

Supplementary Material

Nucleophilic ability of 5-aminopyrazoles in the multicomponent synthesis of pyrazolodihydropyridines and pyrazolodihydropyrimidines

Mahdi Ahmadi Varzaneh^A, Hamid R. Memarian^{A,}, Hadi Amiri Rudbari^A and Olivier Blacque^B*

^ADepartment of Chemistry, University of Isfahan, 81746-73441 Isfahan, Islamic Republic of Iran.

^BDepartment of Chemistry, University of Zurich, Winterthurerstrasse 190, CH 8057, Zurich, Switzerland.

*Correspondence to: Email: memarian@sci.ui.ac.ir

Nucleophilic ability of 5-aminopyrazoles in the multicomponent synthesis of pyrazolodihydropyridines and pyrazolodihydropyrimidines

Mahdi Ahmadi Varzaneh,^a Hamid R. Memarian*,^a Hadi Amiri Rudbari^a and Olivier Blacque^b

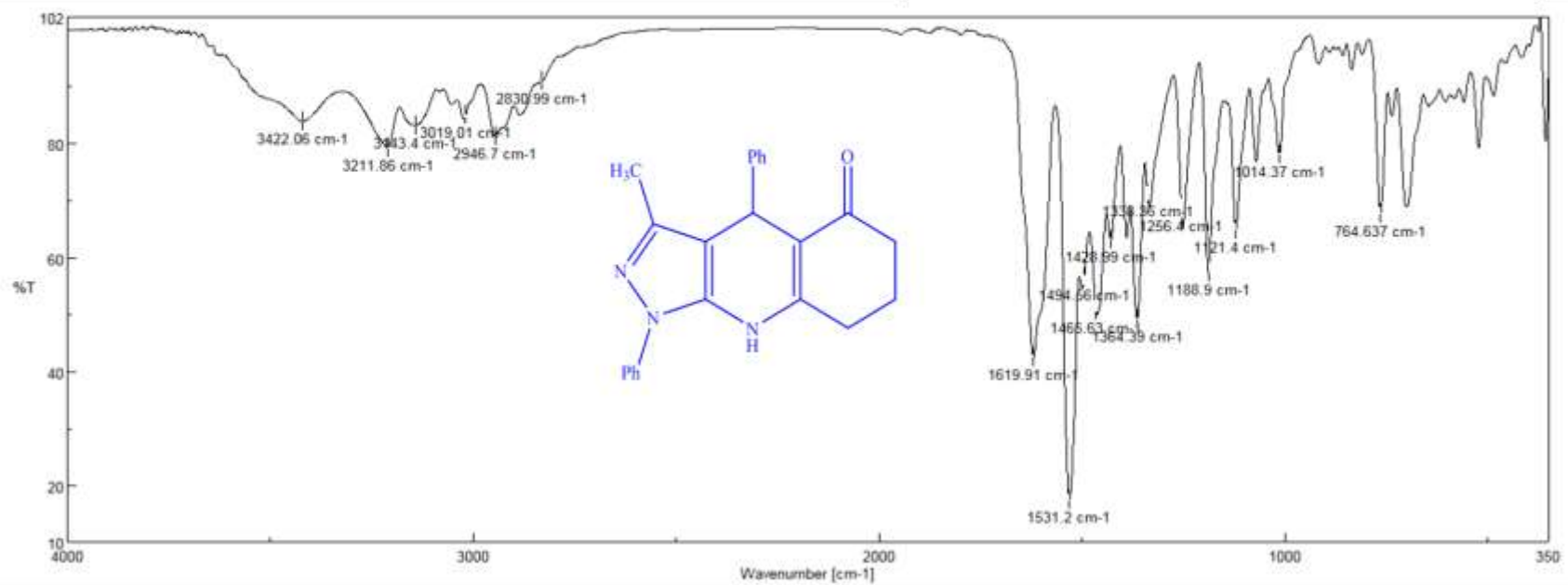
^a*Department of Chemistry, University of Isfahan, 81746-73441 Isfahan, I. R. Iran.*

^b*Department of Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057, Zurich, Switzerland.*

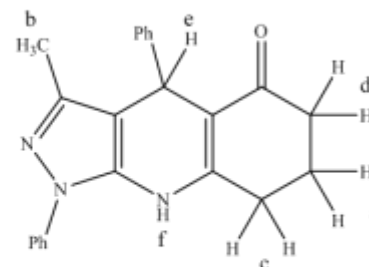
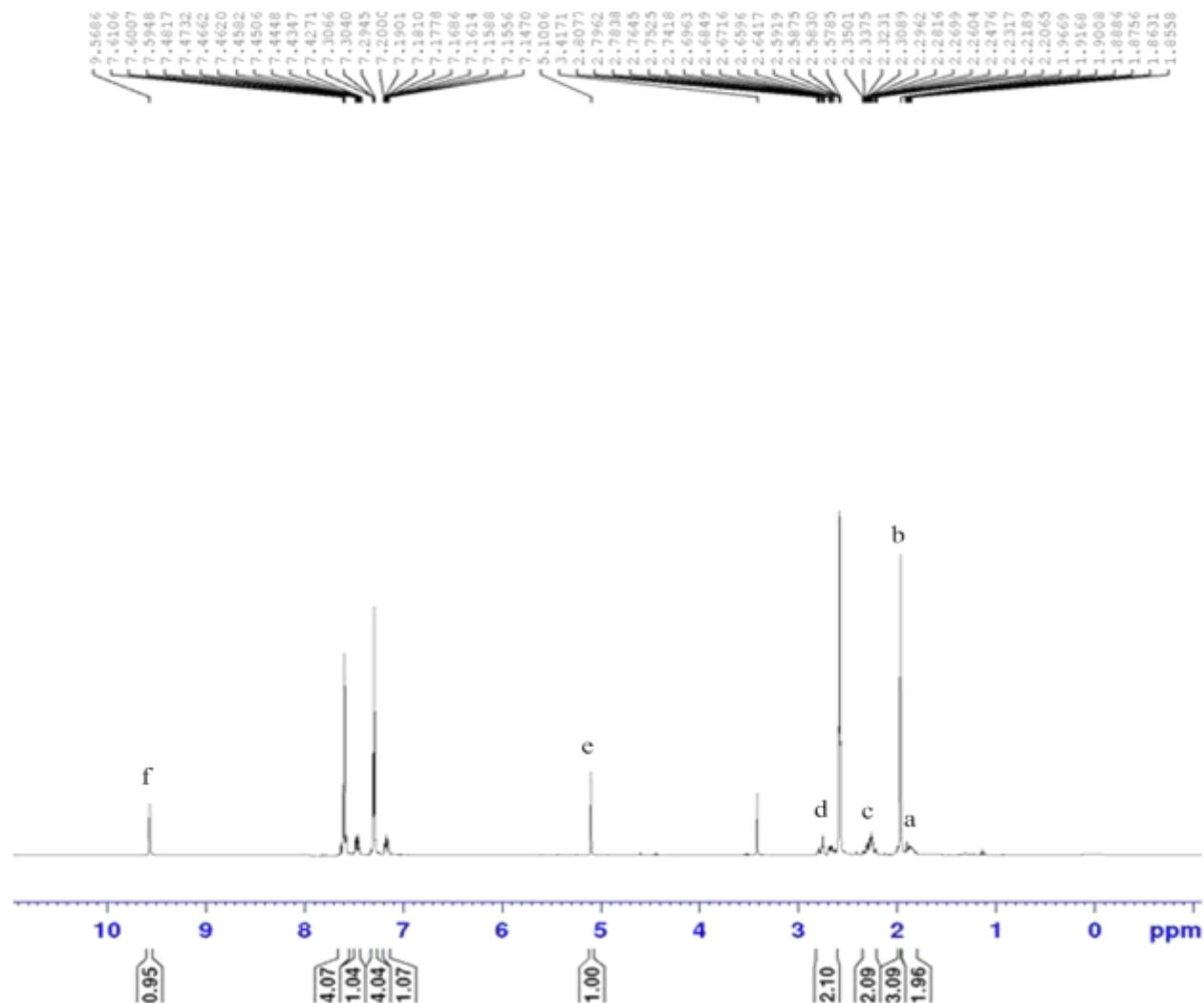
Title	Page
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4a	3-9
¹ H NMR, and UV Spectra of 4b	10-13
¹ H NMR, ¹³ C NMR and UV Spectra of 4c	14-20
¹ H NMR, ¹³ C NMR and UV Spectra of 4d	21-27
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4e	28-36
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4f	37-45
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4g	46-53
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4h	54-61
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4i	62-69
¹ H NMR and UV Spectra of 4j	70-73
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4k	74-82
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4l	83-90
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4m	91-98

¹ H NMR and UV Spectra of 4n	99-102
¹ H NMR and UV Spectra of 4o	103-106
¹ H NMR and UV Spectra of 4p	107-110
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4q	111-117
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4r	118-123
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4s	124-131
¹ H NMR and UV Spectra of 4t	132-135
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4u	136-141
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4v	142-150
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 4w	151-157
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 5a	158-165
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 5b	166-173
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 5c	174-181
IR, ¹ H NMR, ¹³ C NMR and UV Spectra of 5d	182-189
IR, ¹ H NMR, ¹³ C NMR, UV, Spectra and Crystallography data of 5e	190-199

IR-Spectrum of compound 4a



¹H NMR Spectrum of compound 4a

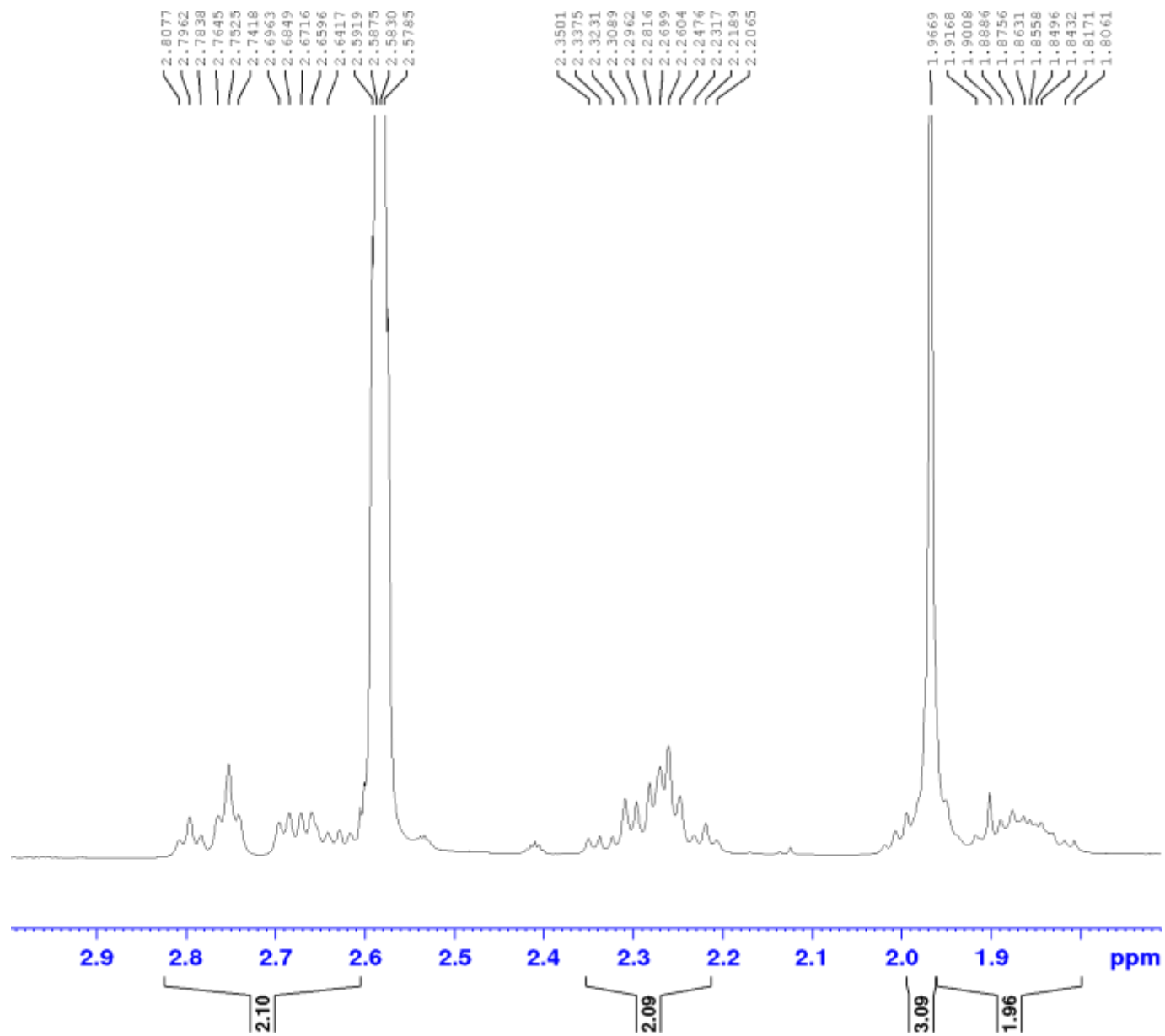


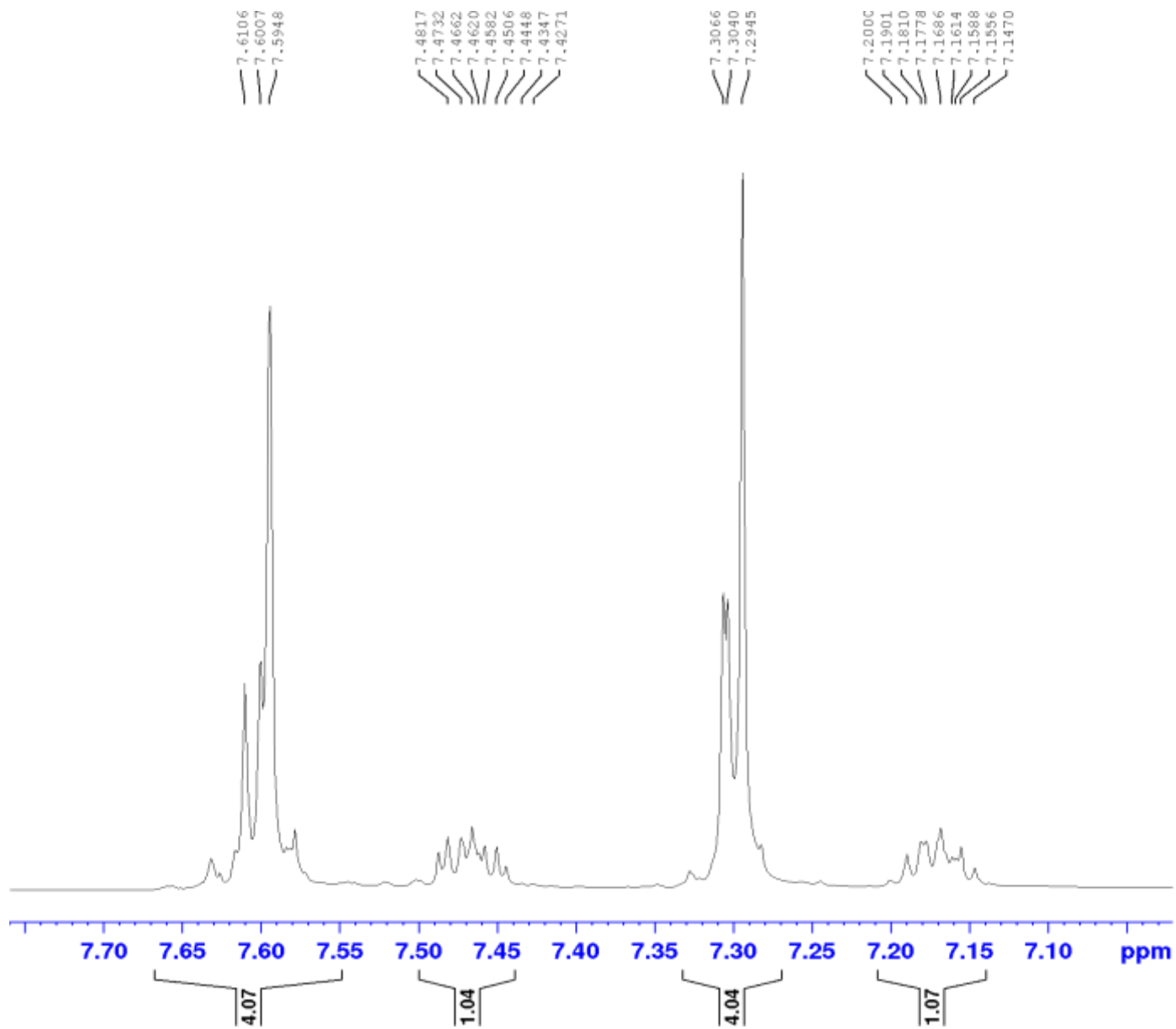
Current Data Parameters
 NAME Ahmadi- Mehdi-IN96100
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20171225
 Time 11.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg
 TD 50504
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8417.509 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999375 sec
 RG 64
 DW 59.400 usec
 DE 6.50 usec
 TE 295.3 K
 D1 5.0000000 sec
 TD0 1

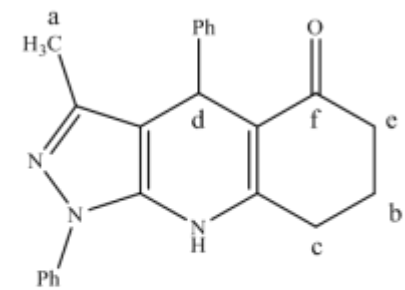
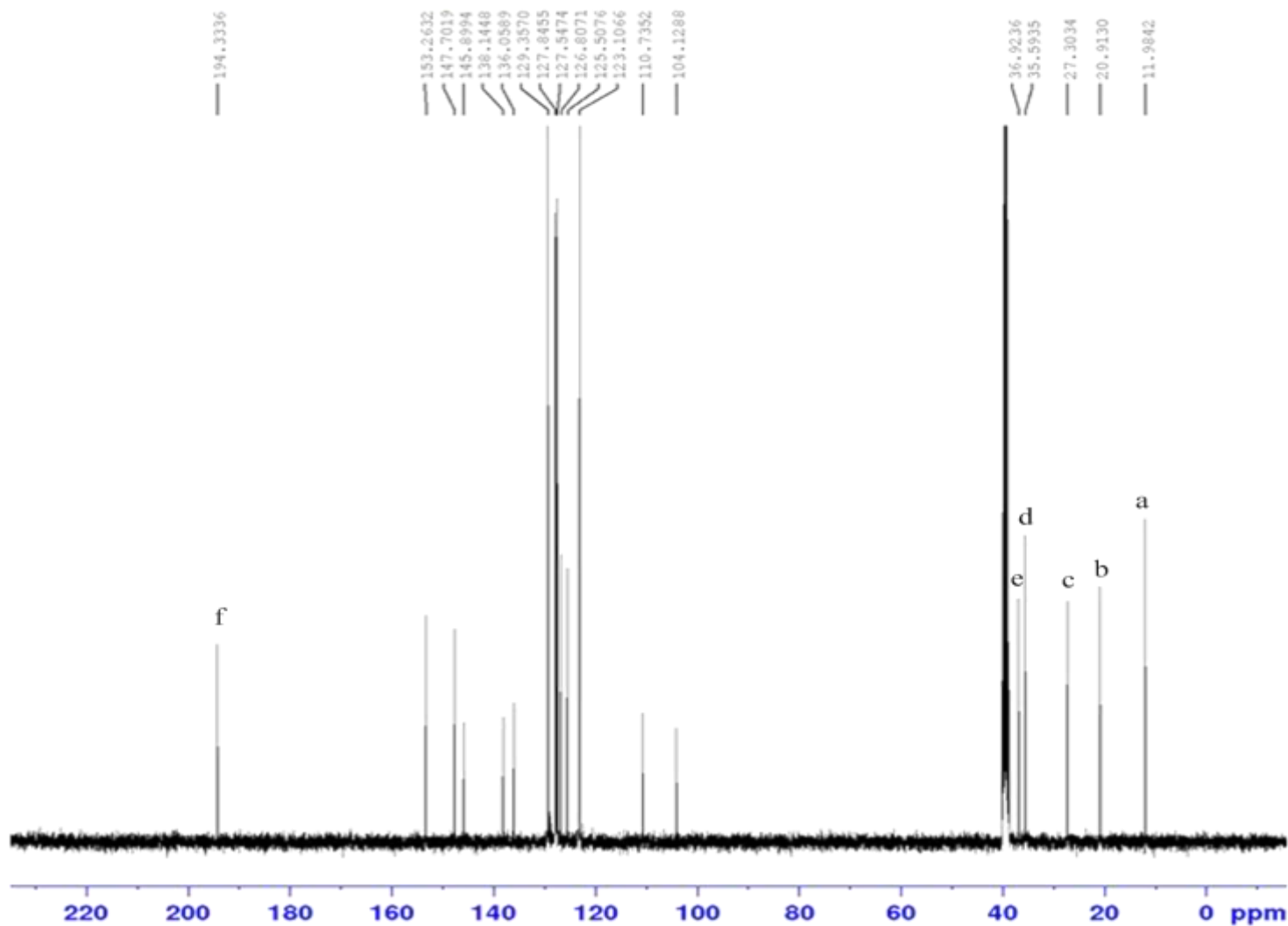
***** CHANNEL f1 *****
 NUC1 1H
 P1 11.00 usec
 PL1 -2.00 dB
 PL1W 17.51671600 W
 SFO1 400.1326008 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1299701 MHz
 NQW RM
 SSB 0
 LB 0.30 Hz
 GB 0





¹³C NMR Spectrum of compound 4a



```

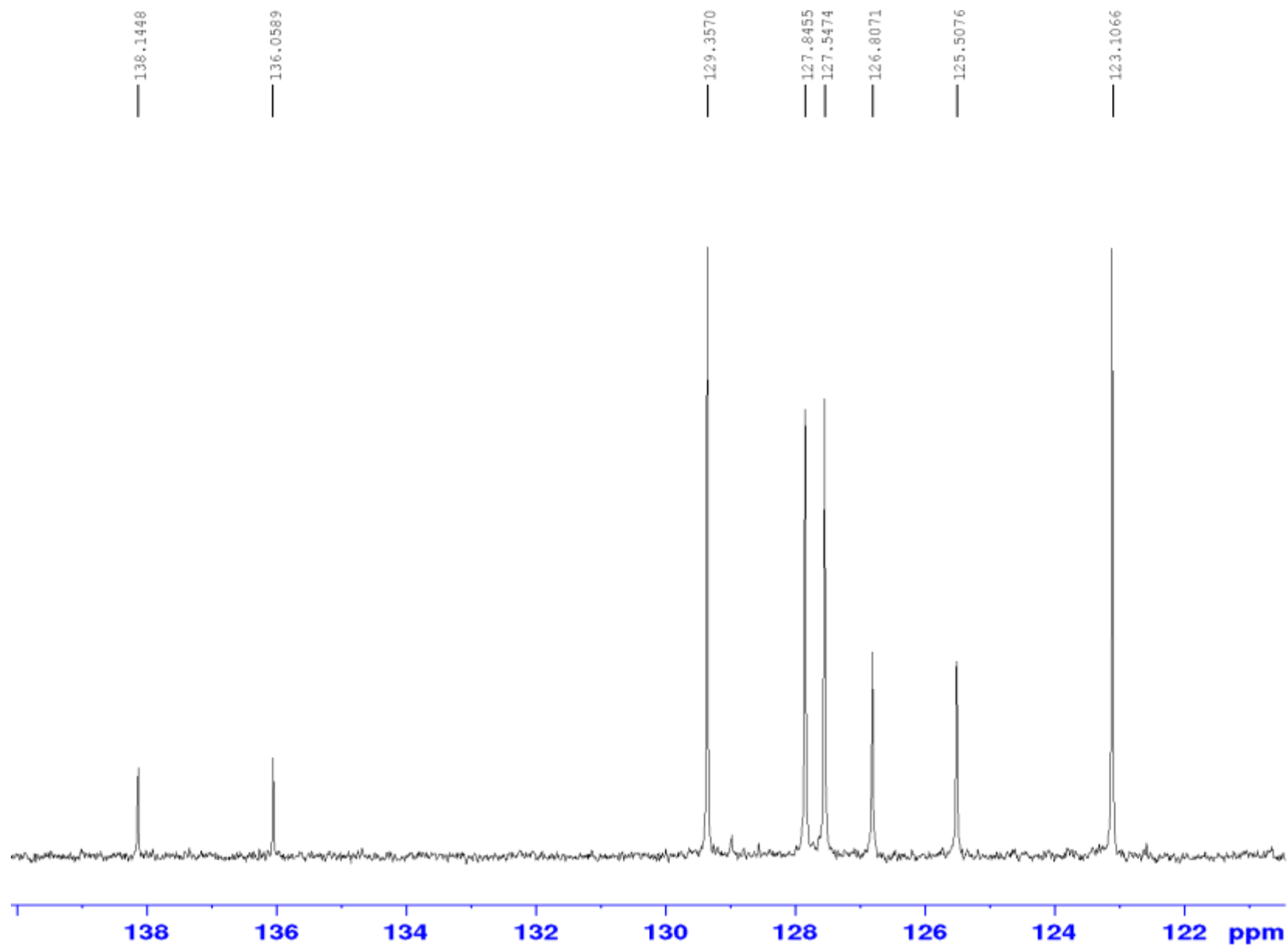
Current Data Parameters
NAME          11 cmz
EXPNO         10
PROCNO        1

F2 - Acquisition Parameters
Date_         20180228
Time_         14.50
INSTRUM       spect
PROBHD        5 mm FARRC BB-
PULPROG       zgpg
TD            50502
SOLVENT       DMSO
NS            2151
DS            2
SWH           25252.525 Hz
FIDRES        0.500030 Hz
AQ            0.9999396 sec
RG            45.2
DW            19.800 usec
DE            6.50 usec
TE            294.4 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0           1

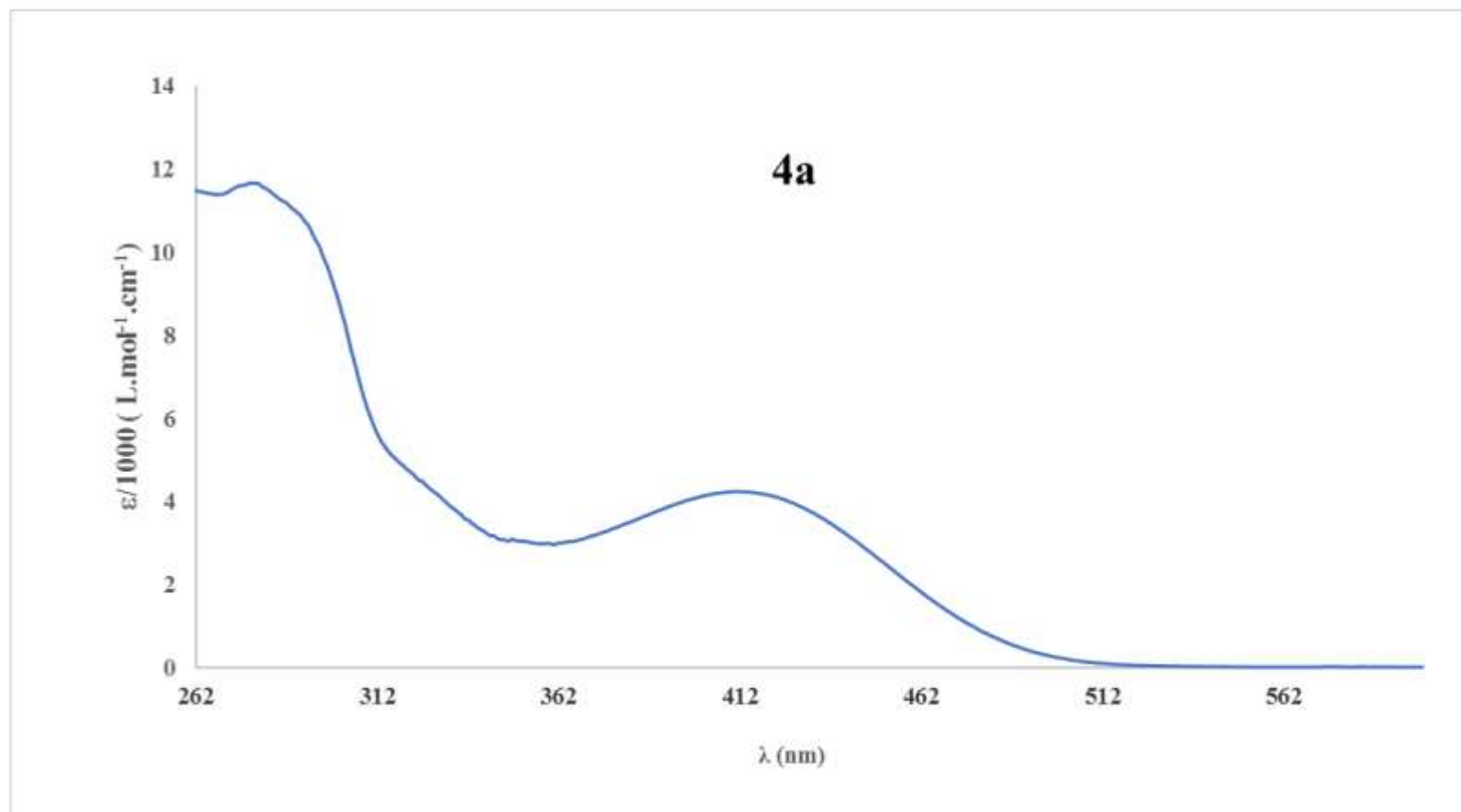
===== CHANNEL f1 =====
NUC1           13C
P1             8.70 usec
PL1            -1.00 dB
PL1W           42.69075012 W
SFO1           100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG[2]     waltz16
NUC2           1H
PCPD2          80.00 usec
PL2            0 dB
PL12           15.26 dB
PL13           18.26 dB
PL2W           11.05230045 W
PL12W          0.32919458 W
PL13W          0.16498812 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI             32768
SF            100.6128193 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
PC             1.40
    
```

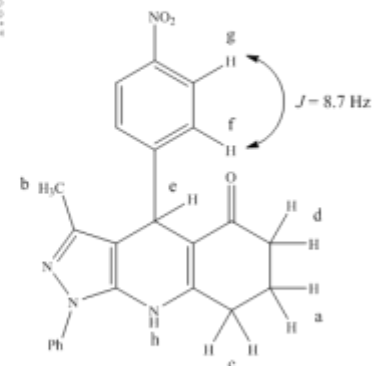
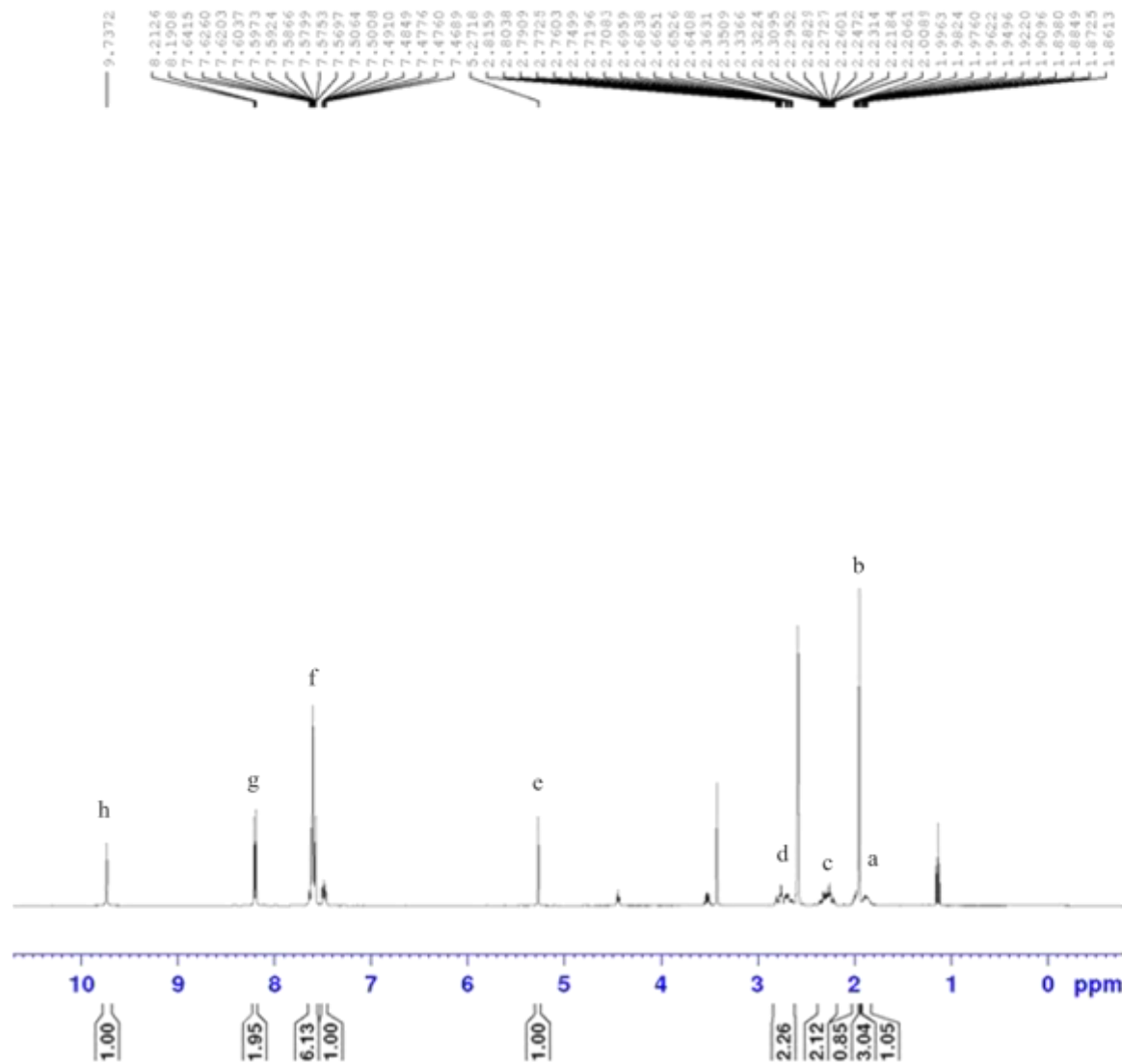



UV-Spectrum of compound **4a**



UV-absorption spectrum of **4a** in CHCl_3

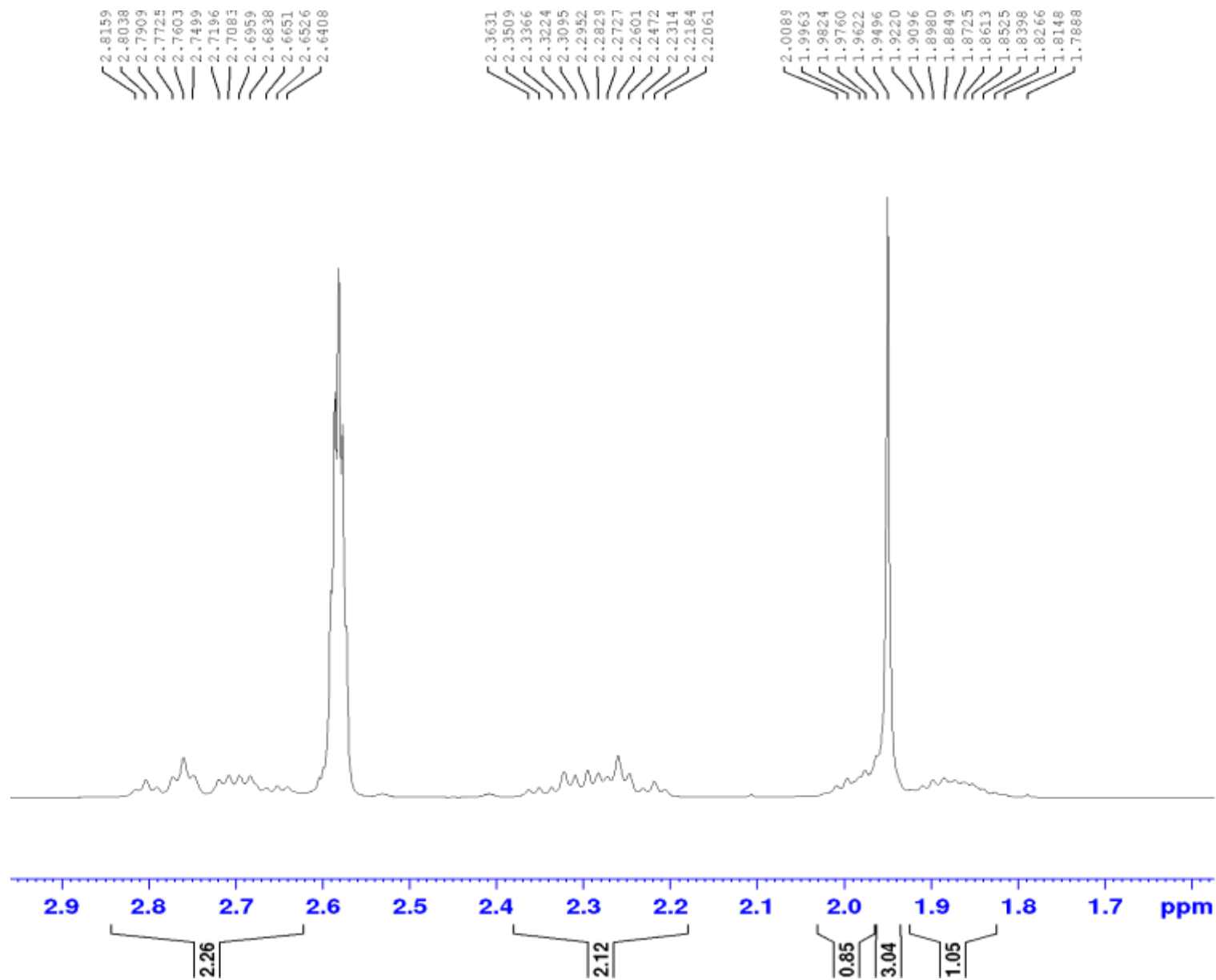
¹H NMR Spectrum of compound 4b

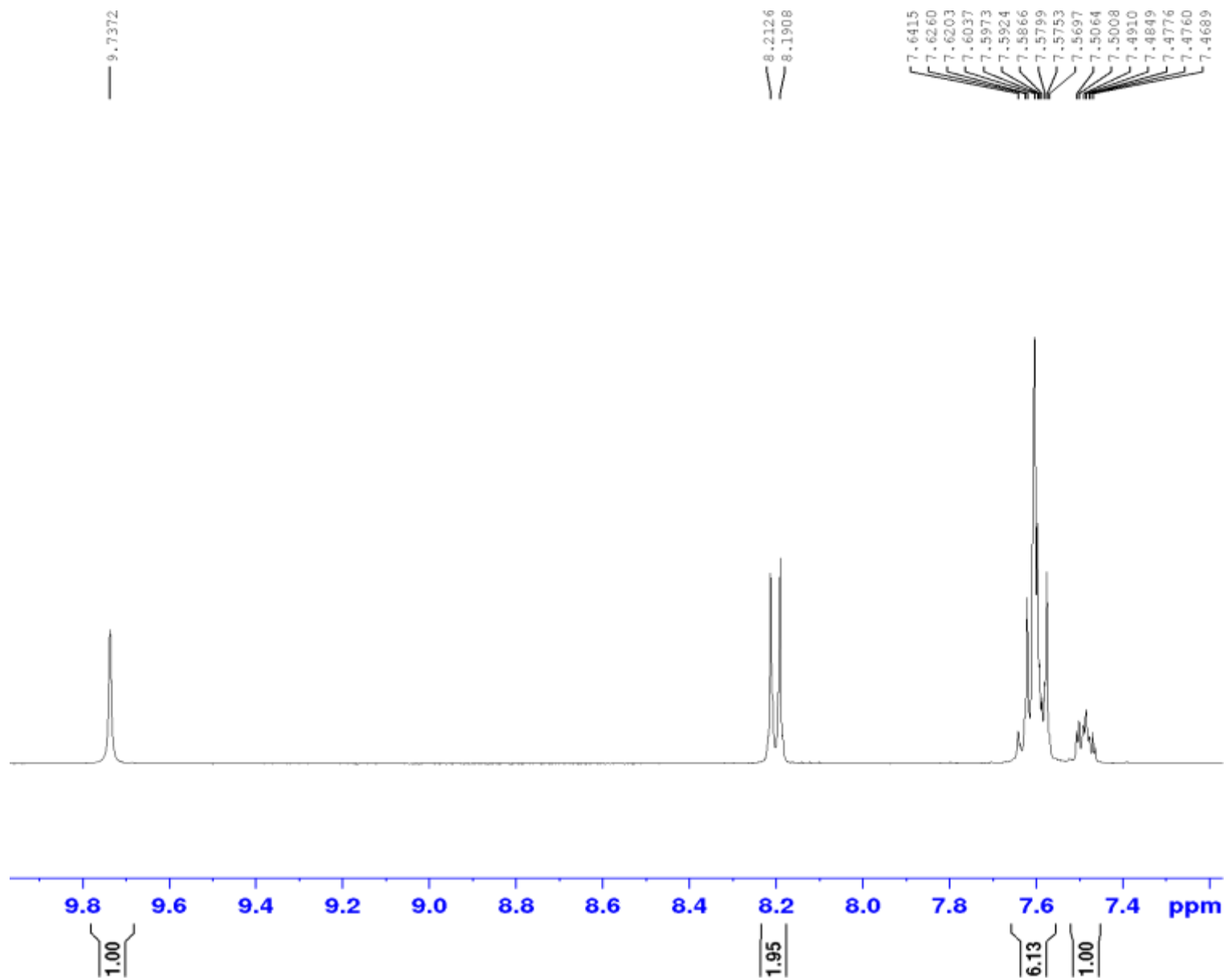


NAME H NMR 104
EXPNO 10
PROCNO 1

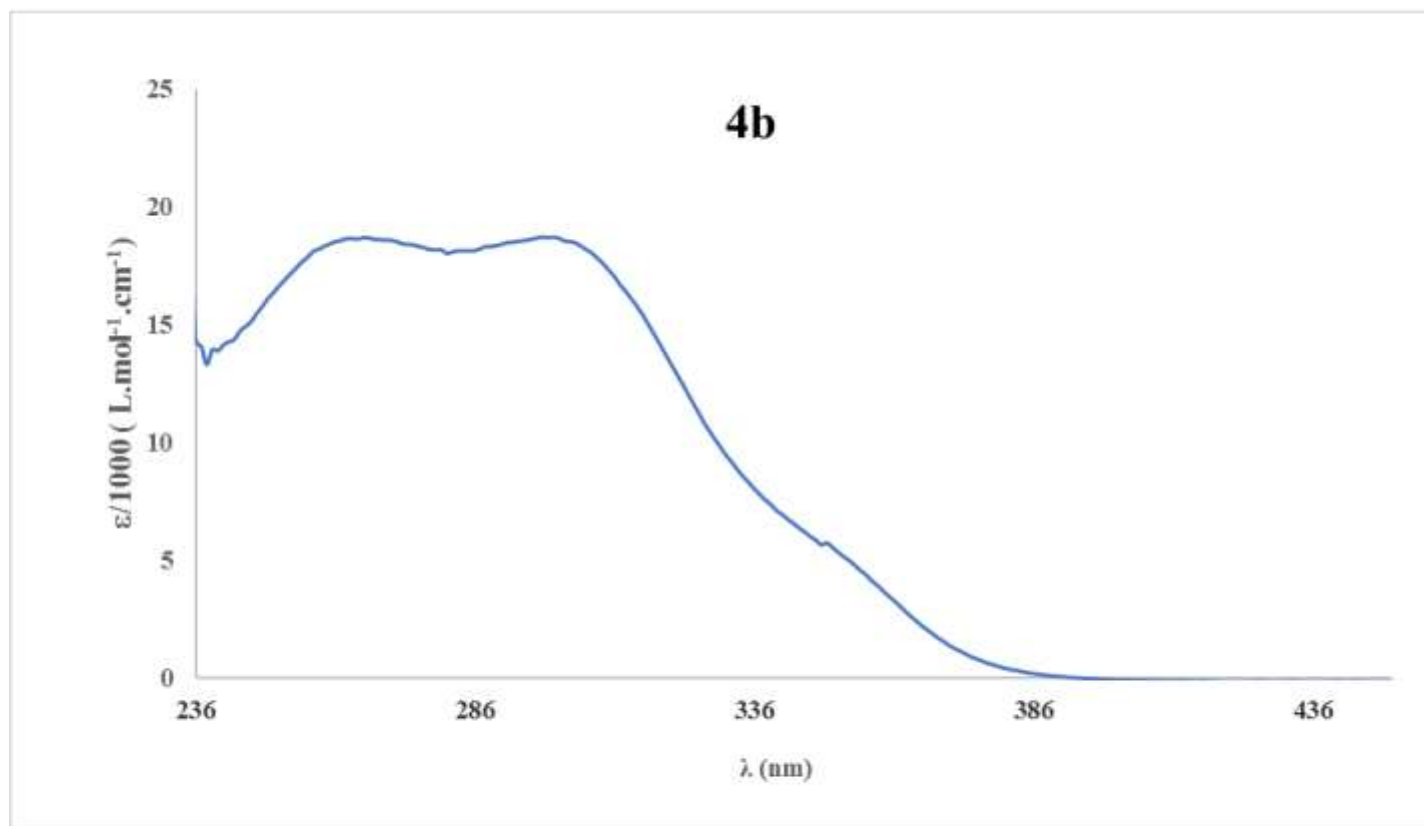
F2 - Acquisition Parameters
Date_ 20180128
Time 14.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 50504
SOLVENT DMSO
NS 32
DS 2
SWH 8417.509 Hz
FIDRES 0.166670 Hz
AQ 2.9999375 sec
RG 80.6
DW 59.400 usec
DE 6.50 usec
TE 294.7 K
D1 5.00000000 sec
TDO 1

***** CHANNEL f1 *****
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
PL1W 17.51671600 W
SF01 400.1326008 MHz
F2 - Processing parameters
SI 32768
SF 400.1299706 MHz
WDW EM
SSB 0
TA 0.10 Hz



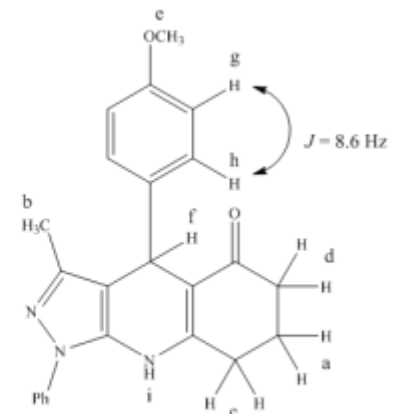
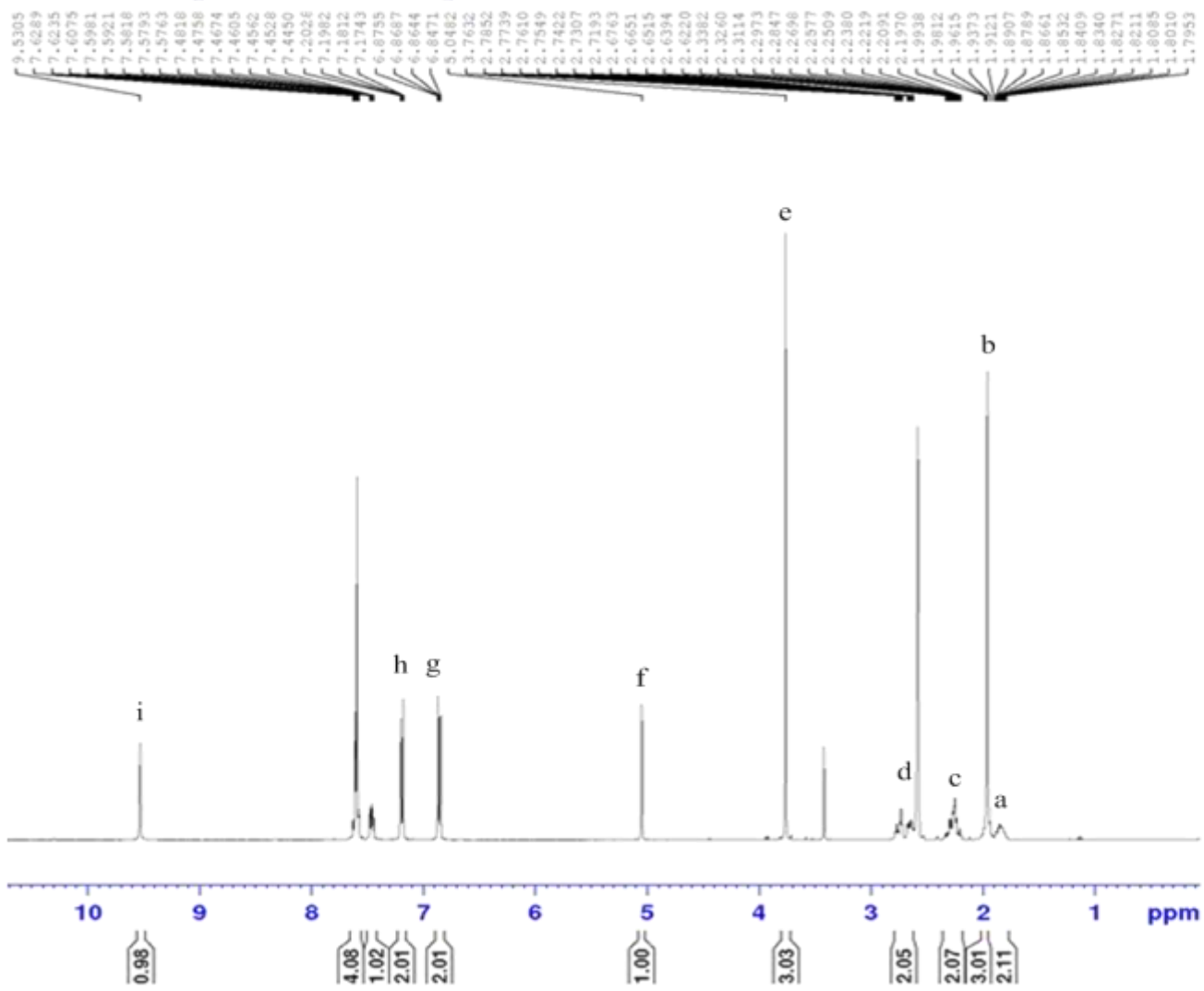


UV-Spectrum of compound **4b**



UV-absorption spectrum of **4b** in CHCl_3

¹H NMR Spectrum of compound 4c



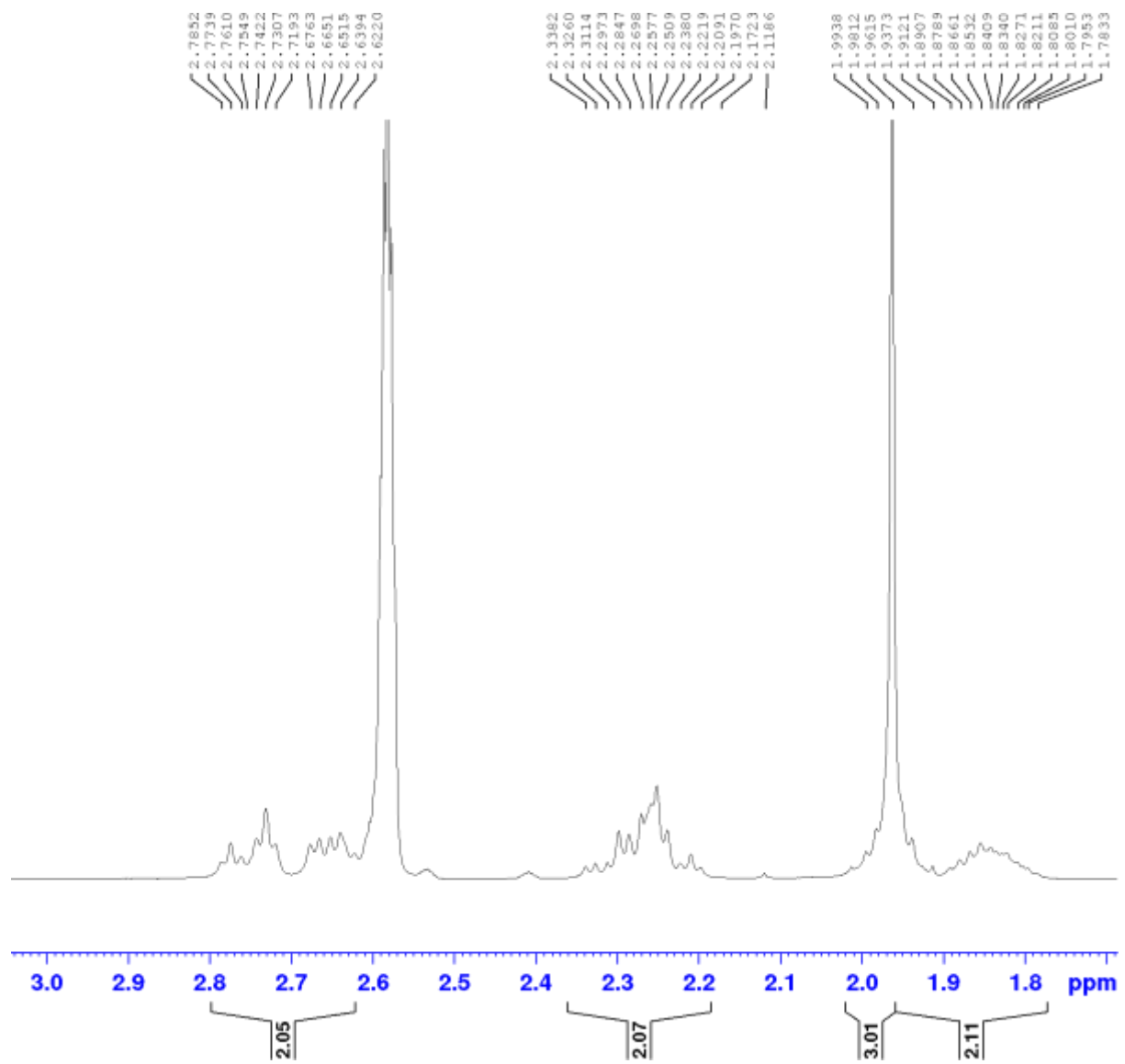
```

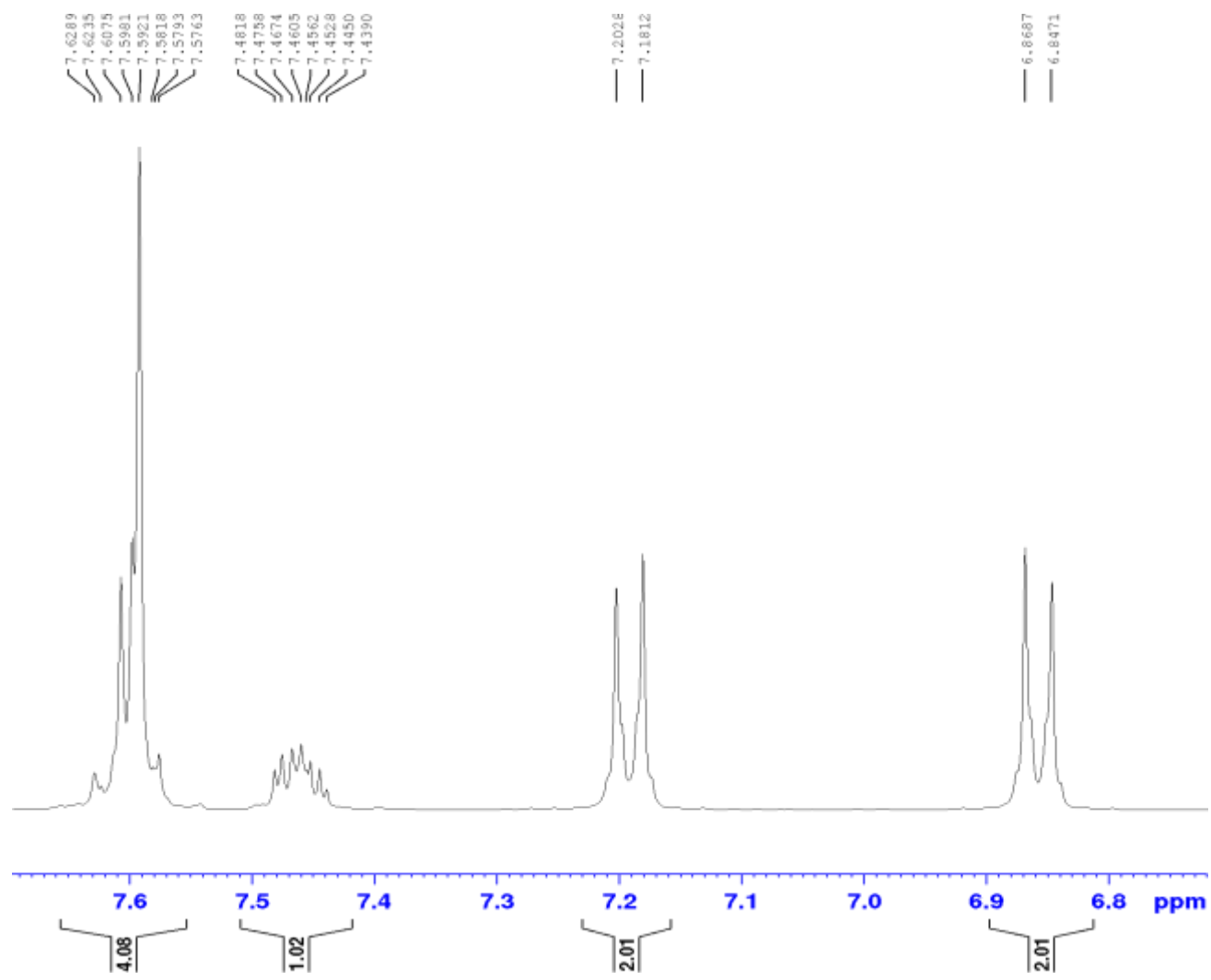
NAME          HNMR 105
EXPNO         20
PROCNO        1

F2 - Acquisition Parameters
Date_         20180128
Time          14.11
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg
TD            50504
SOLVENT       DMSO
NS            32
DS            2
SWH           8417.509 Hz
FIDRES        0.166670 Hz
AQ            2.9999375 sec
RG            80.6
DW            59.400 usec
DE            6.50 usec
TE            294.7 K
D1            5.00000000 sec
TD0           1

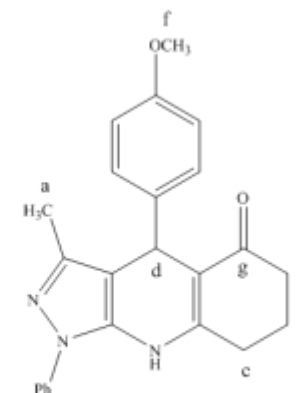
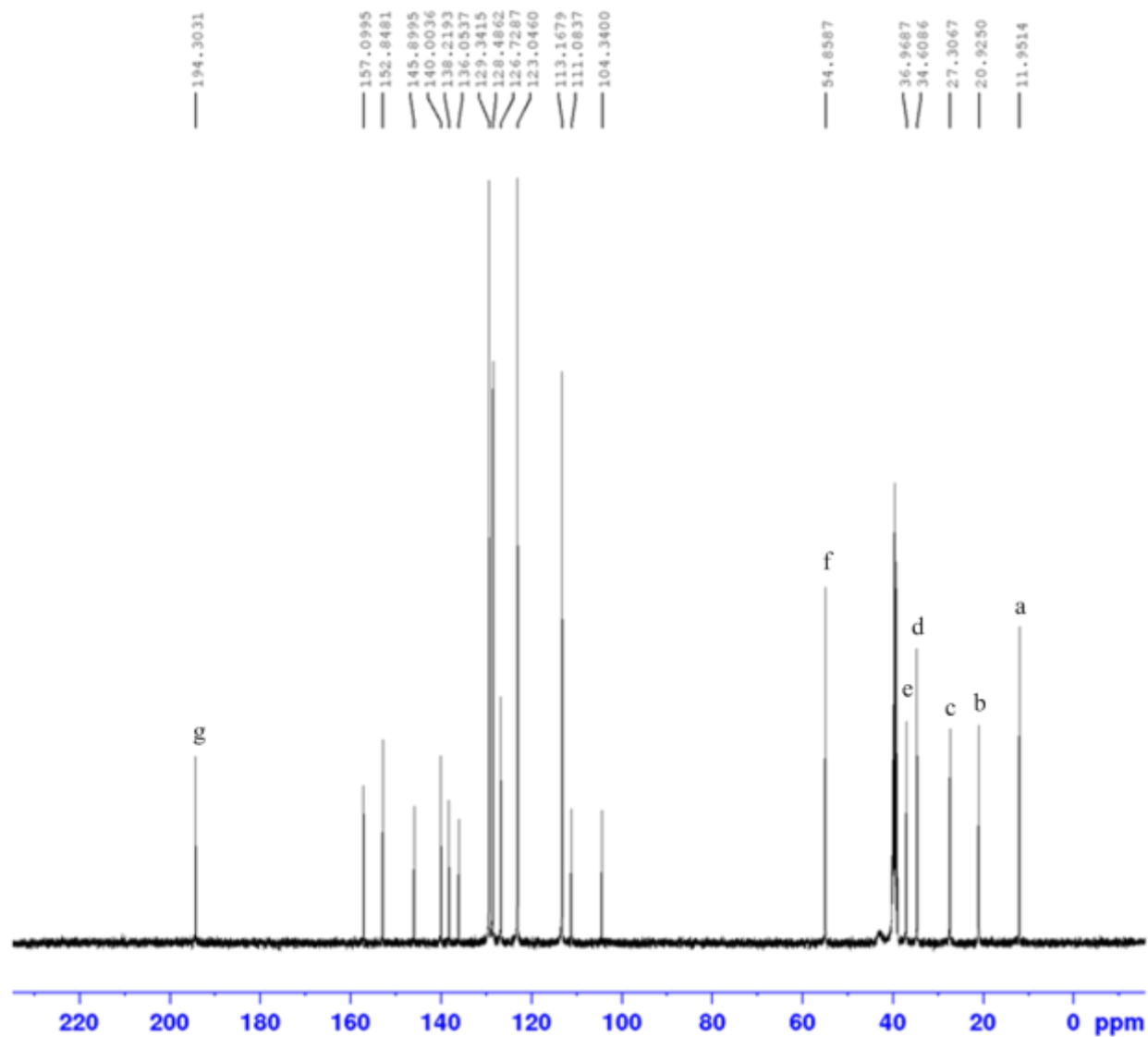
===== CHANNEL f1 =====
NUC1          1H
P1            11.00 usec
PL1           -2.00 dB
PL1W          17.51671600 W
SFO1          400.1326008 MHz

F2 - Processing parameters
SI            32768
SF            400.1299708 MHz
WDW           EM
SSB           0
GB            0.70 Hz
    
```





¹³C NMR Spectrum of compound 4c



```

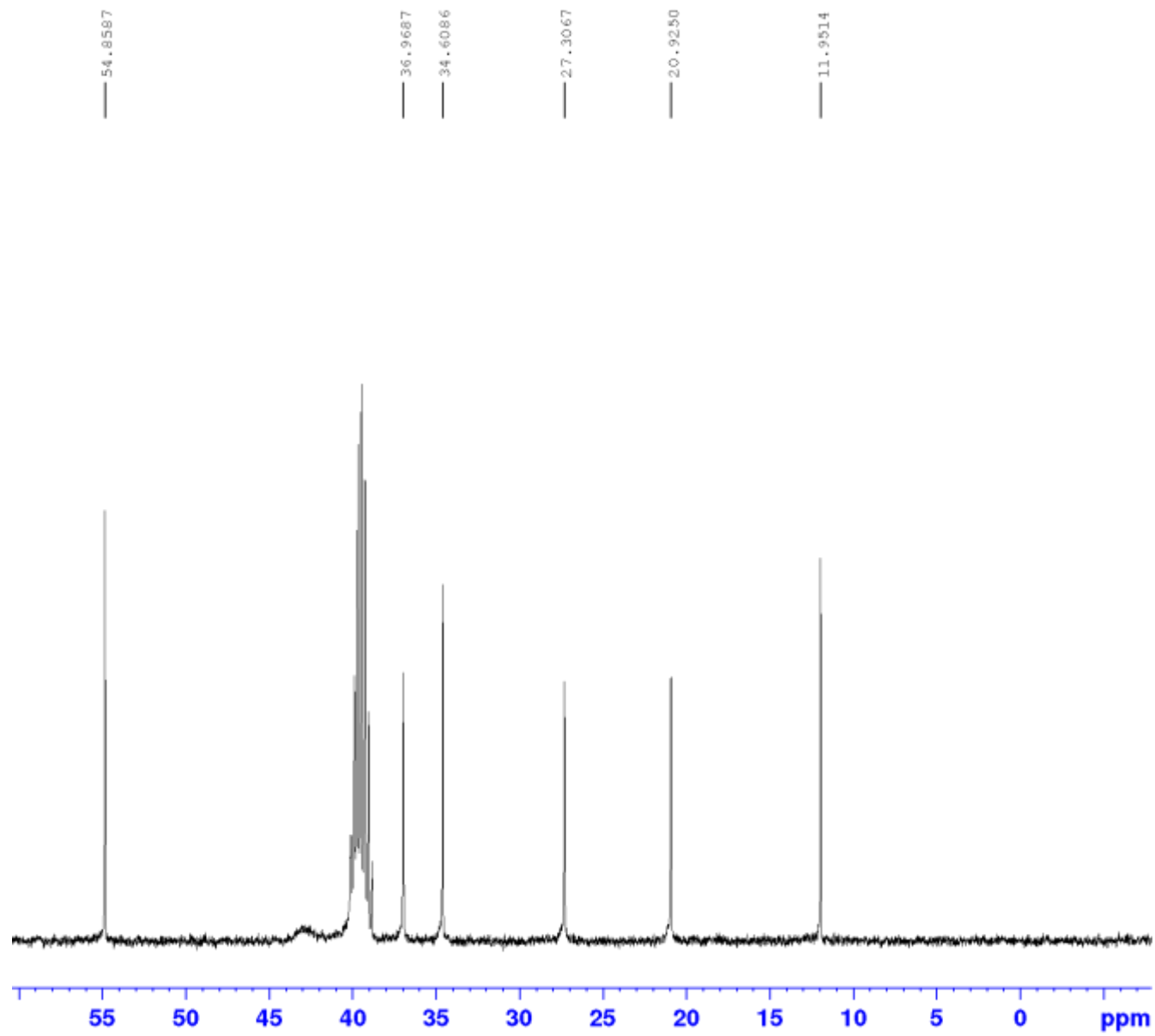
Current Data Parameters
NAME          CMMR 105
EXPNO         41
PROCNO        1

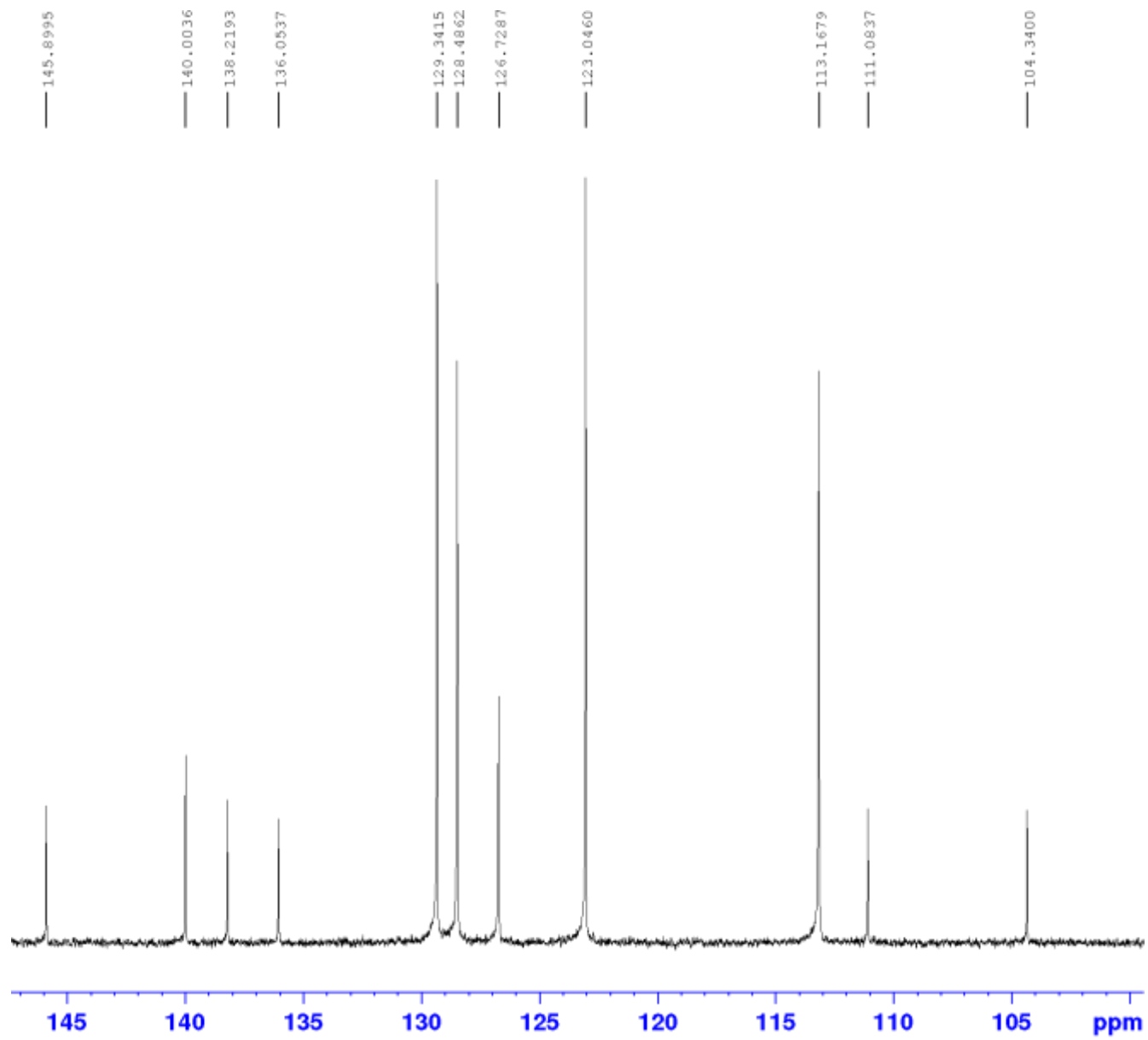
F2 - Acquisition Parameters
Date_         20180221
Time          12.53
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zgpg
TD           50502
SOLVENT      DMSO
NS           2564
DS           2
SWH          25252.525 Hz
FIDRES       0.500030 Hz
AQ           0.9999396 sec
RG           90.5
DW           19.800 usec
DE           6.50 usec
TE           296.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1          13C
P1            8.70 usec
PL1           -1.00 dB
PL1W          42.69075012 W
SFO1          100.628364 MHz

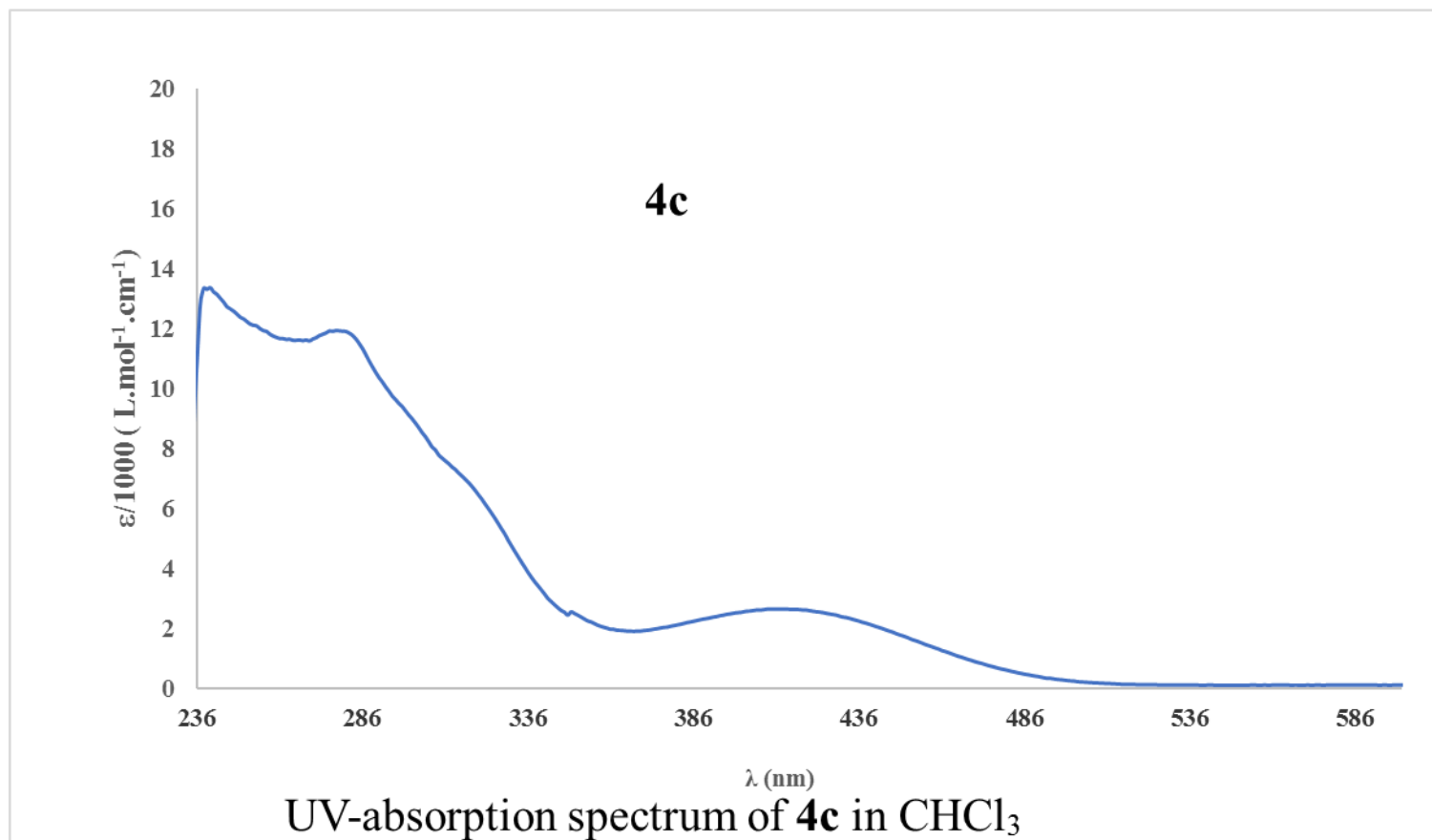
===== CHANNEL f2 =====
CPDPRG[2]    waltz16
NUC2          1H
PCPD2        80.00 usec
PL2           0 dB
PL12         15.26 dB
PL13         18.26 dB
PL2W         11.05230045 W
PL12W        0.32919458 W
PL13W        0.16498812 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI            32768
SF            100.6128193 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
    
```

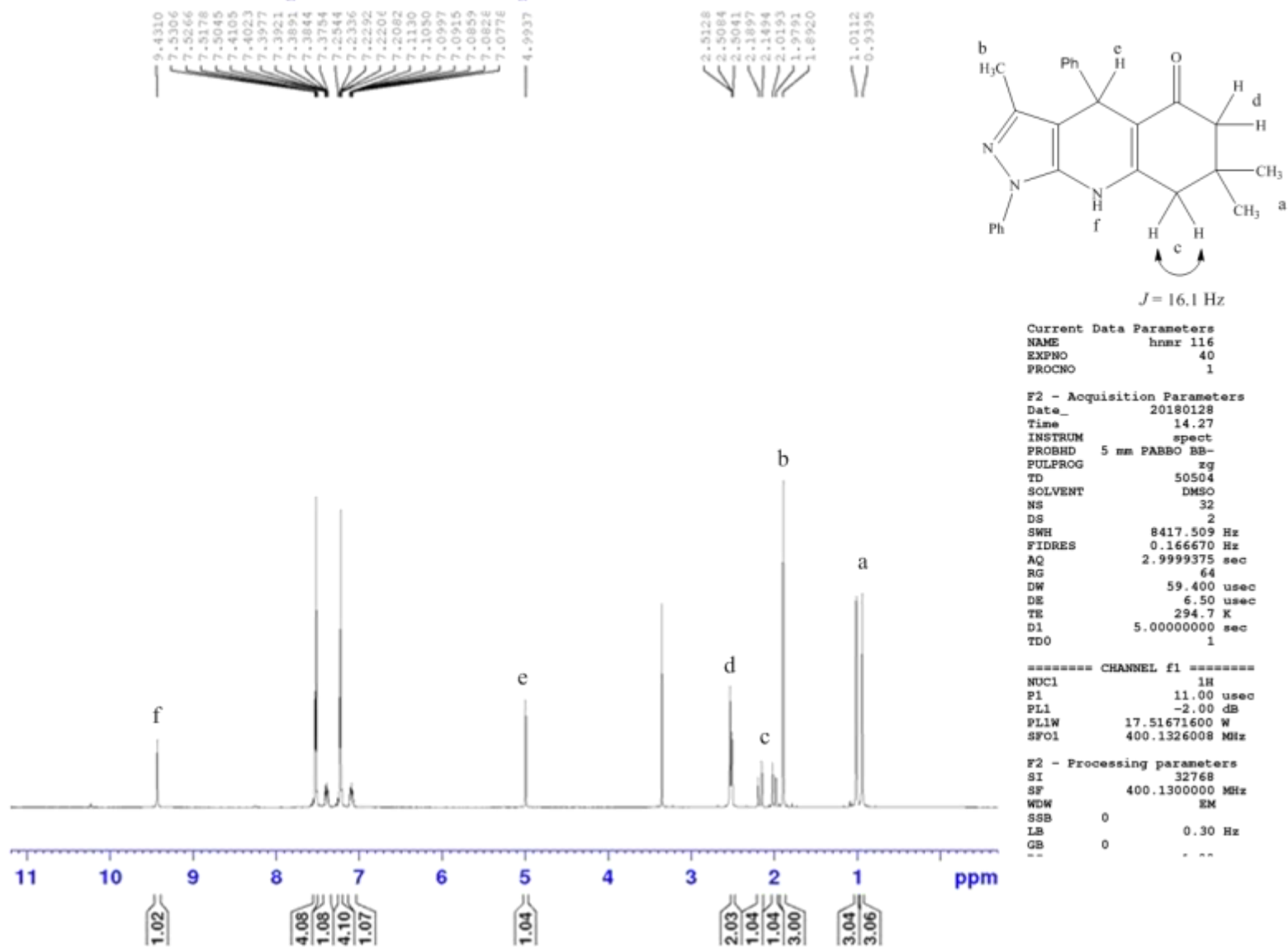


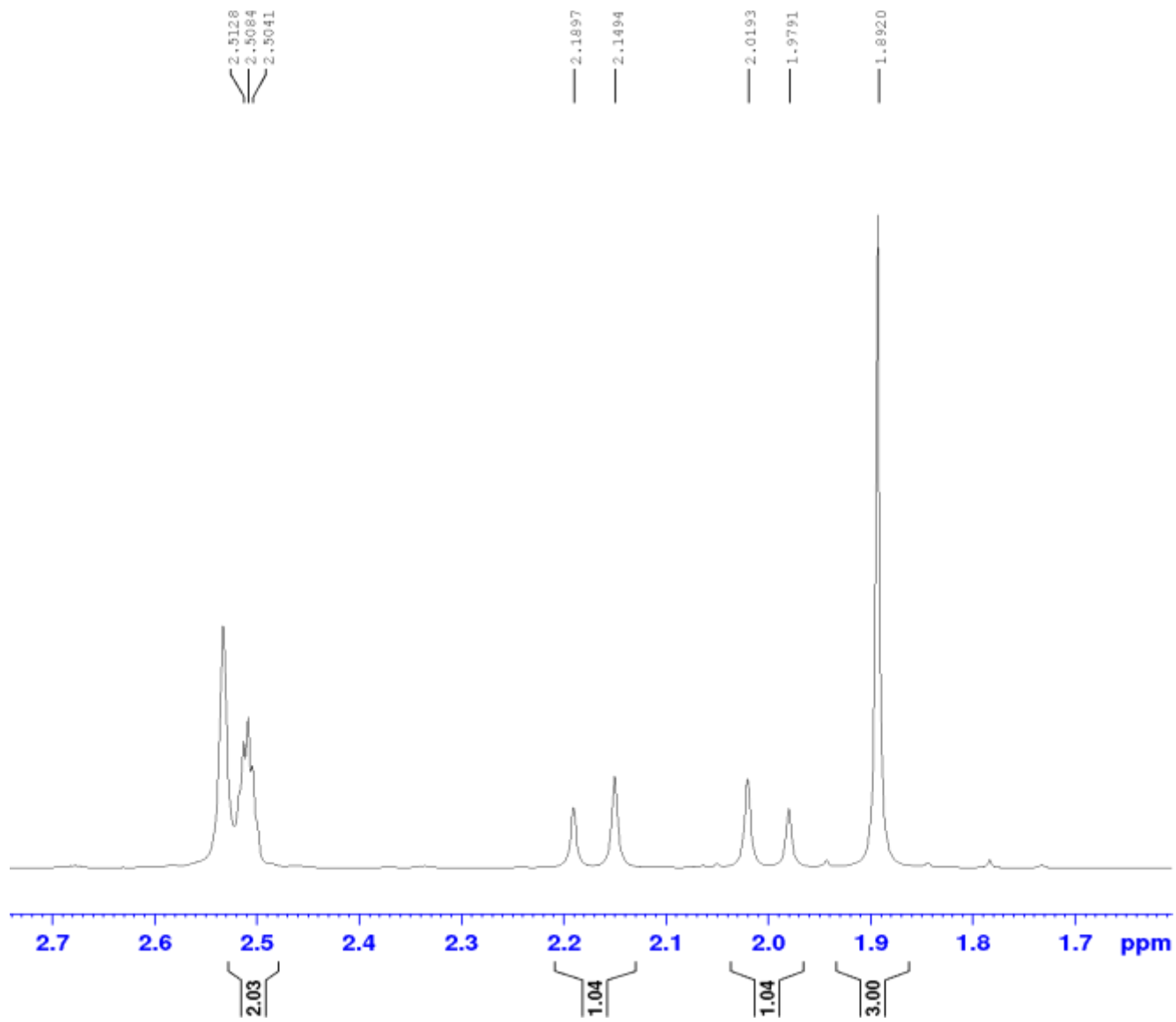


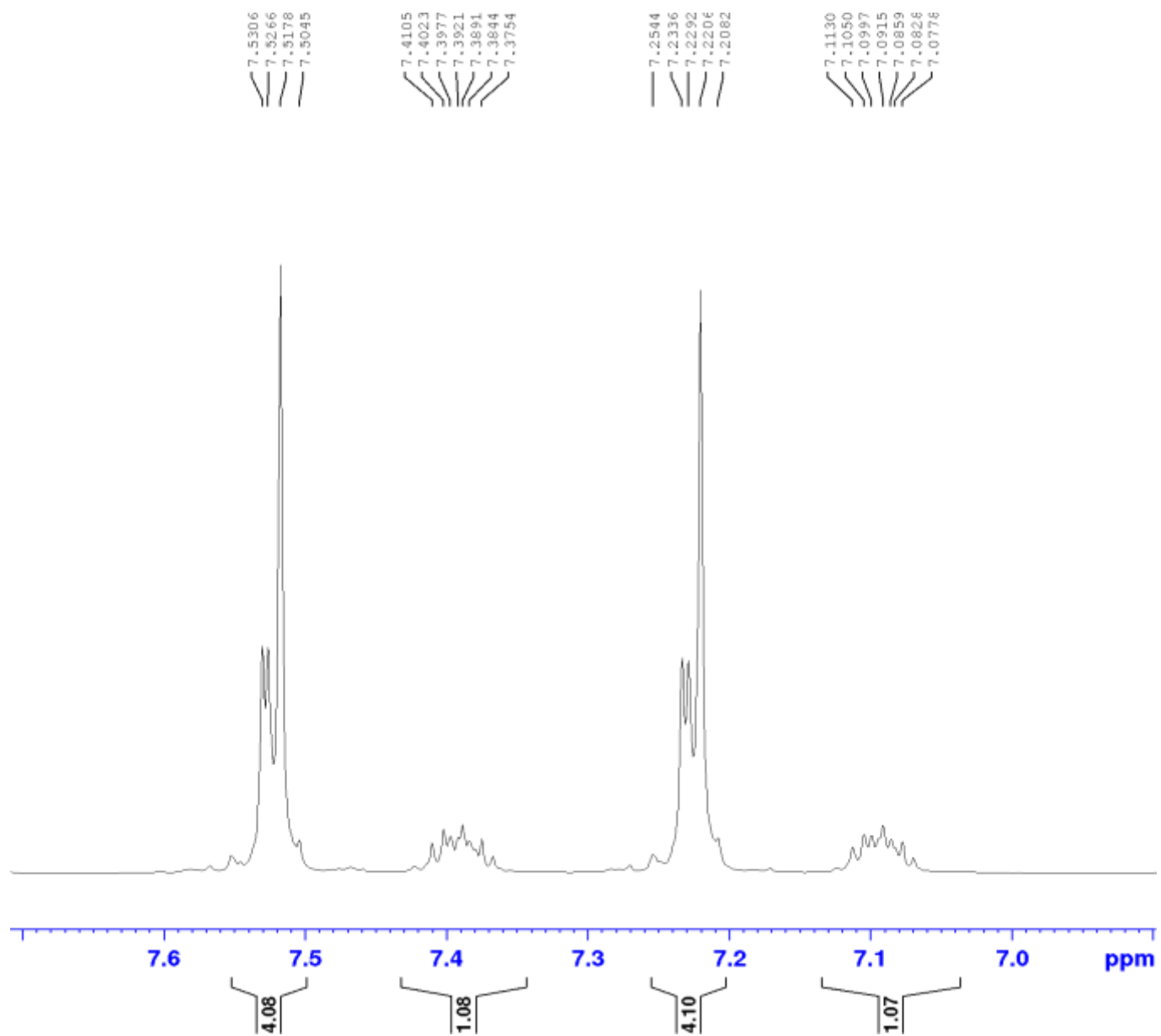
UV-Spectrum of compound **4c**



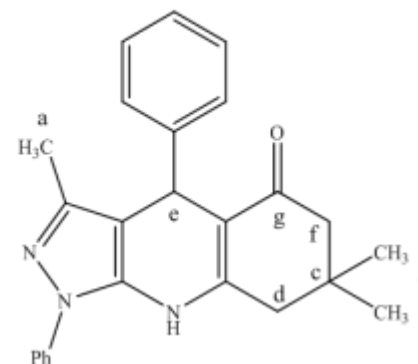
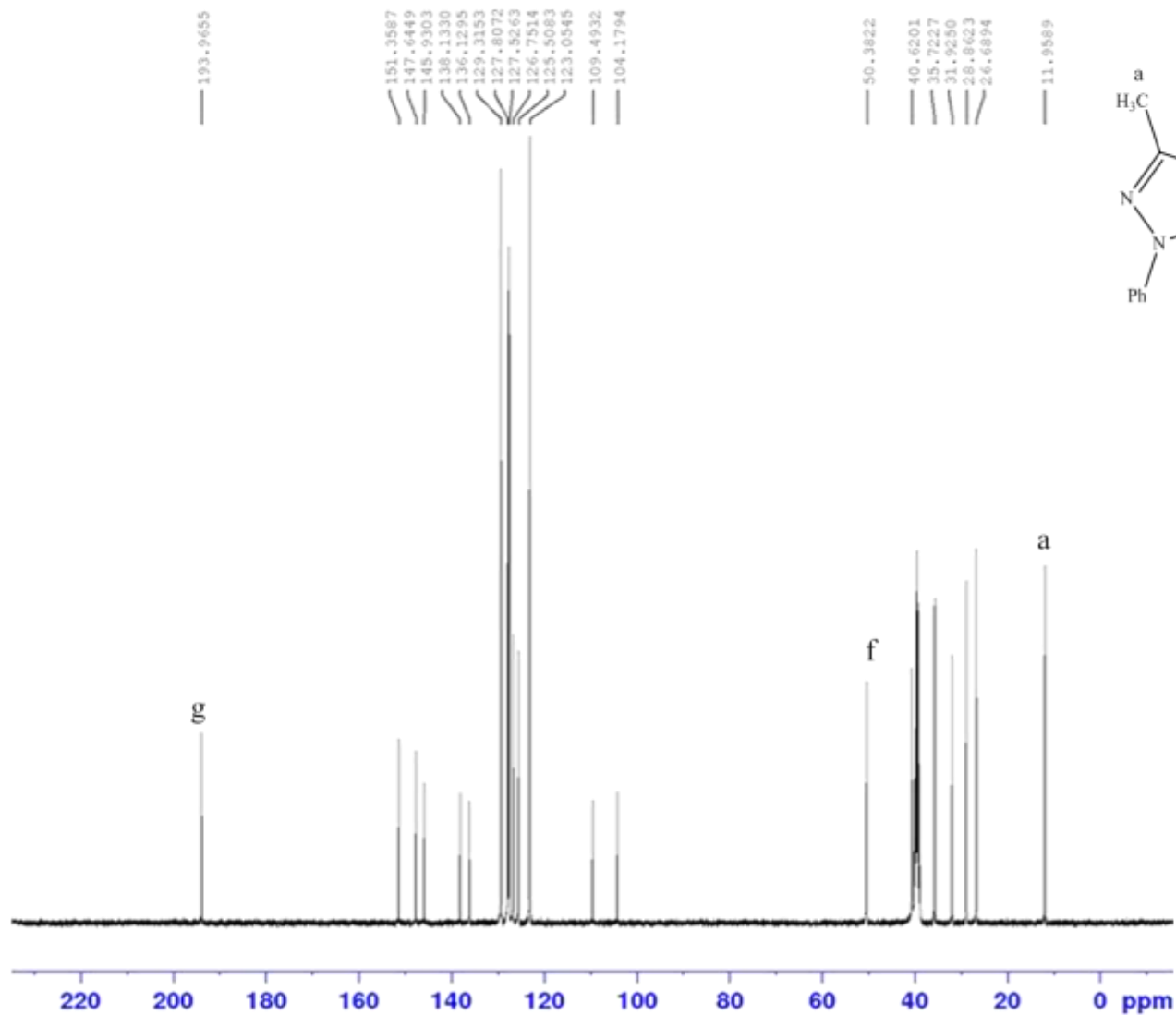
¹H NMR Spectrum of compound 4d







¹³C NMR Spectrum of compound 4d



```

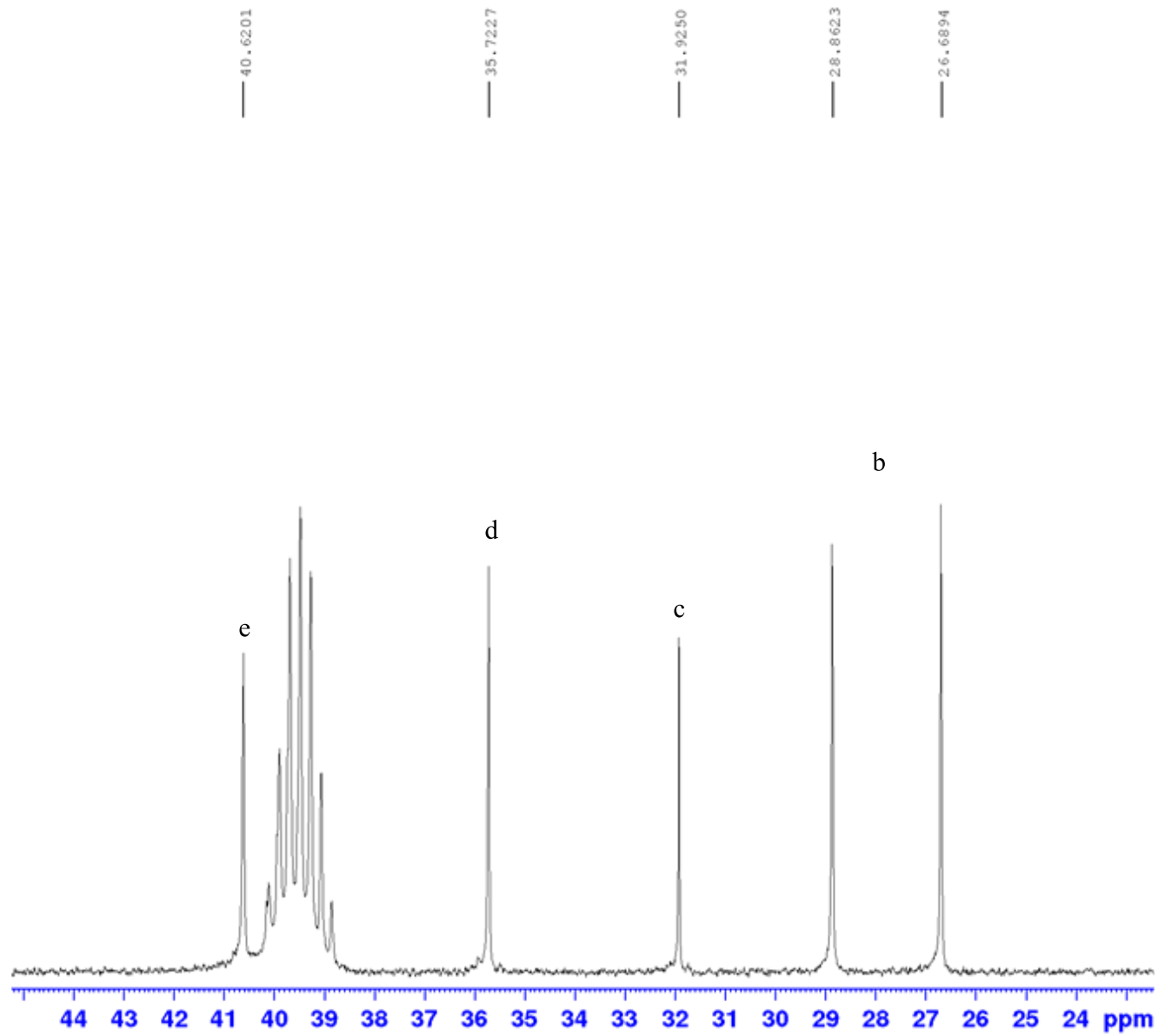
Current Data Parameters
NAME          cnmr 114
EXPNO        61
PROCNO       1

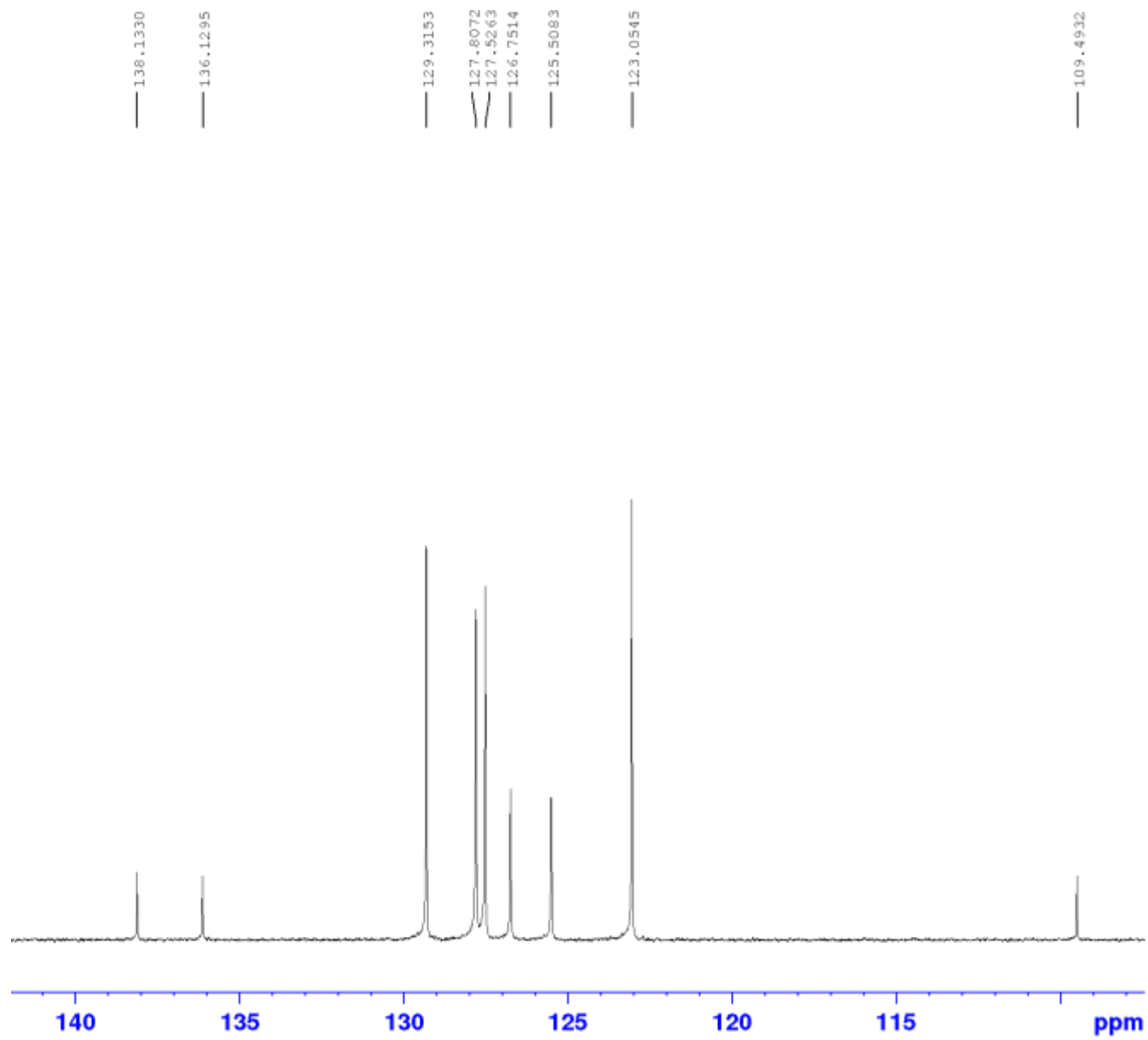
F2 - Acquisition Parameters
Date_        20180221
Time         16.11
INSTRUM      spect
PROBHD       5 mm FAMB0 BB-
PULPROG      zgpg
TD           50502
SOLVENT      DMSO
NS           3000
DS           2
SWH          25252.525 Hz
FIDRES       0.500030 Hz
AQ           0.9999394 sec
RG           71.8
DW           19.800 usec
DE           6.50 usec
TE           296.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TDO          1

===== CHANNEL f1 =====
NUC1          13C
P1            8.70 usec
PL1           -1.00 dB
PL1W          42.69075012 W
SFO1          100.6238364 MHz

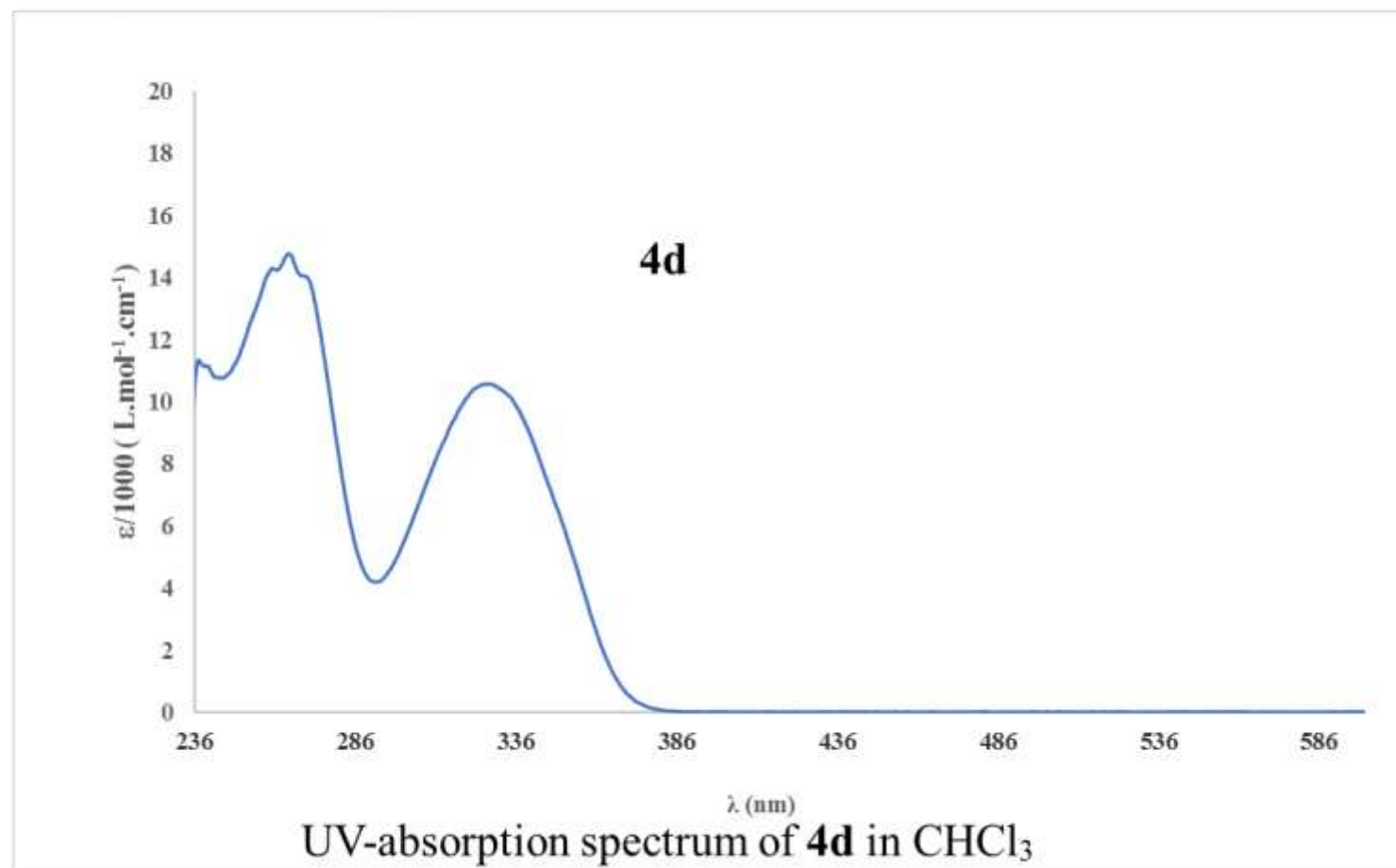
===== CHANNEL f2 =====
CPDPRG2[2]   waltz16
NUC2          1H
PCPD2         80.00 usec
PL2           0 dB
PL12          15.26 dB
PL13          18.26 dB
PL2W          11.05230045 W
PL12W         0.32919458 W
PL13W         0.16498812 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI            32768
SF            100.6128193 MHz
MDW          2M
SSB           0
LB            1.00 Hz
GB            0
    
```

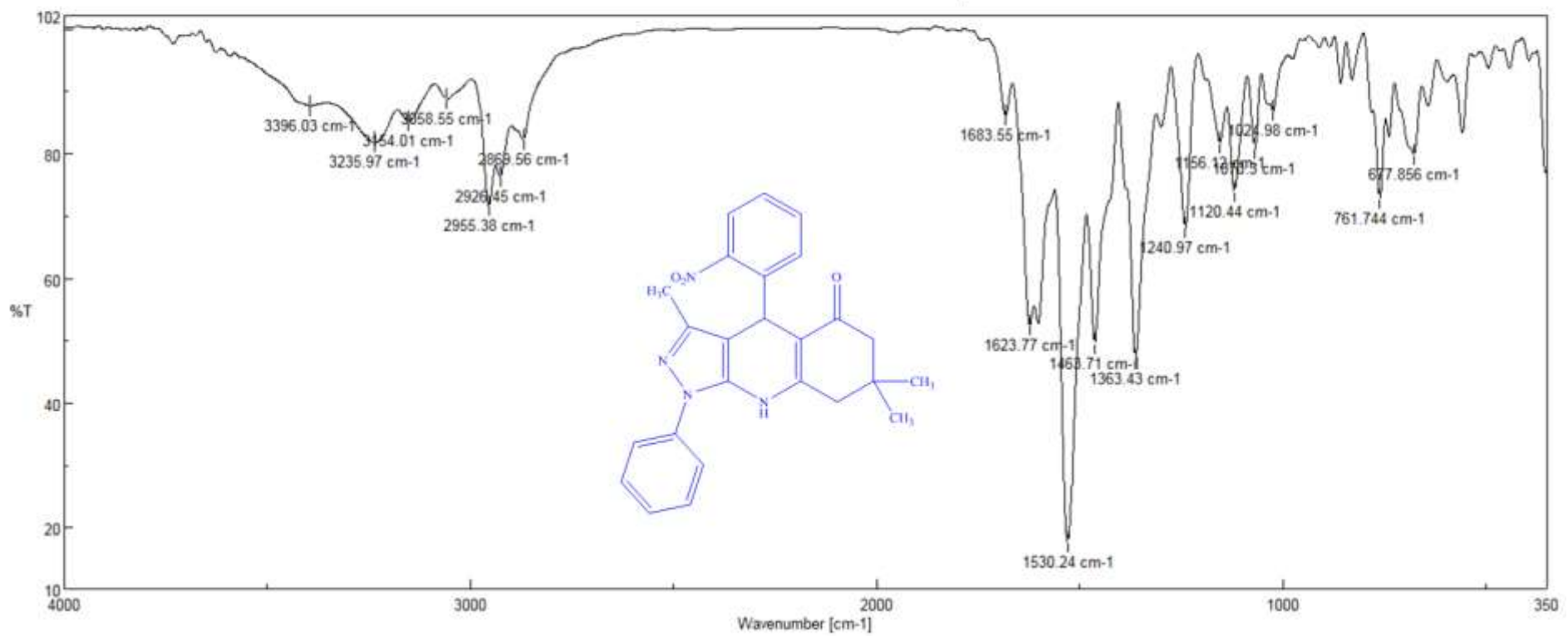




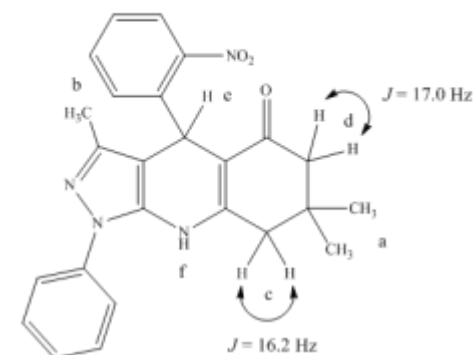
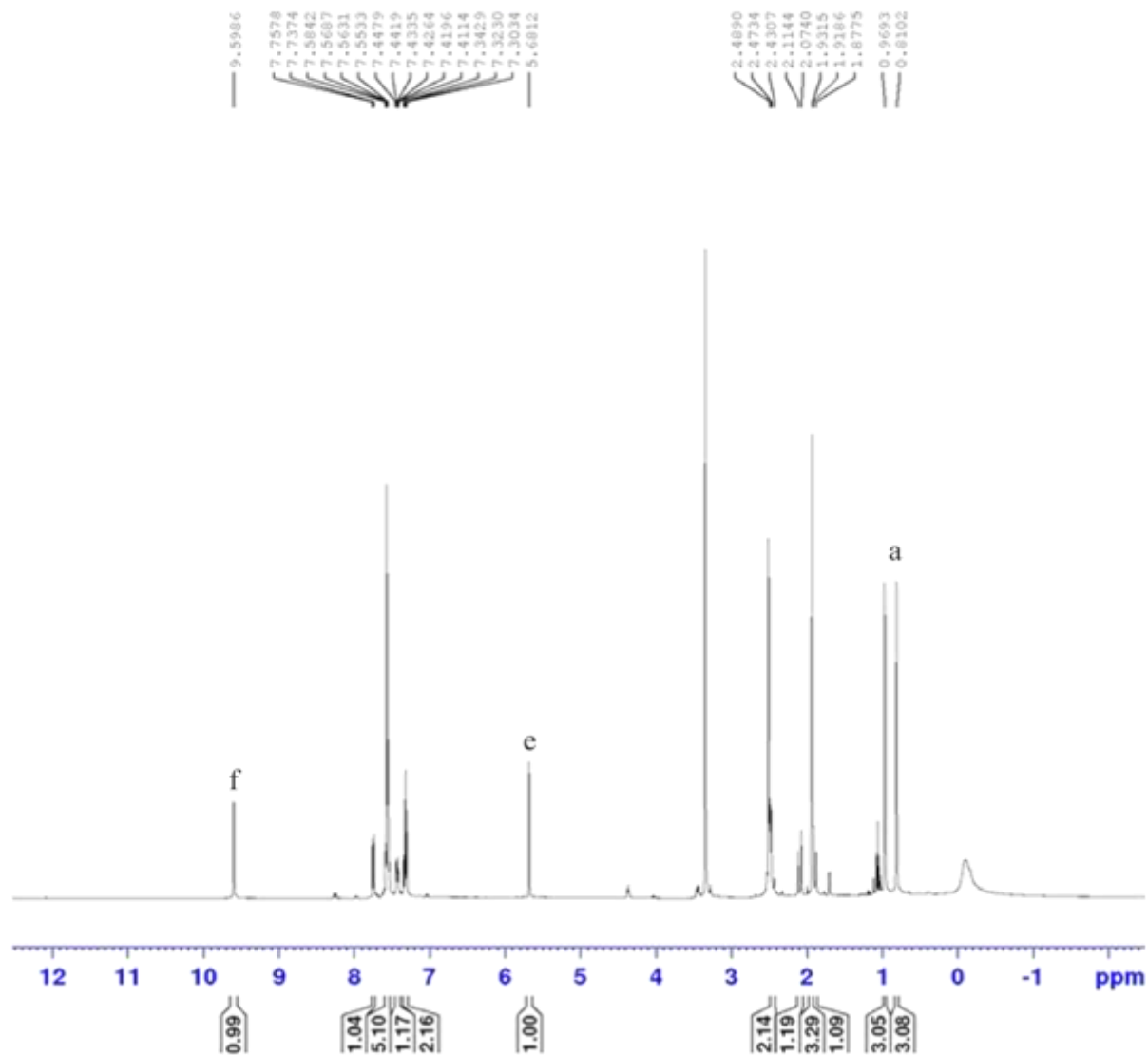
UV-Spectrum of compound **4d**



IR-Spectrum of compound 4e



¹H NMR Spectrum of compound 4e



NAME Ahmadi- Mehdi-IN97082
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters

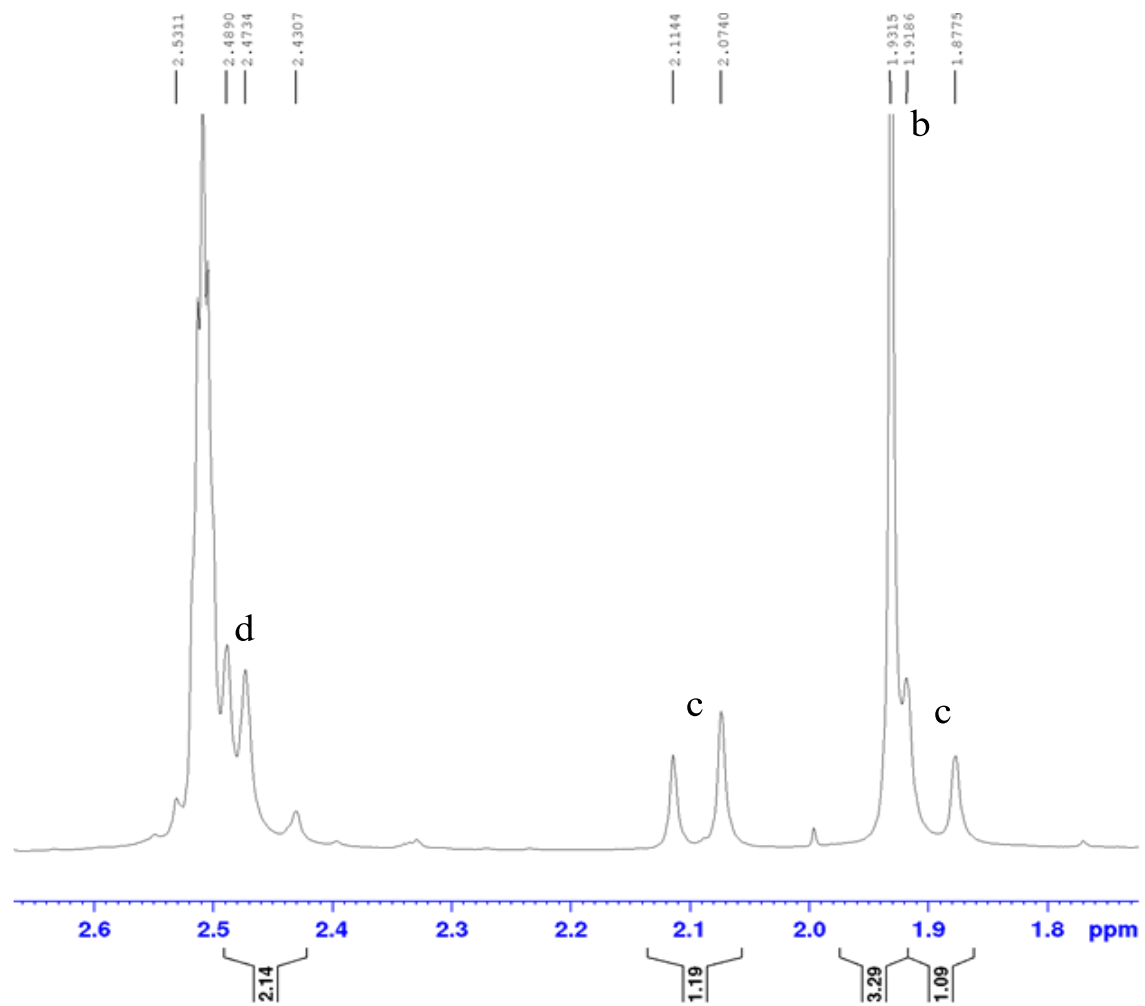
Date_ 20181119
 Time 17.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg
 TD 50504
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8802.817 Hz
 FIDRES 0.174299 Hz
 AQ 2.8686273 sec
 RG 71.8
 DW 56.800 usec
 DE 6.50 usec
 TE 295.0 K
 D1 5.00000000 sec
 TD0 1

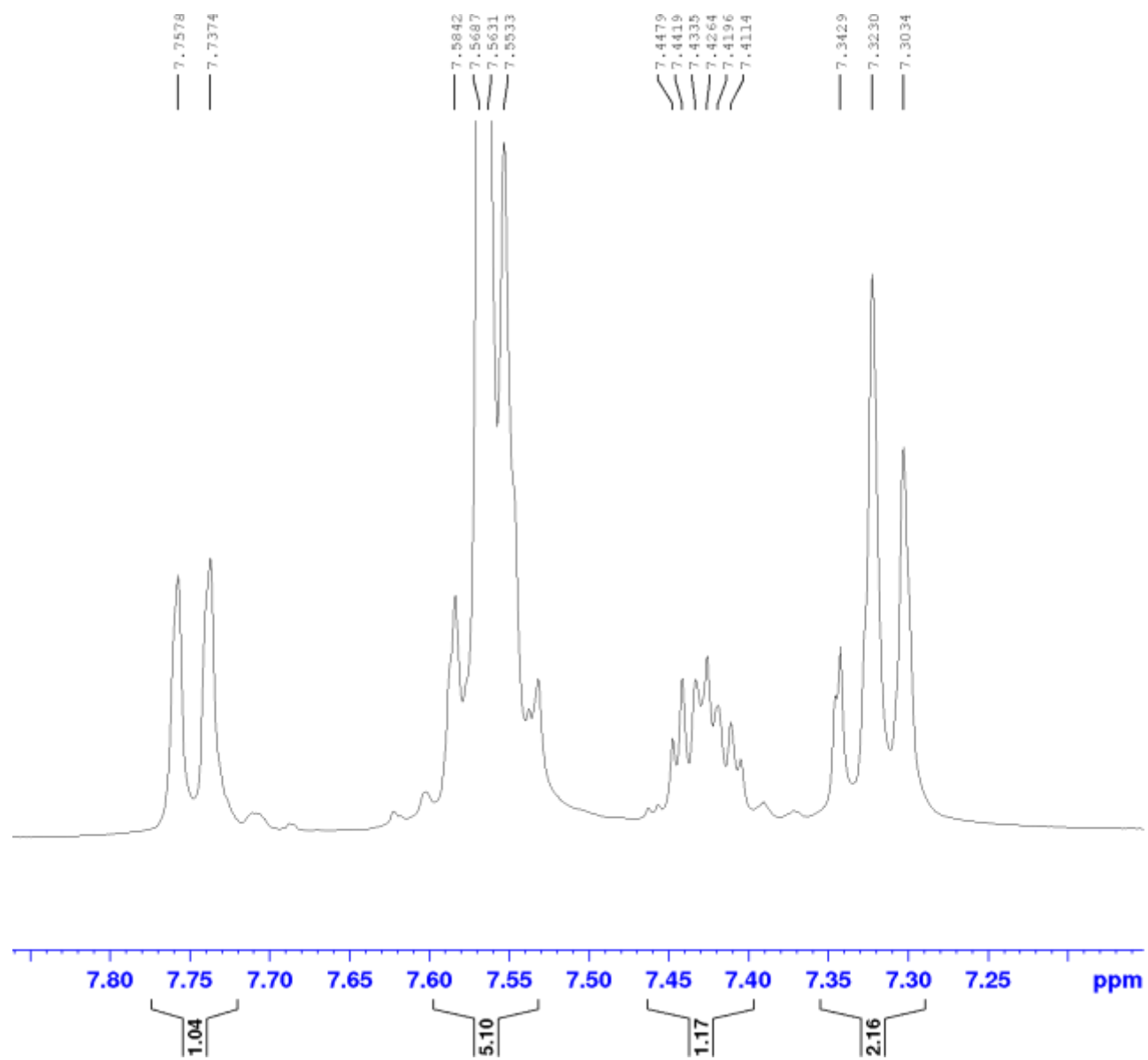
===== CHANNEL f1 =====

NUC1 1H
 P1 11.00 usec
 PL1 -2.00 dB
 PL1W 17.51671600 W
 SFO1 400.1326008 MHz

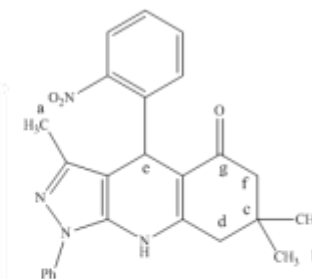
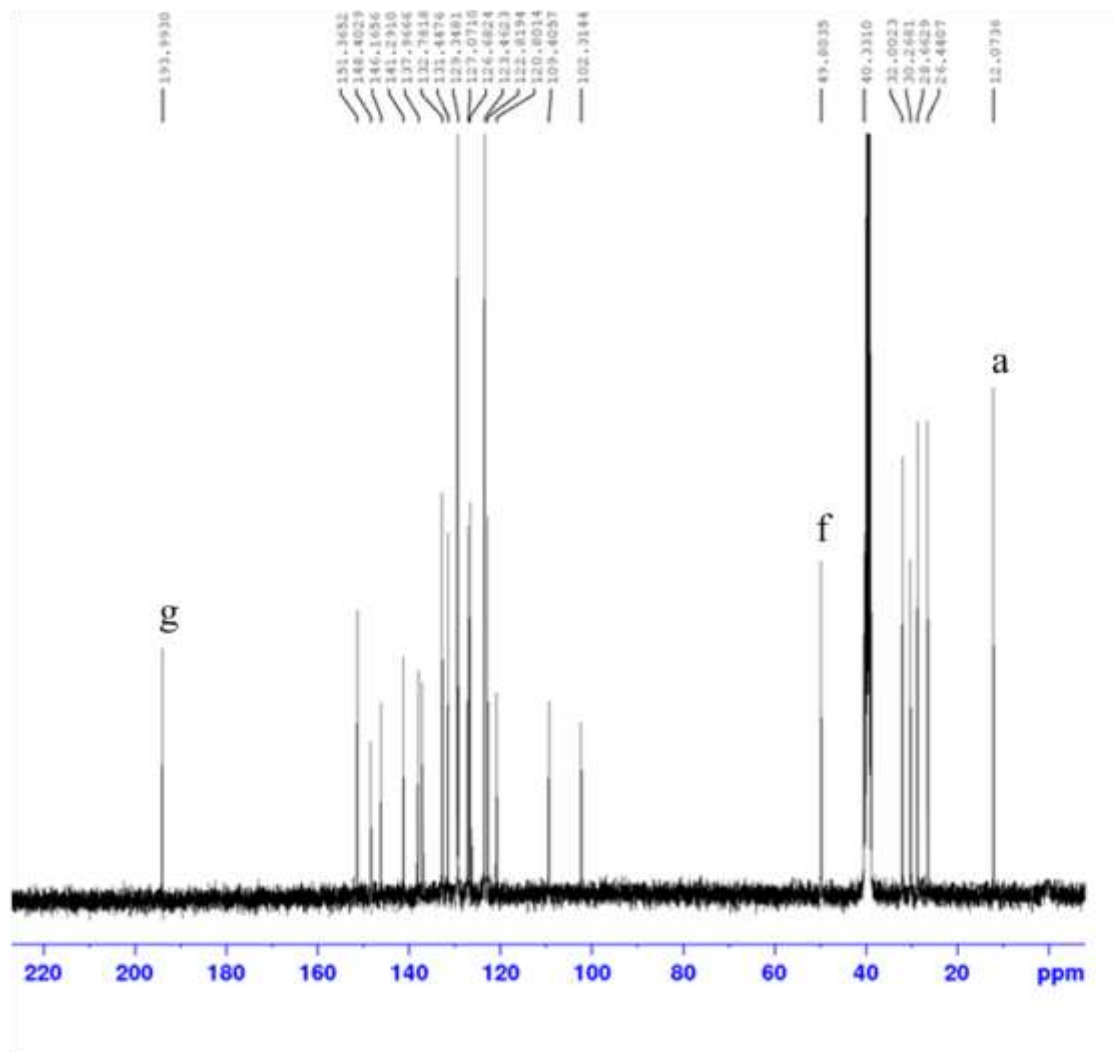
F2 - Processing parameters

SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 GB 0.30 Hz





¹³C NMR Spectrum of compound 4e

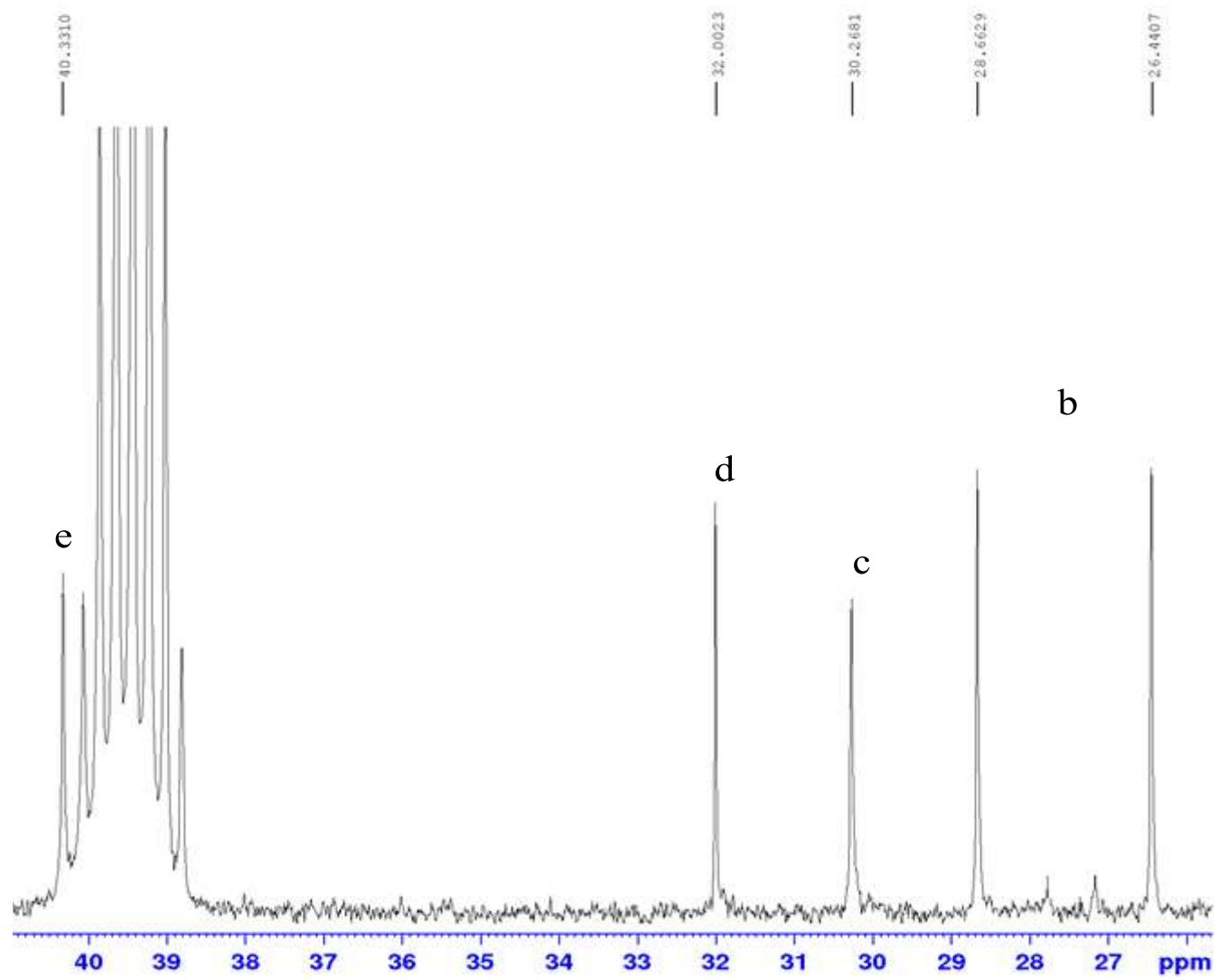


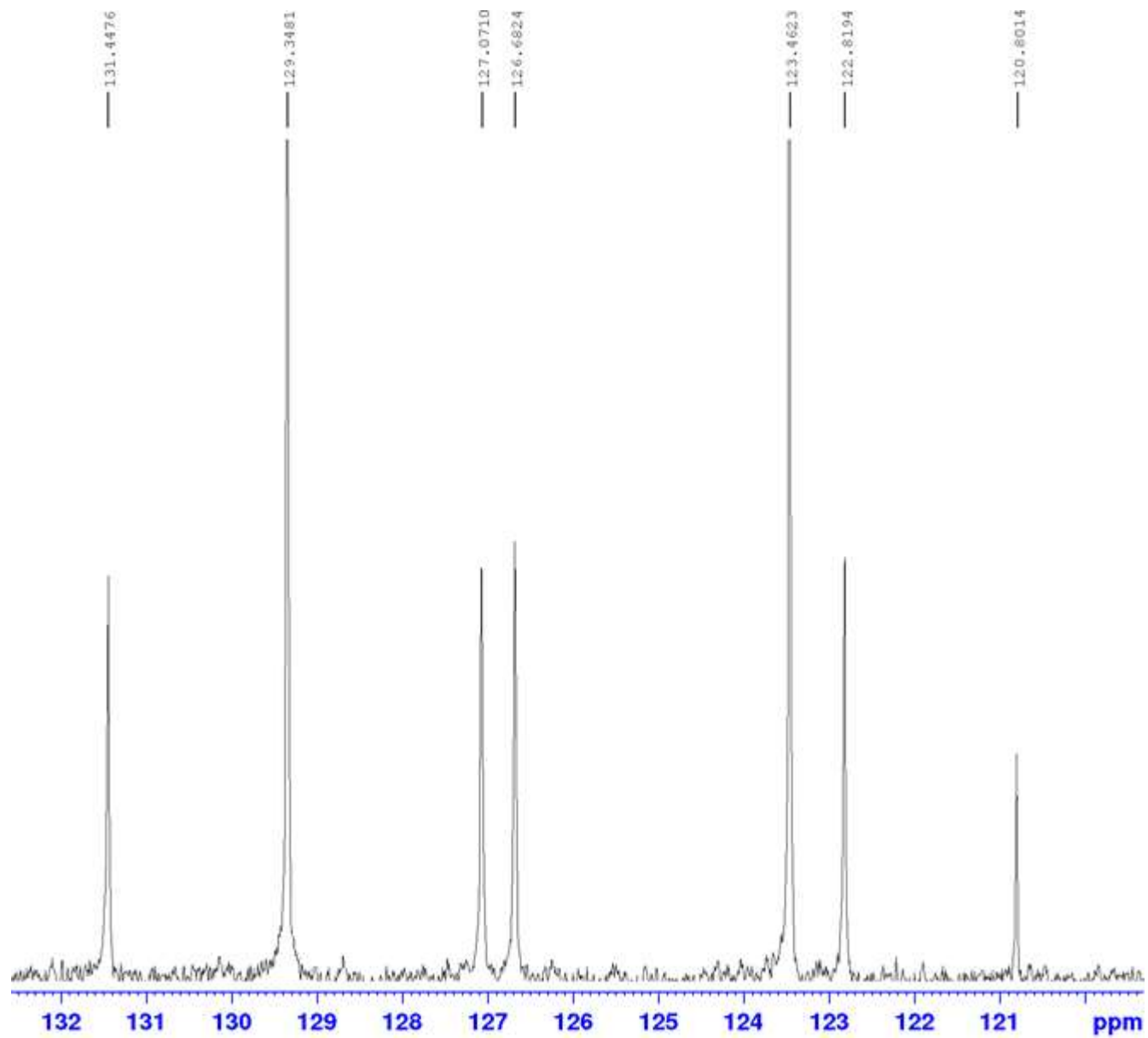
Current Data Parameters
 NAME Ahmadi-Mehdi-IN970830
 EXPNO 11
 PROCNO 1

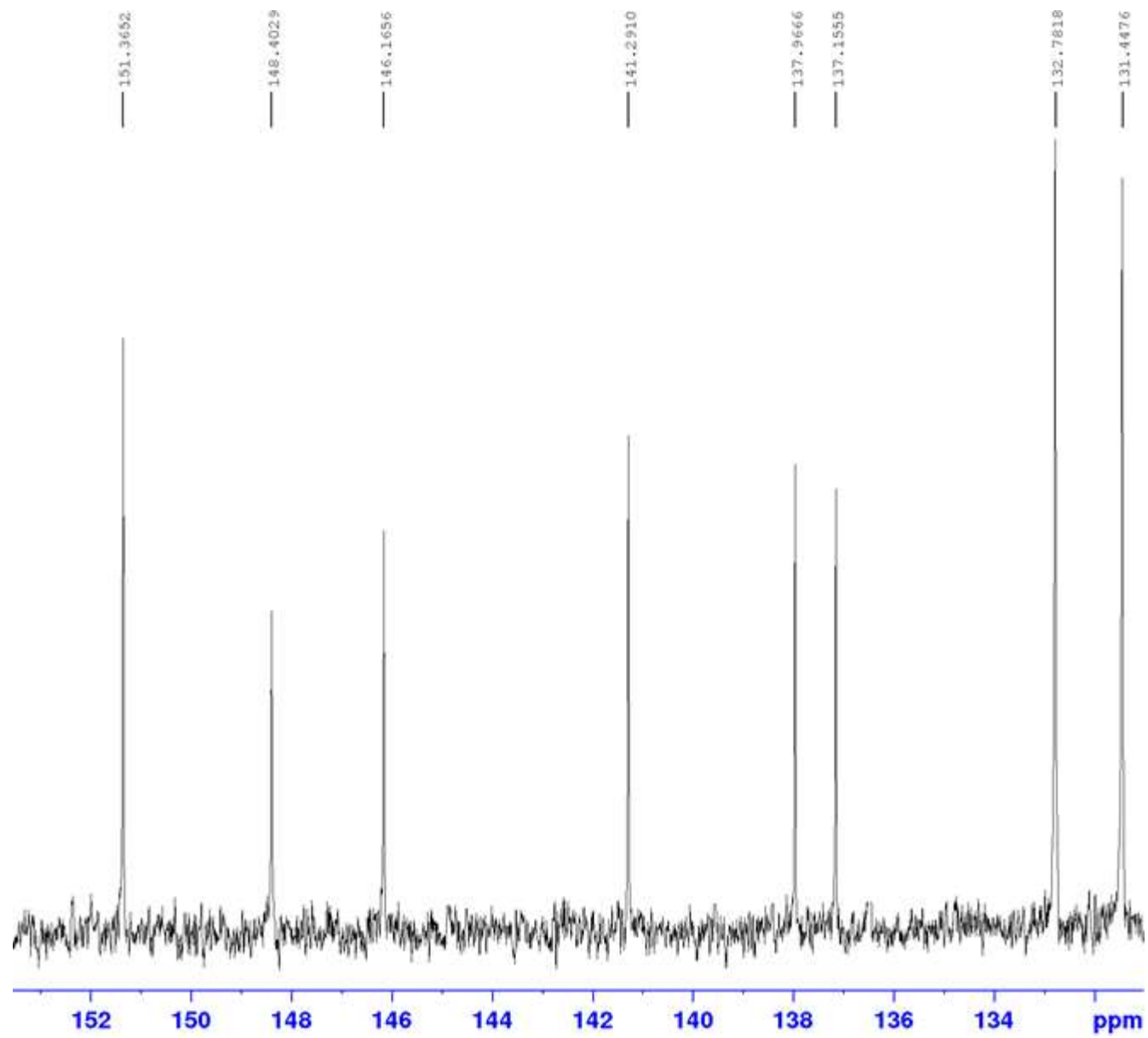
F2 - Acquisition Parameters
 Date_ 20181124
 Time 9.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 50502
 SOLVENT DMSO
 NS 2901
 DS 2
 SWH 25252.525 Hz
 FIDRES 0.500030 Hz
 AQ 0.9999396 sec
 RG 2050
 DW 19.800 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -1.00 dB
 PL1W 42.69075012 W
 SFO1 100.6238364 MHz

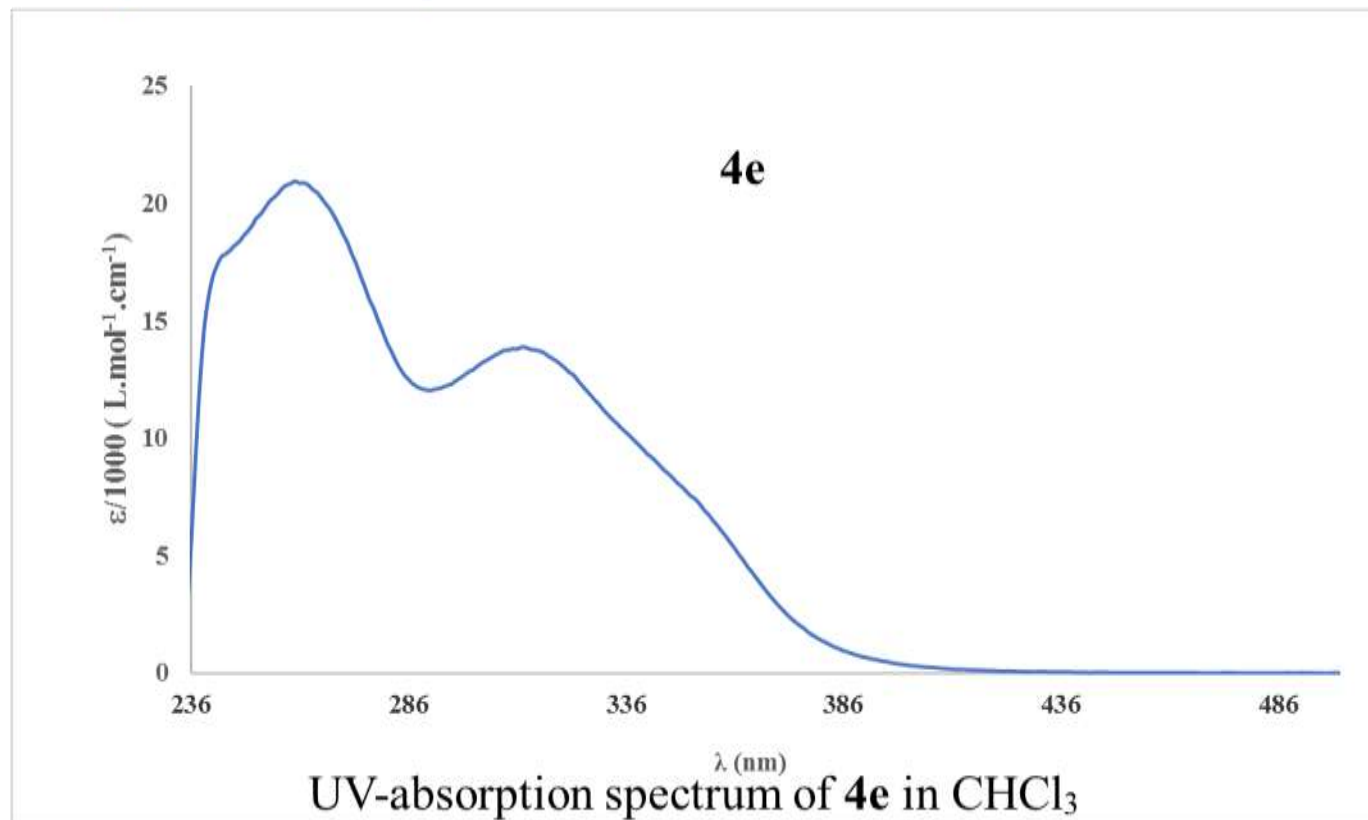
===== CHANNEL f2 =====
 CPDPRG[2] waltz16







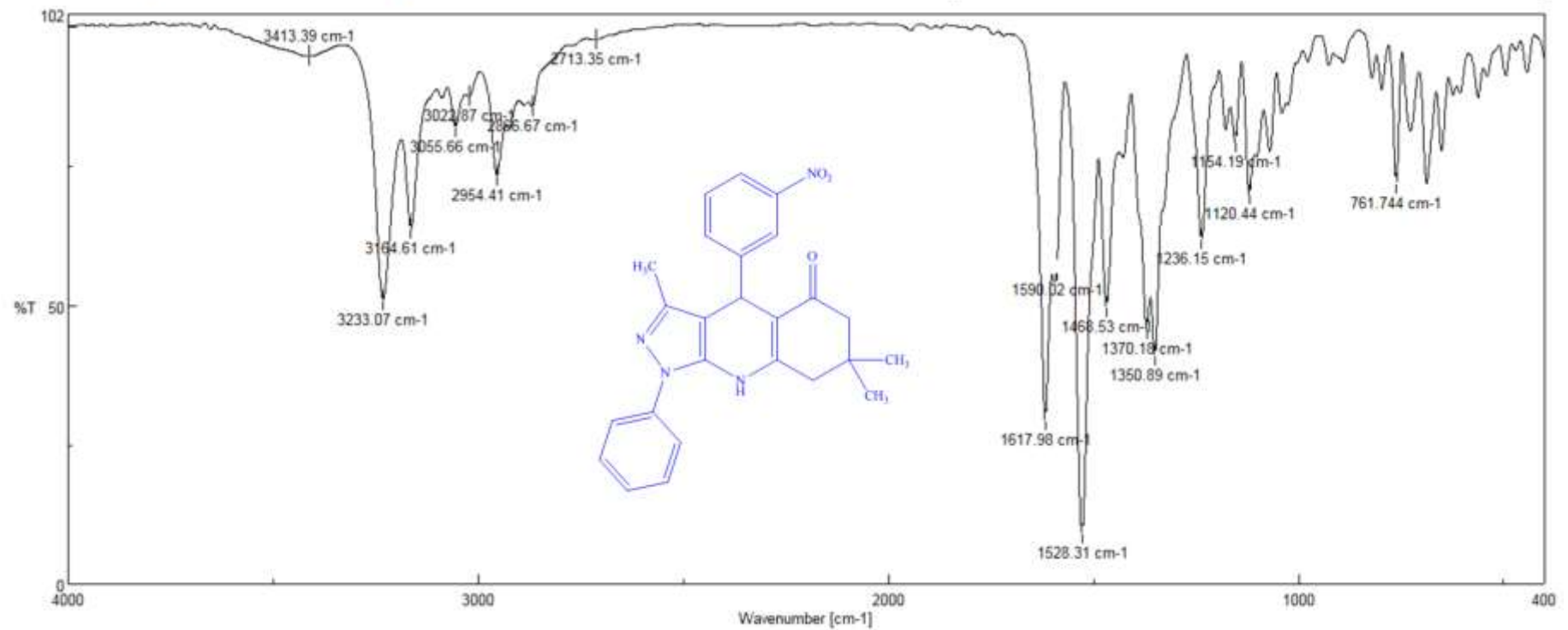
UV-Spectrum of compound **4e**



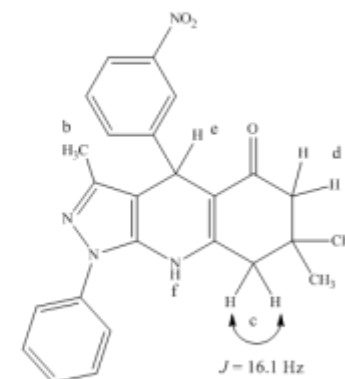
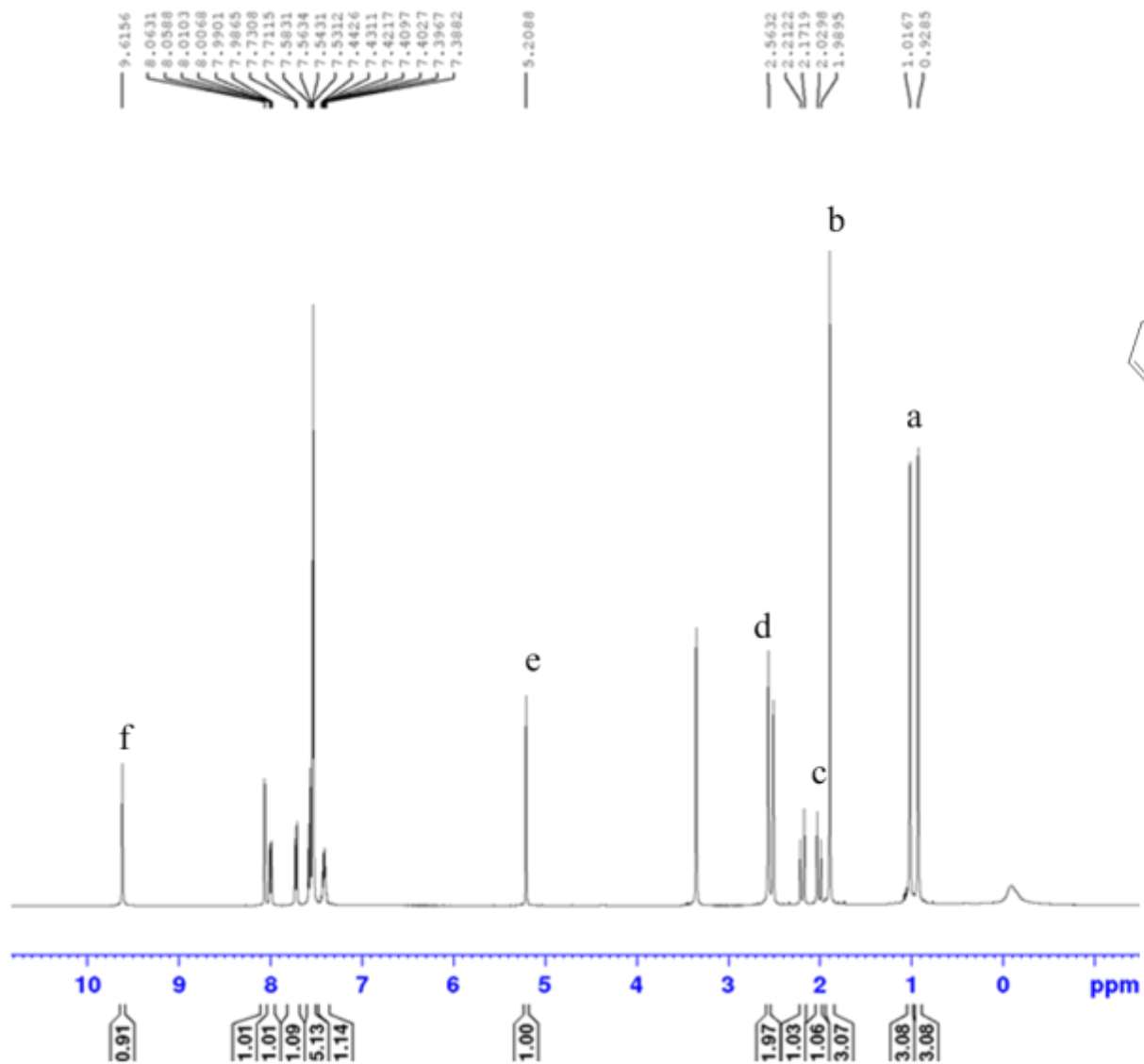
Instrument Specifications

FT Infrared Spectroscopy, JASCO, FT/IR-6300 (400-4000 cm^{-1}), Japan

IR-Spectrum of compound **4f**



¹H NMR Spectrum of compound 4f



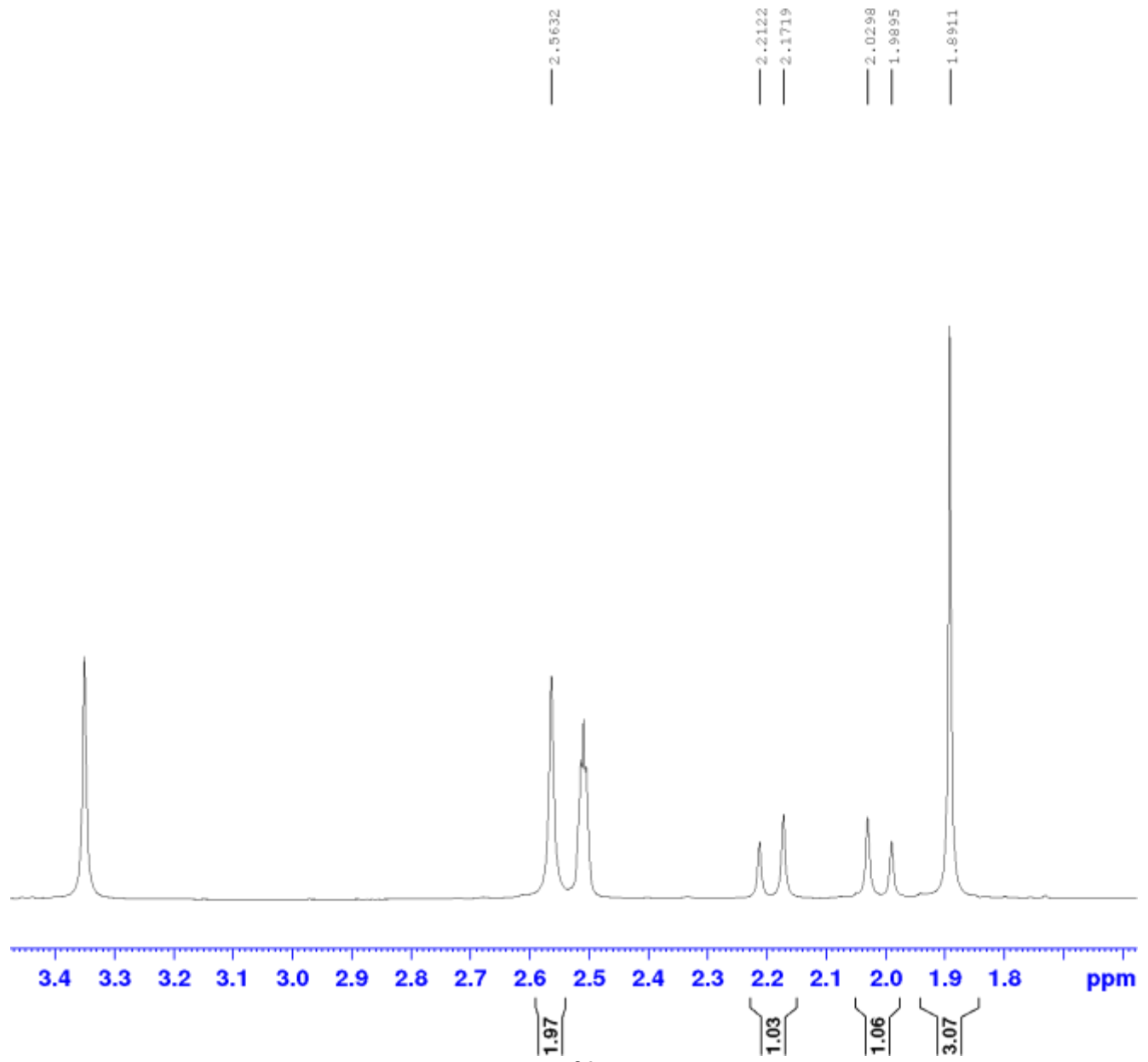
```

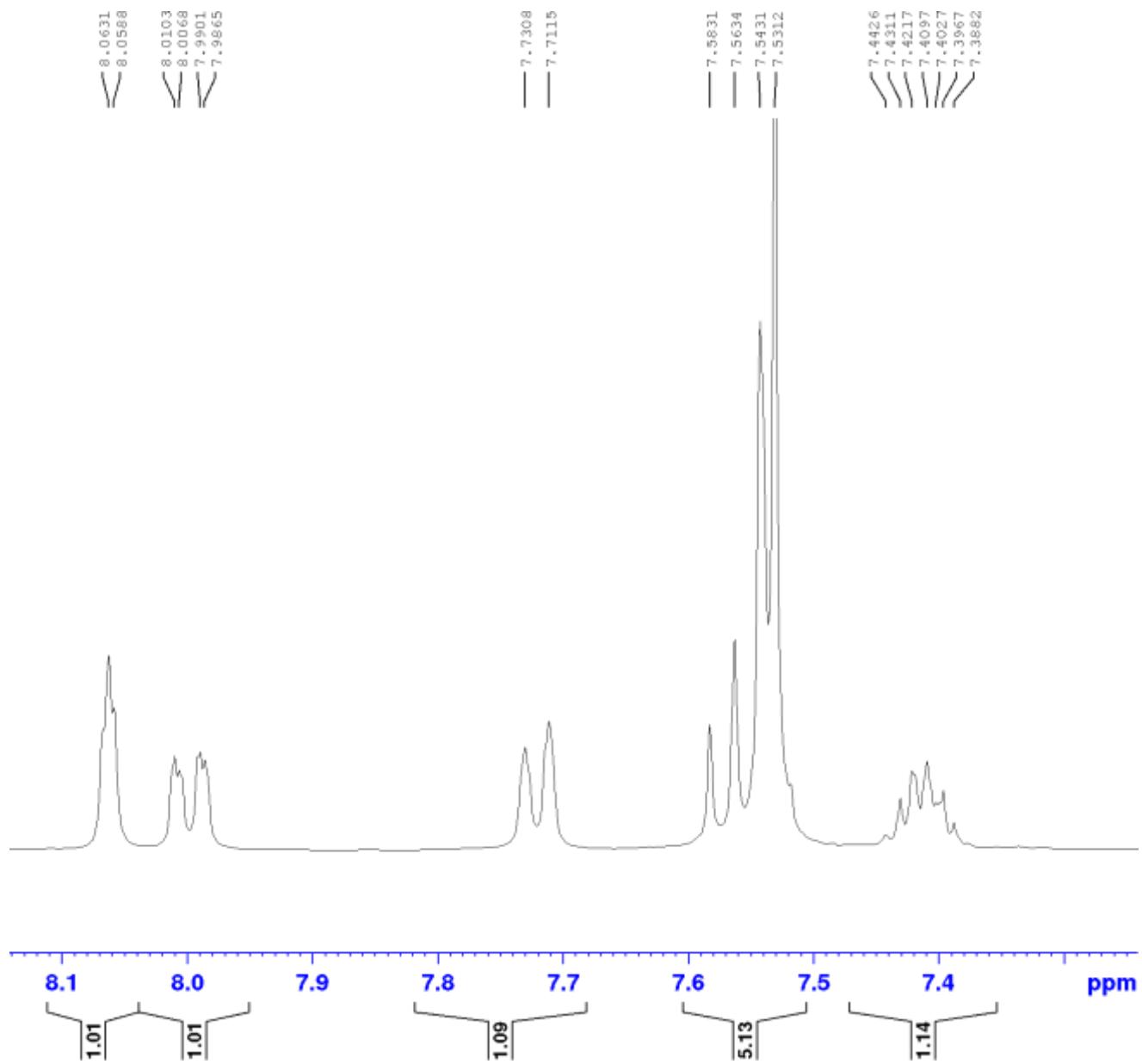
NAME      Ahmadi- Mehdi-IN97082
EXPNO     20
PROCNO    1

F2 - Acquisition Parameters
Date_     20181119
Time      17.34
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg
TD         50504
SOLVENT   DMSO
NS         32
DS         2
SWH        8802.817 Hz
FIDRES     0.174299 Hz
AQ         2.8486273 sec
RG         71.8
DW         56.800 usec
DE         6.50 usec
TE         294.9 K
D1         5.00000000 sec
TD0        1

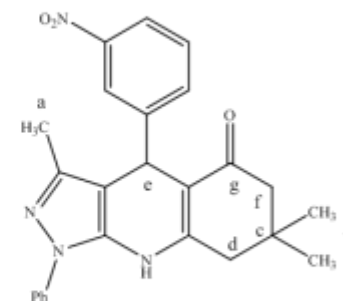
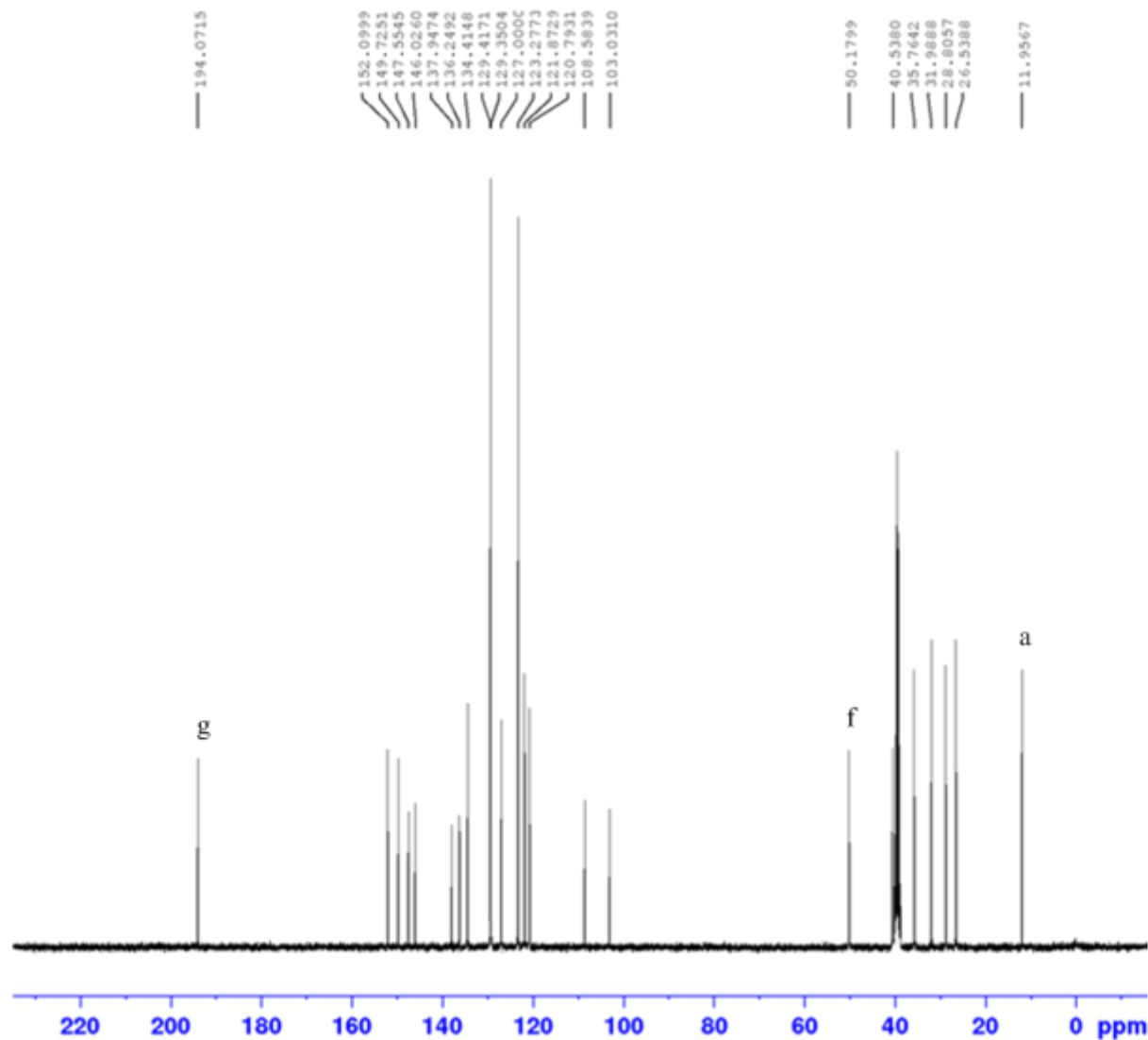
===== CHANNEL f1 =====
NUC1       1H
P1         11.00 usec
PL1        -2.00 dB
PL1W       17.51671600 W
SFO1       400.1326008 MHz

F2 - Processing parameters
SI         32768
SF         400.1300000 MHz
WDW        EM
SSB        0
GB         0.30 Hz
    
```





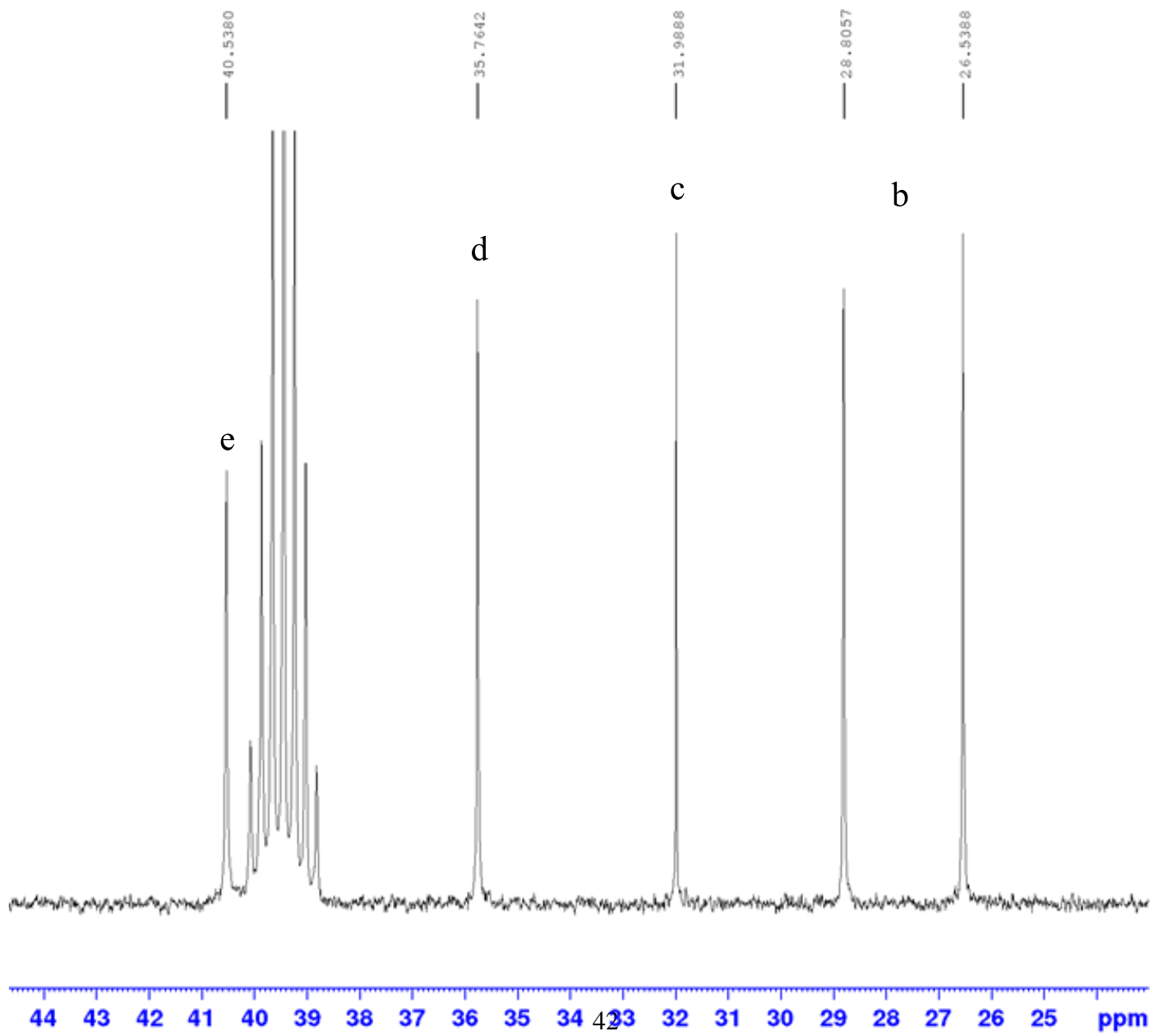
¹³C NMR Spectrum of compound 4f

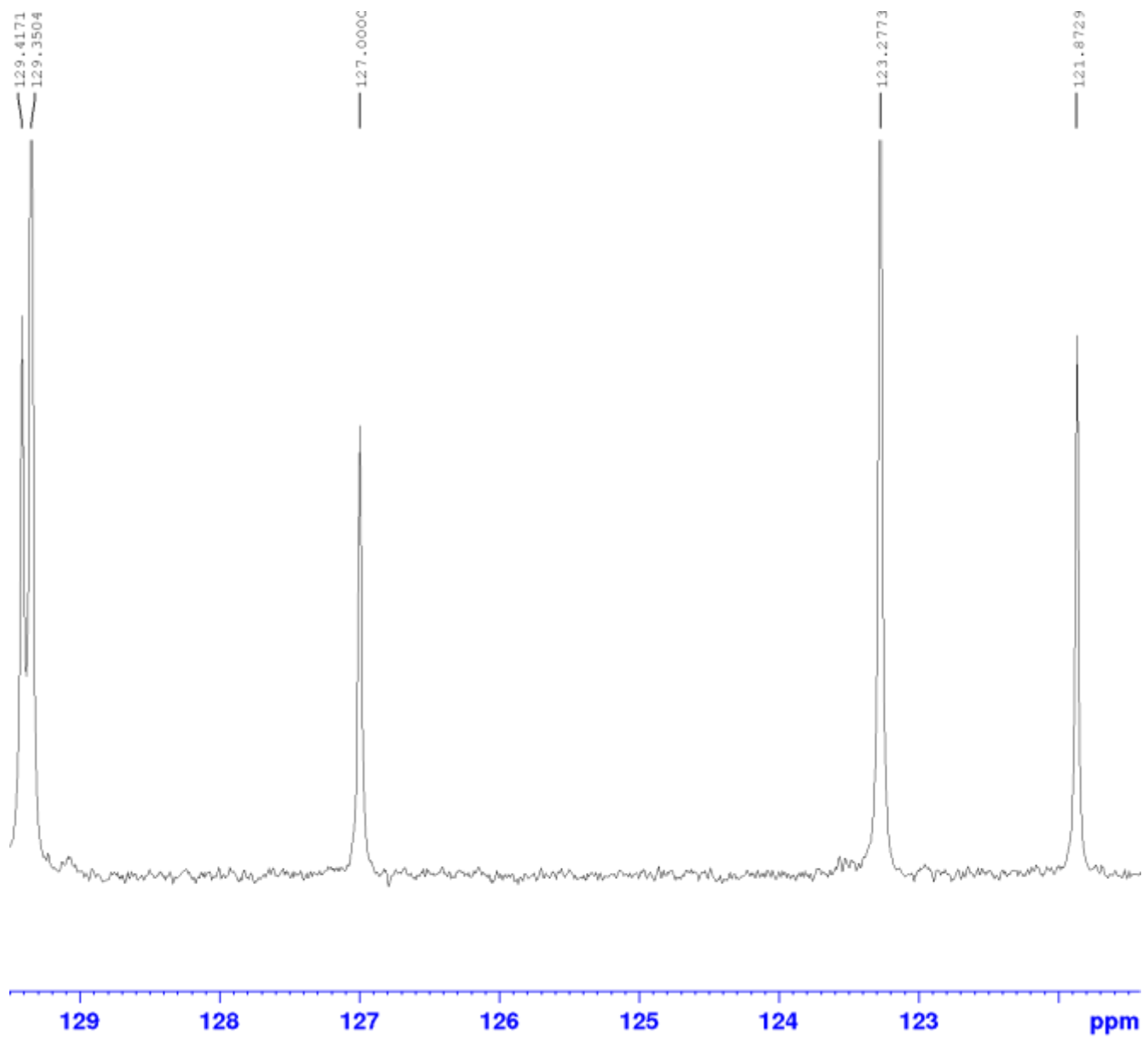


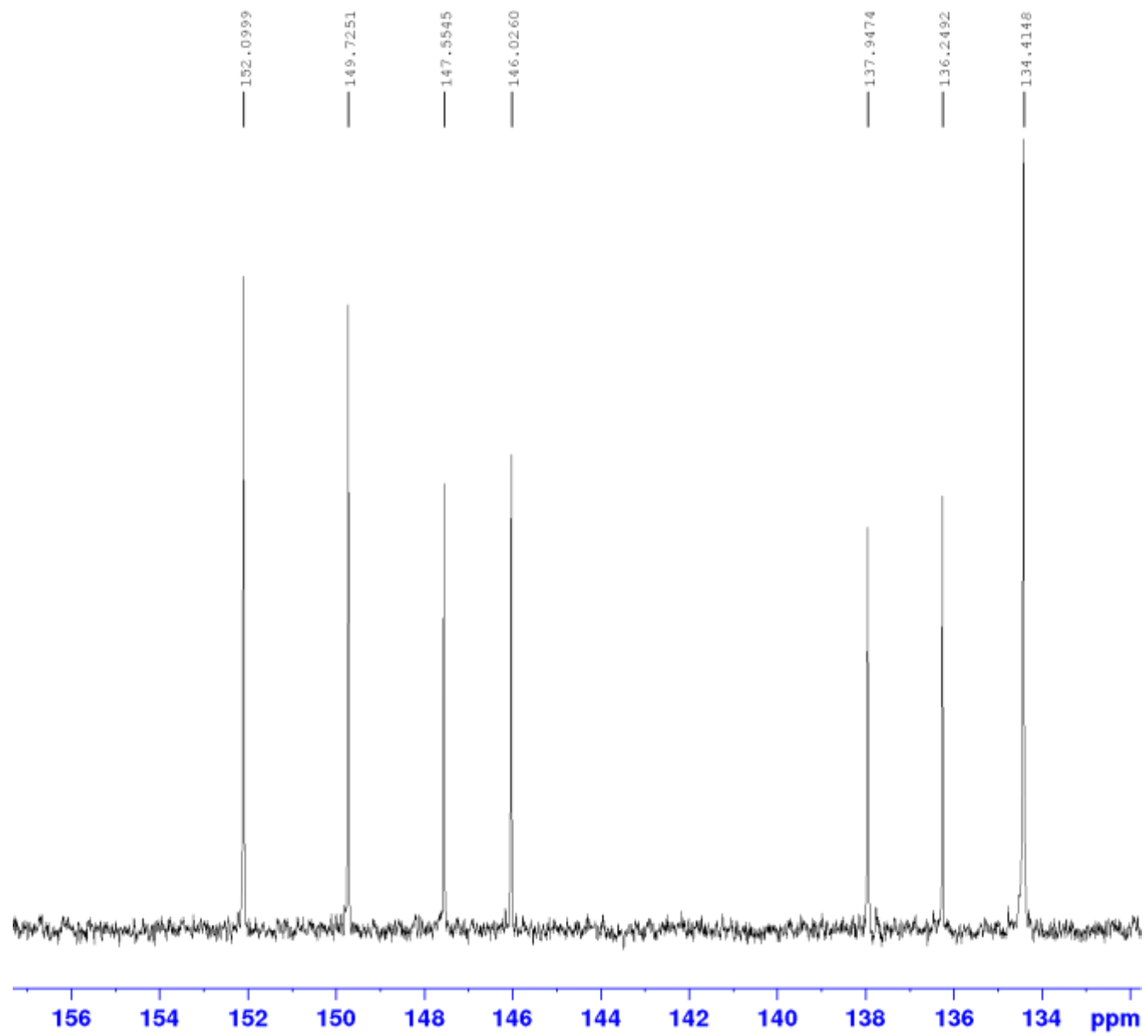
Current Data Parameters
 NAME cnmr 136
 EXPNO 21
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20181124
 Time 10.15
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 50502
 SOLVENT DMSO
 NS 1112
 DS 2
 SWH 25252.525 Hz
 FIDRES 0.500030 Hz
 AQ 0.9999396 sec
 RG 2050
 DW 19.800 usec
 DE 6.50 usec
 TE 294.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TD0 1

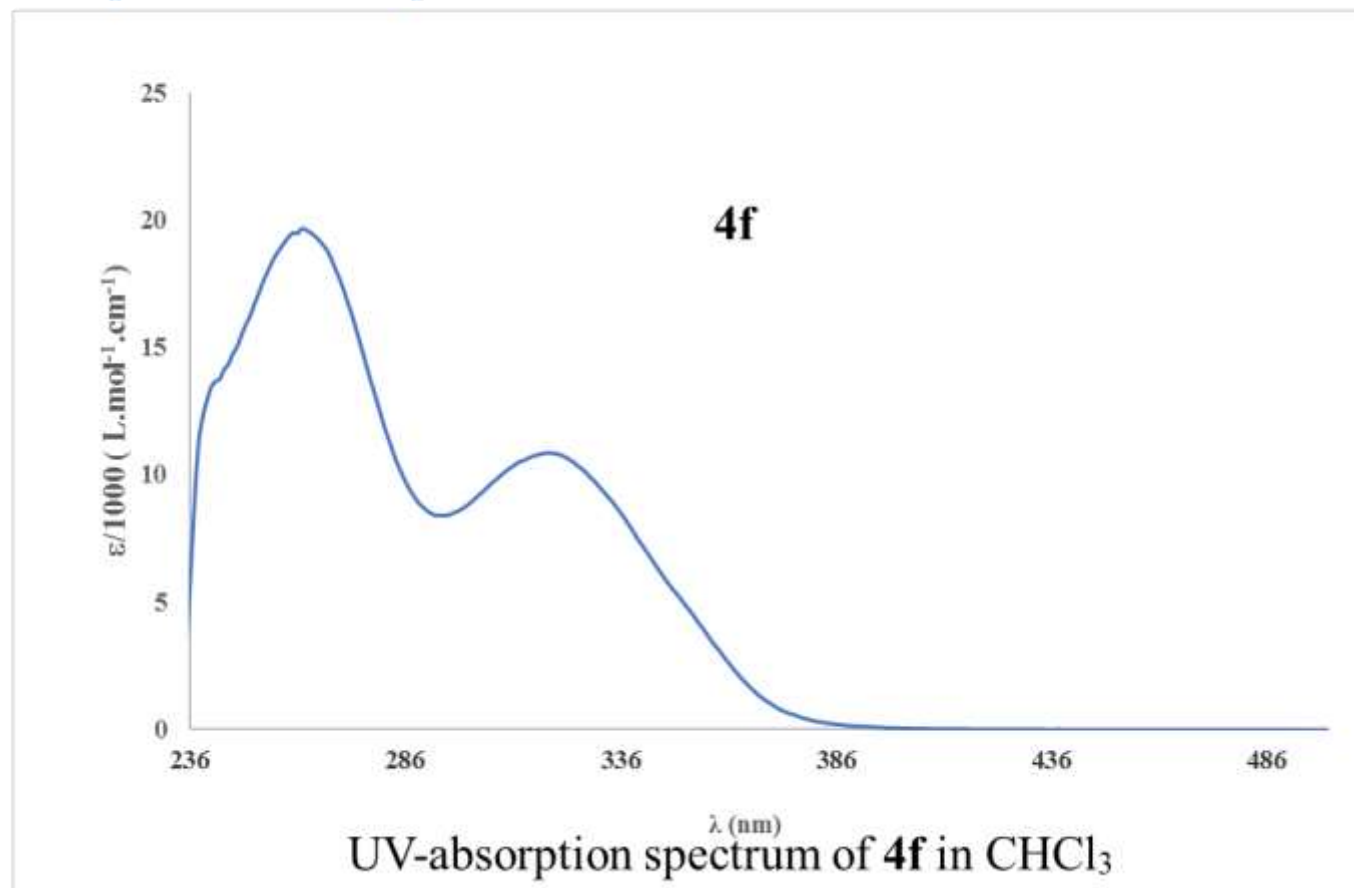
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -1.00 dB
 PL1W 42.69075012 W
 SFO1 100.6238364 MHz



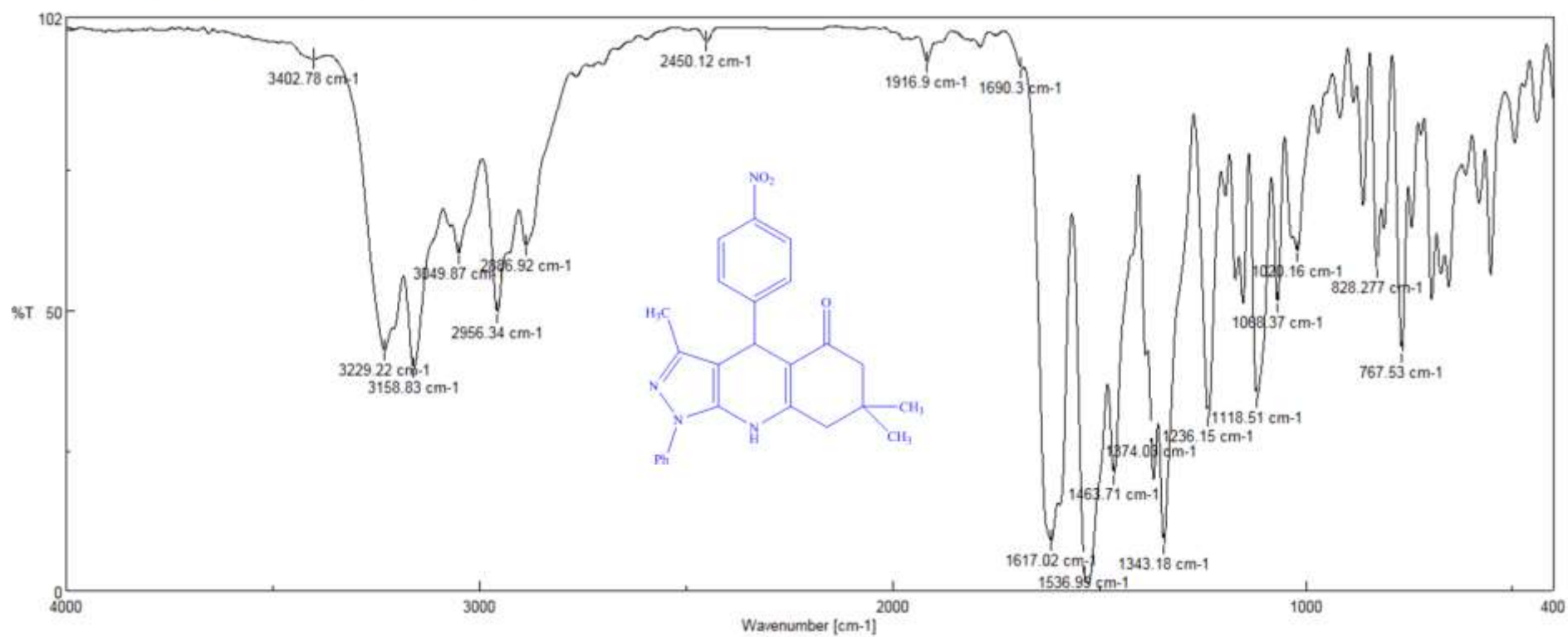




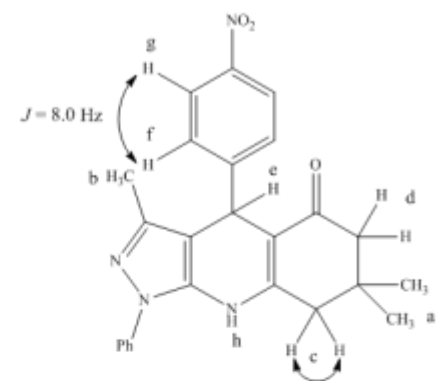
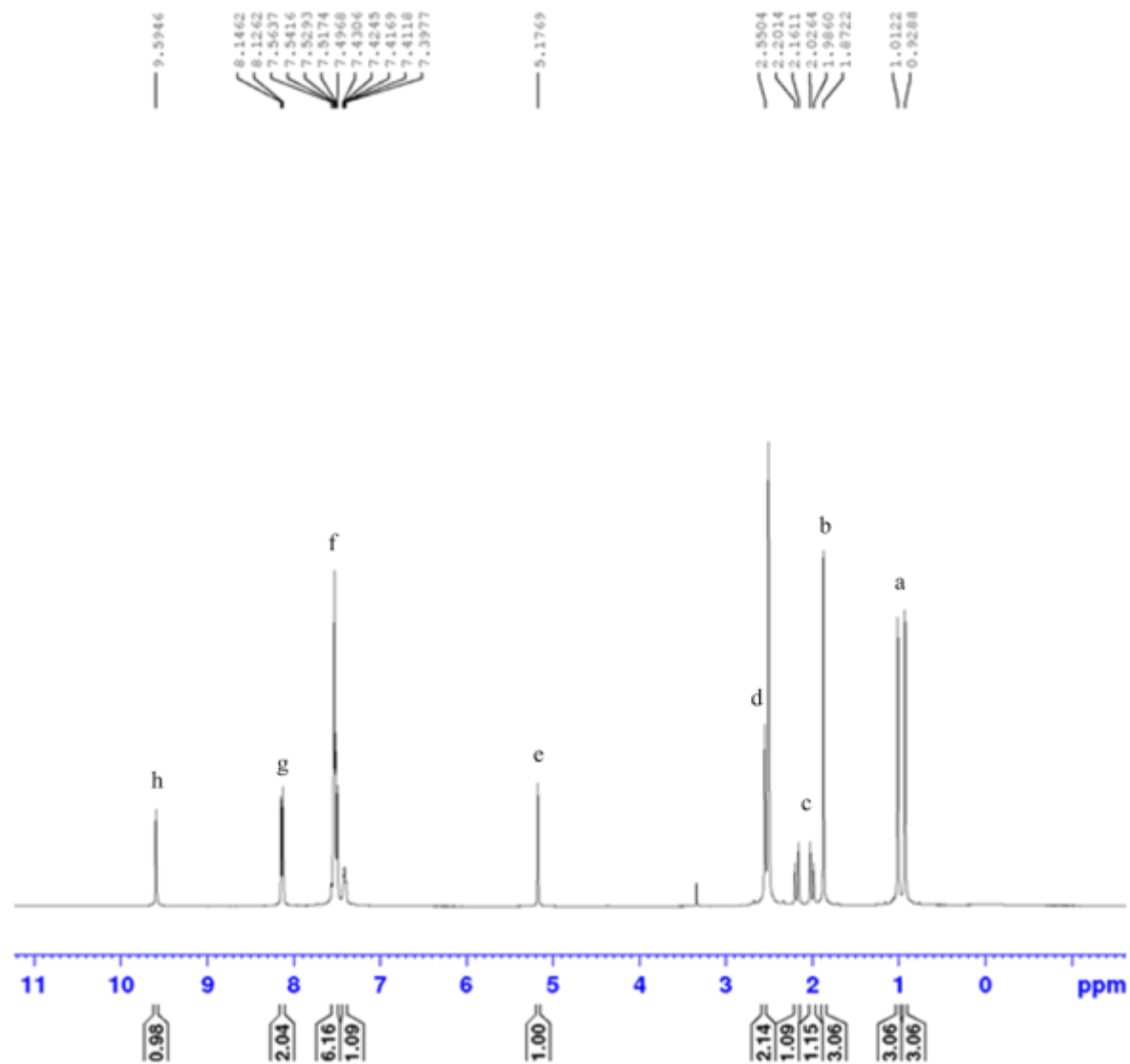
UV-Spectrum of compound **4f**



IR-Spectrum of compound 4g



¹H NMR Spectrum of compound 4g



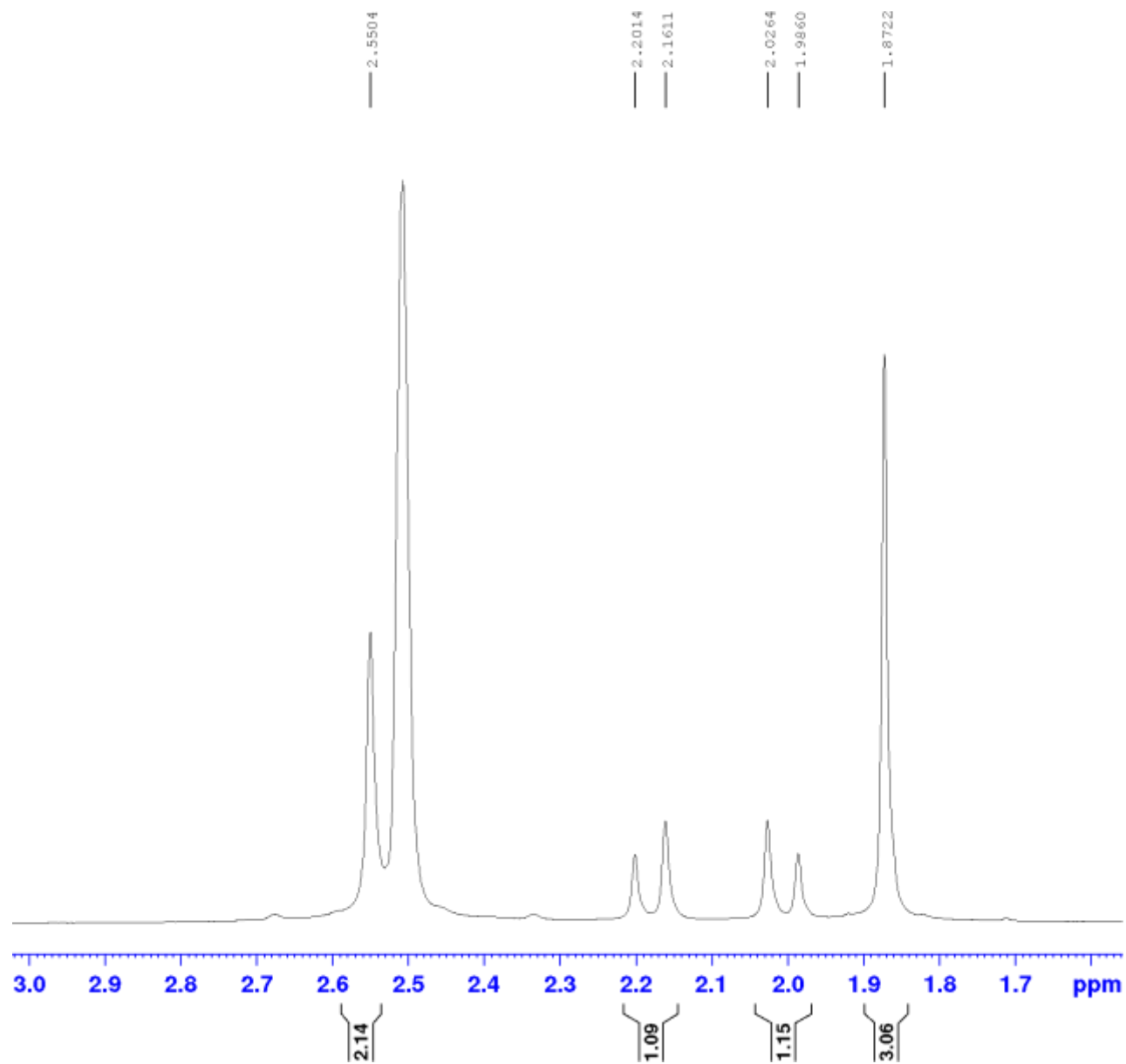
$J = 16.1 \text{ Hz}$

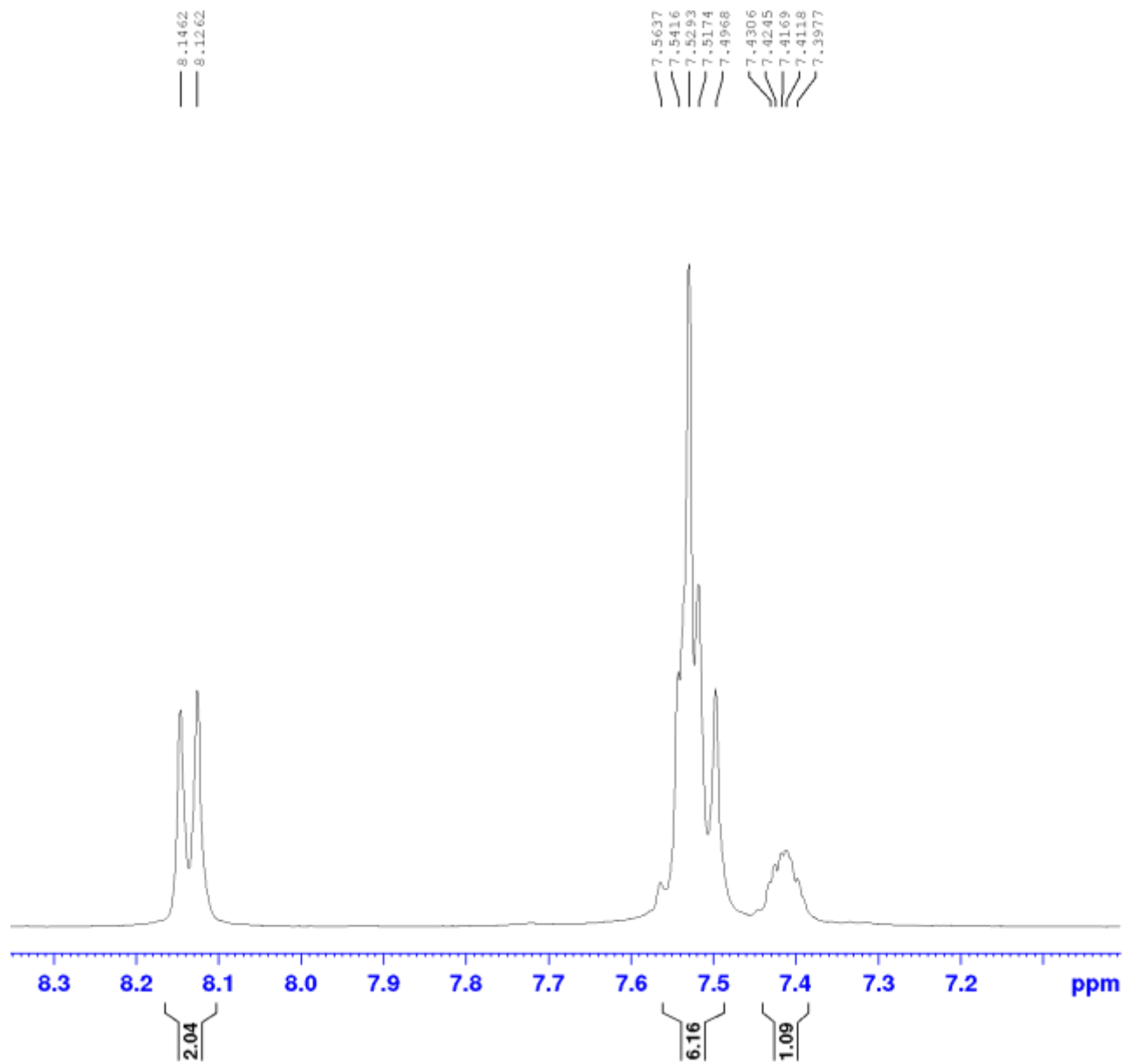
Current Data Parameters
 NAME Ahmadi- Mehdi-IN97012
 EXPNO 20
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180421
 Time 14.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg
 TD 50504
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8417.509 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999375 sec
 RG 71.8
 DW 59.400 usec
 DE 6.50 usec
 TE 295.8 K
 D1 5.0000000 sec
 TD0 1

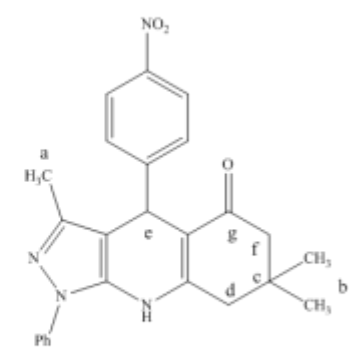
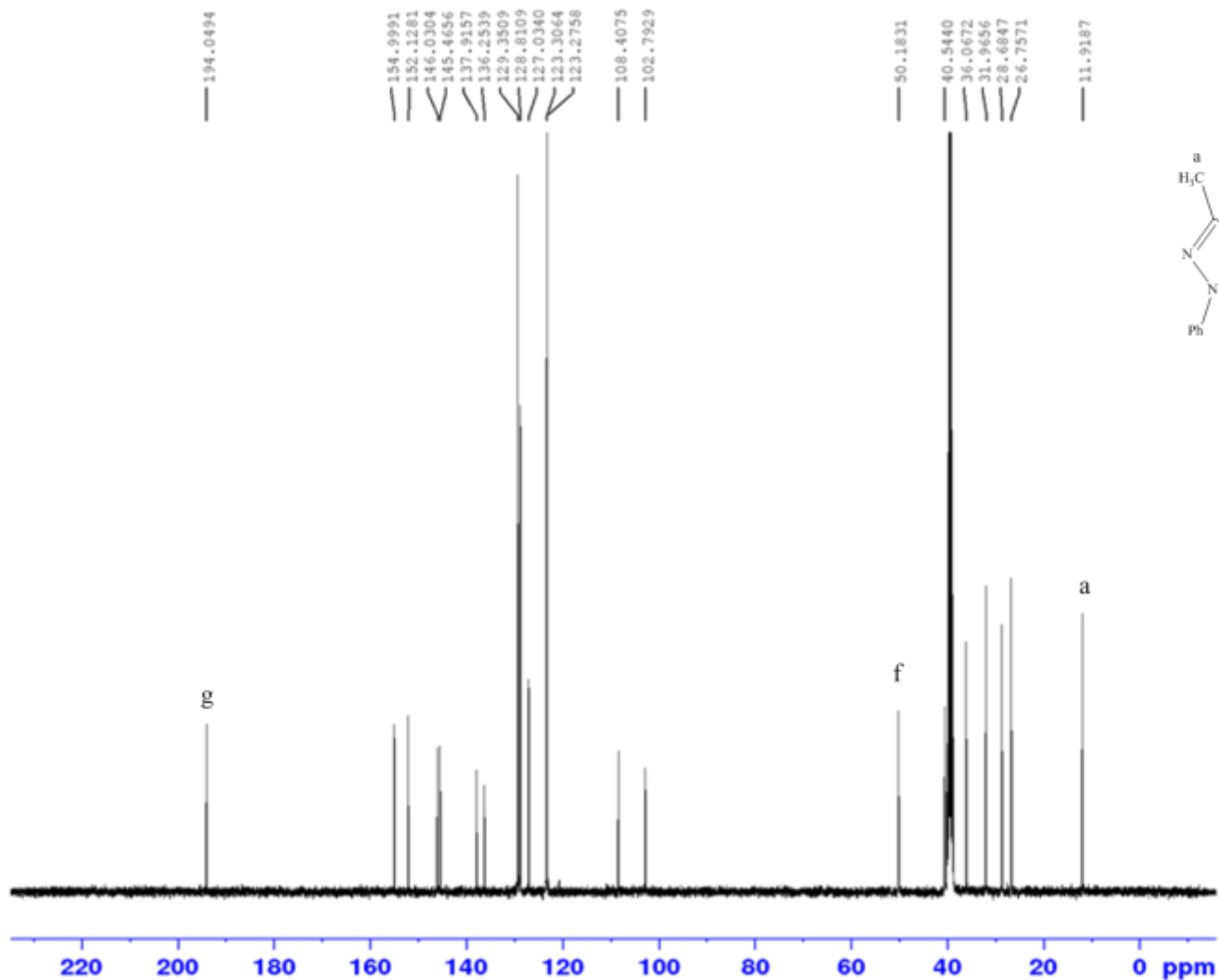
===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 -2.00 dB
 PL1W 17.51671600 W
 SFO1 400.1326008 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0





¹³C NMR Spectrum of compound 4g



```

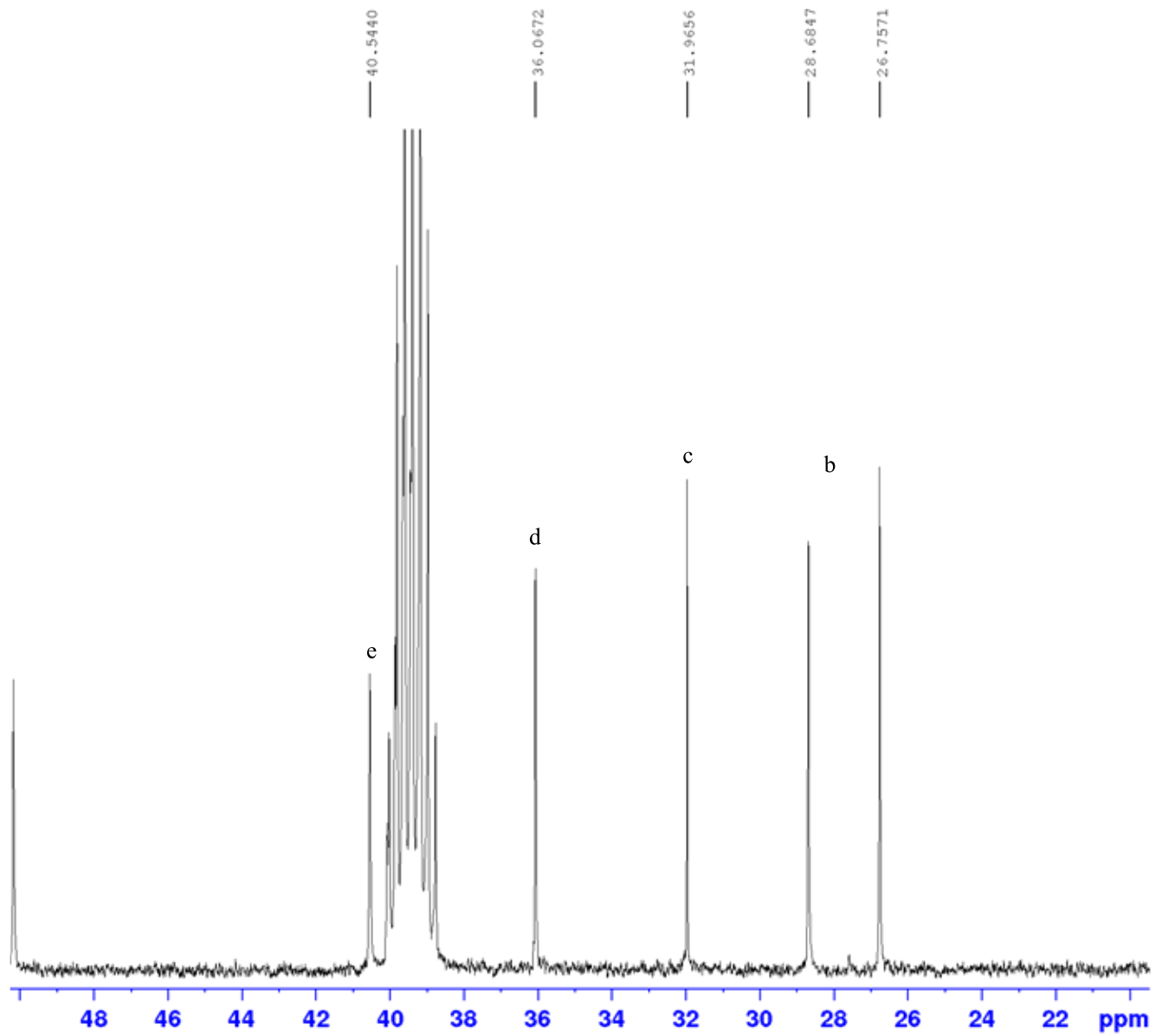
Current Data Parameters
NAME      Ahmadi- Mehdi-1M9702C
EXPNO    10
PROCNO   1

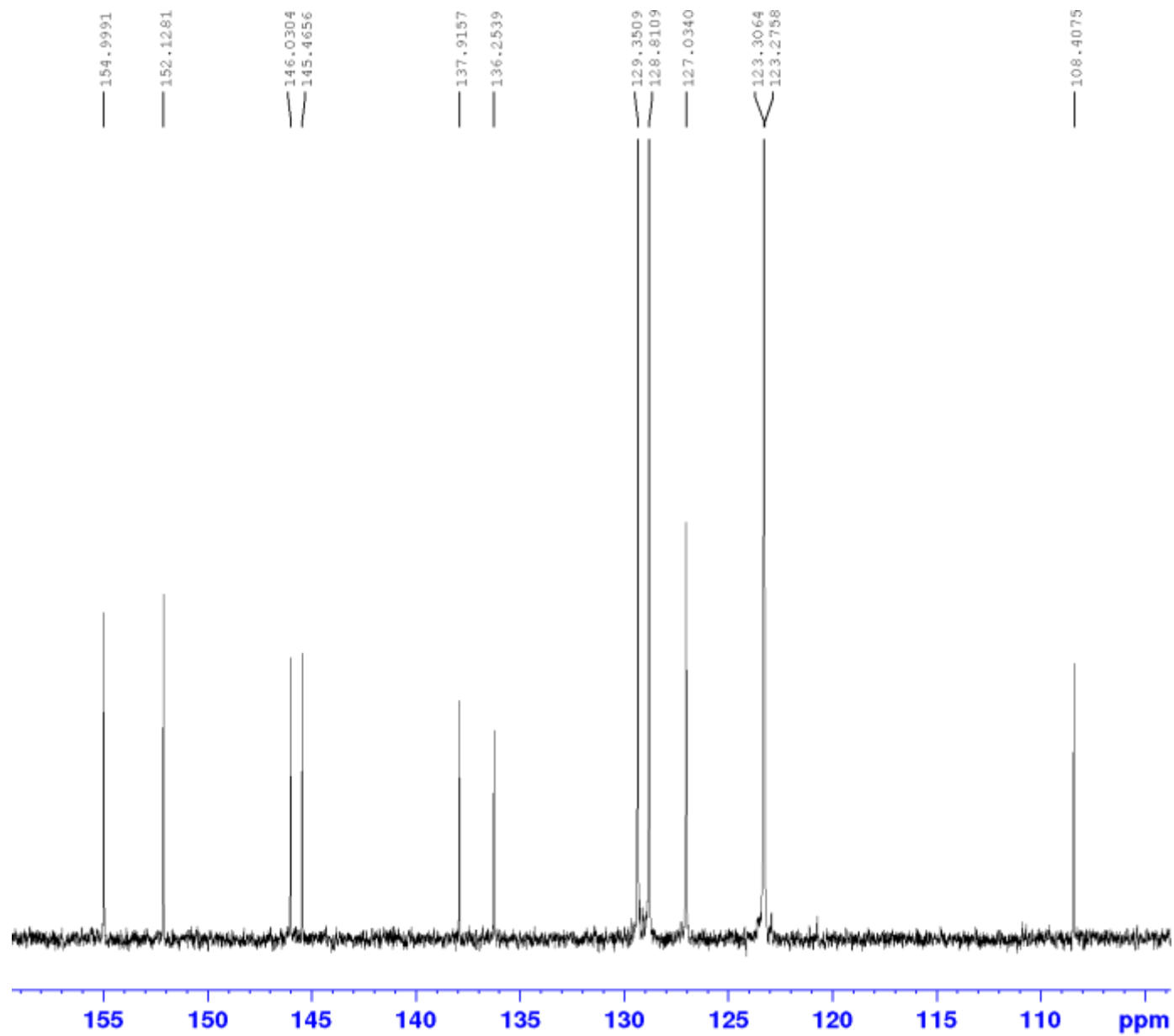
F2 - Acquisition Parameters
Date_    20180430
Time     2.36
INSTRUM  spect
PROBHD   5 mm F400 MR-
PULPROG  zgpg
TD        50502
SOLVENT  DMSO
NS        3000
DS        2
SWH       25252.525 Hz
FIDRES    0.500030 Hz
AQ        0.9999396 sec
RG         1030
DW        19.800 usec
DE         6.50 usec
TE        293.7 K
D1         1.00000000 sec
D11        0.93000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1      13C
P1        8.70 usec
PL1       -1.00 dB
PL1W      42.69075012 W
SFO1      100.6238364 MHz

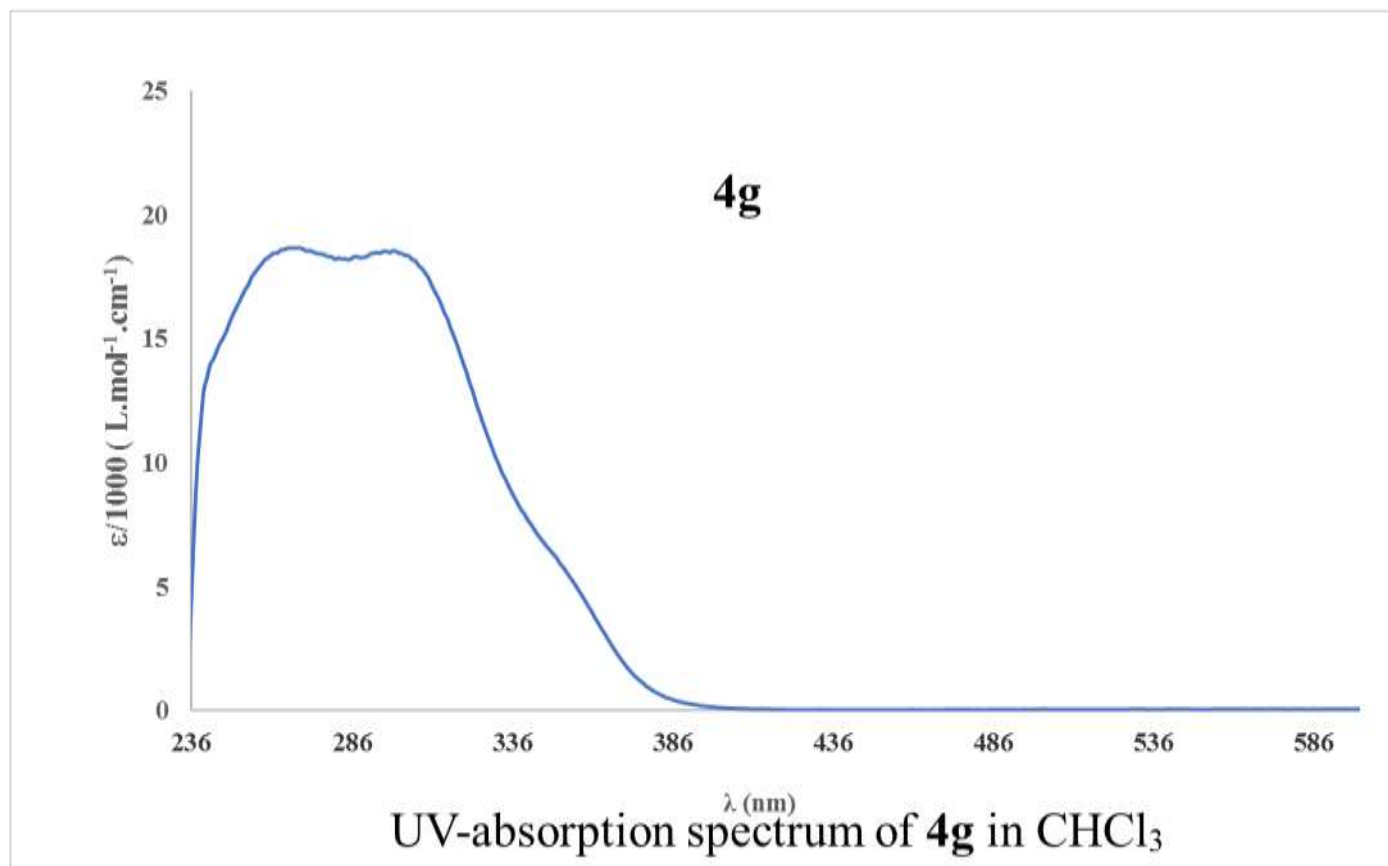
===== CHANNEL f2 =====
PCPD2[2]  waltz14
NUC2      1H
PCPD2     80.00 usec
PL2        0 dB
PL12       15.26 dB
PL13       18.26 dB
PL2W      11.05230045 W
PL12W     0.32919458 W
PL13W     0.14498812 W
SFO2      400.1316005 MHz

F2 - Processing parameters
SI         32768
SF        100.6128193 MHz
WDW        EM
SFB        0
LB         1.00 Hz
GB         0
  
```

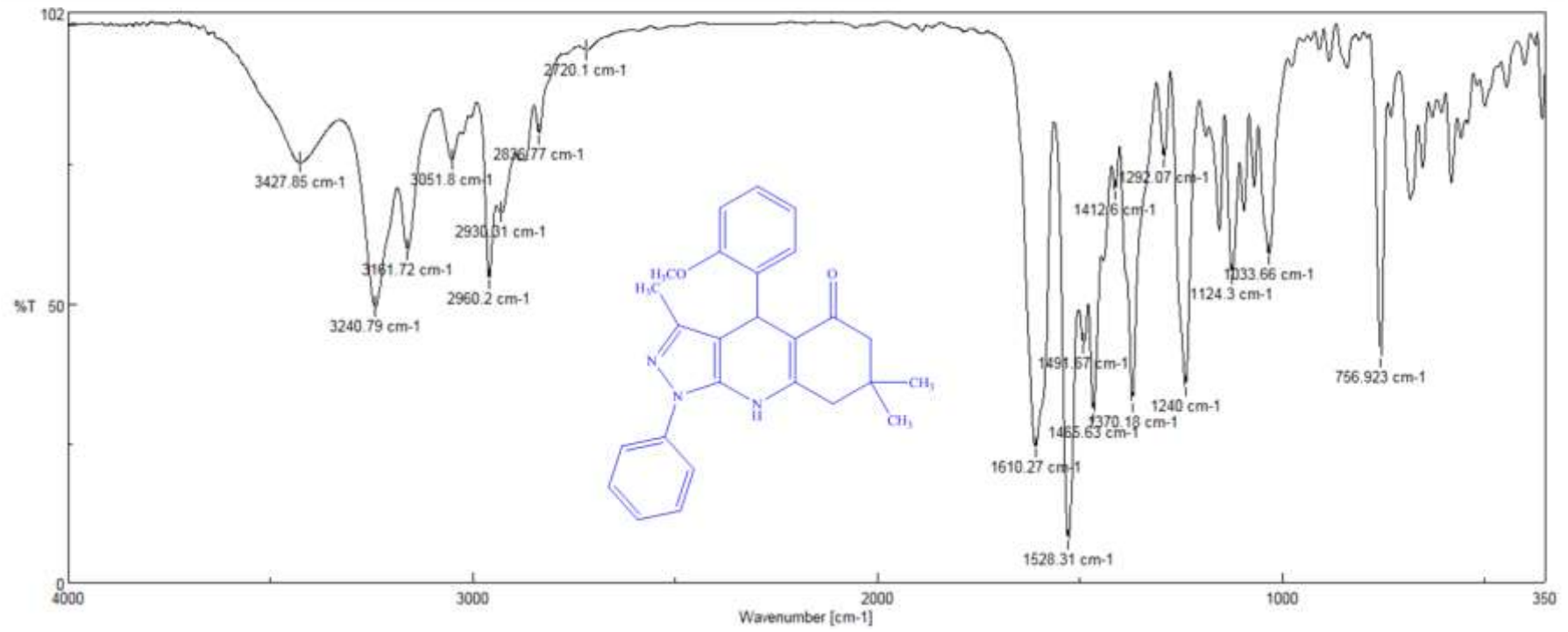




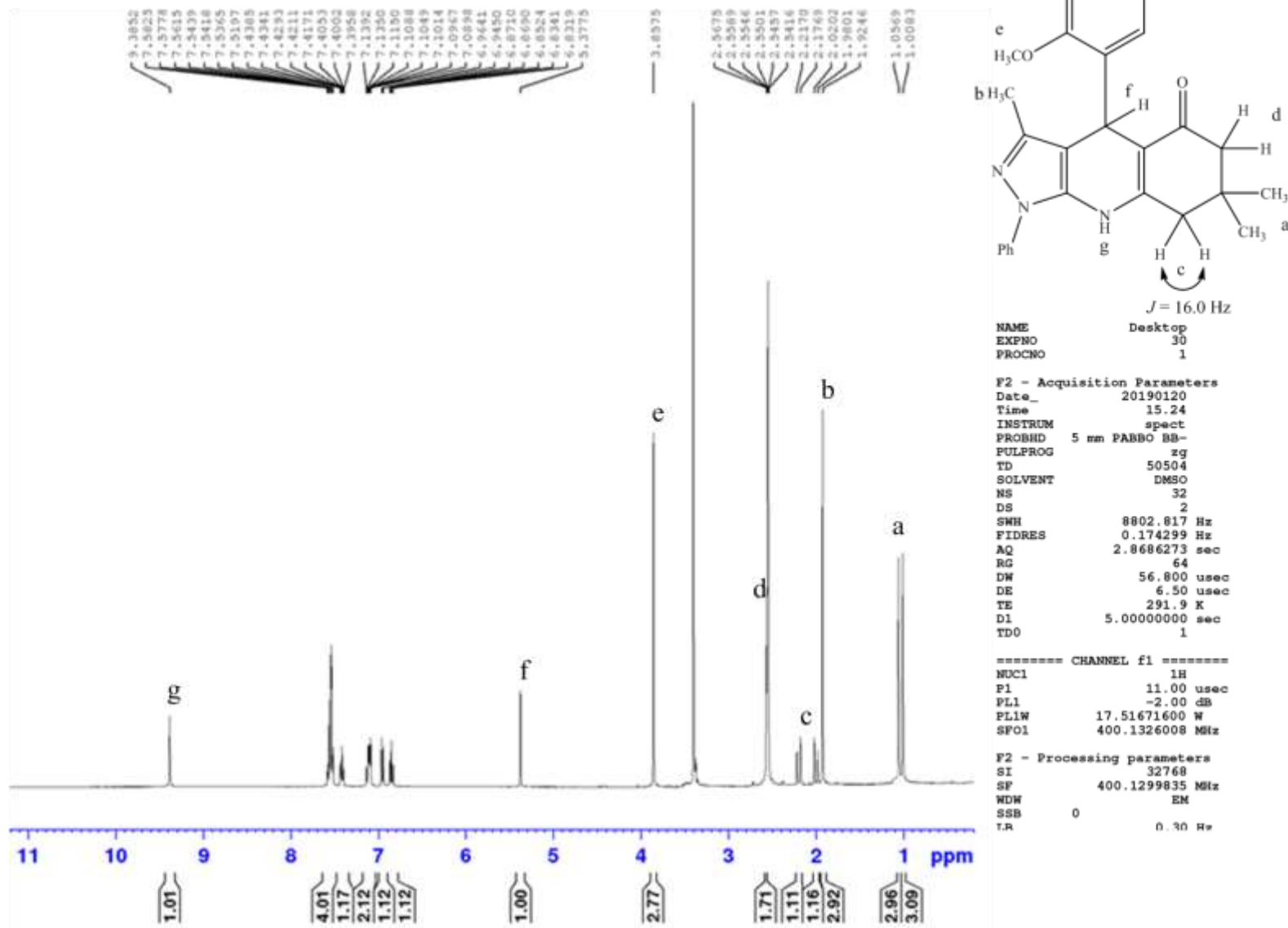
UV-Spectrum of compound **4g**

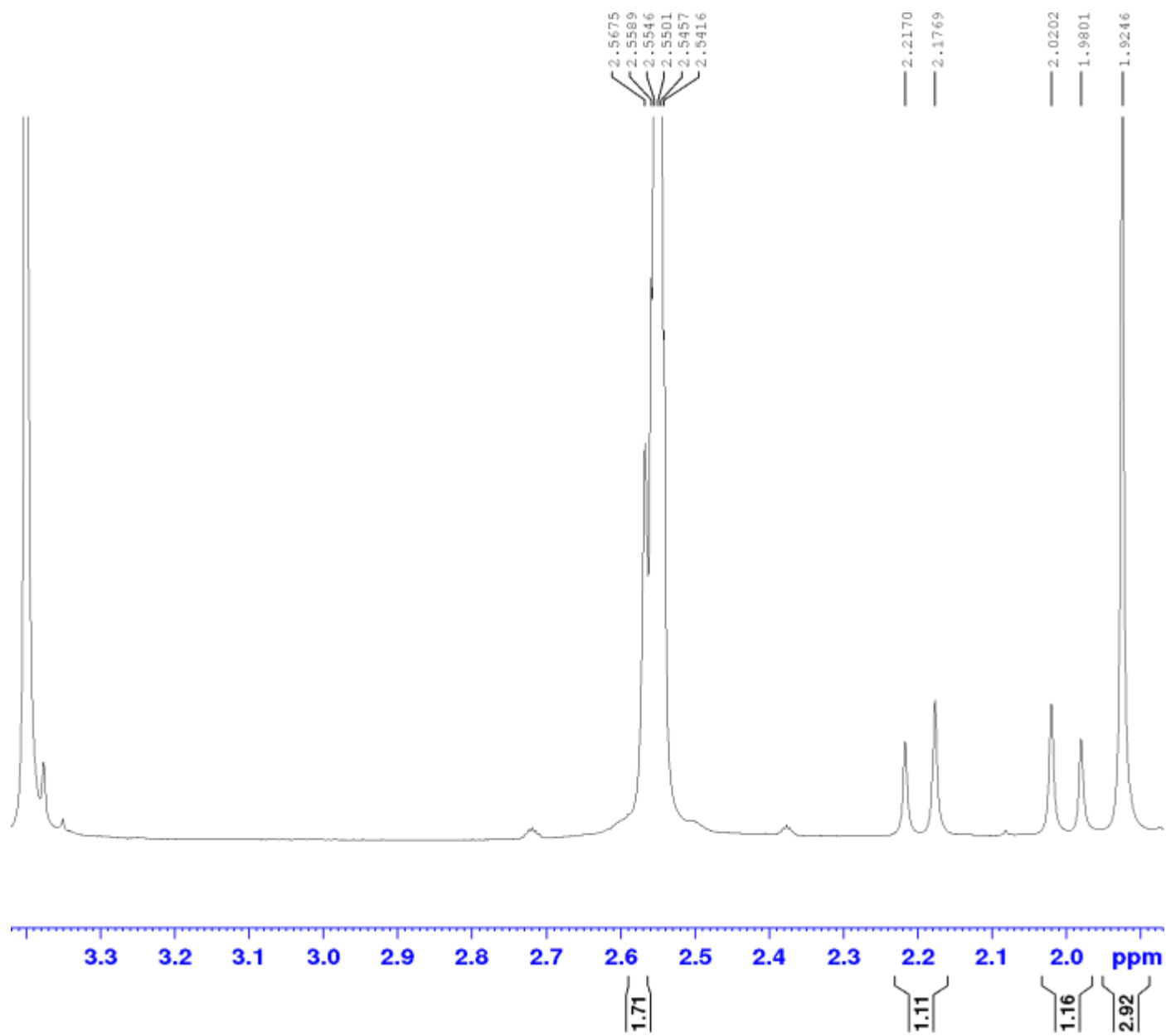


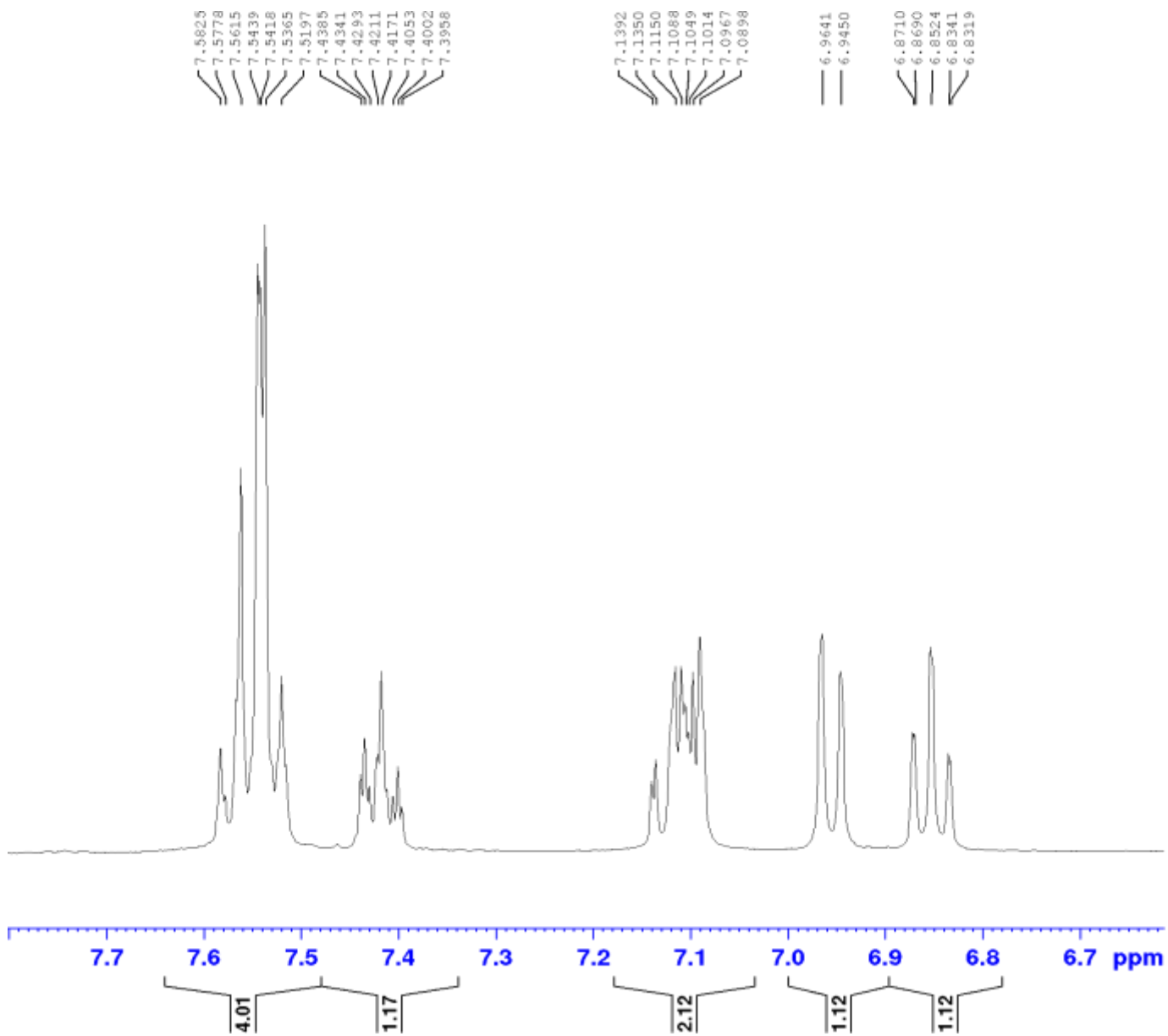
IR-Spectrum of compound 4h



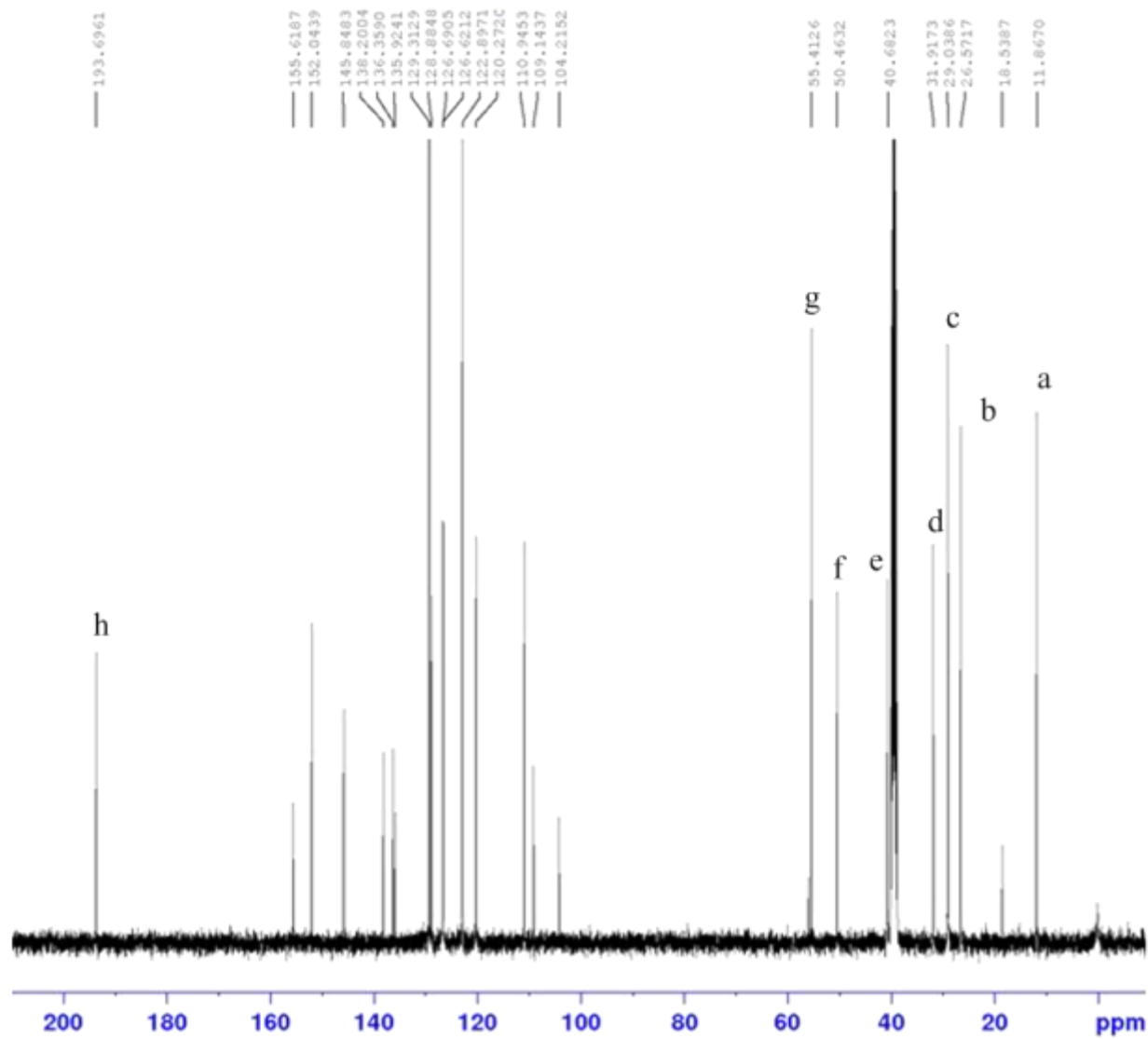
¹H NMR Spectrum of compound 4h







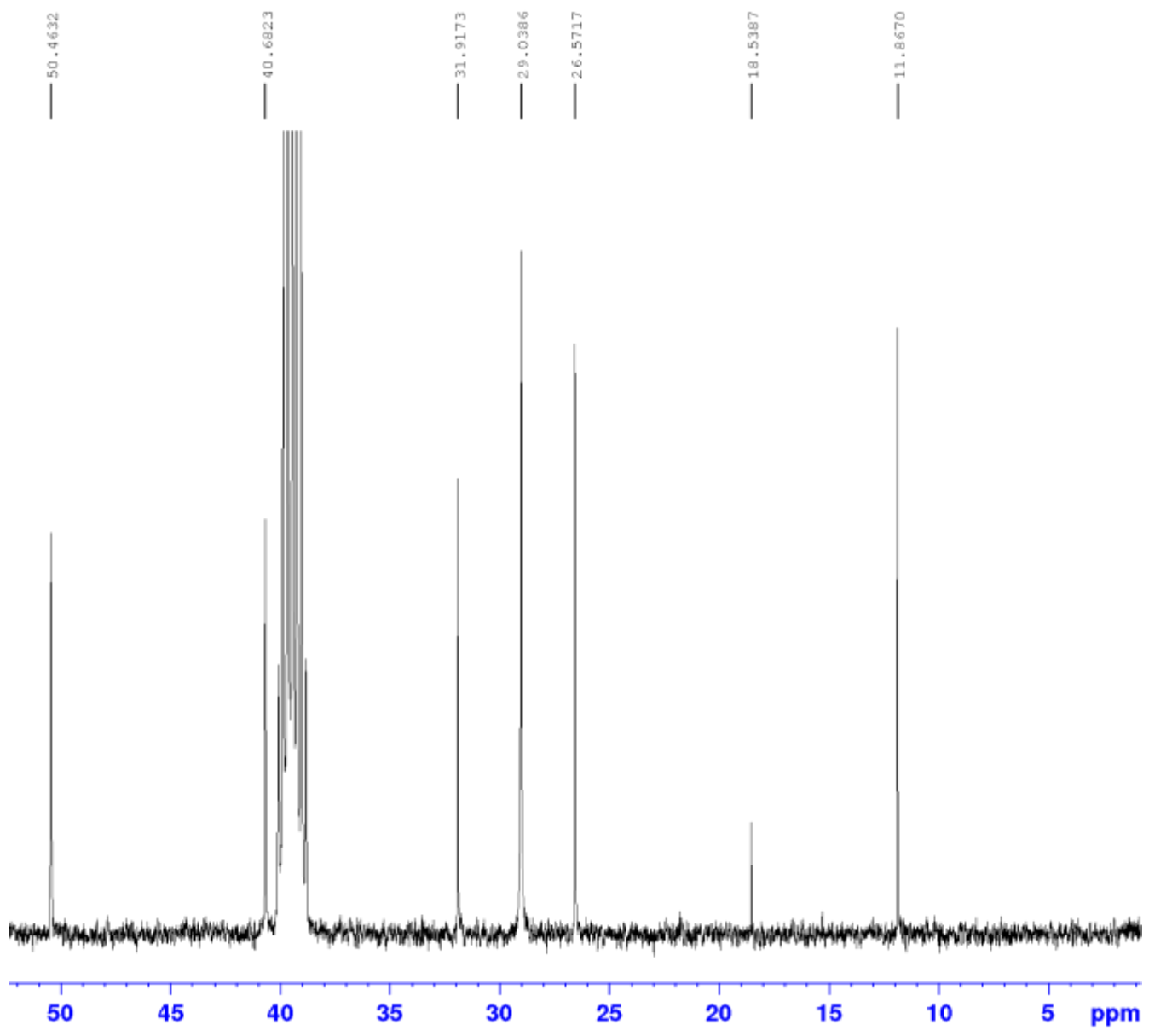
¹³C NMR Spectrum of compound 4h

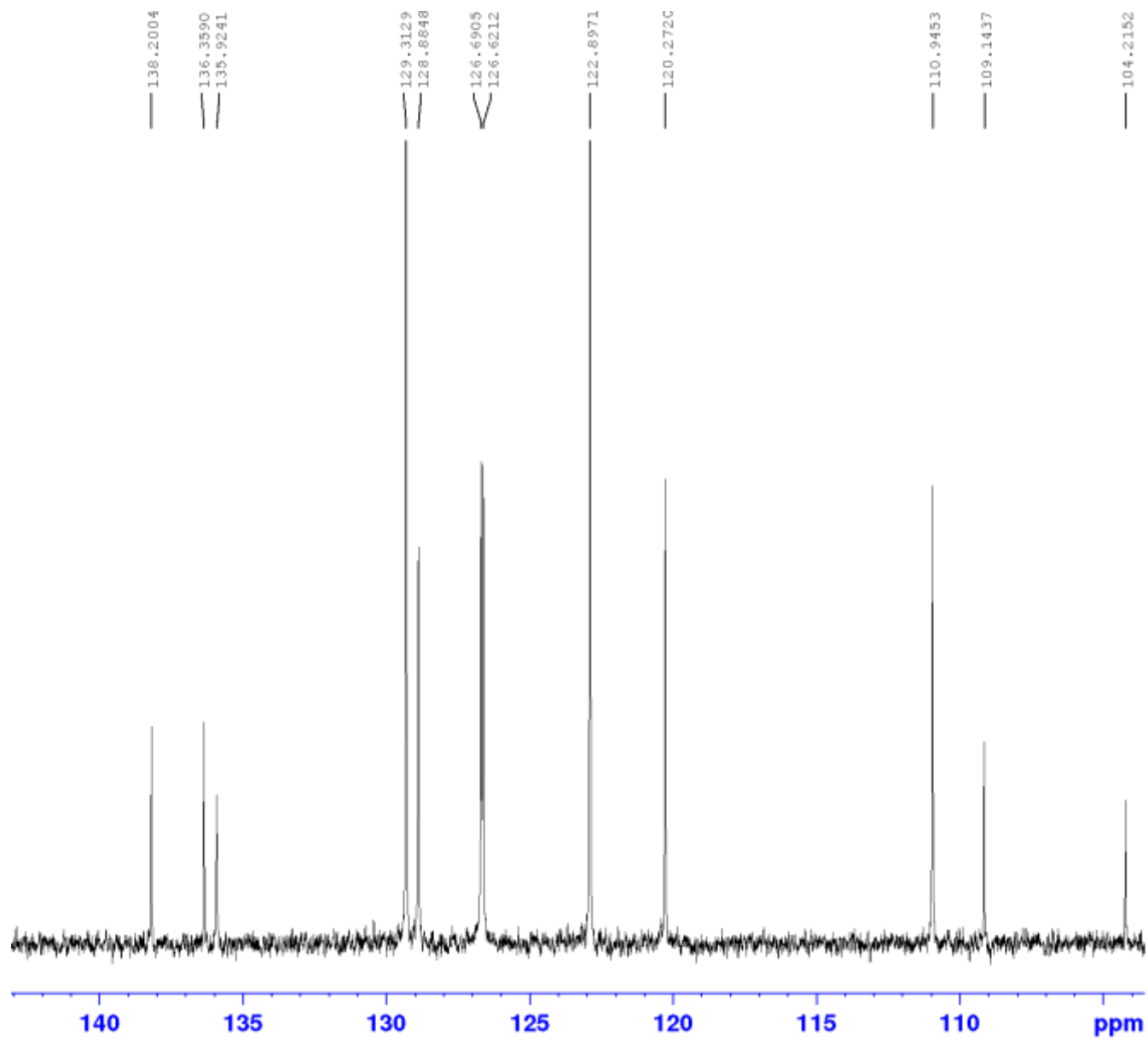


Current Data Parameters
 NAME Ahmadi-mahdi-IN971124
 EXPNO 40
 PROCNO 1

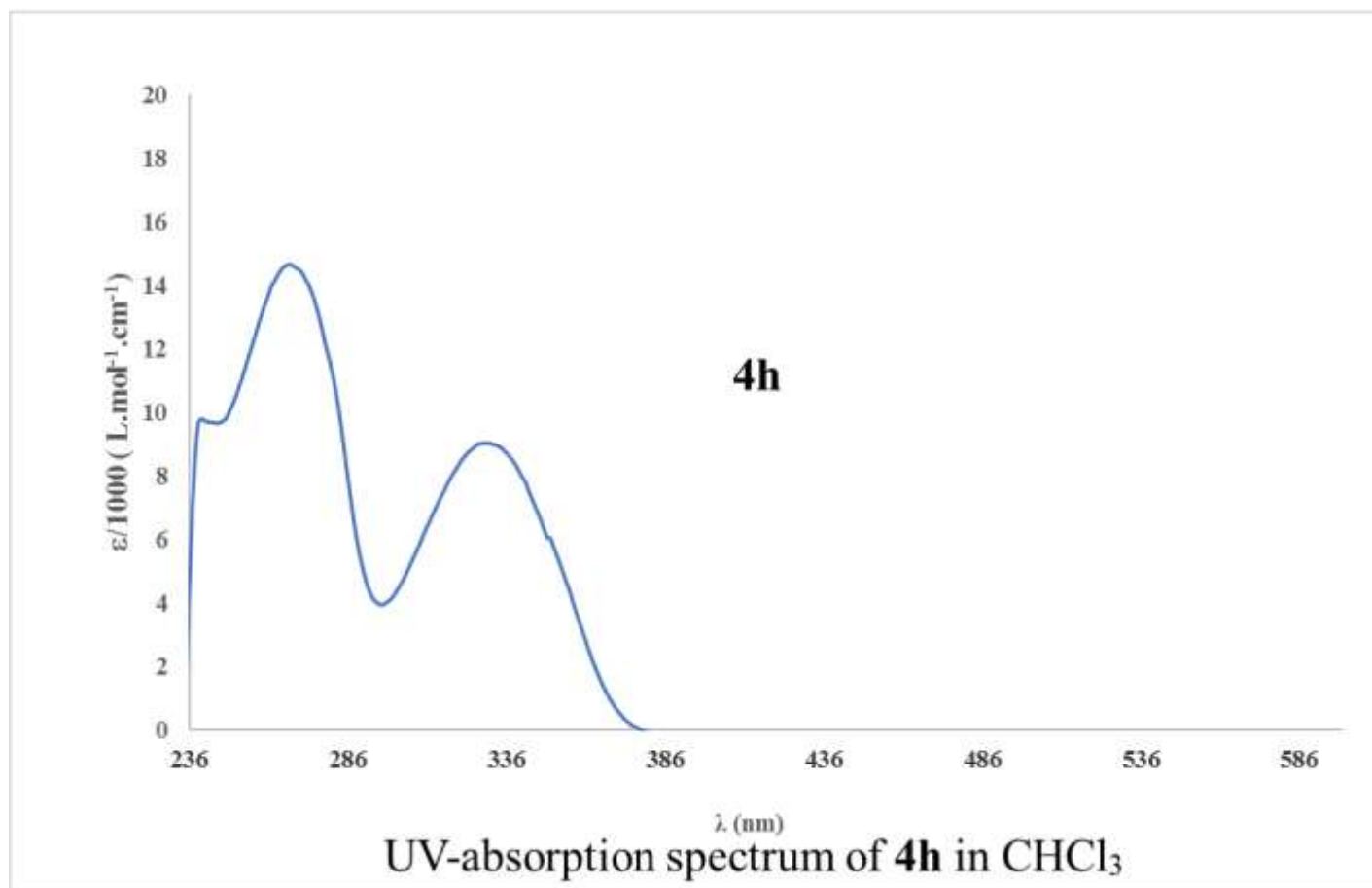
F2 - Acquisition Parameters
 Date_ 20190217
 Time 20.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 50502
 SOLVENT DMSO
 NS 2000
 DS 2
 SWH 25252.525 Hz
 FIDRES 0.500030 Hz
 AQ 0.9999396 sec
 RG 2050
 DW 19.800 usec
 DE 6.50 usec
 TE 294.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -1.00 dB
 PLLW 42.69075012 W
 SFO1 100.628264 MHz

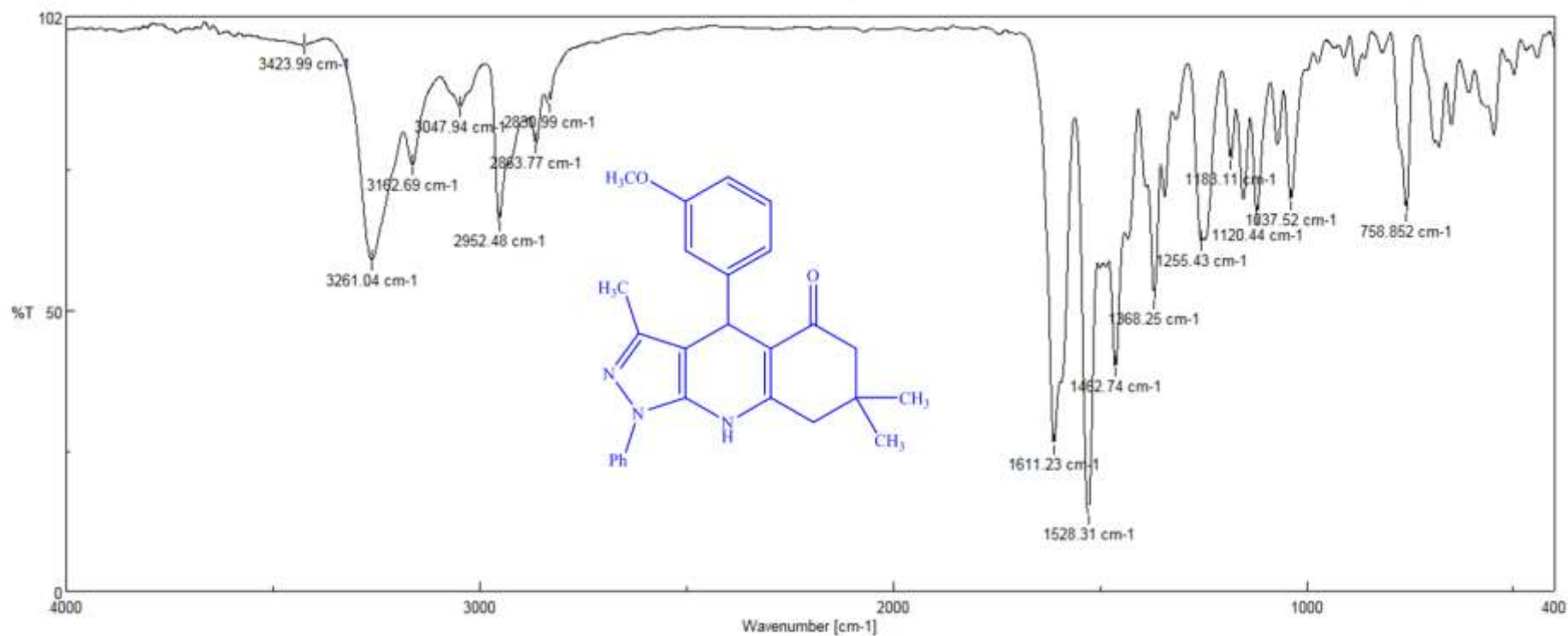




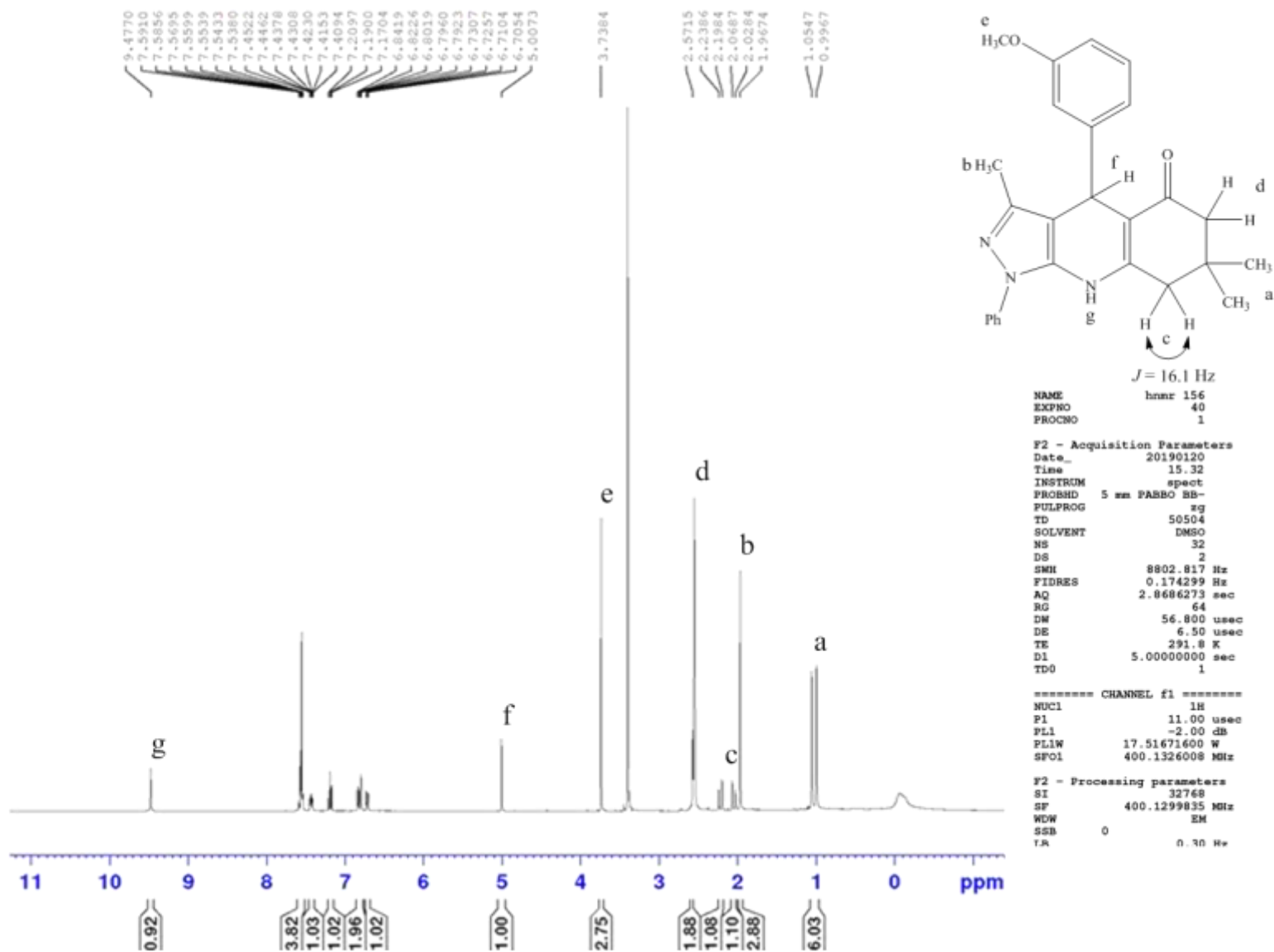
UV-Spectrum of compound **4h**

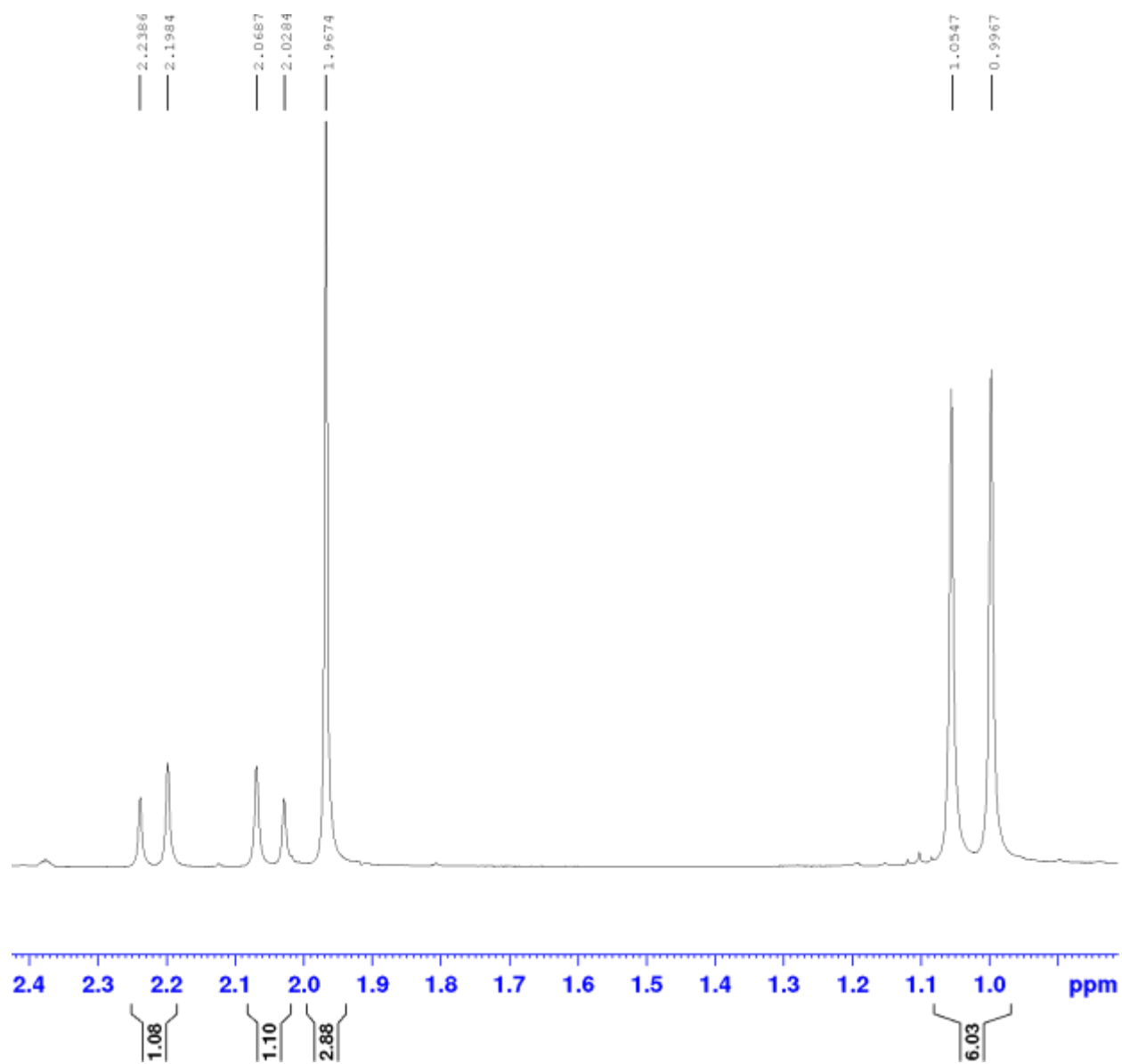


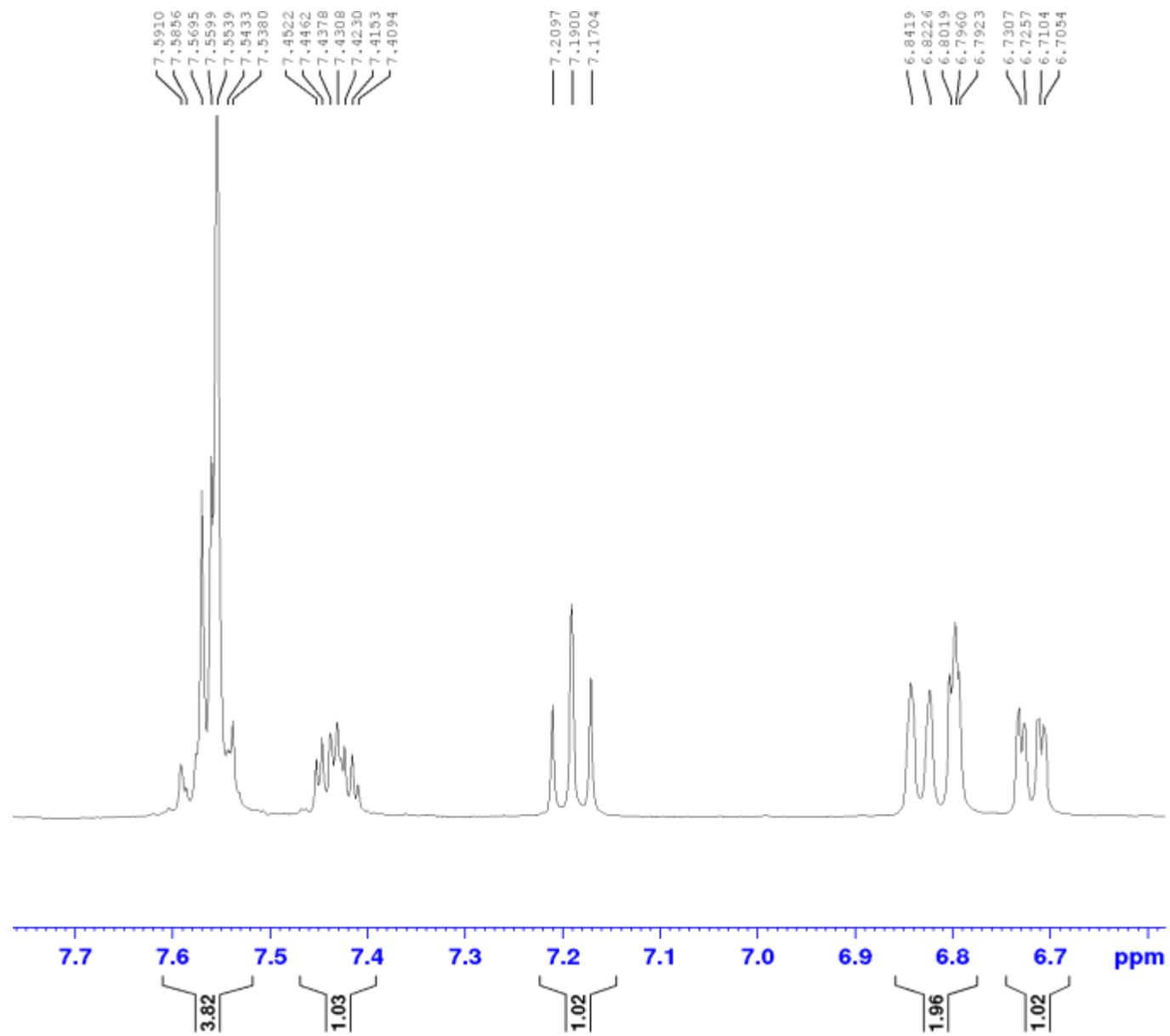
IR-Spectrum of compound 4i



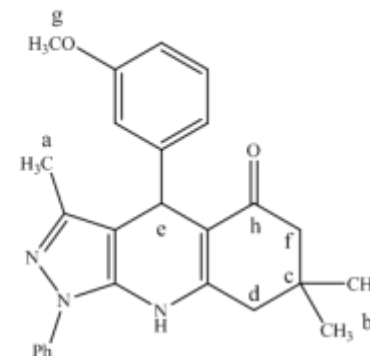
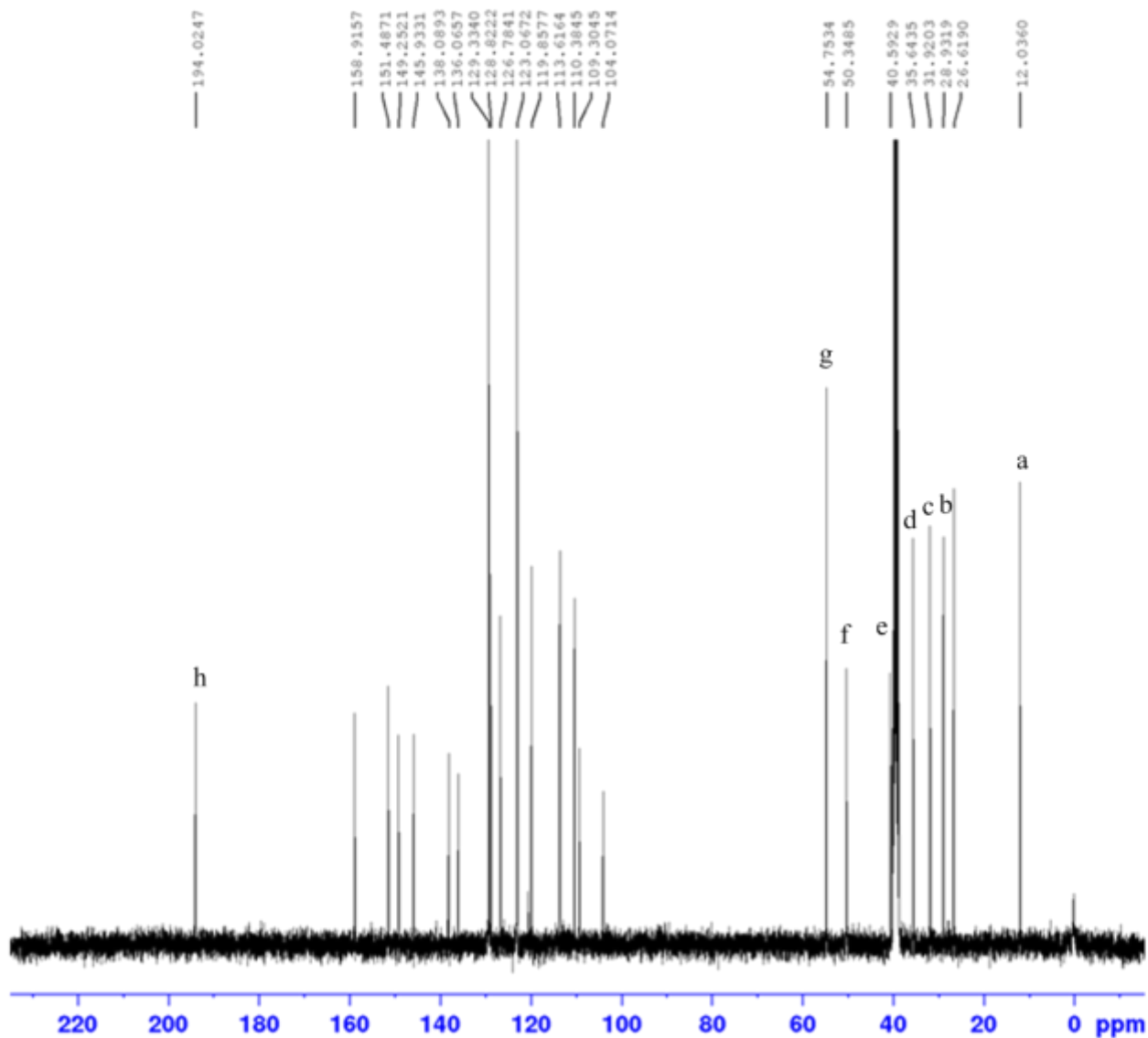
¹H NMR Spectrum of compound 4i







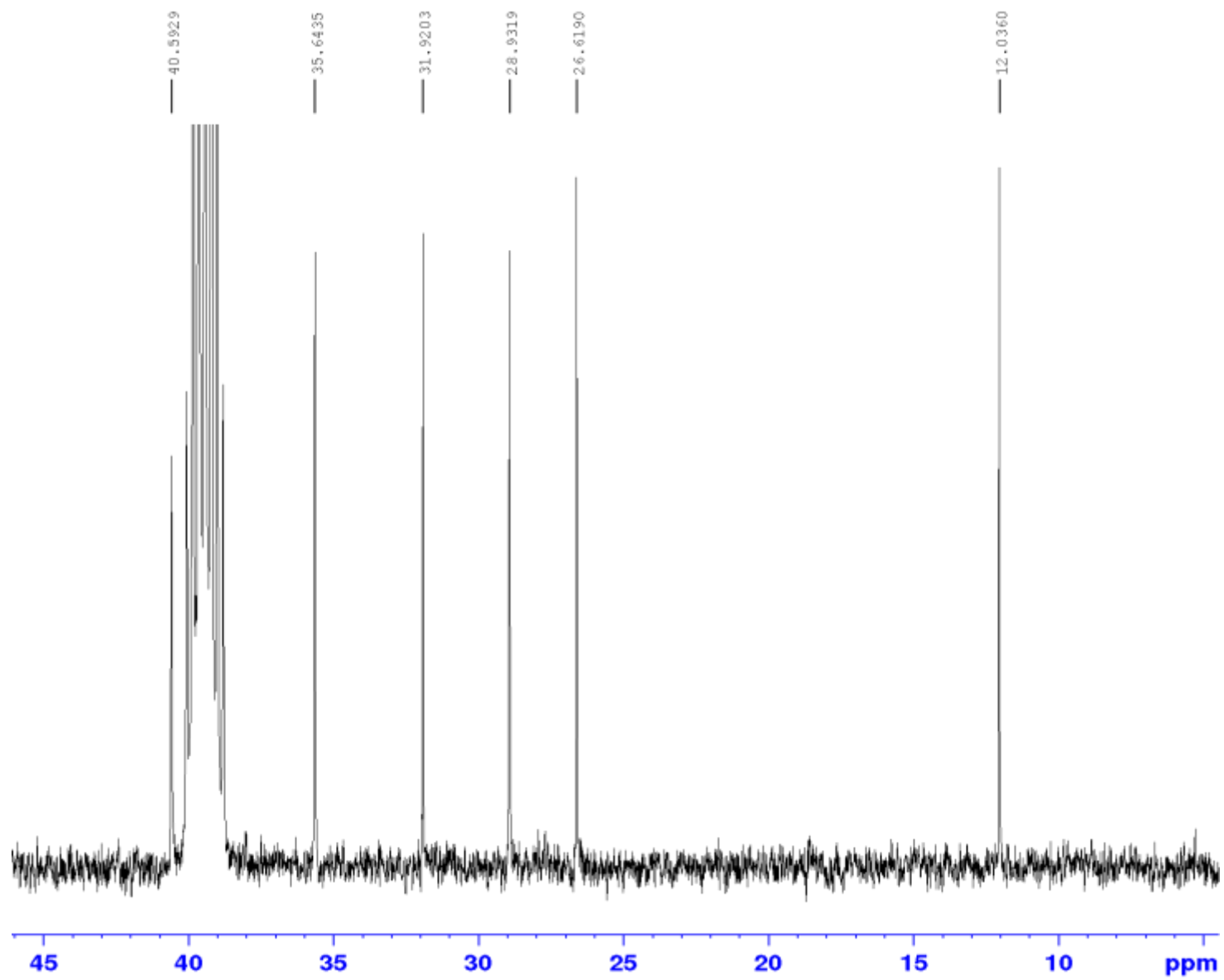
¹³C NMR Spectrum of compound 4i

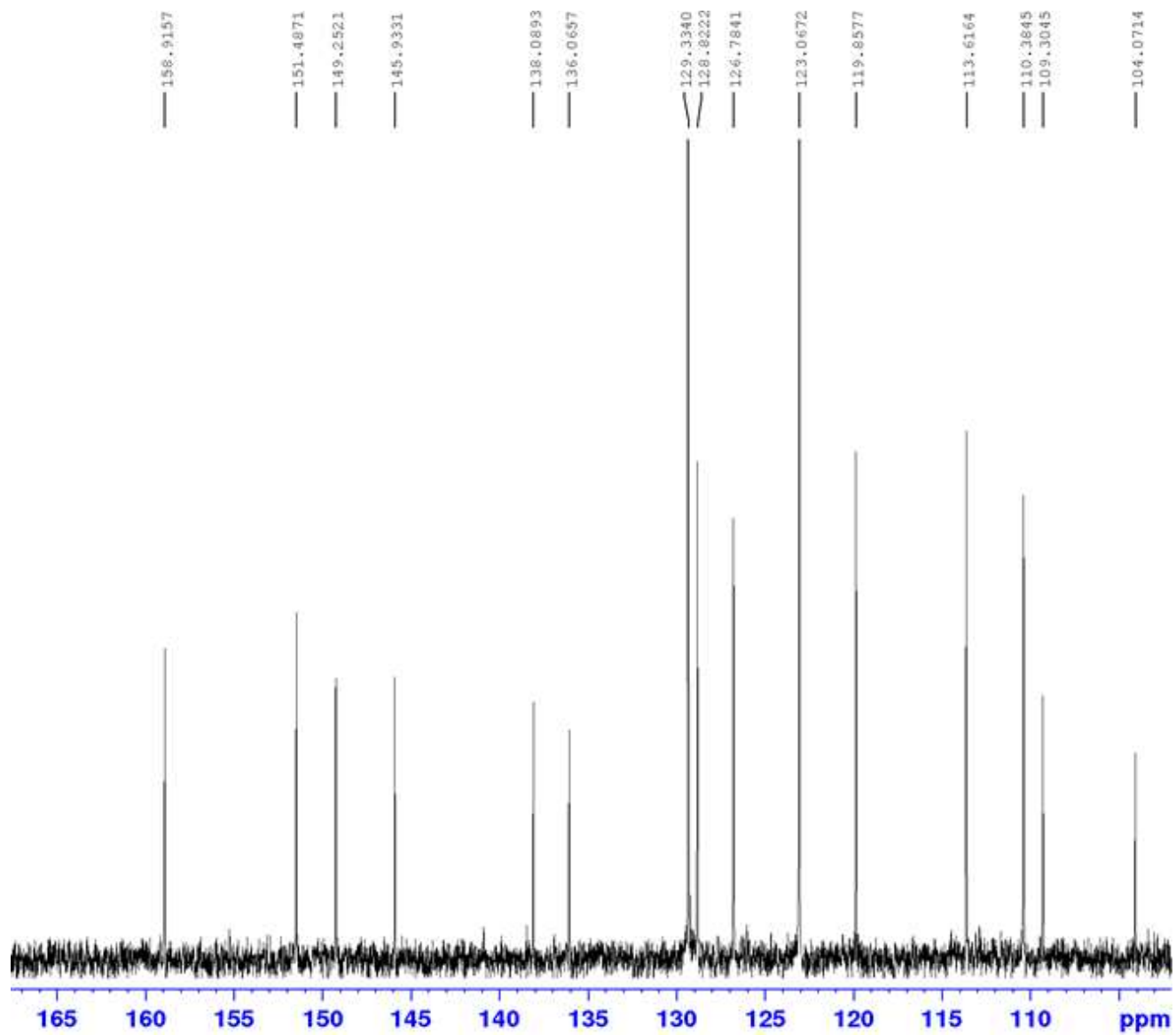


Current Data Parameters
 NAME Ahmadi-mahdi-IN971124
 EXPNO 50
 PROCNO 1

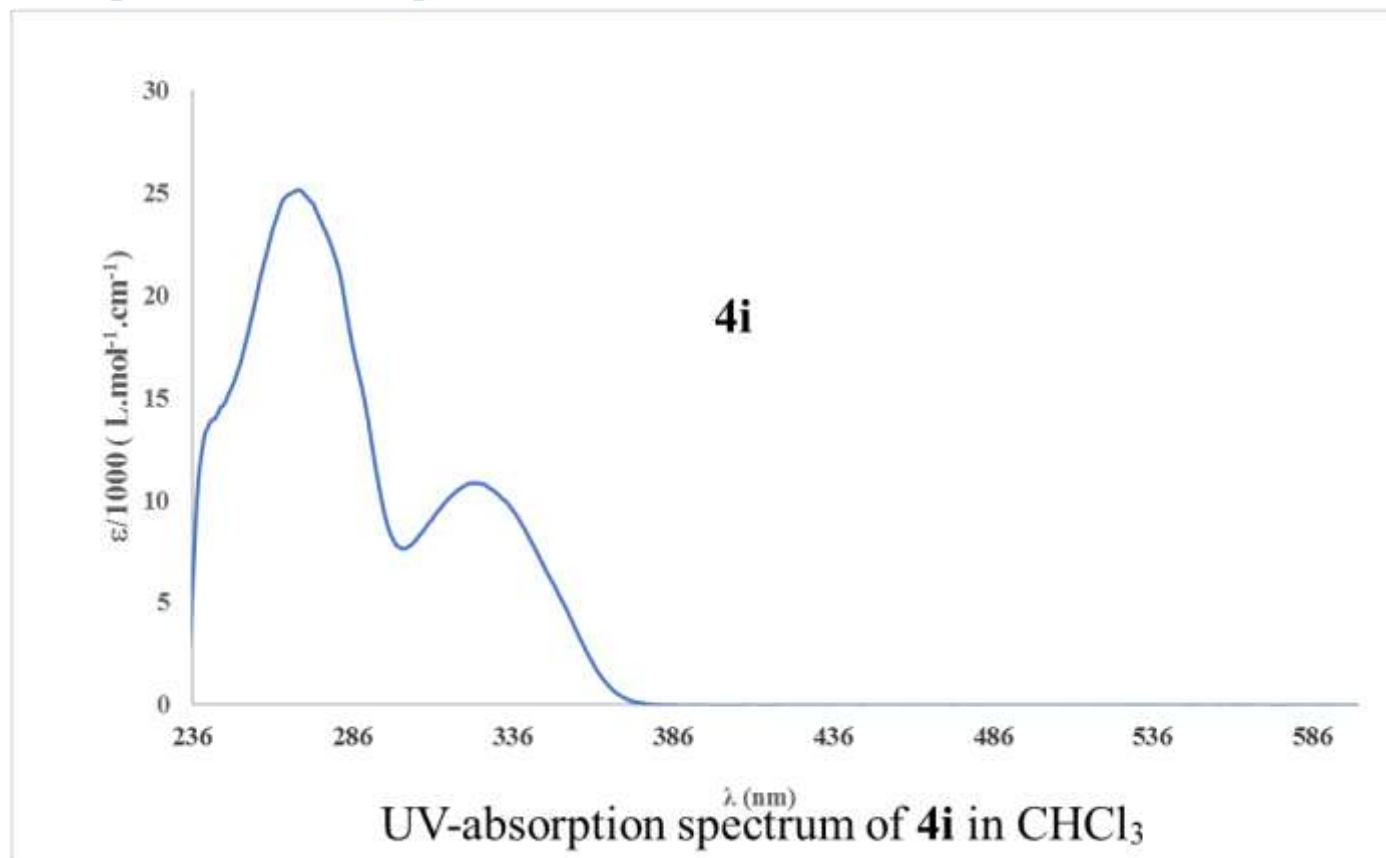
F2 - Acquisition Parameters
 Date_ 20190217
 Time 22.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 50502
 SOLVENT DMSO
 NS 2000
 DS 2
 SWH 25252.525 Hz
 FIDRES 0.500030 Hz
 AQ 0.9999396 sec
 RG 2050
 DW 19.800 usec
 DE 6.50 usec
 TE 293.9 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.50 usec
 PL1 -1.00 dB
 PLLW 42.69075012 W
 SFO1 100.6238364 MHz

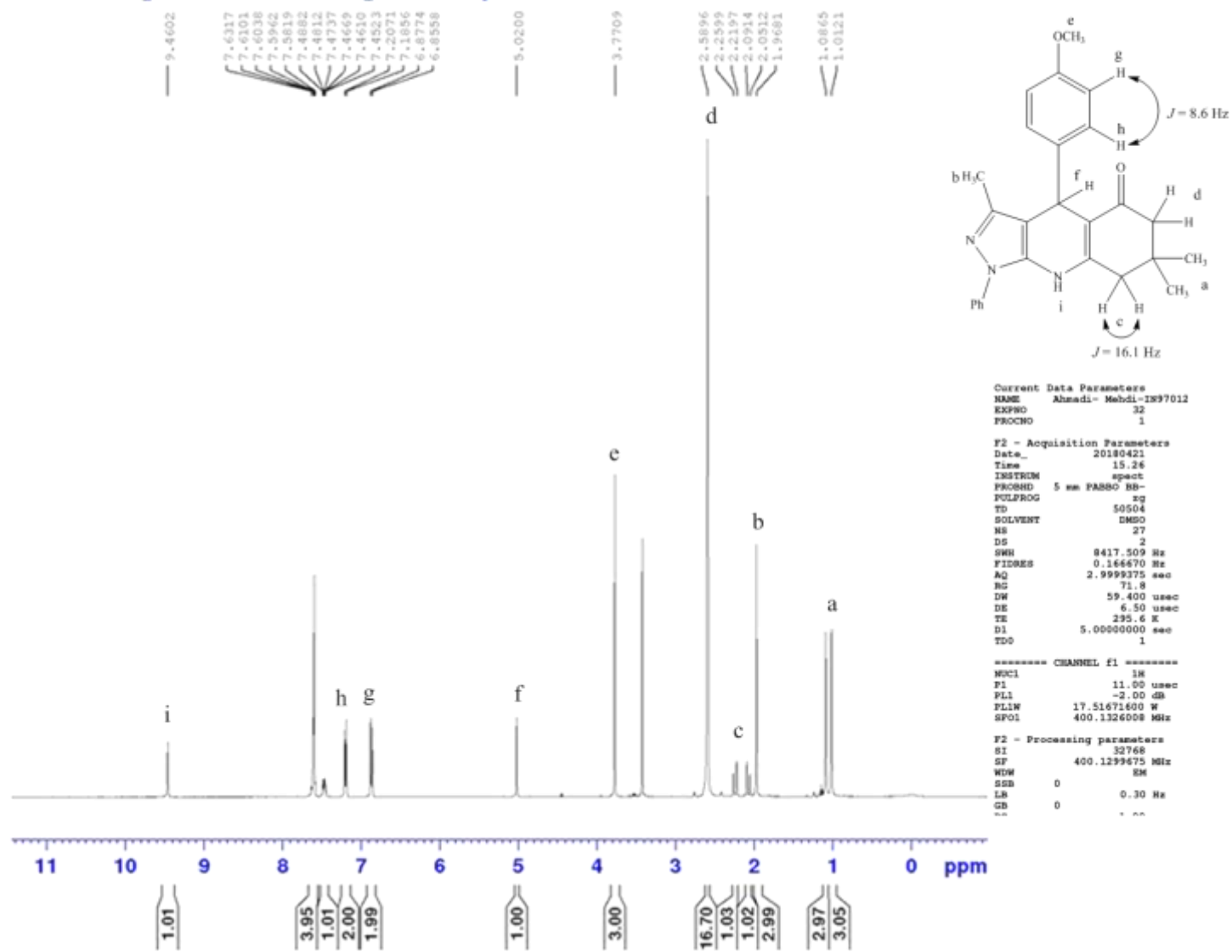


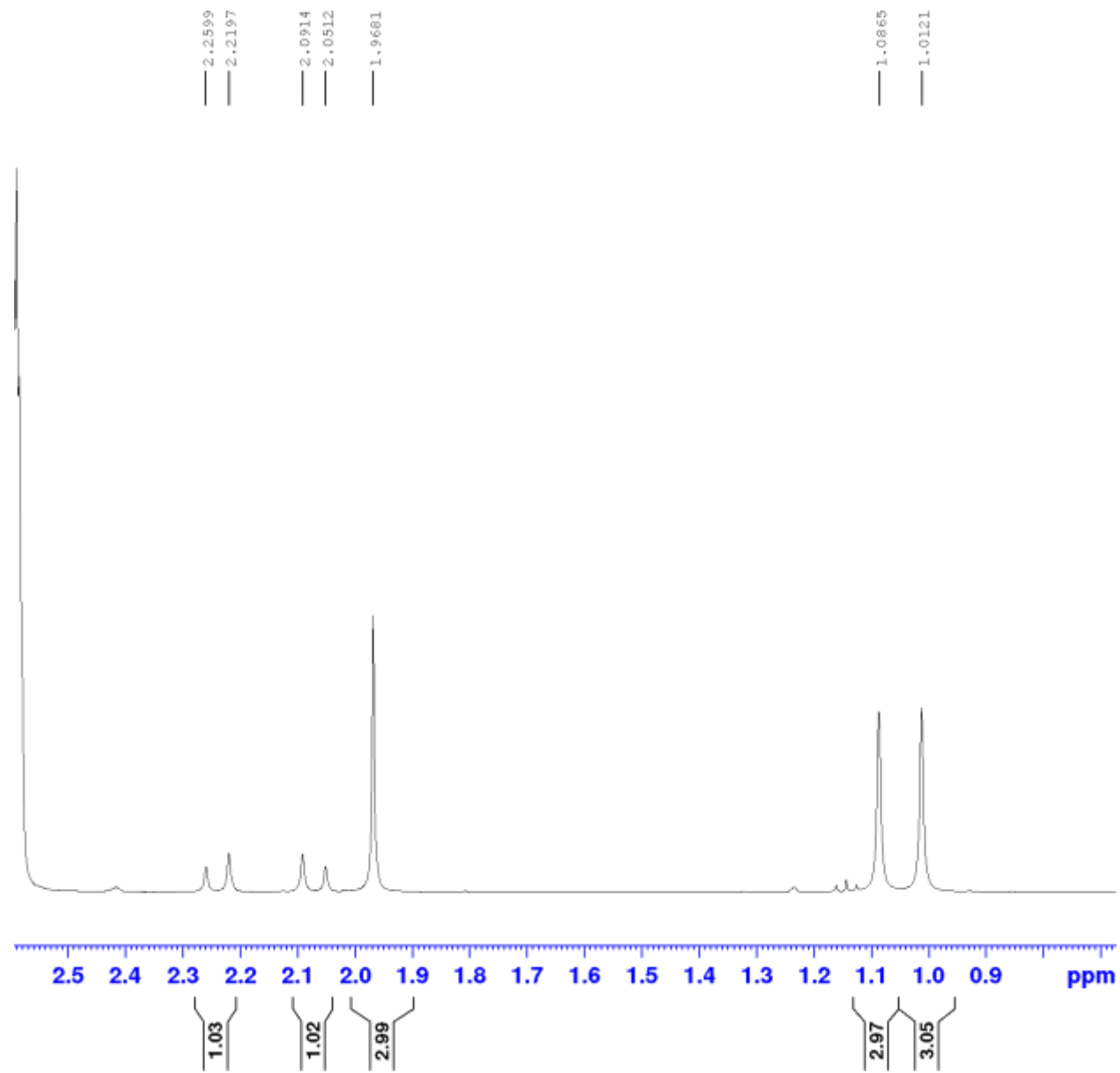


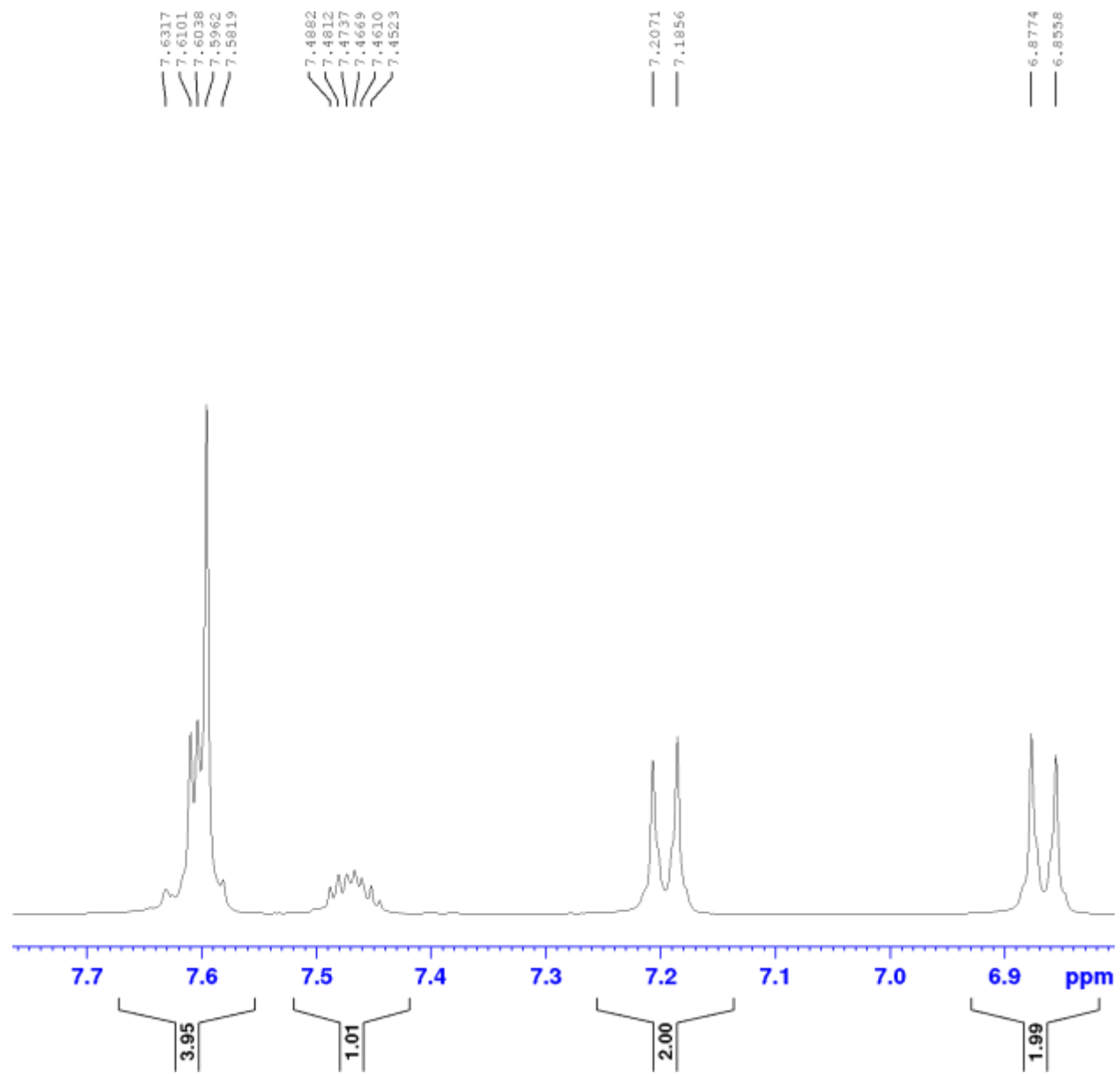
UV-Spectrum of compound **4i**



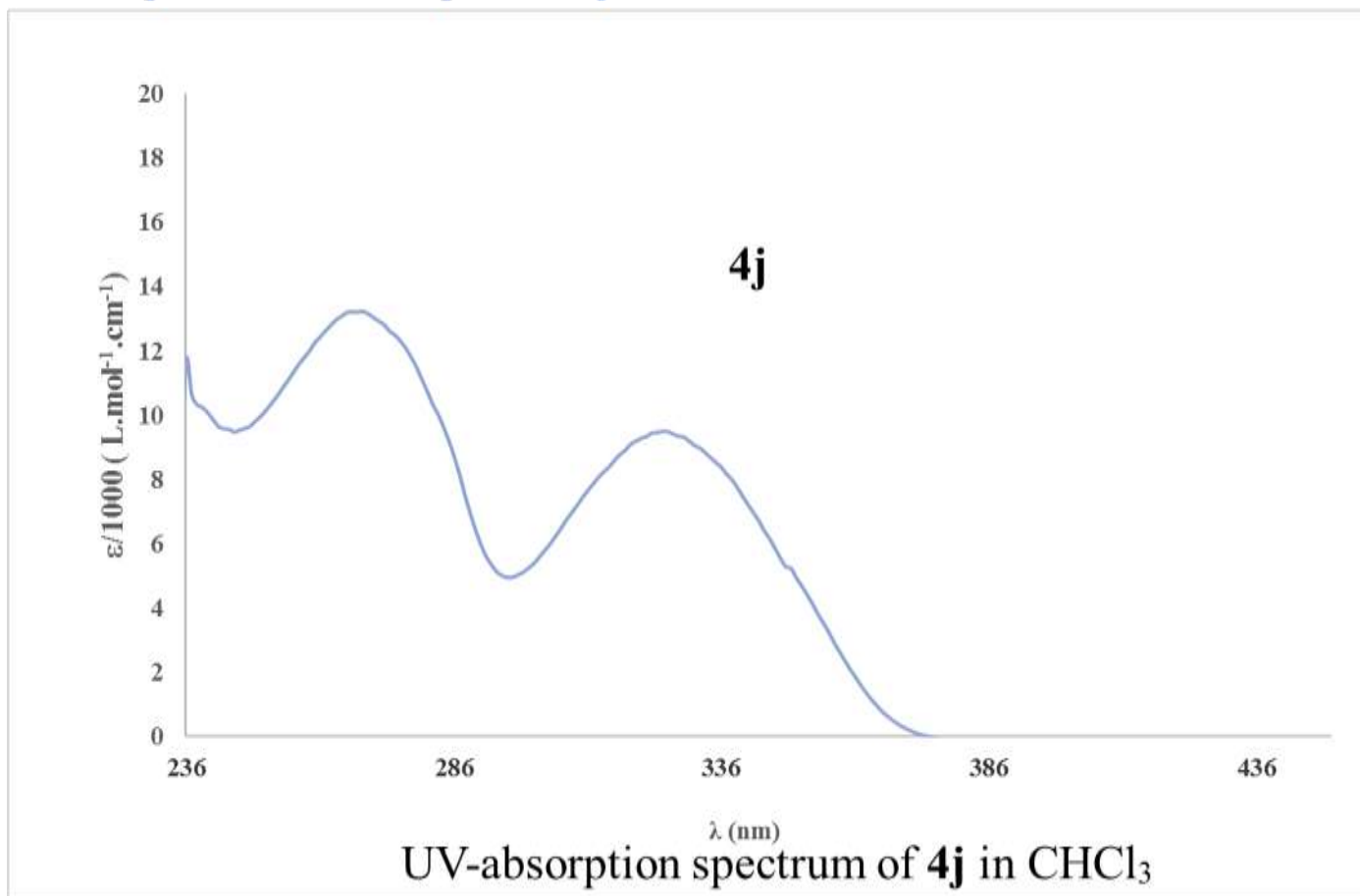
¹H NMR Spectrum of compound 4j



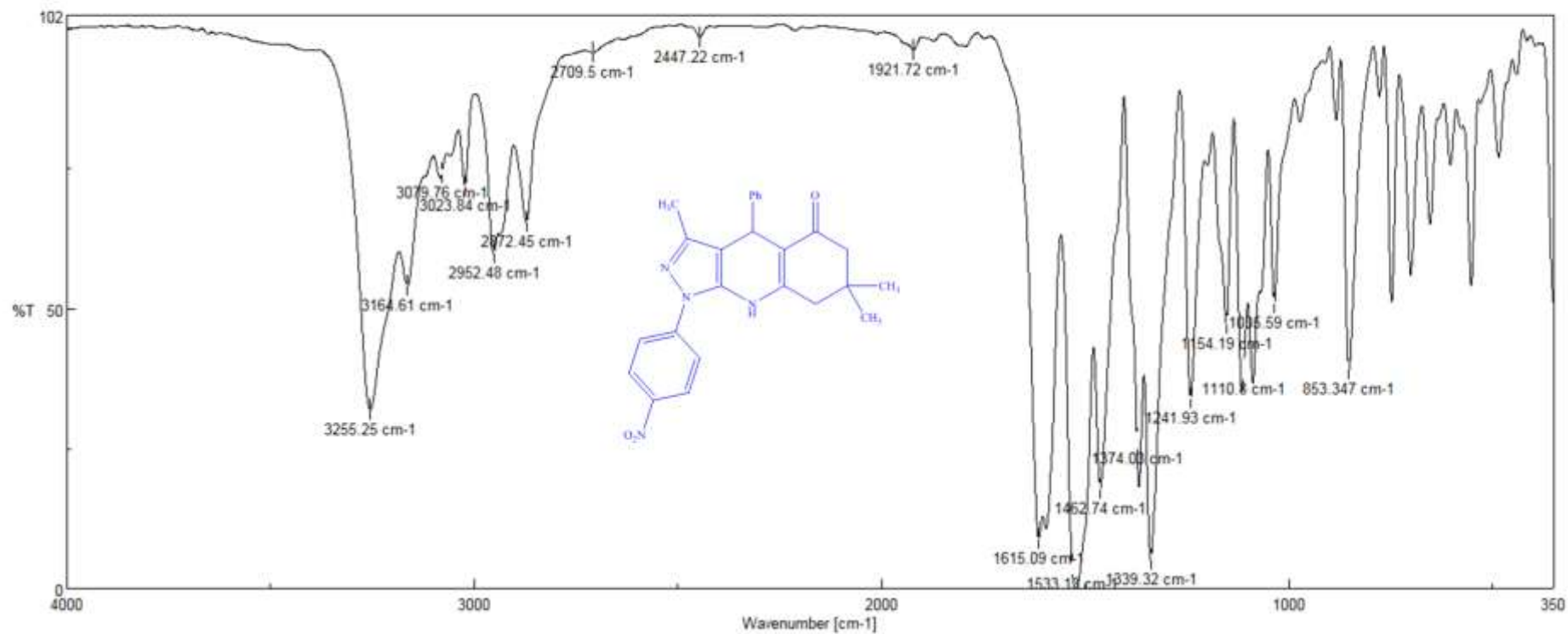




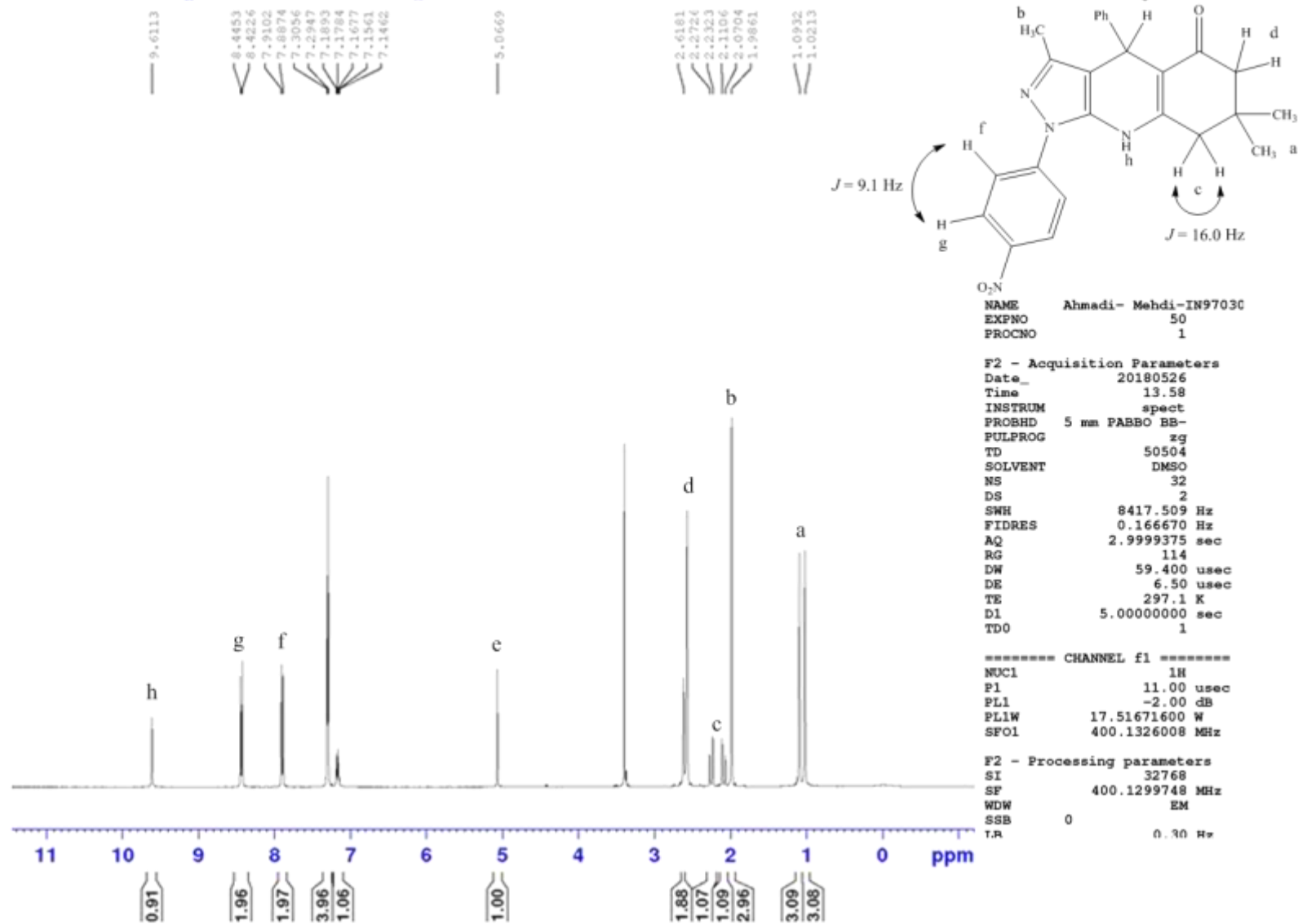
UV-Spectrum of compound **4j**

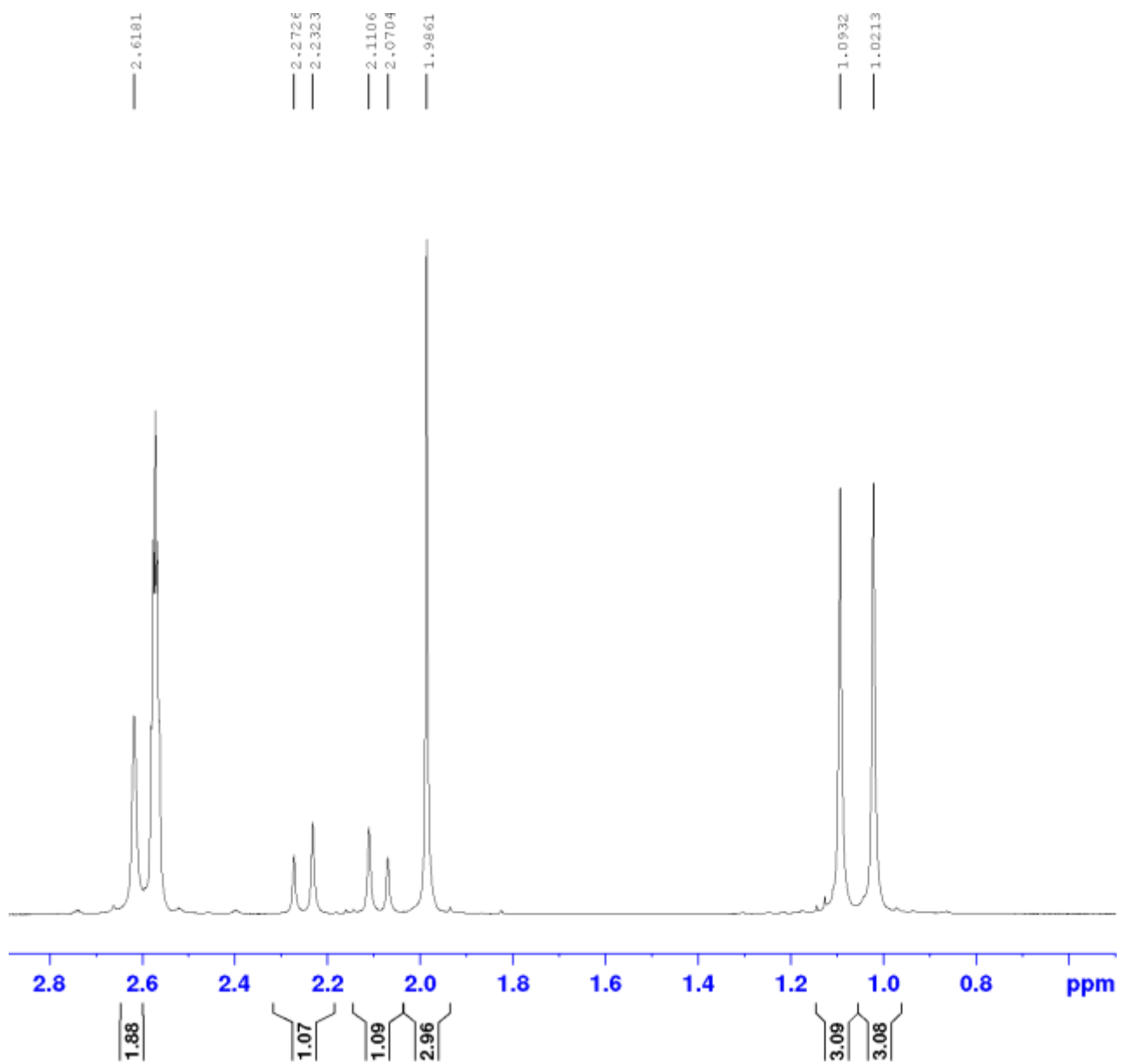


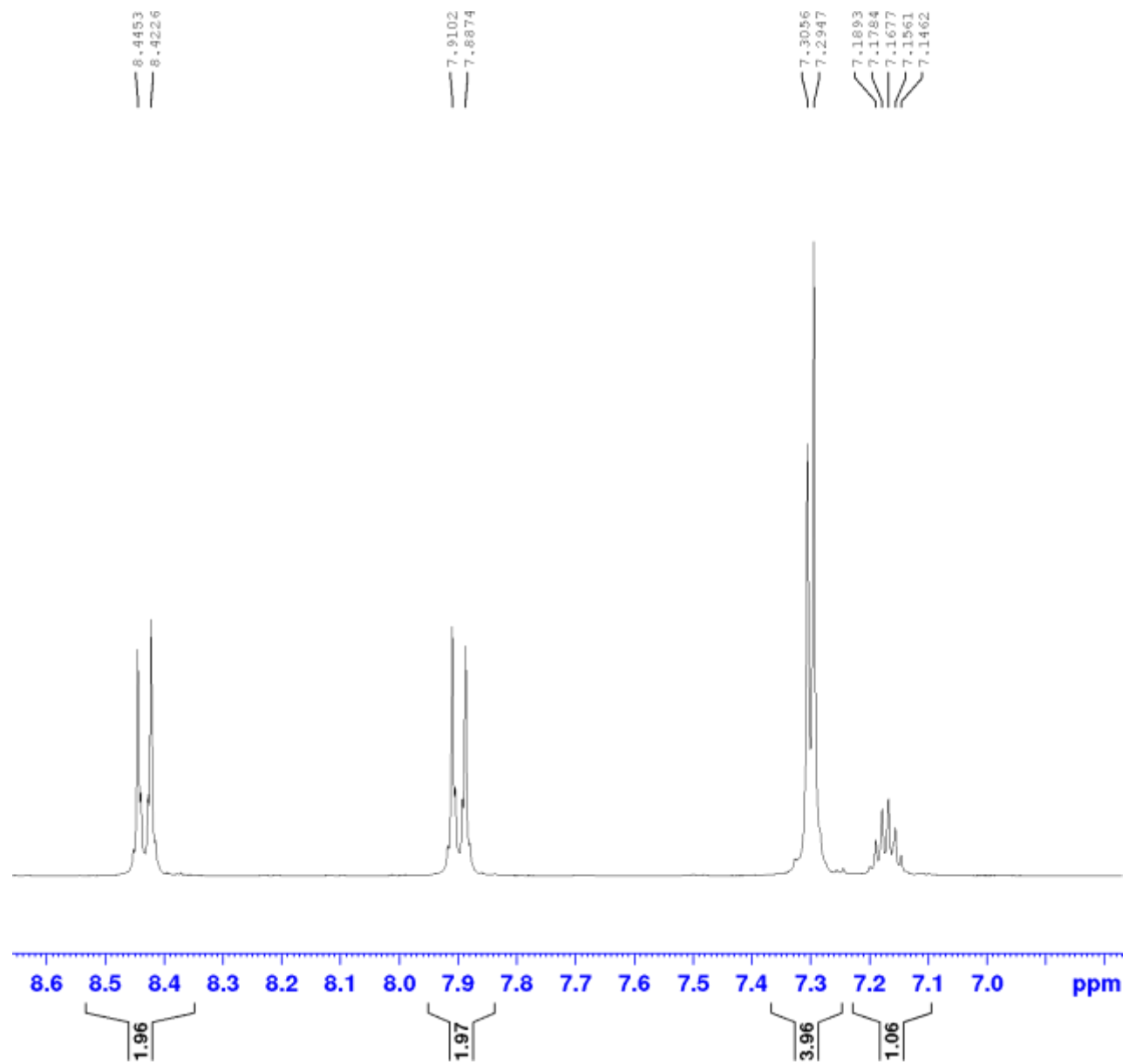
IR-Spectrum of compound 4k



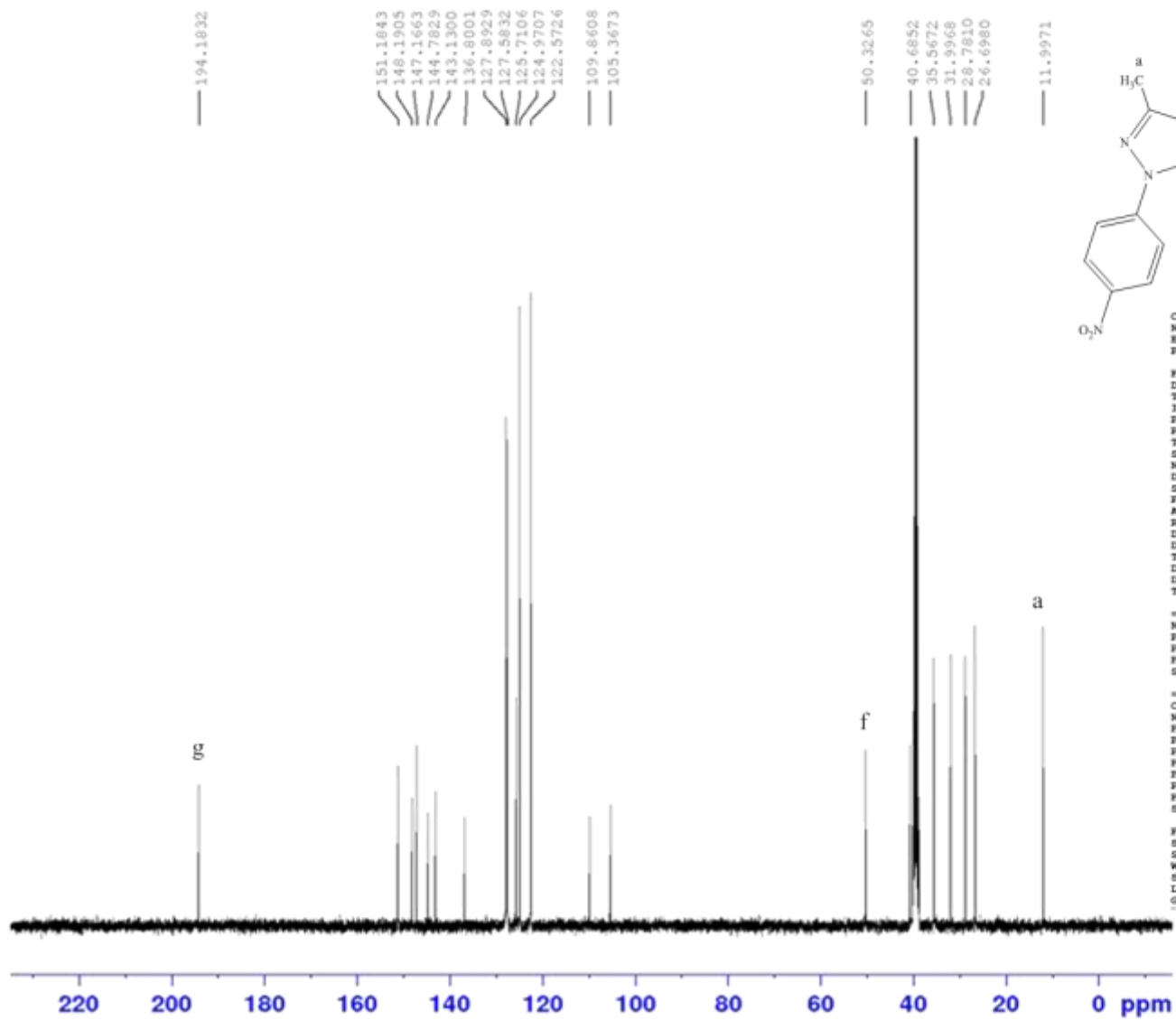
¹H NMR Spectrum of compound **4k**

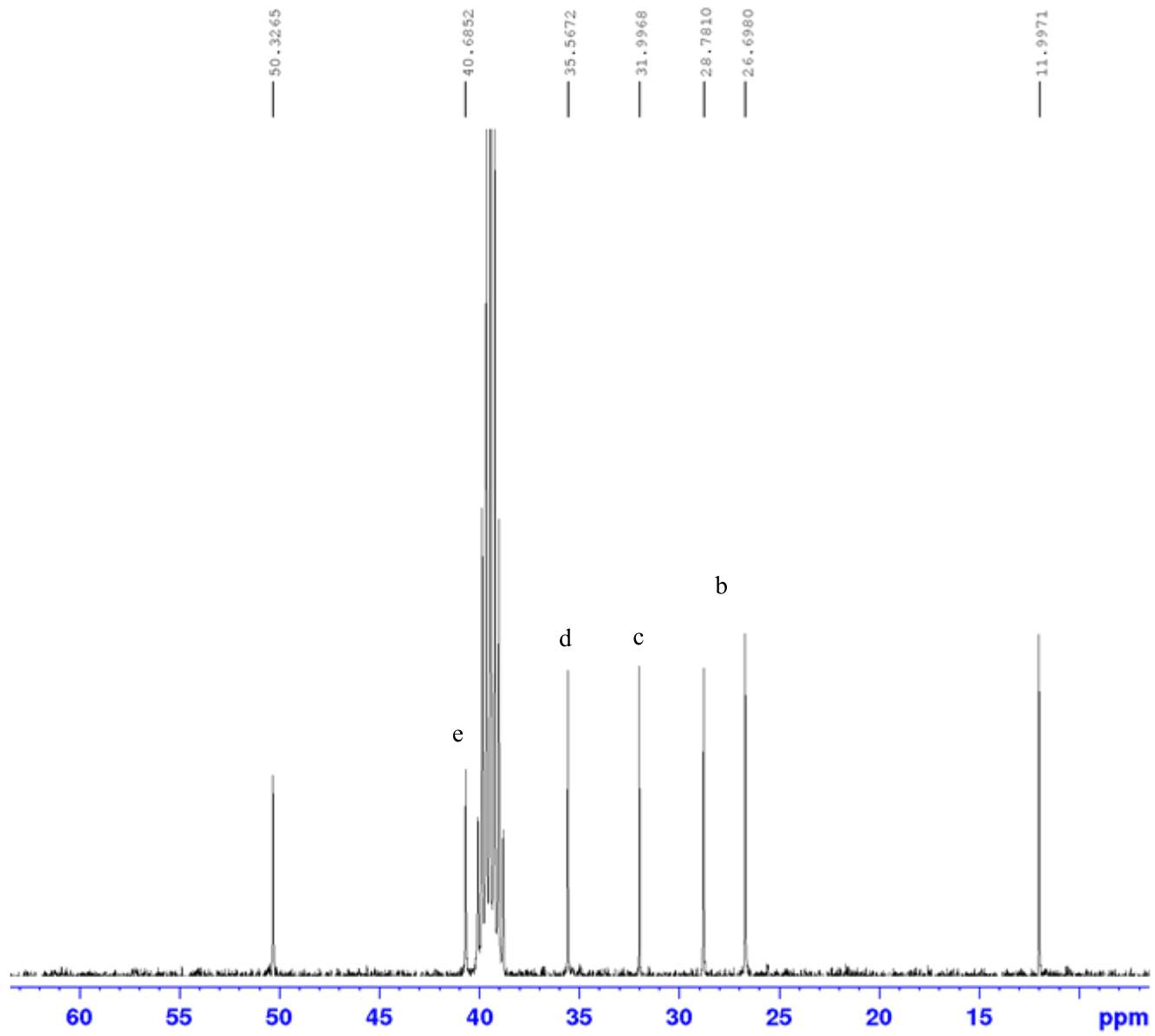


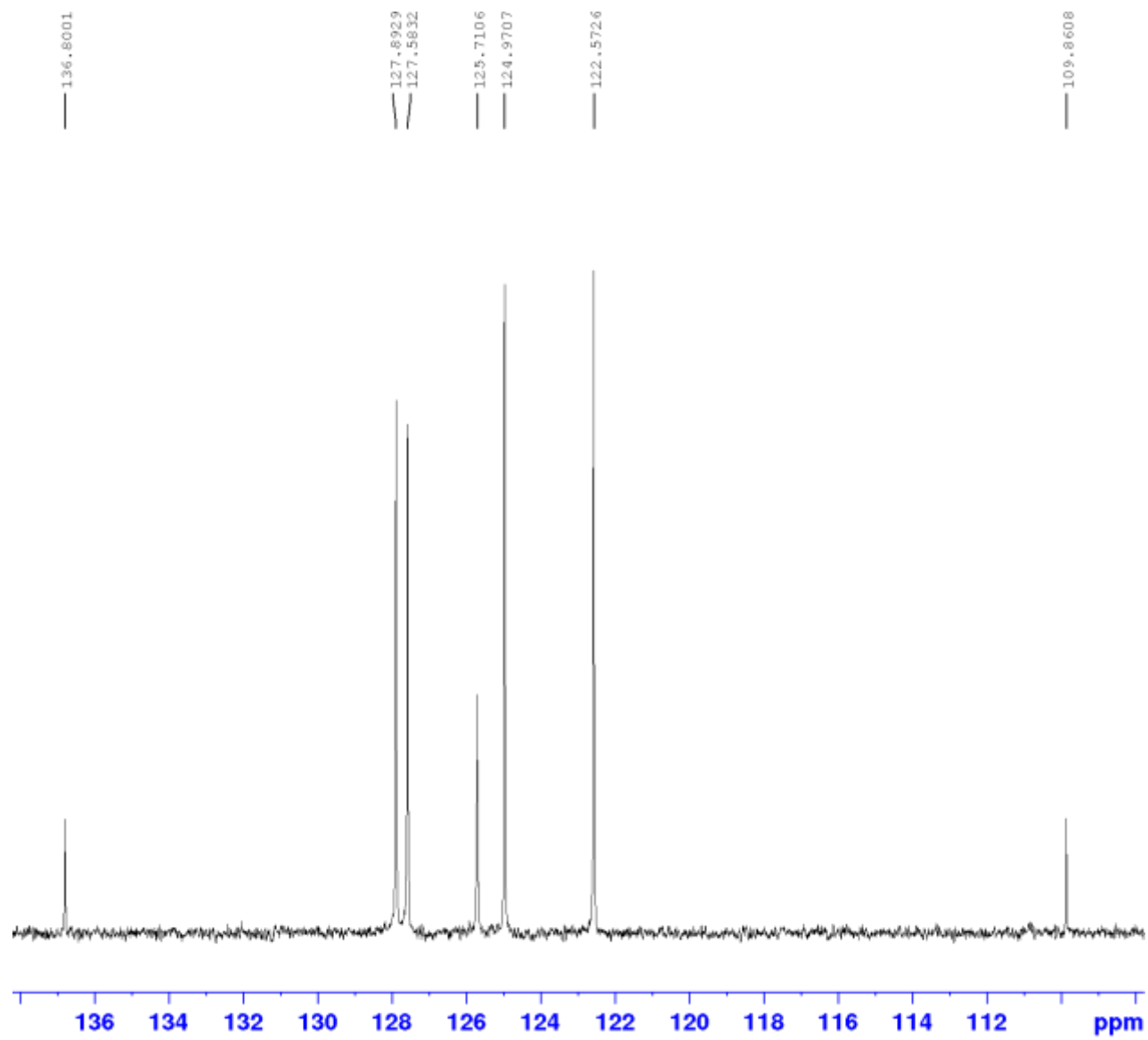


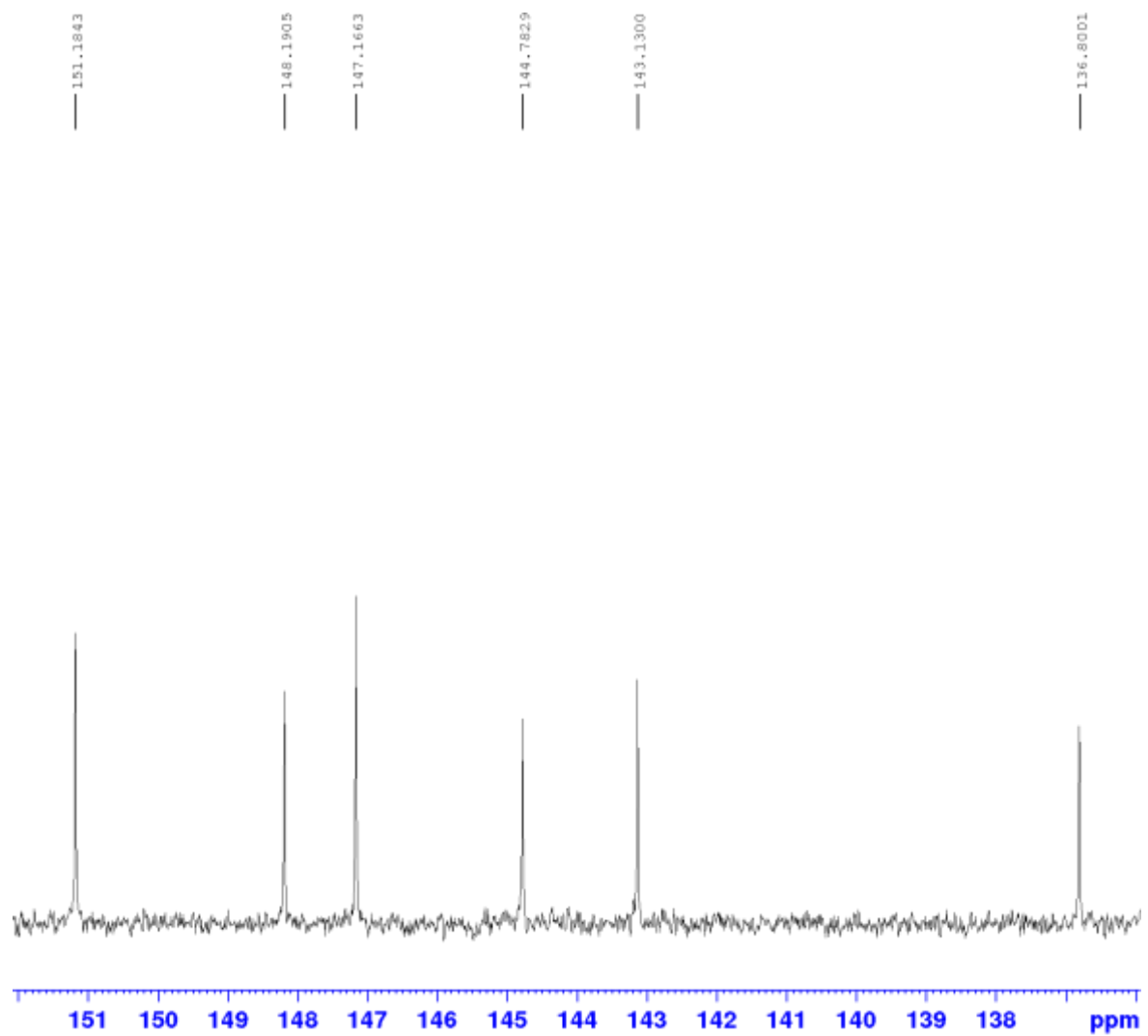


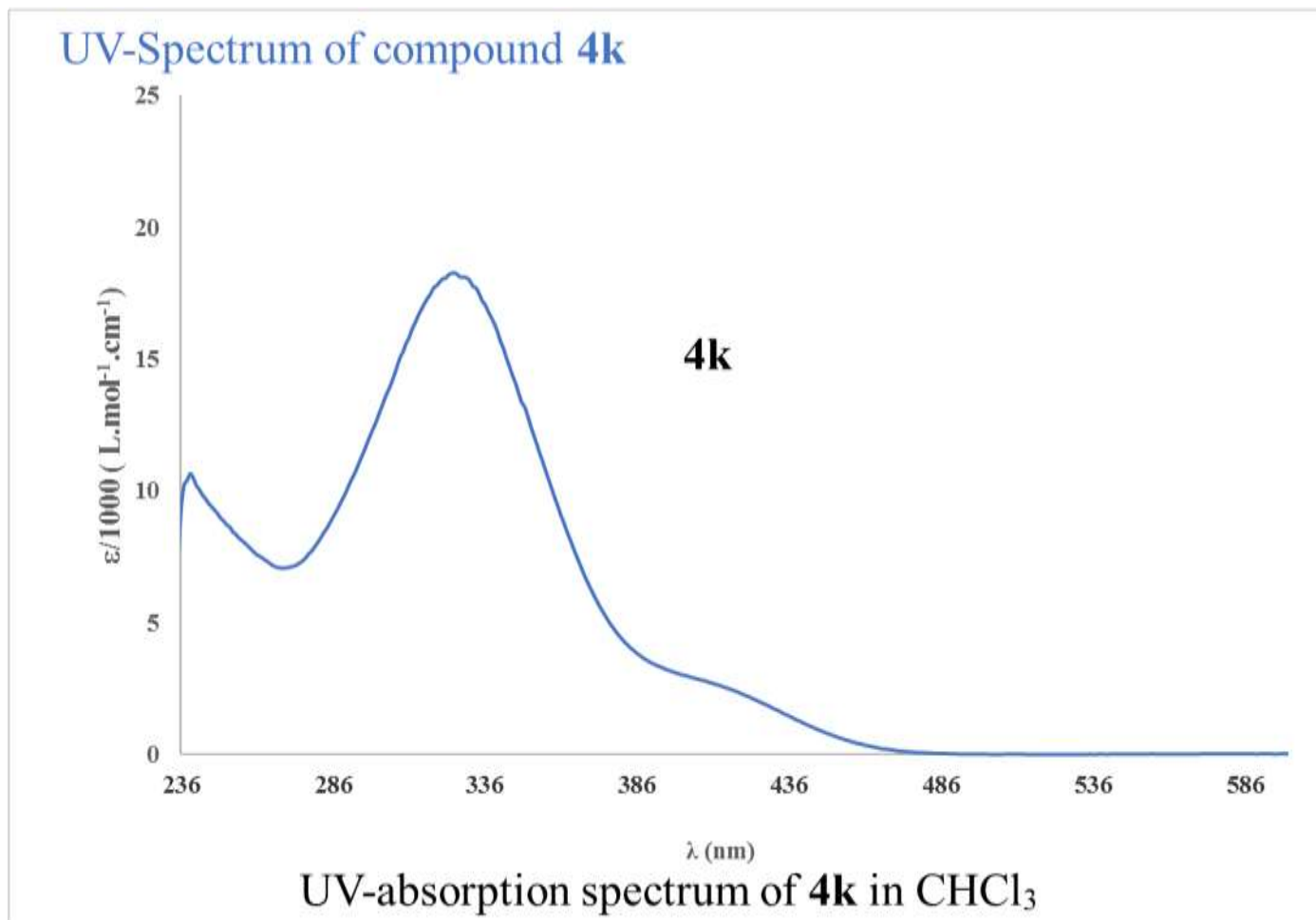
¹³C NMR Spectrum of compound 4k



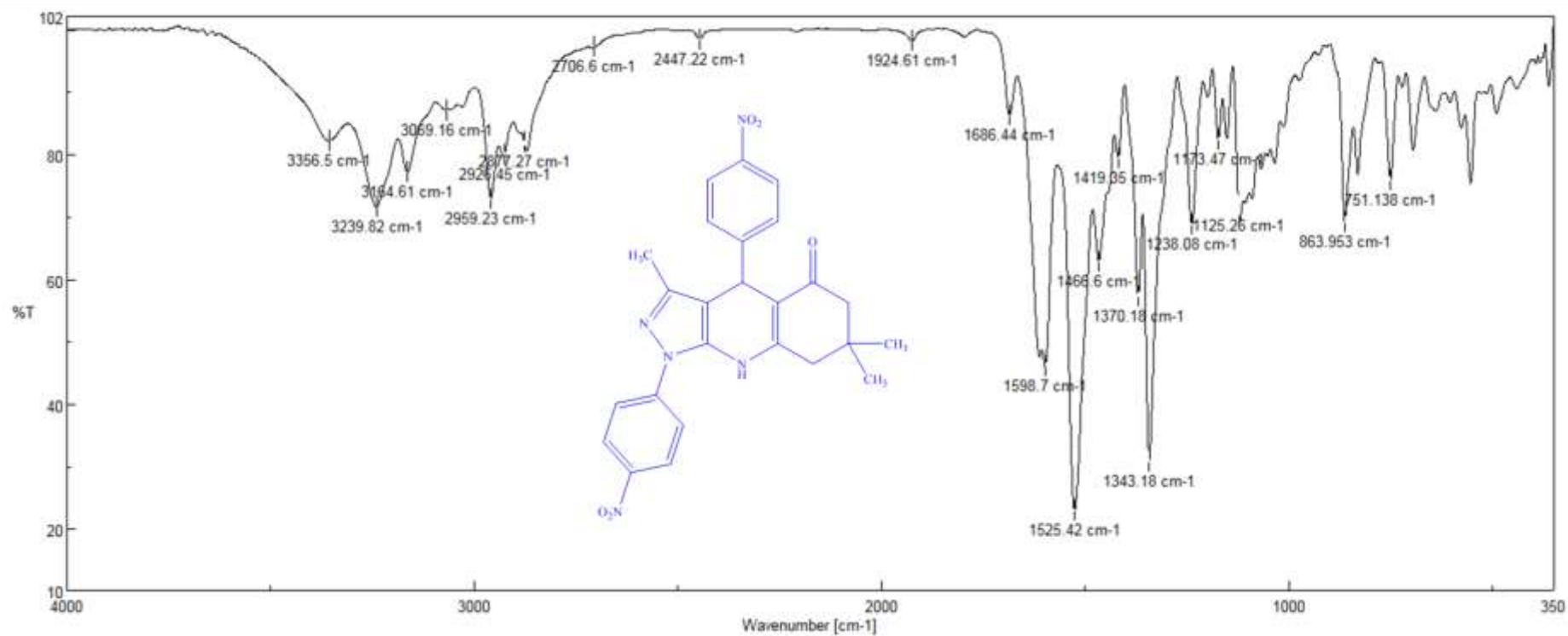




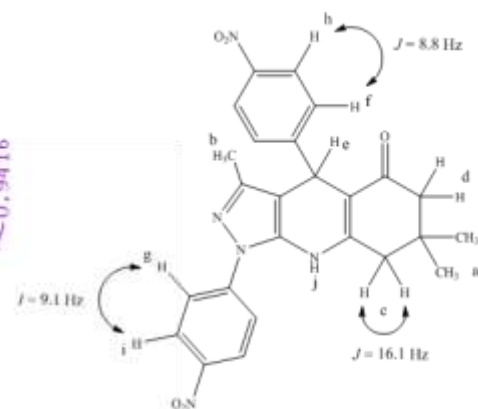
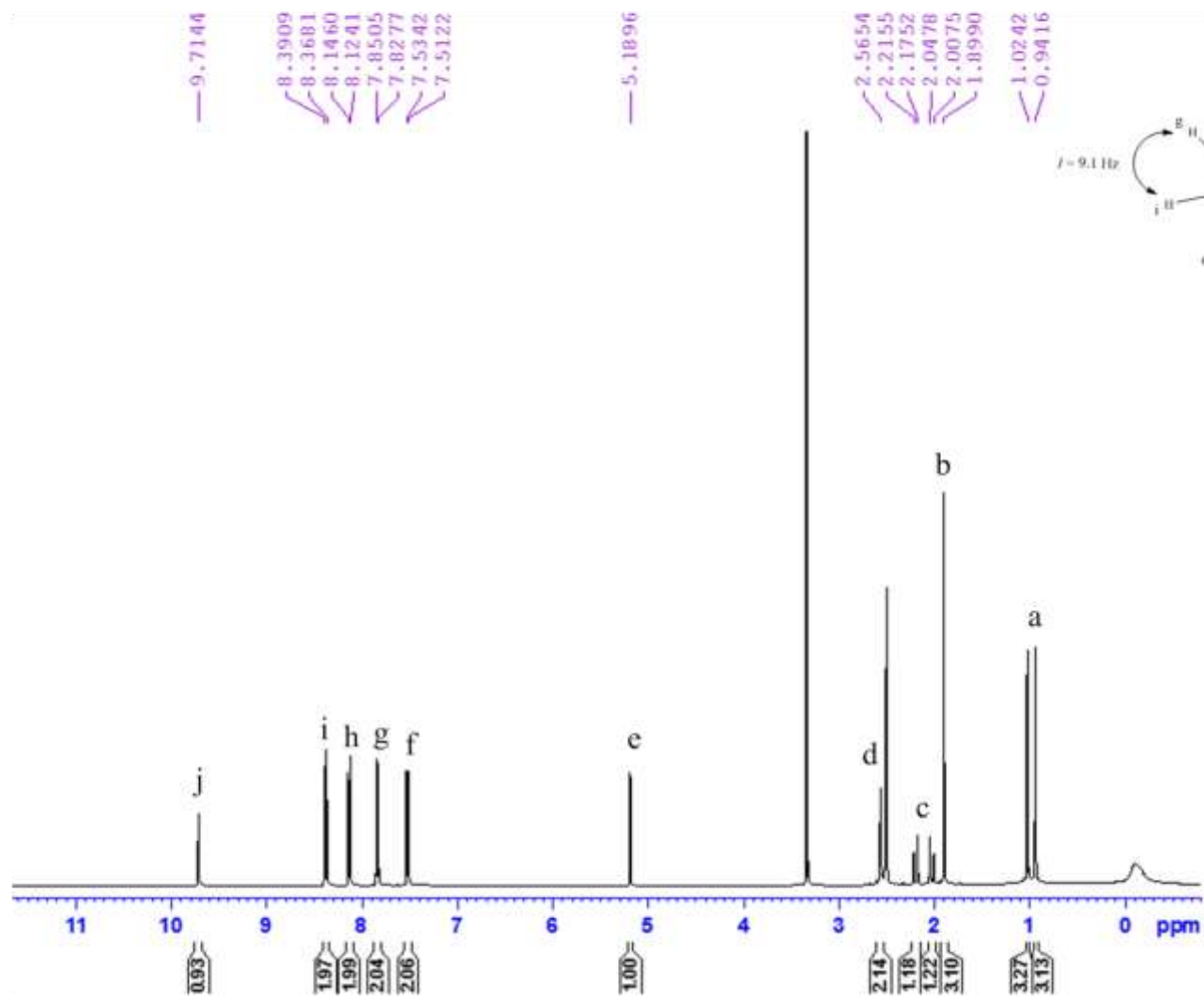




IR-Spectrum of compound 4I



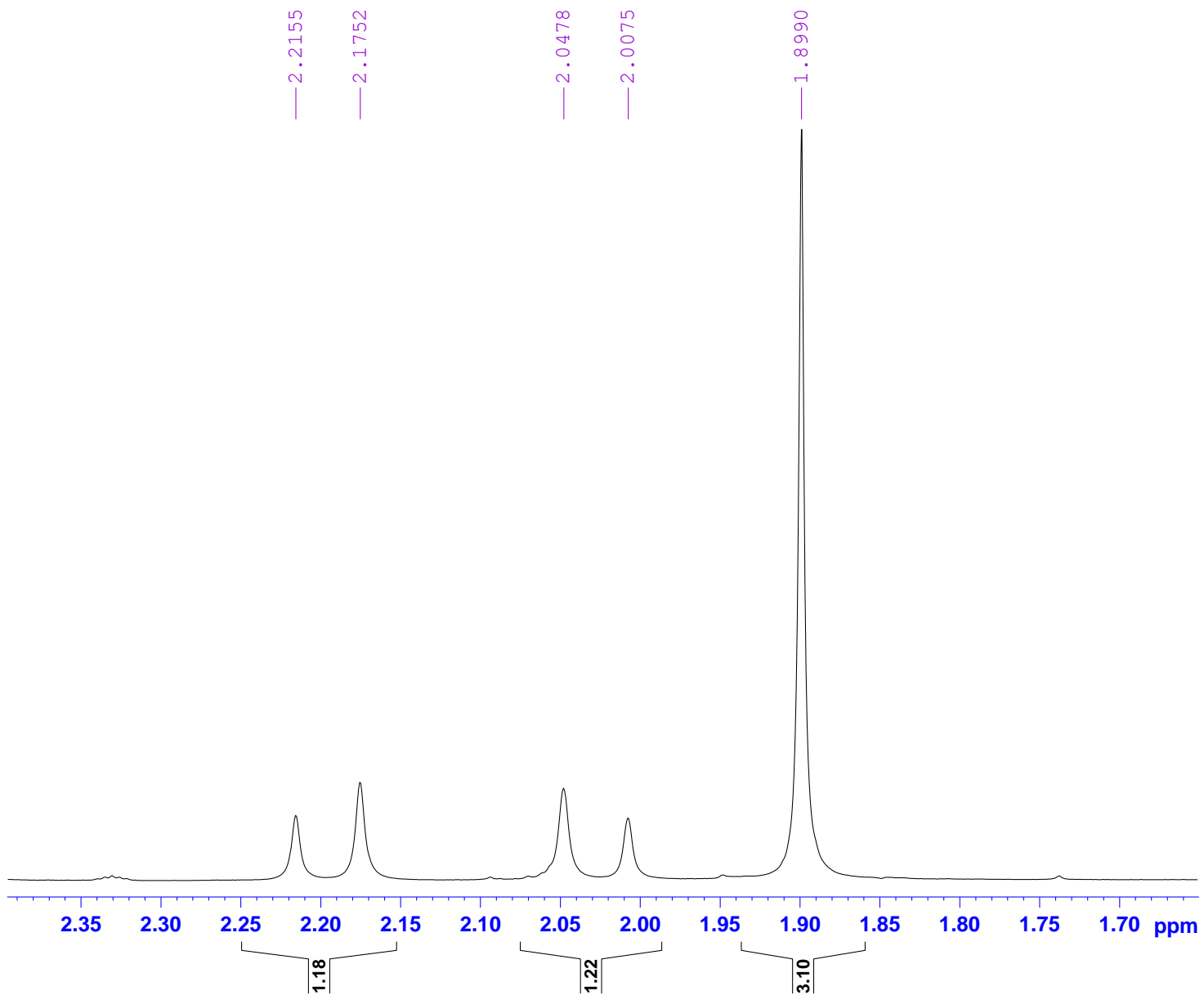
¹H NMR Spectrum of compound 4I

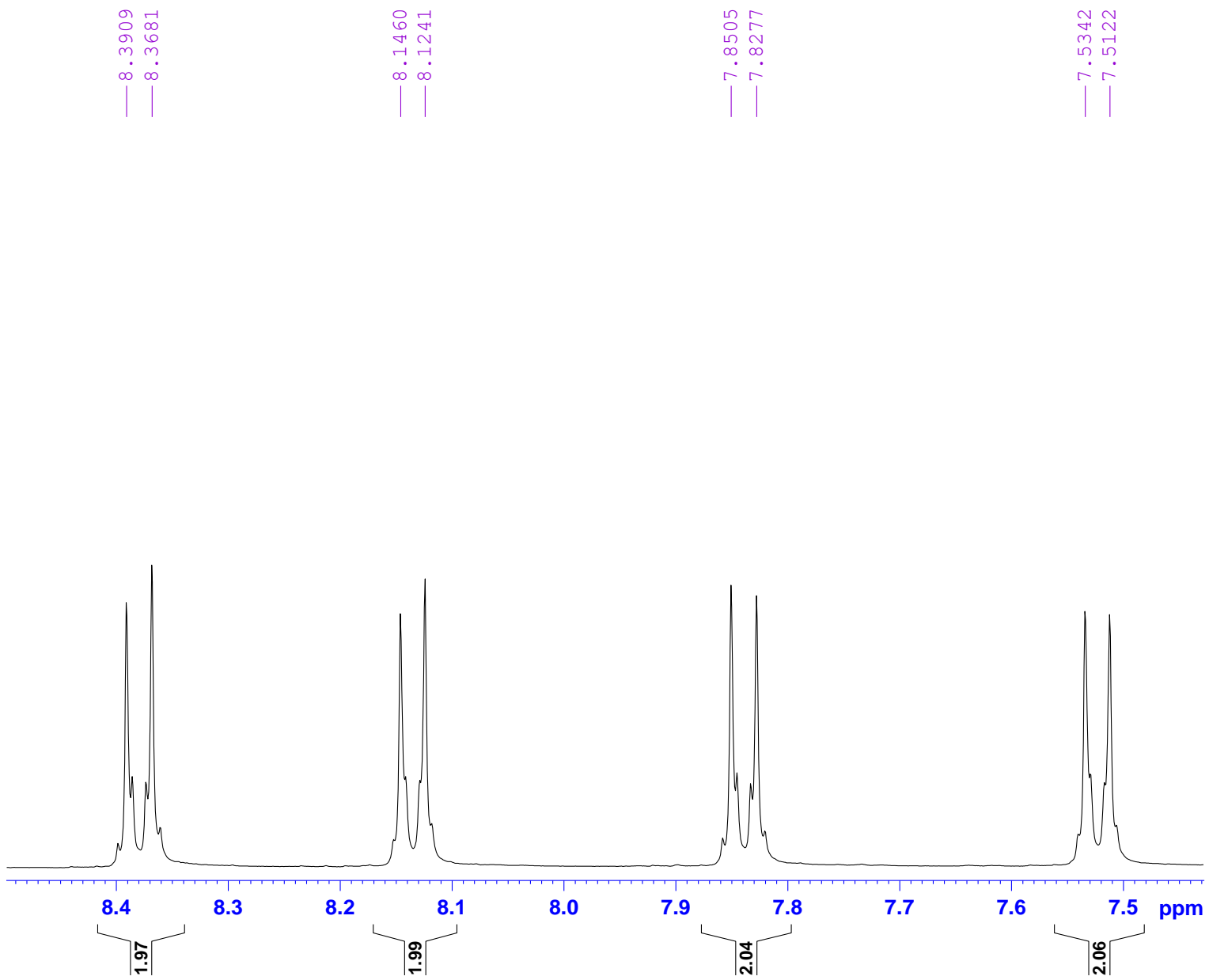


```

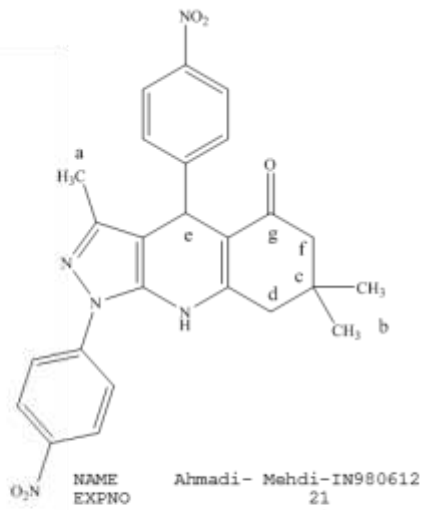
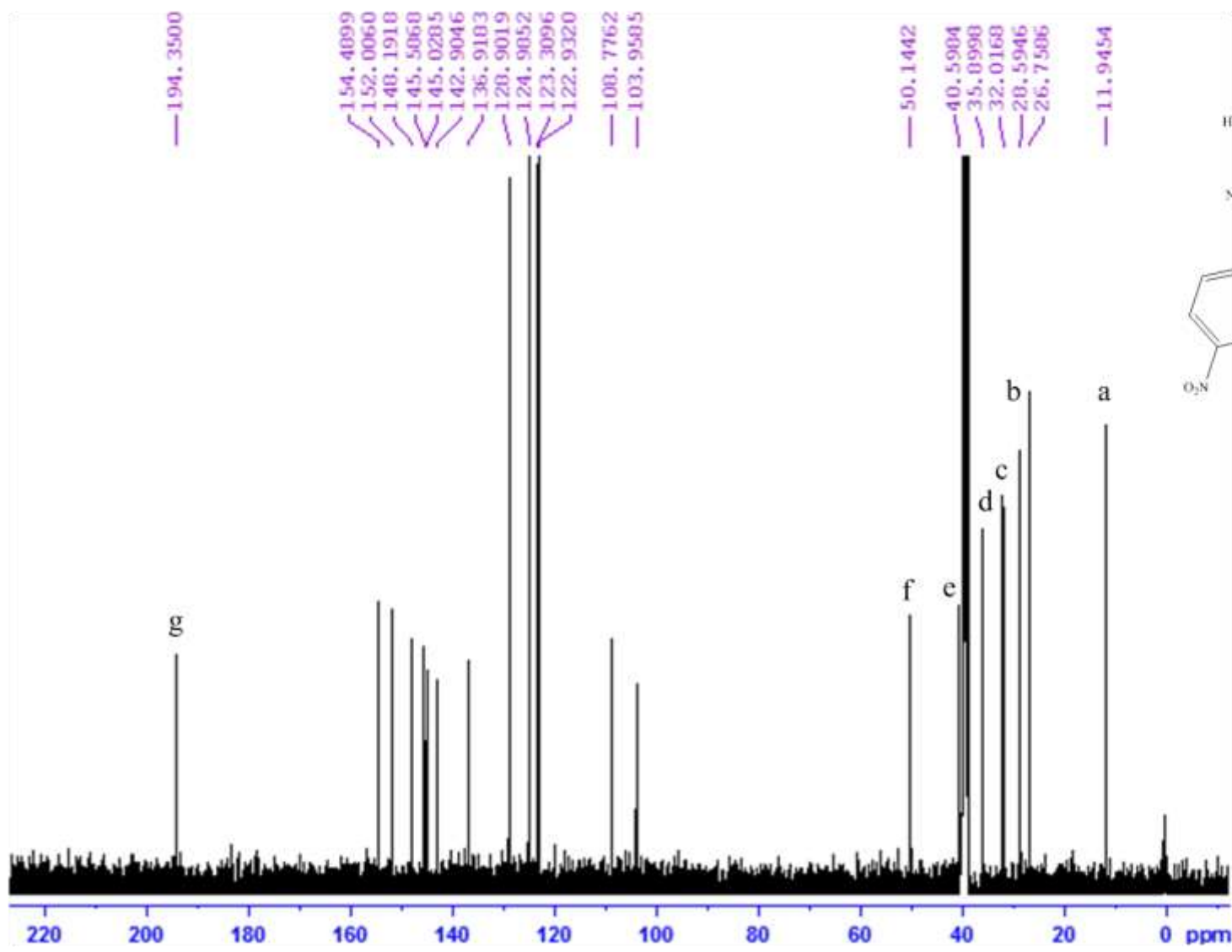
NAME      Ahmadi- Mehdi-IN980501
EXPNO     10
PROCNO    1
Date_     20190723
Time      13.31
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg
TD         50504
SOLVENT   DMSO
NS         32
DS         2
SWH        8802.817 Hz
FIDRES     0.174299 Hz
AQ         2.8686771 sec
RG         57
DW         56.800 usec
DE         6.50 usec
TE         295.1 K
D1         5.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         11.00 usec
PL1        -2.00 dB
PL1W       17.51671600 W
SFO1       400.1326008 MHz
SI         32768
SF         400.1300021 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```





¹³C NMR Spectrum of compound 4l

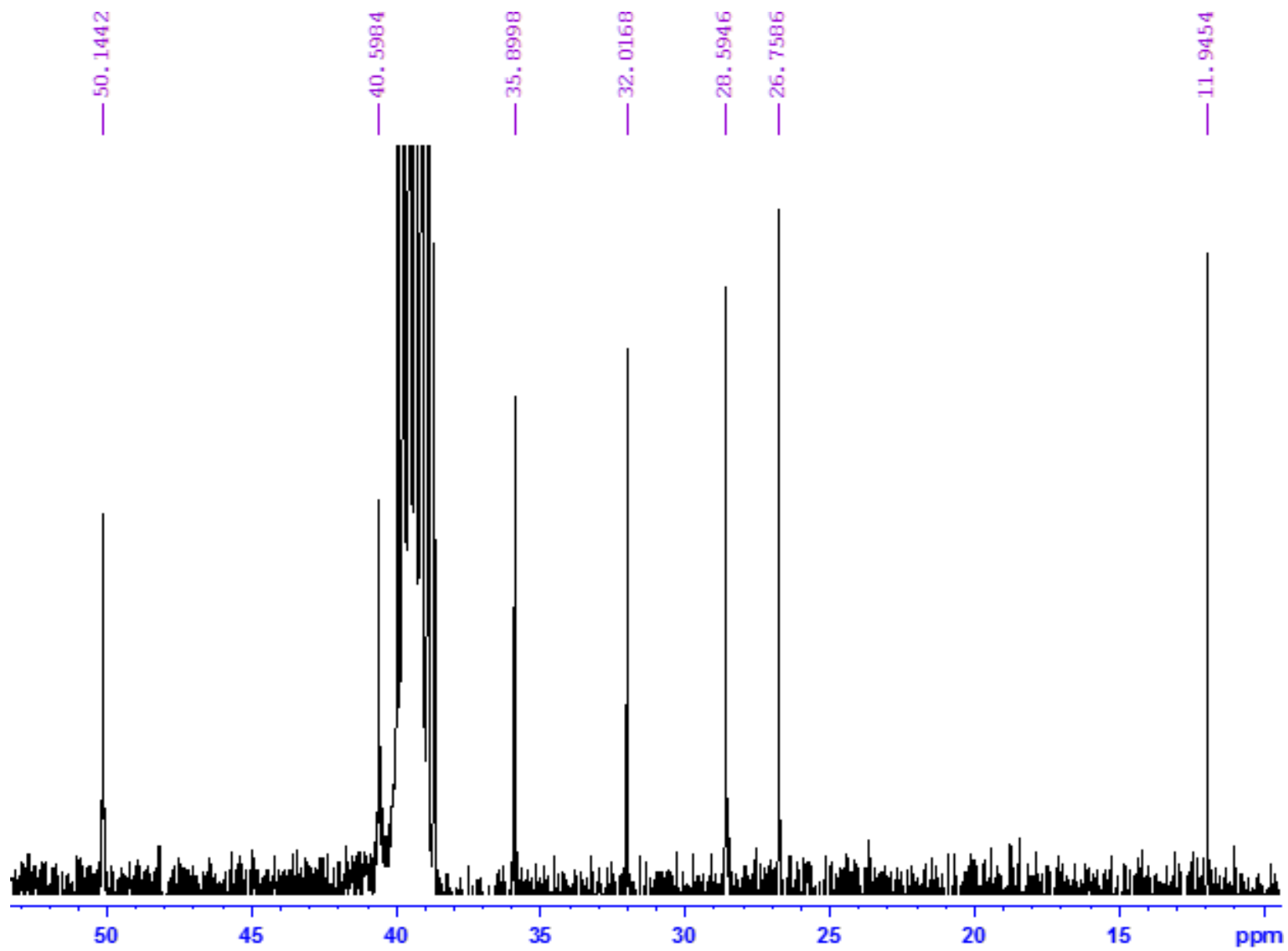


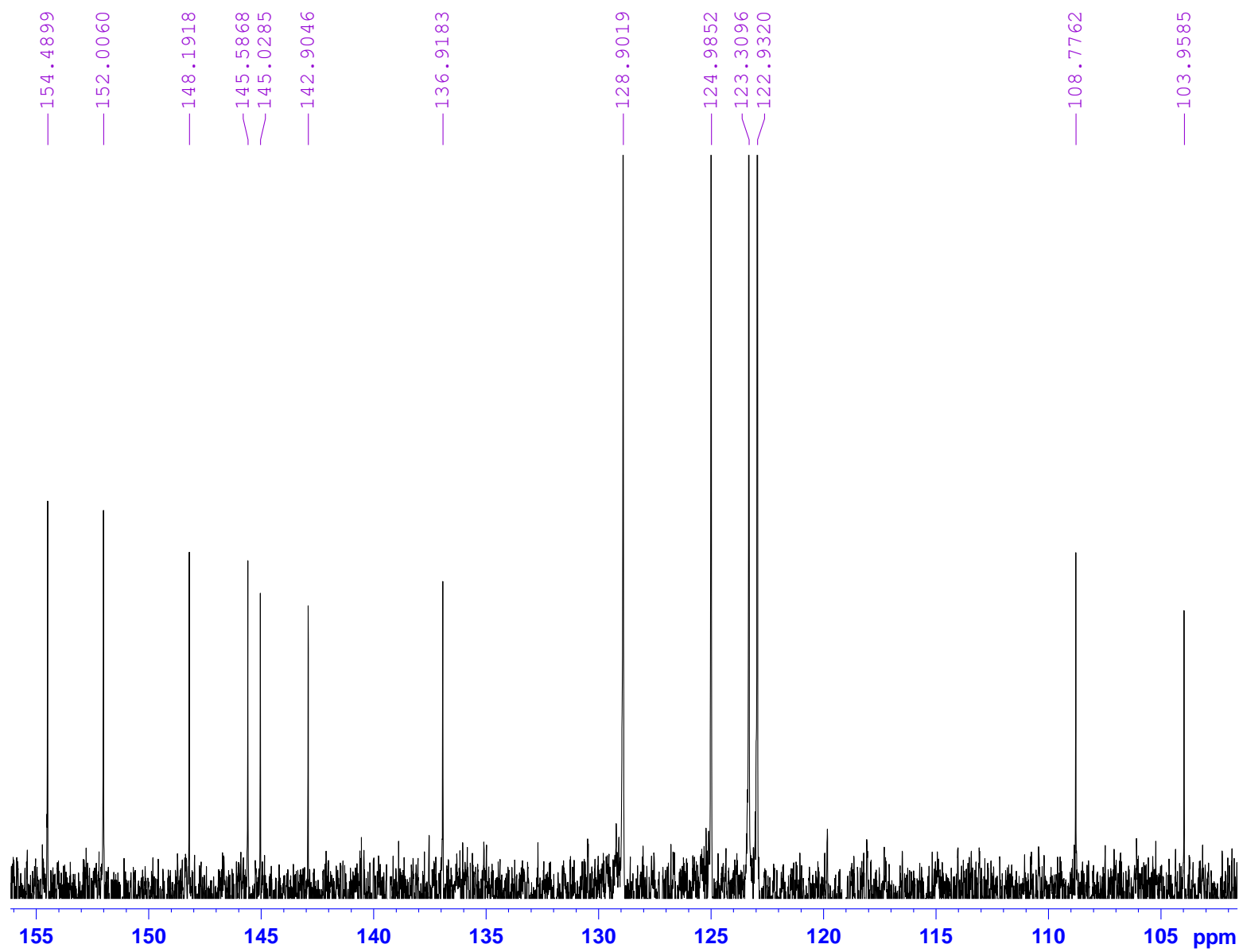
```

NAME      Ahmadi- Mehdi-IN980612
EXPNO     21
PROCNO    1
Date_     20190903
Time      14.27
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         50502
SOLVENT   DMSO
NS         1500
DS         2
SWH        25252.525 Hz
FIDRES     0.500030 Hz
AQ         0.9999896 sec
RG         2050
DW         19.800 usec
DE         6.50 usec
TE         294.8 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

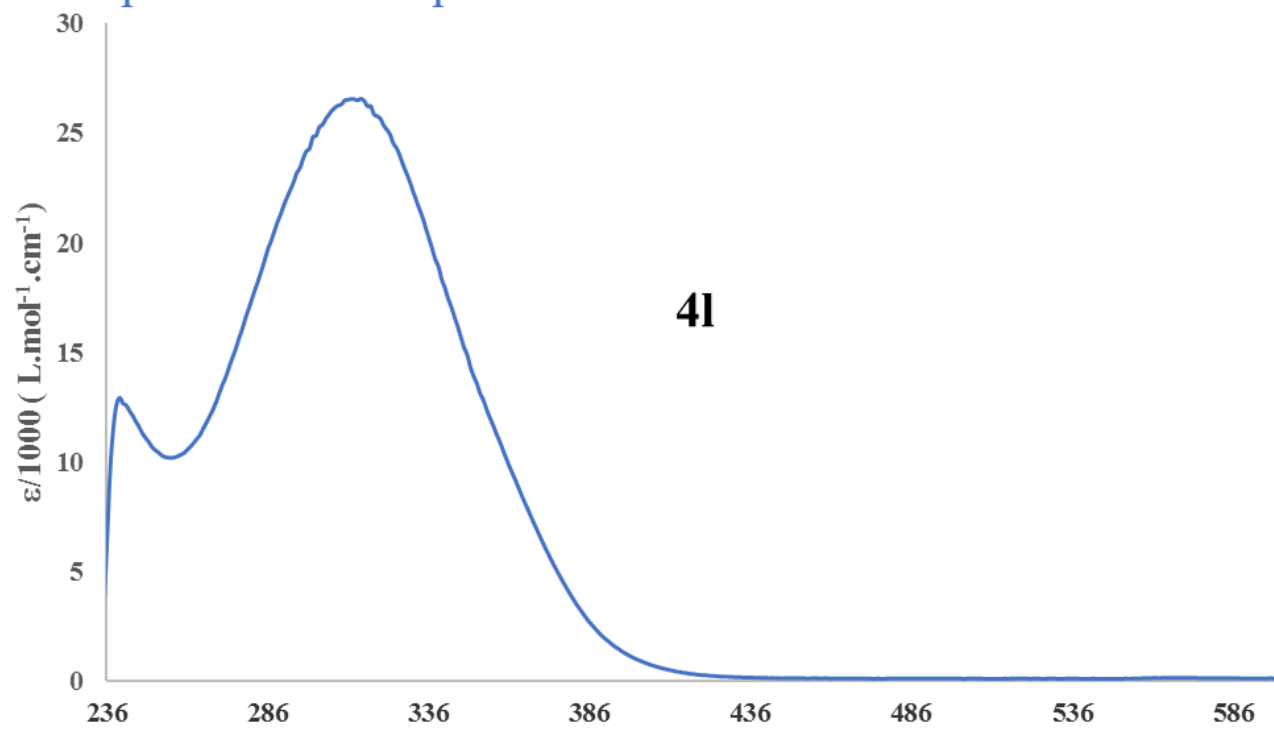
===== CHANNEL f1 =====
NUC1      13C
P1         9.50 usec
PL1        -1.00 dB
PL1W      42.69075012 W
SFO1      100.6238364 MHz

===== CHANNEL f2 =====
    
```



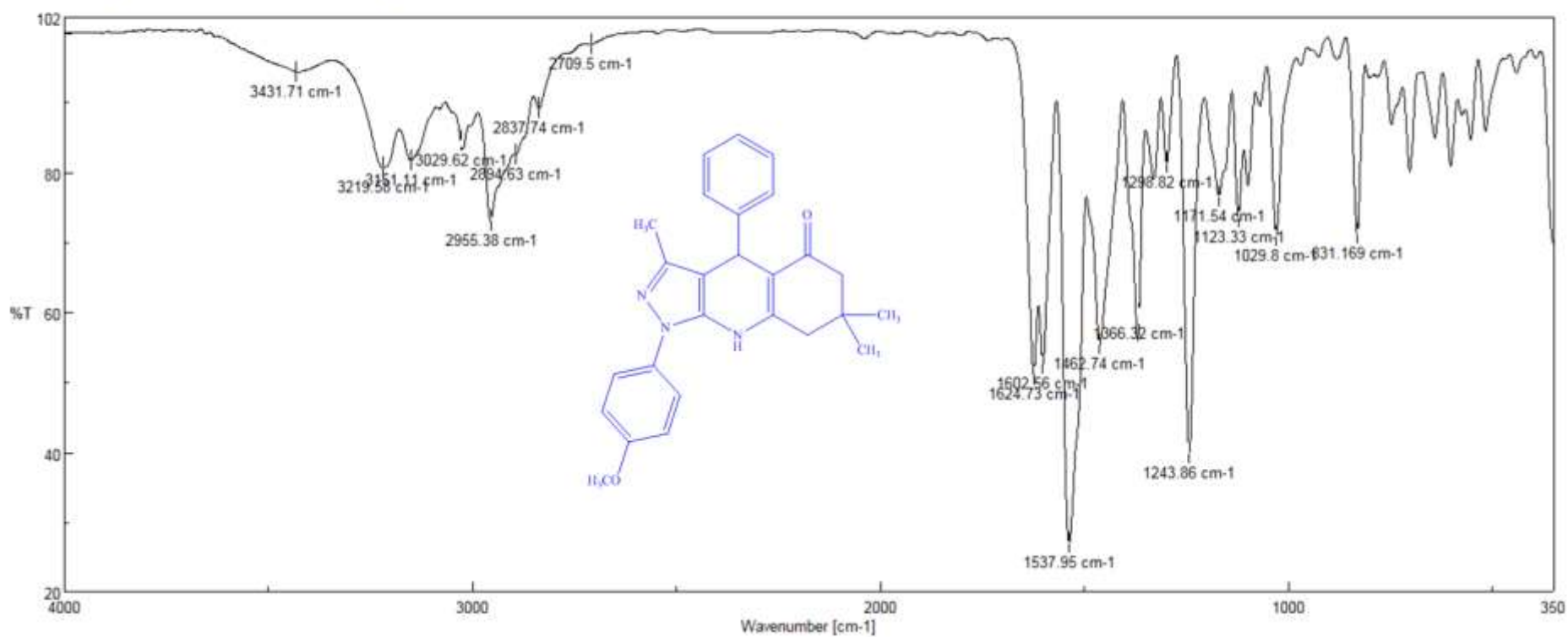
UV-Spectrum of compound **4l**



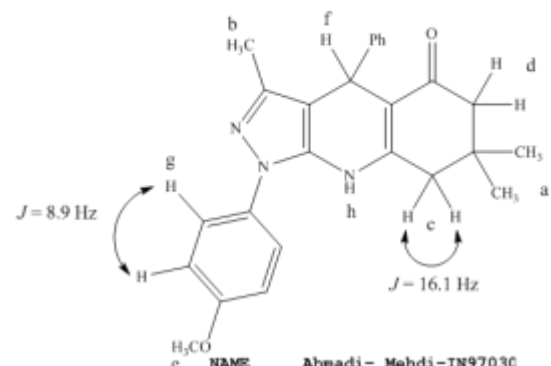
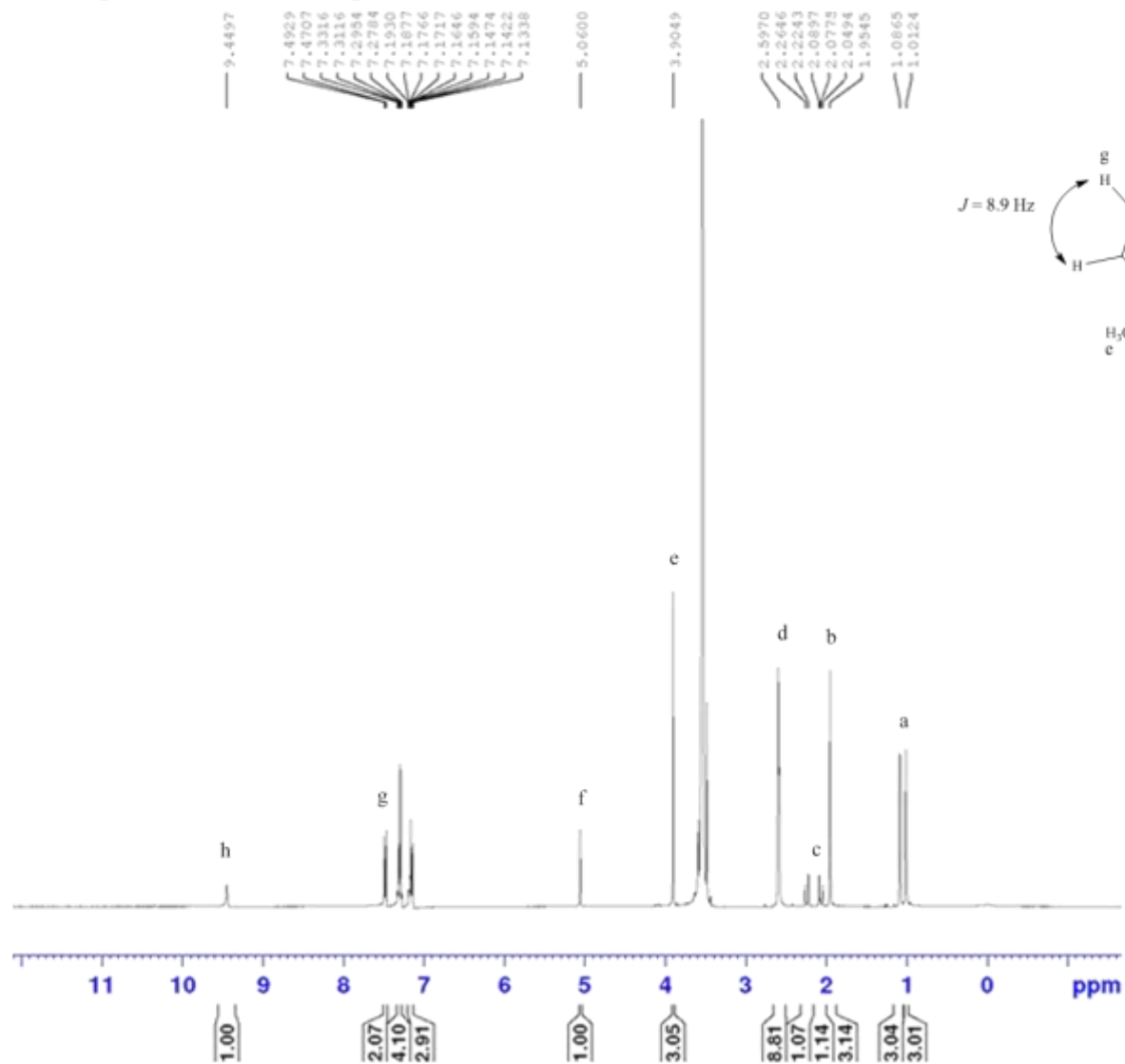
4l

UV-absorption spectrum of **4l** in CHCl_3

IR-Spectrum of compound 4m



¹H NMR Spectrum of compound 4m



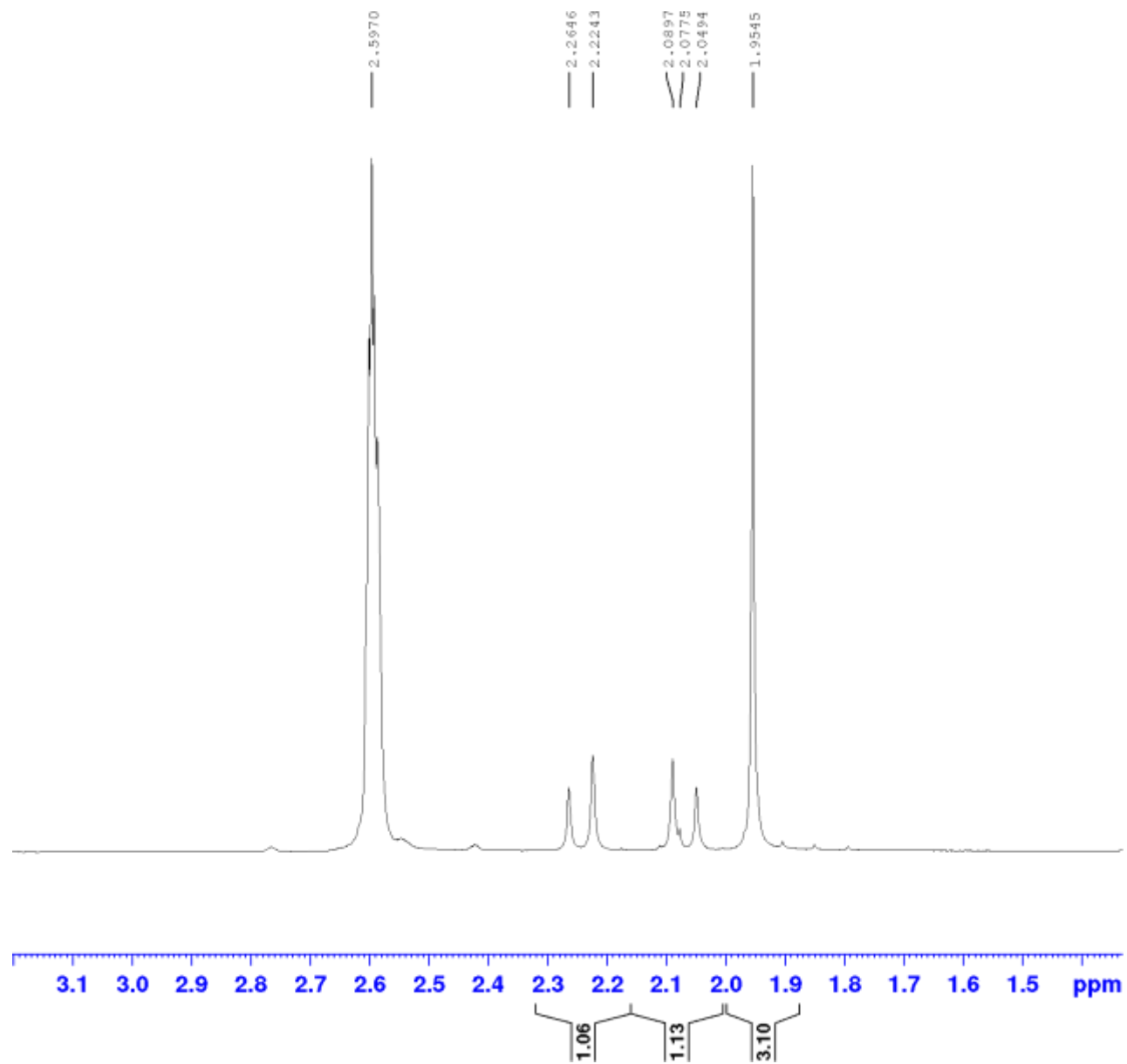
```

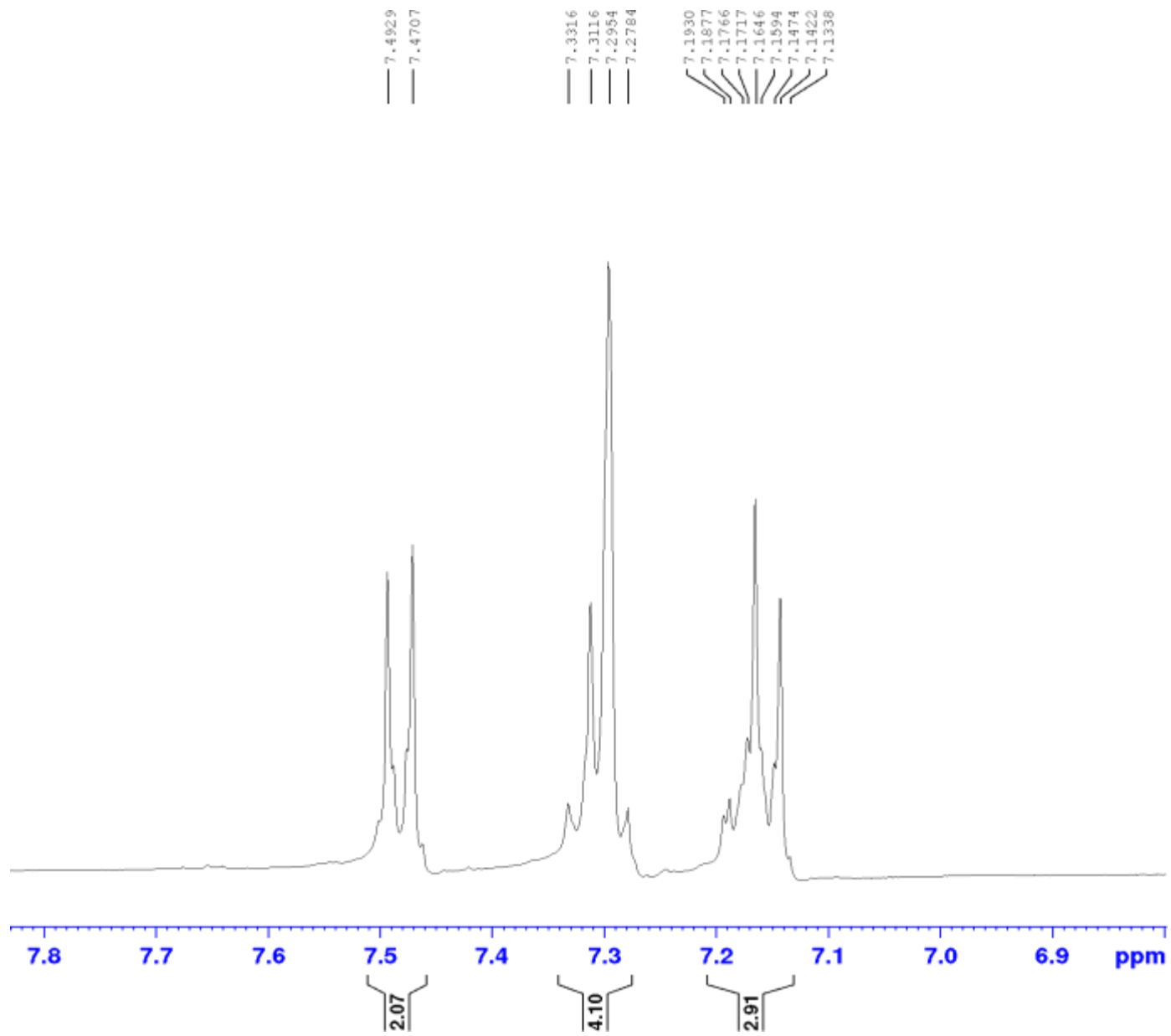
NAME      Ahmadi- Mehdi-IN97030
EXPNO    61
PROCNO   1

F2 - Acquisition Parameters
Date_    20180526
Time     14.29
INSTRUM  spect
PROBHD   5 mm PABBO BB-
PULPROG  zg
TD        50504
SOLVENT  DMSO
NS        32
DS        2
SWH       8417.509 Hz
FIDRES    0.166670 Hz
AQ        2.9999375 sec
RG        36
DW        59.400 usec
DE        6.50 usec
TE        296.4 K
D1        5.00000000 sec
TD0       1

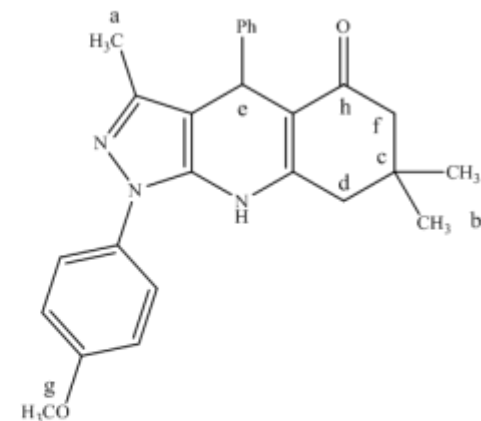
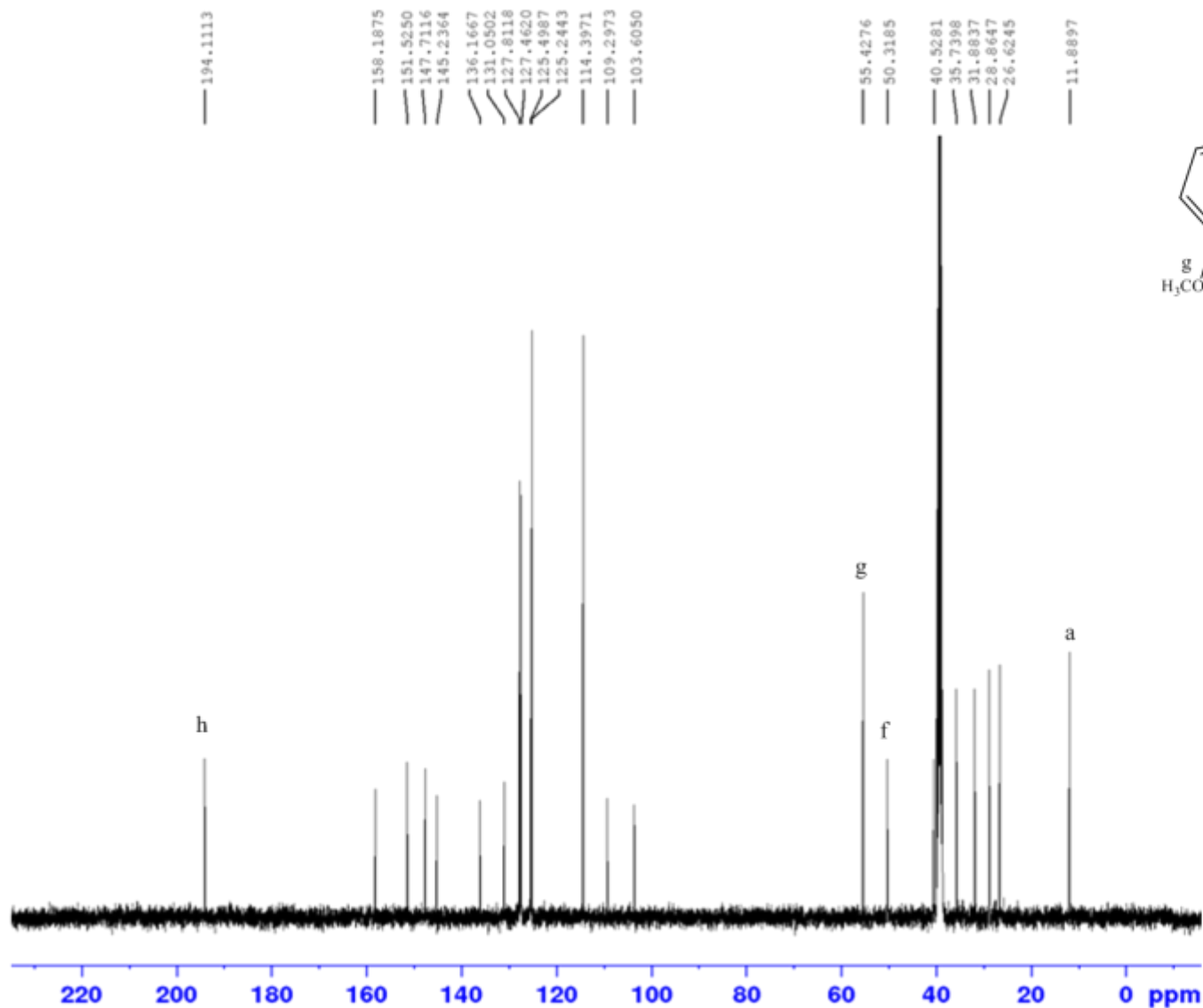
===== CHANNEL f1 =====
NUC1      1H
P1        11.00 usec
PL1       -2.00 dB
PL1W      17.51671600 W
SFO1      400.1326008 MHz

F2 - Processing parameters
SI        32768
SF        400.1299650 MHz
WDW       EM
SSB       0
GB        0.30 Hz
    
```





¹³C NMR Spectrum of compound 4m



```

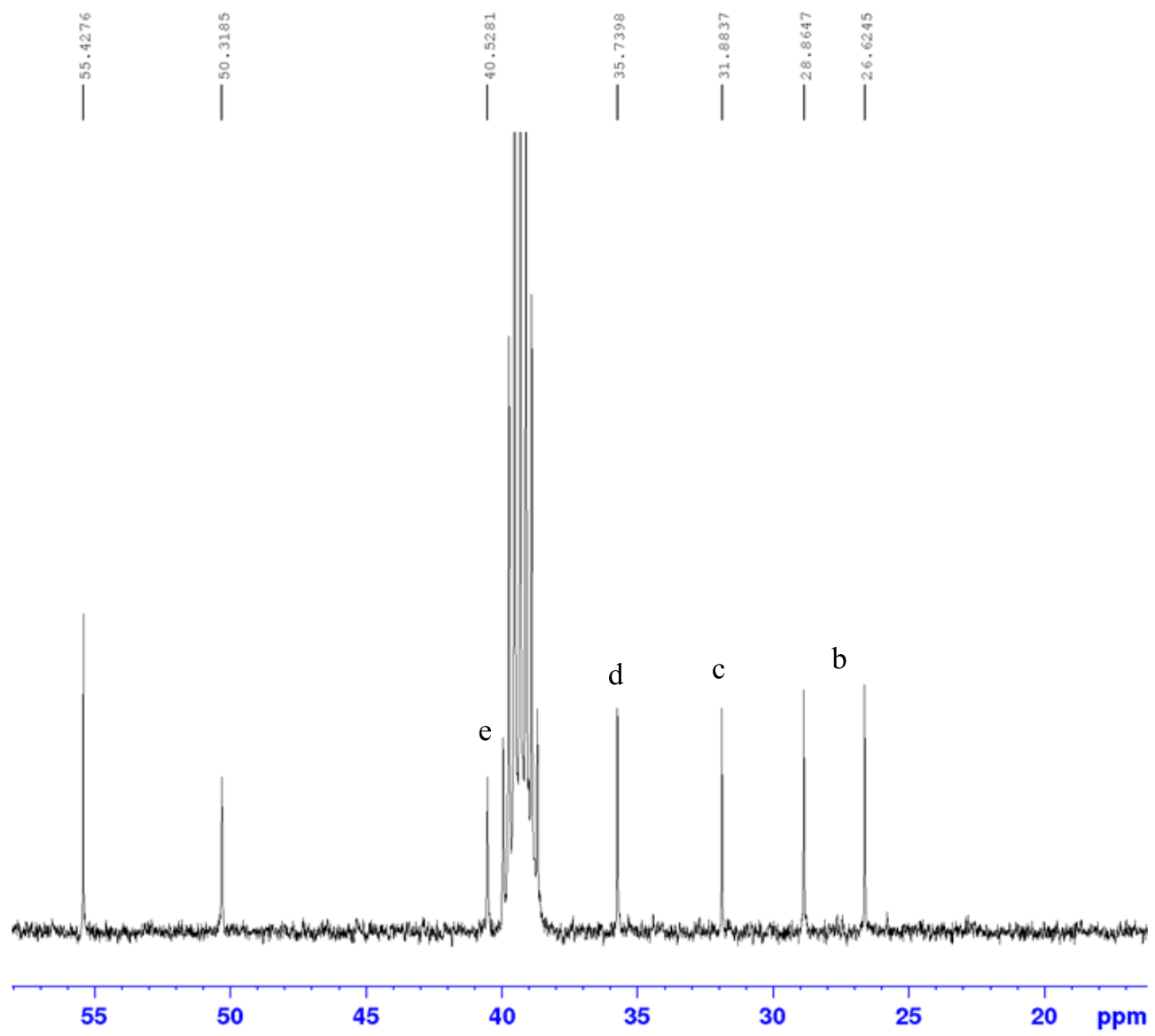
Current Data Parameters
NAME      Ahmadi- Mehdi-IN9703C
EXPNO     21
PROCNO    1

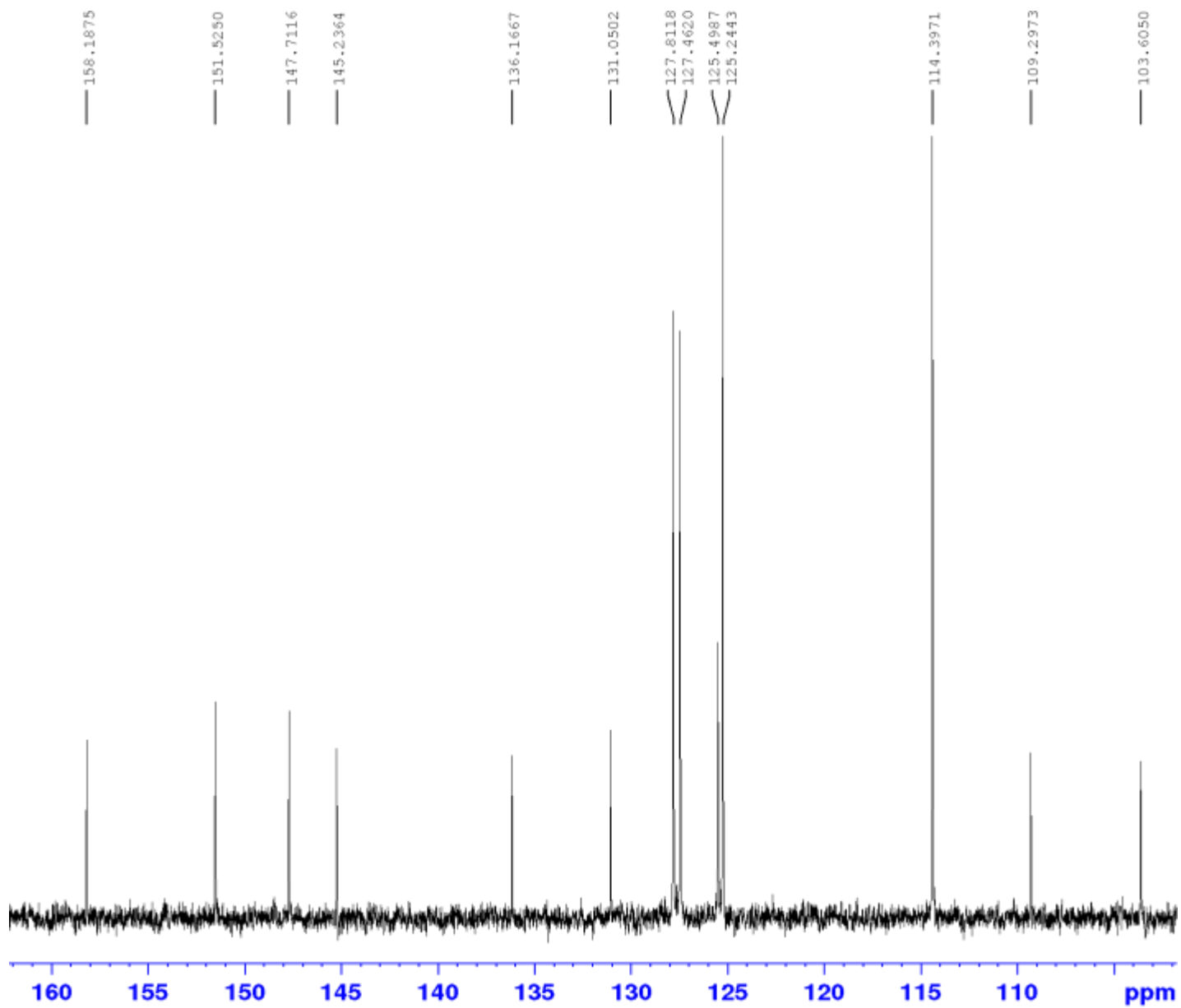
F2 - Acquisition Parameters
Date_     20180602
Time      9.20
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg3
TD         50502
SOLVENT   DMSO
NS         1500
DS         2
SWH        25252.525 Hz
FIDRES     0.500030 Hz
AQ         0.9999396 sec
RG         2050
DW         19.800 usec
DE         6.50 usec
TE         294.7 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

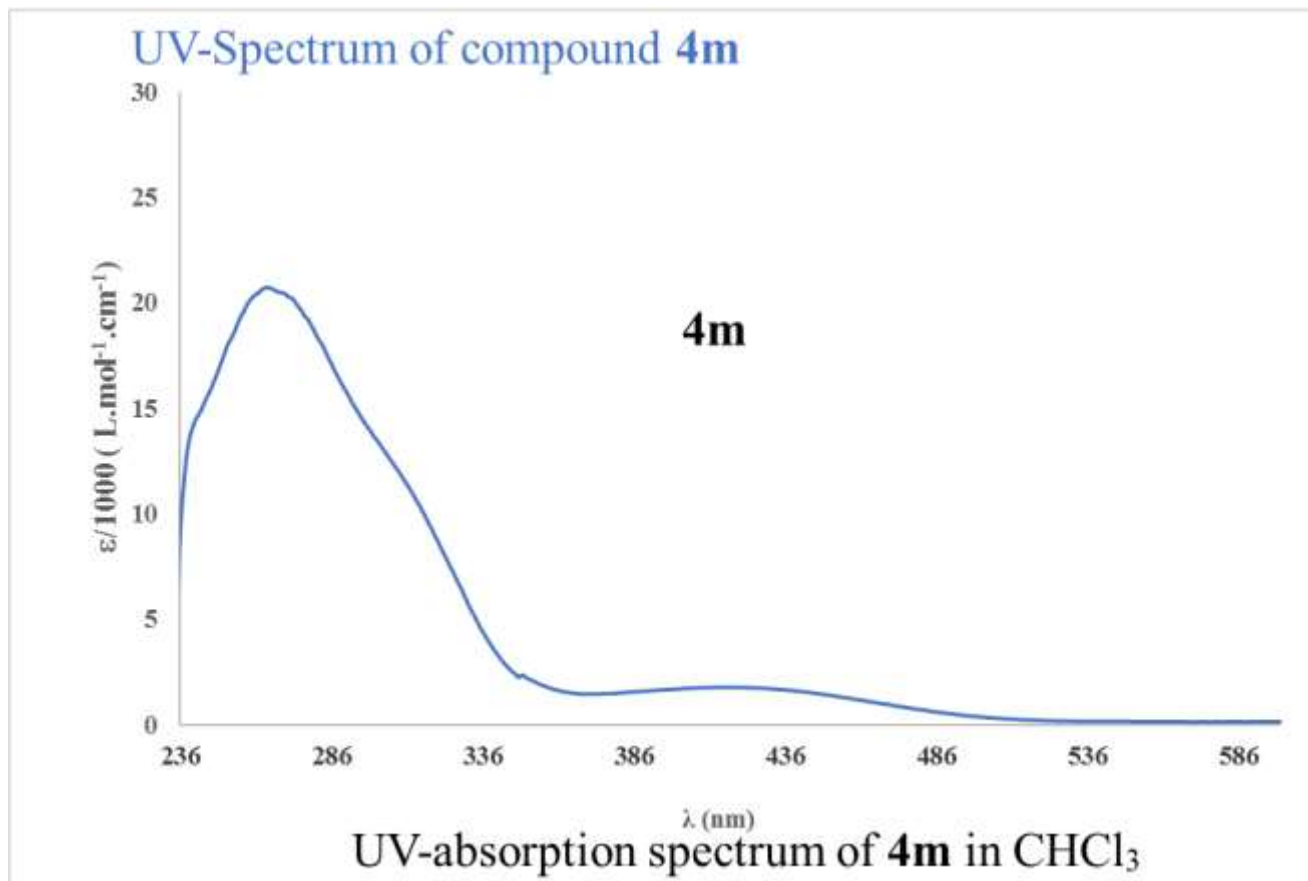
===== CHANNEL f1 =====
NUC1       13C
P1         8.70 usec
PL1        -1.00 dB
PL1W       42.69075012 W
SFO1       100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2         0 dB
PL12        15.26 dB
PL13        18.26 dB
PL1W       11.05230045 W
PL12W      0.32919458 W
PL13W      0.16498812 W
SFO2       400.1316005 MHz

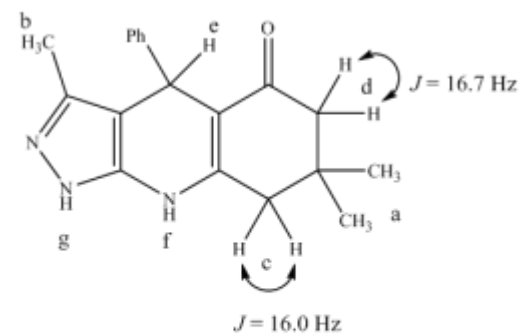
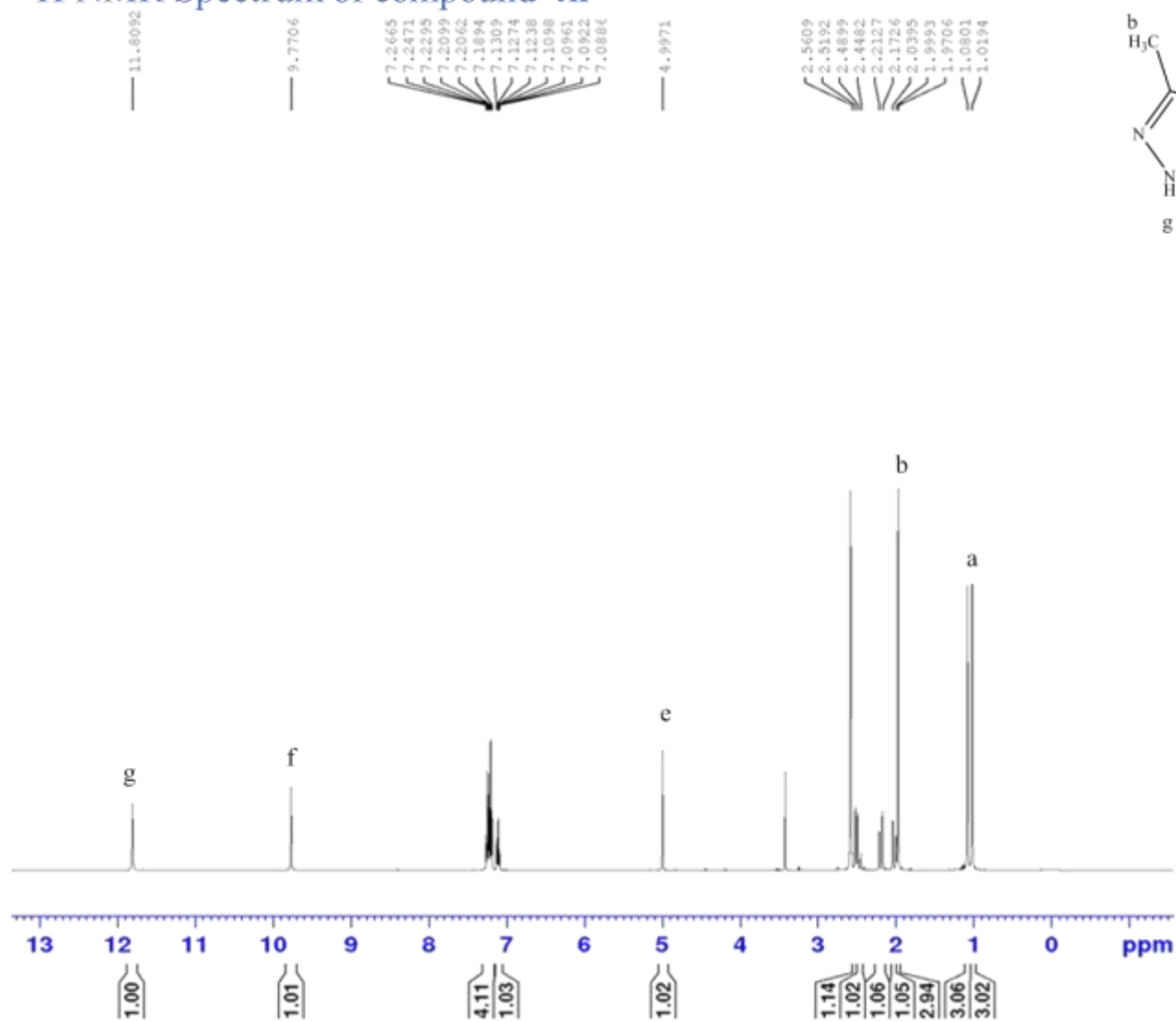
F2 - Processing parameters
SI         32768
SF         100.6128123 MHz
WDW        EM
SSB         0
LB         1.00 Hz
GB         0
  
```





¹H NMR Spectrum of compound 4n

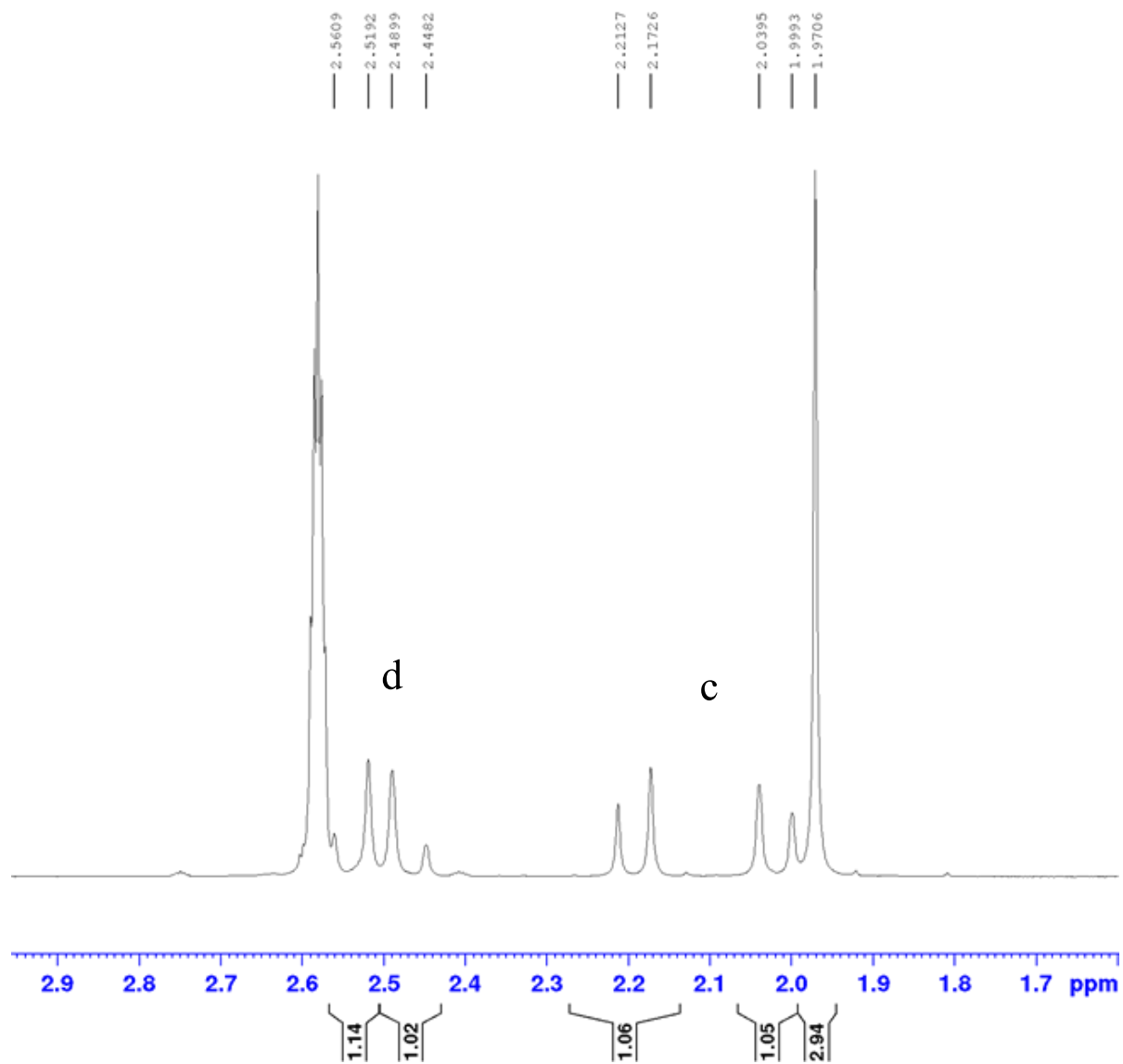


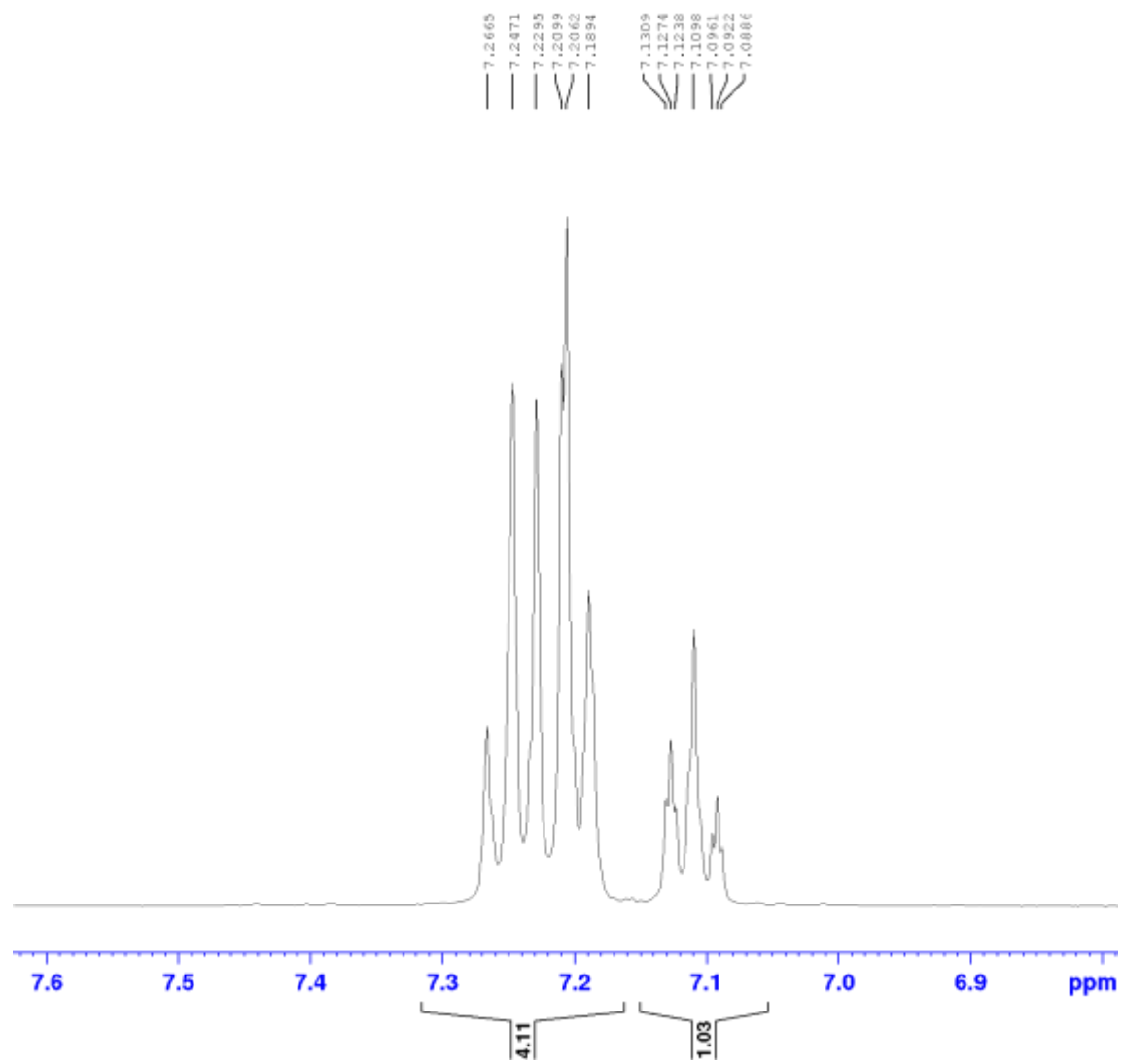
NAME HNMR 115
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180128
Time 14.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 50504
SOLVENT DMSO
NS 32
DS 2
SWH 8417.509 Hz
FIDRES 0.166670 Hz
AQ 2.9999375 sec
RG 80.6
DW 59.400 usec
DE 6.50 usec
TE 294.6 K
D1 5.00000000 sec
TD0 1

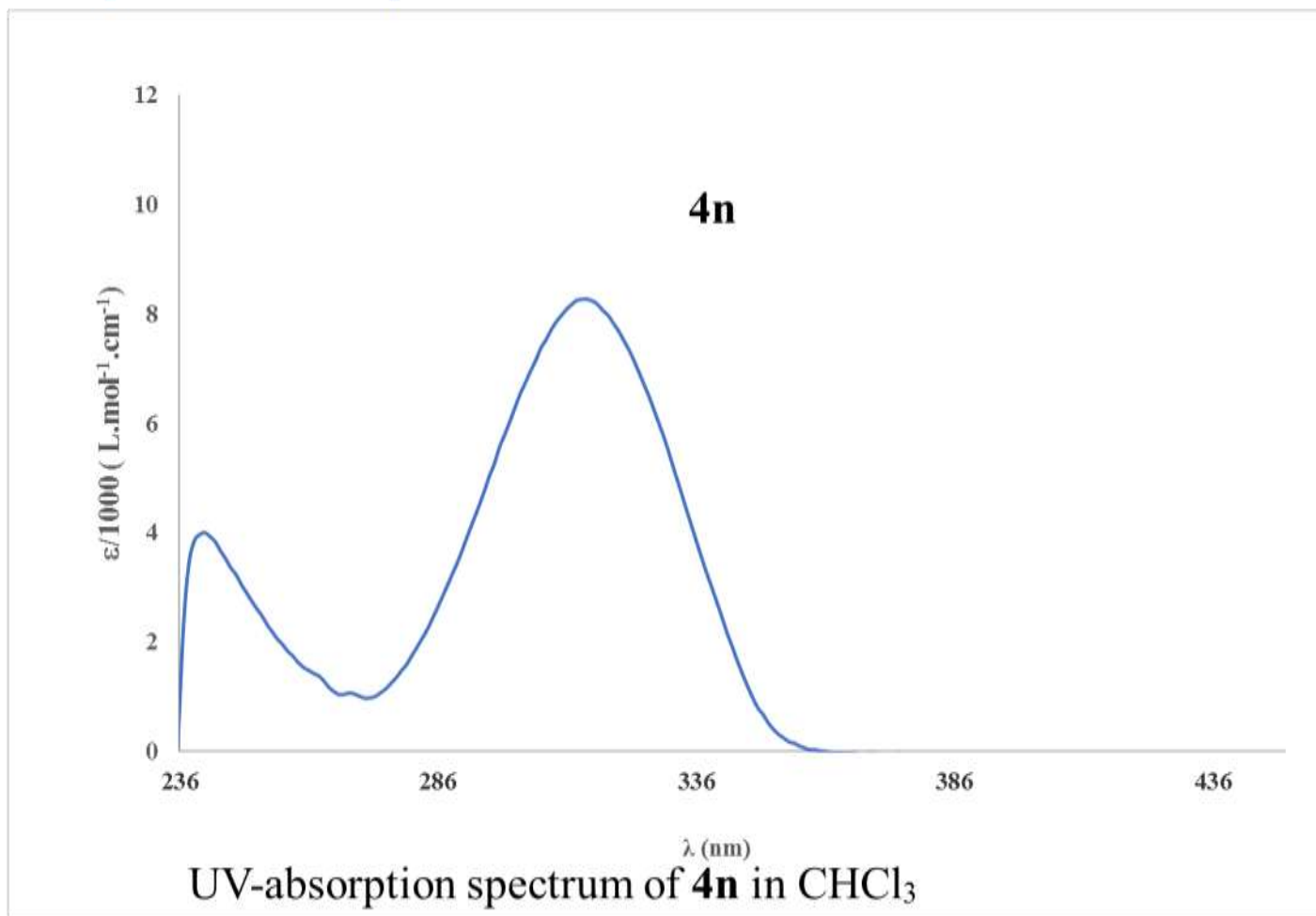
----- CHANNEL f1 -----
NUC1 1H
P1 11.00 usec
PL1 -2.00 dB
PL1W 17.51671600 W
SF01 400.1326008 MHz

F2 - Processing parameters
SI 32768
SF 400.1299709 MHz
WDW EM
SSB 0
GB 0.30 Hz

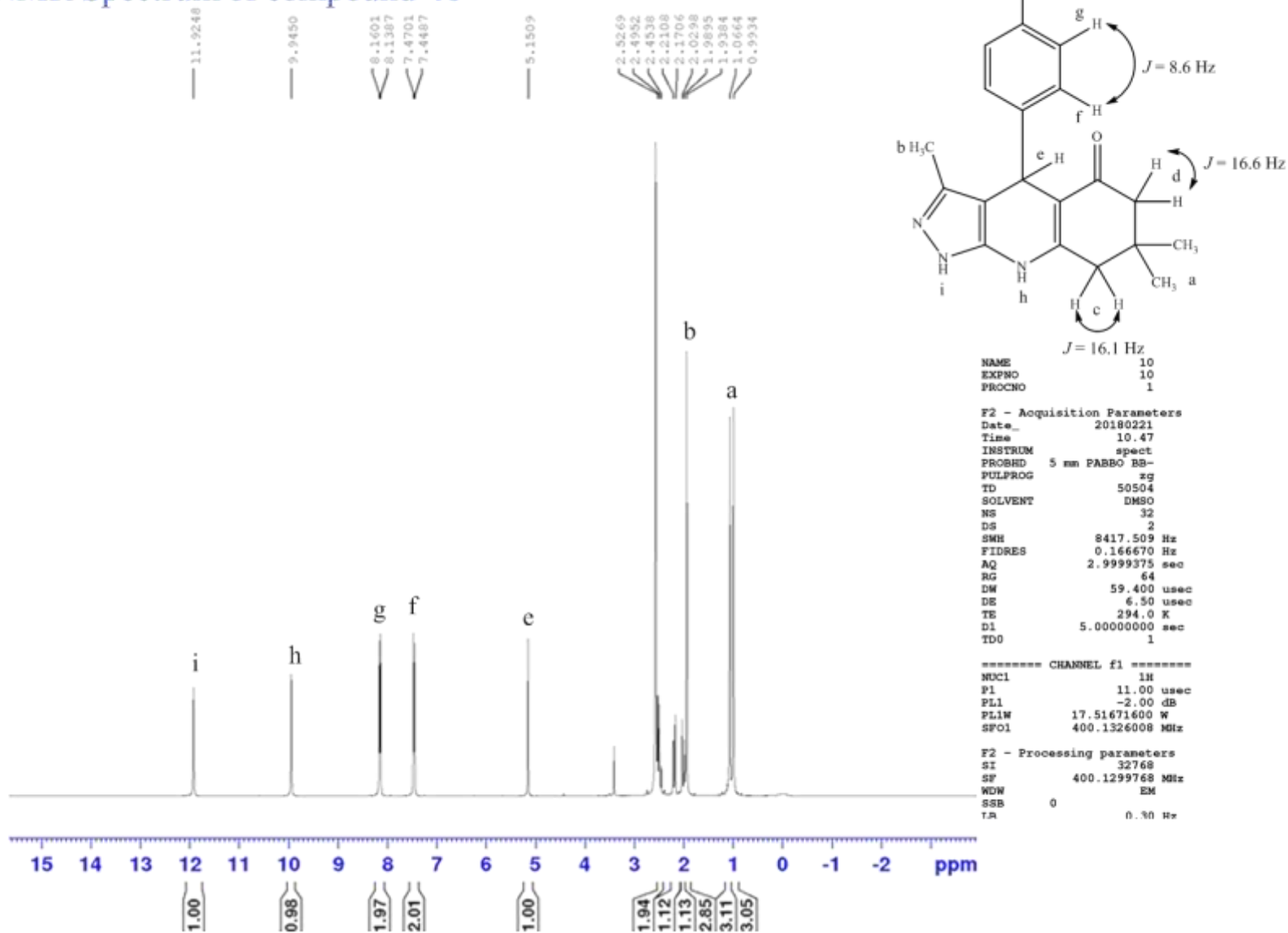


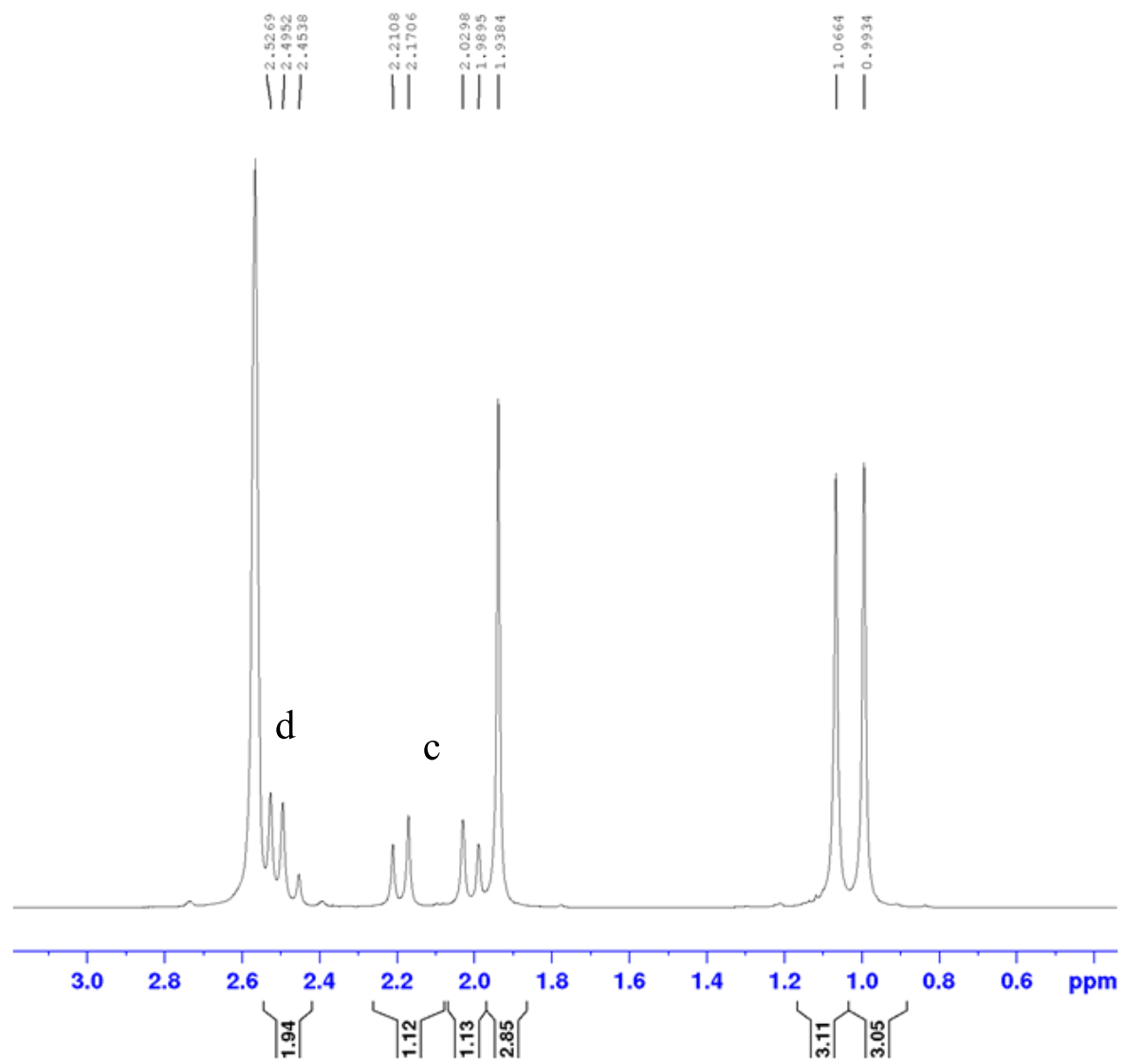


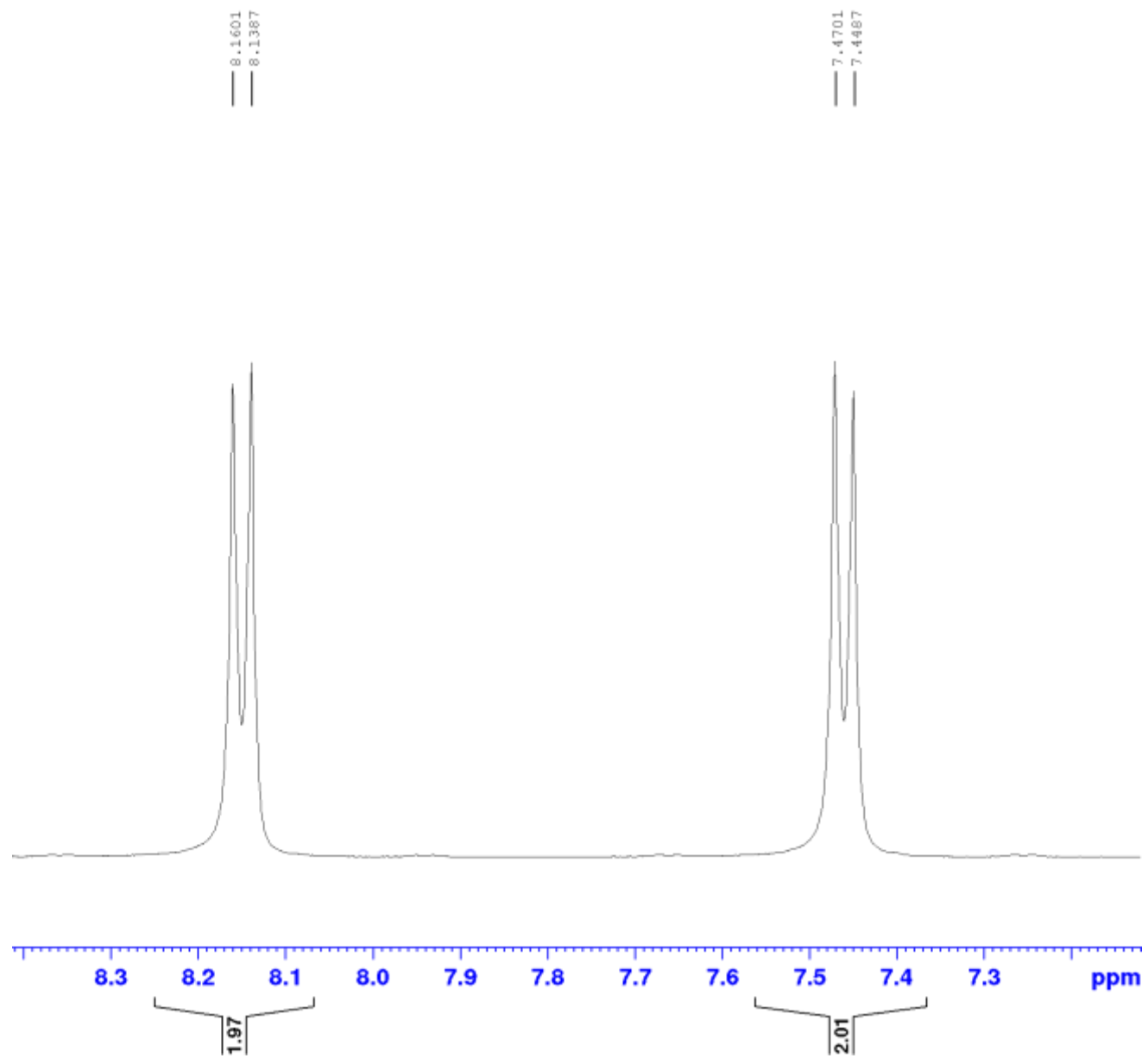
UV-Spectrum of compound **4n**



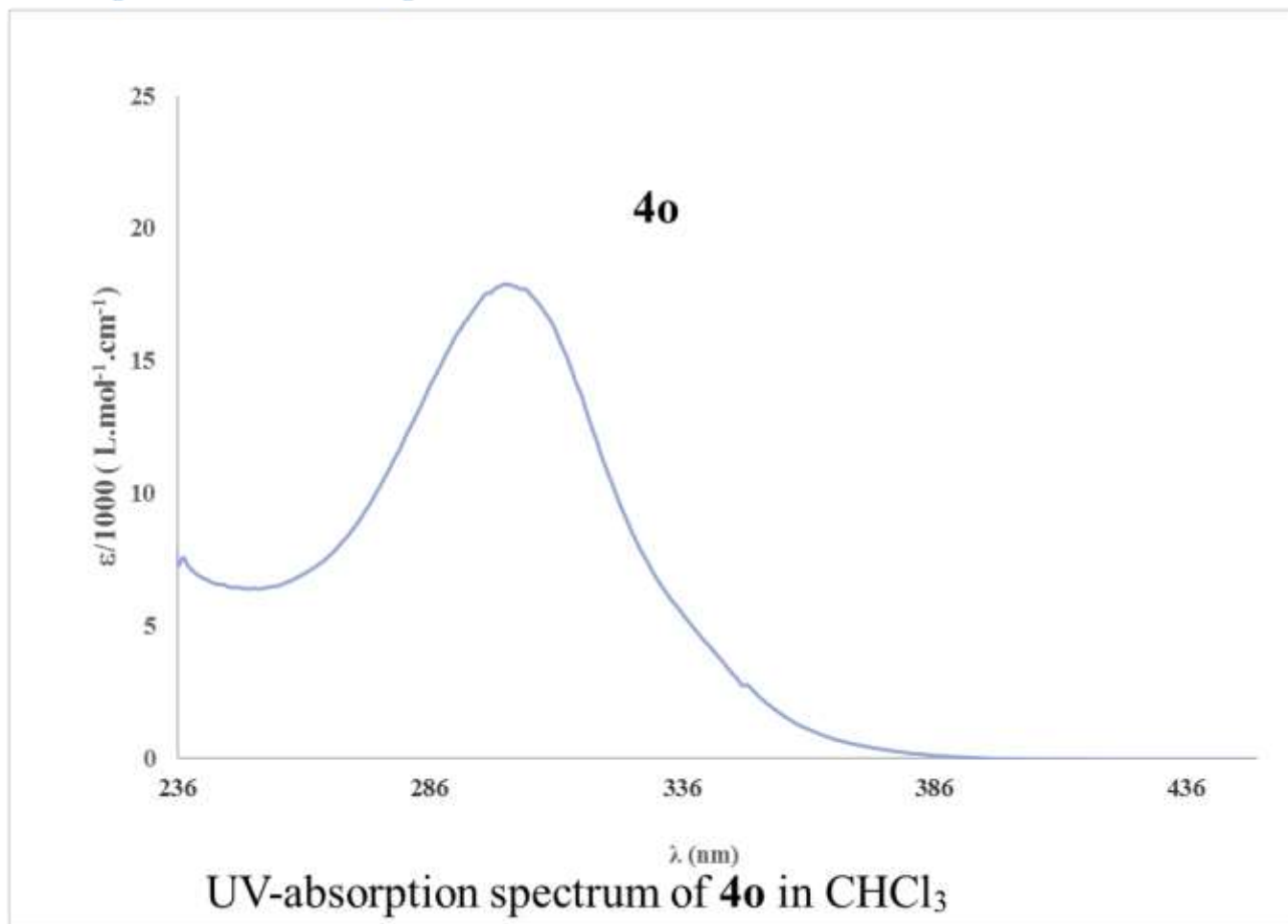
¹H NMR Spectrum of compound 4o



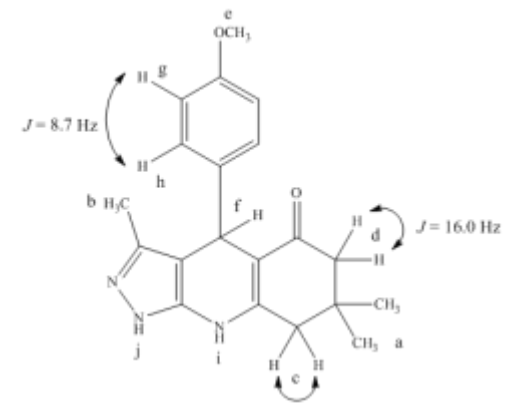
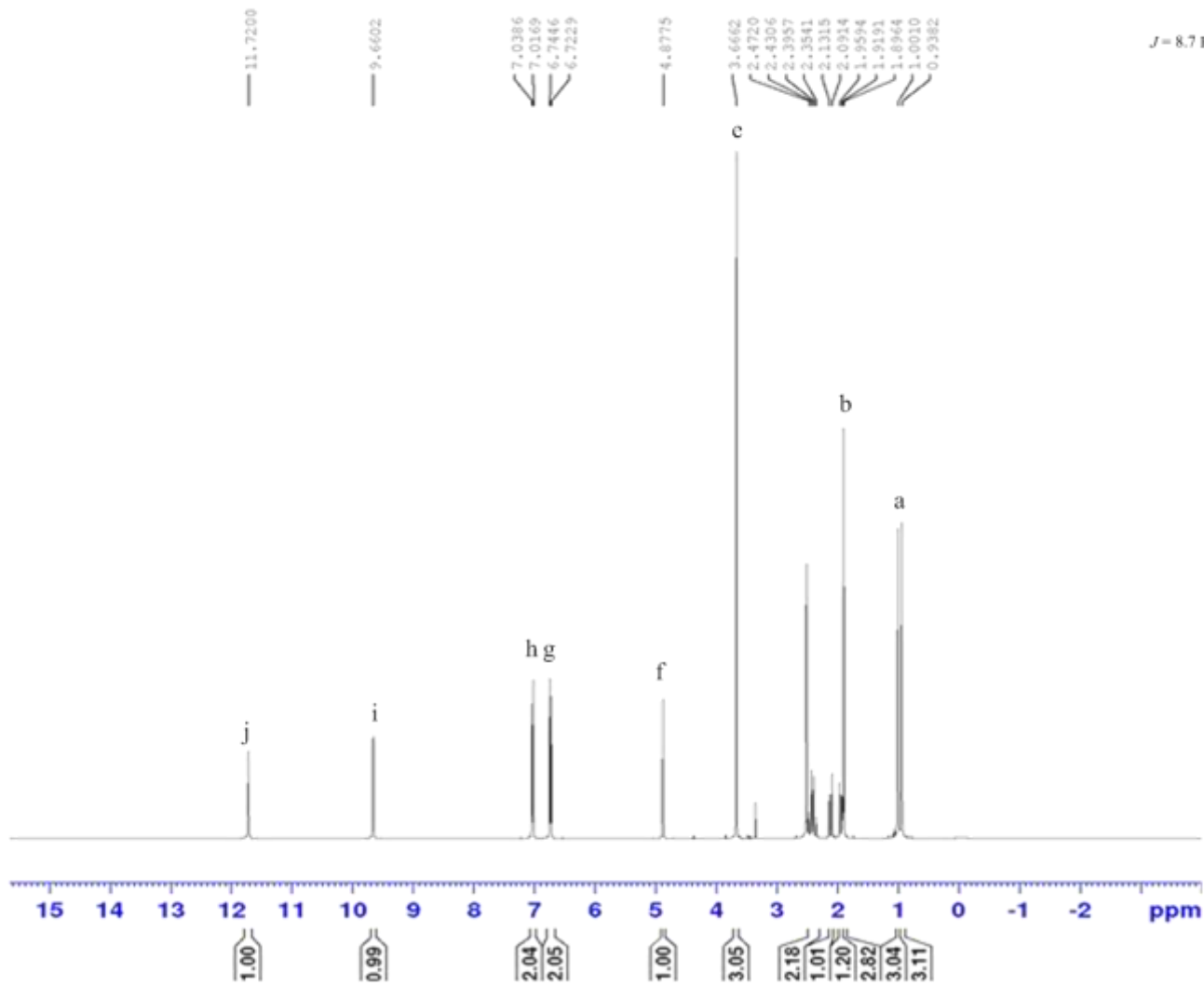




UV-Spectrum of compound **4o**



¹H NMR Spectrum of compound 4p



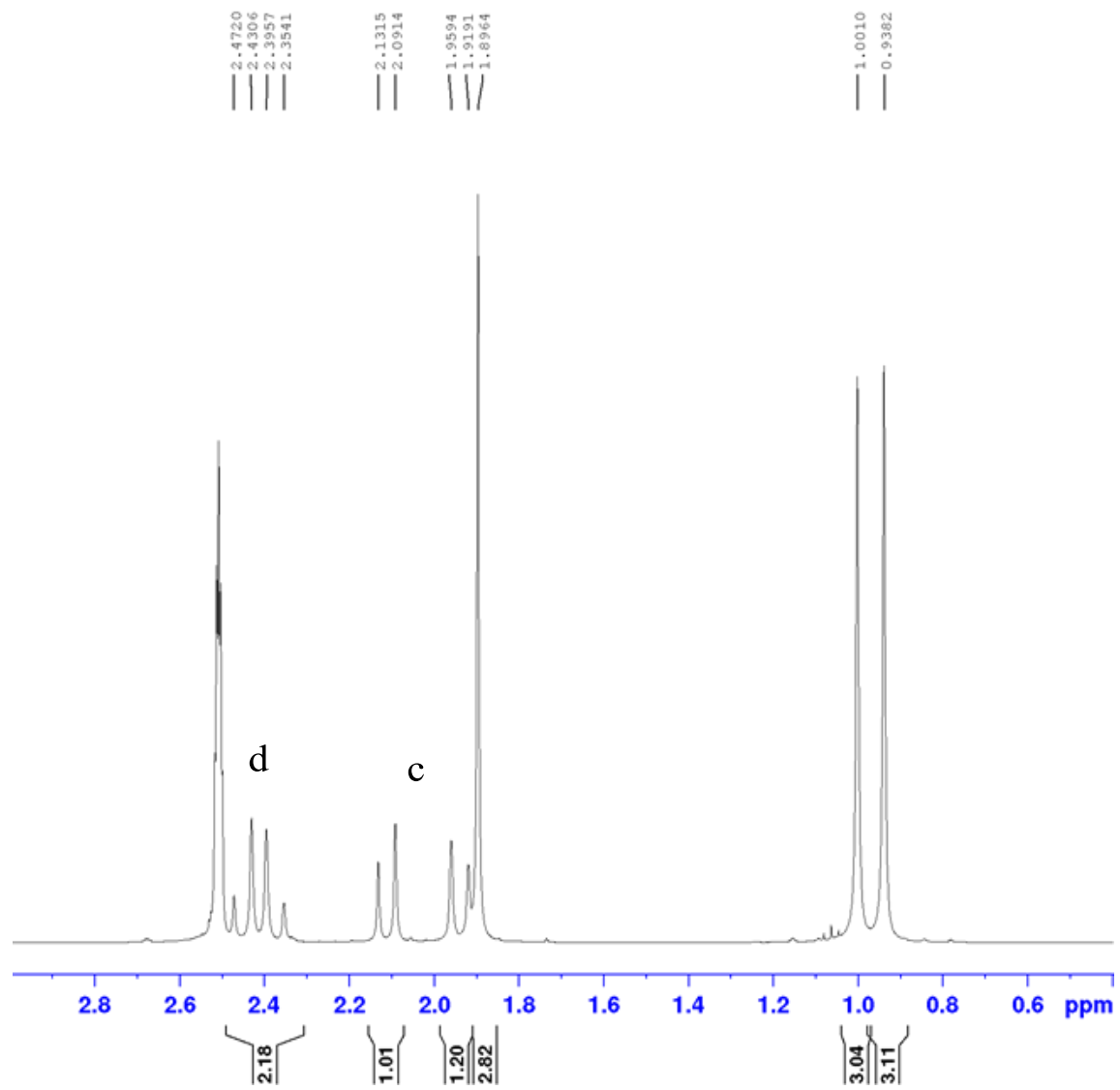
```

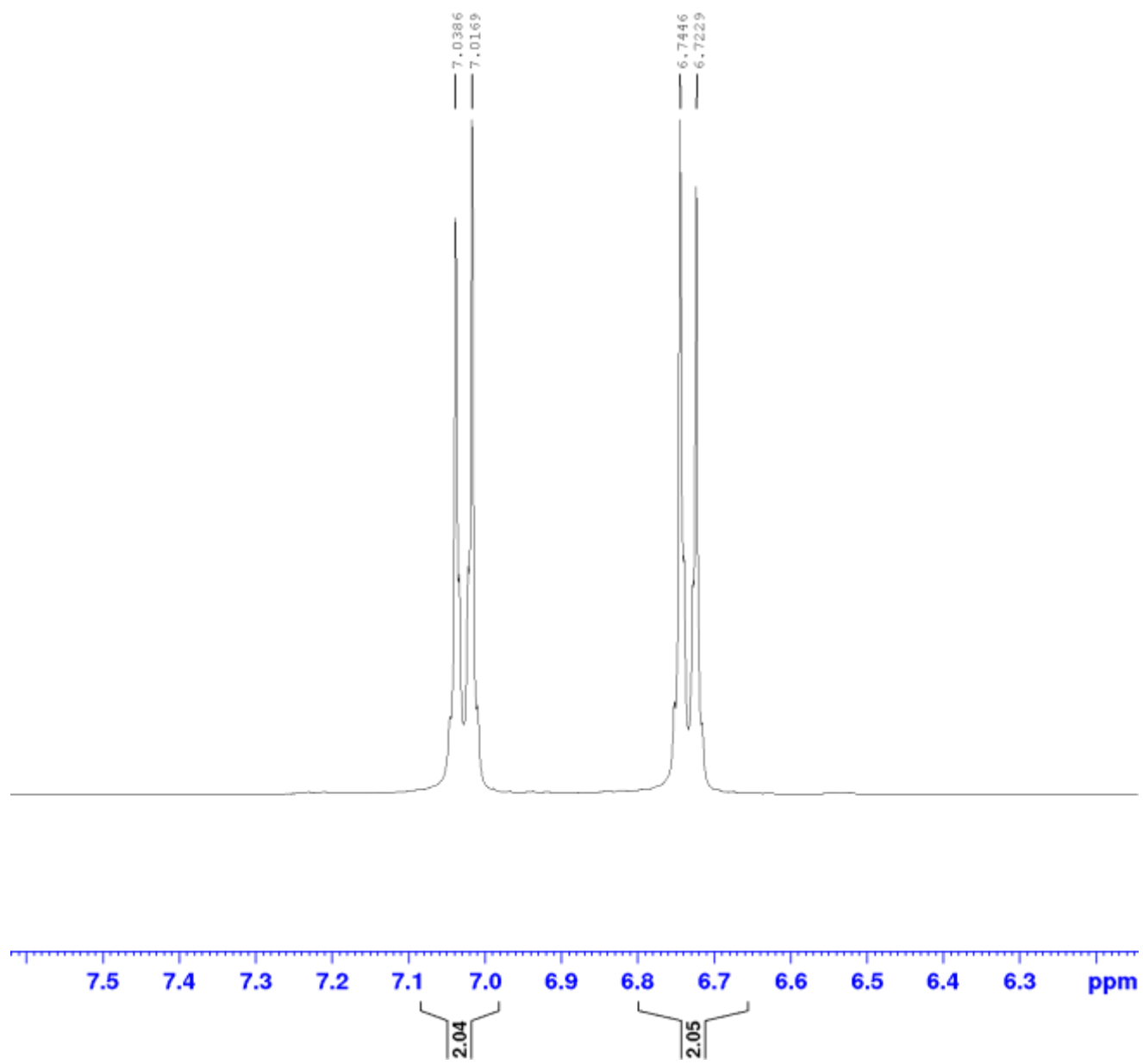
NAME          hnmr 119
EXPNO         20
PROCNO        1

F2 - Acquisition Parameters
Date_         20180221
Time          10.55
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg
TD           50504
SOLVENT      DMSO
NS           32
DS           2
SWH          8417.509 Hz
FIDRES       0.166670 Hz
AQ           2.9999375 sec
RG           50.8
DW           59.400 usec
DE           6.50 usec
TE           294.1 K
D1           5.00000000 sec
TD0          1

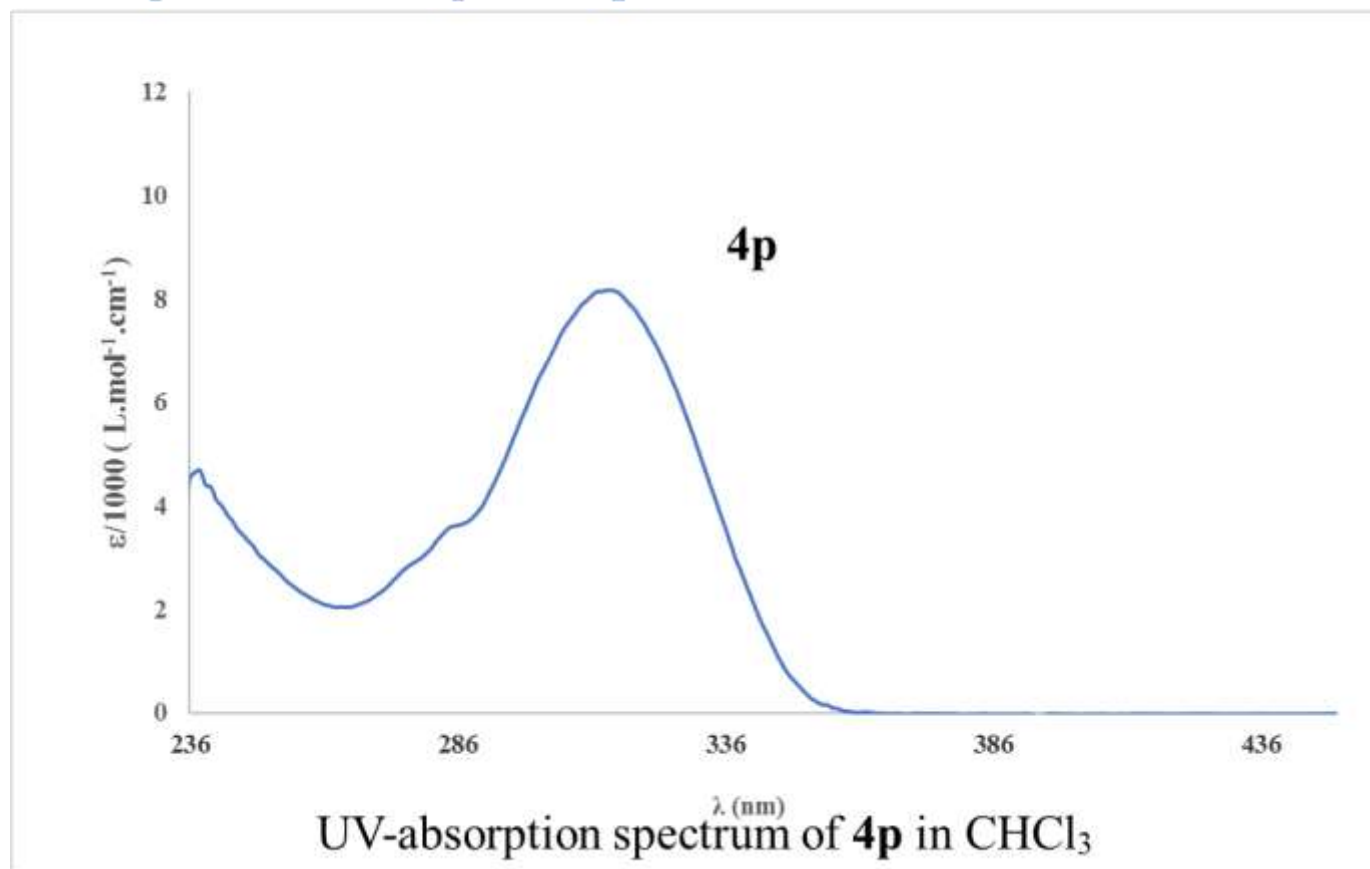
===== CHANNEL f1 =====
NUC1          1H
P1            11.00 usec
PL1           -2.00 dB
PLLW          17.51671600 W
SFO1          400.1326008 MHz

F2 - