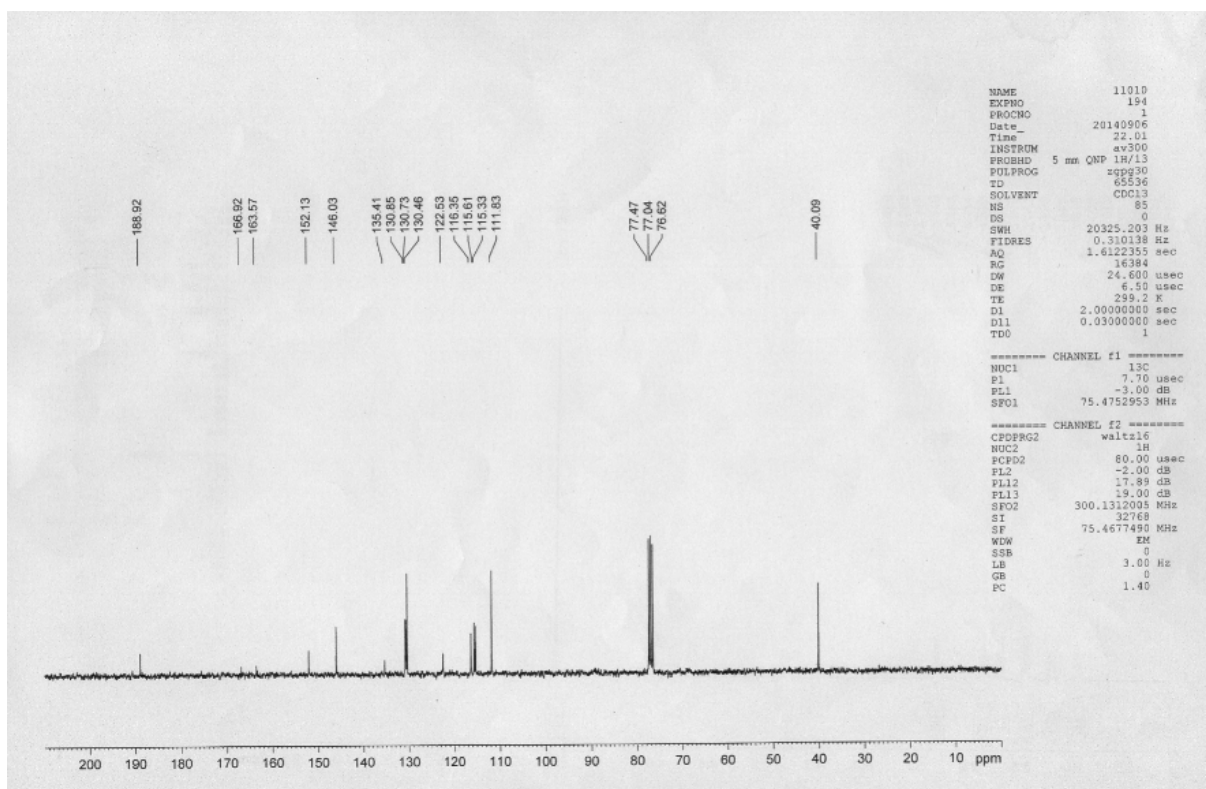
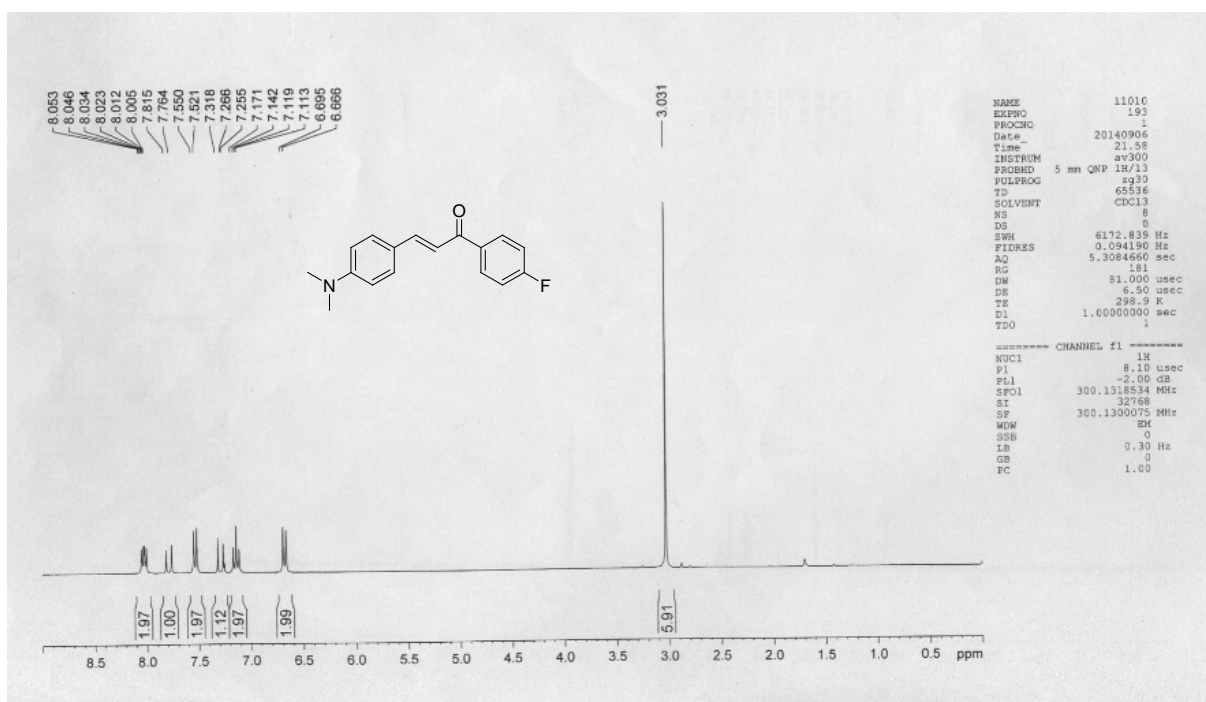
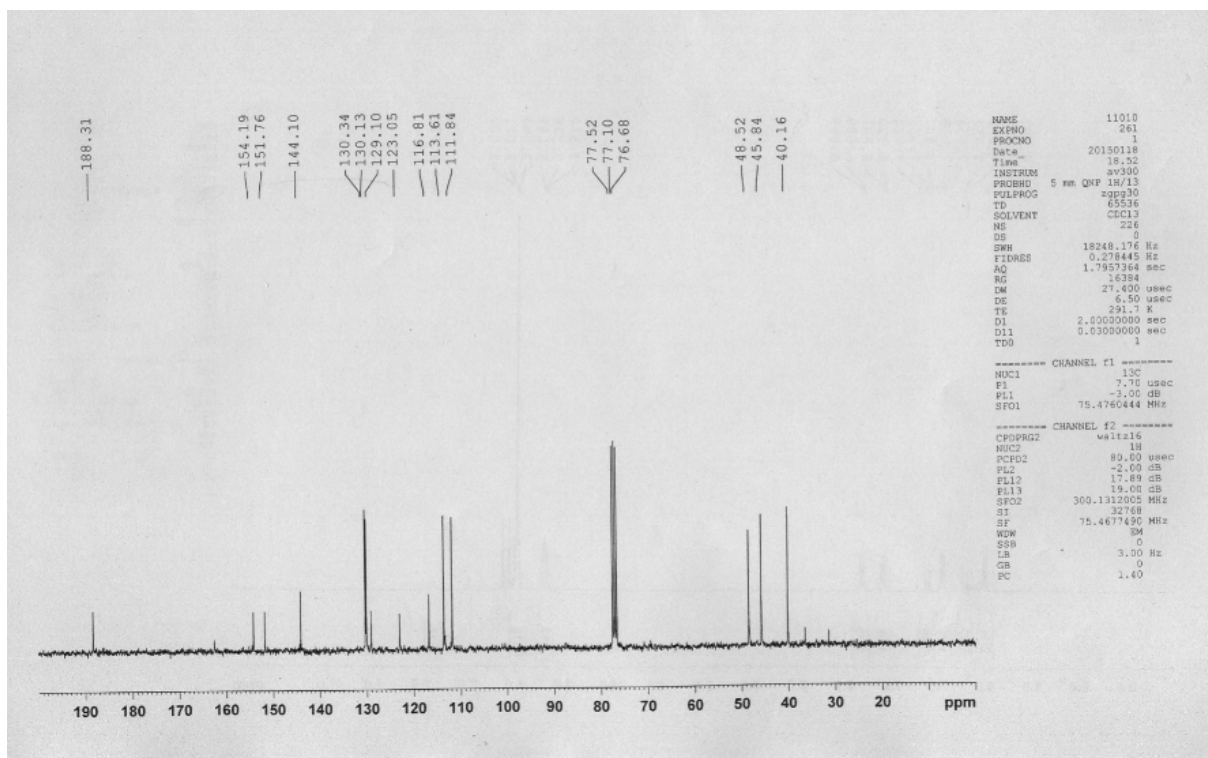
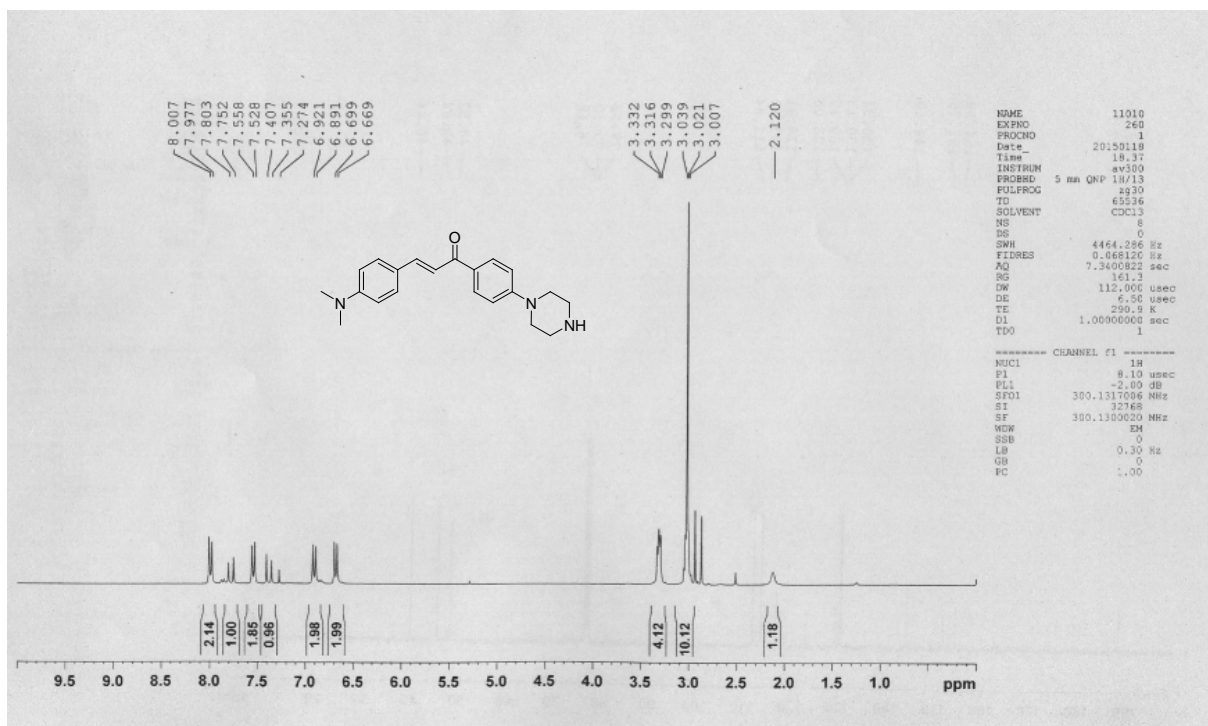
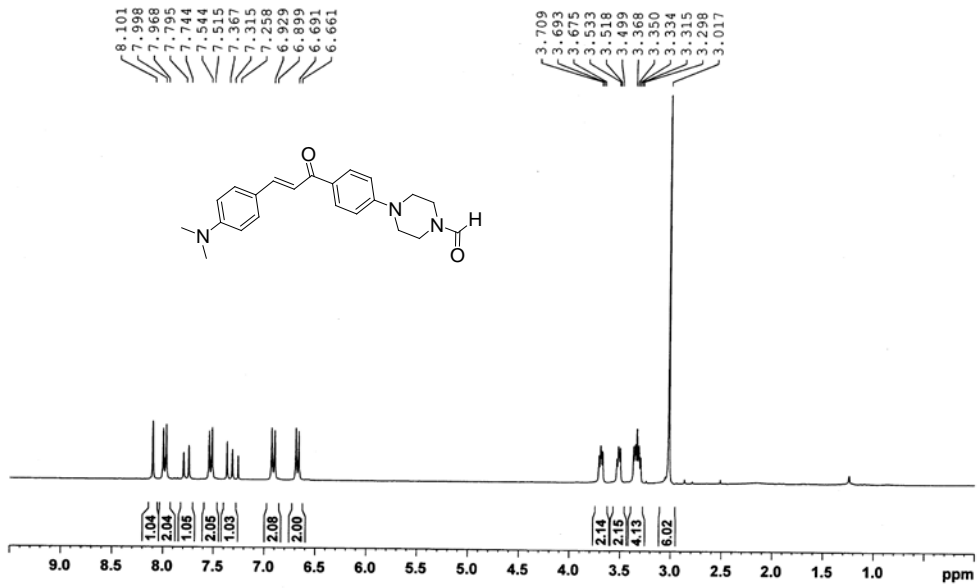


3. NMR and HRMS spectra





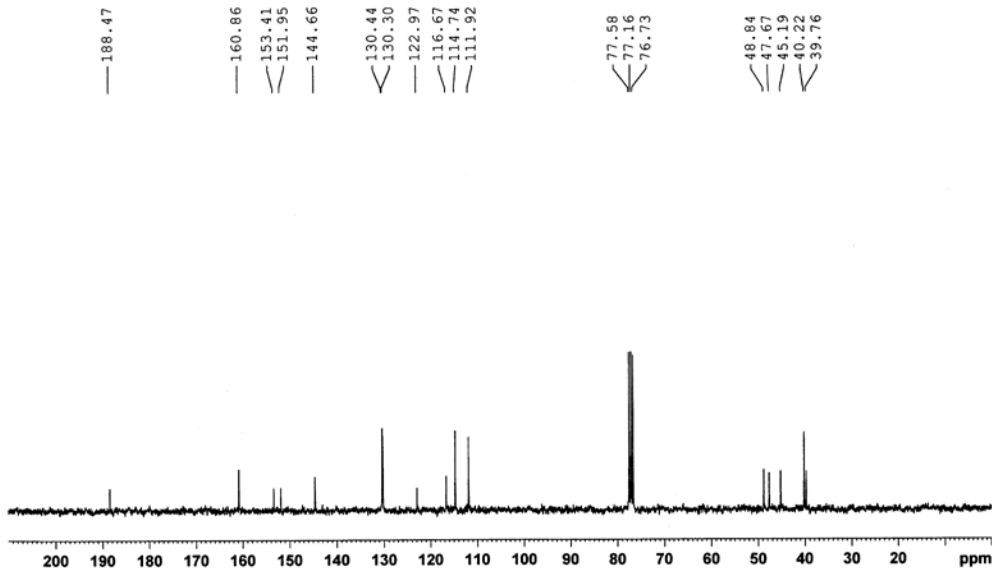


```

NAME          11010
EXPNO         332
PROCNO        1
Date_         20150903
Time          17.43
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           4464.286 Hz
FIDRES        0.068120 Hz
AQ            7.3400822 sec
RG            161.3
DW            112.000 usec
DE            6.50 usec
TE            297.1 K
D1            1.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          1H
P1            8.13 usec
PL1           -2.00 dB
SFO1         300.1317006 MHz
SI            32768
SF           300.1300127 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



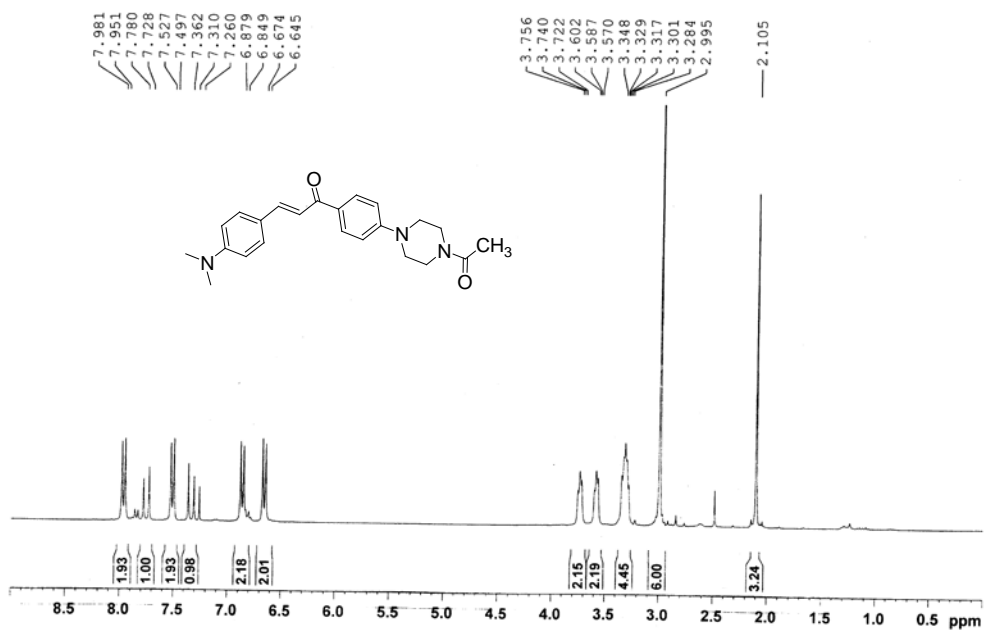
```

NAME          11010
EXPNO         333
PROCNO        1
Date_         20150903
Time          17.47
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            79
DS            0
SWH           18248.176 Hz
FIDRES        0.278445 Hz
AQ            1.7957364 sec
RG            16384
DW            27.400 usec
DE            6.50 usec
TE            297.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          13C
P1            8.10 usec
PL1           -3.00 dB
SFO1         75.4760444 MHz

----- CHANNEL f2 -----
CFDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           -2.00 dB
PL12         17.96 dB
PL13         19.00 dB
SFO2         300.1312005 MHz
SI            32768
SF           75.4677451 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40

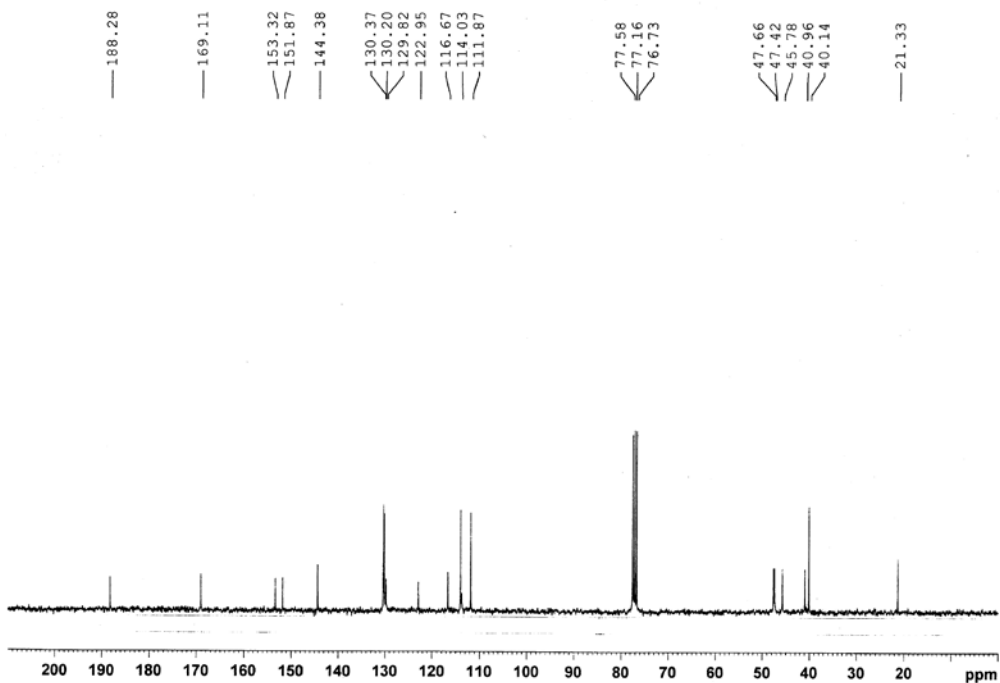
```



```

NAME          11010
EXPNO         286
PROCNO        1
Date_         20150815
Time          7.22
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           4464.286 Hz
FIDRES        0.068120 Hz
AQ            7.3400822 sec
RG            90.5
DM           113.600 usec
DE            6.50 usec
TE            298.2 K
D1            1.00000000 sec
TDO           1
----- CHANNEL f1 -----
NUC1          1H
P1            9.28 usec
PL1           -2.00 dB
SFO1         300.1317006 MHz
SI            32768
SF           300.1300119 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

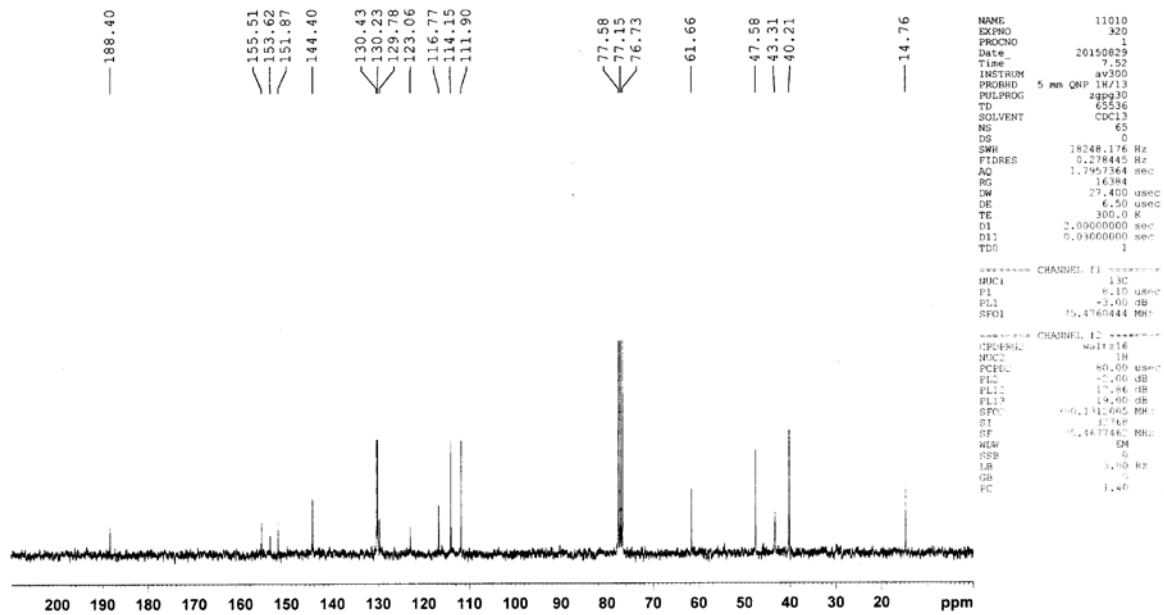
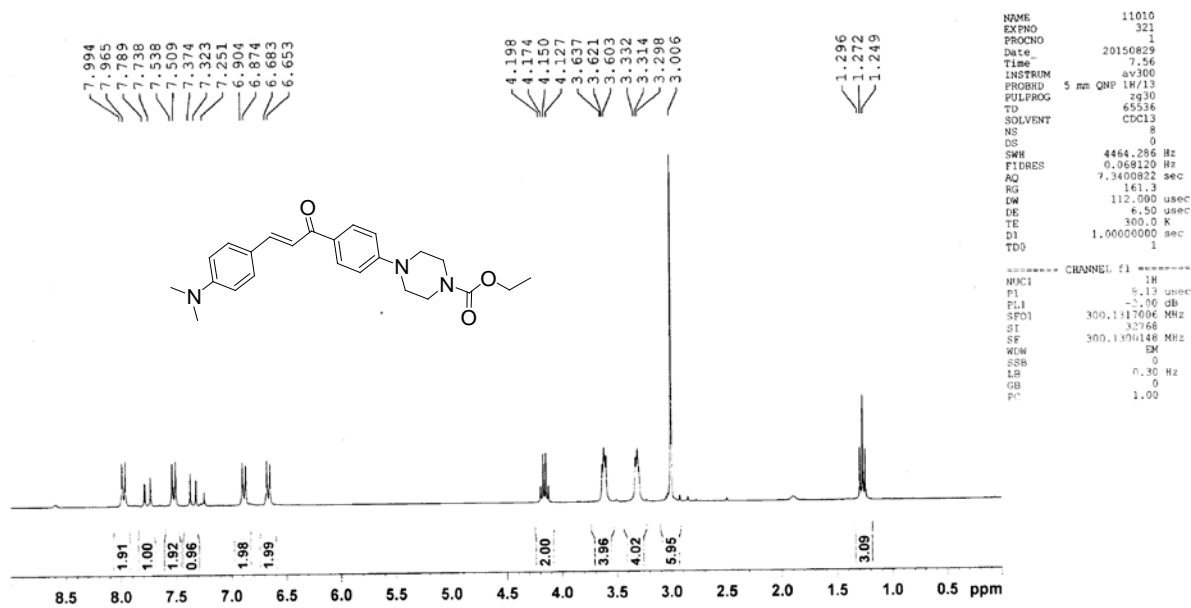
```

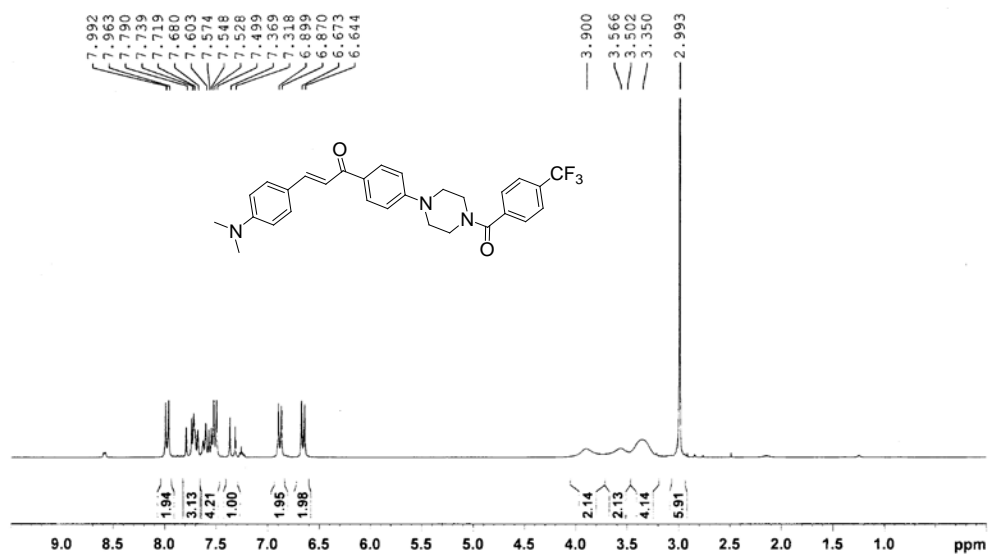


```

NAME          11010
EXPNO         287
PROCNO        1
Date_         20150815
Time          7.19
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            121
DS            0
SWH           18248.176 Hz
FIDRES        0.278445 Hz
AQ            1.7957364 sec
RG            16384
DM           27.400 usec
DE            6.50 usec
TE            298.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1
----- CHANNEL f1 -----
NUC1          13C
P1            7.70 usec
PL1           -3.00 dB
SFO1         75.4760444 MHz
----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
EPCPD2        80.00 usec
PL2           -2.00 dB
PL12          17.70 dB
PL13          19.00 dB
SFO2         300.1312005 MHz
SI            32768
SF           75.4677450 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40

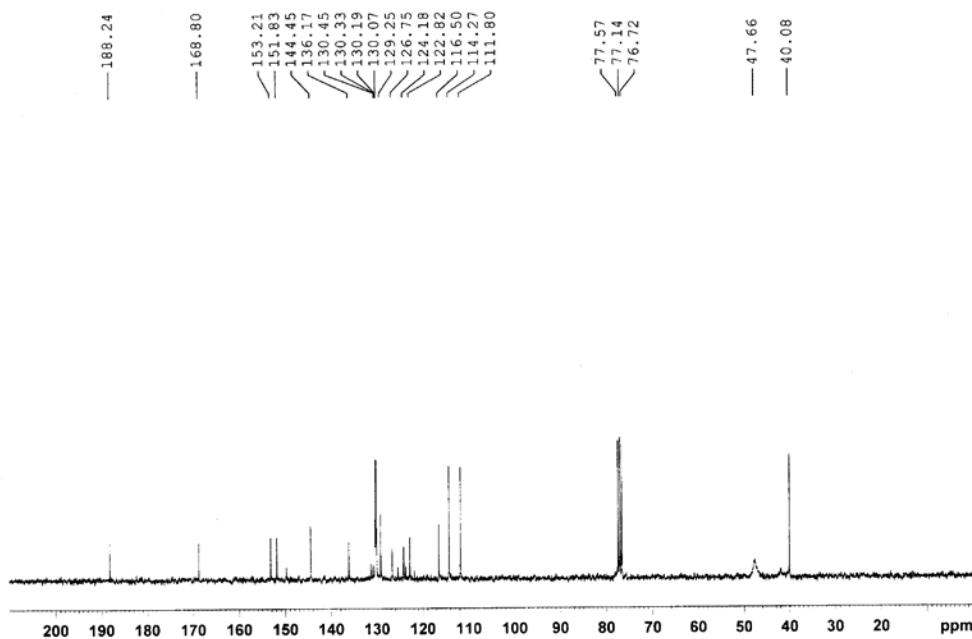
```





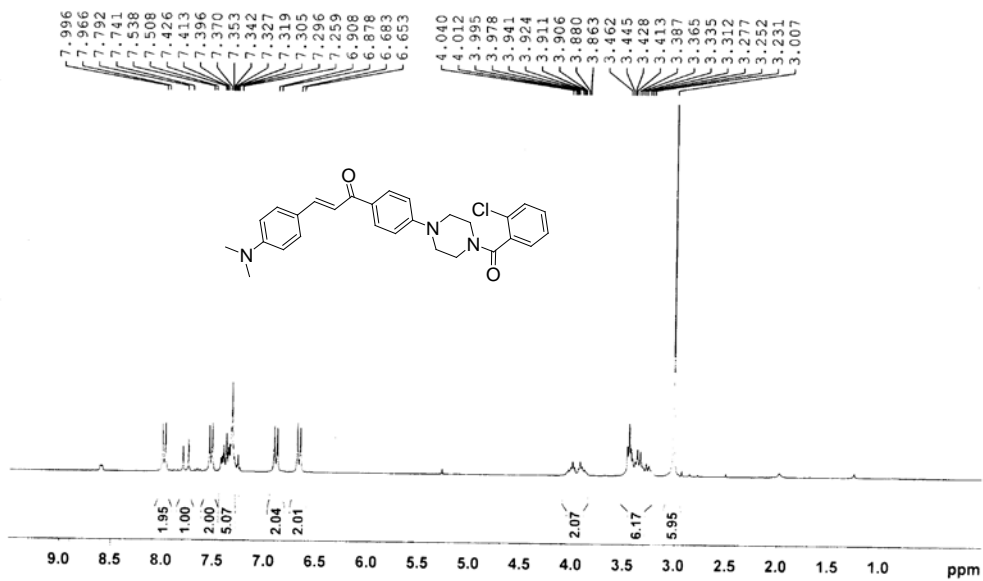
```

NAME      11010
EXPNO     319
PROCNO    1
Date_     20150829
Time      7.45
INSTRUM   av300
PROBHD    5 mm QNP 1H/13
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        4464.286 Hz
FIDRES     0.068120 Hz
AQ         7.3400822 sec
RG         71.8
DM         112.000 usec
DE         6.50 usec
TE         300.0 K
D1         1.00000000 sec
TDO        1
----- CHANNEL f1 -----
NUC1       1H
P1         8.13 usec
PL1        -1.90 dB
SFO1       405.1317096 MHz
SI         32768
SF         300.1300113 MHz
KW         SM
SR         0
LB         0.30 Hz
GB         0
PC         1.00
  
```



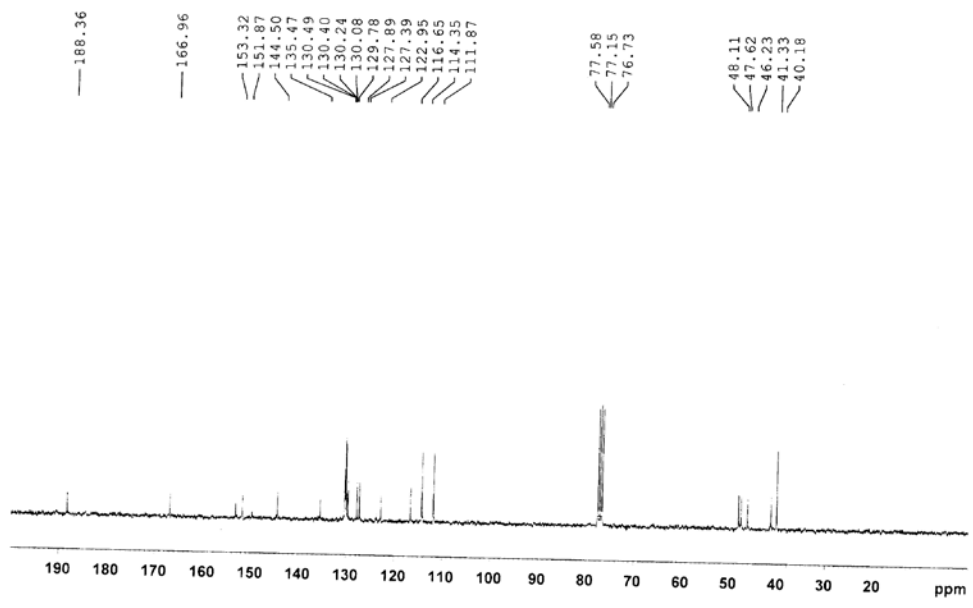
```

NAME      11010
EXPNO     318
PROCNO    1
Date_     20150829
Time      7.43
INSTRUM   av300
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         67
DS         0
SWH        18248.176 Hz
FIDRES     0.278445 Hz
AQ         1.7957364 sec
RG         16384
DM         27.400 usec
DE         6.50 usec
TE         300.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
----- CHANNEL f1 -----
NUC1       13C
P1         8.10 usec
PL1        -1.50 dB
SFO1       75.4760444 MHz
----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.70 usec
PL2        -1.00 dB
PL12      17.00 dB
PL13      17.00 dB
SFO2       400.1317096 MHz
SI         32768
SF         75.4677175 MHz
KW         SM
SR         0
LB         0.30 Hz
GB         0
PC         1.00
  
```



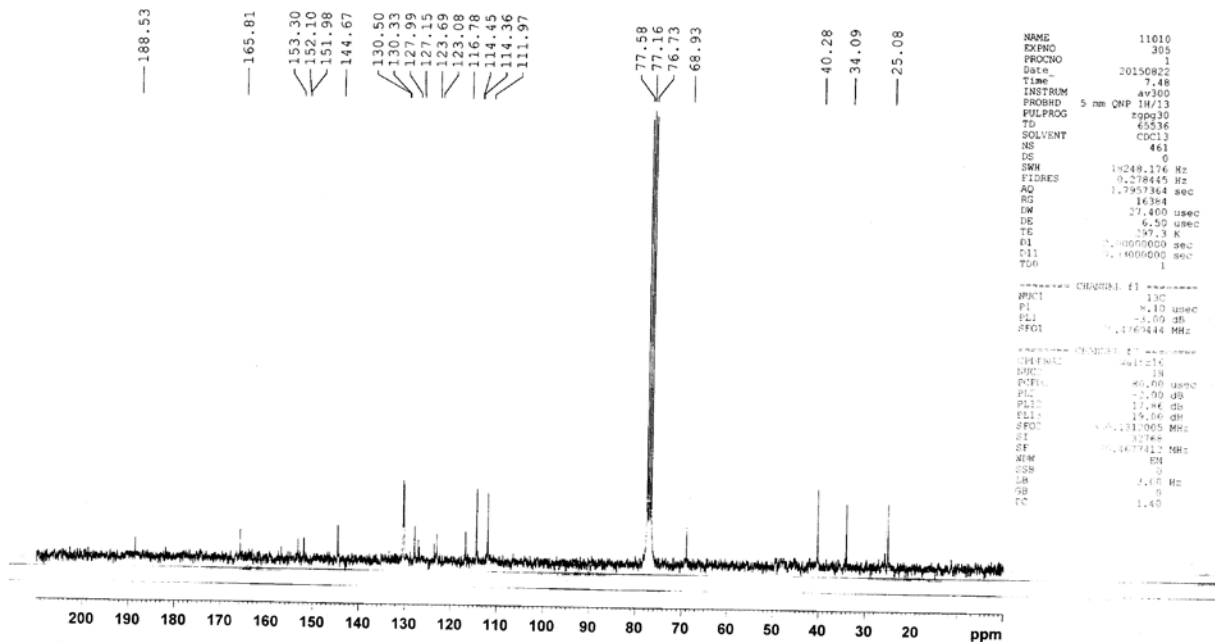
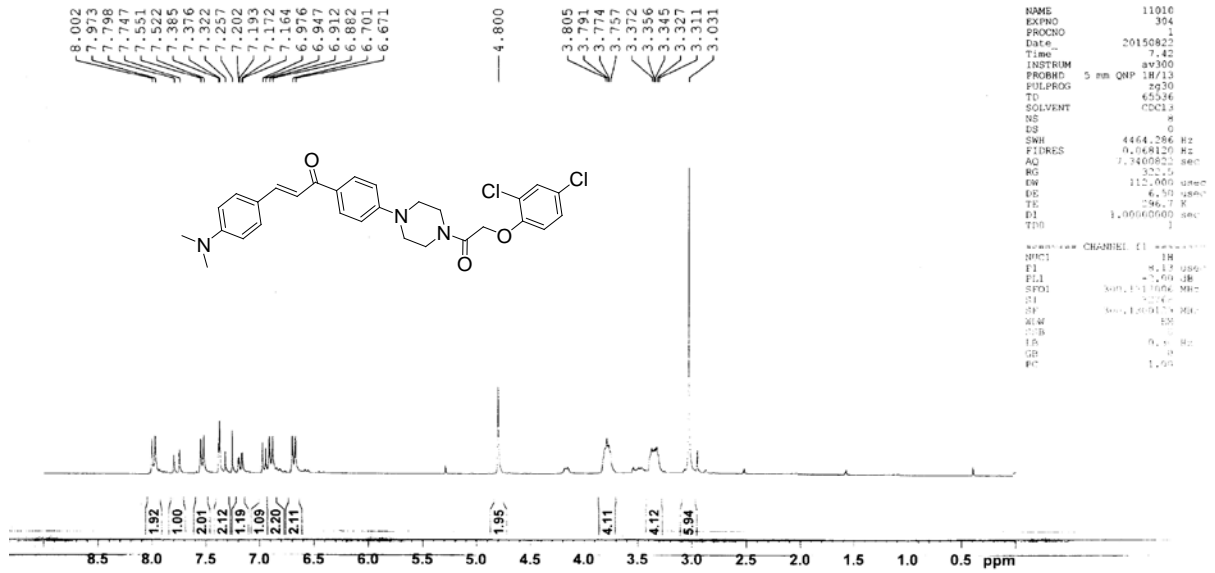
```

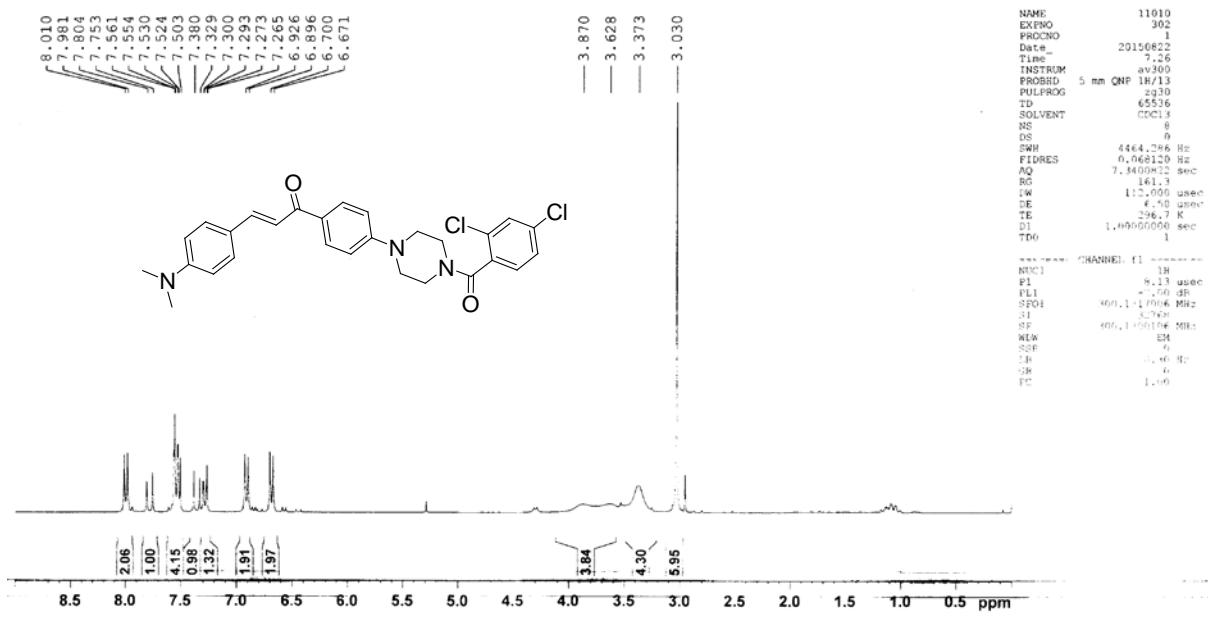
NAME          11010
EXPNO         311
PROCNO        1
Date_         20150829
Time          6.55
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD             65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           4464.286 Hz
FIDRES        0.068120 Hz
AQ            7.3400822 sec
RG            161.3
DE            112.000 use
TE            6.50 use
TD            296.0 K
SI            1.00000000 sec
TQ            1
  
```



```

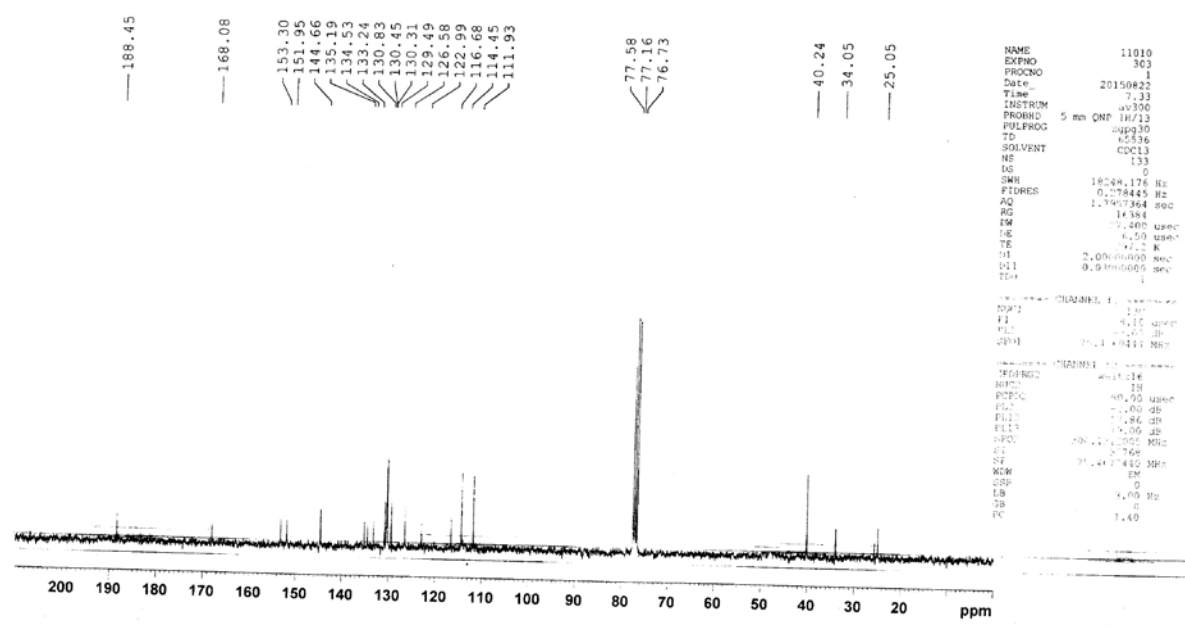
NAME          11010
EXPNO         312
PROCNO        1
Date_         20150829
Time          7.02
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD             65536
SOLVENT       CDCl3
NS            111
DS            0
SWH           16249.176 Hz
FIDRES        0.238445 Hz
AQ            1.7957364 sec
RG            16384
DE            27.400 usec
TE            6.50 usec
TD            296.6 K
SI            1.00000000 sec
D1            0.03000000 sec
D11           0.03000000 sec
TQ            1
  
```





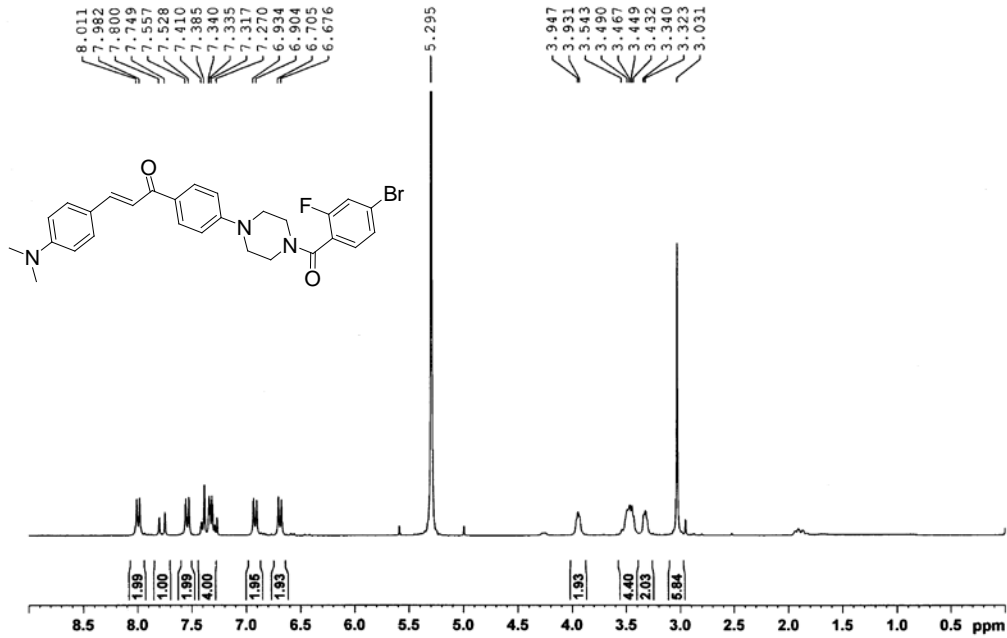
```

