SUPPLEMENTAL SECTION

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

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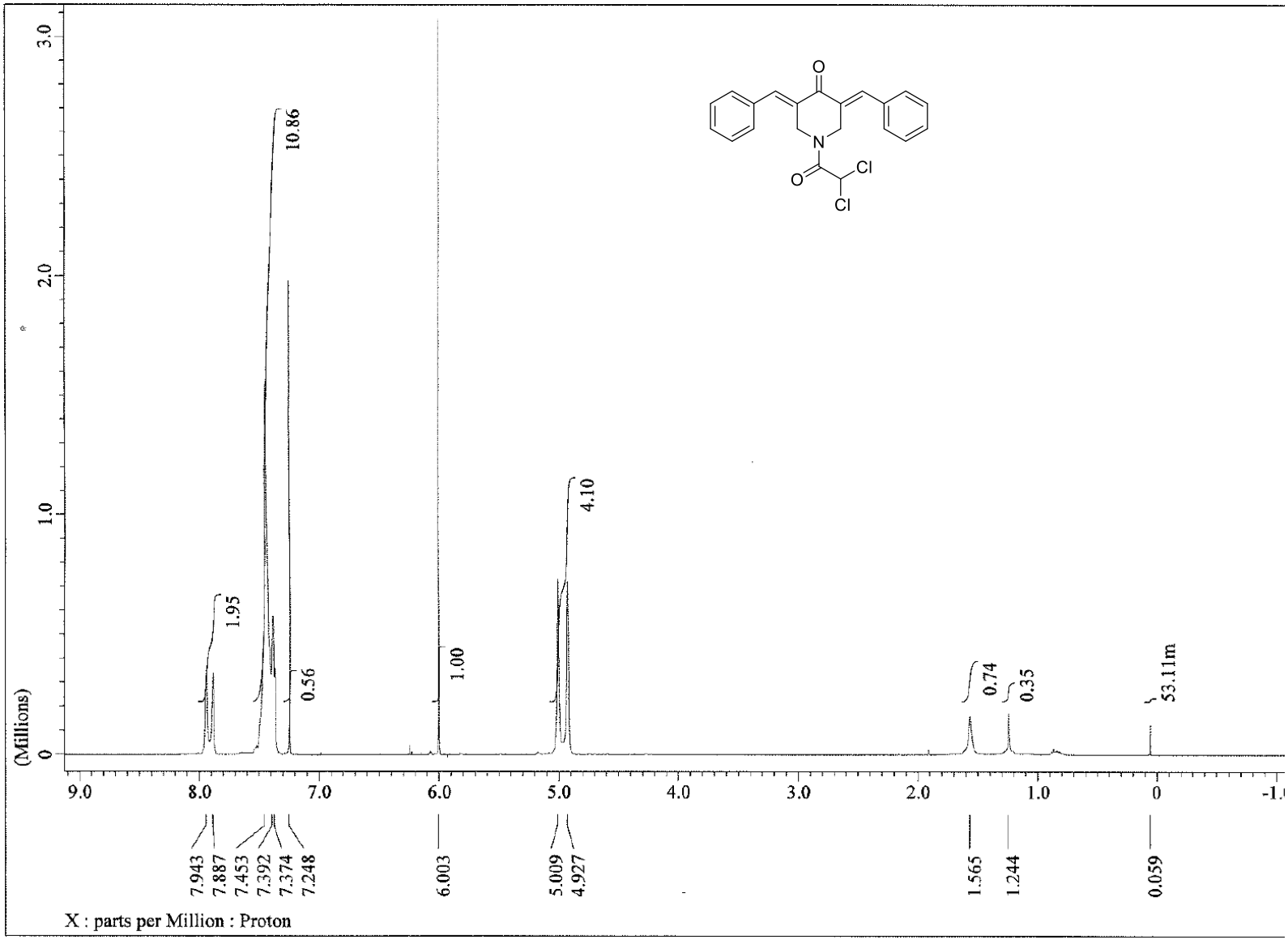
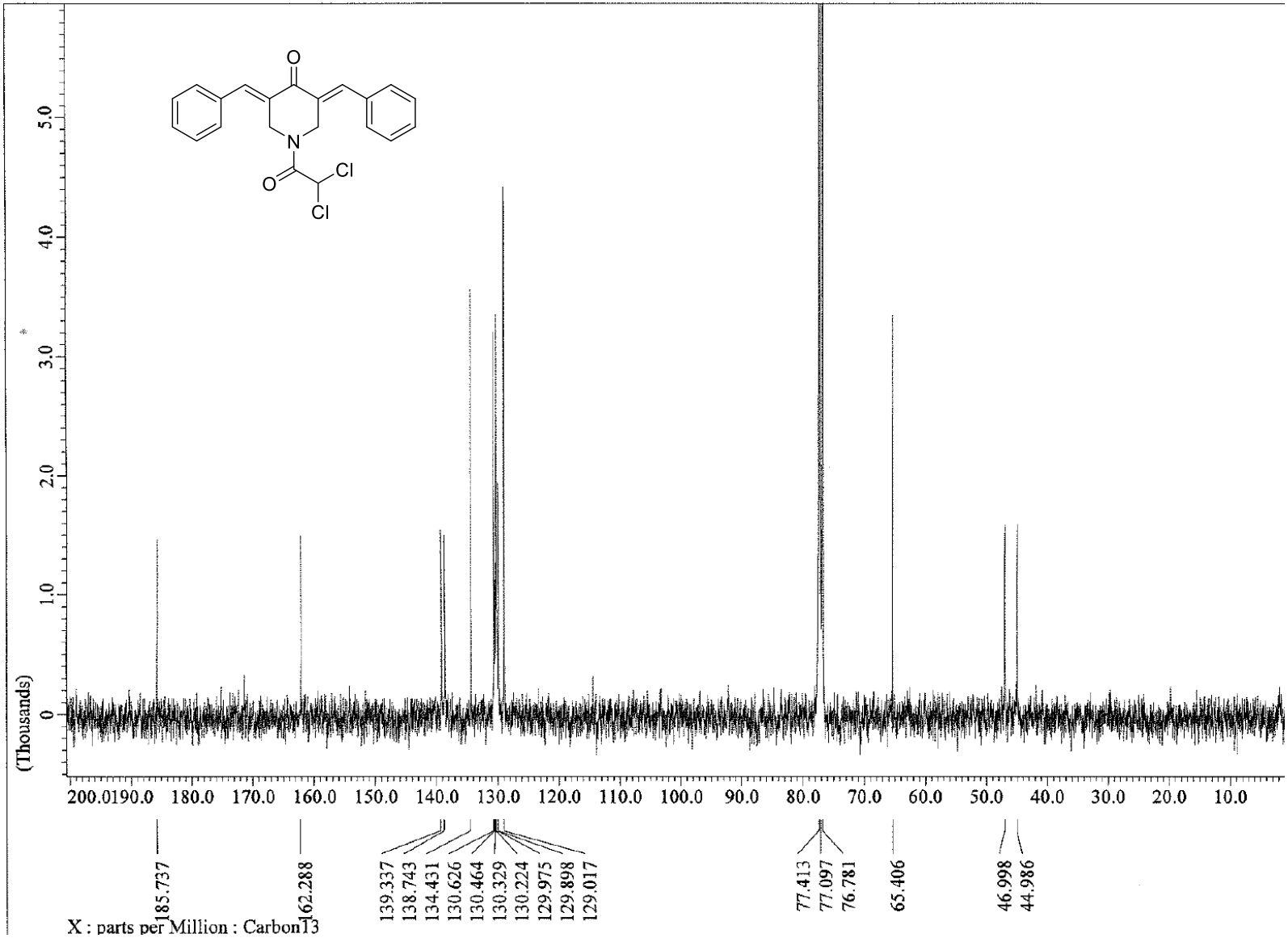
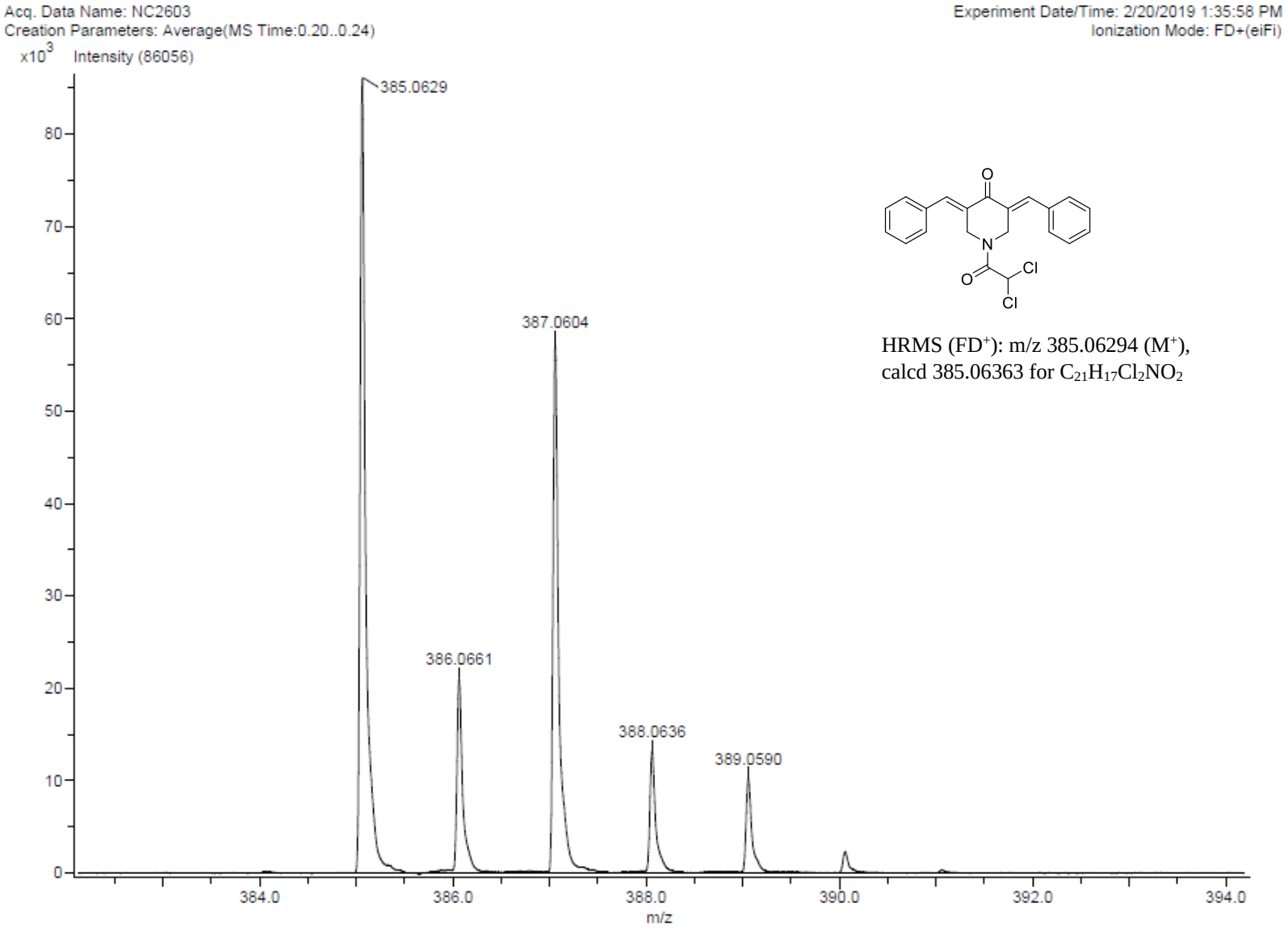
^{1}H NMR ($CDCl_3$) spectrum of (3*E*,5*E*)-3,5-dibenzylidene-1-(2,2-dichloroacetyl)piperidin-4-one (**1a**)



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

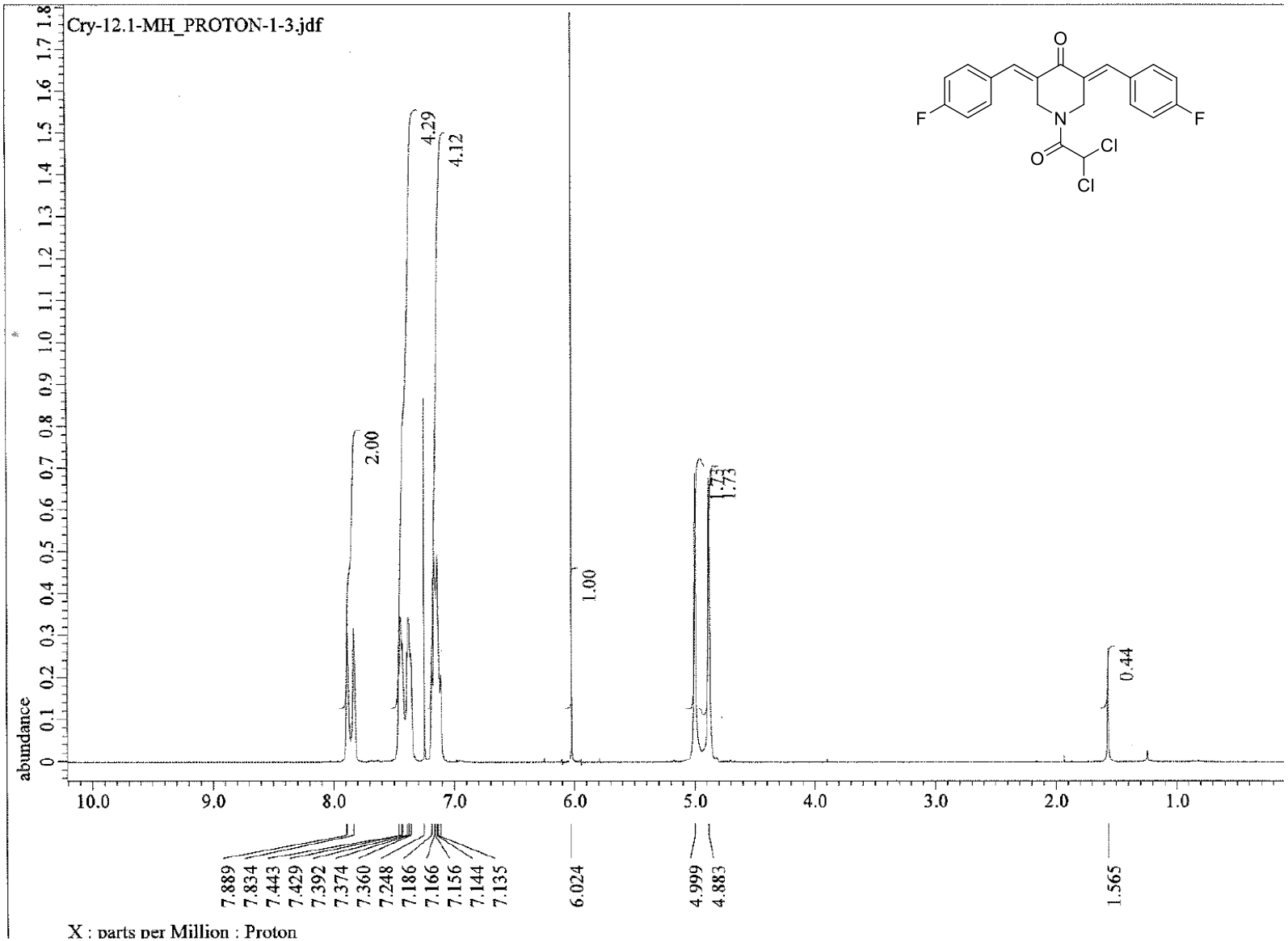


Mass spectrum of (3*E*,5*E*)-3,5-dibenzylidene-1-(2,2-dichloroacetyl)piperidin-4-one (**1a**)

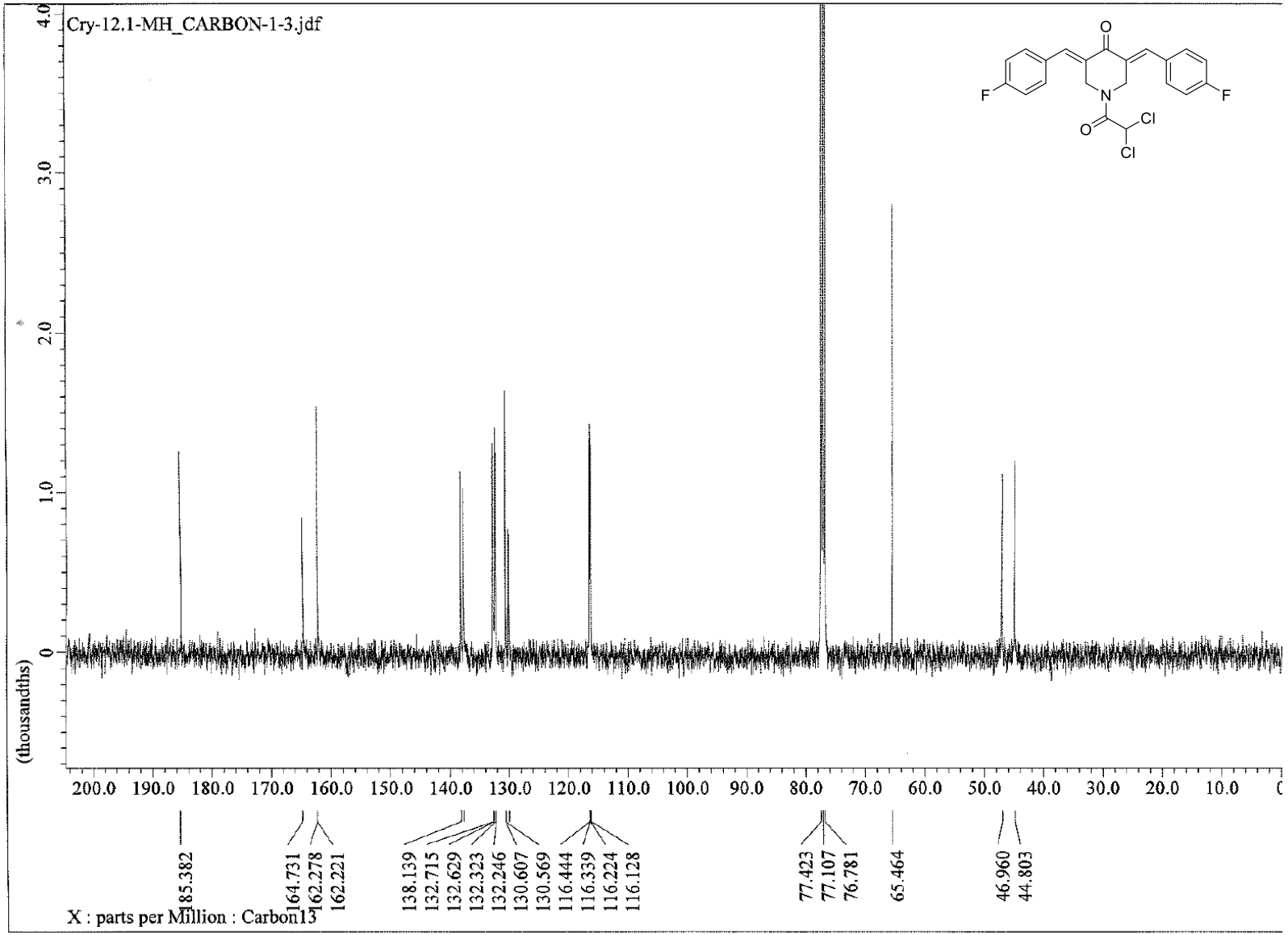


HRMS (FD$^+$): m/z 385.06294 (M^+),
calcd 385.06363 for $C_{21}H_{17}Cl_2NO_2$

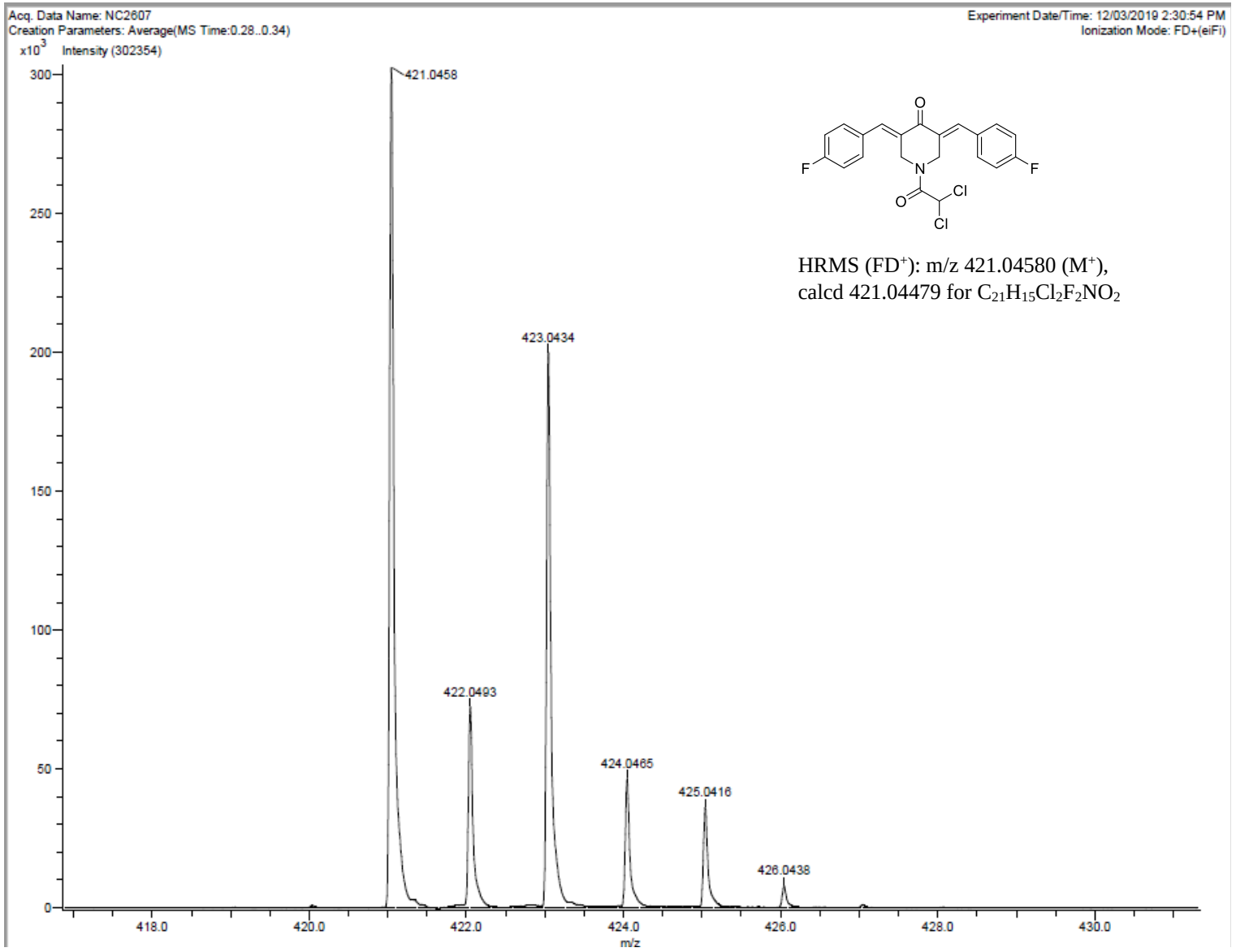
^{1}H NMR ($CDCl_3$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-fluorobenzylidene)piperidin-4-one (**1b**)



