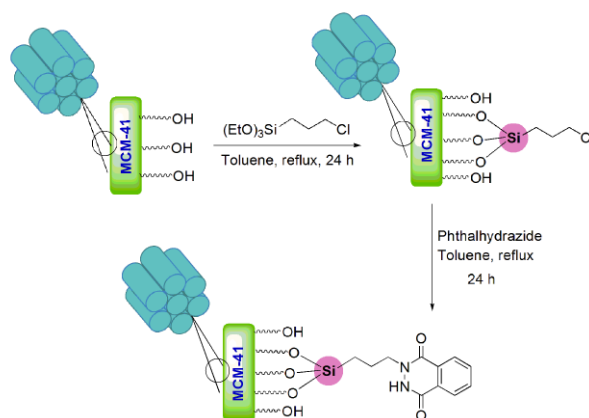


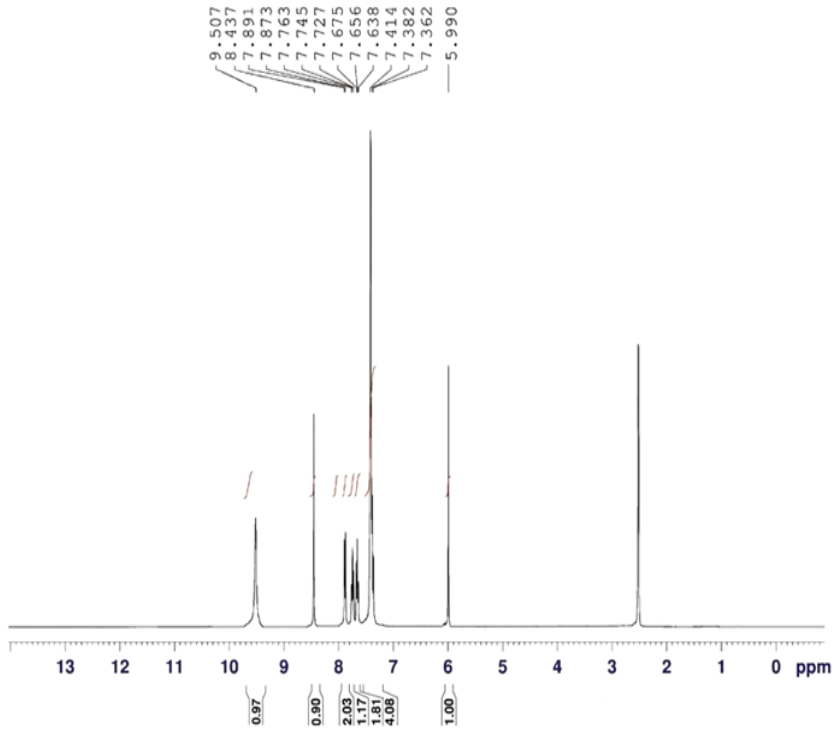
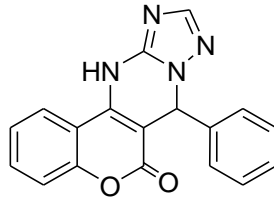
Supplementary data

Preparation and characterization of novel phthalhydrazide functionalized MCM-41 and its application in the one-pot synthesis of 4-hydroxycoumarin fused triazolopyrimidines

Sedigheh Akrami, Bahador Karami* and Mahnaz Farahi



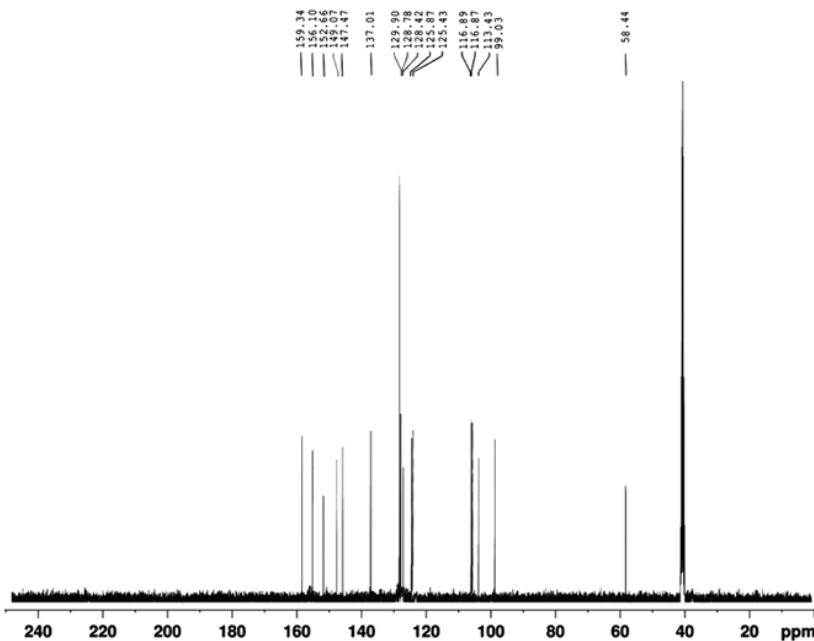
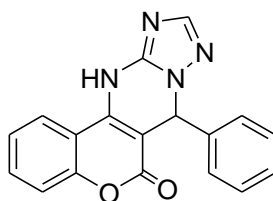
¹H NMR (DMSO-d₆, 400 MHz)



NAME Yasooj UN
EXPNO 101
PROCNO 1
Date_ 20150420
Time 14.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
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 295.6 K
D1 6.0000000 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

¹³C NMR (DMSO-d₆, 100 MHz)

