

**Aspergilins A–B, Including a Unique Orsellinic Acid–Ribose–
Pyridazinone-*N*-oxide Hybrid, from the Mangrove Endophytic
Fungus *Aspergillus* sp. A1E3**

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Guangzhou 510515, PR China

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(Guangying Chen)

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HR-ESIMS for 1

Mass Spectrum SmartFormula Report

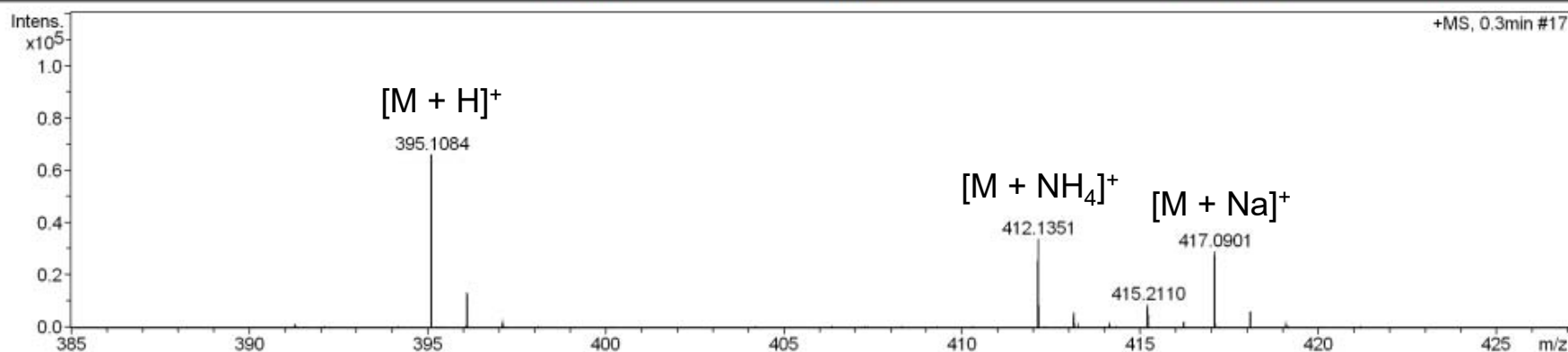
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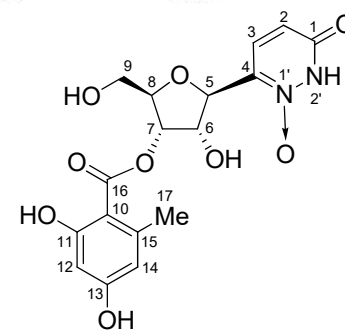
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printed: 10/27/2021 4:47:14 PM

by: SCSIO

Page 1 of 1

S4

HR-ESIMS for 1

Generic Display Report

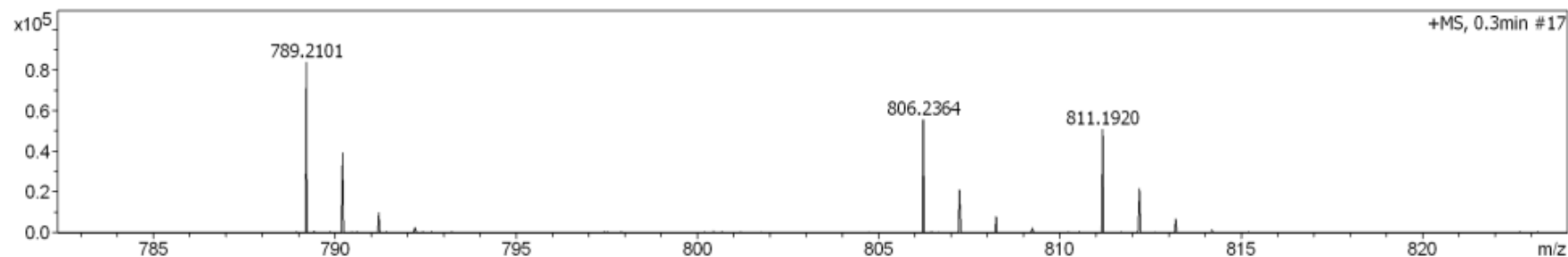
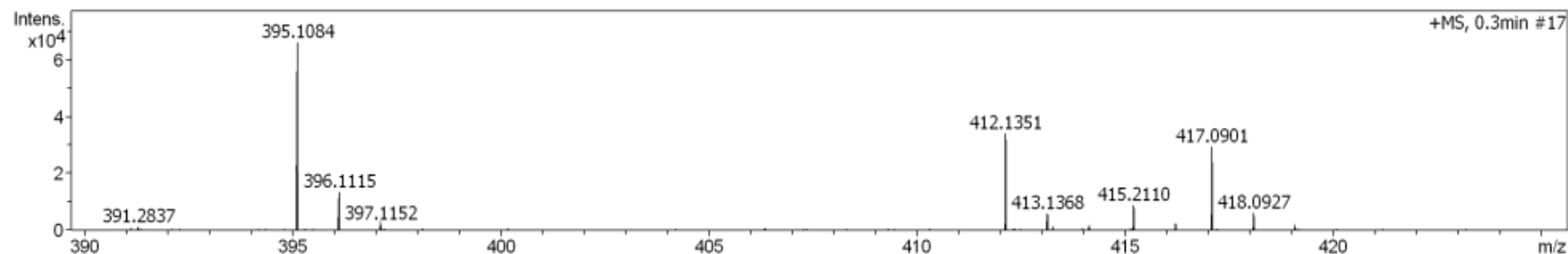
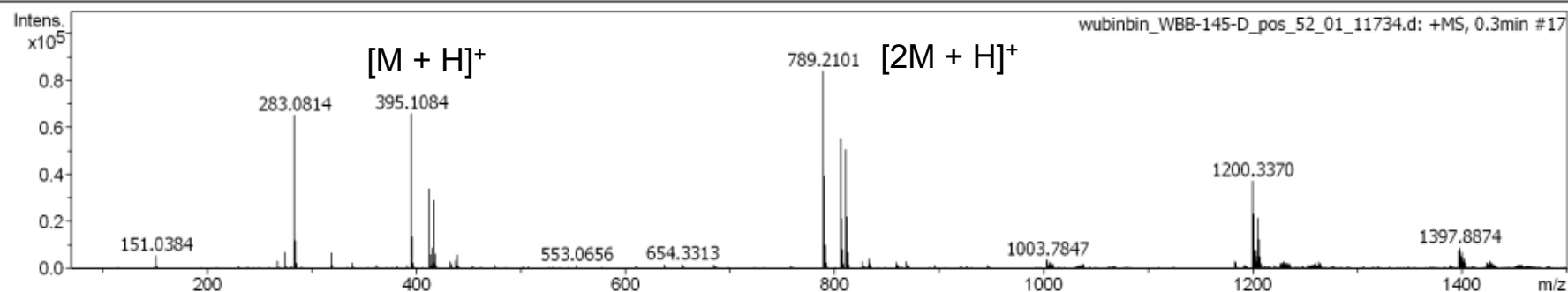
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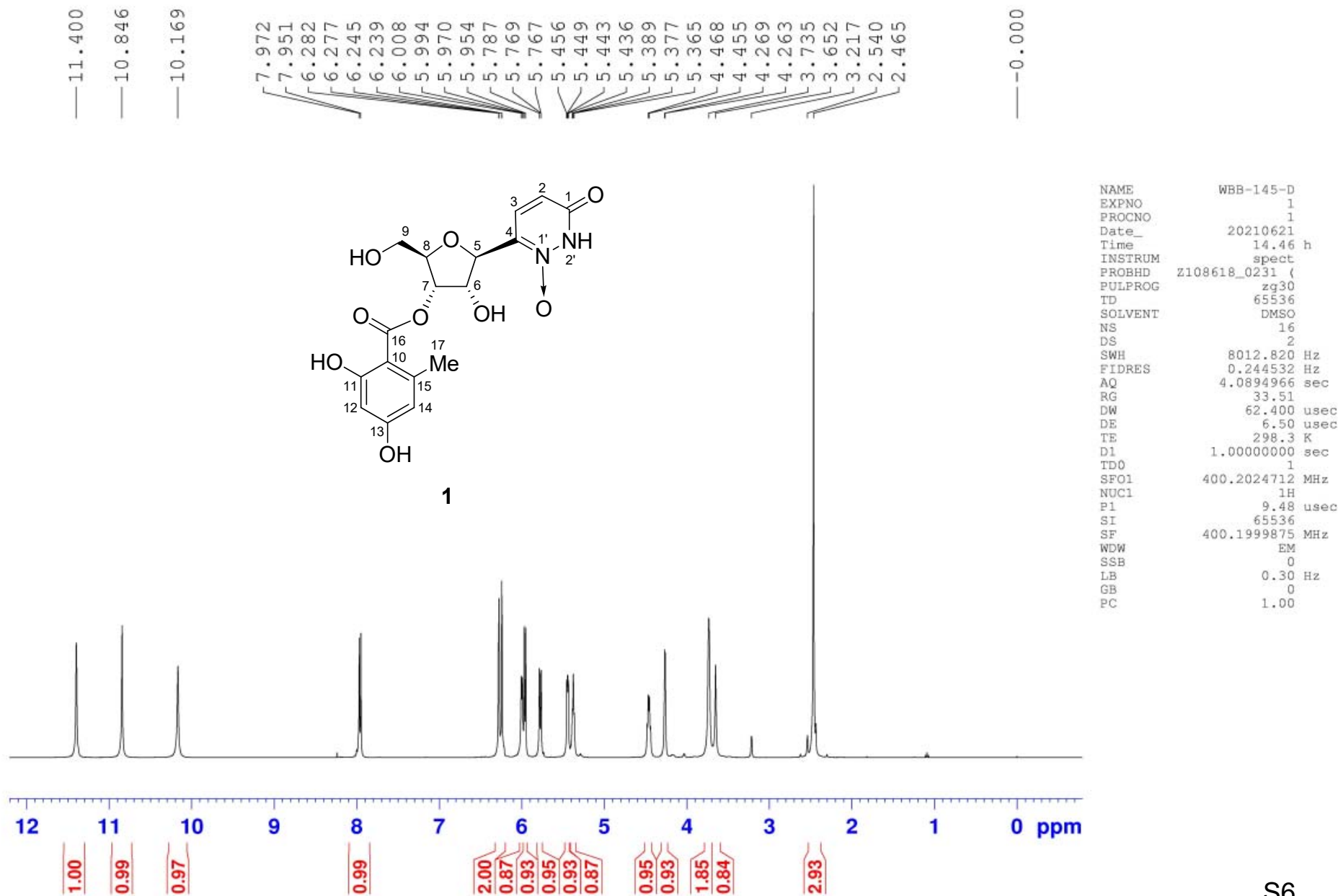
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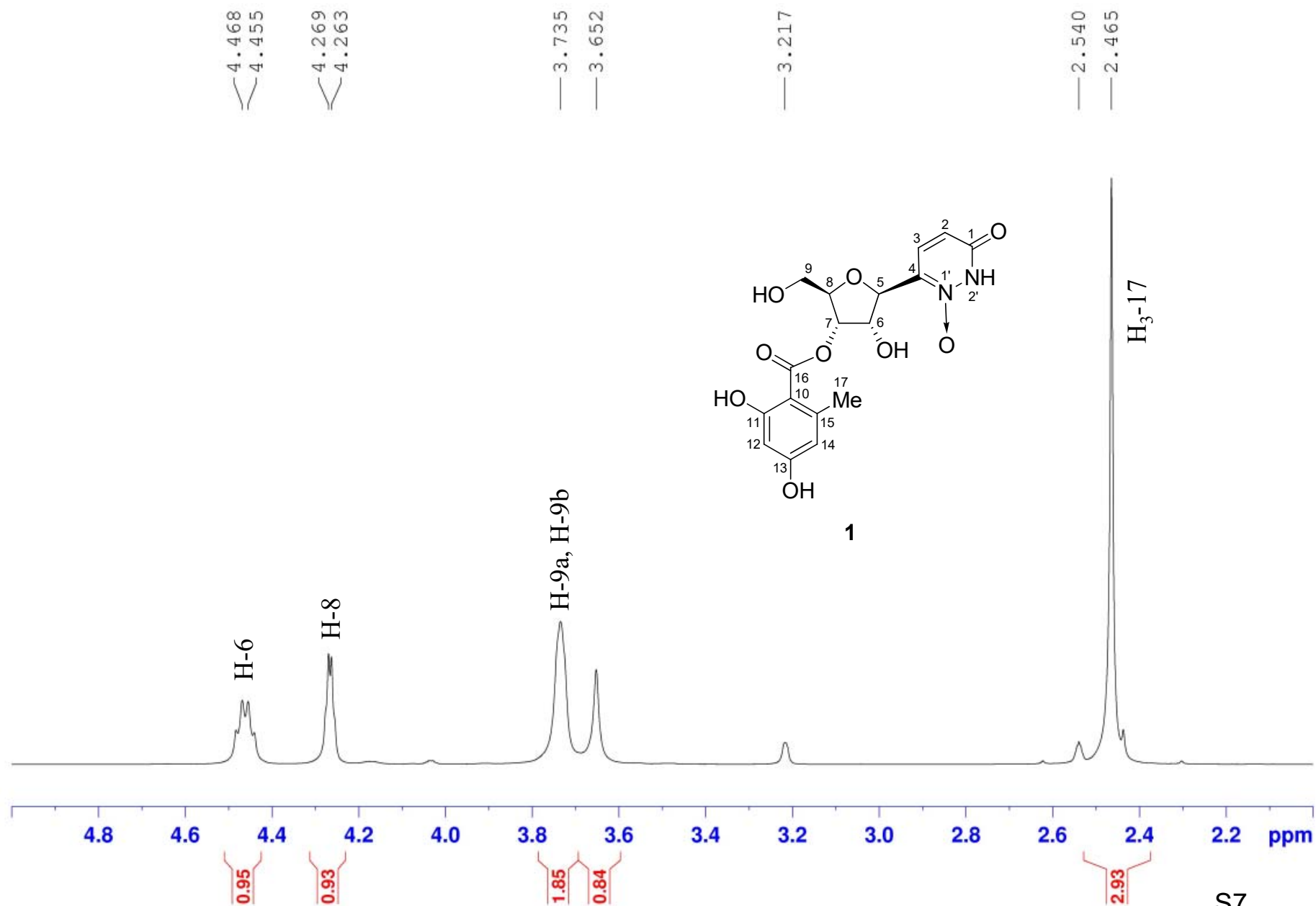
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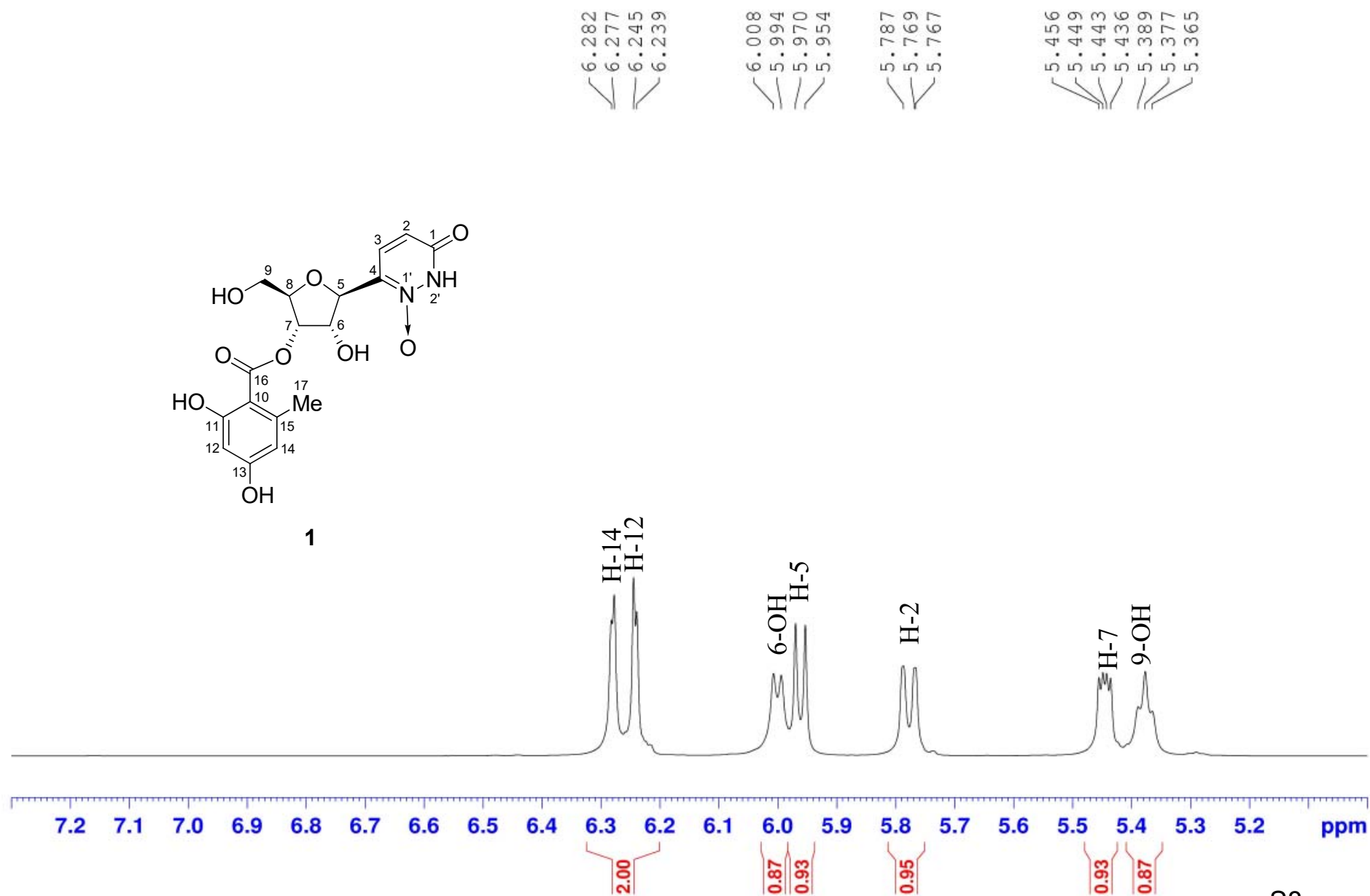
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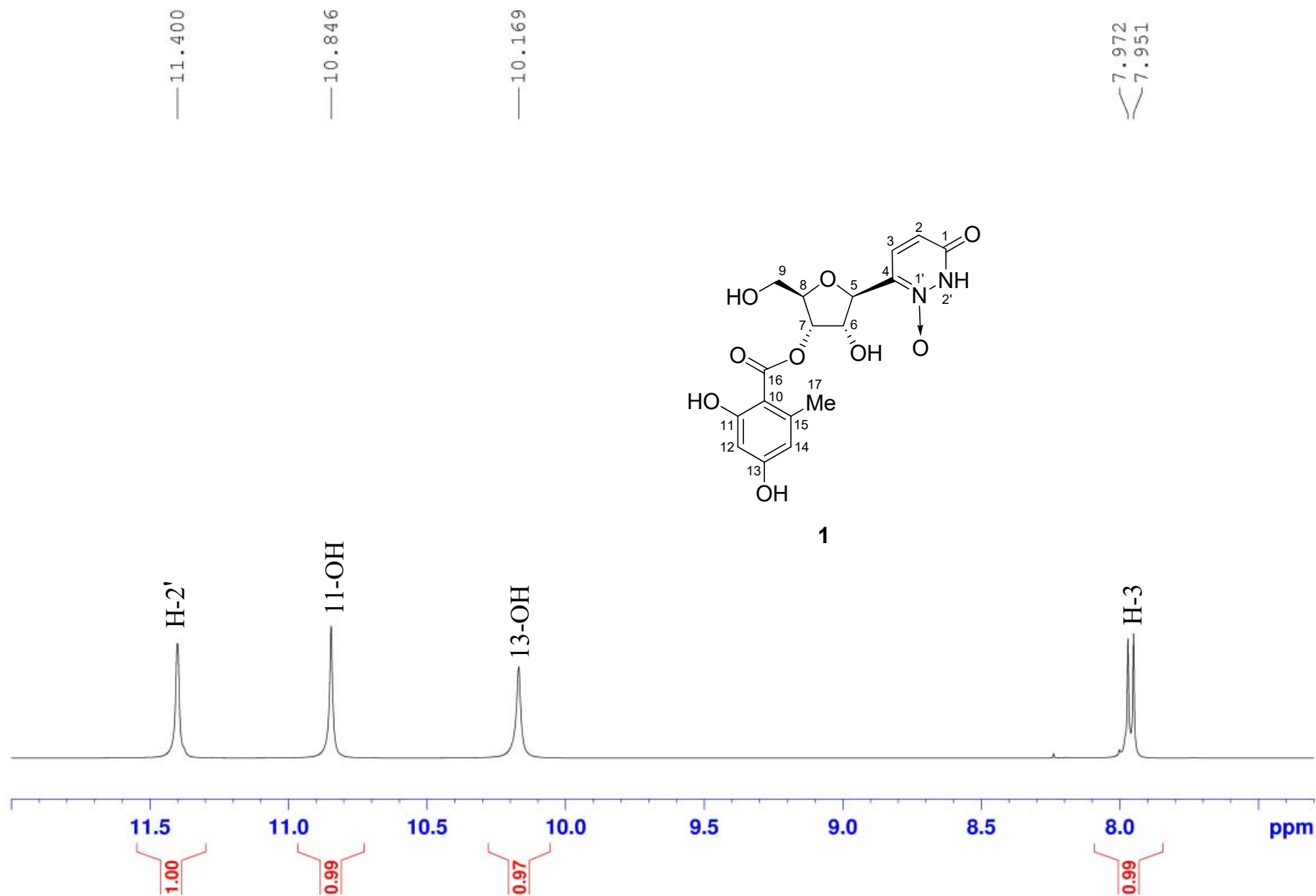
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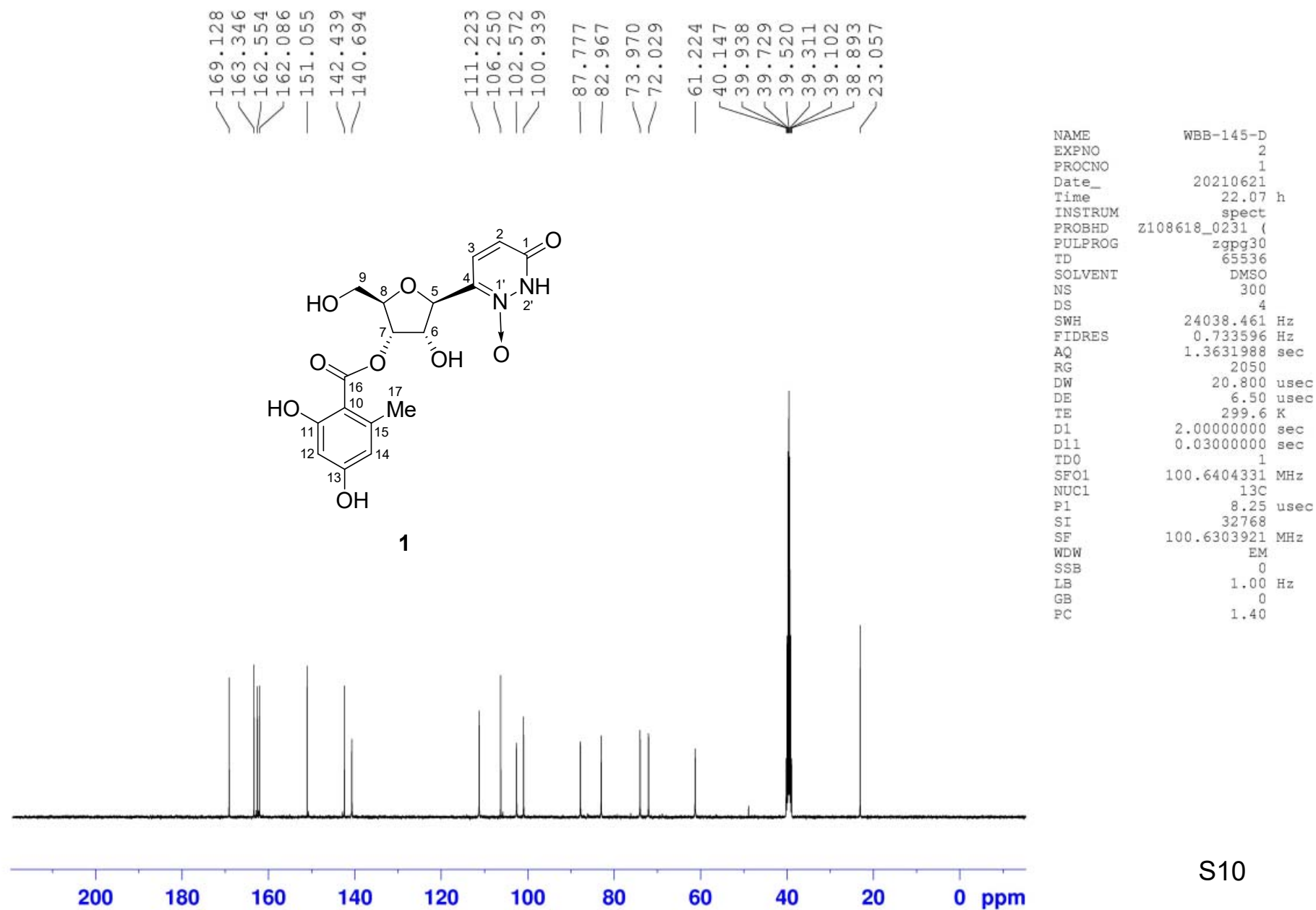
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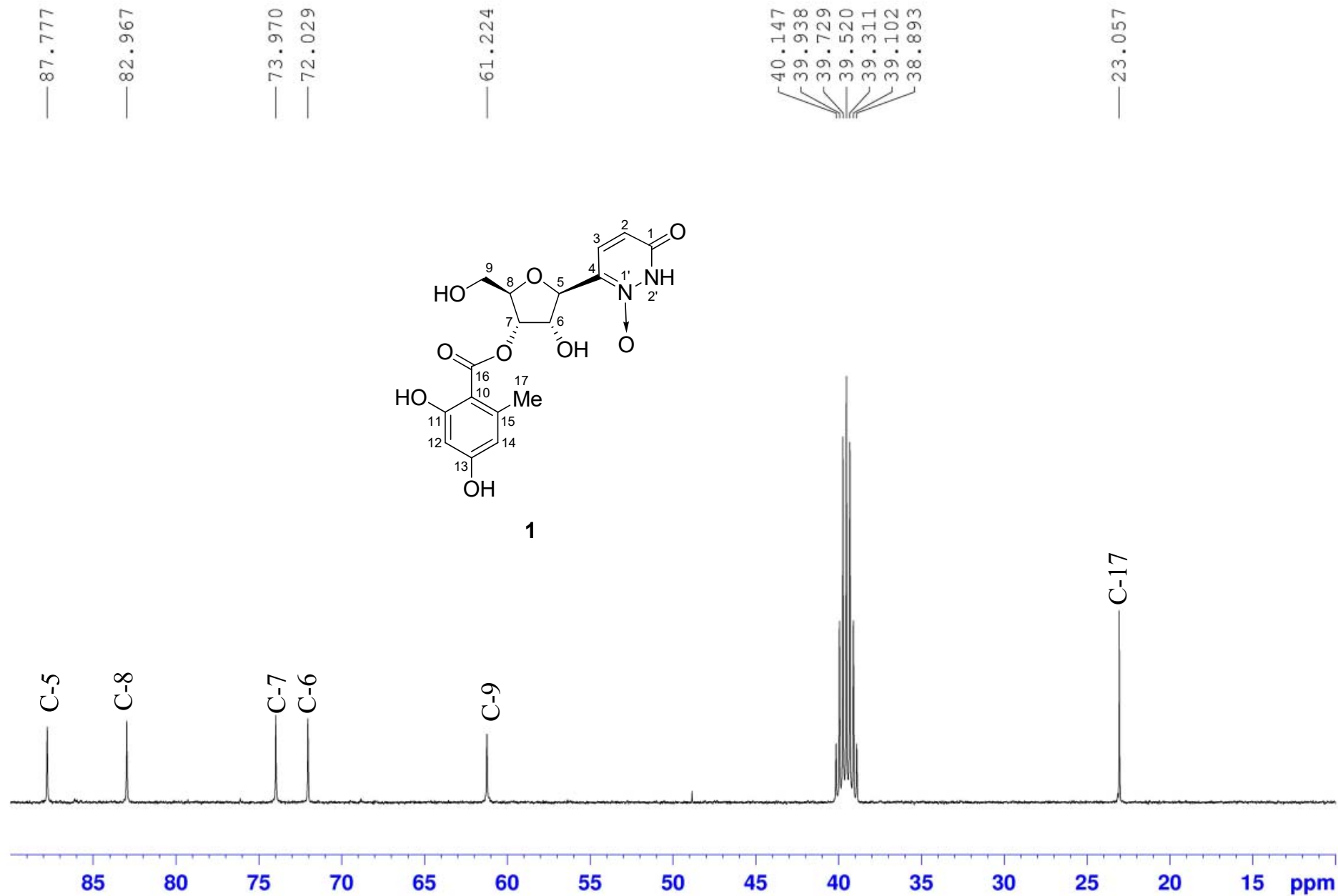
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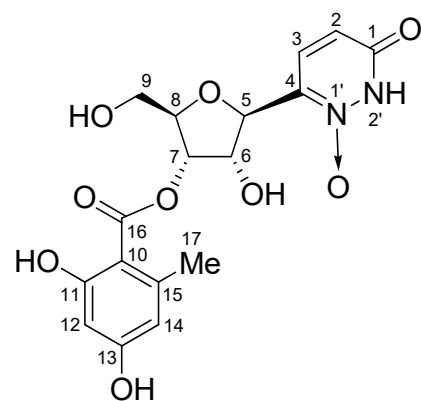
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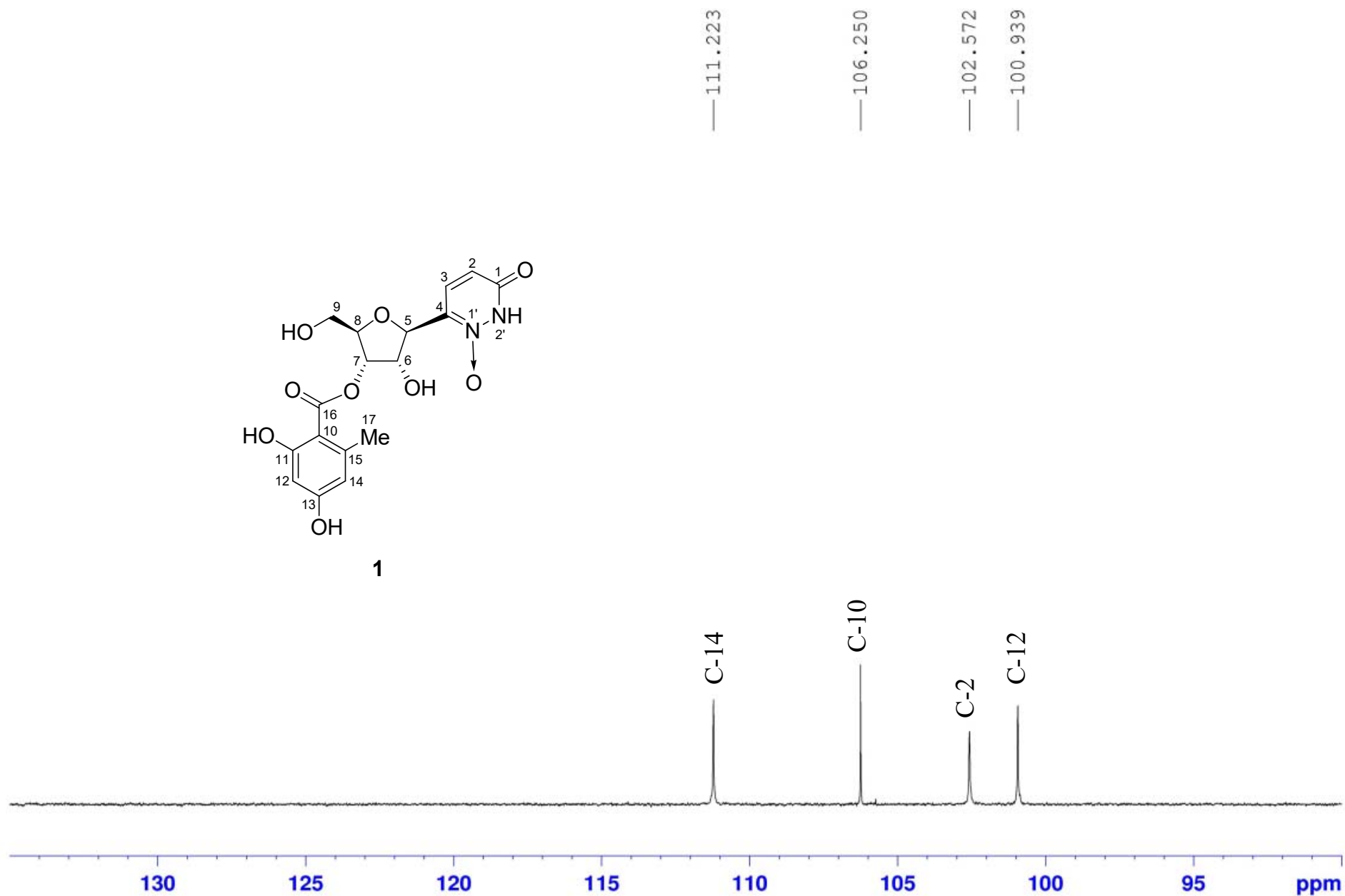
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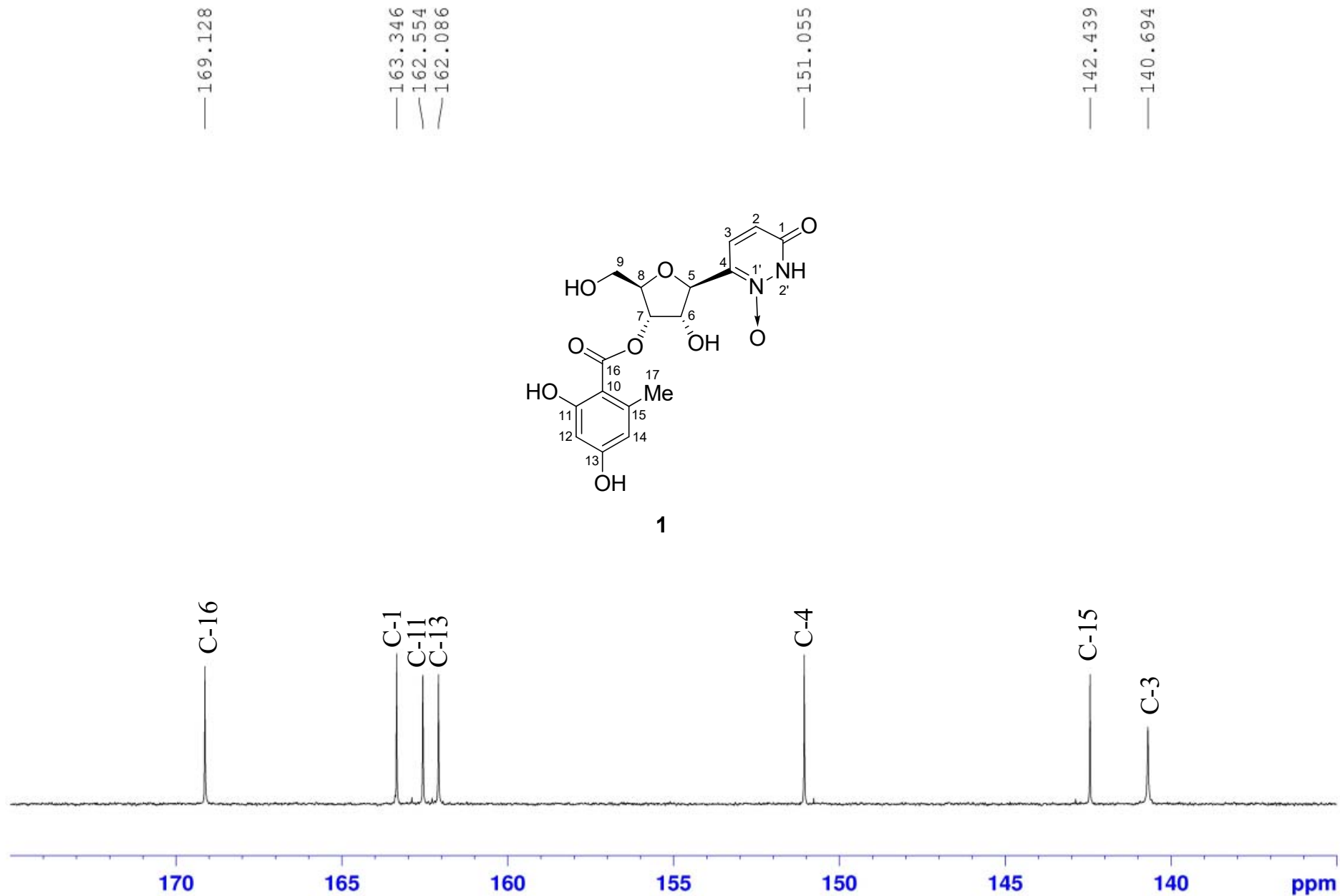
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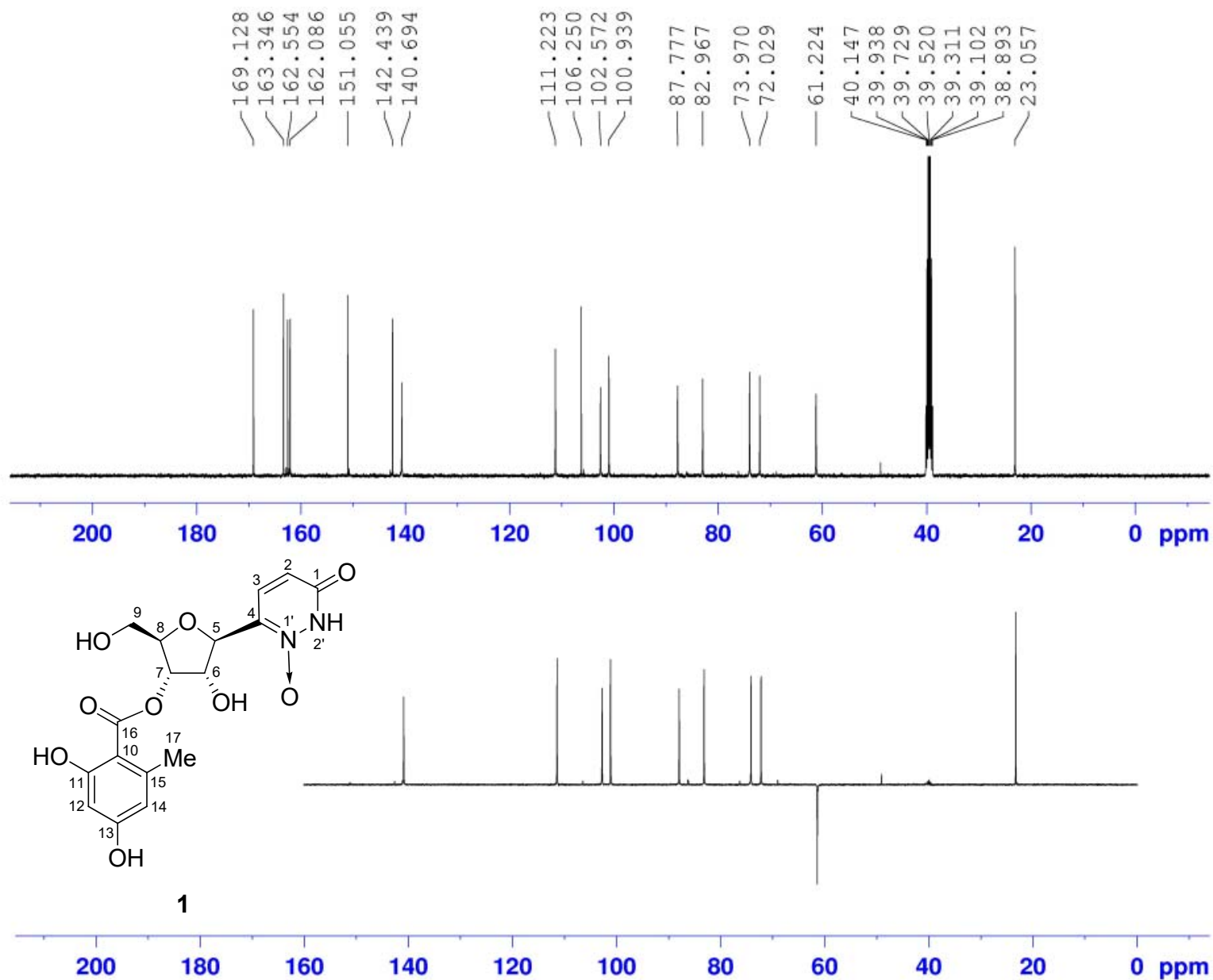
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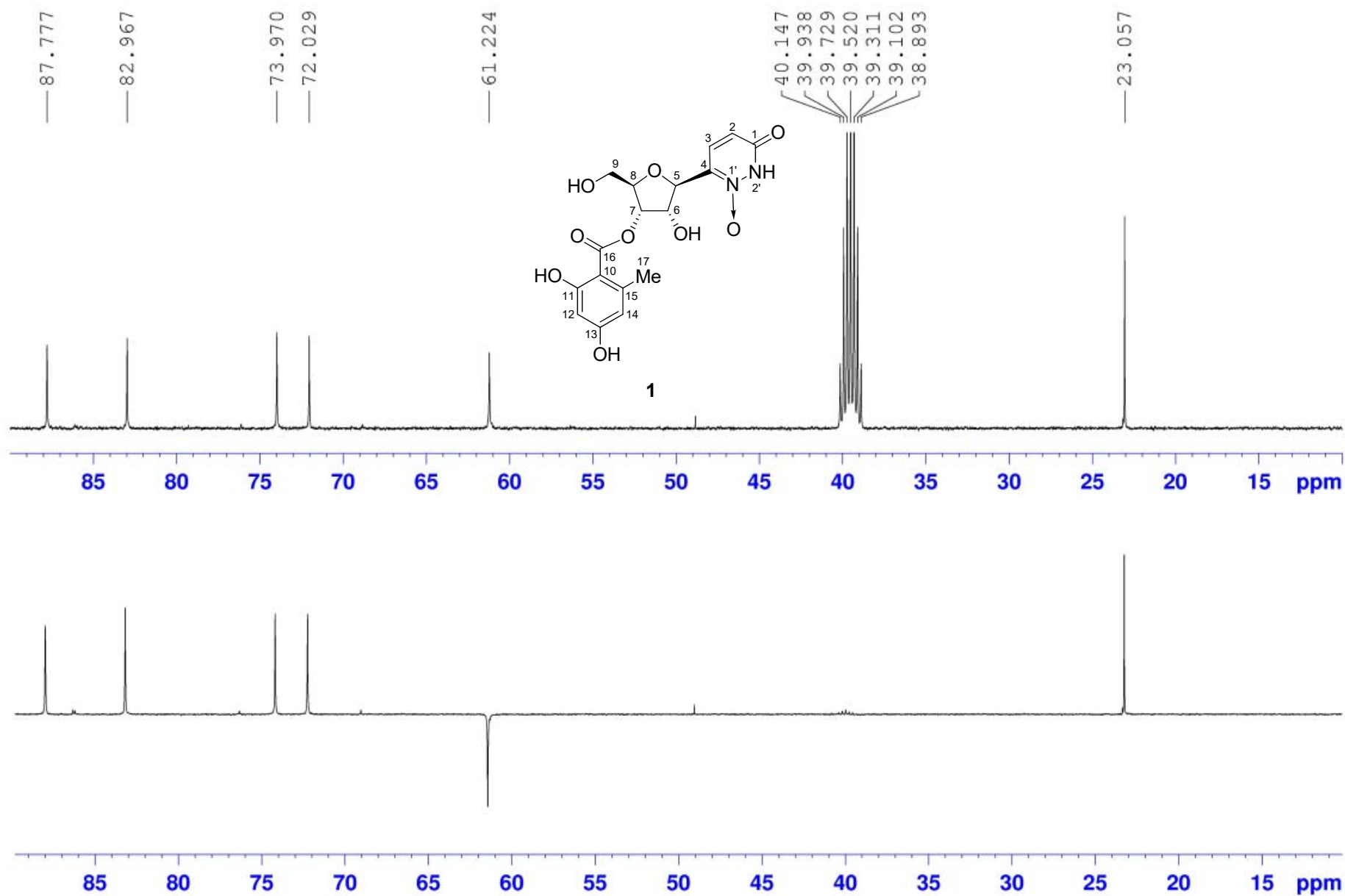
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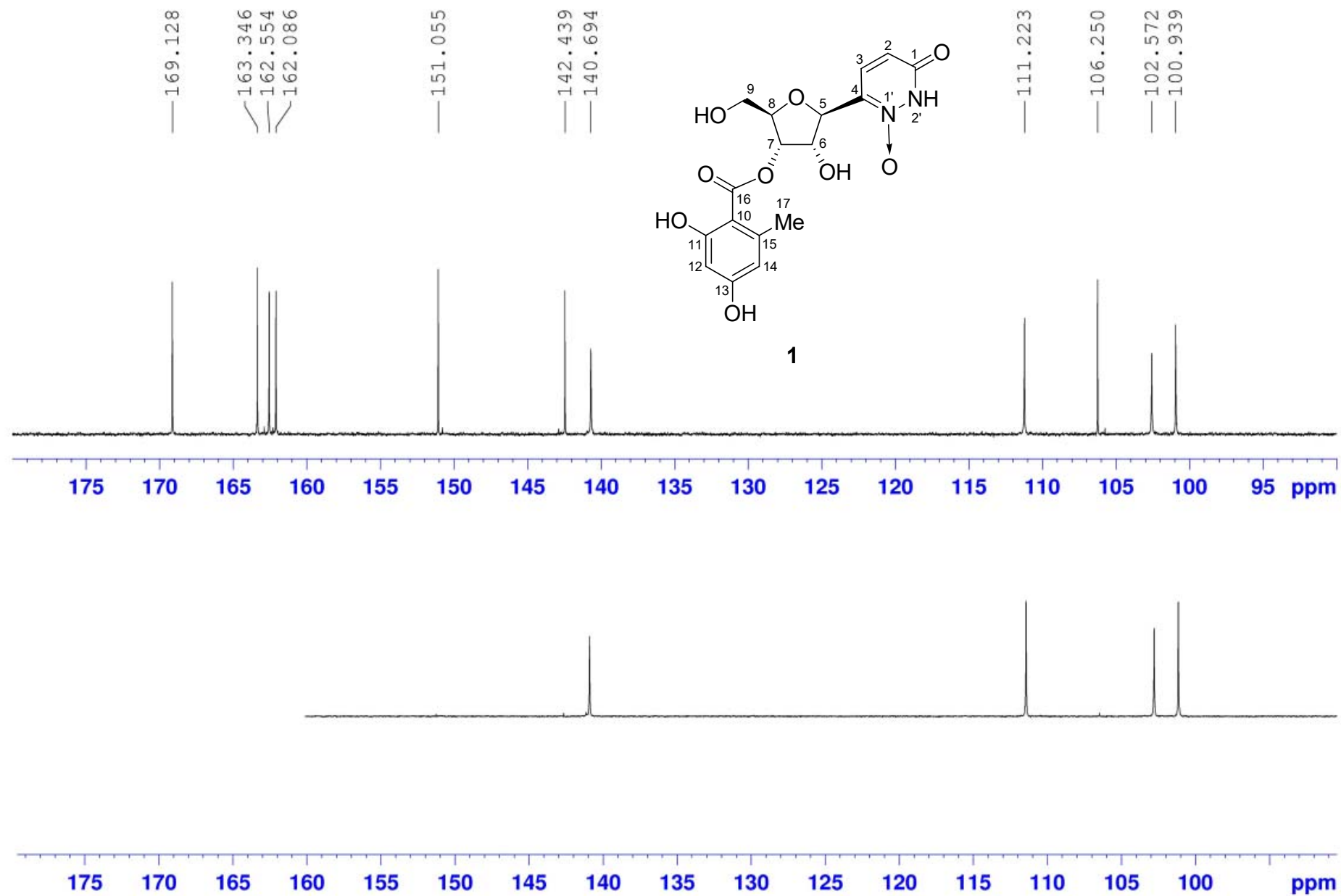
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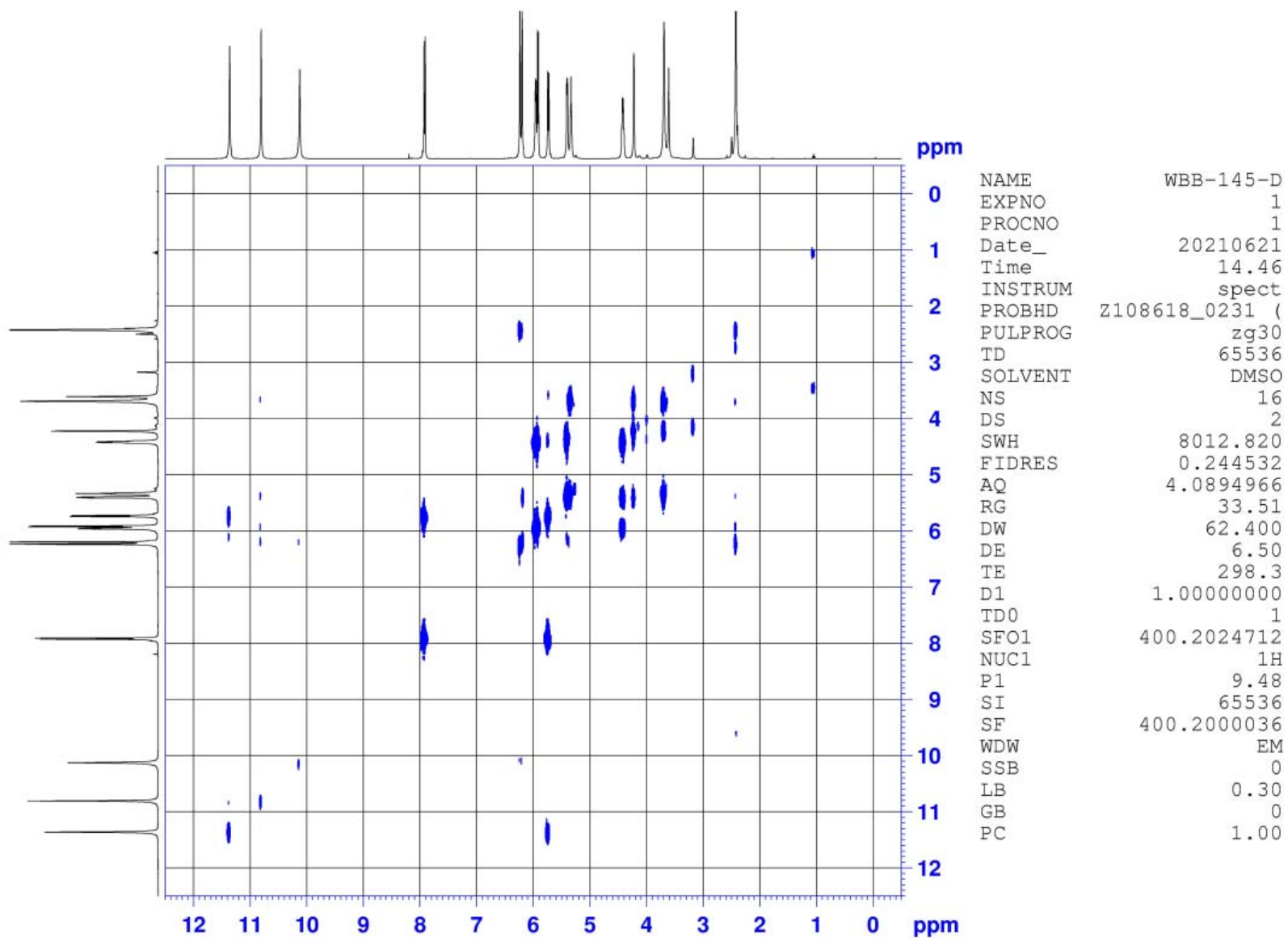
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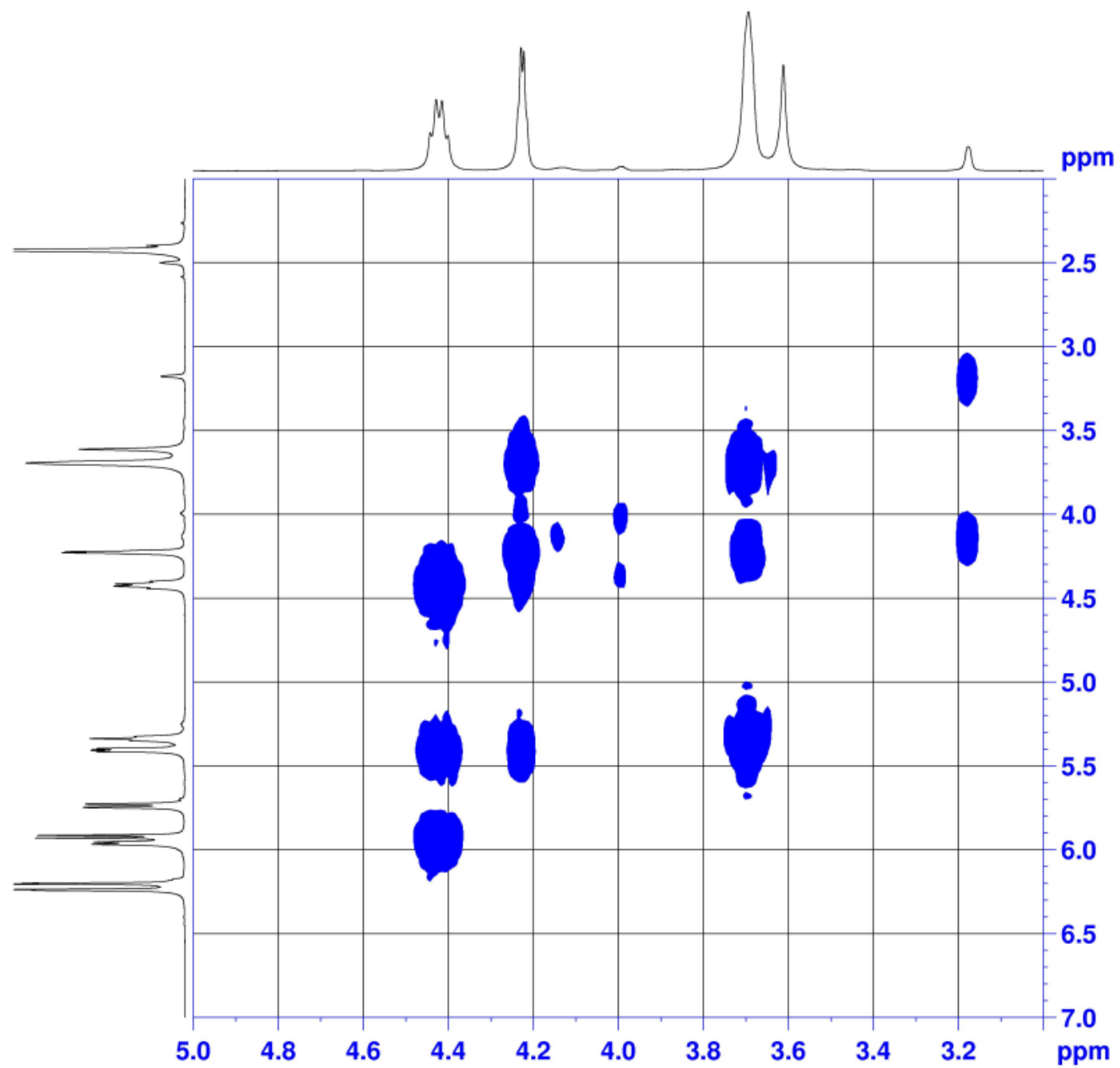
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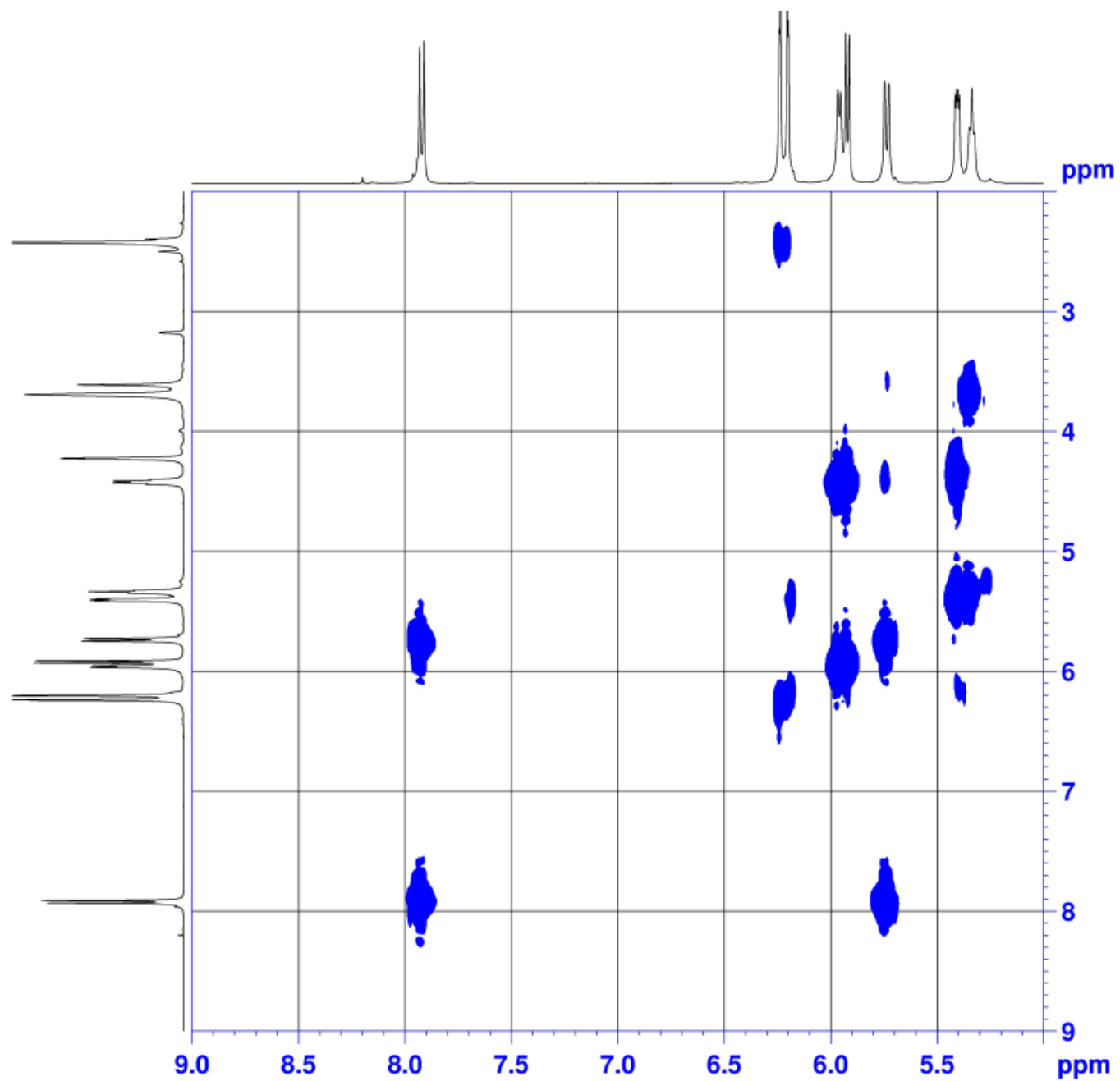
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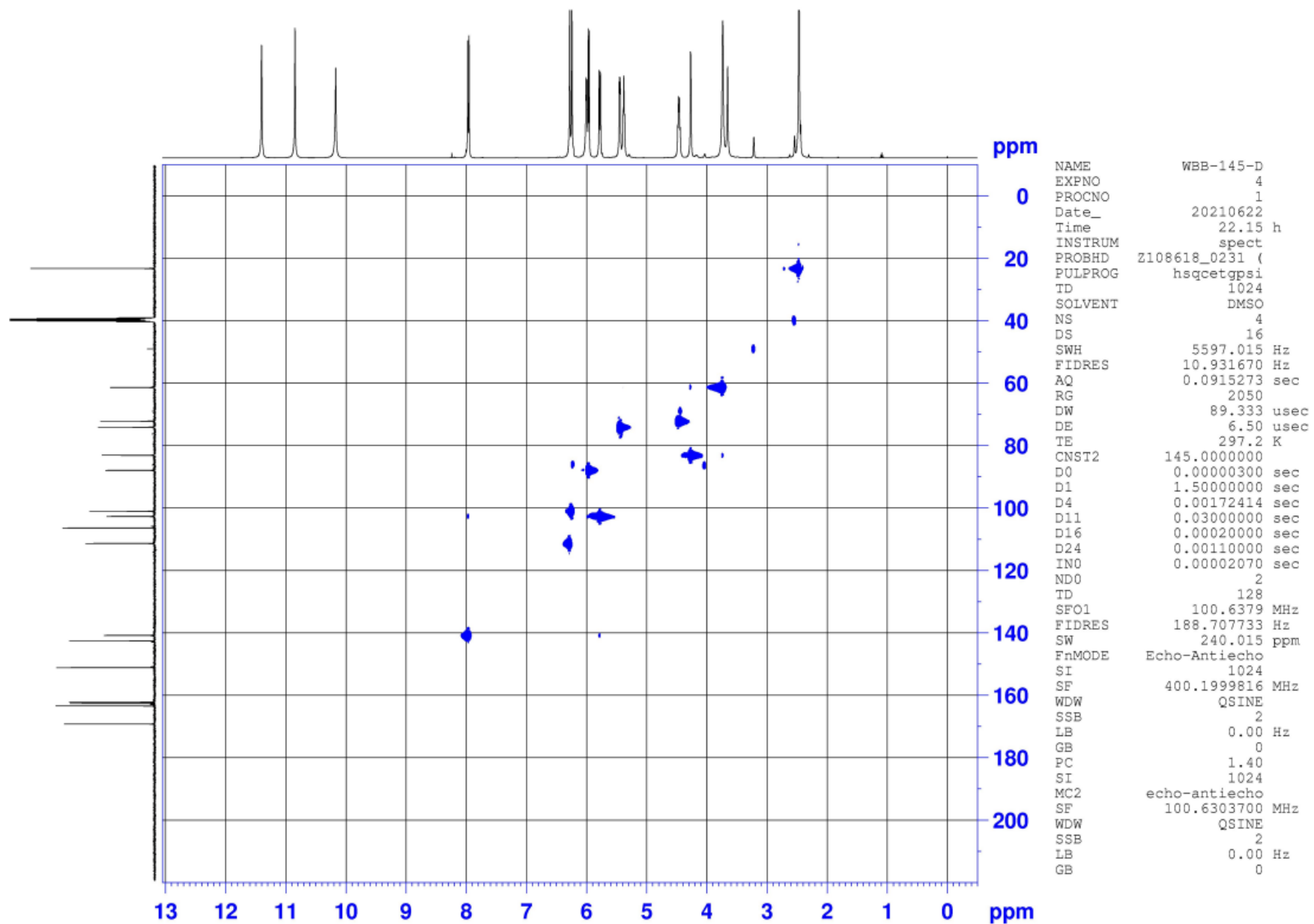
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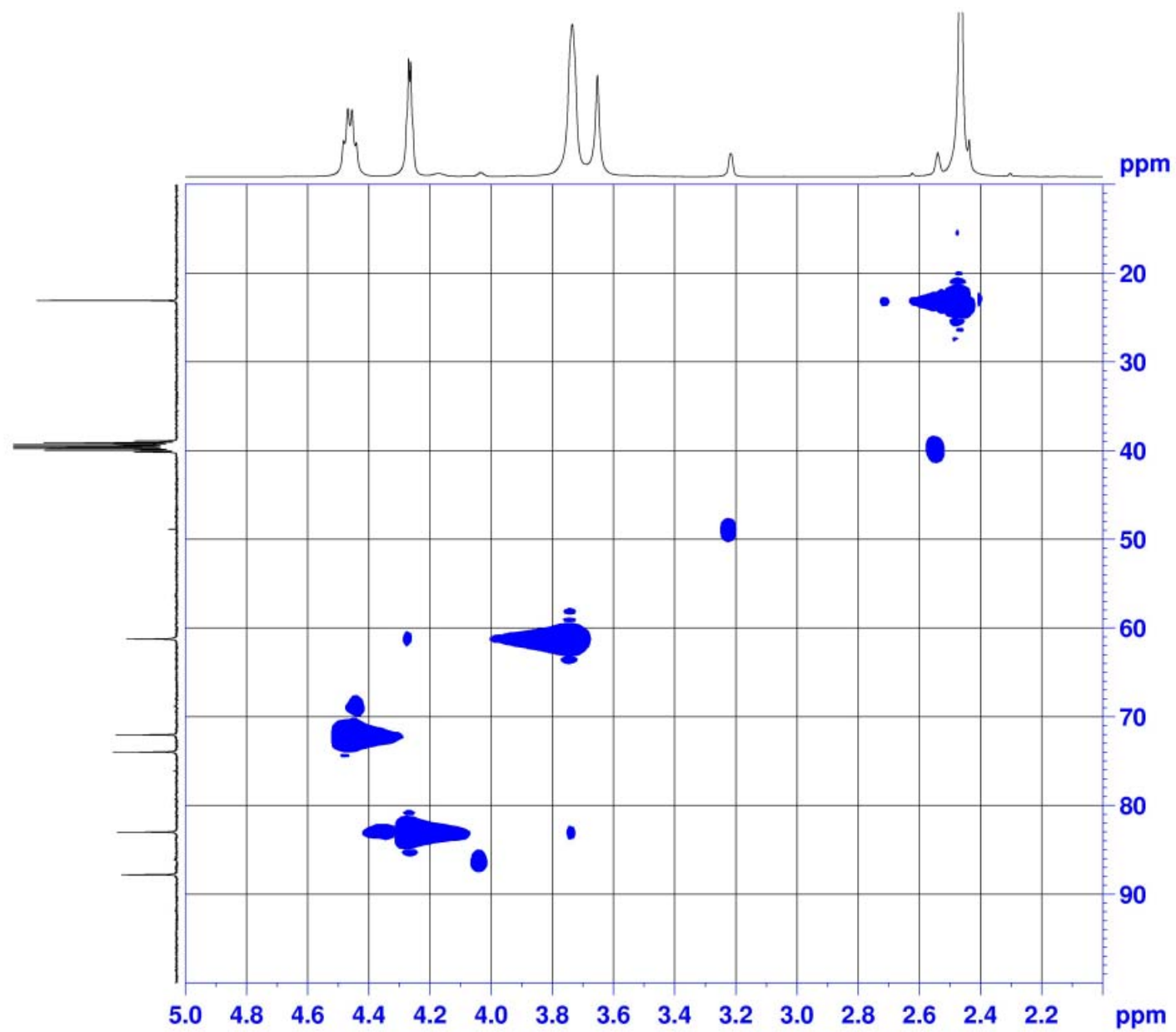
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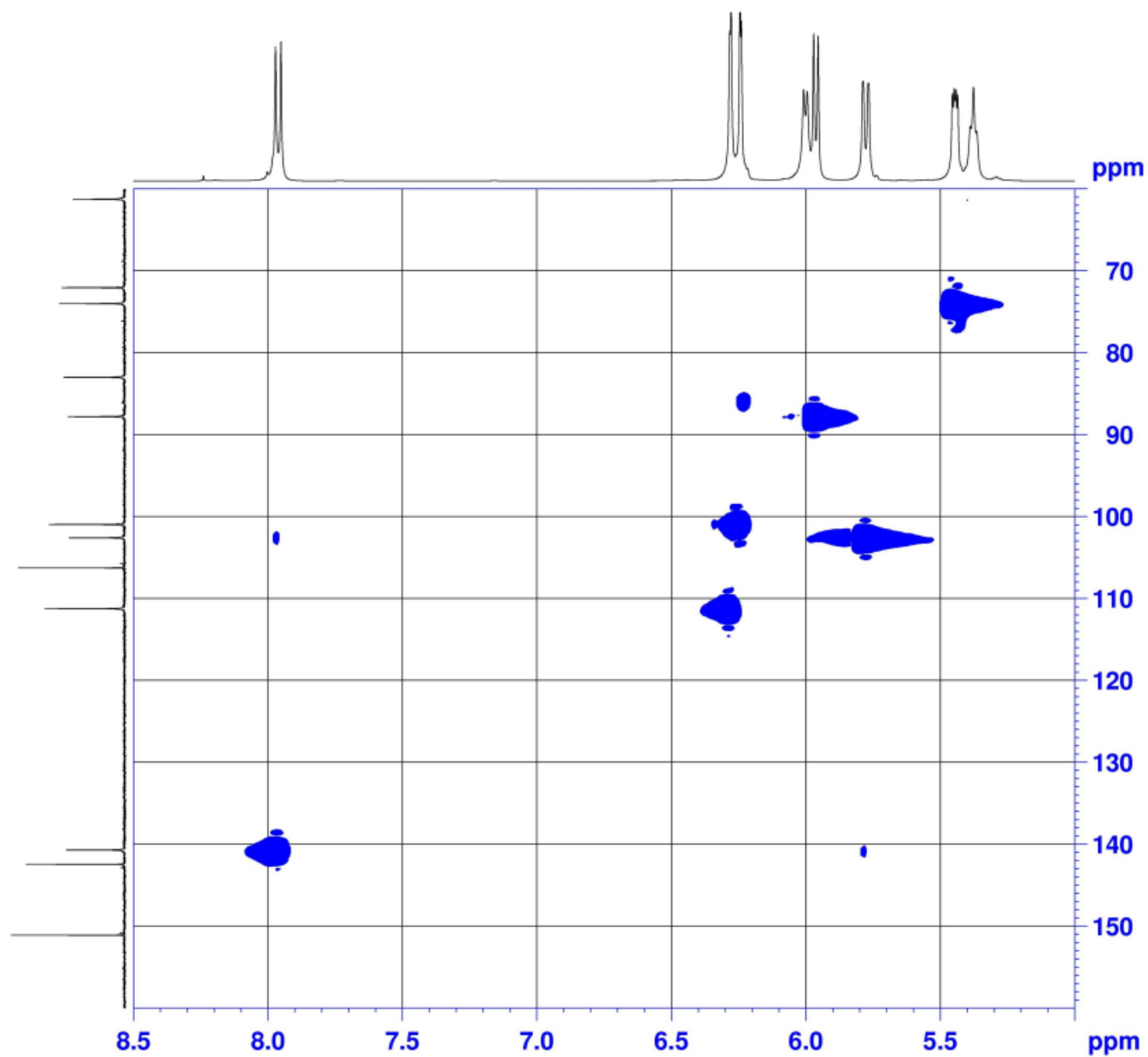
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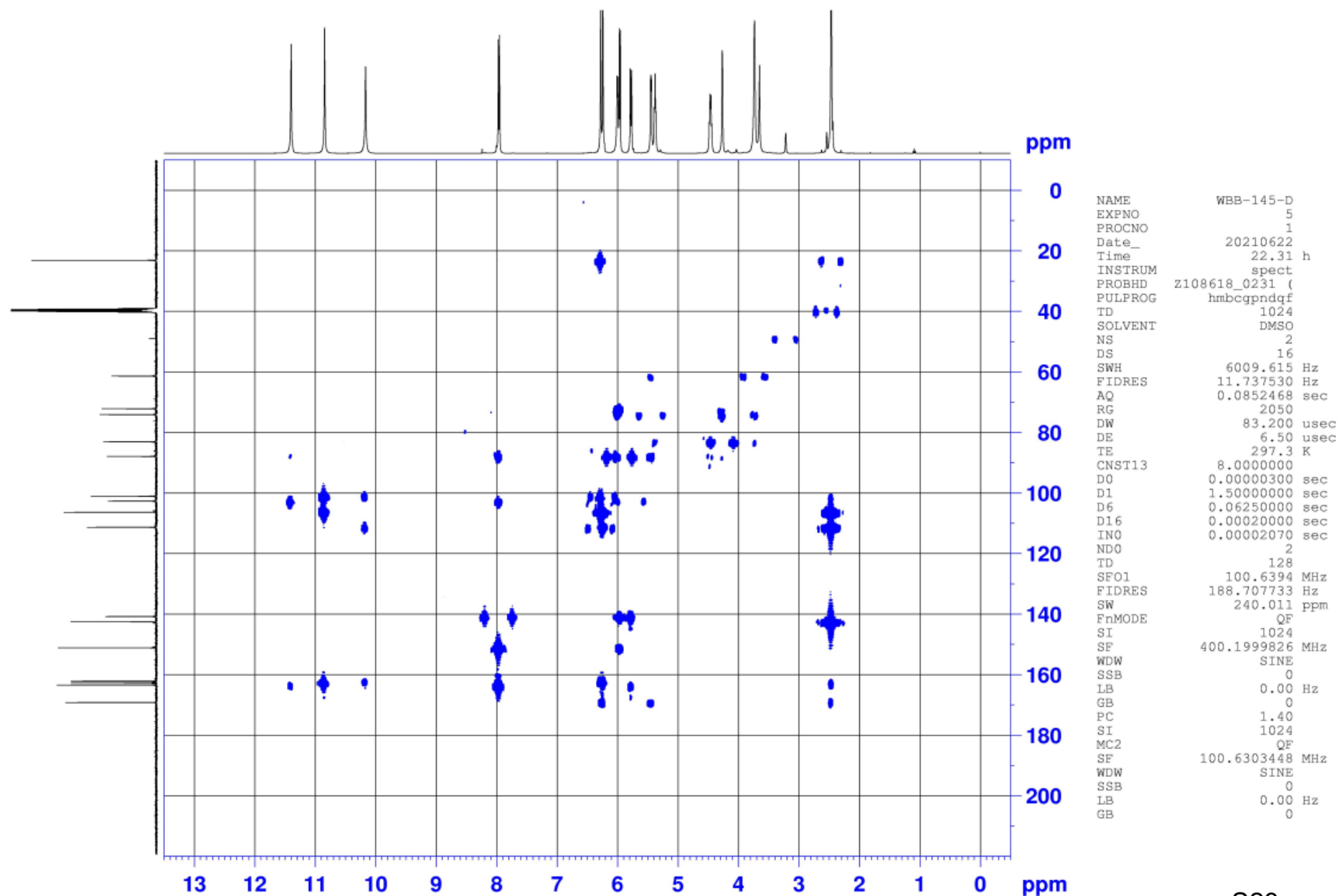
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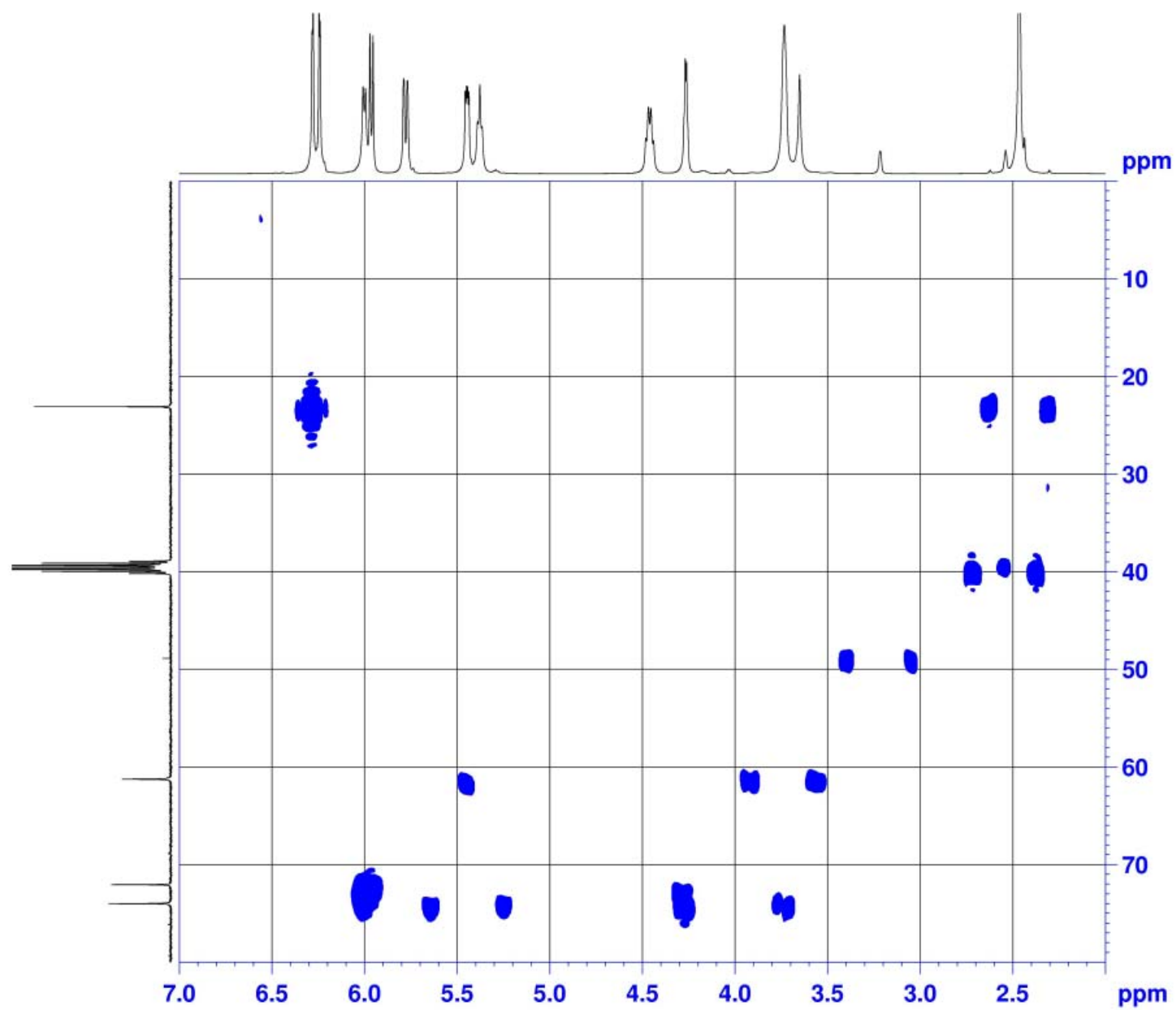
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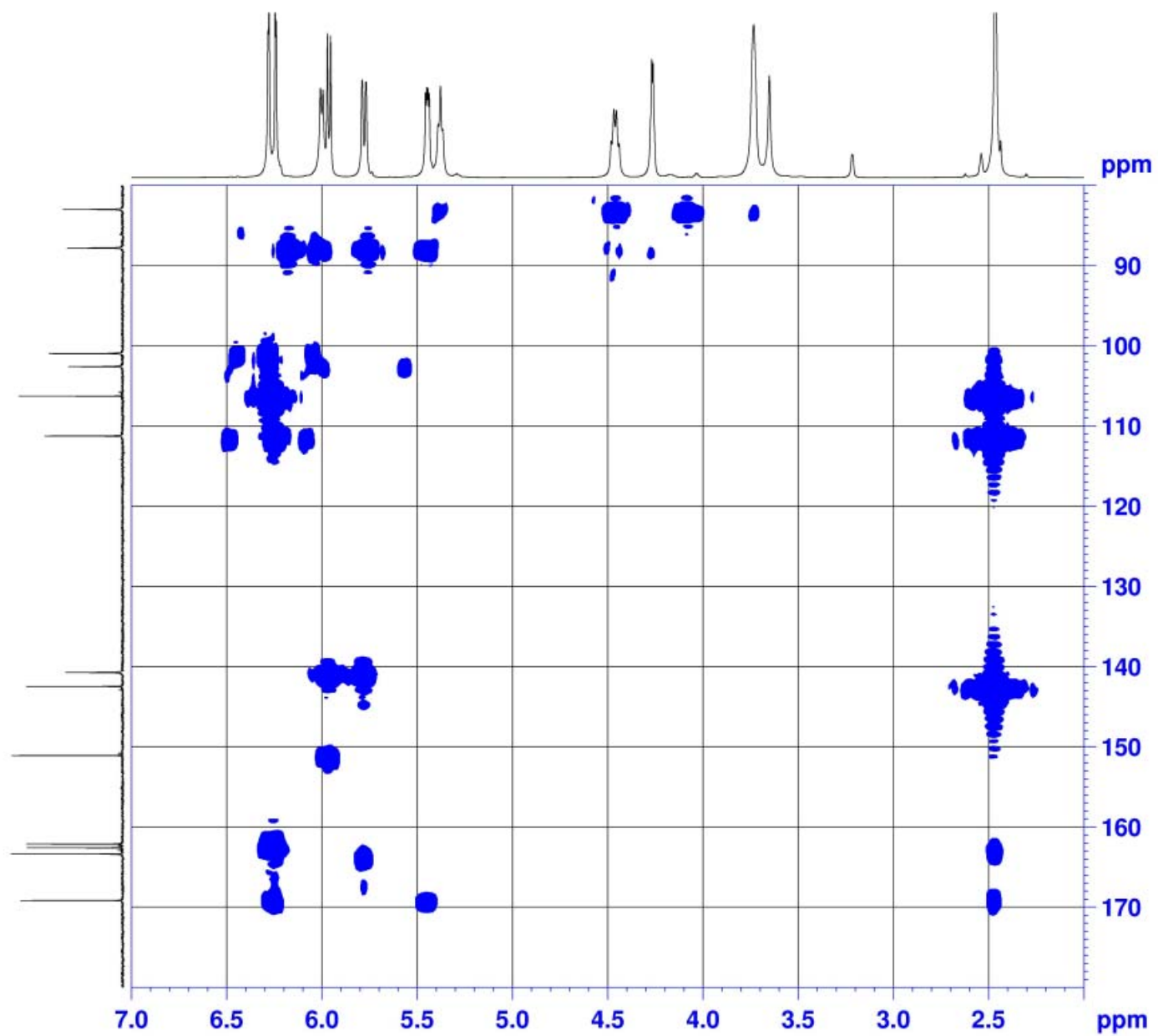
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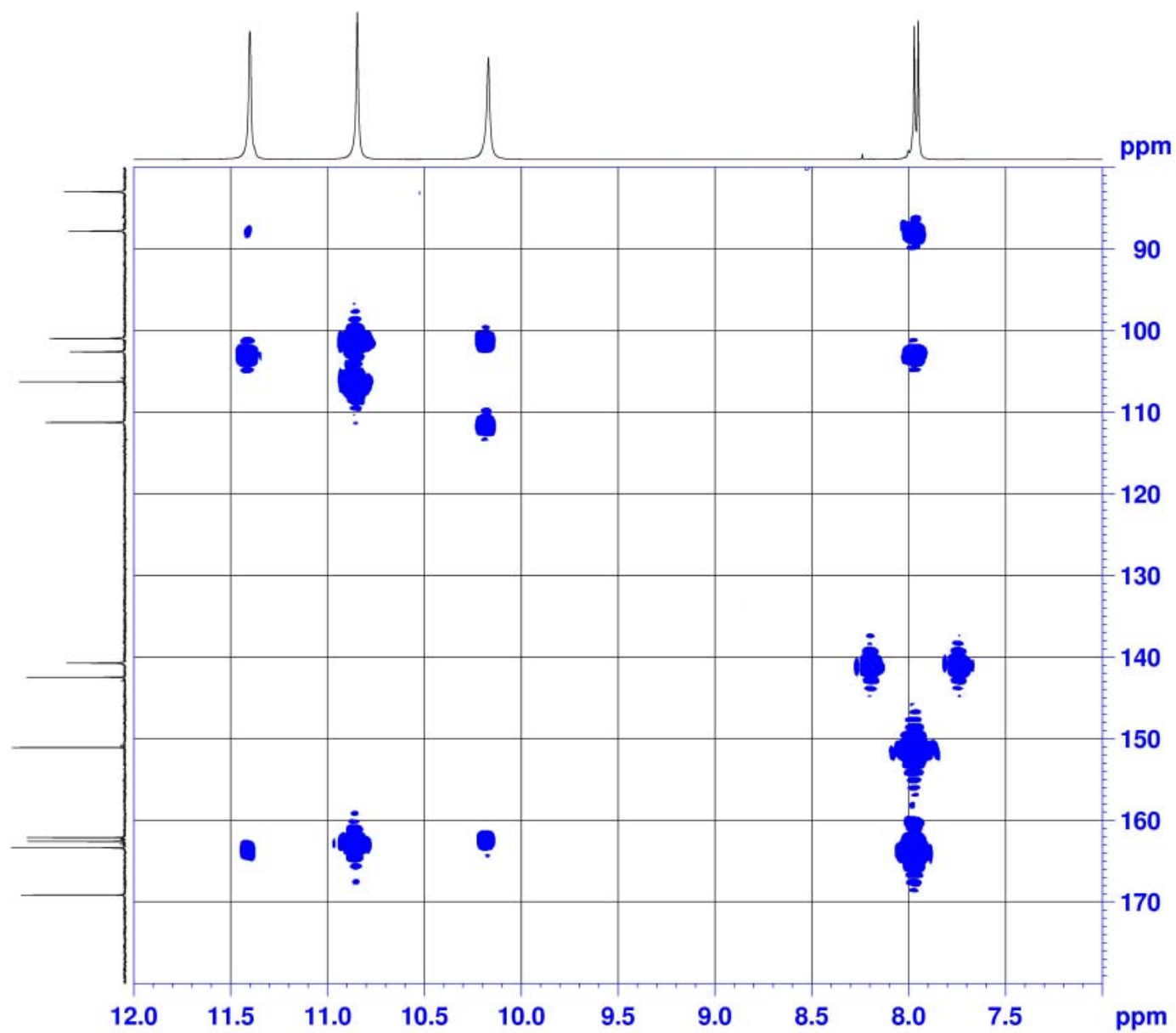
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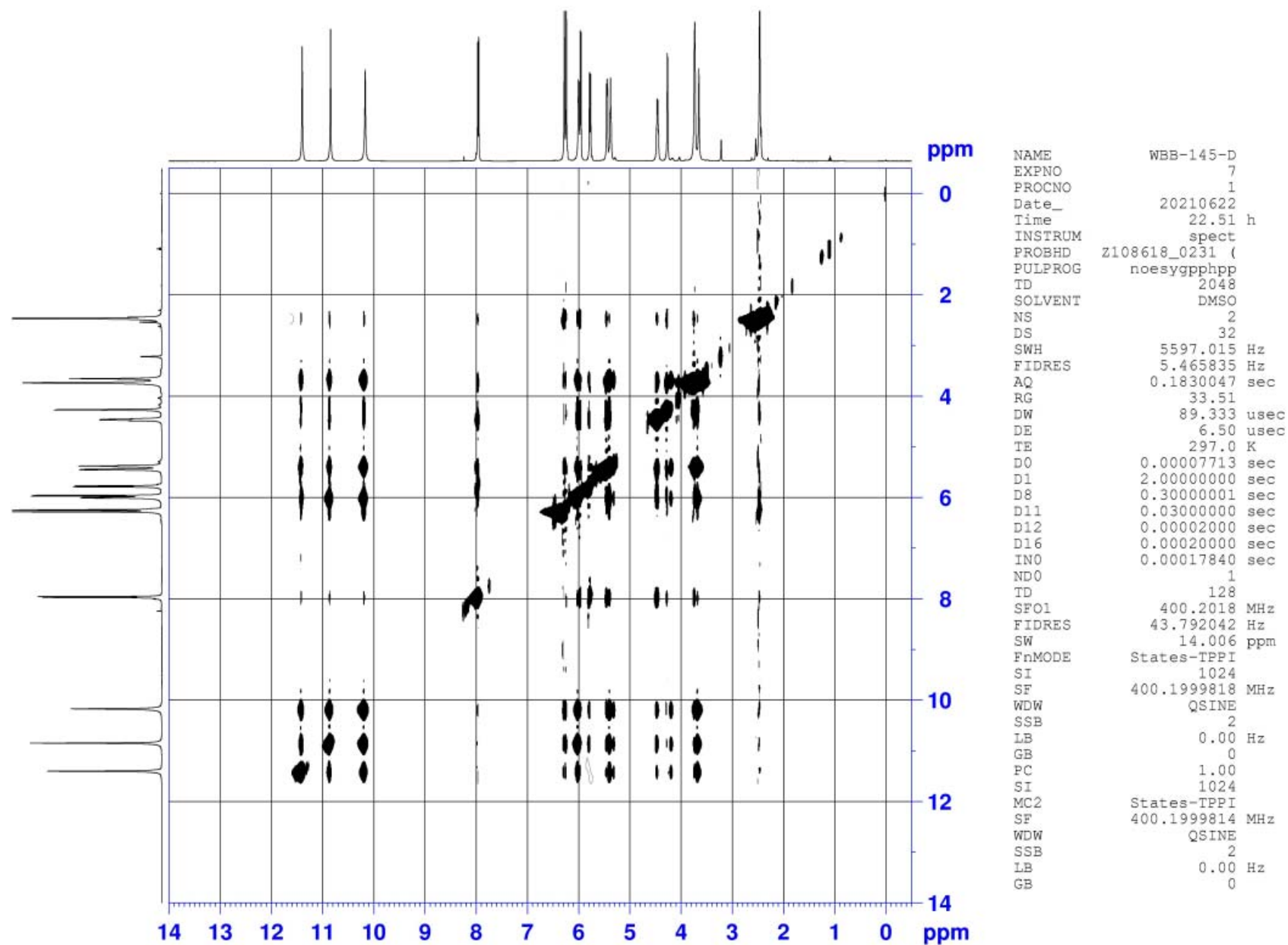
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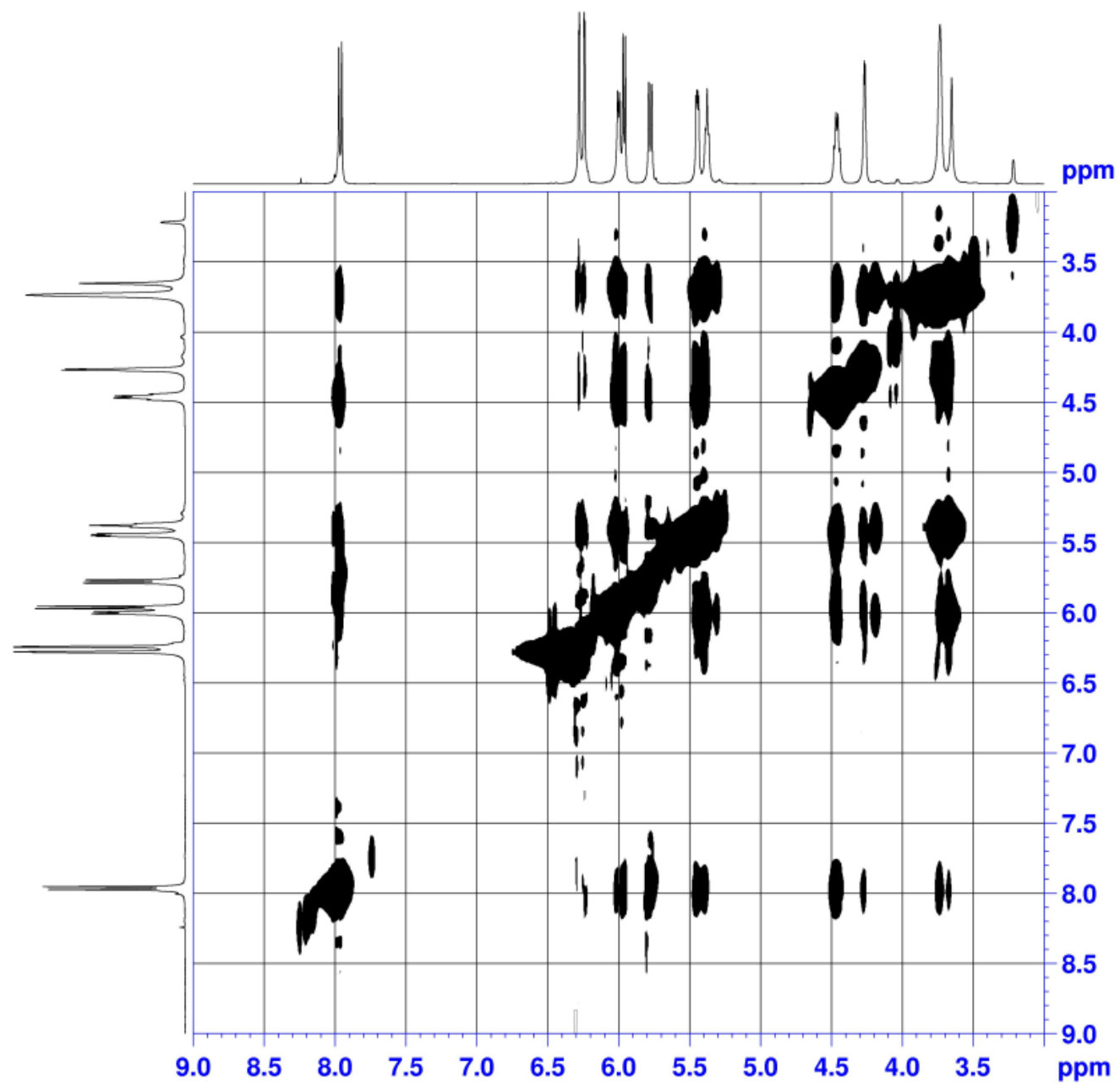
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NOESY (400 MHz) spectrum of **1** in DMSO-*d*₆