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



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



HRMS (FD^+): m/z 421.04580 (M^+),
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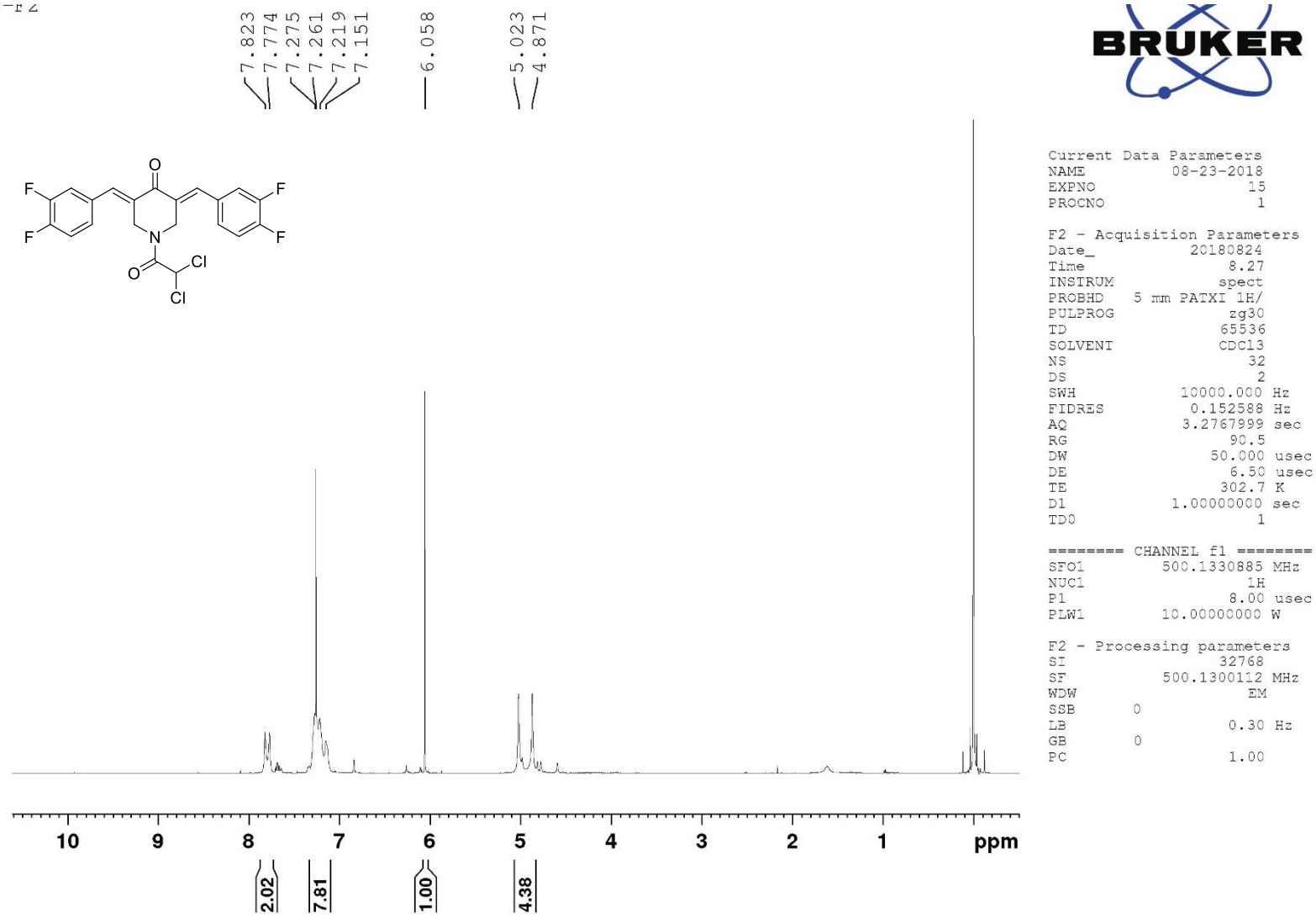
^{1}H NMR ($CDCl_3$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-difluorobenzylidene)piperidin-4-one (**1c**)

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DS                     2
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FIDRES          0.152588 Hz
AQ             3.2767999 sec
RG                  90.5
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TE                302.7 K
D1           1.00000000 sec
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NUC1                  1H
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PLW1        10.00000000 W

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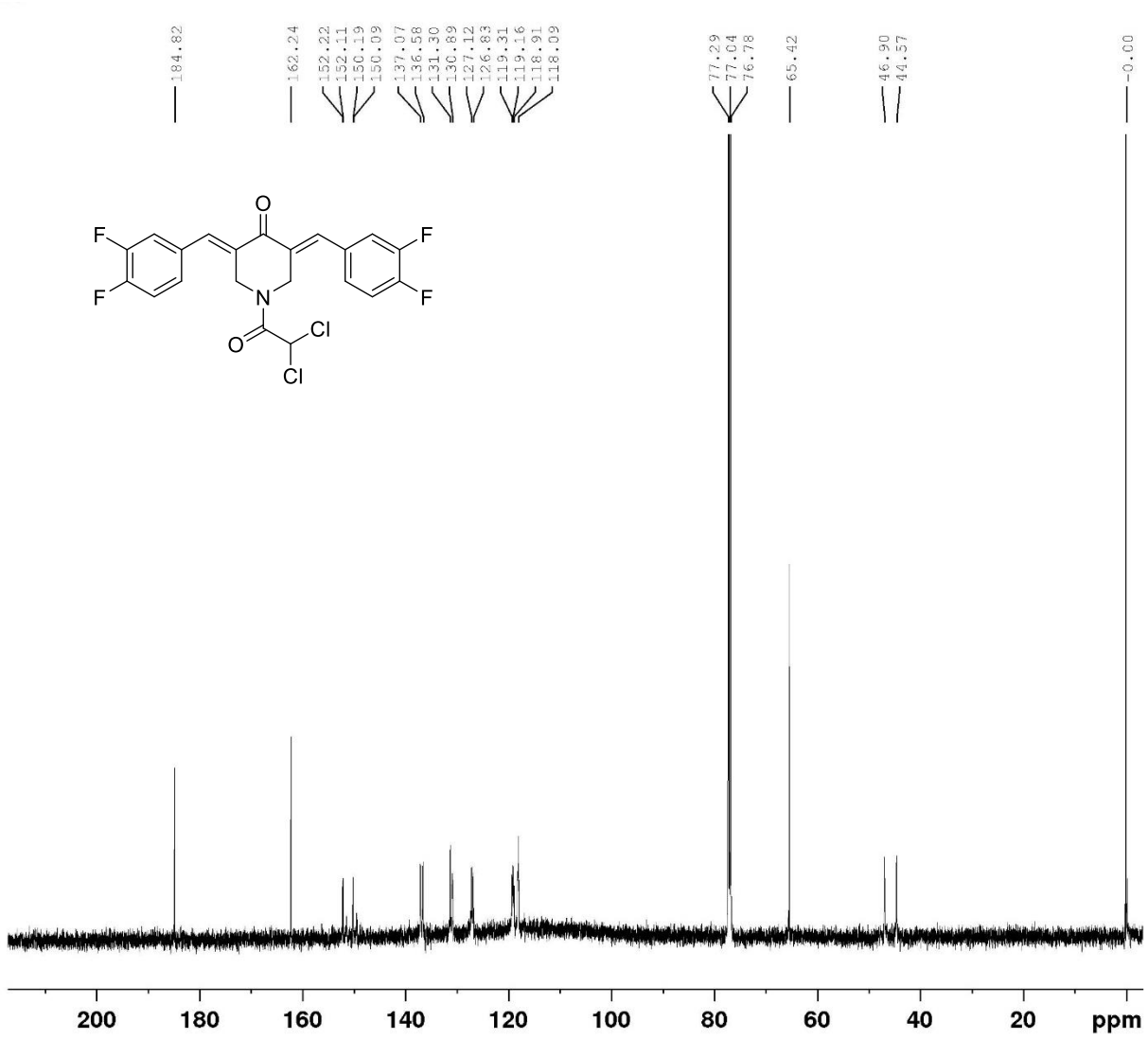
^{13}C NMR ($CDCl_3$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-difluorobenzylidene)piperidin-4-one (**1c**)



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DS                             4
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RG                           575
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F2 - Processing parameters
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WDW                           EM
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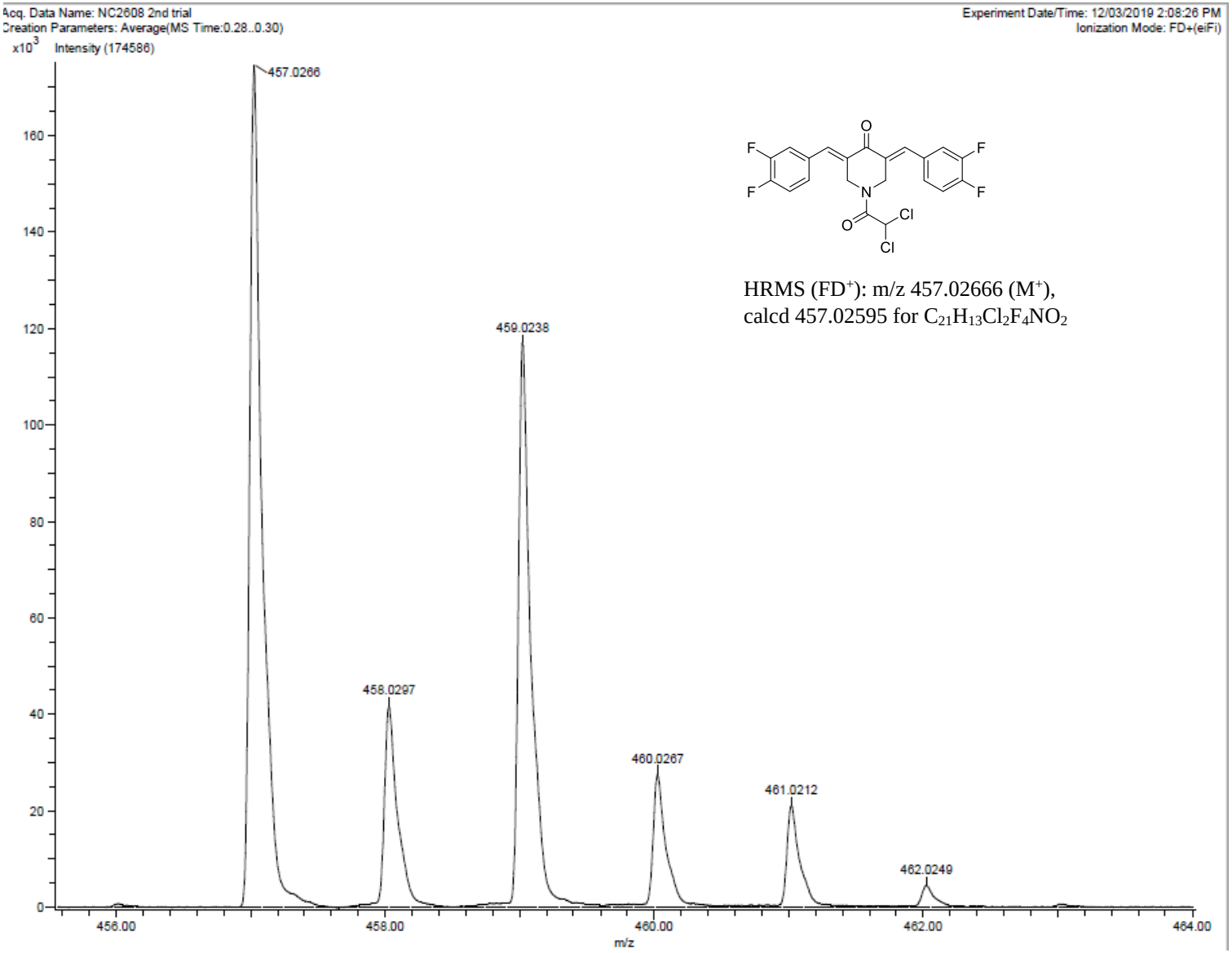
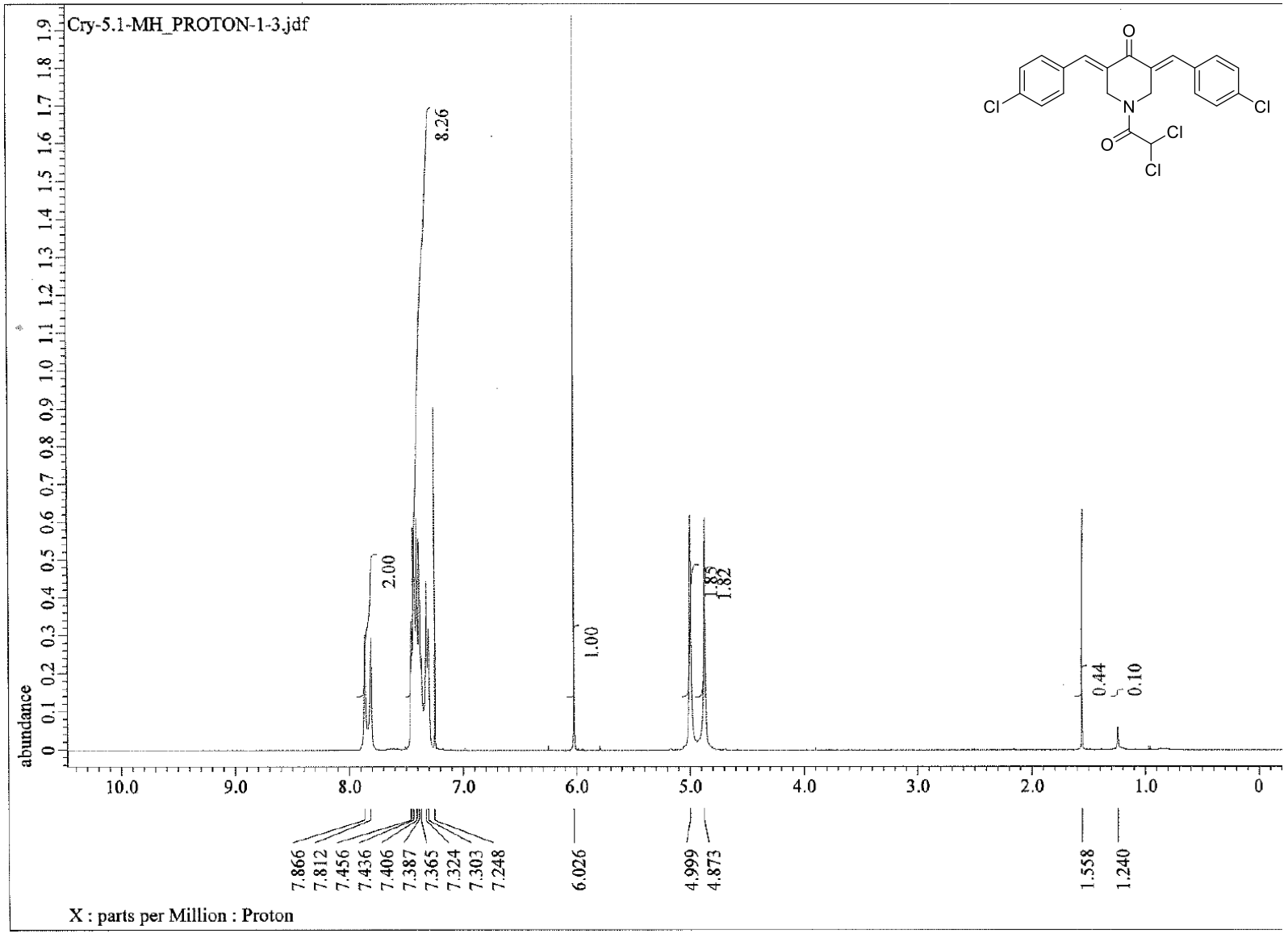
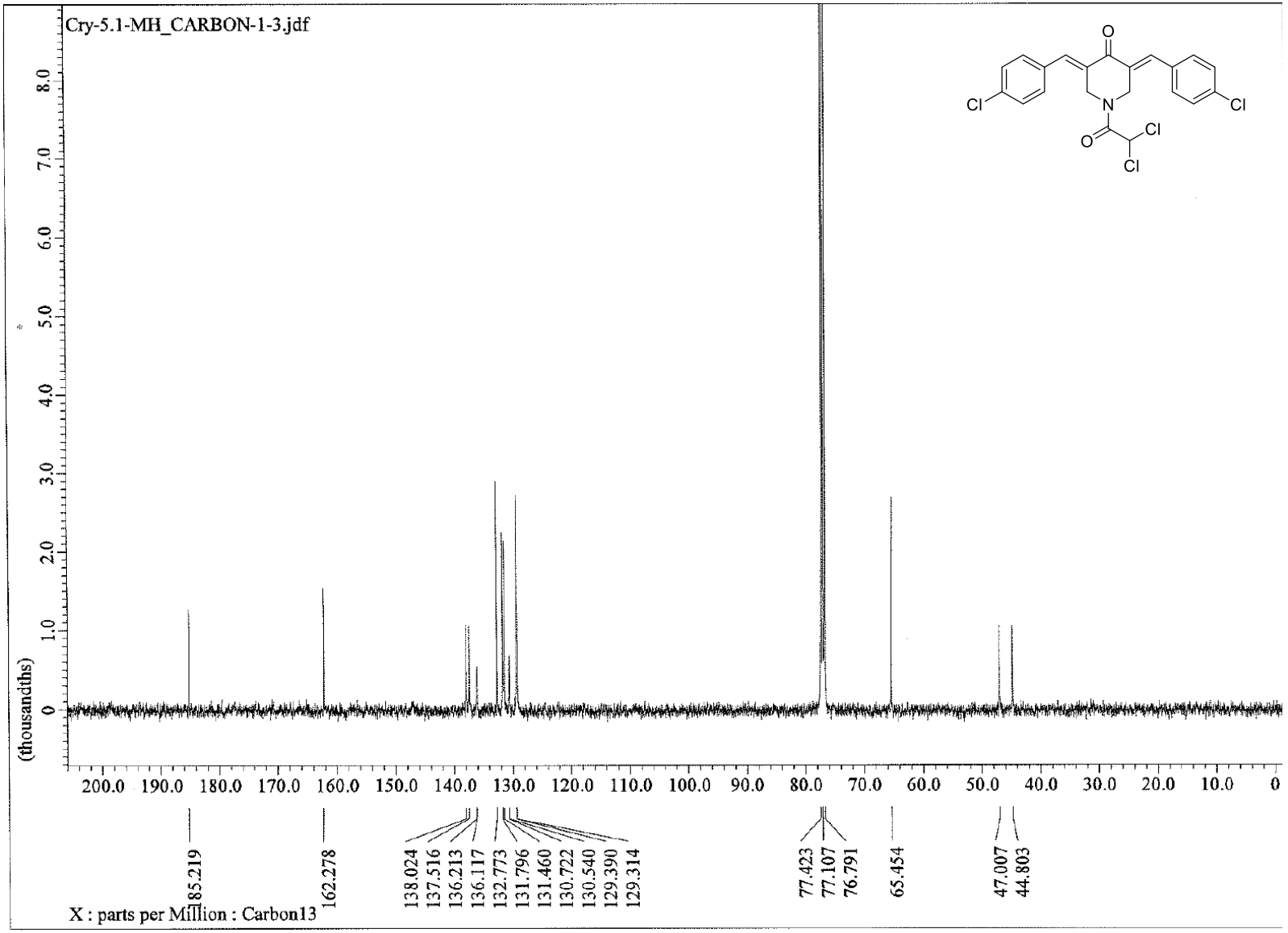
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-difluorobenzylidene)piperidin-4-one (**1c**)



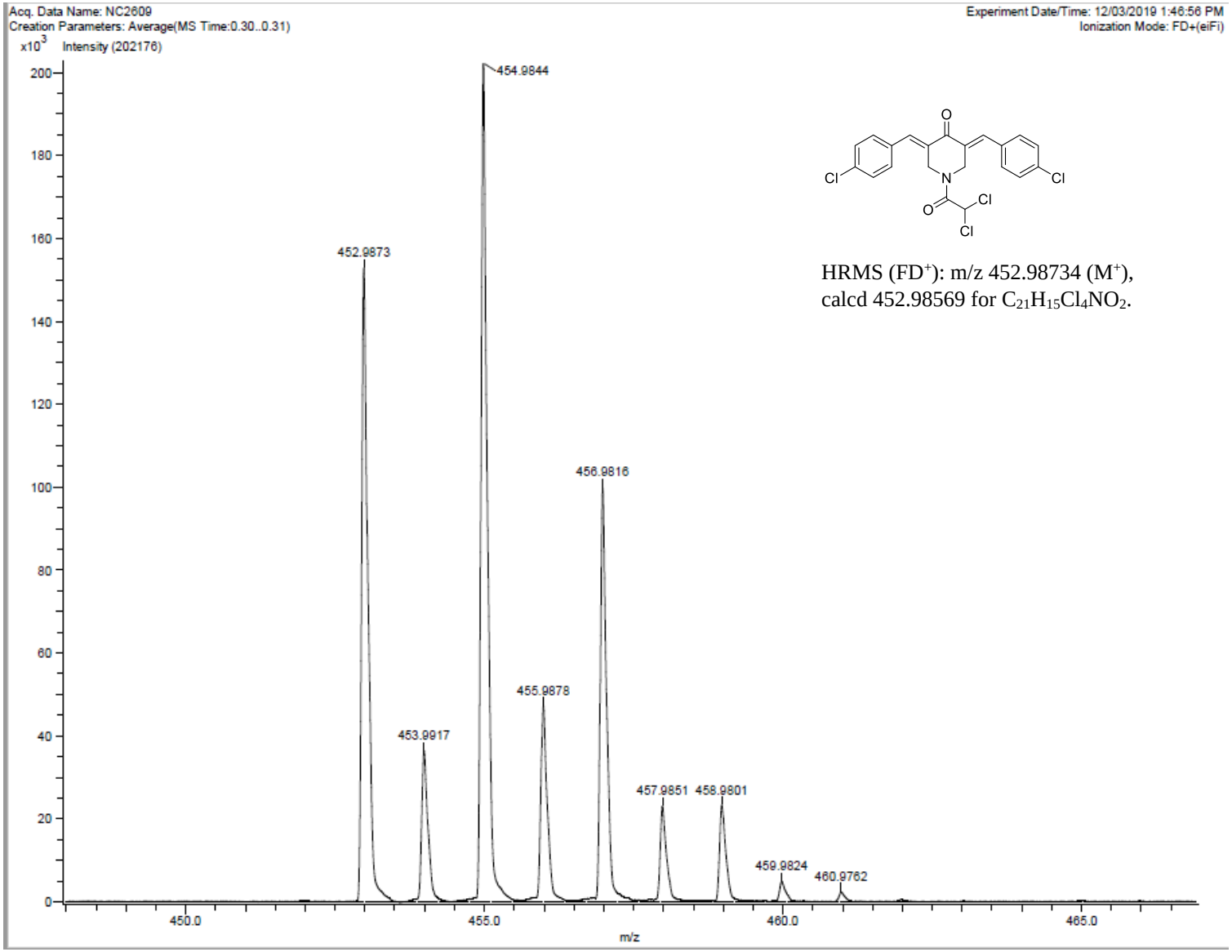
^{1}H NMR ($CDCl_3$) spectrum of 3,5-bis((*E*)-4-chlorobenzylidene)-1-(2,2-dichloroacetyl)piperidin-4-one (**1d**)



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

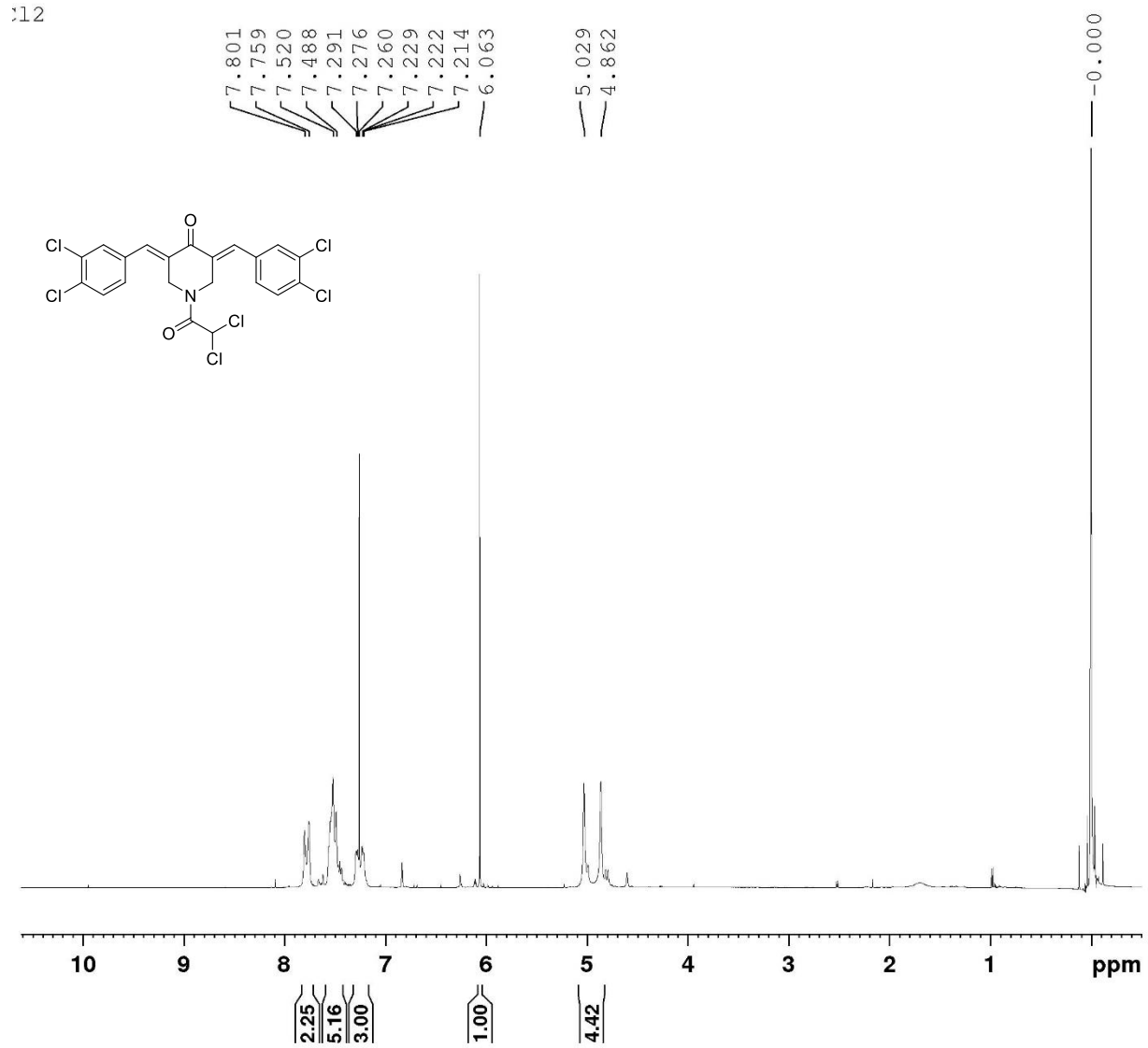


Mass spectrum of 3,5-bis((*E*)-4-chlorobenzylidene)-1-(2,2-dichloroacetyl)piperidin-4-one (**1d**)



HRMS (FD^+): m/z 452.98734 (M^+),
calcd 452.98569 for $C_{21}H_{15}Cl_4NO_2$.

^{1}H NMR ($CDCl_3$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-dichlorobenzylidene)piperidin-4-one (**1e**)

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RG                 80.6
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TE                302.5 K
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F2 - Processing parameters
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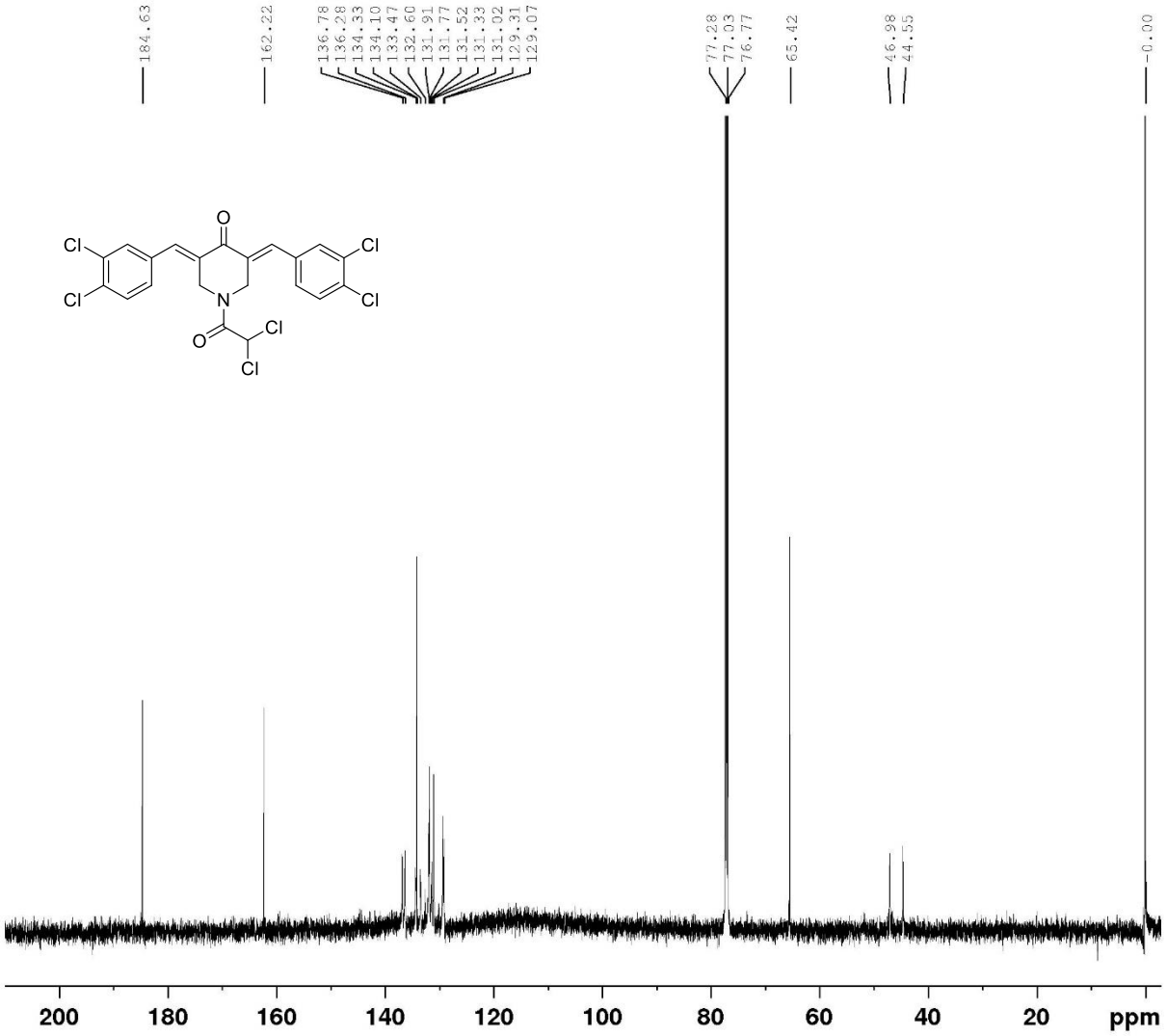
^{13}C NMR ($CDCl_3$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-dichlorobenzylidene)piperidin-4-one (**1e**)

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NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
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RG                  575
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======== CHANNEL f2 ========
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PLW12        0.10000000 W
PLW13        0.06400000 W

F2 - Processing parameters
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WDW                EM
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LB                1.00 Hz
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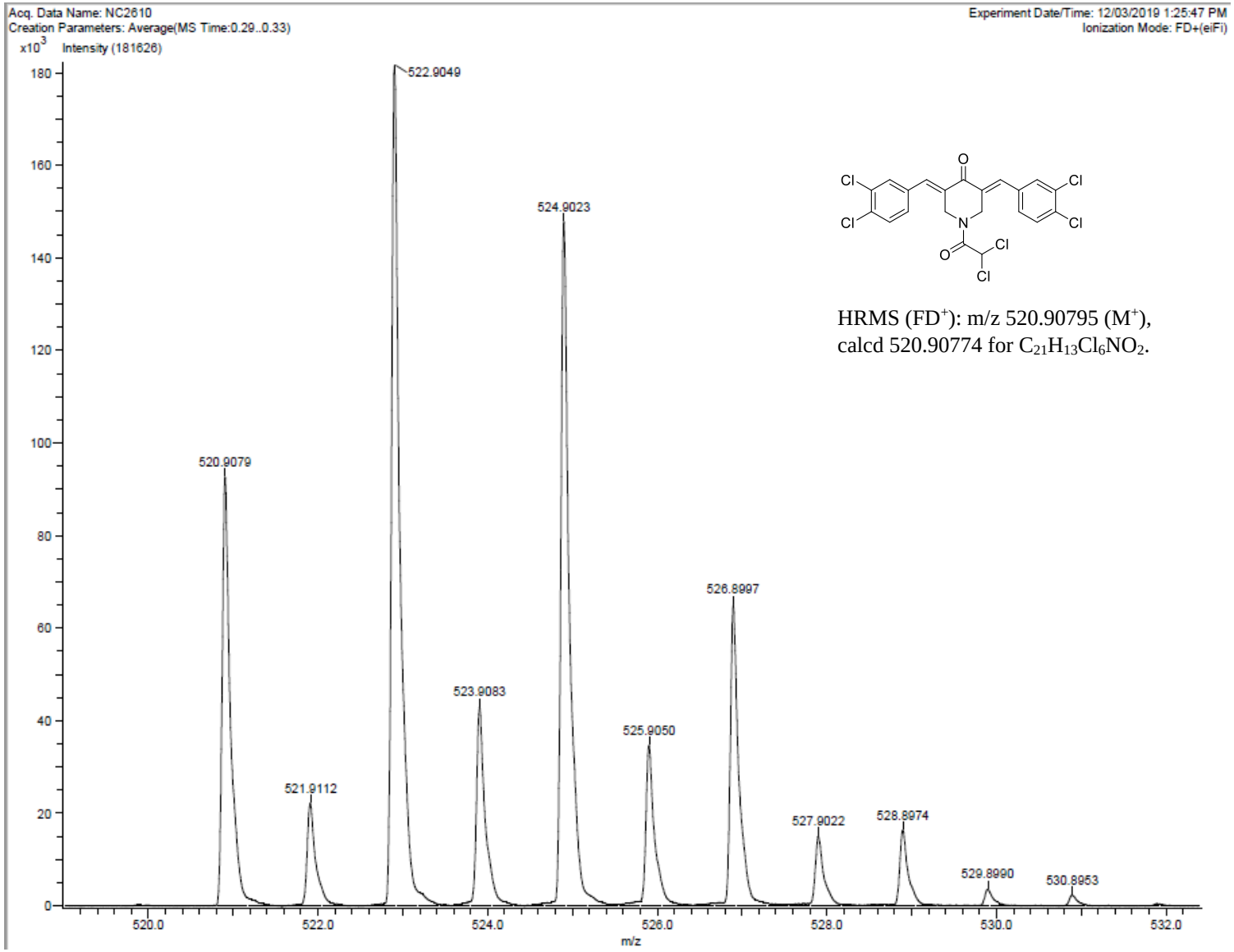
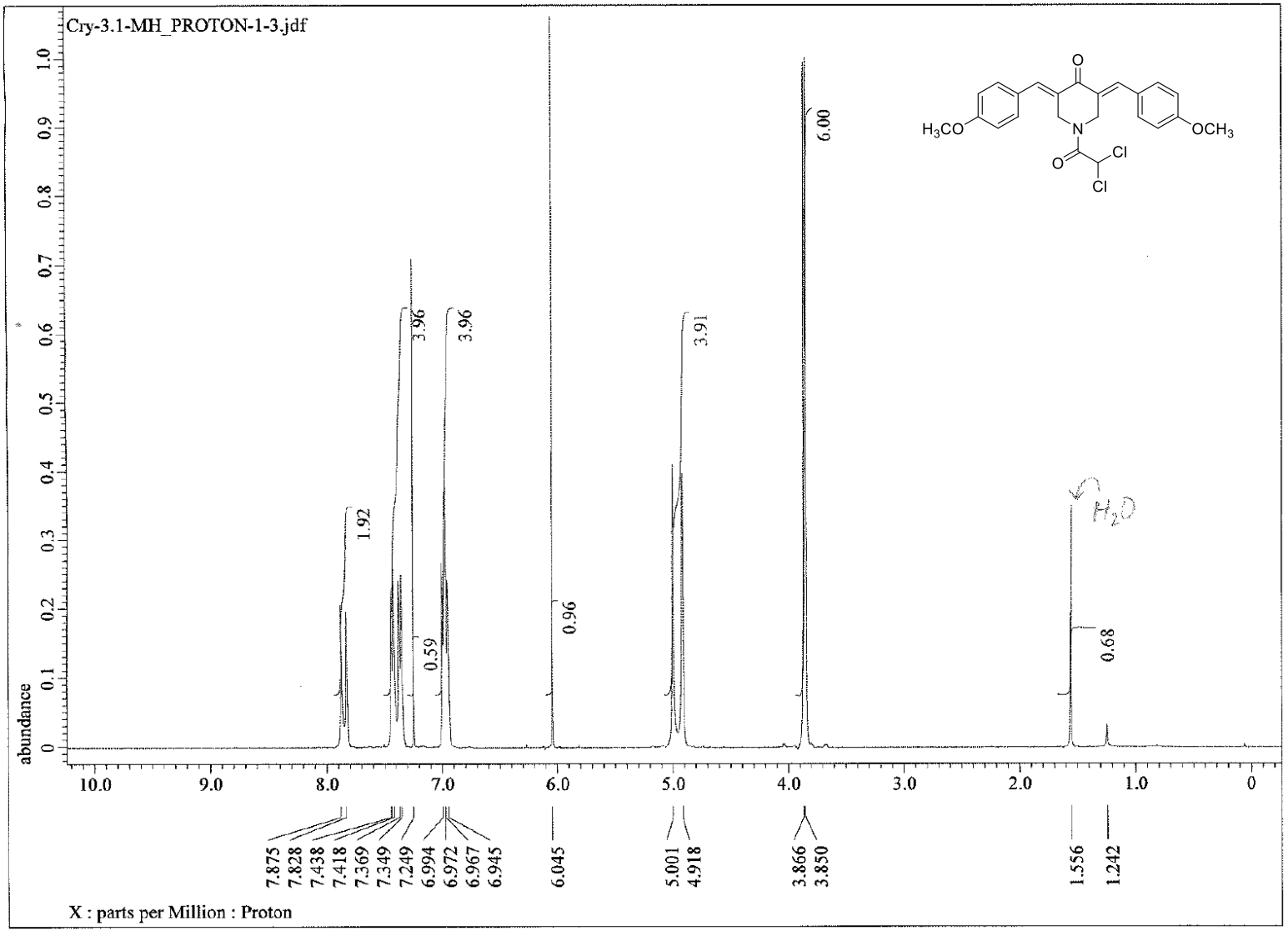
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-dichlorobenzylidene)piperidin-4-one (**1e**)

