Synthesis of blue emissive functionalized 9,9-disubstituted fluorene derivatives via $BF_3.OEt_2$ mediated reaction of co-planar 9-(phenylethynyl)-9H-fluoren-9-ols with isatin imines

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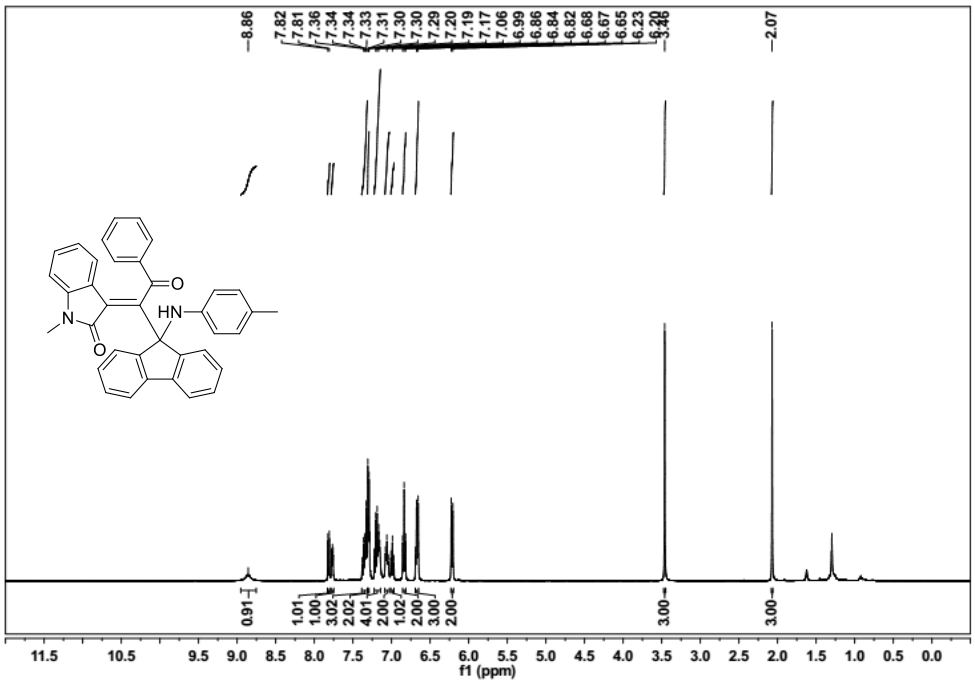
Content

1. Scanned copies of spectra (^{1}H and ^{13}C, DEPT-135 NMR, HRMS)



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Current Data Parameters
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EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20200227
Time              15.08
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                99.98
DW               62.400 usec
DE                6.50 usec
TE               295.4 K
D1           1.00000000 sec
TD0                   1

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NUC1                  1H
P1                12.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                65536
SF          400.2300000 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
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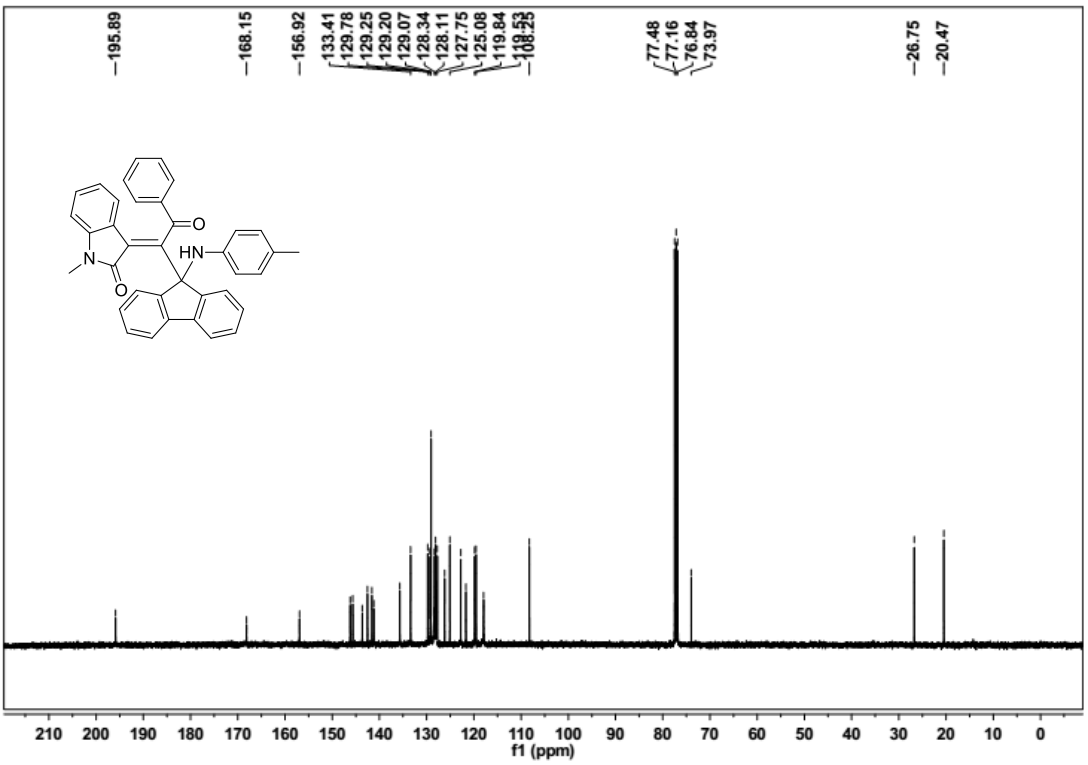
^{1}H NMR spectrum of compound **3a**



BRUKER

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Current Data Parameters
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EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
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Time                19.32
INSTRUM             spect
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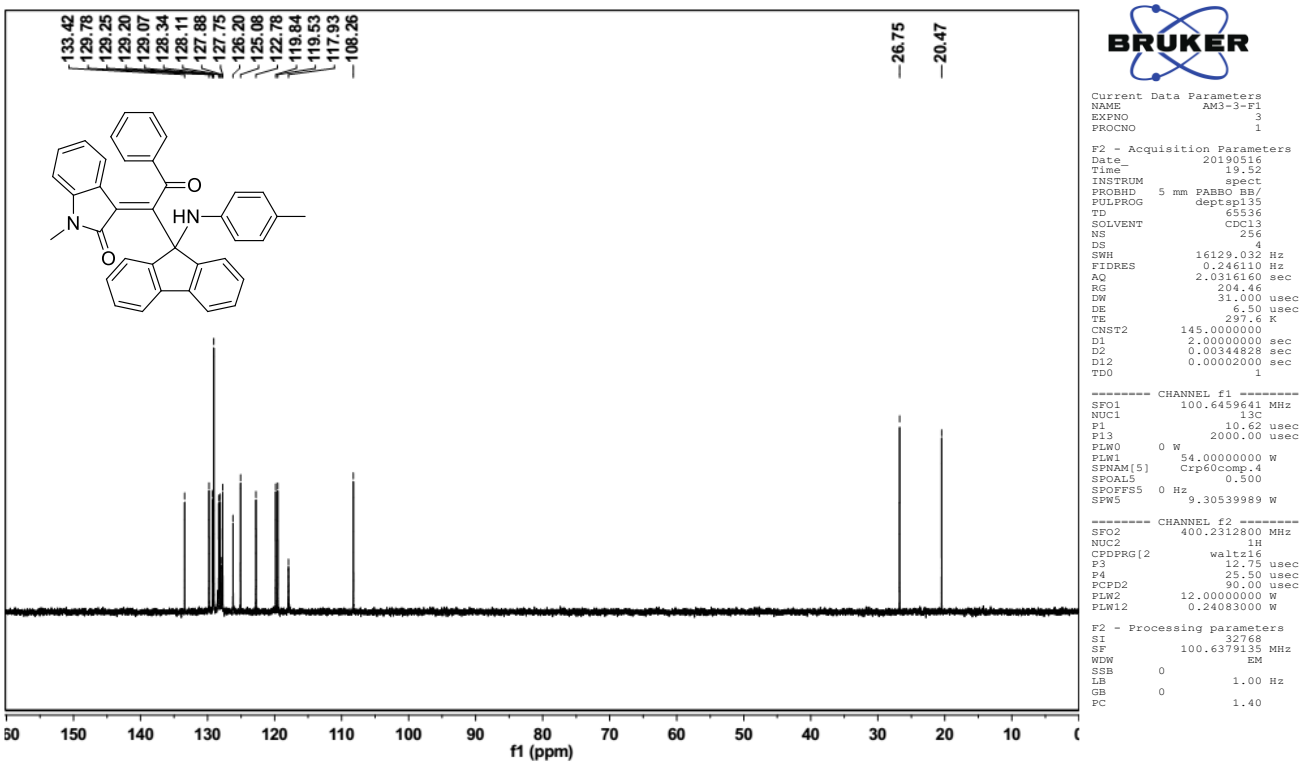
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    512
DS                      4
SWH             24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                 204.46
DW                20.800 usec
DE                 6.50 usec
TE                 298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6479769 MHz
NUC1                   13C
P1                  10.62 usec
PLW1          54.00000000 W

======== CHANNEL f2 ========
SFO2          400.2316009 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.00000000 W
PLW12          0.24083000 W
PLW13          0.19508000 W

F2 - Processing parameters
SI                  32768
SF            100.6379135 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

^{13} C NMR Spectrum of compound **3a**

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EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
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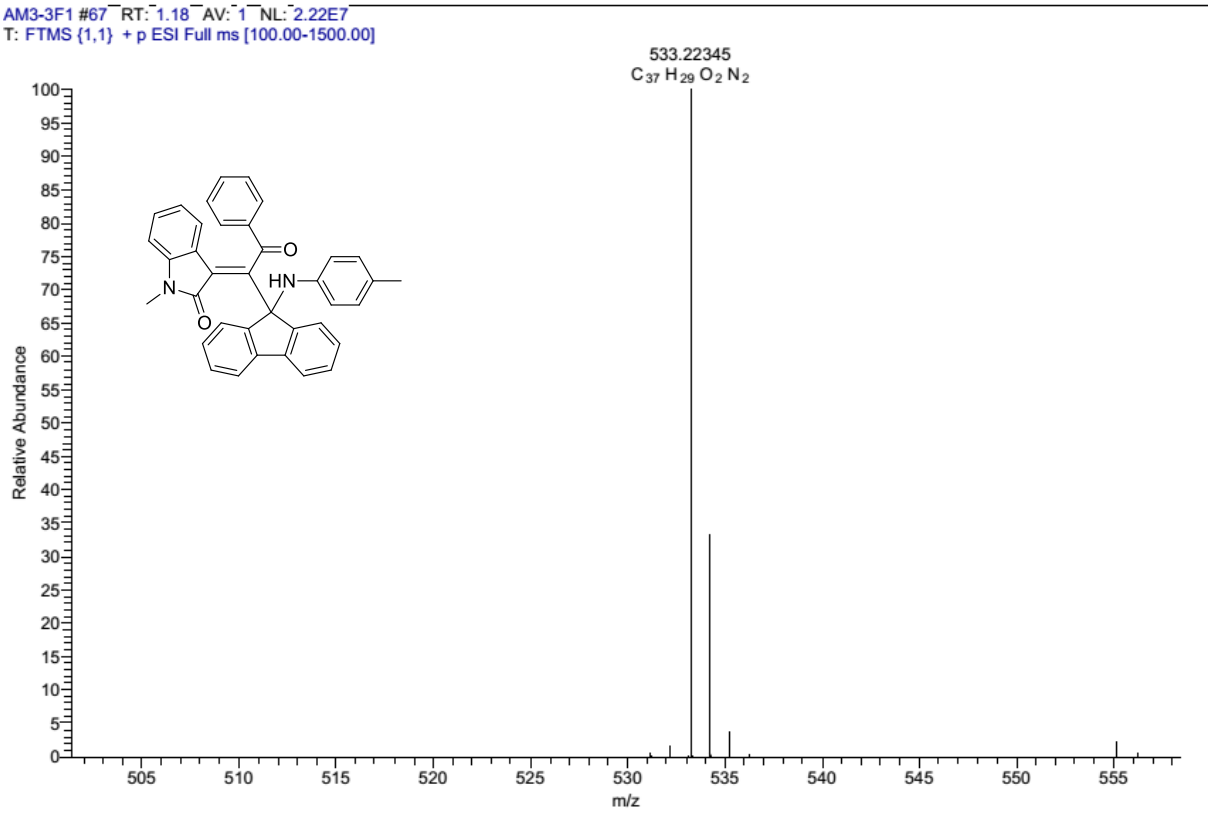
Time                   19.52
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG          deptsp135
TD                   65536
SOLVENT              CDCl3
NS                     256
DS                       4
SWH              16129.032 Hz
FIDRES           0.246110 Hz
AQ               2.0316160 sec
RG                  204.46
DW                  31.000 usec
DE                   6.50 usec
TE                  297.6 K
CNST2           145.0000000
D1               2.00000000 sec
D2               0.00344828 sec
D12              0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            100.6459641 MHz
NUC1                    13C
P1                    10.62 usec
P13                2000.00 usec
PLW0       0 W
PLW1          54.00000000 W
SPNAM[5]      Crp60comp.4
SPOAL5              0.500
SPOFFS5    0 Hz
SPW5           9.30539989 W

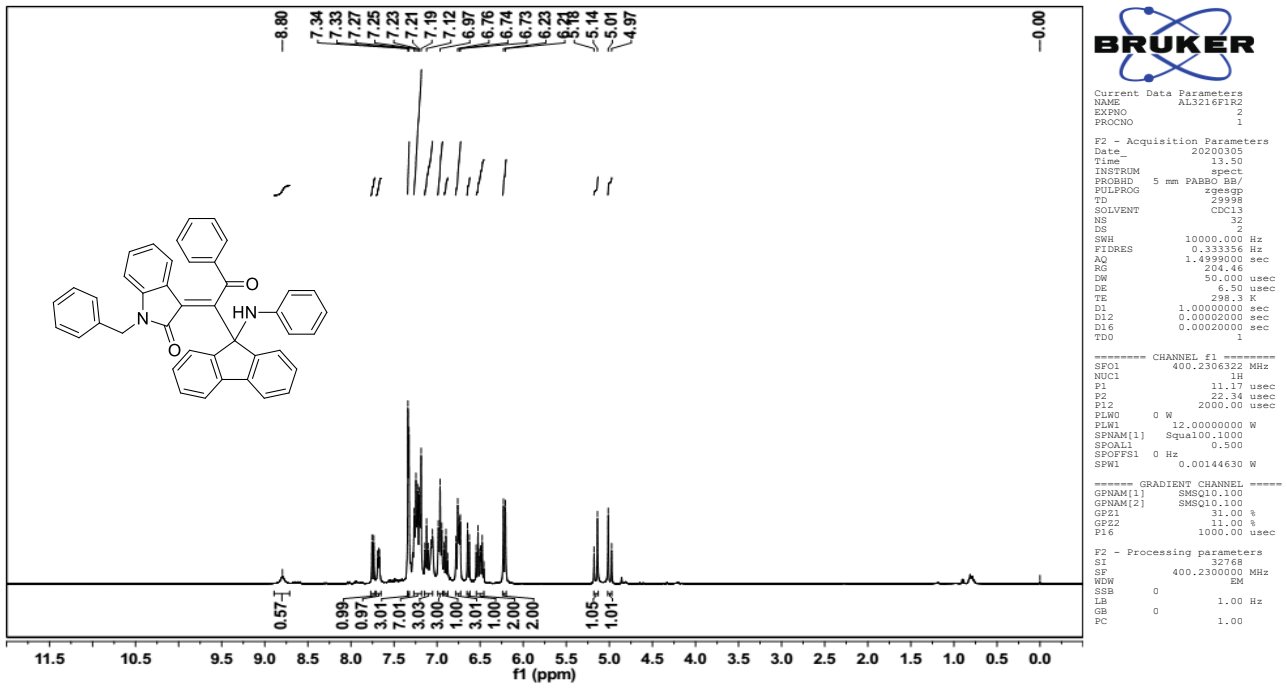
======== CHANNEL f2 ========
SFO2            400.2312800 MHz
NUC2                    1H
CPDPRG[2            waltz16
P3                    12.75 usec
P4                    25.50 usec
PCPD2                 90.00 usec
PLW2           12.00000000 W
PLW12           0.24083000 W

F2 - Processing parameters
SI                    32768
SF              100.6379135 MHz
WDW                     EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    1.40
```

DEPT- 135 Spectrum of compound **3a**



HRMS Spectrum of Compound **3a**



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Current Data Parameters
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EXPNO                          2
PROCNO                         1

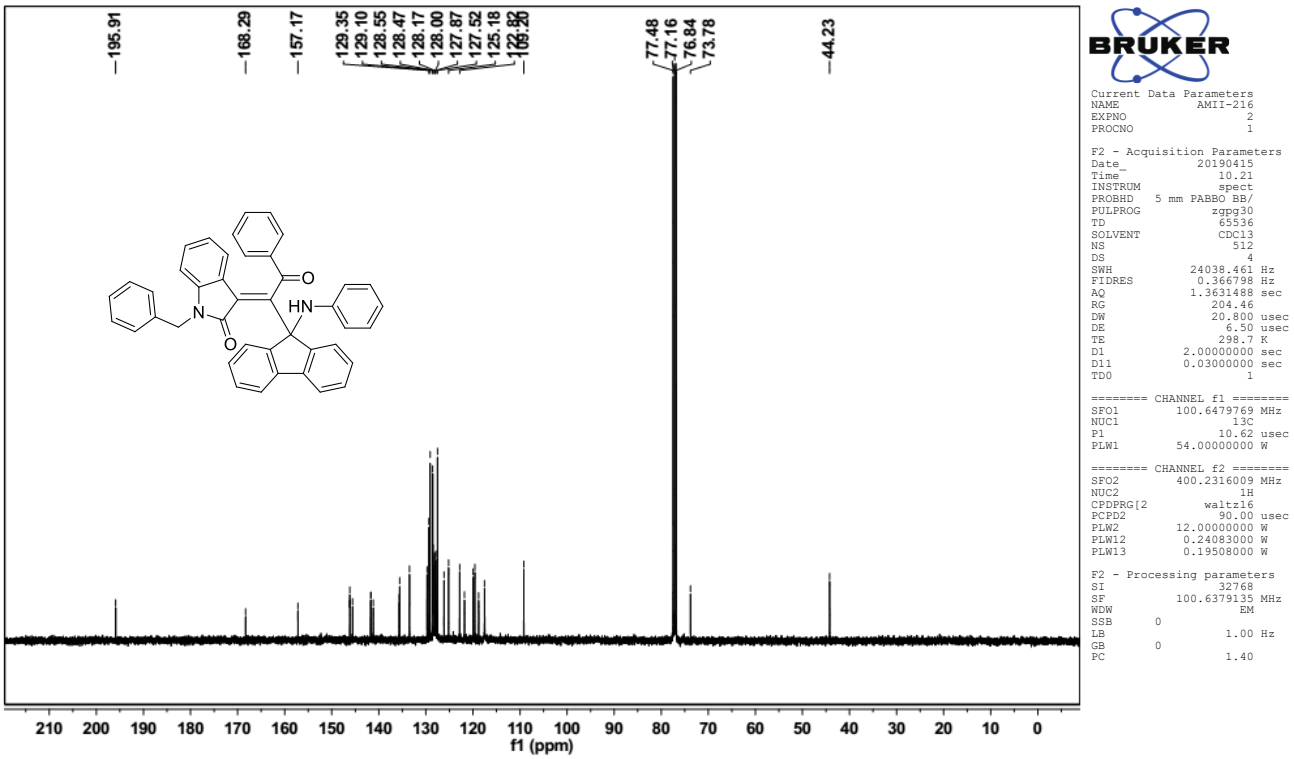
F2 - Acquisition Parameters
Date_               20200305
Time                   13.50
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgesgp
TD                     29998
SOLVENT                CDCl3
NS                        32
DS                         2
SWH                10000.000 Hz
FIDRES             0.333356 Hz
AQ                 1.4999000 sec
RG                    204.46
DW                    50.000 usec
DE                     6.50 usec
TE                    298.3 K
D1                 1.00000000 sec
D12                0.00002000 sec
D16                0.00020000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             400.2306322 MHz
NUC1                       1H
P1                      11.17 usec
P2                      22.34 usec
P12                   2000.00 usec
PLW0        0 W
PLW1              12.00000000 W
SPNAM[1]    Squa100.1000
SPOAL1                  0.500
SPOFFS1     0 Hz
SPW1               0.00144630 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPNAM[2]       SMSQ10.100
GPZ1                   31.00 %
GPZ2                   11.00 %
P16                  1000.00 usec

F2 - Processing parameters
SI                        32768
SF                 400.2300000 MHz
WDW                          EM
SSB         0
LB                      1.00 Hz
GB          0
PC                      1.00
```

^{1}H NMR spectrum of compound **3b**



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Current Data Parameters
NAME                   AMIT-216
EXPNO                          2
PROCNO                         1

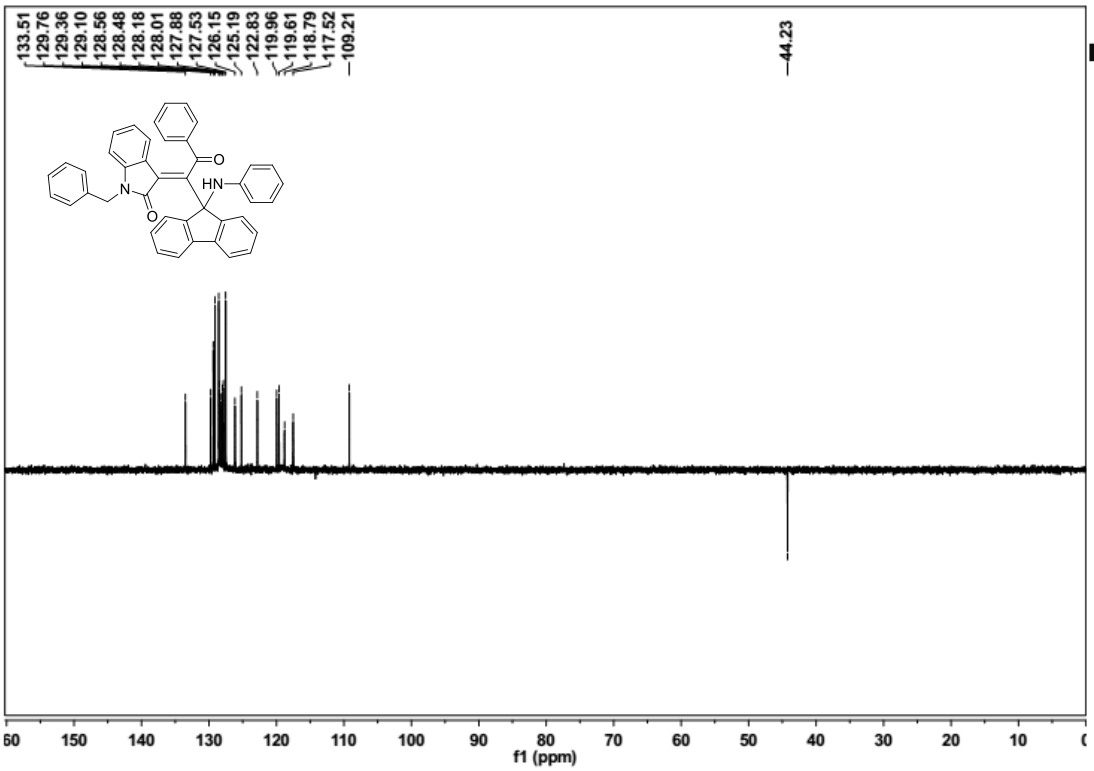
F2 - Acquisition Parameters
Date_               20190415
Time                   10.21
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       512
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    204.46
DW                    20.800 usec
DE                     6.50 usec
TE                    298.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             100.6479769 MHz
NUC1                      13C
P1                      10.62 usec
PLW1              54.00000000 W

======== CHANNEL f2 ========
SFO2             400.2316009 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                  90.00 usec
PLW2              12.00000000 W
PLW12              0.24083000 W
PLW13              0.19508000 W

F2 - Processing parameters
SI                        32768
SF                 100.6379135 MHz
WDW                          EM
SSB         0
LB                      1.00 Hz
GB          0
PC                      1.40
```

^{13} C NMR Spectrum of compound **3b**



Current Data Parameters
NAME AMII-216
EXPNO 3
PROCNO 1

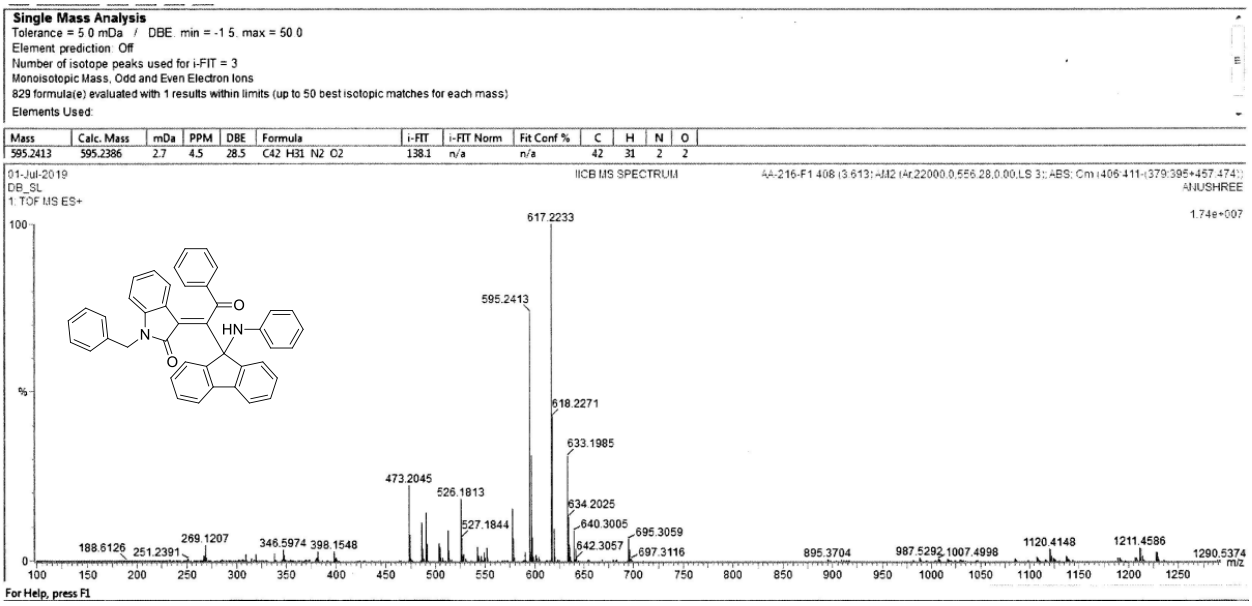
F2 - Acquisition Parameters
Date_ 20190415
Time 10.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 204.46
DW 31.000 usec
DE 6.50 usec
TE 298.3 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6459641 MHz
NUC1 13C
P1 10.62 usec
P13 2000.00 usec
PLW0 0 W
PLW1 54.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.30539989 W

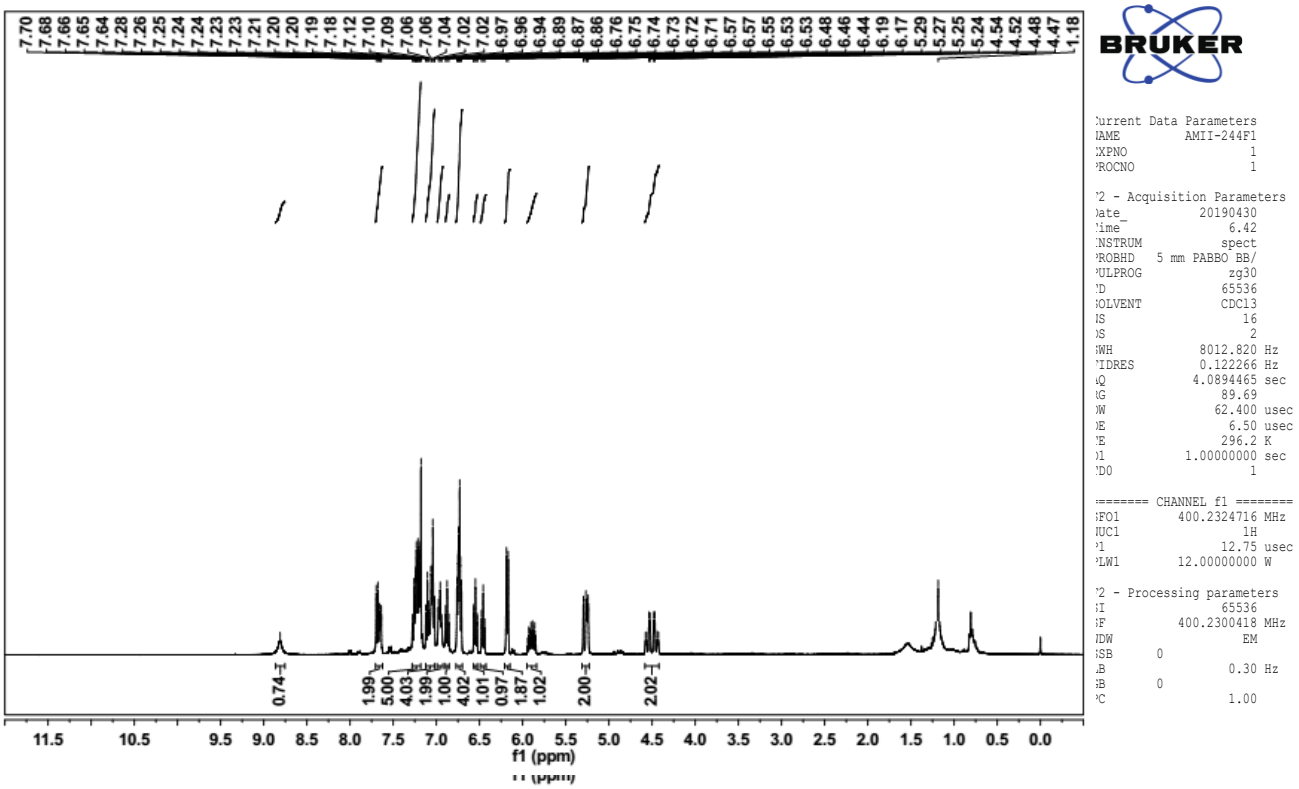
======== CHANNEL f2 ========
SFO2 400.2312800 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 12.75 usec
P4 25.50 usec
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

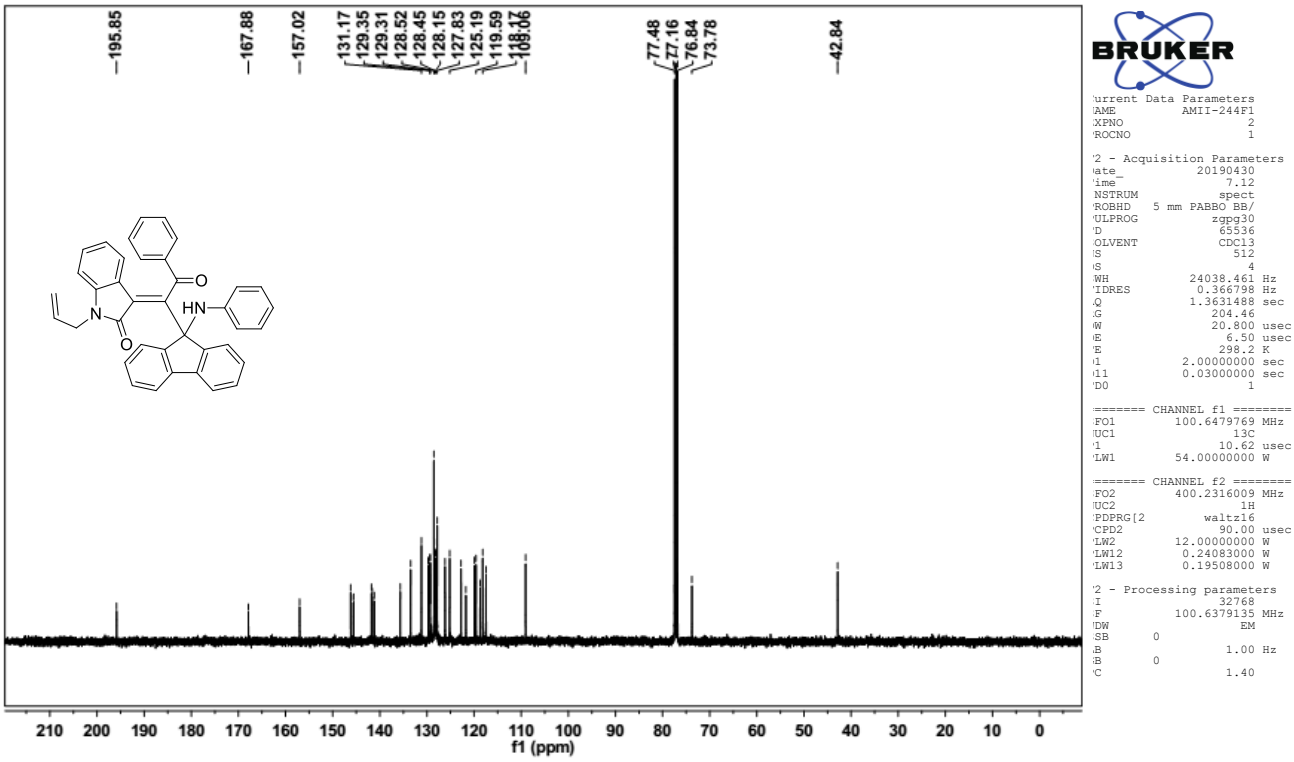
DEPT- 135 Spectrum of compound **3b**



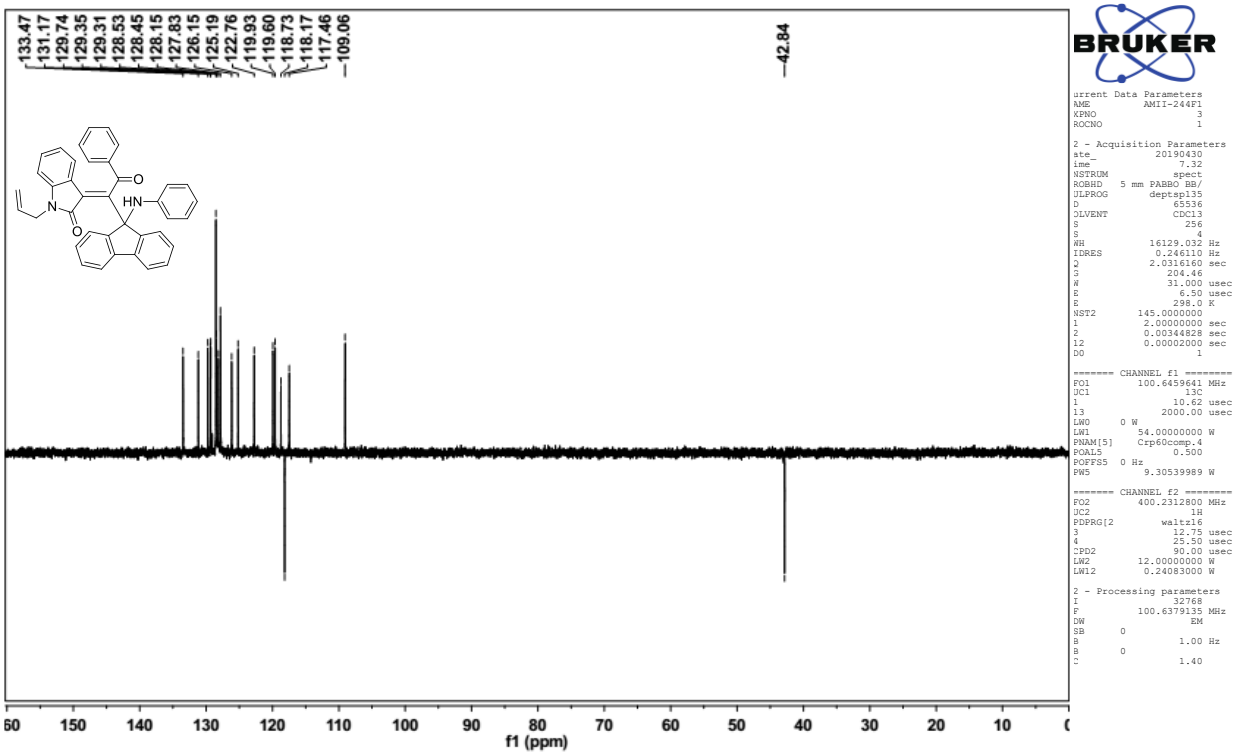
HRMS Spectrum of Compound **3b**



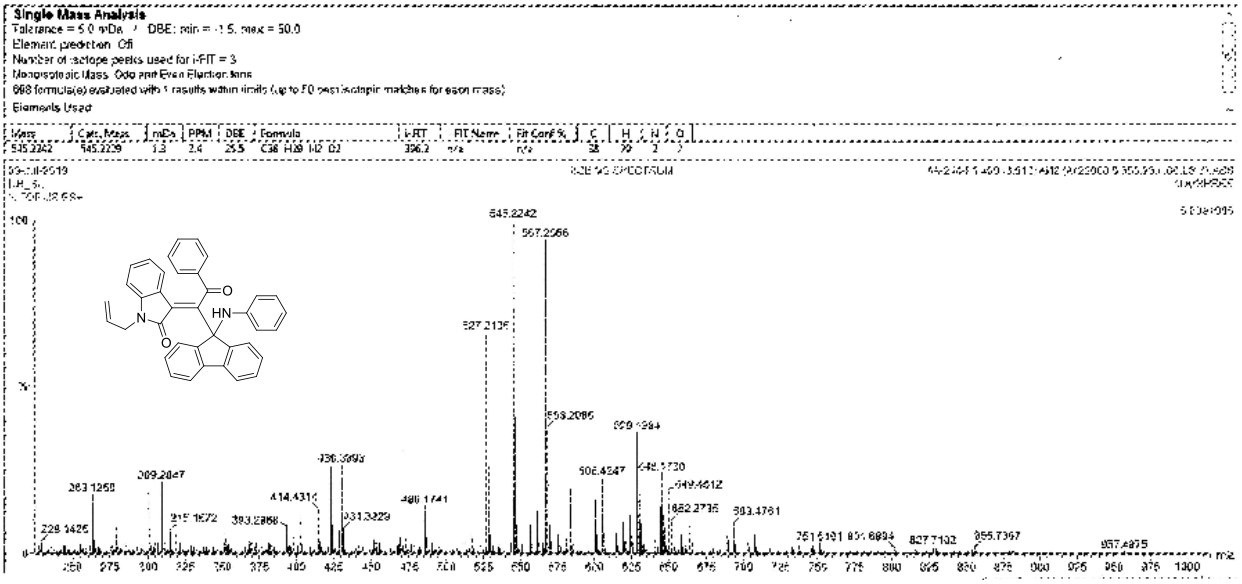
^{1}H NMR spectrum of compound **3c**



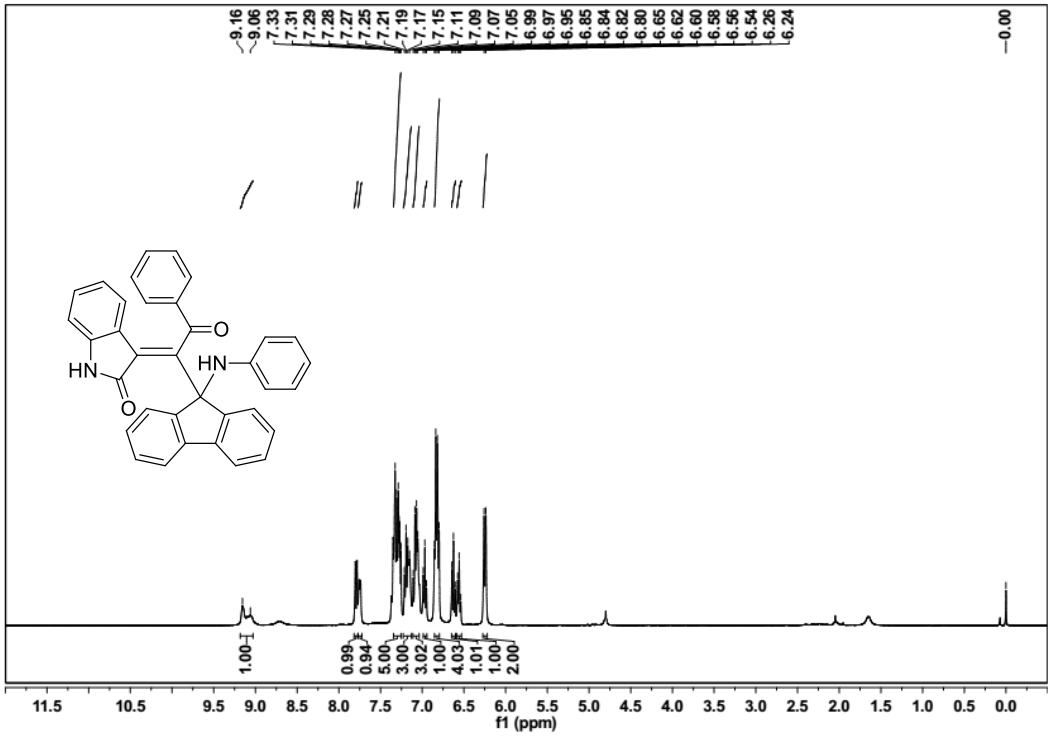
^{13} C NMR Spectrum of compound **3c**



DEPT- 135 Spectrum of compound **3c**



HRMS Spectrum of Compound **3c**



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Current Data Parameters
NAME            AM3240F2
EXPNO                  4
PROCNO                 1

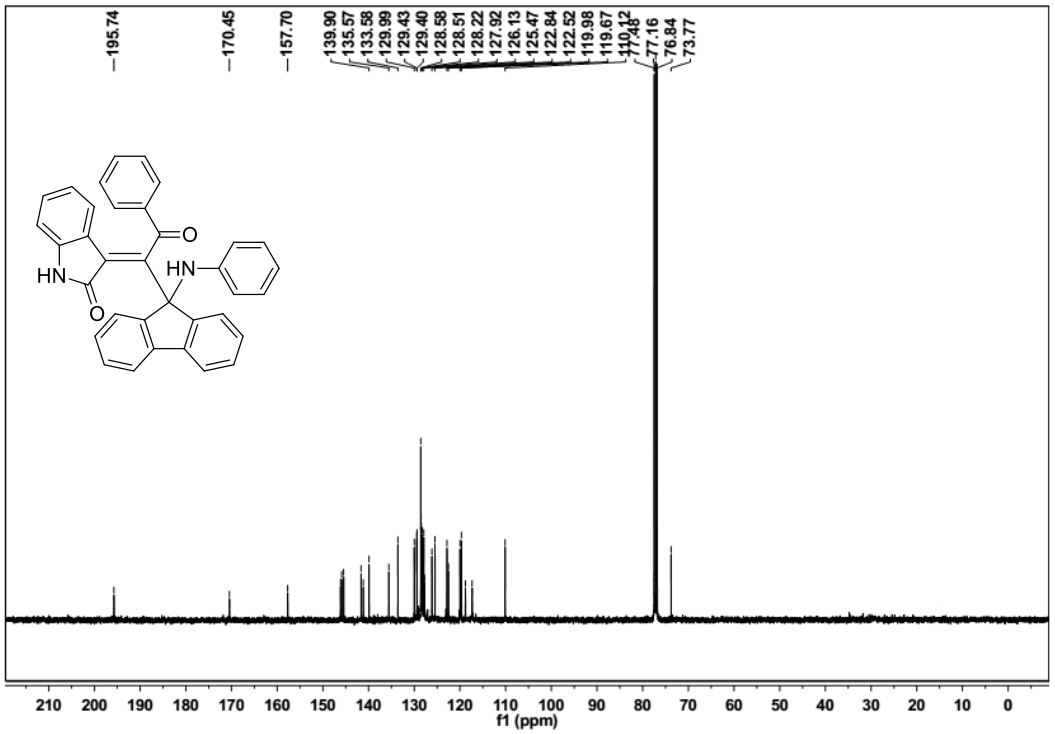
F2 - Acquisition Parameters
Date_           20200313
Time                7.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgesgp
TD                 29998
SOLVENT             CDCl3
NS                    64
DS                     2
SWH            10000.000 Hz
FIDRES             0.333356 Hz
AQ              1.4999000 sec
RG                 204.46
DW                 50.000 usec
DE                  6.50 usec
TE                297.2 K
D1             1.00000000 sec
D12            0.00002000 sec
D16            0.00020000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.2306625 MHz
NUC1                   1H
P1                  11.17 usec
P2                  22.34 usec
P12               2000.00 usec
PLW0      0 W
PLW1       12.00000000 W
SPNAM[1]   Squa100.1000
SPOAL1              0.500
SPOFFS1   0 Hz
SPW1           0.00144630 W

====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPNAM[2]       SMSQ10.100
GPZ1                31.00 %
GPZ2                11.00 %
P16               1000.00 usec

F2 - Processing parameters
SI                    32768
SF           400.2300000 MHz
WDW                     EM
SSB       0
LB                   0.20 Hz
GB        0
PC                   1.00
```

^{1}H NMR spectrum of compound **3d**



BRUKER

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Current Data Parameters
NAME         AMII-240-F1R
EXPNO                   2
PROCNO                  1

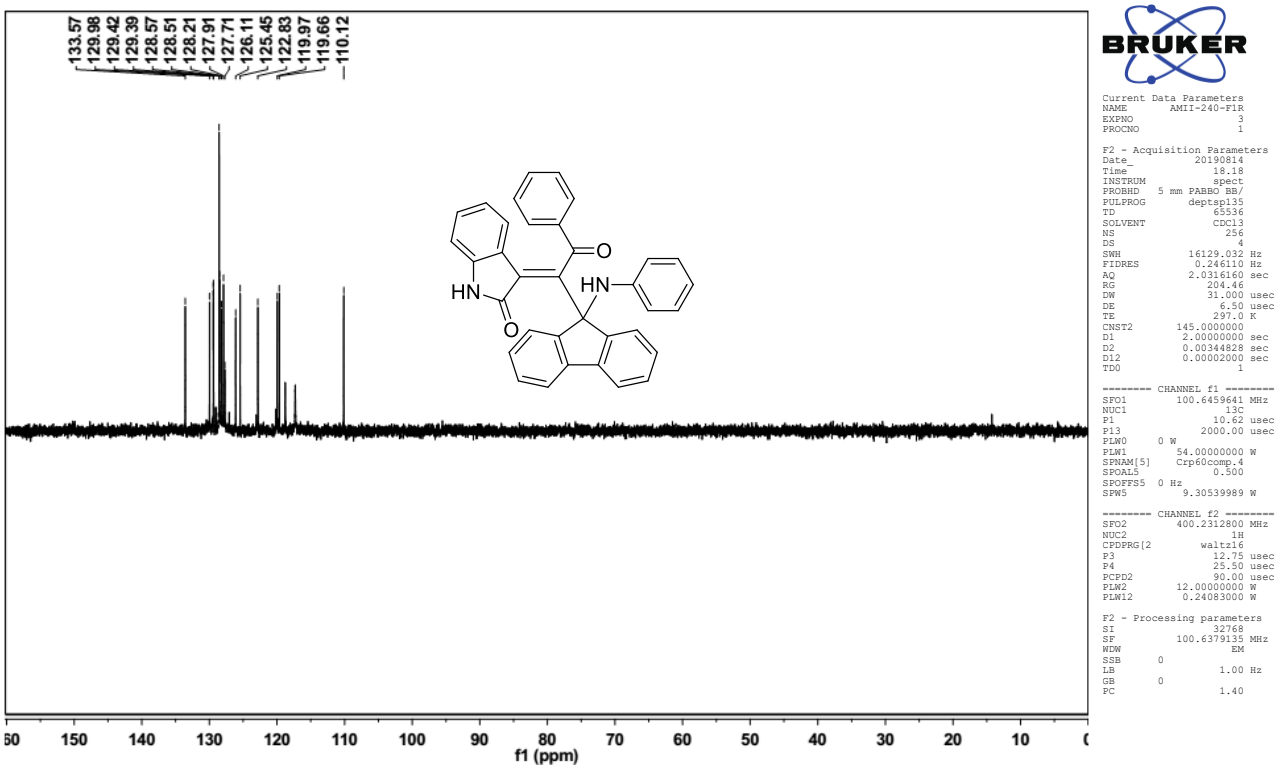
F2 - Acquisition Parameters
Date_           20190814
Time               17.59
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT             CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631488 sec
RG                 204.46
DW                 20.800 usec
DE                  6.50 usec
TE                297.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6479769 MHz
NUC1                  13C
P1                  10.62 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2         400.2316009 MHz
NUC2                   1H
CPDPRG[2         waltz16
PCPD2               90.00 usec
PLW2        12.00000000 W
PLW12        0.24083000 W
PLW13        0.19508000 W

F2 - Processing parameters
SI                    32768
SF           100.6379135 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

^{13}C NMR spectrum of compound **3d**



BRUKER

Current Data Parameters
NAME AMI-240-P1R
EXPNO 3
PROCNO 1

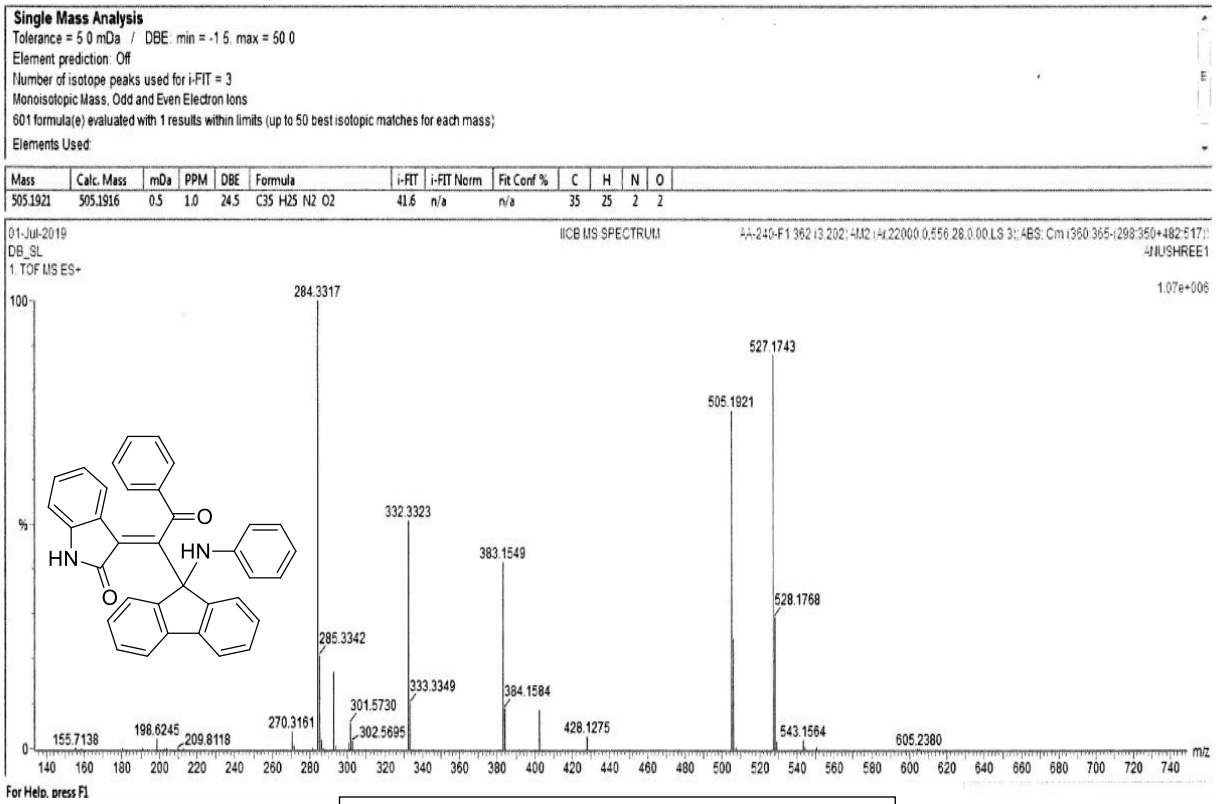
F2 - Acquisition Parameters
Date_ 20190814
Time 18.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 204.46
DW 31.000 usec
DE 6.50 usec
TE 297.0 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6459641 MHz
NUC1 13C
P1 10.62 usec
P13 2000.00 usec
PLW0 0 W
PLW1 54.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.30539989 W

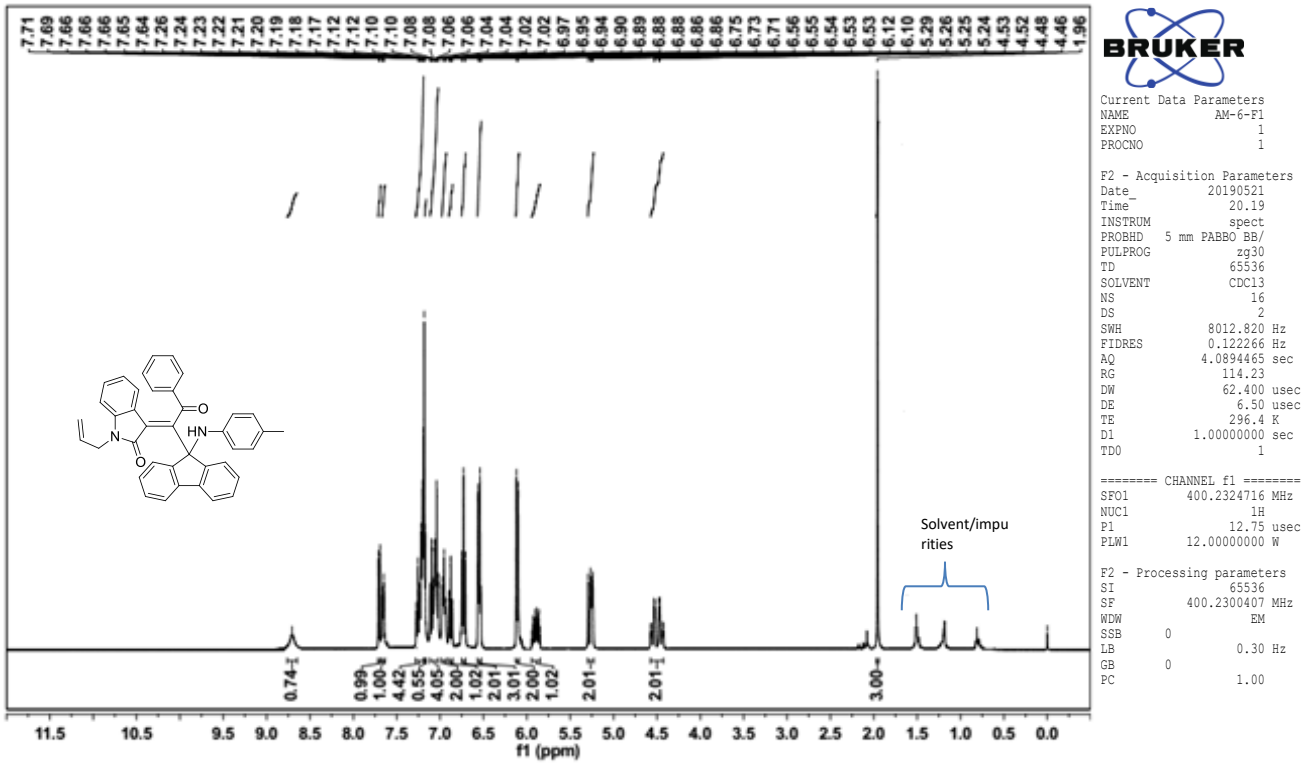
======== CHANNEL f2 ========
SFO2 400.2312800 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 12.75 usec
P4 25.50 usec
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT- 135 Spectrum of compound **3d**



HRMS Spectrum of Compound **3d**



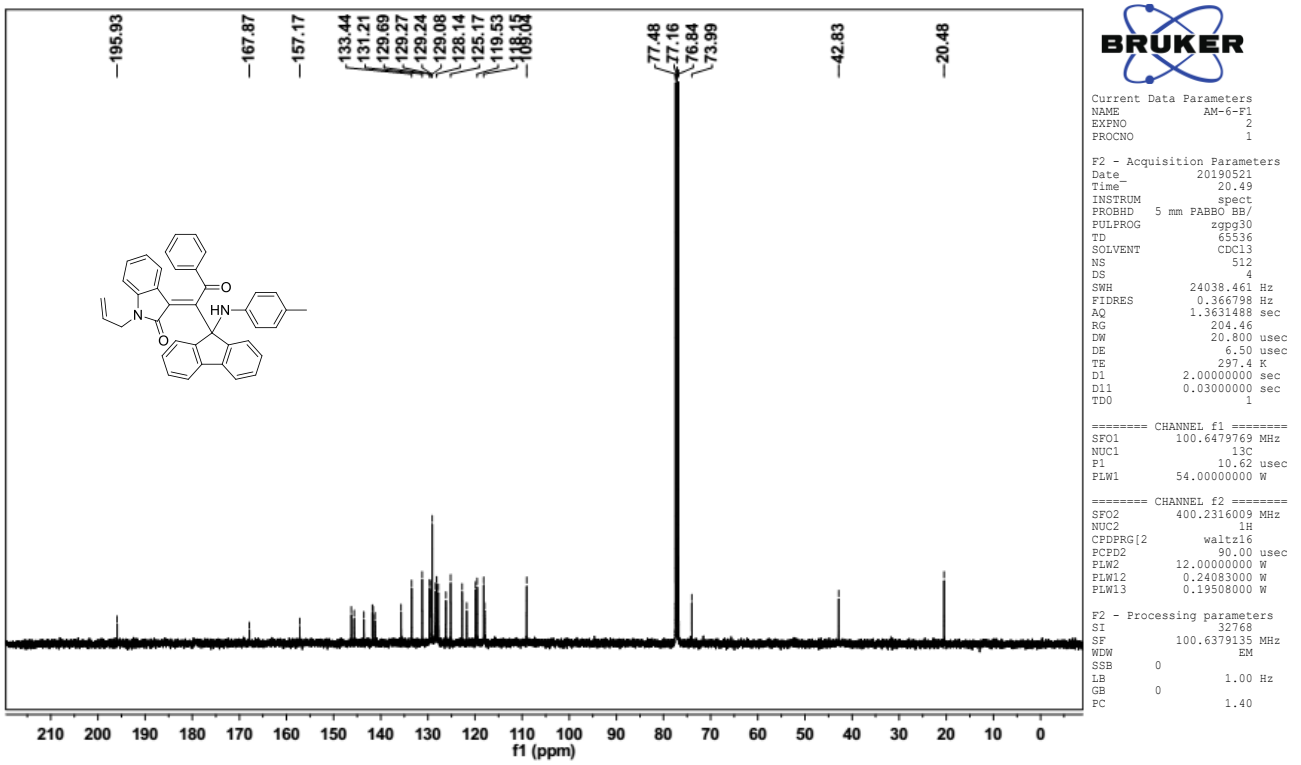
Current Data Parameters
NAME AM-6-F1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190521
Time 20.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114.23
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2324716 MHz
NUC1 1H
P1 12.75 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2300407 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR spectrum of compound **3e**



Current Data Parameters
NAME AM-6-F1
EXPNO 2
PROCNO 1

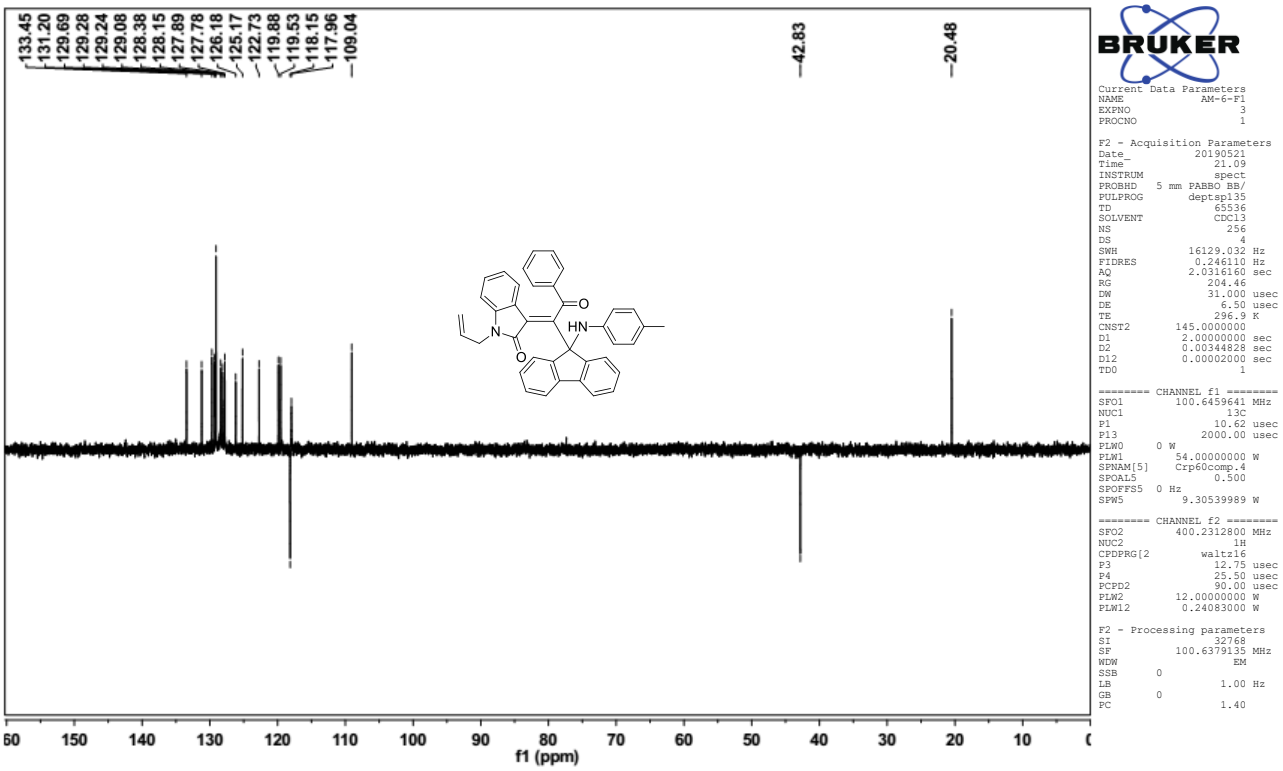
F2 - Acquisition Parameters
Date_ 20190521
Time 20.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 204.46
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6479769 MHz
NUC1 13C
P1 10.62 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W
PLW13 0.19508000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13} C NMR Spectrum of compound **3e**



Current Data Parameters
NAME AM-6-F1
EXPNO 3
PROCNO 1

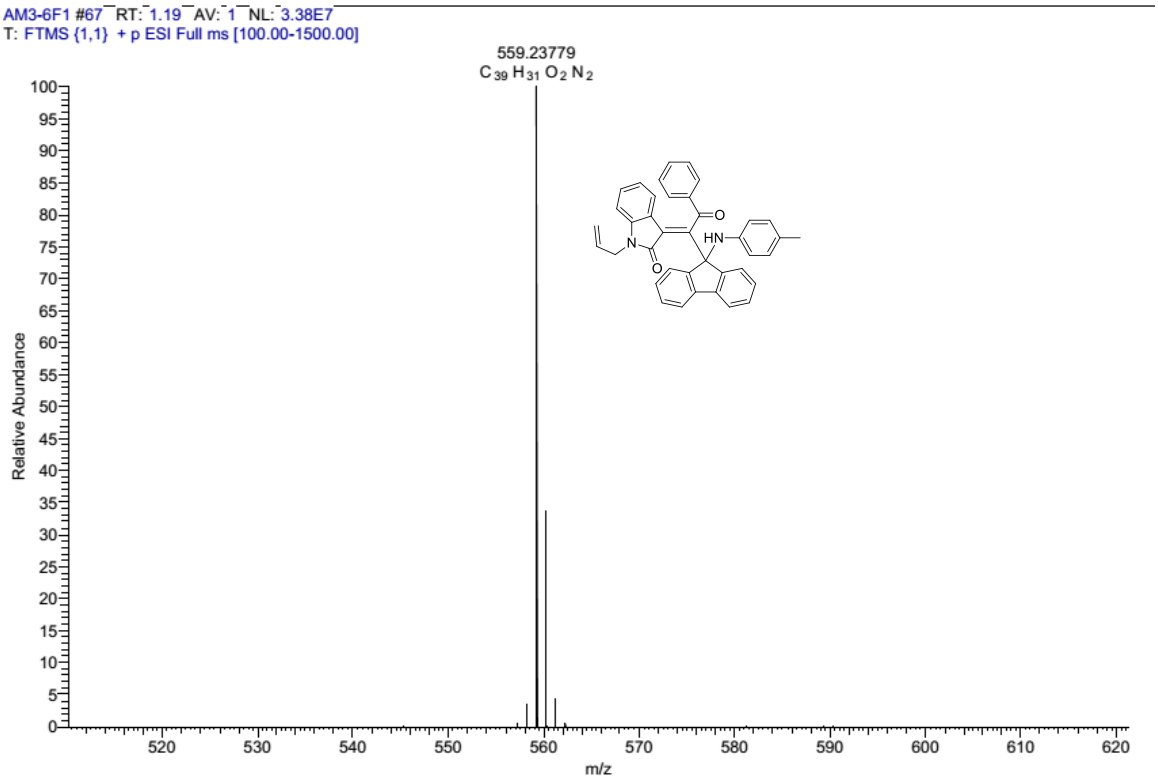
F2 - Acquisition Parameters
Date_ 20190521
Time 21.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 204.46
DW 31.000 usec
DE 6.50 usec
TE 296.9 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6459641 MHz
NUC1 13C
P1 10.62 usec
P13 2000.00 usec
PLW0 0 W
PLW1 54.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.30539989 W

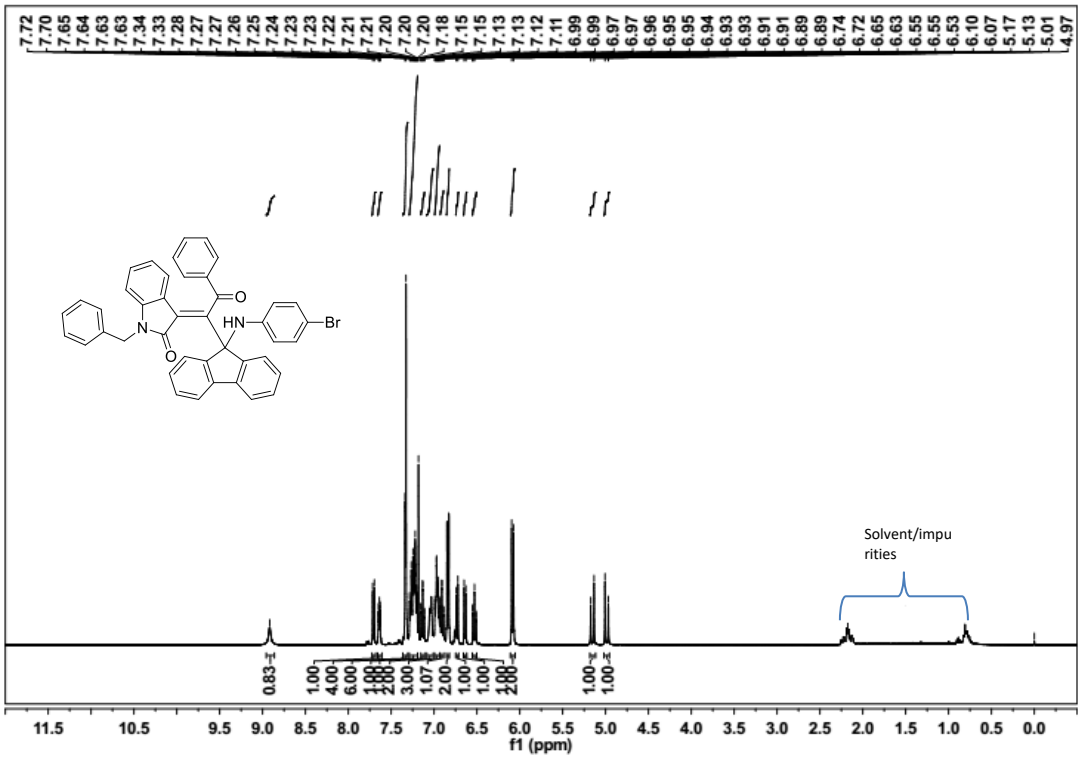
======== CHANNEL f2 ========
SFO2 400.2312800 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 12.75 usec
P4 25.50 usec
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT- 135 Spectrum of compound **3e**



HRMS Spectrum of Compound **3e**



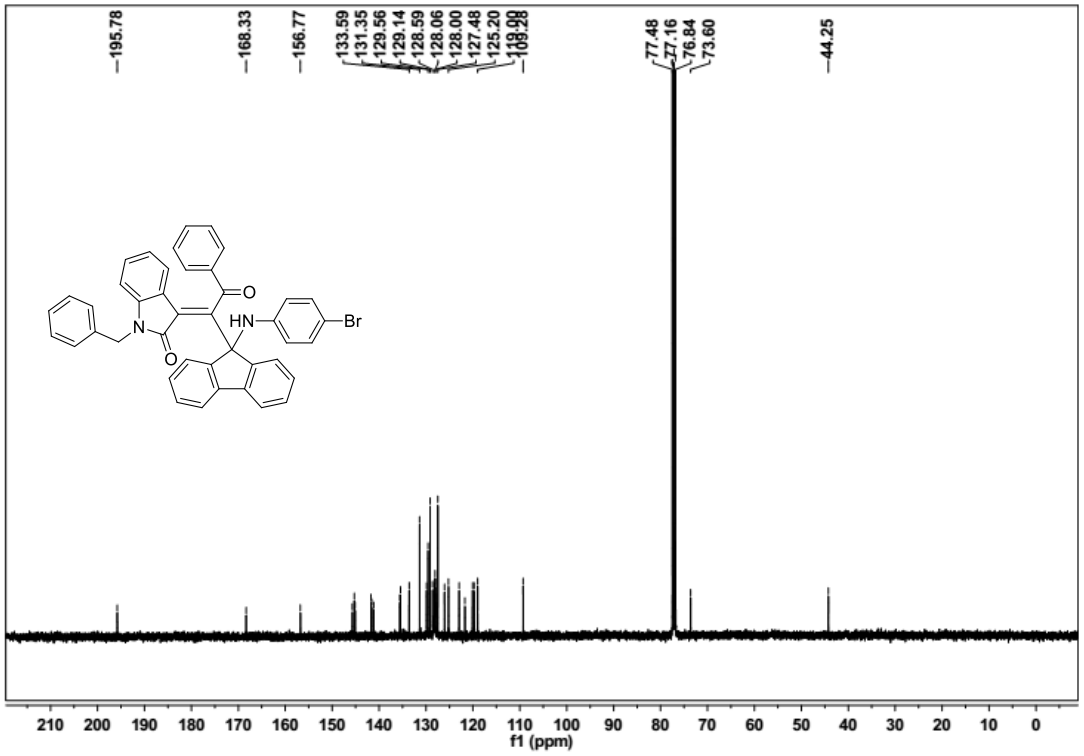
Current Data Parameters
NAME AM3-9-F1R
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190528
Time 23.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114.23
DW 62.400 usec
DE 6.50 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2324716 MHz
NUC1 1H
P1 12.75 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2300411 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR spectrum of compound **3f**



Current Data Parameters
NAME AM3-9-F1R
EXPNO 2
PROCNO 1

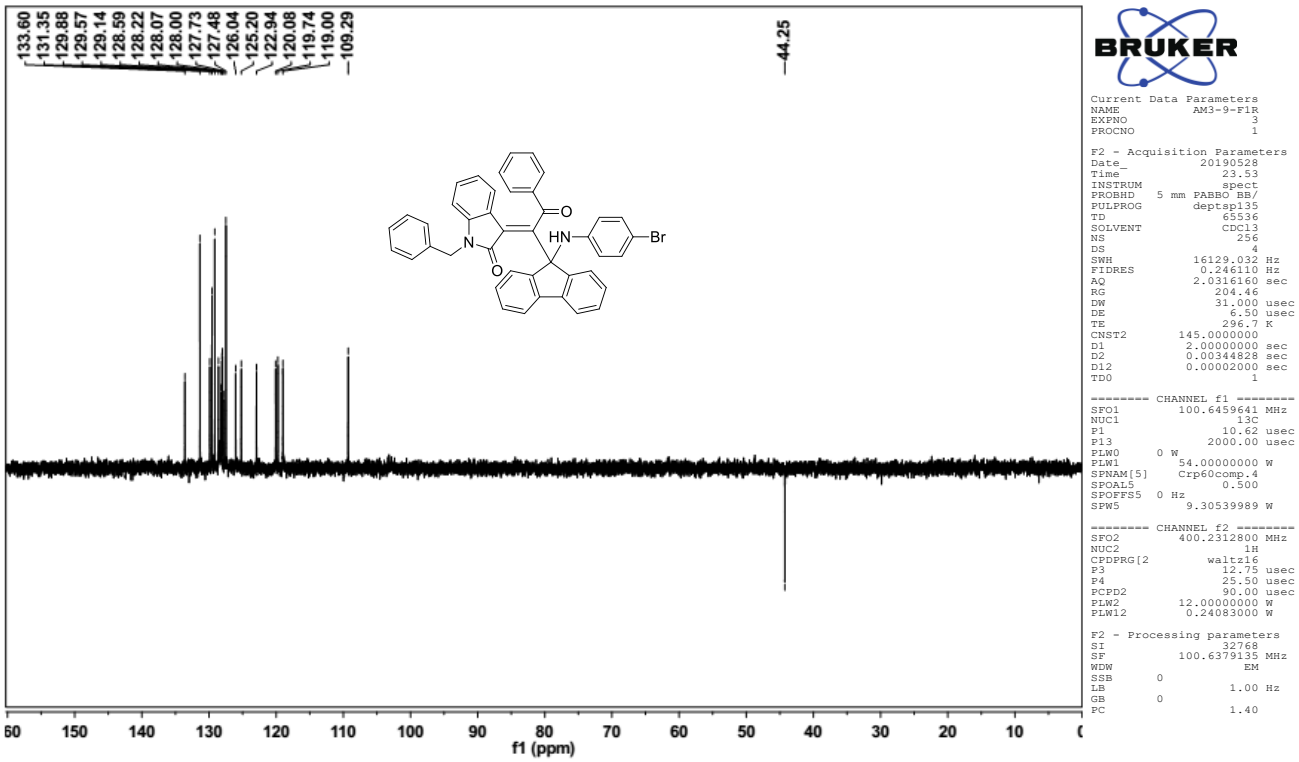
F2 - Acquisition Parameters
Date_ 20190528
Time 23.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 204.46
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6479769 MHz
NUC1 13C
P1 10.62 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W
PLW13 0.19508000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13}C NMR Spectrum of compound **3f**



BRUKER

Current Data Parameters
NAME AM3-9-F1R
EXPNO 3
PROCNO 1

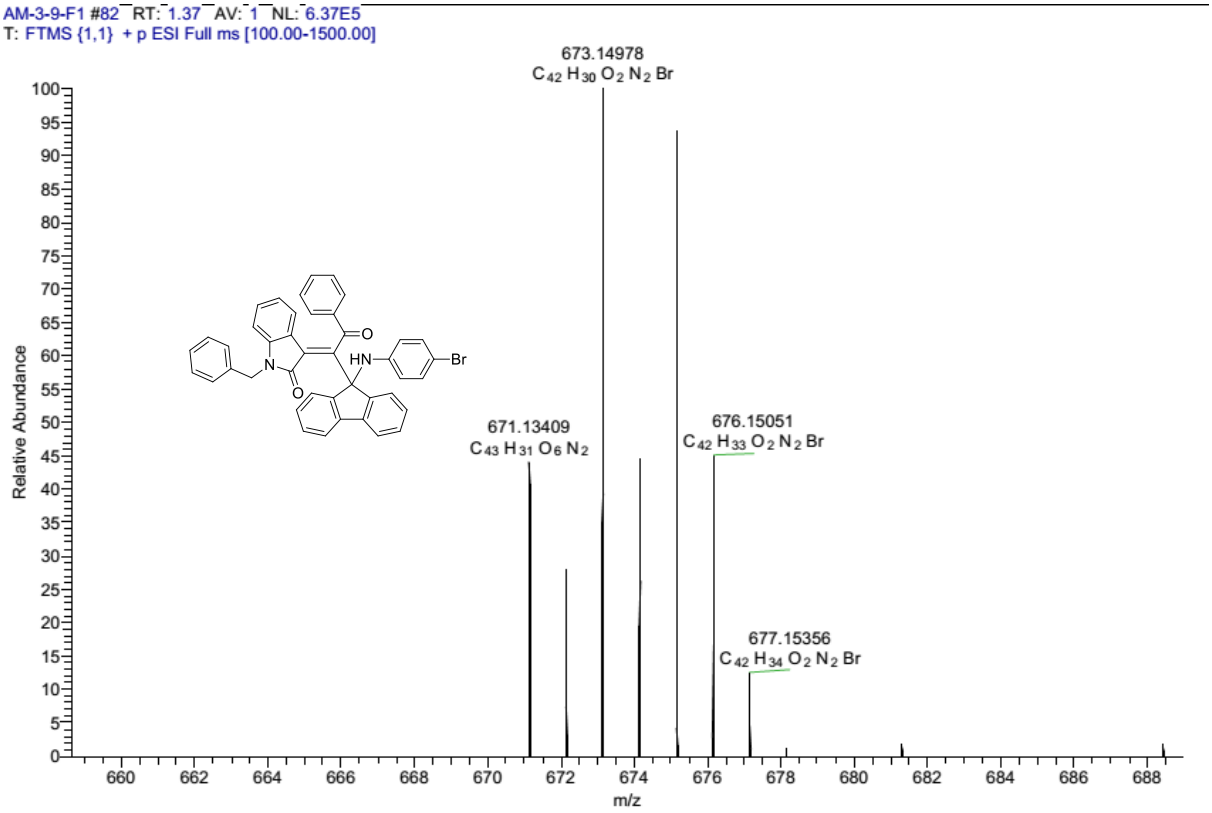
F2 - Acquisition Parameters
Date_ 20190528
Time 23.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 204.46
DW 31.000 usec
DE 6.50 usec
TE 296.7 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6459641 MHz
NUC1 13C
P1 10.62 usec
P13 2000.00 usec
PLW0 0 W
PLW1 54.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.30539989 W

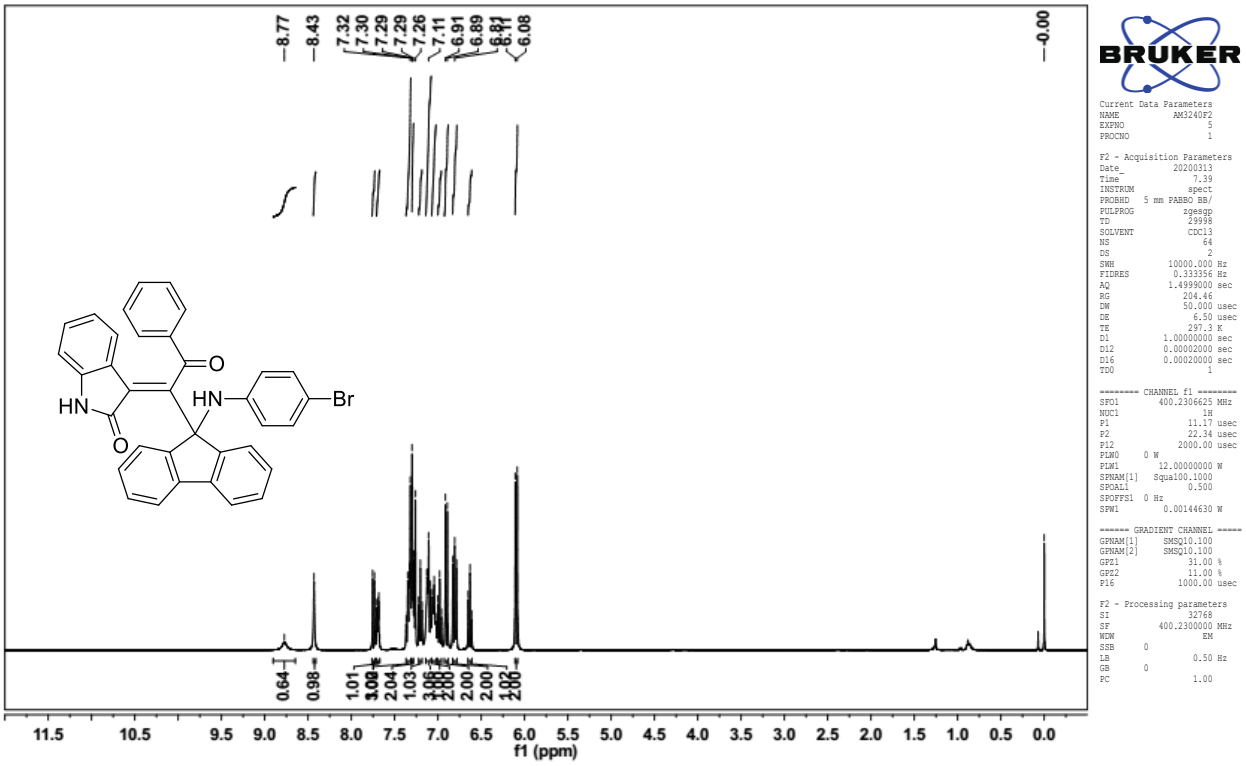
======== CHANNEL f2 ========
SFO2 400.2312800 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 12.75 usec
P4 25.50 usec
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT- 135 Spectrum of compound **3f**



HRMS Spectrum of Compound **3f**




```
Current Data Parameters
NAME                  AM3240F2
EXPNO                        5
PROCNO                       1

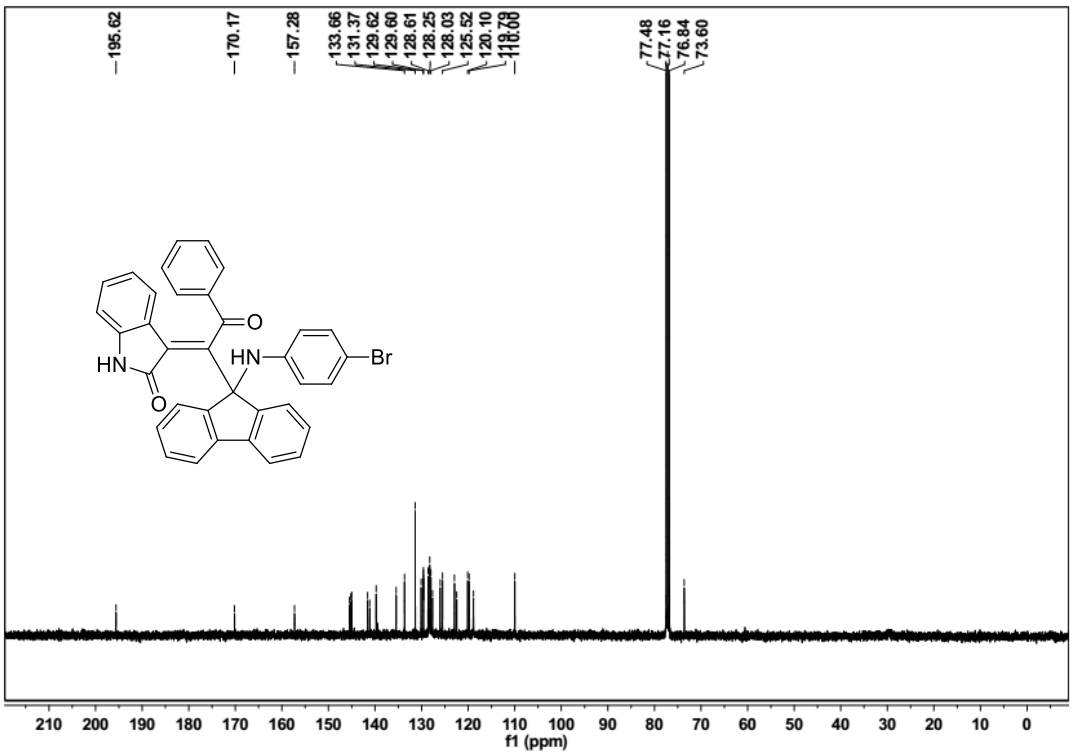
F2 - Acquisition Parameters
Date_               20200313
Time                    7.39
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgesgp
TD                     29998
SOLVENT                CDCl3
NS                        64
DS                         2
SWH                10000.000 Hz
FIDRES             0.333356 Hz
AQ                 1.4999000 sec
RG                     204.46
DW                   50.000 usec
DE                    6.50 usec
TE                    297.3 K
D1                 1.00000000 sec
D12                0.00002000 sec
D16                0.00020000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             400.2306625 MHz
NUC1                       1H
P1                      11.17 usec
P2                      22.34 usec
P12                  2000.00 usec
PLW0         0 W
PLW1            12.00000000 W
SPNAM[1]    Squa100.1000
SPOAL1                  0.500
SPOFFS1    0 Hz
SPW1                0.00144630 W

====== GRADIENT CHANNEL =====
GPNAM[1]         SMSQ10.100
GPNAM[2]         SMSQ10.100
GPZ1                    31.00 %
GPZ2                    11.00 %
P16                   1000.00 usec

F2 - Processing parameters
SI                        32768
SF                400.2300000 MHz
WDW                          EM
SSB          0
LB                       0.50 Hz
GB           0
PC                       1.00
```

^{1}H NMR spectrum of compound **3g**




```
Current Data Parameters
NAME                  AM3-12-F1
EXPNO                        2
PROCNO                       1

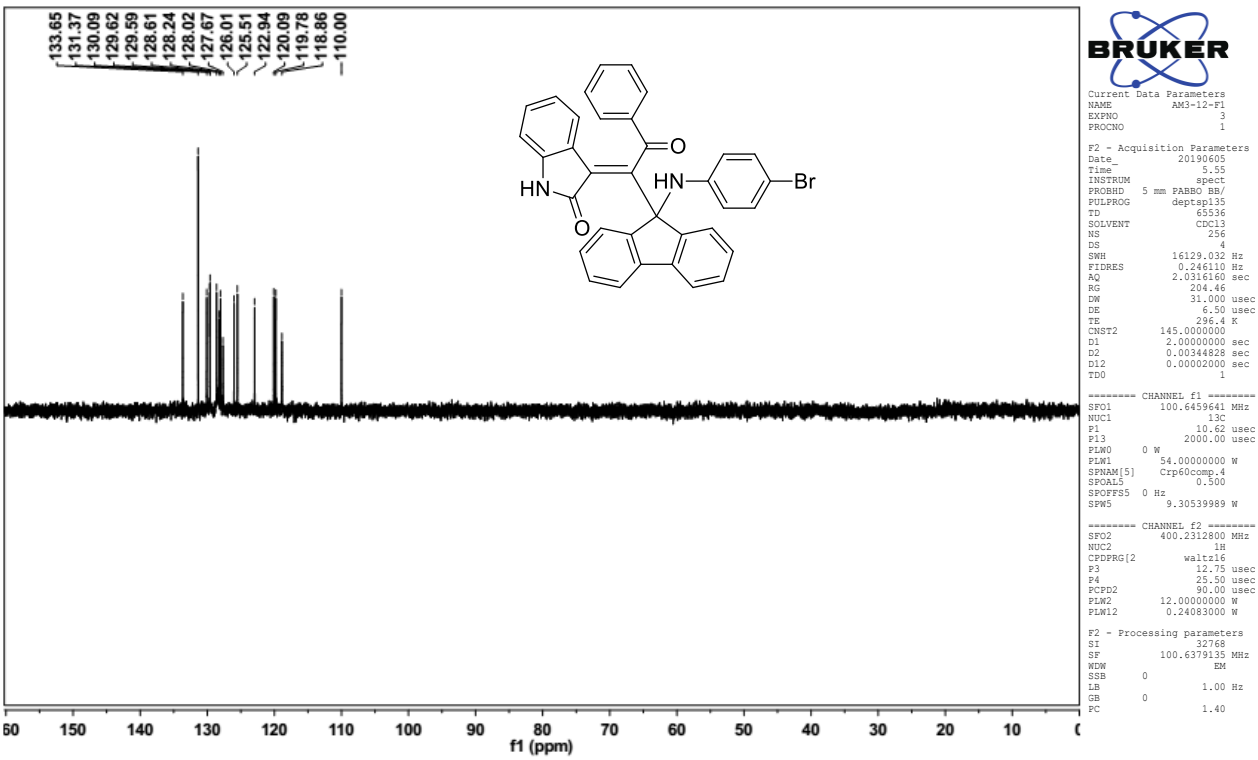
F2 - Acquisition Parameters
Date_               20190605
Time                    5.36
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                     204.46
DW                   20.800 usec
DE                    6.50 usec
TE                    296.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1             100.6479769 MHz
NUC1                      13C
P1                      10.62 usec
PLW1            54.00000000 W

======== CHANNEL f2 ========
SFO2             400.2316009 MHz
NUC2                       1H
CPDPRG[2          waltz16
PCPD2                   90.00 usec
PLW2            12.00000000 W
PLW12            0.24083000 W
PLW13            0.19508000 W

F2 - Processing parameters
SI                        32768
SF                100.6379135 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```

^{13} C NMR Spectrum of compound **3g**



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Current Data Parameters
NAME AM3-12-F1
EXPNO 3
PROCNO 1

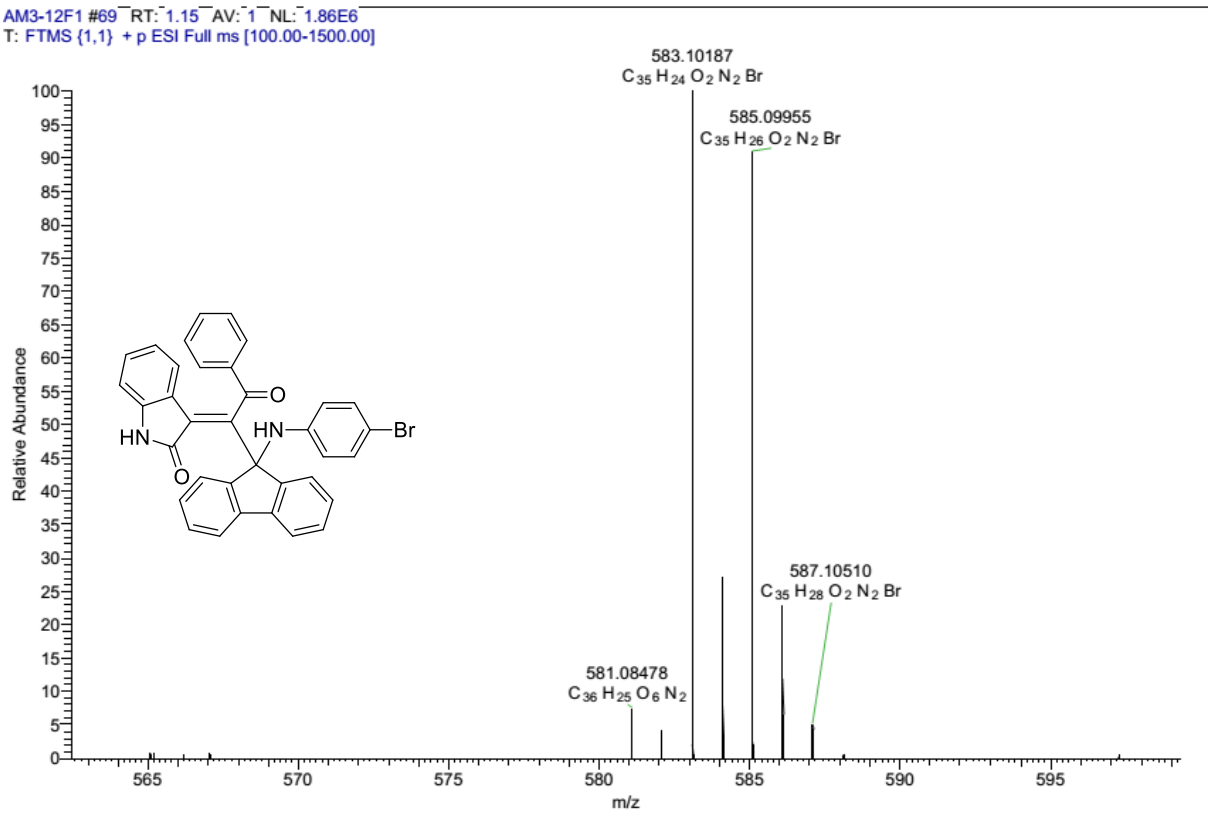
F2 - Acquisition Parameters
Date_ 20190605
Time_ 5.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 204.46
DW 31.000 usec
DE 6.50 usec
TE 296.4 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6459641 MHz
NUC1 13C
P1 10.62 usec
P13 2000.00 usec
PLW0 0 W
PLW1 54.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.30539989 W

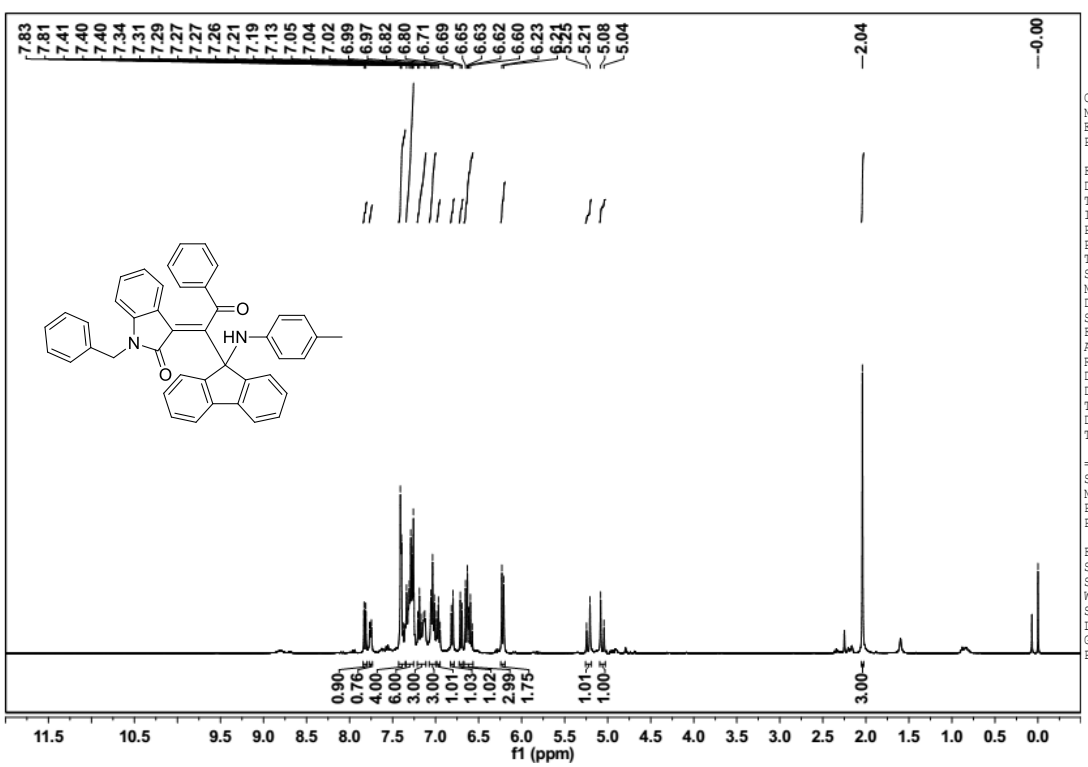
======== CHANNEL f2 ========
SFO2 400.2312800 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 12.75 usec
P4 25.50 usec
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT- 135 Spectrum of compound **3g**



HRMS Spectrum of Compound **3g**



BRUKER

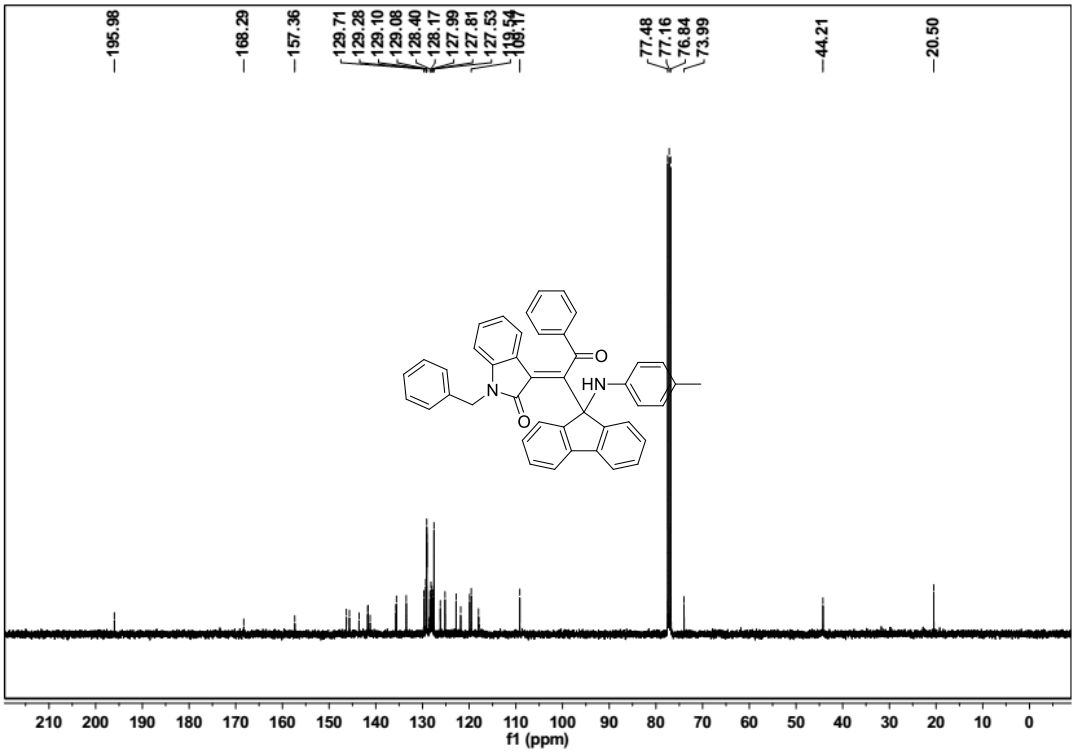
```
Current Data Parameters
NAME          AM242F1r5
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20200318
Time               9.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG               114.23
DW               62.400 usec
DE                6.50 usec
TE               292.9 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        400.2324716 MHz
NUC1                1H
P1                12.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                65536
SF          400.2300104 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{1}H NMR spectrum of compound **3h**



BRUKER

```
Current Data Parameters
NAME          AMII-242-F1
EXPNO                   2
PROCNO                  1

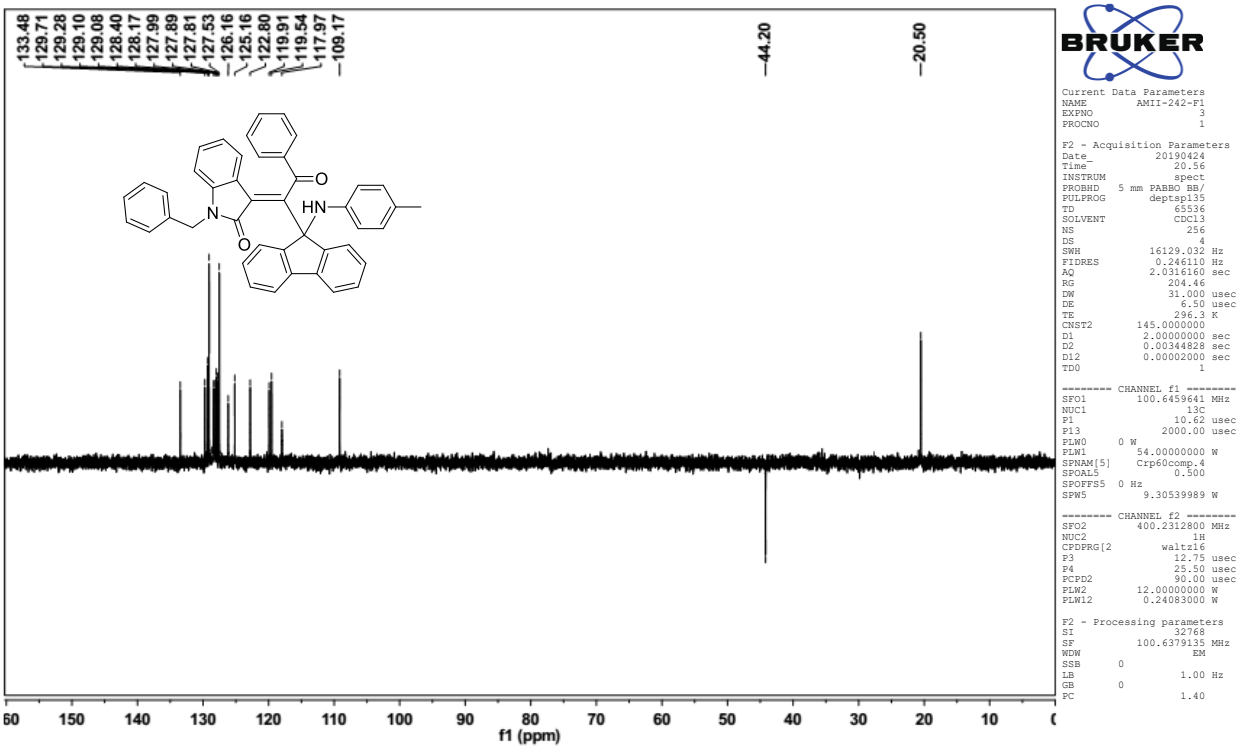
F2 - Acquisition Parameters
Date_          20190424
Time               15.40
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG               204.46
DW               20.800 usec
DE                6.50 usec
TE               297.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6479769 MHz
NUC1                13C
P1                10.62 usec
PLW1        54.00000000 W

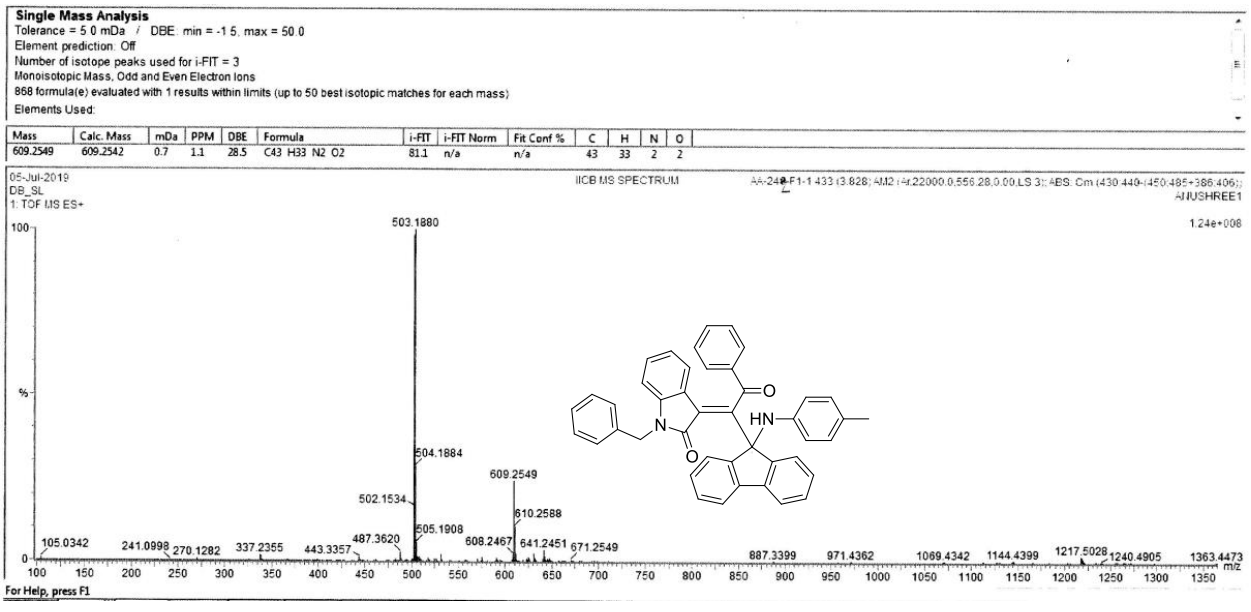
======== CHANNEL f2 ========
SFO2        400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        12.00000000 W
PLW12        0.24083000 W
PLW13        0.19508000 W

F2 - Processing parameters
SI                32768
SF          100.6379135 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

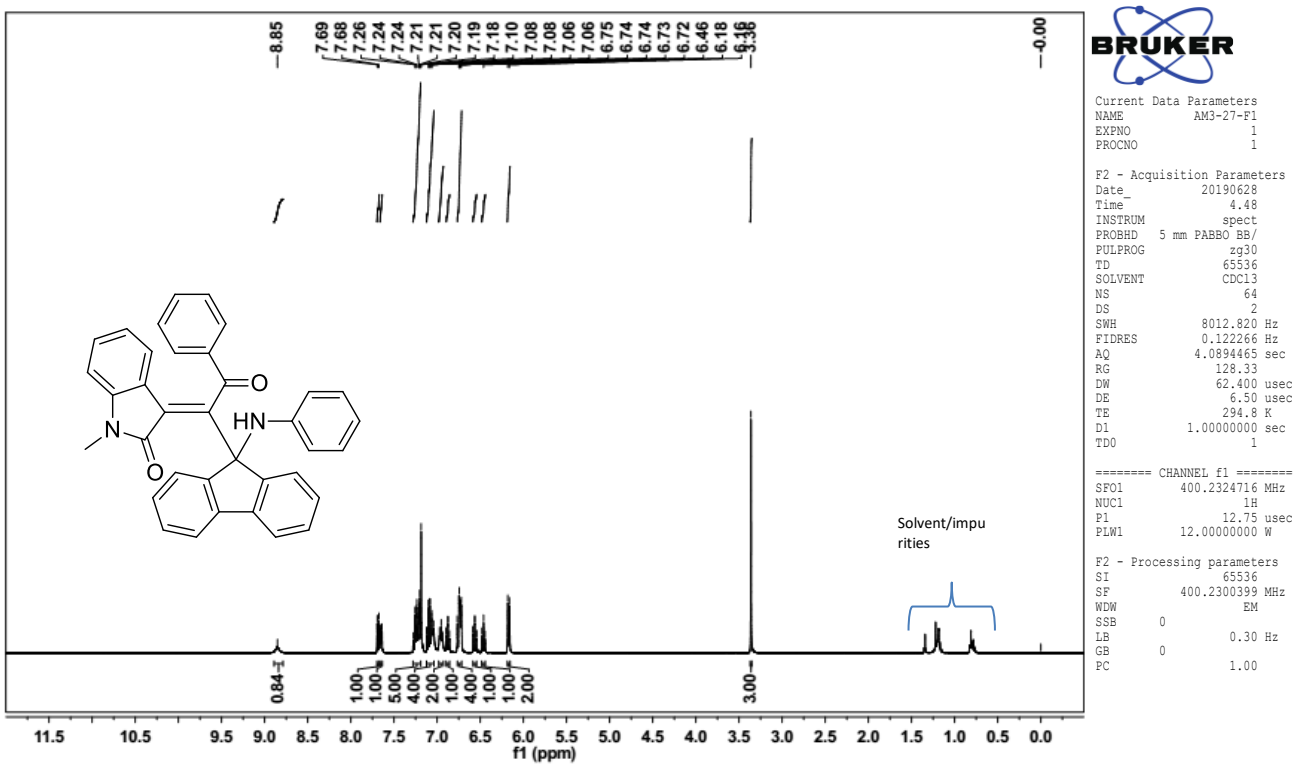
^{13}C NMR Spectrum of compound **3h**



DEPT- 135 Spectrum of compound **3h**



HRMS Spectrum of Compound **3h**



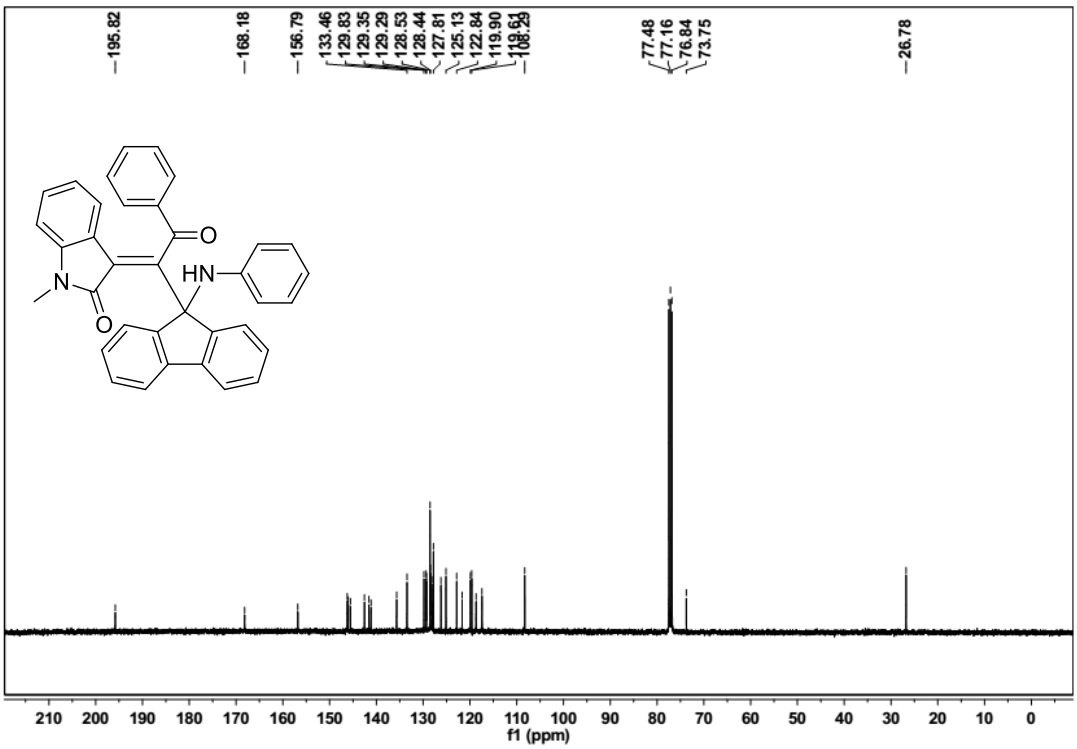

```
Current Data Parameters
NAME            AM3-27-F1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190628
Time                4.48
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    64
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                 128.33
DW                 62.400 usec
DE                  6.50 usec
TE                294.8 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.2324716 MHz
NUC1                   1H
P1                  12.75 usec
PLW1          12.00000000 W

F2 - Processing parameters
SI                 65536
SF            400.2300399 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

