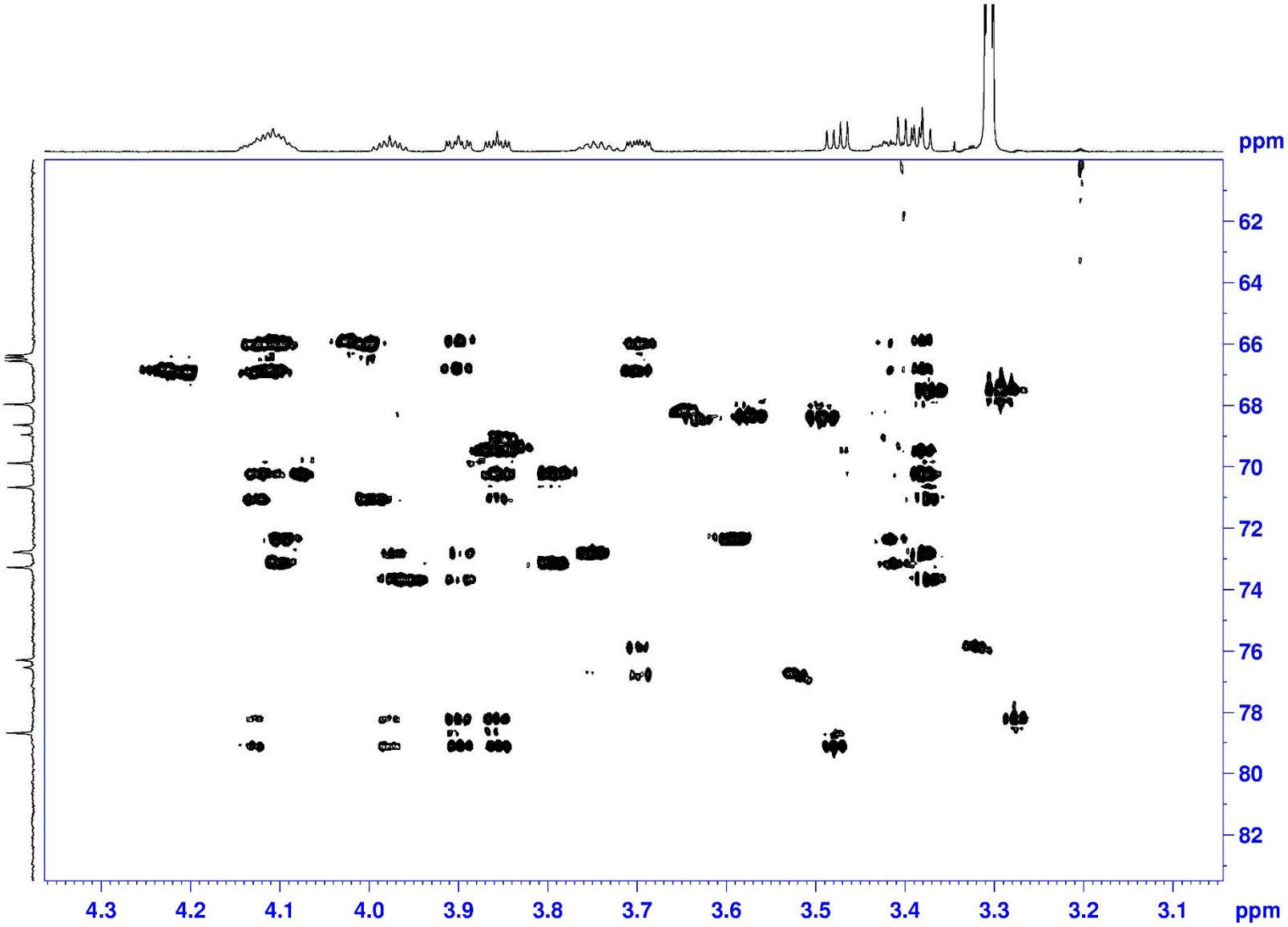
HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



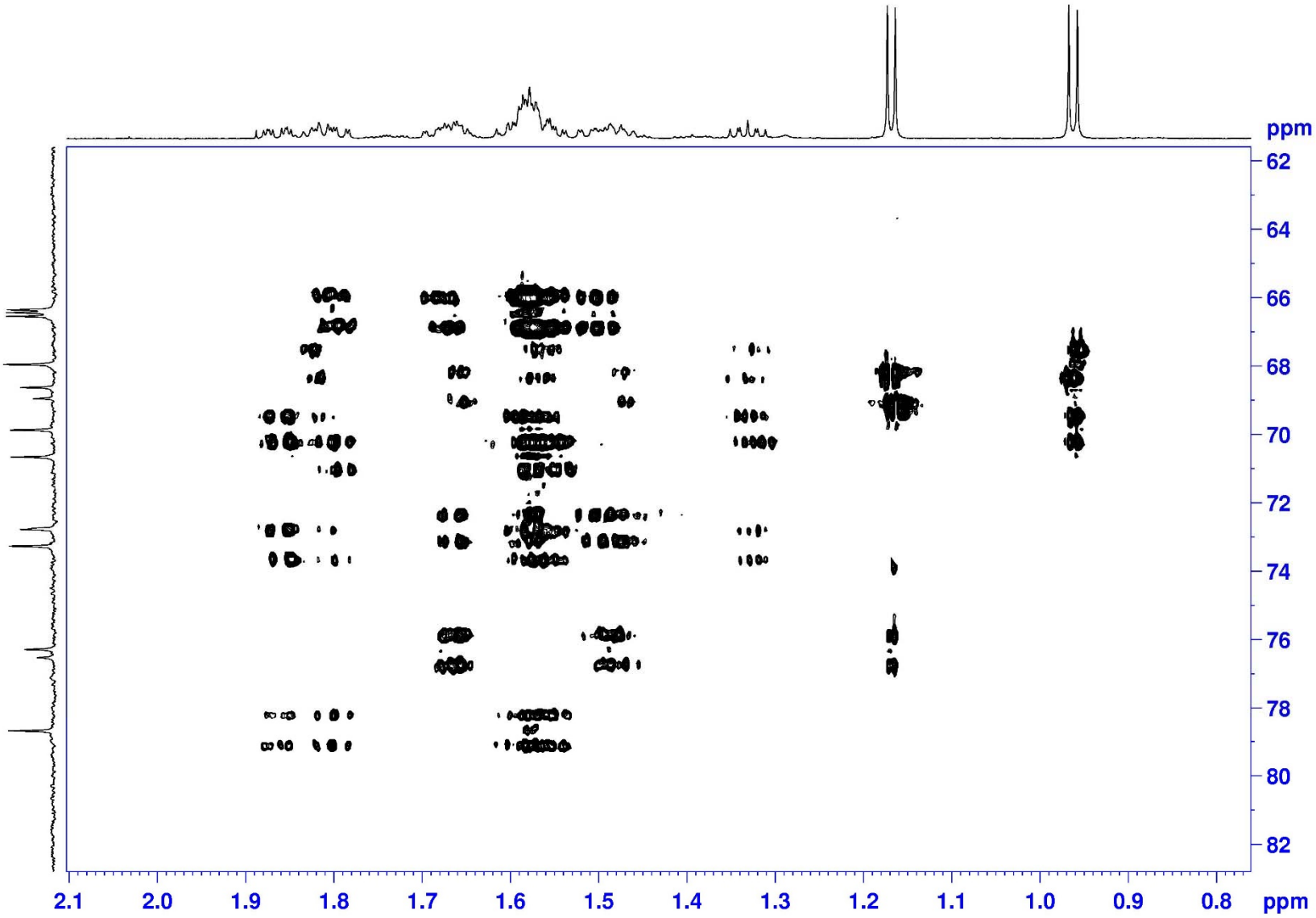


NAME	liwanshan-40-2-2-03-
EXPNO	29
PROCNO	1
Date_	20200819
Time	14.17 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hsqcdietgpjcndsisp
TD	4096
SOLVENT	MeOD
NS	56
DS	16
SWH	5136.986 Hz
FIDRES	2.508294 Hz
AQ	0.3987273 sec
RG	181.26
DW	97.333 usec
DE	10.00 usec
TE	298.0 K
CNST2	145.0000000
CNST16	1.0000000
CNST17	-0.5000000
D0	0.00000300 sec
D1	1.00000000 sec
D2	0.00344828 sec
D4	0.00172414 sec
D9	0.08000000 sec
D16	0.00020000 sec
D20	0.00000300 sec
D24	0.00089000 sec
IN0	0.00002430 sec
IN20	0.00002430 sec
L0	1
L1	28
ND0	2
TD	512
SFO1	176.0685 MHz
FIDRES	40.187756 Hz
SW	116.864 ppm
FnMODE	Echo-Antiecho
SI	8192
SF	700.1800183 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	176.0601399 MHz
WDW	QSINE
SSB	2

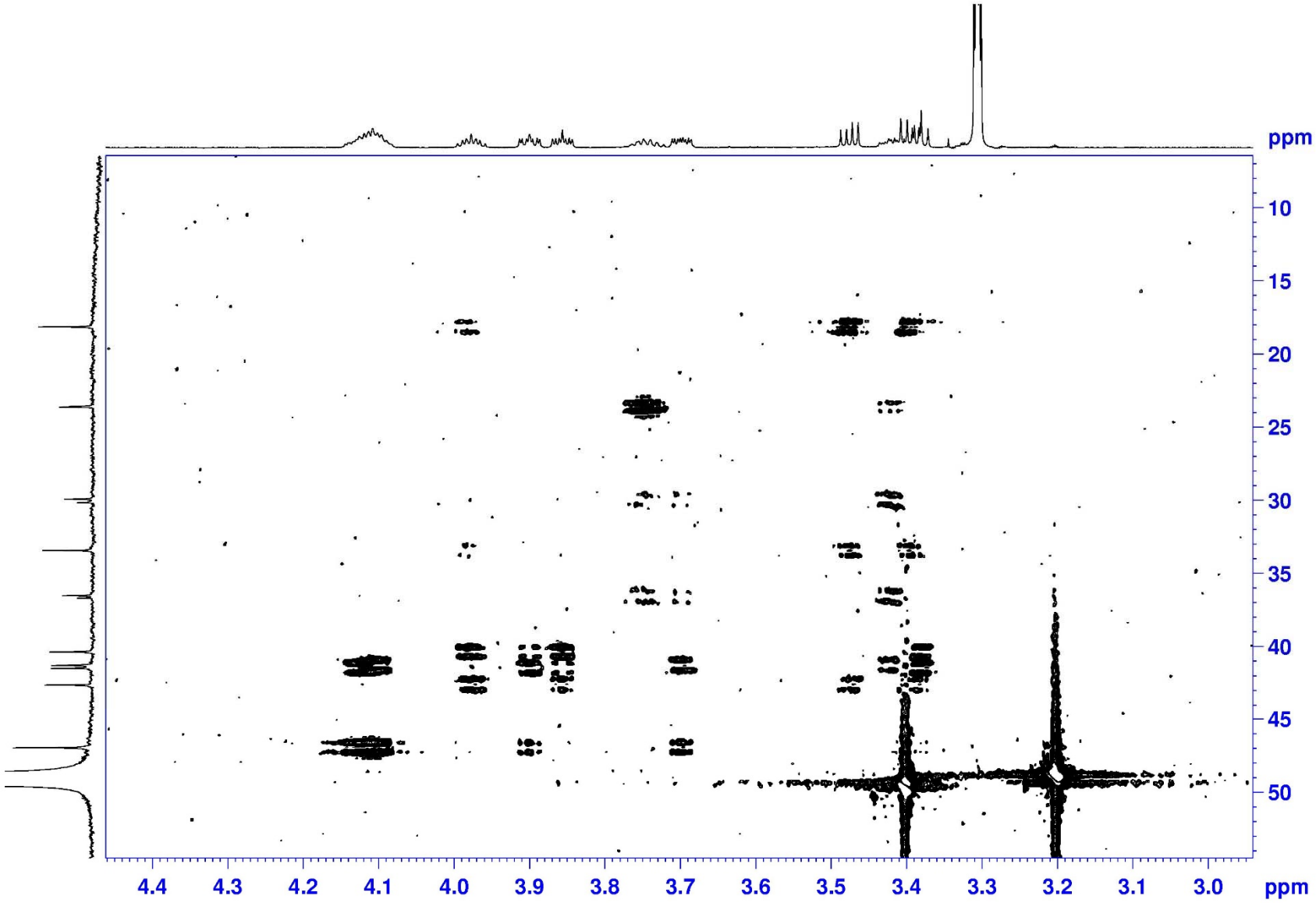
HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



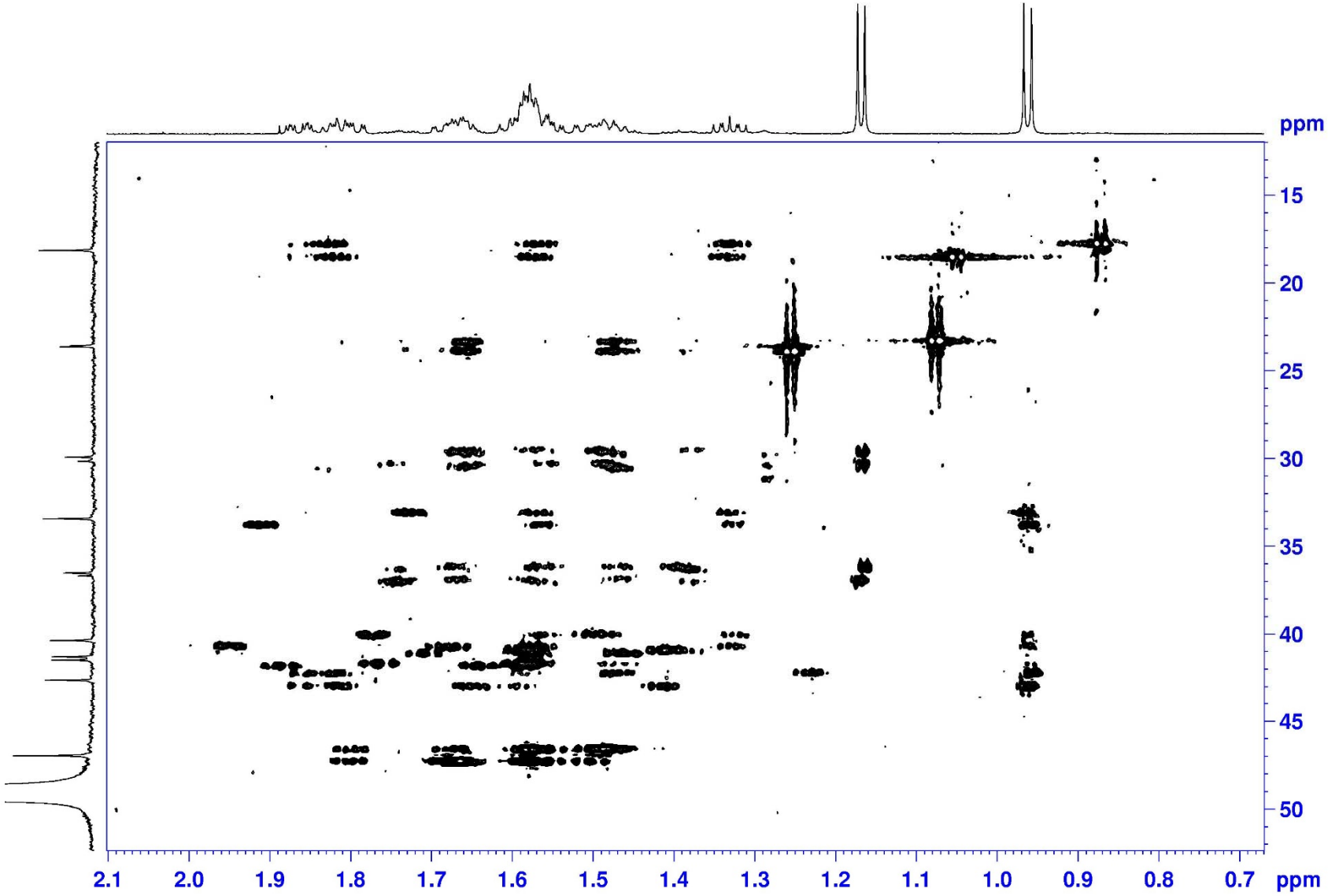
HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



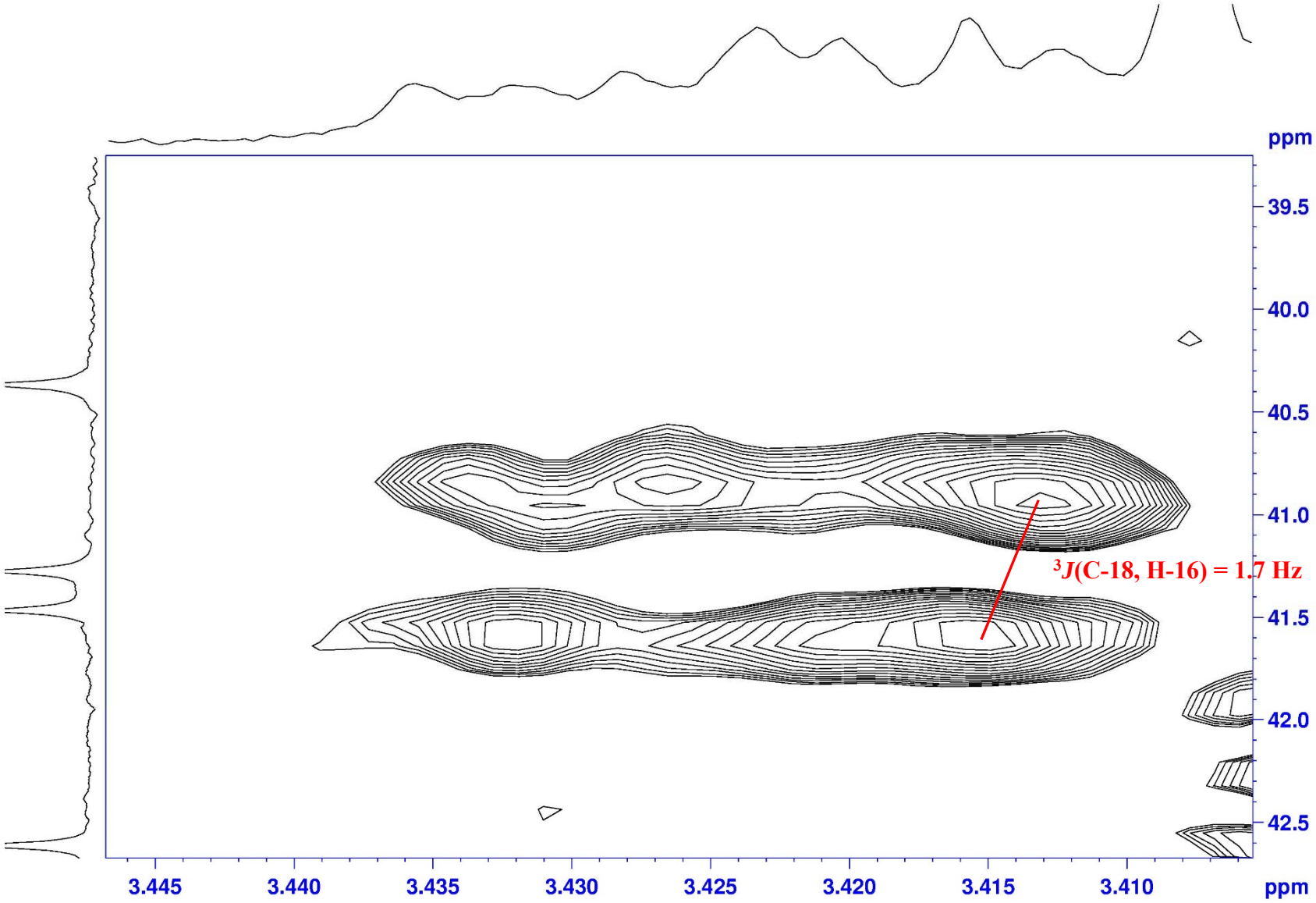
HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



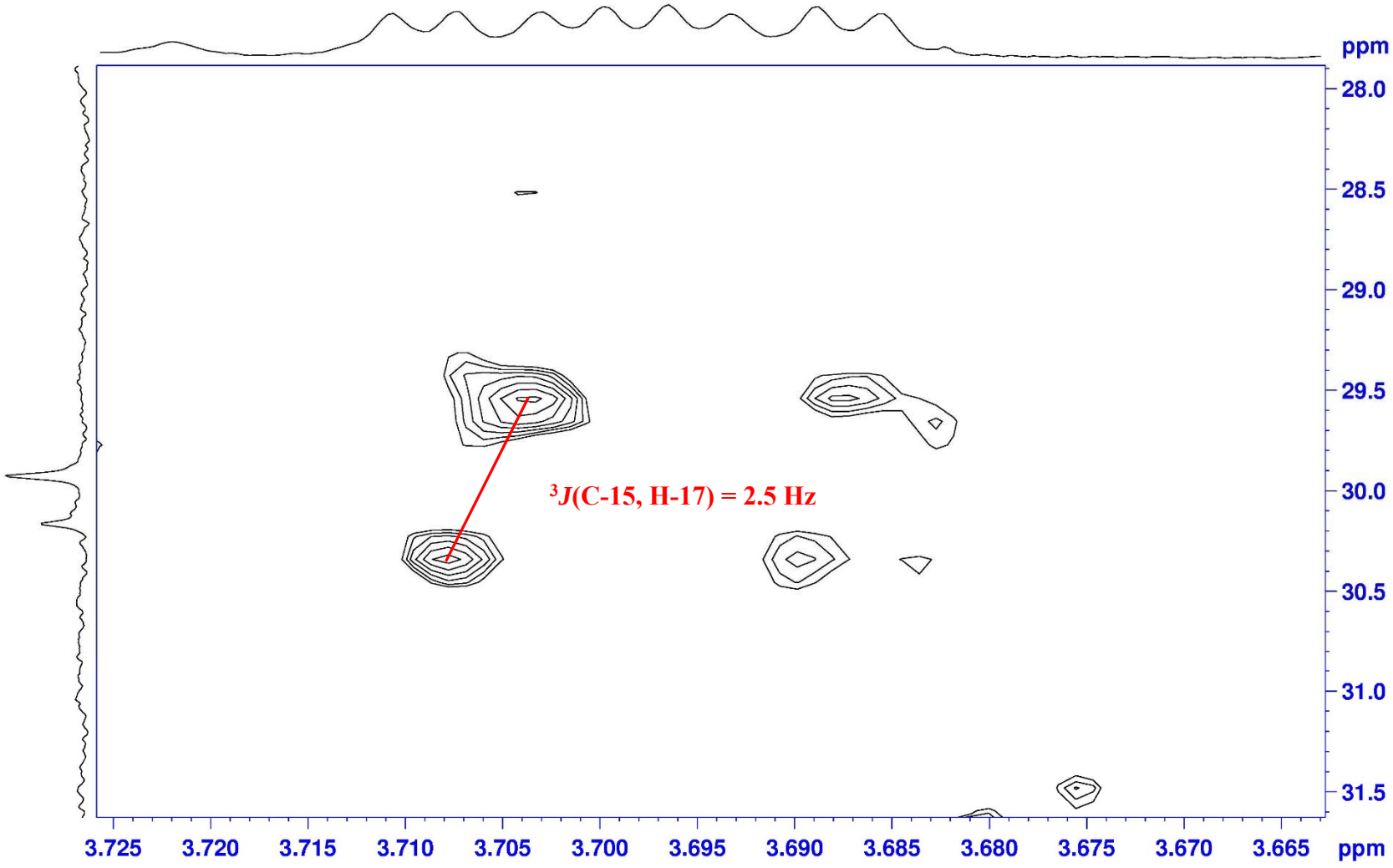
HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



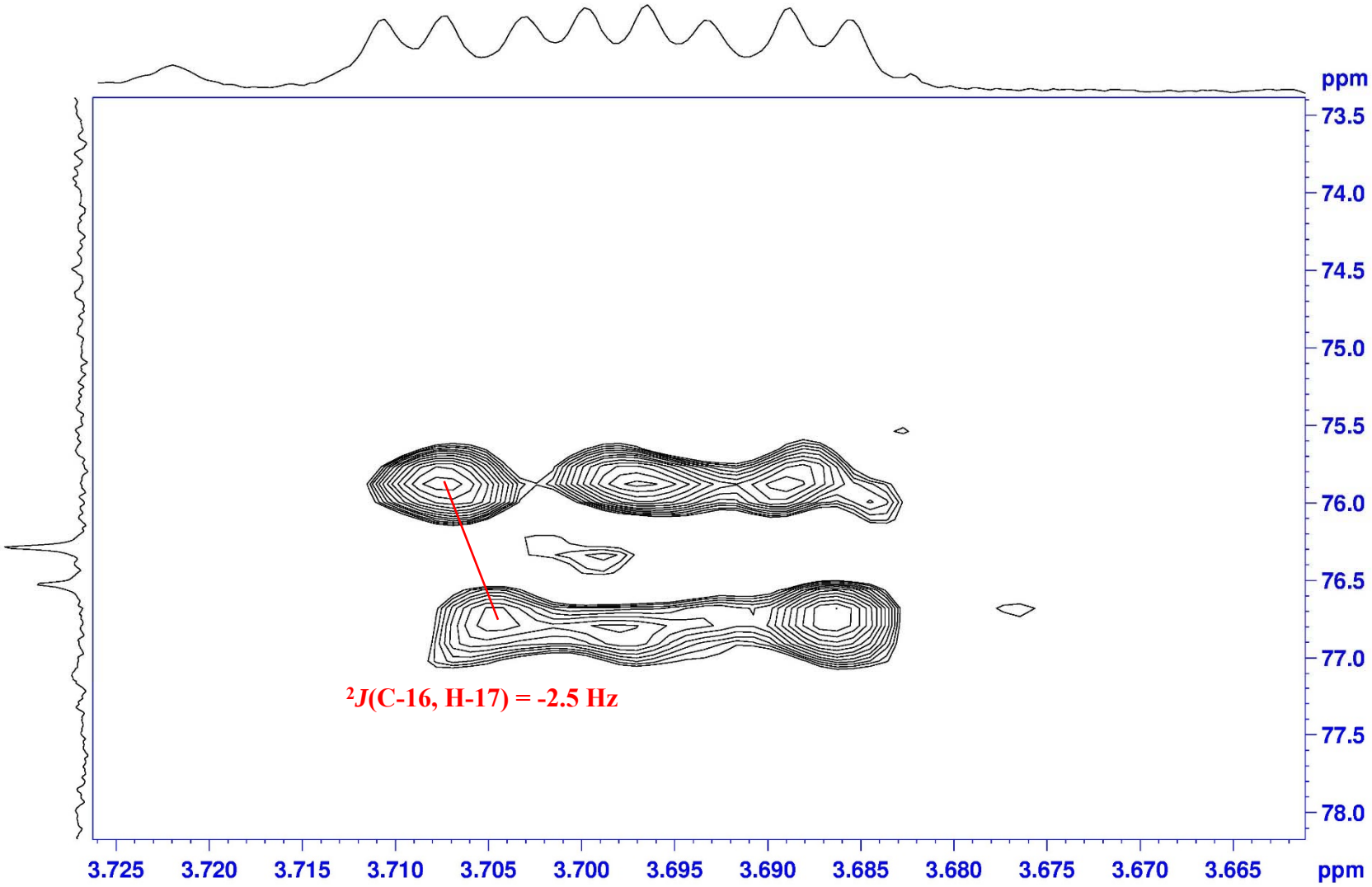
HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



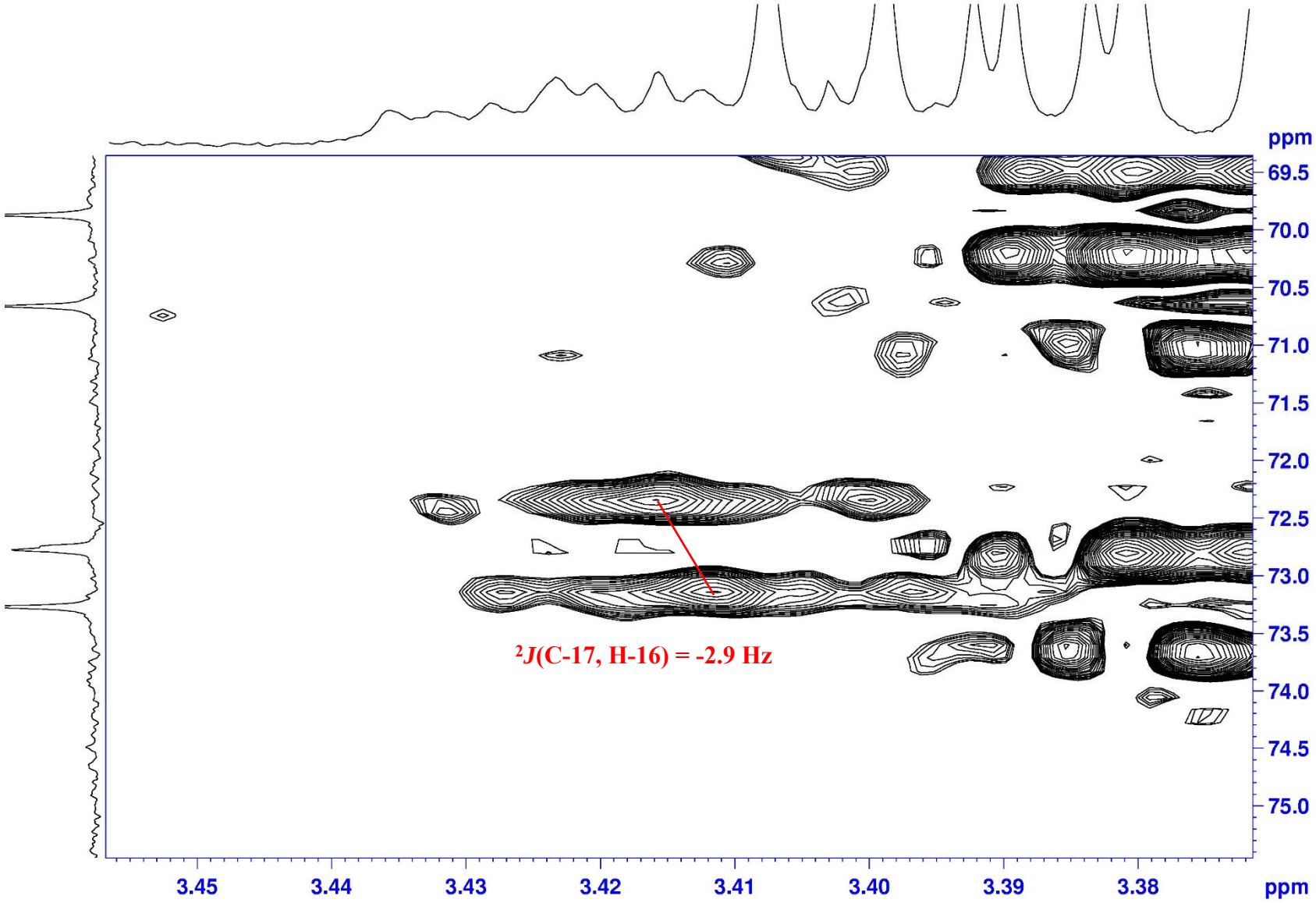
HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



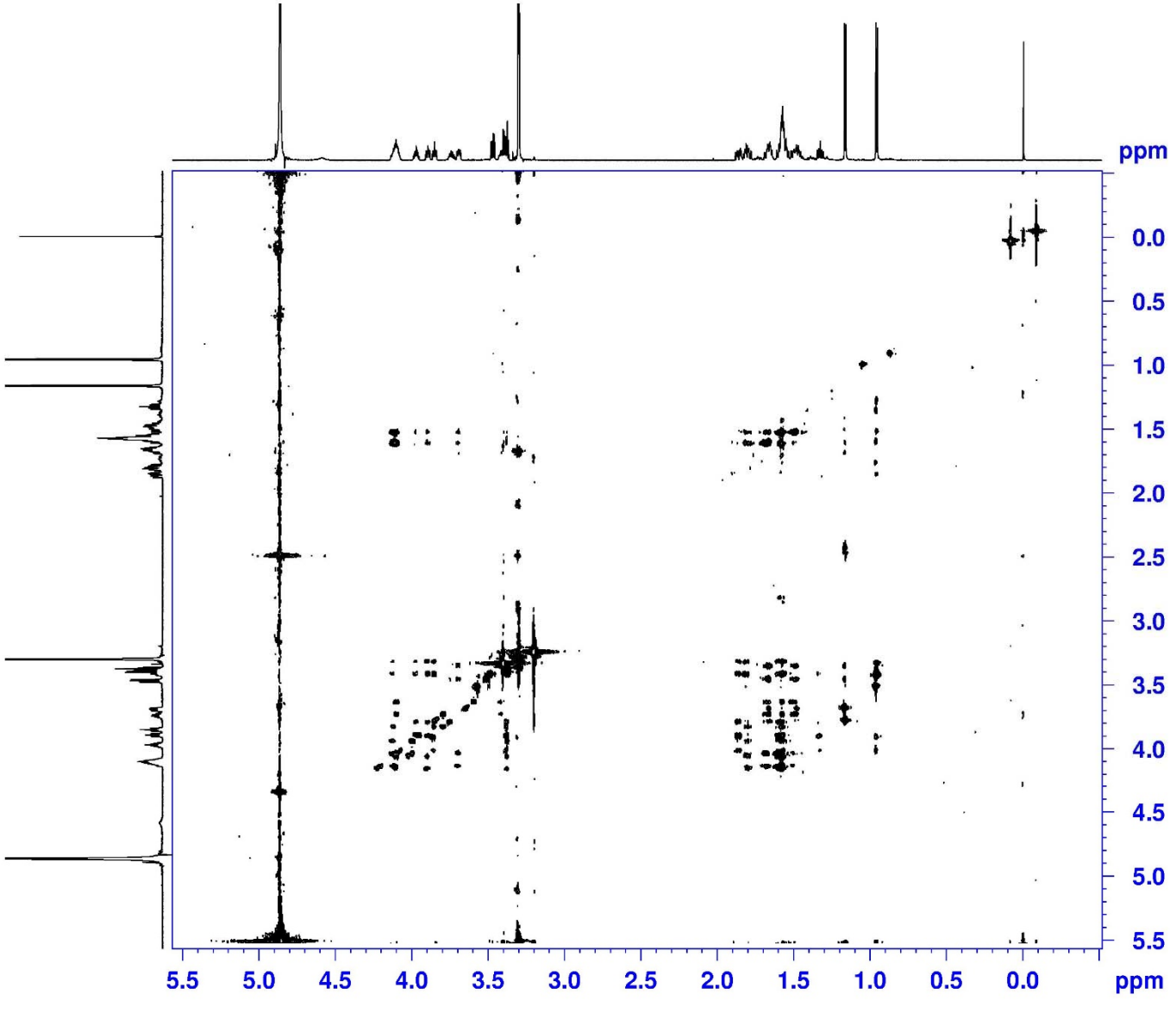
HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



HECADE (700 MHz) spectrum of the fragment **1b** in CD_3OD



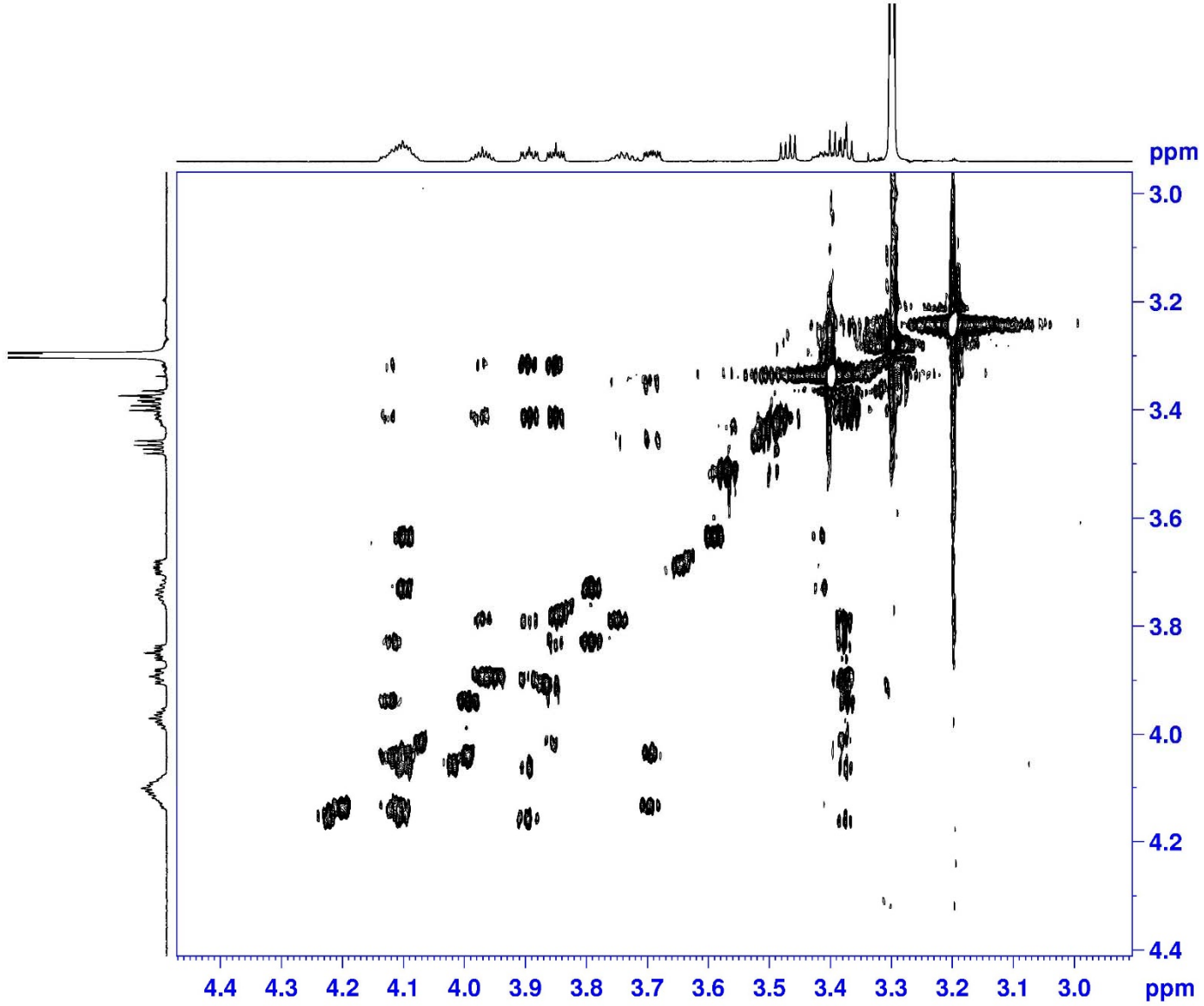
HETLOC (700 MHz) spectrum of the fragment **1b** in CD_3OD



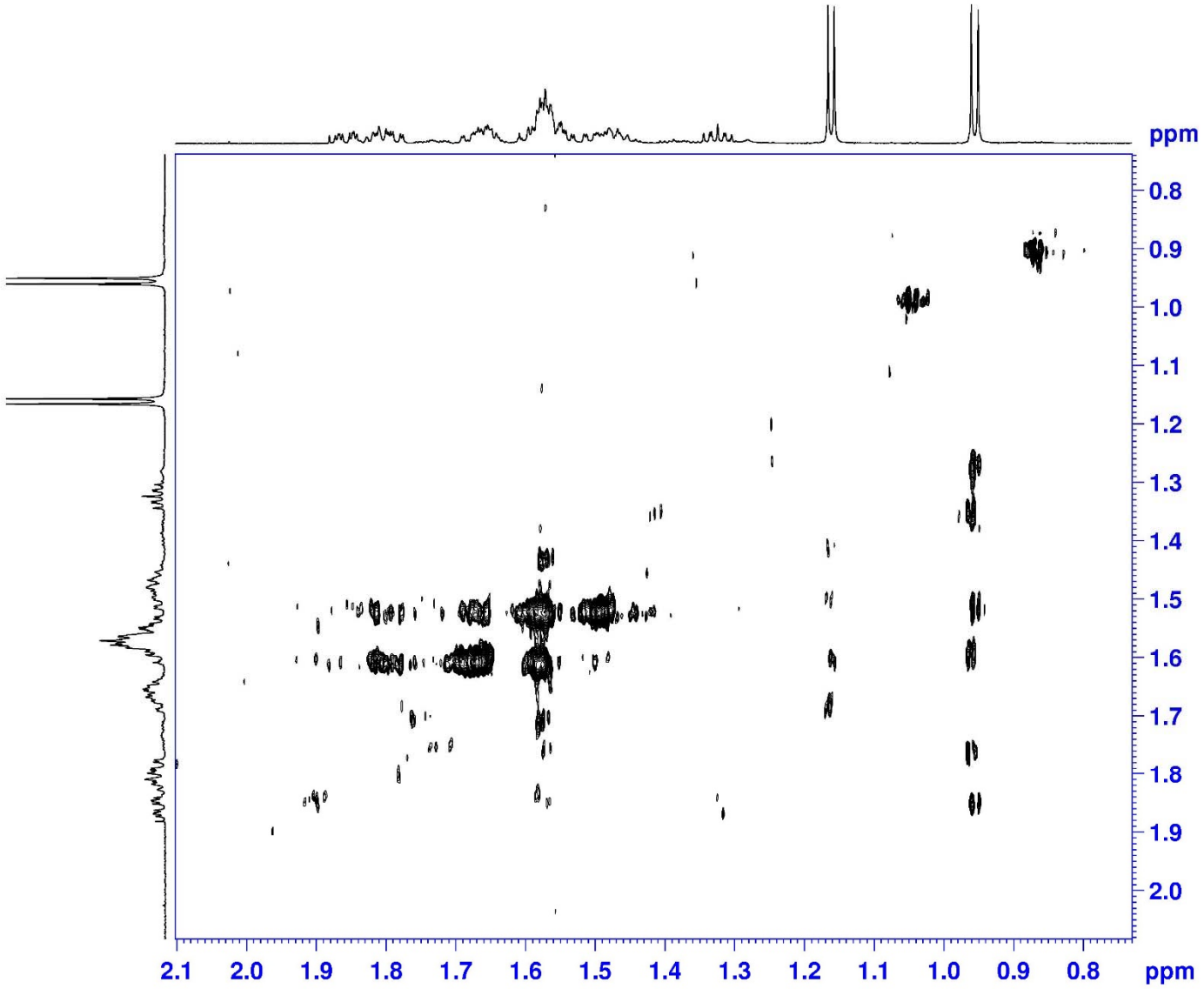
BRUKER

NAME	liwanshan-40-2-2-03-2
EXPNO	23
PROCNO	1
Date_	20200325
Time	22.38 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	dipsi2etgpjcsix1
TD	4096
SOLVENT	MeOD
NS	48
DS	16
SWH	4261.364 Hz
FIDRES	2.080744 Hz
AQ	0.4806473 sec
RG	181.26
DW	117.333 usec
DE	10.00 usec
TE	298.0 K
CNST2	145.0000000
CNST16	0.5000000
D0	0.00000300 sec
D1	1.00000000 sec
D2	0.00344828 sec
D4	0.00172414 sec
D9	0.08000000 sec
D11	0.03000000 sec
D16	0.00020000 sec
D20	0.00000300 sec
D28	0.00000300 sec
IN0	0.00011730 sec
IN20	0.00005865 sec
IN28	0.00005865 sec
L1	28
ND0	2
TD	256
SFO1	700.1818 MHz
FIDRES	16.650682 Hz
SW	6.088 ppm
FnMODE	Echo-Antiecho
SI	8192
SF	700.1800227 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	700.1800262 MHz
WDW	QSINE
SSB	2

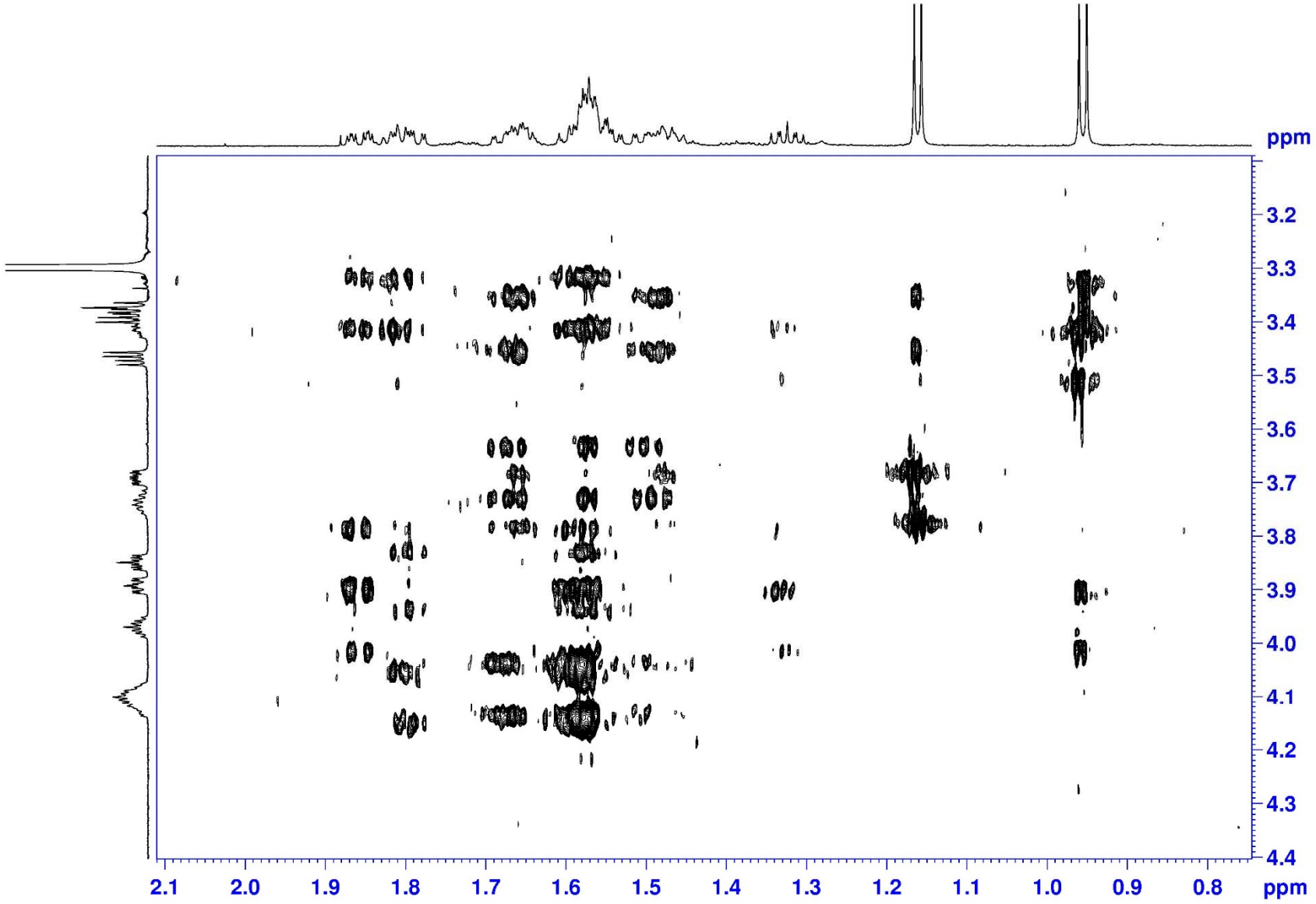
HETLOC (700 MHz) spectrum of the fragment **1b** in CD_3OD



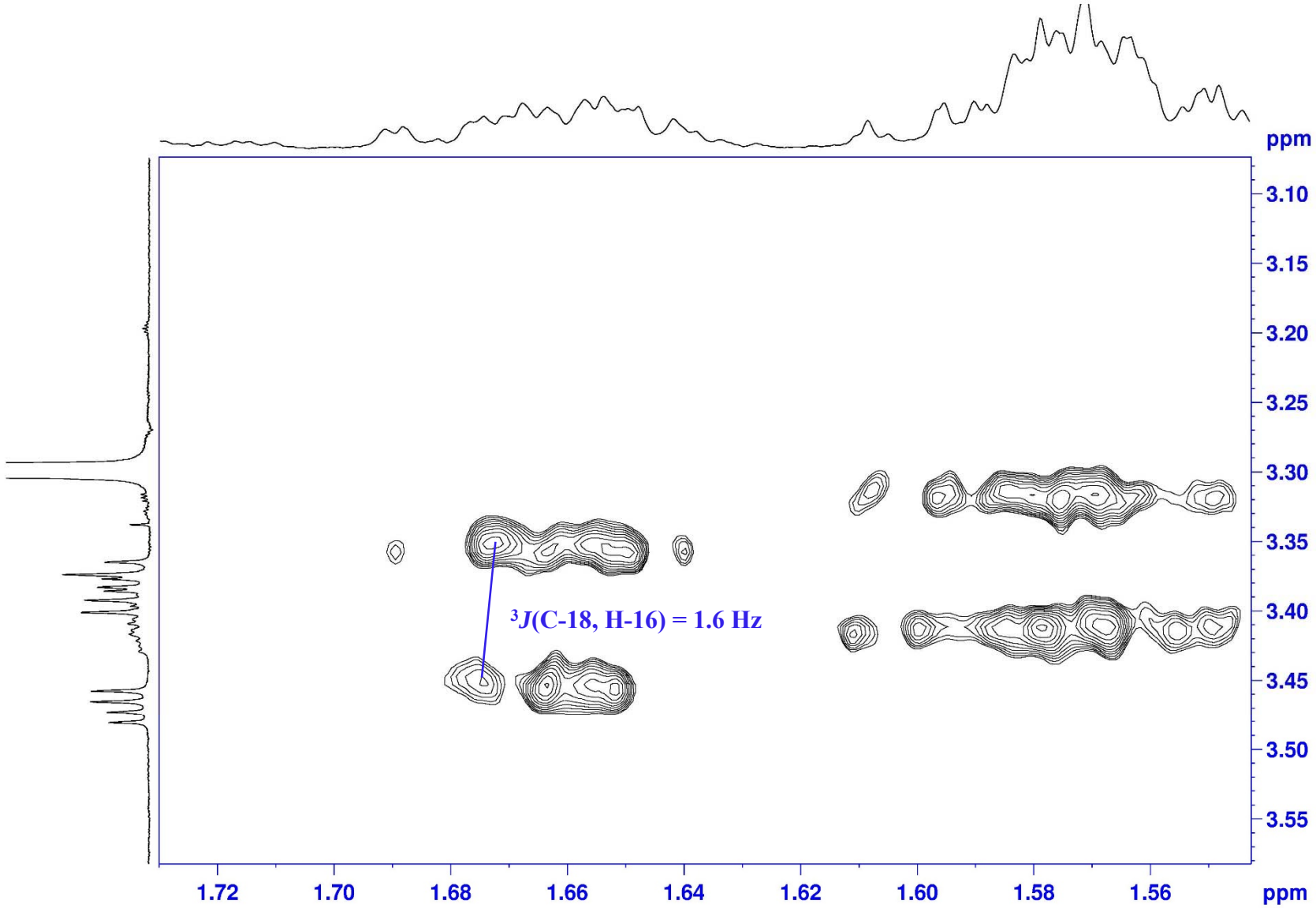
HETLOC (700 MHz) spectrum of the fragment **1b** in CD_3OD



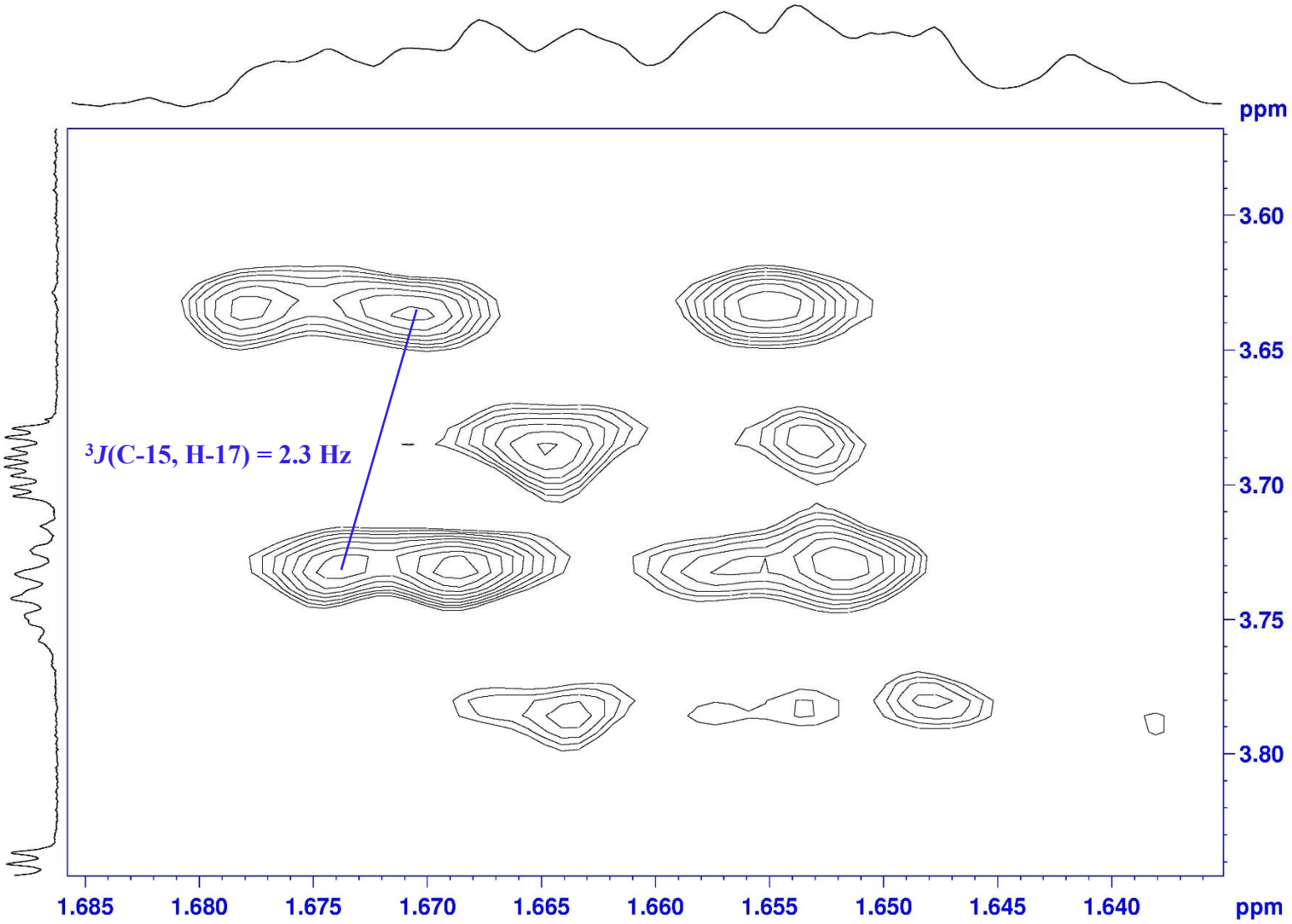
HETLOC (700 MHz) spectrum of the fragment **1b** in CD_3OD



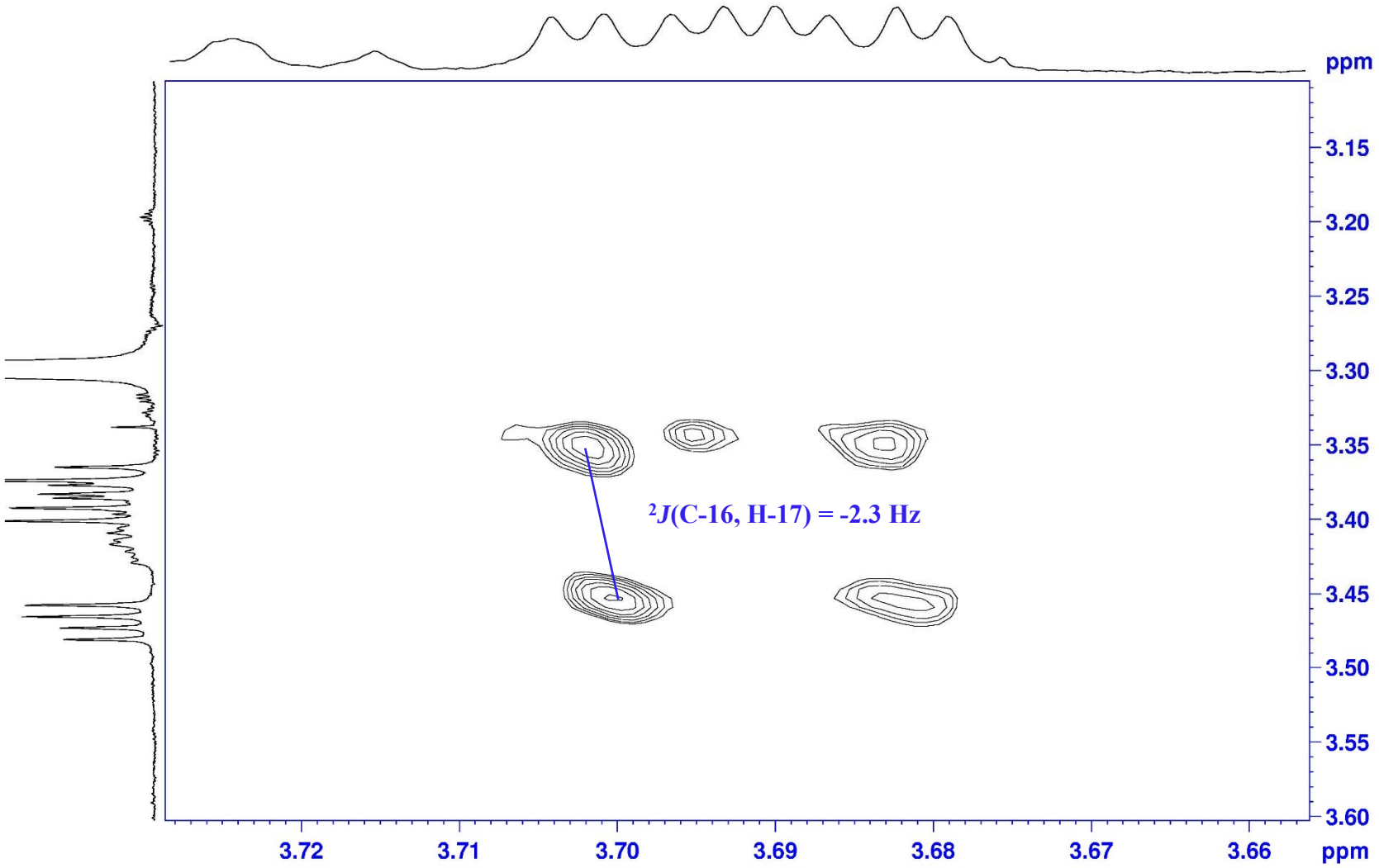
HETLOC (700 MHz) spectrum of the fragment **1b** in CD_3OD



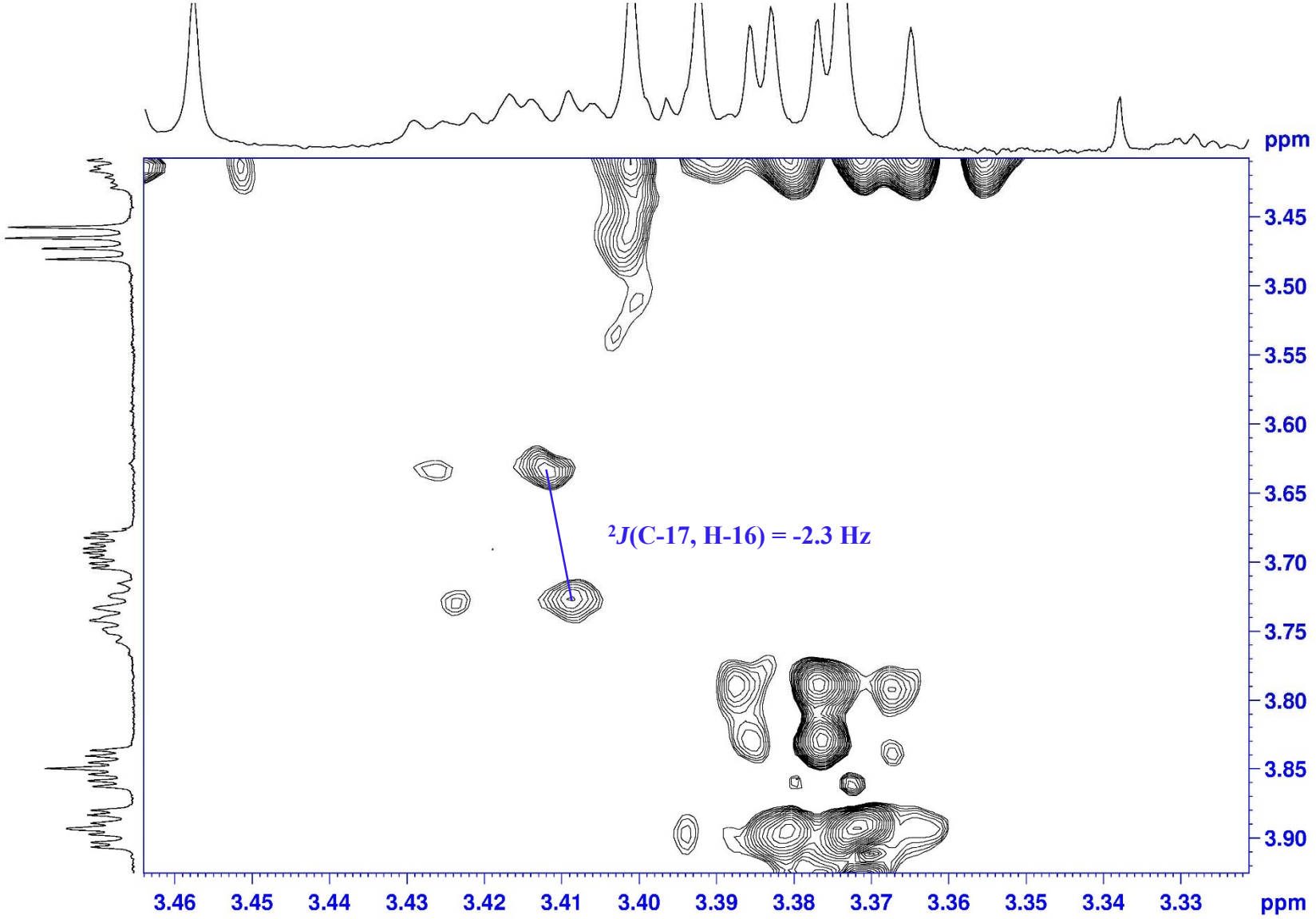
HETLOC (700 MHz) spectrum of the fragment **1b** in CD_3OD



HETLOC (700 MHz) spectrum of the fragment **1b** in CD_3OD



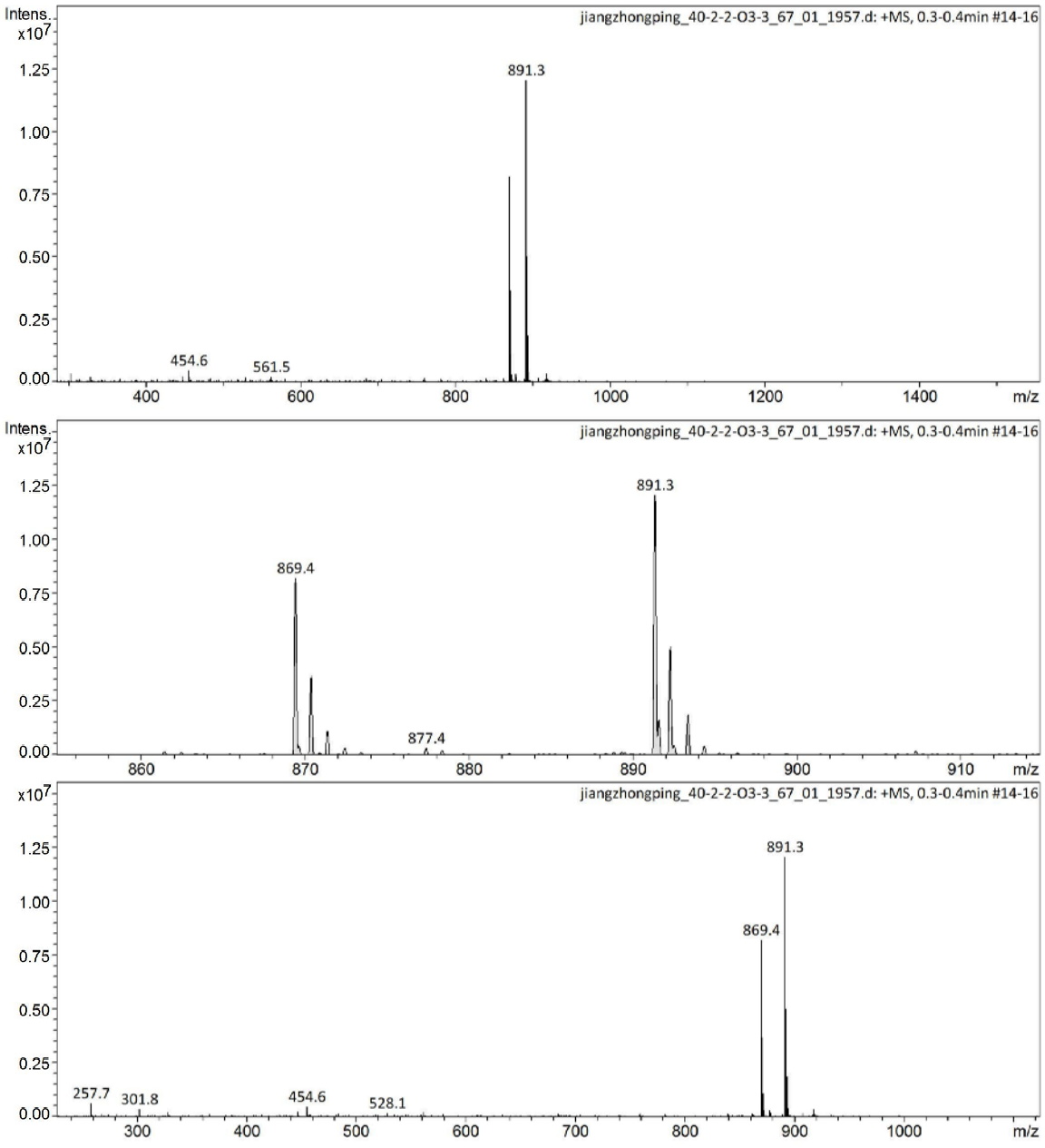
HETLOC (700 MHz) spectrum of the fragment **1b** in CD_3OD



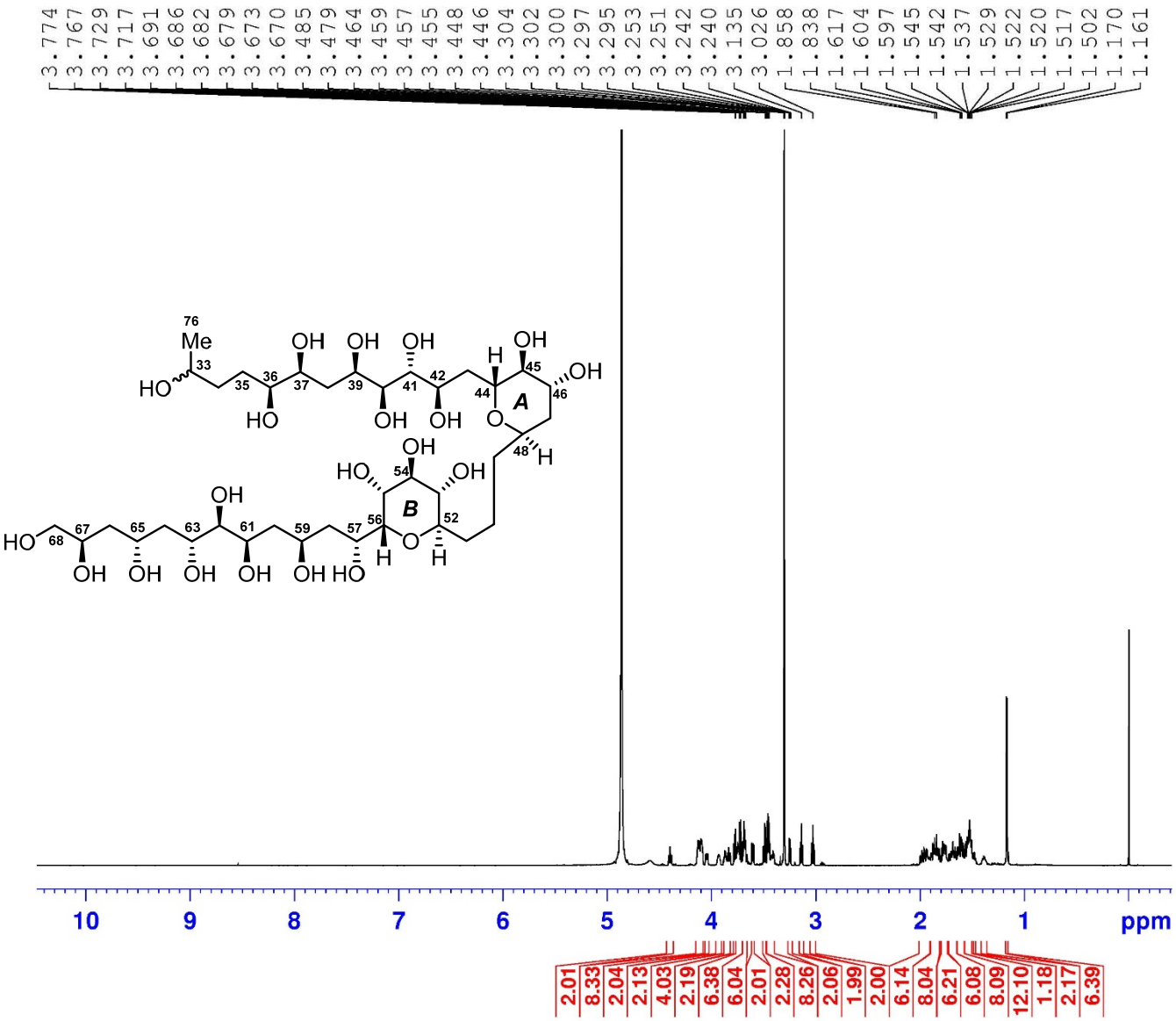
Generic Display Report

Analysis Info

Analysis Name	D:\Data\amaZon SL\MS\data\202007\jiangzhongping_40-2-2-O3-3_67_01_1957.d	Acquisition Date	2020-07-13 15:56:49
Method	1957.m	Operator	bruker
Sample Name	jiangzhongping_40-2-2-O3-3	Instrument	amaZon SL
Comment			



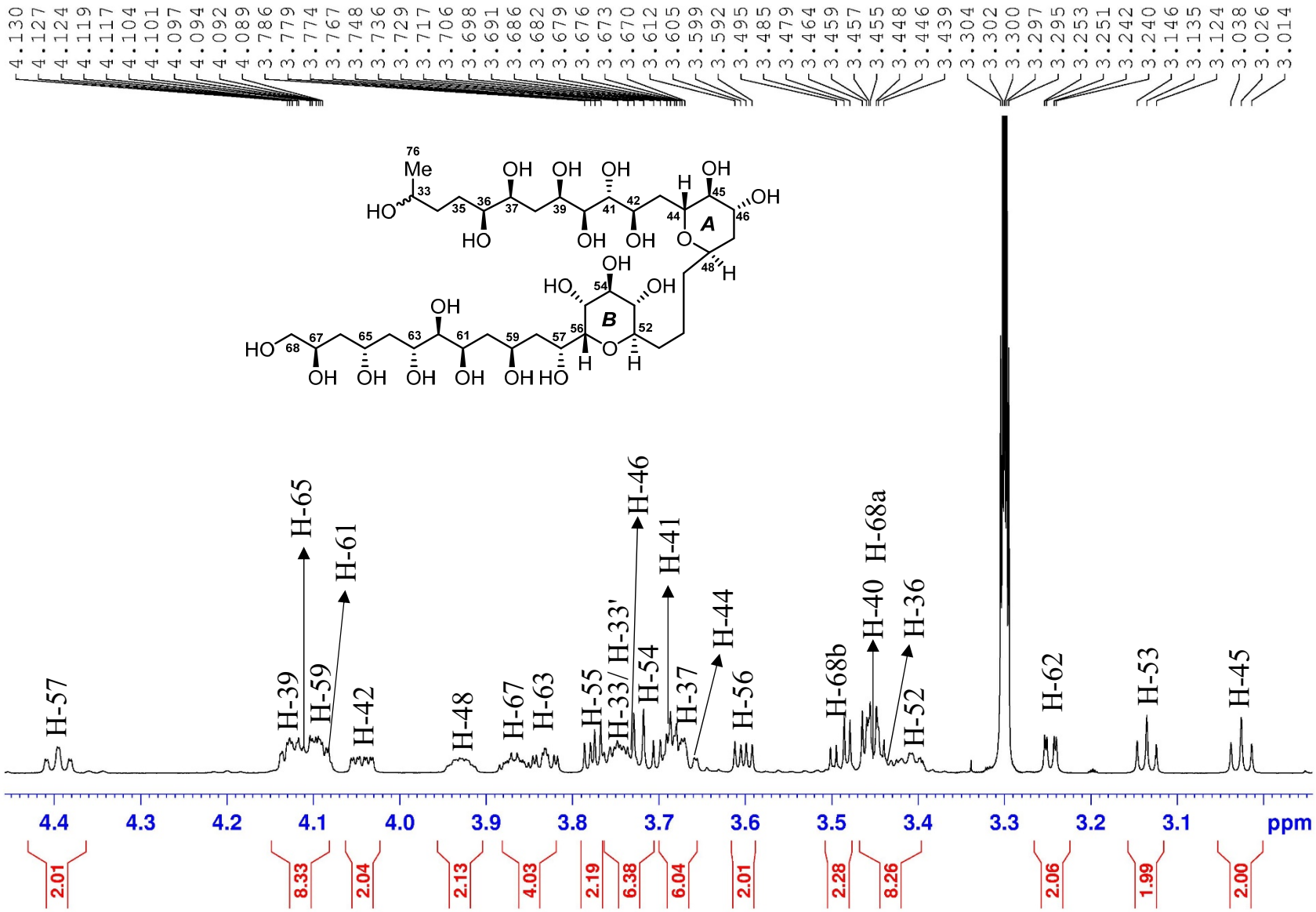
^{1}H (700 MHz) NMR spectrum of the fragment **1c** in CD_3OD



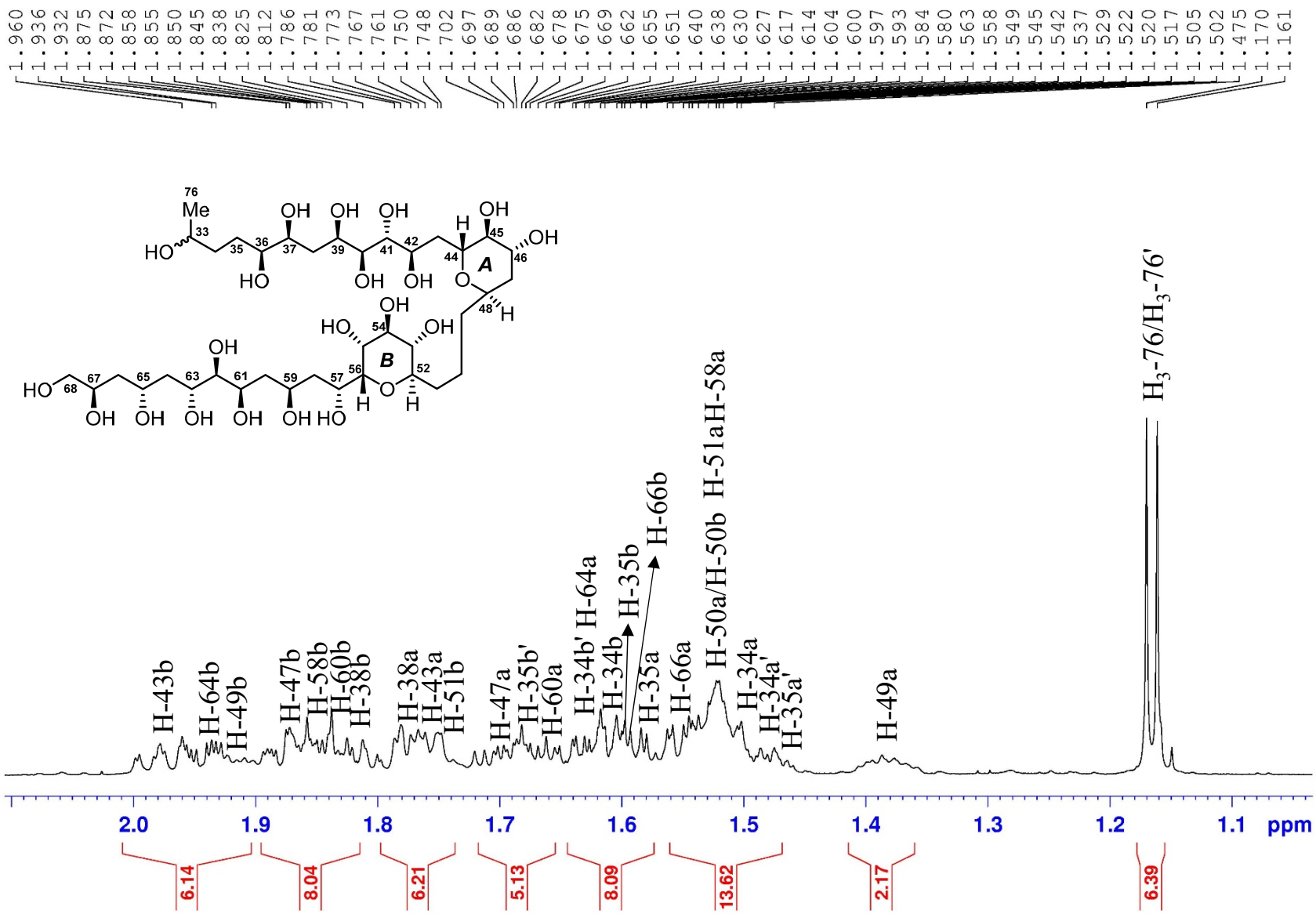
BRUKER

NAME	liwanshan-40-2-2-03-
EXPNO	12
PROCNO	1
Date_	20200321
Time	14.57 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	32
DS	2
SWH	14097.744 Hz
FIDRES	0.430229 Hz
AQ	2.3243935 sec
RG	4.29
DW	35.467 usec
DE	10.00 usec
TE	298.0 K
D1	1.50000000 sec
TD0	1
SFO1	700.1843236 MHz
NUC1	1H
P1	7.55 usec
SI	65536
SF	700.1800209 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

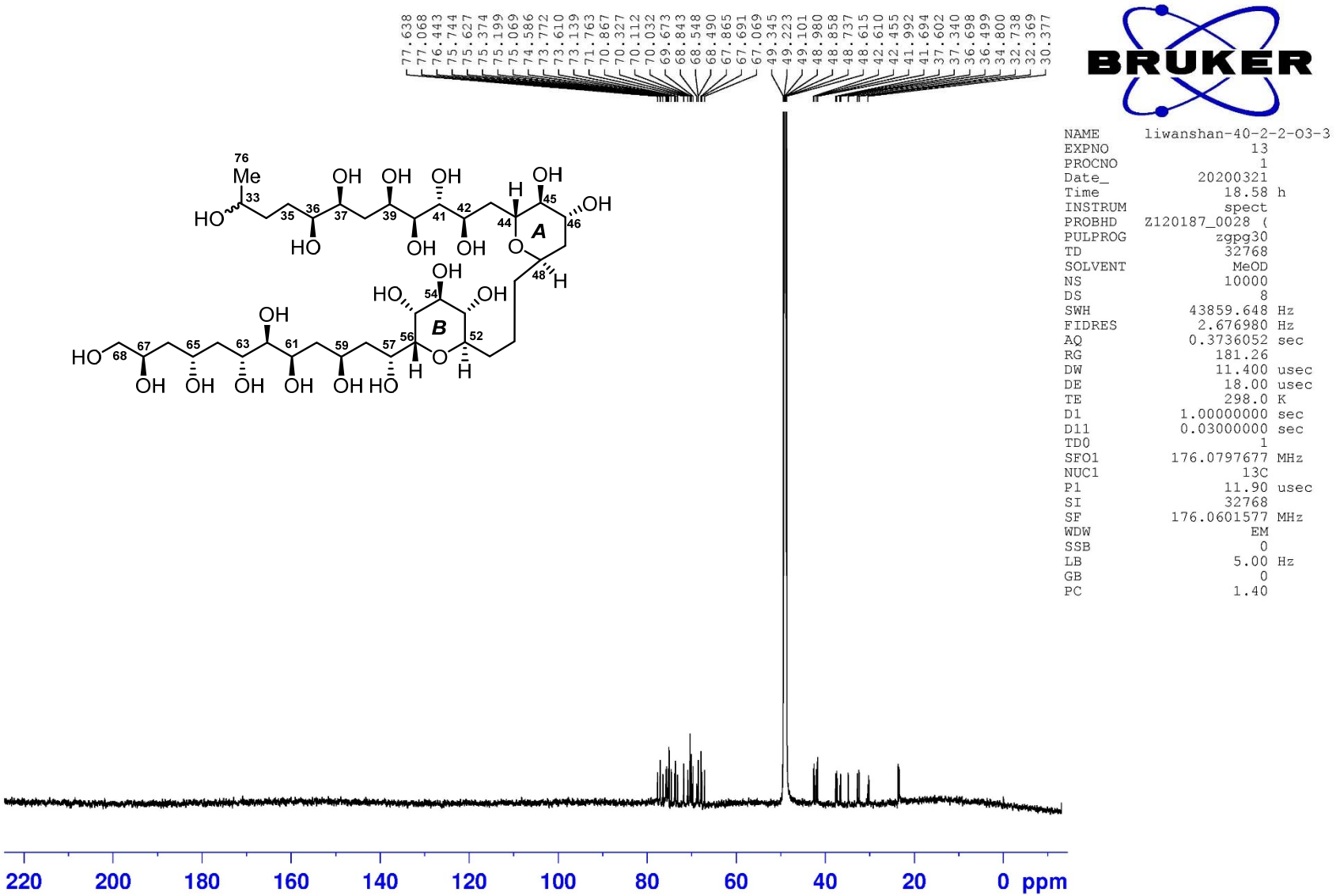
^{1}H (700 MHz) NMR spectrum of the fragment **1c** in CD_3OD



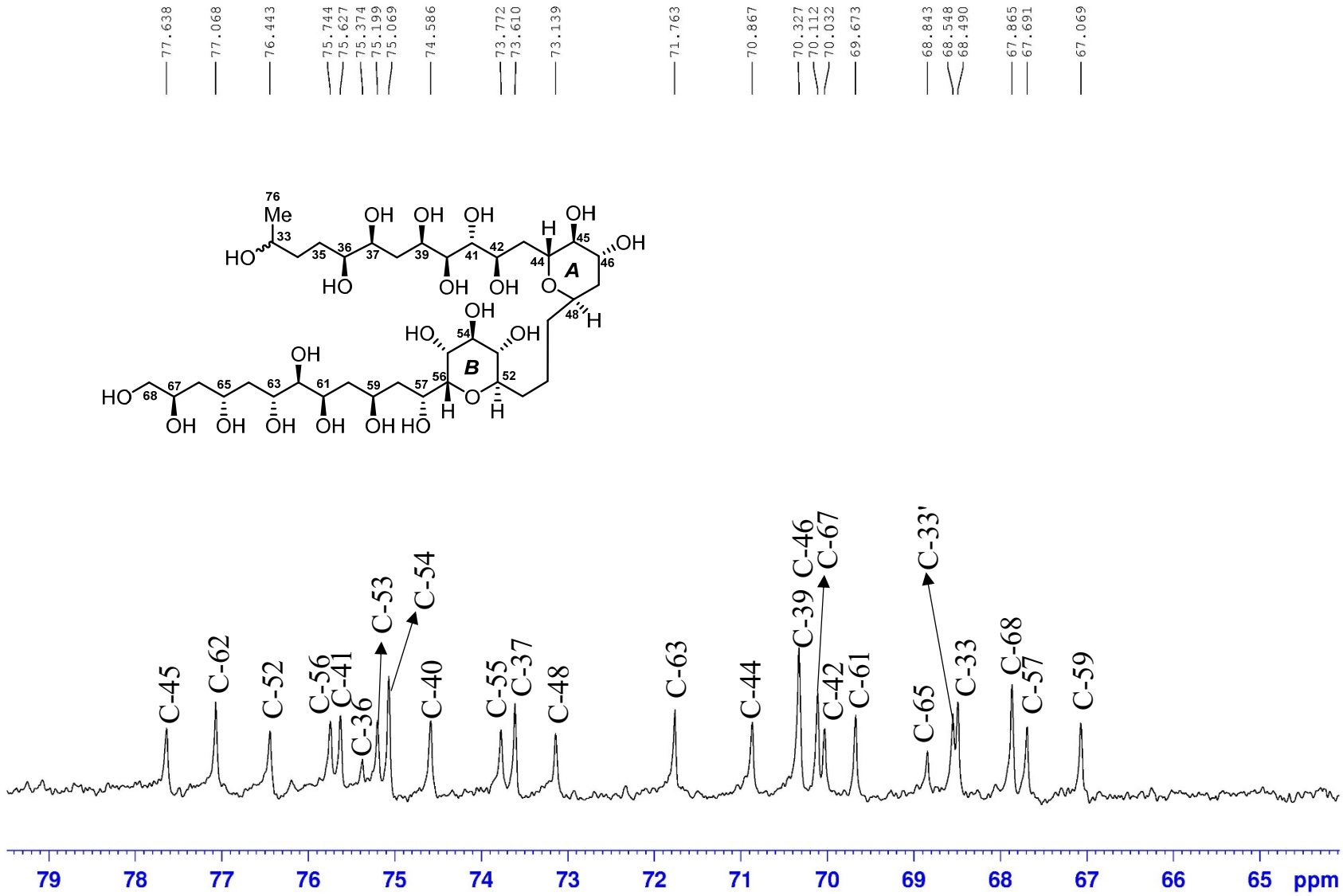
^{1}H (700 MHz) NMR spectrum of the fragment **1c** in CD_3OD



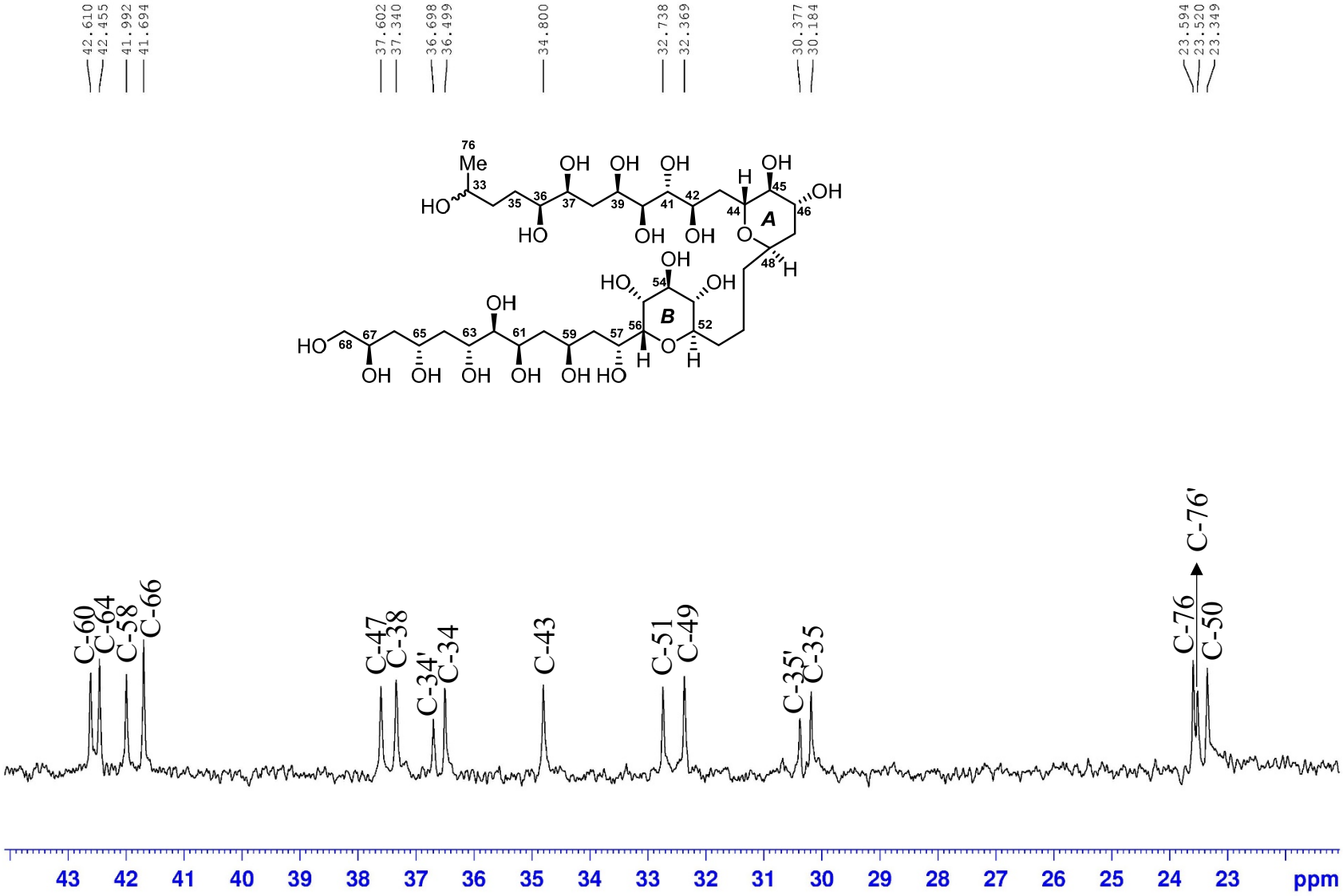
^{13}C (175 MHz) NMR spectrum of the fragment **1c** in CD_3OD



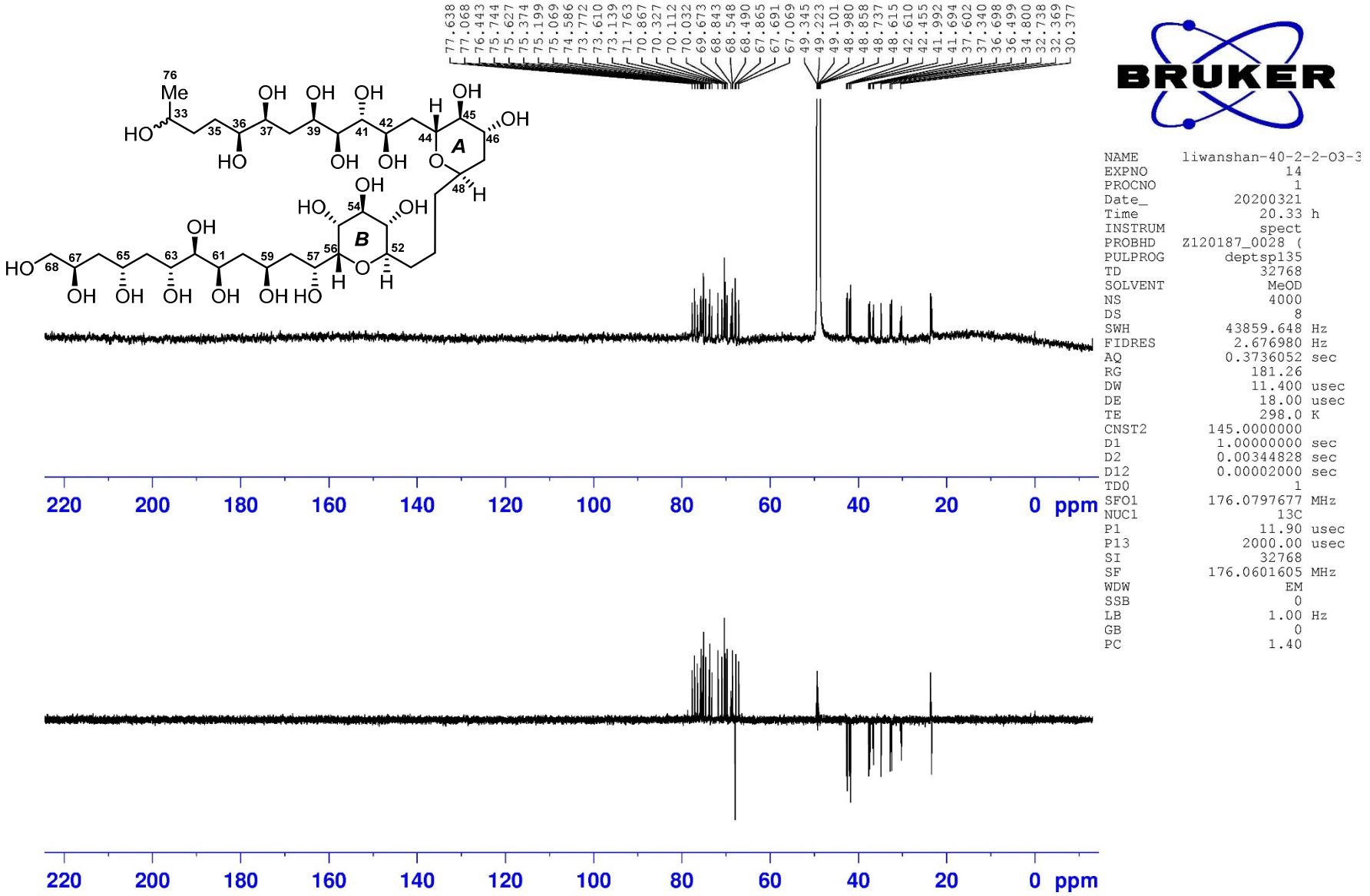
^{13}C (175 MHz) NMR spectrum of the fragment **1c** in CD_3OD