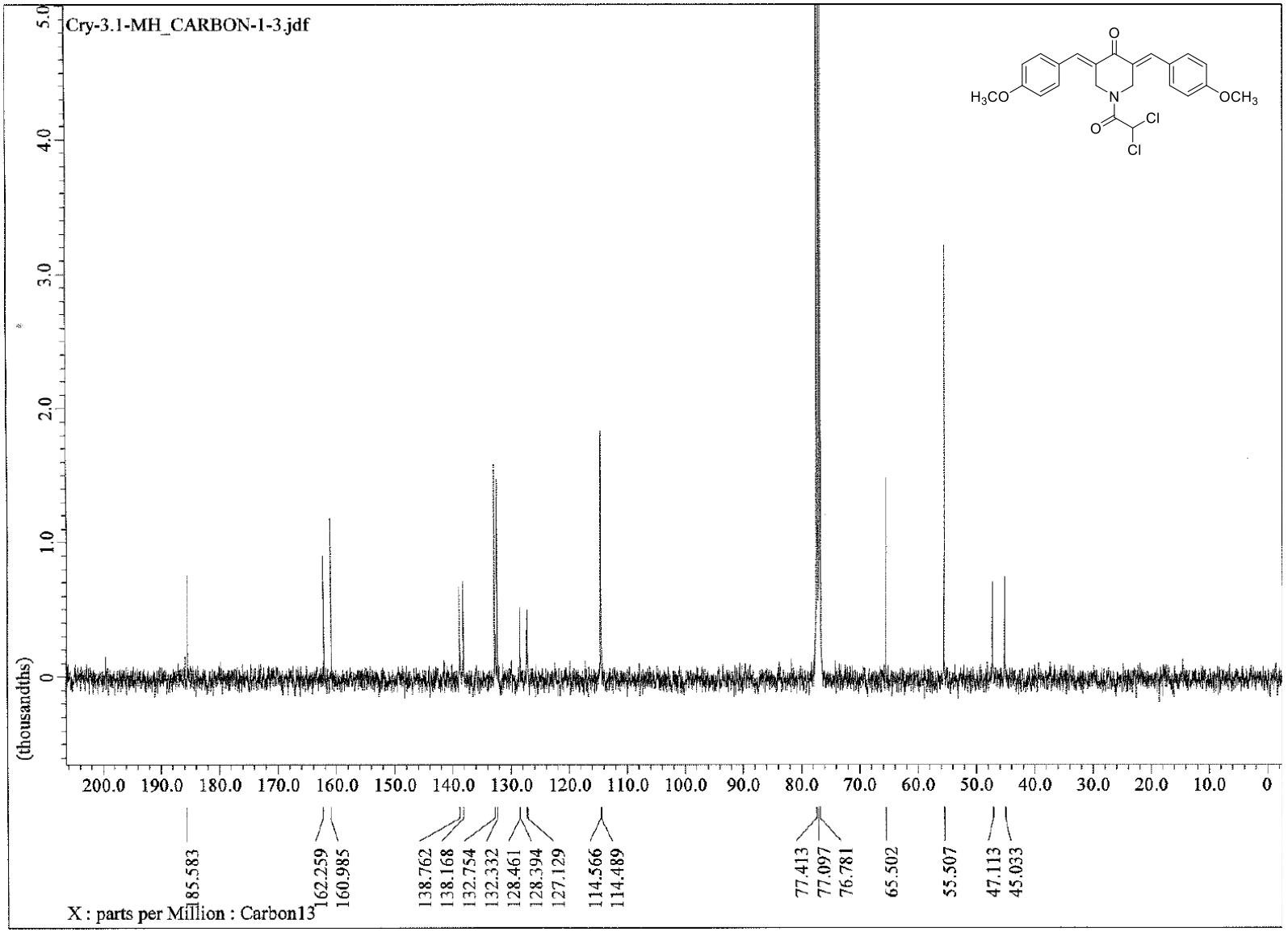


HRMS (FD^+): m/z 520.90795 (M^+), calcd 520.90774 for $C_{21}H_{13}Cl_6NO_2$.

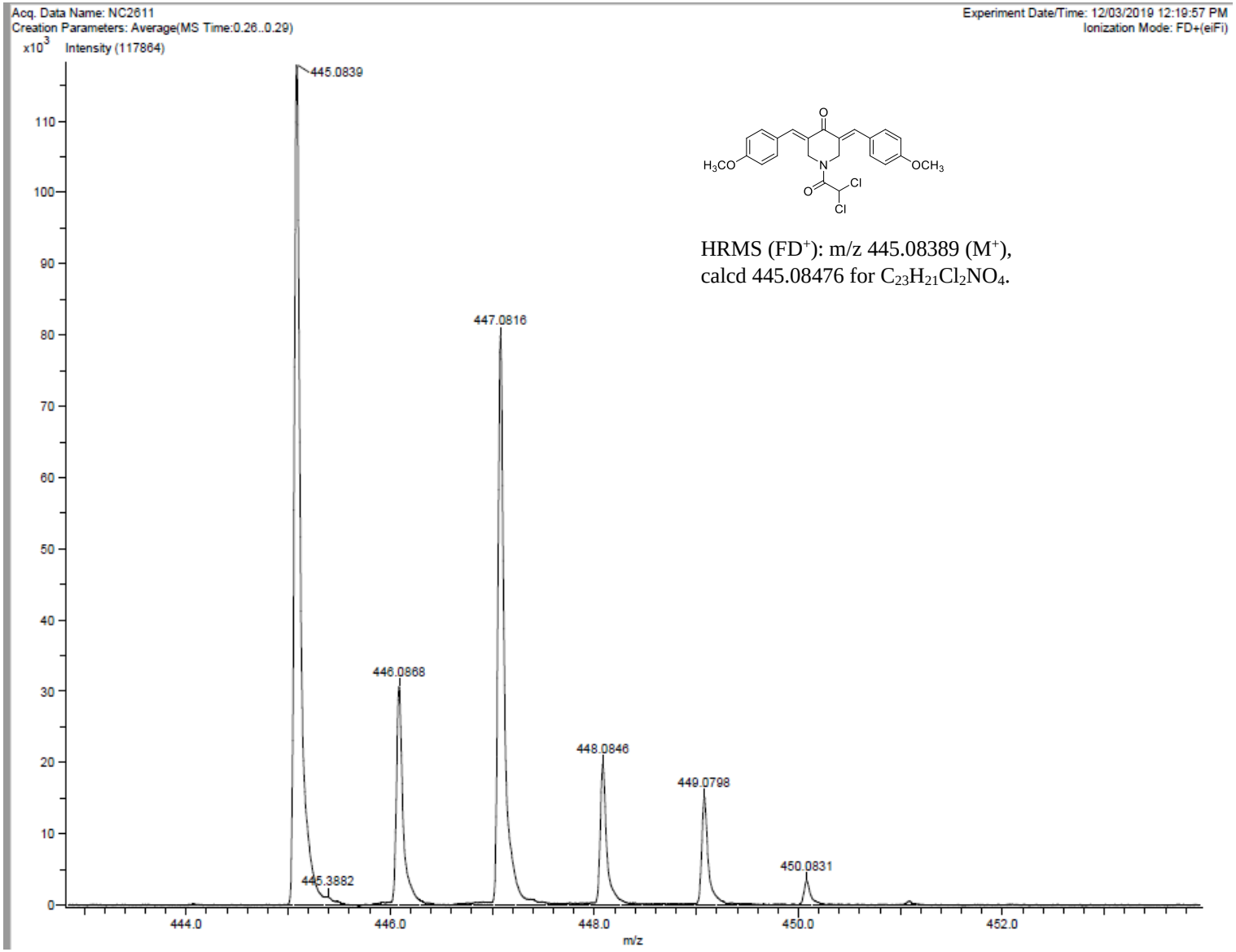
^{1}H NMR ($CDCl_3$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-methoxybenzylidene)piperidin-4-one (**1f**)



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

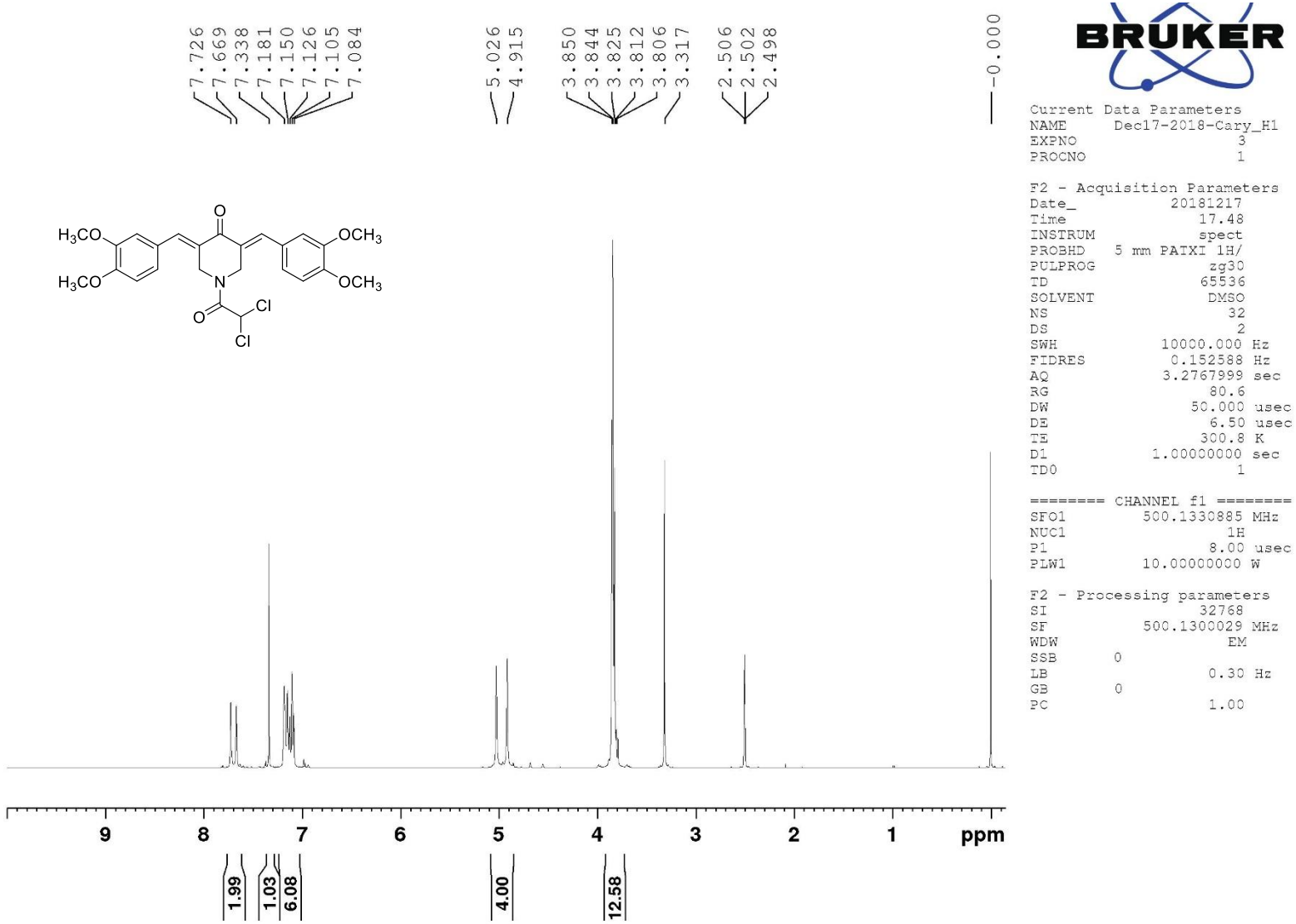


Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-methoxybenzylidene)piperidin-4-one (**1f**)



HRMS (FD$^+$): m/z 445.08389 (M^+),
calcd 445.08476 for $C_{23}H_{21}Cl_2NO_4$.

^{1}H NMR ((CD$_3$)$_2$SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-dimethoxybenzylidene)piperidin-4-one (**1g**)

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TD0                    1

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P1                  8.00 usec
PLW1         10.00000000 W

F2 - Processing parameters
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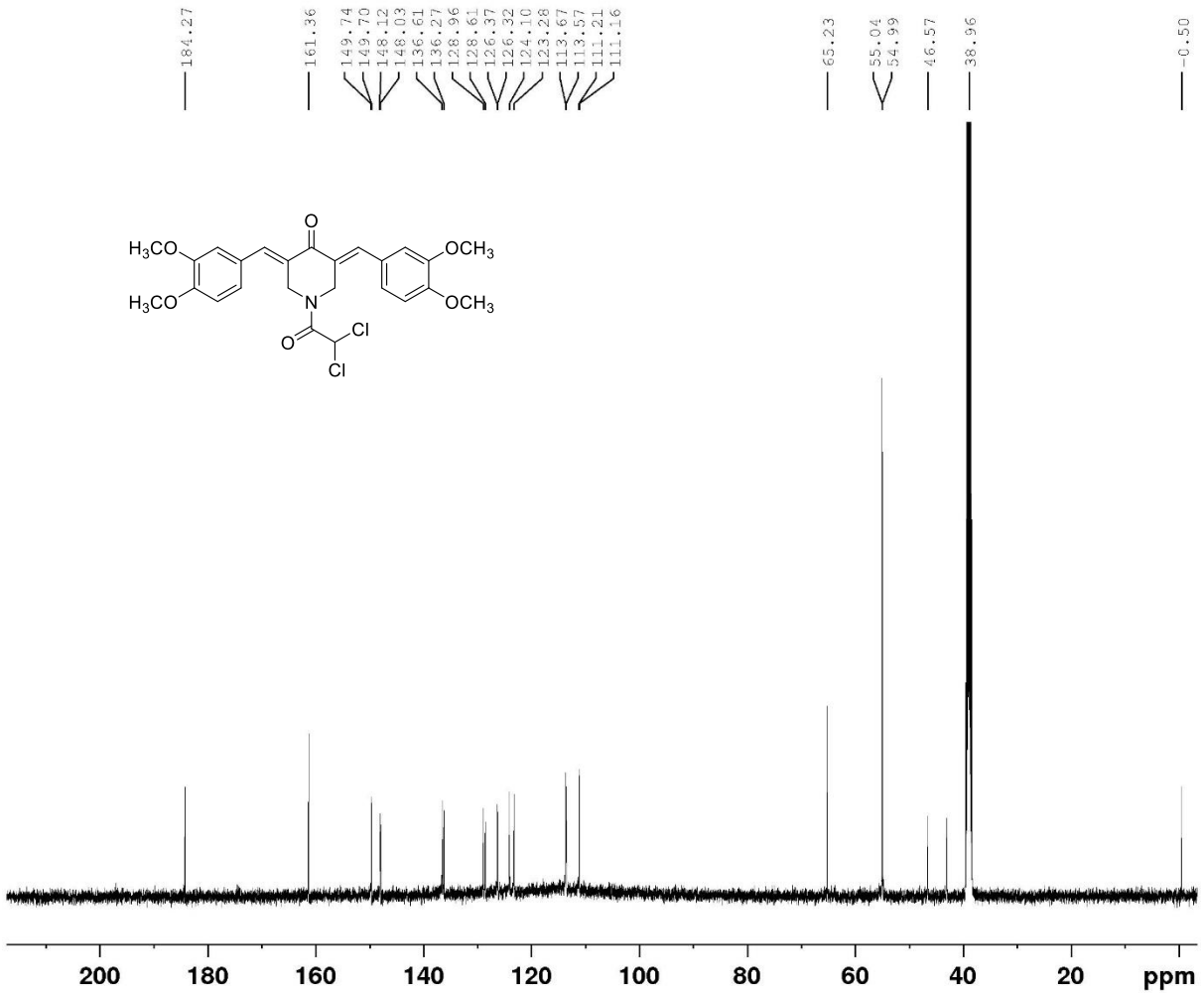
^{13}C NMR ($(CD_3)_2SO$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-dimethoxybenzylidene)piperidin-4-one (**1g**)

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RG                      575
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NUC1                    13C
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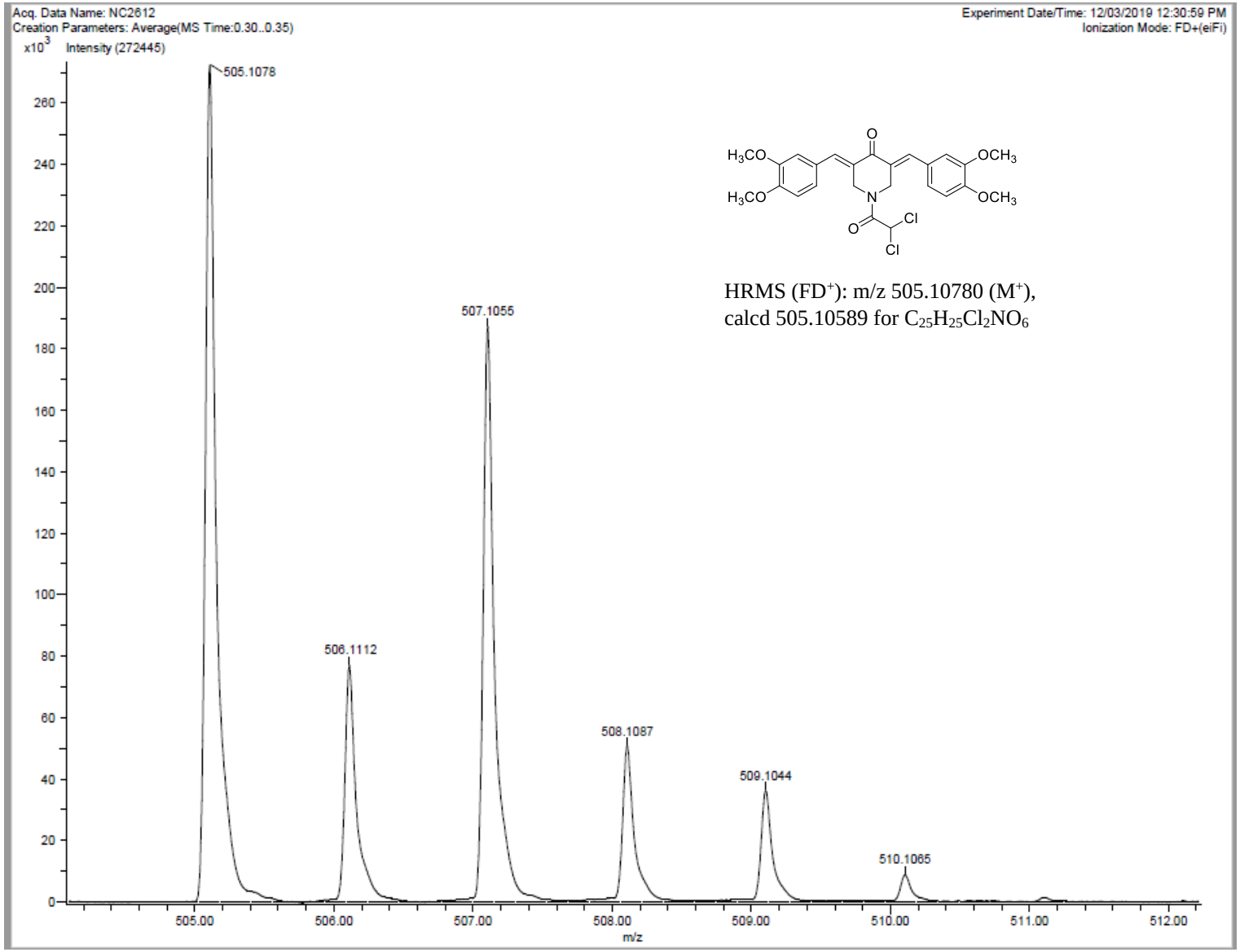
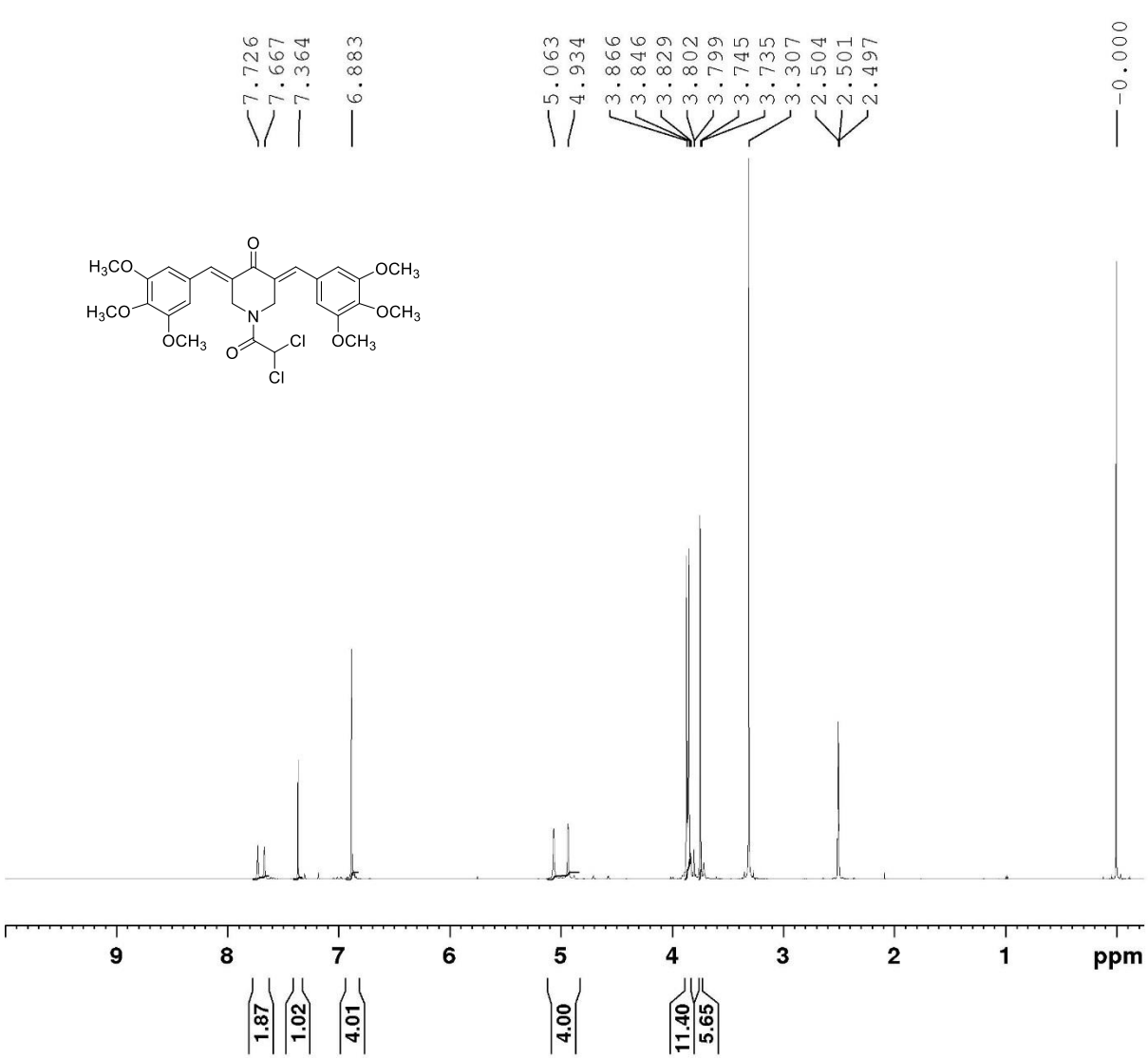
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-dimethoxybenzylidene)piperidin-4-one (**1g**)



