

SUPPLEMENTAL SECTION

Dichloroacetyl amides of 3,5-bis(benzylidene)-4-piperidones displaying greater toxicity to neoplasms than non-malignant cells

Mohammad Hossain ^a, Praveen K. Roayapalley ^{b,*}, Hiroshi Sakagami ^c, Keitaro Satoh ^c, Kenjiro Bandow ^c, Umashankar Das ^b, Jonathan R. Dimmock ^b

^a *School of Sciences, Indiana University Kokomo, Kokomo, IN 46904, USA*

^b *Drug Discovery and Development Research Cluster, University of Saskatchewan, Saskatoon, Saskatchewan S7N 5E5, Canada*

^c *Meikai University Research Institute of Odontology, Sakado, Saitama 350-0283, Japan*

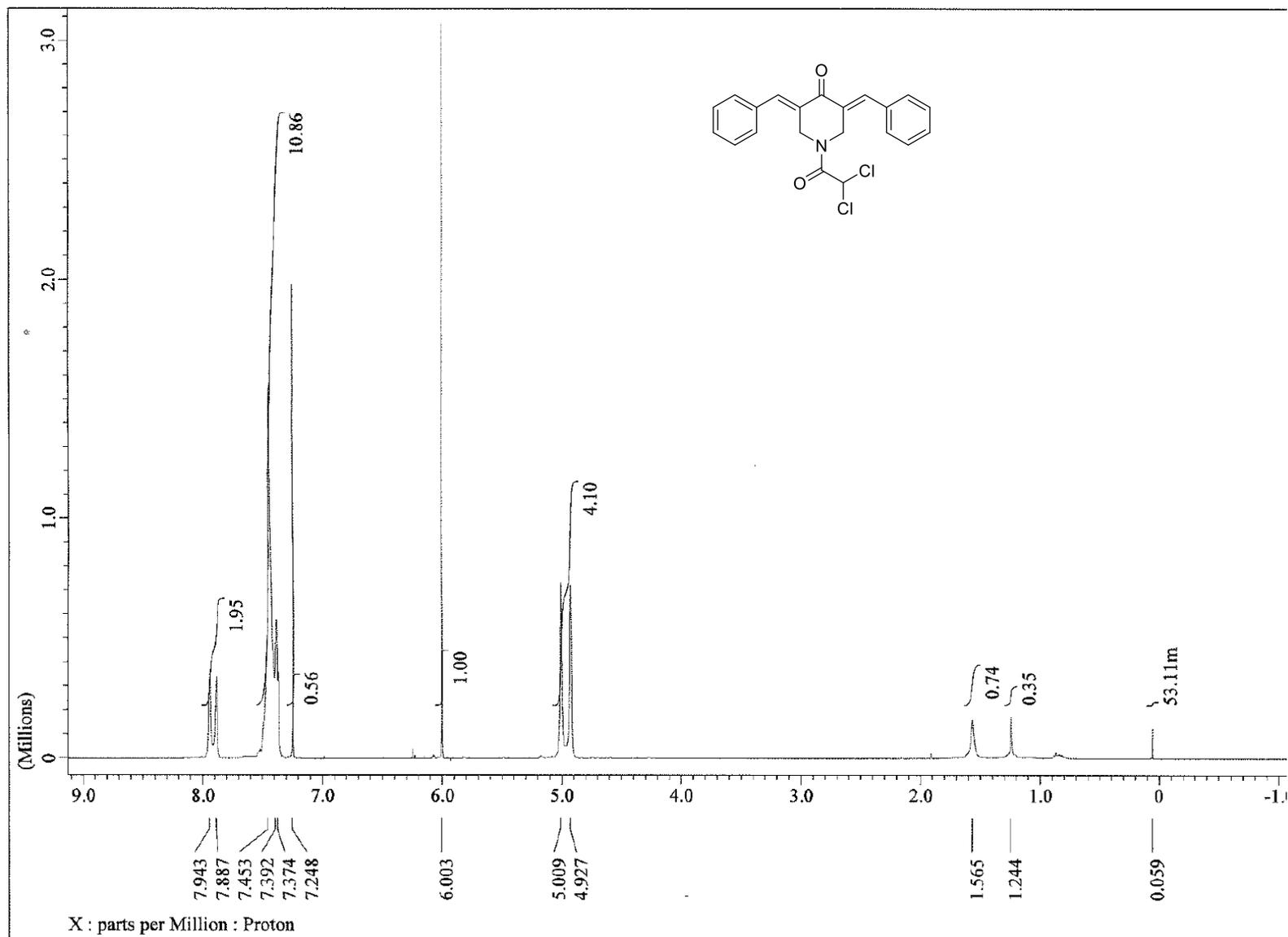
*Corresponding author: E-mail : rpraveen.sp@usask.ca Tel.: +1-306-715-4217

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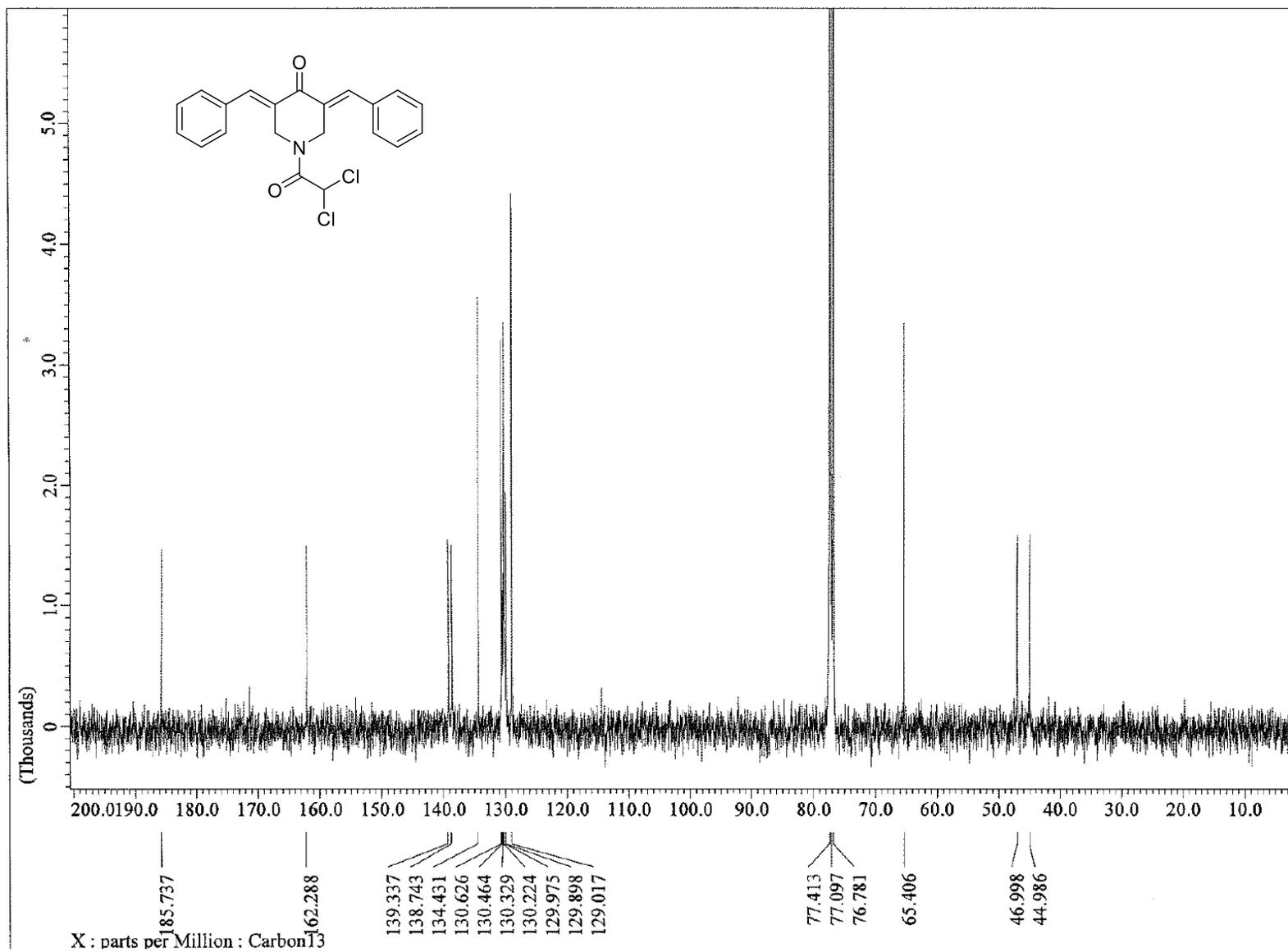
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^1H NMR (CDCl_3) spectrum of (3*E*,5*E*)-3,5-dibenzylidene-1-(2,2-dichloroacetyl)piperidin-4-one (**1a**)



^{13}C NMR (CDCl_3) spectrum of (3E,5E)-3,5-dibenzylidene-1-(2,2-dichloroacetyl)piperidin-4-one (**1a**)

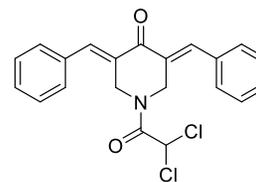
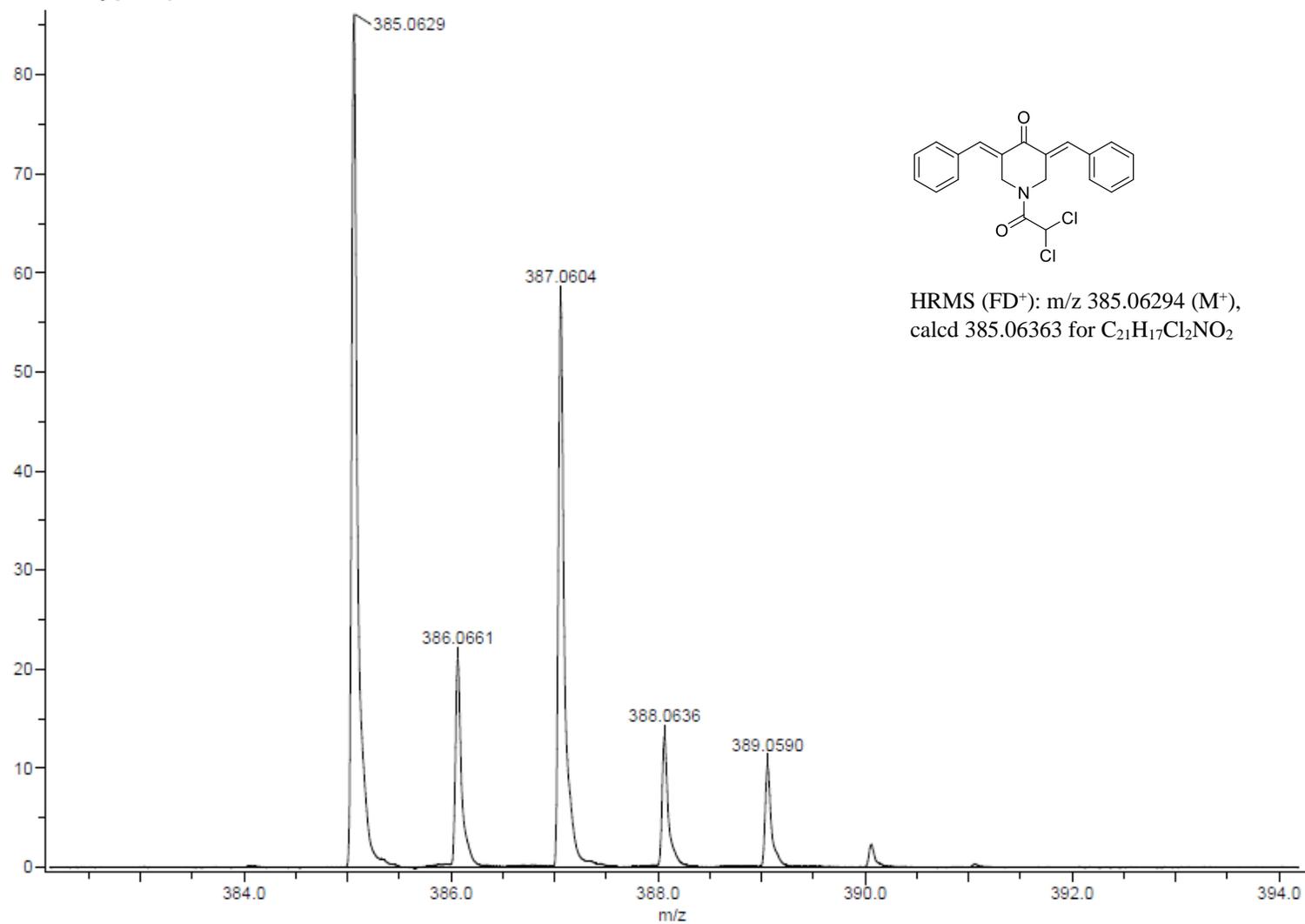


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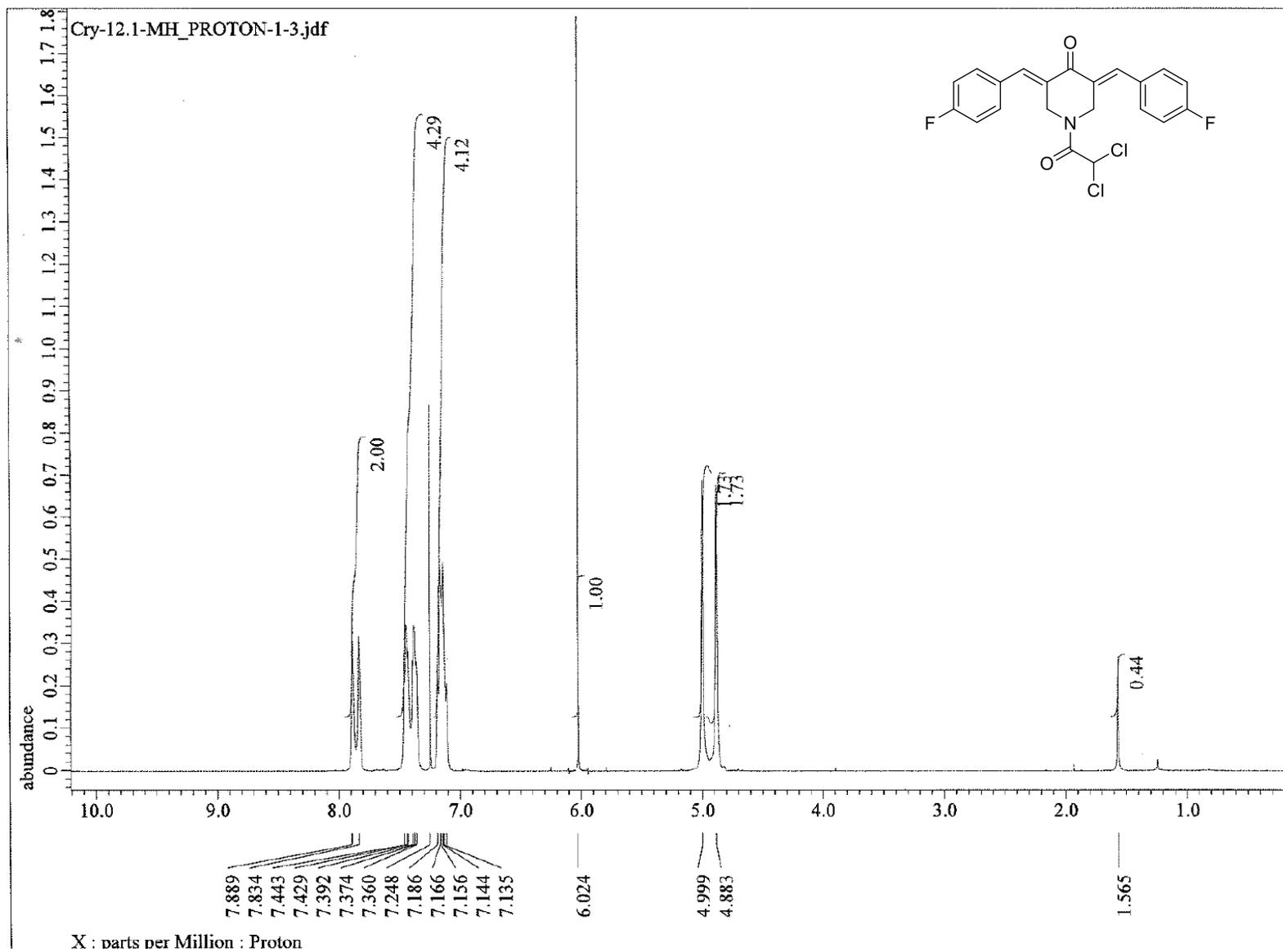
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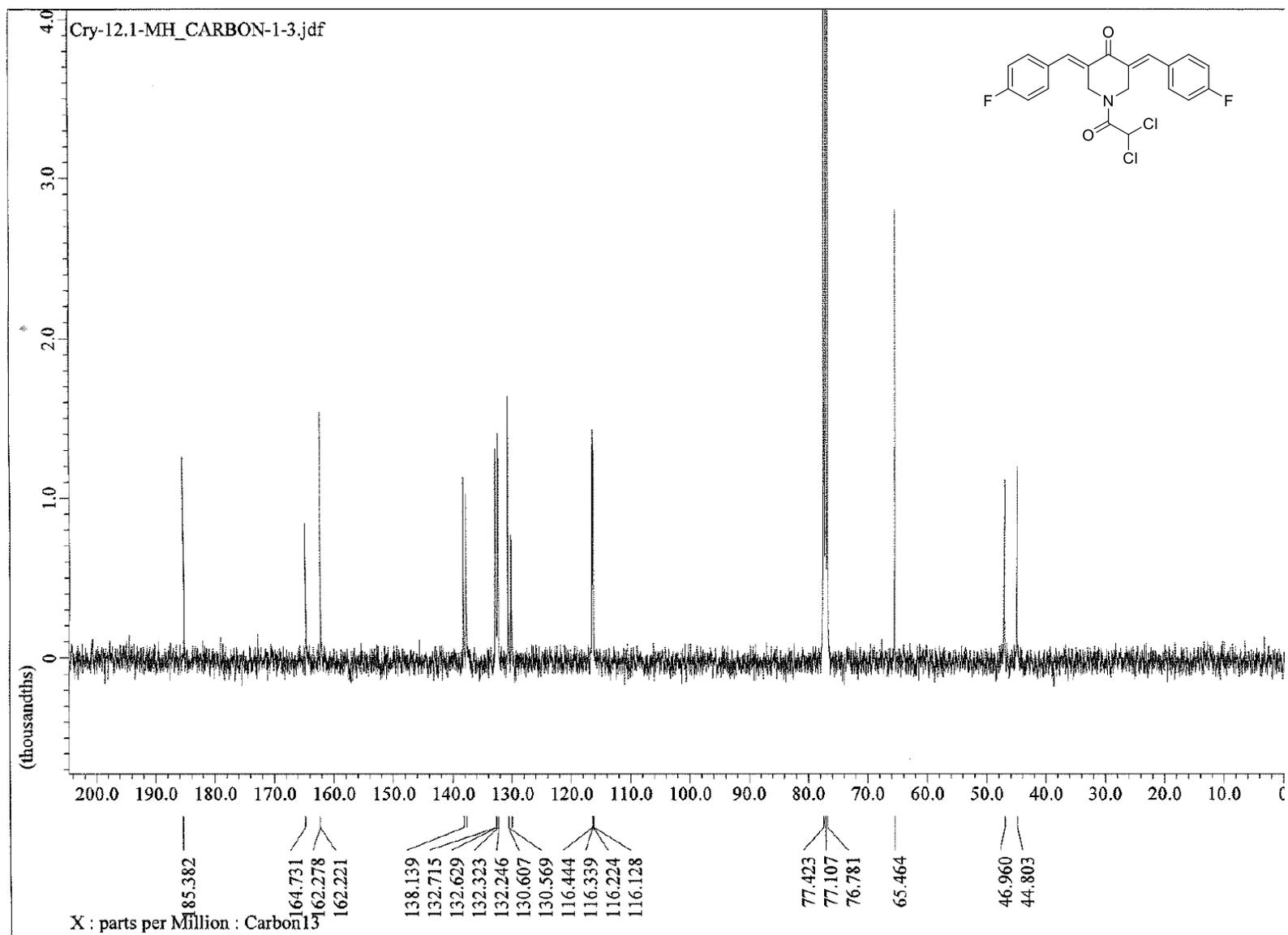


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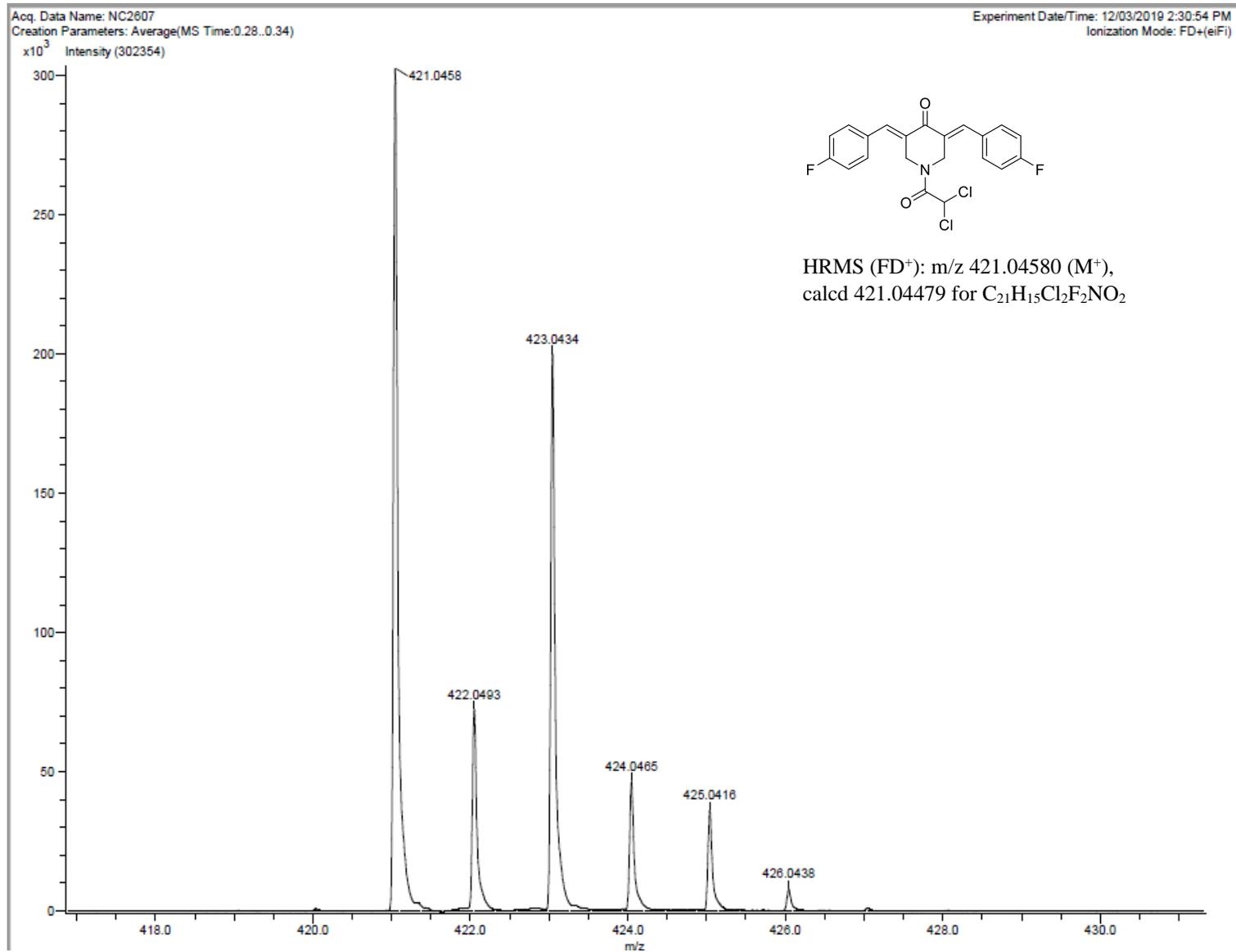
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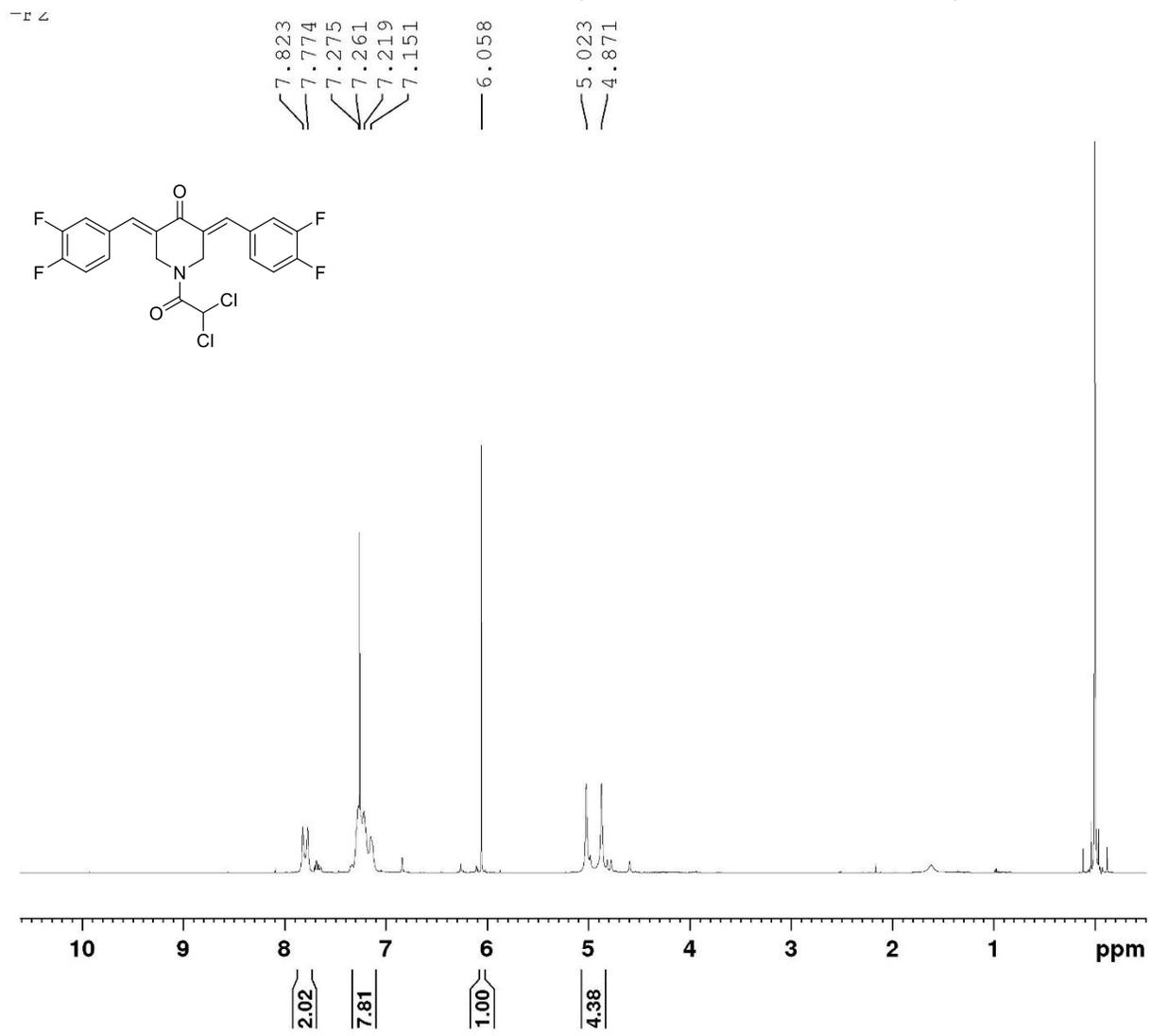
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Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-fluorobenzylidene)piperidin-4-one (**1b**)



¹H NMR (CDCl₃) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-difluorobenzylidene)piperidin-4-one (**1c**)



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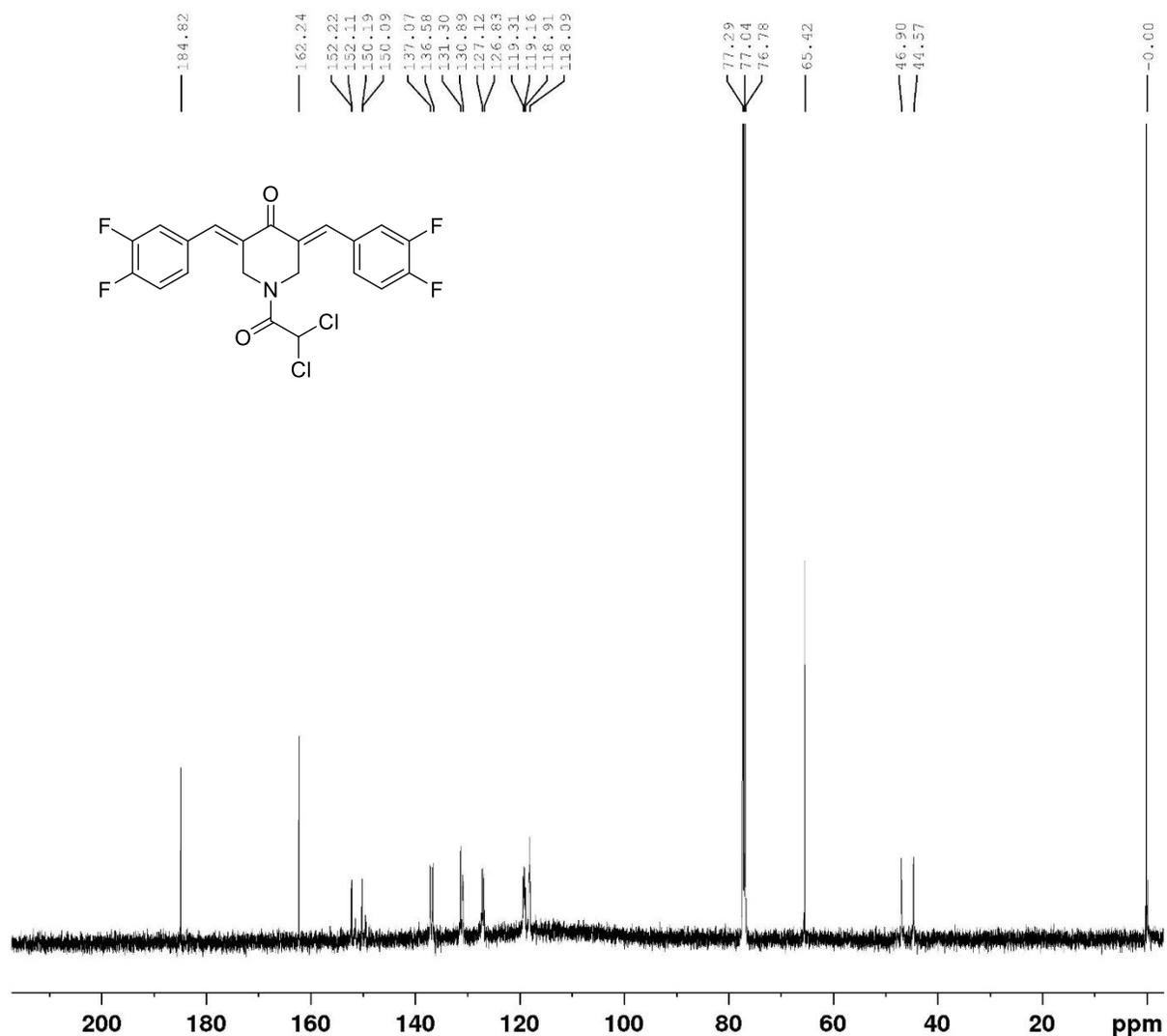
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¹³C NMR (CDCl₃) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-difluorobenzylidene)piperidin-4-one (1c)



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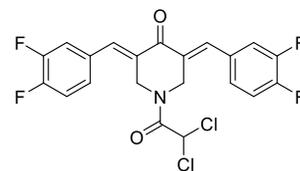
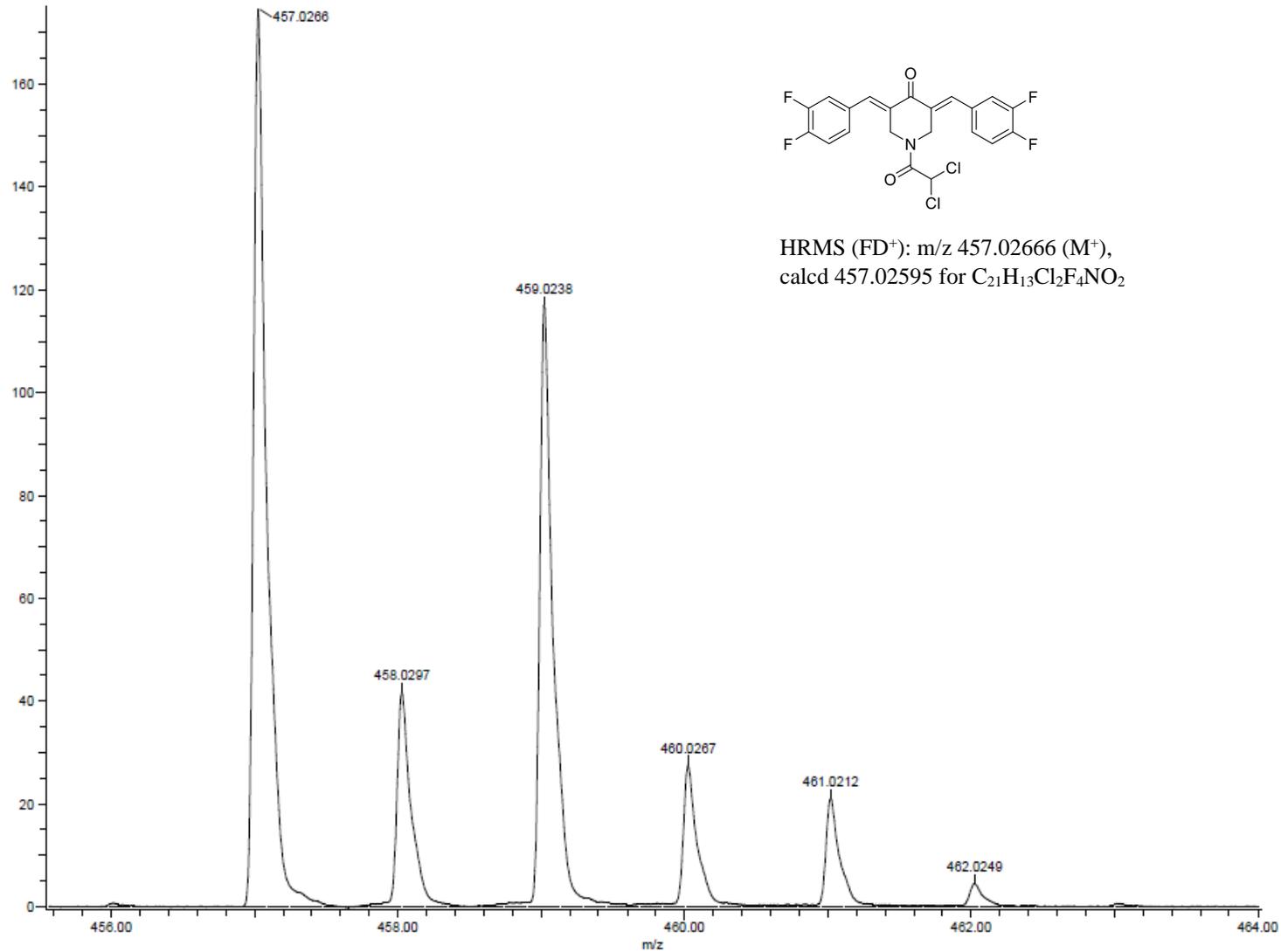
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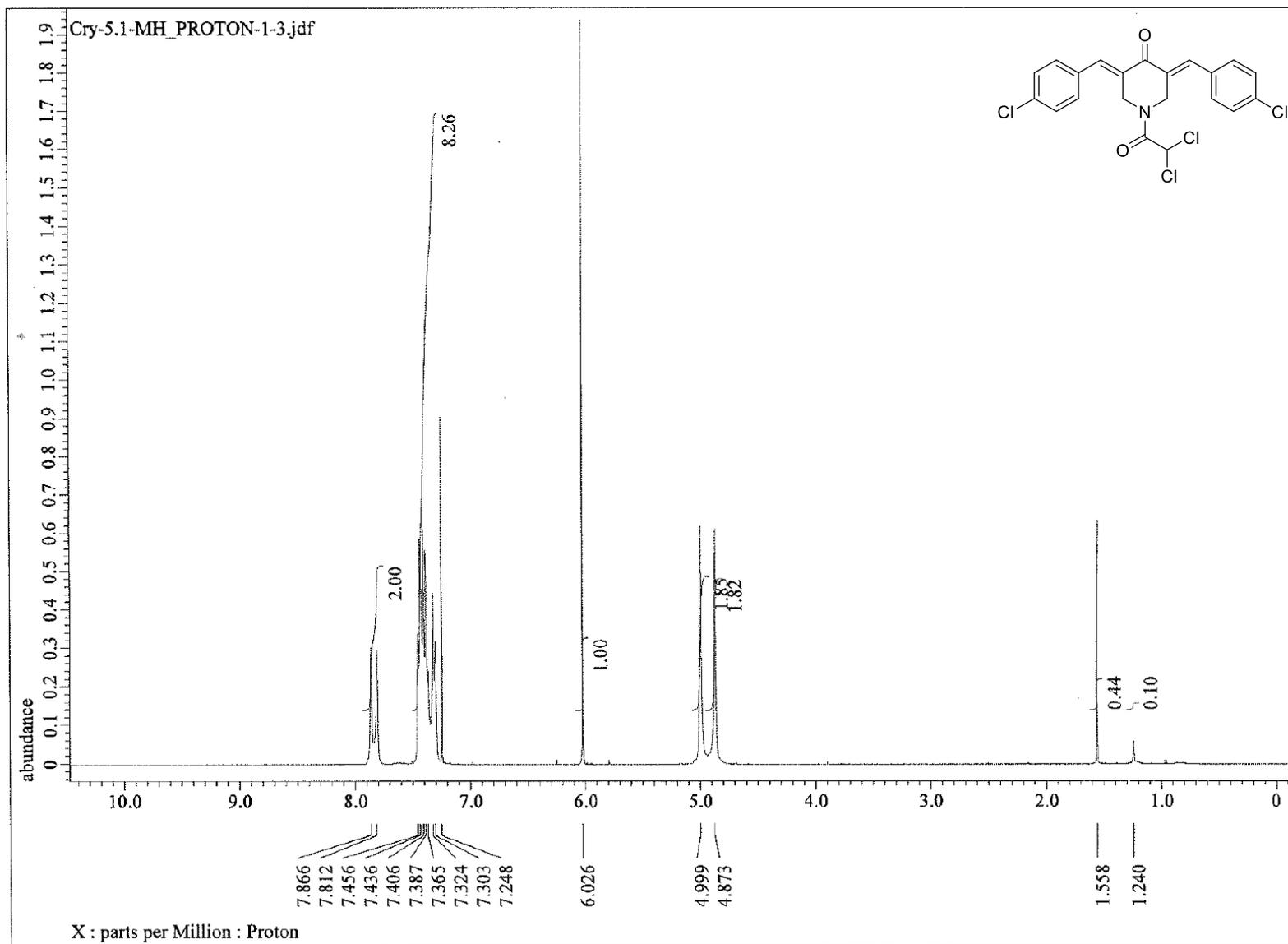
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-difluorobenzylidene)piperidin-4-one (**1c**)

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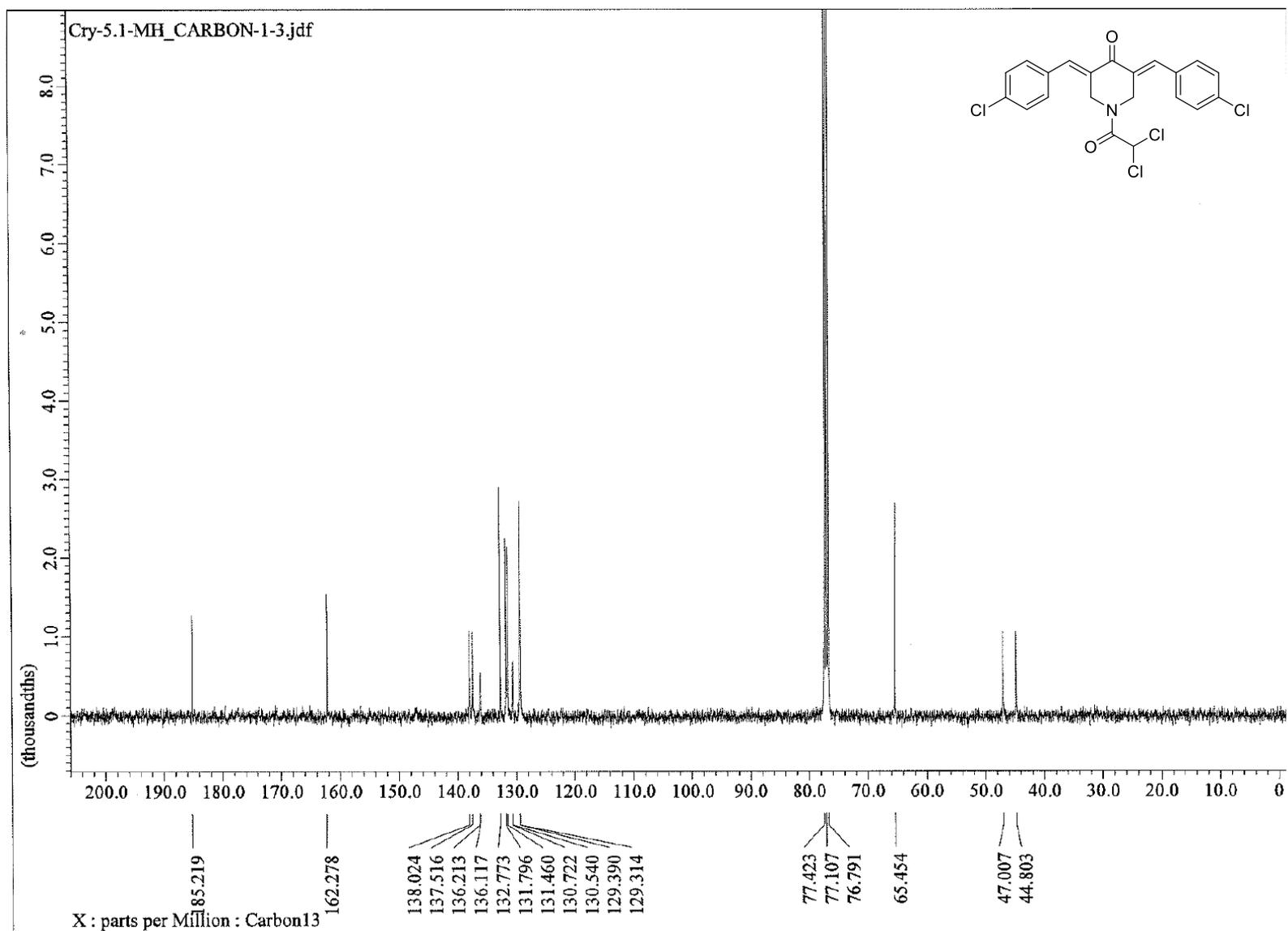
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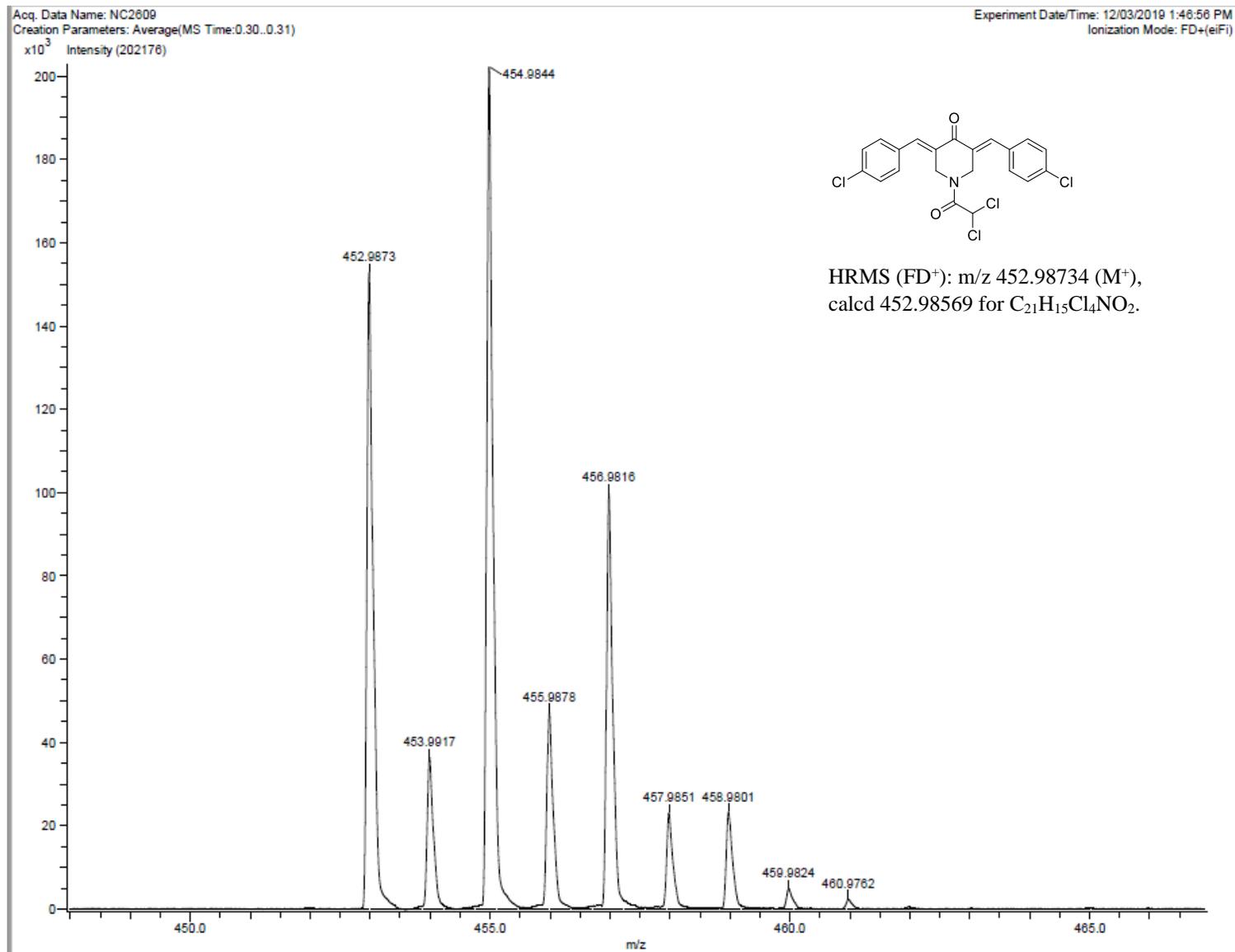
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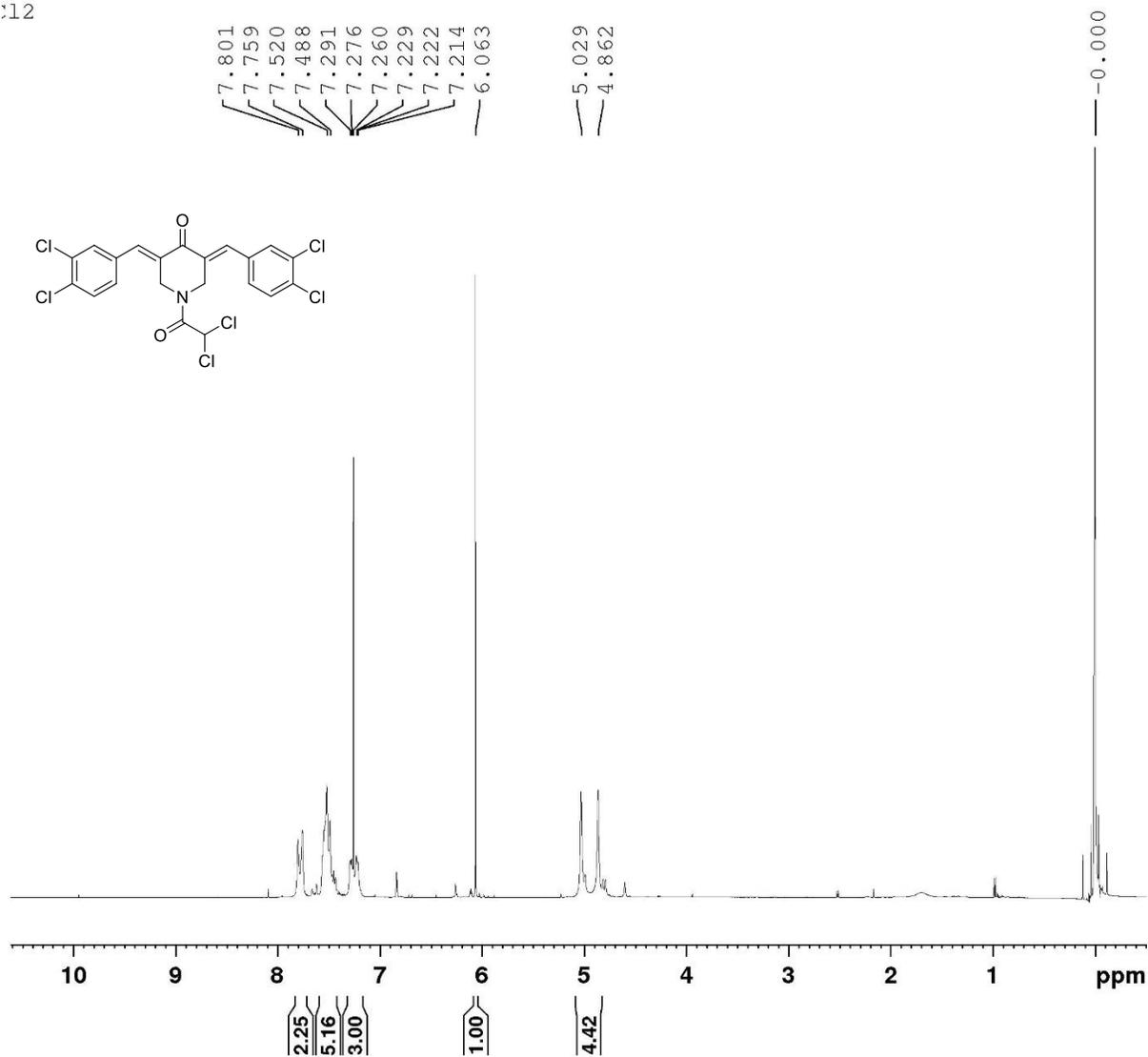


Mass spectrum of 3,5-bis((*E*)-4-chlorobenzylidene)-1-(2,2-dichloroacetyl)piperidin-4-one (**1d**)



¹H NMR (CDCl₃) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-dichlorobenzylidene)piperidin-4-one (1e)

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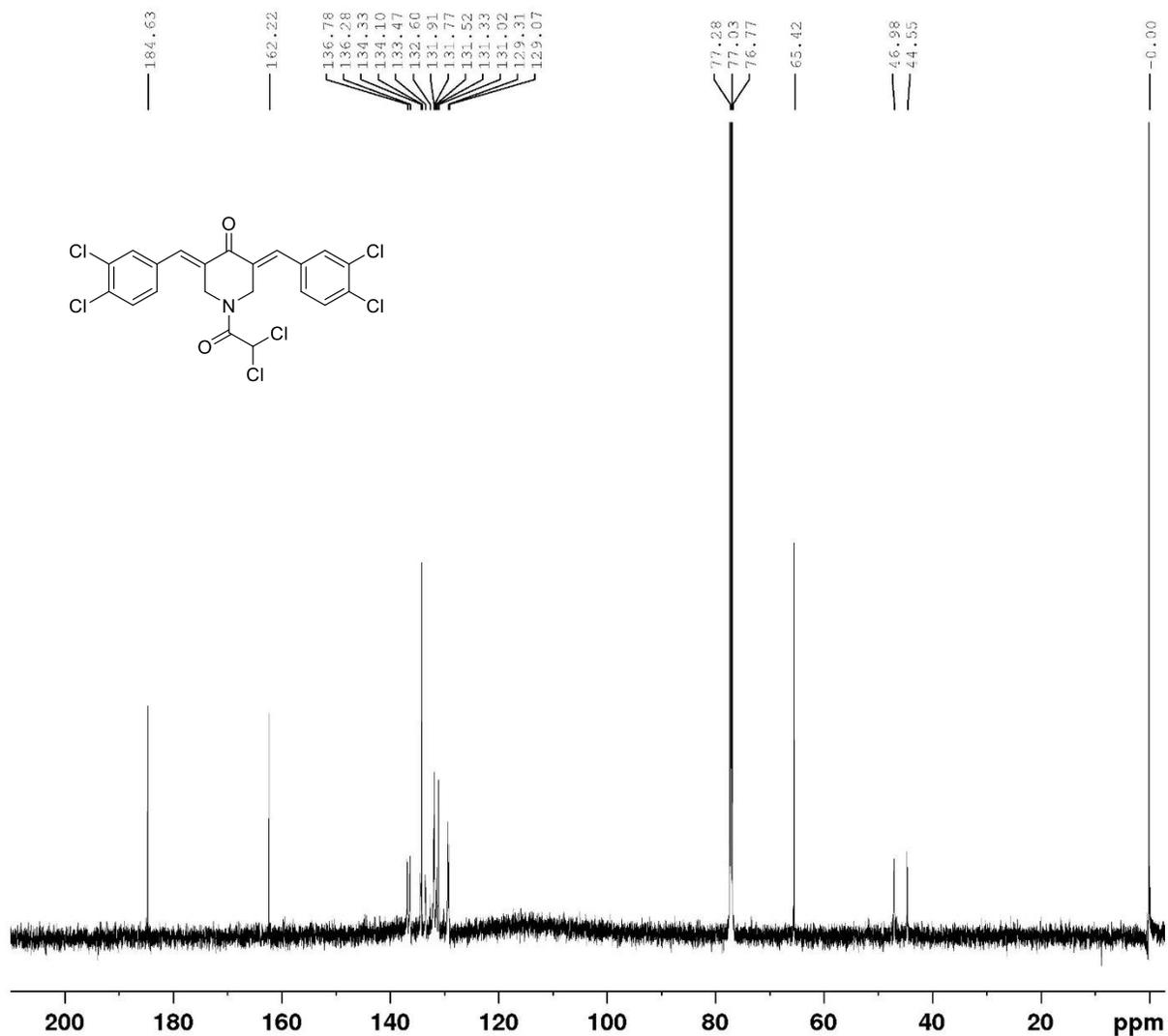
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¹³C NMR (CDCl₃) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-dichlorobenzylidene)piperidin-4-one (1e)



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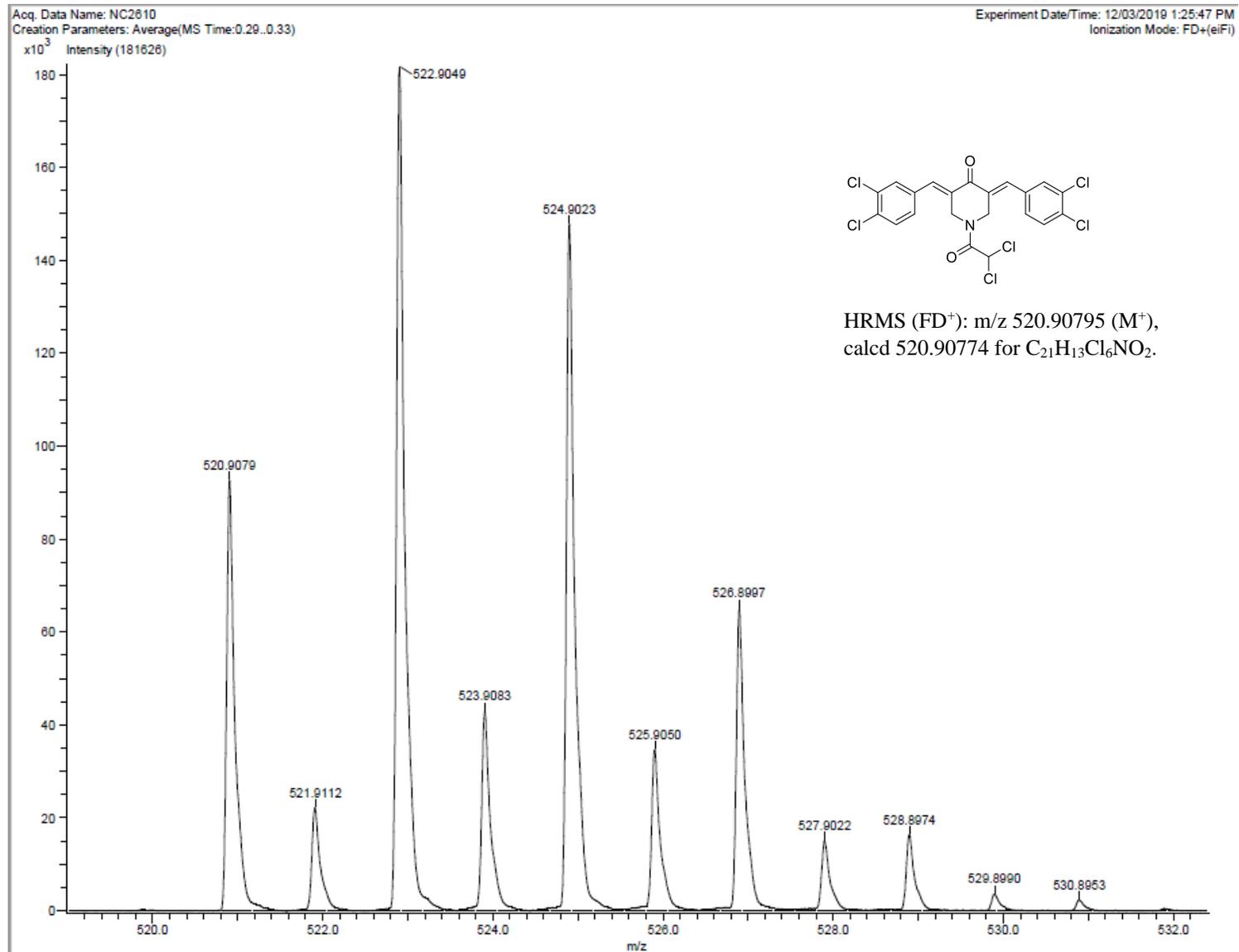
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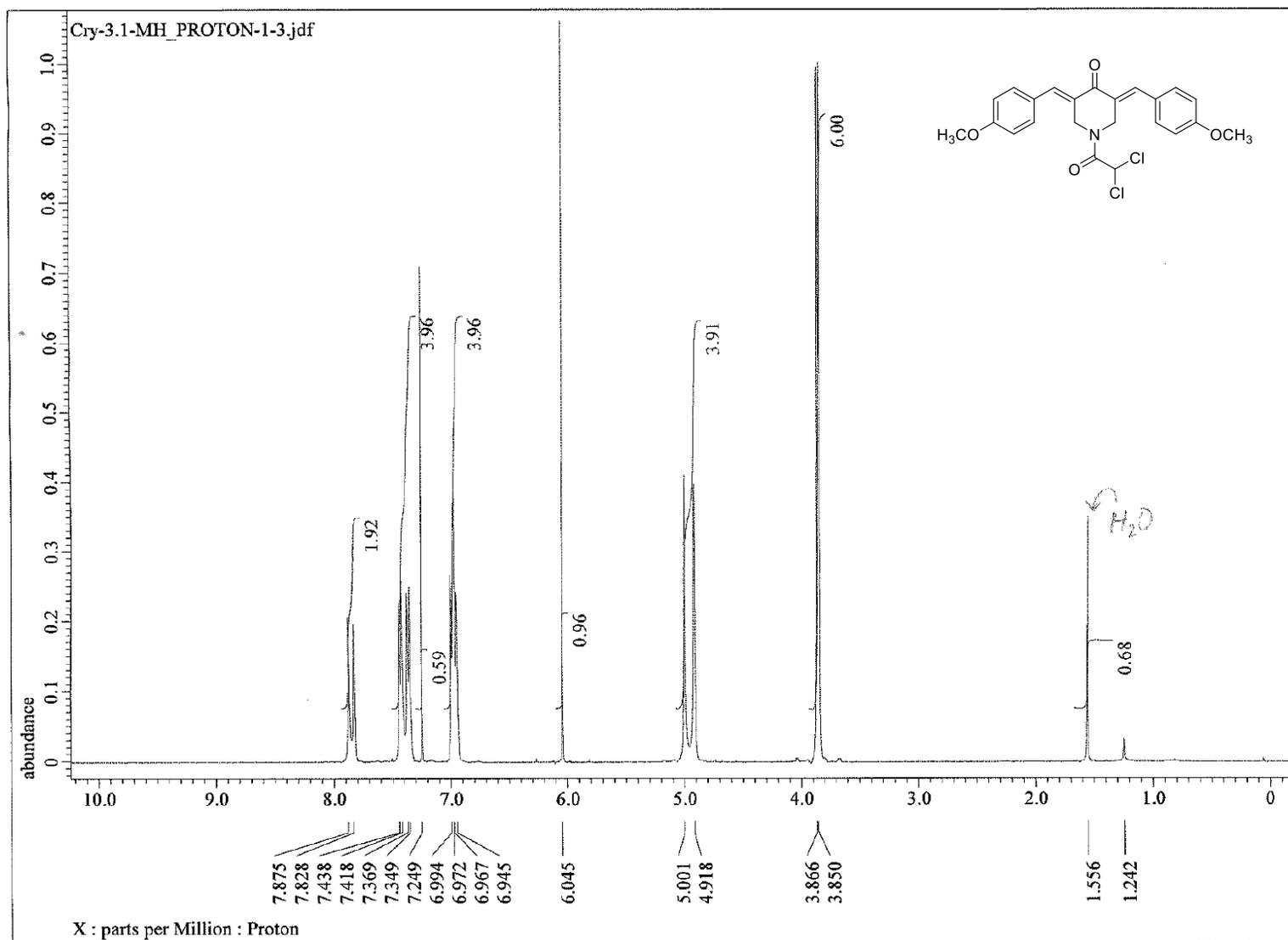
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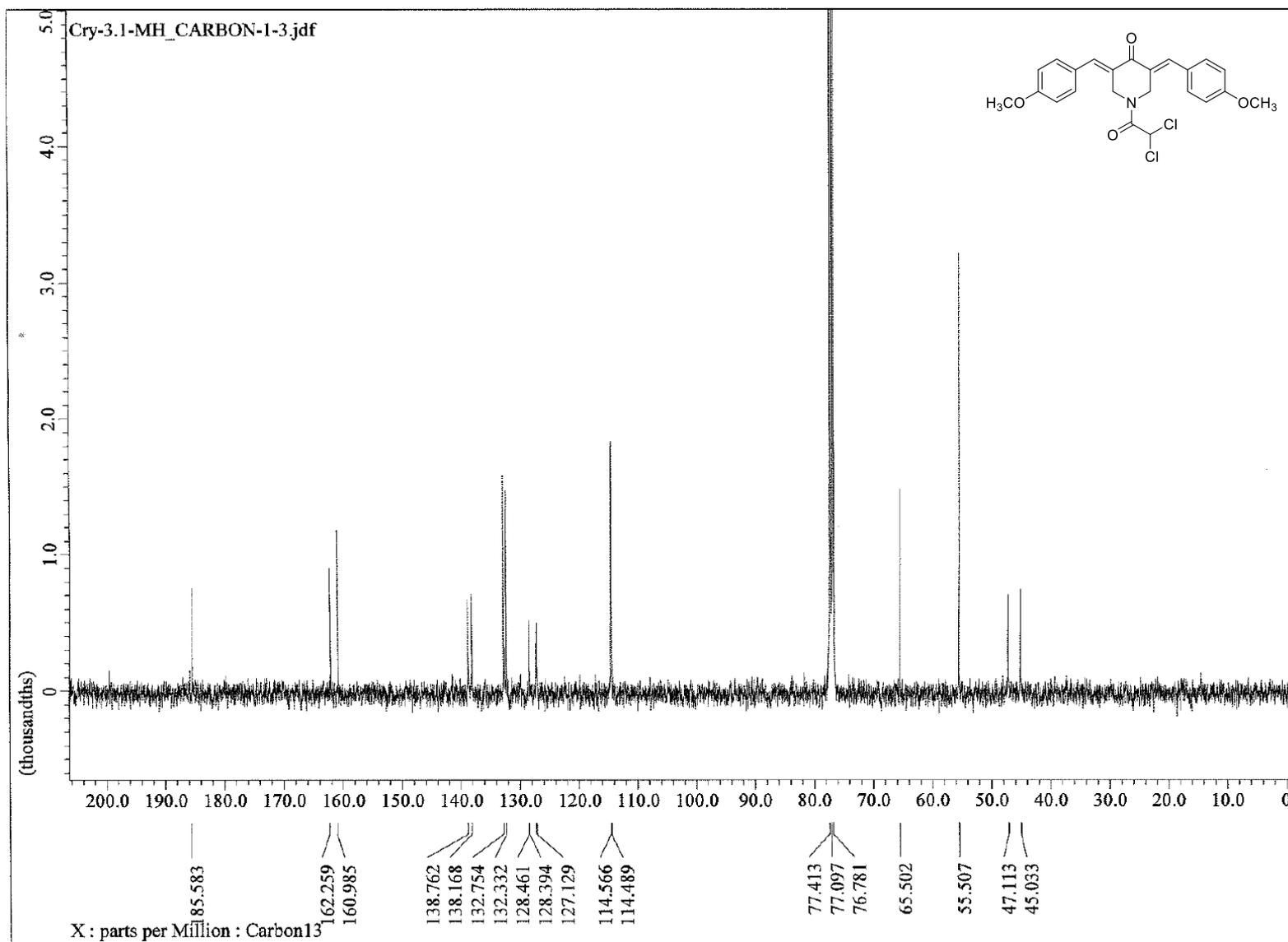
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-dichlorobenzylidene)piperidin-4-one (**1e**)



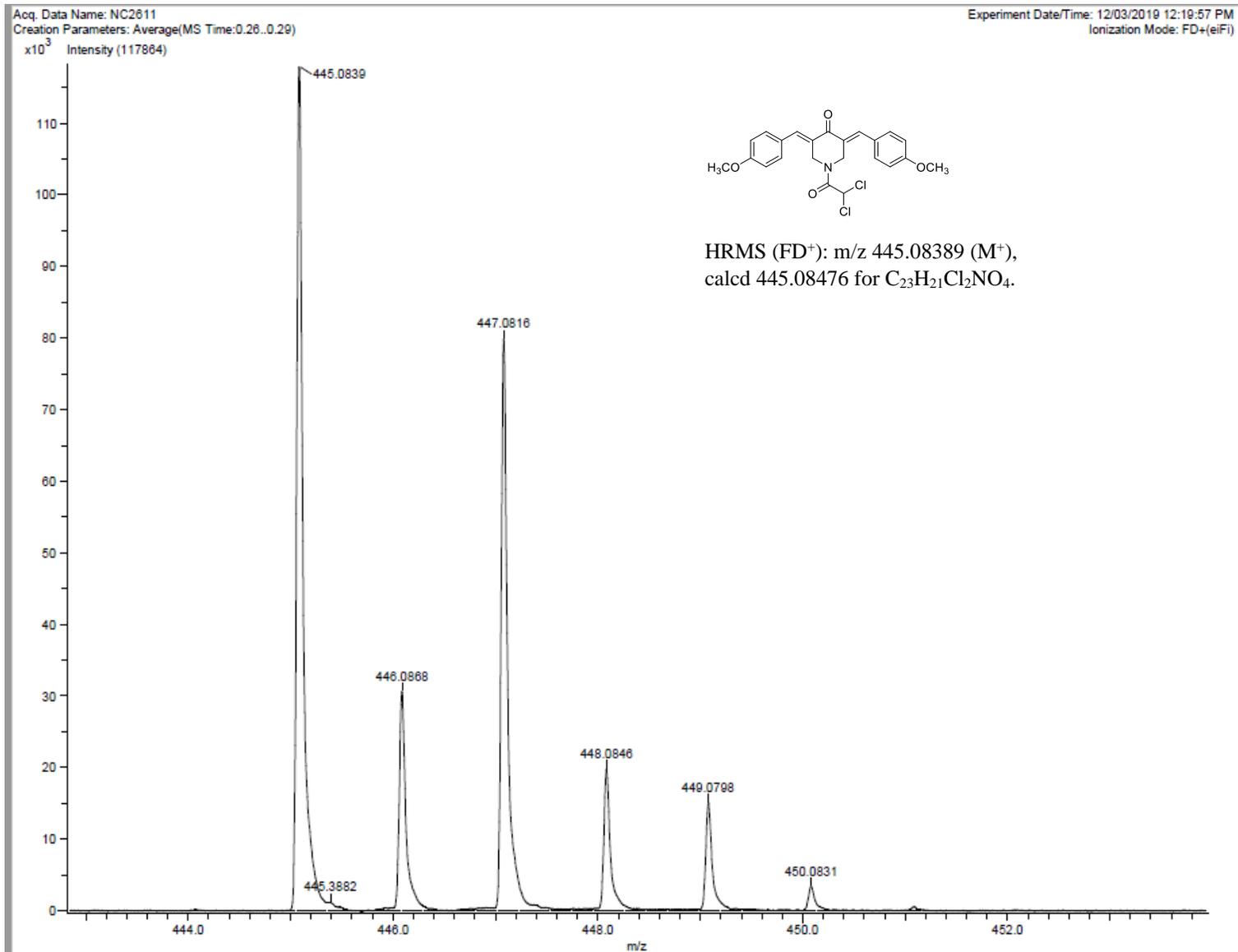
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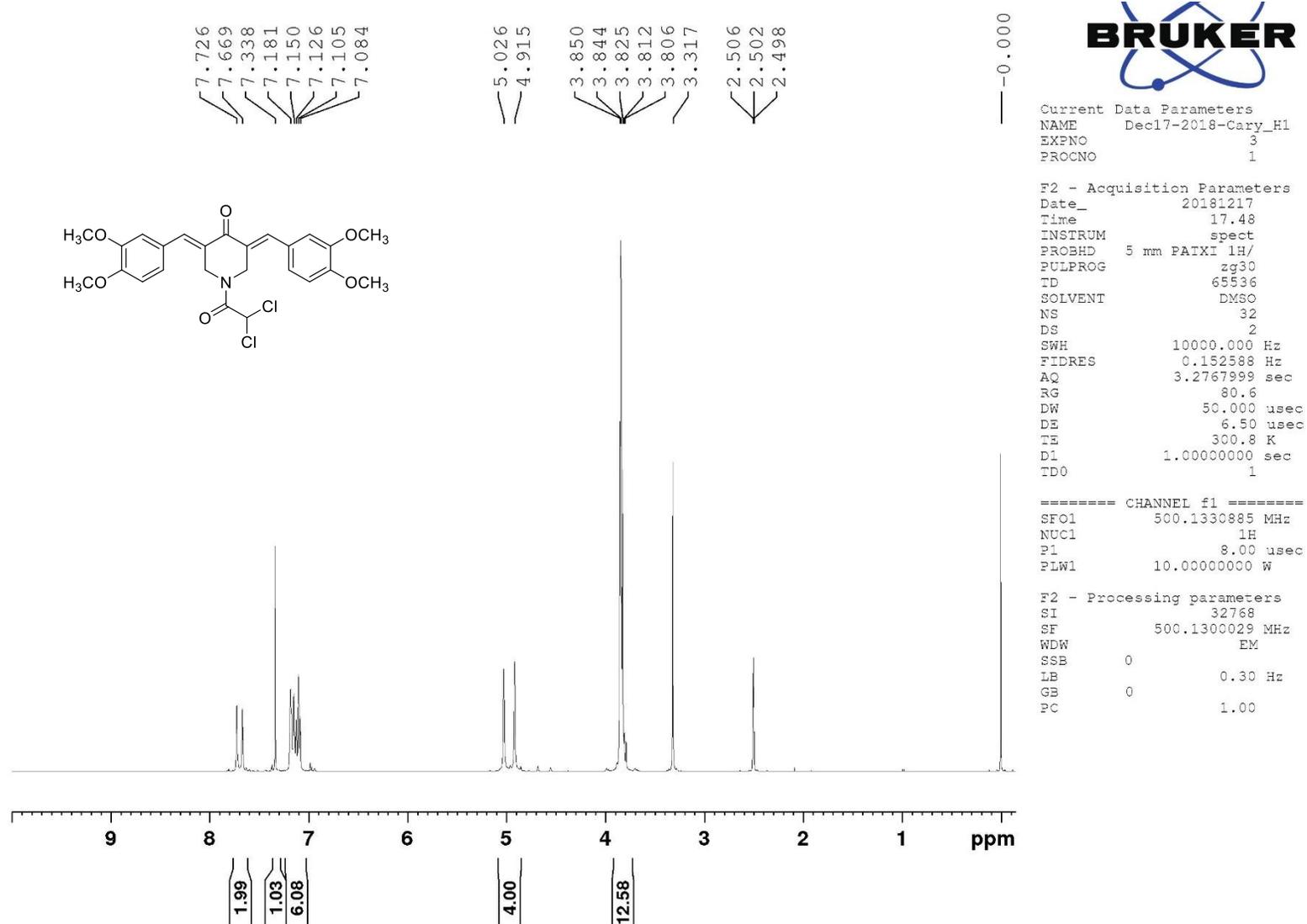
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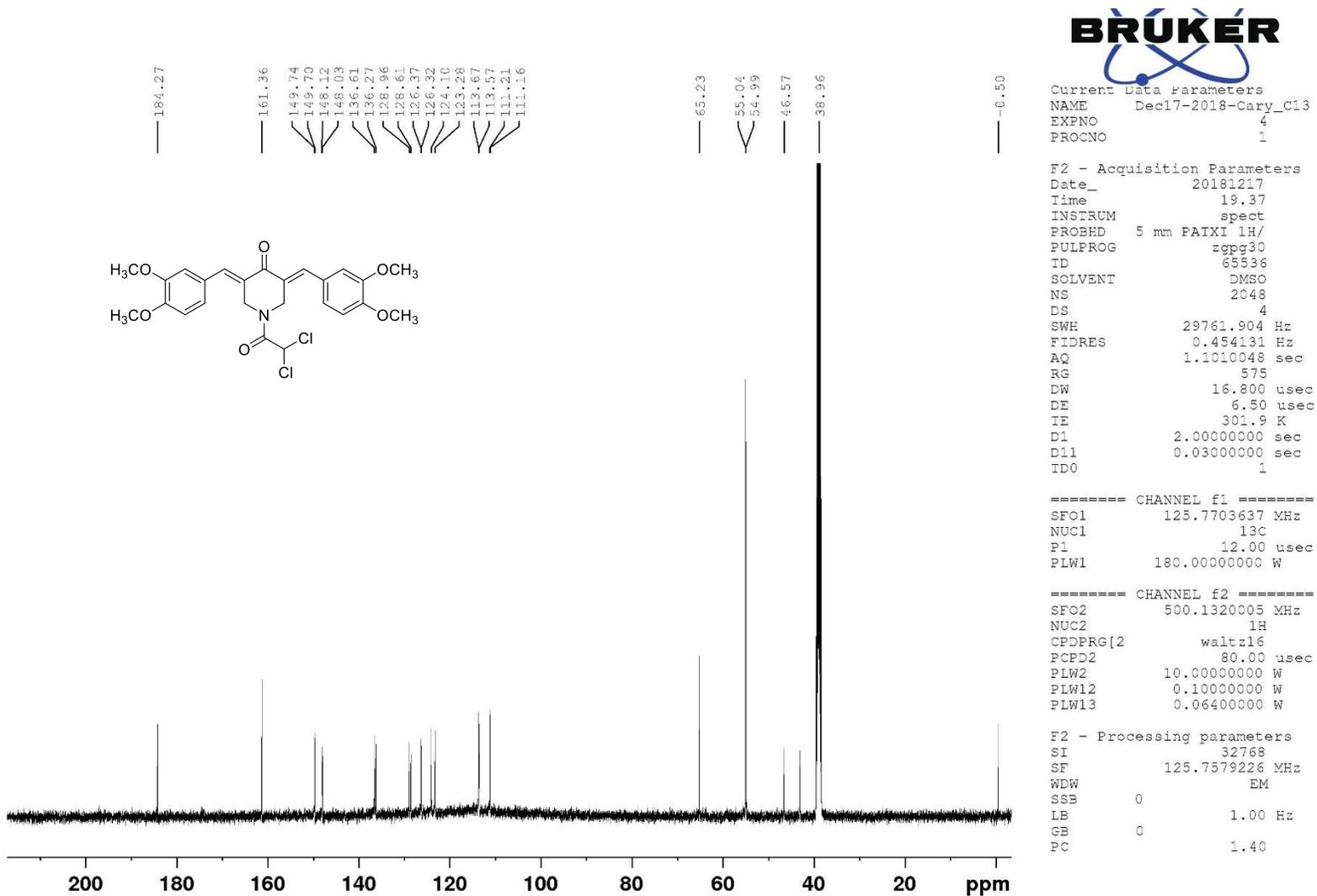
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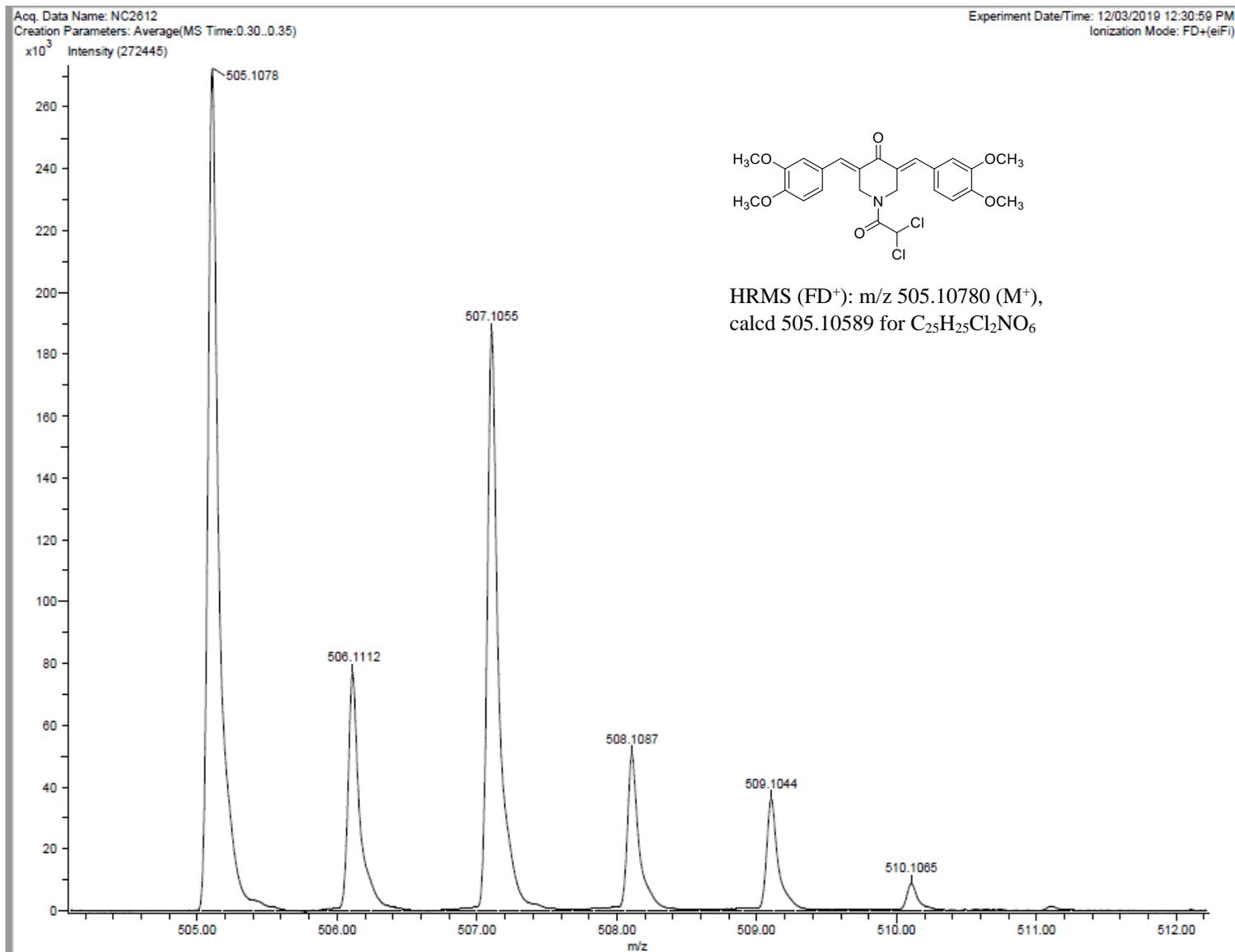
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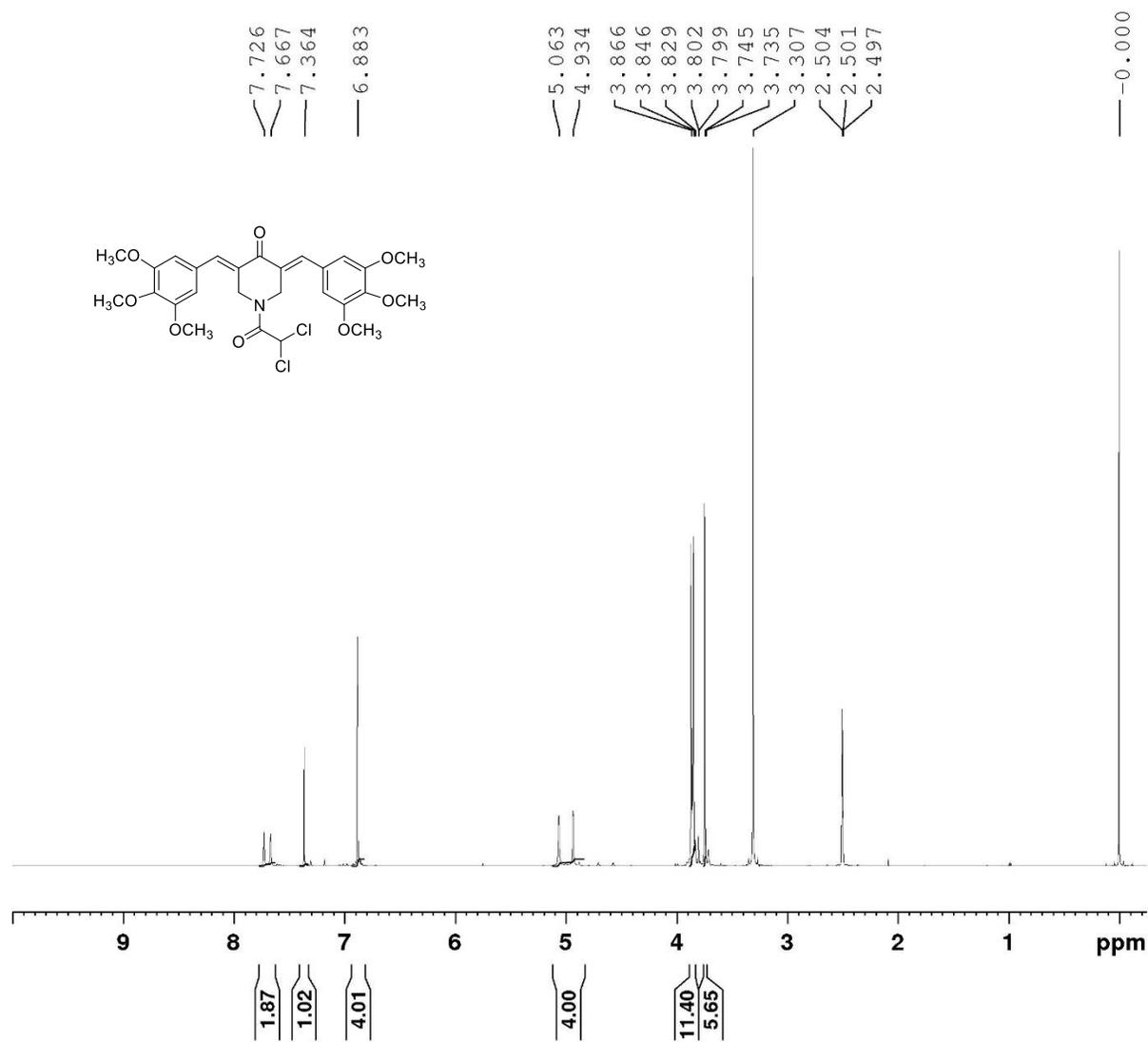
¹³C NMR ((CD₃)₂SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-dimethoxybenzylidene)piperidin-4-one (**1g**)



Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-dimethoxybenzylidene)piperidin-4-one (**1g**)



¹H NMR ((CD₃)₂SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4,5-trimethoxybenzylidene)piperidin-4-one (**1h**)



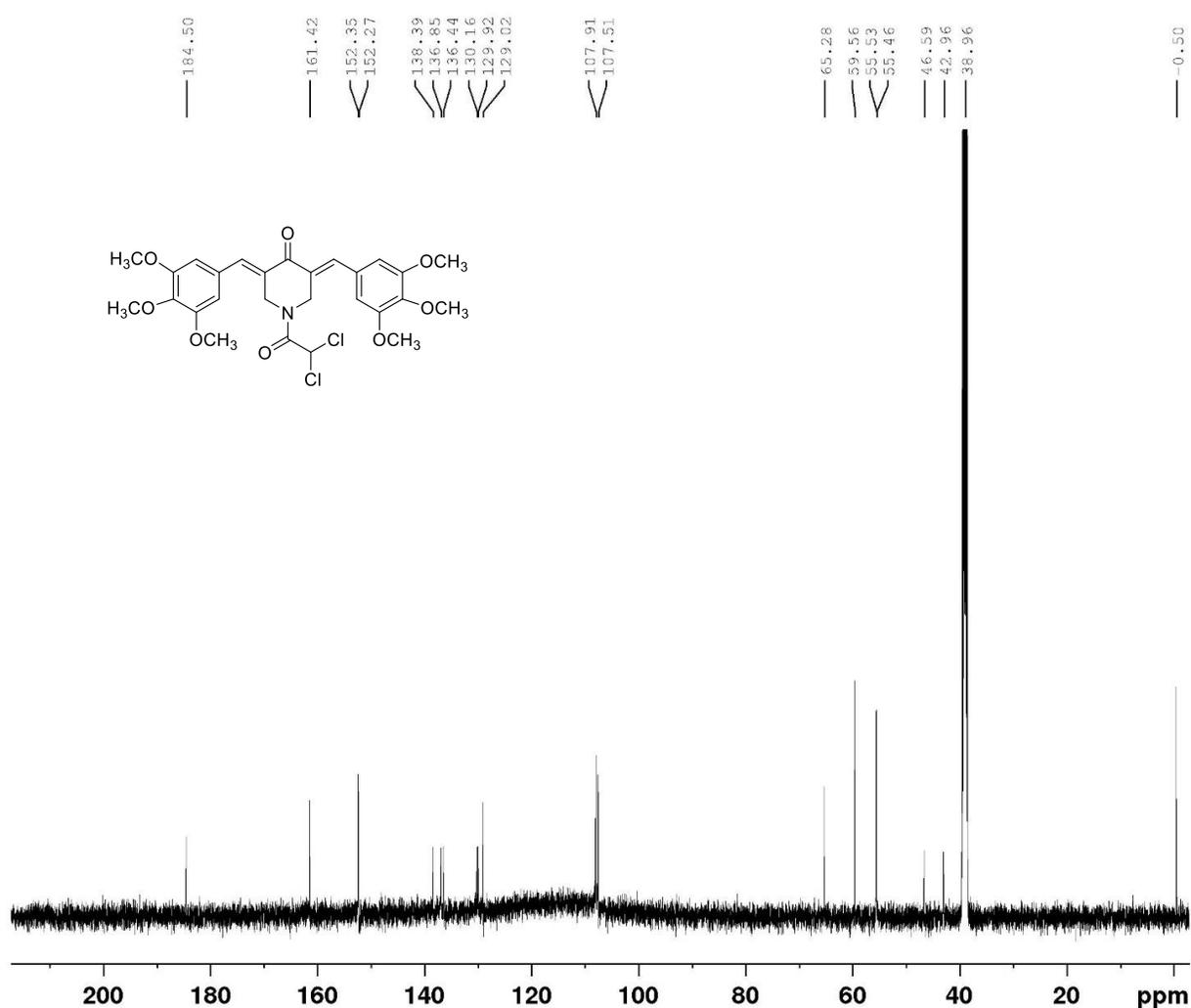
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¹³C NMR ((CD₃)₂SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4,5-trimethoxybenzylidene)piperidin-4-one (**1h**)



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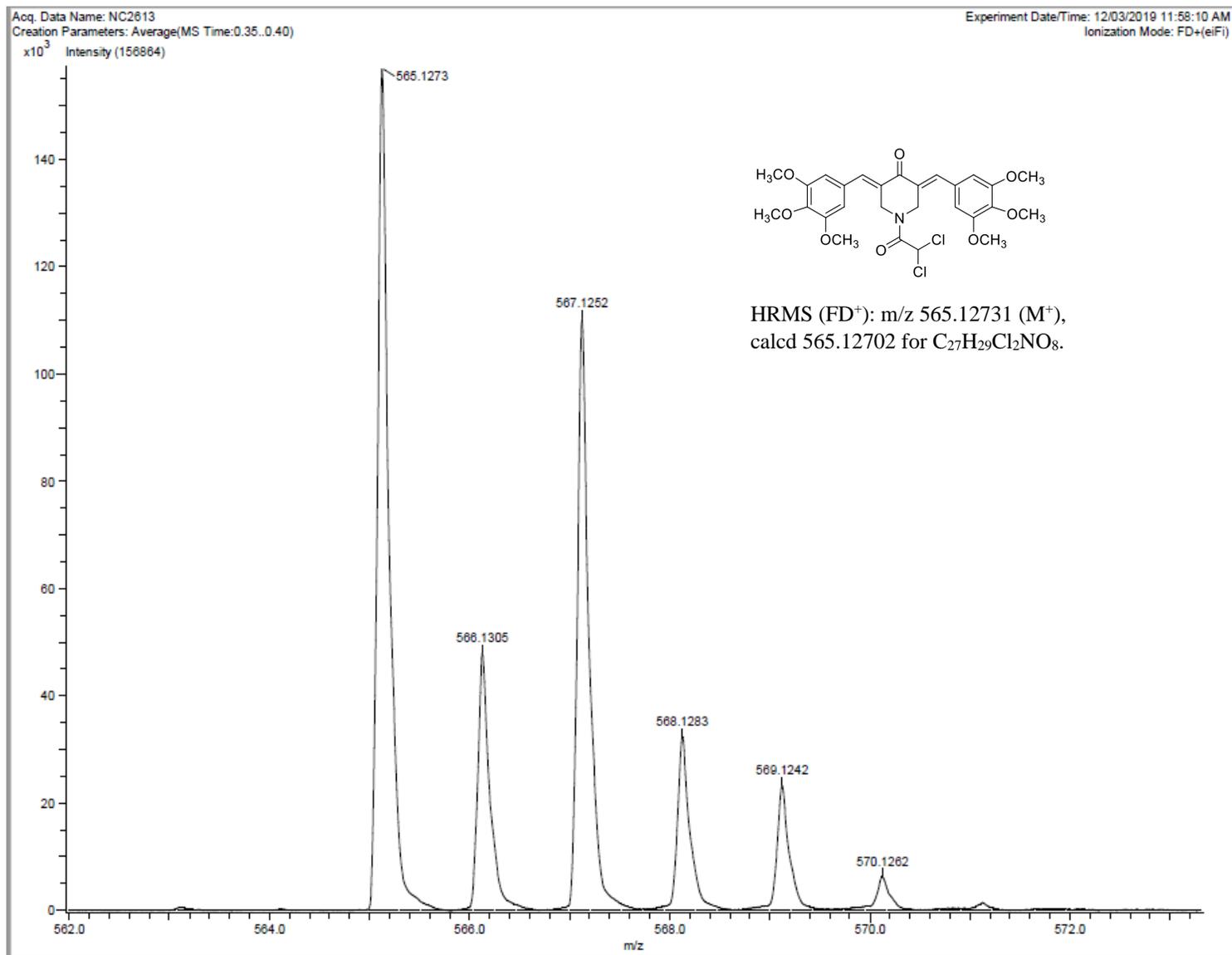
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 PLW2 10.00000000 W
 PLW12 0.10000000 W
 PLW13 0.06400000 W

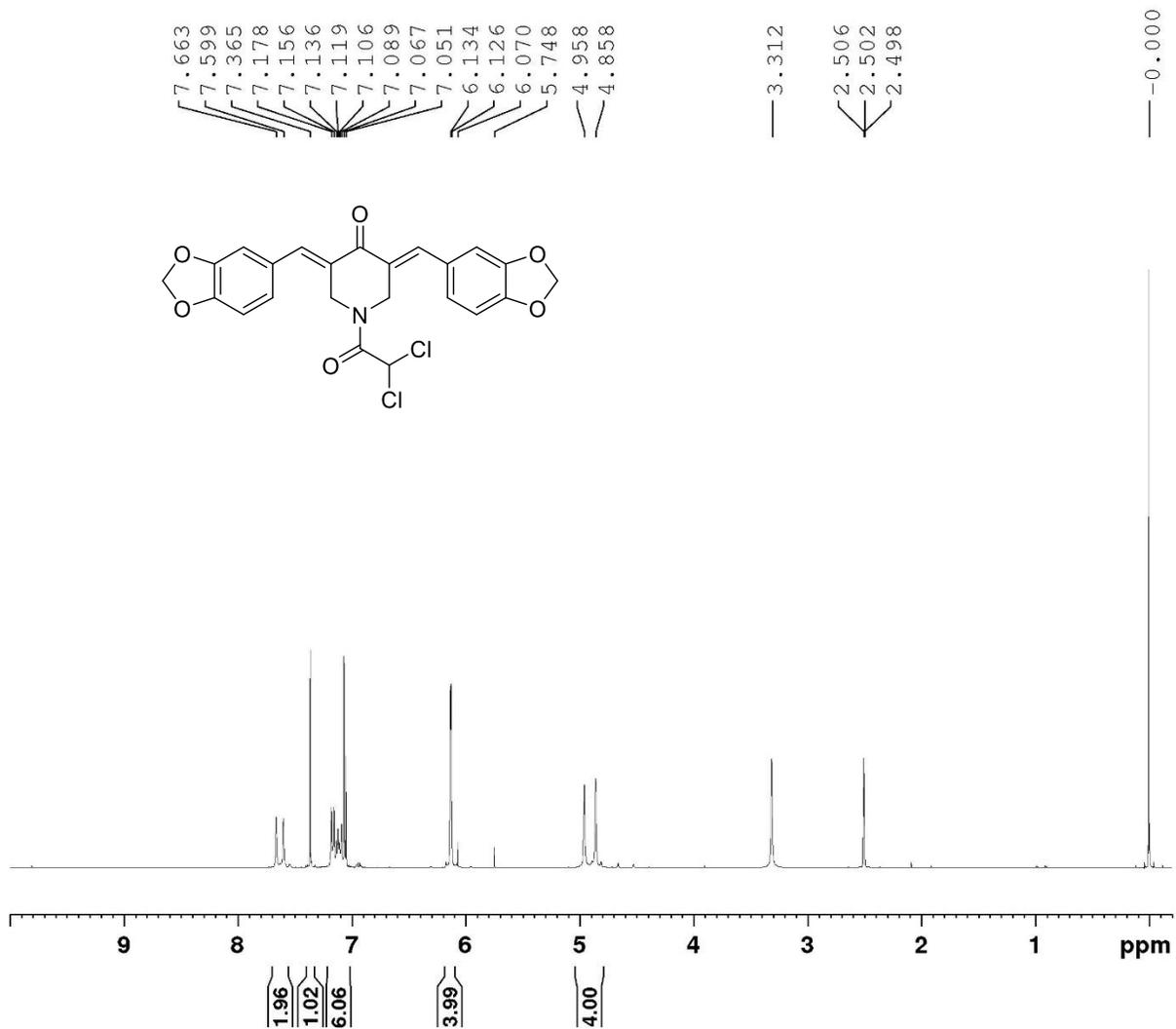
F2 - Processing parameters

SI 32768
 SF 125.7579232 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4,5-trimethoxybenzylidene)piperidin-4-one (**1h**)



¹H NMR ((CD₃)₂SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-methylenedioxybenzylidene)piperidin-4-one (**1i**)



BRUKER

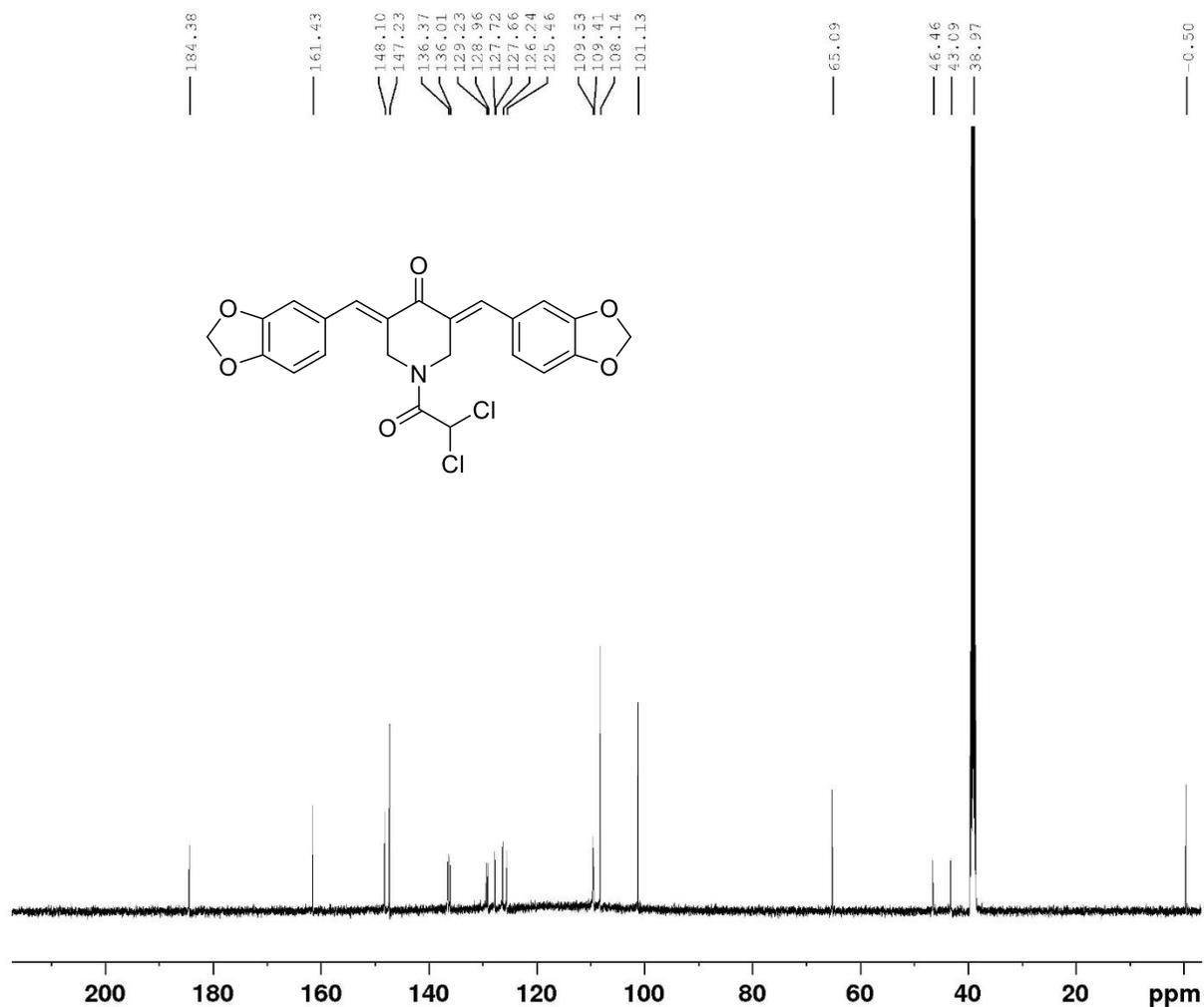
Current Data Parameters
 NAME Dec17-2018-Cary_H1
 EXPNO 8
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181217
 Time 21.38
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 101
 DW 50.000 usec
 DE 6.50 usec
 TE 302.2 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 32768
 SF 500.1300029 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR ((CD₃)₂SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-methylenedioxybenzylidene)piperidin-4-one (**1i**)



Current Data Parameters
NAME Dec17-2018-Cary_H1
EXPNO 9
PROCNO 1

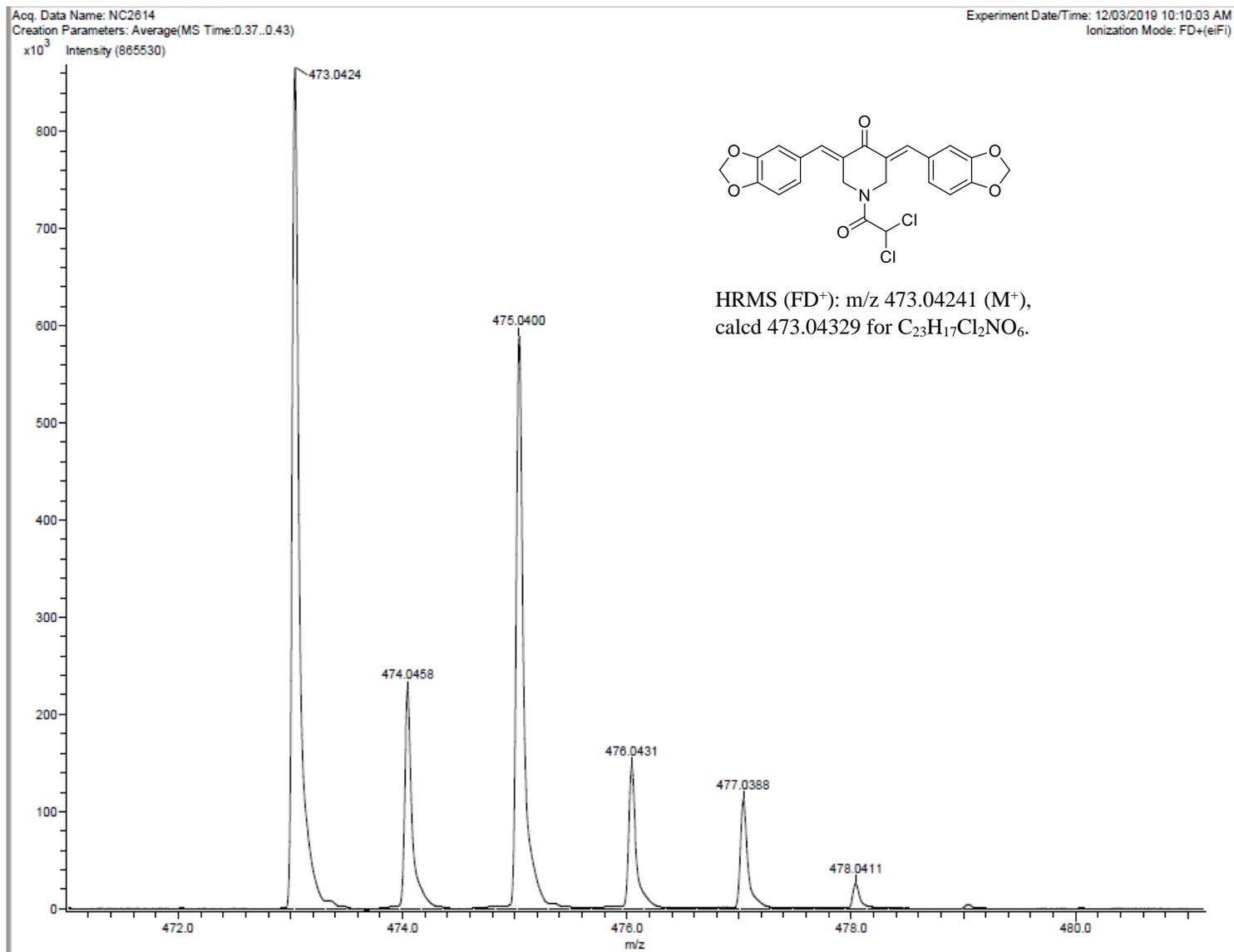
F2 - Acquisition Parameters
Date_ 20181217
Time 23.27
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 575
DW 16.800 usec
DE 6.50 usec
TE 302.8 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 125.7703637 MHz
NUC1 13C
P1 12.00 usec
PLW1 180.0000000 W

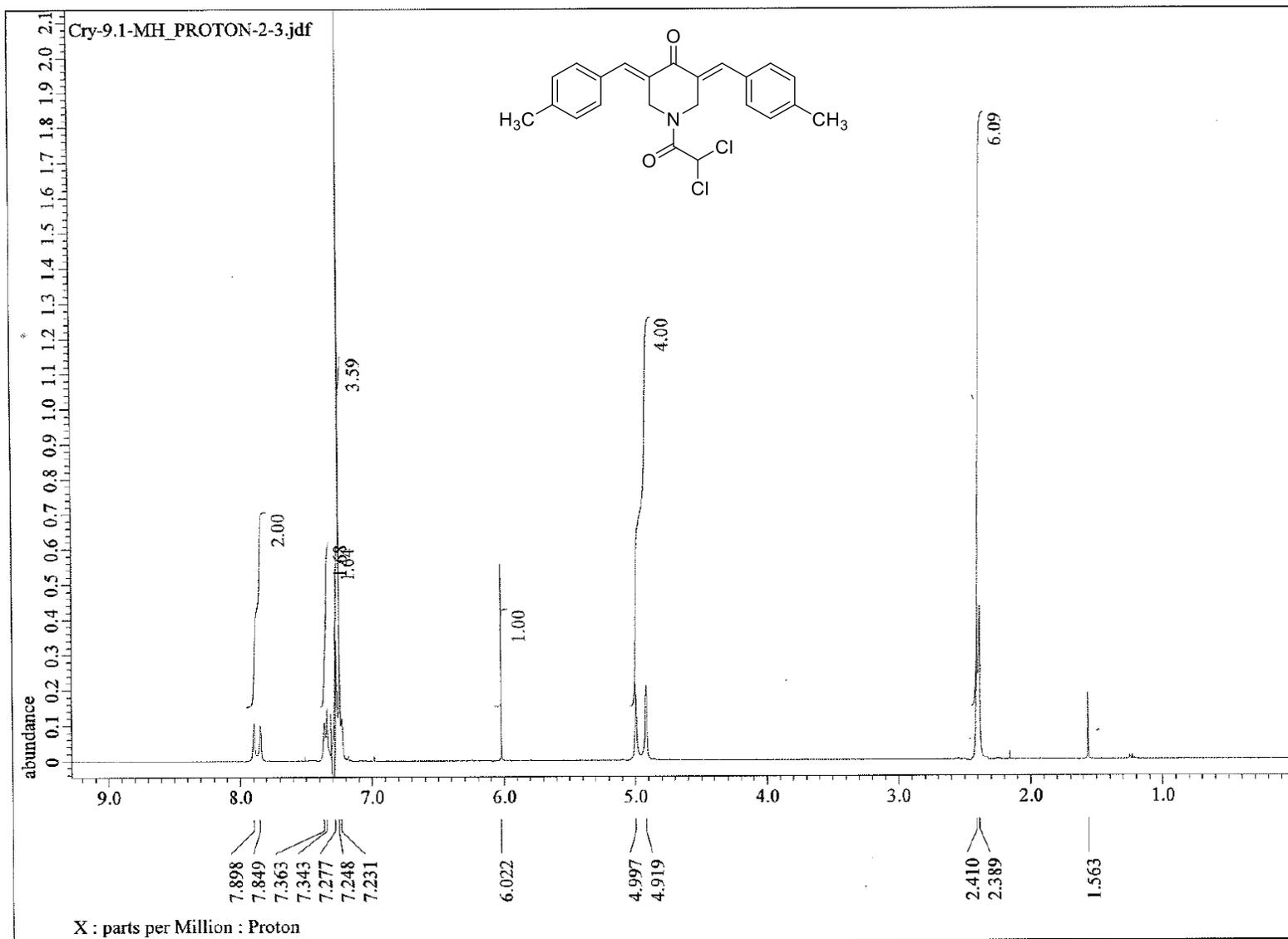
===== CHANNEL f2 =====
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 10.0000000 W
PLW12 0.1000000 W
PLW13 0.0640000 W

F2 - Processing parameters
SI 32768
SF 125.7579226 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

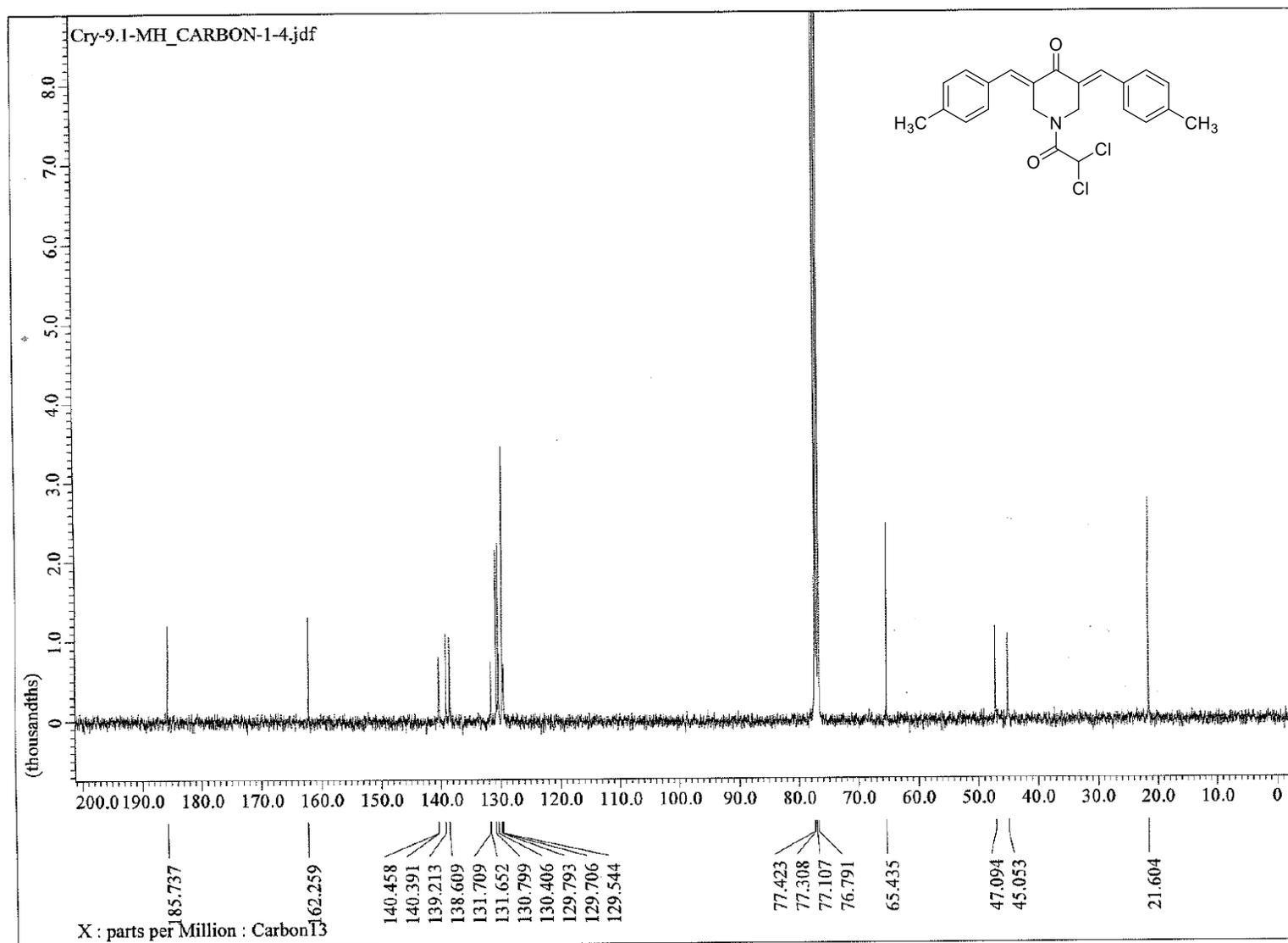
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-3,4-methylenedioxybenzylidene)piperidin-4-one (**1i**)



^1H NMR (CDCl_3) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-methylbenzylidene)piperidin-4-one (**1j**)



^{13}C NMR (CDCl_3) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-methylbenzylidene)piperidin-4-one (**1j**)

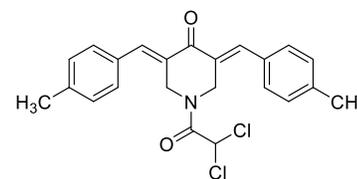
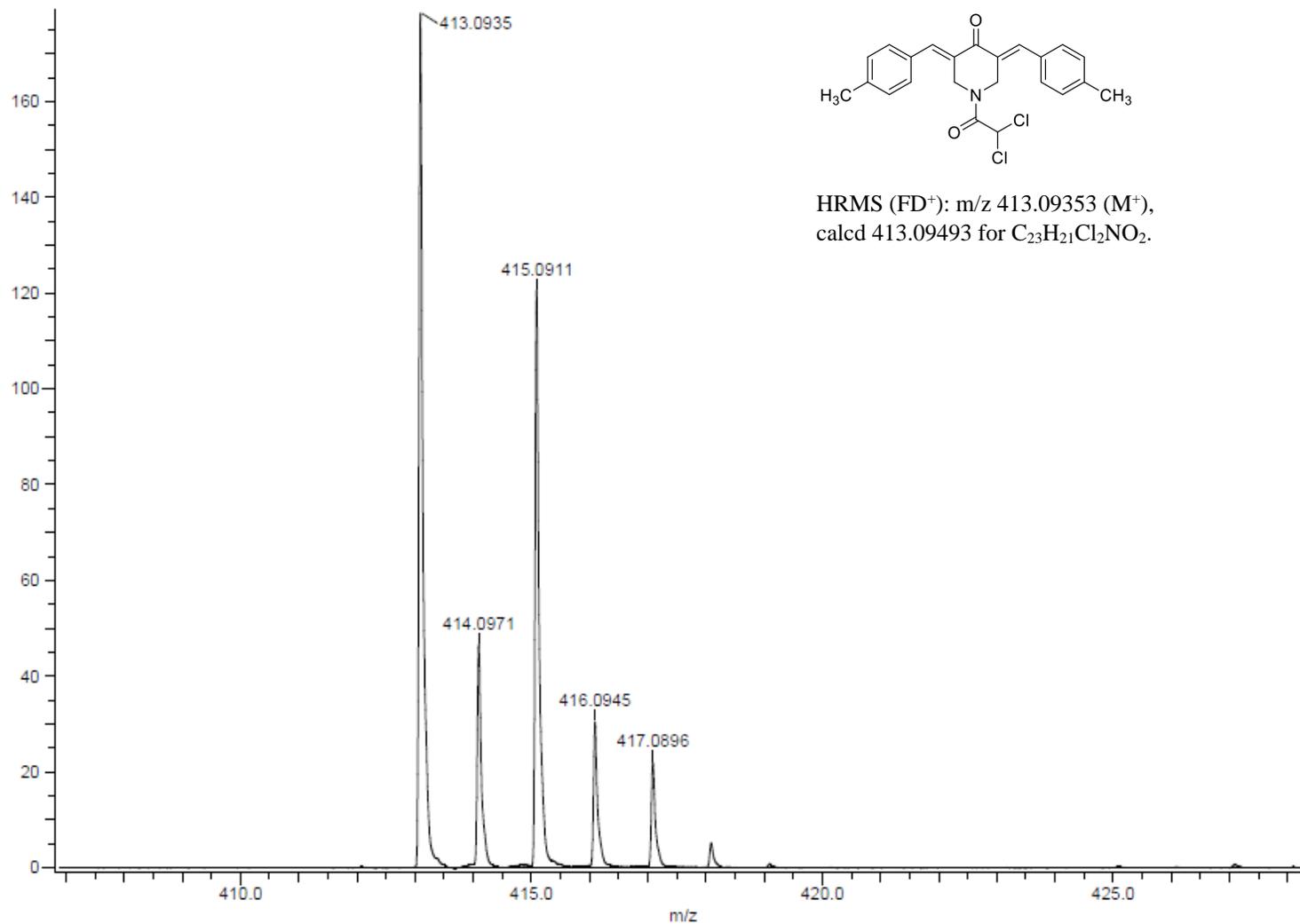


Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-methylbenzylidene)piperidin-4-one (**1j**)

Acq. Data Name: NC2604
Creation Parameters: Average(MS Time:0.33..0.37)

Experiment Date/Time: 2/20/2019 1:51:00 PM
Ionization Mode: FD+(eiFi)

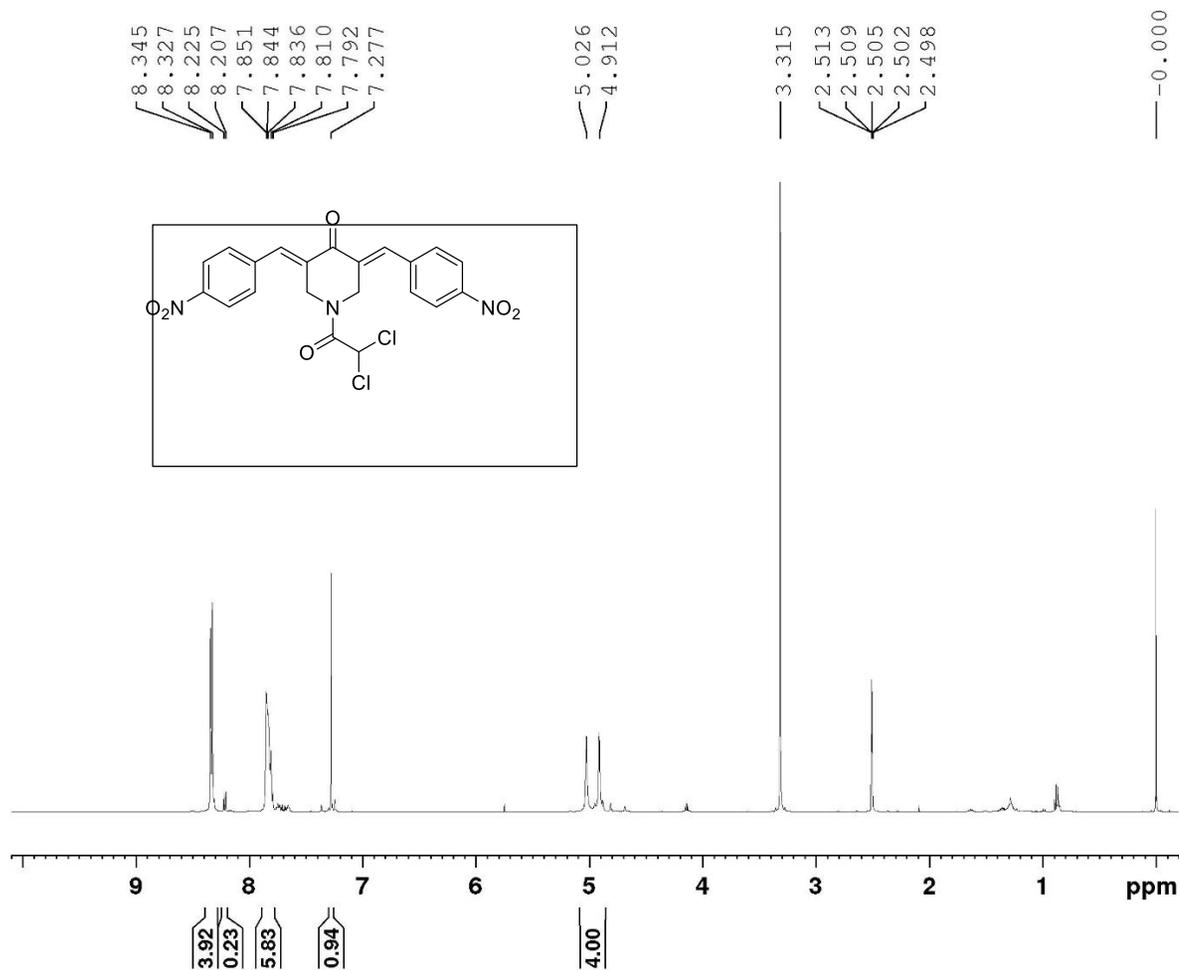
$\times 10^3$ Intensity (178375)



HRMS (FD⁺): m/z 413.09353 (M⁺),
calcd 413.09493 for C₂₃H₂₁Cl₂NO₂.

¹H NMR ((CD₃)₂SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-nitrobenzylidene)piperidin-4-one (1k)

Cry-44.1-MH_NO2_1H_Full



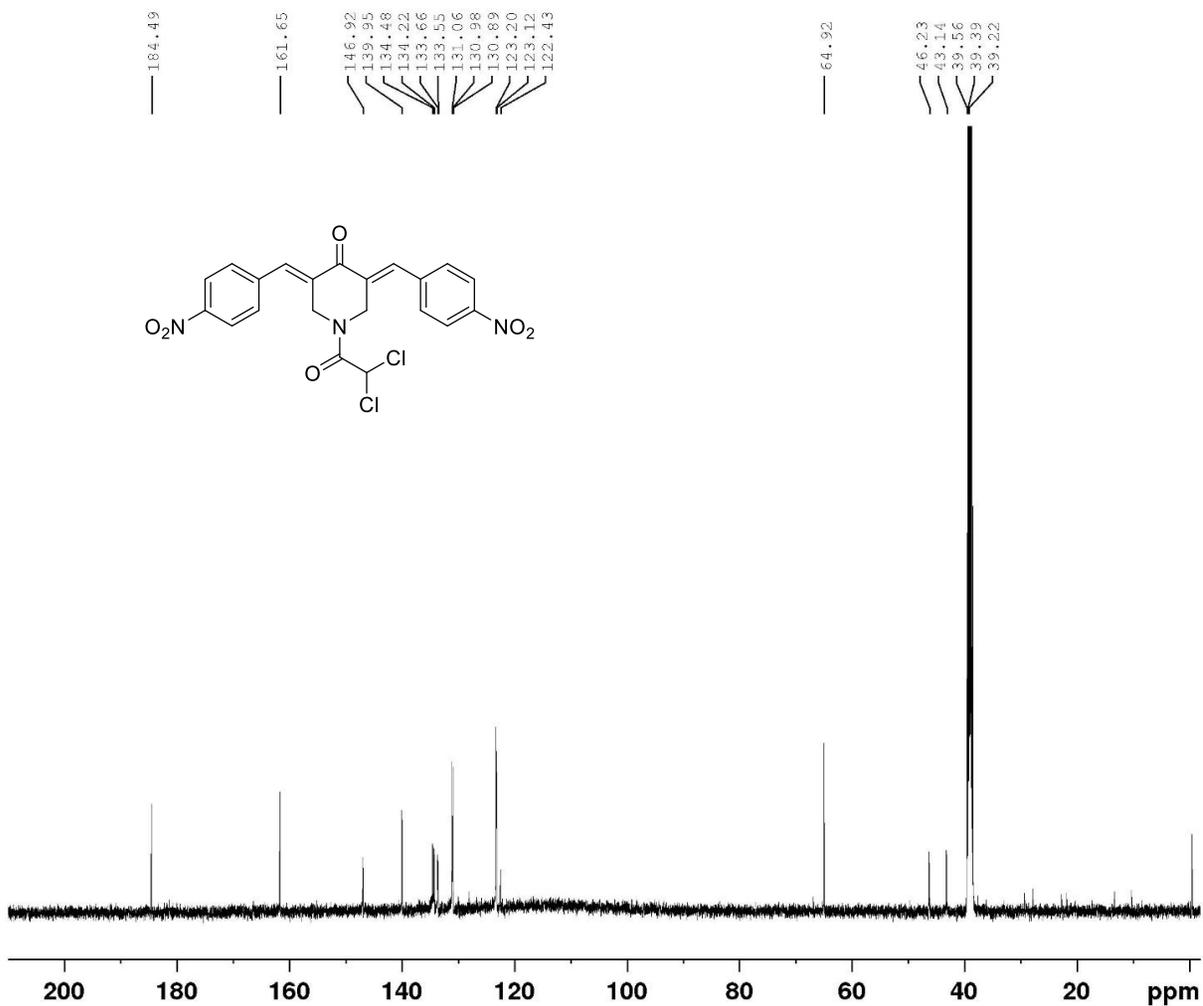
Current Data Parameters
 NAME Dec17-2018-Cary
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181217
 Time 15.52
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 128
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 101
 DW 50.000 usec
 DE 6.50 usec
 TE 301.9 K
 D1 1.00000000 sec
 ID0 1

----- CHANNEL f1 -----
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 8.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 32768
 SF 500.1300013 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR ((CD₃)₂SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-nitrobenzylidene)piperidin-4-one (**1k**)



Cu: 500.1320005 MHz, 13C
 NAL: 20181217
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20181217
 Time 17.42
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 2048
 DS 4
 SWH 29761.904 Hz
 FIDRES 0.454131 Hz
 AQ 1.1010048 sec
 RG 575
 DW 16.800 usec
 DE 6.50 usec
 TE 301.1 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====

SFO1 125.7703637 MHz
 NUC1 13C
 P1 12.00 usec
 PLW1 180.0000000 W

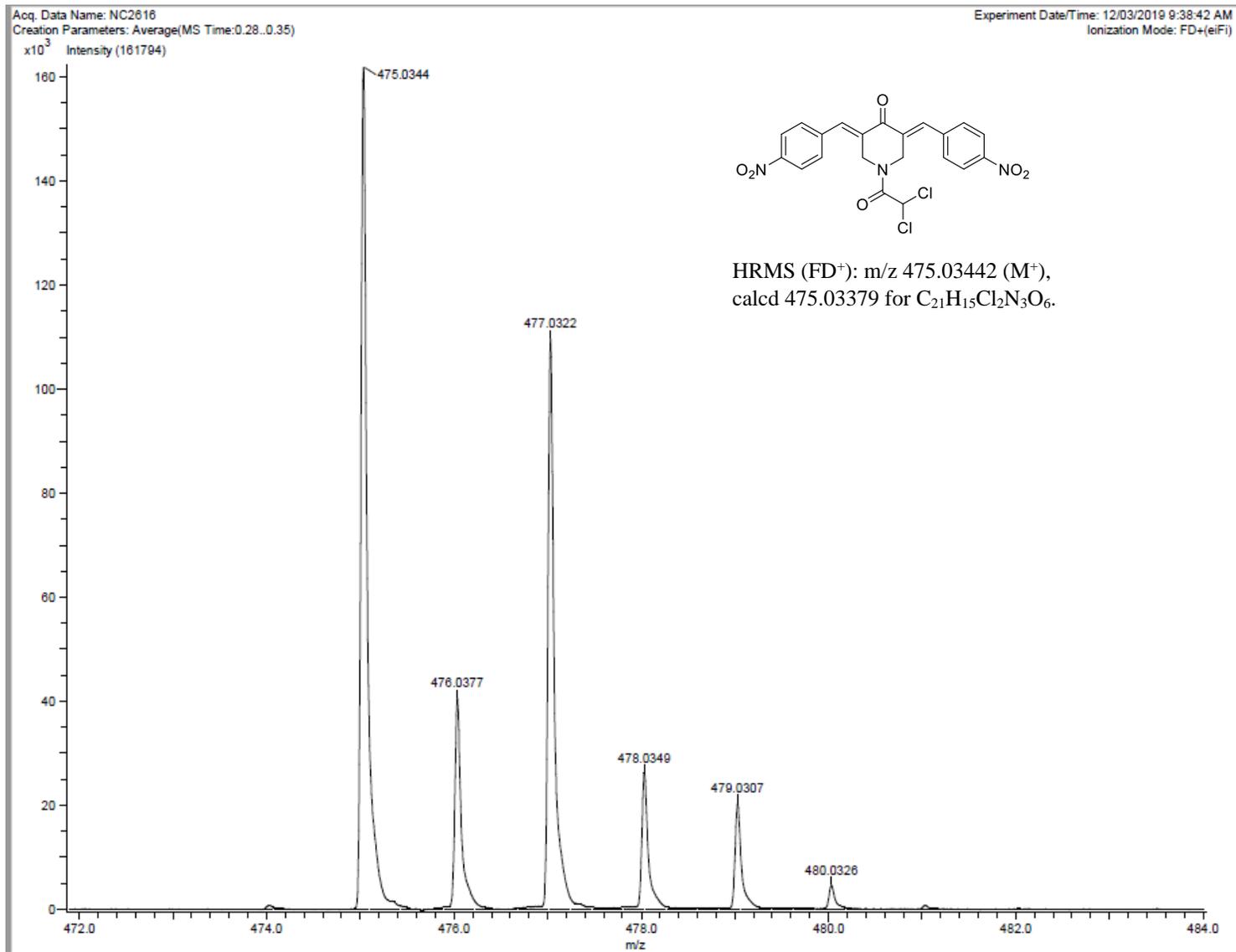
==== CHANNEL f2 =====

SFO2 500.1320005 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 10.00000000 W
 PLW12 0.10000000 W
 PLW13 0.06400000 W

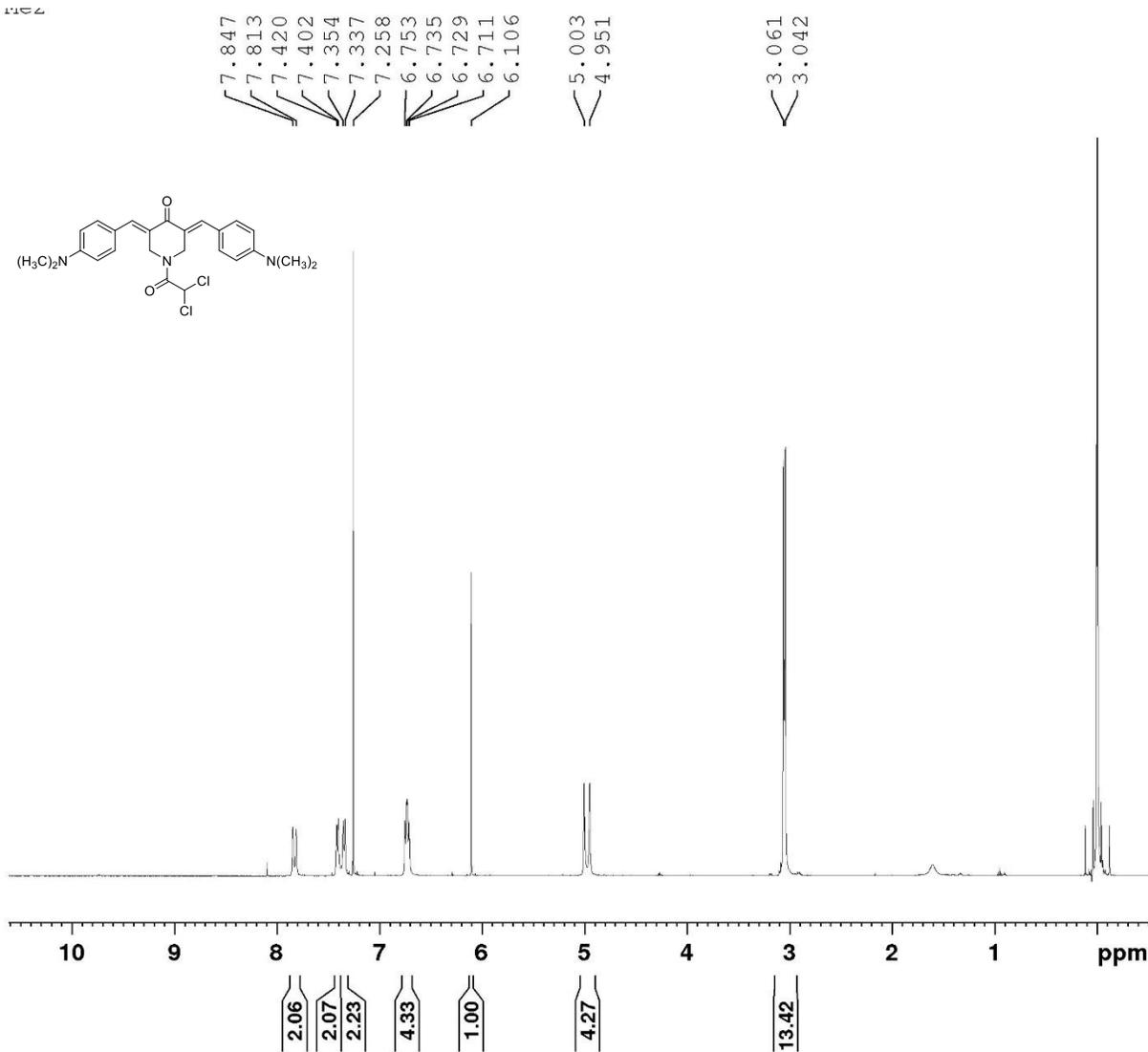
F2 - Processing parameters

SI 32768
 SF 125.7579217 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-nitrobenzylidene)piperidin-4-one (**1k**)



¹H NMR (CDCl₃) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-(dimethylamino)benzylidene)piperidin-4-one (11)



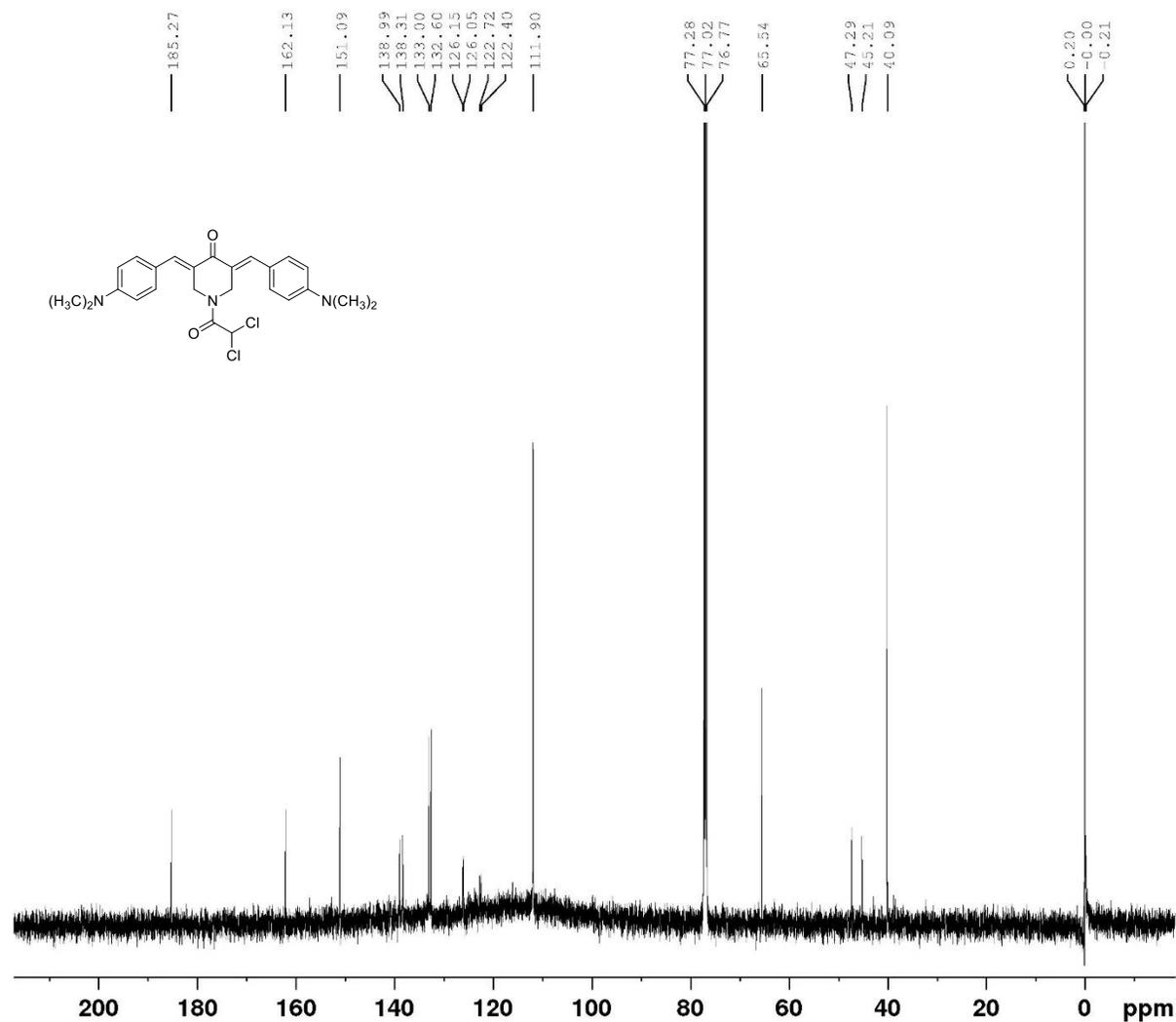
Current Data Parameters
 NAME 08-23-2018
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180823
 Time 20.12
 INSTRUM spect
 PROBHD 5 mm PATXI 1H/
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 90.5
 DW 50.000 usec
 DE 6.50 usec
 TE 299.7 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 SF01 500.1330885 MHz
 NUCL1 1H
 P1 8.00 usec
 PLW1 10.00000000 W

F2 - Processing parameters
 SI 32768
 SF 500.1300129 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

¹³C NMR (CDCl₃) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-(dimethylamino)benzylidene)piperidin-4-one (11)



```

Current Data Parameters
NAME          08-23-2018
EXPNO         6
PROCNO        1

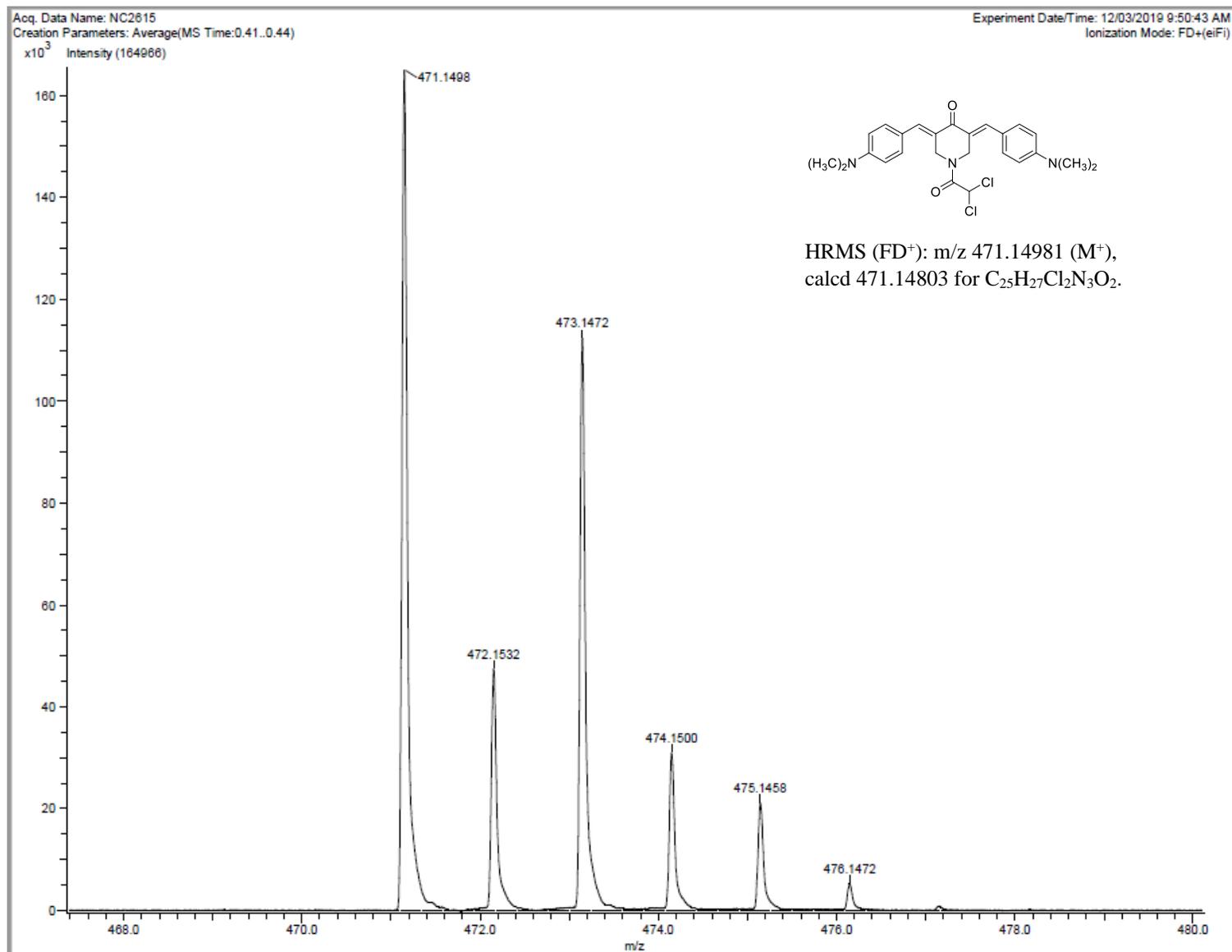
F2 - Acquisition Parameters
Date_         20180823
Time          22.52
INSTRUM       spect
PROBHD        5 mm PAIXI 1H/
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            3000
DS            4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG            575
DW            16.800 usec
DE            6.50 usec
TE            301.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

===== CHANNEL f1 =====
SFO1          125.7703637 MHz
NUC1           13C
P1            12.00 usec
PLW1          180.0000000 W

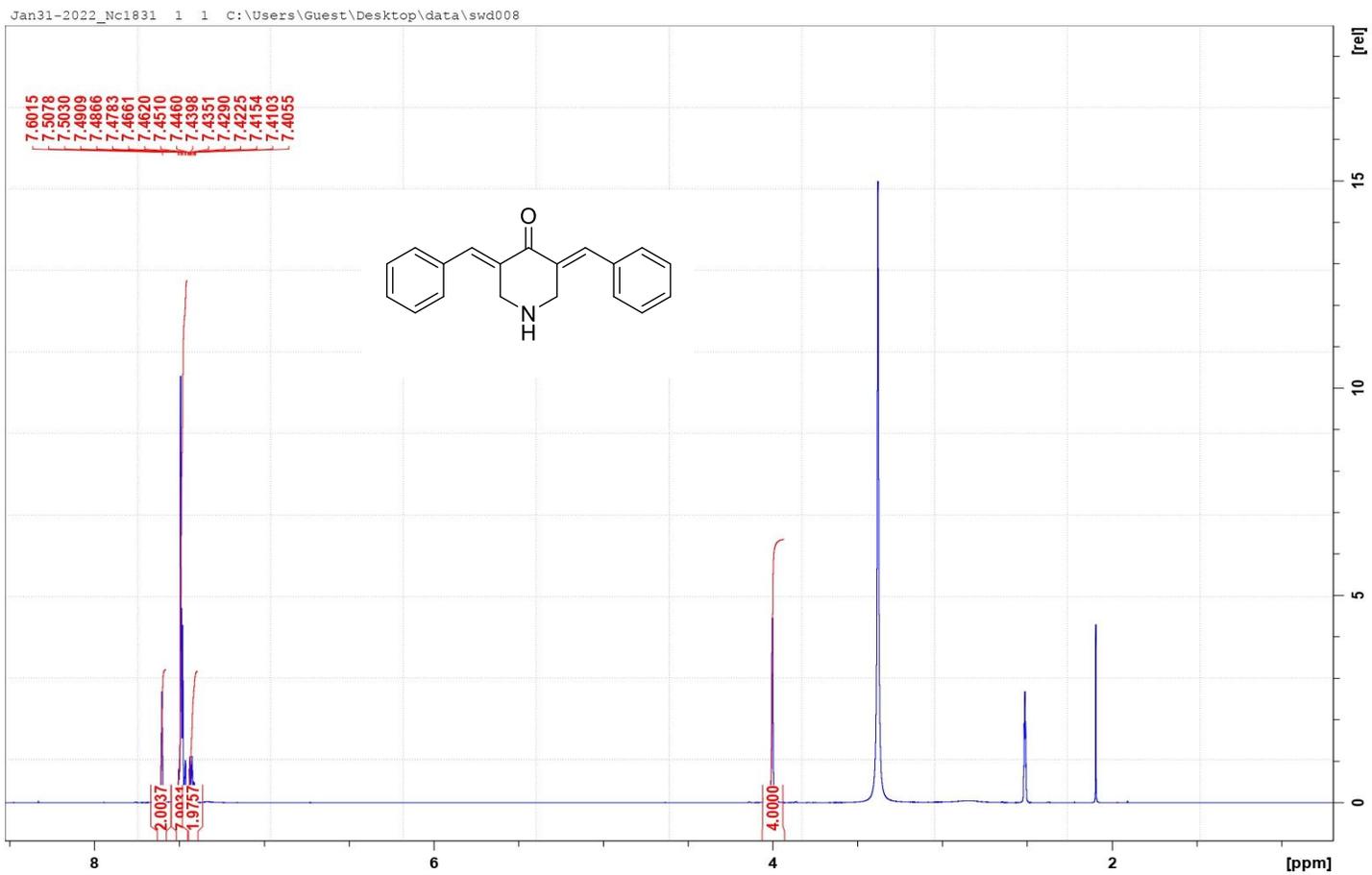
===== CHANNEL f2 =====
SFO2          500.1320005 MHz
NUC2           1H
CPDPRG[2]     waltz16
PCPD2         80.00 usec
PLW2          10.0000000 W
PLW12         0.1000000 W
PLW13         0.06400000 W

F2 - Processing parameters
SI            32768
SF            125.7577871 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-(dimethylamino)benzylidene)piperidin-4-one (**11**)

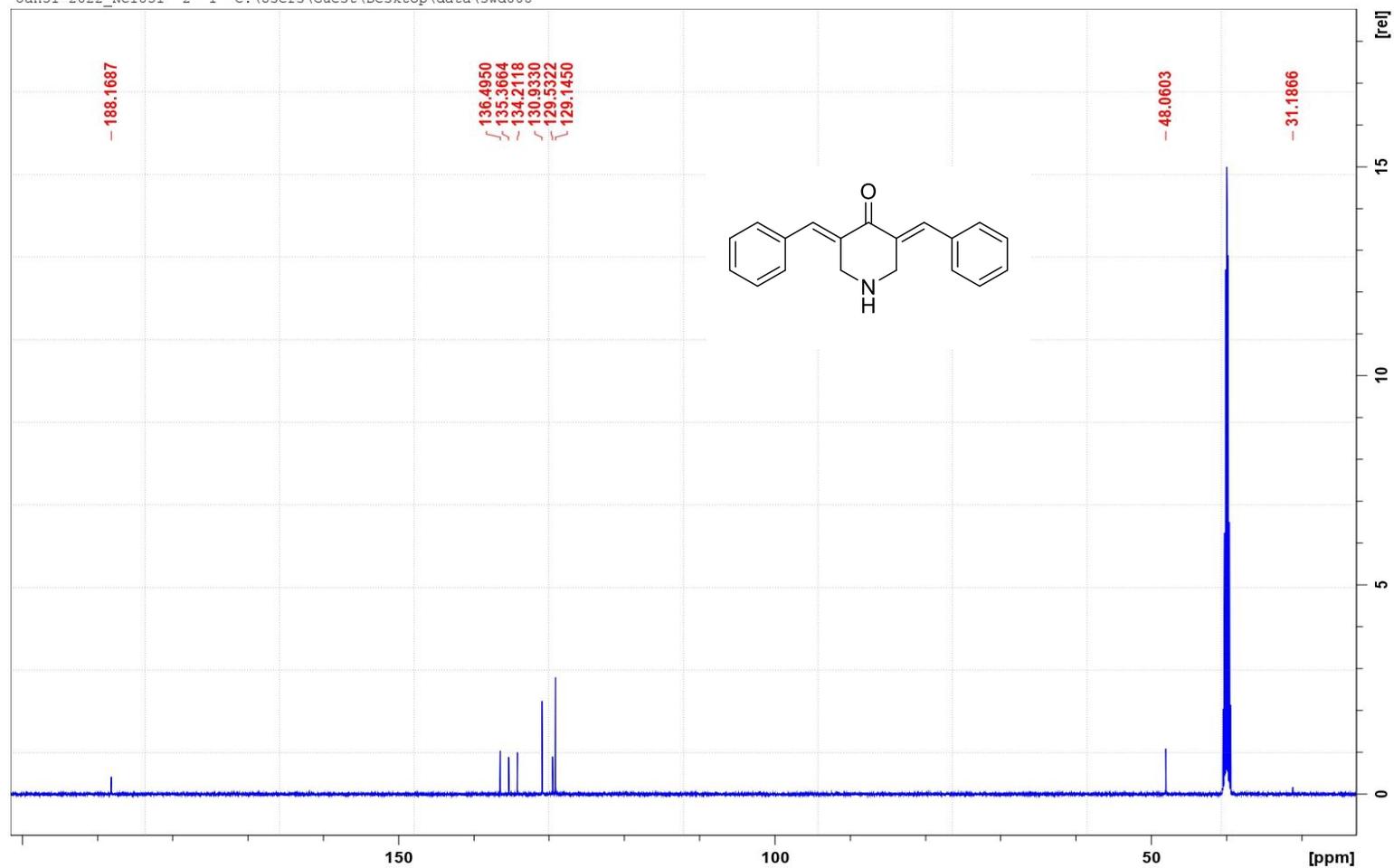


^1H NMR ($(\text{CD}_3)_2\text{SO}$) spectrum of 3,5-di((E)-benzylidene)piperidin-4-one (**2a**)



^{13}C NMR ($(\text{CD}_3)_2\text{SO}$) spectrum of 3,5-di((E)-benzylidene)piperidin-4-one (**2a**)

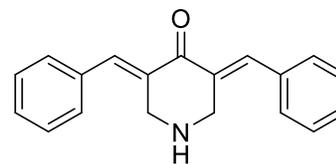
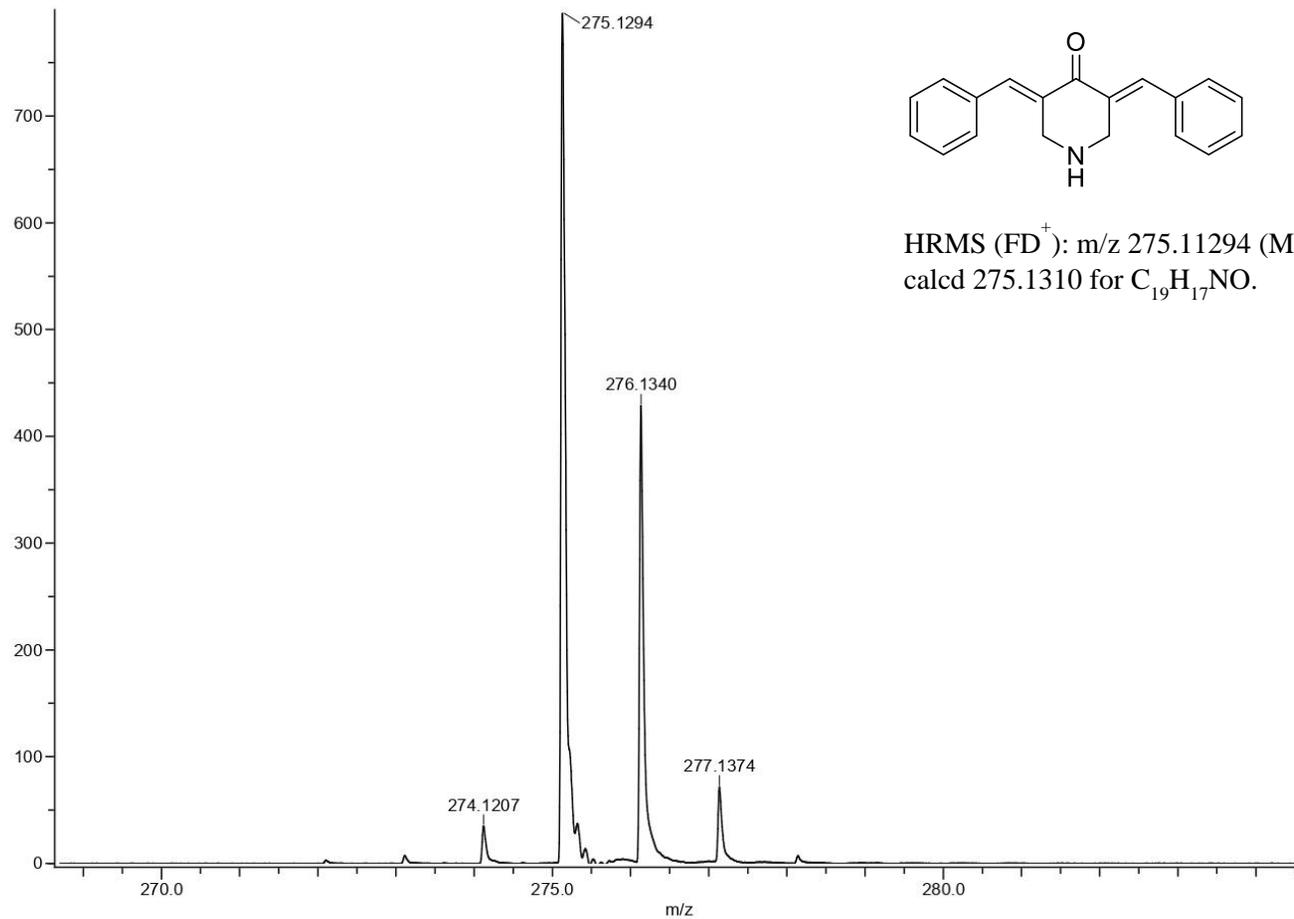
Jan31-2022_Nc1831 2 1 C:\Users\Guest\Desktop\data\swd008



Mass spectrum of 3,5-di((E)-benzylidene)piperidin-4-one (**2a**)

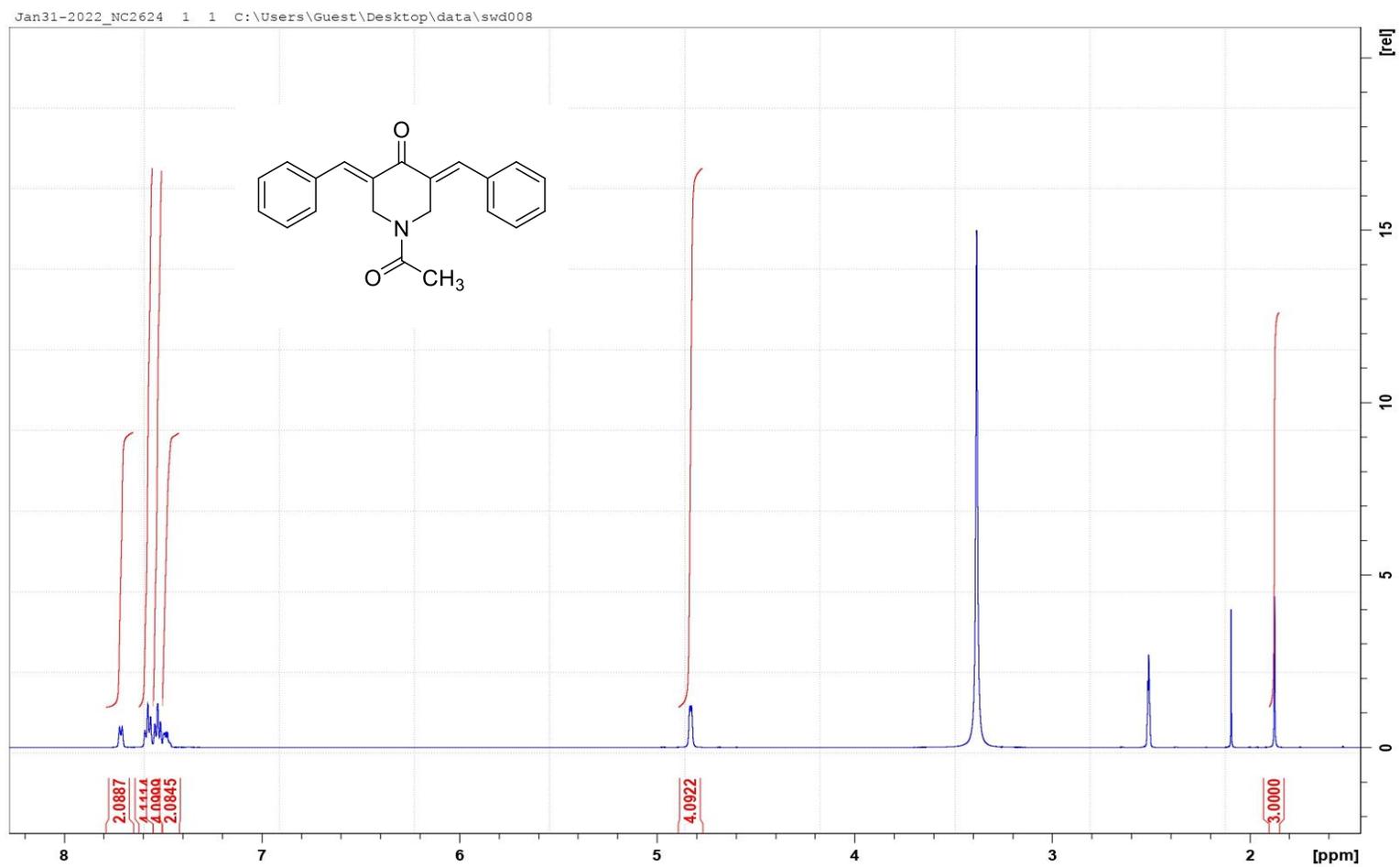
Acq. Data Name: NC1831
Creation Parameters: Average(MS Time:0.41..0.42)
x10³ Intensity (796251)

Experiment Date/Time: 2/1/2022 9:18:45 AM
Ionization Mode: FD+(eiFi)

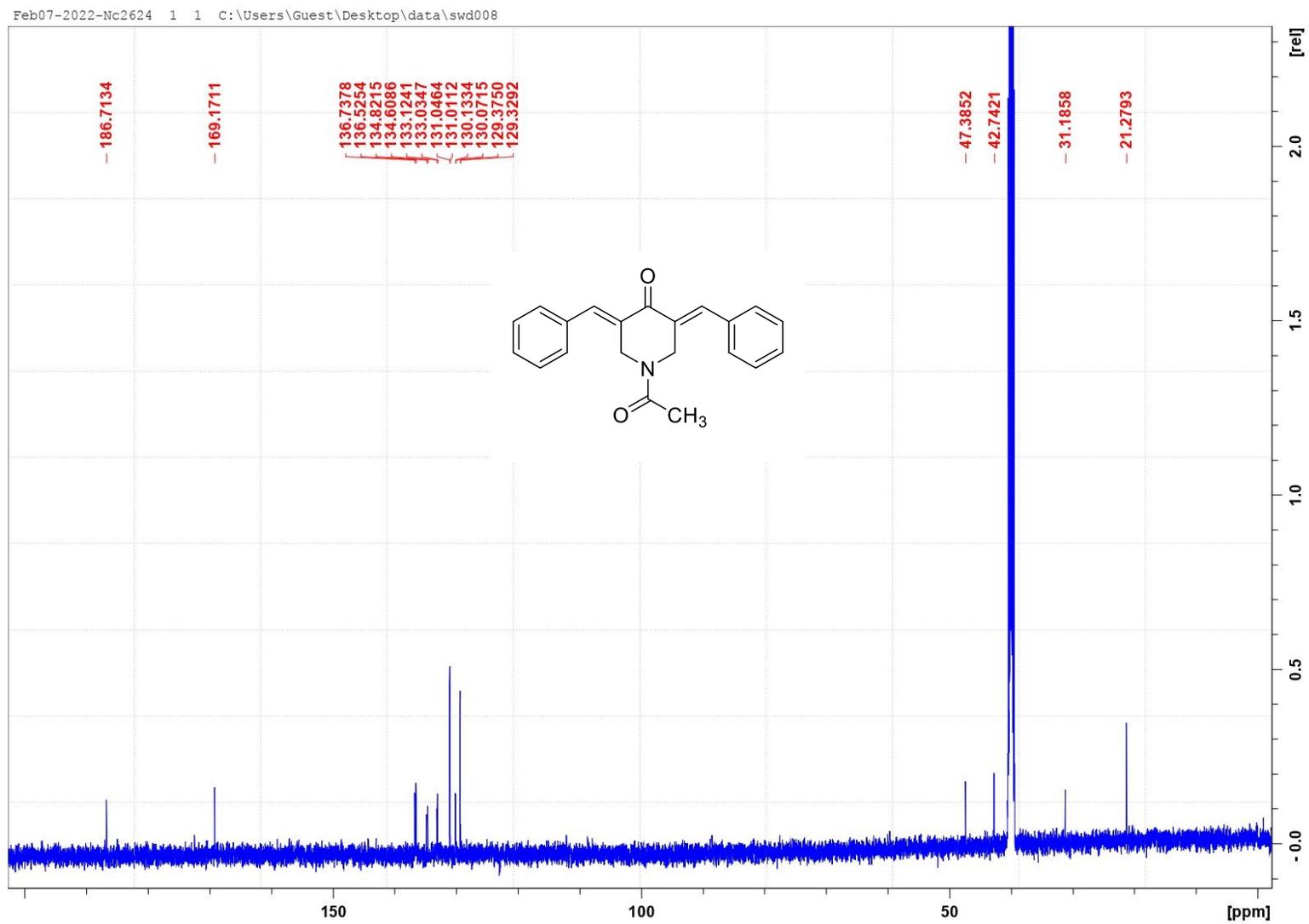


HRMS (FD⁺): m/z 275.11294 (M⁺),
calcd 275.1310 for C₁₉H₁₇NO.

^1H NMR ($(\text{CD}_3)_2\text{SO}$) of 1-acetyl-3,5-di((E)-benzylidene)piperidin-4-one (**2b**)



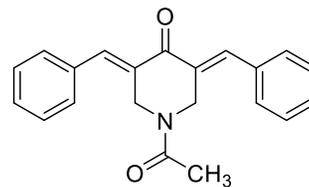
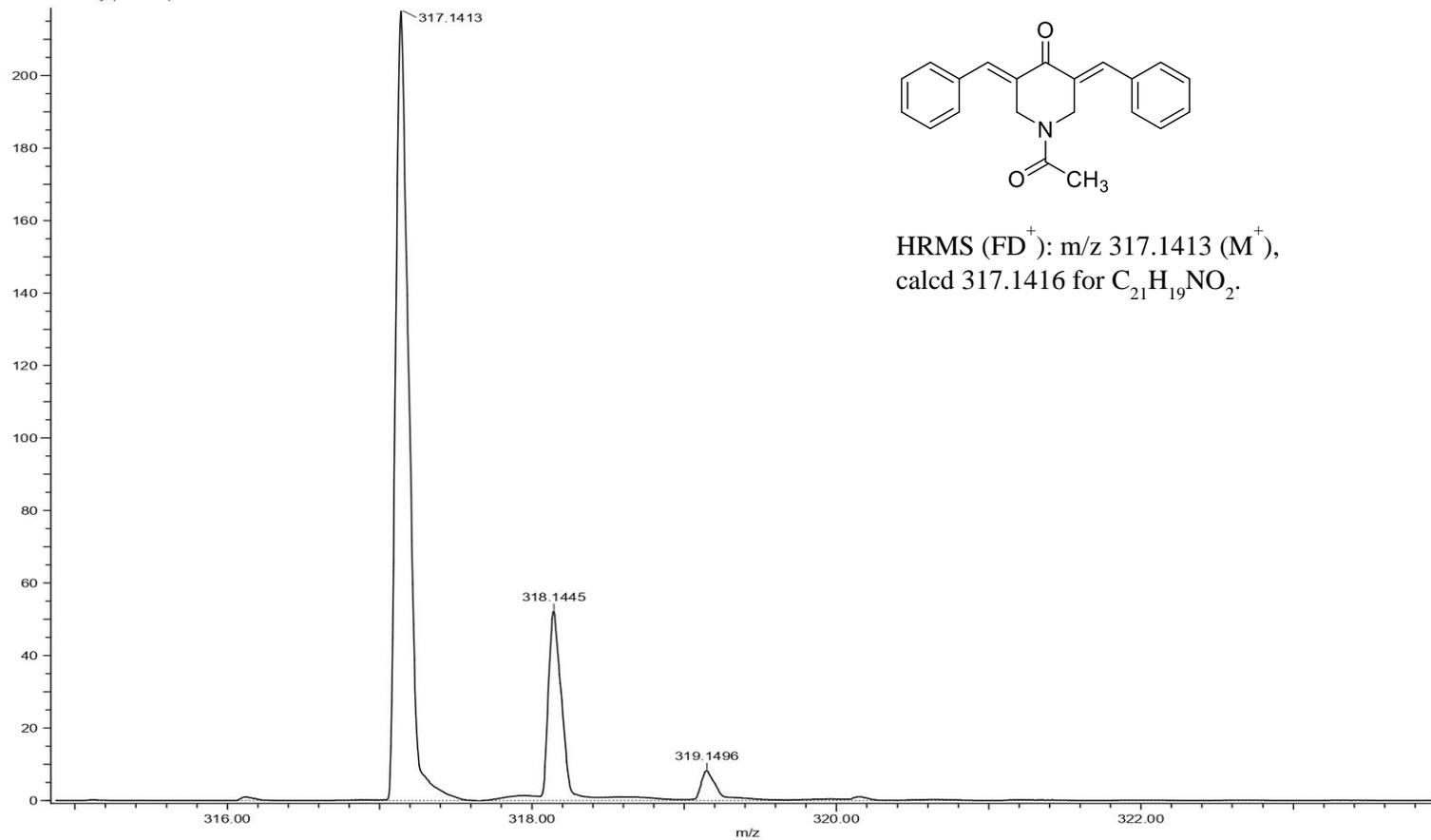
^{13}C NMR ($(\text{CD}_3)_2\text{SO}$) spectrum of 1-acetyl-3,5-di((E)-benzylidene)piperidin-4-one (**2b**)



Mass spectrum of 1-acetyl-3,5-di((E)-benzylidene)piperidin-4-one (**2b**)

Acq. Data Name: NC2624
Creation Parameters: Average(MS Time:0.20..0.33)
x10³ Intensity (217877)

Experiment Date/Time: 12/03/2019 8:56:24 AM
Ionization Mode: FD+(eIFi)



HRMS (FD⁺): m/z 317.1413 (M⁺),
calcd 317.1416 for C₂₁H₁₉NO₂.