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



HR-ESIMS for 2

Mass Spectrum SmartFormula Report

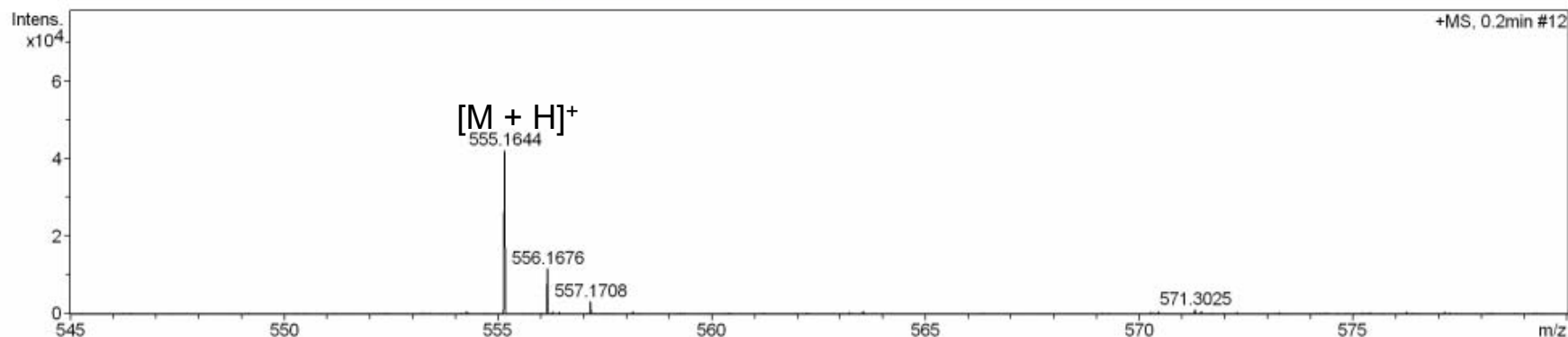
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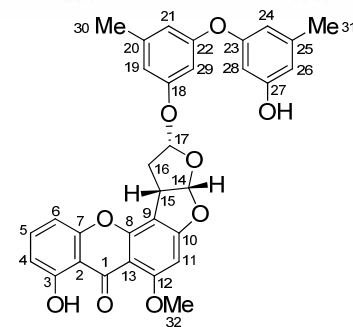
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2

S29

HR-ESIMS for 2

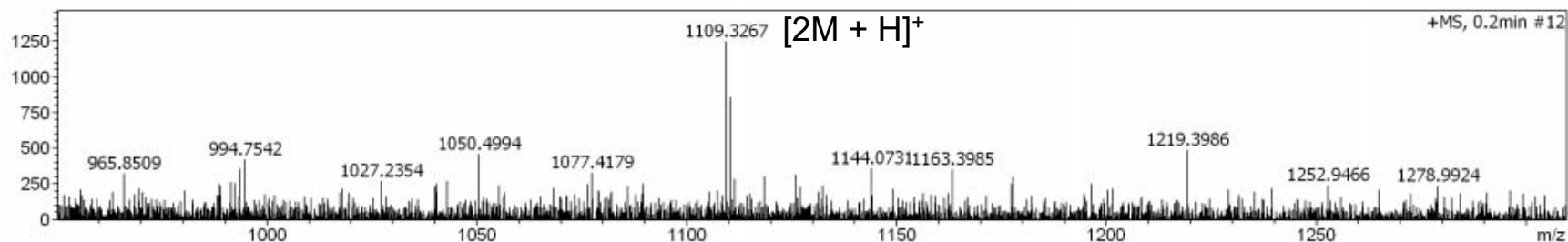
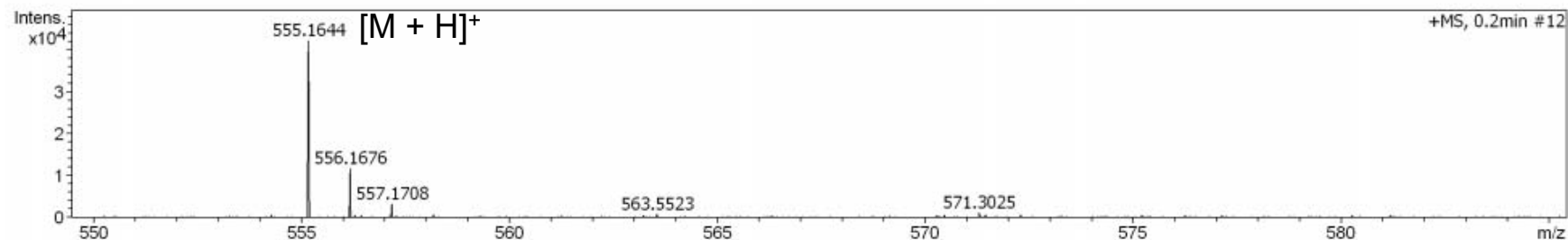
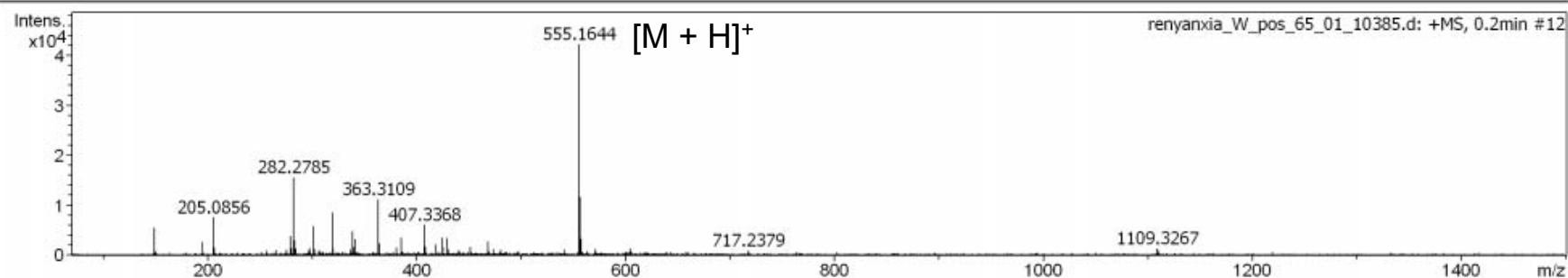
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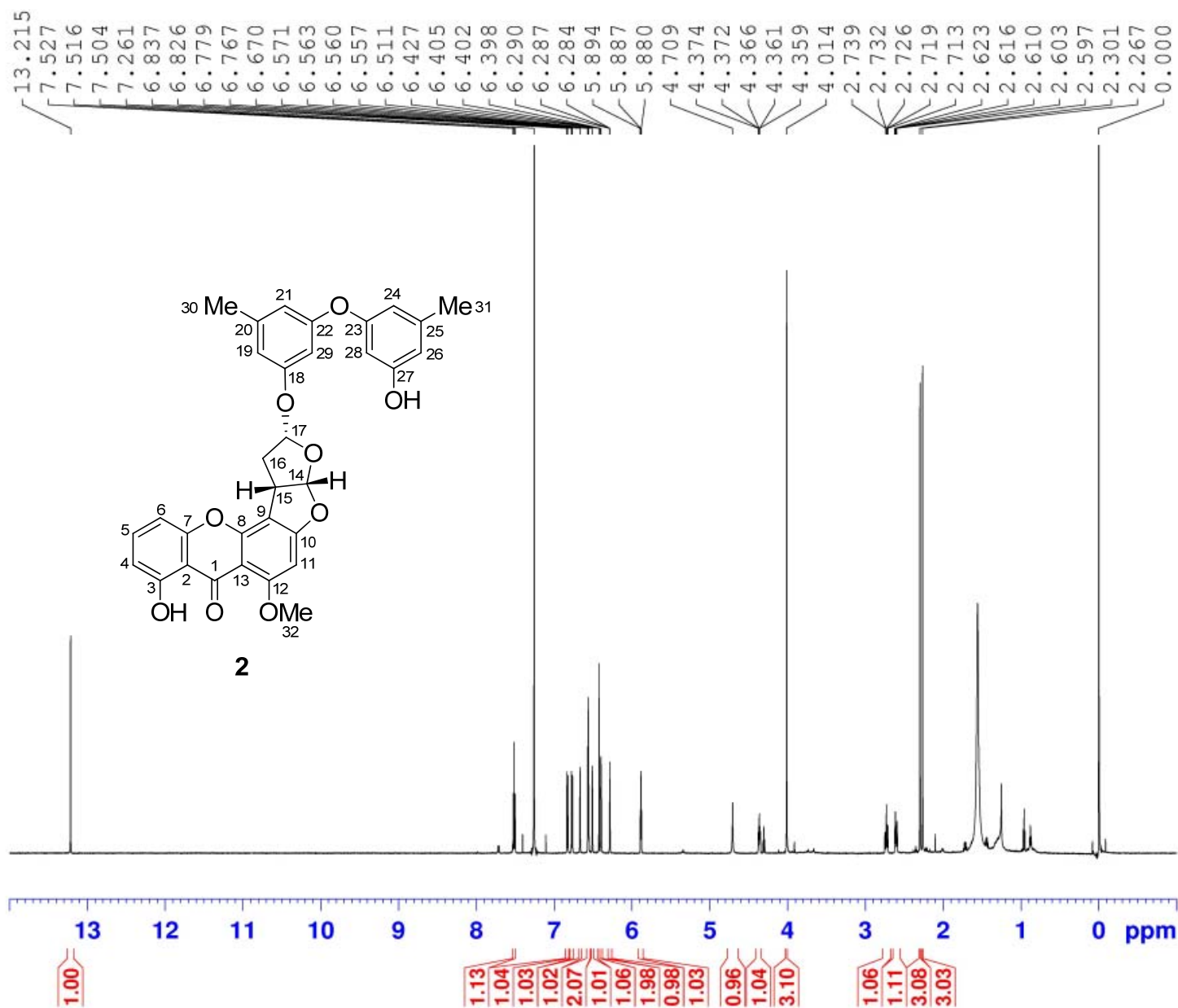
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Operator SCSIO
Instrument maXis



