

Supporting Information

Efficient One-Pot synthesis and Dehydrogenation of Tricyclic Dihydropyrimidines Catalyzed by OMS-2-SO₃H, and Application of the Products as Colorimetric Chemosensors

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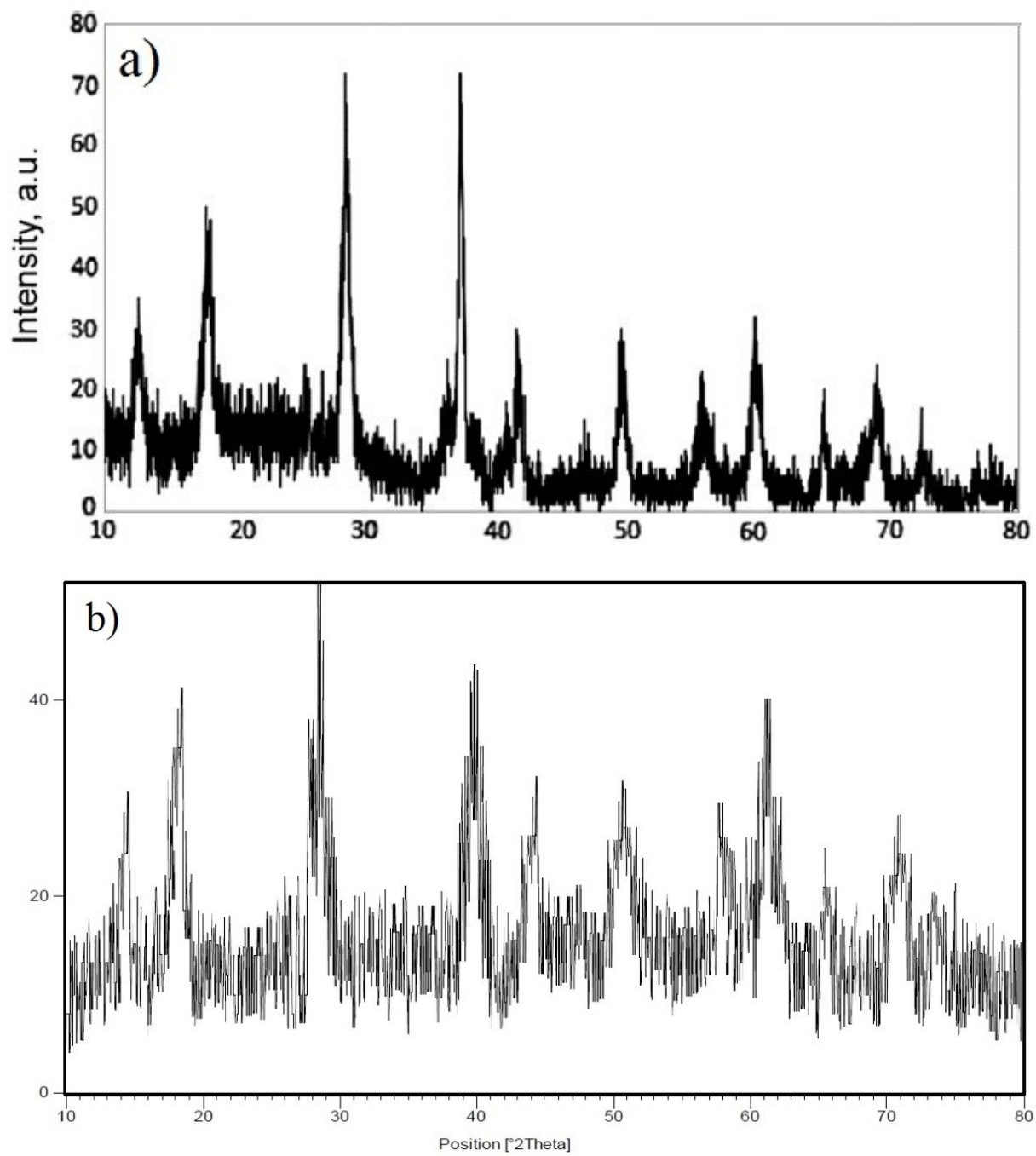


Fig. s1 X-ray diffraction patterns for the OMS-2 (a) and its sulfonated form (b).

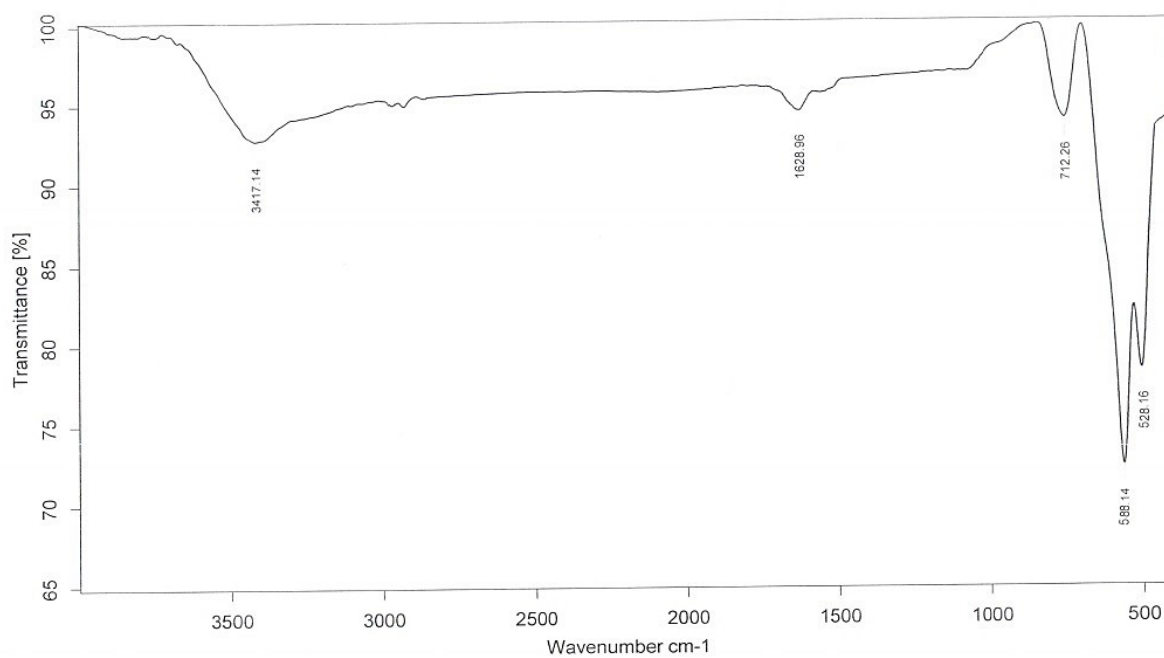
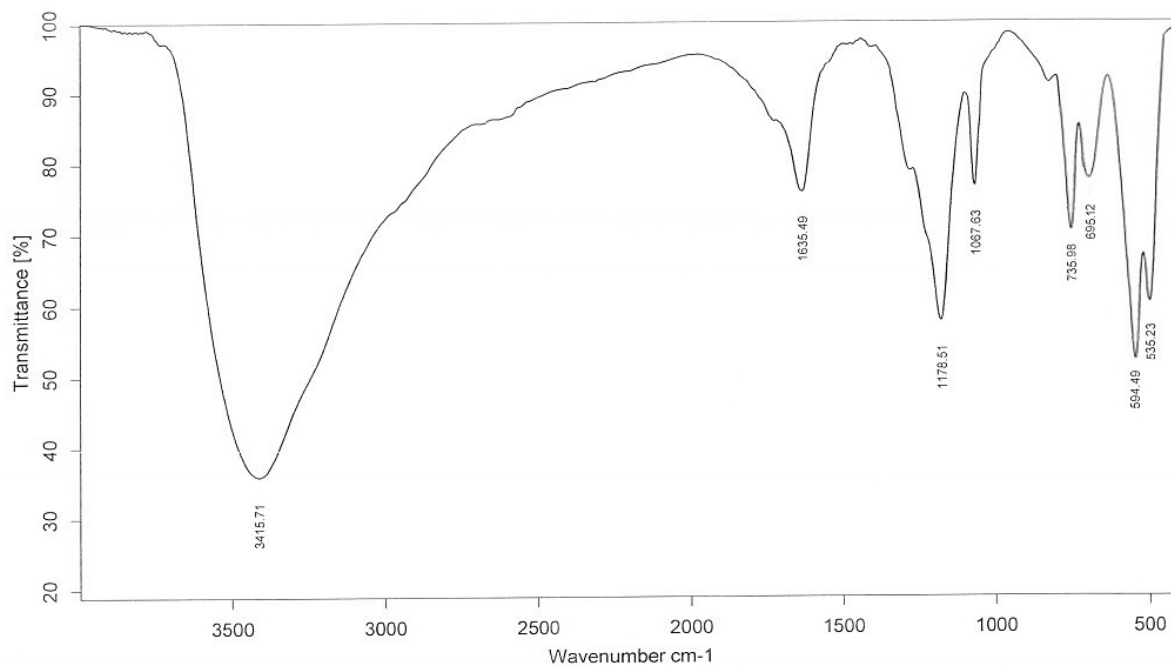


Fig. s2 FT-IR spectra of OMS-2-SO₃H (top) and OMS-2 (bottom).

Spectral data of 5a

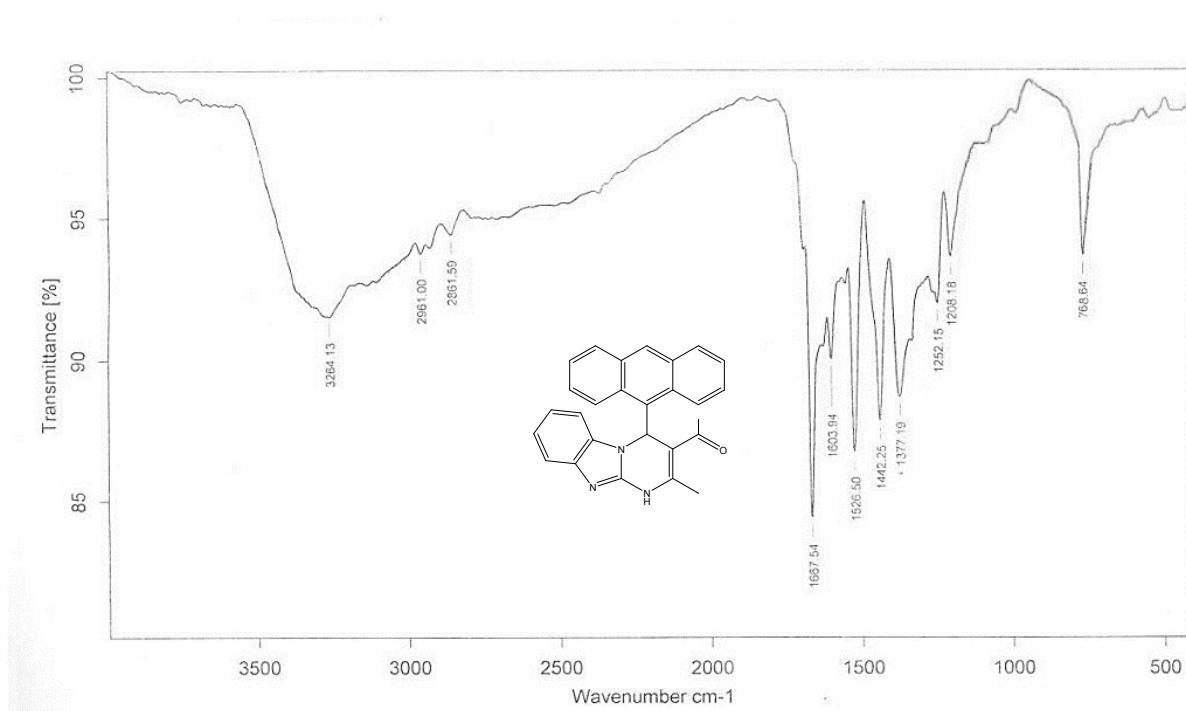


Fig. s3 FTIR spectrum of 5a

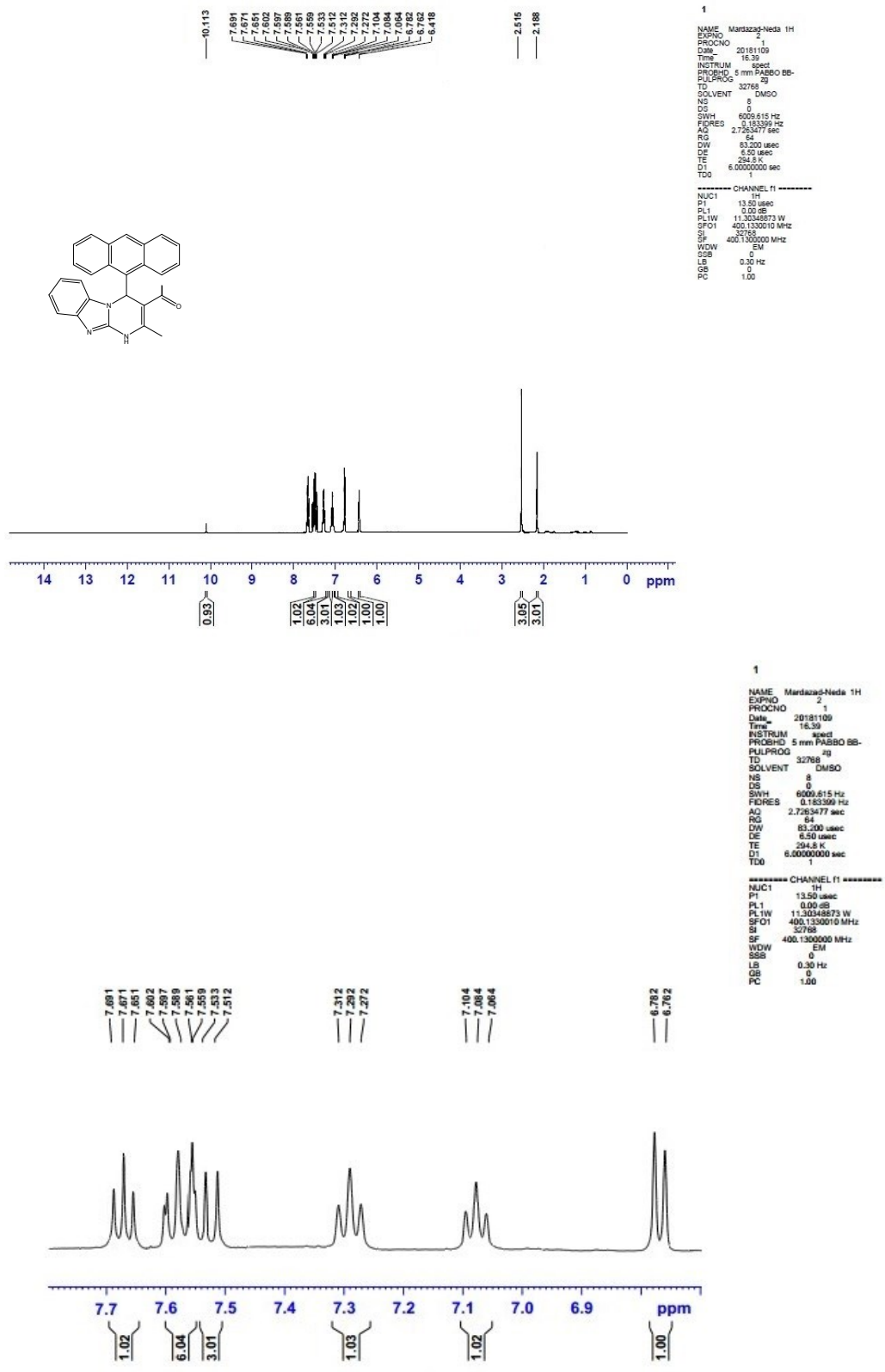


Fig s4 ¹H-NMR spectrum of 5a

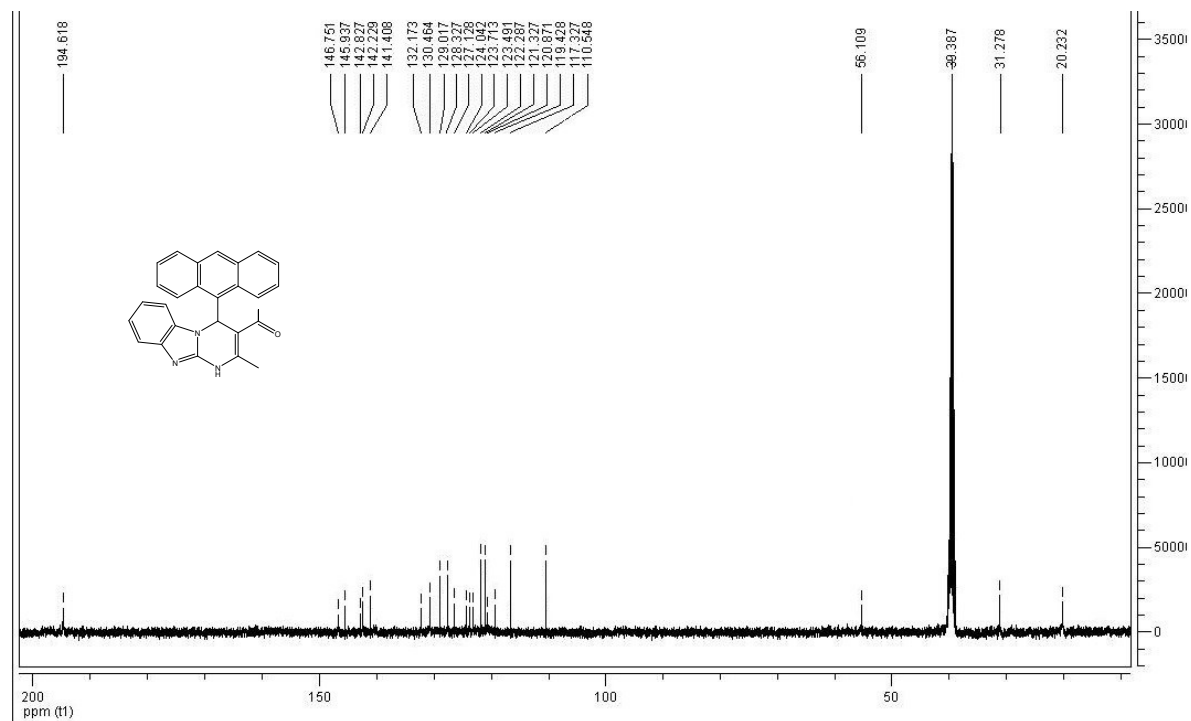


Fig s5 ¹³C-NMR spectrum of 5a

Spectral data of 5b

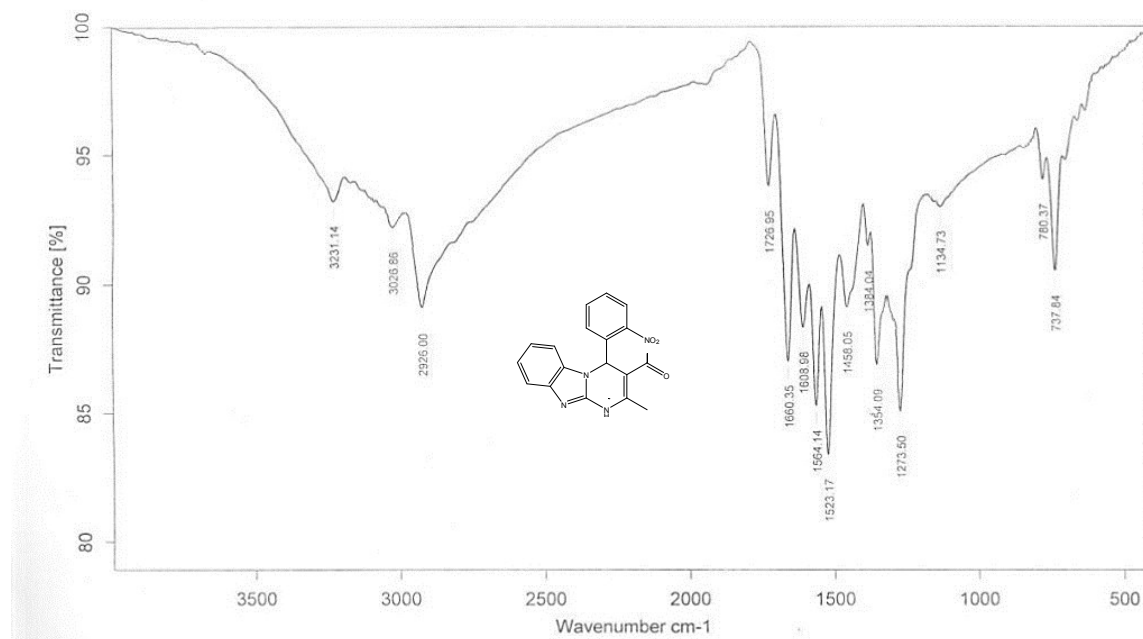


Fig. s6 FTIR spectrum of 5b

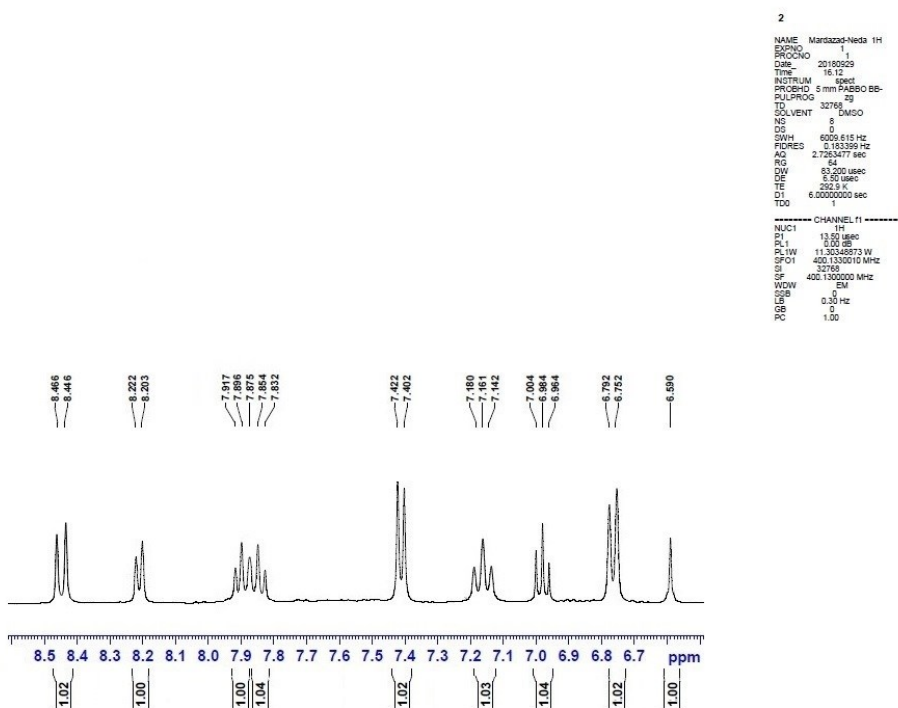
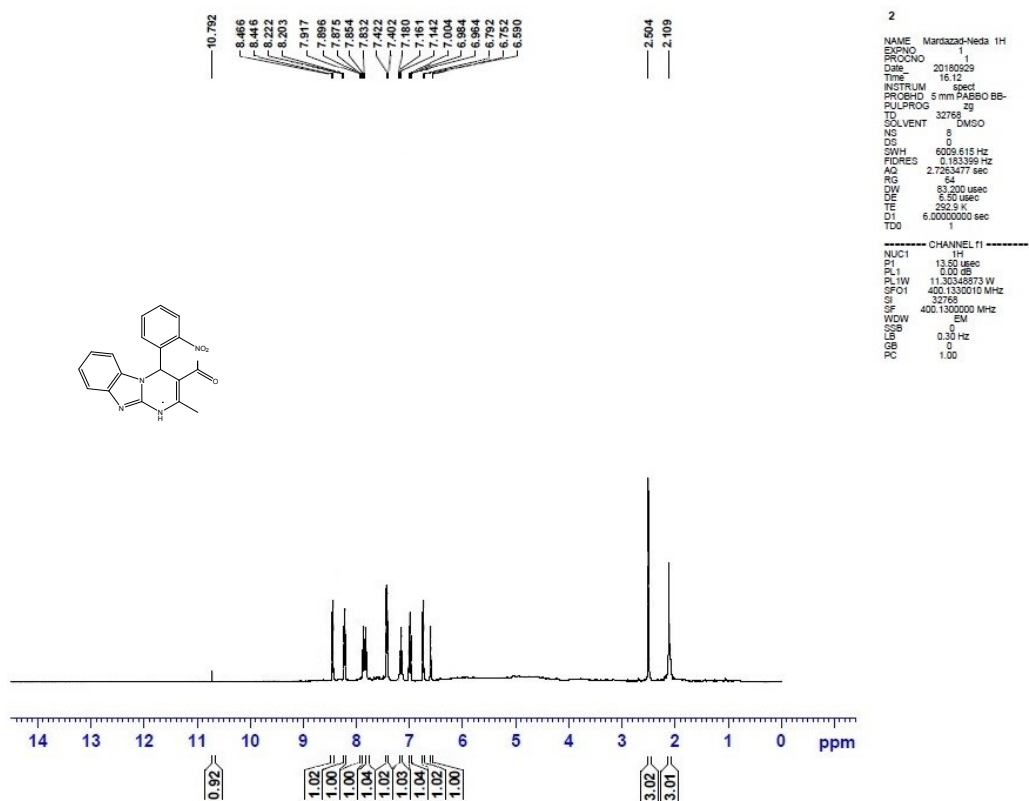


Fig s7 ¹H-NMR spectrum of 5b

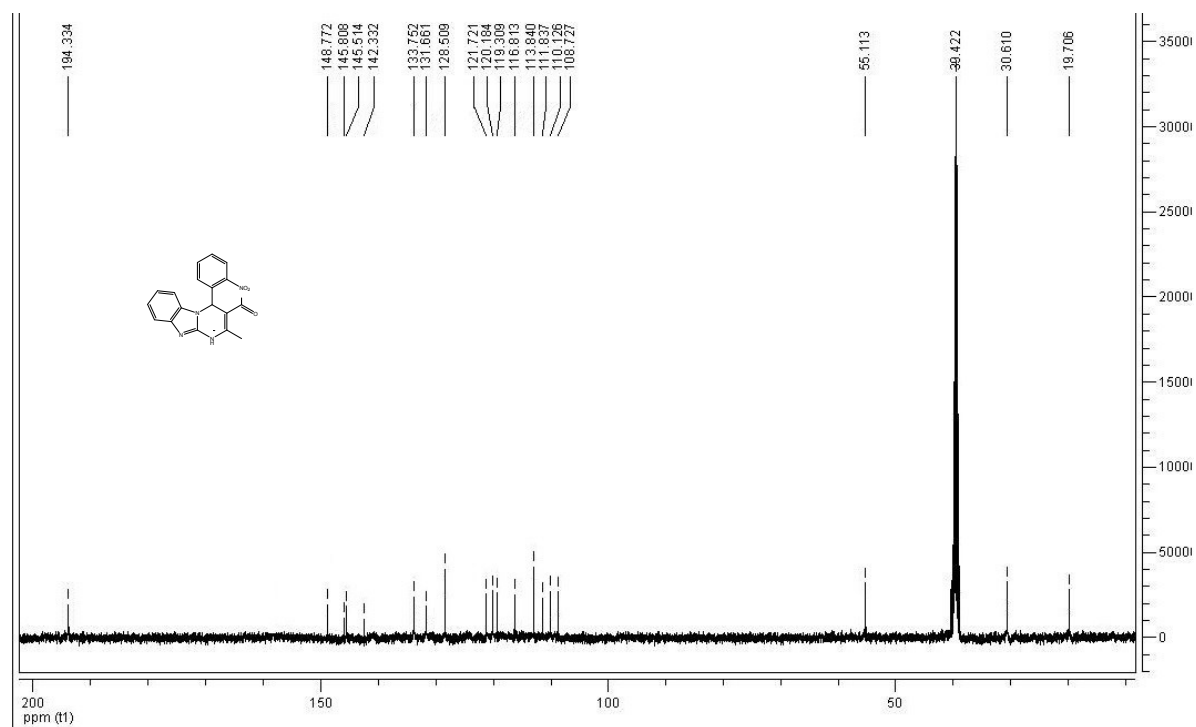


Fig s8 ¹³C-NMR spectrum of 5b

Spectral data of 5c

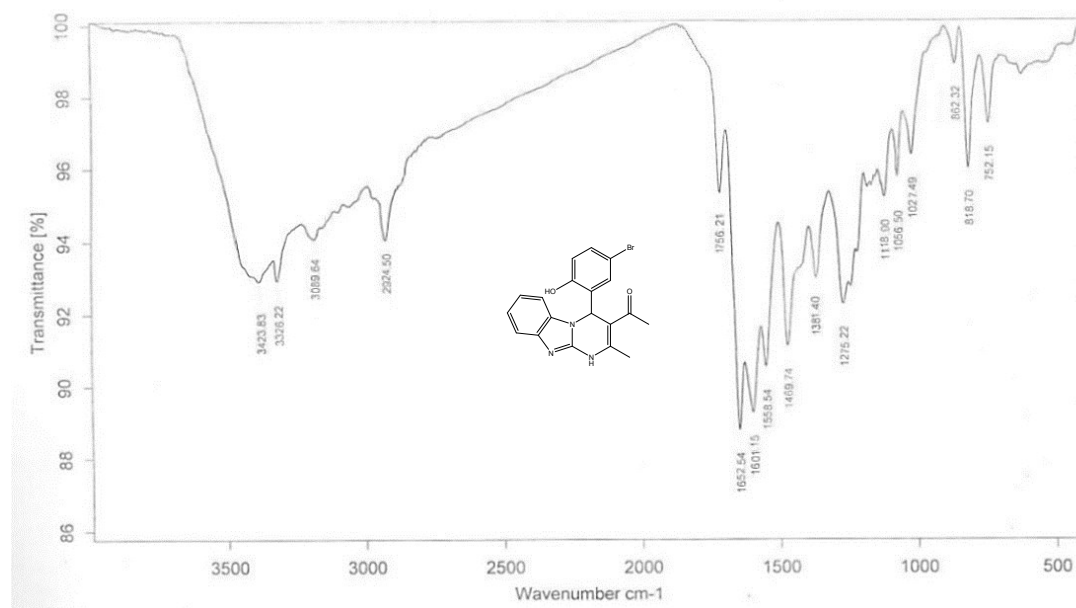


Fig. s9 FTIR spectrum of 5c

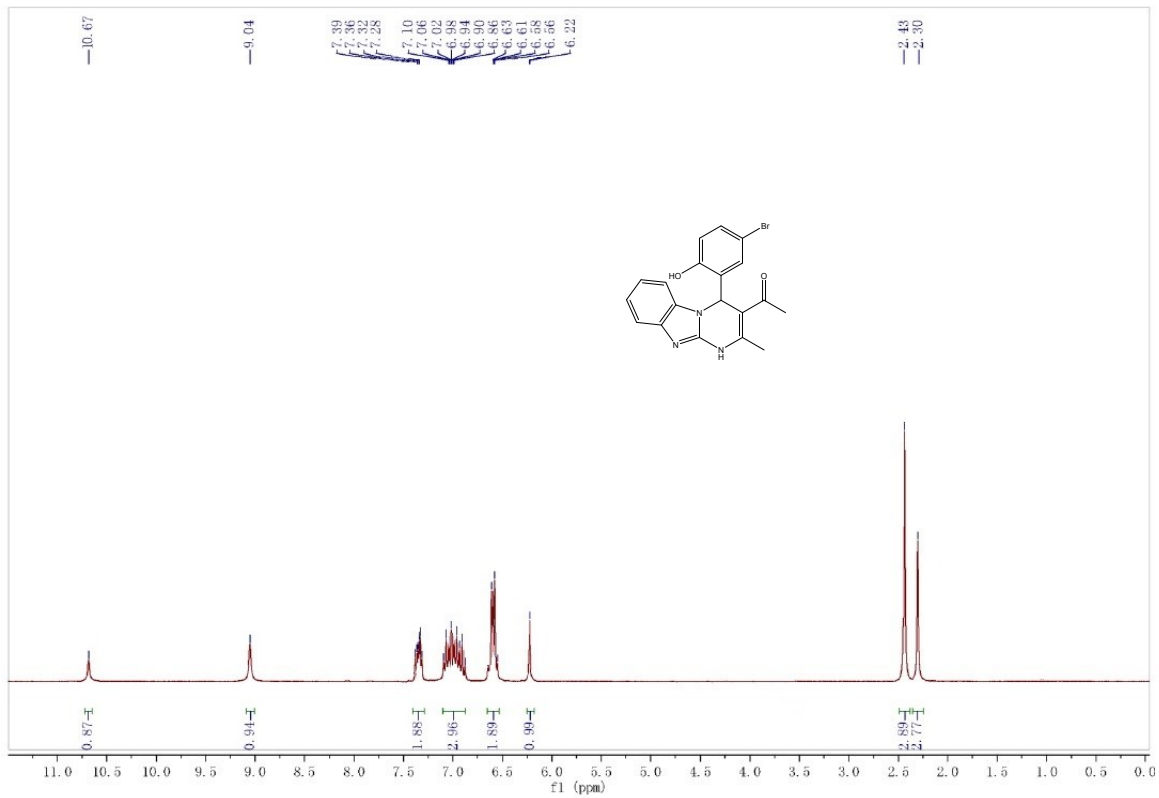


Fig s10 ¹H-NMR spectrum of 5c

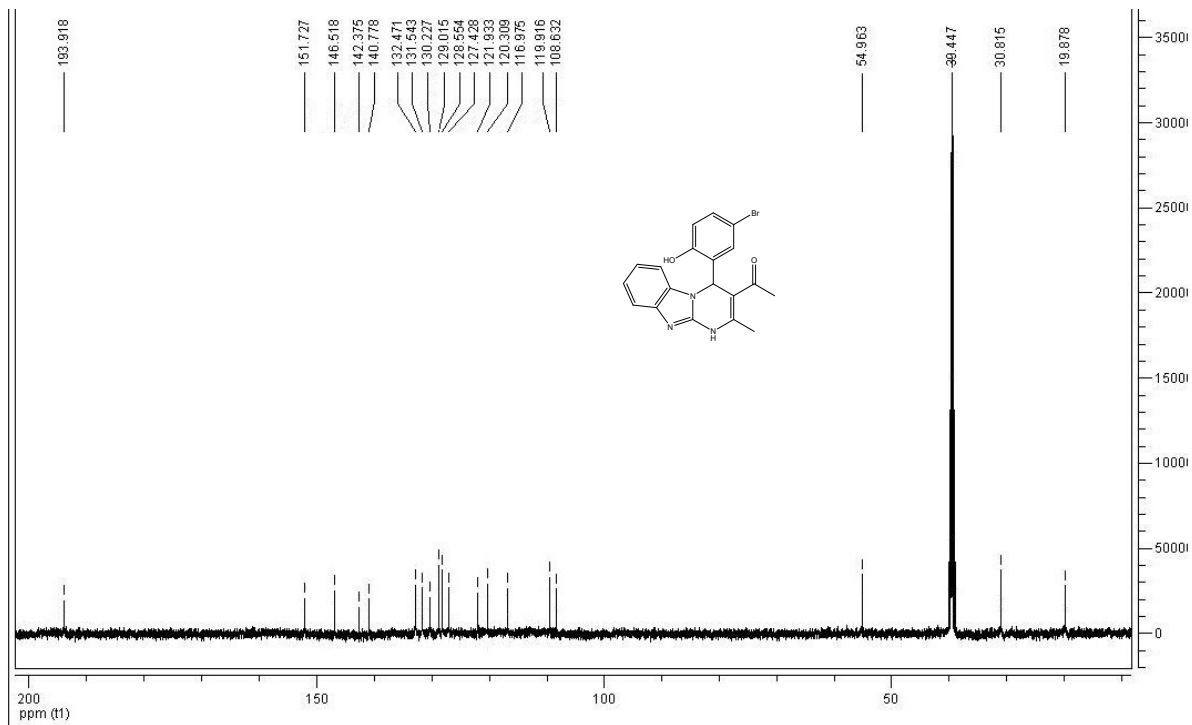


Fig s11 ¹³C-NMR spectrum of 5c

Spectral data of 5d

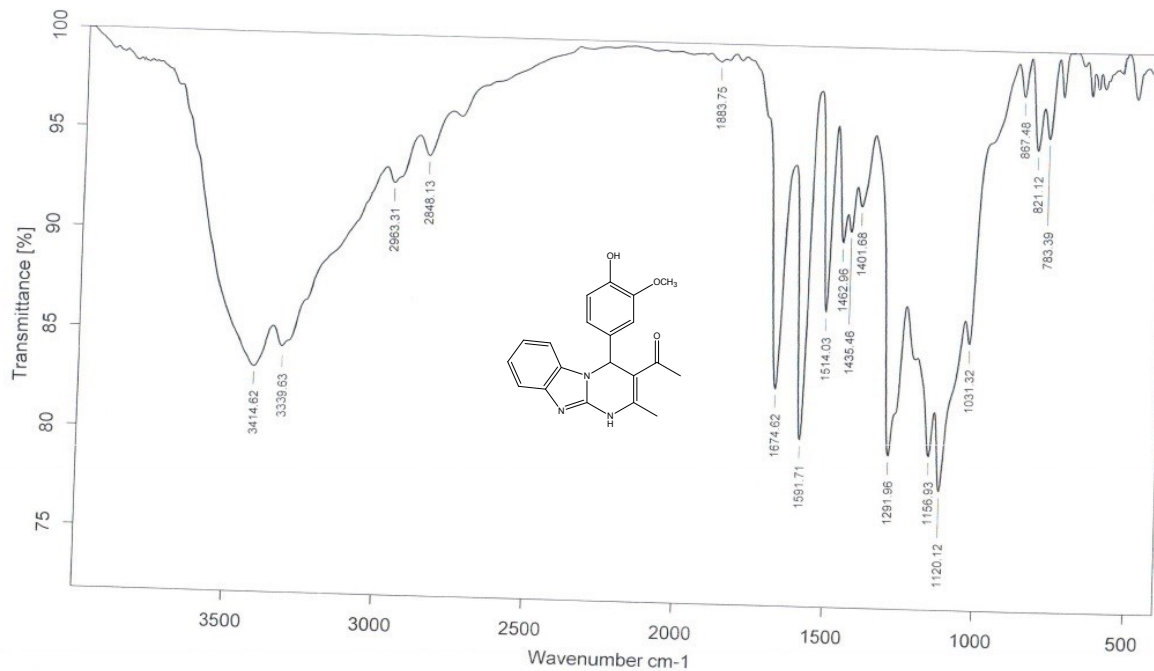


Fig. s12 FTIR spectrum of 5d

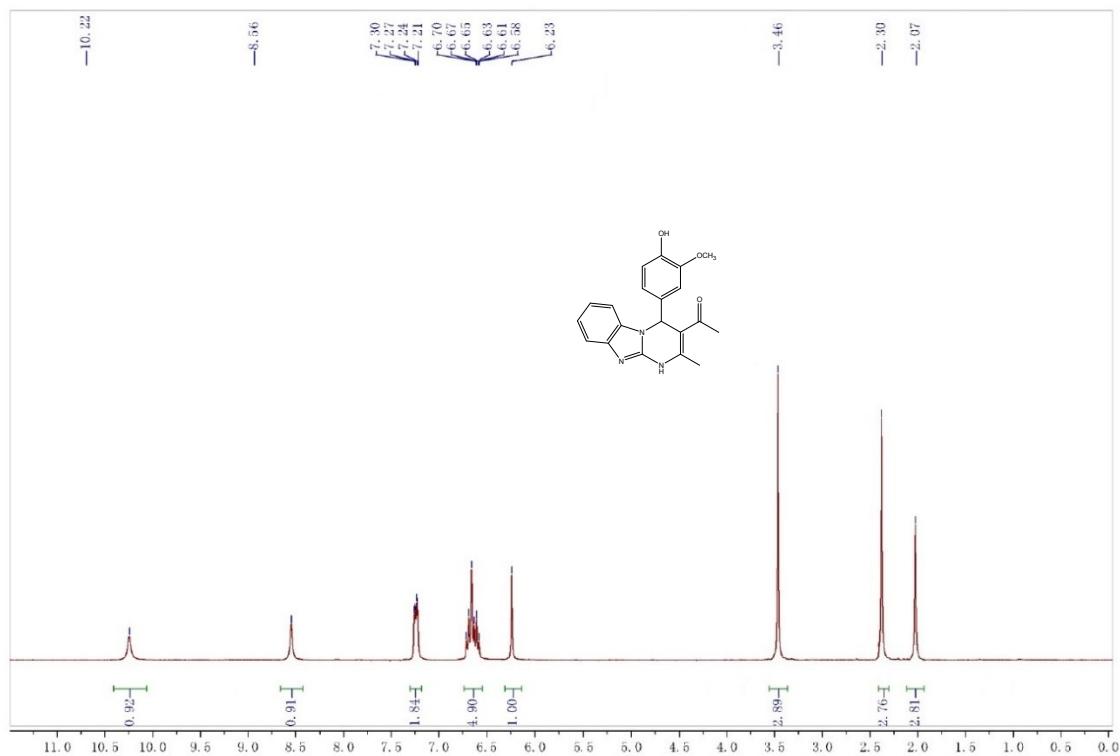


Fig s13 ¹H-NMR spectrum of 5d

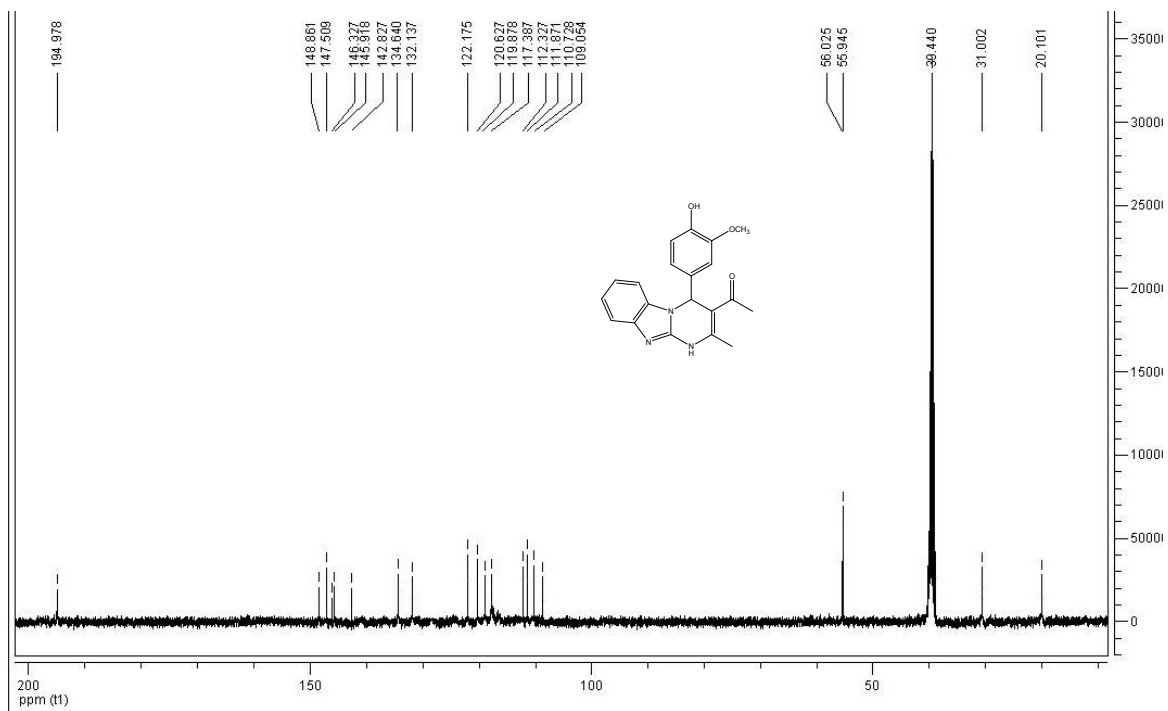


Fig s14 ^{13}C -NMR spectrum of 5d

Spectral data of 6a

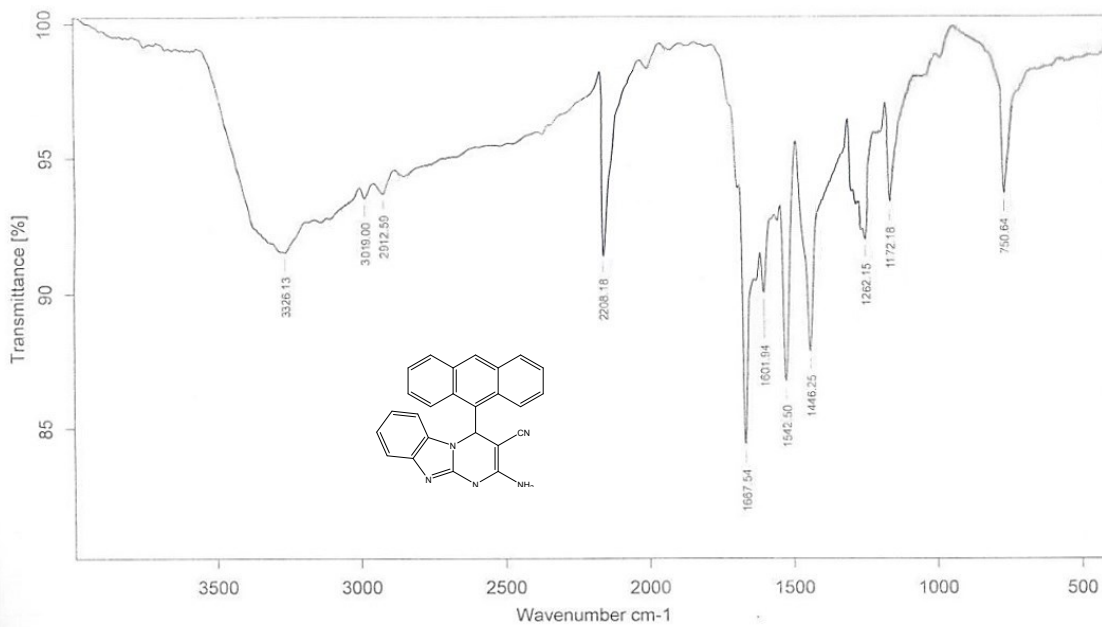
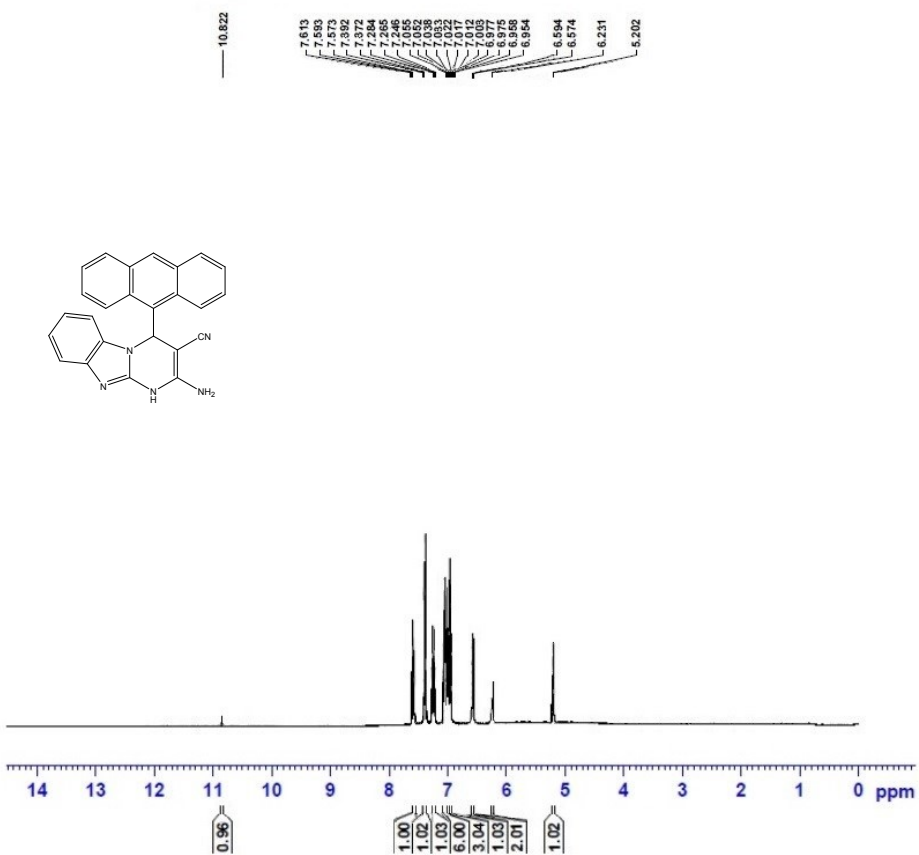


Fig. s15 FTIR spectrum of 6a

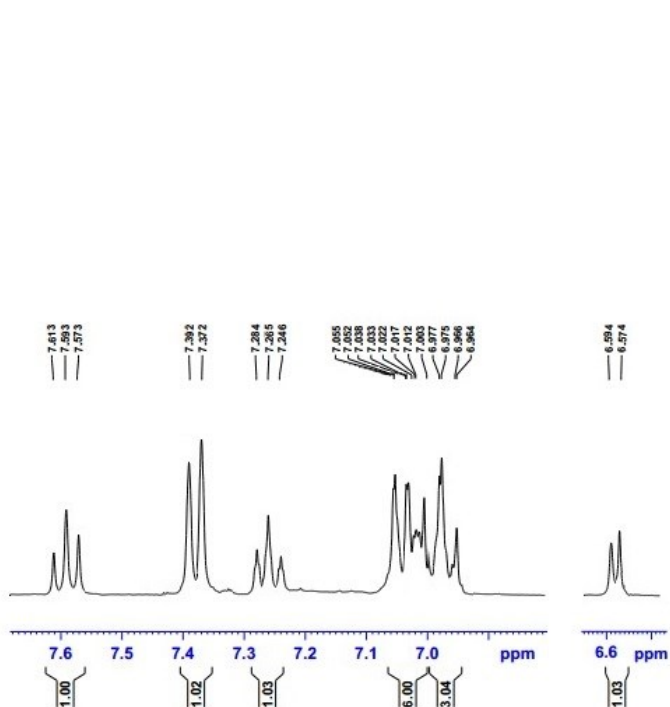


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PROCNO  1
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PULPROG  zg
TD  32768
SOLVENT  DMSO
NS  8
DS  0
SWH  6009.615 Hz
FIDRES  0.183399 Hz
AQ  2.7283477 sec
RG  64
DW  63.200 usec
DE  6.50 usec
TE  295.9 K
D1  6.0000000 sec
TD0  1

----- CHANNEL f1 -----
NUC1  1H
P1  13.50 usec
PL1  0.00 dB
PL1W  11.30348873 W
SFO1  400.1300010 MHz
SI  32768
SF  400.1300000 MHz
WDW  EM
SSB  0
LB  0.30 Hz
GB  0
PC  1.00

```



```

NAME  Martazad-Neda 1H
EXPNO  4
PROCNO  1
Date_  20181211
Time_  13.39
INSTRUM  spect
PROBHD  5 mm PABBO BB-
PULPROG  zg
TD  32768
SOLVENT  DMSO
NS  8
DS  0
SWH  6009.615 Hz
FIDRES  0.183399 Hz
AQ  2.7283477 sec
RG  64
DW  63.200 usec
DE  6.50 usec
TE  295.9 K
D1  6.0000000 sec
TD0  1

----- CHANNEL f1 -----
NUC1  1H
P1  13.50 usec
PL1  0.00 dB
PL1W  11.30348873 W
SFO1  400.1300010 MHz
SI  32768
SF  400.1300000 MHz
WDW  EM
SSB  0
LB  0.30 Hz
GB  0
PC  1.00

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Fig s16 ¹H-NMR spectrum of 6a

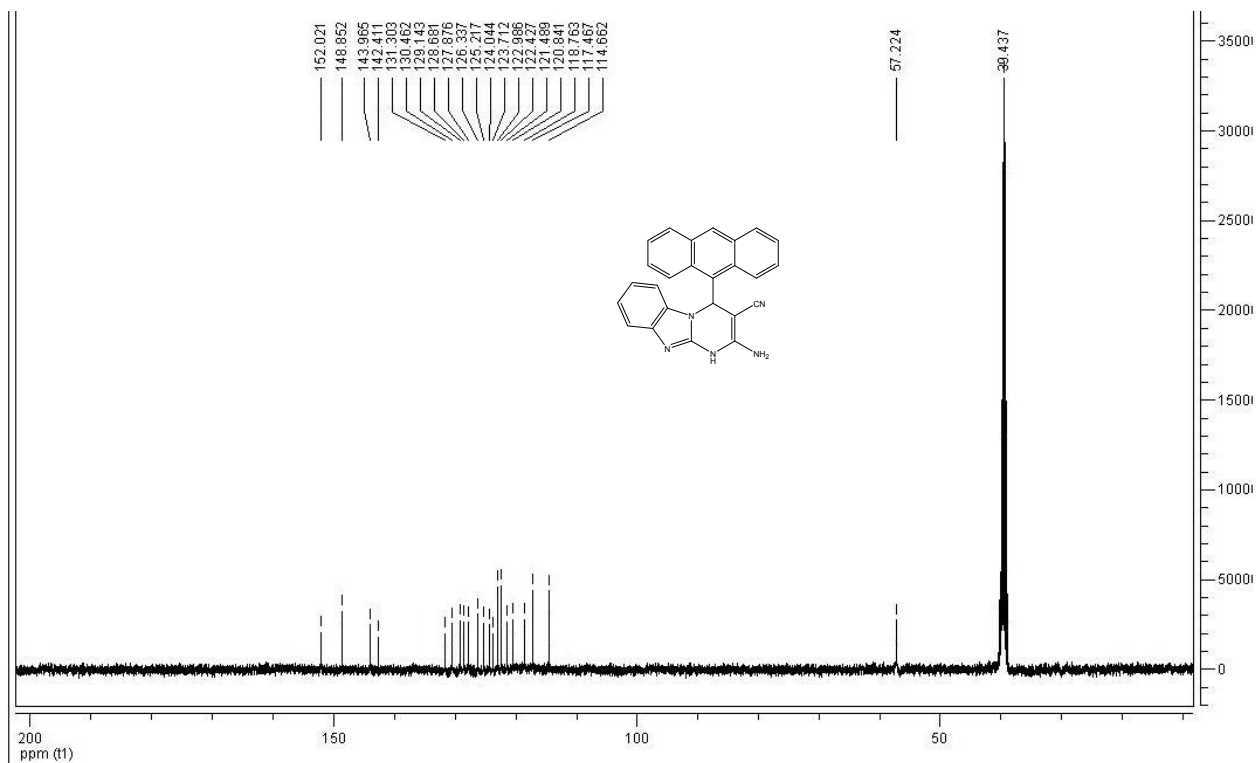


Fig s17 ^{13}C -NMR spectrum of 6a

Spectral data of 6b

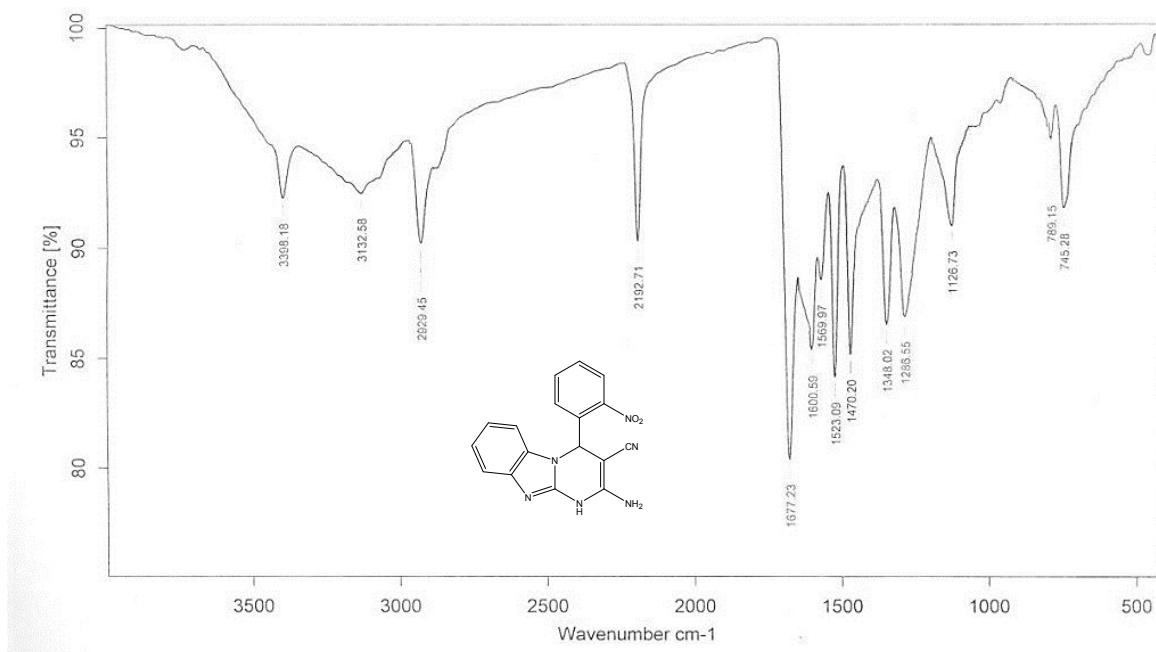
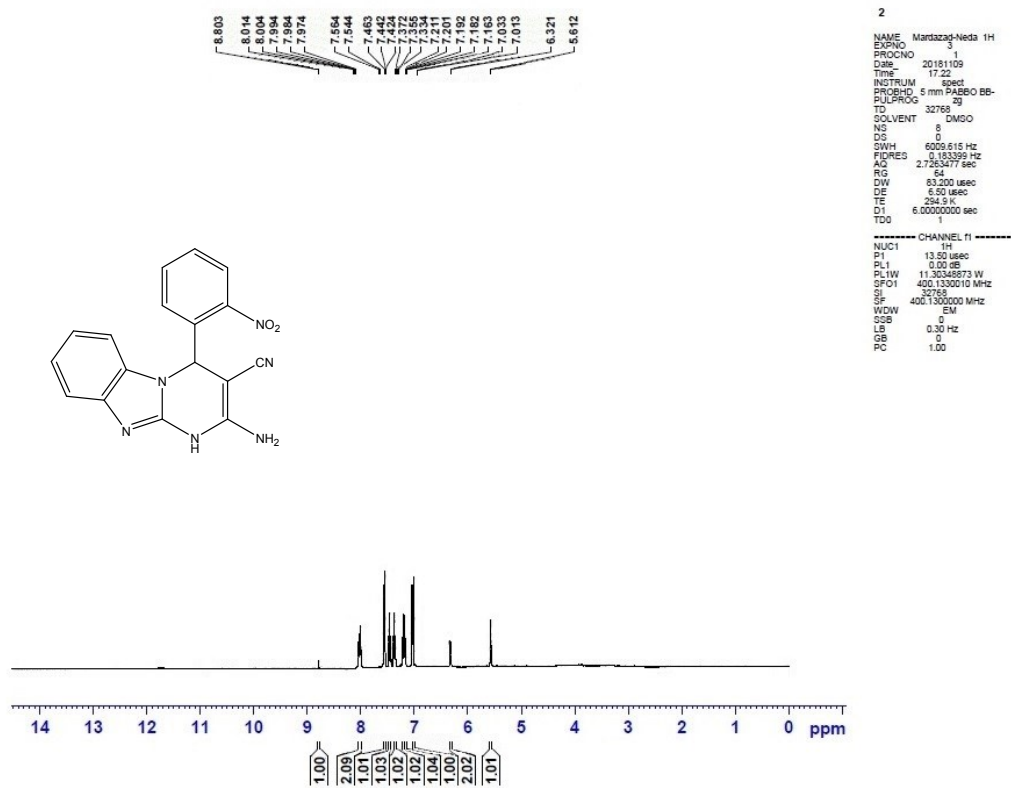


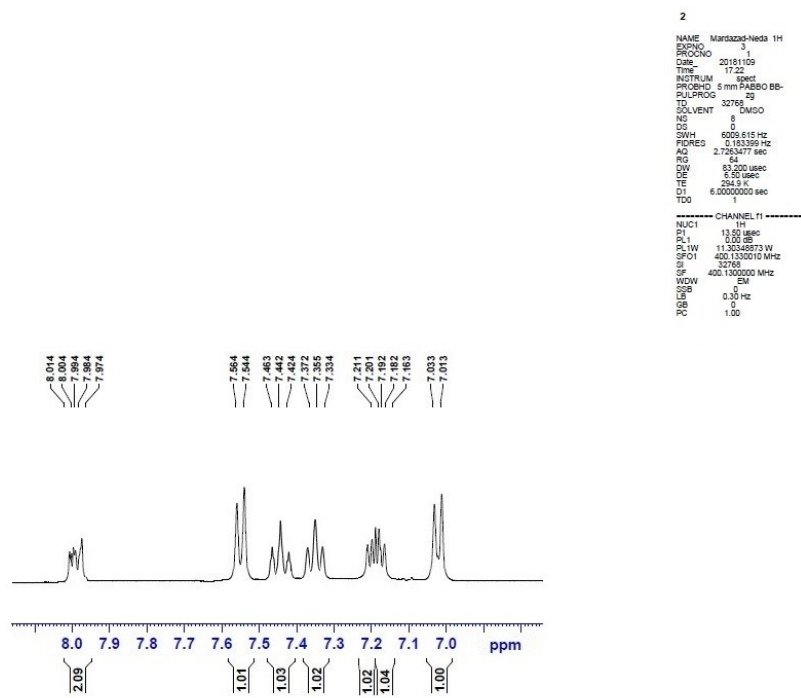
Fig. s18 FTIR spectrum of 6b



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PROCNO 1
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PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 6005.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 64
DW 63.200 usec
DE 6.50 usec
TE 294.2 K
D1 6.0000000 sec
TDO 1
----- CHANNEL f1 -----
NUC1 1H
P1 13.50 usec
PL1 0.00 dB
PL1W 11.30345873 W
SFO1 400.1300010 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```



```

2
NAME Maroqaz-Neda 1H
EXPNO 1
PROCNO 1
Date_ 20181109
Time 17.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 6005.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 64
DW 63.200 usec
DE 6.50 usec
TE 294.2 K
D1 6.0000000 sec
TDO 1
----- CHANNEL f1 -----
NUC1 1H
P1 13.50 usec
PL1 0.00 dB
PL1W 11.30345873 W
SFO1 400.1300010 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```

Fig s19 ¹H-NMR spectrum of 6b

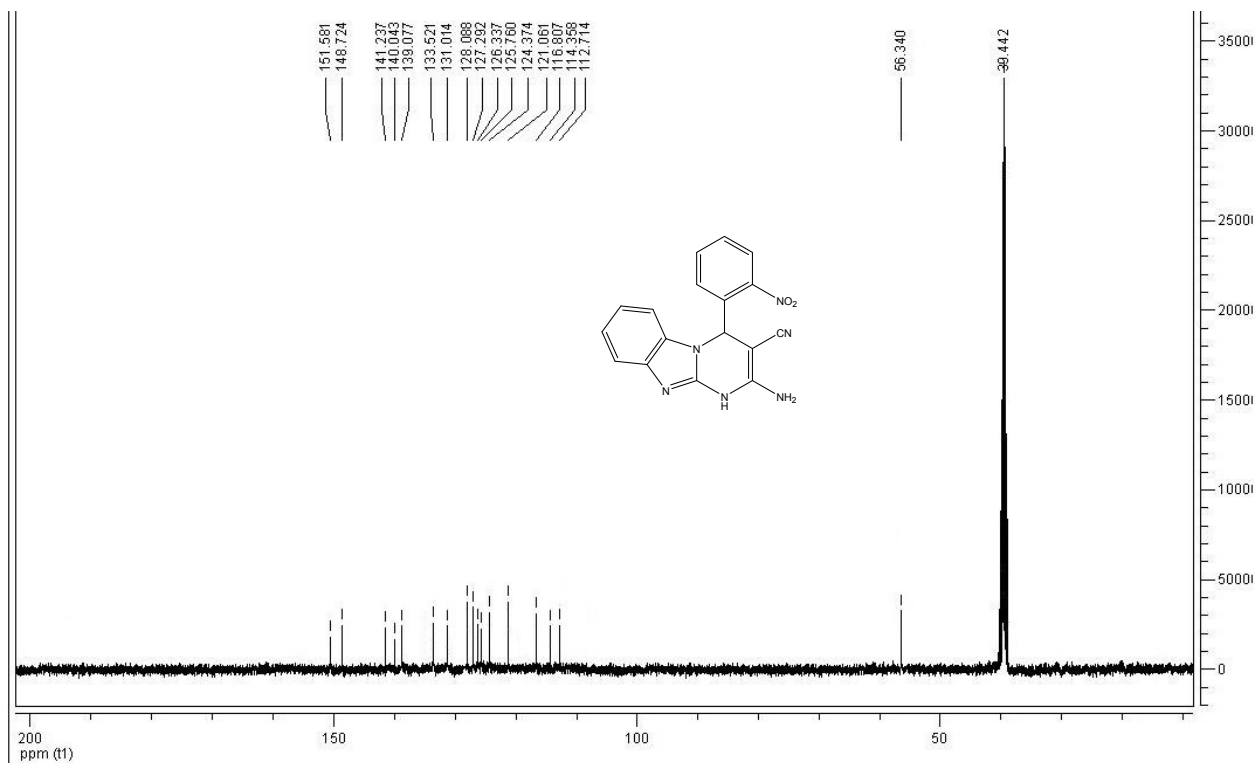


Fig s20 $^{13}\text{C-NMR}$ spectrum of 6b

Spectral data of 6c

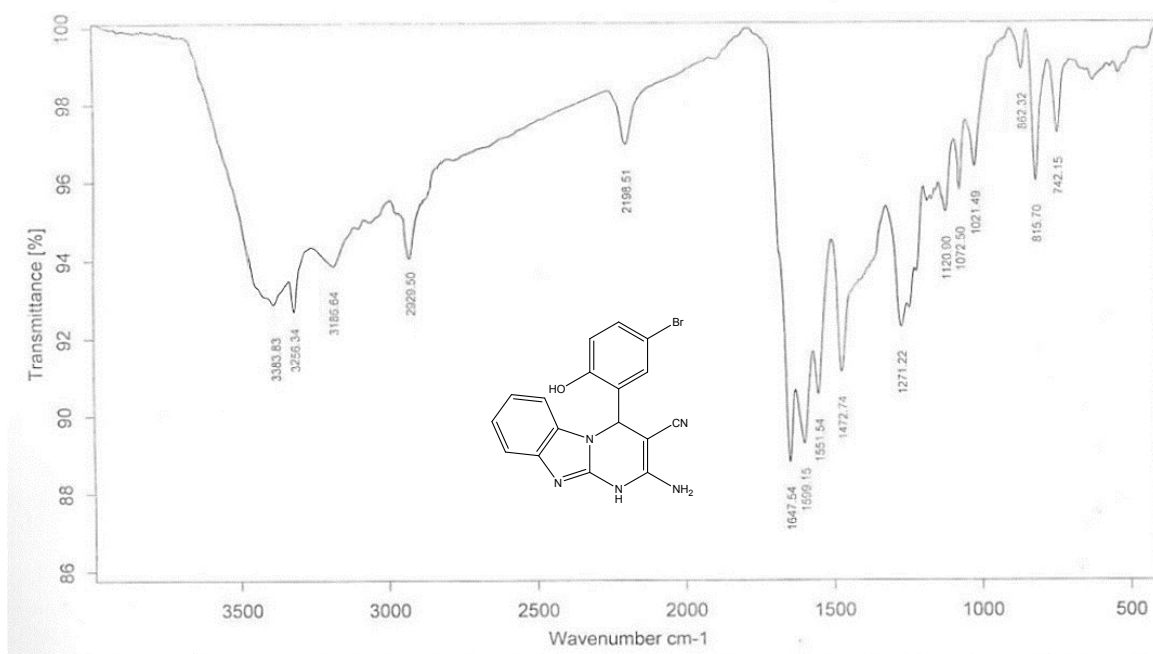


Fig. s21 FTIR spectrum of 6c

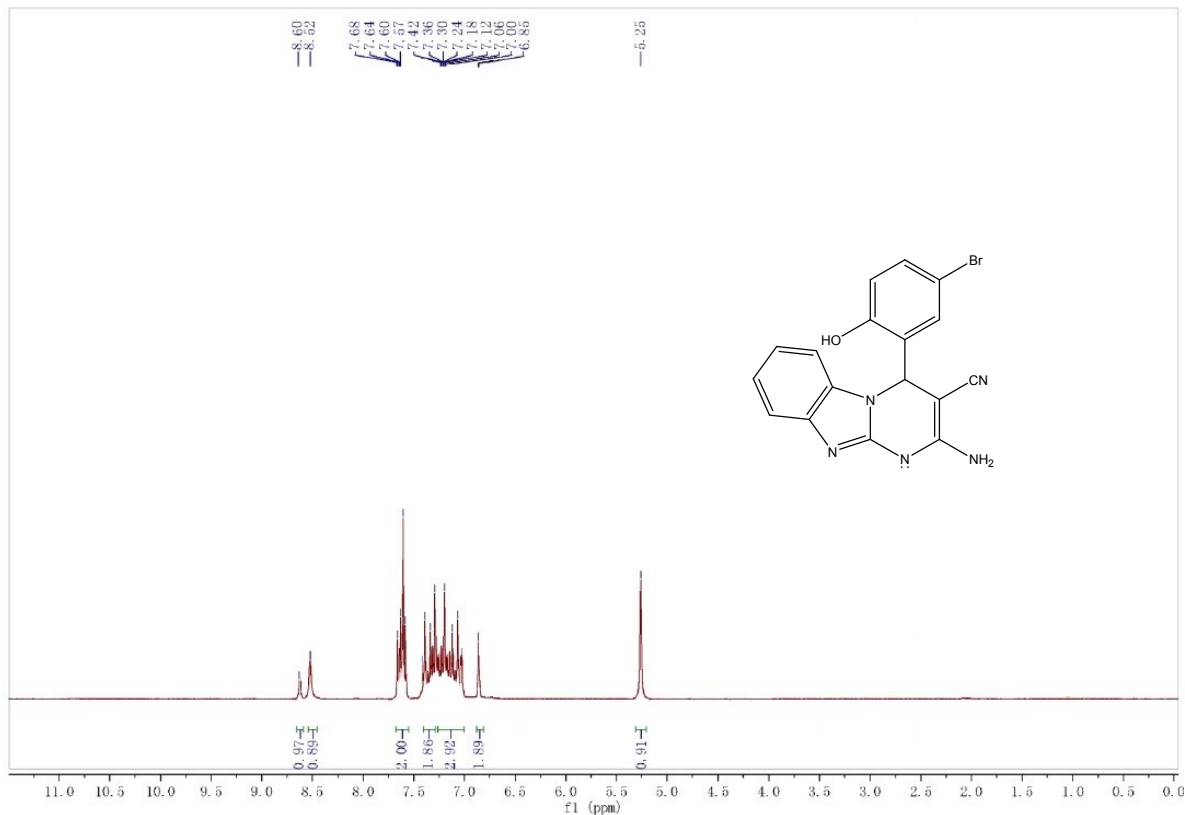


Fig s22 ¹H-NMR spectrum of 6c

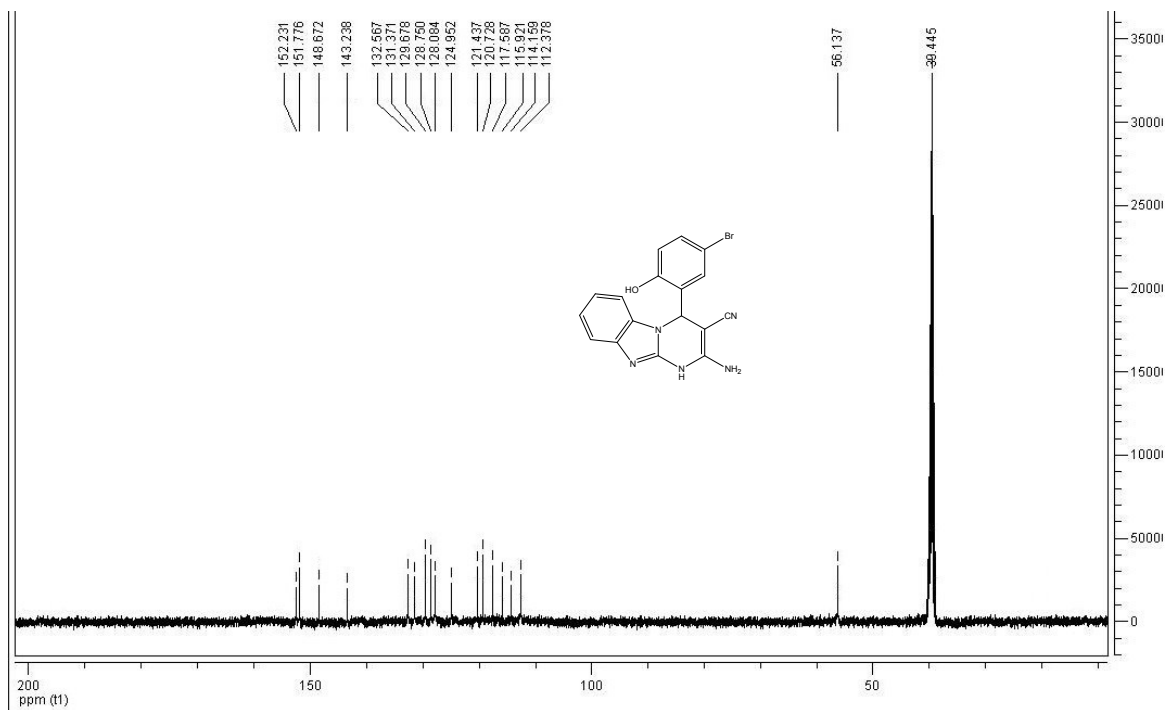


Fig s23 ¹³C-NMR spectrum of 6c

Spectral data of 6d

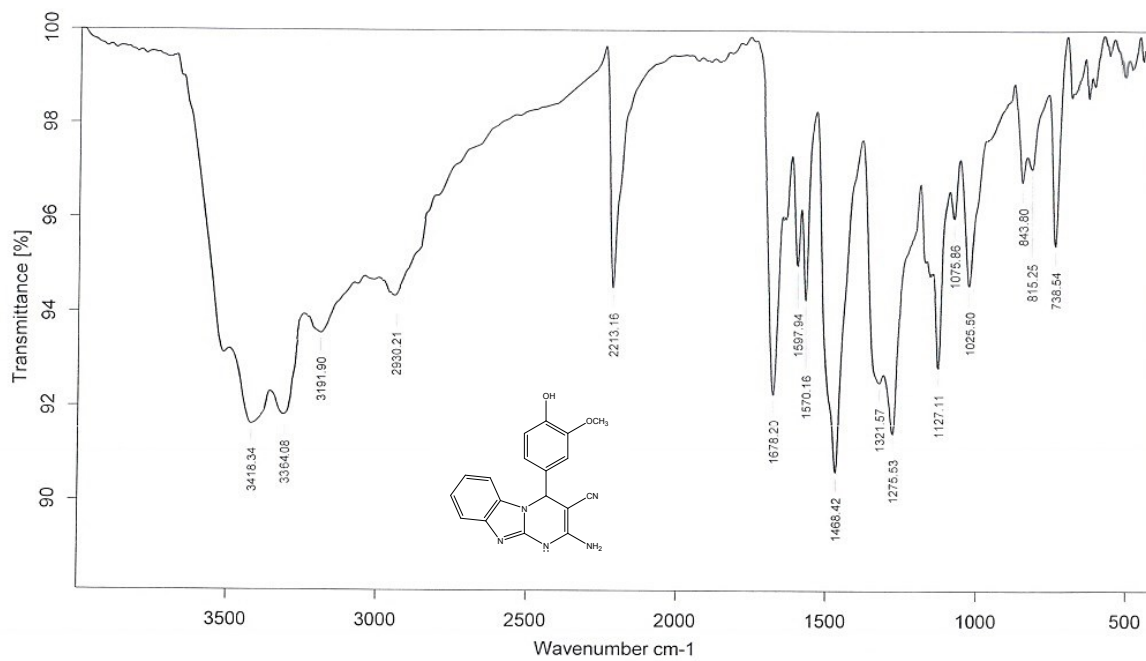


Fig. s24 FTIR spectrum of 6d

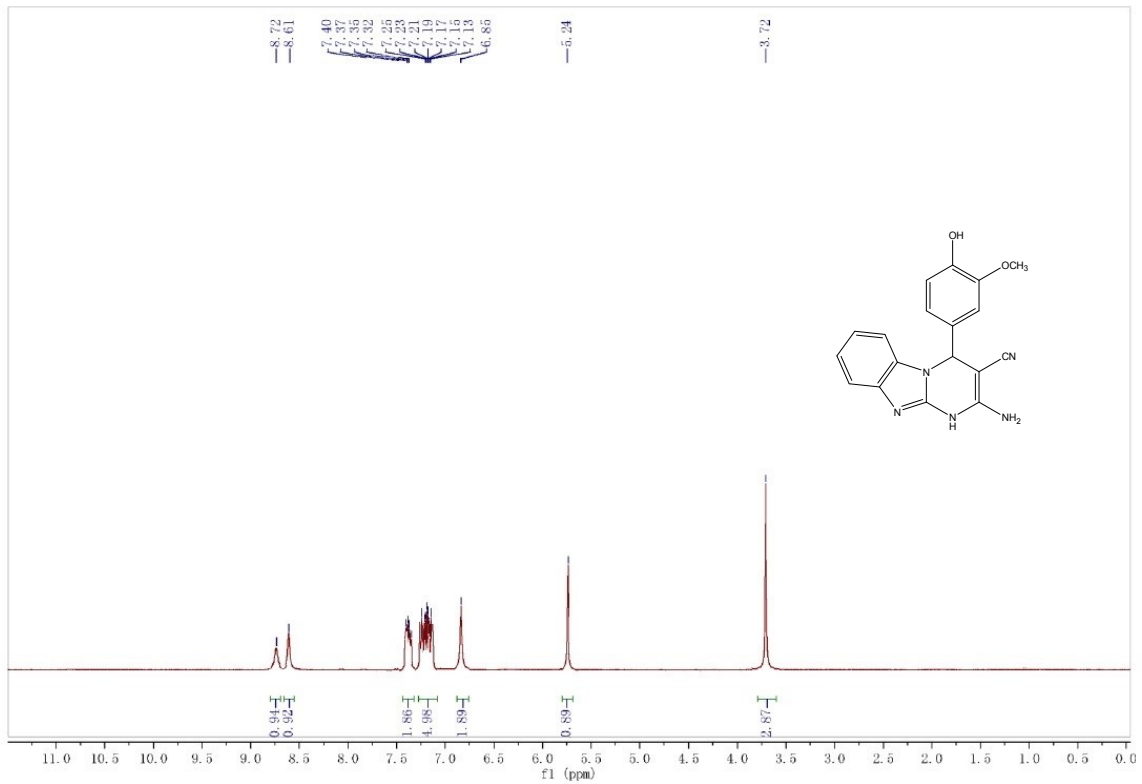


Fig s25 ¹H-NMR spectrum of 6d

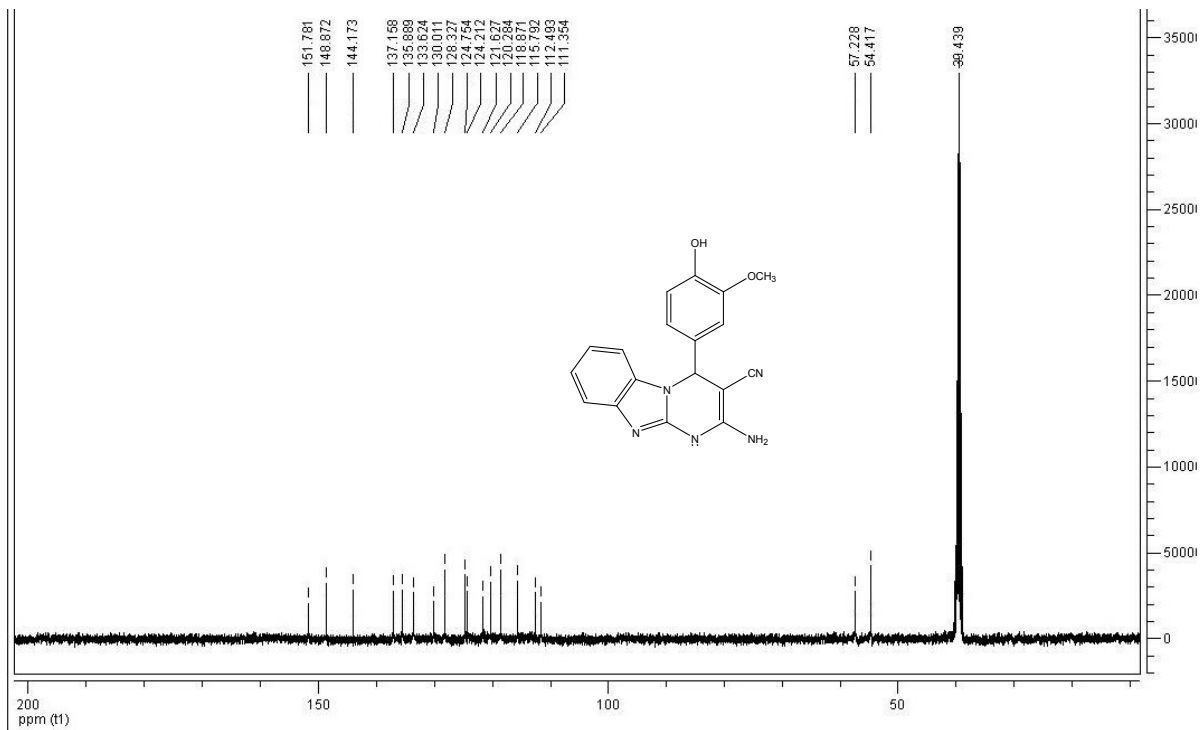


Fig s26 ¹³C-NMR spectrum of 6d

Spectral data of 7a

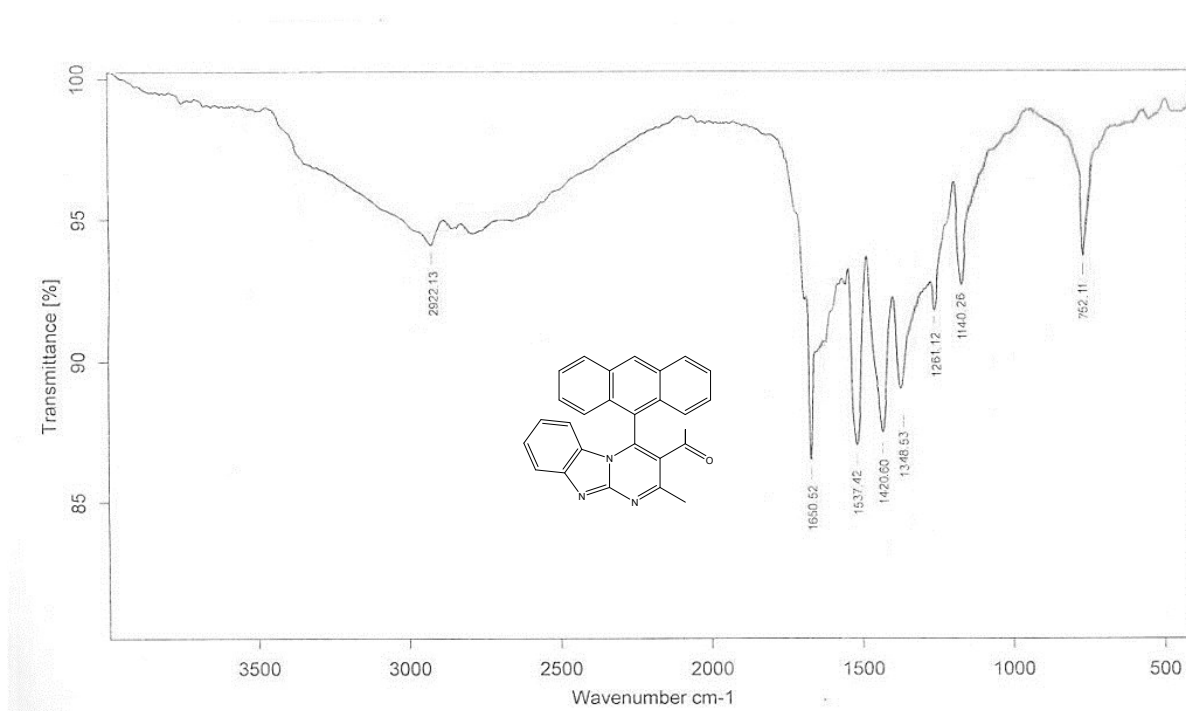


Fig. s27 FTIR spectrum of 7a

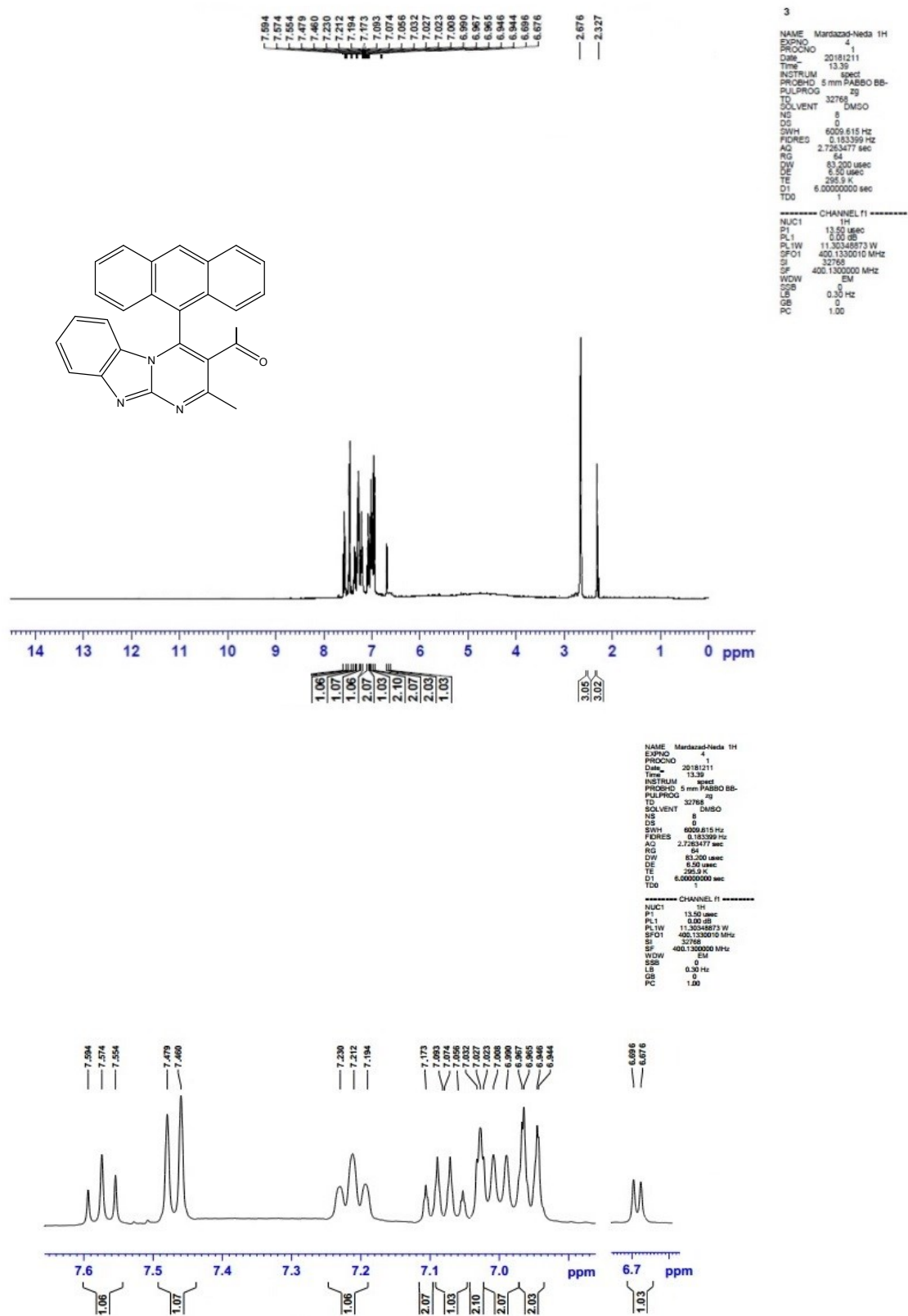


Fig s28 ¹H-NMR spectrum of 7a

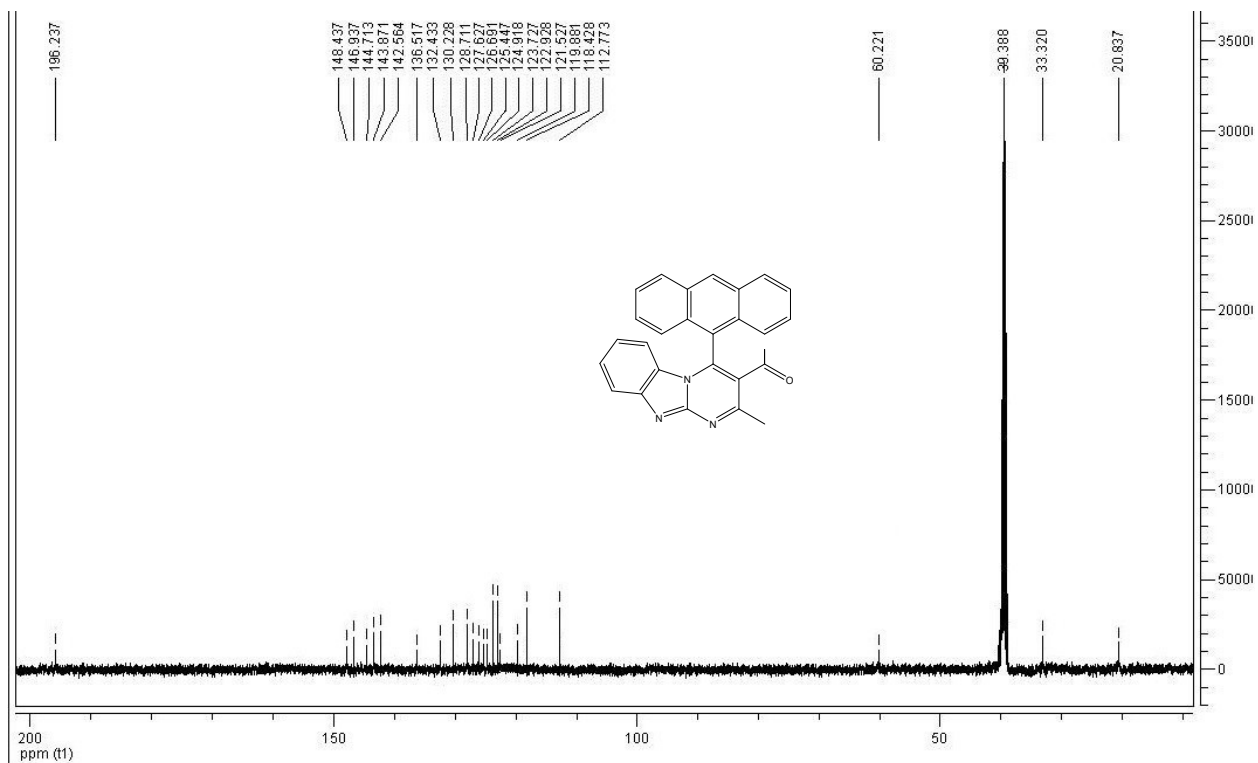


Fig s29 ¹³C-NMR spectrum of 7a

Spectral data of 7b

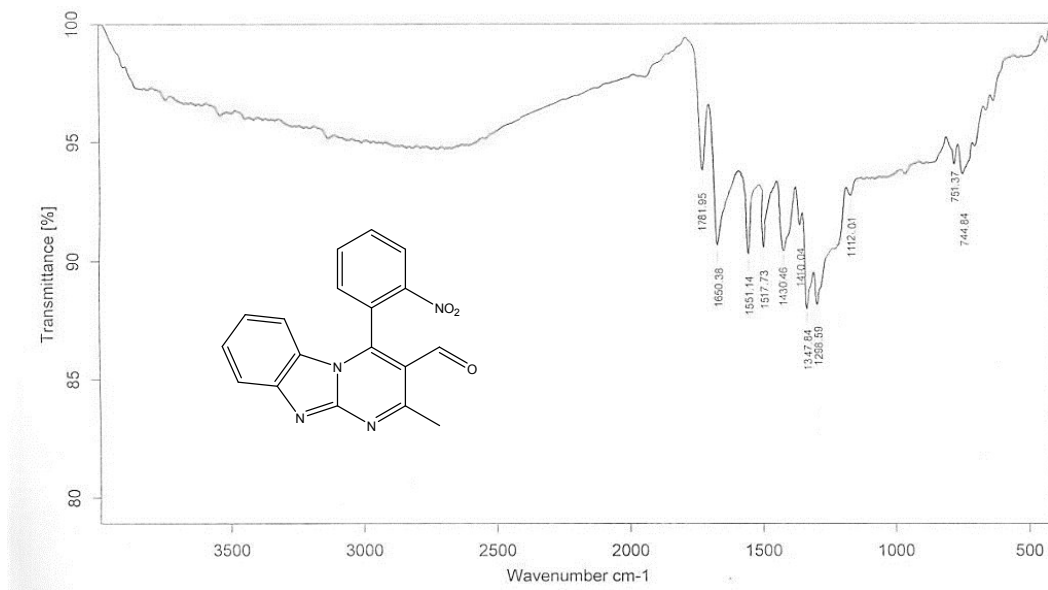


Fig. s30 FTIR spectrum of 7b

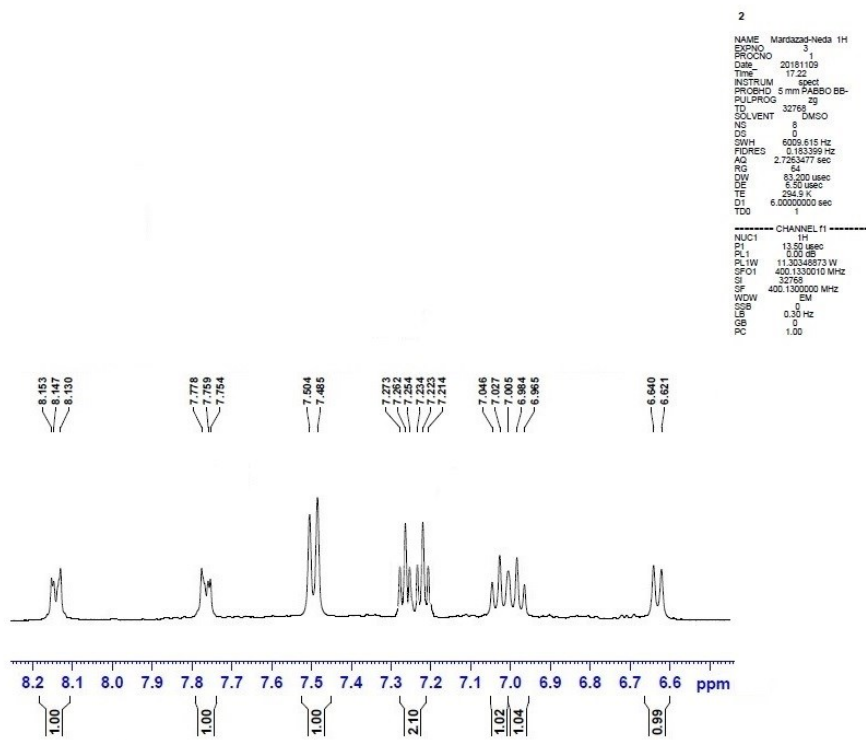
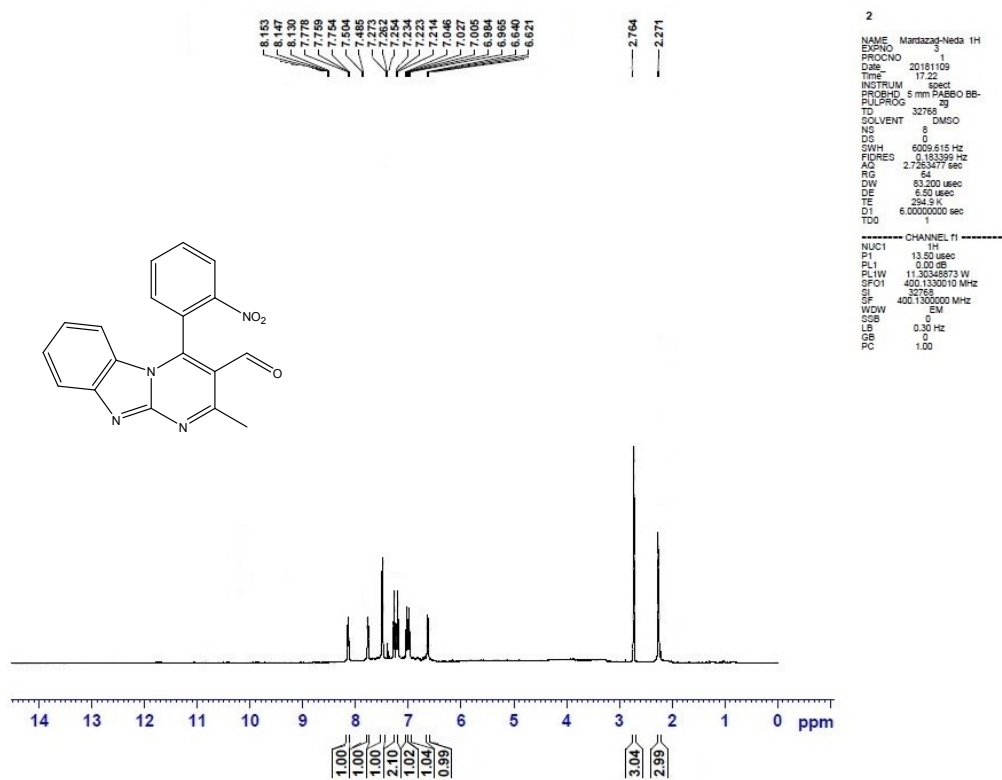


Fig s31 ¹H-NMR spectrum of 7b

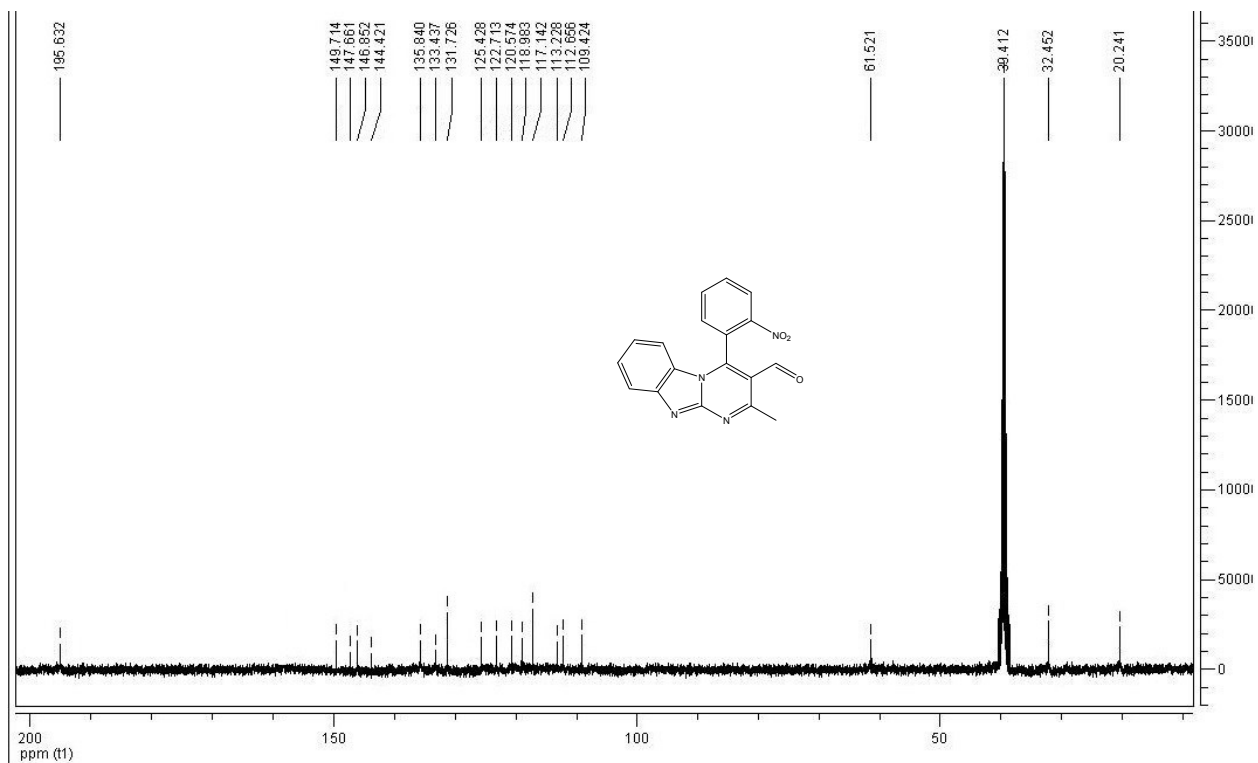


Fig s32 ¹³C-NMR spectrum of 7b

Spectral data of 7c

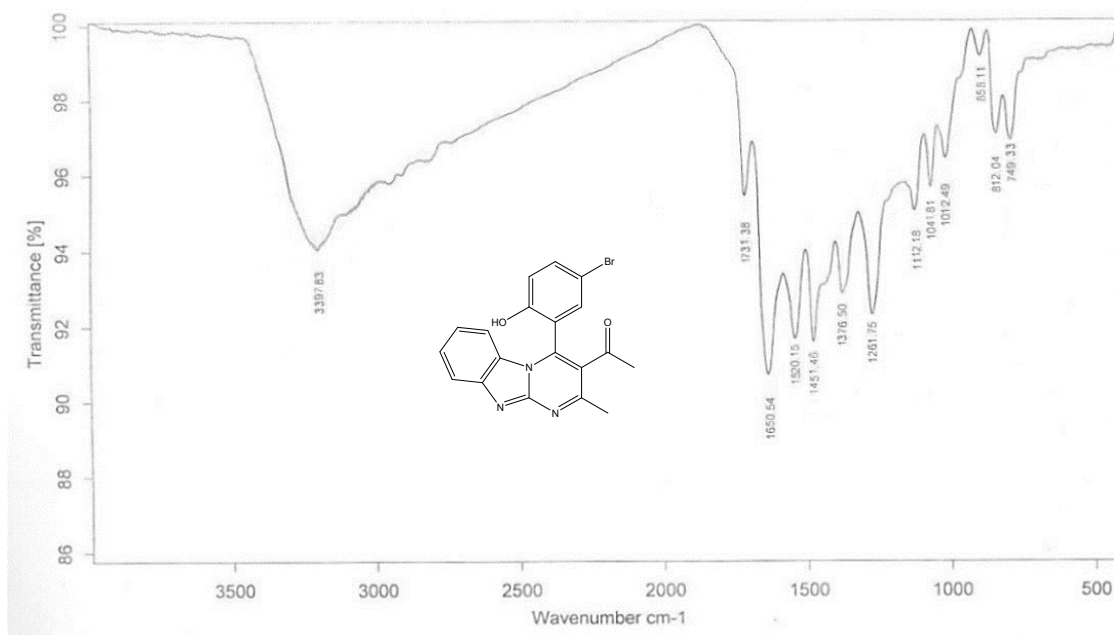
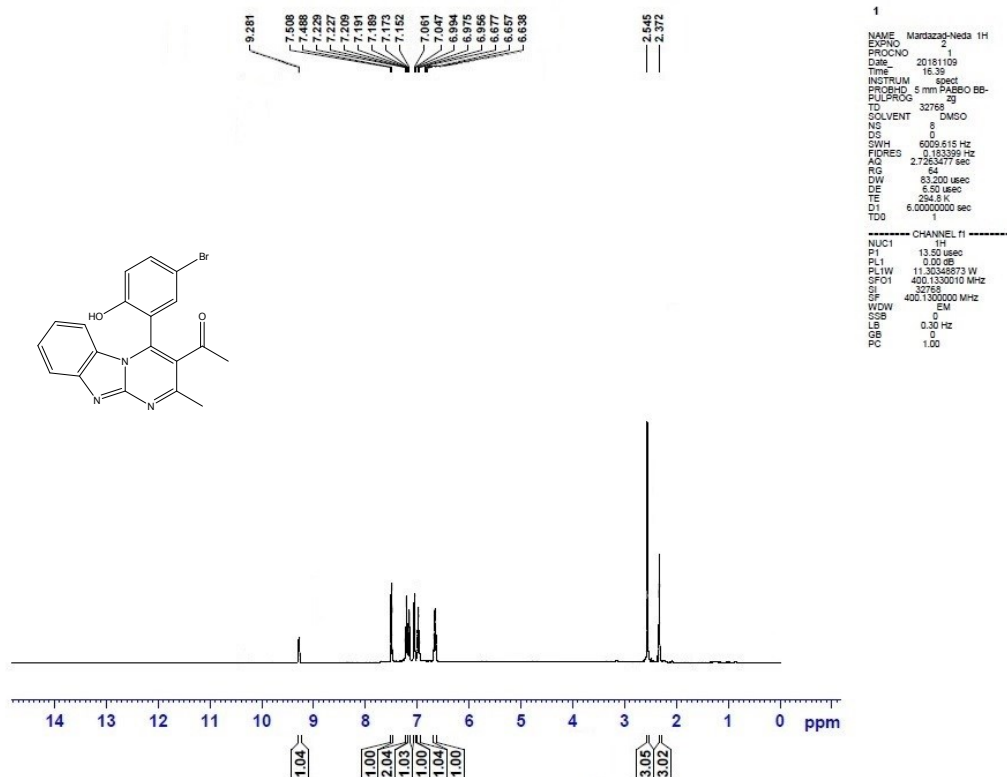


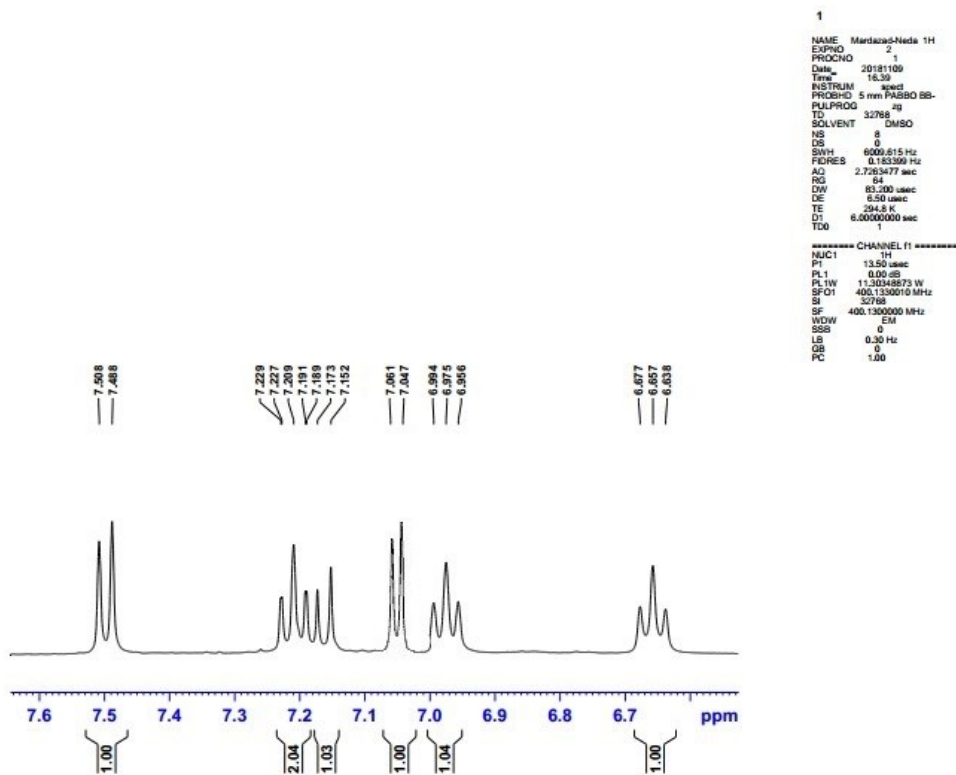
Fig. s33 FTIR spectrum of 7c



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EXPNO 2
PROCNO 1
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PULPROG zg
TD 32768
SOLVENT DMSO
NS 8
DS 8
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 64
DW 83.200 usec
DE 6.50 usec
TE 294.2 K
D1 6.0000000 sec
TDO
----- CHANNEL f1 -----
NUC1 1H
P1 13.50 usec
PL1 0.00 dB
PL1W 11.30348873 W
SFO1 400.1300010 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```



```

1
NAME Mardazad-Neda 1H
EXPNO 2
PROCNO 1
Date_ 20181109
Time 16.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT DMSO
NS 8
DS 8
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 64
DW 83.200 usec
DE 6.50 usec
TE 294.2 K
D1 6.0000000 sec
TDO 1
----- CHANNEL f1 -----
NUC1 1H
P1 13.50 usec
PL1 0.00 dB
PL1W 11.30348873 W
SFO1 400.1300010 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

```

Fig s34 ¹H-NMR spectrum of 7c

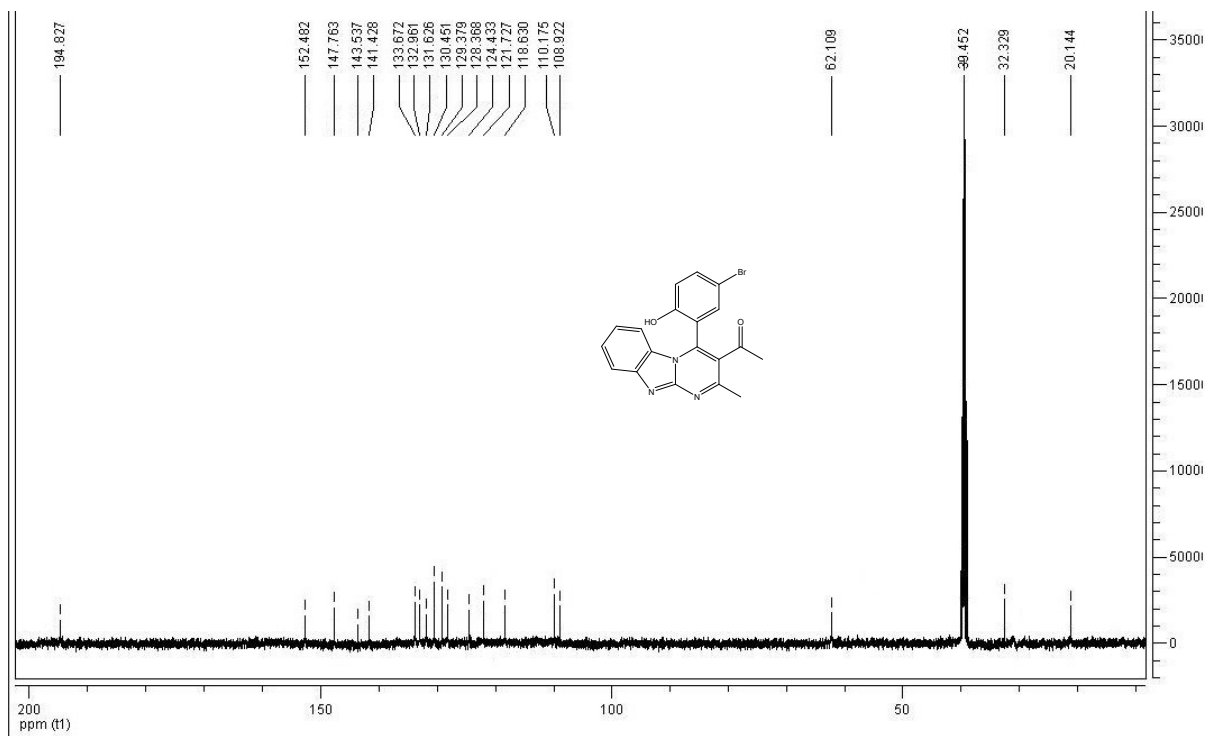


Fig s35 ¹³C-NMR spectrum of 7c

Spectral data of 7d

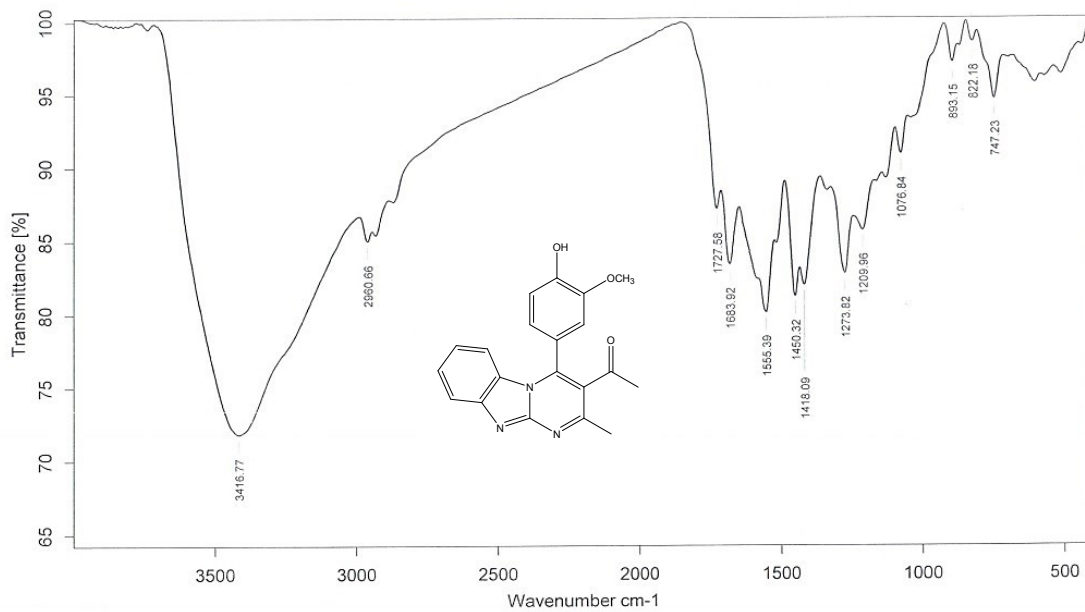


Fig. s36 FTIR spectrum of 7d

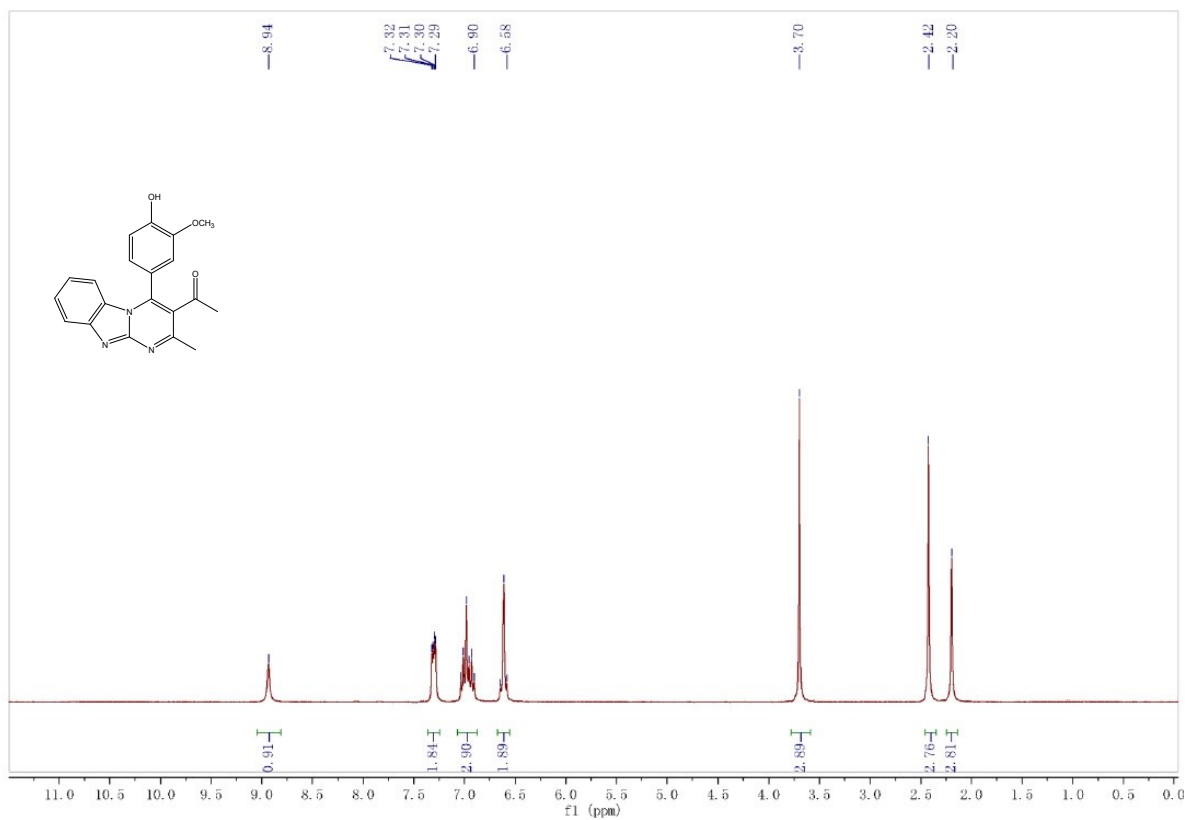


Fig s37 ¹H-NMR spectrum of 7d

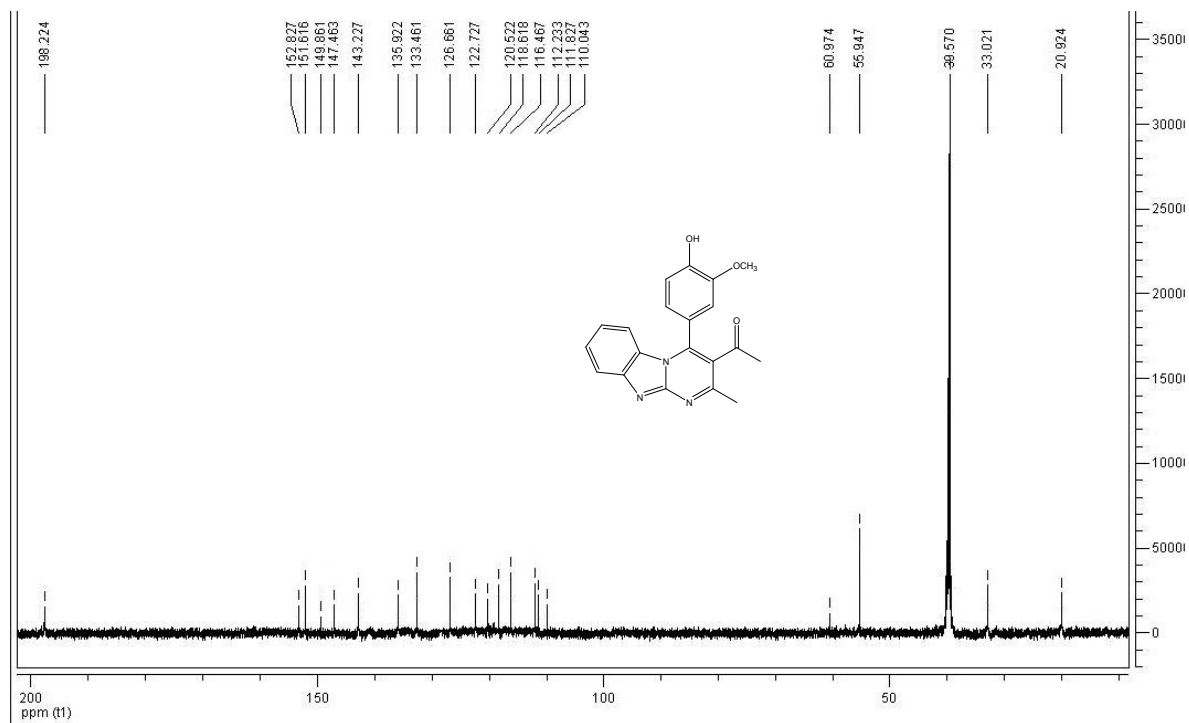


Fig s38 ¹³C-NMR spectrum of 7d

Spectral data of 8a

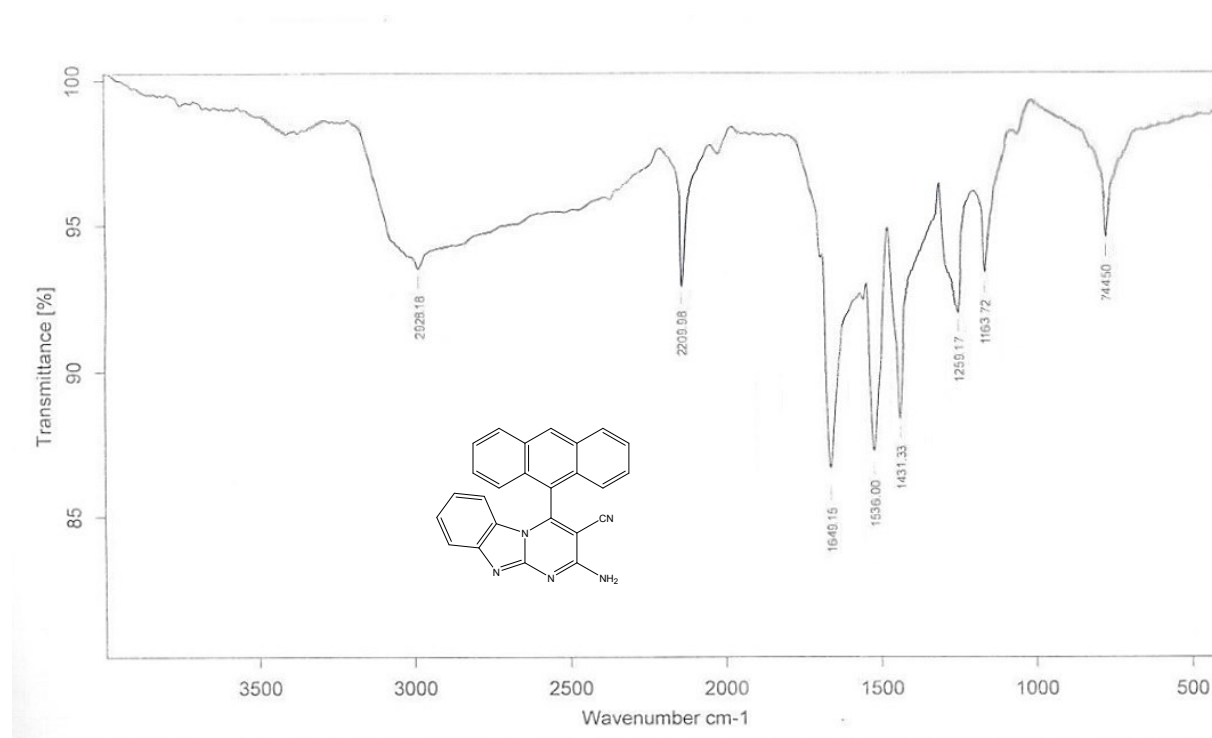


Fig. s39 FTIR spectrum of 8a

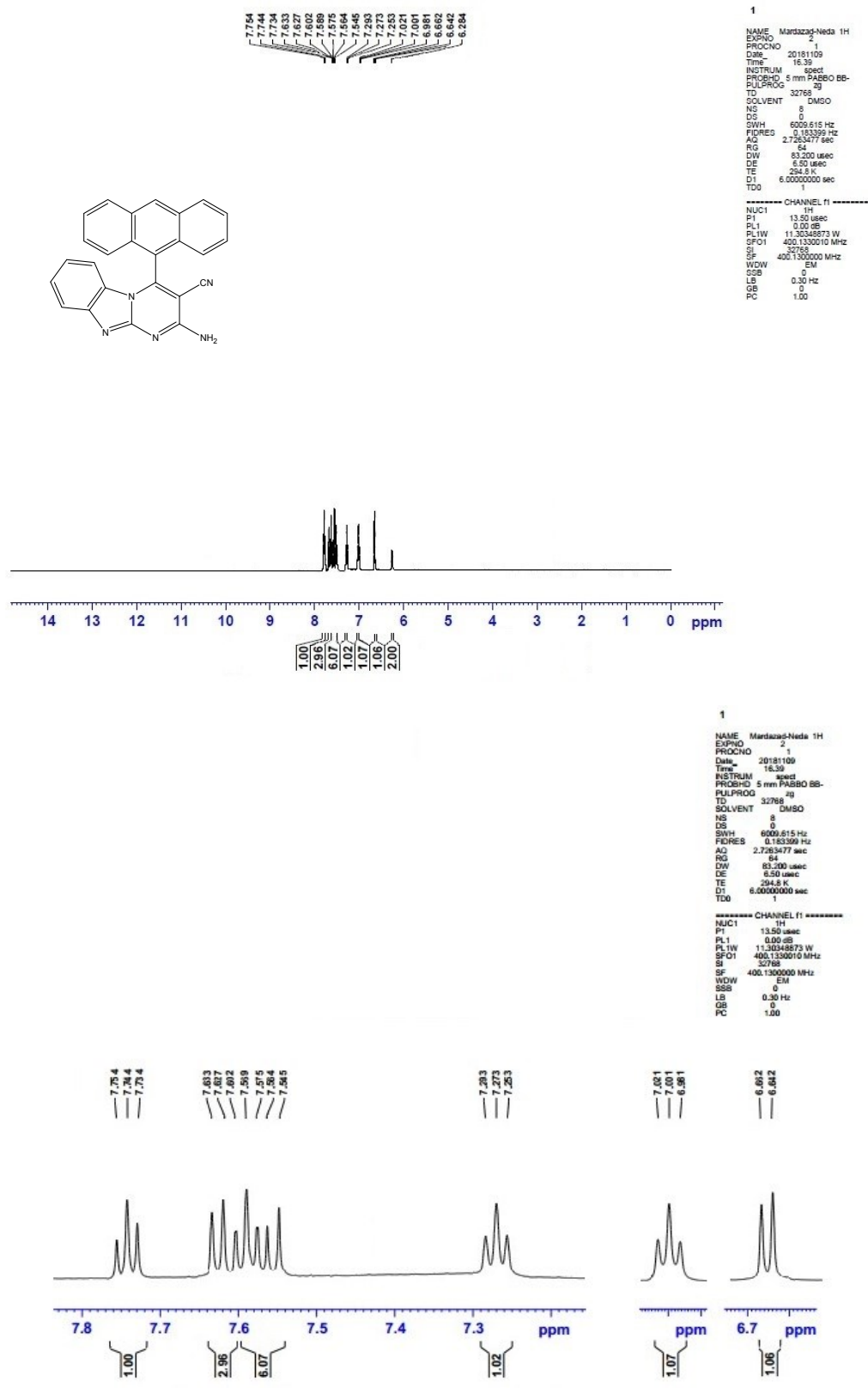


Fig s40 ¹H-NMR spectrum of 8a

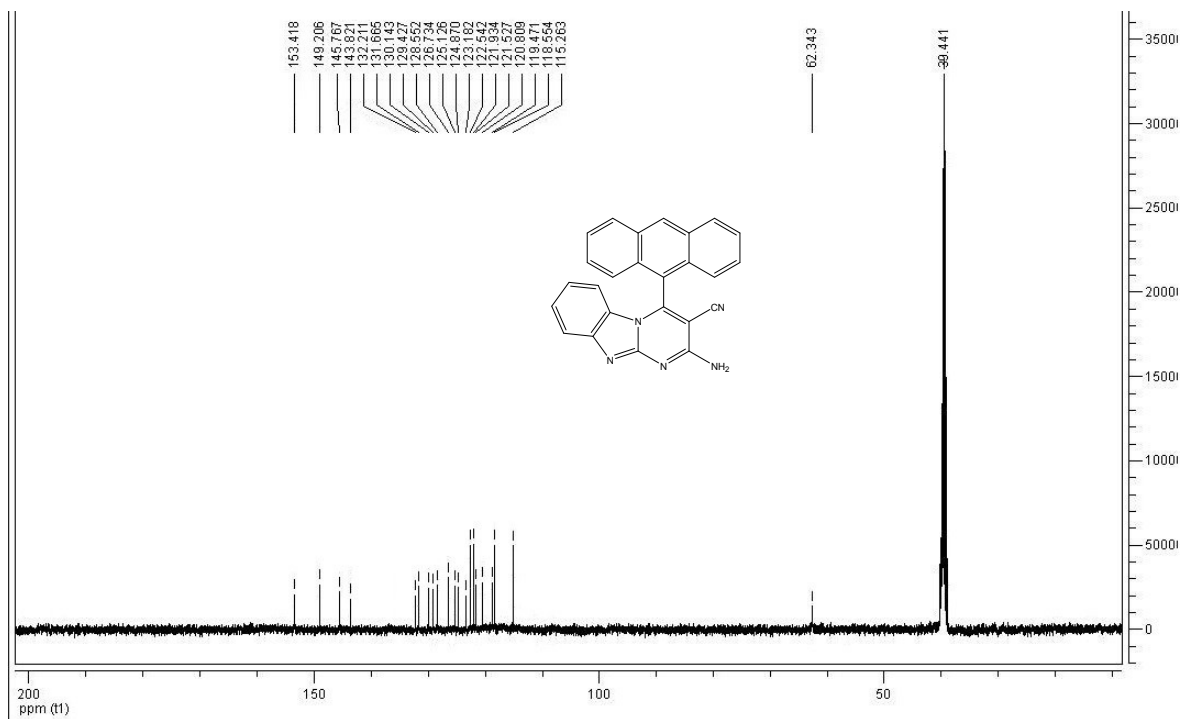


Fig s41 ^{13}C -NMR spectrum of 8a

Spectral data of 8b

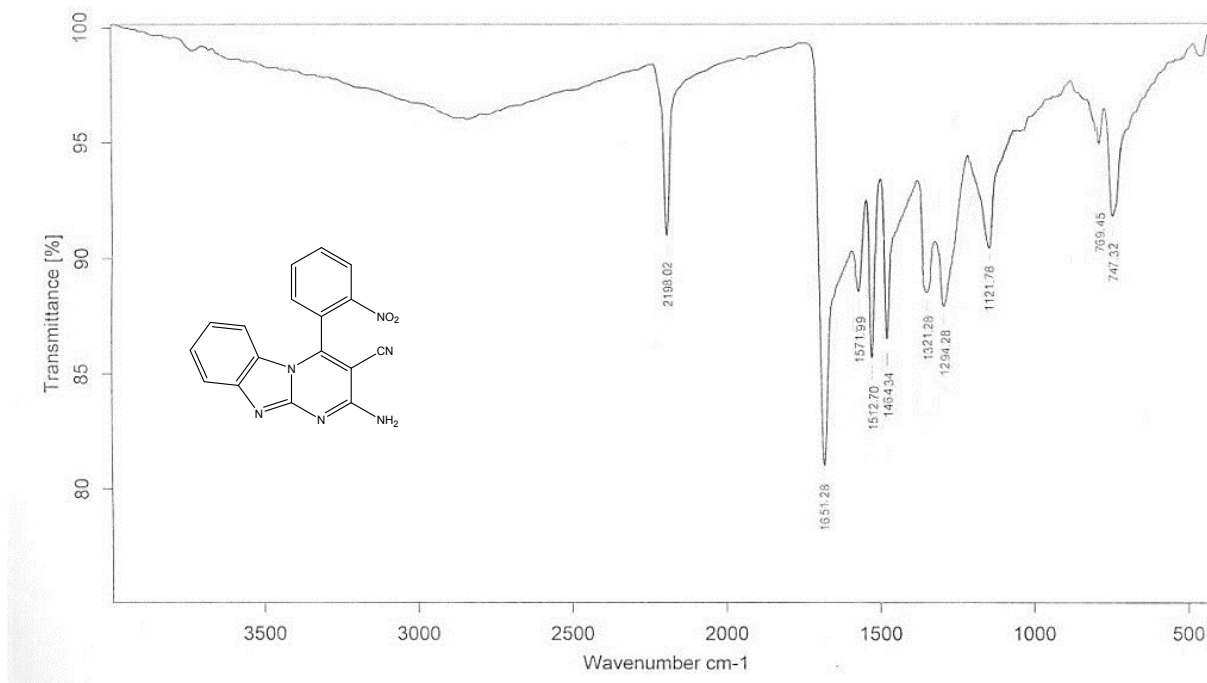
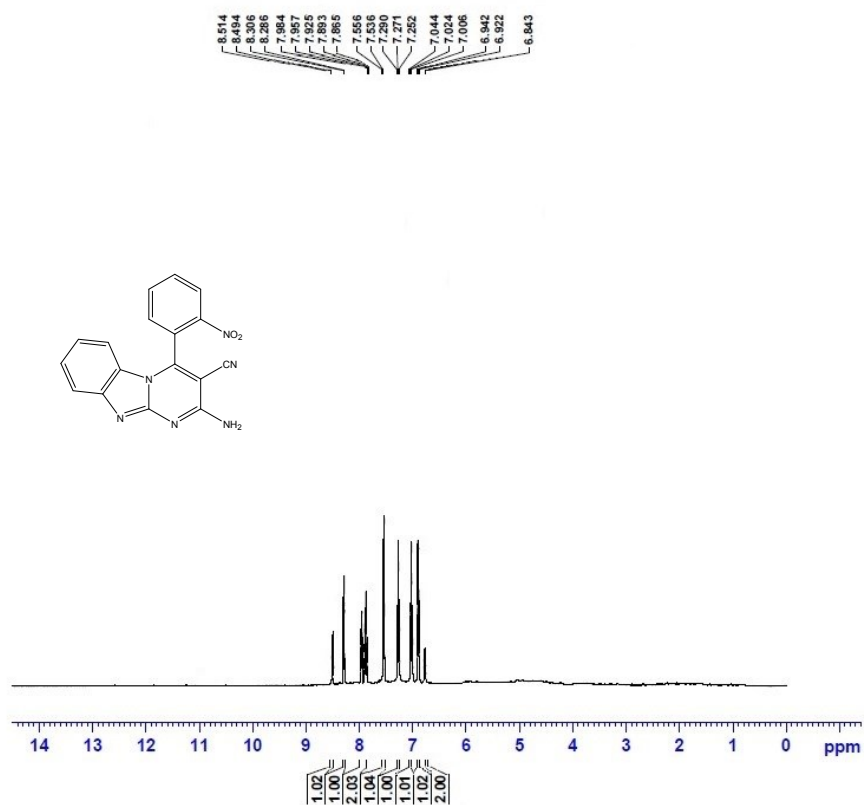


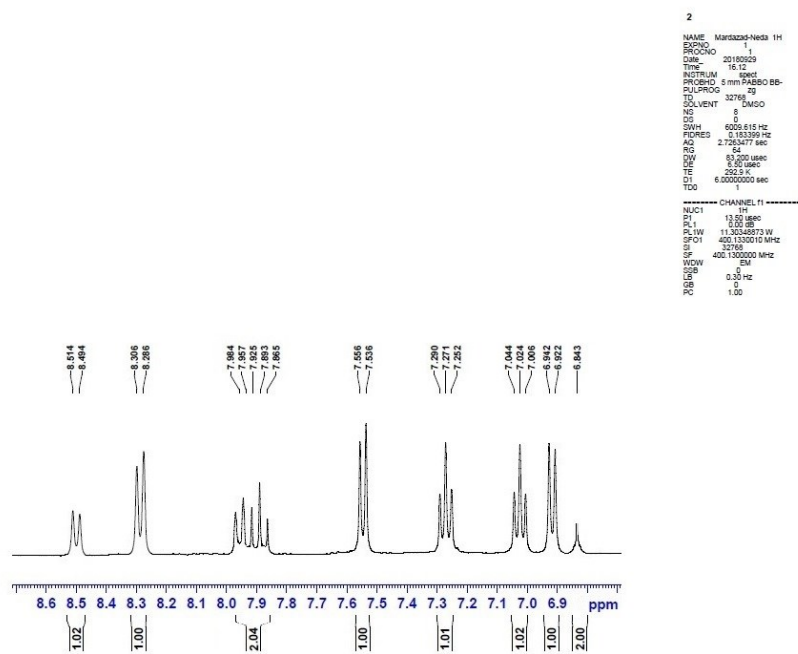
Fig. s42 FTIR spectrum of 8b



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PROCNO 1
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PULPROG zg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.193399 Hz
AQ 2.7263477 sec
RG 64
DQ 81.200 usec
DE 6.30 usec
TE 292.5 K
D1 6.0000000 sec
TDO 1
----- CHANNEL f1 -----
NUC1 1H
P1 13.50 usec
PL1 0.00 dB
PL1W 11.30348873 W
SFO1 400.1330010 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
GB 0.30 Hz
PC 1.00

```



```

2
NAME Mar0323-Neda 1H
EXPNO 1
PROCNO 1
Date_ 20180929
Time 16:12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.193399 Hz
AQ 2.7263477 sec
RG 64
DQ 81.200 usec
DE 6.30 usec
TE 292.5 K
D1 6.0000000 sec
TDO 1
----- CHANNEL f1 -----
NUC1 1H
P1 13.50 usec
PL1 0.00 dB
PL1W 11.30348873 W
SFO1 400.1330010 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
GB 0.30 Hz
PC 1.00

```

Fig s43 ¹H-NMR spectrum of 8b

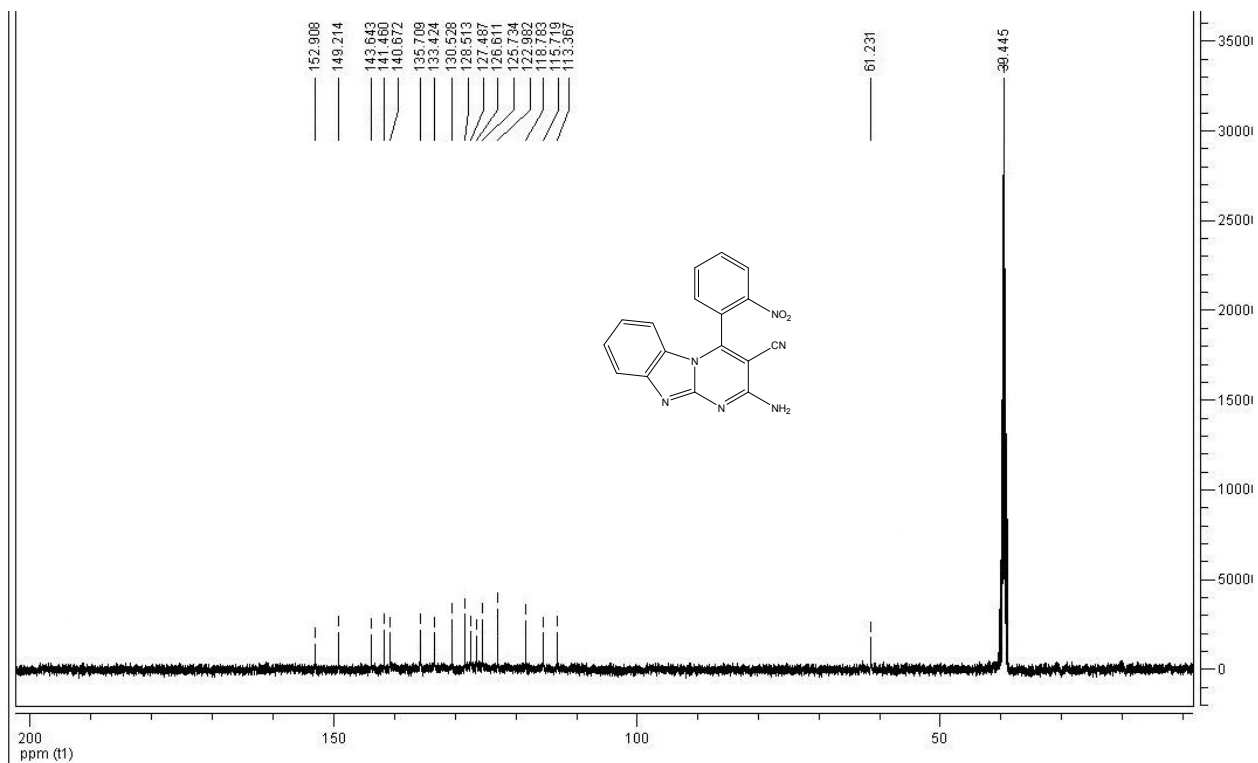


Fig s44 ^{13}C -NMR spectrum of 8b

Spectral data of 8c

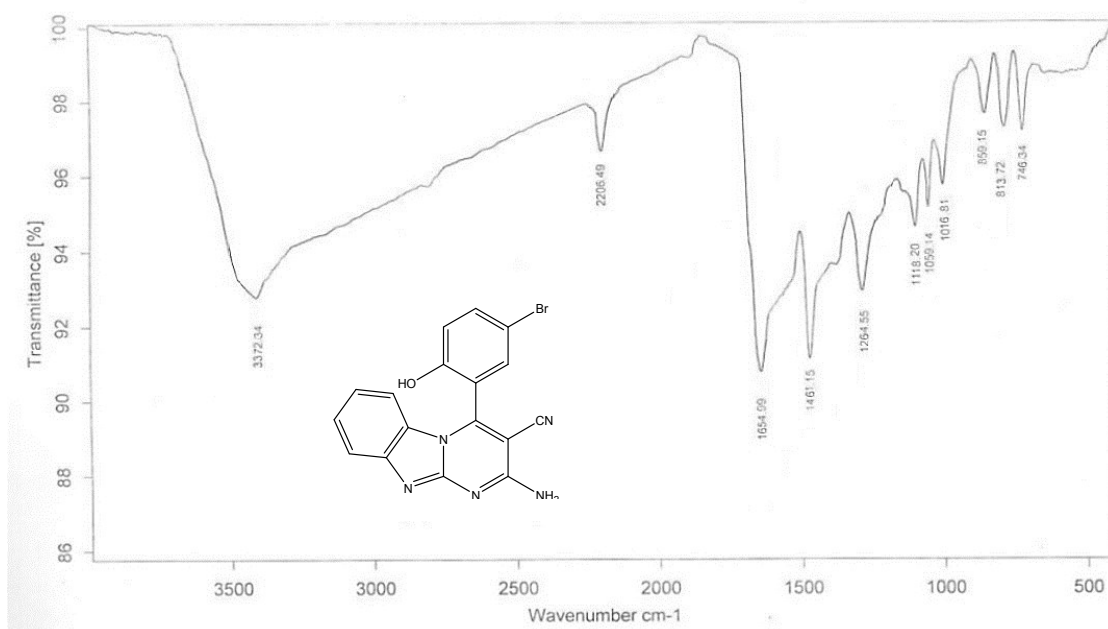
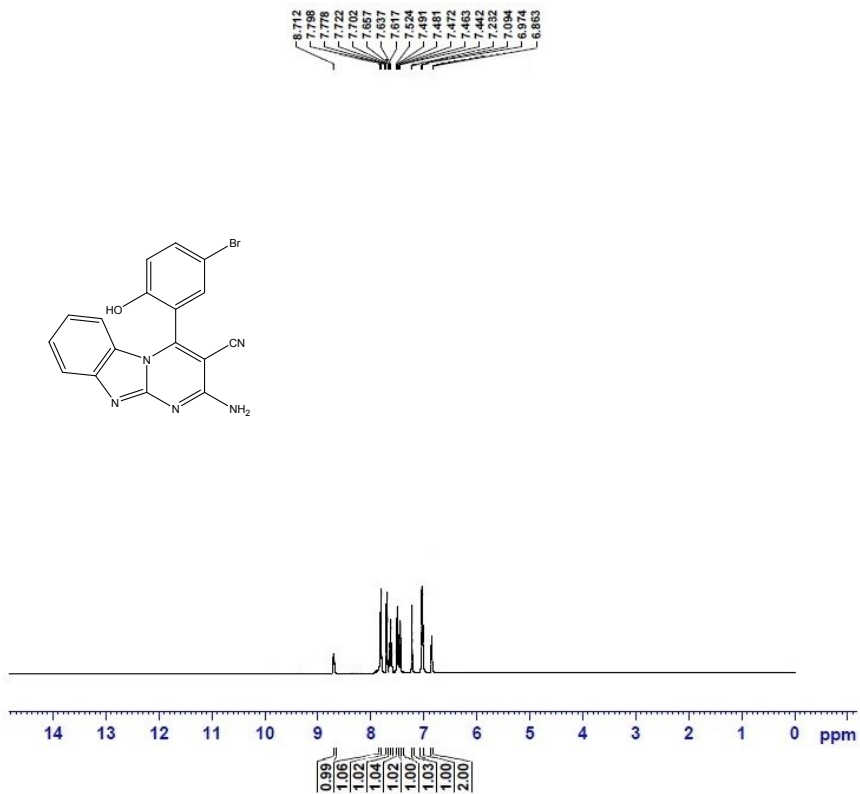


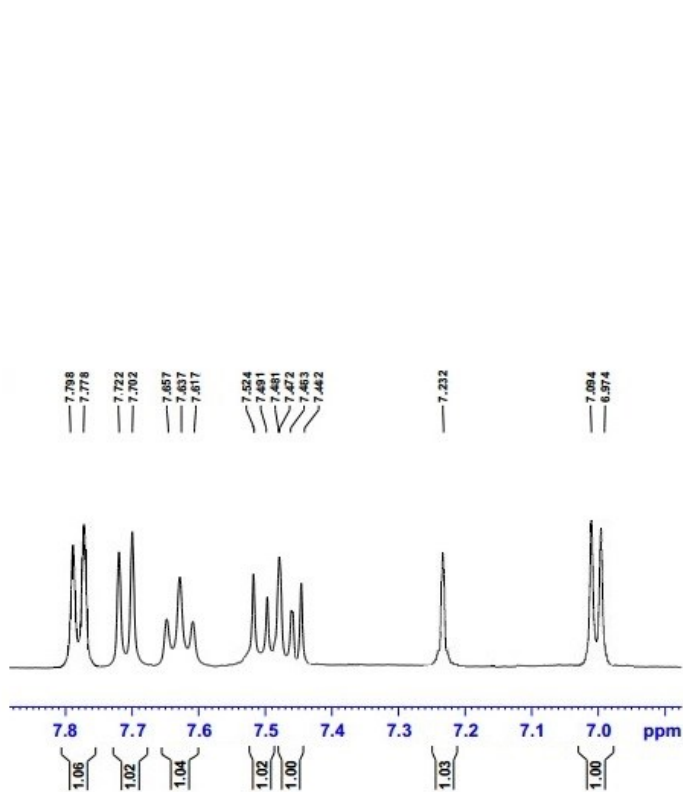
Fig. s45 FTIR spectrum of 8c



```

1
NAME  Mardazad-Neda 1H
EXPNO  2
PROCNO  1
Date_   20181109
Time    16.39
INSTRUM spect
PROBHD  5 mm PABBO BB-
PULPROG zg
TD       32768
SOLVENT DMSO
DS       0
NS       8
SWH     6009.615 Hz
FIDRES  0.183399 Hz
AQ      2.7283477 sec
RG       64
DW      83.200 usec
DE       6.50 usec
TE      294.8 K
D1      6.00000000 sec
TD0     1
----- CHANNEL f1 -----
NUC1    1H
P1      13.50 usec
PL1     0.00 dB
PL1W    11.30348873 W
SFO1    400.1330010 MHz
SI      32768
SF      400.1300000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00

```



```

1
NAME  Mardazad-Neda 1H
EXPNO  2
PROCNO  1
Date_   20181109
Time    16.39
INSTRUM spect
PROBHD  5 mm PABBO BB-
PULPROG zg
TD       32768
SOLVENT DMSO
DS       0
NS       8
SWH     6009.615 Hz
FIDRES  0.183399 Hz
AQ      2.7283477 sec
RG       64
DW      83.200 usec
DE       6.50 usec
TE      294.8 K
D1      6.00000000 sec
TD0     1
----- CHANNEL f1 -----
NUC1    1H
P1      13.50 usec
PL1     0.00 dB
PL1W    11.30348873 W
SFO1    400.1330010 MHz
SI      32768
SF      400.1300000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00

```

Fig s46 ¹H-NMR spectrum of 8c

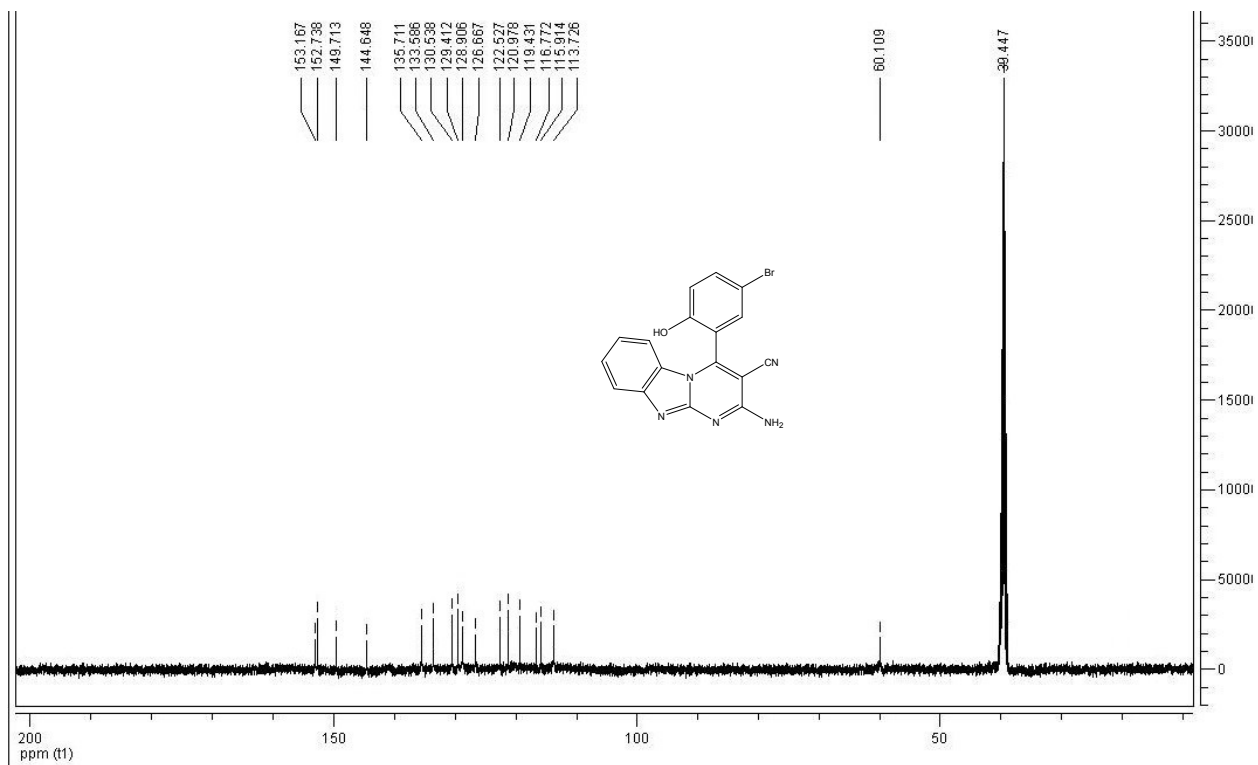


Fig s47 ^{13}C -NMR spectrum of 8c

Spectral data of 8d

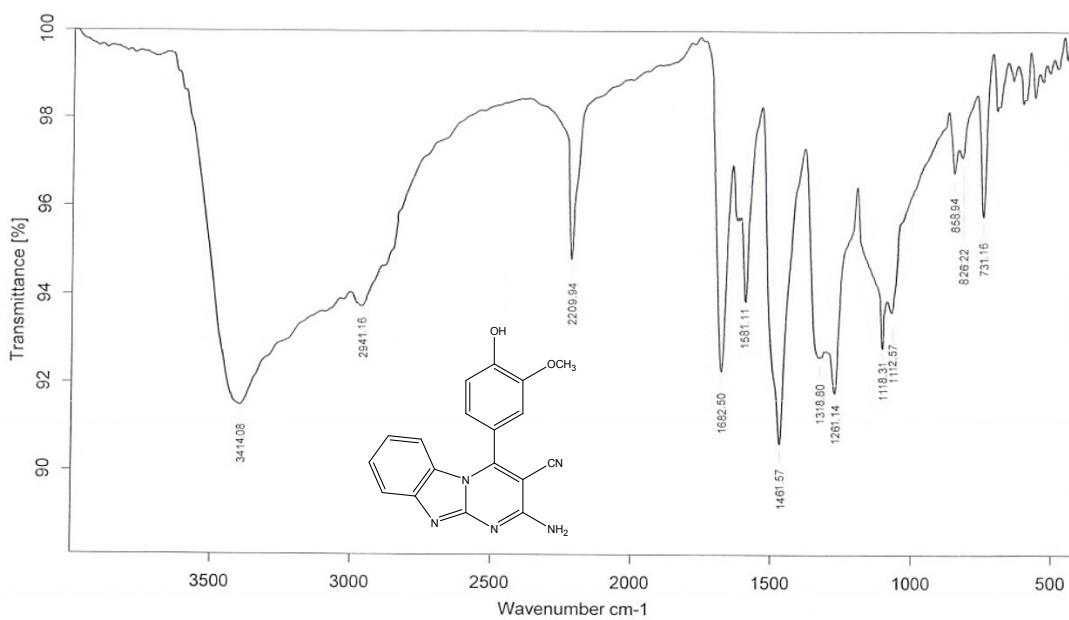


Fig. s48 FTIR spectrum of 8d

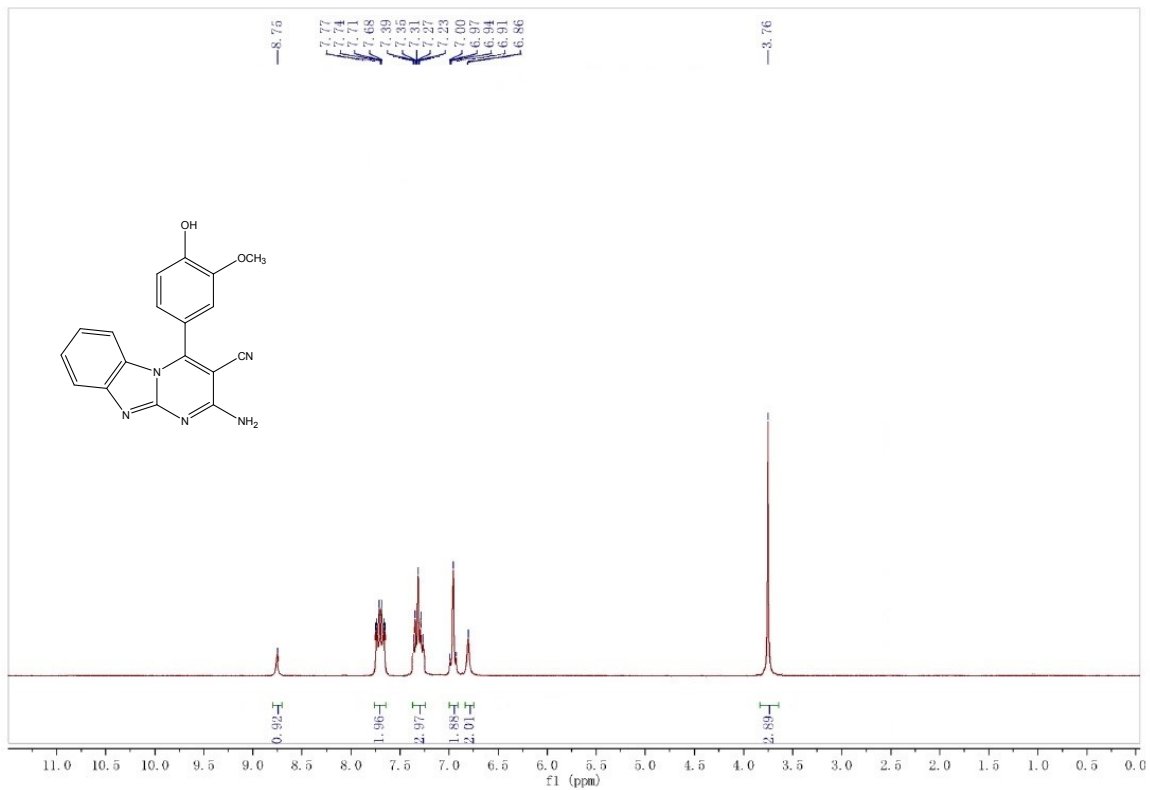


Fig s49 ¹H-NMR spectrum of 8d

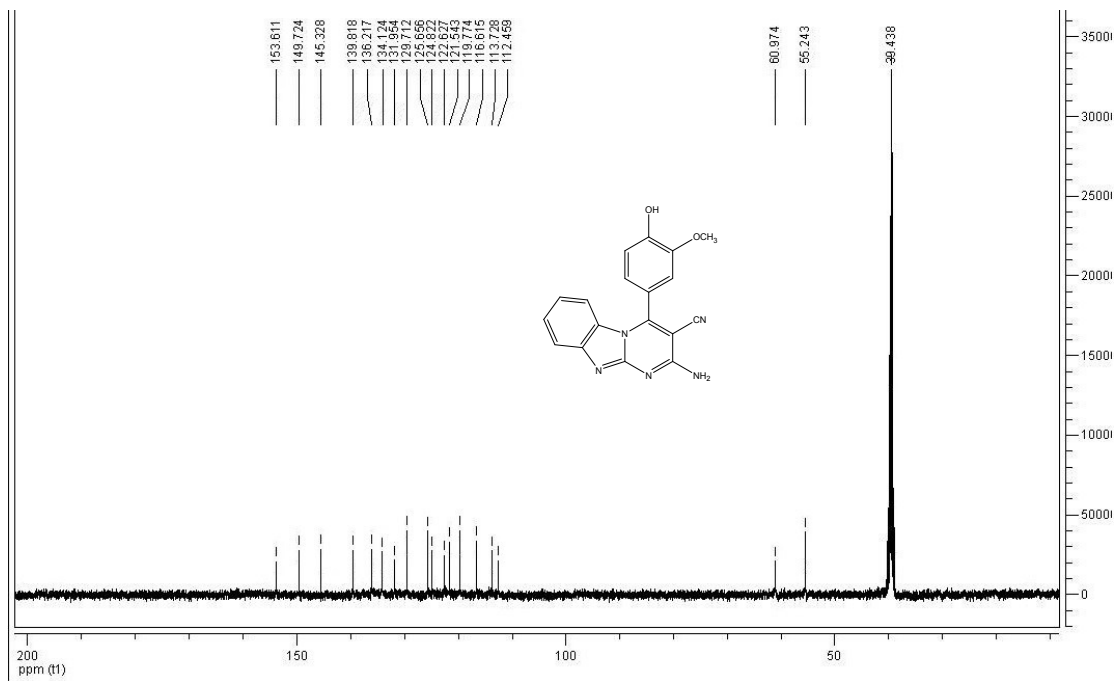


Fig s50 ¹³C-NMR spectrum of 8d