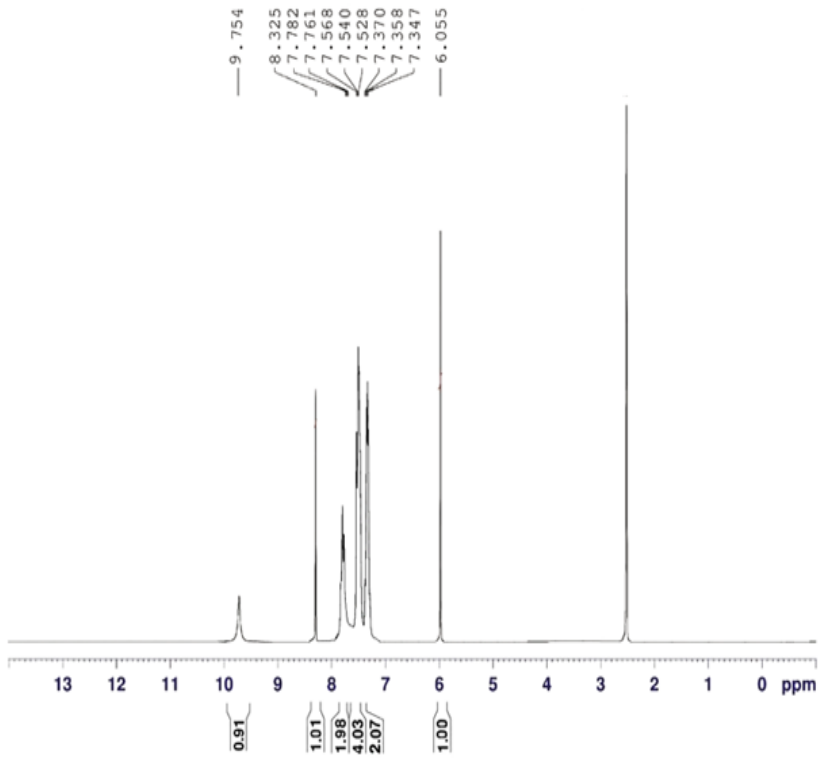
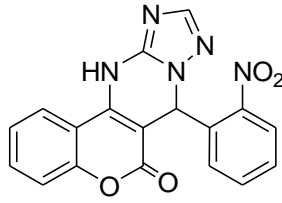


```
NAME      Yasooj UN
EXPNO     102
PROCNO    1
Date_     20150420
Time      14.57
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         65536
SOLVENT   DMSO
NS         70
DS         0
SWH        25252.525 Hz
FIDRES    0.385323 Hz
AQ         1.2976629 sec
RG         2050
DM         19.800 usec
DE         6.50 usec
TE         296.1 K
D1         3.0000000 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
PL1W      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
```

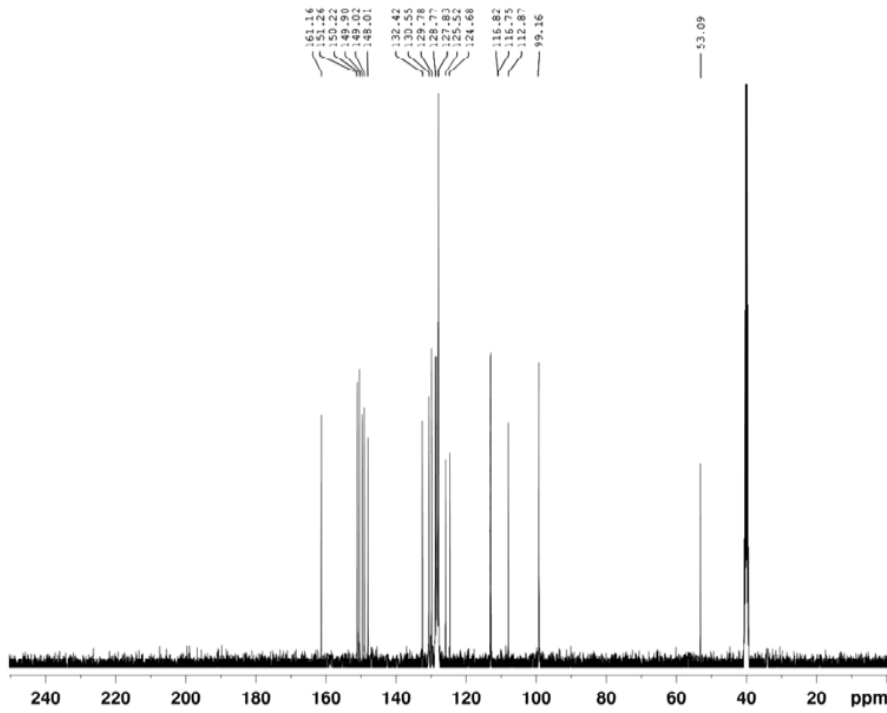
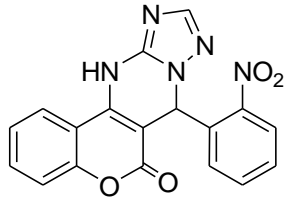
¹H NMR (DMSO-d₆, 400 MHz)



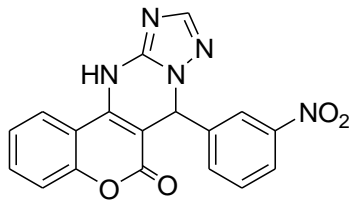
```
NAME      Yasooj UN
EXPNO     103
PROCNO    1
Date_     20150420
Time      15.19
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         32
DS         0
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ         4.0894966 sec
RG         203
DW         62.400 usec
DE         6.50 usec
TE         295.6 K
D1         6.00000000 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
```

¹³C NMR (DMSO-d₆, 100 MHz)



¹H NMR (DMSO-d₆, 400 MHz)