^{1}H NMR spectrum of compound **3i**




```
Current Data Parameters
NAME            AM3-27-F1
EXPNO                   2
PROCNO                  1

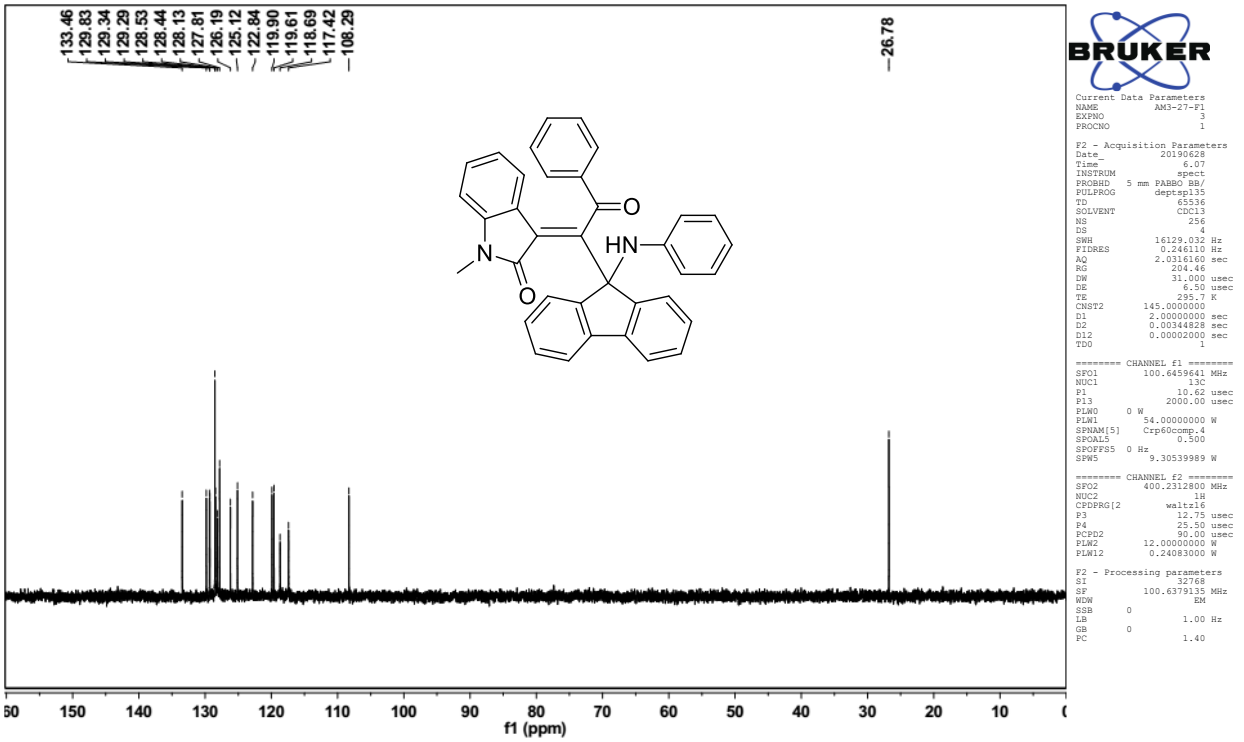
F2 - Acquisition Parameters
Date_            20190628
Time                5.48
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ              1.3631488 sec
RG                 204.46
DW                 20.800 usec
DE                  6.50 usec
TE                296.2 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6479769 MHz
NUC1                   13C
P1                  10.62 usec
PLW1          54.00000000 W

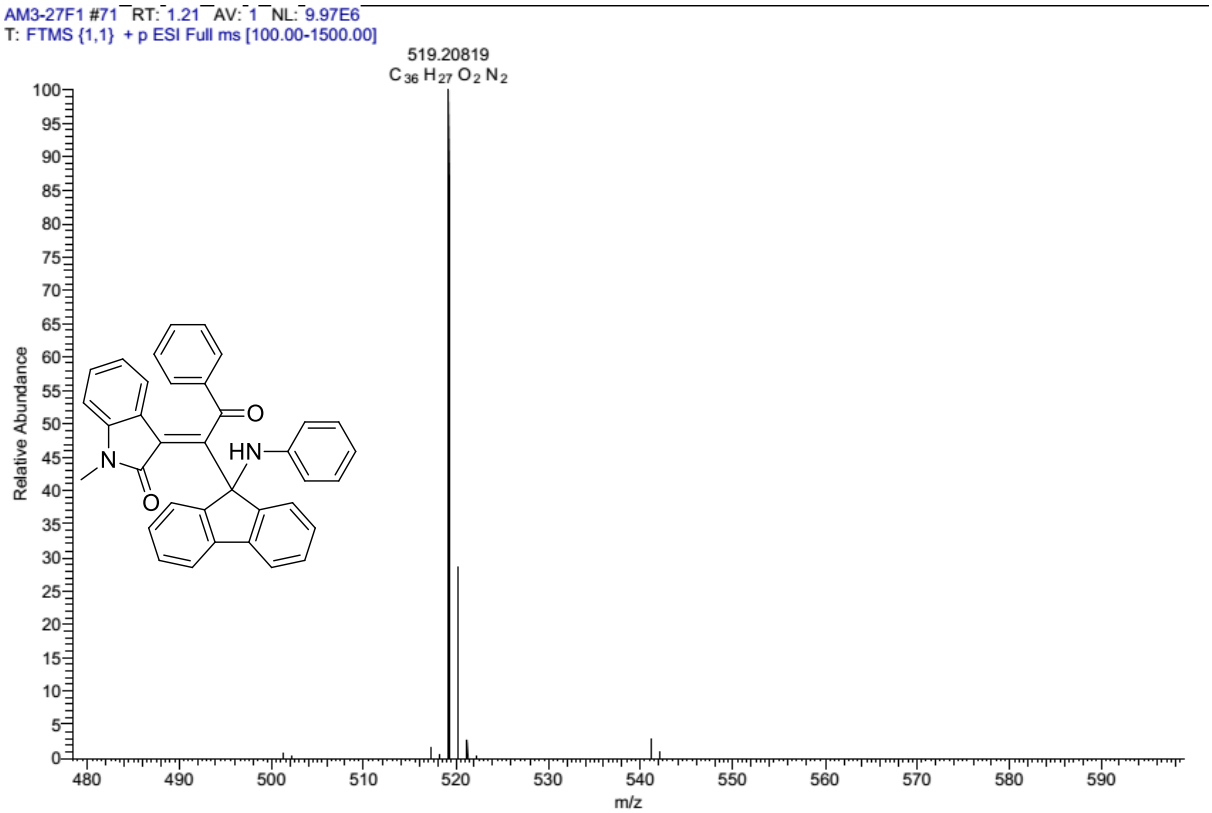
======== CHANNEL f2 ========
SFO2          400.2316009 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.00000000 W
PLW12          0.24083000 W
PLW13          0.19508000 W

F2 - Processing parameters
SI                 32768
SF            100.6379135 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

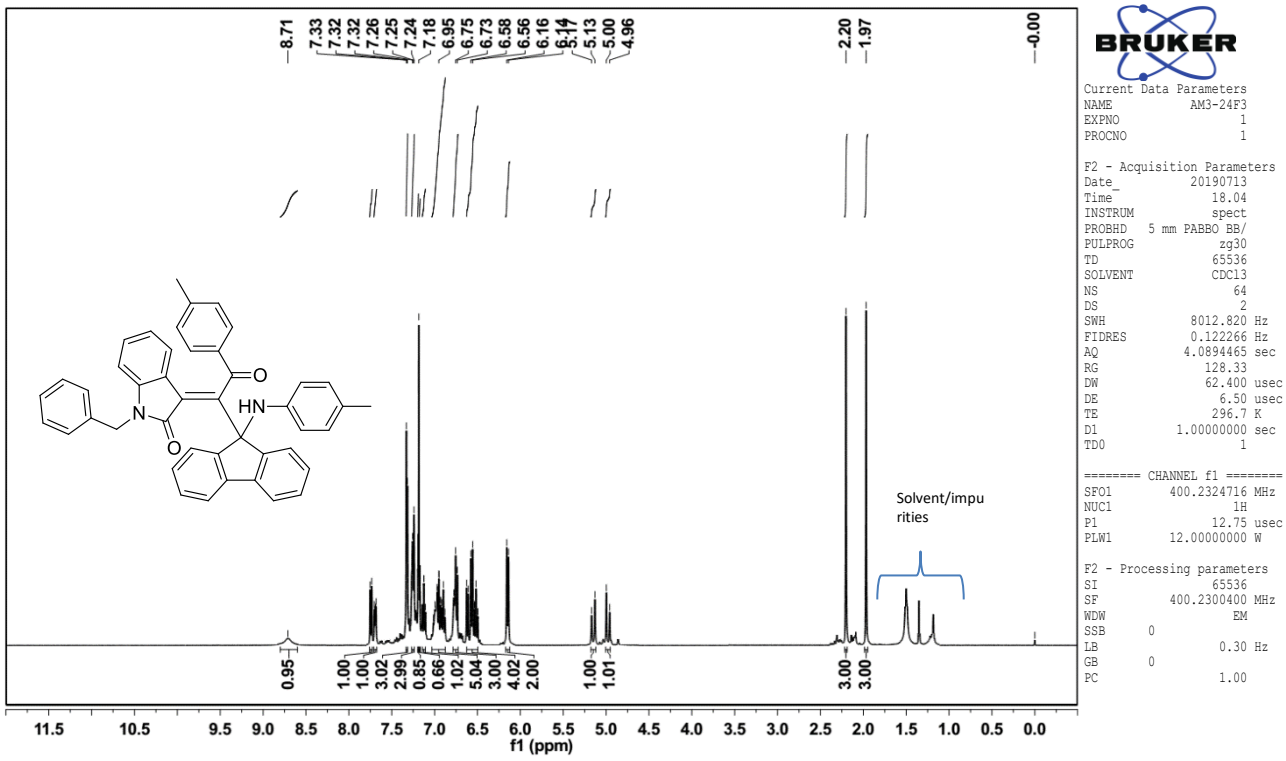
^{13}C NMR Spectrum of compound **3i**



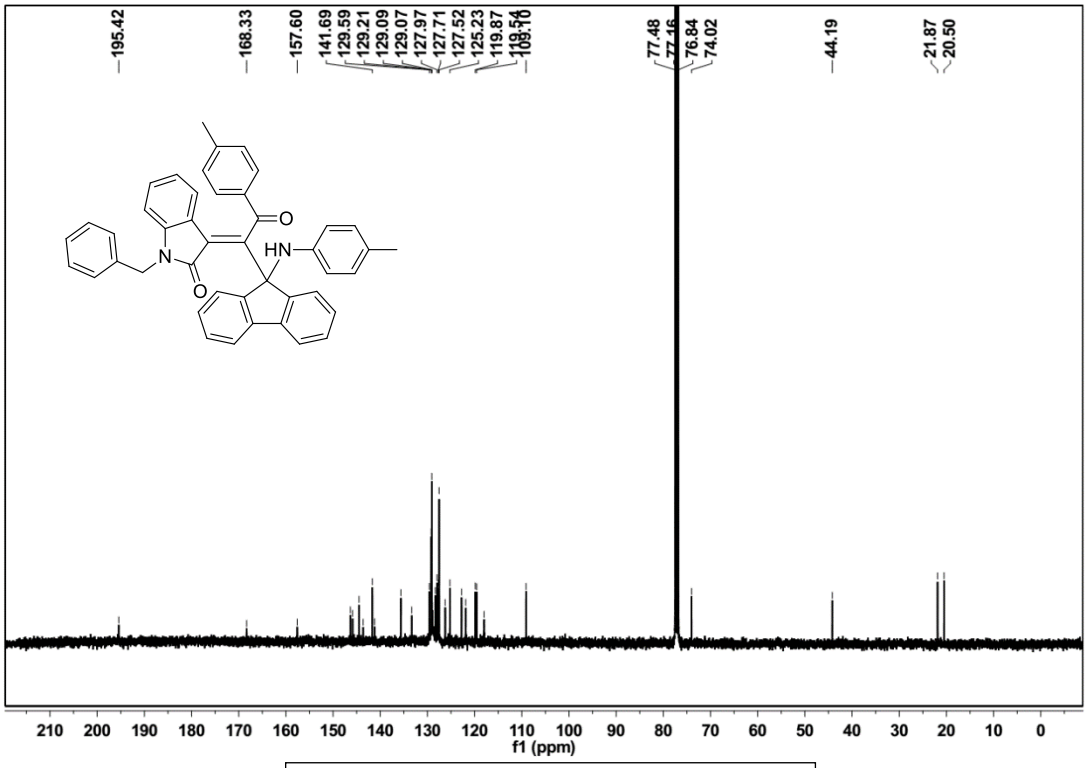
DEPT- 135 Spectrum of compound **3i**

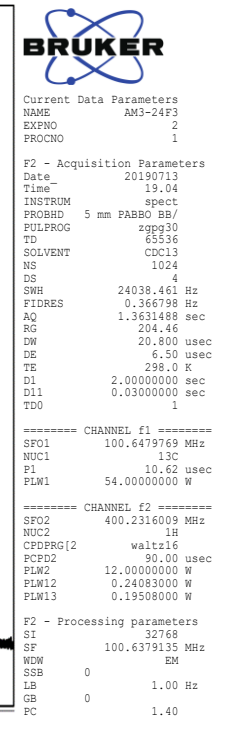


HRMS Spectrum of Compound **3i**

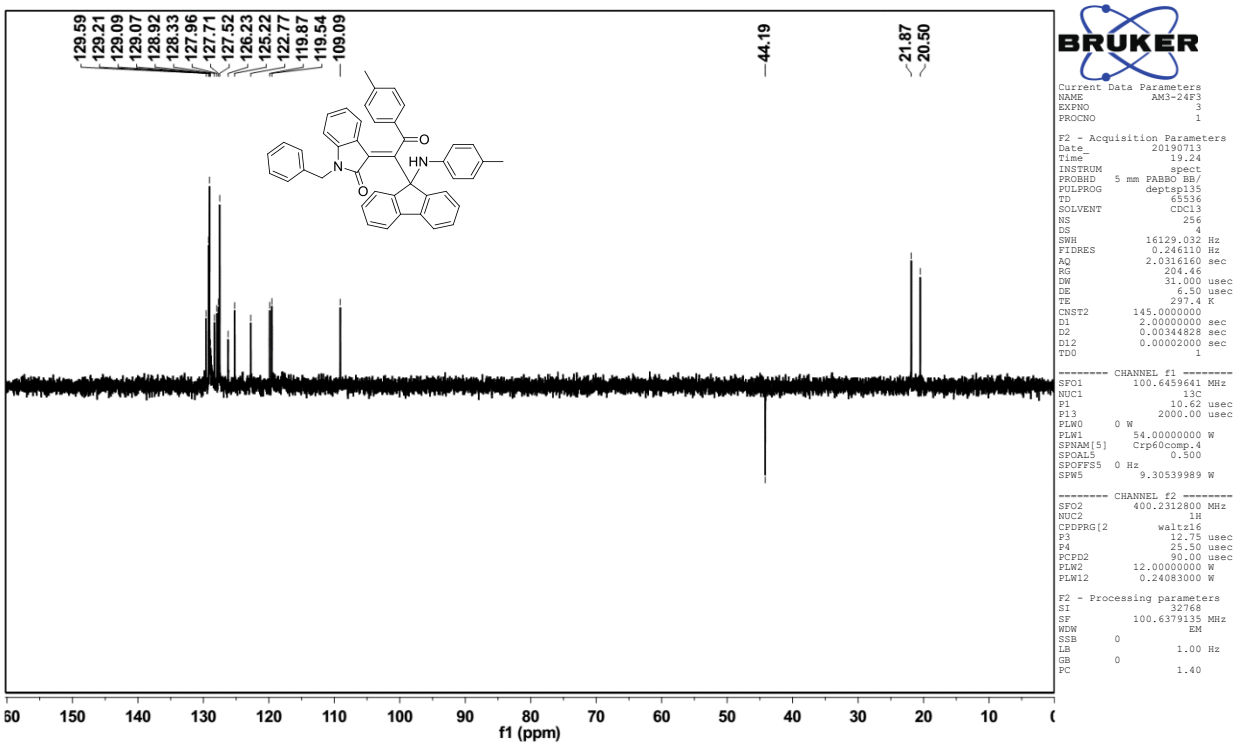


^{1}H NMR spectrum of compound **3j**

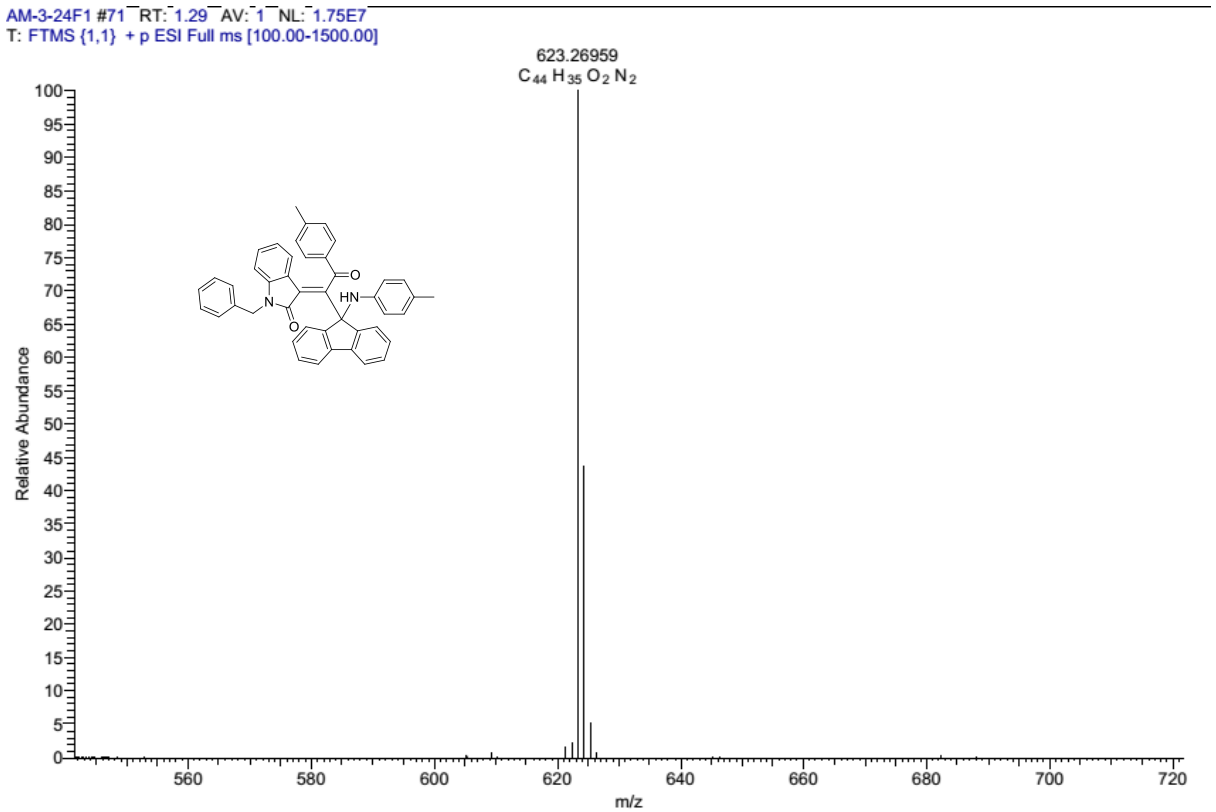




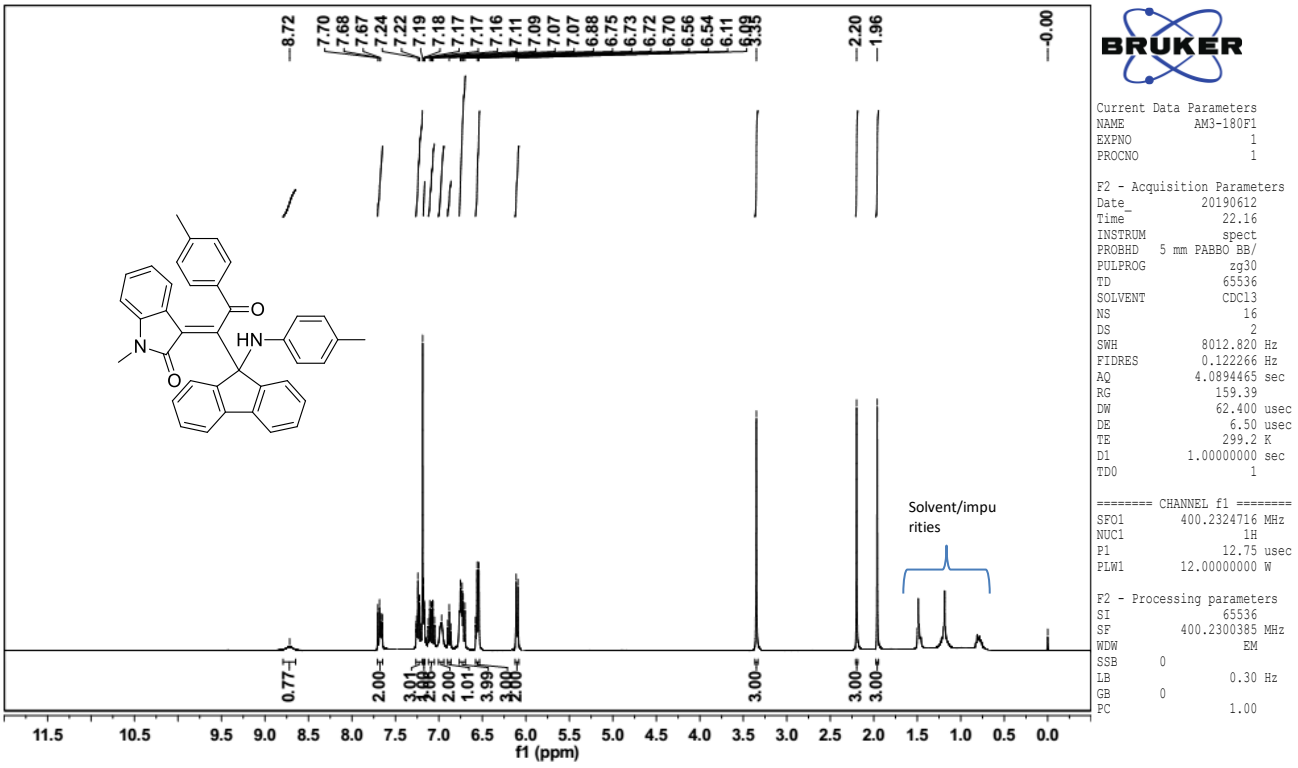
^{13} C NMR Spectrum of compound **3j**



DEPT- 135 Spectrum of compound **3j**



HRMS Spectrum of Compound **3j**



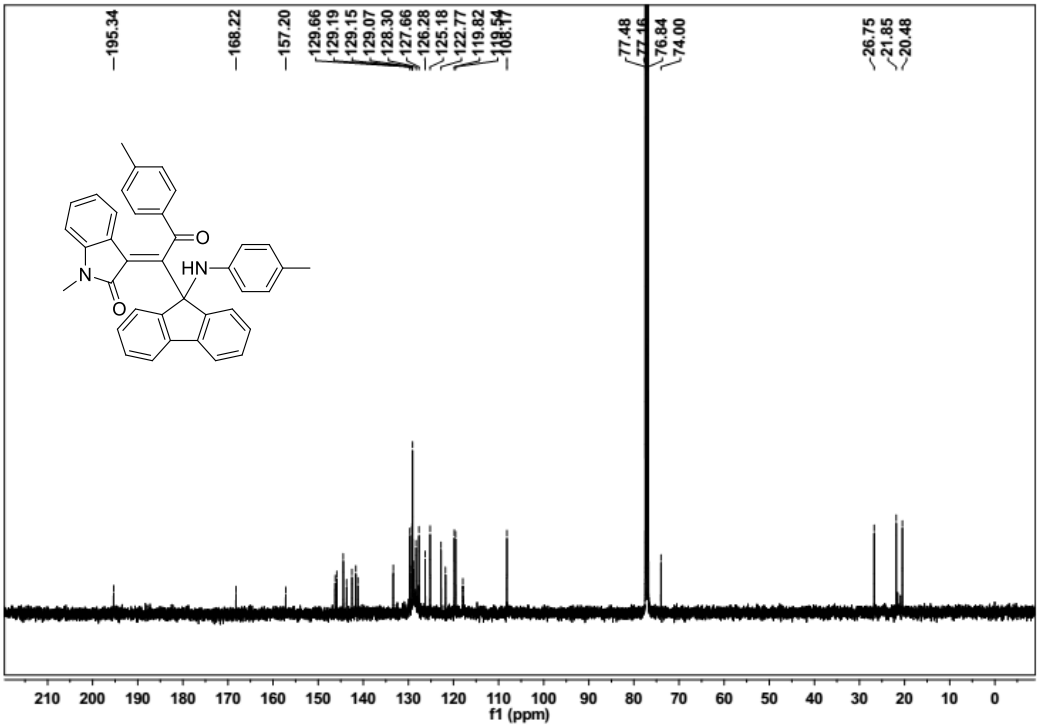