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



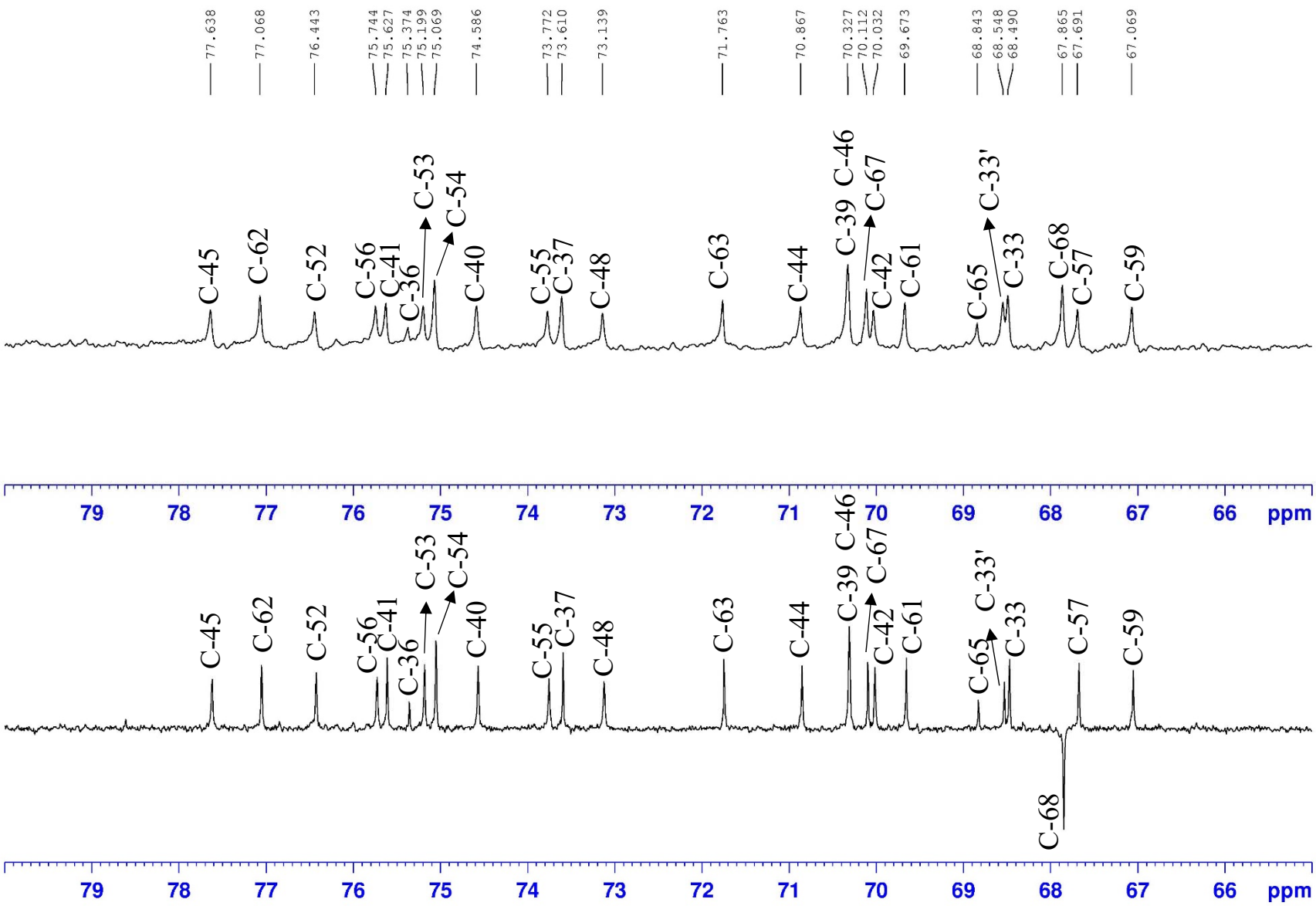
DEPT135 (175 MHz) spectrum of the fragment **1c** in CD_3OD



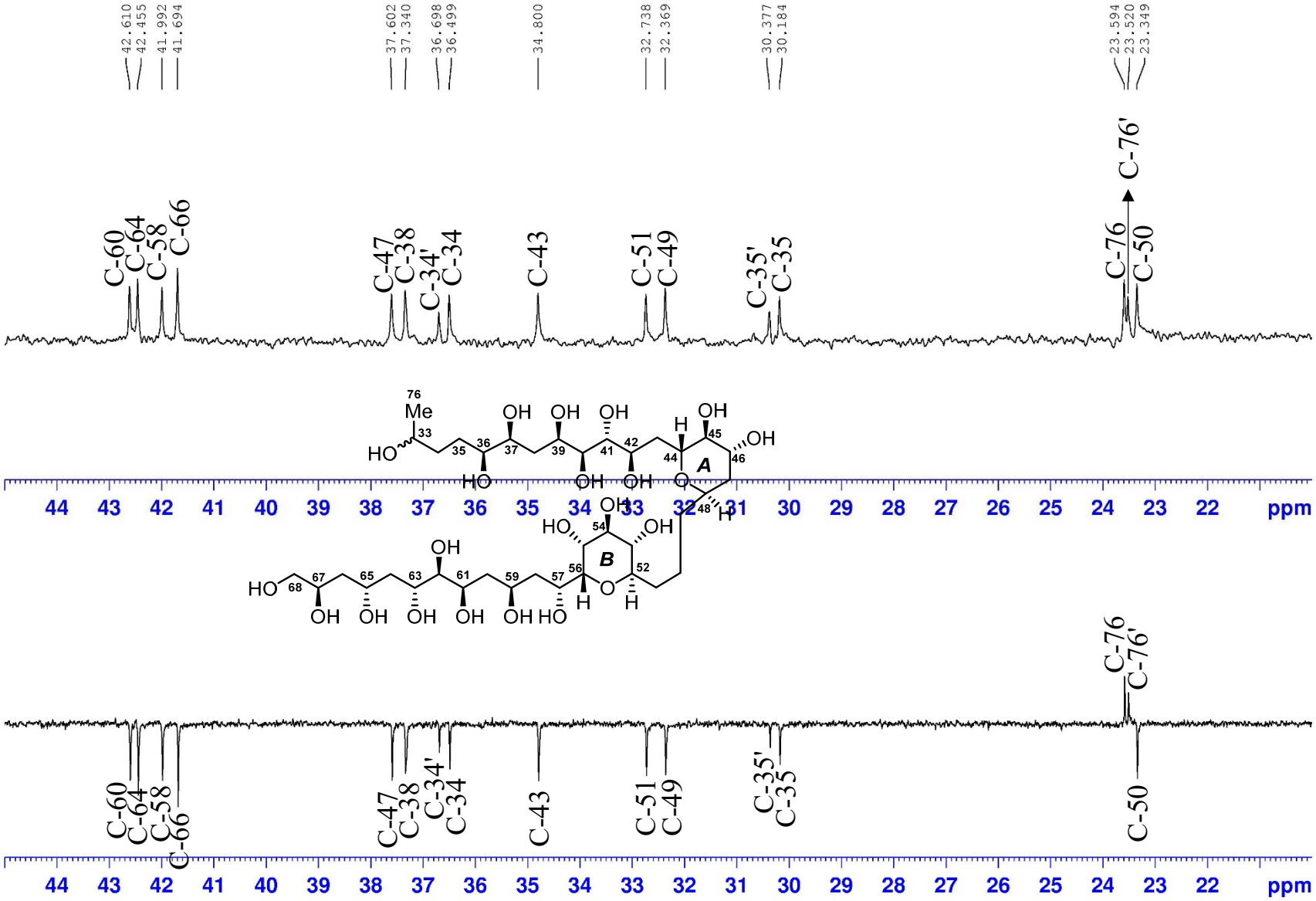
BRUKER

NAME	liwanshan-40-2-2-03-3
EXPNO	14
PROCNO	1
Date_	20200321
Time	20.33 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	deptsp135
TD	32768
SOLVENT	MeOD
NS	4000
DS	8
SWH	43859.648 Hz
FIDRES	2.676980 Hz
AQ	0.3736052 sec
RG	181.26
DW	11.400 usec
DE	18.00 usec
TE	298.0 K
CNST2	145.0000000
D1	1.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
SFO1	176.0797677 MHz
NUC1	13C
P1	11.90 usec
P13	2000.00 usec
SI	32768
SF	176.0601605 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

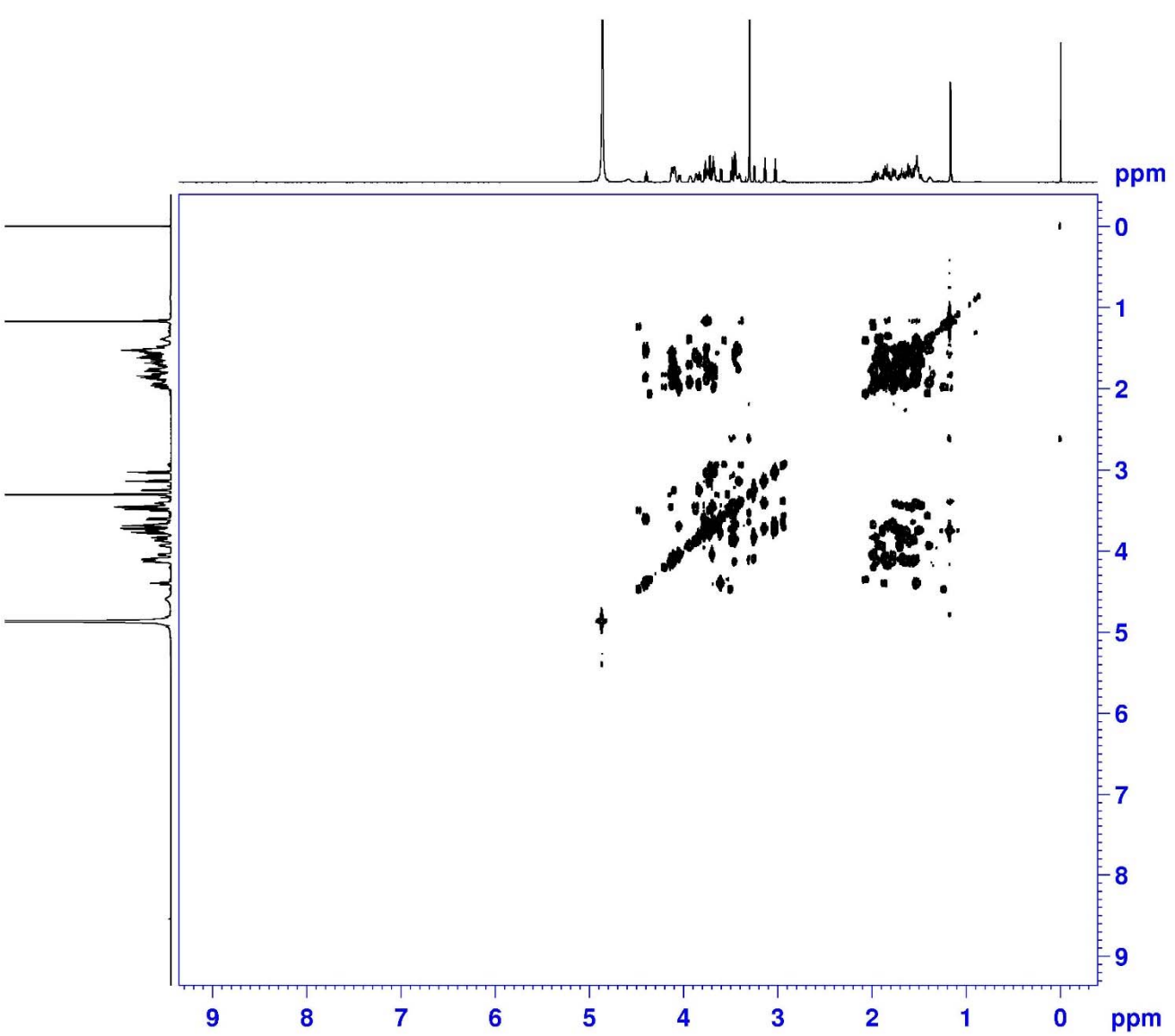
DEPT135 (175 MHz) spectrum of the fragment **1c** in CD_3OD



DEPT135 (175 MHz) spectrum of the fragment **1c** in CD_3OD



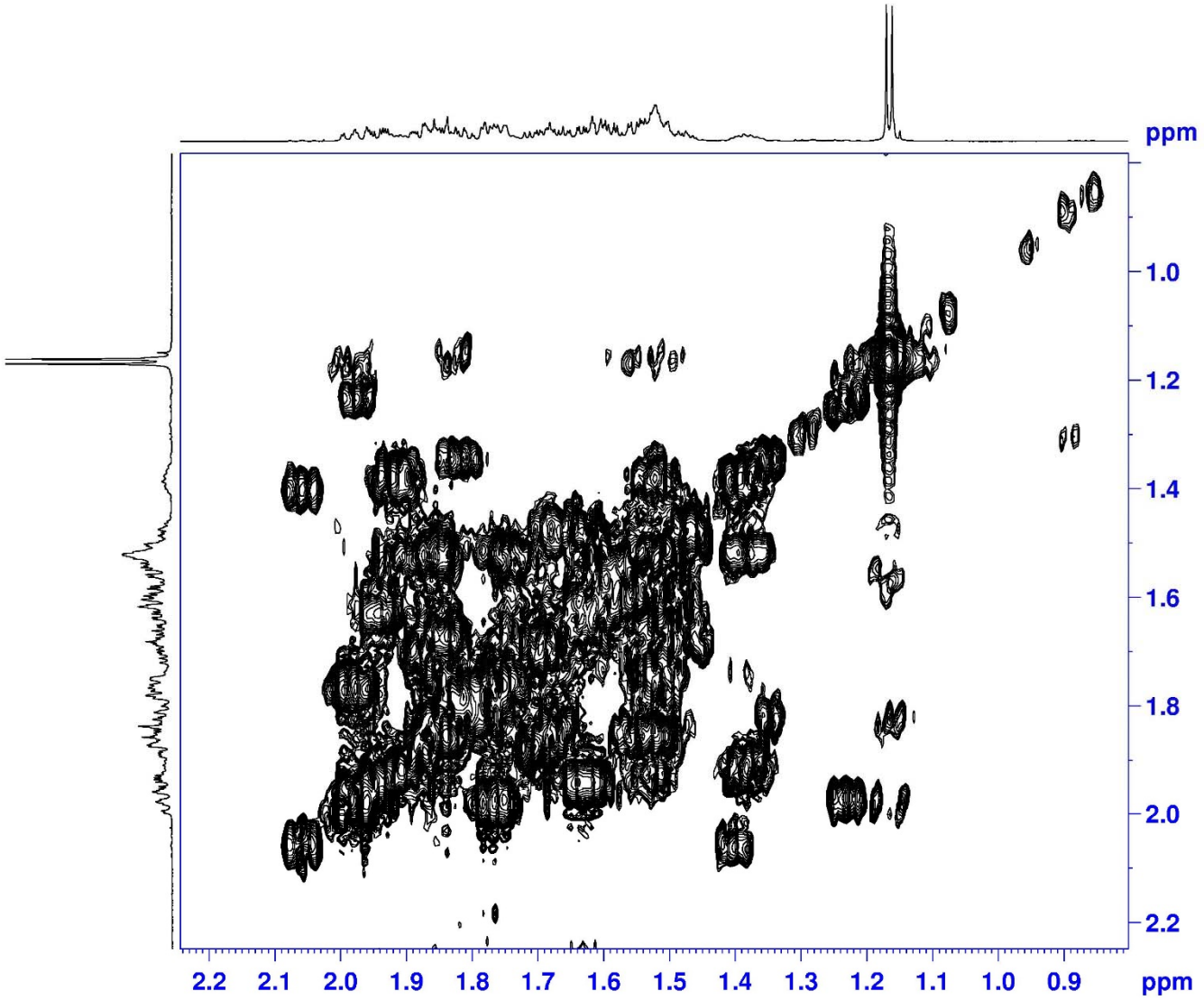
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1c** in CD_3OD



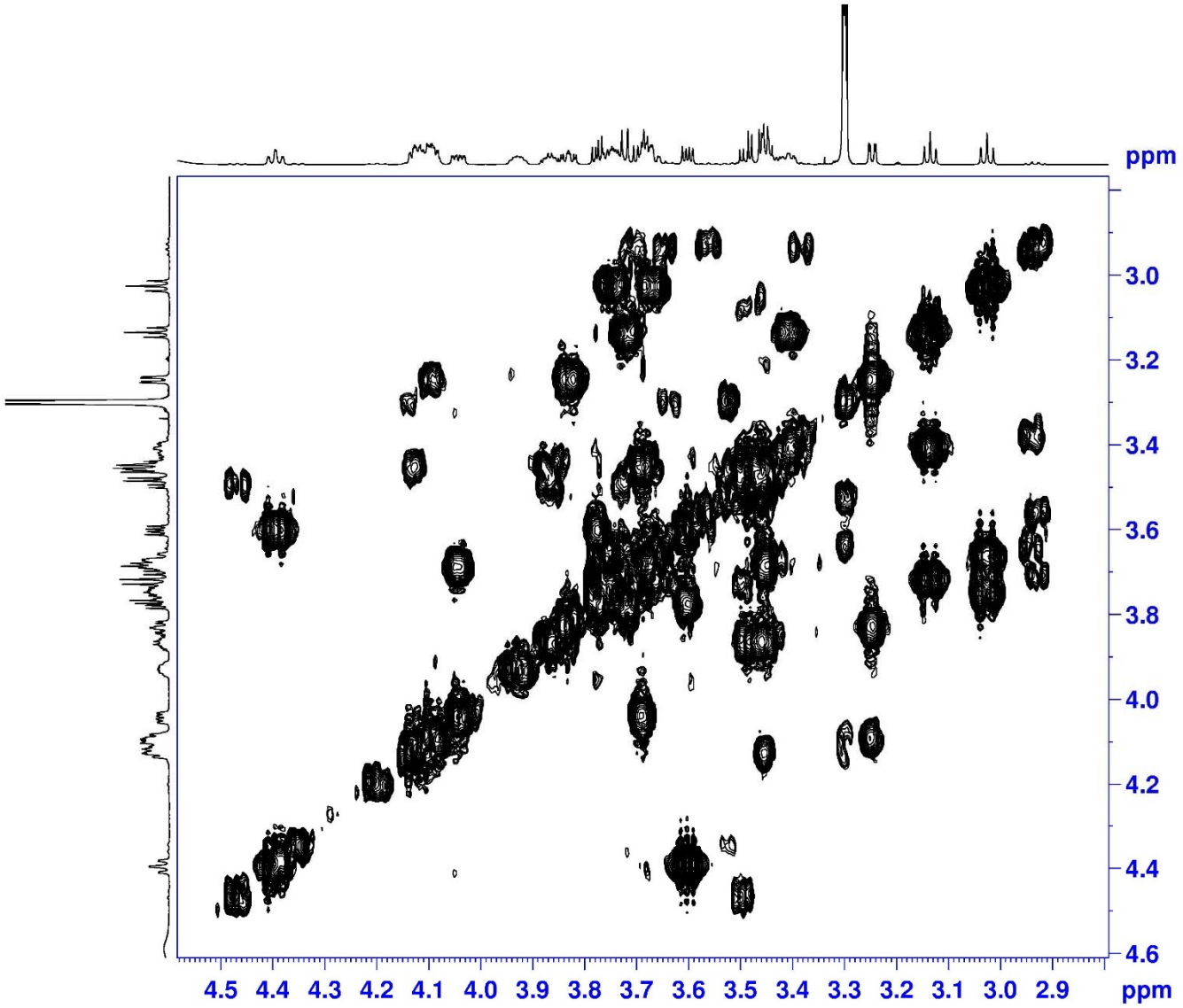
BRUKER

NAME	liwanshan-40-2-2-O3-3
EXPNO	15
PROCNO	1
Date_	20200321
Time	20.35 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	cosygpmfqf
TD	2048
SOLVENT	MeOD
NS	32
DS	16
SWH	4347.826 Hz
FIDRES	4.245924 Hz
AQ	0.2355700 sec
RG	181.26
DW	115.000 usec
DE	10.00 usec
TE	298.0 K
D0	0.00000300 sec
D1	1.00000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00023000 sec
ND0	1
TD	128
SFO1	700.1819 MHz
FIDRES	33.967392 Hz
SW	6.210 ppm
FnMODE	QF
SI	1024
SF	700.1800209 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
ST	1024
MC2	QF
SF	700.1800209 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

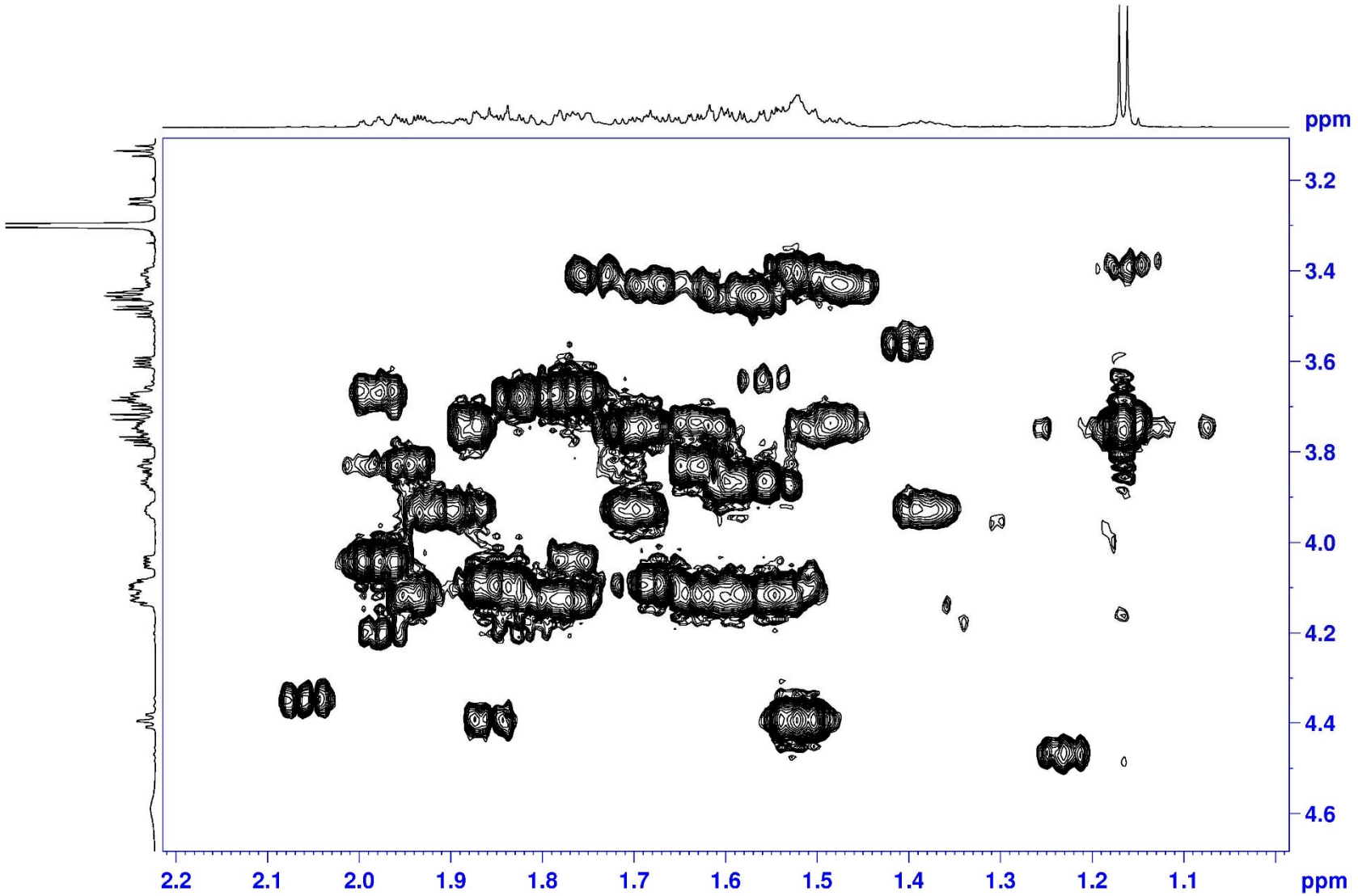
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1c** in CD_3OD



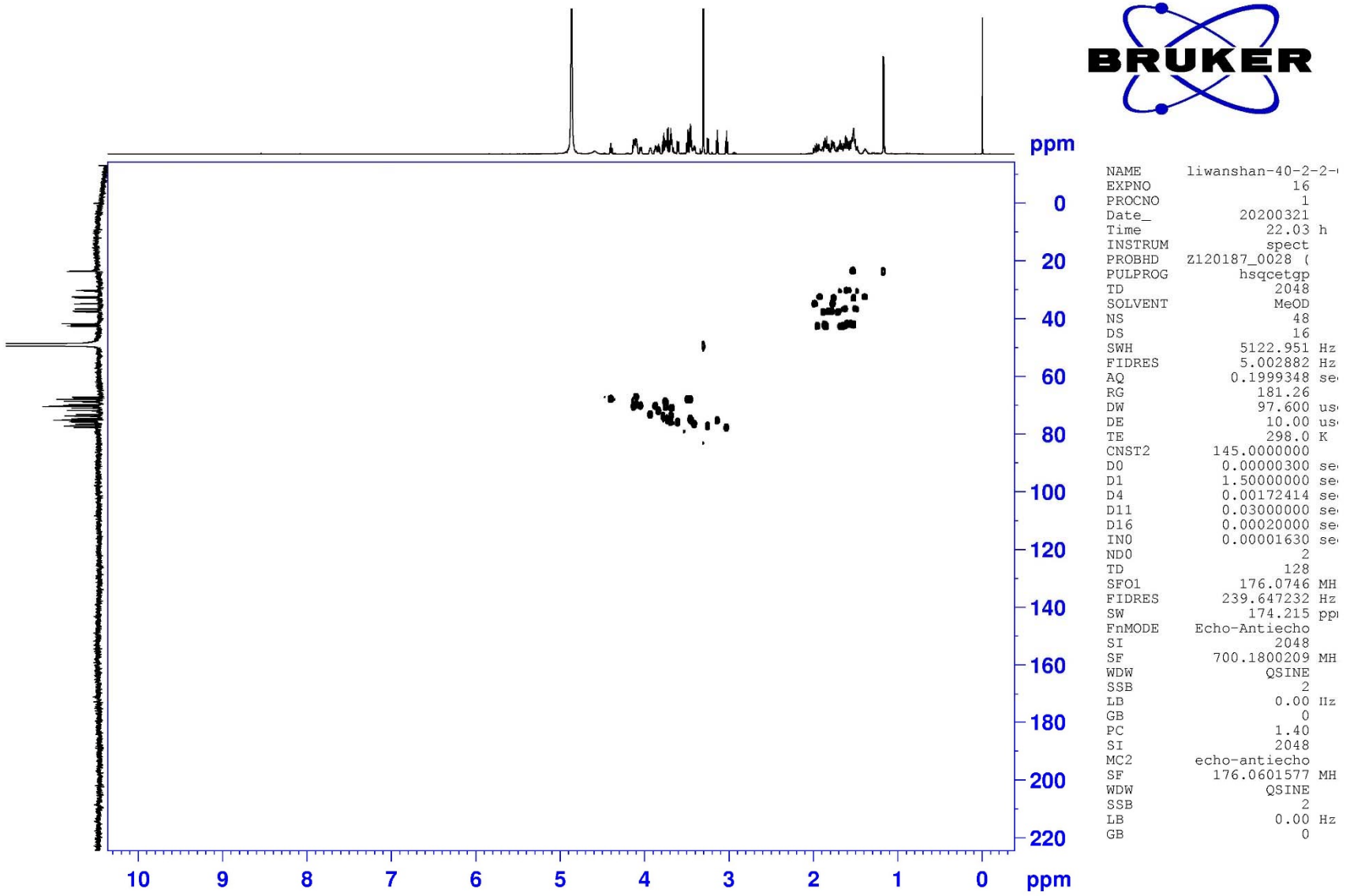
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1c** in CD_3OD



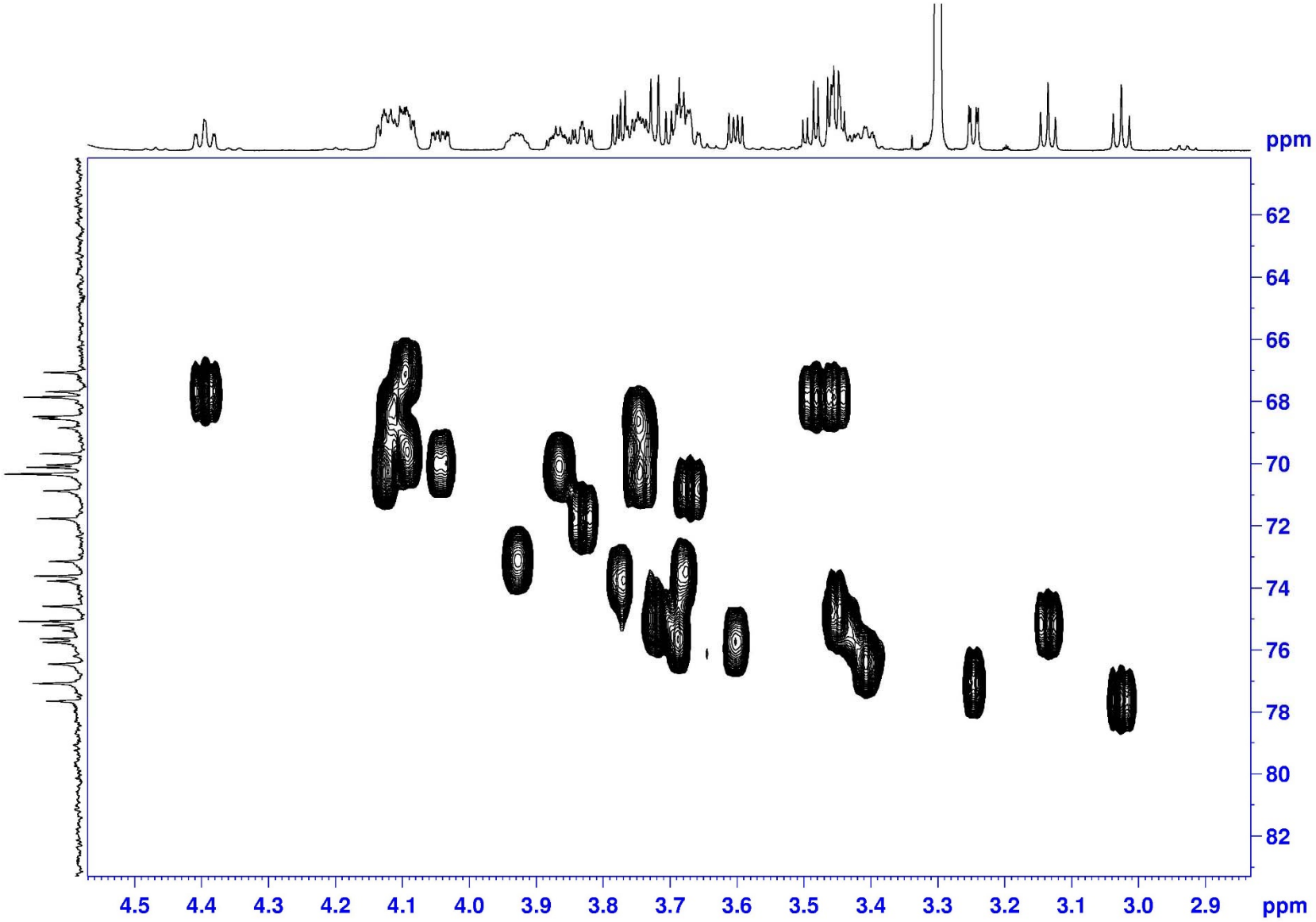
$^{1}H–^{1}H$ COSY (700 MHz) spectrum of the fragment **1c** in CD_3OD



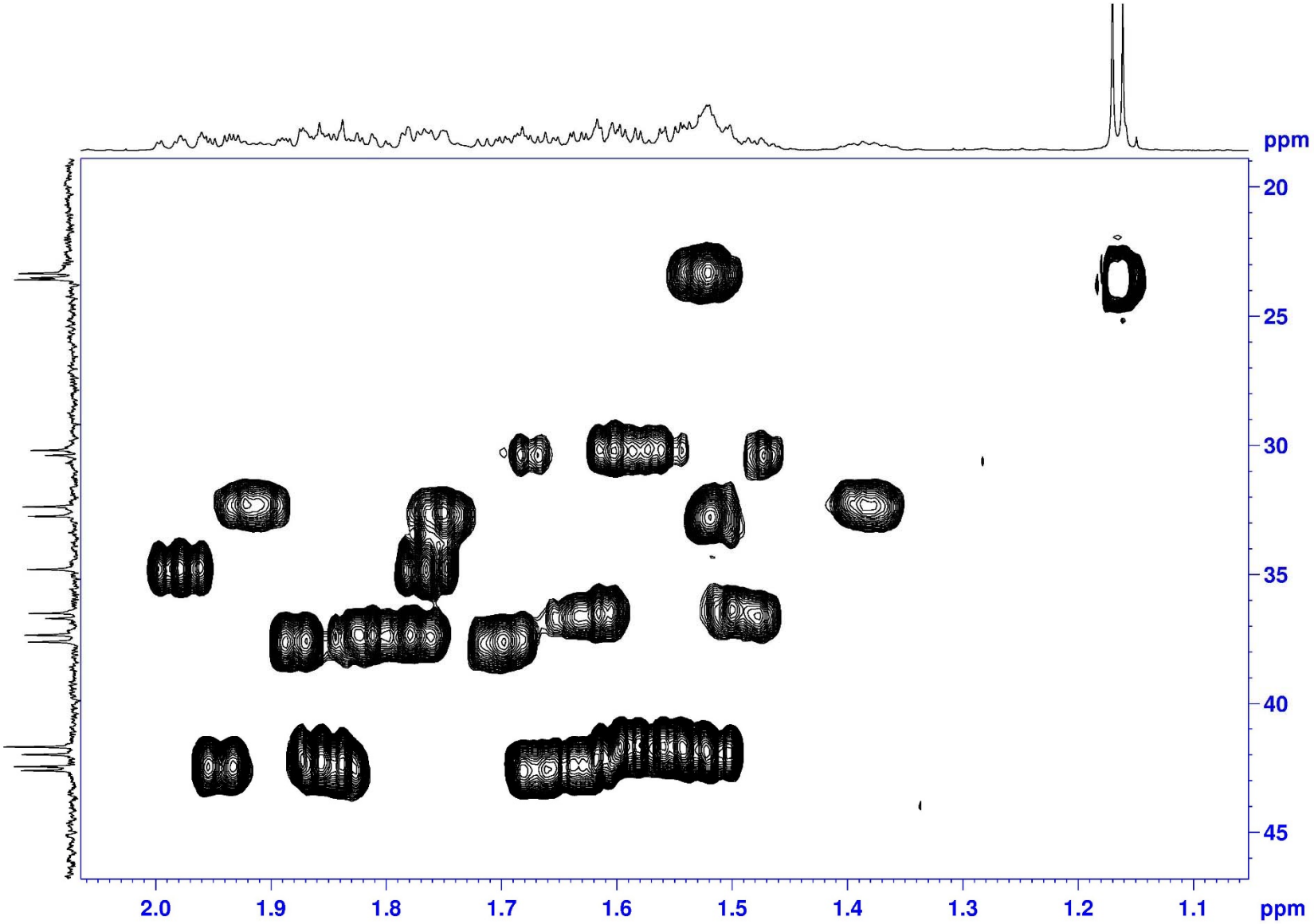
HSQC (700 MHz) spectrum of the fragment **1c** in CD_3OD



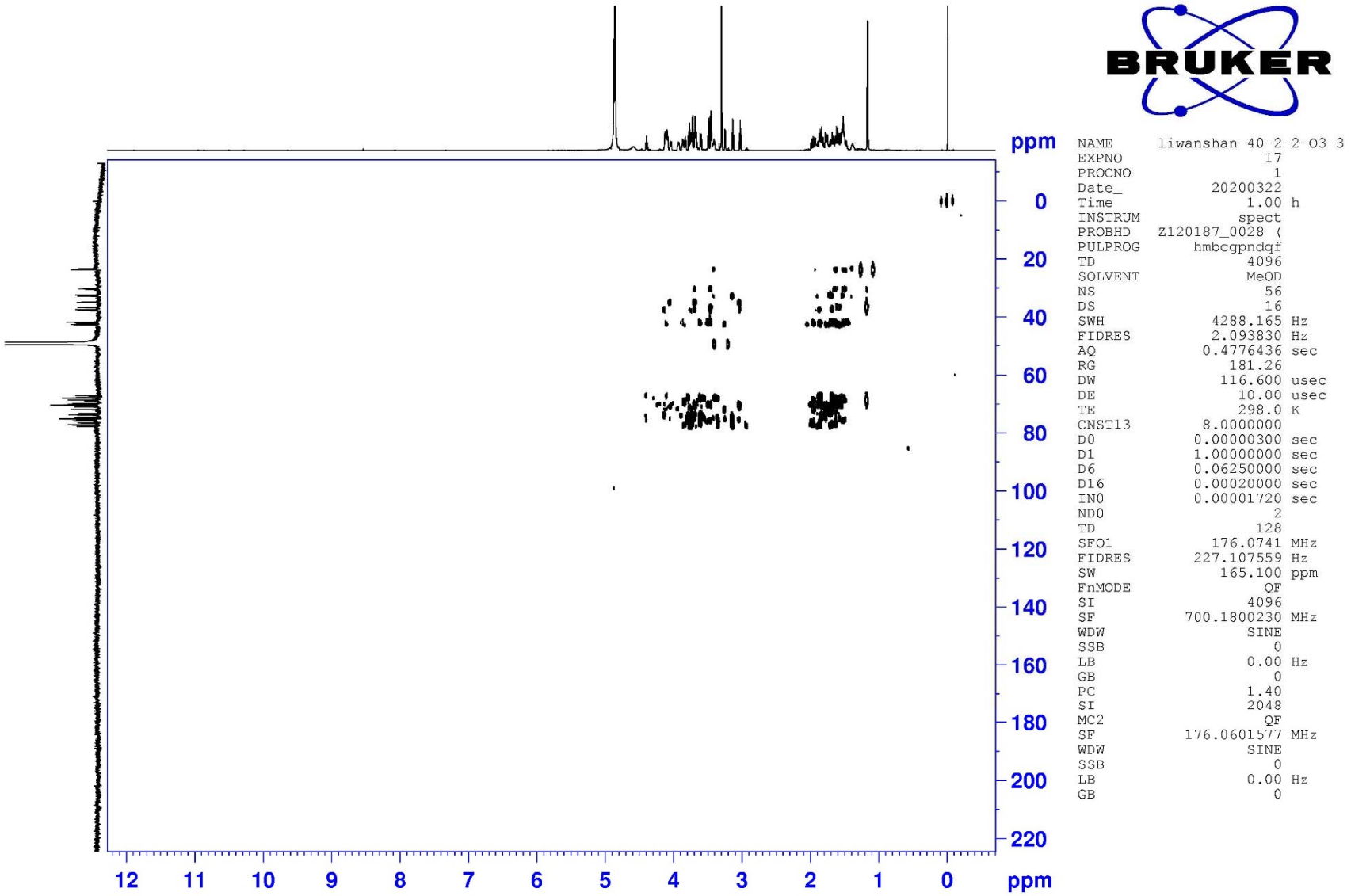
HSQC (700 MHz) spectrum of the fragment **1c** in CD_3OD



HSQC (700 MHz) spectrum of the fragment **1c** in CD_3OD

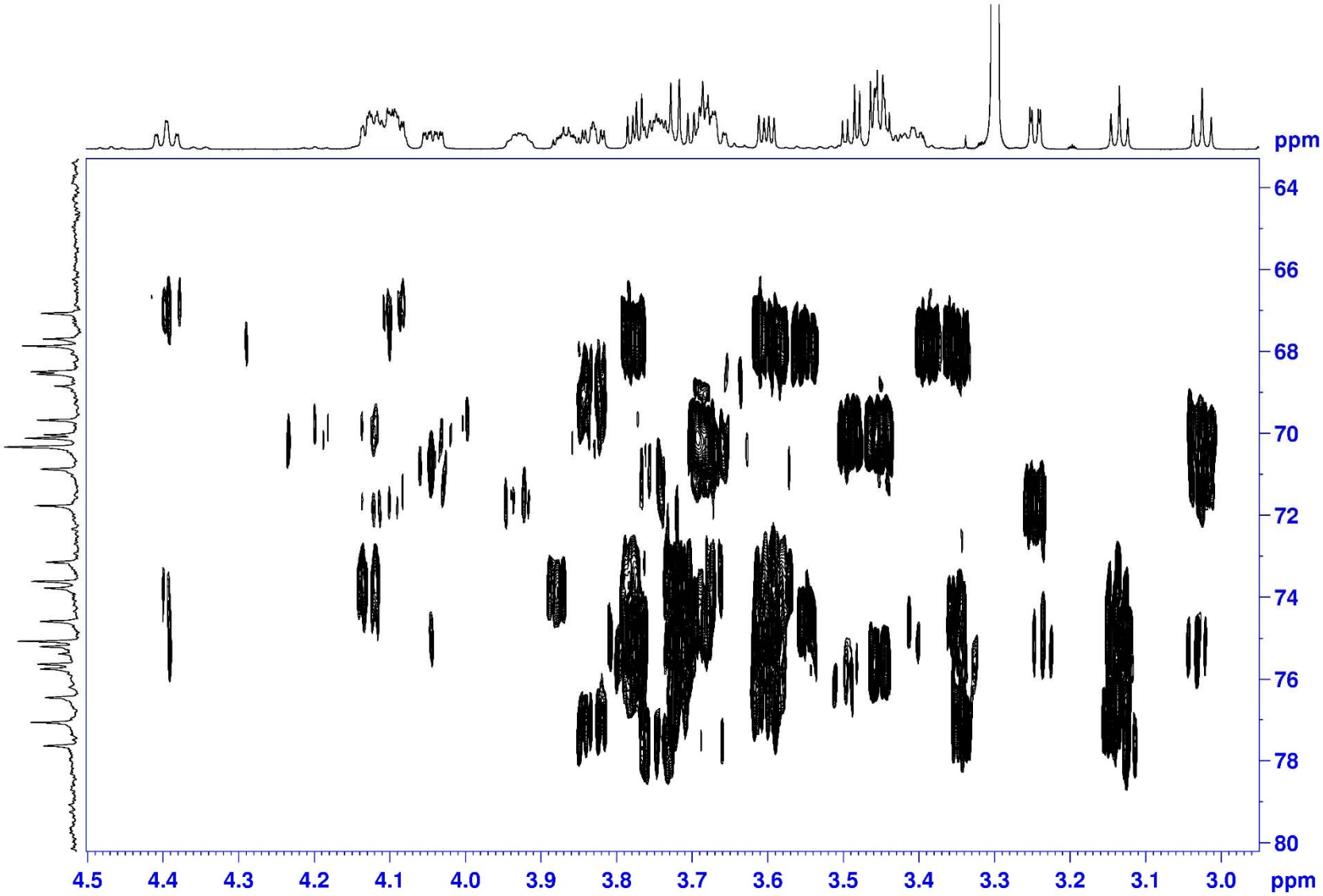


HMBC (700 MHz) spectrum of the fragment **1c** in CD_3OD

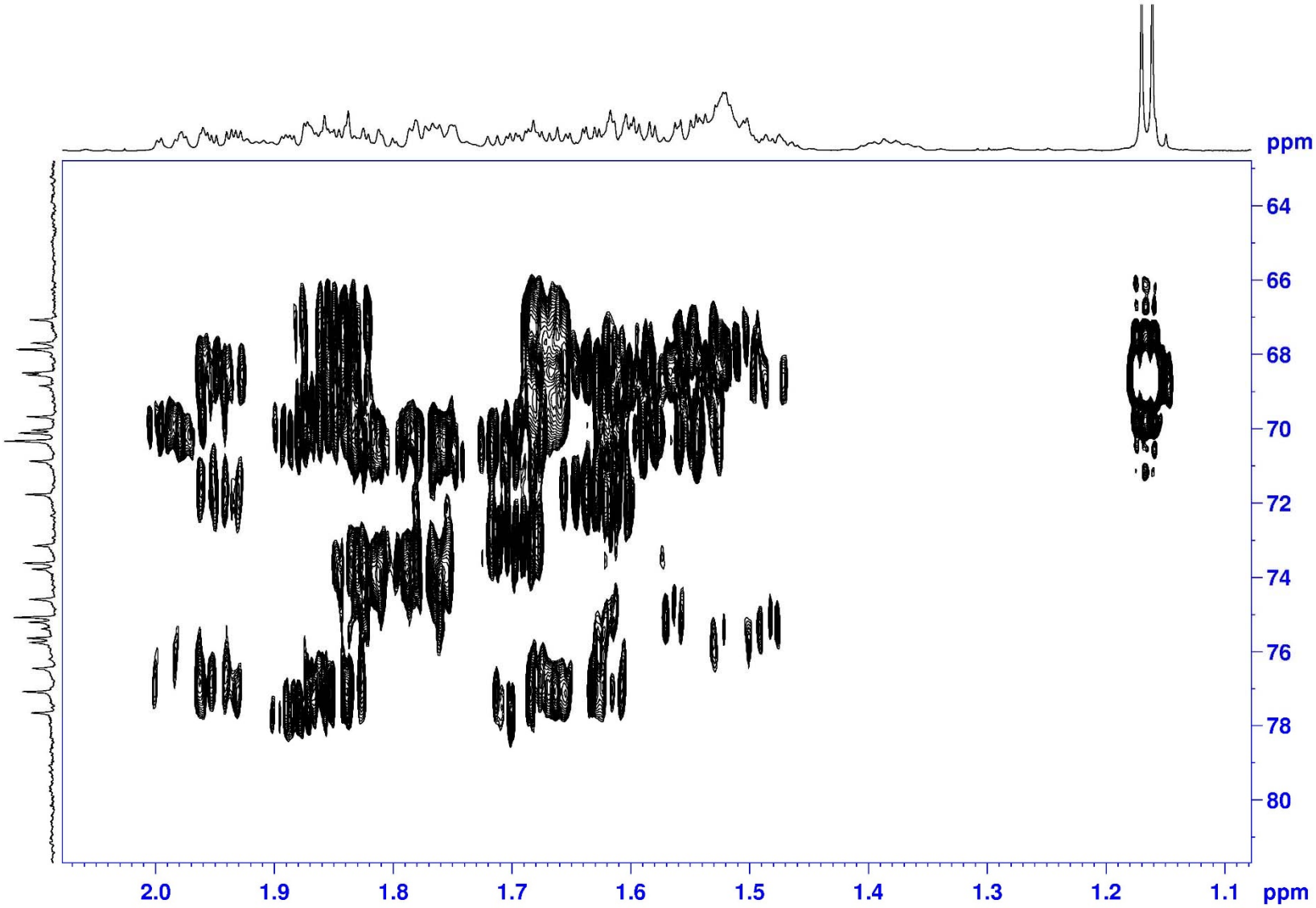


NAME	liwanshan-40-2-2-03-3
EXPNO	17
PROCNO	1
Date_	20200322
Time	1.00 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hmbcgpndqf
TD	4096
SOLVENT	MeOD
NS	56
DS	16
SWH	4288.165 Hz
FIDRES	2.093830 Hz
AQ	0.4776436 sec
RG	181.26
DW	116.600 usec
DE	10.00 usec
TE	298.0 K
CNST13	8.0000000
D0	0.00000300 sec
D1	1.00000000 sec
D6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00001720 sec
ND0	2
TD	128
SFO1	176.0741 MHz
FIDRES	227.107559 Hz
SW	165.100 ppm
FnMODE	QF
SI	4096
SF	700.1800230 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	2048
MC2	QF
SF	176.0601577 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

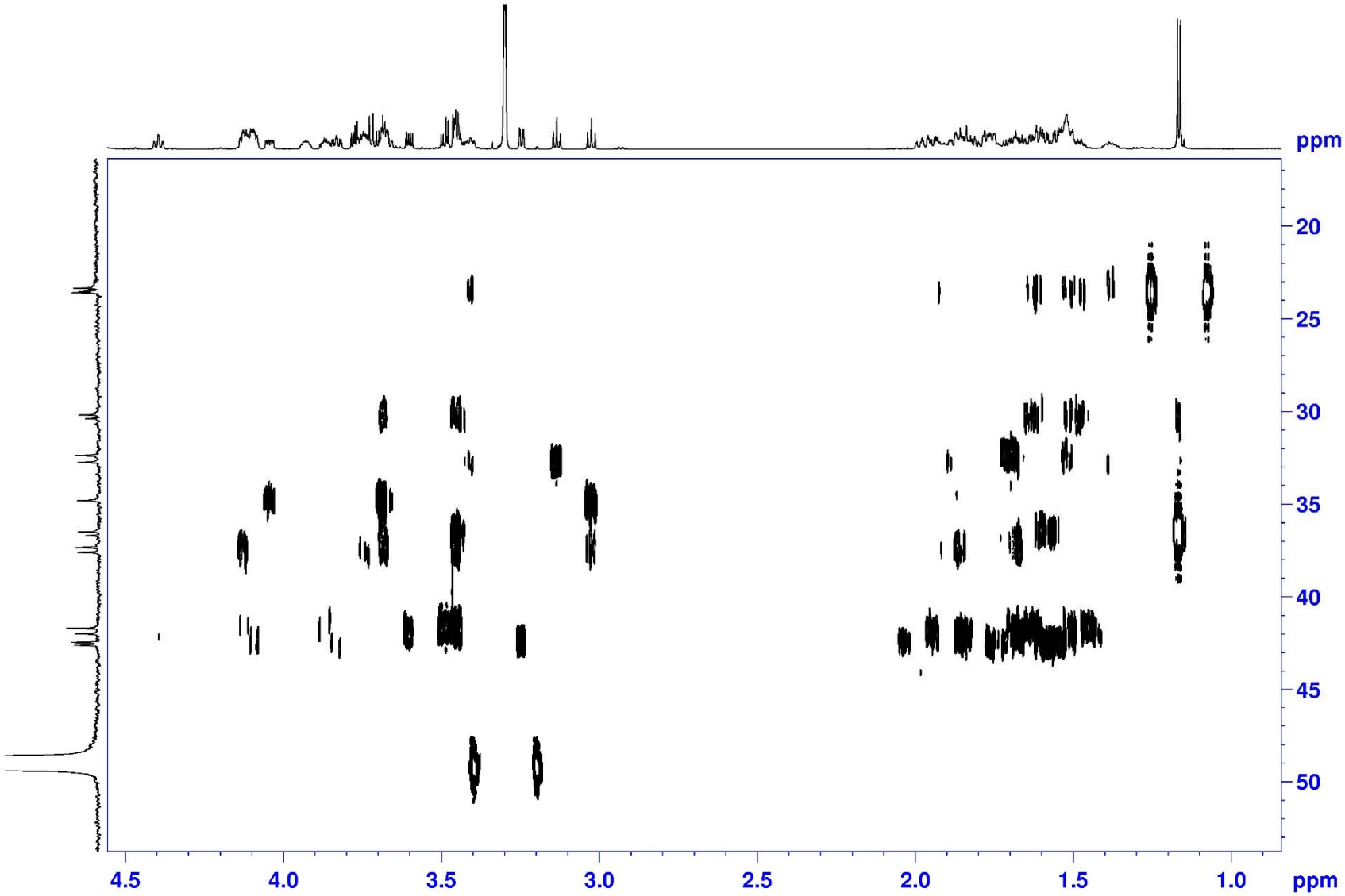
HMBC (700 MHz) spectrum of the fragment **1c** in CD_3OD



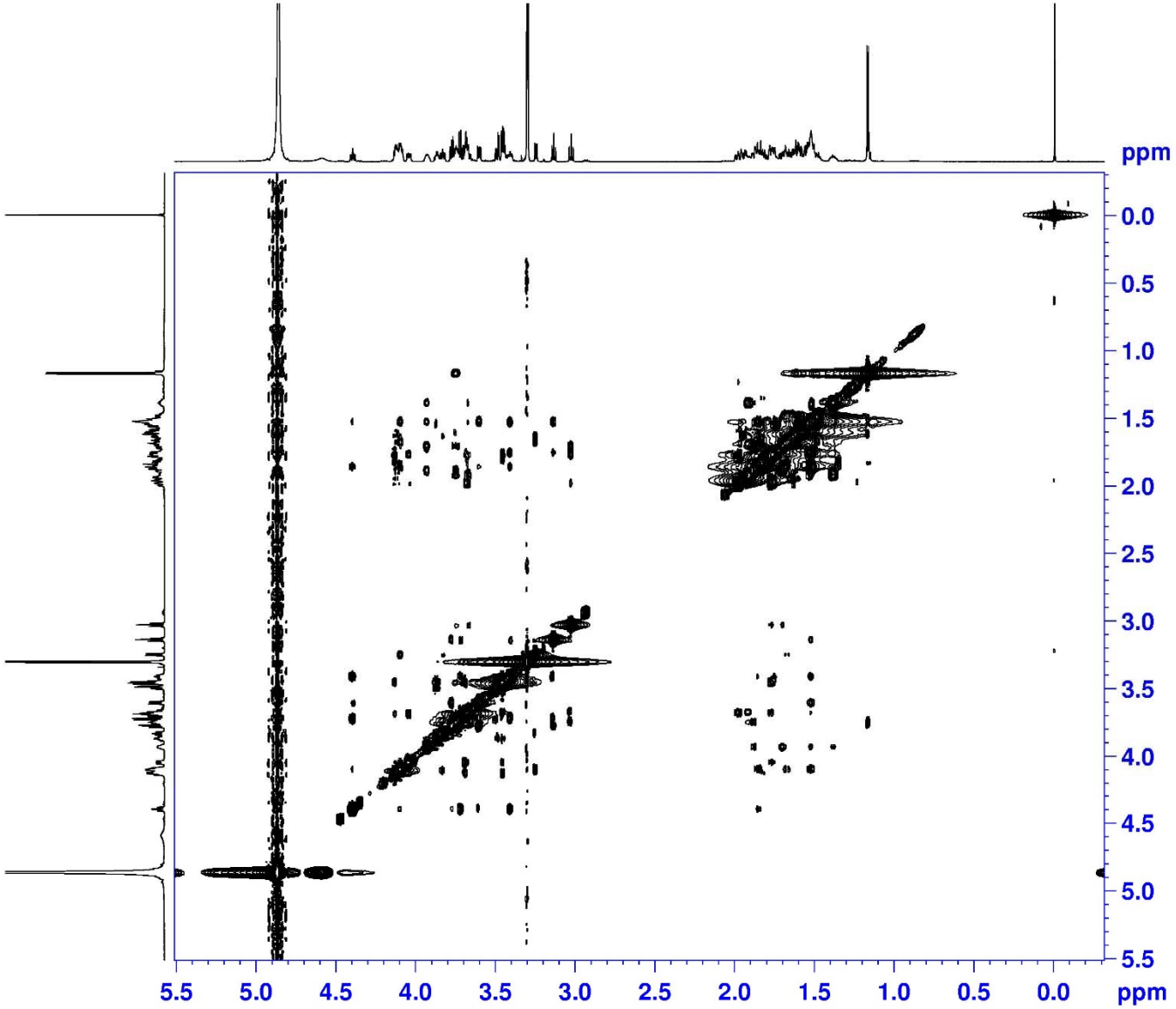
HMBC (700 MHz) spectrum of the fragment **1c** in CD_3OD



HMBC (700 MHz) spectrum of the fragment **1c** in CD_3OD



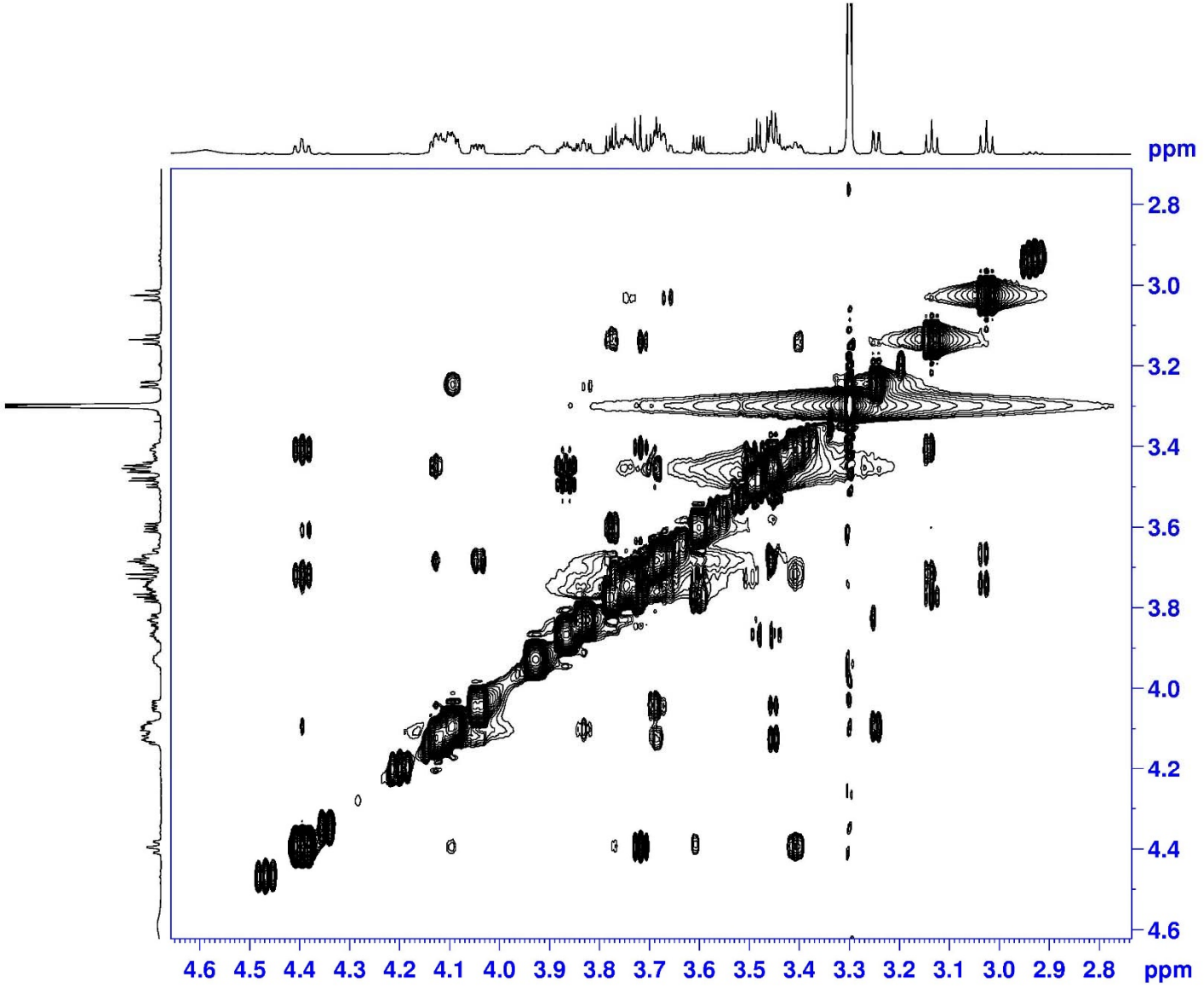
NOESY (700 MHz) spectrum of the fragment **1c** in CD_3OD



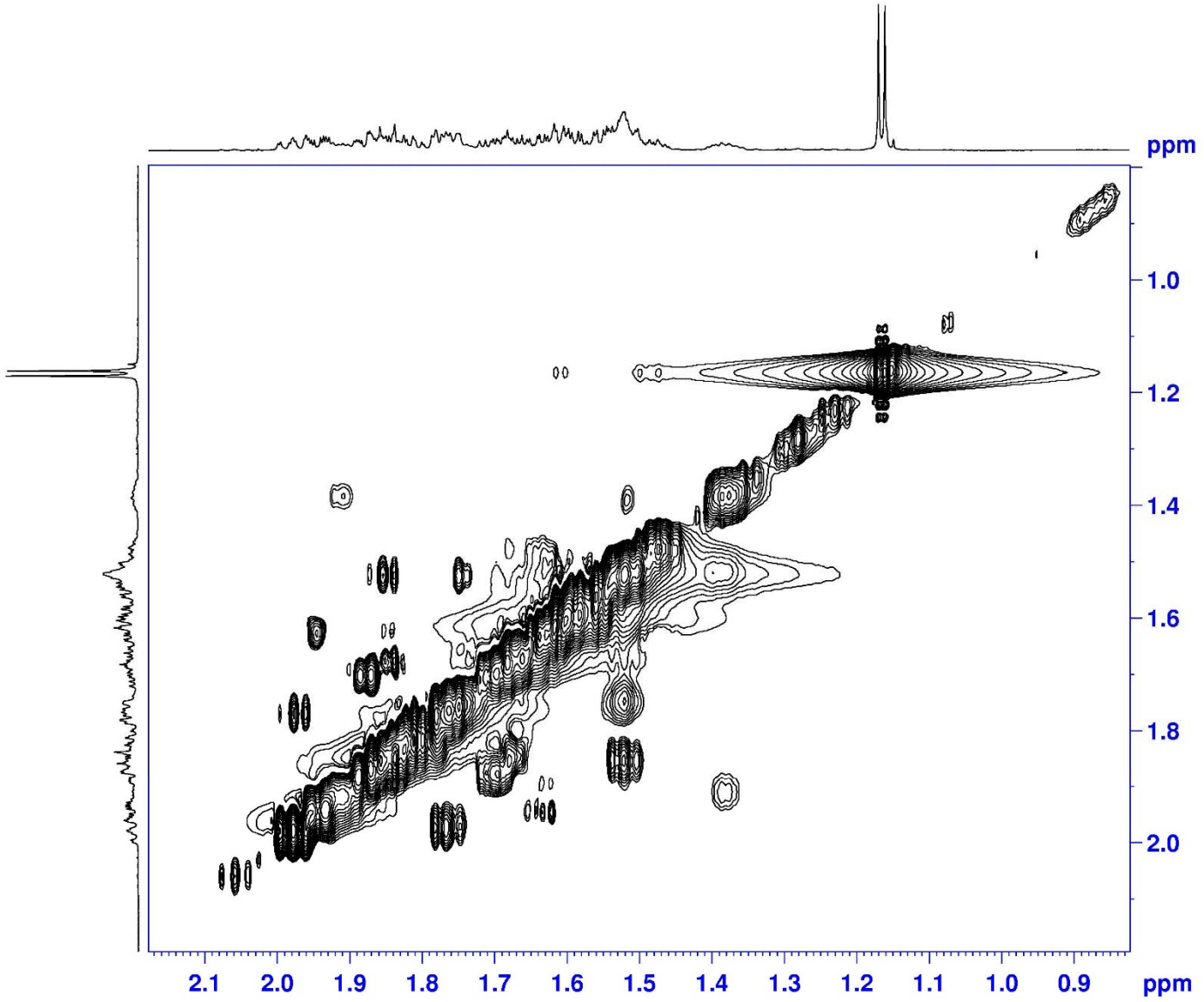
BRUKER

NAME	liwanshan-40-2-2-03-
EXPNO	23
PROCNO	1
Date_	20200330
Time	18.43 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	noesygpph
TD	2048
SOLVENT	MeOD
NS	24
DS	16
SWH	4084.967 Hz
FIDRES	3.989226 Hz
AQ	0.2507252 sec
RG	15.56
DW	122.400 usec
DE	10.00 usec
TE	298.0 K
D0	0.00011279 sec
D1	1.50000000 sec
D8	0.60000002 sec
D16	0.00020000 sec
IN0	0.00024480 sec
ND0	1
TD	256
SFO1	700.1818 MHz
FIDRES	15.956903 Hz
SW	5.834 ppm
FnMODE	TPPI
SI	2048
SF	700.1800209 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	2048
MC2	TPPI
SF	700.1800209 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

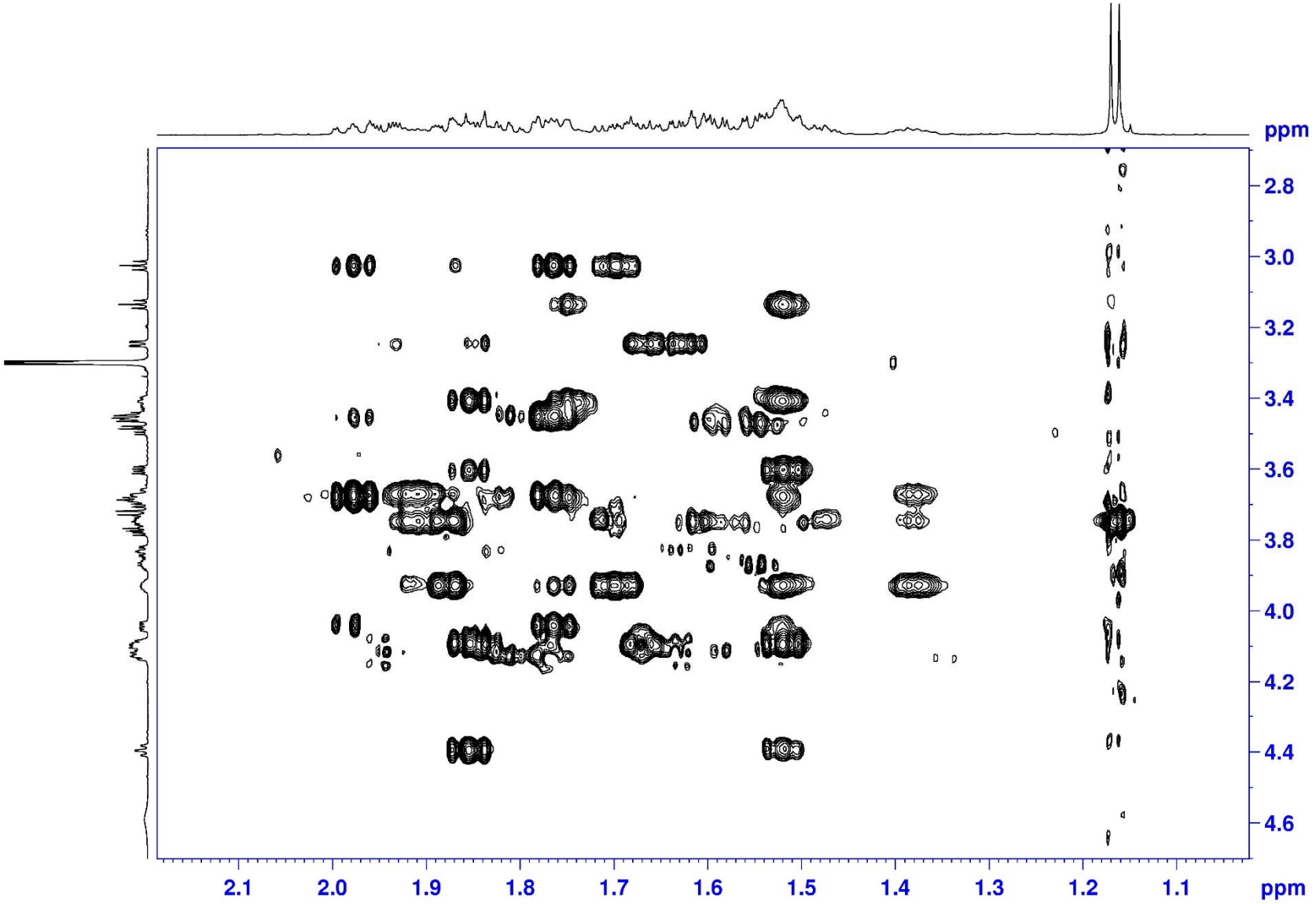
NOESY (700 MHz) spectrum of the fragment **1c** in CD_3OD



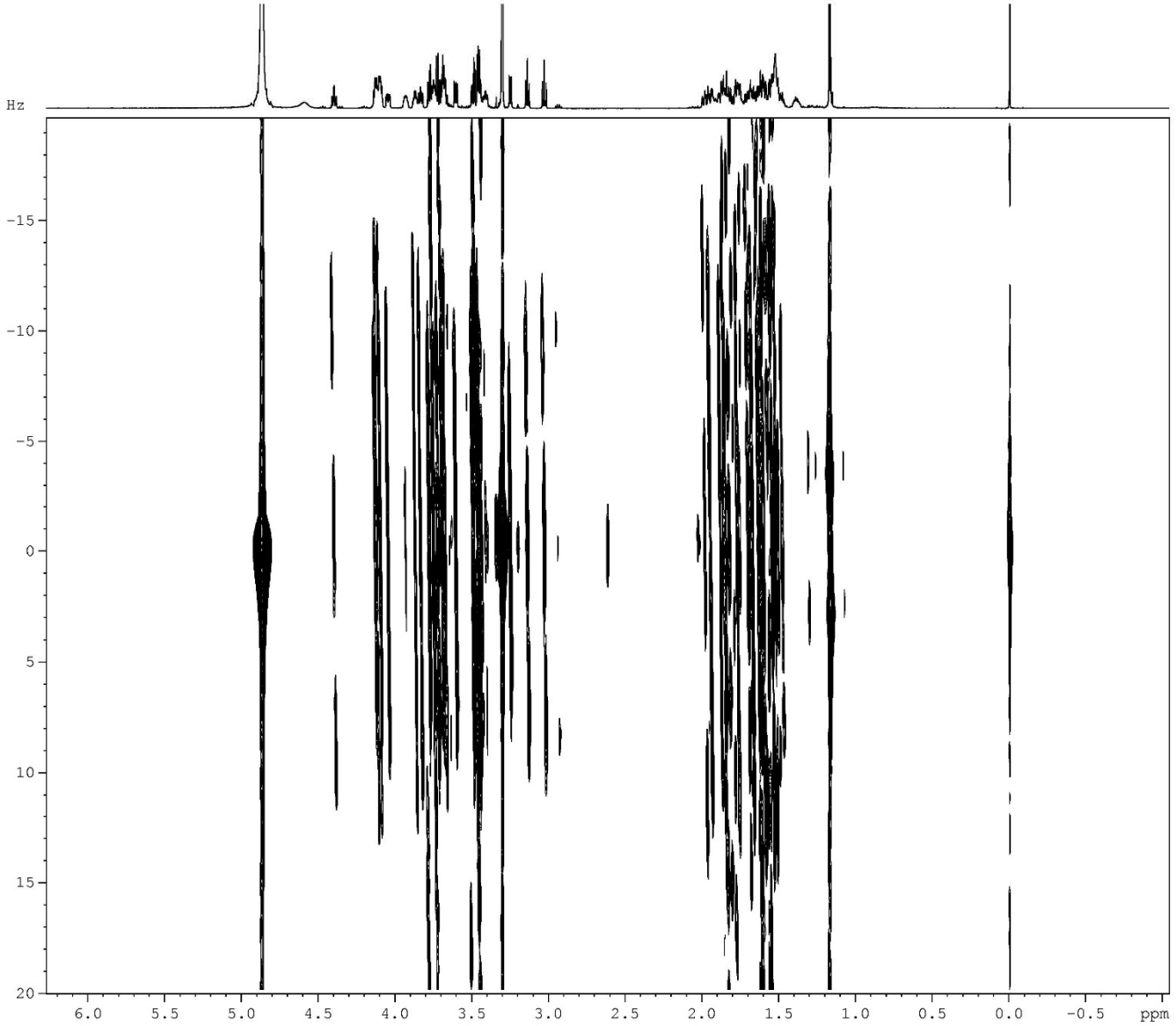
NOESY (700 MHz) spectrum of the fragment **1c** in CD_3OD



NOESY (700 MHz) spectrum of the fragment **1c** in CD_3OD

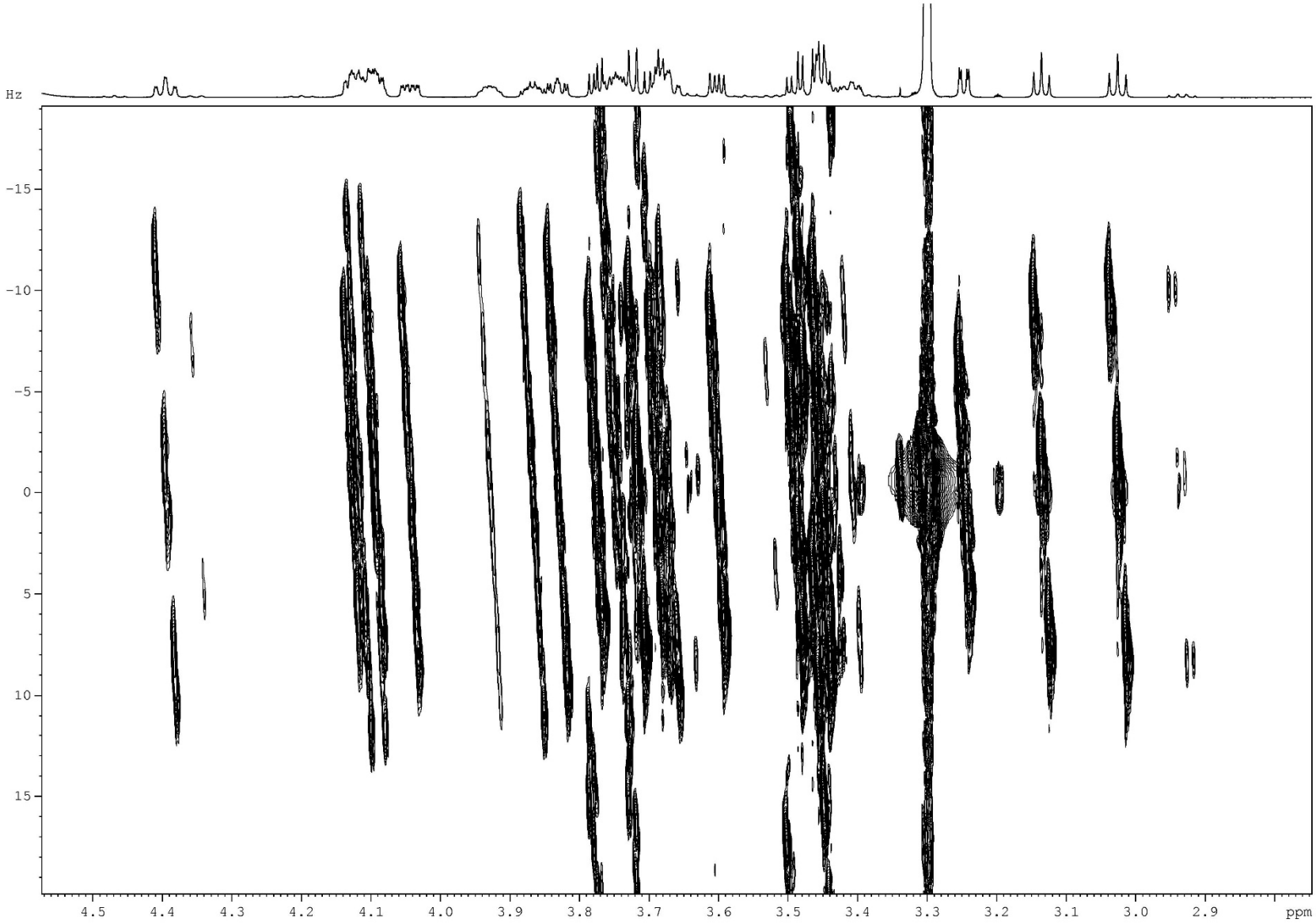


2D *J*RES (700 MHz) spectrum of the fragment **1c** in CD_3OD

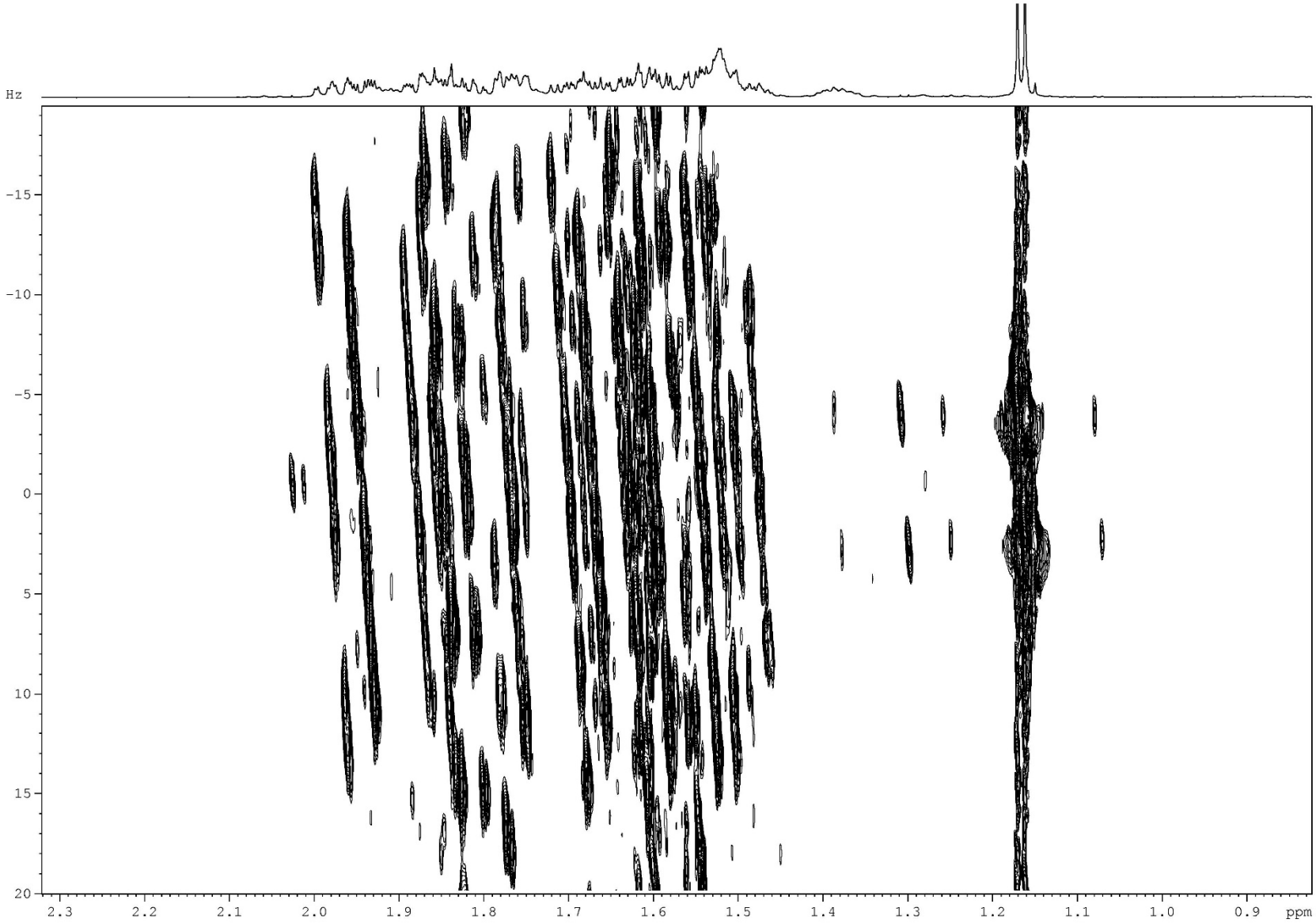


NAME	liwanshan-40-2-2-O
EXPNO	22
PROCNO	1
Date_	20200330
Time	15.26 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	jresgpprqf
TD	8192
SOLVENT	MeOD
NS	128
DS	16
SWH	5122.951 Hz
FIDRES	1.250720 Hz
AQ	0.7995892 sec
RG	136.72
DW	97.600 use
DE	10.00 use
TE	298.0 K
D0	0.00000300 sec
D1	1.00000000 sec
D11	0.03000000 sec
D12	0.00002000 sec
D16	0.00020000 sec
IN0	0.01250000 sec
ND0	2
TD	40
SFO1	700.1819 MHz
FIDRES	1.000000 Hz
SW	0.057 ppm
FnMODE	QF
SI	16384
SF	700.1800232 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.00
SI	128
MC2	QF
SF	700.1818520 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

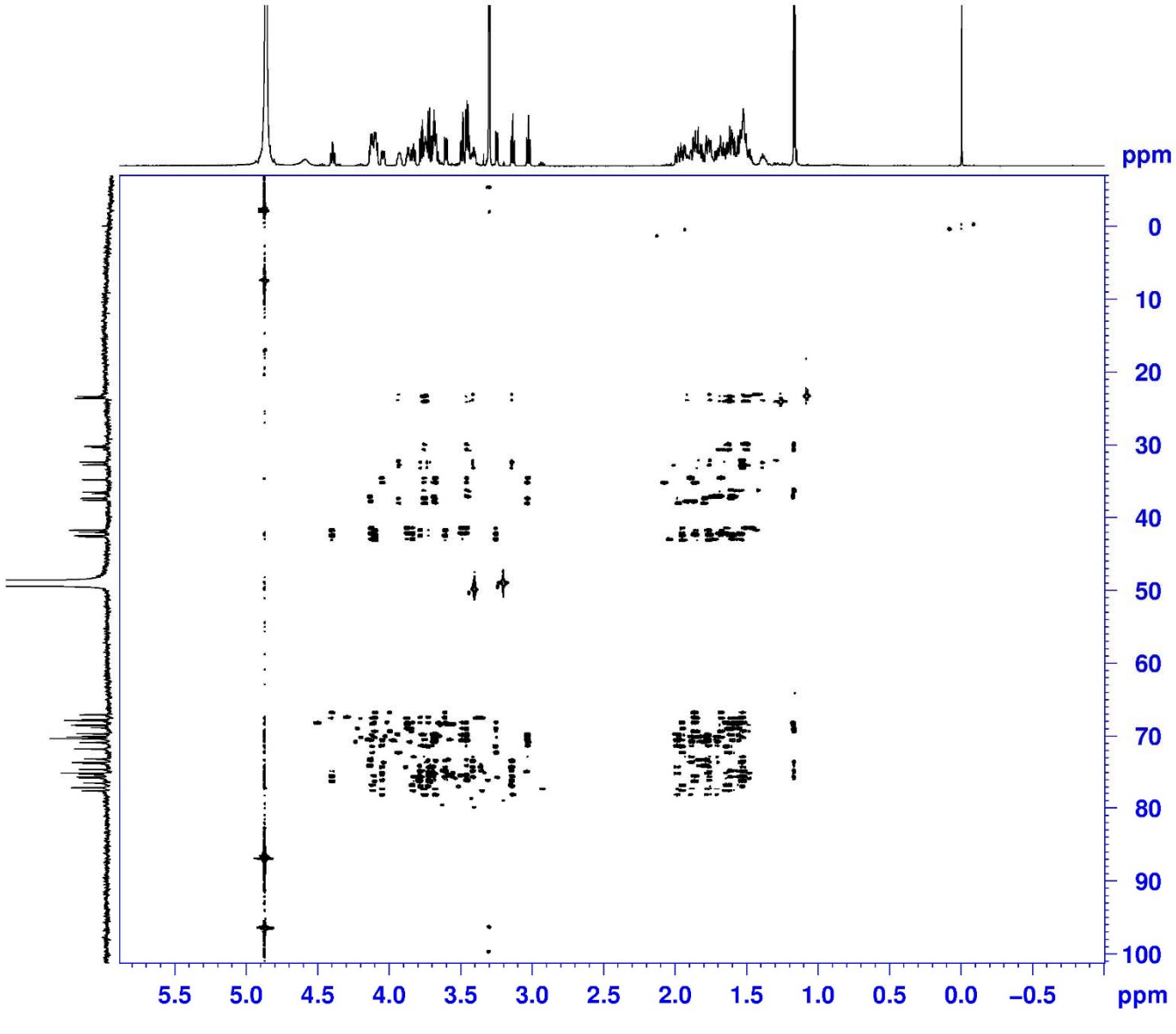
2D *J*RES (700 MHz) spectrum of the fragment **1c** in CD_3OD



2D *J*RES (700 MHz) spectrum of the fragment **1c** in CD_3OD



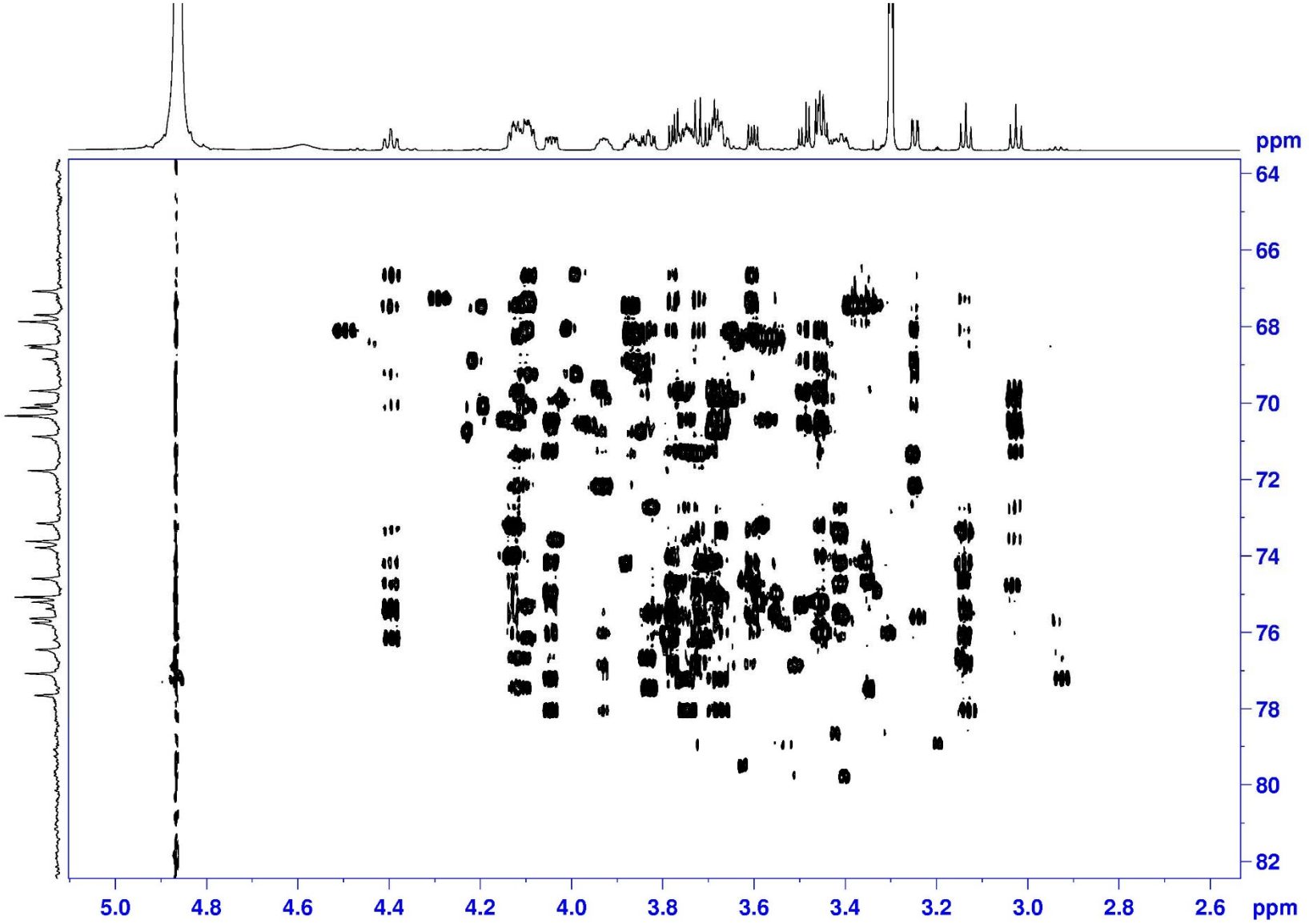
HECADE (700 MHz) spectrum of the fragment **1c** in CD_3OD



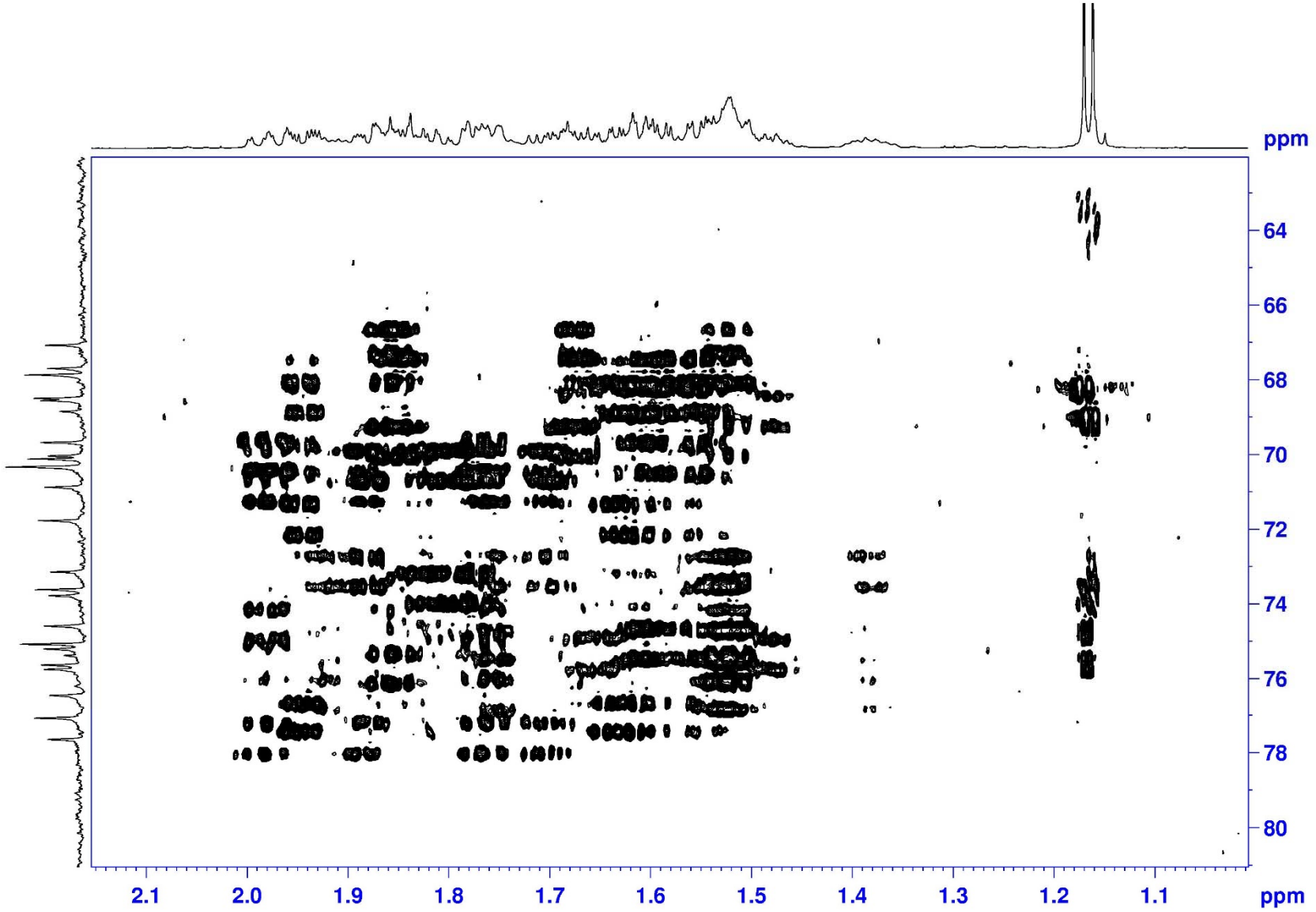
BRUKER

NAME	liwanshan-40-2-2-03-3
EXPNO	25
PROCNO	1
Date_	20200820
Time	2.37 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hsqcdietgpjcndsisp
TD	4096
SOLVENT	MeOD
NS	56
DS	16
SWH	4826.255 Hz
FIDRES	2.356570 Hz
AQ	0.4243956 sec
RG	181.26
DW	103.600 usec
DE	10.00 usec
TE	298.0 K
CNST2	145.0000000
CNST16	1.0000000
CNST17	-0.5000000
D0	0.00000300 sec
D1	1.00000000 sec
D2	0.00344828 sec
D4	0.00172414 sec
D9	0.08000000 sec
D16	0.00020000 sec
D20	0.00000300 sec
D24	0.00089000 sec
IN0	0.00002620 sec
IN20	0.00002620 sec
L0	1
L1	28
ND0	2
TD	512
SFO1	176.0684 MHz
FIDRES	37.273376 Hz
SW	108.389 ppm
FnMODE	Echo-Antiecho
SI	8192
SF	700.1800200 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	176.0601510 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz

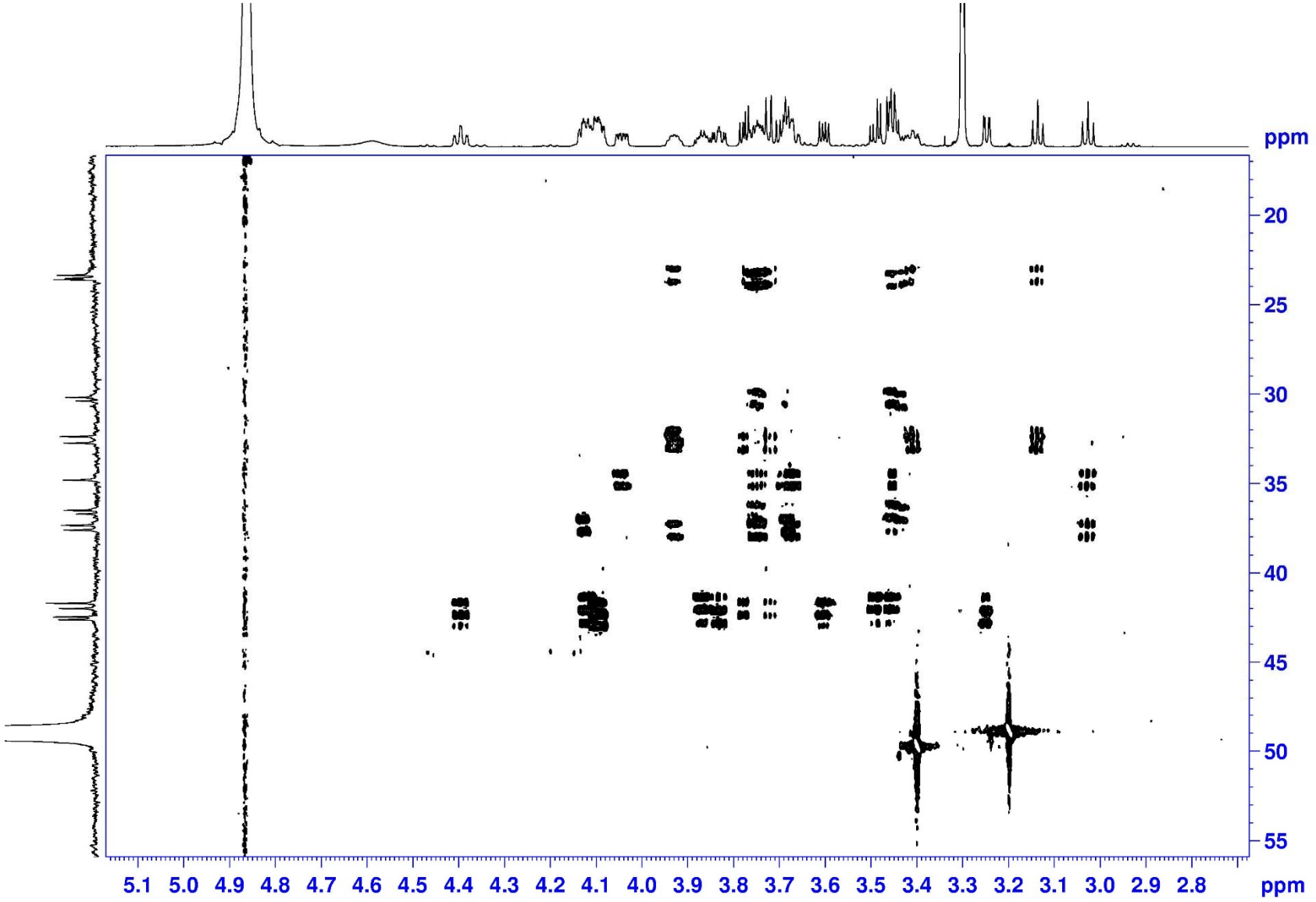
HECADE (700 MHz) spectrum of the fragment **1c** in CD_3OD



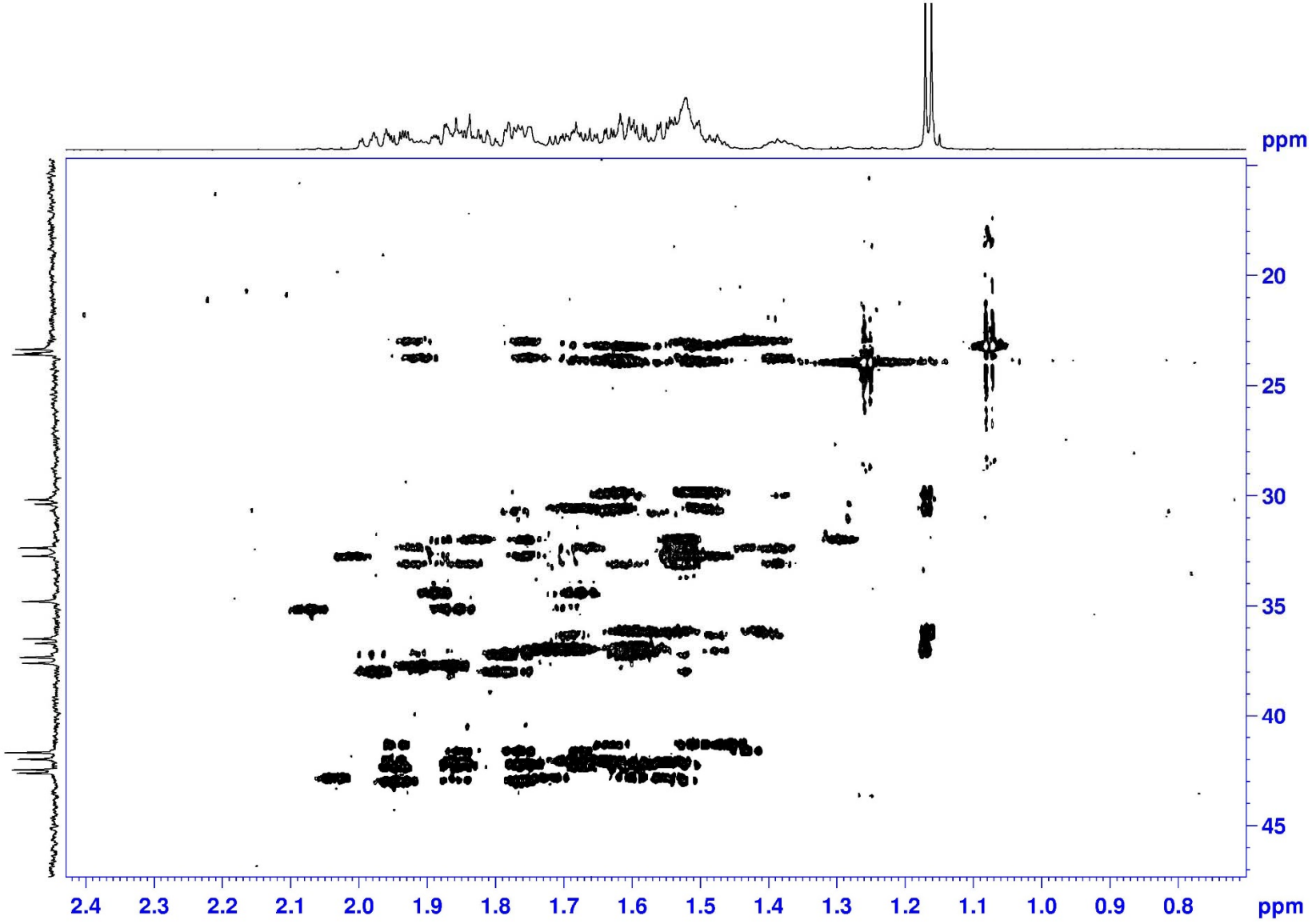
HECADE (700 MHz) spectrum of the fragment **1c** in CD_3OD



HECADE (700 MHz) spectrum of the fragment **1c** in CD_3OD



HECADE (700 MHz) spectrum of the fragment **1c** in CD_3OD

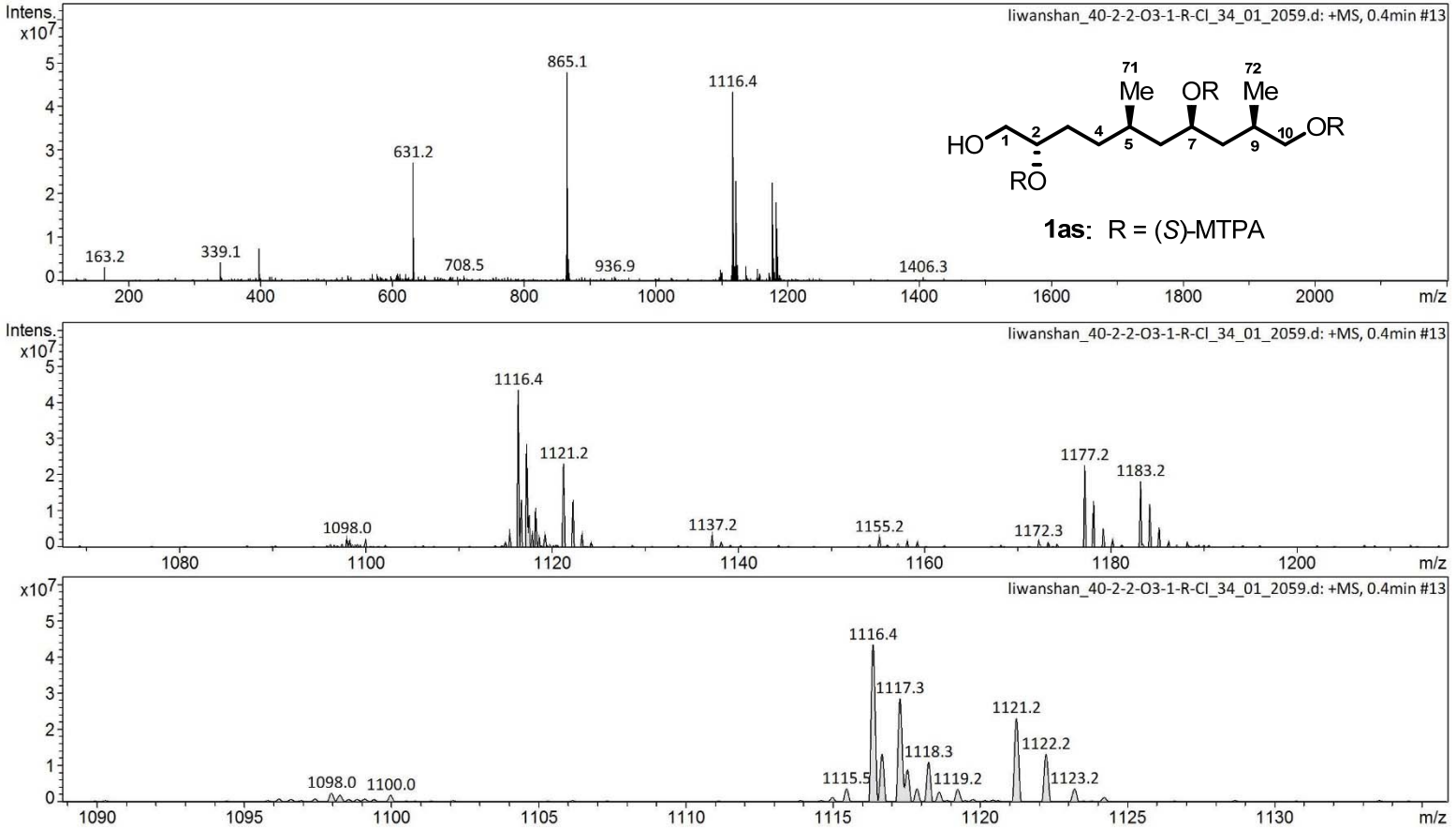


LR-ESI-MS for the fragment **1as**

Generic Display Report

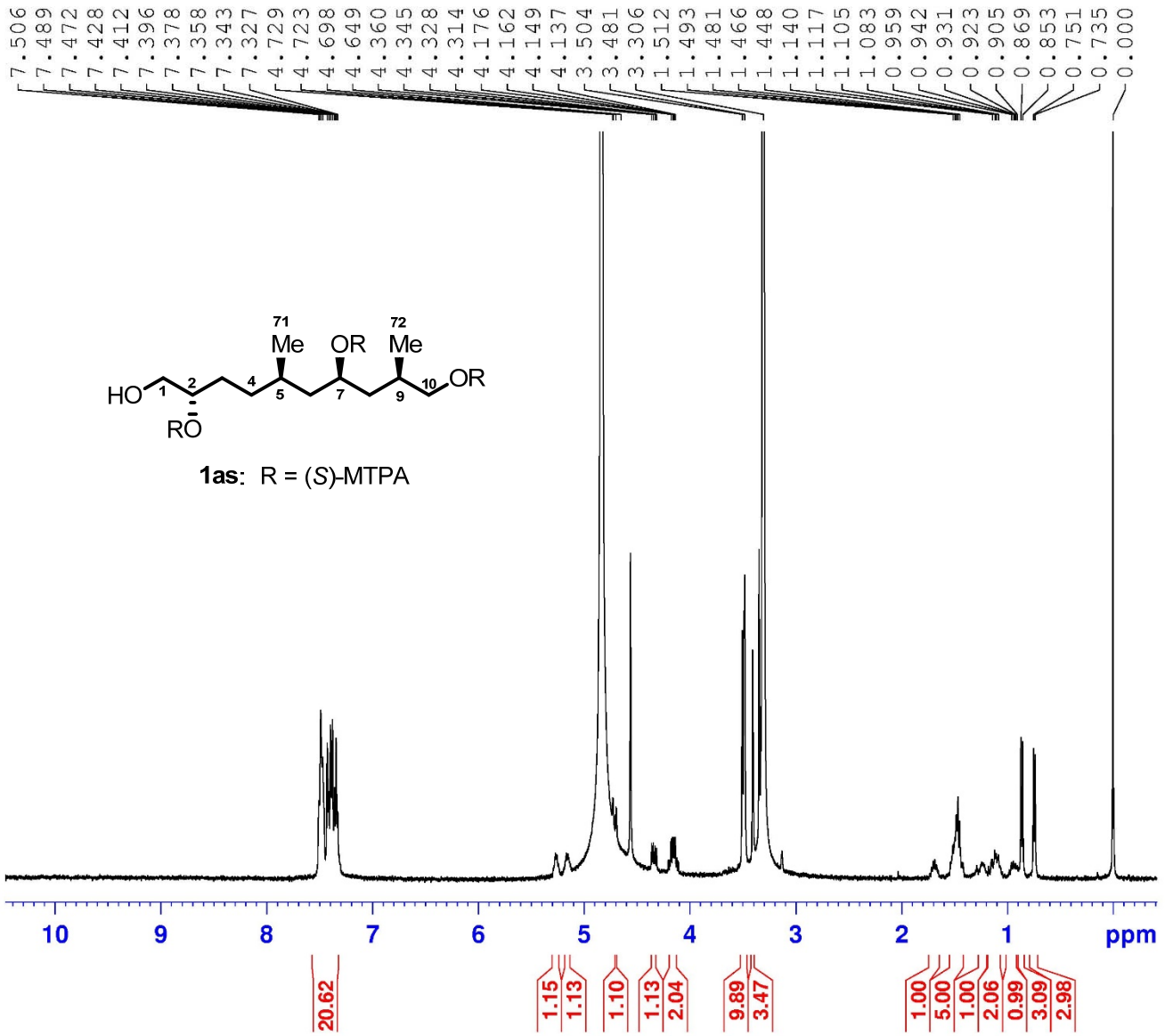
Analysis Info

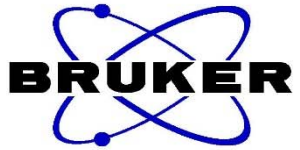
Analysis Name	D:\Data\amaZon SL\MS\data\202008\liwanshan_40-2-2-O3-1-R-Cl_34_01_2059.d	Acquisition Date	2020-08-21 16:35:57
Method	2059.m	Operator	bruker
Sample Name	liwanshan_40-2-2-O3-1-R-Cl	Instrument	amaZon SL
Comment			



Bruker Compass DataAnalysis 4.4 printed: 2020-08-21 16:45:28 by: bruker Page 1 of 1

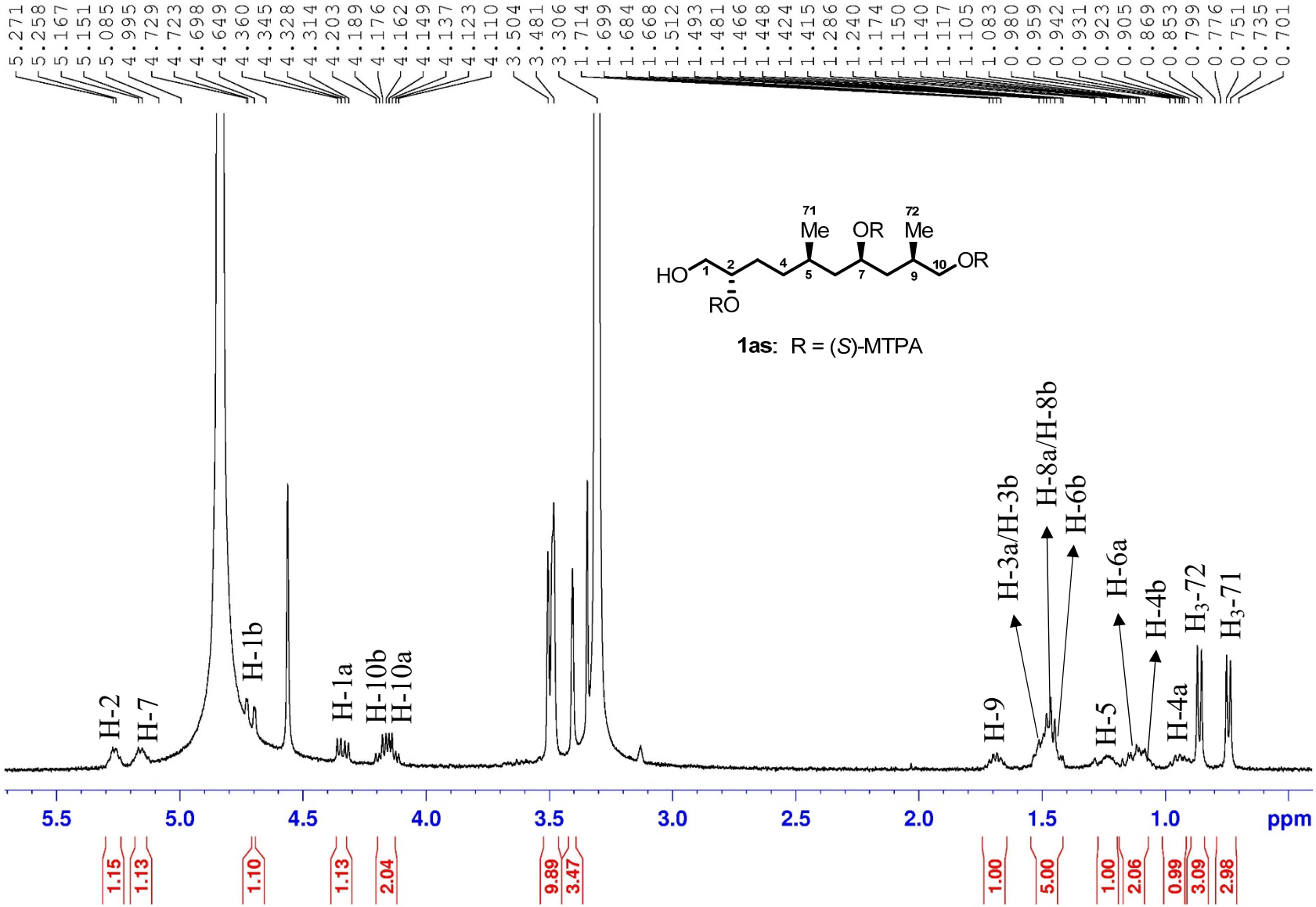
^{1}H (400 MHz) NMR spectrum of the fragment **1as** in CD_3OD



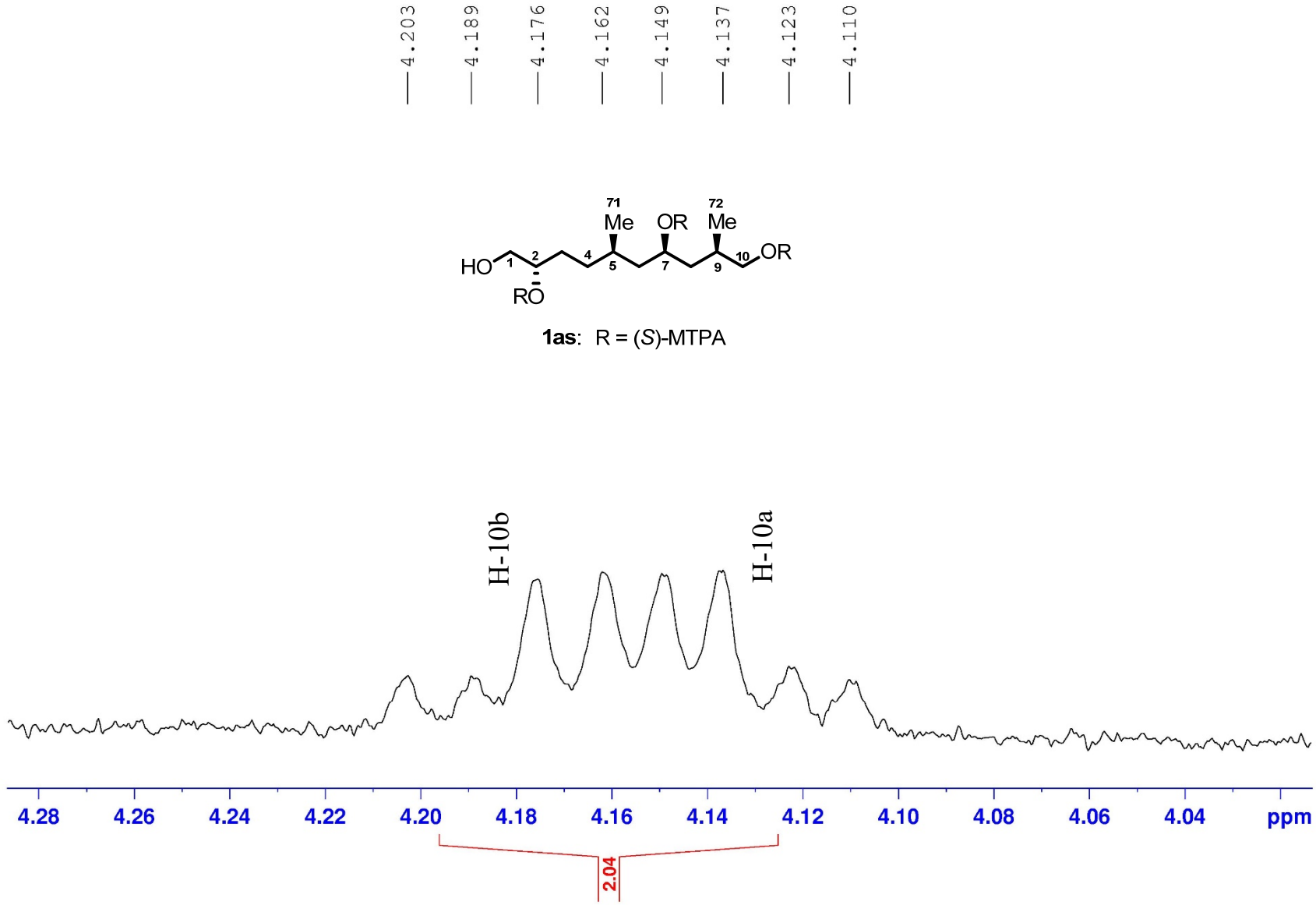


NAME	40-2-2-O3-1-R-Cl
EXPNO	1
PROCNO	1
Date_	20200425
Time	10.26
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	32
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	177.07
DW	62.400 use
DE	6.50 use
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
SFO1	400.1324710 MHz
NUC1	1H
P1	9.73 use
SI	65536
SF	400.1300091 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

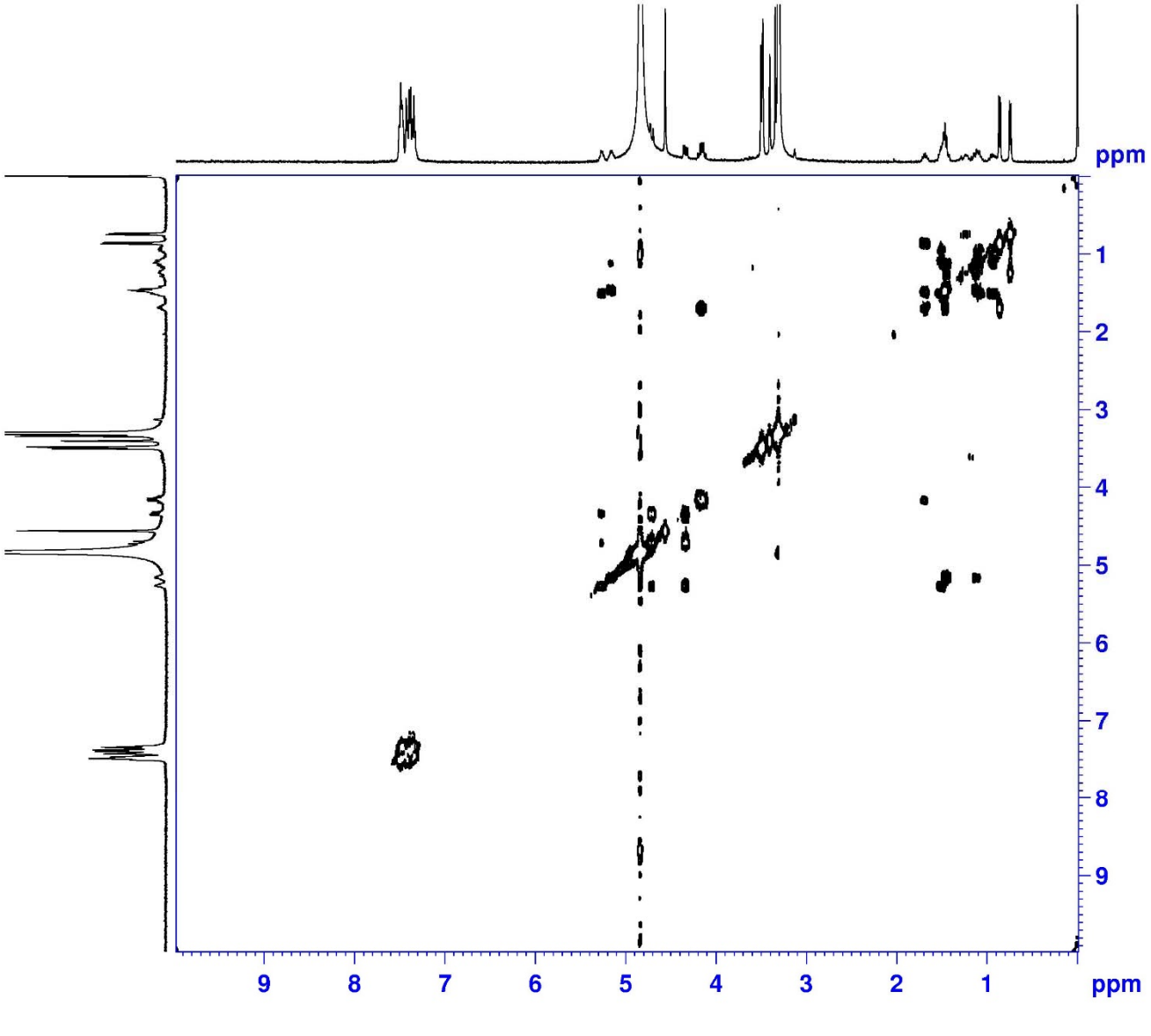
^{1}H (400 MHz) NMR spectrum of the fragment **1as** in CD_3OD



^{1}H (400 MHz) NMR spectrum of the fragment **1as** in CD_3OD

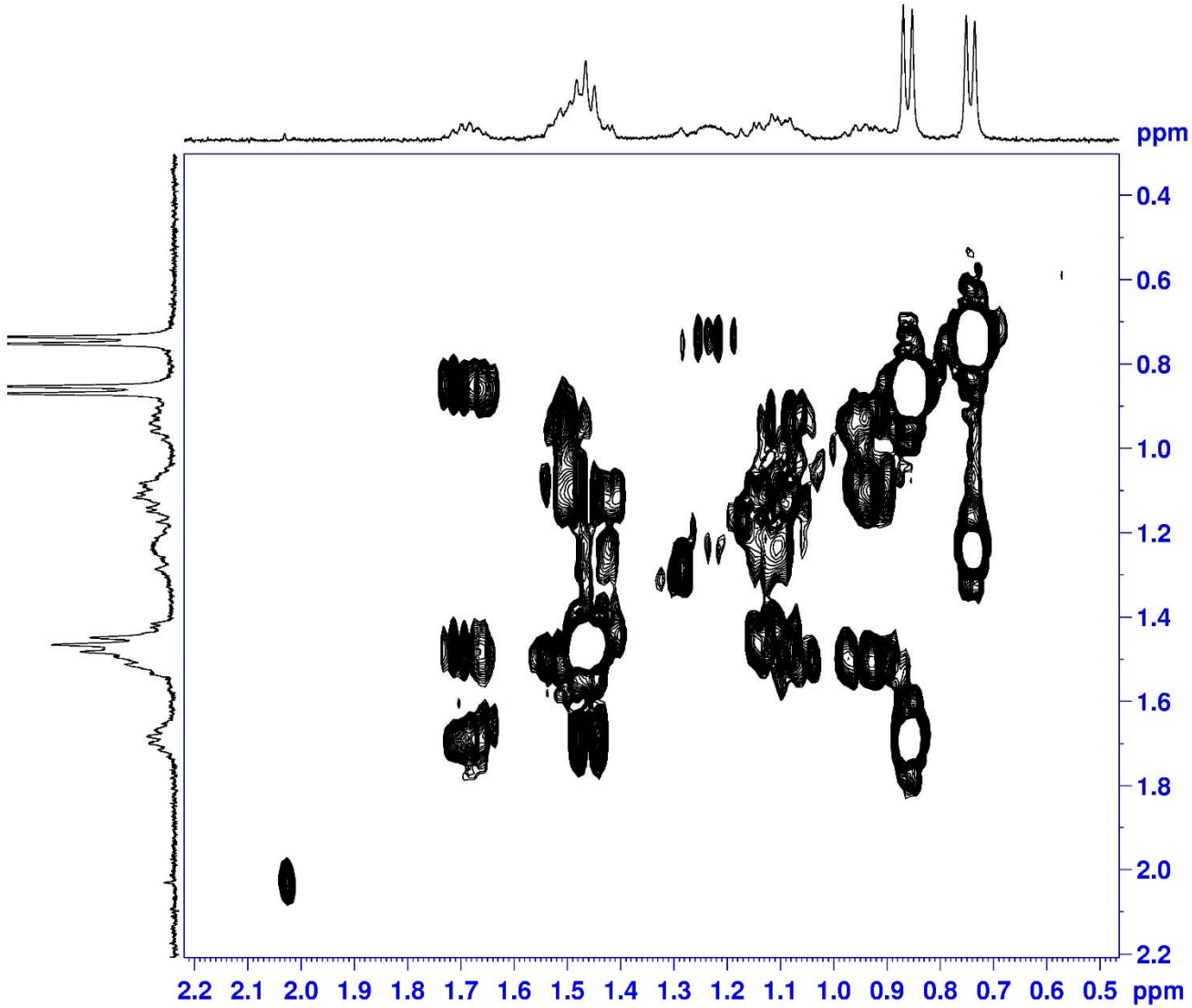


^{1}H–^{1}H COSY (400 MHz) spectrum of the fragment **1as** in CD_3OD

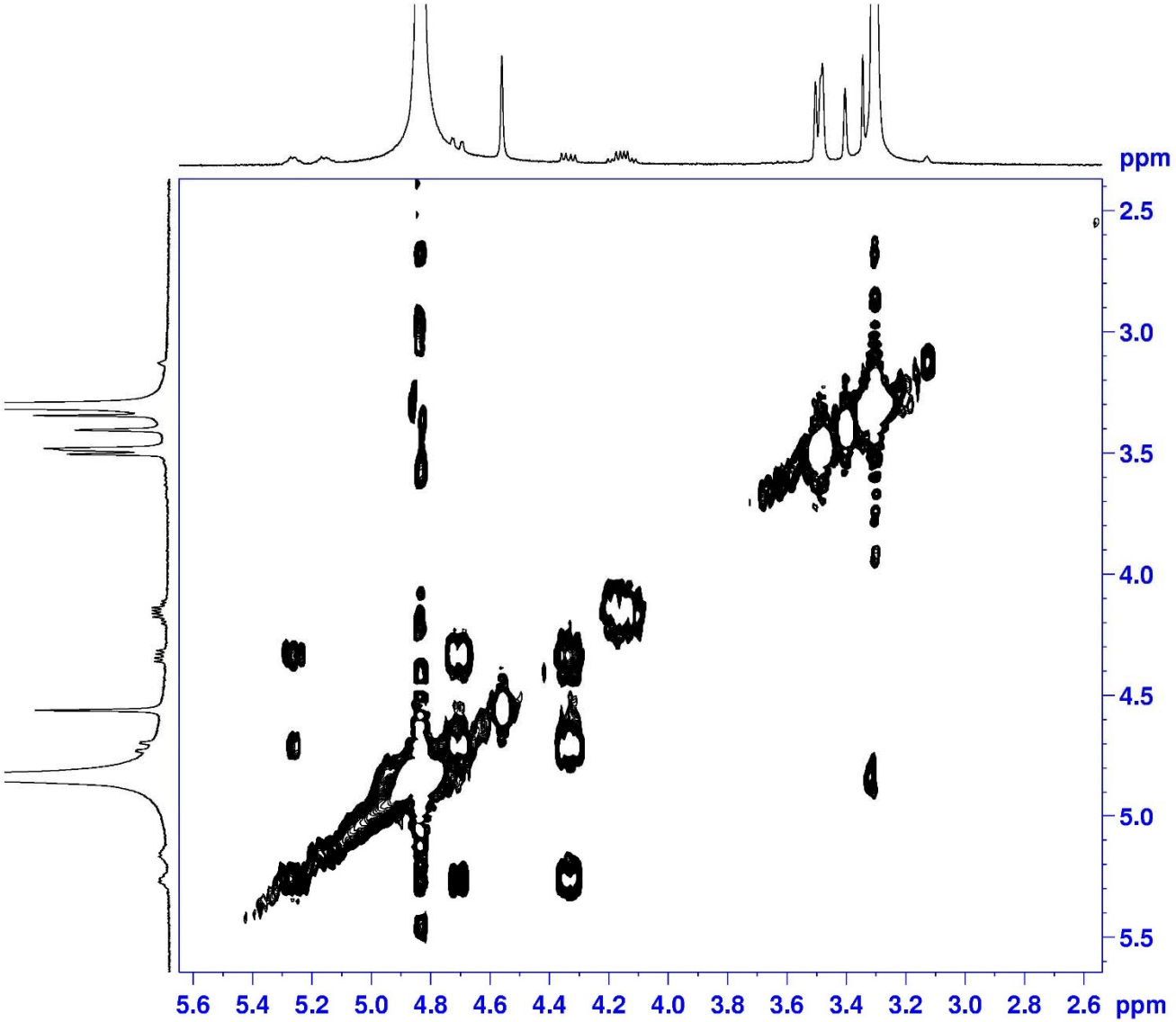



```
NAME        40-2-2-03-1-R-Cl
EXPNO                      2
PROCNO                     1
Date_               20200425
Time                   10.34
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             cosygpqf
TD                      2048
SOLVENT                 MeOD
NS                       100
DS                         8
SWH                4000.000 Hz
FIDRES                1.953125 Hz
AQ                 0.2560500 sec
RG                     202.1
DW                  125.000 usec
DE                    6.50 usec
TE                    300.0 K
D0                 0.00000300 sec
D1                 2.00000000 sec
D13                0.00000400 sec
D16                0.00020000 sec
IN0                0.00025000 sec

======== CHANNEL f1 ========
SFO1              400.1320007 MHz
NUC1                       1H
P0                    9.73 usec
P1                    9.73 usec
ND0                        1
TD                       128
SFO1                400.132 MHz
FIDRES               31.250000 Hz
SW                     9.997 ppm
FnMODE                    QF
SI                       1024
SF                400.1300091 MHz
WDW                    QSINE
SSB                        0
LB                     0.00 Hz
GB                         0
PC                     1.40
SI                       1024
MC2                       QF
SF                400.1300091 MHz
WDW                    QSINE
SSB                        0
LB                     0.00 Hz
```

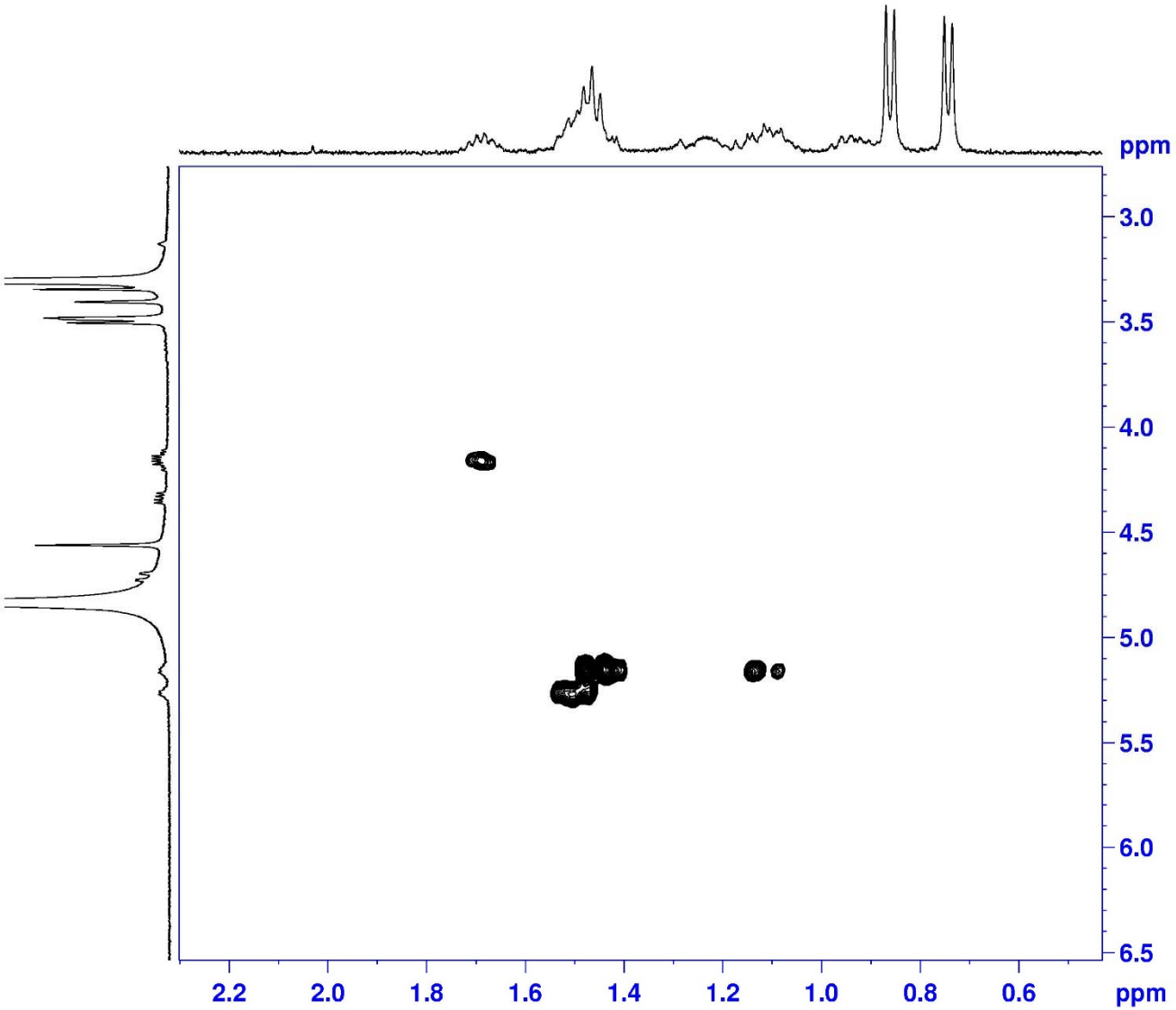
$^{1}H–^{1}H$ COSY (400 MHz) spectrum of the fragment **1as** in CD_3OD



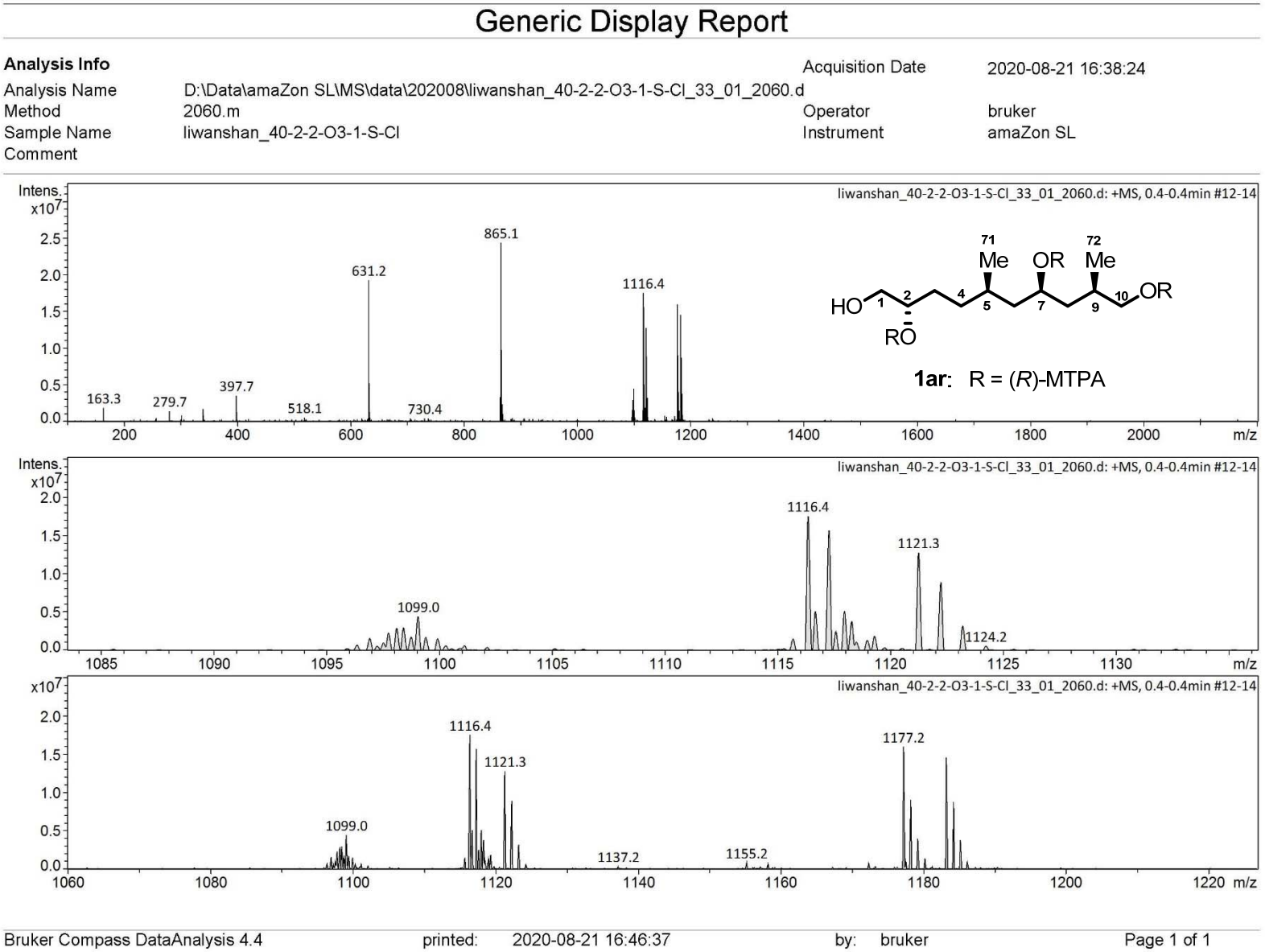
$^{1}H–^{1}H$ COSY (400 MHz) spectrum of the fragment **1as** in CD_3OD



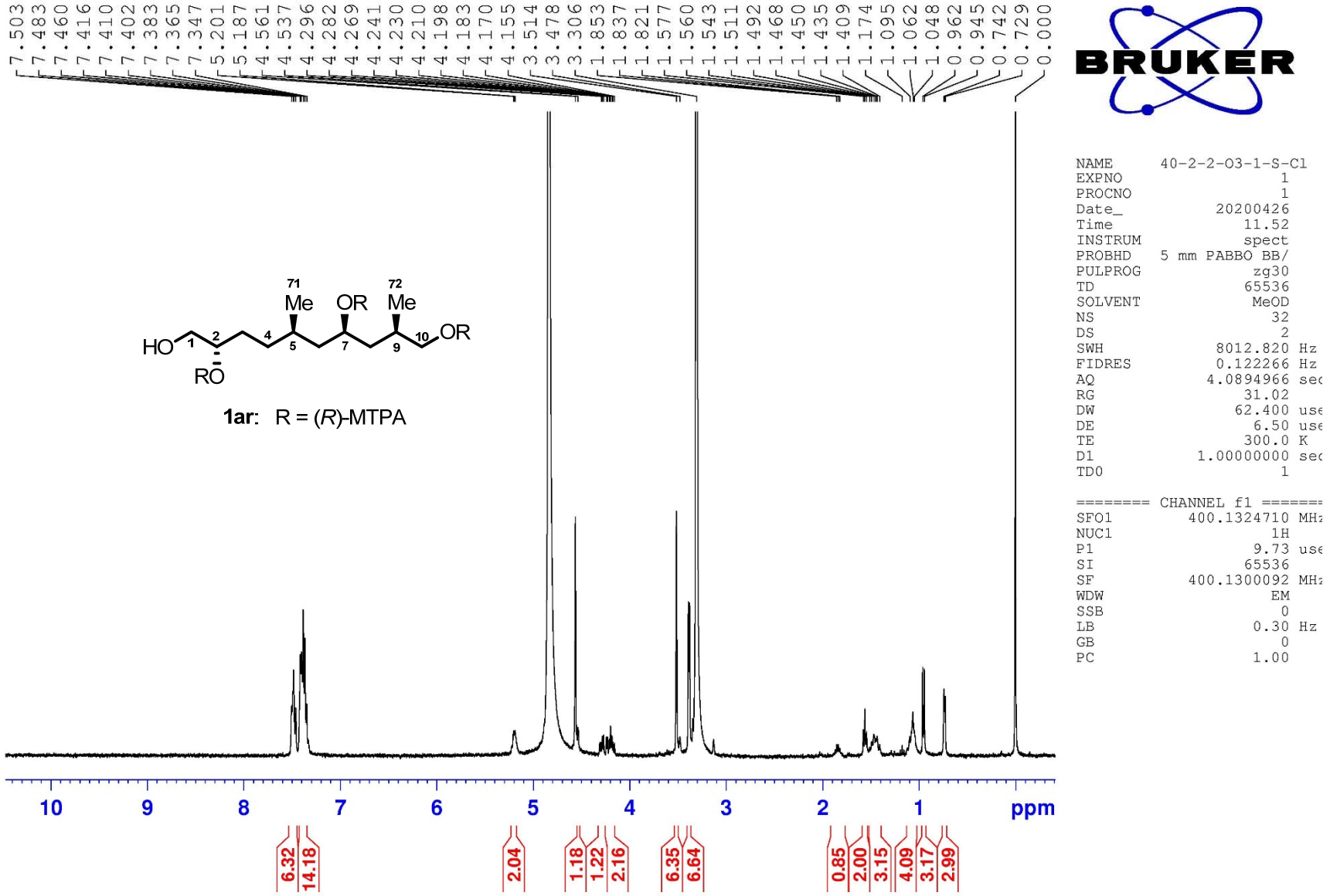
$^{1}H–^{1}H$ COSY (400 MHz) spectrum of the fragment **1as** in CD_3OD



LR-ESI-MS for the fragment **1ar**

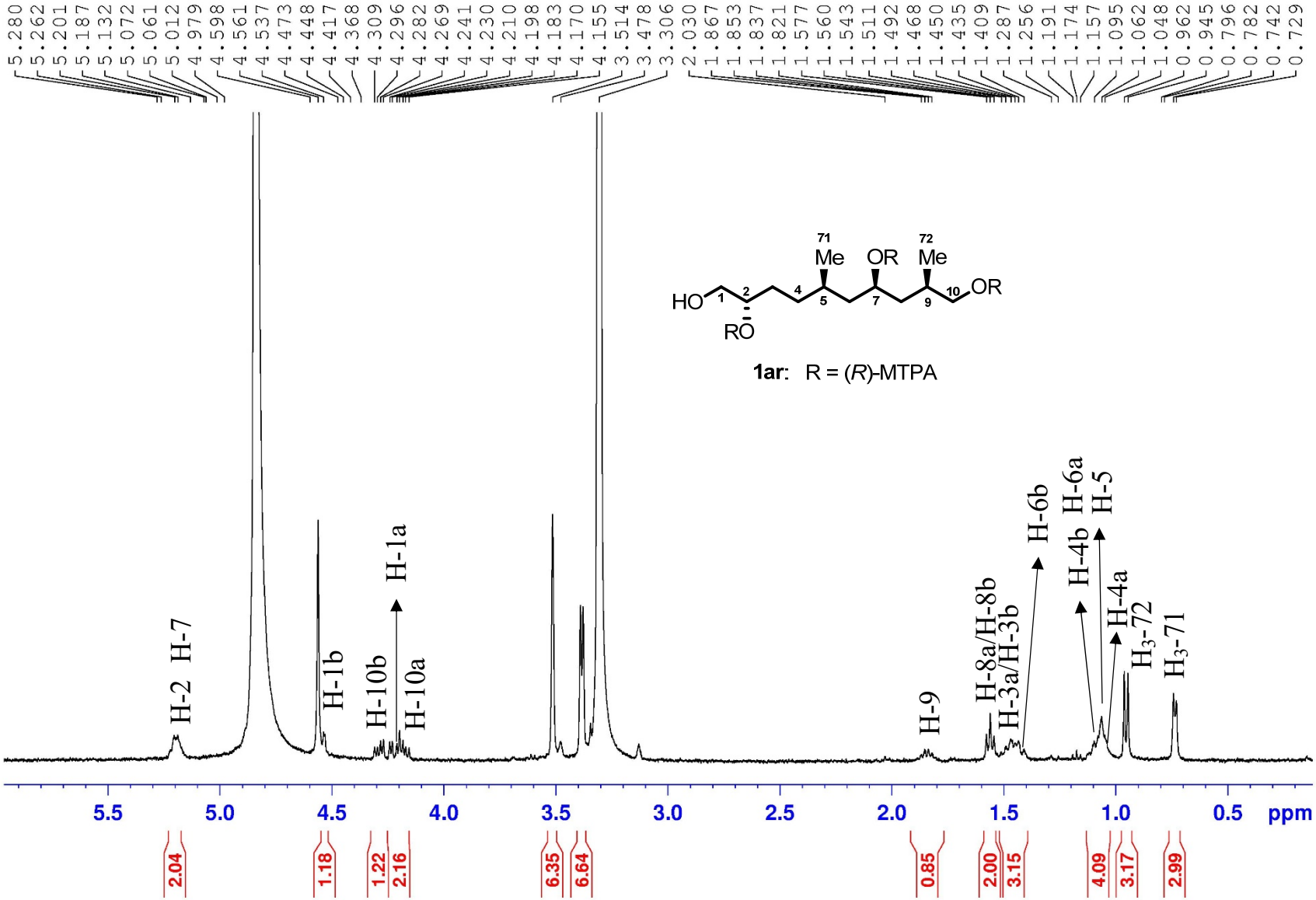


^{1}H (400 MHz) NMR spectrum of the fragment **1ar** in CD_3OD

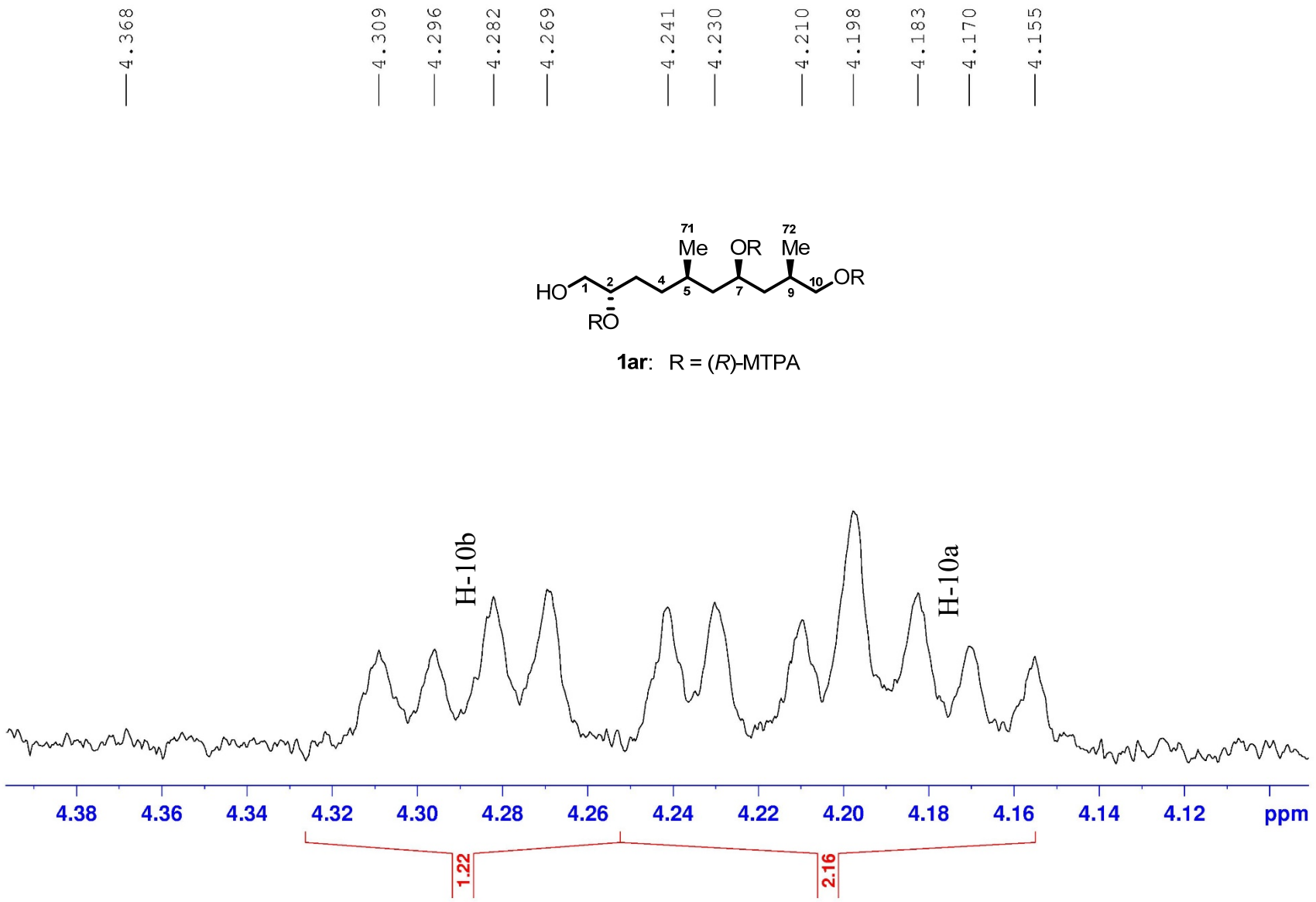


NAME	40-2-2-O3-1-S-Cl
EXPNO	1
PROCNO	1
Date_	20200426
Time	11.52
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	MeOD
NS	32
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894966 sec
RG	31.02
DW	62.400 use
DE	6.50 use
TE	300.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 =======	
SFO1	400.1324710 MHz
NUC1	1H
P1	9.73 use
SI	65536
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

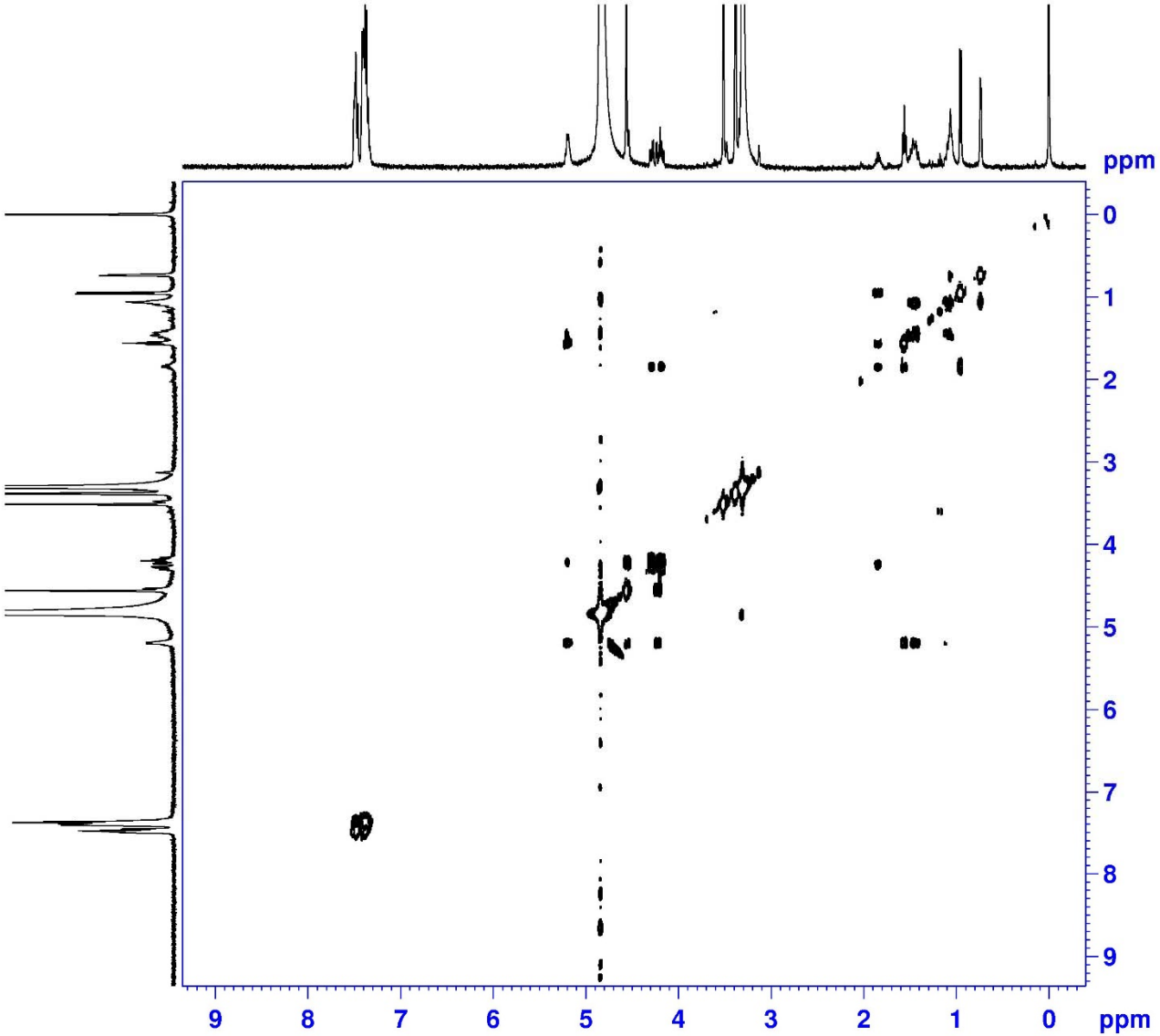
^{1}H (400 MHz) NMR spectrum of the fragment **1ar** in CD_3OD

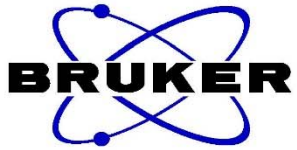


^{1}H (400 MHz) NMR spectrum of the fragment **1ar** in CD_3OD



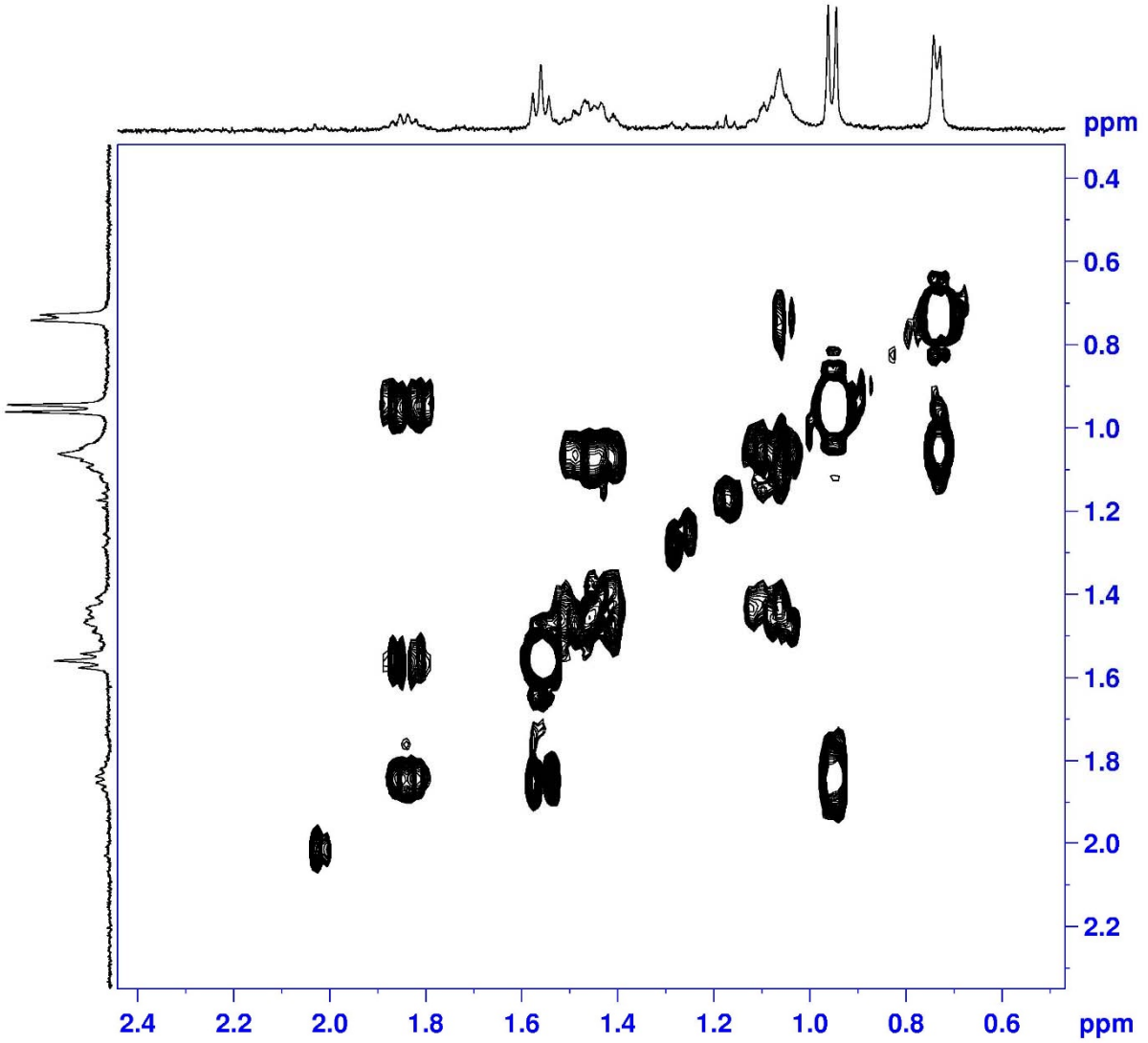
^{1}H–^{1}H COSY (400 MHz) spectrum of the fragment **1ar** in CD_3OD



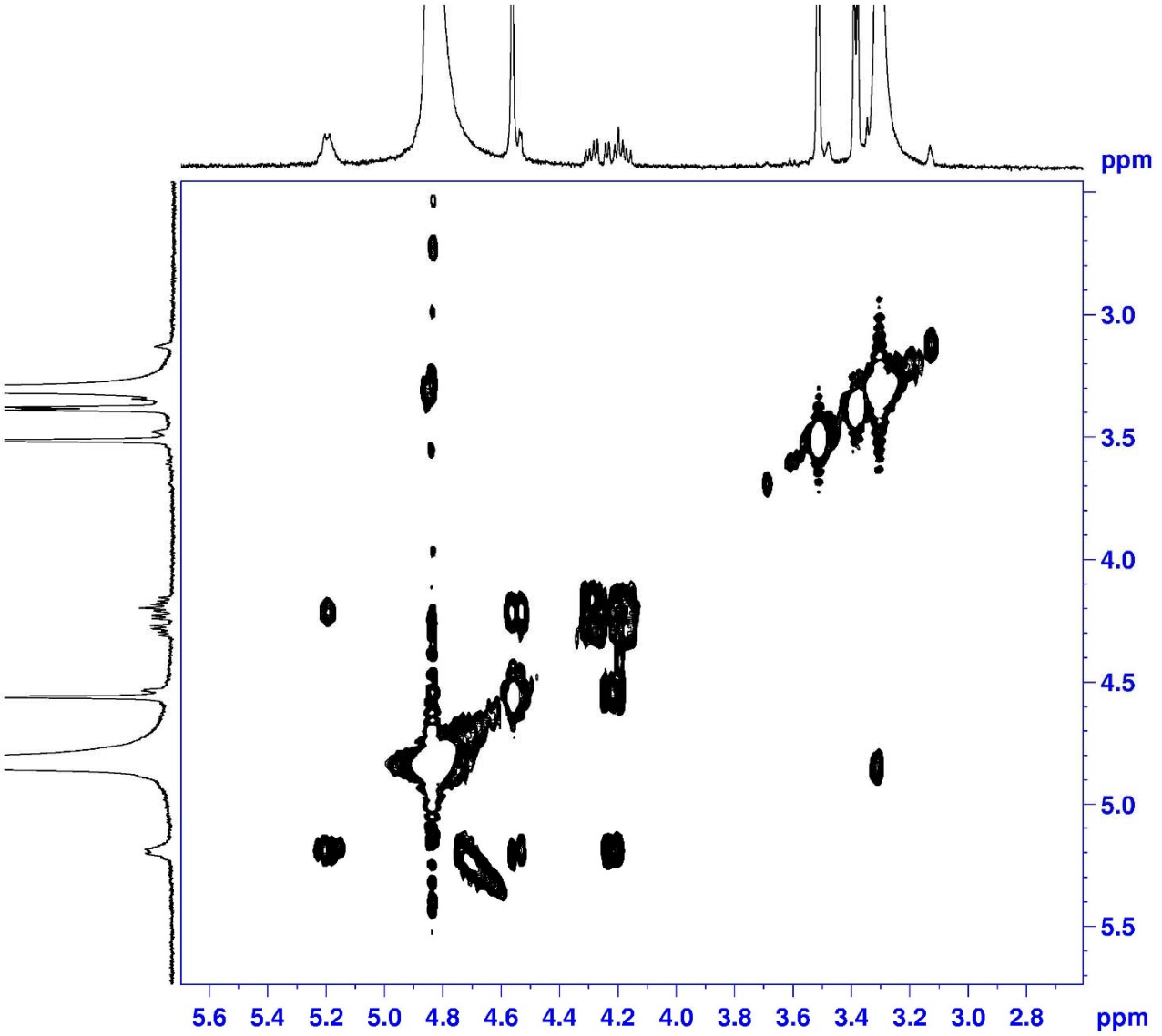



```
NAME          40-2-2-O3-1-S-Cl
EXPNO                        2
PROCNO                       1
Date_                 20200426
Time                     12.00
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG              cosygpqf
TD                       2048
SOLVENT                  MeOD
NS                        100
DS                          8
SWH                  4000.000 Hz
FIDRES               1.953125 Hz
AQ                   0.2560500 sec
RG                       202.1
DW                     125.000 usec
DE                        6.50 usec
TE                       300.0 K
D0                   0.00000300 sec
D1                   2.00000000 sec
D13                  0.00000400 sec
D16                  0.00020000 sec
IN0                  0.00025000 sec

======== CHANNEL f1 ========
SFO1              400.1320007 MHz
NUC1                        1H
P0                        9.73 usec
P1                        9.73 usec
ND0                          1
TD                         128
SFO1                   400.132 MHz
FIDRES               31.250000 Hz
SW                       9.997 ppm
FnMODE                      QF
SI                         1024
SF                400.1300092 MHz
WDW                      QSINE
SSB                          0
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                         1024
MC2                         QF
SF                400.1300092 MHz
WDW                      QSINE
SSB                          0
LB                        0.00 Hz
```

^{1}H–^{1}H COSY (400 MHz) spectrum of the fragment **1ar** in CD_3OD



$^{1}H–^{1}H$ COSY (400 MHz) spectrum of the fragment **1ar** in CD_3OD



$^{1}H–^{1}H$ COSY (400 MHz) spectrum of the fragment **1ar** in CD_3OD