HRMS (FD$^+$): m/z 505.10780 (M^+),
calcd 505.10589 for $C_{25}H_{25}Cl_2NO_6$

^{1}H NMR ((CD$_3$)$_2$SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4,5-trimethoxybenzylidene)piperidin-4-one (**1h**)

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TD                65536
SOLVENT            DMSO
NS                    32
DS                     2
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FIDRES         0.152588 Hz
AQ            3.2767999 sec
RG                   114
DW              50.000 usec
DE               6.50 usec
TE              301.6 K
D1           1.00000000 sec
TD0                    1

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NUC1                1H
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PLW1        10.00000000 W

F2 - Processing parameters
SI                 32768
SF           500.1300036 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
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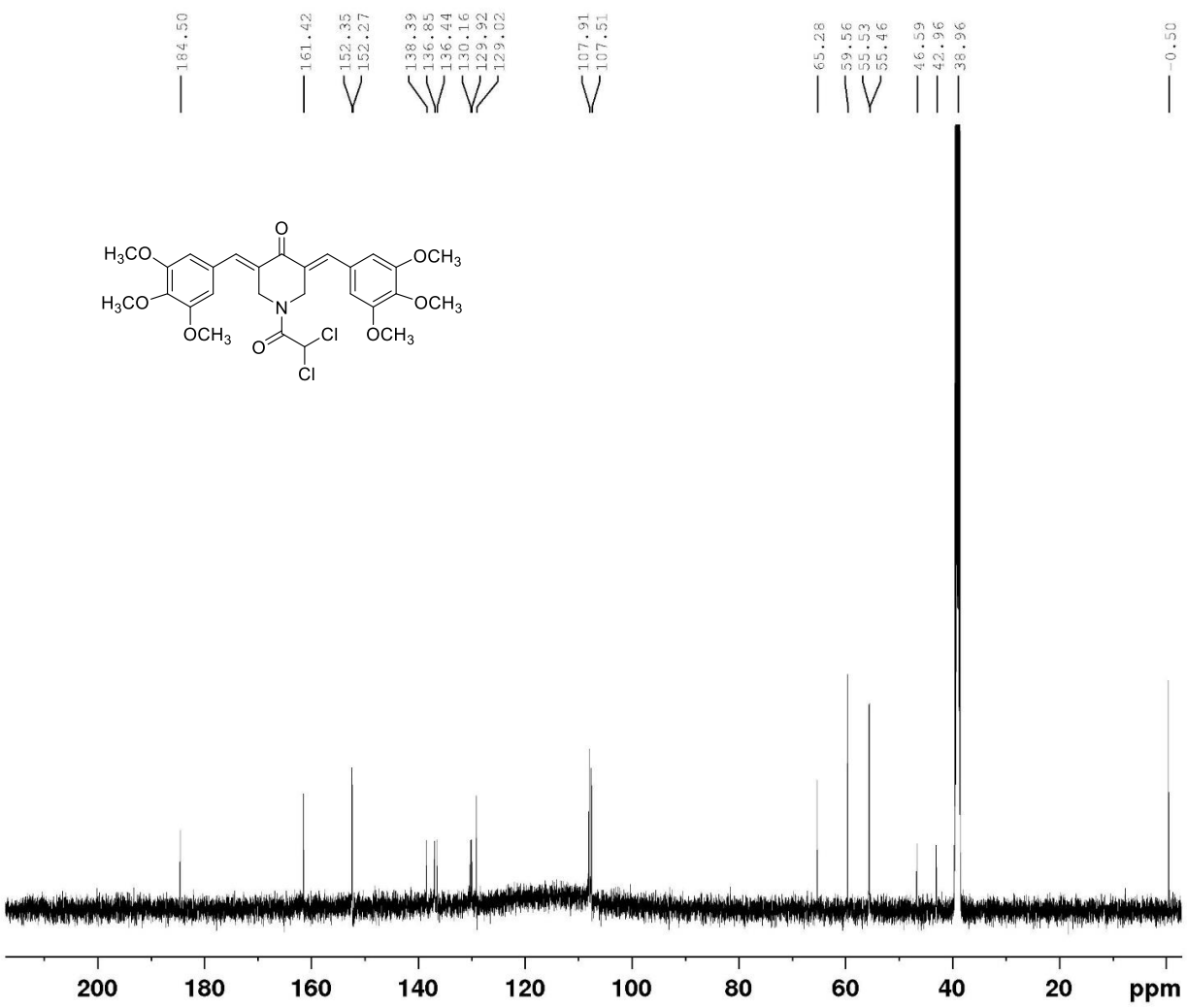
^{13}C NMR ($(CD_3)_2SO$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4,5-trimethoxybenzylidene)piperidin-4-one (**1h**)

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FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                     362
DW                  16.800 usec
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D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

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NUC1                   13C
P1                   12.00 usec
PLW1        180.00000000 W

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NUC2                   1H
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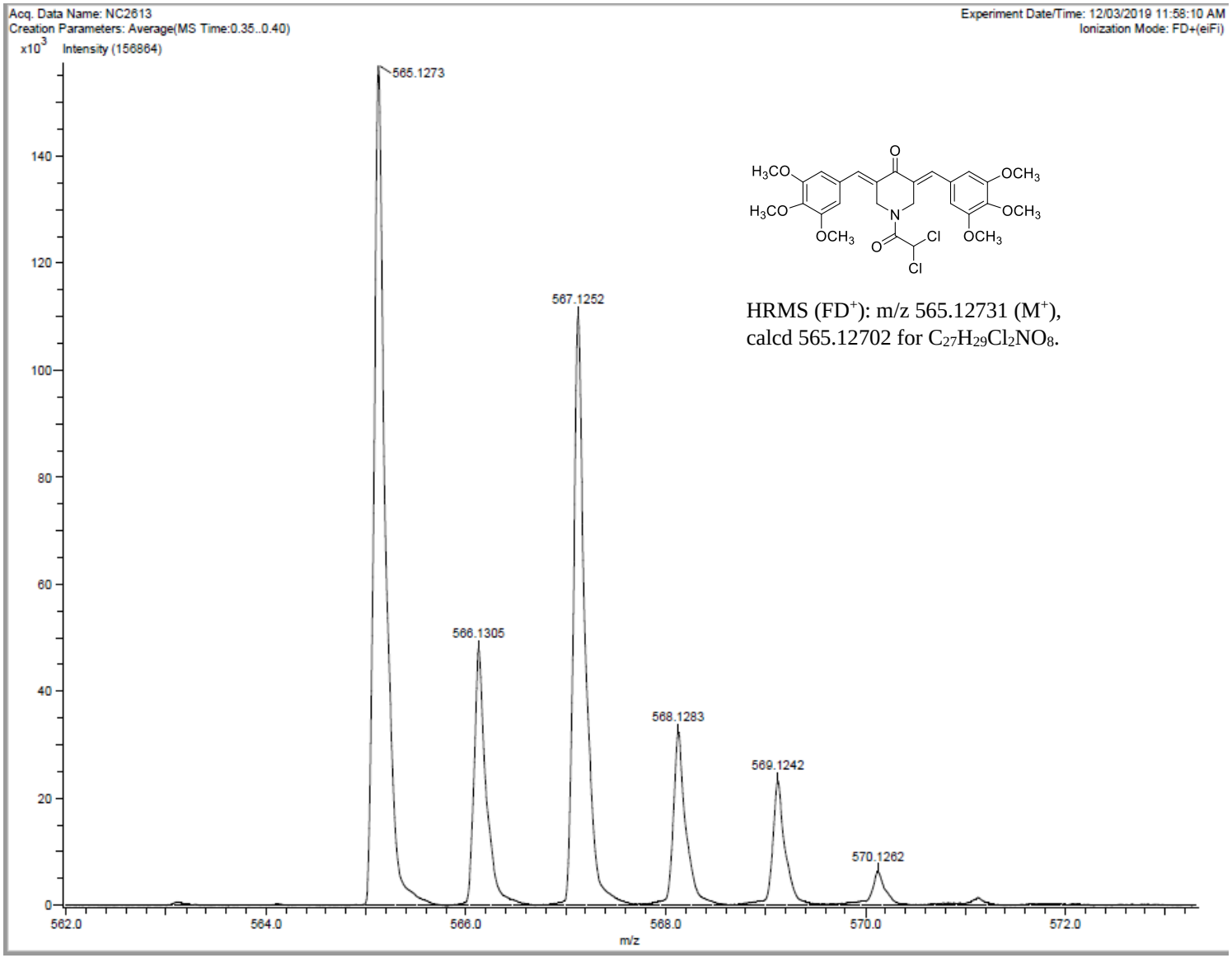
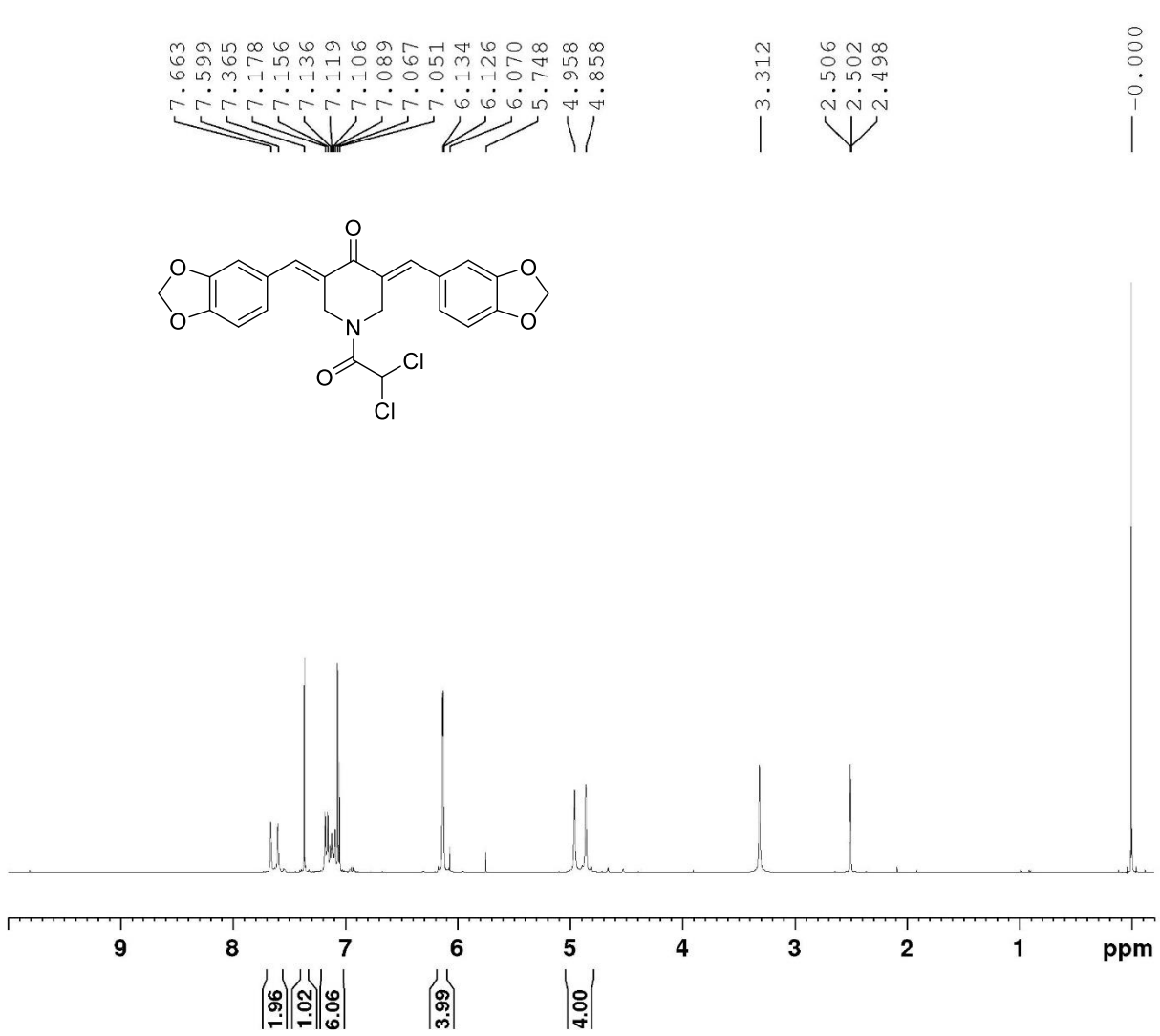
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4,5-trimethoxybenzylidene)piperidin-4-one (**1h**)



^{1}H NMR ((CD$_3$)$_2$SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-methylenedioxybenzylidene)piperidin-4-one (**1i**)



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RG                 101
DW               50.000 usec
DE                6.50 usec
TE               302.2 K
D1           1.00000000 sec
TD0                  1

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NUC1               1H
P1                8.00 usec
PLW1         10.00000000 W

F2 - Processing parameters
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SF           500.1300029 MHz
WDW                EM
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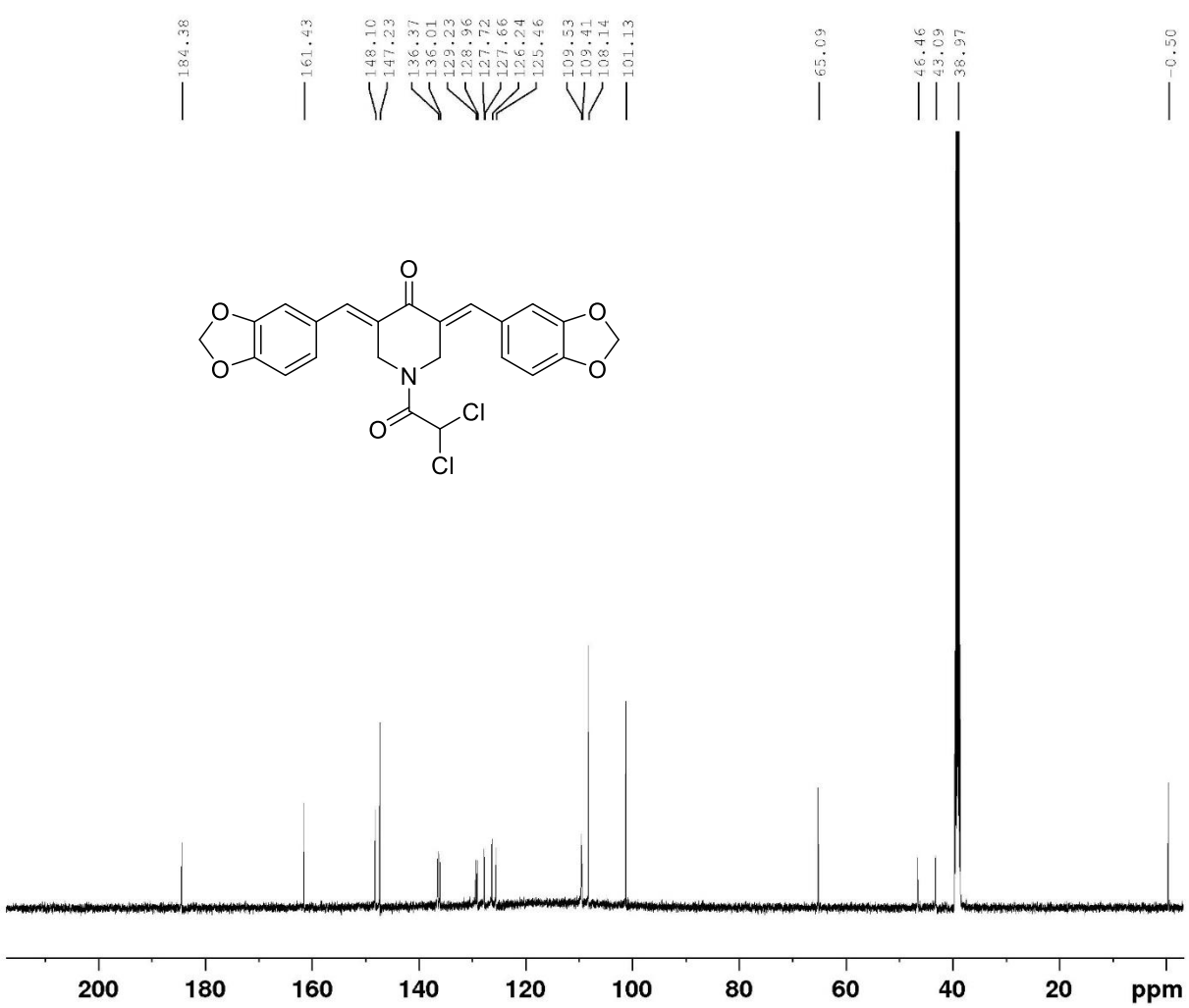
PC                1.00
```

^{13}C NMR ($(CD_3)_2SO$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-methylenedioxybenzylidene)piperidin-4-one (**1i**)

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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           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7703637 MHz
NUC1                 13C
P1                 12.00 usec
PLW1       180.00000000 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           125.7579226 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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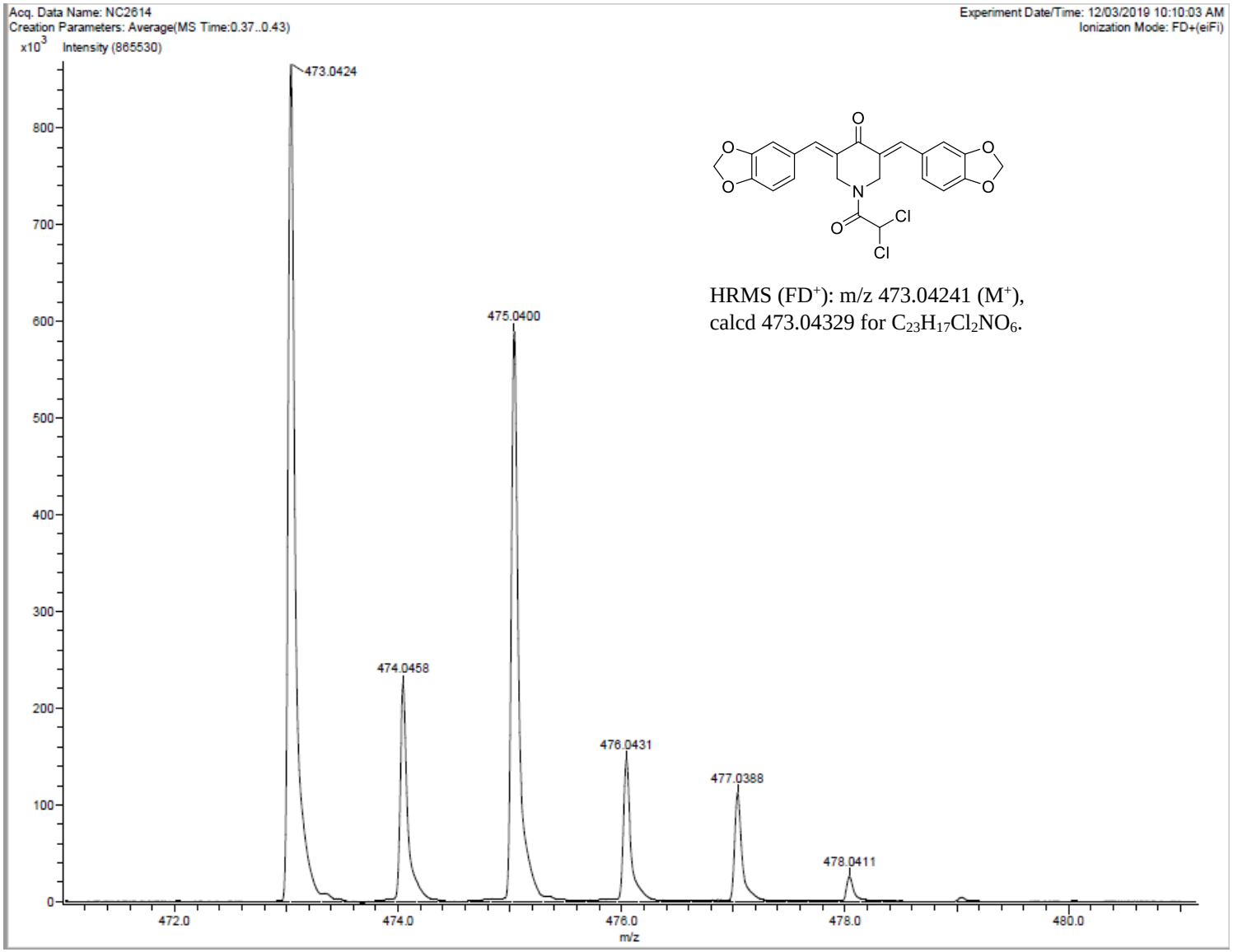
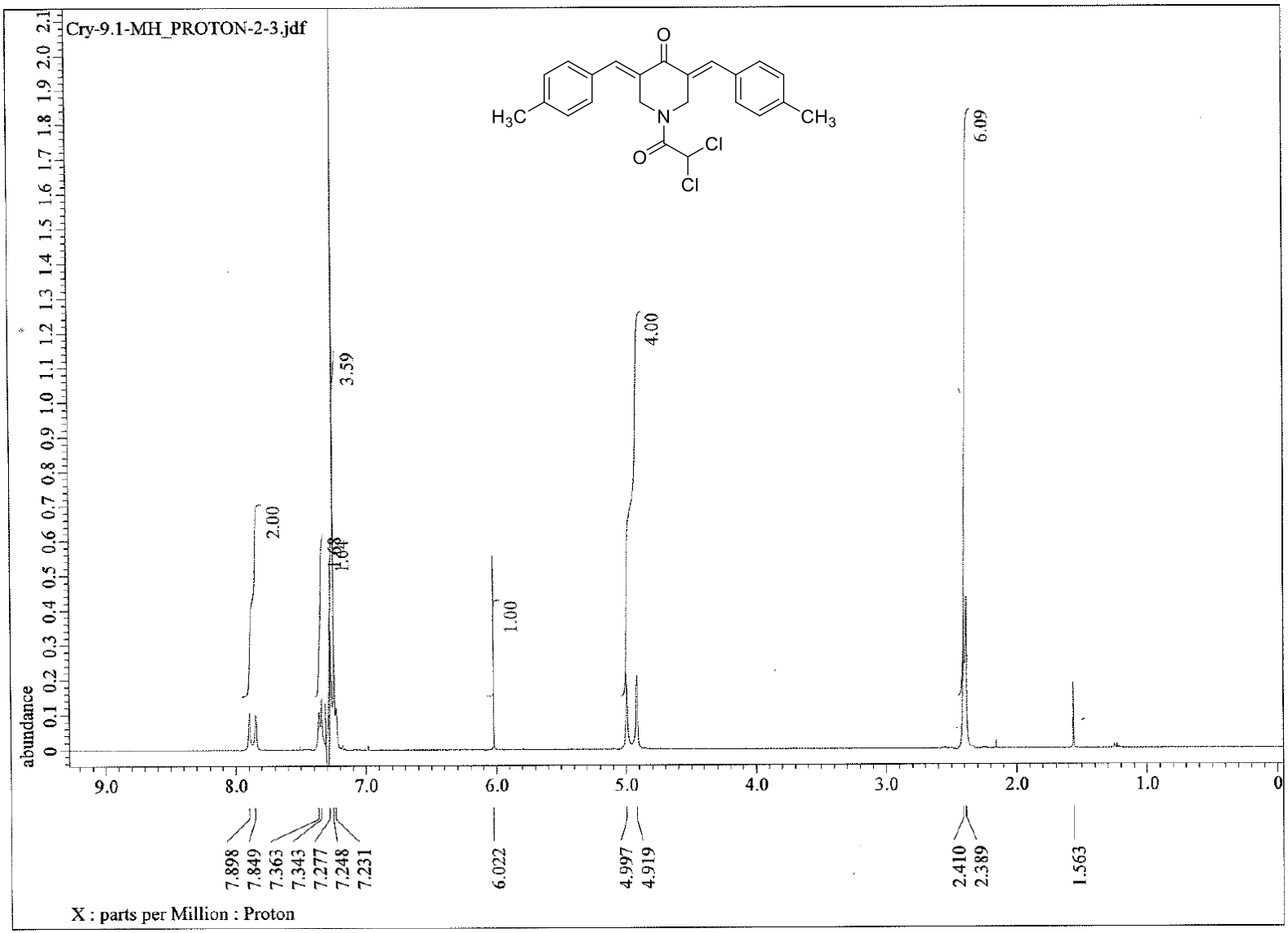
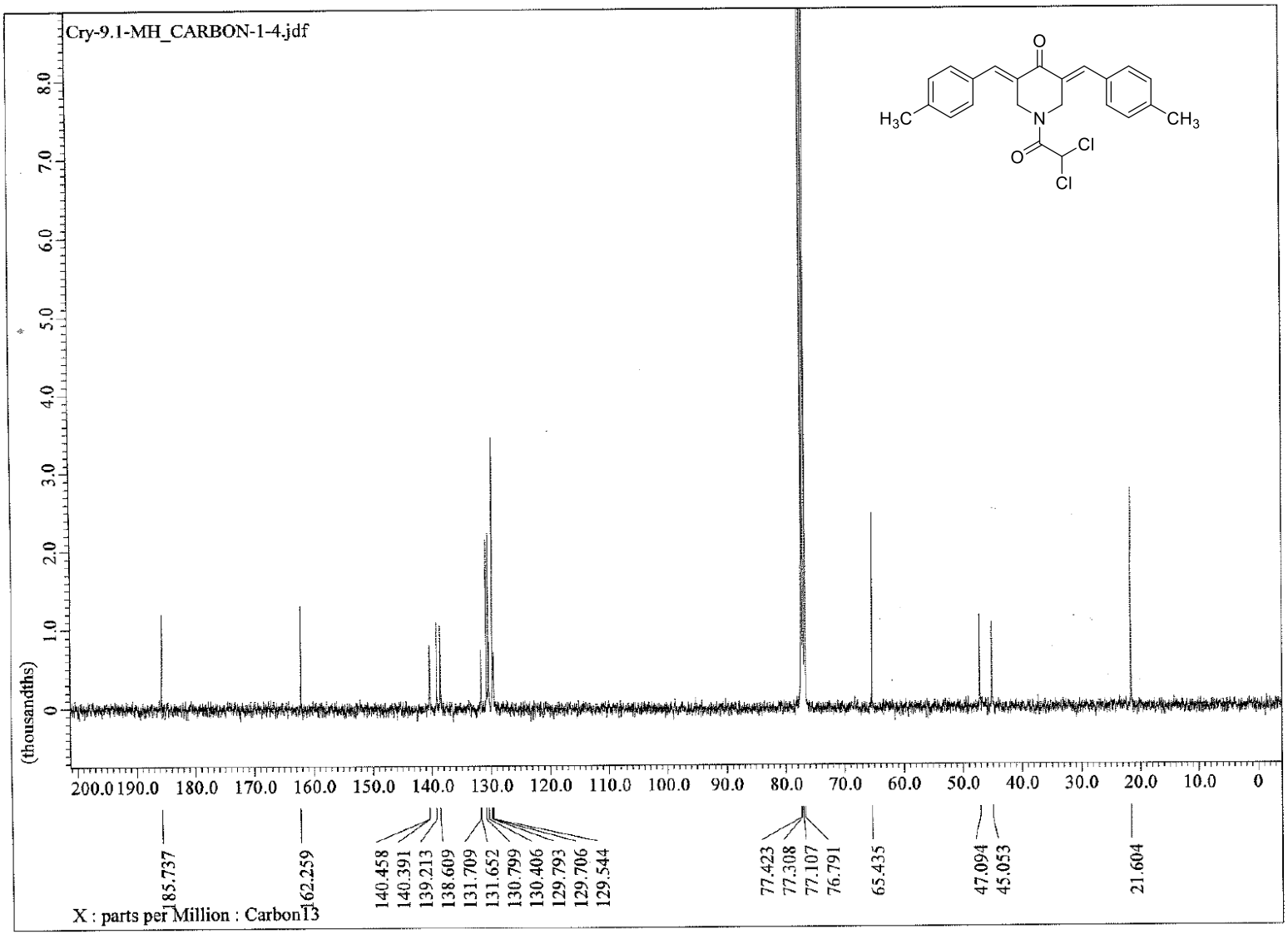
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-3,4-methylenedioxybenzylidene)piperidin-4-one (**1i**)



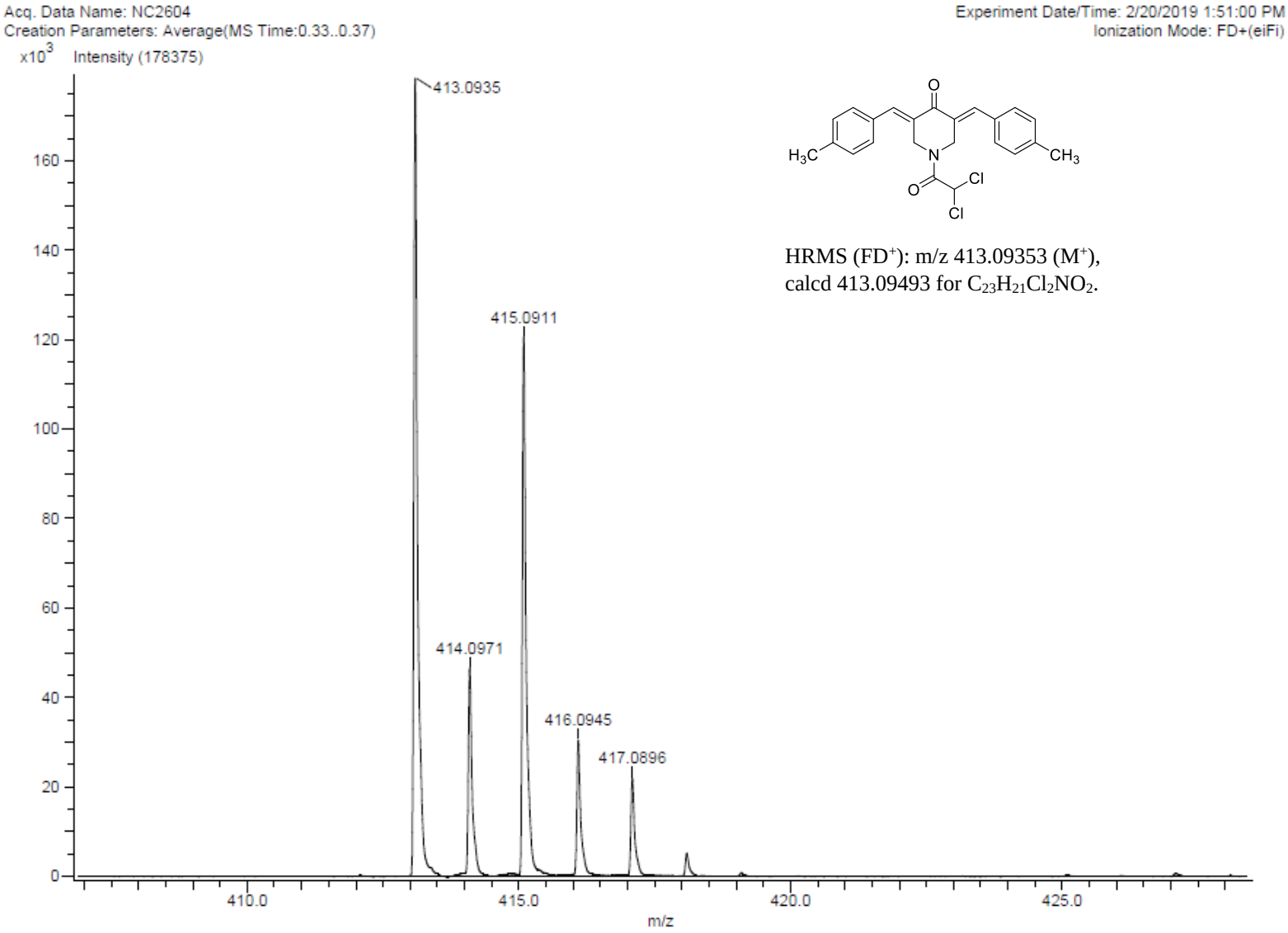
^{1}H NMR ($CDCl_3$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-methylbenzylidene)piperidin-4-one (**1j**)



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

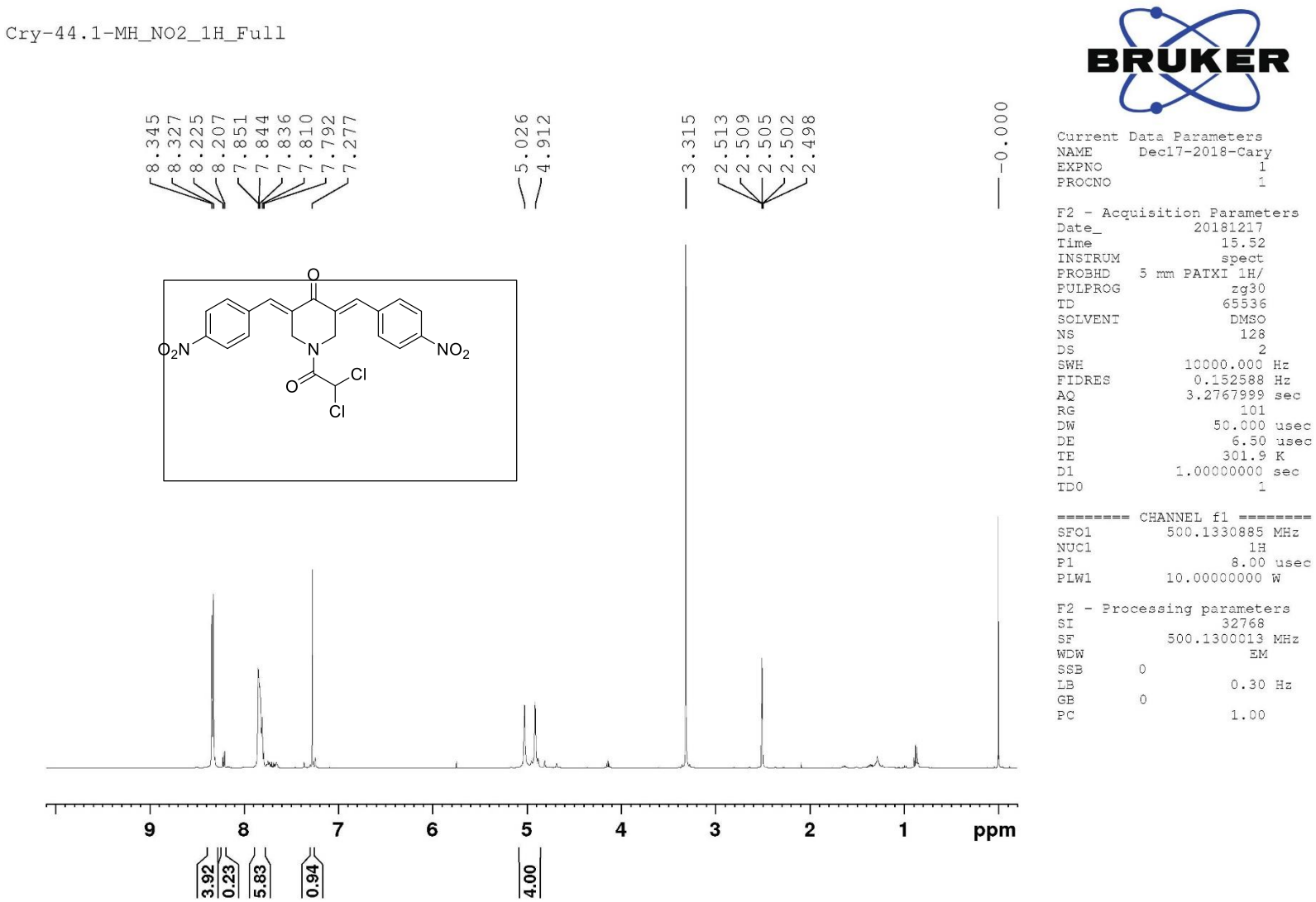


Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-methylbenzylidene)piperidin-4-one (**1j**)



HRMS (FD^+): m/z 413.09353 (M^+), calcd 413.09493 for $C_{23}H_{21}Cl_2NO_2$.

^{1}H NMR ((CD$_3$)$_2$SO) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-nitrobenzylidene)piperidin-4-one (**1k**)

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

F2 - Acquisition Parameters
Date_           20181217
Time               15.52
INSTRUM            spect
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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
TD0                    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
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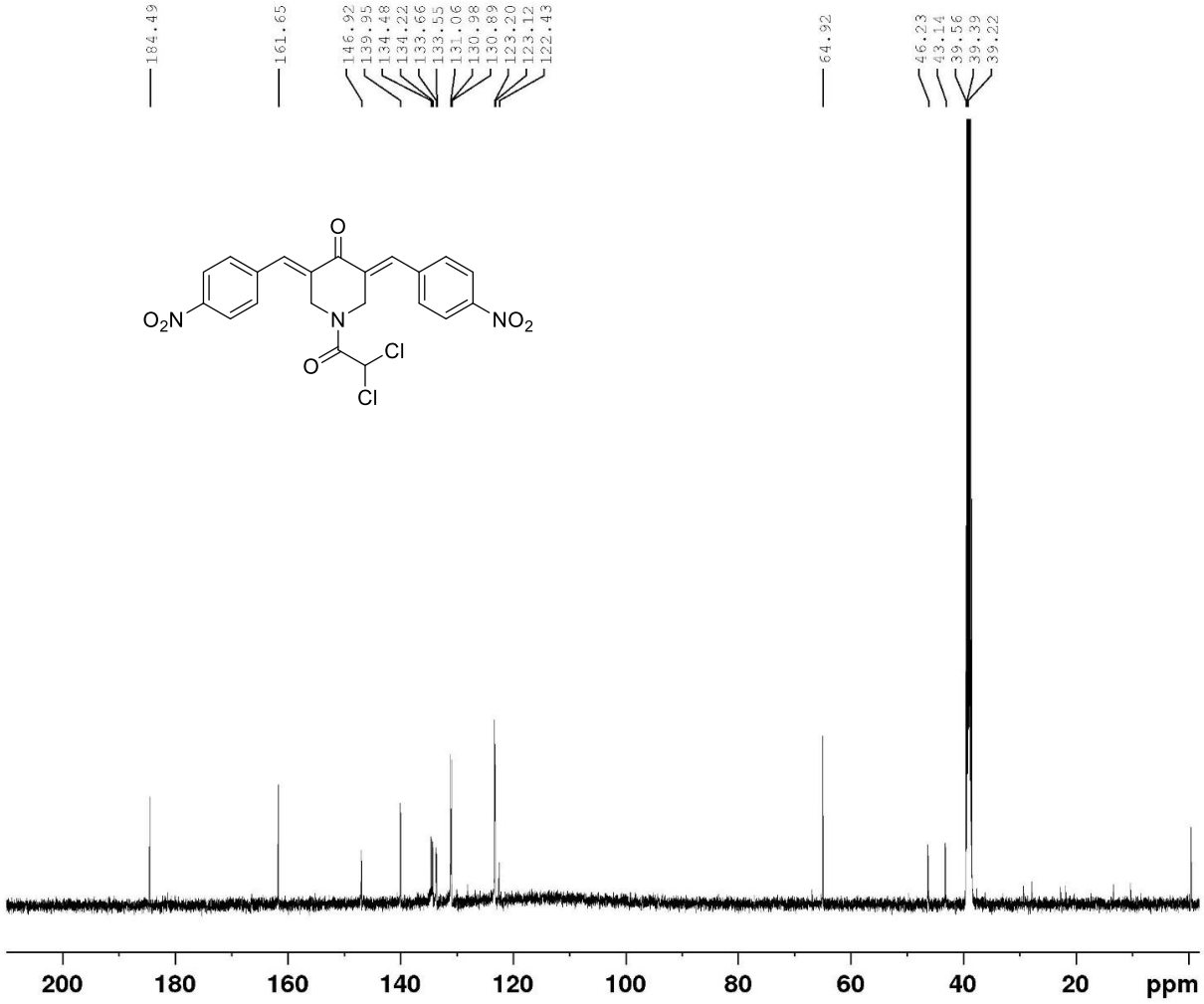
^{13}C NMR ($(CD_3)_2SO$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-nitrobenzylidene)piperidin-4-one (**1k**)

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Cu:
NAME                                  13C
EXPNO                                  2
PROCNO                                 1

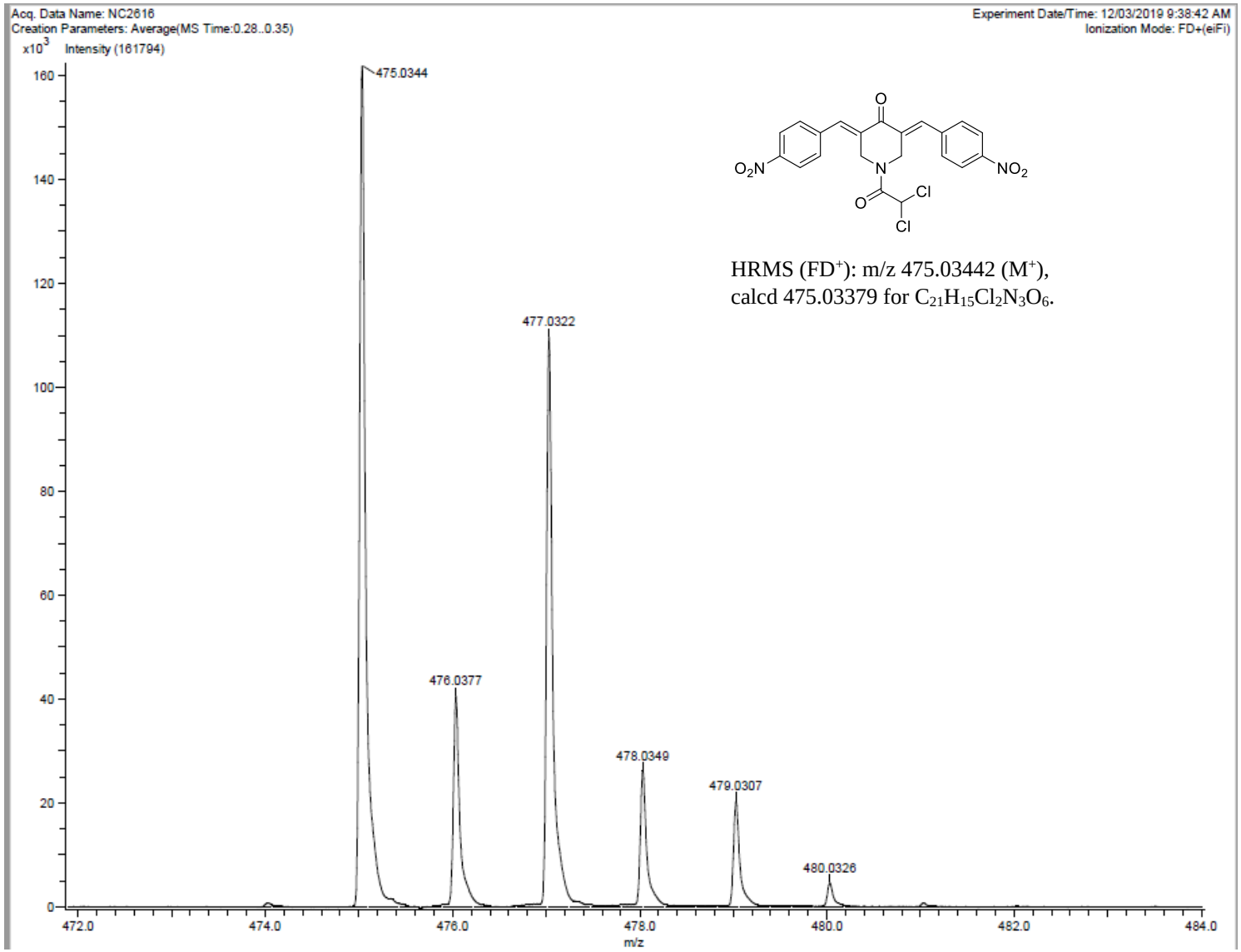
F2 - Acquisition Parameters
Date_                           20181217
Time                               17.42
INSTRUM                            spect
PROBHD    5 mm PATXI 1H/
PULPROG                         zgpg30
TD                                 65536
SOLVENT                             DMSO
NS                                  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                   180.00000000 W

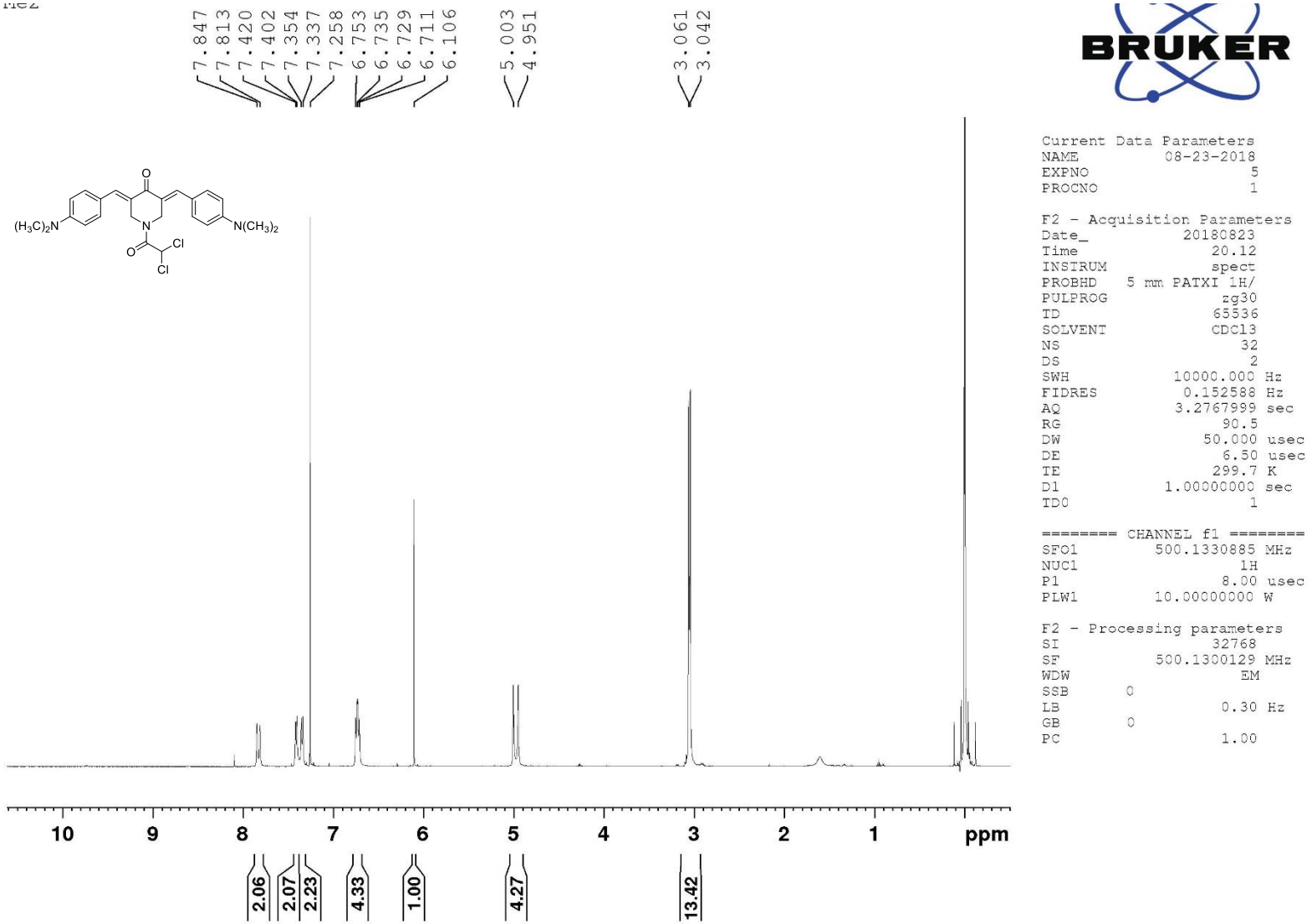
======== CHANNEL f2 ========
SFO2                     500.1320005 MHz
NUC2                               1H
CPDPRG[2                    waltz16
PCPD2                           80.00 usec
PLW2                    10.00000000 W
PLW12                    0.10000000 W
PLW13                    0.06400000 W

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**)



^{1}H NMR ($CDCl_3$) spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((*E*)-4-(dimethylamino)benzylidene)piperidin-4-one (**1l**)

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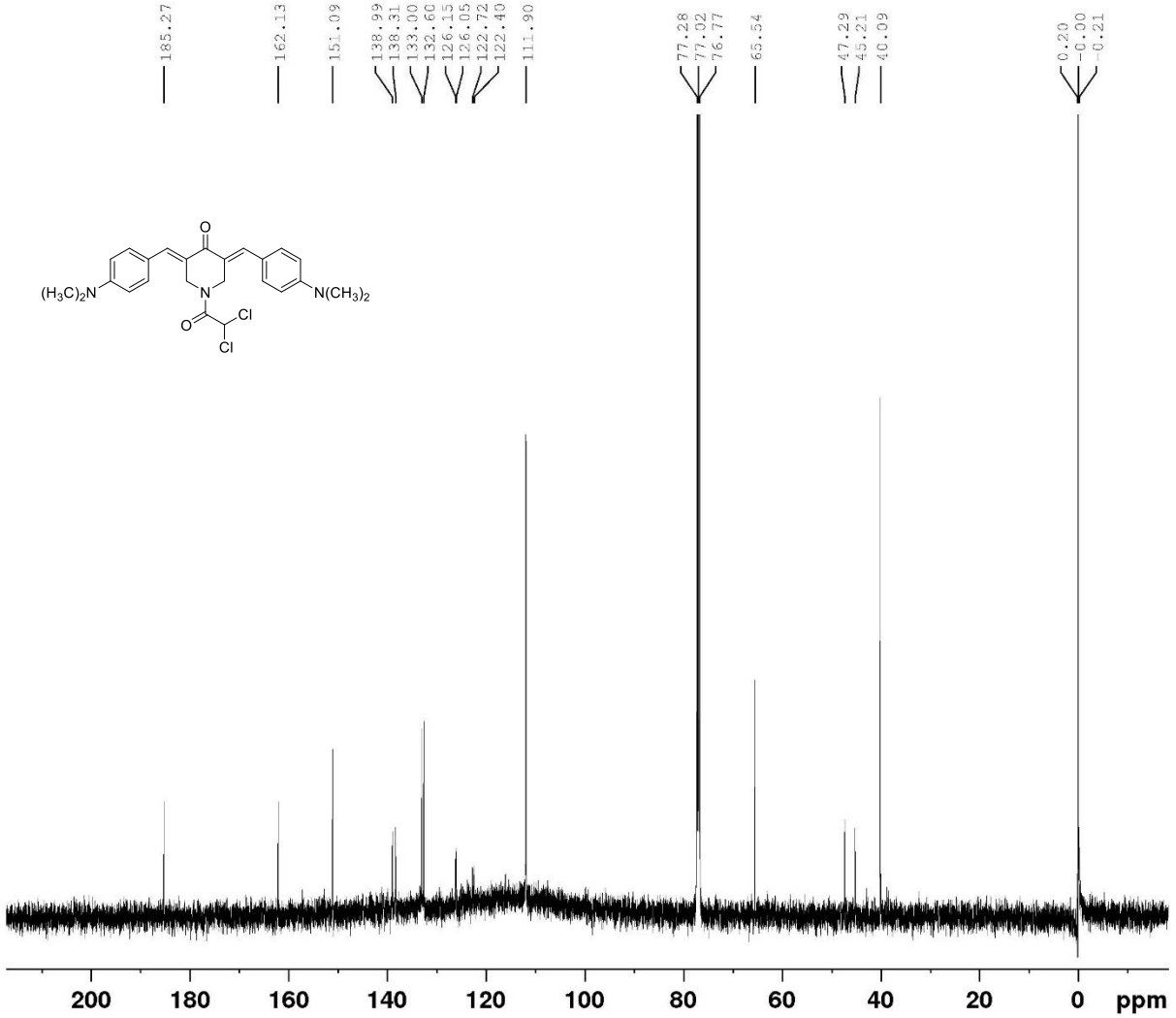
Current Data Parameters
NAME          08-23-2018
EXPNO                  5
PROCNO                 1

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 ========
SFO1         500.1330885 MHz
NUC1                 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
```

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



BRUKER

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

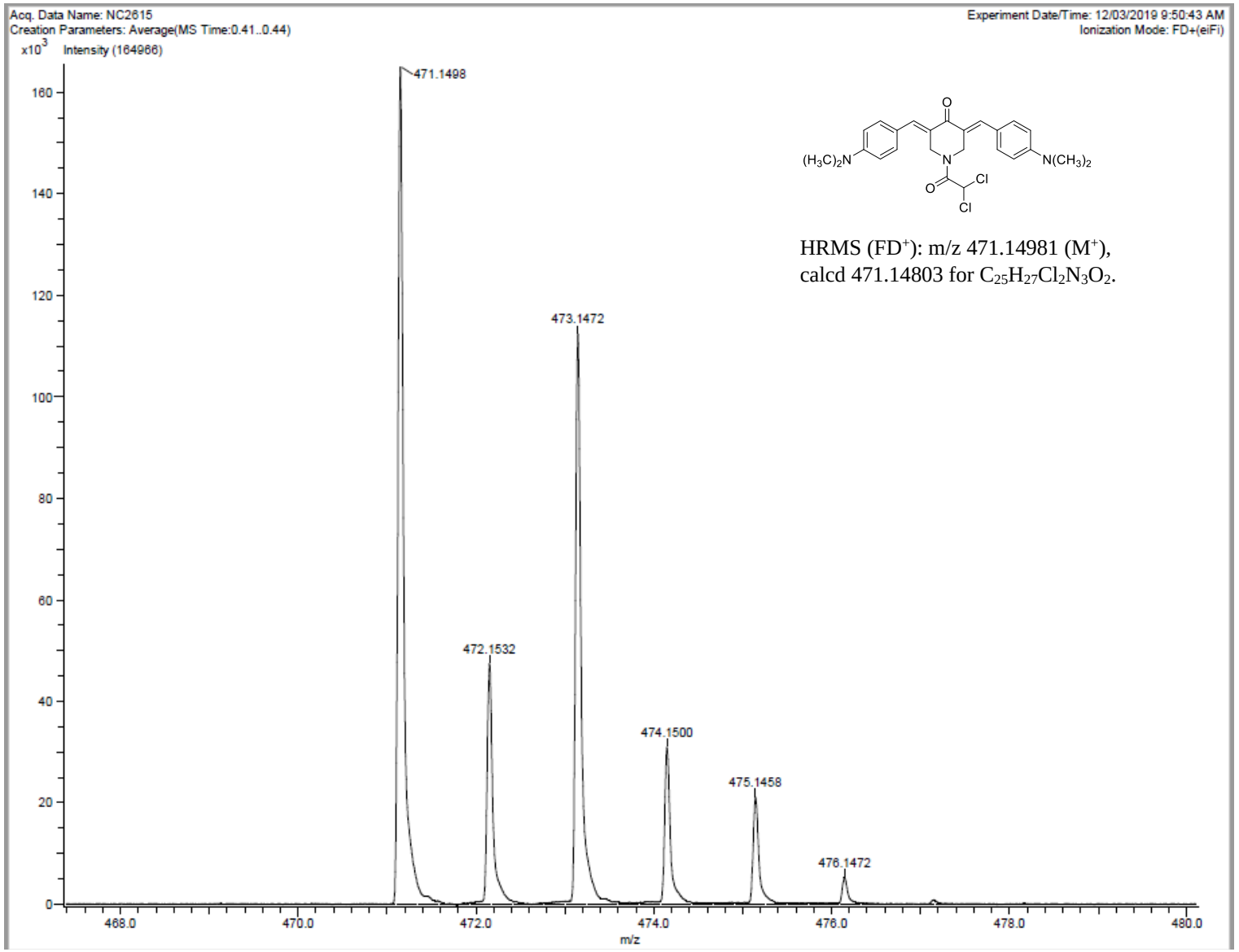
F2 - Acquisition Parameters
Date_           20180823
Time               22.52
INSTRUM            spect
PROBHD   5 mm PATXI 1H/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3000
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
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       180.00000000 W

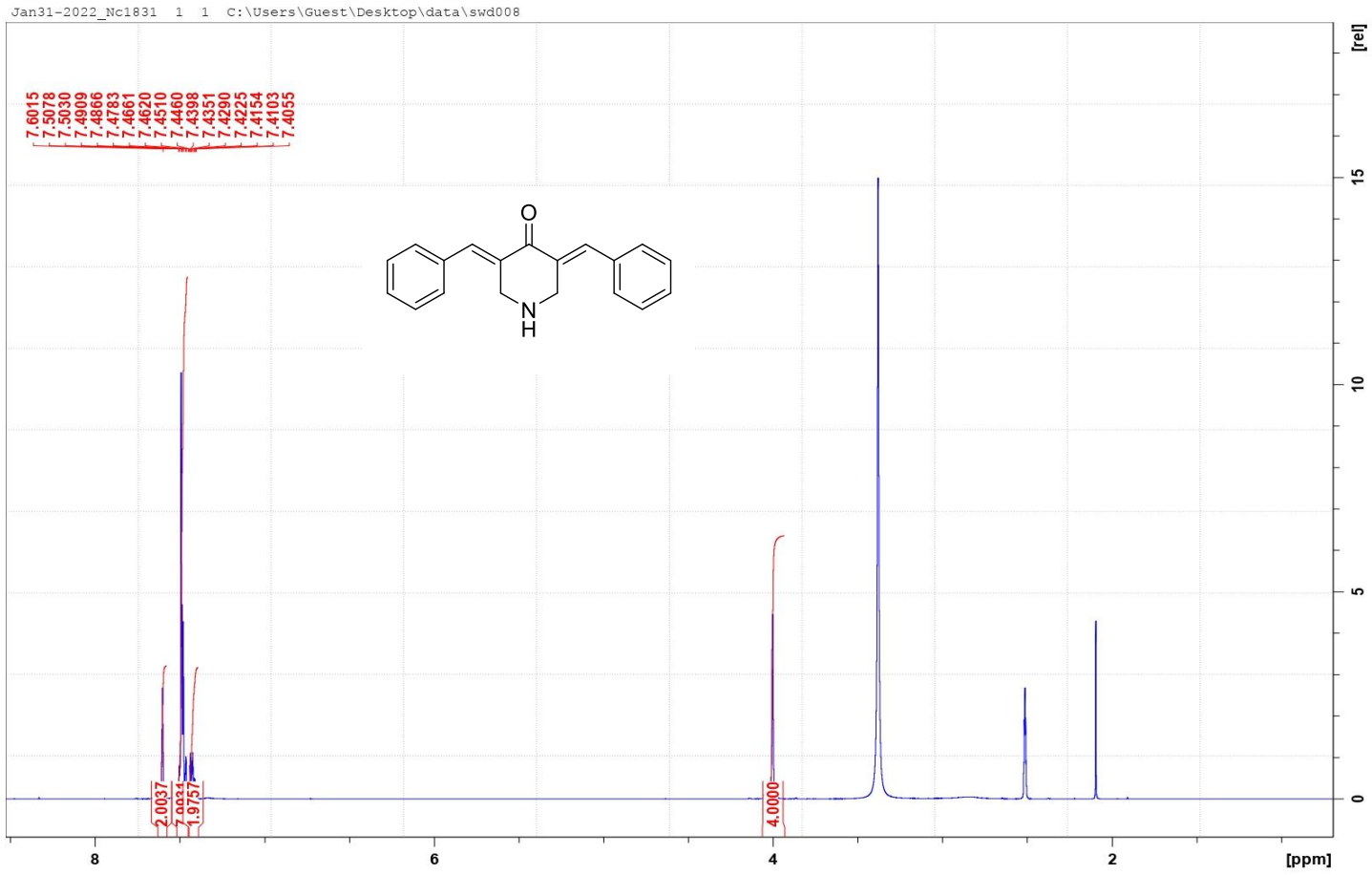
======== CHANNEL f2 ========
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        10.00000000 W
PLW12        0.10000000 W
PLW13        0.06400000 W

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

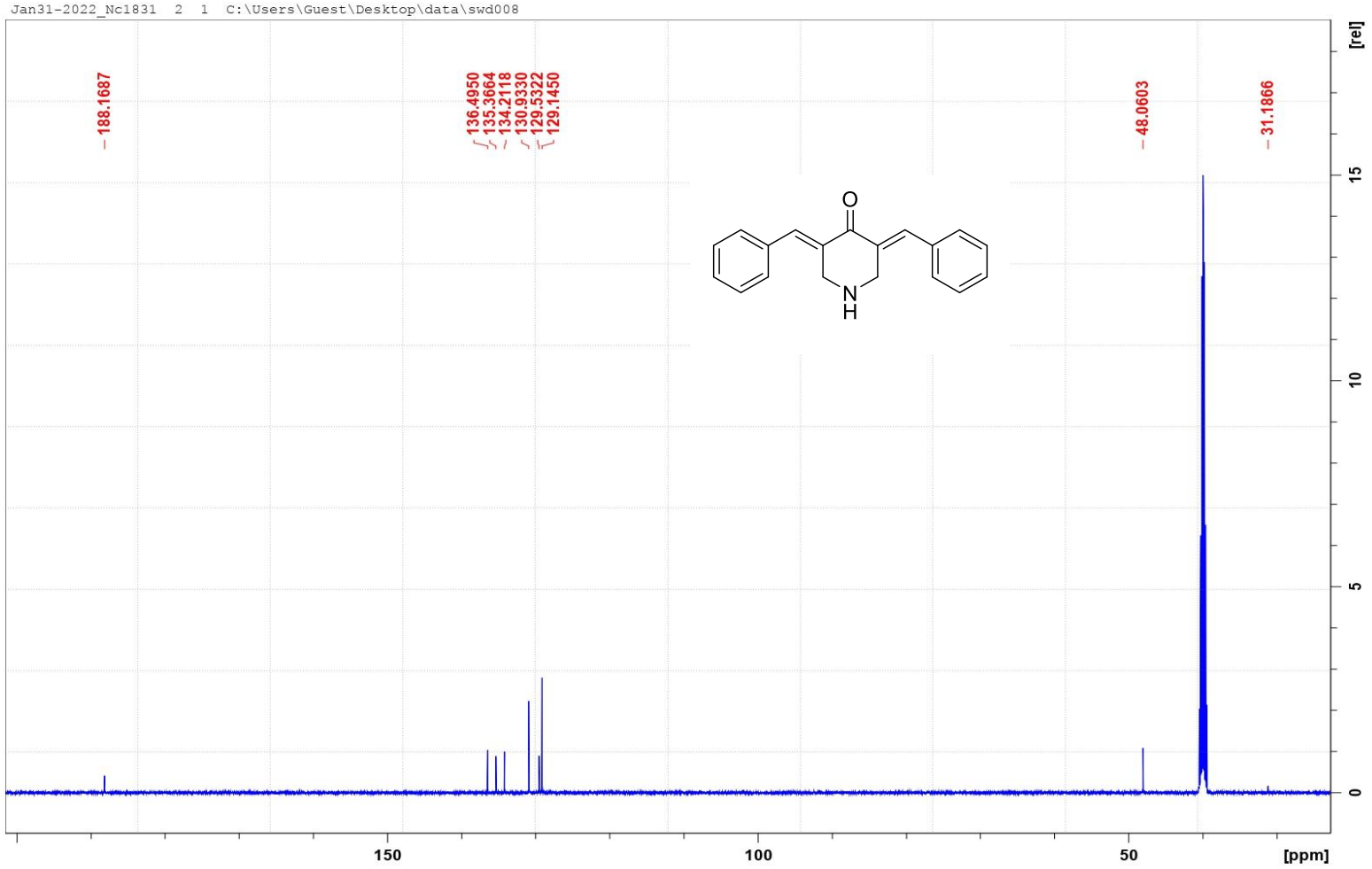
Mass spectrum of 1-(2,2-dichloroacetyl)-3,5-bis((E)-4-(dimethylamino)benzylidene)piperidin-4-one (**1l**)



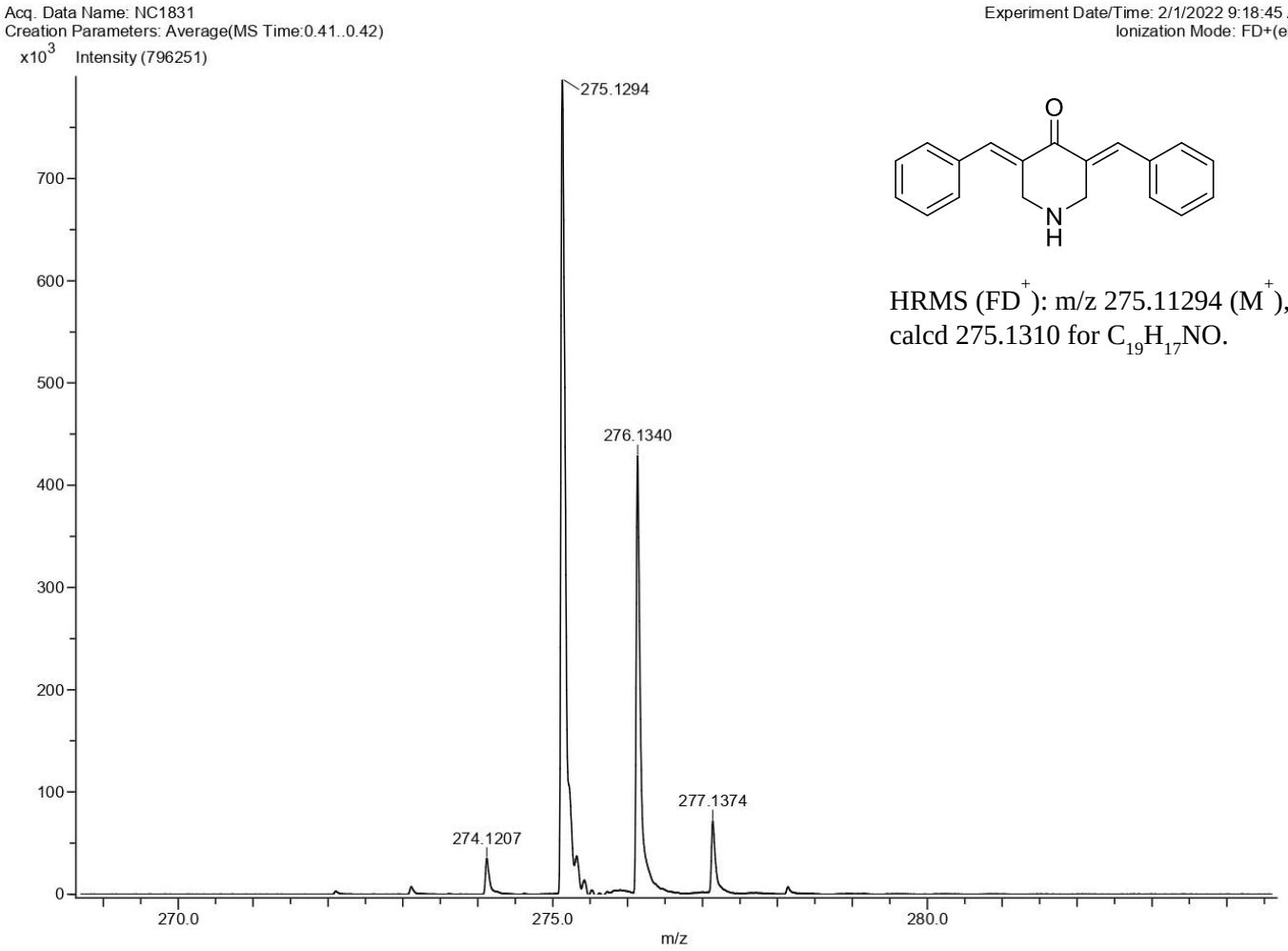
^{1}H NMR ($(CD_3)_2SO$) spectrum of 3,5-di((E)-benzylidene)piperidin-4-one (**2a**)



^{13}C NMR ($(CD_3)_2SO$) spectrum of 3,5-di((E)-benzylidene)piperidin-4-one (**2a**)

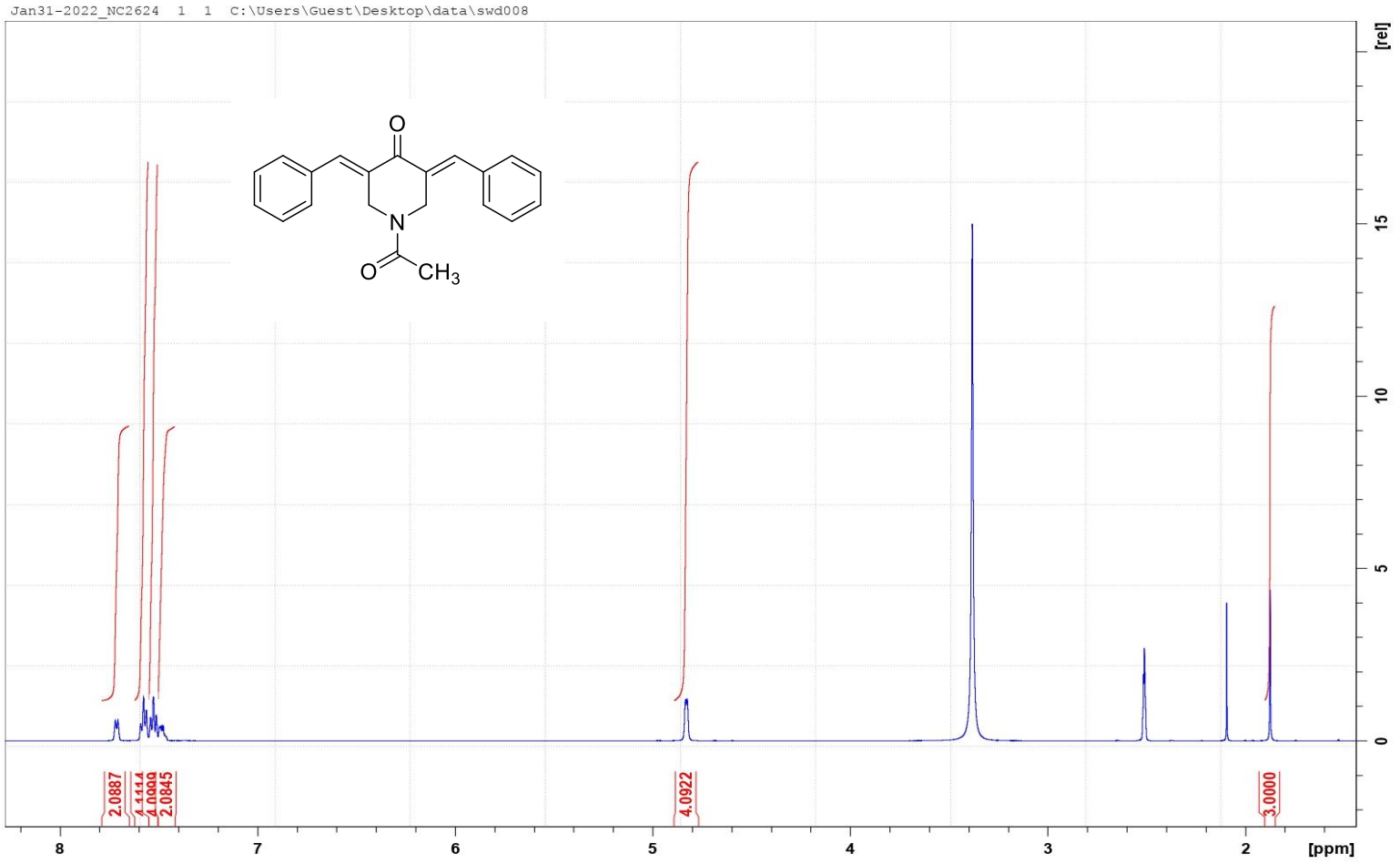


Mass spectrum of 3,5-di((E)-benzylidene)piperidin-4-one (**2a**)

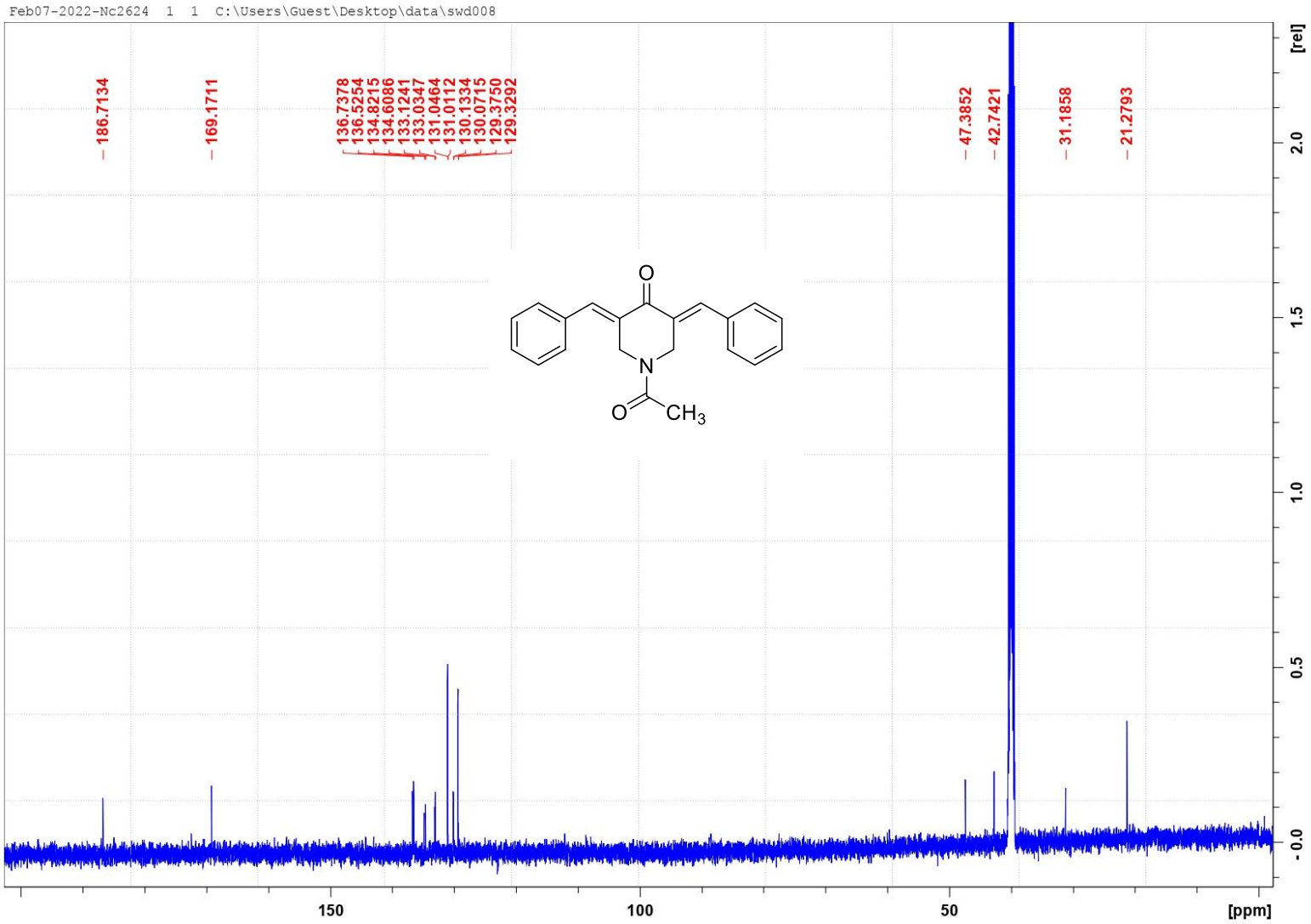


HRMS (FD^+): m/z 275.11294 (M^+), calcd 275.1310 for $C_{19}H_{17}NO$.

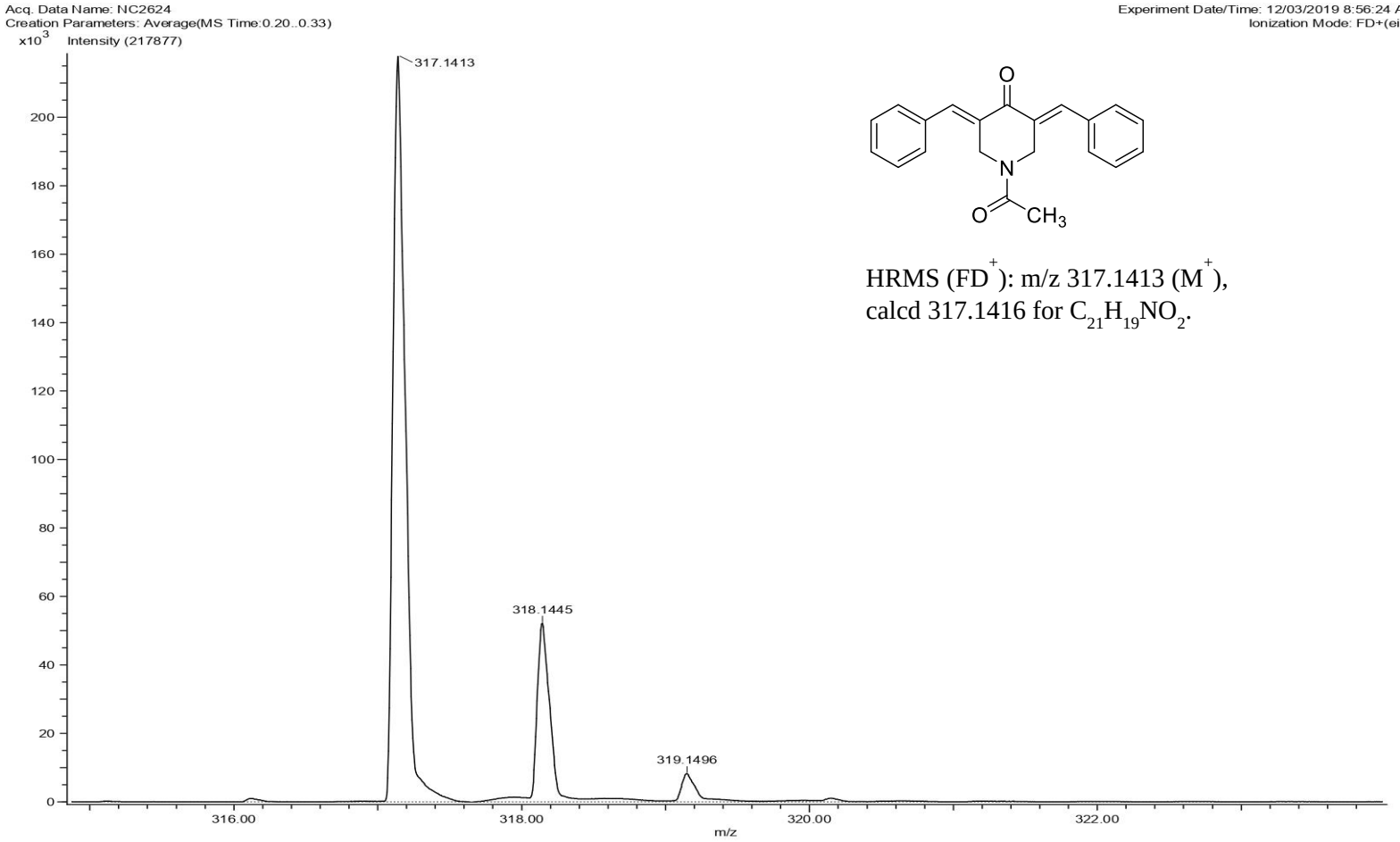
^{1}H NMR ($(CD_3)_2SO$) of 1-acetyl-3,5-di((E)-benzylidene)piperidin-4-one (**2b**)



^{13}C NMR ($(CD_3)_2SO$) 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**)



HRMS (FD^+): m/z 317.1413 (M^+), calcd 317.1416 for $C_{21}H_{19}NO_2$.