Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Solvent and catalyst free ring expansion of indoles: A simple synthesis of highly functionalized benzazepines

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Supplementary Information

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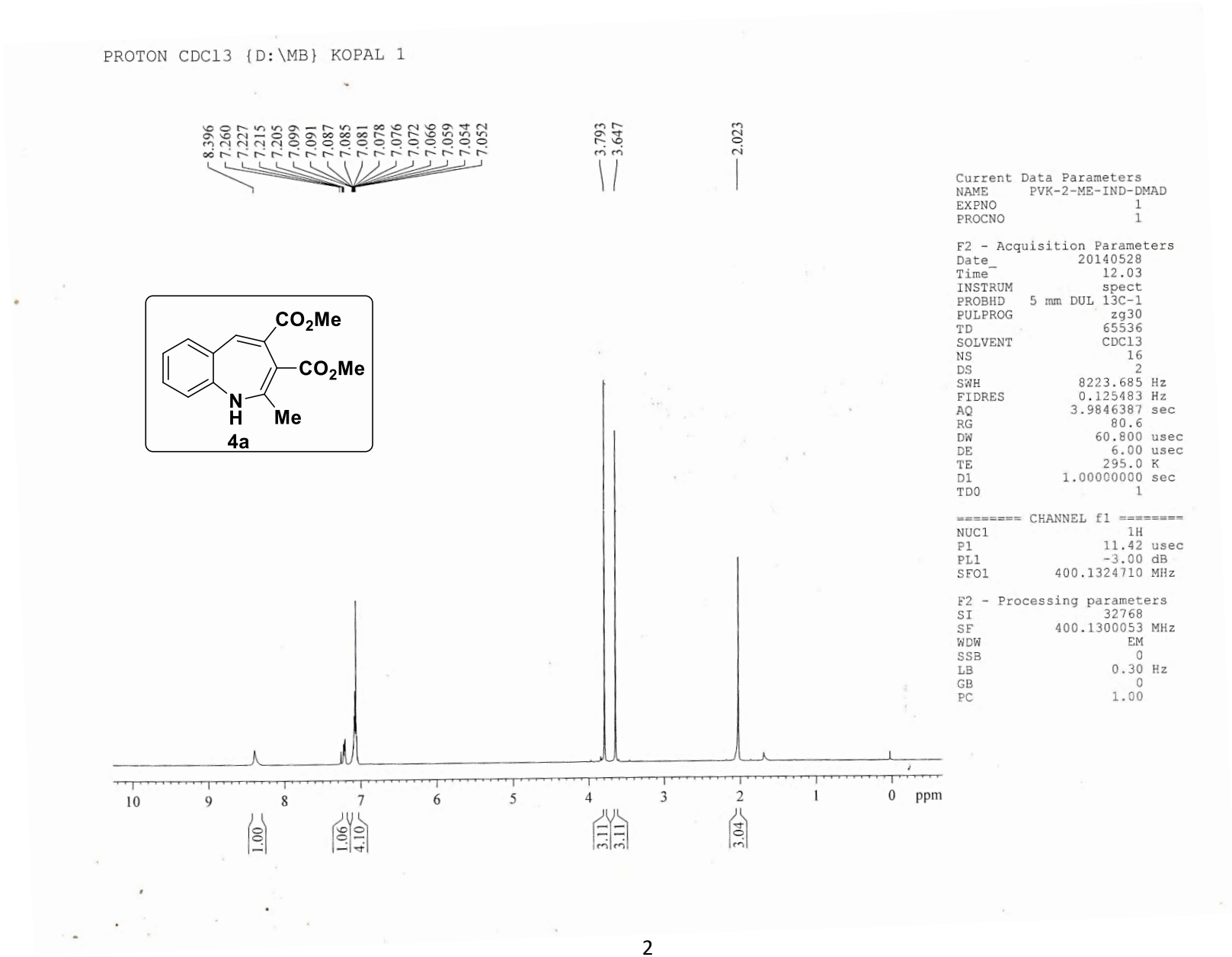
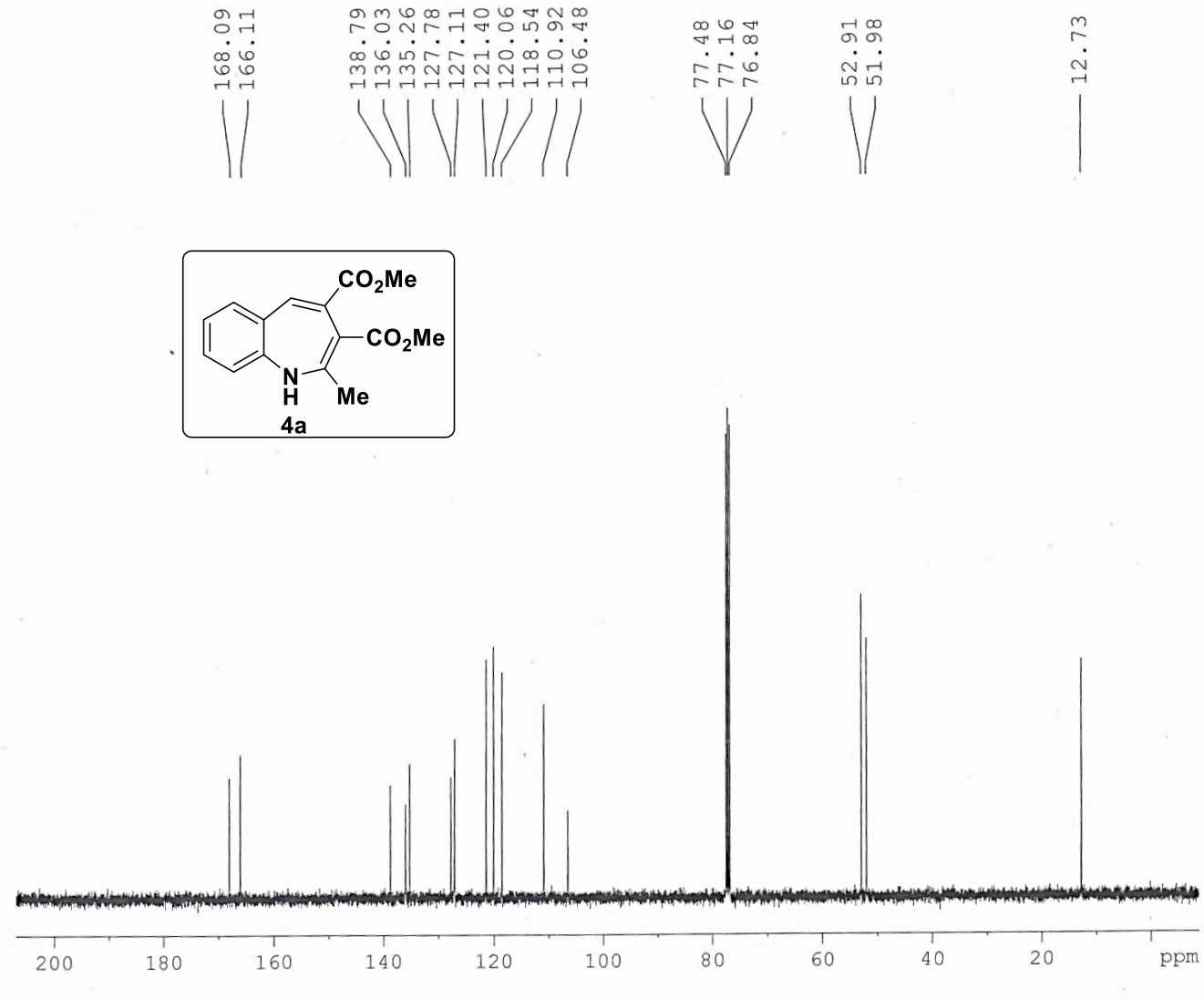
1. ^{1}H , ^{13}C NMR and ESI-HRMS spectra for the compounds 4a-z, 4aa and 5a-d



C13CPD CDCl3 {D:\MB} KOPAL 1

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PROCNO                   1

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PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      88
DS                       4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                      32
DW                20.800 usec
DE                 6.00 usec
TE                295.7 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.15 usec
PL1                   0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL12                 14.90 dB
PL13                 14.90 dB
PL2                  -3.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6127625 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
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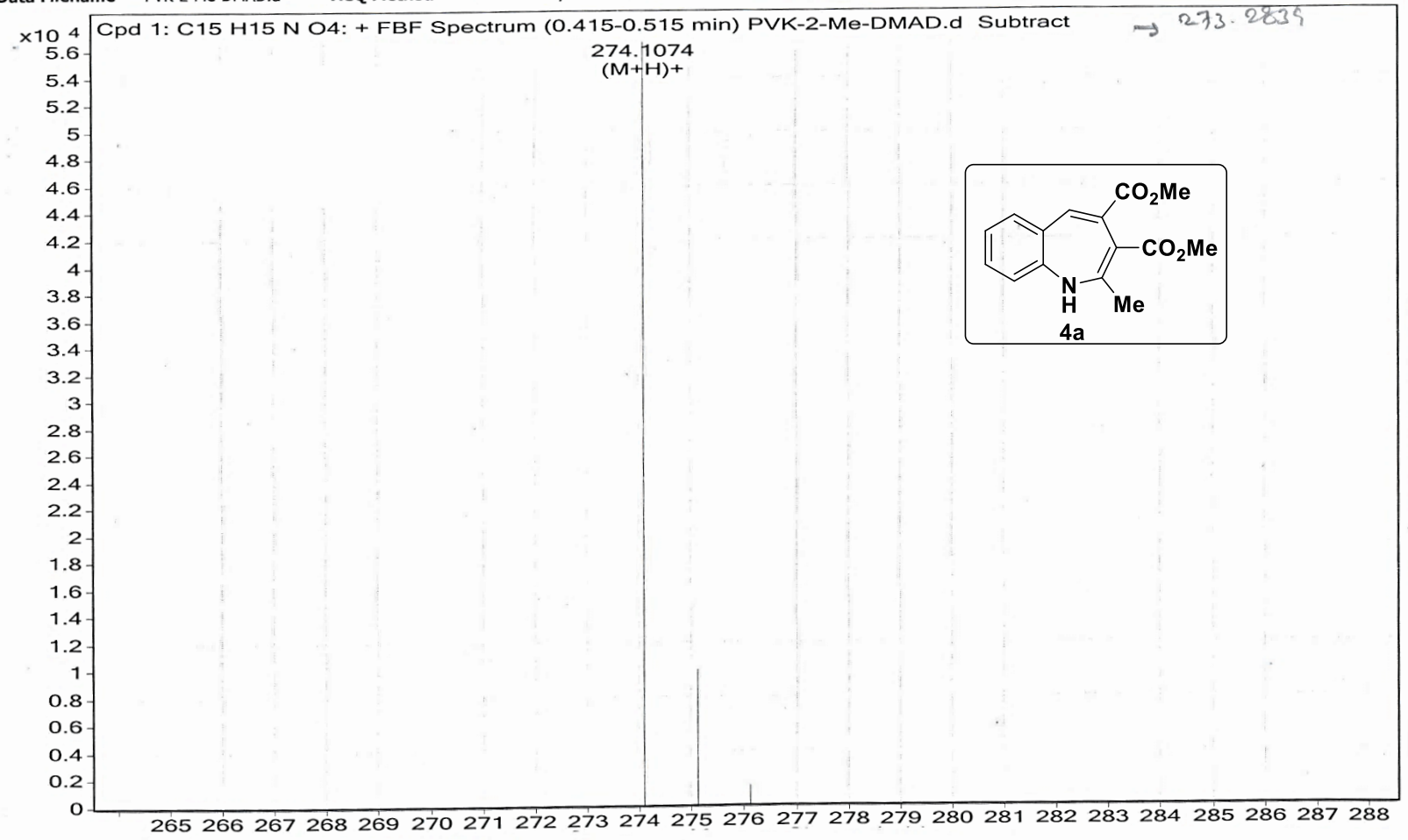
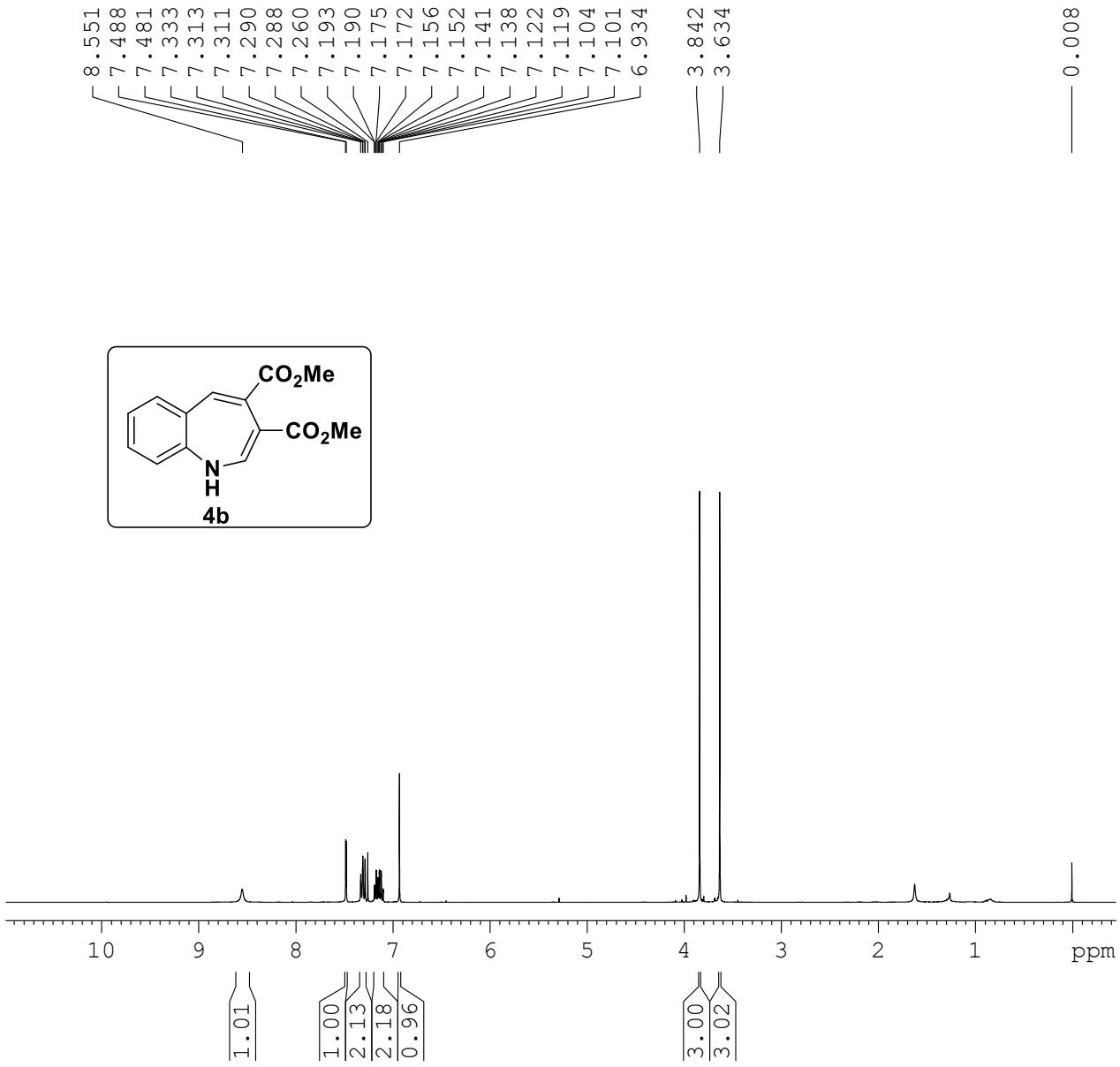


PROTON CDCl3 {D:\MB} KOPAL 1

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PROCNO                 1

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PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ              3.9846387 sec
RG                    181
DW                 60.800 usec
DE                  6.00 usec
TE                 297.5 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.42 usec
PL1                -3.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300051 MHz
WDW                   EM
SSB                    0
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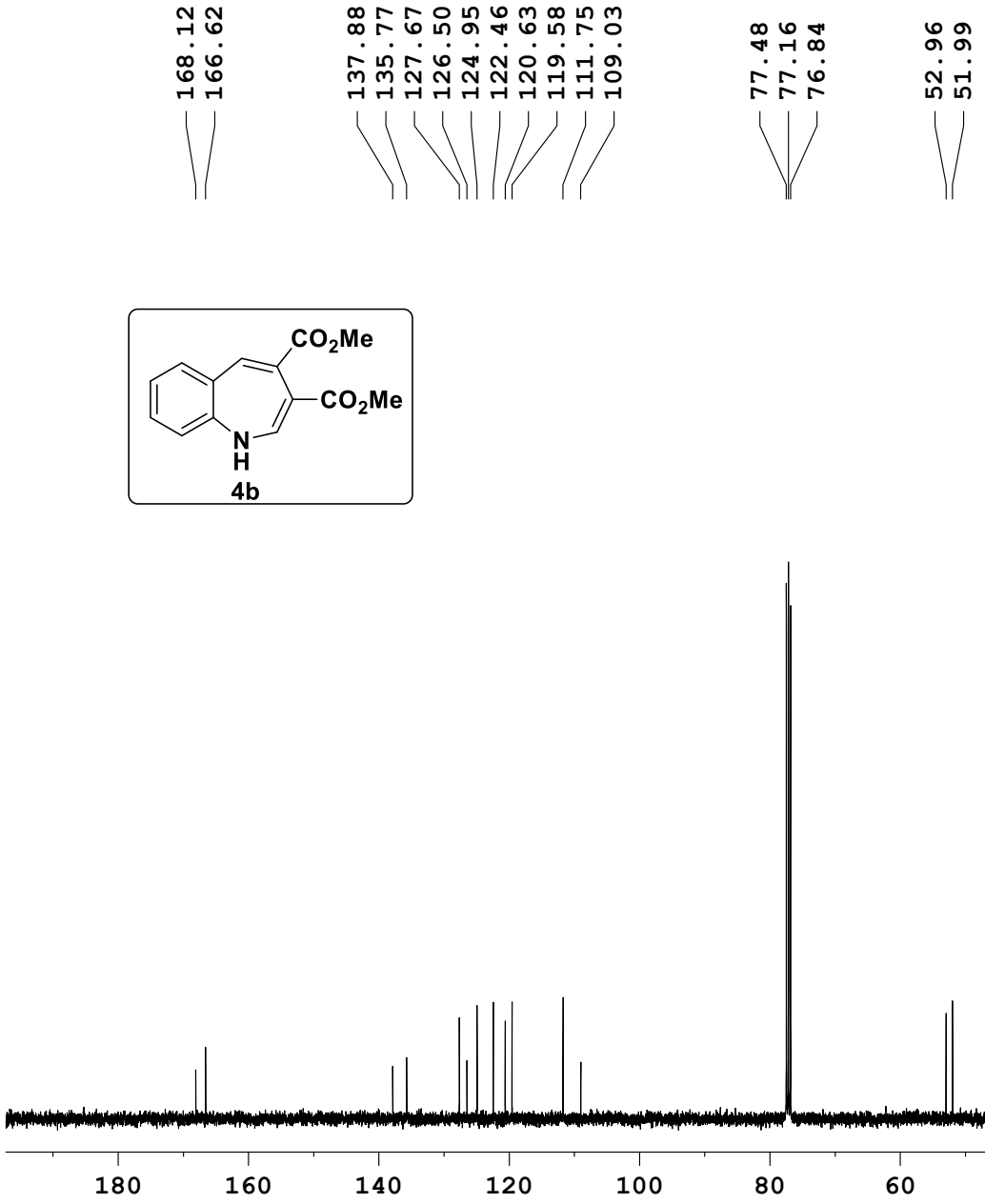


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EXPNO                 2
PROCNO                1

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Time              15.09
INSTRUM           spect
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PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                 28.5
DW                20.800 usec
DE                 6.00 usec
TE                298.2 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127553 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
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Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
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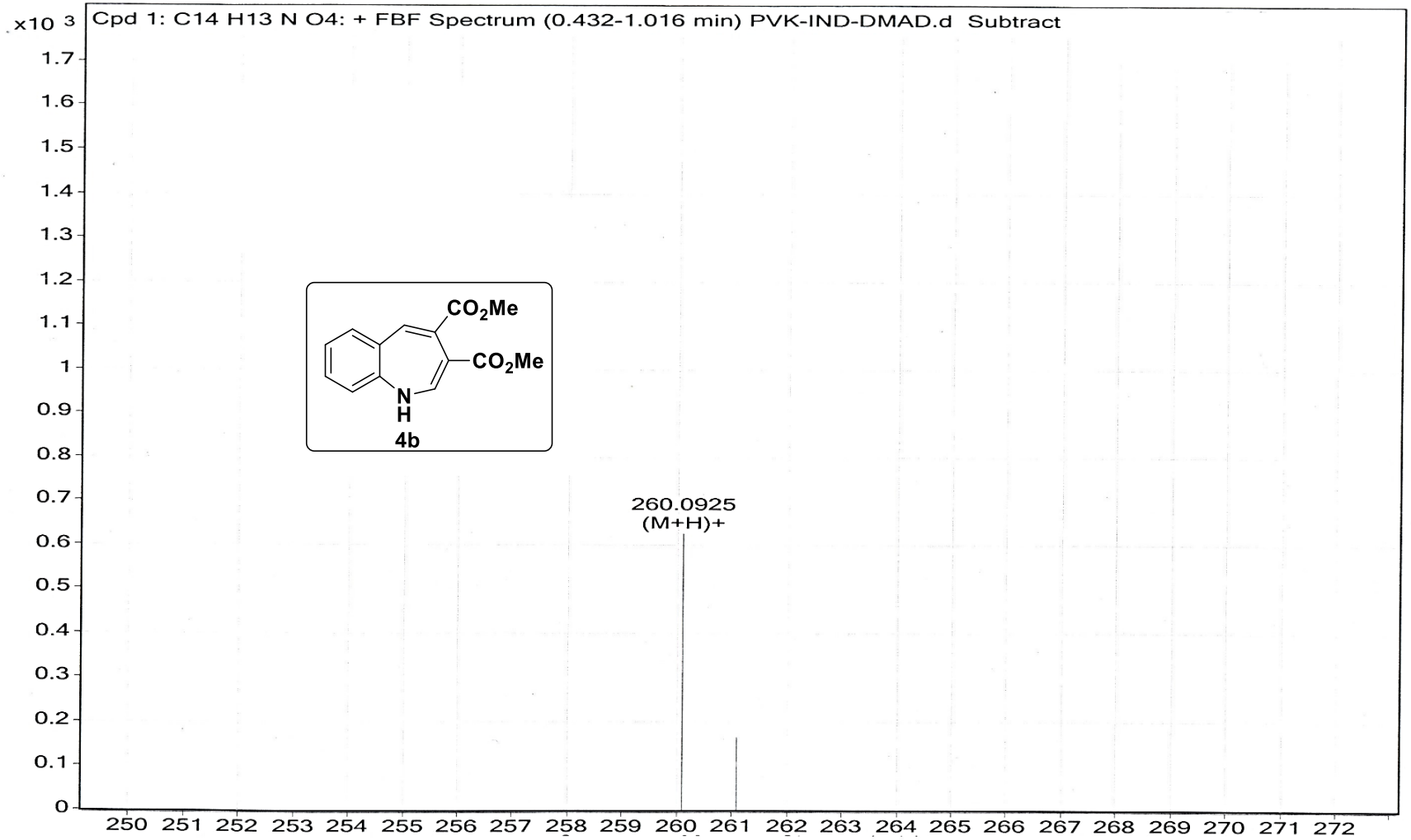

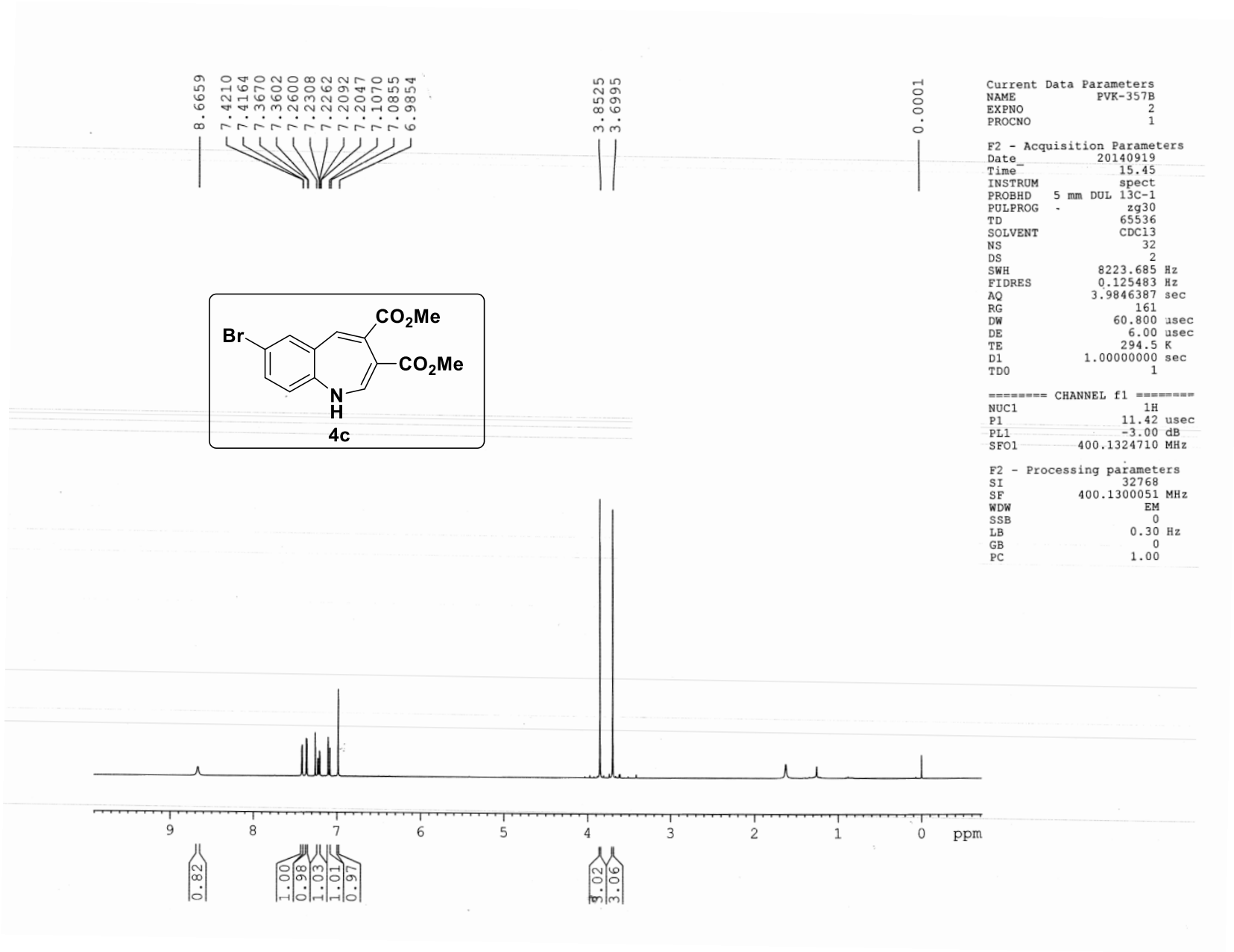

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PROCNO	1

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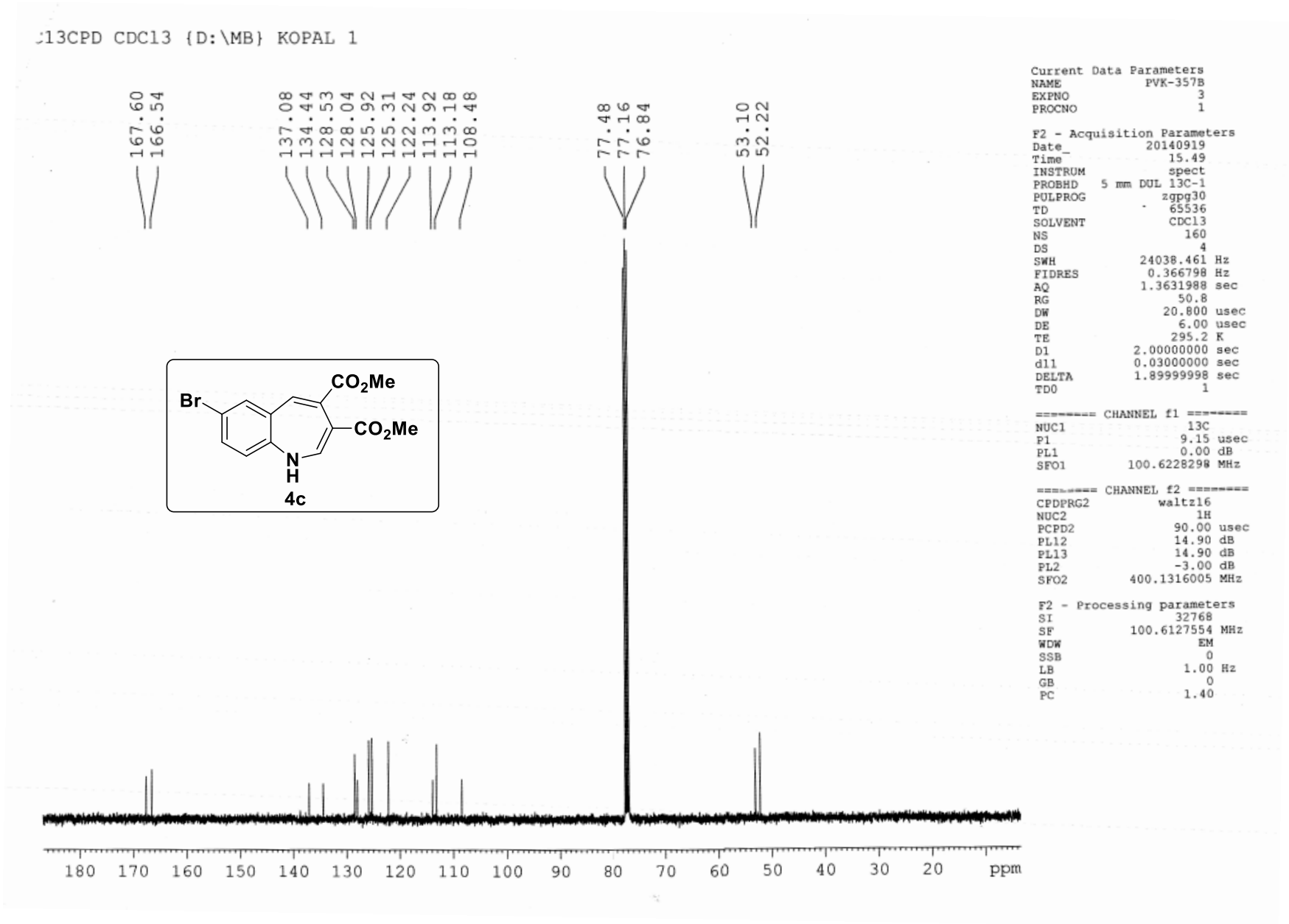
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	161
DW	60.800 usec
DE	6.00 usec
TE	294.5 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 ========

NUC1	1H
P1	11.42 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	32768
SF	400.1300051 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



Current Data Parameters

NAME	PVK-357B
EXPNO	3
PROCNO	1

F2 - Acquisition Parameters

Date_	20140919
Time	15.49
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	160
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	50.8
DW	20.800 usec
DE	6.00 usec
TE	295.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

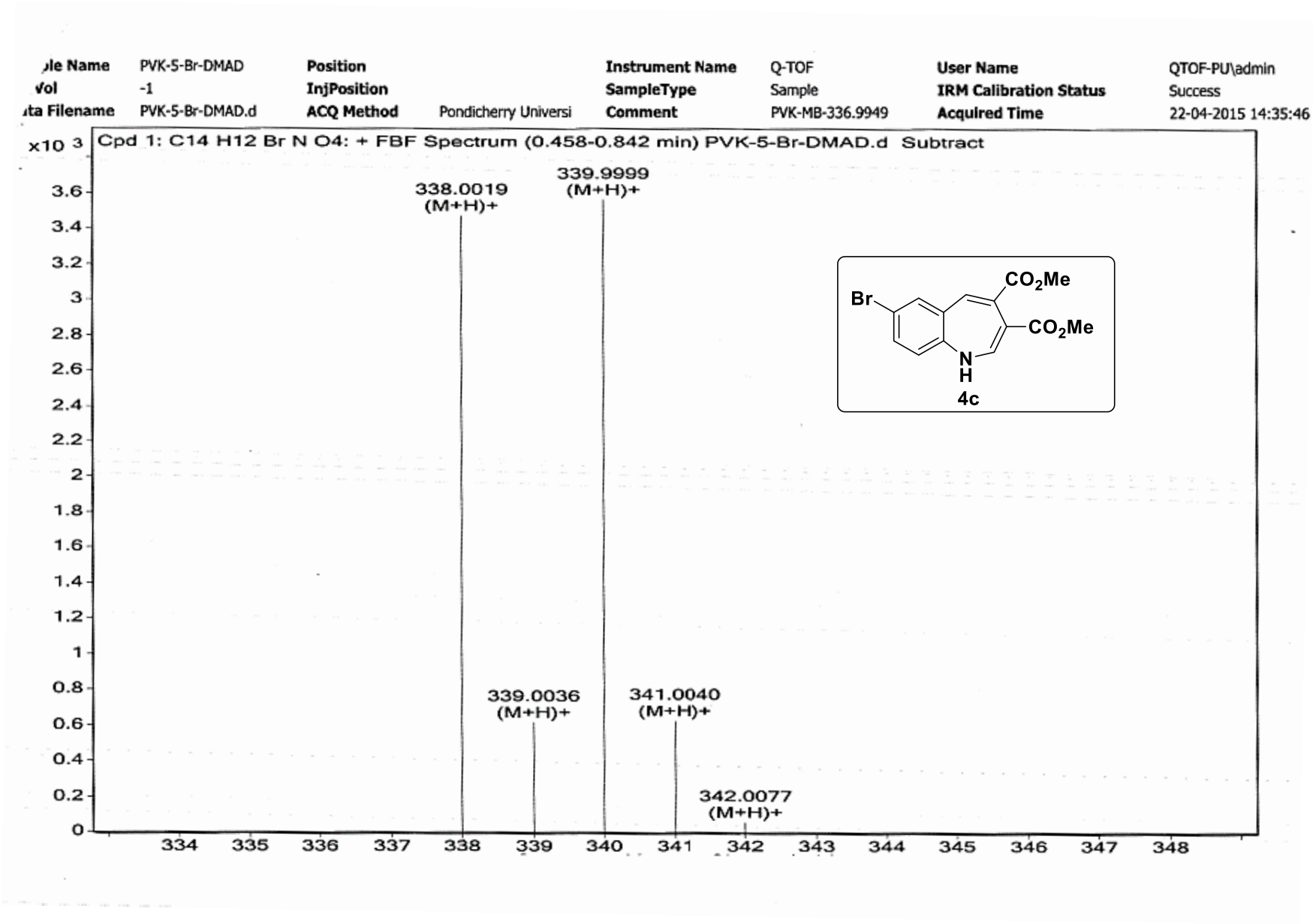
NUC1	13C
P1	9.15 usec
PL1	0.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL12	14.90 dB
PL13	14.90 dB
PL2	-3.00 dB
SFO2	400.1316005 MHz

F2 - Processing parameters

SI	32768
SF	100.6127554 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40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Vol -1
ıta Filename PVK-5-Br-DMAD.d
Position
InjPosition
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Instrument Name Q-TOF
SampleType Sample
Comment PVK-MB-336.9949
User Name QTOF-PU\admin
IRM Calibration Status Success
Acquired Time 22-04-2015 14:35:46
Cpd 1: C14 H12 Br N O4: + FBF Spectrum (0.458-0.842 min) PVK-5-Br-DMAD.d Subtract
x10 3
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339.9999 (M+H)+
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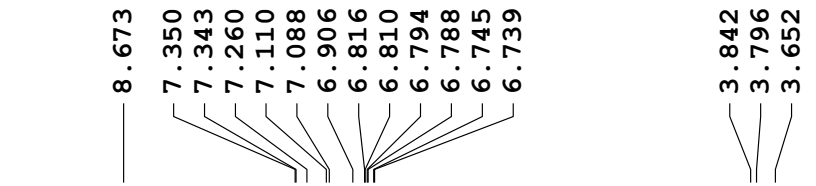
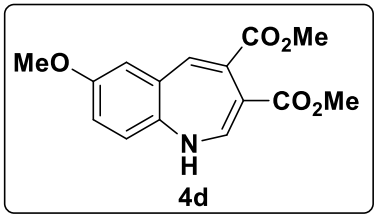
Br
CO2Me
CO2Me
N H
4c





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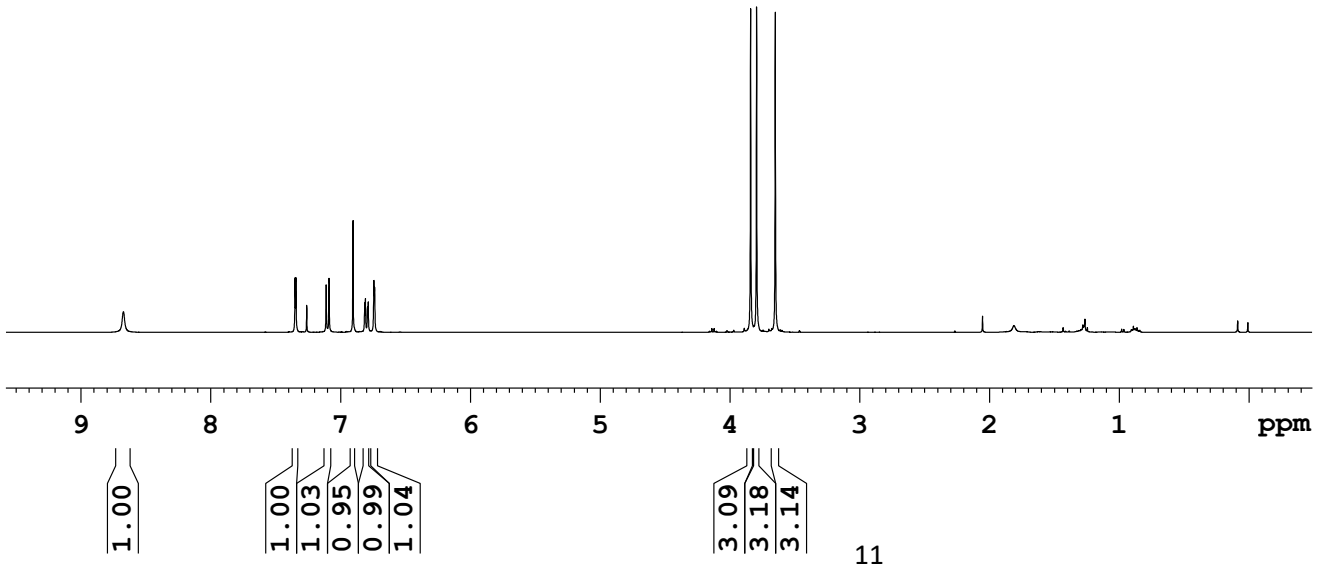


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PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                   128
DW                60.800 usec
DE                 6.00 usec
TE                294.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.35 usec
PL1                -1.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300045 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
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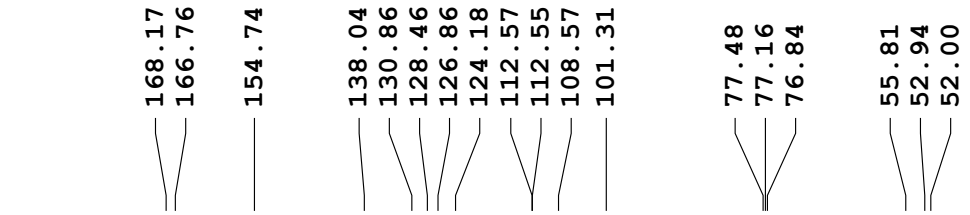

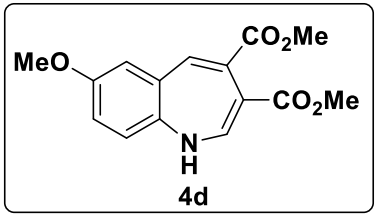


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Current Data Parameters
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EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180831
Time                 12.10
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                     256
DS                       4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                    45.2
DW                  20.800 usec
DE                   6.00 usec
TE                  296.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.95 usec
PL1                  -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2                90.00 usec
PL12                 14.95 dB
PL13                120.00 dB
PL2                  -1.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
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SF           100.6127608 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
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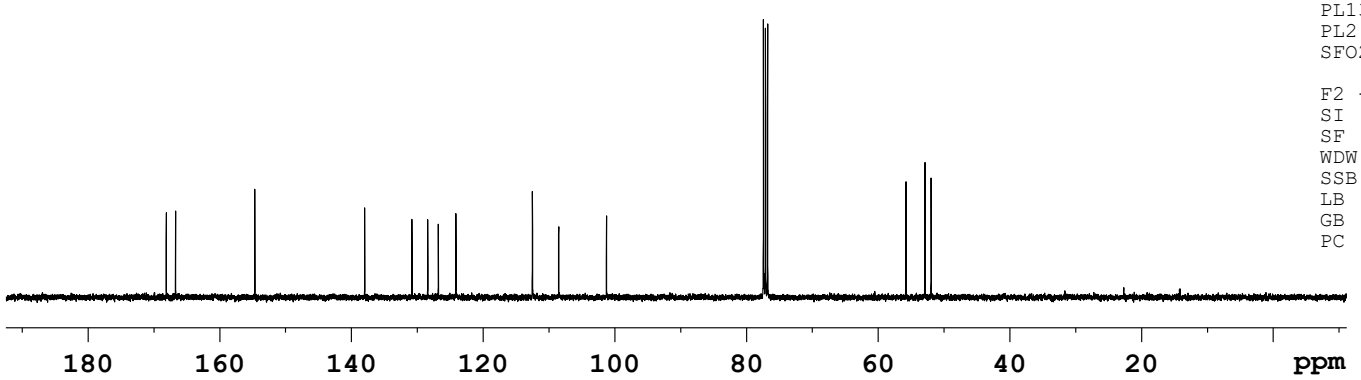

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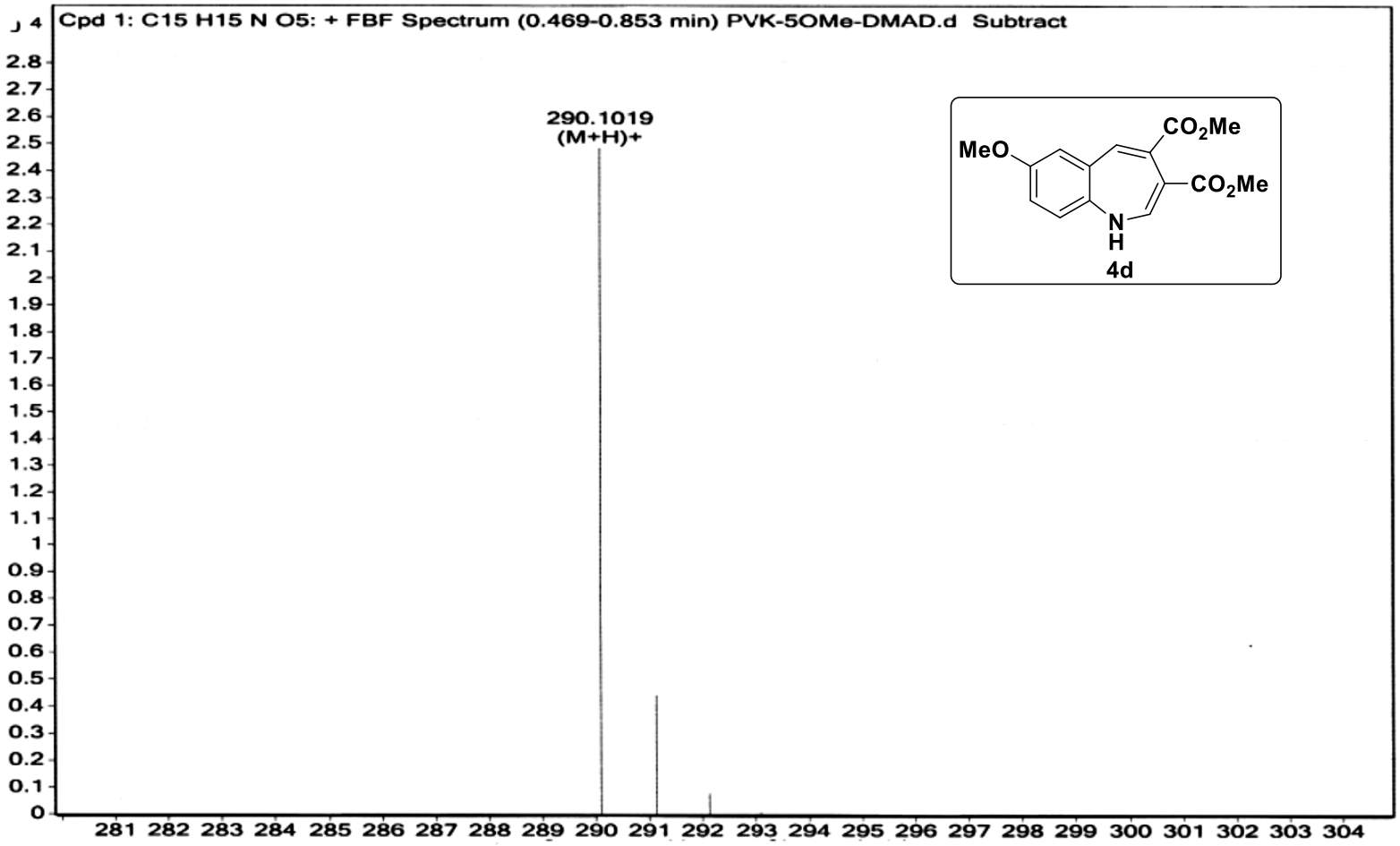
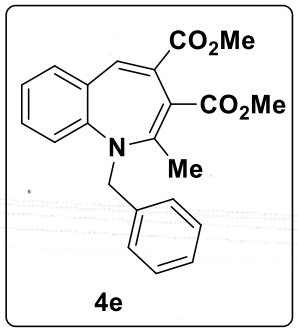


PROTON CDCl3 {D:\MB} KOPAL 1



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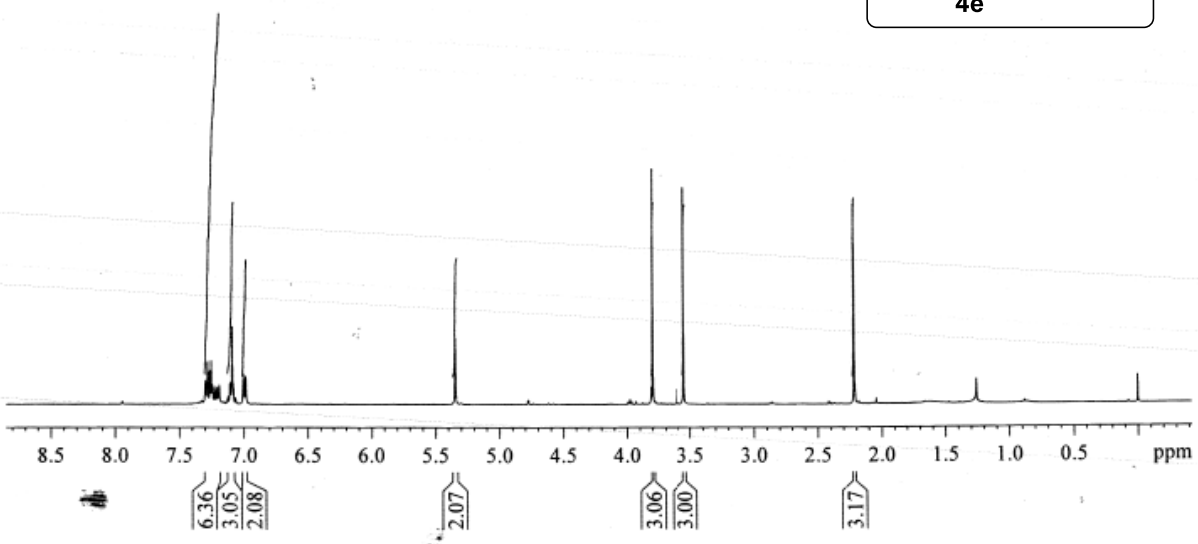


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PROCNO                      1

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PROBHD    5 mm DUL 13C-1
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                        144
DW                     60.800 usec
DE                      6.00 usec
TE                     296.0 K
D1                   1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.42 usec
PL1                    -3.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                      32768
SF             400.1300089 MHz
WDW                        EM
SSB                         0
LB                     0.30 Hz
GB                          0
PC                       1.00
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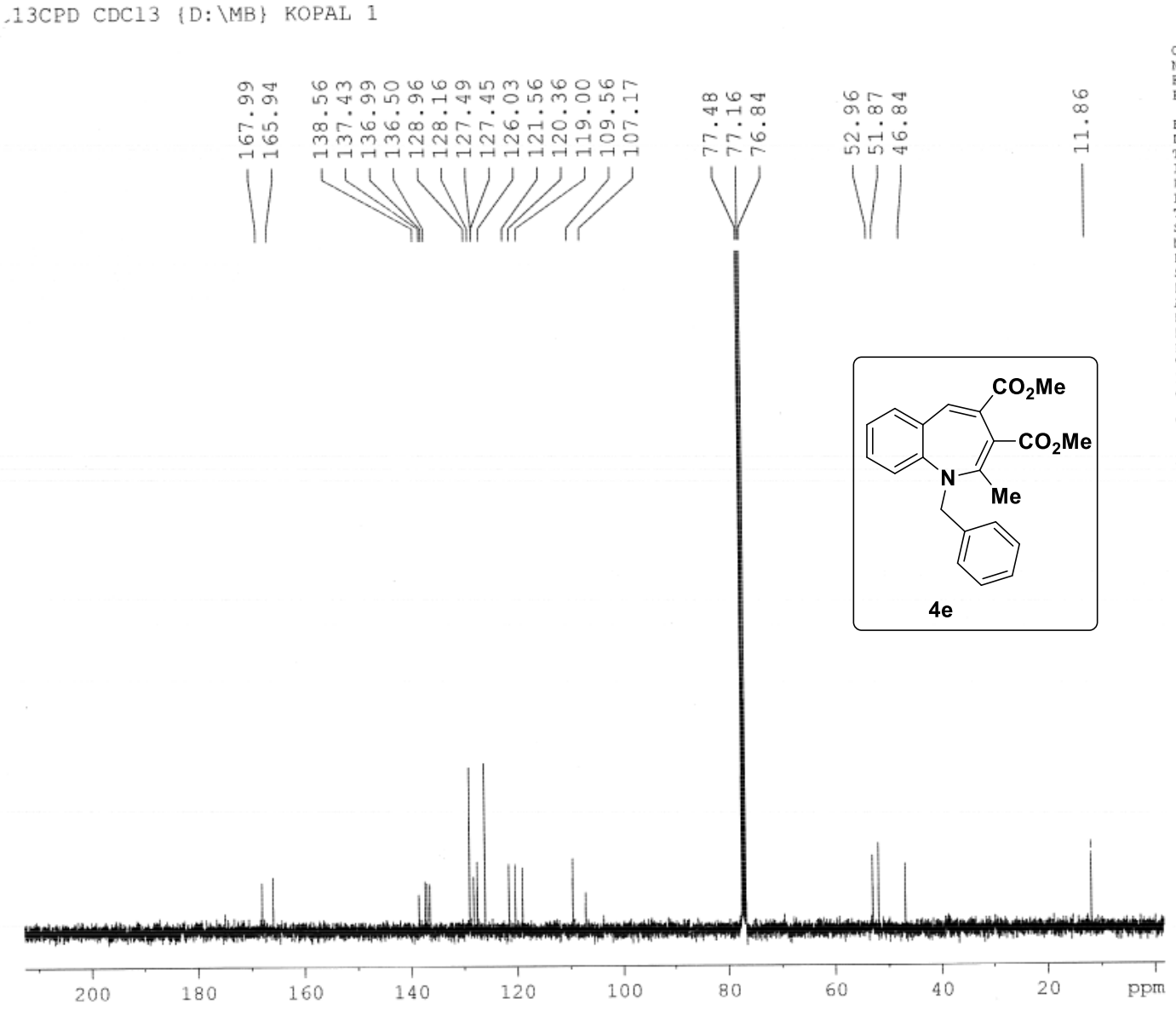


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EXPNO                       7
PROCNO                      1

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Time                    10.46
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PROBHD    5 mm DUL 13C-1
PULPROG                zqpg30
TD                      65536
SOLVENT                 CDC13
NS                        256
DS                          4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                        114
DW                   20.800 usec
DE                    6.00 usec
TE                    296.1 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                     9.15 usec
PL1                    0.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 90.00 usec
PL12                  14.90 dB
PL13                  14.90 dB
PL2                   -3.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127552 MHz
WDW                          EM
SSB                          0
LB                    1.00 Hz
GB                           0
PC                        1.40
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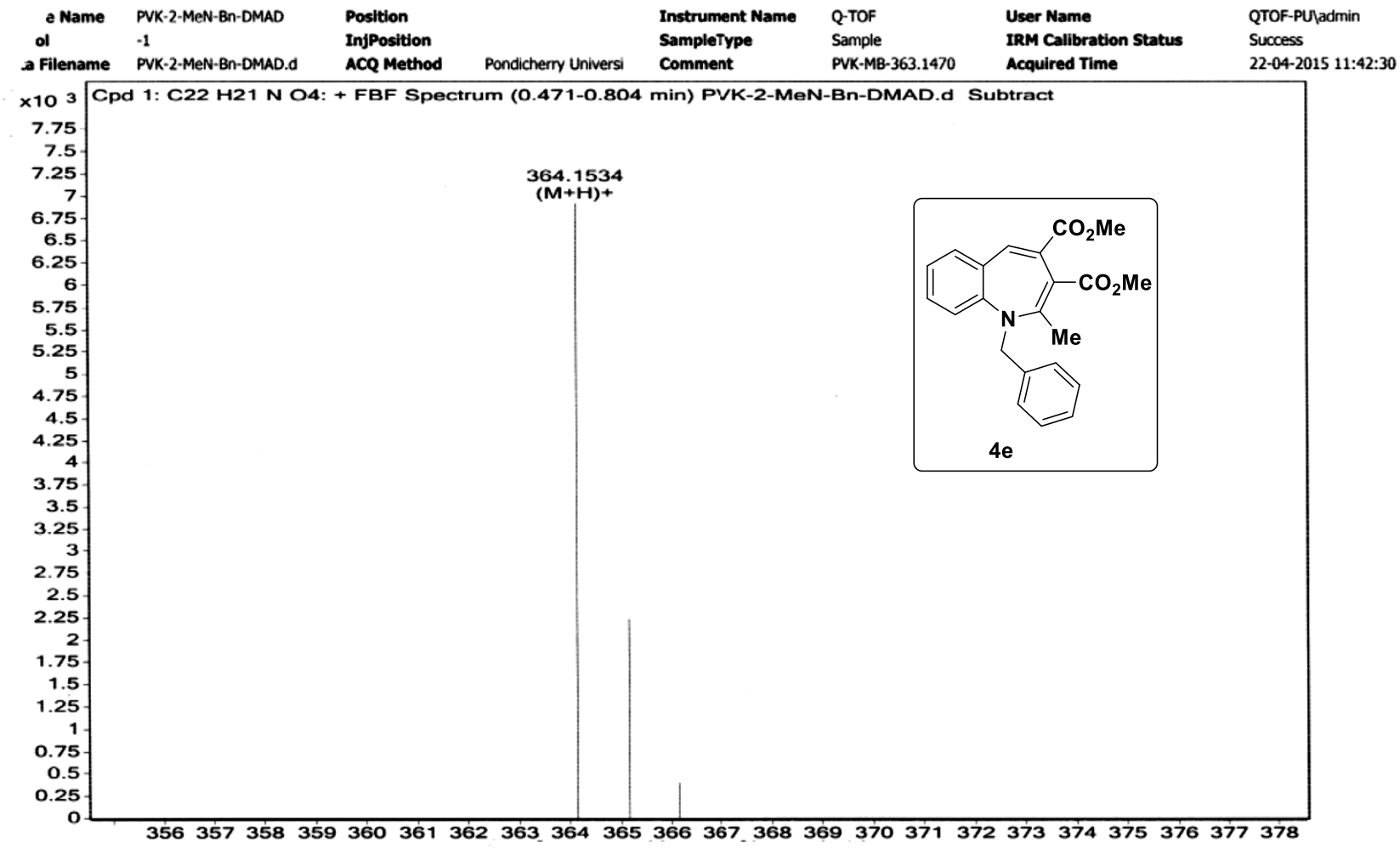
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Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
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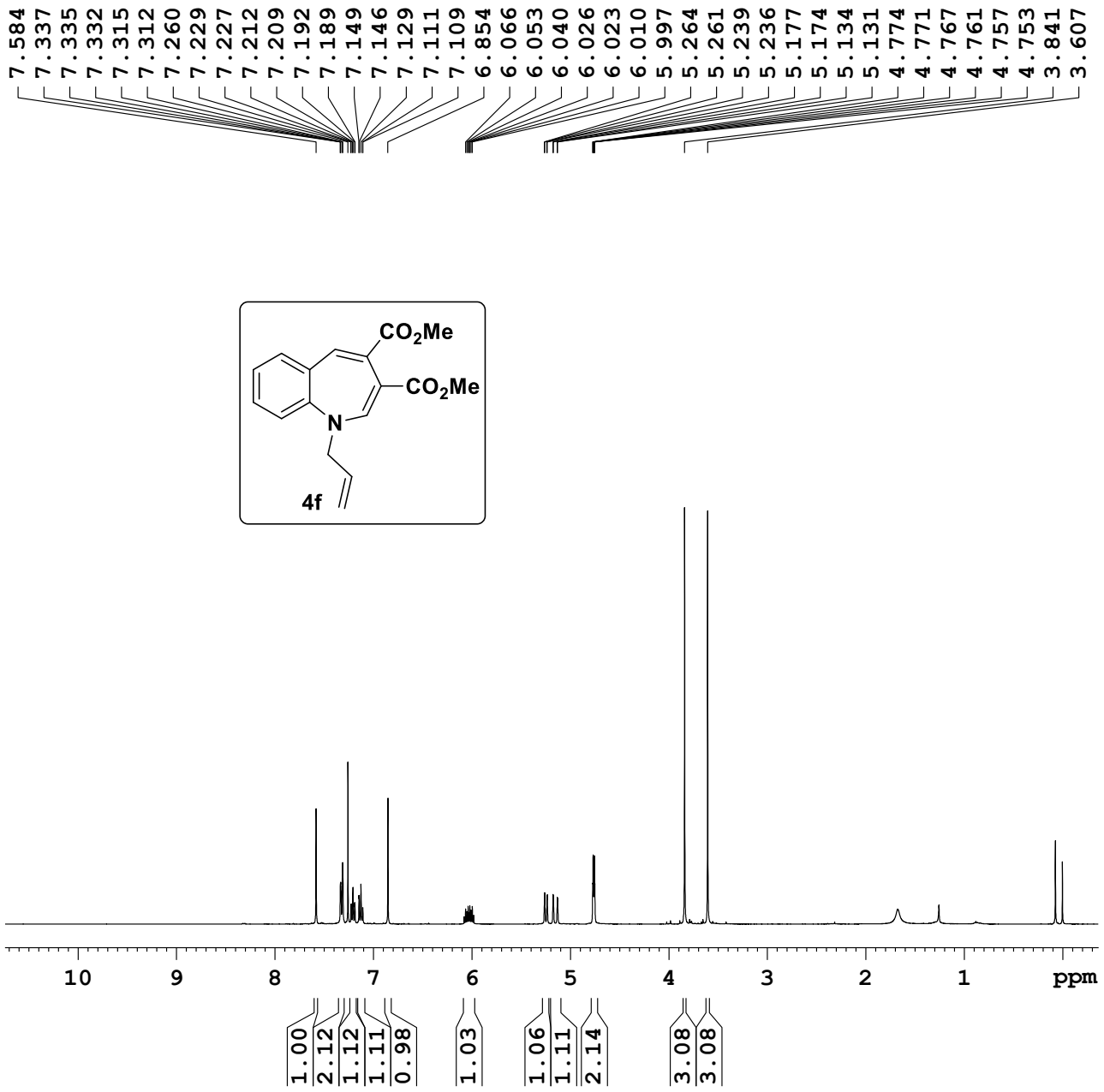
InjPosition
SampleType Sample
IRM Calibration Status Success
a Filename PVK-2-MeN-Bn-DMAD.d
ACQ Method Pondicherry Universi
Comment PVK-MB-363.1470
Acquired Time 22-04-2015 11:42:30
Cpd 1: C22 H21 N O4: + FBF Spectrum (0.471-0.804 min) PVK-2-MeN-Bn-DMAD.d Subtract
x10 3
364.1534
(M+H)+
CO2Me
CO2Me
N
Me
4e

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Current Data Parameters
NAME      TTR-PVK-ALY-IND
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180831
Time                18.23
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                    287
DW                 60.800 usec
DE                  6.00 usec
TE                 295.2 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.35 usec
PL1                 -1.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF           400.1300046 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
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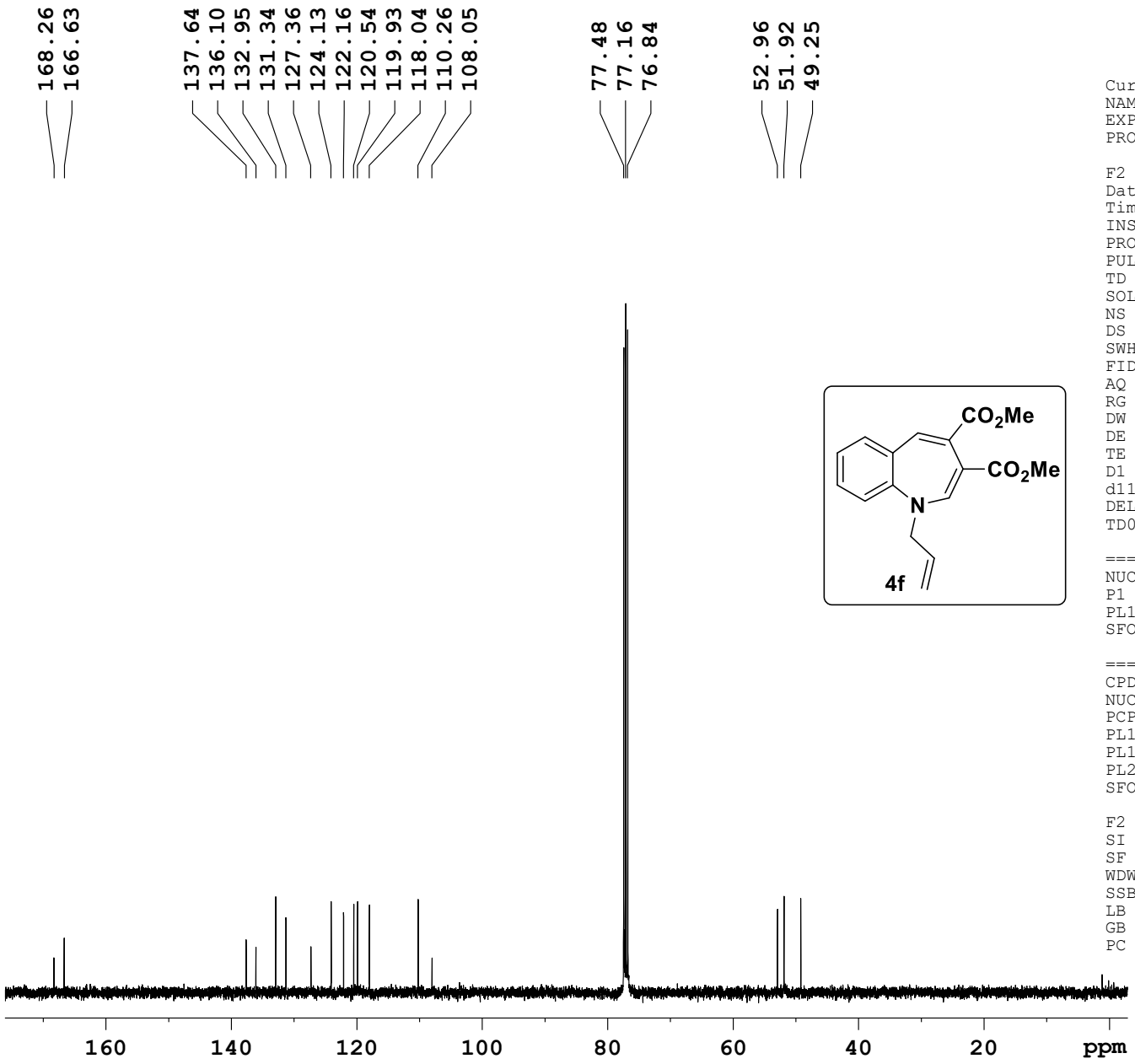


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Current Data Parameters
NAME      TTR-PVK-ALY-IND
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
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Time                23.08
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   534
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                   322
DW                20.800 usec
DE                 6.00 usec
TE                292.3 K
D1            1.00000000 sec
d11           0.03000000 sec
DELTA         0.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.95 usec
PL1                 -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127560 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
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PC                  1.40
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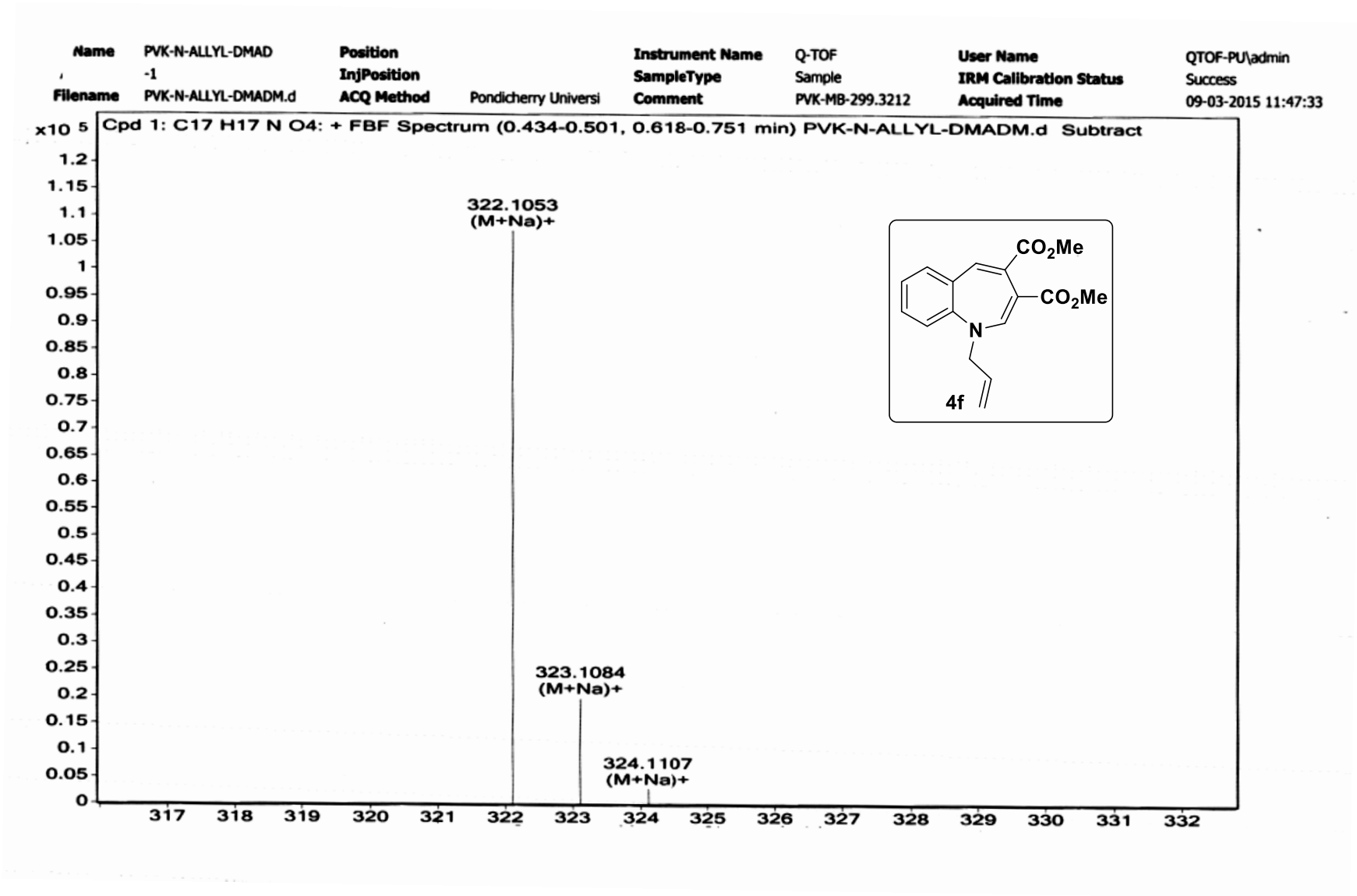
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Position
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User Name QTOF-PU\admin
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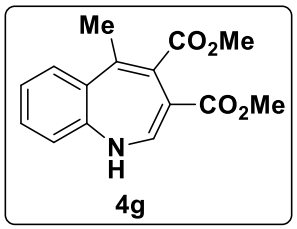
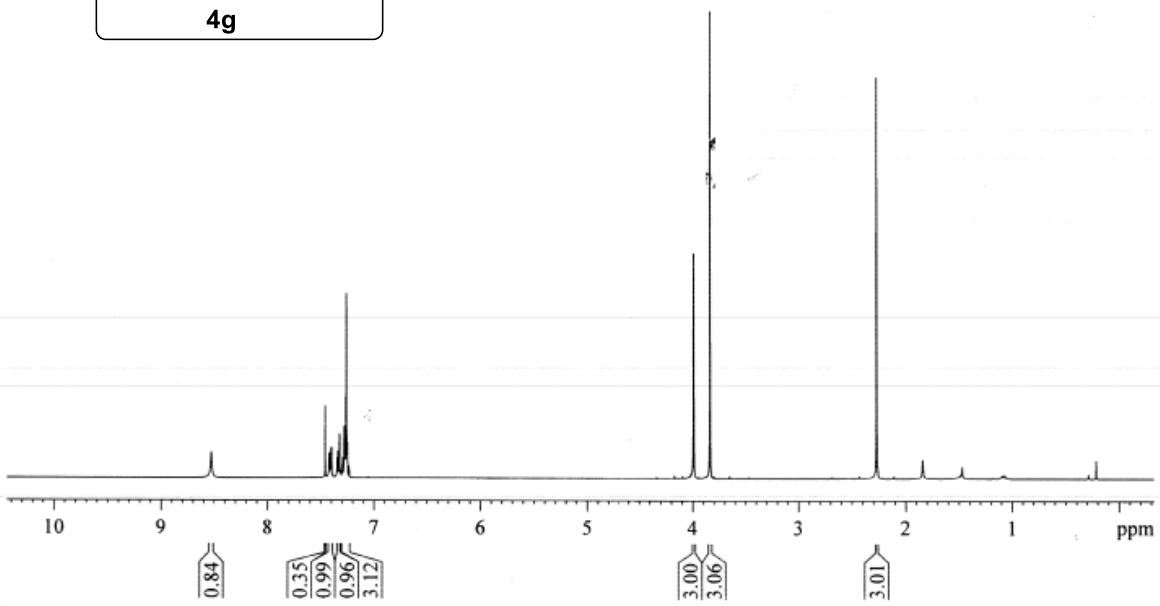
InjPosition
SampleType Sample
IRM Calibration Status Success
Filename PVK-N-ALLYL-DMADM.d
ACQ Method Pondicherry Universi
Comment PVK-MB-299.3212
Acquired Time 09-03-2015 11:47:33
Cpd 1: C17 H17 N O4: + FBF Spectrum (0.434-0.501, 0.618-0.751 min) PVK-N-ALLYL-DMADM.d Subtract
x10 5
322.1053
(M+Na)+
323.1084
(M+Na)+
324.1107
(M+Na)+
CO2Me
CO2Me
N
4f

PROTON CDCl3 {D:\MB} KOPAL 1



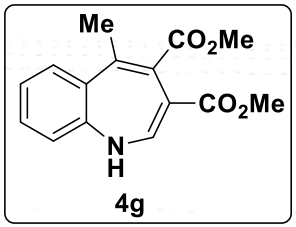
4g



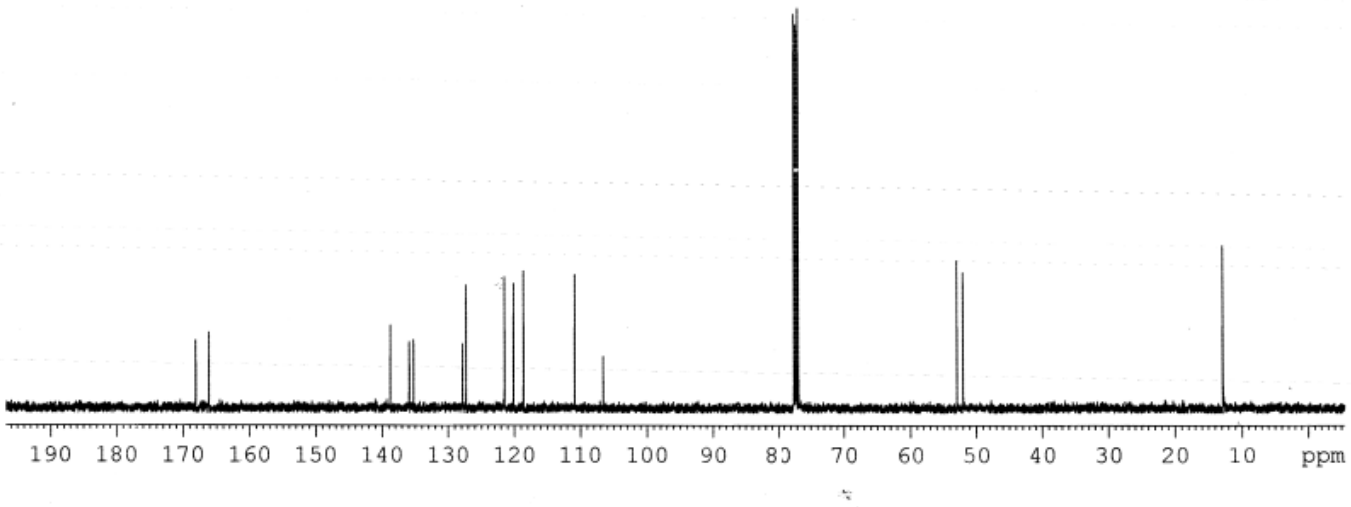

```
Current Data Parameters
NAME                  PVK-427
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140909
Time                  12.45
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      101
DW                 60.800 usec
DE                  6.00 usec
TE                  293.9 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    1H
P1                  11.42 usec
PL1                 -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF            400.1299260 MHz
WDW                     EM
SSB                      0
LB                  0.30 Hz
GB                       0
PC                    1.00
```

C13CPD CDCl3 {D:\MB} KOPAL 1

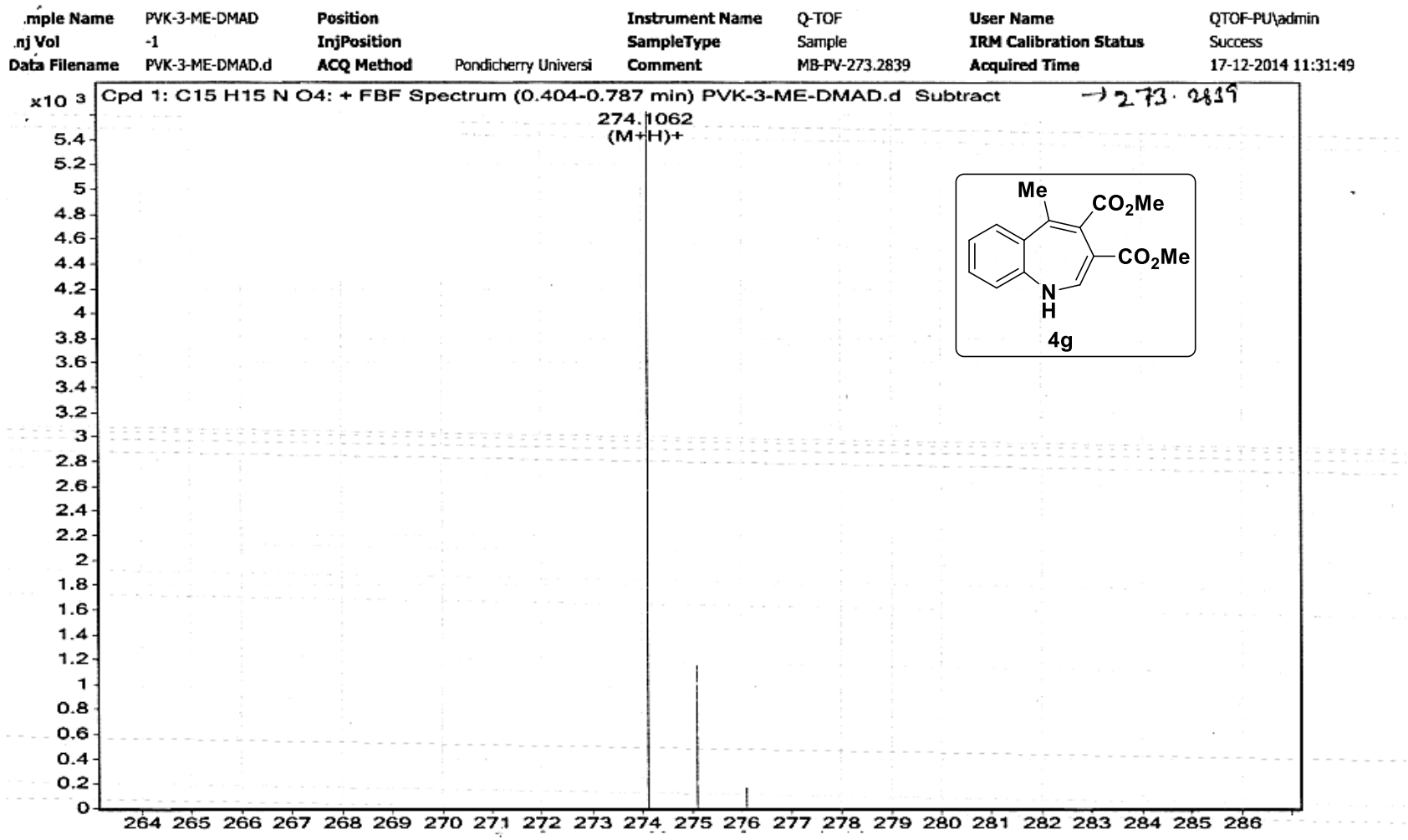
168.06
166.07
138.74
135.91
135.25
127.84
127.29
121.47
120.13
118.62
110.87
106.60
77.48
77.16
76.84
52.94
51.99
12.82

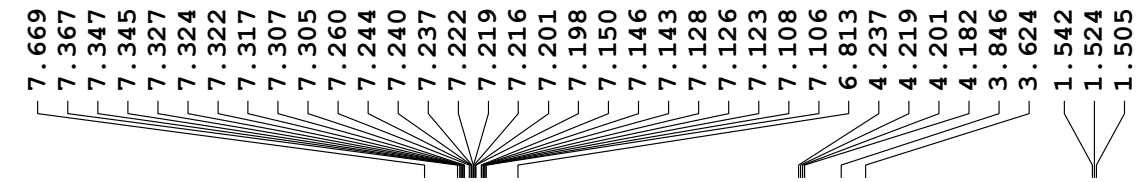


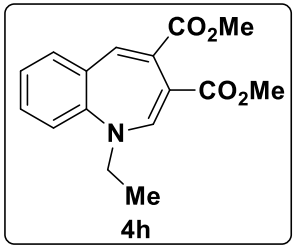
4g



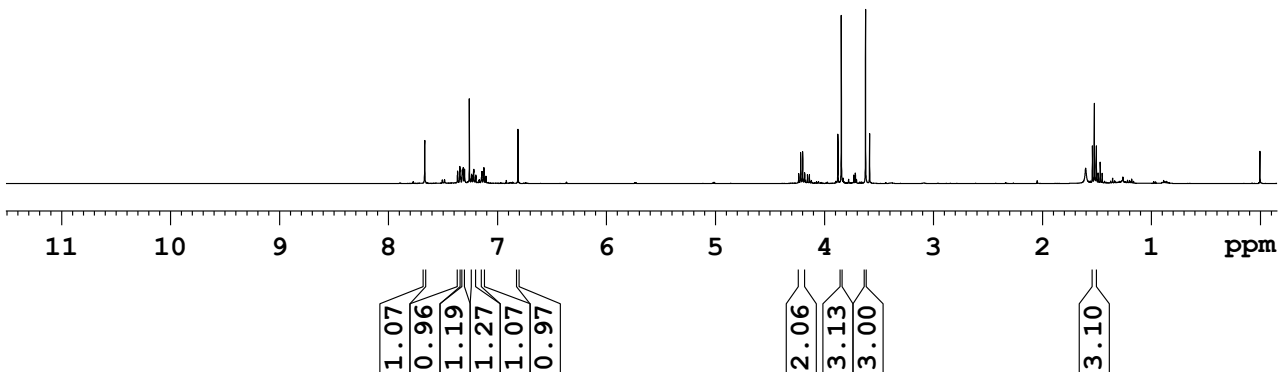

```
Current Data Parameters
NAME                  PVK-427
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140909
Time                   12.48
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                         73
DS                          4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                         57
DW                    20.800 usec
DE                     6.00 usec
TE                    294.6 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.15 usec
PL1                      0.00 dB
SFO1              100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL12                    14.90 dB
PL13                    14.90 dB
PL2                     -3.00 dB
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                100.6127594 MHz
WDW                          EM
SSB                           0
LB                       1.00 Hz
GB                            0
PC                        1.40
```

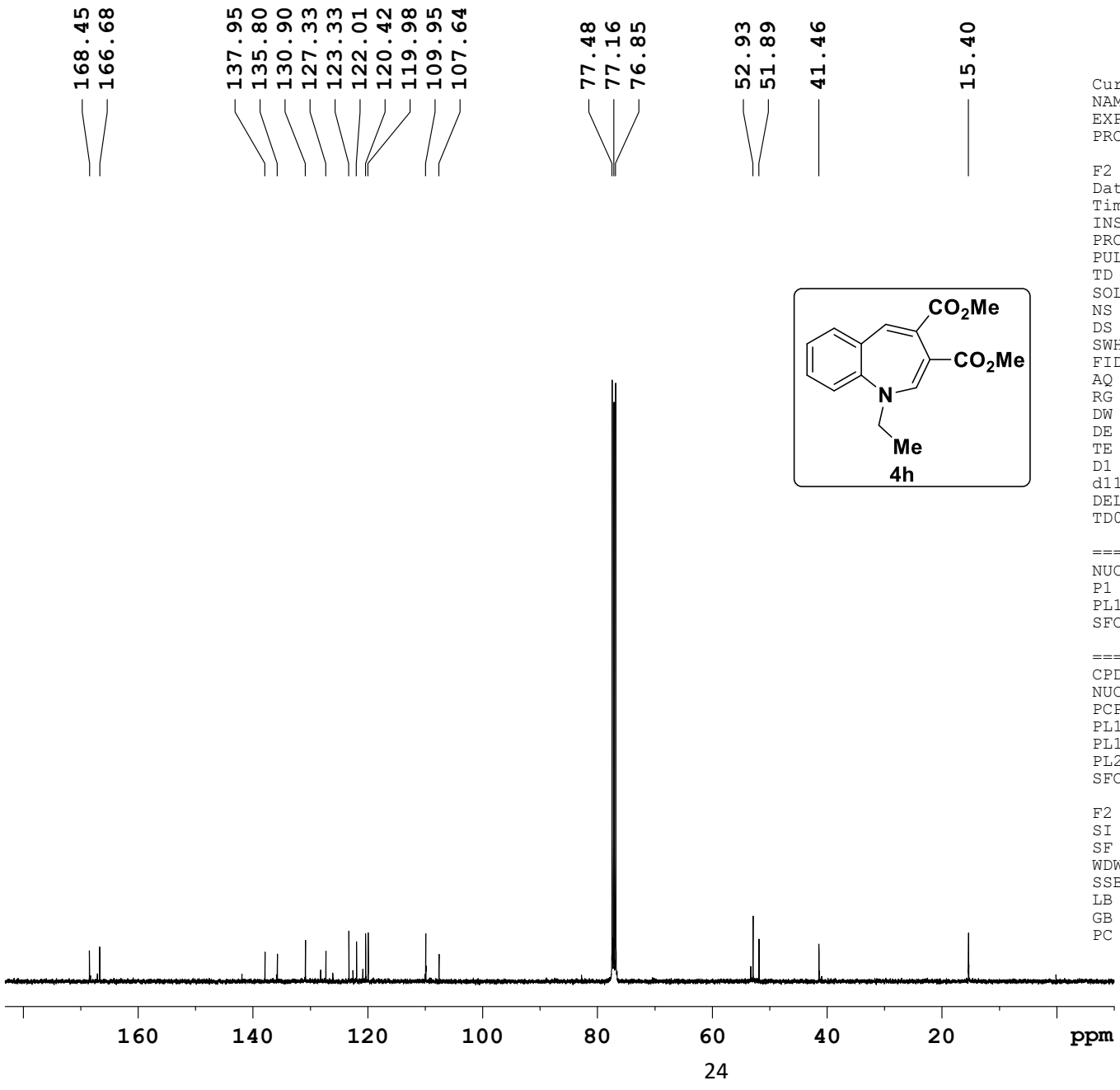

.mple Name PVK-3-ME-DMAD
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
.nj Vol -1
InjPosition
SampleType Sample
IRM Calibration Status Success
Data Filename PVK-3-ME-DMAD.d
ACQ Method Pondicherry Universi
Comment MB-PV-273.2839
Acquired Time 17-12-2014 11:31:49
Cpd 1: C15 H15 N O4: + FBF Spectrum (0.404-0.787 min) PVK-3-ME-DMAD.d Subtract
→ 273.2839
x10 3
274.1062
(M+H)+
Me
CO2Me
CO2Me
N
H
4g
5.4
5.2
5
4.8
4.6
4.4
4.2
4
3.8
3.6
3.4
3.2
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286



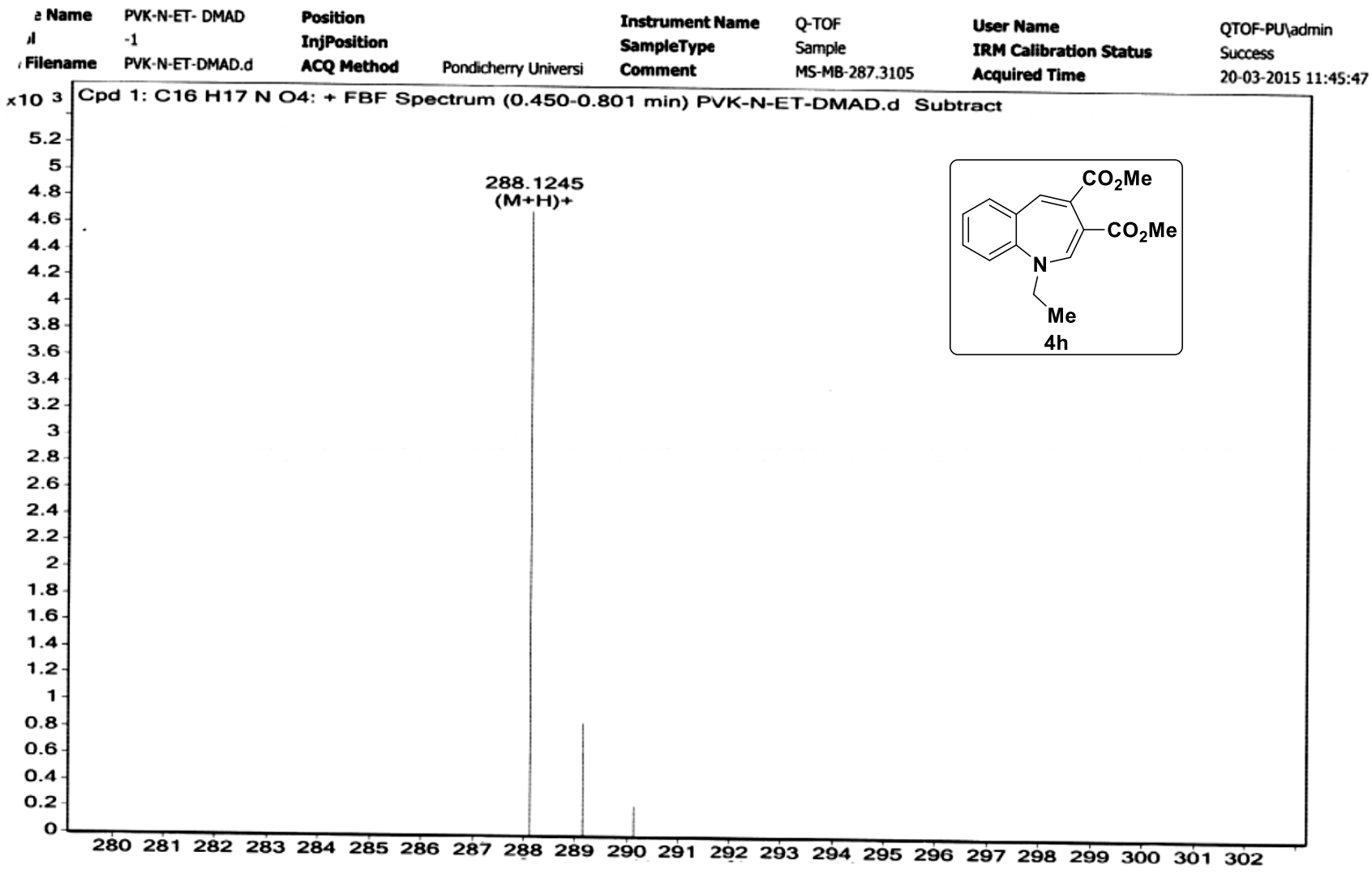


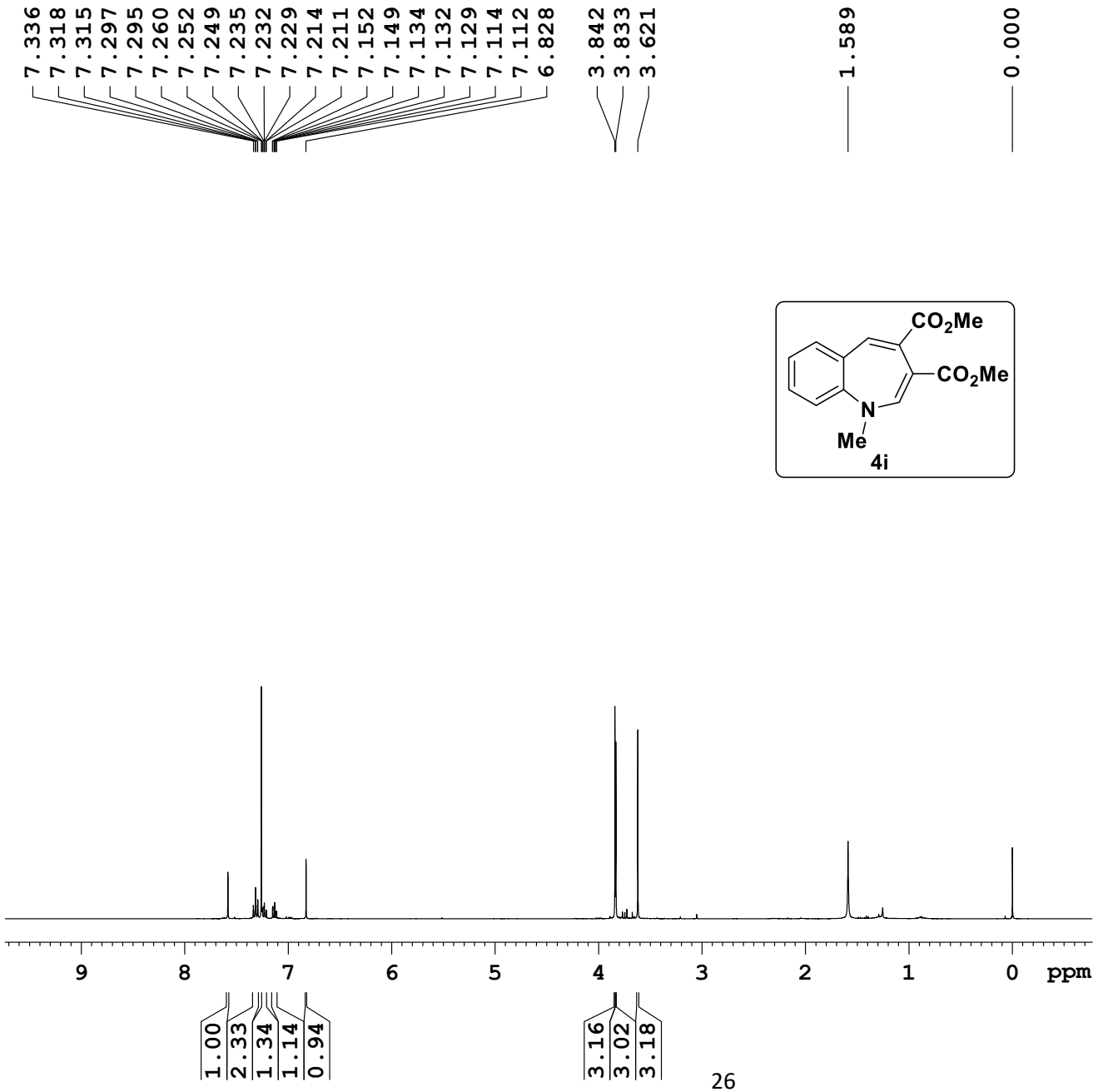

```
Current Data Parameters
NAME      PVK-N-ET-DMAD-IND
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_           20180902
Time              13.07
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8223.685 Hz
FIDRES         0.125483 Hz
AQ            3.9846387 sec
RG                  228
DW               60.800 usec
DE                6.00 usec
TE               294.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.35 usec
PL1               -1.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF          400.1300049 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



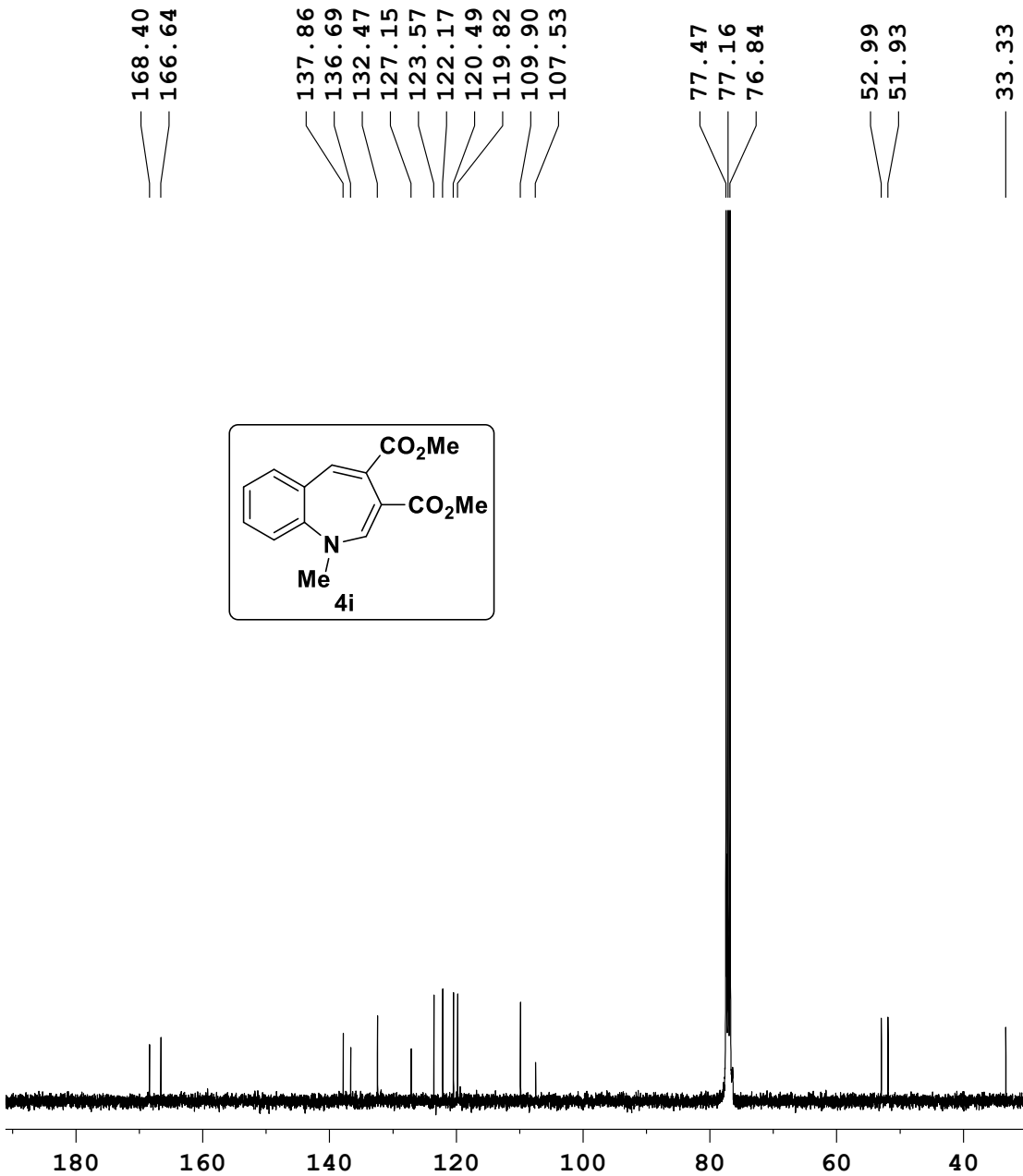



```
Current Data Parameters
NAME      PVK-N-ET-DMAD-IND
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180902
Time                14.53
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1657
DS                      4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                    322
DW                20.800 usec
DE                 6.00 usec
TE                294.5 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.95 usec
PL1               -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL12              14.95 dB
PL13             120.00 dB
PL2               -1.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127560 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

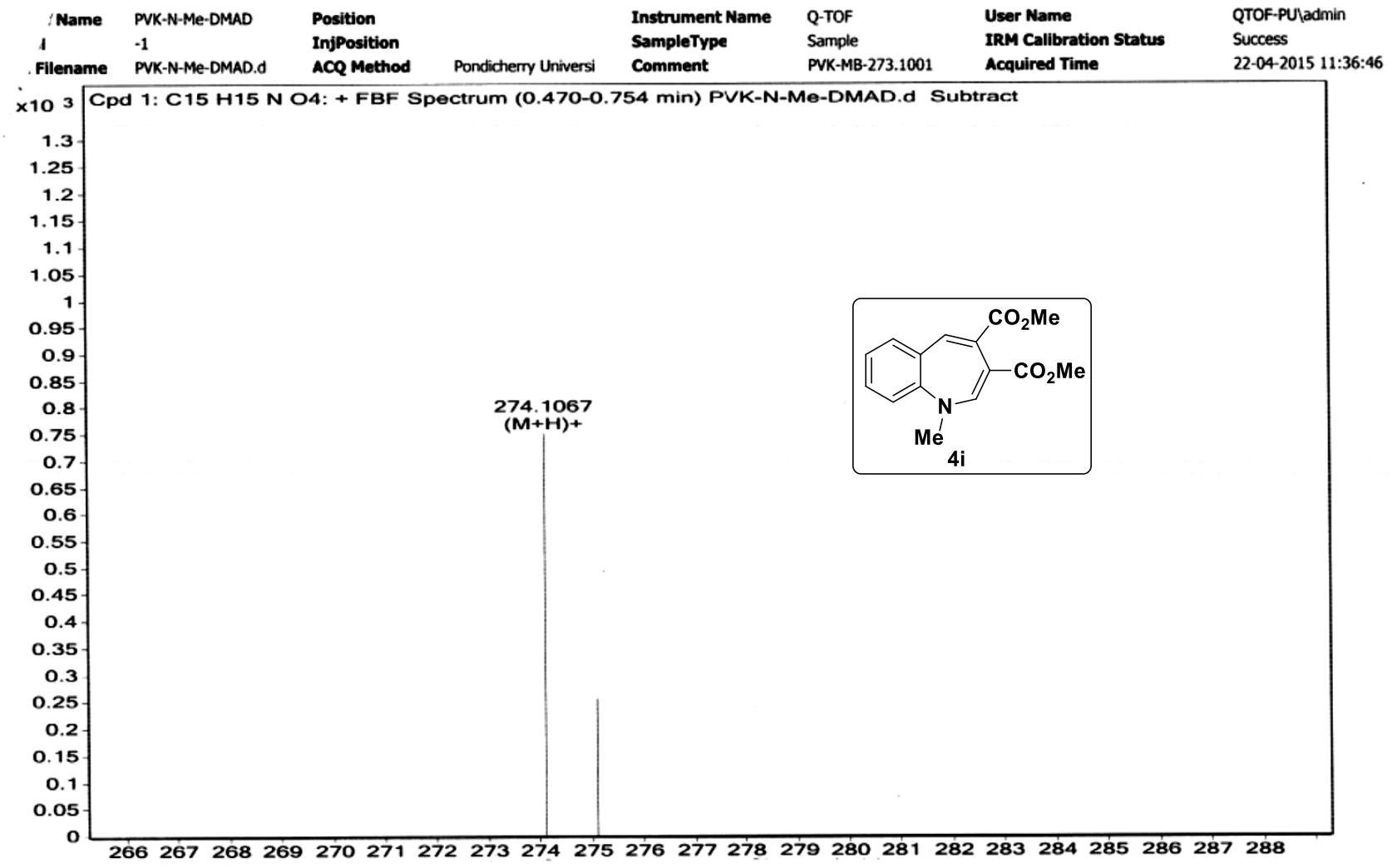

e Name PVK-N-ET- DMAD
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
-1
InjPosition
SampleType Sample
IRM Calibration Status Success
Filename PVK-N-ET-DMAD.d
ACQ Method Pondicherry Universi
Comment MS-MB-287.3105
Acquired Time 20-03-2015 11:45:47
Cpd 1: C16 H17 N O4: + FBF Spectrum (0.450-0.801 min) PVK-N-ET-DMAD.d Subtract
x10 3
288.1245
(M+H)+
CO2Me
CO2Me
N
Me
4h



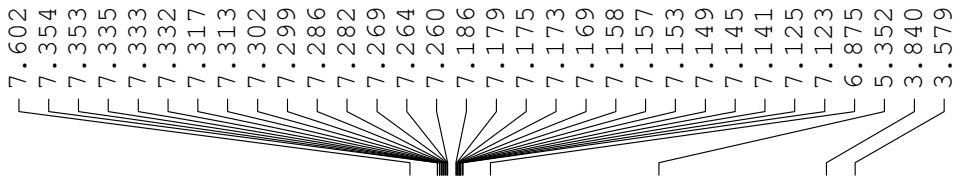

```
Current Data Parameters
NAME      PVK-N-ME-IND-DMAD
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180831
Time               18.36
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                   362
DW                60.800 usec
DE                 6.00 usec
TE                294.9 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                14.35 usec
PL1               -1.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300049 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00
```

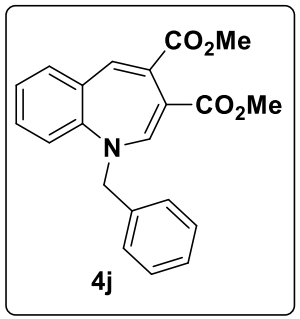


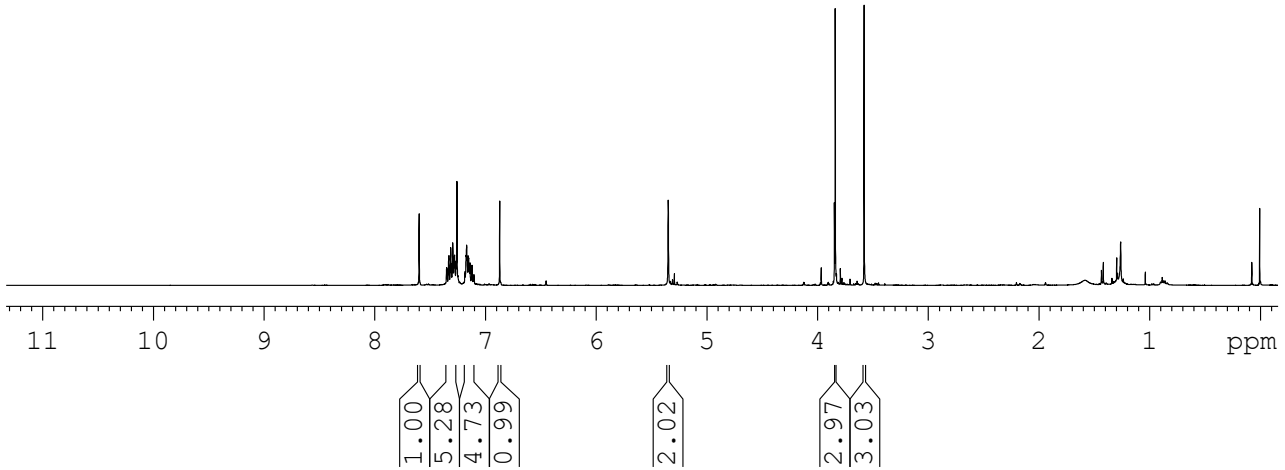

```
Current Data Parameters
NAME      PVK-N-ME-IND-DMAD
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180831
Time                 18.41
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    4262
DS                       4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631988 sec
RG                     362
DW                20.800 usec
DE                 6.00 usec
TE                 294.9 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.95 usec
PL1                  -1.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL12                14.95 dB
PL13               120.00 dB
PL2                 -1.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127554 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```


Name PVK-N-Me-DMAD
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
-1
InjPosition
SampleType Sample
IRM Calibration Status Success
Filename PVK-N-Me-DMAD.d
ACQ Method Pondicherry Universi
Comment PVK-MB-273.1001
Acquired Time 22-04-2015 11:36:46
Cpd 1: C15 H15 N O4: + FBF Spectrum (0.470-0.754 min) PVK-N-Me-DMAD.d Subtract
x10 3
274.1067
(M+H)+
CO2Me
CO2Me
N
Me
4i

PROTON CDCl3 {D:\MB} KOPAL 1







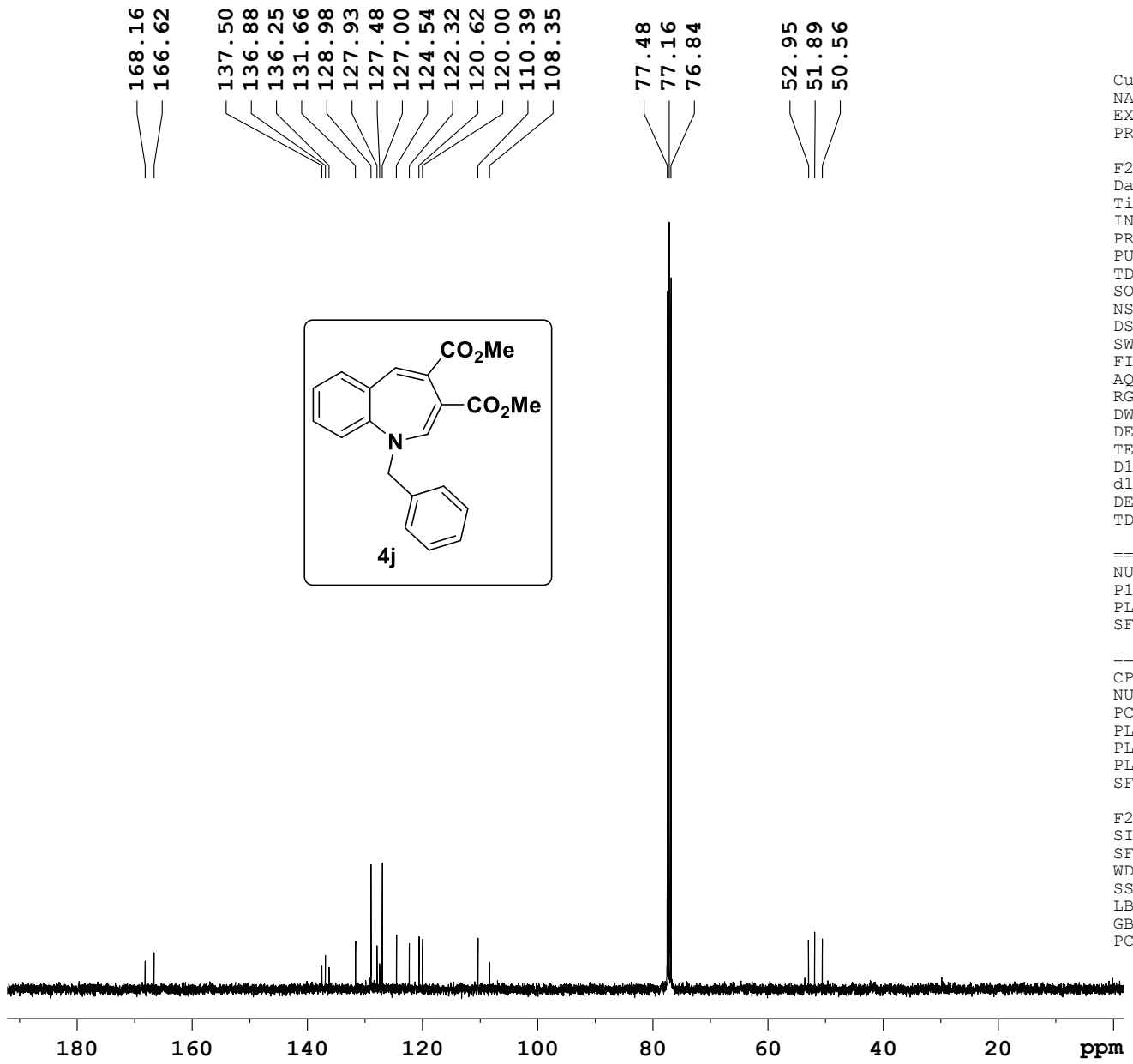
0.006

Current Data Parameters
NAME PVK-N-BN-DEAD
EXPNO 1
PROCNO 1

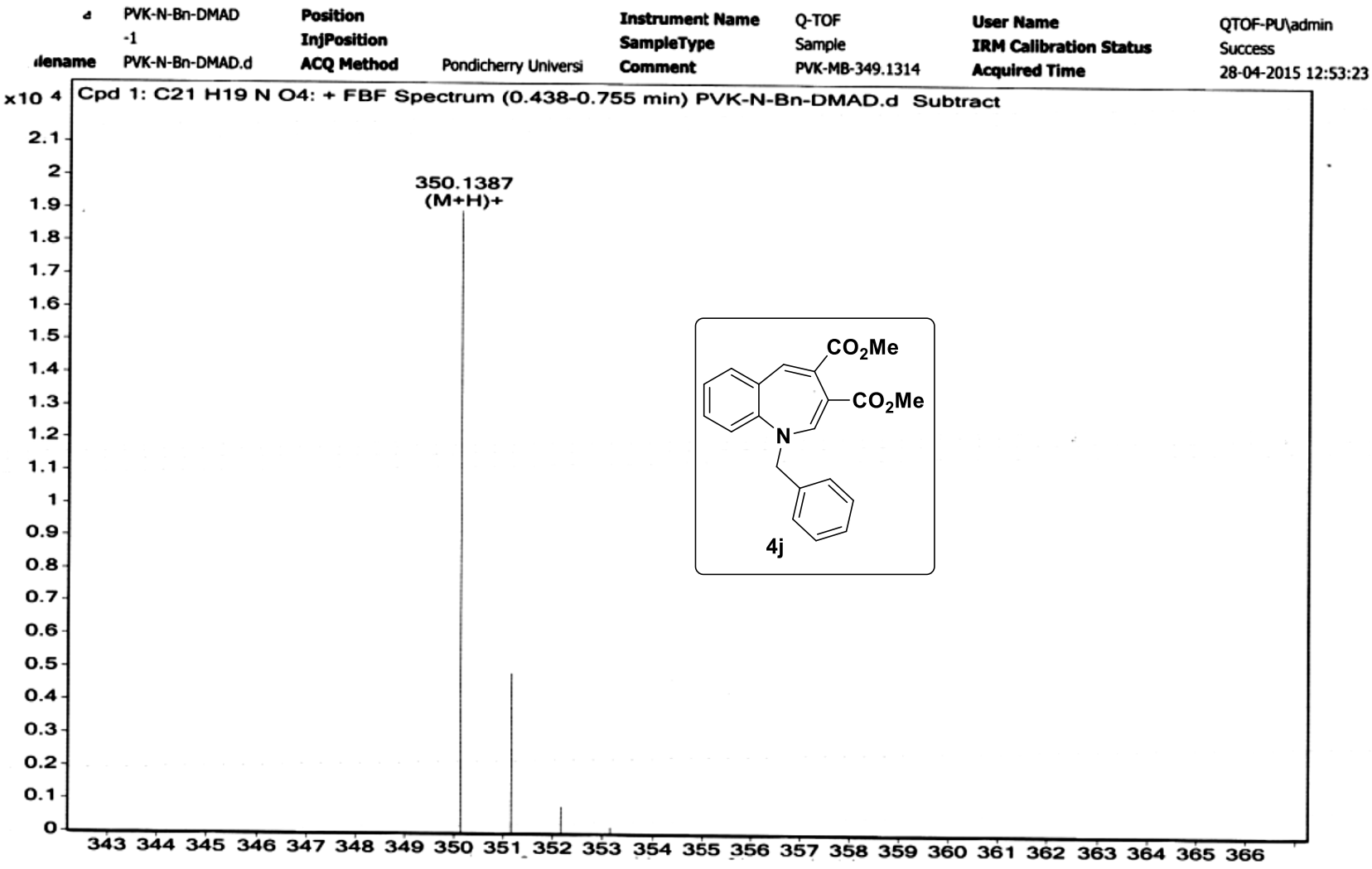
F2 - Acquisition Parameters
Date_ 20150312
Time 16.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

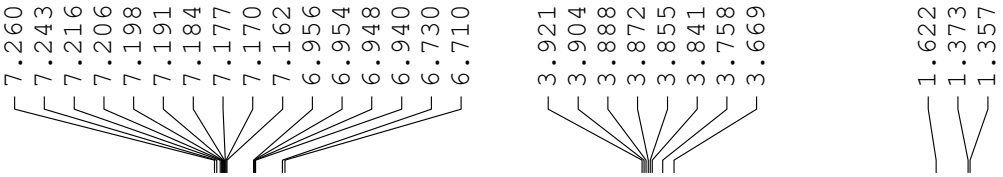
F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

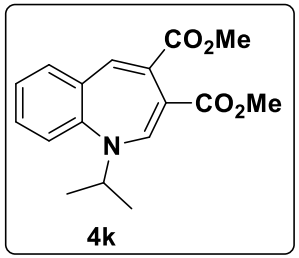



```
Current Data Parameters
NAME       PVK-N-BN-DEAD
EXPNO                  3
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150313
Time               10.13
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                    32
DW                20.800 usec
DE                 6.00 usec
TE                294.7 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.15 usec
PL1                  0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127554 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

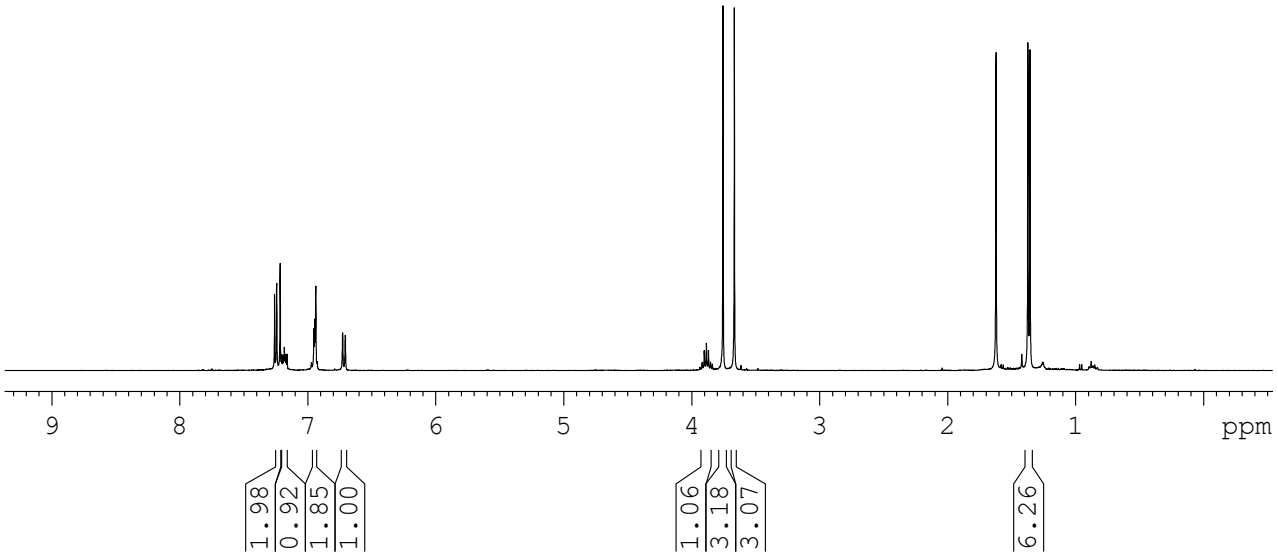

d PVK-N-Bn-DMAD
-1
lename PVK-N-Bn-DMAD.d
Position
InjPosition
ACQ Method
Pondicherry Universi
Instrument Name Q-TOF
SampleType Sample
Comment PVK-MB-349.1314
User Name QTOF-PU\admin
IRM Calibration Status Success
Acquired Time 28-04-2015 12:53:23
Cpd 1: C21 H19 N O4: + FBF Spectrum (0.438-0.755 min) PVK-N-Bn-DMAD.d Subtract
x10 4
350.1387
(M+H)+
CO2Me
CO2Me
N
4j

PROTON CDCl3 {D:\MB} KOPAL 1





4k

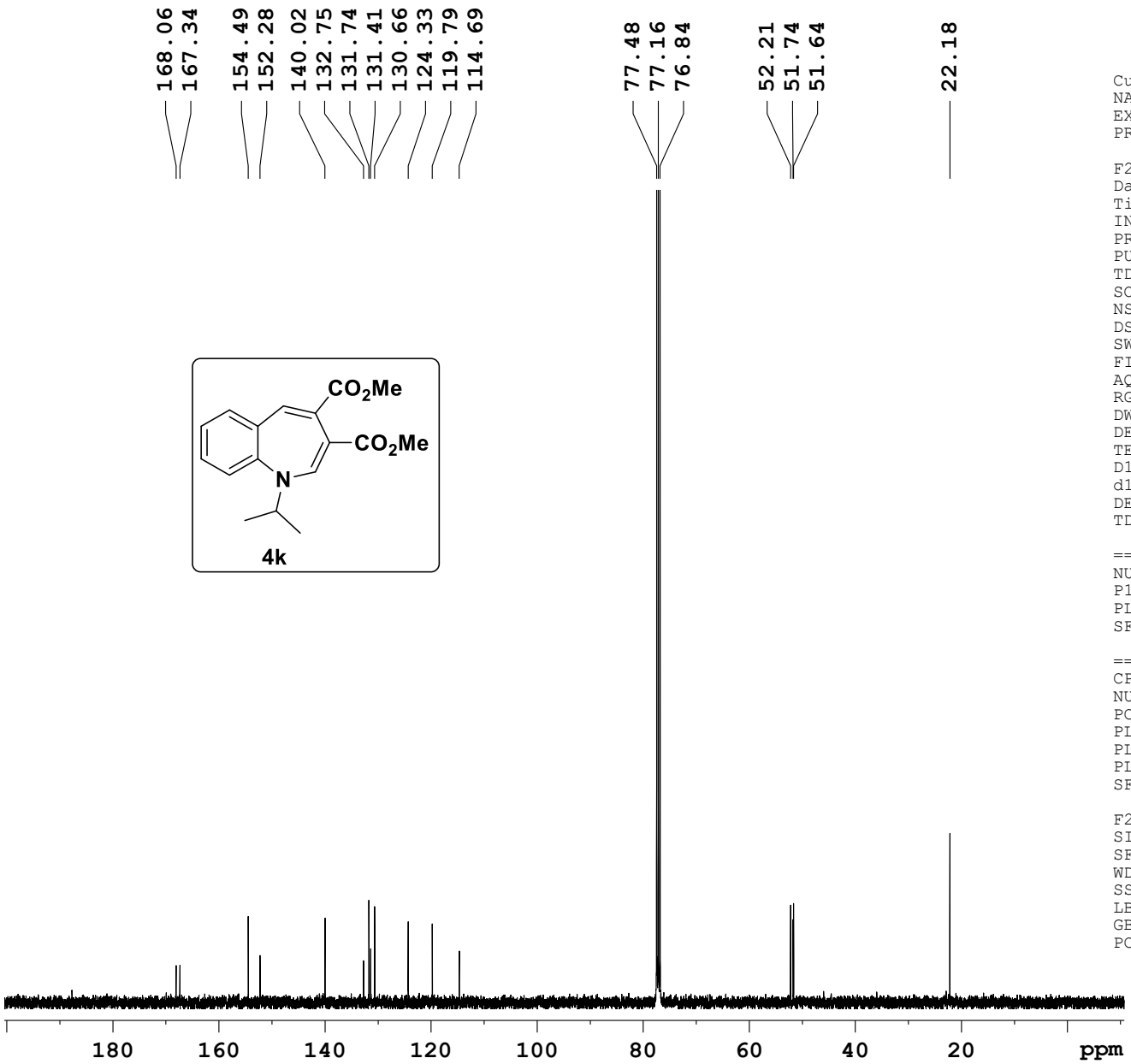


Current Data Parameters
NAME PVK-N-BU-IND-DMAD-D
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170908
Time 16.58
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

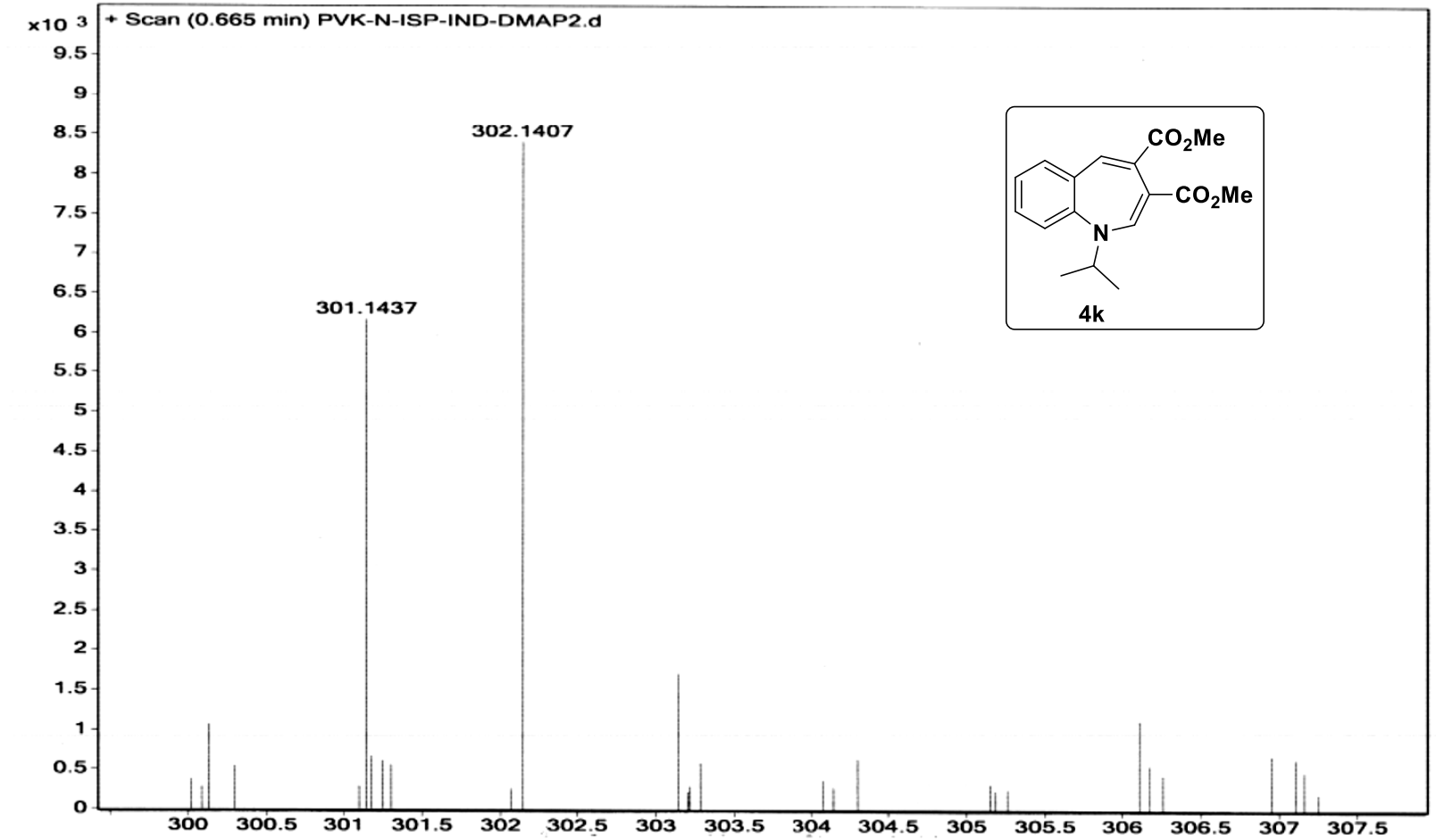
======== CHANNEL f1 ========
NUC1 1H
P1 11.42 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

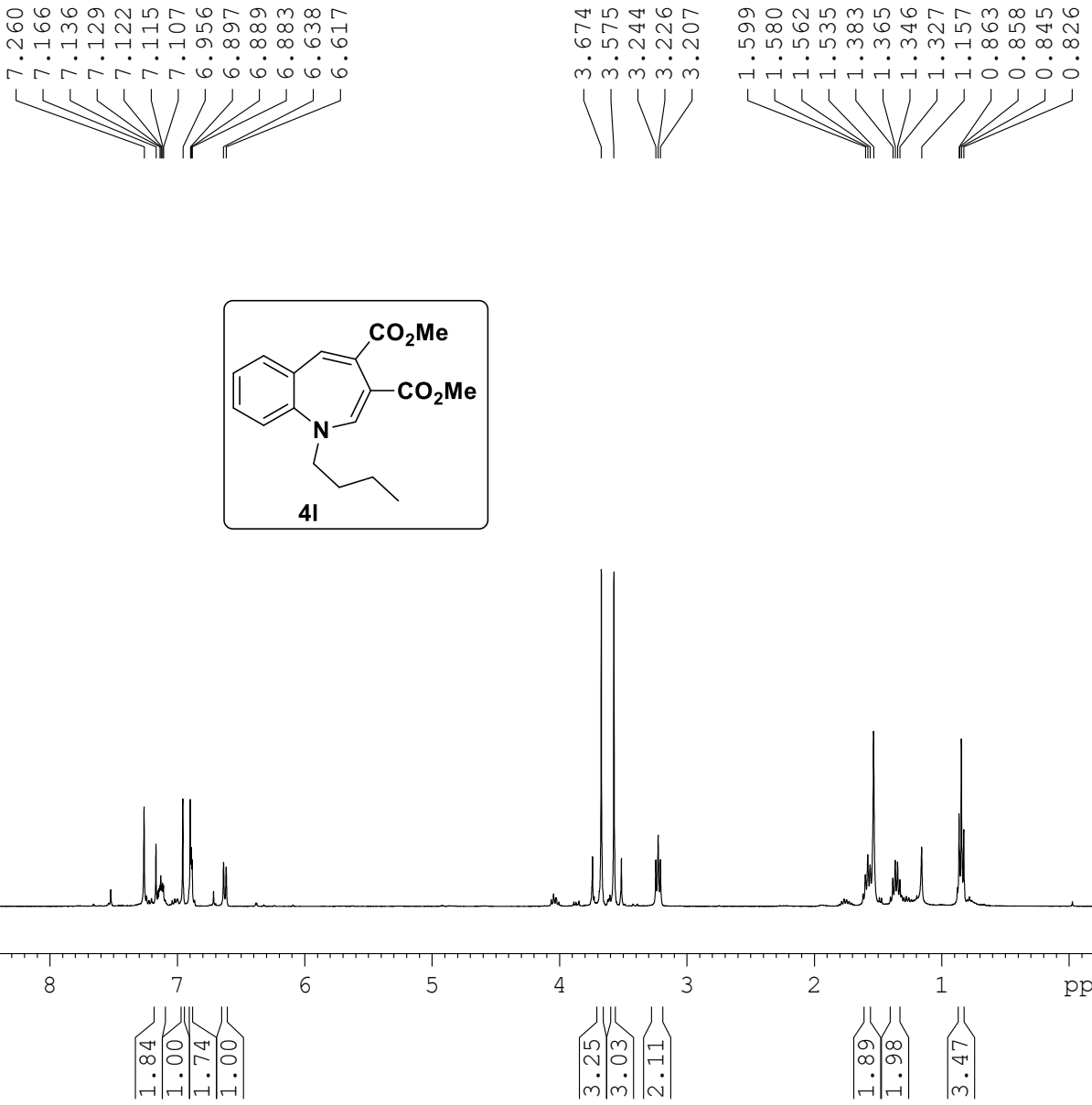



```
Current Data Parameters
NAME      PVK-N-BU-IND-DMAD-D
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20170910
Time                  22.23
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     512
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                      64
DW                  20.800 usec
DE                   6.00 usec
TE                   294.1 K
D1             1.00000000 sec
d11            0.03000000 sec
DELTA          0.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.15 usec
PL1                   0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                90.00 usec
PL12                 14.90 dB
PL13                 14.90 dB
PL2                  -3.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF           100.6127546 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

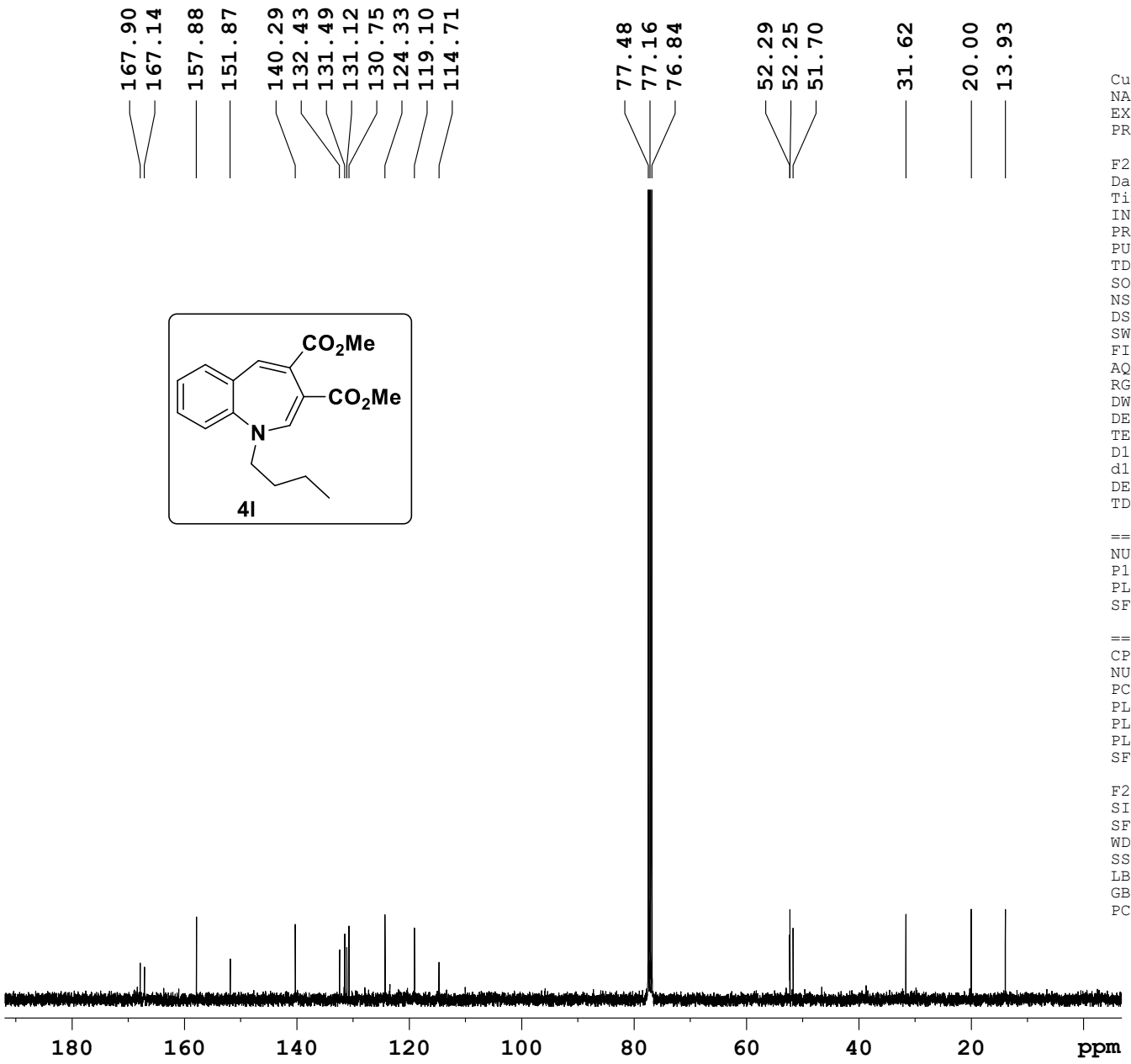
ple Name	PVK-N-ISP-IND-DMAP	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
l Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-N-ISP-IND-DMAP2.	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-302.1392	**Acquired Time**	20-10-2017 12:52:27



PROTON CDCl3 {D:\MB} KOPAL 1

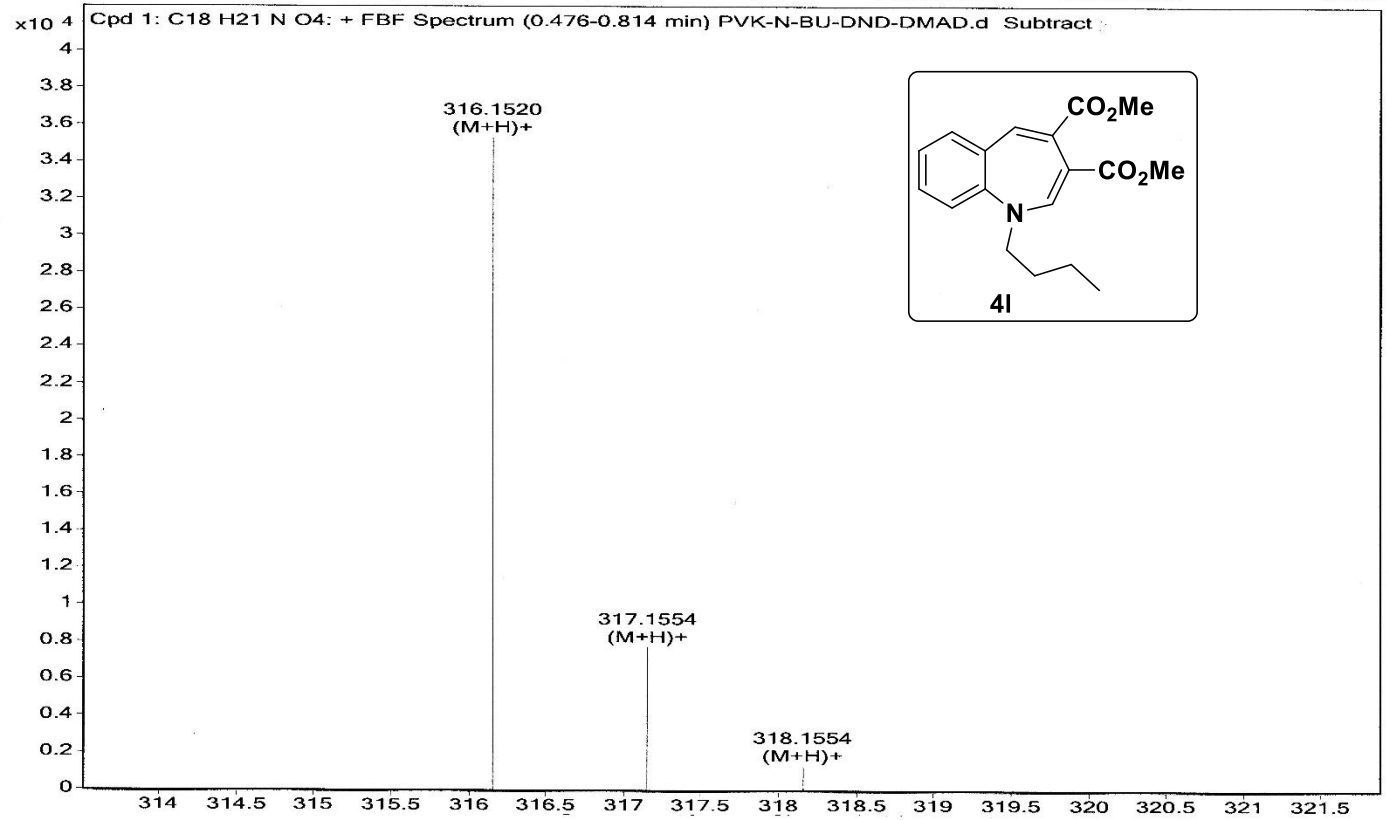


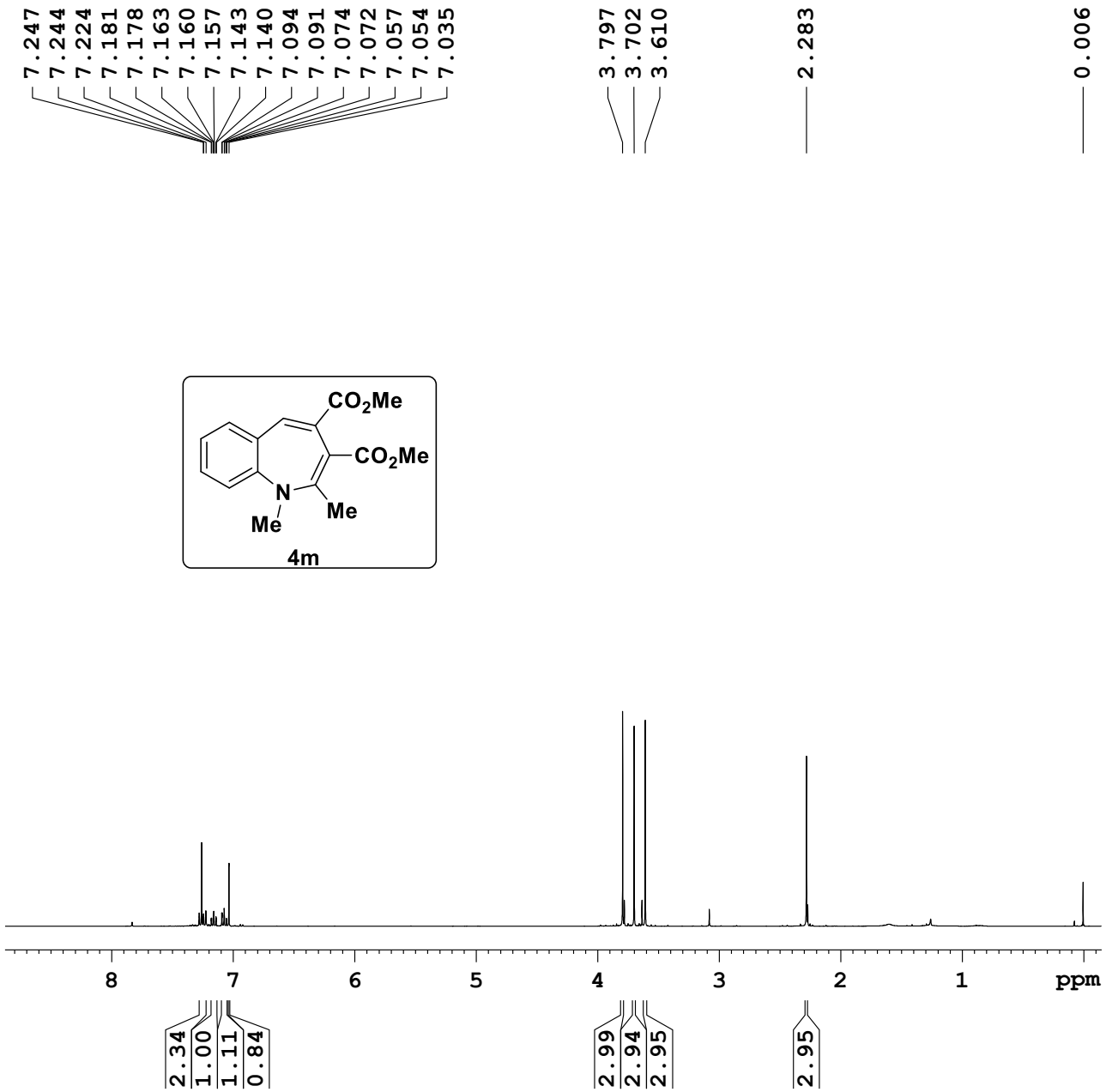

```
Current Data Parameters
NAME      PVK-N-ISP-IND-DMAD-D
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170908
Time                17.04
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ              3.9846387 sec
RG                    181
DW                 60.800 usec
DE                  6.00 usec
TE                 293.6 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.42 usec
PL1                -3.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF           400.1300425 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



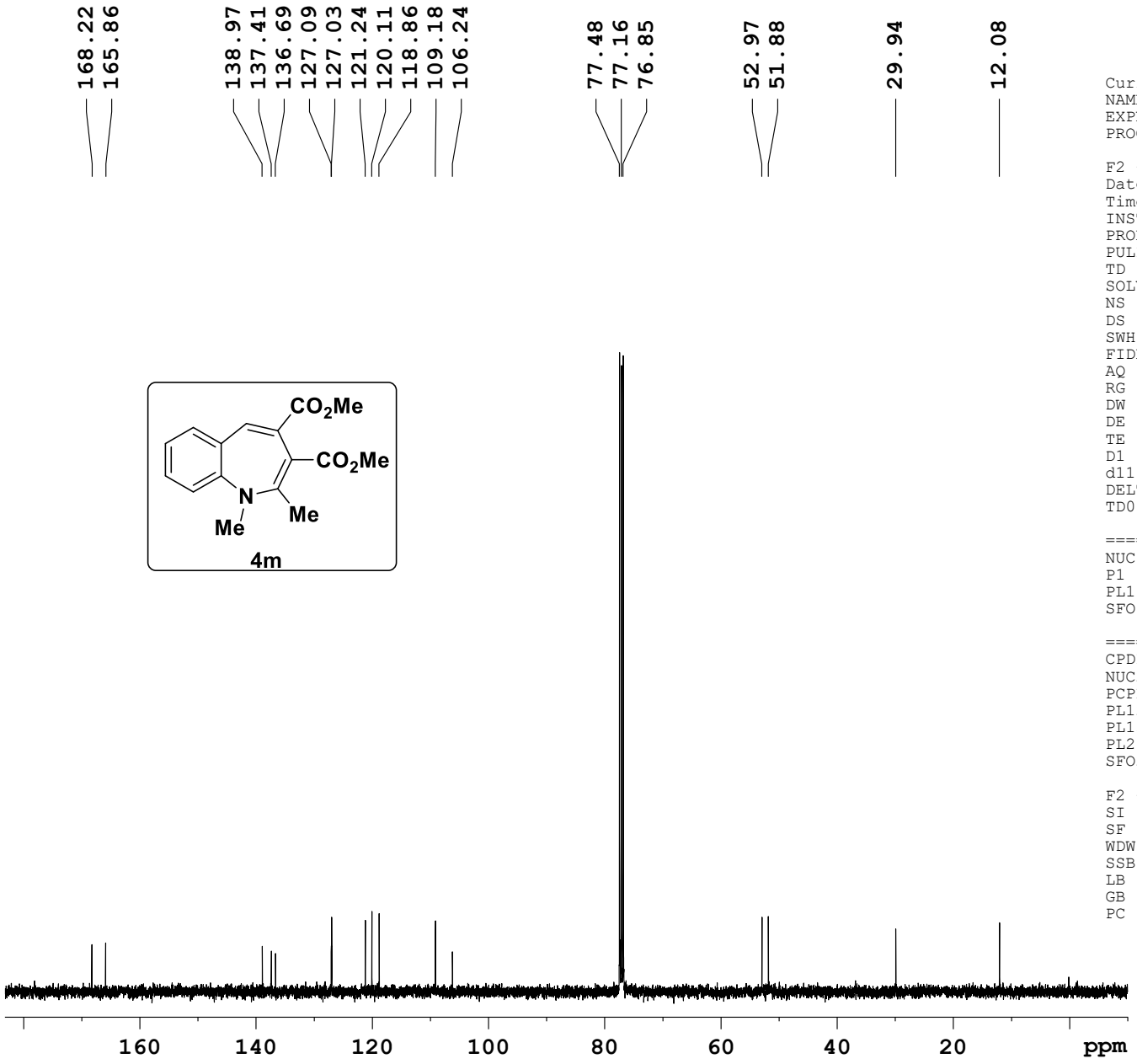

```
Current Data Parameters
NAME      PVK-N-ISP-IND-DMAD-D
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170910
Time                19.15
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                    64
DW                20.800 usec
DE                 6.00 usec
TE                292.8 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127557 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Sample Name	PVK-N-BU-DND-DMAD	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-N-BU-DND-DMAD.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-315.1471	**Acquired Time**	09-05-2018 11:43:53



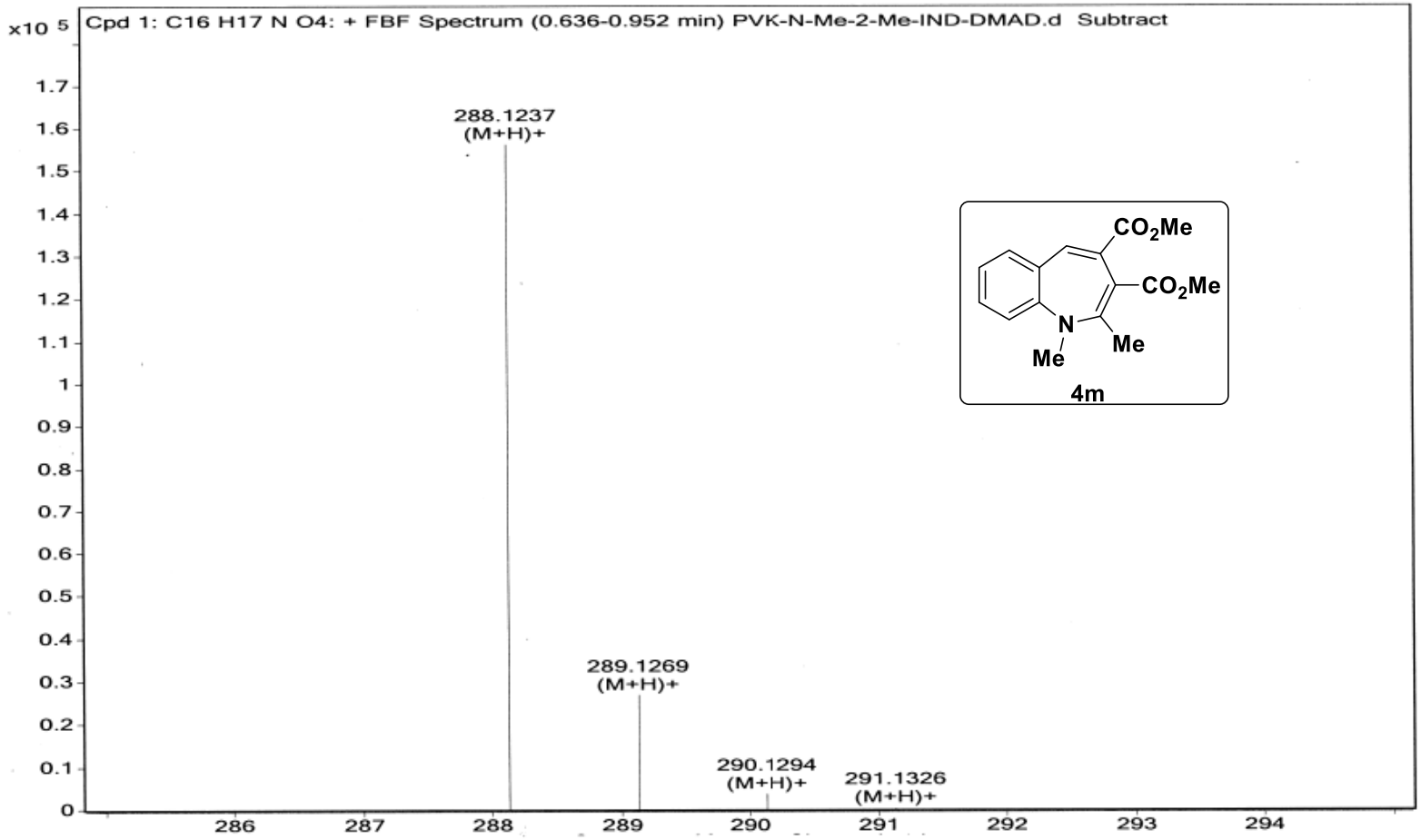



```
Current Data Parameters
NAME      PVK-ME-N-ME-IND-DMAD
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20180827
Time                  10.15
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                       256
DW                    60.800 usec
DE                     6.00 usec
TE                    291.1 K
D1              1.00000000 sec
TD0                       1

========= CHANNEL f1 =========
NUC1                     1H
P1                    14.35 usec
PL1                   -1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300049 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

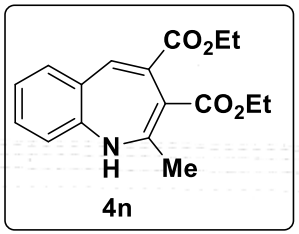



```
Current Data Parameters
NAME      PVK-ME-N-ME-IND-DMAD
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180827
Time               10.18
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                 90.5
DW                20.800 usec
DE                 6.00 usec
TE                291.4 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.95 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6127566 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Sample Name	PVK-N-Me-2-Me-IND-DM	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-N-Me-2-Me-IND-DM	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-287.1158	**Acquired Time**	31-08-2018 12:17:12

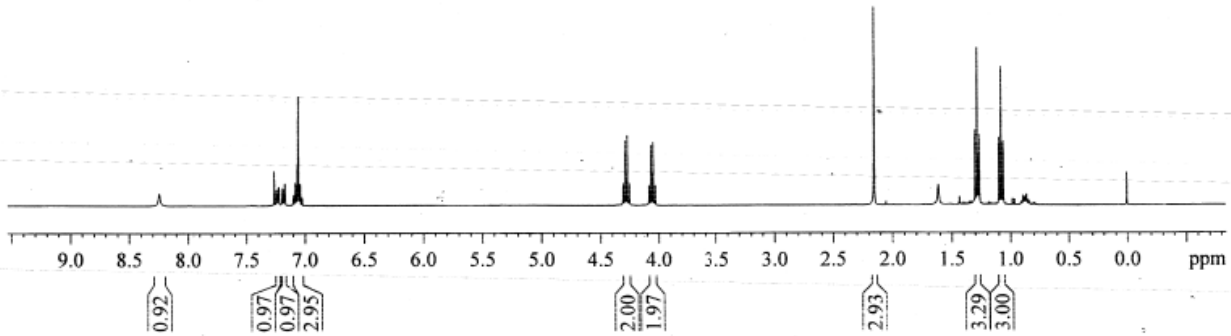


PROTON CDCl3 {D:\MB} KOPAL 1

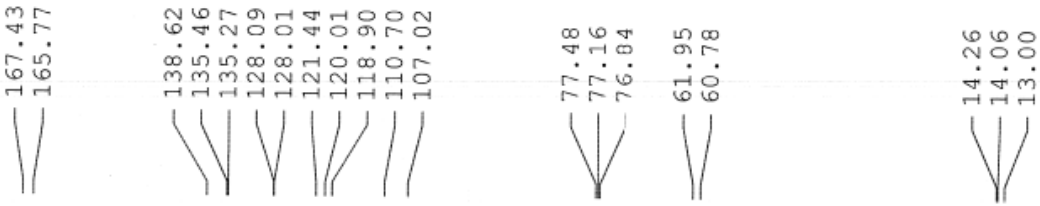


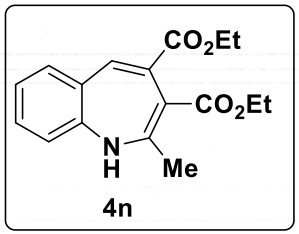
4n

```
Current Data Parameters
NAME                  PVK-408
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20140811
Time                    15.19
INSTRUM                 spect
PROBHD    5 mm DUL 13C-1
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                3.9846387 sec
RG                        144
DW                   60.800 usec
DE                    6.00 usec
TE                    295.3 K
D1                1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                      11.42 usec
PL1                     -3.00 dB
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                      32768
SF                400.1300051 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```



C13CPD CDCl3 {D:\MB} KOPAL 1

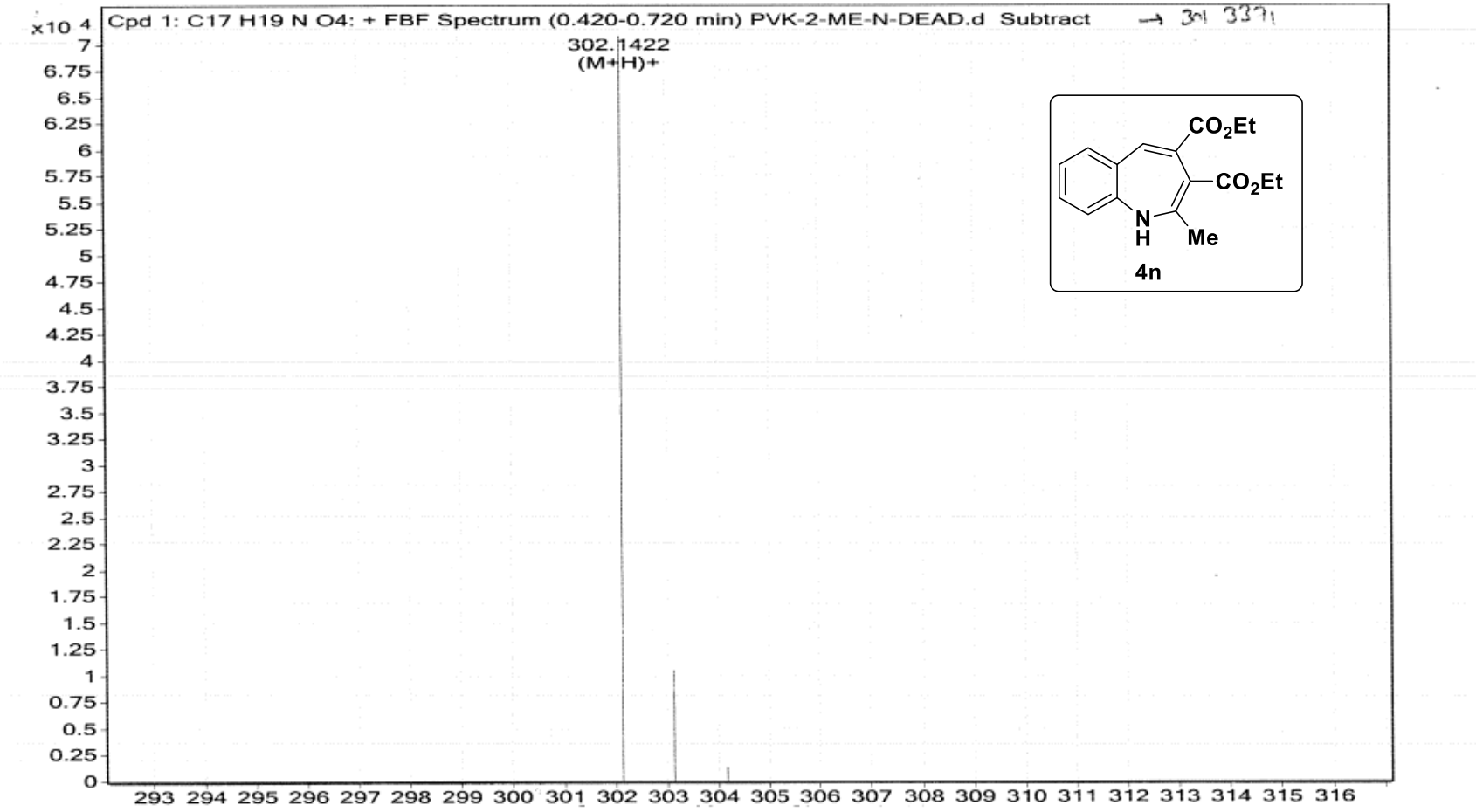


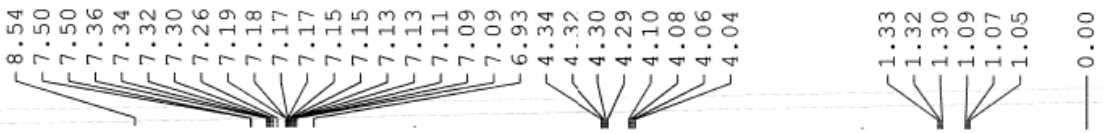


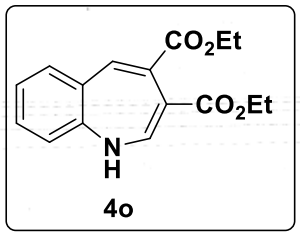
4n


```
Current Data Parameters
NAME                  PVK-408
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140811
Time                   15.30
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        174
DS                          4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                       45.2
DW                     20.800 usec
DE                      6.00 usec
TE                     295.8 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                       9.15 usec
PL1                      0.00 dB
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   90.00 usec
PL12                    14.90 dB
PL13                    14.90 dB
PL2                     -3.00 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127558 MHz
WDW                          EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

mple Name	PVK-2-ME-N-DEAD	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
nj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Data Filename	PVK-2-ME-N-DEAD.d	ACQ Method	Pondicherry Universi	Comment	MB-PV-273.2839	Acquired Time	17-12-2014 11:38:03

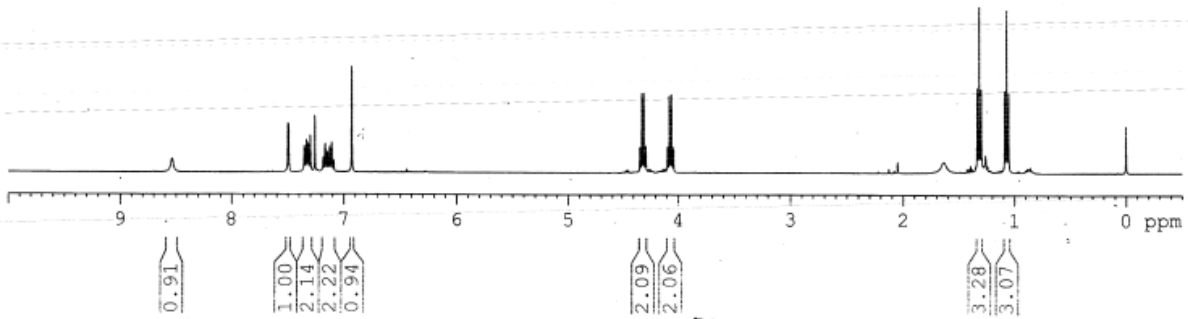


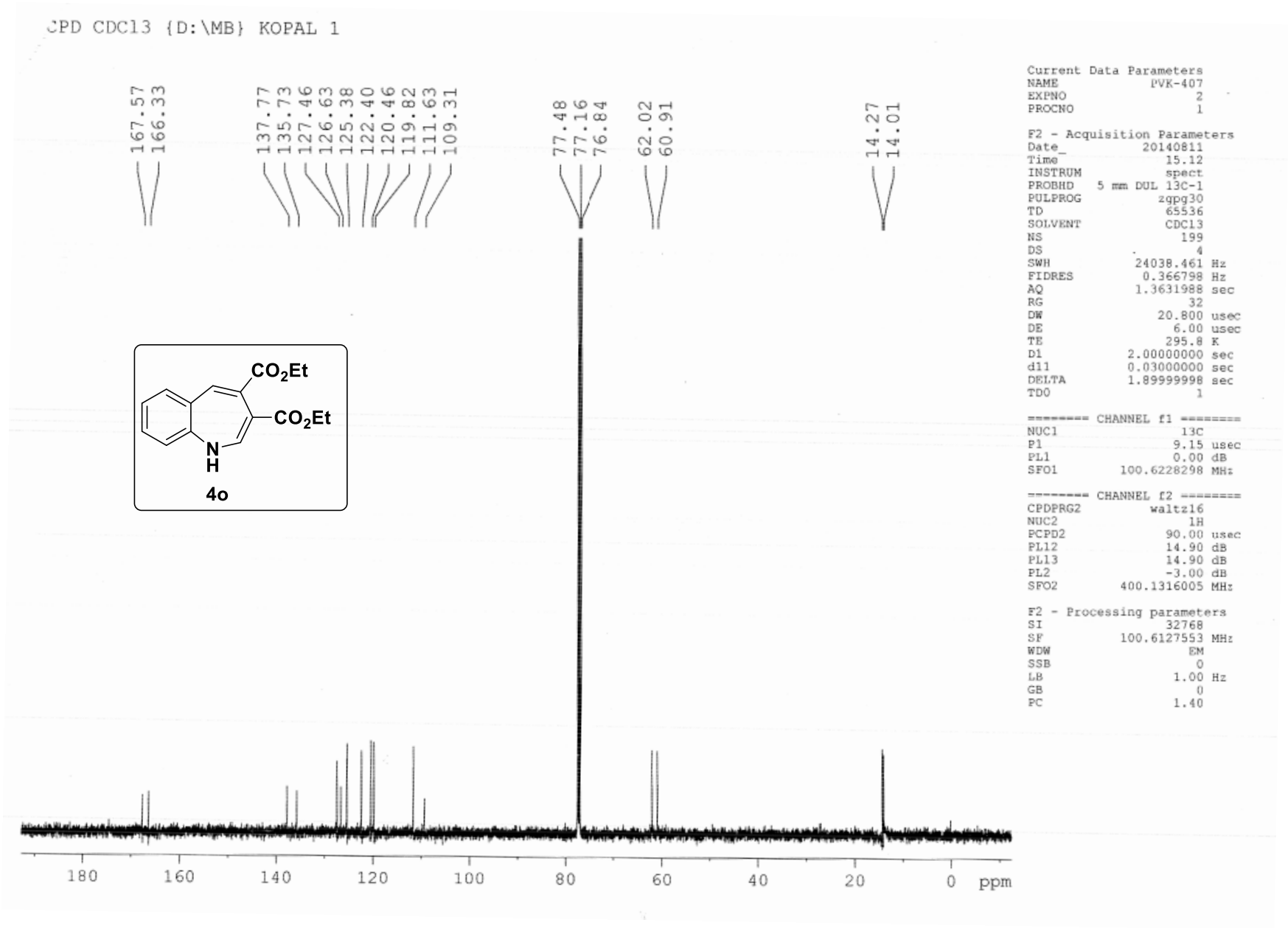


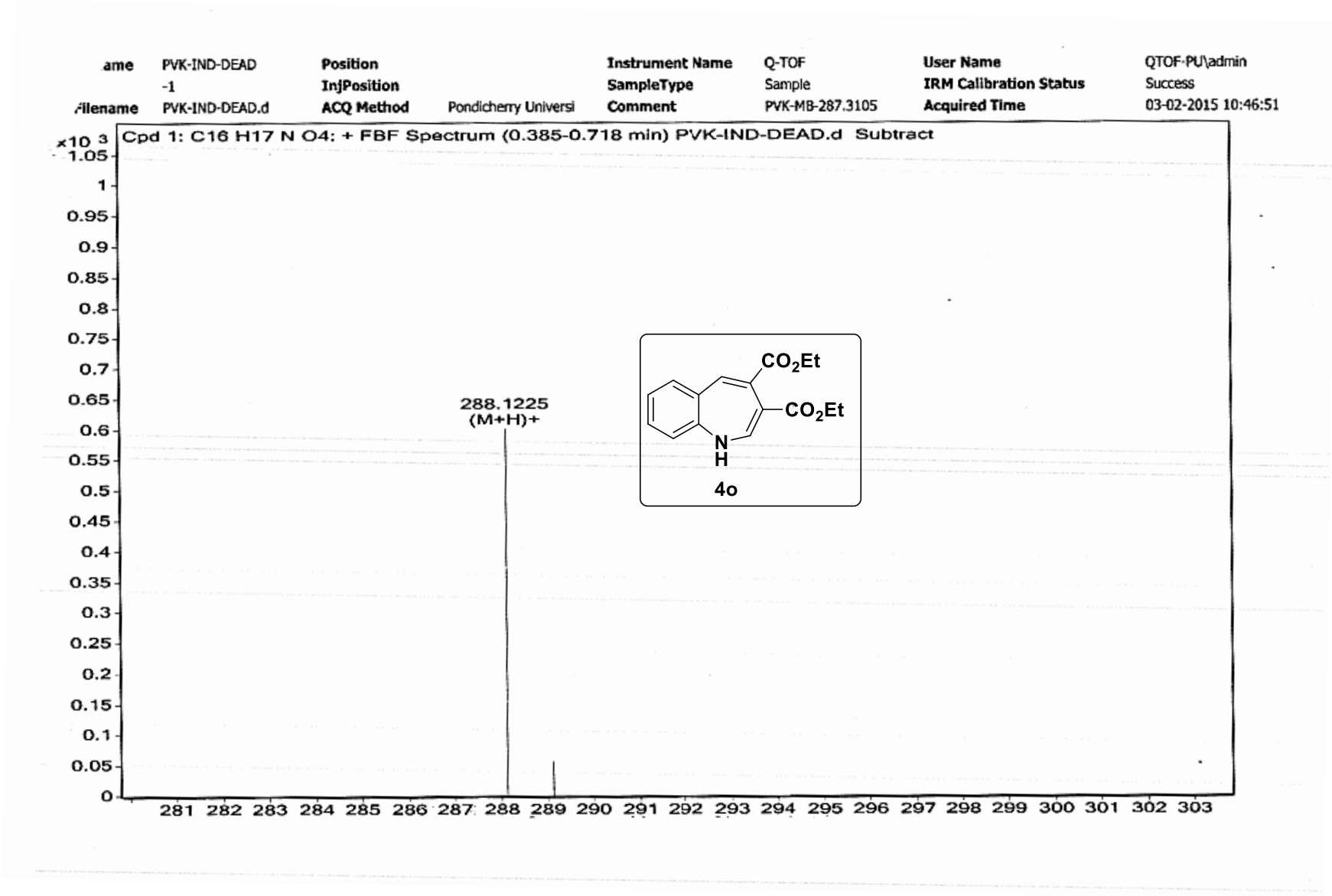


4o

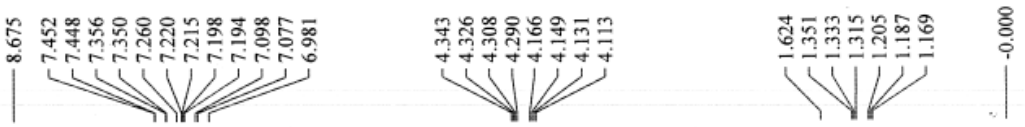
```
Current Data Parameters
NAME                  PVK-407
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              .20140811
Time                   15.00
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9846387 sec
RG                       161
DW                    60.800 usec
DE                     6.00 usec
TE                    295.3 K
D1                 1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.42 usec
PL1                    -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                      32768
SF            400.1300051 MHz
WDW                        EM
SSB                         0
LB                     0.30 Hz
GB                          0
PC                      1.00
```

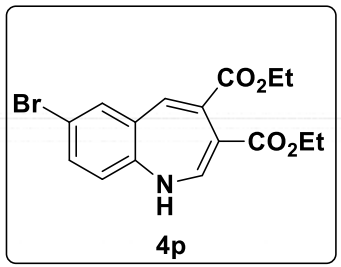



CPD CDCl3 {D:\MB} KOPAL 1
167.57
166.33
137.77
135.73
127.46
126.63
125.38
122.40
120.46
119.82
111.63
109.31
77.48
77.16
76.84
62.02
60.91
14.27
14.01
CO2Et
CO2Et
N
H
4o
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME PVK-407
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140811
Time 15.12
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 199
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 32
DW 20.800 usec
DE 6.00 usec
TE 295.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127553 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


ame PVK-IND-DEAD Position Instrument Name Q-TOF User Name QTOF-PU\admin
-1 InjPosition SampleType Sample IRM Calibration Status Success
Filename PVK-IND-DEAD.d ACQ Method Pondicherry Universi Comment PVK-MB-287.3105 Acquired Time 03-02-2015 10:46:51
Cpd 1: C16 H17 N O4: + FBF Spectrum (0.385-0.718 min) PVK-IND-DEAD.d Subtract
x10 3
288.1225
(M+H)+
CO2Et
CO2Et
N
H
4o

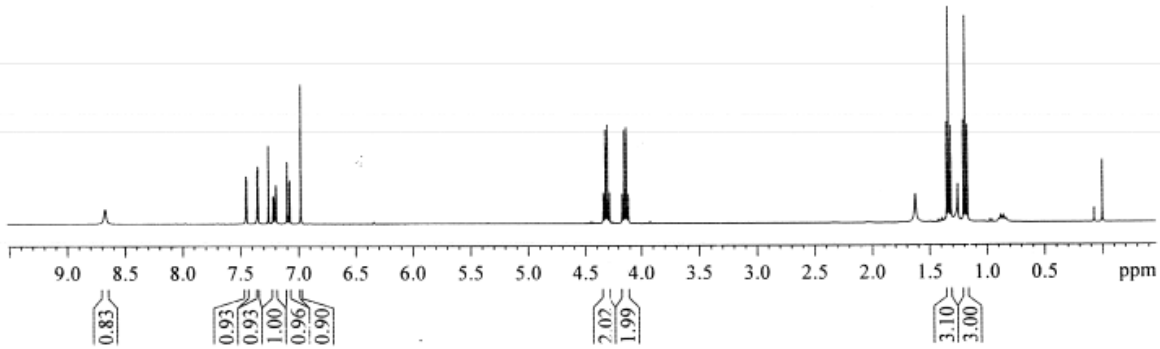
PROTON CDCl3 {D:\MB} KOPAL 1



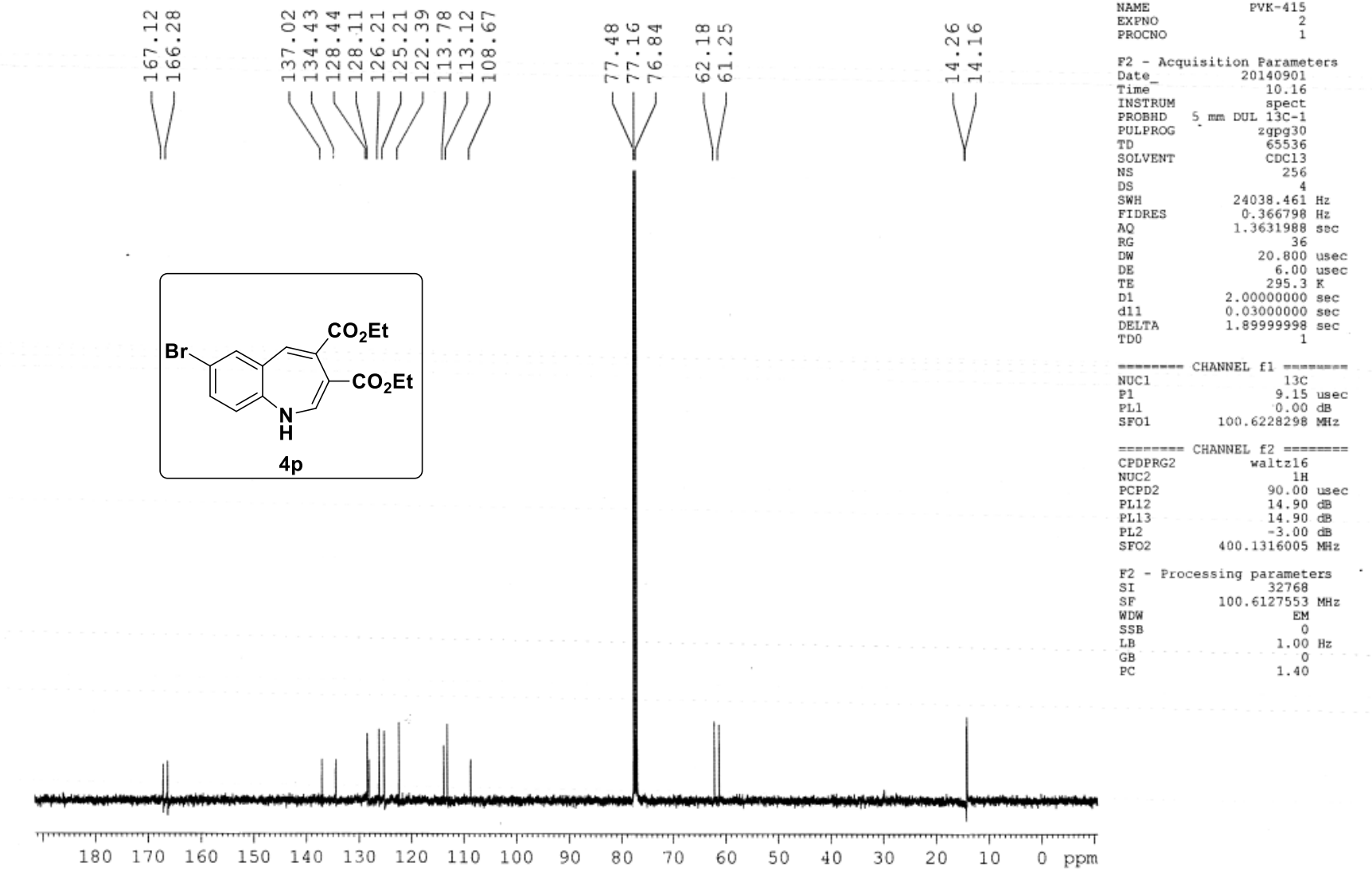


4p

```
Current Data Parameters
NAME                  PVK-415
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20140830
Time                    12.07
INSTRUM                 spect
PROBHD    5 mm DUL 13C-1
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9846387 sec
RG                        161
DW                     60.800 usec
DE                      6.00 usec
TE                     294.5 K
D1                   1.00000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       1H
P1                     11.42 usec
PL1                    -3.00 dB
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                      32768
SF               400.1300051 MHz
WDW                        EM
SSB                         0
LB                      0.30 Hz
GB                          0
FC                       1.00
```

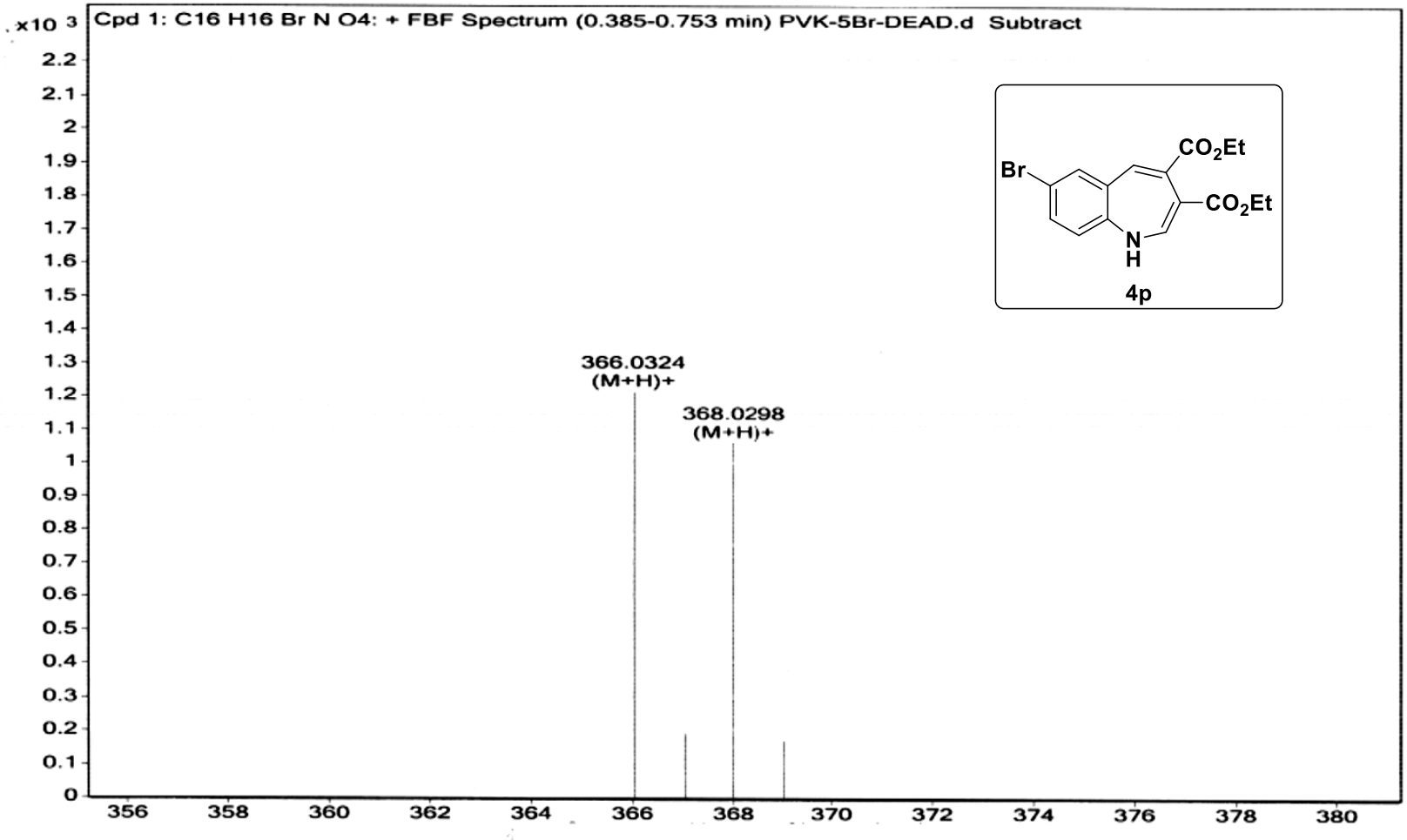


C13CPD CDCl3 {D:\MB} KOPAL 1

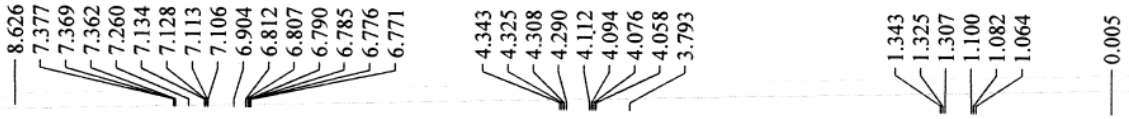


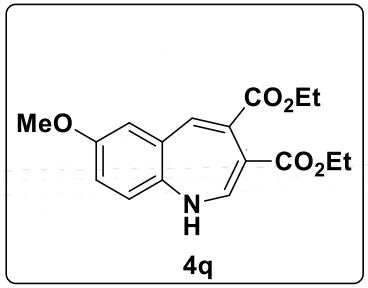

```
Current Data Parameters
NAME                  PVK-415
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_                20140901
Time                    10.16
INSTRUM                 spect
PROBHD   5 mm DUL 13C-1
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        256
DS                          4
SWH                 24038.461 Hz
FIDRES                0.366798 Hz
AQ                    1.3631988 sec
RG                         36
DW                    20.800 usec
DE                     6.00 usec
TE                     295.3 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                       13C
P1                    9.15 usec
PL1                    0.00 dB
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 90.00 usec
PL12                  14.90 dB
PL13                  14.90 dB
PL2                   -3.00 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127553 MHz
WDW                          EM
SSB                           0
LB                    1.00 Hz
GB                            0
PC                         1.40
```

ole Name	PVK-5Br-DEAD	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
ta Filename	PVK-5Br-DEAD.d	ACQ Method	Pondicherry Universi	Comment	MM-MB-366.2065	Acquired Time	02-01-2015 11:51:35

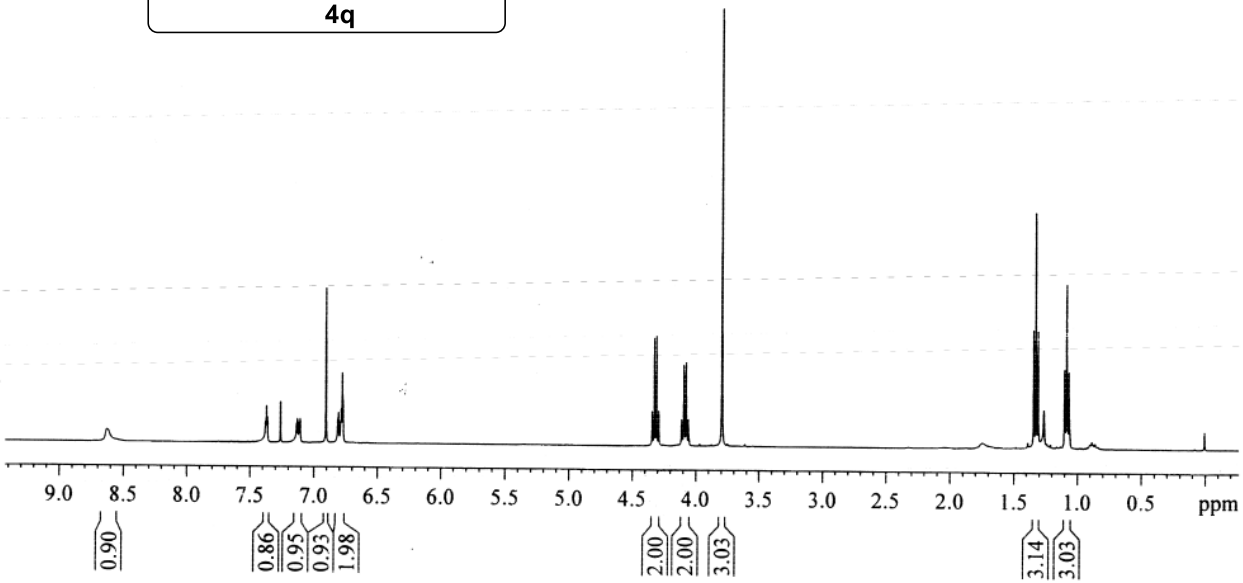


PROTON CDCl3 {D:\MB} KOPAL 1

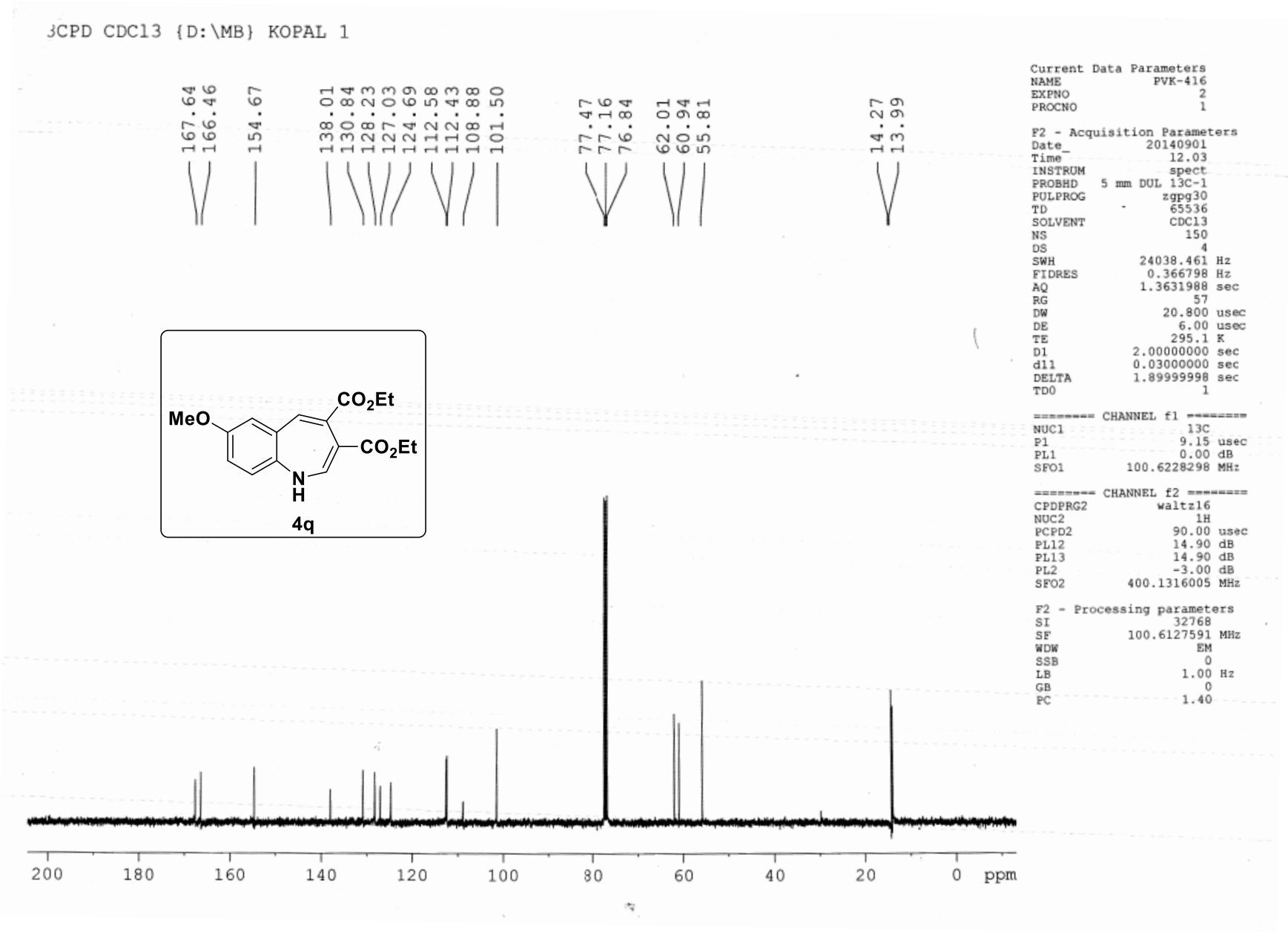


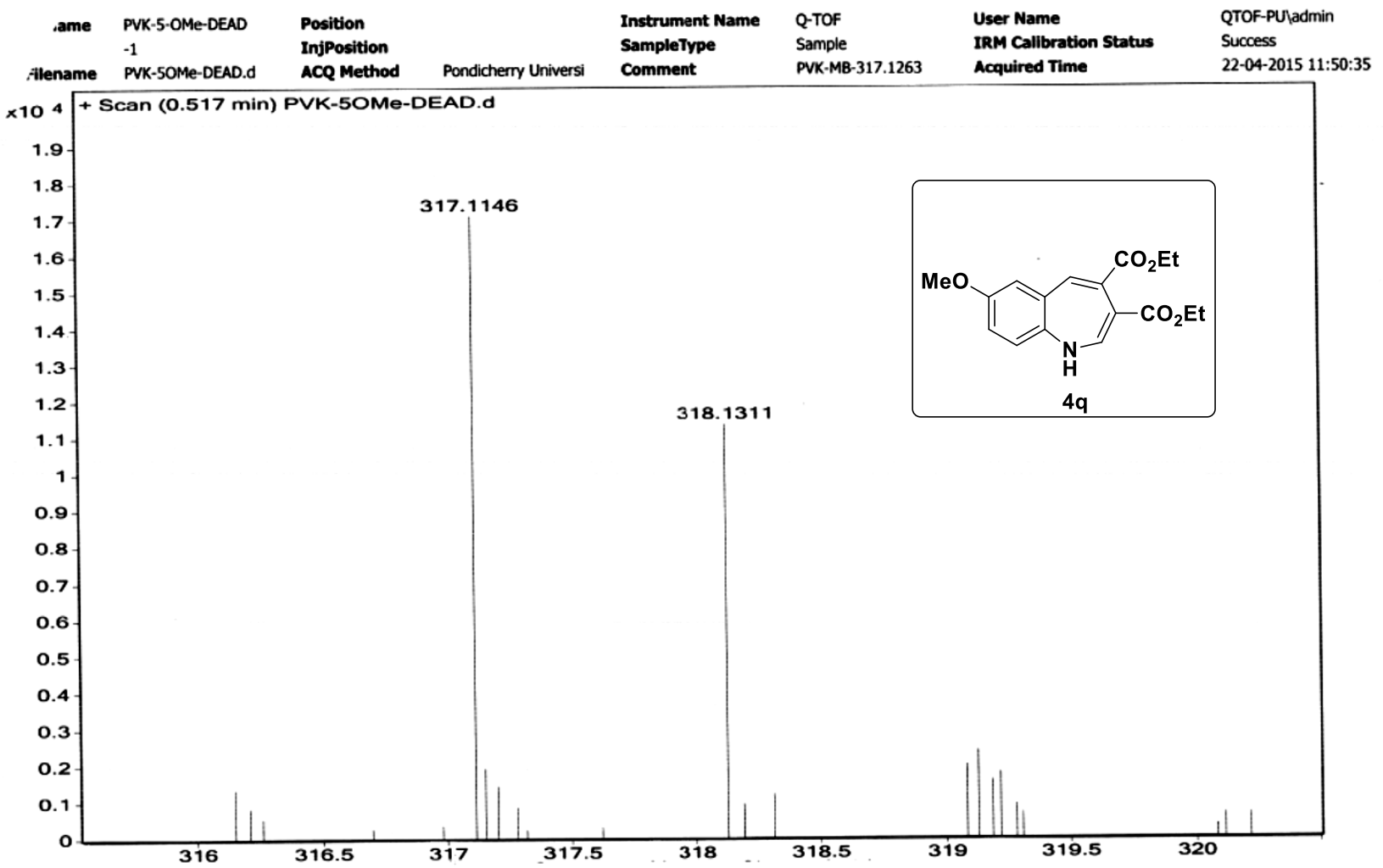


4q

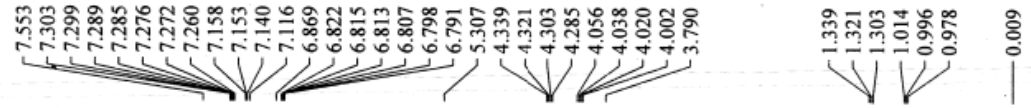


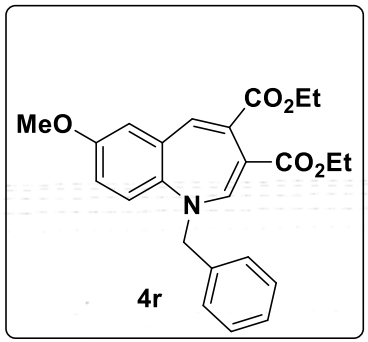

```
Current Data Parameters
NAME                  PVK-416
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140901
Time                   11.54
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                     90.5
DW                   60.800 usec
DE                    6.00 usec
TE                   294.7 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.42 usec
PL1                    -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300049 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

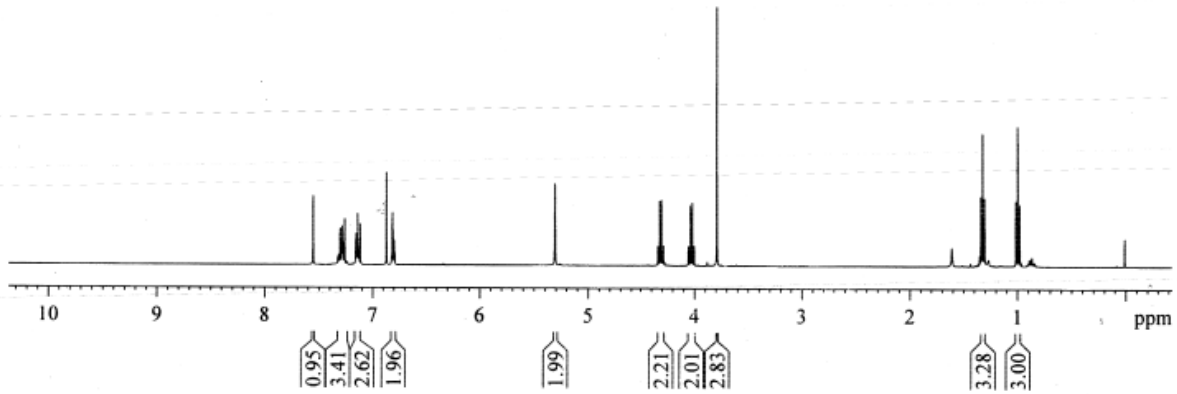

3CPD CDC13 {D:\MB} KOPAL 1
167.64
166.46
154.67
138.01
130.84
128.23
127.03
124.69
112.58
112.43
108.88
101.50
77.47
77.16
76.84
62.01
60.94
55.81
14.27
13.99
MeO
CO2Et
CO2Et
N
H
4q
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME PVK-416
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140901
Time 12.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 150
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 57
DW 20.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127591 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


ame PVK-5-OMe-DEAD
-1
Filename PVK-5OMe-DEAD.d
Position
InjPosition
ACQ Method
Pondicherry Universi
Instrument Name Q-TOF
SampleType Sample
Comment PVK-MB-317.1263
User Name QTOF-PU\admin
IRM Calibration Status Success
Acquired Time 22-04-2015 11:50:35
+ Scan (0.517 min) PVK-5OMe-DEAD.d
x10 4
317.1146
318.1311
MeO
CO2Et
CO2Et
N
H
4q

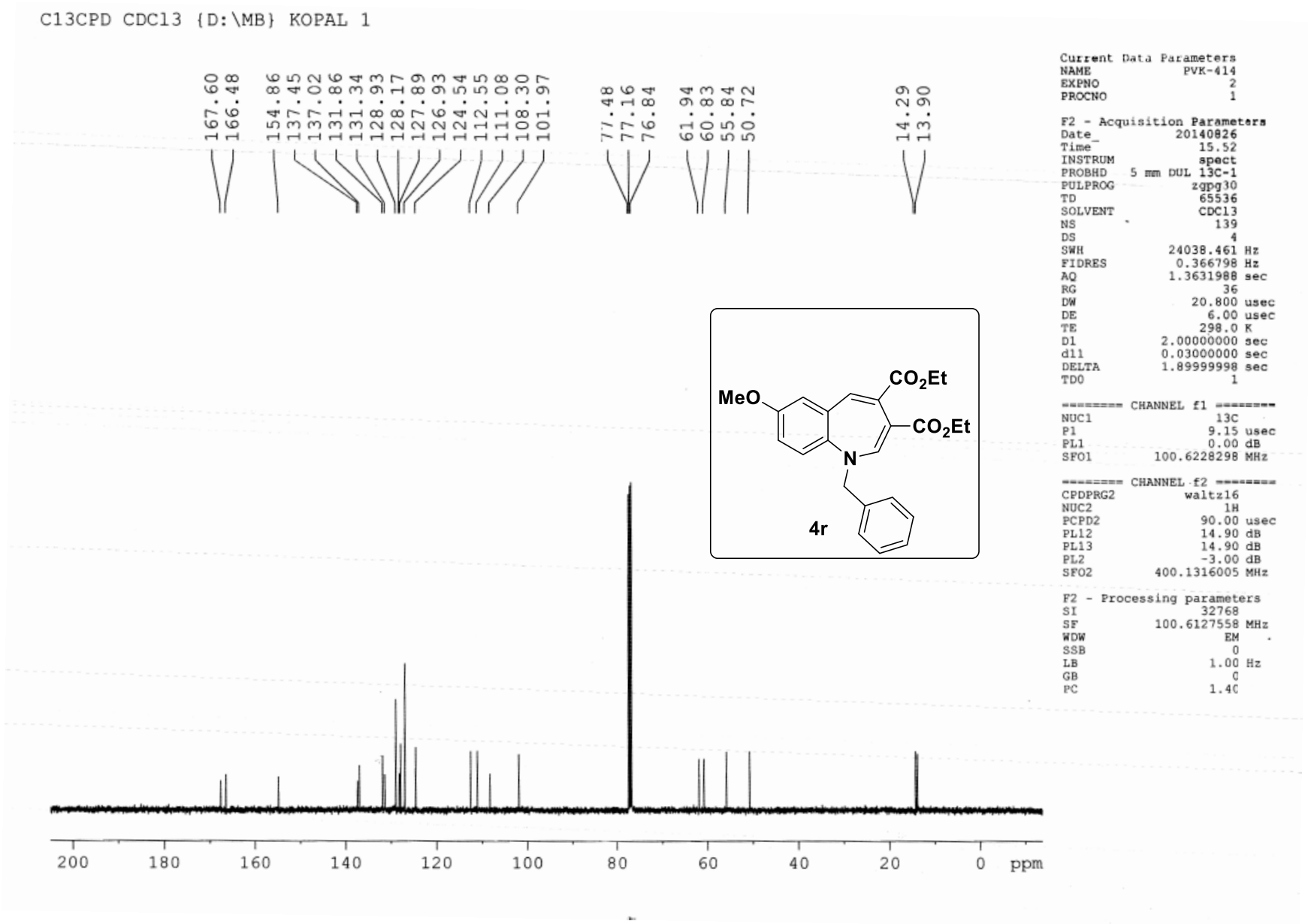
PROTON CDCl3 {D:\MB} KOPAL 1

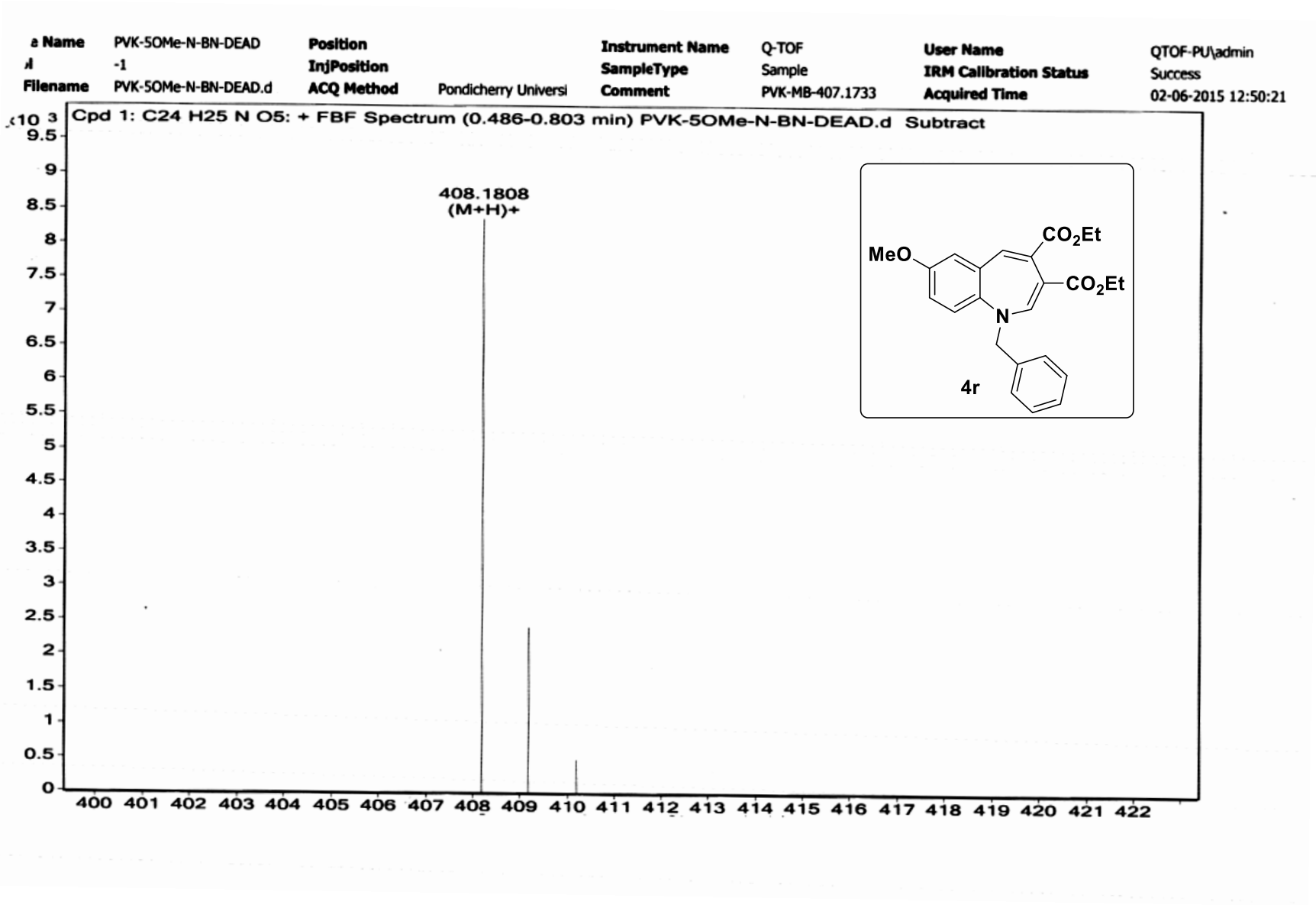




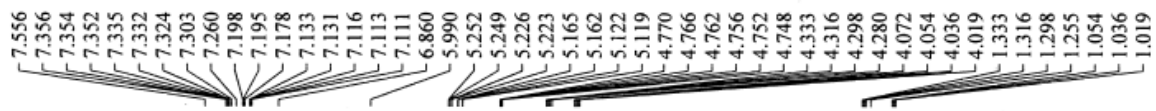


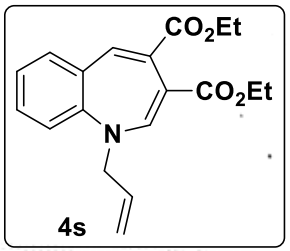

```
Current Data Parameters
NAME                  PVK-414
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20140826
Time                  15.43
INSTRUM               spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                      114
DW                   60.800 usec
DE                    6.00 usec
TE                   297.4 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     11.42 usec
PL1                    -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF            400.1300048 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```


C13CPD CDCl3 {D:\MB} KOPAL 1
167.60
166.48
154.86
137.45
137.02
131.86
131.34
128.93
128.17
127.89
126.93
124.54
112.55
111.08
108.30
101.97
77.48
77.16
76.84
61.94
60.83
55.84
50.72
14.29
13.90
MeO
CO2Et
CO2Et
N
4r
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME PVK-414
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140826
Time 15.52
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 139
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 36
DW 20.800 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127558 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


a Name PVK-5OMe-N-BN-DEAD
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
-1
InjPosition
SampleType Sample
IRM Calibration Status Success
Filename PVK-5OMe-N-BN-DEAD.d
ACQ Method
Pondicherry Universi
Comment PVK-MB-407.1733
Acquired Time 02-06-2015 12:50:21
Cpd 1: C24 H25 N O5: + FBF Spectrum (0.486-0.803 min) PVK-5OMe-N-BN-DEAD.d Subtract
408.1808
(M+H)+
MeO
CO2Et
CO2Et
N
4r

PROTON CDCl3 {D:\MB} KOPAL 1





Current Data Parameters

NAME	PVK-413
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

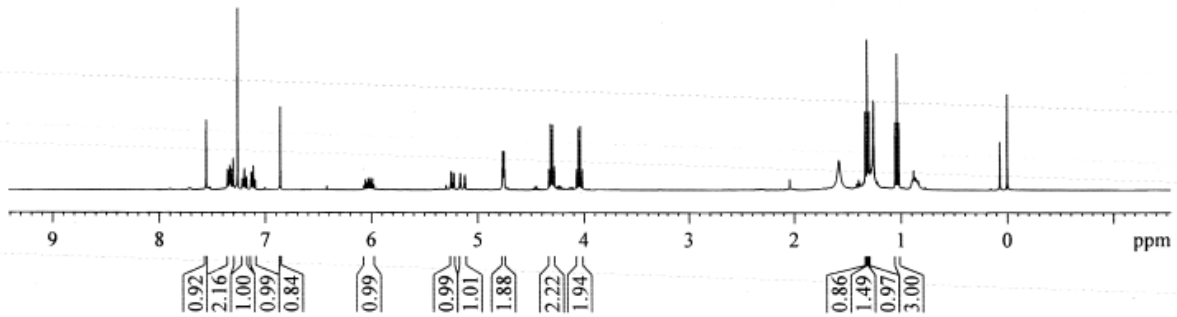
Date_	20140825
Time	12.33
INSTRUM	spect
PROBHD	5 mm BUL 13C-1
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	228
DW	60.800 usec
DE	6.00 usec
TE	296.2 K
D1	1.00000000 sec
TD0	1

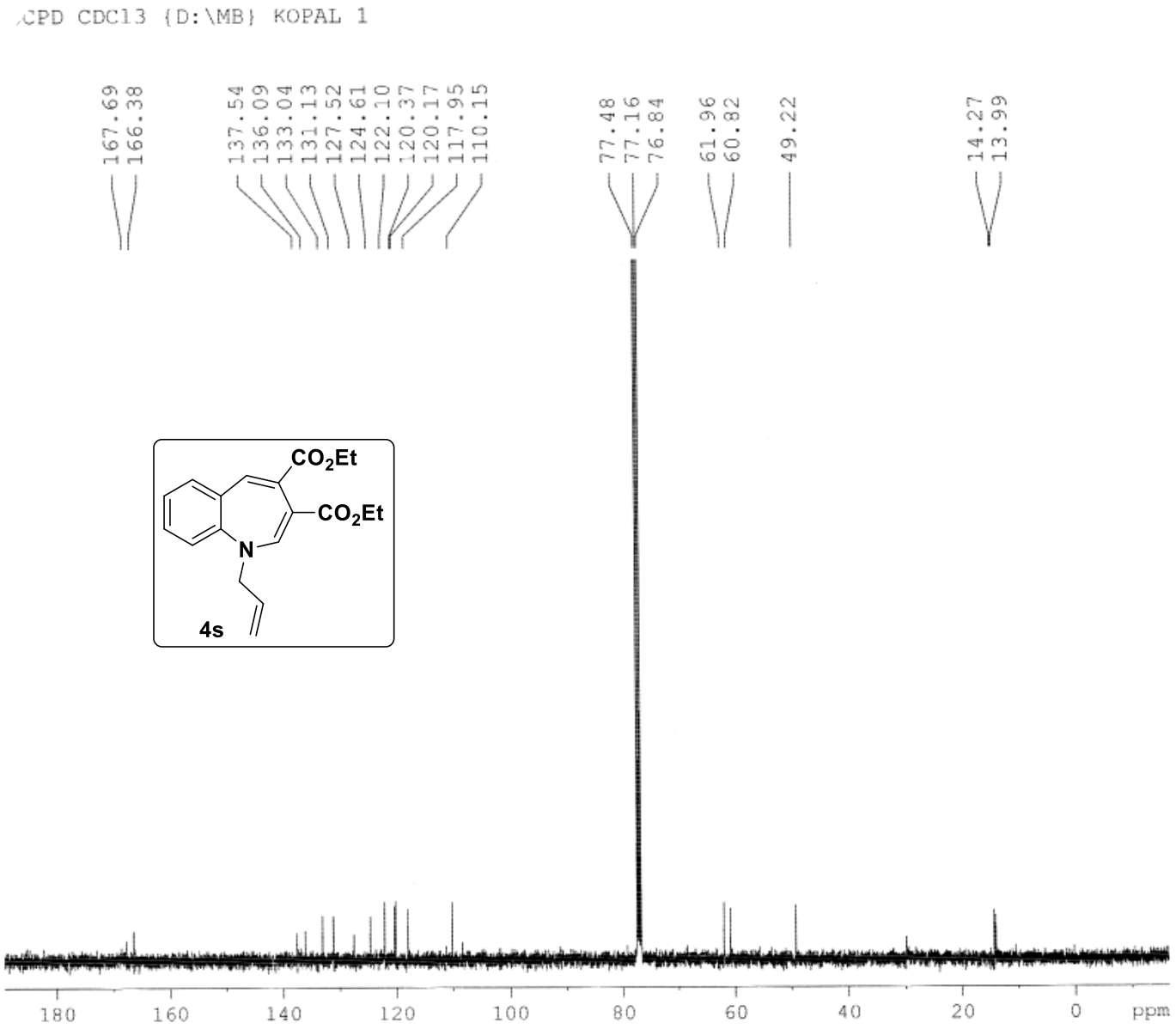
======== CHANNEL f1 ========

NUC1	1H
P1	11.42 usec
PL1	-3.00 dB
SFO1	400.1324710 MHz

F2 - Processing parameters

SI	32768
SF	400.1300051 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00





Current Data Parameters
NAME PVF 411
EXPNO 1
PROCNO 1

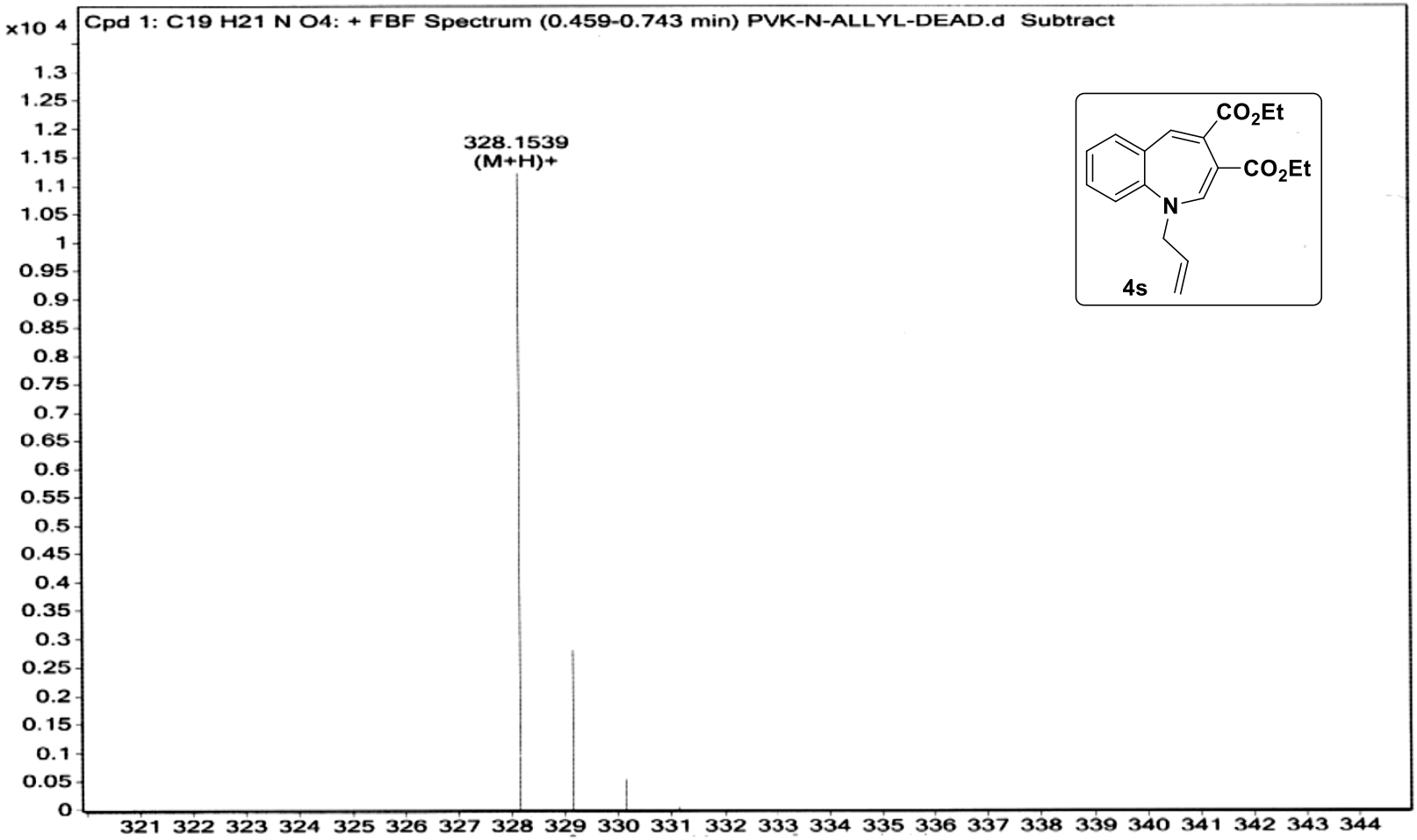
F2 - Acquisition Parameters
Date_ 20140825
Time 13.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 64
DW 20.800 usec
DE 6.00 usec
TE 296.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.15 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

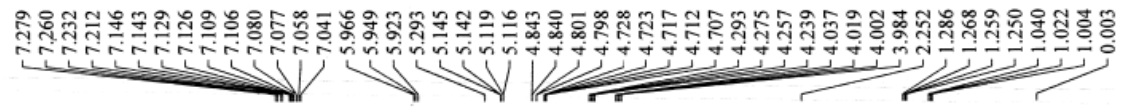
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

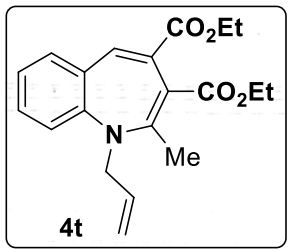
F2 - Processing parameters
SI 32768
SF 100.6127533 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Name	PVK-N-Allyl-DEAD	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Jl	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
ta Filename	PVK-N-ALLYL-DEAD.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-327.1770	**Acquired Time**	22-04-2015 14:31:00

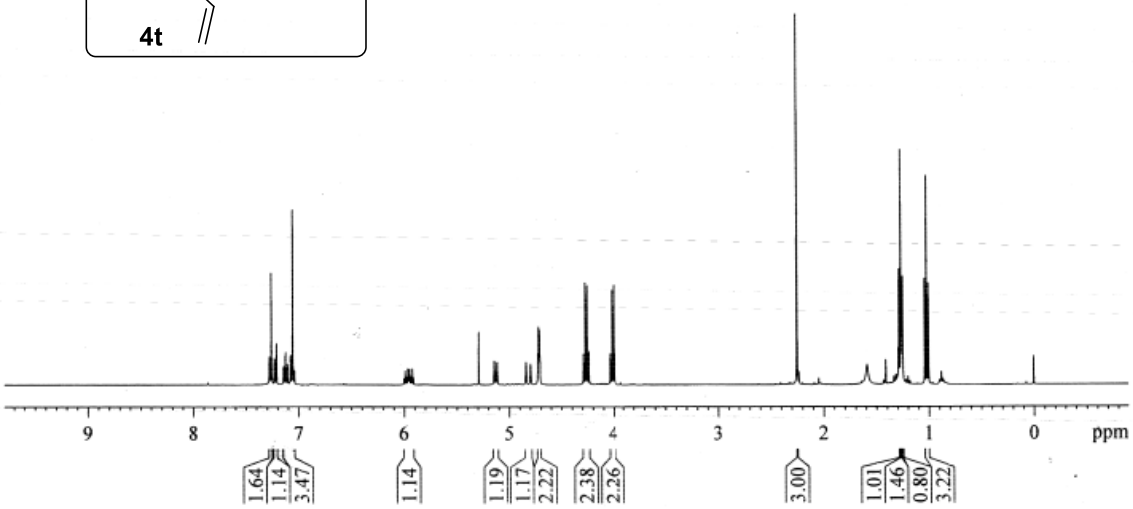


PROTON CDCl3 {D:\MB} KOPAL 1

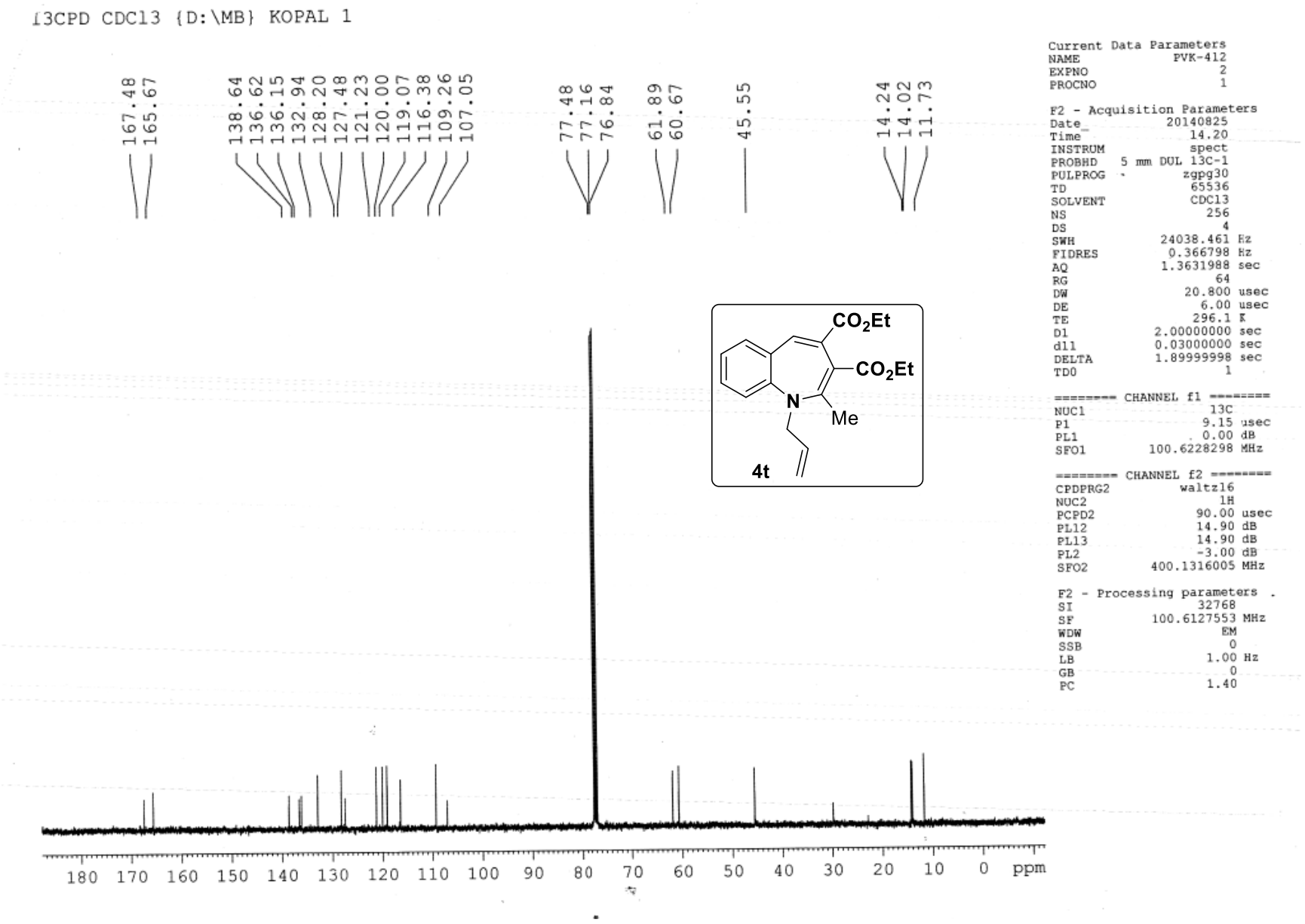




4t




```
Current Data Parameters
NAME                  PVK-412
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20140825
Time                    14.10
INSTRUM                 spect
PROBHD    5 mm DUL 13C-1
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                3.9846387 sec
RG                       128
DW                  60.800 usec
DE                   6.00 usec
TE                   295.3 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                   11.42 usec
PL1                  -3.00 dB
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                     32768
SF                400.1300051 MHz
WDW                       EM
SSB                        0
LB                    0.30 Hz
GB                         0
PC                      1.00
```



Current Data Parameters

NAME	PVK-412
EXPNO	2
PROCNO	1

F2 - Acquisition Parameters

Date_	20140825
Time	14.20
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDC13
NS	256
DS	4
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3631988 sec
RG	64
DW	20.800 usec
DE	6.00 usec
TE	296.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1

======== CHANNEL f1 ========

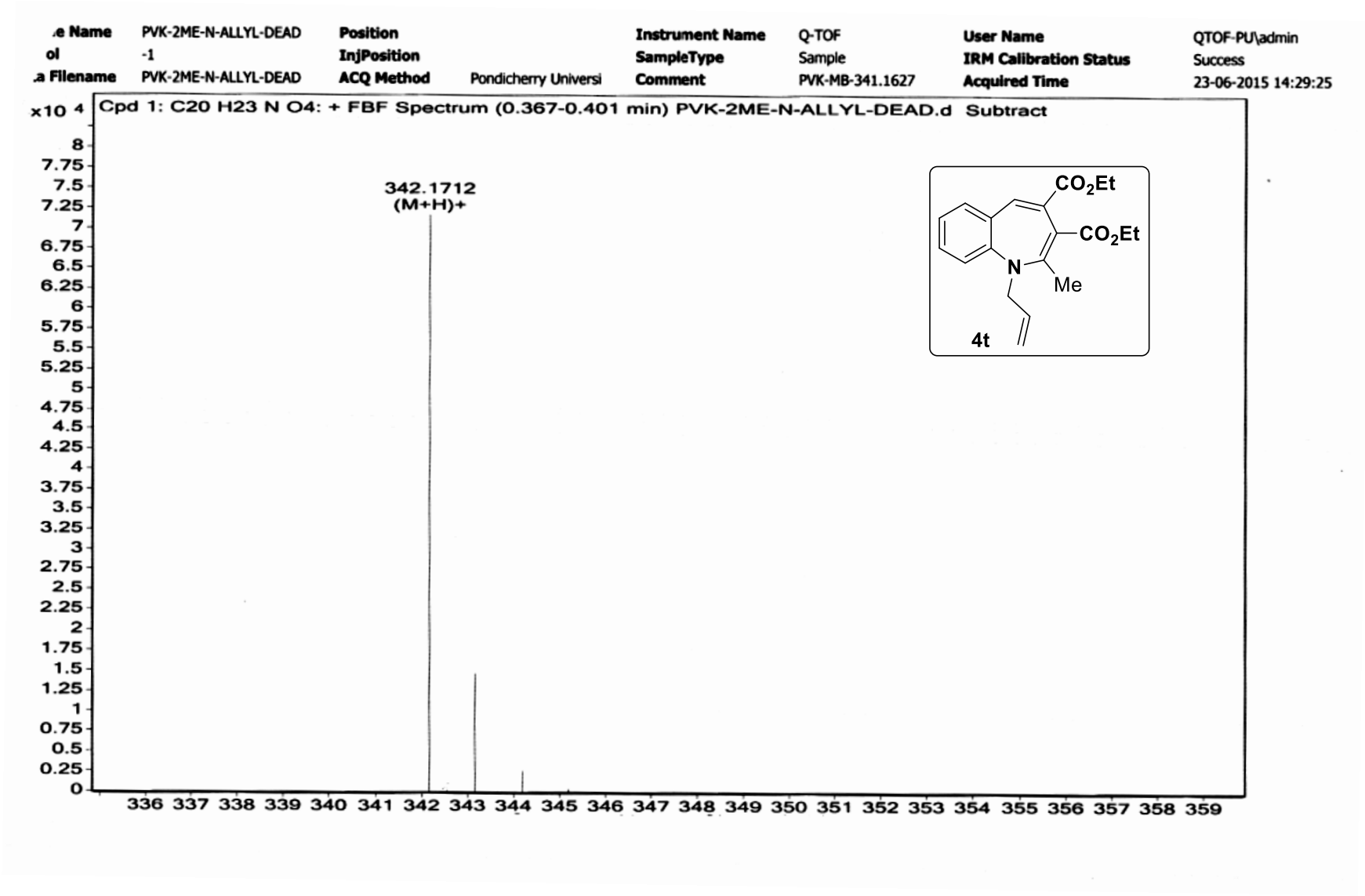
NUC1	13C
P1	9.15 usec
PL1	0.00 dB
SFO1	100.6228298 MHz

======== CHANNEL f2 ========

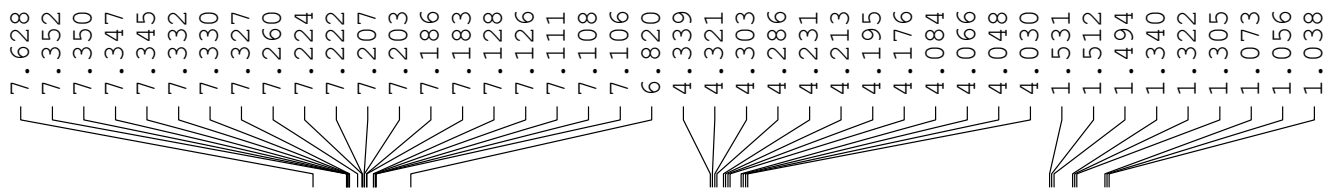
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL12	14.90 dB
PL13	14.90 dB
PL2	-3.00 dB
SFO2	400.1316005 MHz

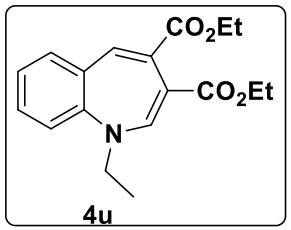
F2 - Processing parameters

SI	32768
SF	100.6127553 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

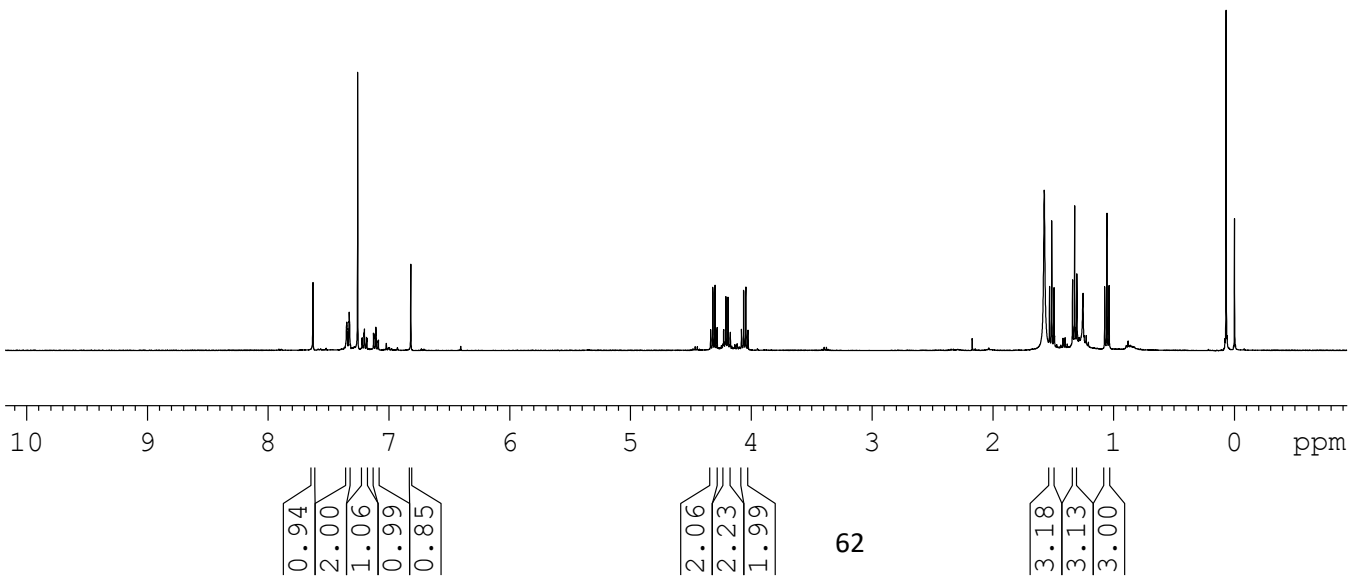

e Name PVK-2ME-N-ALLYL-DEAD
Position
Instrument Name Q-TOF
User Name QTOF-PU\admin
ol -1
InjPosition
SampleType Sample
IRM Calibration Status Success
a Filename PVK-2ME-N-ALLYL-DEAD
ACQ Method Pondicherry Universi
Comment PVK-MB-341.1627
Acquired Time 23-06-2015 14:29:25
Cpd 1: C20 H23 N O4: + FBF Spectrum (0.367-0.401 min) PVK-2ME-N-ALLYL-DEAD.d Subtract
x10 4
342.1712
(M+H)+
CO2Et
CO2Et
N
Me
4t
8
7.75
7.5
7.25
7
6.75
6.5
6.25
6
5.75
5.5
5.25
5
4.75
4.5
4.25
4
3.75
3.5
3.25
3
2.75
2.5
2.25
2
1.75
1.5
1.25
1
0.75
0.5
0.25
0
336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 354 355 356 357 358 359

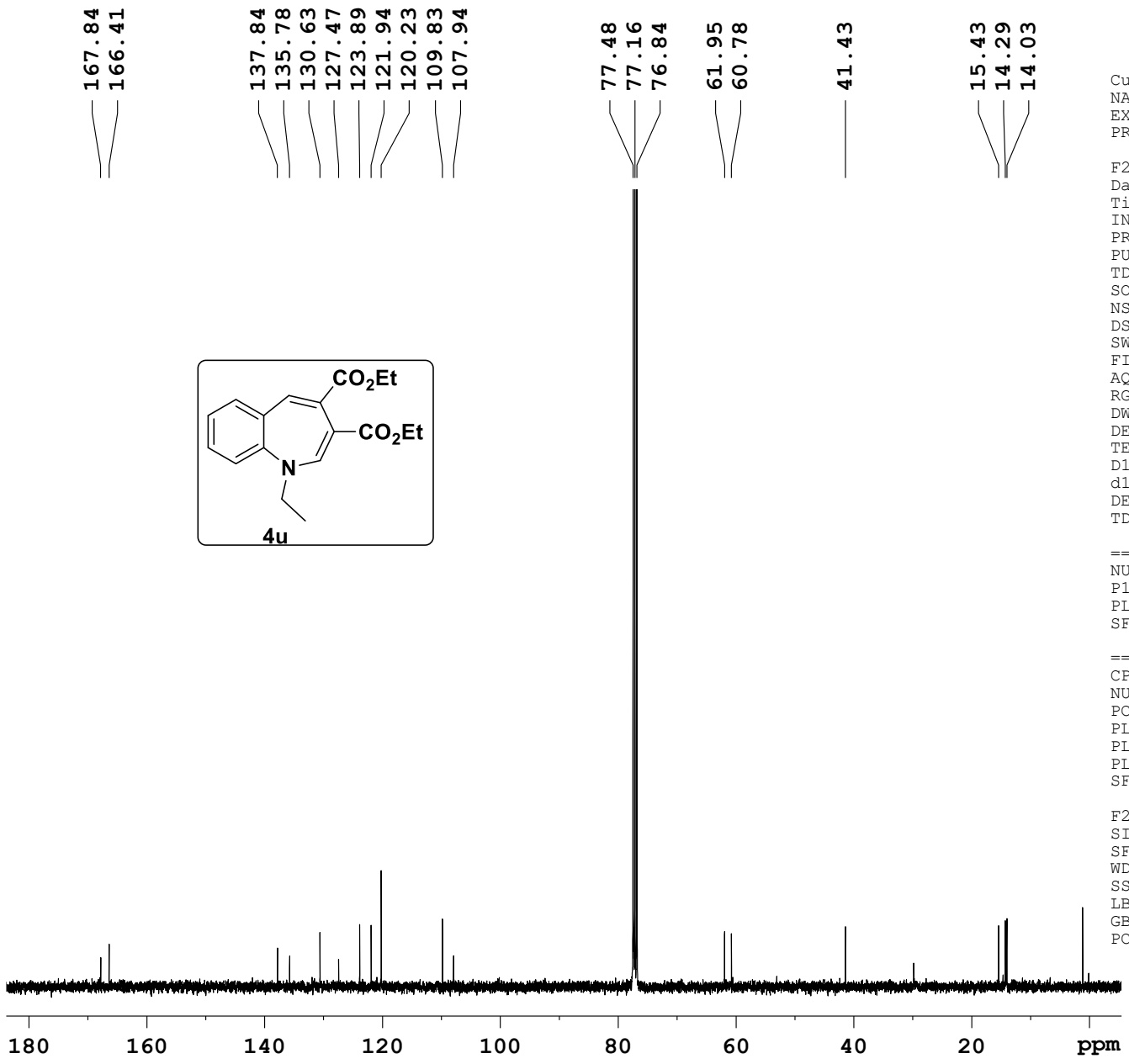
PROTON CDCl3 {D:\MB} KOPAL 1





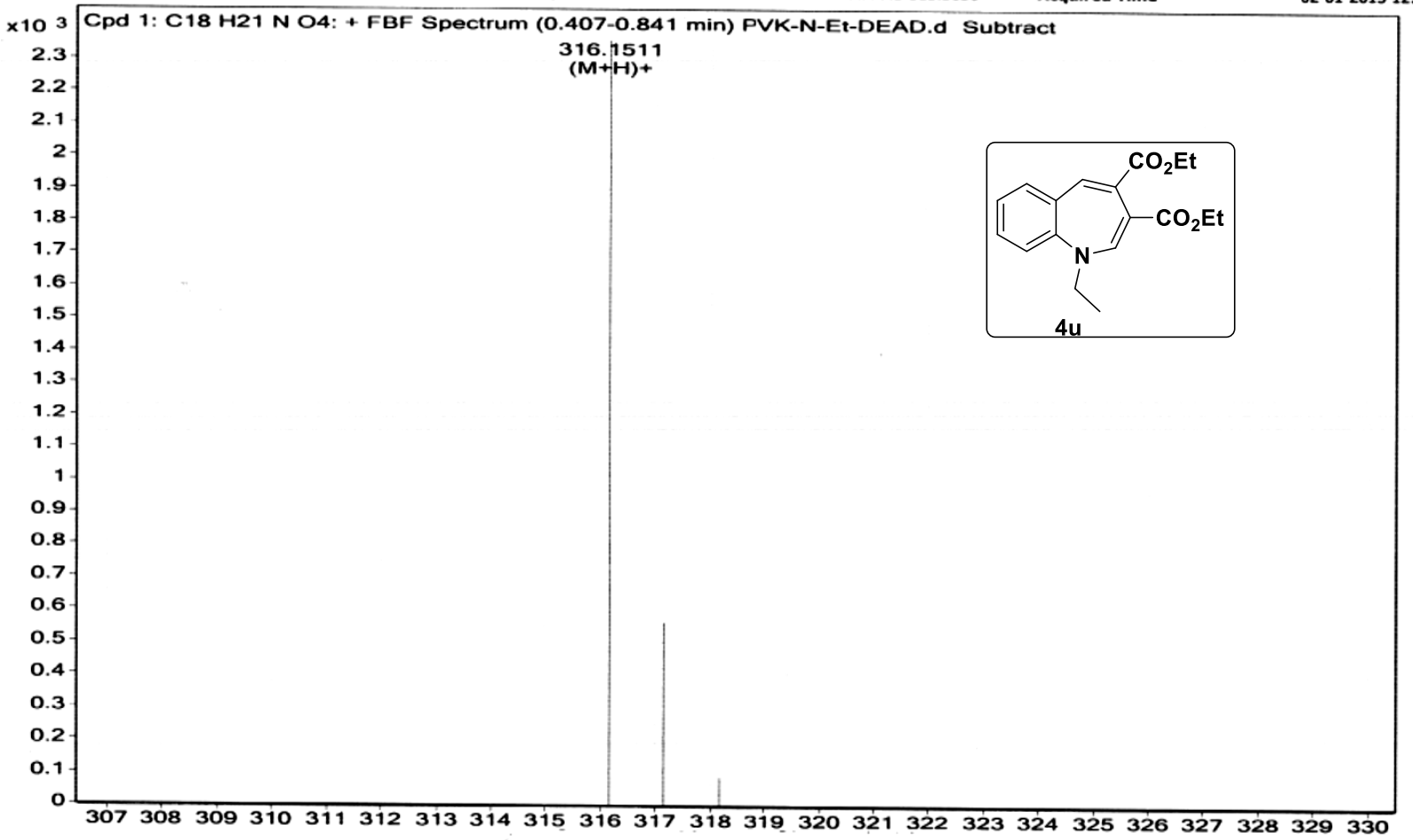

```
Current Data Parameters
NAME      PVK-N-ET-DEAD-II
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20150415
Time                 14.43
INSTRUM              spect
PROBHD   5 mm DUL 13C-1
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9846387 sec
RG                     228
DW                  60.800 usec
DE                   6.00 usec
TE                  296.2 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   11.42 usec
PL1                  -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                   32768
SF            400.1300051 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



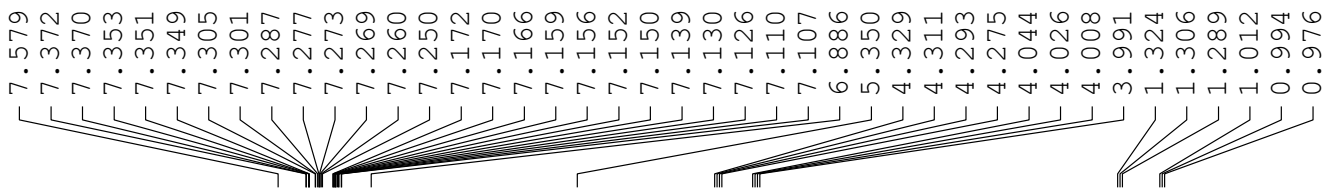


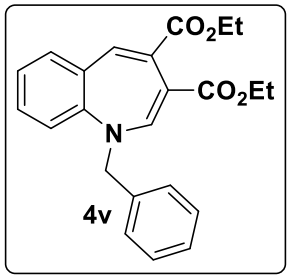

```
Current Data Parameters
NAME      PVK-N-ET-DEAD-III
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20150420
Time               13.54
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   32
DW                20.800 usec
DE                 6.00 usec
TE                296.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127538 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

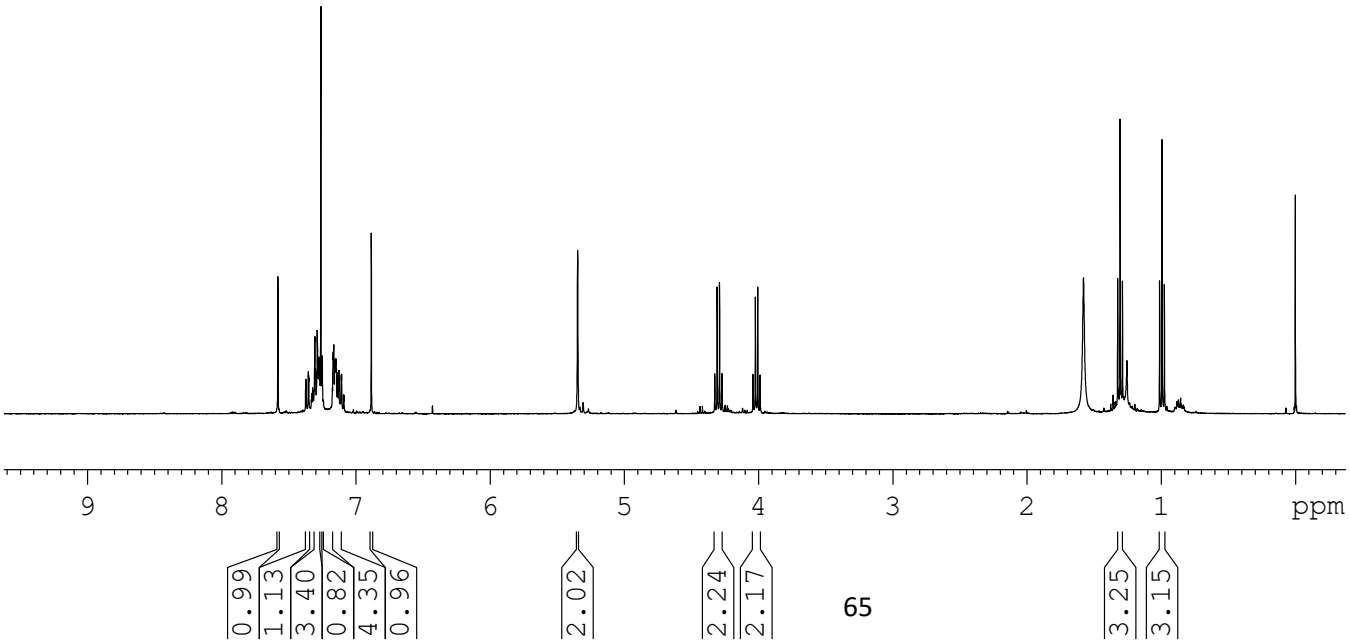
ame	PVK-N-Et-DEAD	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
Filename	PVK-N-Et-DEAD.d	ACQ Method	Pondicherry Universi	Comment	MM-MB-315.3636	Acquired Time	02-01-2015 12:06:49



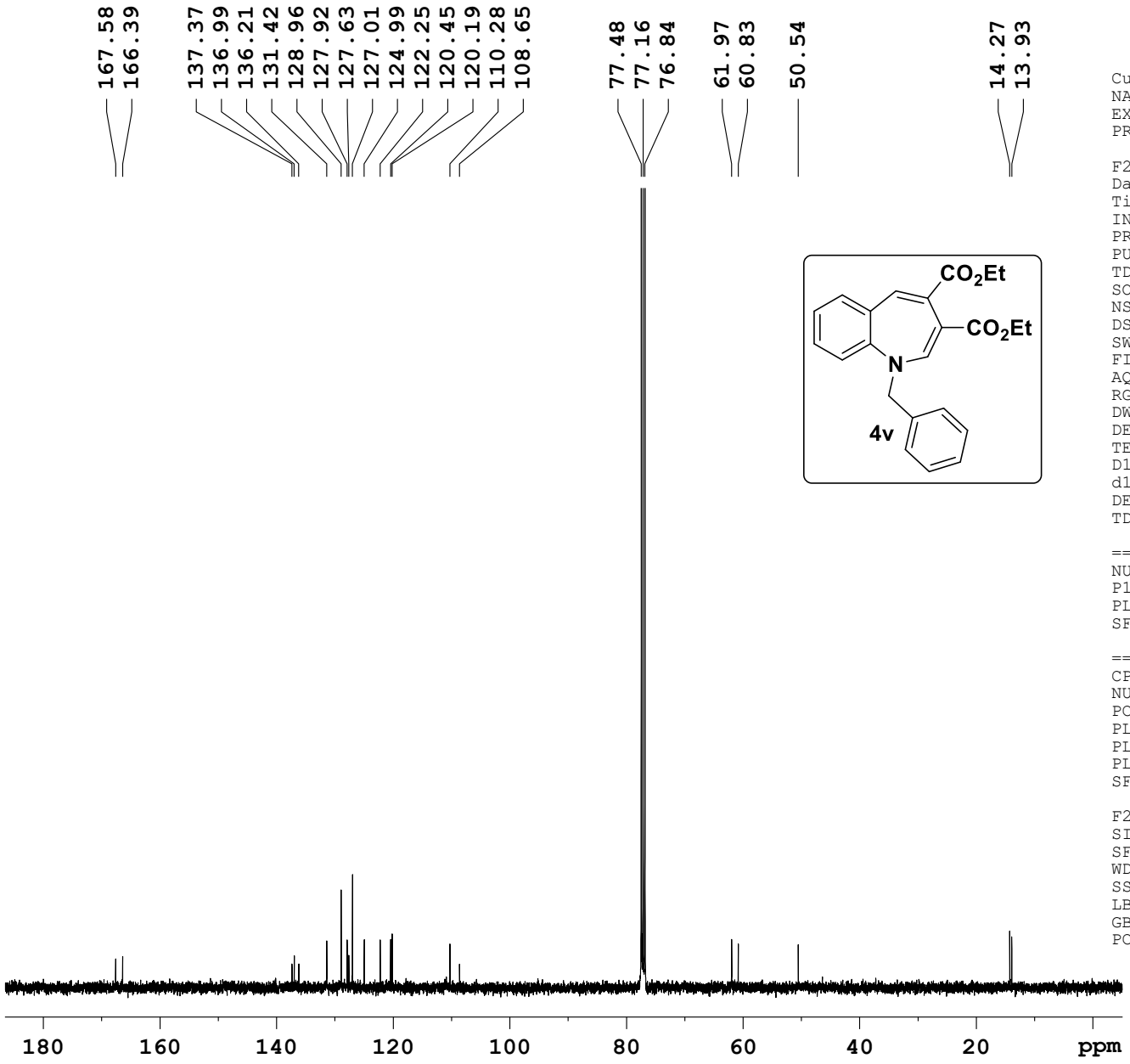
PROTON CDCl3 {D:\MB} KOPAL 1





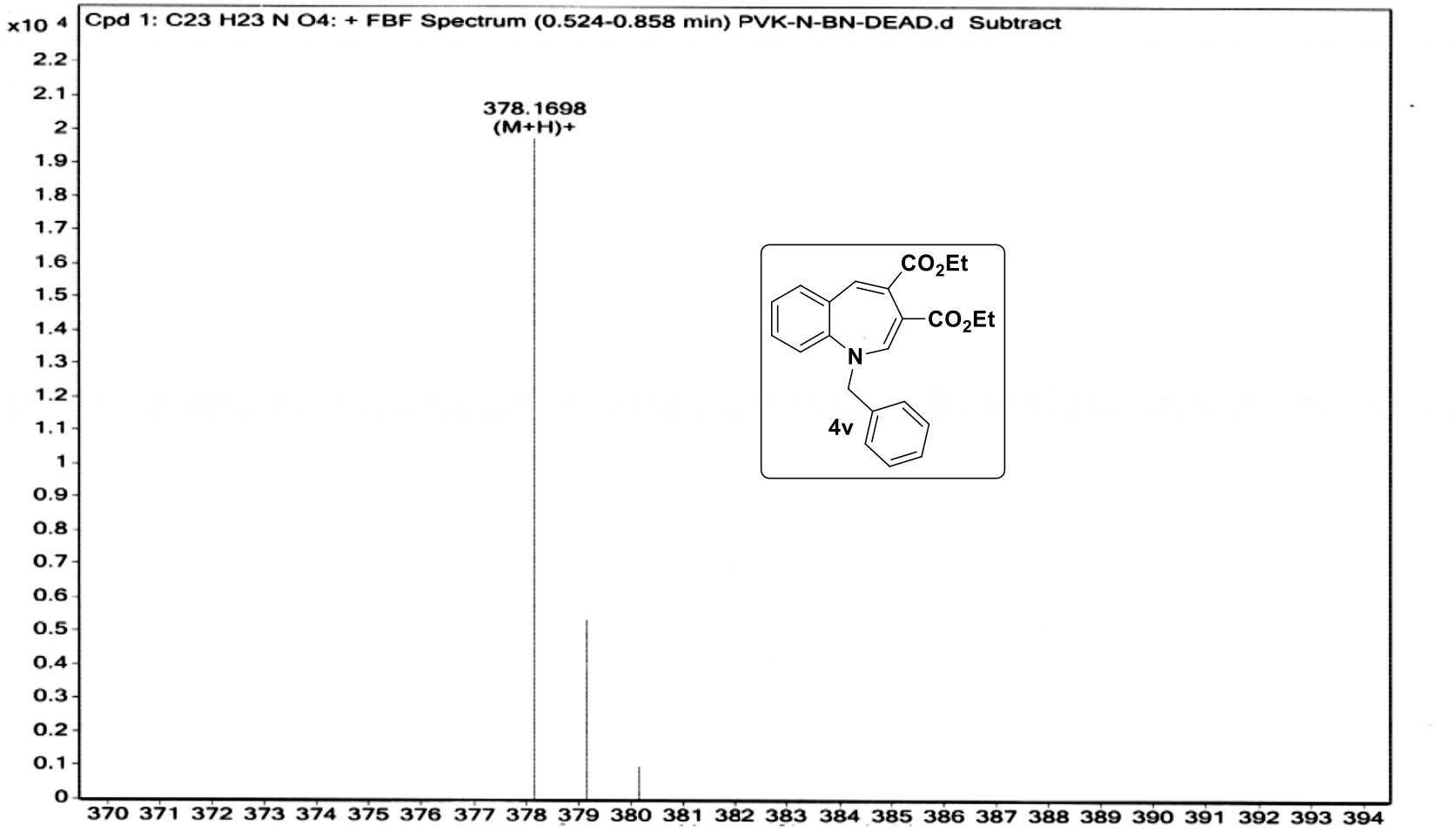



```
Current Data Parameters
NAME       PVK-N-BN-DEAD
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150413
Time              16.12
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ           3.9846387 sec
RG                  228
DW               60.800 usec
DE                6.00 usec
TE               295.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.42 usec
PL1               -3.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                32768
SF        400.1300051 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

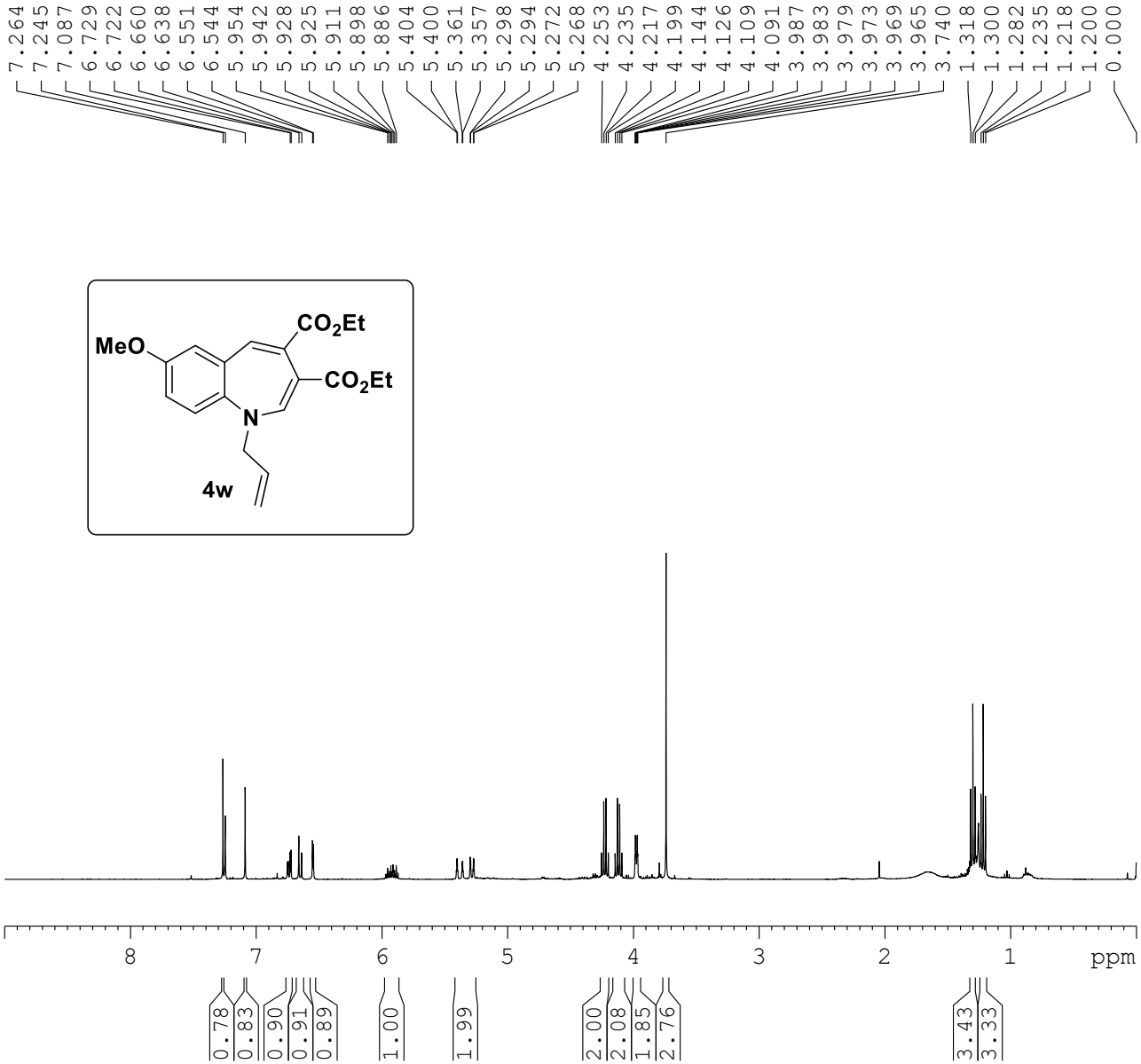



```
Current Data Parameters
NAME       PVK-N-BN-DEAD
EXPNO                  8
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150416
Time               13.18
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  512
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                   32
DW                20.800 usec
DE                 6.00 usec
TE                297.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.15 usec
PL1                 0.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.90 dB
PL13               14.90 dB
PL2                -3.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127535 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

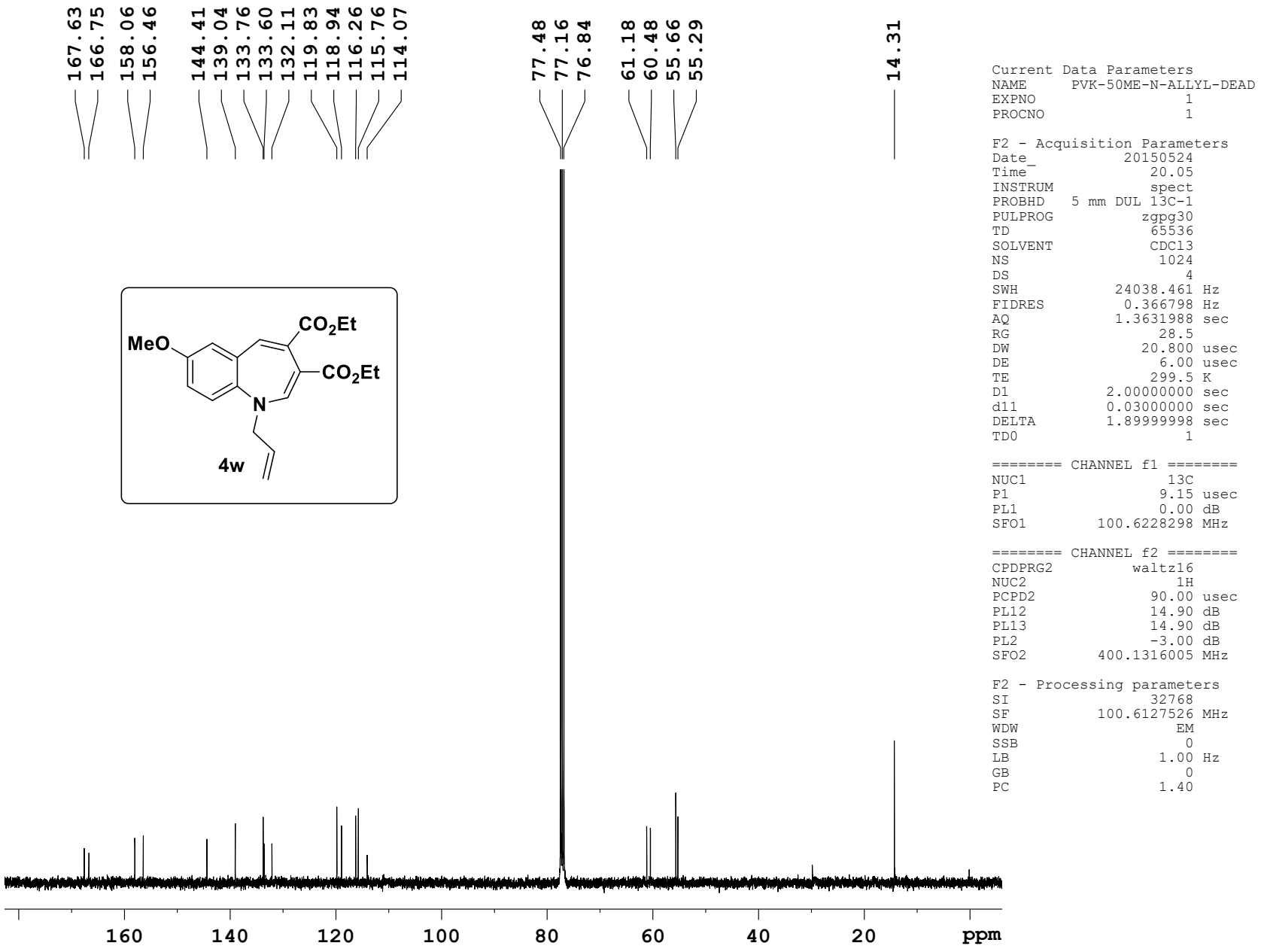
Name	PVK-N-BN-DEAD	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
d	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
a Filename	PVK-N-BN-DEAD.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-377.1627	**Acquired Time**	02-06-2015 12:46:09



PROTON CDCl3 {D:\MB} KOPAL 1

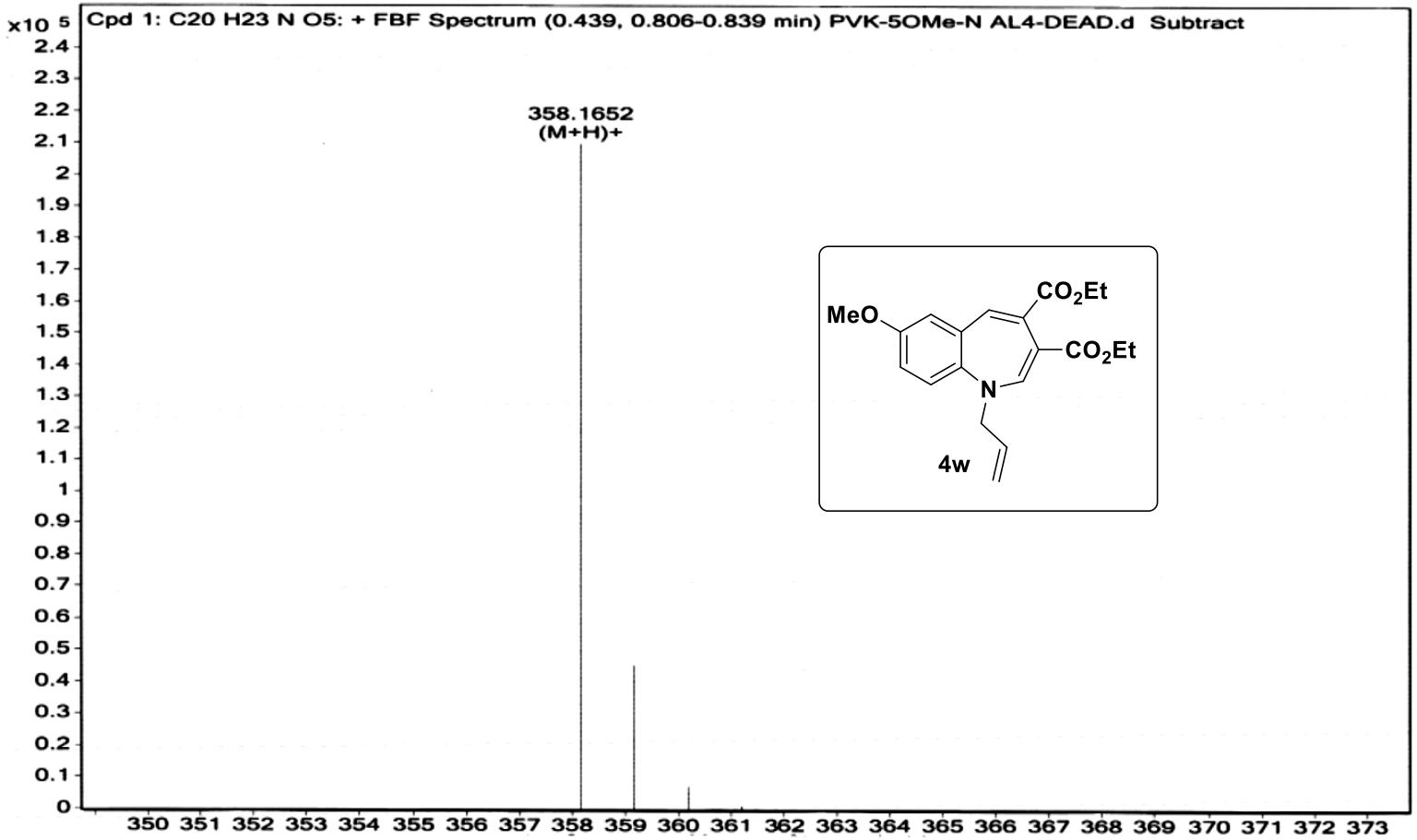


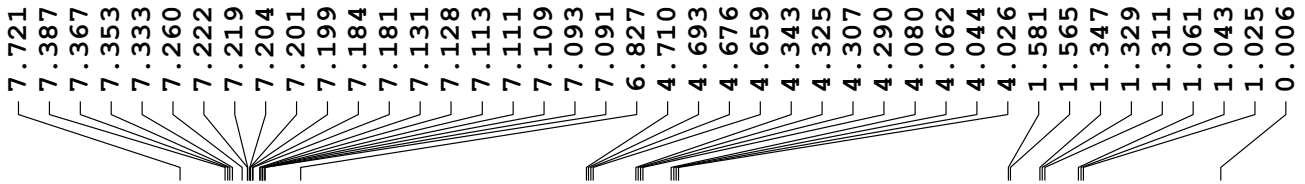

```
Current Data Parameters
NAME      PVK-50ME-N-ALY-DEAD
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150524
Time                  18.46
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                      203
DW                   60.800 usec
DE                    6.00 usec
TE                   297.7 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    11.42 usec
PL1                   -3.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                        32768
SF            400.1300036 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

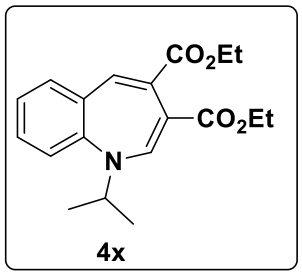



```
Current Data Parameters
NAME      PVK-50ME-N-ALLYL-DEAD
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20150524
Time                   20.05
INSTRUM                spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                 1.3631988 sec
RG                      28.5
DW                    20.800 usec
DE                     6.00 usec
TE                     299.5 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                     9.15 usec
PL1                    0.00 dB
SFO1             100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 90.00 usec
PL12                  14.90 dB
PL13                  14.90 dB
PL2                   -3.00 dB
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF               100.6127526 MHz
WDW                         EM
SSB                          0
LB                     1.00 Hz
GB                           0
PC                     1.40
```

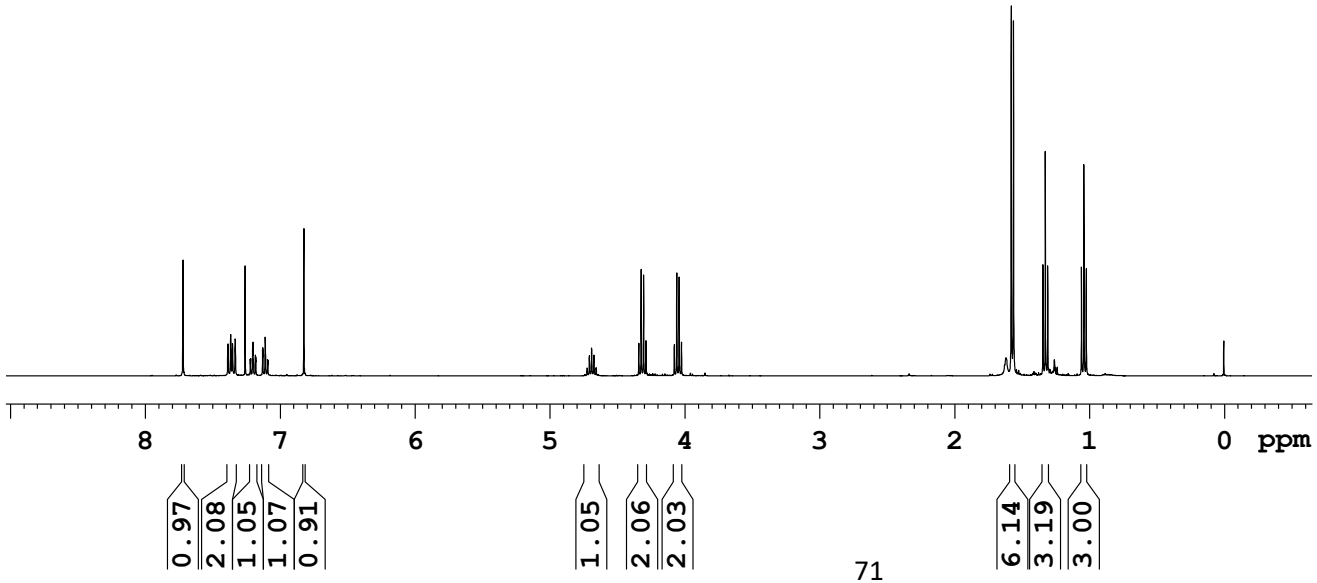
ıe	PVK-5OMe-N AL4-DEAD	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
ilename	PVK-5OMe-N AL4-DEAD.	ACQ Method	Pondicherry Universi	Comment	PVK-MB-357.1576	Acquired Time	02-06-2015 12:59:31



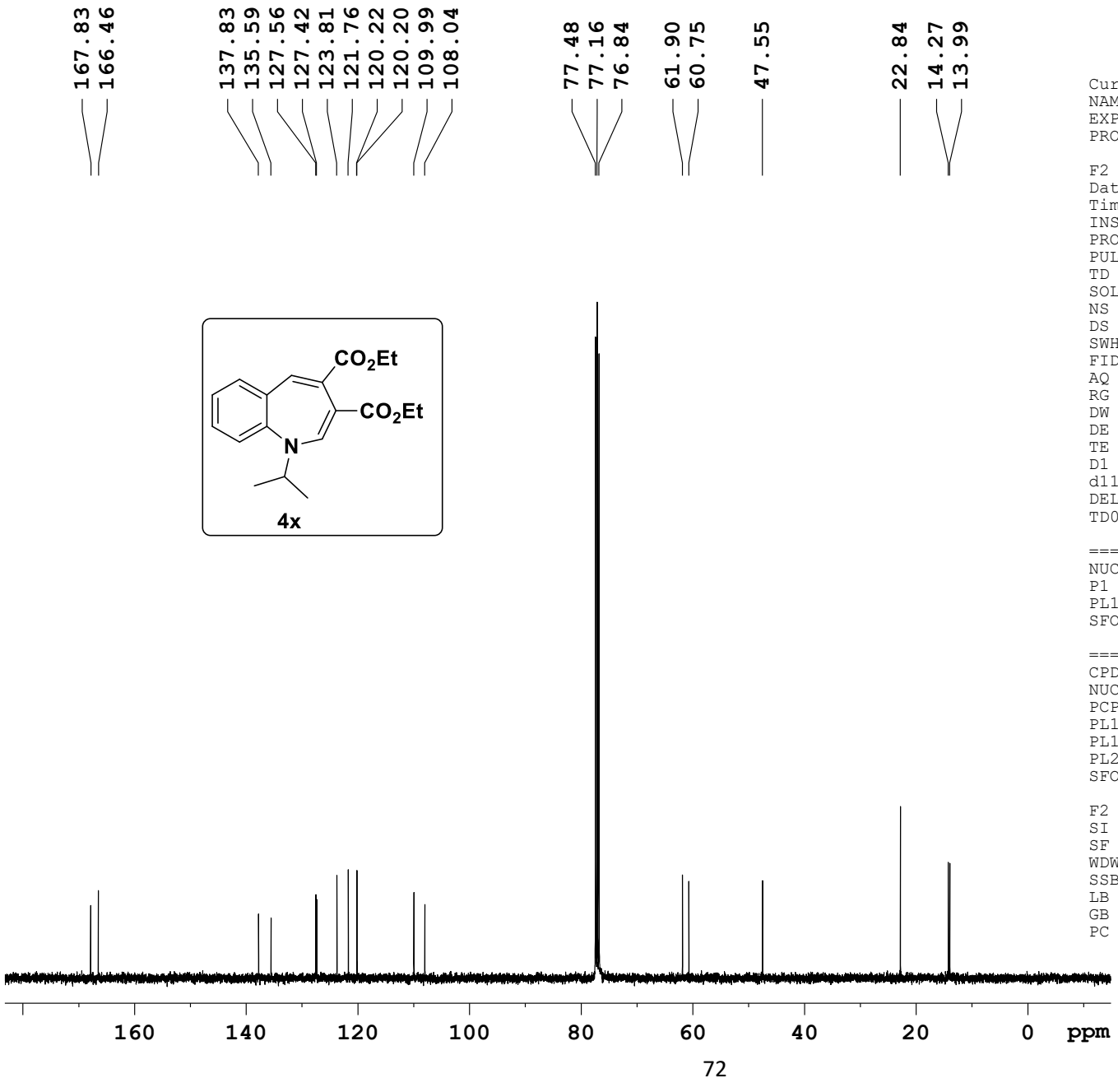




4x

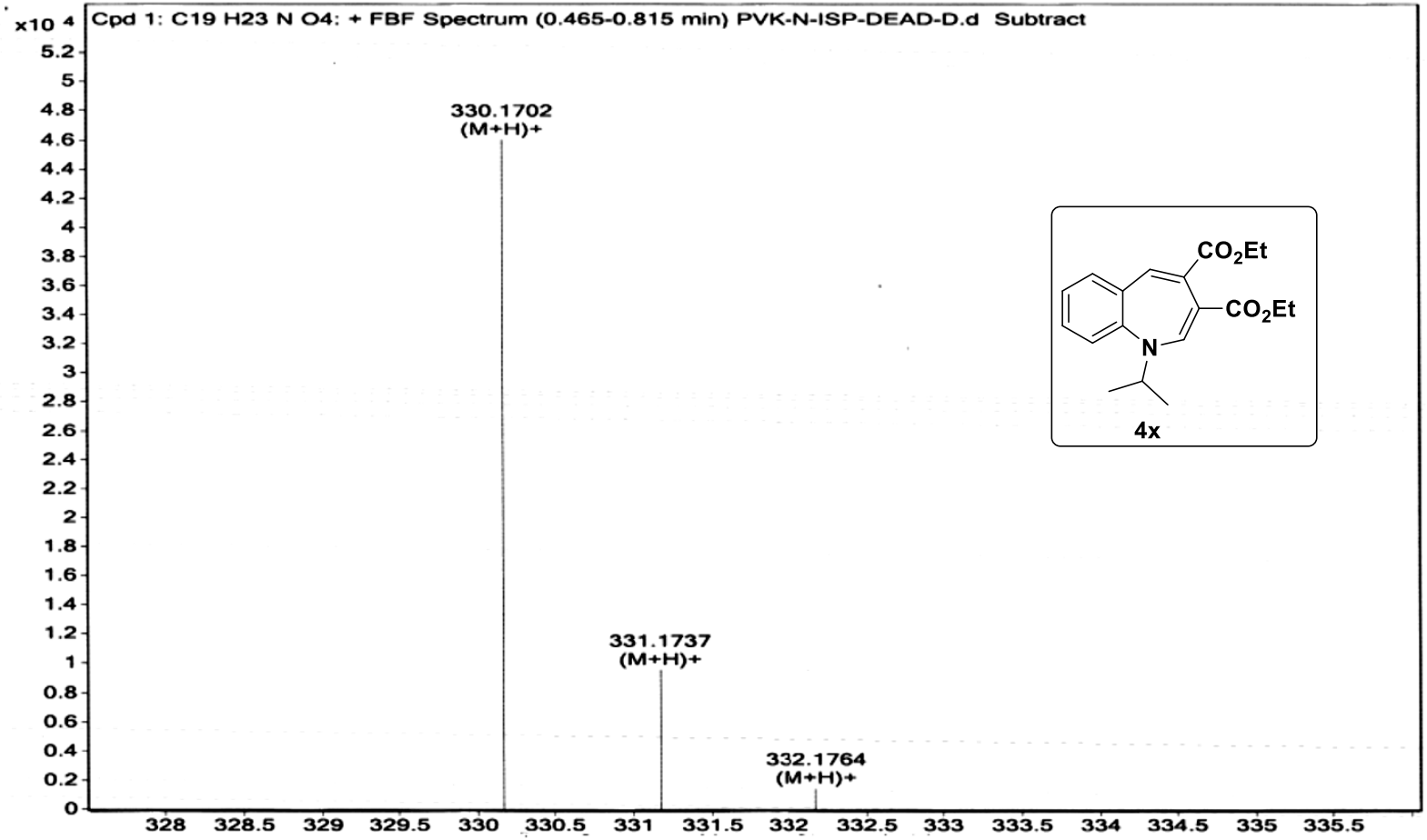



```
Current Data Parameters
NAME      TTR-PVK-N-ISP-DEAD
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180831
Time                   1.16
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9846387 sec
RG                       203
DW                    60.800 usec
DE                     6.00 usec
TE                    294.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                    14.35 usec
PL1                   -1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300048 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

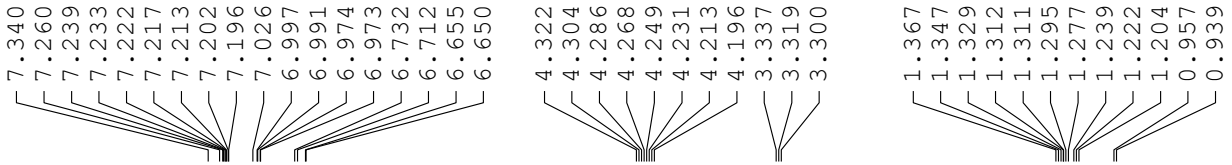


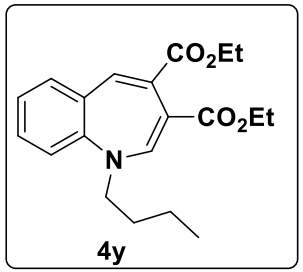

```
Current Data Parameters
NAME      TTR-PVK-N-ISP-DEAD
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180831
Time                1.57
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                  45.2
DW                20.800 usec
DE                 6.00 usec
TE                294.6 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.95 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127569 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Name	PVK-N-ISP-DEAD-D	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
A	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
a Filename	PVK-N-ISP-DEAD-D.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-329.1627	**Acquired Time**	11-09-2017 12:31:40

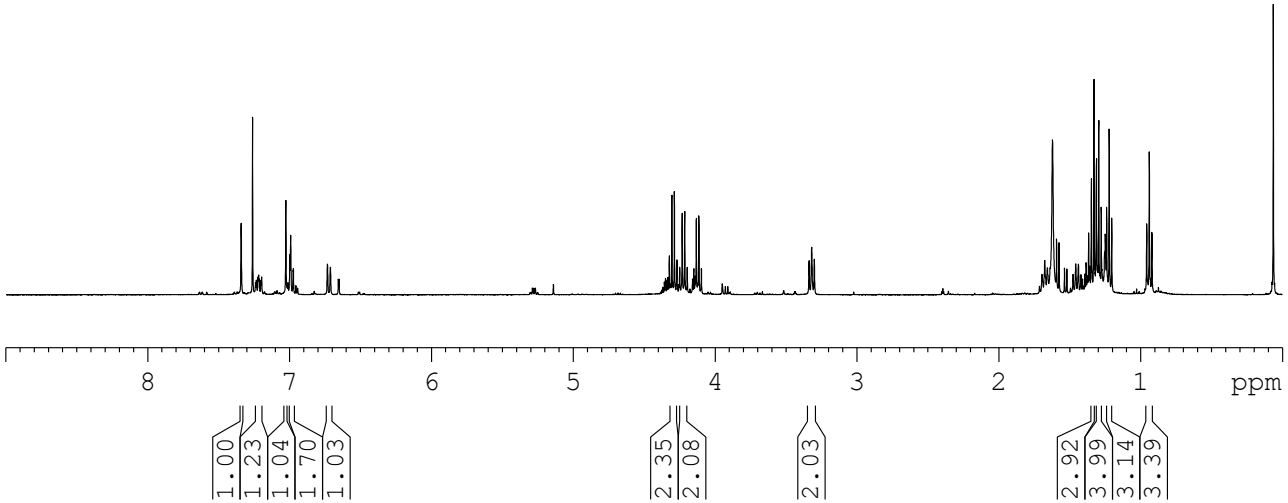


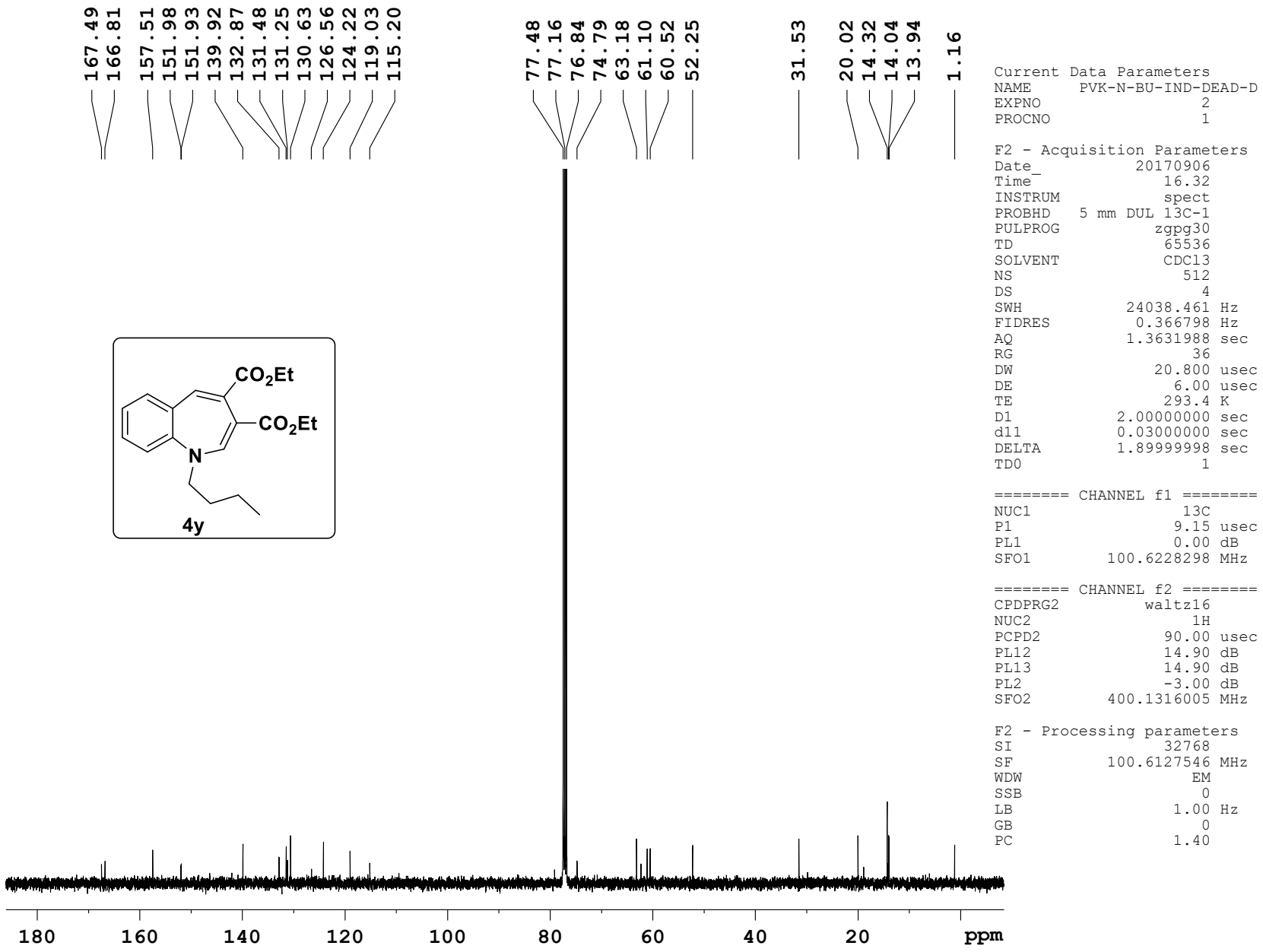
PROTON CDCl3 {D:\MB} KOPAL 1





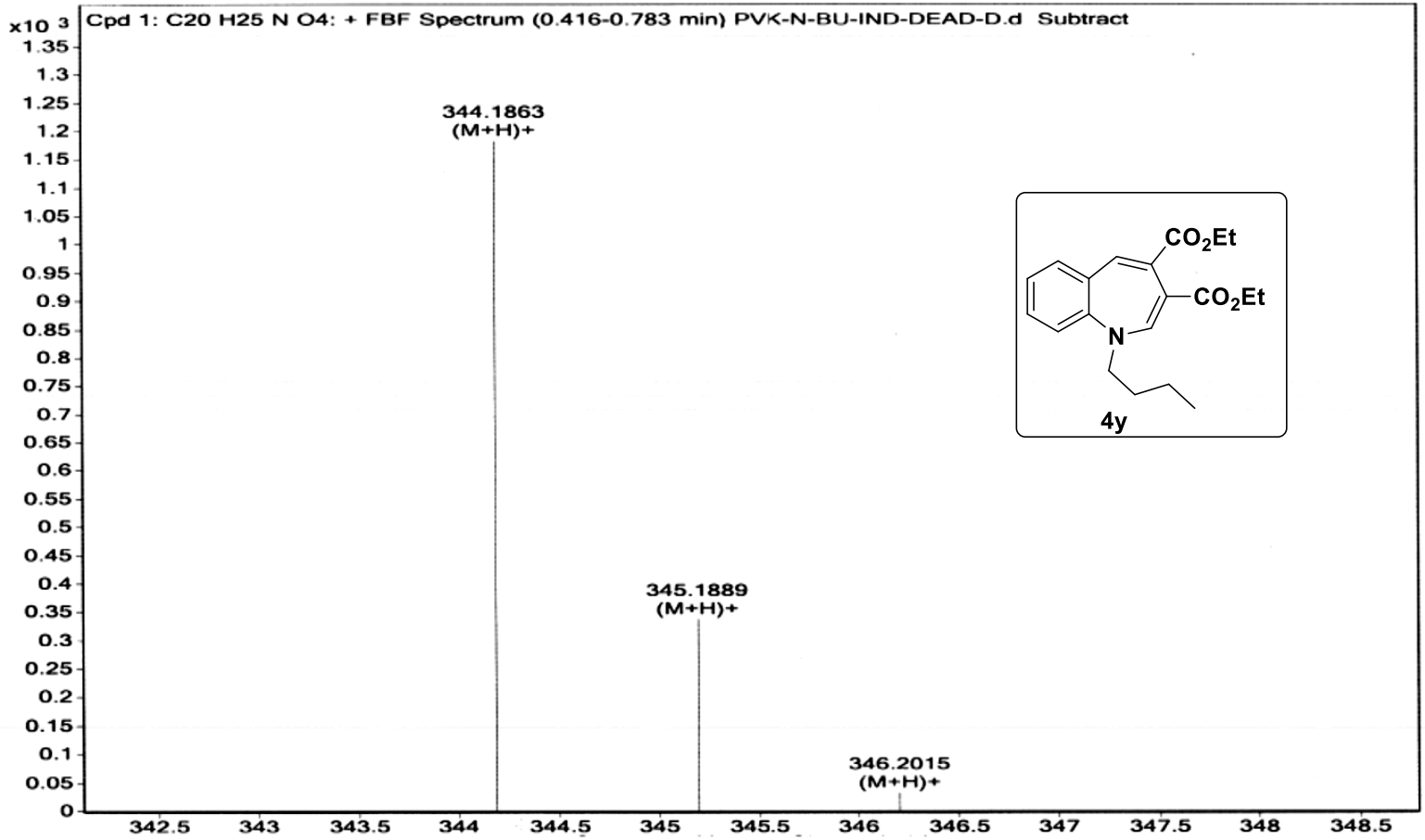

```
Current Data Parameters
NAME      PVK-N-BU-IND-DEAD-D
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170906
Time               16.19
INSTRUM            spect
PROBHD   5 mm DUL 13C-1
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                   203
DW                60.800 usec
DE                 6.00 usec
TE                292.8 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.42 usec
PL1                -3.00 dB
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300051 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

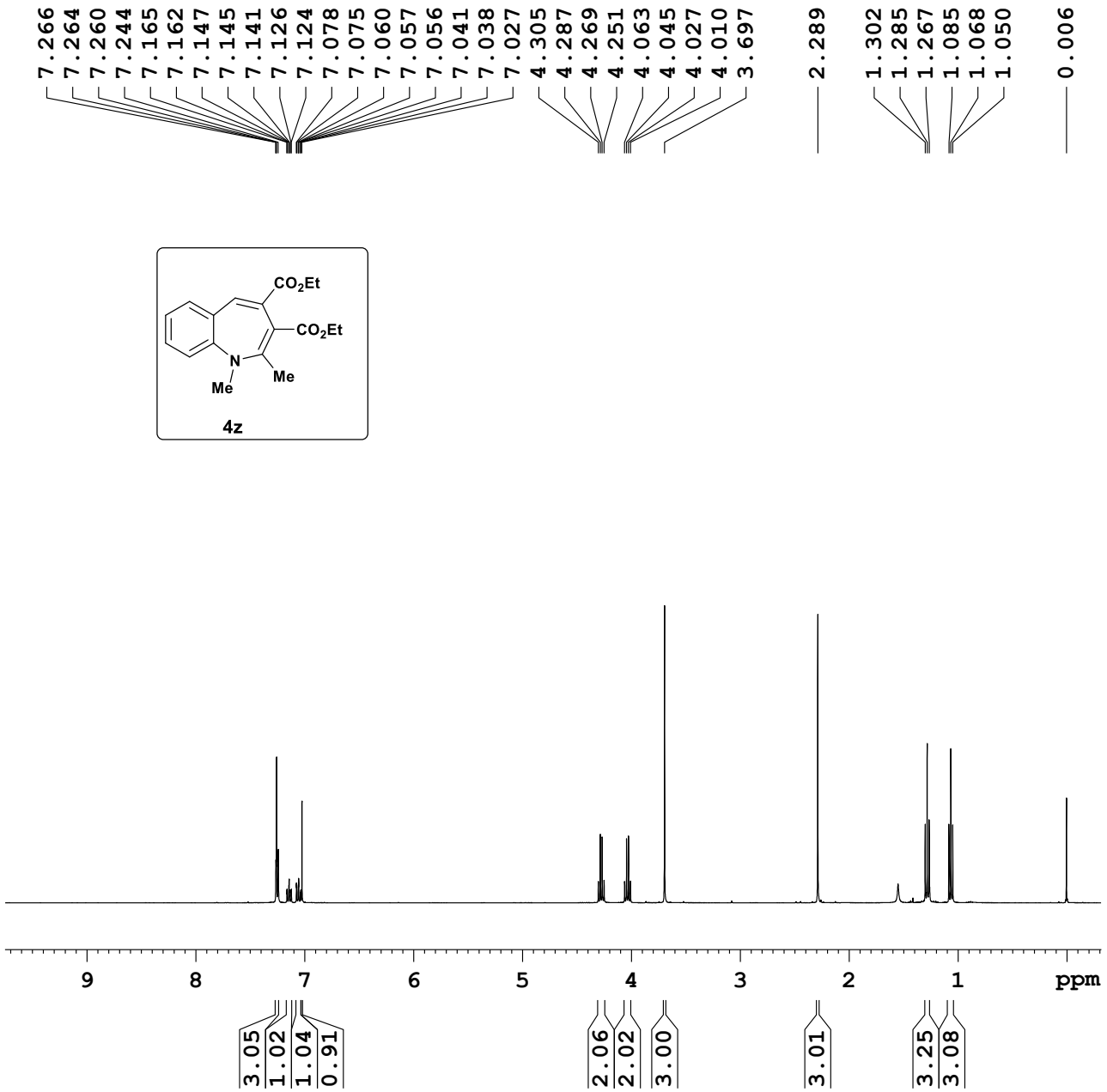




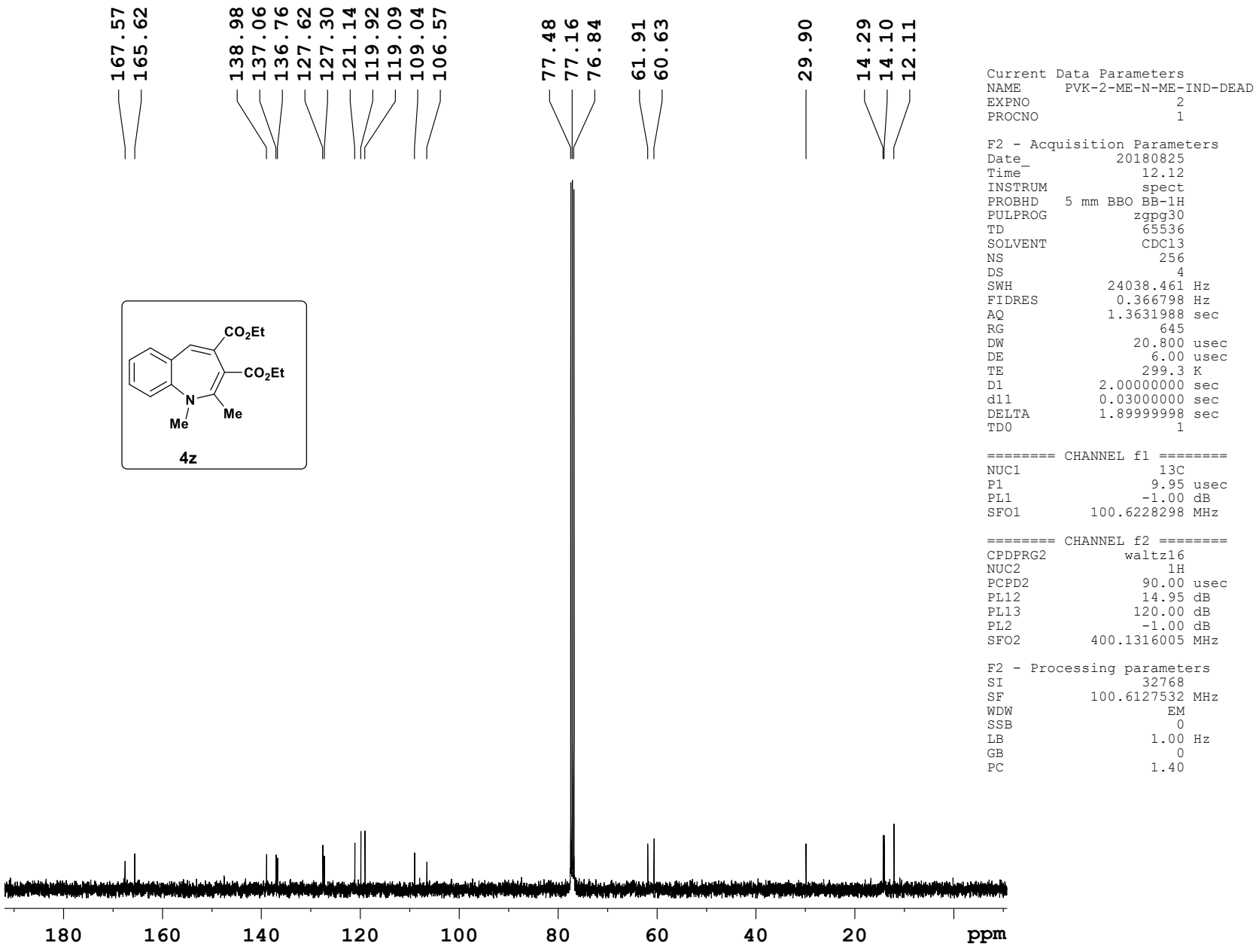

```
Current Data Parameters
NAME      PVK-N-BU-IND-DEAD-D
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20170906
Time                  16.32
INSTRUM               spect
PROBHD   5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     512
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631988 sec
RG                      36
DW                 20.800 usec
DE                  6.00 usec
TE                 293.4 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.15 usec
PL1                   0.00 dB
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                90.00 usec
PL12                 14.90 dB
PL13                 14.90 dB
PL2                  -3.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6127546 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

ame	PVK-N-BU-IND-DEAD-D	Position		Instrument Name	Q-TOF	User Name	QTOF-PU\admin
	-1	InjPosition		SampleType	Sample	IRM Calibration Status	Success
a Filename	PVK-N-BU-IND-DEAD-D.	ACQ Method	Pondicherry Universi	Comment	PVK-MB-343.1784	Acquired Time	11-09-2017 12:35:38



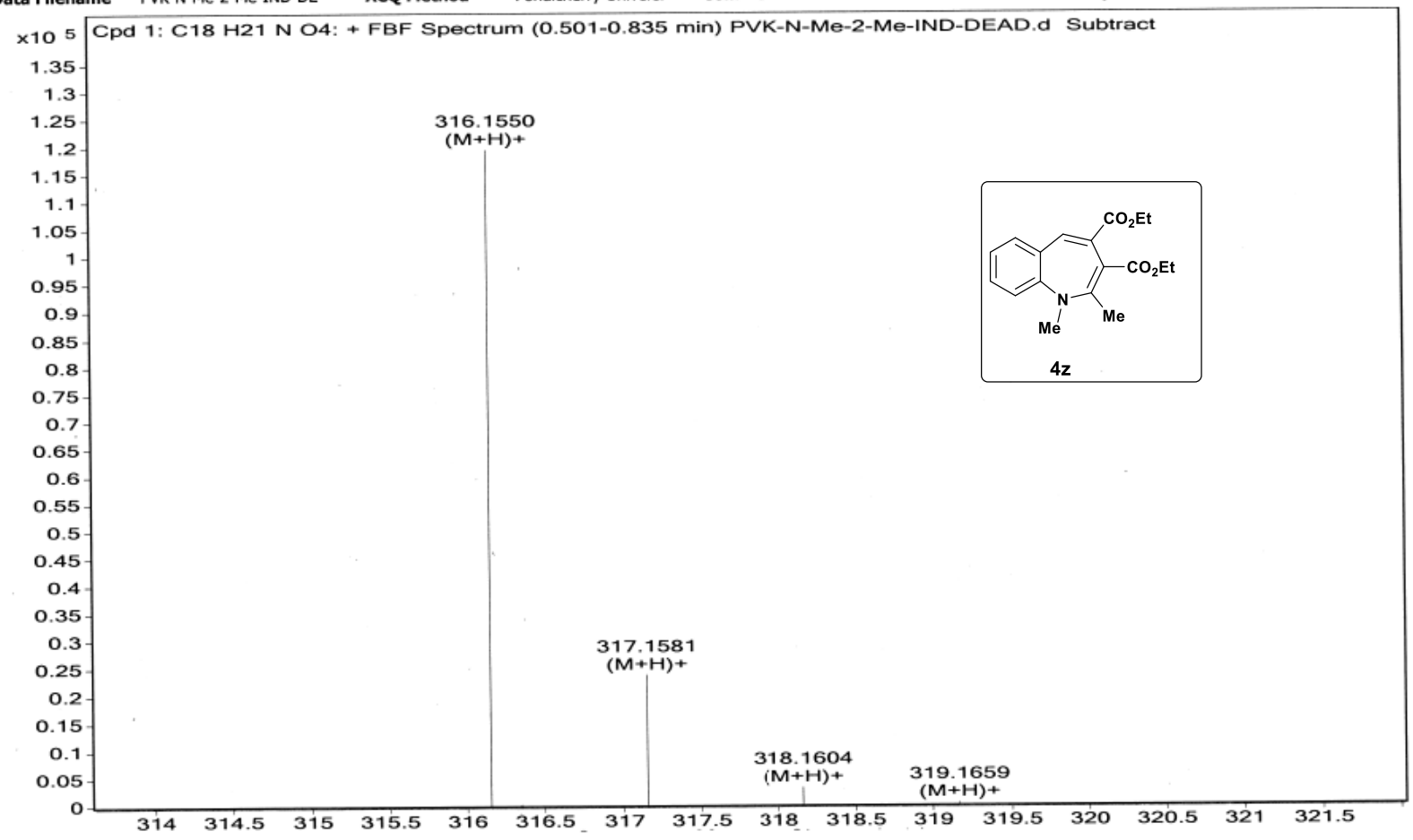


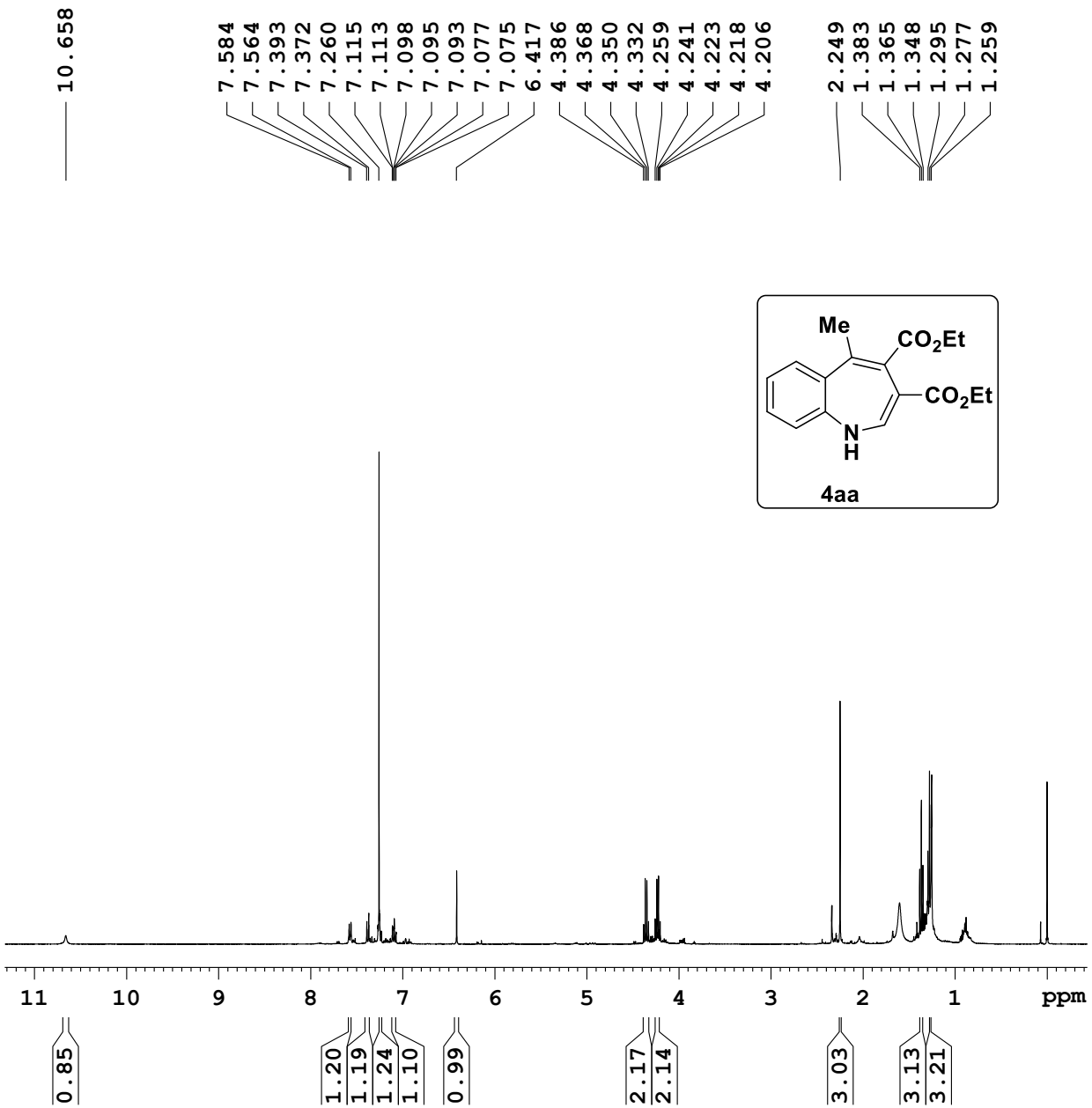

```
Current Data Parameters
NAME      PVK-2-ME-N-ME-IND-DEAD
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20180825
Time                       11.55
INSTRUM                    spect
PROBHD   5 mm BBO BB-1H
PULPROG                     zg30
TD                         65536
SOLVENT                    CDCl3
NS                            16
DS                             2
SWH                     8223.685 Hz
FIDRES                  0.125483 Hz
AQ                    3.9846387 sec
RG                           406
DW                        60.800 usec
DE                         6.00 usec
TE                        299.2 K
D1                   1.00000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                          1H
P1                        14.35 usec
PL1                       -1.00 dB
SFO1                400.1324710 MHz

F2 - Processing parameters
SI                         32768
SF                  400.1300046 MHz
WDW                           EM
SSB                            0
LB                         0.30 Hz
GB                             0
PC                          1.00
```



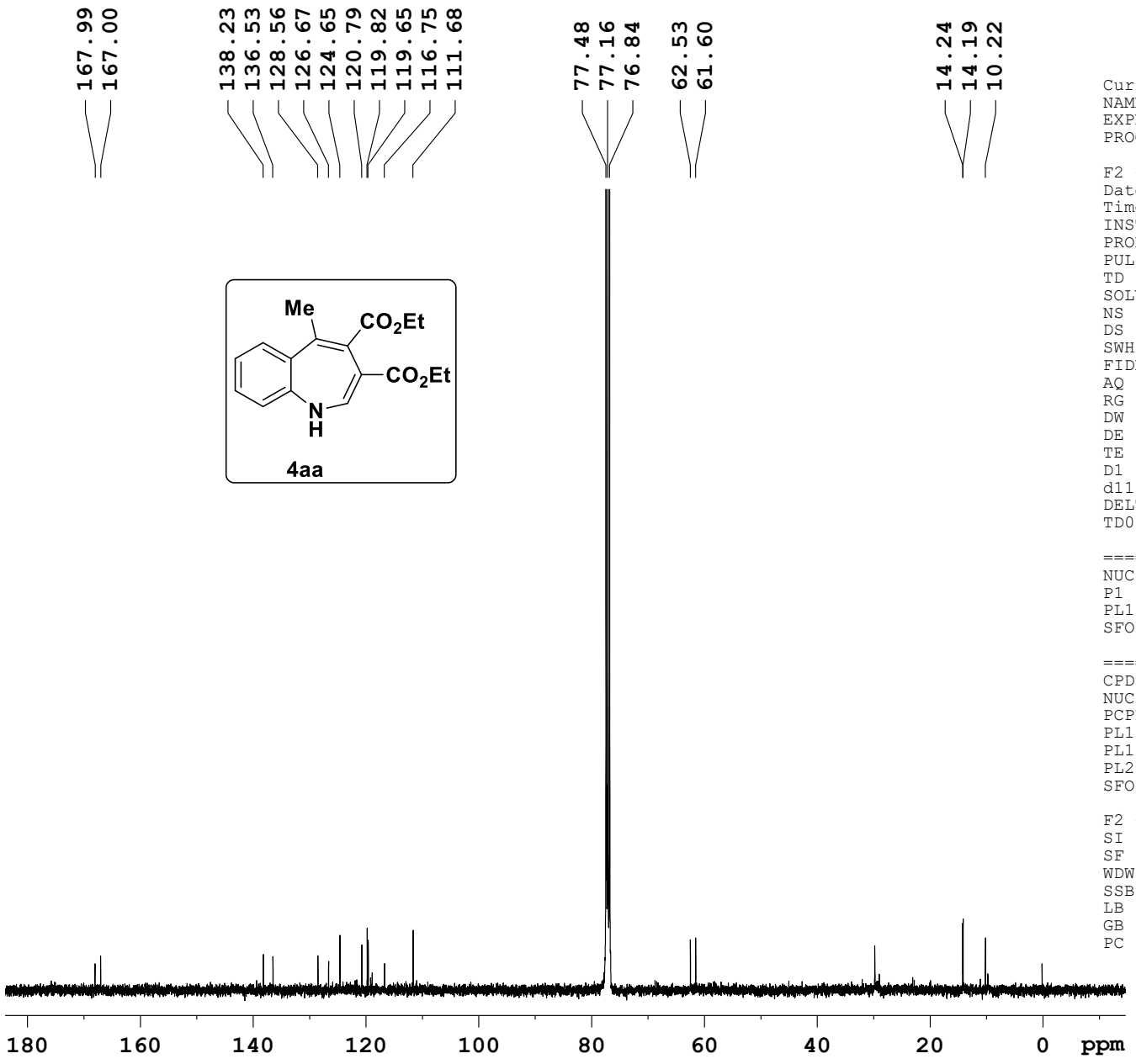

```
Current Data Parameters
NAME      PVK-2-ME-N-ME-IND-DEAD
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20180825
Time                       12.12
INSTRUM                    spect
PROBHD   5 mm BBO BB-1H
PULPROG                  zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                           256
DS                             4
SWH                    24038.461 Hz
FIDRES                  0.366798 Hz
AQ                     1.3631988 sec
RG                           645
DW                        20.800 usec
DE                         6.00 usec
TE                        299.3 K
D1                   2.00000000 sec
d11                  0.03000000 sec
DELTA                1.89999998 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         13C
P1                         9.95 usec
PL1                       -1.00 dB
SFO1                100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                         1H
PCPD2                     90.00 usec
PL12                      14.95 dB
PL13                     120.00 dB
PL2                       -1.00 dB
SFO2                400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                  100.6127532 MHz
WDW                           EM
SSB                            0
LB                         1.00 Hz
GB                             0
PC                         1.40
```

Sample Name	PVK-N-Me-2-Me-IND-DE	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-N-Me-2-Me-IND-DE	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-315.1471	**Acquired Time**	31-08-2018 12:14:07



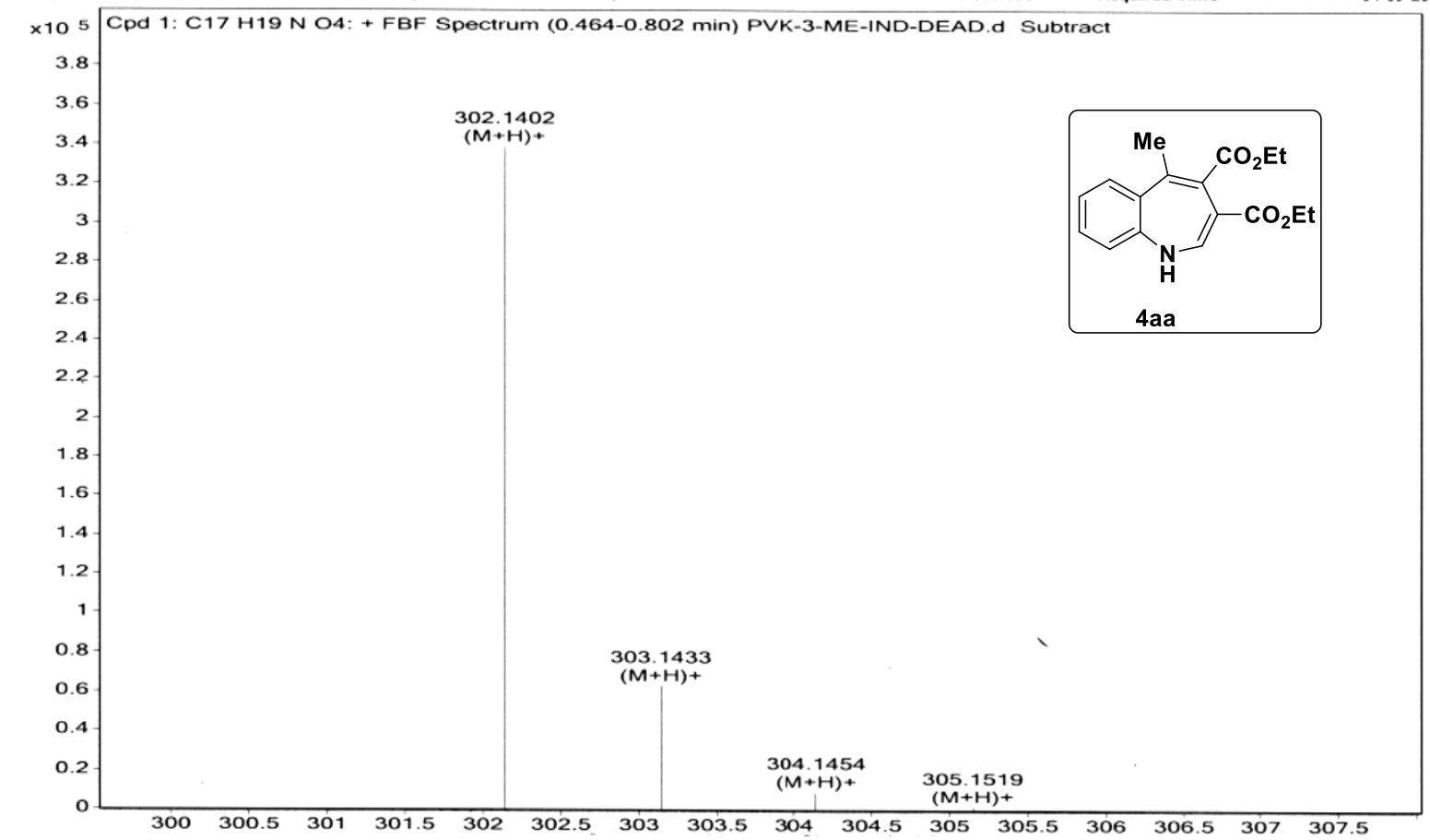


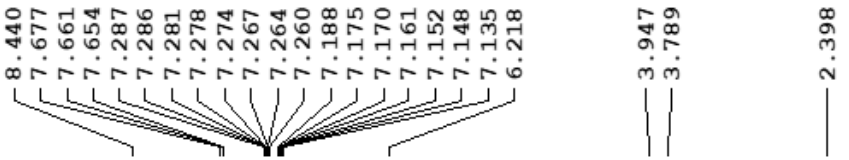

```
Current Data Parameters
NAME      PVK-3-ME-DEAD-IND
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20180902
Time                   2.43
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      287
DW                   60.800 usec
DE                    6.00 usec
TE                   294.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                   14.35 usec
PL1                  -1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300049 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

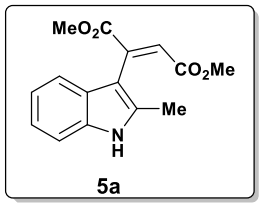



```
Current Data Parameters
NAME      PVK-3-ME-DEAD-IND
EXPNO                     3
PROCNO                    1

F2 - Acquisition Parameters
Date_           20180902
Time                9.33
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  7000
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631988 sec
RG                  45.2
DW                20.800 usec
DE                 6.00 usec
TE                294.5 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.95 usec
PL1                 -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              90.00 usec
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6127545 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

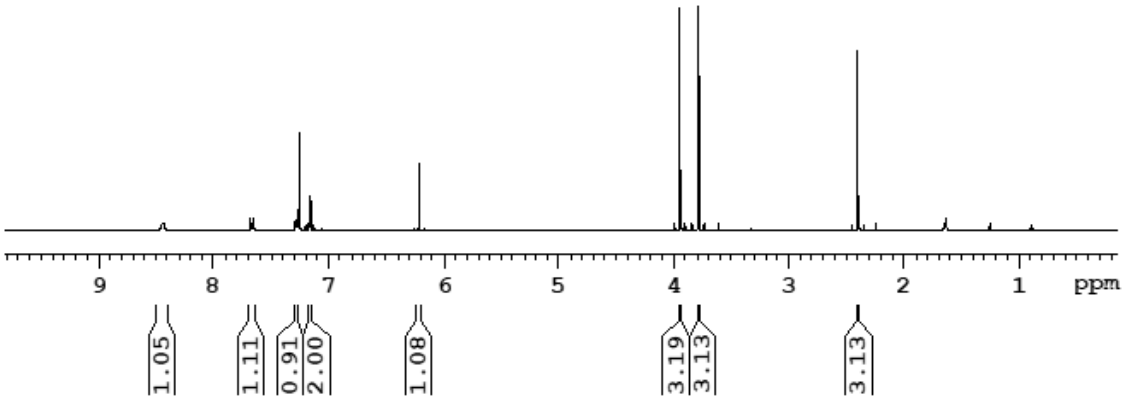
Sample Name	PVK-3-ME-IND-DEAD	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-3-ME-IND-DEAD.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-301.1314	**Acquired Time**	04-09-2018 11:23:34



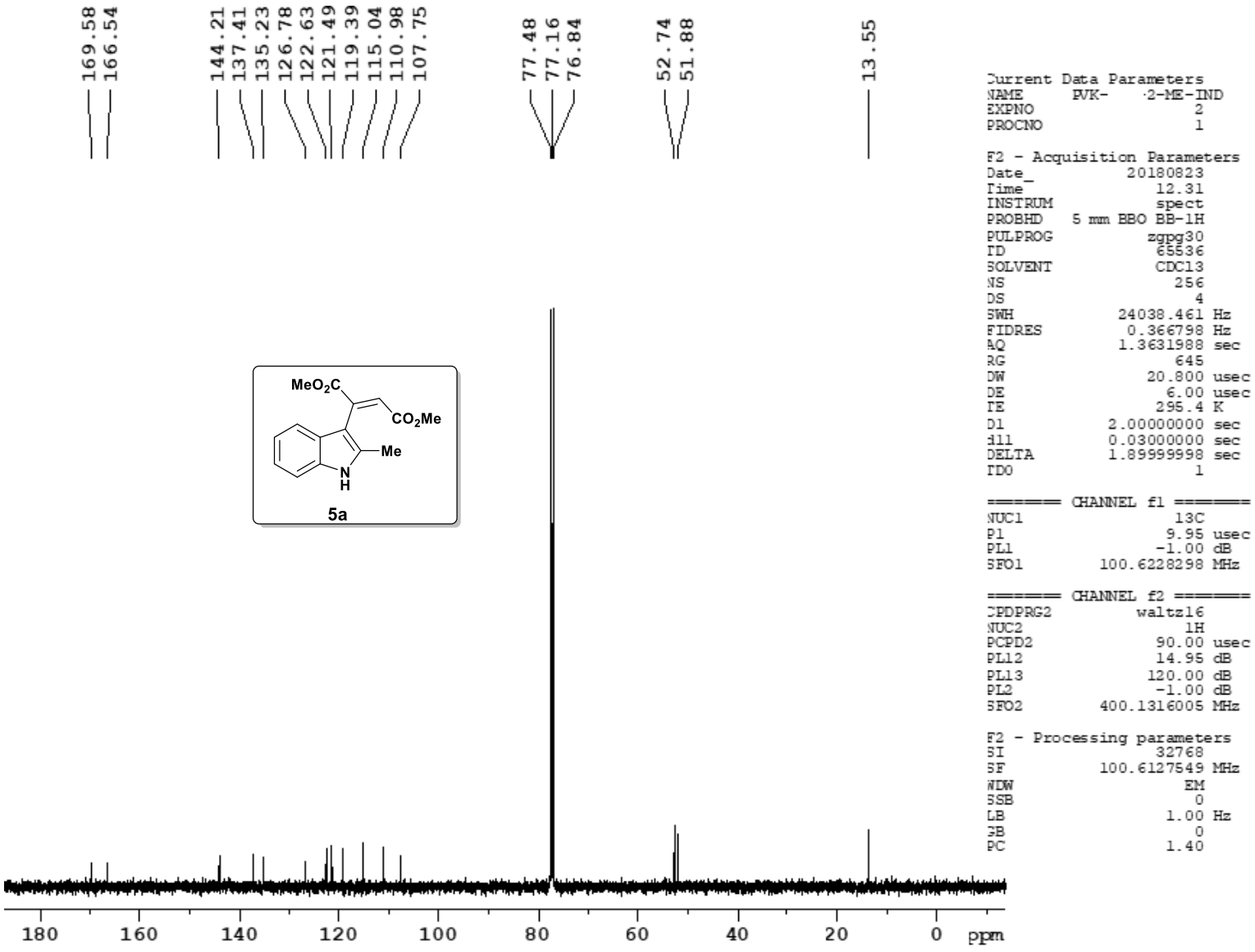




5a

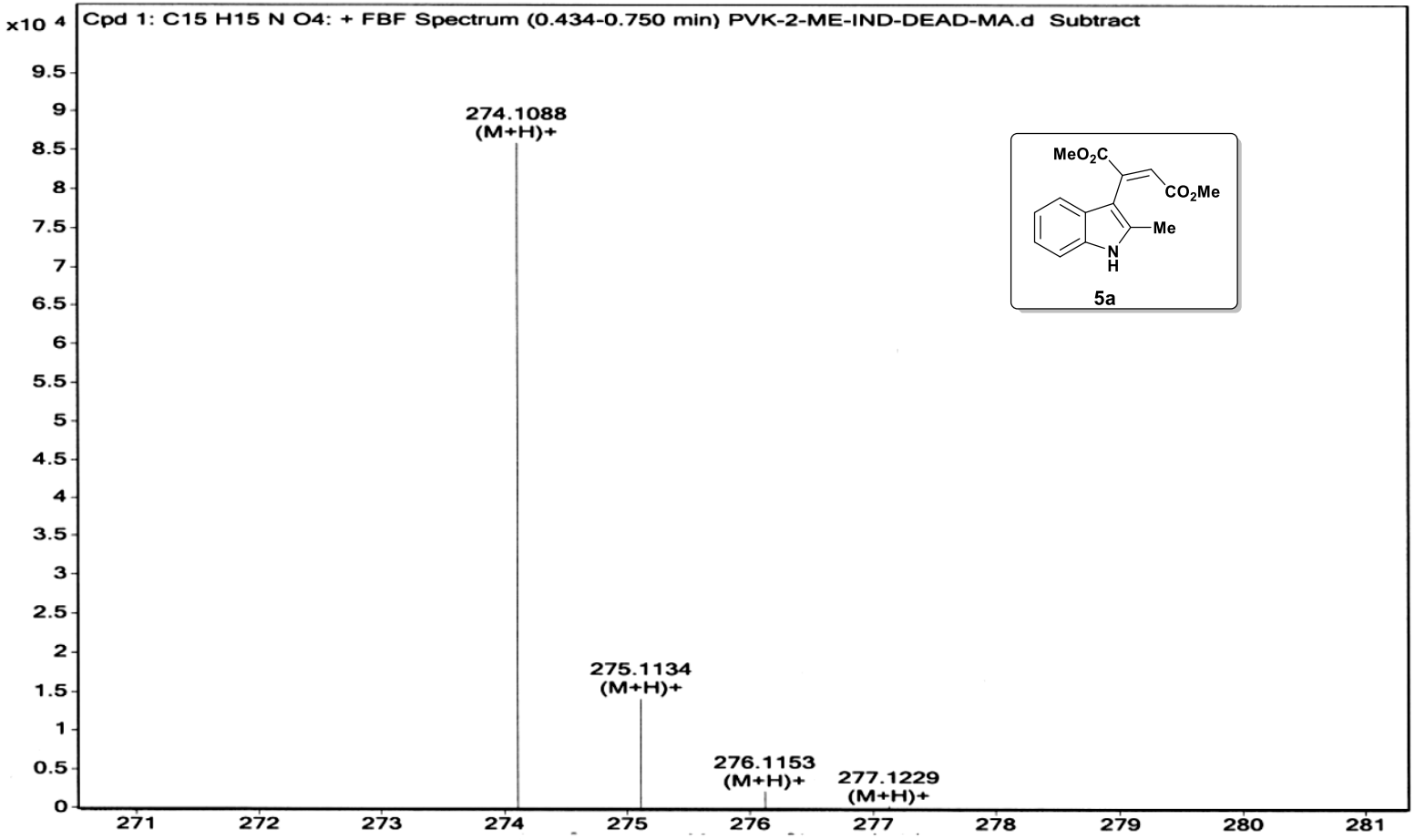



```
Current Data Parameters
NAME      PVK-    2-ME-IND
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20180823
Time               12.25
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ              3.9846387 sec
RG                   287
DW                60.800 usec
DE                 6.00 usec
TE                295.3 K
D1             1.00000000 sec
TD0                    1

====== CHANNEL f1 ======
NUC1                  1H
P1                 14.35 usec
PL1                -1.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300048 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

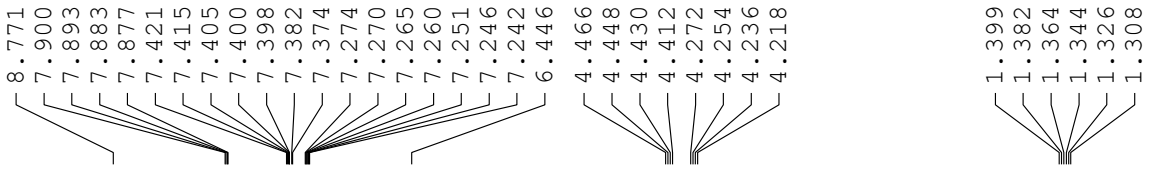


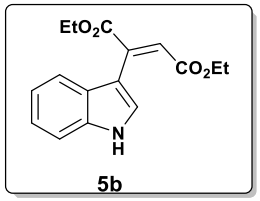

```
Current Data Parameters
NAME      PVK-    2-ME-IND
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20180823
Time              12.31
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                  645
DW               20.800 usec
DE                6.00 usec
TE               295.4 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                9.95 usec
PL1              -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            90.00 usec
PL12             14.95 dB
PL13            120.00 dB
PL2              -1.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127549 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

Sample Name	PVK-2-ME-IND-DEAD-MA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-2-ME-IND-DEAD-MA	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-302.1392	**Acquired Time**	25-04-2018 16:00:40



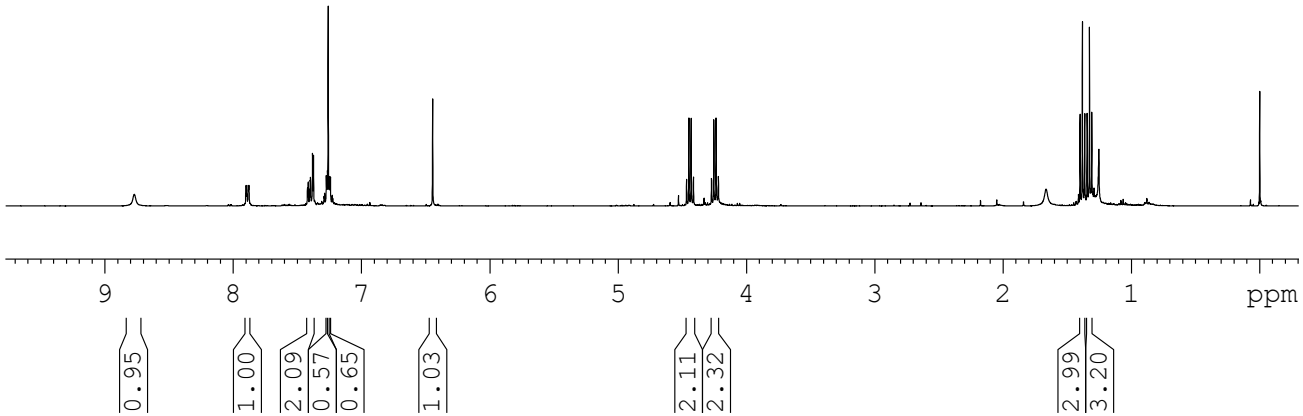
PROTON CDCl3 {D:\MB} KOPAL 1

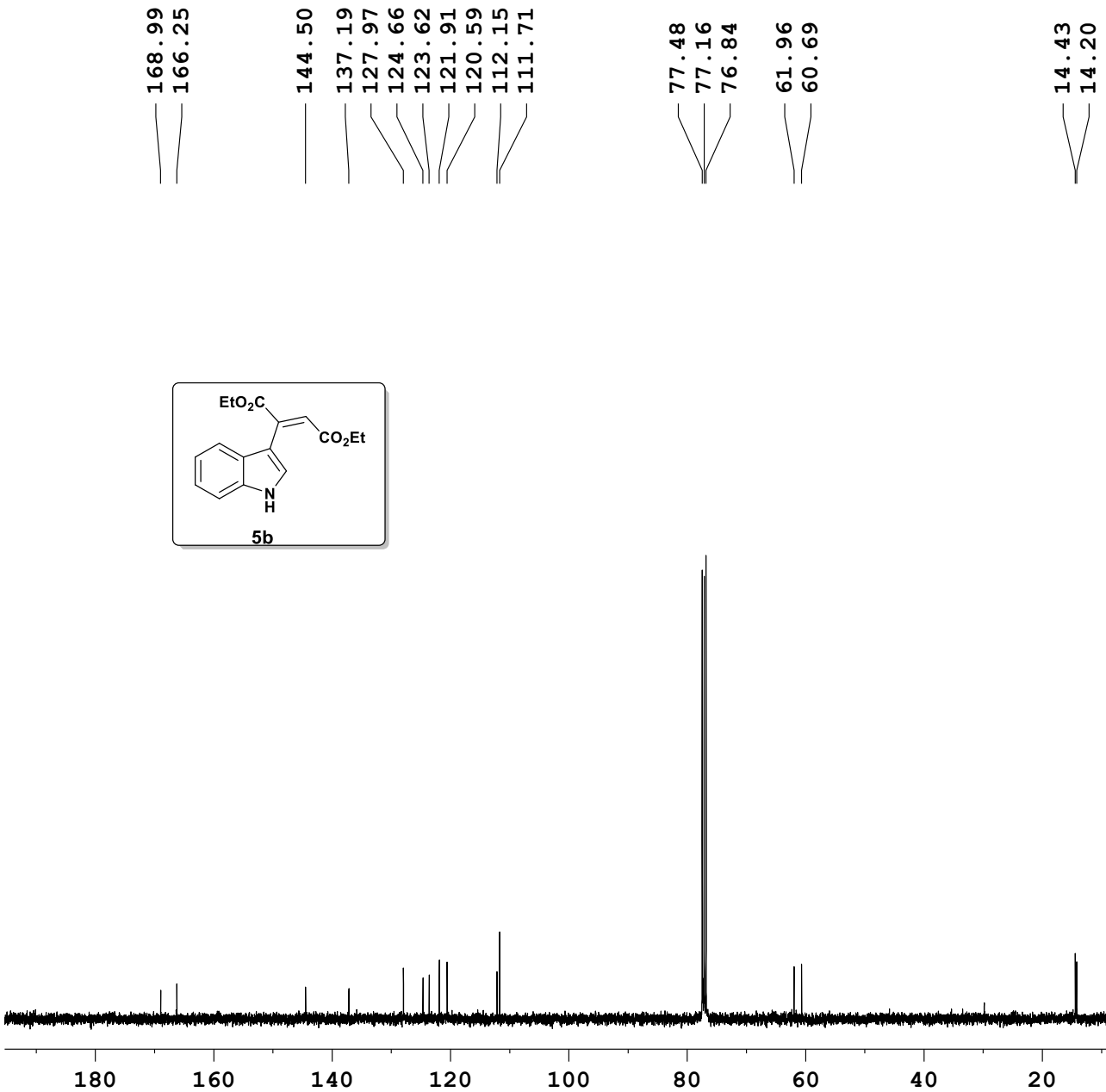




5b

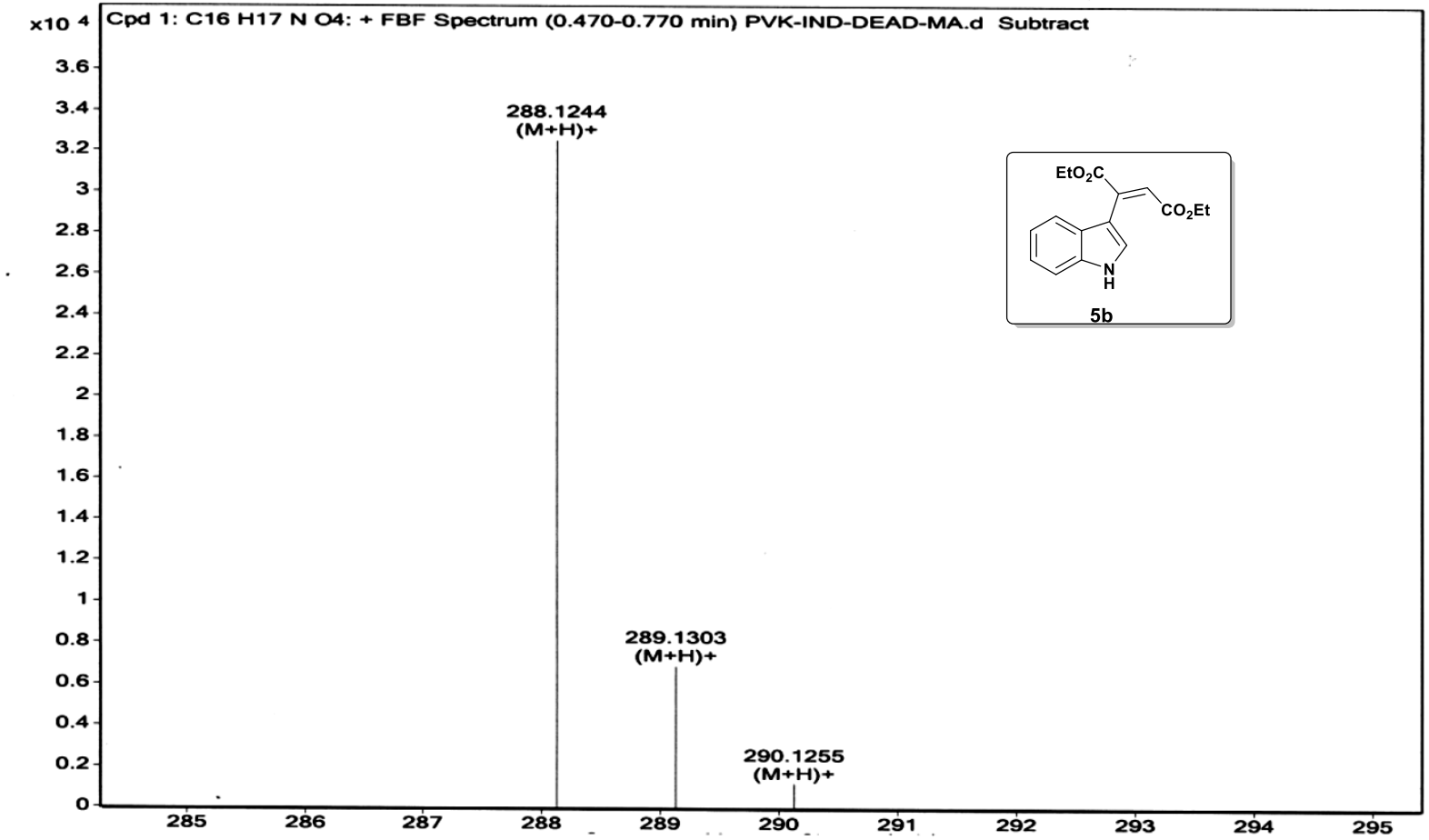
```
Current Data Parameters
NAME      PVK-IND-DEAD-D
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180408
Time               12.26
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.125483 Hz
AQ             3.9846387 sec
RG                   256
DW                60.800 usec
DE                 6.00 usec
TE                291.9 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 14.35 usec
PL1                -1.00 dB
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300049 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



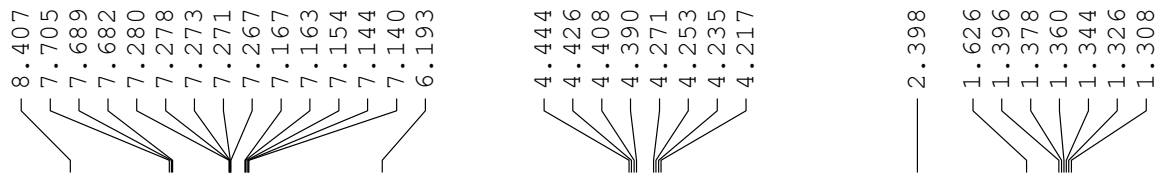


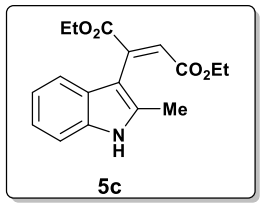

```
Current Data Parameters
NAME      PVK-IND-DEAD-D
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180410
Time              10.44
INSTRUM           spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  256
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631988 sec
RG                 45.2
DW                20.800 usec
DE                 6.00 usec
TE                293.2 K
D1           1.00000000 sec
d11          0.03000000 sec
DELTA        0.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.95 usec
PL1                -1.00 dB
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6127560 MHz
WDW                    EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Sample Name	PVK-IND-DEAD-MA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-IND-DEAD-MA.d	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-288.1236	**Acquired Time**	25-04-2018 16:17:35



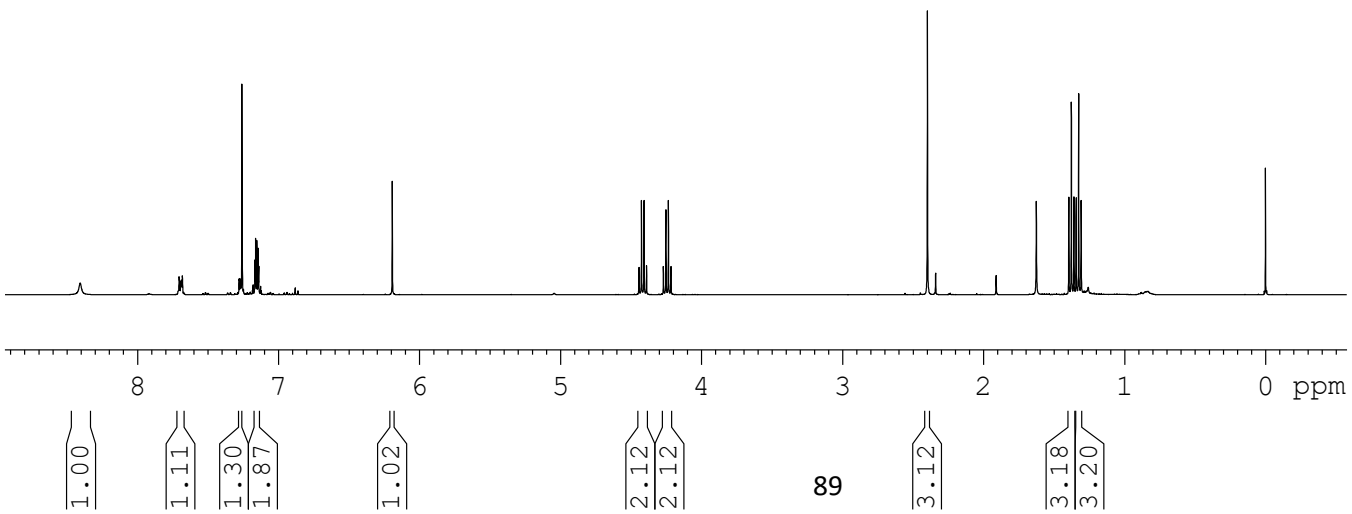
PROTON CDCl3 {D:\MB} KOPAL 1

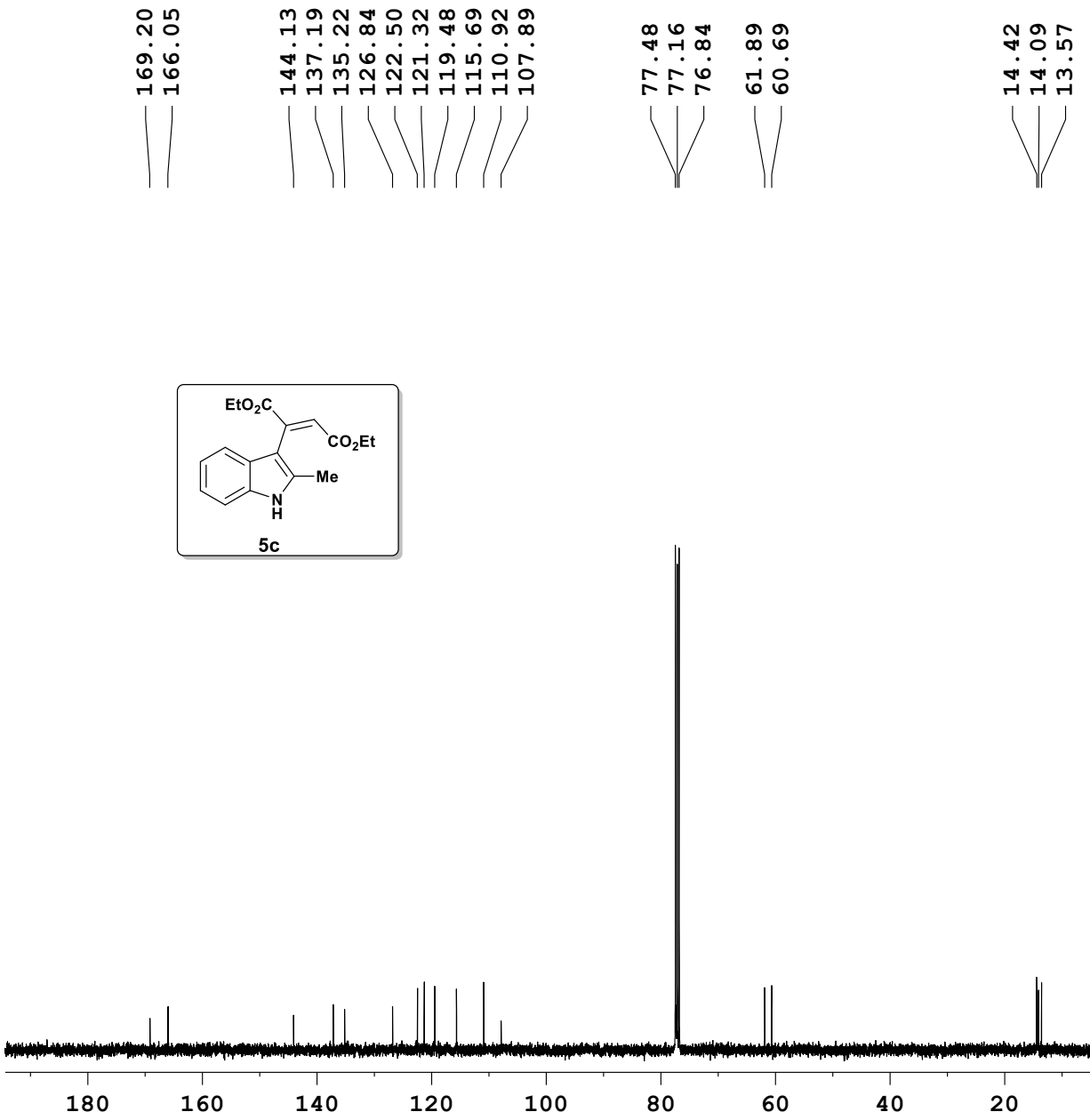




5c

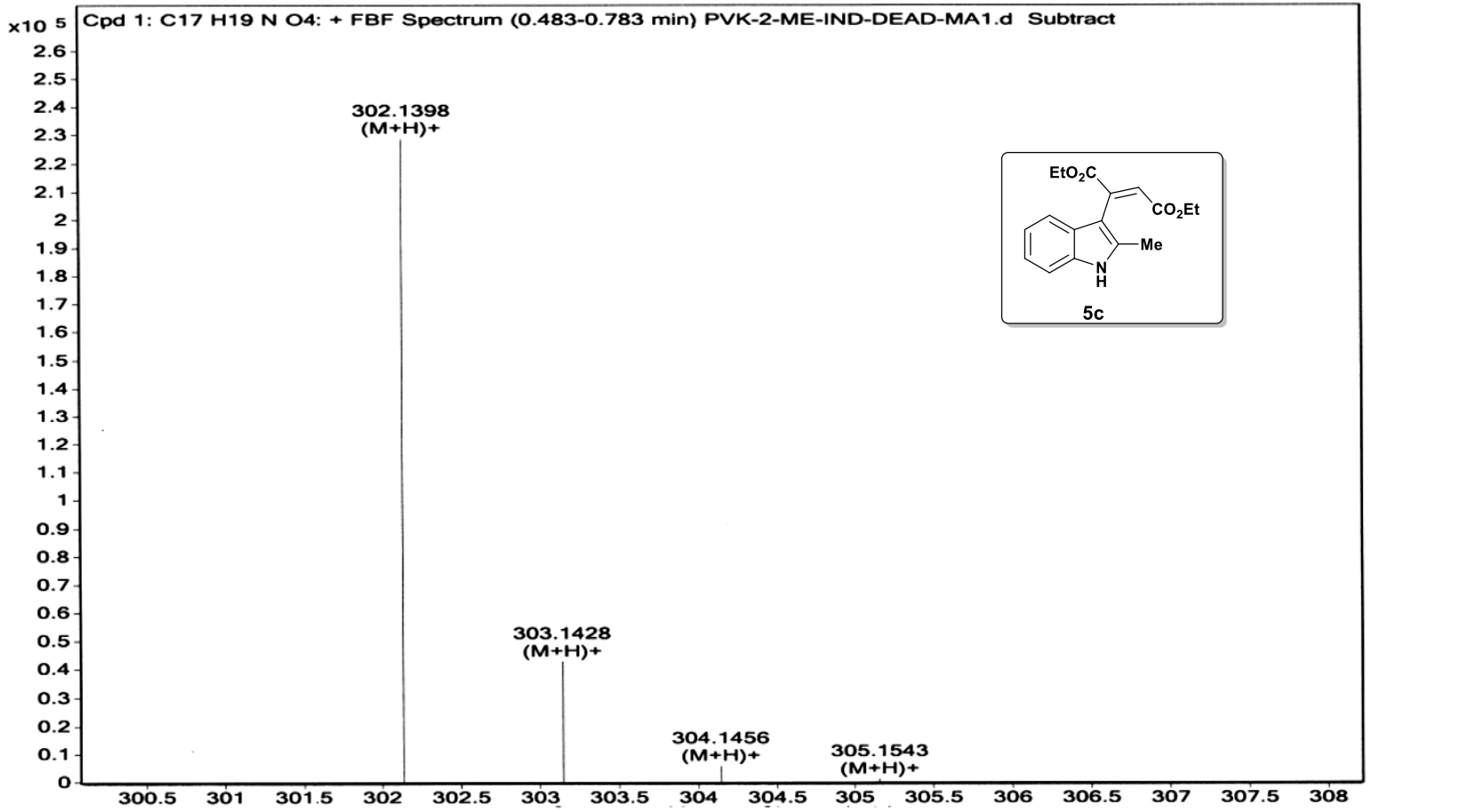
```
Current Data Parameters
NAME      PVK-2-Me-IND-DEAD-D
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20180408
Time                  22.44
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9846387 sec
RG                      287
DW                   60.800 usec
DE                    6.00 usec
TE                   295.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                   14.35 usec
PL1                  -1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300048 MHz
WDW                      EM
SSB                       0
LB                    0.30 Hz
GB                        0
PC                     1.00
```



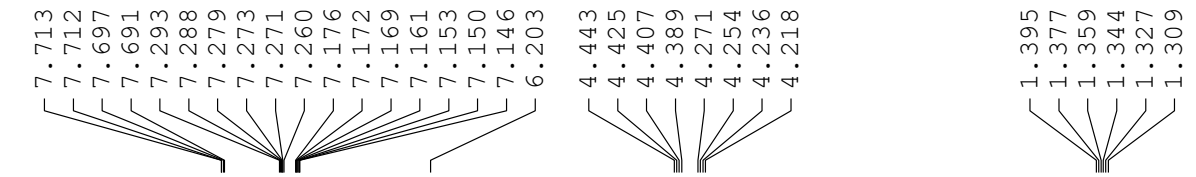


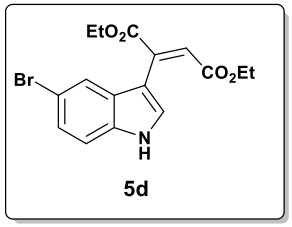

```
Current Data Parameters
NAME      PVK-2-Me-IND-DEAD-D
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20180410
Time                  10.31
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgpg30
TD                   65536
SOLVENT              CDC13
NS                     243
DS                       4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631988 sec
RG                     362
DW                  20.800 usec
DE                   6.00 usec
TE                  292.8 K
D1               1.00000000 sec
d11              0.03000000 sec
DELTA            0.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.95 usec
PL1                  -1.00 dB
SFO1           100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2                90.00 usec
PL12                 14.95 dB
PL13                120.00 dB
PL2                  -1.00 dB
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF             100.6127555 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

Sample Name	PVK-2-ME-IND-DEAD-MA	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-2-ME-IND-DEAD-MA	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-302.1392	**Acquired Time**	25-04-2018 16:06:42



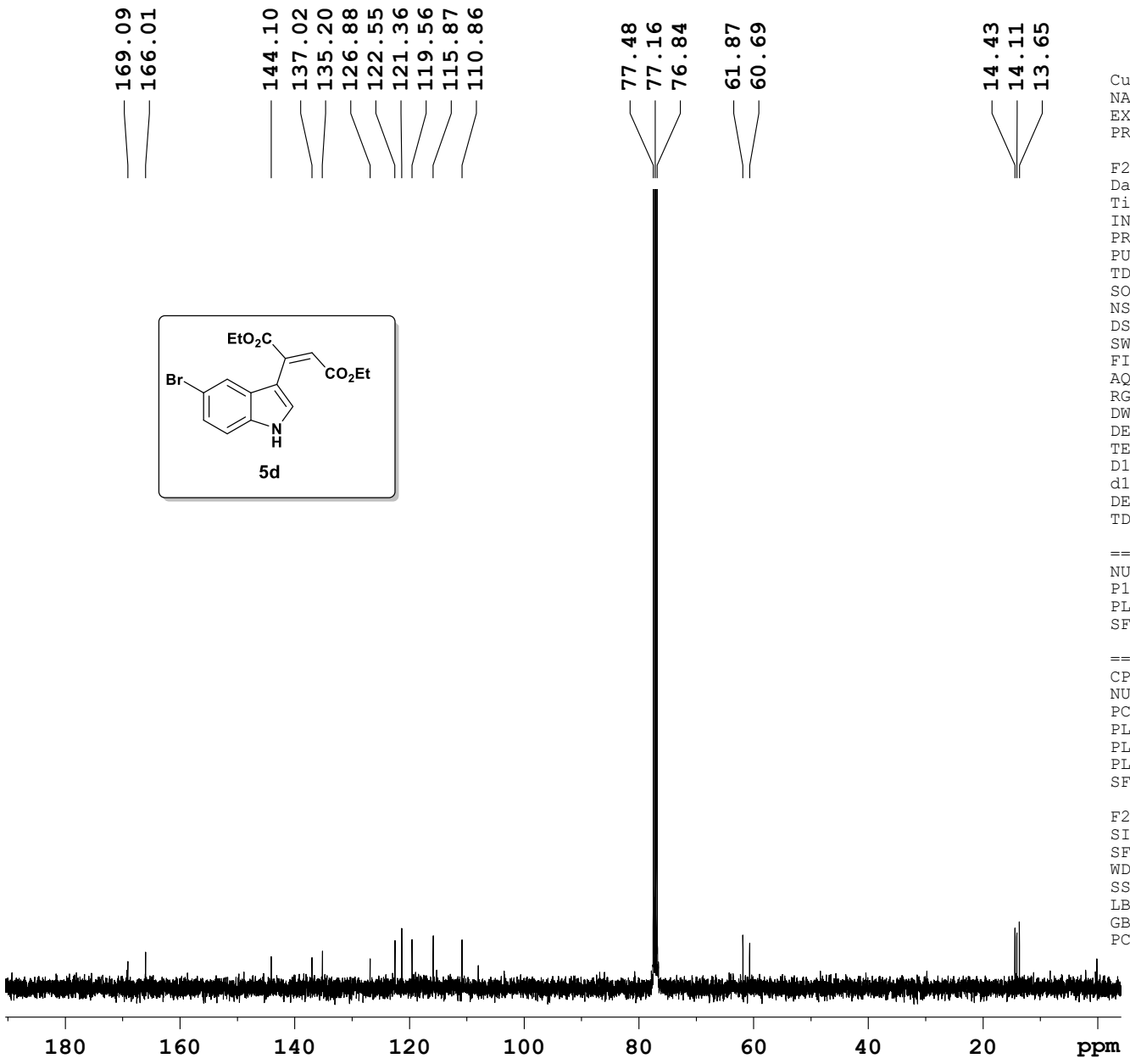
PROTON CDCl3 {D:\MB} KOPAL 1





5d


```
Current Data Parameters
NAME      PVK-5-Br-IND-DEAD
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20180408
Time                 12.30
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8223.685 Hz
FIDRES            0.125483 Hz
AQ               3.9846387 sec
RG                    362
DW                 60.800 usec
DE                  6.00 usec
TE                 292.1 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  14.35 usec
PL1                 -1.00 dB
SFO1          400.1324710 MHz

F2 - Processing parameters
SI                  32768
SF            400.1300048 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```




```
Current Data Parameters
NAME      PVK-5-Br-IND-DEAD
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180408
Time               12.38
INSTRUM            spect
PROBHD   5 mm BBO BB-1H
PULPROG          zgpg30
TD                65536
SOLVENT           CDC13
NS                  350
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                  322
DW               20.800 usec
DE                6.00 usec
TE               292.4 K
D1            1.00000000 sec
d11           0.03000000 sec
DELTA         0.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.95 usec
PL1                -1.00 dB
SFO1         100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              90.00 usec
PL12               14.95 dB
PL13              120.00 dB
PL2                -1.00 dB
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF           100.6127547 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

Sample Name	PVK-5-Br-IND-DEAD-RP	**Position**		**Instrument Name**	Q-TOF	**User Name**	QTOF-PU\admin
Inj Vol	-1	**InjPosition**		**SampleType**	Sample	**IRM Calibration Status**	Success
Data Filename	PVK-5-Br-IND-DEAD-RP	**ACQ Method**	Pondicherry Universi	**Comment**	PVK-MB-365.2303	**Acquired Time**	09-05-2018 14:51:28