

L-proline-promoted three-component reaction of anilines, aldehydes and barbituric acids/malononitrile: Regioselective synthesis of 5-arylpyrimido[4,5-b]quinoline-diones and 2-amino-4-arylquinoline-3-carbonitriles in water

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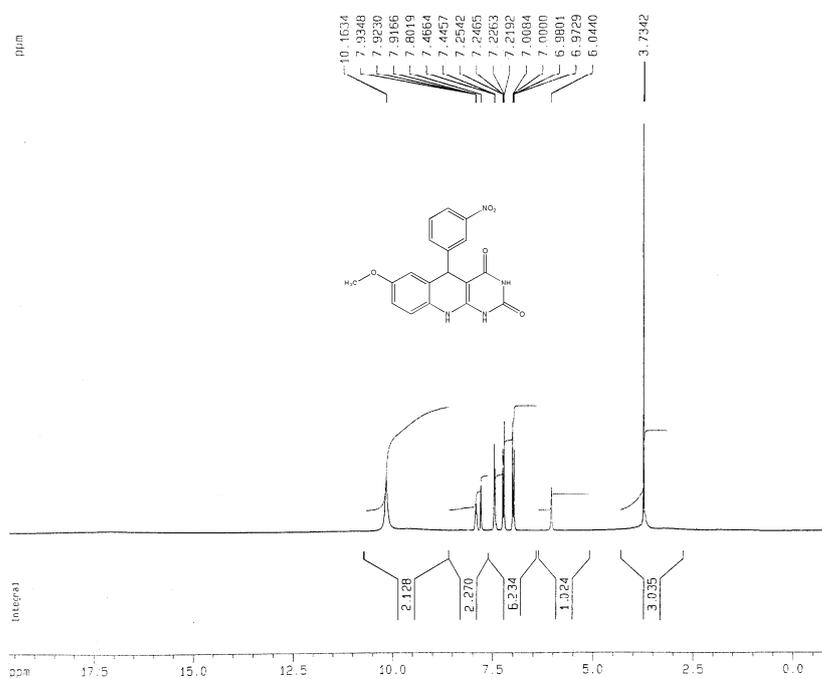
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Copy of ¹H NMR and ¹³C NMR of synthesized compounds:

1. Compound 4a:



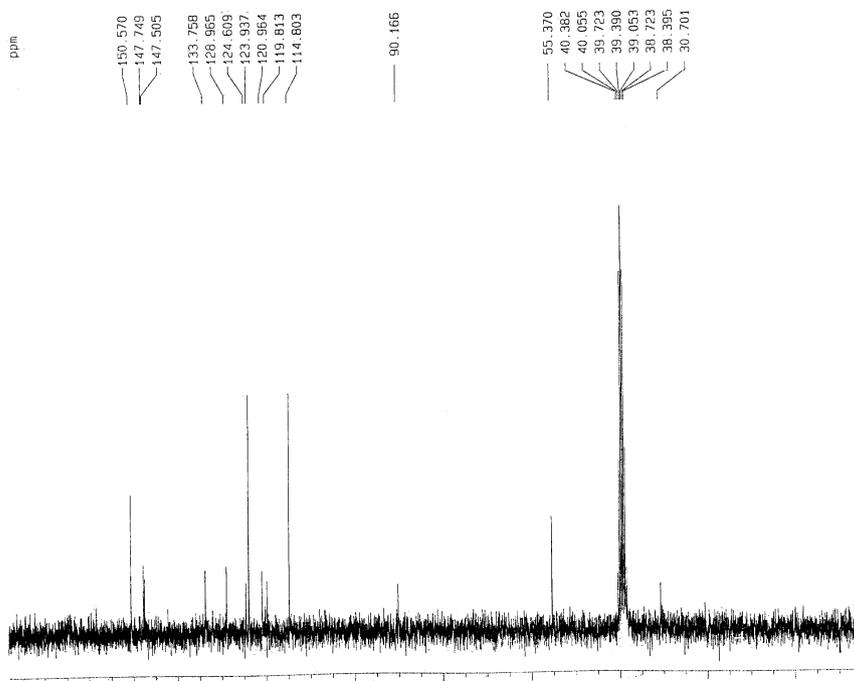
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 10.28
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zg
TD 31054
SOLVENT DMSO
NS 10
DS 0
SWH 7485.030 Hz
FIDRES 0.241033 Hz
AQ 2.0744572 sec
RG 181
DM 66.800 usec
DE 6.00 usec
TE 0.0 K
D1 2.0000000 sec
MCREST 0.0000000 sec
MCNKR 0.0150000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.70 usec
PL1 -3.00 dB
SFO1 250.1315447 MHz

F2 - Processing parameters
SI 32768
SF 250.1300000 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.50

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 19.644 ppm
F1 4913.45 Hz
F2P -0.975 ppm
F2 -243.85 Hz
PPMCM 1.03092 ppm/cm
HZCM 257.66517 Hz/cm
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Current Data Parameters
NAME sarikhani-C-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110201
Time 9.46
INSTRUM spect
PROBHD 5 mm Dual 13C/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 10
DS 0
SWH 10050.241 Hz
FIDRES 0.324241 Hz
AQ 1.2989623 sec
RG 32768
DM 33.200 usec
DE 6.00 usec
TE 0.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8950998 sec
MCREST 0.0000000 sec
MCNKR 0.0150000 sec

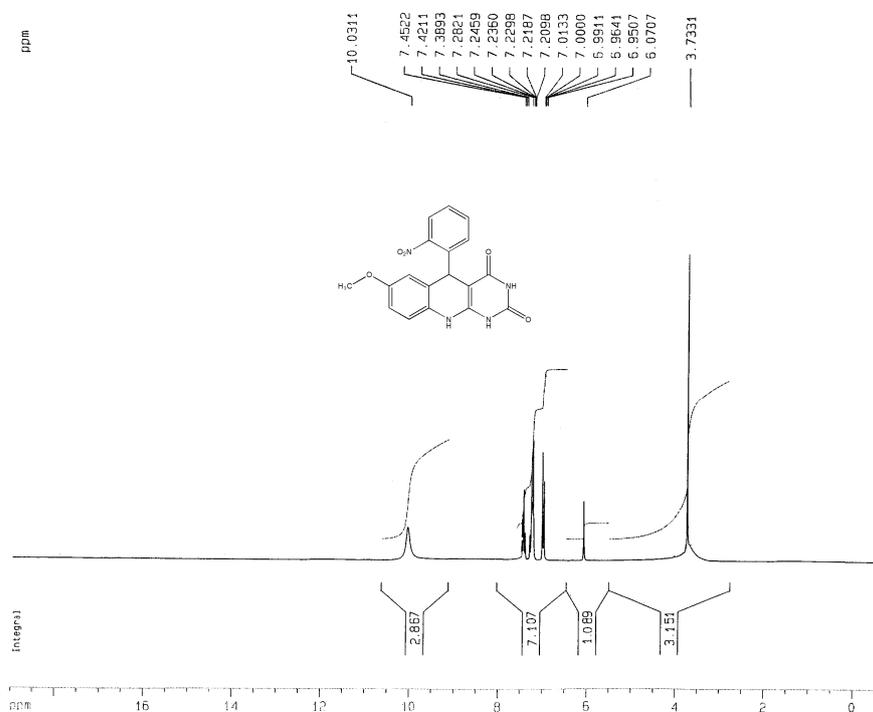
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NUC1 13C
P1 10.20 usec
PL1 -1.00 dB
SFO1 62.9015230 MHz

===== CHANNEL f2 =====
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NUC2 1H
PCPD2 97.00 usec
PL2 -3.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 250.1310005 MHz

F2 - Processing parameters
SI 32768
SF 62.8952704 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 170.627 ppm
F1 11205.65 Hz
F2P -14.767 ppm
F2 -928.77 Hz
PPMCM 5.61271 ppm/cm
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2. Compound 4b:



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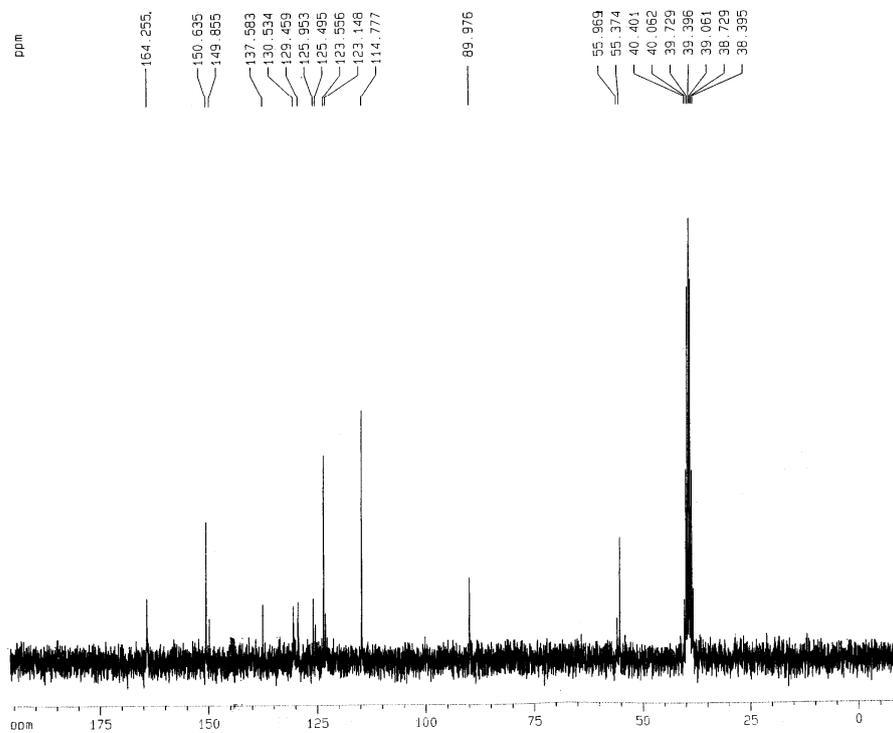
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EXPNO    1
PROCNO   1

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Date_    20110102
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INSTRUM  spect
PROBHD   5 mm Dual 13C/
PULPROG  zgpg
TD        31054
SOLVENT  DMSO
NS        10
DS        0
SWH       7485.030 Hz
FIDRES    0.241033 Hz
AQ        2.0744572 sec
RG        143.7
DW        66.800 usec
DE        6.00 usec
TE        0.0 K
D1        2.0000000 sec
MCREST    0.0000000 sec
MCWRK    0.0150000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        11.70 usec
PL1       3.00 dB
SFO1      250.1315447 MHz

F2 - Processing parameters
SI        32768
SF        250.1300000 MHz
WDW       EM
SSB       0
LB        0.00 Hz
GB        0
PC        1.50

1D NMR plot parameters
CX        20.00 cm
CY        10.00 cm
F1P       19.003 ppm
F1        4753.29 Hz
F2P       -0.719 ppm
F2        -179.78 Hz
PPMCM     0.98610 ppm/cm
HZCM      246.65364 Hz/cm
    
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Current Data Parameters
NAME      Sarikhani-C 1
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20110103
Time     9.22
INSTRUM  spect
PROBHD   5 mm Dual 13C/
PULPROG  zgpg
TD        39154
SOLVENT  DMSO
NS        100
DS        0
SWH       15060.241 Hz
FIDRES    0.384641 Hz
AQ        1.2999628 sec
RG        32768
DW        33.200 usec
DE        6.00 usec
TE        0.0 K
D1        2.0000000 sec
d11       0.0300000 sec
DELTA     1.89999998 sec
MCREST    0.0000000 sec
MCWRK    0.0150000 sec

