

Supplementary Material

Synthesis and characterization of some new thieno[2,3-*b*]pyridines, thieno[2,3-*c*][2,7]naphthyridinones and pyrazolo[3,4-*c*][2,7]naphthyridinones with expected biological activity

Safiyah A. H. Al-Waleedy,^{a,b} Osama Younis,^c Shams H. Abdel-Hafez,^d and Etify A. Bakhite,^{a*}

^aDepartment of Chemistry, Faculty of Science, Assiut University, Assiut, Egypt. ^bDepartment of Chemistry, Faculty of Science, Taiz University, Taiz, Yemen..^cChemistry Department, Faculty of Science, New Valley University, El-Kharja, Egypt

^dDepartment of Chemistry, College of Science, Taif University, Taif 21944, Saudi Arabia
Email: etafy@aun.edu.eg

Table of Contents

IR, ¹H NMR and ¹³C NMR and MS spectra of synthesized compounds S2

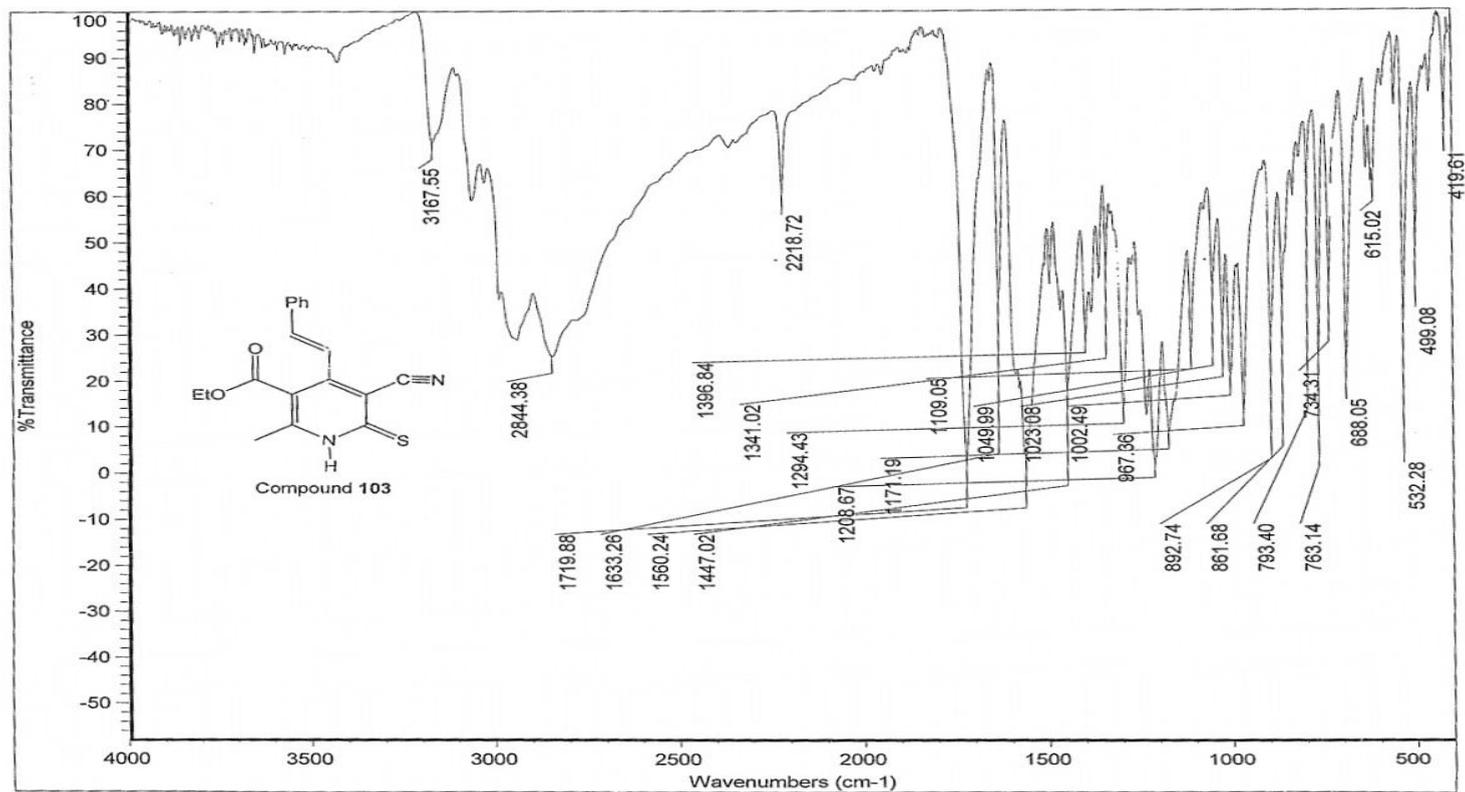


Figure S1: IR spectrum of compound 2.

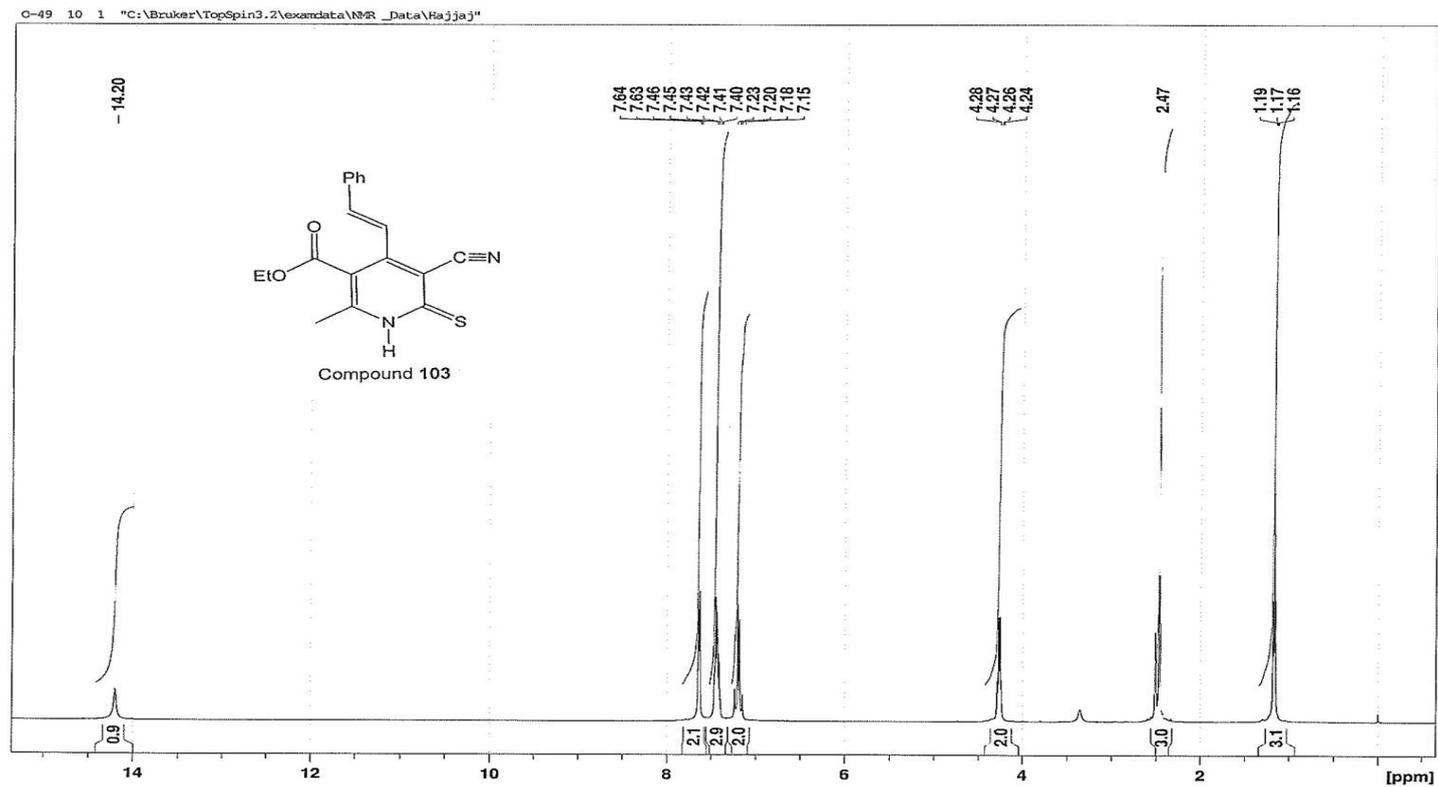


Figure S2: ^1H NMR spectrum of compound 2 in $\text{DMSO-}d_6$.

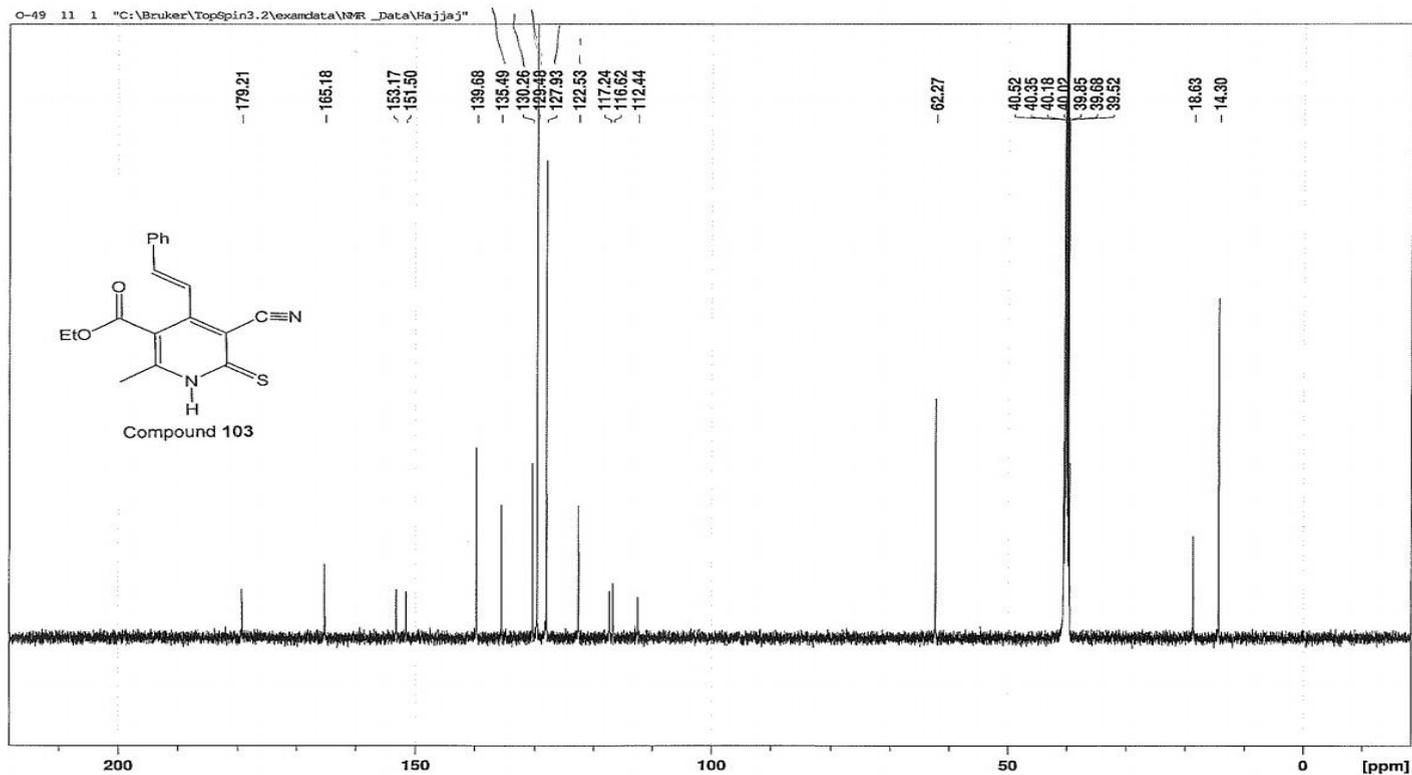


Figure S3: ^{13}C NMR spectrum of compound 2 in $\text{DMSO-}d_6$.

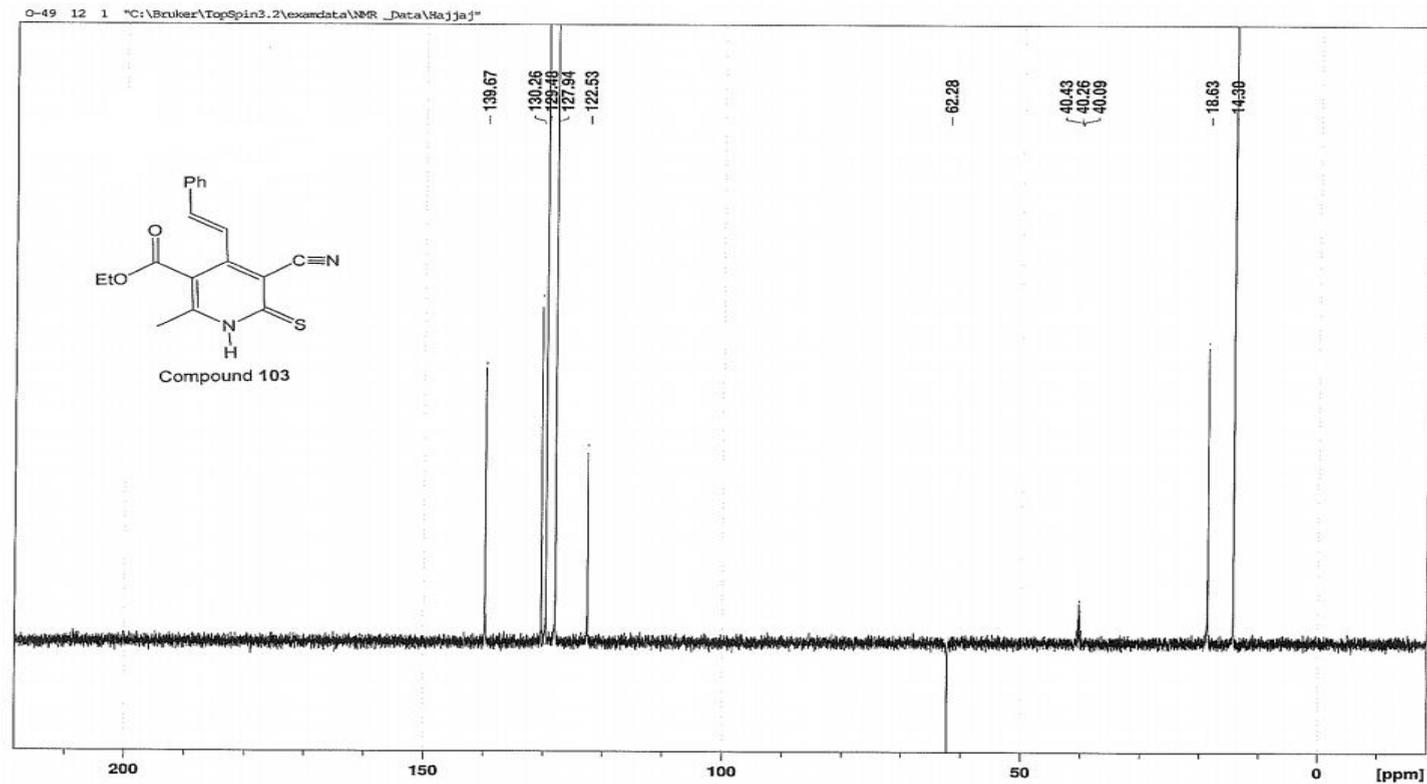


Figure S4: DEPT 135 spectrum of compound 2 in DMSO- d_6 .

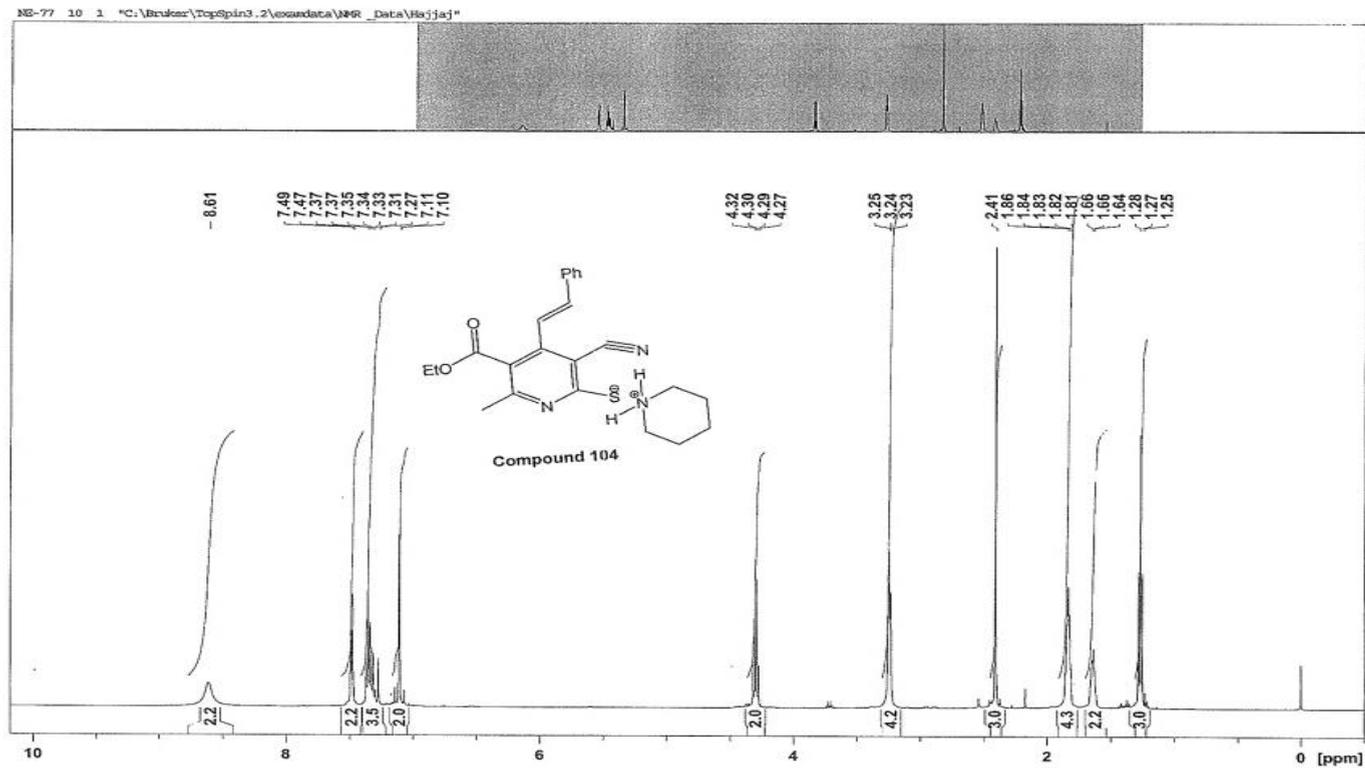


Figure S5: ^1H NMR spectrum of compound 3 in CDCl_3 .

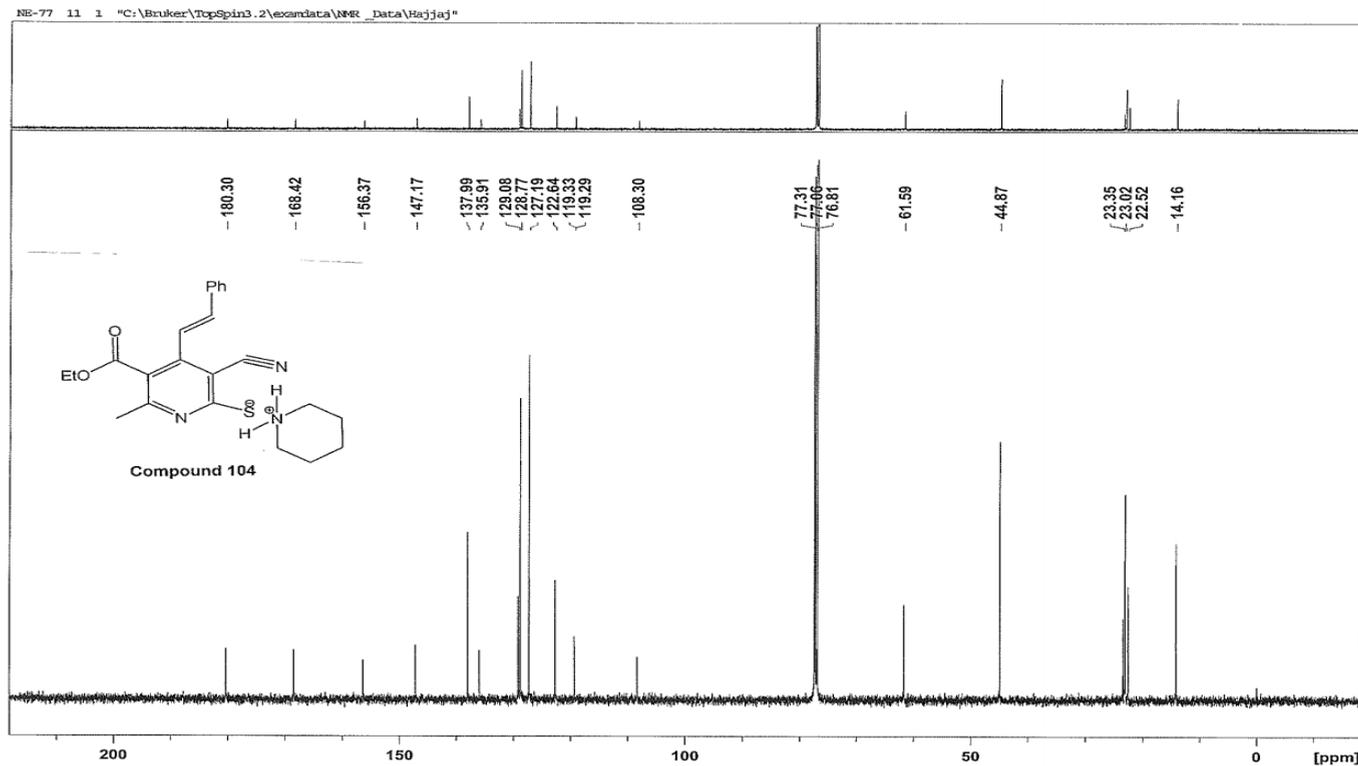


Figure S6: ^{13}C NMR spectrum of compound 3 in CDCl_3 .

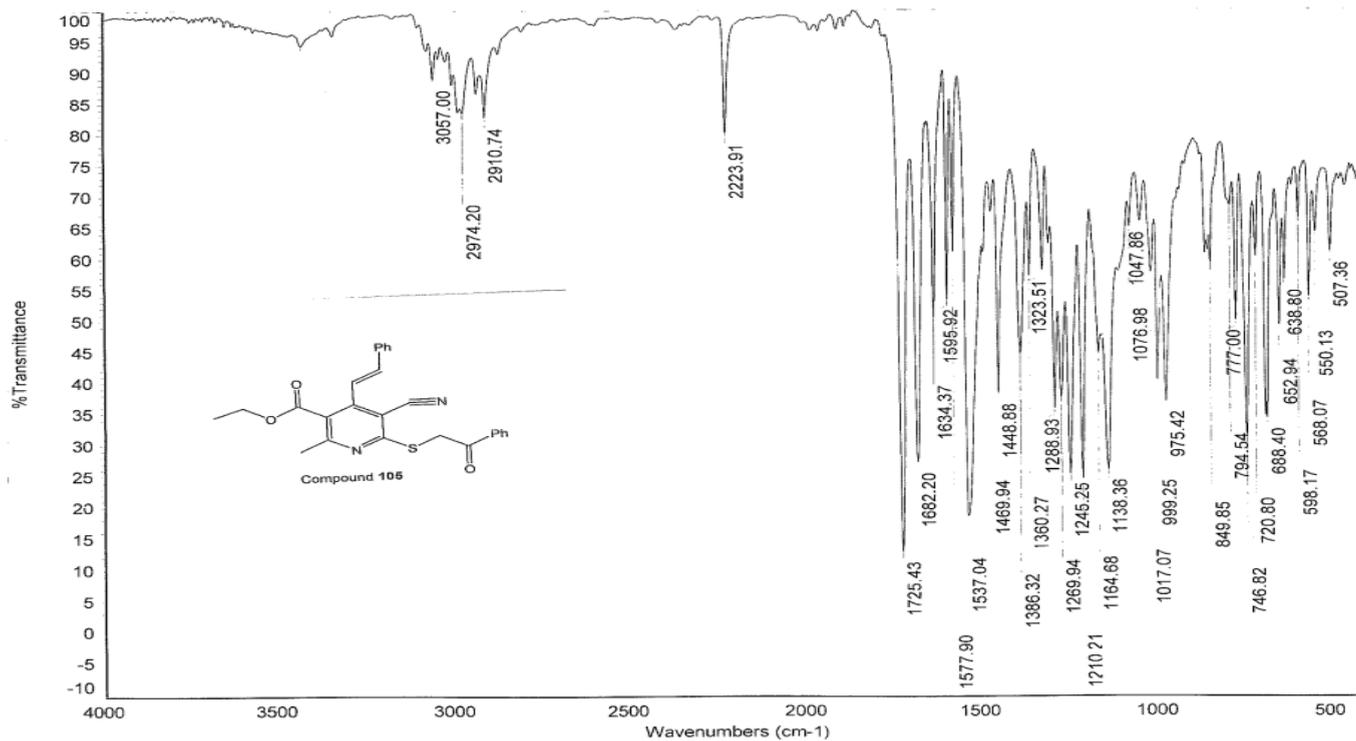


Figure. S7: IR spectrum of compound 5.

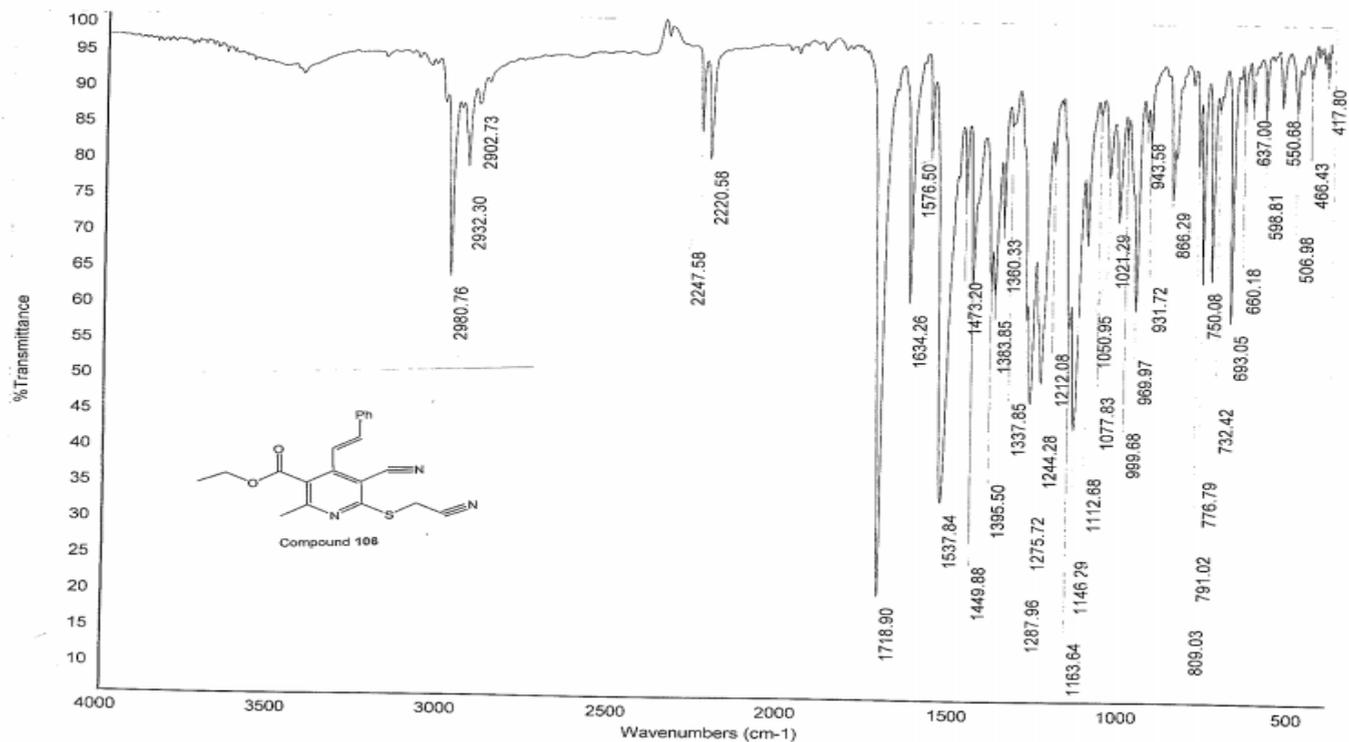


Figure S8: IR spectrum of compound 6.

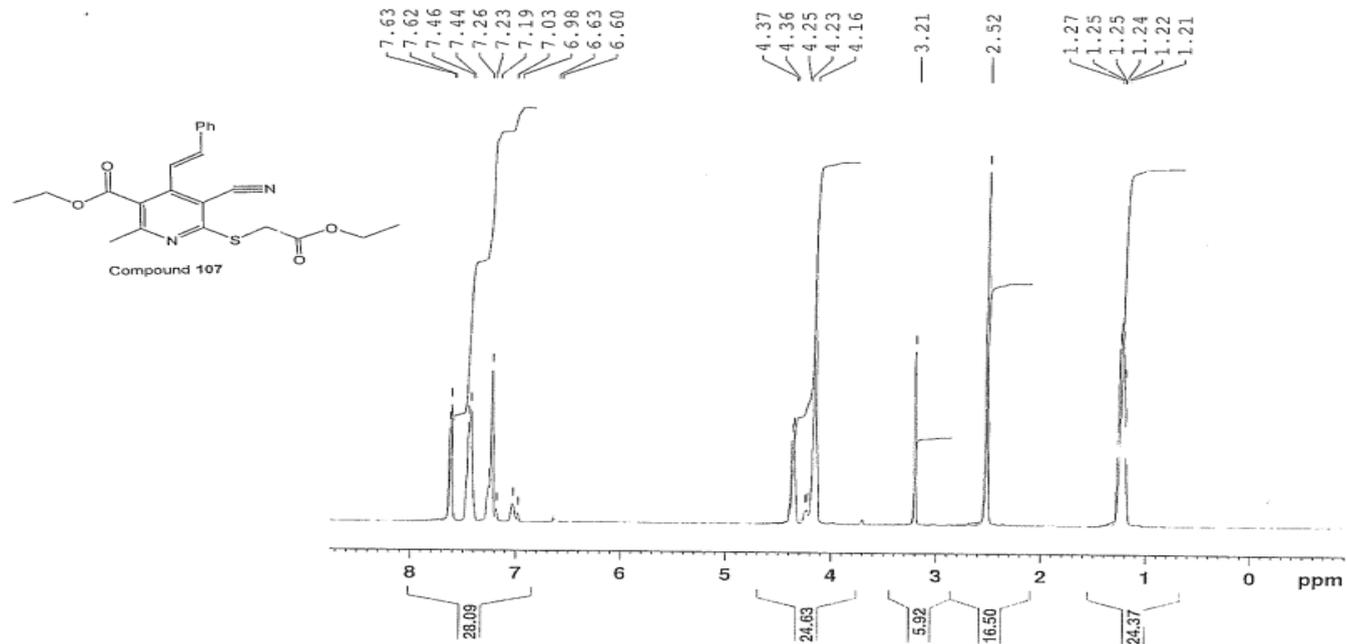


Figure S9: ¹H NMR spectrum of compound 7 in DMSO-*d*₆.

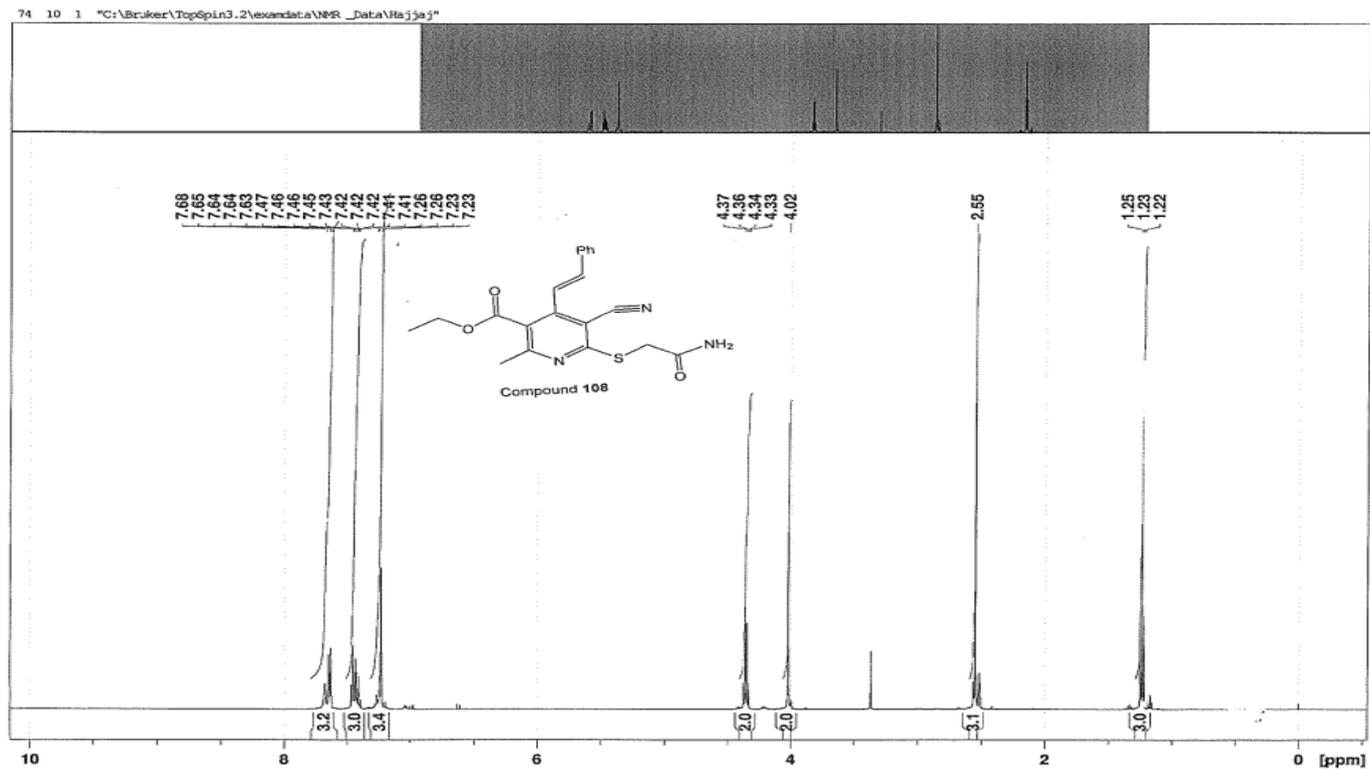


Figure S10: ^1H NMR spectrum of compound 8 in $\text{DMSO-}d_6$.

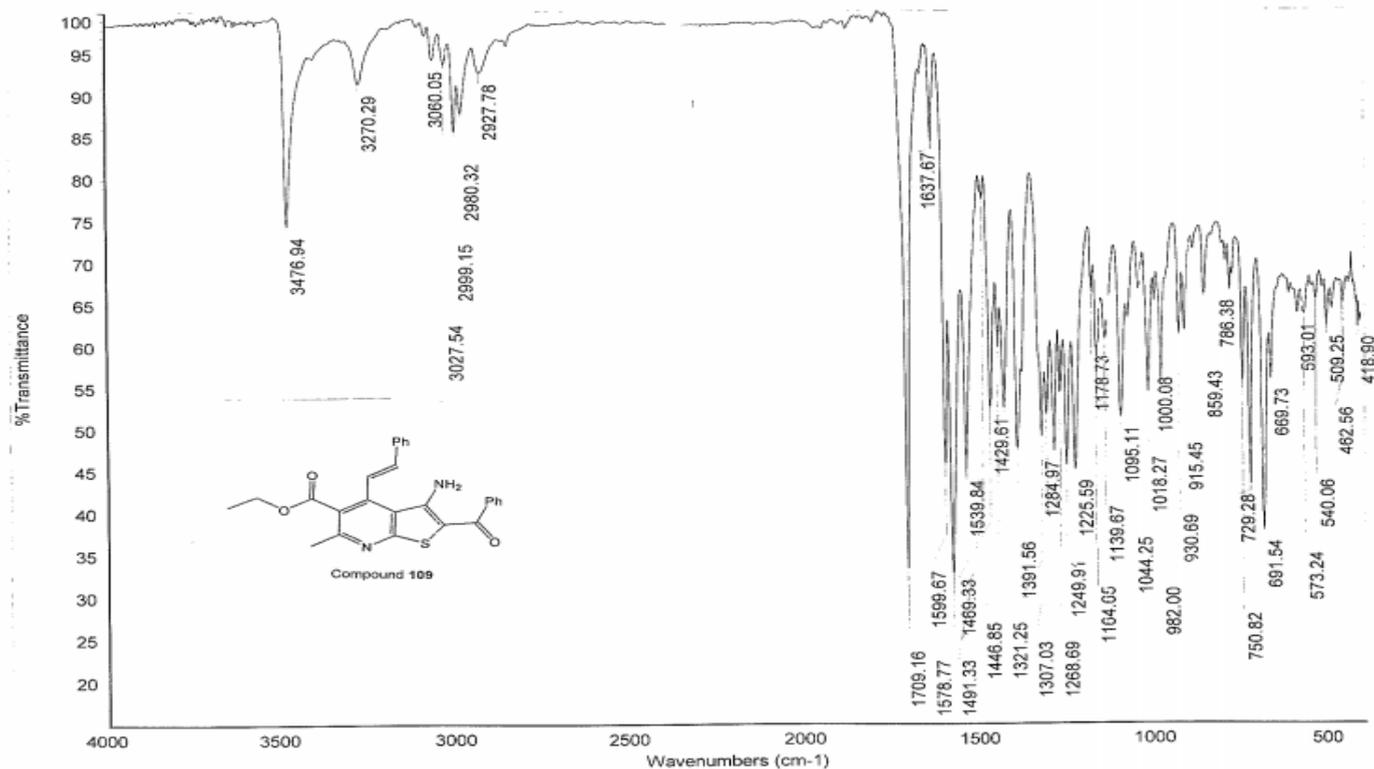


Figure S11: IR spectrum of compound 9.

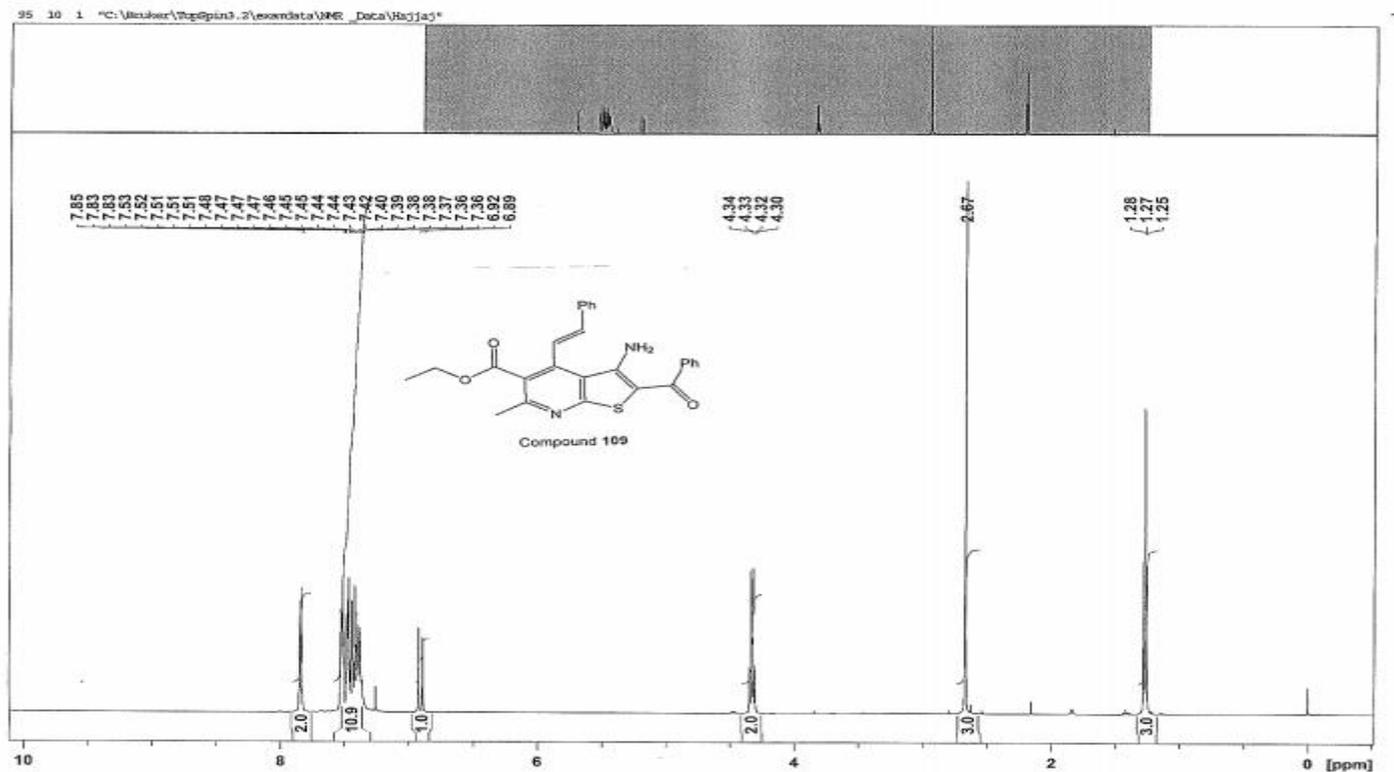


Figure S12: ^1H NMR spectrum of compound 9 in CDCl_3 .

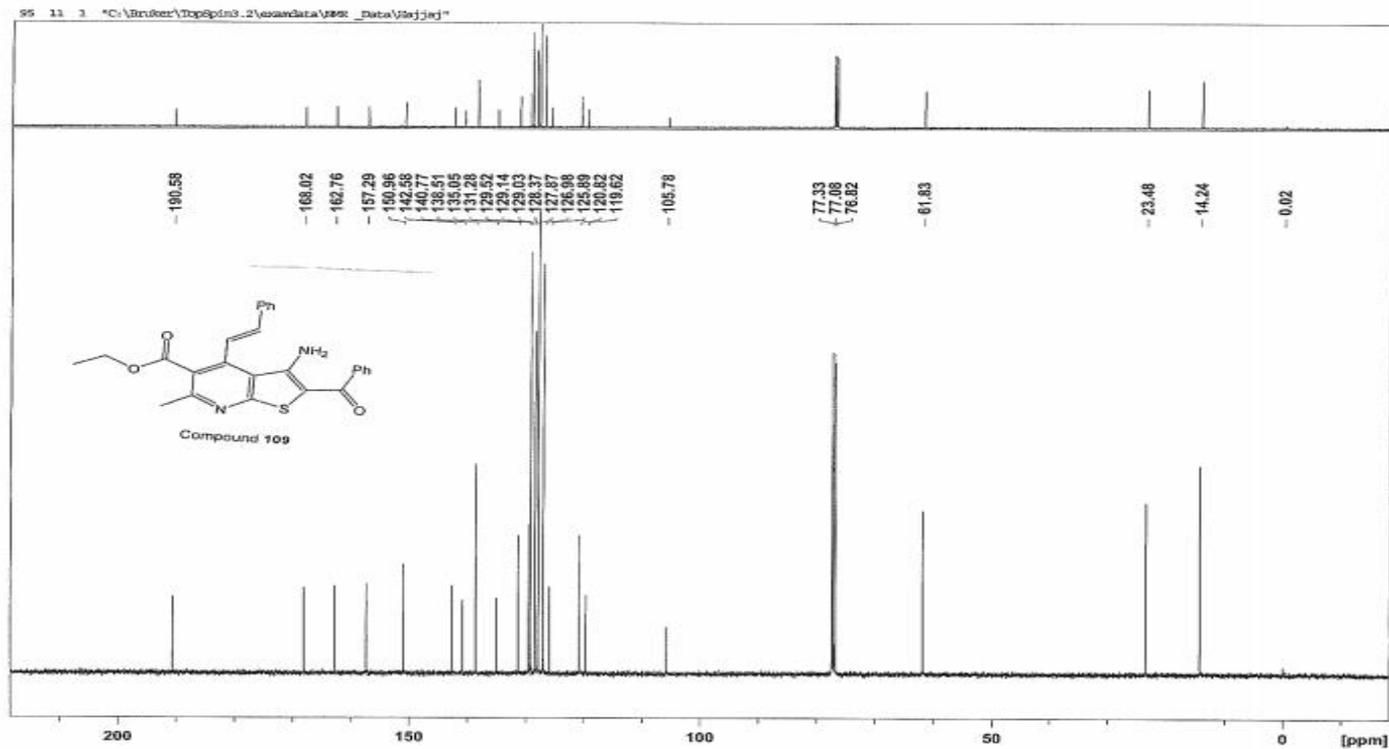


Figure S13: ^{13}C NMR spectrum of compound 9 in CDCl_3 .

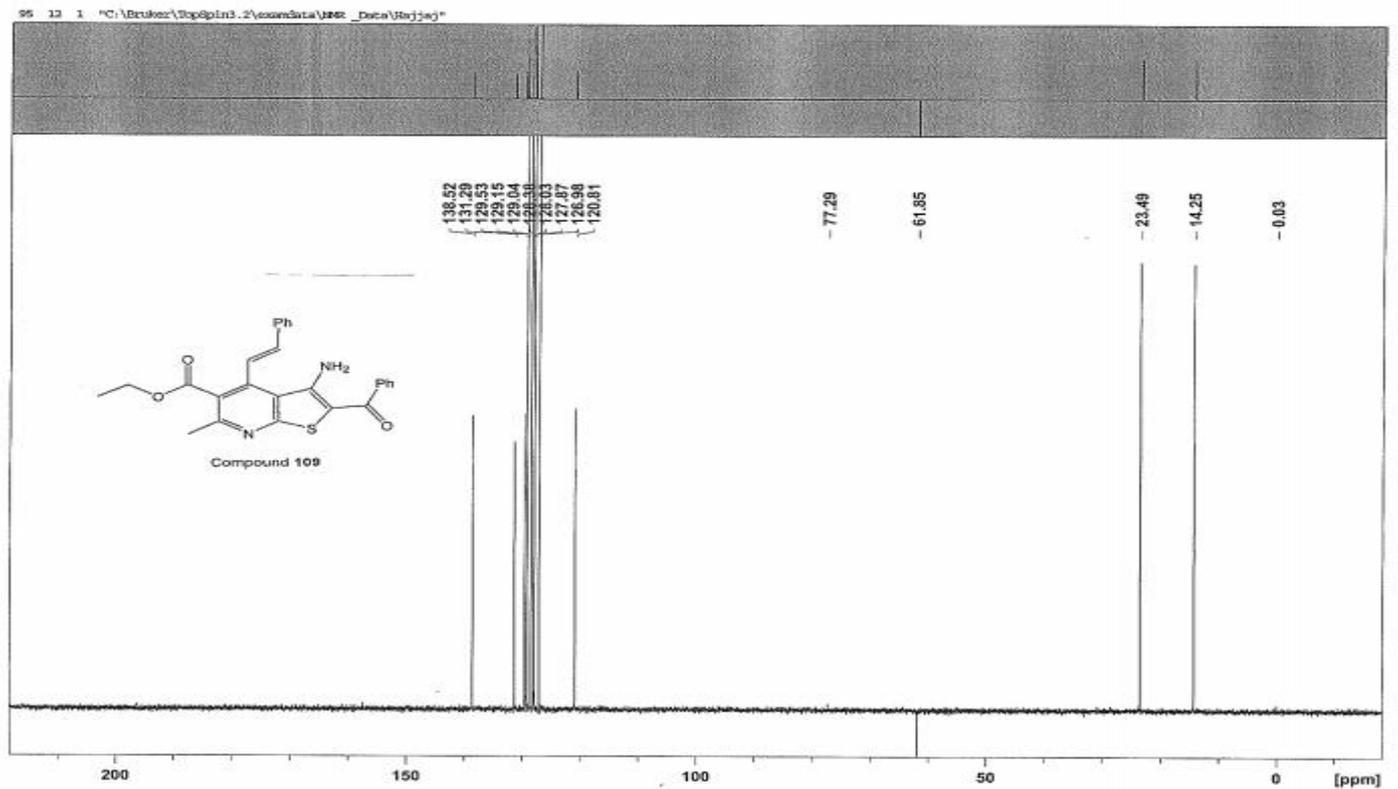


Figure S14: DEPT 135 spectrum of compound 9 in CDCl₃.

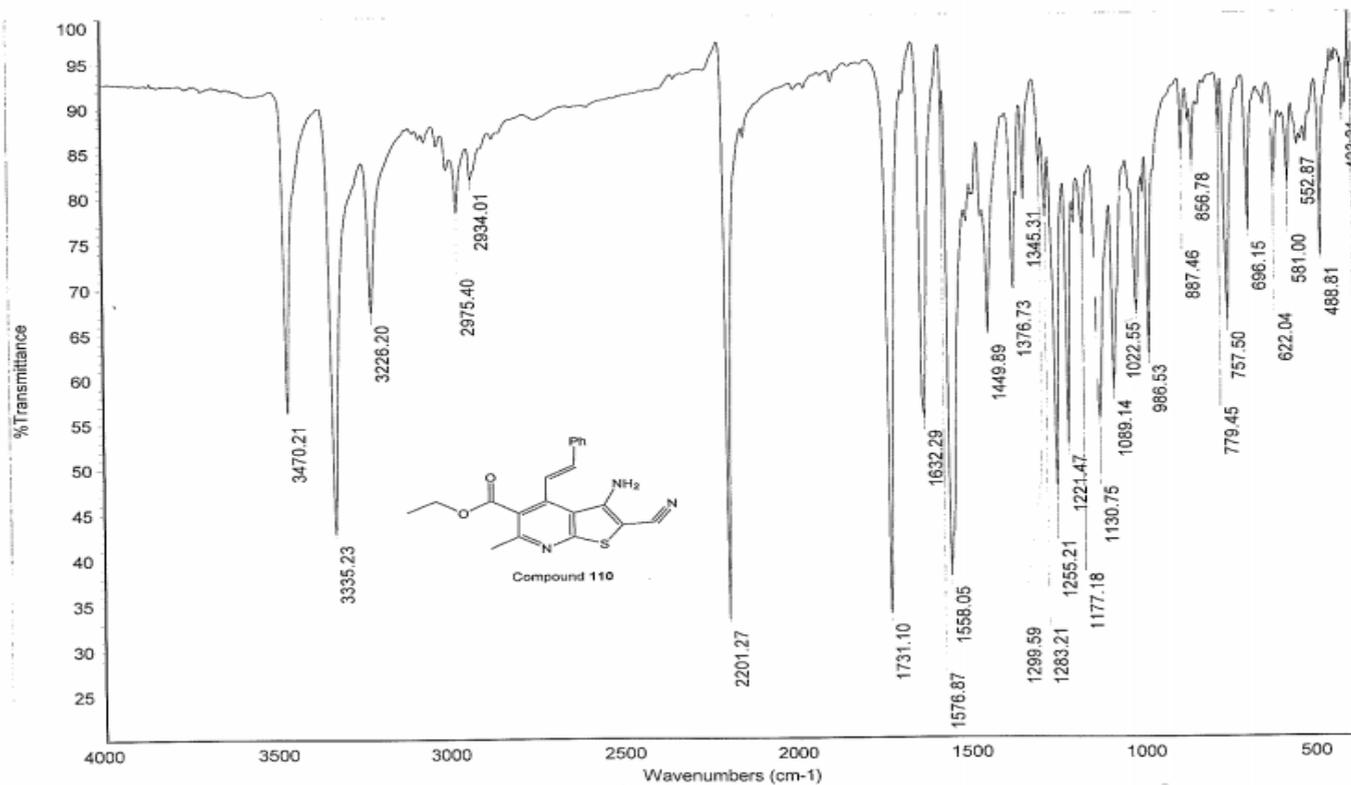


Figure S15: IR spectrum of compound 10.

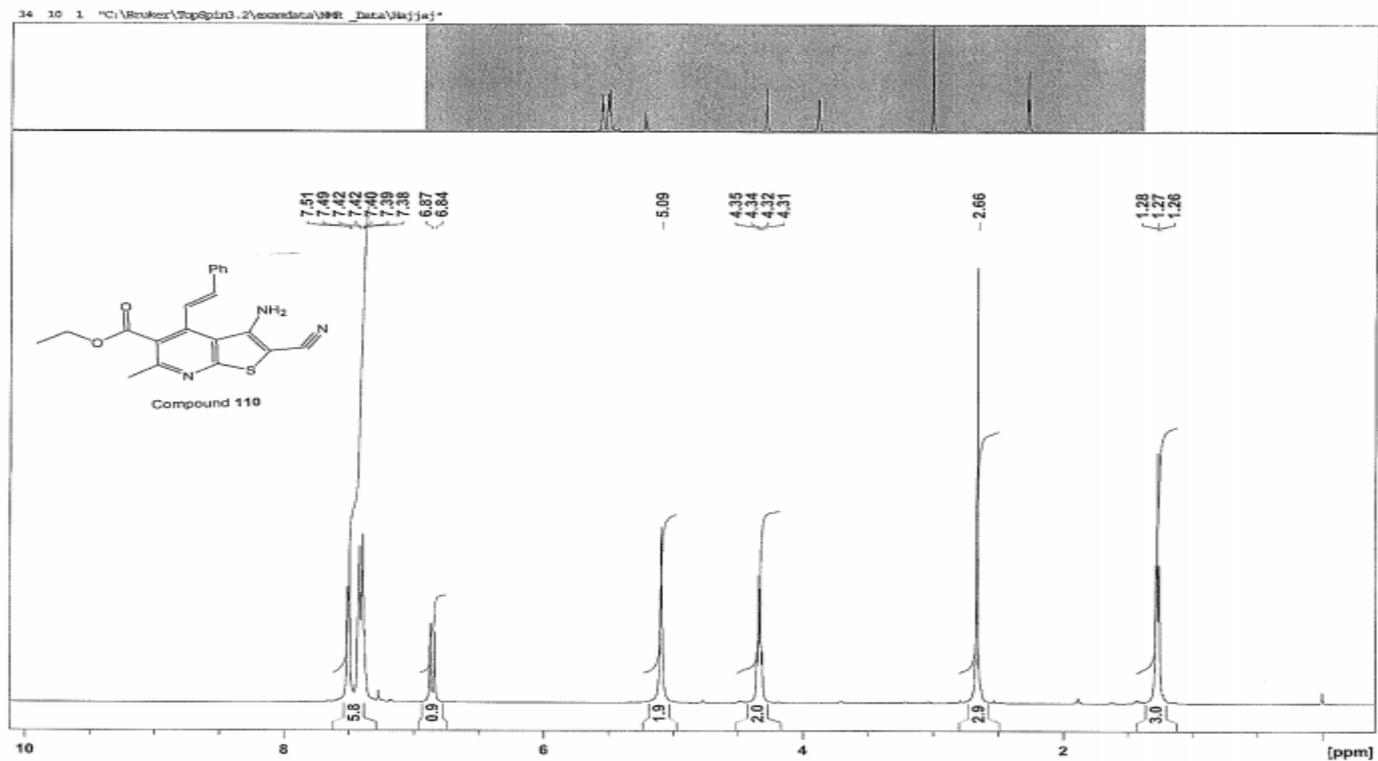


Figure S16: ^1H NMR spectrum of compound 10 in CDCl_3 .

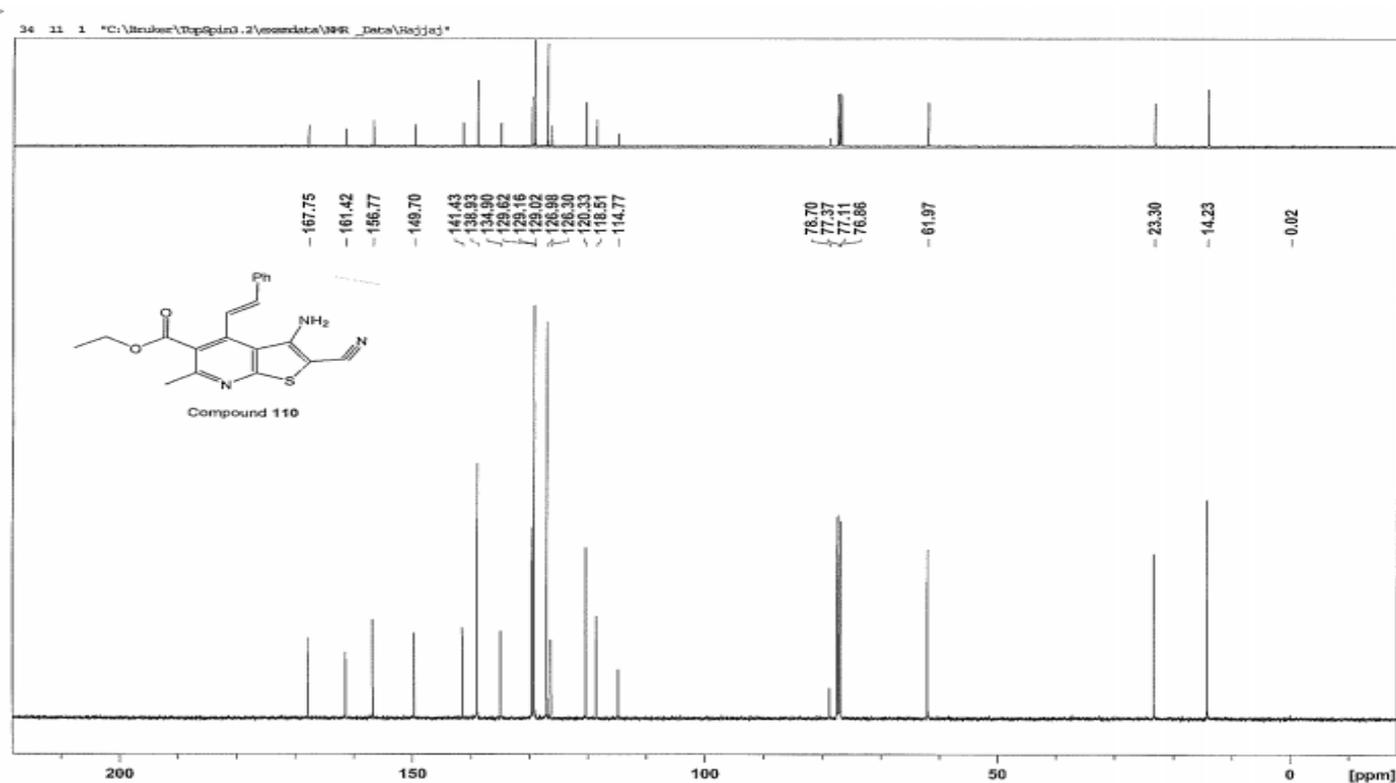


Figure S17: ^{13}C NMR spectrum of compound 10 in CDCl_3 .

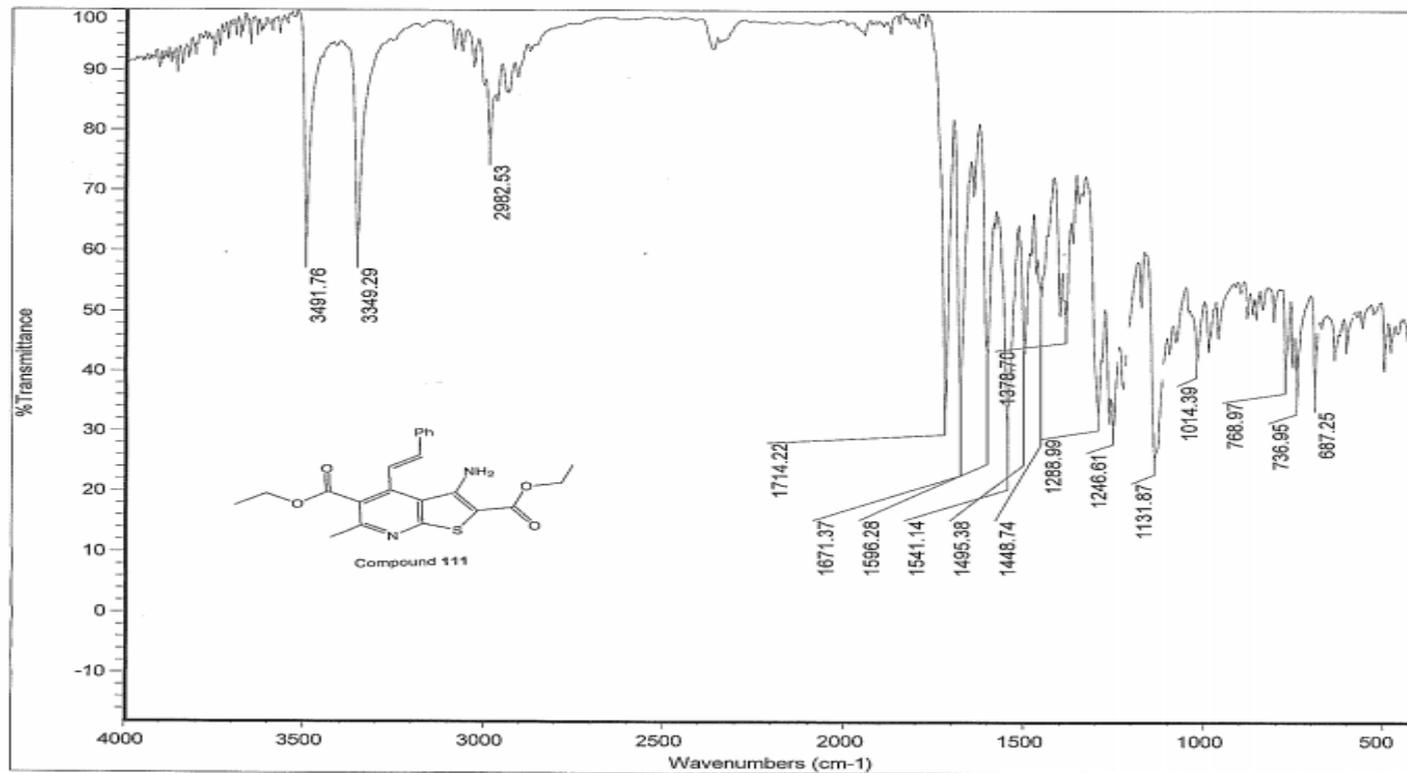


Figure S18: IR spectrum of compound 11.

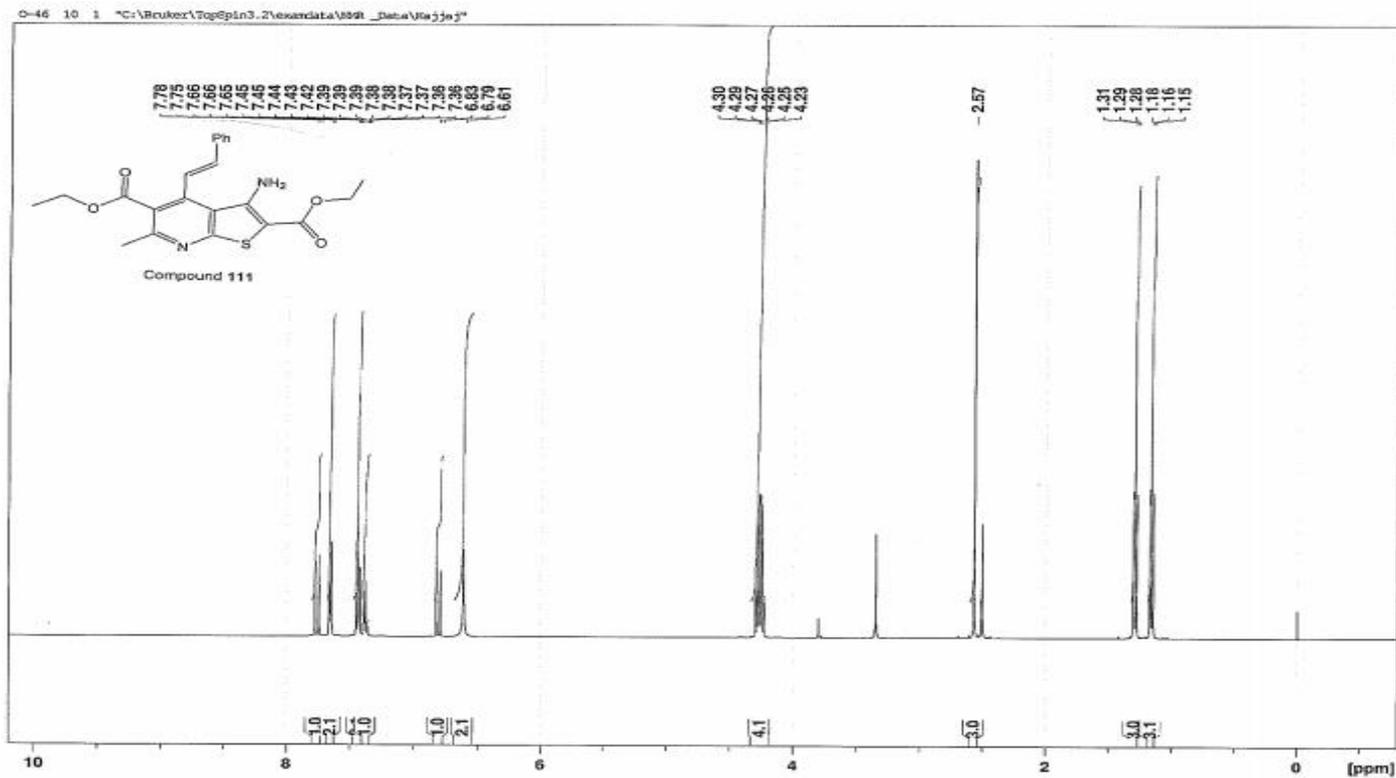


Figure S19: ^1H NMR spectrum of compound 11 in $\text{DMSO-}d_6$.

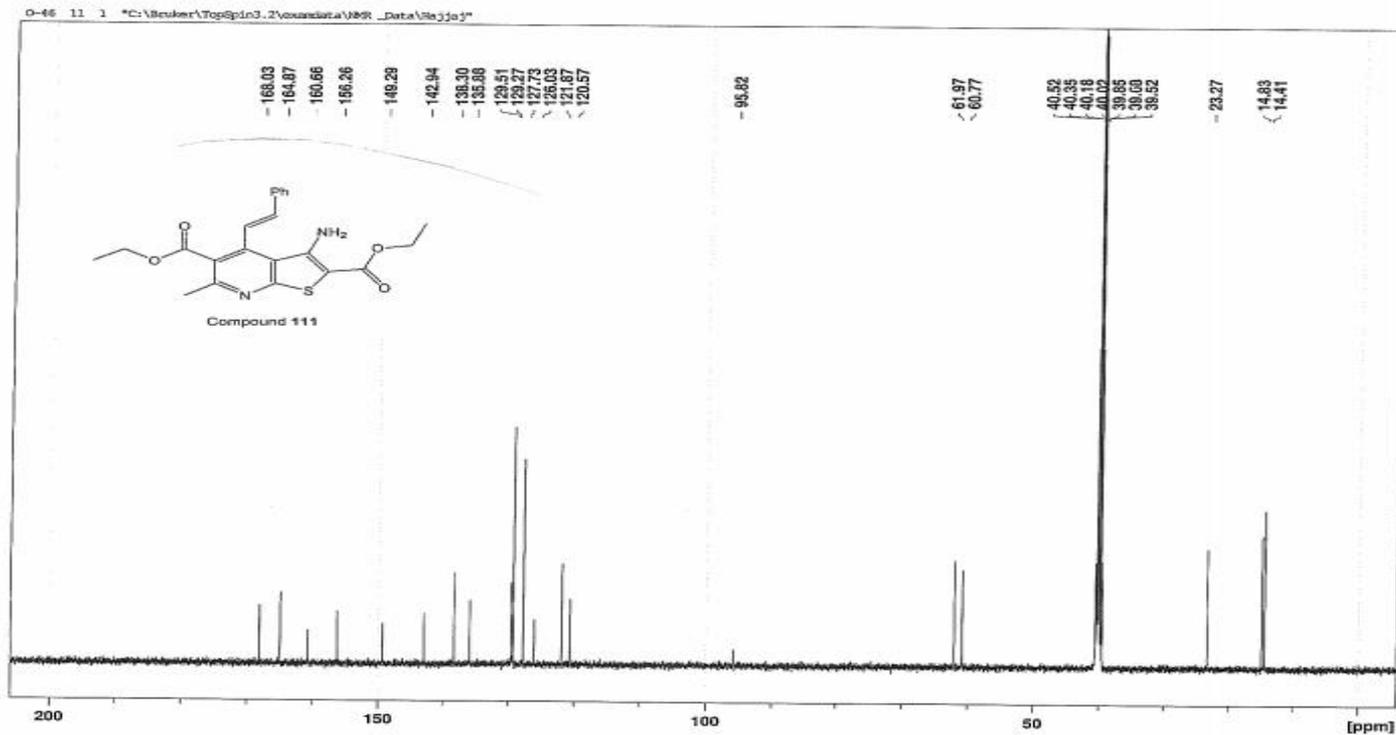


Figure S20: ^{13}C NMR spectrum of compound 11 in $\text{DMSO-}d_6$.

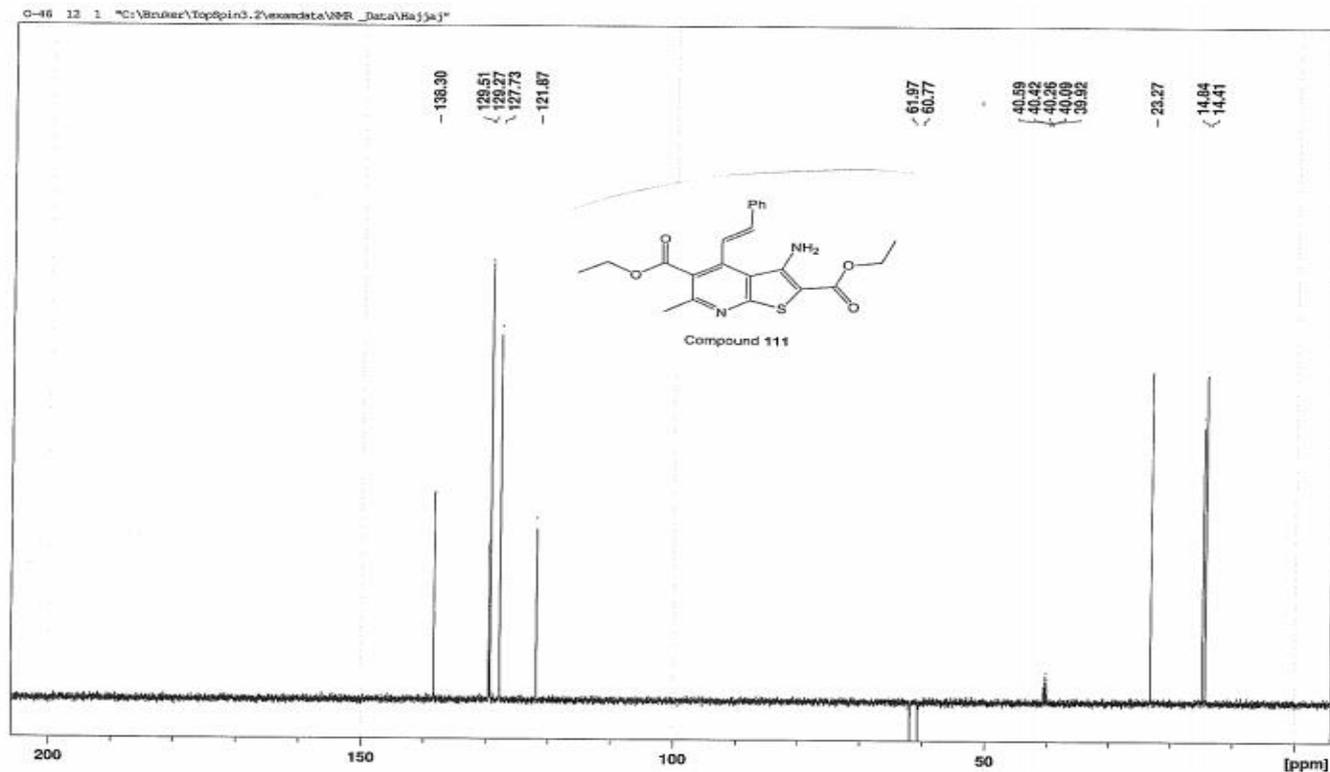


Figure S21: DEPT 135 NMR spectrum of compound 11 in DMSO-

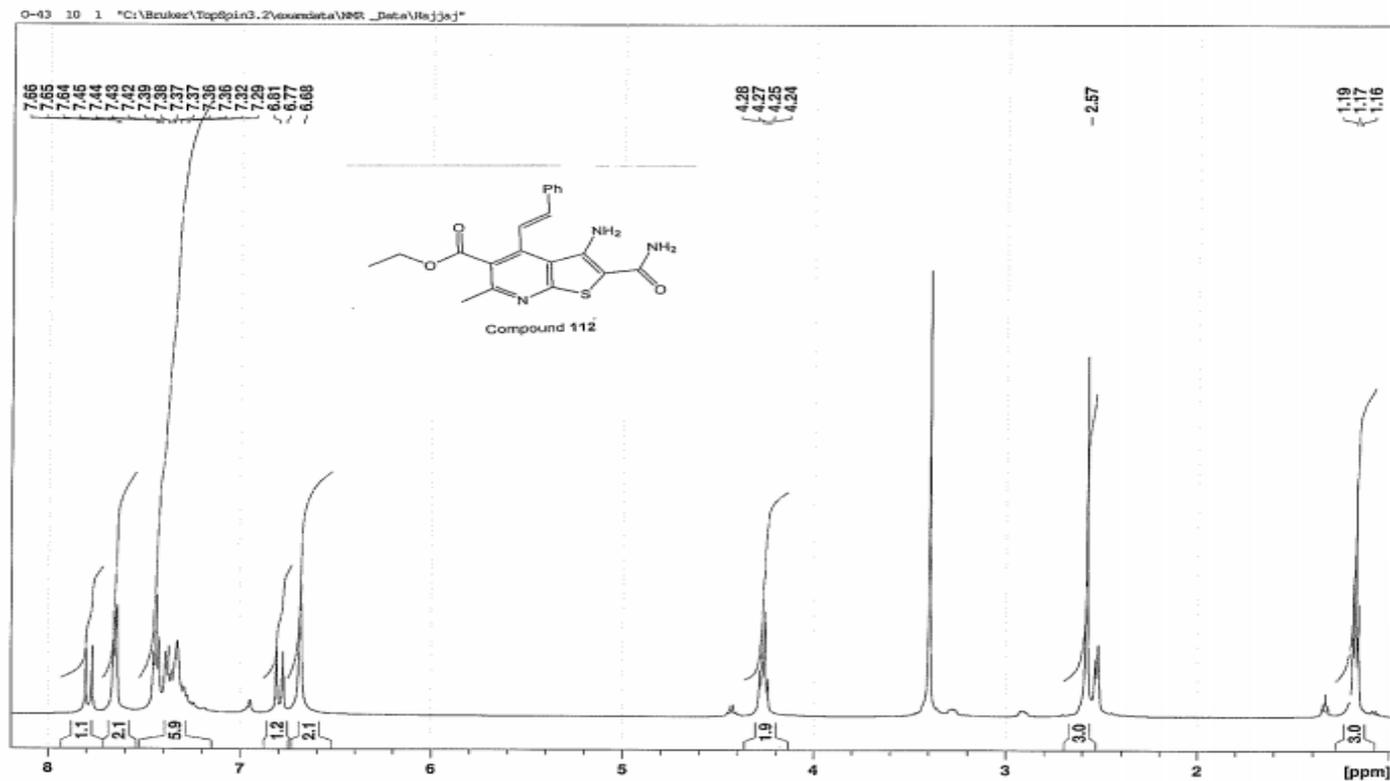


Figure S22: ^1H NMR spectrum of compound 12 in $\text{DMSO-}d_6$.

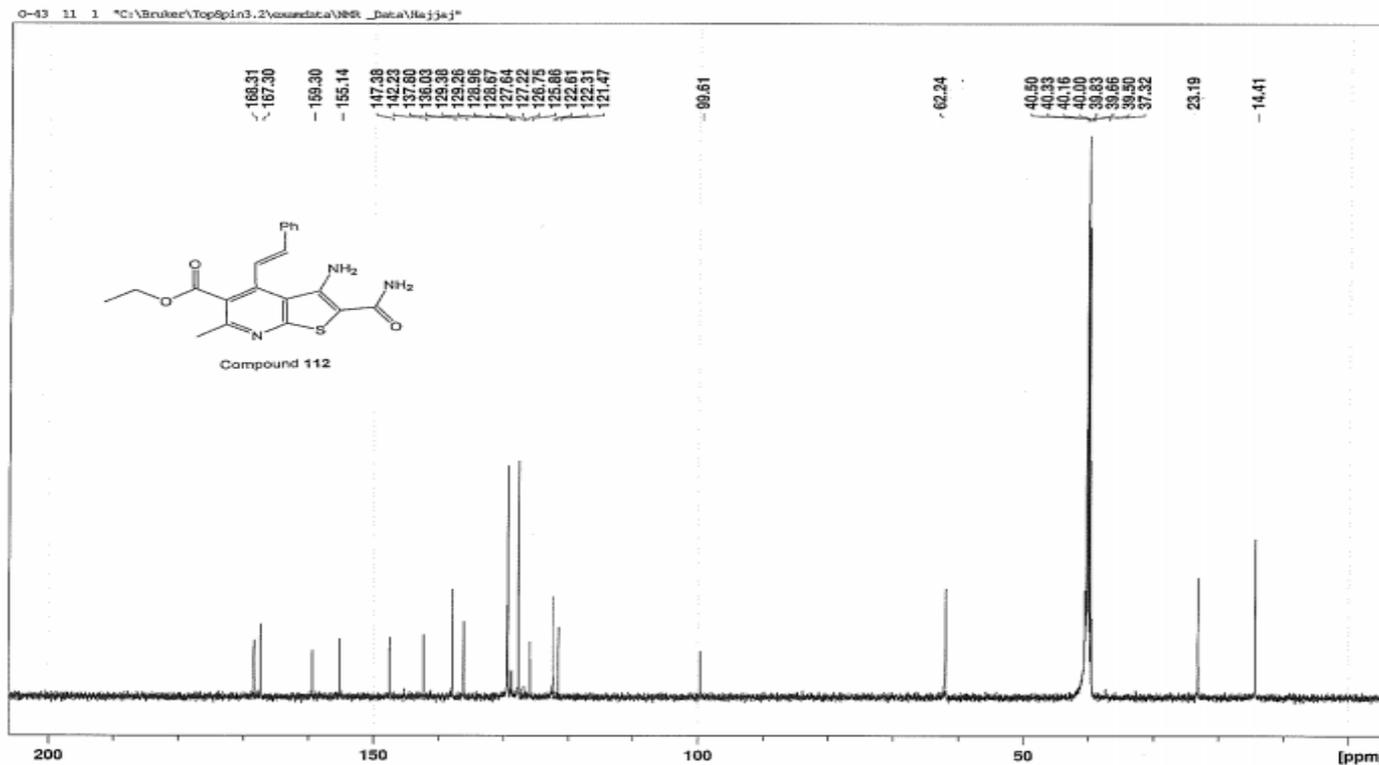


Figure S23: ^{13}C NMR spectrum of compound 12 in $\text{DMSO-}d_6$.

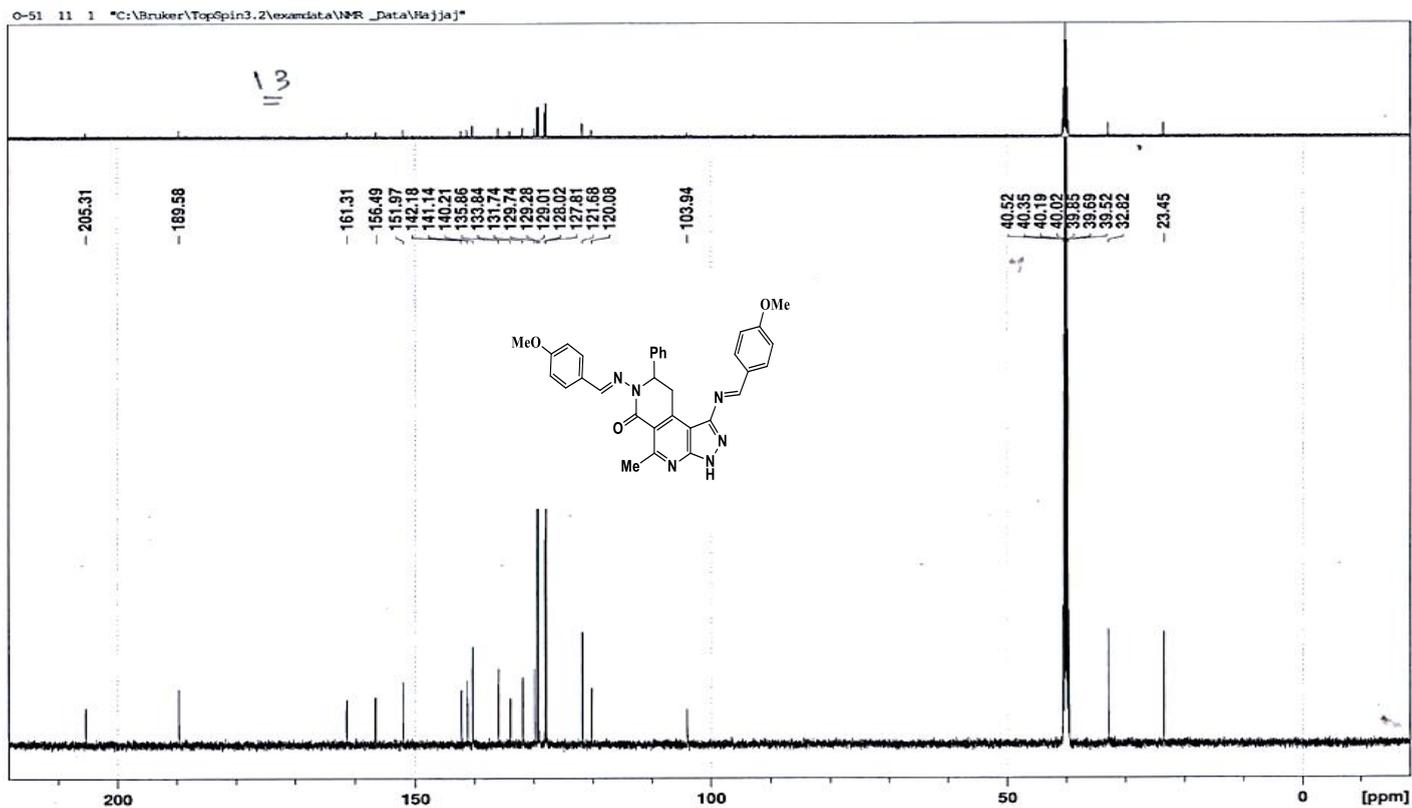


Figure S25: ^{13}C NMR spectrum of compound 13 in $\text{DMSO-}d_6$.

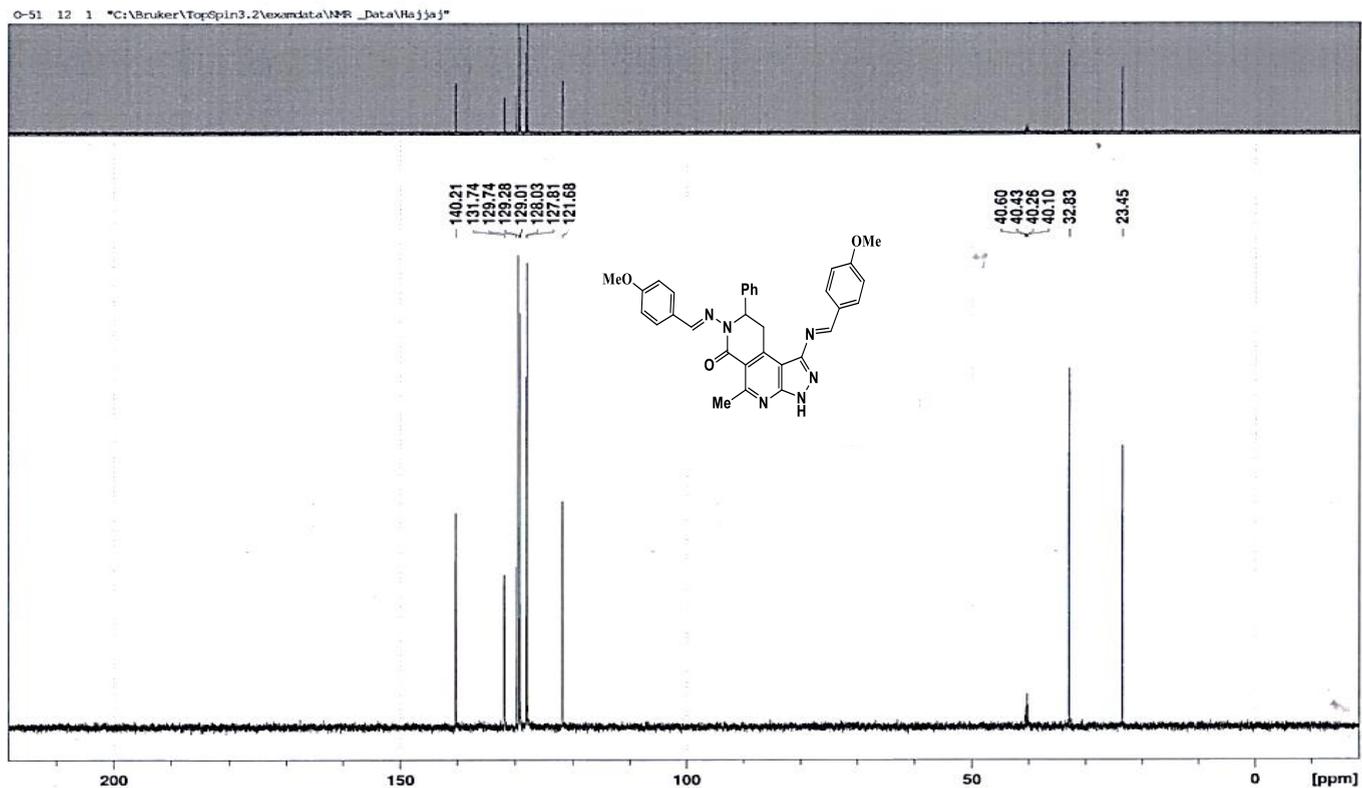


Figure S26: DEPT-135 spectrum of compound 13 in DMSO- d_6 .

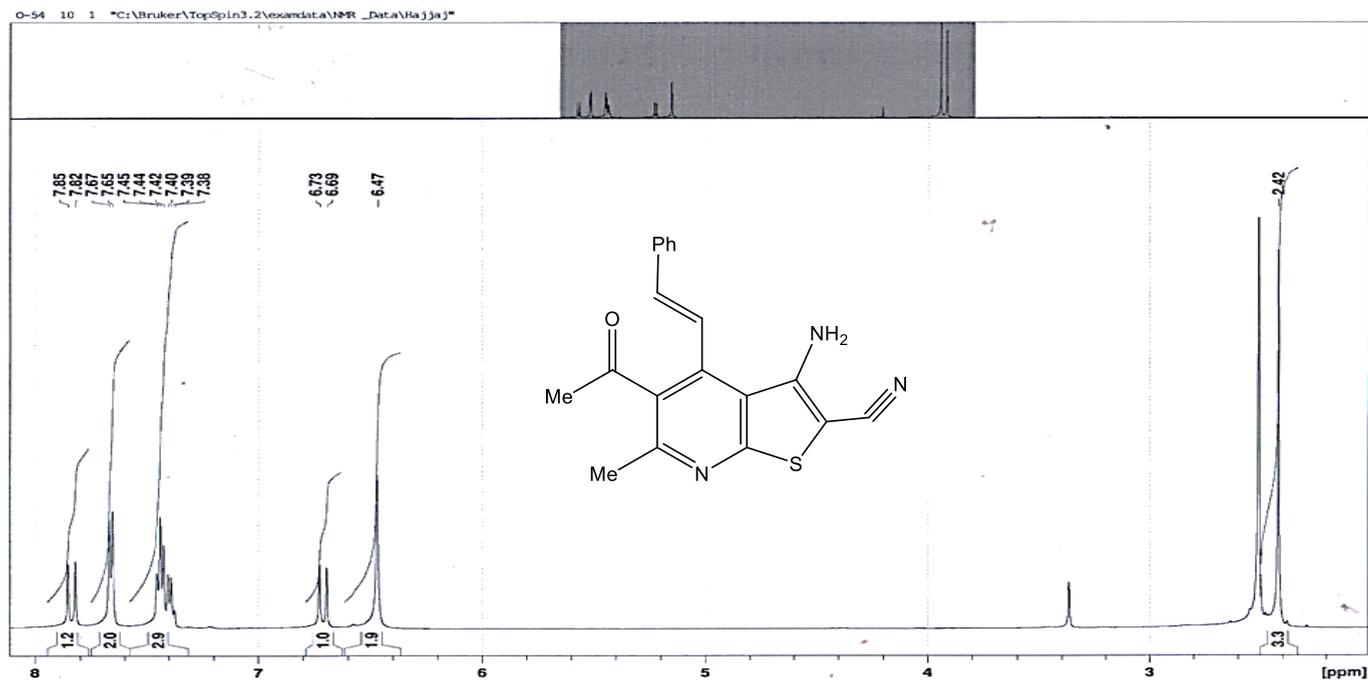


Figure S27: ^1H NMR spectrum of compound 14 in $\text{DMSO-}d_6$.

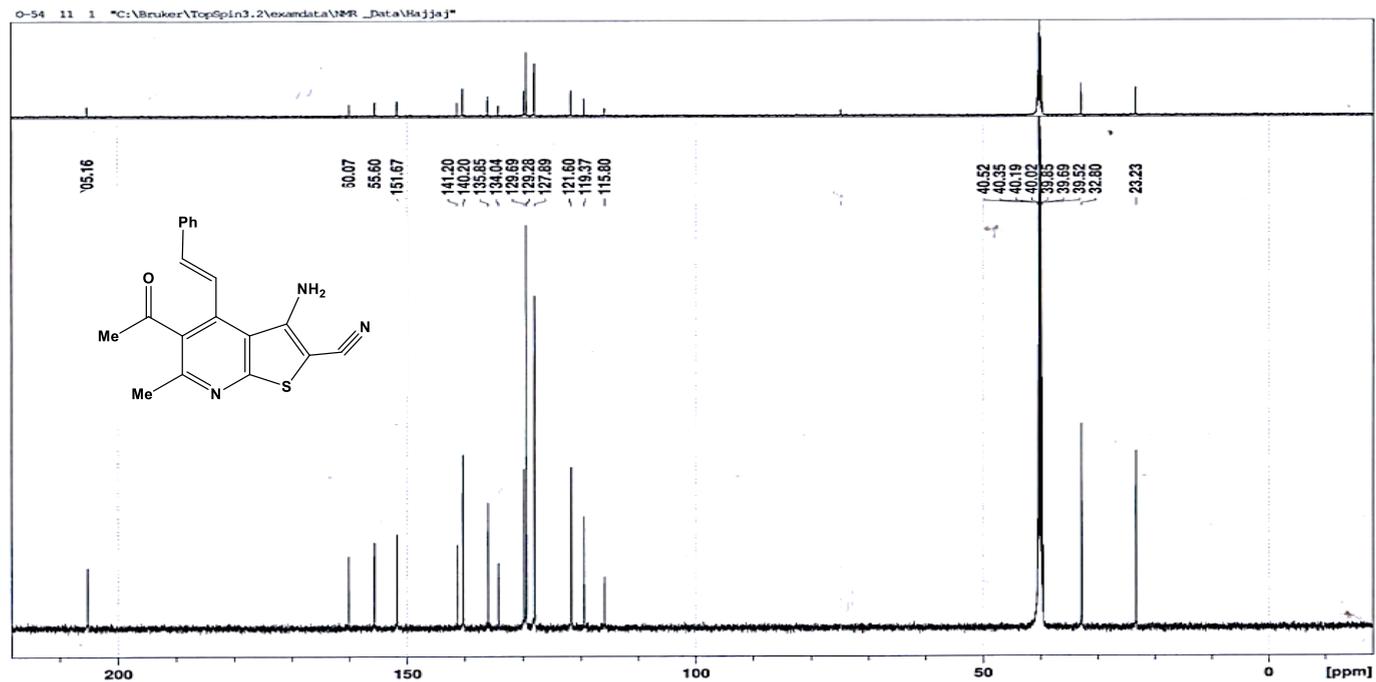


Figure S28: ¹³C NMR spectrum of compound 14 in DMSO-*d*₆.

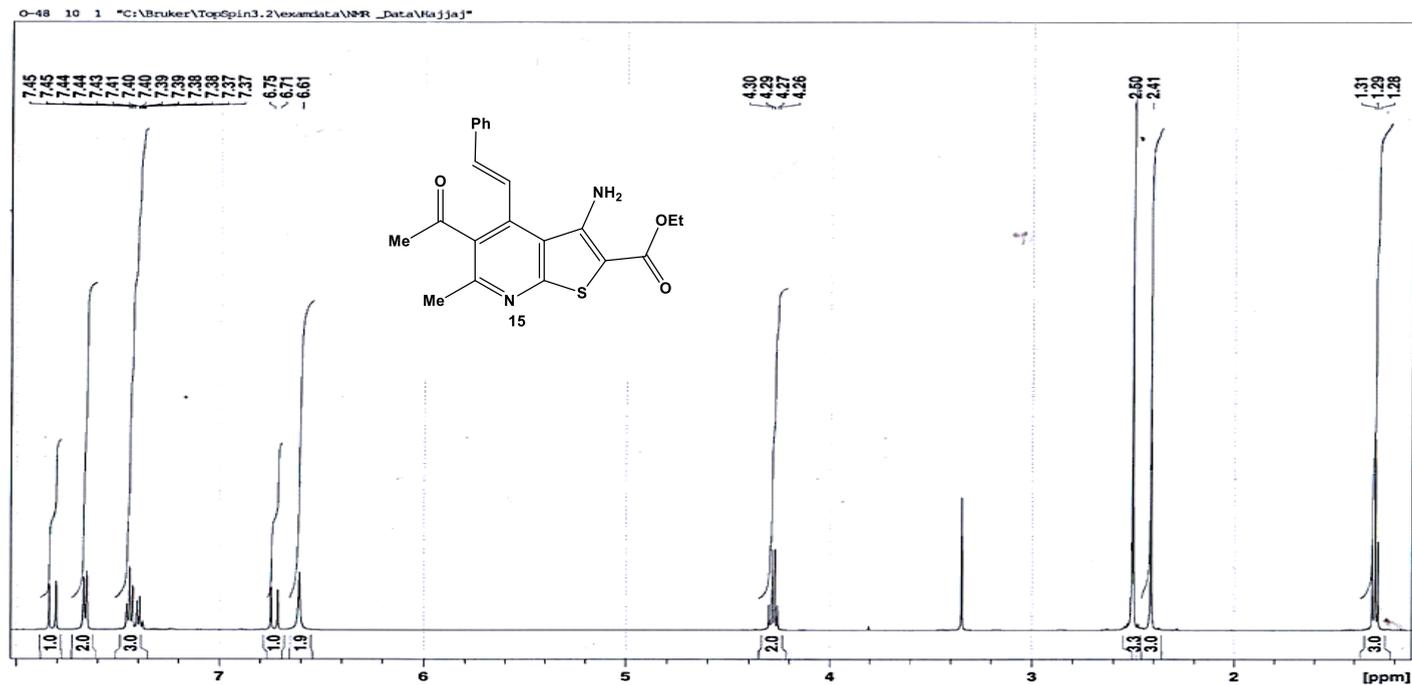


Figure S29: ¹H NMR spectrum of compound 15 in DMSO-*d*₆.

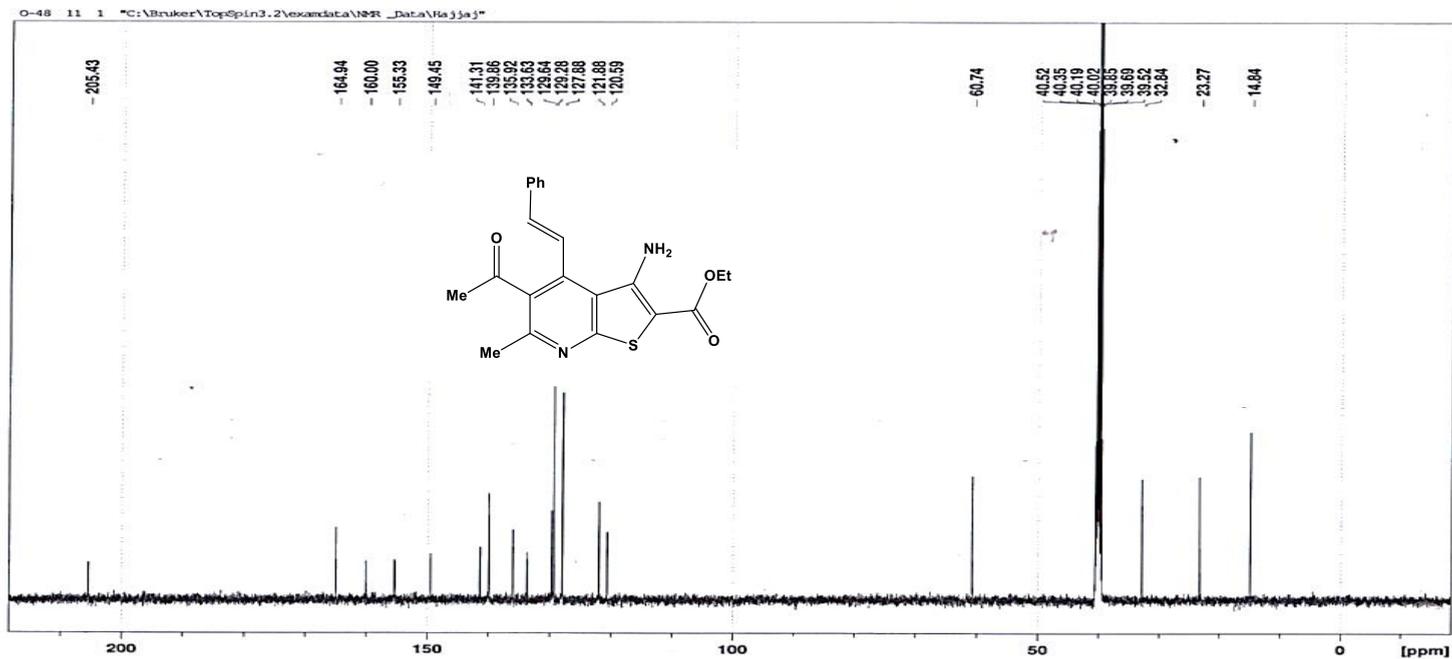


Figure S30: ^{13}C NMR spectrum of compound 15 in $\text{DMSO-}d_6$.

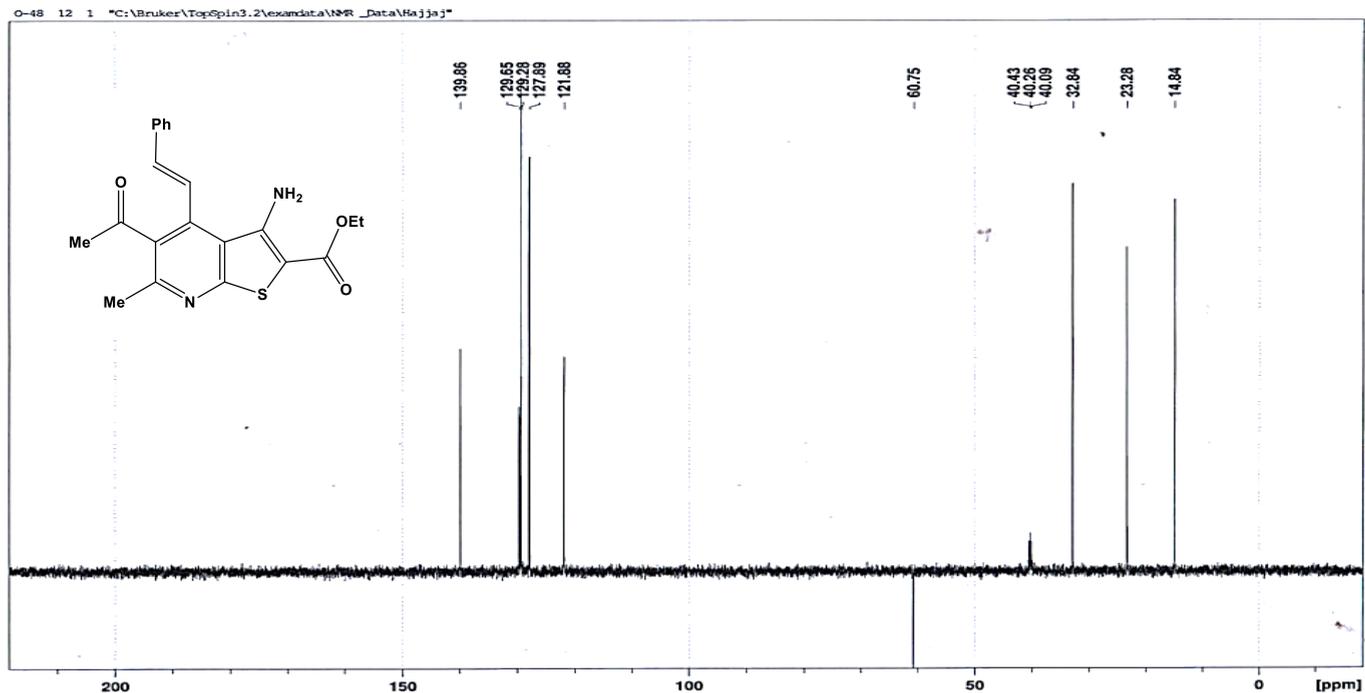


Figure S31: DEPT-135 spectrum of compound 15 in DMSO- d_6 .

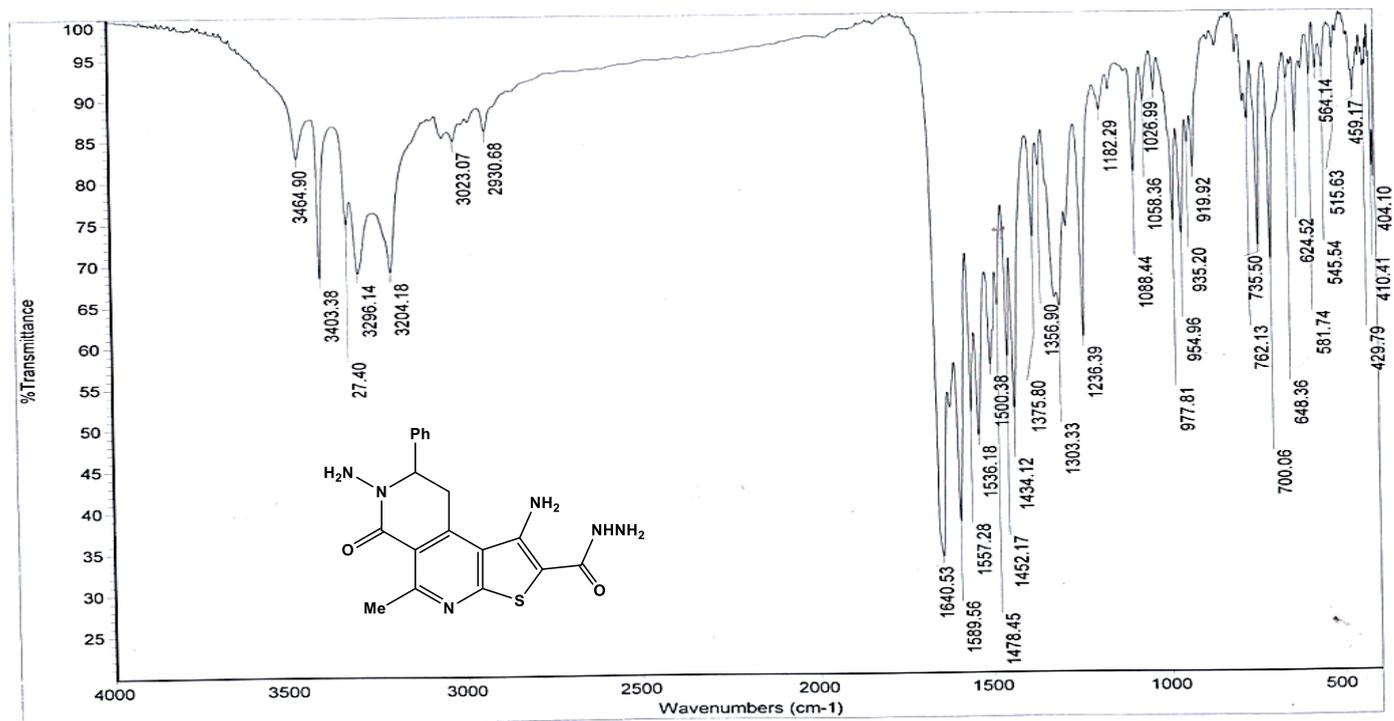
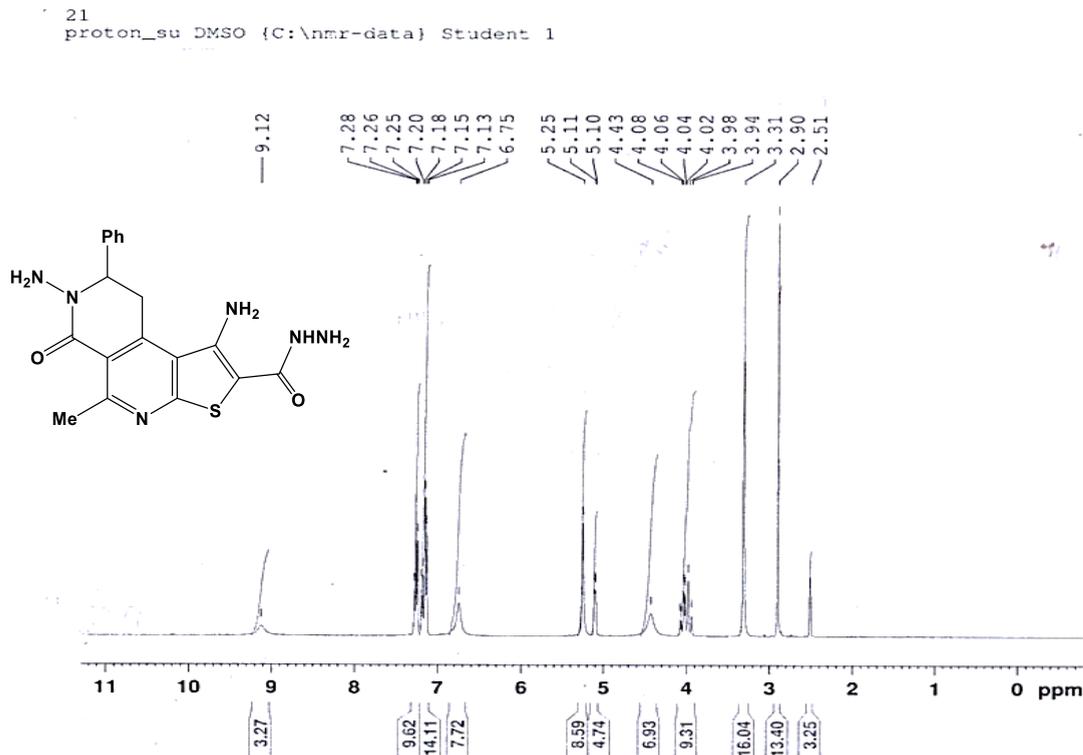


Figure S32: FT-IR spectrum of compound 17 .



Current Data Parameters
 NAME Dec01-2019
 EXPNO 130
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20191201
 Time 10.38
 INSTRUM spect
 PROBHD 5 mm FABBO BB/
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 20
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.122266 Hz
 AQ 4.0894465 sec
 RG 135
 DW 62.400 usec
 DE 6.50 usec
 TE 309.1 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SFO1 400.1324710 MHz
 NUC1 1H
 P1 12.00 usec
 PLW1 22.00000000 W

F2 - Processing parameters
 SI 65536
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S33: ^1H NMR spectrum of compound 17 in $\text{DMSO-}d_6$.

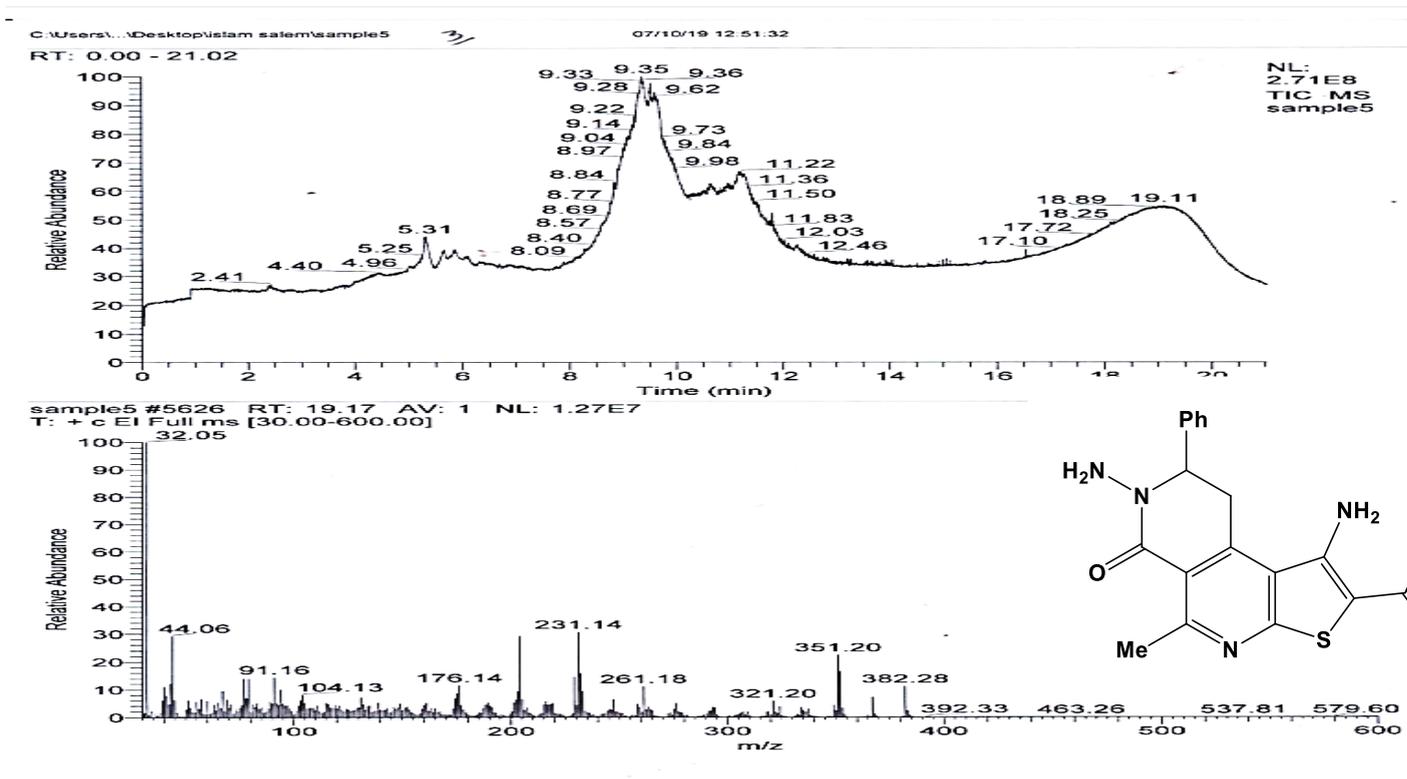


Figure S34: mass spectrometry of compound 17

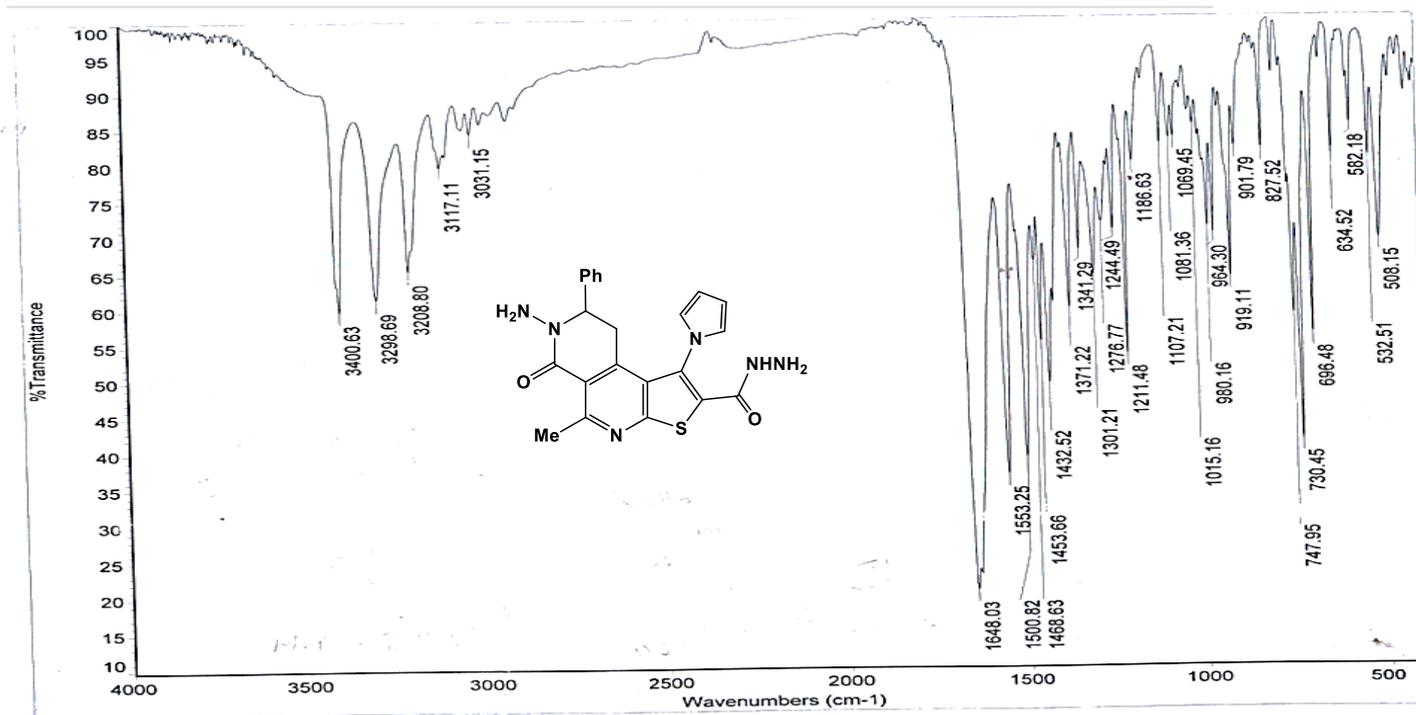
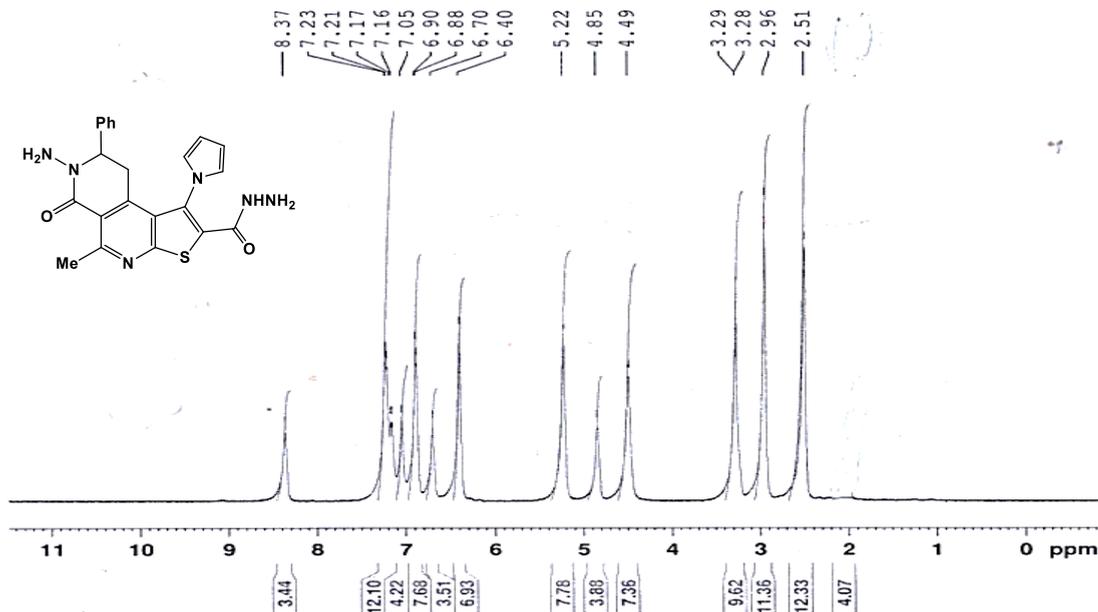


Figure S35: FT-IR spectrum of compound 19 .

30
proton_su DMSO {C:\nmr-data} Student 20



```

Current Data Parameters
NAME      Dec08-2019
EXPNO    210
PROCNO   1

F2 - Acquisition Parameters
Date_    20191208
Time     14.10
INSTRUM  spect
PROBHD   5 mm PABBO Bb/
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        20
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894465 sec
RG        139.04
DW        62.400 usec
DE        6.50 usec
TE        308.1 K
D1        1.0000000 sec
TDO       1

===== CHANNEL f1 =====
SFO1     400.1524710 MHz
NUC1     1H
P1       12.00 usec
PLW1     22.0000000 W

F2 - Processing parameters
SI       65536
SF       400.1300000 MHz
WDW      EM
SSB      0
LB       0.30 Hz
GB       0
PC       1.00

```

Figure S36: ^1H NMR spectrum of compound 19 in $\text{DMSO-}d_6$.

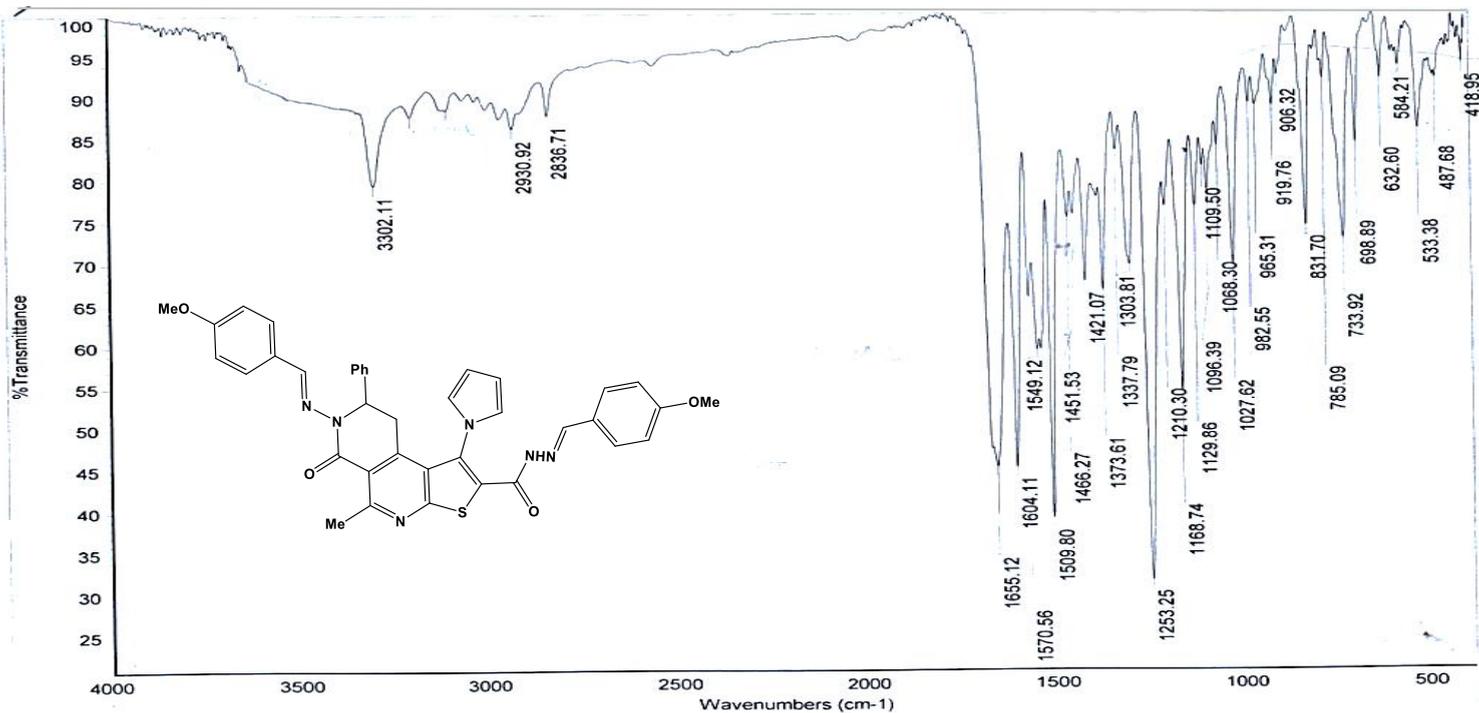


Figure S37: FT-IR spectrum of compound 20 .

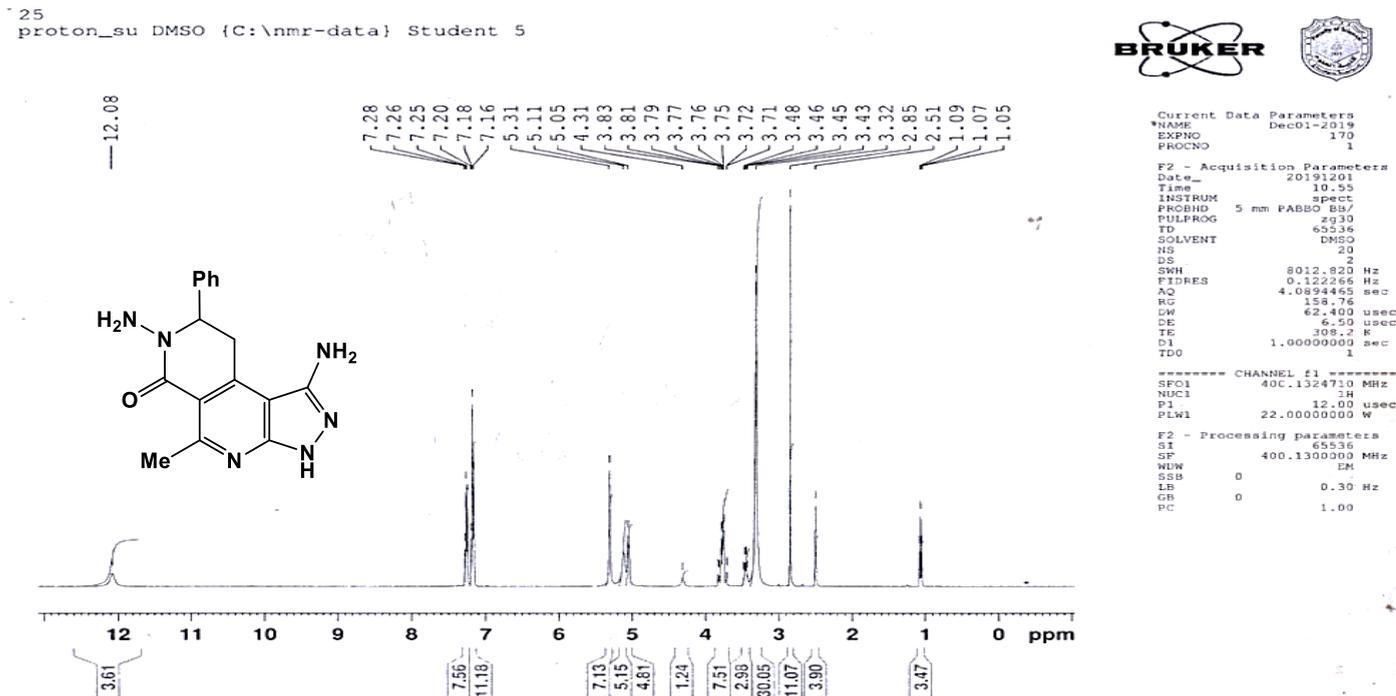


Figure S38: ^1H NMR spectrum of compound 24 in $\text{DMSO-}d_6$.

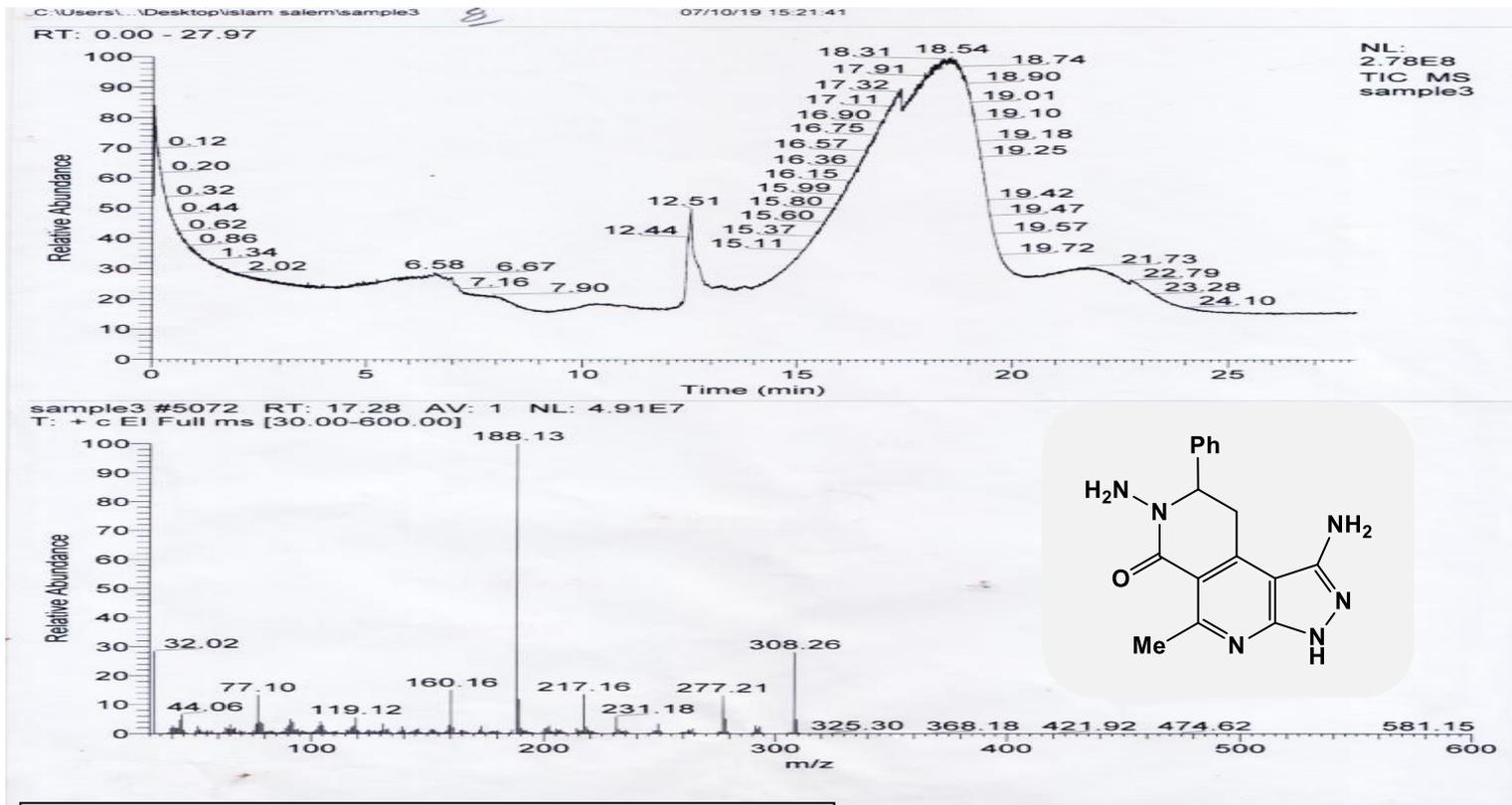


Figure S39: mass spectrometry of compound 24

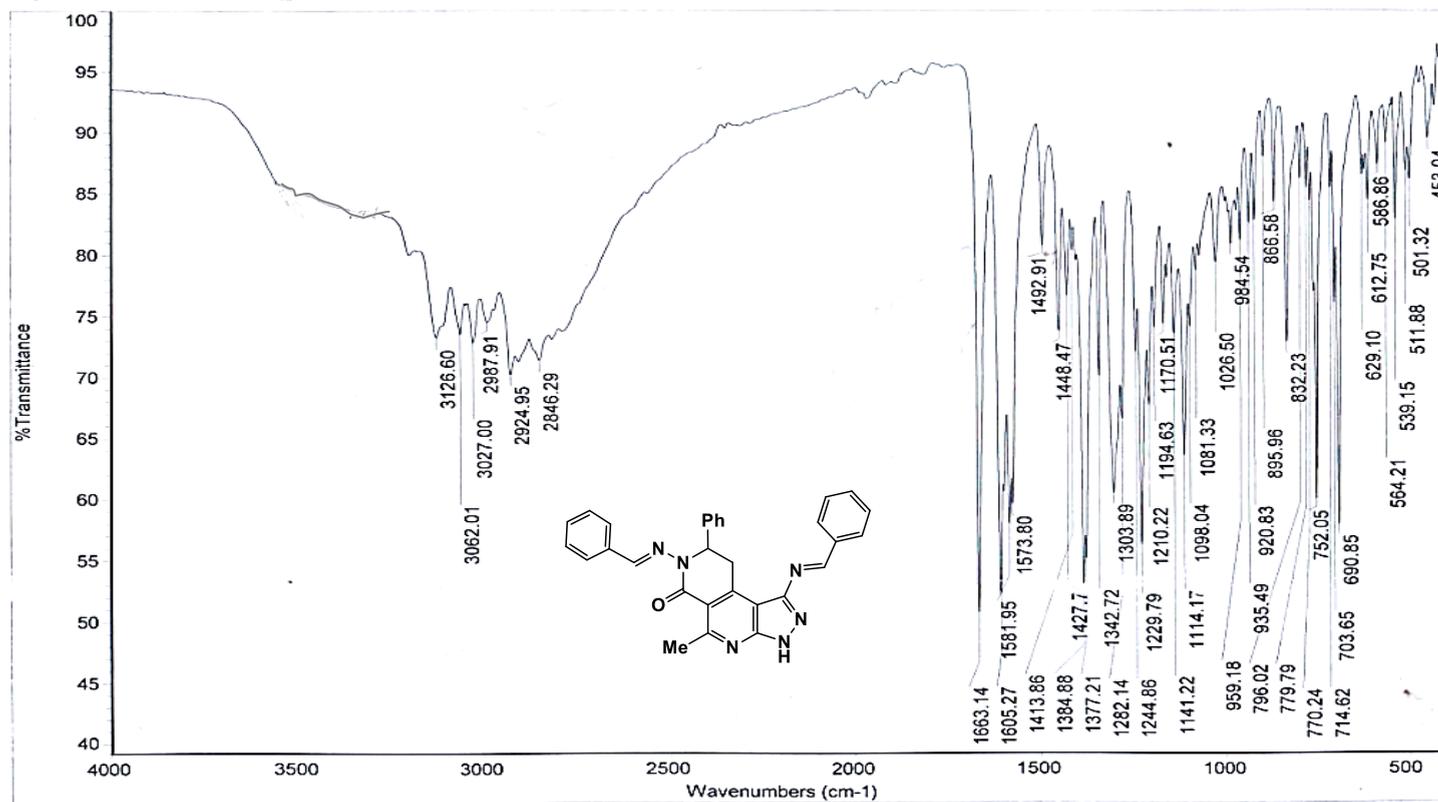
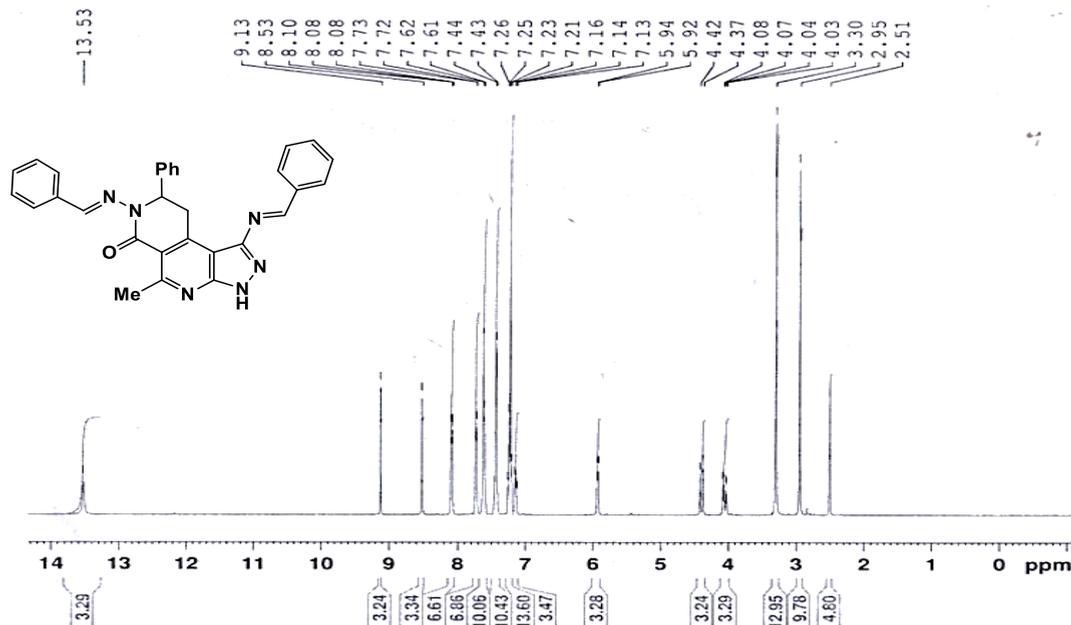


Figure S40: FT-IR spectrum of compound 25a .

26
proton_su DMSO {C:\nmr-data} Student 6



```

Current Data Parameters
NAME      Dec01-2019
EXPNO    180
PROCNO   1

F2 - Acquisition Parameters
Date_    20191201
Time     10.59
INSTRUM  spect
PROBHD   5 mm F400 BB/
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        20
DS        2
SWH       8012.820 Hz
FIDRES    0.122266 Hz
AQ        4.0894465 sec
RG        175.84
DW        62.400 usec
DE        6.50 usec
TE        308.2 K
DI        1.00000000 sec
TD0       1

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
P1       12.00 usec
PLW1     22.00000000 W

F2 - Processing parameters
SI       65536
SF       400.1300000 MHz
WCM      EM
SSB      0
LB       0.30 Hz
GR       0
PC       1.00
    
```

Figure S41: ¹H NMR spectrum of compound 25a in DMSO-d₆.

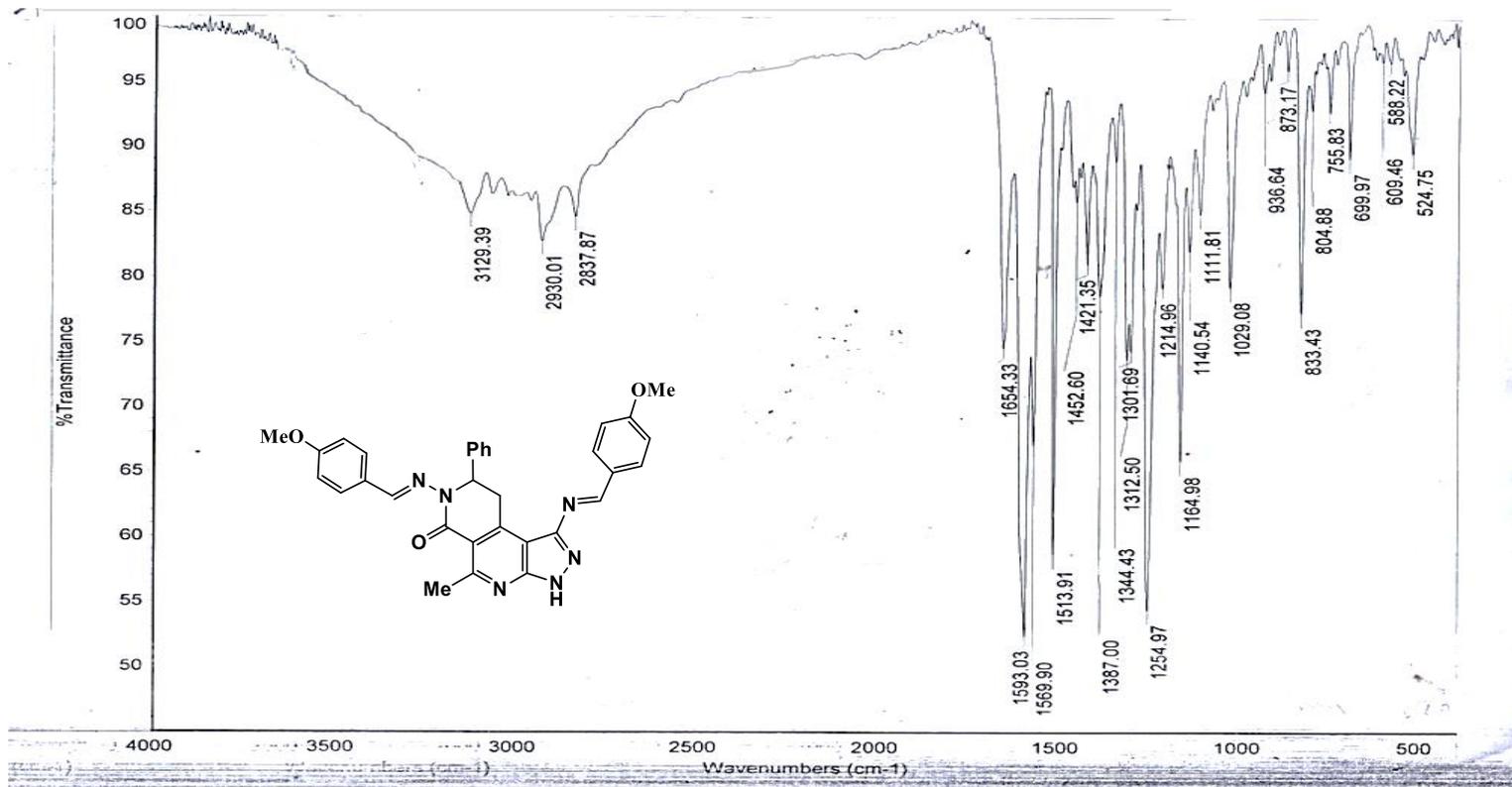


Figure S42: FT-IR spectrum of compound 25b .

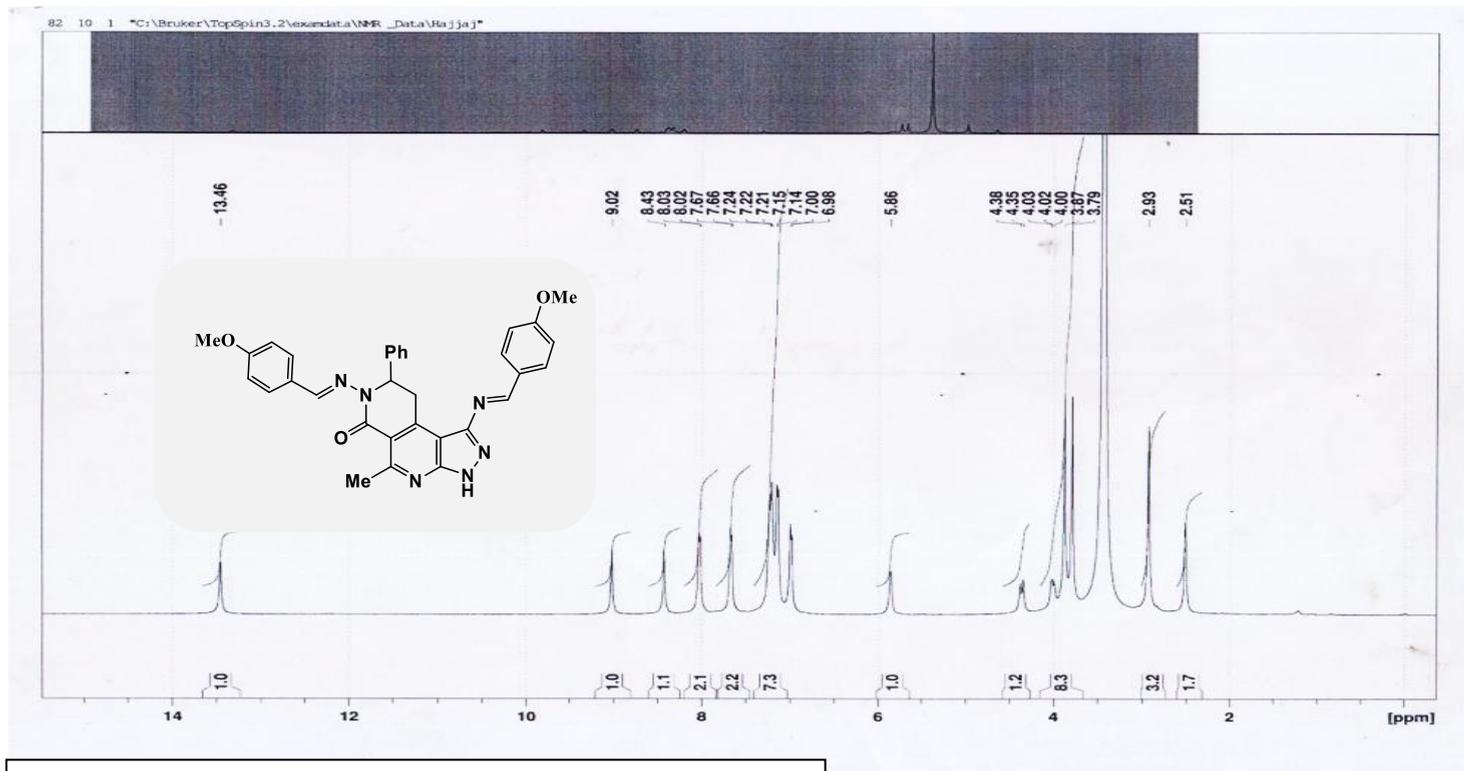


Figure S43: ^1H NMR spectrum of compound 25b in $\text{DMSO-}d_6$.

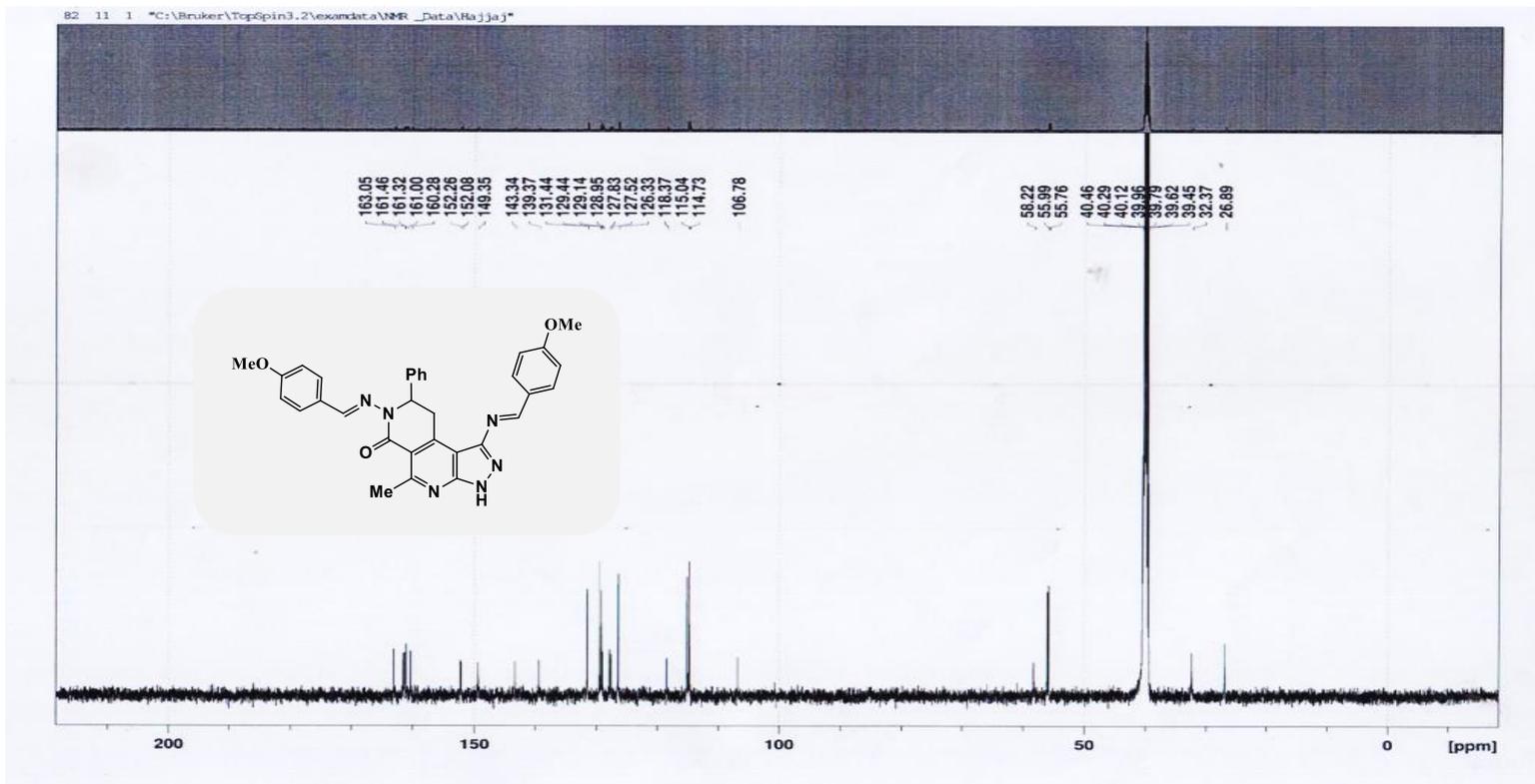


Figure S44: ^{13}C NMR spectrum of compound 25b in $\text{DMSO-}d_6$.

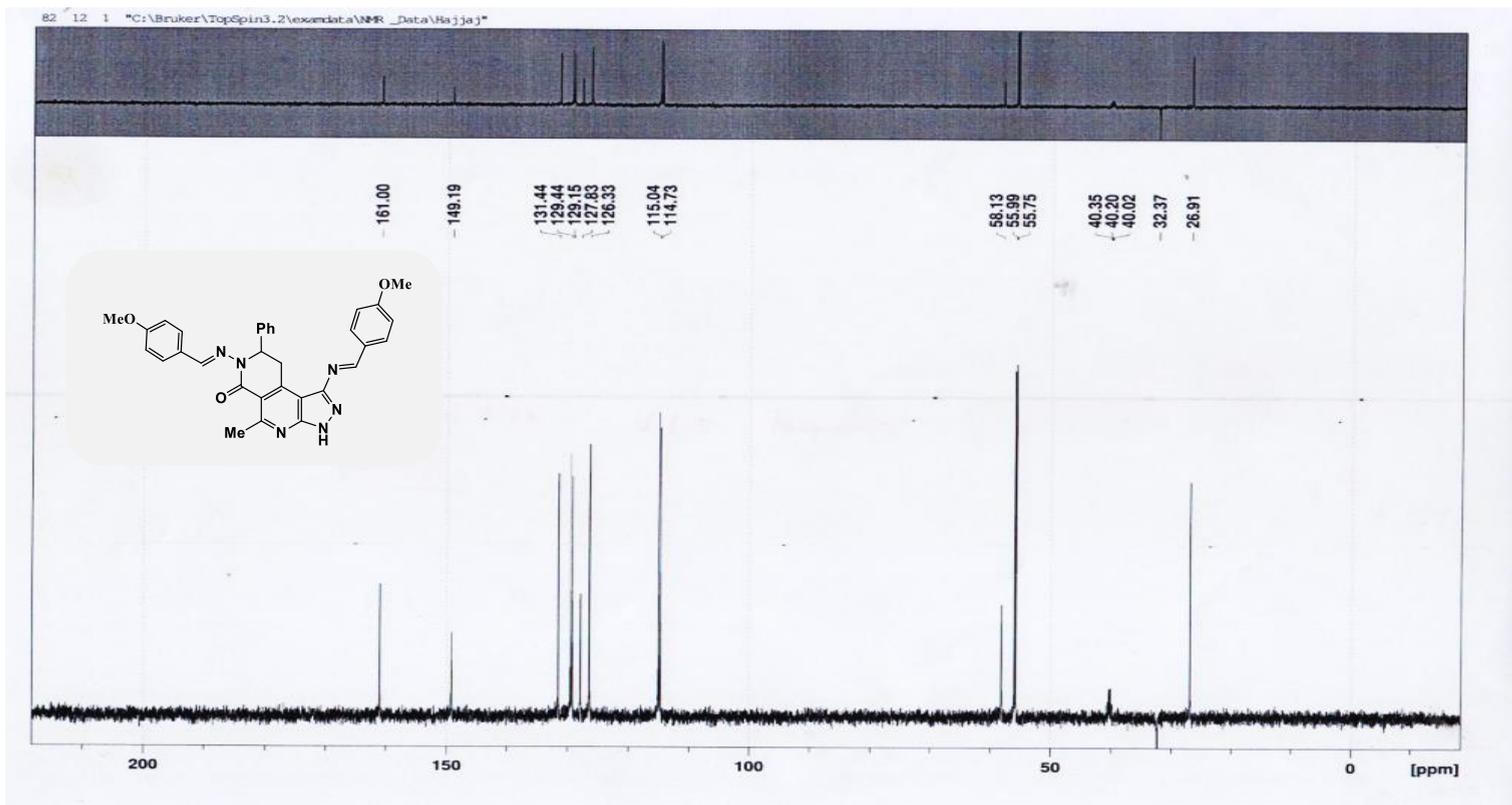


Figure S45: DEPT-135 spectrum of compound 25b in DMSO- d_6 .

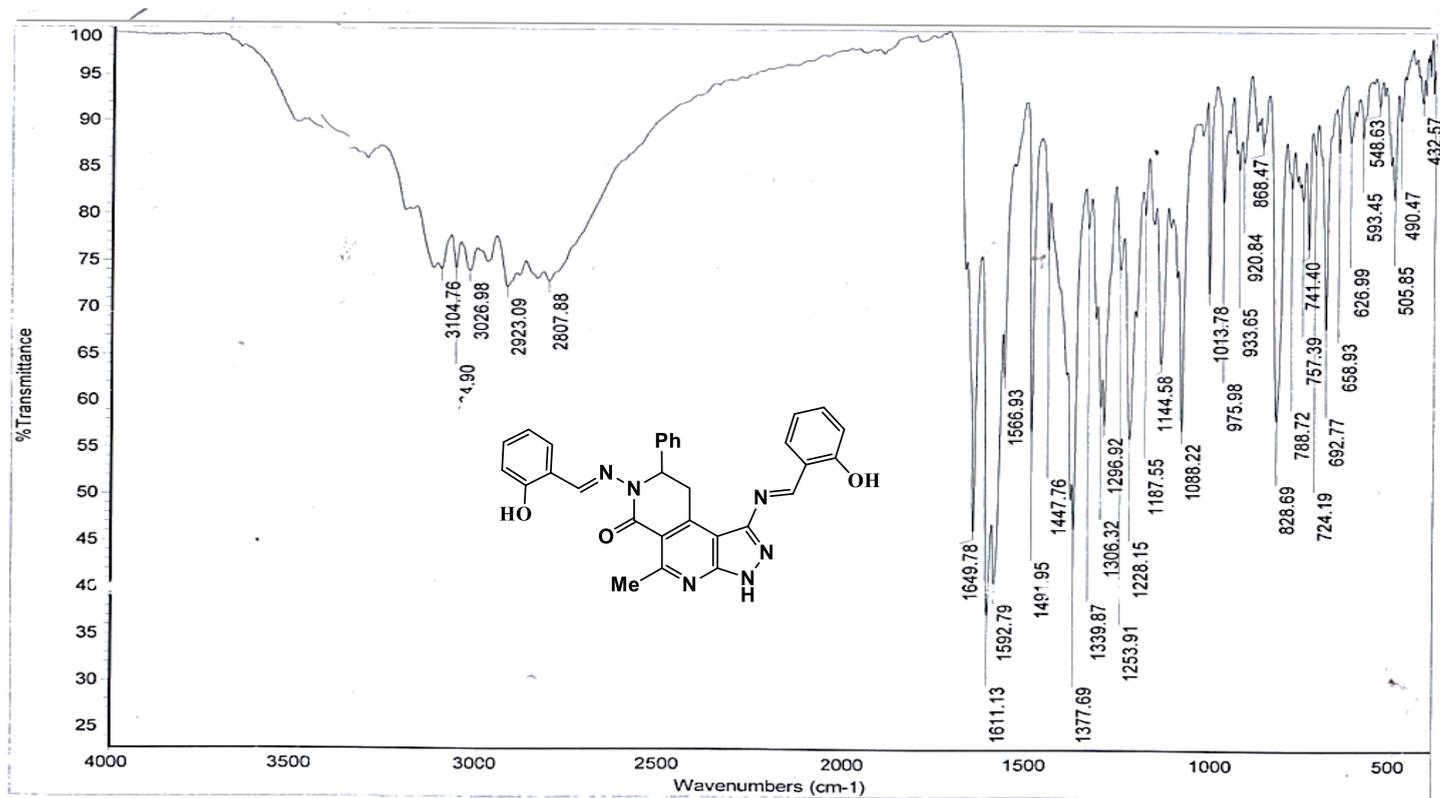
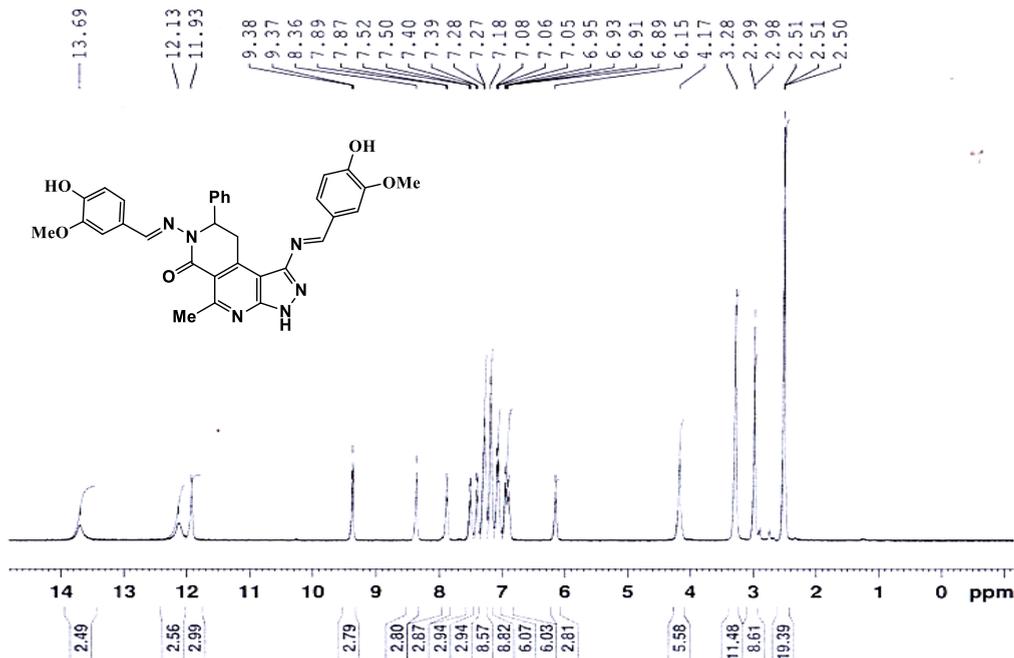


Figure S46: FT-IR spectrum of compound 25bd.

28

proton_su DMSO (C:\nmr-data) Student 18



```

Current Data Parameters
NAME      Dec08-2019
EXPNO    190
PROCNO   1

F2 - Acquisition Parameters
Date_    20191208
Time     14.00
INSTRUM spect
PROBHD   5 mm F400 BBO
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       20
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.089465 sec
RG       199.04
LW       62.400 usec
GB       6.50 usec
TE       300.2 K
D1       1.0000000 sec
TDC      1

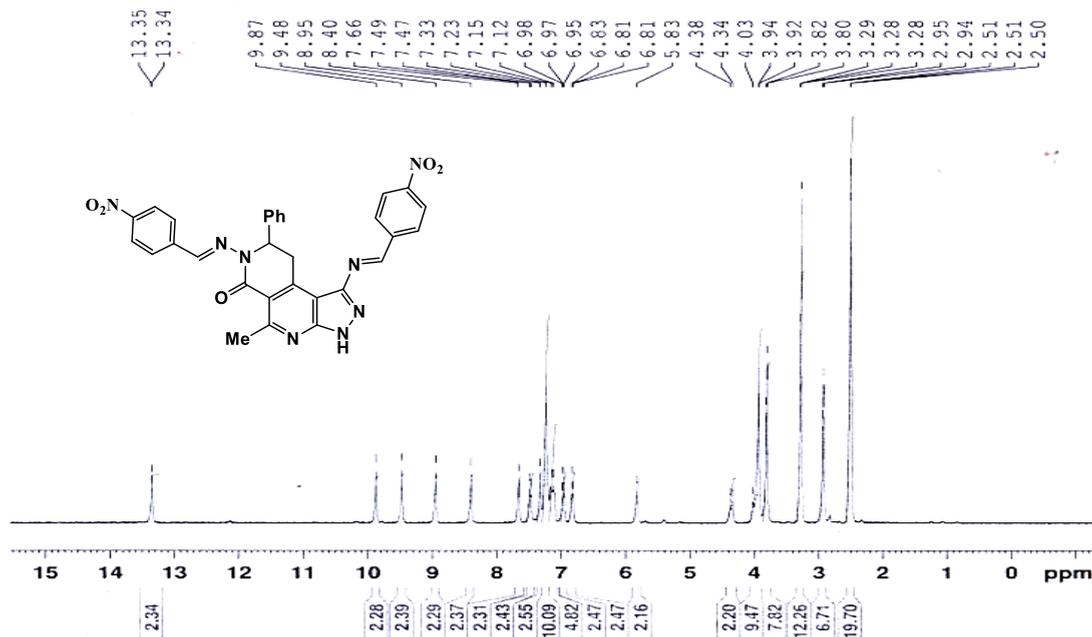
----- CHANNEL f1 -----
SFO1    400.1324710 MHz
NUC1    1H
P1      12.00 usec
PLW1    22.00000000 W

F2 - Processing parameters
SI      65536
SF      400.1300000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00

```

Figure S47: ¹H NMR spectrum of compound 25e in DMSO-*d*₆.

31
proton_su DMSO (C:\nmr-data) Student 21



```

Current Data Parameters
NAME      Dec08-2019
EXPNO    220
PROCNO   1

F2 - Acquisition Parameters
Date_    20191208
Time     14.15
INSTRUM  spect
PROBHD   5 mm PABBO BB/
PULPROG  zg30
TD       65536
SOLVENT  DMSO
NS       20
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0694465 sec
RG       129.04
SW       62.400 usec
DE       6.50 usec
TE       308.2 K
TE       1.00000000 sec
TD0      1

===== CHANNEL f1 =====
SFO1     400.1324710 MHz
NUC1     1H
PI       12.00 usec
PLW1     22.00000000 W

F2 - Processing parameters
SI       65536
SF       400.1300000 MHz
WDW      EM
SFR      0
LB       0.30 Hz
GB       0
PC       1.00

```

Figure S48: ^1H NMR spectrum of compound 25f in $\text{DMSO-}d_6$.

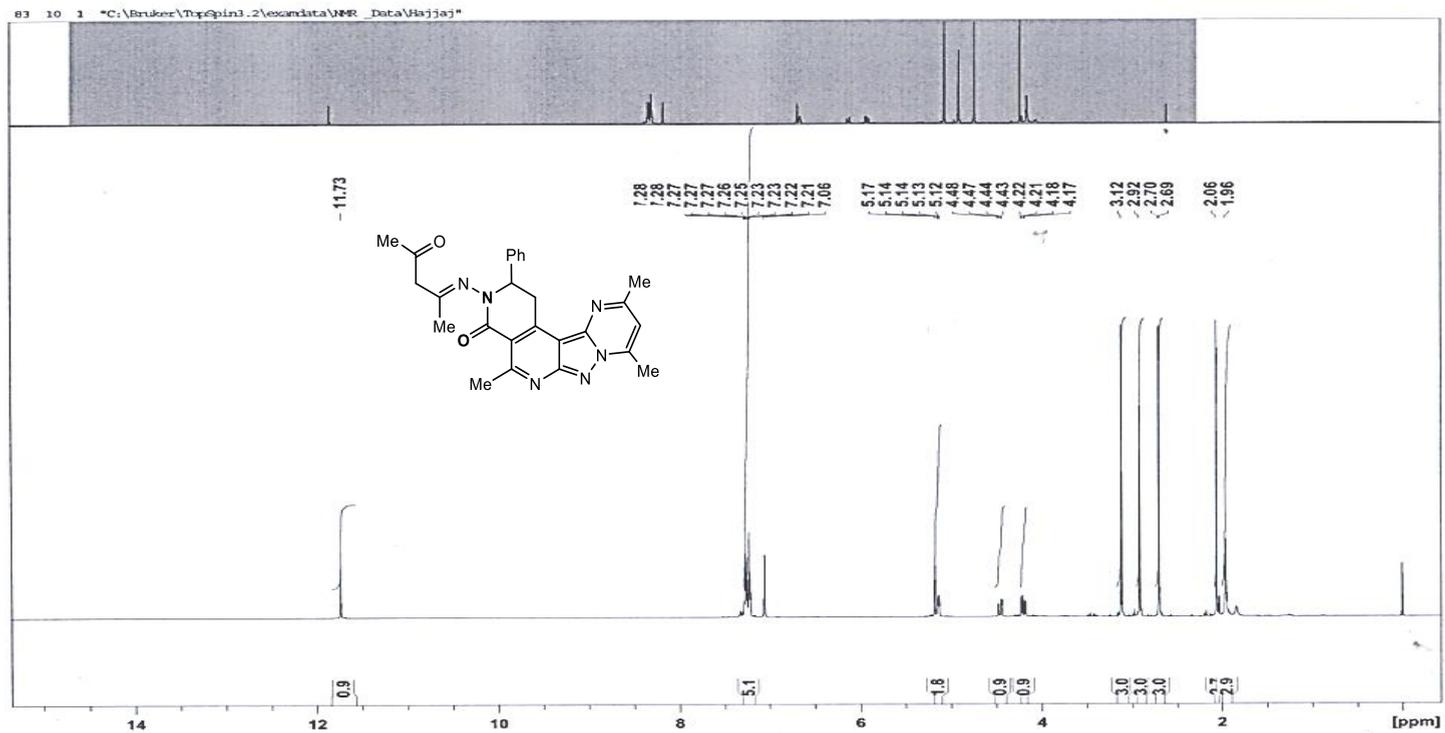


Figure S49: ^1H NMR spectrum of compound 26 in $\text{DMSO-}d_6$.

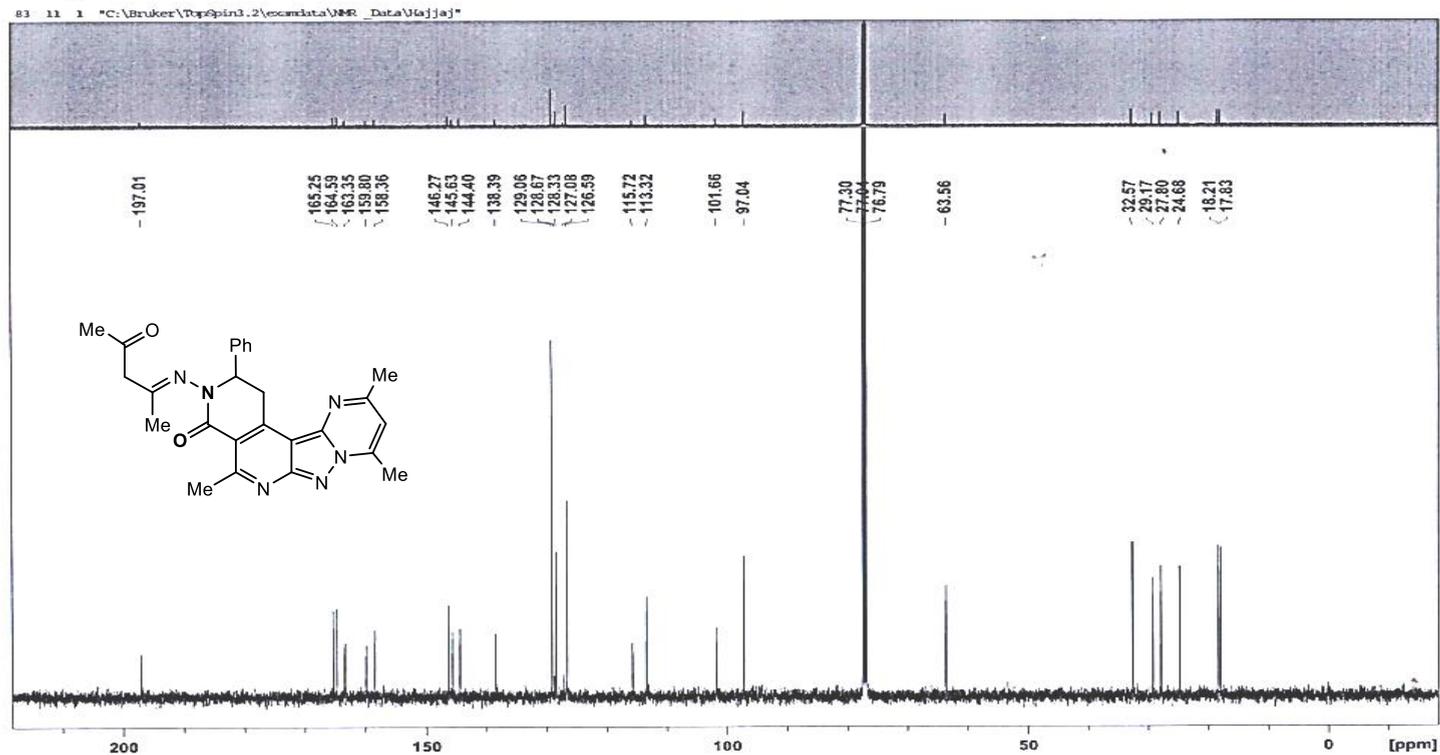


Figure S50: ^{13}C NMR spectrum of compound 26 in $\text{DMSO-}d_6$.

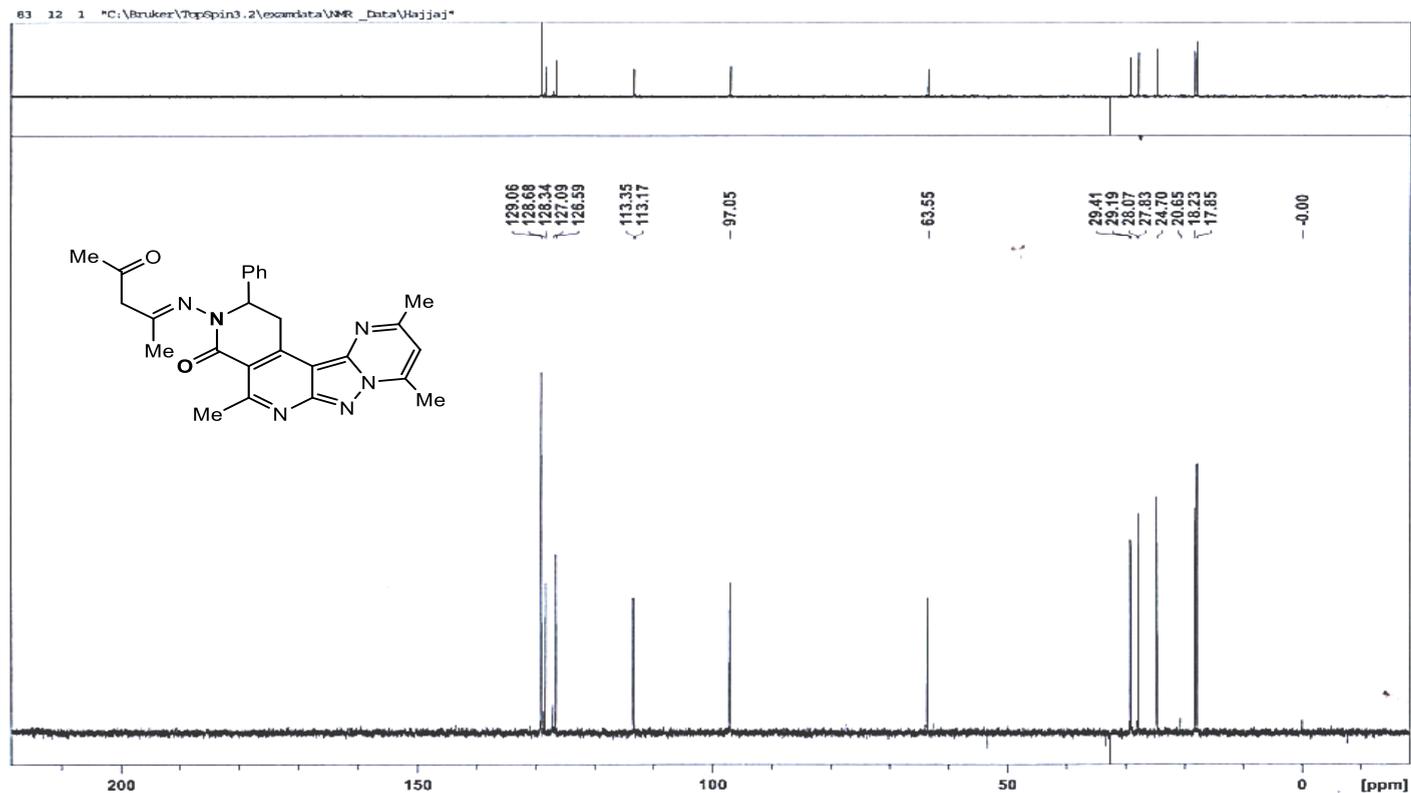


Figure S51: DEPT-135 spectrum of compound 26 in DMSO- d_6 .