```
Current Data Parameters
NAME          AM3-180F1
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20190612
Time              22.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG               159.39
DW               62.400 usec
DE                6.50 usec
TE                299.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.2324716 MHz
NUC1                 1H
P1                12.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                65536
SF           400.2300385 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{1}H NMR spectrum of compound **3k**




```
Current Data Parameters
NAME          13C Final
EXPNO                 1
PROCNO                1

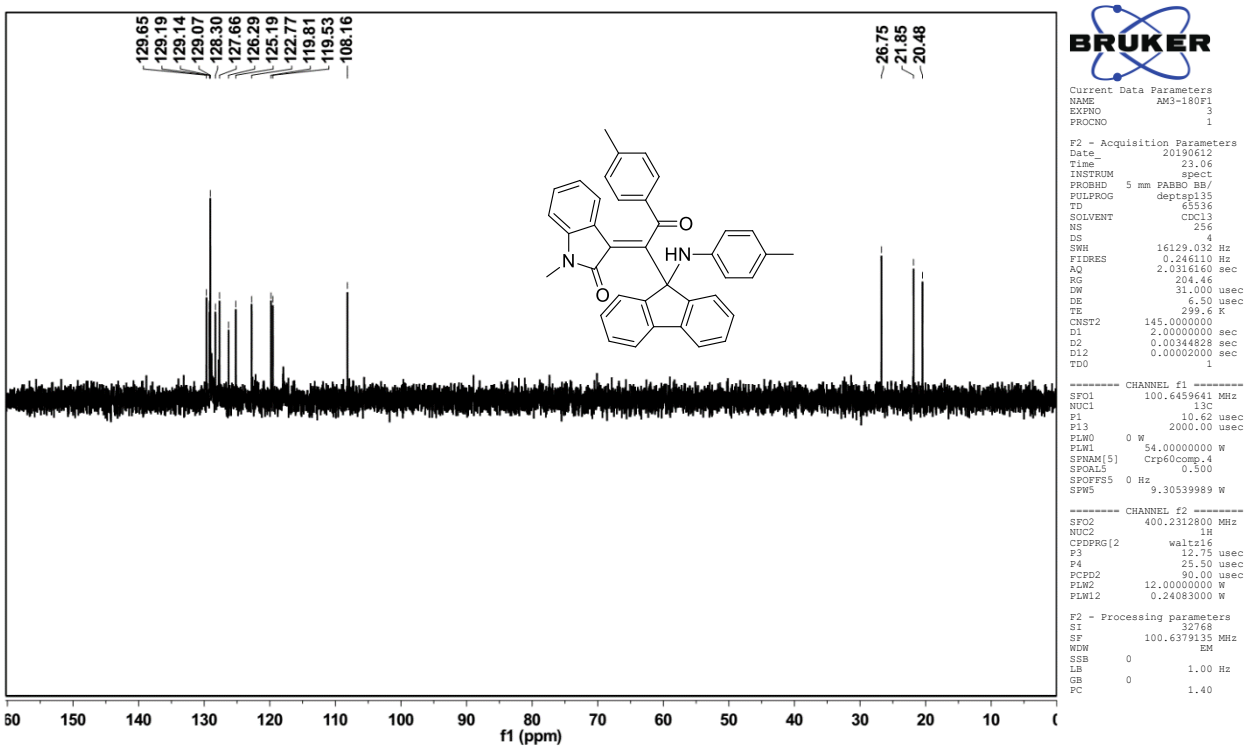
F2 - Acquisition Parameters
Date_          20190711
Time              15.26
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG               204.46
DW               20.800 usec
DE                6.50 usec
TE                297.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6479769 MHz
NUC1                 13C
P1                10.62 usec
PLW1         54.00000000 W

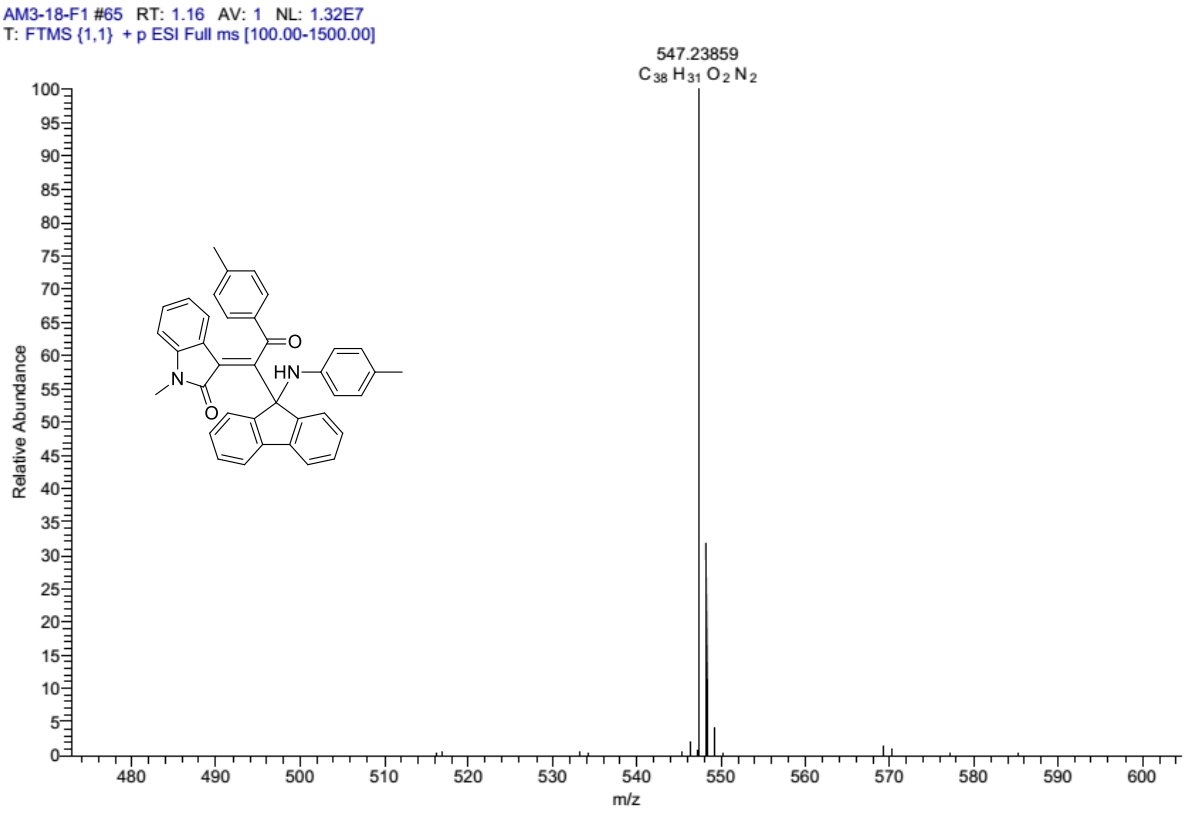
======== CHANNEL f2 ========
SFO2         400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         12.00000000 W
PLW12         0.24083000 W
PLW13         0.19508000 W

F2 - Processing parameters
SI                32768
SF           100.6379135 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

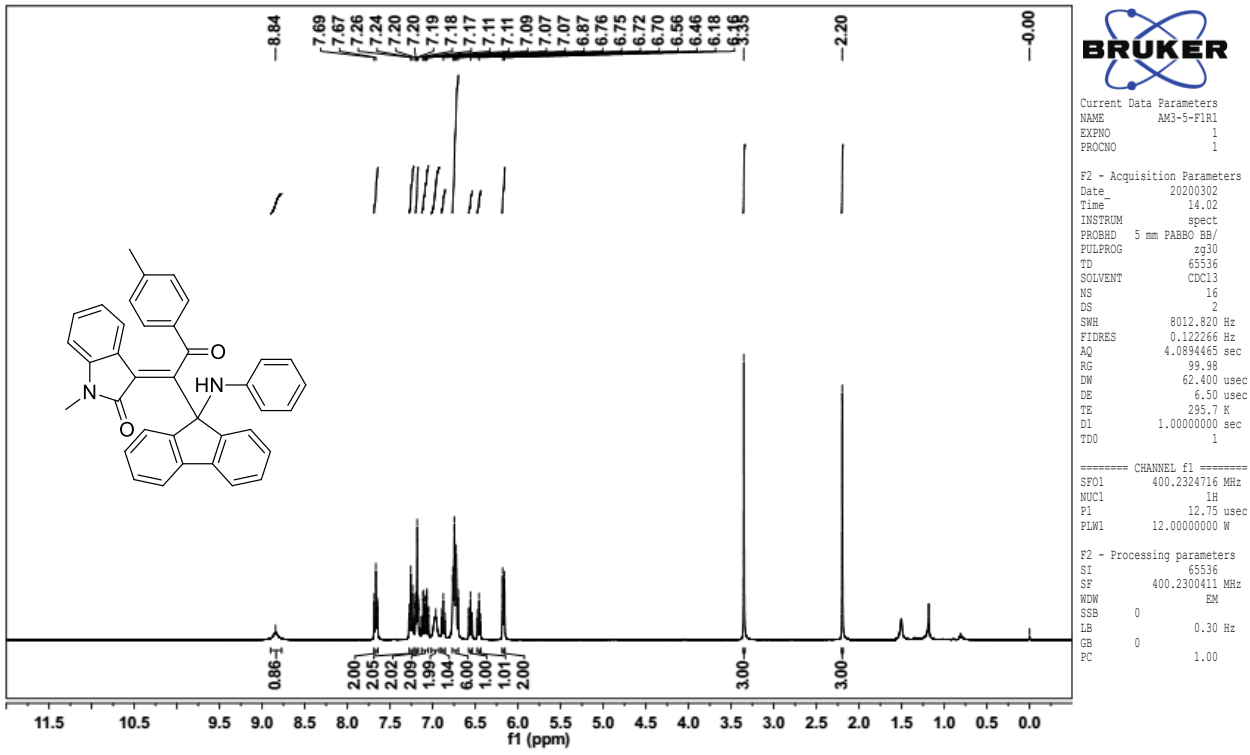
^{13} C NMR Spectrum of compound **3k**



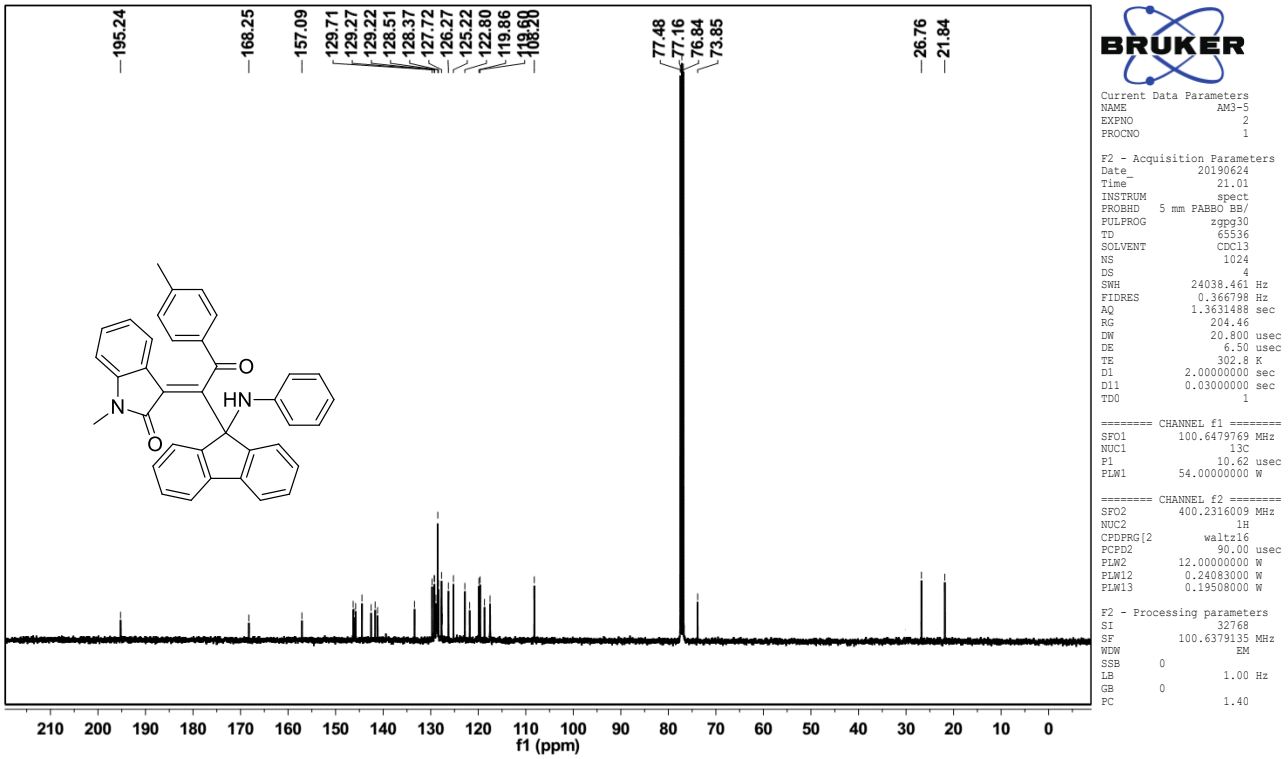
DEPT- 135 Spectrum of compound **3k**



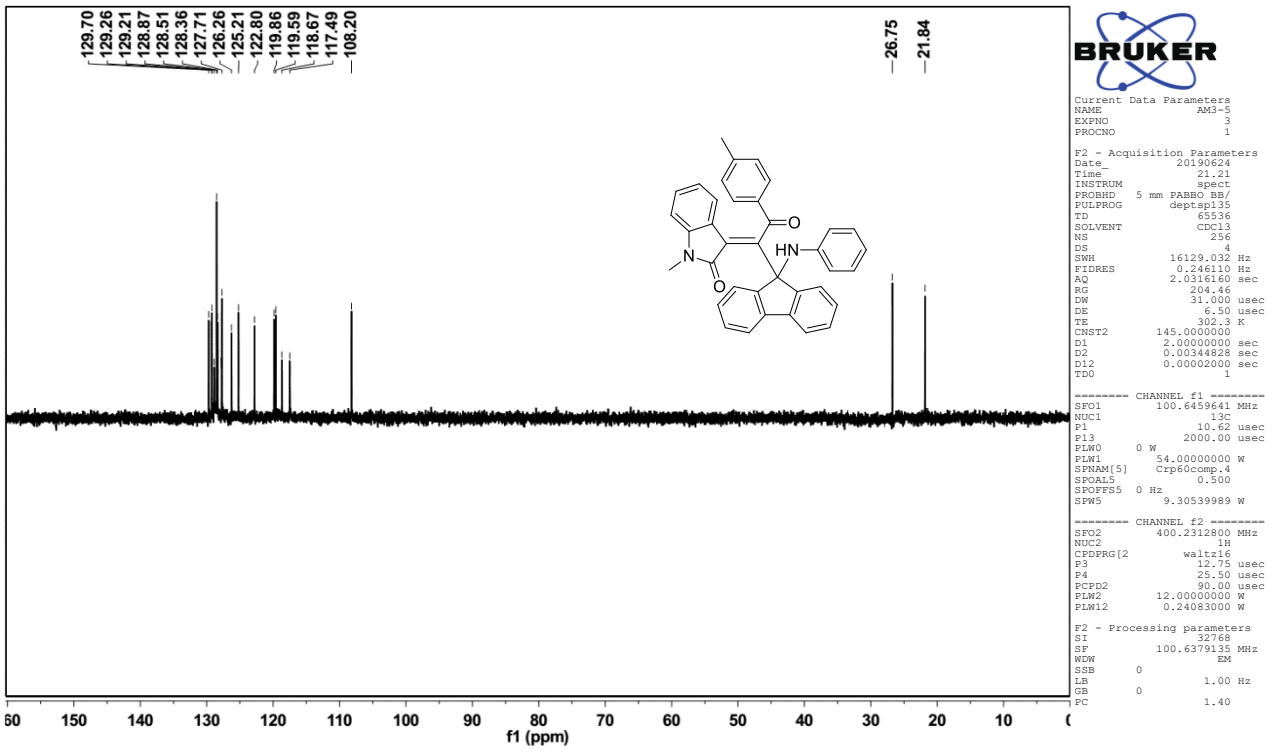
HRMS Spectrum of Compound **3k**



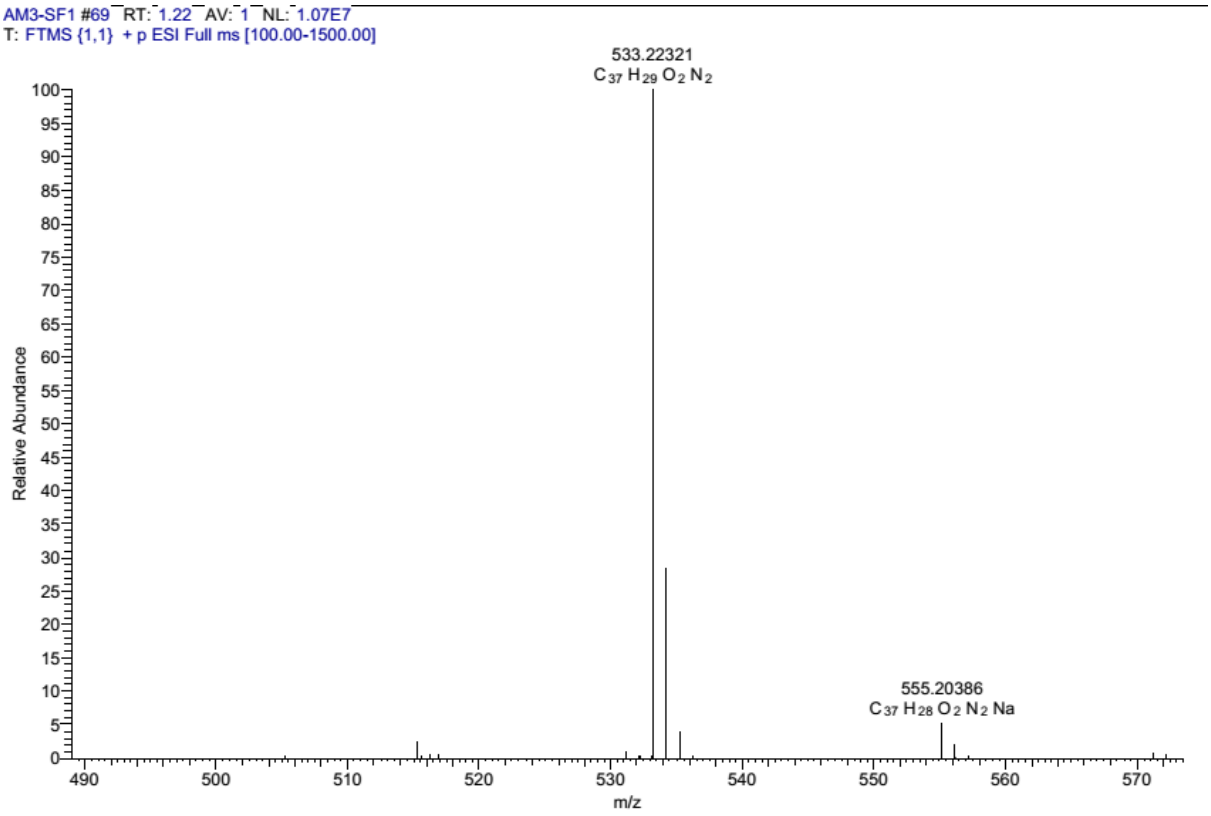
^{1}H NMR spectrum of compound **3l**



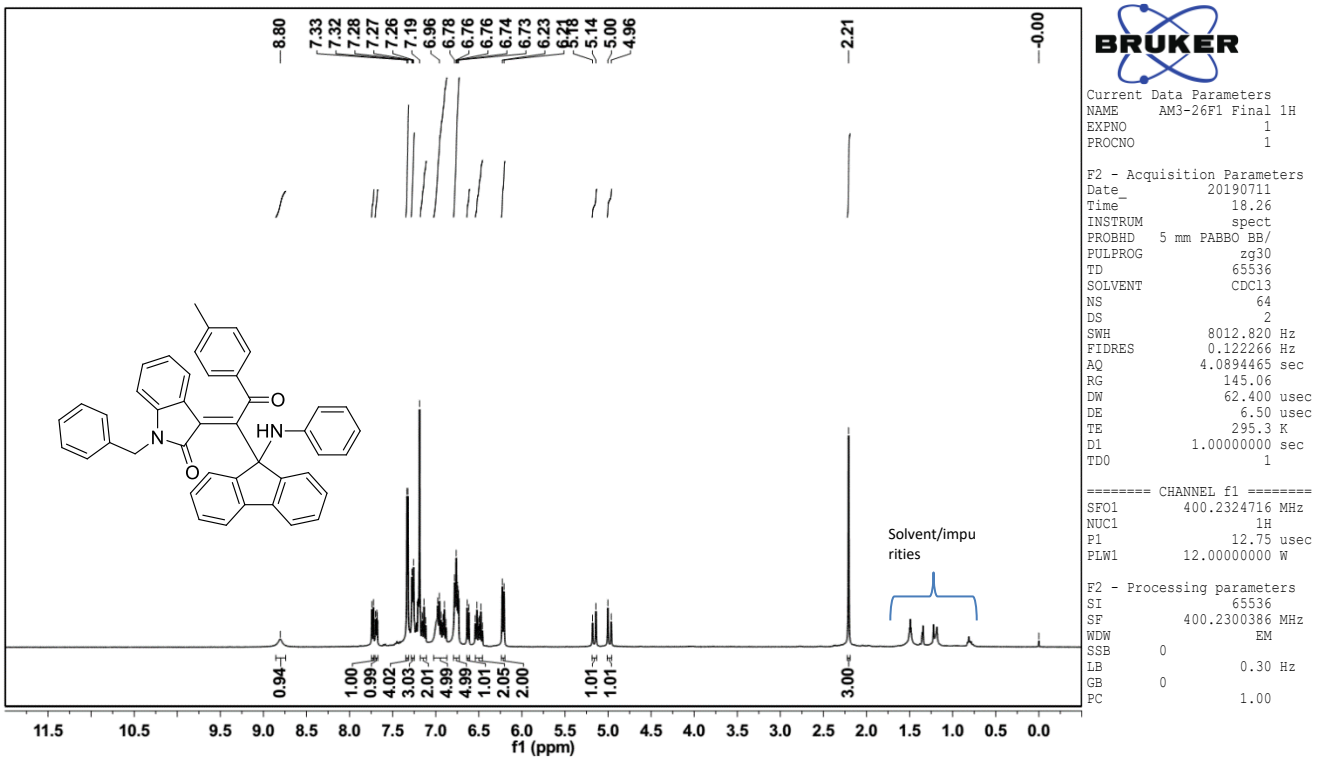
^{13} C NMR Spectrum of compound **3l**



DEPT- 135 Spectrum of compound **3l**



HRMS Spectrum of Compound **3l**



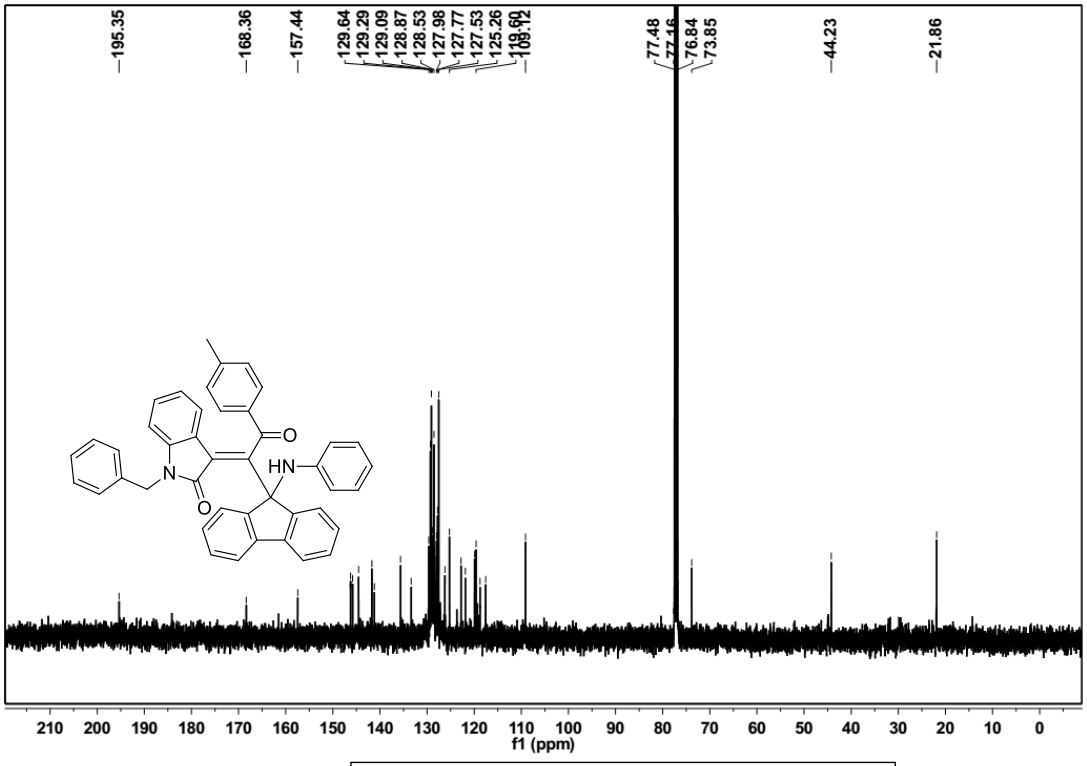

```
Current Data Parameters
NAME      AM3-26F1 Final 1H
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20190711
Time                18.26
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    64
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                145.06
DW                62.400 usec
DE                 6.50 usec
TE                295.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.2324716 MHz
NUC1                   1H
P1                  12.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2300386 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H NMR spectrum of compound **3m**




```
Current Data Parameters
NAME          AM3-26-F1
EXPNO                 2
PROCNO                1

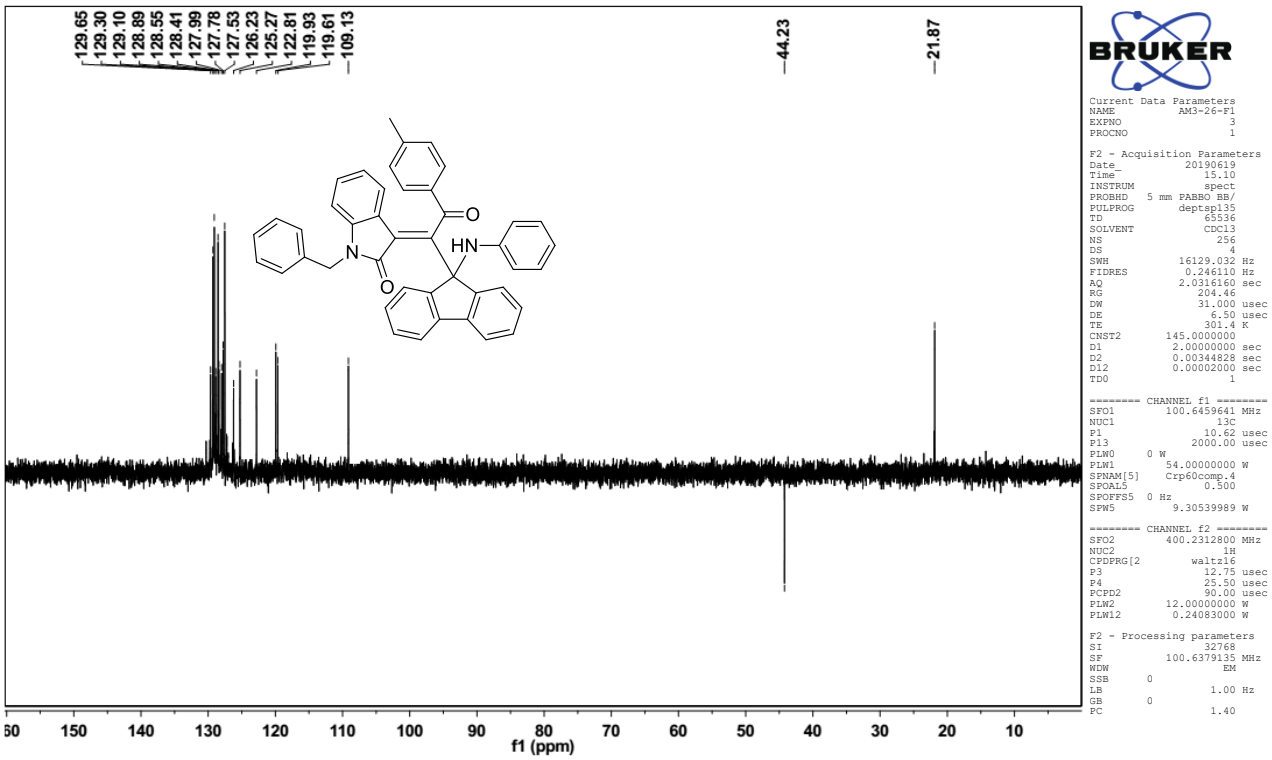
F2 - Acquisition Parameters
Date_            20190619
Time                14.50
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                204.46
DW                20.800 usec
DE                 6.50 usec
TE                302.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6479769 MHz
NUC1                  13C
P1                 10.62 usec
PLW1         54.00000000 W

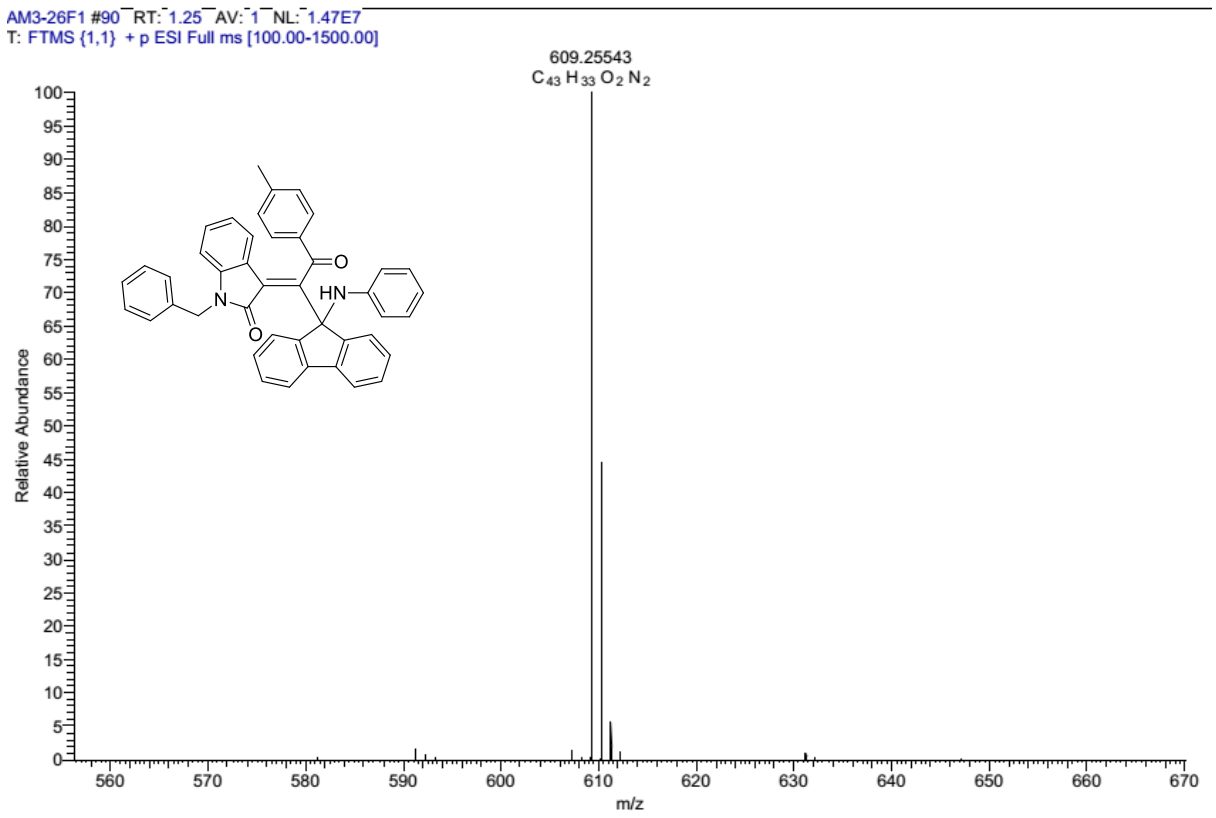
======== CHANNEL f2 ========
SFO2         400.2316009 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         12.00000000 W
PLW12         0.24083000 W
PLW13         0.19508000 W

F2 - Processing parameters
SI                 32768
SF           100.6379135 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

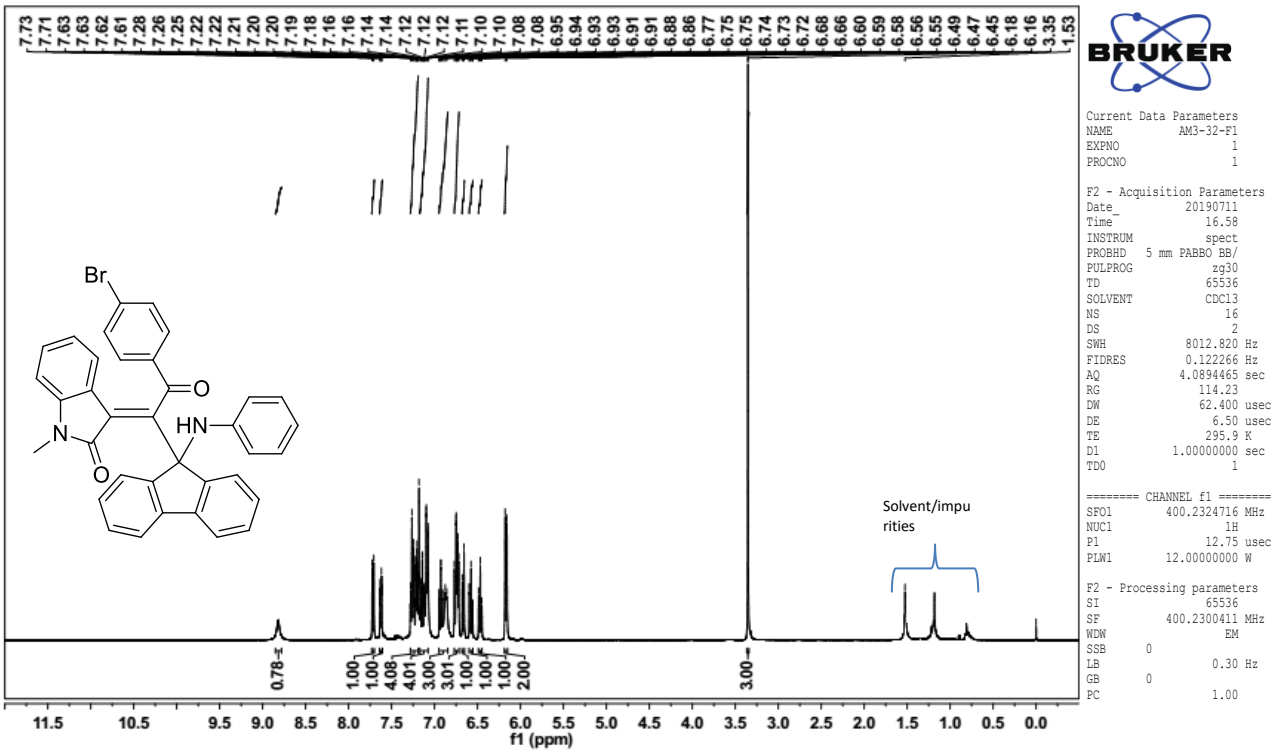
^{13}C NMR spectrum of compound **3m**



DEPT- 135 Spectrum of compound **3m**



HRMS Spectrum of Compound **3m**



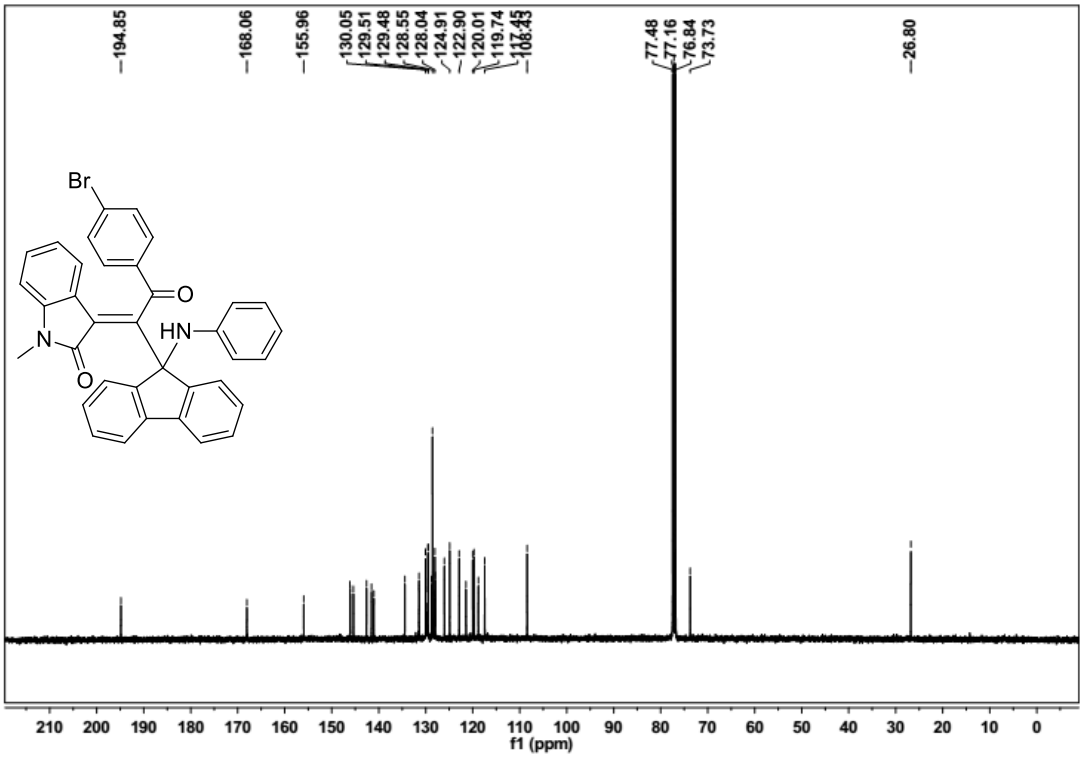
Current Data Parameters
NAME AM3-32-F1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190711
Time 16.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114.23
DW 62.400 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2324716 MHz
NUC1 1H
P1 12.75 usec
PLW1 12.00000000 W

F2 - Processing parameters
SI 65536
SF 400.2300411 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

^{1}H NMR spectrum of compound **3n**



Current Data Parameters
NAME AM3-32-F1
EXPNO 2
PROCNO 1

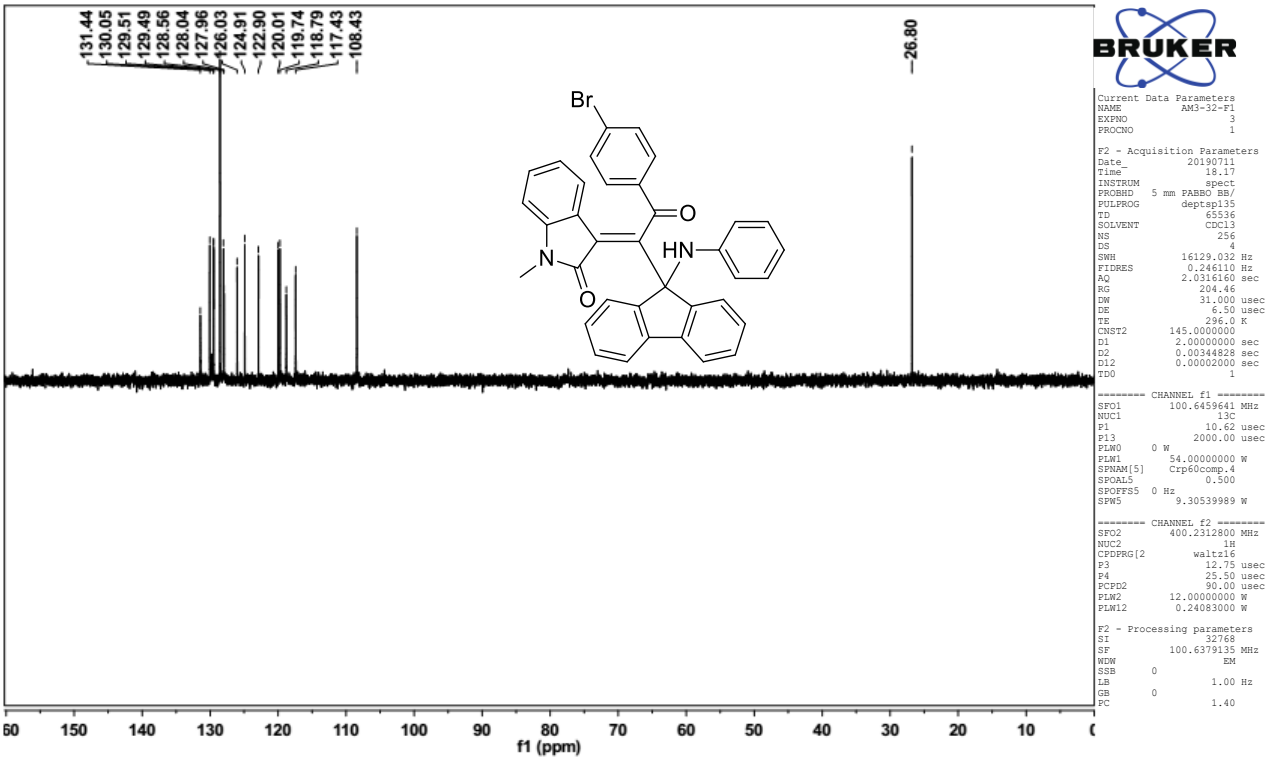
F2 - Acquisition Parameters
Date_ 20190711
Time 17.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 204.46
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6479769 MHz
NUC1 13C
P1 10.62 usec
PLW1 54.00000000 W

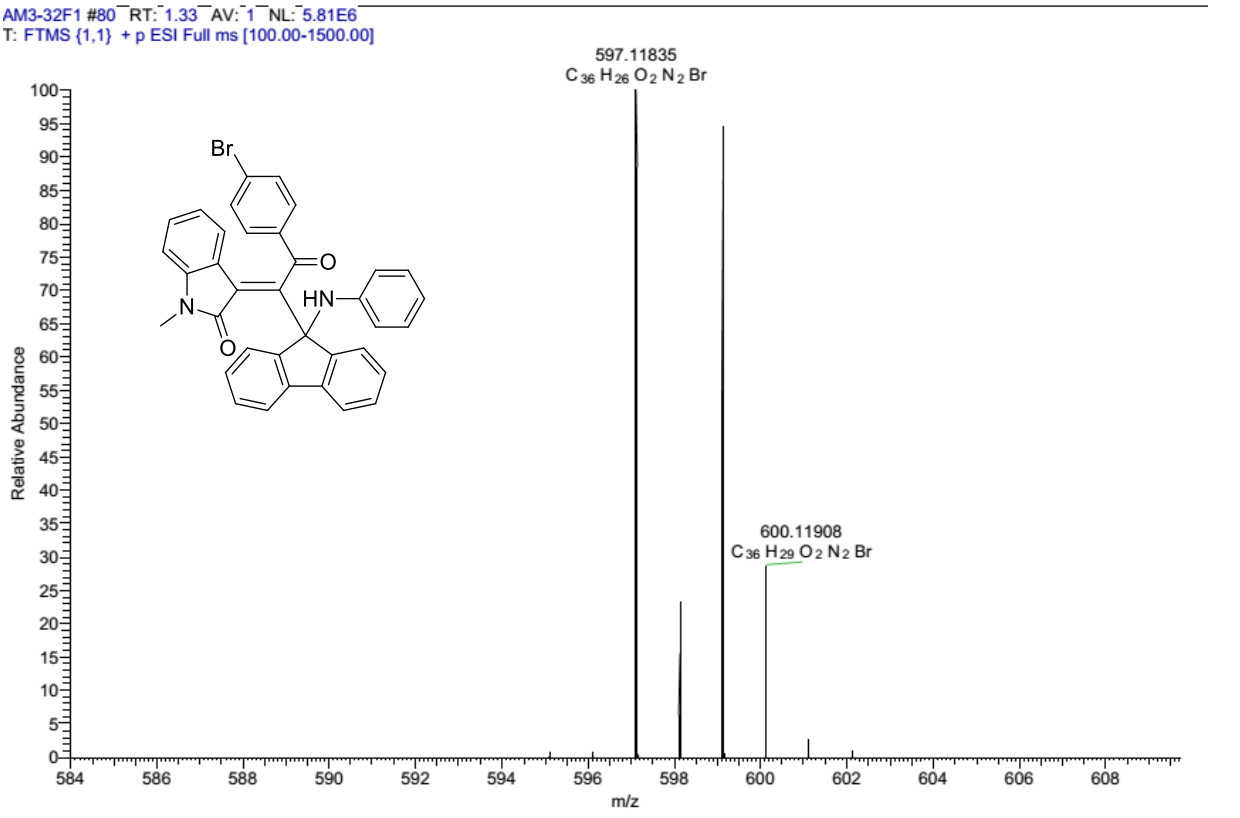
======== CHANNEL f2 ========
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W
PLW13 0.19508000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

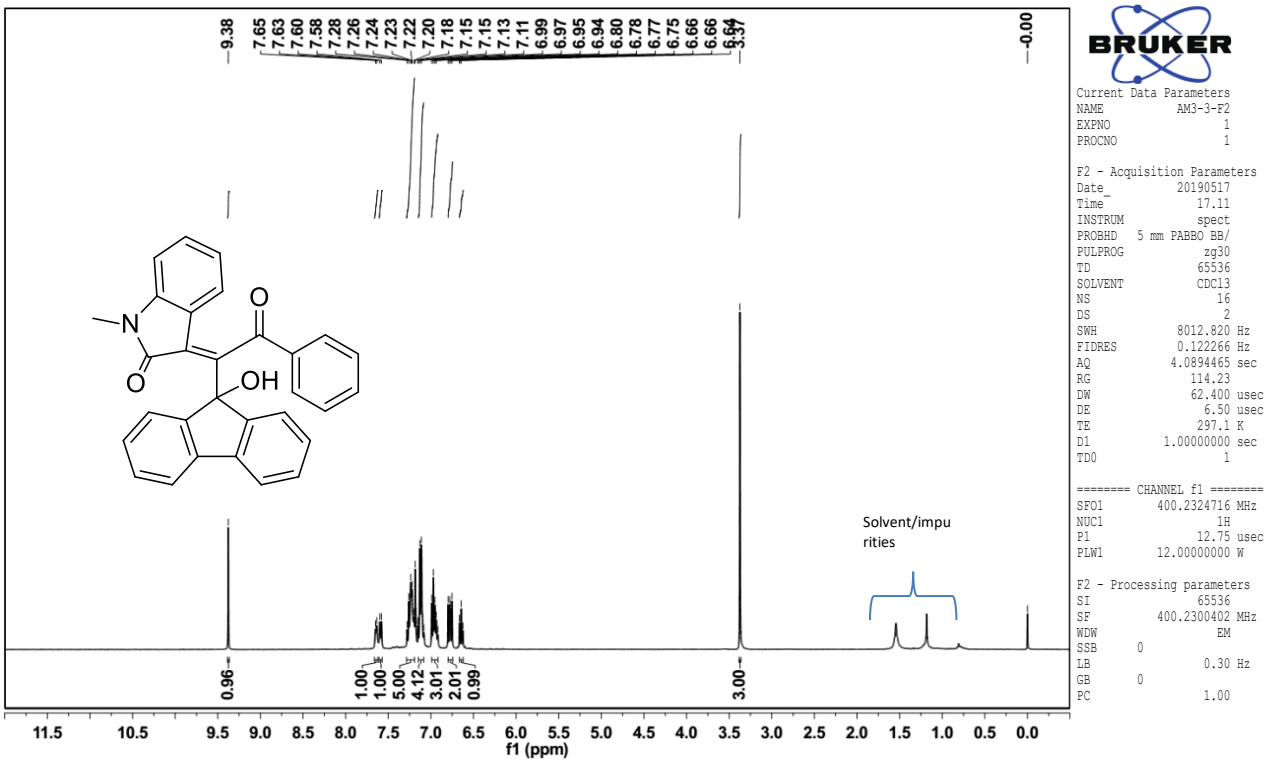
^{13}C NMR Spectrum of compound **3n**



DEPT- 135 Spectrum of compound **3n**



HRMS Spectrum of Compound **3n**



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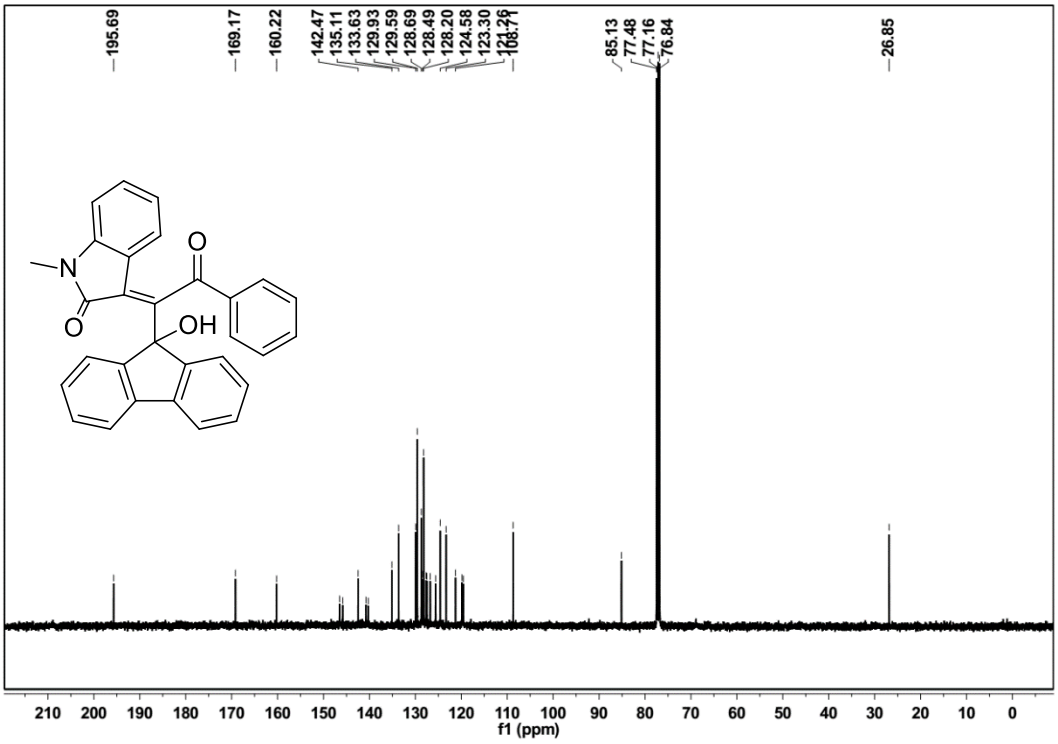
```
Current Data Parameters
NAME            AM3-3-F2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190517
Time               17.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                114.23
DW                62.400 usec
DE                 6.50 usec
TE                297.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.2324716 MHz
NUC1                   1H
P1                 12.75 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.2300402 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{1}H NMR spectrum of compound **4a**