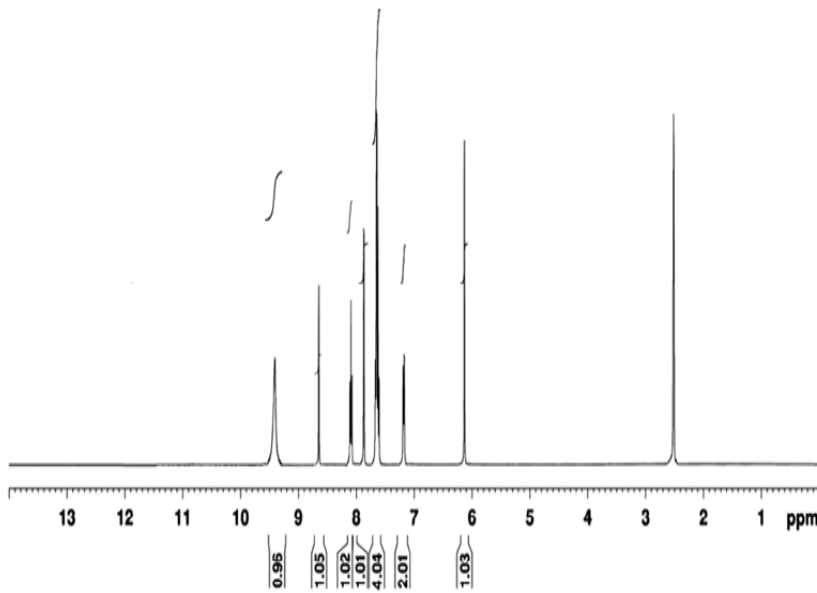


8.461
8.061
8.111
8.107
8.092
7.863
7.671
7.652
7.646
7.626
7.607
7.195
7.176
6.112

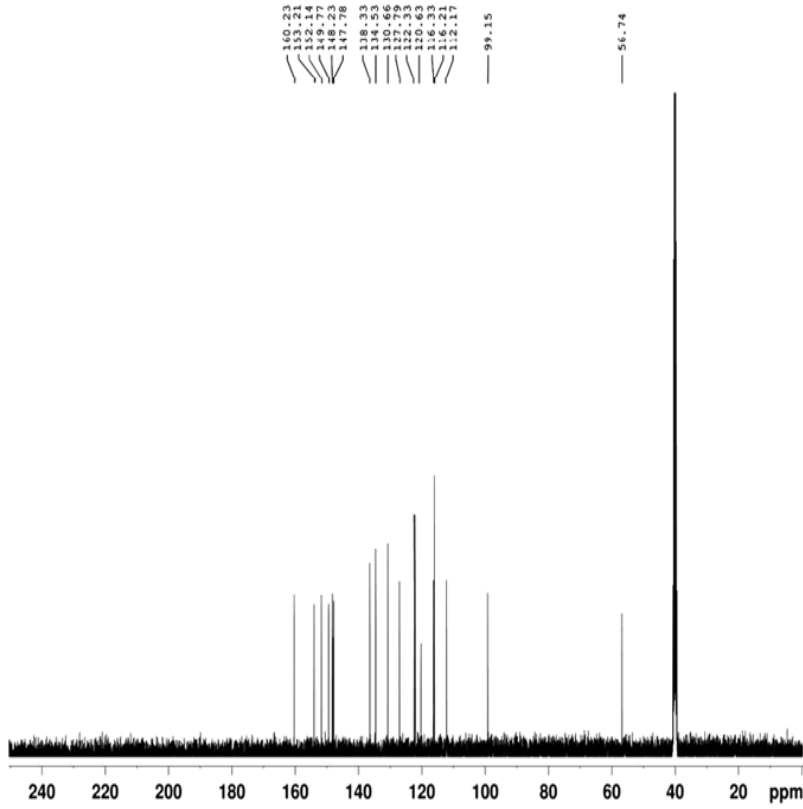
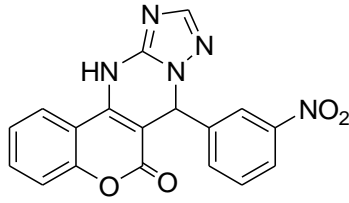


NAME YASOOJ UN
EXPNO 107
PROCNO 1
Date_ 20150420
Time 13.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
ID 65536
SOLVENT DMSO
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.6 K
D1 6.0000000 sec
TD 1

***** 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



¹³C NMR (DMSO-d₆, 100 MHz)

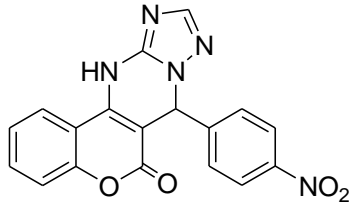


NAME Yasoo1 UN
EXPNO 108
PROCNO 1
Date_ 20150420
Time 16.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 70
DS 0
SWH 25252.325 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DM 19.800 usec
DE 6.50 usec
TE 296.1 K
D1 3.0000000 sec
D11 0.0300000 sec
TDO 1

----- 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
Pz2 -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
S1 32768
SF 100.6353990 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹H NMR (DMSO-d₆, 400 MHz)

