Supporting Information

Table of Contents:

HR-ESIMS for **1**

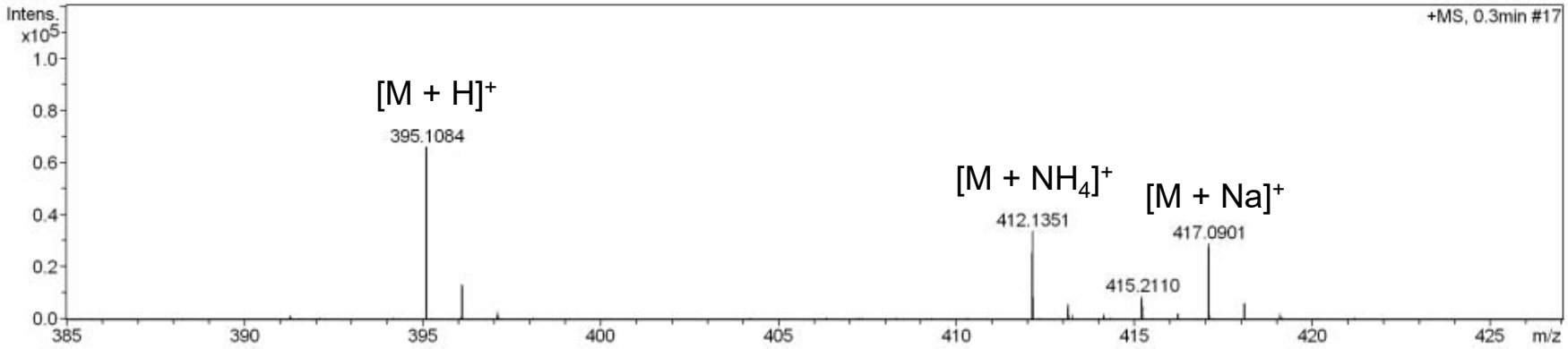
Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\MS\data\202110\wubinbin_WBB-145-D_pos_52_01_11734.d	Acquisition Date	10/27/2021 4:41:37 PM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	wubinbin_WBB-145-D_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



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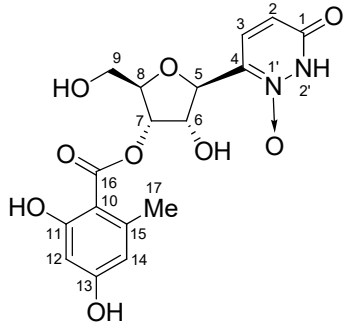
417.0901	1	C17H18N2NaO9	100.00	417.0905	0.8	0.4	6.1	9.5	even	ok



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wubinbin_WBB-145-D_pos_52_01_11734.d

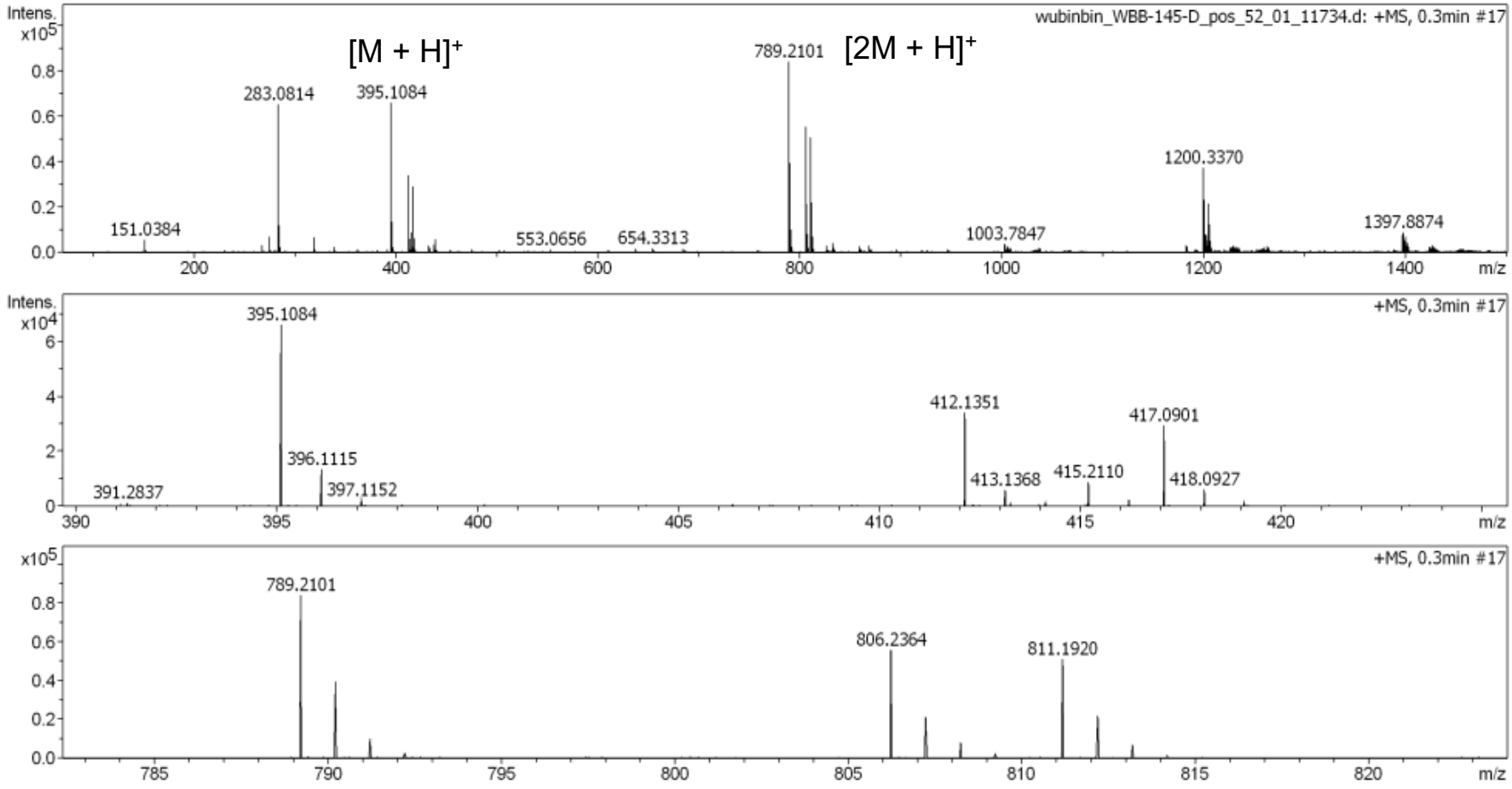
Bruker Compass DataAnalysis 4.1 printed: 10/27/2021 4:47:14 PM by: SCSIO Page 1 of 1

HR-ESIMS for **1**

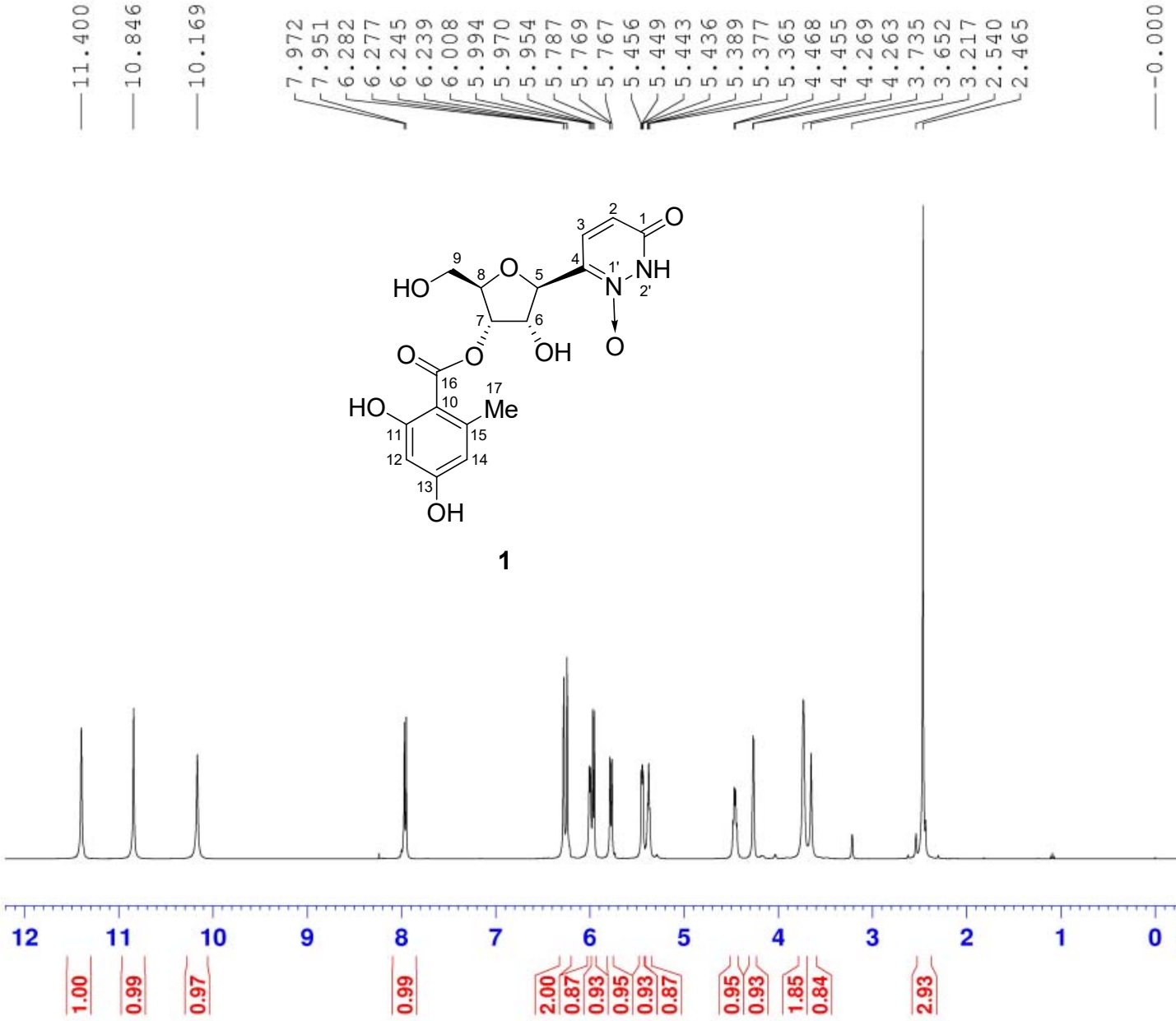
Generic Display Report

Analysis Info

Analysis Name	D:\Data\MS\data\202110\wubinbin_WBB-145-D_pos_52_01_11734.d	Acquisition Date	10/27/2021 4:41:37 PM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	wubinbin_WBB-145-D_pos	Instrument	maXis
Comment			



^{1}H (400 MHz) NMR spectrum of **1** in DMSO-d_6



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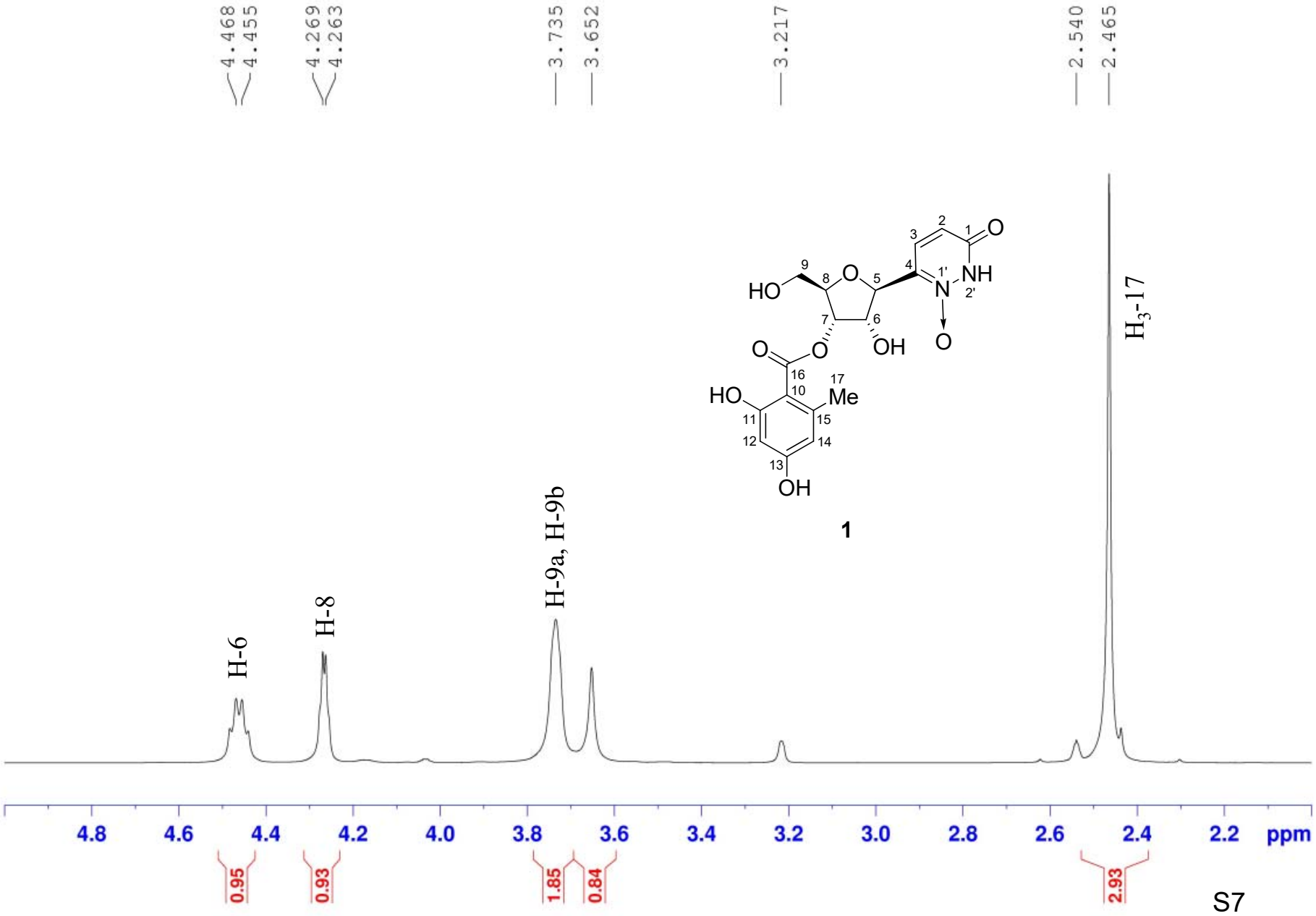
NAME	WBB-145-D
EXPNO	1
PROCNO	1
Date_	20210621
Time	14.46 h
INSTRUM	spect
PROBHD	Z108618_0231 (
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.244532 Hz
AQ	4.0894966 sec
RG	33.51
DW	62.400 usec
DE	6.50 usec
TE	298.3 K
D1	1.00000000 sec
TD0	1
SFO1	400.2024712 MHz
NUC1	1H
P1	9.48 usec
SI	65536
SF	400.1999875 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{1}H (400 MHz) NMR spectrum of **1** in DMSO-d_6



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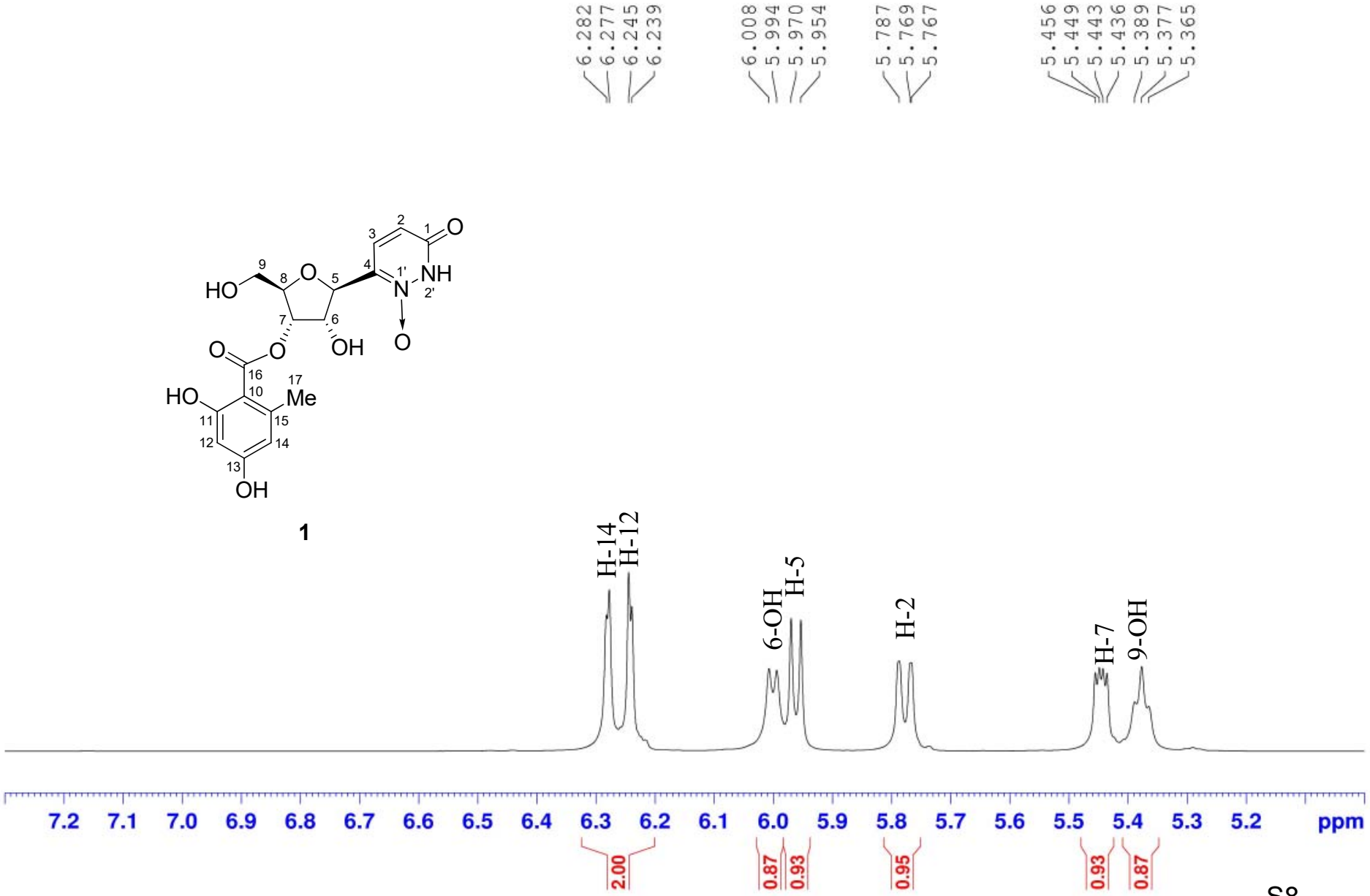
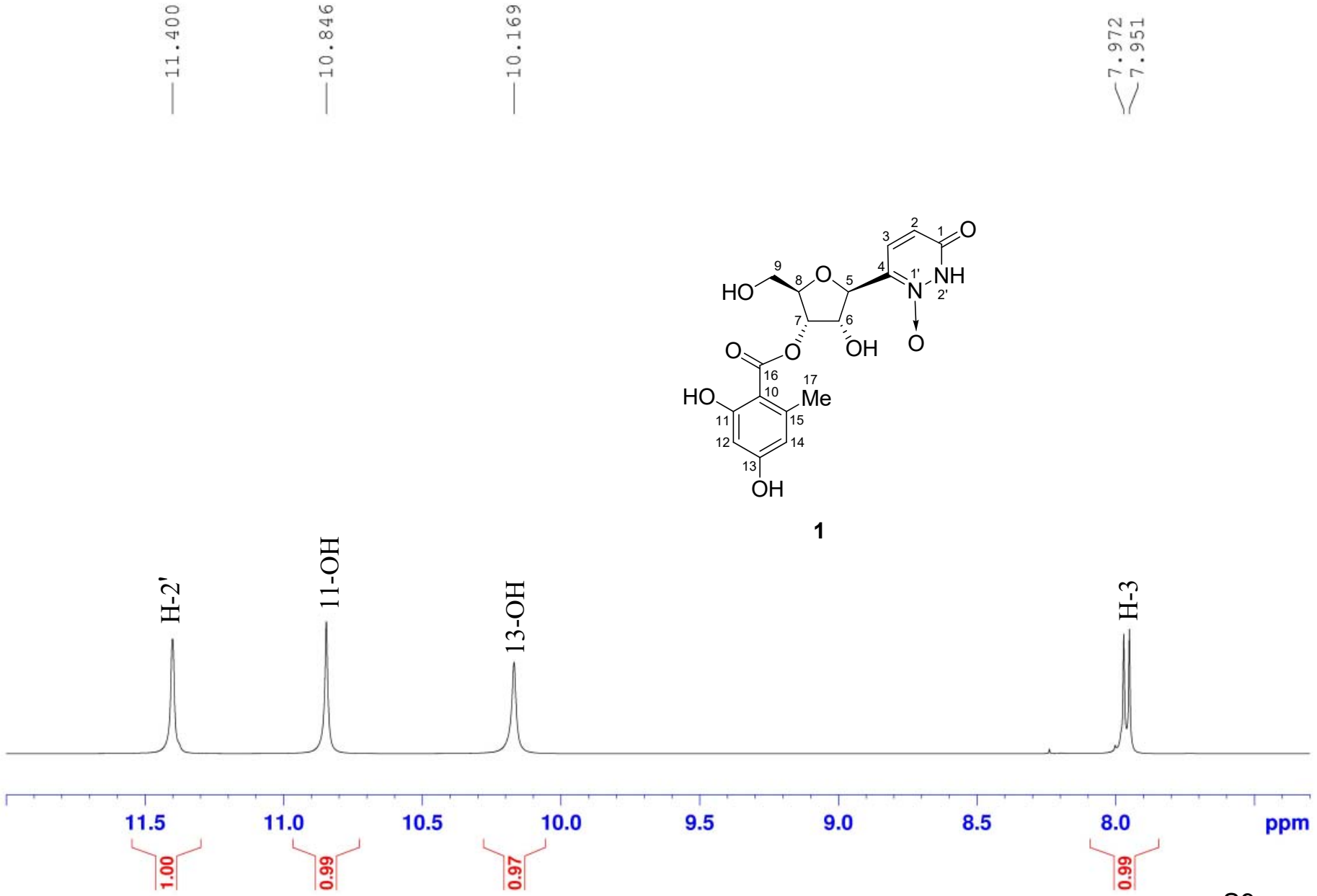
^{1}H (400 MHz) NMR spectrum of **1** in DMSO-d_6



^{1}H (400 MHz) NMR spectrum of **1** in DMSO-d_6



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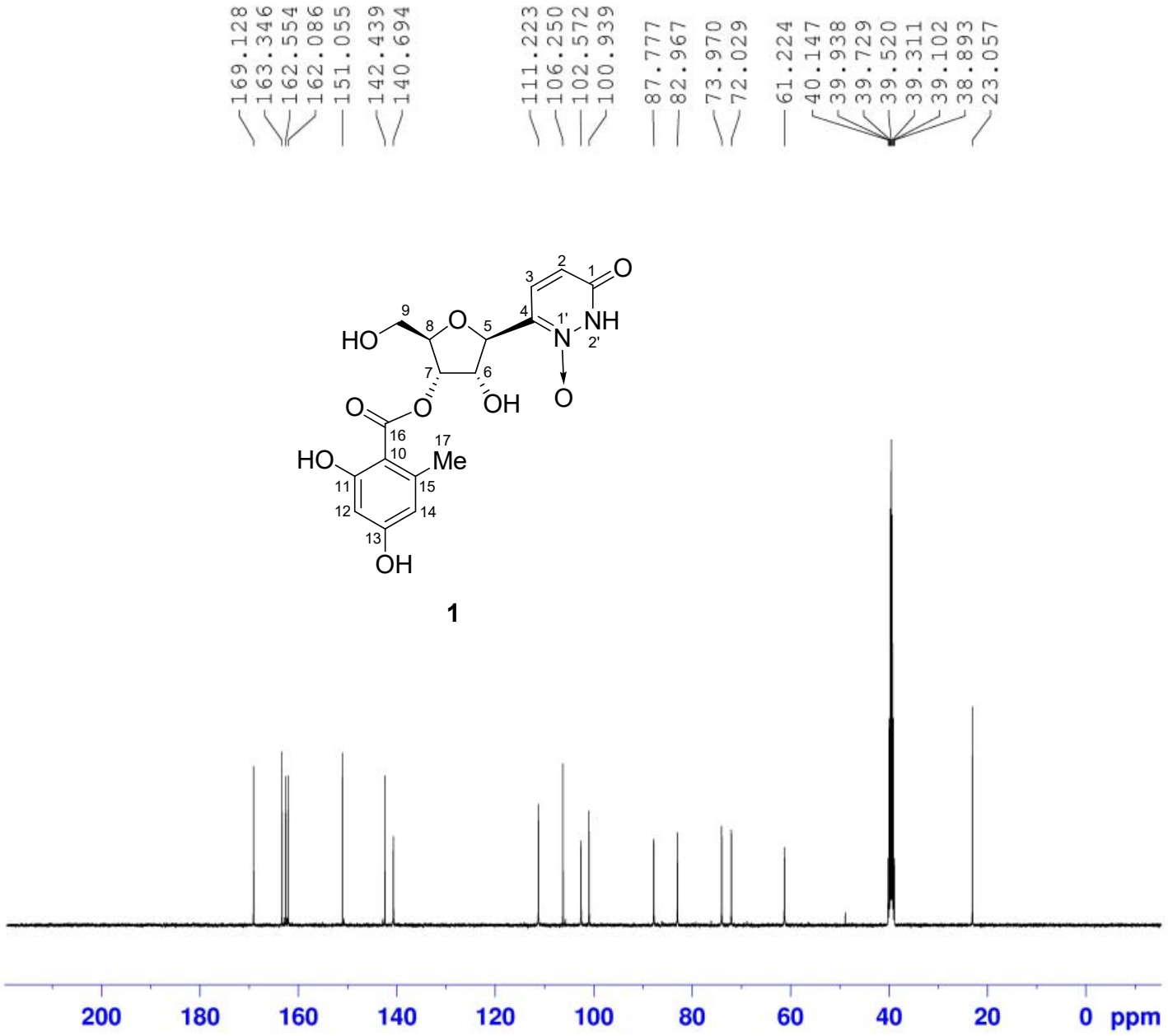
^{13}C (100 MHz) NMR spectrum of **1** in DMSO-d_6



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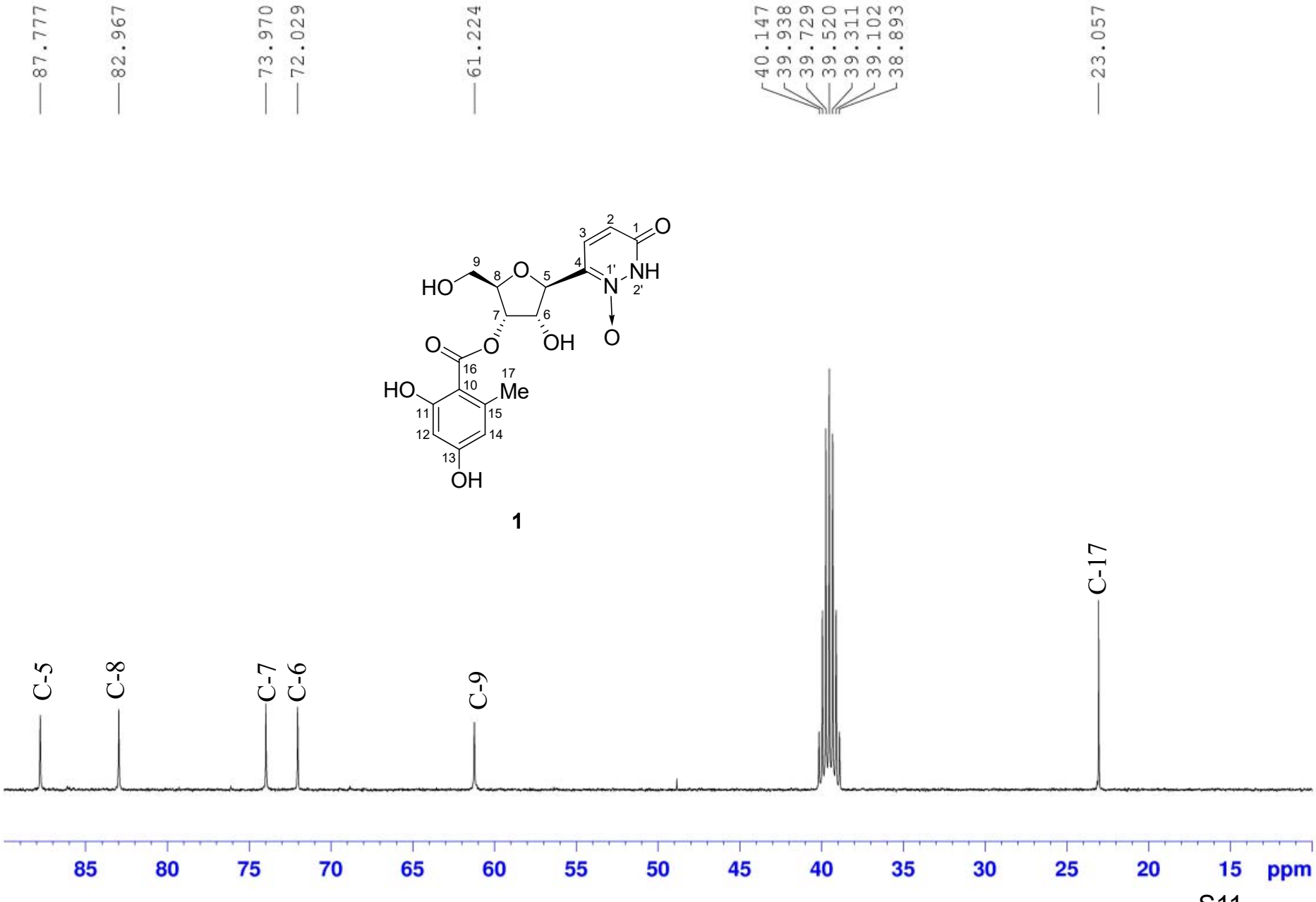
EXPNO	2
PROCNO	1
Date_	20210621
Time	22.07 h
INSTRUM	spect
PROBHD	Z108618_0231 (
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	300
DS	4
SWH	24038.461 Hz
FIDRES	0.733596 Hz
AQ	1.3631988 sec
RG	2050
DW	20.800 usec
DE	6.50 usec
TE	299.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	100.6404331 MHz
NUC1	13C
P1	8.25 usec
SI	32768
SF	100.6303921 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

^{13}C (100 MHz) NMR spectrum of **1** in DMSO-d_6



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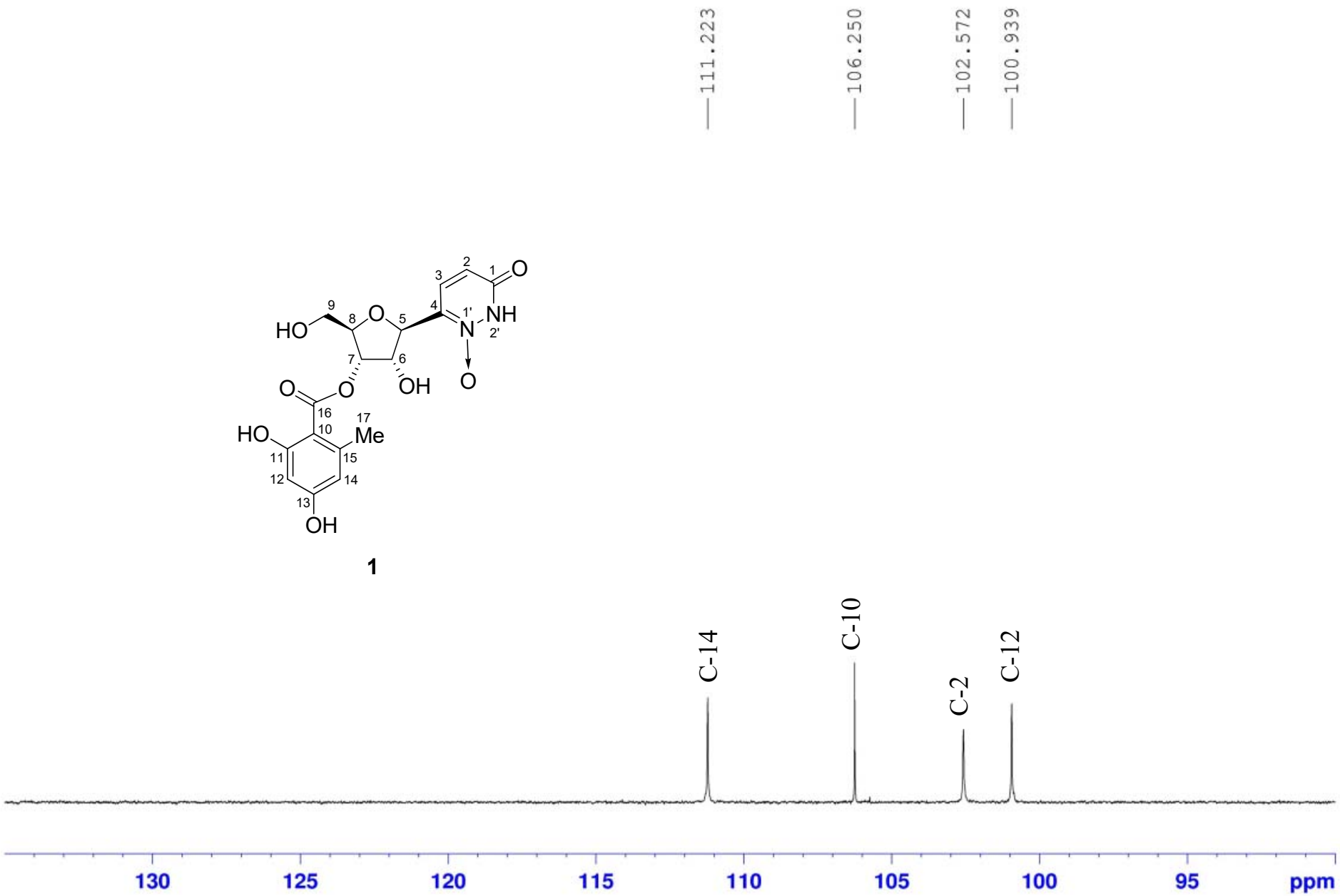
^{13}C (100 MHz) NMR spectrum of **1** in DMSO-d_6



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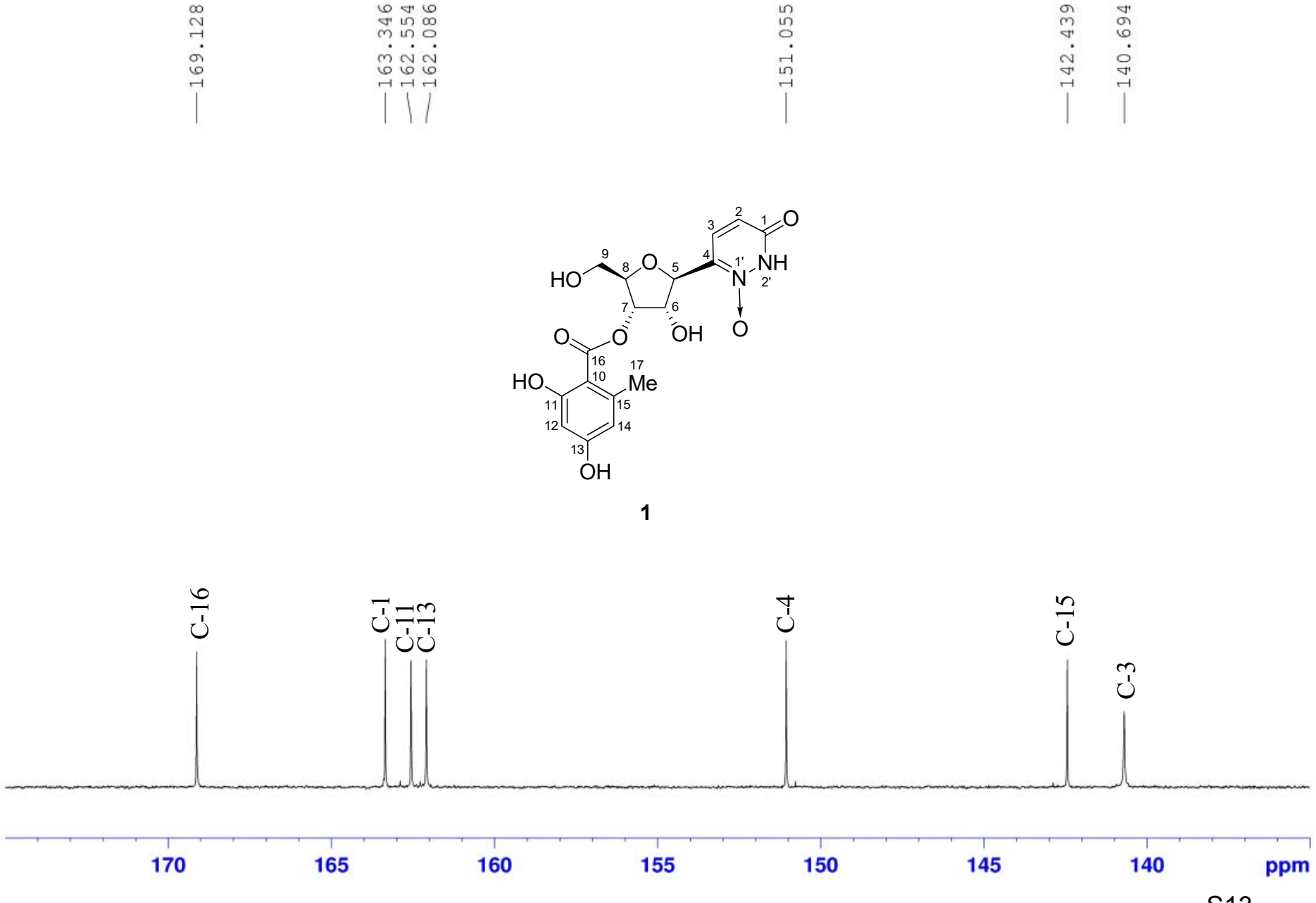
^{13}C (100 MHz) NMR spectrum of **1** in DMSO-d_6



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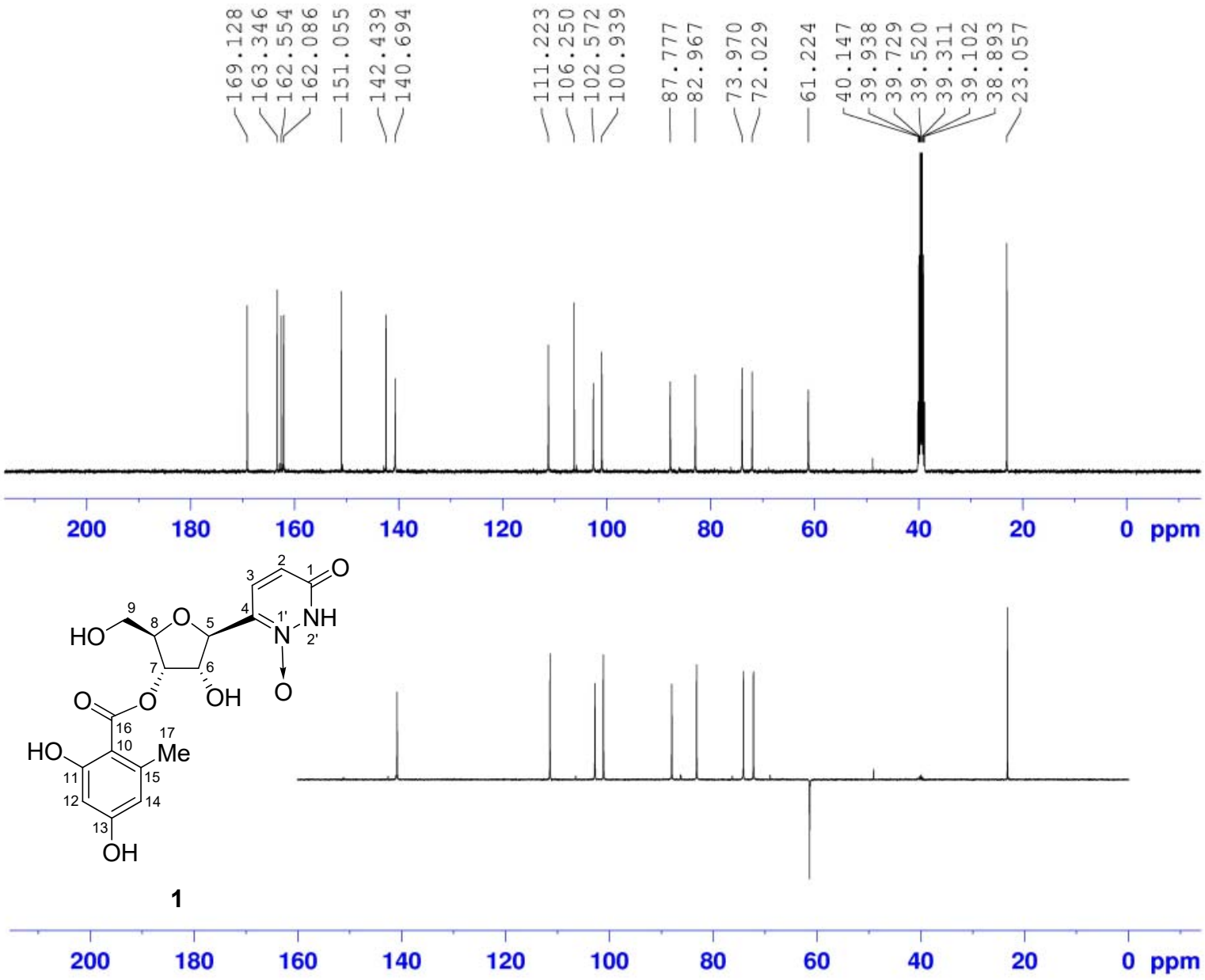
DEPT135 (100 MHz) spectrum of **1** in DMSO-d_6



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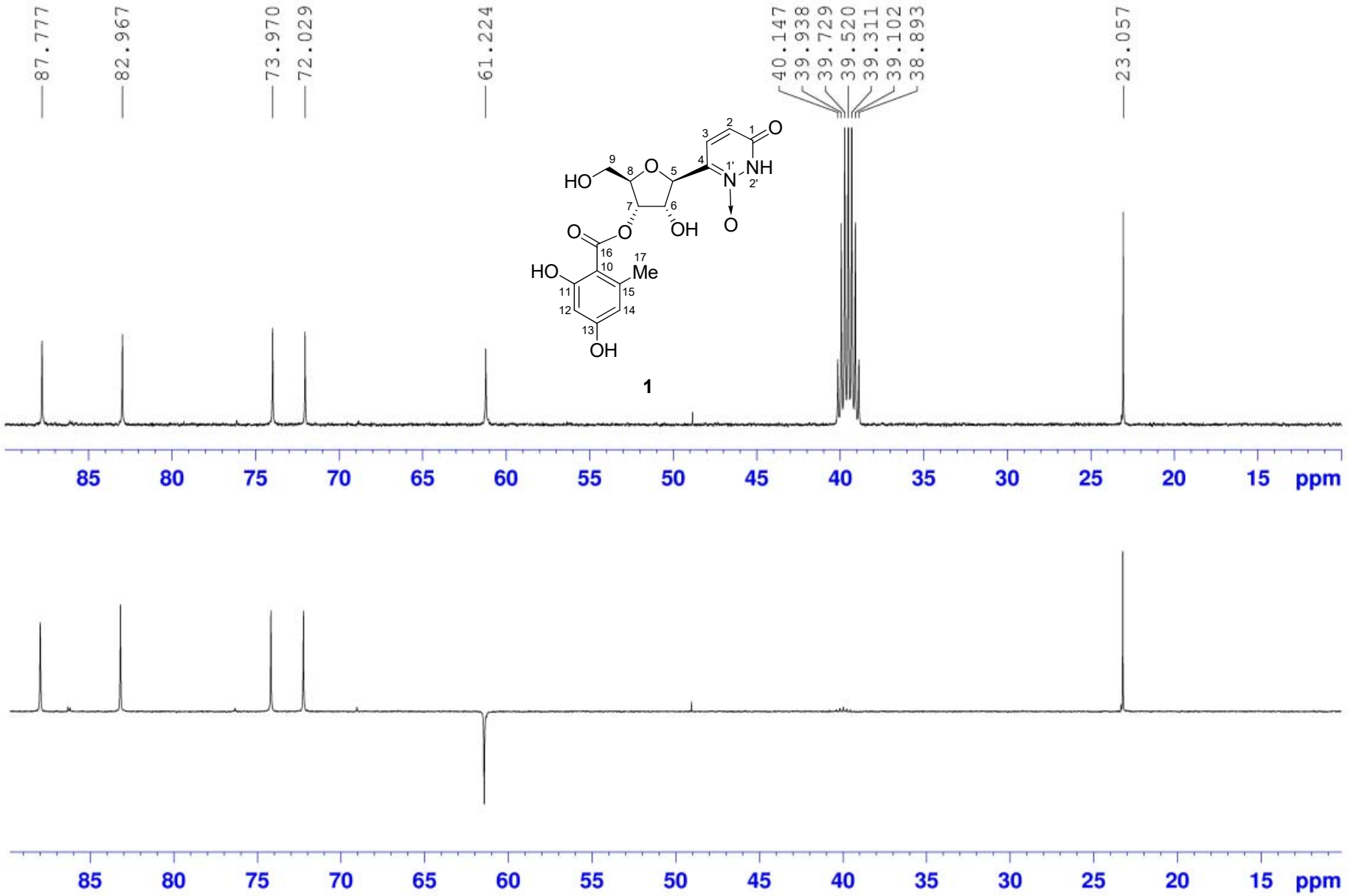
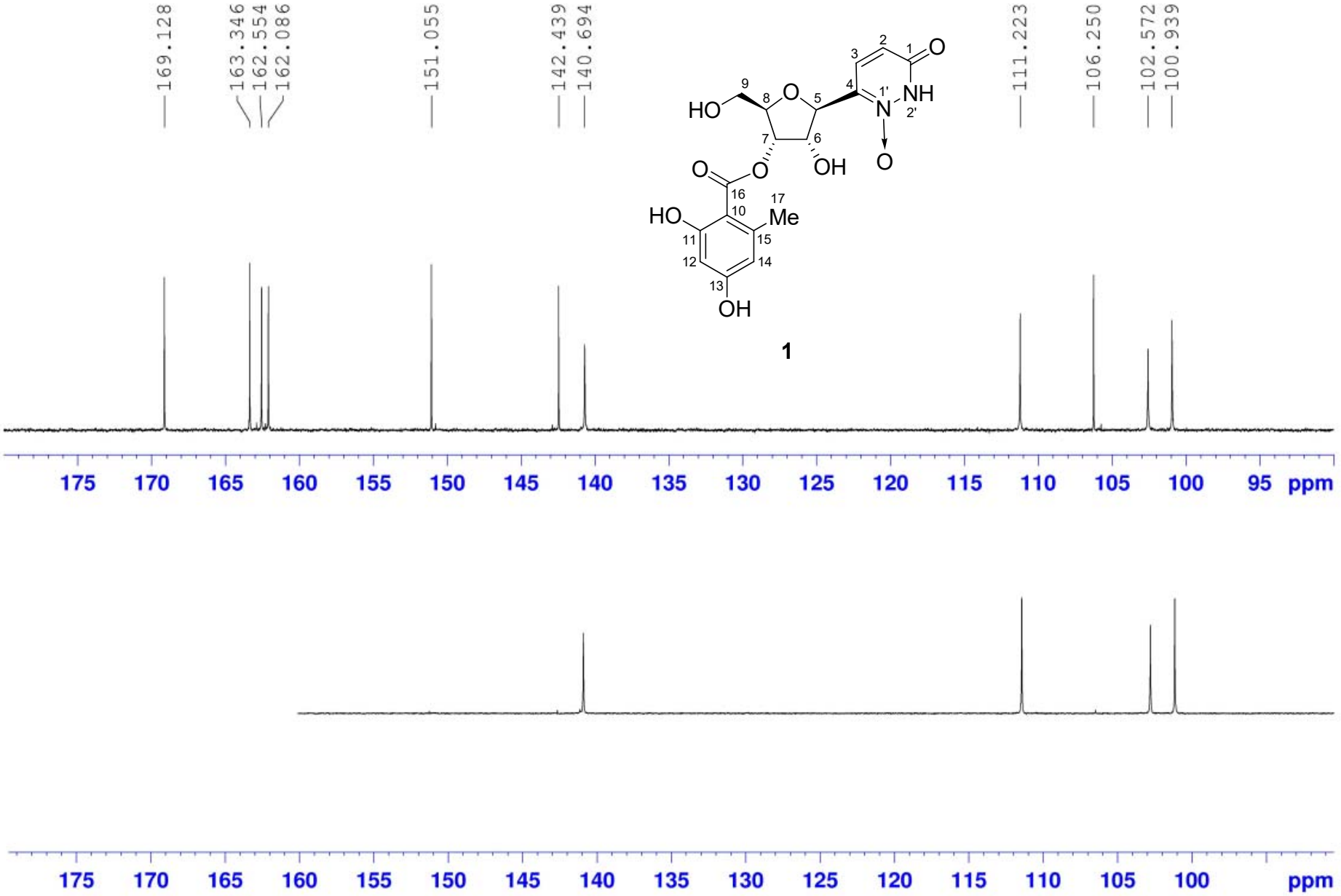
PROCNO	1
Date_	20210621
Time	22.30 h
INSTRUM	spect
PROBHD	Z108618_0231 (
PULPROG	deptsp135
TD	65536
SOLVENT	DMSO
NS	150
DS	8
SWH	16129.032 Hz
FIDRES	0.492219 Hz
AQ	2.0316660 sec
RG	2050
DW	31.000 usec
DE	6.50 usec
TE	299.3 K
CNST2	145.0000000
D1	2.00000000 sec
D2	0.00344828 sec
D12	0.00002000 sec
TD0	1
SFO1	100.6384205 MHz
NUC1	13C
P1	8.25 usec
P13	2000.00 usec
SI	32768
SF	100.6303700 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

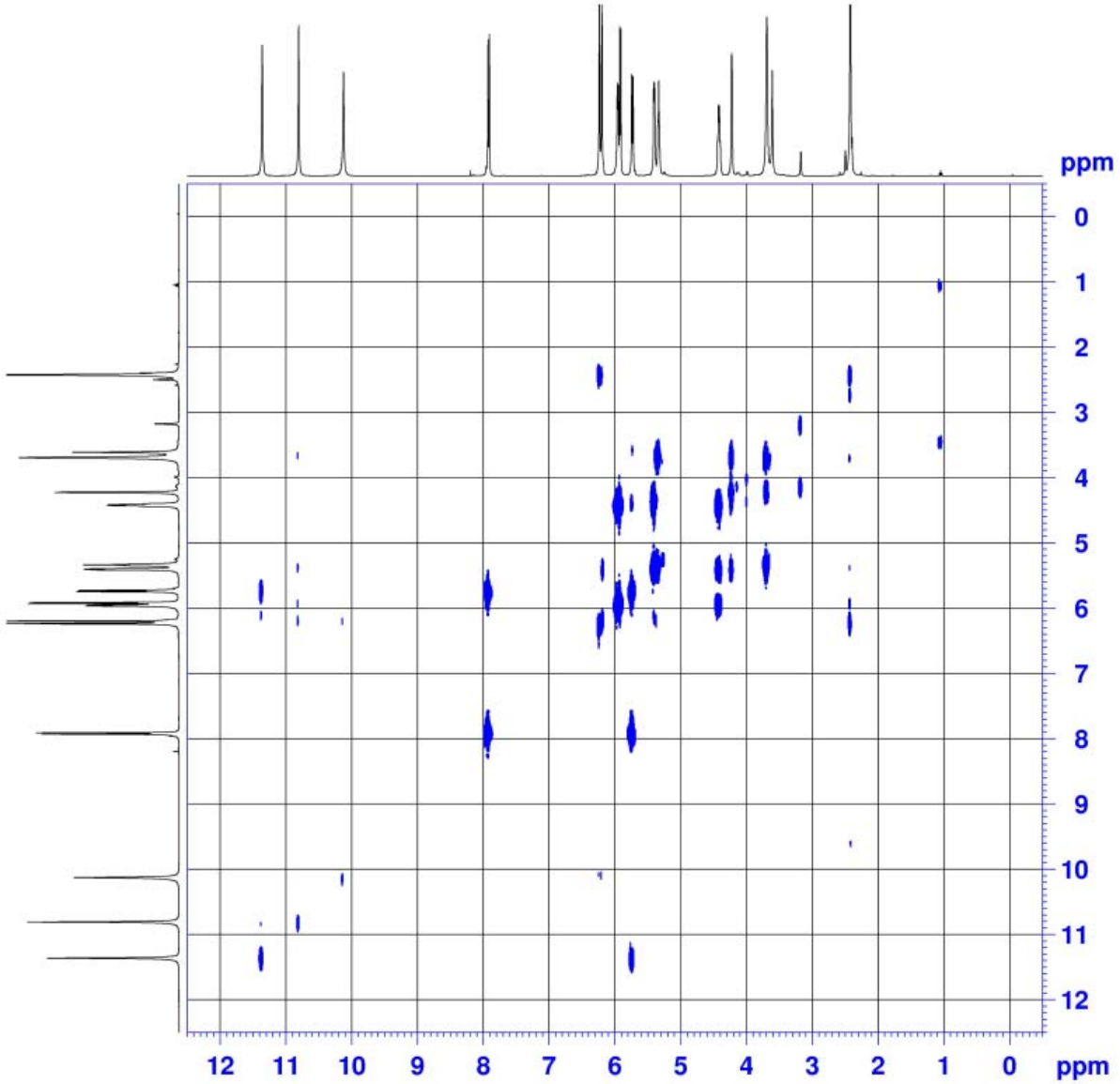
DEPT135 (100 MHz) spectrum of **1** in DMSO-d_6



DEPT135 (100 MHz) spectrum of **1** in DMSO-d_6

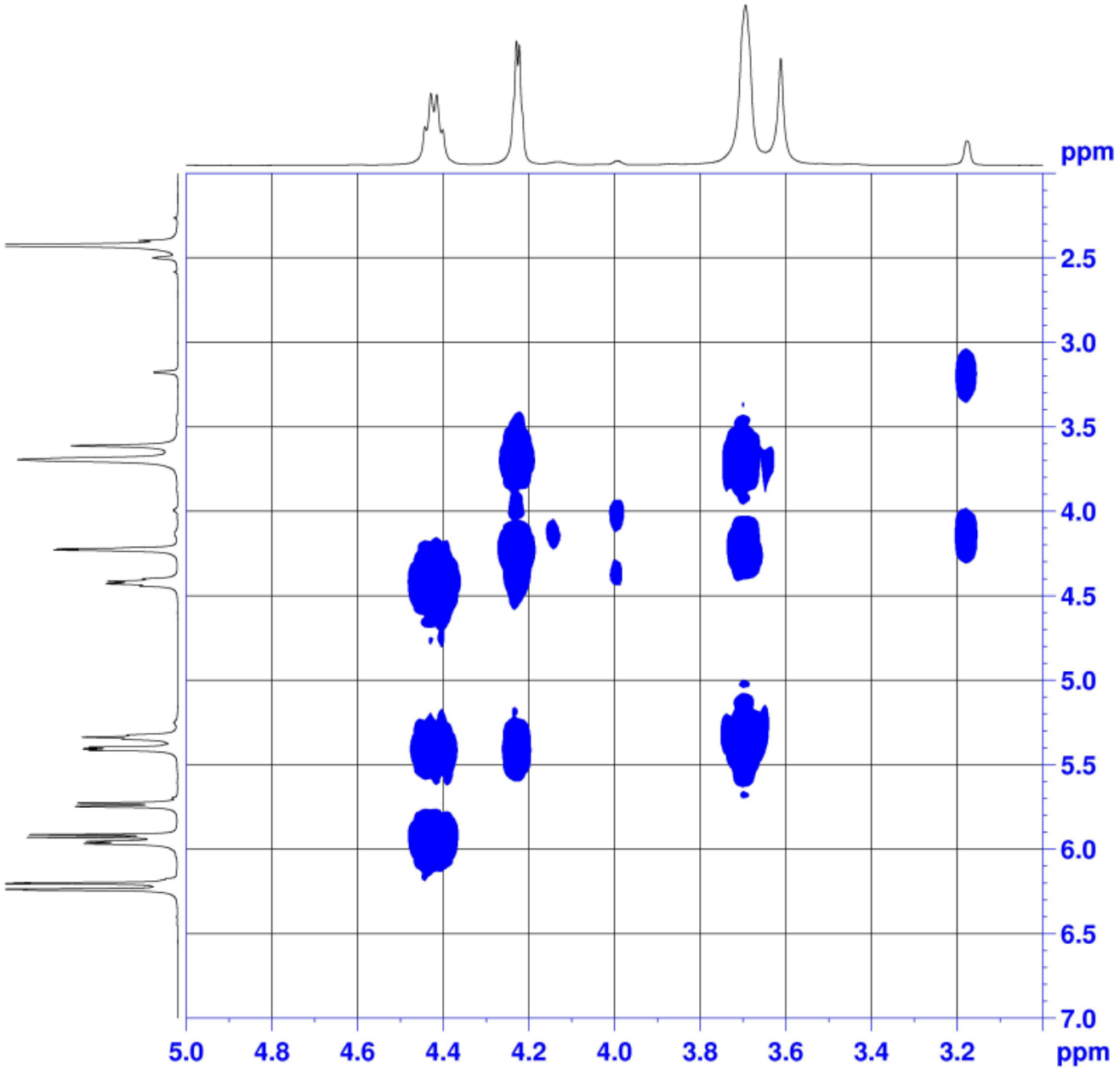


^{1}H–^{1}H COSY (400 MHz) spectrum of **1** in DMSO-d_6

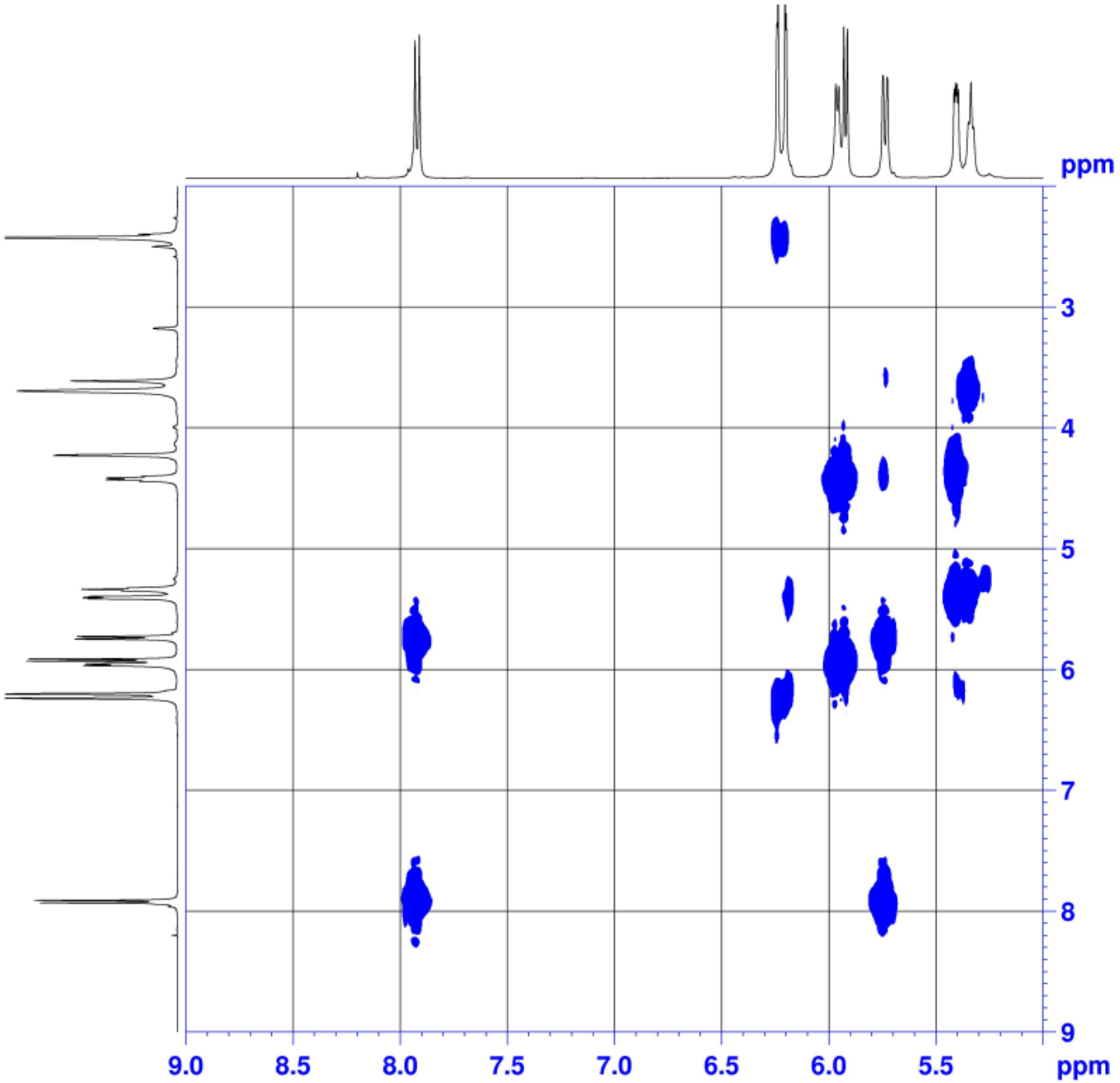


NAME	WBB-145-D
EXPNO	1
PROCNO	1
Date_	20210621
Time	14.46
INSTRUM	spect
PROBHD	Z108618_0231 (
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8012.820
FIDRES	0.244532
AQ	4.0894966
RG	33.51
DW	62.400
DE	6.50
TE	298.3
D1	1.00000000
TD0	1
SFO1	400.2024712
NUC1	1H
P1	9.48
SI	65536
SF	400.2000036
WDW	EM
SSB	0
LB	0.30
GB	0
PC	1.00

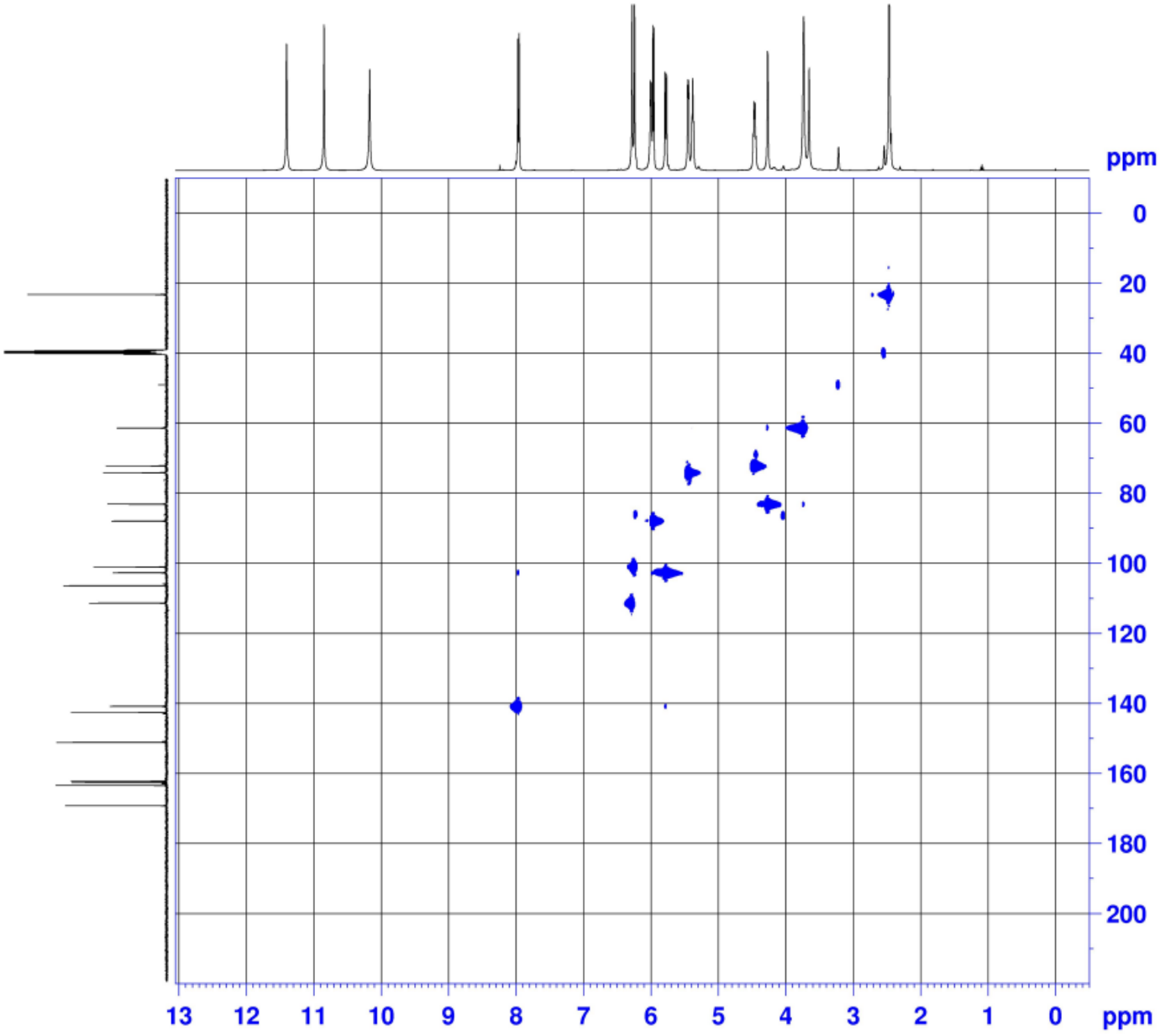
^{1}H–^{1}H COSY (400 MHz) spectrum of **1** in DMSO-d_6



^{1}H–^{1}H COSY (400 MHz) spectrum of **1** in DMSO-d_6



HSQC (400 MHz) spectrum of **1** in DMSO-d_6



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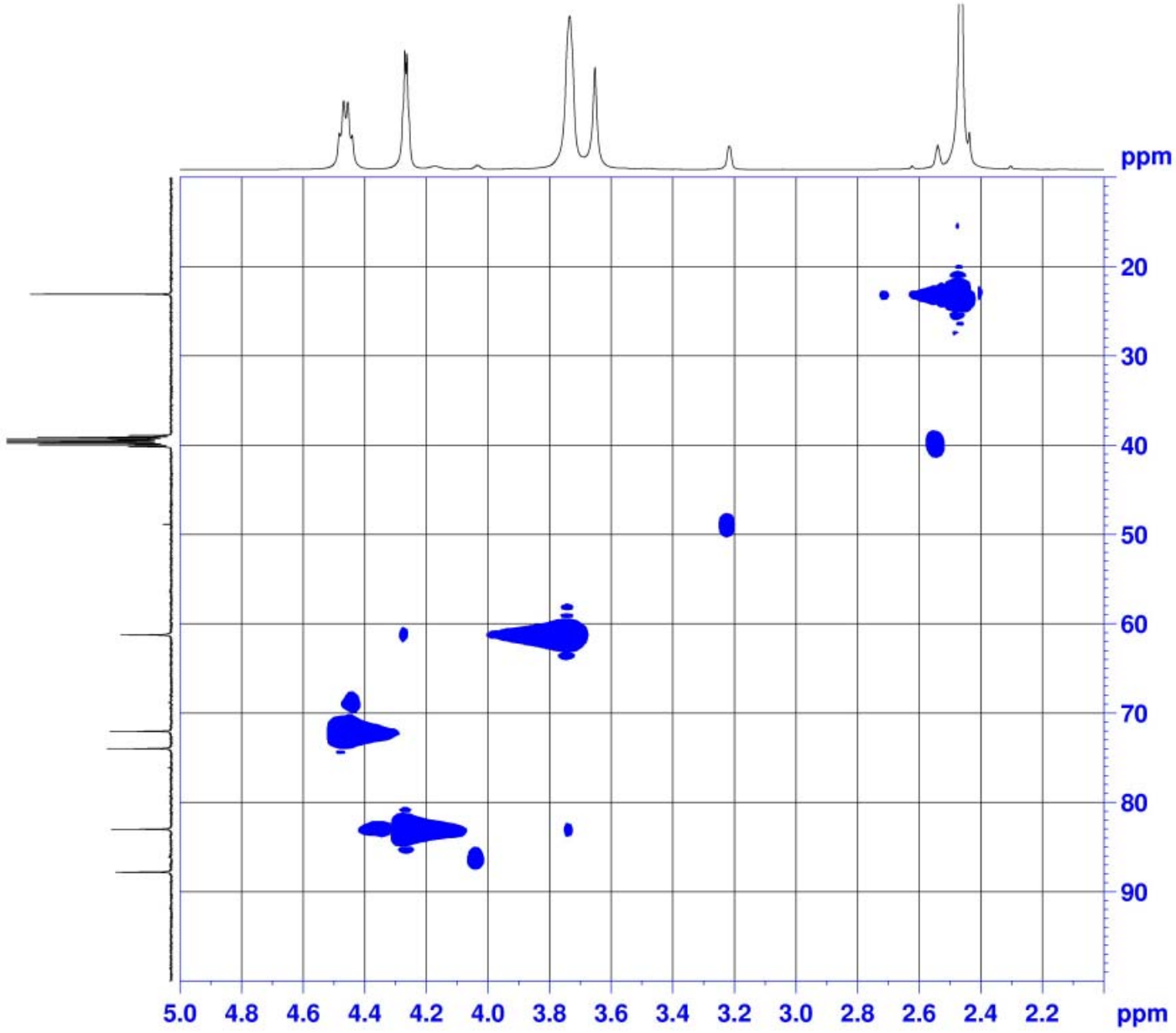
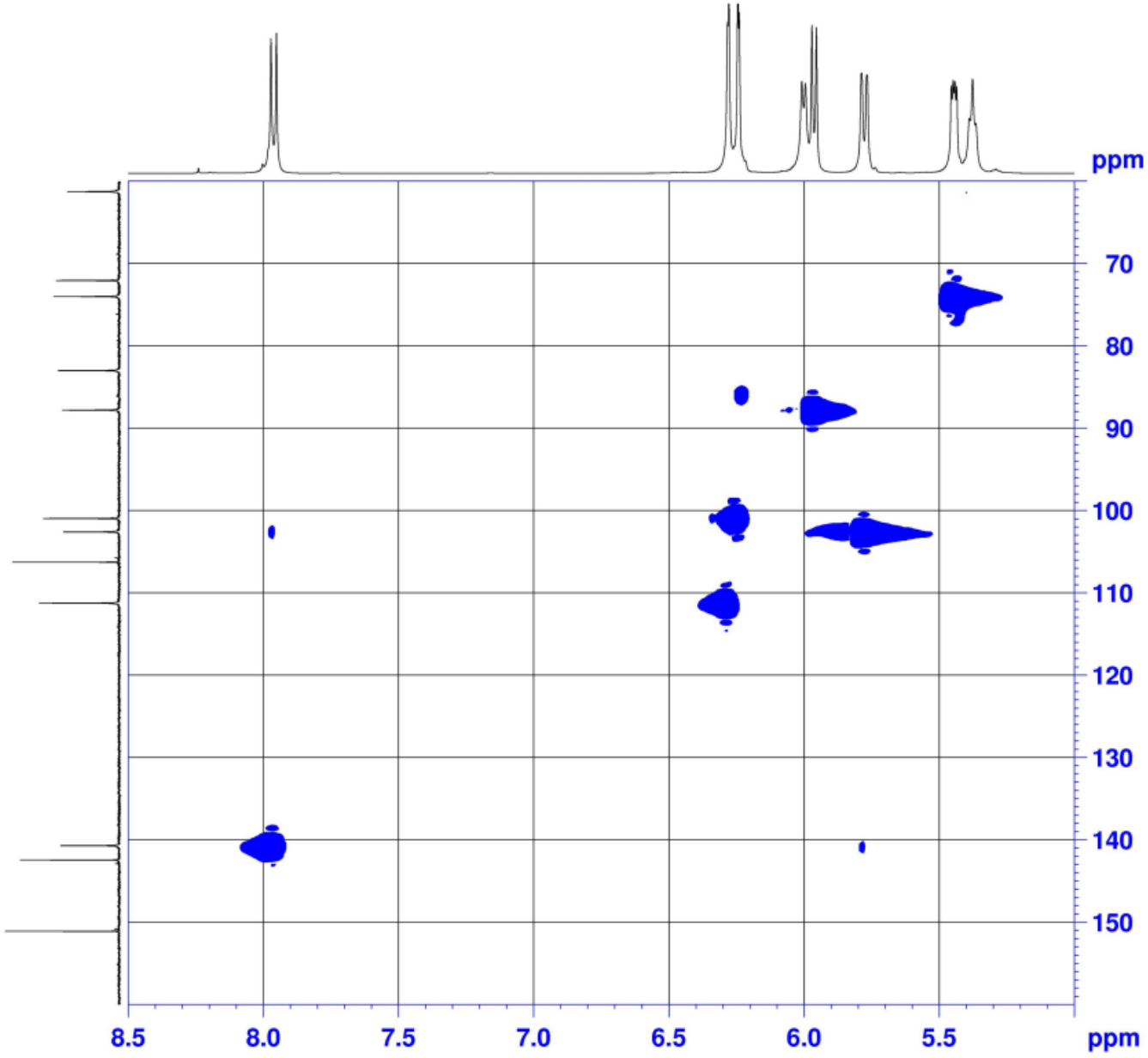
EXPNO	4
PROCNO	1
Date_	20210622
Time	22.15 h
INSTRUM	spect
PROBHD	Z108618_0231 (
PULPROG	hsqcetgpsi
TD	1024
SOLVENT	DMSO
NS	4
DS	16
SWH	5597.015 Hz
FIDRES	10.931670 Hz
AQ	0.0915273 sec
RG	2050
DW	89.333 usec
DE	6.50 usec
TE	297.2 K
CNST2	145.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D4	0.00172414 sec
D11	0.03000000 sec
D16	0.00020000 sec
D24	0.00110000 sec
IN0	0.00002070 sec
ND0	2
TD	128
SFO1	100.6379 MHz
FIDRES	188.707733 Hz
SW	240.015 ppm
FnMODE	Echo-Antiecho
SI	1024
SF	400.1999816 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	100.6303700 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

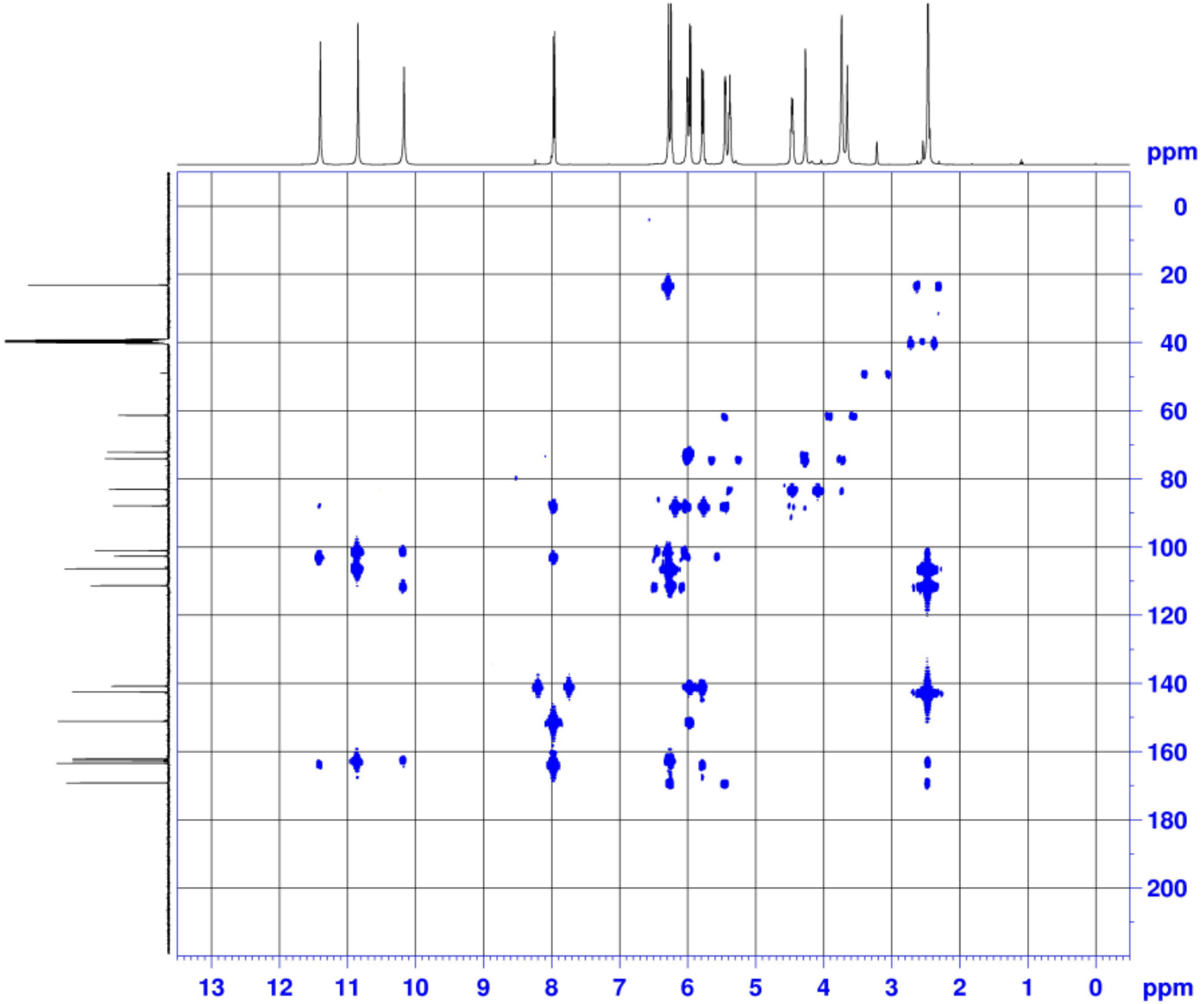
HSQC (400 MHz) spectrum of **1** in DMSO-d_6



HSQC (400 MHz) spectrum of **1** in DMSO-d_6



HMBC (400 MHz) spectrum of **1** in DMSO-d_6



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INSTRUM	spect
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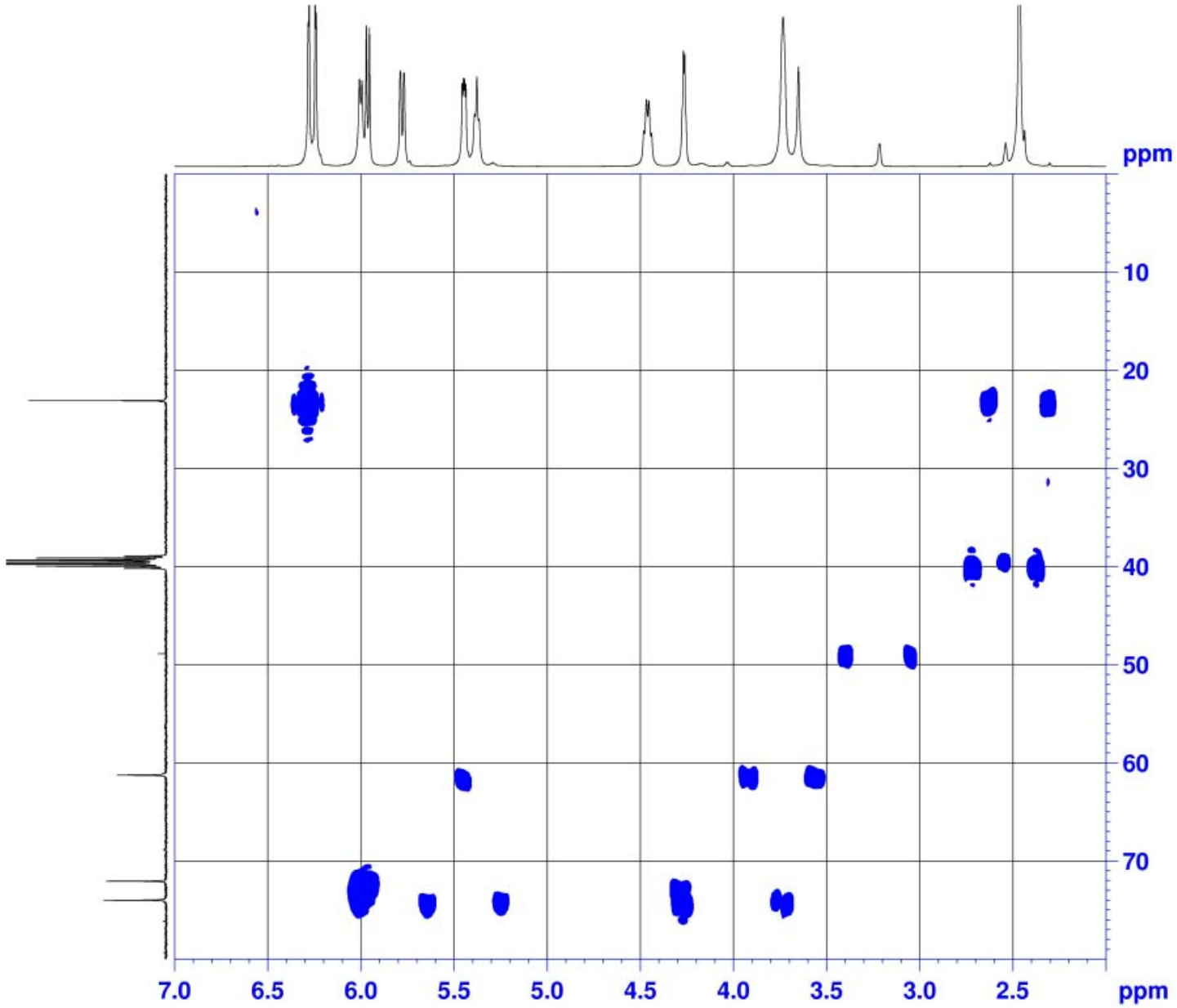
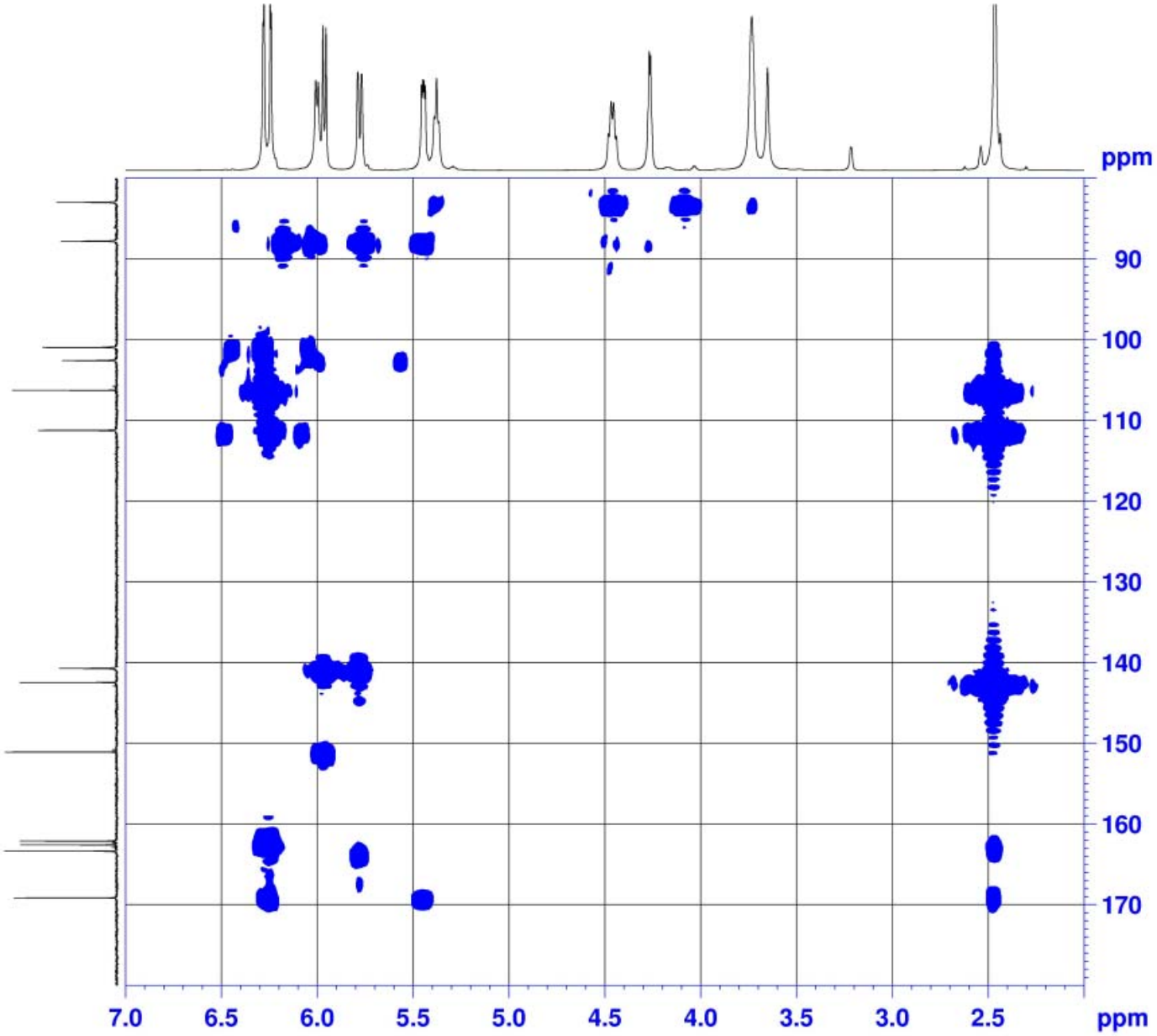
PULPROG	hmbcgpndqf
TD	1024
SOLVENT	DMSO
NS	2
DS	16
SWH	6009.615 Hz
FIDRES	11.737530 Hz
AQ	0.0852468 sec
RG	2050
DW	83.200 usec
DE	6.50 usec
TE	297.3 K
CNST13	8.0000000
D0	0.00000300 sec
D1	1.50000000 sec
D6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00002070 sec
ND0	2
TD	128
SFO1	100.6394 MHz
FIDRES	188.707733 Hz
SW	240.011 ppm
FnMODE	QF
SI	1024
SF	400.1999826 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	100.6303448 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

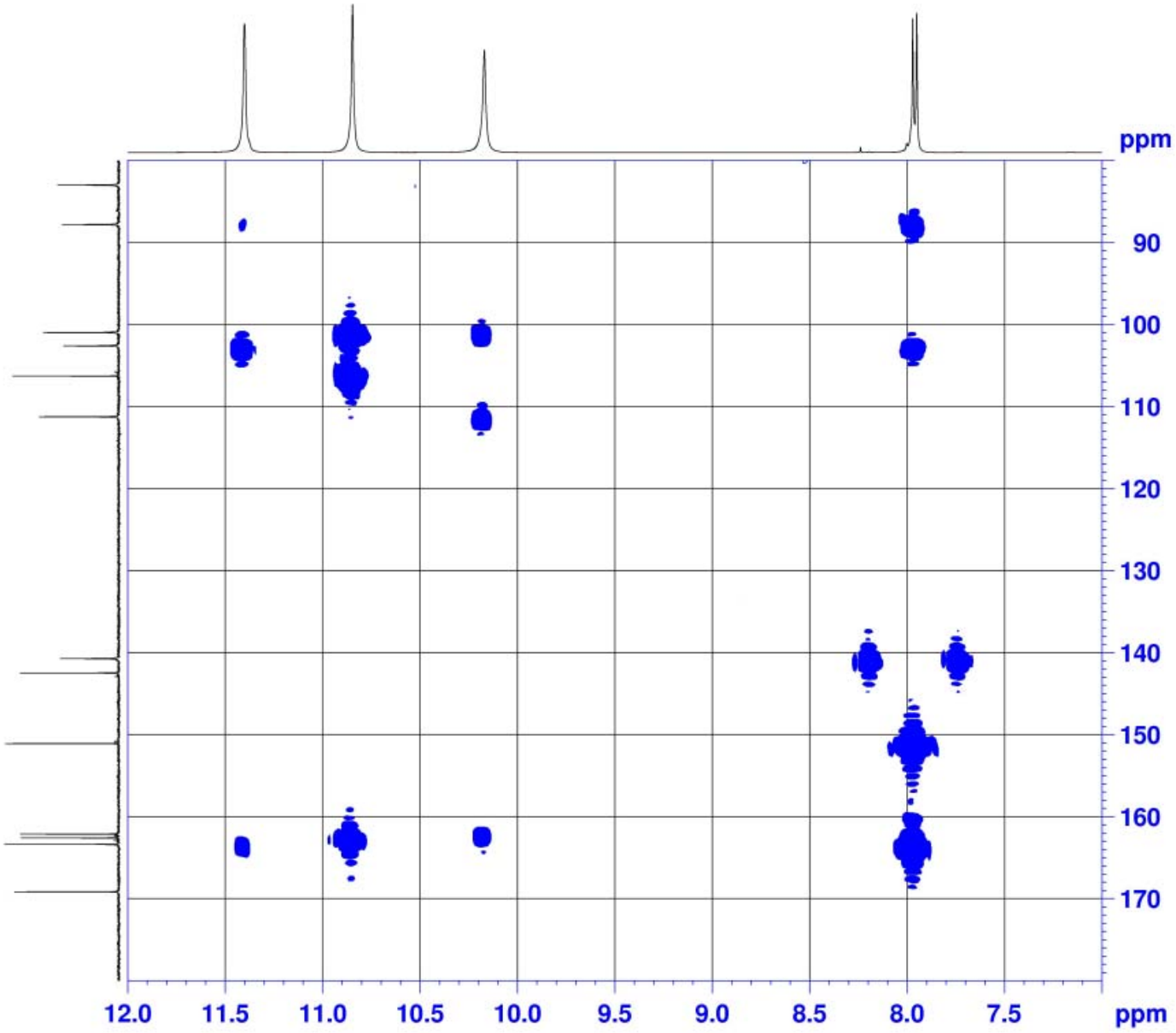
HMBC (400 MHz) spectrum of **1** in DMSO-d_6



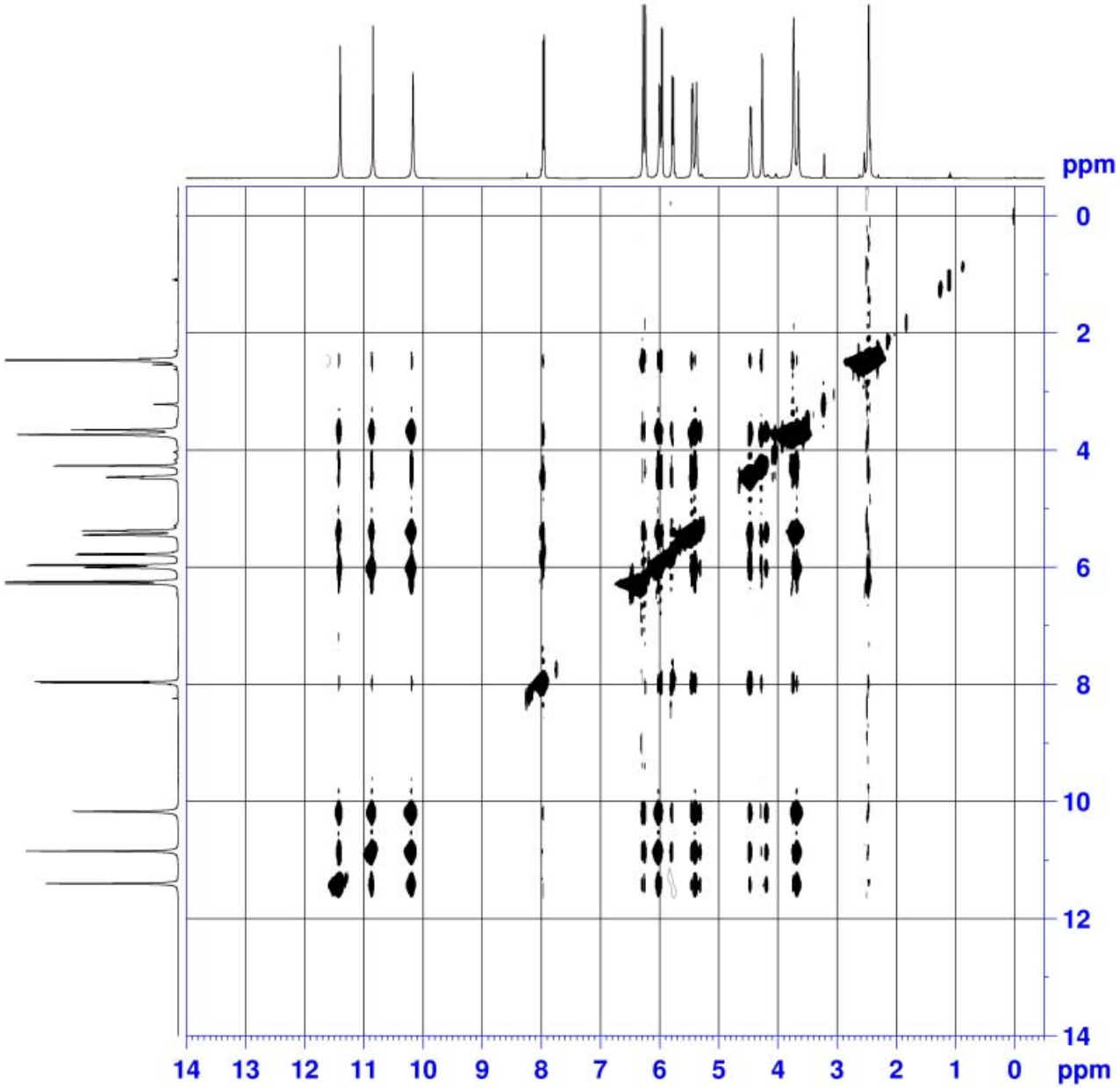
HMBC (400 MHz) spectrum of **1** in DMSO-d_6



HMBC (400 MHz) spectrum of **1** in DMSO-d_6



NOESY (400 MHz) spectrum of **1** in DMSO-d_6



NAME	WBB-145-D	
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INSTRUM	spect	
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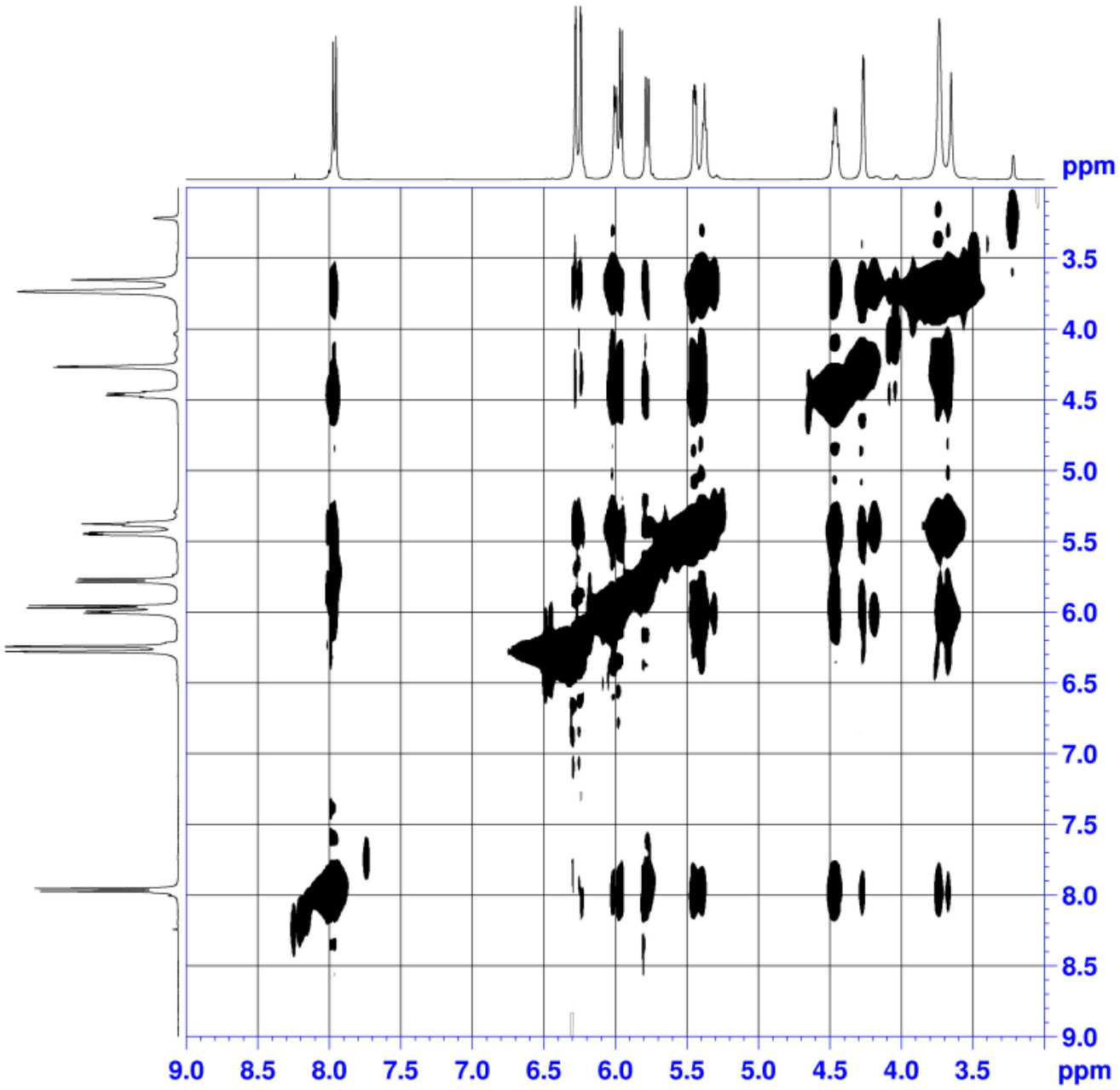
PULPROG	noesygpphpp	
TD	2048	
SOLVENT	DMSO	
NS	2	
DS	32	
SWH	5597.015	Hz
FIDRES	5.465835	Hz
AQ	0.1830047	sec
RG	33.51	
DW	89.333	usec
DE	6.50	usec
TE	297.0	K
D0	0.00007713	sec
D1	2.00000000	sec
D8	0.30000001	sec
D11	0.03000000	sec
D12	0.00002000	sec
D16	0.00020000	sec
IN0	0.00017840	sec
ND0	1	
TD	128	
SFO1	400.2018	MHz
FIDRES	43.792042	Hz
SW	14.006	ppm
FnMODE	States-TPPI	
SI	1024	
SF	400.1999818	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	
PC	1.00	
SI	1024	
MC2	States-TPPI	
SF	400.1999814	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	

NOESY (400 MHz) spectrum of **1** in DMSO-d_6



HR-ESIMS for **2**

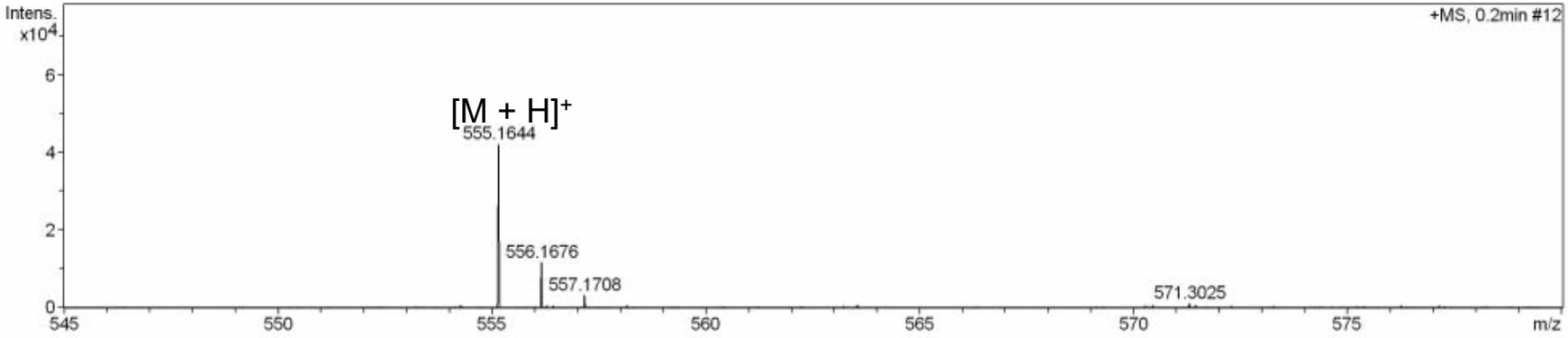
Mass Spectrum SmartFormula Report

Analysis Info

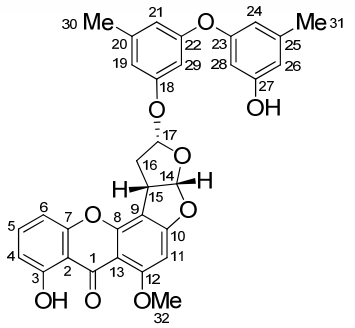
Analysis Name	D:\Data\MS\data\202104\renyanxia_W_pos_65_01_10385.d	Acquisition Date	4/1/2021 5:30:07 PM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	renyanxia_W_pos	Instrument	maXis 255552.00029
Comment			

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
555.1644	1	C32H27O9	100.00	555.1650	-1.1	-0.6	37.1	19.5	even	ok



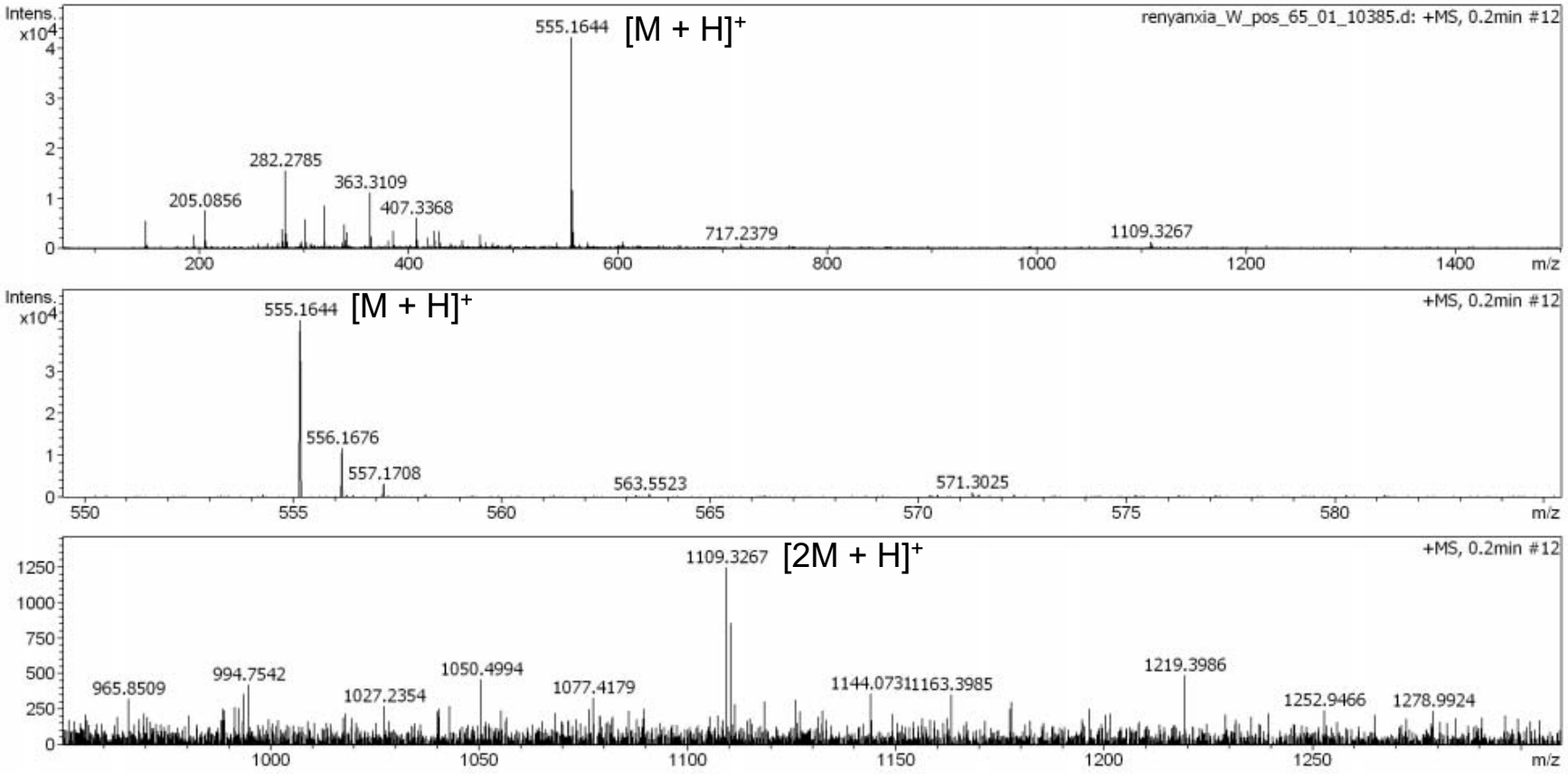
2

HR-ESIMS for **2**

Generic Display Report

Analysis Info

Analysis Name	D:\Data\MS\data\202104\renyanxia_W_pos_65_01_10385.d	Acquisition Date	4/1/2021 5:30:07 PM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	renyanxia_W_pos	Instrument	maXis
Comment			



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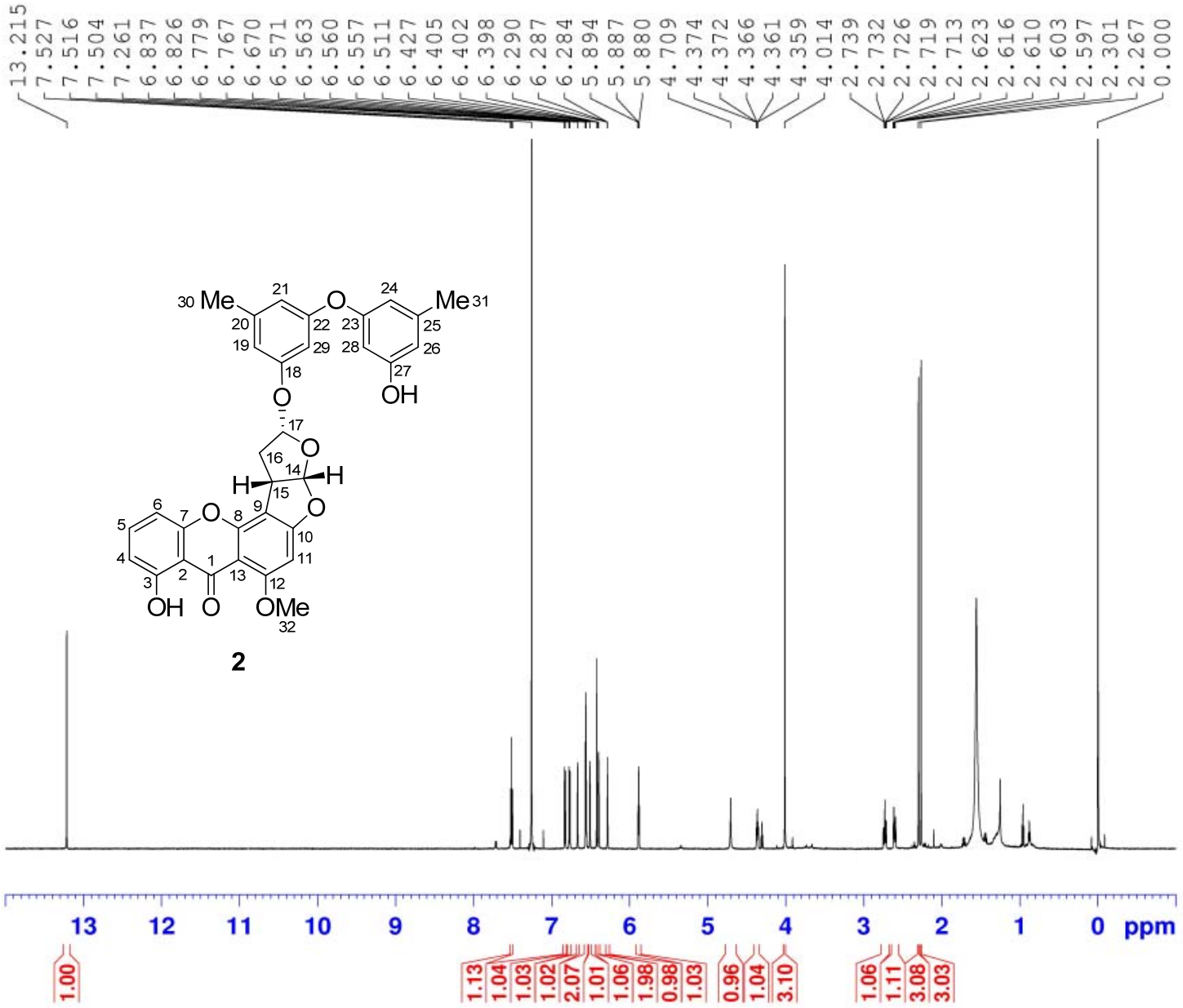
^{1}H (700 MHz) NMR spectrum of **2** in $CDCl_3$



2

NAME	wubibbib-WBB-42-22-9
EXPNO	10
PROCNO	1
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Time	15.25 h
INSTRUM	spect
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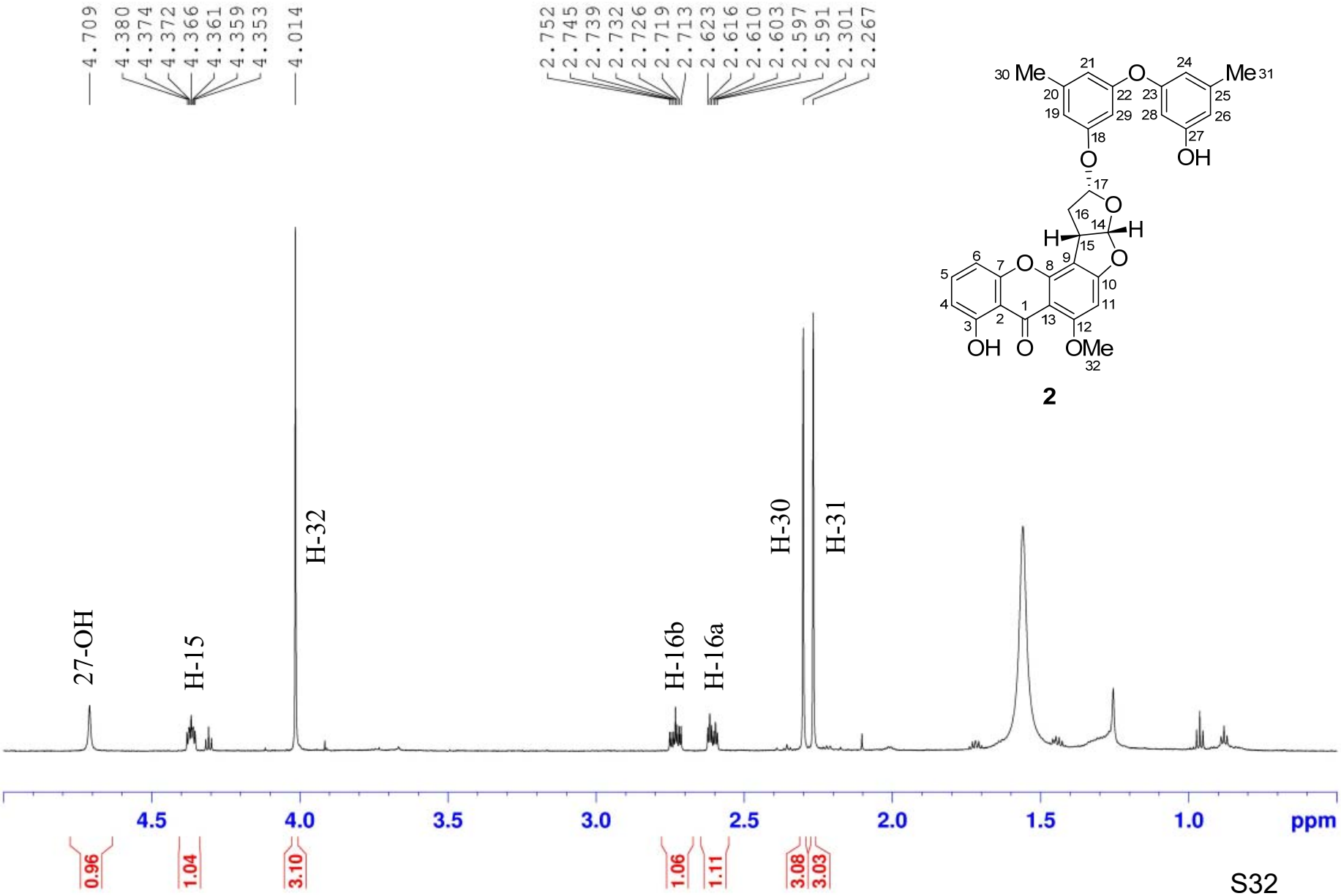
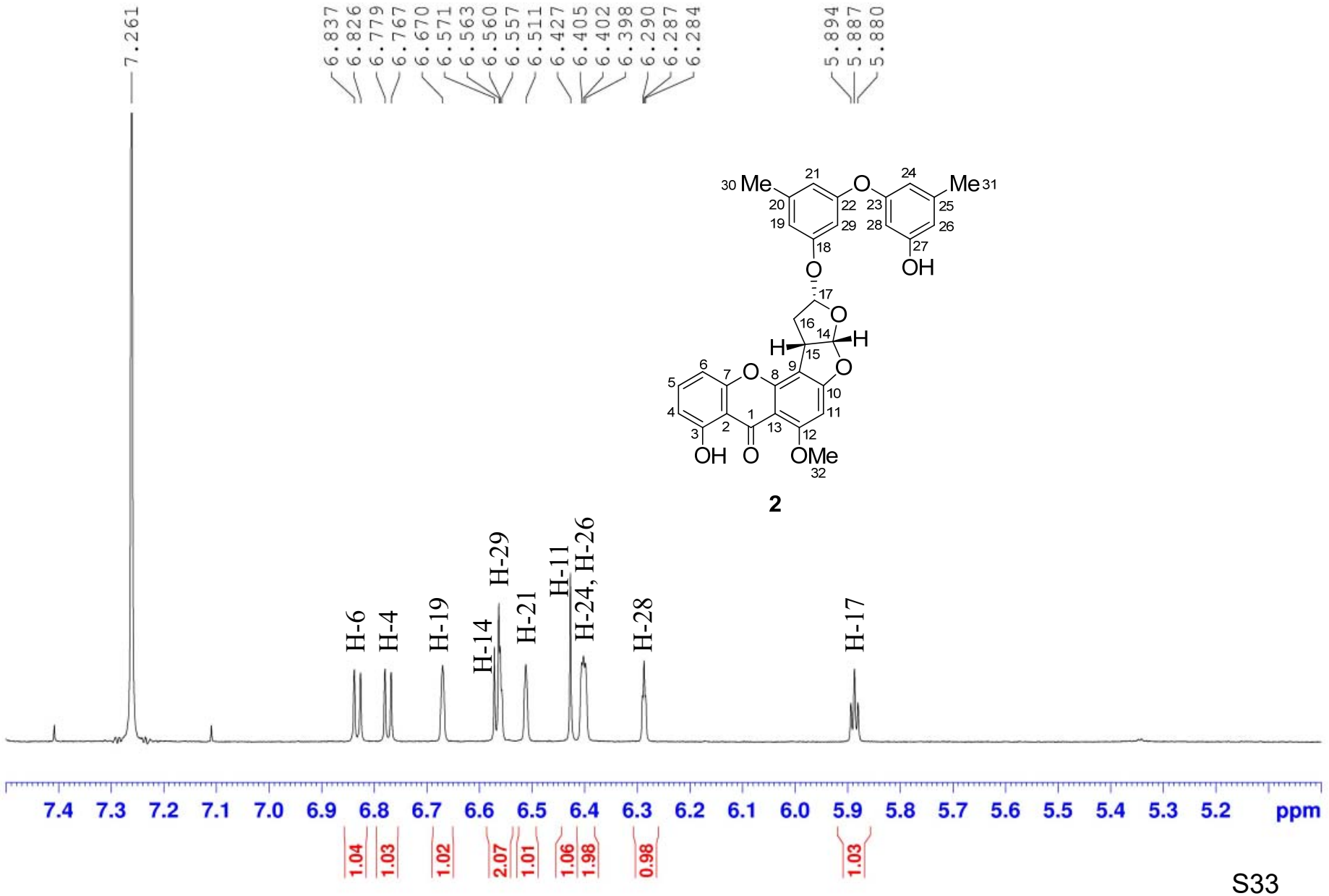
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	2
SWH	14097.744 Hz
FIDRES	0.430229 Hz
AQ	2.3243935 sec
RG	4.87
DW	35.467 usec
DE	10.00 usec
TE	298.0 K
D1	1.00000000 sec
TD0	1
SFO1	700.1849013 MHz
NUC1	1H
P1	7.55 usec
SI	65536
SF	700.1800174 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

^{1}H (700 MHz) NMR spectrum of **2** in $CDCl_3$



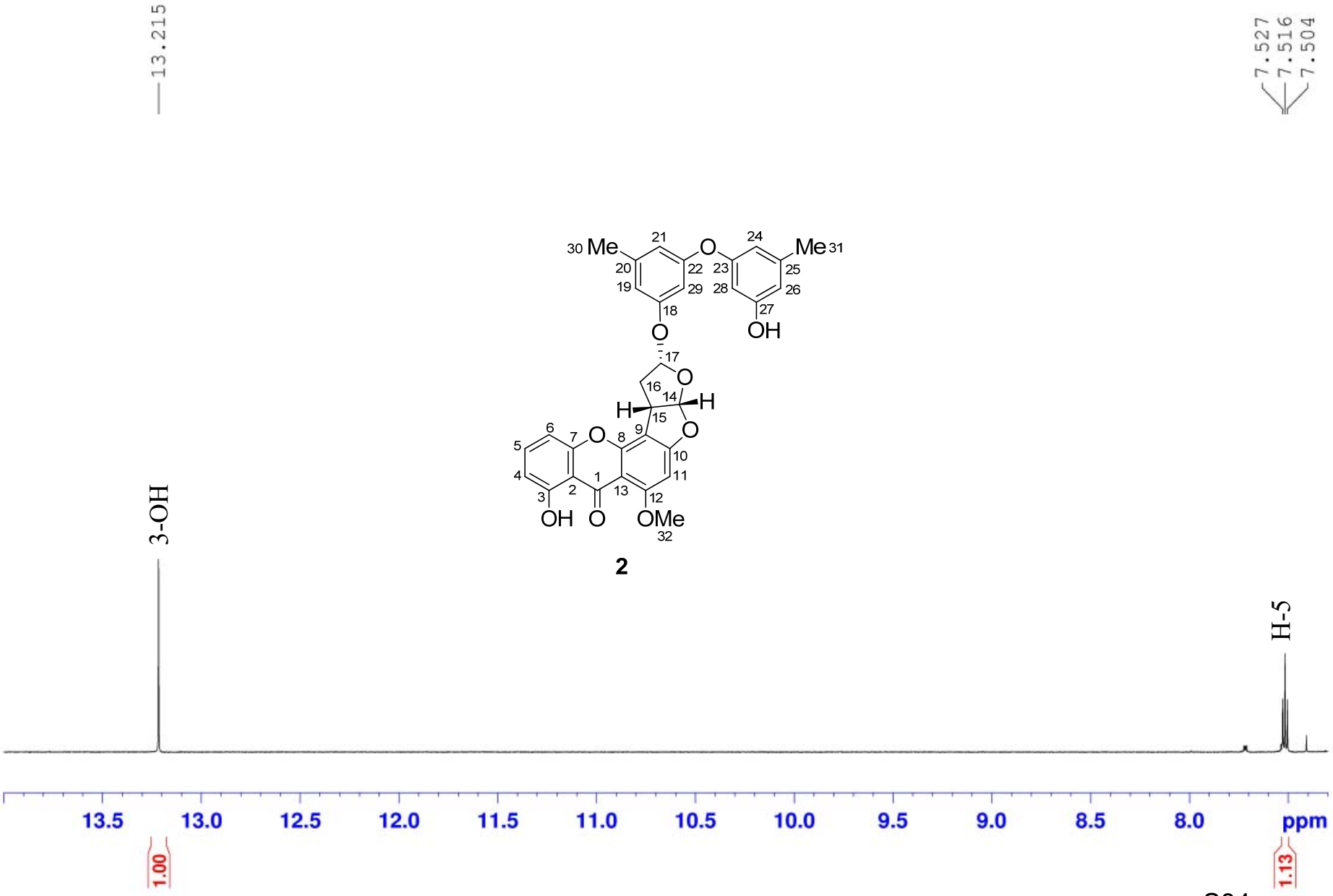
2

^{1}H (700 MHz) NMR spectrum of **2** in $CDCl_3$



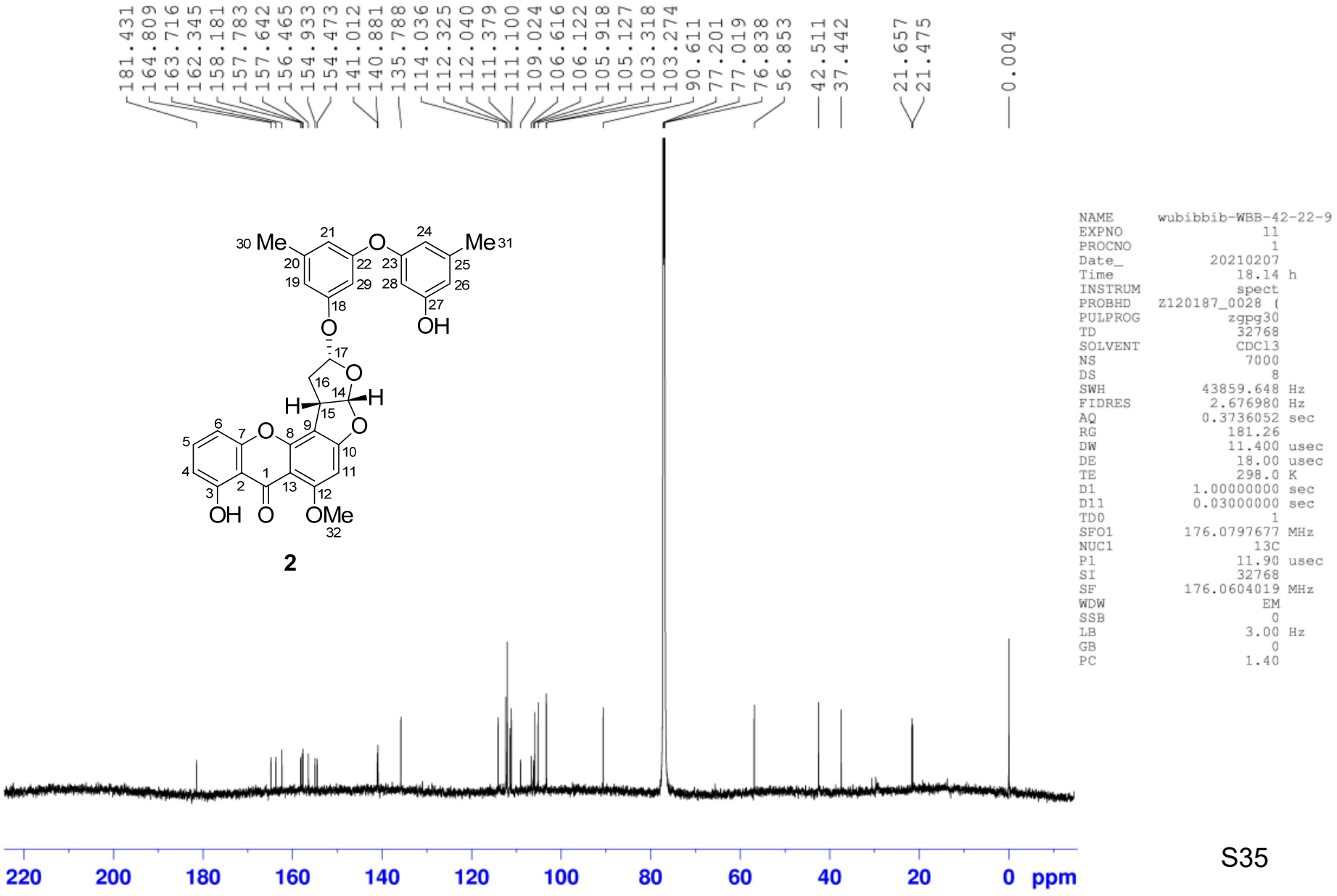
2

^{1}H (700 MHz) NMR spectrum of **2** in $CDCl_3$



2

^{13}C (175 MHz) NMR spectrum of **2** in $CDCl_3$



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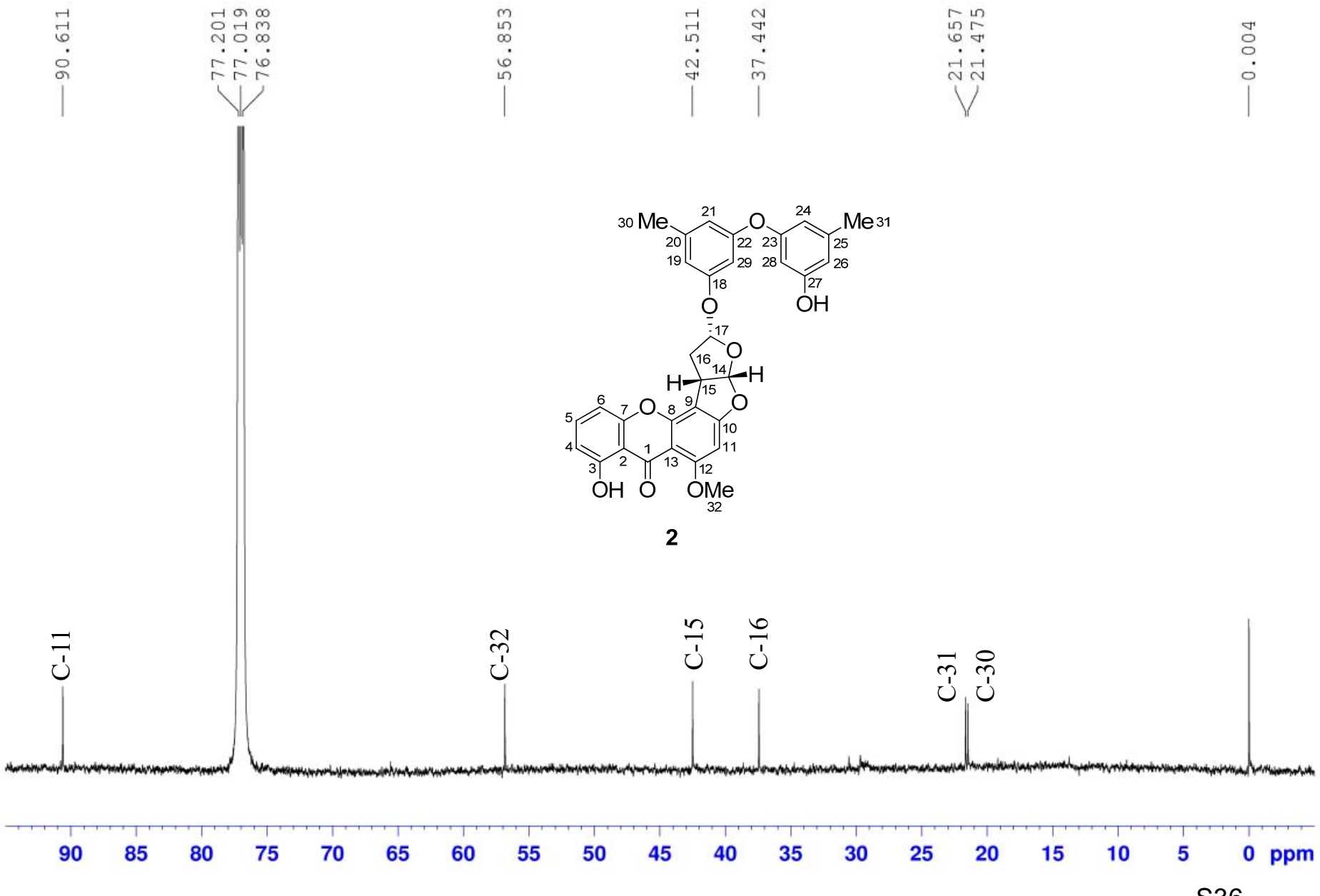
^{13}C (175 MHz) NMR spectrum of **2** in $CDCl_3$



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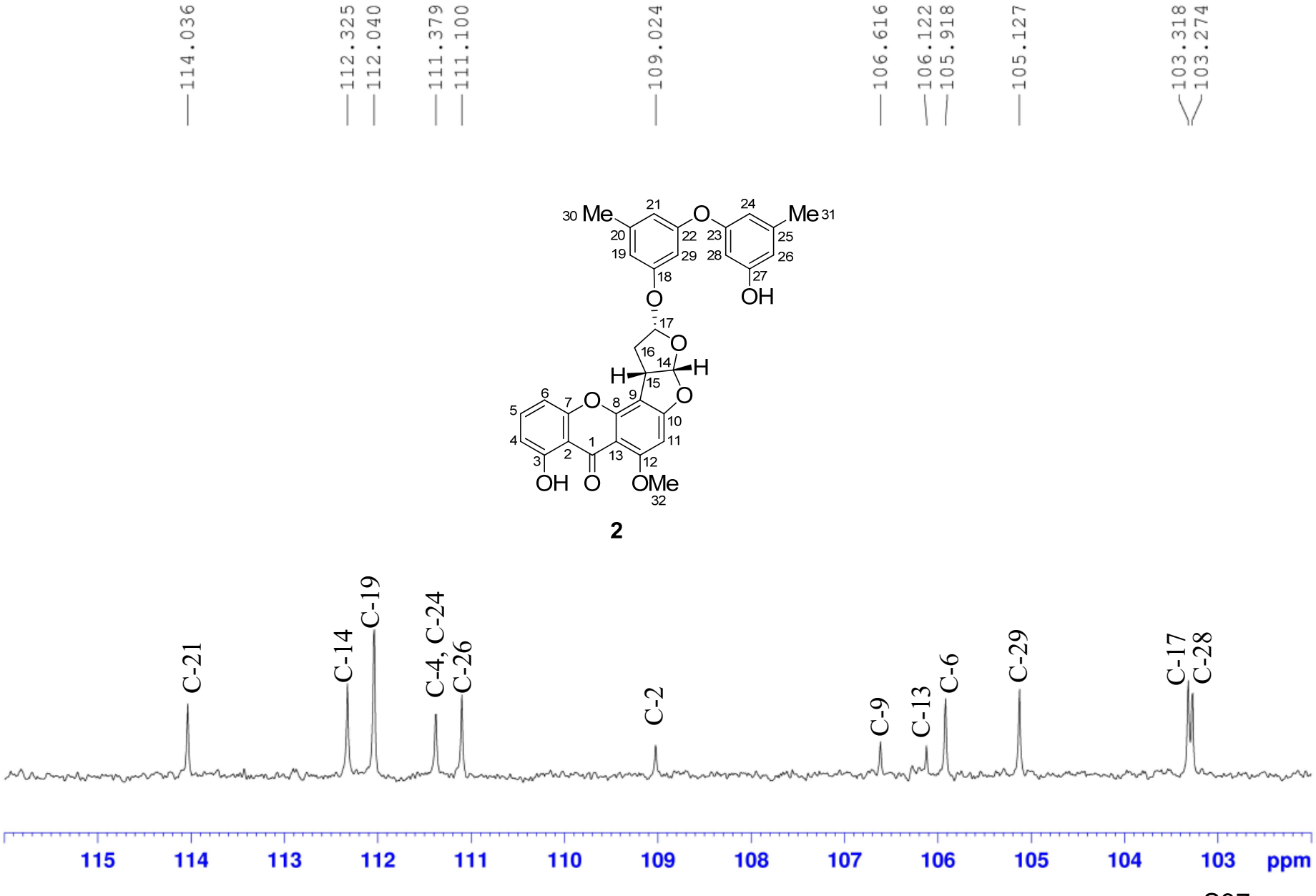
^{13}C (175 MHz) NMR spectrum of **2** in $CDCl_3$



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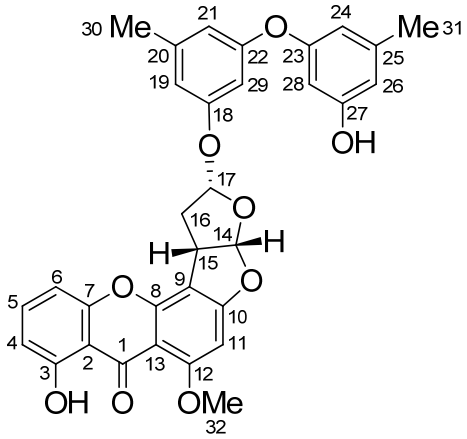
^{13}C (175 MHz) NMR spectrum of **2** in $CDCl_3$



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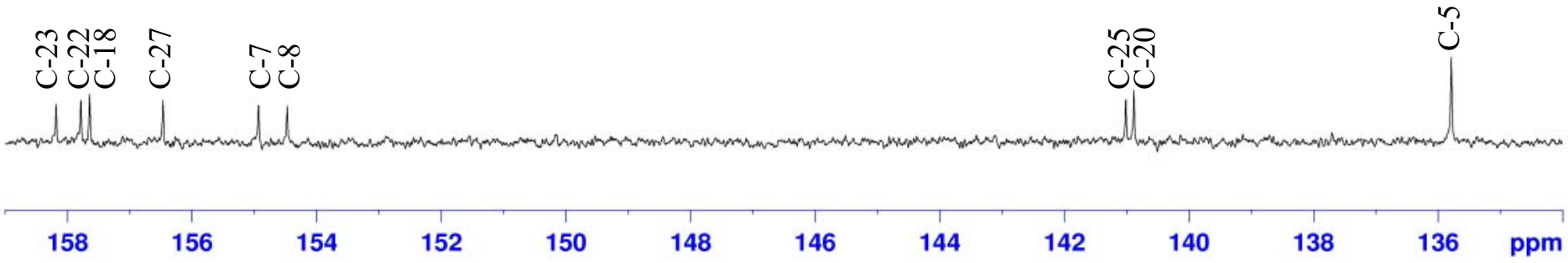
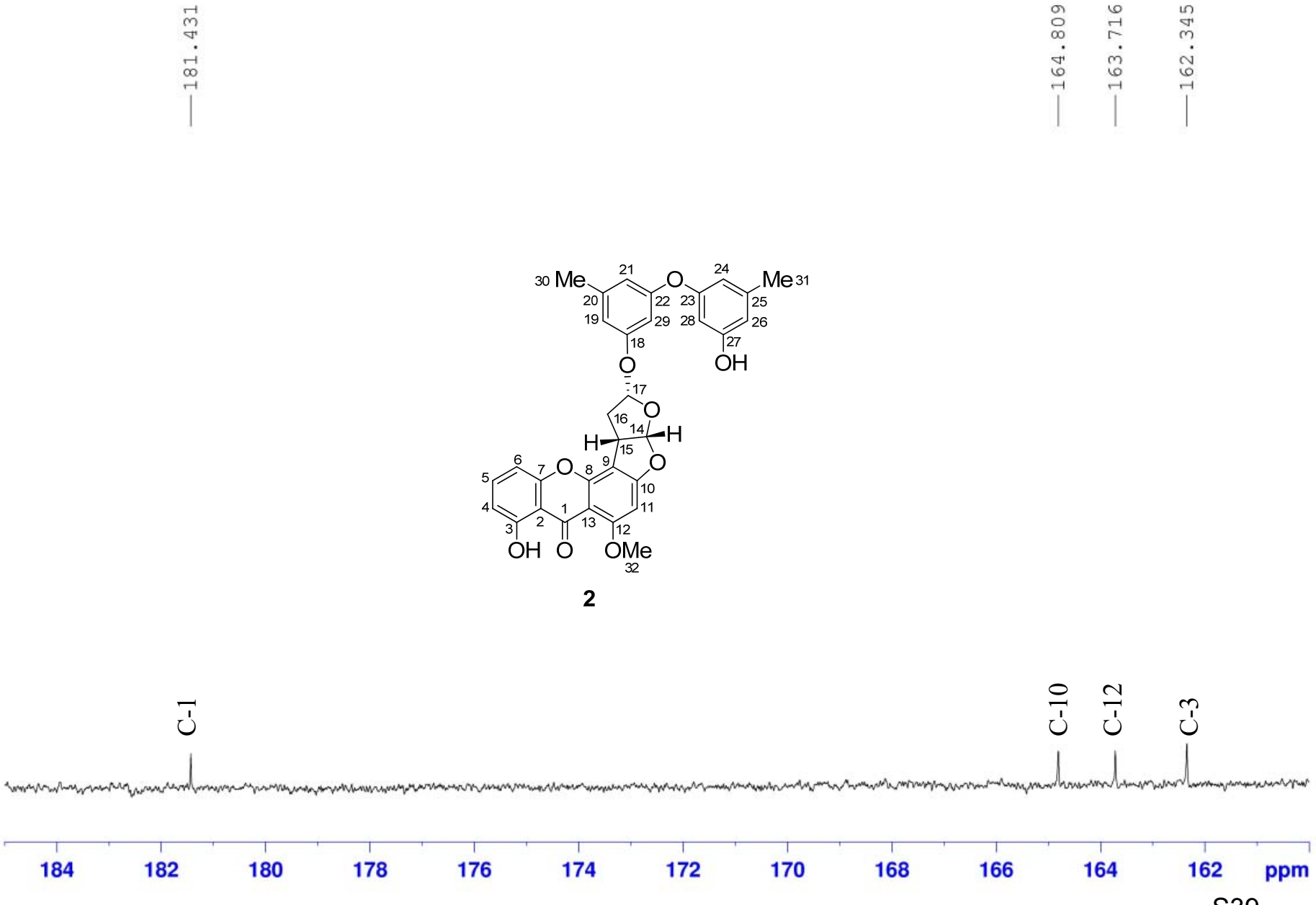
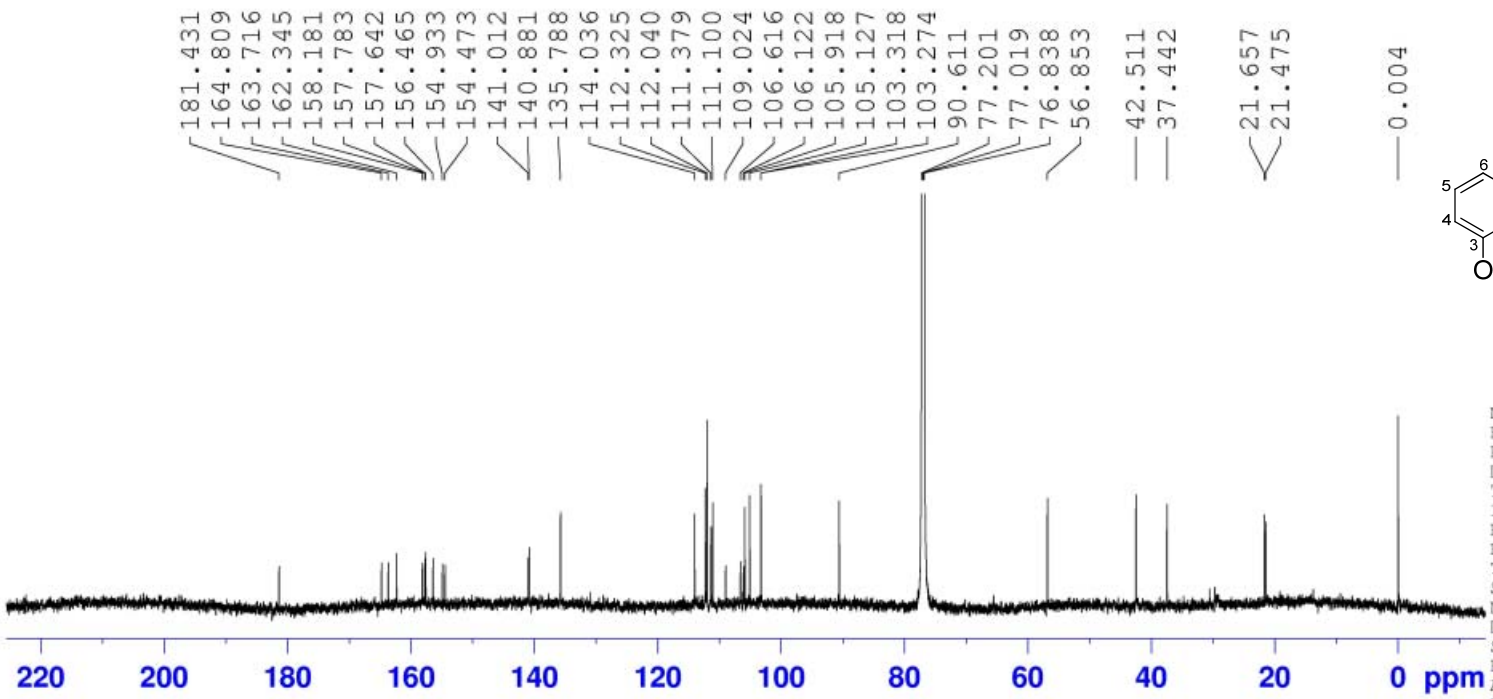
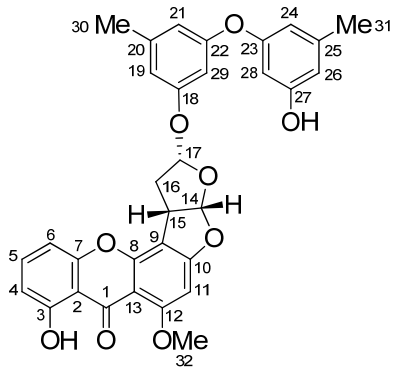


^{13}C (175 MHz) NMR spectrum of **2** in $CDCl_3$



DEPT135 (175 MHz) spectrum of **2** in $CDCl_3$

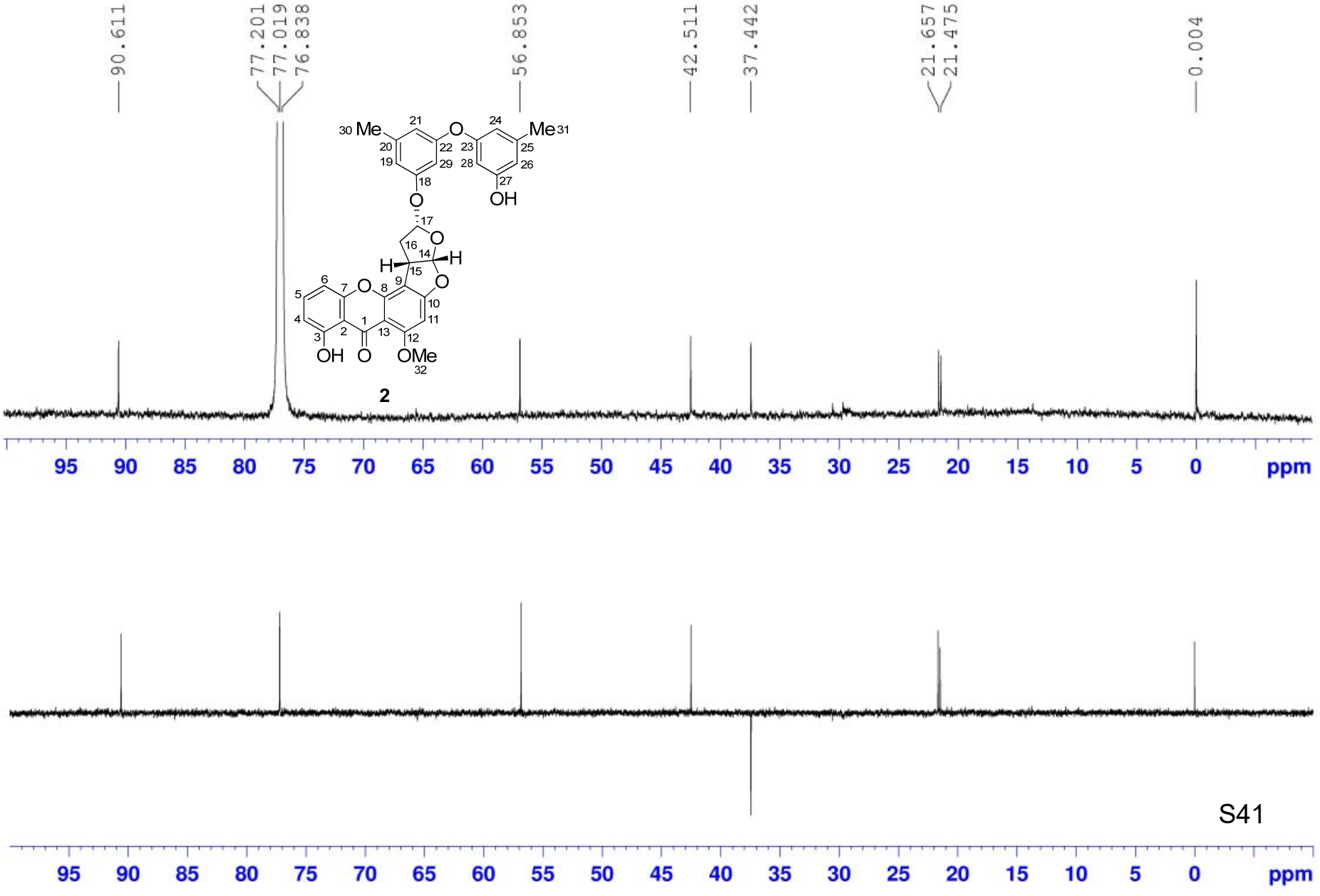




2

NAME	wubibbib-WBB-42-22-9
EXPNO	12
PROCNO	1
Date_	20210207
Time	19.38 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	deptsp135
TD	32768
SOLVENT	CDCl3
NS	3500
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	176.0604026 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

DEPT135 (175 MHz) spectrum of **2** in $CDCl_3$



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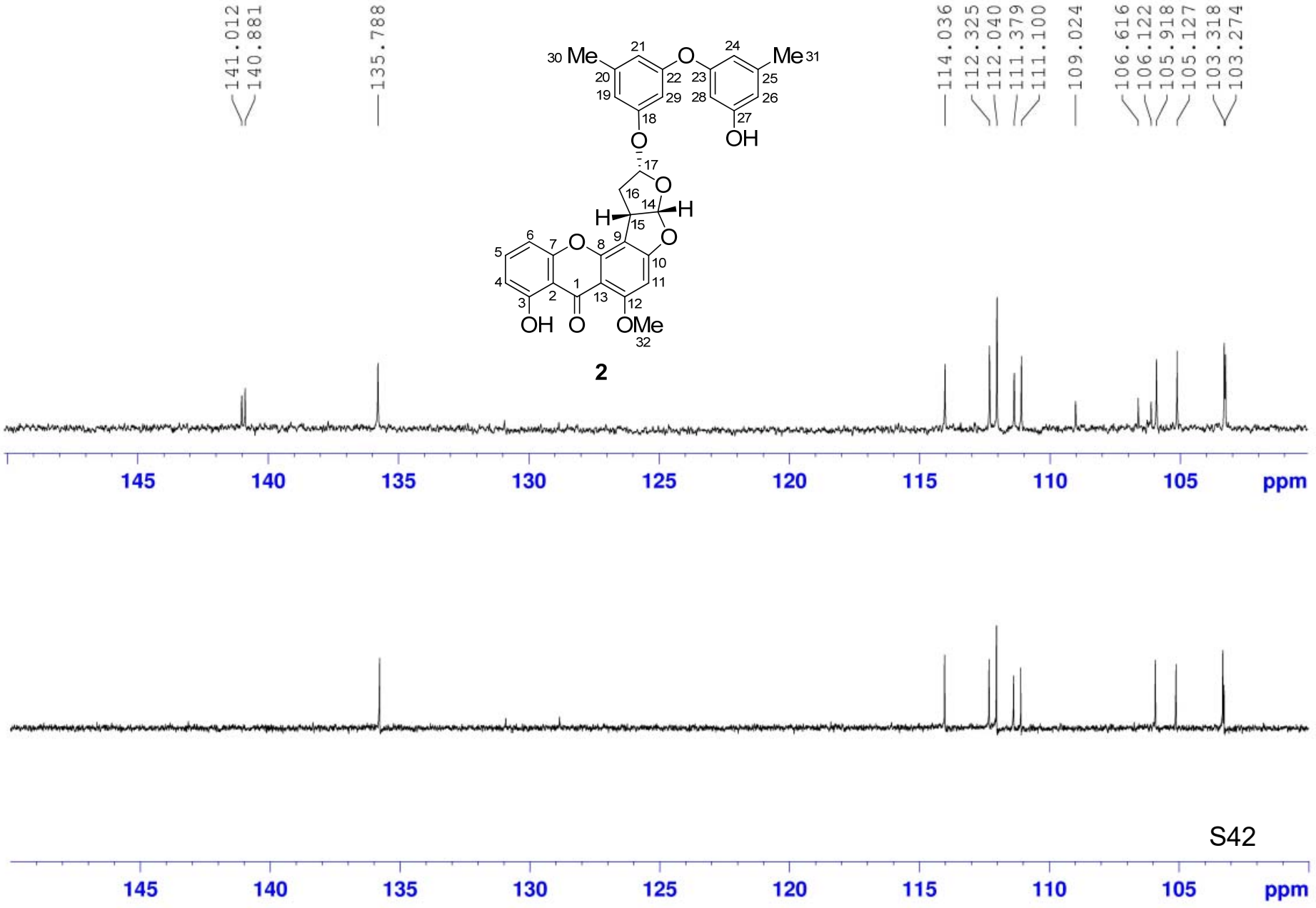
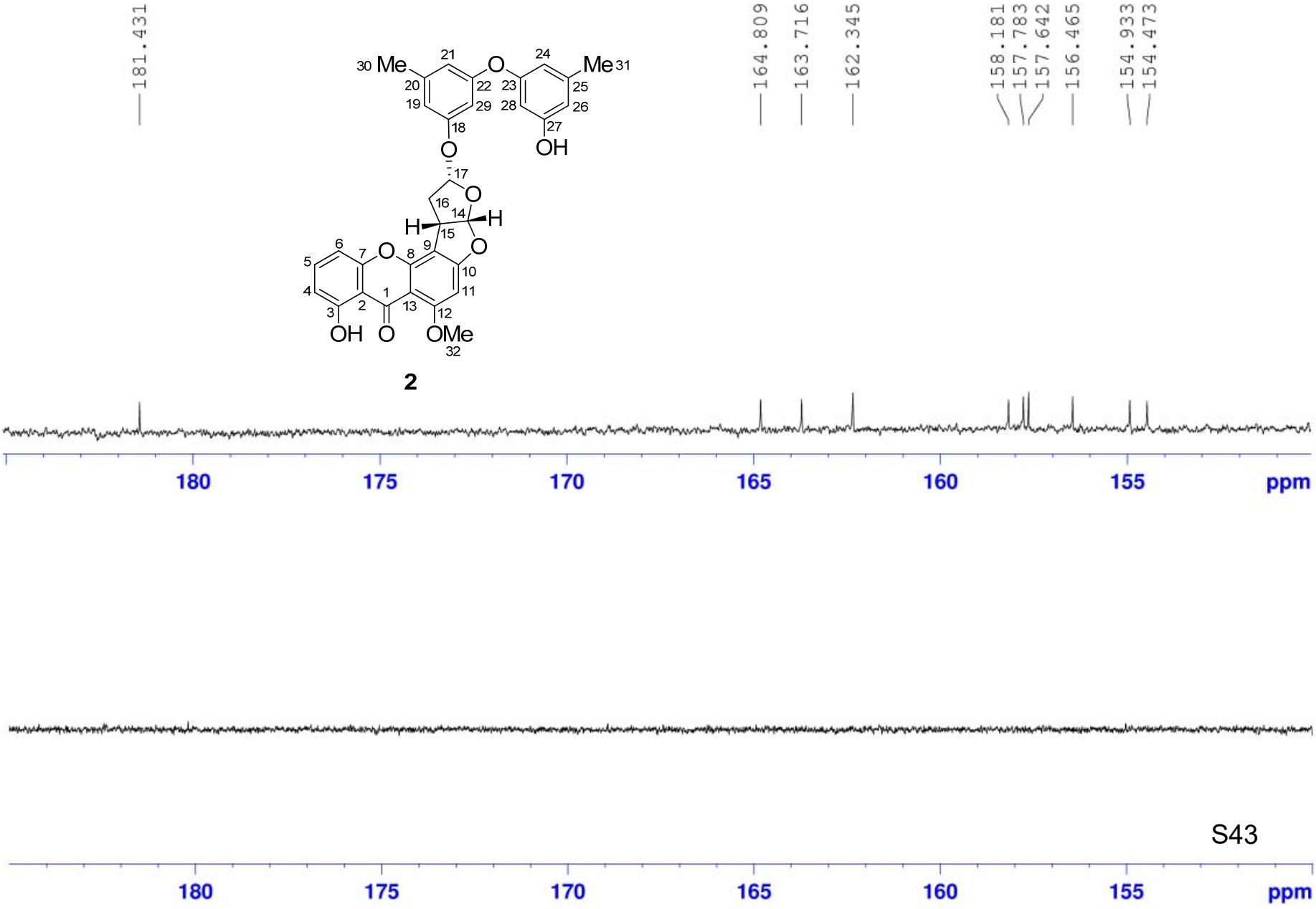
DEPT135 (175 MHz) spectrum of **2** in $CDCl_3$

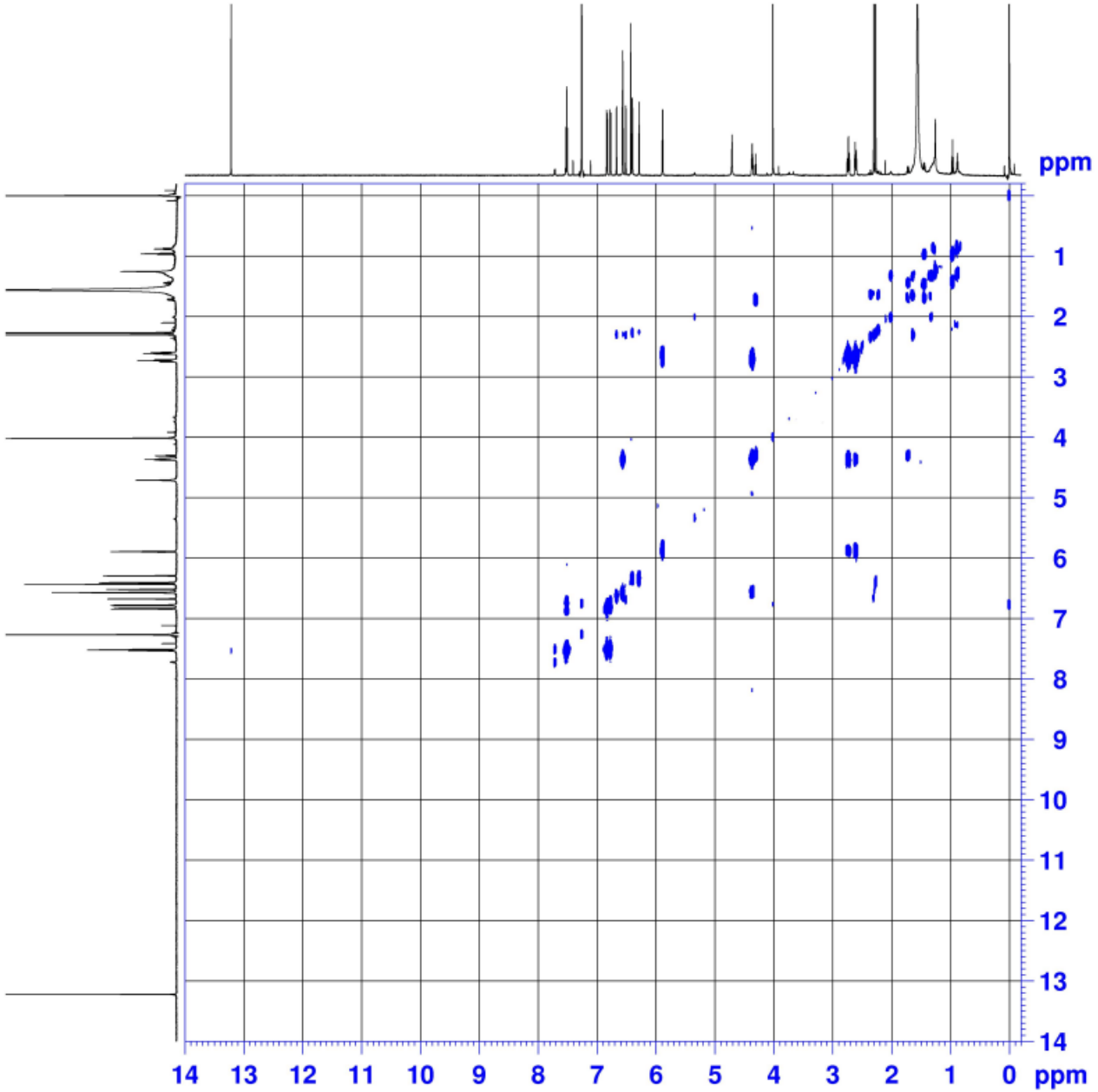


DEPT135 (175 MHz) spectrum of **2** in $CDCl_3$



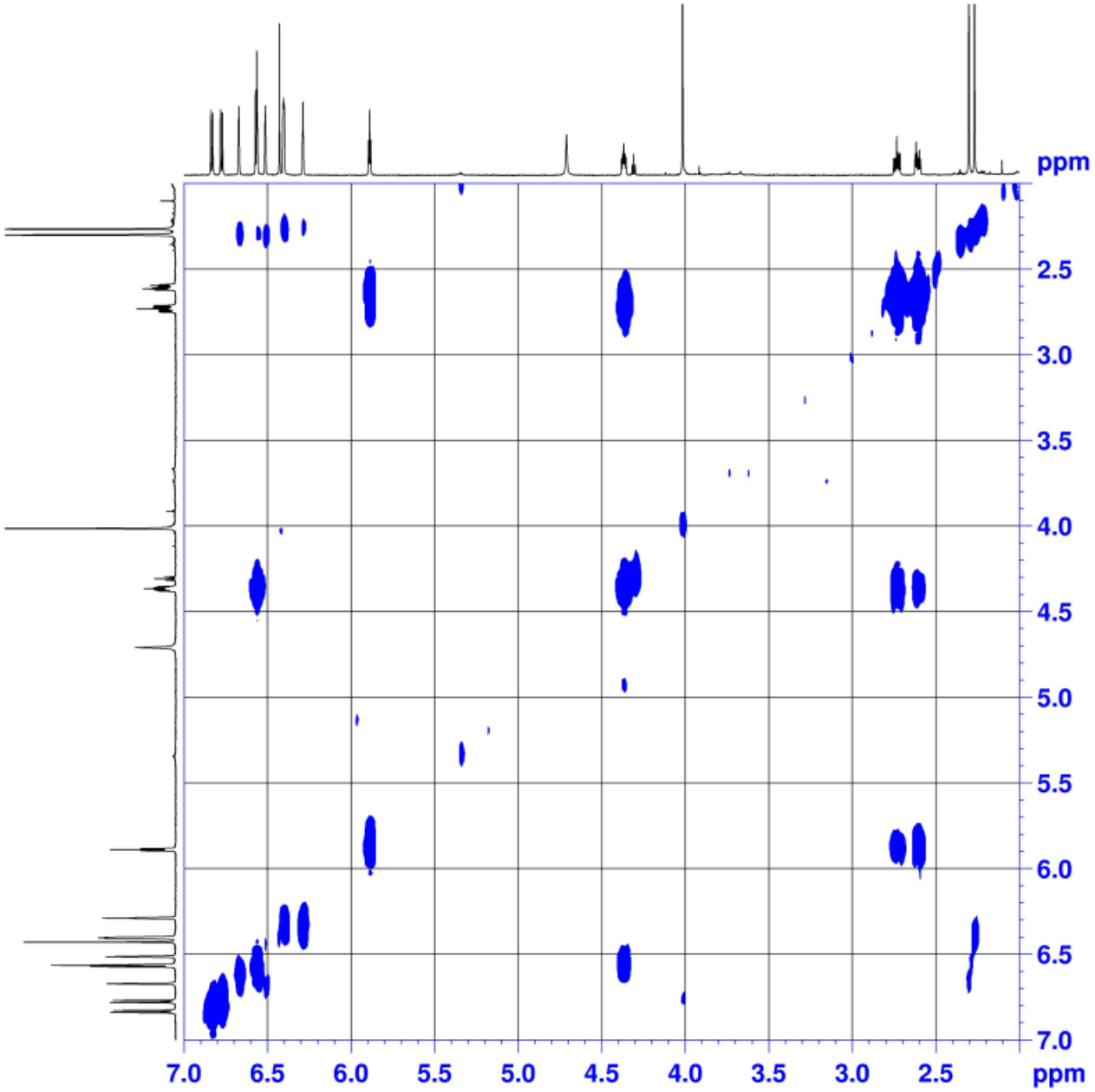
2

^{1}H–^{1}H COSY (700 MHz) spectrum of **2** in $CDCl_3$

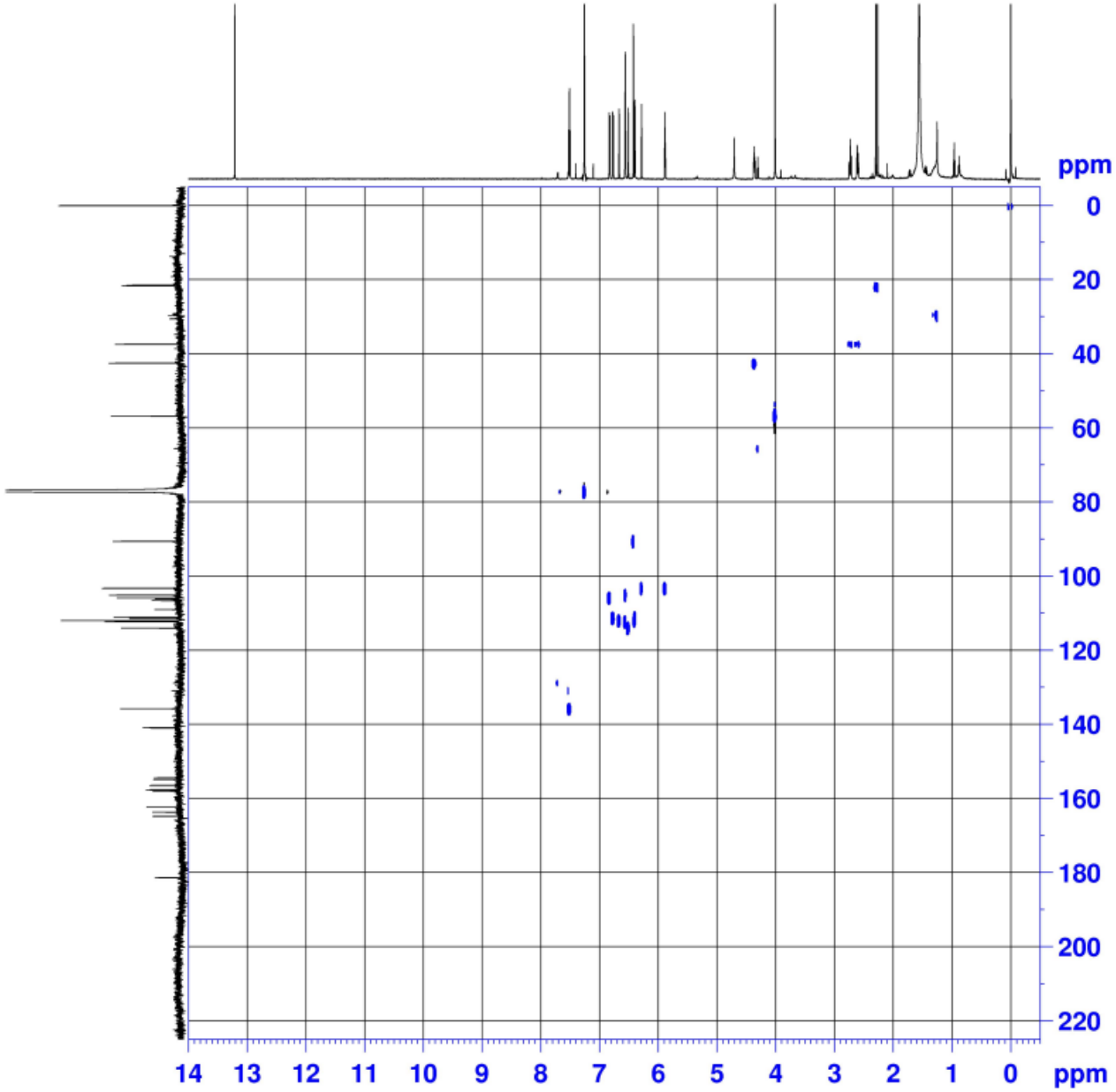


NAME	wubibbib-WBB-42-22-9
EXPNO	13
PROCNO	1
Date_	20210207
Time	19.39 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	cosygpmfqf
TD	2048
SOLVENT	CDCl3
NS	24
DS	16
SWH	11520.737 Hz
FIDRES	11.250720 Hz
AQ	0.0889332 sec
RG	181.26
DW	43.400 usec
DE	10.00 usec
TE	298.0 K
D0	0.00000300 sec
D1	1.00000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00008680 sec
ND0	1
TD	128
SFO1	700.1847 MHz
FIDRES	90.005760 Hz
SW	16.454 ppm
FnMODE	QF
SI	1024
SF	700.1800175 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	700.1800175 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

^{1}H–^{1}H COSY (700 MHz) spectrum of **2** in $CDCl_3$

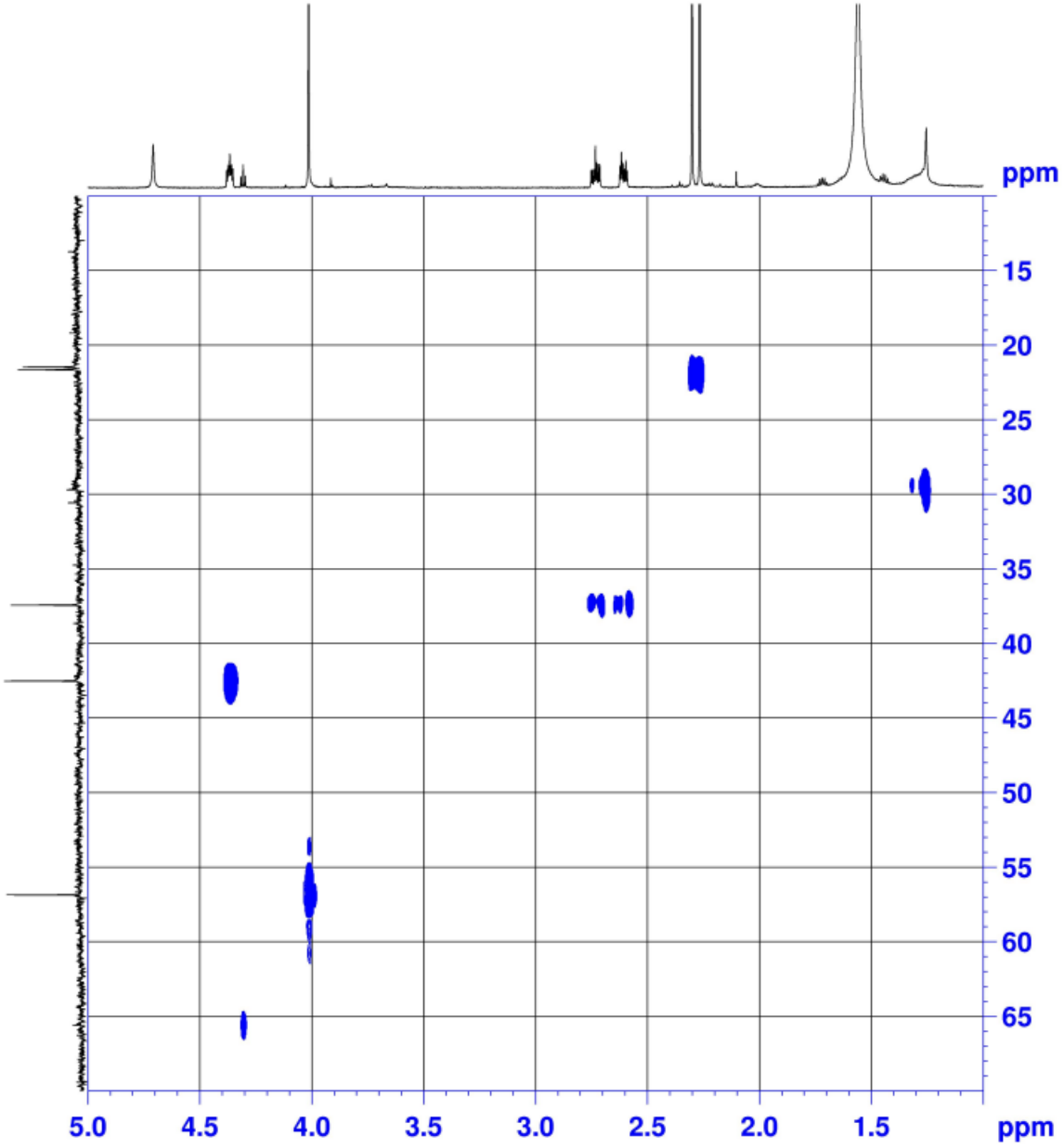


HSQC (700 MHz) spectrum of **2** in $CDCl_3$

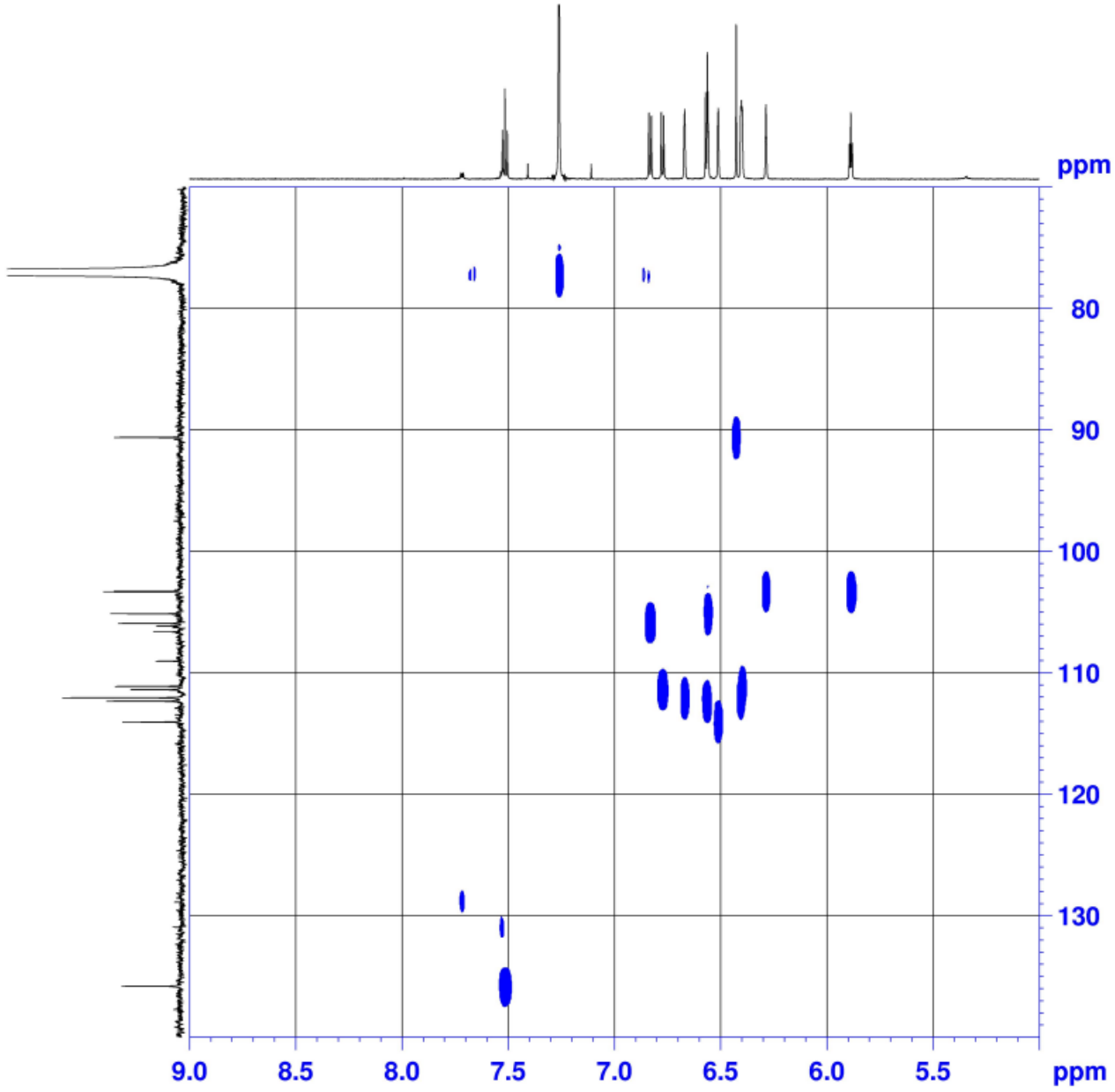


NAME	wubibbib-WBB-42-22-9	
EXPNO	16	
PROCNO	1	
Date_	20210207	
Time	23.43	h
INSTRUM	spect	
PROBHD	Z120187_0028 (	
PULPROG	hsqcetgp	
TD	2048	
SOLVENT	CDCl3	
NS	28	
DS	16	
SWH	11432.927	Hz
FIDRES	11.164968	Hz
AQ	0.0896159	sec
RG	181.26	
DW	43.733	usec
DE	10.00	usec
TE	298.0	K
CNST2	145.0000000	
D0	0.00000300	sec
D1	1.00000000	sec
D4	0.00172414	sec
D11	0.03000000	sec
D16	0.00020000	sec
IN0	0.00001180	sec
ND0	2	
TD	128	
SFO1	176.0796	MHz
FIDRES	331.038147	Hz
SW	240.646	ppm
FnMODE	Echo-Antiecho	
SI	2048	
SF	700.1800175	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	
PC	1.40	
SI	2048	
MC2	echo-antiecho	
SF	176.0604010	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	

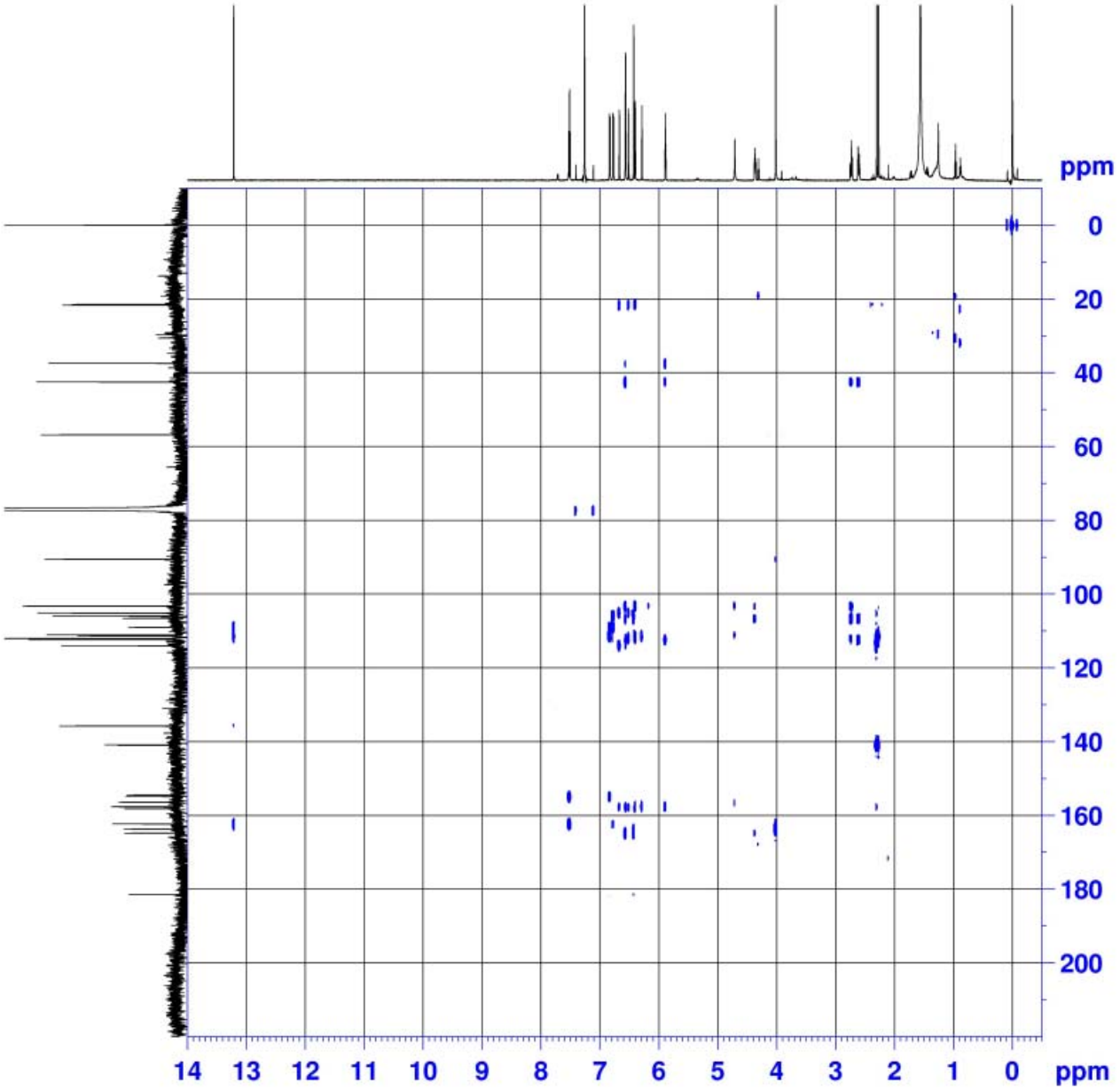
HSQC (700 MHz) spectrum of **2** in $CDCl_3$



HSQC (700 MHz) spectrum of **2** in $CDCl_3$

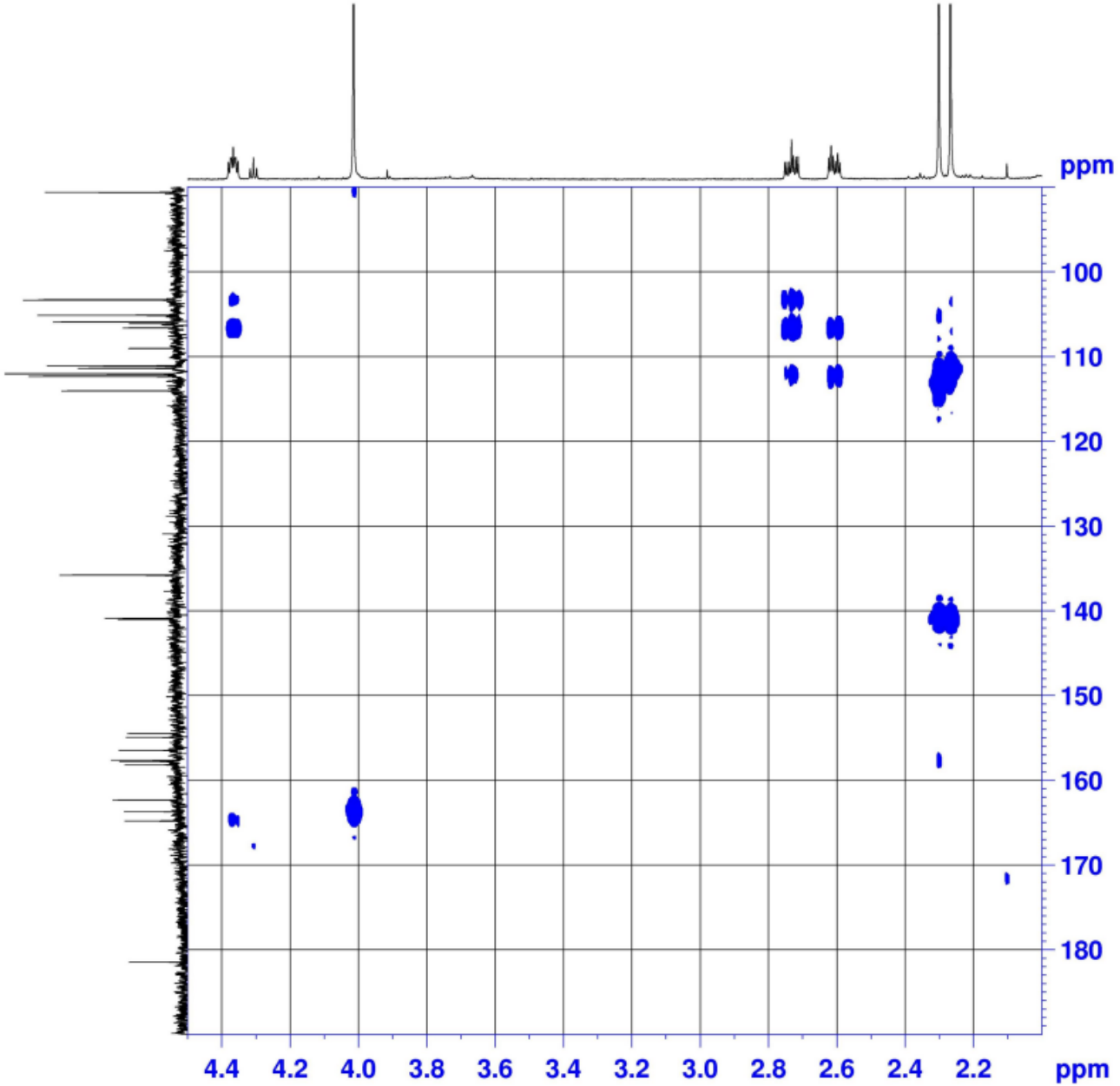


HMBC (700 MHz) spectrum of **2** in $CDCl_3$

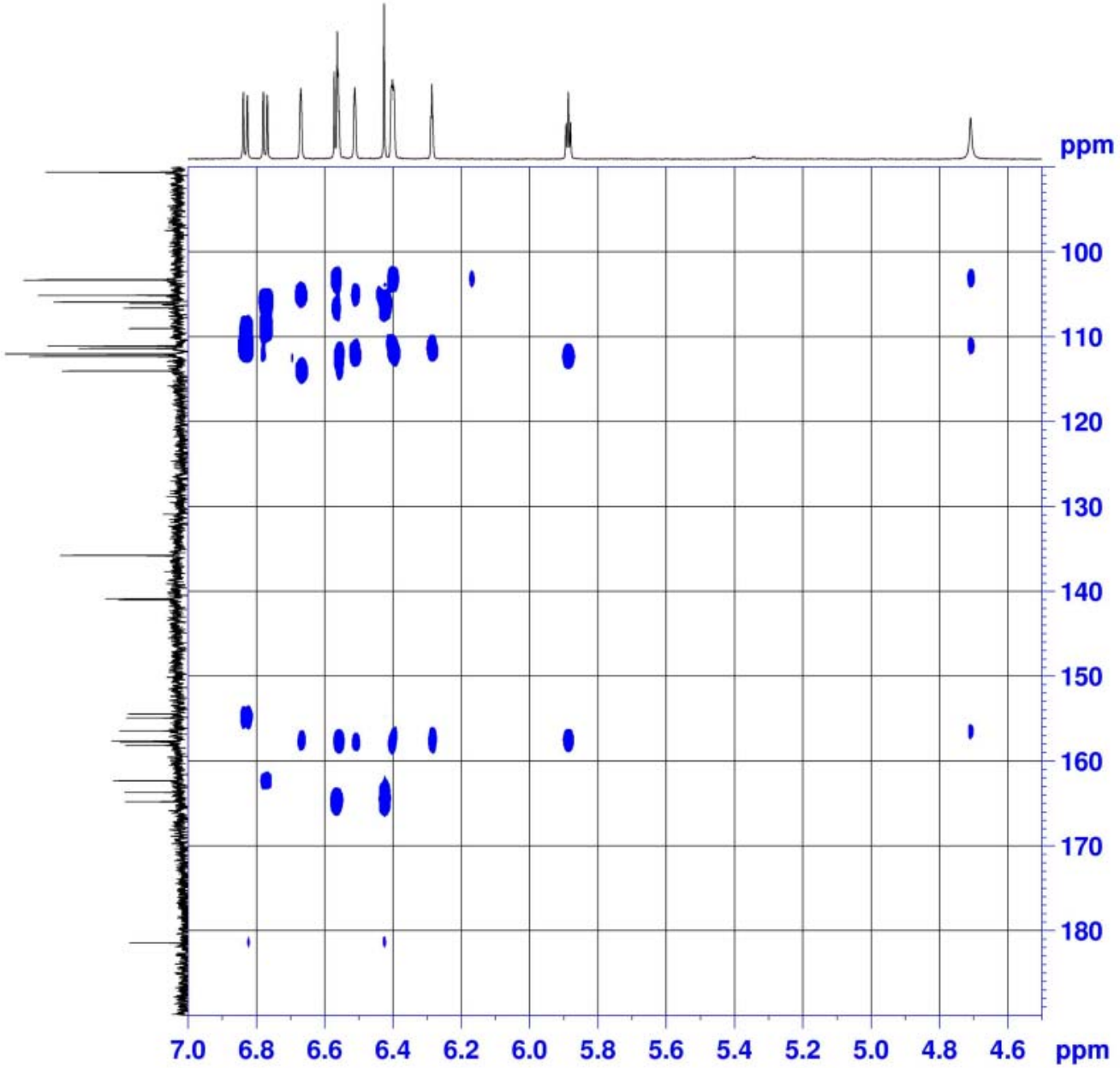


NAME	wubibbib-WBB-42-22-9
EXPNO	15
PROCNO	1
Date_	20210207
Time	22.05 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hmbcetgpl3nd
TD	4096
SOLVENT	CDCl3
NS	36
DS	16
SWH	11432.927 Hz
FIDRES	5.582484 Hz
AQ	0.1791817 sec
RG	181.26
DW	43.733 usec
DE	10.00 usec
TE	298.0 K
CNST6	120.0000000
CNST7	165.0000000
CNST13	8.0000000
D0	0.00000300 sec
D1	1.00000000 sec
D6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00001180 sec
ND0	2
TD	128
SFO1	176.0797 MHz
FIDRES	331.038147 Hz
SW	240.646 ppm
FnMODE	Echo-Antiecho
SI	2048
SF	700.1800175 MHz
WDW	SINE
SSB	4
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	176.0604010 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

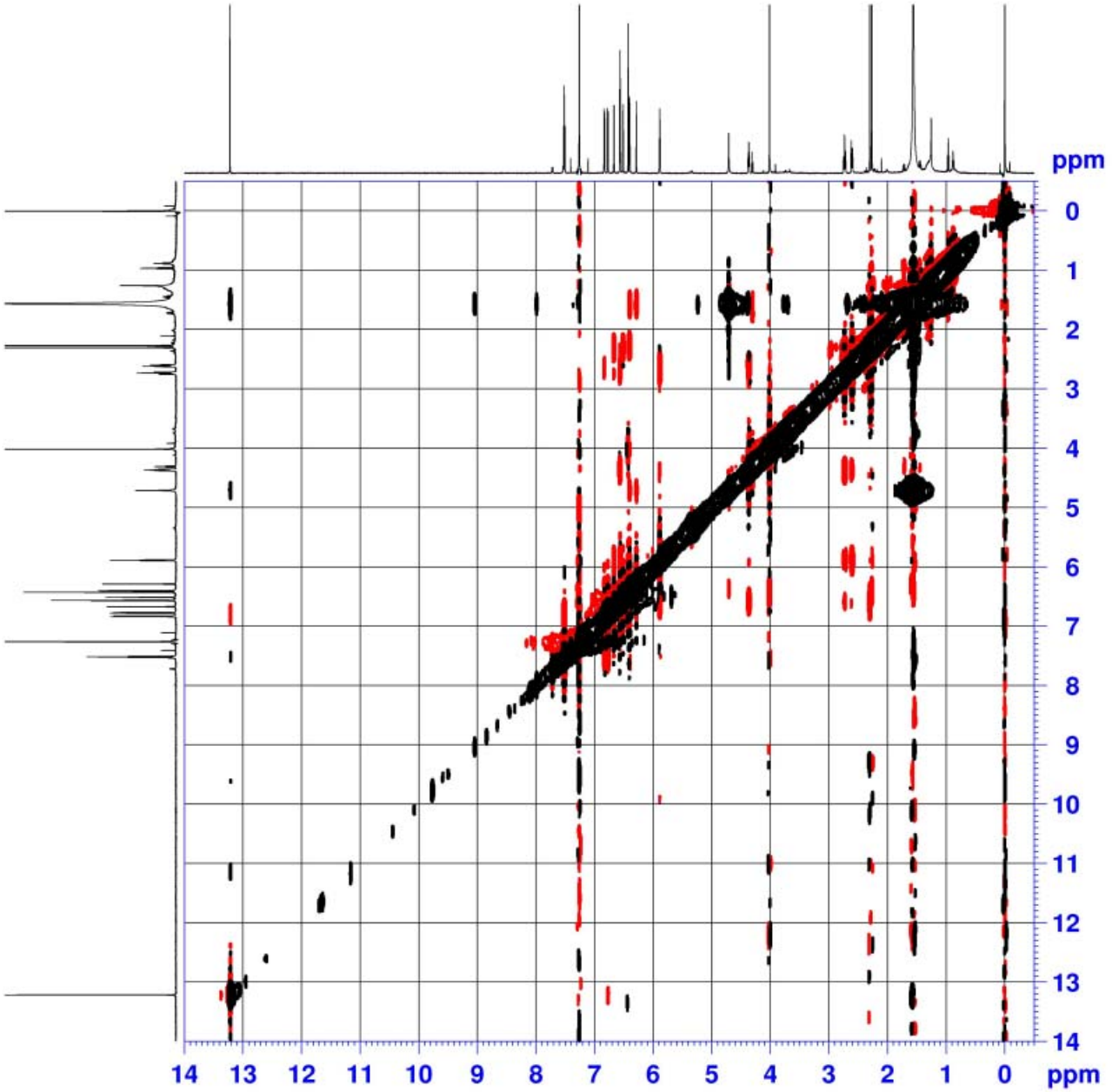
HMBC (700 MHz) spectrum of **2** in $CDCl_3$



HMBC (700 MHz) spectrum of **2** in $CDCl_3$

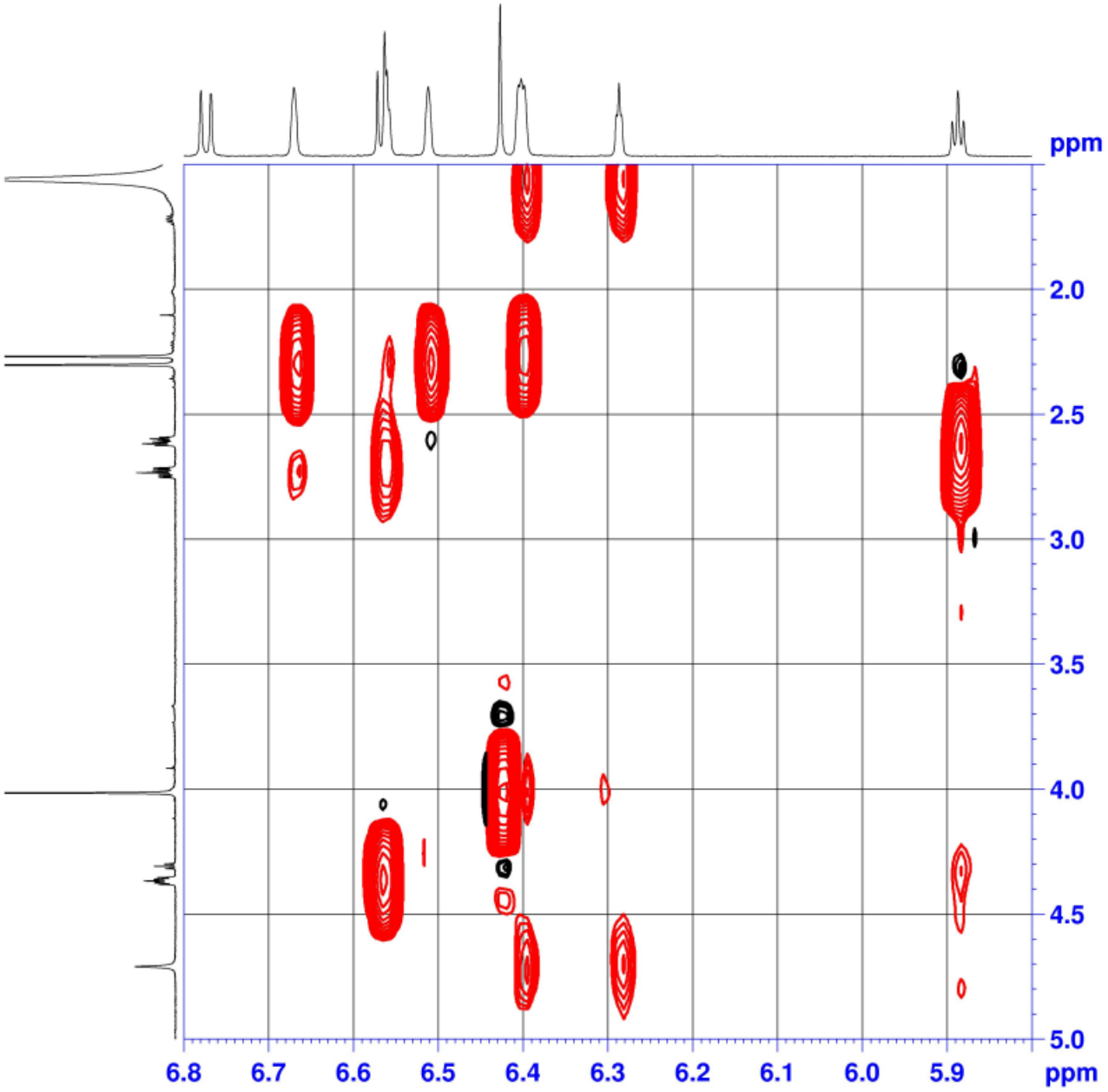


NOESY (700 MHz) spectrum of **2** in $CDCl_3$

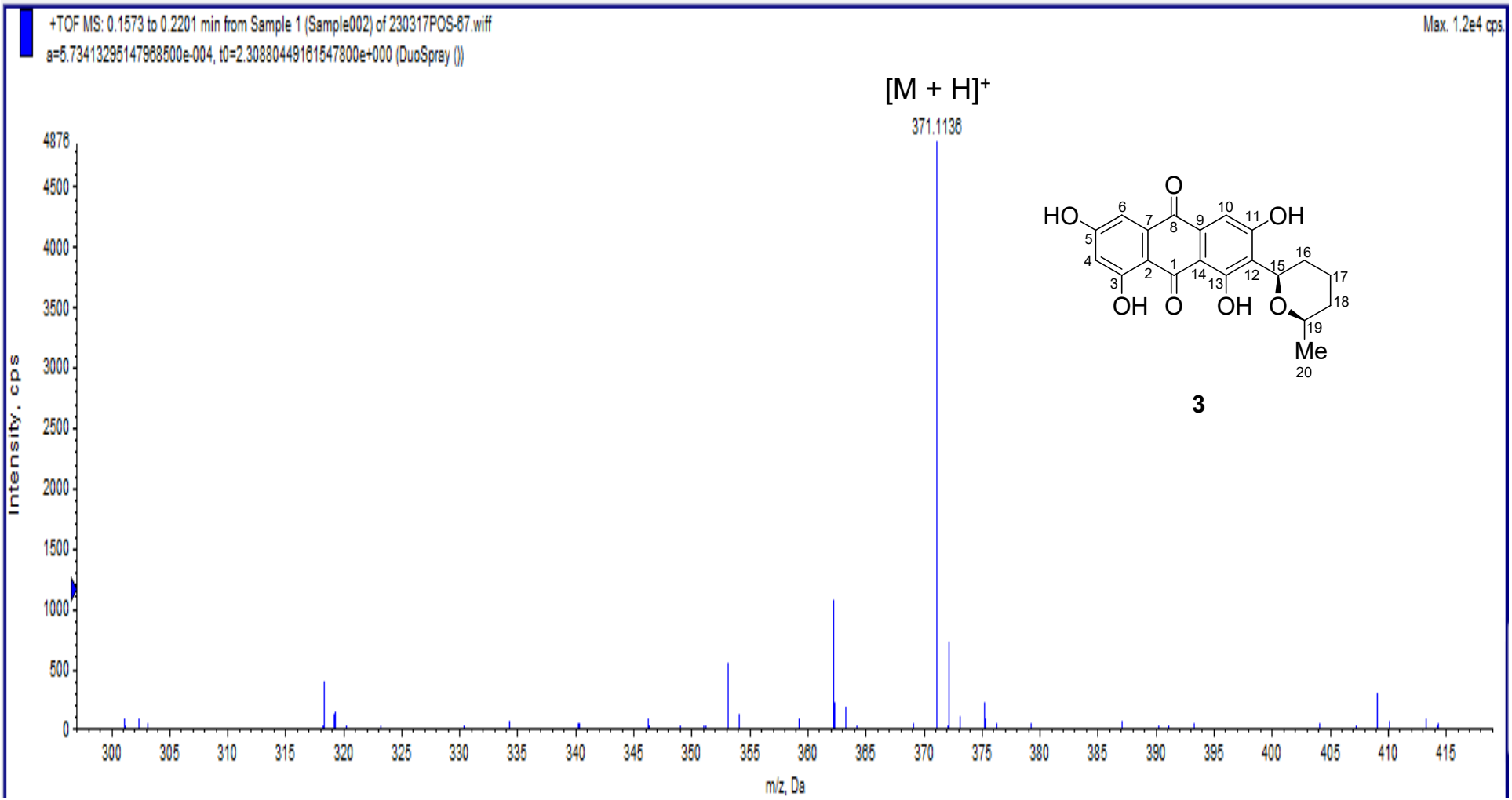


NAME	wubibbib-WBB-42-22-9
EXPNO	14
PROCNO	1
Date_	20210207
Time	20.37 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	noesygpph
TD	2048
SOLVENT	CDCl3
NS	24
DS	16
SWH	11645.963 Hz
FIDRES	11.373011 Hz
AQ	0.0879775 sec
RG	15.56
DW	42.933 usec
DE	10.00 usec
TE	298.0 K
D0	0.00003329 sec
D1	1.00000000 sec
D8	0.60000002 sec
D16	0.00020000 sec
IN0	0.00008580 sec
ND0	1
TD	128
SFO1	700.1847 MHz
FIDRES	91.054779 Hz
SW	16.646 ppm
FnMODE	TPPI
SI	2048
SF	700.1800175 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0
PC	1.00
SI	2048
MC2	TPPI
SF	700.1800175 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

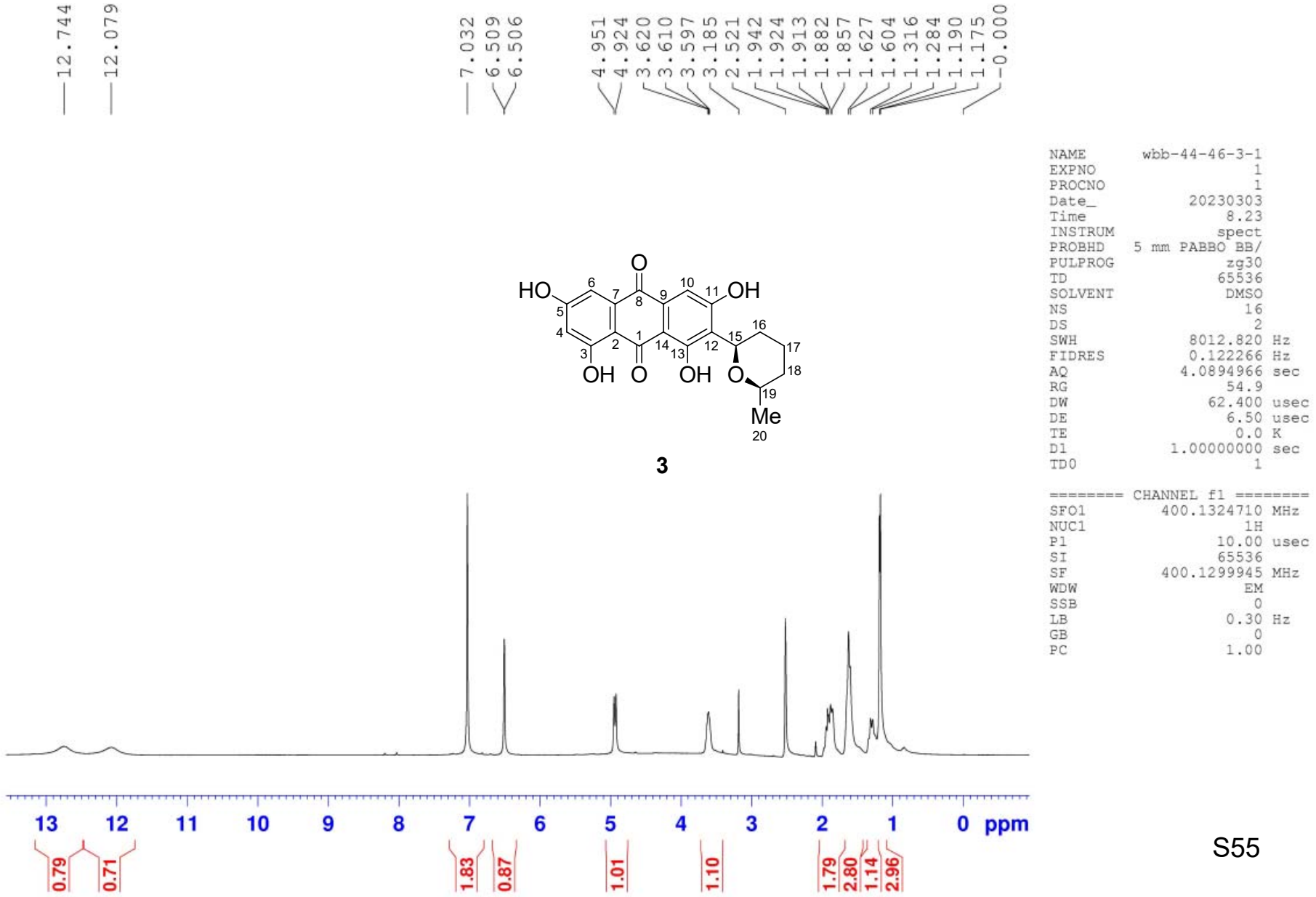
NOESY (700 MHz) spectrum of **2** in $CDCl_3$



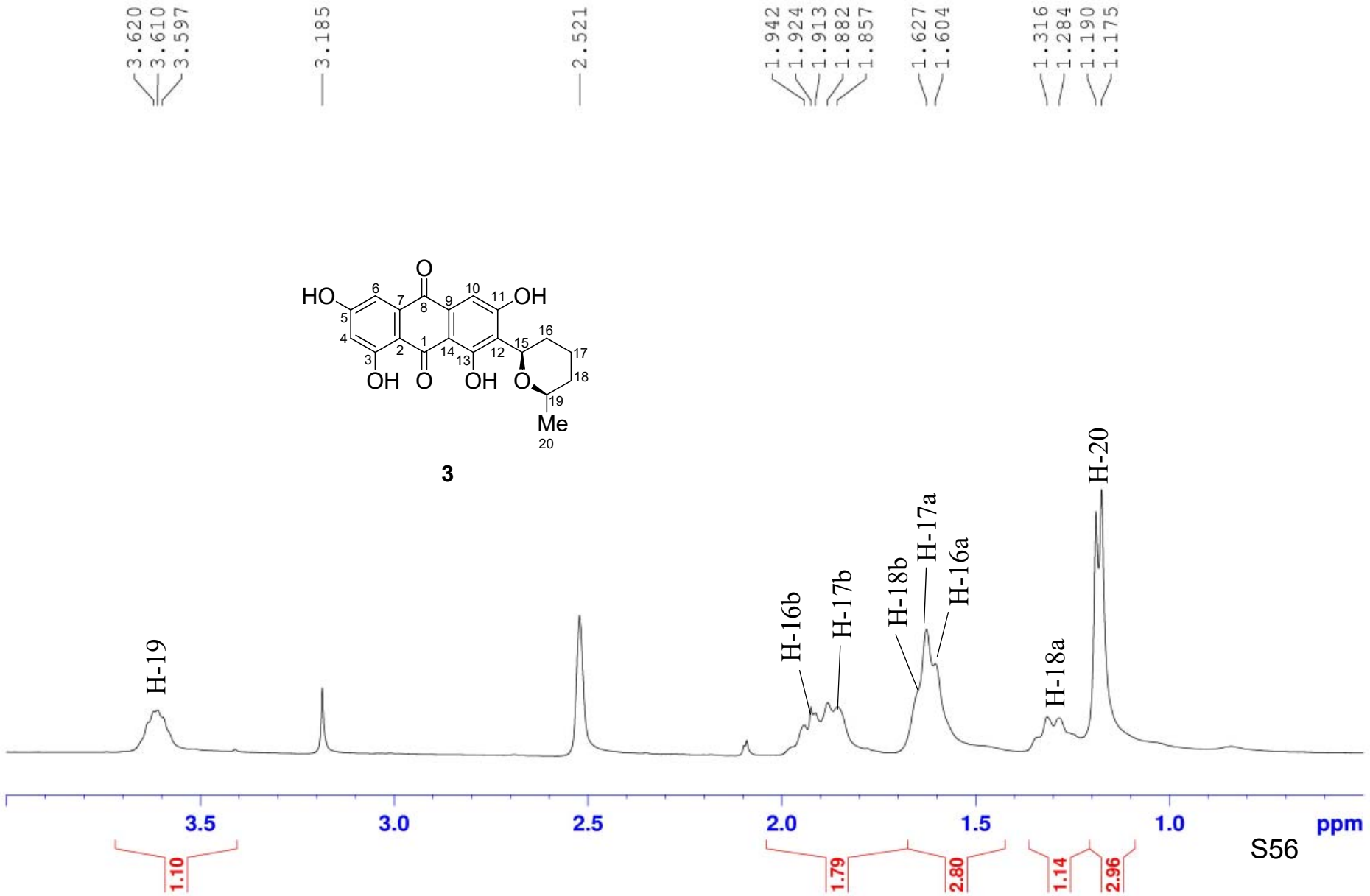
HR-ESIMS for **3**



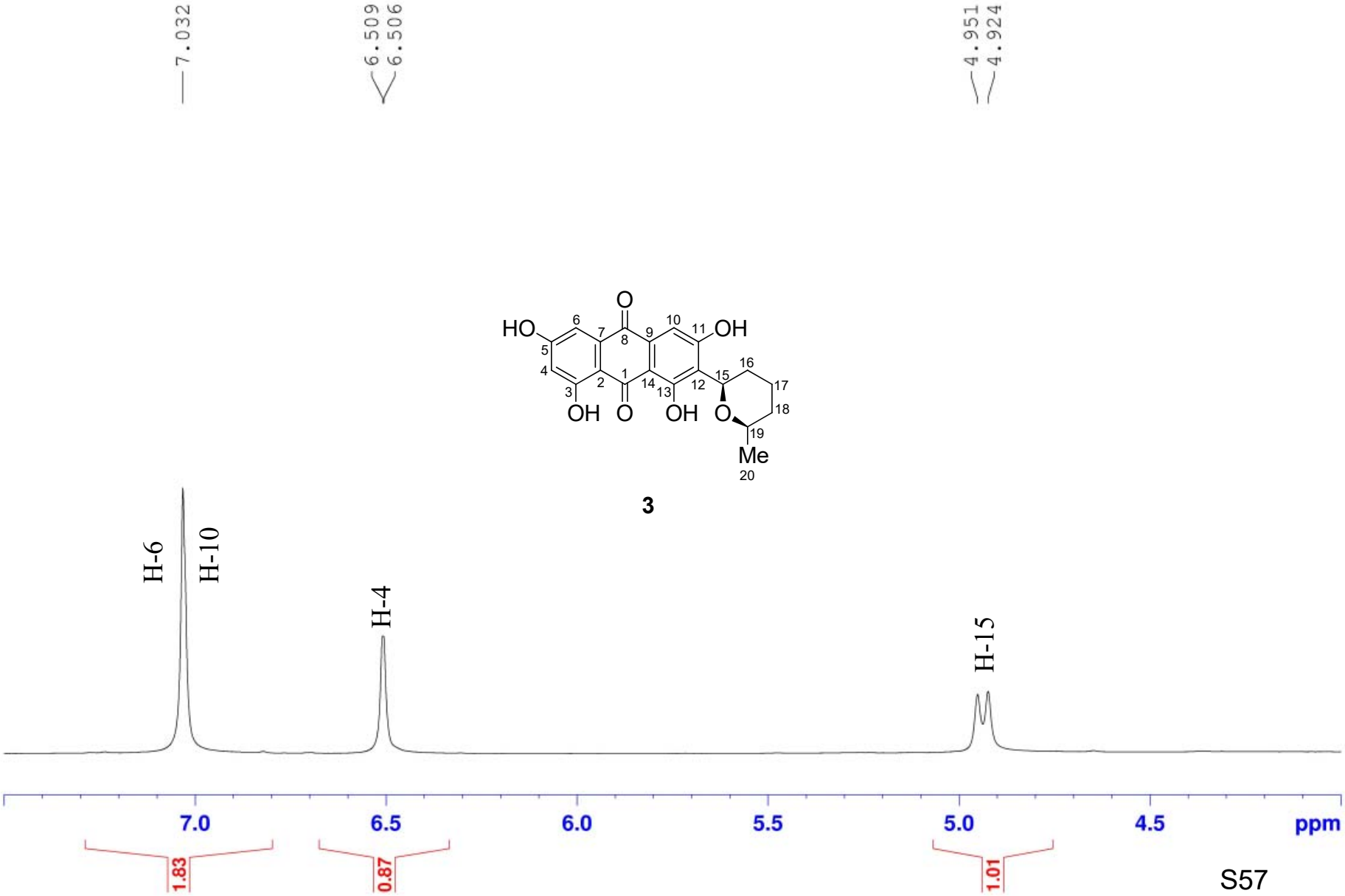
^{1}H (400 MHz) NMR spectrum of **3** in DMSO-d_6



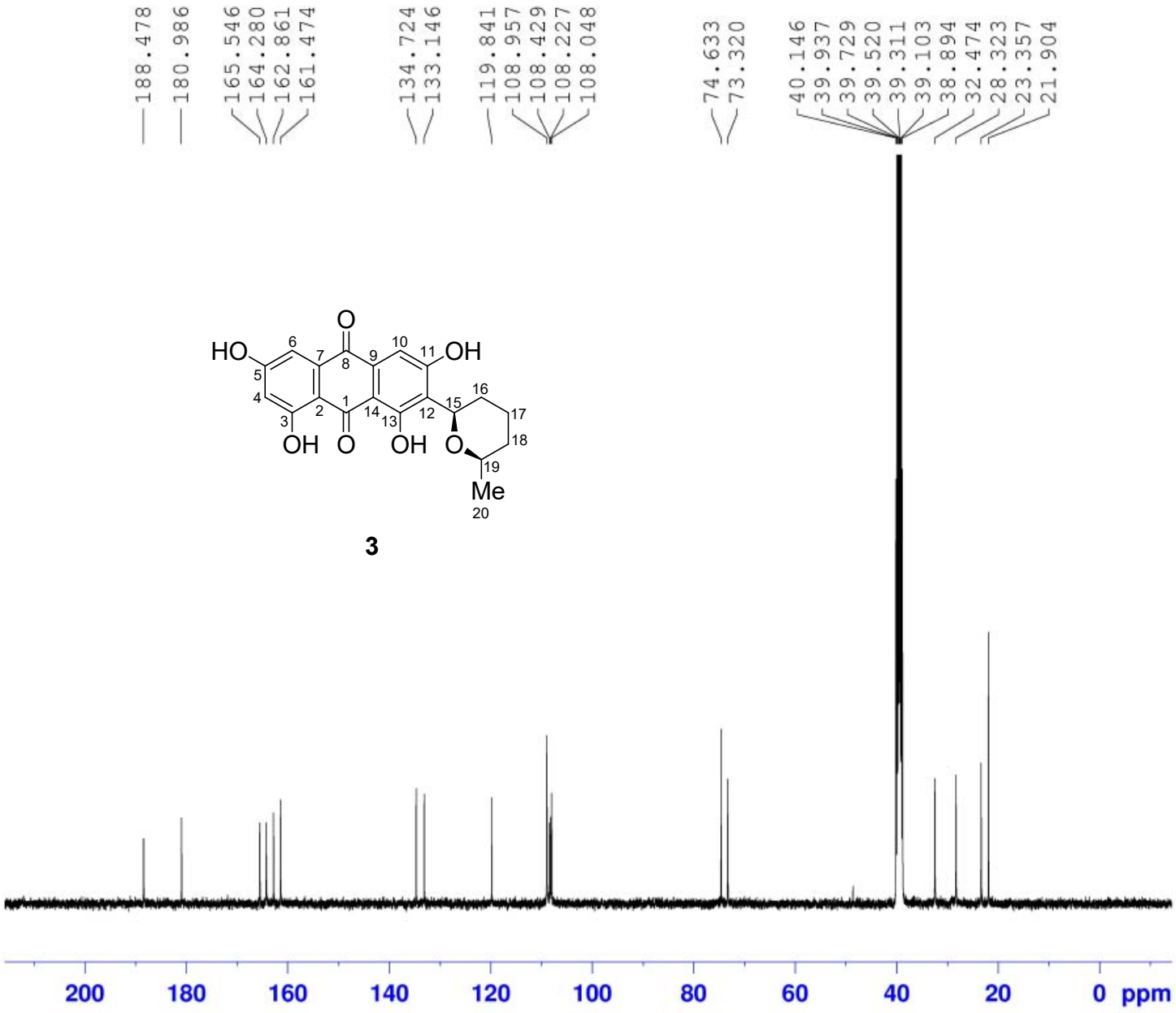
^{1}H (400 MHz) NMR spectrum of **3** in DMSO-d_6



^{1}H (400 MHz) NMR spectrum of **3** in DMSO-d_6



^{13}C (100 MHz) NMR spectrum of **3** in DMSO-d_6

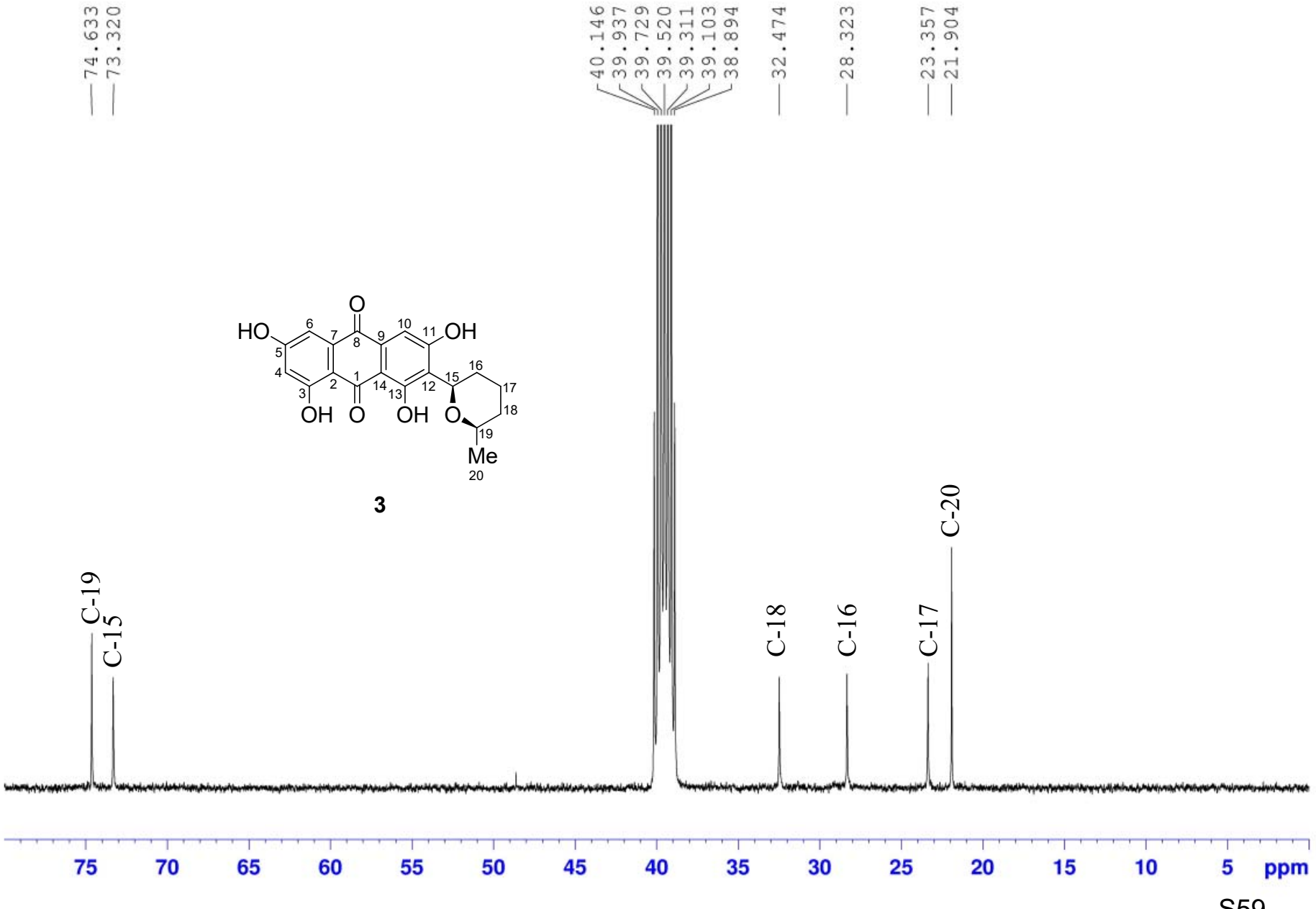


3

```
NAME          wbb-44-46-3-1
EXPNO                     2
PROCNO                    1
Date_              20230303
Time                   8.34
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                     195.9
DW                    20.800 usec
DE                     6.50 usec
TE                      0.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

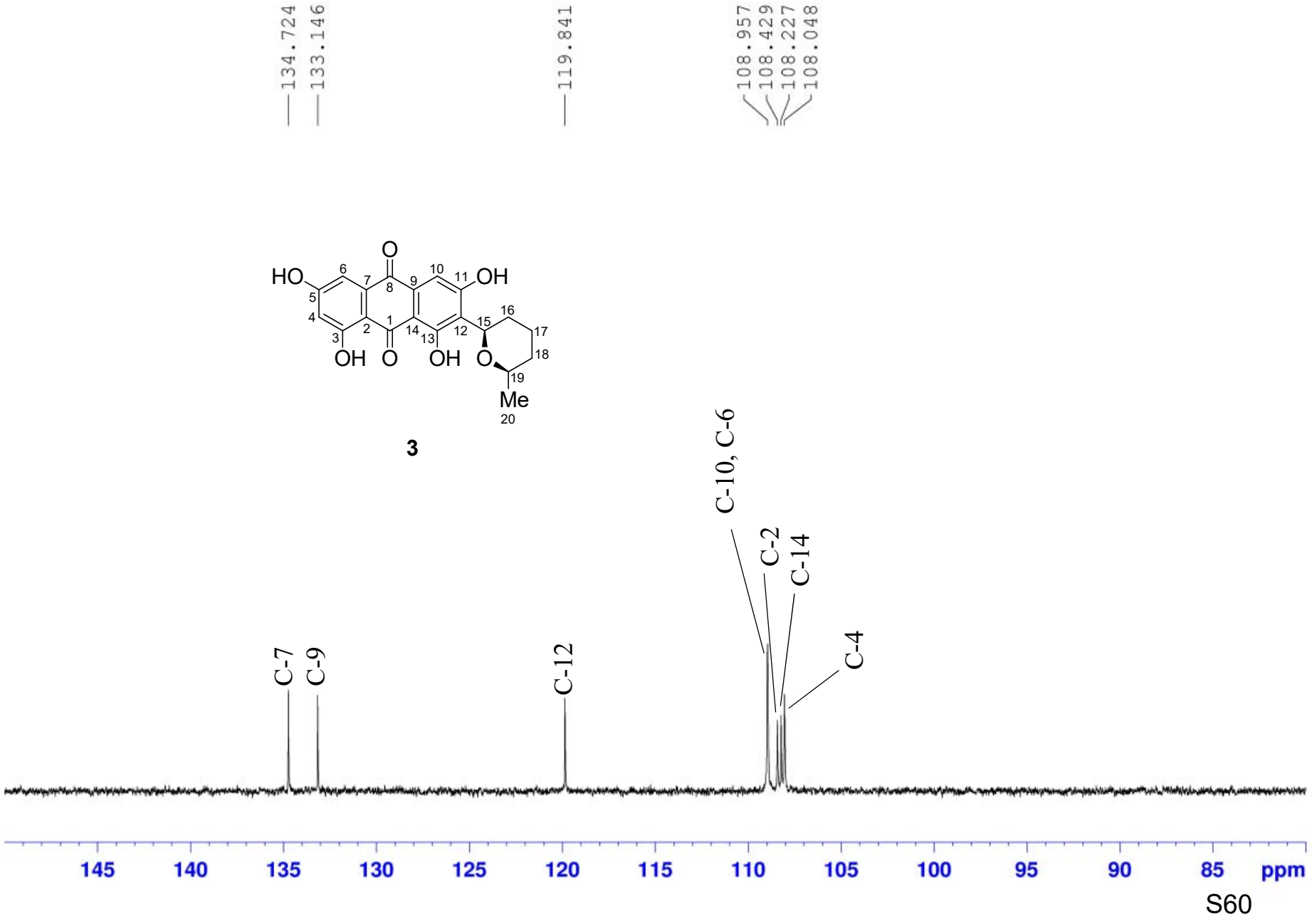
======== CHANNEL f1 ========
SFO1           100.6228293 MHz
NUC1                    13C
P1                    10.00 usec
SI                    32768
SF             100.6128123 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

^{13}C (100 MHz) NMR spectrum of **3** in DMSO-d_6

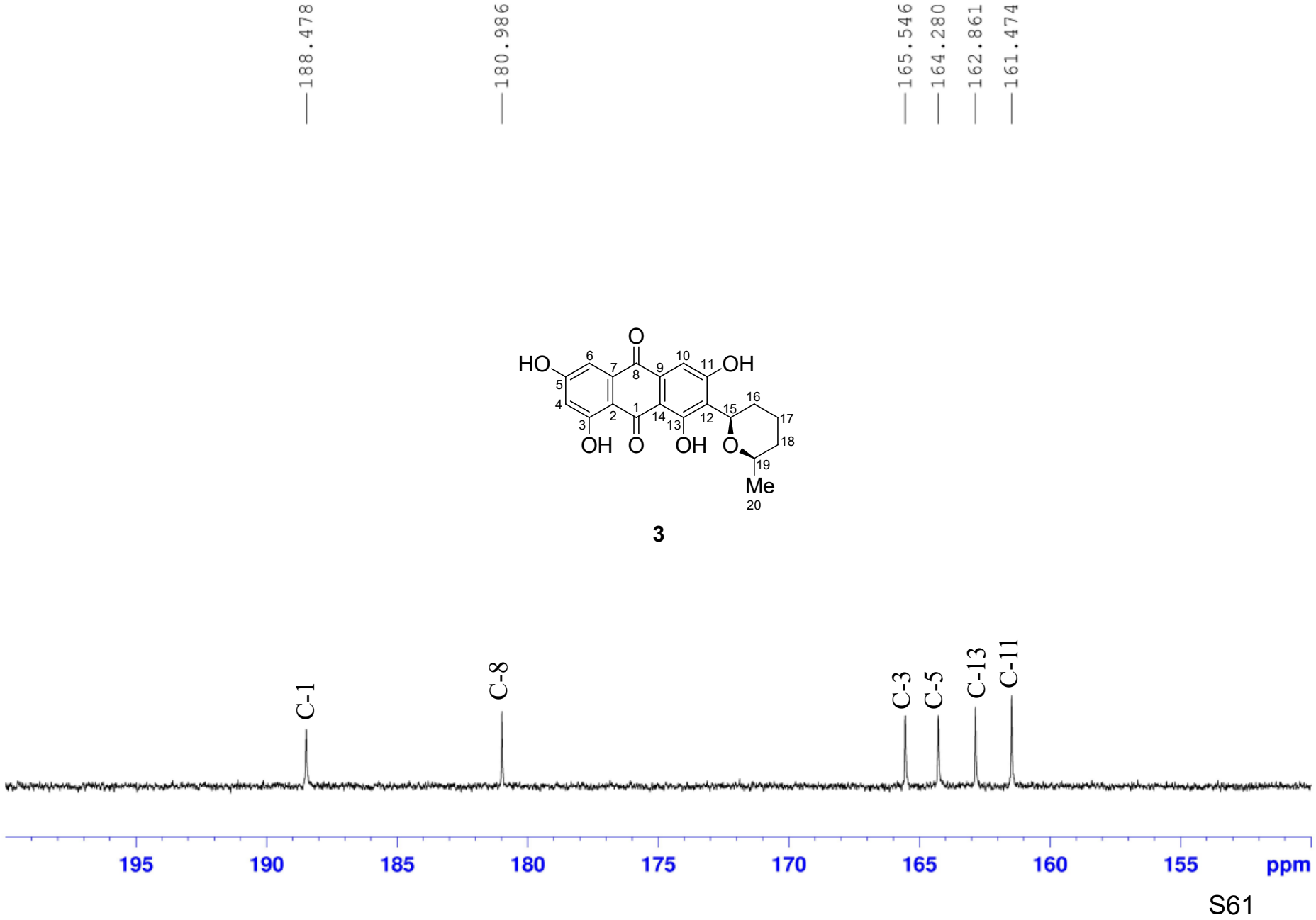


3

^{13}C (100 MHz) NMR spectrum of **3** in DMSO-d_6

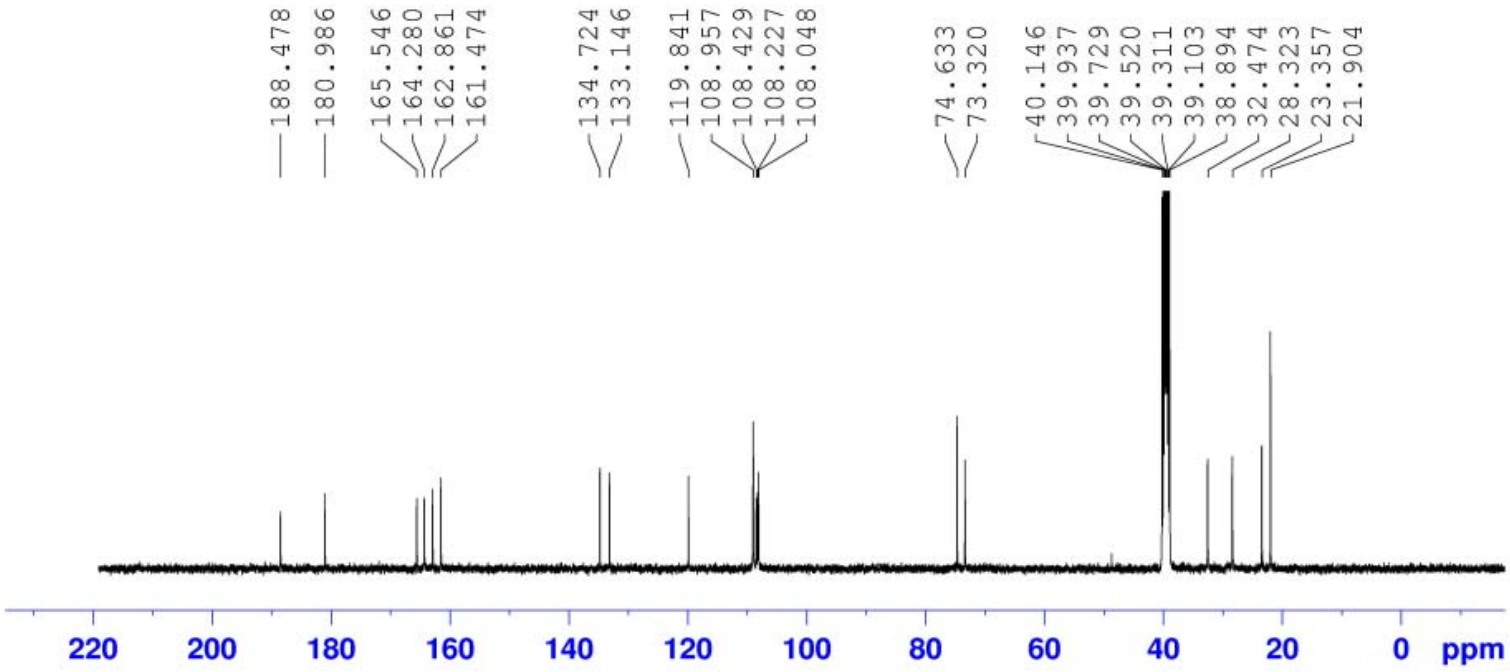


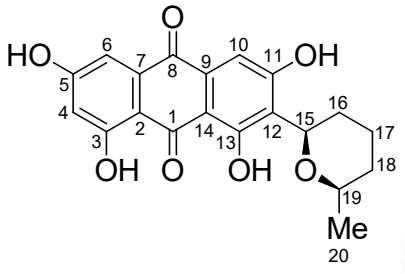
^{13}C (100 MHz) NMR spectrum of **3** in DMSO-d_6



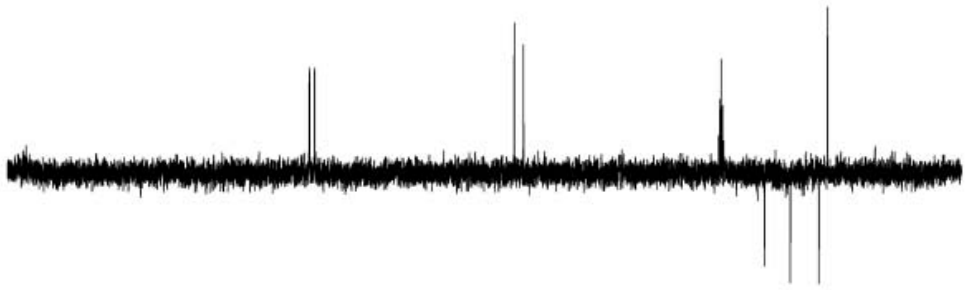
3

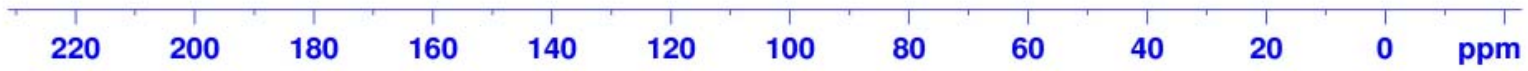
DEPT135 (100 MHz) spectrum of **3** in DMSO-d_6





3



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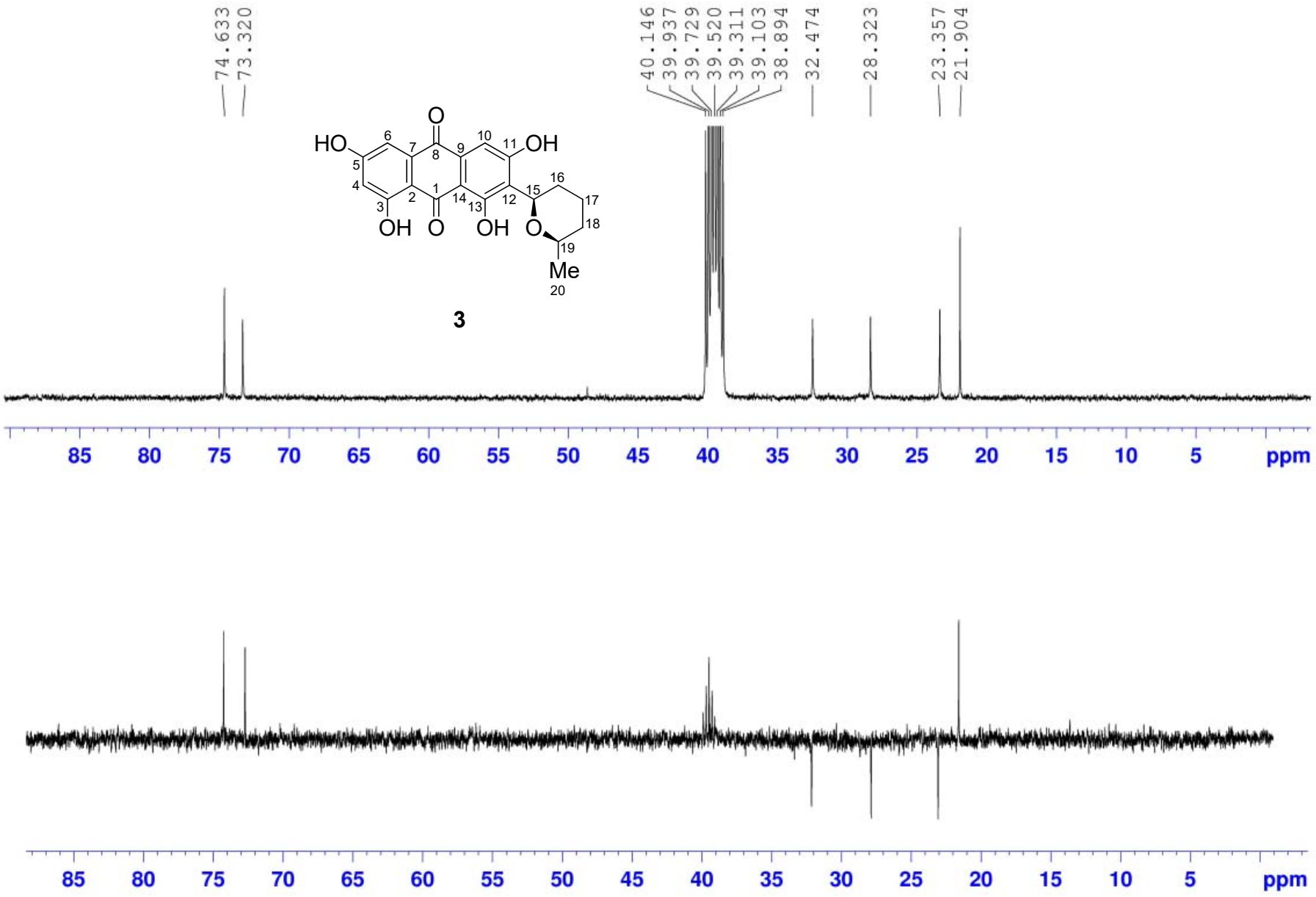
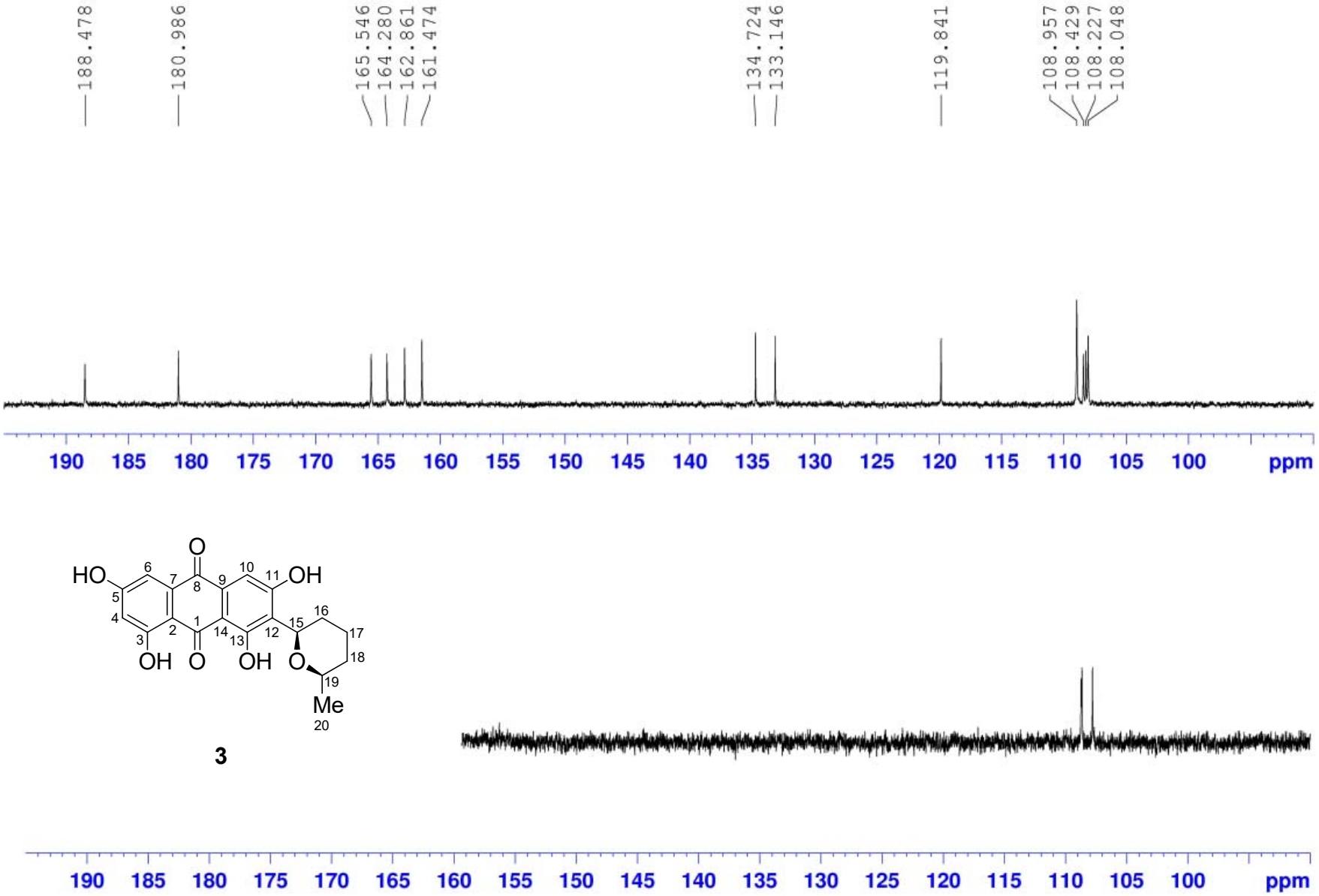
NAME        wbb-47-17-1-r
EXPNO                   6
PROCNO                  1
Date_            20210518
Time                4.37 h
INSTRUM             spect
PROBHD    Z108618_0231 (
PULPROG         deptsp135
TD                  65536
SOLVENT               DMSO
NS                    450
DS                      8
SWH             16129.032 Hz
FIDRES          0.492219 Hz
AQ              2.0316660 sec
RG                   2050
DW                 31.000 usec
DE                  6.50 usec
TE                 298.8 K
CNST2          145.0000000
D1               2.00000000 sec
D2               0.00344828 sec
D12              0.00002000 sec
TD0                     1
SFO1           100.6384205 MHz
NUC1                  13C
P1                  8.25 usec
P13              2000.00 usec
SI                   32768
SF             100.6303705 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

DEPT135 (100 MHz) spectrum of **3** in DMSO-d_6

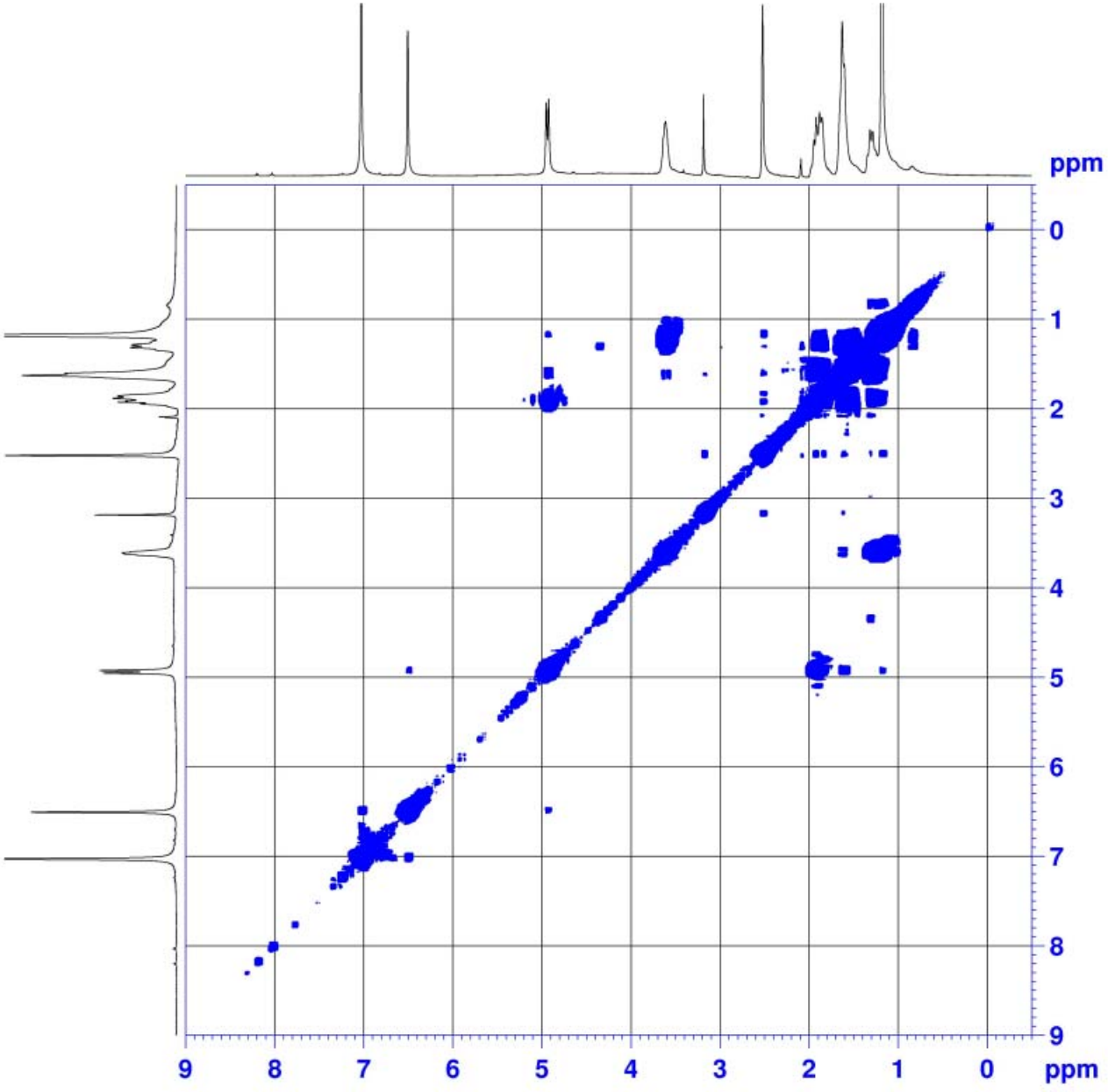


DEPT135 (100 MHz) spectrum of **3** in DMSO-d_6



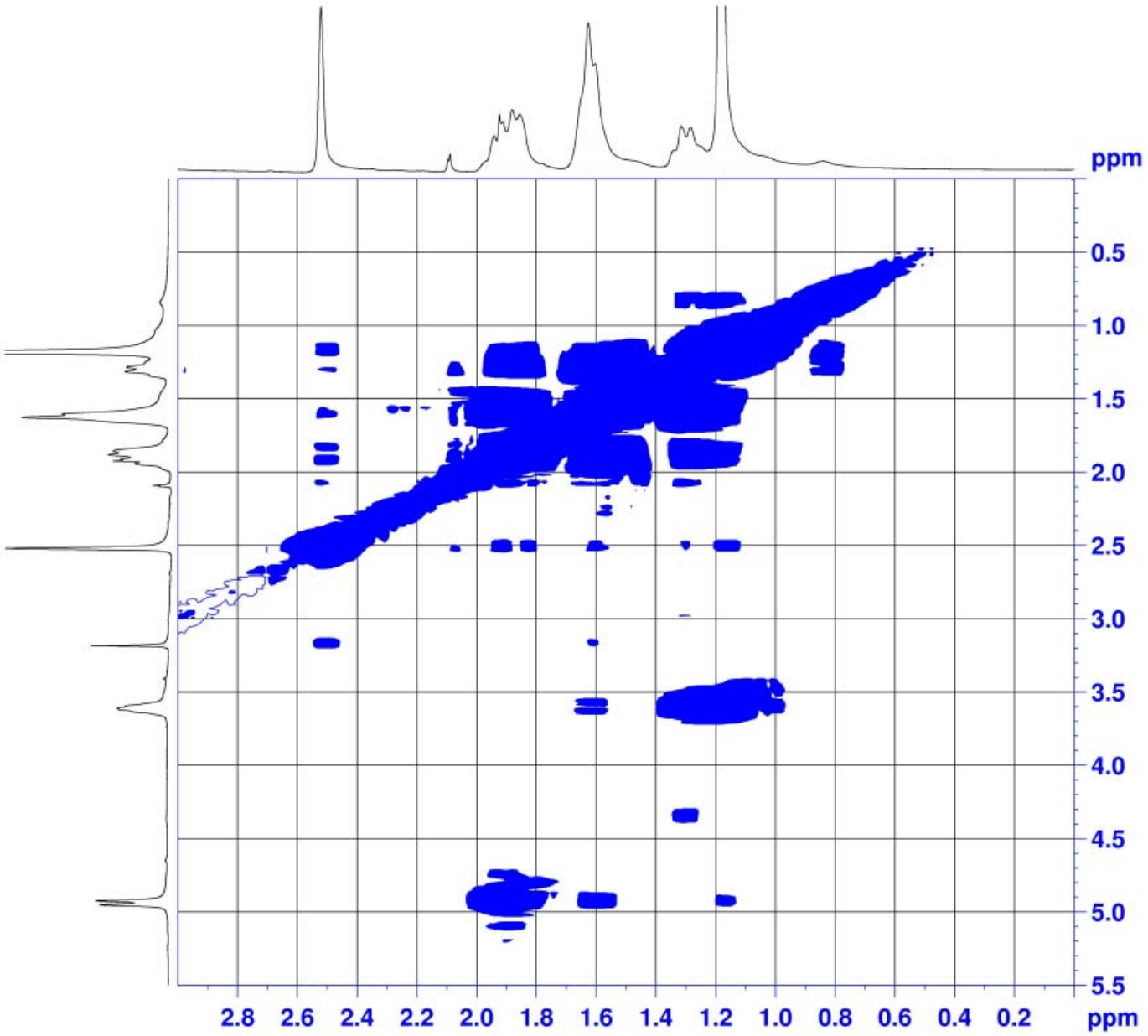
3

^{1}H–^{1}H COSY (400 MHz) spectrum of **3** in DMSO-d_6

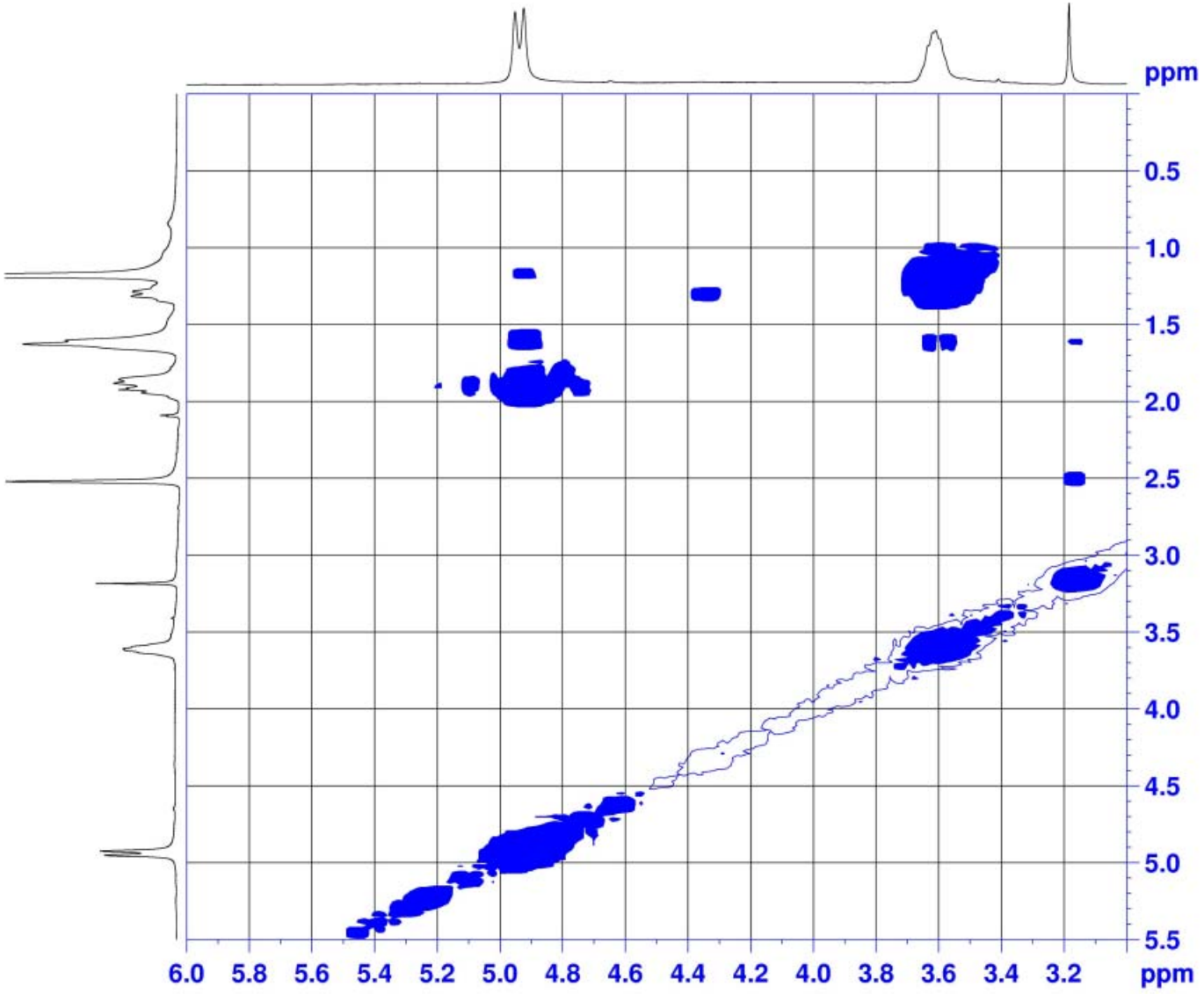


NAME	wbb-44-46-3-1
EXPNO	3
PROCNO	1
Date_	20230303
Time	9.26
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	cosygpppqf
TD	2048
SOLVENT	DMSO
NS	8
DS	8
SWH	6250.000 Hz
FIDRES	3.051758 Hz
AQ	0.1638900 sec
RG	25.73
DW	80.000 usec
DE	6.50 usec
TE	0.0 K
D0	0.00000300 sec
D1	2.02785301 sec
D11	0.03000000 sec
D12	0.00002000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00016000 sec
======== CHANNEL f1 ========	
SFO1	400.1327442 MHz
NUC1	1H
P0	10.00 usec
P1	10.00 usec
P17	2500.00 usec
ND0	1
TD	128
SFO1	400.1327 MHz
FIDRES	48.828125 Hz
SW	15.620 ppm
FnMODE	QF
SI	1024
SF	400.1300000 MHz
WDW	QSINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	400.1300000 MHz
WDW	QSINE
SSB	0
LB	0.00 Hz
GB	0

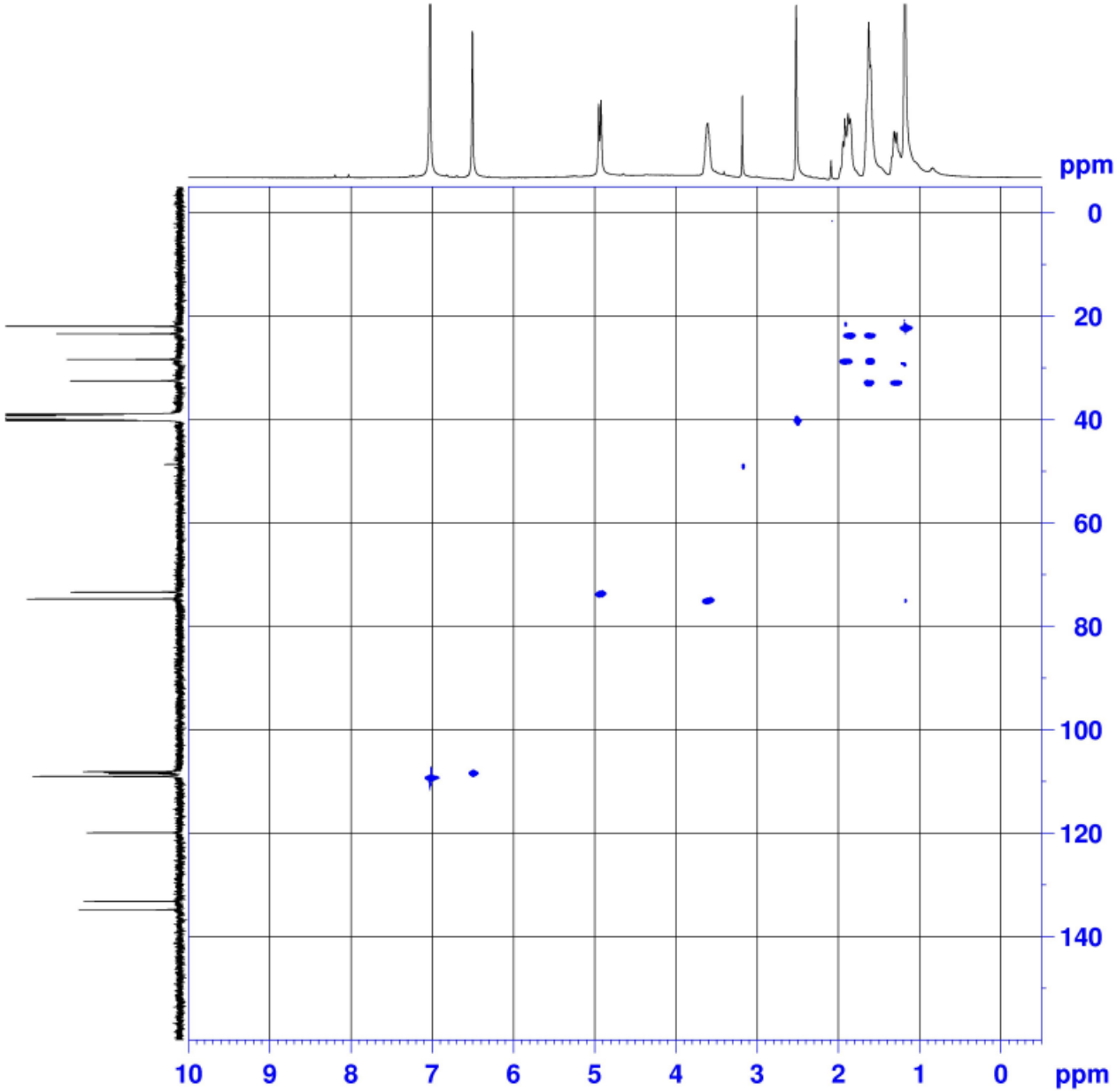
^{1}H–^{1}H COSY (400 MHz) spectrum of **3** in DMSO-d_6



^{1}H–^{1}H COSY (400 MHz) spectrum of **3** in DMSO-d_6



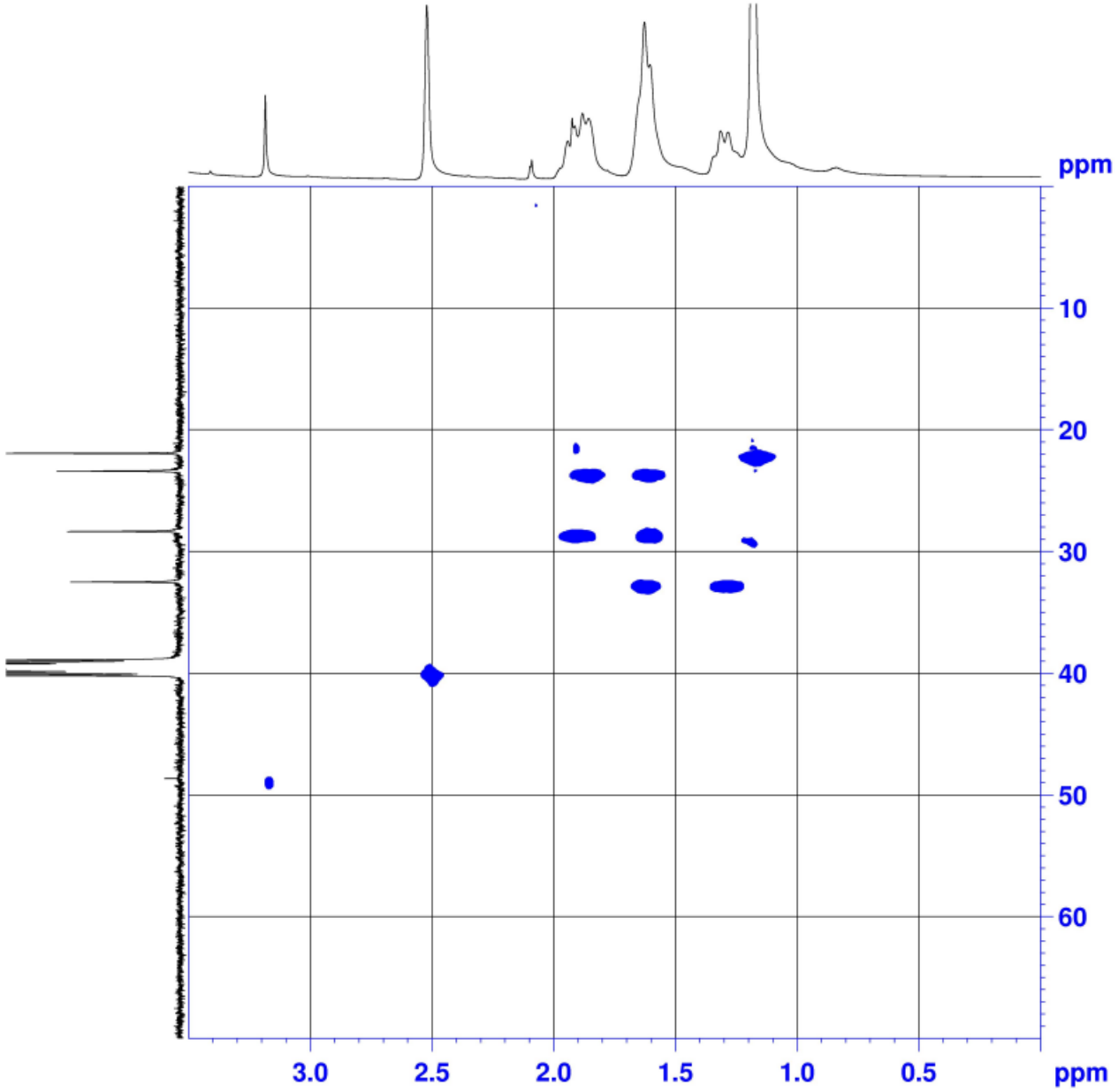
HSQC (400 MHz) spectrum of **3** in DMSO-d_6



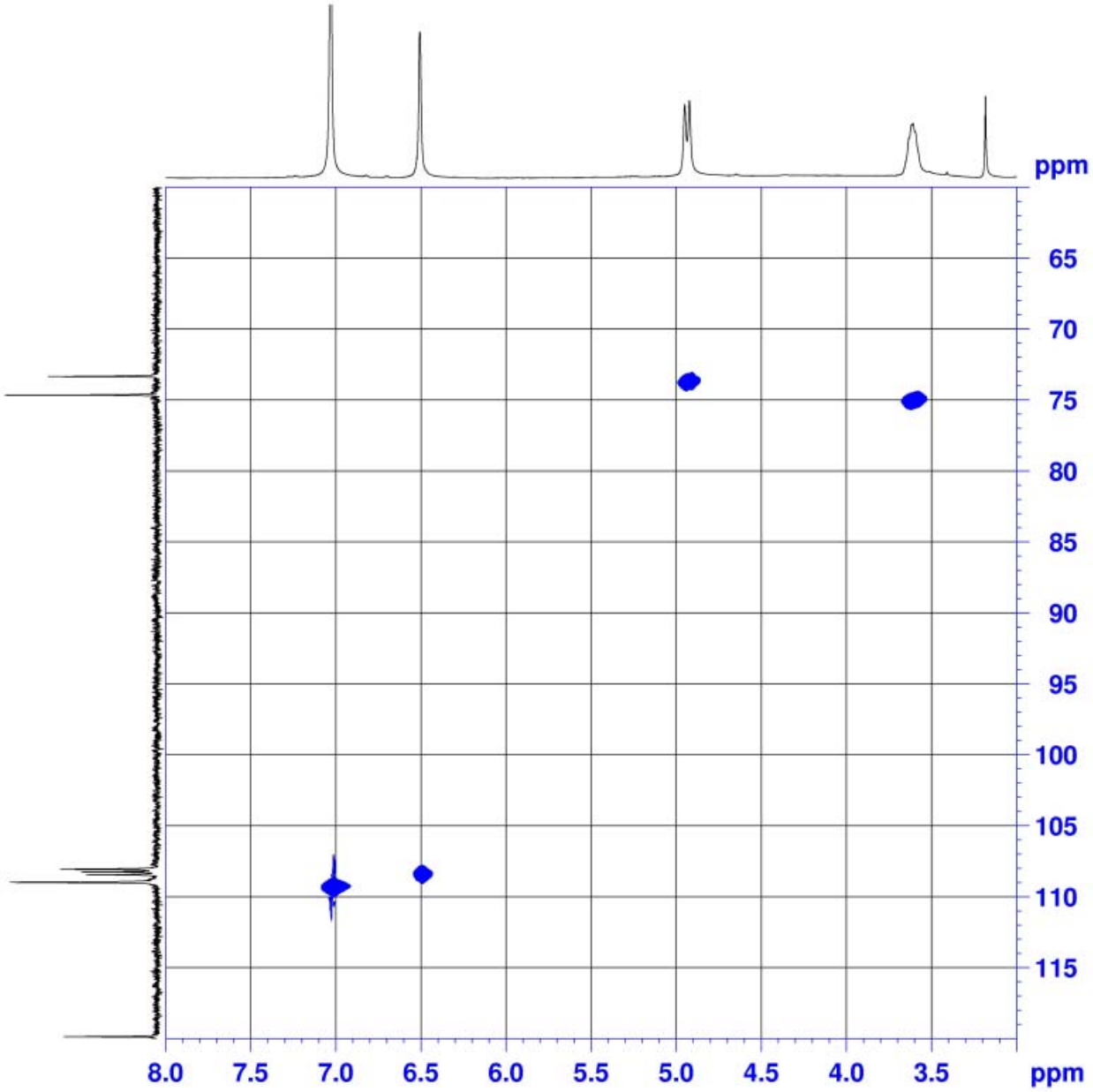

```
NAME        wbb-44-46-3-1
EXPNO                   5
PROCNO                  1
Date_            20230303
Time                10.40
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG   hsqcedetgpsisp2.3
TD                   2048
SOLVENT              DMSO
NS                      4
DS                     32
SWH             4795.396 Hz
FIDRES          2.341502 Hz
AQ             0.2135881 sec
RG                  195.9
DW                104.267 usec
DE                   6.50 usec
TE                    0.0 K
CNST2         145.0000000
CNST17         -0.5000000
D0            0.00000300 sec
D1            2.00000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D21           0.00360000 sec
D24           0.00089000 sec
IN0           0.00003010 sec

======== CHANNEL f1 ========
SFO1       400.1318806 MHz
NUC1                   1H
P1                  10.00 usec
P2                  20.00 usec
P28               1000.00 usec
ND0                    2
TD                   256
SFO1            100.6198 MHz
FIDRES          64.887871 Hz
SW                165.090 ppm
FnMODE     Echo-Antiecho
SI                  1024
SF         400.1300000 MHz
WDW                 QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
PC                  1.40
SI                  1024
MC2         echo-antiecho
SF           100.6127685 MHz
WDW                 QSINE
SSB                    2
LB                  0.00 Hz
GB                     0
```

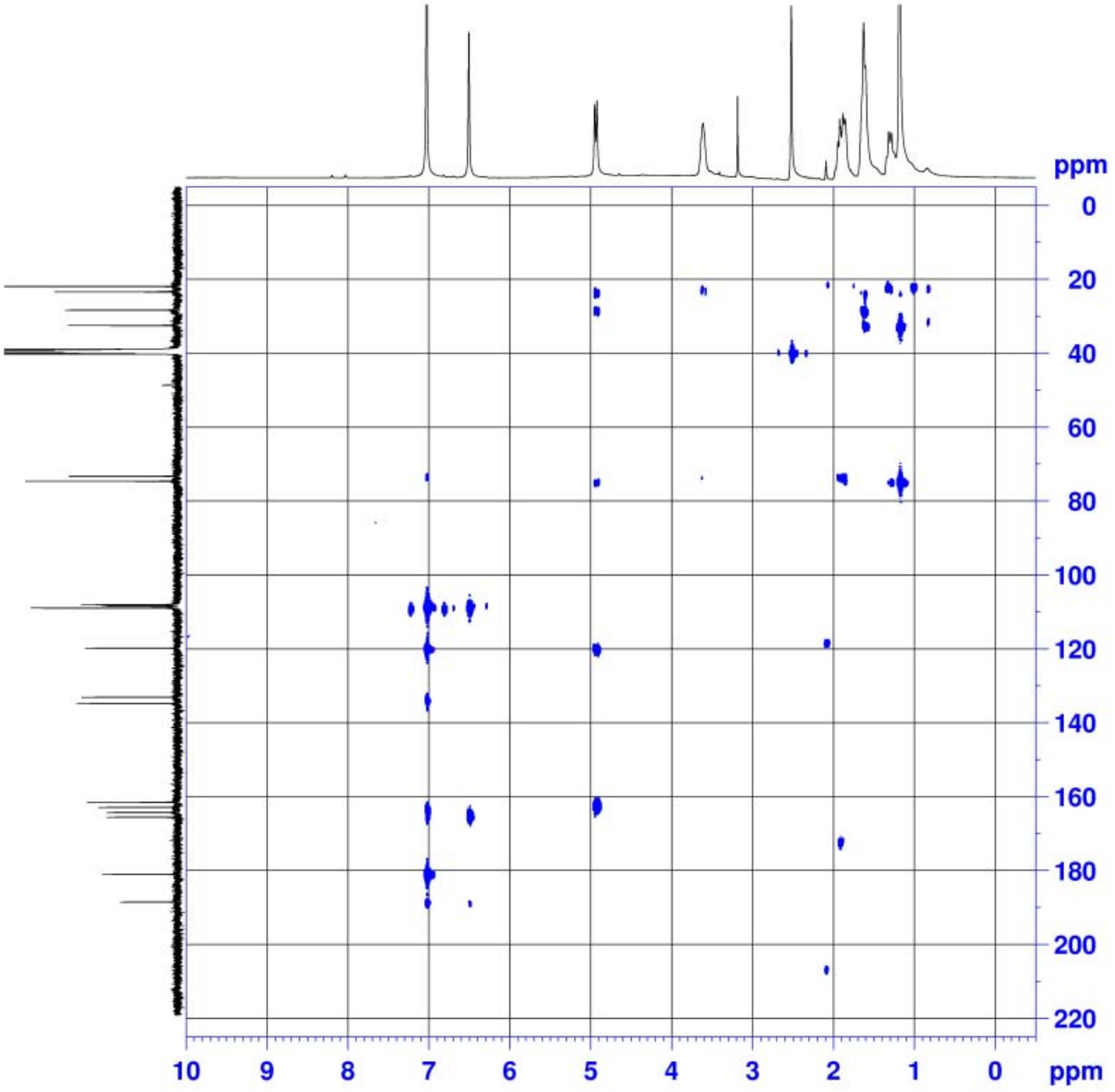
HSQC (400 MHz) spectrum of **3** in DMSO-d_6



HSQC (400 MHz) spectrum of **3** in DMSO-d_6



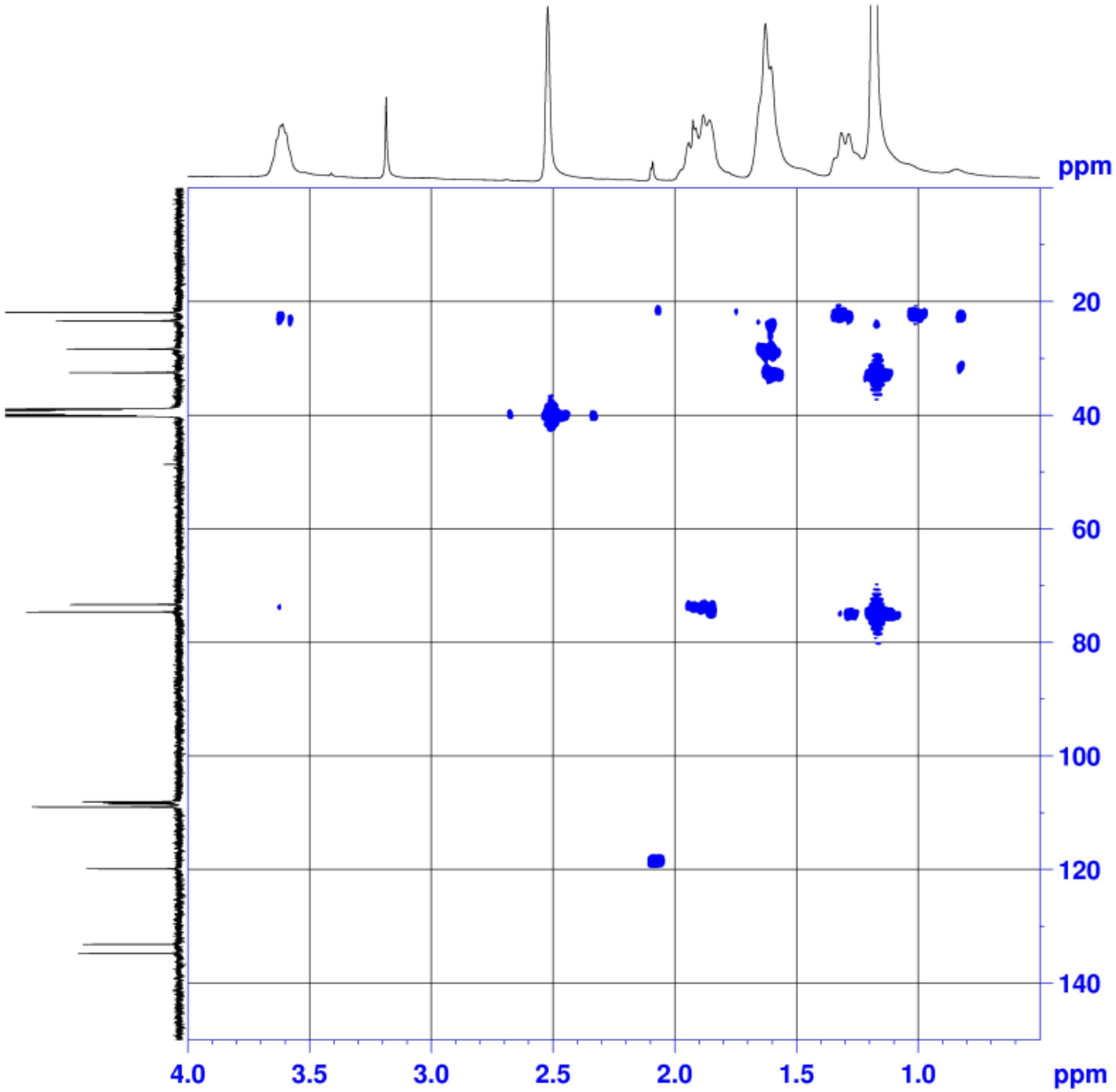
HMBC (400 MHz) spectrum of **3** in DMSO-d_6



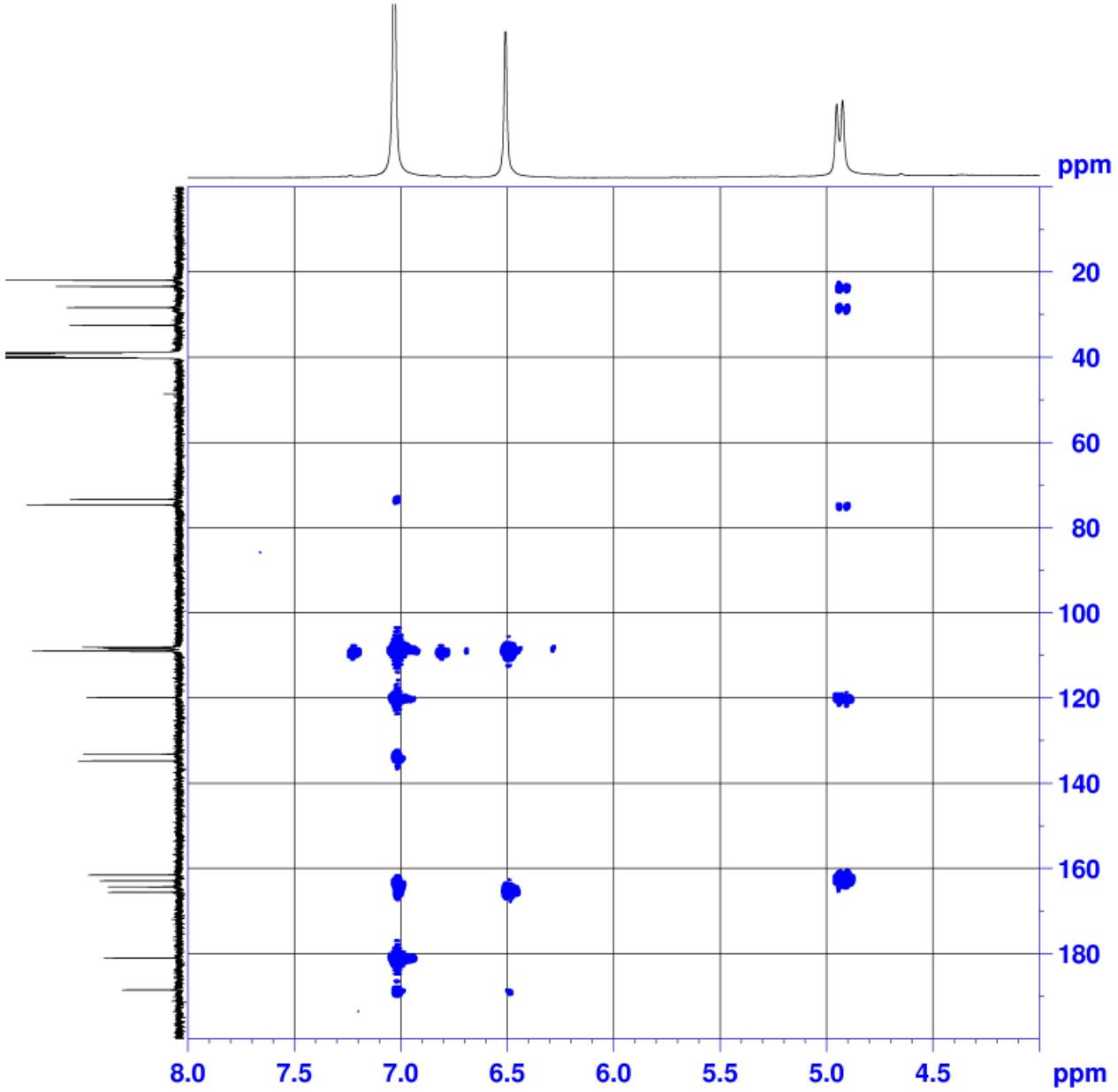

```
NAME          wbb-44-46-3-1
EXPNO                     4
PROCNO                    1
Date_              20230303
Time                 10.07
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG     hmbcgplpndqf
TD                     2048
SOLVENT                DMSO
NS                        8
DS                       16
SWH                6250.000 Hz
FIDRES                3.051758 Hz
AQ                 0.1638900 sec
RG                     195.9
DW                    80.000 usec
DE                     6.50 usec
TE                      0.0 K
CNST2              145.0000000
CNST13              10.0000000
D0                  0.00000300 sec
D1                  1.53317797 sec
D2                  0.00344828 sec
D6                  0.05000000 sec
D16                 0.00020000 sec
IN0                 0.00002240 sec

======== CHANNEL f1 ========
SFO1               400.1327442 MHz
NUC1                       1H
P1                      10.00 usec
P2                      20.00 usec
ND0                        2
TD                       128
SFO1                100.6228 MHz
FIDRES              174.386154 Hz
SW                   221.833 ppm
FnMODE                    QF
SI                       2048
SF                 400.1300000 MHz
WDW                     SINE
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.40
SI                      1024
MC2                       QF
SF                 100.6127685 MHz
WDW                     SINE
SSB                        0
LB                      0.00 Hz
GB                         0
```

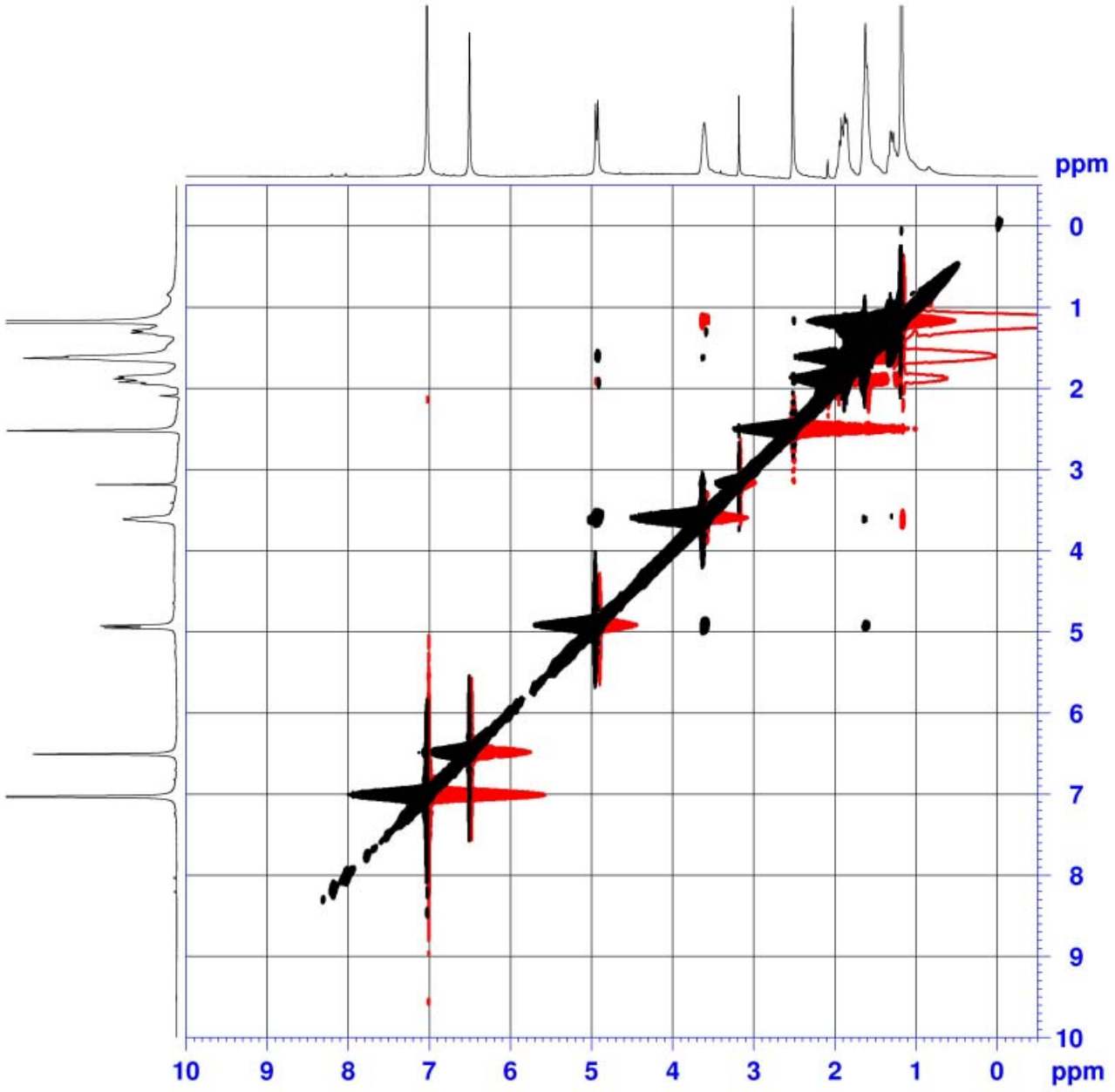
HMBC (400 MHz) spectrum of **3** in DMSO-d_6



HMBC (400 MHz) spectrum of **3** in DMSO-d_6

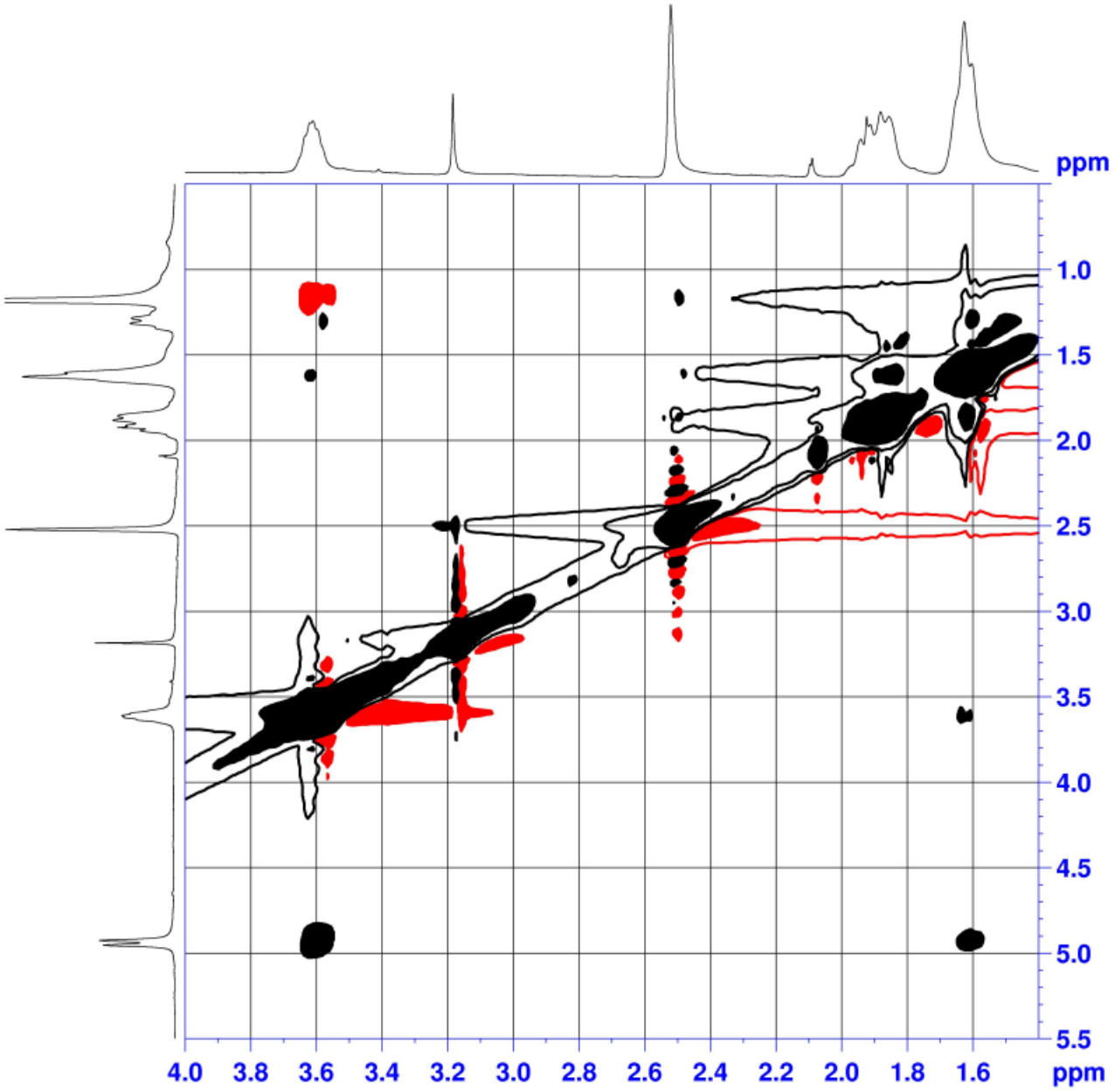


NOESY (400 MHz) spectrum of **3** in DMSO-d_6



NAME	wbb-44-46-3-1	
EXPNO	6	
PROCNO	1	
Date_	20230303	
Time	11.21	
INSTRUM	spect	
PROBHD	5 mm PABBO BB/	
PULPROG	noesygpphpp	
TD	2048	
SOLVENT	DMSO	
NS	4	
DS	32	
SWH	6172.839	Hz
FIDRES	3.014082	Hz
AQ	0.1659380	sec
RG	25.73	
DW	81.000	usec
DE	6.50	usec
TE	0.0	K
D0	0.00006827	sec
D1	2.09011102	sec
D8	0.30000001	sec
D11	0.03000000	sec
D12	0.00002000	sec
D16	0.00020000	sec
IN0	0.00016200	sec
========	CHANNEL f1 ========	
SFO1	400.1327617	MHz
NUC1	1H	
P1	10.00	usec
P2	20.00	usec
P17	2500.00	usec
ND0	1	
TD	256	
SFO1	400.1328	MHz
FIDRES	24.112654	Hz
SW	15.427	ppm
FnMODE	States-TPPI	
SI	1024	
SF	400.1300000	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	
PC	1.00	
SI	1024	
MC2	States-TPPI	
SF	400.1300000	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	

NOESY (400 MHz) spectrum of **3** in DMSO-d_6



HR-ESIMS for **4**

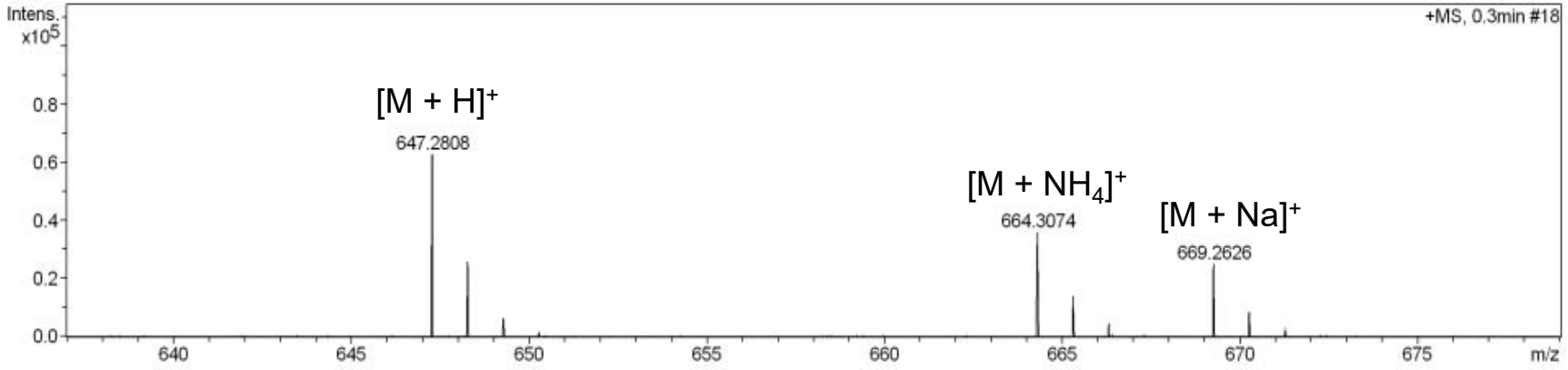
Mass Spectrum SmartFormula Report

Analysis Info

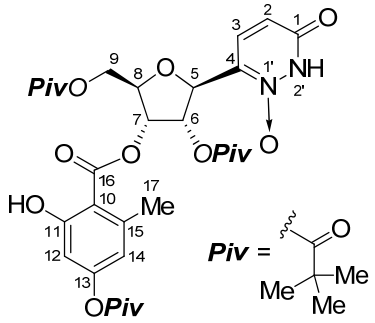
Analysis Name	D:\Data\MS\data\202110\wubinbin_WBB-145-D-R-6_pos_51_01_11733.d	Acquisition Date	10/27/2021 4:38:12 PM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	wubinbin_WBB-145-D-R-6_pos	Instrument	maXis 255552.00029
Comment			

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
647.2808	1	C32H43N2O12	100.00	647.2811	-0.4	-0.2	26.3	12.5	even	ok
669.2626	1	C32H42N2NaO12	100.00	669.2630	-0.6	-0.4	14.4	12.5	even	ok



4

wubinbin_WBB-145-D-R-6_pos_51_01_11733.d

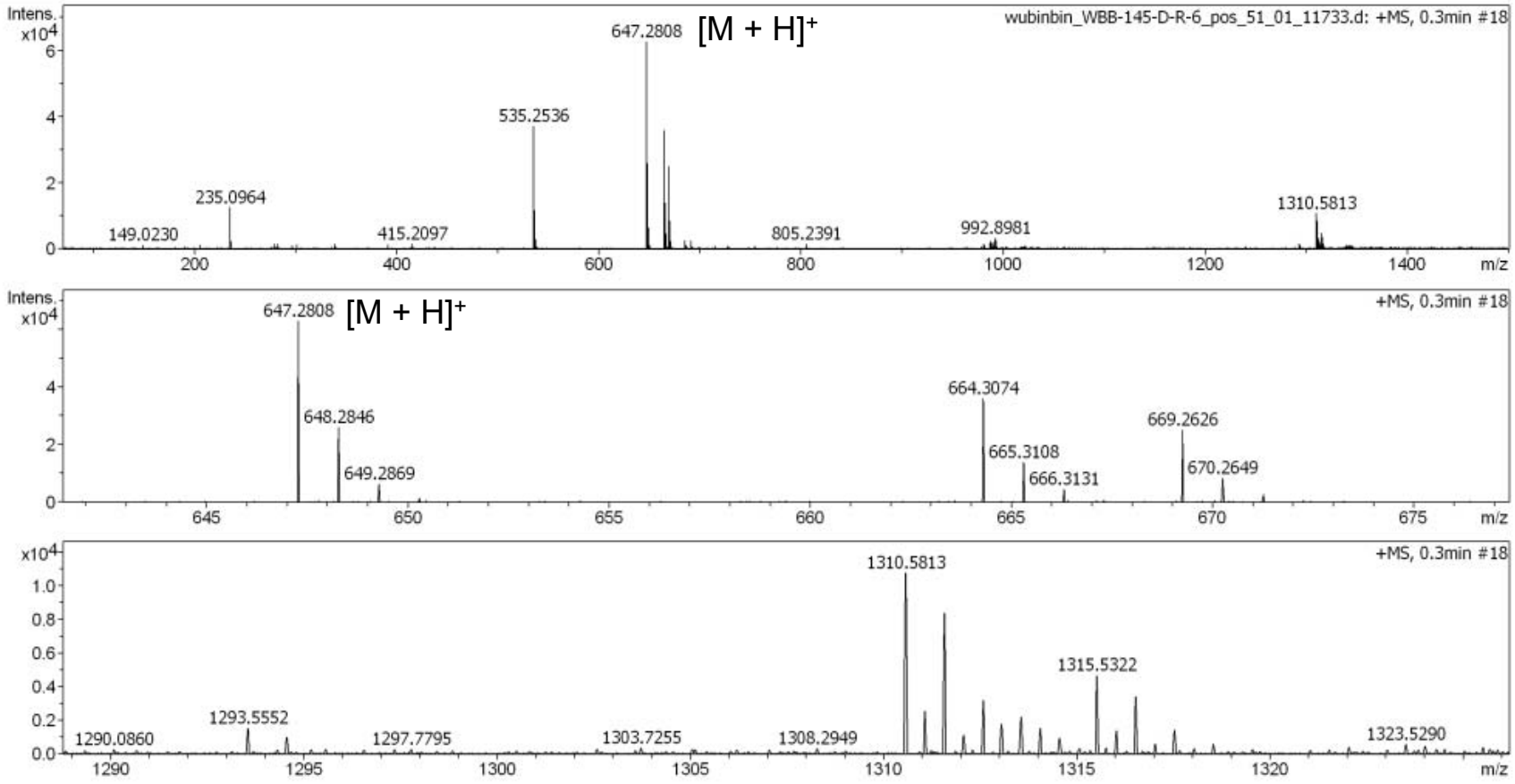
Bruker Compass DataAnalysis 4.1 printed: 10/27/2021 4:45:18 PM by: SCSIO Page 1 of 1

HR-ESIMS for **4**

Generic Display Report

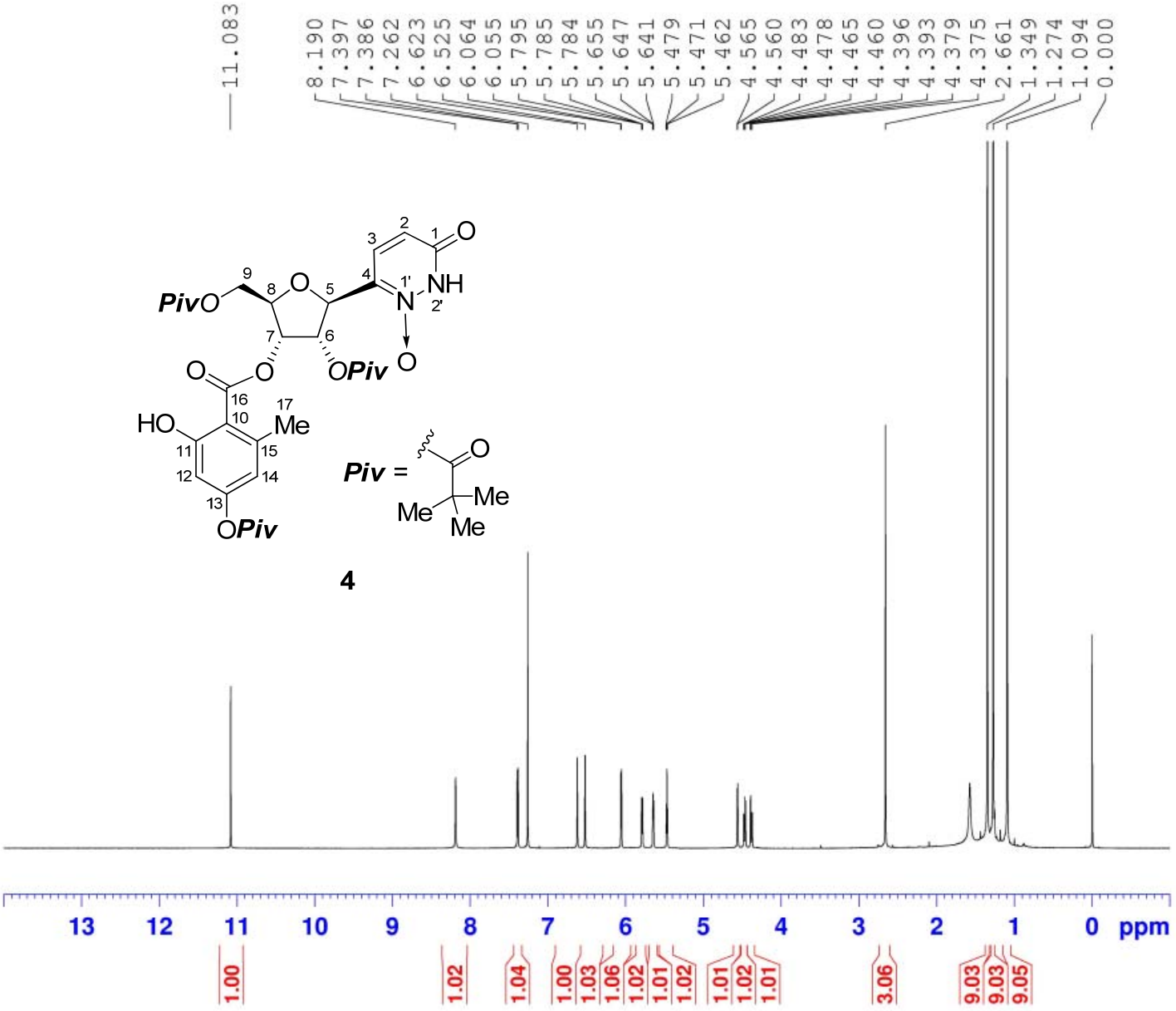
Analysis Info

Analysis Name	D:\Data\MS\data\202110\wubinbin_WBB-145-D-R-6_pos_51_01_11733.d	Acquisition Date	10/27/2021 4:38:12 PM
Method	LC_Direct Infusion_pos_70-500mz.m	Operator	SCSIO
Sample Name	wubinbin_WBB-145-D-R-6_pos	Instrument	maXis
Comment			



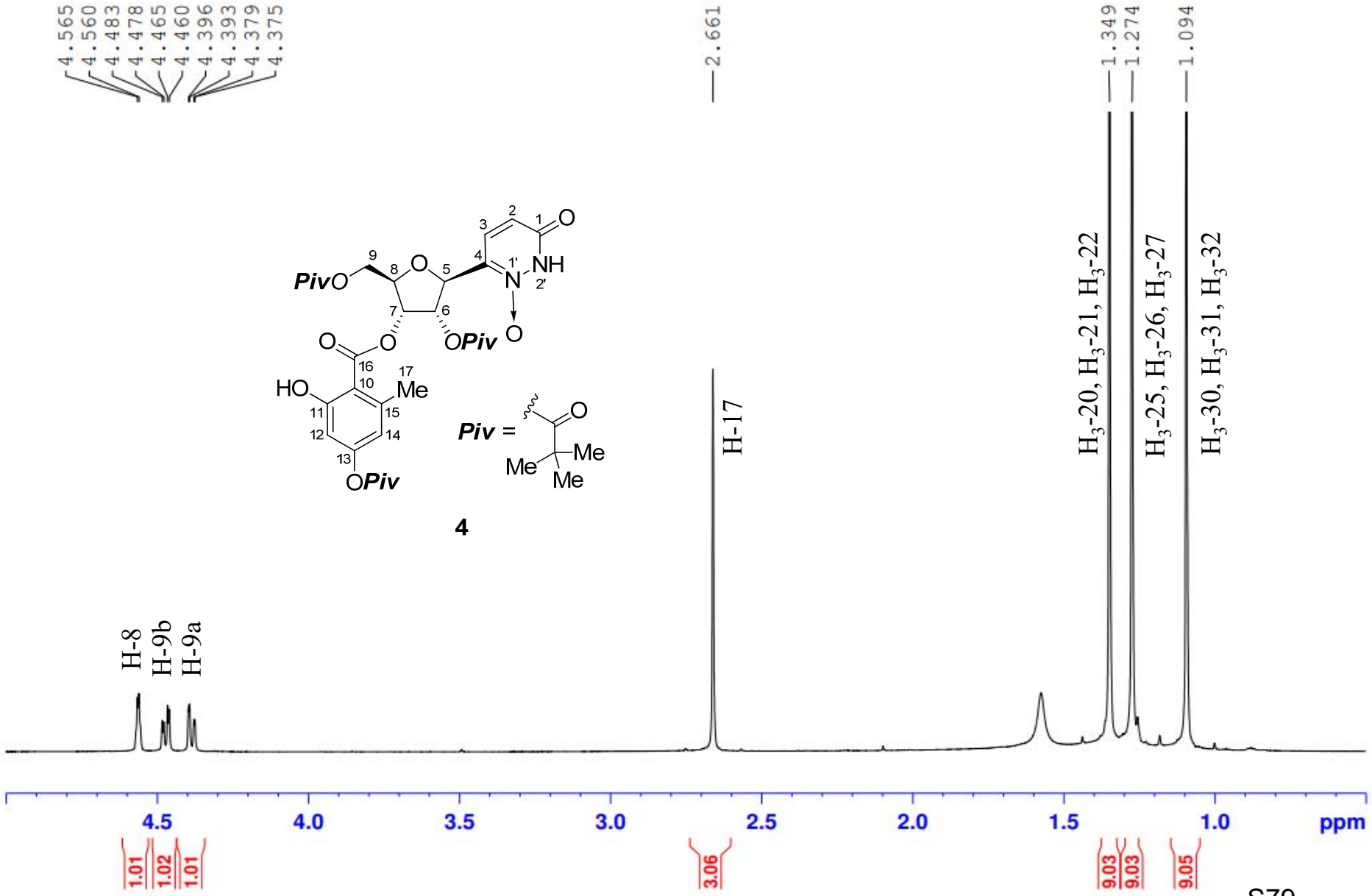
Bruker Compass DataAnalysis 4.1 printed: 10/27/2021 4:45:56 PM by: SCSIO Page 1 of 1

^{1}H (700 MHz) NMR spectrum of **4** in $CDCl_3$

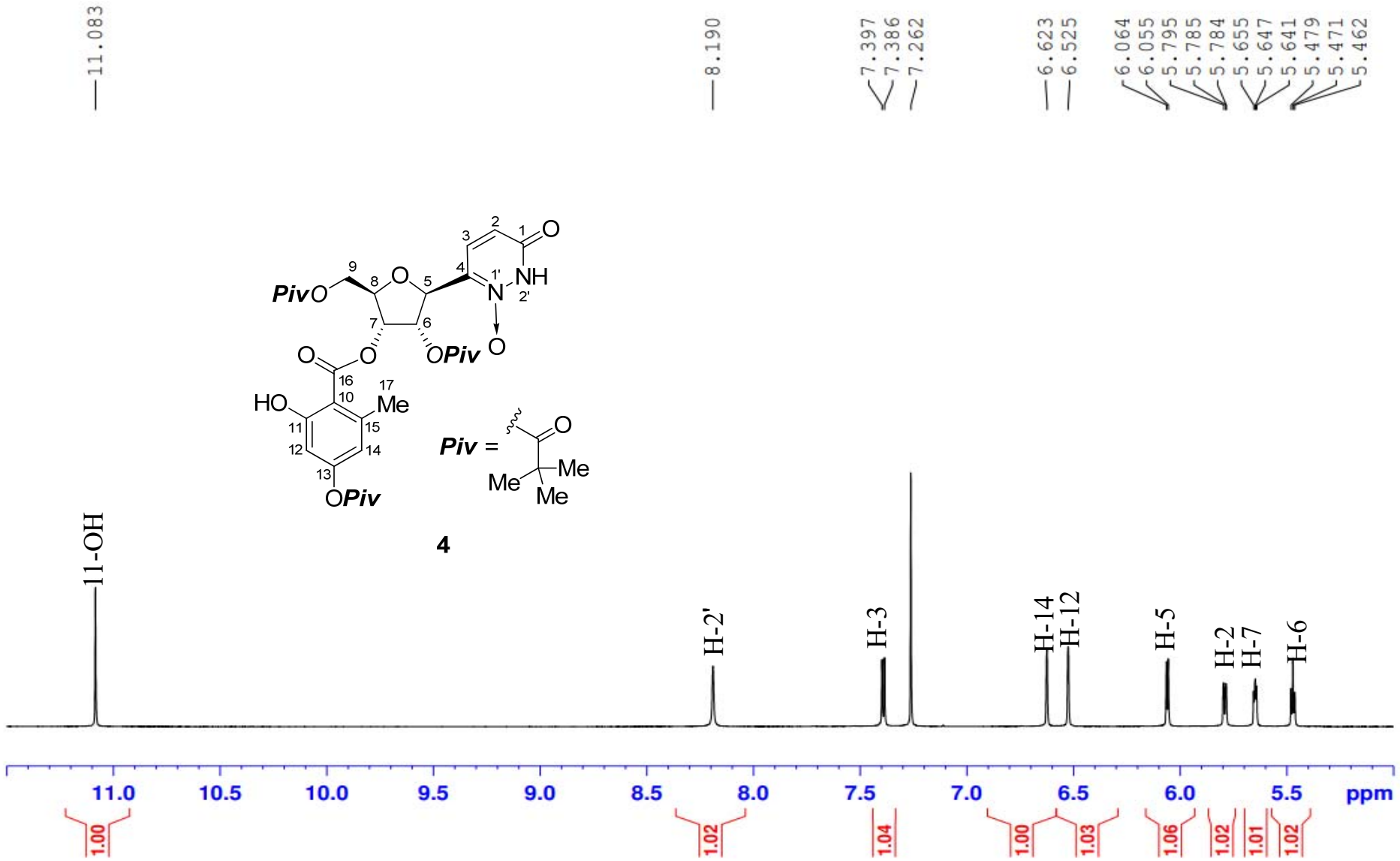



```
NAME        wubinbin-145D-R-6-1
EXPNO                        23
PROCNO                        1
Date_                  20211031
Time                      15.25 h
INSTRUM                   spect
PROBHD    Z120187_0028 (
PULPROG                   zg30
TD                       65536
SOLVENT                  CDCl3
NS                          16
DS                           2
SWH                  14097.744 Hz
FIDRES               0.430229 Hz
AQ                   2.3243935 sec
RG                        4.87
DW                      35.467 usec
DE                      10.00 usec
TE                      298.0 K
D1                   1.00000000 sec
TD0                           1
SFO1               700.1849013 MHz
NUC1                         1H
P0                       2.52 usec
P1                       7.55 usec
SI                       65536
SF                 700.1800162 MHz
WDW                          EM
SSB                           0
LB                       0.30 Hz
GB                            0
PC                        1.00
```

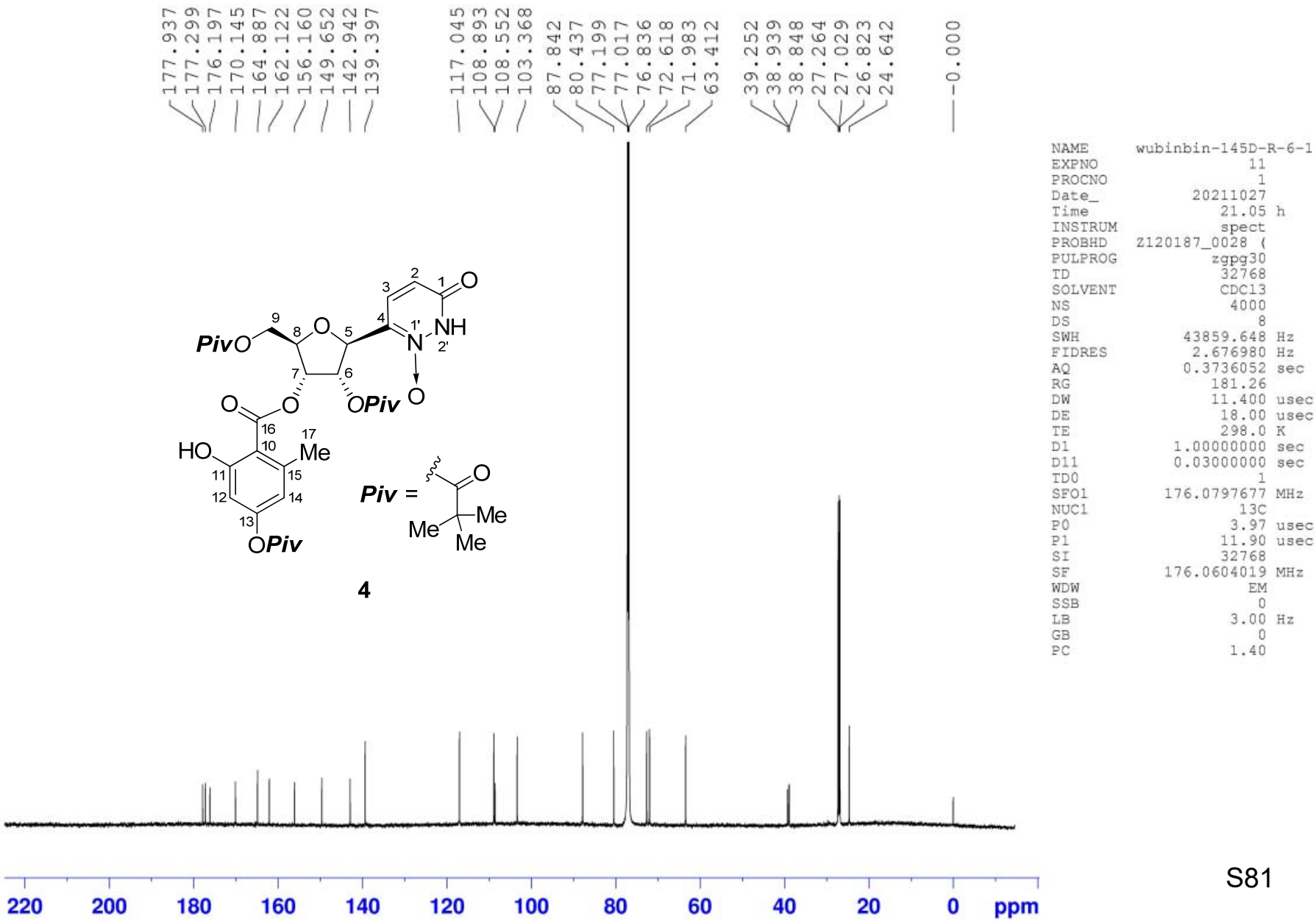
^{1}H (700 MHz) NMR spectrum of **4** in $CDCl_3$



^{1}H (700 MHz) NMR spectrum of **4** in $CDCl_3$

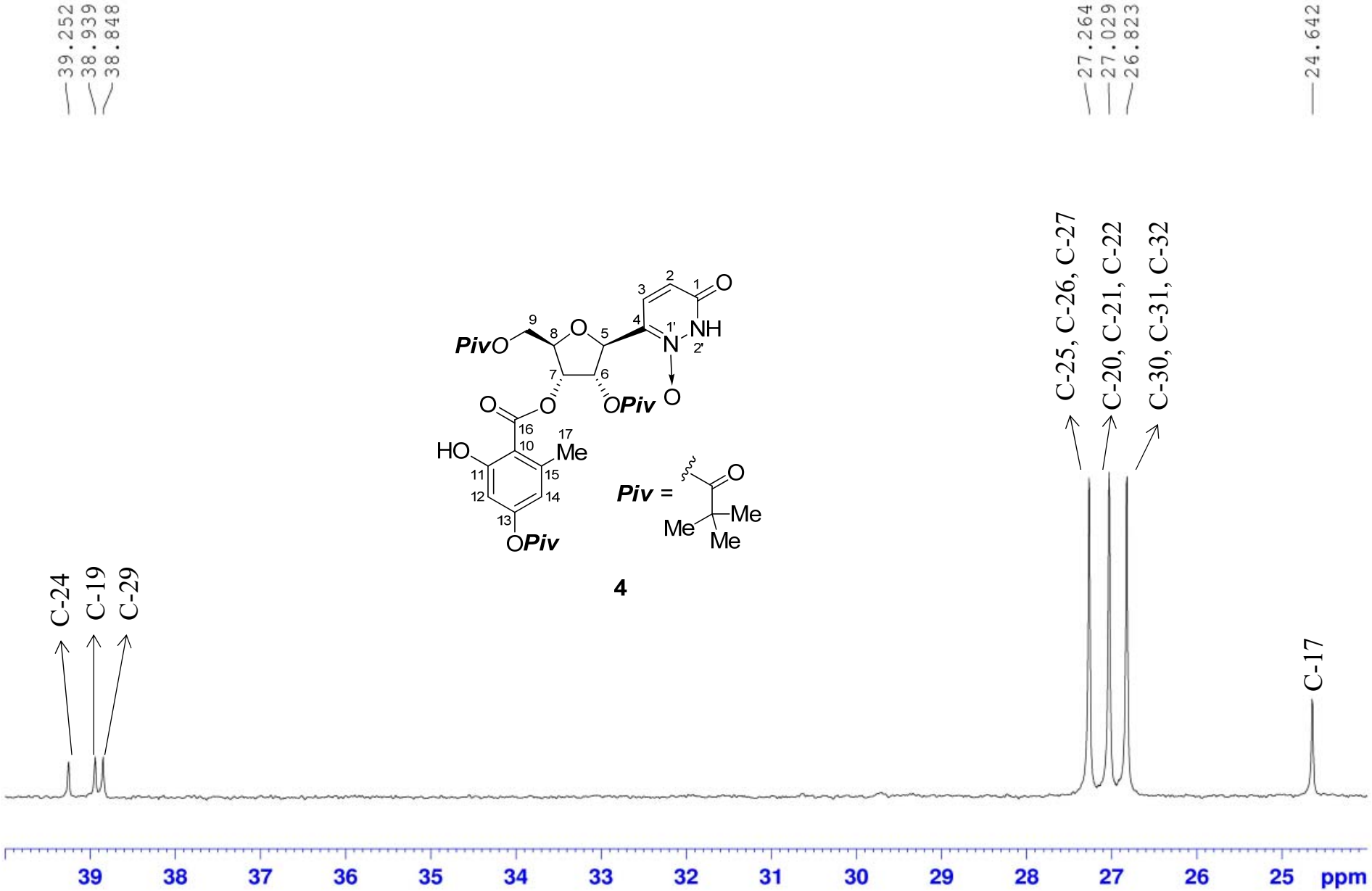


^{13}C (175 MHz) NMR spectrum of **4** in $CDCl_3$



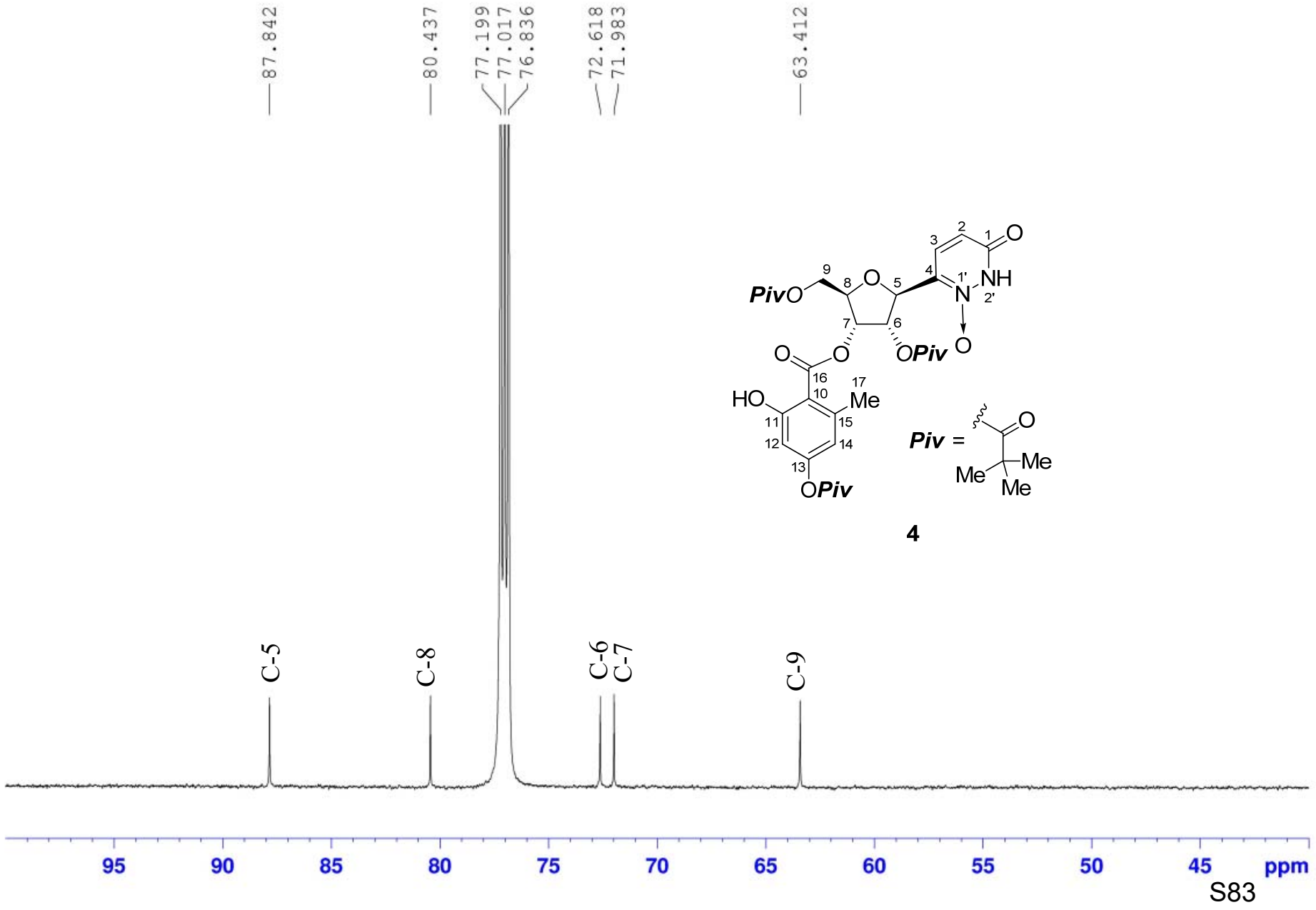
NAME	wubinbin-145D-R-6-1
EXPNO	11
PROCNO	1
Date_	20211027
Time	21.05 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	zgpg30
TD	32768
SOLVENT	CDC13
NS	4000
DS	8
SWH	43859.648 Hz
FIDRES	2.676980 Hz
AQ	0.3736052 sec
RG	181.26
DW	11.400 usec
DE	18.00 usec
TE	298.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	176.0797677 MHz
NUC1	13C
P0	3.97 usec
P1	11.90 usec
SI	32768
SF	176.0604019 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.40

^{13}C (175 MHz) NMR spectrum of **4** in $CDCl_3$



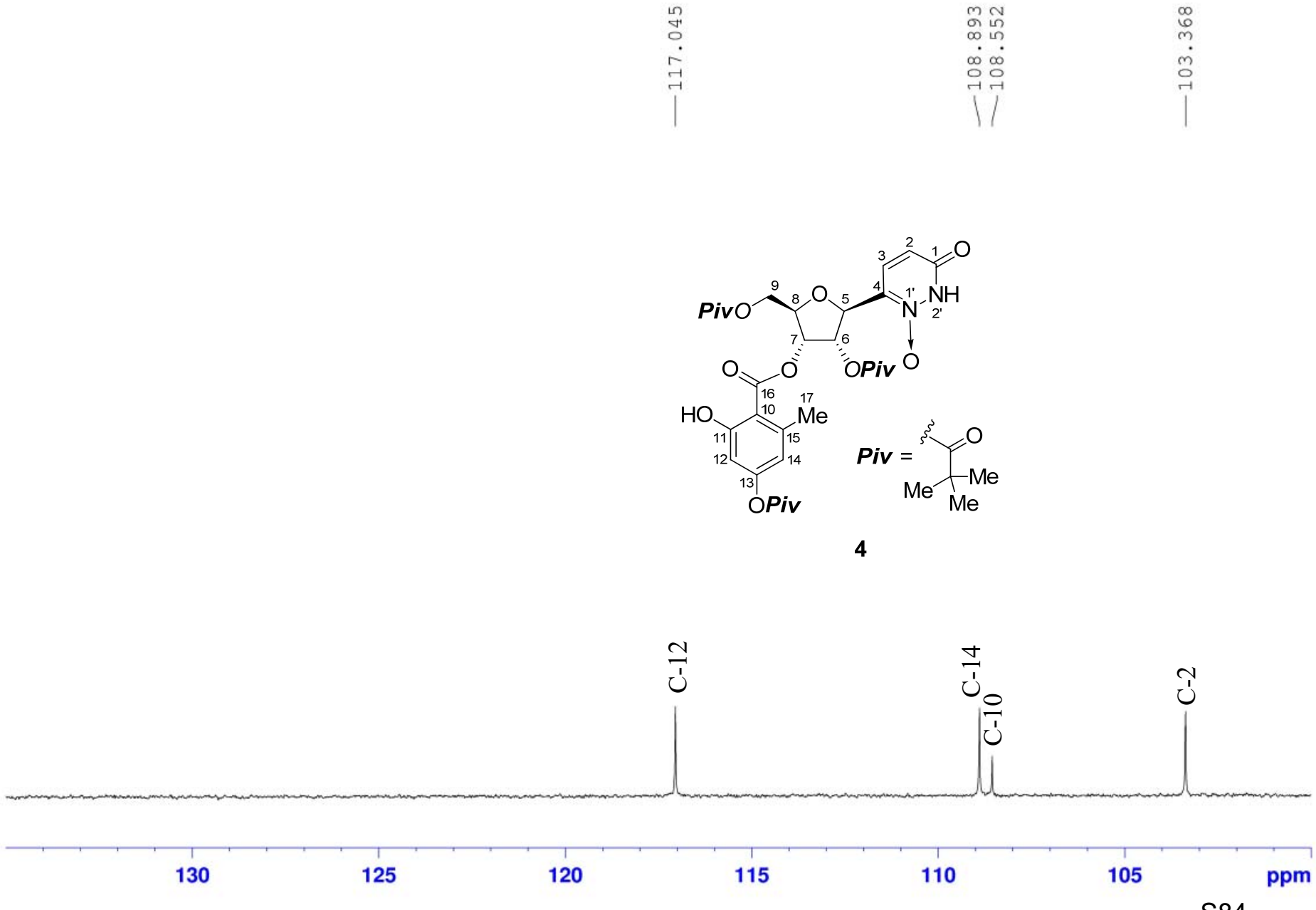
4

^{13}C (175 MHz) NMR spectrum of **4** in $CDCl_3$

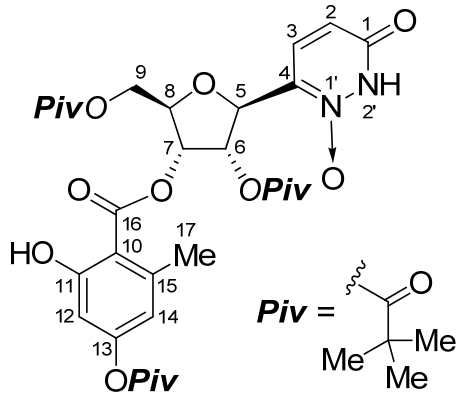


4

^{13}C (175 MHz) NMR spectrum of **4** in $CDCl_3$



^{13}C (175 MHz) NMR spectrum of **4** in $CDCl_3$



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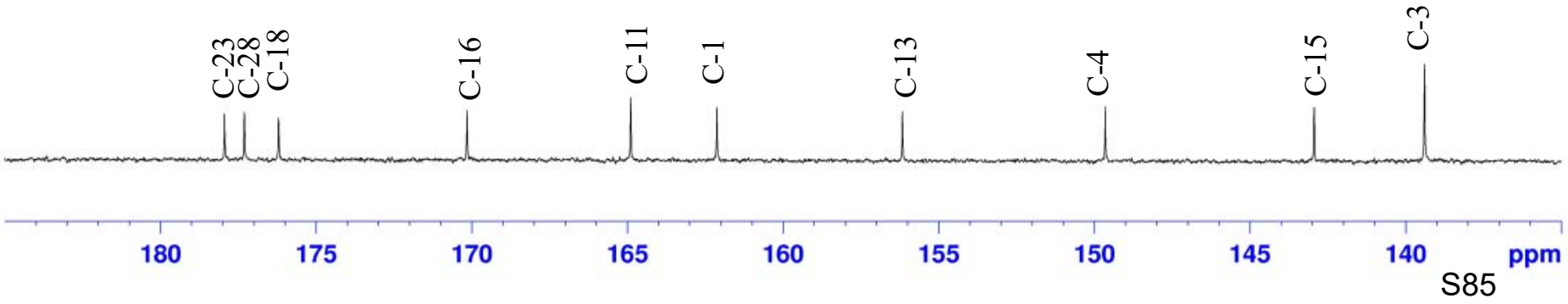
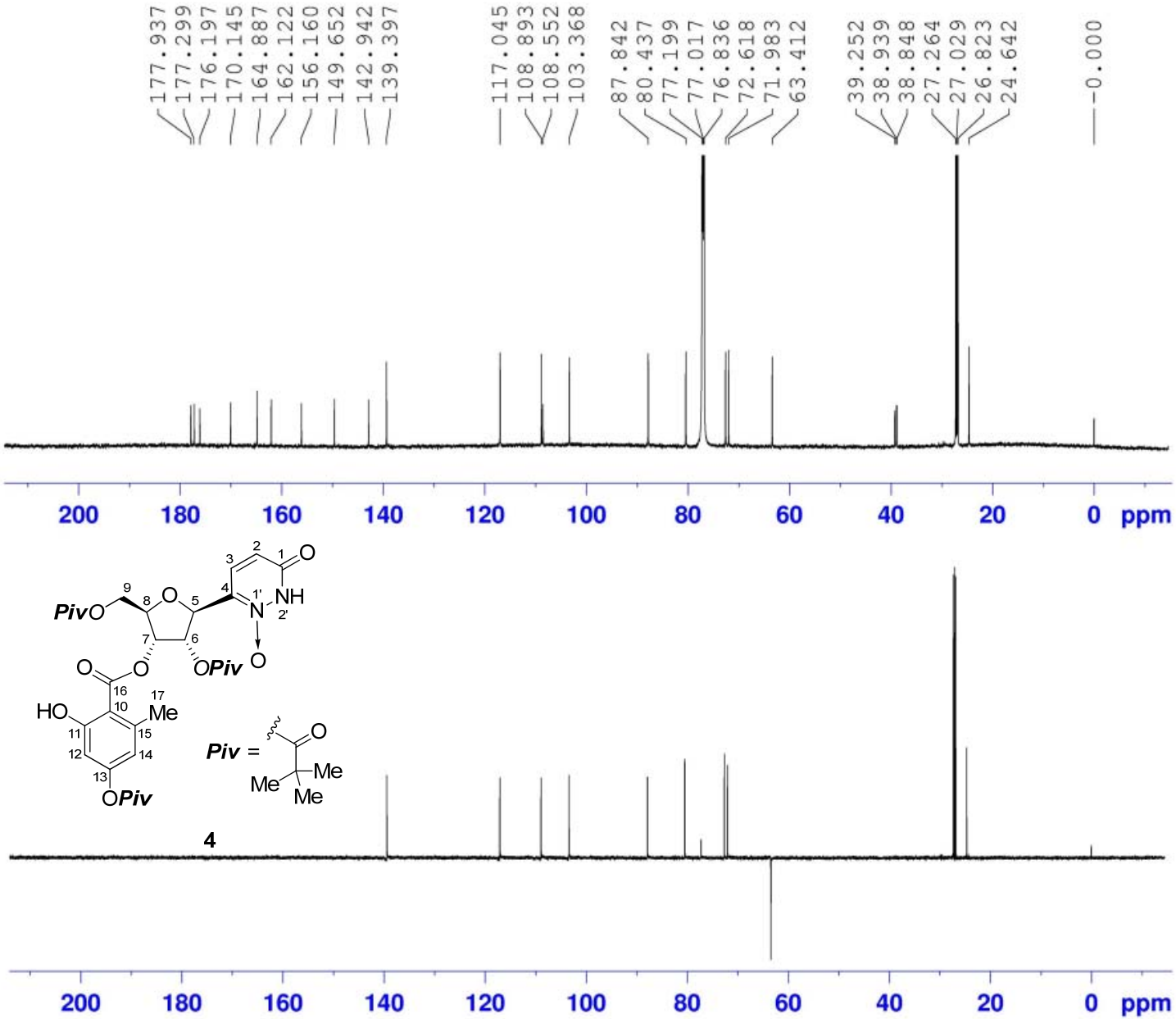
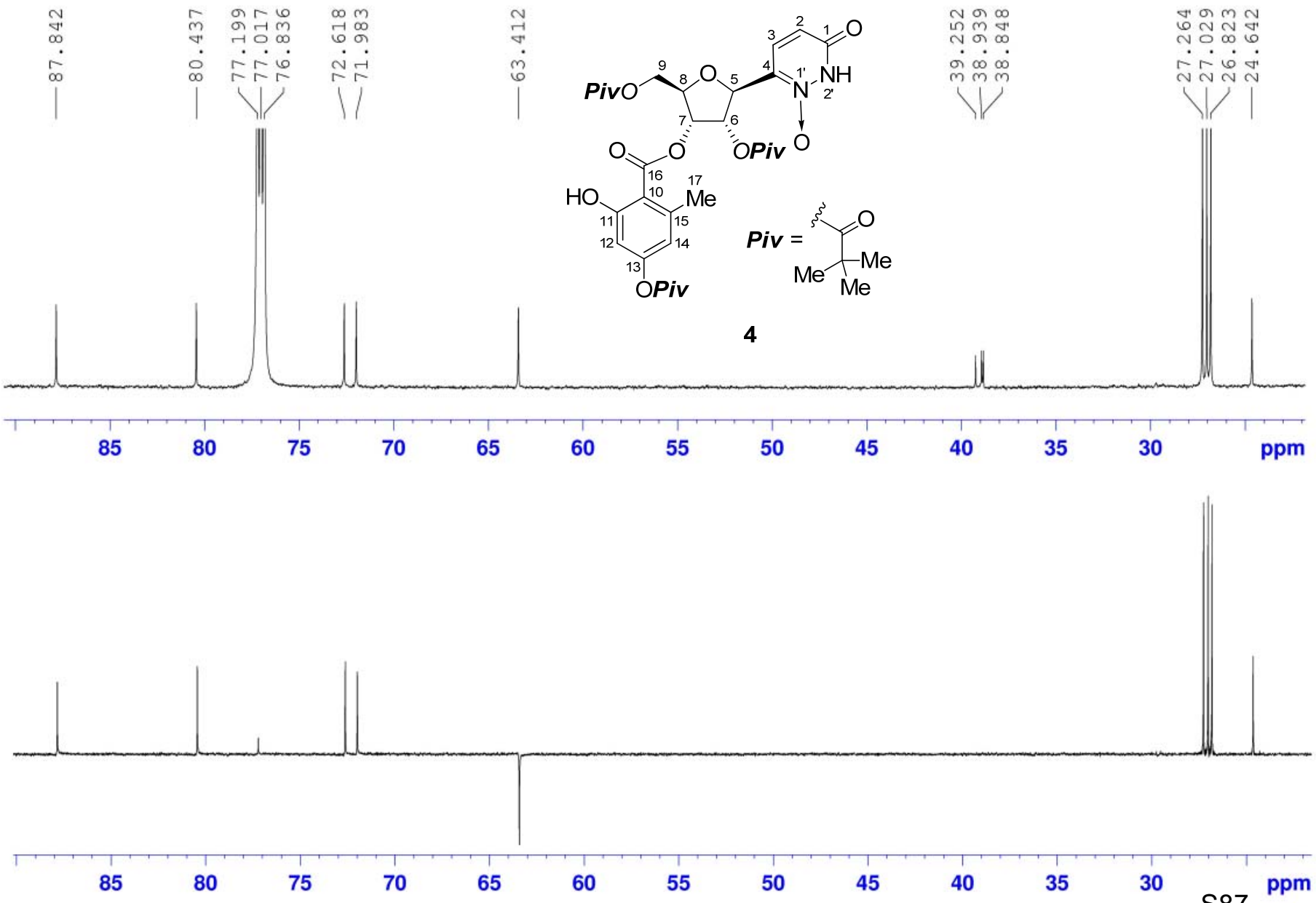


DEPT135 (175 MHz) spectrum of **4** in $CDCl_3$

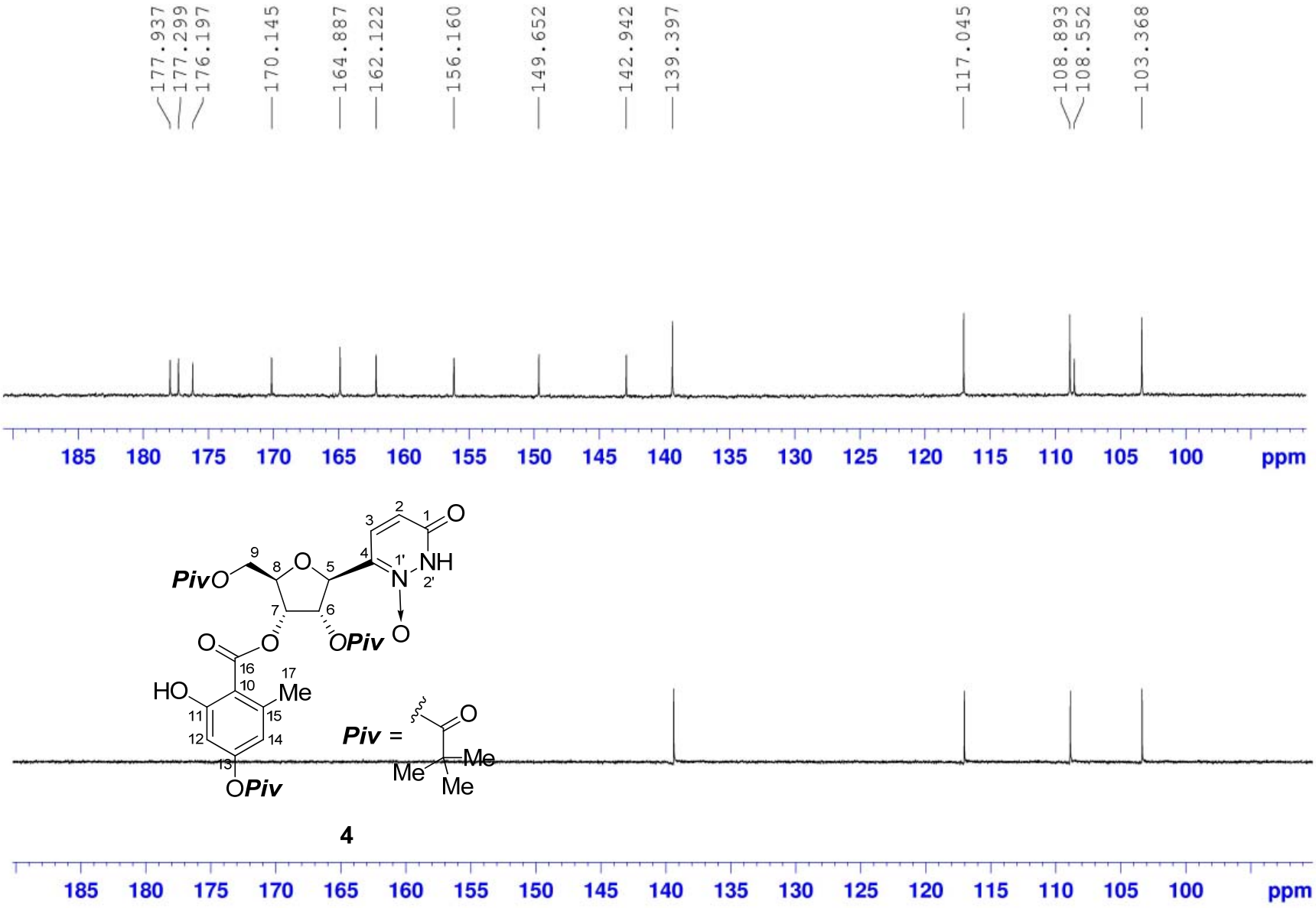


NAME	wubinbin-145D-R-6-1
EXPNO	12
PROCNO	1
Date_	20211027
Time	21.54 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	deptsp135
TD	32768
SOLVENT	CDCl3
NS	2000
DS	8
SWH	43859.648 Hz
FIDRES	2.676980 Hz
AQ	0.3736052 sec
RG	181.26
DW	11.400 usec
DE	18.00 usec
TE	298.0 K
CNST2	145.0000000
D1	1.00000000 sec
D2	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	176.0604010 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

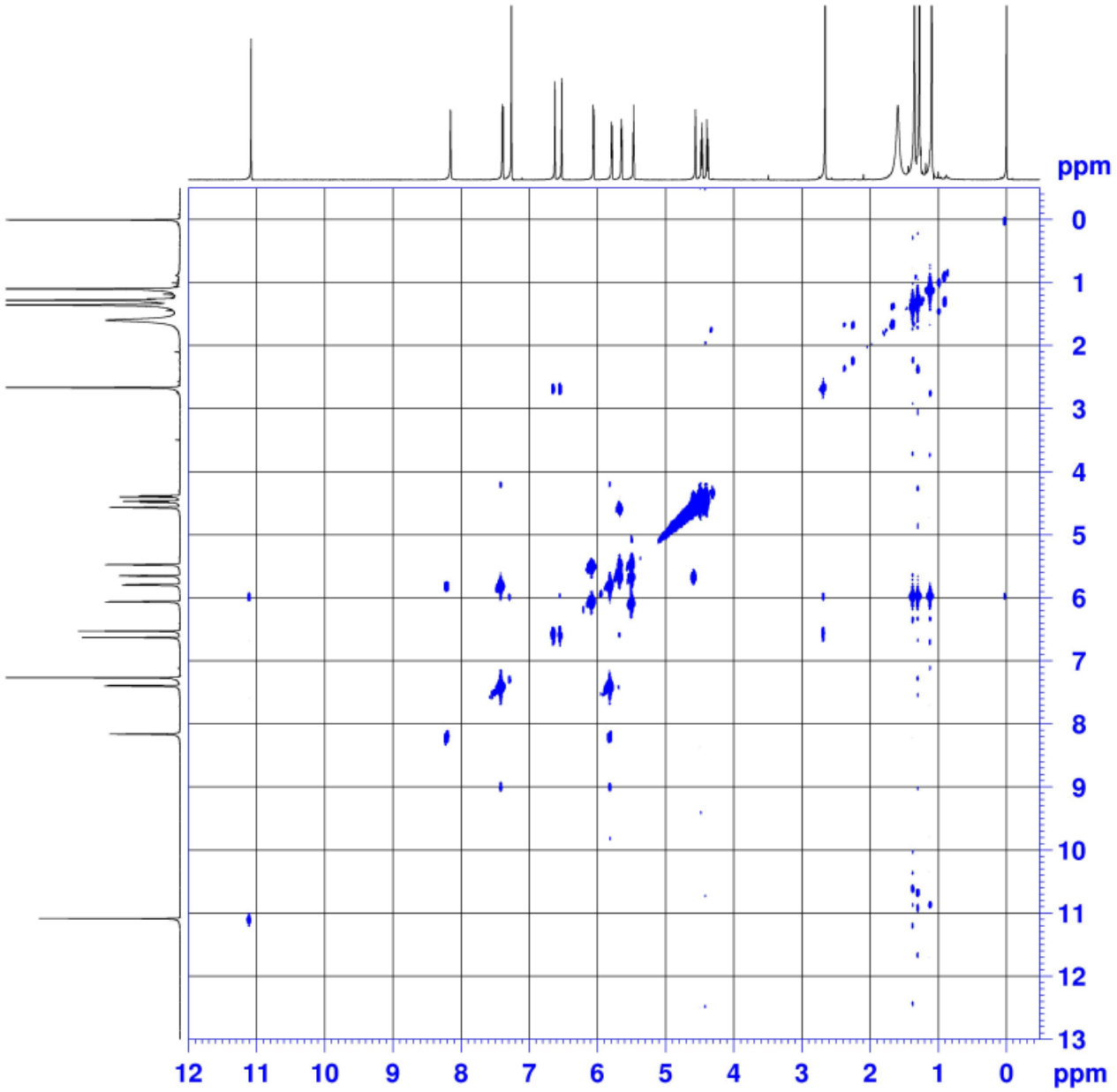
DEPT135 (175 MHz) spectrum of **4** in $CDCl_3$



DEPT135 (175 MHz) spectrum of **4** in $CDCl_3$

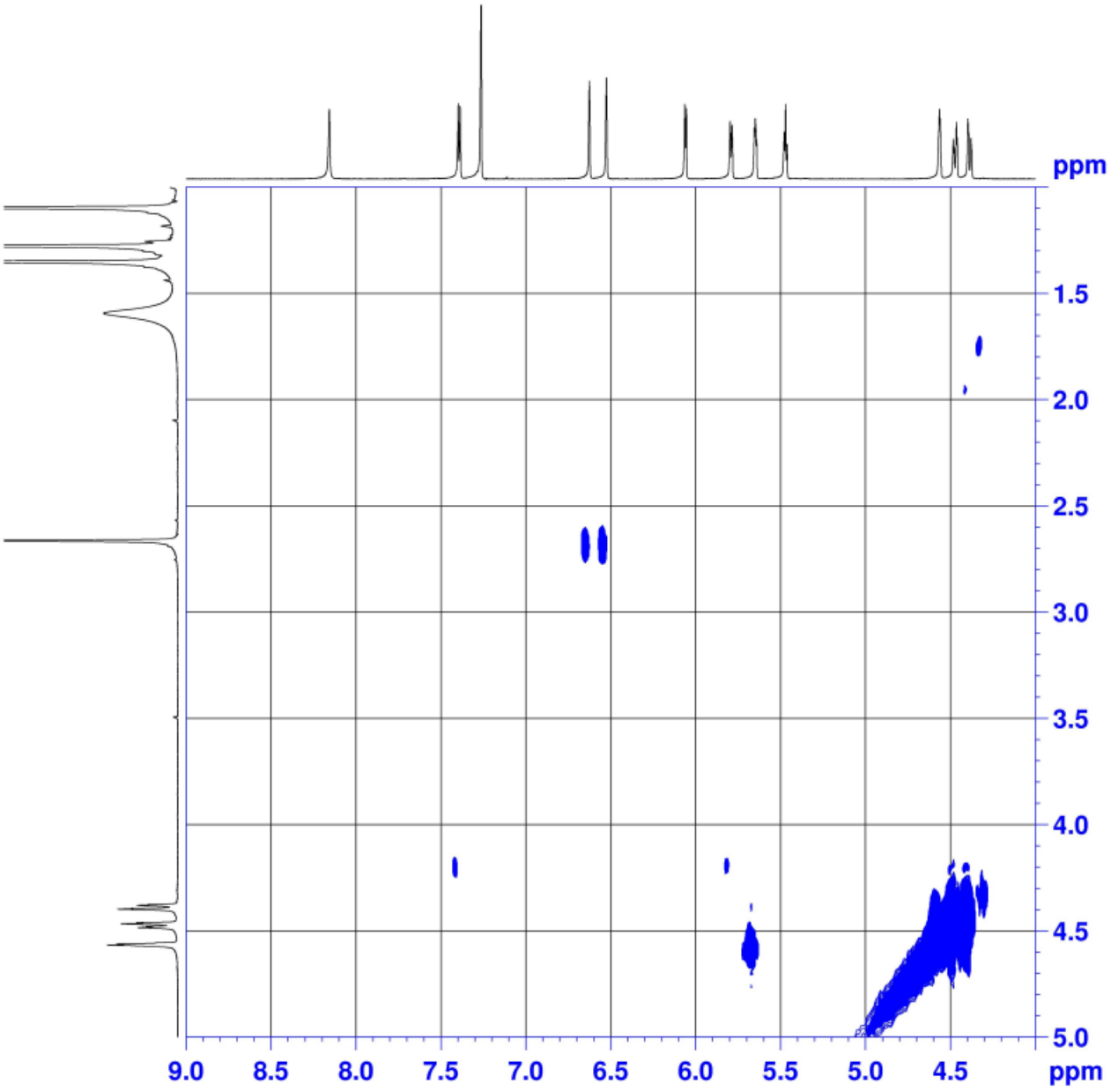


^{1}H–^{1}H COSY (700 MHz) spectrum of **4** in $CDCl_3$

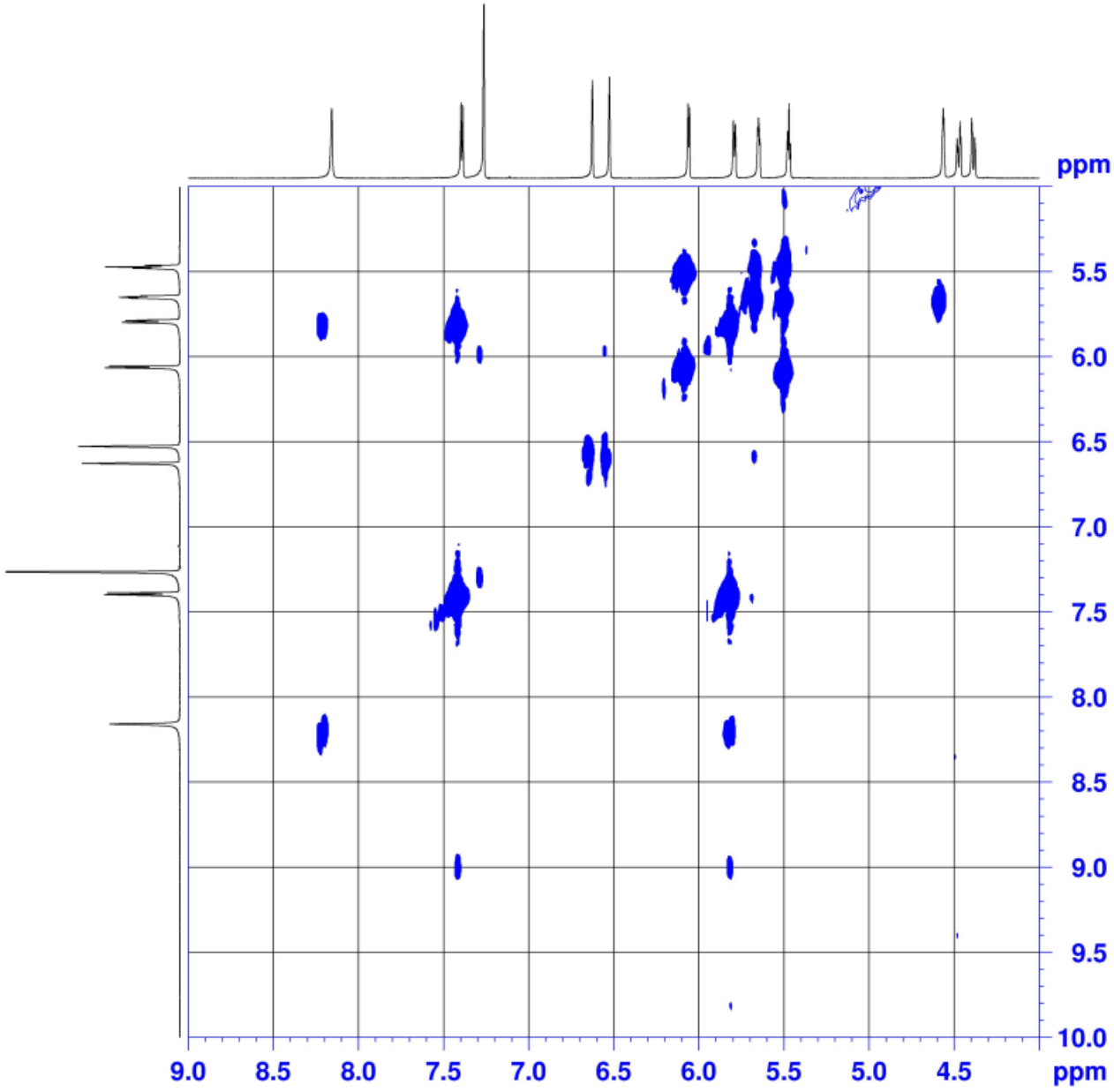


NAME	wubinbin-145D-R-6-1
EXPNO	17
PROCNO	1
Date_	20211029
Time	21.22 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	cosygpmfqf
TD	2048
SOLVENT	CDCl3
NS	16
DS	16
SWH	9090.909 Hz
FIDRES	8.877841 Hz
AQ	0.1126900 sec
RG	181.26
DW	55.000 usec
DE	10.00 usec
TE	298.0 K
D0	0.00000300 sec
D1	1.00000000 sec
D13	0.00000400 sec
D16	0.00020000 sec
IN0	0.00010980 sec
ND0	1
TD	128
SFO1	700.1842 MHz
FIDRES	71.152092 Hz
SW	13.007 ppm
FnMODE	QF
SI	1024
SF	700.1799963 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	QF
SF	700.1799963 MHz
WDW	SINE
SSB	0
LB	0.00 Hz
GB	0

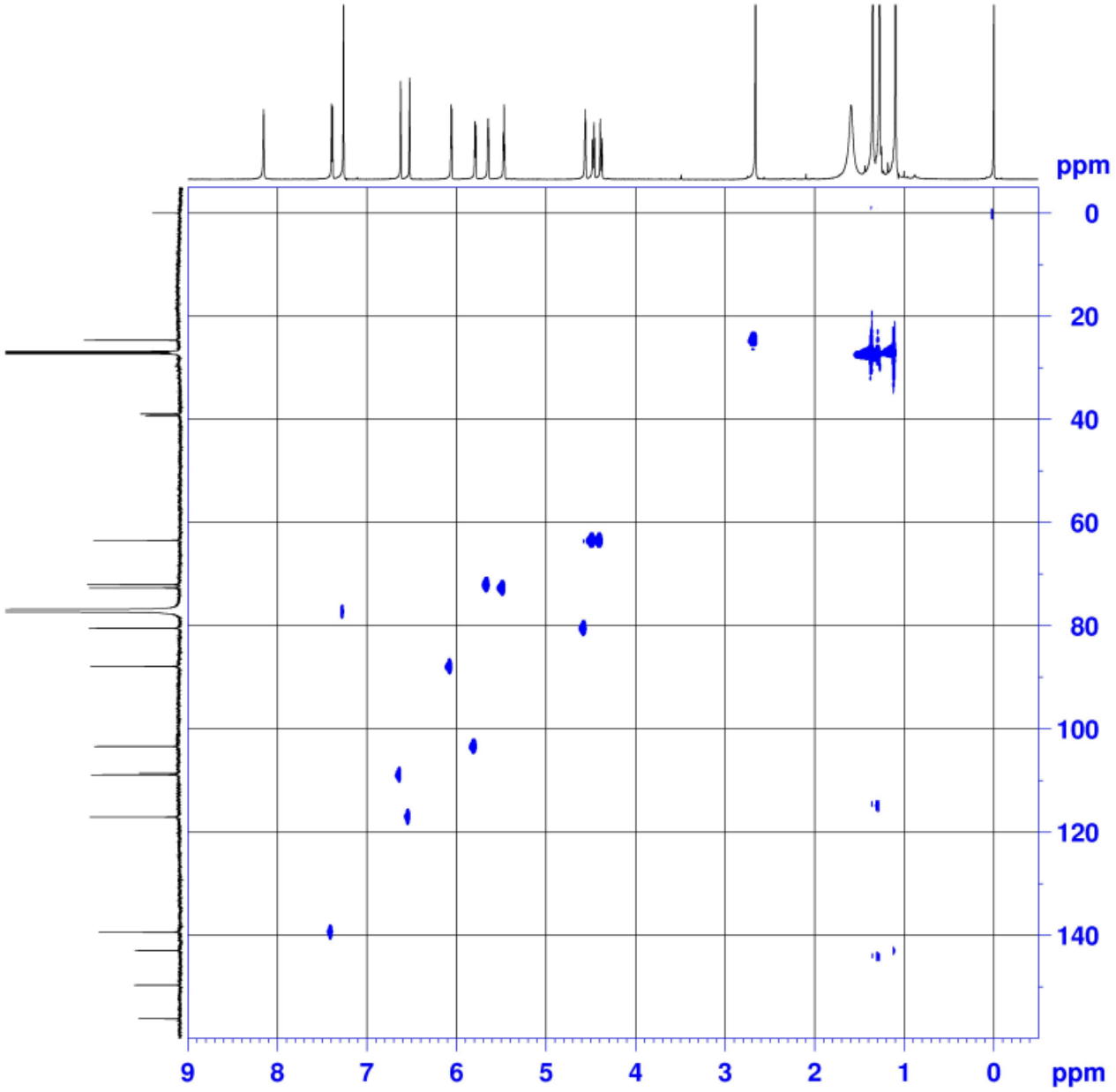
^{1}H–^{1}H COSY (700 MHz) spectrum of **4** in $CDCl_3$



^{1}H–^{1}H COSY (700 MHz) spectrum of **4** in $CDCl_3$

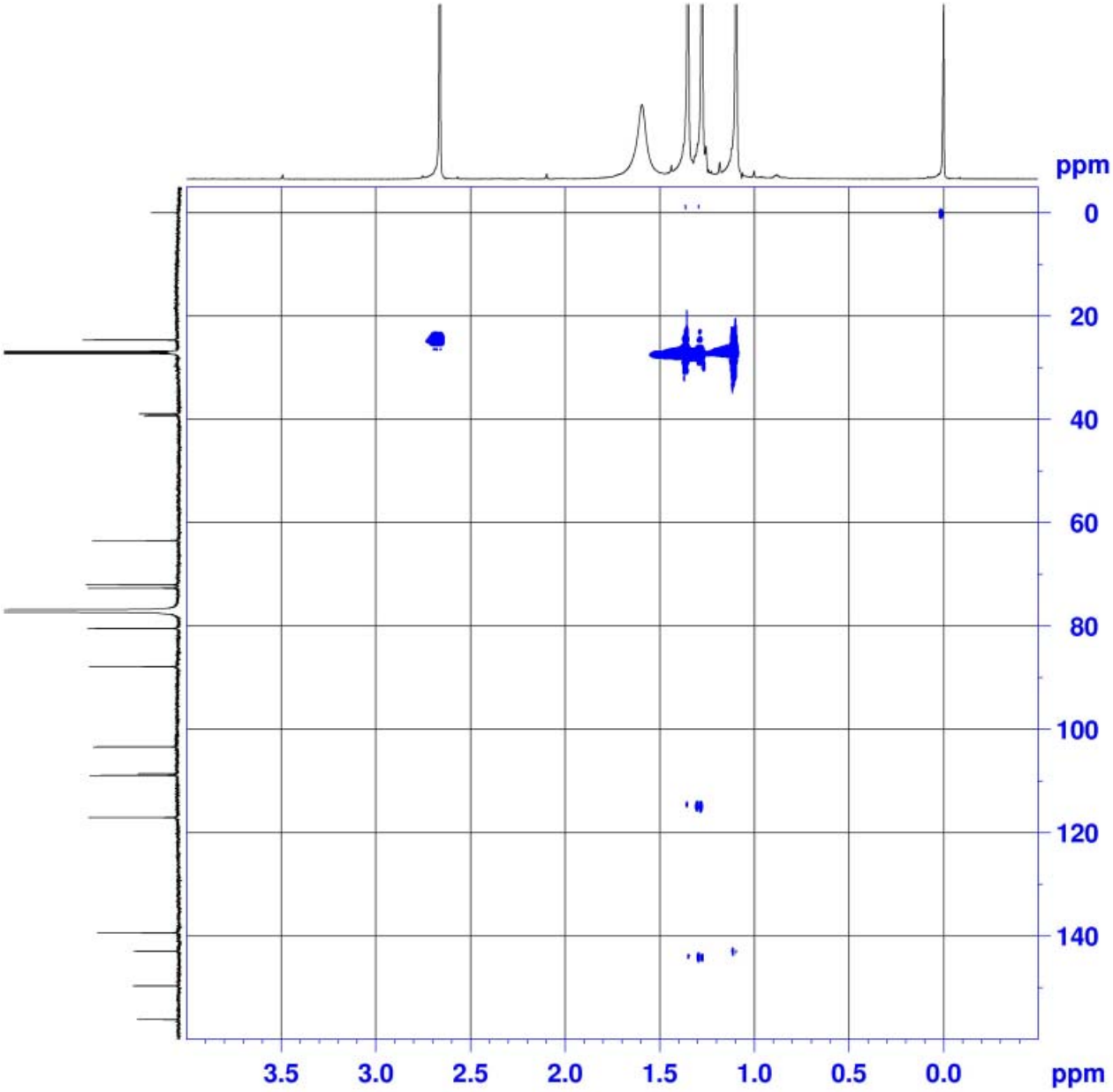


HSQC (700 MHz) spectrum of **4** in $CDCl_3$

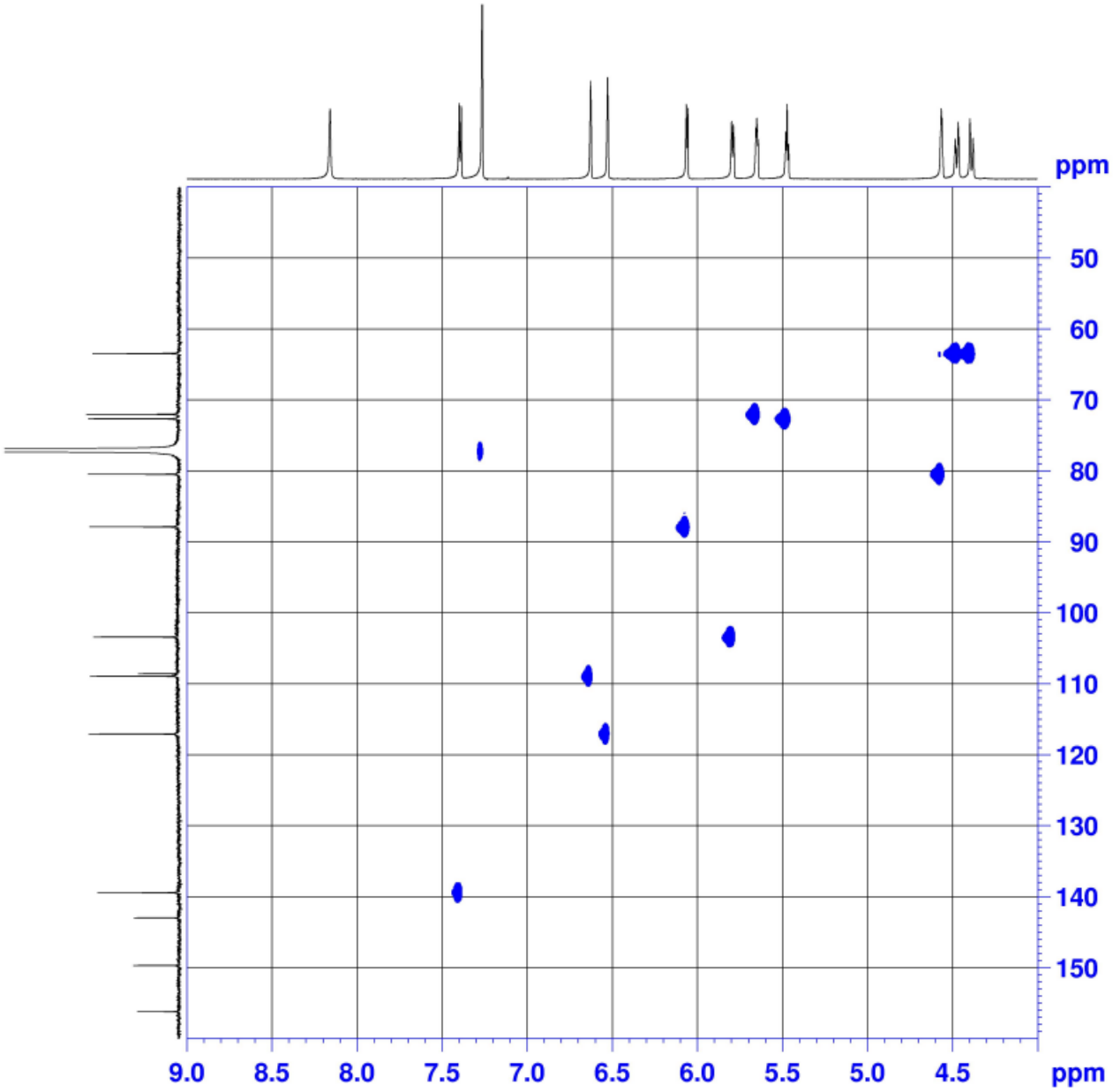



```
NAME        wubinbin-145D-R-6-1
EXPNO                        16
PROCNO                        1
Date_                  20211029
Time                      20.42 h
INSTRUM                   spect
PROBHD     Z120187_0028 (
PULPROG                hsqcetgp
TD                         2048
SOLVENT                   CDCl3
NS                           16
DS                           16
SWH                    9090.909 Hz
FIDRES                 8.877841 Hz
AQ                     0.1126900 sec
RG                        181.26
DW                        55.000 usec
DE                        10.00 usec
TE                        298.0 K
CNST2                145.0000000
D0                    0.00000300 sec
D1                    1.00000000 sec
D4                    0.00172414 sec
D11                   0.03000000 sec
D16                   0.00020000 sec
IN0                   0.00001390 sec
ND0                          2
TD                         128
SFO1                   176.0768 MHz
FIDRES                 281.025177 Hz
SW                        204.293 ppm
FnMODE          Echo-Antiecho
SI                         2048
SF                     700.1800042 MHz
WDW                       QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
PC                        1.40
SI                         2048
MC2               echo-antiecho
SF                     176.0604010 MHz
WDW                       QSINE
SSB                          2
LB                        0.00 Hz
GB                           0
```

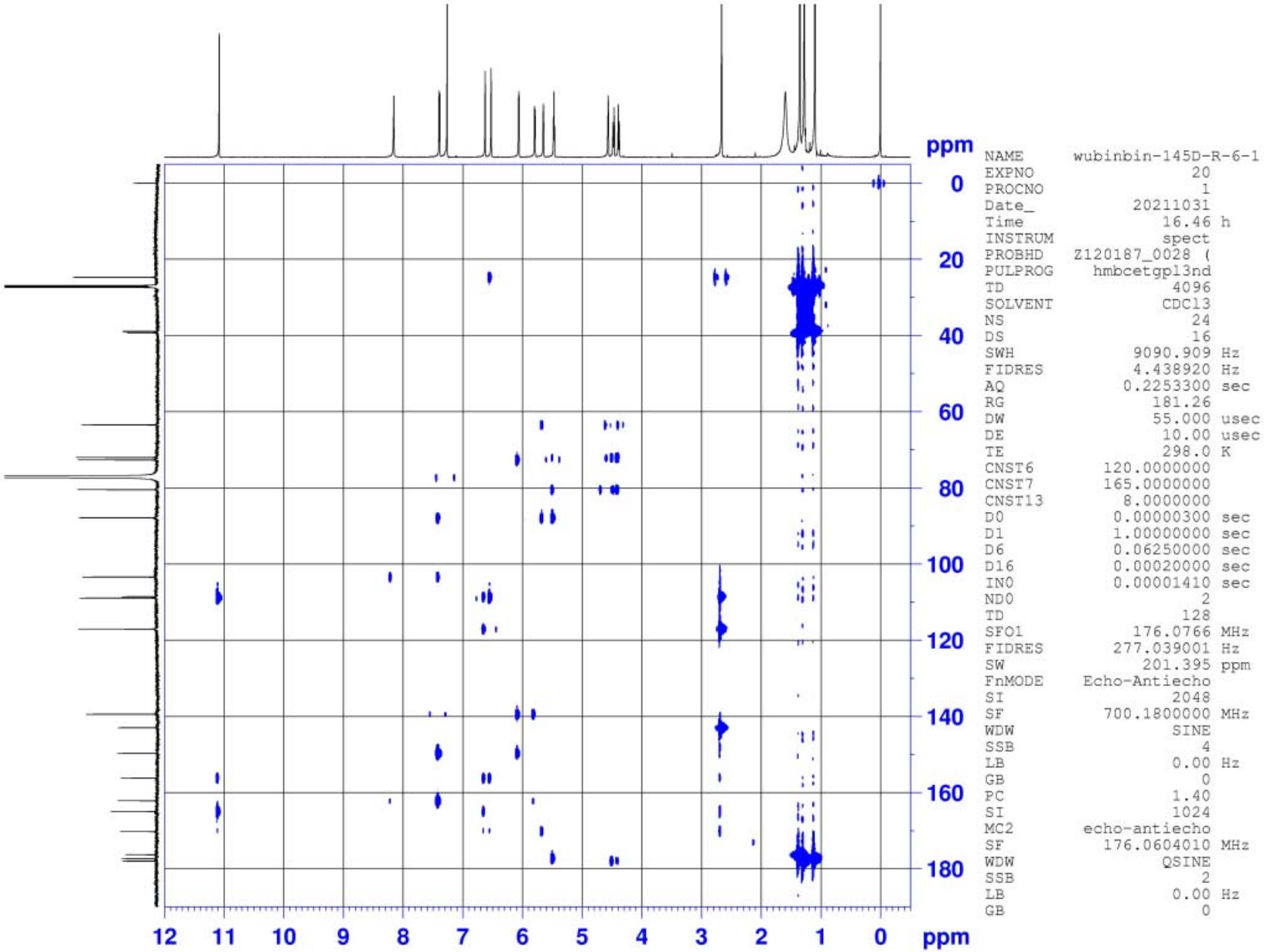
HSQC (700 MHz) spectrum of **4** in $CDCl_3$



HSQC (700 MHz) spectrum of **4** in $CDCl_3$

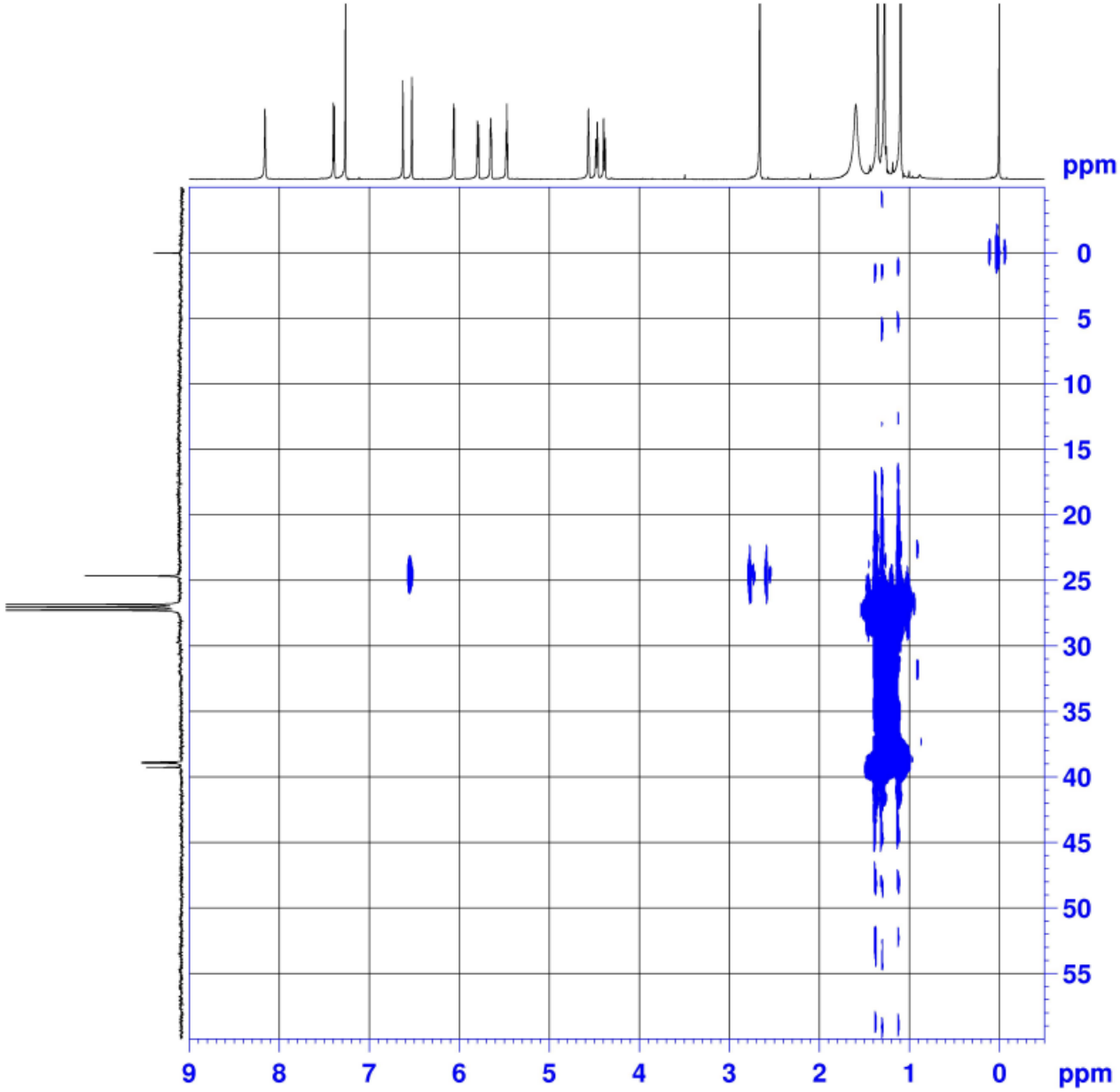


HMBC (700 MHz) spectrum of **4** in $CDCl_3$

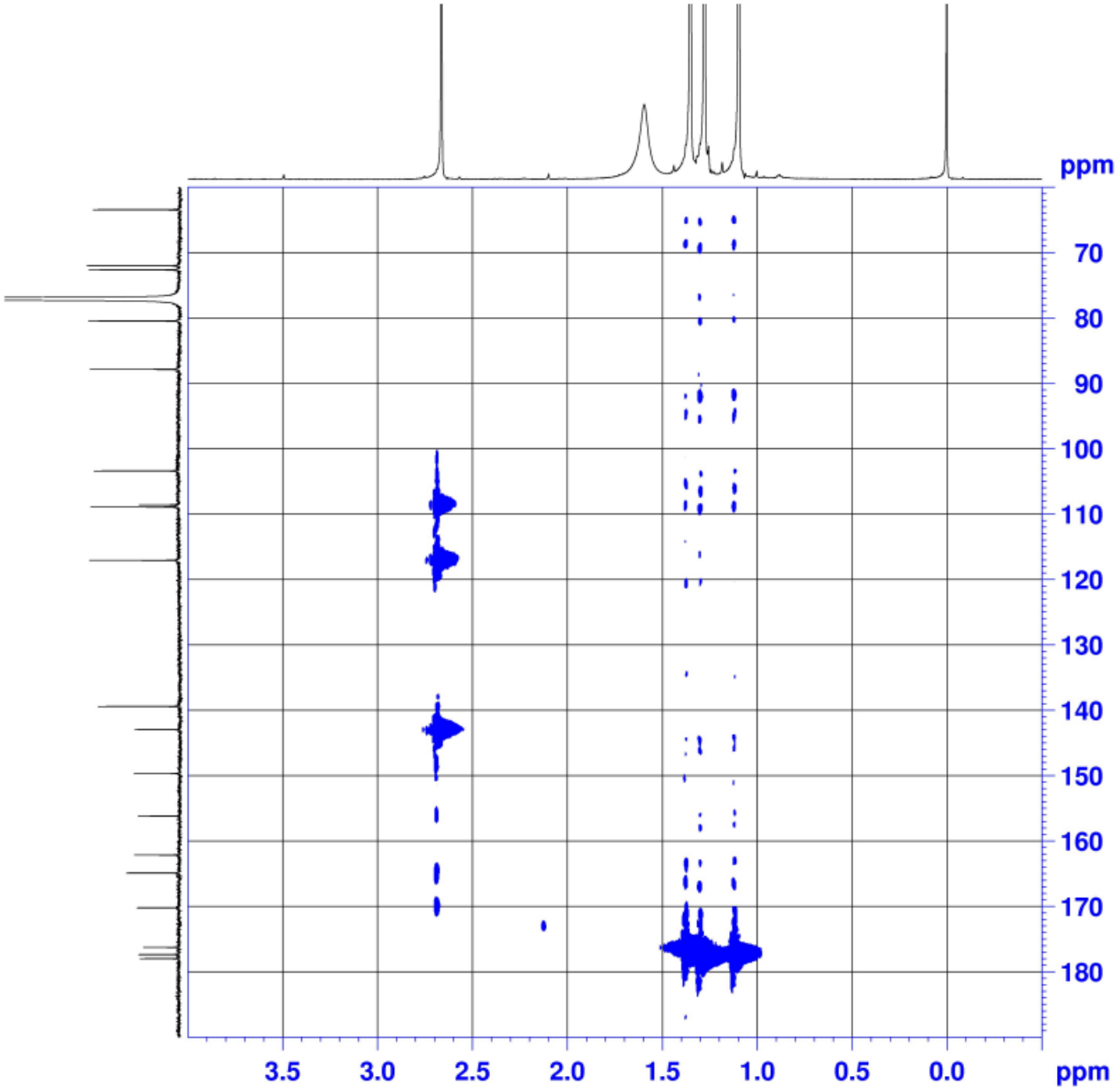


NAME	wubinbin-145D-R-6-1
EXPNO	20
PROCNO	1
Date_	20211031
Time	16.46 h
INSTRUM	spect
PROBHD	Z120187_0028 (
PULPROG	hmbcetgpl3nd
TD	4096
SOLVENT	CDCl3
NS	24
DS	16
SWH	9090.909 Hz
FIDRES	4.438920 Hz
AQ	0.2253300 sec
RG	181.26
DW	55.000 usec
DE	10.00 usec
TE	298.0 K
CNST6	120.0000000
CNST7	165.0000000
CNST13	8.0000000
D0	0.00000300 sec
D1	1.00000000 sec
D6	0.06250000 sec
D16	0.00020000 sec
IN0	0.00001410 sec
ND0	2
TD	128
SFO1	176.0766 MHz
FIDRES	277.039001 Hz
SW	201.395 ppm
FnMODE	Echo-Antiecho
SI	2048
SF	700.1800000 MHz
WDW	SINE
SSB	4
LB	0.00 Hz
GB	0
PC	1.40
SI	1024
MC2	echo-antiecho
SF	176.0604010 MHz
WDW	QSINE
SSB	2
LB	0.00 Hz
GB	0

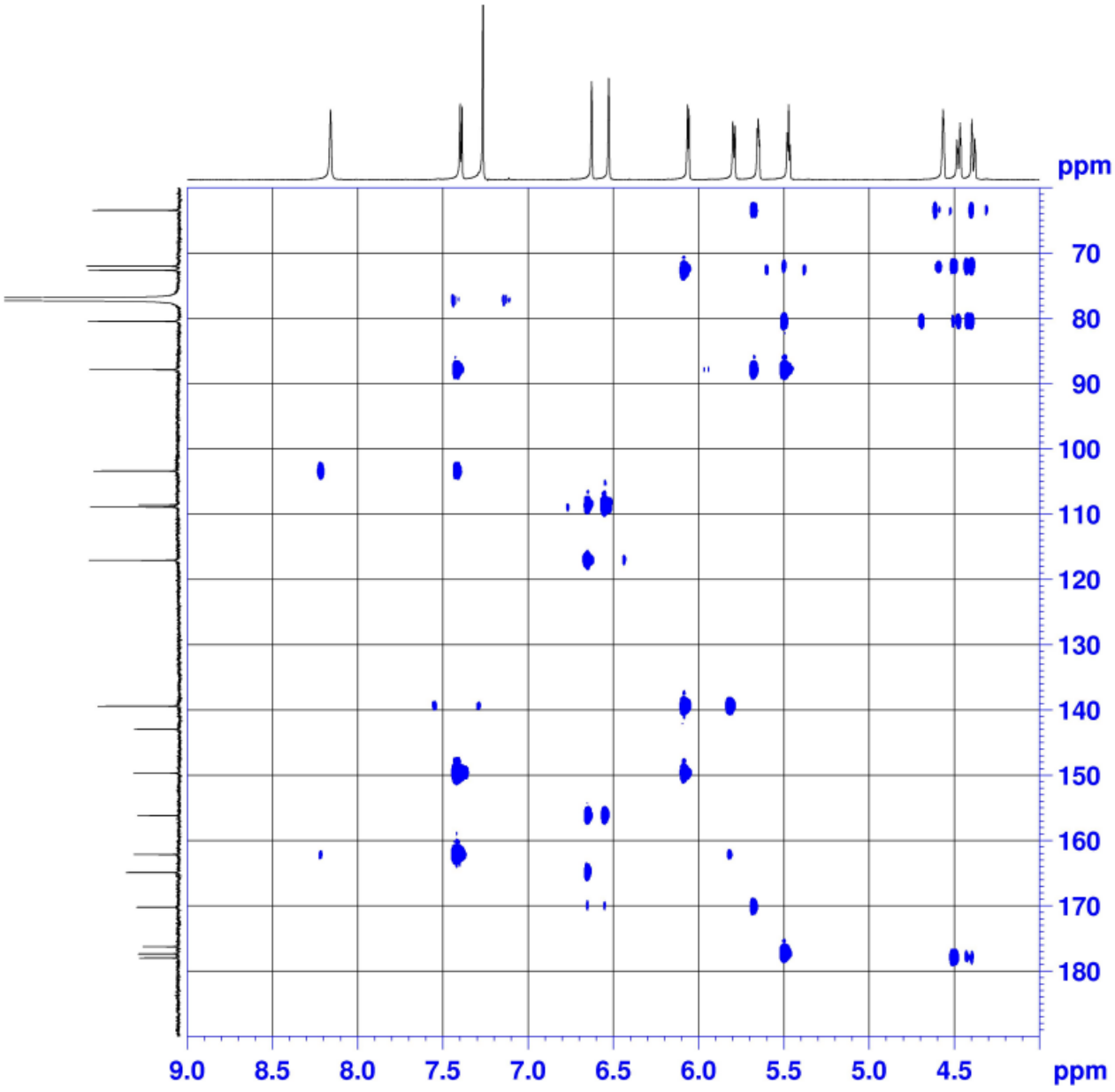
HMBC (700 MHz) spectrum of **4** in $CDCl_3$



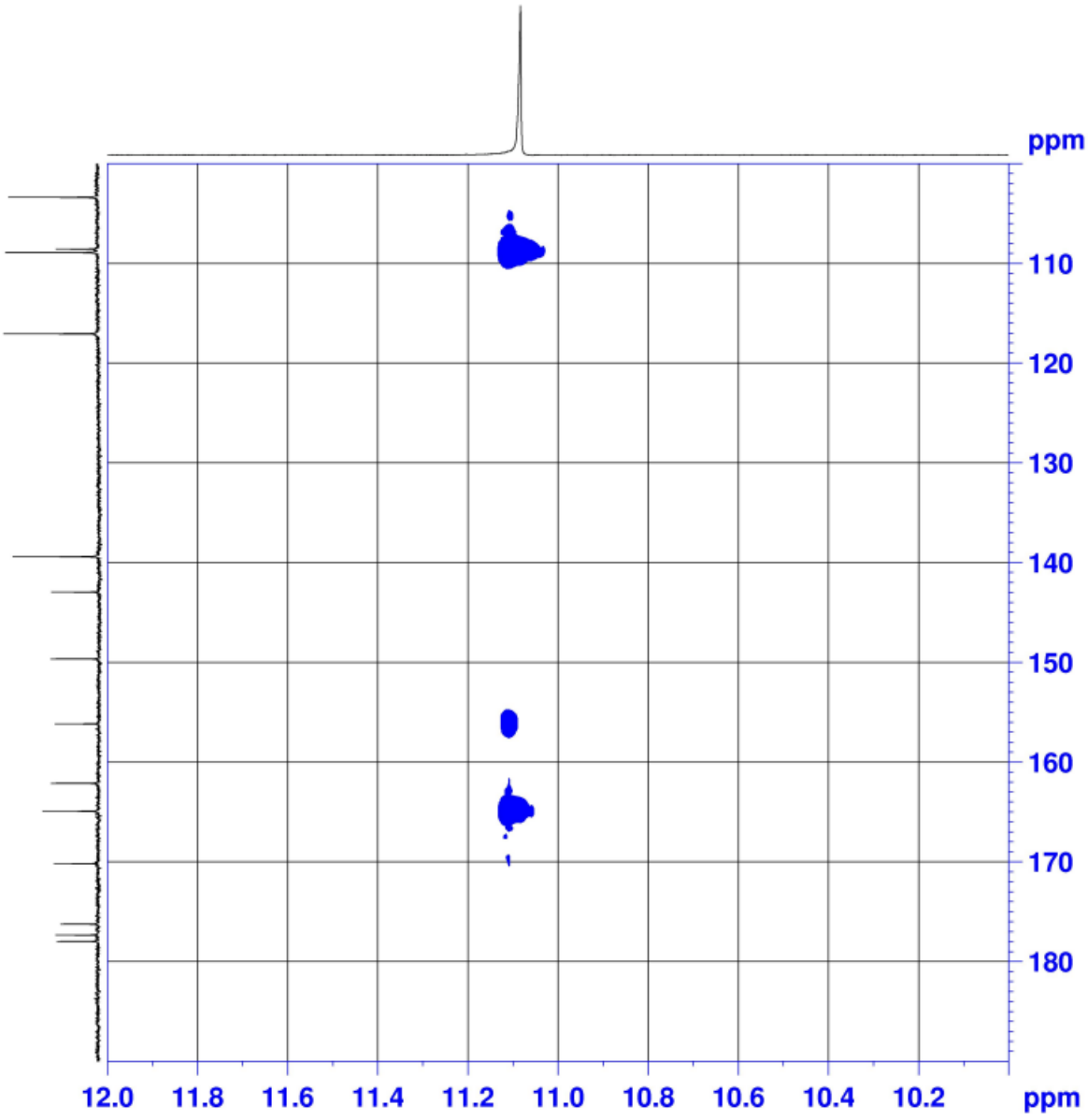
HMBC (700 MHz) spectrum of **4** in $CDCl_3$



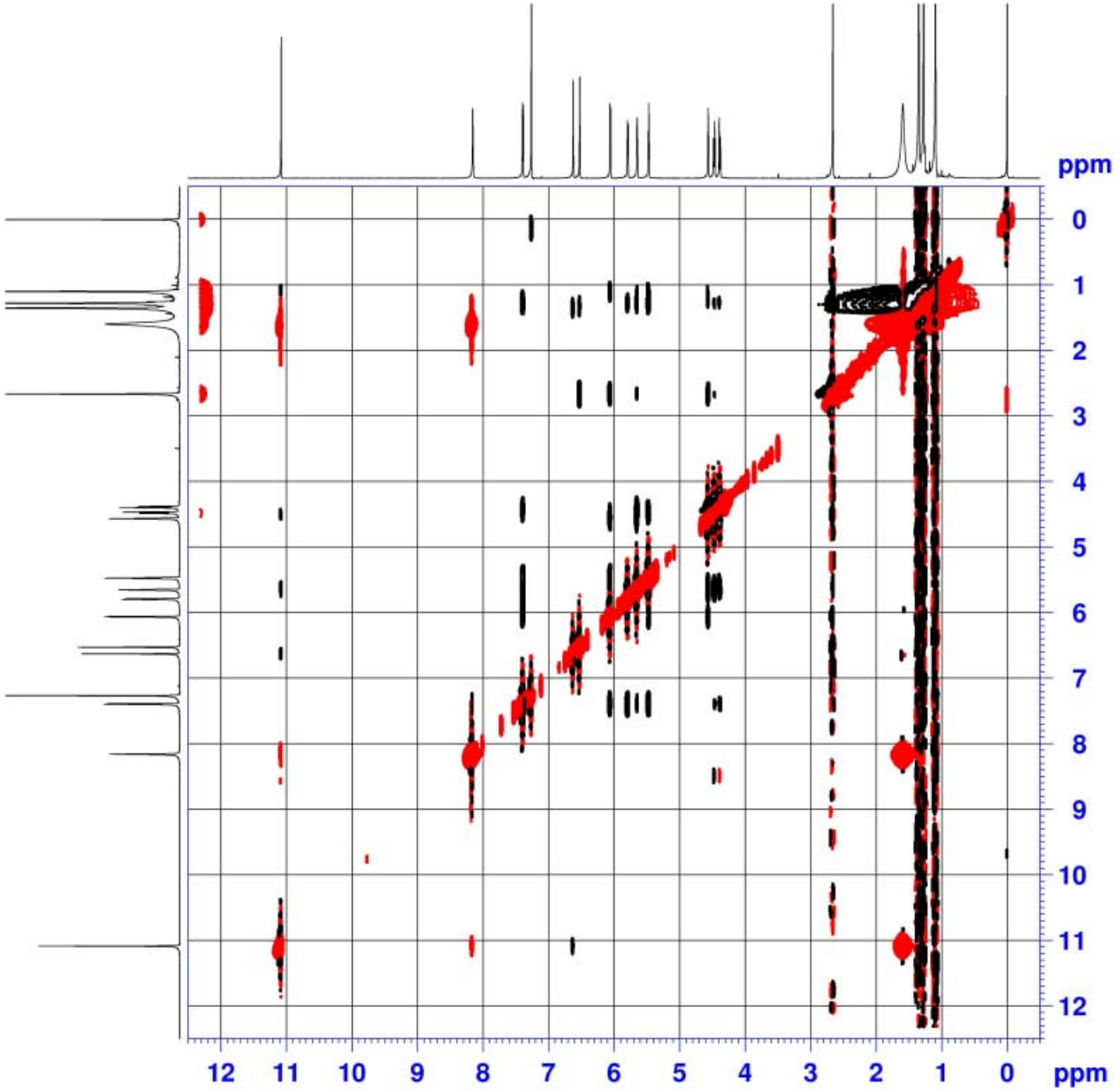
HMBC (700 MHz) spectrum of **4** in $CDCl_3$



HMBC (700 MHz) spectrum of **4** in $CDCl_3$

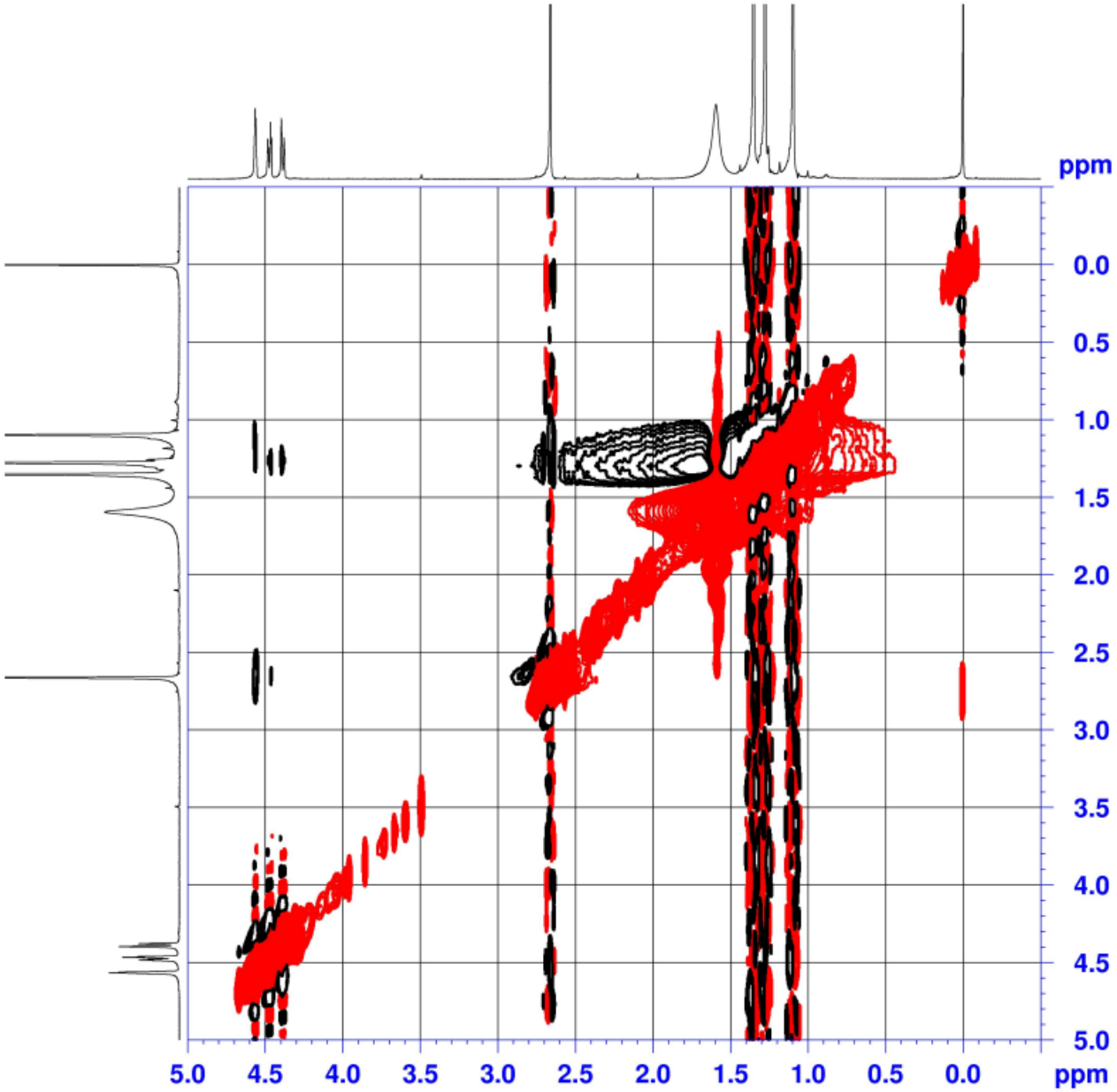


NOESY (700 MHz) spectrum of **4** in $CDCl_3$

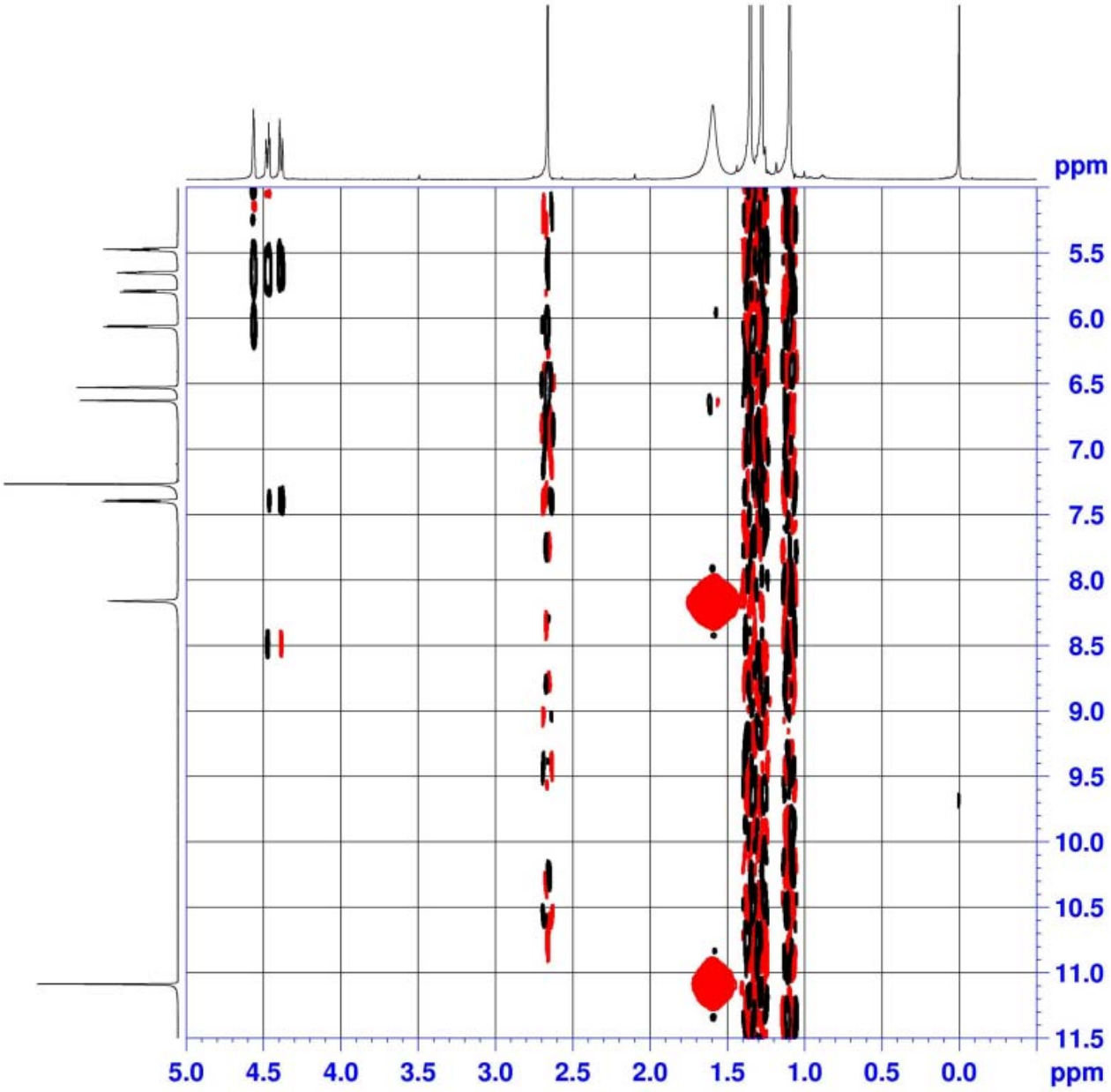


NAME	wubinbin-145D-R-6-1	
EXPNO	14	
PROCNO	1	
Date_	20211028	
Time	13.55	h
INSTRUM	spect	
PROBHD	Z120187_0028 (	
PULPROG	noesygpph	
TD	2048	
SOLVENT	CDCl3	
NS	24	
DS	16	
SWH	9578.544	Hz
FIDRES	9.354047	Hz
AQ	0.1069556	sec
RG	9.62	
DW	52.200	usec
DE	10.00	usec
TE	298.0	K
D0	0.00004232	sec
D1	1.00000000	sec
D8	0.60000002	sec
D16	0.00020000	sec
IN0	0.00010420	sec
ND0	1	
TD	128	
SFO1	700.1839	MHz
FIDRES	74.976006	Hz
SW	13.706	ppm
FnMODE	TPPI	
SI	2048	
SF	700.1800154	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	
PC	1.00	
SI	2048	
MC2	TPPI	
SF	700.1800154	MHz
WDW	QSINE	
SSB	2	
LB	0.00	Hz
GB	0	

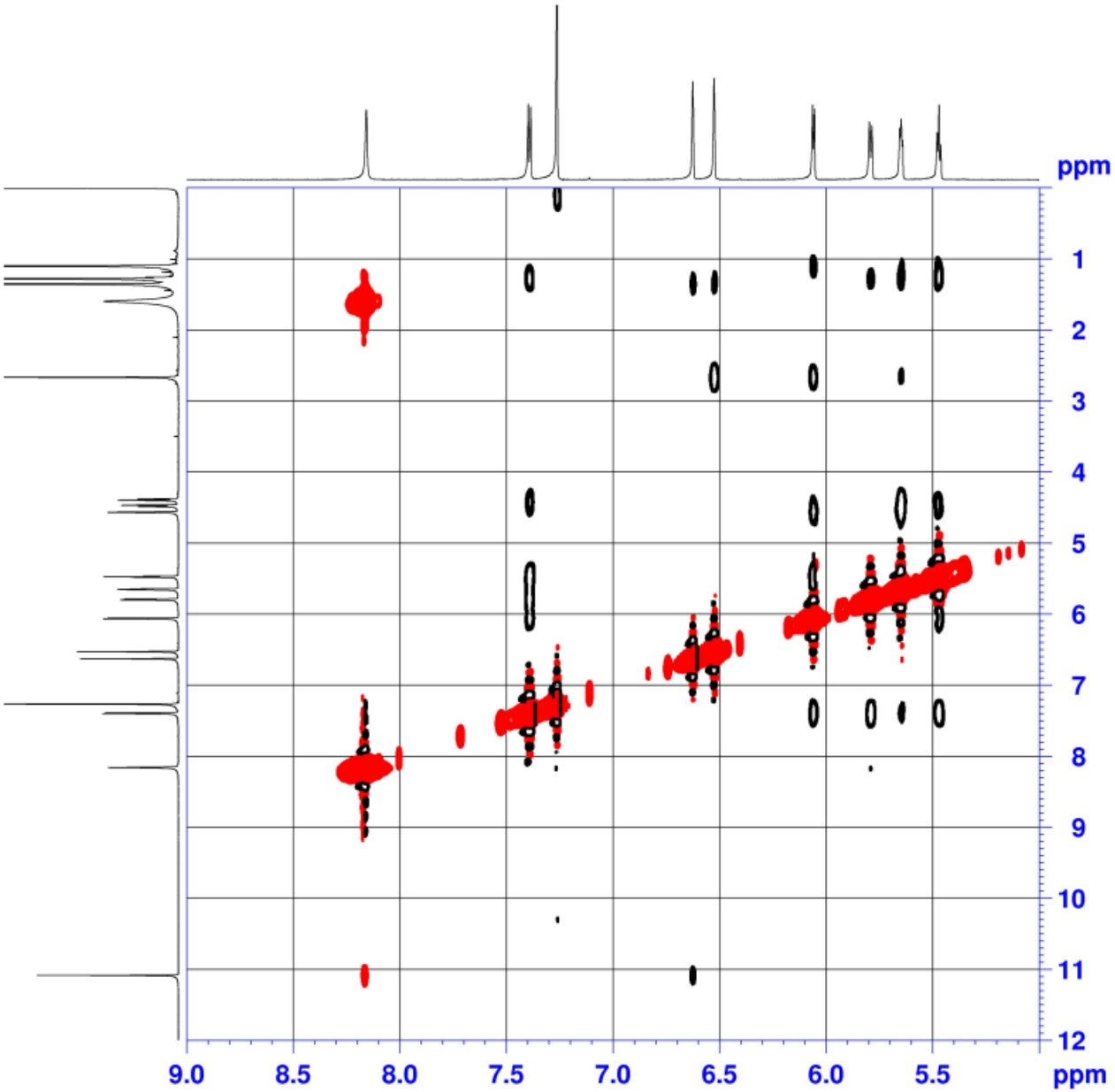
NOESY (700 MHz) spectrum of **4** in $CDCl_3$



NOESY (700 MHz) spectrum of **4** in $CDCl_3$



NOESY (700 MHz) spectrum of **4** in $CDCl_3$



NOESY (700 MHz) spectrum of **4** in $CDCl_3$

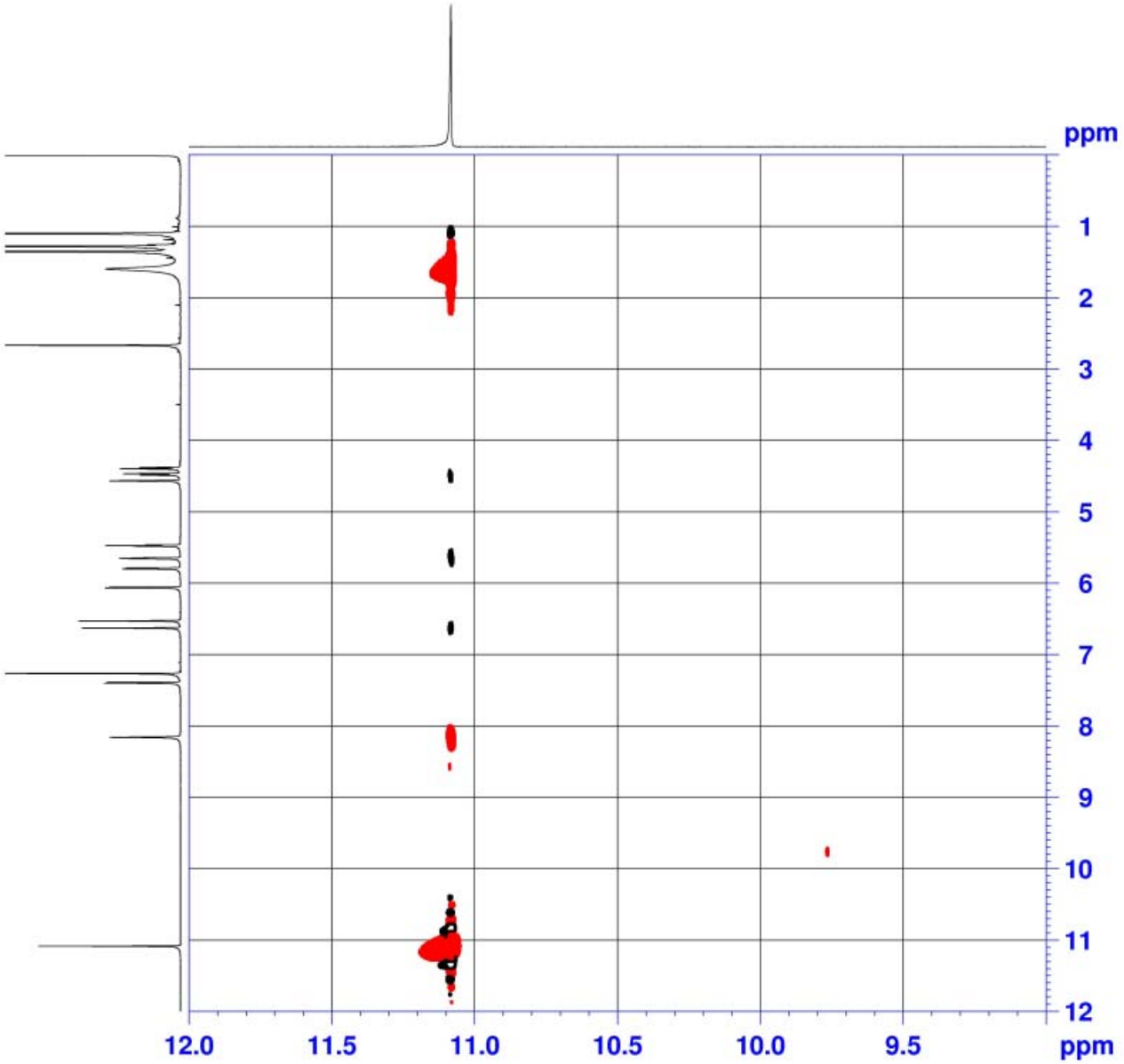


Figure S1. Energy analyses of conformers (14*S*,15*S*,17*R*)-2A to (14*S*,15*S*,17*R*)-2J

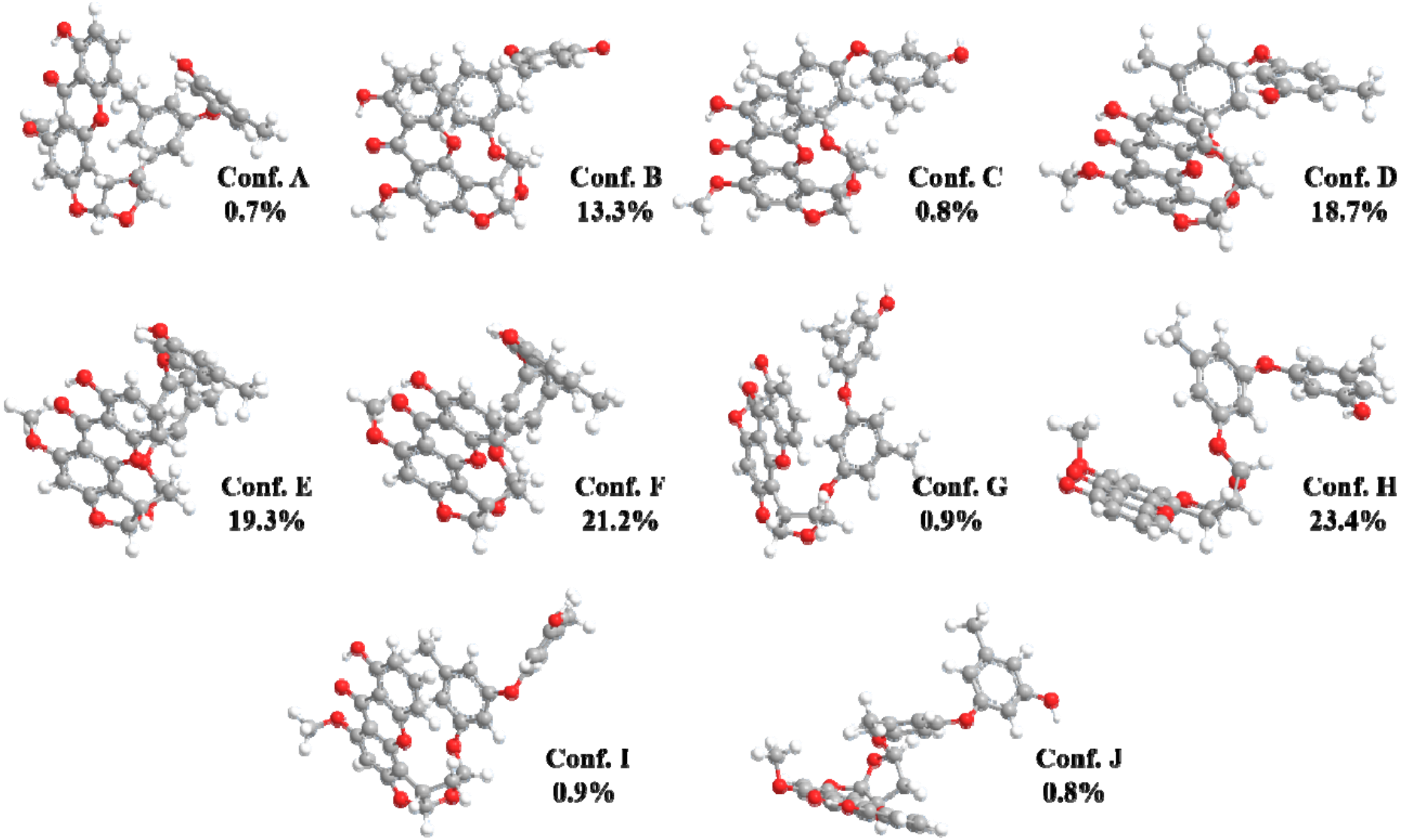


Figure S2. Energy analyses of conformers (15*R*,19*R*)-3A to (15*R*,19*R*)-3E

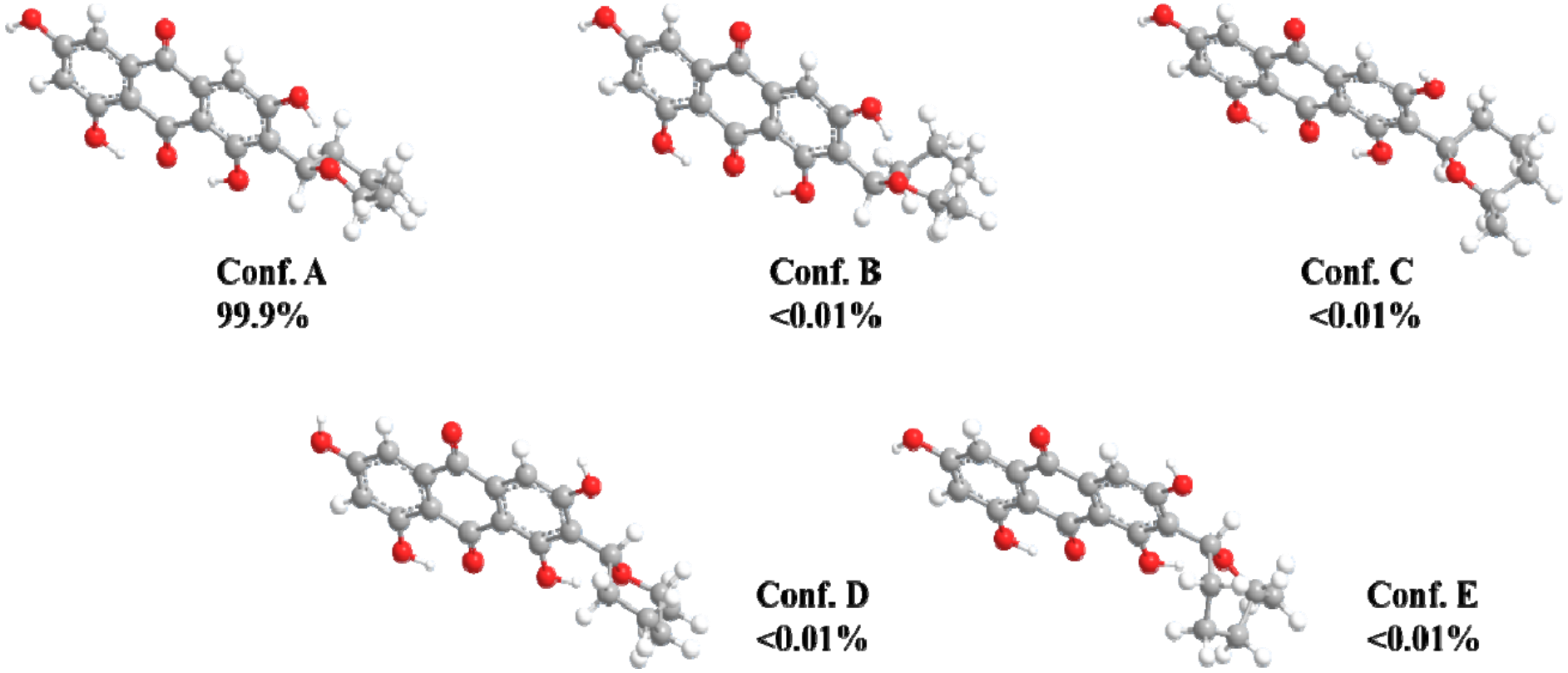
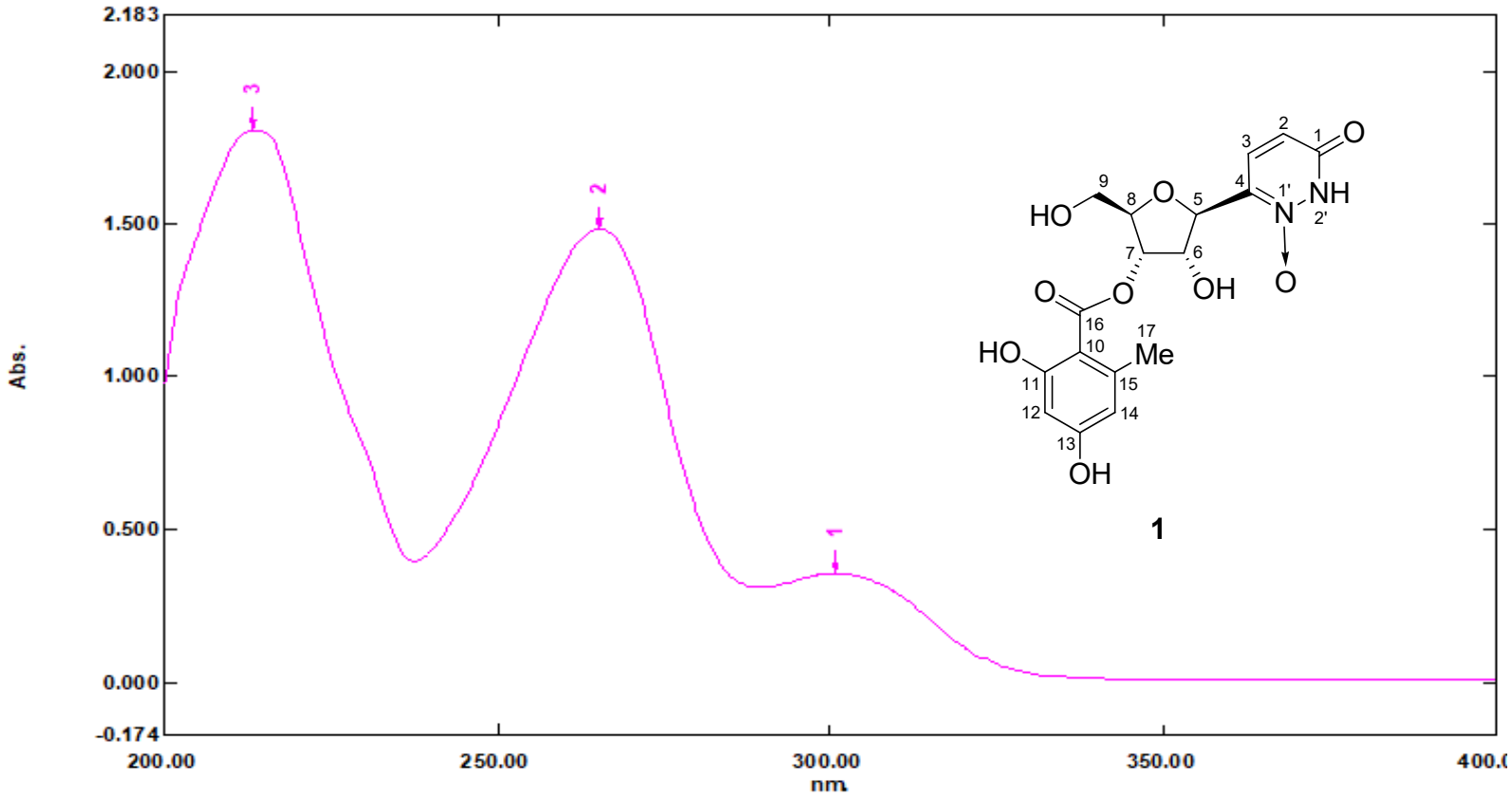
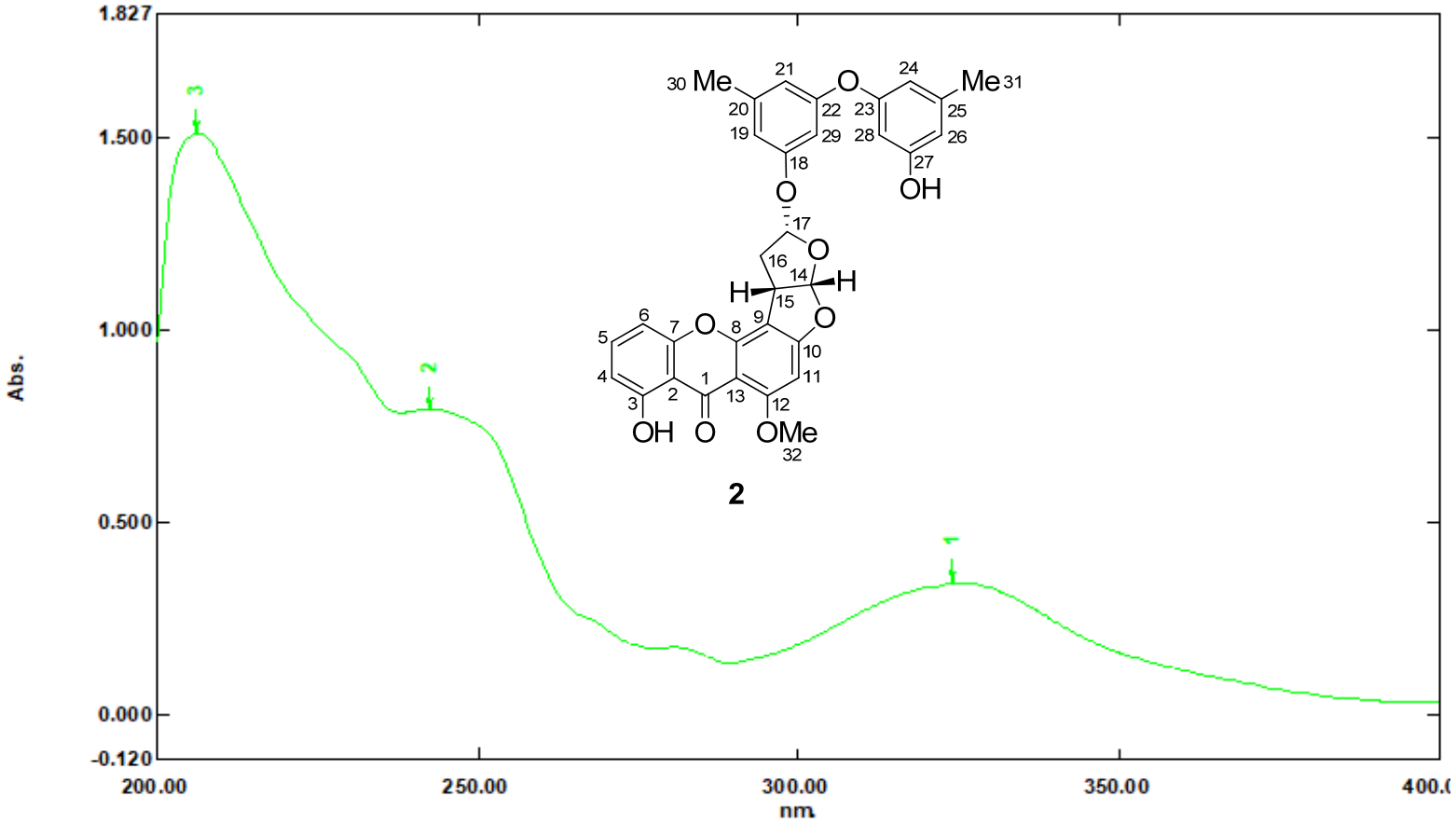


Figure S3. The UV spectrum of **1**



No.	P/V wavelength (nm)	Abs.
1	300.80	0.355
2	265.40	1.482
3	213.40	1.805

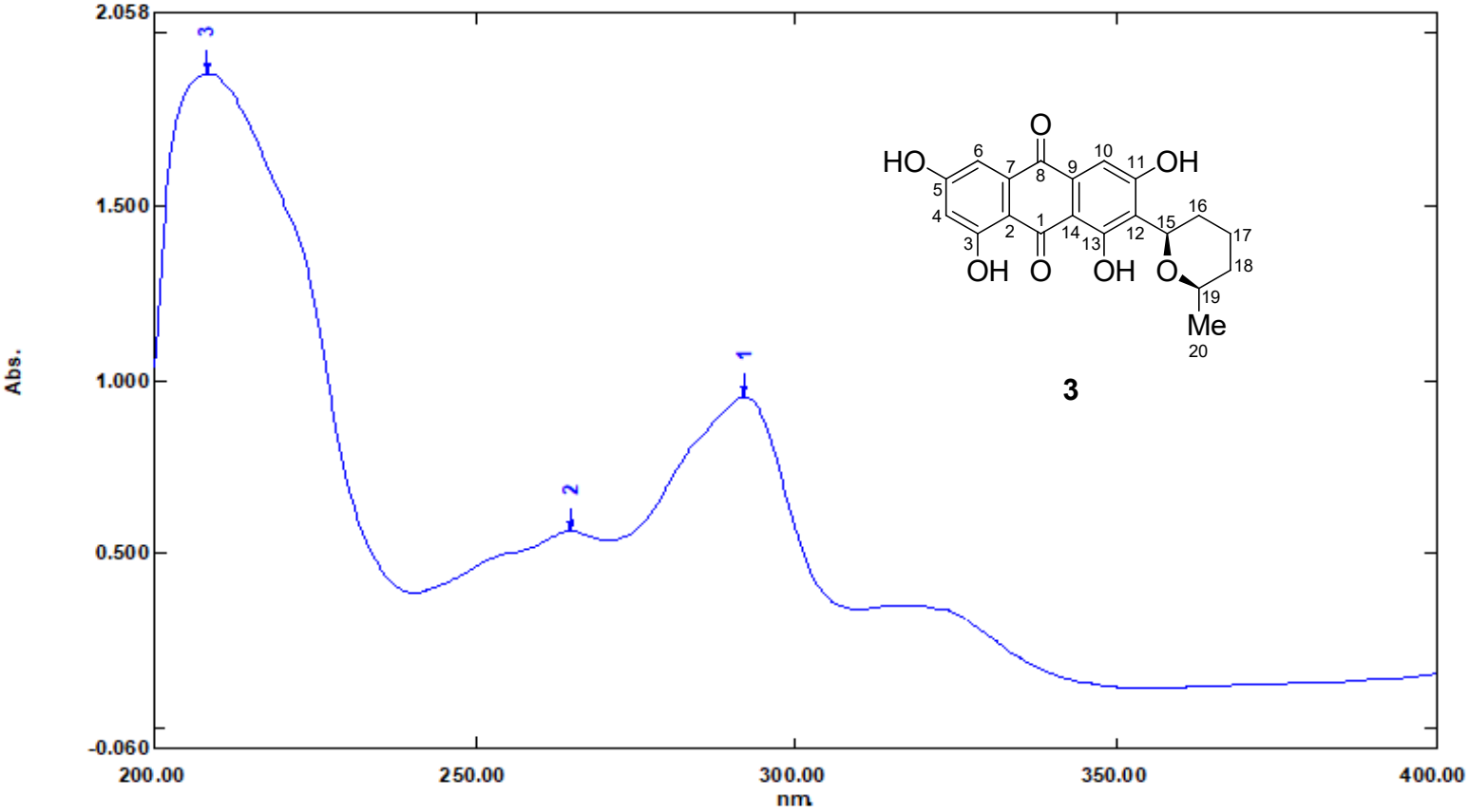
Figure S4. The UV spectrum of **2**



2

No.	P/V wavelength (nm)	Abs.
1	324.20	0.343
2	242.60	0.794
3	206.20	1.515

Figure S5. The UV spectrum of **3**



No.	P/V wavelength (nm)	Abs.
1	292.00	0.951
2	264.80	0.564
3	208.20	1.882

Figure S6. The IR spectrum of **1**

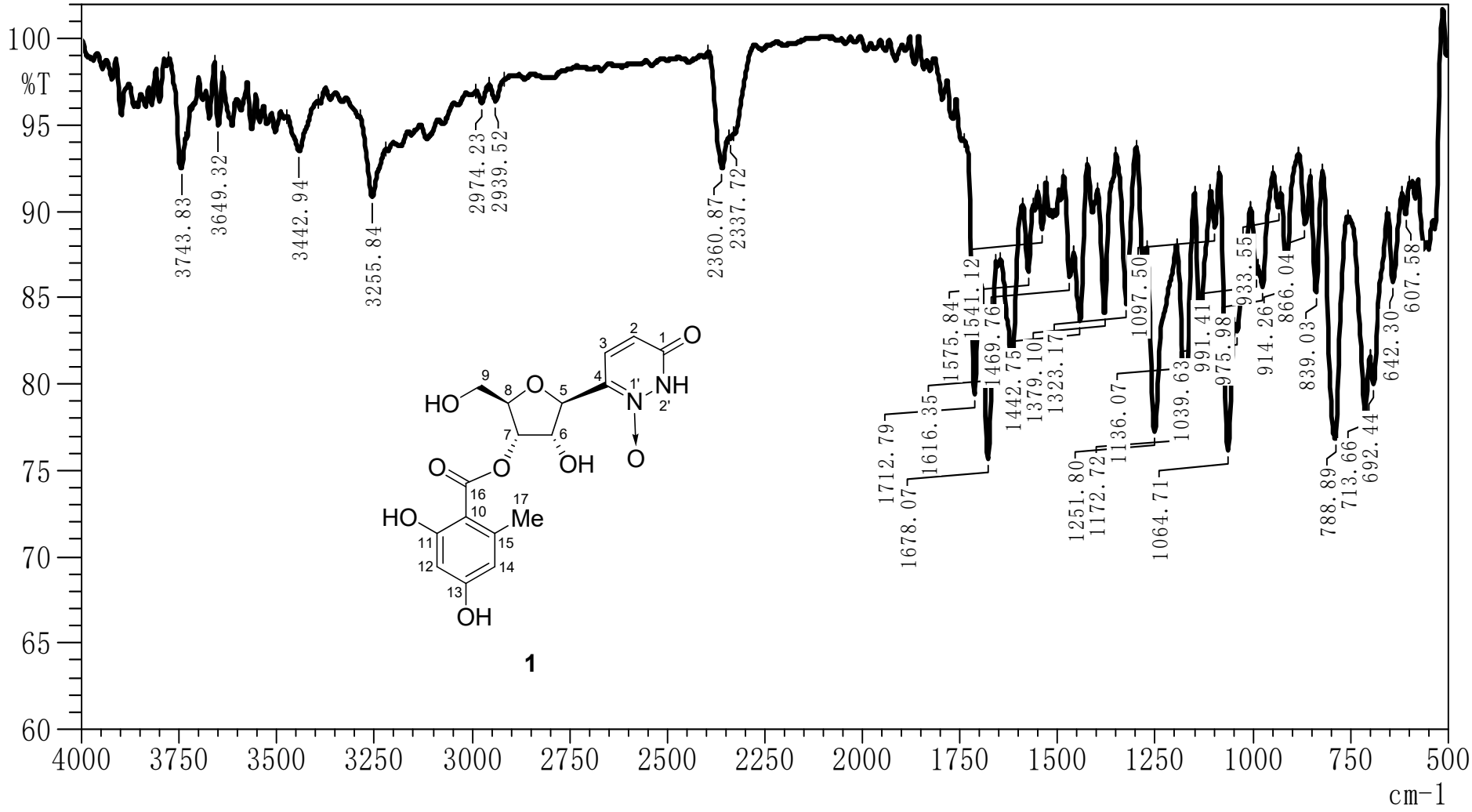


Figure S7. The IR spectrum of **2**

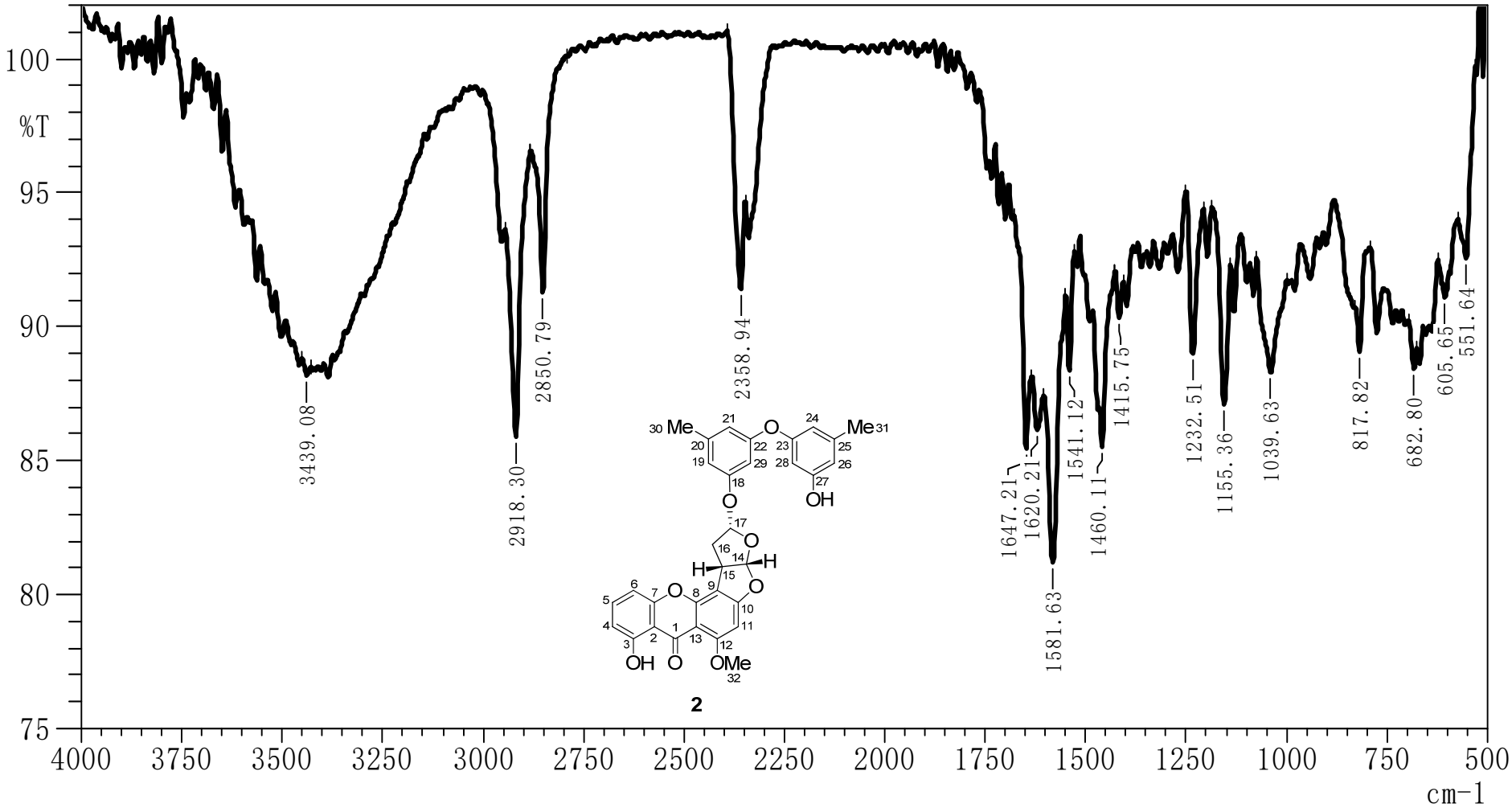


Figure S8. The IR spectrum of **3**