NAME      11010
EXPNO    302
PROCNO   1
Date_    20150822
Time     7.26
INSTRUM  av300
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD       65536
SOLVENT  CDCl3
NS       8
DS       0
SWH      4464.286 Hz
FIDRES   0.068120 Hz
AQ       7.8409812 sec
RG       161.3
IW       112.000 usec
DE       4.50 usec
TE       296.2 K
D1       1.0000000 sec
TD0      1
----- CHANNEL f1 -----
NUC1     13C
P1       9.13 usec
PL1     -1.00 dB
SFO1    101.625361 MHz
SI       32768
SF       101.625361 MHz
WLM      EM
SSB      0
LB       0.00 Hz
GB       0
PC       1.00
  
```



```

NAME      11010
EXPNO    303
PROCNO   1
Date_    20150822
Time     7.33
INSTRUM  av300
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD       65536
SOLVENT  CDCl3
NS       133
DS       0
SWH      18048.176 Hz
FIDRES   0.278445 Hz
AQ       1.7907364 sec
RG       16384
IW       17.400 usec
DE       4.50 usec
TE       296.2 K
D1       2.0000000 sec
D11     0.5000000 sec
TD0      1
----- CHANNEL f1 -----
NUC1     13C
P1       9.13 usec
PL1     -1.00 dB
SFO1    101.625361 MHz
SI       32768
SF       101.625361 MHz
WLM      EM
SSB      0
LB       0.00 Hz
GB       0
PC       1.40
  
```

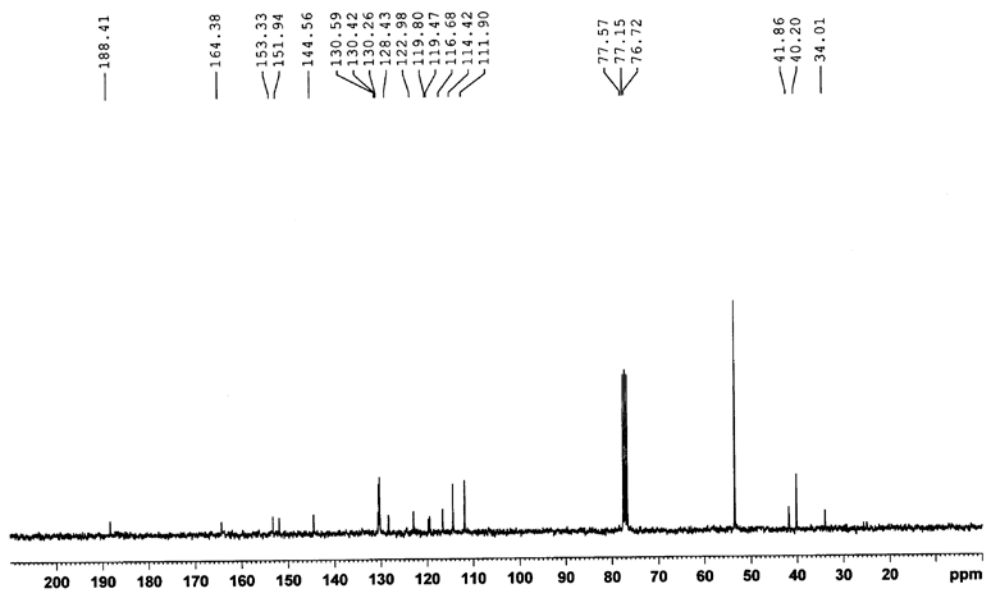


```

NAME      11010
EXPNO    330
PROCNO   1
Date_    20150903
Time     17.28
INSTRUM  av300
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        0
SWH       4464.286 Hz
FIDRES   0.968120 Hz
AQ        7.3400822 sec
RG        161.3
DW        112.000 usec
DE        6.50 usec
TE        297.0 K
D1        1.00000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      1H
P1        8.13 usec
PL1       -2.00 dB
SFO1     300.1317006 MHz
S1        32768
SF        300.1300092 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00

```



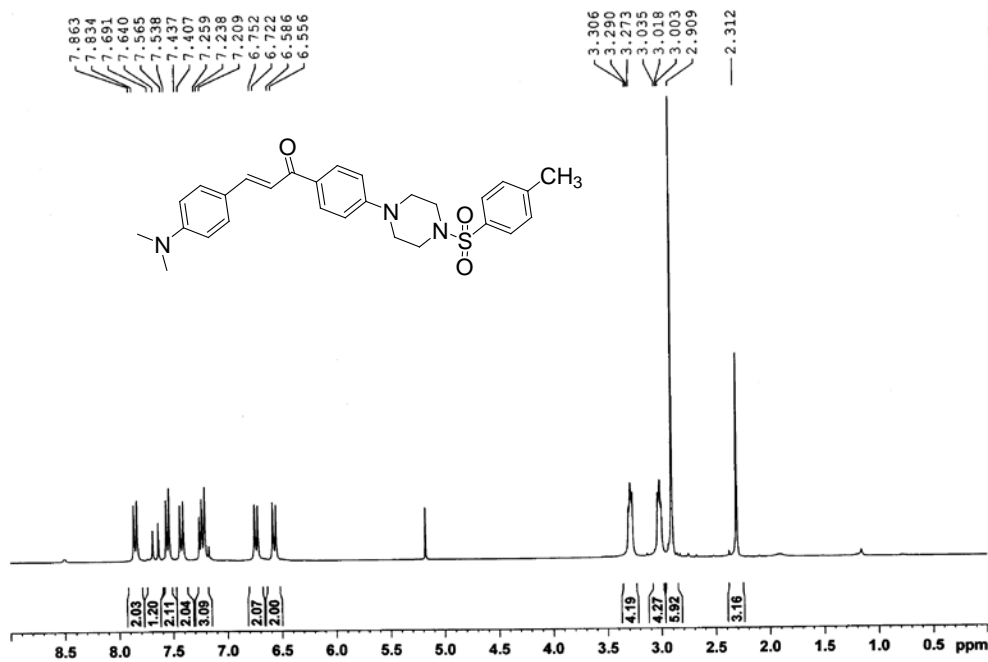
```

NAME      11010
EXPNO    331
PROCNO   1
Date_    20150903
Time     17.36
INSTRUM  av300
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        150
DS        0
SWH       18248.176 Hz
FIDRES   0.278445 Hz
AQ        1.7957364 sec
RG        16384
DW        27.400 usec
DE        6.50 usec
TE        297.6 K
D1        2.00000000 sec
D11      0.03000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      13C
P1        8.10 usec
PL1       -3.00 dB
SFO1     75.4760444 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       -2.00 dB
PL12     17.86 dB
PL13     19.00 dB
SFO2     300.1312005 MHz
S1        32768
SF        75.4677453 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40

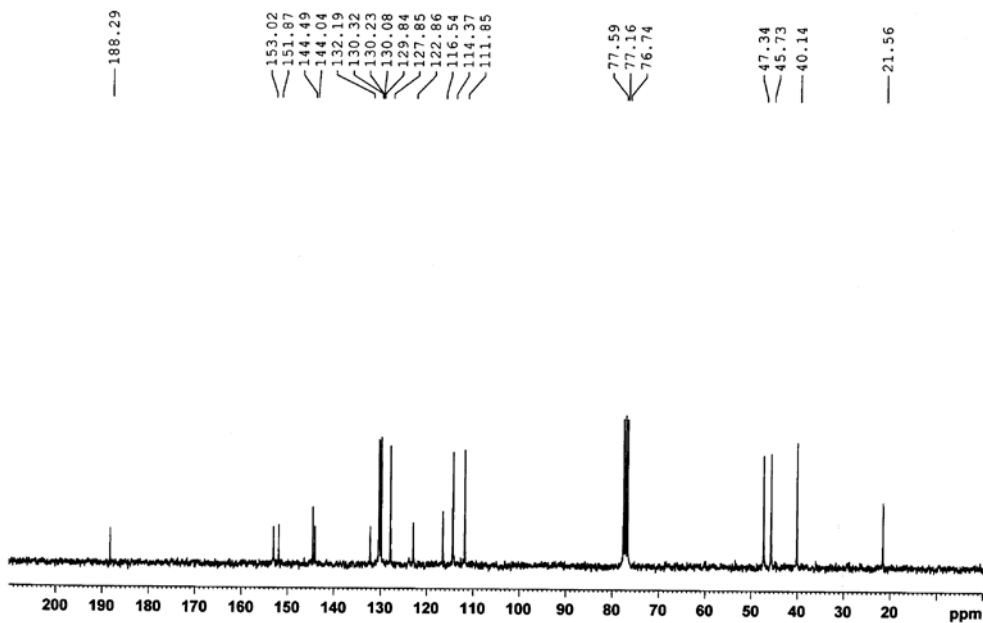
```



```

NAME          11010
EXPNO         336
PROCNO        1
Date_         20150903
Time          19.44
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           4464.286 Hz
FIDRES        0.068120 Hz
AQ            7.3400822 sec
RG            90.5
DW           112.000 usec
DE            6.50 usec
TE            297.3 K
D1            1.00000000 sec
TDO           1

----- CHANNEL f1 -----
NUC1          13C
P1            8.13 usec
PL1           -2.00 dB
SFO1         300.1317006 MHz
SI            32768
SF           300.1300387 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```

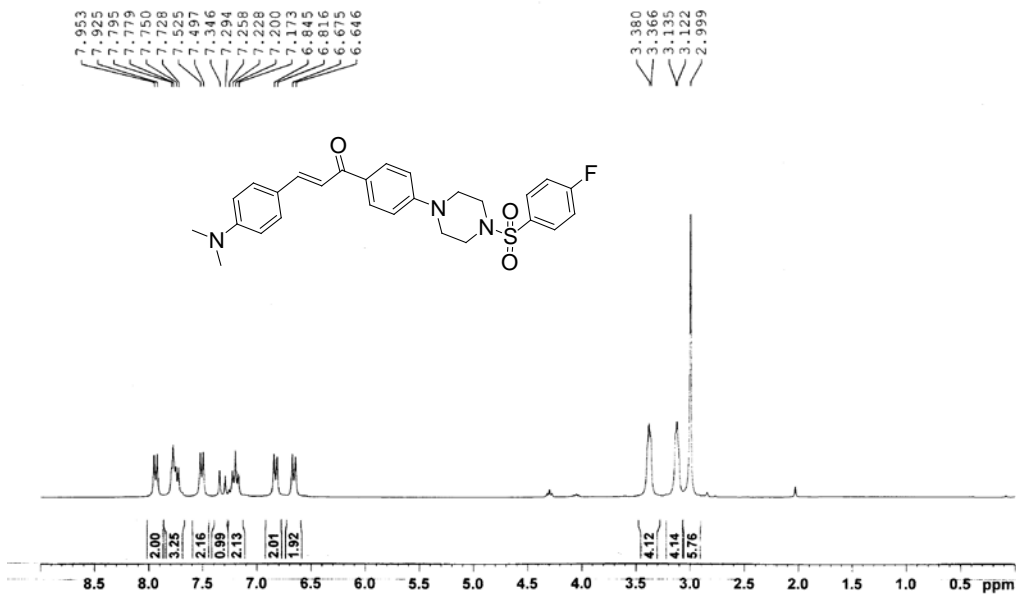


```

NAME          11010
EXPNO         337
PROCNO        1
Date_         20150903
Time          18.50
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            82
DS            0
SWH           18248.176 Hz
FIDRES        0.278445 Hz
AQ            1.7957364 sec
RG            16384
DW           27.400 usec
DE            6.50 usec
TE            297.9 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1

----- CHANNEL f1 -----
NUC1          13C
P1            8.10 usec
PL1           -3.00 dB
SFO1         75.4760444 MHz

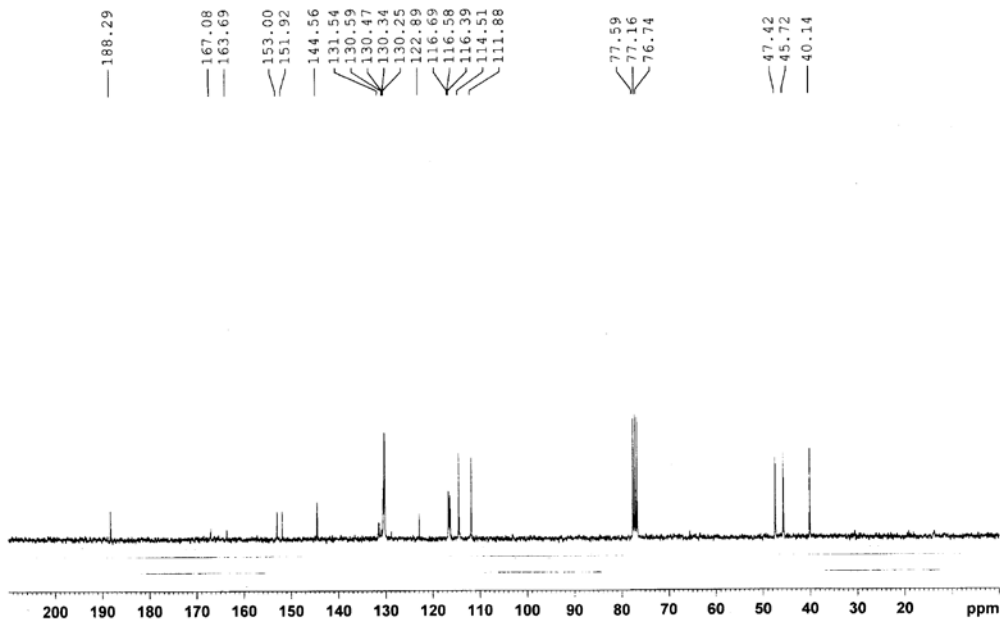
----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.00 dB
PL12          17.86 dB
PL13          19.00 dB
SFO2         300.1312005 MHz
SI            32768
SF           75.4677501 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40
  
```



```

NAME      11010
EXPNO     292
PROCNO    1
Date_     20150816
Time      7.40
INSTRUM   av300
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         8
DS         0
SWH        4464.286 Hz
FIDRES    0.068120 Hz
AQ         7.3400822 sec
RG         90.5
LW         112.000 usec
DE         6.50 usec
TE         293.4 K
D1         1.00000000 sec
TD0        1
----- CHANNEL f1 -----
NUC1       1H
P1         8.28 usec
PL1        -2.00 dB
SFO1       300.1317006 MHz
SI         32768
SF         300.1300133 MHz
WUW        0
GB         0
LB         0.30 Hz
GB         0
PC         1.00

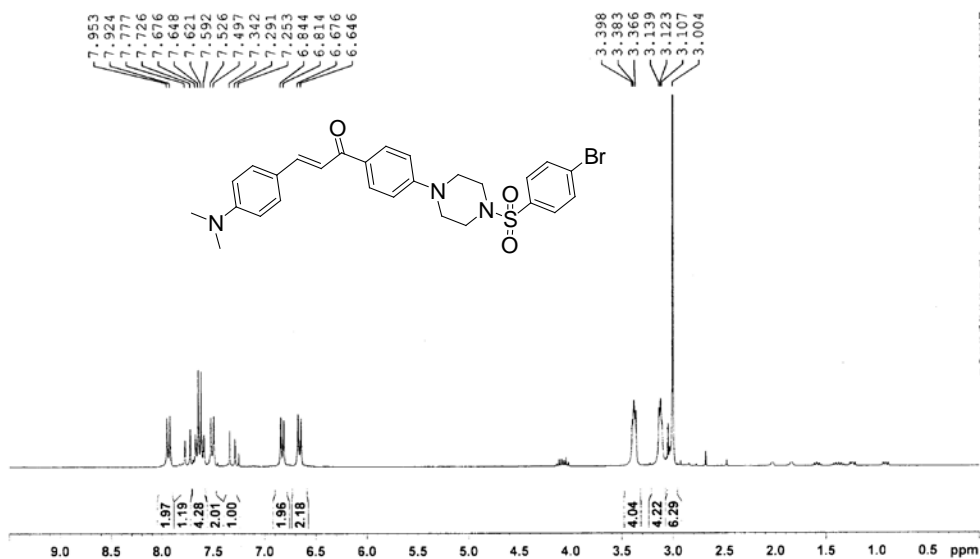
```



```

NAME      11010
EXPNO     297
PROCNO    1
Date_     20150816
Time      8.07
INSTRUM   av300
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         93
DS         0
SWH        18248.176 Hz
FIDRES    0.278445 Hz
AQ         1.7957364 sec
RG         16384
LW         37.400 usec
DE         6.50 usec
TE         298.2 K
D1         2.00000000 sec
L11       0.02000000 sec
TD0        1
----- CHANNEL f1 -----
NUC1       13C
P1         7.70 usec
PL1        -3.00 dB
SFO1       101.4761144 MHz
----- CHANNEL f2 -----
SFO2       wait116
NUC2       1H
PCPD2     80.00 usec
PL2       -2.00 dB
PL12      17.70 dB
PL13      19.00 dB
SFO2      500.1312092 MHz
SI         32768
SF         25.4677480 MHz
WUW        0
GB         0
LB         3.00 Hz
GB         0
PC         1.40

```

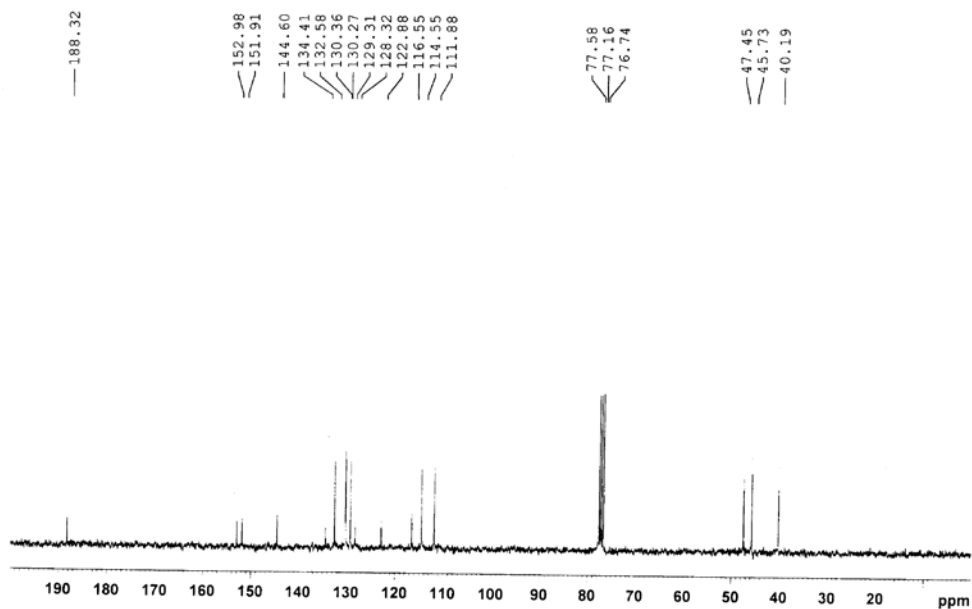


```

NAME          11010
EXPNO         313
PROCNO        1
Date_         20150829
Time          7.09
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           4464.286 Hz
FIDRES        0.066120 Hz
AQ            7.3400822 sec
RG            161.3
RW           112.000 usec
DE            6.50 usec
TE            296.1 K
D1            1.00000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          13C
P1            0.13 usec
PL1           -2.00 dB
SFO1         100.611004 MHz
SI            32768
SF           100.6100139 MHz
WFWD         64
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

```



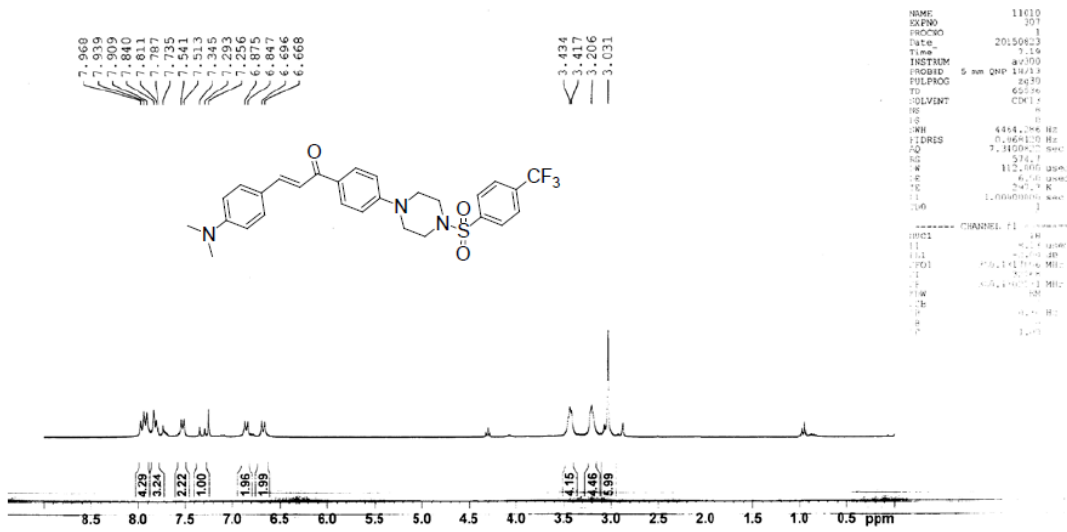
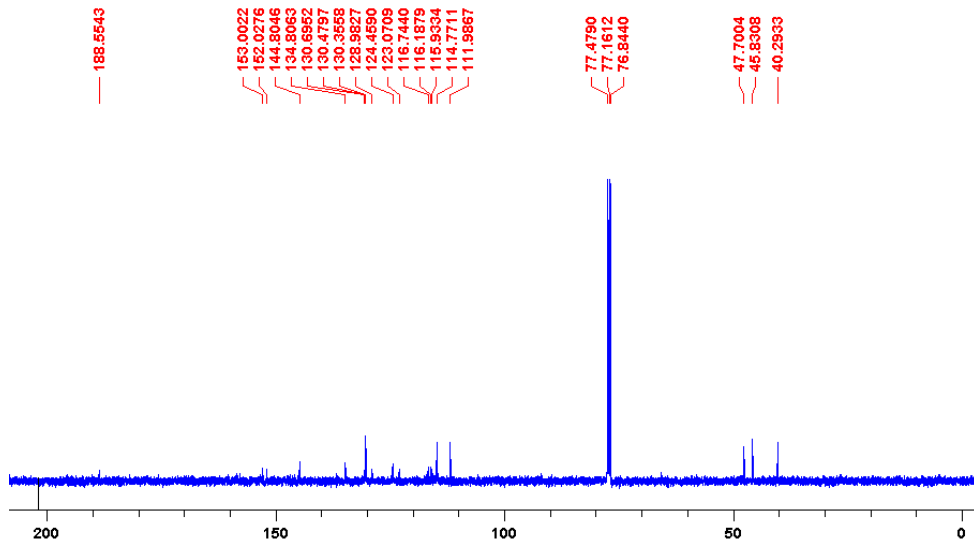
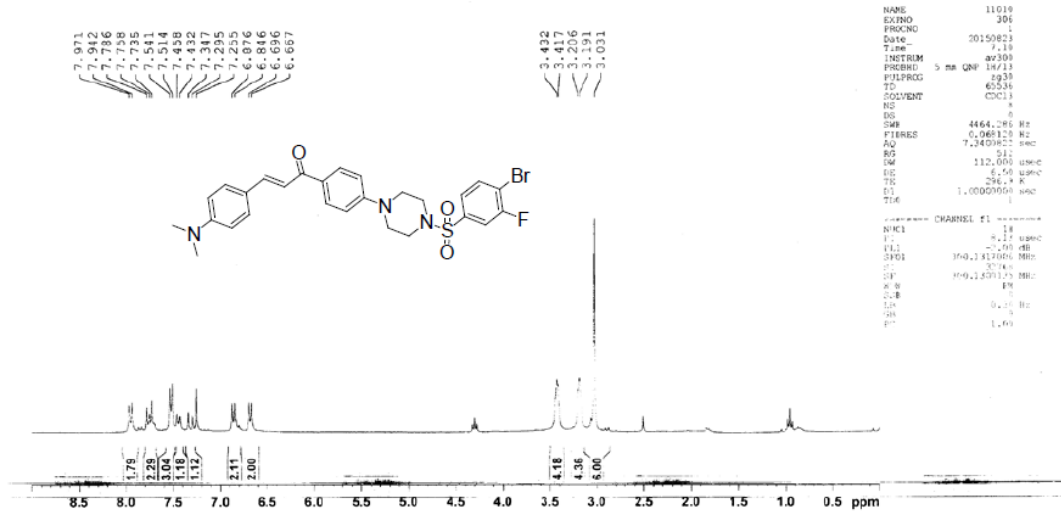
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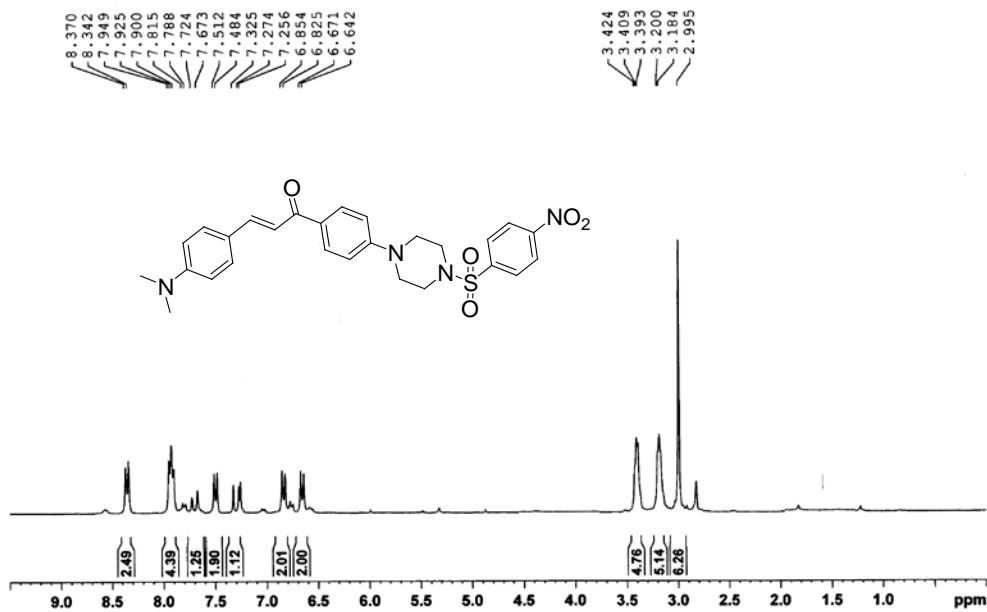
NAME          11010
EXPNO         317
PROCNO        1
Date_         20150829
Time          7.33
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            68
DS            0
SWH           18248.176 Hz
FIDRES        0.278445 Hz
AQ            1.7957364 sec
RG            16394
RW           27.400 usec
DE            8.50 usec
TE            300.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           1

----- CHANNEL f1 -----
NUC1          13C
P1            8.10 usec
PL1           -3.00 dB
SFO1         75.4760444 MHz

----- CHANNEL f2 -----
NUC2          1H
P2            80.00 usec
PL2           -2.00 dB
SFO2         400.1419970 MHz
SI            32768
SF           400.1419970 MHz
WFWD         64
SSB           0
LB            3.00 Hz
GB            0
PC            1.00

```



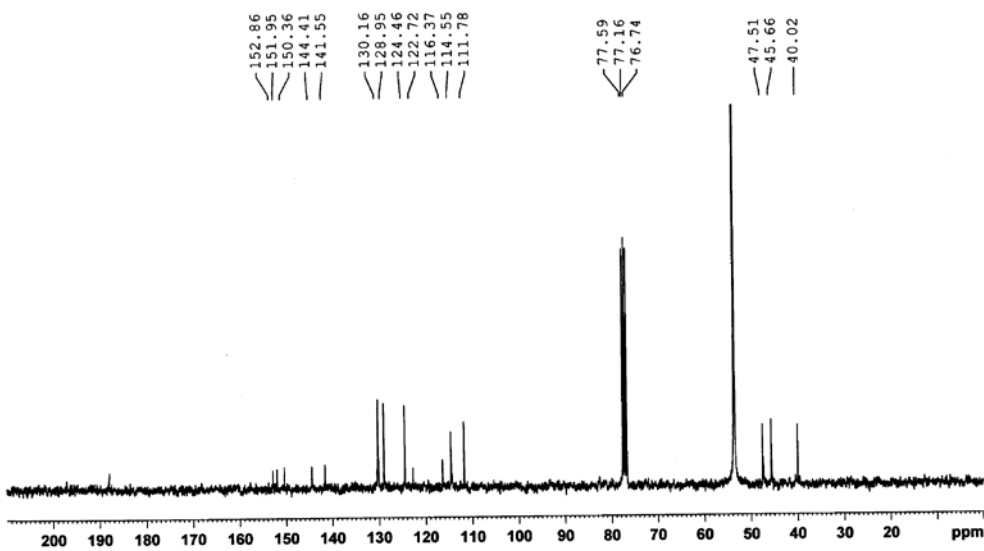


```

NAME          11010
EXPNO         334
PROCNO        1
Date_         20150903
Time          17.55
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           4464.286 Hz
FIDRES        0.068120 Hz
AQ            7.3400823 sec
RG            45.3
DW            112.000 usec
DE            6.50 usec
TE            297.0 K
D1            1.00000000 sec
TDO           1

----- CHANNEL f1 -----
NUC1          13C
P1            8.13 usec
PL1          -2.00 dB
SFO1         300.1317006 MHz
SI           32768
SF           300.1300131 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

```



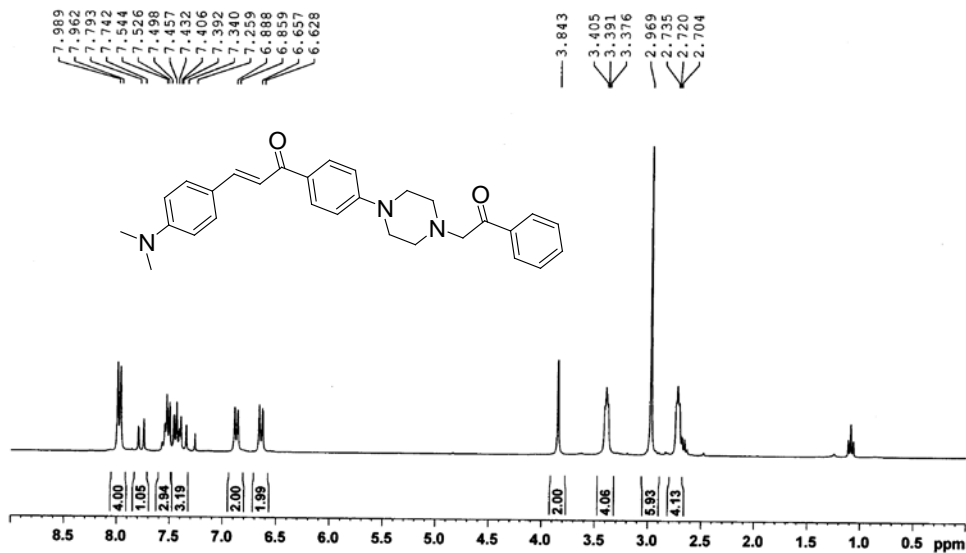
```

NAME          11010
EXPNO         335
PROCNO        1
Date_         20150903
Time          18.10
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            555
DS            0
SWH           18248.176 Hz
FIDRES        0.278445 Hz
AQ            1.7957364 sec
RG            16384
DW            27.400 usec
DE            6.50 usec
TE            297.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1

----- CHANNEL f1 -----
NUC1          13C
P1            8.10 usec
PL1          -3.00 dB
SFO1         75.4760444 MHz

----- CHANNEL f2 -----
CPDPRG2       waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           -2.00 dB
PL12          17.86 dB
PL13          19.00 dB
SFO2         300.1312005 MHz
SI           32768
SF           75.4677490 MHz
WDW          EM
SSB          0
LB           3.00 Hz
GB           0
PC           1.40

```

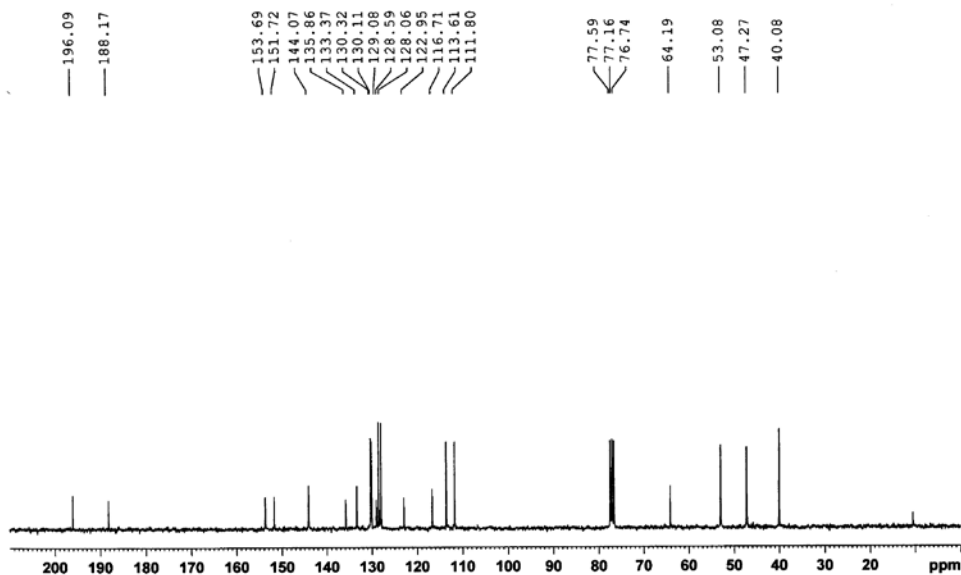


```

NAME          11010
EXPNO         322
PROCNO        1
Date_         20150903
Time          16.24
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           4464.286 Hz
FIDRES        0.068120 Hz
AQ            7.3400822 sec
RG            71.8
DW           112.000 usec
DE            6.50 usec
TE            296.9 K
D1            1.00000000 sec
TDO           1
  
```

```

----- CHANNEL f1 -----
NUC1          1H
P1            8.13 usec
PL1          -2.00 dB
SFO1         300.1311008 MHz
SI           32768
SF           300.1300120 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00
  
```



```

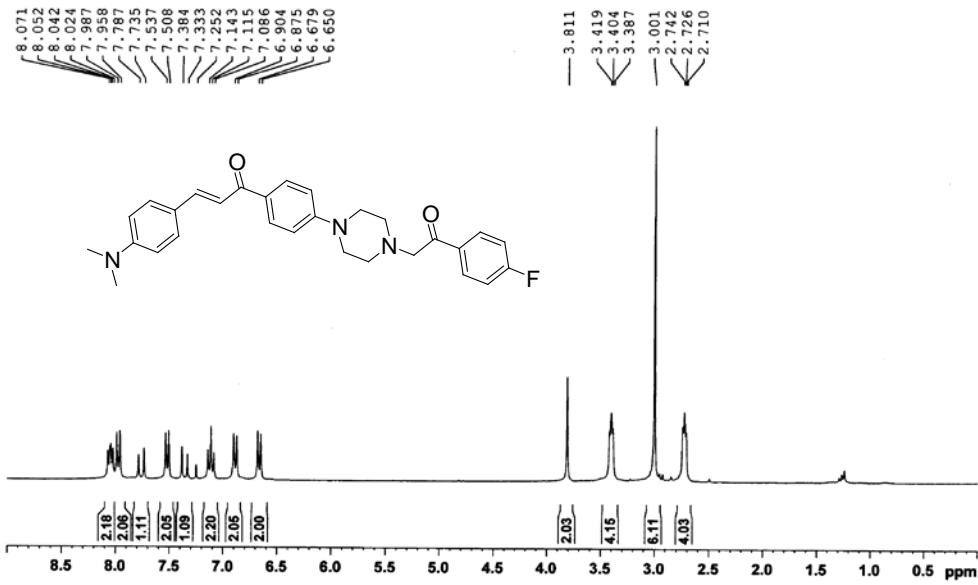
NAME          11010
EXPNO         323
PROCNO        1
Date_         20150903
Time          16.30
INSTRUM       av300
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
TD            65536
SOLVENT       CDCl3
NS            86
DS            0
SWH           18248.176 Hz
FIDRES        0.279445 Hz
AQ            1.7957364 sec
RG            16384
DW           27.400 usec
DE            6.50 usec
TE            297.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TDO           1
  
```

```

----- CHANNEL f1 -----
NUC1          13C
P1            9.10 usec
PL1          -3.00 dB
SFO1         75.4760444 MHz
  
```

```

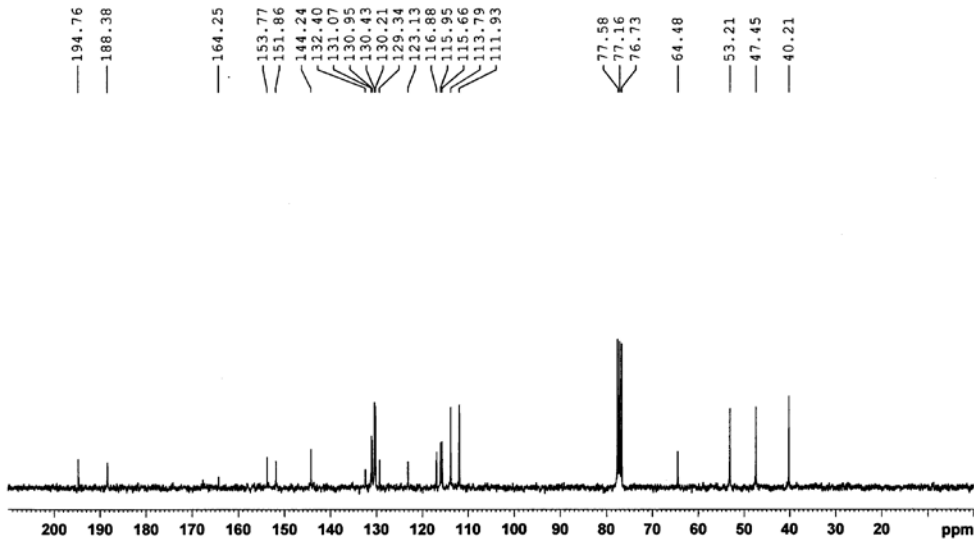
----- CHANNEL f2 -----
CPDPRG2      waltz16
NUC2          1H
PCPD2        80.00 usec
PL2          -2.00 dB
PL12         17.86 dB
PL13         19.00 dB
SFO2         300.1312005 MHz
SI           32768
SF           75.4677540 MHz
WDW           EM
SSB           0
LB            3.00 Hz
GB            0
PC            1.40
  
```

```

NAME      11010
EXPNO    324
PROCNO    1
Date_     20150903
Time      16.36
INSTRUM   av300
PROBHD    5 mm QNP 1H/13
PULPROG   zg30
TD         65536
SOLVENT    CDCl3
NS         8
DS         0
SWH        4464.286 Hz
FIDRES     0.068120 Hz
AQ         7.3400822 sec
RG         161.3
DW         112.000 usec
DE         6.50 usec
TE         296.5 K
D1         1.00000000 sec
D11        1
----- CHANNEL f1 -----
NUC1       1H
P1         8.13 usec
PL1        -2.00 dB
SFO1       300.1317006 MHz
SI         32768
SF         300.1300145 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

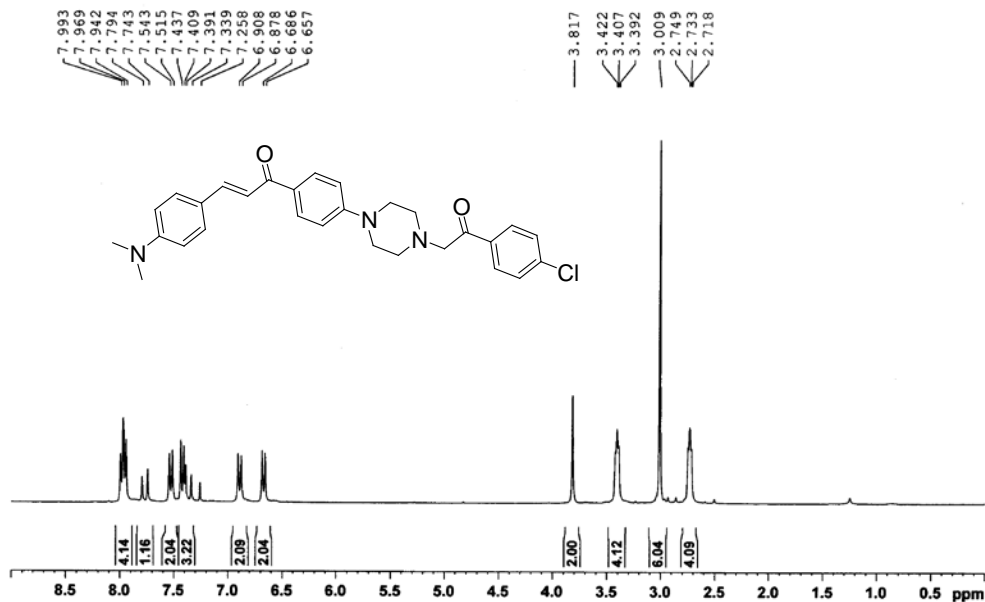
```



```

NAME      11010
EXPNO    325
PROCNO    1
Date_     20150903
Time      16.44
INSTRUM   av300
PROBHD    5 mm QNP 1H/13
PULPROG   zgpg30
TD         65536
SOLVENT    CDCl3
NS         155
DS         0
SWH        18248.176 Hz
FIDRES     0.278445 Hz
AQ         1.7957364 sec
RG         16384
DW         27.400 usec
DE         6.50 usec
TE         297.5 K
D1         2.00000000 sec
D11        0.03000000 sec
D10        1
----- CHANNEL f1 -----
NUC1       13C
P1         8.10 usec
PL1        -3.00 dB
SFO1       75.4760444 MHz
----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2       1H
PCPD2     80.00 usec
PL2        -2.00 dB
PL12       17.86 dB
PL13       19.00 dB
SFO2       300.1312005 MHz
SI         32768
SF         75.4677451 MHz
WDW        DM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40

```

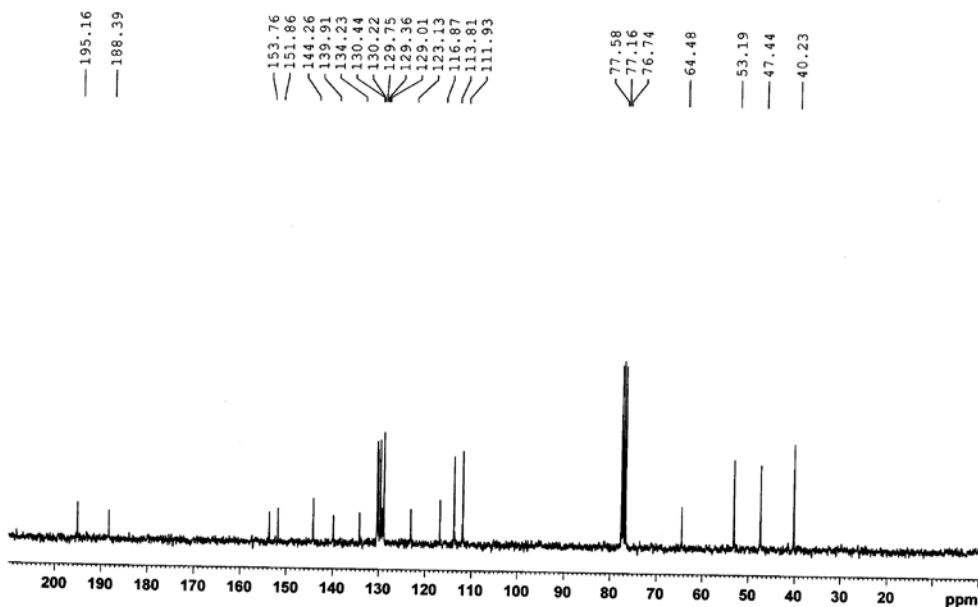


```

NAME      11010
EXPNO    326
PROCNO   1
Date_    20150903
Time     16.59
INSTRUM  av300
PROBHD   5 mm QNP 1H/13
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        0
SWH       4464.286 Hz
FIDRES    0.068120 Hz
AQ        7.3409822 sec
RG        161.3
DW        112.000 usec
DE        6.50 usec
TE        296.3 K
D1        1.00000000 sec
D11       1
TDO       1
  
```

```

----- CHANNEL f1 -----
NUC1      1H
P1        8.13 usec
PL1       -2.00 dB
SFO1     300.1317006 MHz
SI        32768
SF        300.1300128 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```



```

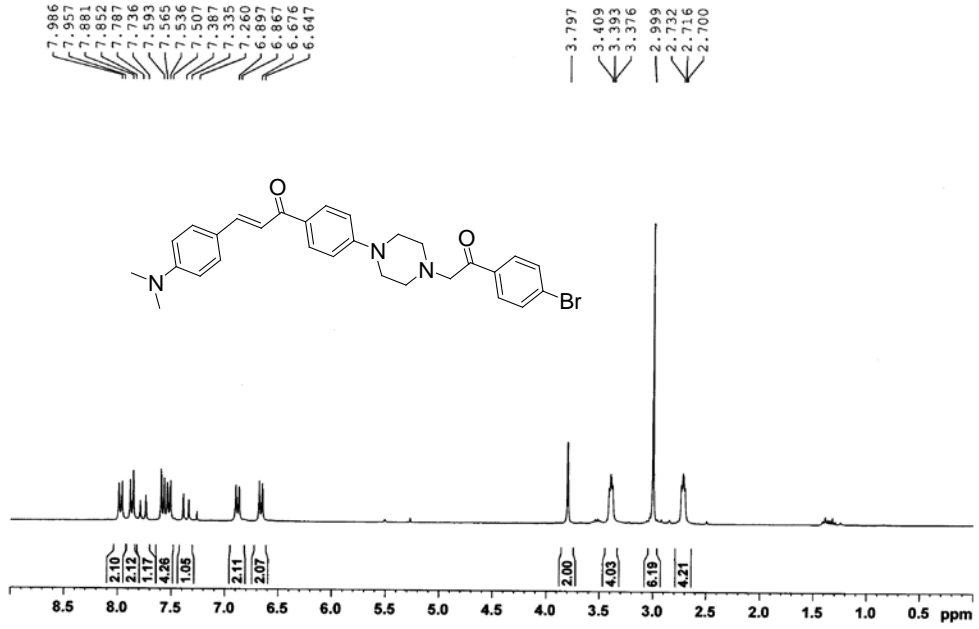
NAME      11010
EXPNO    327
PROCNO   1
Date_    20150903
Time     17.08
INSTRUM  av300
PROBHD   5 mm QNP 1H/13
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        135
DS        0
SWH       18248.176 Hz
FIDRES    0.278445 Hz
AQ        1.7957364 sec
RG        16384
DW        27.400 usec
DE        6.50 usec
TE        297.6 K
D1        2.00000000 sec
D11       1
TDO       0.03000000 sec
  
```

```

----- CHANNEL f1 -----
NUC1      13C
P1        8.10 usec
PL1       -3.00 dB
SFO1     75.4760444 MHz
  
```

```

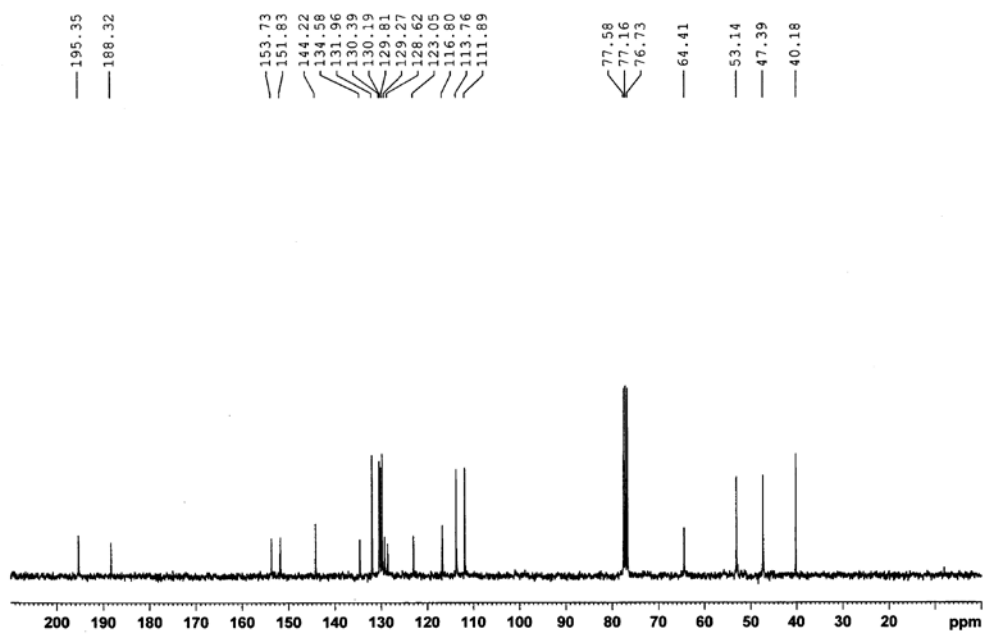
----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2      1H
PCPD2    80.00 usec
PL2       -2.00 dB
PL12     17.86 dB
PL13     19.00 dB
SFO2     300.1312005 MHz
SI        32768
SF        75.4677446 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40
  
```



```

NAME 11010
EXPNO 328
PROCNO 1
Date_ 20150903
Time 17.14
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 4464.286 Hz
FIDRES 0.088120 Hz
AQ 7.3400822 sec
RG 161.3
DW 112.000 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 1H
P1 8.13 usec
PL1 -2.00 dB
SFO1 300.1311905 MHz
SI 32768
SF 300.1300119 MHz
WVW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```



```

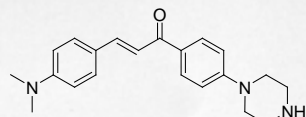
NAME 11010
EXPNO 329
PROCNO 1
Date_ 20150903
Time 17.23
INSTRUM av300
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 132
DS 0
SWH 18248.176 Hz
FIDRES 0.278445 Hz
AQ 1.7957364 sec
RG 16384
DW 27.400 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
----- CHANNEL f1 -----
NUC1 13C
P1 8.10 usec
PL1 -3.00 dB
SFO1 75.4760444 MHz
----- CHANNEL f2 -----
CFPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -2.00 dB
PL12 17.86 dB
PL13 19.00 dB
SFO2 300.1312005 MHz
SI 32768
SF 75.4677473 MHz
WVW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

```

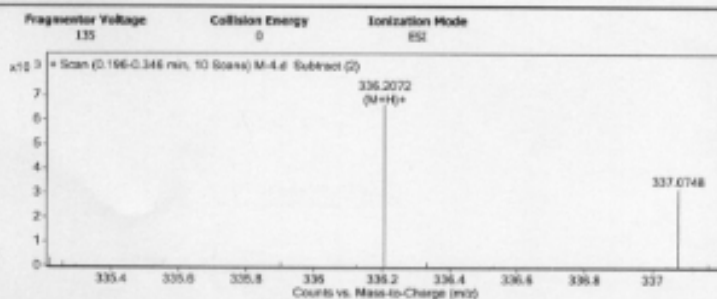
Qualitative Analysis Report

Data Filename	M-4.d	Sample Name	M-4
Sample Type	Sample	Position	P1-C5
Instrument Name	Instrument 1	User Name	
Acq Method	SIBLm	Acquired Time	3/18/2015 2:29:45 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group: Info.
 Acquisition SW: 6200 series TOF/6500 series
 Version: Q-TOF B.05.01 (85125.2)



User Spectra



Peak List

m/z	z	Abund	Formula	Ion
102.1277	1	4945.88		
336.2072	1	6619.3	C21 H25 N3 O	[M+H] ⁺
337.0748	1	3188.03		
374.1029	1	2550.54		
411.0932	1	3379.24		
427.0674	1	2320.66		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	10
N	0	10

Formula Calculator Results

Formula	CalculatedMass	CalculatedHz	Hz	Diff. (mDa)	Diff. (ppm)	DBE
C21 H25 N3 O	335.1998	336.2070	336.2072	-0.3	-0.8	11.9000

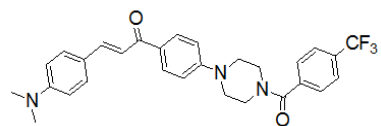
--- End Of Report ---

Qualitative Analysis Report

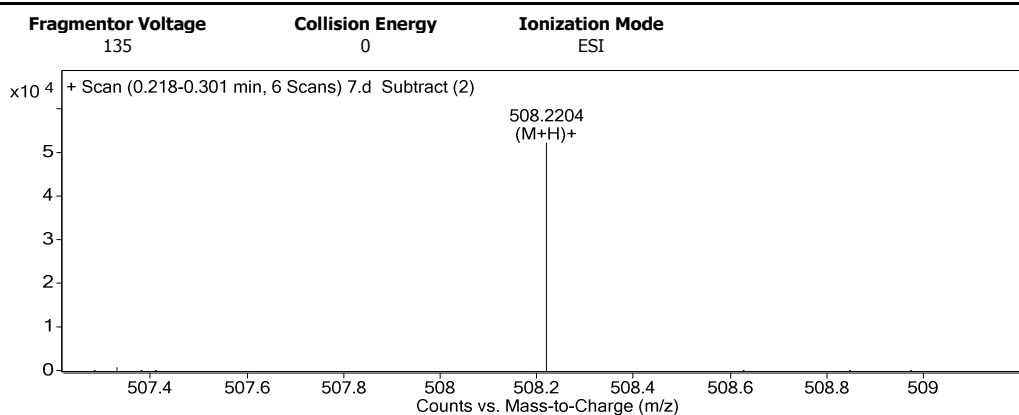
Data Filename	7.d	Sample Name	7
Sample Type	Sample	Position	P1-B2
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	9/22/2015 11:24:23 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group Info.

Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.2)



User Spectra



Peak List

m/z	z	Abund	Formula	Ion
104.107	1	16364.21		
163.1231	1	14463.81		
205.1337	1	22028.3		
219.1744	1	14829.66		
264.2322	1	40861.31		
508.2204	1	52101.79	C ₂₉ H ₂₈ F ₃ N ₃ O ₂	(M+H) ⁺
509.2235	1	16546.87	C ₂₉ H ₂₈ F ₃ N ₃ O ₂	(M+H) ⁺
530.2026	1	10914.45		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₉ H ₂₈ F ₃ N ₃ O ₂	507.2134	508.2206	508.2204	0.2	0.4	16.0000

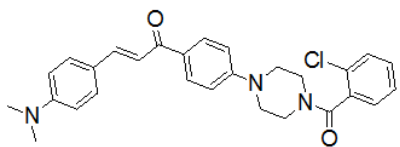
--- End Of Report ---

Qualitative Analysis Report

Data Filename	2.d	Sample Name	2
Sample Type	Sample	Position	P1-A6
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	9/22/2015 11:16:59 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

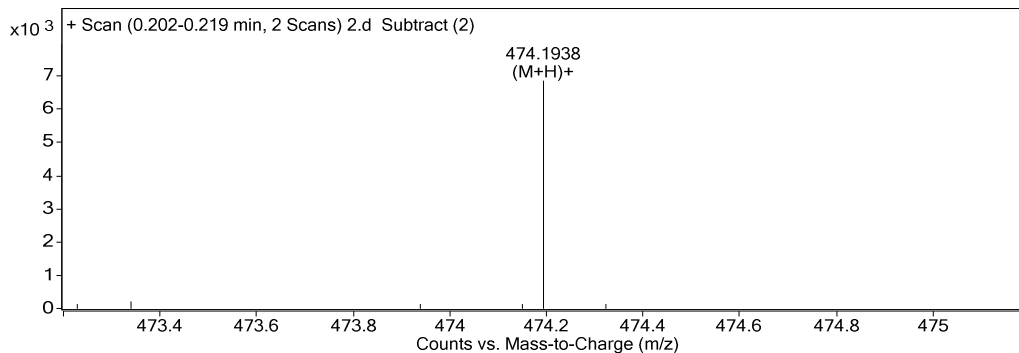
Sample Group Info.

Acquisition SW Version 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2)



User Spectra

Fragmentor Voltage 135
Collision Energy 0
Ionization Mode ESI



Peak List

m/z	z	Abund	Formula	Ion
147.0915		4302.41		
163.1234	1	13246.98		
179.1166	1	4469.47		
217.1048		3700.42		
417.202	1	71671.53		
418.2051	1	16742.54		
455.1571	1	3062.89		
474.1938	1	6860.73	C28 H28 Cl N3 O2	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
Cl	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C28 H28 Cl N3 O2	473.1870	474.1943	474.1938	0.4	0.9	16.0000

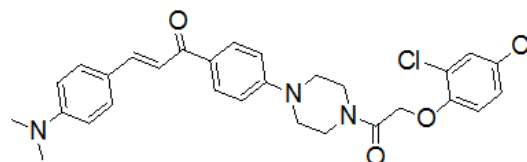
--- End Of Report ---

Qualitative Analysis Report

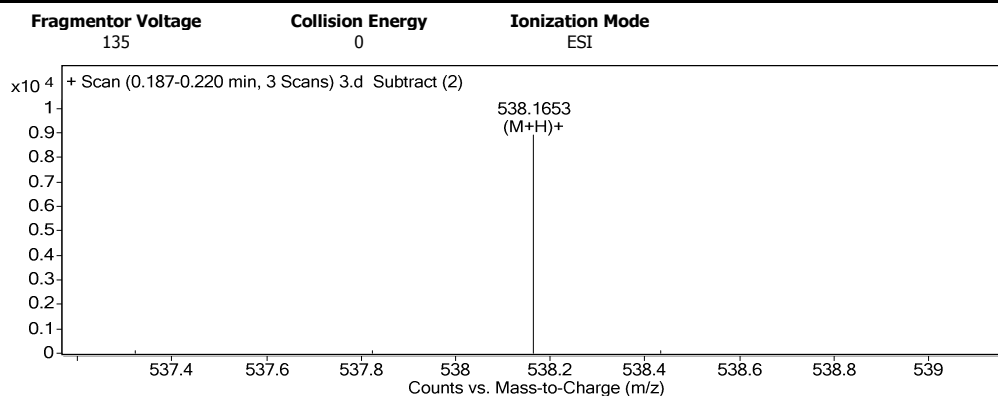
Data Filename 3.d **Sample Name** 3
Sample Type Sample **Position** P1-A7
Instrument Name Instrument 1 **User Name**
Acq Method SIBU.m **Acquired Time** 9/22/2015 11:18:29 AM
IRM Calibration Status Success **DA Method** ESI+.m
Comment

Sample Group
Acquisition SW Version 6200 series TOF/6500 series
 Q-TOF B.05.01 (B5125.2)

Info.



User Spectra



Peak List

m/z	z	Abund	Formula	Ion
163.1247	1	5443.68		
205.1339	1	9516.44		
225.196	1	18063.5		
264.2321	1	13487.84		
417.2018	1	23556.56		
418.2051	1	5931.01		
538.1653	1	8919.39	C ₂₉ H ₂₉ Cl ₂ N ₃ O ₃	(M+H) ⁺
540.1631	1	5846.32	C ₂₉ H ₂₉ Cl ₂ N ₃ O ₃	(M+H) ⁺

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
Cl	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₉ H ₂₉ Cl ₂ N ₃ O ₃	537.1586	538.1659	538.1653	0.4	0.8	16.0000

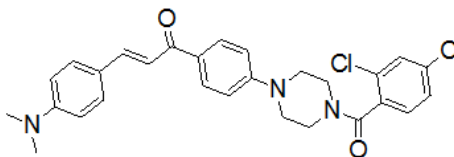
--- End Of Report ---

Qualitative Analysis Report

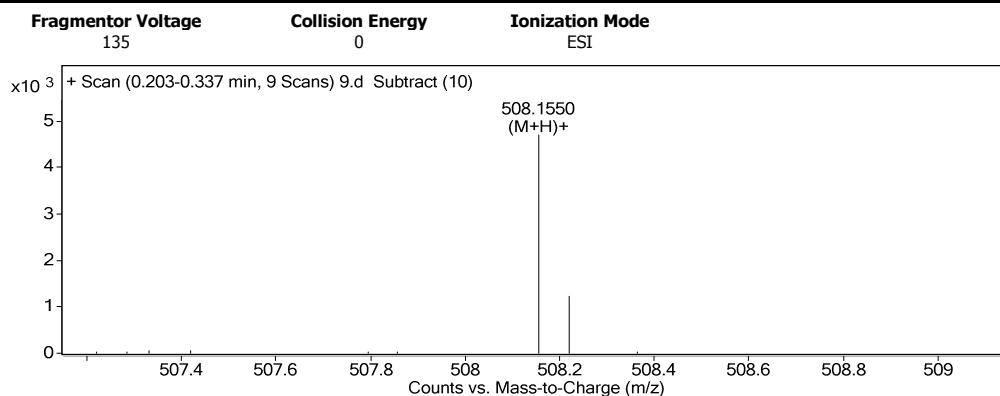
Data Filename	9.d	Sample Name	9
Sample Type	Sample	Position	P1-B4
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	9/22/2015 11:30:47 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group
Acquisition SW Version
 6200 series TOF/6500 series
 Q-TOF B.05.01 (B5125.2)

Info.



User Spectra



Peak List

m/z	z	Abund	Formula	Ion
205.1341	1	4591.31		
225.1961	1	46765.62		
226.1997	1	7031.34		
247.1779	1	13344.19		
264.233		4688.65		
417.2062	1	5476.2		
508.155	1	4703.89	C28 H27 Cl2 N3 O2	(M+H)+
510.1526	1	3319.7	C28 H27 Cl2 N3 O2	(M+H)+

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
Cl	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C28 H27 Cl2 N3 O2	507.1480	508.1553	508.1550	0.4	0.8	16.0000

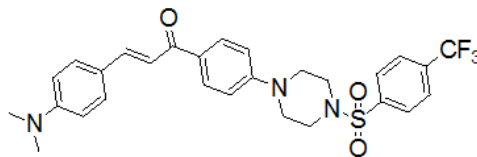
--- End Of Report ---

Qualitative Analysis Report

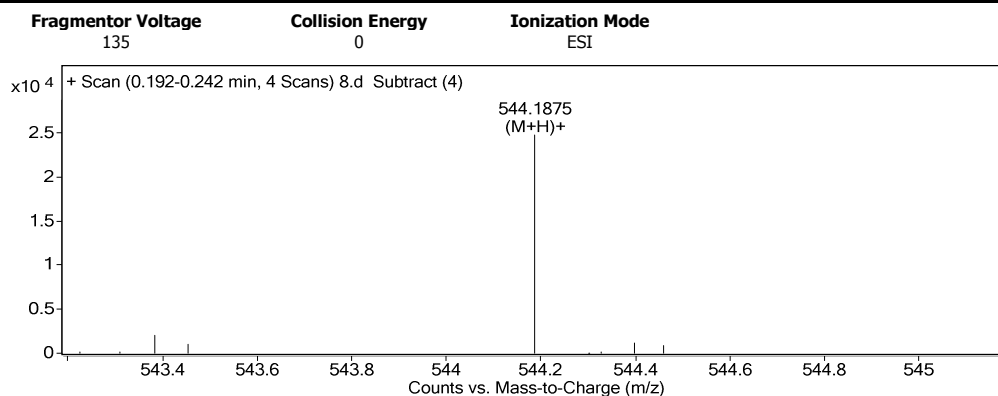
Data Filename 8.d **Sample Name** 8
Sample Type Sample **Position** P1-B3
Instrument Name Instrument 1 **User Name**
Acq Method SIBU.m **Acquired Time** 9/22/2015 2:37:35 PM
IRM Calibration Status Success **DA Method** ESI+.m
Comment

Sample Group
Acquisition SW Version 6200 series TOF/6500 series
 Q-TOF B.05.01 (B5125.2)

Info.



User Spectra



Peak List

m/z	z	Abund
104.1071		49710.88
160.112	1	34749.2
205.1336	1	114895.16
212.1182	1	84987.07
219.1746	1	144089.28
264.2326	1	362742.84
265.2369	1	60987.03
308.2949	1	32857.08

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	0	5
S	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₈ H ₂₈ F ₃ N ₃ O ₃ S	543.1804	544.1876	544.1875	0.3	0.5	15.0000

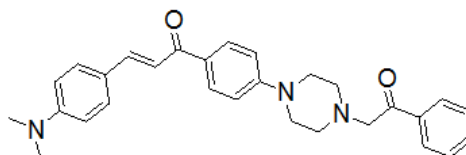
--- End Of Report ---

Qualitative Analysis Report

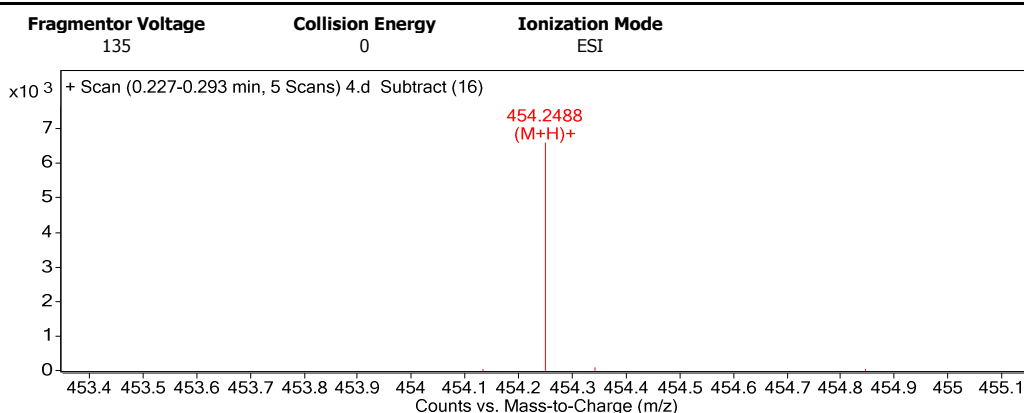
Data Filename	4.d	Sample Name	4
Sample Type	Sample	Position	P1-A8
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	9/22/2015 11:19:58 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group Info.

Acquisition SW Version 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2)



User Spectra



Peak List

m/z	z	Abund	Formula	Ion
104.107	1	11165.61		
160.1118	1	8425.55		
205.1327	1	26426.91		
219.174	1	12312.93		
264.2325		40457.69		
417.2019	1	31933.33		
418.2052	1	7505.92		
454.2488	1	6606.53	C ₂₉ H ₃₁ N ₃ O ₂	(M+H) ⁺

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
Cl	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₉ H ₃₁ N ₃ O ₂	453.2416	454.2489	454.2488	0.1	0.2	16.0000

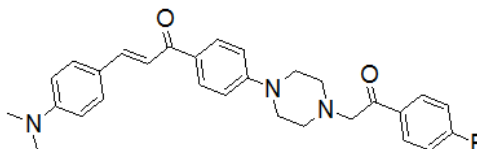
--- End Of Report ---

Qualitative Analysis Report

Data Filename	1.d	Sample Name	1
Sample Type	Sample	Position	P1-A5
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	9/22/2015 11:13:40 AM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

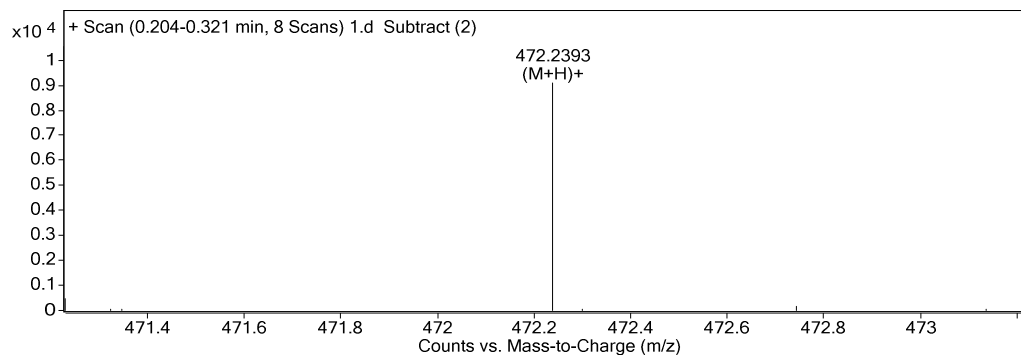
Sample Group
Acquisition SW Version 6200 series TOF/6500 series
 Q-TOF B.05.01 (B5125.2)

Info.



User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
102.1276		3484.19		
163.1244	1	7424.51		
179.1176	1	5906.1		
217.1051	1	3262.65		
417.2019	1	49809.26		
418.205	1	11317.32		
472.2393	1	9103.09	C ₂₉ H ₃₀ F N ₃ O ₂	(M+H) ⁺
473.2424	1	2900.38	C ₂₉ H ₃₀ F N ₃ O ₂	(M+H) ⁺

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
F	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₉ H ₃₀ F N ₃ O ₂	471.2322	472.2395	472.2393	0.2	0.5	16.0000

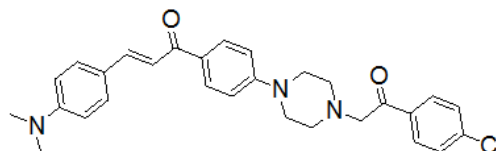
--- End Of Report ---

Qualitative Analysis Report

Data Filename	5+.d	Sample Name	5
Sample Type	Sample	Position	P1-A9
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	9/22/2015 2:46:41 PM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

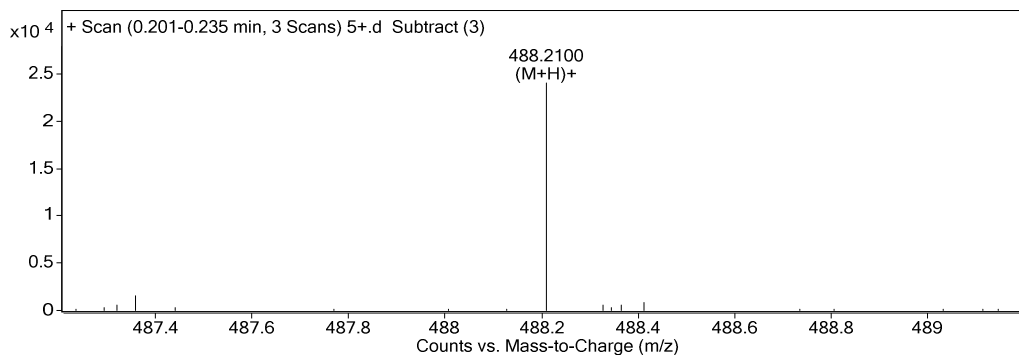
Sample Group Info.

Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125.2)



User Spectra

Fragmentor Voltage 135
Collision Energy 0
Ionization Mode ESI



Peak List

m/z	z	Abund
104.1071		85433.3
160.1118	1	68488.69
205.1337	1	226194.86
219.1745	1	342475.84
220.1778	1	56010.65
264.2325	1	1012433.5
265.236	1	178969.31
563.4356	1	36889.39

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
Cl	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₉ H ₃₀ Cl N ₃ O ₂	487.2027	488.2099	488.2100	0.1	0.1	16.0000

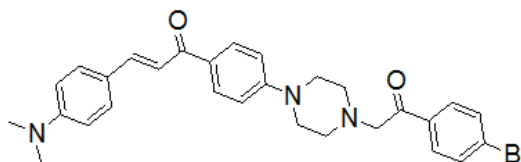
--- End Of Report ---

Qualitative Analysis Report

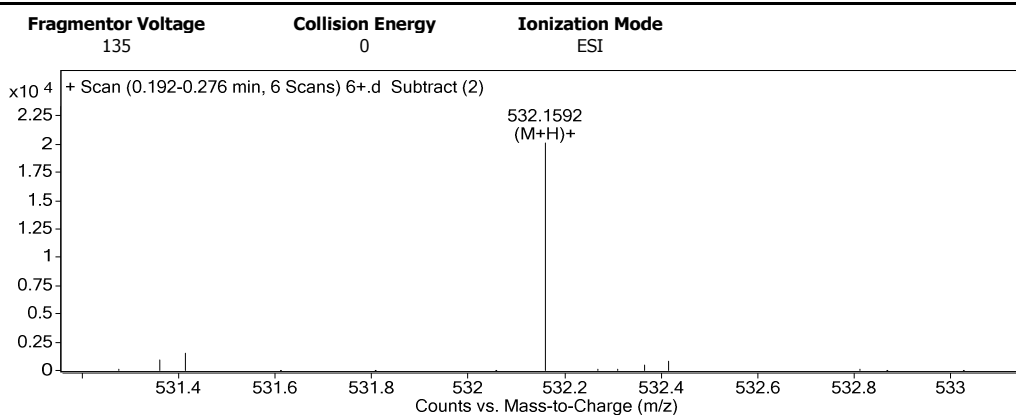
Data Filename	6+.d	Sample Name	6
Sample Type	Sample	Position	P1-B1
Instrument Name	Instrument 1	User Name	
Acq Method	SIBU.m	Acquired Time	9/22/2015 2:48:12 PM
IRM Calibration Status	Success	DA Method	ESI+.m
Comment			

Sample Group Info.

Acquisition SW Version 6200 series TOF/6500 series
Q-TOF B.05.01 (B5125.2)



User Spectra



Peak List

m/z	z	Abund
102.1276	1	166006.39
104.1071	1	81451.66
118.1223	1	62890.13
150.1043	1	453020.66
152.1014	1	139537.52
205.1336	1	130481.8
219.1743	1	89405.04
264.2323	1	237515.94

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30
Br	0	3

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C ₂₉ H ₃₀ Br N ₃ O ₂	531.1521	532.1594	532.1592	0.2	0.3	16.0000

--- End Of Report ---