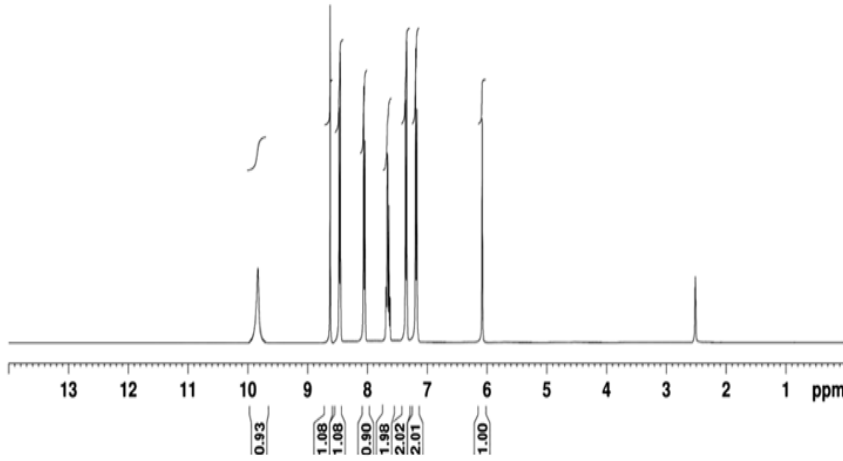


9.821
8.611
8.492
8.476
8.086
8.062
7.671
7.652
7.646
7.626
7.507
7.504
7.543
7.195
7.174
6.081

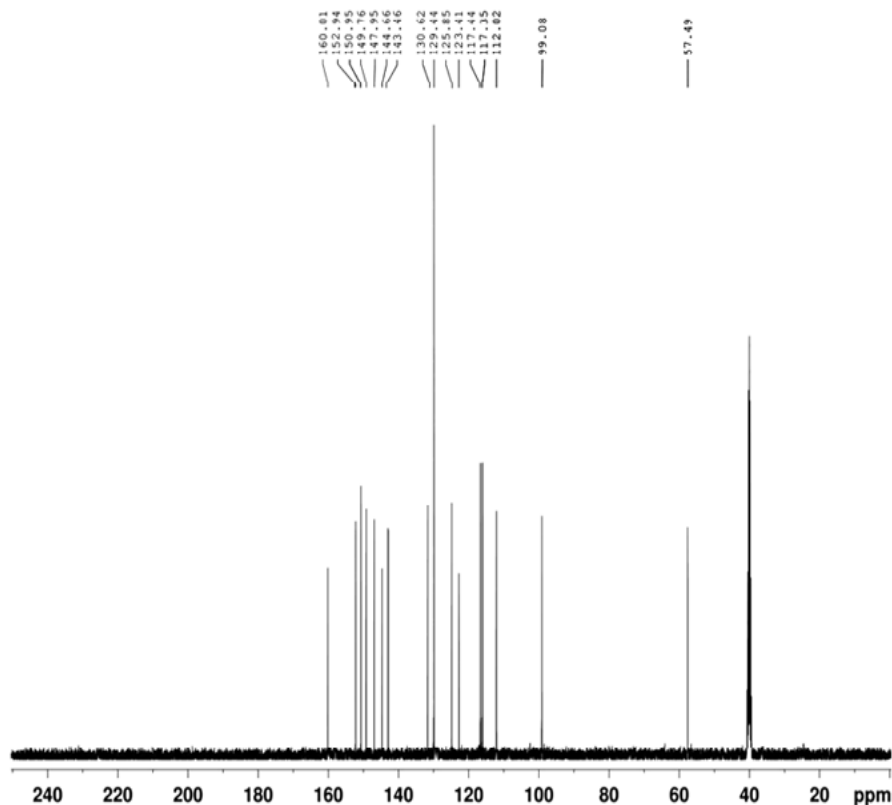
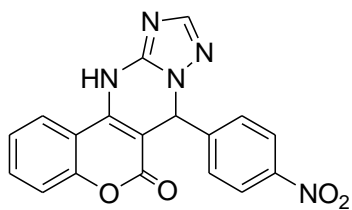


NAME Yasooj UN
EXPNO 105
PROCNO 1
Date_ 20150420
Time 15.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.6 K
D1 6.00000000 sec
TDO 1

***** 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



¹³C NMR (DMSO-d₆, 100 MHz)

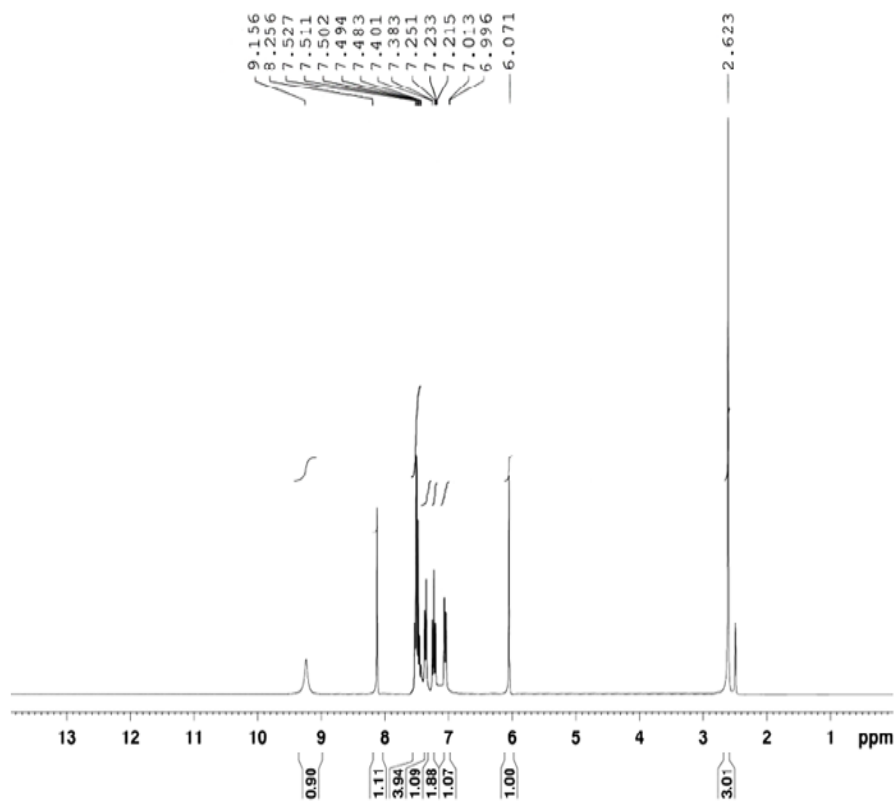
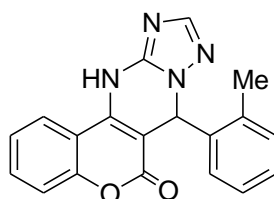


```
NAME          Yasooj UN
EXPNO          106
PROCNO         1
Date_          20150420
Time           15.43
INSTRUM        spect
PROBHD         5 mm PABBO BB-
PULPROG        zgpg
TD              65536
SOLVENT        DMSO
NS              70
DS              0
SWH            25252.525 Hz
FIDRES         0.385323 Hz
AQ             1.2976629 sec
RG             2050
DW             19.800 usec
DE             6.50 usec
TE             296.1 K
D1             3.0000000 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
PCPDZ          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
```

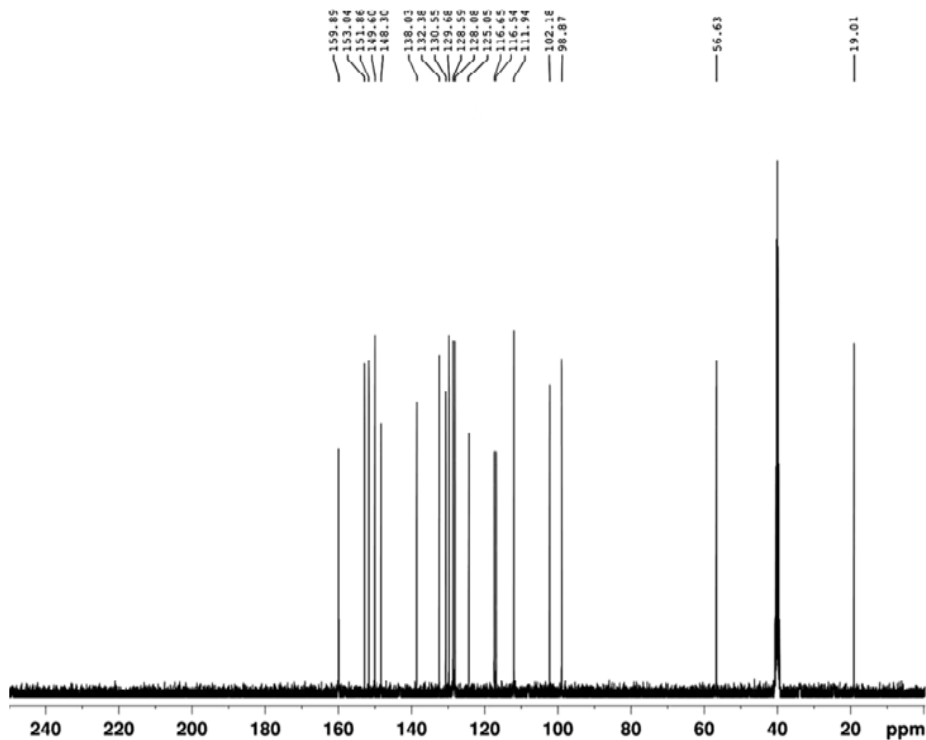
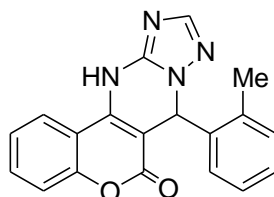
¹H NMR (DMSO-d₆, 400 MHz)



```
NAME      Yasooj UN
EXPNO     109
PROCNO    1
Date_     20150420
Time      16.34
INSTRUM   spect
PROBHD    5 mm PABBO DD-
PULPROG   zg30
TD        65536
SOLVENT   DMSO
NS        32
DS        0
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        203
NW        62.400 usec
DE        6.50 usec
TE        295.6 K
D1        6.00000000 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
```

¹³C NMR (DMSO-d₆, 100 MHz)



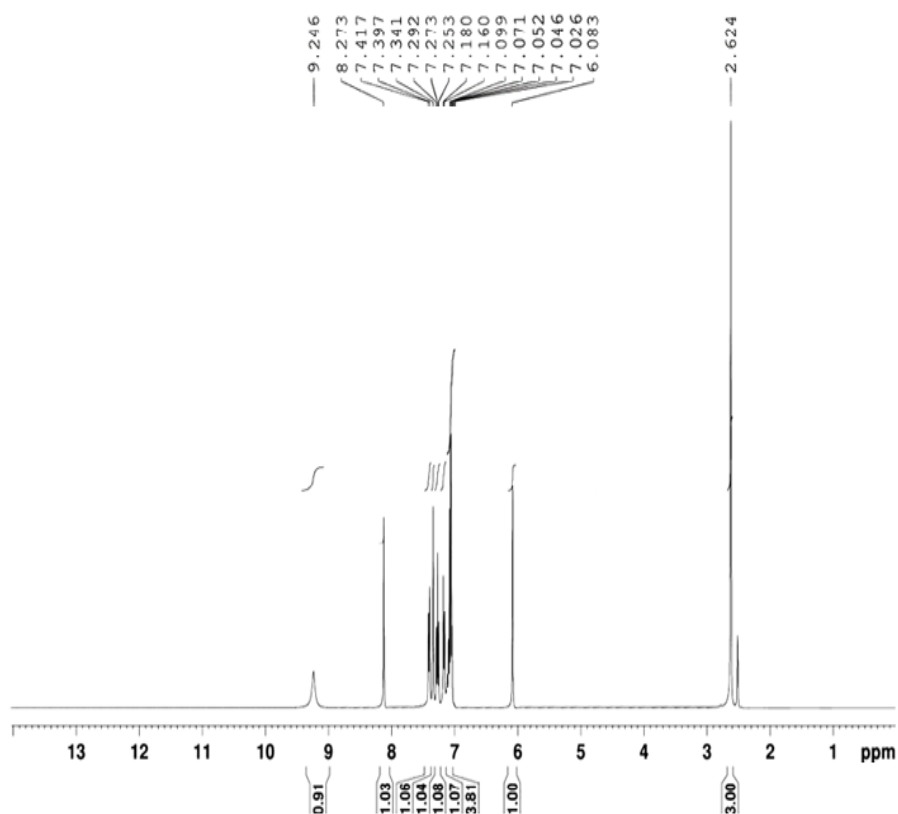
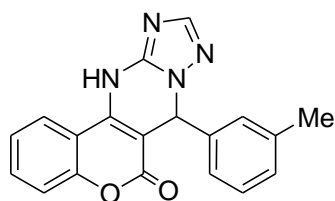
```

NAME          Yaxooj UN
EXPNO         110
PROCNO        1
Date_         20150420
Time          16.39
INSTRUM       spect
PROBHD        5 mm PABBO BBO
PULPROG       zgpg
ID            65536
SOLVENT       DMSO
NS            70
DS            0
SWH           25252.525 Hz
FIDRES        0.385323 Hz
AQ            1.2976629 sec
RG            2050
DW            19.800 usec
DE            6.30 usec
TE            296.1 K
D1            3.0000000 sec
d11           0.0300000 sec
TDO           1

----- CHANNEL f1 -----
NUC1          13C
P1            9.00 usec
PL1           -0.30 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          17.30 dB
PL2W          11.86359406 W
PL12W         0.28722104 W
PL13W         0.12139934 W
SFO2          400.2216009 MHz
SI            32768
SF            100.6353990 MHz
WDW           BH
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

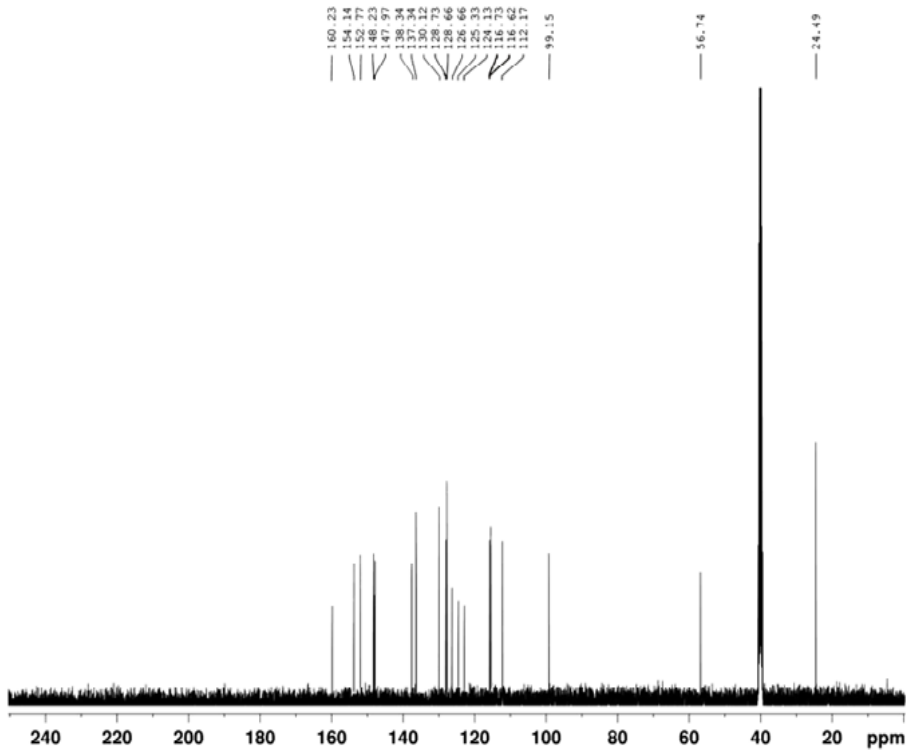
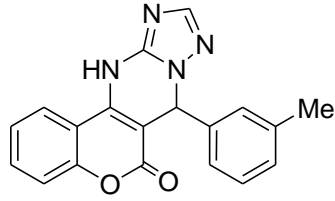
¹H NMR (DMSO-d₆, 400 MHz)



```
NAME      Yasooj UN
EXPNO     111
PROCNO    1
Date_     20150421
Time      08.14
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         32
DS         0
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         203
DM         62.400 usec
DE         6.50 usec
TE         295.6 K
D1         6.00000000 sec
TD0        1
```

```
***** CHANNEL f1 *****
NUC1      1H
P1        14.00 usec
PL1       -2.00 dB
PL1W      11.86339406 W
SFO1      400.2236020 MHz
SI        32768
SF        400.2200000 MHz
WDW       EM
SSD        0
LB         0.30 Hz
GB         0
PC         1.00
```

¹³C NMR (DMSO-d₆, 100 MHz)



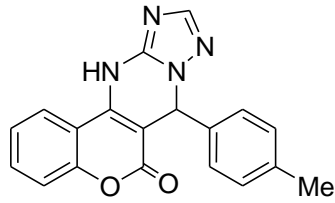
```

NAME      Yasoo1 UN
EXPNO     112
PROCNO    1
Date_     20160421
Time      08.19
INSTRUM   spect
PROBHD    5 mm PABBO DD-
PULPROG   zgpg
ID         65536
SOLVENT   DMSO
NS         70
DS         0
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DM         19.800 usec
DE         6.50 usec
TE         296.1 K
D1         3.0000000 sec
D11        0.0300000 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
FL2        -2.00 dB
FL12       14.10 dB
PL13       17.30 dB
PL2W       11.86359405 W
PL12W      0.28722104 W
PL13W      0.12139534 W
SFO2       400.2216009 MHz
SI         32768
SF         100.6353990 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GD         0
FC         1.40
    
```

¹H NMR (DMSO-d₆, 400 MHz)



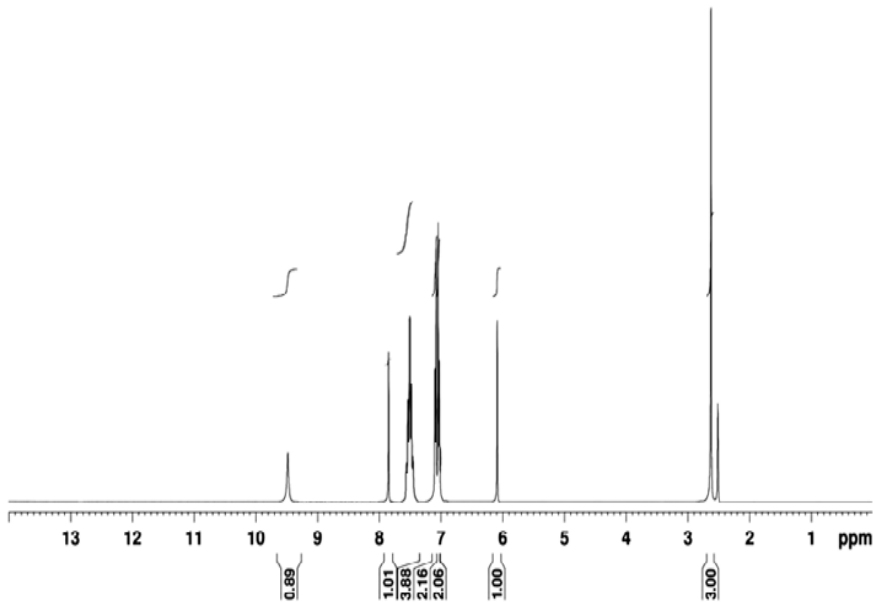
9.492
7.853
7.697
7.682
7.679
7.663
7.650
7.101
7.081
7.047
7.027
— 6.091

— 2.628

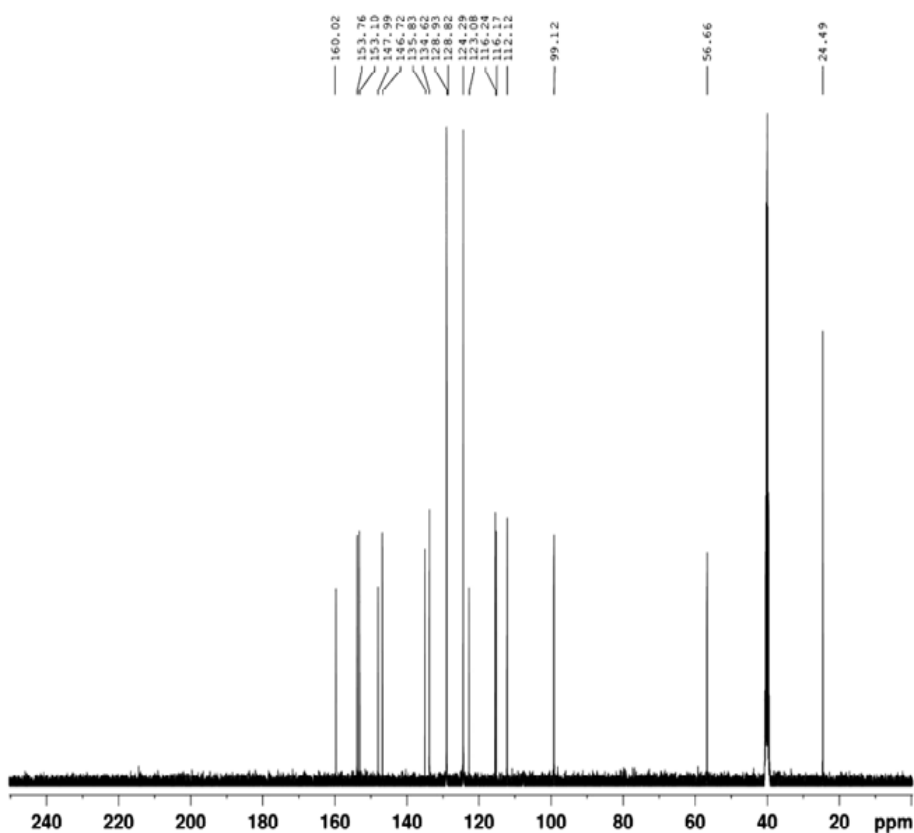
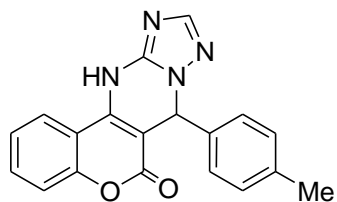


```
NAME      Yasooj UN
EXPNO     113
PROCNO    1
Date_     20150421
Time      08.48
INSTRUM   spect
PROBHD    5 mm PABBO BBI-
PULPROG   zg30
TD         65536
SOLVENT   DMSO
NS         32
DS         0
SWH        8012.820 Hz
FIDRES     0.122266 Hz
AQ         4.0894966 sec
RG         203
DM         62.400 usec
DE         6.50 usec
TE         295.6 K
D1         6.0000000 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
```



¹³C NMR (DMSO-d₆, 100 MHz)



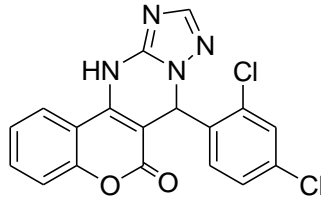
```

NAME      Yasoo1 UN
EXPNO     114
PROCNO    1
Date_     20150421
Time      08.43
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         65536
SOLVENT   DMSO
NS         70
DS         0
SWH       25252.525 Hz
FIDRES    0.385323 Hz
AQ         1.2976629 sec
RG         2050
DM         19.800 usec
DE         6.50 usec
TE         296.1 K
D1         3.0000000 sec
D11        0.0300000 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         100.6333990 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
DC         1.40
    
```

¹H NMR (DMSO-d₆, 400 MHz)



— 10.917

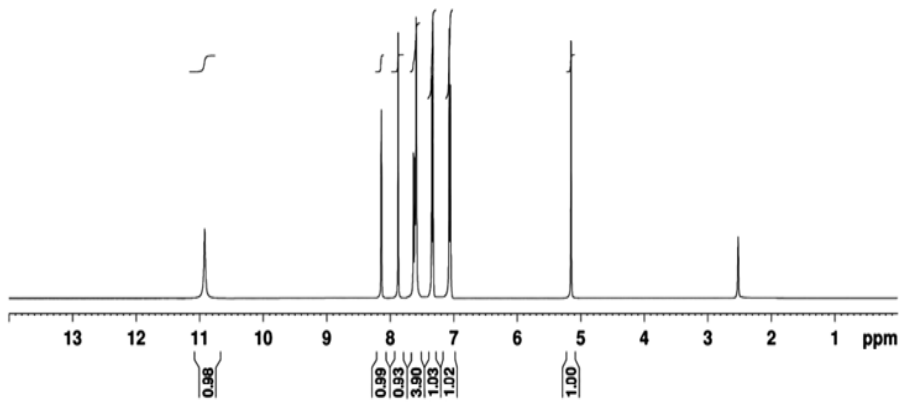
8.256
7.862
7.654
7.636
7.613
7.335
7.313
7.052
7.030

— 5.345

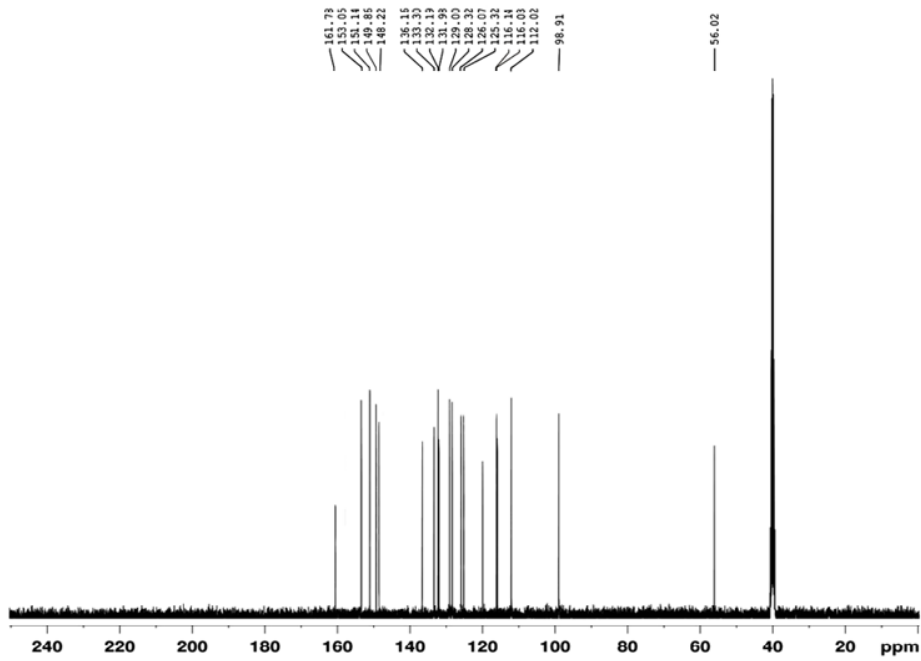
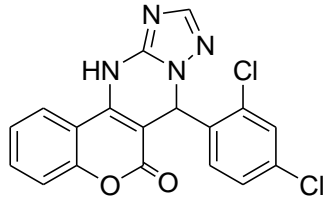


```
NAME      Yasooj UN
EXPNO     117
PROCNO    1
Date_     20150421
Time      09.29
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg30
TD        65536
SOLVENT   DMSO
NS        32
DS        0
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894966 sec
RG        233
DW        62.400 usec
DE        6.50 usec
TE        295.6 K
D1        6.0000000 sec
TDO       1
```

```
----- CHANNEL f1 -----
NUC1      1H
P1        14.00 usec
PL1       -2.00 dB
PLW       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
```



¹³C NMR (DMSO-d₆, 100 MHz)



```

NAME      Yassuj UN
EXPNO     118
PROCNO    1
Date_     20150421
Time      09:39
INSTRUM   spect
PROBHD    5 mm PABBO BBI
PULPROG   zgpg
TD         65536
SOLVENT   DMSO
NS         70
DS         0
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
TM         19.800 usec
DE         6.50 usec
TE         296.1 K
D1         3.0000000 sec
d11        0.0300000 sec
TD0        1

----- CHANNEL f1 -----
NUC1       13C
P1         9.00 usec
PL1        -0.90 dB
PL1H       42.02801895 W
SFO1       100.6479784 MHz

----- CHANNEL f2 -----
CFDPFG2   waltz16
NUC2       1H
PCPD2     90.00 usec
PL2        -2.00 dB
PL12       14.16 dB
PL13       17.90 dB
PL12H     11.86359406 W
PL12W     0.28722104 W
PL13W     0.12139934 W
SFO2       400.2216009 MHz
SI         32768
SE         100.6353990 MHz
RGW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
    
```