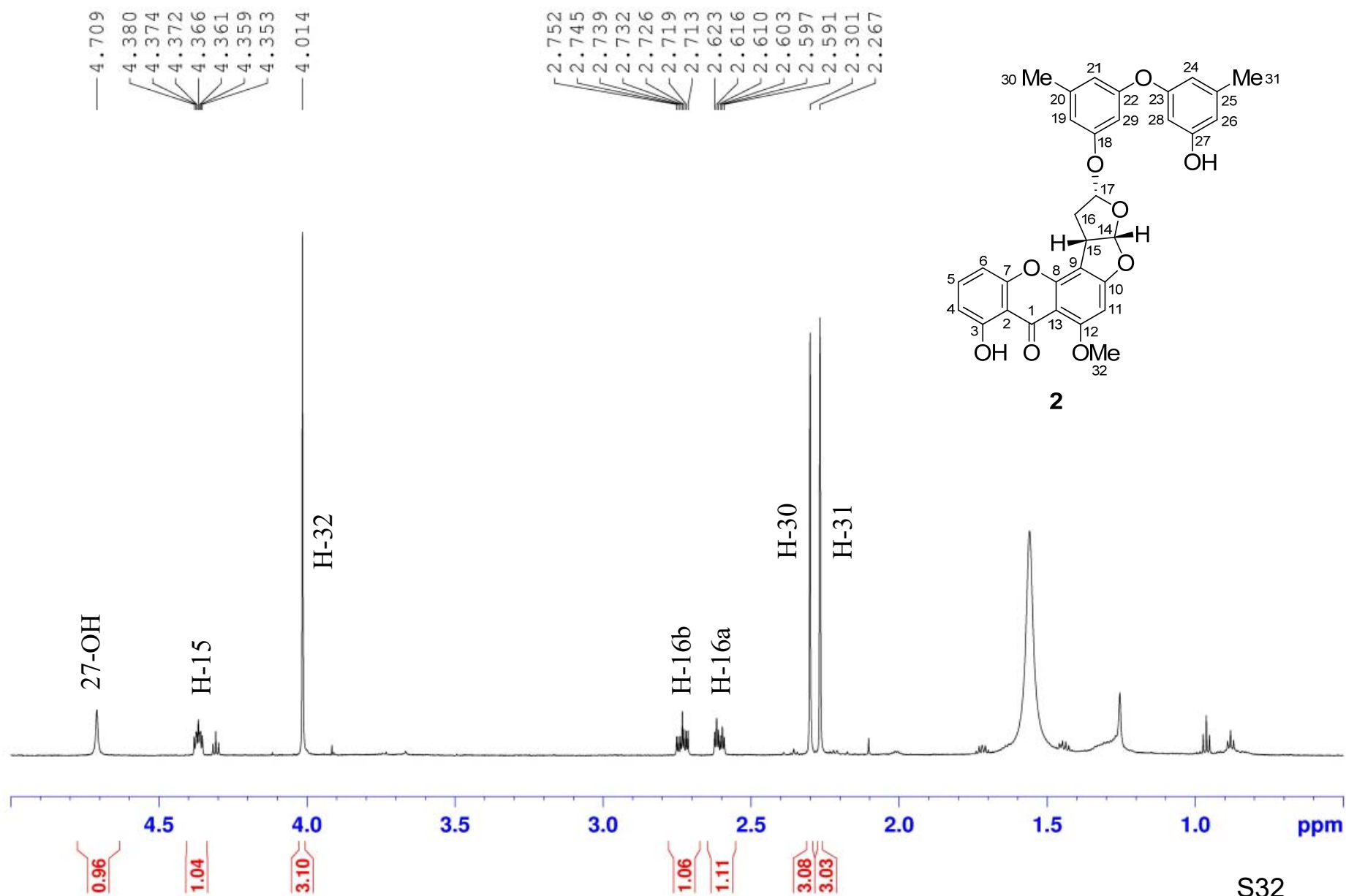
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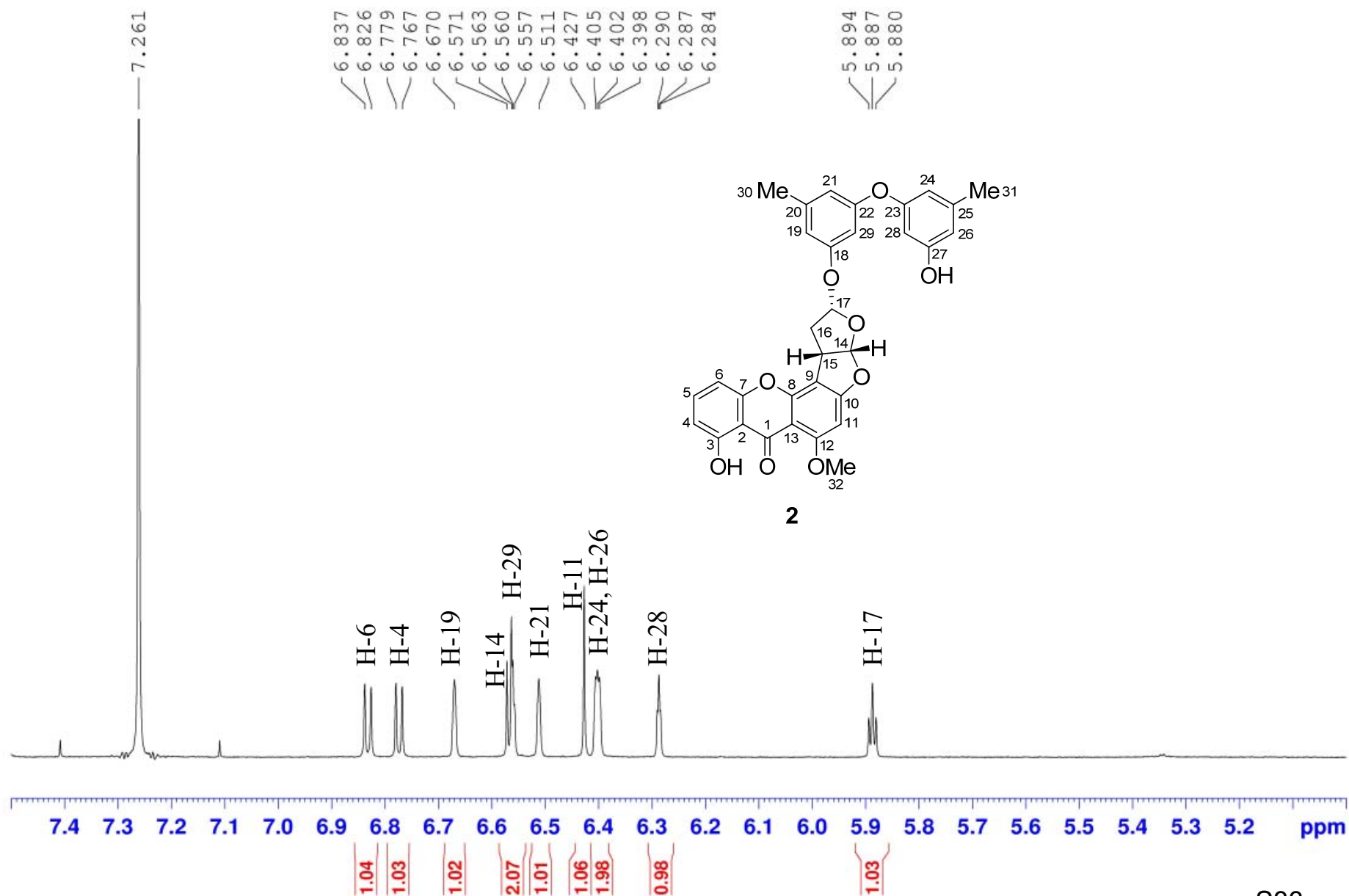
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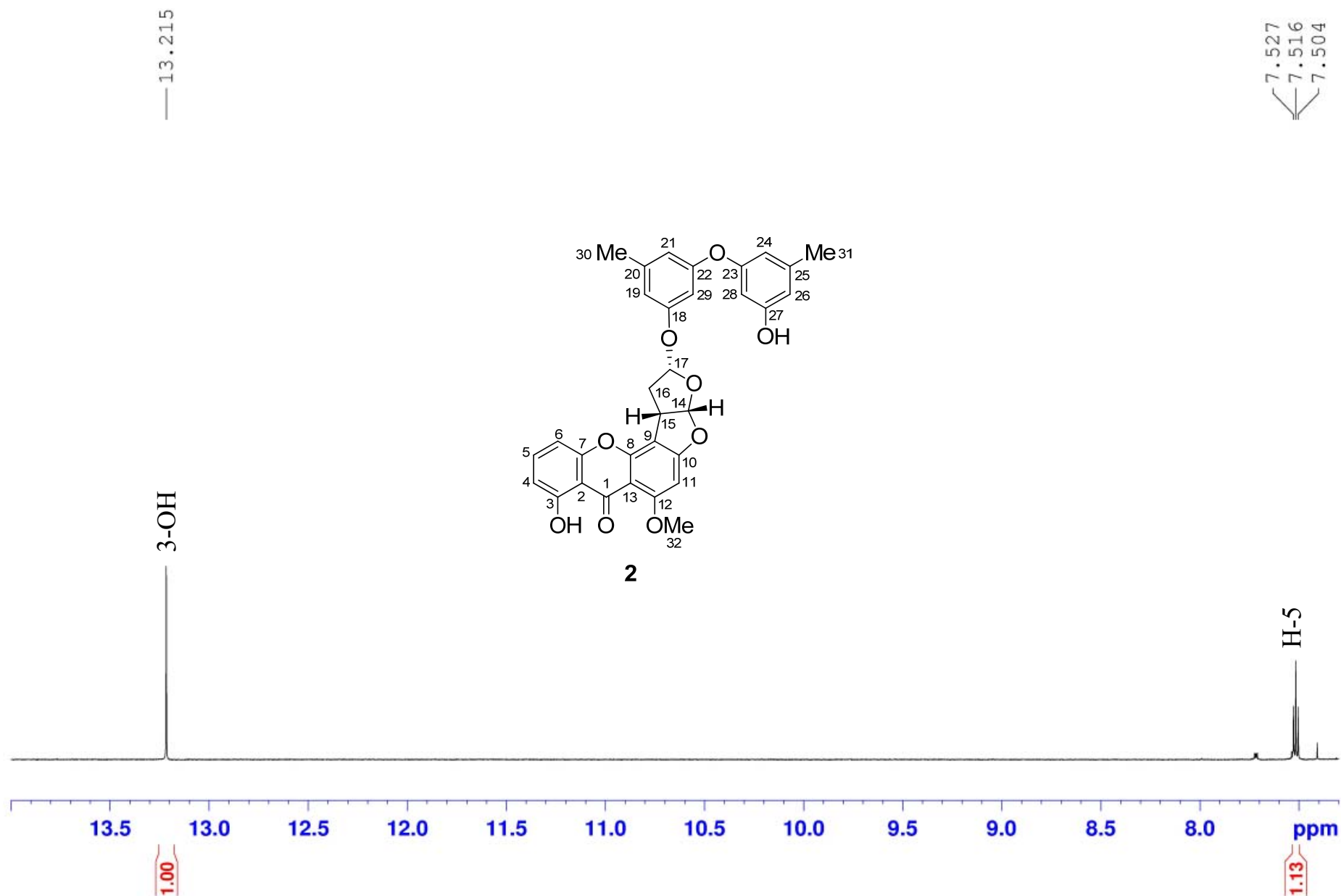
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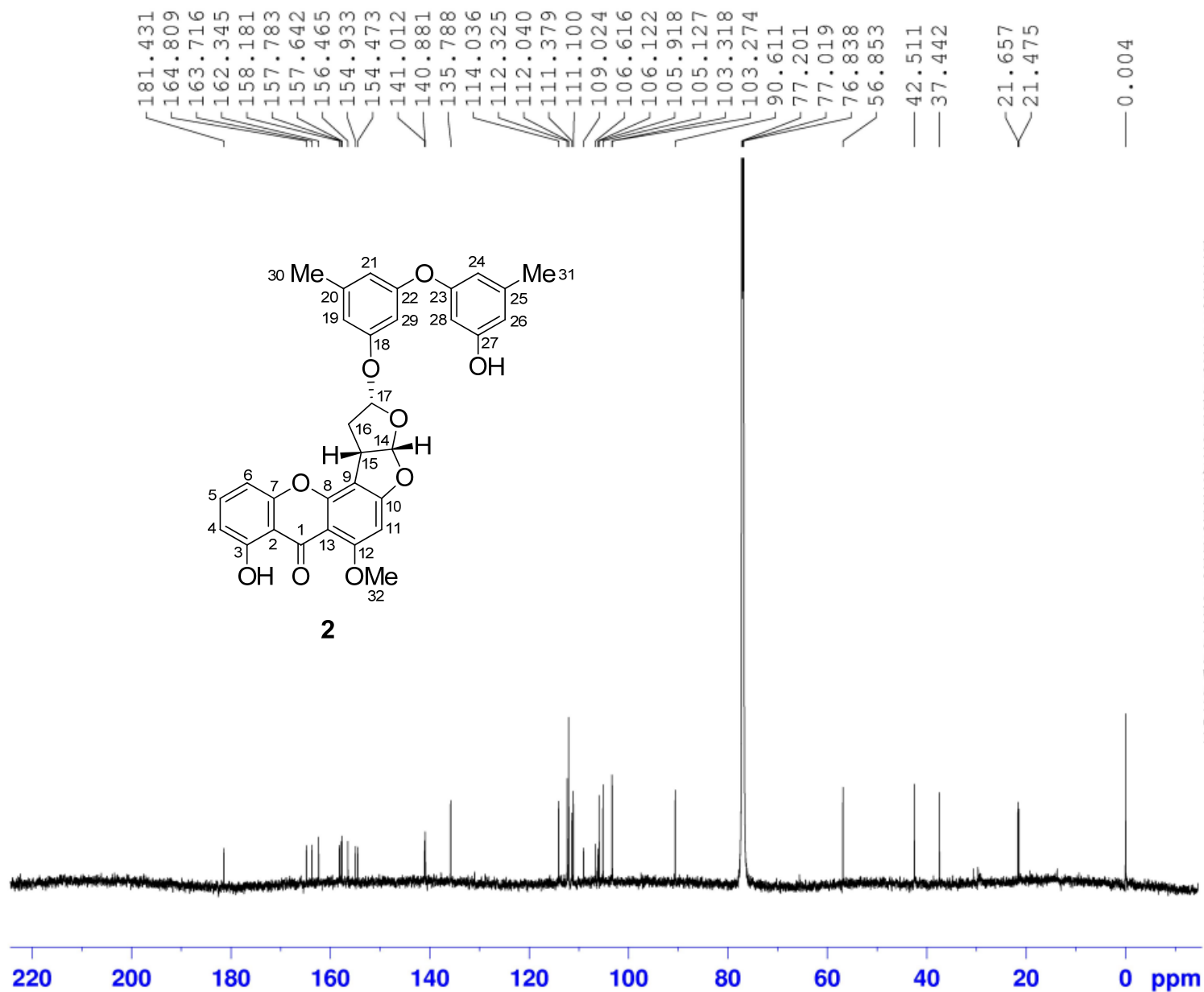
^1H (700 MHz) NMR spectrum of **2** in CDCl_3



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



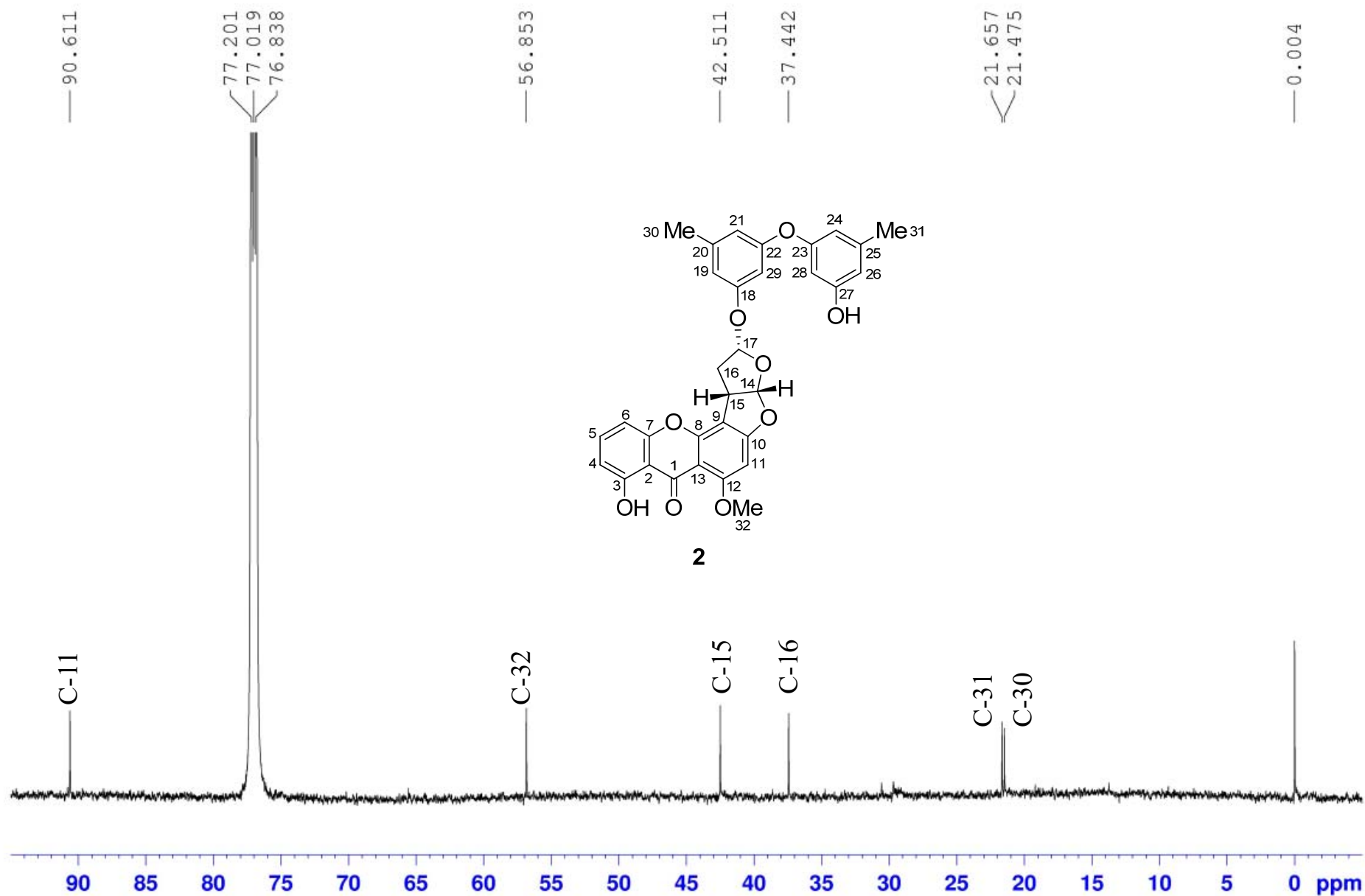
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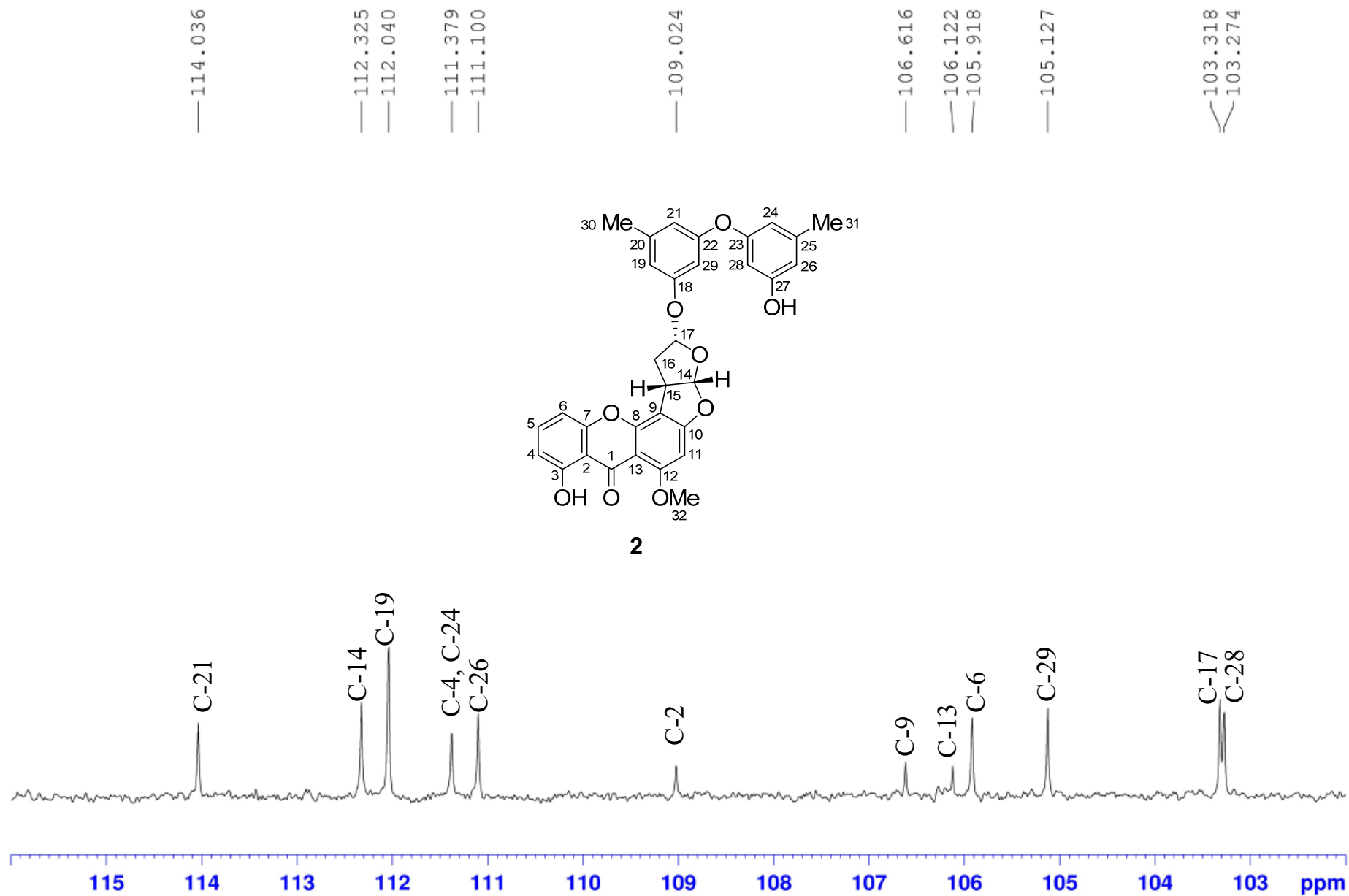
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^{13}C (175 MHz) NMR spectrum of **2** in CDCl_3



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



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

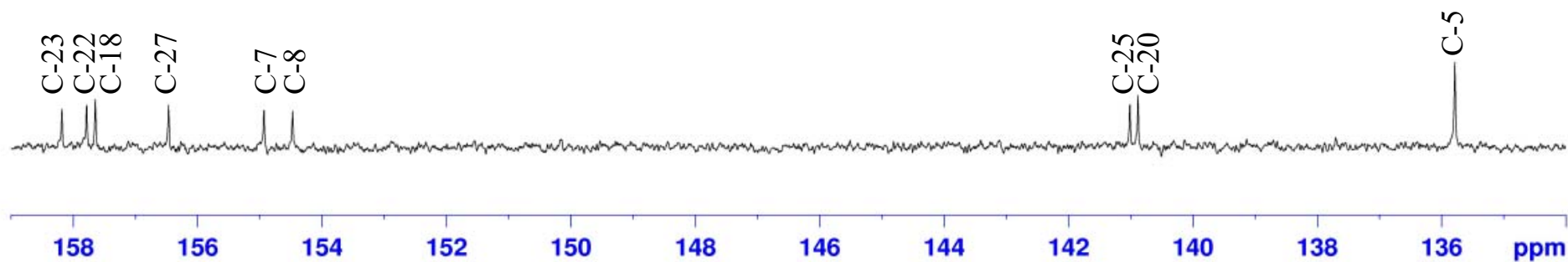
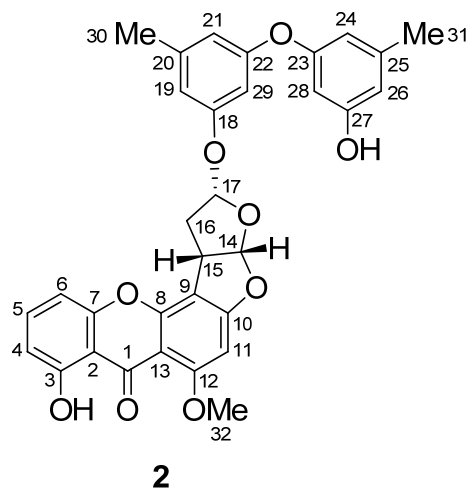
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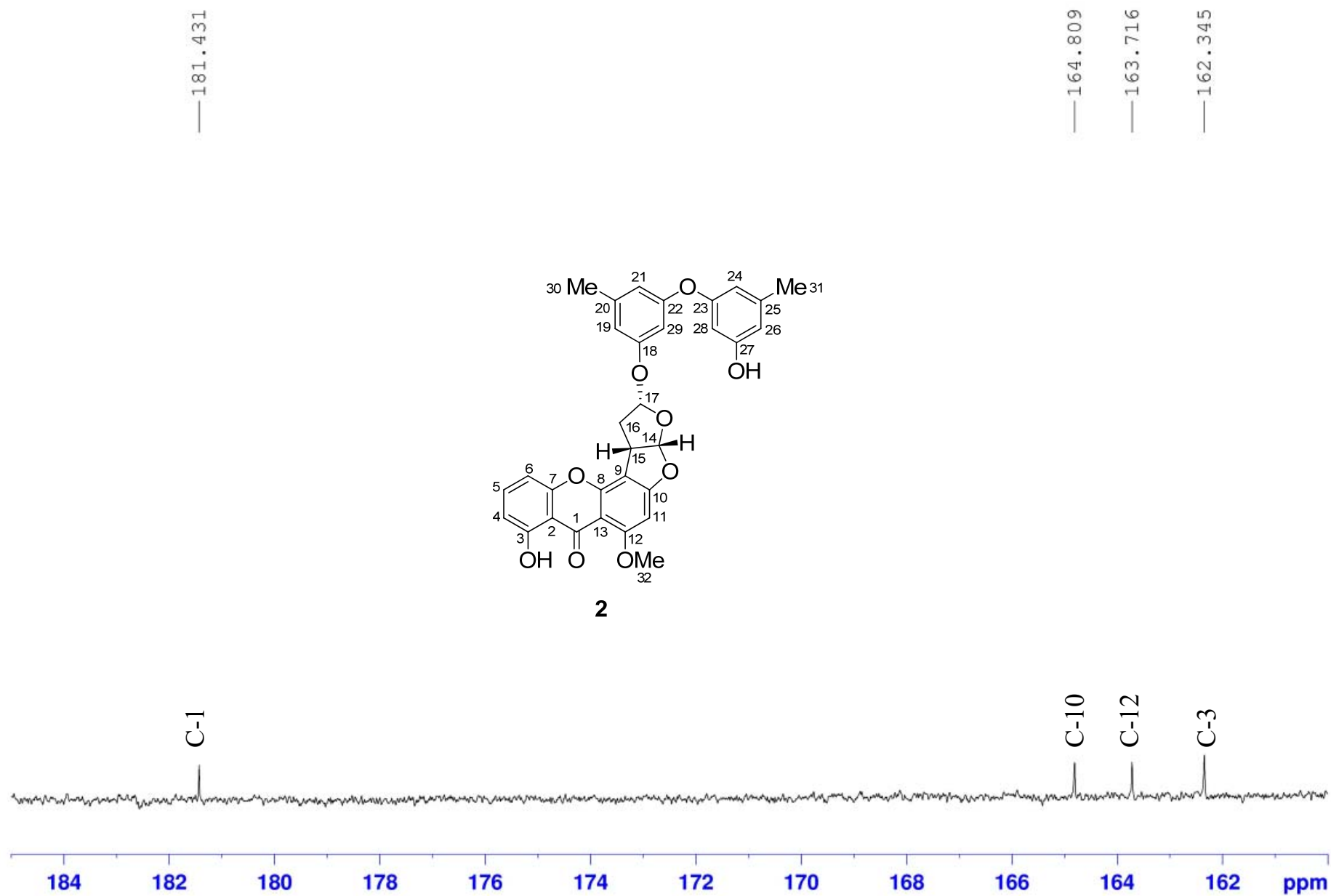
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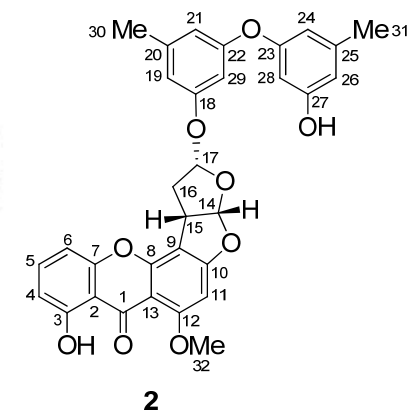
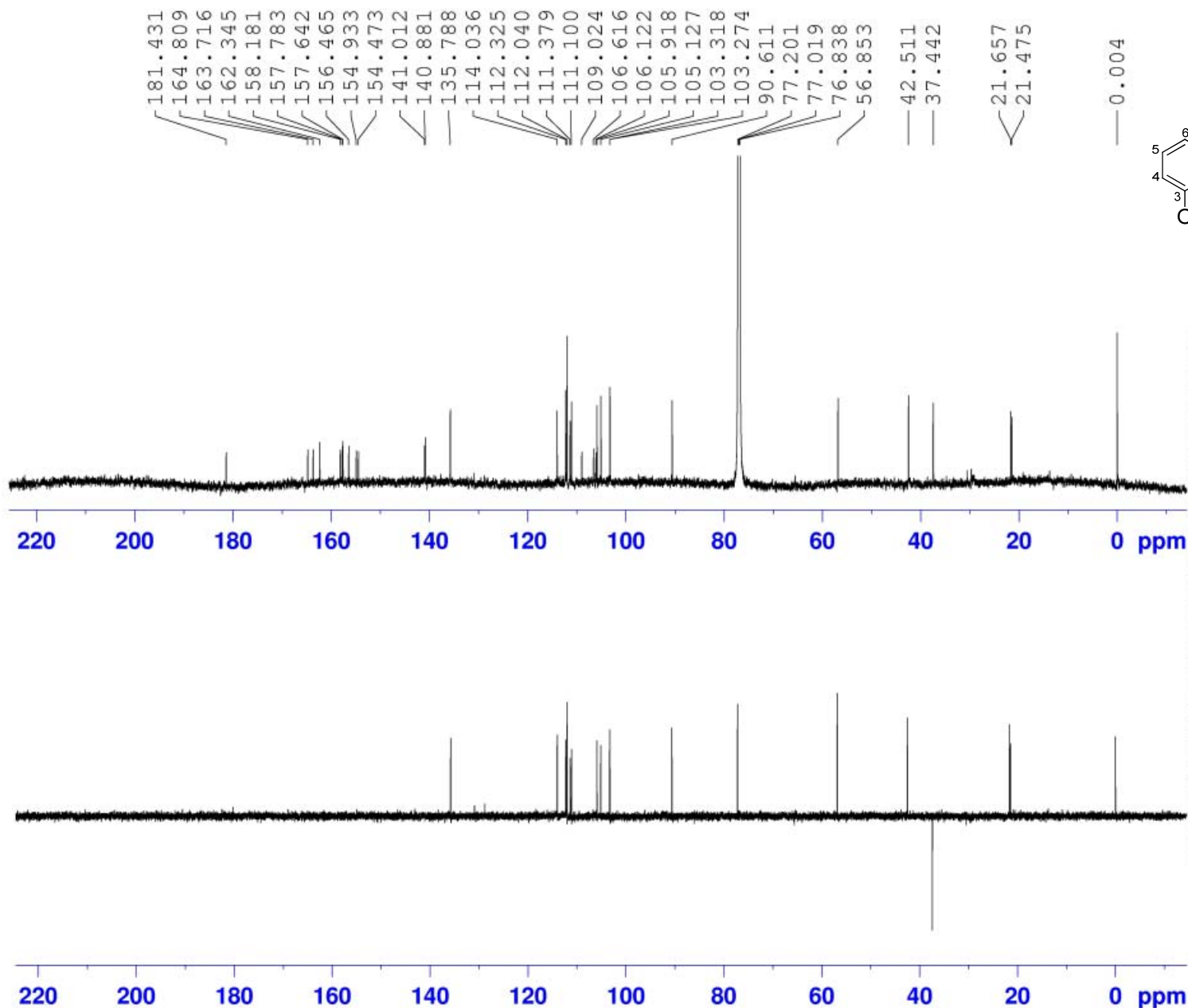
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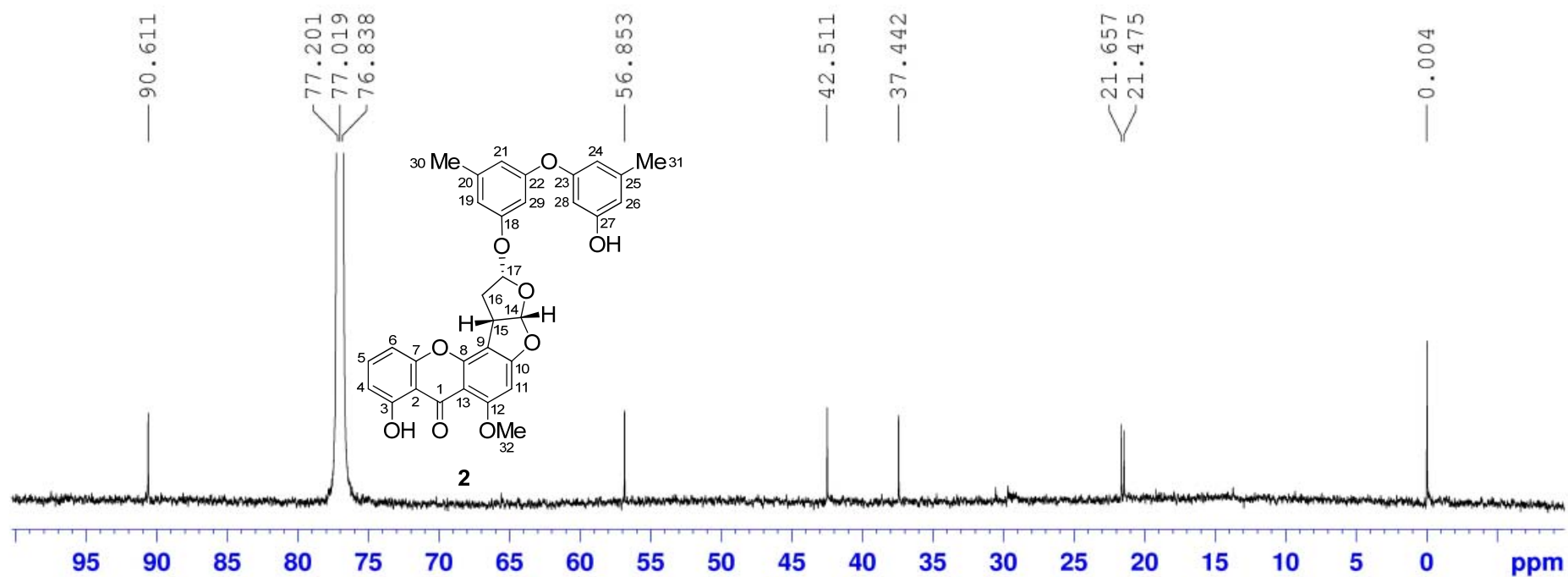


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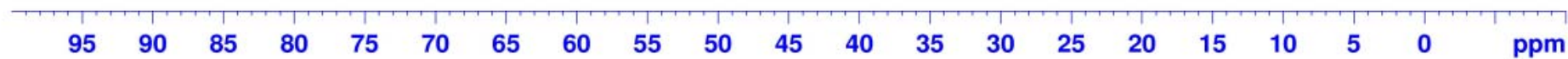


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 PROBHD z120187_0028 (
 PULPROG deptsp135
 TD 32768
 SOLVENT CDCl3
 NS 3500
 DS 8
 SWH 43859.648 Hz
 FIDRES 2.676980 Hz
 AQ 0.3736052 sec
 RG 181.26
 DW 11.400 usec
 DE 18.00 usec
 TE 298.0 K
 CNST2 145.000000
 D1 1.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 TD0 1
 SFO1 176.0797677 MHz
 NUC1 13C
 P1 11.90 usec
 P13 2000.00 usec
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 SSB 0
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 PC 1.40

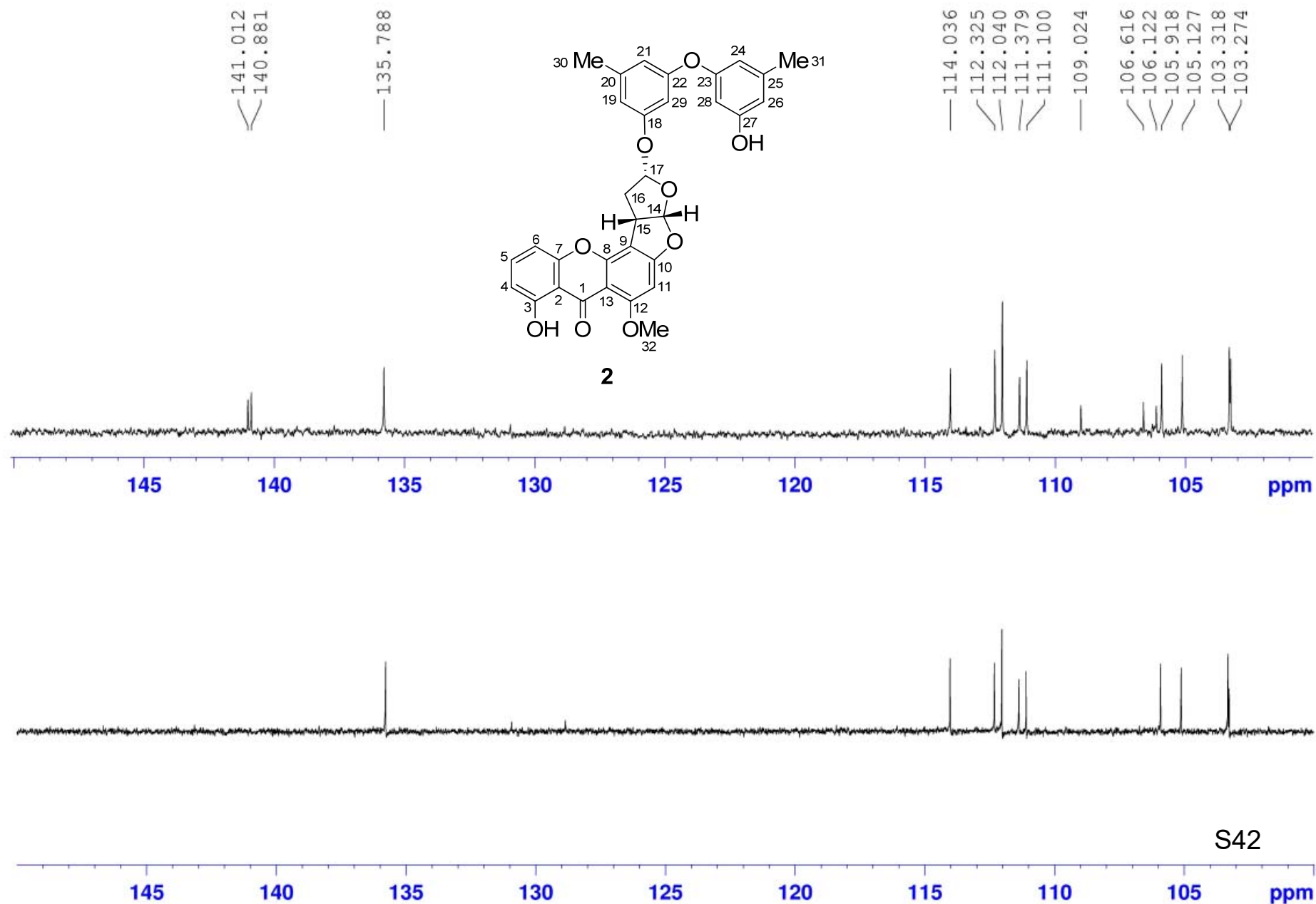
DEPT135 (175 MHz) spectrum of **2** in CDCl₃



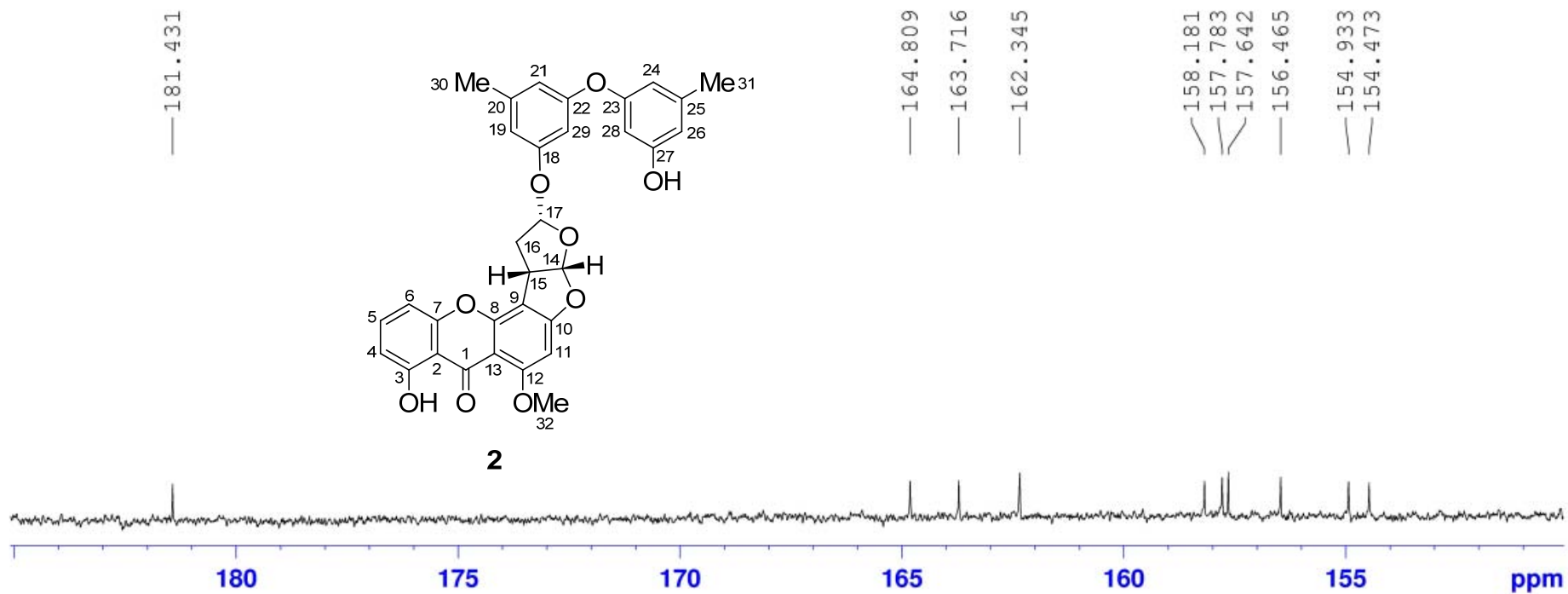
S41



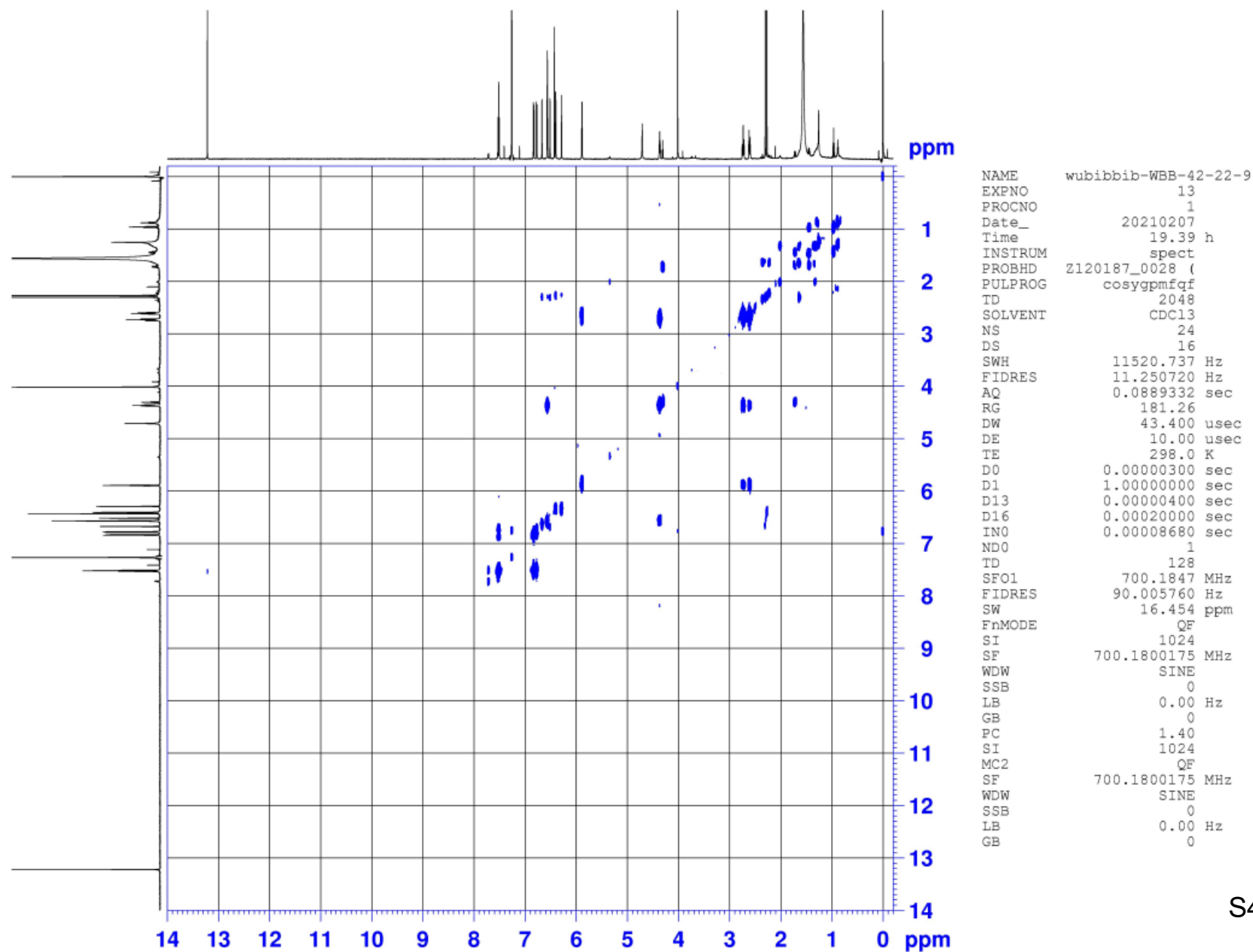
DEPT135 (175 MHz) spectrum of **2** in CDCl₃



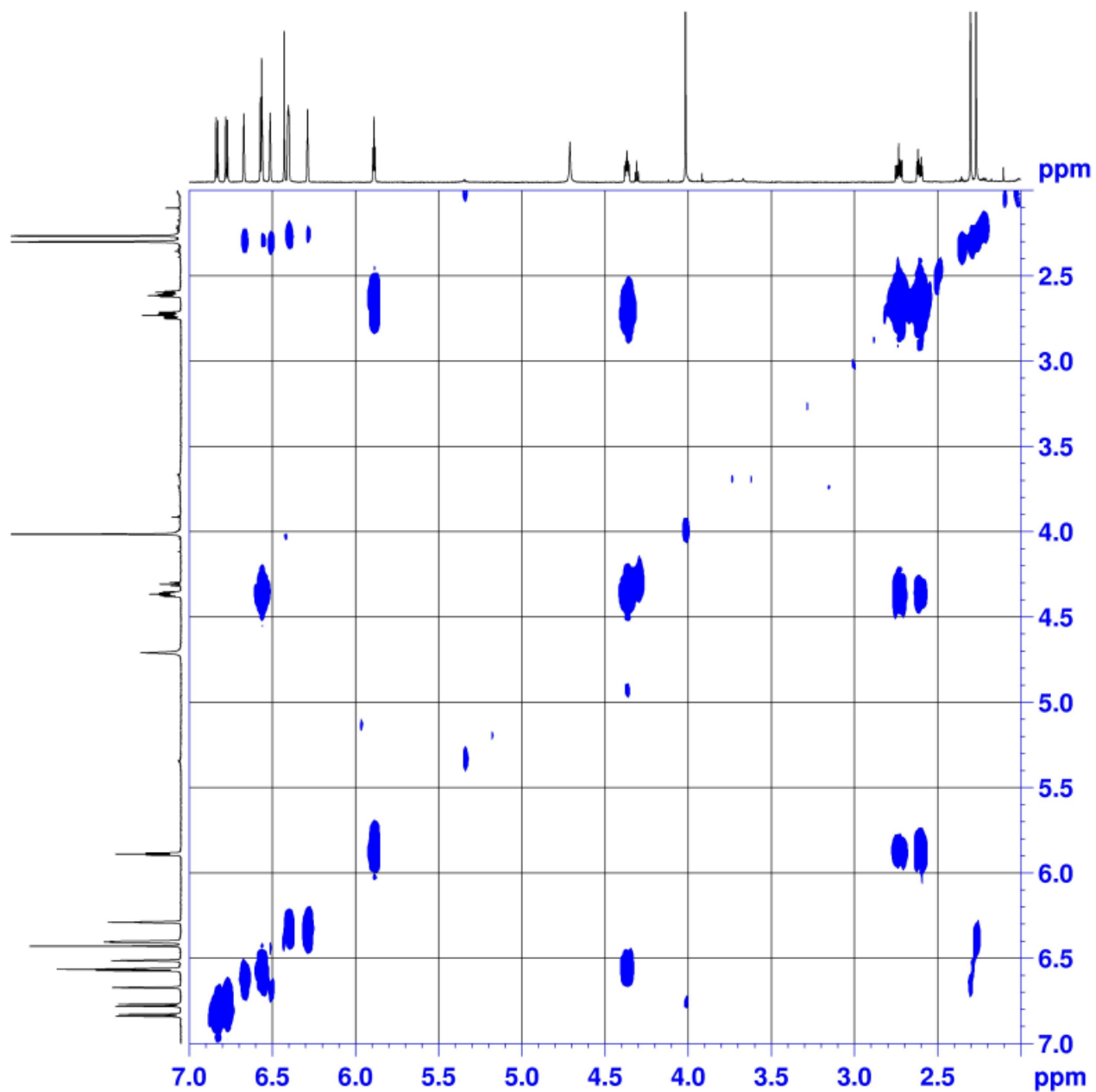
DEPT135 (175 MHz) spectrum of **2** in CDCl₃



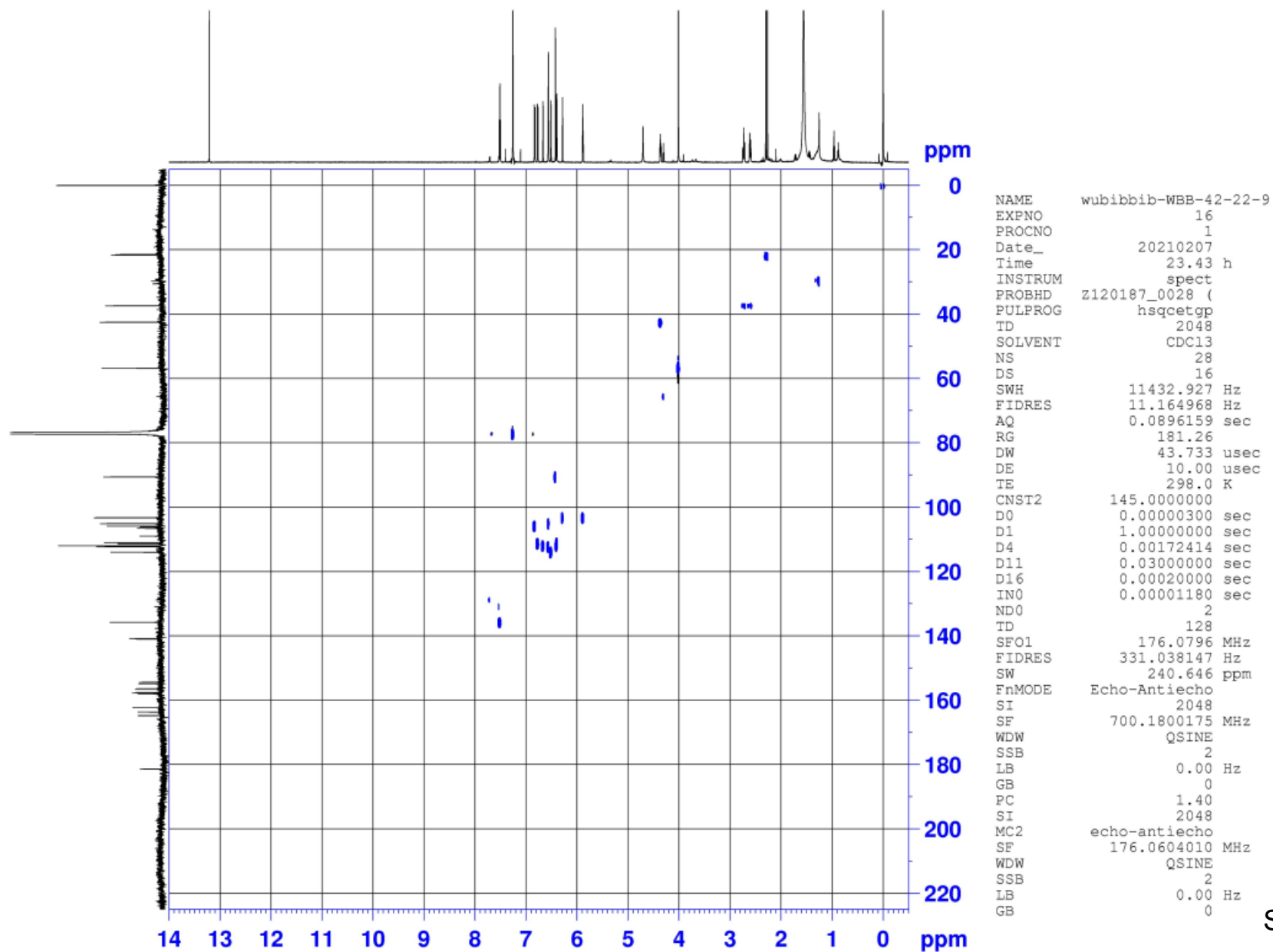
^1H - ^1H COSY (700 MHz) spectrum of **2** in CDCl_3



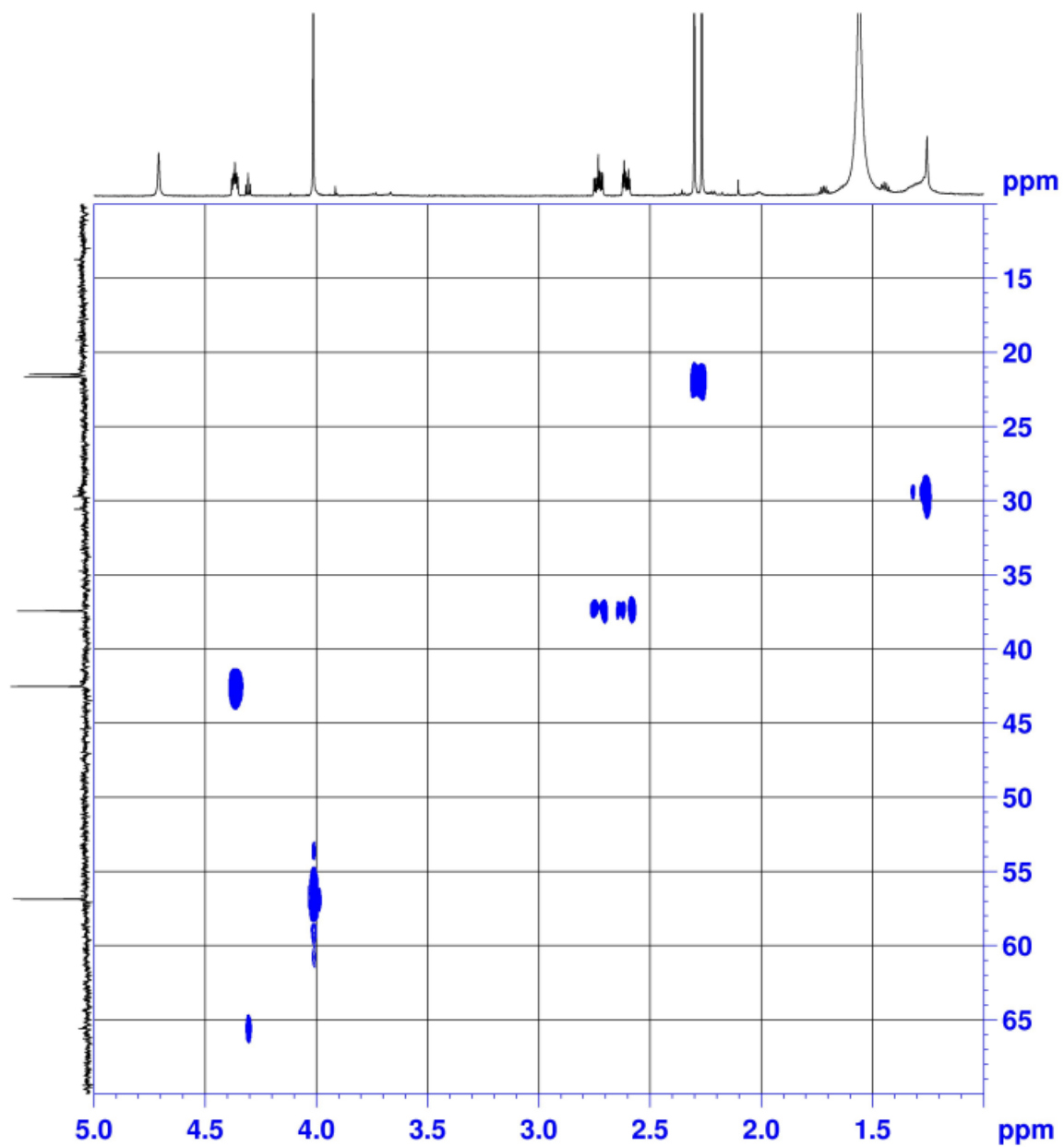
^1H - ^1H COSY (700 MHz) spectrum of **2** in CDCl_3



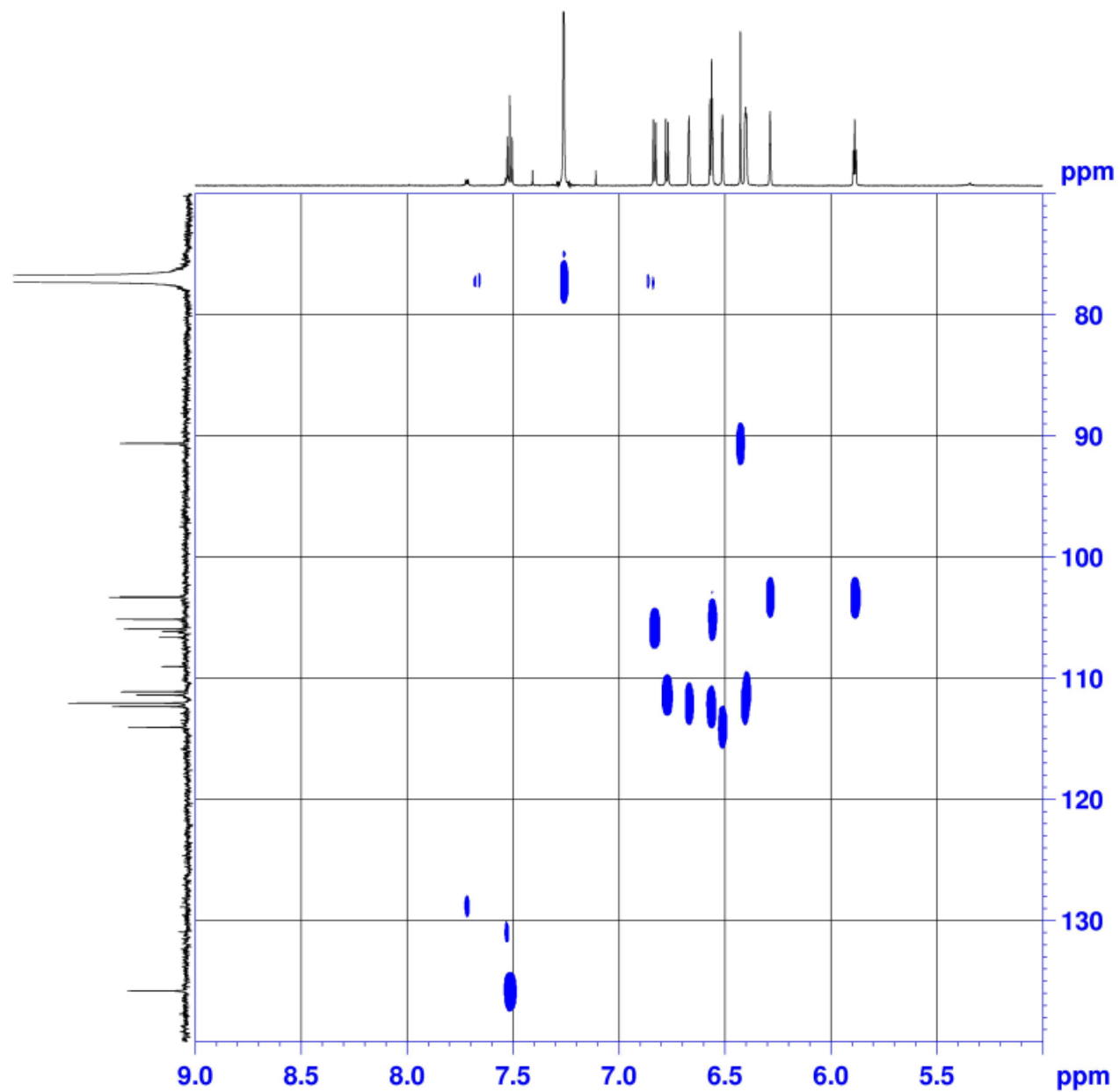
HSQC (700 MHz) spectrum of **2** in CDCl₃



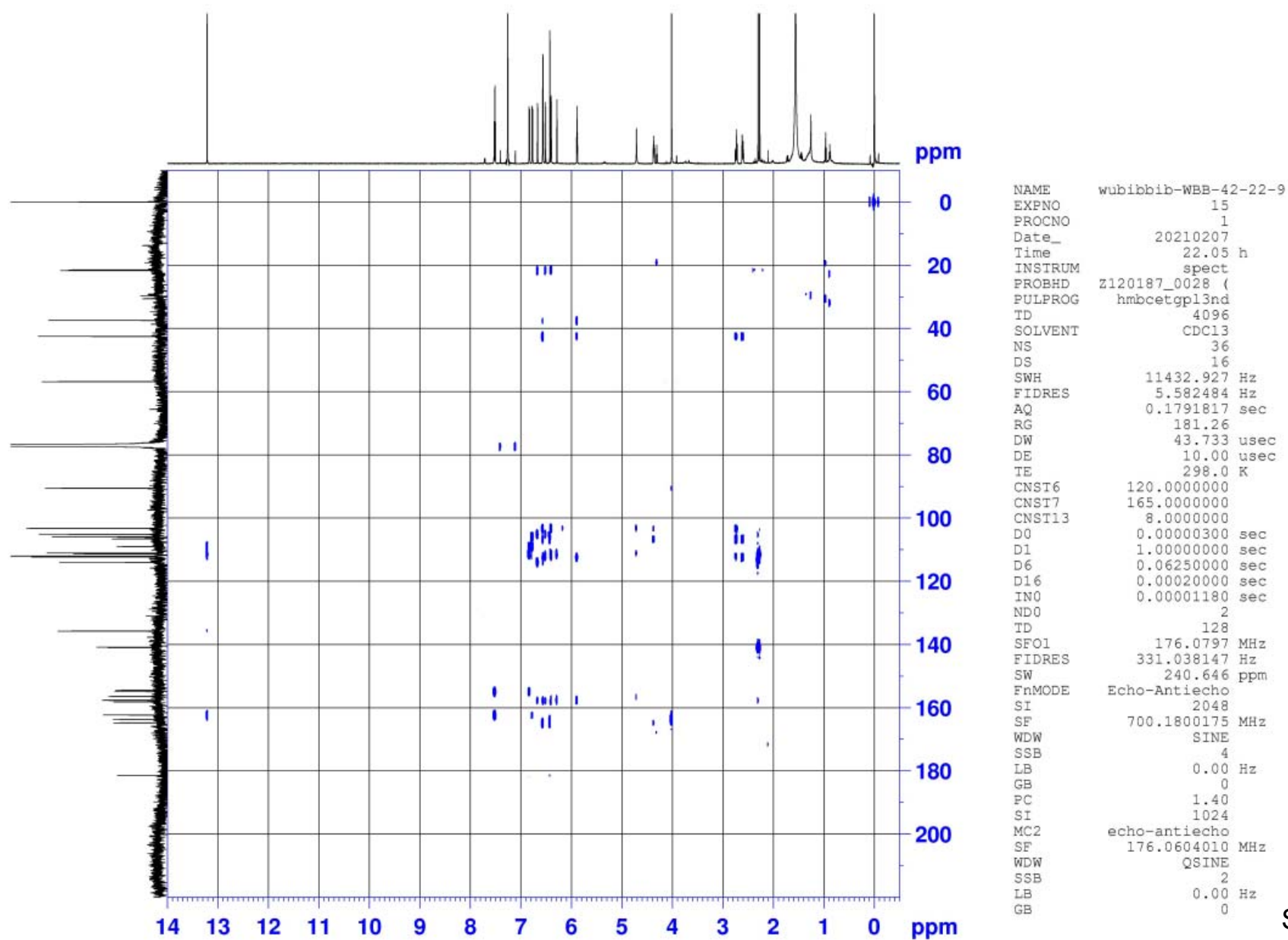
HSQC (700 MHz) spectrum of **2** in CDCl₃



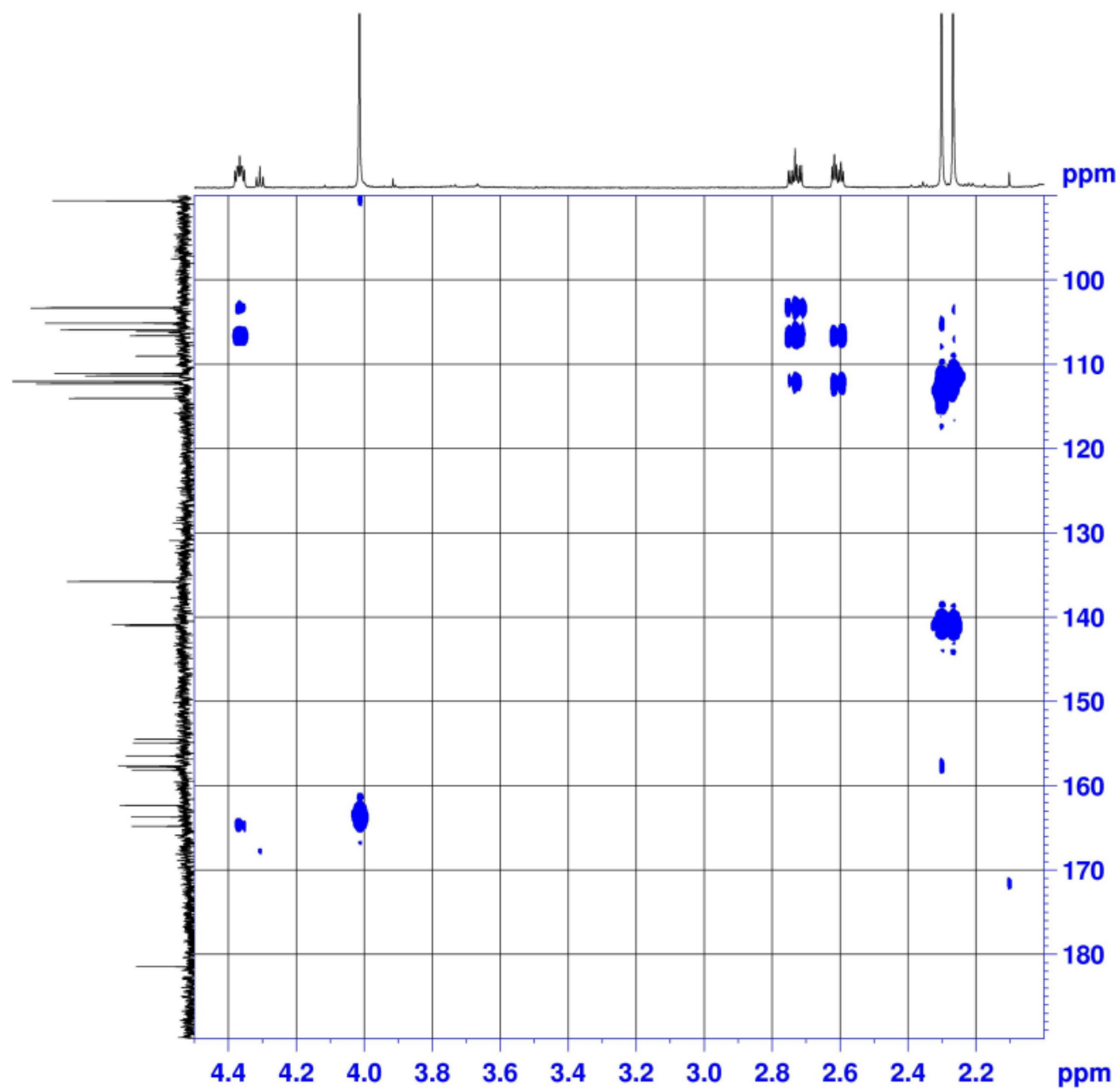
HSQC (700 MHz) spectrum of **2** in CDCl₃



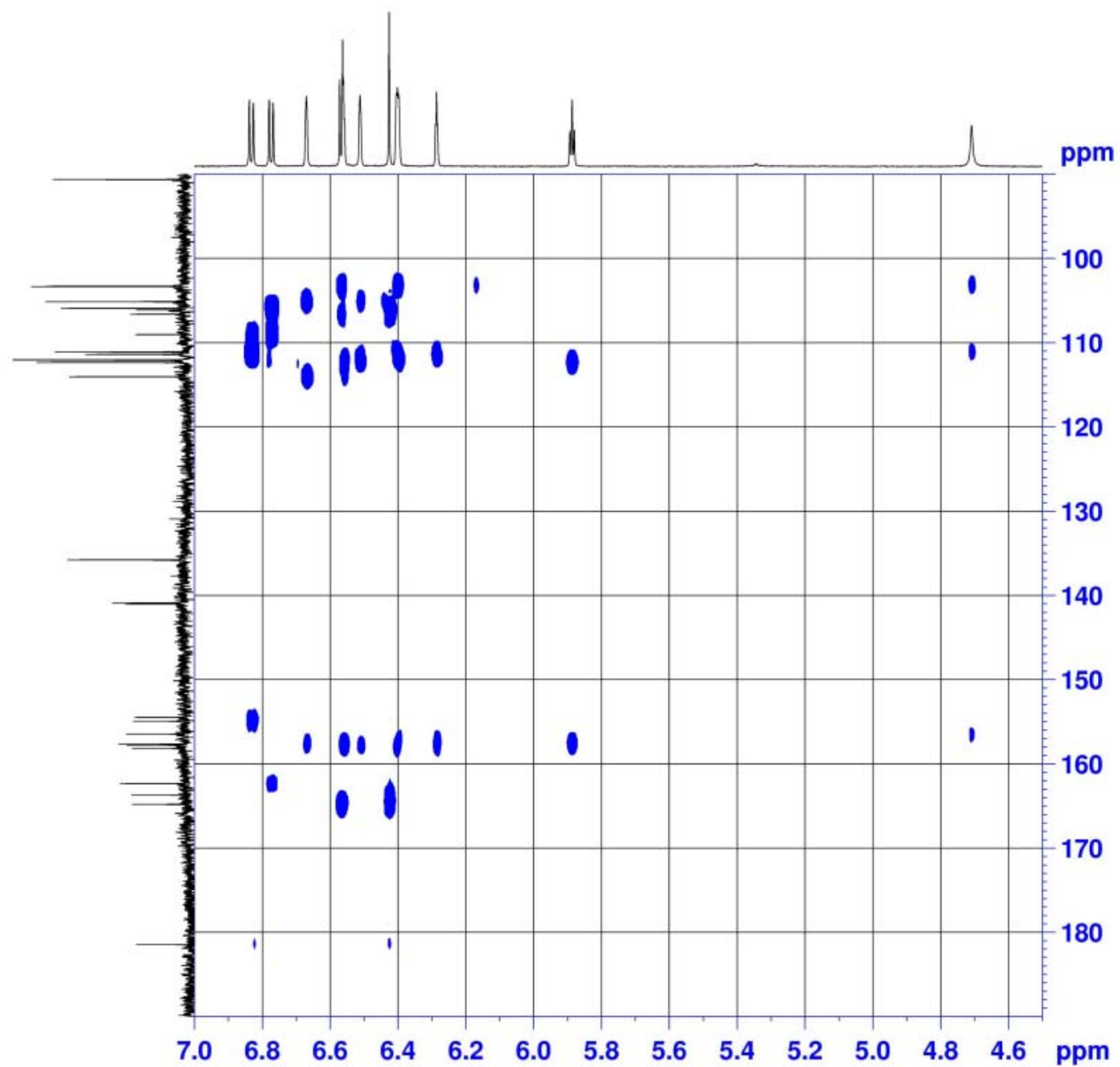
HMBC (700 MHz) spectrum of **2** in CDCl₃



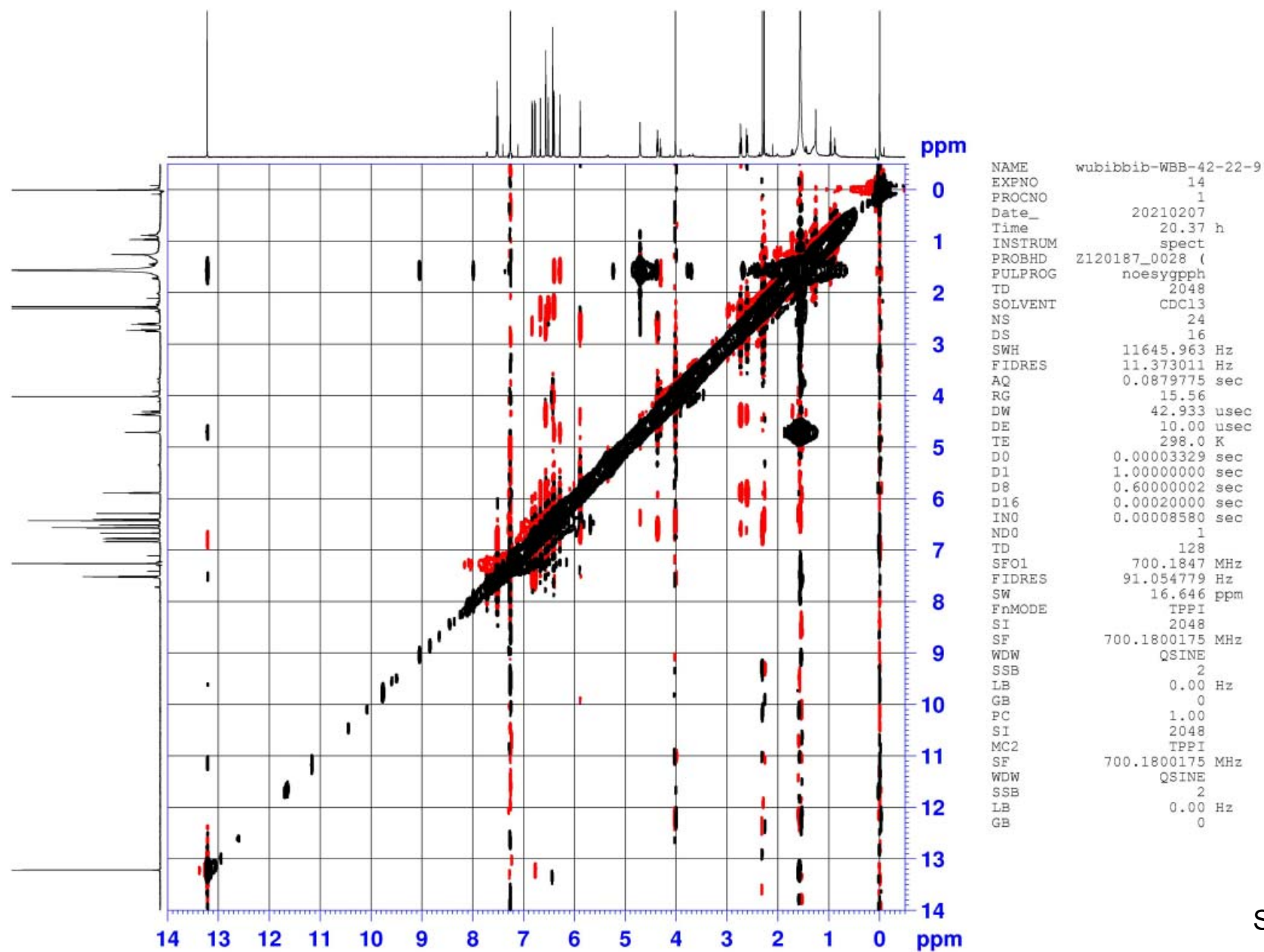
HMBC (700 MHz) spectrum of **2** in CDCl₃



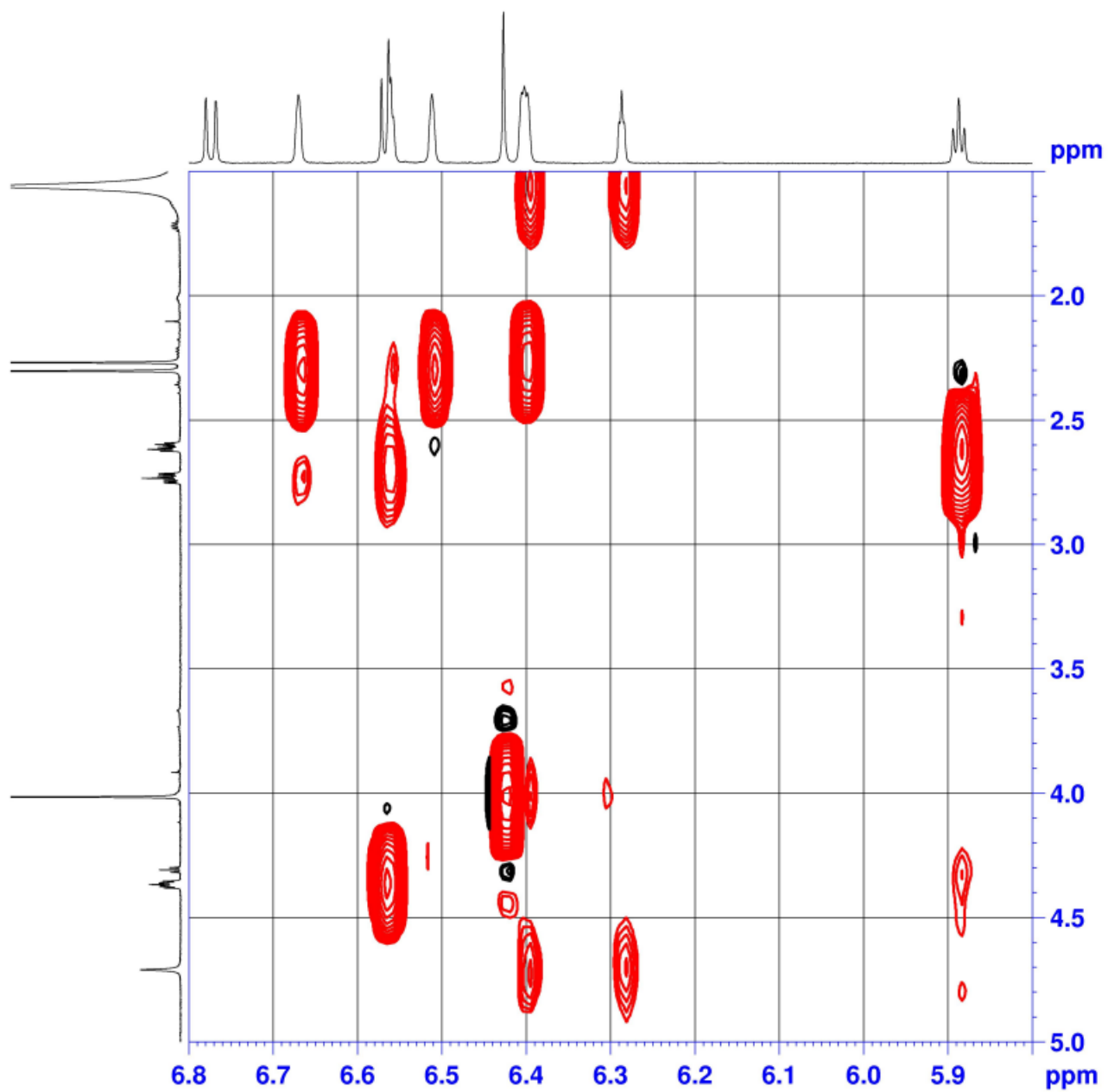
HMBC (700 MHz) spectrum of **2** in CDCl₃



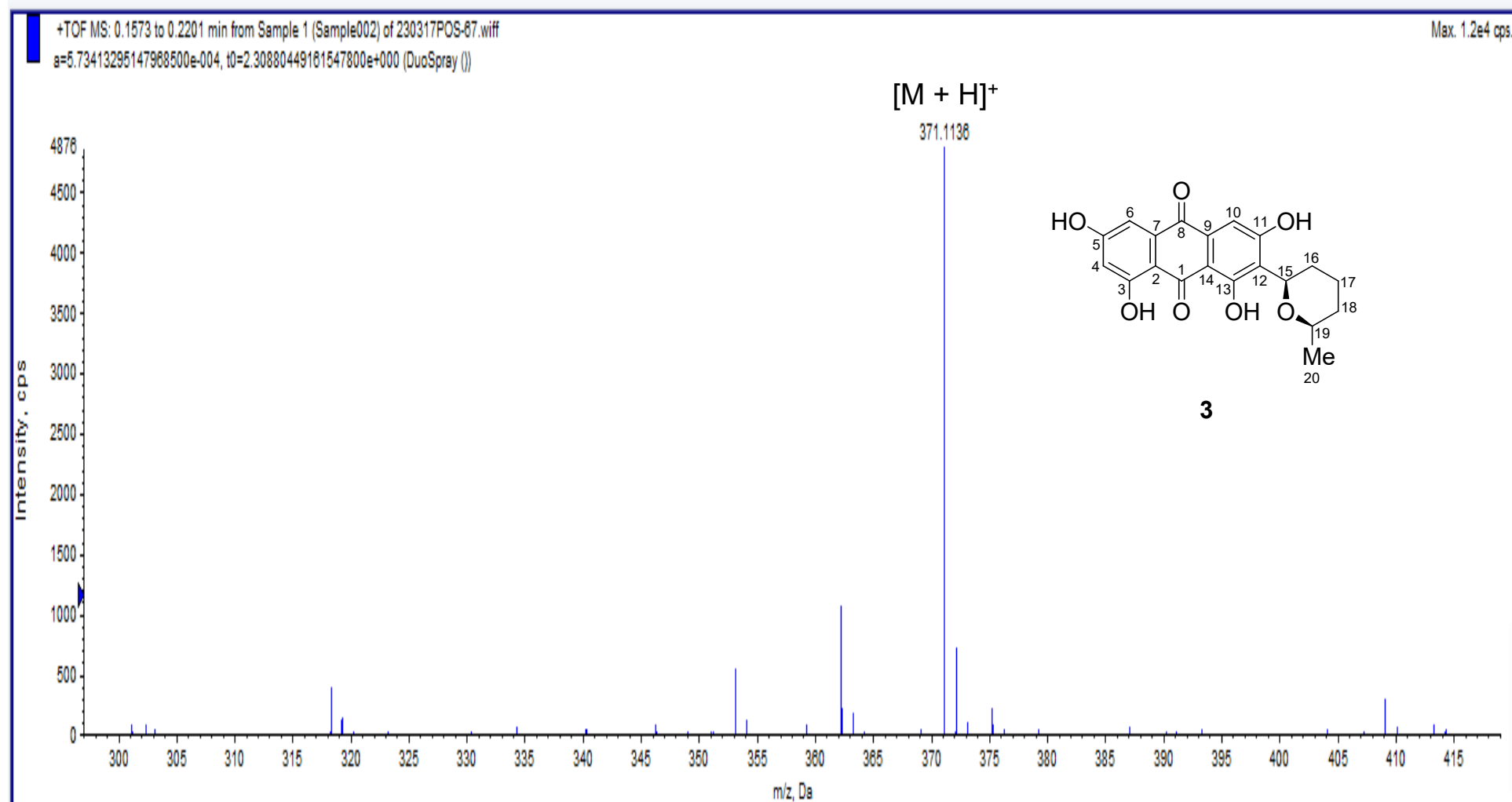
NOESY (700 MHz) spectrum of **2** in CDCl₃



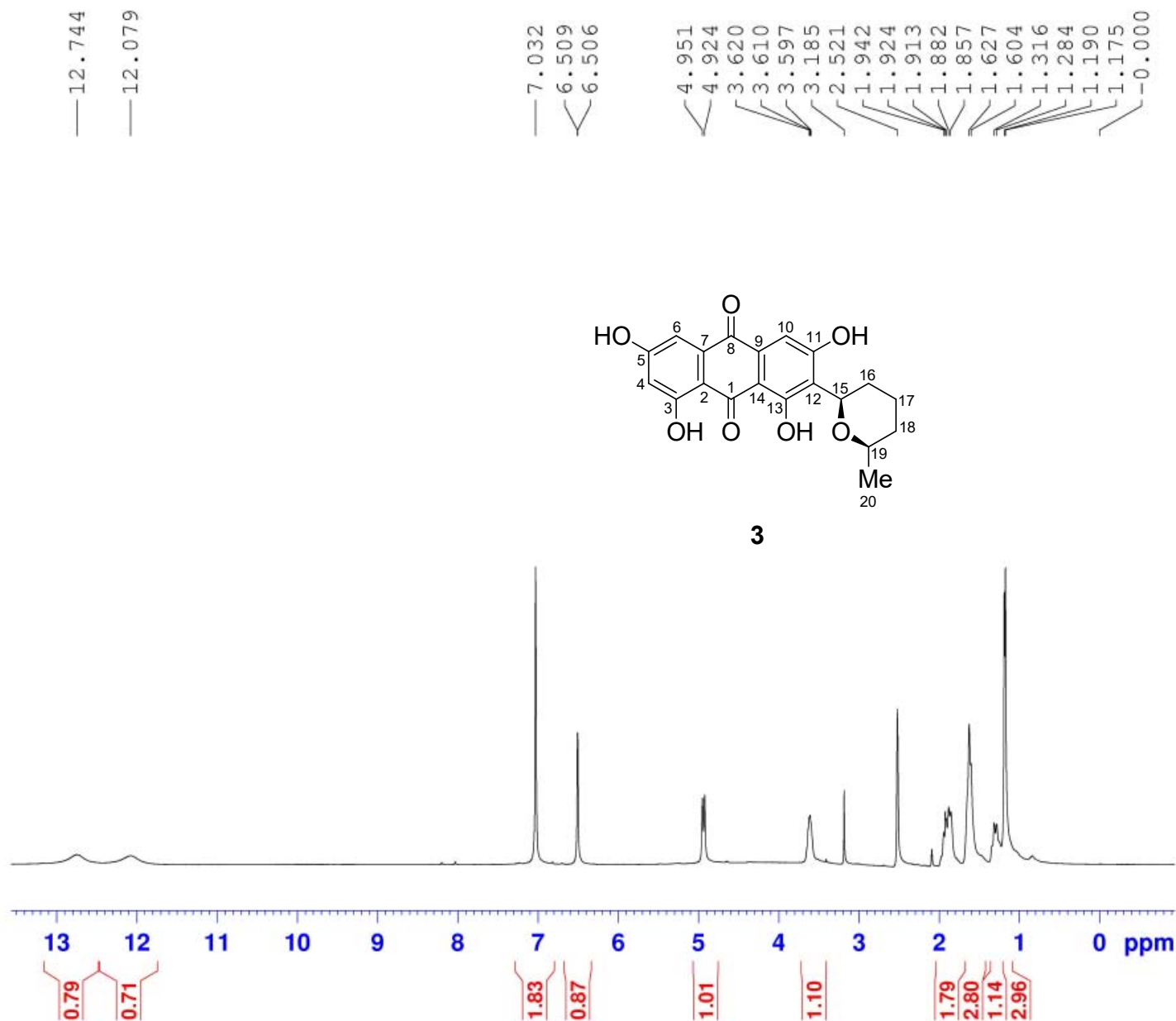
NOESY (700 MHz) spectrum of **2** in CDCl₃



HR-ESIMS for **3**



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



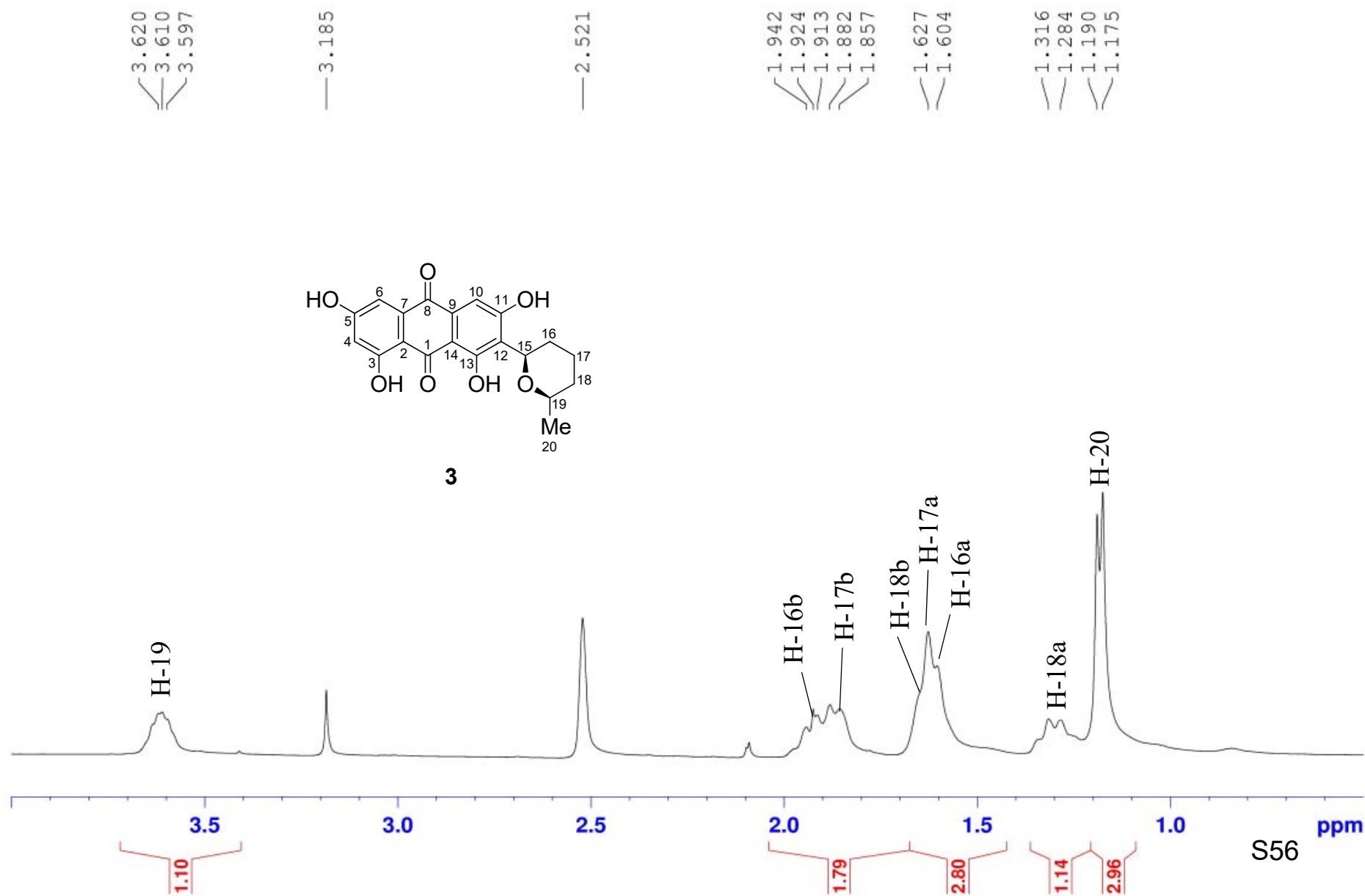
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PROCNO    1
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Time      8.23
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PULPROG   zg30
TD        65536
SOLVENT   DMSO
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        54.9
DW        62.400 usec
DE        6.50 usec
TE        0.0 K
D1        1.00000000 sec
TD0       1
    
```

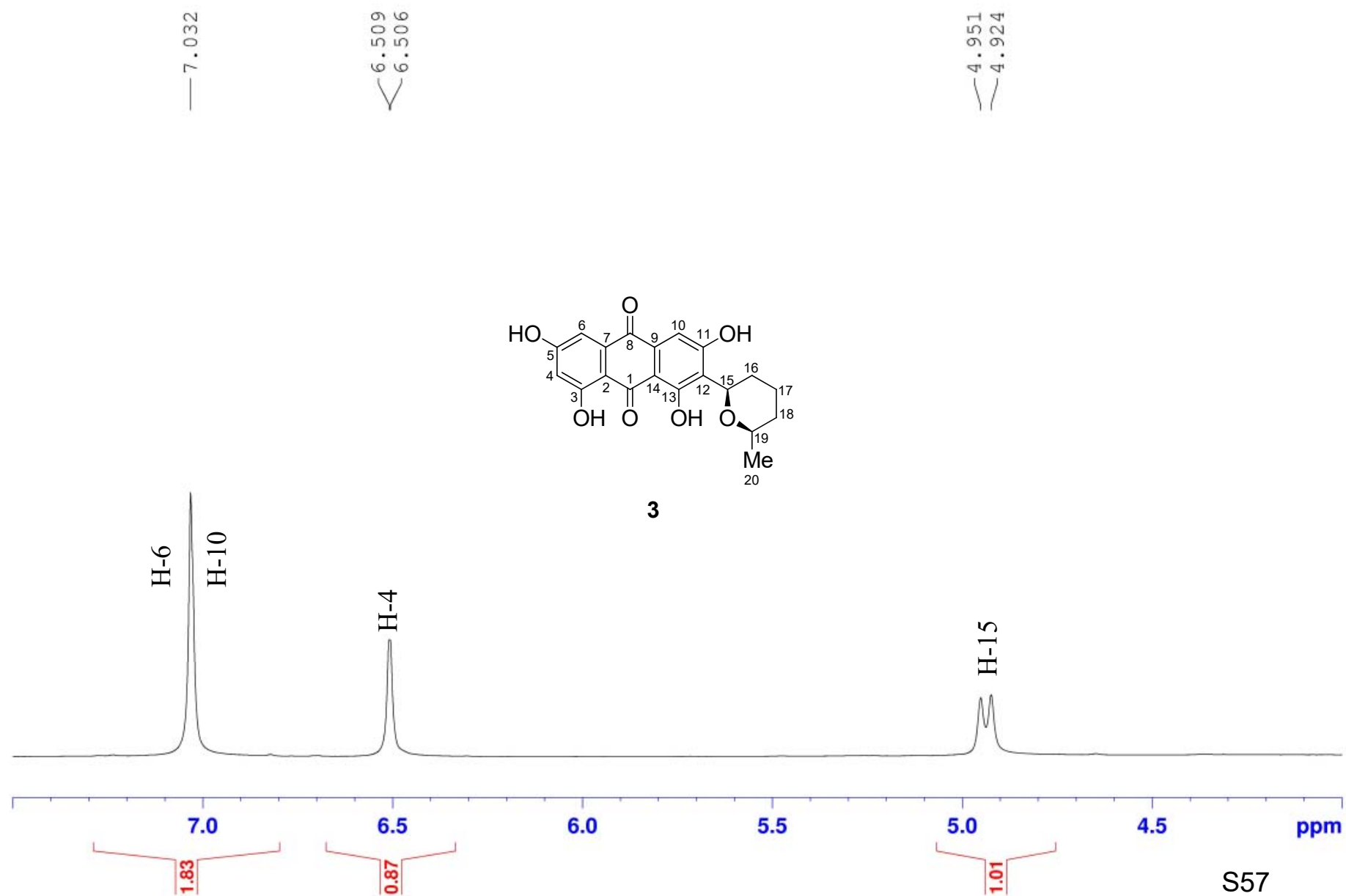
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NUC1      1H
P1        10.00 usec
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SF        400.1299945 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

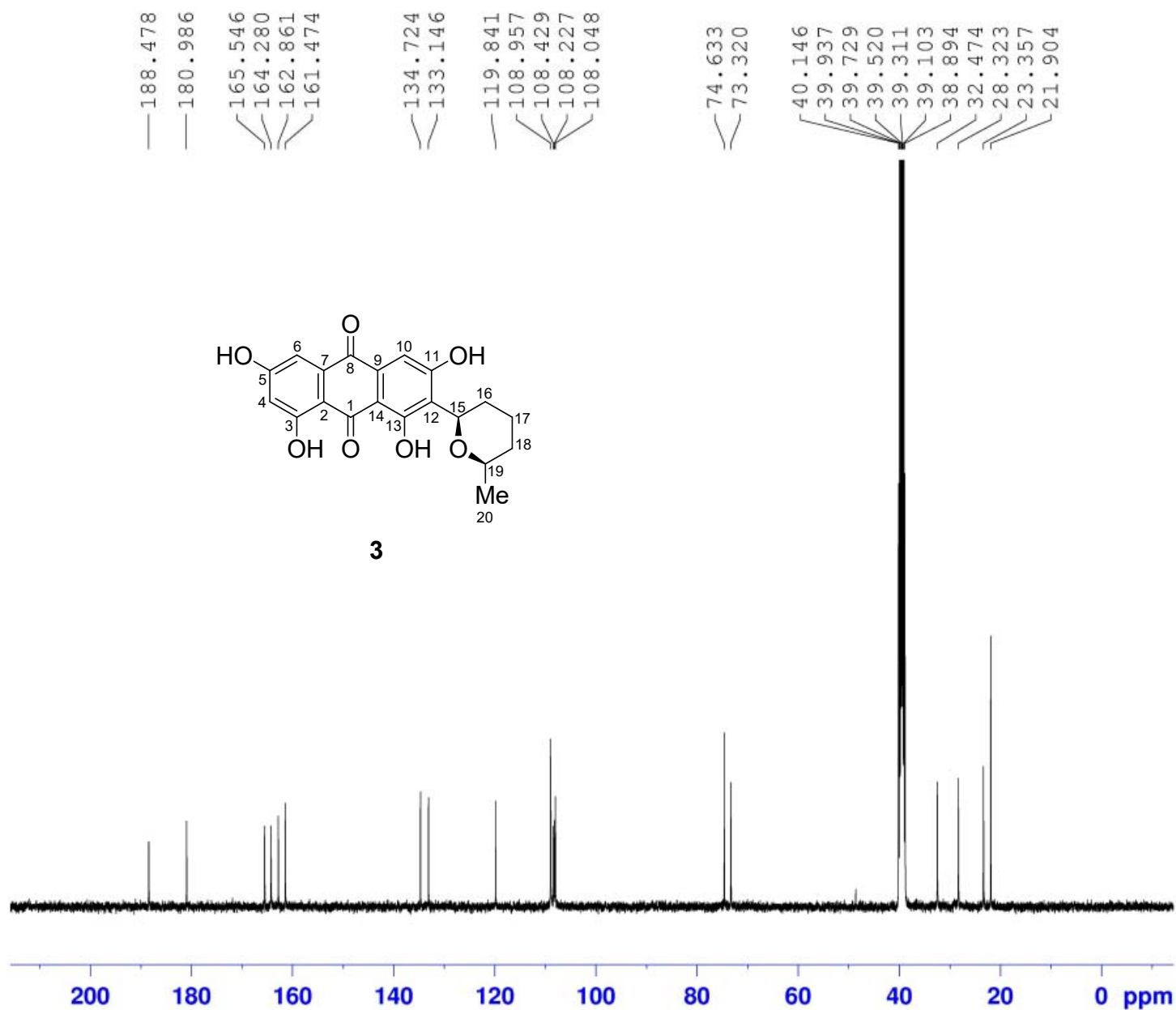
^1H (400 MHz) NMR spectrum of **3** in $\text{DMSO-}d_6$



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



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



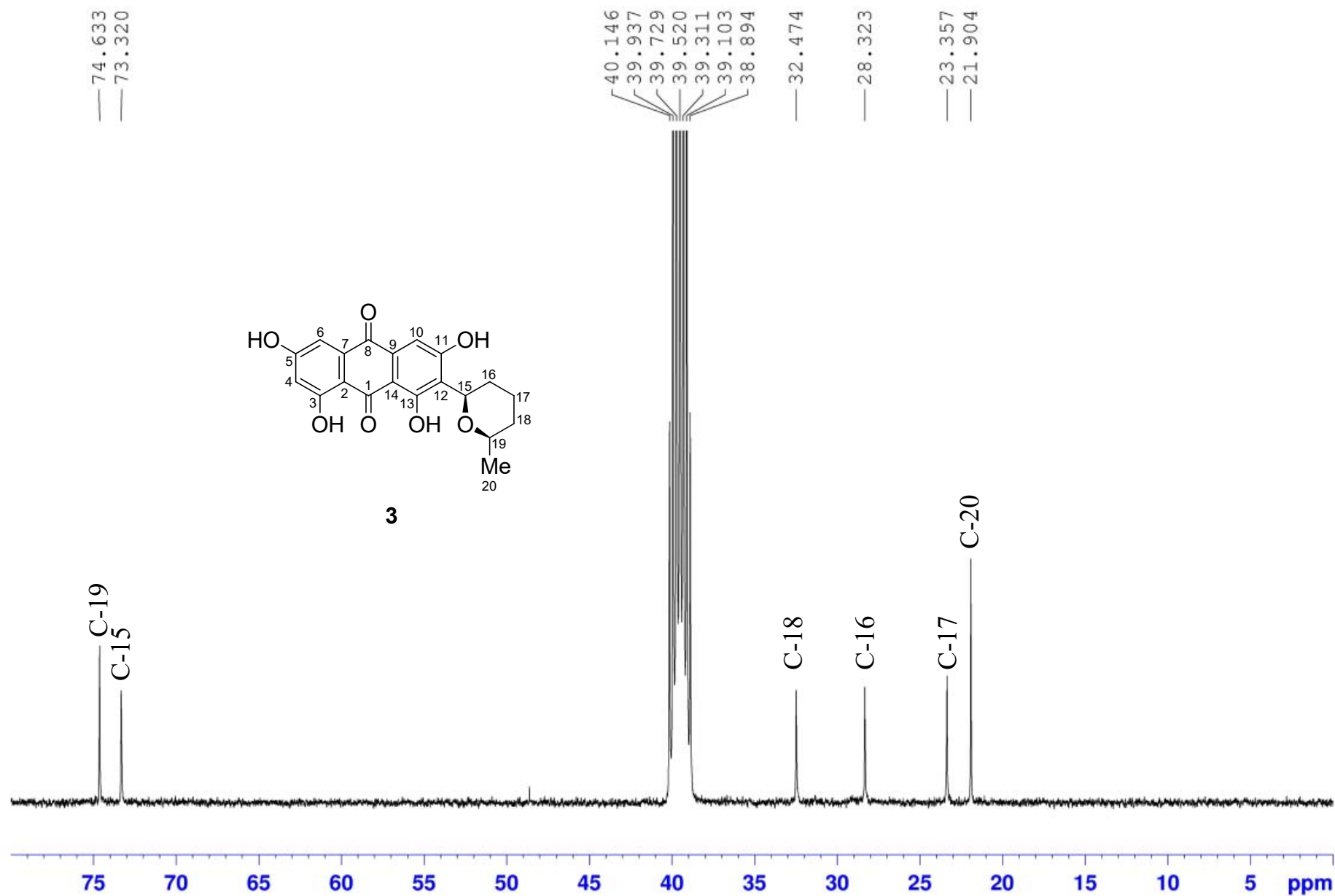
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PROCNO    1
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PULPROG    zgpg30
TD         65536
SOLVENT    DMSO
NS         1024
DS         4
SWH        24038.461 Hz
FIDRES     0.366798 Hz
AQ         1.3631988 sec
RG         195.9
DW         20.800 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
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LB        1.00 Hz
GB        0
PC        1.40
    
```

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

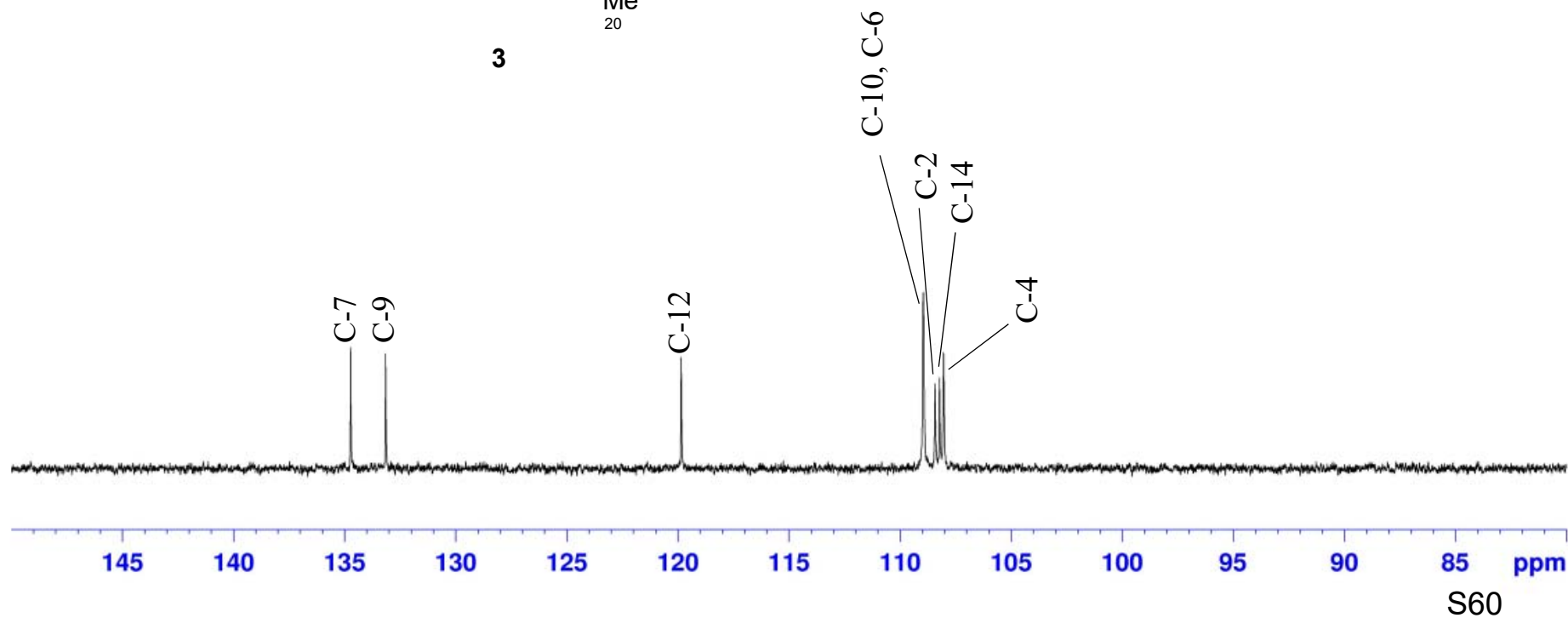
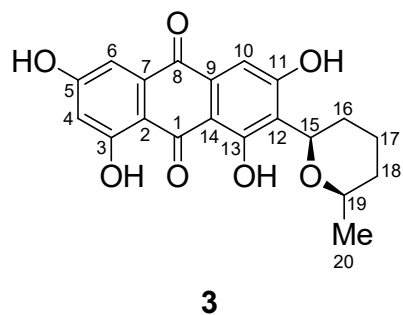


^{13}C (100 MHz) NMR spectrum of **3** in $\text{DMSO-}d_6$

— 134.724
— 133.146

— 119.841

108.957
108.429
108.227
108.048



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

—188.478

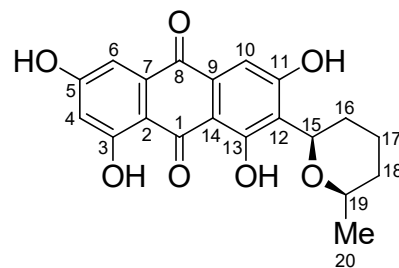
—180.986

—165.546

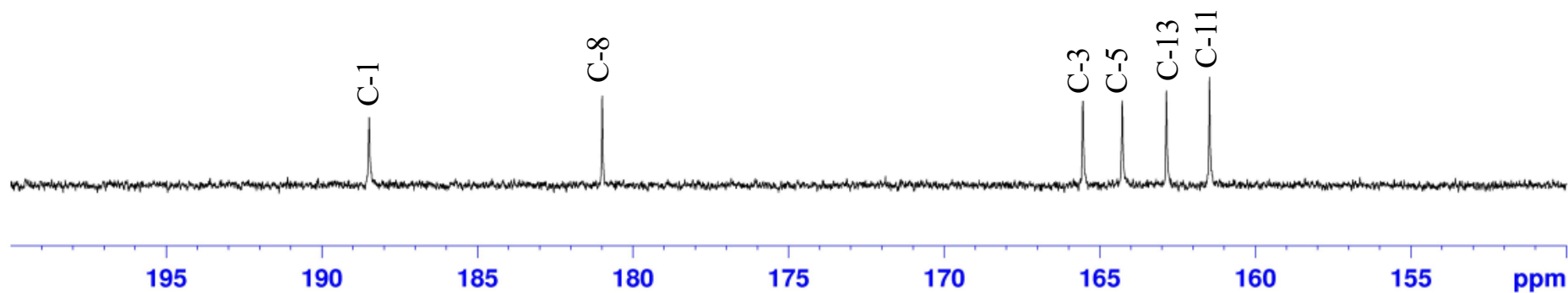
—164.280

—162.861

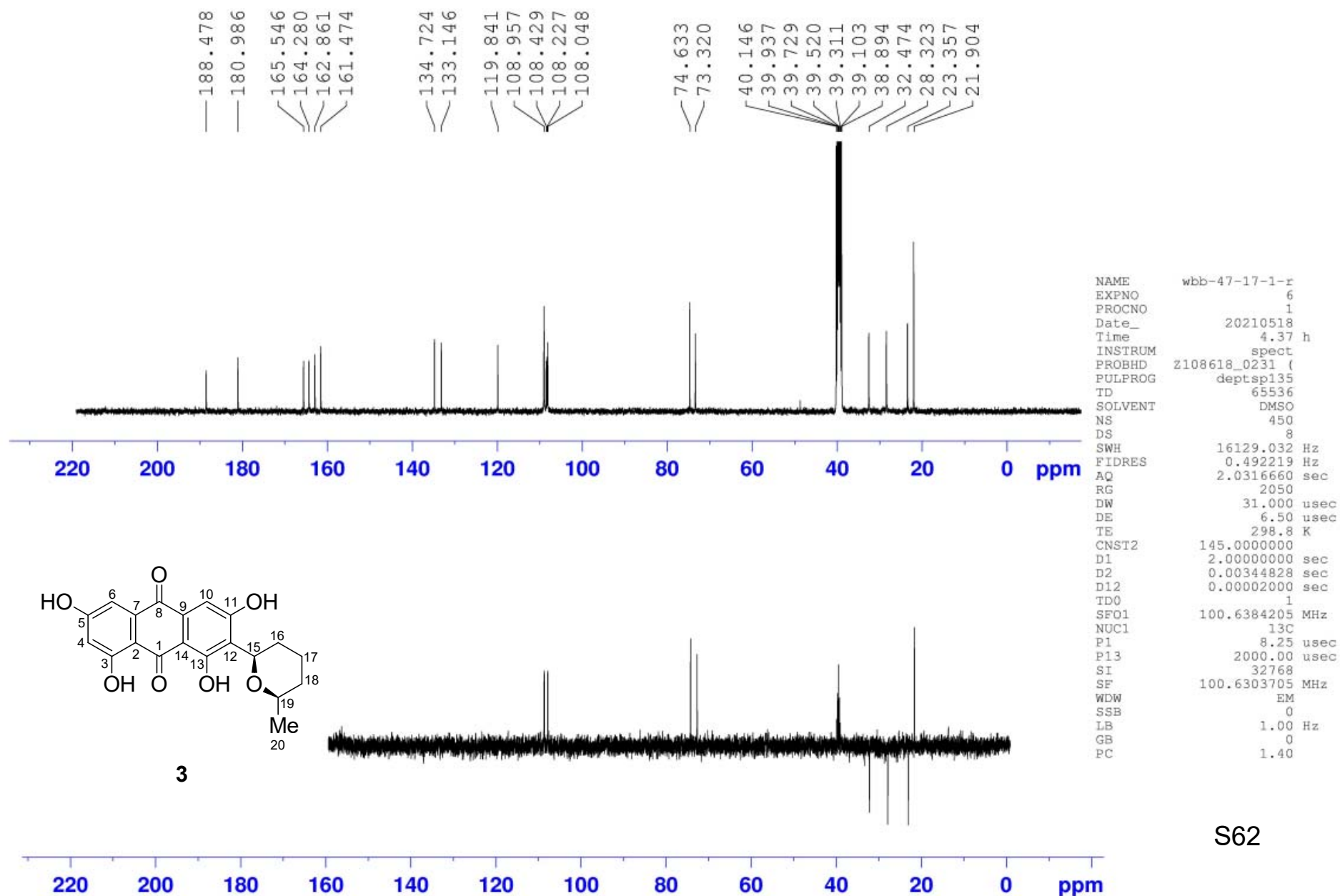
—161.474



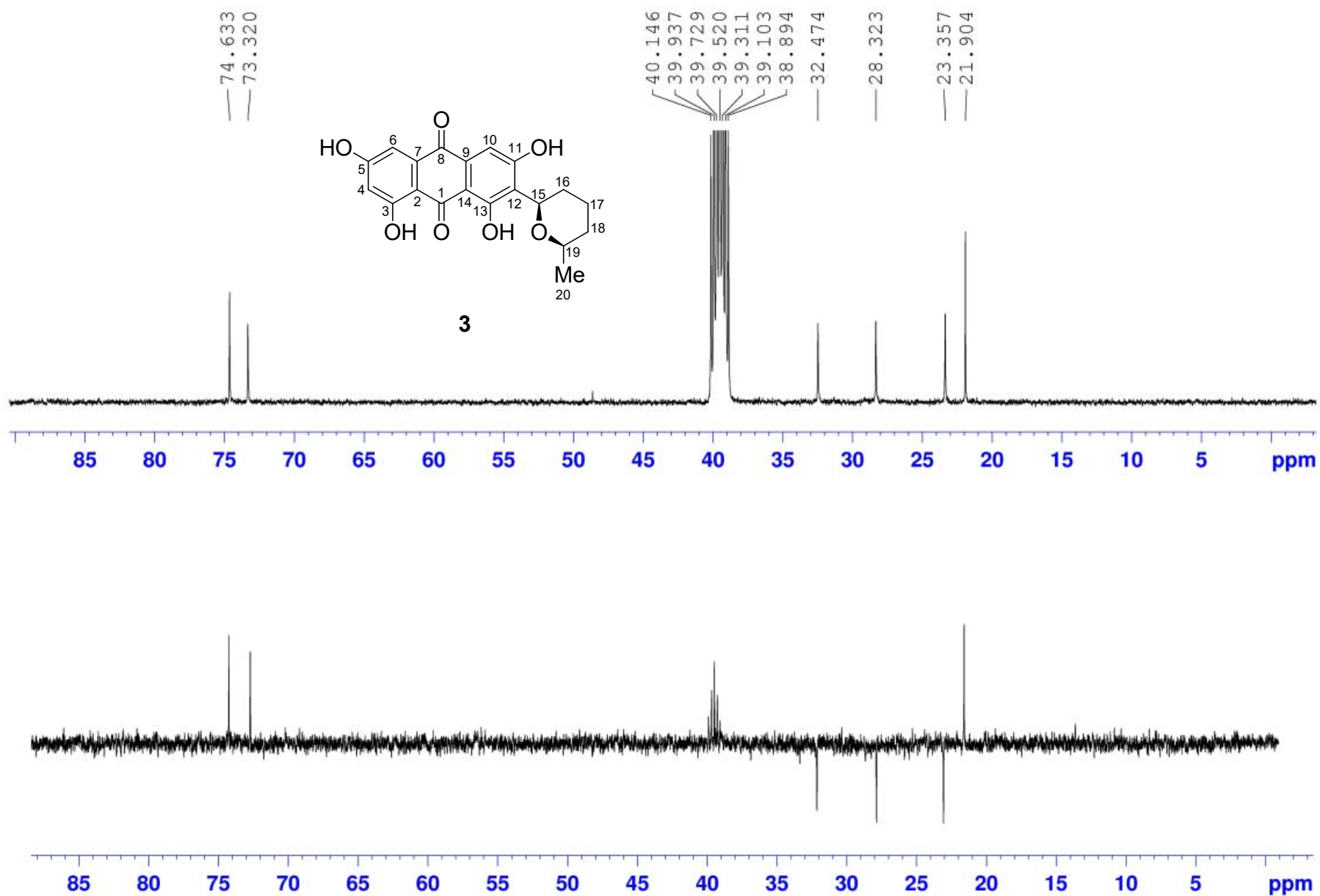
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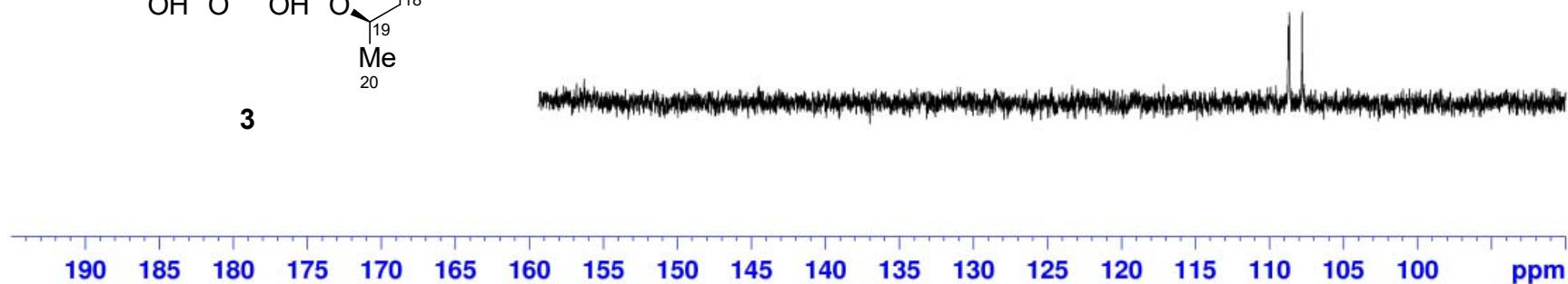
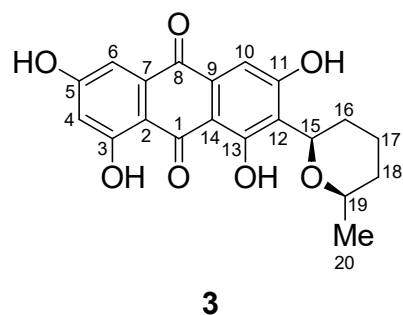
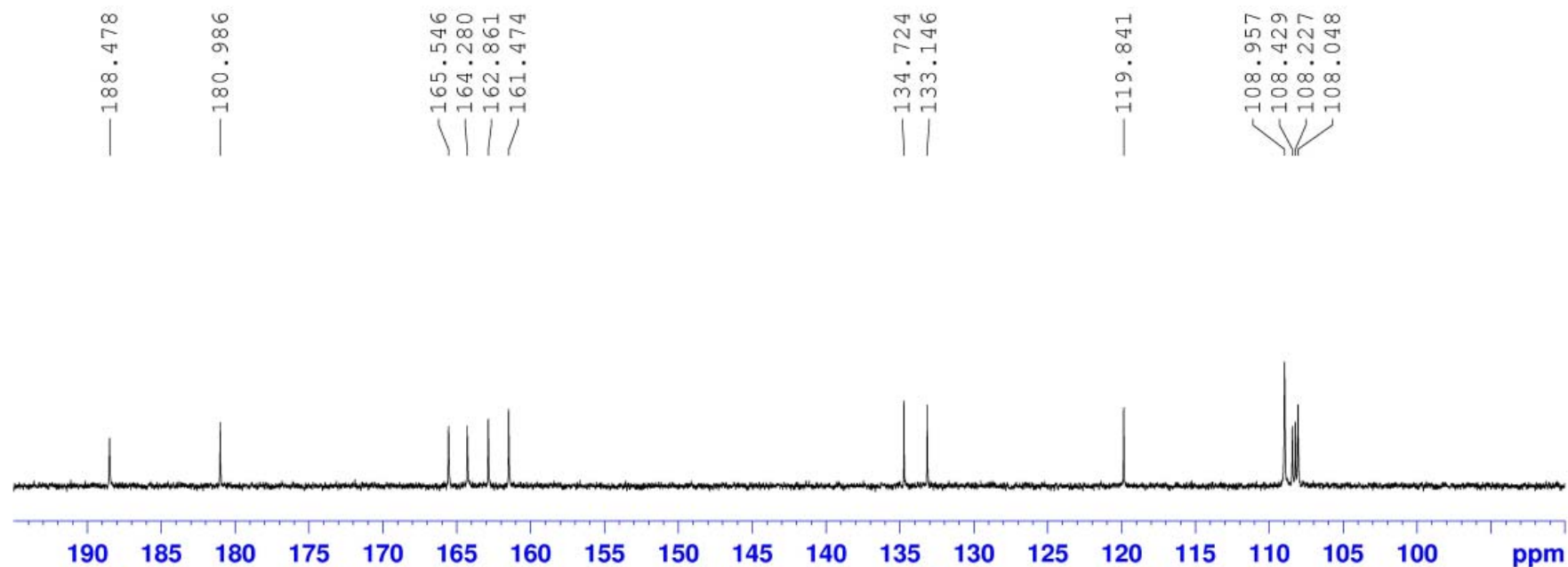
DEPT135 (100 MHz) spectrum of **3** in DMSO- d_6



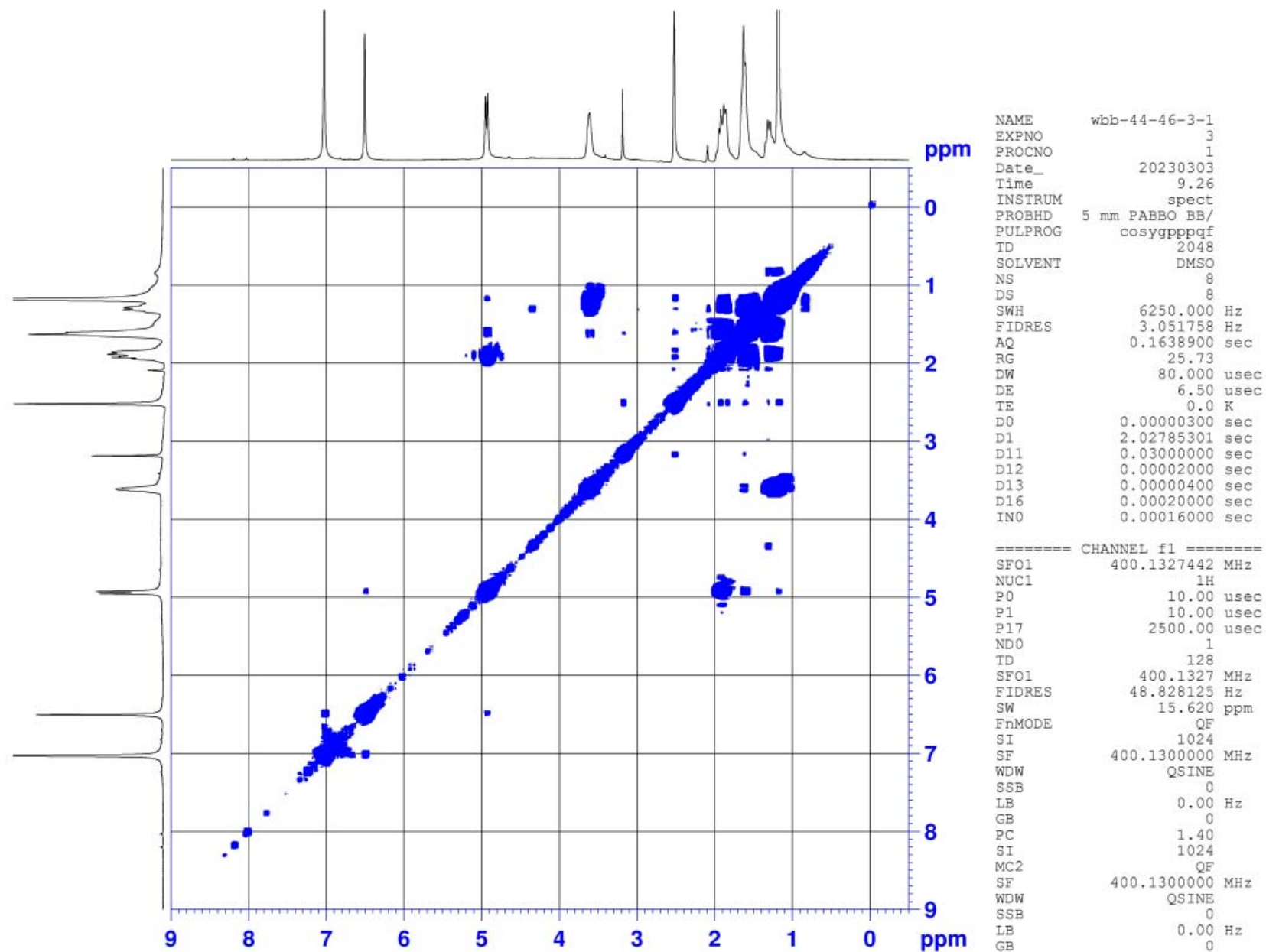
DEPT135 (100 MHz) spectrum of **3** in DMSO- d_6



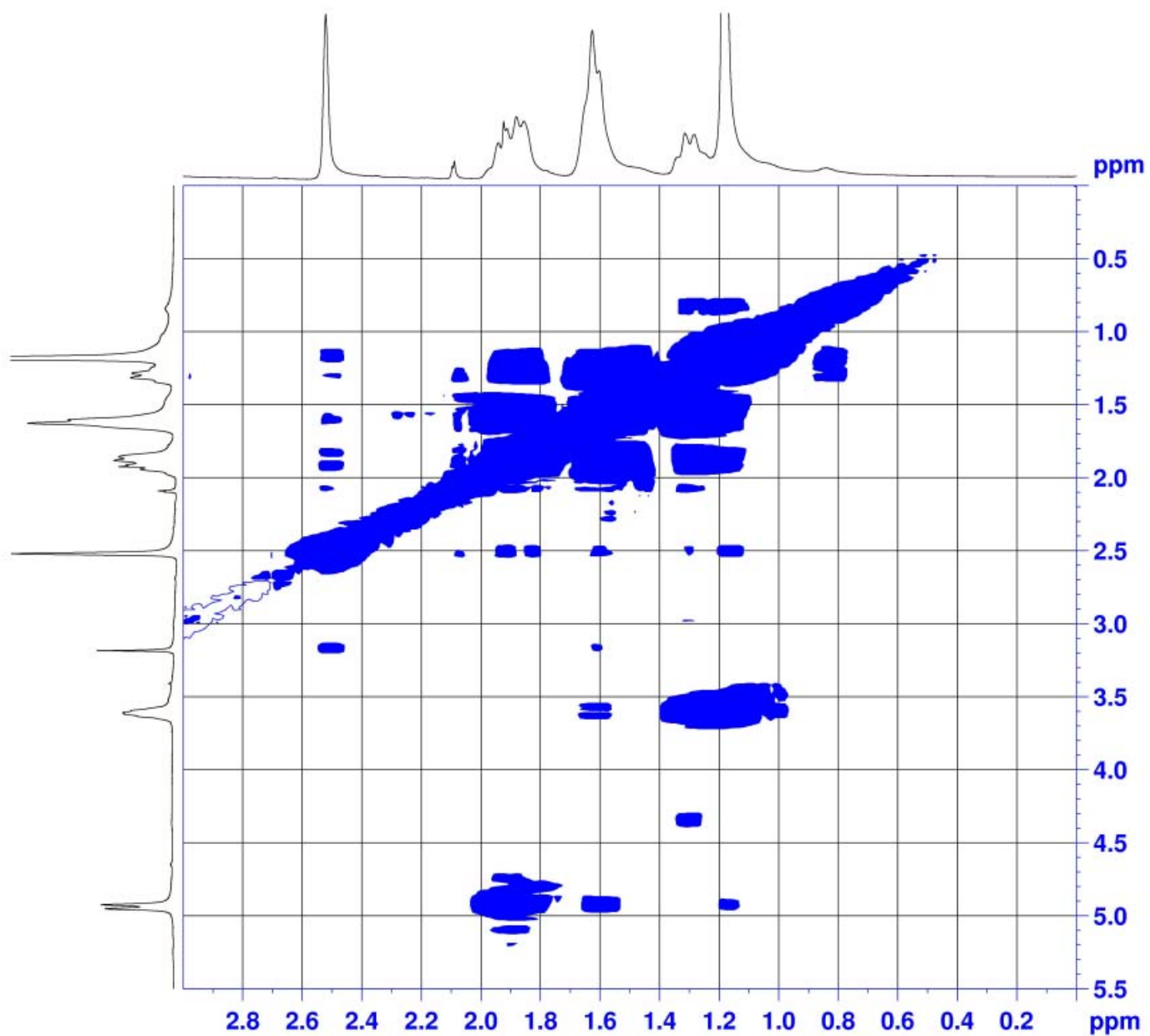
DEPT135 (100 MHz) spectrum of **3** in DMSO- d_6



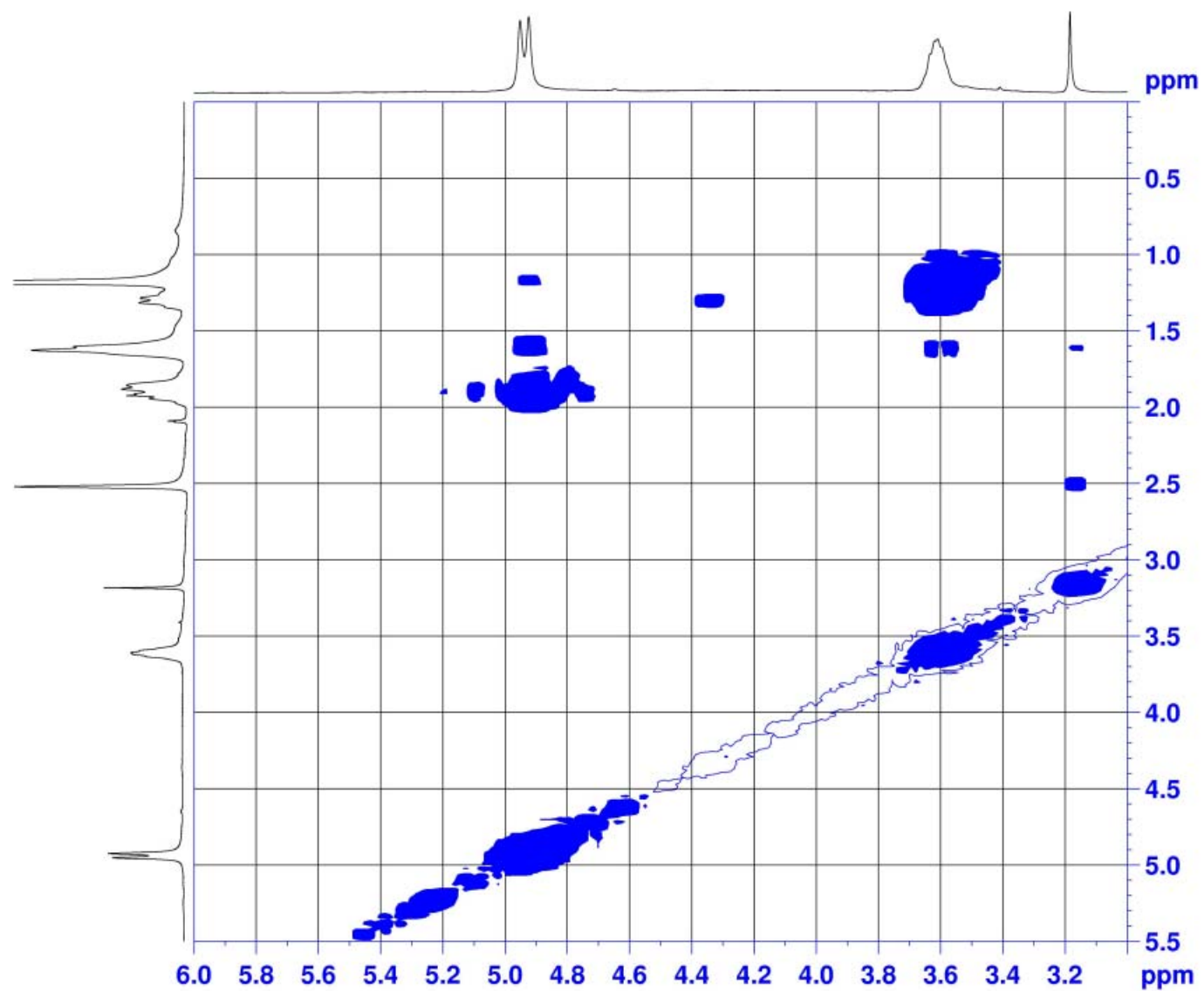
^1H - ^1H COSY (400 MHz) spectrum of **3** in $\text{DMSO-}d_6$



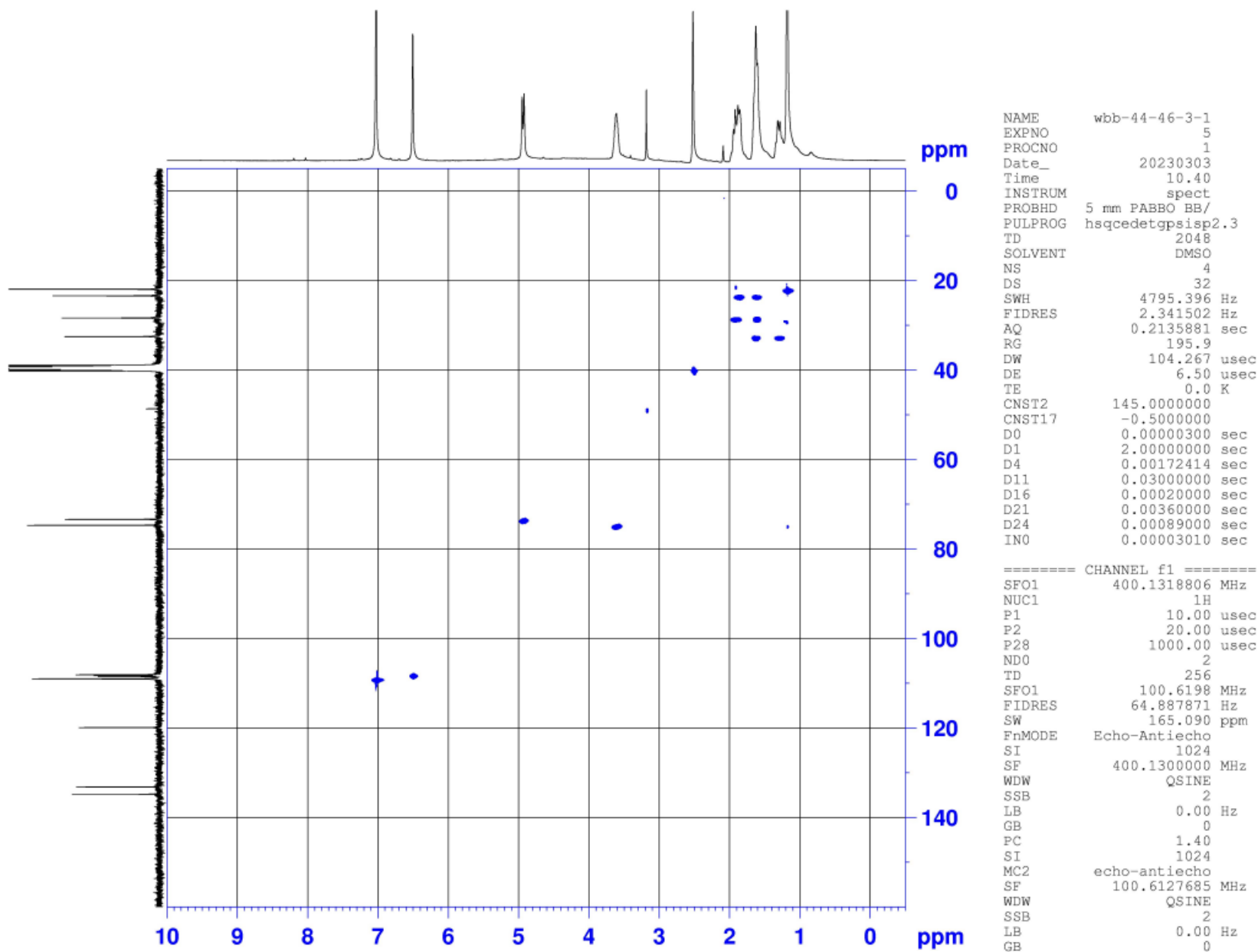
^1H - ^1H COSY (400 MHz) spectrum of **3** in $\text{DMSO-}d_6$



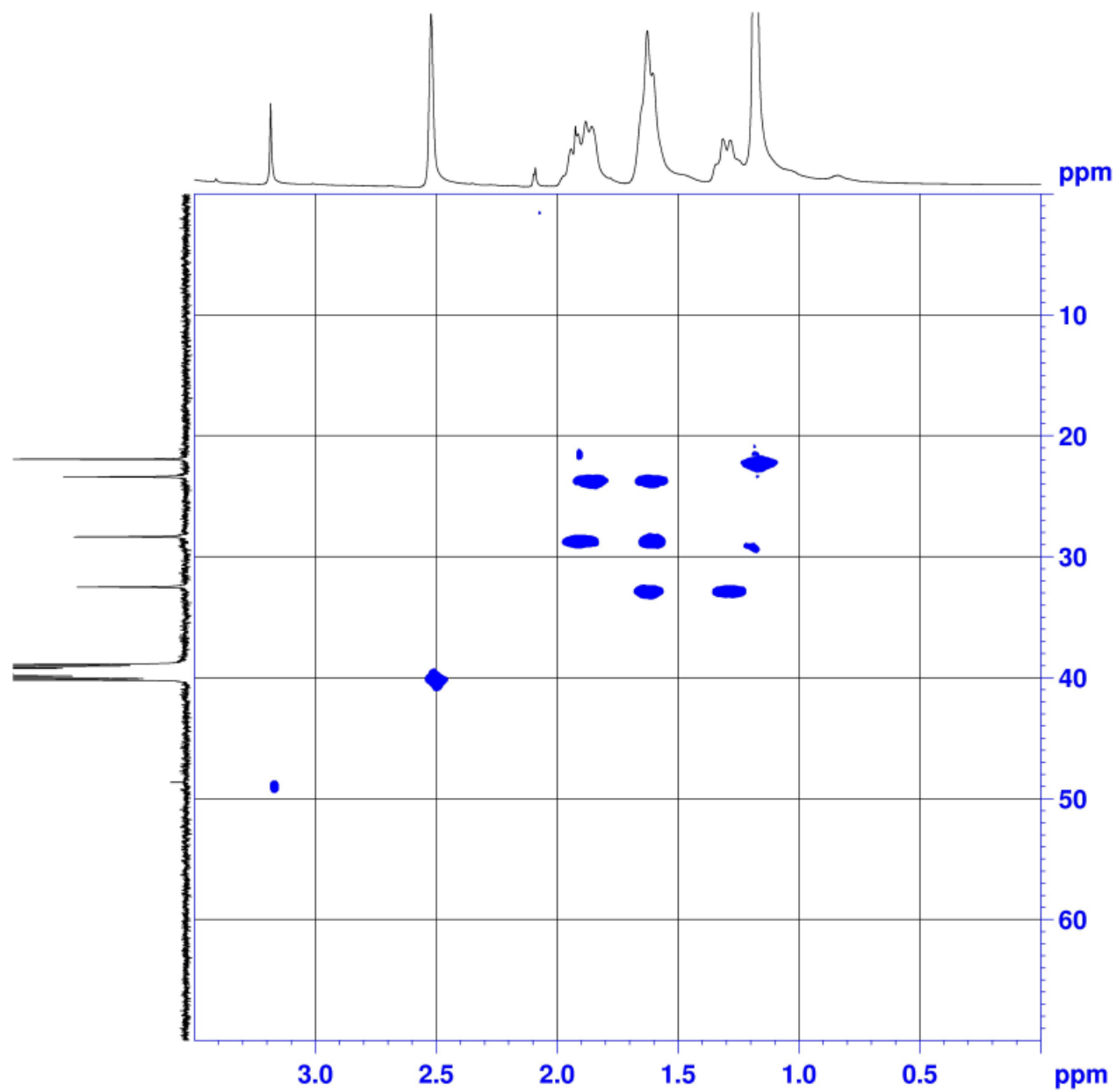
^1H - ^1H COSY (400 MHz) spectrum of **3** in $\text{DMSO-}d_6$



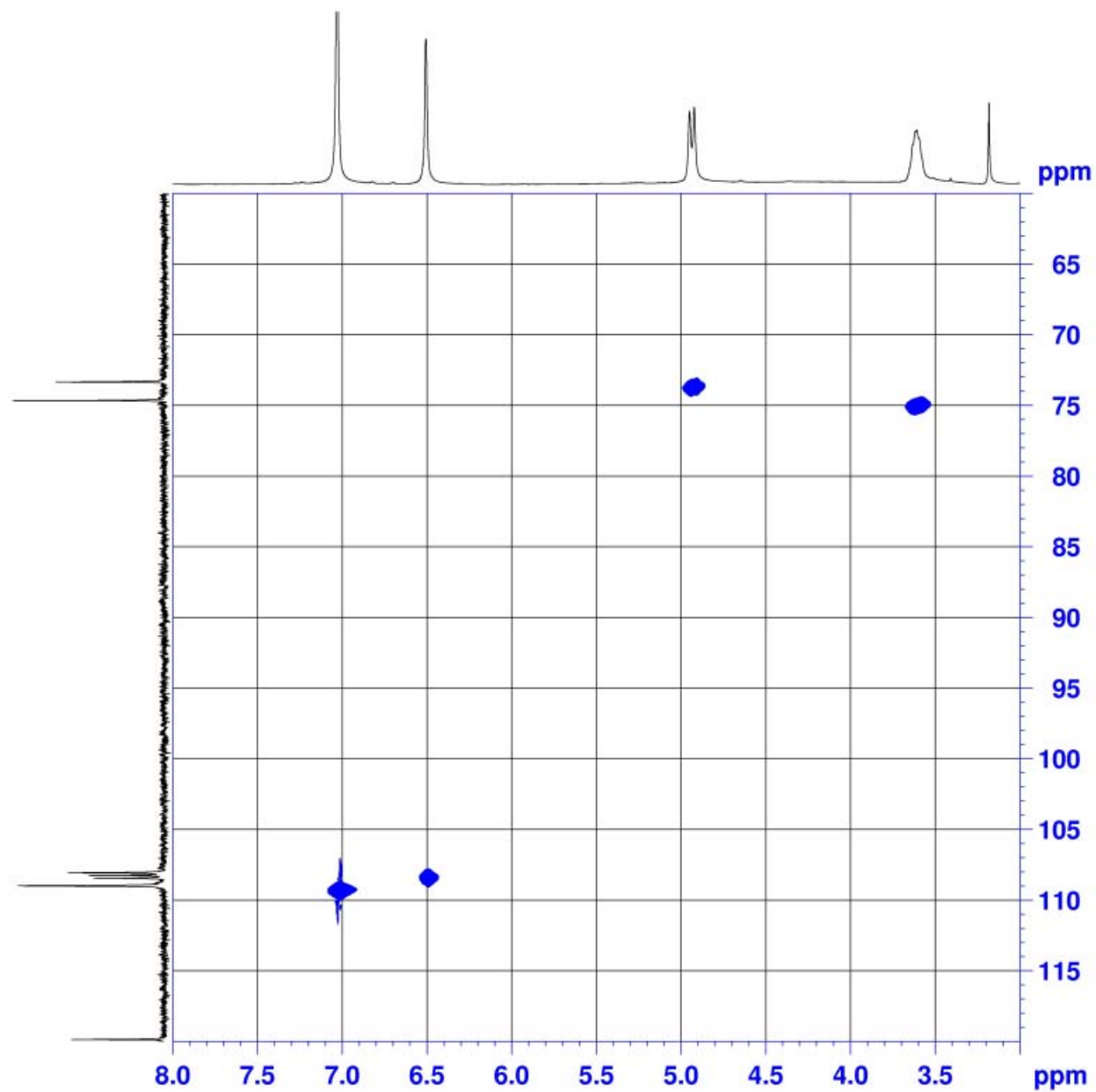
HSQC (400 MHz) spectrum of **3** in DMSO-*d*₆



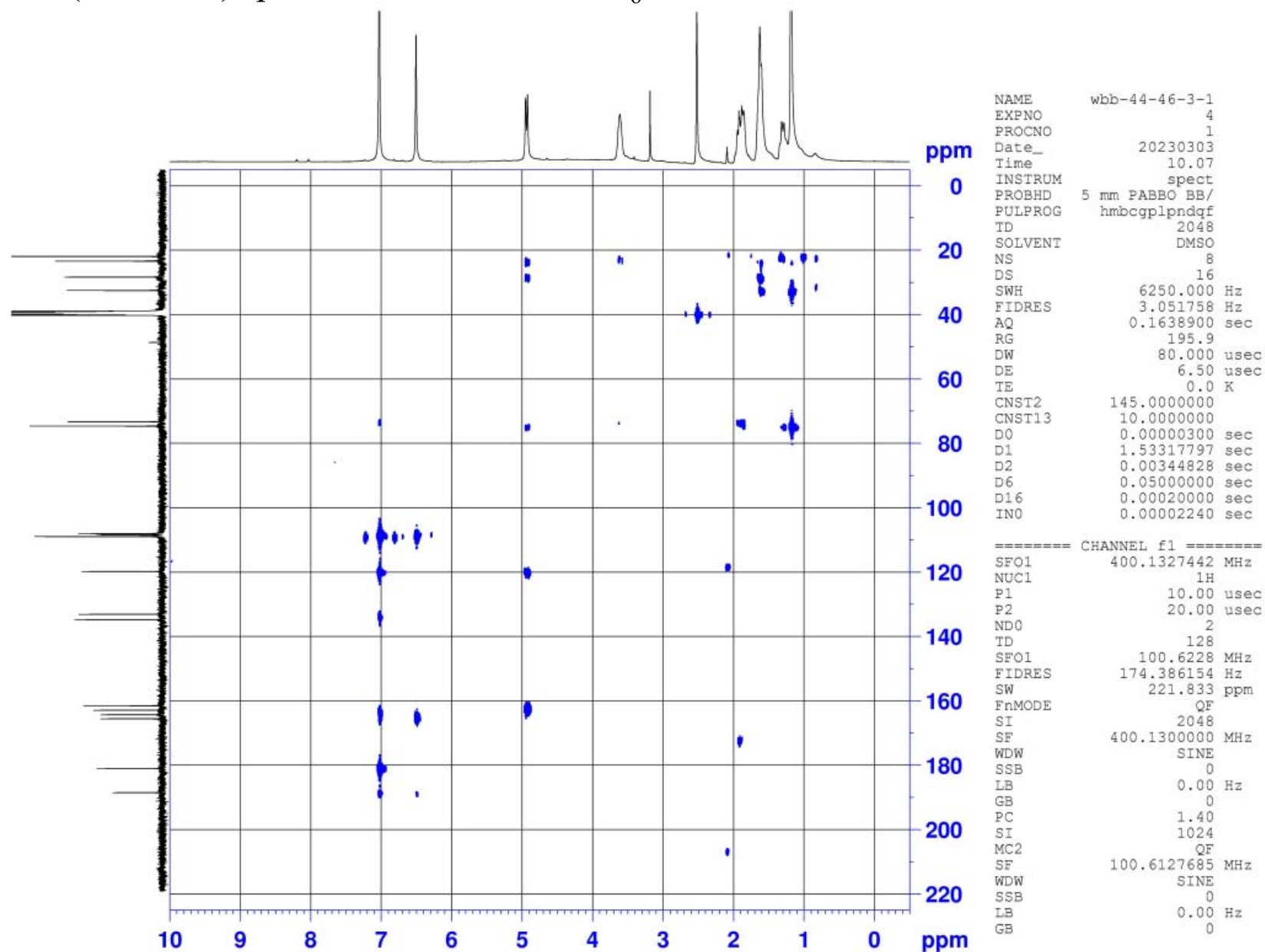
HSQC (400 MHz) spectrum of **3** in DMSO- d_6



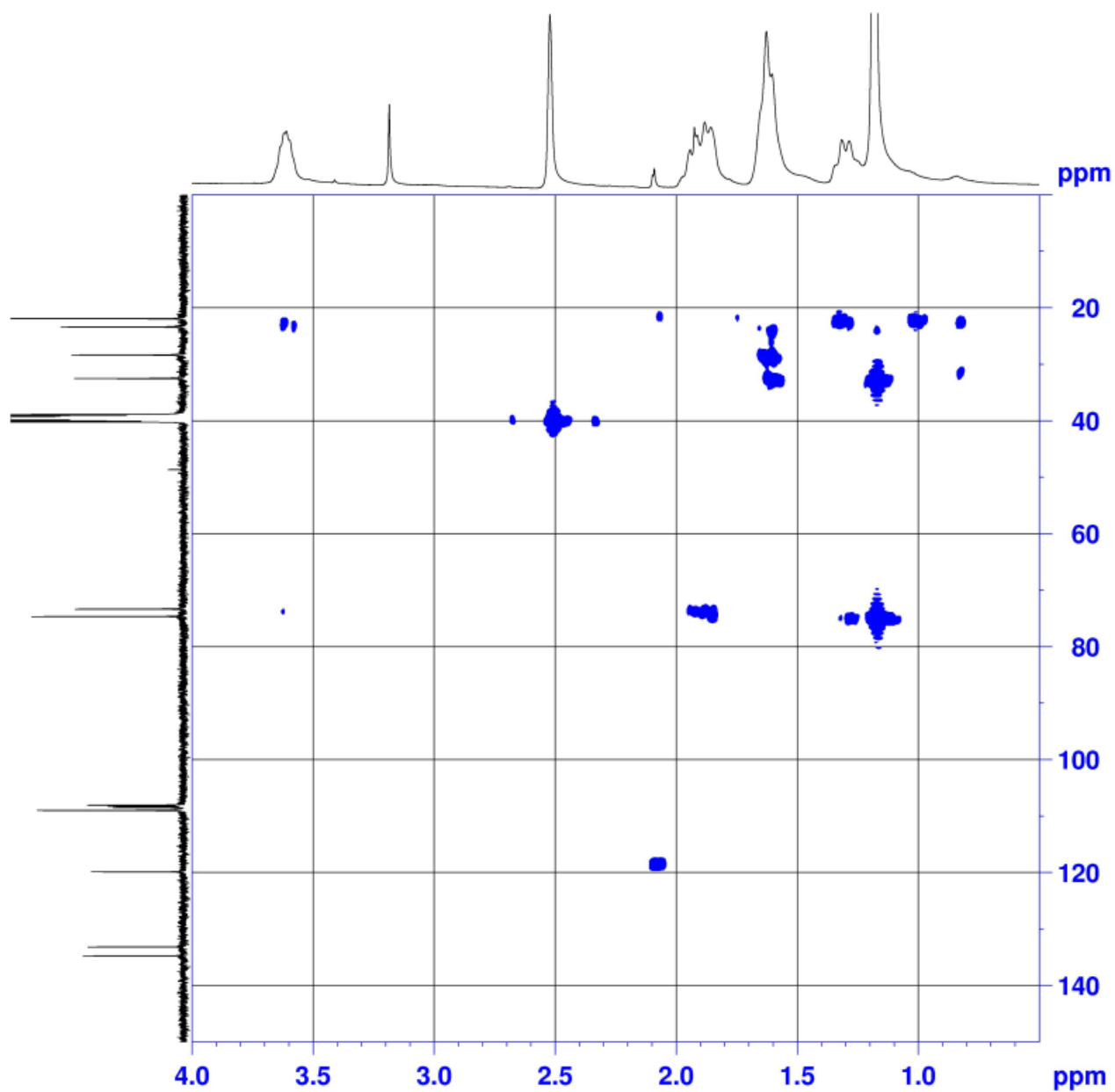
HSQC (400 MHz) spectrum of **3** in DMSO- d_6



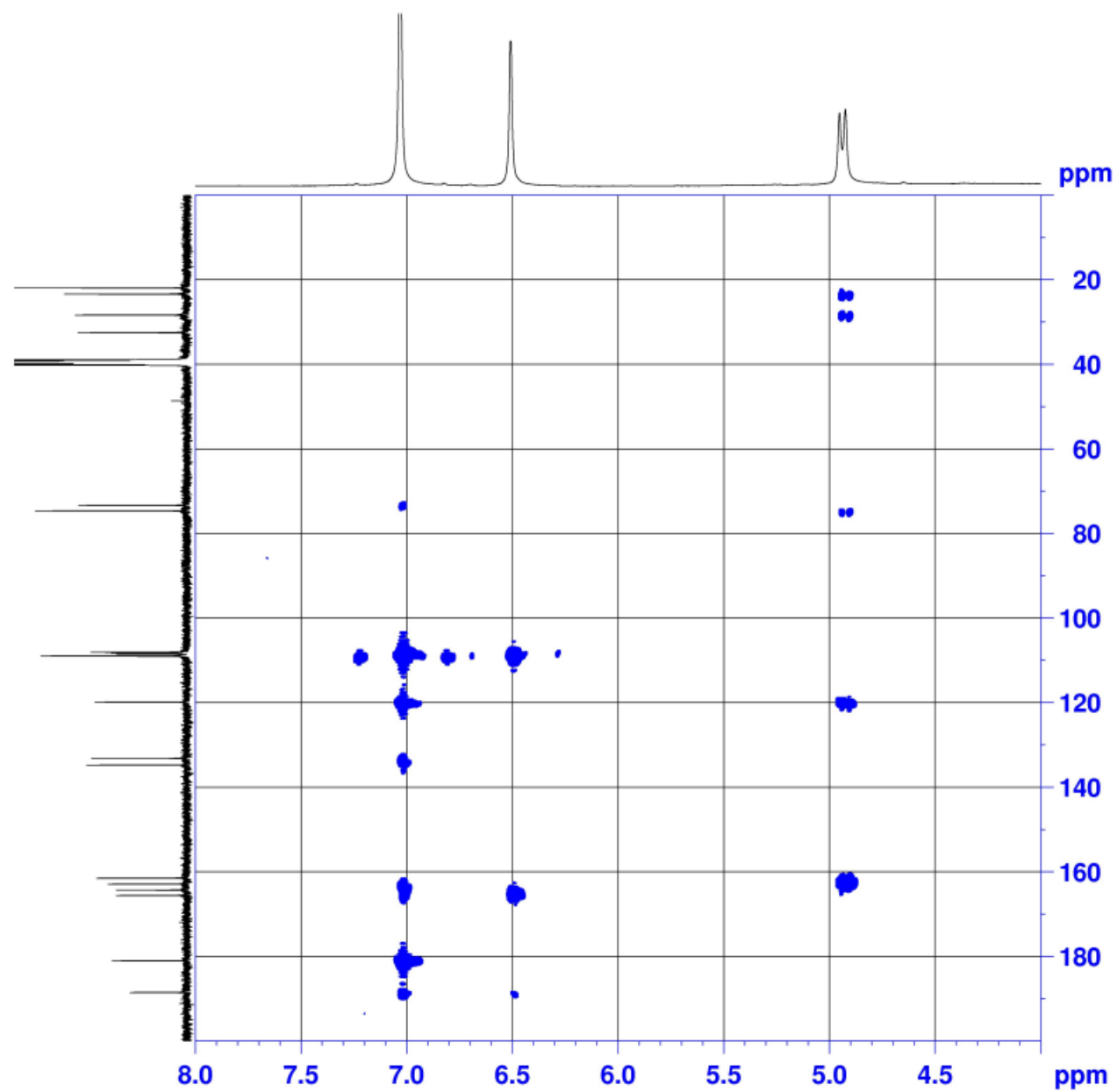
HMBC (400 MHz) spectrum of **3** in DMSO-*d*₆



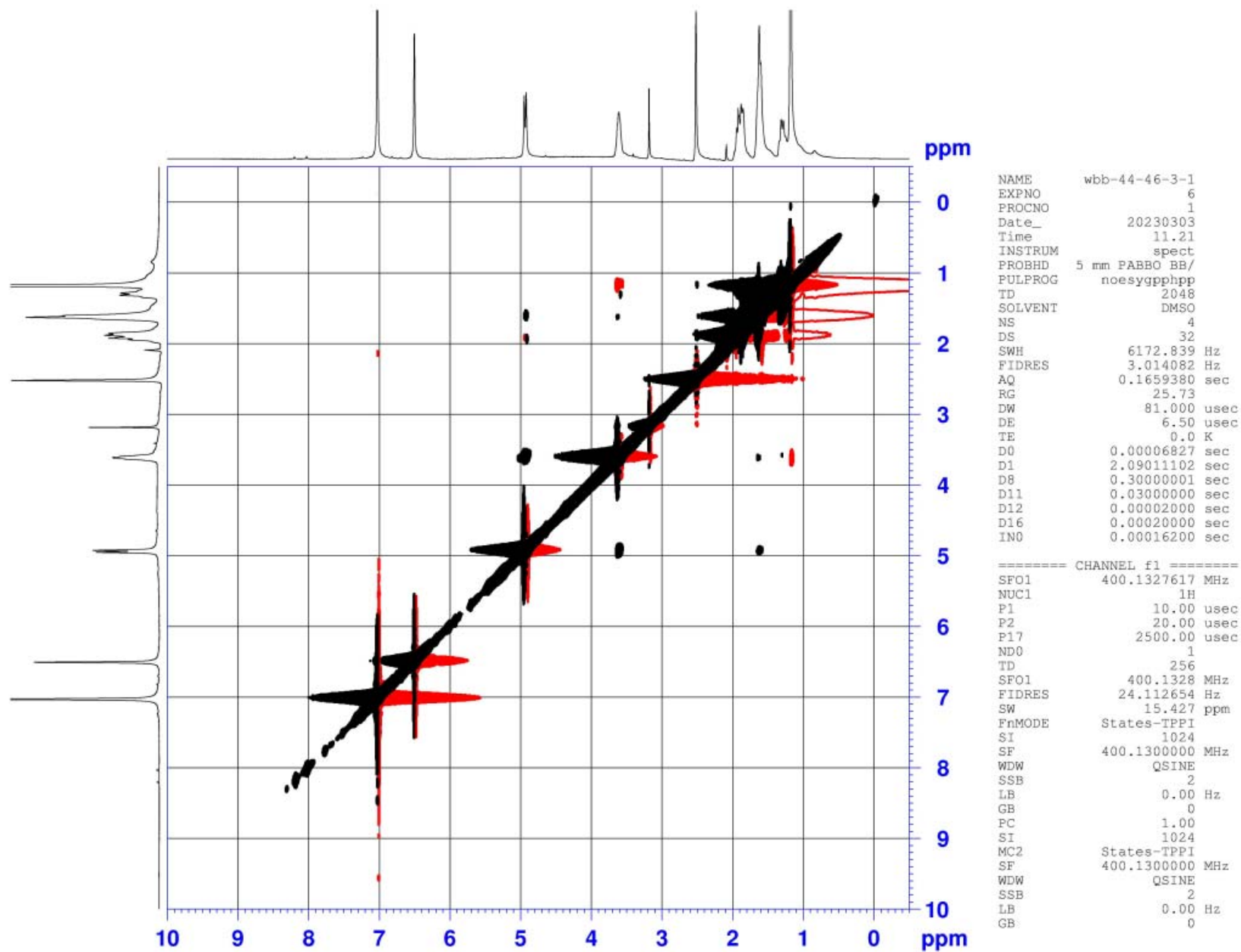
HMBC (400 MHz) spectrum of **3** in DMSO- d_6



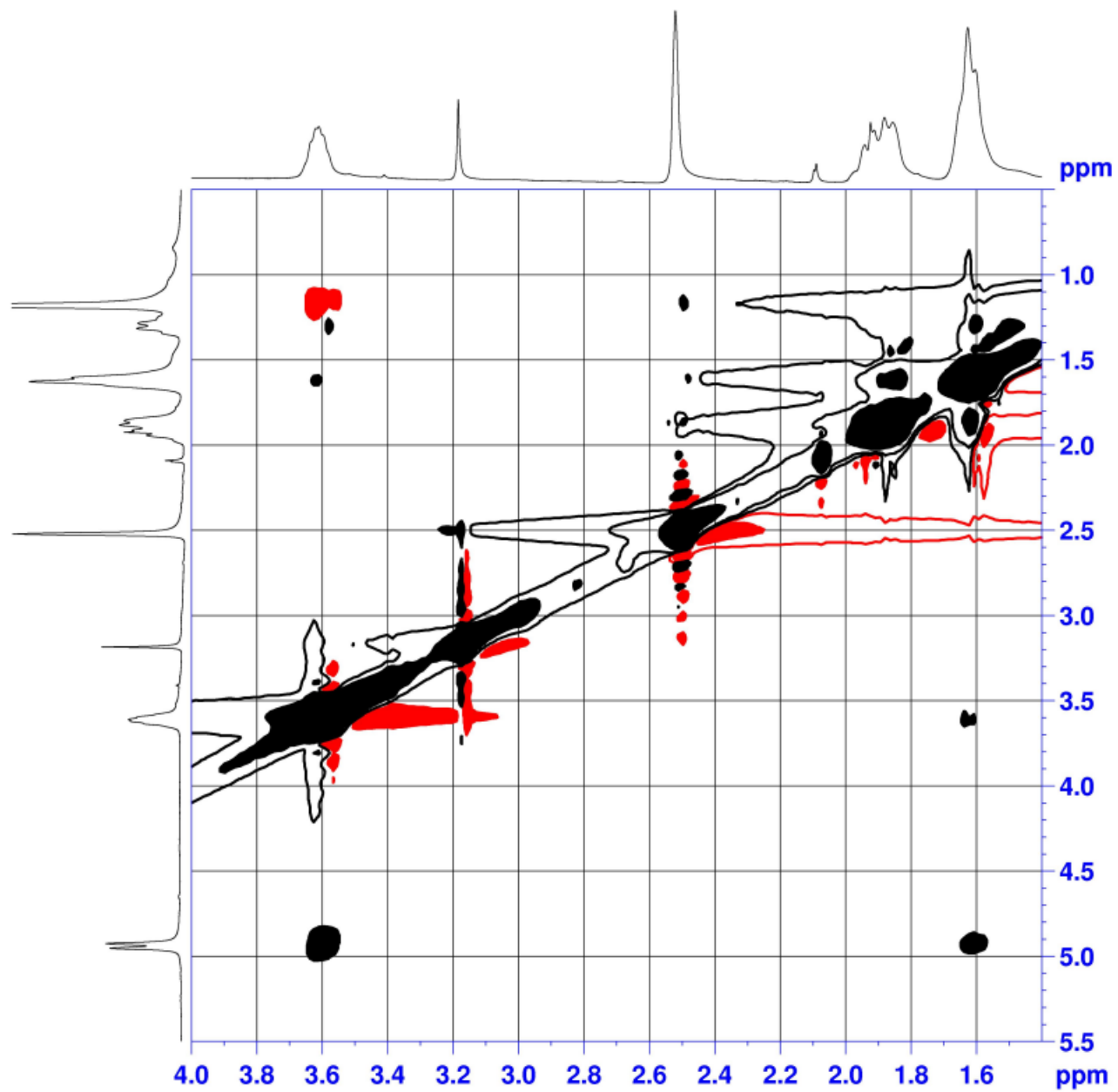
HMBC (400 MHz) spectrum of **3** in DMSO- d_6



NOESY (400 MHz) spectrum of **3** in DMSO-*d*₆



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



HR-ESIMS for 4

Mass Spectrum SmartFormula Report

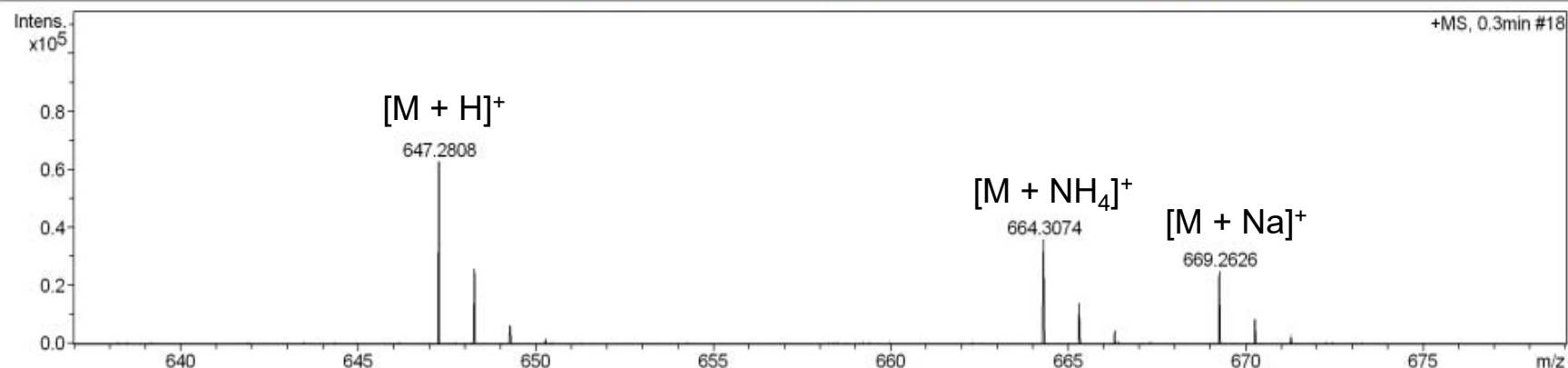
Analysis Info

Analysis Name D:\Data\MS\data\202110\wubinbin_WBB-145-D-R-6_pos_51_01_11733.d
 Method LC_Direct Infusion_pos_70-500mz.m
 Sample Name wubinbin_WBB-145-D-R-6_pos
 Comment

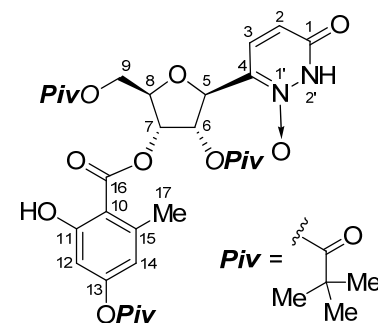
Acquisition Date 10/27/2021 4:38:12 PM
 Operator SCSIO
 Instrument maXis 255552.00029

Acquisition Parameter

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



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e ⁻ Conf	N-Rule
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

S76

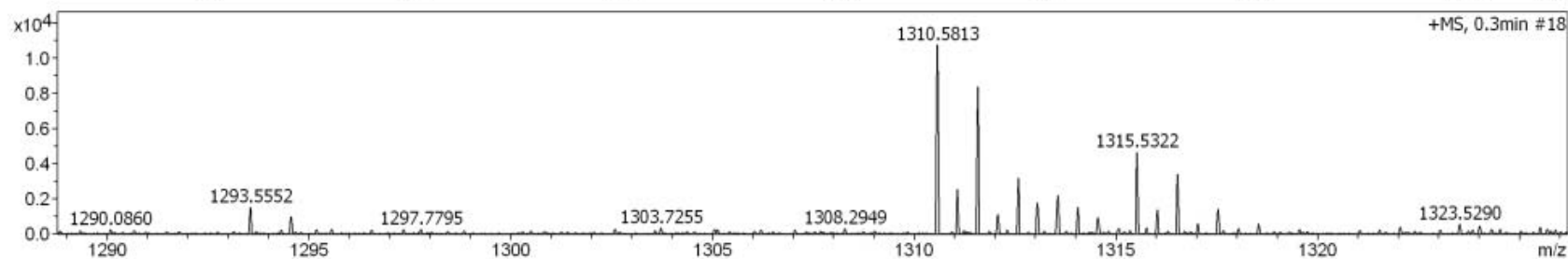
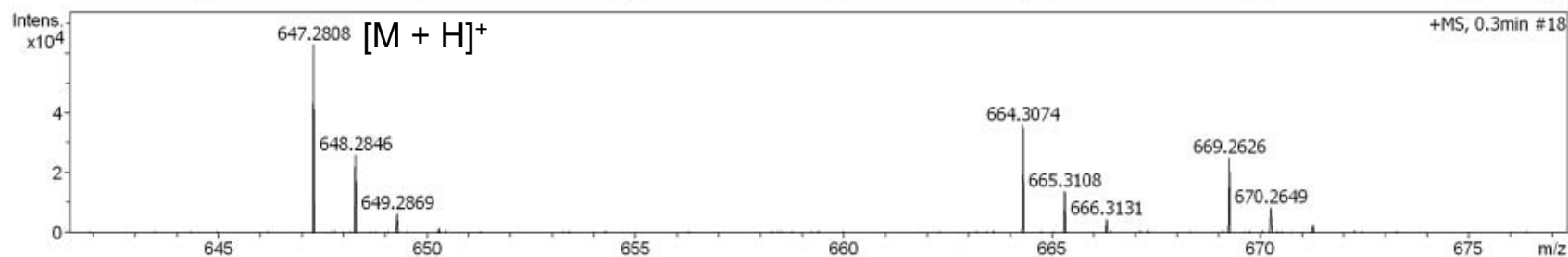
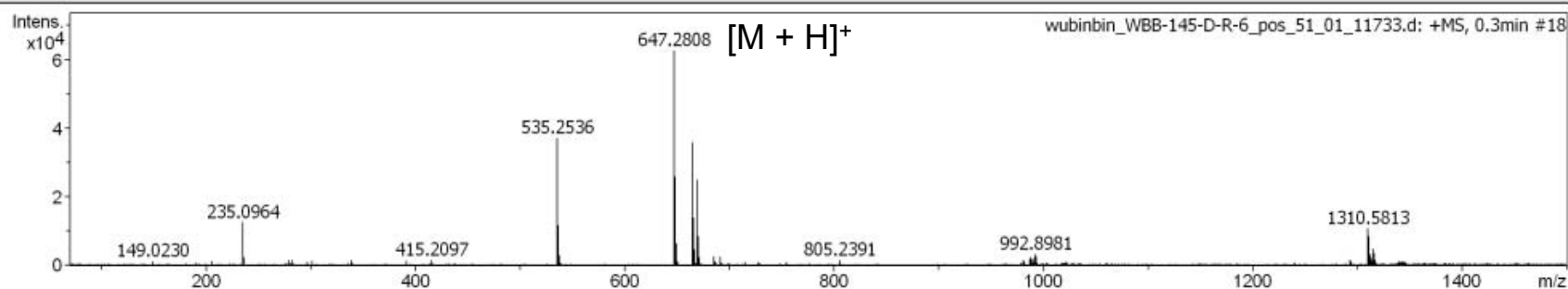
HR-ESIMS for 4

Generic Display Report

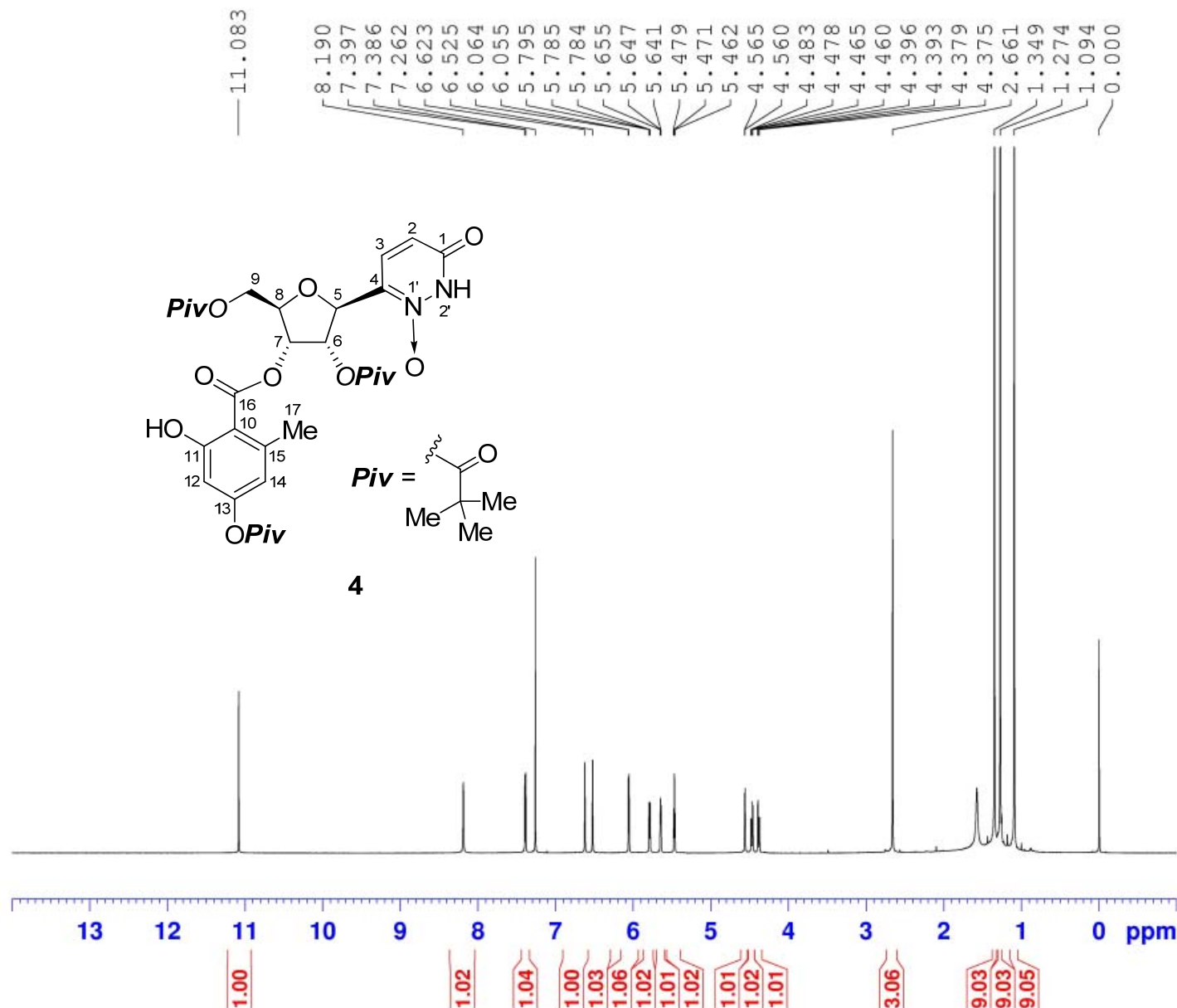
Analysis Info

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Method LC_Direct Infusion_pos_70-500mz.m
Sample Name wubinbin_WBB-145-D-R-6_pos
Comment

Acquisition Date 10/27/2021 4:38:12 PM
Operator SCSIO
Instrument maXis

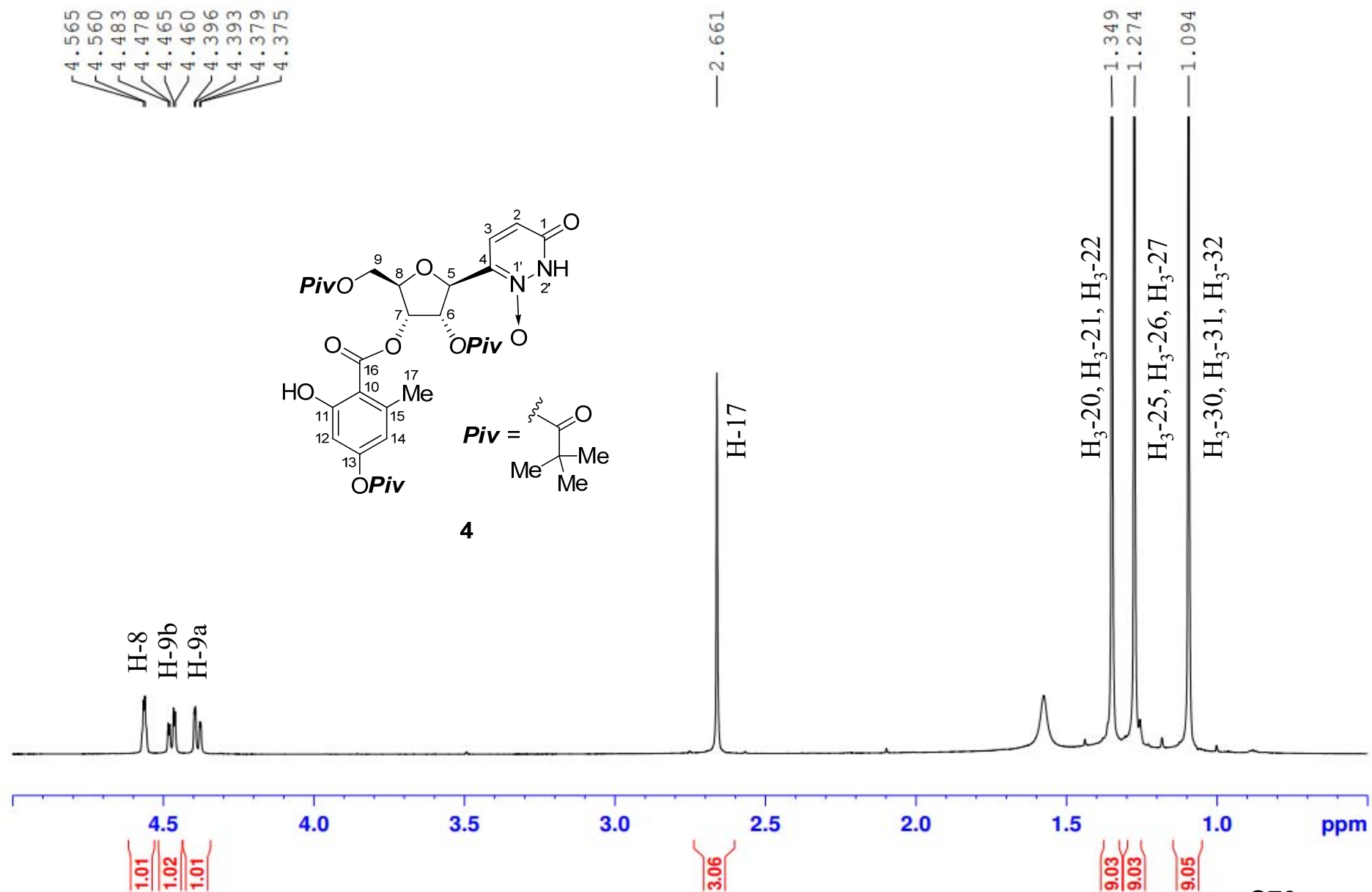


^1H (700 MHz) NMR spectrum of **4** in CDCl_3

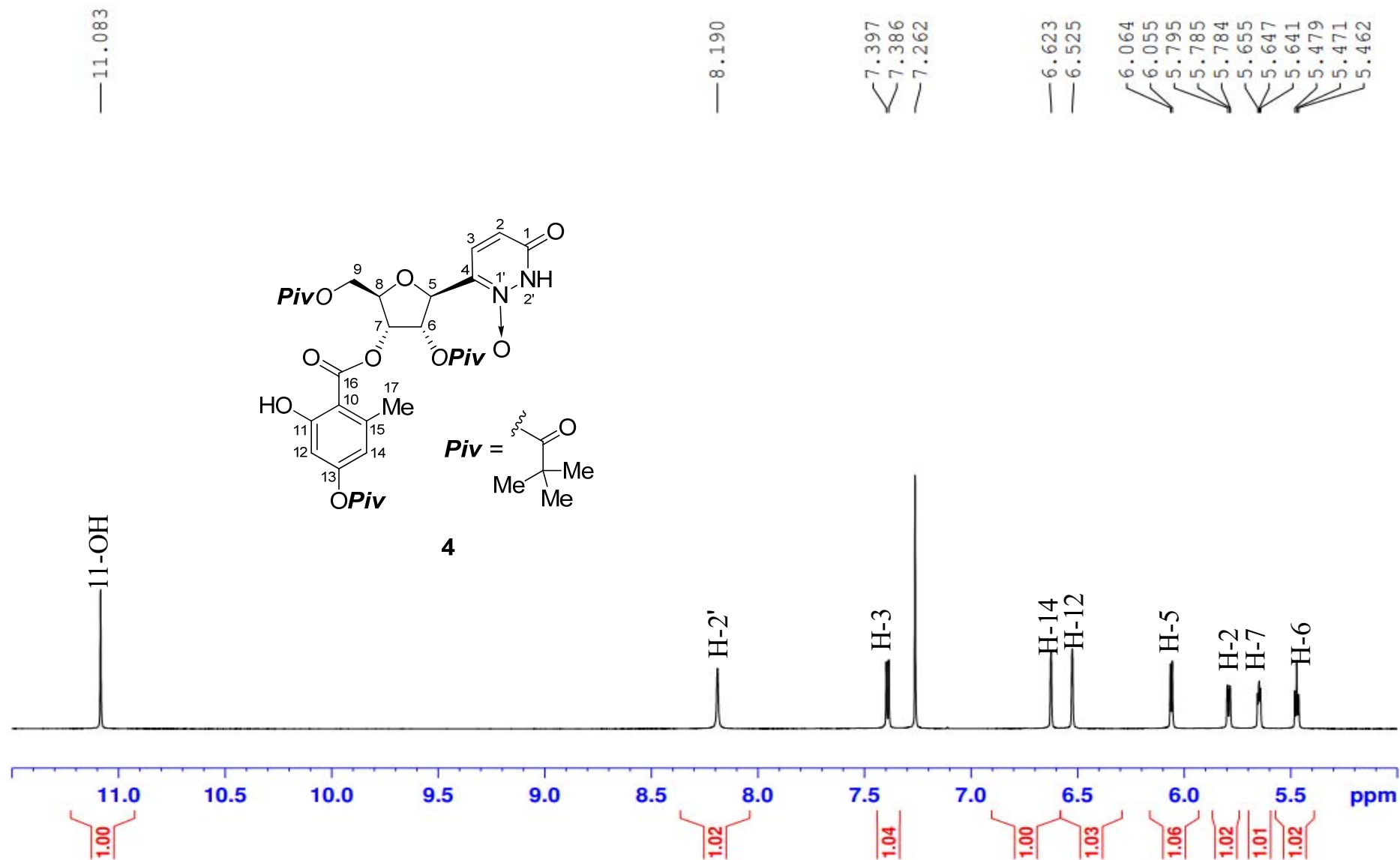


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 PROCNO 1
 Date_ 20211031
 Time 15.25 h
 INSTRUM spect
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl_3
 NS 16
 DS 2
 SWH 14097.744 Hz
 FIDRES 0.430229 Hz
 AQ 2.3243935 sec
 RG 4.87
 DW 35.467 usec
 DE 10.00 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
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 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

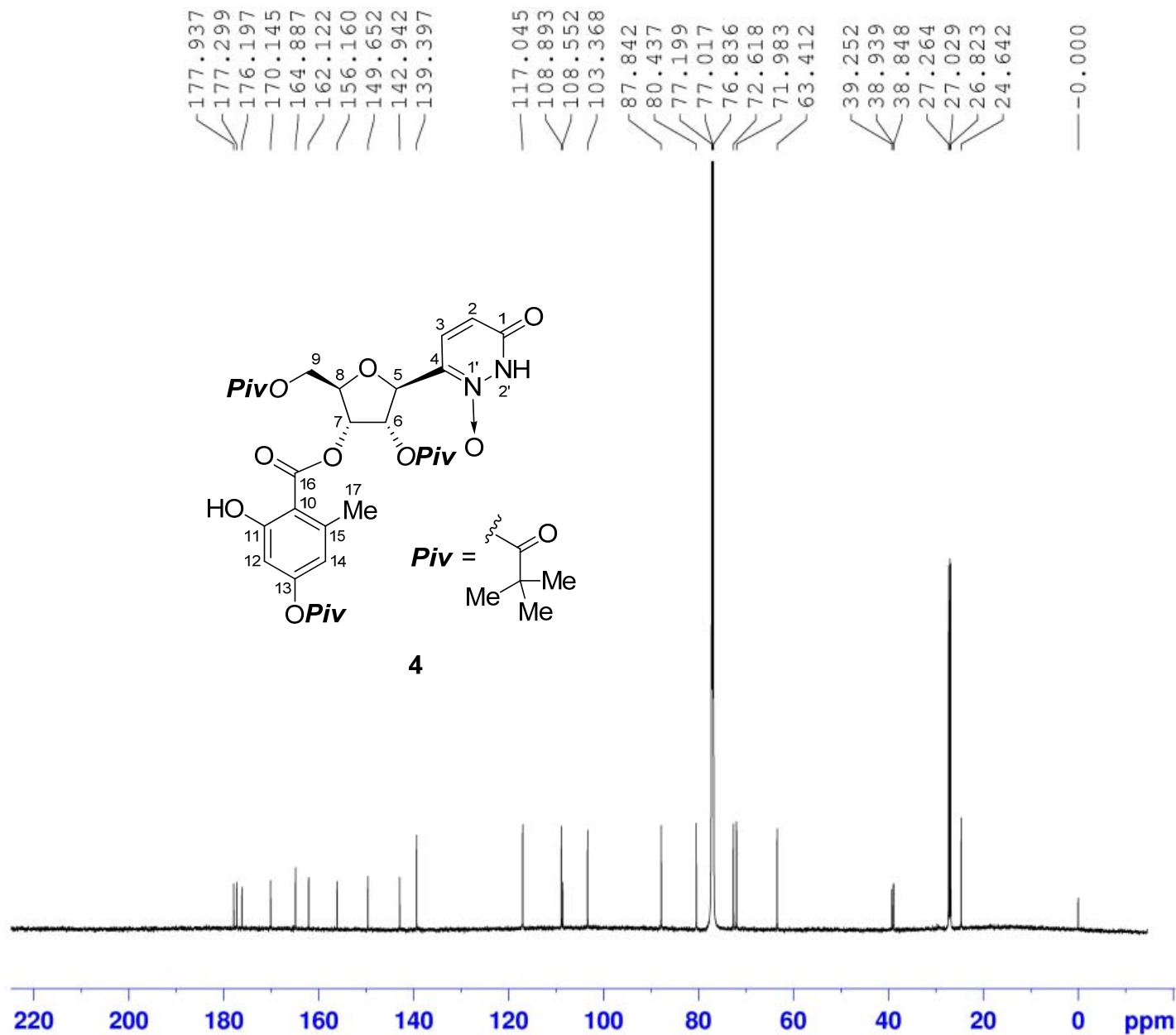
^1H (700 MHz) NMR spectrum of **4** in CDCl_3



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



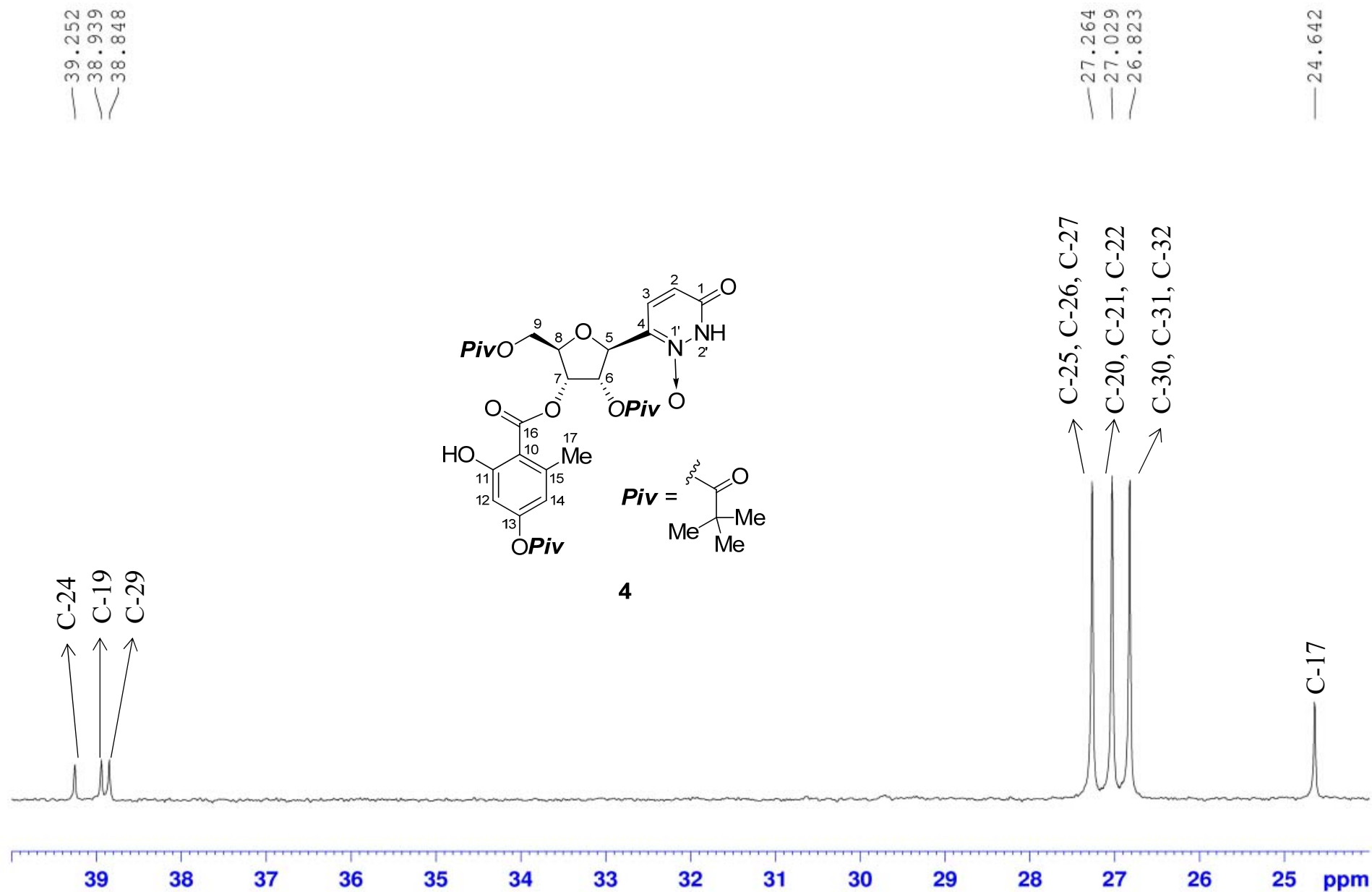
^{13}C (175 MHz) NMR spectrum of **4** in CDCl_3



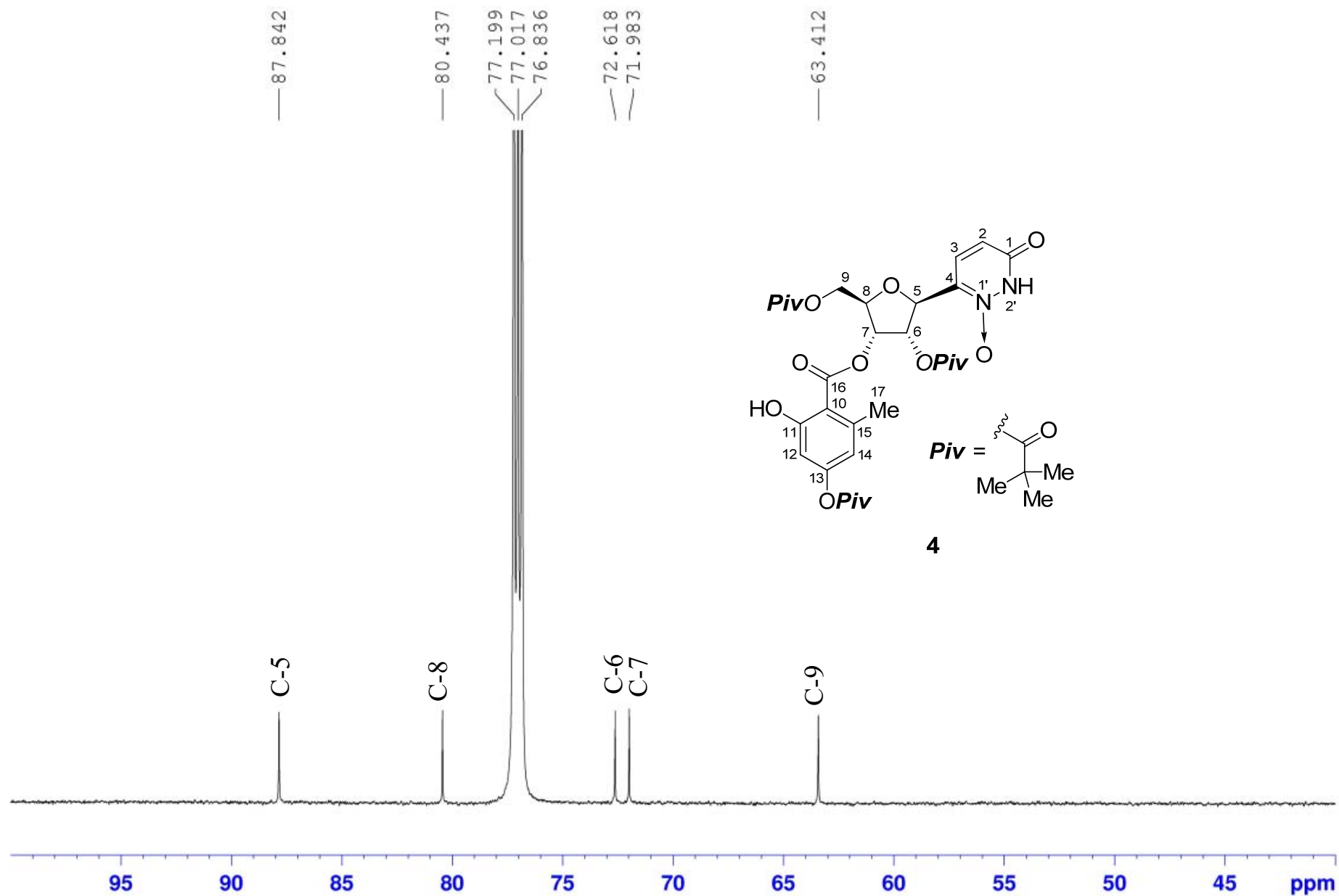
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PROCNO    1
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PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         4000
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SWH        43859.648 Hz
FIDRES     2.676980 Hz
AQ         0.3736052 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
    
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^{13}C (175 MHz) NMR spectrum of **4** in CDCl_3



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

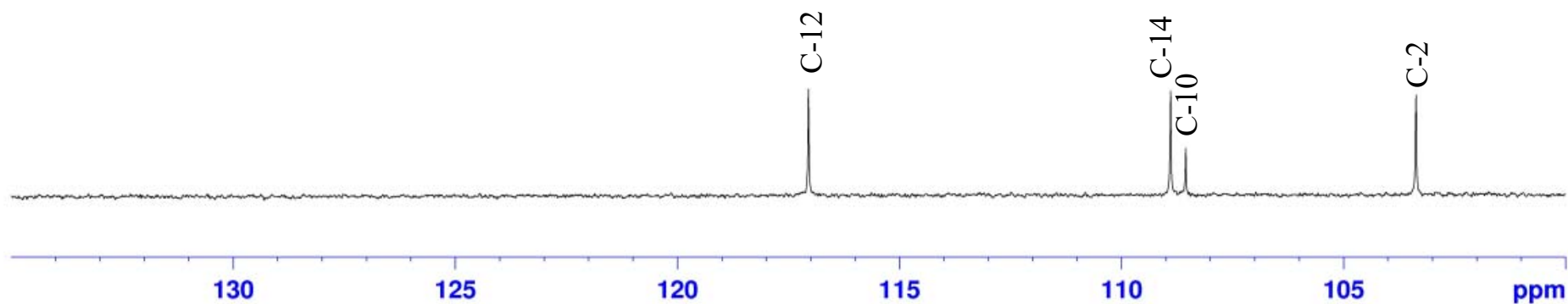
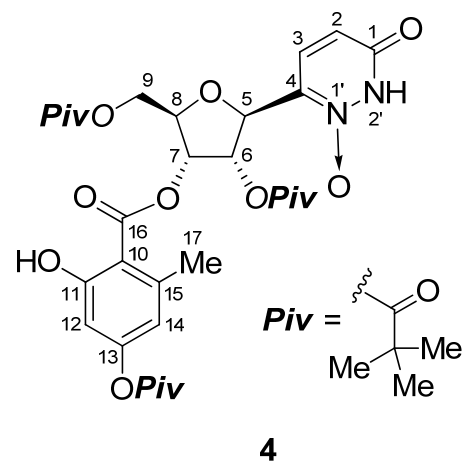


^{13}C (175 MHz) NMR spectrum of **4** in CDCl_3

—117.045

—108.893
—108.552

—103.368



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

—177.937
—177.299
—176.197

—170.145

—164.887

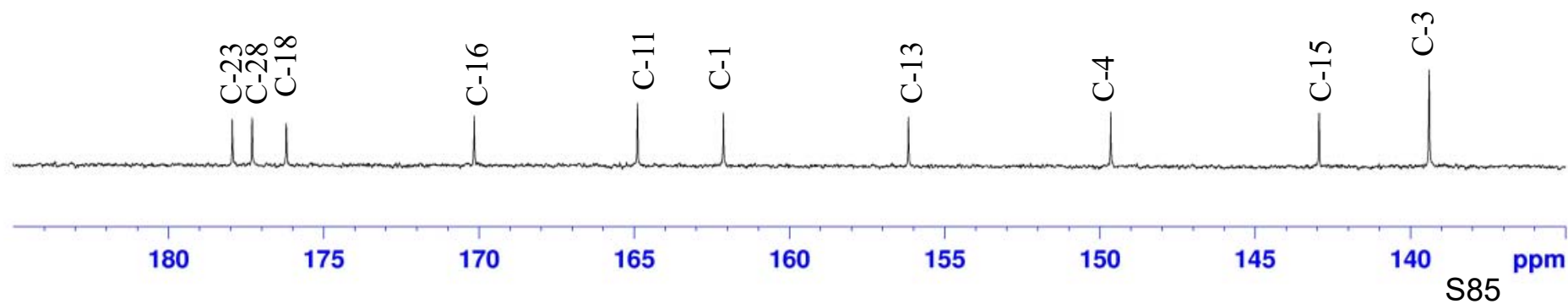
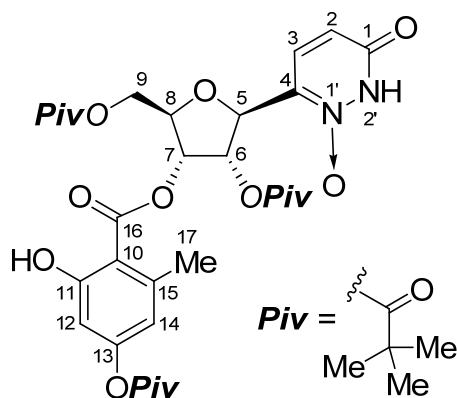
—162.122

—156.160

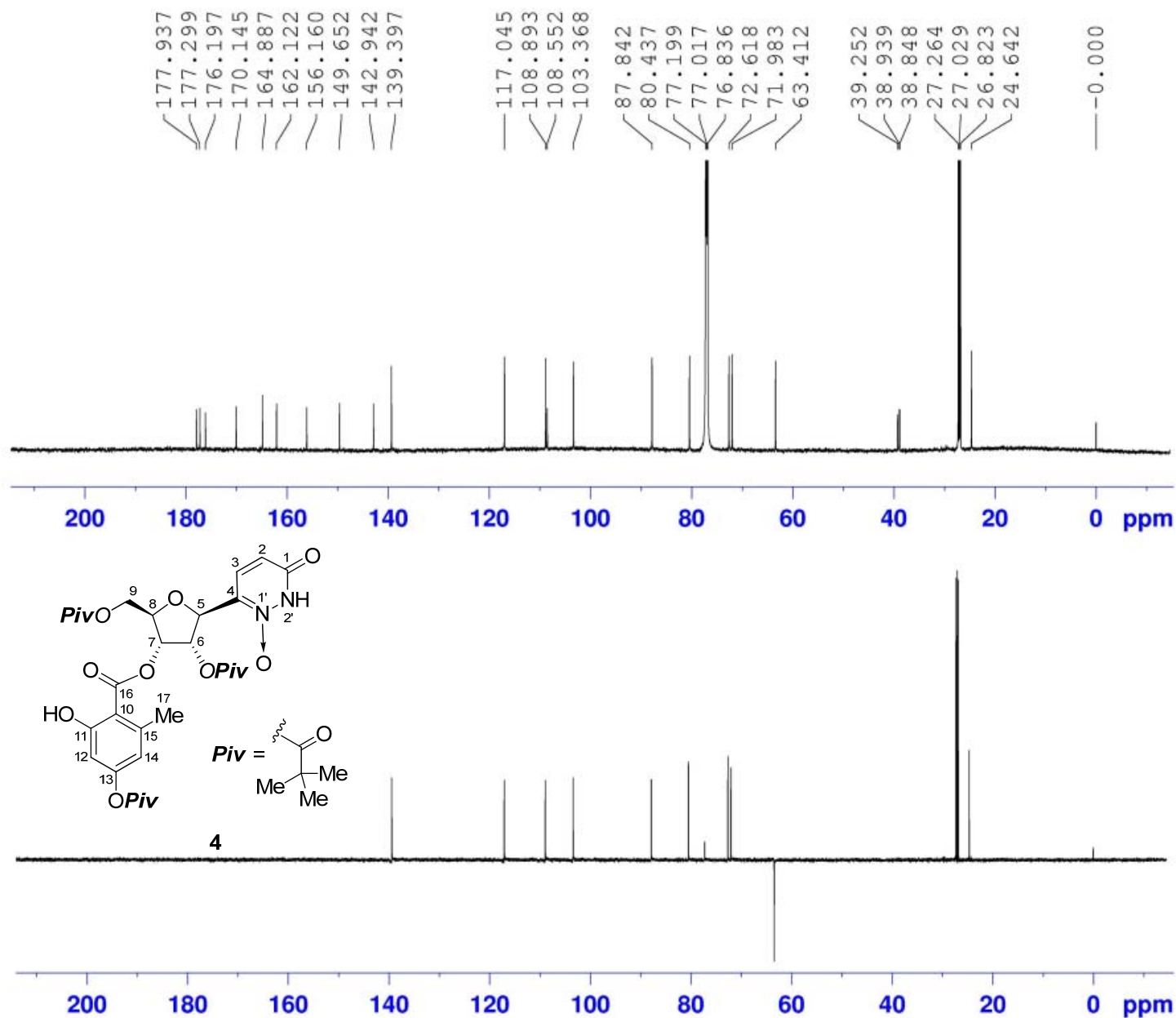
—149.652

—142.942

—139.397



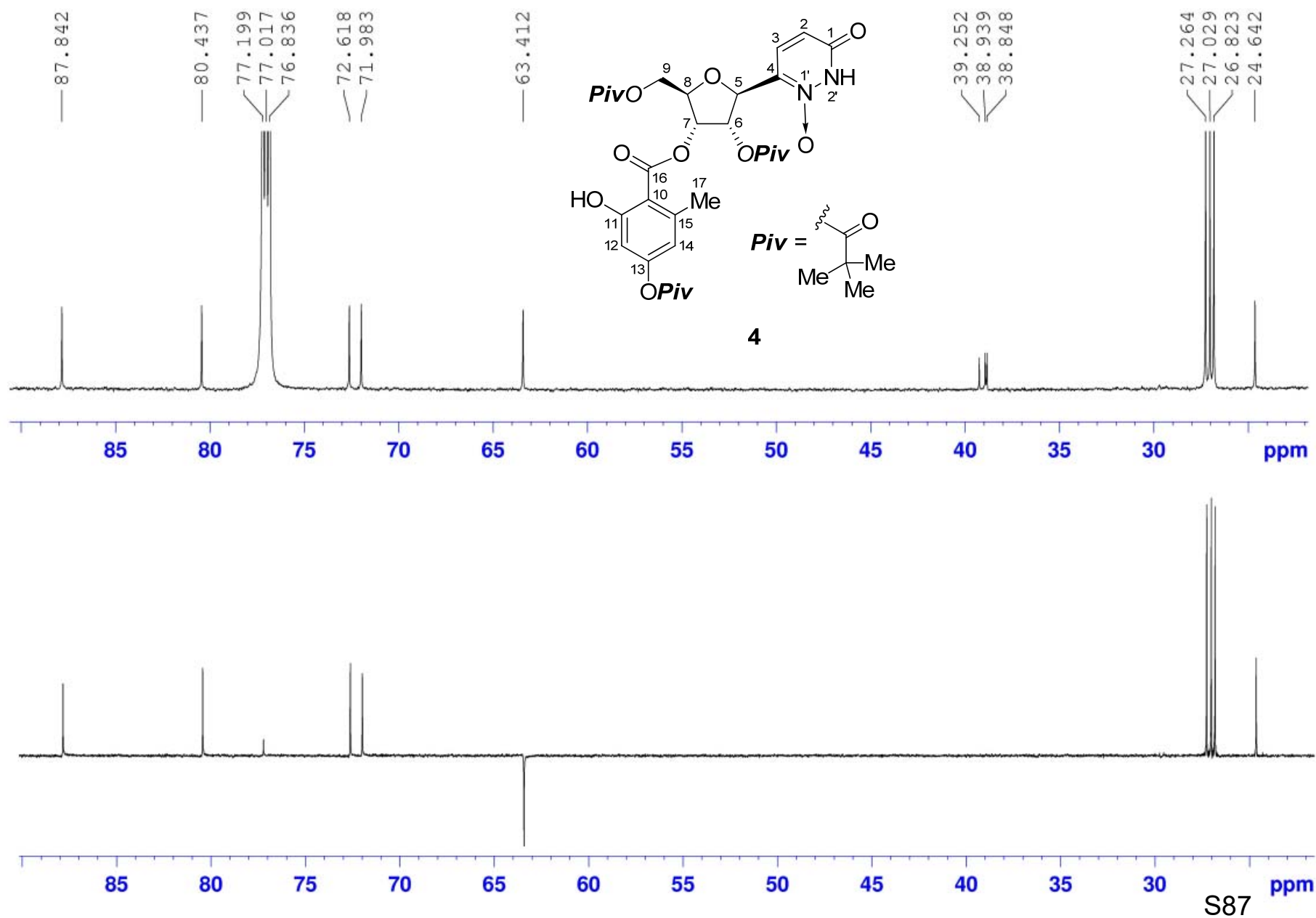
DEPT135 (175 MHz) spectrum of **4** in CDCl₃



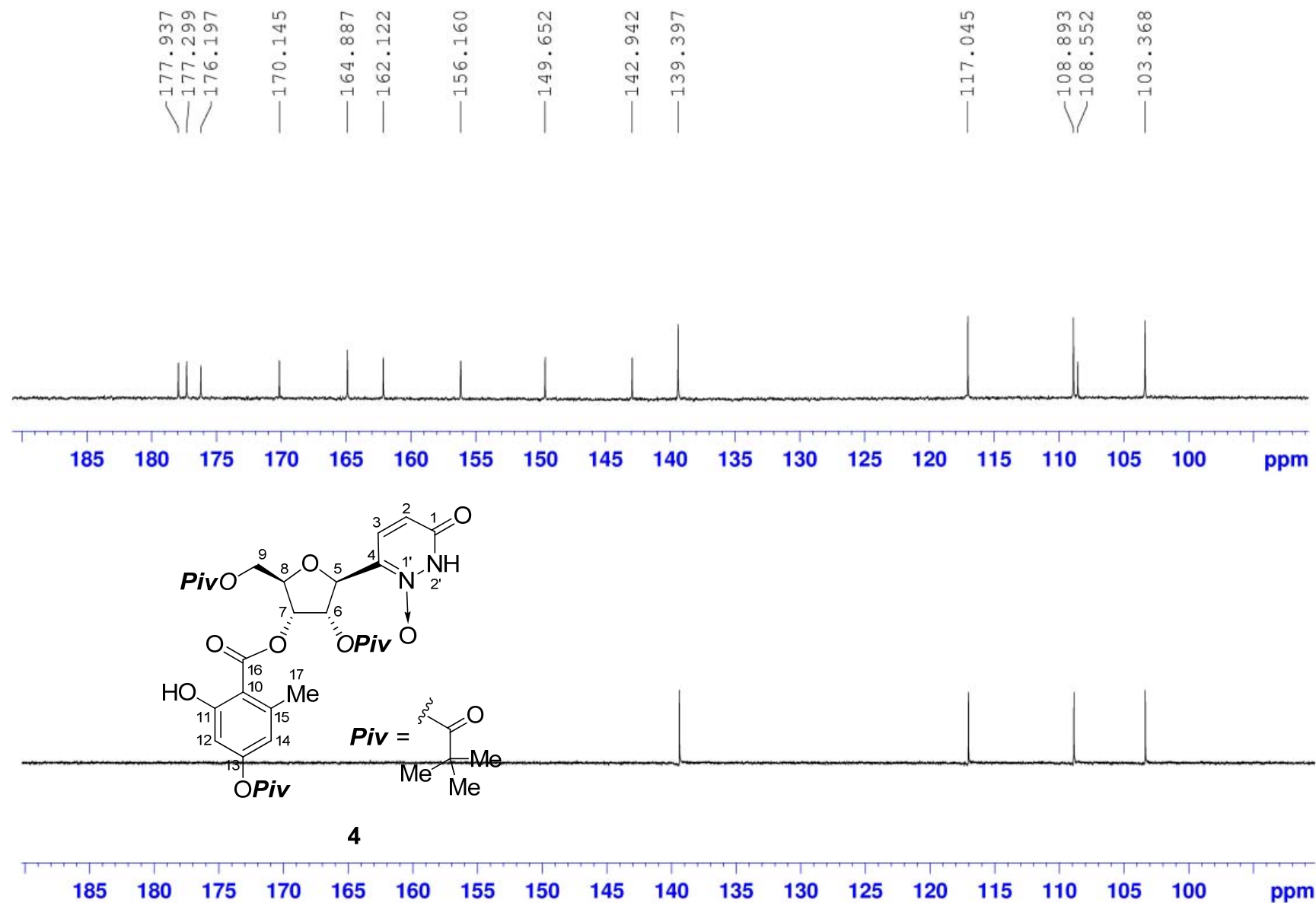
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PROCNO    1
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PULPROG   deptsp135
TD         32768
SOLVENT   CDCl3
NS         2000
DS         8
SWH        43859.648 Hz
FIDRES     2.676980 Hz
AQ         0.3736052 sec
RG         181.26
DW         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
    
```

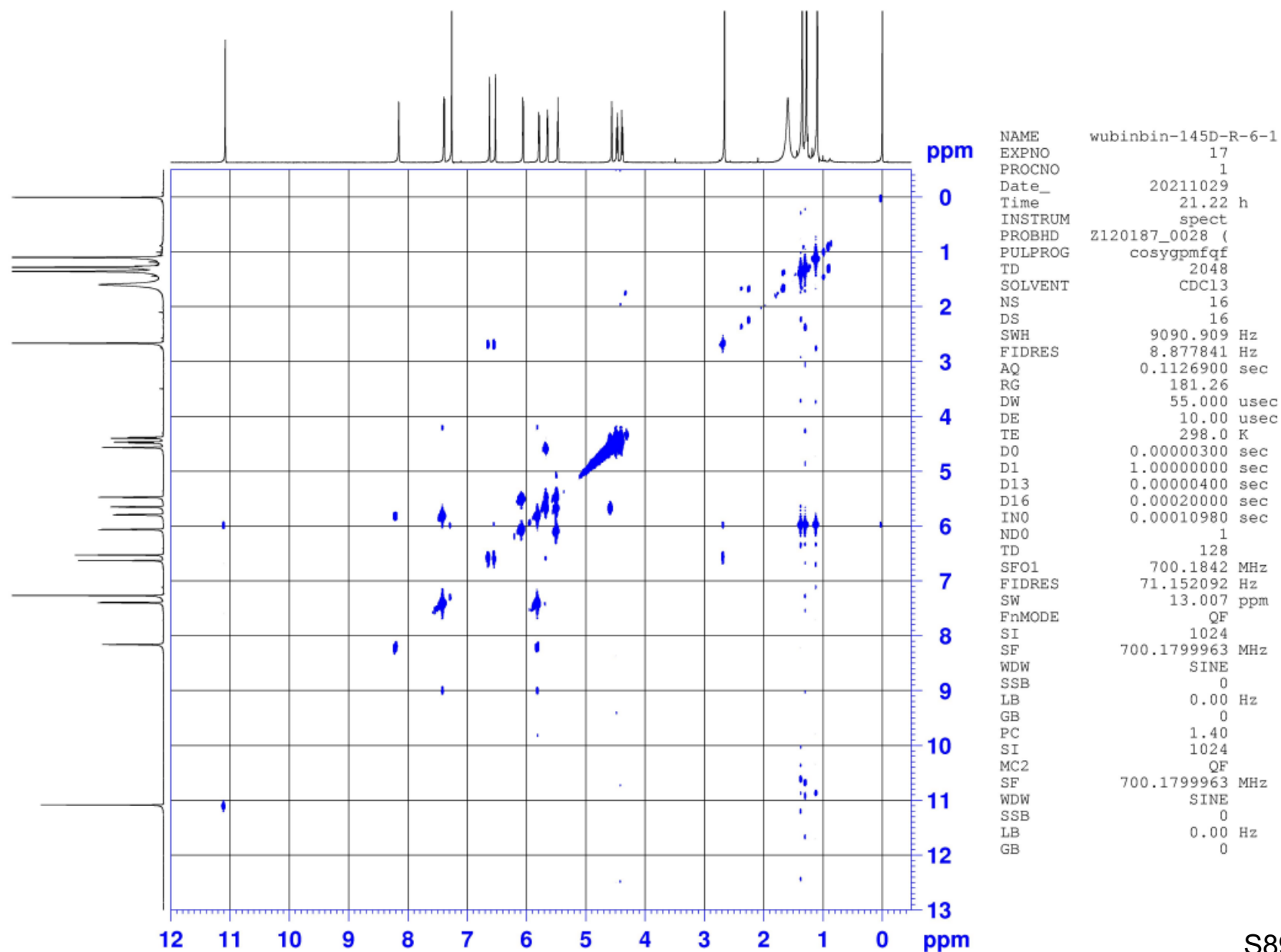
DEPT135 (175 MHz) spectrum of **4** in CDCl₃



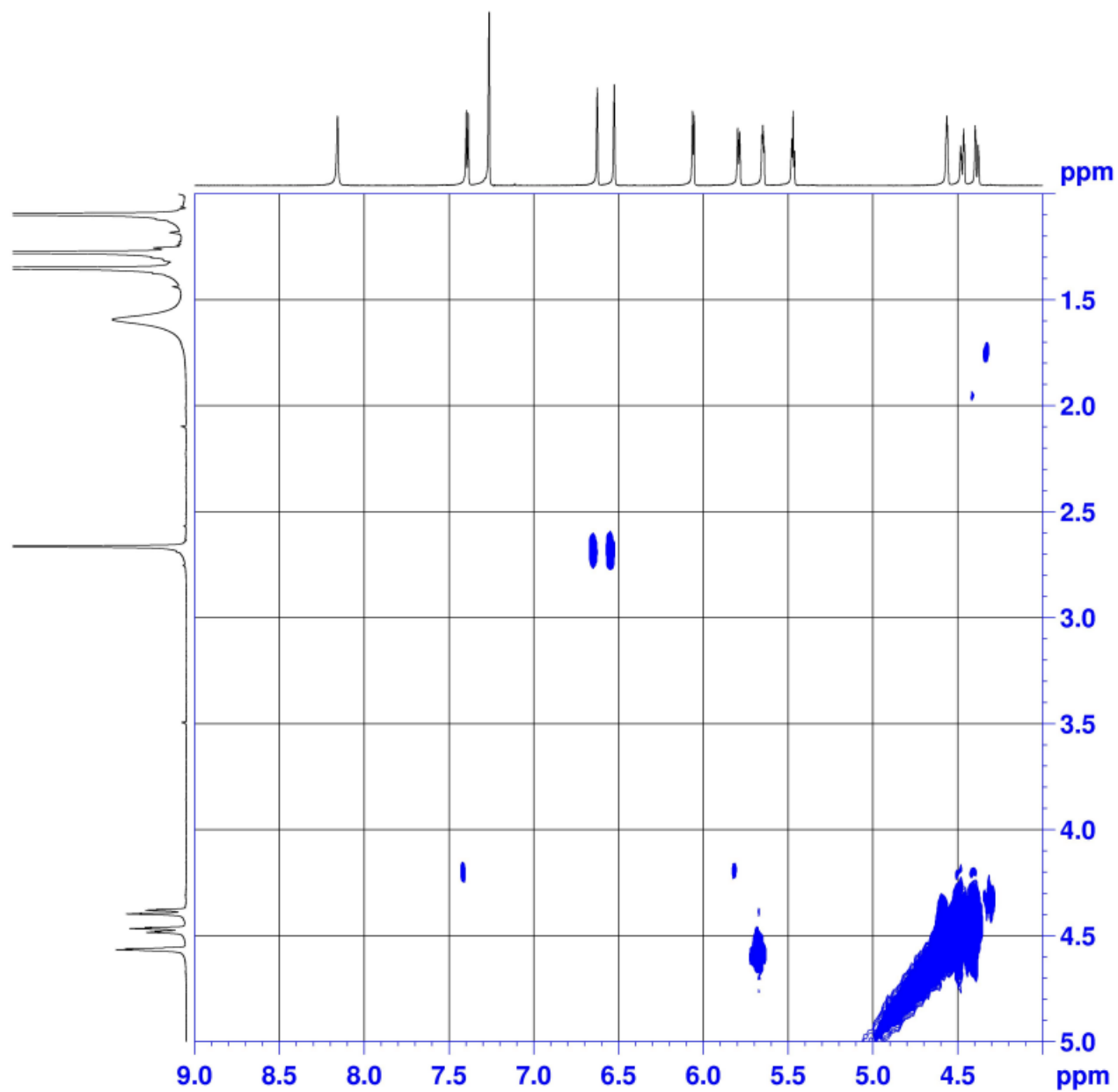
DEPT135 (175 MHz) spectrum of **4** in CDCl₃



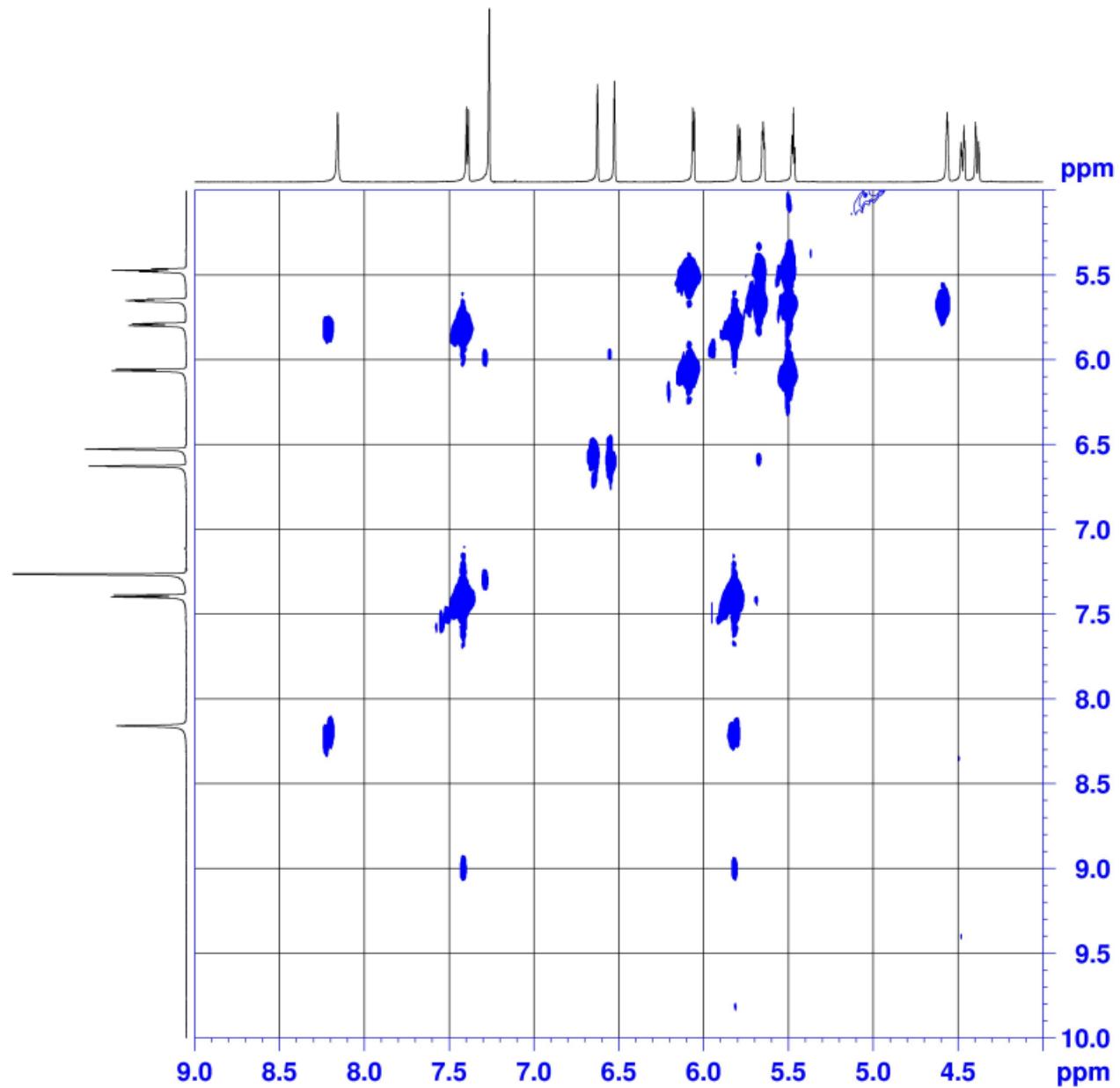
^1H - ^1H COSY (700 MHz) spectrum of **4** in CDCl_3



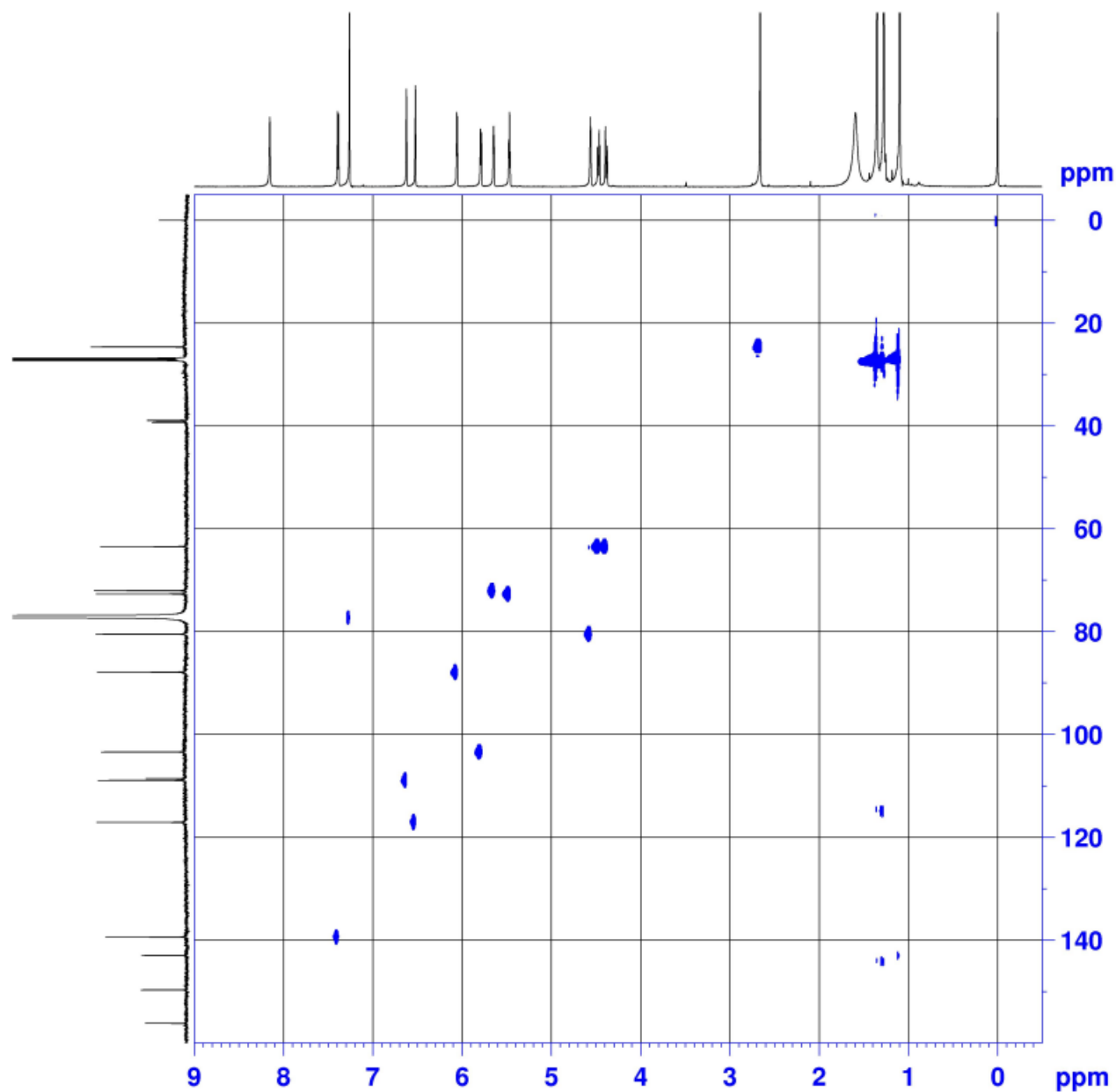
^1H - ^1H COSY (700 MHz) spectrum of **4** in CDCl_3



^1H - ^1H COSY (700 MHz) spectrum of **4** in CDCl_3



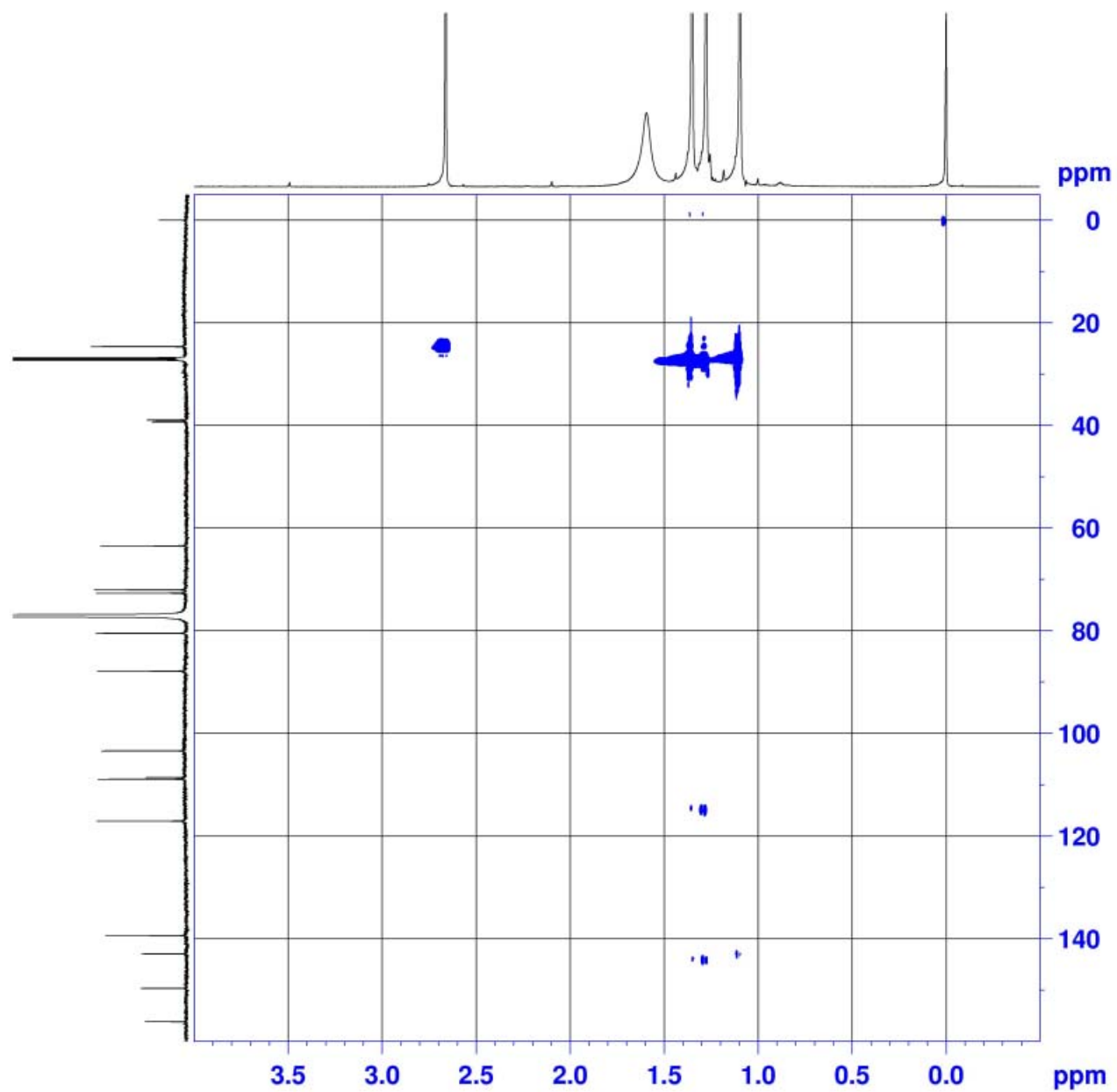
HSQC (700 MHz) spectrum of **4** in CDCl₃



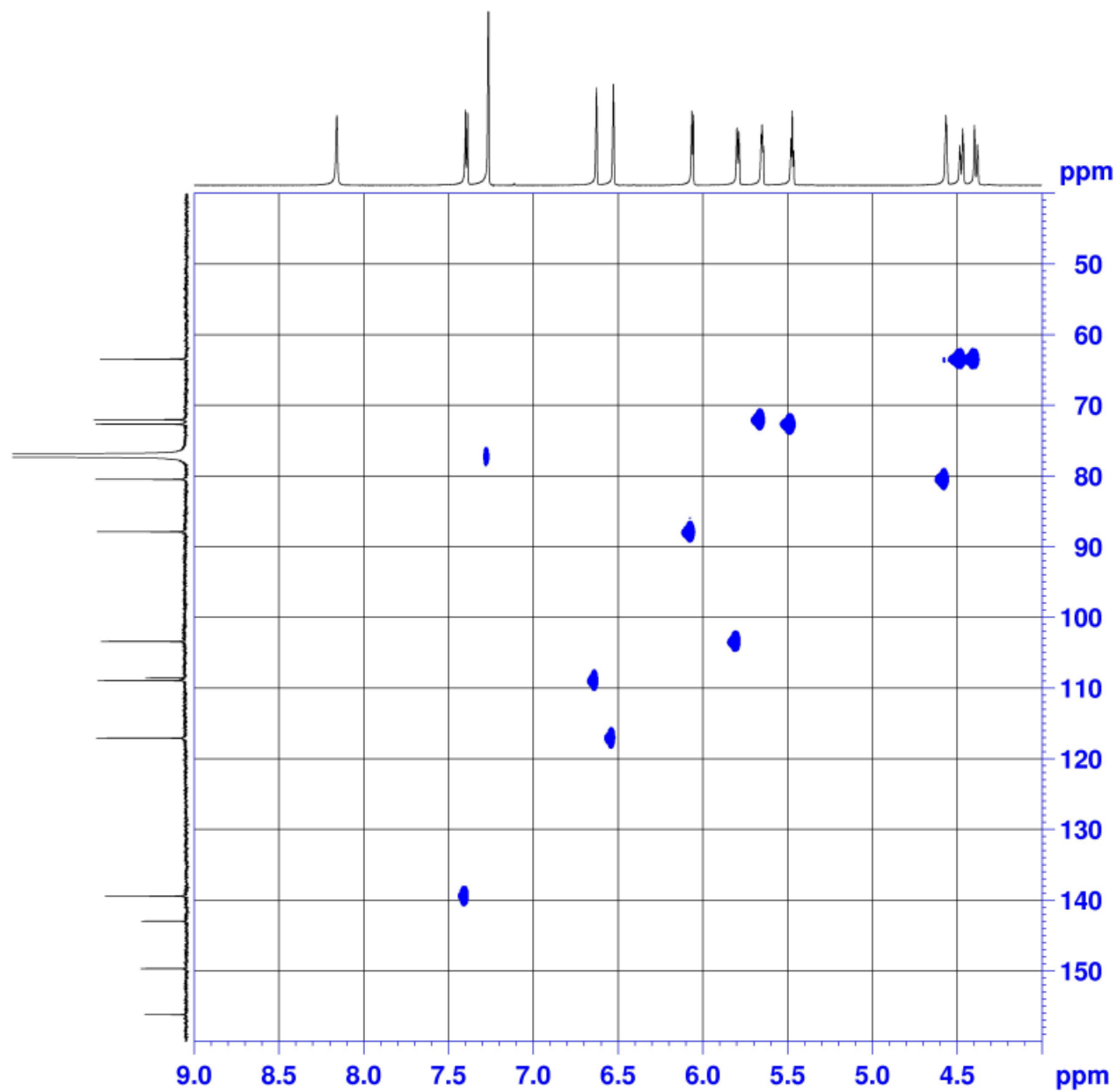
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NAME      wubinbin-145D-R-6-1
EXPNO     16
PROCNO    1
Date_     20211029
Time      20.42 h
INSTRUM   spect
PROBHD    z120187_0028 (
PULPROG   hsqcetgp
TD         2048
SOLVENT   CDC13
NS         16
DS         16
SWH        9090.909 Hz
FIDRES     8.877841 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
    
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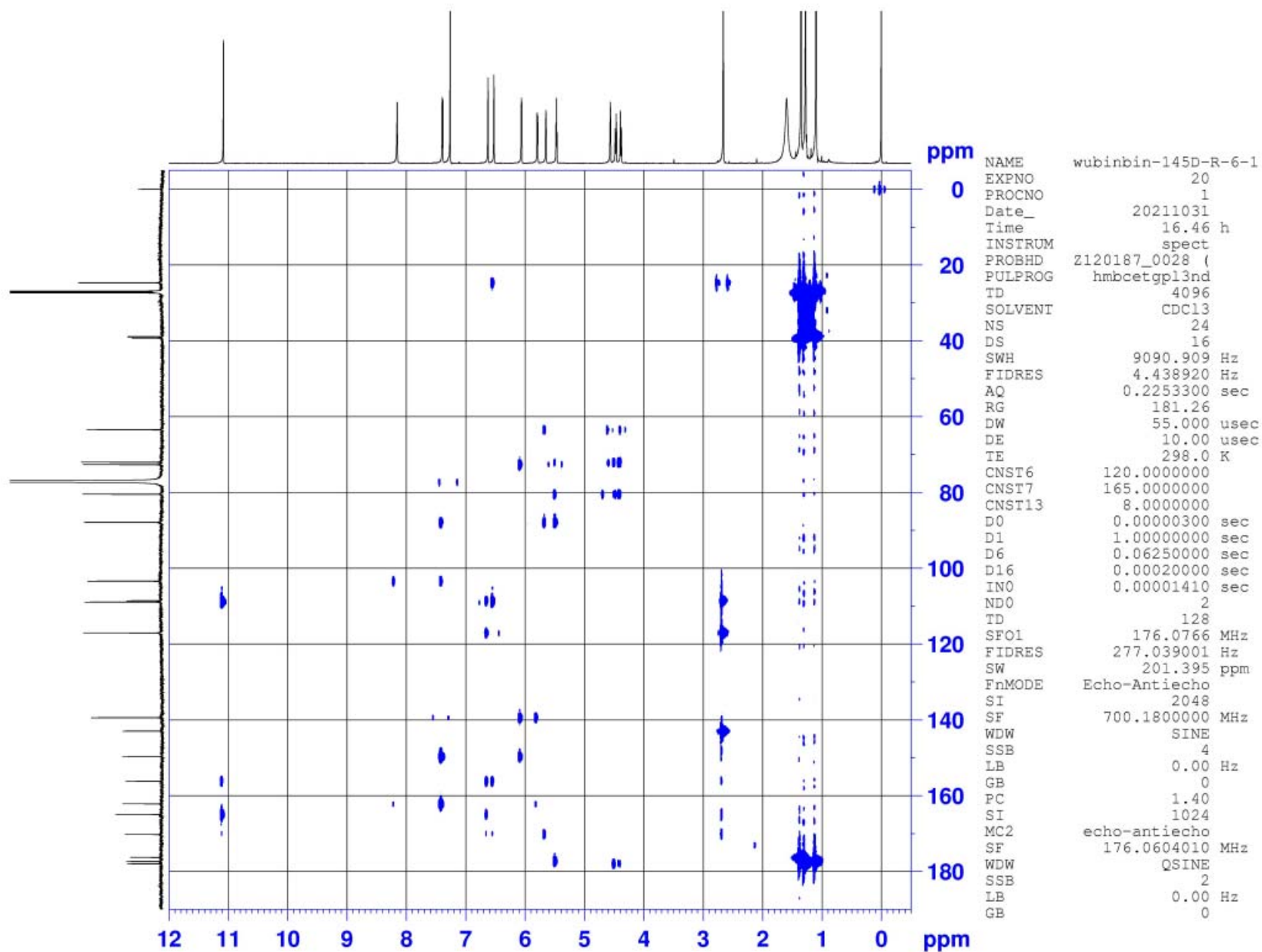
HSQC (700 MHz) spectrum of **4** in CDCl_3



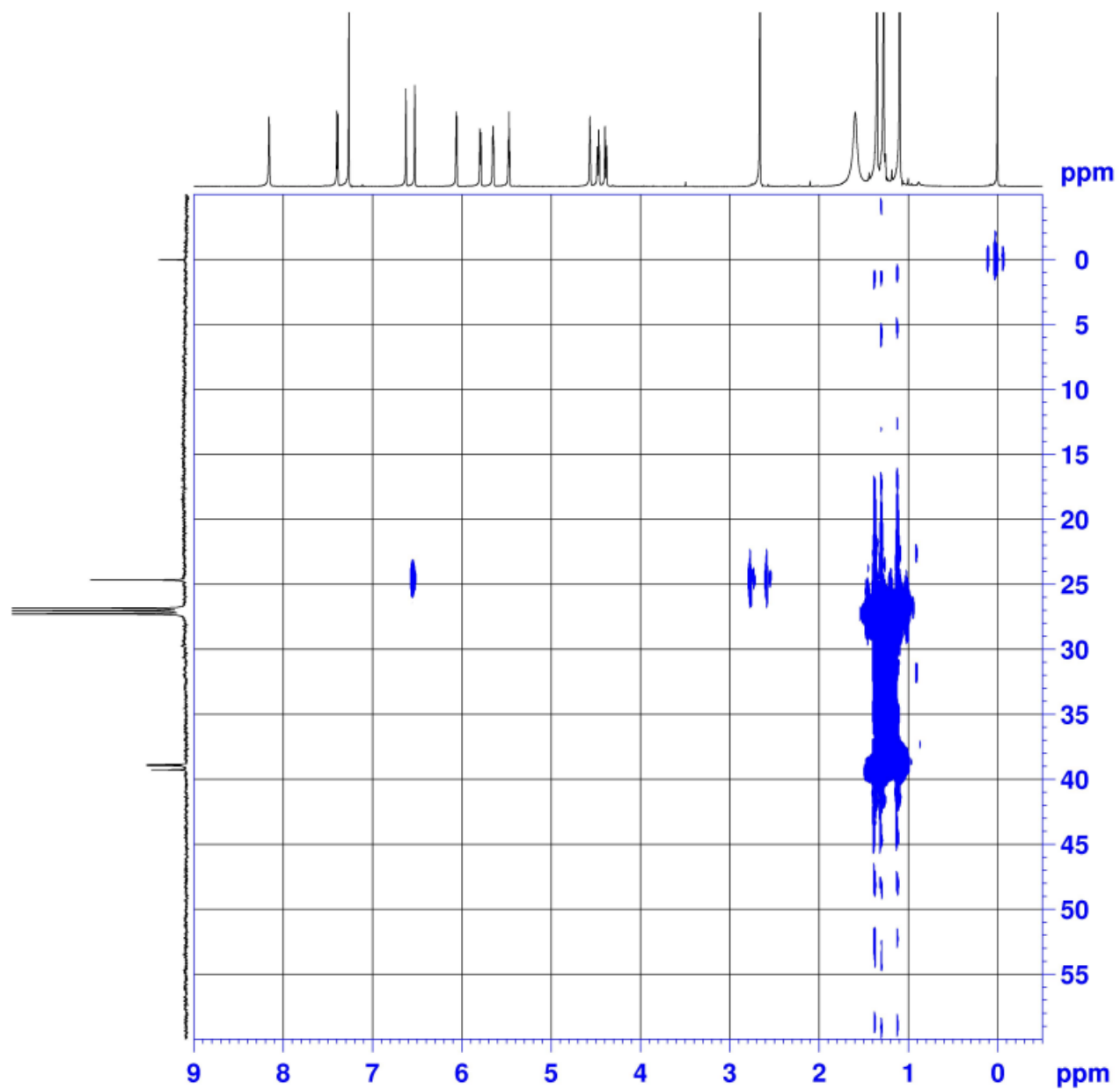
HSQC (700 MHz) spectrum of **4** in CDCl_3



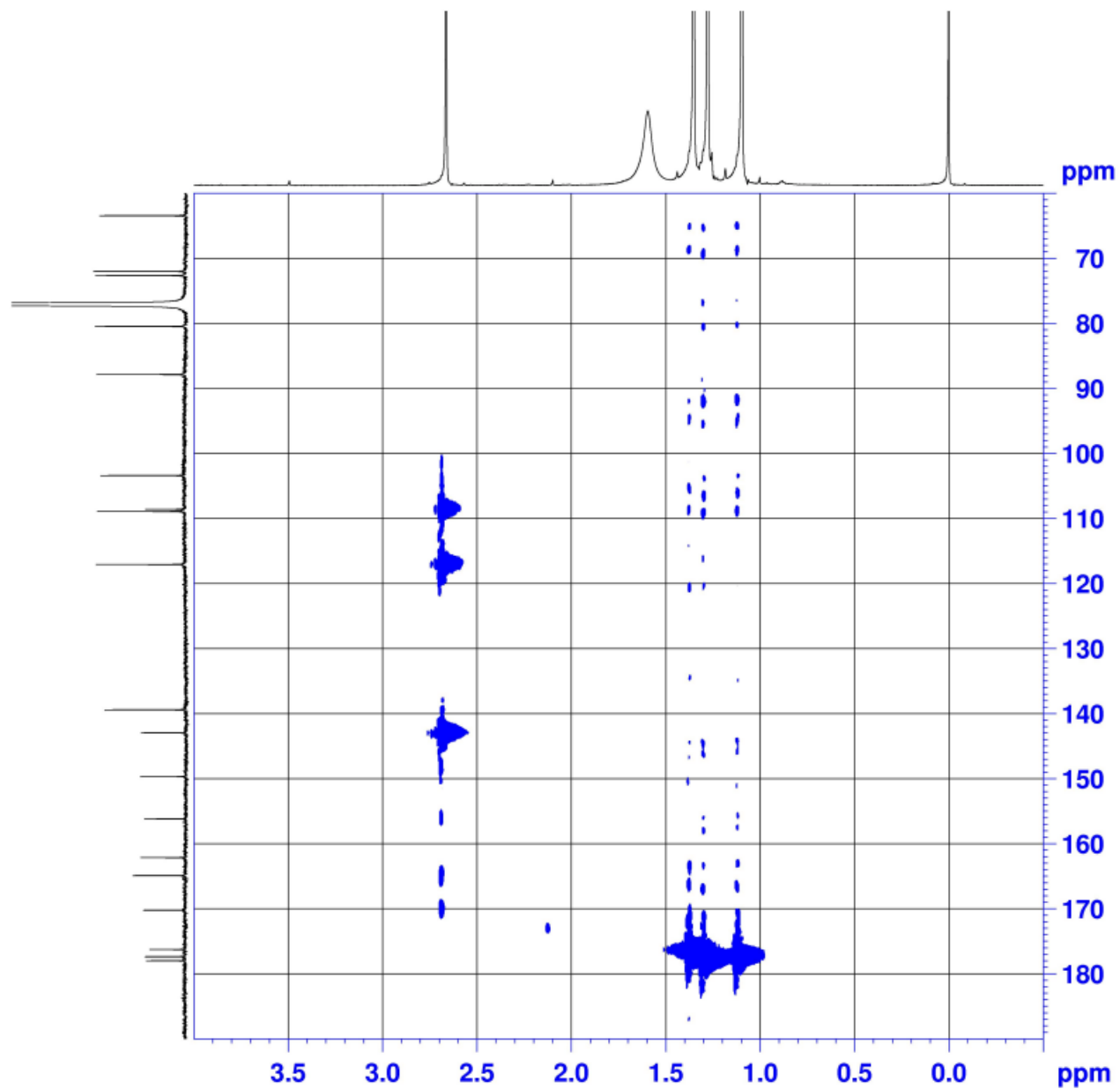
HMBC (700 MHz) spectrum of **4** in CDCl₃



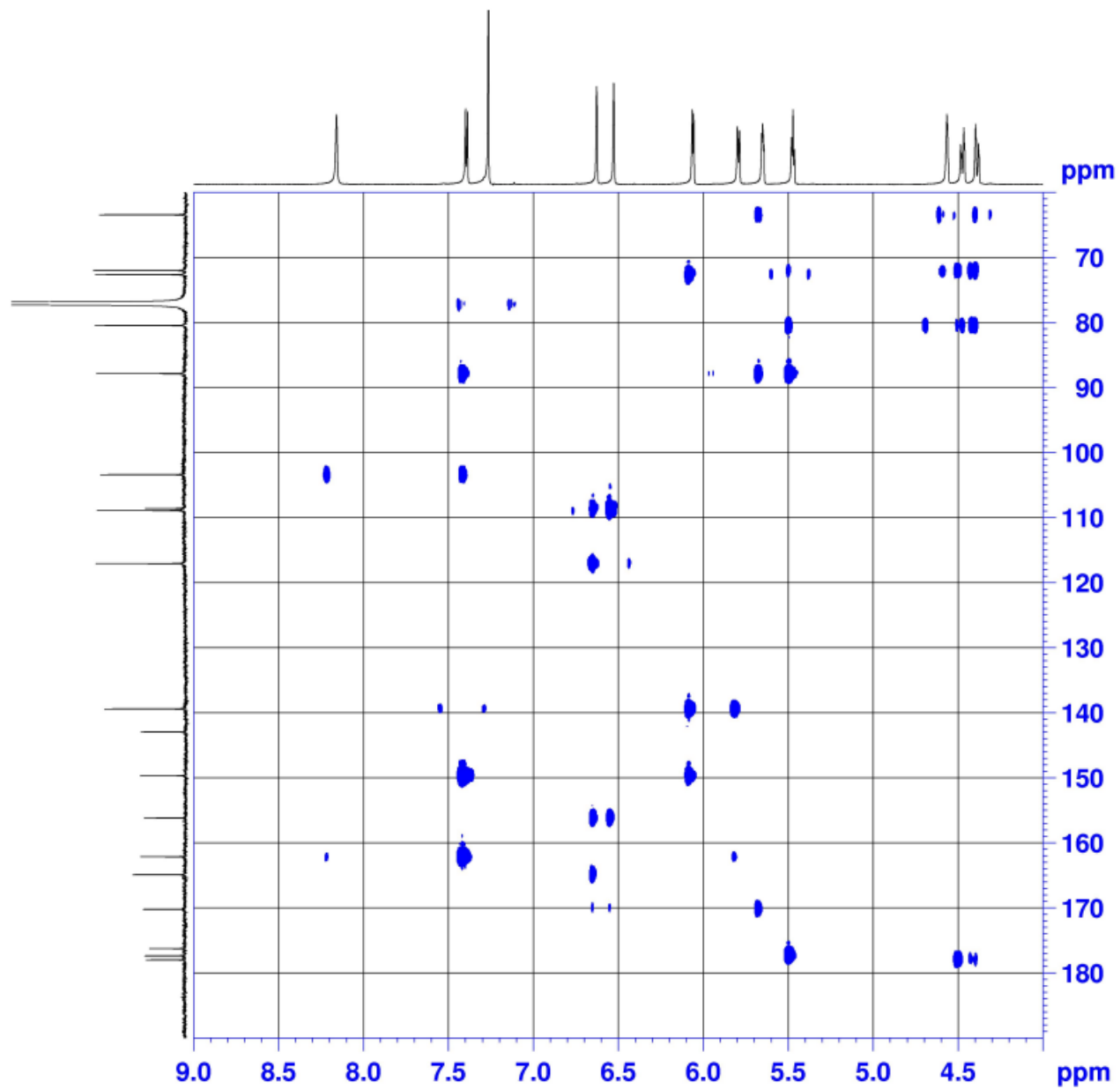
HMBC (700 MHz) spectrum of **4** in CDCl_3



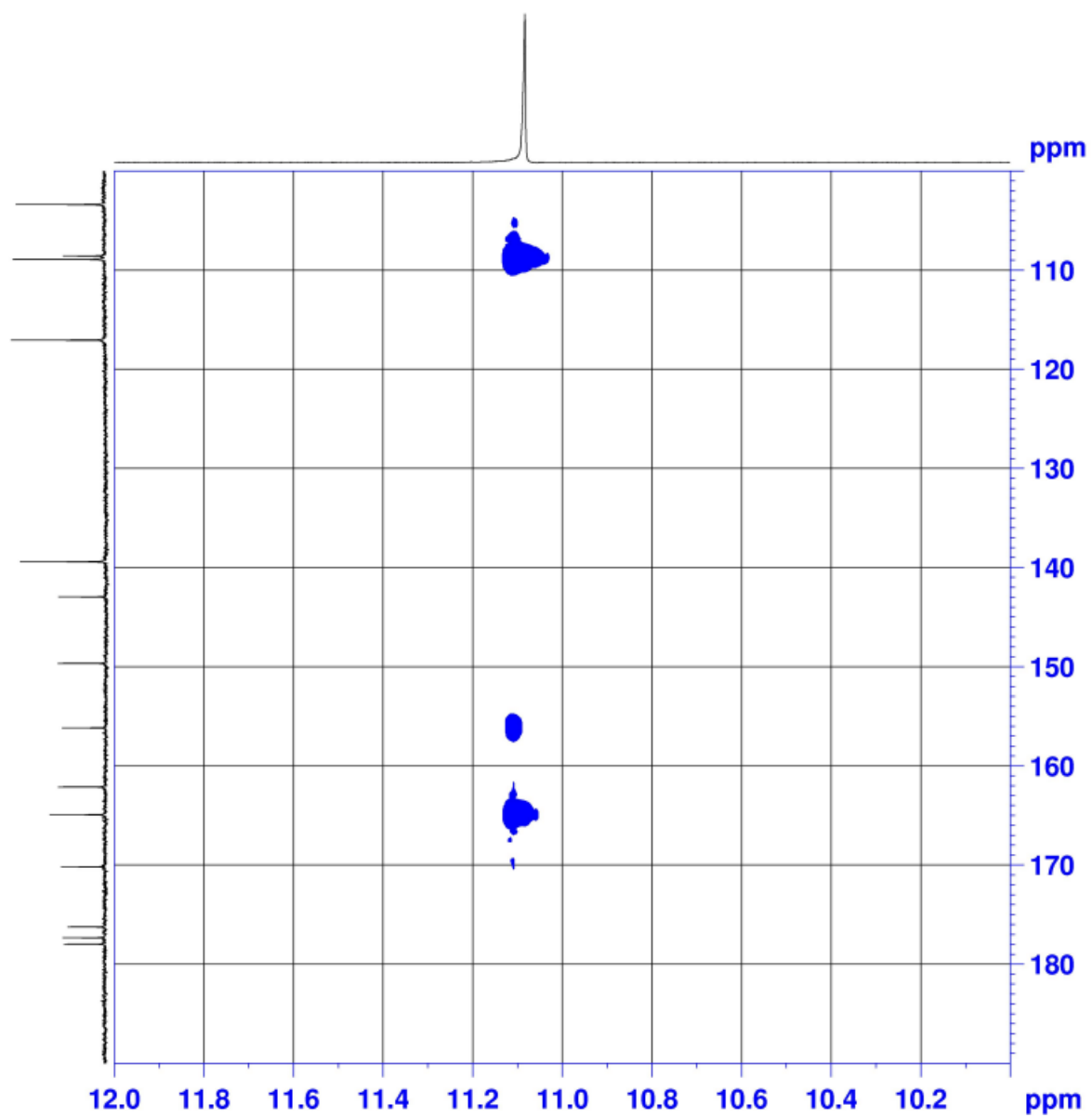
HMBC (700 MHz) spectrum of **4** in CDCl₃



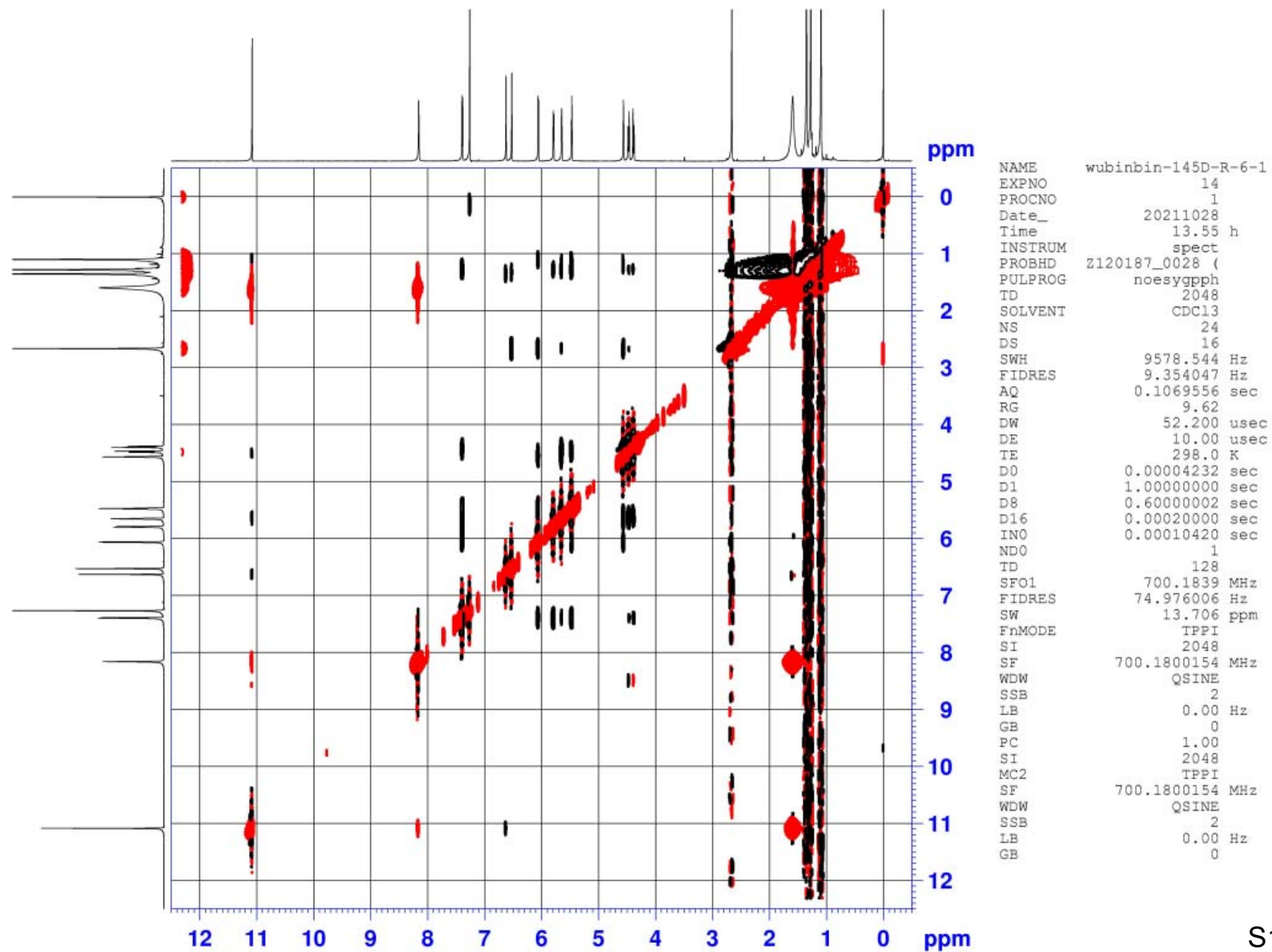
HMBC (700 MHz) spectrum of **4** in CDCl₃



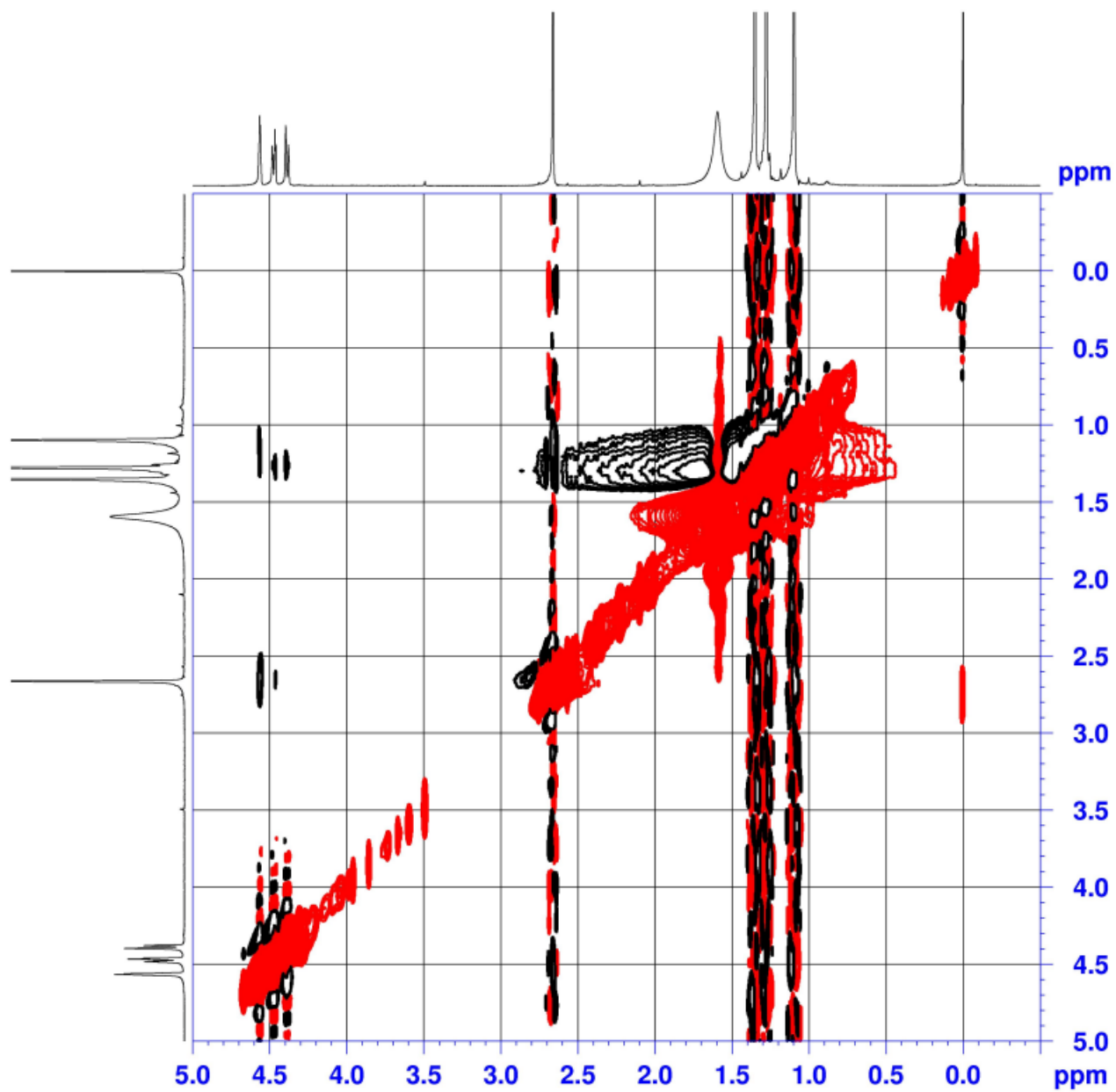
HMBC (700 MHz) spectrum of **4** in CDCl_3



NOESY (700 MHz) spectrum of **4** in CDCl₃

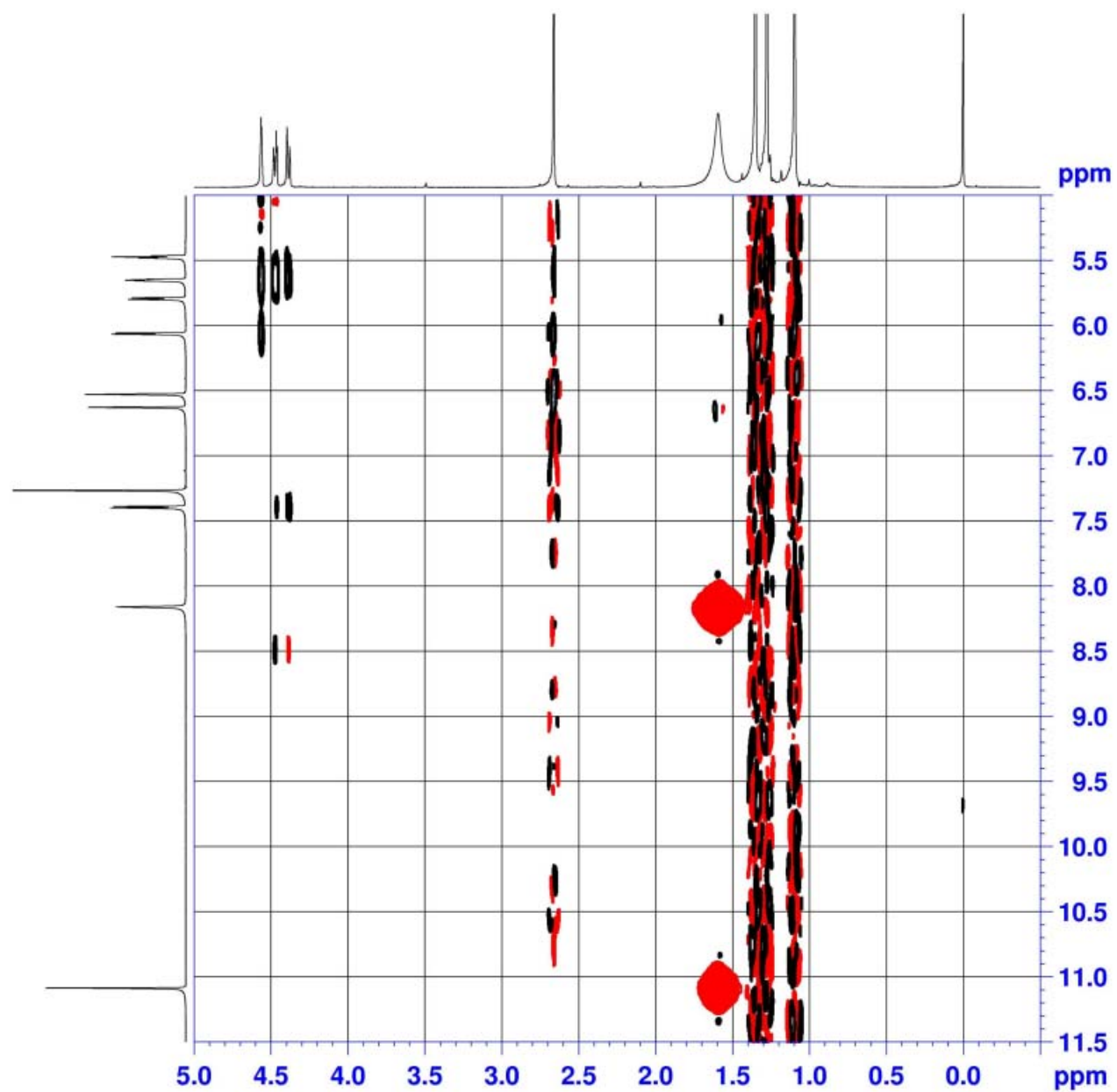


NOESY (700 MHz) spectrum of **4** in CDCl_3

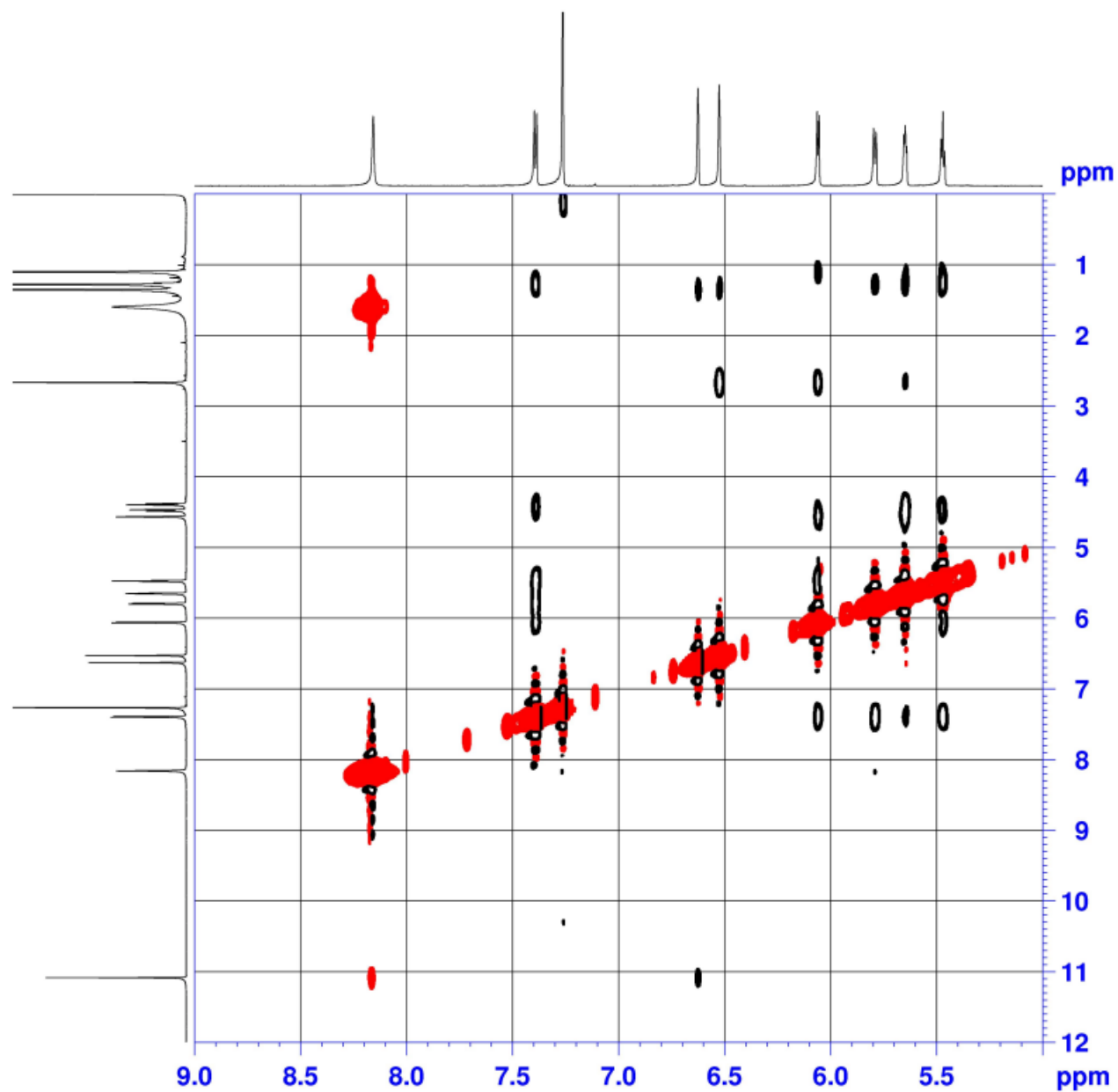


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NOESY (700 MHz) spectrum of **4** in CDCl_3



NOESY (700 MHz) spectrum of **4** in CDCl₃



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

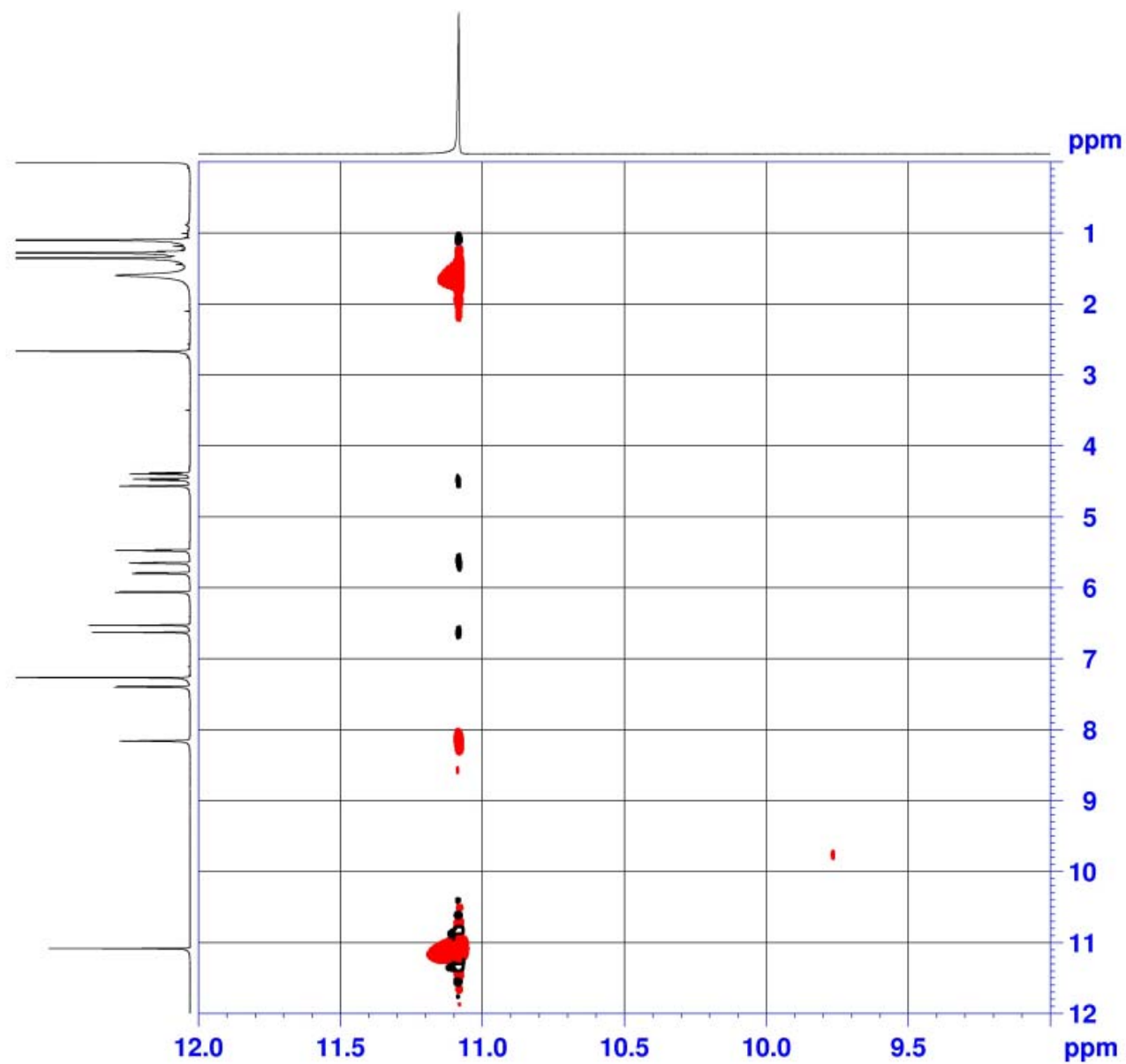


Figure S1. Energy analyses of conformers (14*S*,15*S*,17*R*)-2A to (14*S*,15*S*,17*R*)-2J

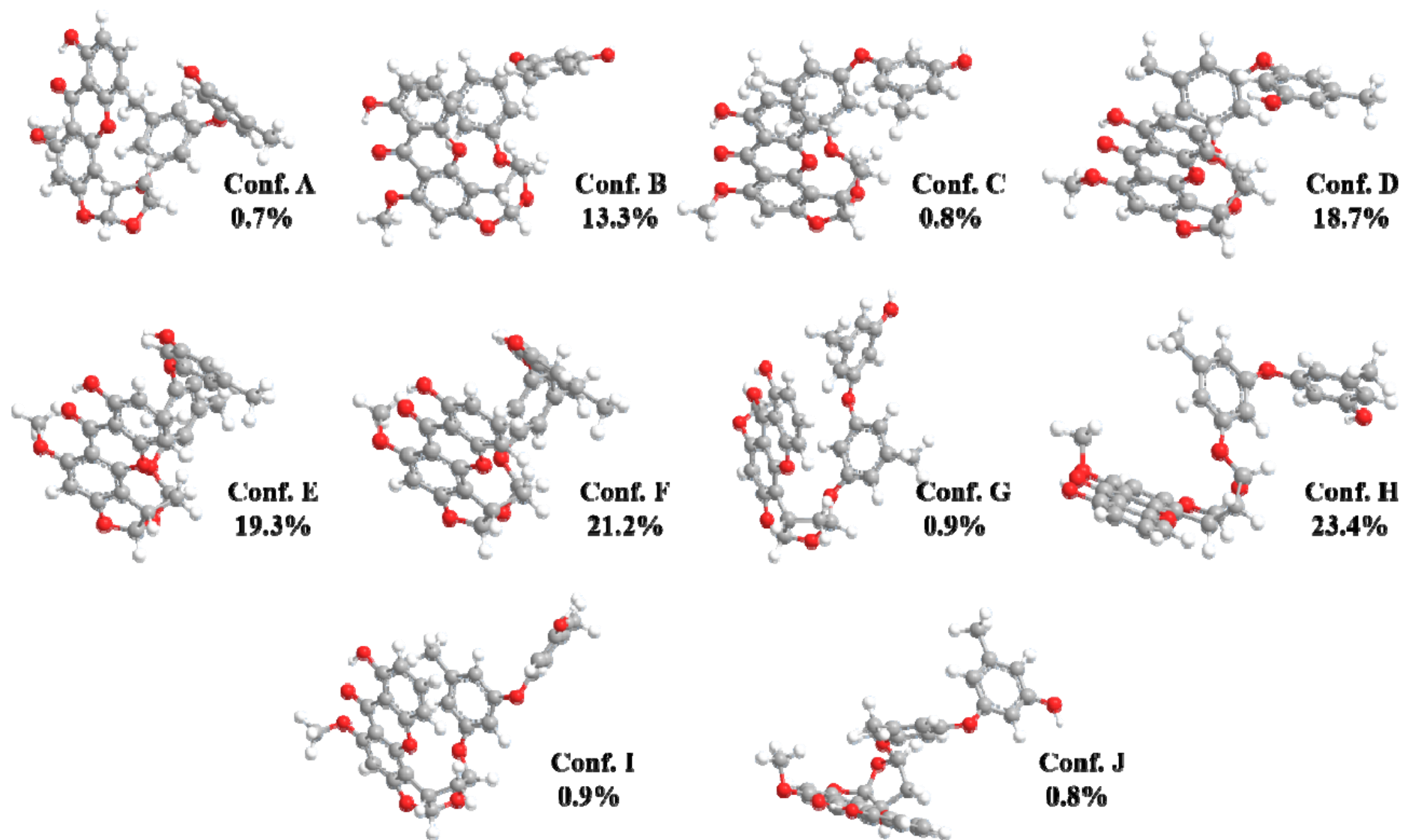
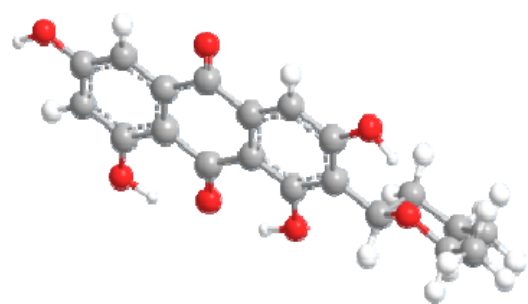
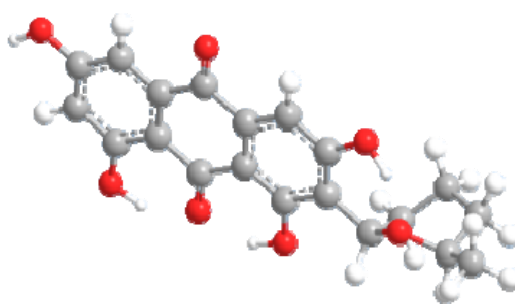


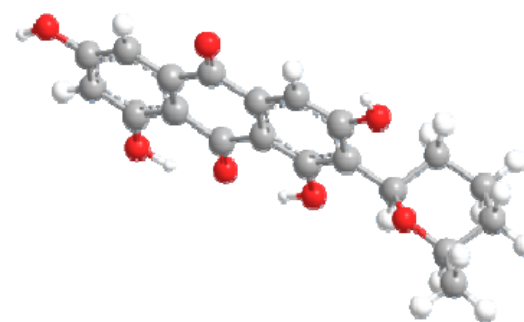
Figure S2. Energy analyses of conformers (15*R*,19*R*)-3A to (15*R*,19*R*)-3E



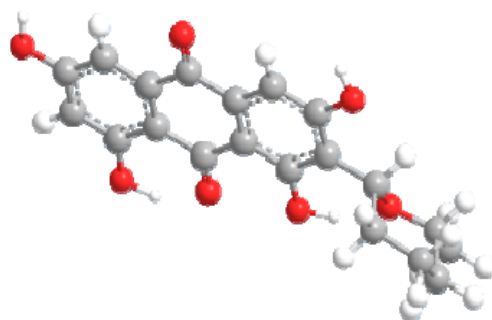
Conf. A
99.9%



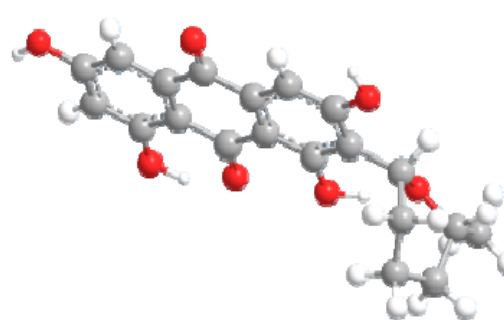
Conf. B
<0.01%



Conf. C
<0.01%

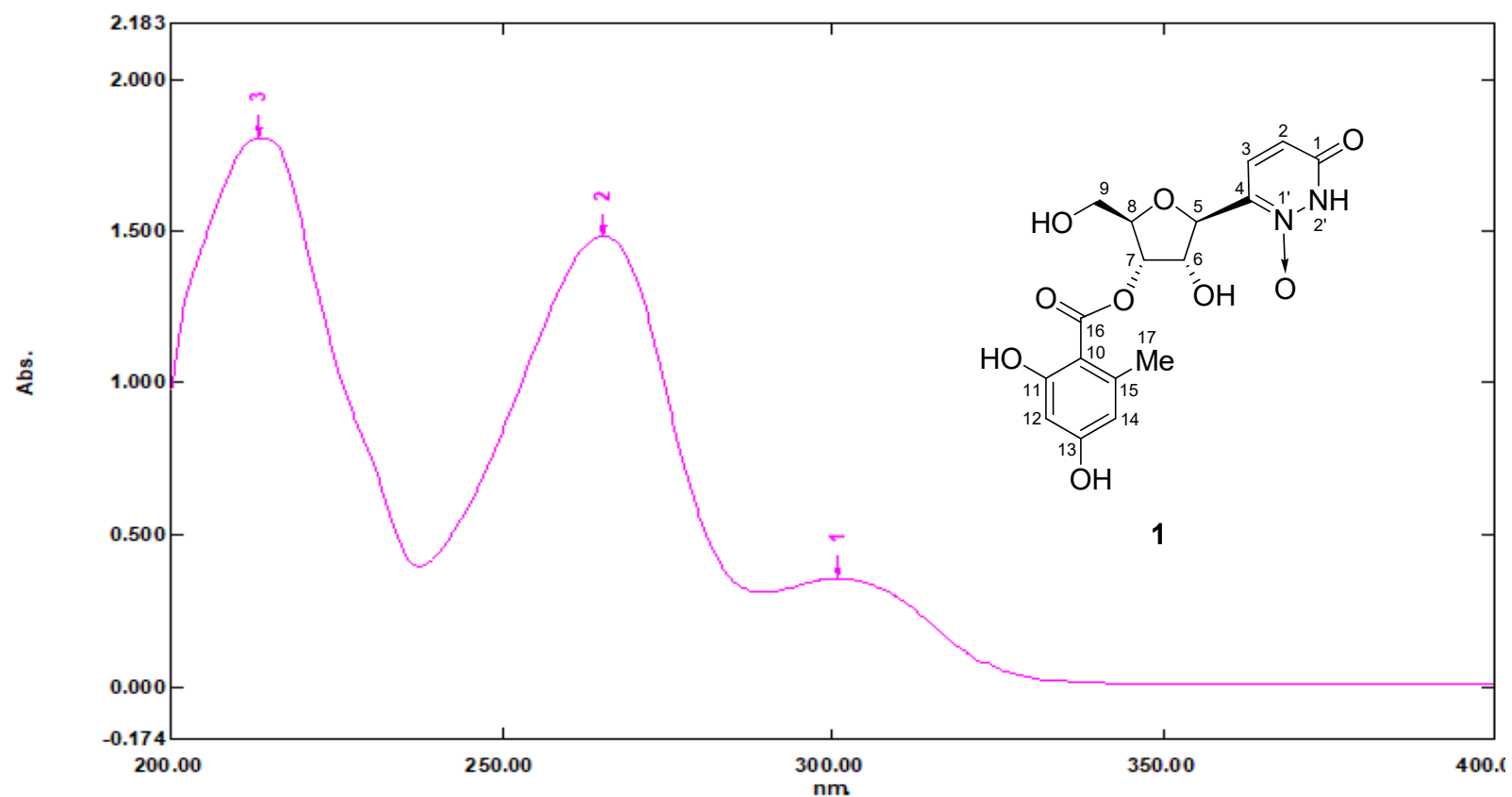


Conf. D
<0.01%



Conf. E
<0.01%

Figure S3. The UV spectrum of Compound **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 Compound **2**

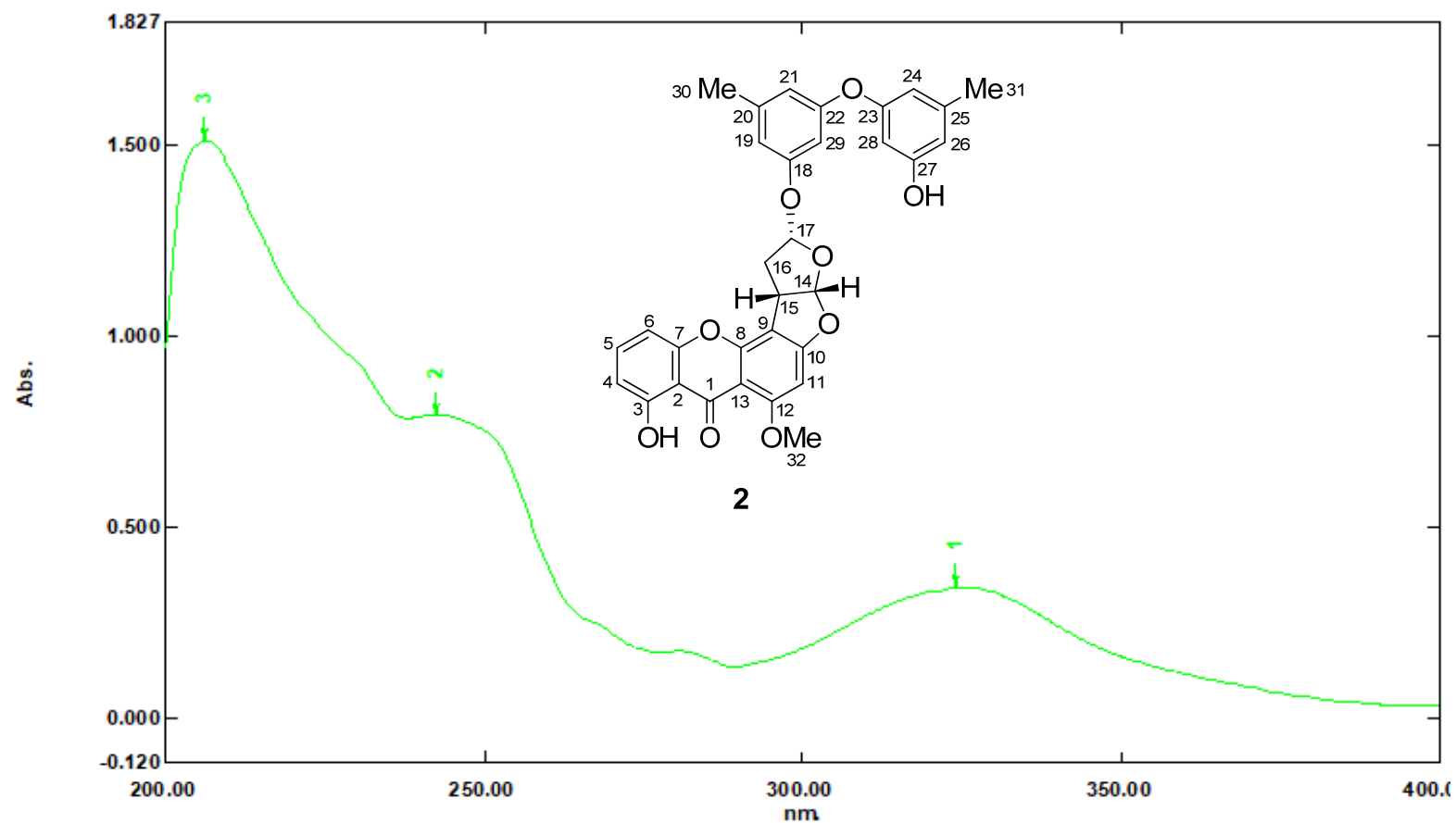
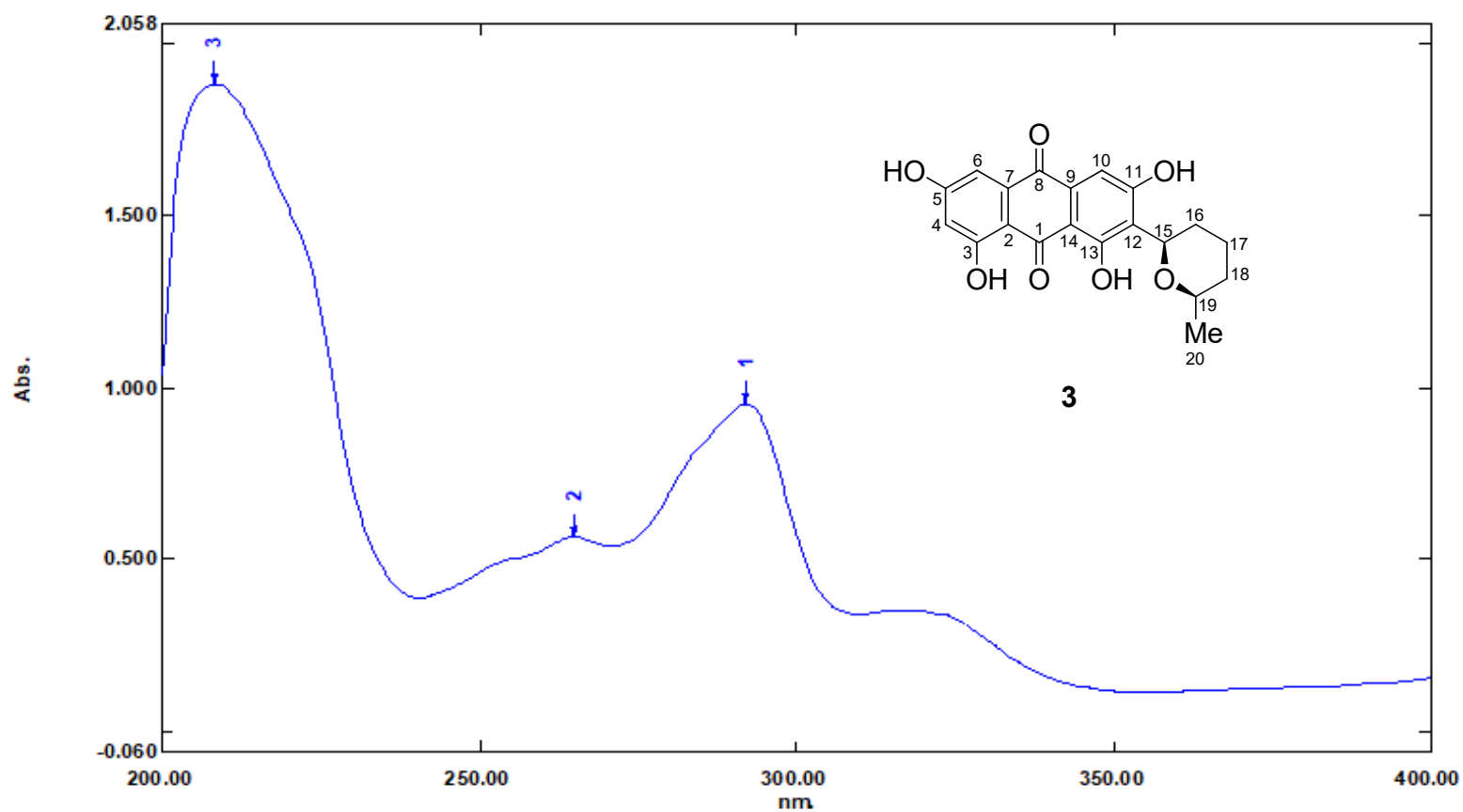


Figure S5. The UV spectrum of Compound 3



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 Compound **1**

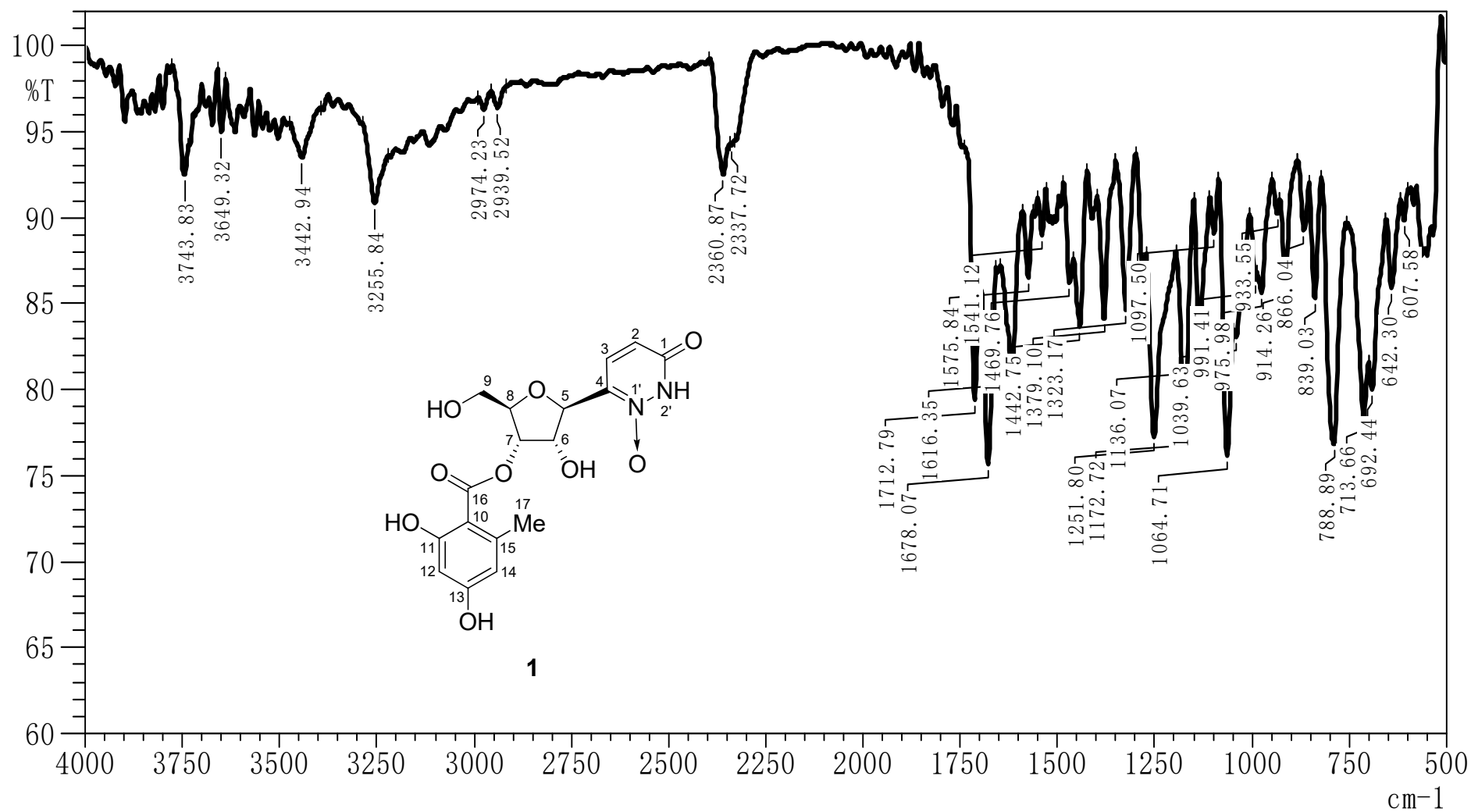


Figure S7. The IR spectrum of Compound 2

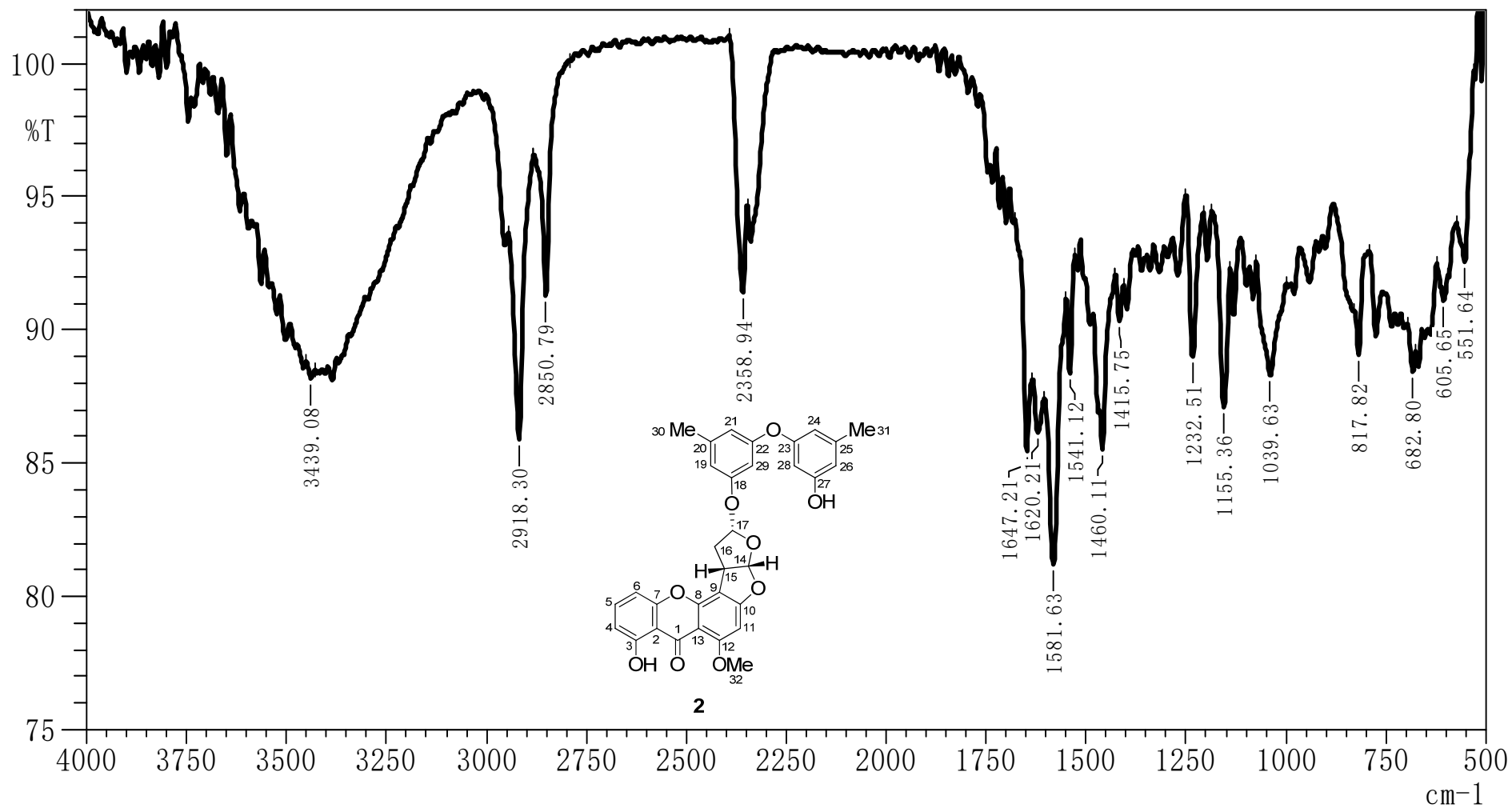


Figure S8. The IR spectrum of Compound **3**