BRUKER

```
Current Data Parameters
NAME            AM3-3-F2
EXPNO                  3
PROCNO                 1

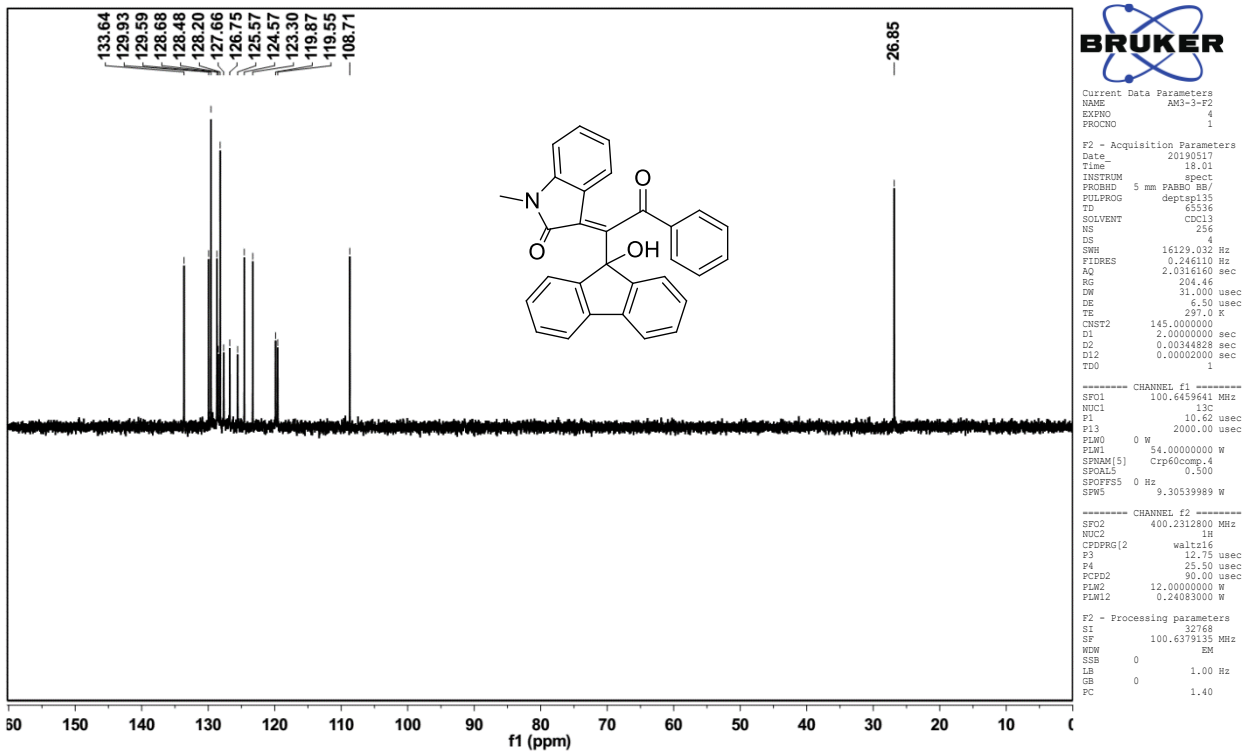
F2 - Acquisition Parameters
Date_           20190517
Time               17.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                204.46
DW                20.800 usec
DE                 6.50 usec
TE                297.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6479769 MHz
NUC1                   13C
P1                10.62 usec
PLW1         54.00000000 W

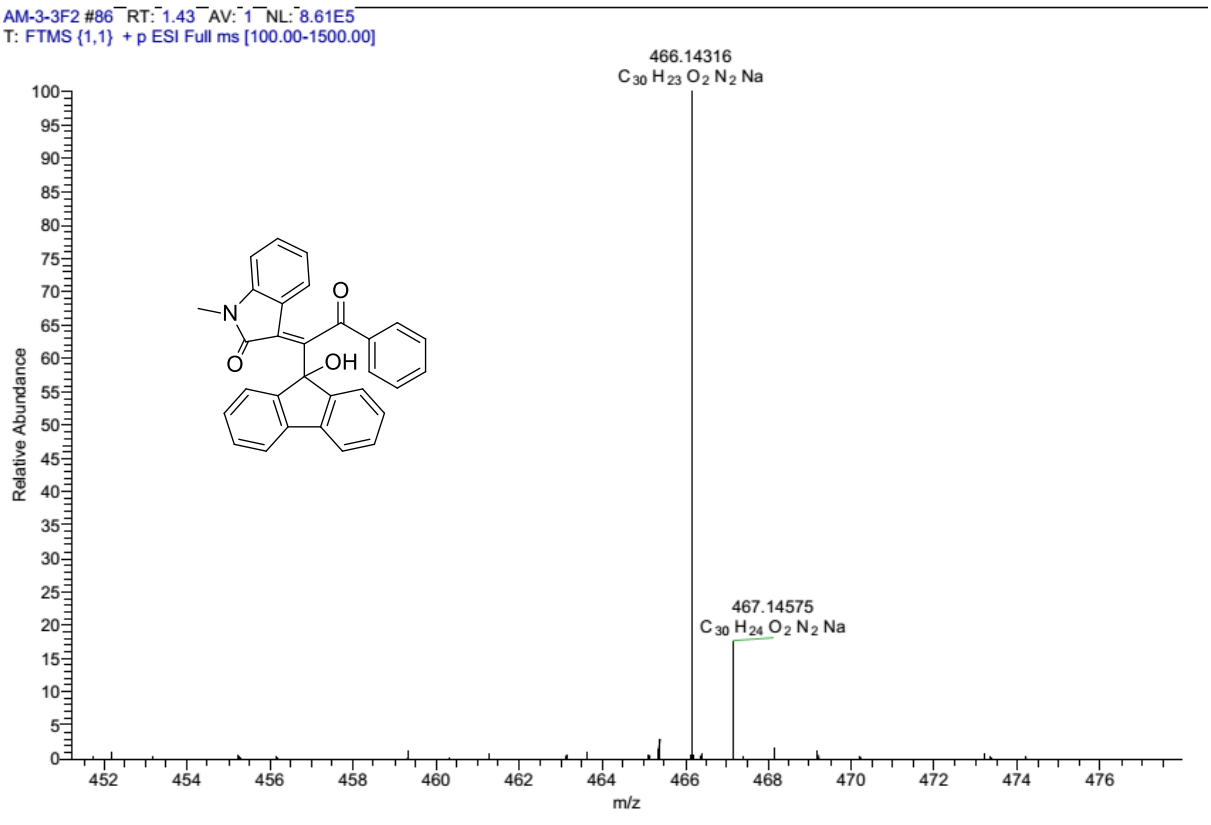
======== CHANNEL f2 ========
SFO2         400.2316009 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         12.00000000 W
PLW12         0.24083000 W
PLW13         0.19508000 W

F2 - Processing parameters
SI                 32768
SF           100.6379135 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

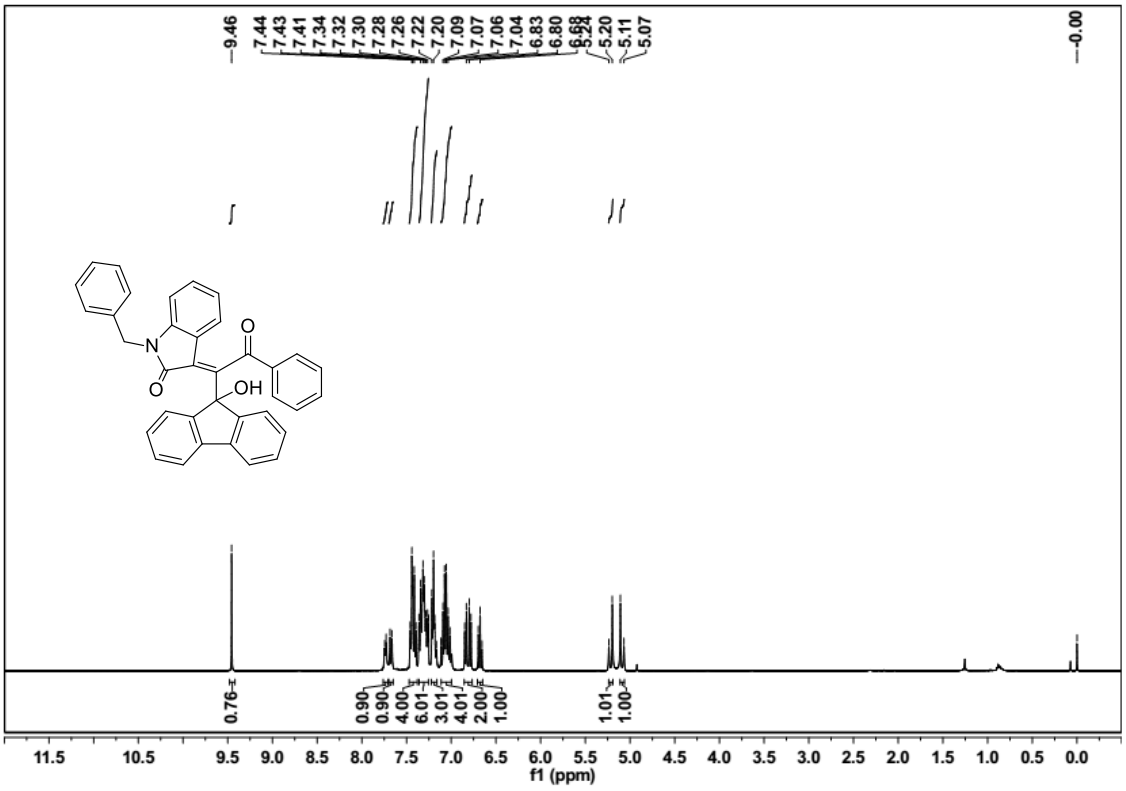
^{13} C NMR Spectrum of compound **4a**



DEPT- 135 Spectrum of compound **4a**



HRMS Spectrum of Compound **4a**



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```
Current Data Parameters
NAME            AM3240F2
EXPNO                  7
PROCNO                 1

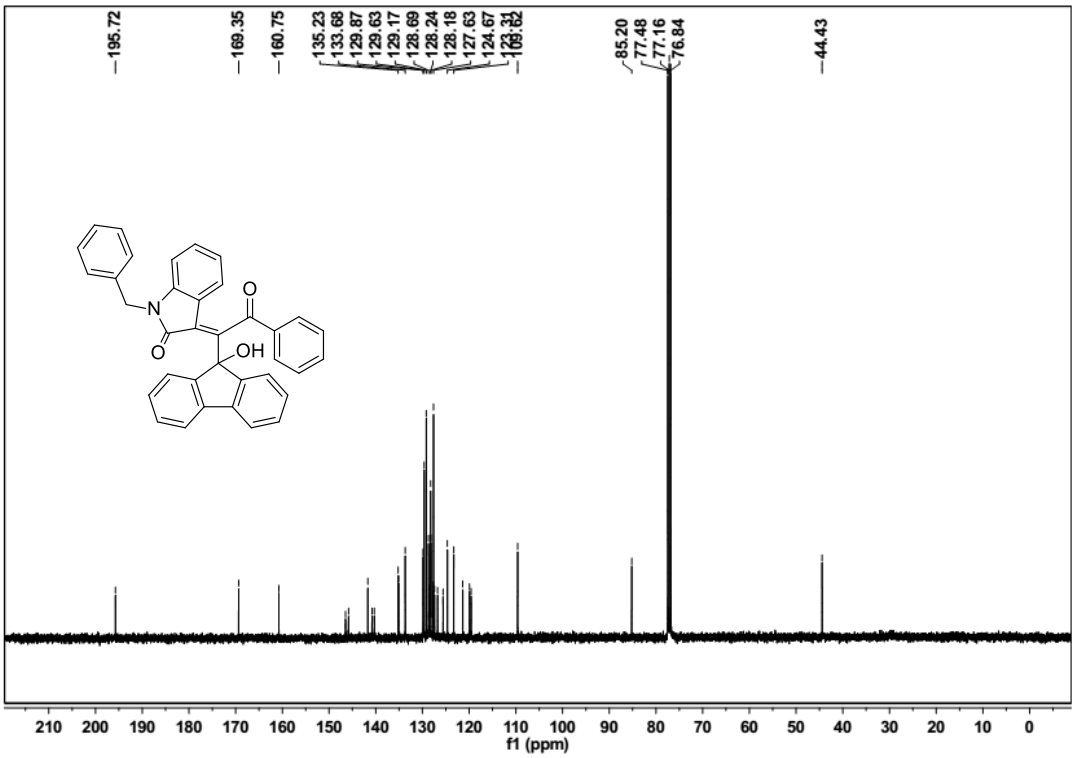
F2 - Acquisition Parameters
Date_           20200313
Time                8.10
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgesgp
TD                 29998
SOLVENT             CDCl3
NS                    64
DS                     2
SWH            10000.000 Hz
FIDRES             0.333356 Hz
AQ             1.4999000 sec
RG                145.06
DW                 50.000 usec
DE                  6.50 usec
TE                297.5 K
D1             1.00000000 sec
D12            0.00002000 sec
D16            0.00020000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.2306625 MHz
NUC1                   1H
P1                  11.17 usec
P2                  22.34 usec
P12               2000.00 usec
PLW0       0 W
PLW1      12.00000000 W
SPNAM[1]   Squa100.1000
SPOAL1              0.500
SPOFFS1    0 Hz
SPW1          0.00144630 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPZ1               31.00 %
GPZ2               11.00 %
P16              1000.00 usec

F2 - Processing parameters
SI                 32768
SF           400.2300000 MHz
WDW                   EM
SSB        0
LB                  0.50 Hz
GB         0
PC                  1.00
```

^{1}H NMR spectrum of compound **4b**



BRUKER

```
Current Data Parameters
NAME          AMII-242-F2
EXPNO                   5
PROCNO                  1

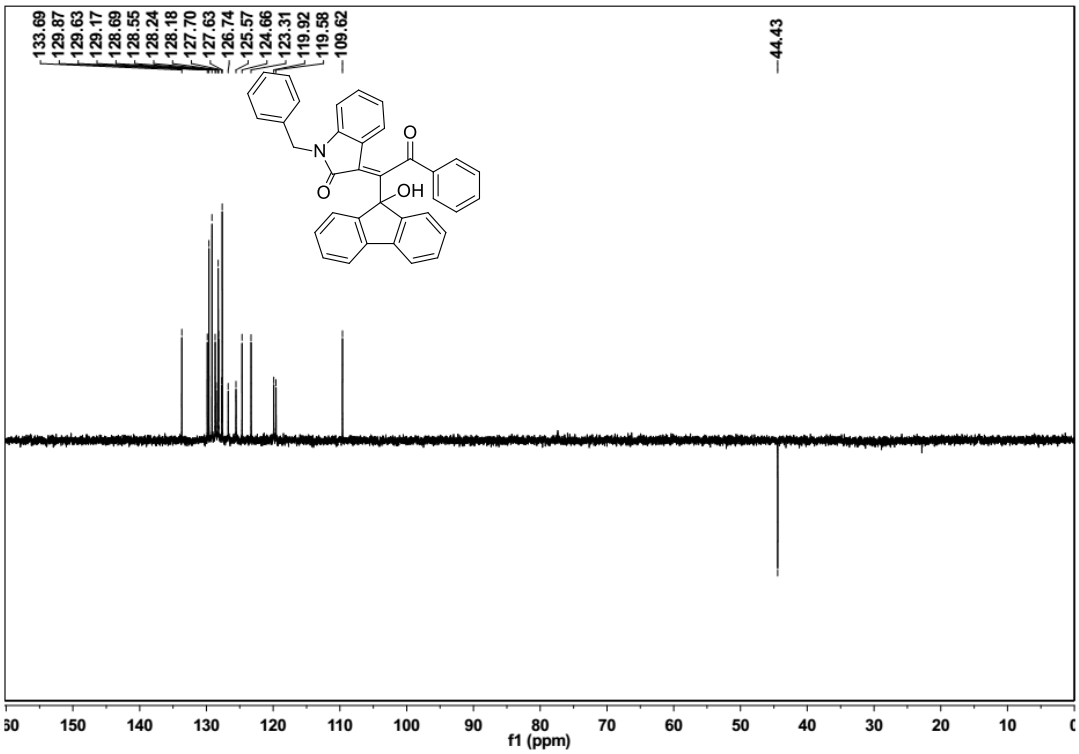
F2 - Acquisition Parameters
Date_           20190425
Time               17.55
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT             CDCl3
NS                   512
DS                     4
SWH            24038.461 Hz
FIDRES             0.366798 Hz
AQ             1.3631488 sec
RG                204.46
DW                 20.800 usec
DE                  6.50 usec
TE                297.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

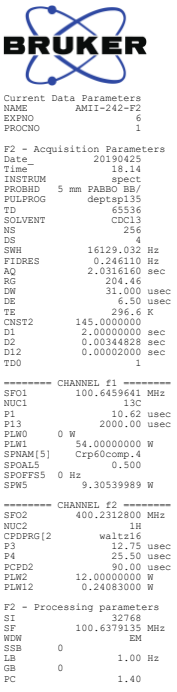
======== CHANNEL f1 ========
SFO1         100.6479769 MHz
NUC1                  13C
P1                  10.62 usec
PLW1          54.00000000 W

======== CHANNEL f2 ========
SFO2         400.2316009 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.00000000 W
PLW12          0.24083000 W
PLW13          0.19508000 W

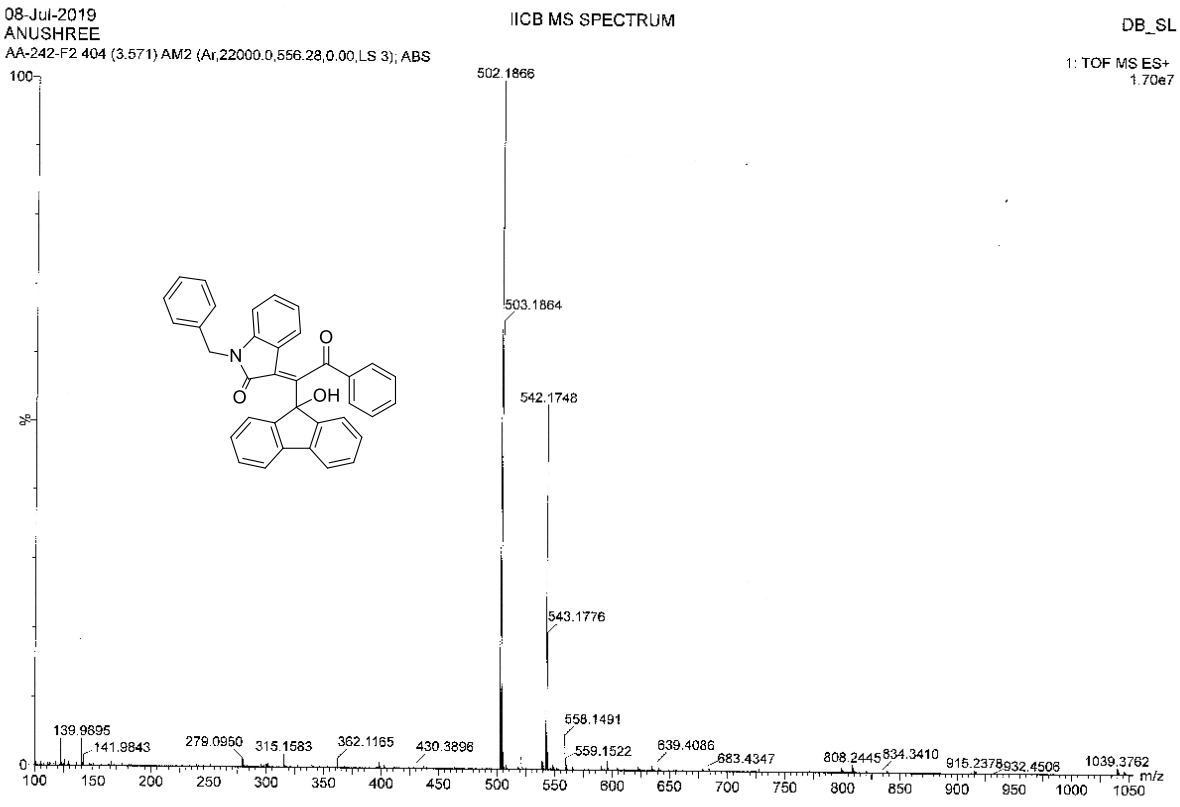
F2 - Processing parameters
SI                 32768
SF           100.6379135 MHz
WDW                   EM
SSB        0
LB                  1.00 Hz
GB         0
PC                  1.40
```

^{13} C NMR Spectrum of compound **4b**

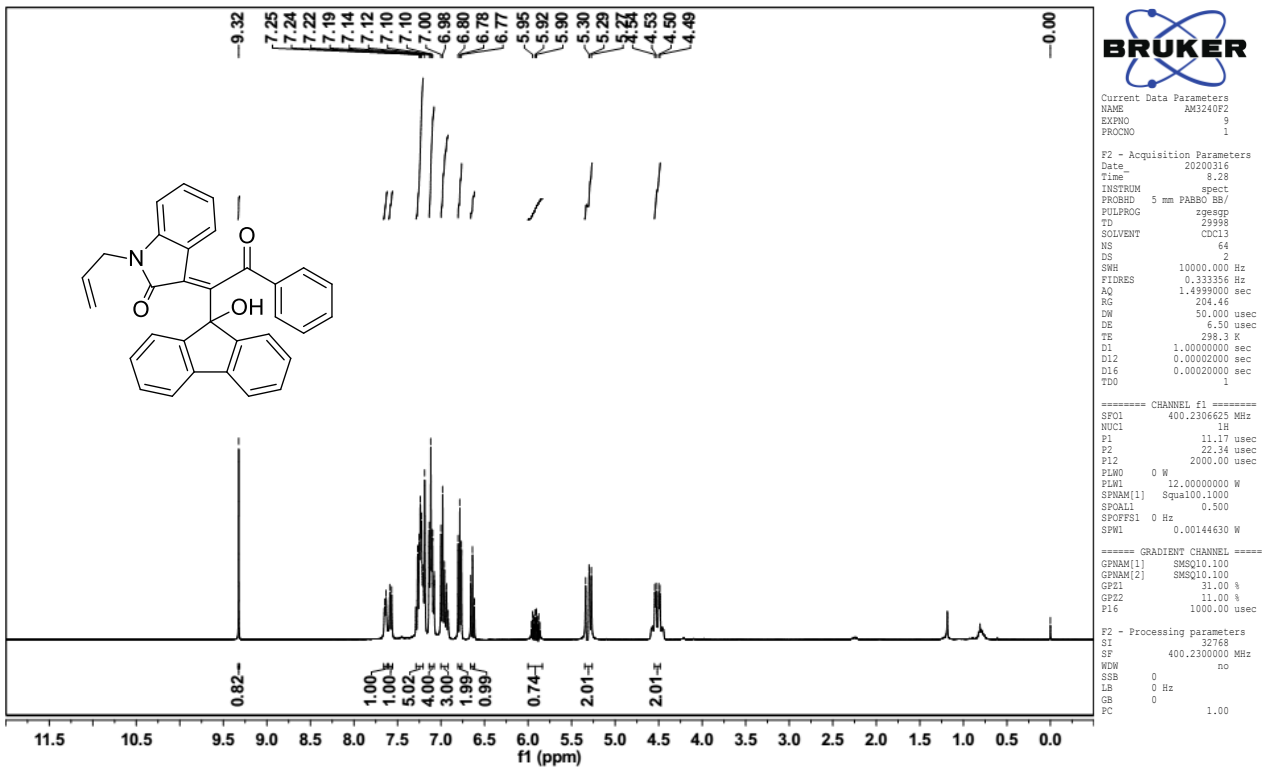




DEPT- 135 Spectrum of compound **4b**



HRMS Spectrum of Compound **4b**



Current Data Parameters
NAME AM3240F2
EXPNO 9
PROCNO 1

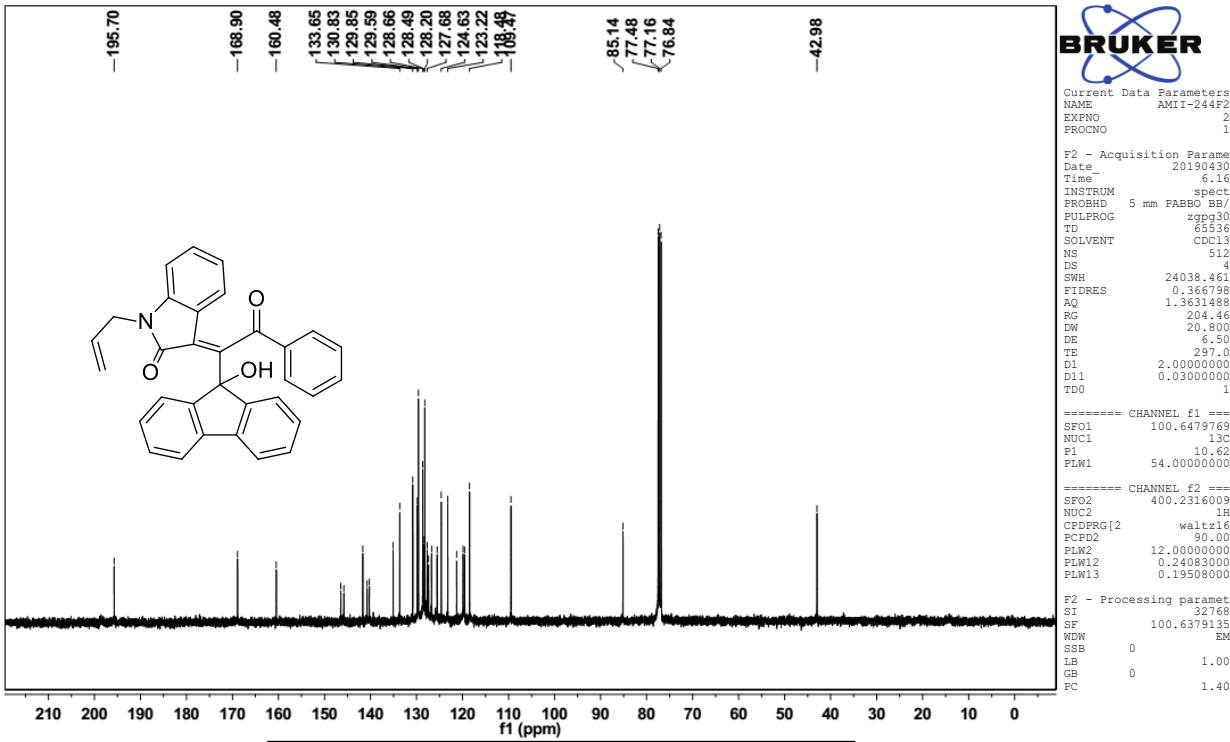
F2 - Acquisition Parameters
Date_ 20200316
Time 8.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgesgp
TD 29998
SOLVENT CDCl3
NS 64
DS 2
SWH 10000.000 Hz
FIDRES 0.333356 Hz
AQ 1.4999000 sec
RG 204.46
DW 50.000 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
D12 0.00002000 sec
D16 0.00020000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.2306625 MHz
NUC1 1H
P1 11.17 usec
P2 22.34 usec
P12 2000.00 usec
PLW0 0 W
PLW1 12.00000000 W
SPNAM[1] Squa100.1000
SPOAL1 0.500
SPOFFS1 0 Hz
SPW1 0.00144630 W

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPZ1 31.00 %
GPZ2 11.00 %
P16 1000.00 usec

F2 - Processing parameters
SI 32768
SF 400.2300000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

^{1}H NMR spectrum of compound **4c**



Current Data Parameters
NAME AMII-244F2
EXPNO 2
PROCNO 1

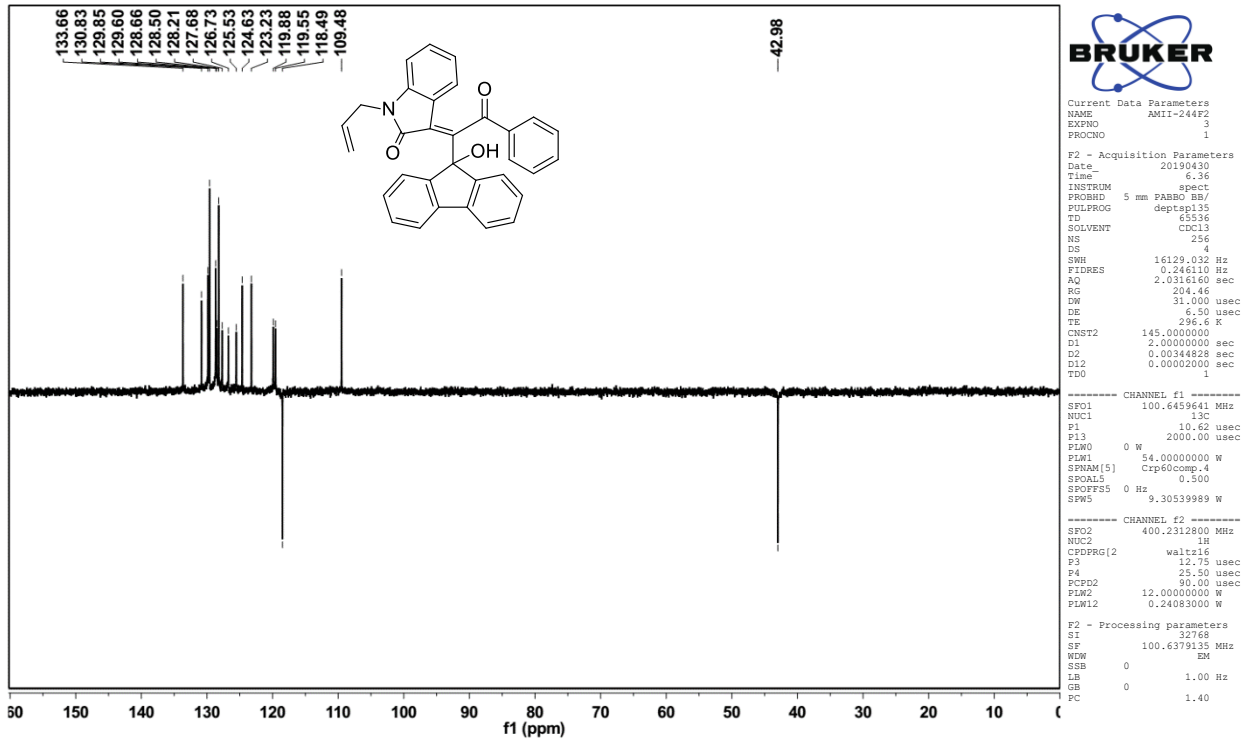
F2 - Acquisition Parameters
Date_ 20190430
Time 6.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 204.46
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6479769 MHz
NUC1 13C
P1 10.62 usec
PLW1 54.00000000 W

======== CHANNEL f2 ========
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W
PLW13 0.19508000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

^{13} C NMR Spectrum of compound **4c**



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Current Data Parameters
NAME AMII-244F2
EXPNO 3
PROCNO 1

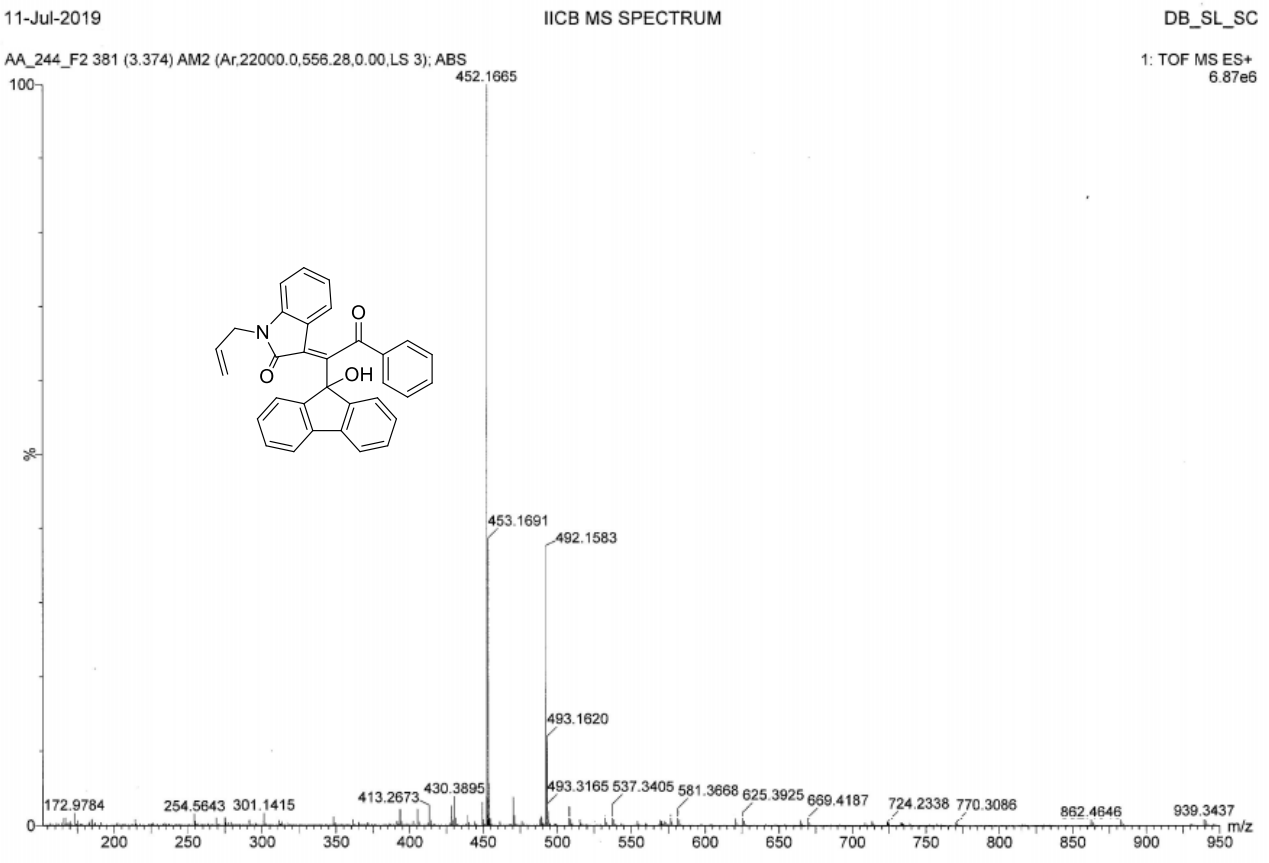
F2 - Acquisition Parameters
Date_ 20190430
Time 6.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 204.46
DW 31.000 usec
DE 6.50 usec
TE 296.6 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6459641 MHz
NUC1 13C
P1 10.62 usec
P13 2000.00 usec
PLW0 0 W
PLW1 54.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.30539989 W

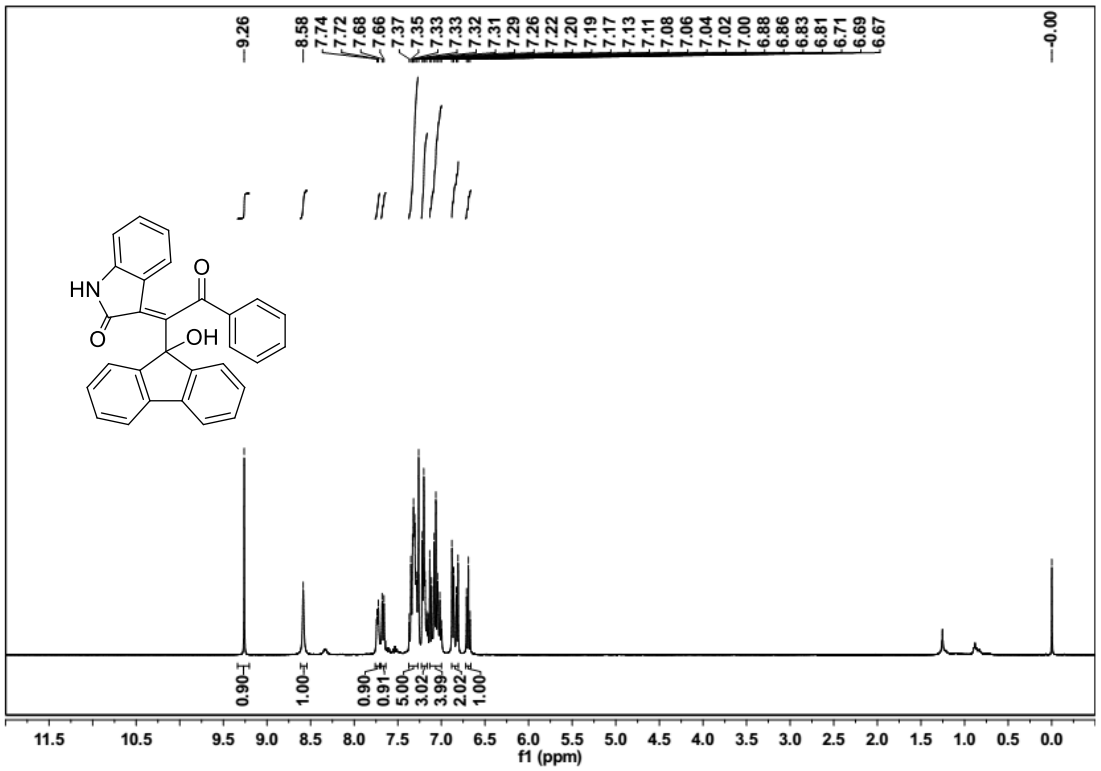
======== CHANNEL f2 ========
SFO2 400.2312800 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 12.75 usec
P4 25.50 usec
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT- 135 Spectrum of compound **4c**



HRMS Spectrum of compound **4c**



BRUKER

```
Current Data Parameters
NAME            AM3240F2
EXPNO                  2
PROCNO                 1

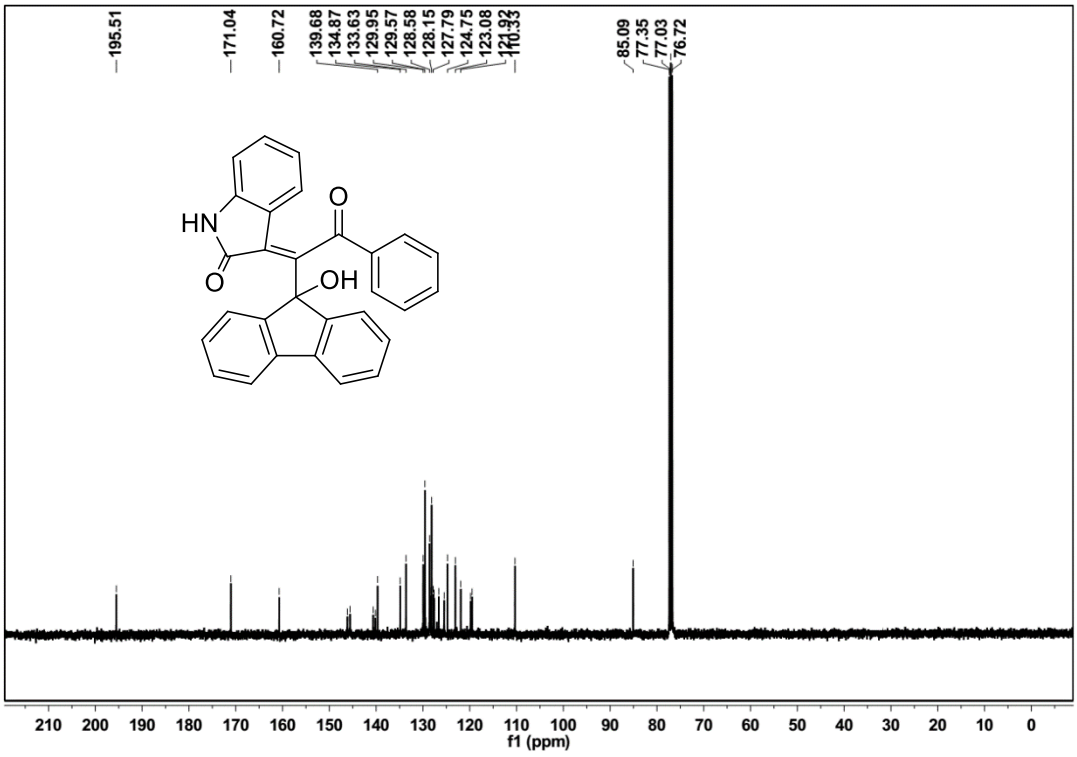
F2 - Acquisition Parameters
Date_           20200313
Time                7.16
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgesgp
TD                 29998
SOLVENT             CDC13
NS                    64
DS                     2
SWH           10000.000 Hz
FIDRES            0.333356 Hz
AQ             1.4999000 sec
RG                204.46
DW                50.000 usec
DE                 6.50 usec
TE                297.1 K
D1            1.00000000 sec
D12           0.00002000 sec
D16           0.00020000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.2306625 MHz
NUC1                   1H
P1                 11.17 usec
P2                 22.34 usec
P12              2000.00 usec
PLW0       0 W
PLW1         12.00000000 W
SPNAM[1]   Squa100.1000
SPOAL1             0.500
SPOFFS1  0 Hz
SPW1          0.00144630 W

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPZ1               31.00 %
GPZ2               11.00 %
P16              1000.00 usec

F2 - Processing parameters
SI                 32768
SF            400.2300000 MHz
WDW                   EM
SSB        0
LB                  0.50 Hz
GB         0
PC                  1.00
```

^{1}H NMR spectrum of compound **4d**



BRUKER

```
Current Data Parameters
NAME          AMII-240F2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190424
Time                19.20
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT             CDC13
NS                   512
DS                     4
SWH           24038.461 Hz
FIDRES            0.366798 Hz
AQ             1.3631488 sec
RG                204.46
DW                20.800 usec
DE                 6.50 usec
TE                297.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6479769 MHz
NUC1                   13C
P1                10.62 usec
PLW1          54.00000000 W

======== CHANNEL f2 ========
SFO2          400.2316009 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          12.00000000 W
PLW12          0.24083000 W
PLW13          0.19508000 W

F2 - Processing parameters
SI                 32768
SF            100.6379135 MHz
WDW                   EM
SSB        0
LB                  1.00 Hz
GB         0
PC                  1.40
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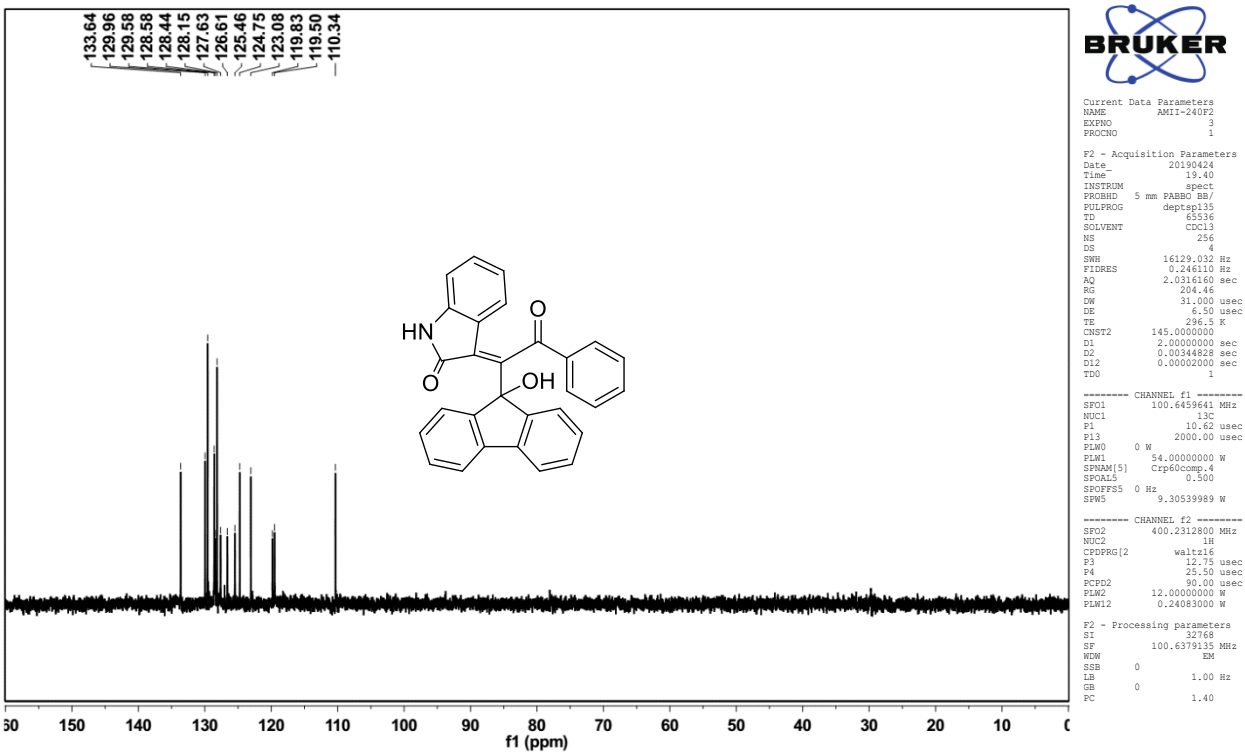
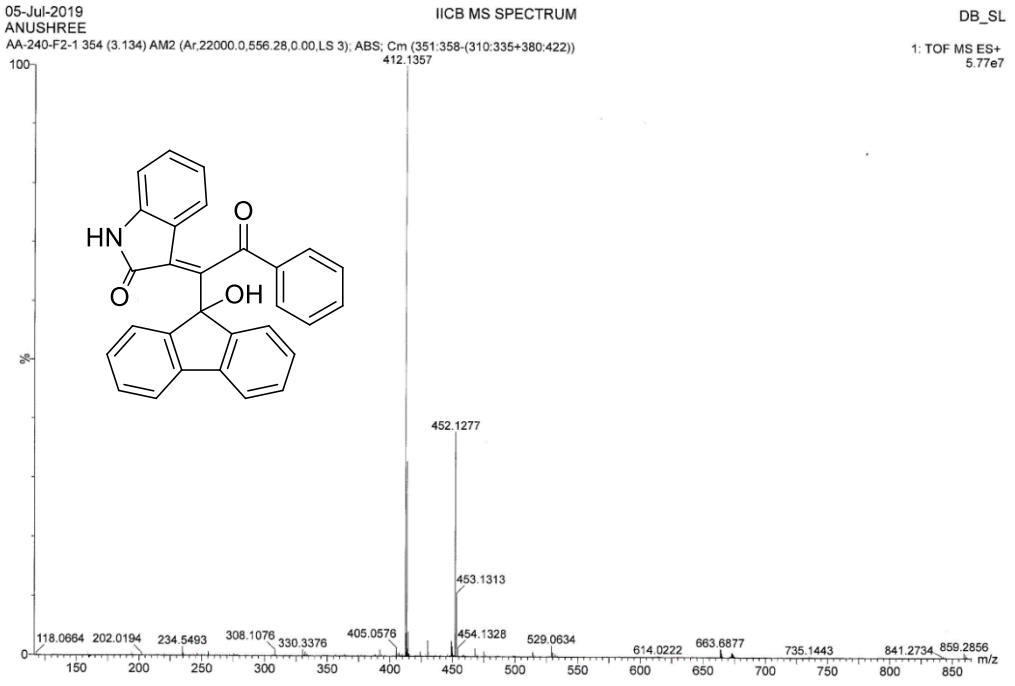
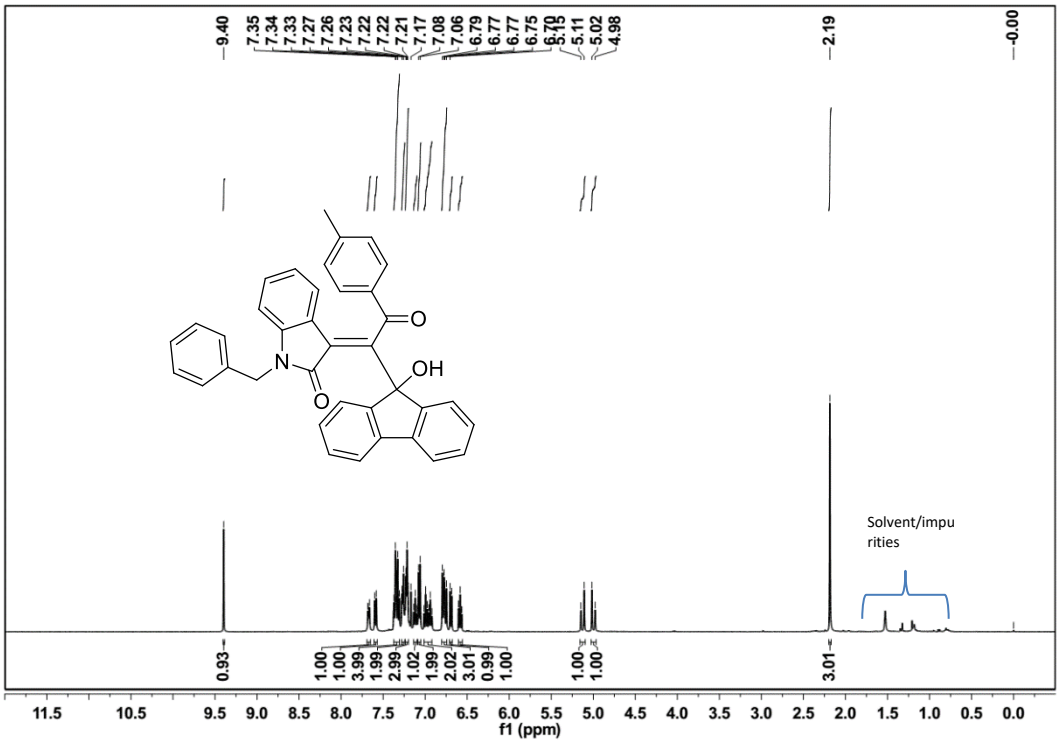
^{13} C NMR Spectrum of compound **4d**



DEPT- 135 Spectrum of compound **4d**



HRMS Spectrum of Compound **4d**



BRUKER

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Current Data Parameters
NAME          AM3-26 F2
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
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Time             19.28
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                79.6
DW              62.400 usec
DE               6.50 usec
TE              296.8 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.2324716 MHz
NUC1                   1H
P1                 12.75 usec
PLW1        12.00000000 W

F2 - Processing parameters
SI                 65536
SF          400.2300463 MHz
WDW                   EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
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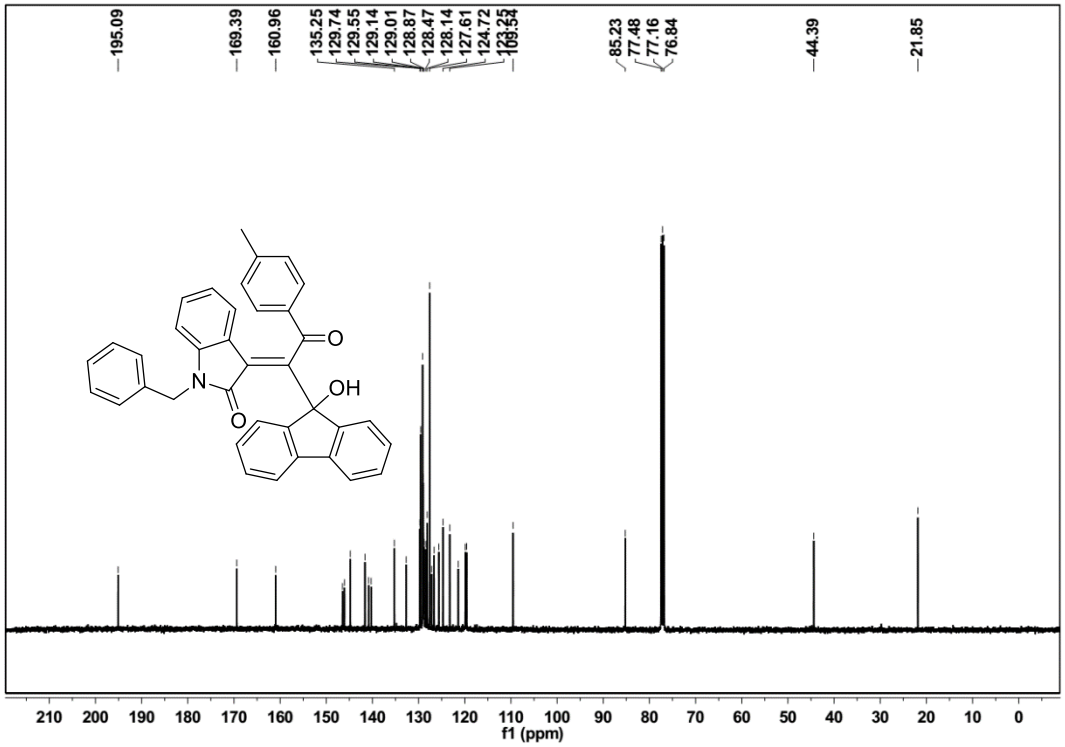
^{1} H NMR Spectrum of compound **4e**



BRUKER

```
Current Data Parameters
NAME          AM3-26 F2
EXPNO                5
PROCNO               1

F2 - Acquisition Parameters
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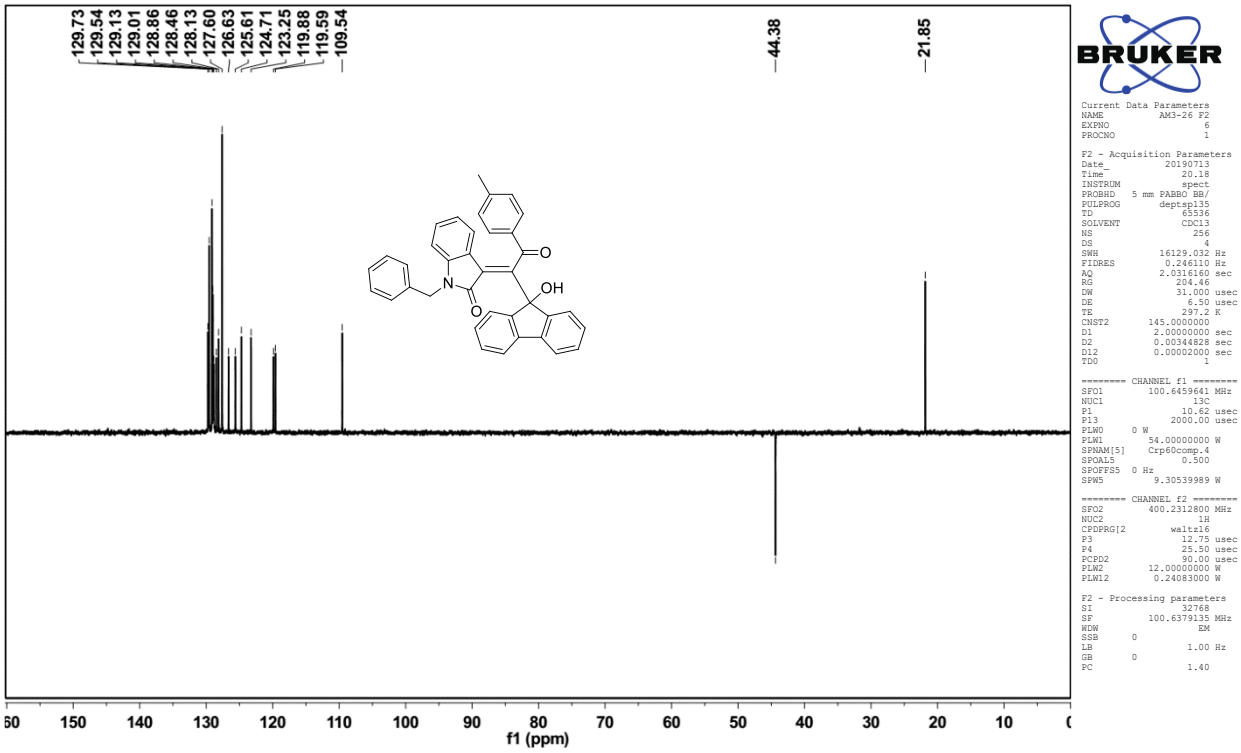
Time             19.59
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 512
DS                   4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG                204.46
DW              20.800 usec
DE               6.50 usec
TE              297.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6479769 MHz
NUC1                  13C
P1                10.62 usec
PLW1        54.00000000 W

======== CHANNEL f2 ========
SFO2        400.2316009 MHz
NUC2                  1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        12.00000000 W
PLW12        0.24083000 W
PLW13        0.19508000 W

F2 - Processing parameters
SI                 32768
SF          100.6379135 MHz
WDW                   EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

^{13} C NMR Spectrum of compound **4e**



Current Data Parameters
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EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
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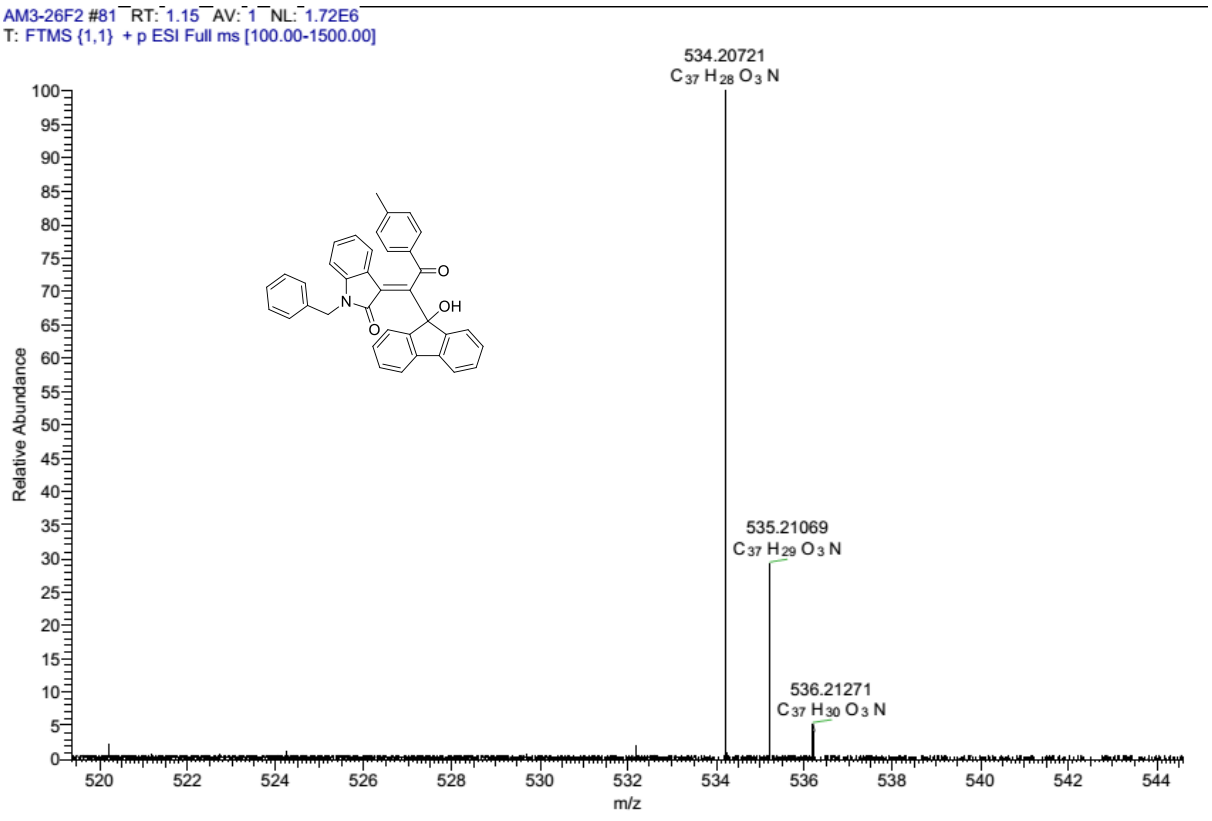
Time 20.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG deptsp135
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 204.46
DW 31.000 usec
DE 6.50 usec
TE 297.2 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6459641 MHz
NUC1 13C
P1 10.62 usec
P13 2000.00 usec
PLW0 0 W
PLW1 54.00000000 W
SPNAM[5] Crp60comp.4
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.30539989 W

======== CHANNEL f2 ========
SFO2 400.2312800 MHz
NUC2 1H
CPDPRG[2 waltz16
P3 12.75 usec
P4 25.50 usec
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W

F2 - Processing parameters
SI 32768
SF 100.6379135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

DEPT- 135 Spectrum of compound **4e**



HRMS Spectrum of Compound **4e**

Table 1. Crystal data and structure refinement for **3a**

Identification code	**3a**	
Empirical formula	C37 H28 N2 O2	
Formula weight	532.61	
Temperature	296(2) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.867(3) Å	α= 90°.
	b = 12.900(3) Å	β= 98.427(17)°.
	c = 18.148(6) Å	γ = 90°.
Volume	2748.3(12) $Å^3$	
Z	4	
Density (calculated)	1.287 Mg/m^3	
Absorption coefficient	0.626 mm^{-1}	
F(000)	1120	
Crystal size	0.150 x 0.150 x 0.100 mm^3	
Theta range for data collection	4.187 to 69.999°.	
Index ranges	-14<=h<=14, -15<=k<=15, -22<=l<=22	
Reflections collected	33648	
Independent reflections	5186 [R(int) = 0.0807]	
Completeness to theta = 67.684°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7536 and 0.6903	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5186 / 0 / 377	
Goodness-of-fit on F^2	1.093	
Final R indices [I>2sigma(I)]	R1 = 0.0643, wR2 = 0.1688	
R indices (all data)	R1 = 0.0982, wR2 = 0.1986	
Extinction coefficient	0.0096(8)	
Largest diff. peak and hole	0.190 and -0.172 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for AM. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3860(2)	4442(3)	3639(2)	81(1)
C(2)	3321(3)	3738(3)	3131(2)	89(1)
C(3)	3900(3)	3146(3)	2685(2)	78(1)
C(4)	5067(3)	3282(3)	2772(2)	81(1)
C(5)	5626(2)	3979(2)	3287(2)	76(1)
C(6)	5025(2)	4581(2)	3725(2)	60(1)
C(7)	6370(2)	6037(2)	4068(1)	53(1)
C(8)	7524(2)	5527(2)	4013(2)	56(1)
C(9)	8118(2)	4833(2)	4504(2)	69(1)
C(10)	9165(3)	4498(3)	4359(2)	83(1)
C(11)	9607(2)	4851(3)	3754(2)	86(1)
C(12)	9005(2)	5522(2)	3243(2)	77(1)
C(13)	7934(2)	5853(2)	3382(2)	60(1)
C(14)	7056(2)	6471(2)	2927(1)	60(1)
C(15)	7033(3)	6917(2)	2228(2)	77(1)
C(16)	6054(4)	7386(3)	1898(2)	90(1)
C(17)	5100(3)	7417(3)	2245(2)	87(1)
C(18)	5116(3)	7002(2)	2955(2)	70(1)
C(19)	6103(2)	6533(2)	3292(1)	56(1)
C(20)	7664(2)	8604(2)	3883(2)	63(1)
C(21)	8146(3)	9377(2)	3512(2)	79(1)
C(22)	9274(3)	9614(3)	3703(2)	93(1)
C(23)	9924(3)	9079(3)	4269(3)	105(1)
C(24)	9455(3)	8302(3)	4645(2)	84(1)
C(25)	8309(2)	8054(2)	4450(2)	61(1)
C(26)	7813(2)	7227(2)	4876(2)	58(1)
C(27)	6574(2)	6926(2)	4648(1)	57(1)
C(28)	5818(2)	7490(2)	4975(2)	62(1)
C(29)	6069(3)	8362(2)	5507(2)	68(1)
C(30)	7041(3)	8793(3)	5902(2)	83(1)
C(31)	6967(4)	9629(3)	6373(2)	102(1)
C(32)	5925(4)	10038(3)	6460(2)	110(1)
C(33)	4942(4)	9614(3)	6090(2)	102(1)

C(34)	5016(3)	8770(3)	5626(2)	79(1)
C(35)	2924(3)	8409(4)	5199(2)	112(1)
C(36)	4535(3)	7426(3)	4826(2)	69(1)
C(37)	3310(3)	2399(3)	2122(2)	103(1)
N(1)	5543(2)	5290(2)	4272(1)	63(1)
N(2)	4133(2)	8218(2)	5214(2)	81(1)
O(1)	8365(2)	6811(2)	5416(1)	70(1)
O(2)	3915(2)	6823(2)	4434(1)	83(1)

Table 3. Bond lengths [Å] and angles [°] for AM.

C(1)-C(6)	1.380(4)
C(1)-C(2)	1.383(5)
C(1)-H(1)	0.9300
C(2)-C(3)	1.369(5)
C(2)-H(2)	0.9300
C(3)-C(4)	1.382(4)
C(3)-C(37)	1.502(5)
C(4)-C(5)	1.392(4)
C(4)-H(4)	0.9300
C(5)-C(6)	1.381(4)
C(5)-H(5)	0.9300
C(6)-N(1)	1.421(4)
C(7)-N(1)	1.461(3)
C(7)-C(8)	1.536(3)
C(7)-C(19)	1.537(3)
C(7)-C(27)	1.552(4)
C(8)-C(13)	1.375(4)
C(8)-C(9)	1.381(4)
C(9)-C(10)	1.377(4)
C(9)-H(9)	0.9300
C(10)-C(11)	1.364(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.387(5)
C(11)-H(11)	0.9300
C(12)-C(13)	1.398(4)
C(12)-H(12)	0.9300
C(13)-C(14)	1.467(4)
C(14)-C(15)	1.390(4)

C(14)-C(19)	1.393(3)
C(15)-C(16)	1.367(5)
C(15)-H(15)	0.9300
C(16)-C(17)	1.375(5)
C(16)-H(16)	0.9300
C(17)-C(18)	1.393(4)
C(17)-H(17)	0.9300
C(18)-C(19)	1.379(3)
C(18)-H(18)	0.9300
C(20)-C(21)	1.374(4)
C(20)-C(25)	1.385(4)
C(20)-H(20)	0.9300
C(21)-C(22)	1.367(4)
C(21)-H(21)	0.9300
C(22)-C(23)	1.377(5)
C(22)-H(22)	0.9300
C(23)-C(24)	1.374(5)
C(23)-H(23)	0.9300
C(24)-C(25)	1.391(4)
C(24)-H(24)	0.9300
C(25)-C(26)	1.489(4)
C(26)-O(1)	1.220(3)
C(26)-C(27)	1.519(4)
C(27)-C(28)	1.358(4)
C(28)-C(29)	1.484(4)
C(28)-C(36)	1.509(4)
C(29)-C(30)	1.382(4)
C(29)-C(34)	1.402(4)
C(30)-C(31)	1.387(4)
C(30)-H(30)	0.9300
C(31)-C(32)	1.375(5)
C(31)-H(31)	0.9300
C(32)-C(33)	1.371(5)
C(32)-H(32)	0.9300
C(33)-C(34)	1.387(5)
C(33)-H(33)	0.9300
C(34)-N(2)	1.391(4)
C(35)-N(2)	1.453(4)

C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(36)-O(2)	1.225(4)
C(36)-N(2)	1.365(4)
C(37)-H(37A)	0.9600
C(37)-H(37B)	0.9600
C(37)-H(37C)	0.9600
N(1)-H(1A)	0.94(3)

C(6)-C(1)-C(2)	121.3(3)
C(6)-C(1)-H(1)	119.4
C(2)-C(1)-H(1)	119.4
C(3)-C(2)-C(1)	122.4(3)
C(3)-C(2)-H(2)	118.8
C(1)-C(2)-H(2)	118.8
C(2)-C(3)-C(4)	116.3(3)
C(2)-C(3)-C(37)	122.4(3)
C(4)-C(3)-C(37)	121.2(3)
C(3)-C(4)-C(5)	122.0(3)
C(3)-C(4)-H(4)	119.0
C(5)-C(4)-H(4)	119.0
C(6)-C(5)-C(4)	120.9(3)
C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
C(1)-C(6)-C(5)	117.1(3)
C(1)-C(6)-N(1)	119.1(3)
C(5)-C(6)-N(1)	123.8(2)
N(1)-C(7)-C(8)	111.8(2)
N(1)-C(7)-C(19)	116.8(2)
C(8)-C(7)-C(19)	100.6(2)
N(1)-C(7)-C(27)	111.1(2)
C(8)-C(7)-C(27)	107.98(19)
C(19)-C(7)-C(27)	107.7(2)
C(13)-C(8)-C(9)	121.8(3)
C(13)-C(8)-C(7)	110.5(2)
C(9)-C(8)-C(7)	127.7(3)
C(10)-C(9)-C(8)	118.0(3)

C(10)-C(9)-H(9)	121.0
C(8)-C(9)-H(9)	121.0
C(11)-C(10)-C(9)	120.9(3)
C(11)-C(10)-H(10)	119.6
C(9)-C(10)-H(10)	119.6
C(10)-C(11)-C(12)	121.7(3)
C(10)-C(11)-H(11)	119.2
C(12)-C(11)-H(11)	119.2
C(11)-C(12)-C(13)	117.6(3)
C(11)-C(12)-H(12)	121.2
C(13)-C(12)-H(12)	121.2
C(8)-C(13)-C(12)	119.9(3)
C(8)-C(13)-C(14)	109.0(2)
C(12)-C(13)-C(14)	130.9(3)
C(15)-C(14)-C(19)	120.1(3)
C(15)-C(14)-C(13)	131.0(3)
C(19)-C(14)-C(13)	108.9(2)
C(16)-C(15)-C(14)	119.1(3)
C(16)-C(15)-H(15)	120.5
C(14)-C(15)-H(15)	120.5
C(15)-C(16)-C(17)	121.0(3)
C(15)-C(16)-H(16)	119.5
C(17)-C(16)-H(16)	119.5
C(16)-C(17)-C(18)	120.8(3)
C(16)-C(17)-H(17)	119.6
C(18)-C(17)-H(17)	119.6
C(19)-C(18)-C(17)	118.3(3)
C(19)-C(18)-H(18)	120.8
C(17)-C(18)-H(18)	120.8
C(18)-C(19)-C(14)	120.7(3)
C(18)-C(19)-C(7)	129.5(2)
C(14)-C(19)-C(7)	109.8(2)
C(21)-C(20)-C(25)	120.7(3)
C(21)-C(20)-H(20)	119.6
C(25)-C(20)-H(20)	119.6
C(22)-C(21)-C(20)	120.1(3)
C(22)-C(21)-H(21)	120.0
C(20)-C(21)-H(21)	120.0

C(21)-C(22)-C(23)	119.9(3)
C(21)-C(22)-H(22)	120.1
C(23)-C(22)-H(22)	120.1
C(24)-C(23)-C(22)	120.8(3)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(23)-C(24)-C(25)	119.6(3)
C(23)-C(24)-H(24)	120.2
C(25)-C(24)-H(24)	120.2
C(20)-C(25)-C(24)	119.0(3)
C(20)-C(25)-C(26)	122.4(2)
C(24)-C(25)-C(26)	118.6(3)
O(1)-C(26)-C(25)	121.7(3)
O(1)-C(26)-C(27)	119.4(3)
C(25)-C(26)-C(27)	118.9(2)
C(28)-C(27)-C(26)	114.8(2)
C(28)-C(27)-C(7)	130.2(2)
C(26)-C(27)-C(7)	115.0(2)
C(27)-C(28)-C(29)	127.5(3)
C(27)-C(28)-C(36)	127.3(3)
C(29)-C(28)-C(36)	105.1(2)
C(30)-C(29)-C(34)	117.7(3)
C(30)-C(29)-C(28)	135.7(3)
C(34)-C(29)-C(28)	106.6(3)
C(29)-C(30)-C(31)	120.6(3)
C(29)-C(30)-H(30)	119.7
C(31)-C(30)-H(30)	119.7
C(32)-C(31)-C(30)	120.5(4)
C(32)-C(31)-H(31)	119.7
C(30)-C(31)-H(31)	119.7
C(33)-C(32)-C(31)	120.4(4)
C(33)-C(32)-H(32)	119.8
C(31)-C(32)-H(32)	119.8
C(32)-C(33)-C(34)	119.1(4)
C(32)-C(33)-H(33)	120.5
C(34)-C(33)-H(33)	120.5
C(33)-C(34)-N(2)	128.3(3)
C(33)-C(34)-C(29)	121.7(4)

N(2)-C(34)-C(29)	110.0(3)
N(2)-C(35)-H(35A)	109.5
N(2)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
N(2)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
O(2)-C(36)-N(2)	123.3(3)
O(2)-C(36)-C(28)	130.1(3)
N(2)-C(36)-C(28)	106.6(3)
C(3)-C(37)-H(37A)	109.5
C(3)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(3)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(6)-N(1)-C(7)	119.1(2)
C(6)-N(1)-H(1A)	109(2)
C(7)-N(1)-H(1A)	109(2)
C(36)-N(2)-C(34)	111.6(3)
C(36)-N(2)-C(35)	122.4(3)
C(34)-N(2)-C(35)	125.9(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for AM. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	60(2)	103(2)	81(2)	-1(2)	11(2)	-2(2)
C(2)	57(2)	114(3)	93(3)	-2(2)	5(2)	-15(2)
C(3)	72(2)	79(2)	76(2)	11(2)	-5(2)	-12(2)
C(4)	70(2)	76(2)	96(2)	-10(2)	5(2)	-5(2)
C(5)	58(2)	78(2)	91(2)	-10(2)	4(2)	-3(1)
C(6)	60(1)	65(2)	55(2)	13(1)	6(1)	-1(1)
C(7)	50(1)	58(1)	50(1)	6(1)	5(1)	7(1)
C(8)	51(1)	58(1)	57(2)	-7(1)	0(1)	4(1)

C(9)	66(2)	64(2)	70(2)	-9(1)	-12(1)	14(1)
C(10)	72(2)	71(2)	96(3)	-26(2)	-20(2)	18(2)
C(11)	52(2)	82(2)	120(3)	-36(2)	-1(2)	15(2)
C(12)	60(2)	77(2)	97(2)	-28(2)	23(2)	-5(1)
C(13)	55(1)	59(2)	67(2)	-12(1)	8(1)	-2(1)
C(14)	70(2)	57(2)	53(2)	-4(1)	13(1)	-4(1)
C(15)	105(2)	68(2)	63(2)	0(1)	28(2)	-5(2)
C(16)	139(3)	76(2)	59(2)	17(2)	20(2)	20(2)
C(17)	109(3)	82(2)	66(2)	13(2)	-2(2)	30(2)
C(18)	71(2)	76(2)	60(2)	10(1)	0(1)	17(1)
C(19)	56(1)	59(2)	51(1)	2(1)	4(1)	2(1)
C(20)	63(2)	58(2)	68(2)	2(1)	6(1)	7(1)
C(21)	84(2)	67(2)	87(2)	11(2)	12(2)	4(2)
C(22)	89(2)	79(2)	114(3)	14(2)	24(2)	-5(2)
C(23)	67(2)	97(3)	150(4)	13(3)	6(2)	-13(2)
C(24)	64(2)	78(2)	104(3)	5(2)	-6(2)	1(2)
C(25)	61(2)	56(2)	65(2)	-6(1)	4(1)	7(1)
C(26)	61(2)	56(1)	54(2)	-5(1)	-1(1)	14(1)
C(27)	60(1)	61(2)	49(1)	8(1)	4(1)	15(1)
C(28)	66(2)	67(2)	52(2)	6(1)	9(1)	16(1)
C(29)	80(2)	70(2)	57(2)	7(1)	17(1)	24(2)
C(30)	95(2)	84(2)	72(2)	-14(2)	16(2)	14(2)
C(31)	134(3)	89(3)	84(3)	-22(2)	24(2)	6(2)
C(32)	150(4)	92(3)	94(3)	-23(2)	36(3)	22(3)
C(33)	128(3)	94(3)	90(3)	-3(2)	39(2)	45(2)
C(34)	98(2)	83(2)	58(2)	8(2)	23(2)	31(2)
C(35)	86(2)	153(4)	102(3)	7(3)	33(2)	47(2)
C(36)	72(2)	78(2)	59(2)	13(1)	15(1)	22(2)
C(37)	93(3)	108(3)	101(3)	-8(2)	-7(2)	-26(2)
N(1)	63(1)	68(1)	58(1)	6(1)	11(1)	0(1)
N(2)	76(2)	98(2)	73(2)	10(2)	24(1)	35(2)
O(1)	72(1)	71(1)	61(1)	3(1)	-6(1)	17(1)
O(2)	62(1)	102(2)	85(2)	0(1)	14(1)	17(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for AM.

	x	y	z	U(eq)
H(1)	3430	4830	3928	97
H(2)	2535	3663	3092	107
H(4)	5492	2897	2478	97
H(5)	6415	4040	3337	92
H(9)	7819	4600	4920	82
H(10)	9576	4024	4679	100
H(11)	10330	4636	3681	104
H(12)	9303	5743	2824	92
H(15)	7673	6897	1989	93
H(16)	6034	7688	1431	109
H(17)	4436	7719	2002	105
H(18)	4478	7041	3196	84
H(20)	6896	8447	3751	76
H(21)	7706	9739	3130	95
H(22)	9601	10137	3452	112
H(23)	10690	9245	4400	127
H(24)	9901	7944	5026	101
H(30)	7750	8520	5851	100
H(31)	7628	9916	6631	122
H(32)	5886	10605	6772	132
H(33)	4237	9889	6150	122
H(35A)	2495	7967	4835	167
H(35B)	2758	9121	5072	167
H(35C)	2718	8265	5681	167
H(37A)	3052	1810	2373	155
H(37B)	3832	2175	1797	155
H(37C)	2669	2735	1834	155
H(1A)	4970(30)	5650(30)	4465(19)	109(13)

Table 6. Torsion angles [°] for AM.

C(6)-C(1)-C(2)-C(3)	-0.4(5)
C(1)-C(2)-C(3)-C(4)	0.6(5)
C(1)-C(2)-C(3)-C(37)	-178.5(3)
C(2)-C(3)-C(4)-C(5)	0.3(5)
C(37)-C(3)-C(4)-C(5)	179.4(3)
C(3)-C(4)-C(5)-C(6)	-1.3(5)
C(2)-C(1)-C(6)-C(5)	-0.6(5)
C(2)-C(1)-C(6)-N(1)	-178.0(3)
C(4)-C(5)-C(6)-C(1)	1.4(5)
C(4)-C(5)-C(6)-N(1)	178.6(3)
N(1)-C(7)-C(8)-C(13)	135.0(2)
C(19)-C(7)-C(8)-C(13)	10.3(3)
C(27)-C(7)-C(8)-C(13)	-102.5(2)
N(1)-C(7)-C(8)-C(9)	-44.9(4)
C(19)-C(7)-C(8)-C(9)	-169.7(3)
C(27)-C(7)-C(8)-C(9)	77.6(3)
C(13)-C(8)-C(9)-C(10)	2.3(4)
C(7)-C(8)-C(9)-C(10)	-177.8(3)
C(8)-C(9)-C(10)-C(11)	0.8(4)
C(9)-C(10)-C(11)-C(12)	-2.9(5)
C(10)-C(11)-C(12)-C(13)	1.8(4)
C(9)-C(8)-C(13)-C(12)	-3.3(4)
C(7)-C(8)-C(13)-C(12)	176.7(2)
C(9)-C(8)-C(13)-C(14)	172.6(2)
C(7)-C(8)-C(13)-C(14)	-7.3(3)
C(11)-C(12)-C(13)-C(8)	1.2(4)
C(11)-C(12)-C(13)-C(14)	-173.7(3)
C(8)-C(13)-C(14)-C(15)	-175.9(3)
C(12)-C(13)-C(14)-C(15)	-0.5(5)
C(8)-C(13)-C(14)-C(19)	0.7(3)
C(12)-C(13)-C(14)-C(19)	176.0(3)
C(19)-C(14)-C(15)-C(16)	-2.0(4)
C(13)-C(14)-C(15)-C(16)	174.3(3)
C(14)-C(15)-C(16)-C(17)	-0.3(5)
C(15)-C(16)-C(17)-C(18)	2.2(6)
C(16)-C(17)-C(18)-C(19)	-1.9(5)

C(17)-C(18)-C(19)-C(14)	-0.4(4)
C(17)-C(18)-C(19)-C(7)	178.6(3)
C(15)-C(14)-C(19)-C(18)	2.3(4)
C(13)-C(14)-C(19)-C(18)	-174.7(2)
C(15)-C(14)-C(19)-C(7)	-176.8(2)
C(13)-C(14)-C(19)-C(7)	6.2(3)
N(1)-C(7)-C(19)-C(18)	49.9(4)
C(8)-C(7)-C(19)-C(18)	171.2(3)
C(27)-C(7)-C(19)-C(18)	-75.9(3)
N(1)-C(7)-C(19)-C(14)	-131.0(2)
C(8)-C(7)-C(19)-C(14)	-9.8(3)
C(27)-C(7)-C(19)-C(14)	103.2(2)
C(25)-C(20)-C(21)-C(22)	-0.3(5)
C(20)-C(21)-C(22)-C(23)	-0.1(5)
C(21)-C(22)-C(23)-C(24)	0.3(6)
C(22)-C(23)-C(24)-C(25)	-0.1(6)
C(21)-C(20)-C(25)-C(24)	0.5(4)
C(21)-C(20)-C(25)-C(26)	178.6(3)
C(23)-C(24)-C(25)-C(20)	-0.3(5)
C(23)-C(24)-C(25)-C(26)	-178.6(3)
C(20)-C(25)-C(26)-O(1)	-173.6(2)
C(24)-C(25)-C(26)-O(1)	4.6(4)
C(20)-C(25)-C(26)-C(27)	4.1(4)
C(24)-C(25)-C(26)-C(27)	-177.8(3)
O(1)-C(26)-C(27)-C(28)	89.3(3)
C(25)-C(26)-C(27)-C(28)	-88.4(3)
O(1)-C(26)-C(27)-C(7)	-91.8(3)
C(25)-C(26)-C(27)-C(7)	90.5(3)
N(1)-C(7)-C(27)-C(28)	-45.4(3)
C(8)-C(7)-C(27)-C(28)	-168.4(3)
C(19)-C(7)-C(27)-C(28)	83.7(3)
N(1)-C(7)-C(27)-C(26)	135.9(2)
C(8)-C(7)-C(27)-C(26)	12.9(3)
C(19)-C(7)-C(27)-C(26)	-95.0(2)
C(26)-C(27)-C(28)-C(29)	1.3(4)
C(7)-C(27)-C(28)-C(29)	-177.4(2)
C(26)-C(27)-C(28)-C(36)	175.6(2)
C(7)-C(27)-C(28)-C(36)	-3.1(5)

C(27)-C(28)-C(29)-C(30)	-9.5(5)
C(36)-C(28)-C(29)-C(30)	175.2(3)
C(27)-C(28)-C(29)-C(34)	173.6(3)
C(36)-C(28)-C(29)-C(34)	-1.7(3)
C(34)-C(29)-C(30)-C(31)	-2.7(5)
C(28)-C(29)-C(30)-C(31)	-179.4(3)
C(29)-C(30)-C(31)-C(32)	0.6(6)
C(30)-C(31)-C(32)-C(33)	0.9(7)
C(31)-C(32)-C(33)-C(34)	-0.1(6)
C(32)-C(33)-C(34)-N(2)	178.8(4)
C(32)-C(33)-C(34)-C(29)	-2.1(6)
C(30)-C(29)-C(34)-C(33)	3.5(5)
C(28)-C(29)-C(34)-C(33)	-178.9(3)
C(30)-C(29)-C(34)-N(2)	-177.2(3)
C(28)-C(29)-C(34)-N(2)	0.3(3)
C(27)-C(28)-C(36)-O(2)	5.9(5)
C(29)-C(28)-C(36)-O(2)	-178.7(3)
C(27)-C(28)-C(36)-N(2)	-172.8(3)
C(29)-C(28)-C(36)-N(2)	2.5(3)
C(1)-C(6)-N(1)-C(7)	-132.8(3)
C(5)-C(6)-N(1)-C(7)	49.9(4)
C(8)-C(7)-N(1)-C(6)	-75.5(3)
C(19)-C(7)-N(1)-C(6)	39.7(3)
C(27)-C(7)-N(1)-C(6)	163.8(2)
O(2)-C(36)-N(2)-C(34)	178.7(3)
C(28)-C(36)-N(2)-C(34)	-2.4(3)
O(2)-C(36)-N(2)-C(35)	0.6(5)
C(28)-C(36)-N(2)-C(35)	179.5(3)
C(33)-C(34)-N(2)-C(36)	-179.4(3)
C(29)-C(34)-N(2)-C(36)	1.4(4)
C(33)-C(34)-N(2)-C(35)	-1.4(6)
C(29)-C(34)-N(2)-C(35)	179.4(3)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for AM [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1A)...O(2)	0.94(3)	1.96(4)	2.810(3)	151(3)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for **4b**

Identification code	**4b**	
Empirical formula	C36 H25 N O3	
Formula weight	519.57	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.7530(5) Å	α= 90°.
	b = 19.4993(9) Å	β= 94.635(2)°.
	c = 14.0108(7) Å	γ = 90°.
Volume	2655.8(2) $Å^3$	
Z	4	
Density (calculated)	1.299 Mg/m^3	
Absorption coefficient	0.082 mm^{-1}	
F(000)	1088	
Crystal size	0.150 x 0.150 x 0.100 mm^3	
Theta range for data collection	3.457 to 26.000°.	
Index ranges	-12<=h<=12, -24<=k<=24, -17<=l<=17	
Reflections collected	61272	
Independent reflections	5187 [R(int) = 0.0607]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6751	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5187 / 0 / 366	
Goodness-of-fit on F^2	1.095	
Final R indices [I>2sigma(I)]	R1 = 0.0481, wR2 = 0.1017	
R indices (all data)	R1 = 0.0675, wR2 = 0.1121	
Extinction coefficient	0.0263(14)	
Largest diff. peak and hole	0.199 and -0.165 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 242. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	9293(2)	6391(1)	1604(1)	39(1)
C(2)	9980(2)	5941(1)	1045(1)	49(1)
C(3)	9895(2)	6044(1)	60(2)	59(1)
C(4)	9139(2)	6583(1)	-346(2)	63(1)
C(5)	8465(2)	7037(1)	208(1)	56(1)
C(6)	8550(2)	6941(1)	1195(1)	42(1)
C(7)	7977(2)	7337(1)	1955(1)	42(1)
C(8)	7170(2)	7926(1)	1920(2)	57(1)
C(9)	6805(2)	8206(1)	2765(2)	65(1)
C(10)	7226(2)	7912(1)	3633(2)	58(1)
C(11)	8010(2)	7319(1)	3679(1)	48(1)
C(12)	8385(2)	7034(1)	2837(1)	38(1)
C(13)	9200(2)	6374(1)	2683(1)	36(1)
C(14)	8319(2)	5762(1)	2984(1)	33(1)
C(15)	7448(2)	5448(1)	2152(1)	35(1)
C(16)	6128(2)	5789(1)	1829(1)	36(1)
C(17)	5445(2)	6200(1)	2442(1)	46(1)
C(18)	4200(2)	6495(1)	2140(2)	58(1)
C(19)	3651(2)	6395(1)	1220(2)	70(1)
C(20)	4331(3)	5995(1)	600(2)	79(1)
C(21)	5561(2)	5688(1)	903(1)	59(1)
C(22)	8231(2)	5503(1)	3868(1)	32(1)
C(23)	7321(2)	4953(1)	4169(1)	33(1)
C(24)	6393(2)	4513(1)	3683(1)	42(1)
C(25)	5678(2)	4046(1)	4198(1)	49(1)
C(26)	5888(2)	4010(1)	5178(1)	50(1)
C(27)	6808(2)	4443(1)	5685(1)	45(1)
C(28)	7505(2)	4906(1)	5170(1)	35(1)
C(29)	8992(2)	5750(1)	4788(1)	35(1)
C(30)	8957(2)	5492(1)	6525(1)	41(1)
C(31)	7952(2)	5903(1)	7056(1)	38(1)
C(32)	7778(2)	6600(1)	6890(1)	47(1)
C(33)	6846(2)	6972(1)	7378(2)	56(1)

C(34)	6079(2)	6653(1)	8025(2)	61(1)
C(35)	6244(2)	5964(1)	8199(1)	59(1)
C(36)	7176(2)	5591(1)	7717(1)	48(1)
N(1)	8503(1)	5388(1)	5515(1)	37(1)
O(1)	9880(1)	6197(1)	4905(1)	46(1)
O(2)	7858(1)	4942(1)	1758(1)	49(1)
O(3)	10559(1)	6363(1)	3127(1)	44(1)

Table 3. Bond lengths [Å] and angles [°] for 242.

C(1)-C(2)	1.385(2)
C(1)-C(6)	1.392(2)
C(1)-C(13)	1.522(2)
C(2)-C(3)	1.389(3)
C(2)-H(2)	0.9300
C(3)-C(4)	1.380(3)
C(3)-H(3)	0.9300
C(4)-C(5)	1.380(3)
C(4)-H(4)	0.9300
C(5)-C(6)	1.391(3)
C(5)-H(5)	0.9300
C(6)-C(7)	1.462(3)
C(7)-C(8)	1.391(3)
C(7)-C(12)	1.398(2)
C(8)-C(9)	1.376(3)
C(8)-H(8)	0.9300
C(9)-C(10)	1.376(3)
C(9)-H(9)	0.9300
C(10)-C(11)	1.386(3)
C(10)-H(10)	0.9300
C(11)-C(12)	1.380(2)
C(11)-H(11)	0.9300
C(12)-C(13)	1.536(2)
C(13)-O(3)	1.4177(19)
C(13)-C(14)	1.549(2)
C(14)-C(22)	1.348(2)
C(14)-C(15)	1.515(2)
C(15)-O(2)	1.2143(19)

C(15)-C(16)	1.487(2)
C(16)-C(21)	1.383(2)
C(16)-C(17)	1.383(2)
C(17)-C(18)	1.379(3)
C(17)-H(17)	0.9300
C(18)-C(19)	1.369(3)
C(18)-H(18)	0.9300
C(19)-C(20)	1.377(3)
C(19)-H(19)	0.9300
C(20)-C(21)	1.376(3)
C(20)-H(20)	0.9300
C(21)-H(21)	0.9300
C(22)-C(23)	1.475(2)
C(22)-C(29)	1.513(2)
C(23)-C(24)	1.385(2)
C(23)-C(28)	1.402(2)
C(24)-C(25)	1.385(2)
C(24)-H(24)	0.9300
C(25)-C(26)	1.373(3)
C(25)-H(25)	0.9300
C(26)-C(27)	1.386(3)
C(26)-H(26)	0.9300
C(27)-C(28)	1.369(2)
C(27)-H(27)	0.9300
C(28)-N(1)	1.410(2)
C(29)-O(1)	1.2304(19)
C(29)-N(1)	1.357(2)
C(30)-N(1)	1.463(2)
C(30)-C(31)	1.507(2)
C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700
C(31)-C(36)	1.383(2)
C(31)-C(32)	1.387(2)
C(32)-C(33)	1.386(3)
C(32)-H(32)	0.9300
C(33)-C(34)	1.371(3)
C(33)-H(33)	0.9300
C(34)-C(35)	1.372(3)

C(34)-H(34)	0.9300
C(35)-C(36)	1.382(3)
C(35)-H(35)	0.9300
C(36)-H(36)	0.9300
O(3)-H(3A)	0.96(3)

C(2)-C(1)-C(6)	120.93(16)
C(2)-C(1)-C(13)	128.30(16)
C(6)-C(1)-C(13)	110.77(15)
C(1)-C(2)-C(3)	118.59(19)
C(1)-C(2)-H(2)	120.7
C(3)-C(2)-H(2)	120.7
C(4)-C(3)-C(2)	120.4(2)
C(4)-C(3)-H(3)	119.8
C(2)-C(3)-H(3)	119.8
C(3)-C(4)-C(5)	121.36(19)
C(3)-C(4)-H(4)	119.3
C(5)-C(4)-H(4)	119.3
C(4)-C(5)-C(6)	118.7(2)
C(4)-C(5)-H(5)	120.7
C(6)-C(5)-H(5)	120.7
C(5)-C(6)-C(1)	120.05(18)
C(5)-C(6)-C(7)	131.09(18)
C(1)-C(6)-C(7)	108.86(15)
C(8)-C(7)-C(12)	119.96(18)
C(8)-C(7)-C(6)	131.20(18)
C(12)-C(7)-C(6)	108.84(15)
C(9)-C(8)-C(7)	118.84(19)
C(9)-C(8)-H(8)	120.6
C(7)-C(8)-H(8)	120.6
C(8)-C(9)-C(10)	121.01(19)
C(8)-C(9)-H(9)	119.5
C(10)-C(9)-H(9)	119.5
C(9)-C(10)-C(11)	120.91(19)
C(9)-C(10)-H(10)	119.5
C(11)-C(10)-H(10)	119.5
C(12)-C(11)-C(10)	118.63(18)
C(12)-C(11)-H(11)	120.7

C(10)-C(11)-H(11)	120.7
C(11)-C(12)-C(7)	120.63(16)
C(11)-C(12)-C(13)	129.27(16)
C(7)-C(12)-C(13)	110.06(15)
O(3)-C(13)-C(1)	107.92(13)
O(3)-C(13)-C(12)	115.32(13)
C(1)-C(13)-C(12)	101.24(13)
O(3)-C(13)-C(14)	112.83(13)
C(1)-C(13)-C(14)	111.40(13)
C(12)-C(13)-C(14)	107.58(12)
C(22)-C(14)-C(15)	118.84(14)
C(22)-C(14)-C(13)	128.11(14)
C(15)-C(14)-C(13)	113.03(13)
O(2)-C(15)-C(16)	122.32(15)
O(2)-C(15)-C(14)	119.58(15)
C(16)-C(15)-C(14)	118.07(14)
C(21)-C(16)-C(17)	119.25(17)
C(21)-C(16)-C(15)	119.50(16)
C(17)-C(16)-C(15)	121.25(15)
C(18)-C(17)-C(16)	120.51(18)
C(18)-C(17)-H(17)	119.7
C(16)-C(17)-H(17)	119.7
C(19)-C(18)-C(17)	119.8(2)
C(19)-C(18)-H(18)	120.1
C(17)-C(18)-H(18)	120.1
C(18)-C(19)-C(20)	120.2(2)
C(18)-C(19)-H(19)	119.9
C(20)-C(19)-H(19)	119.9
C(19)-C(20)-C(21)	120.2(2)
C(19)-C(20)-H(20)	119.9
C(21)-C(20)-H(20)	119.9
C(20)-C(21)-C(16)	120.0(2)
C(20)-C(21)-H(21)	120.0
C(16)-C(21)-H(21)	120.0
C(14)-C(22)-C(23)	128.30(14)
C(14)-C(22)-C(29)	126.87(15)
C(23)-C(22)-C(29)	104.72(13)
C(24)-C(23)-C(28)	118.46(15)

C(24)-C(23)-C(22)	134.00(15)
C(28)-C(23)-C(22)	107.54(13)
C(25)-C(24)-C(23)	119.25(16)
C(25)-C(24)-H(24)	120.4
C(23)-C(24)-H(24)	120.4
C(26)-C(25)-C(24)	120.88(17)
C(26)-C(25)-H(25)	119.6
C(24)-C(25)-H(25)	119.6
C(25)-C(26)-C(27)	121.28(17)
C(25)-C(26)-H(26)	119.4
C(27)-C(26)-H(26)	119.4
C(28)-C(27)-C(26)	117.40(16)
C(28)-C(27)-H(27)	121.3
C(26)-C(27)-H(27)	121.3
C(27)-C(28)-C(23)	122.73(16)
C(27)-C(28)-N(1)	128.09(15)
C(23)-C(28)-N(1)	109.18(14)
O(1)-C(29)-N(1)	123.73(15)
O(1)-C(29)-C(22)	129.12(15)
N(1)-C(29)-C(22)	107.15(13)
N(1)-C(30)-C(31)	113.13(13)
N(1)-C(30)-H(30A)	109.0
C(31)-C(30)-H(30A)	109.0
N(1)-C(30)-H(30B)	109.0
C(31)-C(30)-H(30B)	109.0
H(30A)-C(30)-H(30B)	107.8
C(36)-C(31)-C(32)	118.44(16)
C(36)-C(31)-C(30)	120.65(16)
C(32)-C(31)-C(30)	120.91(16)
C(33)-C(32)-C(31)	120.50(18)
C(33)-C(32)-H(32)	119.8
C(31)-C(32)-H(32)	119.8
C(34)-C(33)-C(32)	120.19(19)
C(34)-C(33)-H(33)	119.9
C(32)-C(33)-H(33)	119.9
C(33)-C(34)-C(35)	119.95(19)
C(33)-C(34)-H(34)	120.0
C(35)-C(34)-H(34)	120.0

C(34)-C(35)-C(36)	120.1(2)
C(34)-C(35)-H(35)	120.0
C(36)-C(35)-H(35)	120.0
C(35)-C(36)-C(31)	120.85(19)
C(35)-C(36)-H(36)	119.6
C(31)-C(36)-H(36)	119.6
C(29)-N(1)-C(28)	111.38(13)
C(29)-N(1)-C(30)	123.82(14)
C(28)-N(1)-C(30)	124.80(14)
C(13)-O(3)-H(3A)	105.8(15)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 242. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	38(1)	42(1)	38(1)	2(1)	6(1)	-6(1)
C(2)	48(1)	56(1)	45(1)	0(1)	12(1)	-3(1)
C(3)	58(1)	74(1)	48(1)	-9(1)	19(1)	-13(1)
C(4)	64(1)	90(2)	37(1)	4(1)	6(1)	-20(1)
C(5)	57(1)	67(1)	44(1)	15(1)	0(1)	-9(1)
C(6)	40(1)	46(1)	41(1)	7(1)	2(1)	-10(1)
C(7)	40(1)	37(1)	49(1)	6(1)	1(1)	-5(1)
C(8)	60(1)	43(1)	68(1)	13(1)	-3(1)	3(1)
C(9)	64(1)	42(1)	86(2)	-1(1)	2(1)	14(1)
C(10)	58(1)	49(1)	67(1)	-14(1)	6(1)	10(1)
C(11)	51(1)	44(1)	47(1)	-3(1)	2(1)	4(1)
C(12)	36(1)	35(1)	44(1)	0(1)	3(1)	-4(1)
C(13)	33(1)	38(1)	37(1)	2(1)	2(1)	0(1)
C(14)	31(1)	34(1)	34(1)	-1(1)	4(1)	6(1)
C(15)	41(1)	34(1)	31(1)	1(1)	7(1)	-4(1)
C(16)	37(1)	39(1)	33(1)	3(1)	2(1)	-6(1)
C(17)	41(1)	58(1)	39(1)	2(1)	2(1)	4(1)
C(18)	45(1)	70(1)	58(1)	5(1)	6(1)	14(1)
C(19)	49(1)	89(2)	69(2)	10(1)	-13(1)	13(1)
C(20)	75(2)	104(2)	53(1)	-5(1)	-28(1)	15(1)

C(21)	63(1)	71(1)	41(1)	-9(1)	-9(1)	6(1)
C(22)	31(1)	33(1)	32(1)	-1(1)	3(1)	5(1)
C(23)	32(1)	33(1)	34(1)	-1(1)	5(1)	5(1)
C(24)	44(1)	46(1)	37(1)	-2(1)	3(1)	-7(1)
C(25)	49(1)	51(1)	48(1)	-4(1)	7(1)	-13(1)
C(26)	55(1)	47(1)	51(1)	1(1)	19(1)	-10(1)
C(27)	55(1)	48(1)	34(1)	2(1)	11(1)	-1(1)
C(28)	36(1)	35(1)	34(1)	-1(1)	6(1)	5(1)
C(29)	32(1)	36(1)	36(1)	-2(1)	2(1)	5(1)
C(30)	43(1)	48(1)	31(1)	-2(1)	-2(1)	8(1)
C(31)	38(1)	45(1)	29(1)	-4(1)	-2(1)	2(1)
C(32)	46(1)	44(1)	50(1)	-2(1)	2(1)	-2(1)
C(33)	52(1)	45(1)	71(1)	-12(1)	-3(1)	6(1)
C(34)	48(1)	73(2)	62(1)	-23(1)	6(1)	11(1)
C(35)	56(1)	78(2)	44(1)	-4(1)	14(1)	-1(1)
C(36)	58(1)	48(1)	37(1)	-1(1)	4(1)	3(1)
N(1)	42(1)	41(1)	29(1)	-3(1)	2(1)	1(1)
O(1)	44(1)	50(1)	42(1)	-2(1)	-3(1)	-9(1)
O(2)	60(1)	42(1)	46(1)	-10(1)	8(1)	3(1)
O(3)	33(1)	54(1)	46(1)	4(1)	1(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 242.

	x	y	z	U(eq)
H(2)	10488	5579	1322	59
H(3)	10349	5747	-327	71
H(4)	9083	6641	-1007	76
H(5)	7963	7401	-72	68
H(8)	6882	8127	1337	69
H(9)	6265	8599	2750	78
H(10)	6982	8115	4195	70
H(11)	8279	7116	4266	57
H(17)	5828	6277	3062	55
H(18)	3735	6762	2560	70
H(19)	2816	6598	1014	84

H(20)	3957	5932	-26	95
H(21)	6010	5413	485	71
H(24)	6252	4531	3020	51
H(25)	5047	3752	3876	59
H(26)	5403	3689	5507	60
H(27)	6947	4421	6348	55
H(30A)	9837	5727	6570	49
H(30B)	9091	5049	6832	49
H(32)	8291	6819	6449	56
H(33)	6740	7440	7265	68
H(34)	5448	6904	8347	73
H(35)	5728	5748	8641	70
H(36)	7282	5125	7839	58
H(3A)	10470(30)	6370(12)	3802(19)	85(8)

Table 6. Torsion angles [°] for 242.

C(6)-C(1)-C(2)-C(3)	-1.1(3)
C(13)-C(1)-C(2)-C(3)	178.21(17)
C(1)-C(2)-C(3)-C(4)	0.0(3)
C(2)-C(3)-C(4)-C(5)	0.8(3)
C(3)-C(4)-C(5)-C(6)	-0.4(3)
C(4)-C(5)-C(6)-C(1)	-0.7(3)
C(4)-C(5)-C(6)-C(7)	178.86(18)
C(2)-C(1)-C(6)-C(5)	1.5(3)
C(13)-C(1)-C(6)-C(5)	-177.97(15)
C(2)-C(1)-C(6)-C(7)	-178.17(15)
C(13)-C(1)-C(6)-C(7)	2.41(19)
C(5)-C(6)-C(7)-C(8)	0.3(3)
C(1)-C(6)-C(7)-C(8)	179.88(18)
C(5)-C(6)-C(7)-C(12)	-178.74(18)
C(1)-C(6)-C(7)-C(12)	0.83(19)
C(12)-C(7)-C(8)-C(9)	1.0(3)
C(6)-C(7)-C(8)-C(9)	-177.98(19)
C(7)-C(8)-C(9)-C(10)	0.0(3)
C(8)-C(9)-C(10)-C(11)	-1.2(3)
C(9)-C(10)-C(11)-C(12)	1.3(3)
C(10)-C(11)-C(12)-C(7)	-0.2(3)

C(10)-C(11)-C(12)-C(13)	-177.82(17)
C(8)-C(7)-C(12)-C(11)	-0.9(3)
C(6)-C(7)-C(12)-C(11)	178.30(16)
C(8)-C(7)-C(12)-C(13)	177.13(15)
C(6)-C(7)-C(12)-C(13)	-3.70(18)
C(2)-C(1)-C(13)-O(3)	54.8(2)
C(6)-C(1)-C(13)-O(3)	-125.81(15)
C(2)-C(1)-C(13)-C(12)	176.32(17)
C(6)-C(1)-C(13)-C(12)	-4.31(17)
C(2)-C(1)-C(13)-C(14)	-69.6(2)
C(6)-C(1)-C(13)-C(14)	109.81(15)
C(11)-C(12)-C(13)-O(3)	-61.2(2)
C(7)-C(12)-C(13)-O(3)	120.98(16)
C(11)-C(12)-C(13)-C(1)	-177.42(17)
C(7)-C(12)-C(13)-C(1)	4.80(17)
C(11)-C(12)-C(13)-C(14)	65.6(2)
C(7)-C(12)-C(13)-C(14)	-112.15(15)
O(3)-C(13)-C(14)-C(22)	44.0(2)
C(1)-C(13)-C(14)-C(22)	165.52(15)
C(12)-C(13)-C(14)-C(22)	-84.37(19)
O(3)-C(13)-C(14)-C(15)	-137.48(14)
C(1)-C(13)-C(14)-C(15)	-15.91(18)
C(12)-C(13)-C(14)-C(15)	94.20(15)
C(22)-C(14)-C(15)-O(2)	-84.13(19)
C(13)-C(14)-C(15)-O(2)	97.16(17)
C(22)-C(14)-C(15)-C(16)	97.64(17)
C(13)-C(14)-C(15)-C(16)	-81.07(17)
O(2)-C(15)-C(16)-C(21)	-21.6(2)
C(14)-C(15)-C(16)-C(21)	156.58(16)
O(2)-C(15)-C(16)-C(17)	157.52(17)
C(14)-C(15)-C(16)-C(17)	-24.3(2)
C(21)-C(16)-C(17)-C(18)	1.2(3)
C(15)-C(16)-C(17)-C(18)	-177.94(17)
C(16)-C(17)-C(18)-C(19)	-1.5(3)
C(17)-C(18)-C(19)-C(20)	0.7(4)
C(18)-C(19)-C(20)-C(21)	0.6(4)
C(19)-C(20)-C(21)-C(16)	-0.9(4)
C(17)-C(16)-C(21)-C(20)	0.1(3)

C(15)-C(16)-C(21)-C(20)	179.2(2)
C(15)-C(14)-C(22)-C(23)	-3.3(2)
C(13)-C(14)-C(22)-C(23)	175.18(14)
C(15)-C(14)-C(22)-C(29)	-179.01(14)
C(13)-C(14)-C(22)-C(29)	-0.5(3)
C(14)-C(22)-C(23)-C(24)	5.3(3)
C(29)-C(22)-C(23)-C(24)	-178.22(17)
C(14)-C(22)-C(23)-C(28)	-174.45(15)
C(29)-C(22)-C(23)-C(28)	1.99(16)
C(28)-C(23)-C(24)-C(25)	0.2(2)
C(22)-C(23)-C(24)-C(25)	-179.55(17)
C(23)-C(24)-C(25)-C(26)	-0.6(3)
C(24)-C(25)-C(26)-C(27)	0.7(3)
C(25)-C(26)-C(27)-C(28)	-0.3(3)
C(26)-C(27)-C(28)-C(23)	-0.1(3)
C(26)-C(27)-C(28)-N(1)	-178.73(16)
C(24)-C(23)-C(28)-C(27)	0.1(2)
C(22)-C(23)-C(28)-C(27)	179.96(15)
C(24)-C(23)-C(28)-N(1)	179.00(14)
C(22)-C(23)-C(28)-N(1)	-1.17(17)
C(14)-C(22)-C(29)-O(1)	-4.7(3)
C(23)-C(22)-C(29)-O(1)	178.84(16)
C(14)-C(22)-C(29)-N(1)	174.36(15)
C(23)-C(22)-C(29)-N(1)	-2.15(16)
N(1)-C(30)-C(31)-C(36)	108.26(18)
N(1)-C(30)-C(31)-C(32)	-71.5(2)
C(36)-C(31)-C(32)-C(33)	-0.1(3)
C(30)-C(31)-C(32)-C(33)	179.63(16)
C(31)-C(32)-C(33)-C(34)	-0.4(3)
C(32)-C(33)-C(34)-C(35)	0.6(3)
C(33)-C(34)-C(35)-C(36)	-0.4(3)
C(34)-C(35)-C(36)-C(31)	-0.1(3)
C(32)-C(31)-C(36)-C(35)	0.3(3)
C(30)-C(31)-C(36)-C(35)	-179.42(17)
O(1)-C(29)-N(1)-C(28)	-179.39(15)
C(22)-C(29)-N(1)-C(28)	1.53(17)
O(1)-C(29)-N(1)-C(30)	0.9(2)
C(22)-C(29)-N(1)-C(30)	-178.18(13)

C(27)-C(28)-N(1)-C(29)	178.53(16)
C(23)-C(28)-N(1)-C(29)	-0.26(18)
C(27)-C(28)-N(1)-C(30)	-1.8(3)
C(23)-C(28)-N(1)-C(30)	179.45(14)
C(31)-C(30)-N(1)-C(29)	101.89(18)
C(31)-C(30)-N(1)-C(28)	-77.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 242 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3A)...O(1)	0.96(3)	1.72(3)	2.6474(18)	161(2)

Symmetry transformations used to generate equivalent atoms: