Supporting information

Catalyst-free reactions of anilines with *β*-chloroenones: Synthesis of *α*-chloroenaminones and 1,4-benzodiazepines

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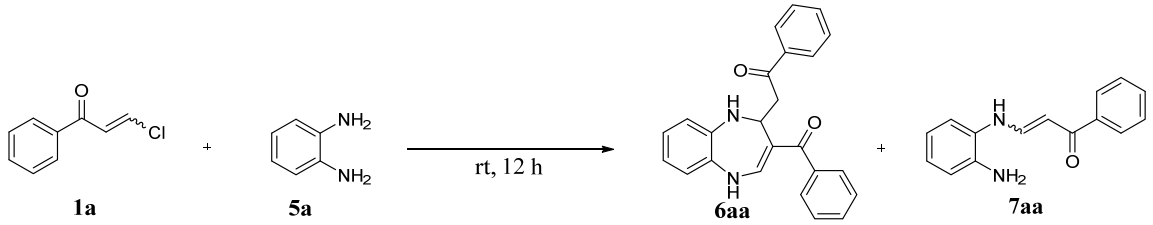
1. Optimization of the reaction conditions[a]



1a **5a** **6aa** **7aa**

Entry	Catalyst	Solvent	Time	Yield[b] **6aa**	Yield[b] **7**
1	-	DMSO	12	44 (40)[c]	10
2	-	DMSO	24	37	3
3	-	DMF	12	42	8
4	-	DMA	12	40	12
5	-	NMP	12	39	12
6	-	Ethyl acetate	12	-	34 (28)[c]
7[d]		DMSO	12	23	4
8	$TsOH•H_2O$ (30 mol%)	DMSO	12	-	-
9	$FeCl_3$ (30 mol%)	DMSO	12	33	3
10	$ZnCl_2$ (30 mol%)	DMSO	12	41	8

All of the reactions were carried out using **1a** (0.25 mmol, 42 mg), **2a** (0.25 mmol, 27 mg) and solvent (2 mL). [b]The yields were determined by ^1H NMR analyses of the crude reaction mixtures using CH_2Br_2 as the internal standard. [c]Isolated yield. [d]2 equiv. of **1a** (0.5 mmol, 83 mg) was used. DMSO = Dimethyl sulfoxide, DMF = Dimethylformamide, DMA = Dimethylacetamide, NMP = *N*-Methyl-2-pyrrolidone.

2. Single crystal X-ray analytical data

A solvent mixture of ethyl acetate and dichloromethane was used to obtain crystals of **3aa** by a slow evaporation method at ambient temperature. In the case of **3af**, a mixture of hexanes and dichloromethane was used. The crystals of **6ea** were obtained using ethyl acetate as a solvent system. X-ray reflections were collected using Mo Kα X-radiation (λ = 0.71073 Å) on the single crystals at 200 K using a Bruker Kappa APEX-II diffractometer. All the crystal structures were solved and refined using SHELX-97. The details of crystals data collections and data refinement parameters are given in Table S1, S2 and S3.

Ortep (ellipsoid counter 30% probability**) diagram and crystal data of compound 3aa: CCDC Number 2334143**

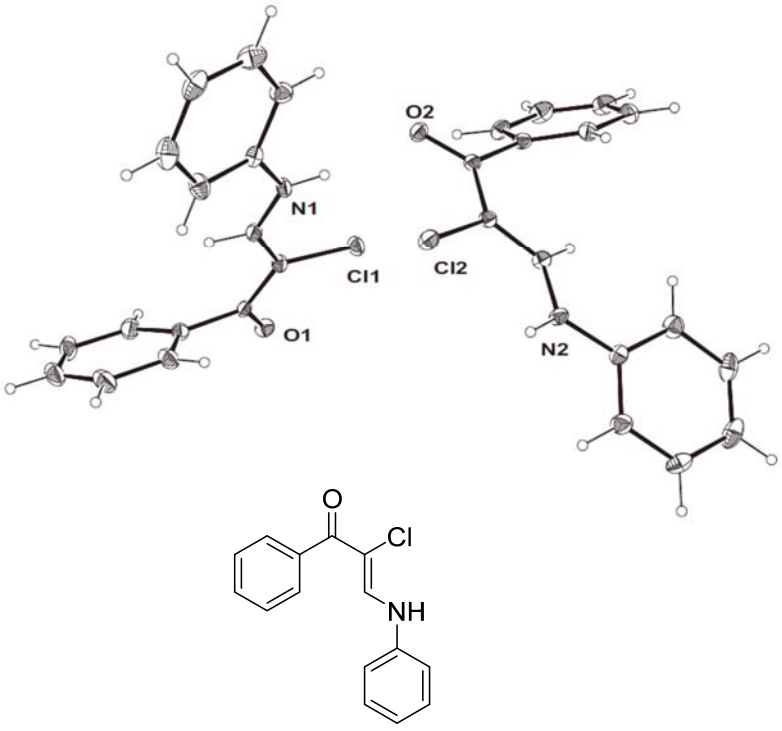
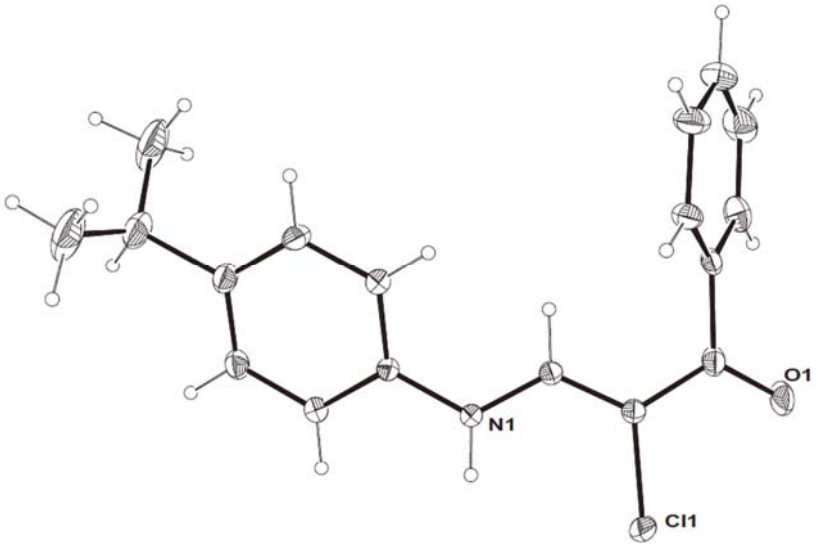


Table S1. Crystal data and structure refinement for d24546 (**3aa**).

Identification code	d24546	
Empirical formula	$C_{15}H_{12}BrClNO$	
Formula weight	257.71	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P c a 21	
Unit cell dimensions	a = 20.4024(11) Å	α= 90°.
	b = 8.0914(4) Å	β= 90°.
	c = 16.3490(8) Å	γ = 90°.
Volume	2699.0(2) $Å^3$	
Z	8	
Density (calculated)	1.268 Mg/m^3	
Absorption coefficient	0.270 mm^{-1}	
F(000)	1072	
Crystal size	0.52 x 0.48 x 0.30 mm^3	
Theta range for data collection	2.00 to 25.00°.	
Index ranges	-24<=h<=23, -8<=k<=9, -16<=l<=19	
Reflections collected	19163	
Independent reflections	4314 [R(int) = 0.0842]	
Completeness to theta = 25.00°	99.6 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9234 and 0.8725	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4314 / 1 / 325	
Goodness-of-fit on F^2	1.002	
Final R indices [I>2sigma(I)]	R1 = 0.0435, wR2 = 0.1049	
R indices (all data)	R1 = 0.0635, wR2 = 0.1140	
Absolute structure parameter	0.06(7)	
Largest diff. peak and hole	0.604 and -0.176 $e.Å^{-3}$	

Ortep (ellipsoid counter 30% probability**) diagram and crystal data of compound 3af: CCDC Number 2370736**



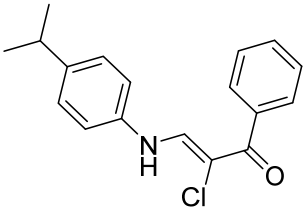


Table S2. Crystal data and structure refinement for 25152 (**3af**).

Identification code	d25152	
Empirical formula	$C_{18}H_{18}ClNO$	
Formula weight	299.78	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 9.9614(6) Å	α= 90°.
	b = 15.4727(9) Å	β= 109.434(2)°.
	c = 11.3672(7) Å	γ = 90°.
Volume	1652.20(17) $Å^3$	
Z	4	
Density (calculated)	1.205 Mg/m^3	
Absorption coefficient	0.230 mm^{-1}	
F(000)	632	
Crystal size	0.53 x 0.44 x 0.03 mm^3	
Theta range for data collection	2.31 to 25.05°.	
Index ranges	-11<=h<=11, -18<=k<=18, -13<=l<=13	
Reflections collected	34591	
Independent reflections	2917 [R(int) = 0.0954]	
Completeness to theta = 25.05°	99.7 %	
Absorption correction	None	
Max. and min. transmission	0.9931 and 0.8880	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2917 / 0 / 186	
Goodness-of-fit on F^2	1.149	
Final R indices [I>2sigma(I)]	R1 = 0.0576, wR2 = 0.1394	
R indices (all data)	R1 = 0.0746, wR2 = 0.1516	
Largest diff. peak and hole	0.503 and -0.540 $e.Å^{-3}$	

Ortep (ellipsoid counter 30% probability**) diagram and crystal data of compound 6ea: CCDC Number 2360356**

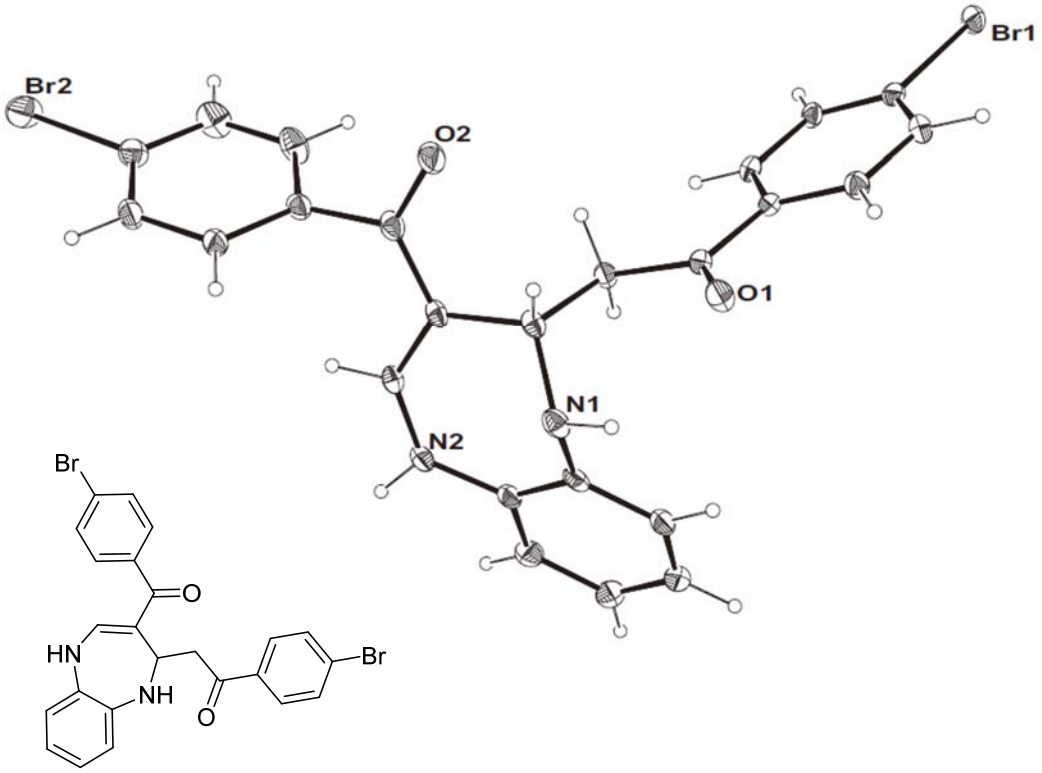


Table S3. Crystal data and structure refinement for d25025 (**6ea**).

Identification code	d25025	
Empirical formula	C_{24} H_{18} Br_2 N_2 O_2	
Formula weight	526.22	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 32.4571(15) Å	α= 90°.
	b = 13.4666(5) Å	β= 110.33°.
	c = 11.2783(5) Å	γ = 90°.
Volume	4622.4(3) $Å^3$	
Z	8	
Density (calculated)	1.512 Mg/m^3	
Absorption coefficient	3.529 mm^{-1}	
F(000)	2096	
Crystal size	0.21 x 0.10 x 0.03 mm^3	
Theta range for data collection	2.36 to 25.07°.	
Index ranges	-38<=h<=38, -16<=k<=14, -13<=l<=13	
Reflections collected	23074	
Independent reflections	4072 [R(int) = 0.0642]	
Completeness to theta = 25.07°	99.4 %	
Absorption correction	None	
Max. and min. transmission	0.9015 and 0.5244	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4072 / 0 / 271	
Goodness-of-fit on F^2	0.685	
Final R indices [I>2sigma(I)]	R1 = 0.0355, wR2 = 0.0960	
R indices (all data)	R1 = 0.0431, wR2 = 0.1038	
Largest diff. peak and hole	0.546 and -1.033 $e.Å^{-3}$	

Comments on checkcif:

Checkcif highlighted A level alerts which have been commented on here

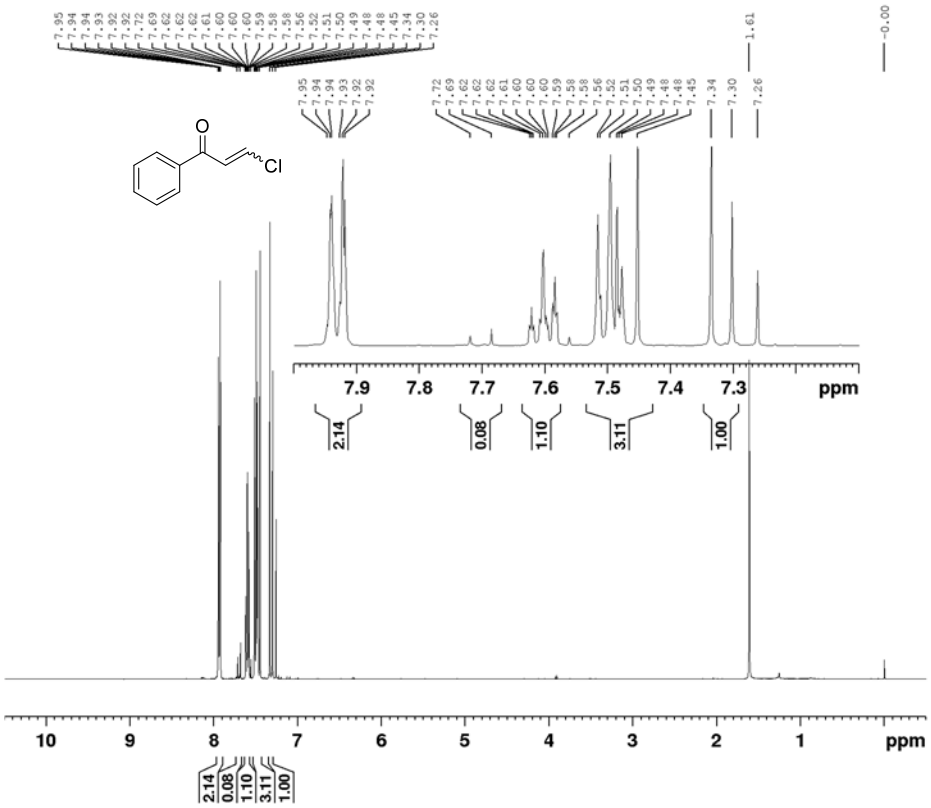
Compound 6ea

PLAT601_ALERT_2_A Unit Cell Contains Solvent Accessible VOIDS of. 272 Ang**3

Author response: The highest peak in the final difference map is just 0.55 e/A^3 and no model could be found for any solvent.

3. NMR Spectra copies

3-chloro-1-phenylprop-2-en-1-one (1a)

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Current Data Parameters
NAME                  Enaminone
EXPNO                        48
PROCNO                        1

F2 - Acquisition Parameters
Date_               20231223
Time                    15.37
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                7211.539 Hz
FIDRES             0.220079 Hz
AQ                 2.2719147 sec
RG                     128.9
DW                  69.333 usec
DE                  10.06 usec
TE                  297.4 K
D1                 2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            400.1324008 MHz
NUC1                      1H
P1                    15.00 usec
PLW1           13.50000000 W

F2 - Processing parameters
SI                     16384
SF              400.1300090 MHz
WDW                       EM
SSB                        0
LB                         0 Hz
GB                         0
PC                      1.00
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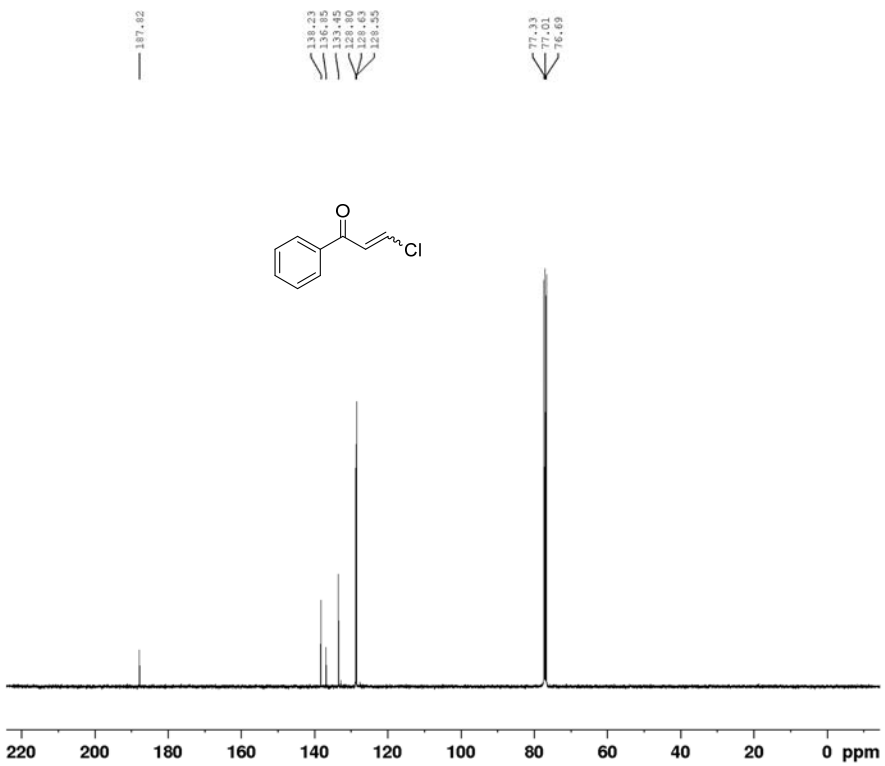


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Current Data Parameters
NAME                  Enaminone
EXPNO                        24
PROCNO                        1

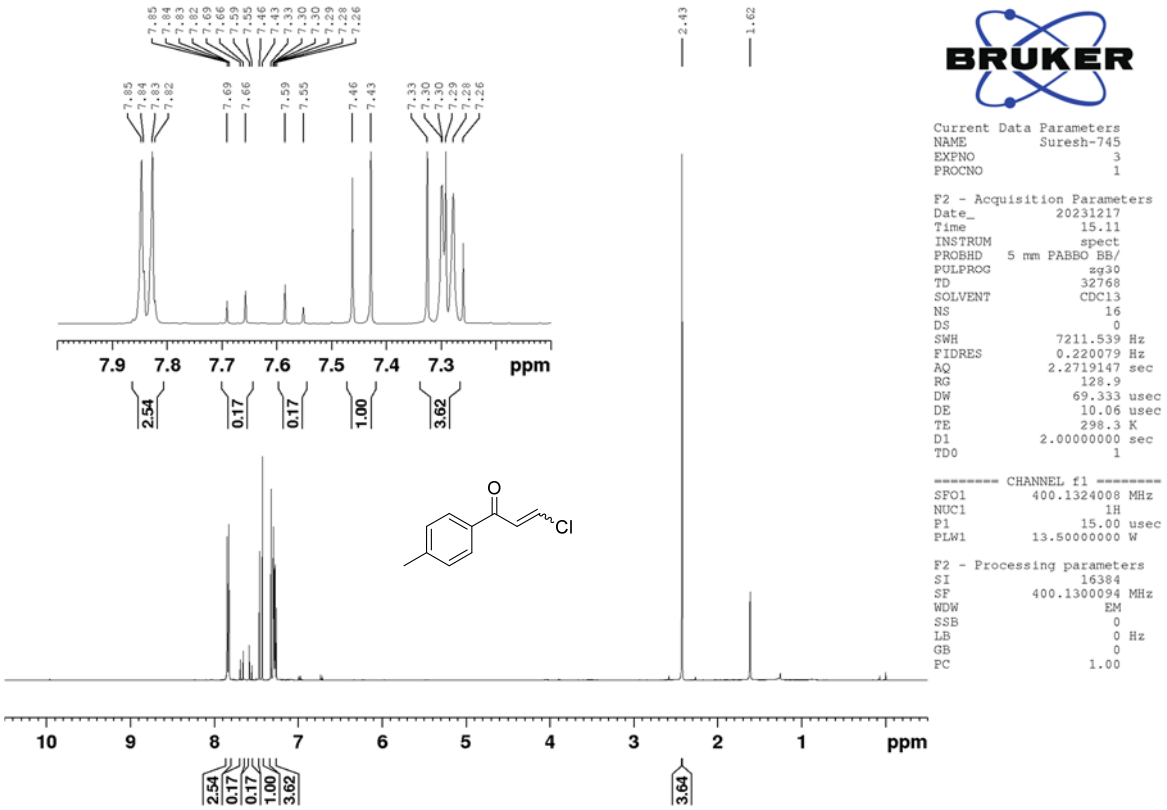
F2 - Acquisition Parameters
Date_               20231223
Time                    17.14
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      2048
DS                         0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                     32768
DW                  20.800 usec
DE                   6.50 usec
TE                  297.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                   10.00 usec
PL1                   4.20 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                      1H
PCPD2                90.00 usec
PL2                  10.20 dB
PL12                 26.00 dB
PL13                 29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF              100.6127690 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                      1.00
```

3-chloro-1-(*p*-tolyl)prop-2-en-1-one (1b)

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Current Data Parameters
NAME          Suresh-745
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231217
Time               15.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 128.9
DW                69.333 usec
DE                10.06 usec
TE                298.3 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324008 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          13.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300094 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
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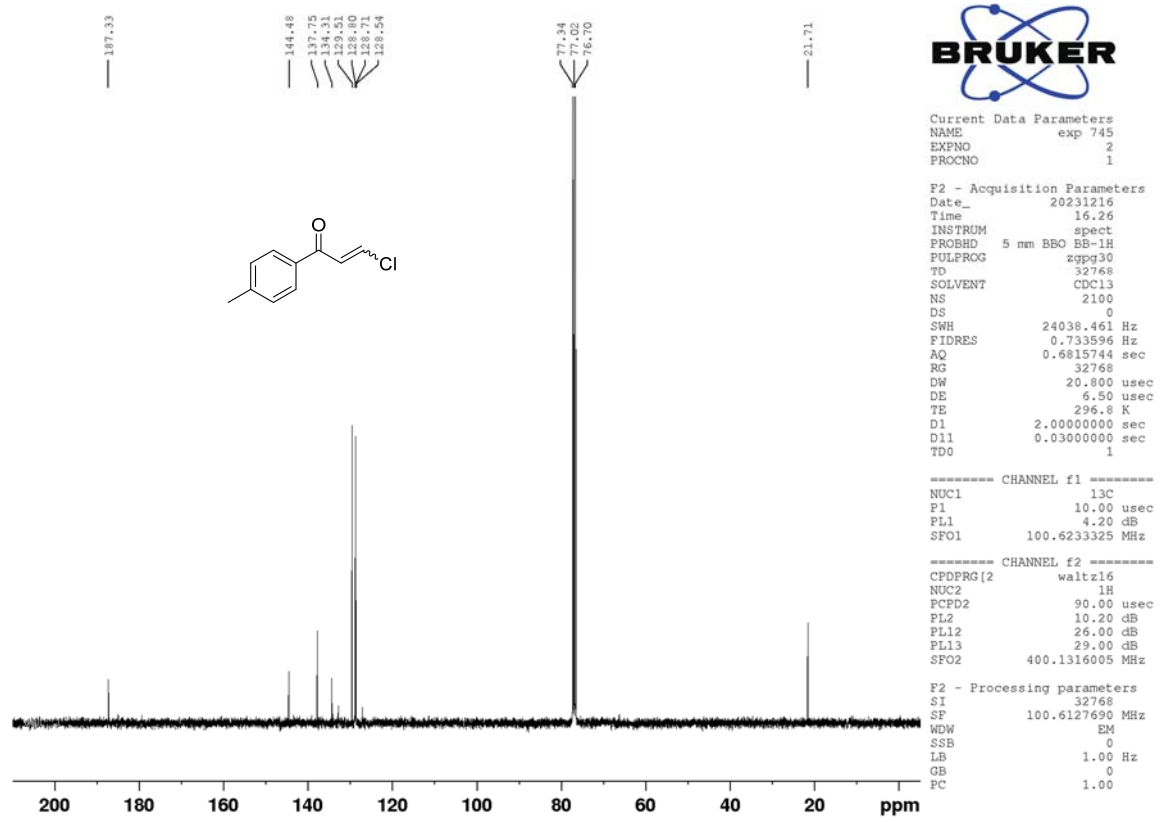


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Current Data Parameters
NAME             exp 745
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231216
Time               16.26
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                  2100
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 32768
DW                20.800 usec
DE                 6.50 usec
TE                296.8 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 4.20 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```
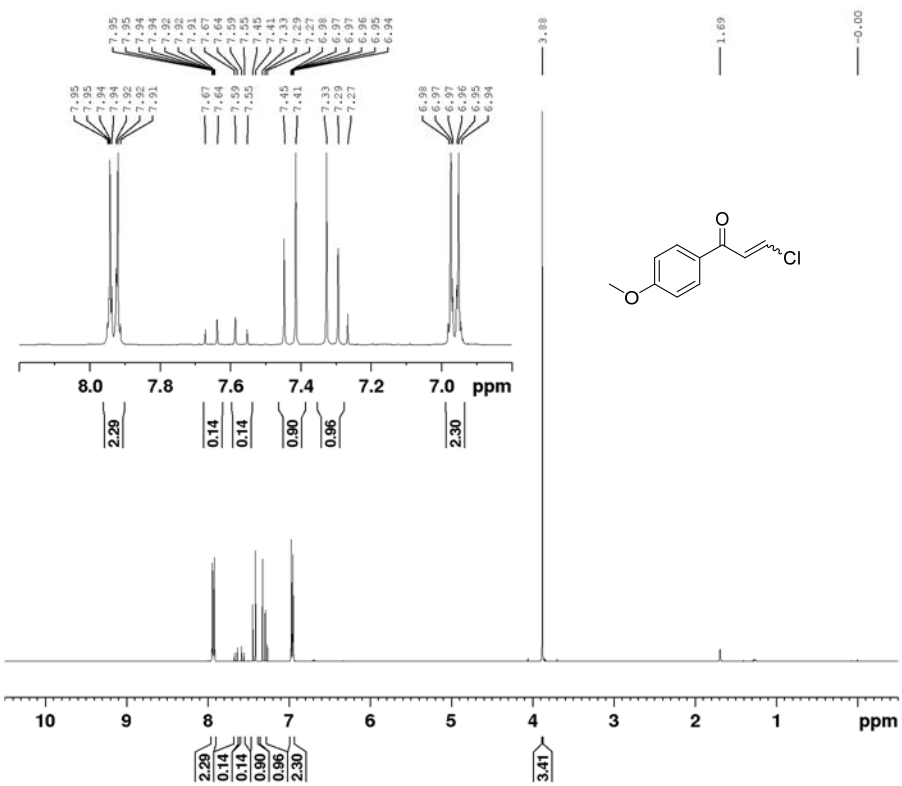

3-chloro-1-(4-methoxyphenyl)prop-2-en-1-one (1c)



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Current Data Parameters
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EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231207
Time               21.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 89.08
DW                69.333 usec
DE                10.06 usec
TE                298.3 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                  15.00 usec
PLW1          13.50000000 W

F2 - Processing parameters
SI                 16384
SF           400.1300072 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
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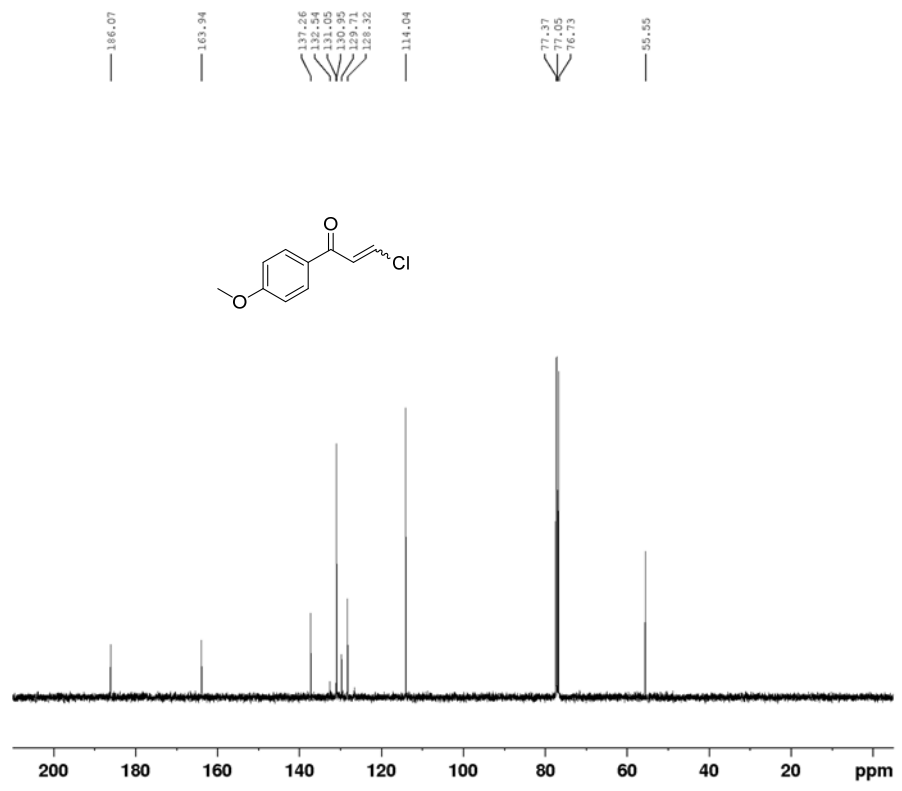

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Current Data Parameters
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EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20231207
Time               20.58
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDC13
NS                   151
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 32768
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                4.20 dB
SFO1         100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
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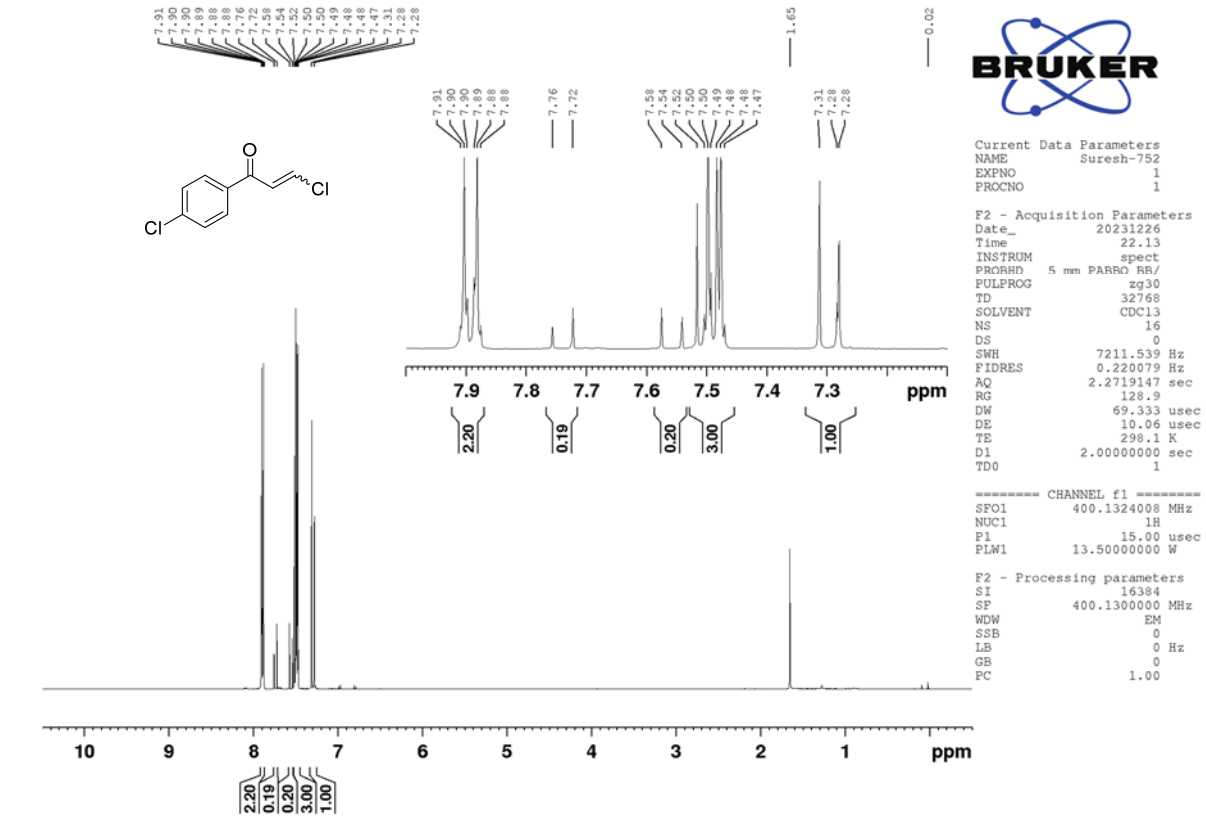
3-chloro-1-(4-chlorophenyl)prop-2-en-1-one (1d)

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Current Data Parameters
NAME                 Suresh-752
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20231226
Time                   22.13
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                7211.539 Hz
FIDRES             0.220079 Hz
AQ                 2.2719147 sec
RG                     128.9
DW                    69.333 usec
DE                    10.06 usec
TE                    298.1 K
D1                 2.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1              400.1324008 MHz
NUC1                        1H
P1                       15.00 usec
PLW1              13.50000000 W

F2 - Processing parameters
SI                        16384
SF                400.1300000 MHz
WDW                          EM
SSB                           0
LB                         0 Hz
GB                            0
PC                         1.00
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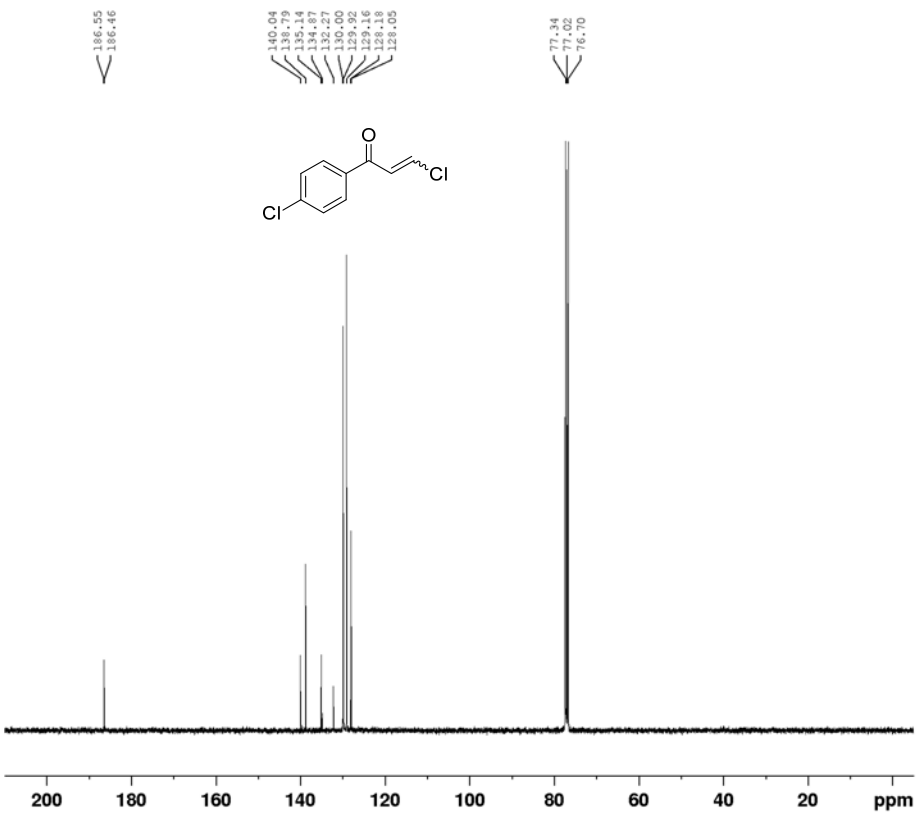


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Current Data Parameters
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EXPNO                        2
PROCNO                       1

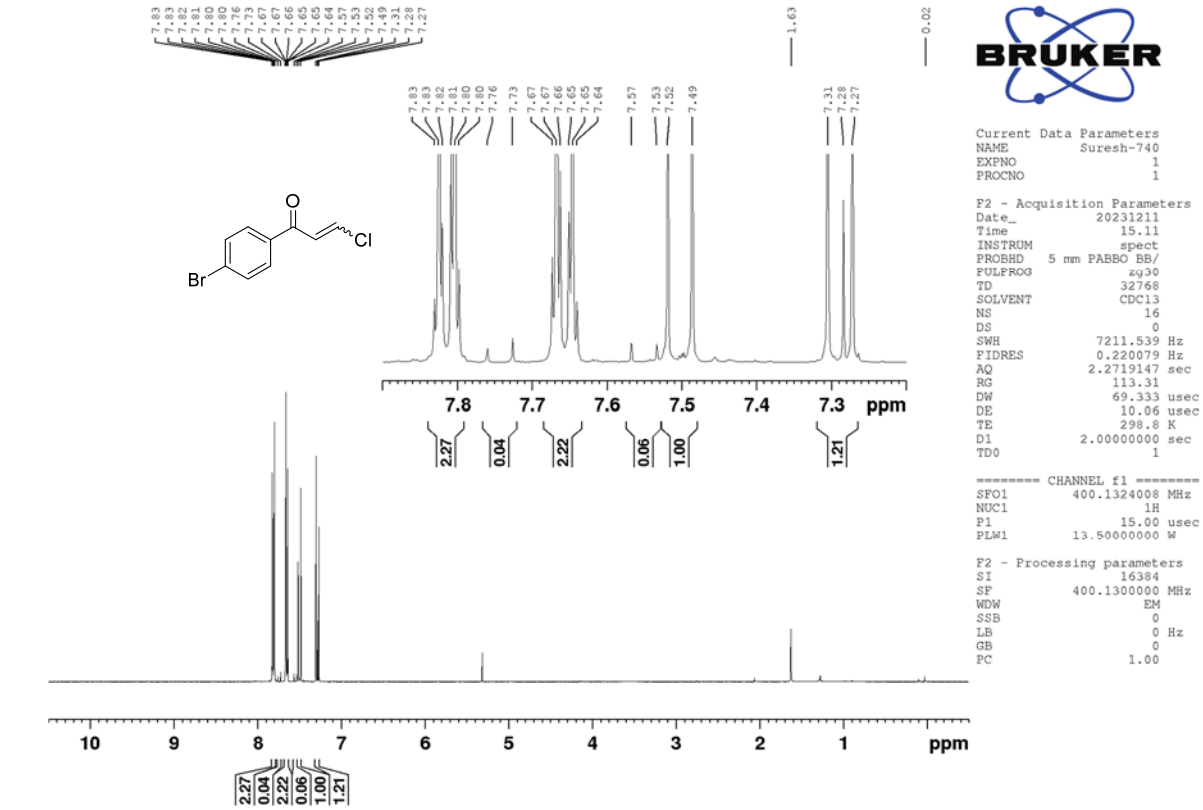
F2 - Acquisition Parameters
Date_               20231227
Time                   12.10
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     1392
DS                        0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                    32768
DW                   20.800 usec
DE                    6.50 usec
TE                    298.4 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
NUC1                        13C
P1                       10.00 usec
PL1                       4.20 dB
SFO1              100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                        1H
PCPD2                    90.00 usec
PL2                      10.20 dB
PL12                     26.00 dB
PL13                     29.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127690 MHz
WDW                          EM
SSB                           0
LB                         1.00 Hz
GB                            0
PC                         1.00
```

1-(4-bromophenyl)-3-chloroprop-2-en-1-one (1e)



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Current Data Parameters
NAME          Suresh-740
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231211
Time               15.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG               113.31
DW               69.333 usec
DE               10.06 usec
TE               298.8 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                   1H
P1                15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
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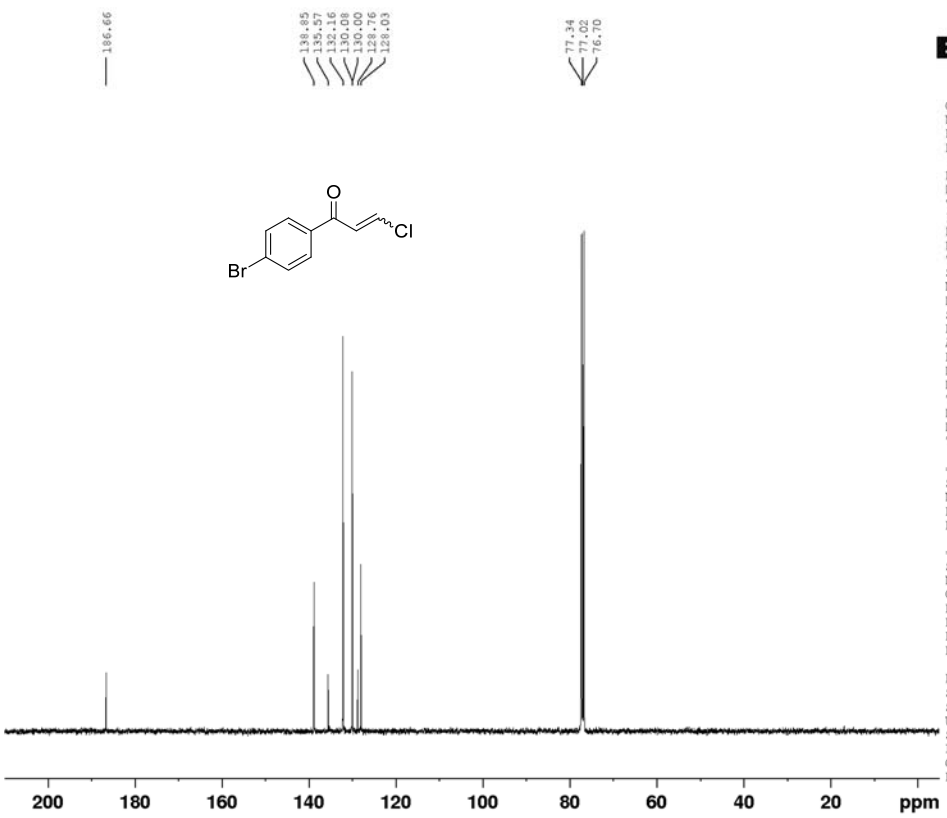

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```
Current Data Parameters
NAME          Suresh-740
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231211
Time               17.20
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  512
DS                    0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE               298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                   13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
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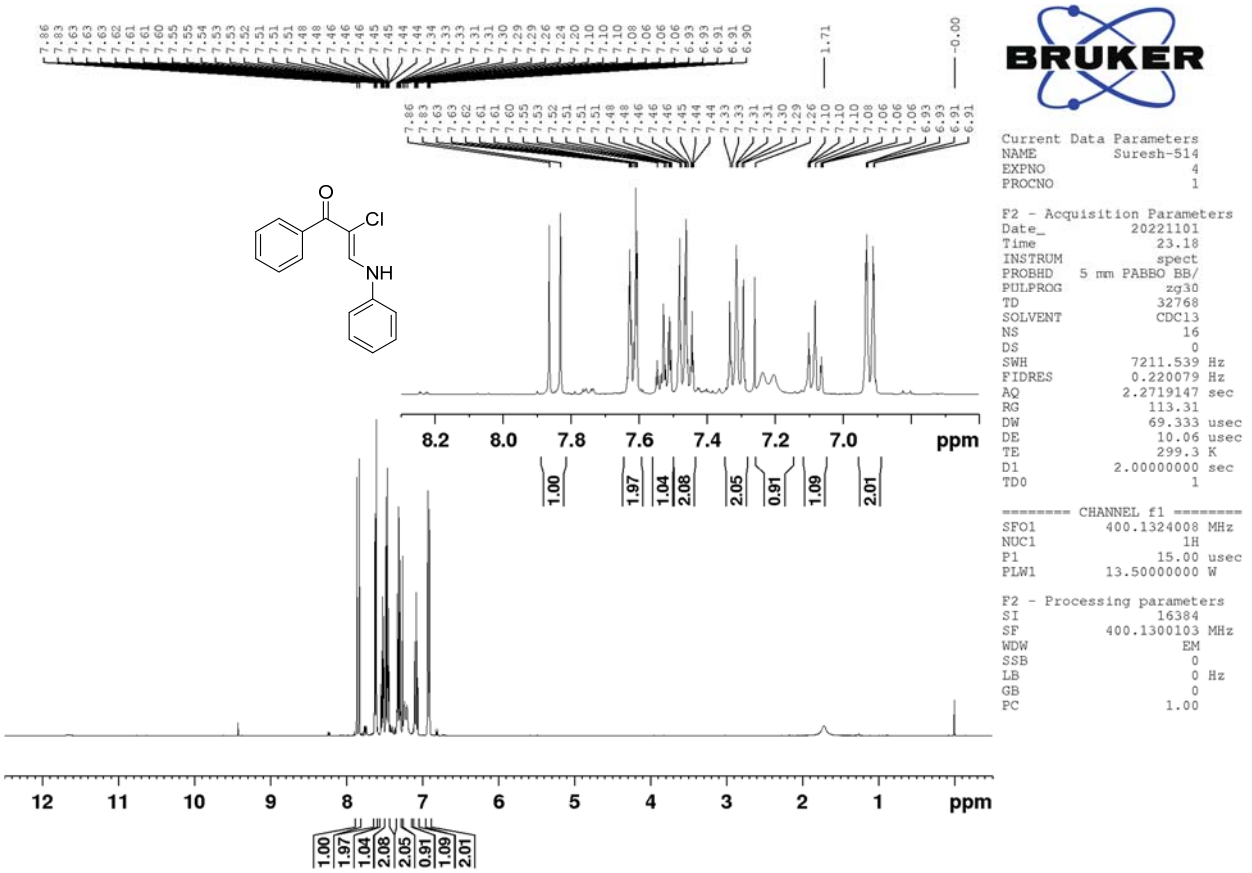
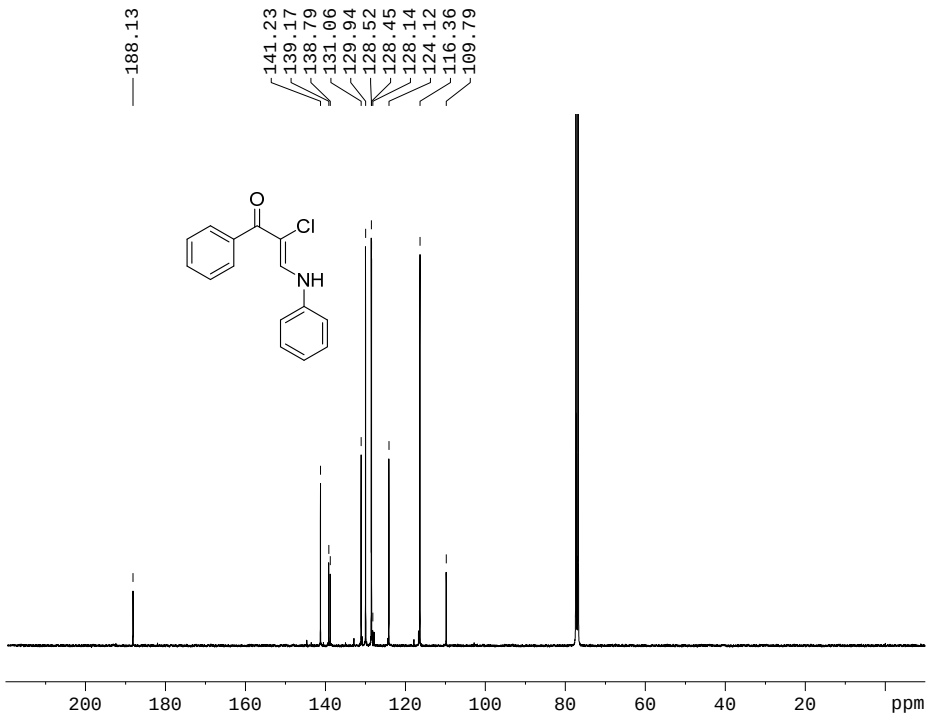
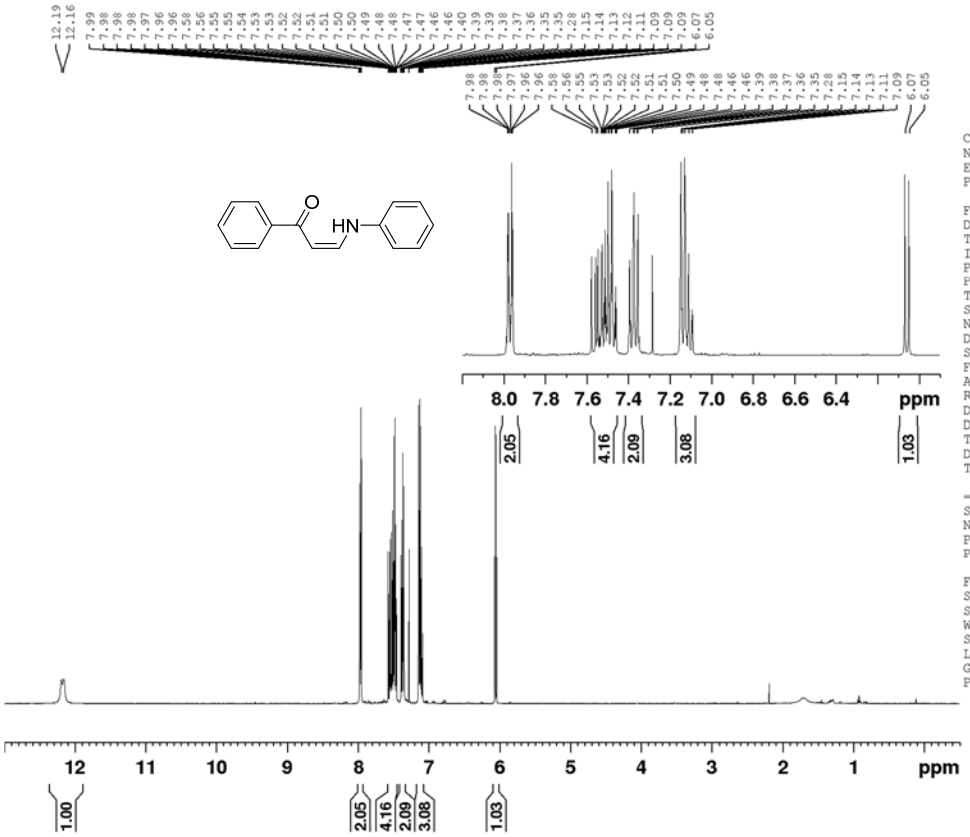
(*Z*)-2-chloro-1-phenyl-3-(phenylamino)prop-2-en-1-one (3aa)





(*Z*)-1-phenyl-3-(phenylamino)prop-2-en-1-one (4aa)



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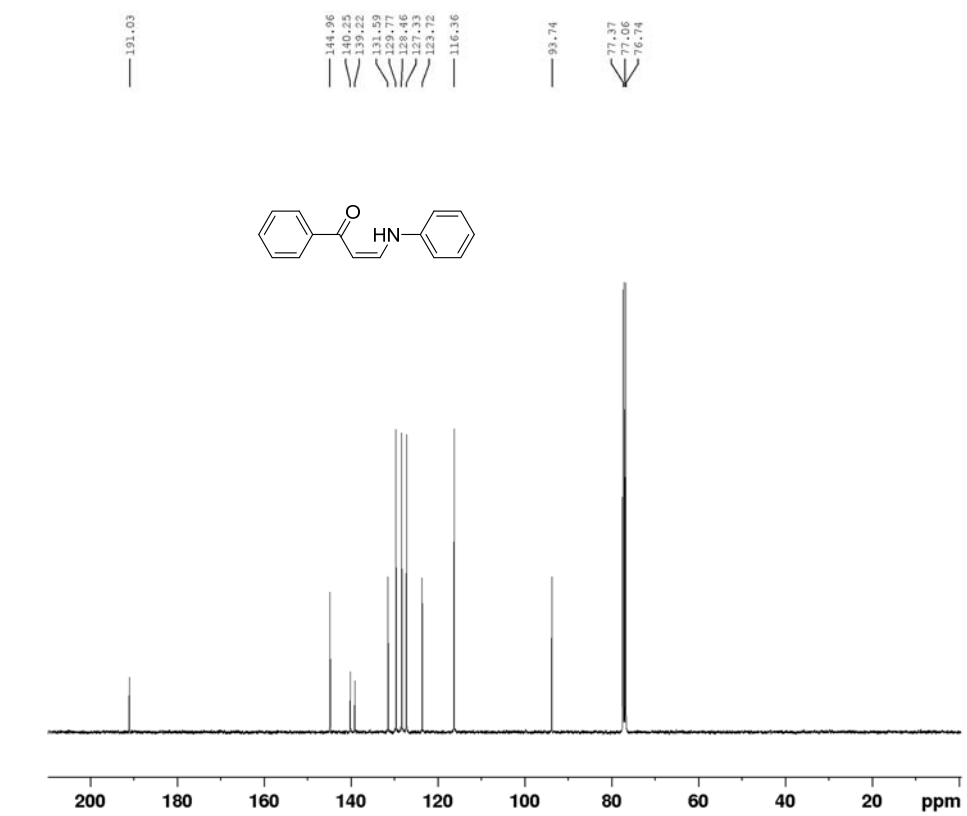
```
Current Data Parameters
NAME          Suresh-515
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221101
Time               22.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    16
DS                     0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                 89.08
DW               69.333 usec
DE                10.06 usec
TE                299.1 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



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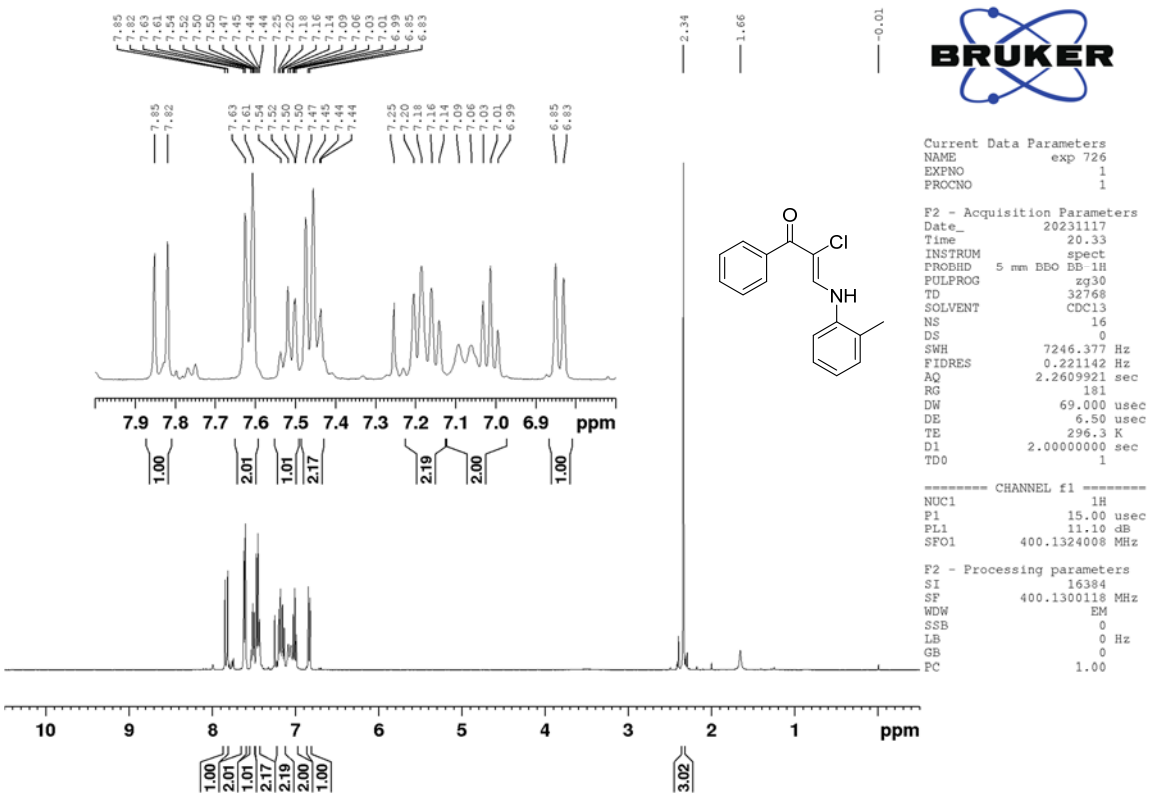
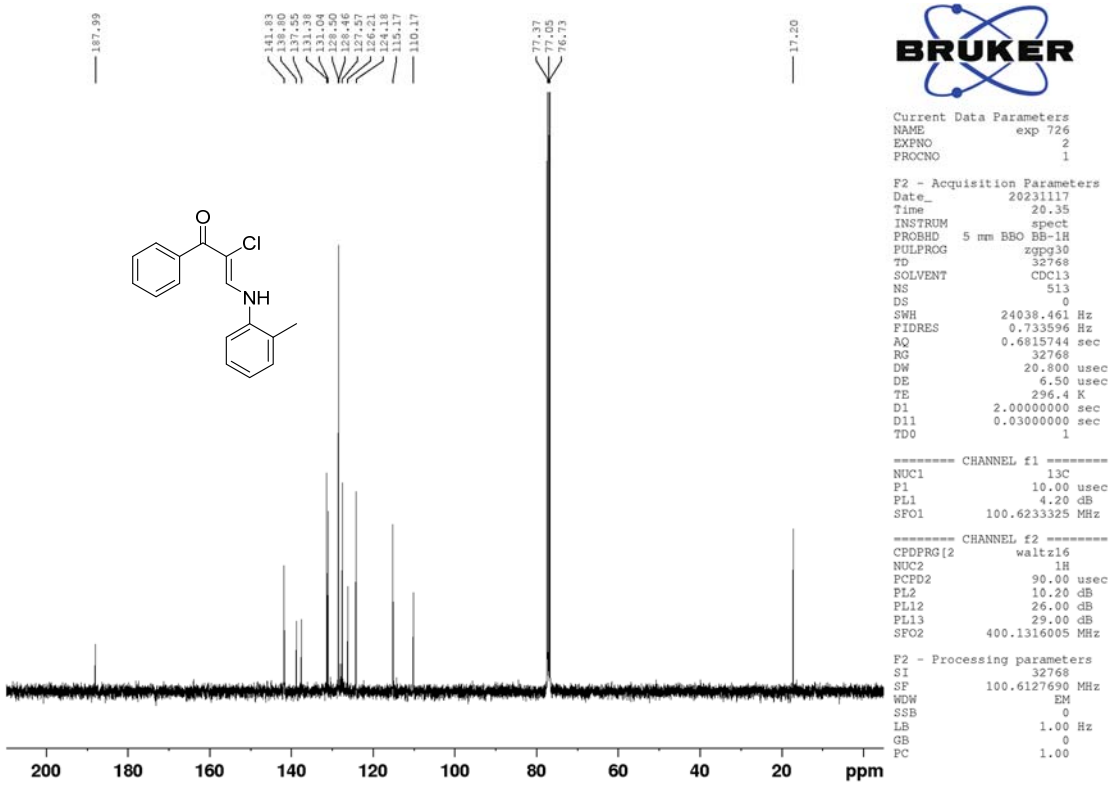
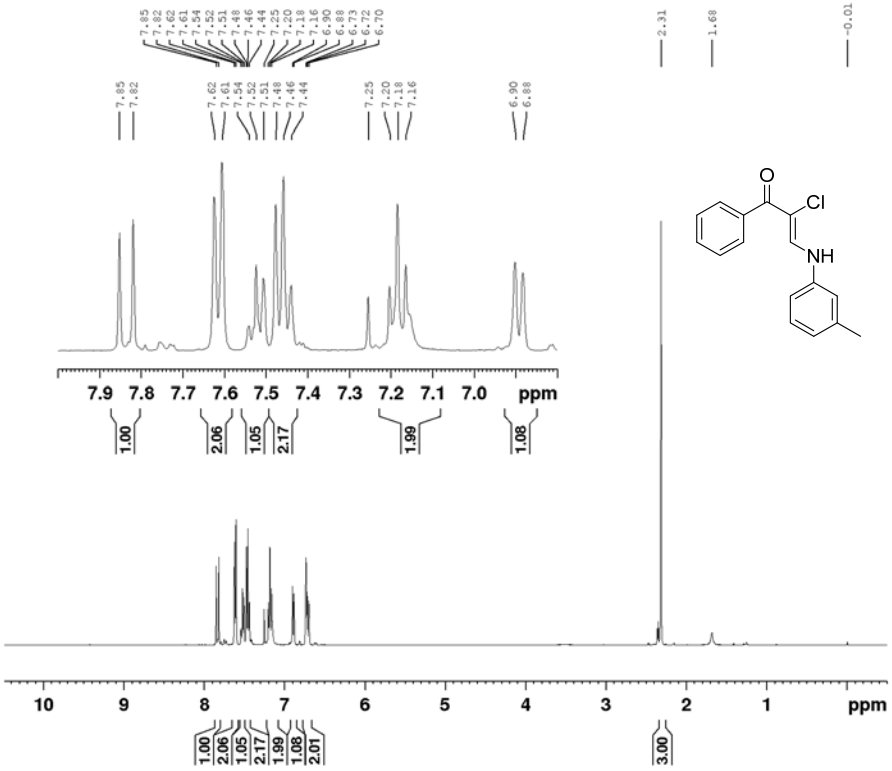
```
Current Data Parameters
NAME          Suresh-515
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20221101
Time               22.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32760
SOLVENT            CDC13
NS                  1024
DS                     0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                299.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                  13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-2-chloro-1-phenyl-3-(*o*-tolylamino)prop-2-en-1-one (3ab)

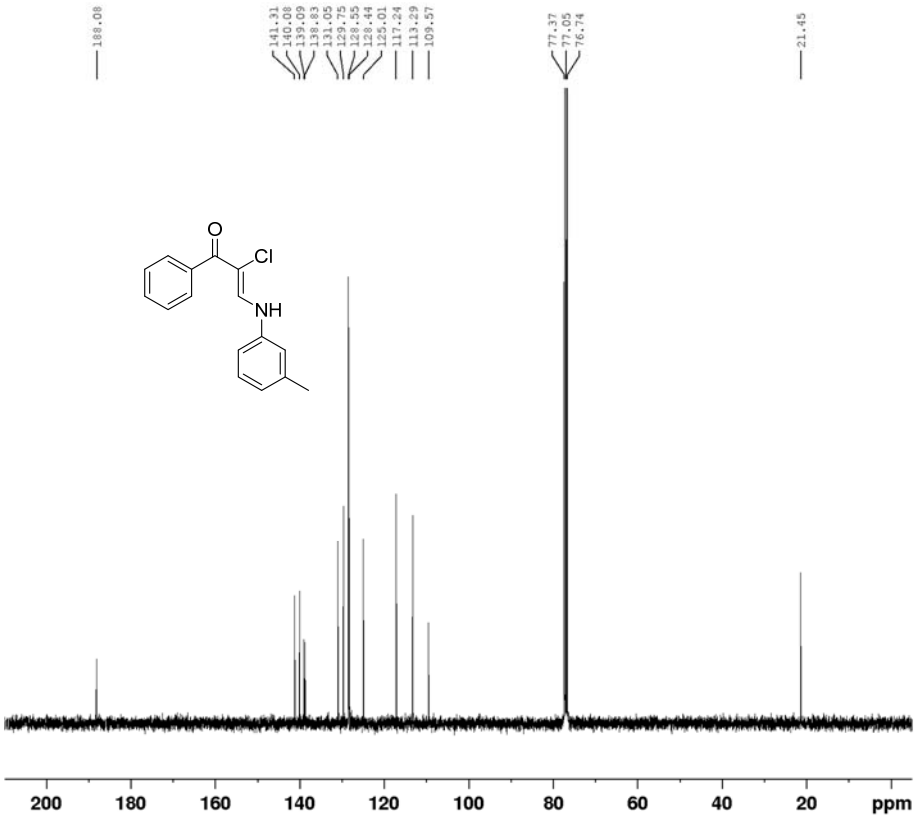




(*Z*)-2-chloro-1-phenyl-3-(*m*-tolylamino)prop-2-en-1-one (3ac)

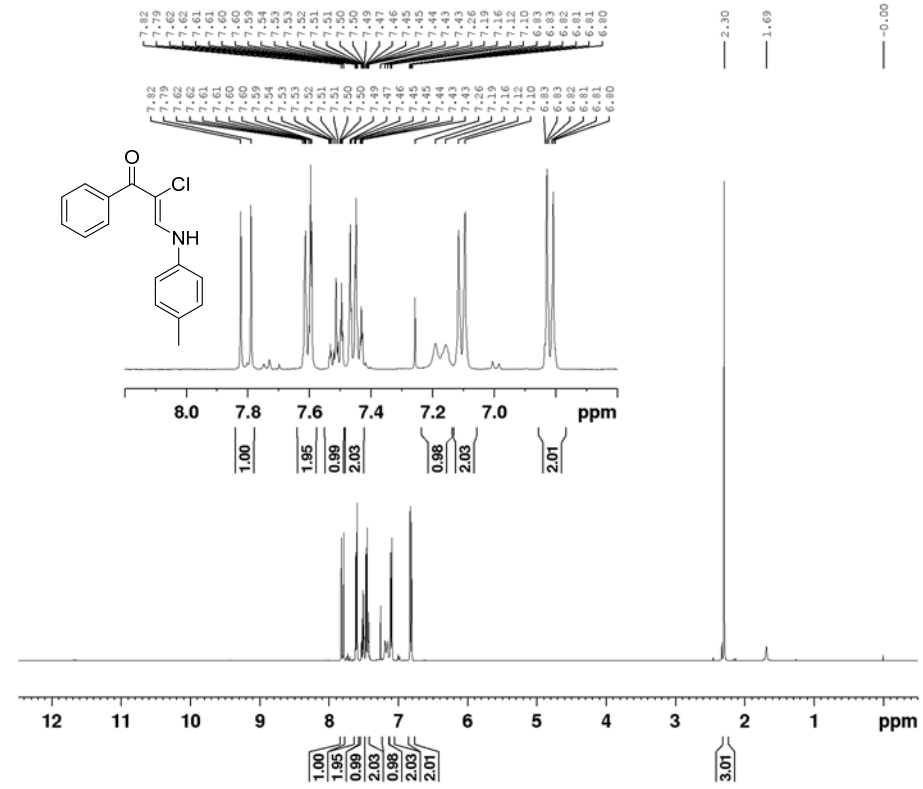



```
Current Data Parameters
NAME                  exp 729
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_               20231120
Time                   17.40
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                     32768
SOLVENT                CDC13
NS                        16
DS                         0
SWH                7246.377 Hz
FIDRES             0.221142 Hz
AQ                 2.2609921 sec
RG                       181
DW                    69.000 usec
DE                     6.50 usec
TE                    296.2 K
D1                 2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PL1                    11.10 dB
SFO1            400.1324008 MHz

F2 - Processing parameters
SI                     16384
SF                400.1300118 MHz
WDW                       EM
SSB                        0
LB                      0 Hz
GB                         0
PC                      1.00
```

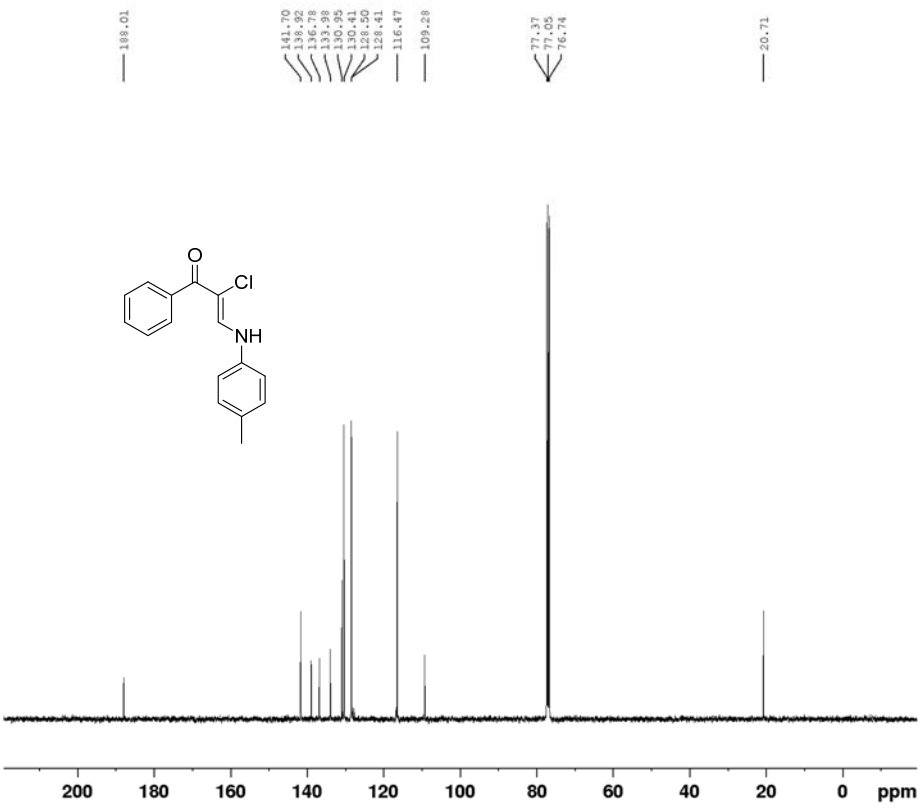



```
Current Data Parameters
NAME                  exp 729
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_               20231120
Time                   17.42
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                     32768
SOLVENT                CDC13
NS                       412
DS                         0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                     32768
DW                    20.800 usec
DE                     6.50 usec
TE                    296.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                     10.00 usec
PL1                     4.20 dB
SFO1           100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                      1H
PCPD2                 90.00 usec
PL2                    10.20 dB
PL12                   26.00 dB
PL13                   29.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                     32768
SF                100.6127690 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.00
```

(*Z*)-2-chloro-1-phenyl-3-(*p*-tolylamino)prop-2-en-1-one (3ad)

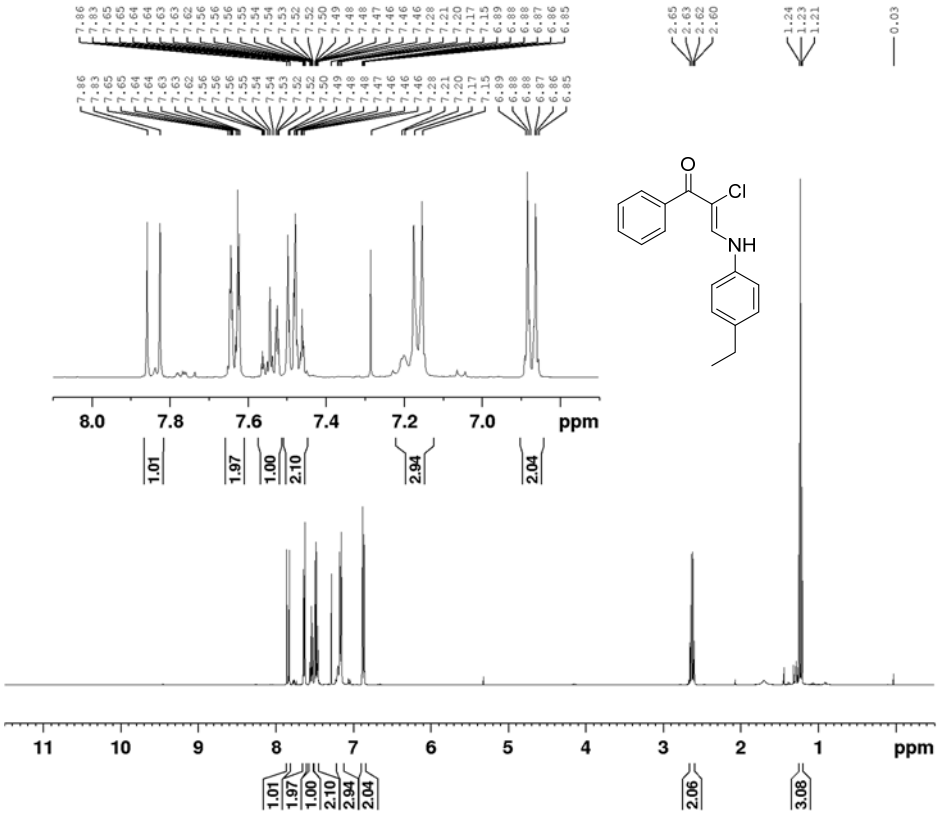


```
Current Data Parameters
NAME          Suresh-730
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231120
Time               12.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 89.08
DW                69.333 usec
DE                10.06 usec
TE                299.4 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                  15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF           400.1300107 MHz
WDW                   EM
SSB                    0
LB                  0 Hz
GB                     0
PC                  1.00
```

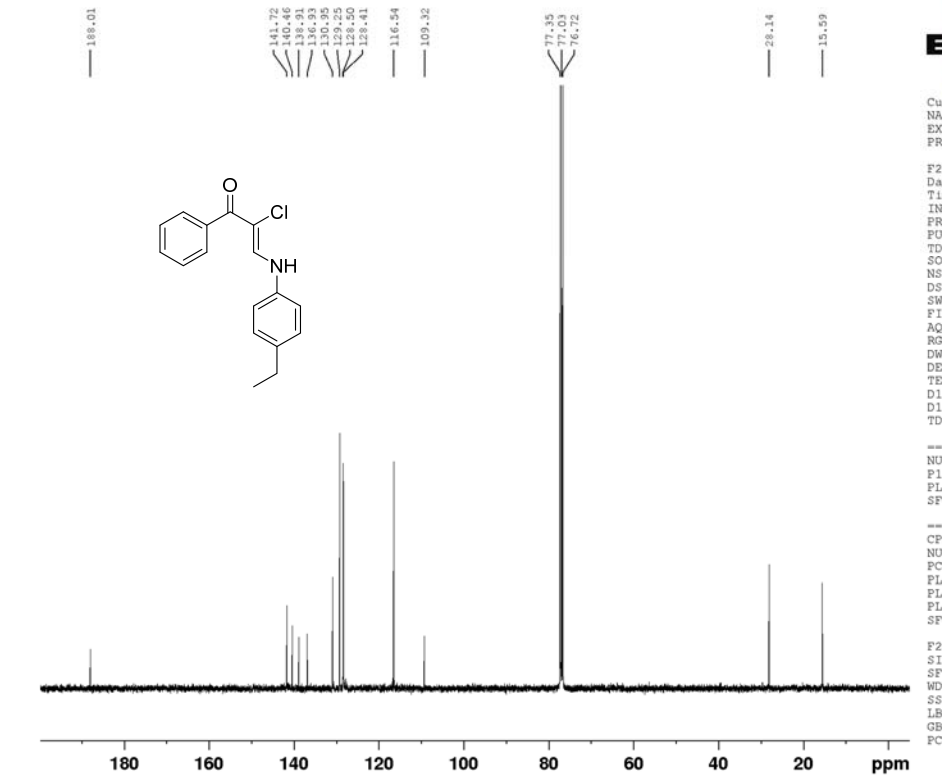


```
Current Data Parameters
NAME          Suresh-730
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231120
Time               12.06
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT            CDC13
NS                   400
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                299.4 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                  10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-2-chloro-3-((4-ethylphenyl)amino)-1-phenylprop-2-en-1-one (3ae)

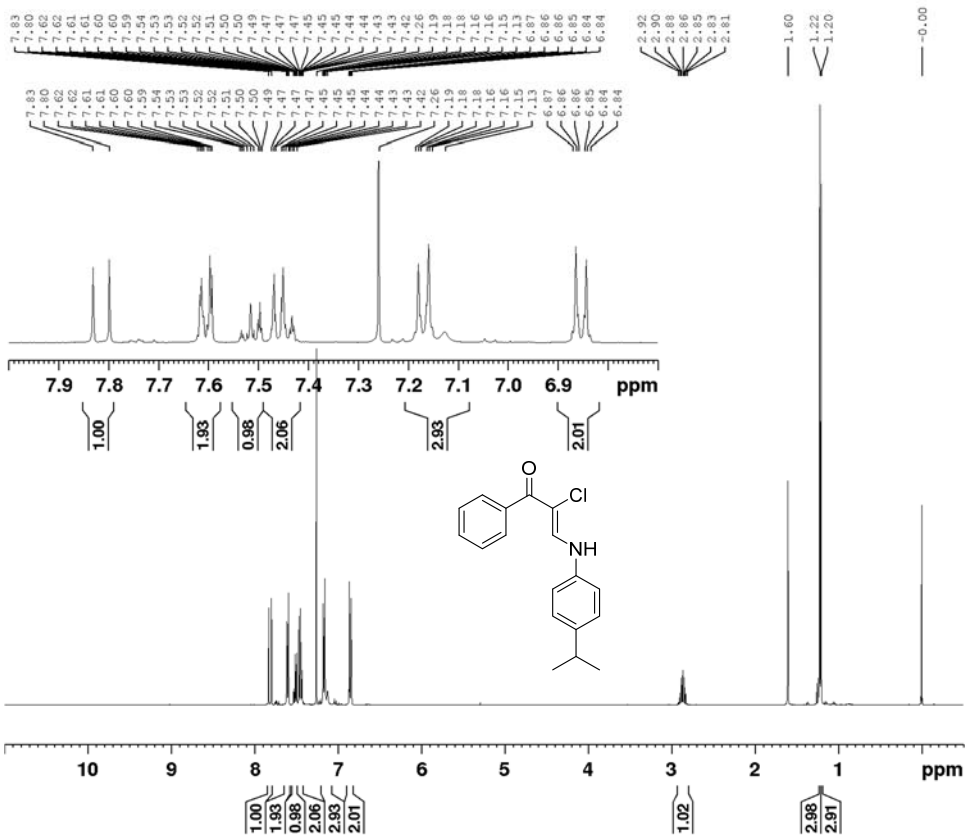


```
Current Data Parameters
NAME                  Enaminone
EXPNO                        22
PROCNO                        1

F2 - Acquisition Parameters
Date_               20231101
Time                    11.19
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                      32768
SOLVENT                 CDC13
NS                         16
DS                          0
SWH                  7211.539 Hz
FIDRES               0.220079 Hz
AQ                   2.2719147 sec
RG                      113.31
DW                      69.333 usec
DE                      10.06 usec
TE                      298.7 K
D1                   2.00000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1            400.1324008 MHz
NUC1                       1H
P1                      15.00 usec
PLW1            13.50000000 W

F2 - Processing parameters
SI                      16384
SF                400.1300000 MHz
WDW                        EM
SSB                         0
LB                          0 Hz
GB                          0
PC                       1.00
```



```
Current Data Parameters
NAME                  Enaminone
EXPNO                        11
PROCNO                        1

F2 - Acquisition Parameters
Date_               20231101
Time                    11.57
INSTRUM                 spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zgpg30
TD                      32768
SOLVENT                 CDC13
NS                       1024
DS                          0
SWH                 24038.461 Hz
FIDRES               0.733596 Hz
AQ                   0.6815744 sec
RG                      32768
DW                      20.800 usec
DE                       6.50 usec
TE                      295.6 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                      10.00 usec
PL1                      4.20 dB
SFO1            100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL2                     10.20 dB
PL12                    26.00 dB
PL13                    29.00 dB
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                      32768
SF                100.6127690 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.00
```

(*Z*)-2-chloro-3-((4-isopropylphenyl)amino)-1-phenylprop-2-en-1-one (3af)



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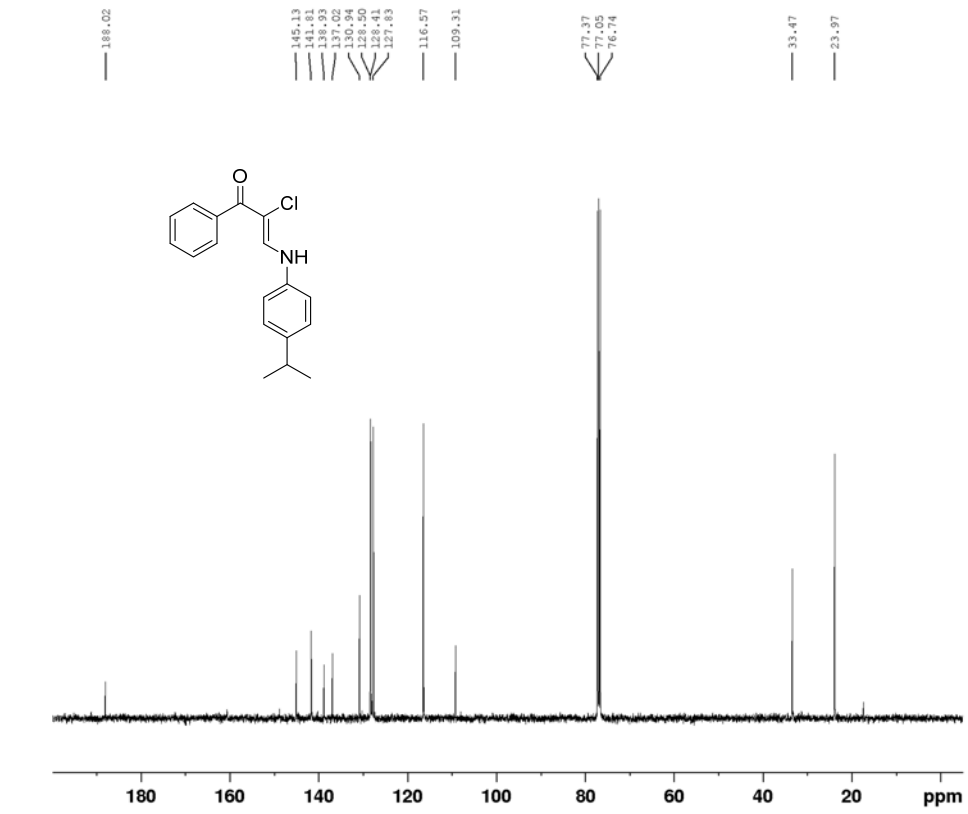
```
Current Data Parameters
NAME            Enaminone
EXPNO                  78
PROCNO                  1

F2 - Acquisition Parameters
Date_            20240705
Time                10.30
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH              7211.539 Hz
FIDRES           0.220079 Hz
AQ               2.2719147 sec
RG                  128.9
DW                 69.333 usec
DE                 10.06 usec
TE                 300.6 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                  15.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                  16384
SF           400.1300103 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```



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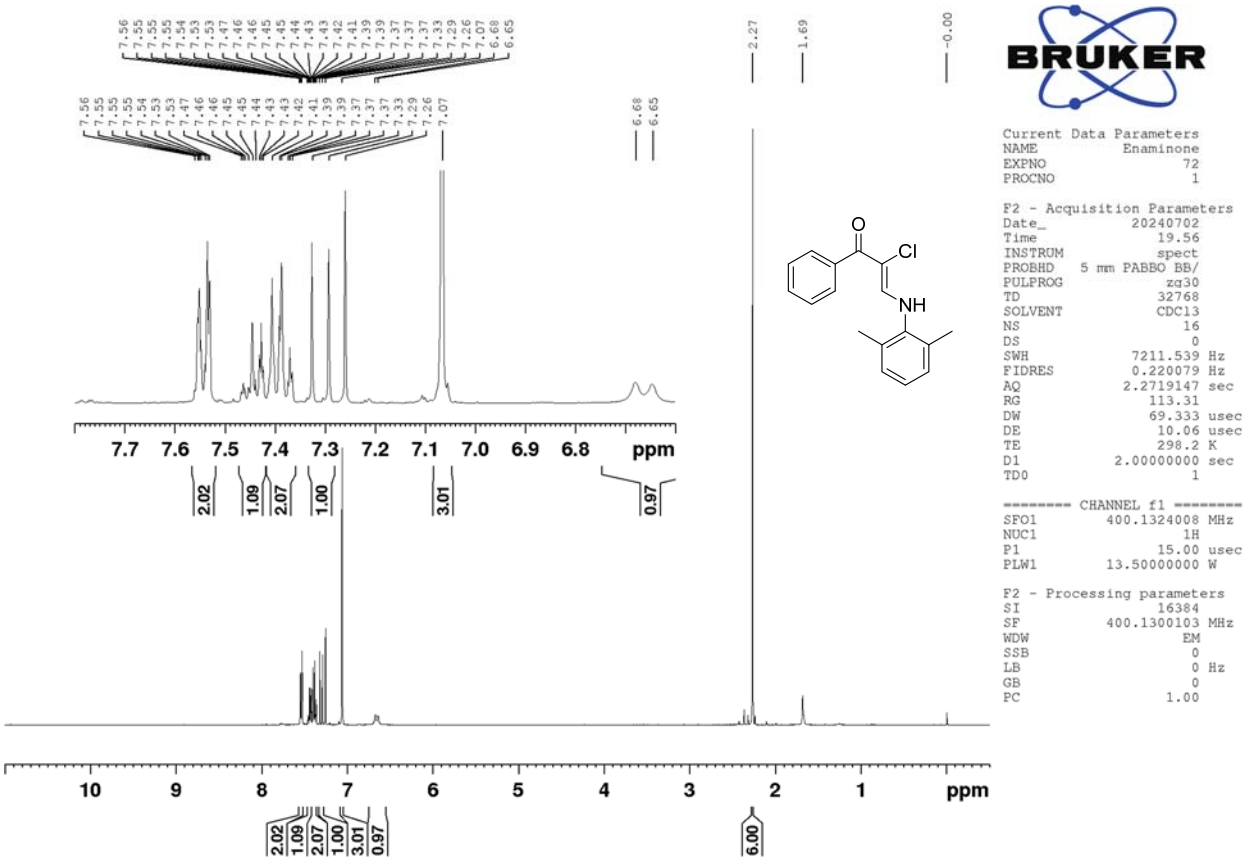
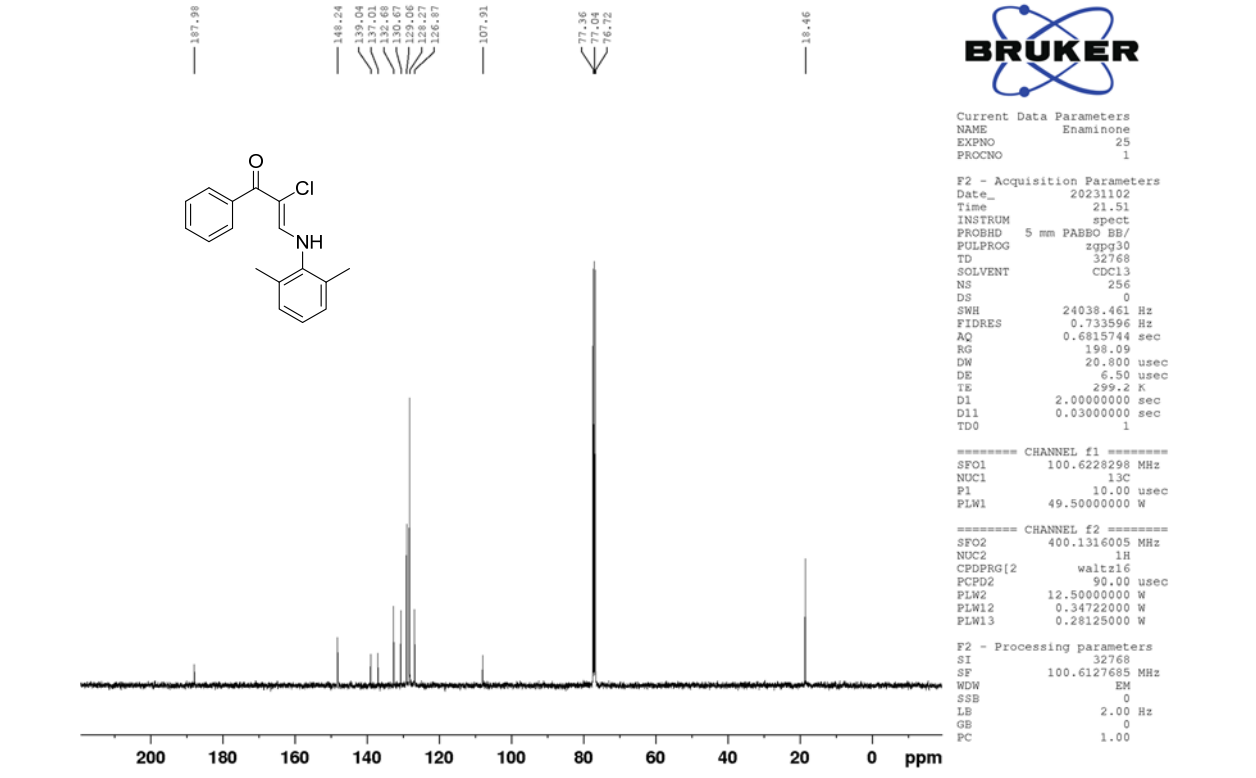
```
Current Data Parameters
NAME          Suresh-701
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_            20231008
Time                13.18
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  32768
SOLVENT             CDCl3
NS                    256
DS                      0
SWH             24038.461 Hz
FIDRES           0.733596 Hz
AQ               0.6815744 sec
RG                  198.09
DW                 20.800 usec
DE                  6.50 usec
TE                 297.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                  10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                  32768
SF           100.6127685 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```

(*Z*)-2-chloro-3-((2,6-dimethylphenyl)amino)-1-phenylprop-2-en-1-one (3ag)



BRUKER

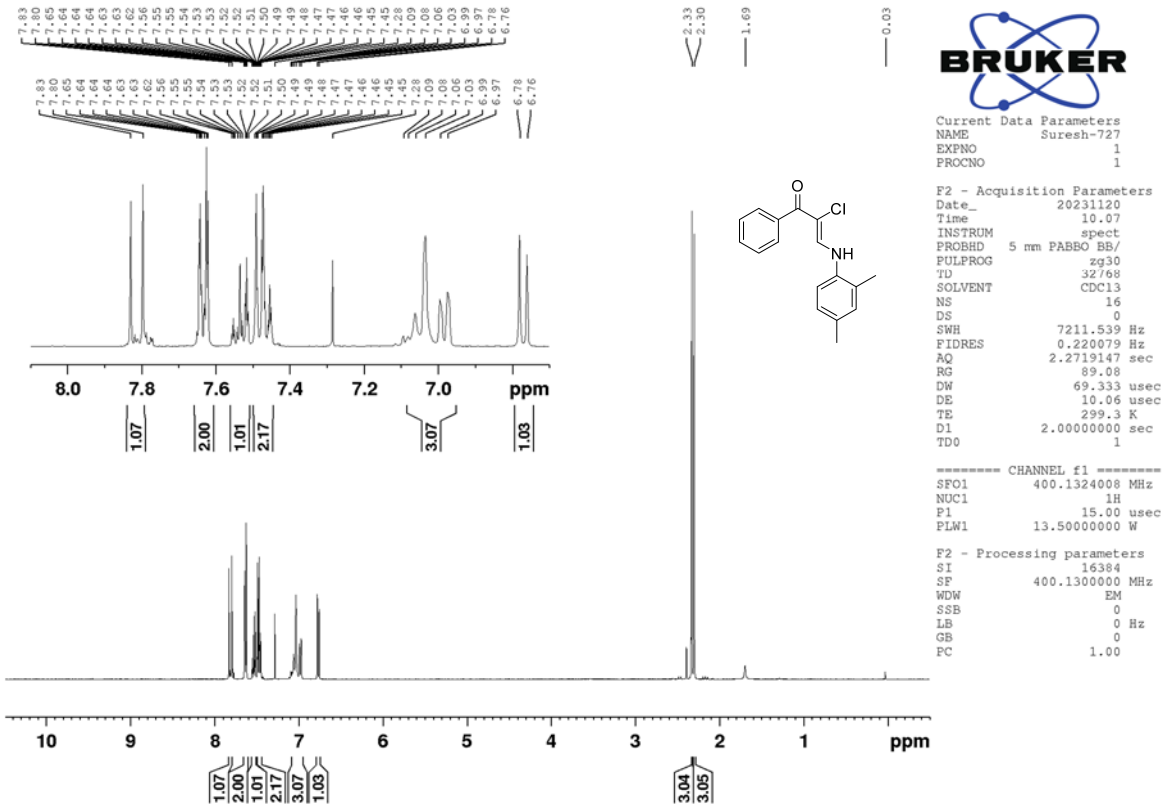
```
Current Data Parameters
NAME                  Enaminone
EXPNO                        72
PROCNO                        1

F2 - Acquisition Parameters
Date_               20240702
Time                   19.56
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 7211.539 Hz
FIDRES                0.220079 Hz
AQ                  2.2719147 sec
RG                     113.31
DW                     69.333 usec
DE                     10.06 usec
TE                     298.2 K
D1                  2.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1           400.1324008 MHz
NUC1                      1H
P1                     15.00 usec
PLW1           13.50000000 W

F2 - Processing parameters
SI                        16384
SF                 400.1300103 MHz
WDW                        EM
SSB                         0
LB                          0 Hz
GB                          0
PC                       1.00
```

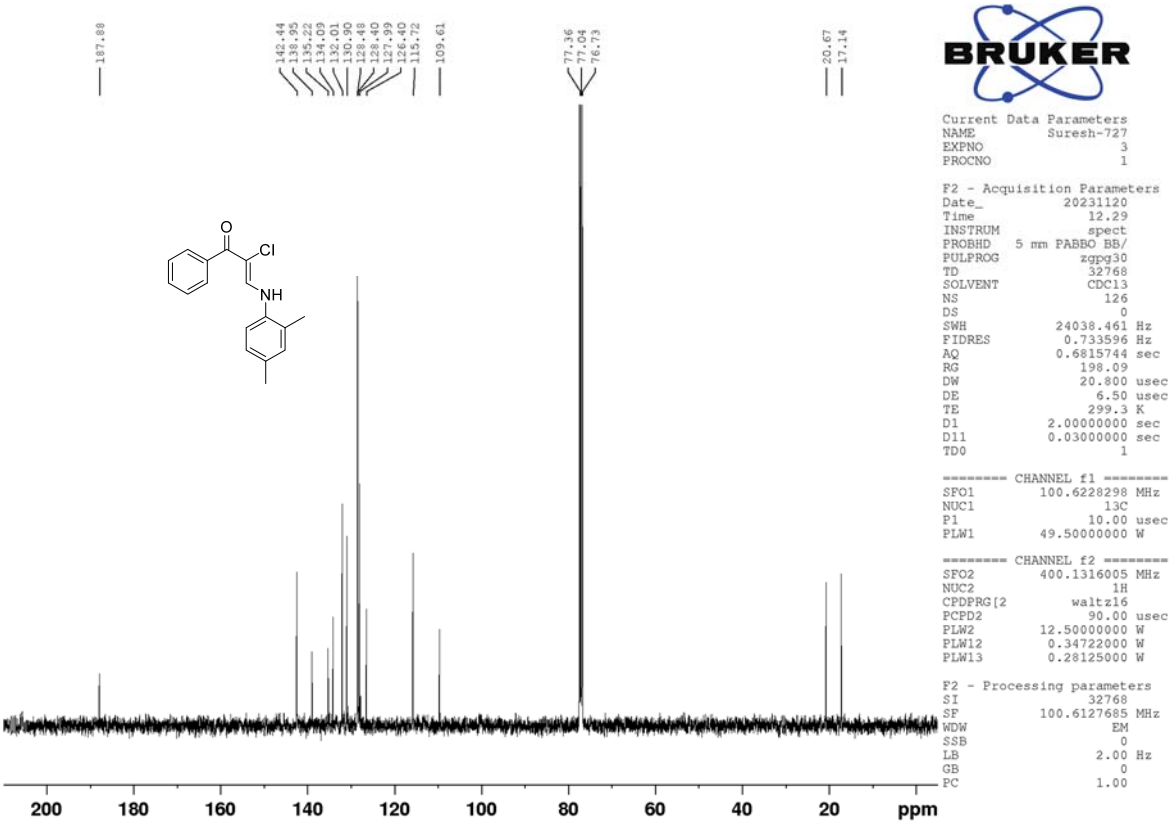


BRUKER

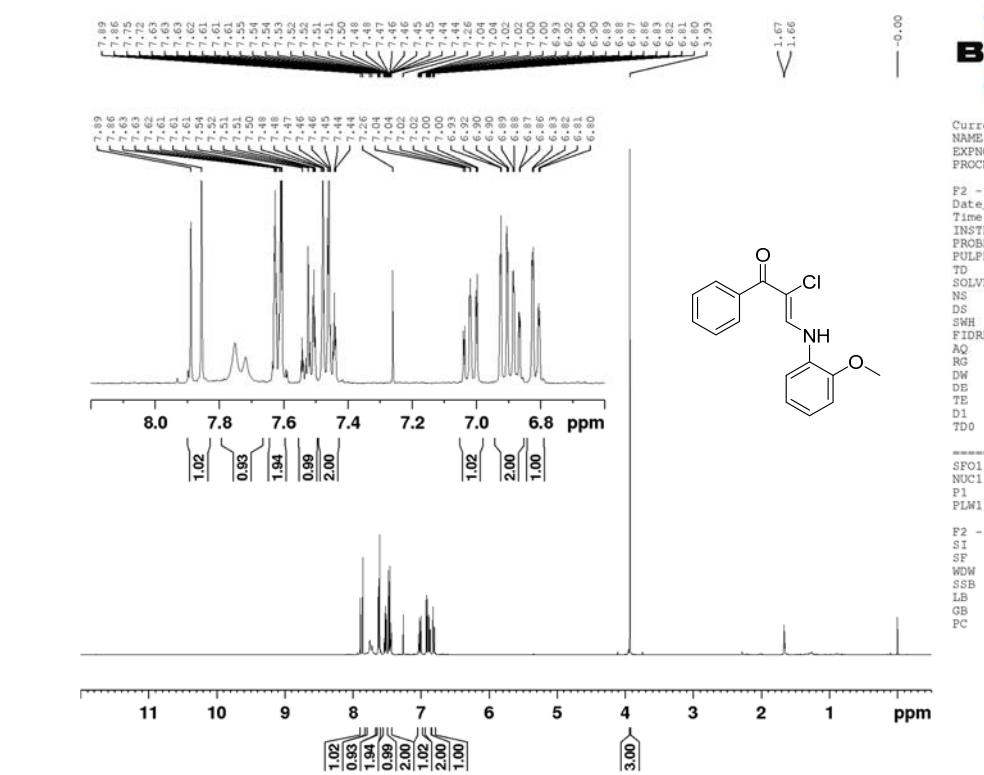
```
Current Data Parameters
NAME                  Enaminone
EXPNO                        25
PROCNO                        1

F2 - Acquisition Parameters
Date_               20231102
Time                   21.51
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                     32768
SOLVENT                CDCl3
NS                       256
DS                         0
SWH                24038.461 Hz
FIDRES                0.733596 Hz
AQ                  0.6815744 sec
RG                     198.09
DW                     20.800 usec
DE                      6.50 usec
TE                     299.2 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1           100.6228298 MHz
NUC1                      13C
P1                     10.00 usec
PLW1           49.50000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2           12.50000000 W
PLW12           0.34722000 W
PLW13           0.28125000 W

F2 - Processing parameters
SI                        32768
SF                 100.6127685 MHz
WDW                        EM
SSB                         0
LB                       2.00 Hz
GB                          0
PC                       1.00
```

(*Z*)-2-chloro-3-((2,4-dimethylphenyl)amino)-1-phenylprop-2-en-1-one (3ah)



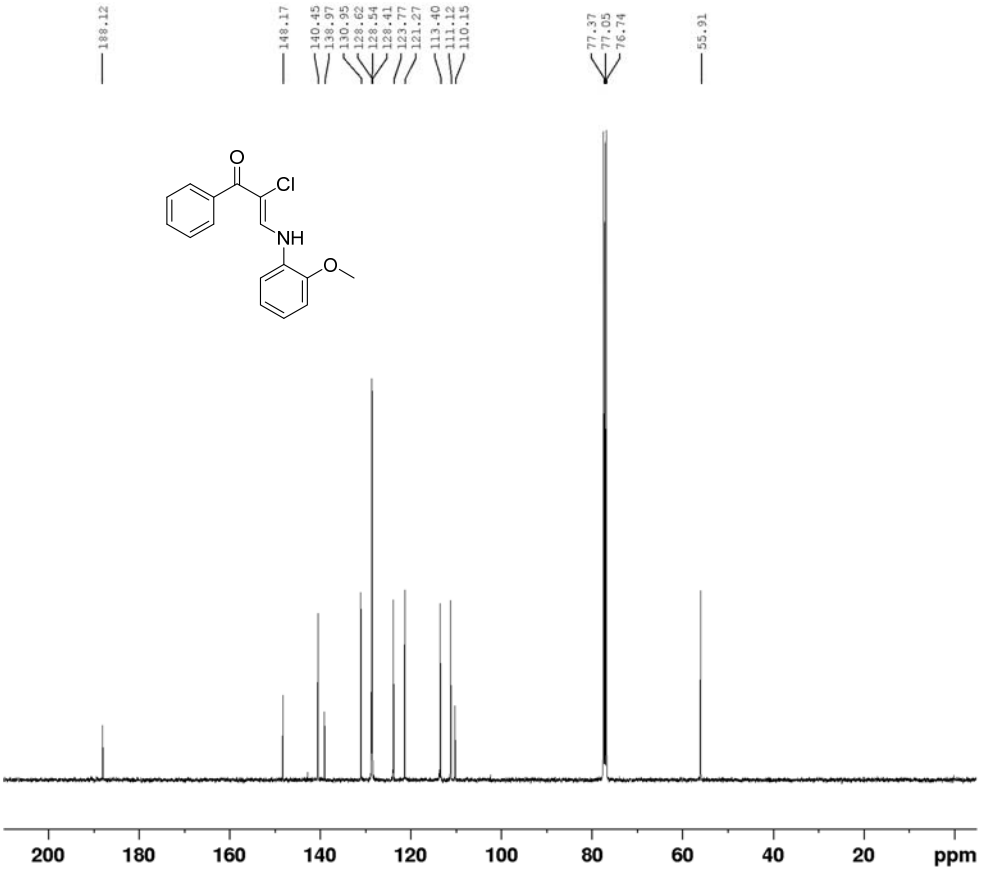


(*Z*)-2-chloro-3-((2-methoxyphenyl)amino)-1-phenylprop-2-en-1-one (3ai)



BRUKER

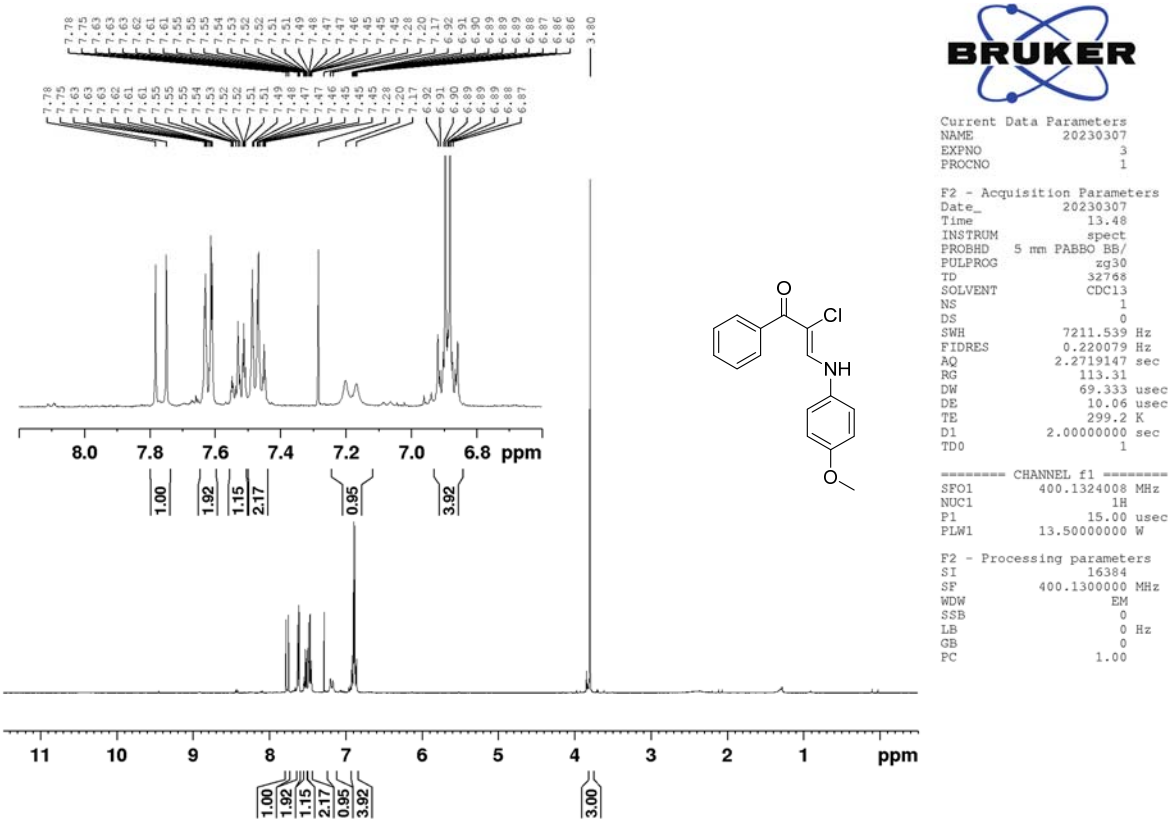
```
Current Data Parameters
NAME          Suresh-512
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_          20221029
Time              15.55
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDC13
NS                  16
DS                   0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                89.08
DW               69.333 usec
DE                10.06 usec
TE                298.2 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                1H
P1                15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                16384
SF          400.1300098 MHz
WDW                  EM
SSB                   0
LB                 0 Hz
GB                    0
PC                 1.00
```



BRUKER

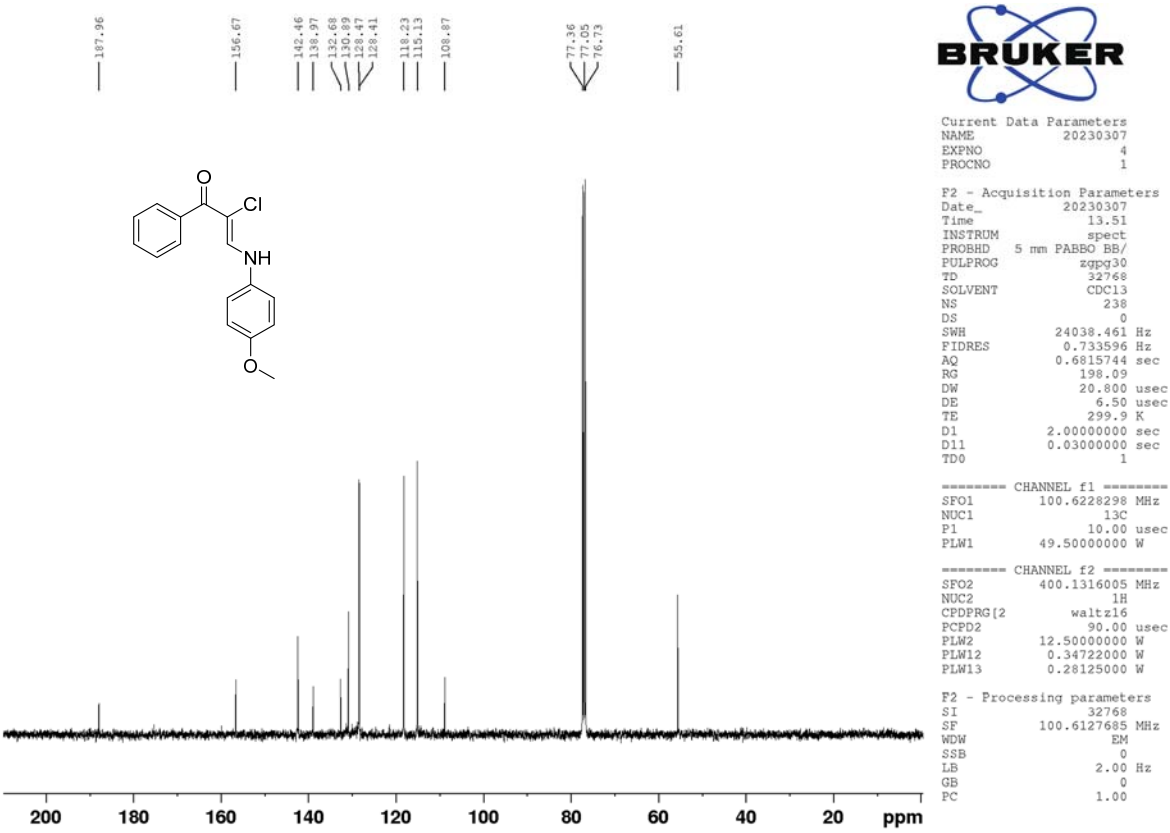
```
Current Data Parameters
NAME          Suresh-512
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_          20221029
Time              16.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDC13
NS                1495
DS                   0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW               20.800 usec
DE                6.50 usec
TE                298.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          100.6127685 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

(*Z*)-2-chloro-3-((4-methoxyphenyl)amino)-1-phenylprop-2-en-1-one (3aj)



BRUKER

```
Current Data Parameters
NAME                 20230307
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230307
Time                   13.48
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        1
DS                        0
SWH                7211.539 Hz
FIDRES             0.220079 Hz
AQ                 2.2719147 sec
RG                    113.31
DW                    69.333 usec
DE                     10.06 usec
TE                     299.2 K
D1                 2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             400.1324008 MHz
NUC1                       1H
P1                     15.00 usec
PLW1            13.50000000 W

F2 - Processing parameters
SI                        16384
SF               400.1300000 MHz
WDW                        EM
SSB                        0
LB                         0 Hz
GB                         0
PC                      1.00
```



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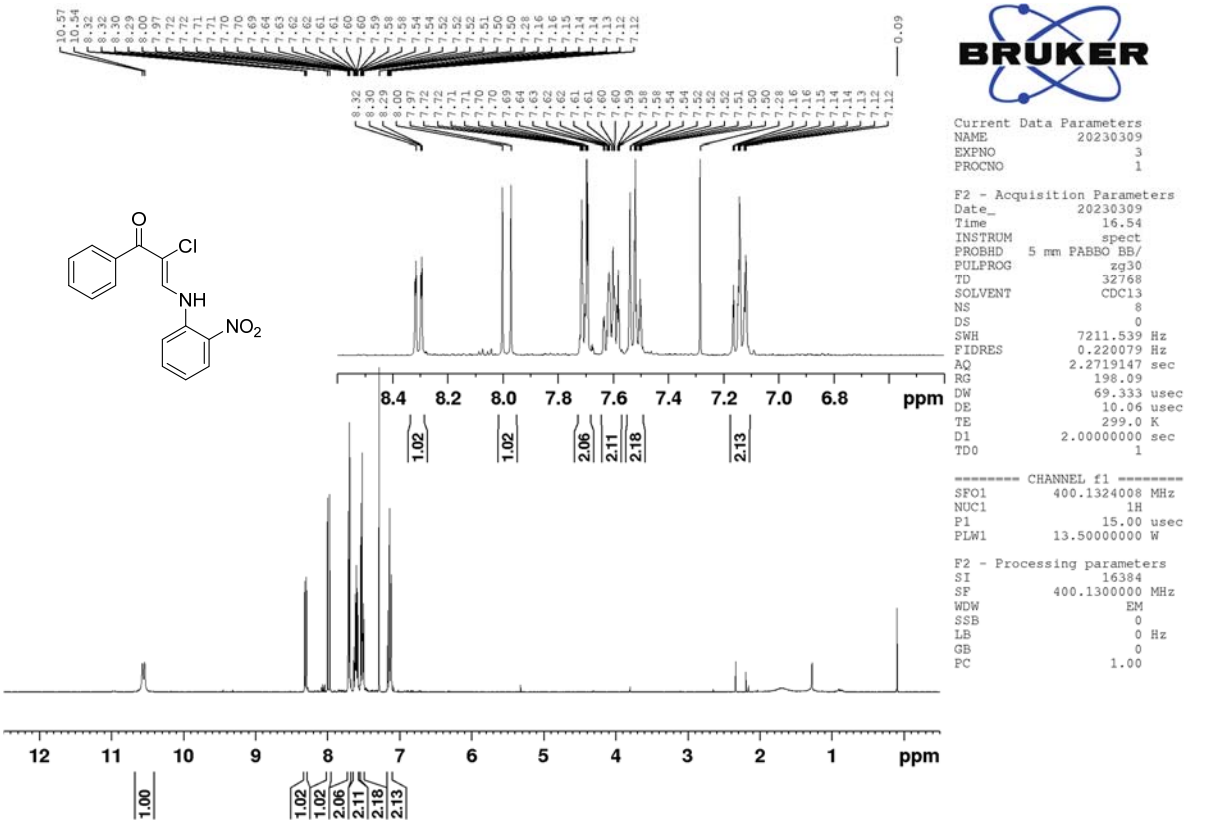
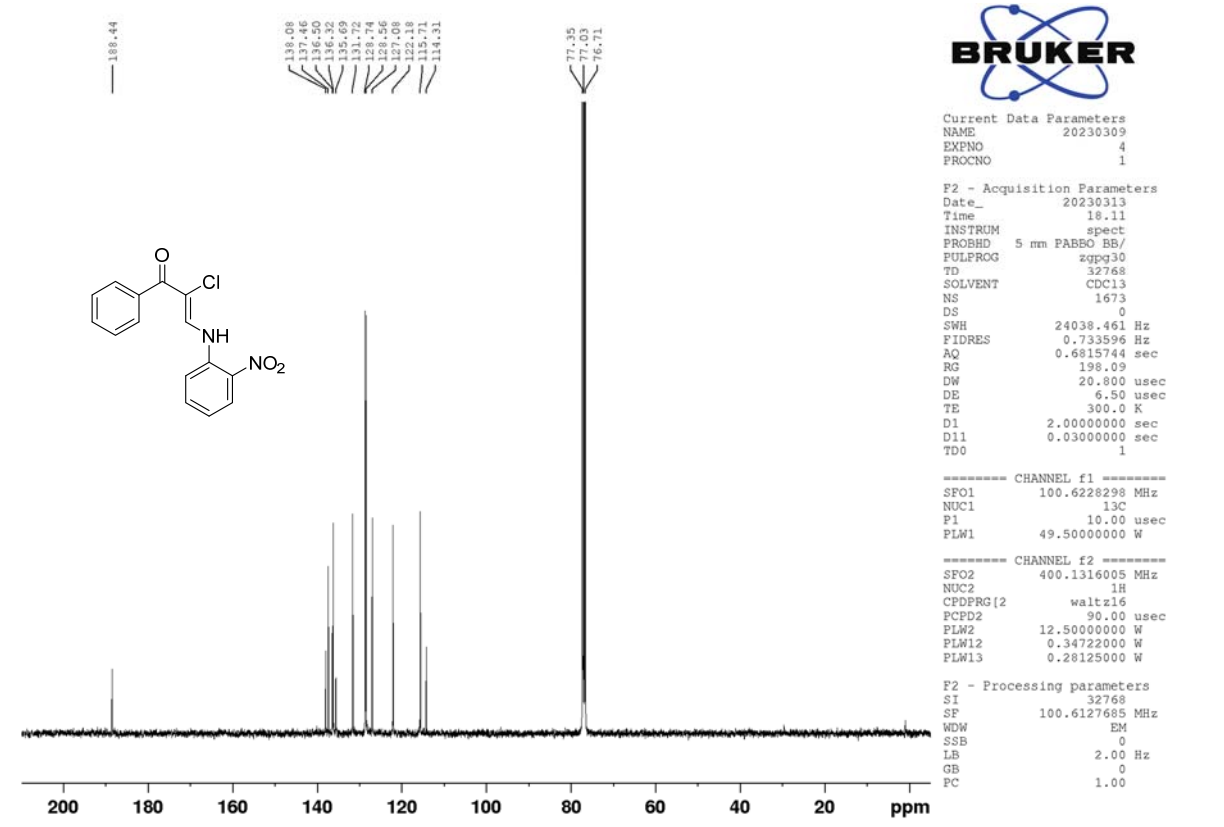
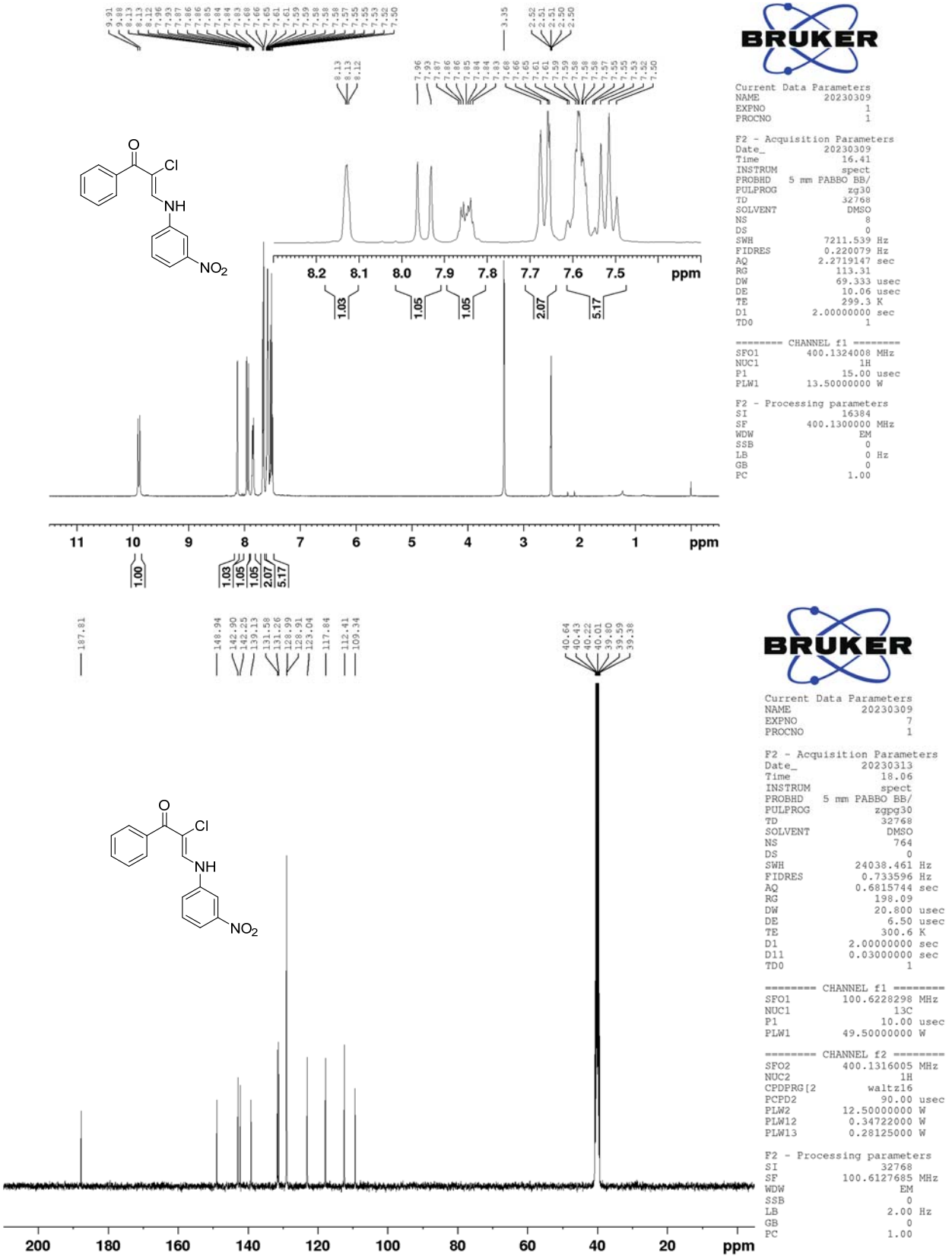
```
Current Data Parameters
NAME                 20230307
EXPNO                       4
PROCNO                      1

F2 - Acquisition Parameters
Date_               20230307
Time                   13.51
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                      238
DS                        0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                    198.09
DW                    20.800 usec
DE                      6.50 usec
TE                     299.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             100.6228298 MHz
NUC1                      13C
P1                     10.00 usec
PLW1            49.50000000 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2            12.50000000 W
PLW12            0.34722000 W
PLW13            0.28125000 W

F2 - Processing parameters
SI                        32768
SF               100.6127685 MHz
WDW                        EM
SSB                        0
LB                      2.00 Hz
GB                         0
PC                      1.00
```

(*Z*)-2-chloro-3-((2-nitrophenyl)amino)-1-phenylprop-2-en-1-one (3ak)

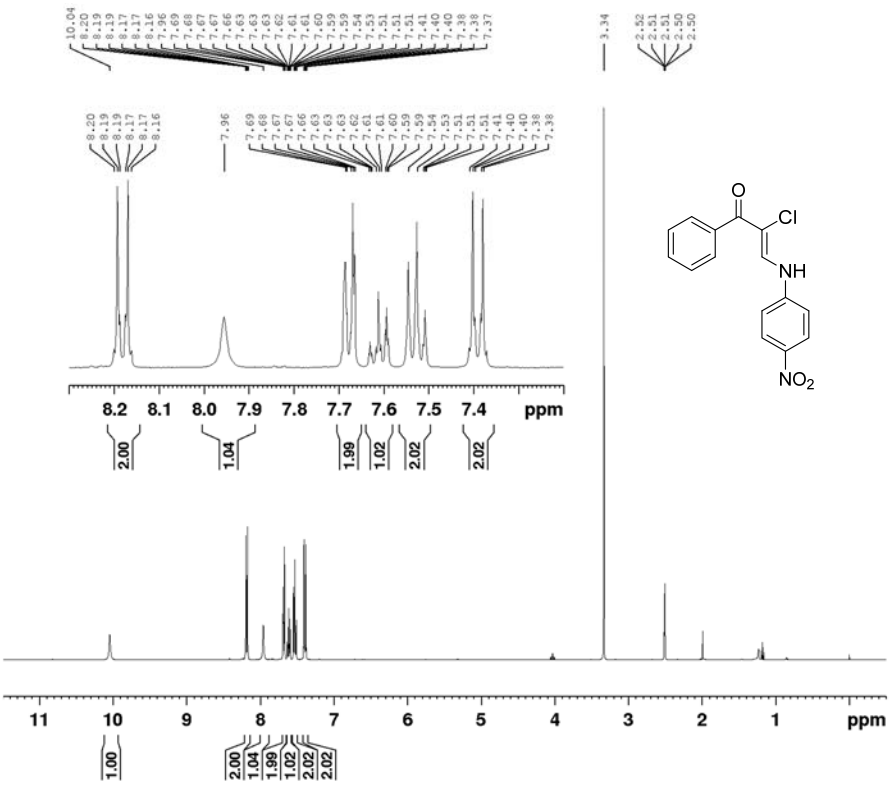




(*Z*)-2-chloro-3-((3-nitrophenyl)amino)-1-phenylprop-2-en-1-one (3al)



(*Z*)-2-chloro-3-((4-nitrophenyl)amino)-1-phenylprop-2-en-1-one (3am)



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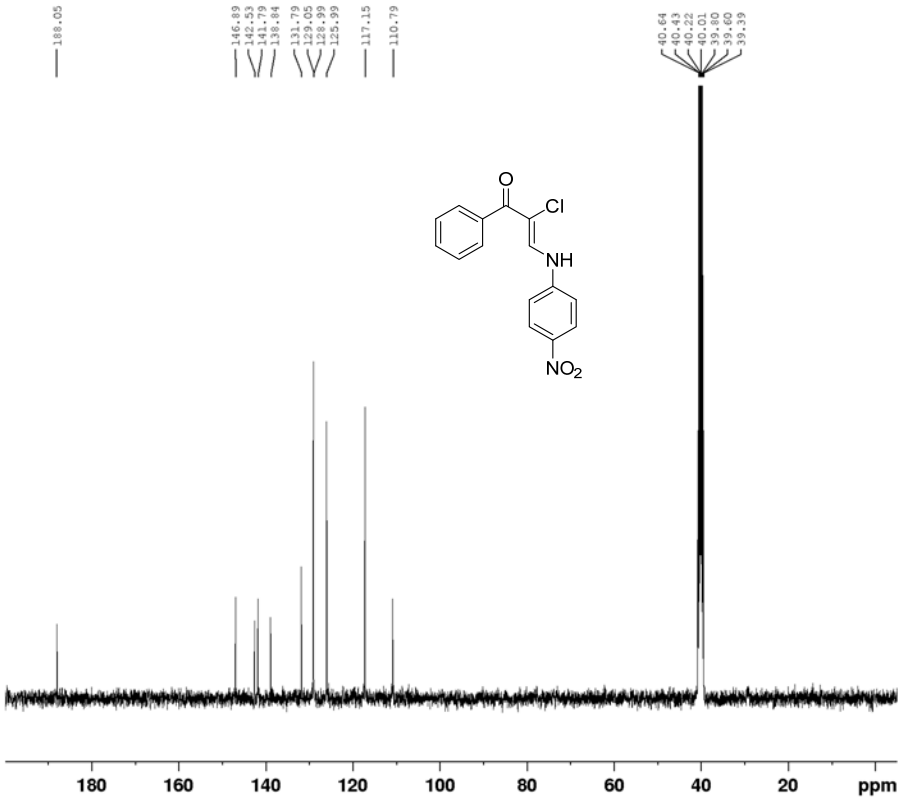
```
Current Data Parameters
NAME                  Enaminone
EXPNO                        33
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20231107
Time                     15.07
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                  zg30
TD                      32768
SOLVENT                  DMSO
NS                          16
DS                           0
SWH                  7211.539 Hz
FIDRES               0.220079 Hz
AQ                   2.2719147 sec
RG                       128.9
DW                      69.333 usec
DE                      10.06 usec
TE                      298.3 K
D1                   2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                400.1324008 MHz
NUC1                        1H
P1                       15.00 usec
PLW1                13.50000000 W

F2 - Processing parameters
SI                       16384
SF                  400.1300000 MHz
WDW                         EM
SSB                          0
LB                           0 Hz
GB                           0
PC                        1.00
```



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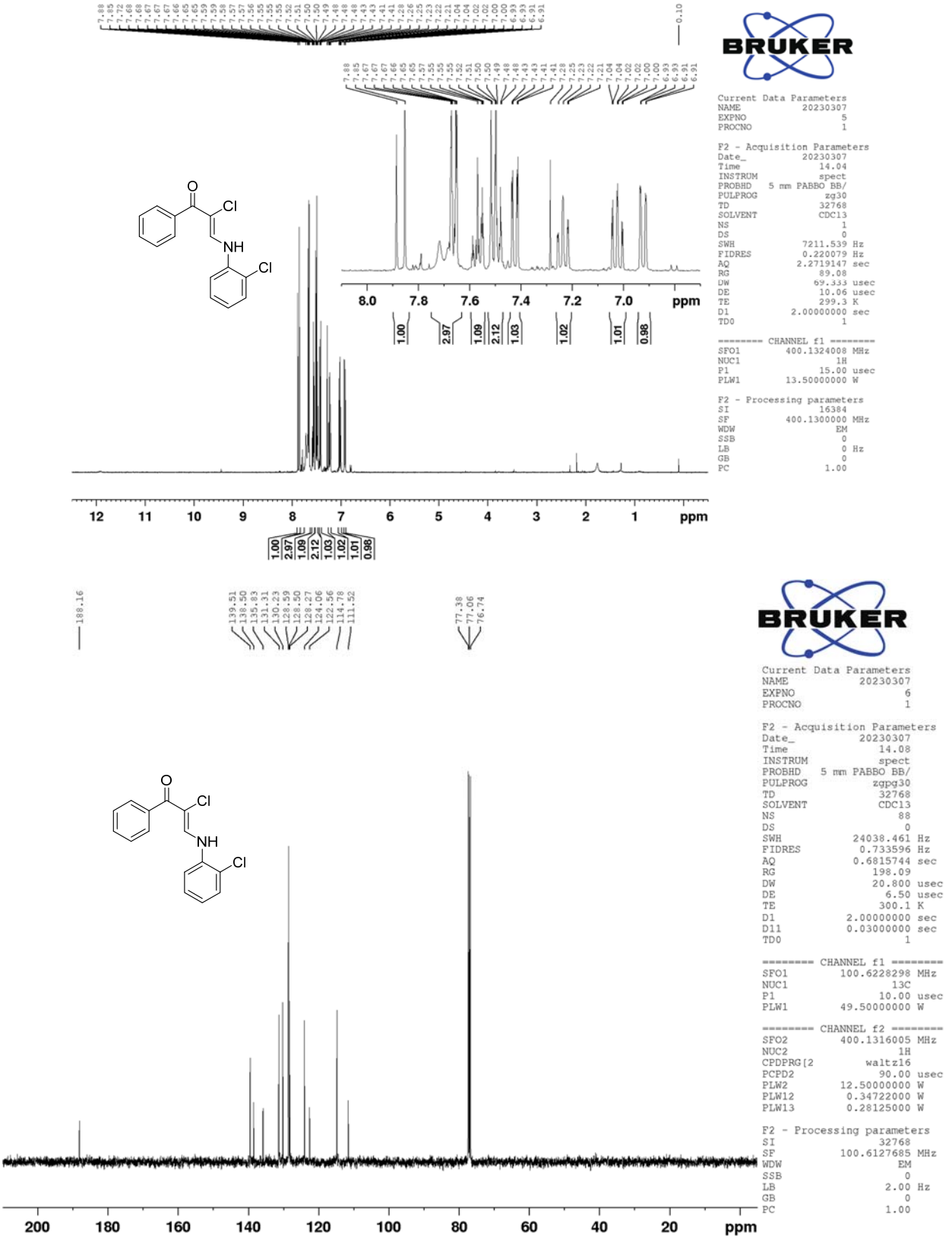
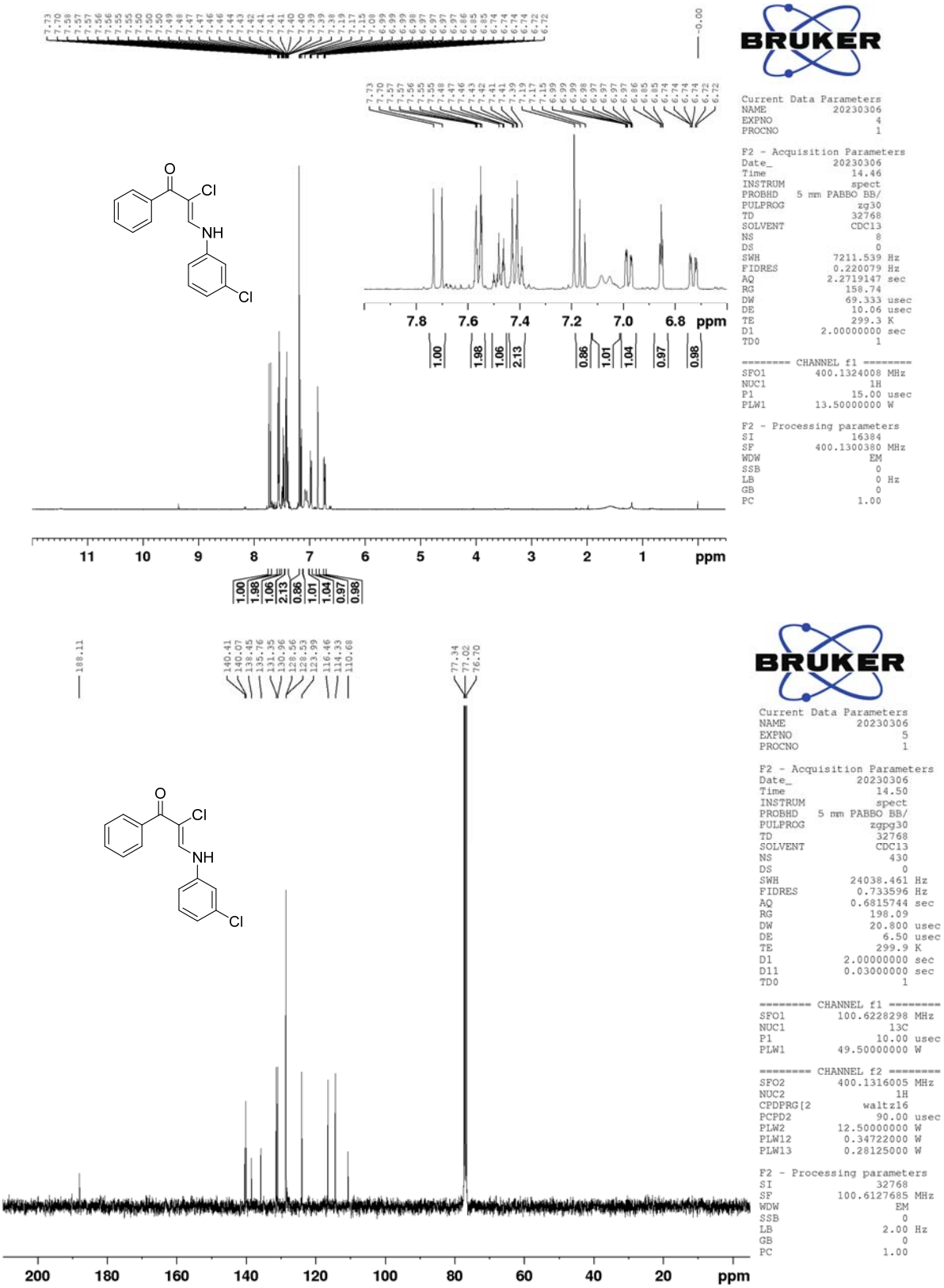
```
Current Data Parameters
NAME                  Enaminone
EXPNO                        32
PROCNO                        1

F2 - Acquisition Parameters
Date_                 20231107
Time                     14.09
INSTRUM                  spect
PROBHD     5 mm PABBO BB/
PULPROG                zgpg30
TD                      32768
SOLVENT                  DMSO
NS                         256
DS                           0
SWH                 24038.461 Hz
FIDRES               0.733596 Hz
AQ                   0.6815744 sec
RG                       198.09
DW                      20.800 usec
DE                       6.50 usec
TE                      298.8 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1                100.6228298 MHz
NUC1                        13C
P1                       10.00 usec
PLW1                49.50000000 W

======== CHANNEL f2 ========
SFO2                400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                12.50000000 W
PLW12                0.34722000 W
PLW13                0.28125000 W

F2 - Processing parameters
SI                       32768
SF                  100.6127685 MHz
WDW                         EM
SSB                          0
LB                        2.00 Hz
GB                           0
PC                        1.00
```

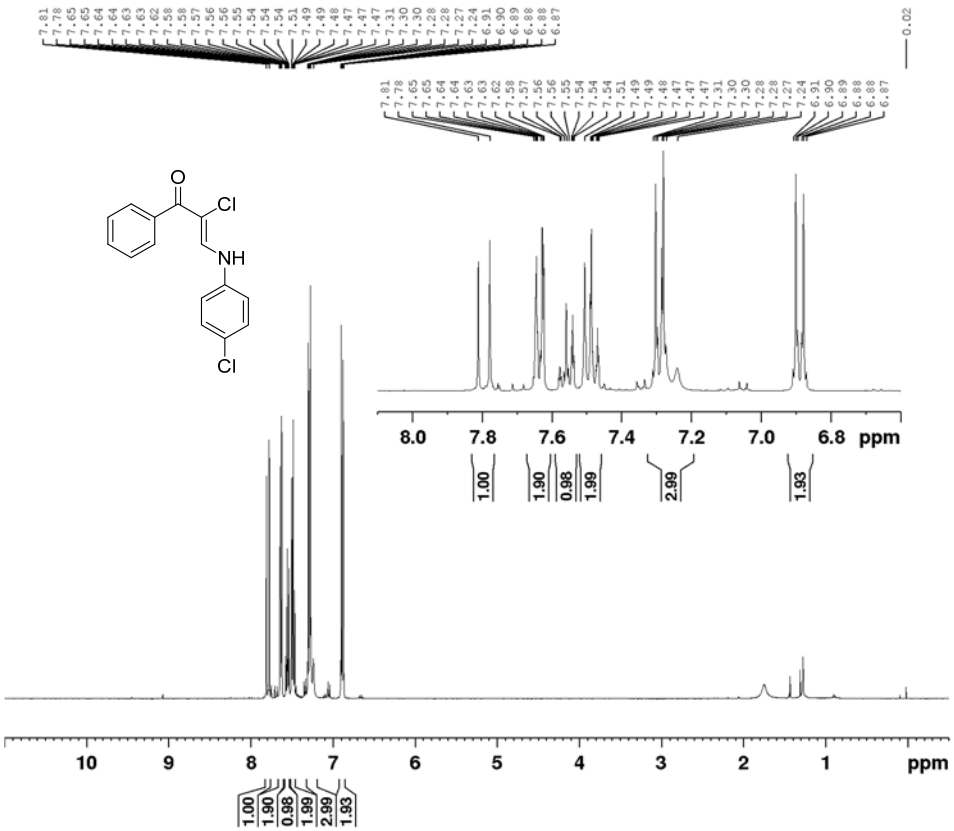
(*Z*)-2-chloro-3-((2-chlorophenyl)amino)-1-phenylprop-2-en-1-one (3an)



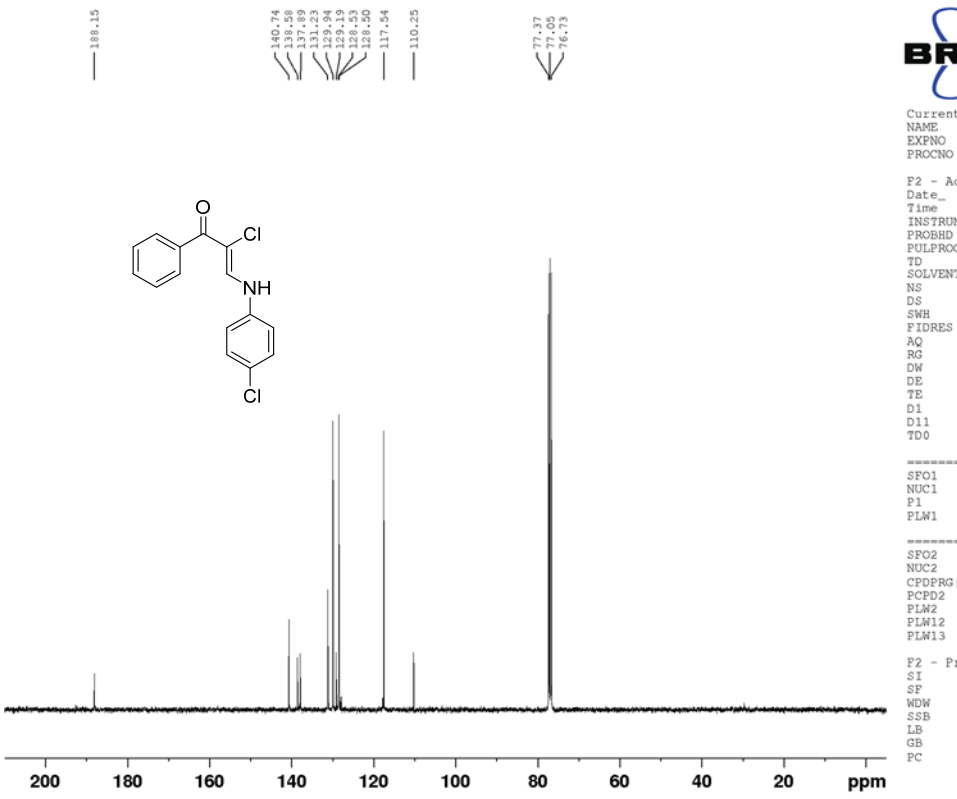
(*Z*)-2-chloro-3-((3-chlorophenyl)amino)-1-phenylprop-2-en-1-one (3ao)



(*Z*)-2-chloro-3-((4-chlorophenyl)amino)-1-phenylprop-2-en-1-one (3ap)

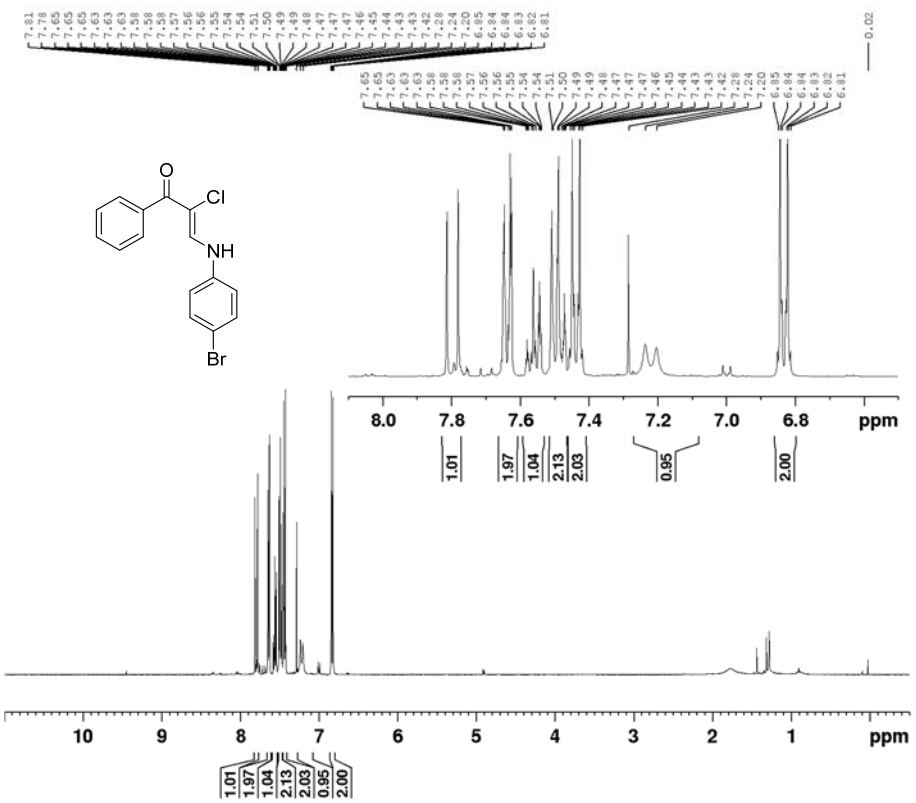


```
Current Data Parameters
NAME          Suresh-722
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231124
Time               21.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                113.31
DW                69.333 usec
DE                10.06 usec
TE                298.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324008 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          13.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



```
Current Data Parameters
NAME          Suresh-722
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231124
Time               21.24
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          49.50000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.50000000 W
PLW12          0.34722000 W
PLW13          0.28125000 W

F2 - Processing parameters
SI                 32768
SF            100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-3-((4-bromophenyl)amino)-2-chloro-1-phenylprop-2-en-1-one (3aq)



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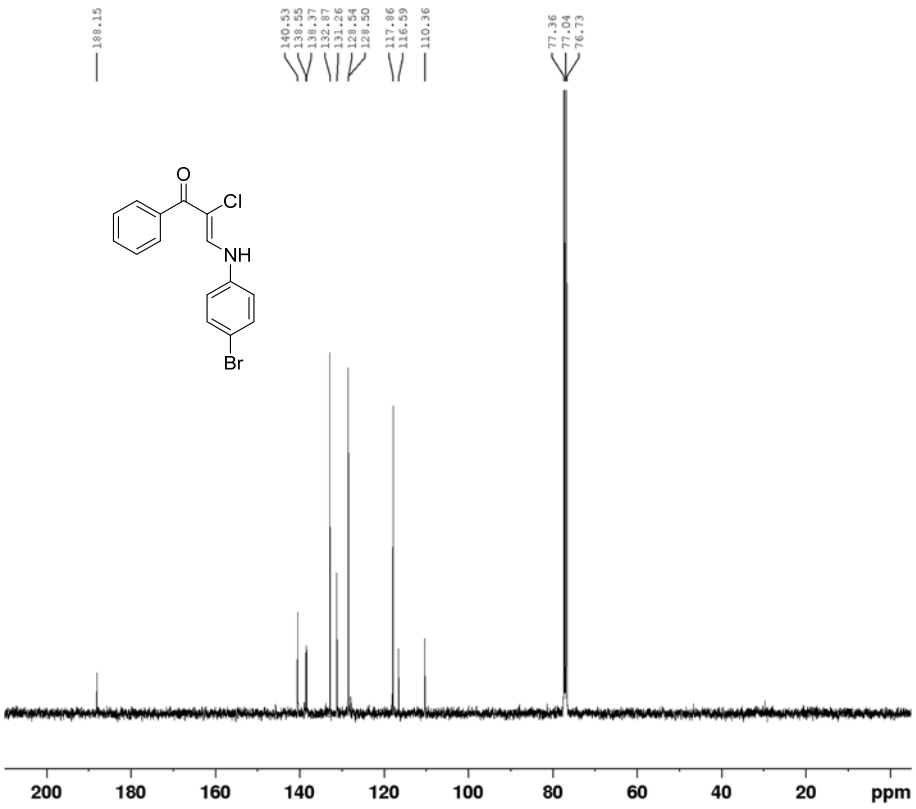
```
Current Data Parameters
NAME          Suresh-734
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231201
Time               11.02
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 128.9
DW                69.333 usec
DE                10.06 usec
TE                298.3 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324008 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          13.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



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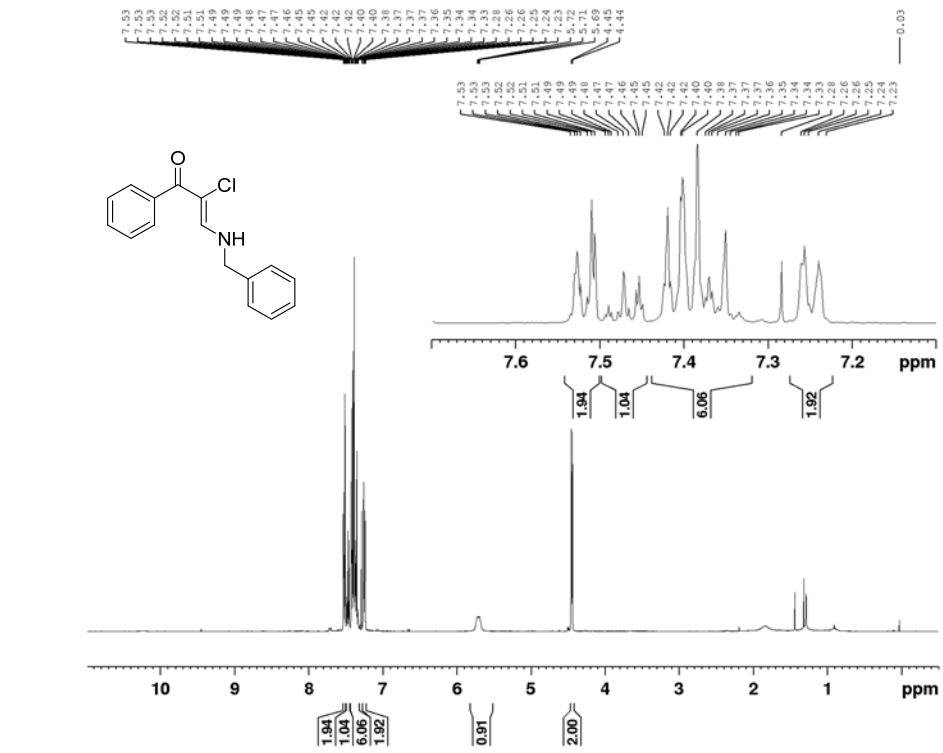
```
Current Data Parameters
NAME          Suresh-734
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231204
Time               21.30
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   302
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          49.50000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.50000000 W
PLW12          0.34722000 W
PLW13          0.28125000 W

F2 - Processing parameters
SI                 32768
SF            100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-3-(benzylamino)-2-chloro-1-phenylprop-2-en-1-one (3ar)



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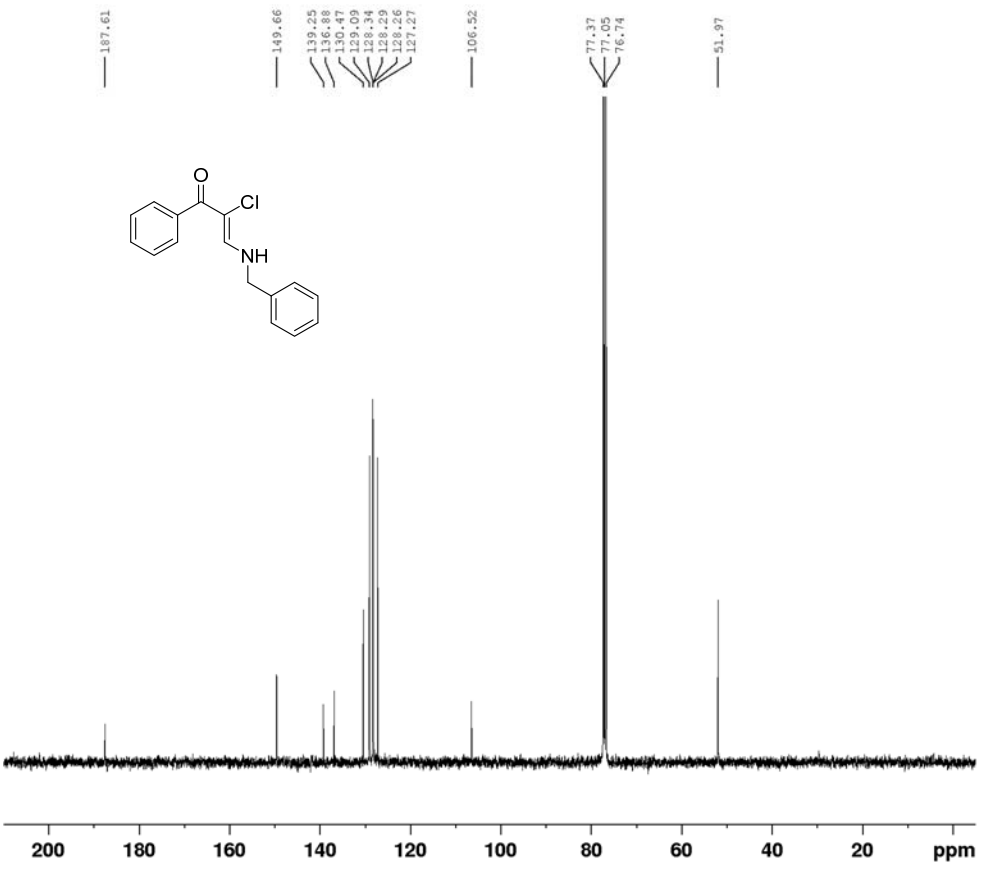
```
Current Data Parameters
NAME          Suresh-733
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231206
Time               14.36
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 99.72
DW                69.333 usec
DE                10.06 usec
TE                298.5 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                 16384
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0 Hz
GB                     0
PC                  1.00
```



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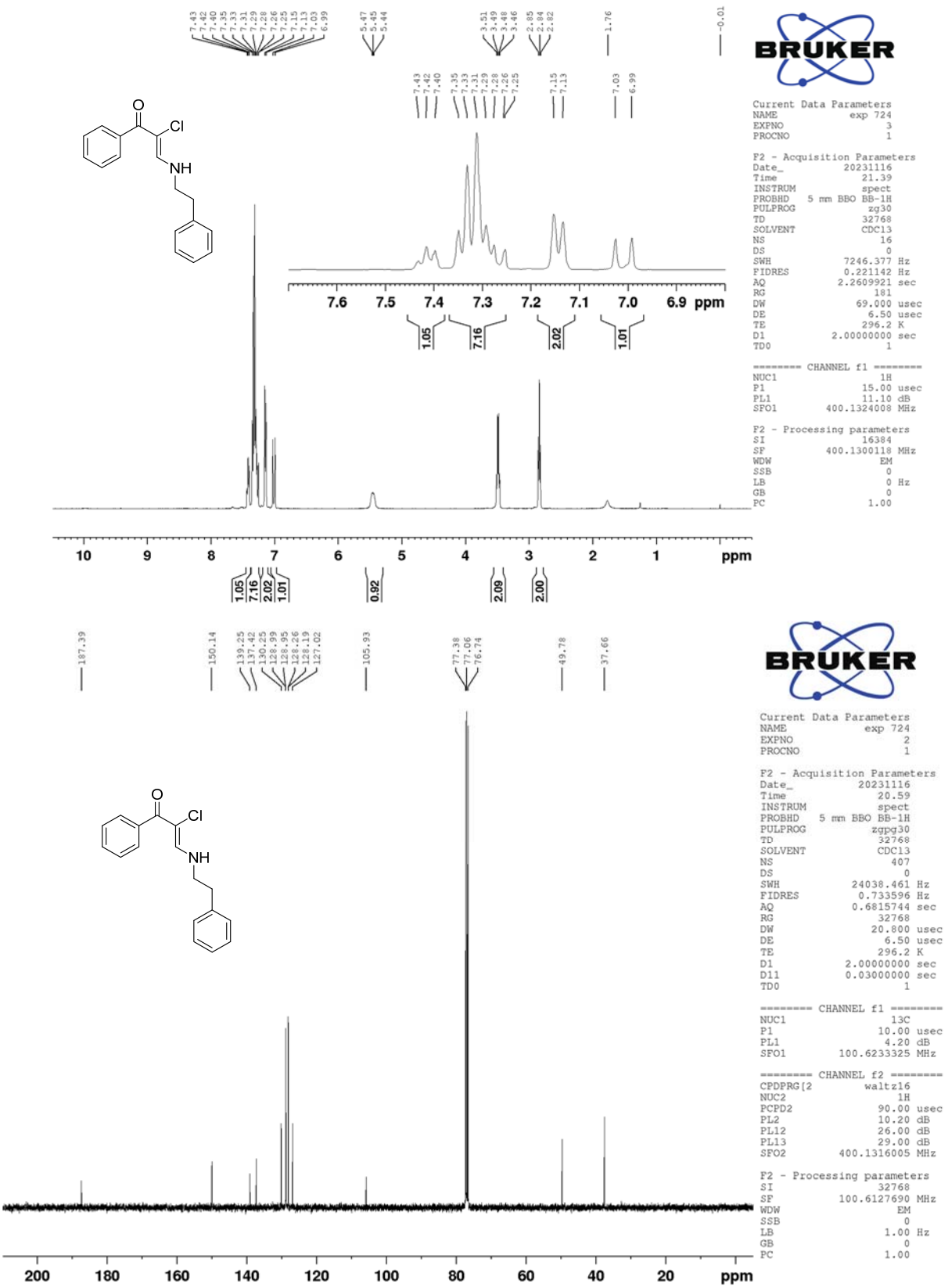
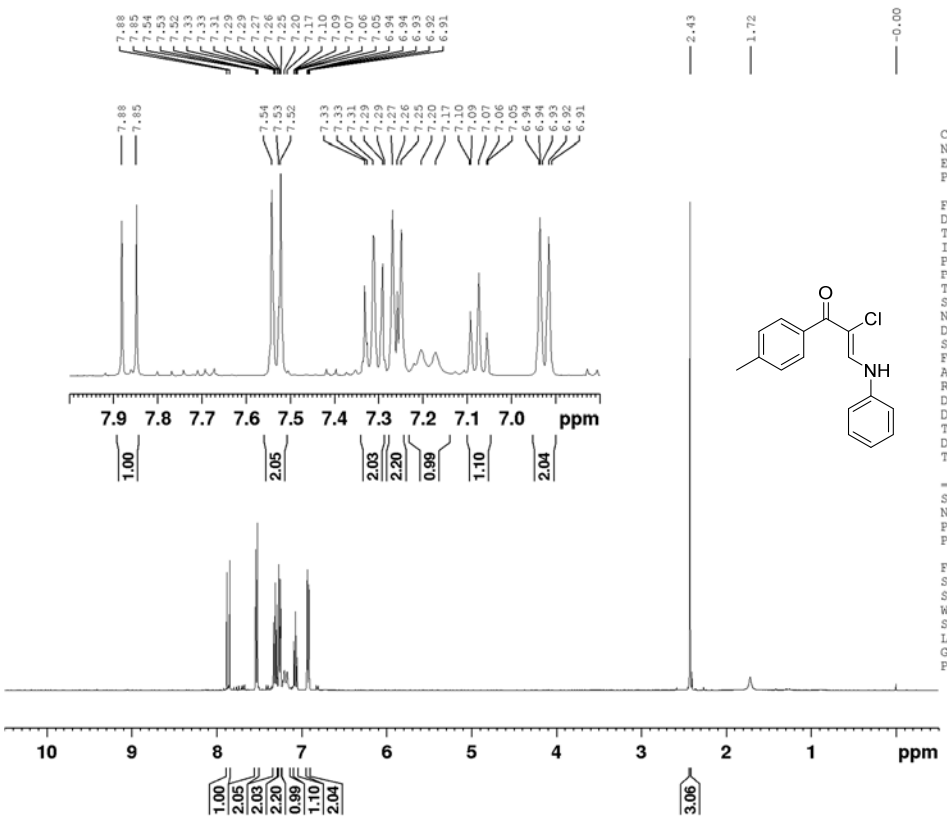
```
Current Data Parameters
NAME          Suresh-733
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231206
Time               14.38
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   230
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

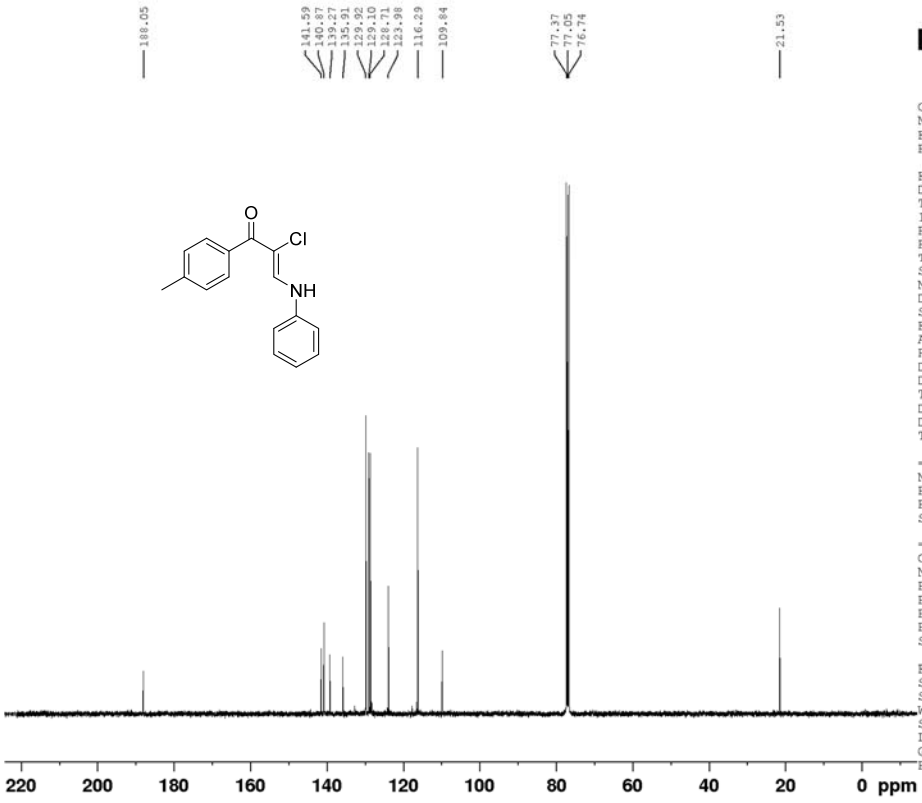
(*Z*)-2-chloro-3-(phenethylamino)-1-phenylprop-2-en-1-one (3as)



(*Z*)-2-chloro-3-(phenylamino)-1-(*p*-tolyl)prop-2-en-1-one (3ba)

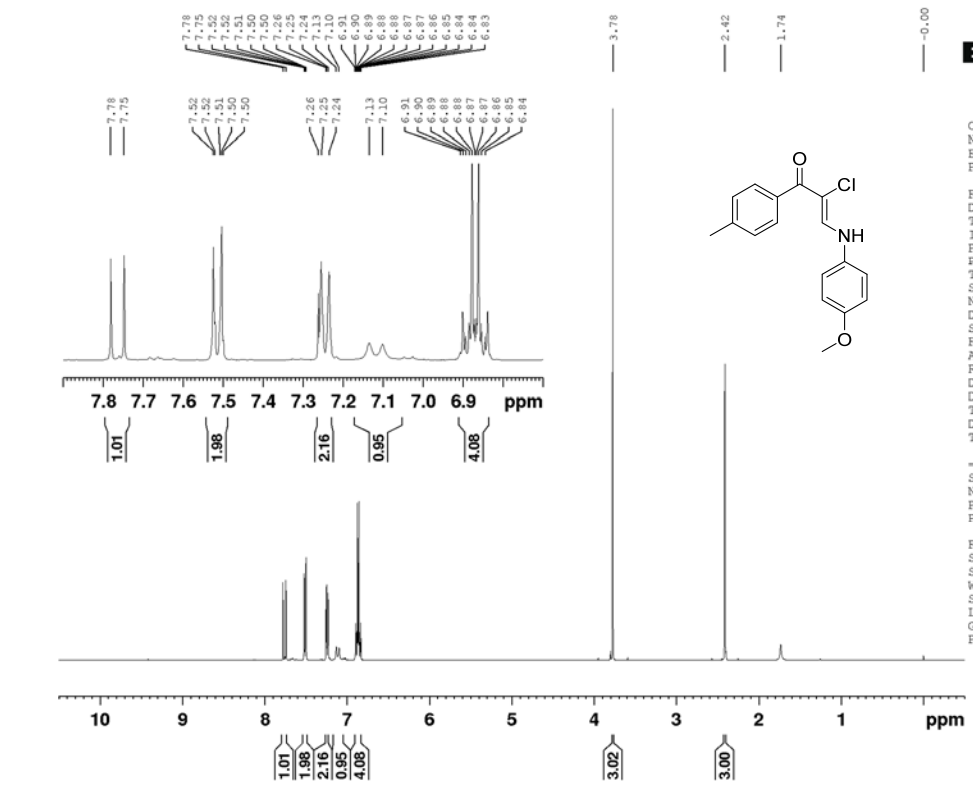



```
Current Data Parameters
NAME                  Suresh-747
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                  20231223
Time                      18.17
INSTRUM                   spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg30
TD                       32768
SOLVENT                  CDC13
NS                          16
DS                           0
SWH                  7211.539 Hz
FIDRES               0.220079 Hz
AQ                   2.2719147 sec
RG                       99.72
DW                      69.333 usec
DE                       10.06 usec
TE                       298.2 K
D1                   2.00000000 sec
TD0                          1

======== CHANNEL f1 ========
SFO1          400.1324008 MHz
NUC1                     1H
P1                    15.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                       16384
SF            400.1300103 MHz
WDW                         EM
SSB                          0
LB                        0 Hz
GB                           0
PC                        1.00
```




```
Current Data Parameters
NAME                   exp 747
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                  20231223
Time                      21.08
INSTRUM                   spect
PROBHD    5 mm BBO BB-1H
PULPROG                 zgpg30
TD                       32768
SOLVENT                  CDC13
NS                        1024
DS                           0
SWH                  24038.461 Hz
FIDRES               0.733596 Hz
AQ                   0.6815744 sec
RG                       32768
DW                      20.800 usec
DE                       6.50 usec
TE                       298.5 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       13C
P1                    10.00 usec
PL1                    4.20 dB
SFO1         100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                       1H
PCPD2                 90.00 usec
PL2                   10.20 dB
PL12                  26.00 dB
PL13                  29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF            100.6127690 MHz
WDW                         EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                        1.00
```

(*Z*)-2-chloro-3-((4-methoxyphenyl)amino)-1-(*p*-tolyl)prop-2-en-1-one (3bj)



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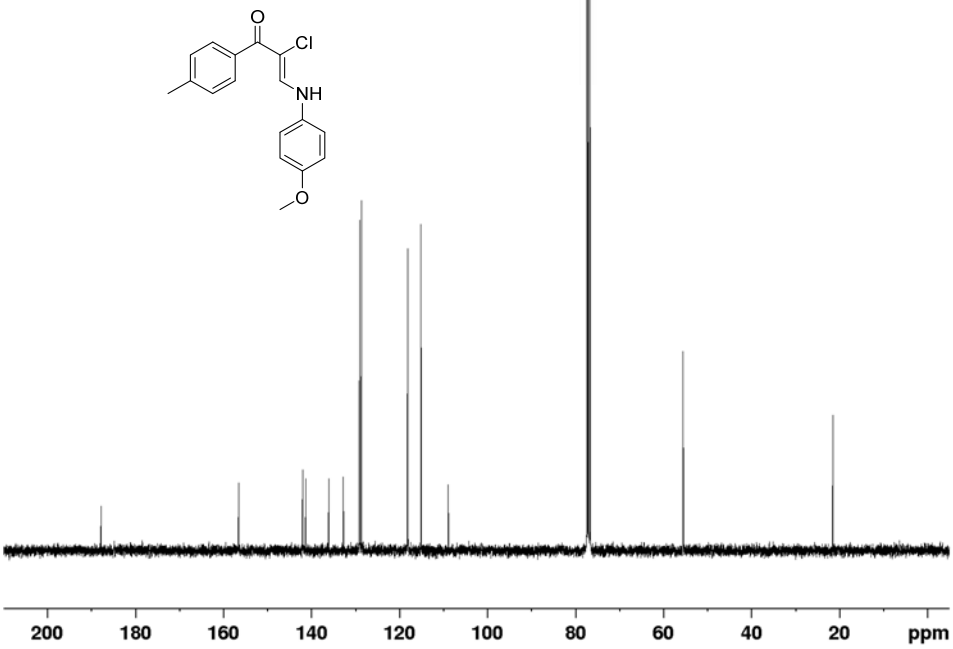
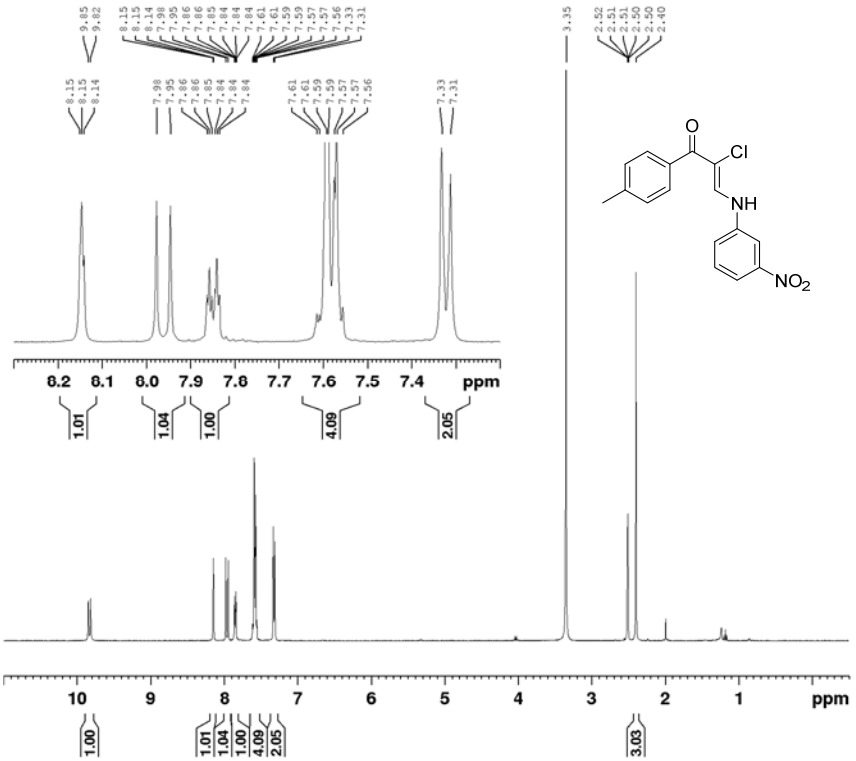
```
Current Data Parameters
NAME          Suresh-748
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231223
Time               17.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 99.72
DW                69.333 usec
DE                10.06 usec
TE                298.1 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324008 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          13.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300089 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



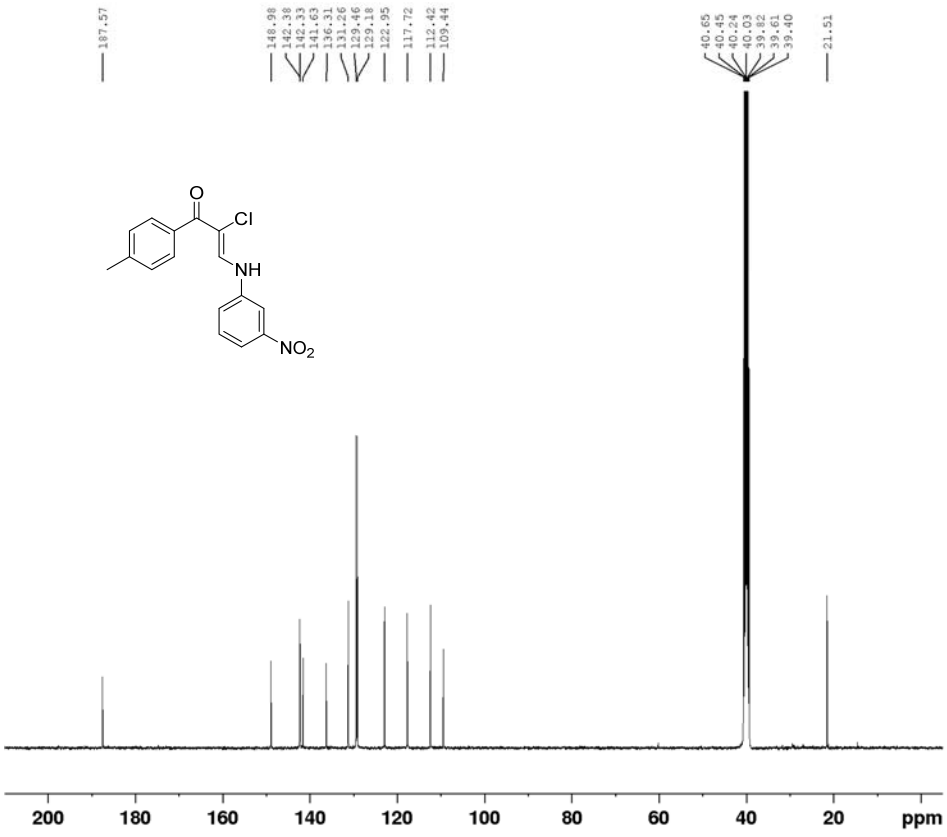
BRUKER

```
Current Data Parameters
NAME             exp 748
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231223
Time               16.46
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   512
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 32768
DW                20.800 usec
DE                 6.50 usec
TE                297.6 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 4.20 dB
SFO1          100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-2-chloro-3-((3-nitrophenyl)amino)-1-(*p*-tolyl)prop-2-en-1-one (3bl)

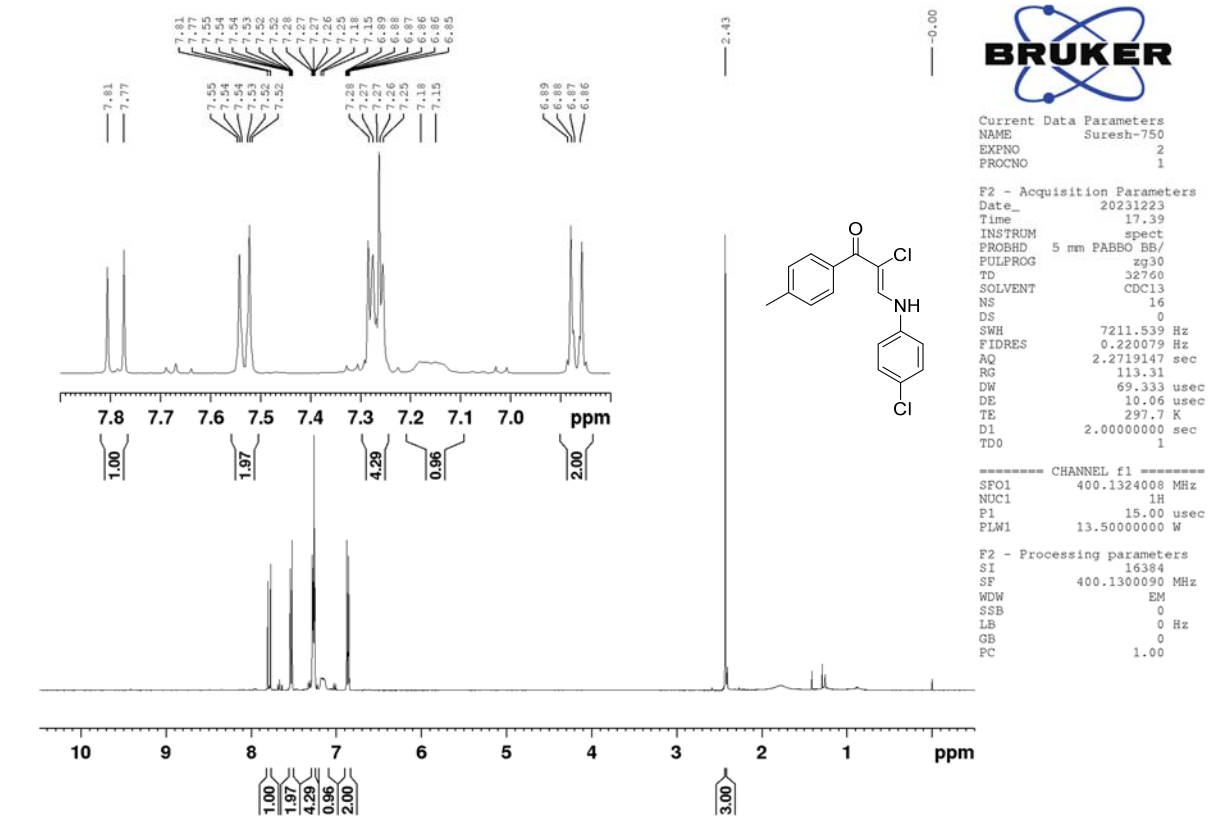



```
Current Data Parameters
NAME                 Suresh-749
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_               20240117
Time                   20.35
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       16
DS                        0
SWH                7211.539 Hz
FIDRES             0.220079 Hz
AQ                 2.2719147 sec
RG                    113.31
DW                  69.333 usec
DE                   10.06 usec
TE                   298.3 K
D1                 2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             400.1324008 MHz
NUC1                     1H
P1                    15.00 usec
PLW1            13.50000000 W

F2 - Processing parameters
SI                    16384
SF               400.1300000 MHz
WDW                      EM
SSB                       0
LB                     0 Hz
GB                        0
PC                     1.00
```




```
Current Data Parameters
NAME                 Suresh-749
EXPNO                         6
PROCNO                        1

F2 - Acquisition Parameters
Date_               20240117
Time                   22.01
INSTRUM                spect
PROBHD     5 mm PABBO BB/
PULPROG             zgpg30
TD                    32768
SOLVENT                DMSO
NS                     12096
DS                        0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                    198.09
DW                  20.800 usec
DE                    6.50 usec
TE                   298.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             100.6228298 MHz
NUC1                     13C
P1                    10.00 usec
PLW1            49.50000000 W

======== CHANNEL f2 ========
SFO2             400.1316005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2            12.50000000 W
PLW12            0.34722000 W
PLW13            0.28125000 W

F2 - Processing parameters
SI                    32768
SF               100.6127685 MHz
WDW                      EM
SSB                       0
LB                     2.00 Hz
GB                        0
PC                     1.00
```

(*Z*)-2-chloro-3-((4-chlorophenyl)amino)-1-(*p*-tolyl)prop-2-en-1-one (3bp)

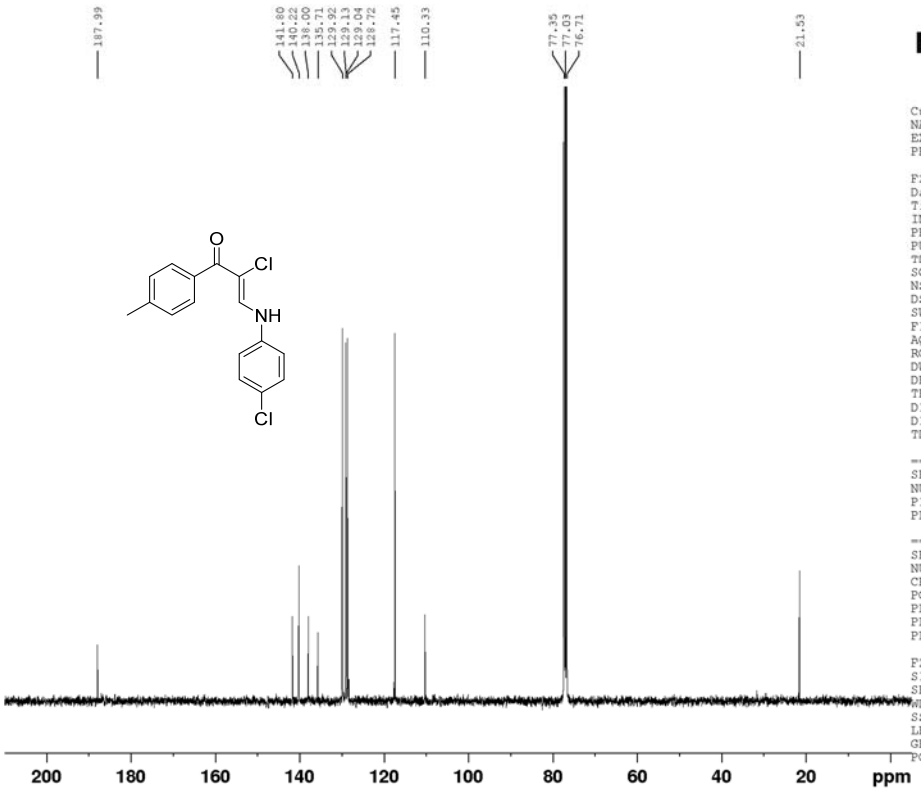


Current Data Parameters
NAME Suresh-750
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20231223
Time 17.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32760
SOLVENT CDCl3
NS 16
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 113.31
DW 69.333 usec
DE 10.06 usec
TE 297.7 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 15.00 usec
PLW1 13.50000000 W

F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME Suresh-750
EXPNO 3
PROCNO 1

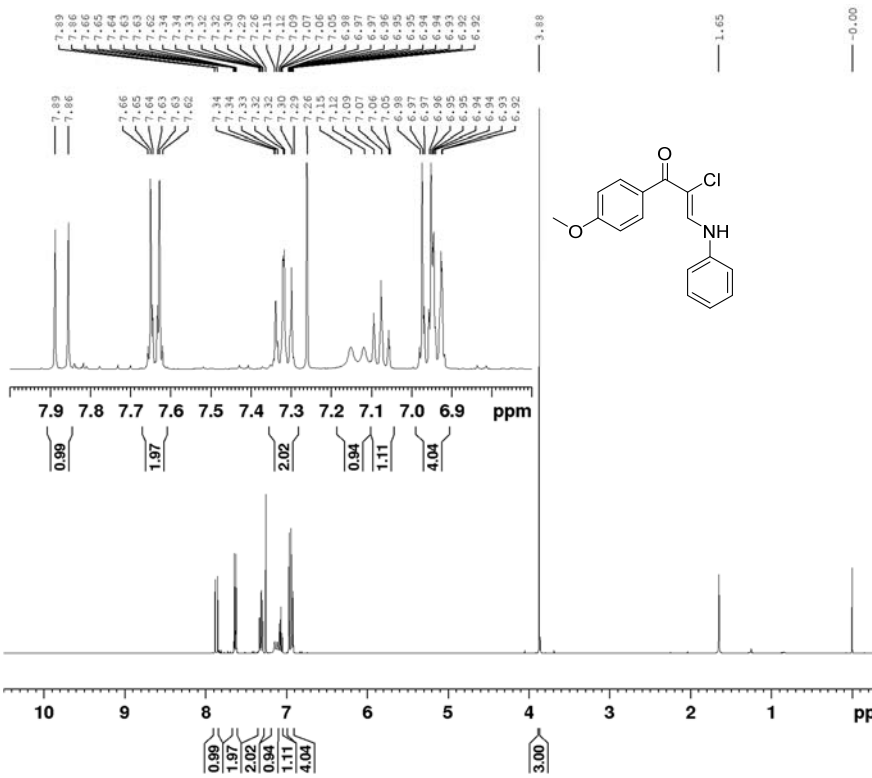
F2 - Acquisition Parameters
Date_ 20231223
Time 18.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32760
SOLVENT CDCl3
NS 682
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 49.50000000 W

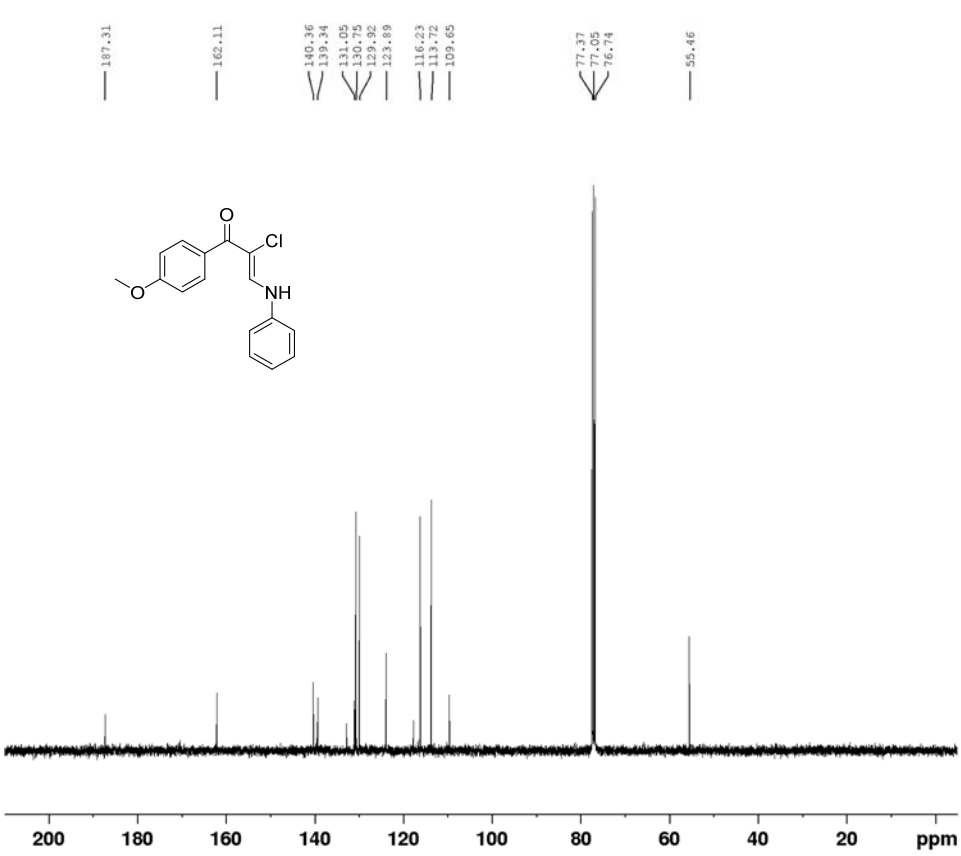
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.50000000 W
PLW12 0.34722000 W
PLW13 0.28125000 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

(*Z*)-2-chloro-1-(4-methoxyphenyl)-3-(phenylamino)prop-2-en-1-one (3ca)

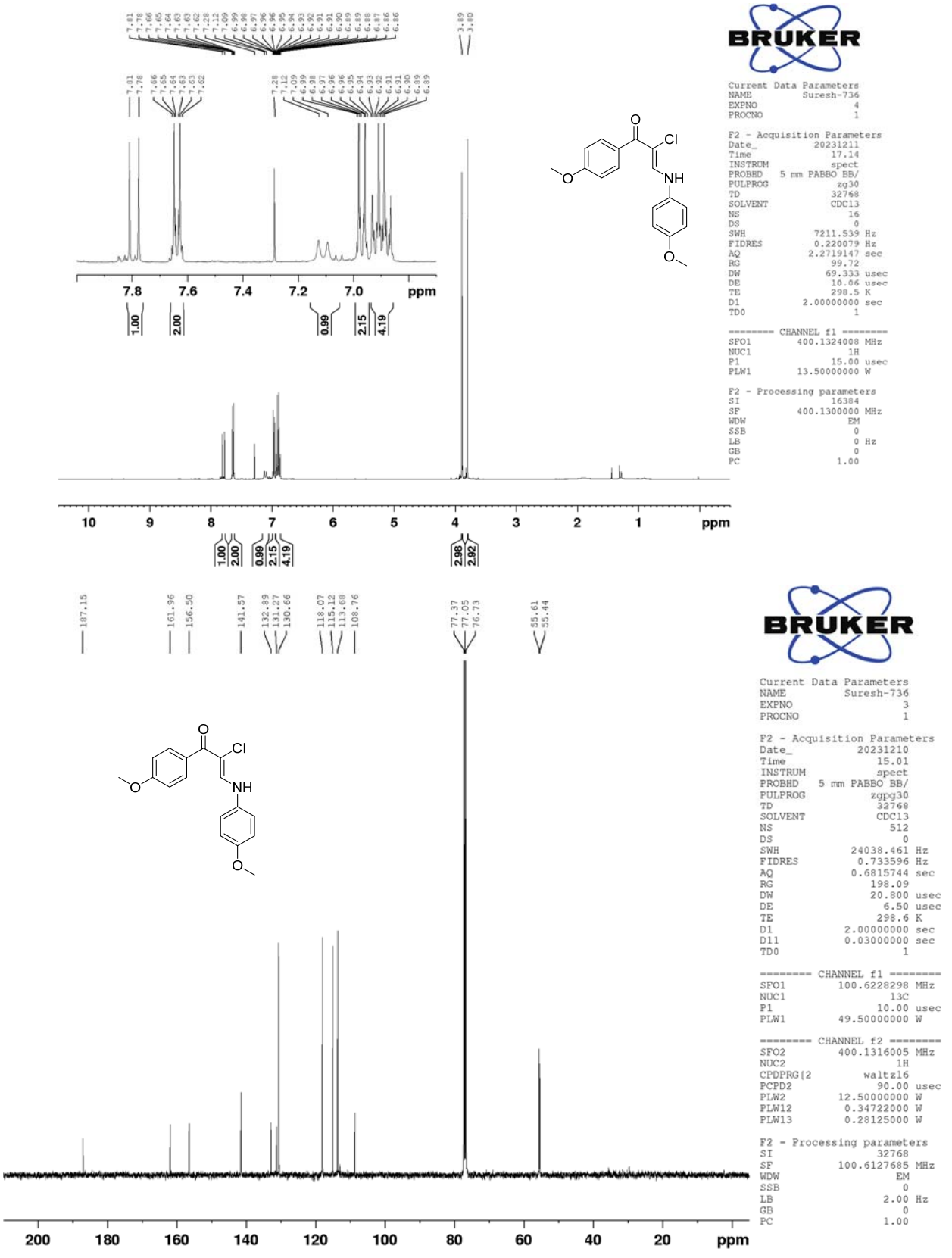



```
Current Data Parameters
NAME            Enaminone
EXPNO                  87
PROCNO                  1

F2 - Acquisition Parameters
Date_           20240710
Time               14.15
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                 128.9
DW                69.333 usec
DE                10.06 usec
TE                299.6 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF           400.1300098 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

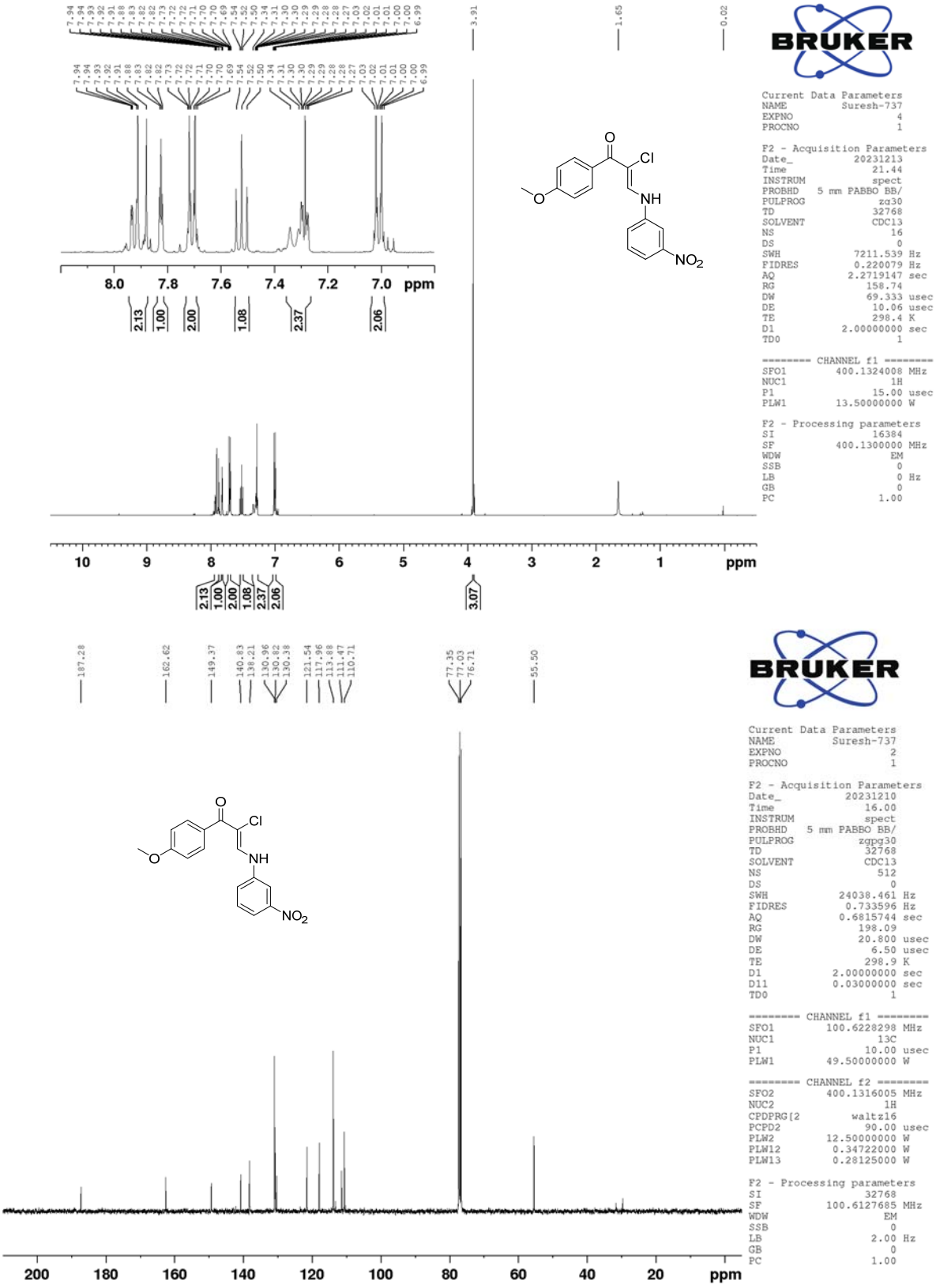



```
Current Data Parameters
NAME              exp 738
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20231213
Time               21.54
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT            CDC13
NS                   232
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                 32768
DW                20.800 usec
DE                 6.50 usec
TE                296.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.00 usec
PL1                4.20 dB
SFO1         100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

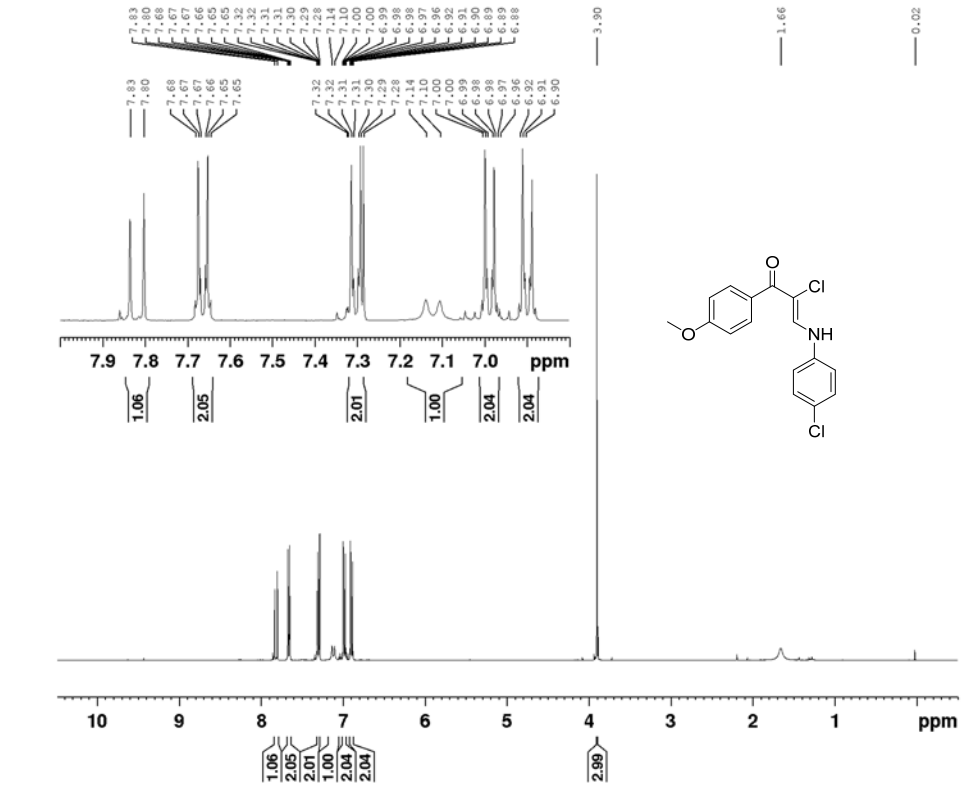
(*Z*)-2-chloro-1-(4-methoxyphenyl)-3-((4-methoxyphenyl)amino)prop-2-en-1-one (3cj)



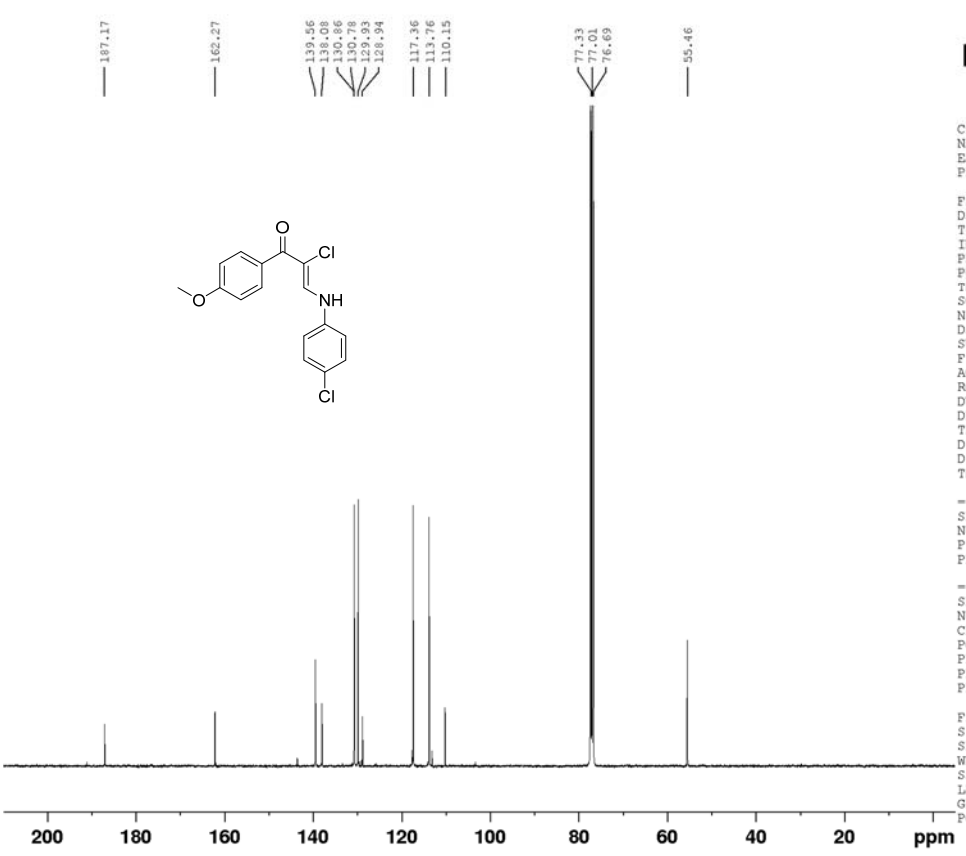
(*Z*)-2-chloro-1-(4-methoxyphenyl)-3-((3-nitrophenyl)amino)prop-2-en-1-one (3cl)



(*Z*)-2-chloro-3-((4-chlorophenyl)amino)-1-(4-methoxyphenyl)prop-2-en-1-one (3cp)

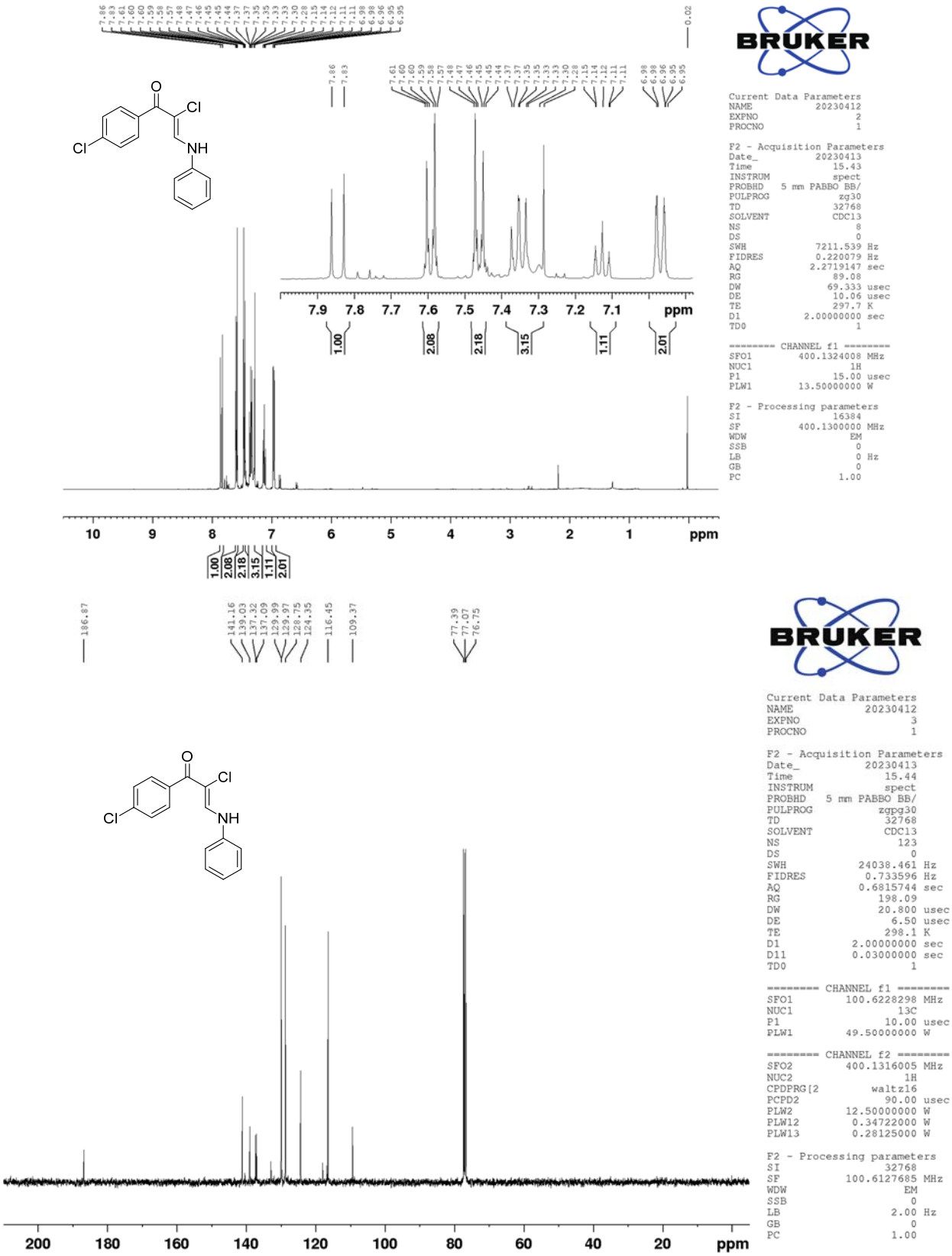



```
Current Data Parameters
NAME          Suresh-739
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231216
Time               21.05
INSTRUM            spect
PROBHD  5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                144.49
DW                69.333 usec
DE                10.06 usec
TE                298.2 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324008 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          13.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

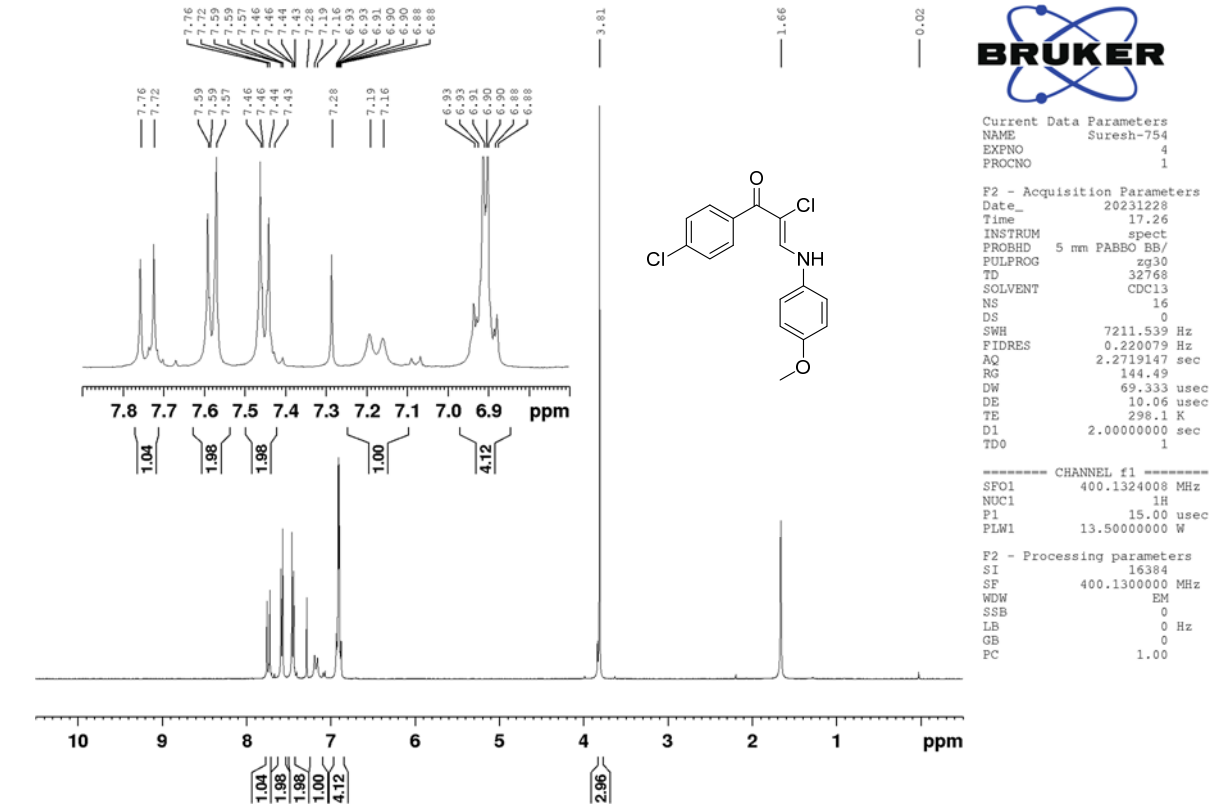



```
Current Data Parameters
NAME          Suresh-739
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231216
Time               21.07
INSTRUM            spect
PROBHD  5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                 15000
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          49.50000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.50000000 W
PLW12          0.34722000 W
PLW13          0.28125000 W

F2 - Processing parameters
SI                 32768
SF            100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

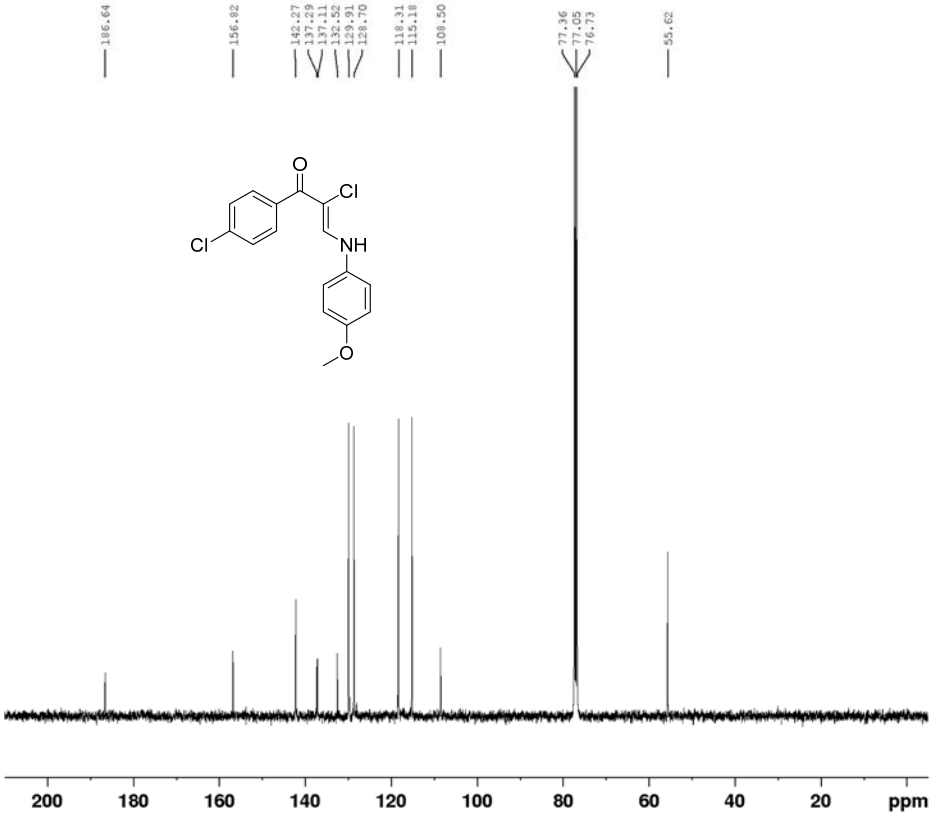
(*Z*)-2-chloro-1-(4-chlorophenyl)-3-(phenylamino)prop-2-en-1-one (3da)



(*Z*)-2-chloro-1-(4-chlorophenyl)-3-((4-methoxyphenyl)amino)prop-2-en-1-one (3dj)

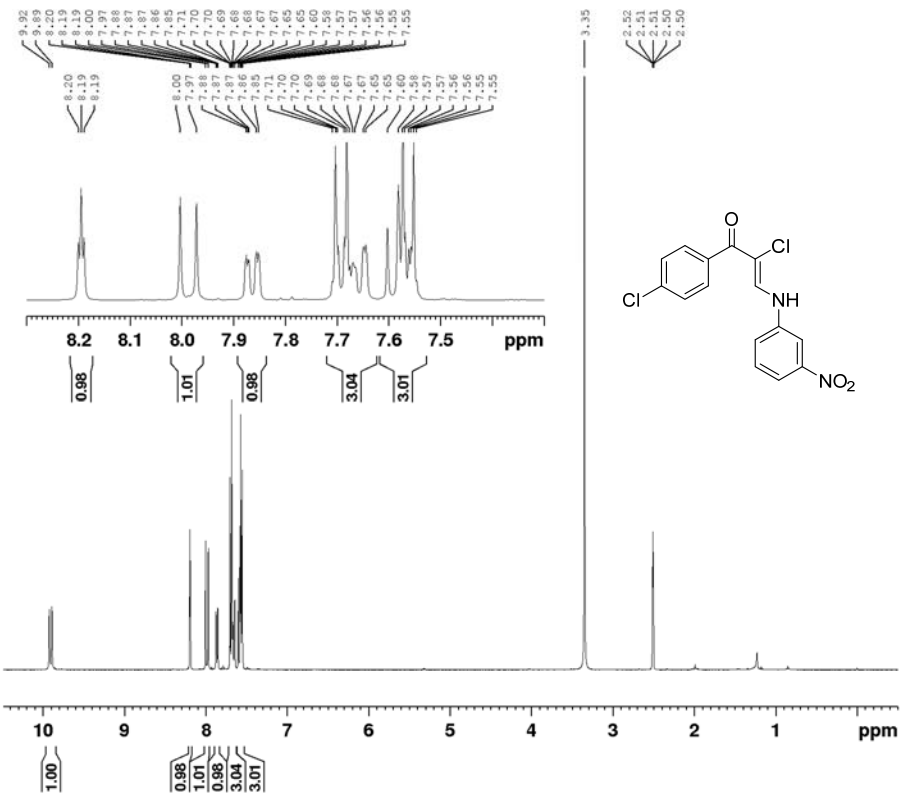



```
Current Data Parameters
NAME          Suresh-754
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231228
Time               17.26
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                144.49
DW                69.333 usec
DE                10.06 usec
TE                298.1 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                  0 Hz
GB                     0
PC                  1.00
```

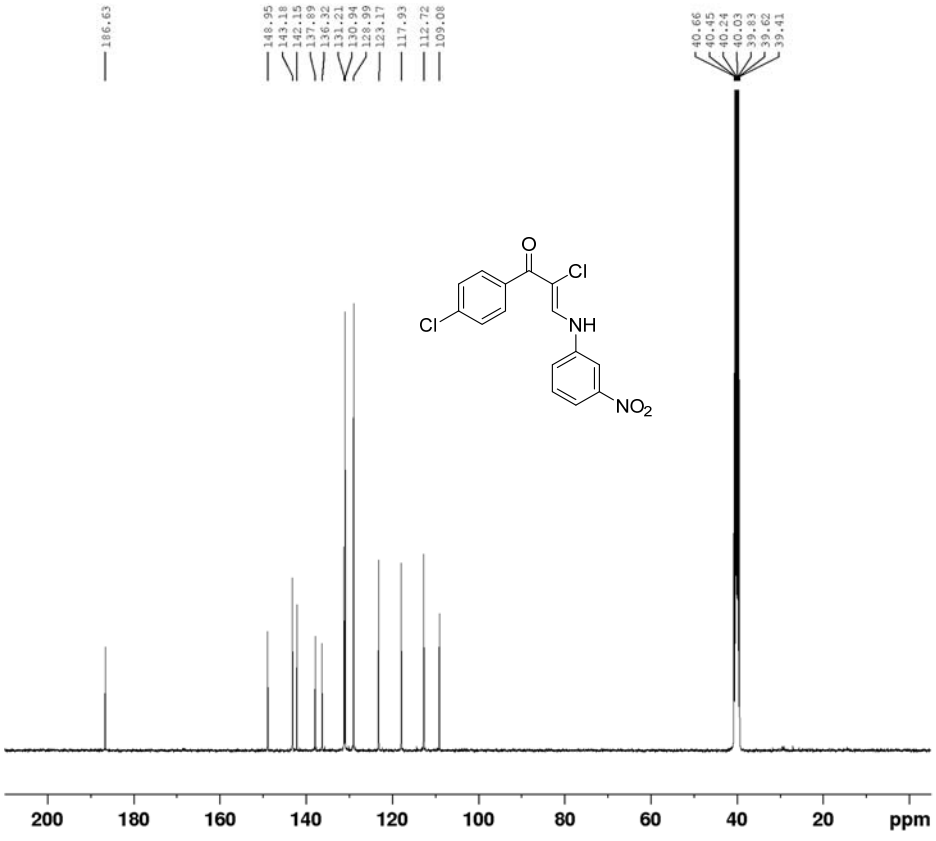



```
Current Data Parameters
NAME          Suresh-754
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231228
Time               15.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDC13
NS                   429
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                   EM
SSB                    0
LB                 2.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-2-chloro-1-(4-chlorophenyl)-3-((3-nitrophenyl)amino)prop-2-en-1-one (3dl)

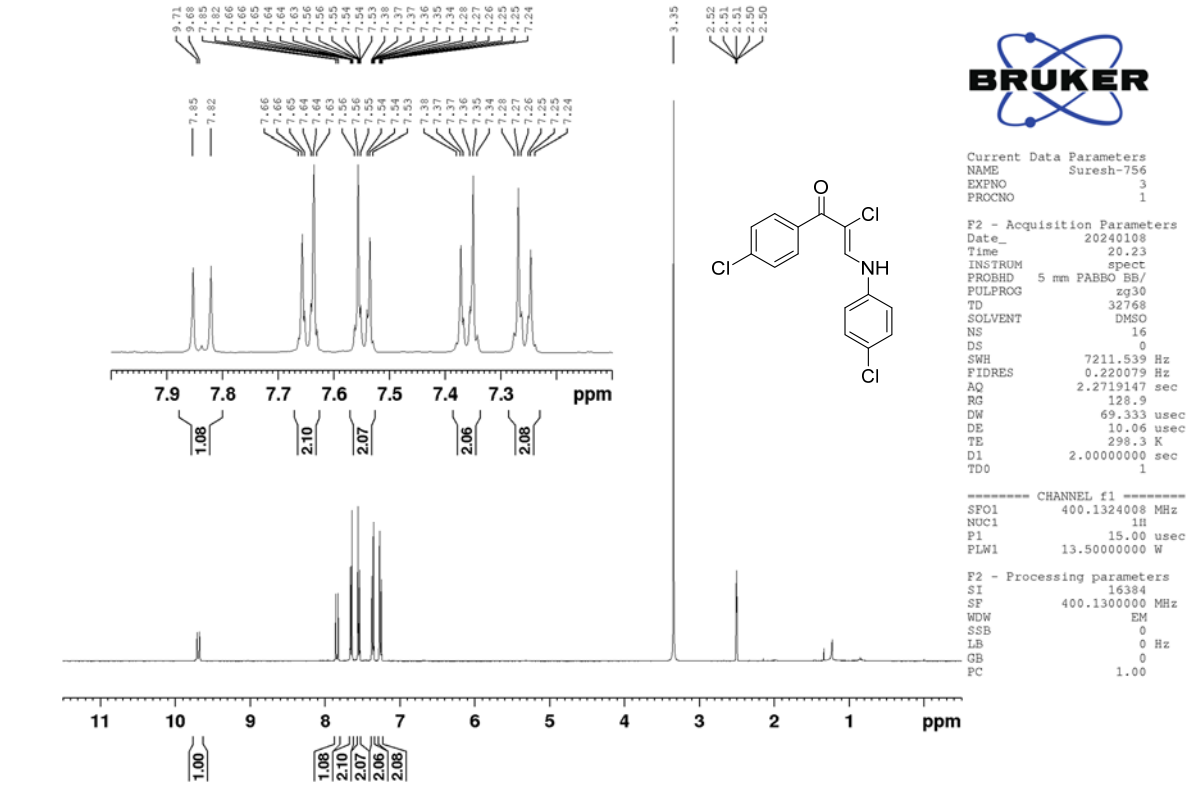


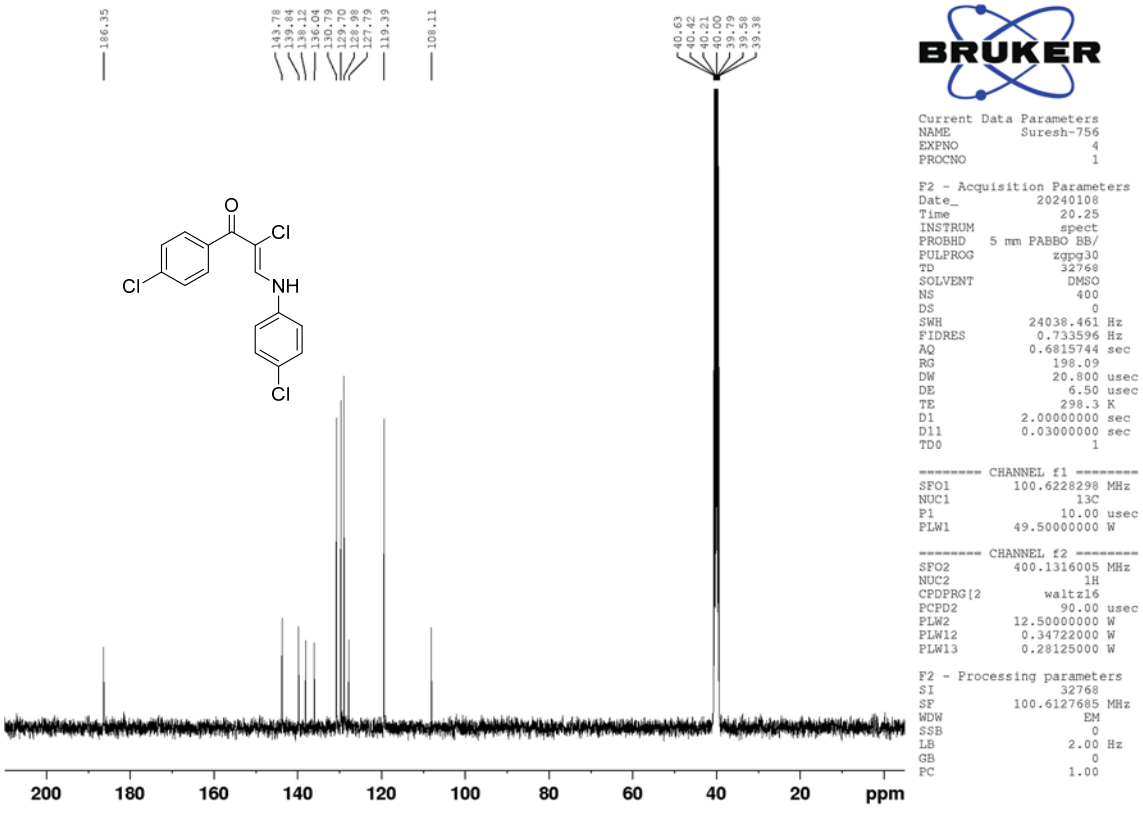

```
Current Data Parameters
NAME          Suresh-755
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240116
Time               22.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                113.31
DW                69.333 usec
DE                10.06 usec
TE                298.1 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324008 MHz
NUC1                  1H
P1                 15.00 usec
PLW1          13.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



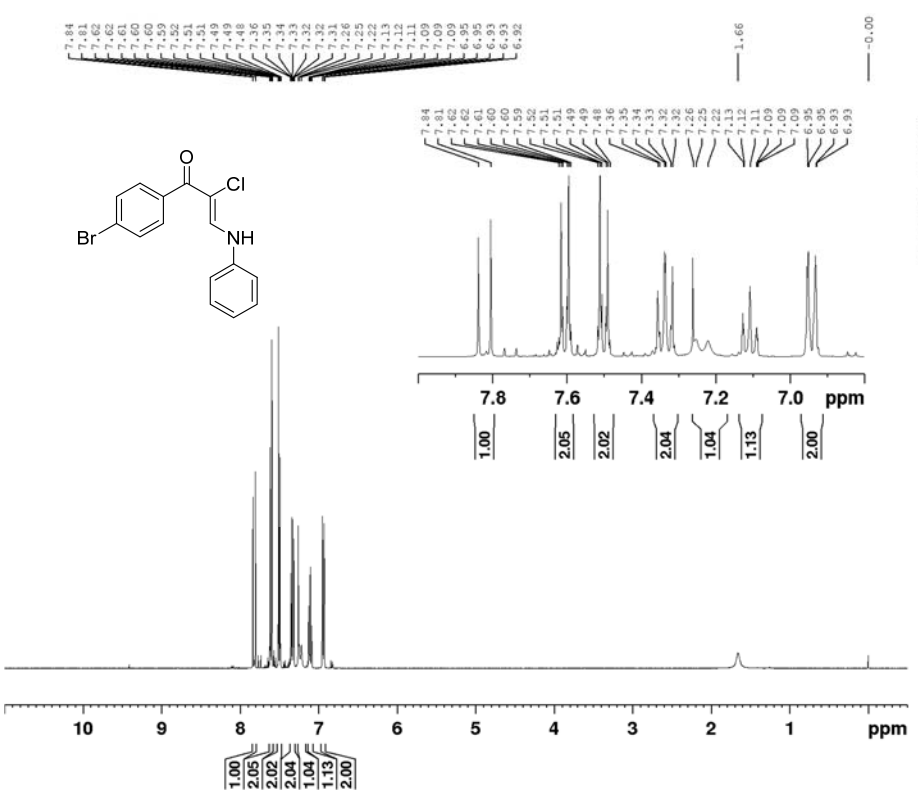

```
Current Data Parameters
NAME          Suresh-755
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240116
Time               22.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                 14950
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          49.50000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          12.50000000 W
PLW12          0.34722000 W
PLW13          0.28125000 W

F2 - Processing parameters
SI                 32768
SF            100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-2-chloro-1-(4-chlorophenyl)-3-((4-chlorophenyl)amino)prop-2-en-1-one (3dp)



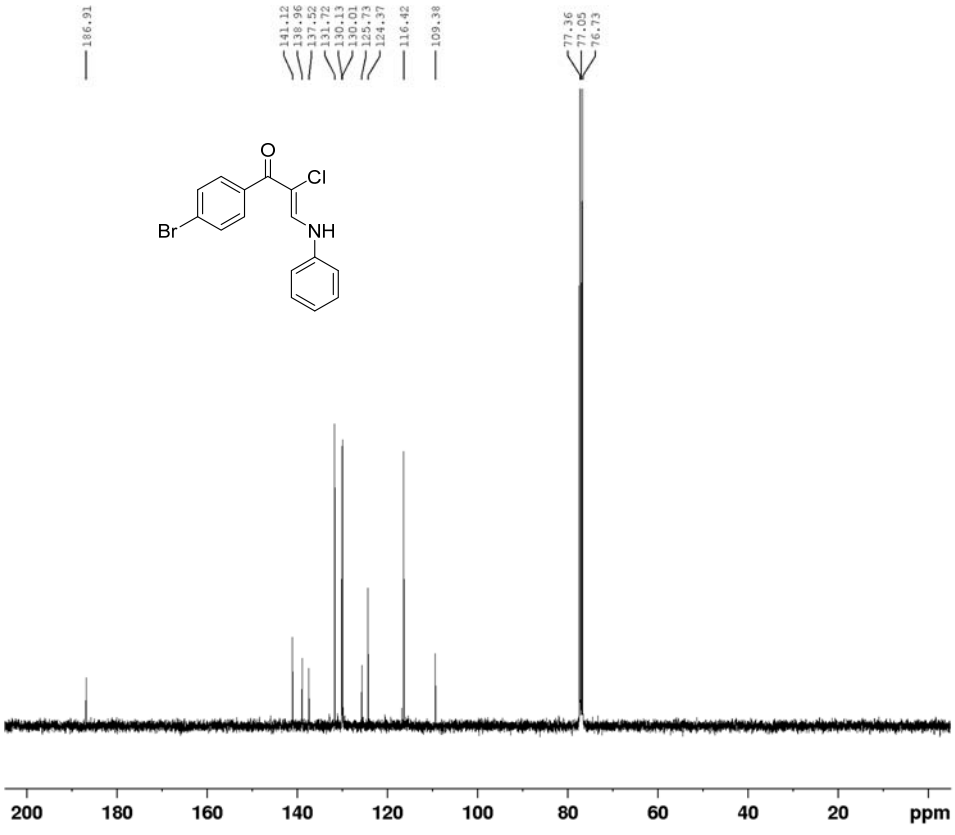


(*Z*)-1-(4-bromophenyl)-2-chloro-3-(phenylamino)prop-2-en-1-one (3ea)



BRUKER

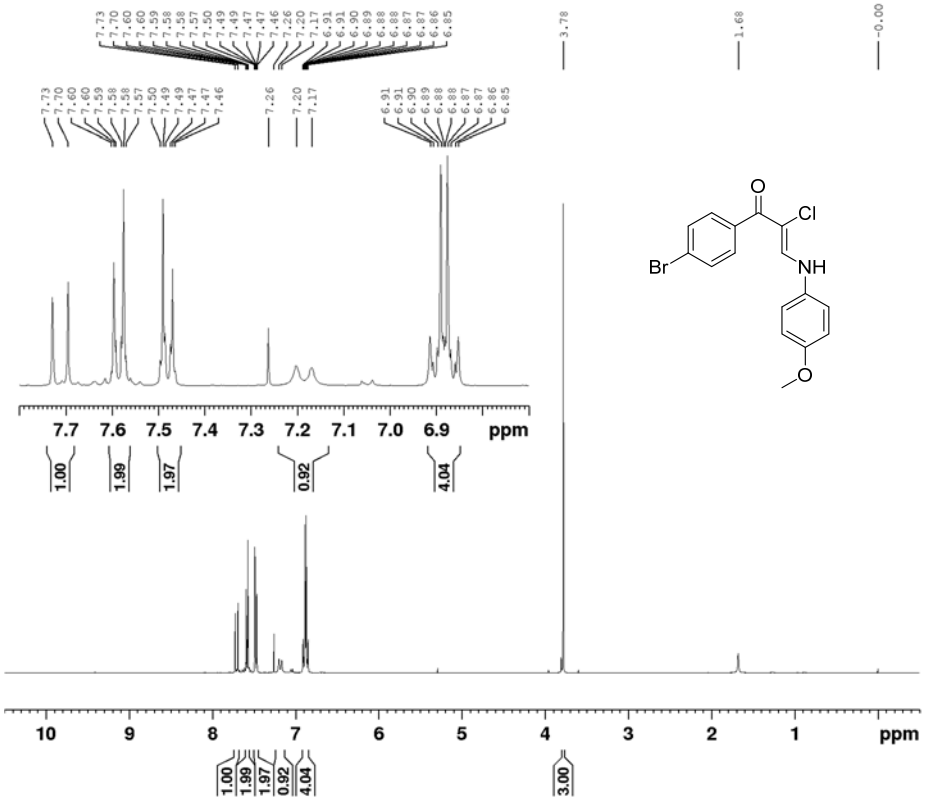
```
Current Data Parameters
NAME          Suresh-741
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231212
Time               11.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    16
DS                     0
SWH           7211.539 Hz
FIDRES          0.220079 Hz
AQ            2.2719147 sec
RG                 128.9
DW                69.333 usec
DE                10.06 usec
TE                298.4 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF          400.1300094 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



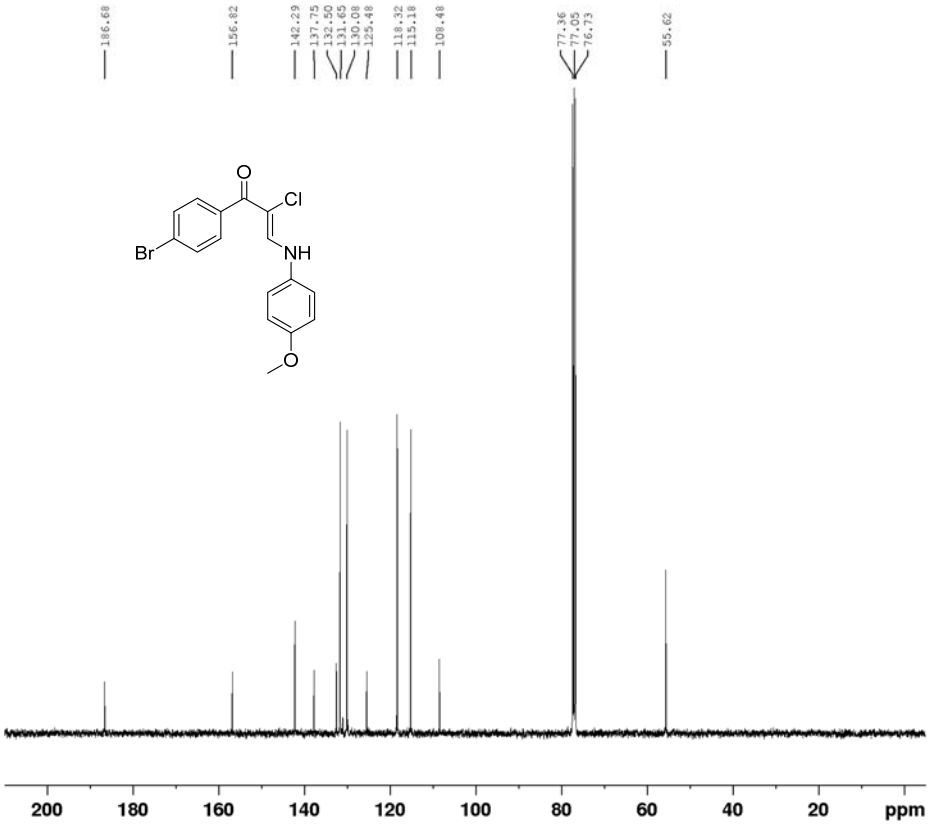
BRUKER

```
Current Data Parameters
NAME             exp 741
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231211
Time               22.14
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                 32768
SOLVENT            CDC13
NS                   512
DS                     0
SWH          24038.461 Hz
FIDRES         0.733596 Hz
AQ            0.6815744 sec
RG                 32768
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.00 usec
PL1                4.20 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                   1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127690 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-1-(4-bromophenyl)-2-chloro-3-((4-methoxyphenyl)amino)prop-2-en-1-one (3ej)

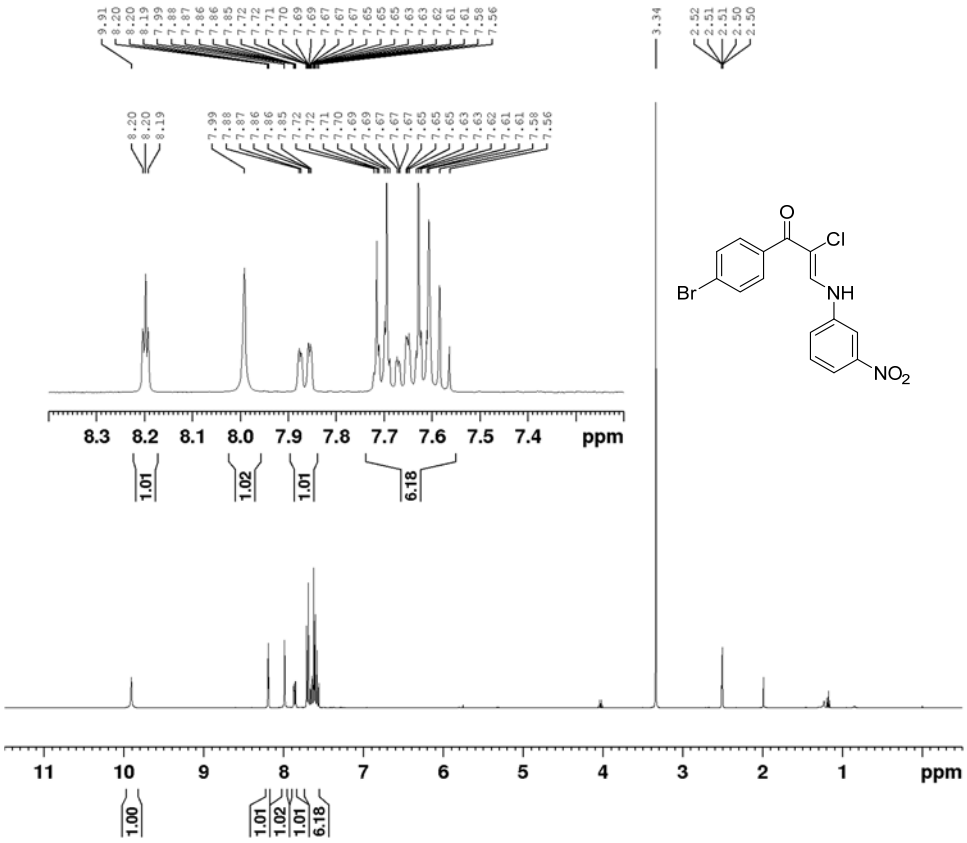


```
Current Data Parameters
NAME          Suresh-742
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231212
Time               18.13
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                113.31
DW                69.333 usec
DE                 10.06 usec
TE                299.3 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                  1H
P1                 15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF          400.1300090 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

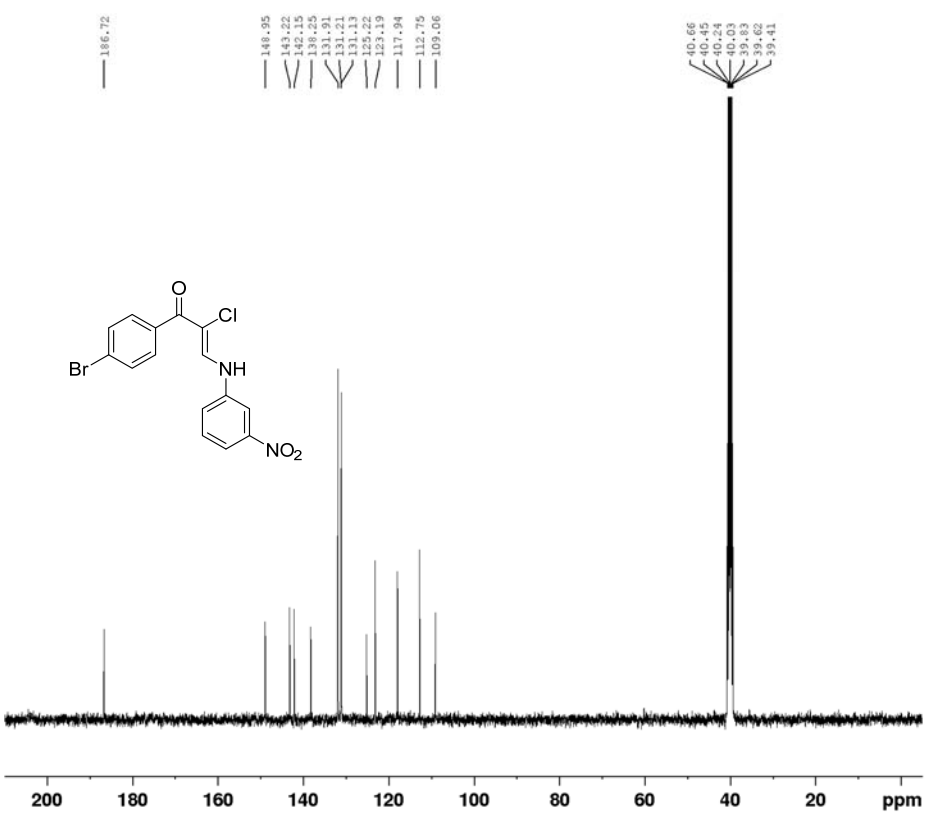


```
Current Data Parameters
NAME          Suresh-742
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231212
Time               18.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDCl3
NS                   412
DS                     0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                299.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                  13C
P1                 10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-1-(4-bromophenyl)-2-chloro-3-((3-nitrophenyl)amino)prop-2-en-1-one (3el)

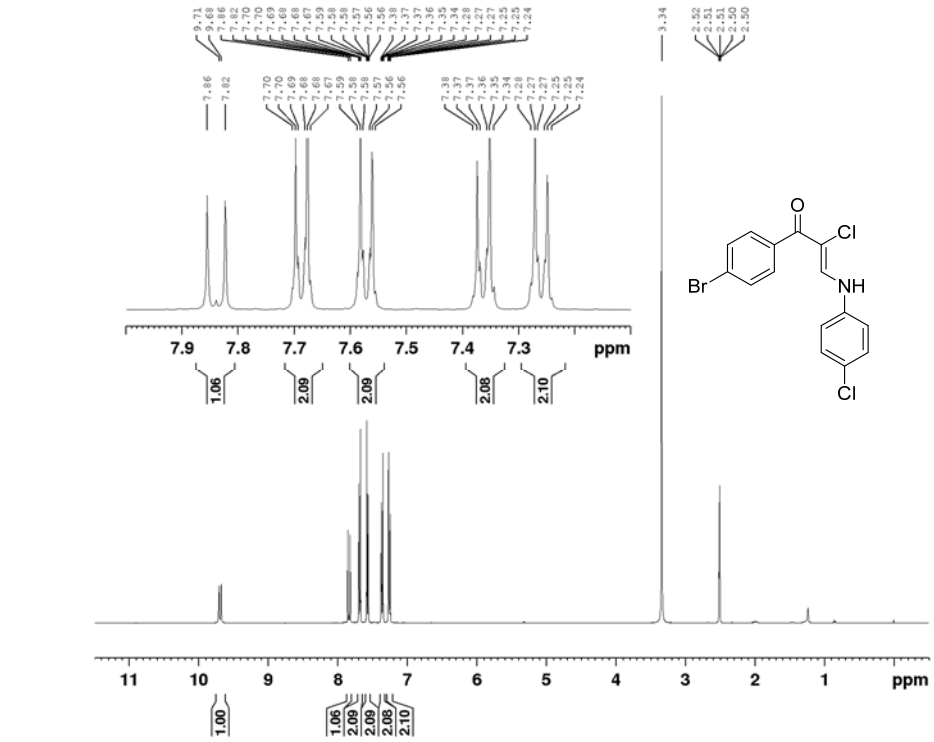



```
Current Data Parameters
NAME          Suresh-744
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231215
Time               10.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                113.31
DW                69.333 usec
DE                10.06 usec
TE                298.3 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                 16384
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

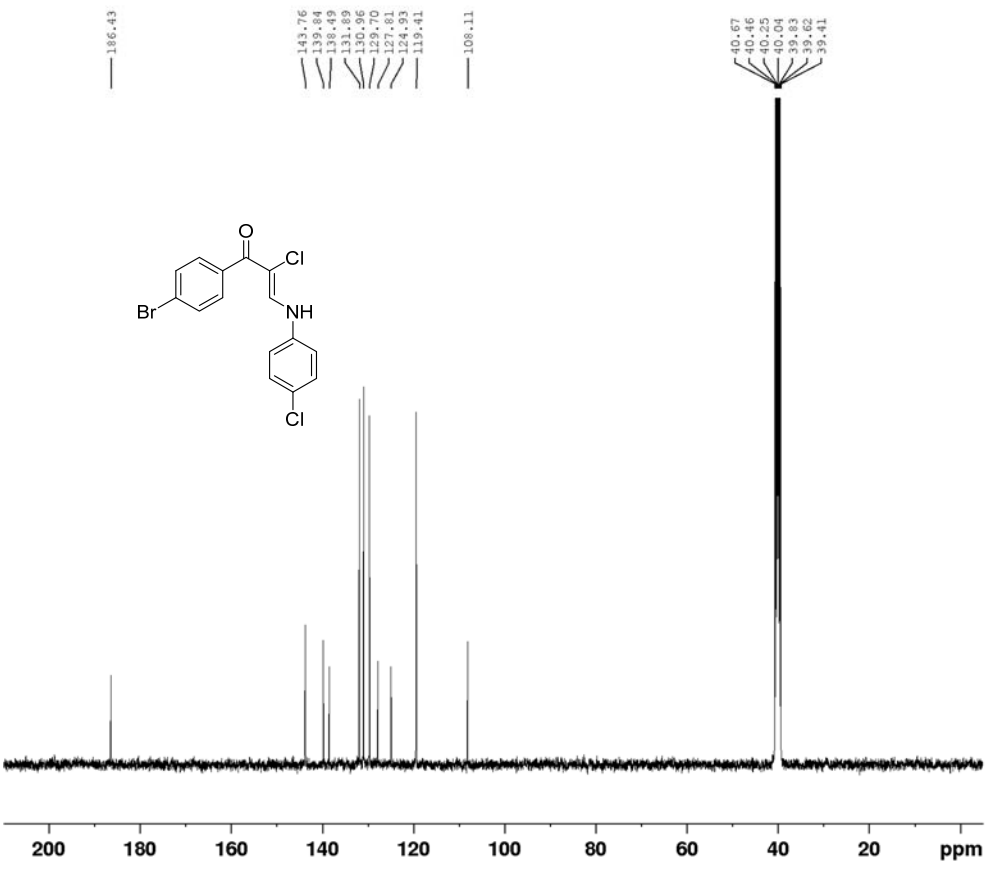



```
Current Data Parameters
NAME          Suresh-744
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231215
Time               10.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                   512
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

(*Z*)-1-(4-bromophenyl)-2-chloro-3-((4-chlorophenyl)amino)prop-2-en-1-one (3ep)

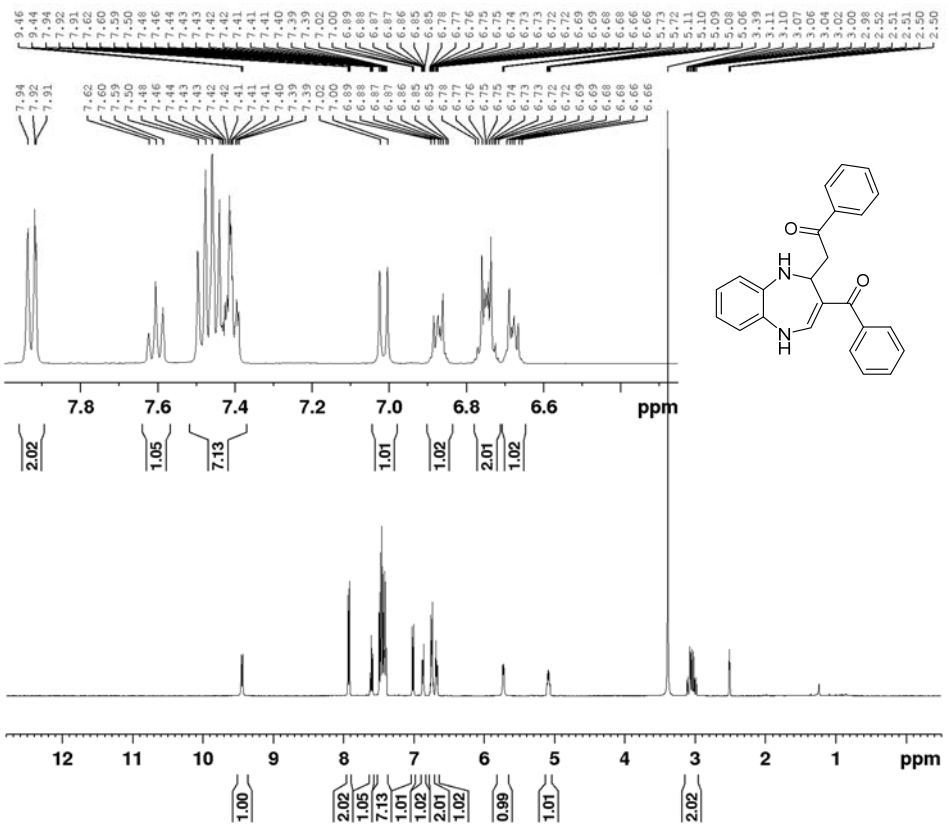


```
Current Data Parameters
NAME          Suresh-743
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231215
Time               11.17
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ             2.2719147 sec
RG                 128.9
DW                69.333 usec
DE                10.06 usec
TE                298.9 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                  15.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                 16384
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

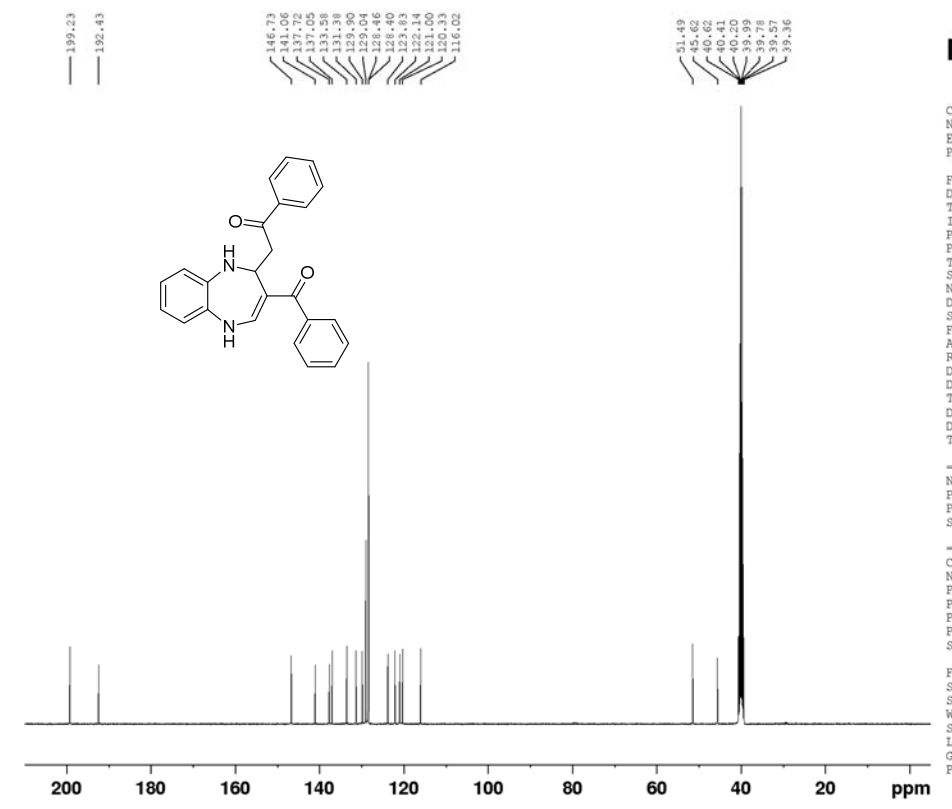


```
Current Data Parameters
NAME          Suresh-743
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20231215
Time               13.05
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                  1324
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ             0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                  13C
P1                  10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

2-(3-benzoyl-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-phenylethan-1-one 6aa

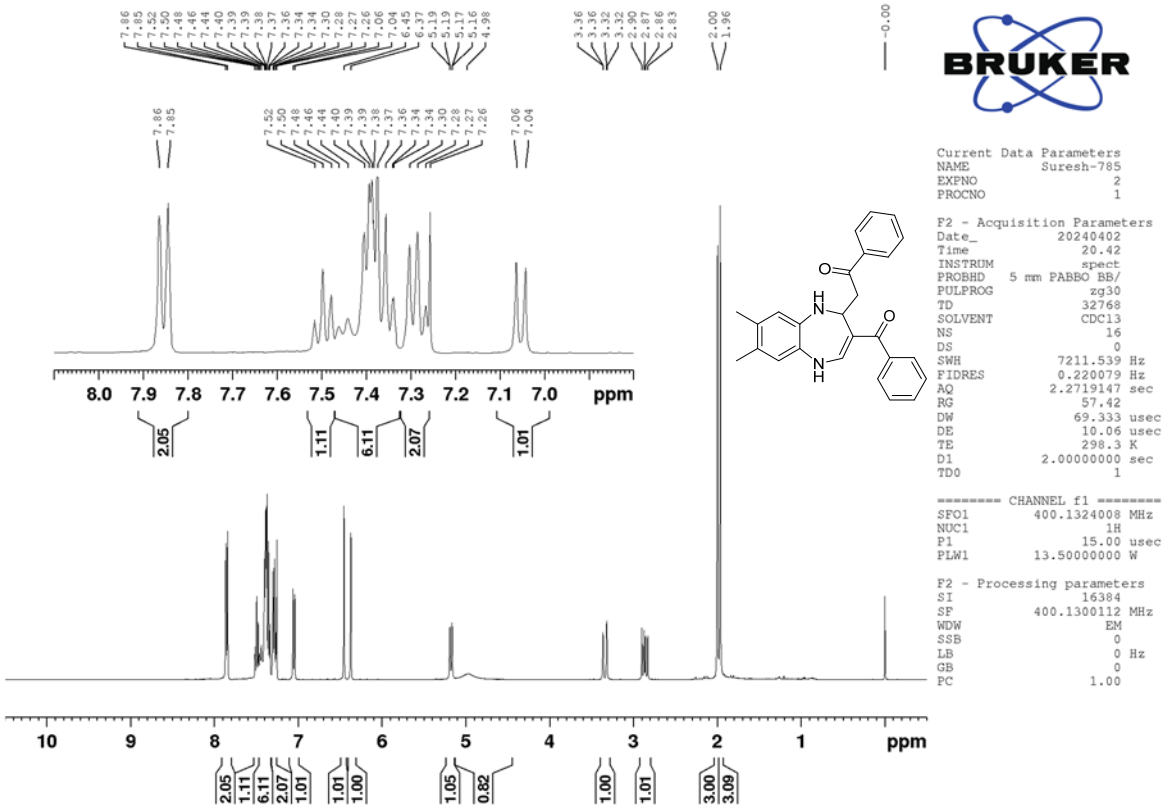


```
Current Data Parameters
NAME          Suresh-777
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240321
Time               21.26
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT            DMSO
NS                   16
DS                    0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                63.58
DW               69.333 usec
DE                10.06 usec
TE                298.2 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                  1H
P1                15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                16384
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0 Hz
GB                    0
PC                 1.00
```



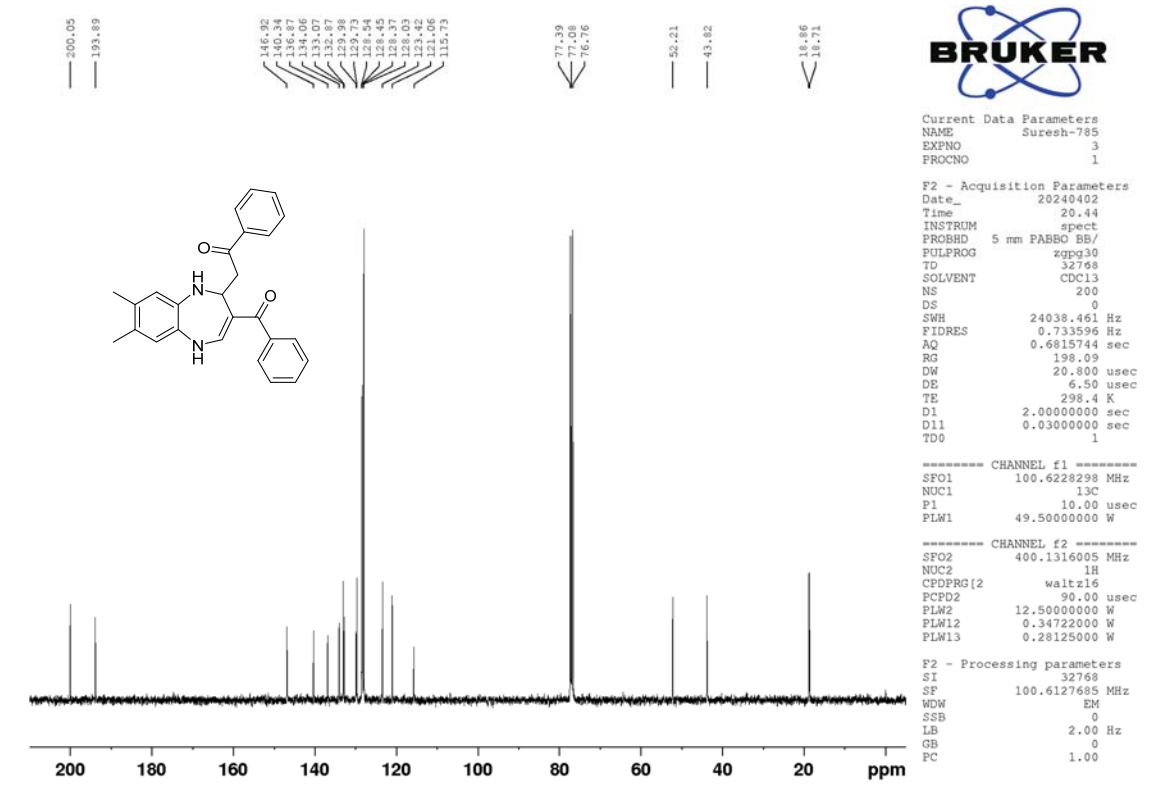
```
Current Data Parameters
NAME             exp 777
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240321
Time               21.51
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                32768
SOLVENT            DMSO
NS                15000
DS                    0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                32768
DW               20.800 usec
DE                6.50 usec
TE                296.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PL1                4.20 dB
SFO1        100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2               10.20 dB
PL12              26.00 dB
PL13              29.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127690 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.00
```

2-(3-benzoyl-7,8-dimethyl-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-phenylethan-1-one
6ab



BRUKER

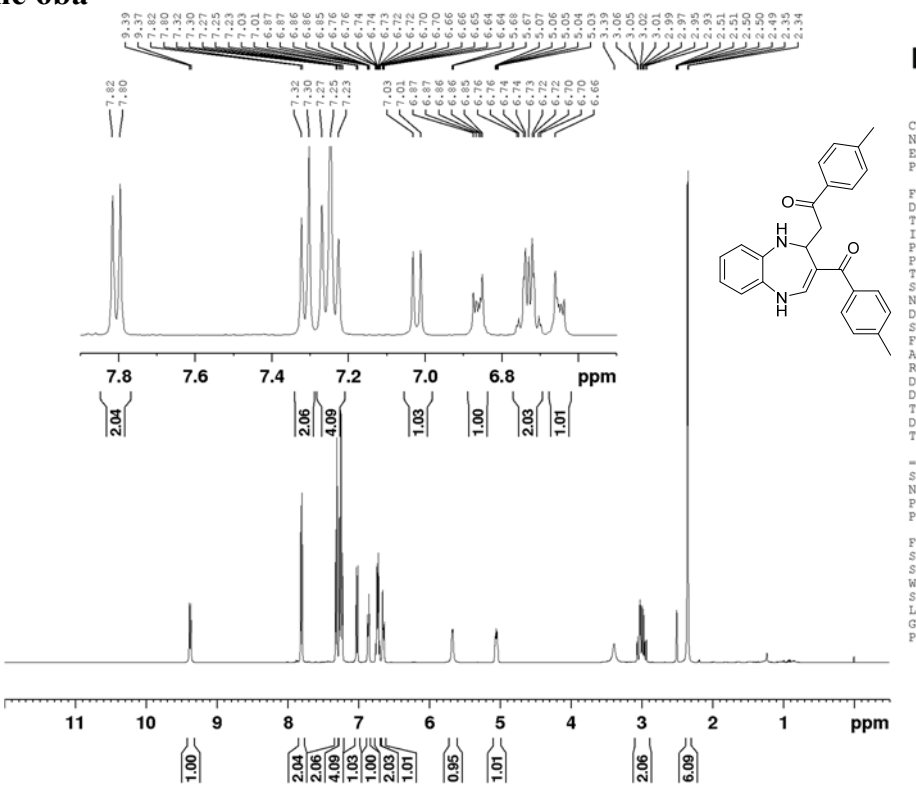
```
Current Data Parameters
NAME          Suresh-785
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240402
Time               20.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT            CDC13
NS                    16
DS                     0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                 57.42
DW                69.333 usec
DE                10.06 usec
TE                298.3 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                 16384
SF            400.1300112 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```



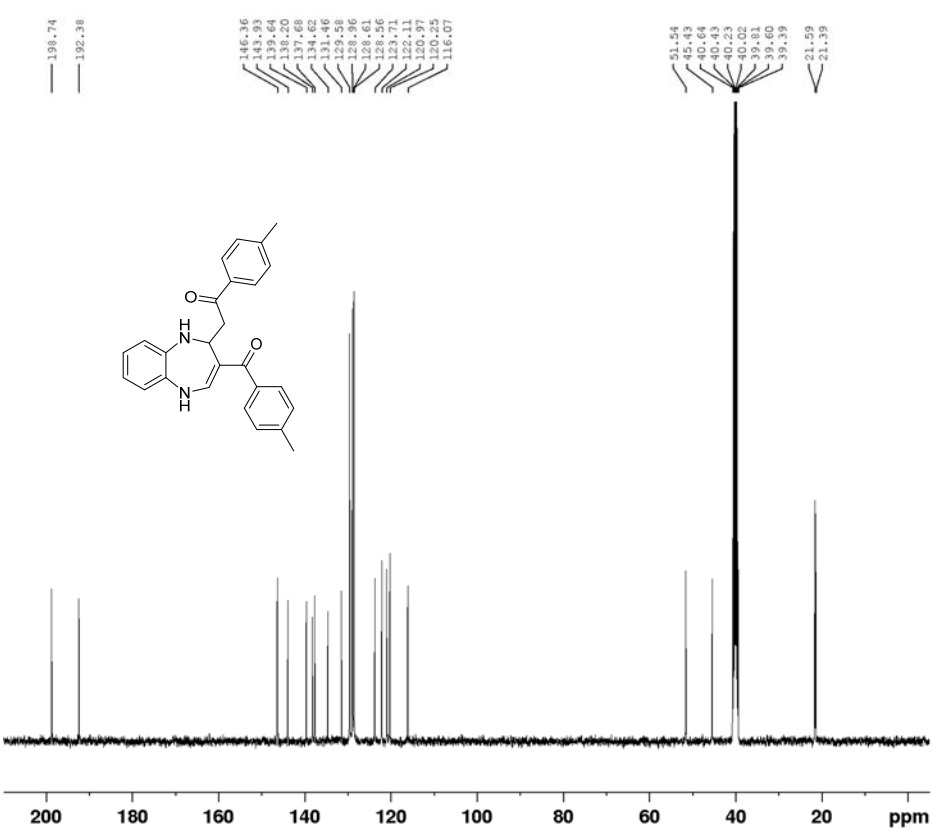
BRUKER

```
Current Data Parameters
NAME          Suresh-785
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240402
Time               20.44
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32768
SOLVENT            CDC13
NS                   200
DS                     0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                 10.00 usec
PLW1         49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2         12.50000000 W
PLW12         0.34722000 W
PLW13         0.28125000 W

F2 - Processing parameters
SI                 32768
SF           100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

2-(3-(4-methylbenzoyl)-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-(*p*-tolyl)ethan-1-one 6ba

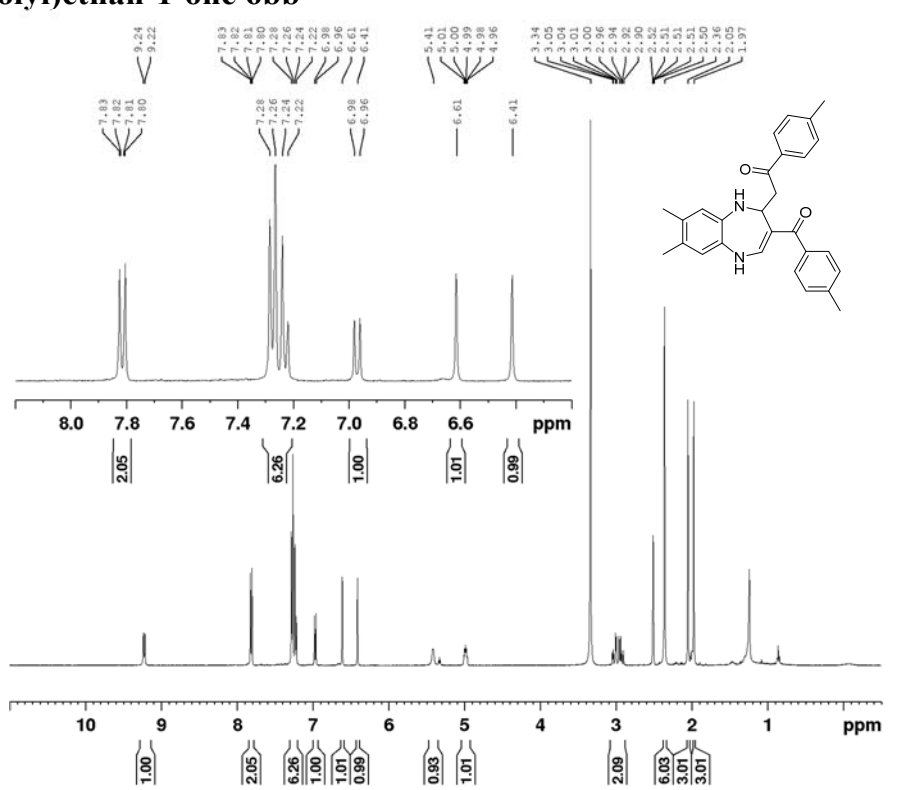


```
Current Data Parameters
NAME          Suresh-833
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240531
Time               11.14
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                57.42
DW               69.333 usec
DE                10.06 usec
TE                298.0 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF          400.1300028 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

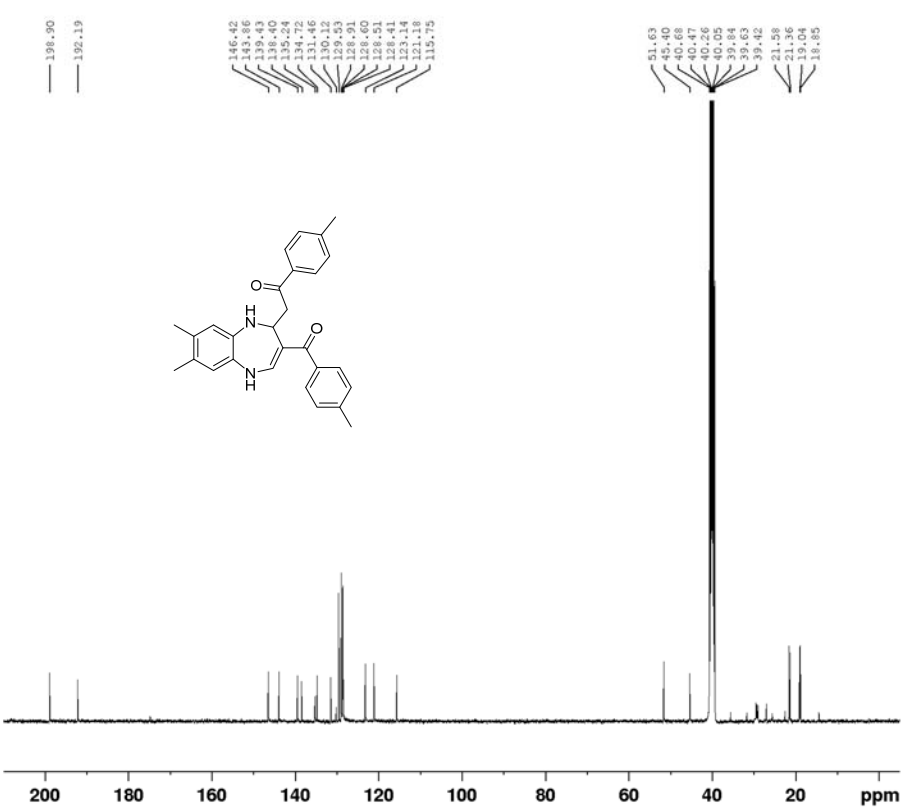


```
Current Data Parameters
NAME          Suresh-833
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240531
Time               11.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                   512
DS                     0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                   13C
P1                 10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

2-(7,8-dimethyl-3-(4-methylbenzoyl)-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-(*p*-tolyl)ethan-1-one 6bb

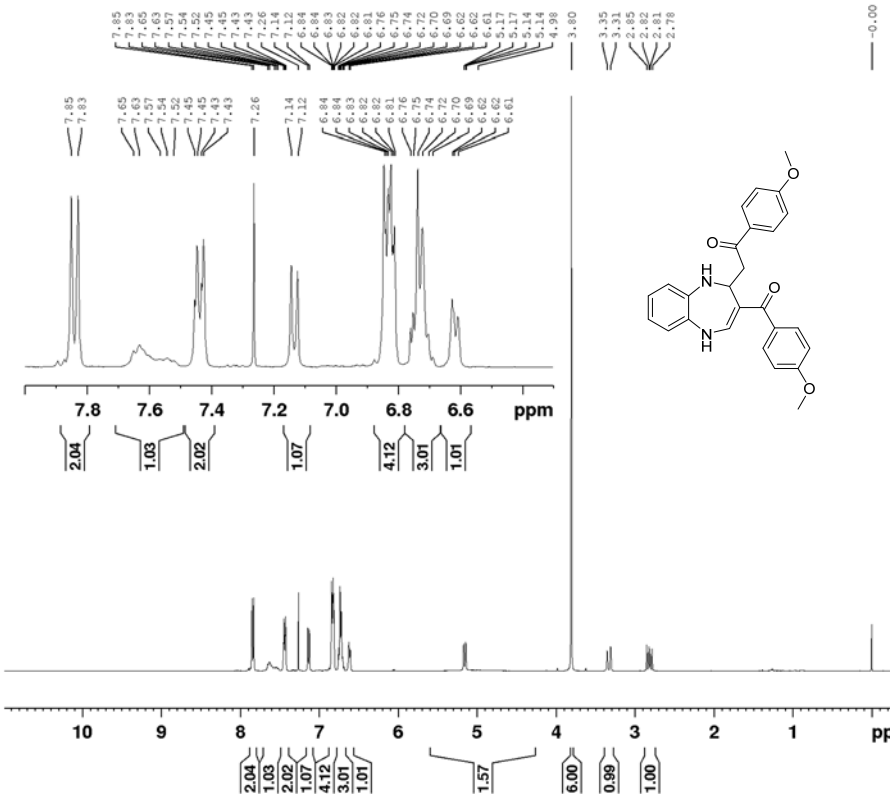


```
Current Data Parameters
NAME      Exp-1-revision work
EXPNO                   26
PROCNO                   1

F2 - Acquisition Parameters
Date_              20240430
Time                 22.04
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32768
SOLVENT              DMSO
NS                      16
DS                       0
SWH               7211.539 Hz
FIDRES            0.220079 Hz
AQ                2.2719147 sec
RG                   128.9
DW                  69.333 usec
DE                  10.06 usec
TE                  298.3 K
D1              2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.1324008 MHz
NUC1                   1H
P1                  15.00 usec
PLW1           13.50000000 W

F2 - Processing parameters
SI                   16384
SF              400.1300000 MHz
WDW                    EM
SSB                     0
LB                      0 Hz
GB                      0
PC                   1.00
```

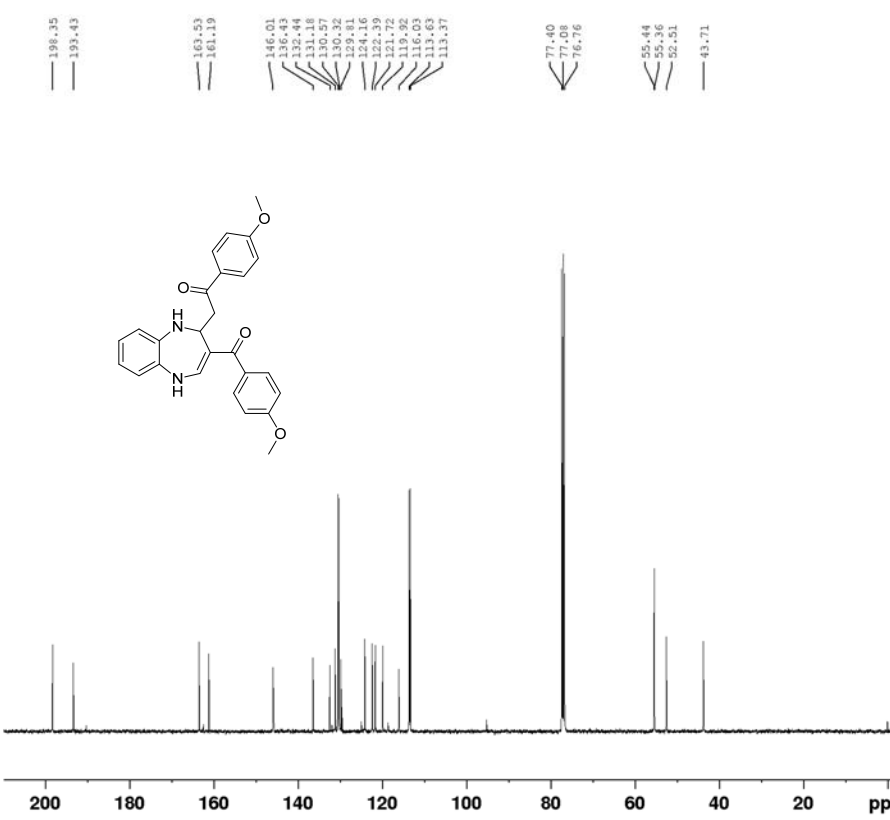


```
Current Data Parameters
NAME      Exp-1-revision work
EXPNO                   27
PROCNO                   2

F2 - Acquisition Parameters
Date_              20240501
Time                  9.32
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgpg30
TD                  32768
SOLVENT              DMSO
NS                   15000
DS                       0
SWH              24038.461 Hz
FIDRES            0.733596 Hz
AQ                0.6815744 sec
RG                   198.09
DW                  20.800 usec
DE                   6.50 usec
TE                  300.4 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6228298 MHz
NUC1                   13C
P1                  10.00 usec
PLW1           49.50000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               90.00 usec
PLW2           12.50000000 W
PLW12           0.34722000 W
PLW13           0.28125000 W

F2 - Processing parameters
SI                   32768
SF              100.6127685 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.00
```

2-(3-(4-methoxybenzoyl)-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-(4-methoxyphenyl)ethan-1-one 6ca

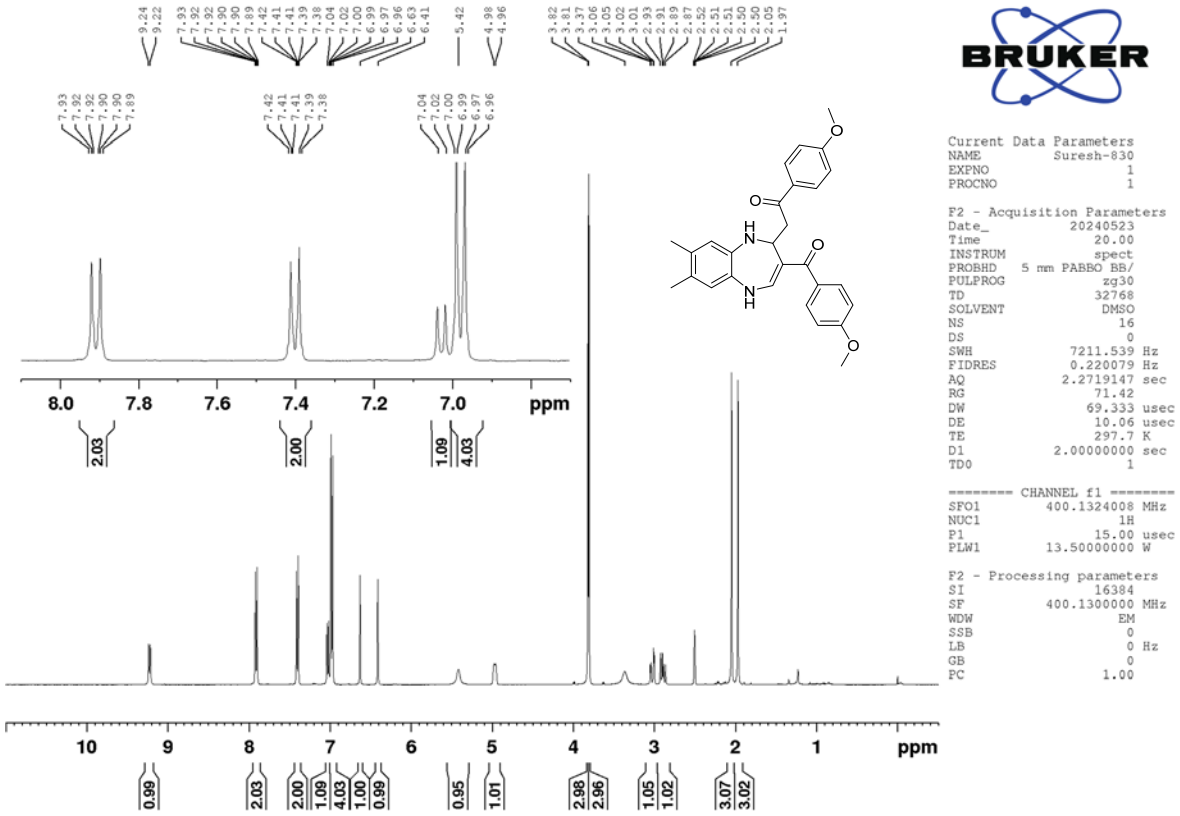


```
Current Data Parameters
NAME          Suresh-829
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240522
Time               17.20
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                63.58
DW              69.333 usec
DE              10.06 usec
TE                297.8 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                   1H
P1                 15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF          400.1300085 MHz
WDW                   EM
SSB                    0
LB                     0 Hz
GB                     0
PC                  1.00
```

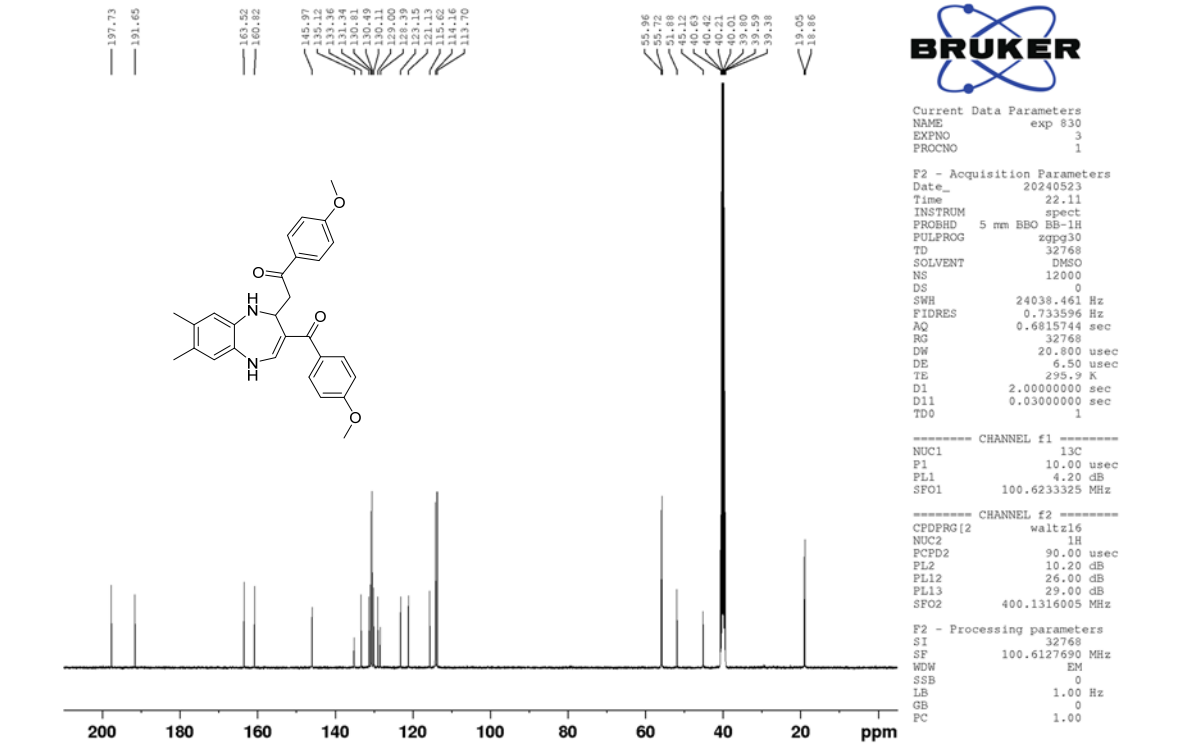


```
Current Data Parameters
NAME          Suresh-829
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240522
Time               17.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  978
DS                    0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW              20.800 usec
DE               6.50 usec
TE                298.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                   13C
P1                 10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

2-(3-(4-methoxybenzoyl)-7,8-dimethyl-2,5-dihydro-1H-benzo[b][1,4]diazepin-2-yl)-1-(4-methoxyphenyl)ethan-1-one 6cb

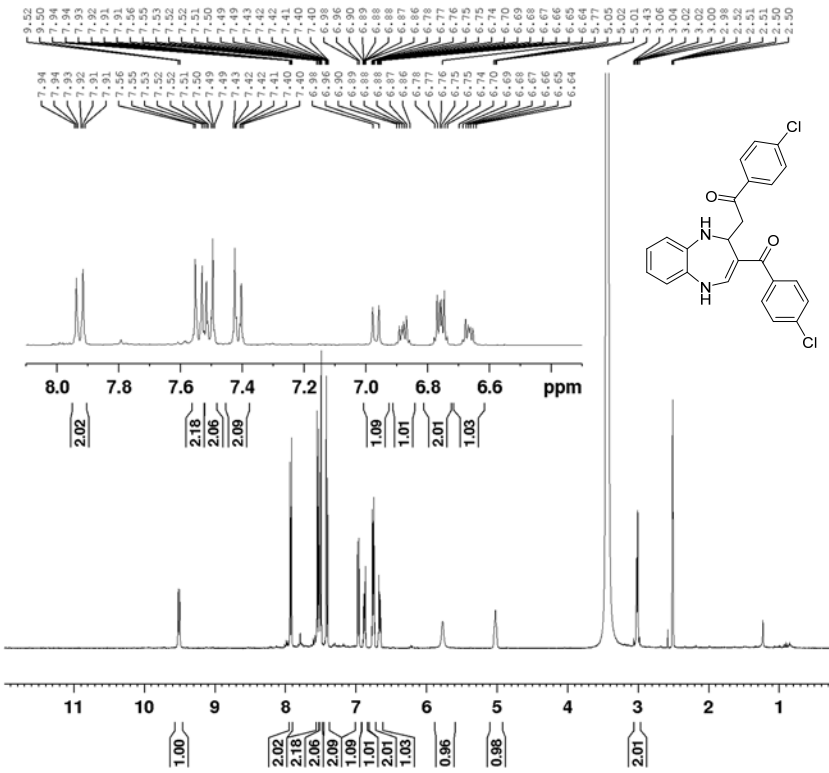


```
Current Data Parameters
NAME                 Suresh-830
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20240523
Time                   20.00
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       16
DS                        0
SWH                7211.539 Hz
FIDRES             0.220079 Hz
AQ                 2.2719147 sec
RG                     71.42
DW                  69.333 usec
DE                   10.06 usec
TE                   297.7 K
D1                 2.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1             400.1324008 MHz
NUC1                       1H
P1                      15.00 usec
PLW1            13.50000000 W

F2 - Processing parameters
SI                        16384
SF               400.1300000 MHz
WDW                        EM
SSB                         0
LB                       0 Hz
GB                          0
PC                       1.00
```

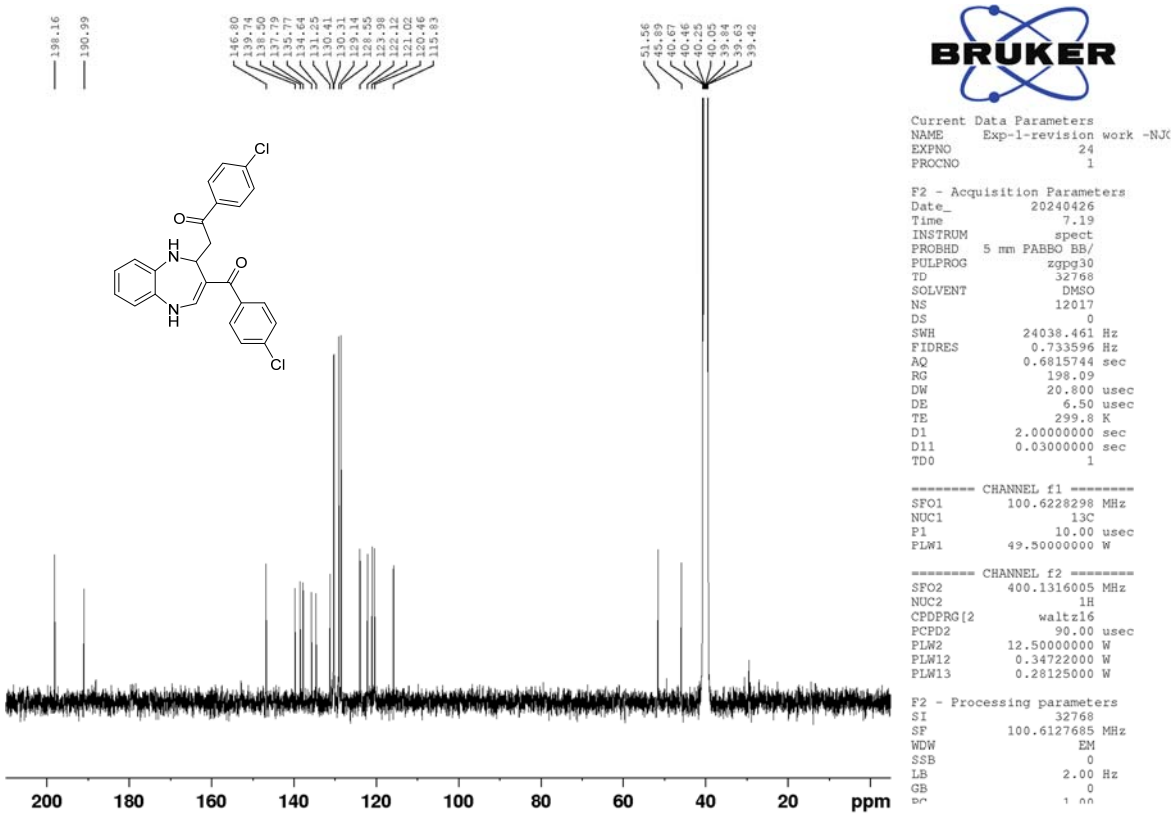


```
Current Data Parameters
NAME                  exp 830
EXPNO                       3
PROCNO                      1

F2 - Acquisition Parameters
Date_               20240523
Time                   22.11
INSTRUM                spect
PROBHD    5 mm BBO BB-1H
PULPROG             zgpg30
TD                    32768
SOLVENT                DMSO
NS                     12000
DS                        0
SWH               24038.461 Hz
FIDRES             0.733596 Hz
AQ                 0.6815744 sec
RG                     32768
DW                  20.800 usec
DE                    6.50 usec
TE                   295.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      13C
P1                      10.00 usec
PL1                      4.20 dB
SFO1            100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL2                     10.20 dB
PL12                    26.00 dB
PL13                    29.00 dB
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF              100.6127690 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.00
```

2-(3-(4-chlorobenzoyl)-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-(4-chlorophenyl)ethan-1-one 6da

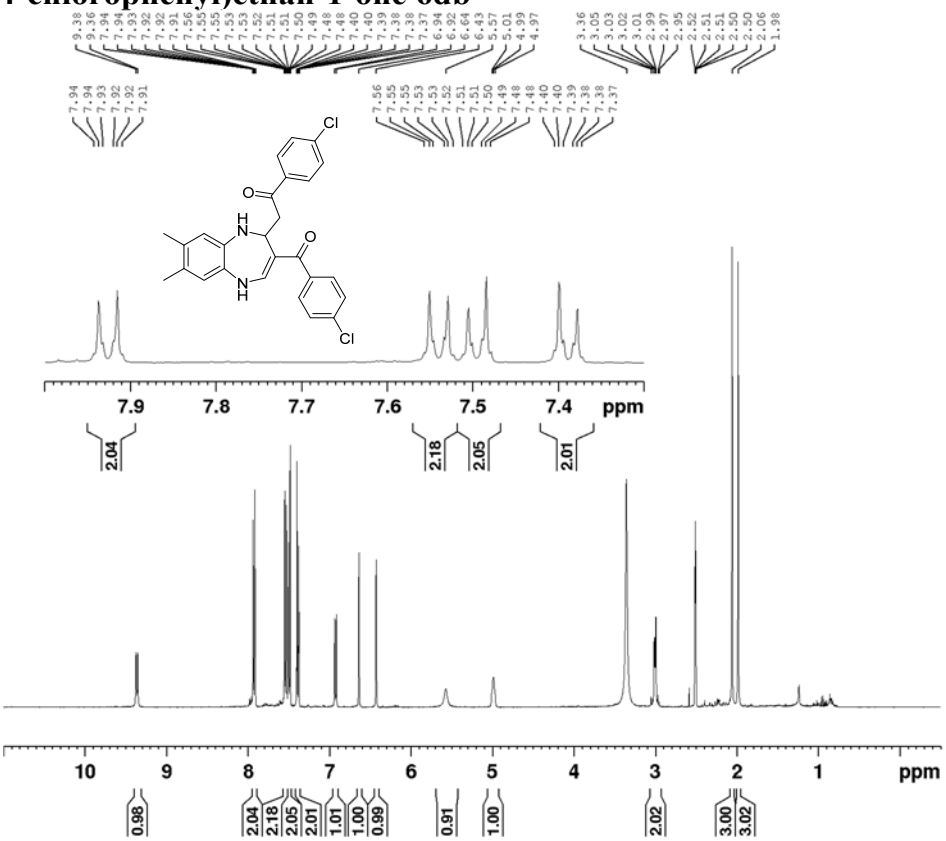


```
Current Data Parameters
NAME      Exp-1-revision work
EXPNO                   22
PROCNO                   1

F2 - Acquisition Parameters
Date_           20240425
Time              20.55
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           DMSO
NS                   16
DS                    0
SWH            7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                71.42
DW               69.333 usec
DE               10.06 usec
TE                298.4 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                1H
P1                15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                16384
SF           400.1300000 MHz
WDW                 EM
SSB                  0
LB                0 Hz
GB                   0
PC                1.00
```

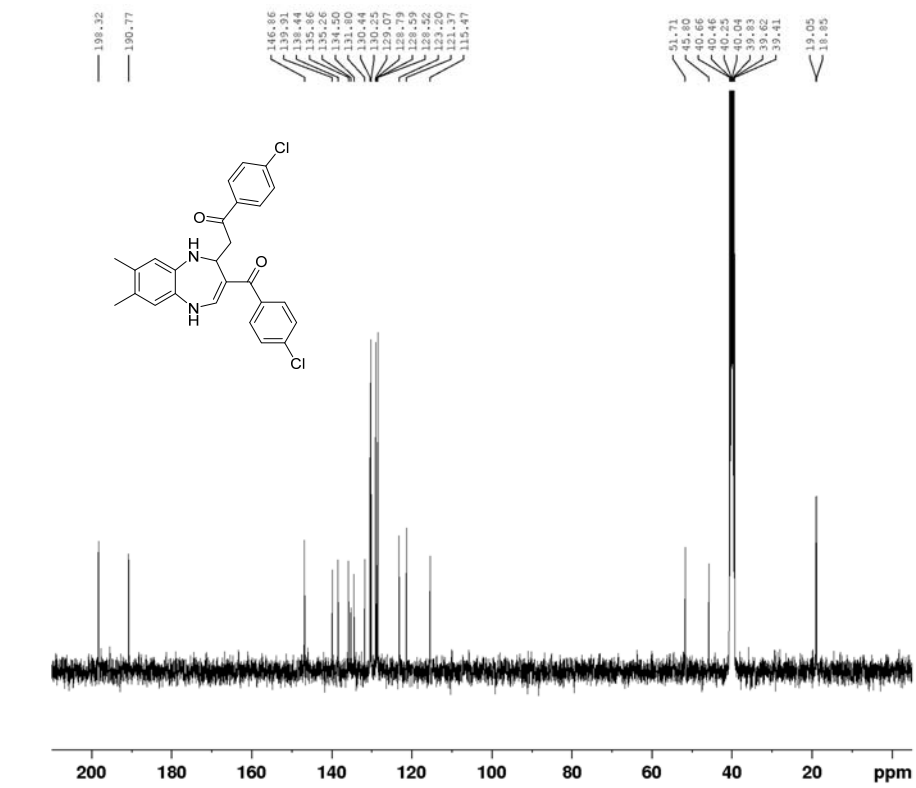


```
Current Data Parameters
NAME      Exp-1-revision work -NJ
EXPNO                   24
PROCNO                   1

F2 - Acquisition Parameters
Date_           20240426
Time              7.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT           DMSO
NS                12017
DS                    0
SWH           24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                198.09
DW               20.800 usec
DE                6.50 usec
TE                299.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF           100.6127685 MHz
WDW                 EM
SSB                  0
LB                2.00 Hz
GB                   0
```

2-(3-(4-chlorobenzoyl)-7,8-dimethyl-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-(4-chlorophenyl)ethan-1-one 6db

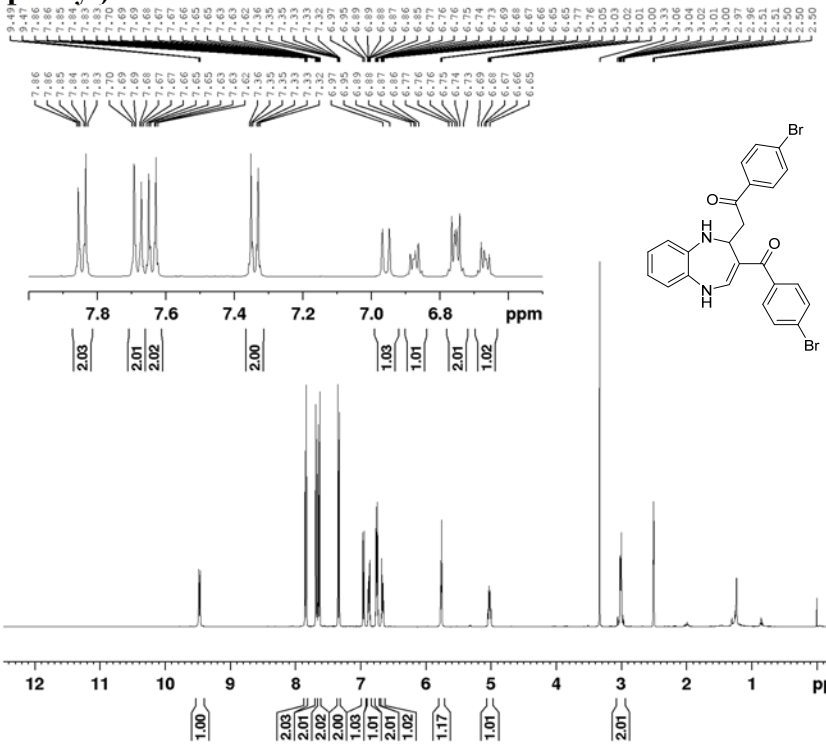


```
Current Data Parameters
NAME      Exp-1-revision work -N
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240425
Time              20.47
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT           DMSO
NS                   20
DS                    0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG               113.31
DW               69.333 usec
DE               10.06 usec
TE               298.4 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                  1H
P1                15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                16384
SF          400.1300000 MHz
WDW                  EM
SSB                   0
LB                 0 Hz
GB                    0
PC                 1.00
```



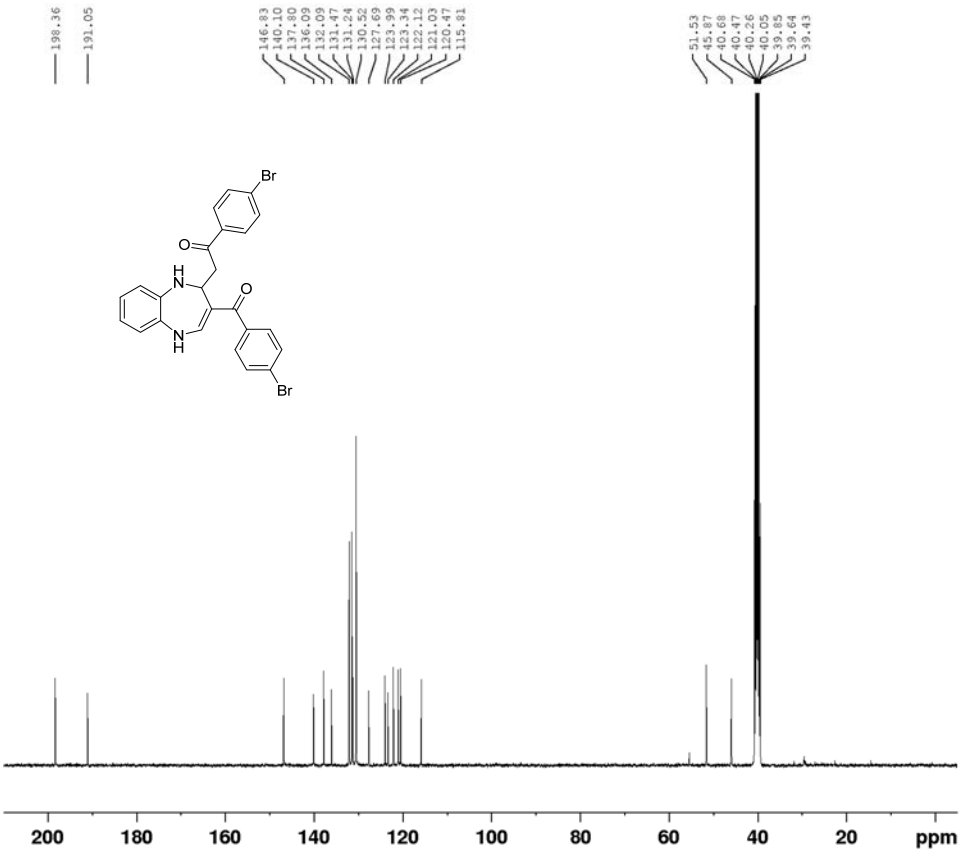
```
Current Data Parameters
NAME      Exp-1-revision work -1
EXPNO                 22
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240425
Time              21.44
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT           DMSO
NS                  505
DS                    0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE               300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                 13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          100.6127685 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.00
```

2-(3-(4-bromobenzoyl)-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-(4-bromophenyl)ethan-1-one 6ea



BRUKER

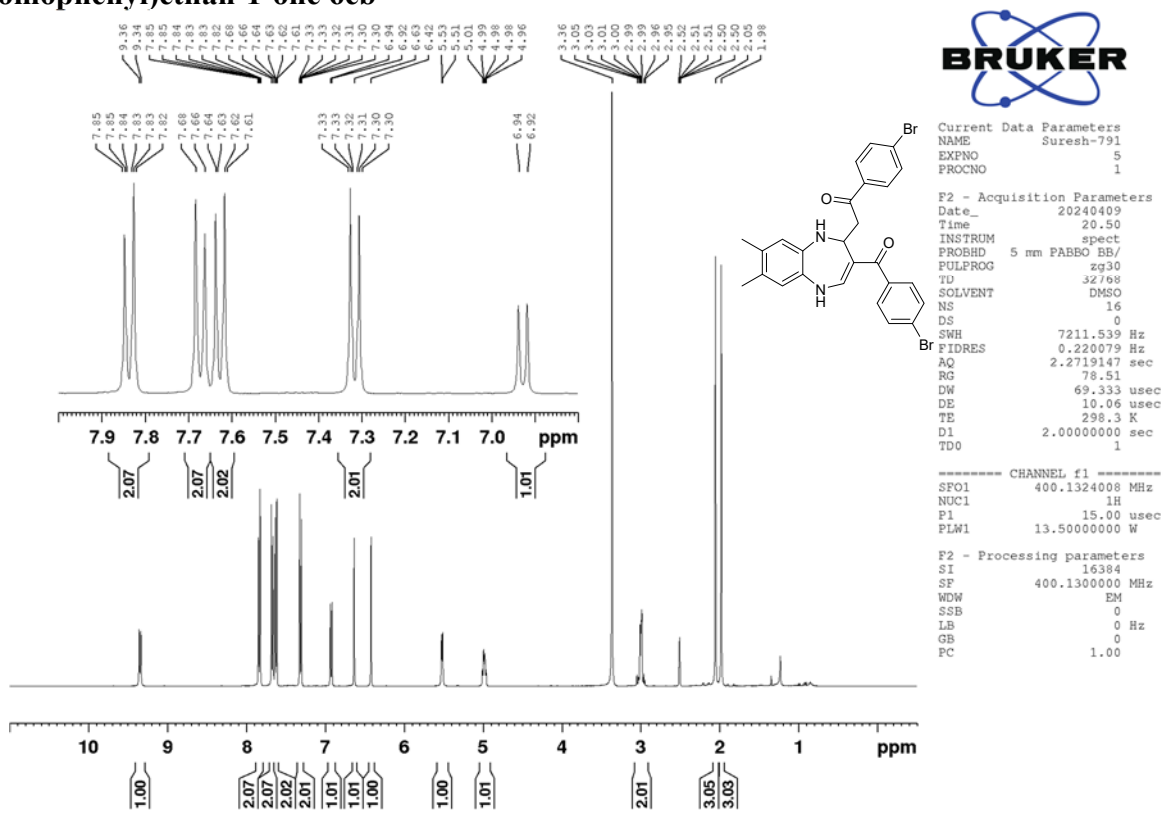
```
Current Data Parameters
NAME          Suresh-787
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240419
Time               15.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH             7211.539 Hz
FIDRES          0.220079 Hz
AQ              2.2719147 sec
RG                113.31
DW                69.333 usec
DE                10.06 usec
TE                298.8 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                  15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                 16384
SF          400.1300019 MHz
WDW                   EM
SSB                    0
LB                  0 Hz
GB                     0
PC                  1.00
```



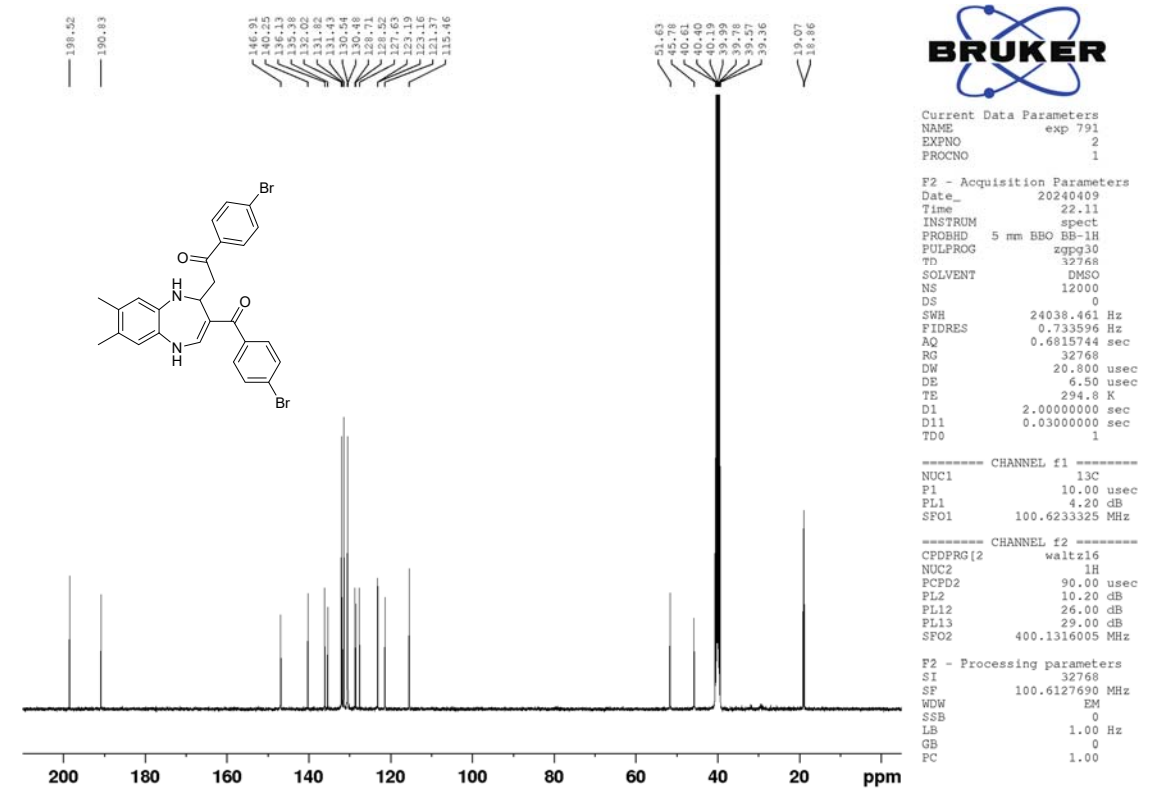
BRUKER

```
Current Data Parameters
NAME          Suresh-787
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240419
Time               21.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 32760
SOLVENT             DMSO
NS                  6000
DS                     0
SWH            24038.461 Hz
FIDRES          0.733596 Hz
AQ              0.6815744 sec
RG                198.09
DW                20.800 usec
DE                 6.50 usec
TE                298.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                   13C
P1                  10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                 32768
SF          100.6127685 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.00
```

2-(3-(4-bromobenzoyl)-7,8-dimethyl-2,5-dihydro-1*H*-benzo[*b*][1,4]diazepin-2-yl)-1-(4-bromophenyl)ethan-1-one 6eb

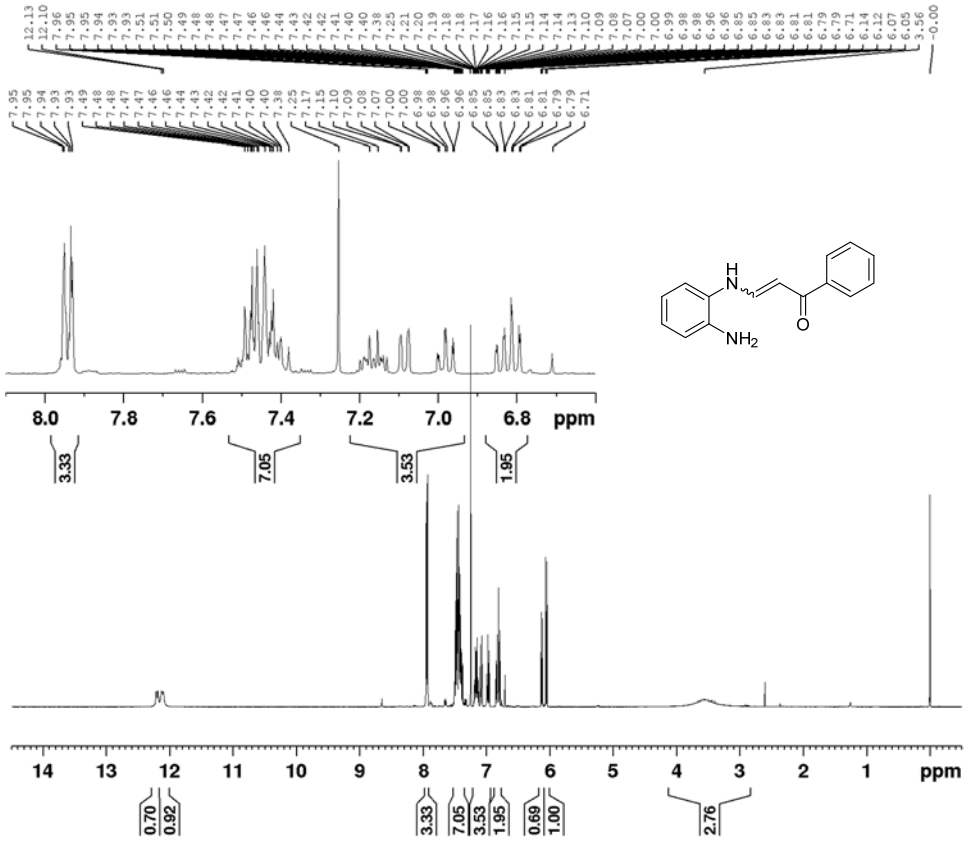


```
Current Data Parameters
NAME          Suresh-791
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240409
Time               20.50
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                 78.51
DW                69.333 usec
DE                10.06 usec
TE                298.3 K
D1            2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324008 MHz
NUC1                   1H
P1                  15.00 usec
PLW1         13.50000000 W

F2 - Processing parameters
SI                 16384
SF           400.1300000 MHz
WDW                   EM
SSB                    0
LB                 0 Hz
GB                     0
PC                  1.00
```

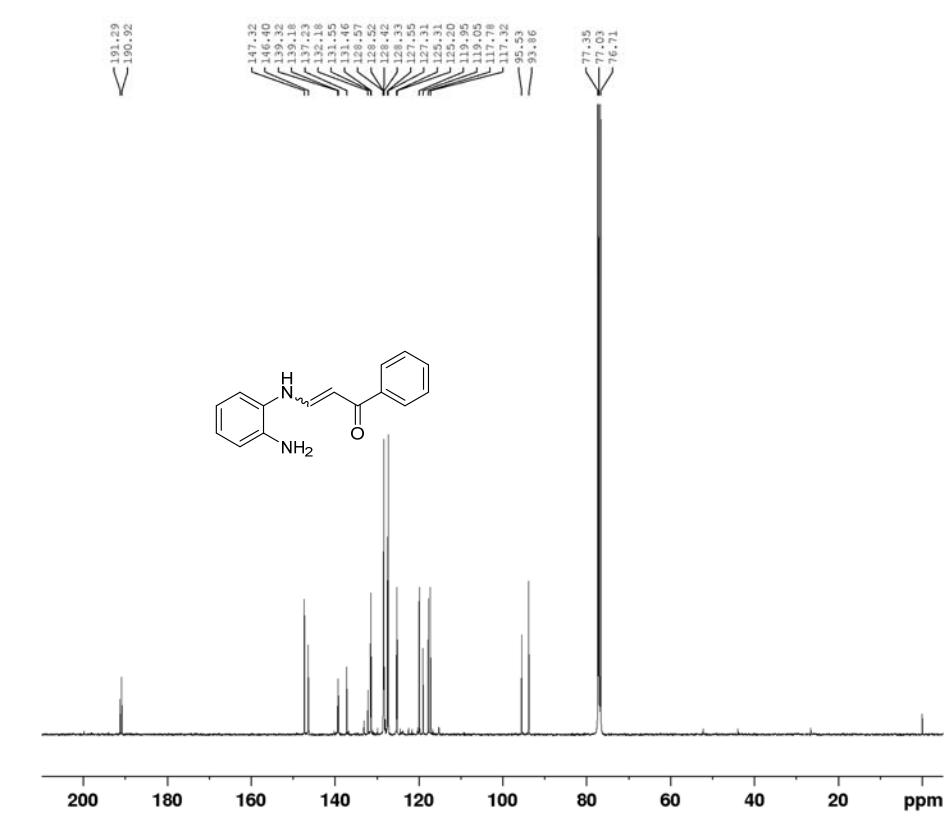


```
Current Data Parameters
NAME             exp 791
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240409
Time               22.11
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                 12000
DS                     0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG                 32768
DW                20.800 usec
DE                 6.50 usec
TE                294.8 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                4.20 dB
SFO1         100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                10.20 dB
PL12               26.00 dB
PL13               29.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127690 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.00
```

3-((2-aminophenyl)amino)-1-phenylprop-2-en-1-one 7aa



```
Current Data Parameters
NAME          Suresh-821
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240515
Time              22.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   0
SWH           7211.539 Hz
FIDRES        0.220079 Hz
AQ            2.2719147 sec
RG                99.72
DW               69.333 usec
DE                10.06 usec
TE                299.4 K
D1           2.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324008 MHz
NUC1                1H
P1                15.00 usec
PLW1        13.50000000 W

F2 - Processing parameters
SI                16384
SF          400.1300125 MHz
WDW                EM
SSB                 0
LB                  0 Hz
GB                  0
PC               1.00
```

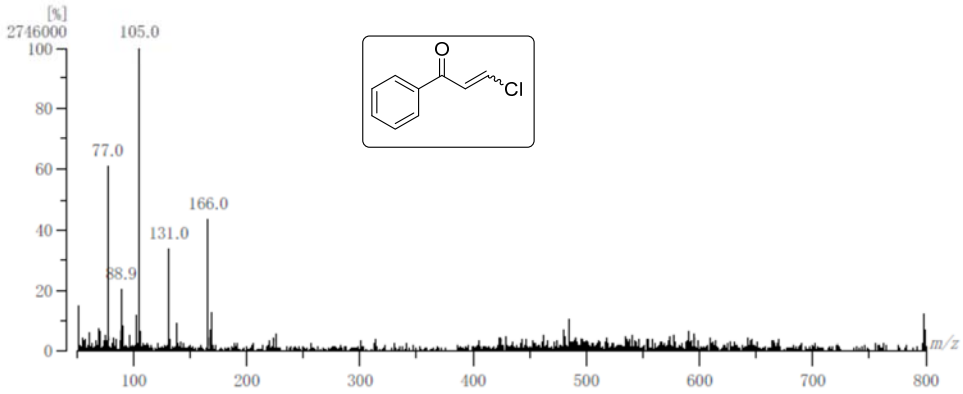


```
Current Data Parameters
NAME          Suresh-821
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20240515
Time              22.08
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32760
SOLVENT          CDCl3
NS               16297
DS                   0
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            0.6815744 sec
RG               198.09
DW               20.800 usec
DE                6.50 usec
TE                300.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        49.50000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        12.50000000 W
PLW12        0.34722000 W
PLW13        0.28125000 W

F2 - Processing parameters
SI                32768
SF          100.6127685 MHz
WDW                EM
SSB                 0
LB               2.00 Hz
GB                  0
PC               1.00
```

4. Mass Spectrometry Data

HRMS of **1a**

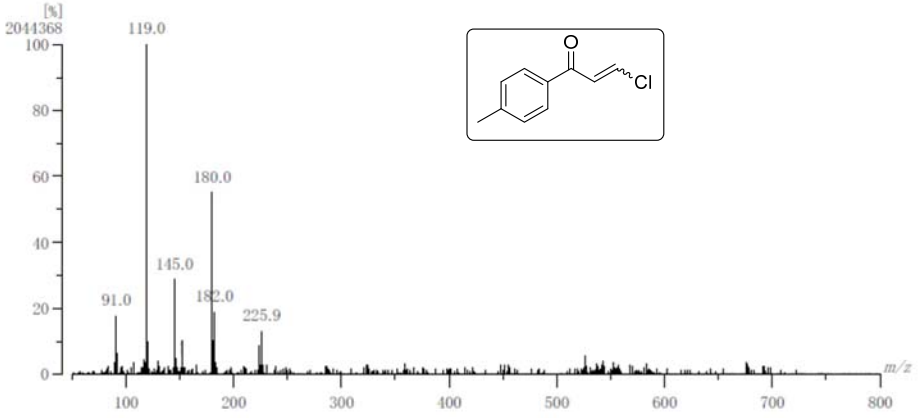
[Mass Spectrum]
Data : 20231128_HREI_2a002 Date : 28-Nov-2023 15:11
RT : 0.00 min Scan# : 1
Elements : C 10/0, H 10/0, 35Cl 1/0, 37Cl 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



	Observed m/z	Int%							
	166.0181	43.36							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	O	
1	166.0130	+30.7 / +5.1	2.0	7	10	1	1	-	
2	166.0185	-2.7 / -0.4	6.0	9	7	1	-	1	

HRMS of **1b**

[Mass Spectrum]
Data : 20231220_HREI_Expt-745001 Date : 20-Dec-2023 16:15
RT : 0.00 min Scan# : 1
Elements : C 10/0, H 10/0, 35Cl 1/0, 37Cl 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

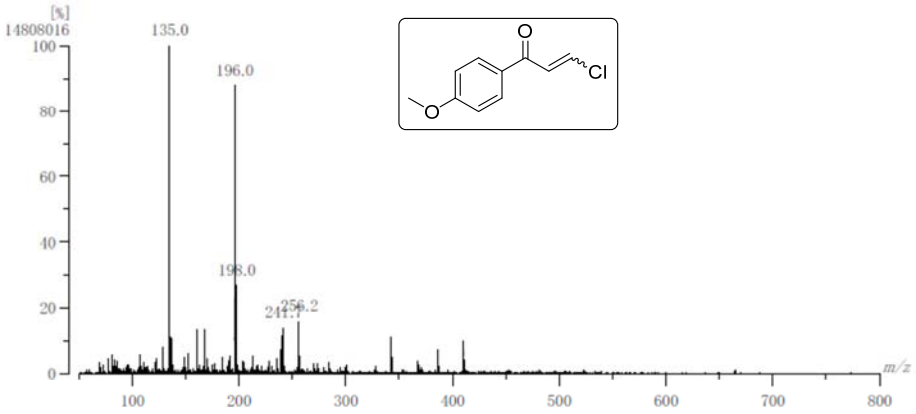


	Observed m/z	Int%							
	180.0338	55.02							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	O	
1	180.0342	-2.2 / -0.4	6.0	10	9	1	-	1	

	Observed m/z	Int%							
	182.0325	18.99							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	O	
2	182.0312	+6.9 / +1.3	6.0	10	9	-	1	1	

HRMS of **1c**

[Mass Spectrum]
Data : 20231220_HREI_Expt-735002 Date : 20-Dec-2023 11:52
RT : 0.15 min Scan# : 2
Elements : C 10/0, H 10/0, 35Cl 1/0, 37Cl 1/0, O 2/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



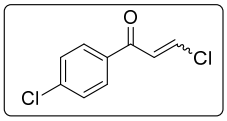
	Observed m/z	Int%							
	196.0284	87.93							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl		O
1	196.0291	-3.6 / -0.7	6.0	10	9	1	-		2
2	196.0105	+91.3 / +17.9	7.0	10	7	-	1		2

	Observed m/z	Int%							
	198.0277	27.00							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl		O
3	198.0262	+7.8 / +1.5	6.0	10	9	-	1		2

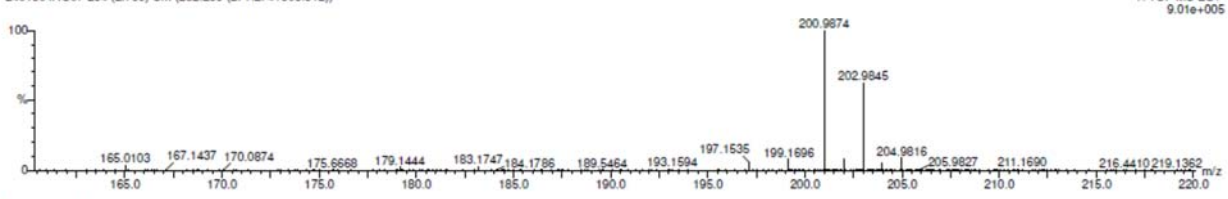
HRMS of **1d**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



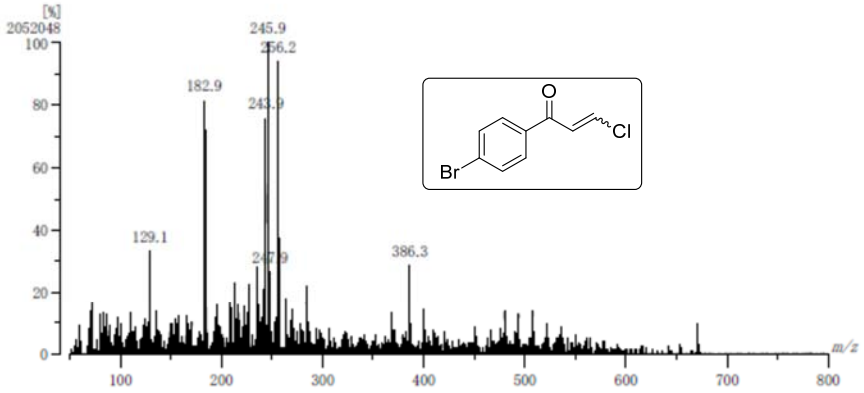
Monoisotopic Mass, Even Electron Ions
35 formula(e) evaluated with 3 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 O: 1-10 Cl: 1-3
Expt-752
240130YAO07 284 (2.769) Cm (282:286-(271:274+308:312))



Minimum:	80.00				-1.5
Maximum:	100.00		10.0	500.0	50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
200.9874	100.00	200.9874	0.0	0.0	5.5	C9 H7 O C12
		200.9802	7.2	35.8	1.5	C4 H6 O7 Cl
		200.9955	-8.1	-40.3	5.5	C8 H6 O4 Cl

HRMS of **1e**

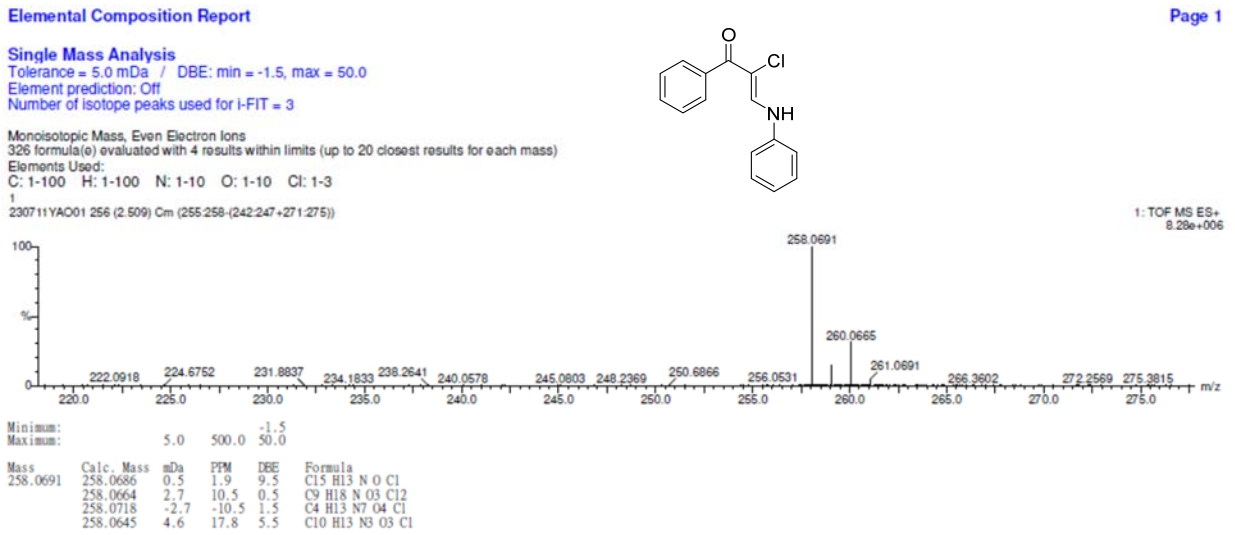


	Observed m/z	Int%									
	243.9287	75.76									
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	35Cl	37Cl	O	
1	243.9477	-78.1 / -19.0	6.0	10	8	-	1	1	-	-	
2	243.9468	-74.4 / -18.1	6.0	10	8	1	-	-	1	-	
3	243.9291	-1.8 / -0.4	7.0	10	6	-	1	-	1	-	
4	243.9235	+21.2 / +5.2	2.0	7	9	1	-	1	1	-	
5	243.9058	+93.8 / +22.9	3.0	7	7	-	1	1	1	-	
6	243.9291	-1.4 / -0.4	6.0	9	6	1	-	1	-	1	
7	243.9114	+71.1 / +17.3	7.0	9	4	-	1	1	-	1	
8	243.9105	+74.8 / +18.2	7.0	9	4	1	-	-	1	1	

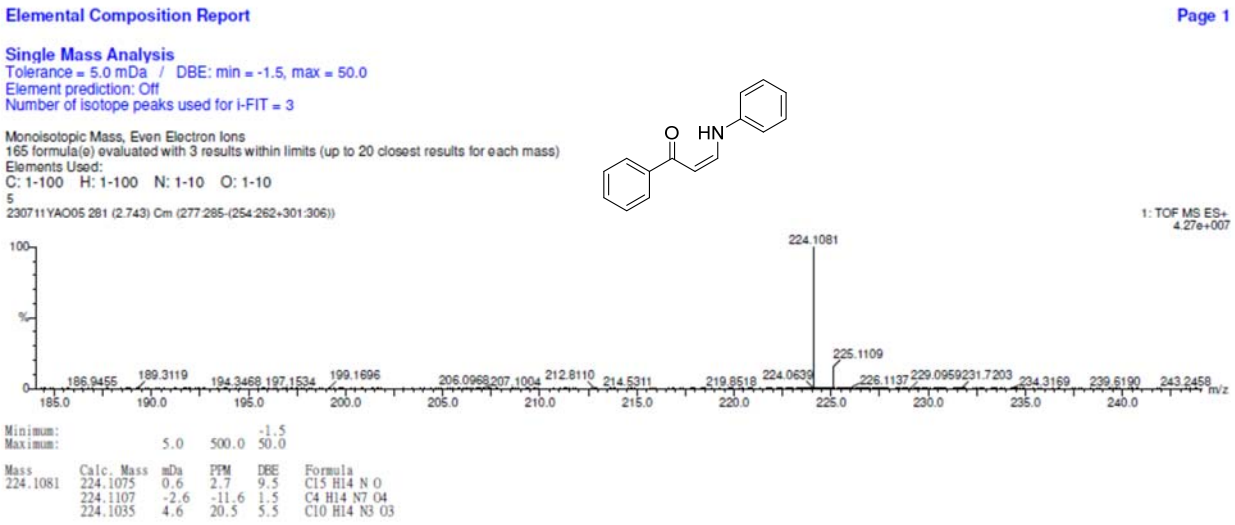
	Observed m/z	Int%									
	245.9276	100.00									
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	35Cl	37Cl	O	
9	245.9448	-69.9 / -17.2	6.0	10	8	-	1	-	1	-	
10	245.9215	+24.9 / +6.1	2.0	7	9	-	1	1	1	-	
11	245.9078	+80.5 / +19.8	0.0	5	10	1	1	-	-	1	
12	245.9447	-69.5 / -17.1	5.0	9	8	1	-	1	-	1	
13	245.9270	+2.4 / +0.6	6.0	9	6	-	1	1	-	1	
14	245.9261	+6.1 / +1.5	6.0	9	6	1	-	-	1	1	
15	245.9084	+78.0 / +19.2	7.0	9	4	-	1	-	1	1	

	Observed m/z	Int%									
	247.9265	26.44									
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	35Cl	37Cl	O	
16	247.9427	-65.2 / -16.2	5.0	9	8	-	1	1	-	1	
17	247.9418	-61.5 / -15.3	5.0	9	8	1	-	-	1	1	
18	247.9241	+9.9 / +2.4	6.0	9	6	-	1	-	1	1	
19	247.9184	+32.5 / +8.1	1.0	6	9	1	-	1	1	1	

HRMS of **3aa**

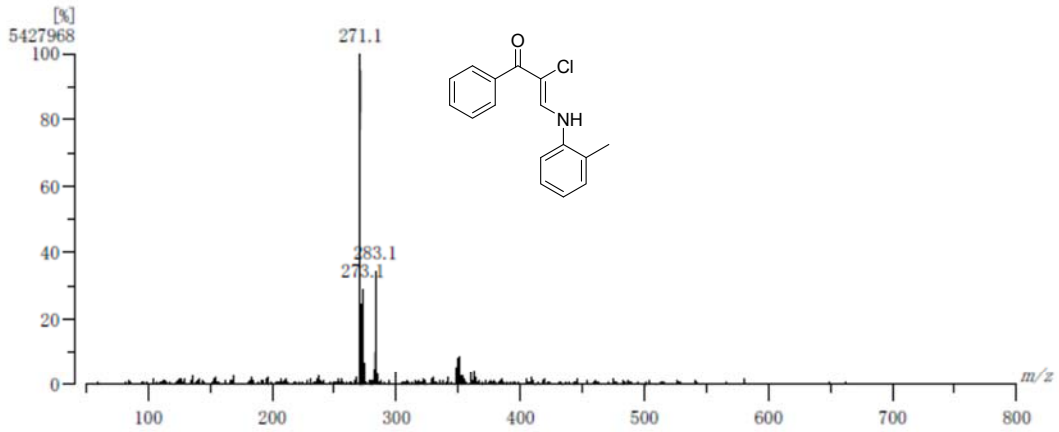


HRMS of **4aa**



HRMS of **3ab**

[Mass Spectrum]
Data : 20231128_HREI_3ab005 Date : 28-Nov-2023 14:44
RT : 0.15 min Scan# : 2
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

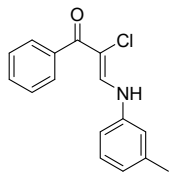


	Observed m/z	Int%								
	271.0758	100.00								
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	271.0834	-28.2 / -7.6	5.5	15	19	1	1	-	-
2	271.0942	-67.8 / -18.4	10.0	17	16	-	1	1	-
3	271.0709	+18.2 / +4.9	6.0	14	17	1	1	1	-
4	271.0890	-48.6 / -13.2	9.5	17	16	1	-	-	1
5	271.0704	+20.0 / +5.4	10.5	17	14	-	1	-	1
6	271.0997	-88.2 / -23.9	14.0	19	13	-	-	1	1
7	271.0764	-2.2 / -0.6	10.0	16	14	1	-	1	1
8	271.0578	+66.4 / +18.0	11.0	16	12	-	1	1	1

	Observed m/z	Int%							
	273.0747	29.06							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
9	273.0865	-43.2 / -11.8	5.0	14	19	1	1	1	-
10	273.0860	-41.4 / -11.3	9.5	17	16	-	1	-	1
11	273.0627	+44.0 / +12.0	5.5	14	17	1	1	-	1
12	273.0920	-63.5 / -17.3	9.0	16	16	1	-	1	1
13	273.0734	+4.6 / +1.3	10.0	16	14	-	1	1	1
14	273.0501	+90.0 / +24.6	6.0	13	15	1	1	1	1

HRMS of **3ac**

[Mass Spectrum]
Data : 20231128_HREI_3ac002 Date : 28-Nov-2023 14:24
RT : 0.30 min Scan# : 3
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

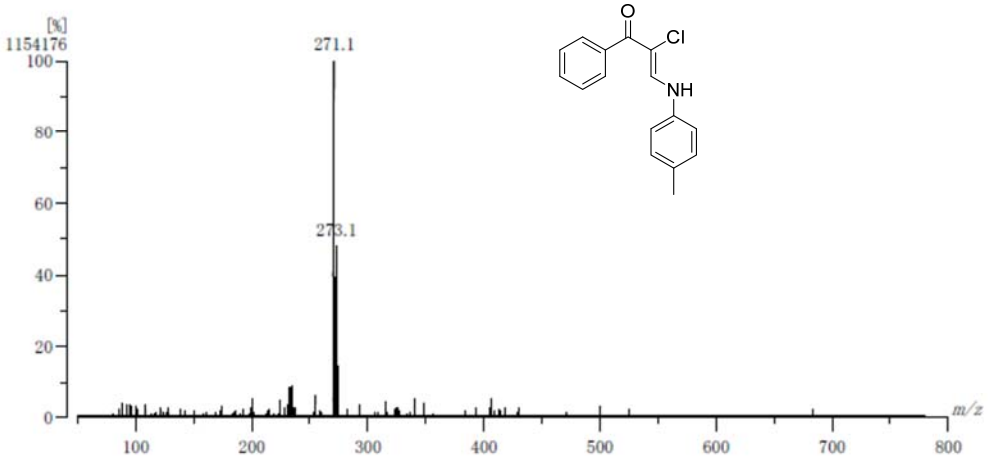


	Observed m/z	Int%								
	271.0780	100.00								
	Estimated m/z	Err[ppm / mmu]		U.S.	C	H	35Cl	37Cl	N	O
1	271.0834	-20.0 /	-5.4	5.5	15	19	1	1	-	-
2	271.0942	-59.7 /	-16.2	10.0	17	16	-	1	1	-
3	271.0709	+26.4 /	+7.1	6.0	14	17	1	1	1	-
4	271.0890	-40.5 /	-11.0	9.5	17	16	1	-	-	1
5	271.0704	+28.2 /	+7.6	10.5	17	14	-	1	-	1
6	271.0997	-80.1 /	-21.7	14.0	19	13	-	-	1	1
7	271.0764	+5.9 /	+1.6	10.0	16	14	1	-	1	1
8	271.0578	+74.5 /	+20.2	11.0	16	12	-	1	1	1

	Observed m/z	Int%								
	273.0772	46.12								
	Estimated m/z	Err[ppm / mmu]		U.S.	C	H	35Cl	37Cl	N	O
9	273.0865	-34.1 /	-9.3	5.0	14	19	1	1	1	-
10	273.0860	-32.3 /	-8.8	9.5	17	16	-	1	-	1
11	273.0627	+53.1 /	+14.5	5.5	14	17	1	1	-	1
12	273.0920	-54.4 /	-14.8	9.0	16	16	1	-	1	1
13	273.0734	+13.8 /	+3.8	10.0	16	14	-	1	1	1
14	273.0501	+99.2 /	+27.1	6.0	13	15	1	1	1	1

HRMS of **3ad**

[Mass Spectrum]
Data : 20231128_HREI_3ad001 Date : 28-Nov-2023 14:54
RT : 0.45 min Scan# : 4
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

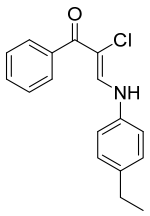


	Observed m/z	Int%								
	271.0755	100.00								
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	271.0834	-29.3 / -7.9	5.5	15	19	1	1	-	-
2	271.0942	-68.9 / -18.7	10.0	17	16	-	1	1	-
3	271.0709	+17.1 / +4.6	6.0	14	17	1	1	1	-
4	271.0890	-49.7 / -13.5	9.5	17	16	1	-	-	1
5	271.0704	+18.9 / +5.1	10.5	17	14	-	1	-	1
6	271.0997	-89.3 / -24.2	14.0	19	13	-	-	1	1
7	271.0764	-3.3 / -0.9	10.0	16	14	1	-	1	1
8	271.0578	+65.3 / +17.7	11.0	16	12	-	1	1	1

	Observed m/z	Int%							
	273.0739	47.75							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
9	273.0471	+98.1 / +26.8	14.5	19	10	1	-	-	-
10	273.0865	-46.2 / -12.6	5.0	14	19	1	1	1	-
11	273.0860	-44.4 / -12.1	9.5	17	16	-	1	-	1
12	273.0627	+41.0 / +11.2	5.5	14	17	1	1	-	1
13	273.0920	-66.4 / -18.1	9.0	16	16	1	-	1	1
14	273.0734	+1.7 / +0.5	10.0	16	14	-	1	1	1
15	273.0501	+87.1 / +23.8	6.0	13	15	1	1	1	1

HRMS of **3ae**

[Mass Spectrum]
Data : 20231128_HREI_3ae001 Date : 28-Nov-2023 15:24
RT : 0.60 min Scan# : 5
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

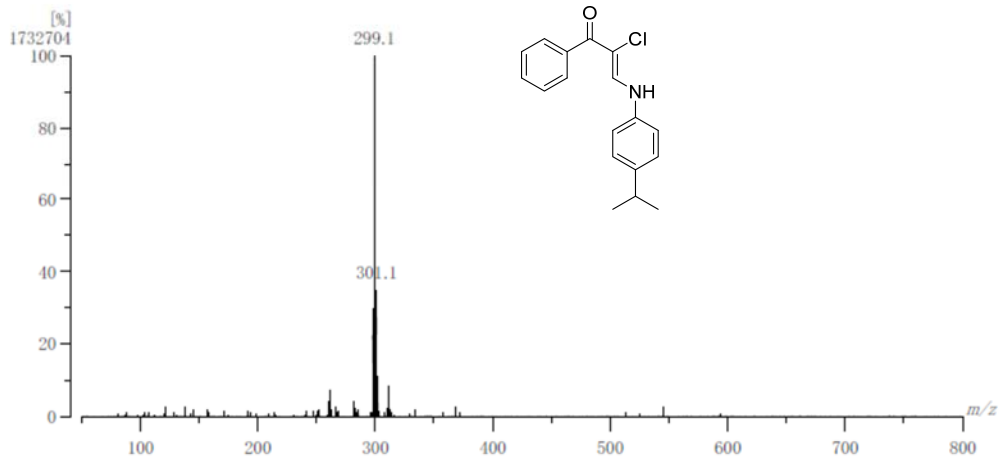


	Observed m/z	Int%							
	285.0913	100.00							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	285.1098	-65.0 / -18.5	10.0	18	18	-	1	1	-
2	285.0865	+16.8 / +4.8	6.0	15	19	1	1	1	-
3	285.1046	-46.7 / -13.3	9.5	18	18	1	-	-	1
4	285.0860	+18.5 / +5.3	10.5	18	16	-	1	-	1
5	285.1154	-84.4 / -24.1	14.0	20	15	-	-	1	1
6	285.0920	-2.6 / -0.7	10.0	17	16	1	-	1	1
7	285.0734	+62.6 / +17.9	11.0	17	14	-	1	1	1

	Observed m/z	Int%							
	287.0902	42.19							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
8	287.0628	+95.6 / +27.4	14.5	20	12	1	-	-	-
9	287.1017	-39.9 / -11.5	9.5	18	18	-	1	-	1
10	287.0783	+41.3 / +11.9	5.5	15	19	1	1	-	1
11	287.1077	-60.9 / -17.5	9.0	17	18	1	-	1	1
12	287.0891	+3.9 / +1.1	10.0	17	16	-	1	1	1
13	287.0658	+85.1 / +24.4	6.0	14	17	1	1	1	1

HRMS of **3af**

[Mass Spectrum]
Data : 20231128_HREI_3af001 Date : 28-Nov-2023 15:34
RT : 0.45 min Scan# : 4
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

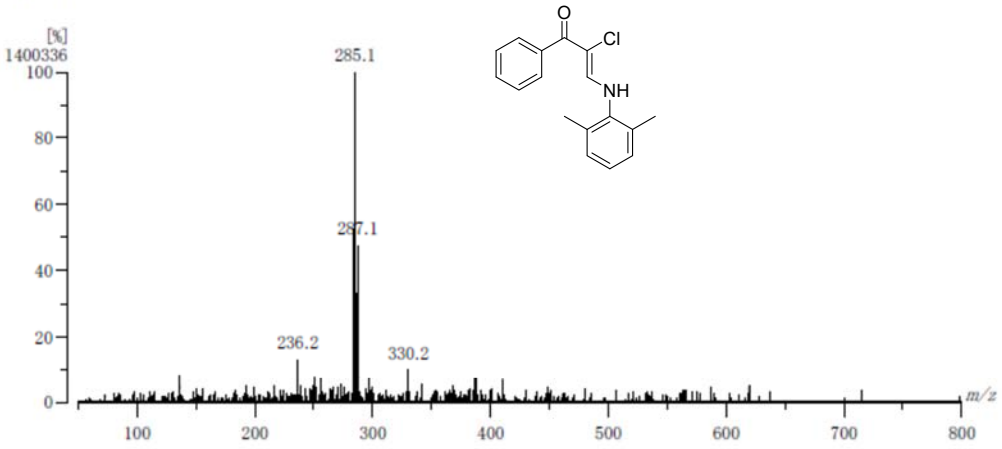


	Observed m/z	Int%							
	299.1074	100.00							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	299.1255	-60.4 / -18.1	10.0	19	20	-	1	1	-
2	299.1203	-43.0 / -12.9	9.5	19	20	1	-	-	1
3	299.1017	+19.2 / +5.7	10.5	19	18	-	1	-	1
4	299.0783	+97.1 / +29.1	6.5	16	19	1	1	-	1
5	299.1077	-1.0 / -0.3	10.0	18	18	1	-	1	1
6	299.0891	+61.2 / +18.3	11.0	18	16	-	1	1	1

	Observed m/z	Int%							
	301.1058	34.80							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
7	301.1173	-38.3 / -11.5	9.5	19	20	-	1	-	1
8	301.1233	-58.3 / -17.5	9.0	18	20	1	-	1	1
9	301.1047	+3.5 / +1.1	10.0	18	18	-	1	1	1
10	301.0814	+81.0 / +24.4	6.0	15	19	1	1	1	1

HRMS of **3ag**

[Mass Spectrum]
Data : 20231128_HREI_3ag001 Date : 28-Nov-2023 15:42
RT : 0.75 min Scan# : 6
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

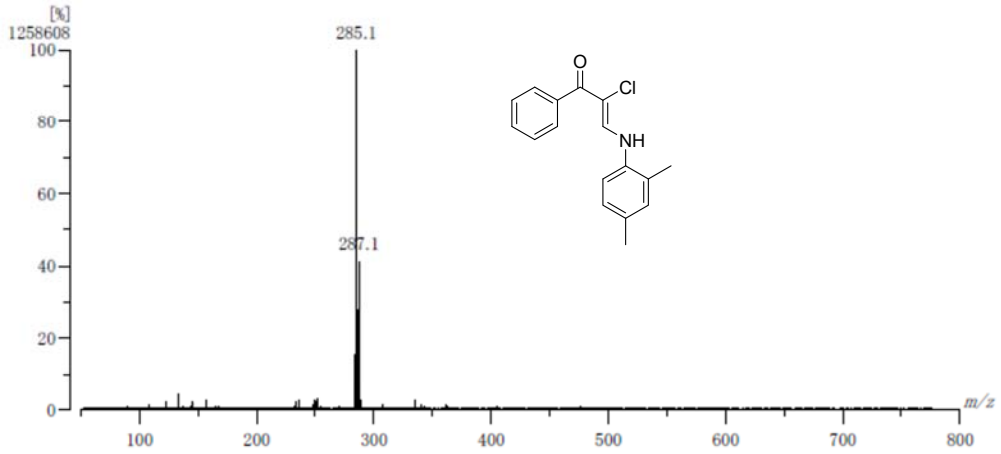


	Observed m/z	Int%								
	285.0910	100.00								
	Estimated m/z	Err[ppm / mmu]		U.S.	C	H	35Cl	37Cl	N	O
1	285.1098	-66.0 / -18.8		10.0	18	18	-	1	1	-
2	285.0865	+15.8 / +4.5		6.0	15	19	1	1	1	-
3	285.1046	-47.8 / -13.6		9.5	18	18	1	-	-	1
4	285.0860	+17.5 / +5.0		10.5	18	16	-	1	-	1
5	285.0627	+99.3 / +28.3		6.5	15	17	1	1	-	1
6	285.1154	-85.5 / -24.4		14.0	20	15	-	-	1	1
7	285.0920	-3.7 / -1.0		10.0	17	16	1	-	1	1
8	285.0734	+61.6 / +17.6		11.0	17	14	-	1	1	1

	Observed m/z	Int%								
	287.0939	47.22								
	Estimated m/z	Err[ppm / mmu]		U.S.	C	H	35Cl	37Cl	N	O
9	287.1203	-91.8 / -26.4		8.5	18	20	1	-	-	1
10	287.1017	-27.1 / -7.8		9.5	18	18	-	1	-	1
11	287.0783	+54.2 / +15.6		5.5	15	19	1	1	-	1
12	287.1077	-48.0 / -13.8		9.0	17	18	1	-	1	1
13	287.0891	+16.7 / +4.8		10.0	17	16	-	1	1	1
14	287.0658	+98.0 / +28.1		6.0	14	17	1	1	1	1

HRMS of **3ah**

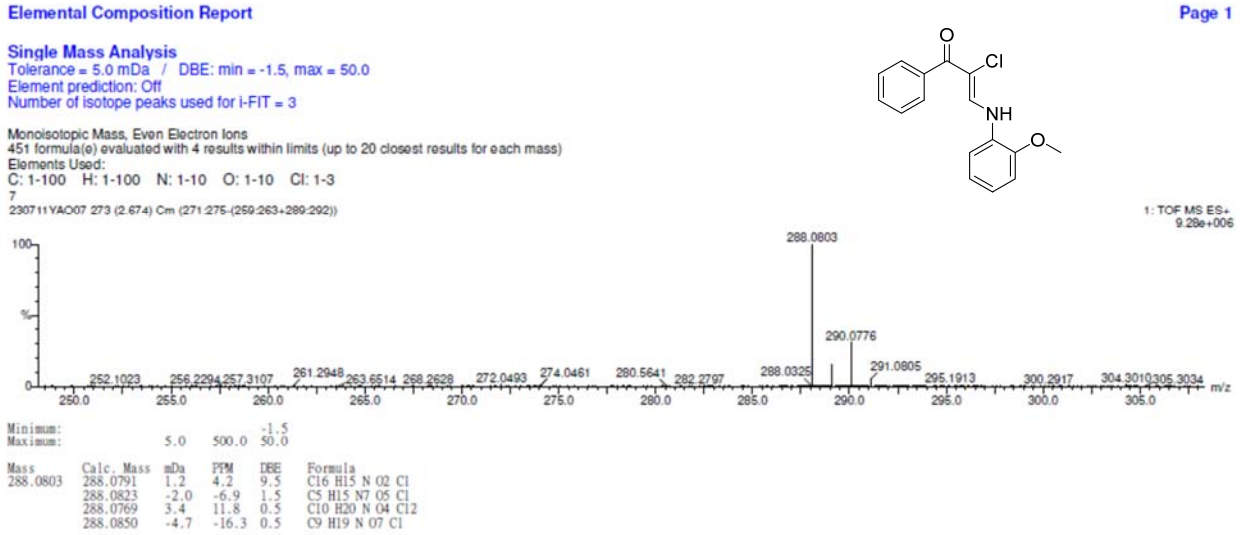
[Mass Spectrum]
Data : 20231128_HREI_3ah001 Date : 28-Nov-2023 15:50
RT : 0.30 min Scan# : 3
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



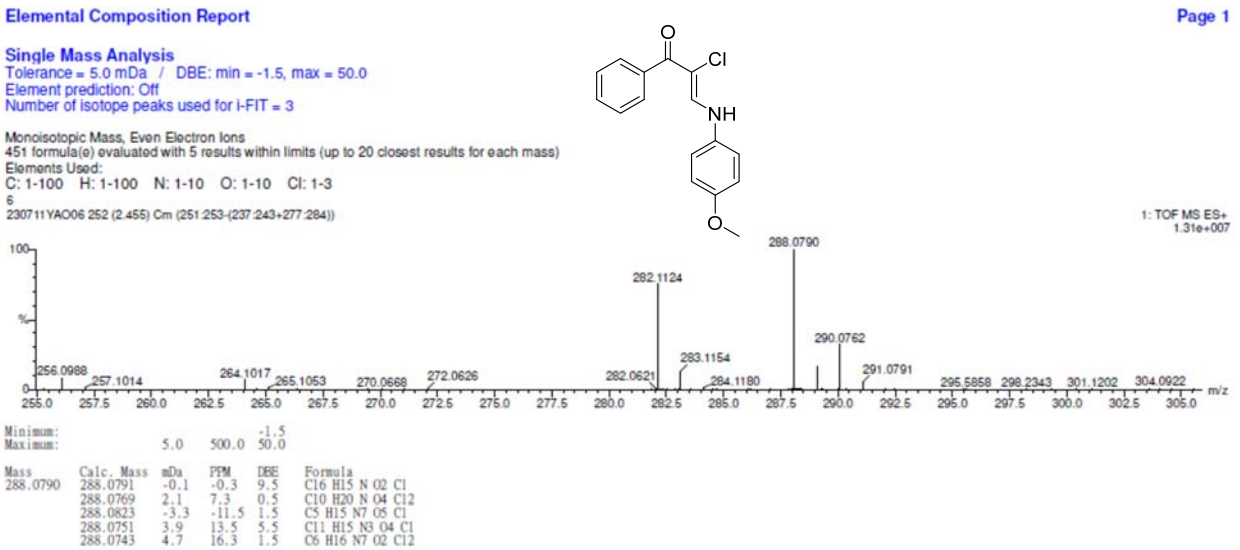
	Observed m/z	Int%								
	285.0910	100.00								
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	285.1098	-66.0 / -18.8	10.0	18	18	-	1	1	-
2	285.0865	+15.8 / +4.5	6.0	15	19	1	1	1	-
3	285.1046	-47.8 / -13.6	9.5	18	18	1	-	-	1
4	285.0860	+17.5 / +5.0	10.5	18	16	-	1	-	1
5	285.0627	+99.3 / +28.3	6.5	15	17	1	1	-	1
6	285.1154	-85.5 / -24.4	14.0	20	15	-	-	1	1
7	285.0920	-3.7 / -1.0	10.0	17	16	1	-	1	1
8	285.0734	+61.6 / +17.6	11.0	17	14	-	1	1	1

	Observed m/z	Int%							
	287.0902	41.13							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
9	287.0628	+95.6 / +27.4	14.5	20	12	1	-	-	-
10	287.1017	-39.9 / -11.5	9.5	18	18	-	1	-	1
11	287.0783	+41.3 / +11.9	5.5	15	19	1	1	-	1
12	287.1077	-60.9 / -17.5	9.0	17	18	1	-	1	1
13	287.0891	+3.9 / +1.1	10.0	17	16	-	1	1	1
14	287.0658	+85.1 / +24.4	6.0	14	17	1	1	1	1

HRMS of **3ai**



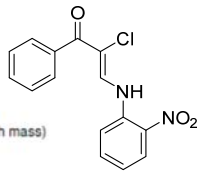
HRMS of **3aj**



HRMS of **3ak**

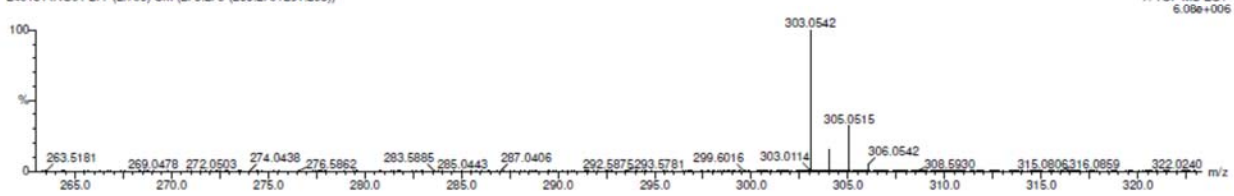
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
512 formula(e) evaluated with 14 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
3ak
240131YAO01 277 (2.709) Cm (275:279-(266:270+291:295))

1: TOF MS ES+
6.08e+006



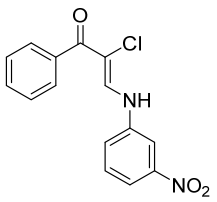
Minimum:	80.00			-1.5	
Maximum:	100.00		10.0	500.0	50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
303.0542	100.00	303.0536	0.6	2.0	10.5	C15 H12 N2 O3 Cl
		303.0515	2.7	8.9	1.5	C9 H17 N2 O5 C12
		303.0595	-5.3	-17.5	1.5	C8 H16 N2 O8 Cl
		303.0546	-0.4	-1.3	1.5	C9 H18 N4 O Cl3
		303.0627	-8.5	-28.0	1.5	C8 H17 N4 O4 C12
		303.0496	4.6	15.2	6.5	C10 H12 N4 O5 Cl
		303.0609	-6.7	-22.1	6.5	C9 H12 N6 O4 Cl
		303.0456	8.6	28.4	2.5	C5 H12 N6 O7 Cl
		303.0528	1.4	4.6	6.5	C10 H13 N6 O C12
		303.0488	5.4	17.8	2.5	C5 H13 N8 O3 C12
		303.0568	-2.6	-8.6	2.5	C4 H12 N8 O6 Cl
		303.0510	3.2	10.6	11.5	C11 H8 N8 O Cl
		303.0469	7.3	24.1	7.5	C6 H8 N10 O3 Cl
		303.0600	-5.8	-19.1	2.5	C4 H13 N10 O2 C12

HRMS of **3al**

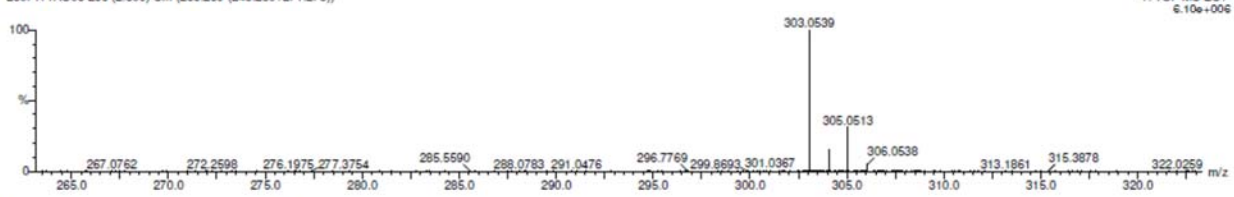
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
512 formula(e) evaluated with 7 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
3
230711YAO03 256 (2.509) Cm (255:259-(245:250+271:275))

1: TOF MS ES+
6.10e+006



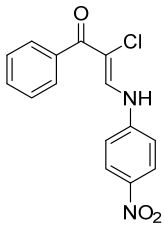
Minimum:				-1.5	
Maximum:		5.0	500.0	50.0	

Mass	Calc. Mass	mDa	PPM	DBE	Formula
303.0539	303.0536	0.3	1.0	10.5	C15 H12 N2 O3 Cl
	303.0546	-0.7	-2.3	1.5	C9 H18 N4 O Cl3
	303.0528	1.1	3.6	6.5	C10 H13 N6 O C12
	303.0515	2.4	7.9	1.5	C9 H17 N2 O5 C12
	303.0568	-2.9	-9.6	2.5	C4 H12 N8 O6 Cl
	303.0510	2.9	9.6	11.5	C11 H8 N8 O Cl
	303.0496	4.3	14.2	6.5	C10 H12 N4 O5 Cl

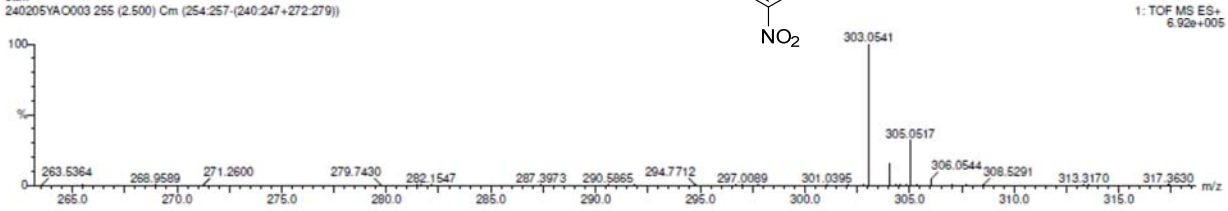
HRMS of **3am**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
512 formula(e) evaluated with 14 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
3am
240205YAO003 255 (2.500) Cm (254:257-(240:247+272:279))

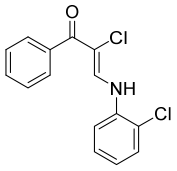


Minimum:	80.00				-1.5	
Maximum:	100.00		10.0	500.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
303.0541	100.00	303.0536	0.5	1.6	10.5	C15 H12 N2 O3 Cl
		303.0546	-0.5	-1.6	1.5	C9 H18 N4 O C13
		303.0528	1.3	4.3	6.5	C10 H13 N6 O C12
		303.0515	2.6	8.6	1.5	C9 H17 N2 O5 C12
		303.0568	-2.7	-8.9	2.5	C4 H12 N8 O6 Cl
		303.0510	3.1	10.2	11.5	C11 H8 N8 O Cl
		303.0496	4.5	14.8	6.5	C10 H12 N4 O5 Cl
		303.0488	5.3	17.5	2.5	C5 H13 N8 O3 C12
		303.0595	-5.4	-17.8	1.5	C8 H16 N2 O8 Cl
		303.0600	-5.9	-19.5	2.5	C4 H13 N10 O2 C12
		303.0609	-6.8	-22.4	6.5	C9 H12 N6 O4 Cl
		303.0469	7.2	23.8	7.5	C6 H8 N10 O3 Cl
		303.0456	8.5	28.0	2.5	C5 H12 N6 O7 Cl
		303.0627	-8.6	-28.4	1.5	C8 H17 N4 O4 C12

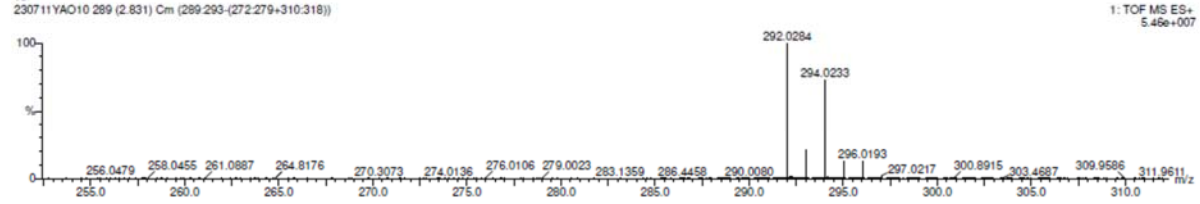
HRMS of **3an**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

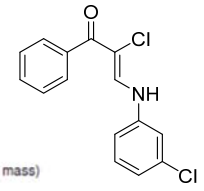


Monoisotopic Mass, Even Electron Ions
469 formula(e) evaluated with 9 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
10
230711YAO10 289 (2.831) Cm (289:293-(272:279+310:318))



Minimum:					-1.5	
Maximum:			5.0	500.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula	
292.0284	292.0296	-1.2	-4.1	9.5	C15 H12 N O C12	
	292.0278	0.6	2.1	14.5	C16 H7 N3 O Cl	
	292.0247	3.7	12.7	1.5	C5 H13 N7 O C13	
	292.0237	4.7	16.1	10.5	C11 H7 N5 O3 Cl	
	292.0256	2.8	9.6	5.5	C10 H12 N3 O3 C12	
	292.0274	1.0	3.4	0.5	C9 H17 N O3 C13	
	292.0310	-2.6	-8.9	6.5	C5 H7 N9 O4 Cl	
	292.0328	-4.4	-15.1	1.5	C4 H12 N7 O4 C12	
	292.0296	-1.2	-4.1	1.5	C4 H11 N5 O8 Cl	

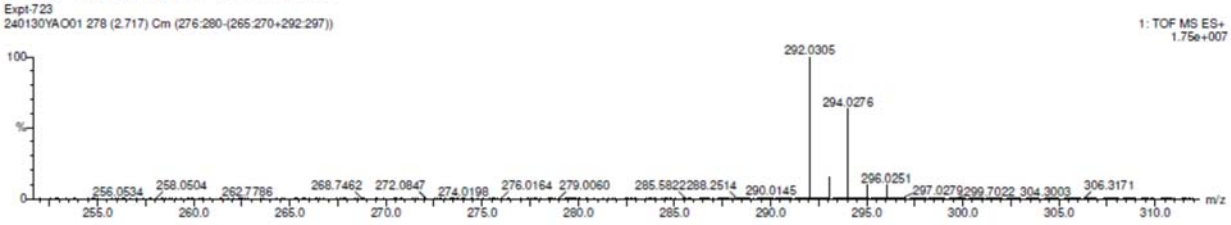
HRMS of **3ao**



Elemental Composition Report Page 1

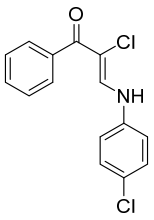
Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
469 formula(e) evaluated with 18 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
Expt-723
240130YAO01 278 (2.717) Cm (276:280-(265:270+292:297))



Minimum:	80.00				-1.5	
Maximum:	100.00		10.0	500.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
292.0305	100.00	292.0296	0.9	3.1	9.5	C15 H12 N O C12
		292.0274	3.1	10.6	0.5	C9 H17 N O3 C13
		292.0224	8.1	27.7	5.5	C10 H11 N O7 Cl
		292.0355	-5.0	-17.1	0.5	C8 H16 N O6 C12
		292.0377	-7.2	-24.7	9.5	C14 H11 N O4 Cl
		292.0256	4.9	16.8	5.5	C10 H12 N3 O3 C12
		292.0386	-8.1	-27.7	0.5	C8 H17 N3 O2 C13
		292.0278	2.7	9.2	14.5	C16 H7 N3 O Cl
		292.0336	-3.1	-10.6	5.5	C9 H11 N3 O6 Cl
		292.0296	0.9	3.1	1.5	C4 H11 N5 O8 Cl
		292.0368	-6.3	-21.6	5.5	C9 H12 N5 O2 C12
		292.0237	6.8	23.3	10.5	C11 H7 N5 O3 Cl
		292.0215	9.0	30.8	1.5	C5 H12 N5 O5 C12
		292.0247	5.8	19.9	1.5	C5 H13 N7 O C13
		292.0350	-4.5	-15.4	10.5	C10 H7 N7 O2 Cl
		292.0328	-2.3	-7.9	1.5	C4 H12 N7 O4 C12
		292.0229	7.6	26.0	6.5	C6 H8 N9 O C12
		292.0310	-0.5	-1.7	6.5	C5 H7 N9 O4 Cl

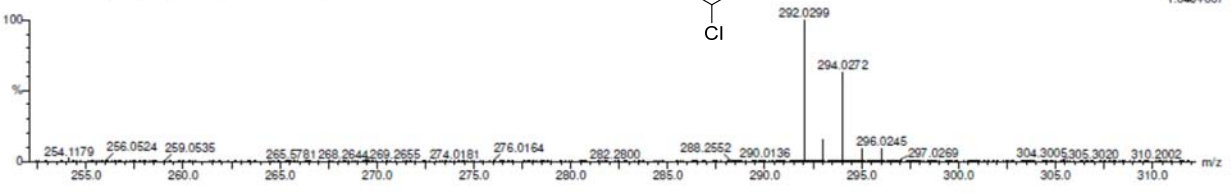
HRMS of **3ap**



Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
469 formula(e) evaluated with 8 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
4
230711YAO04 277 (2.709) Cm (275:279-(266:269+289:292))

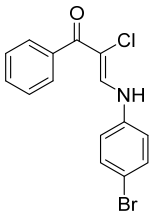


Minimum:				-1.5	
Maximum:		5.0	500.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
292.0299	292.0296	0.3	1.0	9.5	C15 H12 N O C12
	292.0296	0.3	1.0	1.5	C4 H11 N5 O8 Cl
	292.0310	-1.1	-3.8	6.5	C5 H7 N9 O4 Cl
	292.0278	2.1	7.2	14.5	C16 H7 N3 O Cl
	292.0274	2.5	8.6	0.5	C9 H17 N O3 C13
	292.0328	-2.9	-9.9	1.5	C4 H12 N7 O4 C12
	292.0336	-3.7	-12.7	5.5	C9 H11 N3 O6 Cl
	292.0256	4.3	14.7	5.5	C10 H12 N3 O3 C12

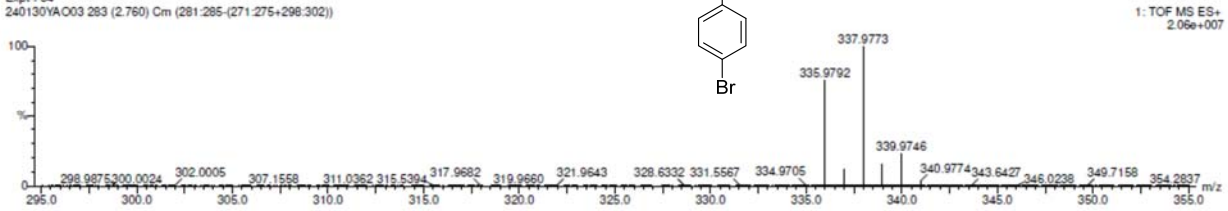
HRMS of **3aq**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
386 formula(e) evaluated with 10 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3 Br: 1-3
Expt-734
240130YAO03 283 (2.760) Cm (281:285-(271:275+298:302))

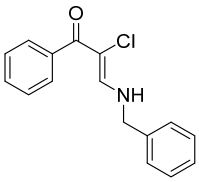


Minimum:			-1.5		
Maximum:		10.0	500.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
335.9792	335.9791	0.1	0.3	9.5	C15 H12 N O Cl Br
	335.9769	2.3	6.8	0.5	C9 H17 N O3 Cl2 Br
	335.9823	-3.1	-9.2	1.5	C4 H12 N7 O4 Cl Br
	335.9751	4.1	12.2	5.5	C10 H12 N3 O3 Cl Br
	335.9742	5.0	14.9	1.5	C5 H13 N7 O Cl2 Br
	335.9850	-5.8	-17.3	0.5	C8 H16 N O6 Cl Br
	335.9724	6.8	20.2	6.5	C6 H8 N9 O Cl Br
	335.9863	-7.1	-21.1	5.5	C9 H12 N5 O2 Cl Br
	335.9710	8.2	24.4	1.5	C5 H12 N5 O5 Cl Br
	335.9881	-8.9	-26.5	0.5	C8 H17 N3 O2 Cl2 Br

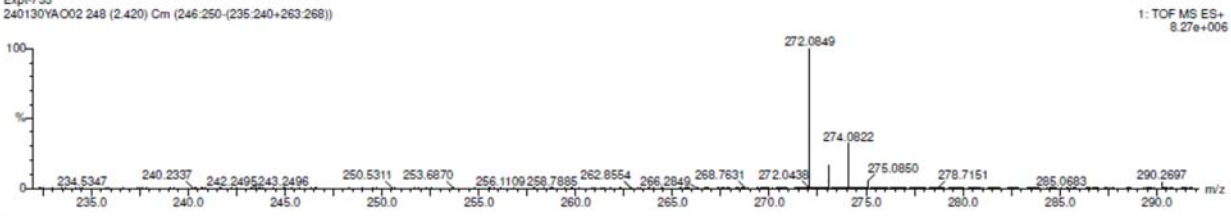
HRMS of **3ar**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



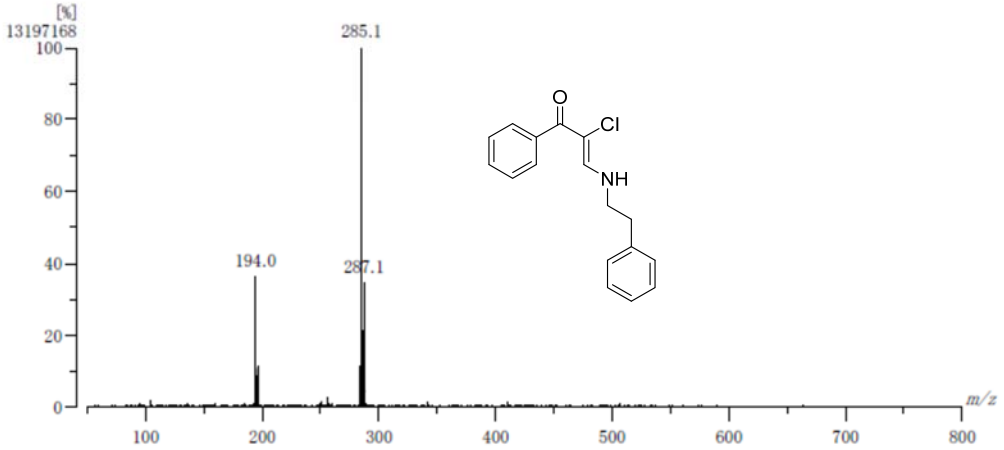
Monoisotopic Mass, Even Electron Ions
381 formula(e) evaluated with 10 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
Expt-733
240130YAO02 248 (2.420) Cm (246:250-(235:240+263:268))



Minimum:	80.00				-1.5	
Maximum:	100.00		10.0	500.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
272.0849	100.00	272.0842	0.7	2.6	9.5	C16 H15 N O Cl
		272.0874	-2.5	-9.2	1.5	C5 H15 N7 O4 Cl
		272.0820	2.9	10.7	0.5	C10 H20 N O3 Cl2
		272.0802	4.7	17.3	5.5	C11 H15 N3 O3 Cl
		272.0901	-5.2	-19.1	0.5	C9 H19 N O6 Cl
		272.0793	5.6	20.6	1.5	C6 H16 N7 O Cl2
		272.0914	-6.5	-23.9	5.5	C10 H15 N5 O2 Cl
		272.0775	7.4	27.2	6.5	C7 H11 N9 O Cl
		272.0933	-8.4	-30.9	0.5	C9 H20 N3 O2 Cl2
		272.0762	8.7	32.0	1.5	C6 H15 N5 O5 Cl

HRMS of **3as**

[Mass Spectrum]
Data : 20231128_HREI_3as001 Date : 28-Nov-2023 15:57
RT : 0.15 min Scan# : 2
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

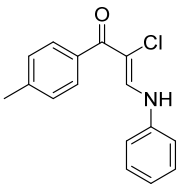


	Observed m/z	Int%								
	285.0912	100.00								
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	285.1098	-65.3 / -18.6	10.0	18	18	-	1	1	-
2	285.0865	+16.5 / +4.7	6.0	15	19	1	1	1	-
3	285.1046	-47.1 / -13.4	9.5	18	18	1	-	-	1
4	285.0860	+18.2 / +5.2	10.5	18	16	-	1	-	1
5	285.0627	+100.0 / +28.5	6.5	15	17	1	1	-	1
6	285.1154	-84.8 / -24.2	14.0	20	15	-	-	1	1
7	285.0920	-3.0 / -0.8	10.0	17	16	1	-	1	1
8	285.0734	+62.3 / +17.8	11.0	17	14	-	1	1	1

	Observed m/z	Int%							
	287.0902	34.43							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
9	287.0628	+95.6 / +27.4	14.5	20	12	1	-	-	-
10	287.1017	-39.9 / -11.5	9.5	18	18	-	1	-	1
11	287.0783	+41.3 / +11.9	5.5	15	19	1	1	-	1
12	287.1077	-60.9 / -17.5	9.0	17	18	1	-	1	1
13	287.0891	+3.9 / +1.1	10.0	17	16	-	1	1	1
14	287.0658	+85.1 / +24.4	6.0	14	17	1	1	1	1

HRMS of **3ba**

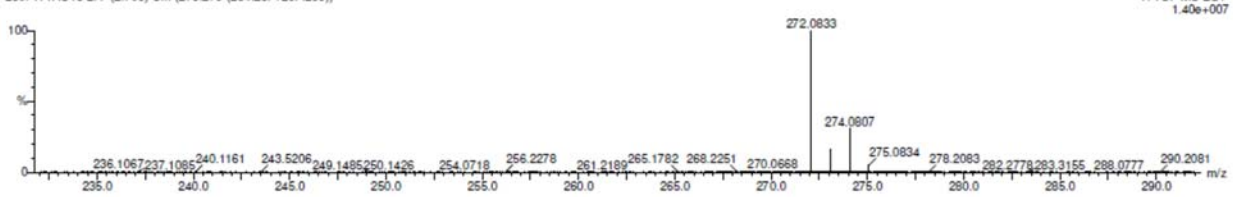
Elemental Composition Report Page 1



Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
381 formula(e) evaluated with 5 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
13
230711YAO13 277 (2.709) Cm (275:279-(254:257+297:299))

1: TOF MS ES+
1.40e+007

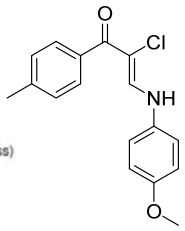


Minimum:			-1.5		
Maximum:		5.0	500.0	50.0	

Mass	Calc. Mass	mDa	PPM	DBE	Formula
272.0833	272.0842	-0.9	-3.3	9.5	C16 H15 N O Cl
	272.0820	1.3	4.8	0.5	C10 H20 N O3 Cl2
	272.0802	3.1	11.4	5.5	C11 H15 N3 O3 Cl
	272.0793	4.0	14.7	1.5	C6 H16 N7 O Cl2
	272.0874	-4.1	-15.1	1.5	C5 H15 N7 O4 Cl

HRMS of **3bj**

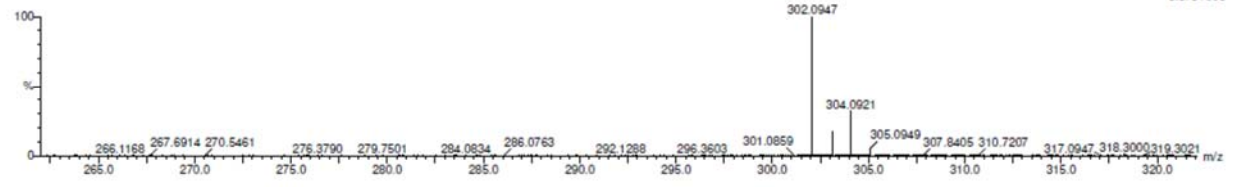
Elemental Composition Report Page 1



Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
509 formula(e) evaluated with 11 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
Expt-748
240130YAO05 268 (2.612) Cm (266:270-(254:259+283:288))

1: TOF MS ES+
5.67e+006

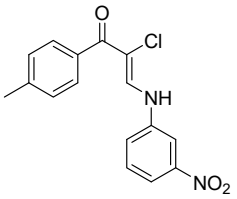


Minimum:	80.00				-1.5	
Maximum:	100.00		10.0	500.0	50.0	

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
302.0947	100.00	302.0948	-0.1	-0.3	9.5	C17 H17 N O2 Cl
		302.0926	2.1	7.0	0.5	C11 H22 N O4 Cl2
		302.0980	-3.3	-10.9	1.5	C6 H17 N7 O5 Cl
		302.0908	3.9	12.9	5.5	C12 H17 N3 O4 Cl
		302.0899	4.8	15.9	1.5	C7 H18 N7 O2 Cl2
		302.1007	-6.0	-19.9	0.5	C10 H21 N O7 Cl
		302.1011	-6.4	-21.2	1.5	C6 H18 N9 O Cl2
		302.0881	6.6	21.8	6.5	C8 H13 N9 O2 Cl
		302.1020	-7.3	-24.2	5.5	C11 H17 N5 O3 Cl
		302.0867	8.0	26.5	1.5	C7 H17 N5 O6 Cl
		302.1038	-9.1	-30.1	0.5	C10 H22 N3 O3 Cl2

HRMS of **3bl**

Elemental Composition Report Page 1

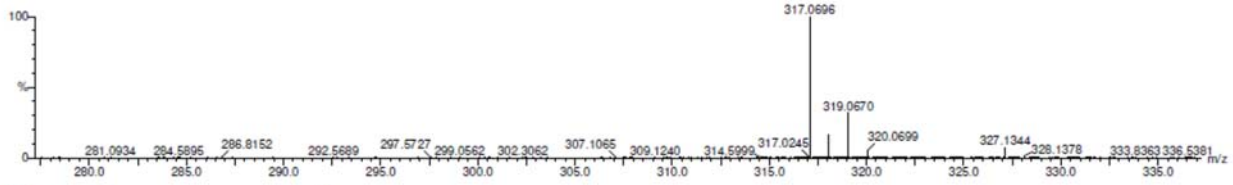


Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
571 formula(e) evaluated with 15 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3

Expt-749
240131YAO03 271 (2.657) Cm (271:273-(260:265+286:290))

1: TOF MS ES+
6.35e+006

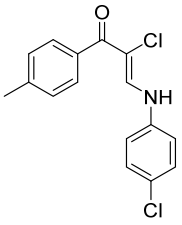


Minimum:	80.00				-1.5
Maximum:	100.00		10.0	500.0	50.0

Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
317.0696	100.00	317.0693	0.3	0.9	10.5	C16 H14 N2 O3 Cl
		317.0703	-0.7	-2.2	1.5	C10 H20 N4 O C13
		317.0684	1.2	3.8	6.5	C11 H15 N6 O C12
		317.0671	2.5	7.9	1.5	C10 H19 N2 O5 C12
		317.0725	-2.9	-9.1	2.5	C5 H14 N8 O6 Cl
		317.0666	3.0	9.5	11.5	C12 H10 N8 O Cl
		317.0653	4.3	13.6	6.5	C11 H14 N4 O5 Cl
		317.0644	5.2	16.4	2.5	C6 H15 N8 O3 C12
		317.0752	-5.6	-17.7	1.5	C9 H18 N2 O8 Cl
		317.0757	-6.1	-19.2	2.5	C5 H15 N10 O2 C12
		317.0765	-6.9	-21.8	6.5	C10 H14 N6 O4 Cl
		317.0626	7.0	22.1	7.5	C7 H10 N10 O3 Cl
		317.0612	8.4	26.5	2.5	C6 H14 N6 O7 Cl
		317.0783	-8.7	-27.4	1.5	C9 H19 N4 O4 C12
		317.0604	9.2	29.0	-1.5	C H15 N10 O5 C12

HRMS of **3bp**

Elemental Composition Report Page 1

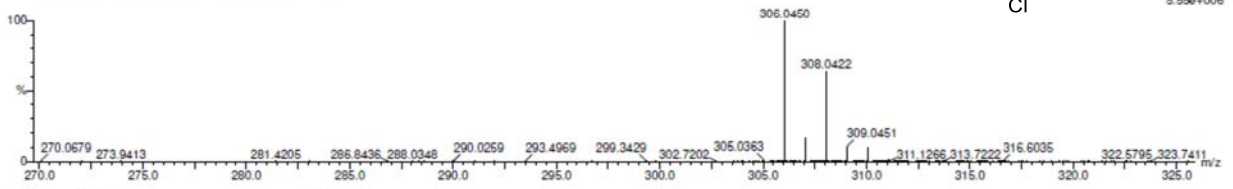


Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
533 formula(e) evaluated with 19 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3

3bp
240205YAO002 289 (2.831) Cm (289:291-(273:281+307:313))

1: TOF MS ES+
5.55e+006



Minimum:	80.00				-1.5
Maximum:	100.00		10.0	500.0	50.0

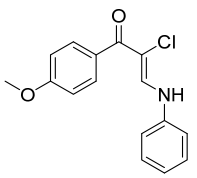
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
306.0450	100.00	306.0452	-0.2	-0.7	9.5	C16 H14 N O C12
		306.0453	-0.3	-1.0	1.5	C5 H13 N5 O8 Cl
		306.0434	1.6	5.2	14.5	C17 H9 N3 O Cl
		306.0466	-1.6	-5.2	6.5	C6 H9 N9 O4 Cl
		306.0431	1.9	6.2	0.5	C10 H19 N O3 C13
		306.0484	-3.4	-11.1	1.5	C5 H14 N7 O4 C12
		306.0412	3.8	12.4	5.5	C11 H14 N3 O3 C12
		306.0493	-4.3	-14.1	5.5	C10 H13 N3 O6 Cl
		306.0404	4.6	15.0	1.5	C6 H15 N7 O C13
		306.0506	-5.6	-18.3	10.5	C11 H9 N7 O2 Cl
		306.0394	5.6	18.3	10.5	C12 H9 N5 O3 Cl
		306.0511	-6.1	-19.9	0.5	C9 H18 N O6 C12
		306.0385	6.5	21.2	6.5	C7 H10 N9 O C12
		306.0381	6.9	22.5	5.5	C11 H13 N O7 Cl
		306.0525	-7.5	-24.5	5.5	C10 H14 N5 O2 C12
		306.0372	7.8	25.5	1.5	C6 H14 N5 O5 C12
		306.0533	-8.3	-27.1	9.5	C15 H13 N O4 Cl
		306.0543	-9.3	-30.4	0.5	C9 H19 N3 O2 C13
		306.0354	9.6	31.4	6.5	C7 H9 N7 O5 Cl

HRMS of **3ca**

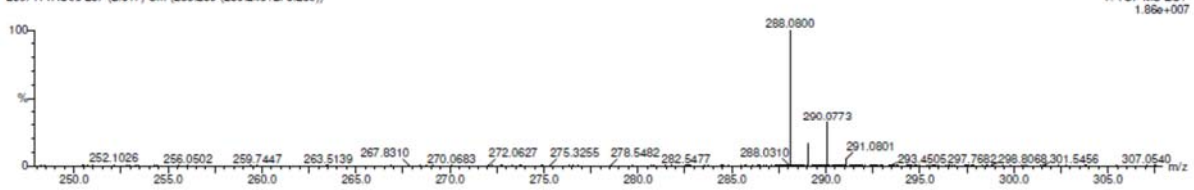
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
451 formula(e) evaluated with 4 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
9
230711YAO09 257 (2.517) Cm (255:259-(239:246+275:280))



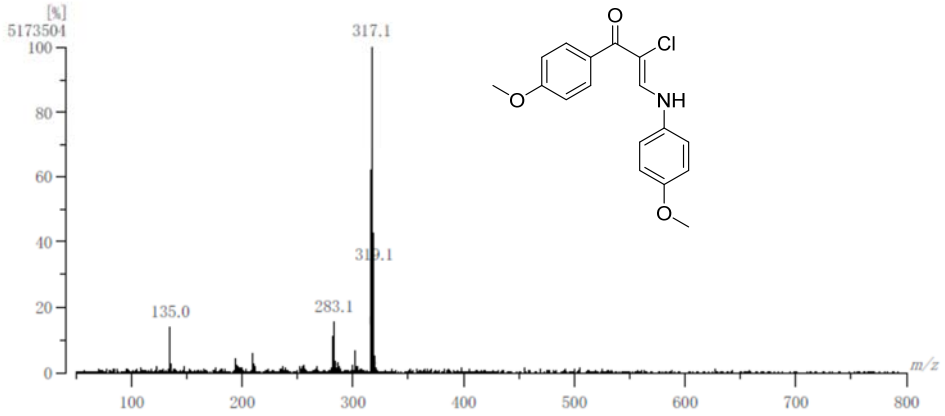
1: TOF MS ES+
1.86e+007



Minimum:				-1.5	
Maximum:		5.0	500.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
288.0800	288.0791	0.9	3.1	9.5	C16 H15 N O2 Cl
	288.0823	-2.3	-8.0	1.5	C5 H15 N7 O5 Cl
	288.0769	3.1	10.8	0.5	C10 H20 N O4 Cl2
	288.0751	4.9	17.0	5.5	C11 H15 N3 O4 Cl

HRMS of **3cj**

[Mass Spectrum]
Data : 20231220_HREI_Expt-736001 Date : 20-Dec-2023 11:59
RT : 0.45 min Scan# : 4
Elements : C 20/0, H 20/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 3/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



Observed m/z 317.0812 Int% 100.00

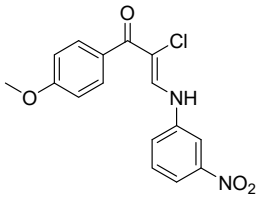
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	317.0678	+42.3 / +13.4	10.5	19	17	1	1	-	-
2	317.0552	+82.0 / +26.0	11.0	18	15	1	1	1	-
3	317.0607	+64.5 / +20.5	15.0	20	12	1	-	1	1
4	317.1122	-97.9 / -31.0	9.5	19	20	-	1	-	2
5	317.0997	-58.2 / -18.5	10.0	18	18	-	1	1	2
6	317.0763	+15.3 / +4.9	6.0	15	19	1	1	1	2
7	317.0944	-41.8 / -13.2	9.5	18	18	1	-	-	3
8	317.0758	+16.9 / +5.4	10.5	18	16	-	1	-	3
9	317.0525	+90.4 / +28.7	6.5	15	17	1	1	-	3
10	317.1052	-75.7 / -24.0	14.0	20	15	-	-	1	3
11	317.0819	-2.1 / -0.7	10.0	17	16	1	-	1	3
12	317.0633	+56.5 / +17.9	11.0	17	14	-	1	1	3

HRMS of **3cl**

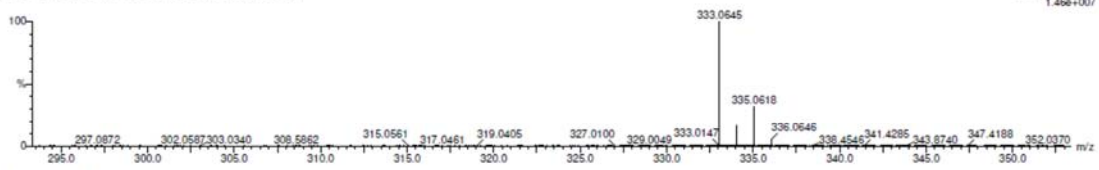
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
643 formula(e) evaluated with 17 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
Expt-737
240131YA002 259 (2.534) Cm (258:261-(247:252+276:281))



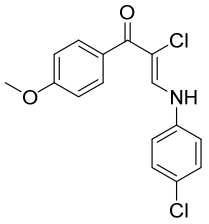
1: TOF MS ES+
1.46e+007



Minimum:	80.00				-1.5	
Maximum:	100.00		10.0	500.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
333.0645	100.00	333.0642	0.3	0.9	10.5	C16 H14 N2 O4 Cl
		333.0652	-0.7	-2.1	1.5	C10 H20 N4 O2 C13
		333.0634	1.1	3.3	6.5	C11 H15 N6 O2 C12
		333.0620	2.5	7.5	1.5	C10 H19 N2 O6 C12
		333.0674	-2.9	-8.7	2.5	C5 H14 N8 O7 Cl
		333.0615	3.0	9.0	11.5	C12 H10 N8 O2 Cl
		333.0602	4.3	12.9	6.5	C11 H14 N4 O6 Cl
		333.0593	5.2	15.6	2.5	C6 H15 N8 O4 C12
		333.0701	-5.6	-16.8	1.5	C9 H18 N2 O9 Cl
		333.0706	-6.1	-18.3	2.5	C5 H15 N10 O3 C12
		333.0714	-6.9	-20.7	6.5	C10 H14 N6 O5 Cl
		333.0575	7.0	21.0	7.5	C7 H10 N10 O4 Cl
		333.0562	8.3	24.9	2.5	C6 H14 N6 O8 Cl
		333.0728	-8.3	-24.9	11.5	C11 H10 N10 O Cl
		333.0561	8.4	25.2	10.5	C17 H15 N2 O C12
		333.0733	-8.8	-26.4	1.5	C9 H19 N4 O5 C12
		333.0553	9.2	27.6	-1.5	C H15 N10 O6 C12

HRMS of **3cp**

[Mass Spectrum]
Data : 20231220_HREI_Expt-739002 Date : 20-Dec-2023 15:01
RT : 0.60 min Scan# : 5
Elements : C 16/0, H 15/0, 35Cl 2/0, 37Cl 2/0, N 1/0, O 2/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



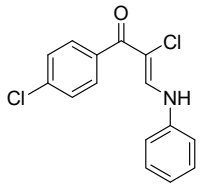
	Observed m/z	Int%							
	321.0318	100.00							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	321.0082	+73.5 / +23.6	7.0	14	14	1	2	1	1
2	321.0030	+89.7 / +28.8	6.5	14	14	2	1	-	2
3	321.0323	-1.7 / -0.5	10.0	16	13	2	-	1	2
4	321.0137	+56.3 / +18.1	11.0	16	11	1	1	1	2

	Observed m/z	Int%							
	322.0260	82.43							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
5	322.0160	+31.0 / +10.0	6.5	14	15	1	2	1	1
6	322.0108	+47.2 / +15.2	6.0	14	15	2	1	-	2
7	322.0402	-44.0 / -14.2	9.5	16	14	2	-	1	2
8	322.0216	+13.8 / +4.4	10.5	16	12	1	1	1	2
9	321.9982	+86.2 / +27.8	6.5	13	13	2	1	1	2
10	322.0030	+71.6 / +23.0	11.5	16	10	-	2	1	2

HRMS of **3da**

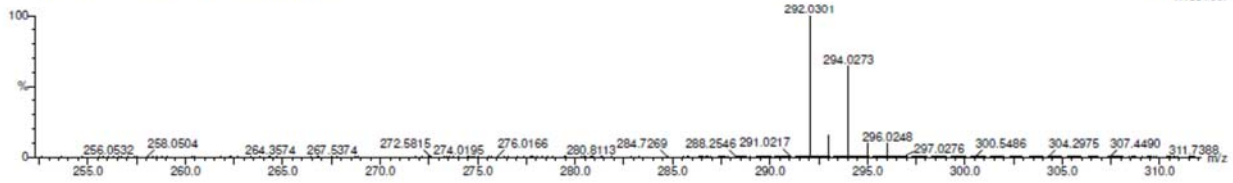
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
469 formula(e) evaluated with 18 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
Expt-753
240130YAO08 279 (2.726) Cm (278:281-(265:270+297:303))

1: TOF MS ES+
1.15e+007

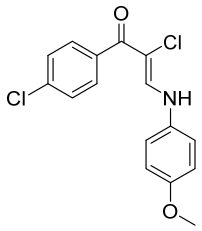


Minimum:	80.00				-1.5	
Maximum:	100.00		10.0	500.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
292.0301	100.00	292.0296	0.5	1.7	9.5	C15 H12 N O Cl2
		292.0296	0.5	1.7	1.5	C4 H11 N5 O8 Cl
		292.0310	-0.9	-3.1	6.5	C5 H7 N9 O4 Cl
		292.0278	2.3	7.9	14.5	C16 H7 N3 O Cl
		292.0328	-2.7	-9.2	1.5	C4 H12 N7 O4 Cl2
		292.0274	2.7	9.2	0.5	C9 H17 N O3 Cl3
		292.0336	-3.5	-12.0	5.5	C9 H11 N3 O6 Cl
		292.0256	4.5	15.4	5.5	C10 H12 N3 O3 Cl2
		292.0350	-4.9	-16.8	10.5	C10 H7 N7 O2 Cl
		292.0355	-5.4	-18.5	0.5	C8 H16 N O6 Cl2
		292.0247	5.4	18.5	1.5	C5 H13 N7 O Cl3
		292.0237	6.4	21.9	10.5	C11 H7 N5 O3 Cl
		292.0368	-6.7	-22.9	5.5	C9 H12 N5 O2 Cl2
		292.0229	7.2	24.7	6.5	C6 H8 N9 O Cl2
		292.0377	-7.6	-26.0	9.5	C14 H11 N O4 Cl
		292.0224	7.7	26.4	5.5	C10 H11 N O7 Cl
		292.0386	-8.5	-29.1	0.5	C8 H17 N3 O2 Cl3
		292.0215	8.6	29.4	1.5	C5 H12 N5 O5 Cl2

HRMS of **3dj**

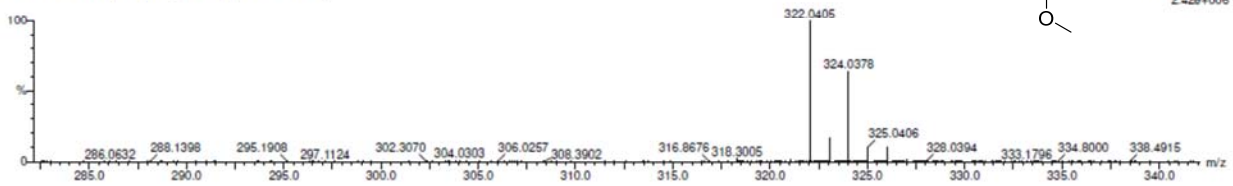
Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
604 formula(e) evaluated with 20 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
Expt-754
240130YAO09 273 (2.674) Cm (271:275-(259:265+291:296))

1: TOF MS ES+
2.42e+006

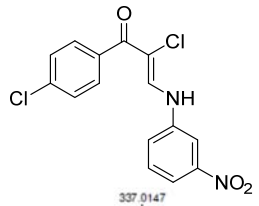


Minimum:	80.00				-1.5	
Maximum:	100.00		10.0	500.0	50.0	
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
322.0405	100.00	322.0402	0.3	0.9	9.5	C16 H14 N O2 Cl2
		322.0402	0.3	0.9	1.5	C5 H13 N5 O9 Cl
		322.0415	-1.0	-3.1	6.5	C6 H9 N9 O5 Cl
		322.0383	2.2	6.8	14.5	C17 H9 N3 O2 Cl
		322.0380	2.5	7.8	0.5	C10 H19 N O4 Cl3
		322.0433	-2.8	-8.7	1.5	C5 H14 N7 O5 Cl2
		322.0442	-3.7	-11.5	5.5	C10 H13 N3 O7 Cl
		322.0361	4.4	13.7	5.5	C11 H14 N3 O4 Cl2
		322.0455	-5.0	-15.5	10.5	C11 H9 N7 O3 Cl
		322.0353	5.2	16.1	1.5	C6 H15 N7 O2 Cl3
		322.0460	-5.5	-17.1	0.5	C9 H18 N O7 Cl2
		322.0465	-6.0	-18.6	1.5	C5 H15 N9 O Cl3
		322.0343	6.2	19.3	10.5	C12 H9 N5 O4 Cl
		322.0474	-6.9	-21.4	5.5	C10 H14 N5 O3 Cl2
		322.0335	7.0	21.7	6.5	C7 H10 N9 O2 Cl2
		322.0330	7.5	23.3	5.5	C11 H13 N O8 Cl
		322.0482	-7.7	-23.9	9.5	C15 H13 N O5 Cl
		322.0321	8.4	26.1	1.5	C6 H14 N5 O6 Cl2
		322.0492	-8.7	-27.0	0.5	C9 H19 N3 O3 Cl3
		322.0496	-9.1	-28.3	14.5	C16 H9 N5 O Cl

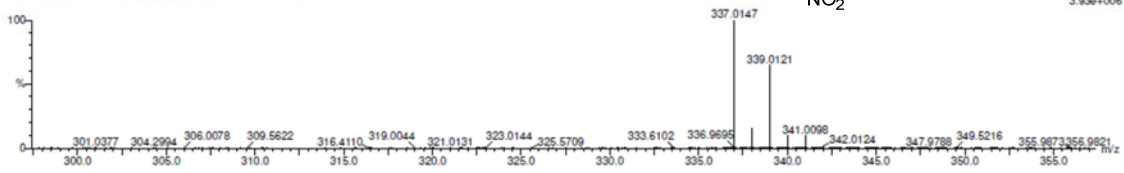
HRMS of **3dl**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



Monoisotopic Mass, Even Electron Ions
661 formula(e) evaluated with 25 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
Expt-755
240131YAO04 277 (2.709) Cm (276:280-(265:270+293:299))

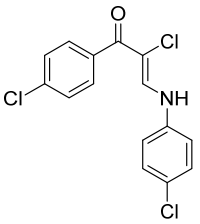


Minimum:		80.00			-1.5	
Maximum:		100.00		10.0	500.0	50.0
Mass	RA	Calc. Mass	mDa	PPM	DBE	Formula
337.0147	100.00	337.0147	0.0	0.0	10.5	C15 H11 N2 O3 C12
		337.0075	7.2	21.4	6.5	C10 H10 N2 O9 C1
		337.0125	2.2	6.5	1.5	C9 H16 N2 O5 C13
		337.0169	-2.2	-6.5	19.5	C21 H6 N2 O Cl
		337.0205	-5.8	-17.2	1.5	C8 H15 N2 O8 C12
		337.0227	-8.0	-23.7	10.5	C14 H10 N2 O6 C1
		337.0128	1.9	5.6	15.5	C16 H6 N4 O3 C1
		337.0187	-4.0	-11.9	6.5	C9 H10 N4 O8 C1
		337.0106	4.1	12.2	6.5	C10 H11 N4 O5 C12
		337.0237	-9.0	-26.7	1.5	C8 H16 N4 O4 C13
		337.0219	-7.2	-21.4	6.5	C9 H11 N6 O4 C12
		337.0147	0.0	0.0	2.5	C4 H10 N6 O10 C1
		337.0138	0.9	2.7	6.5	C10 H12 N6 O C13
		337.0066	8.1	24.0	2.5	C5 H11 N6 O7 C12
		337.0241	-9.4	-27.9	15.5	C15 H6 N6 O2 C1
		337.0088	5.9	17.5	11.5	C11 H6 N6 O5 C1
		337.0179	-3.2	-9.5	2.5	C4 H11 N8 O6 C12
		337.0098	4.9	14.5	2.5	C5 H12 N8 O3 C13
		337.0201	-5.4	-16.0	11.5	C10 H6 N8 O4 C1
		337.0048	9.9	29.4	7.5	C6 H6 N8 O7 C1
		337.0120	2.7	8.0	11.5	C11 H7 N8 O C12
		337.0210	-6.3	-18.7	2.5	C4 H12 N10 O2 C13
		337.0102	4.5	13.4	16.5	C12 H2 N10 O C1
		337.0160	-1.3	-3.9	7.5	C5 H6 N10 O6 C1
		337.0080	6.7	19.9	7.5	C6 H7 N10 O3 C12

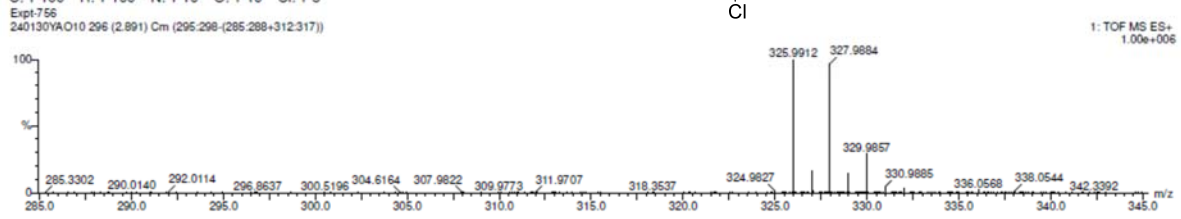
HRMS of **3dp**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3



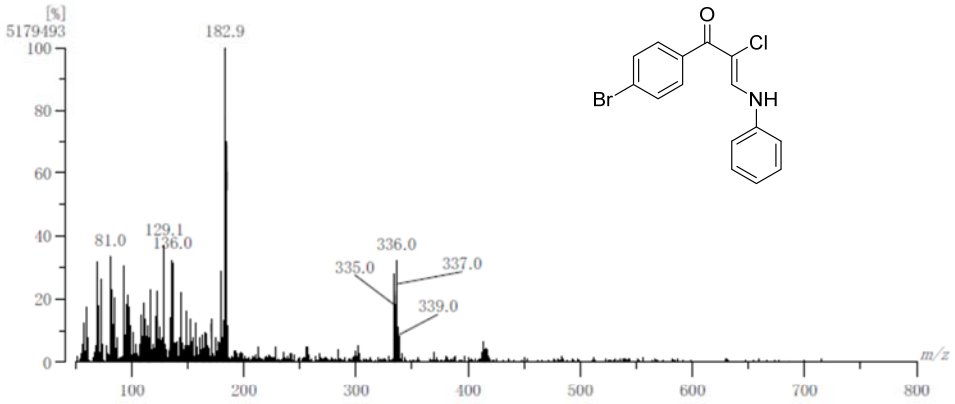
Monoisotopic Mass, Even Electron Ions
615 formula(e) evaluated with 26 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3
Expt-756
240130YAO10 296 (2.891) Cm (295:298-(285:288+312:317))



Minimum:					-1.5	
Maximum:				10.0	500.0	50.0
Mass	Calc. Mass	mDa	PPM	DBE	Formula	
325.9912	325.9906	0.6	1.8	9.5	C15 H11 N O C13	
	325.9834	7.8	23.9	5.5	C10 H10 N O7 C12	
	325.9987	-7.5	-23.0	9.5	C14 H10 N O4 C12	
	325.9965	-5.3	-16.3	0.5	C8 H15 N O6 C13	
	325.9856	5.6	17.2	14.5	C16 H5 N O5 C1	
	325.9915	-0.3	-0.9	5.5	C9 H9 N O10 C1	
	325.9888	2.4	7.4	14.5	C16 H6 N3 O C12	
	325.9969	-5.7	-17.5	14.5	C15 H5 N3 O4 C1	
	325.9816	9.6	29.4	10.5	C11 H5 N3 O7 C1	
	325.9947	-3.5	-10.7	5.5	C9 H10 N3 O6 C12	
	325.9866	4.6	14.1	5.5	C10 H11 N3 O3 C13	
	325.9870	4.2	12.9	19.5	C17 H N5 O C1	
	325.9826	8.6	26.4	1.5	C5 H11 N5 O5 C13	
	325.9978	-6.6	-20.2	5.5	C9 H11 N5 O2 C13	
	325.9848	6.4	19.6	10.5	C11 H6 N5 O3 C12	
	325.9928	-1.6	-4.9	10.5	C10 H5 N5 O6 C1	
	325.9906	0.6	1.8	1.5	C4 H10 N5 O8 C12	
	325.9960	-4.8	-14.7	10.5	C10 H6 N7 O2 C12	
	325.9829	8.3	25.5	15.5	C12 H N7 O3 C1	
	325.9938	-2.6	-8.0	1.5	C4 H11 N7 O4 C13	
	325.9888	2.4	7.4	6.5	C5 H5 N7 O8 C1	
	325.9942	-3.0	-9.2	15.5	C11 H N9 O2 C1	
	326.0000	-8.8	-27.0	6.5	C4 H5 N9 O7 C1	
	325.9839	7.3	22.4	6.5	C6 H7 N9 O C13	
	325.9920	-0.8	-2.5	6.5	C5 H6 N9 O4 C12	

HRMS of **3ea**

[Mass Spectrum]
Data : 20231220_HREI_Expt-741001 Date : 20-Dec-2023 15:33
RT : 0.30 min Scan# : (3,4)
Elements : C 15/0, H 15/0, 79Br 1/0, 81Br 1/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 1/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

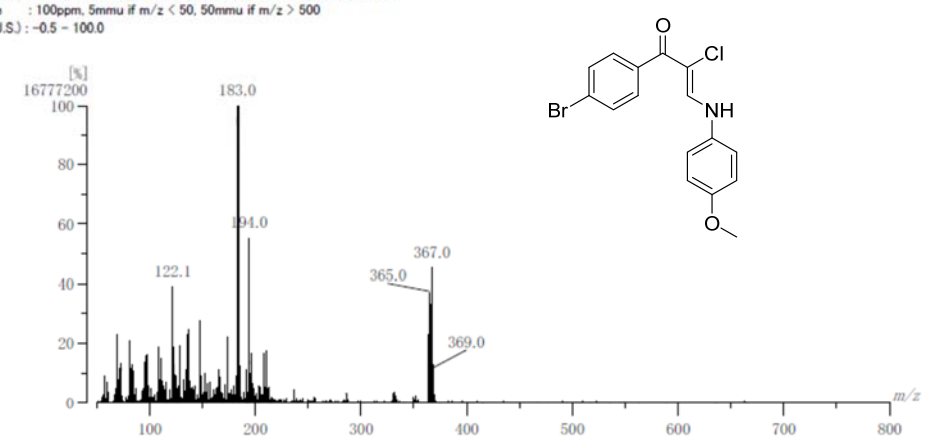


Observed m/z Int%
334.9703 17.49

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	35Cl	37Cl	N	O
1	334.9606	+29.0 / +9.7	6.5	14	14	-	1	1	1	-	-
2	334.9657	+13.7 / +4.6	6.0	13	14	1	-	1	1	1	-
3	334.9480	+66.5 / +22.3	7.0	13	12	-	1	1	1	1	-
4	334.9469	+69.8 / +23.4	4.5	12	15	1	1	-	-	-	1
5	334.9419	+84.8 / +28.4	6.5	13	12	1	-	1	1	-	1
6	334.9713	-2.8 / -1.0	10.0	15	11	1	-	1	-	1	1
7	334.9536	+50.0 / +16.7	11.0	15	9	-	1	1	-	1	1
8	334.9527	+52.7 / +17.6	11.0	15	9	1	-	-	1	1	1

HRMS of **3ej**

[Mass Spectrum]
Data : 20231220_HREI_Expt-742001 Date : 20-Dec-2023 15:48
RT : 0.30 min Scan# : 3
Elements : C 16/0, H 15/0, 79Br 1/0, 81Br 1/0, 35Cl 1/0, 37Cl 1/0, N 1/0, O 2/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

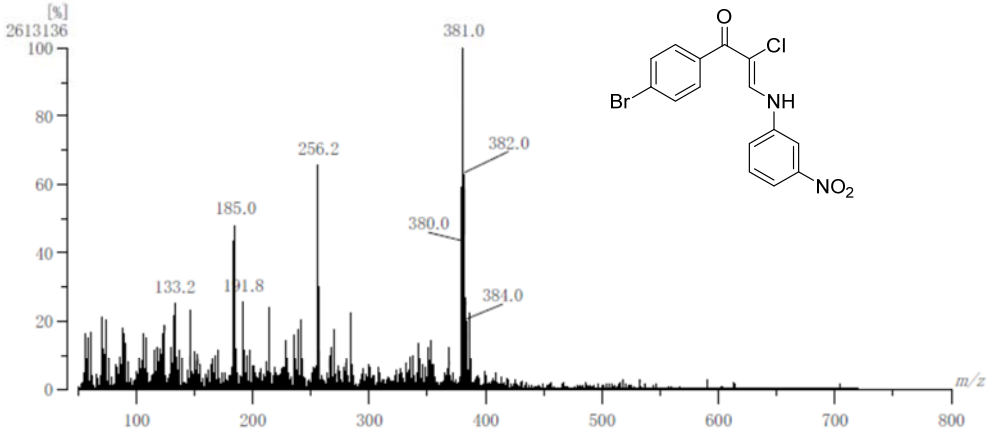


Observed m/z Int%
364.9812 36.93

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	35Cl	37Cl	N	O
1	364.9586	+62.0 / +22.6	7.0	14	14	-	1	1	1	1	1
2	364.9525	+78.7 / +28.7	6.5	14	14	1	-	1	1	-	2
3	364.9449	+99.4 / +36.3	5.0	12	15	1	1	-	-	1	2
4	364.9818	-1.7 / -0.6	10.0	16	13	1	-	1	-	1	2
5	364.9641	+46.8 / +17.1	11.0	16	11	-	1	1	-	1	2
6	364.9632	+49.3 / +18.0	11.0	16	11	1	-	-	1	1	2
7	364.9455	+97.8 / +35.7	12.0	16	9	-	1	-	1	1	2

HRMS of **3el**

[Mass Spectrum]
Data : 20231220_HREI_Expt-744001 Date : 20-Dec-2023 15:55
RT : 0.15 min Scan# : 2
Elements : C 15/0, H 10/0, 79Br 1/0, 81Br 1/0, 35Cl 1/0, 37Cl 1/0, N 2/0, O 3/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



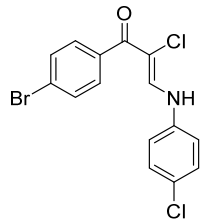
	Observed m/z	Int%								
	379.9554	42.91								
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	35Cl	37Cl	N	O
1	379.9563	-2.5 / -0.9	11.0	15	10	1	-	1	-	2	3
2	379.9386	+44.1 / +16.8	12.0	15	8	-	1	1	-	2	3
3	379.9377	+46.5 / +17.7	12.0	15	8	1	-	-	1	2	3
4	379.9200	+93.1 / +35.4	13.0	15	6	-	1	-	1	2	3

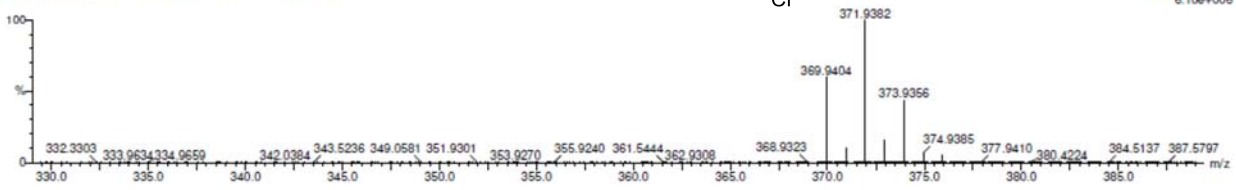
HRMS of **3ep**

Elemental Composition Report Page 1

Single Mass Analysis
Tolerance = 10.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
607 formula(e) evaluated with 20 results within limits (up to 25 closest results for each mass)
Elements Used:
C: 1-100 H: 1-100 N: 1-10 O: 1-10 Cl: 1-3 Br: 1-3
Expt-743
240130YAO04 300 (2.926) Cm (299:303-(287:292+313:317))

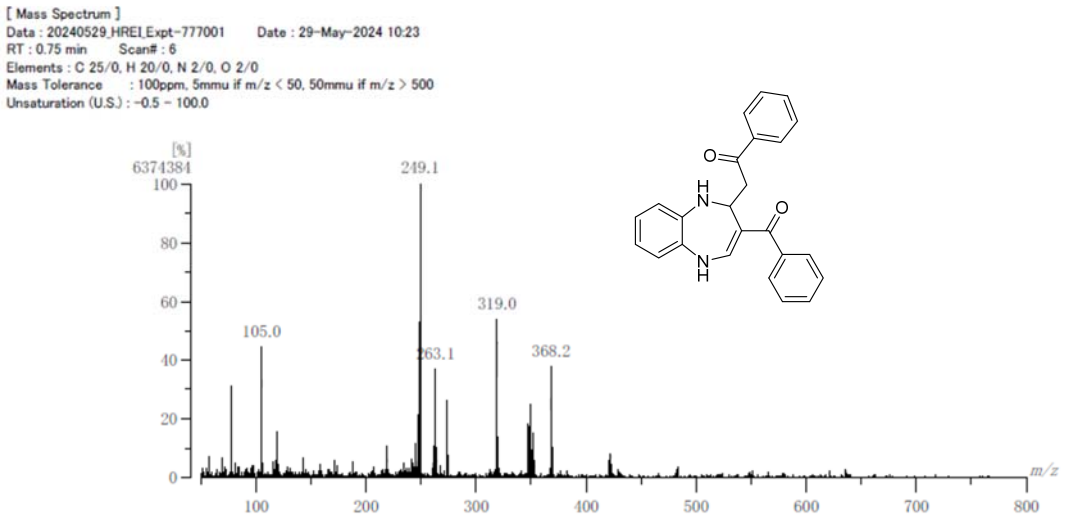




Minimum: -1.5
Maximum: 10.0 500.0 50.0

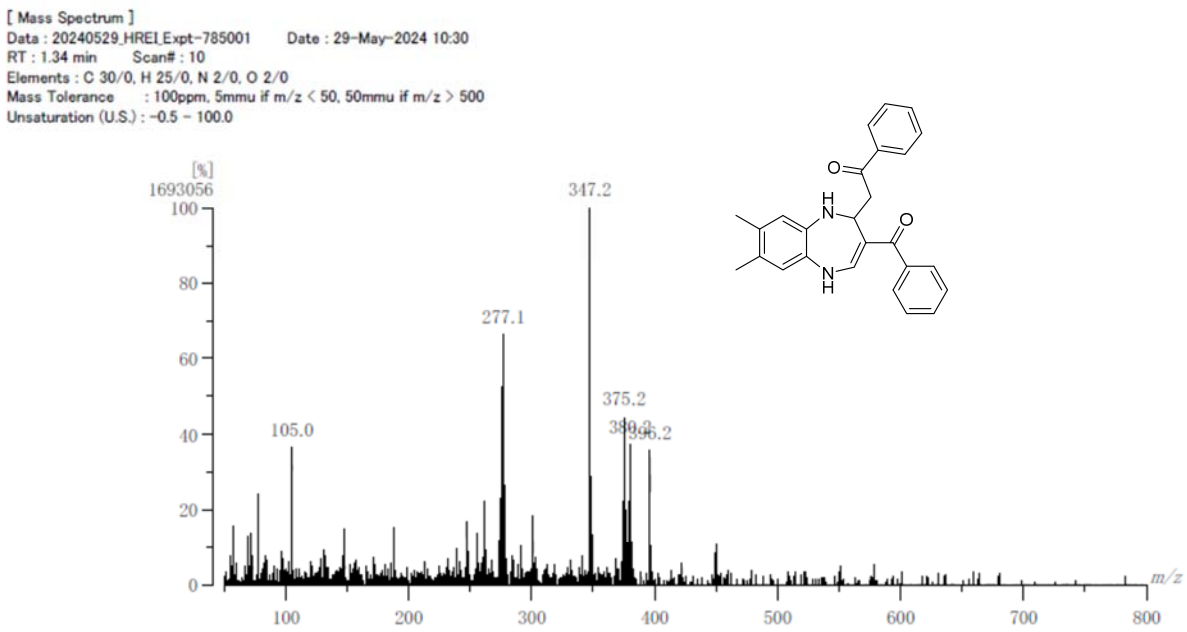
Mass	Calc. Mass	mDa	PPM	DBE	Formula
369.9404	369.9401	0.3	0.8	9.5	C15 H11 N O C12 Br
	369.9401	0.3	0.8	1.5	C4 H10 N5 O8 Cl Br
	369.9415	-1.1	-3.0	6.5	C5 H6 N9 O4 Cl Br
	369.9393	1.1	3.0	-0.5	C4 H15 N7 O Cl Br2
	369.9420	-1.6	-4.3	-1.5	C8 H19 N O3 Cl Br2
	369.9383	2.1	5.7	14.5	C16 H6 N3 O Cl Br
	369.9379	2.5	6.8	0.5	C9 H16 N O3 Cl3 Br
	369.9433	-2.9	-7.8	1.5	C4 H11 N7 O4 Cl2 Br
	369.9442	-3.8	-10.3	5.5	C9 H10 N3 O6 Cl Br
	369.9361	4.3	11.6	5.5	C10 H11 N3 O3 Cl2 Br
	369.9455	-5.1	-13.8	10.5	C10 H6 N7 O2 Cl Br
	369.9352	5.2	14.1	1.5	C5 H12 N7 O Cl3 Br
	369.9460	-5.6	-15.1	0.5	C8 H15 N O6 Cl2 Br
	369.9343	6.1	16.5	10.5	C11 H6 N5 O3 Cl Br
	369.9473	-6.9	-18.7	5.5	C9 H11 N5 O2 Cl2 Br
	369.9334	7.0	18.9	6.5	C6 H7 N9 O Cl2 Br
	369.9329	7.5	20.3	5.5	C10 H10 N O7 Cl Br
	369.9482	-7.8	-21.1	9.5	C14 H10 N O4 Cl Br
	369.9321	8.3	22.4	1.5	C5 H11 N5 O5 Cl2 Br
	369.9491	-8.7	-23.5	0.5	C8 H16 N3 O2 Cl3 Br

HRMS of **6aa**



	Observed m/z	Int%	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
	368.1537	37.77							
1			368.1525	+3.3 / +1.2	16.0	24	20	2	2

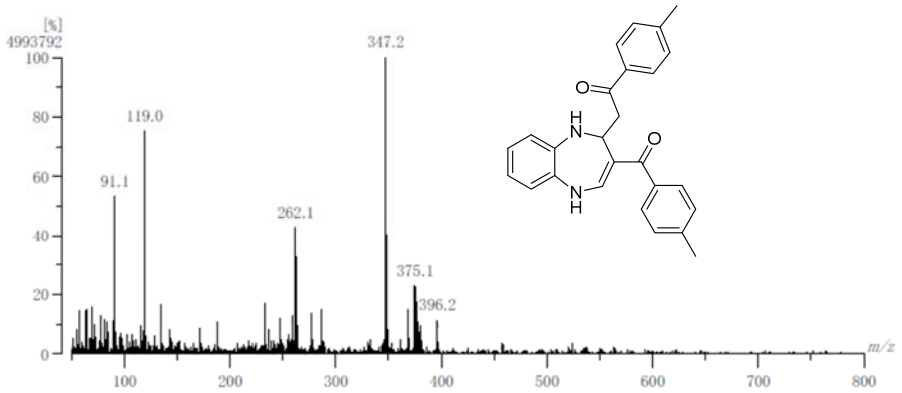
HRMS of **6ab**



	Observed m/z	Int%	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
	396.1834	35.87							
1			396.1752	+20.6 / +8.2	20.5	30	22	1	-
2			396.1626	+52.4 / +20.8	21.0	29	20	2	-
3			396.1514	+80.7 / +32.0	21.0	30	20	-	1
4			396.1838	-1.0 / -0.4	16.0	26	24	2	2

HRMS of **6ba**

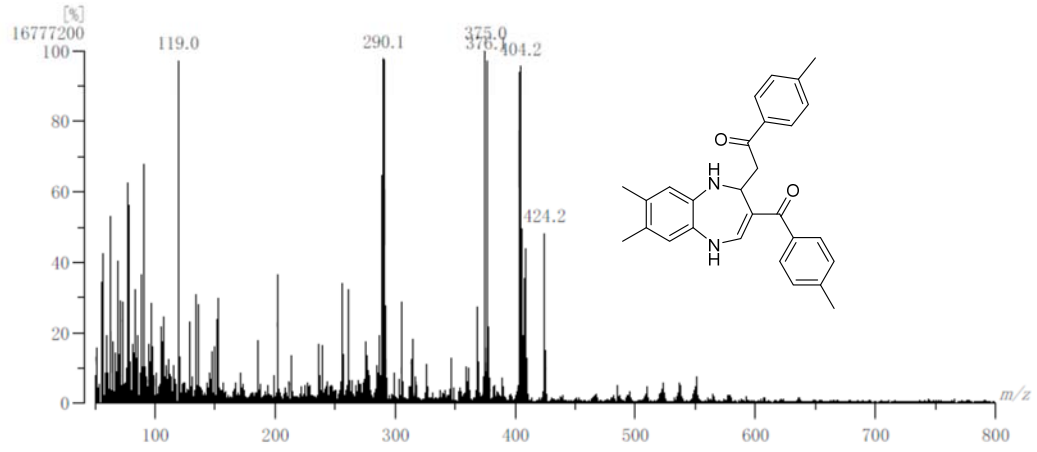
[Mass Spectrum]
Data : 20240603_HREI_6ba001 Date : 03-Jun-2024 10:39
RT : 1.49 min Scan# : 11
Elements : C 30/0, H 30/0, N 2/0, O 2/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



	Observed m/z	Int%				
	396.1850	11.30				
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
1	396.1752	+24.7 / +9.8	20.5	30	22	1	-
2	396.1626	+56.4 / +22.4	21.0	29	20	2	-
3	396.1514	+84.8 / +33.6	21.0	30	20	-	1
4	396.2202	-88.8 / -35.2	15.0	27	28	2	1
5	396.2089	-60.4 / -23.9	15.0	28	28	-	2
6	396.1964	-28.7 / -11.4	15.5	27	26	1	2
7	396.1838	+3.1 / +1.2	16.0	26	24	2	2

HRMS of **6bb**

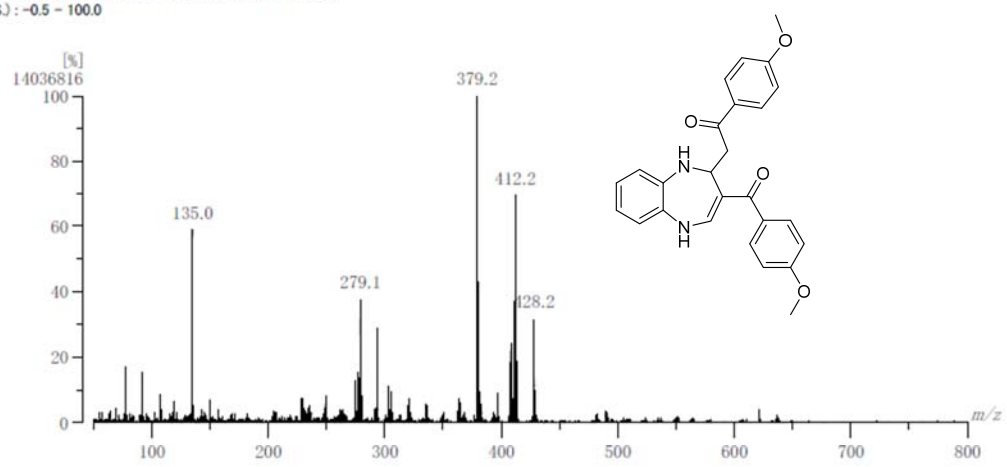
[Mass Spectrum]
Data : 20240603_HREI_6bb001 Date : 03-Jun-2024 10:48
RT : 1.64 min Scan# : 12
Elements : C 30/0, H 30/0, N 2/0, O 2/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



	Observed m/z	Int%				
	424.2136	48.24				
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
1	424.2277	-33.1 / -14.1	15.5	29	30	1	2
2	424.2151	-3.5 / -1.5	16.0	28	28	2	2

HRMS of **6ca**

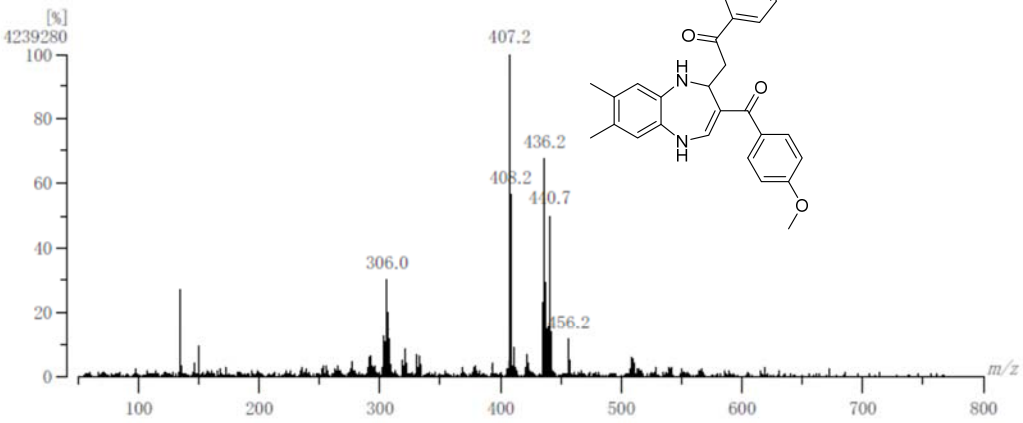
[Mass Spectrum]
Data : 20240529_HREI_Expt-829001 Date : 29-May-2024 10:55
RT : 1.19 min Scan# : 9
Elements : C 30/0, H 30/0, N 2/0, O 4/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



	Observed m/z	Int%					
	428.1731	31.62					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
1	428.1889	-36.8 / -15.8	20.0	30	24	2	1
2	428.1651	+18.8 / +8.0	20.5	30	22	1	2
3	428.1525	+48.2 / +20.6	21.0	29	20	2	2
4	428.1412	+74.4 / +31.9	21.0	30	20	-	3
5	428.2100	-86.2 / -36.9	15.0	27	28	2	3
6	428.1988	-59.9 / -25.7	15.0	28	28	-	4
7	428.1862	-30.6 / -13.1	15.5	27	26	1	4
8	428.1736	-1.2 / -0.5	16.0	26	24	2	4

HRMS of **6cb**

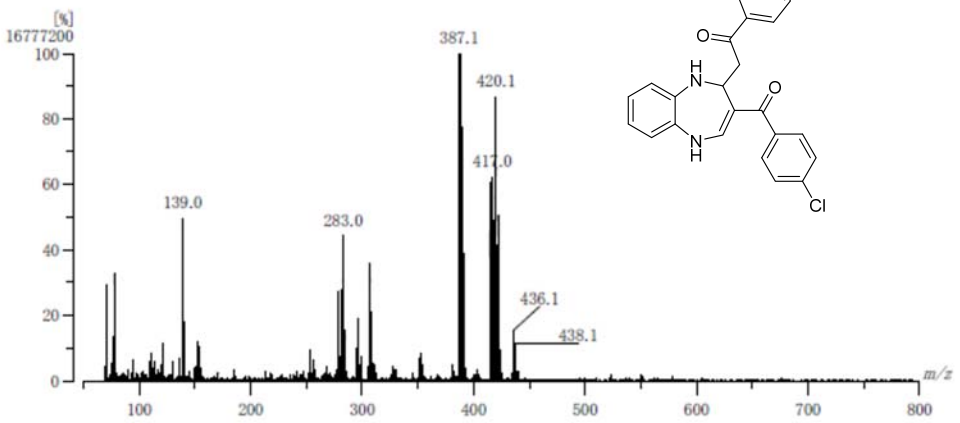
[Mass Spectrum]
Data : 20240529_HREI_Expt-830002 Date : 29-May-2024 11:13
RT : 1.34 min Scan# : 10
Elements : C 30/0, H 30/0, N 2/0, O 4/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0



	Observed m/z	Int%					
	456.2033	11.45					
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	N	O
1	456.2175	-31.1 / -14.2	15.5	29	30	1	4
2	456.2049	-3.5 / -1.6	16.0	28	28	2	4

HRMS of **6da**

[Mass Spectrum]
Data : 20240603_HREI_6da004 Date : 03-Jun-2024 11:34
RT : 0.15 min Scan# : 2
Elements : C 25/0, H 20/0, 35Cl 2/0, 37Cl 2/0, N 2/0, O 2/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

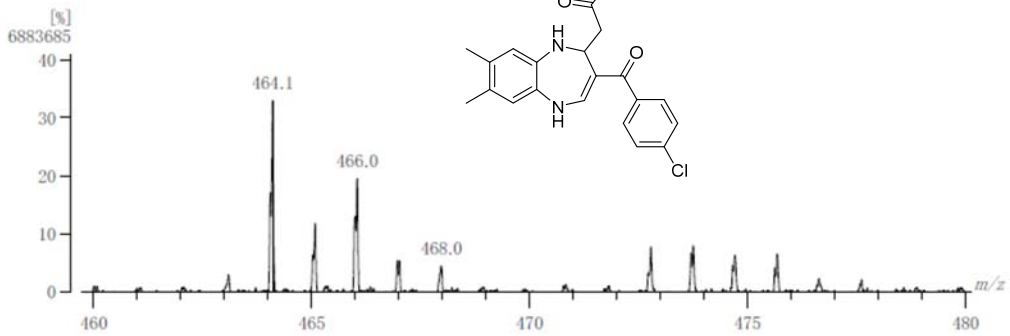


	Observed m/z	Int%								
	436.0736	14.90								
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	436.0923	-42.9 / -18.7	16.0	25	20	1	1	2	1
2	436.0737	-0.3 / -0.1	17.0	25	18	-	2	2	1
3	436.0504	+53.2 / +23.2	13.0	22	19	1	2	2	1
4	436.0392	+79.0 / +34.4	13.0	23	19	1	2	-	2
5	436.0871	-31.0 / -13.5	15.5	25	20	2	-	1	2
6	436.0685	+11.7 / +5.1	16.5	25	18	1	1	1	2
7	436.0452	+65.2 / +28.4	12.5	22	19	2	1	1	2
8	436.0499	+54.3 / +23.7	17.5	25	16	-	2	1	2
9	436.0745	-2.1 / -0.9	16.0	24	18	2	-	2	2
10	436.0559	+40.5 / +17.7	17.0	24	16	1	1	2	2
11	436.0326	+94.0 / +41.0	13.0	21	17	2	1	2	2
12	436.0373	+83.2 / +36.3	18.0	24	14	-	2	2	2

	Observed m/z	Int%							
	438.0722	10.98							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
13	438.0397	+74.2 / +32.5	16.5	25	17	2	1	1	-
14	438.0894	-39.2 / -17.2	16.0	25	20	-	2	2	1
15	438.0842	-27.3 / -12.0	15.5	25	20	1	1	1	2
16	438.0656	+15.2 / +6.6	16.5	25	18	-	2	1	2
17	438.0422	+68.4 / +30.0	12.5	22	19	1	2	1	2
18	438.0902	-41.1 / -18.0	15.0	24	20	2	-	2	2
19	438.0716	+1.4 / +0.6	16.0	24	18	1	1	2	2
20	438.0483	+54.6 / +23.9	12.0	21	19	2	1	2	2
21	438.0530	+43.9 / +19.2	17.0	24	16	-	2	2	2
22	438.0297	+97.1 / +42.5	13.0	21	17	1	2	2	2

HRMS of **6db**

[Mass Spectrum]
Data : 20240429_HREI_1001 Date : 29-Apr-2024 15:32
RT : 1.04 min Scan# : 8
Elements : C 26/0, H 25/0, 35Cl 2/0, 37Cl 2/0, N 2/0, O 2/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

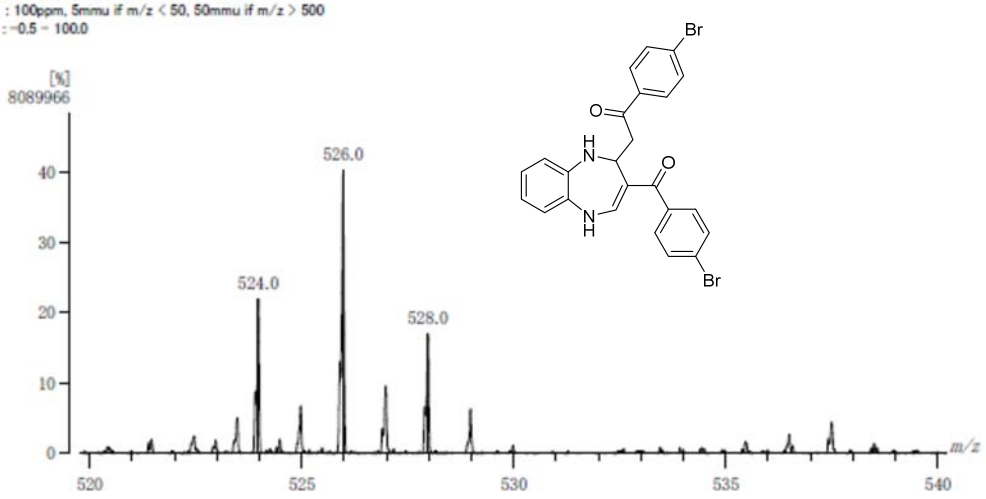


Observed m/z 464.1051 Int% 33.06

	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	35Cl	37Cl	N	O
1	464.0943	+23.3 / +10.8	12.5	25	25	1	2	1	1
2	464.1003	+10.3 / +4.8	12.0	24	25	2	1	2	1
3	464.0817	+50.4 / +23.4	13.0	24	23	1	2	2	1
4	464.0891	+34.6 / +16.0	12.0	25	25	2	1	-	2
5	464.0705	+74.6 / +34.6	13.0	25	23	1	2	-	2
6	464.0765	+61.7 / +28.6	12.5	24	23	2	1	1	2
7	464.1058	-1.6 / -0.7	16.0	26	22	2	-	2	2
8	464.0872	+38.5 / +17.9	17.0	26	20	1	1	2	2
9	464.0639	+88.7 / +41.2	13.0	23	21	2	1	2	2
10	464.0686	+78.6 / +36.5	18.0	26	18	-	2	2	2

HRMS of **6ea**

[Mass Spectrum]
Data : 20240429_HREI_787001 Date : 29-Apr-2024 17:15
RT : 1.19 min Scan# : 9
Elements : C 25/0, H 20/0, 79Br 2/0, 81Br 2/0, N 2/0, O 2/0
Mass Tolerance : 100ppm, 5mmu if m/z < 50, 50mmu if m/z > 500
Unsaturation (U.S.) : -0.5 - 100.0

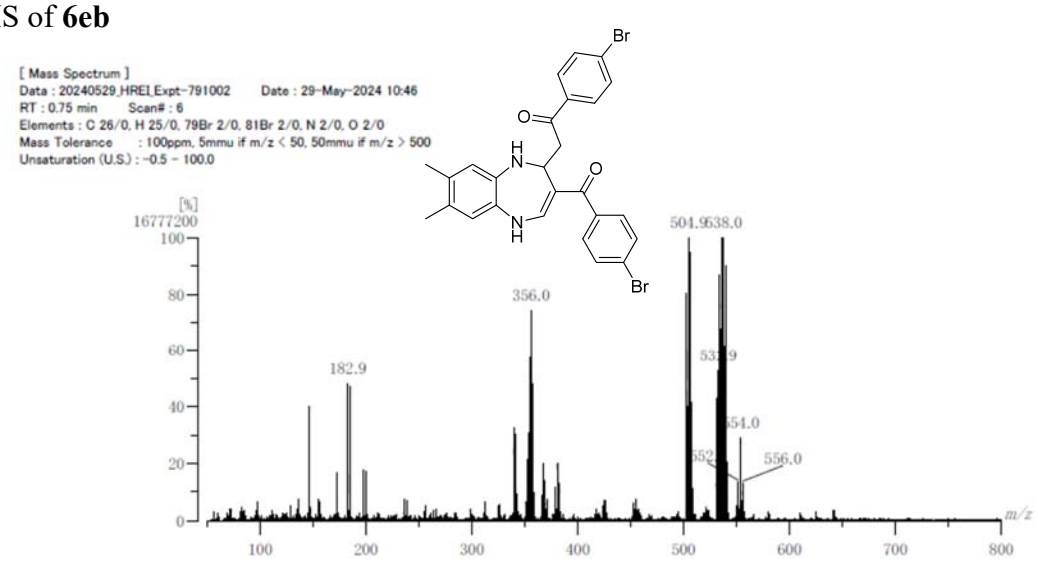


	Observed m/z	Int%								
	523.9738	21.90								
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	N	O
1	523.9922	-35.1 / -18.4	16.0	25	20	1	1	2	1
2	523.9745	-1.3 / -0.7	17.0	25	18	-	2	2	1
3	523.9861	-23.4 / -12.3	15.5	25	20	2	-	1	2
4	523.9684	+10.3 / +5.4	16.5	25	18	1	1	1	2
5	523.9507	+44.1 / +23.1	17.5	25	16	-	2	1	2
6	523.9735	+0.6 / +0.3	16.0	24	18	2	-	2	2
7	523.9558	+34.3 / +18.0	17.0	24	16	1	1	2	2
8	523.9381	+68.1 / +35.7	18.0	24	14	-	2	2	2

	Observed m/z	Int%							
	525.9759	40.19							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	N	O
9	525.9901	-27.1 / -14.2	16.0	25	20	-	2	2	1
10	525.9840	-15.5 / -8.1	15.5	25	20	1	1	1	2
11	525.9663	+18.2 / +9.6	16.5	25	18	-	2	1	2
12	525.9892	-25.2 / -13.3	15.0	24	20	2	-	2	2
13	525.9715	+8.5 / +4.4	16.0	24	18	1	1	2	2
14	525.9538	+42.1 / +22.1	17.0	24	16	-	2	2	2

	Observed m/z	Int%							
	527.9737	16.98							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	N	O
15	527.9820	-15.7 / -8.3	15.5	25	20	-	2	1	2
16	527.9871	-25.4 / -13.4	15.0	24	20	1	1	2	2
17	527.9694	+8.1 / +4.3	16.0	24	18	-	2	2	2

HRMS of **6eb**

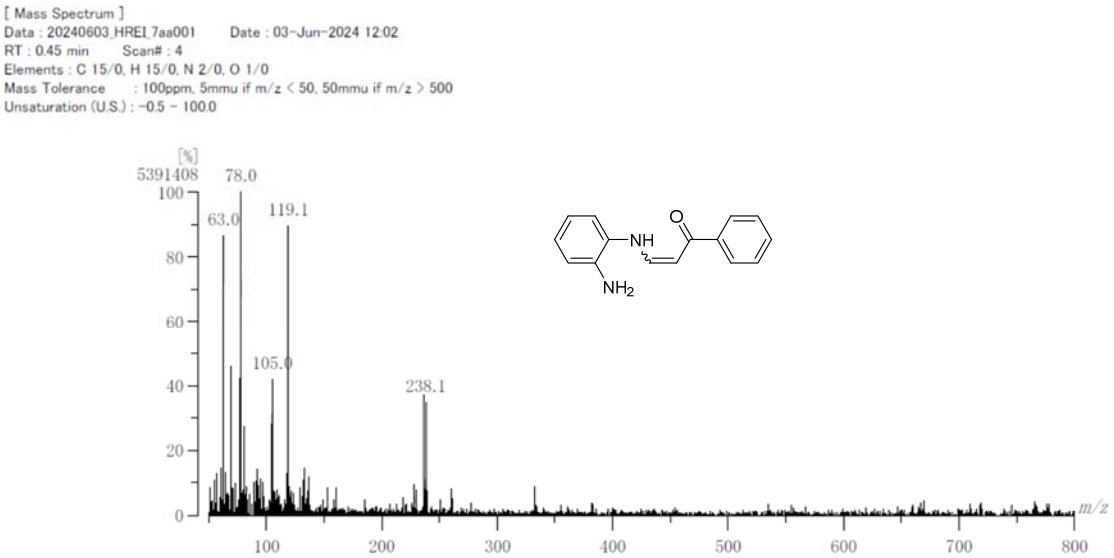


	Observed m/z	Int%							
	552.0033	13.46							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	N	O
1	552.0048	-2.7 / -1.5	16.0	26	22	2	-	2	2
2	551.9871	+29.3 / +16.2	17.0	26	20	1	1	2	2
3	551.9694	+61.4 / +33.9	18.0	26	18	-	2	2	2

	Observed m/z	Int%							
	554.0021	29.01							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	N	O
4	554.0205	-33.1 / -18.4	15.0	26	24	2	-	2	2
5	554.0028	-1.2 / -0.7	16.0	26	22	1	1	2	2
6	553.9851	+30.8 / +17.0	17.0	26	20	-	2	2	2

	Observed m/z	Int%							
	556.0003	13.14							
	Estimated m/z	Err[ppm / mmu]	U.S.	C	H	79Br	81Br	N	O
7	555.9547	+81.9 / +45.6	10.0	22	25	2	1	2	-
8	556.0184	-32.6 / -18.1	15.0	26	24	1	1	2	2
9	556.0007	-0.7 / -0.4	16.0	26	22	-	2	2	2

HRMS of **7aa**



	Observed m/z	Int%	Err[ppm / mmu]	U.S.	Composition
1	238.1102	34.82	-1.7 / -0.4	10.0	C15 H14 N2 O