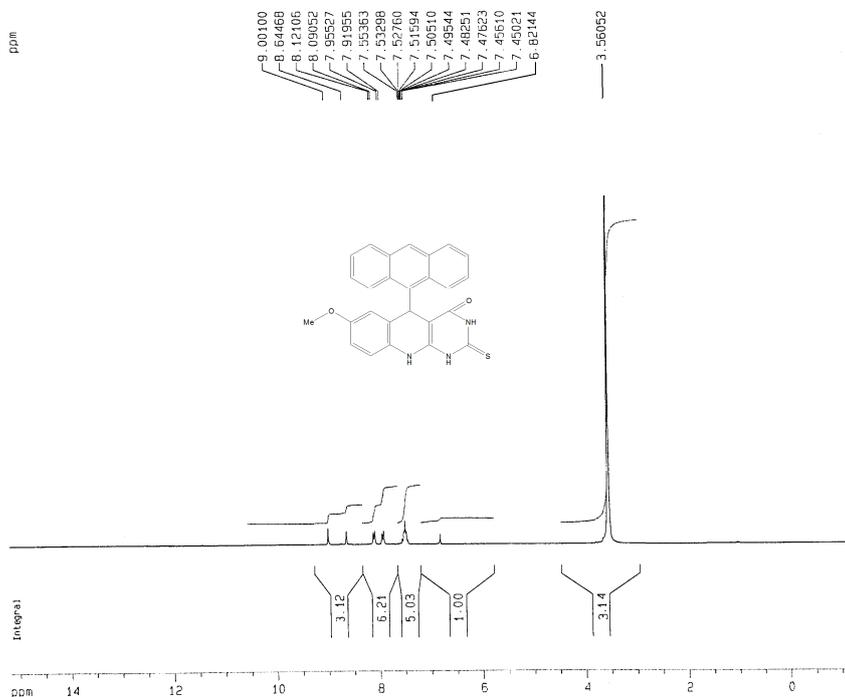
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NUC1      13C
P1        10.50 usec
PL1       -1.00 dB
SFO1      62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2      1H
PCPD2    97.00 usec
PL2       -3.00 dB
PL12     17.00 dB
PL13     17.00 dB
SFO2     250.1310005 MHz

F2 - Processing parameters
SI        32768
SF        62.8993704 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

1D NMR plot parameters
CX        20.00 cm
CY        10.00 cm
F1P       195.990 ppm
F1        12326.82 Hz
F2P       -9.985 ppm
F2        -628.00 Hz
PPMCM     10.29872 ppm/cm
HZCM      647.74078 Hz/cm
    
```

3. Compound 4c:



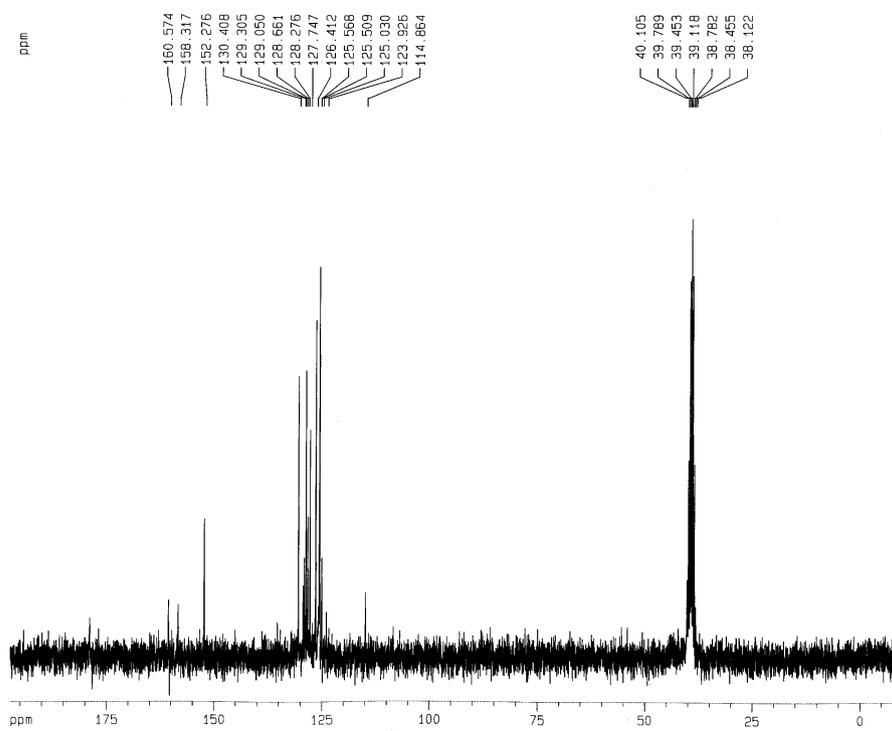
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 NAME Sarikhani-H-8
 EXPNO 1
 PROCNO 1

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 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zg
 TD 31054
 SOLVENT DMSO
 NS 10
 DS 0
 SWH 7485.030 Hz
 FIDRES 0.241033 Hz
 AQ 2.0744572 sec
 RG 128
 DW 66.800 usec
 DE 6.00 usec
 TE 0.0 K
 D1 2.00000000 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

***** CHANNEL f1 *****
 NUC1 1H
 P1 11.70 usec
 PL1 -3.00 dB
 SFO1 250.1315447 MHz

F2 - Processing parameters
 SI 32768
 SF 250.1300000 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.50

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 15.204 ppm
 F1 3682.58 Hz
 F2P -1.231 ppm
 F2 -307.92 Hz
 PPMCM 0.82175 ppm/cm
 HZCM 205.54469 Hz/cm



Current Data Parameters
 NAME Sarikhani-C-8
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20110726
 Time 9.34
 INSTRUM spect
 PROBHD 5 mm Dual 13C/
 PULPROG zgpg
 TD 39154
 SOLVENT DMSO
 NS 100
 DS 0
 SWH 15060.241 Hz
 FIDRES 0.384541 Hz
 AQ 1.2395628 sec
 RG 32768
 DW 33.800 usec
 DE 6.00 usec
 TE 0.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 MCREST 0.00000000 sec
 MCWRR 0.01500000 sec

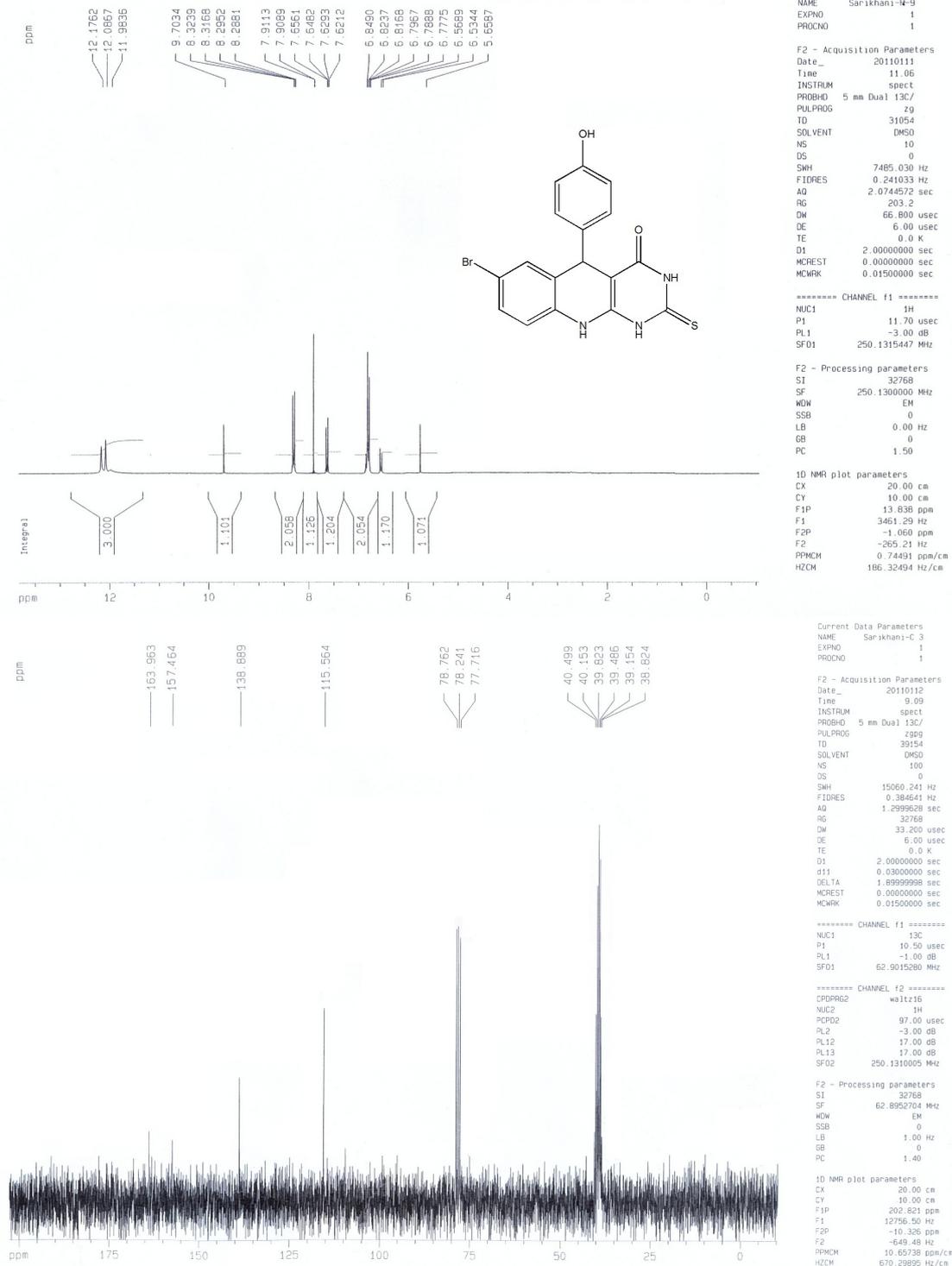
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 NUC1 13C
 P1 10.50 usec
 PL1 -1.00 dB
 SFO1 62.9015280 MHz

***** CHANNEL f2 *****
 CPDPRG2 waltz16
 NUC2 1H
 PPRG2 97.00 usec
 PL2 -3.00 dB
 PL12 17.00 dB
 PL13 17.00 dB
 SFO2 250.1310005 MHz

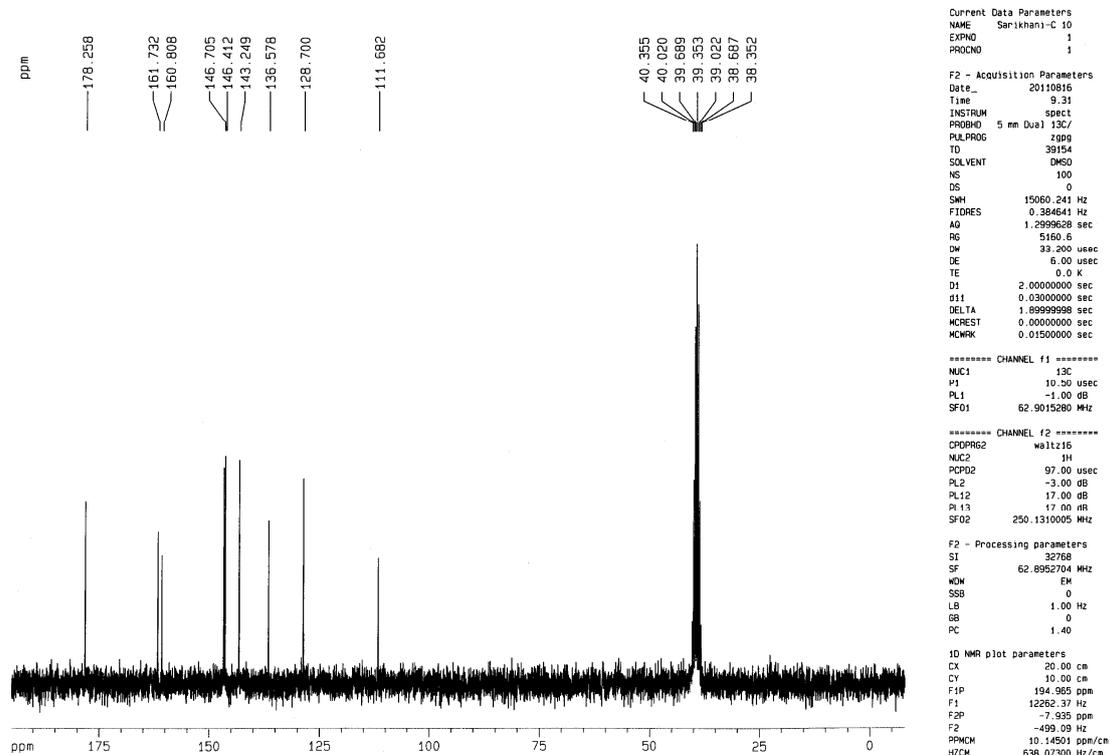
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 SF 62.8952704 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 157.256 ppm
 F1 12412.75 Hz
 F2P -9.302 ppm
 F2 -585.03 Hz
 PPMCM 10.32288 ppm/cm
 HZCM 649.88916 Hz/cm

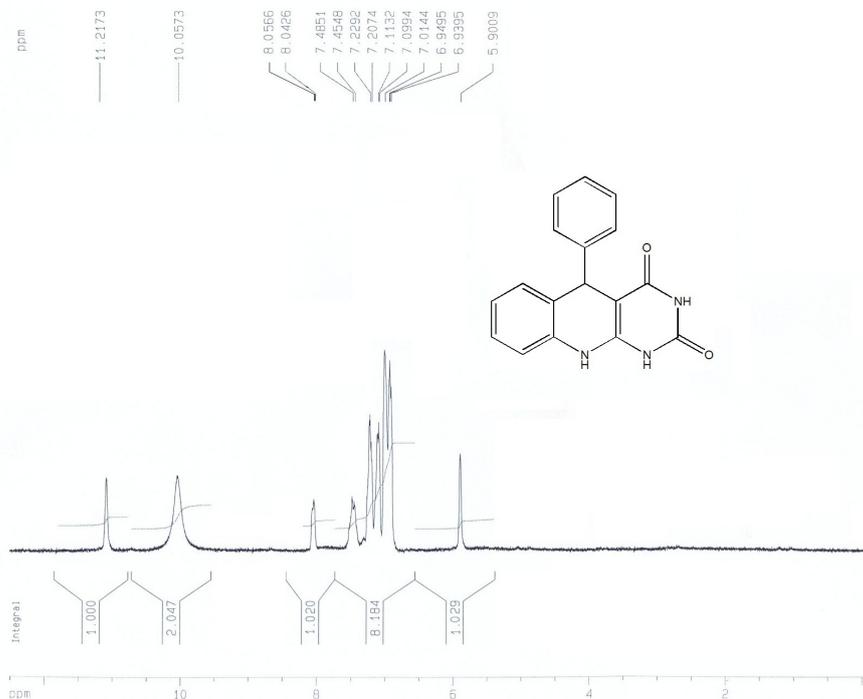
4. Compound 4d:



5. Compound 4e:



6. Compound 4f:



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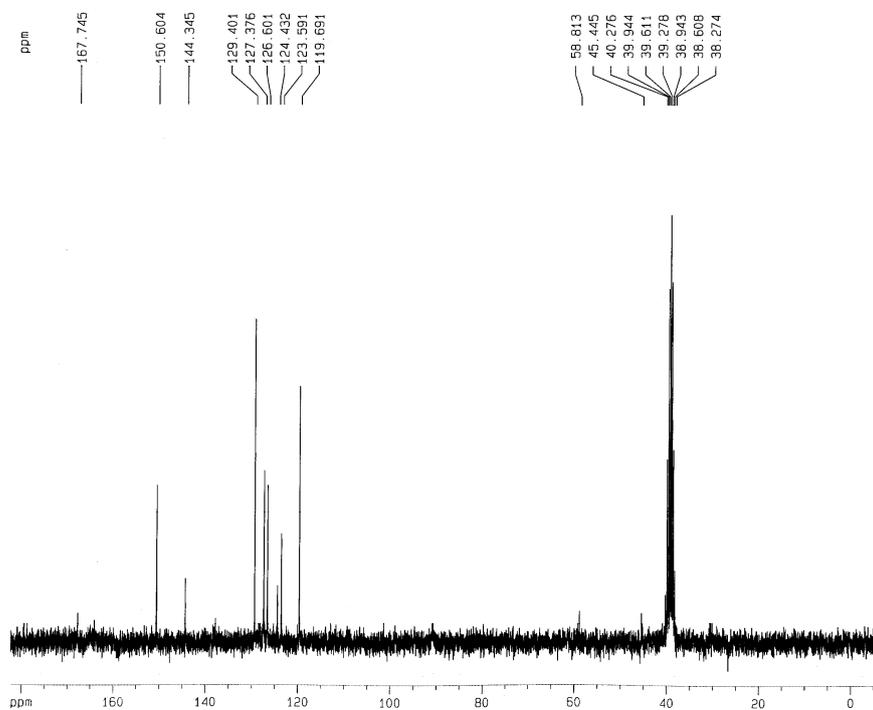
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EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
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Time     10.25
INSTRUM  spect
PROBHD   5 mm Dual 13C/
PULPROG  zg
TD       31054
SOLVENT  DMSO
NS       10
DS       0
SWH      7485.030 Hz
FIDRES   0.241033 Hz
AQ       2.0744572 sec
RG       256
DW       66.800 usec
DE       6.00 usec
TE       0.0 K
D1       2.0000000 sec
MCREST   0.0000000 sec
MCWRK    0.0150000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       11.70 usec
PL1      -3.00 dB
SFO1     250.1315447 MHz

F2 - Processing parameters
SI       32768
SF       250.1300000 MHz
WDW      EM
SSB      0
LB       0.00 Hz
GB       0
PC       1.50

1D NMR plot parameters
CX       20.00 cm
CY       10.00 cm
F1P      12.515 ppm
F1       3130.29 Hz
F2P      -0.121 ppm
F2       -30.30 Hz
PPMCH    0.63179 ppm/cm
HZCM     150.02917 Hz/cm
    
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Current Data Parameters
NAME      Sarikhani-C 11
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20110420
Time     11.49
INSTRUM  spect
PROBHD   5 mm Dual 13C/
PULPROG  zgpg30
TD       39154
SOLVENT  DMSO
NS       100
DS       0
SWH      15060.244 Hz
FIDRES   0.384641 Hz
AQ       1.2999628 sec
RG       1448.2
DW       33.200 usec
DE       6.00 usec
TE       0.0 K
D1       2.0000000 sec
e11      0.0300000 sec
DELTA    1.8999998 sec
MCREST   0.0000000 sec
MCWRK    0.0150000 sec

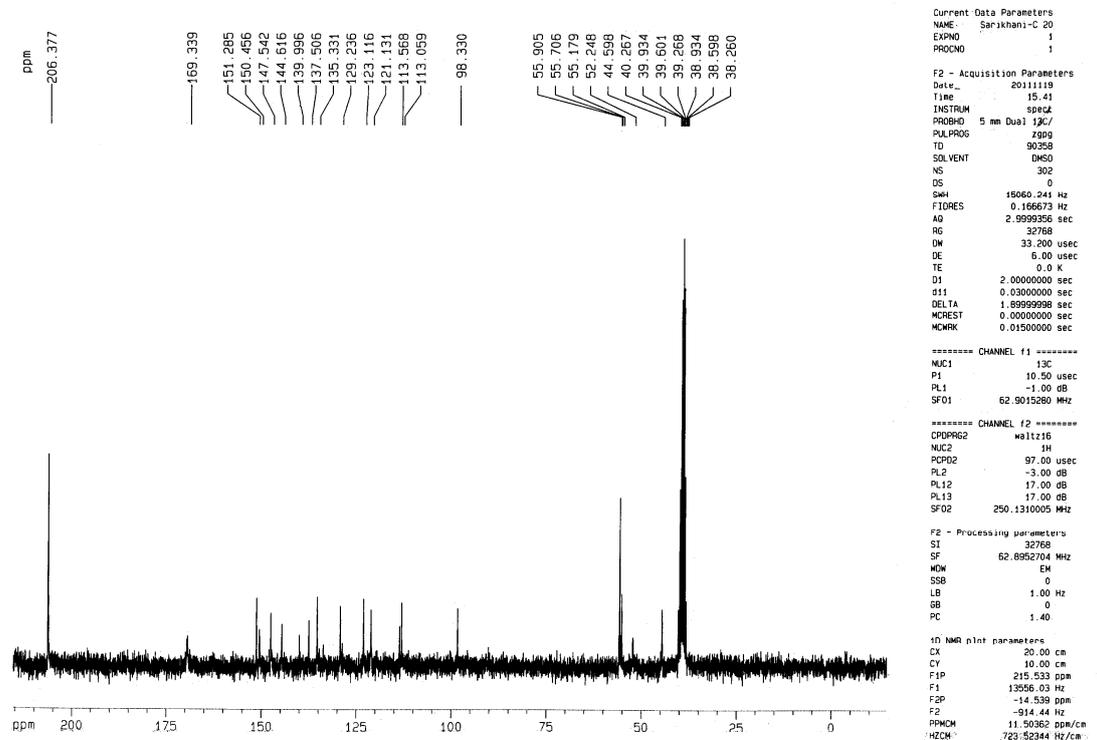
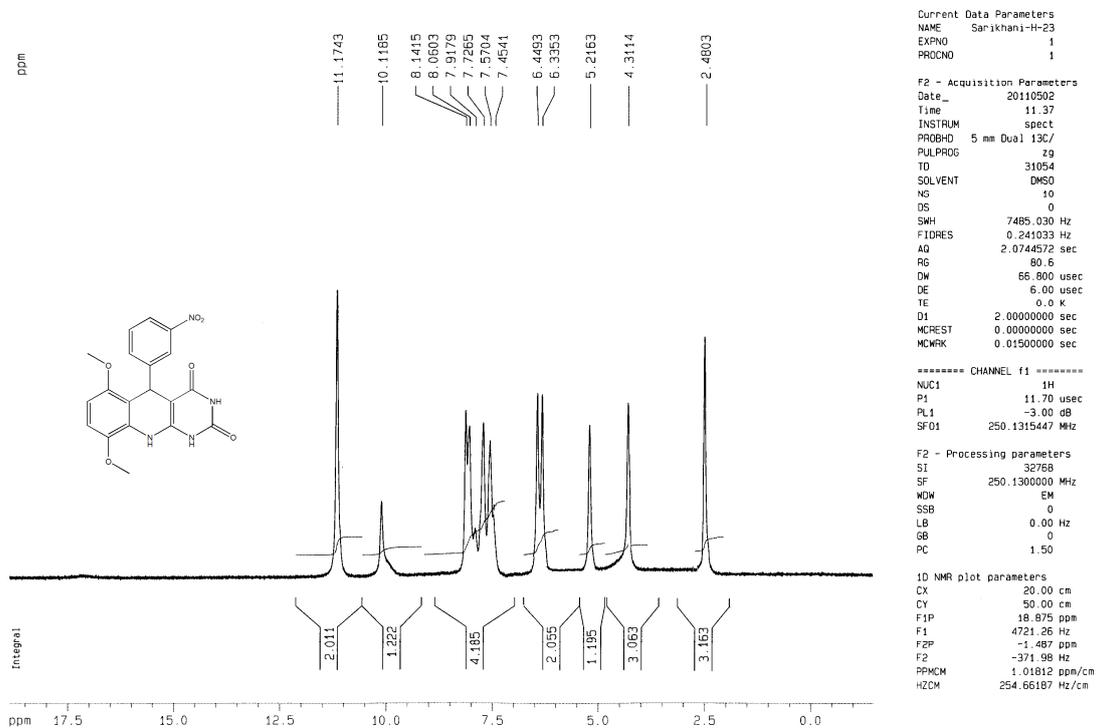
===== CHANNEL f1 =====
NUC1     13C
P1       10.50 usec
PL1      -1.00 dB
SFO1     62.9015280 MHz

===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     1H
PCPD2    97.00 usec
PL2      -3.00 dB
PL12     17.00 dB
PL13     17.00 dB
SFO2     250.1310005 MHz

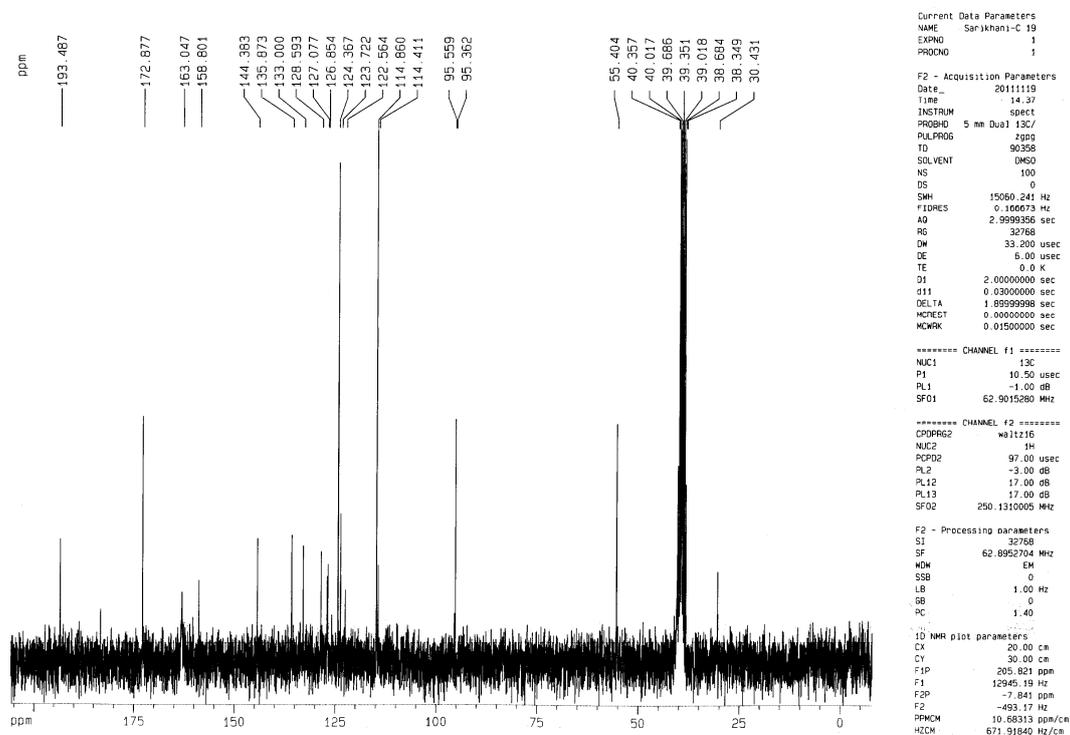
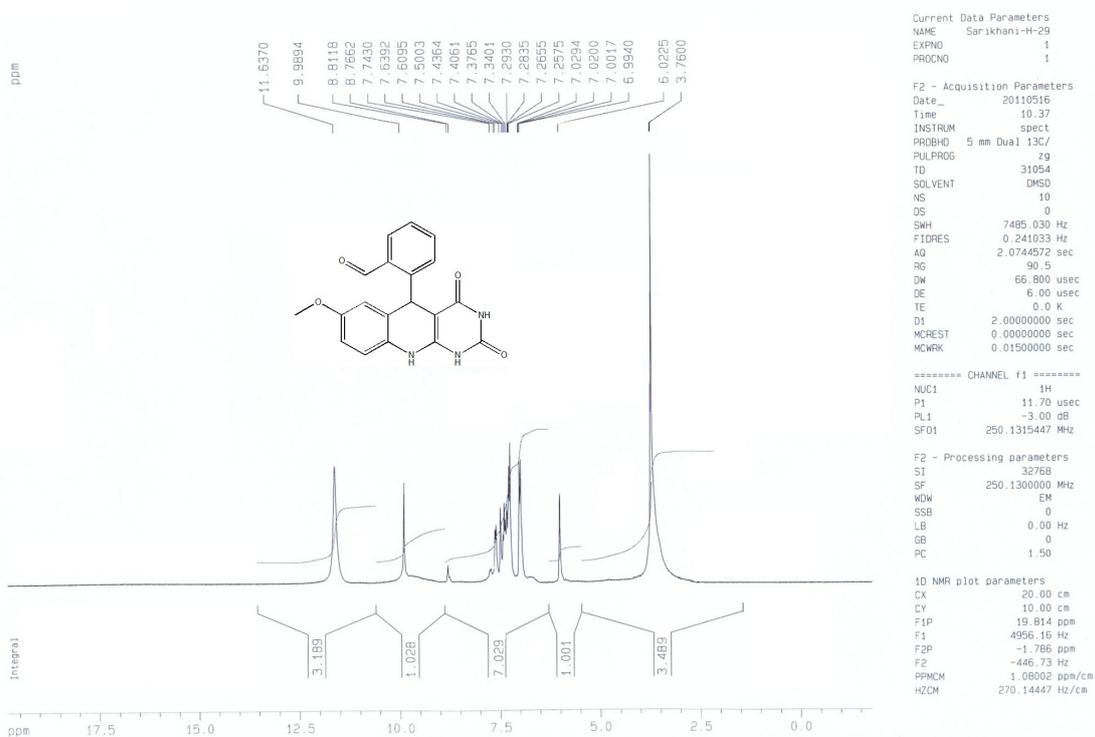
F2 - Processing parameters
SI       32768
SF       62.8952704 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40

1D NMR plot parameters
CX       20.00 cm
CY       10.00 cm
F1P      182.326 ppm
F1       11467.46 Hz
F2P      -6.227 ppm
F2       -391.67 Hz
PPMCH    9.42768 ppm/cm
HZCM     592.95673 Hz/cm
    
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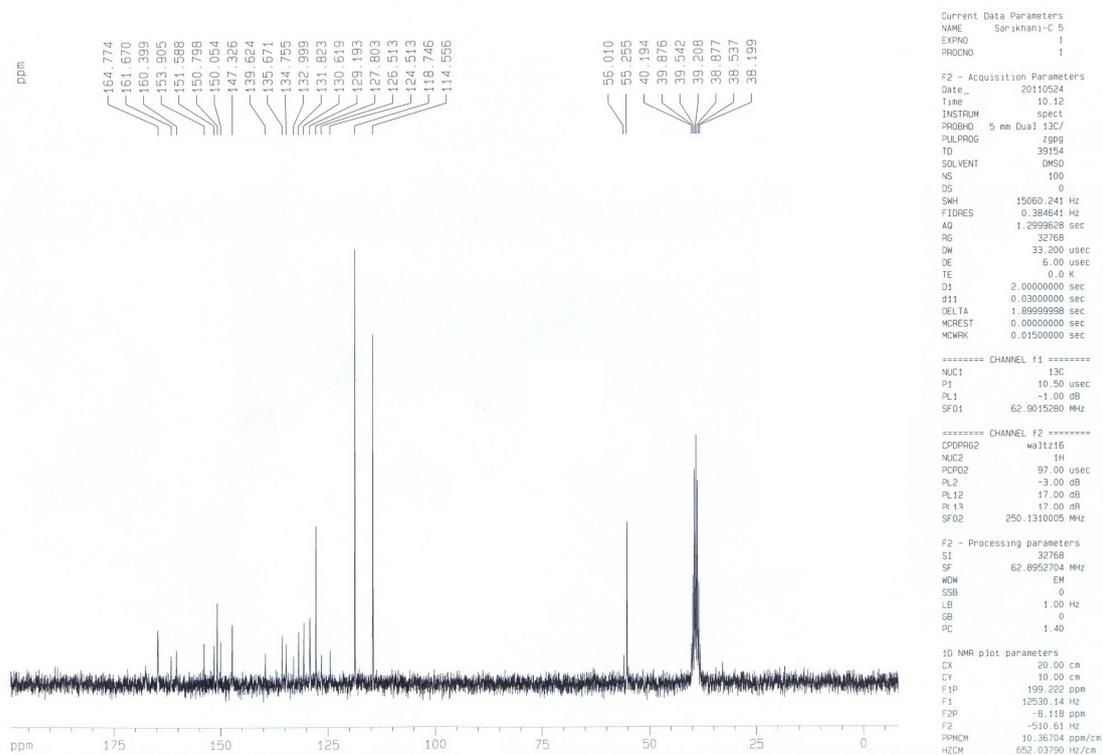
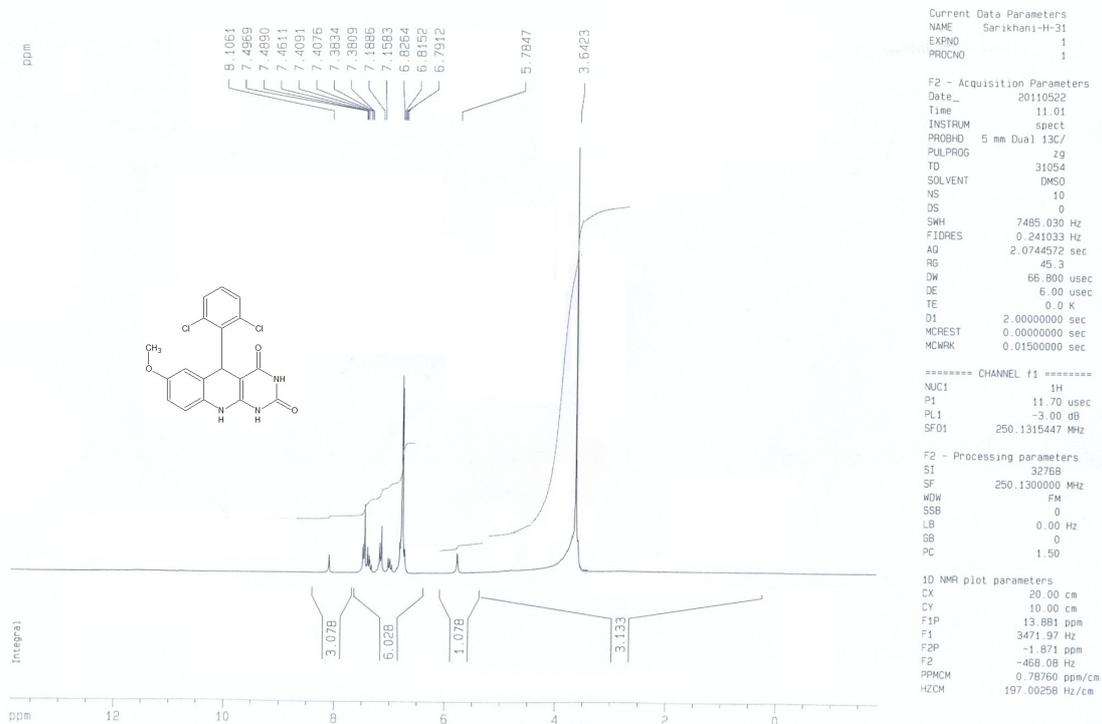
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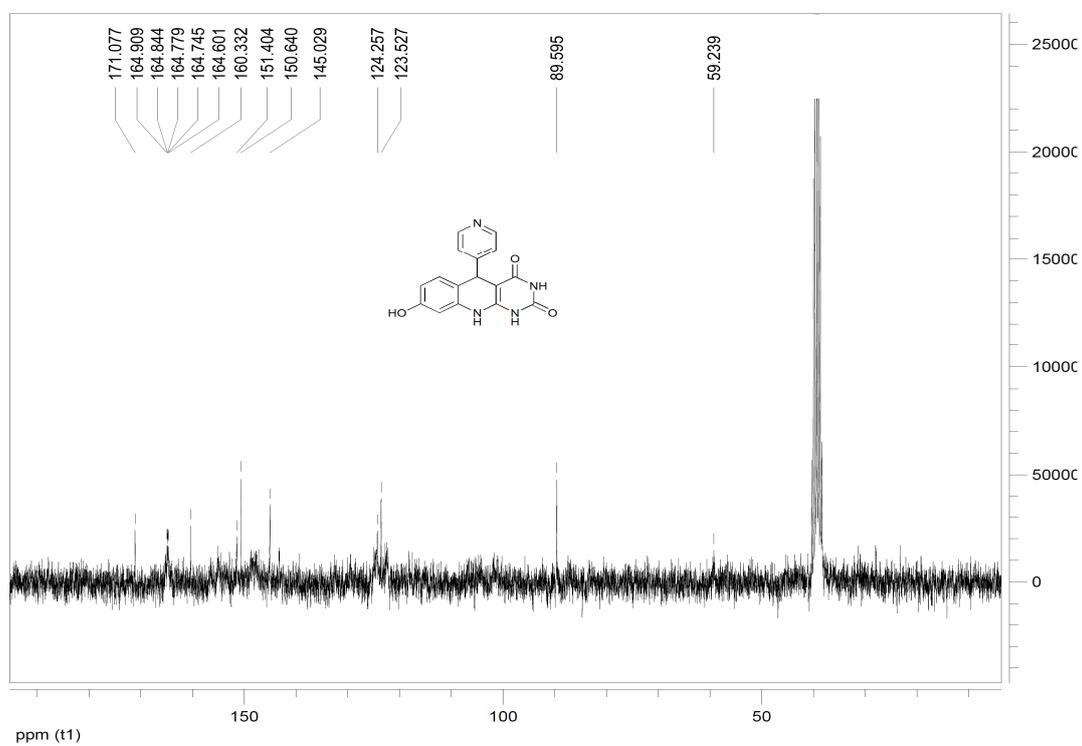
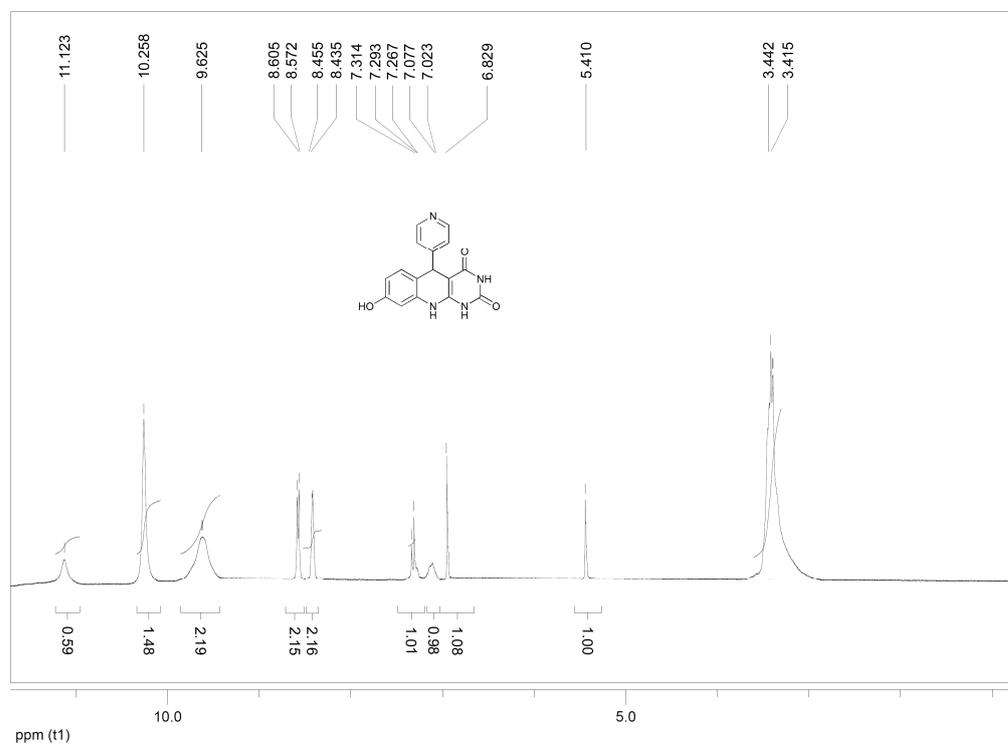
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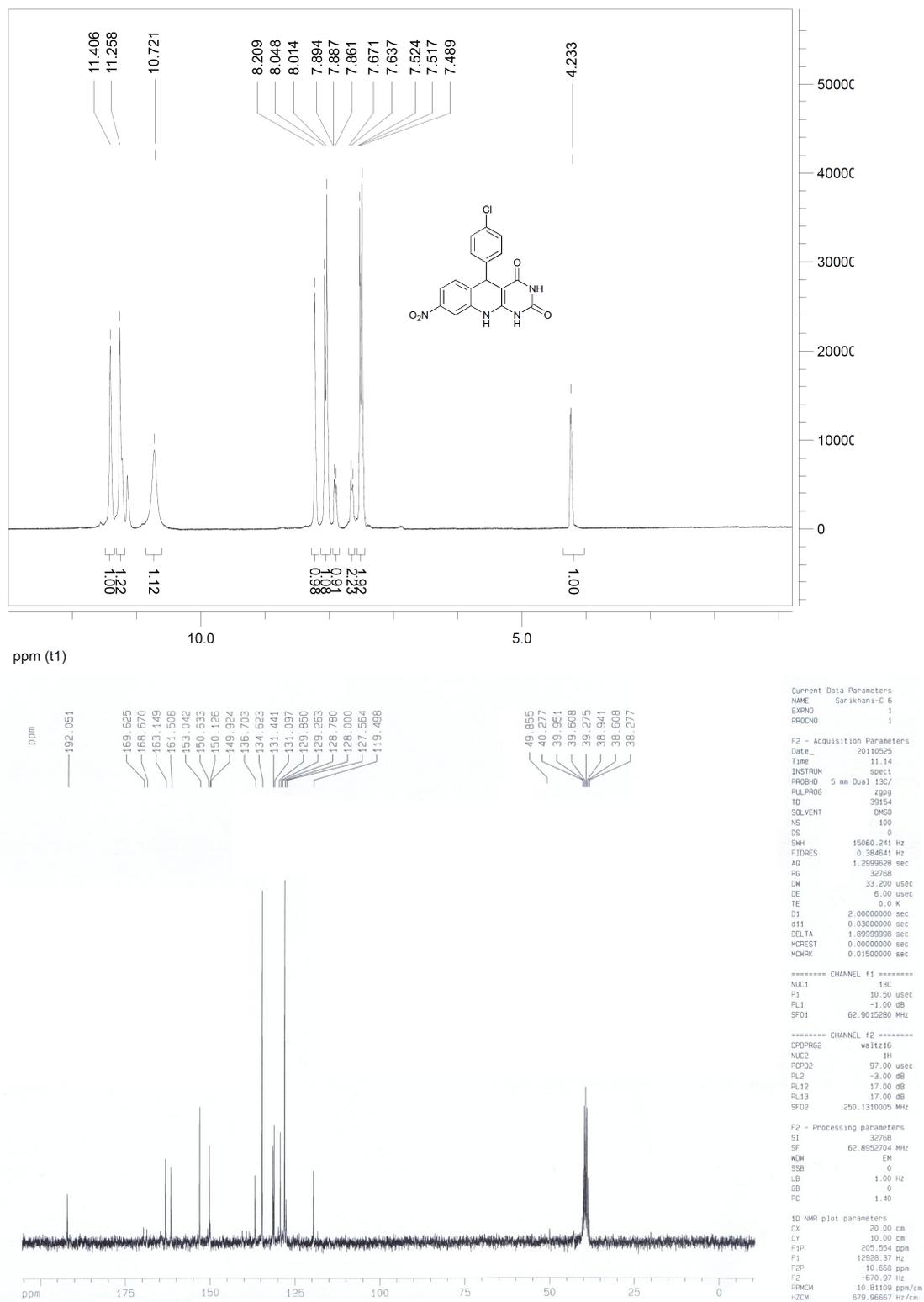
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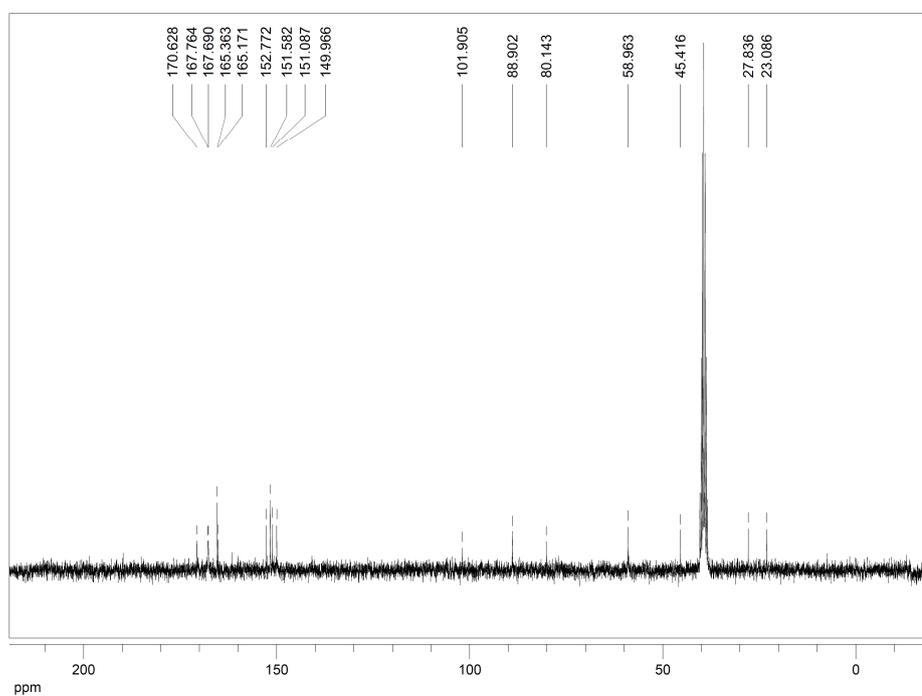
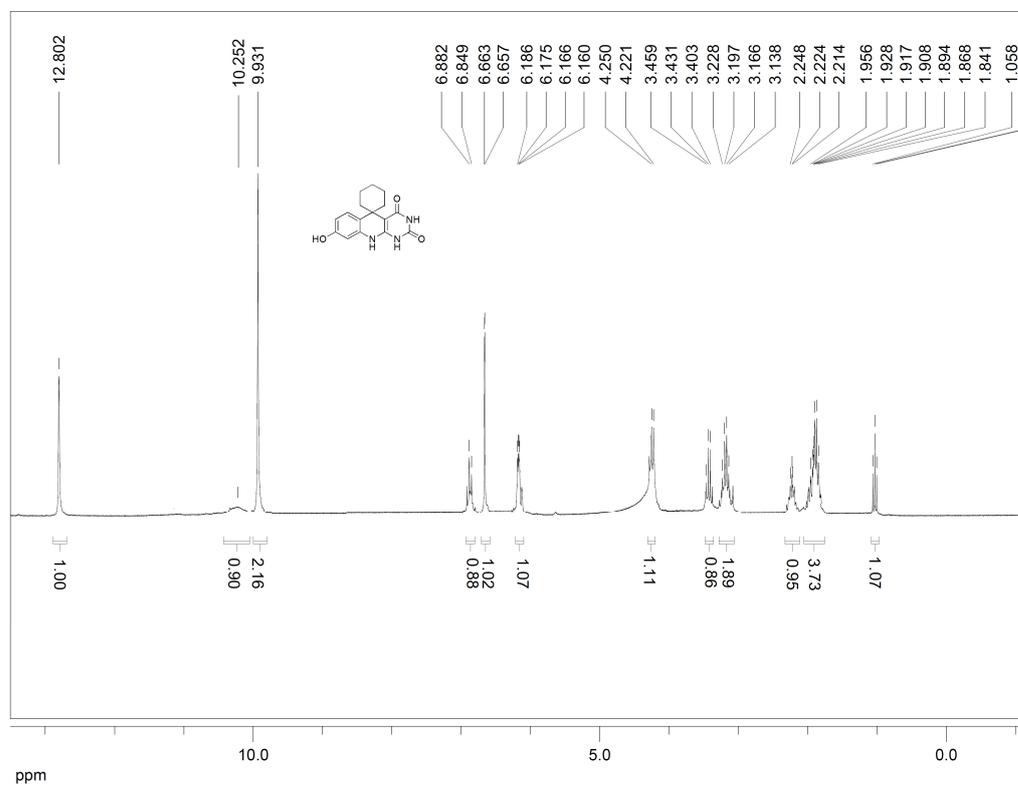
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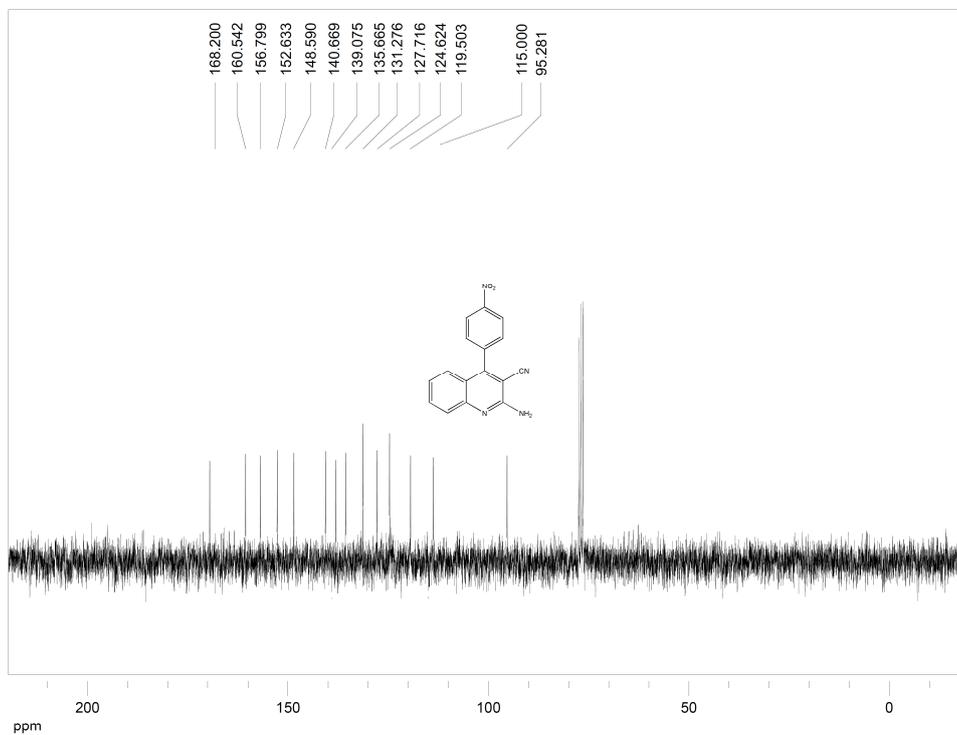
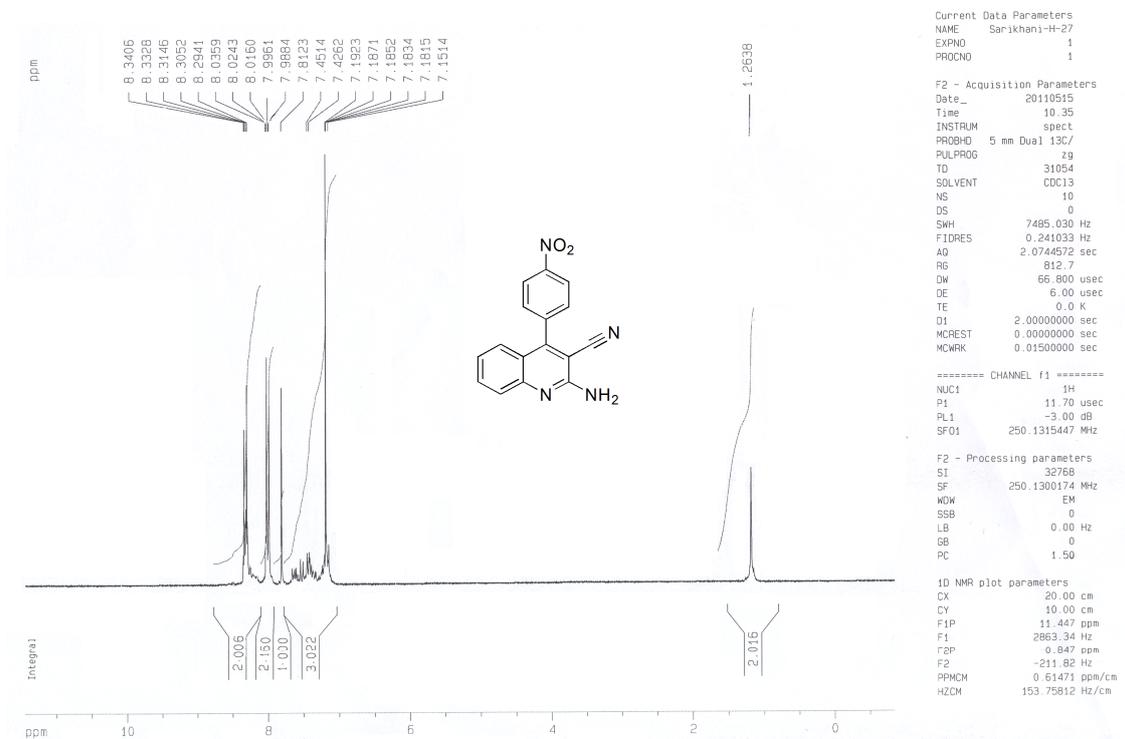
11. Compound 4k:



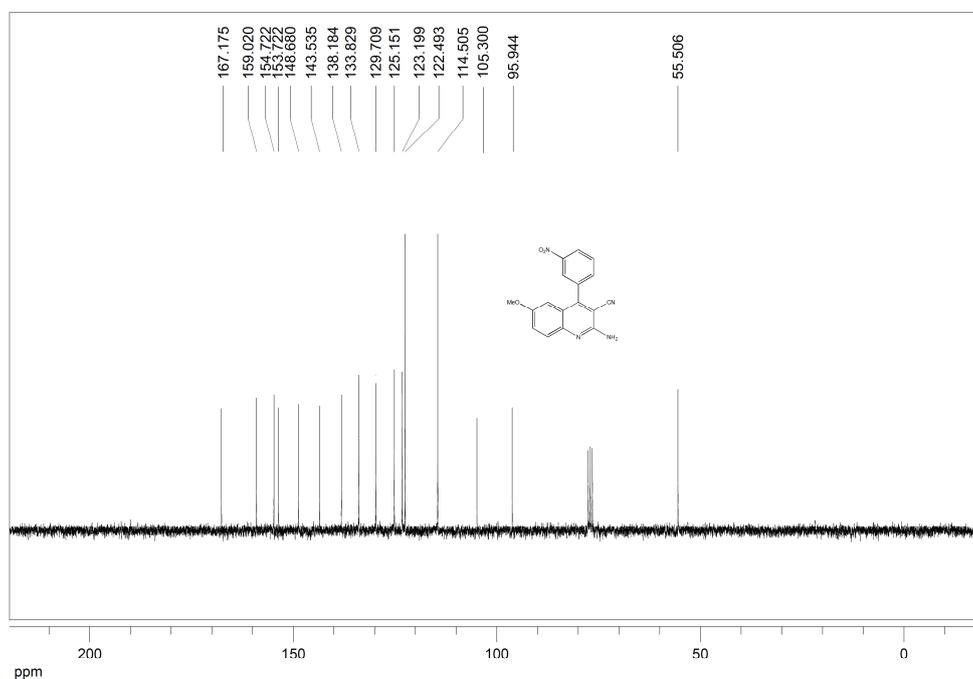
12. Compound 41:



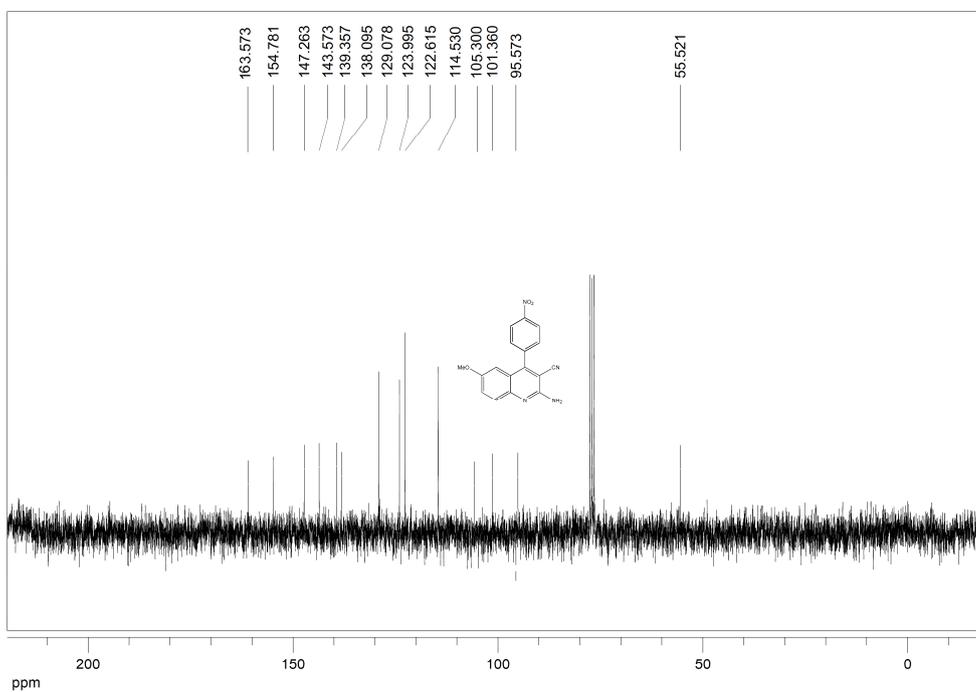
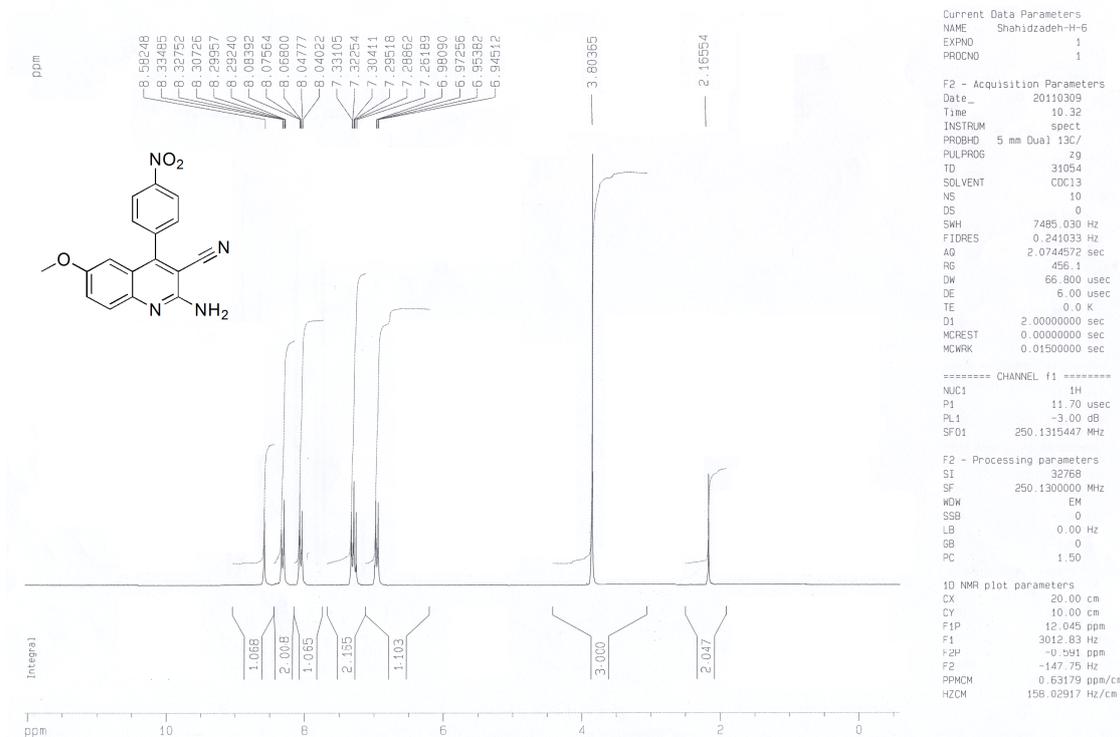
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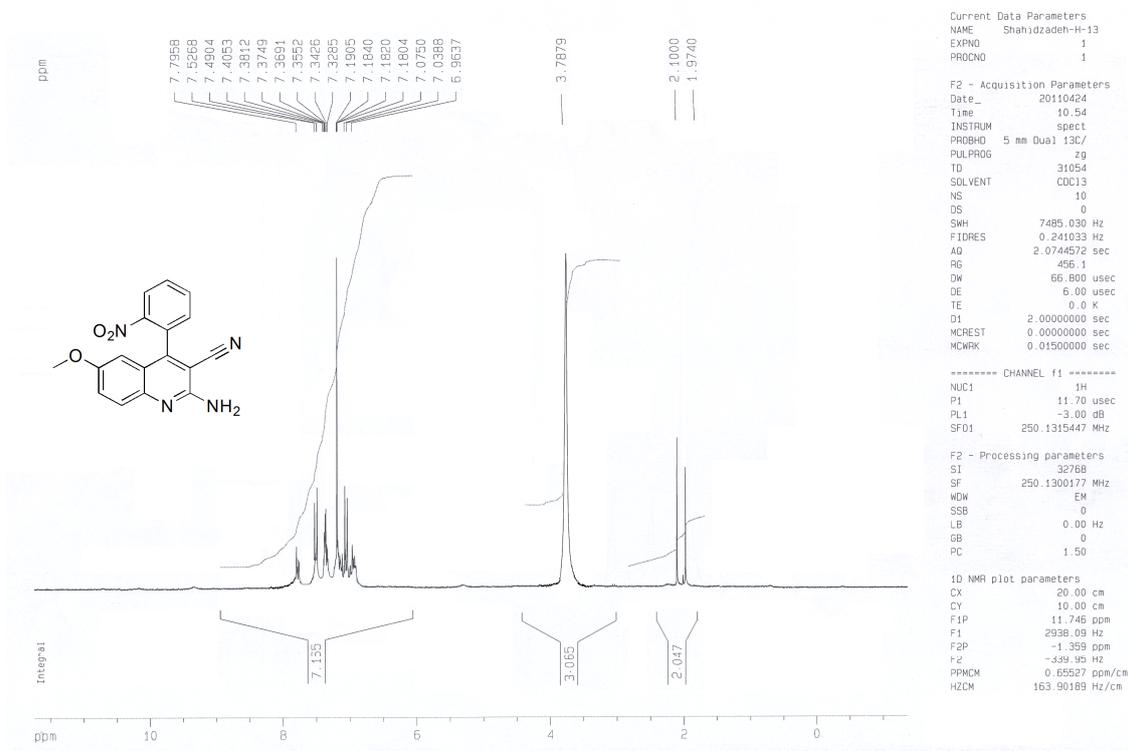
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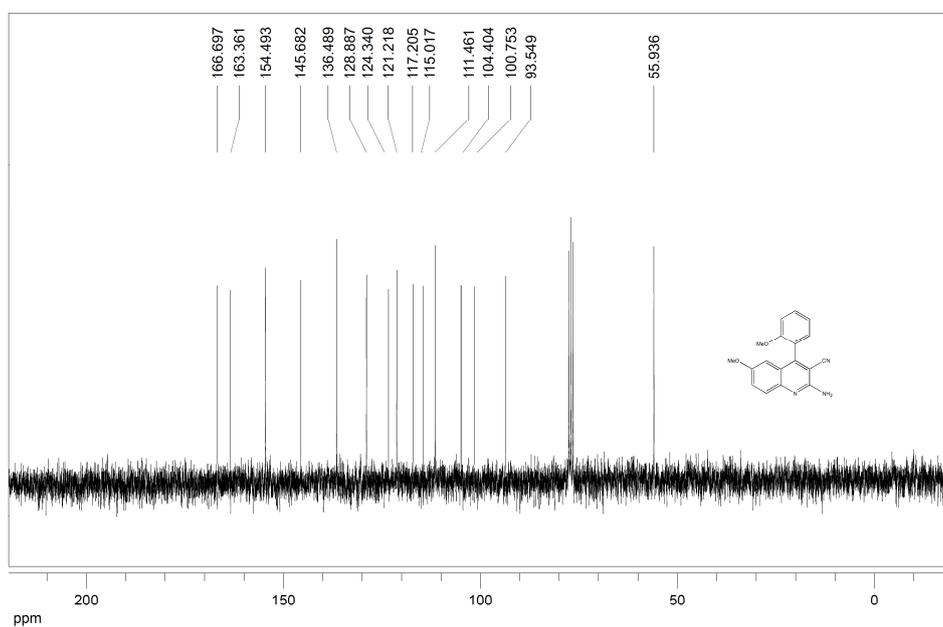
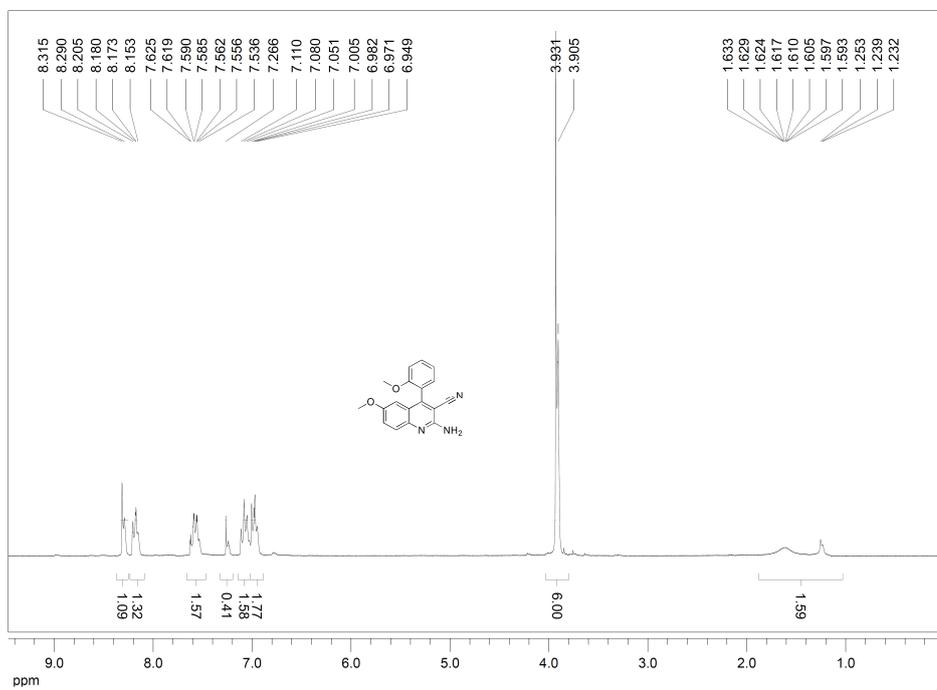
15. Compound 6c:



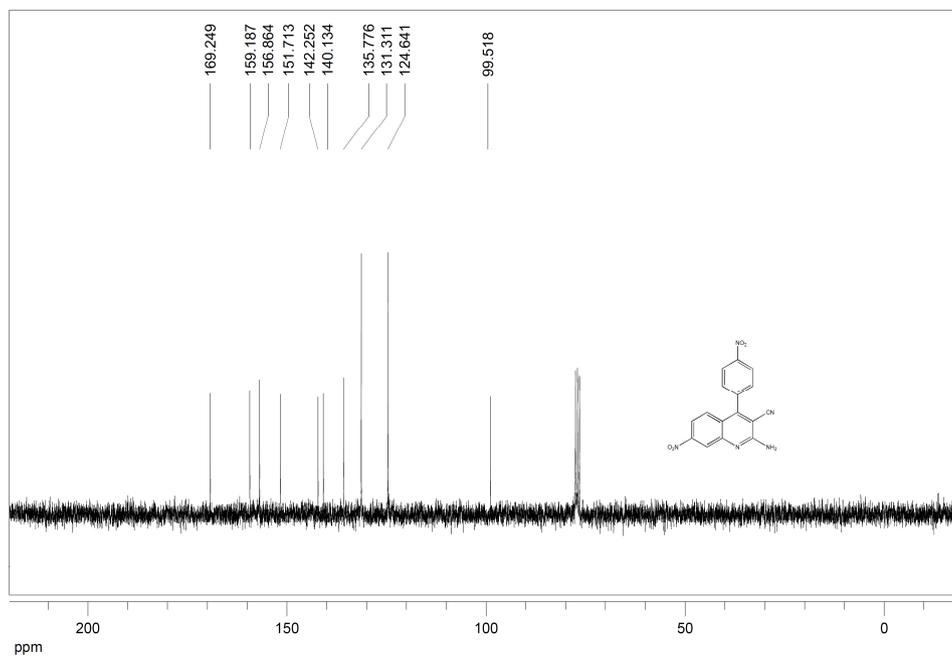
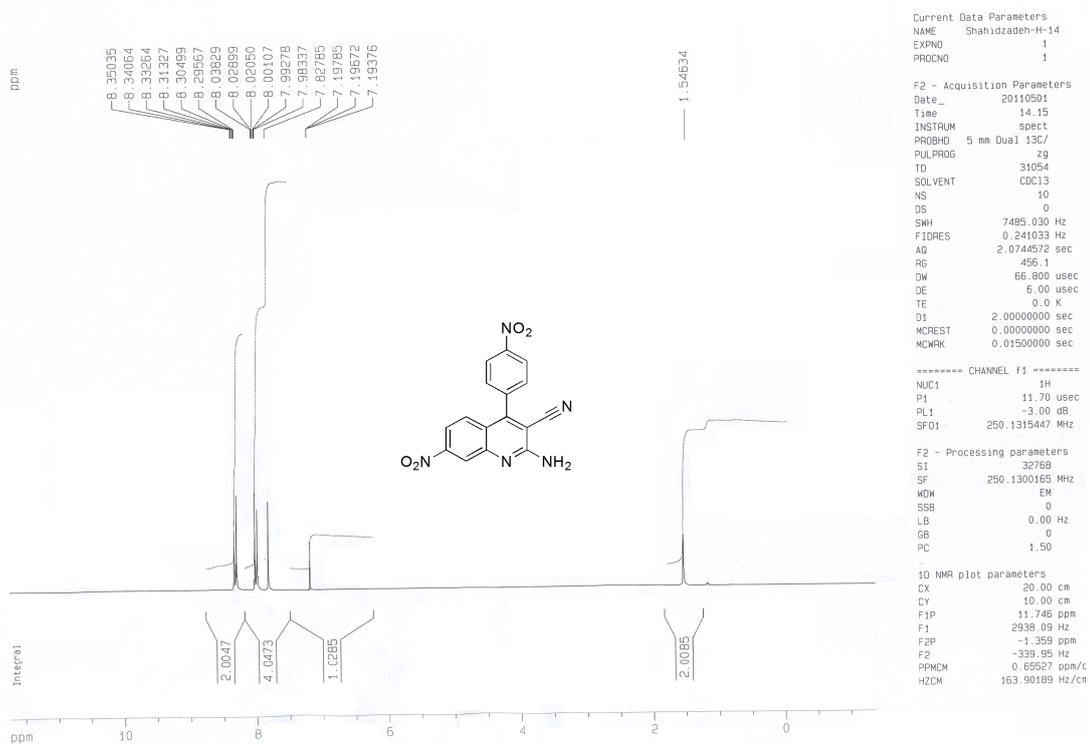
16. Compound 6d:



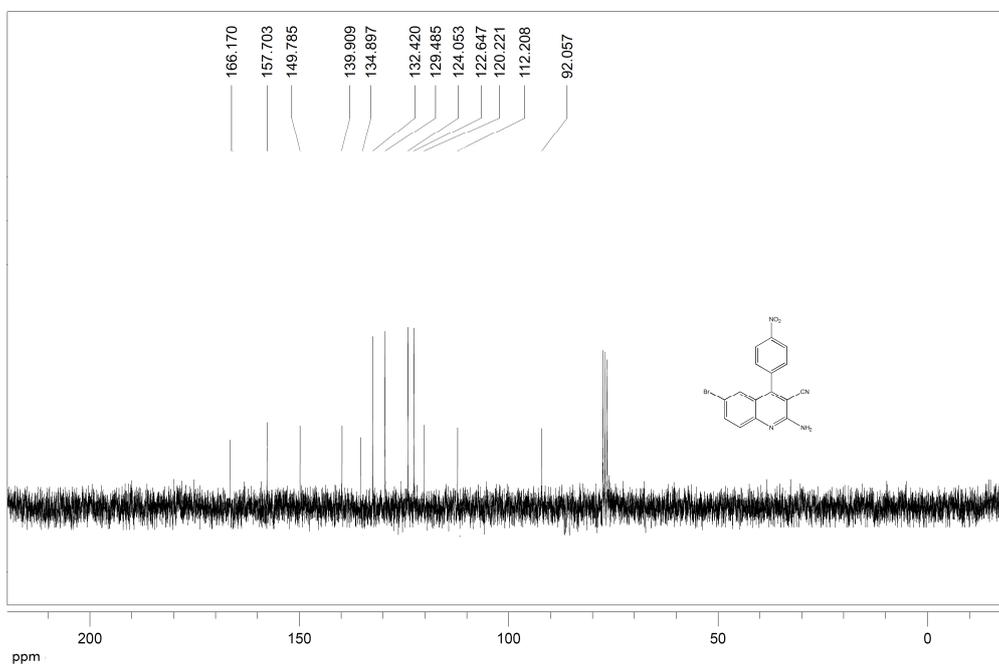
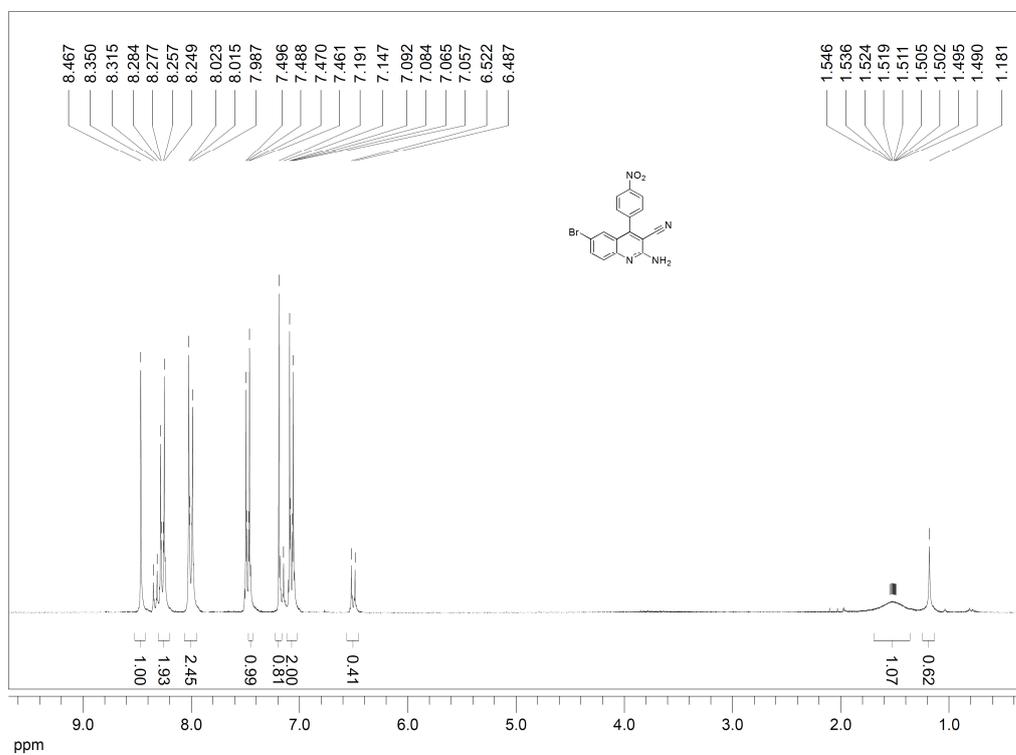
17. Compound **6e**:



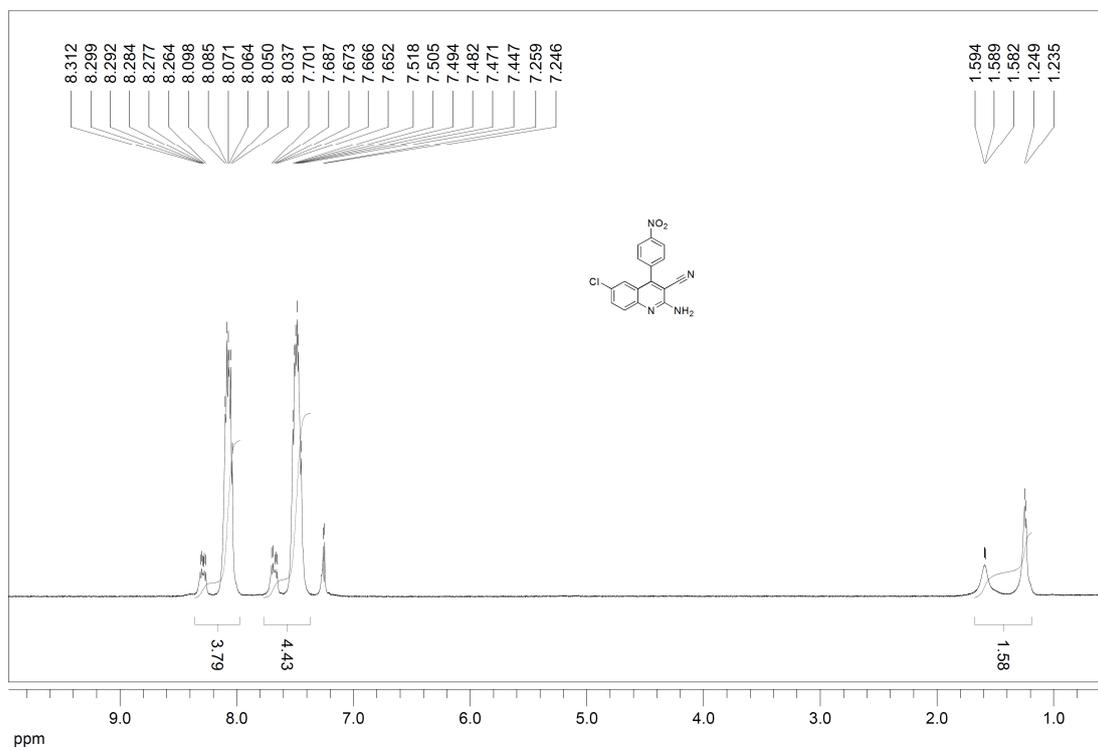
18. Compound 6f:



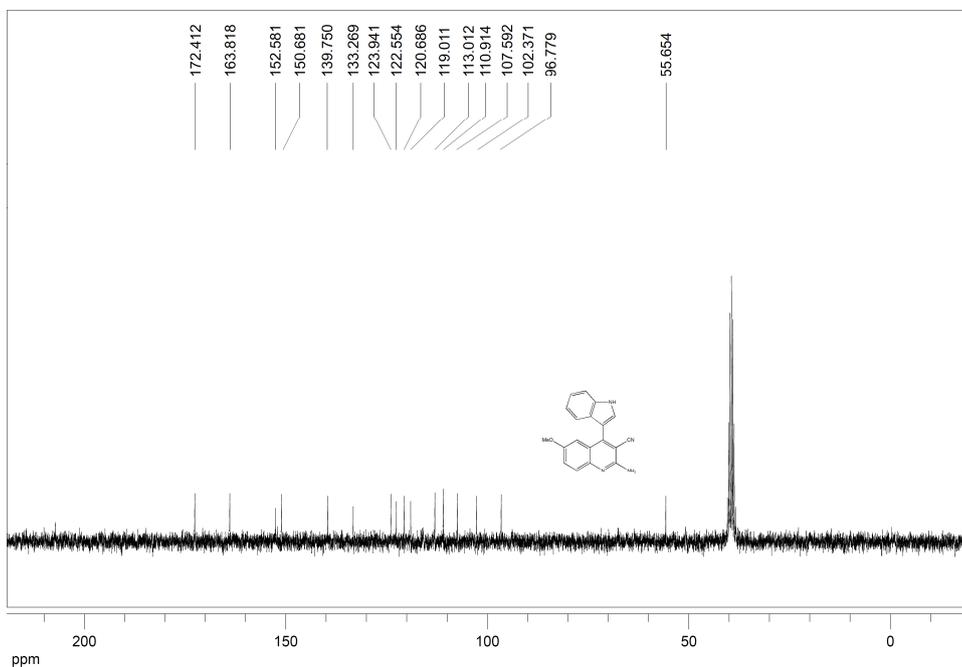
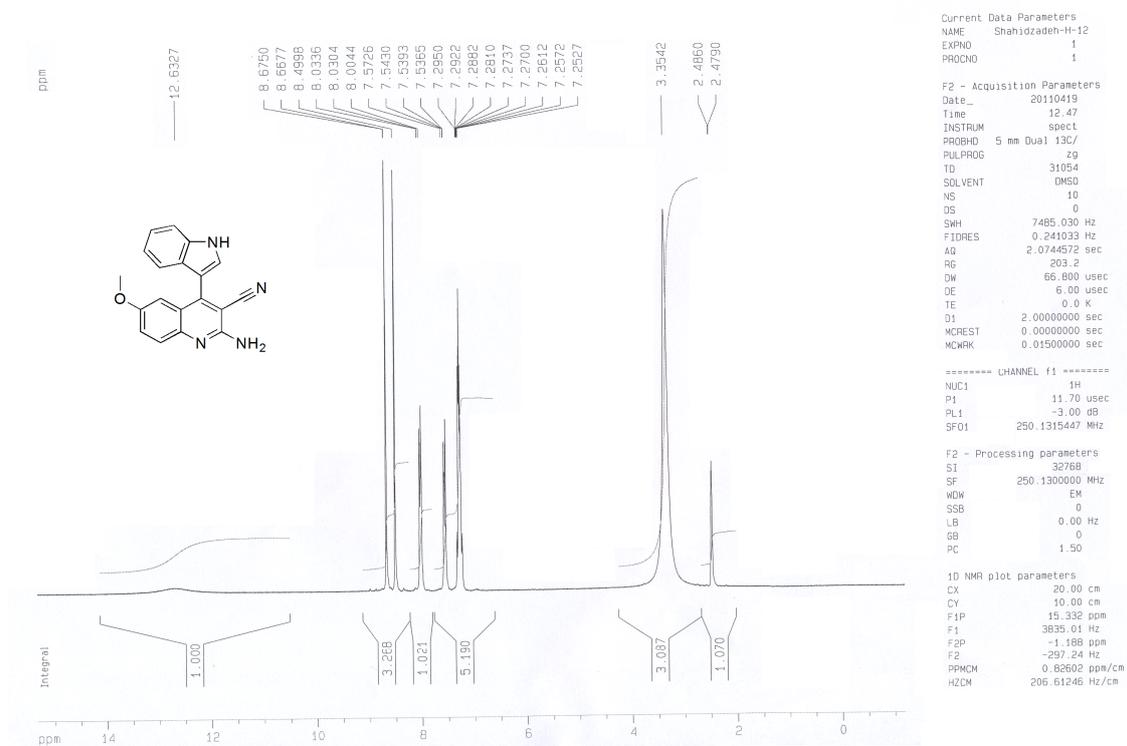
19. Compound **6g**:



20. Compound **6h**:



21. Compound 6i:



22. Compound 6j:

