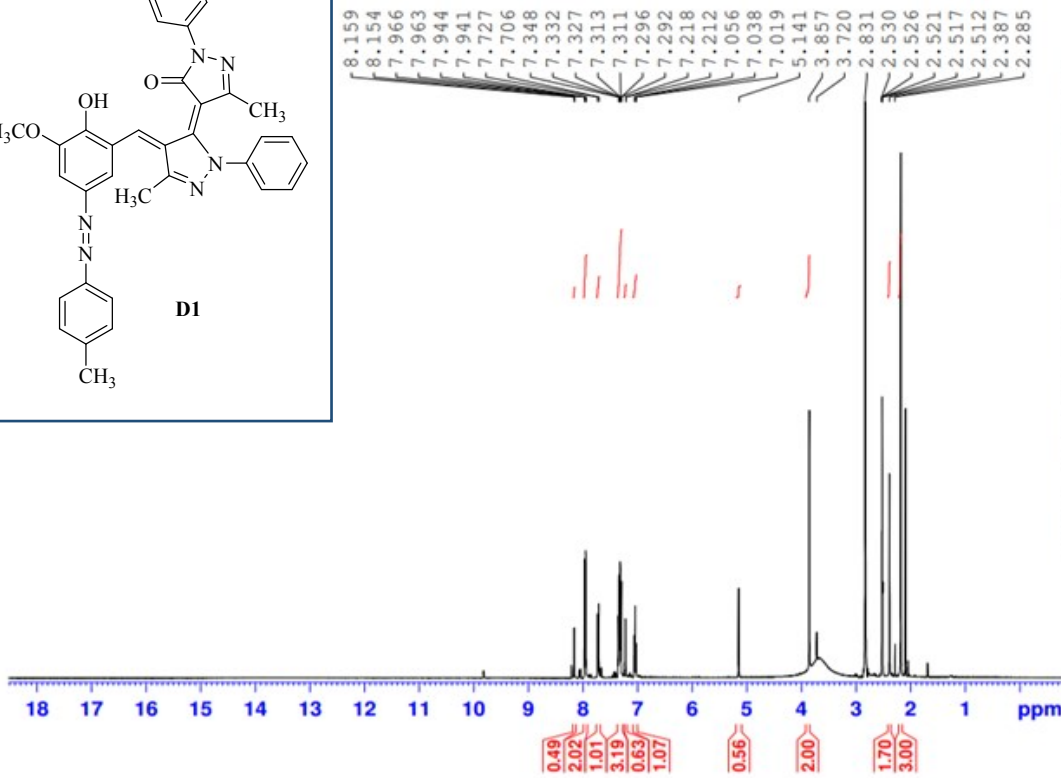
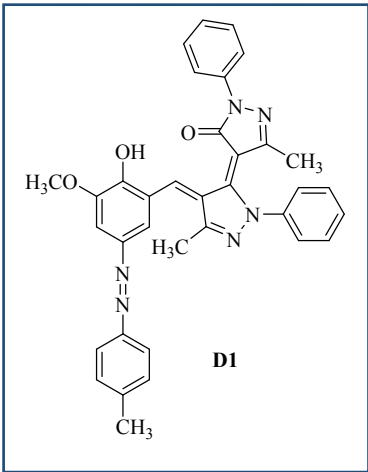


**Novel edaravone-based azo dyes: Efficient synthesis, characterization,  
antibacterial activity, DFT calculations and comprehensive investigation of  
the solvent effect on the absorption spectra**

**Mohammad Amin Davasaz Rabbani, Behzad Khalili, Hamid Saeidian**

**$^1\text{H}$  NMR, and  $^{13}\text{C}$  NMR spectra of Novel edaravone-based azo dyes D1-D10**

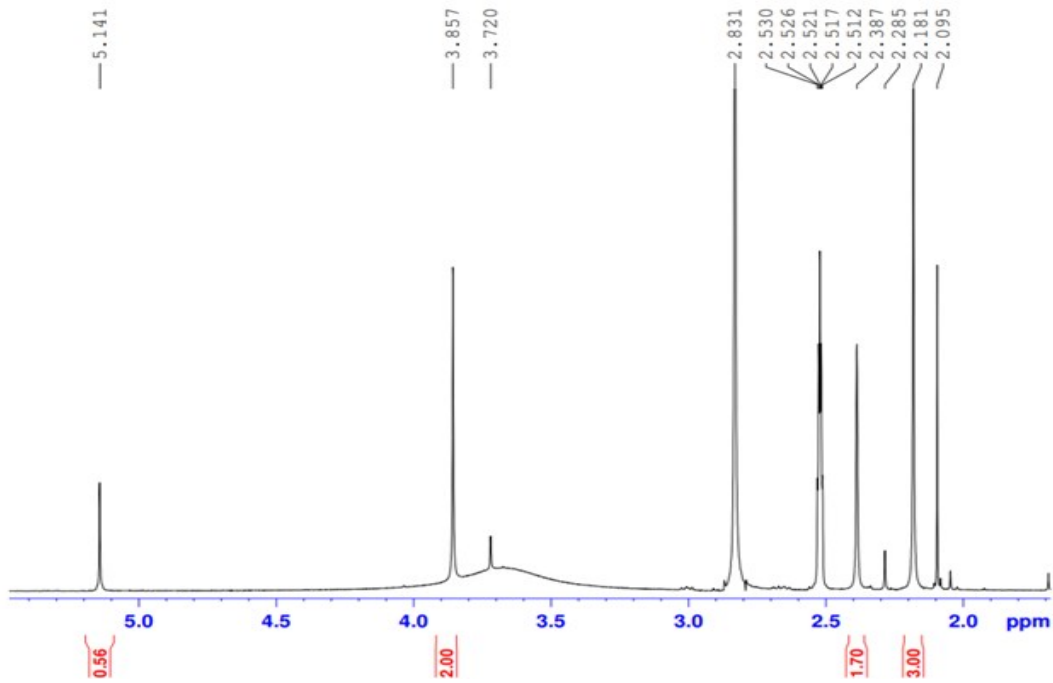


**BRUKER**

NAME PNU-Zanjan  
 EXPNO 422  
 PROCNO 1  
 Date\_ 20190602  
 Time 19.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 4.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -2.00 dB  
 PL1W 11.86359406 W  
 SFO1 400.2236020 MHz  
 SI 32768  
 SF 400.2200000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Sample Code: 2 (Davasaz)



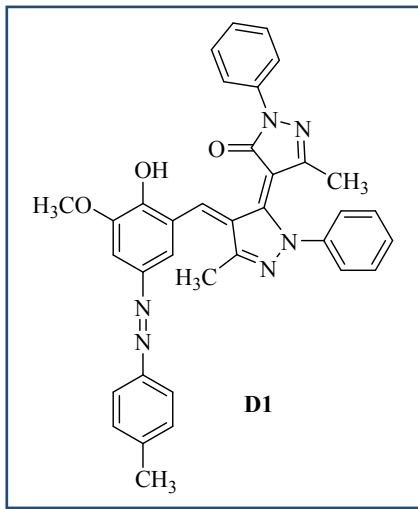
**BRUKER**

NAME PNU-Zanjan  
 EXPNO 422  
 PROCNO 1  
 Date\_ 20190602  
 Time 19.47  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 4.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -2.00 dB  
 PL1W 11.86359406 W  
 SFO1 400.2236020 MHz  
 SI 32768  
 SF 400.2200000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Ac  
Go

Fig <sup>1</sup>H NMR of D1



158.20  
150.62  
148.15  
146.67  
144.16  
134.16  
130.28  
129.04  
128.71  
124.85  
123.22  
122.53  
119.47  
102.12  
97.17

56.17  
45.97  
40.63  
40.42  
40.21  
40.00  
39.79  
39.58  
39.37  
39.16  
28.41  
23.68  
1.64



```

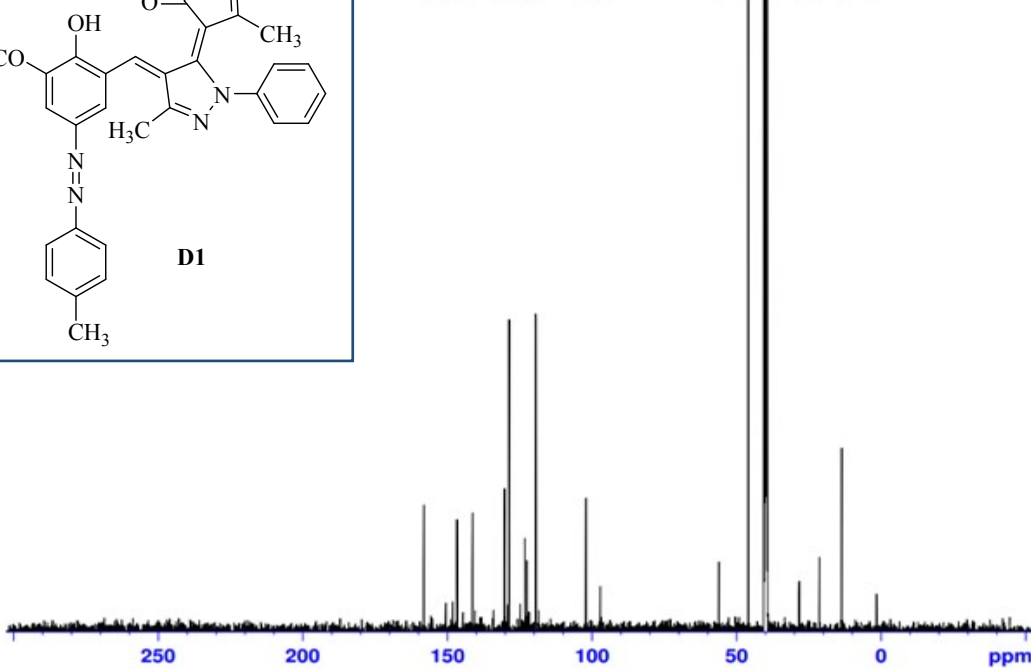
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EXPNO     423
PROCNO    1
Date_     20190602
Time      19.52
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         3983
DS         0
SWH        35714.285 Hz
FIDRES     0.544957 Hz
AQ         0.9175540 sec
RG         2050
DW         14.000 usec
DE         6.50 usec
TE         296.2 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

----- CHANNEL f1 -----
NUC1       13C
P1         9.00 usec
PL1        -0.90 dB
PL1W       42.02801895 W
SFO1       100.6479784 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2    waltz16
NUC2        1H
PCPD2       90.00 usec
PL2         -2.00 dB
PL12        14.16 dB
PL13        17.90 dB
PL2W        11.86359406 W
PL12W       0.28722104 W
PL13W       0.12139934 W
SFO2        400.2216009 MHz
SI          32768
SF          100.6353990 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```



Sample Code: 2 (Davasaz)



```

NAME      PNU-Zanjan
EXPNO     423
PROCNO    1
Date_     20190602
Time      19.52
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD         65536
SOLVENT   DMSO
NS         3983
DS         0
SWH        35714.285 Hz
FIDRES     0.544957 Hz
AQ         0.9175540 sec
RG         2050
DW         14.000 usec
DE         6.50 usec
TE         296.2 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

----- CHANNEL f1 -----
NUC1       13C
P1         9.00 usec
PL1        -0.90 dB
PL1W       42.02801895 W
SFO1       100.6479784 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2    waltz16
NUC2        1H
PCPD2       90.00 usec
PL2         -2.00 dB
PL12        14.16 dB
PL13        17.90 dB
PL2W        11.86359406 W
PL12W       0.28722104 W
PL13W       0.12139934 W
SFO2        400.2216009 MHz
SI          32768
SF          100.6353990 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40
  
```

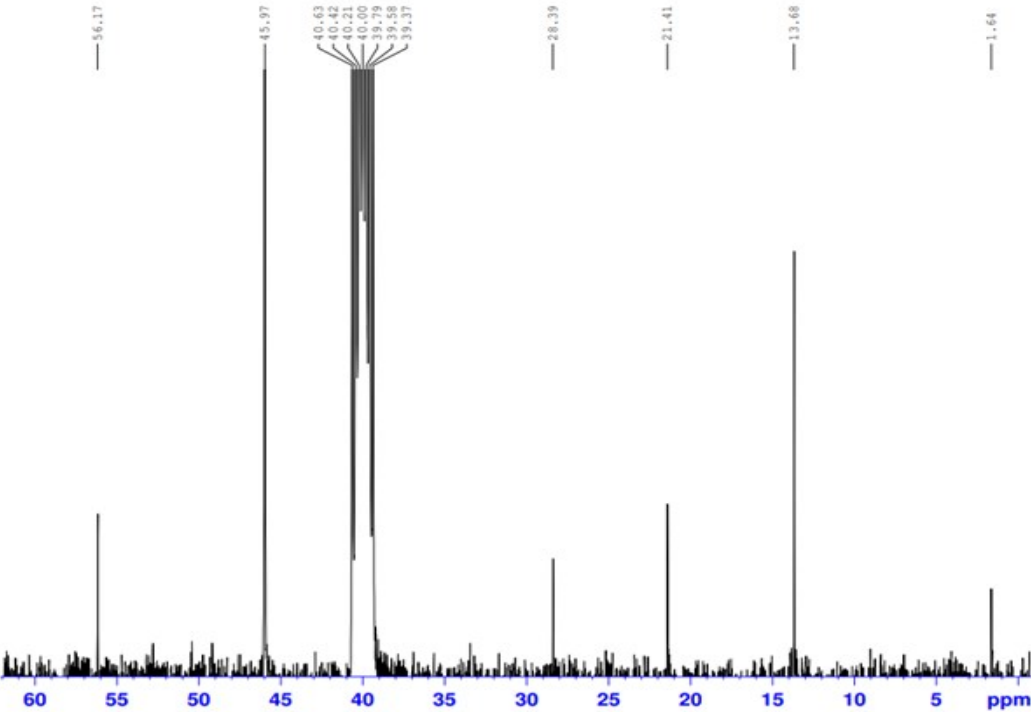
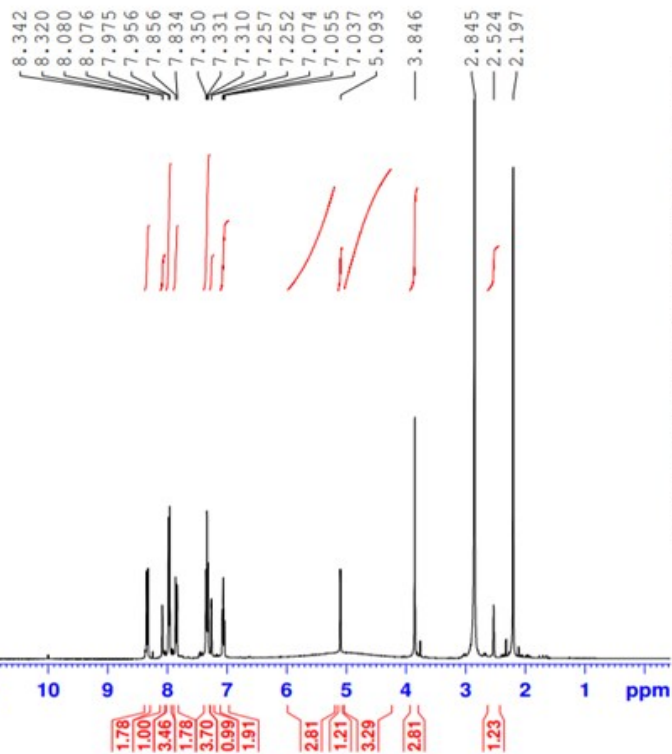
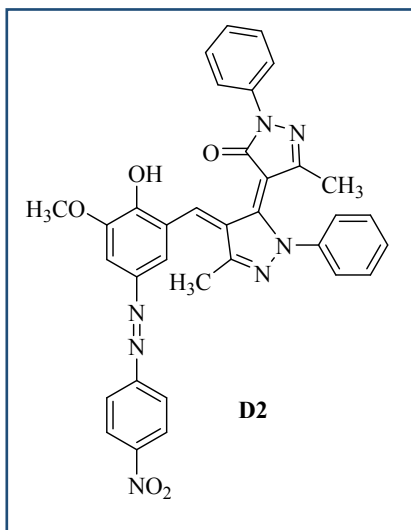


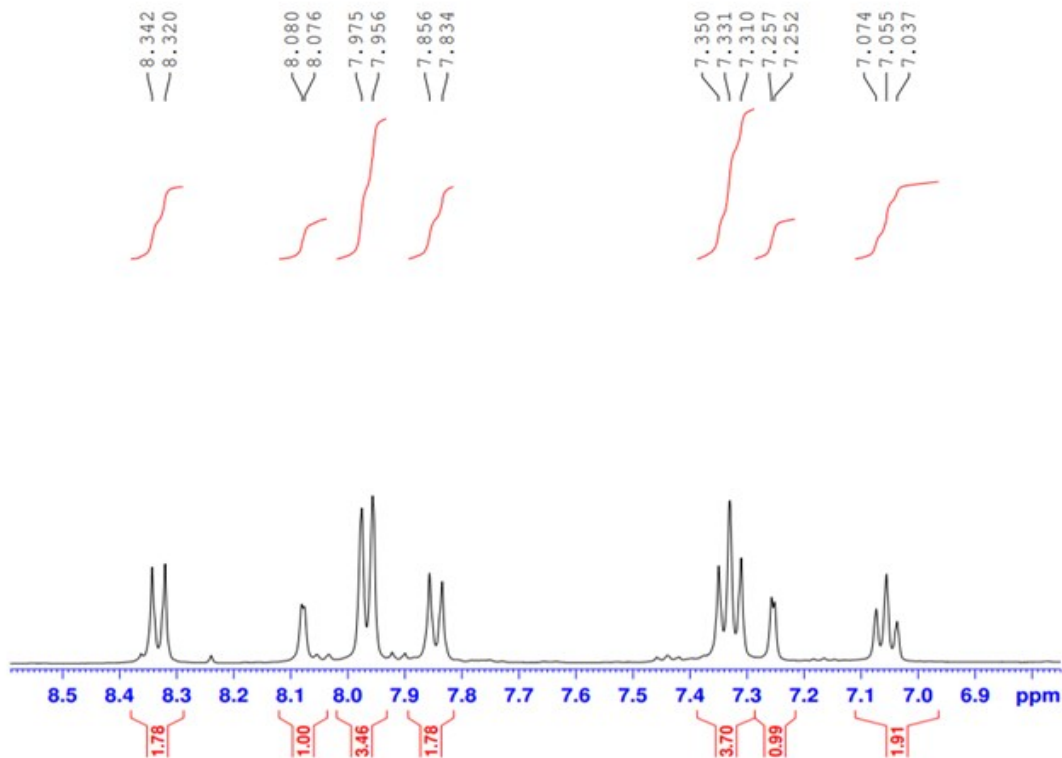
Fig <sup>13</sup>C NMR of D1.



NAME PNU-Zanjan  
 EXPNO 412  
 PROCNO 1  
 Date\_ 20190305  
 Time 13.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 90.5  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.0 K  
 D1 4.00000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -2.00 dB  
 PL1W 11.86359406 W  
 SFO1 400.2236020 MHz  
 SI 32768  
 SF 400.2200000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

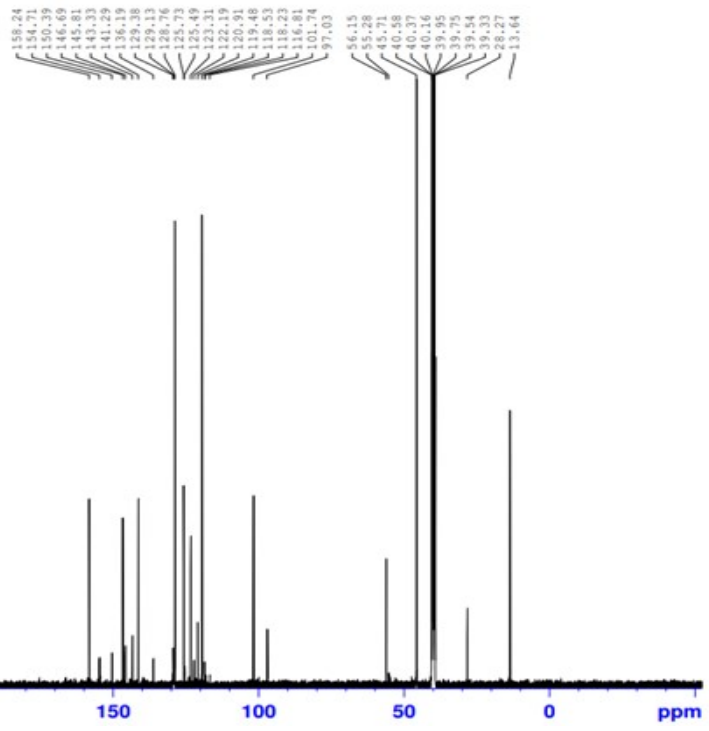
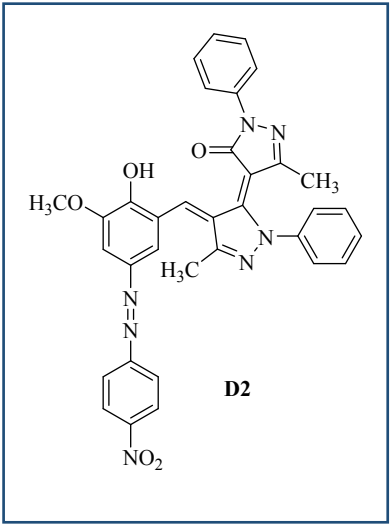
Sample Code: 1 (Davasaz)



NAME PNU-Zanjan  
 EXPNO 412  
 PROCNO 1  
 Date\_ 20190305  
 Time 13.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 90.5  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.0 K  
 D1 4.00000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -2.00 dB  
 PL1W 11.86359406 W  
 SFO1 400.2236020 MHz  
 SI 32768  
 SF 400.2200000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Fig <sup>1</sup>H NMR of D2



**BRUKER**

```

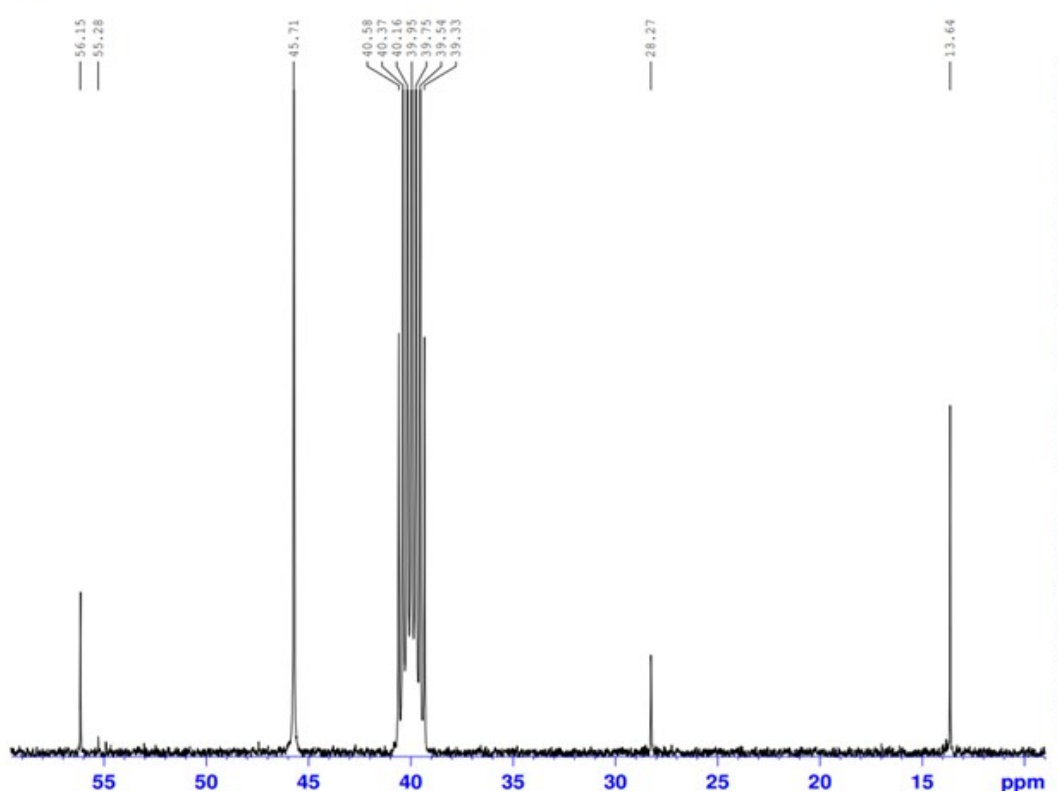
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EXPNO    417
PROCNO   1
Date_    20190309
Time     18.54
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        3856
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ         0.9175540 sec
RG         2050
DW         14.000 usec
DE         6.50 usec
TE         293.0 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1          9.00 usec
PL1         -0.90 dB
PL1W       42.02801895 W
SFO1       100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     90.00 usec
PL2        -2.00 dB
PL12       14.16 dB
PL13       17.90 dB
PL2W      11.86359406 W
PL12W     0.28722104 W
PL13W     0.12139934 W
SFO2       400.2216009 MHz
SI         32768
SF         100.6353990 MHz
WDW        EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.40

```

Sample Code: 1 (Davasaz)



**BRUKER**

```

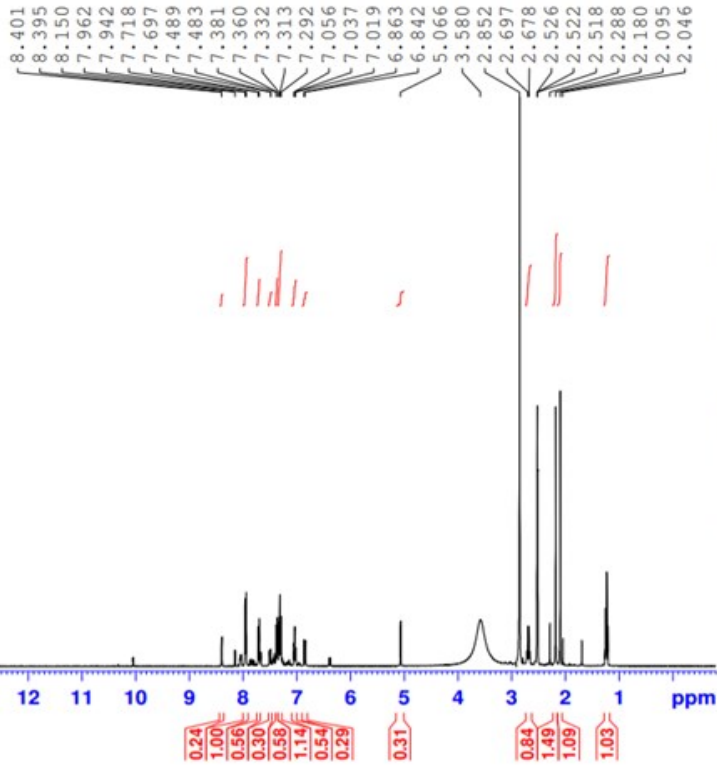
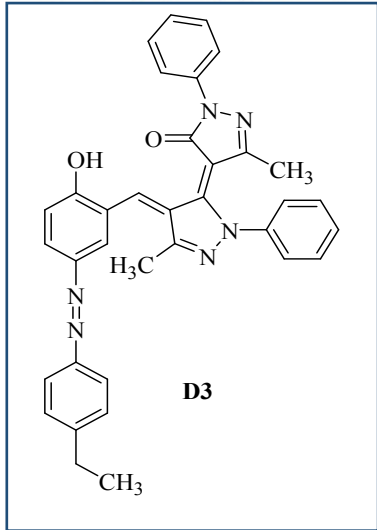
NAME      PNU-Zanjan
EXPNO    417
PROCNO   1
Date_    20190309
Time     18.54
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        3856
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ         0.9175540 sec
RG         2050
DW         14.000 usec
DE         6.50 usec
TE         293.0 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1          9.00 usec
PL1         -0.90 dB
PL1W       42.02801895 W
SFO1       100.6479784 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       1H
PCPD2     90.00 usec
PL2        -2.00 dB
PL12       14.16 dB
PL13       17.90 dB
PL2W      11.86359406 W
PL12W     0.28722104 W
PL13W     0.12139934 W
SFO2       400.2216009 MHz
SI         32768
SF         100.6353990 MHz
WDW        EM
SSB         0
LB          1.00 Hz Act
GB          0
PC          1.40 Go t

```

Fig <sup>13</sup>C NMR of D2.



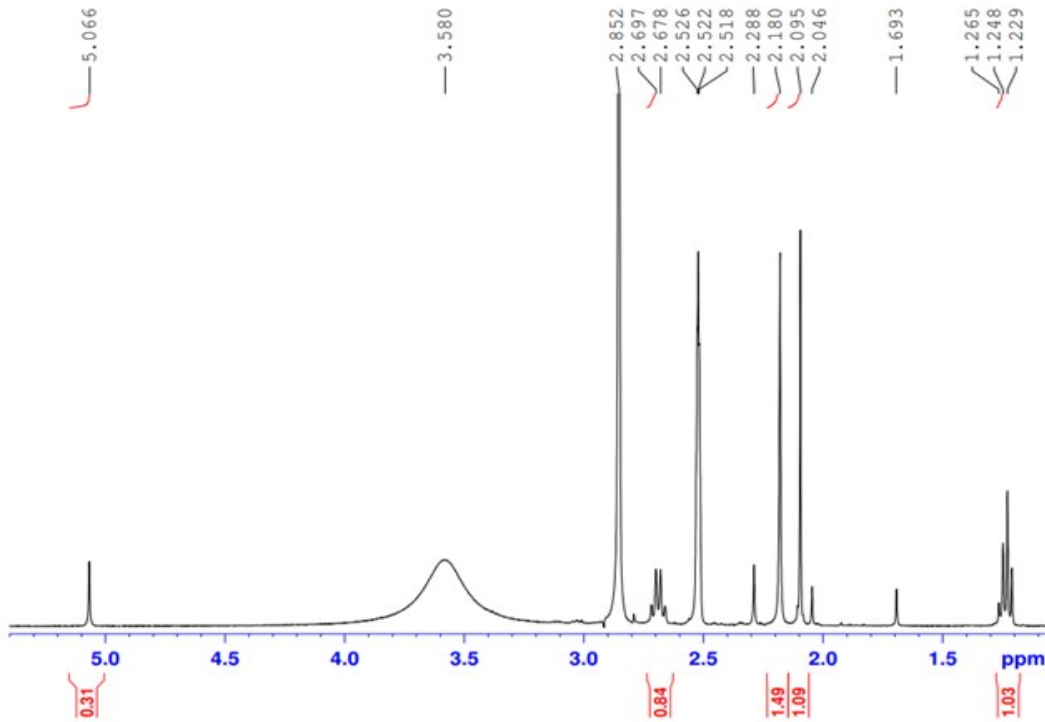
**BRUKER**

```

NAME      PNU-Zanjan
EXPNO    424
PROCNO   1
Date_    20190602
Time     22.06
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        20
DS        0
SWH       8012.820 Hz
FIDRES   0.122266 Hz
AQ        4.0894966 sec
RG        203
DW        62.400 usec
DE        6.50 usec
TE        296.3 K
D1        4.0000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      1H
P1        14.00 usec
PL1       -2.00 dB
PL1W      11.86359406 W
SFO1      400.2236020 MHz
SI        32768
SF        400.2200000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

Sample Code: 3 (Davasaz)



**BRUKER**

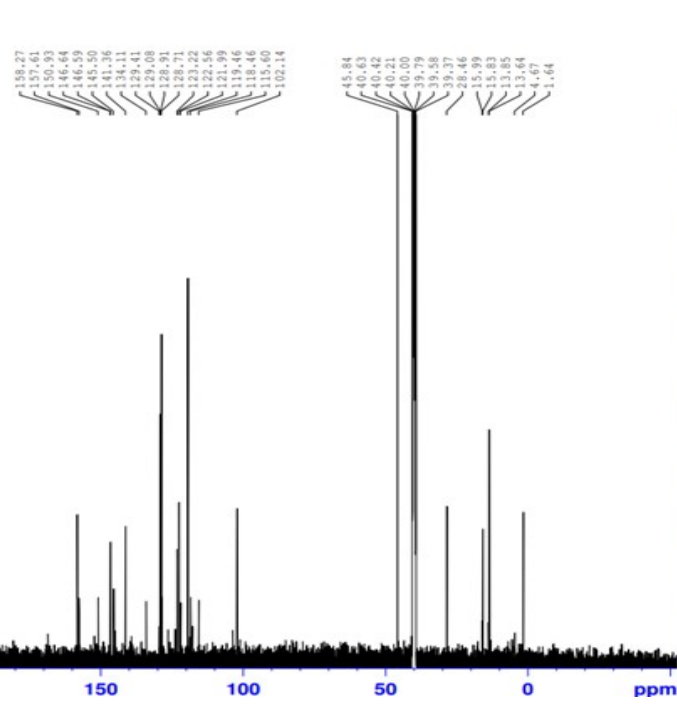
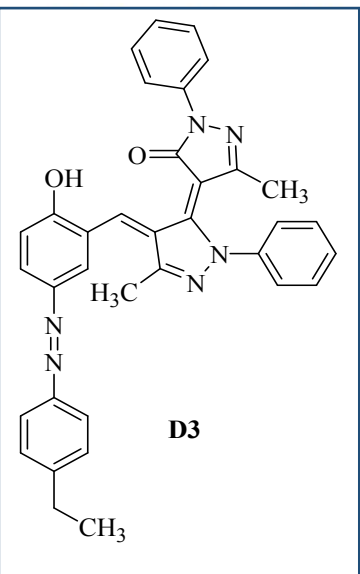
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NAME      PNU-Zanjan
EXPNO    424
PROCNO   1
Date_    20190602
Time     22.06
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        20
DS        0
SWH       8012.820 Hz
FIDRES   0.122266 Hz
AQ        4.0894966 sec
RG        203
DW        62.400 usec
DE        6.50 usec
TE        296.3 K
D1        4.0000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      1H
P1        14.00 usec
PL1       -2.00 dB
PL1W      11.86359406 W
SFO1      400.2236020 MHz
SI        32768
SF        400.2200000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
```

Fig <sup>1</sup>H NMR of D3.





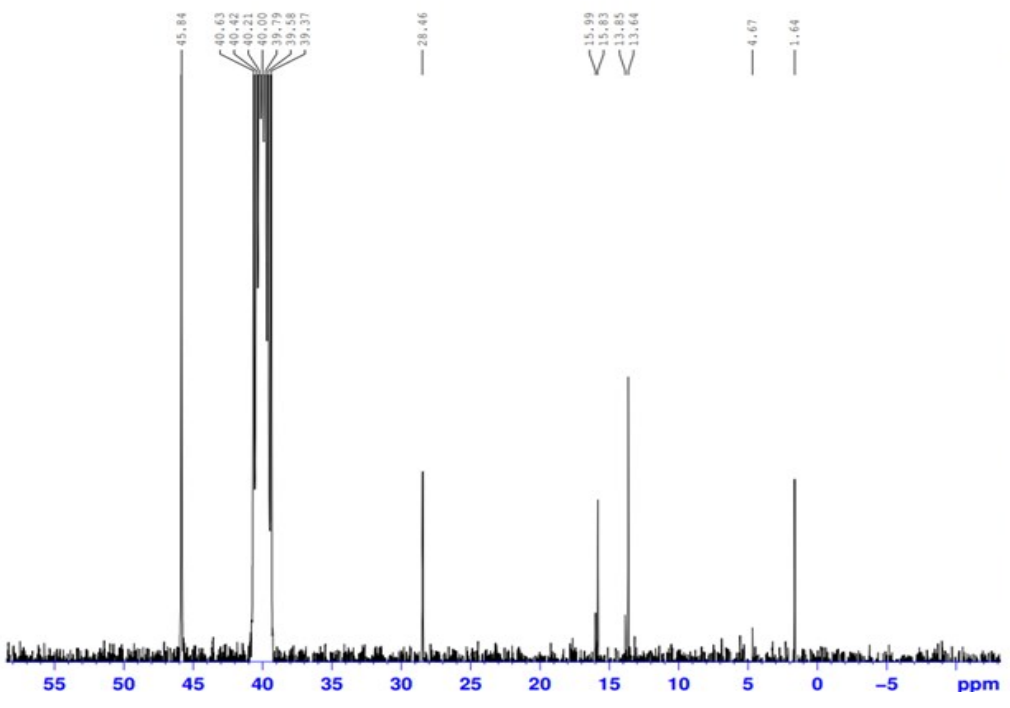
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NAME PNU-Zanjan
EXPNO 425
PROCNO 1
Date_ 20190603
Time 2.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8192
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

Sample Code: 3 (Davasaz)



```

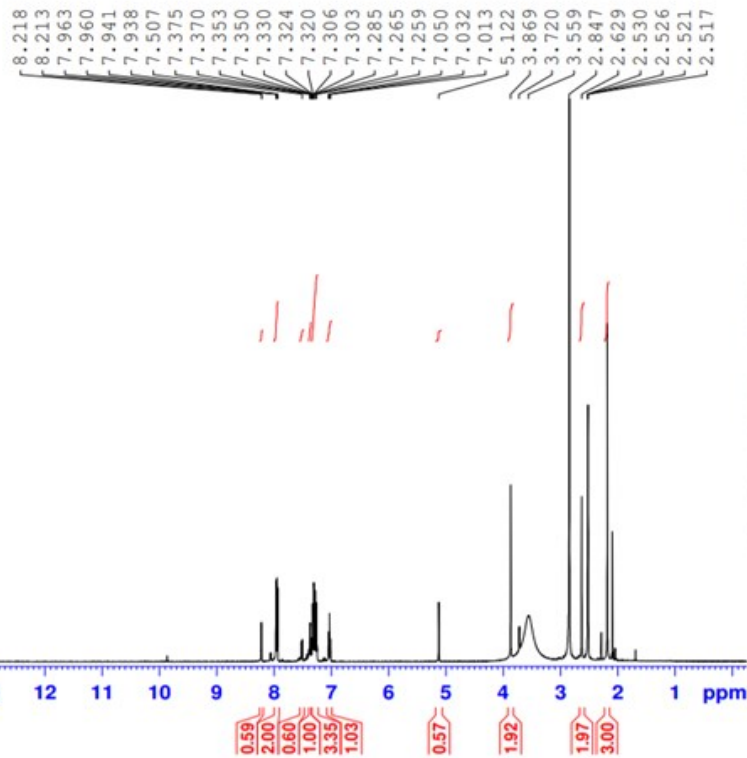
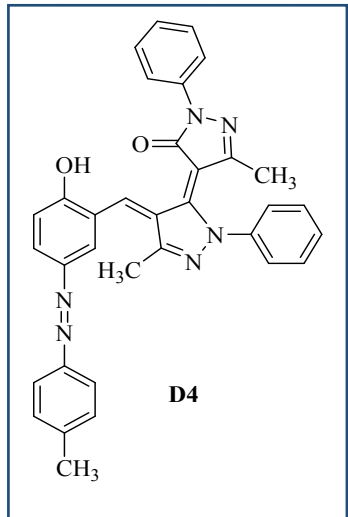
NAME PNU-Zanjan
EXPNO 425
PROCNO 1
Date_ 20190603
Time 2.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 8192
DS 0
SWH 35714.285 Hz
FIDRES 0.544957 Hz
AQ 0.9175540 sec
RG 2050
DW 14.000 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 9.00 usec
PL1 -0.90 dB
PL1W 42.02801895 W
SFO1 100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.00 dB
PL12 14.16 dB
PL13 17.90 dB
PL2W 11.86359406 W
PL12W 0.28722104 W
PL13W 0.12139934 W
SFO2 400.2216009 MHz
SI 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

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Go to Settir

Fig <sup>13</sup>C NMR of D3.

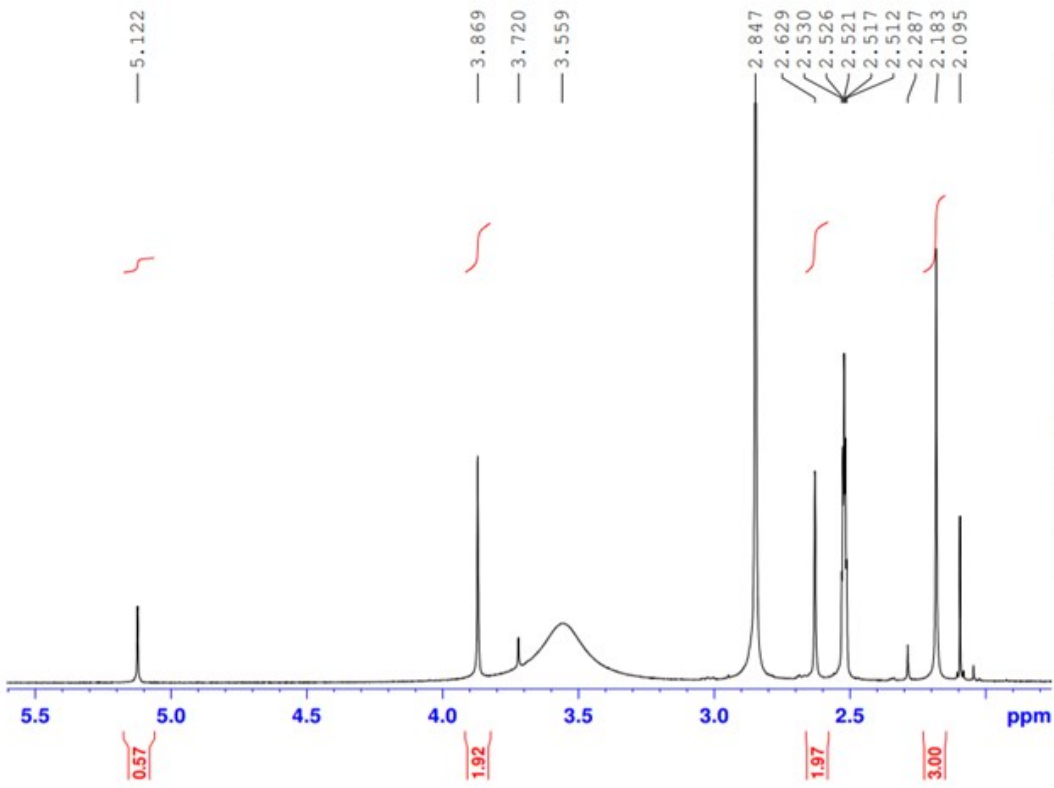


```

NAME      PNU-Zanjan
EXPNO    420
PROCNO   1
Date_    20190602
Time     14.40
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       20
DS       0
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       203
DW       62.400 usec
DE       6.50 usec
TE       295.3 K
D1       4.00000000 sec
TD0     1

----- CHANNEL f1 -----
NUC1     1H
P1       14.00 usec
PL1     -2.00 dB
PL1W    11.86359406 W
SFO1    400.2236020 MHz
SI      32768
SF      400.2200000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
  
```

Sample Code: 1 (Davasaz)



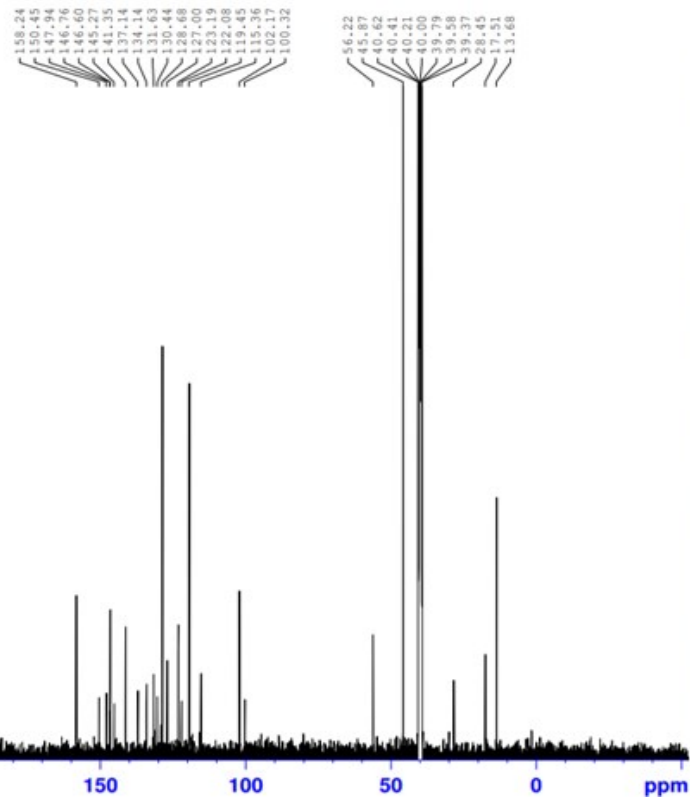
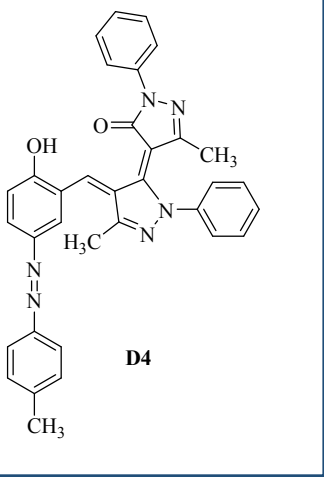
```

NAME      PNU-Zanjan
EXPNO    420
PROCNO   1
Date_    20190602
Time     14.40
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       20
DS       0
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894966 sec
RG       203
DW       62.400 usec
DE       6.50 usec
TE       295.3 K
D1       4.00000000 sec
TD0     1

----- CHANNEL f1 -----
NUC1     1H
P1       14.00 usec
PL1     -2.00 dB
PL1W    11.86359406 W
SFO1    400.2236020 MHz
SI      32768
SF      400.2200000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
  
```

Fig <sup>1</sup>H NMR of D4.





```

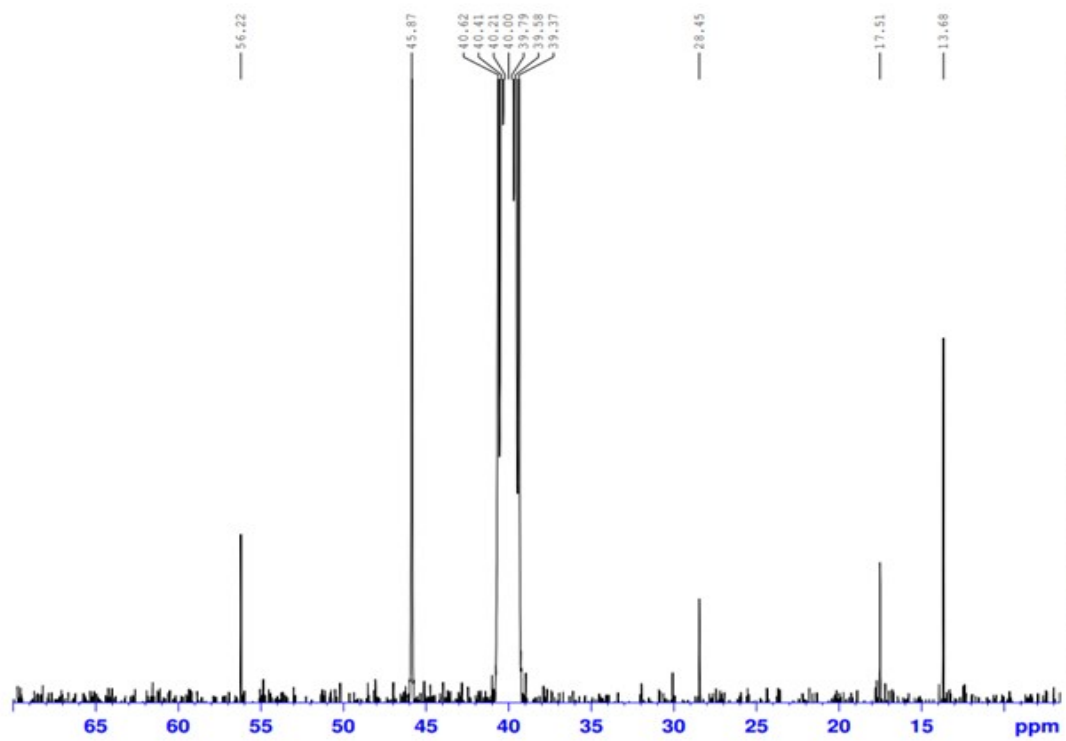
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EXPNO     421
PROCNO    1
Date_     20190602
Time      14.42
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        8192
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        295.7 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1      -0.90 dB
PL1W     42.02801895 W
SFO1     100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W     11.86359406 W
PL12W    0.28722104 W
PL13W    0.12139934 W
SFO2     400.2216009 MHz
SI        32768
SF        100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

Sample Code: 1 (Davasaz)



```

NAME      PNU-Zanjan
EXPNO     421
PROCNO    1
Date_     20190602
Time      14.42
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        8192
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        295.7 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1

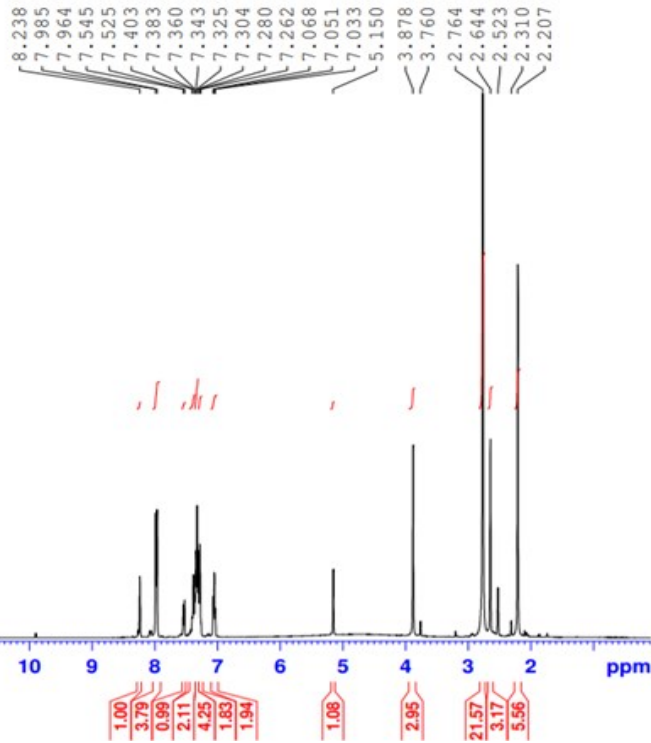
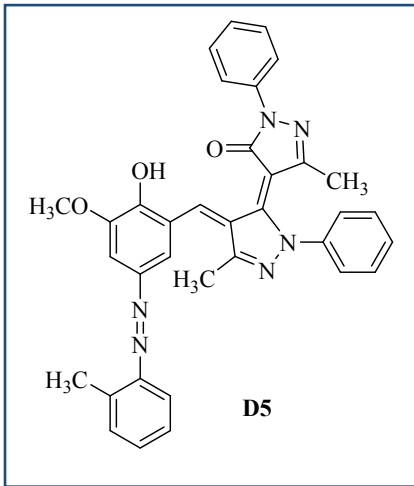
----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1      -0.90 dB
PL1W     42.02801895 W
SFO1     100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W     11.86359406 W
PL12W    0.28722104 W
PL13W    0.12139934 W
SFO2     400.2216009 MHz
SI        32768
SF        100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

Fig <sup>13</sup>C NMR of D4.

Sample Code: 5 (Davasaz)

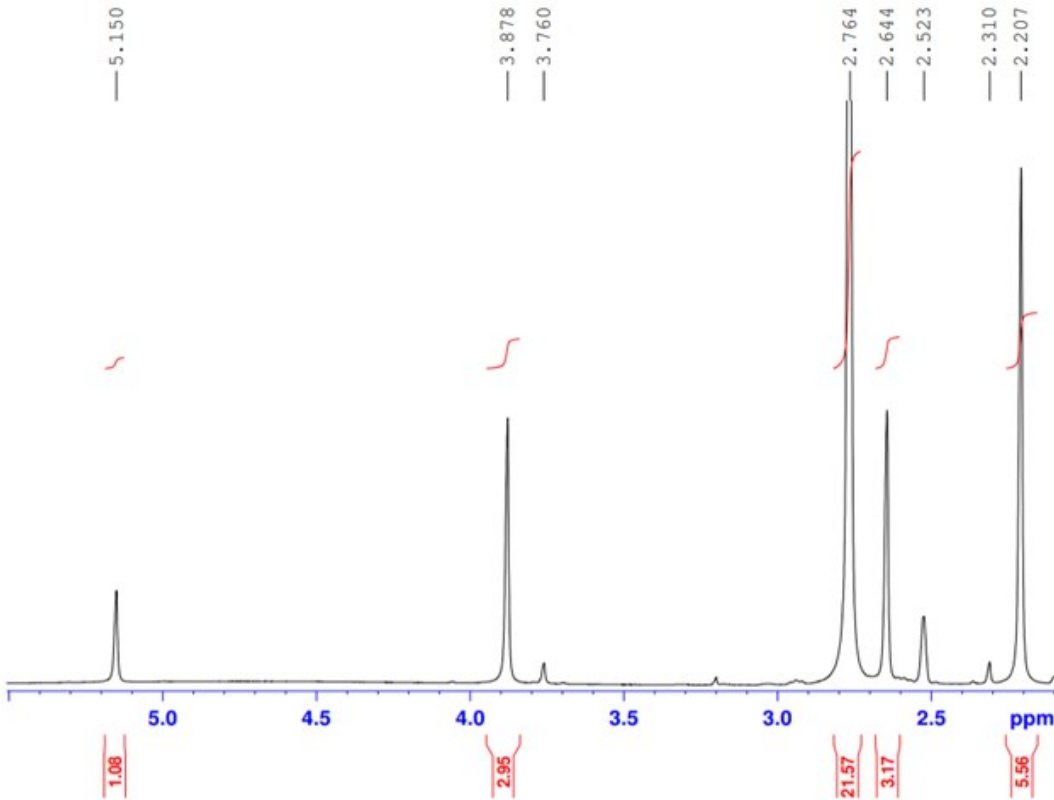


**BRUKER**

NAME PNU-Zanjan  
EXPNO 402  
PROCNO 1  
Date\_ 20181111  
Time 14.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 20  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 71.8  
DW 62.400 usec  
DE 6.50 usec  
TE 293.2 K  
D1 4.0000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.00 usec  
PL1 -2.00 dB  
PL1W 11.86359406 W  
SF01 400.2236020 MHz  
SI 32768  
SF 400.2200000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Sample Code: 5 (Davasaz)

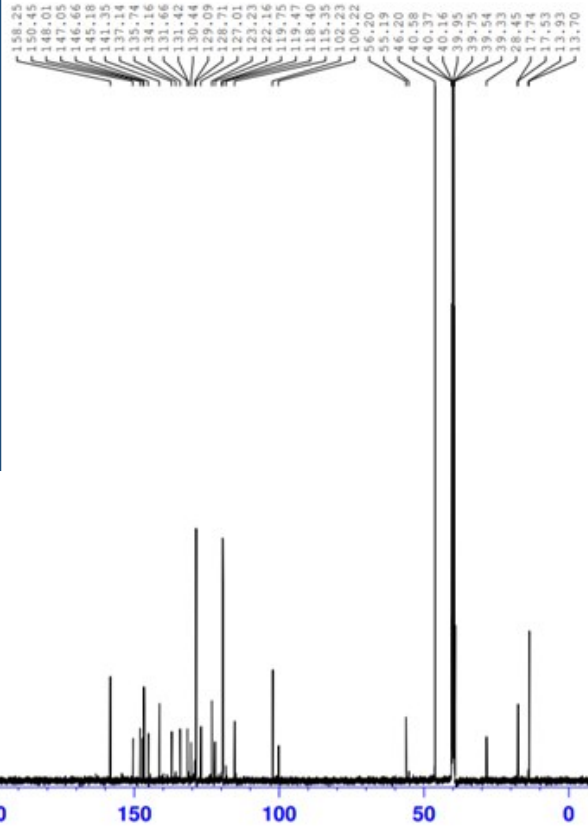
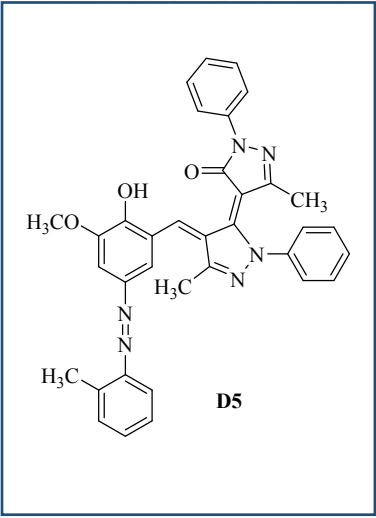


**BRUKER**

NAME PNU-Zanjan  
EXPNO 402  
PROCNO 1  
Date\_ 20181111  
Time 14.21  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 20  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 71.8  
DW 62.400 usec  
DE 6.50 usec  
TE 293.2 K  
D1 4.0000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.00 usec  
PL1 -2.00 dB  
PL1W 11.86359406 W  
SF01 400.2236020 MHz  
SI 32768  
SF 400.2200000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

Fig <sup>1</sup>H NMR of D5



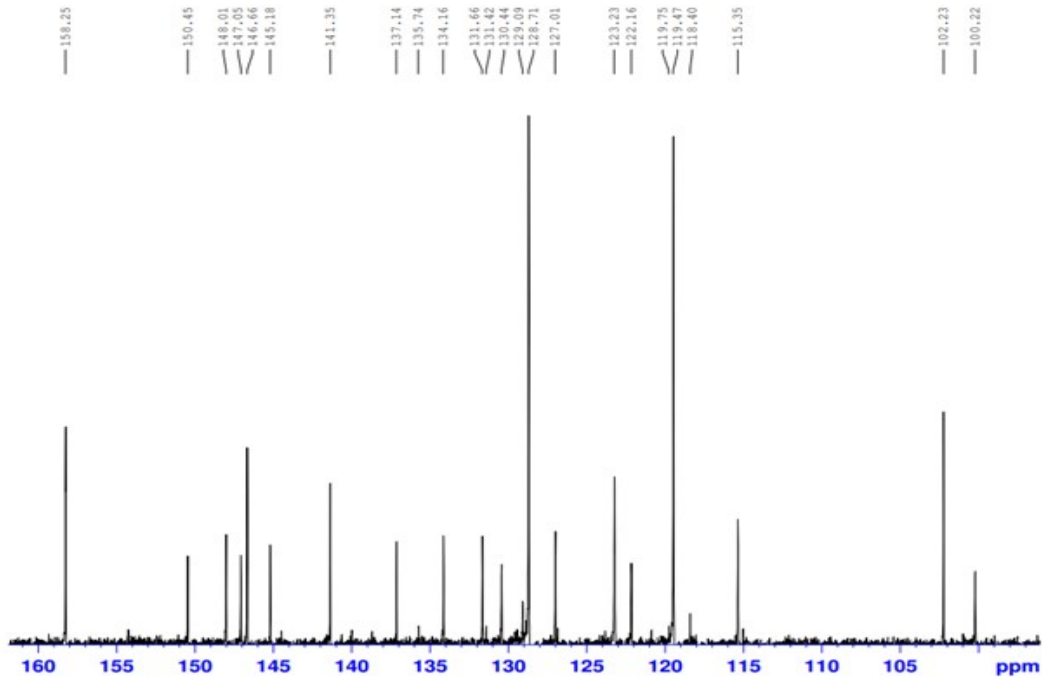
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NAME      PNU-Zanjan
EXPNO    411
PROCNO   1
Date_    20181117
Time     12.41
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       1724
DS       0
SWH      35714.285 Hz
FIDRES   0.544957 Hz
AQ       0.9175540 sec
RG       2050
DW       14.000 usec
DE       6.50 usec
TE       292.4 K
D1       1.0000000 sec
D11      0.0300000 sec
TD0      1

----- CHANNEL f1 -----
NUC1     13C
P1       9.00 usec
PL1      -0.90 dB
PL1W    42.02801895 W
SFO1    100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    90.00 usec
PL2      -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W    11.86359406 W
PL12W   0.28722104 W
PL13W   0.12139934 W
SFO2    400.2216009 MHz
SI       32768
SF      100.6353990 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

Sample Code: 5 (Davasaz)



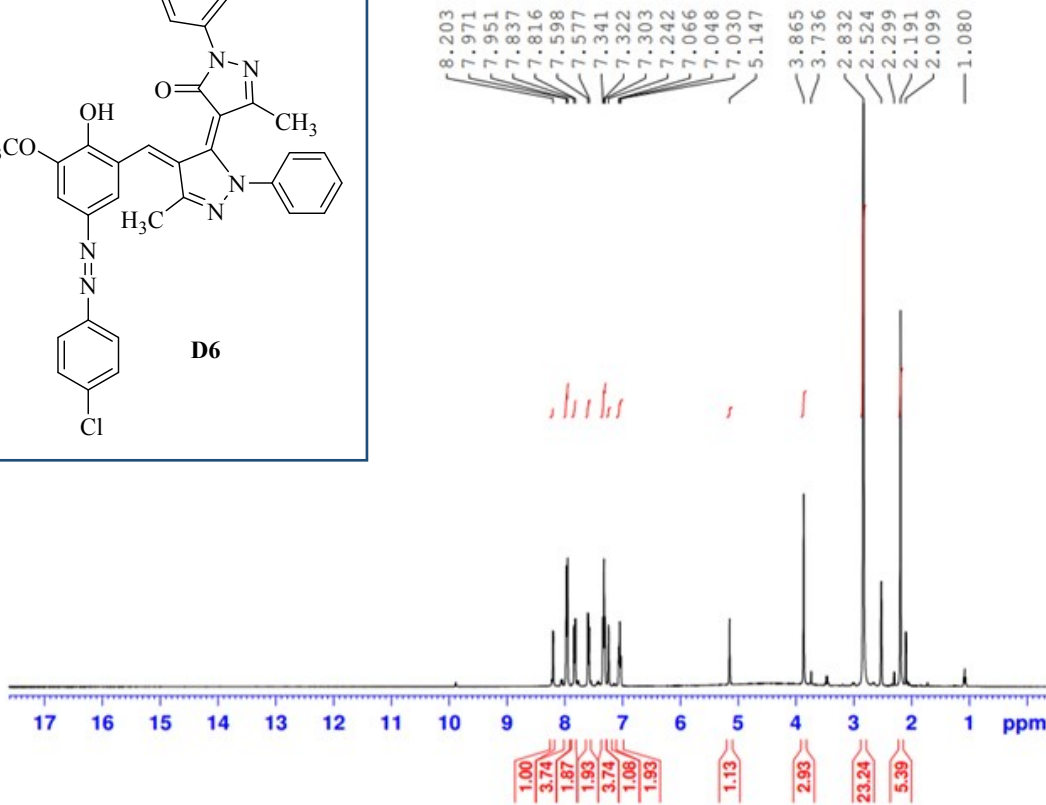
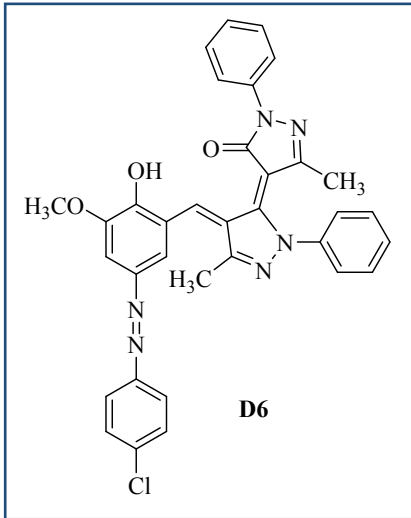
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NAME      PNU-Zanjan
EXPNO    411
PROCNO   1
Date_    20181117
Time     12.41
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zgpg30
TD       65536
SOLVENT  DMSO
NS       1724
DS       0
SWH      35714.285 Hz
FIDRES   0.544957 Hz
AQ       0.9175540 sec
RG       2050
DW       14.000 usec
DE       6.50 usec
TE       292.4 K
D1       1.0000000 sec
D11      0.0300000 sec
TD0      1

----- CHANNEL f1 -----
NUC1     13C
P1       9.00 usec
PL1      -0.90 dB
PL1W    42.02801895 W
SFO1    100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2  waltz16
NUC2     1H
PCPD2    90.00 usec
PL2      -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W    11.86359406 W
PL12W   0.28722104 W
PL13W   0.12139934 W
SFO2    400.2216009 MHz
SI       32768
SF      100.6353990 MHz
WDW      EM
SSB      0
LB       1.00 Hz
GB       0
PC       1.40
  
```

Fig <sup>13</sup>C NMR of D5.



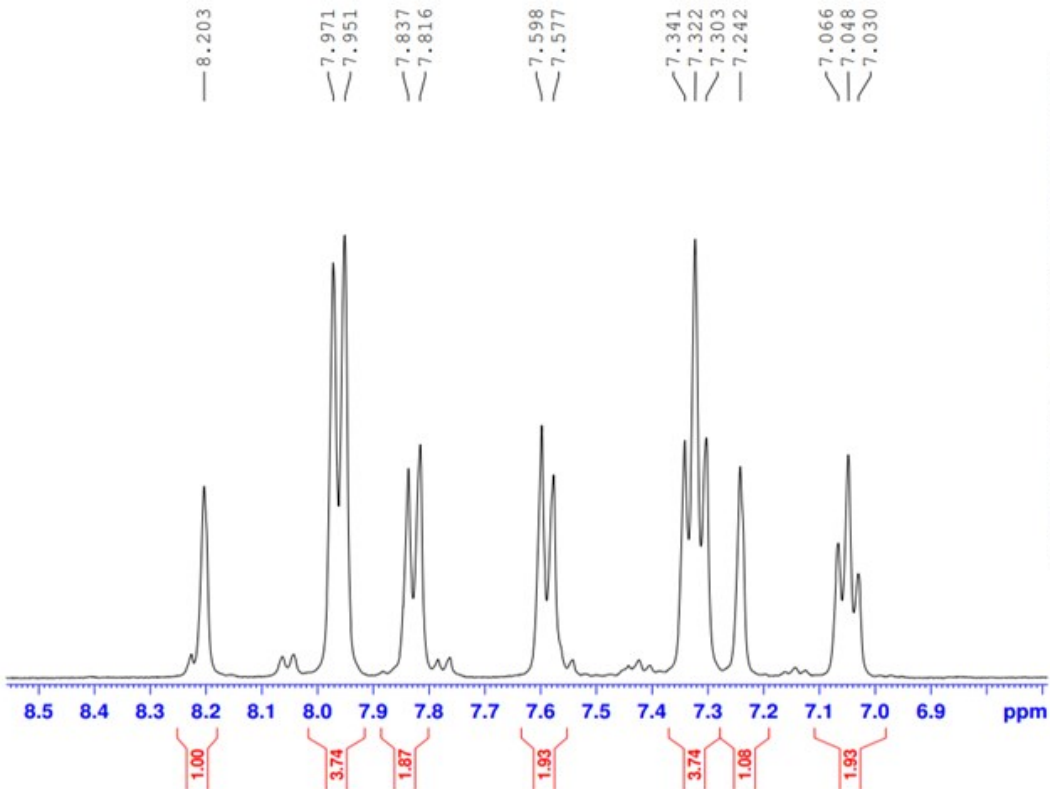
```

NAME      PNU-Zanjan
EXPNO     403
PROCNO    1
Date_     20181111
Time      14.25
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         20
DS         0
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894966 sec
RG         128
DW         62.400 usec
DE         6.50 usec
TE         293.3 K
D1         4.00000000 sec
TD0        1
  
```

```

----- CHANNEL f1 -----
NUC1      1H
P1         14.00 usec
PL1        -2.00 dB
PL1W      11.86359406 W
SFO1      400.2236020 MHz
SI         32768
SF         400.2200000 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```

Sample Code: 4 (Davasaz)



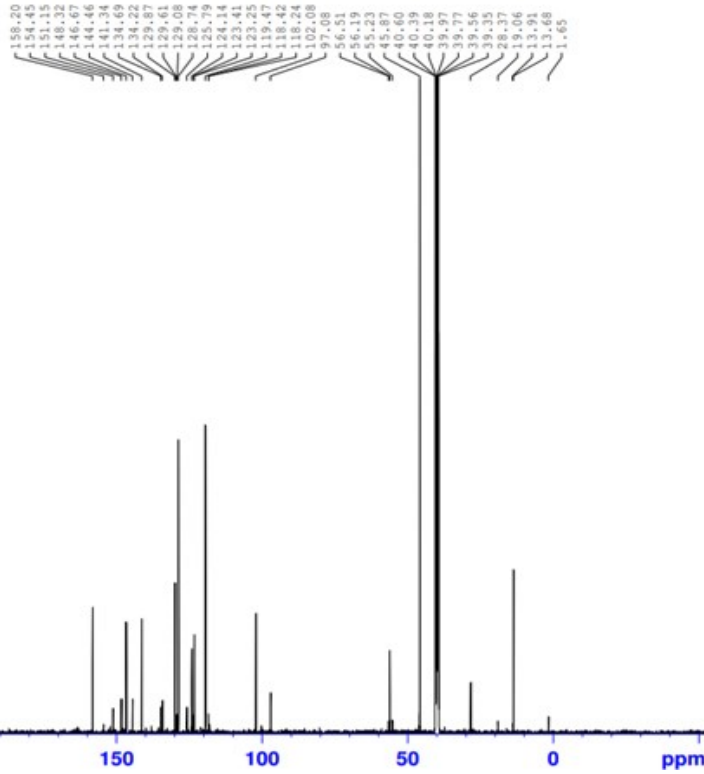
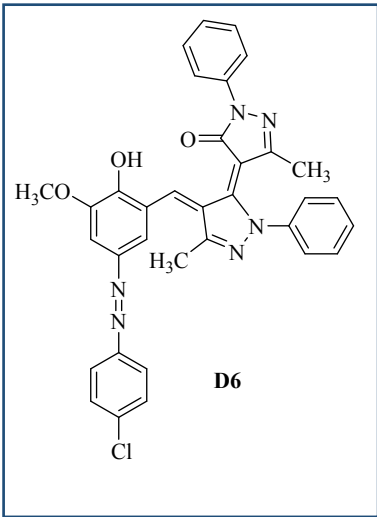
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NAME      PNU-Zanjan
EXPNO     403
PROCNO    1
Date_     20181111
Time      14.25
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         20
DS         0
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894966 sec
RG         128
DW         62.400 usec
DE         6.50 usec
TE         293.3 K
D1         4.00000000 sec
TD0        1
  
```

```

----- CHANNEL f1 -----
NUC1      1H
P1         14.00 usec
PL1        -2.00 dB
PL1W      11.86359406 W
SFO1      400.2236020 MHz
SI         32768
SF         400.2200000 MHz
WDW        EM
SSB         0
LB         0.30 Hz
GB         0
PC         1.00
  
```

Fig <sup>1</sup>H NMR of D6



```

NAME      PNU-Zanjan
EXPNO     409
PROCNO    1
Date_     20181116
Time      15.05
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        8192
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        293.3 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

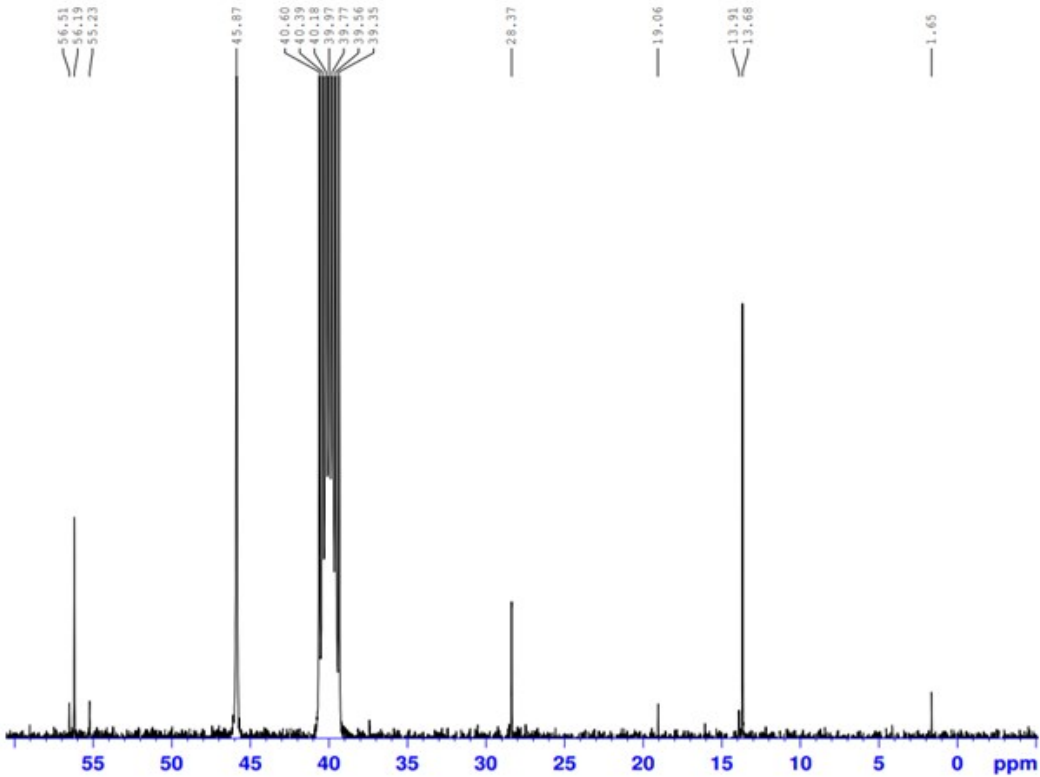
```

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -0.90 dB
PL1W     42.02801895 W
SFO1     100.6479784 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W     11.86359406 W
PL12W    0.28722104 W
PL13W    0.12139934 W
SFO2     400.2216009 MHz
SI        32768
SF       100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

Sample Code: 4 (Davasaz)



```

NAME      PNU-Zanjan
EXPNO     409
PROCNO    1
Date_     20181116
Time      15.05
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        8192
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        293.3 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

```

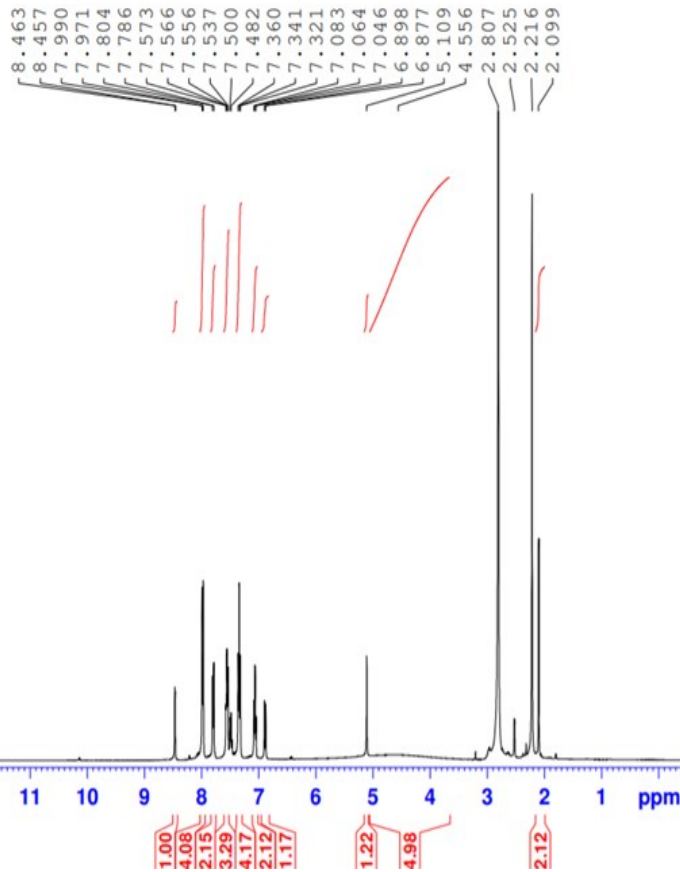
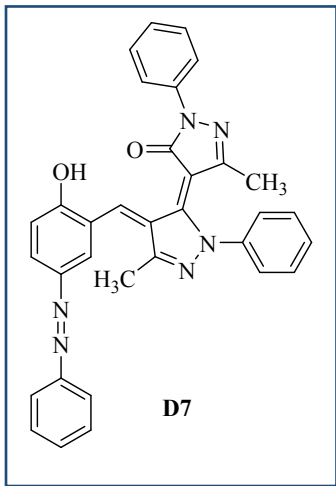
----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -0.90 dB
PL1W     42.02801895 W
SFO1     100.6479784 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W     11.86359406 W
PL12W    0.28722104 W
PL13W    0.12139934 W
SFO2     400.2216009 MHz
SI        32768
SF       100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

Fig <sup>13</sup>C NMR of D6.





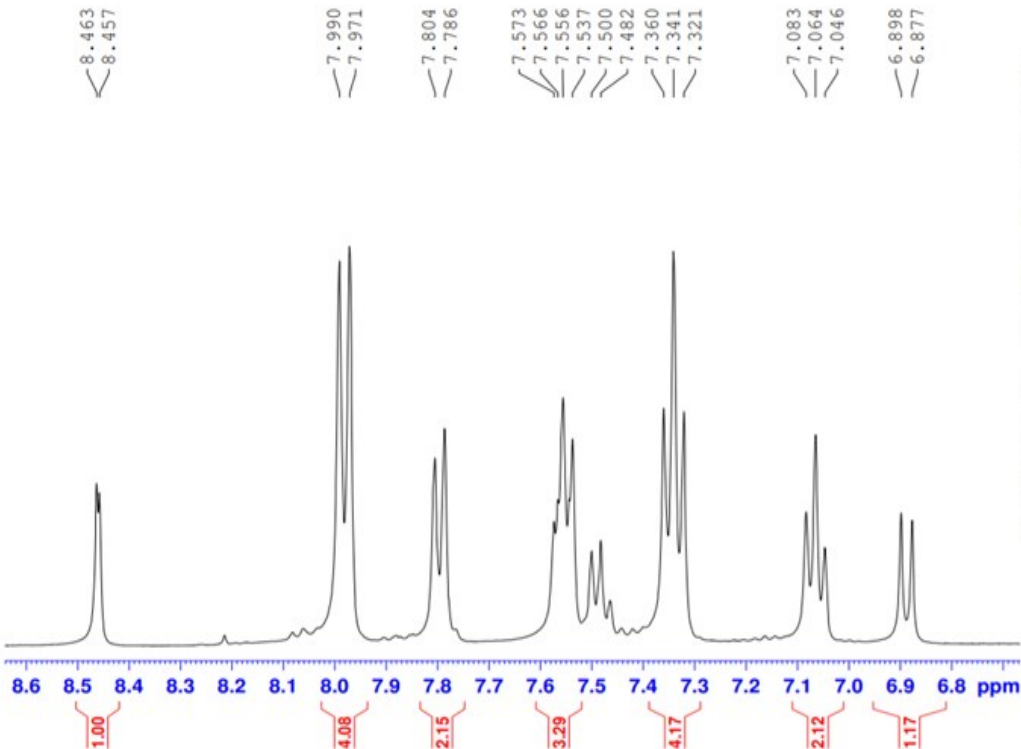
**BRUKER**

NAME PNU-Zanjan  
 EXPNO 413  
 PROCNO 1  
 Date\_ 20190305  
 Time 13.24  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 57  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.2 K  
 D1 4.0000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -2.00 dB  
 PL1W 11.86359406 W  
 SF01 400.2236020 MHz  
 SI 32768  
 SF 400.2200000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Activate  
Go to Settir

Sample Code: 2 (Davasaz)



**BRUKER**

NAME PNU-Zanjan  
 EXPNO 413  
 PROCNO 1  
 Date\_ 20190305  
 Time 13.24  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 57  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 293.2 K  
 D1 4.0000000 sec  
 TD0 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -2.00 dB  
 PL1W 11.86359406 W  
 SF01 400.2236020 MHz  
 SI 32768  
 SF 400.2200000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Activa  
Go to Si

Fig <sup>1</sup>H NMR of D7.



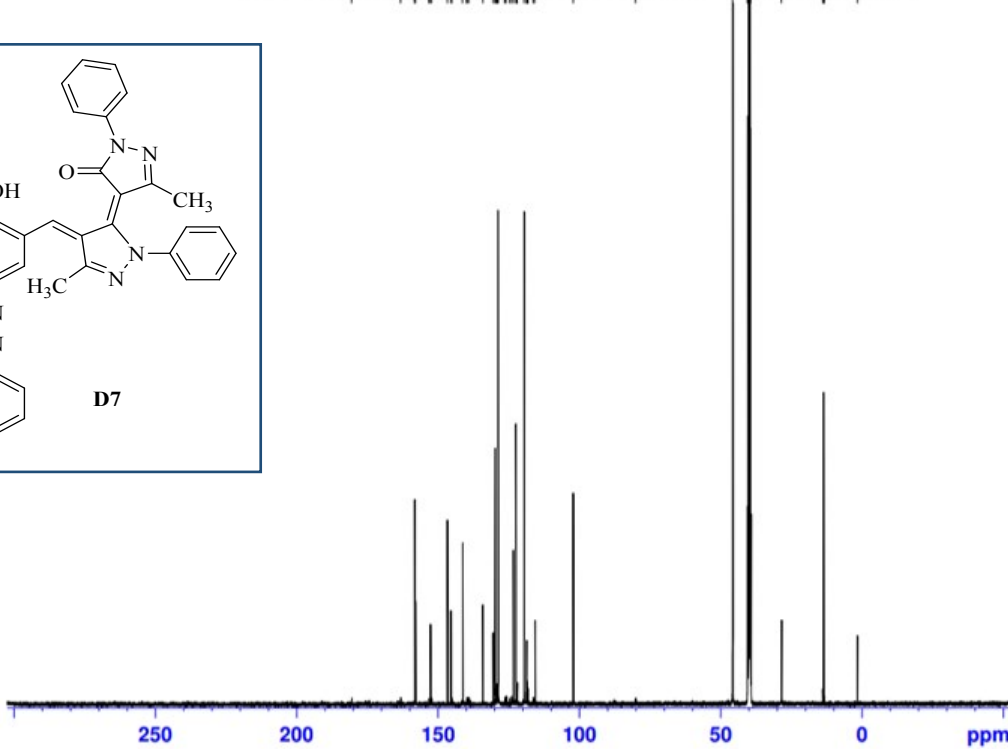
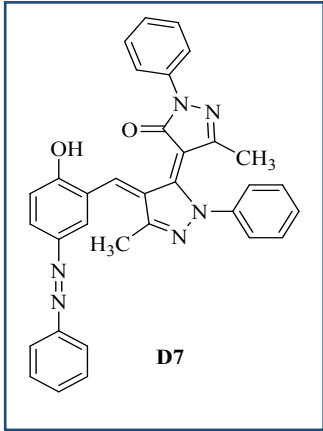
Sample Code: 2 (Davasaz)



NAME PNU-Zanjan  
EXPNO 418  
PROCNO 1  
Date\_ 20190309  
Time 21.10  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 8192  
DS 0  
SWH 35714.285 Hz  
FIDRES 0.544957 Hz  
AQ 0.9175540 sec  
RG 2050  
DW 14.000 usec  
DE 6.50 usec  
TE 293.4 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 13C  
P1 9.00 usec  
PL1 -0.90 dB  
PL1W 42.02801895 W  
SFO1 100.6479784 MHz

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.00 dB  
PL12 14.16 dB  
PL13 17.90 dB  
PL2W 11.86359406 W  
PL12W 0.28722104 W  
PL13W 0.12139934 W  
SFO2 400.2216009 MHz  
SI 32768  
SF 100.6353990 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



Sample Code: 2 (Davasaz)



NAME PNU-Zanjan  
EXPNO 418  
PROCNO 1  
Date\_ 20190309  
Time 21.10  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 8192  
DS 0  
SWH 35714.285 Hz  
FIDRES 0.544957 Hz  
AQ 0.9175540 sec  
RG 2050  
DW 14.000 usec  
DE 6.50 usec  
TE 293.4 K  
D1 1.00000000 sec  
D11 0.03000000 sec  
TDO 1

----- CHANNEL f1 -----  
NUC1 13C  
P1 9.00 usec  
PL1 -0.90 dB  
PL1W 42.02801895 W  
SFO1 100.6479784 MHz

----- CHANNEL f2 -----  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -2.00 dB  
PL12 14.16 dB  
PL13 17.90 dB  
PL2W 11.86359406 W  
PL12W 0.28722104 W  
PL13W 0.12139934 W  
SFO2 400.2216009 MHz  
SI 32768  
SF 100.6353990 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

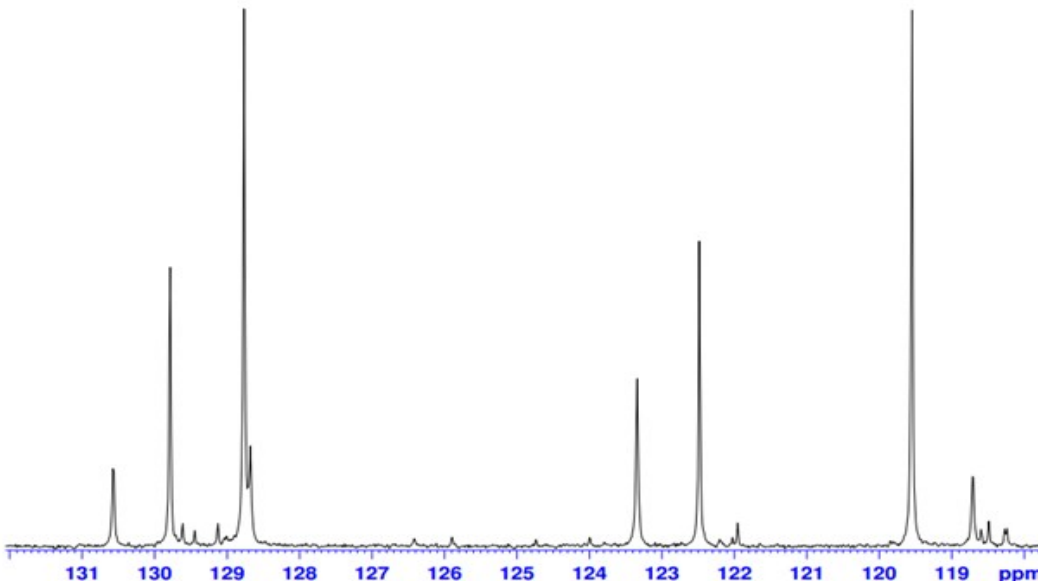
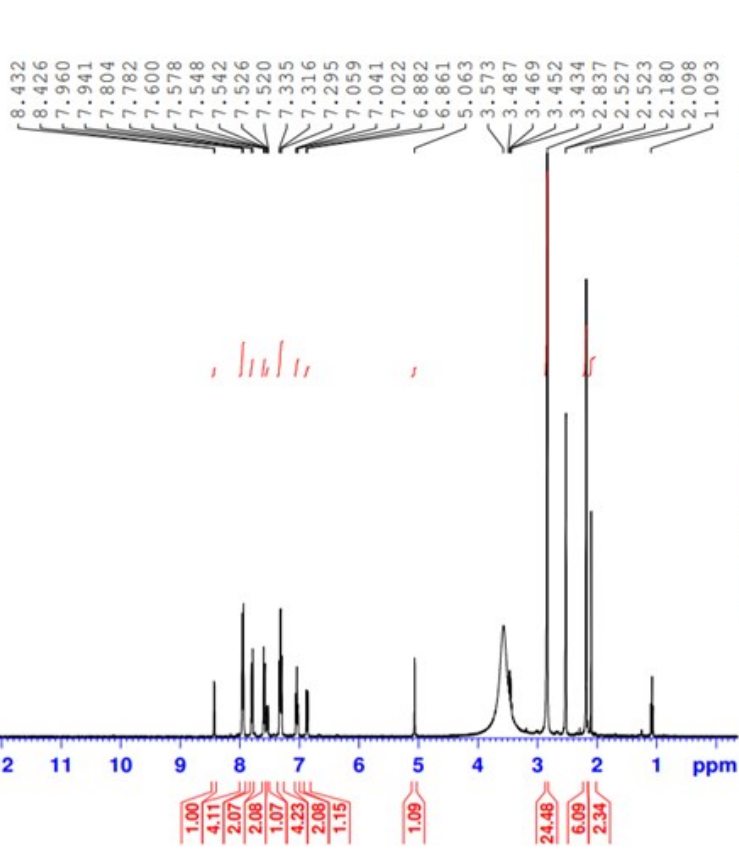
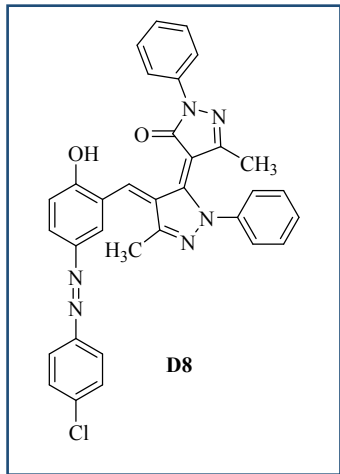


Fig <sup>13</sup>C NMR of D7.

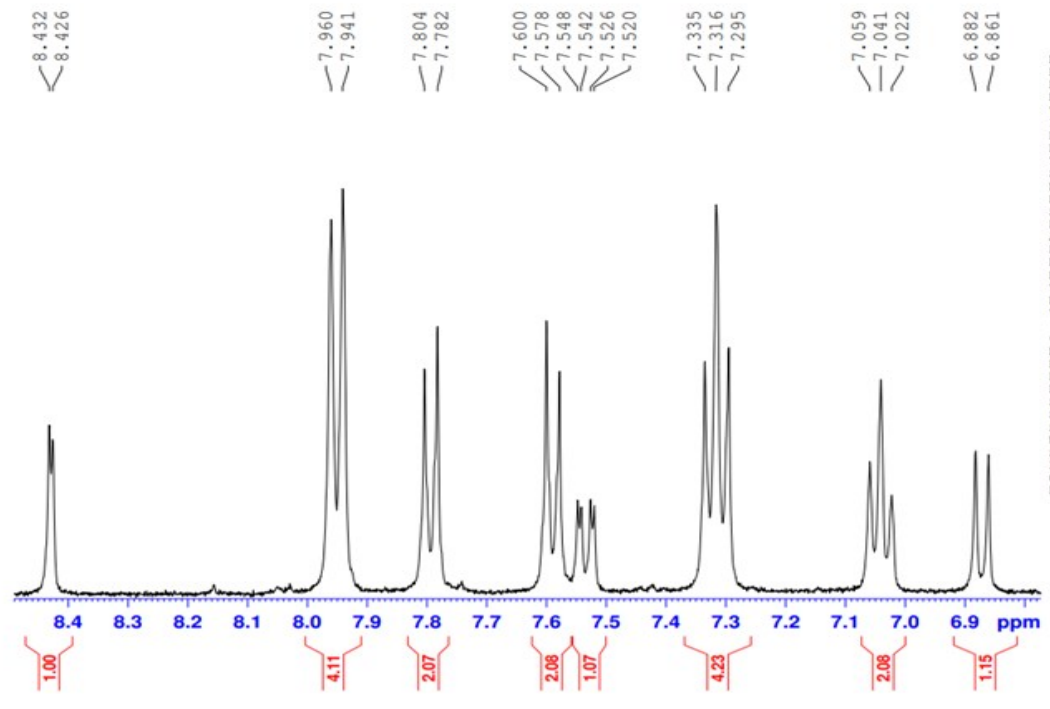


**BRUKER**

NAME PNU-Zanjan  
EXPNO 415  
PROCNO 1  
Date\_ 20190305  
Time 13.44  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 20  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 228  
DW 62.400 usec  
DE 6.50 usec  
TE 293.3 K  
D1 4.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.00 usec  
PL1 -2.00 dB  
PL1W 11.86359406 W  
SF01 400.2236020 MHz  
SI 32768  
SF 400.2200000 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

Sample Code: 4 (Davasaz)

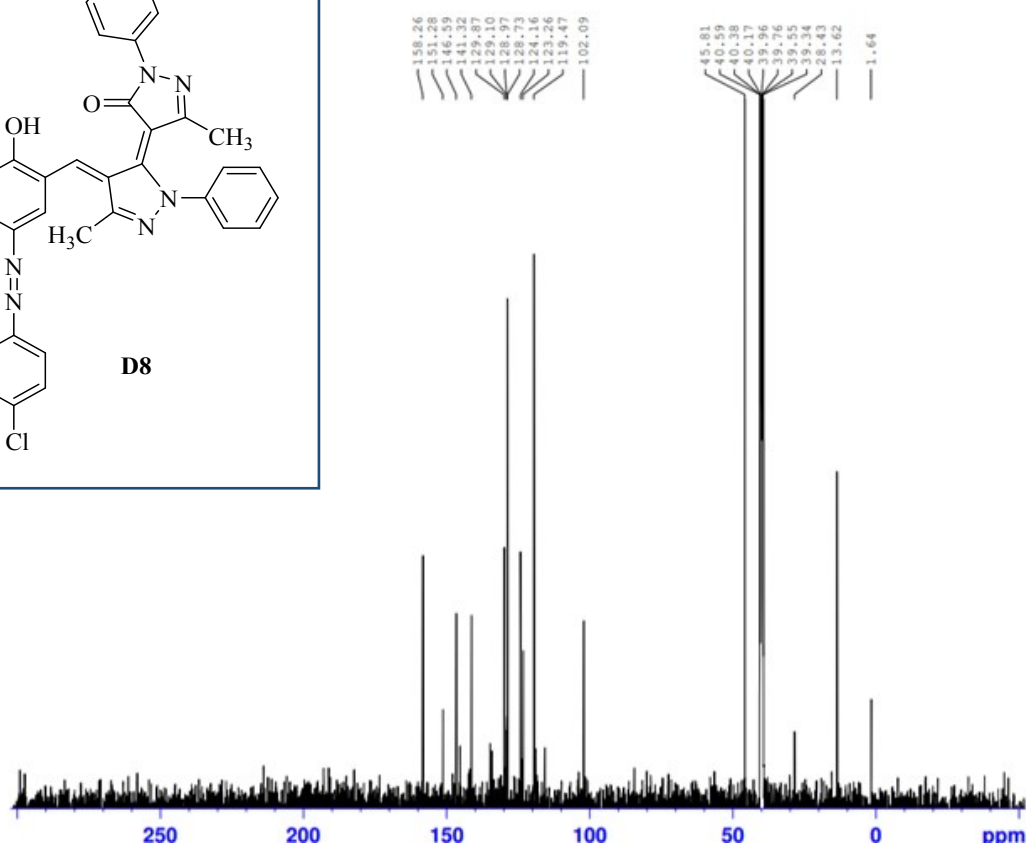
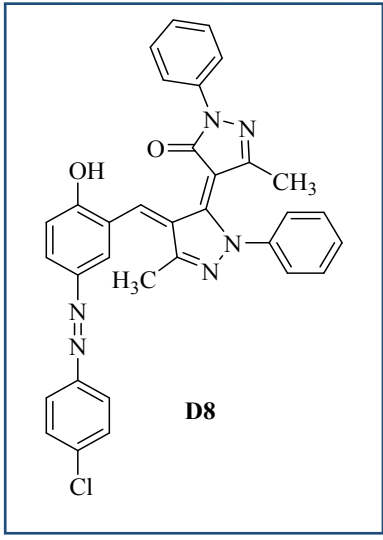


**BRUKER**

NAME PNU-Zanjan  
EXPNO 415  
PROCNO 1  
Date\_ 20190305  
Time 13.44  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 20  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 228  
DW 62.400 usec  
DE 6.50 usec  
TE 293.3 K  
D1 4.00000000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.00 usec  
PL1 -2.00 dB  
PL1W 11.86359406 W  
SF01 400.2236020 MHz  
SI 32768  
SF 400.2200000 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

Fig <sup>1</sup>H NMR of D8.



**BRUKER**

```

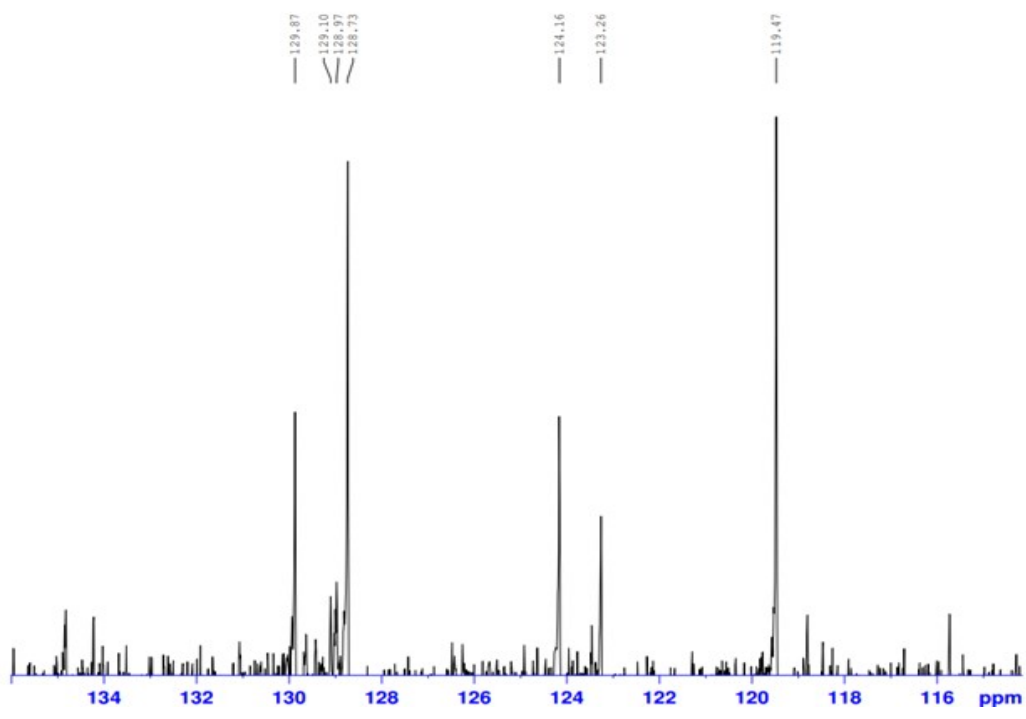
NAME      PNU-Zanjan
EXPNO     419
PROCNO    1
Date_     20190312
Time      19.00
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        2807
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        295.2 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -0.90 dB
PL1W     42.02801895 W
SFO1     100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W     11.86359406 W
PL12W    0.28722104 W
PL13W    0.12139934 W
SFO2     400.2216009 MHz
SI        32768
SF        100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

Sample Code: 4 (Davasaz)



**BRUKER**

```

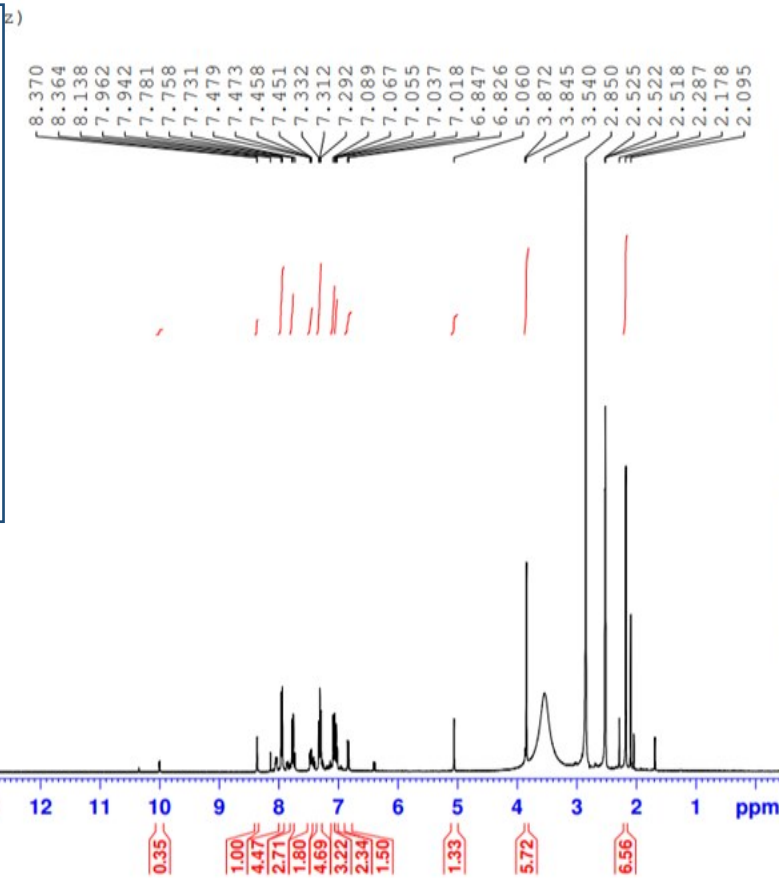
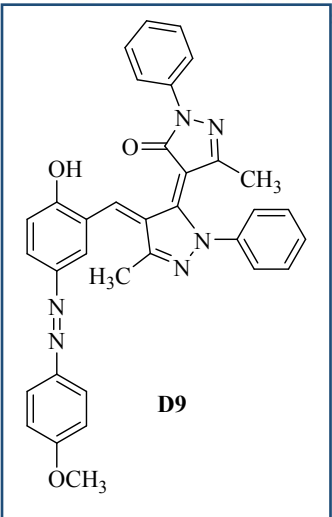
NAME      PNU-Zanjan
EXPNO     419
PROCNO    1
Date_     20190312
Time      19.00
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        2807
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        295.2 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -0.90 dB
PL1W     42.02801895 W
SFO1     100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W     11.86359406 W
PL12W    0.28722104 W
PL13W    0.12139934 W
SFO2     400.2216009 MHz
SI        32768
SF        100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

Fig <sup>13</sup>C NMR of D8.

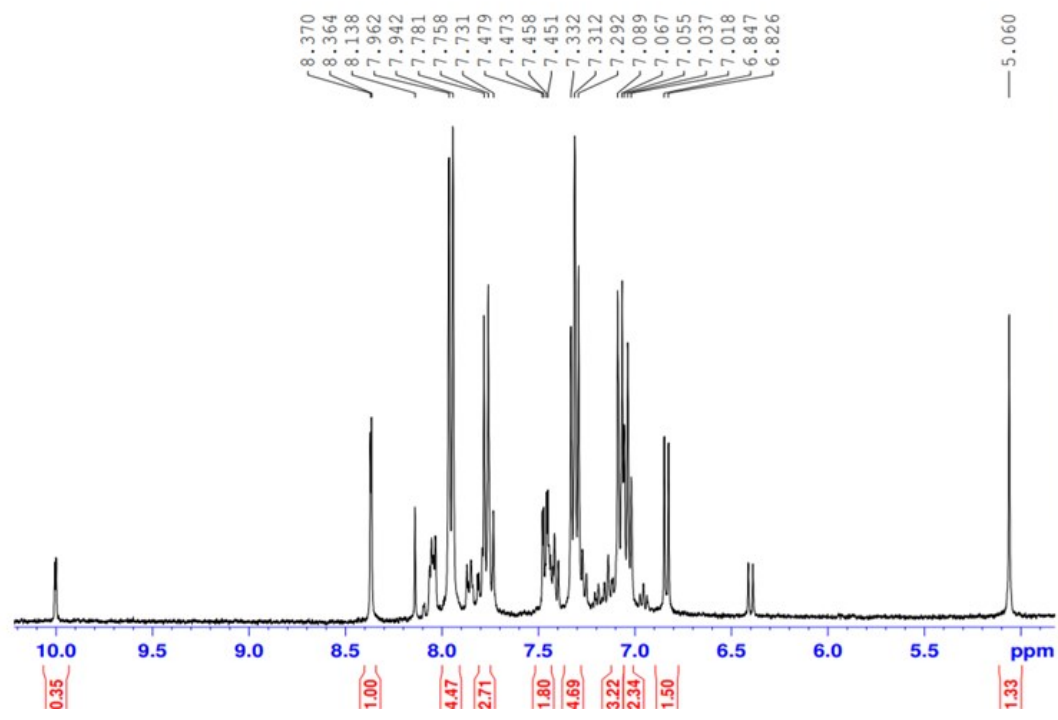


**BRUKER**

NAME PNU-Zanjan  
 EXPNO 426  
 PROCNO 1  
 Date\_ 20190603  
 Time 7.19  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 4.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -2.00 dB  
 PL1W 11.86359406 W  
 SFO1 400.2236020 MHz  
 SI 32768  
 SF 400.2200000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Sample Code: 4 (Davasaz)



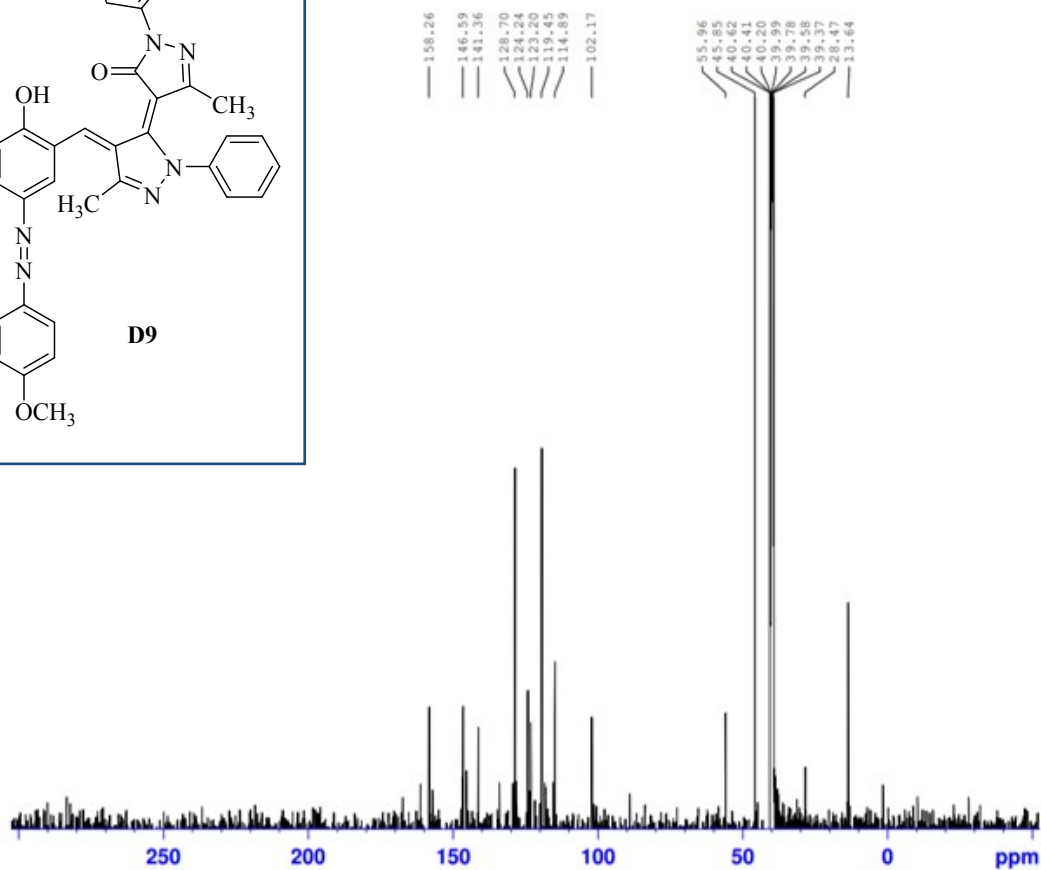
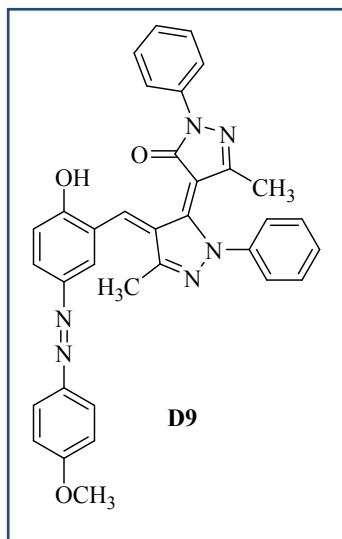
**BRUKER**

NAME PNU-Zanjan  
 EXPNO 426  
 PROCNO 1  
 Date\_ 20190603  
 Time 7.19  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 20  
 DS 0  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 203  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.1 K  
 D1 4.00000000 sec  
 TDO 1

----- CHANNEL f1 -----  
 NUC1 1H  
 P1 14.00 usec  
 PL1 -2.00 dB  
 PL1W 11.86359406 W  
 SFO1 400.2236020 MHz  
 SI 32768  
 SF 400.2200000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

Ac  
Go

Fig <sup>1</sup>H NMR of D9.



```

NAME      PNU-Zanjan
EXPNO     427
PROCNO    1
Date_     20190603
Time      7.30
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        4450
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        296.7 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

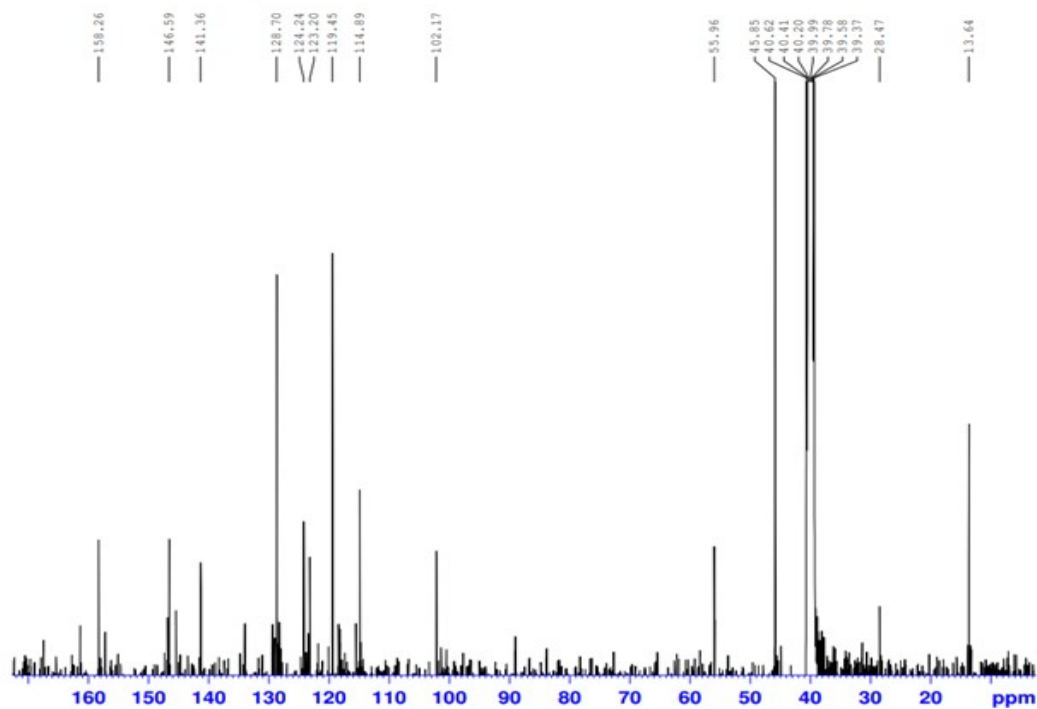
```

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -0.90 dB
PL1W     42.02801895 W
SFO1     100.6479784 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W     11.86359406 W
PL12W    0.28722104 W
PL13W    0.12139934 W
SFO2     400.2216009 MHz
SI        32768
SF       100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

Sample Code: 4 (Davasaz)



```

NAME      PNU-Zanjan
EXPNO     427
PROCNO    1
Date_     20190603
Time      7.30
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        4450
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        296.7 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

```

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -0.90 dB
PL1W     42.02801895 W
SFO1     100.6479784 MHz
  
```

```

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12     14.16 dB
PL13     17.90 dB
PL2W     11.86359406 W
PL12W    0.28722104 W
PL13W    0.12139934 W
SFO2     400.2216009 MHz
SI        32768
SF       100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
  
```

Fig <sup>13</sup>C NMR of D9.

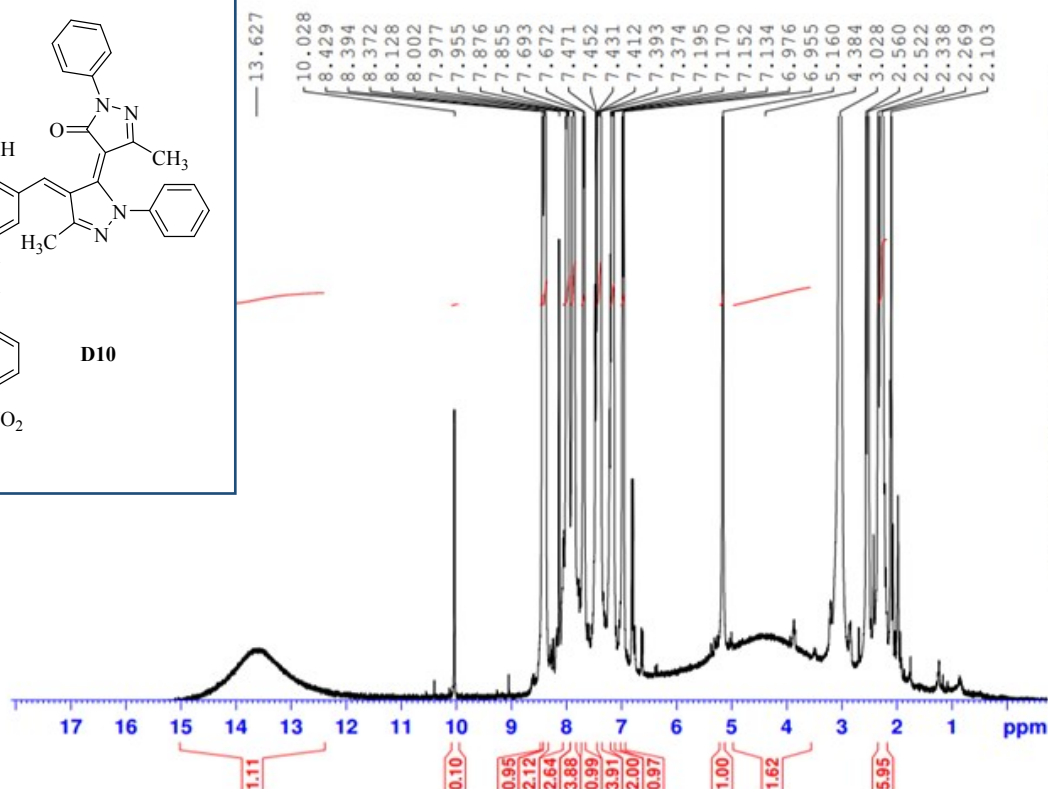
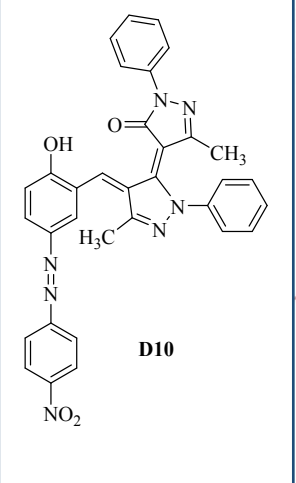


Sample Code:1 (Davasaz-Dr.Saeedian)



NAME PNU-Zanjan  
EXPNO 366  
PROCNO 1  
Date\_ 20180706  
Time 13.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 20  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 114  
DW 62.400 usec  
DE 6.50 usec  
TE 296.4 K  
D1 4.0000000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.00 usec  
PL1 -2.00 dB  
PL1W 11.86359406 W  
SF01 400.2236020 MHz  
SI 32768  
SF 400.2200000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Sample Code:1 (Davasaz-Dr.Saeedian)



NAME PNU-Zanjan  
EXPNO 366  
PROCNO 1  
Date\_ 20180706  
Time 13.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 20  
DS 0  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894966 sec  
RG 114  
DW 62.400 usec  
DE 6.50 usec  
TE 296.4 K  
D1 4.0000000 sec  
TD0 1

----- CHANNEL f1 -----  
NUC1 1H  
P1 14.00 usec  
PL1 -2.00 dB  
PL1W 11.86359406 W  
SF01 400.2236020 MHz  
SI 32768  
SF 400.2200000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

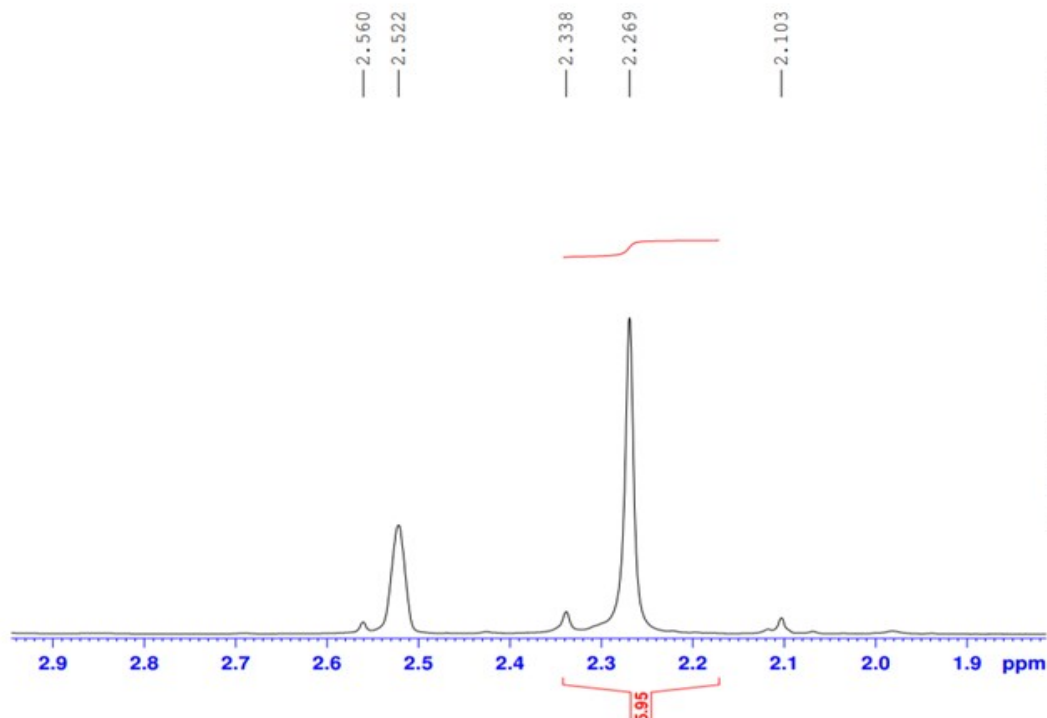
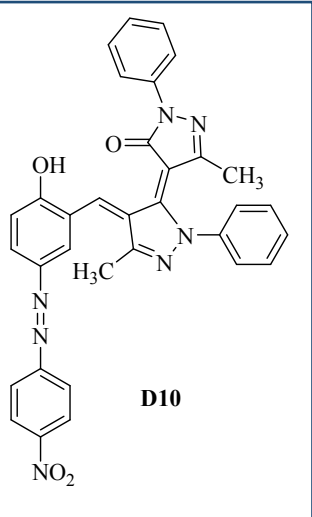
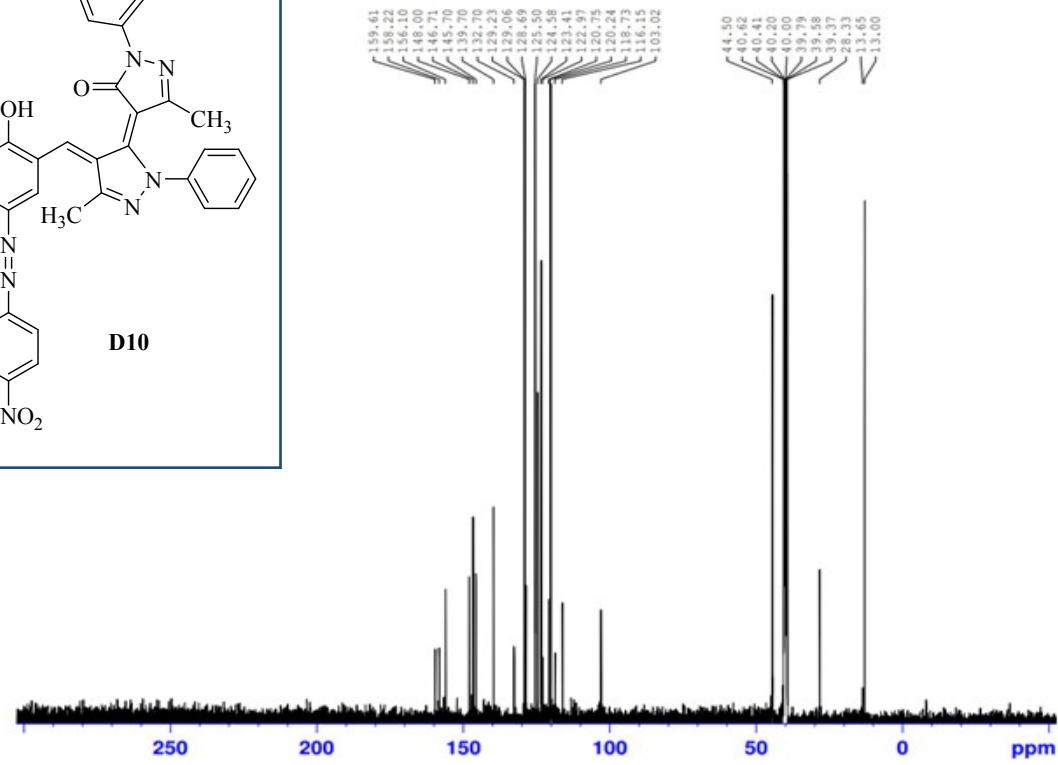


Fig <sup>1</sup>H NMR of D10





-Dr.Saeedian)



```

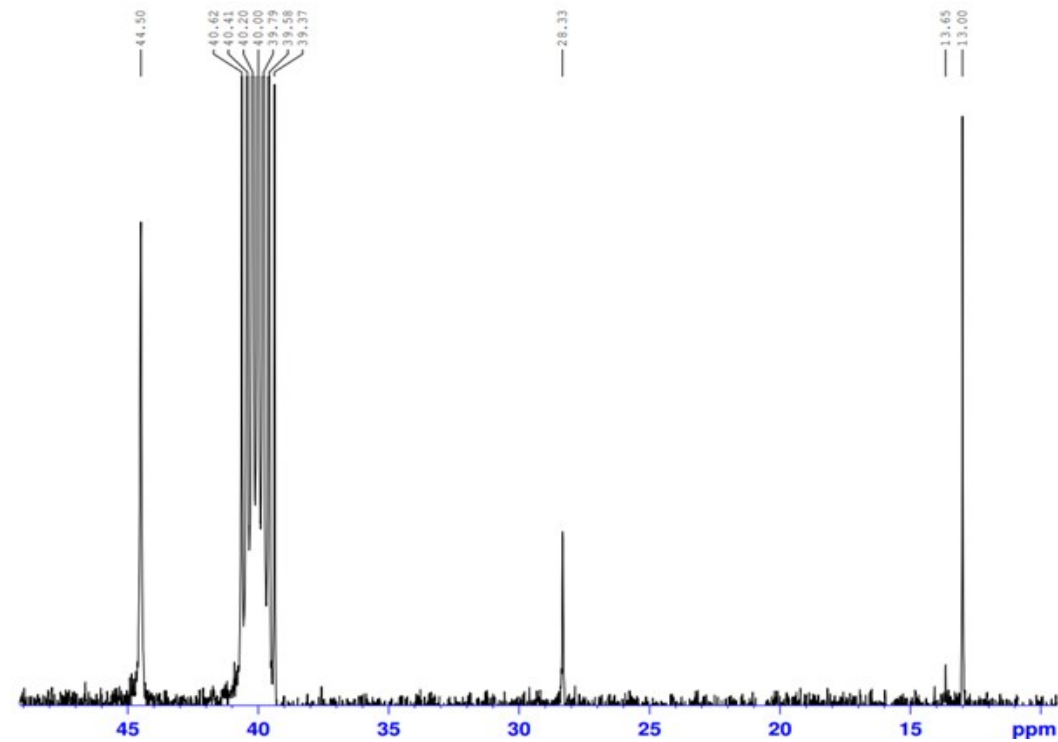
NAME      PNU-Zanjan
EXPNO     367
PROCNO    1
Date_     20180706
Time      13.29
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        1131
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        296.6 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -0.90 dB
PL1W      42.02801895 W
SFO1      100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12      14.48 dB
PL13      17.90 dB
PL2W      11.86359406 W
PL12W     0.26681873 W
PL13W     0.12139934 W
SFO2      400.2216009 MHz
SI        32768
SF        100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

Sample Code:1 (Davasaz-Dr.Saeedian)



```

NAME      PNU-Zanjan
EXPNO     367
PROCNO    1
Date_     20180706
Time      13.29
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg30
TD        65536
SOLVENT   DMSO
NS        1131
DS        0
SWH       35714.285 Hz
FIDRES    0.544957 Hz
AQ        0.9175540 sec
RG        2050
DW        14.000 usec
DE        6.50 usec
TE        296.6 K
D1        1.00000000 sec
D11       0.03000000 sec
TD0       1

----- CHANNEL f1 -----
NUC1      13C
P1        9.00 usec
PL1       -0.90 dB
PL1W      42.02801895 W
SFO1      100.6479784 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     90.00 usec
PL2       -2.00 dB
PL12      14.48 dB
PL13      17.90 dB
PL2W      11.86359406 W
PL12W     0.26681873 W
PL13W     0.12139934 W
SFO2      400.2216009 MHz
SI        32768
SF        100.6353990 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40

```

Fig <sup>13</sup>C NMR of D10.

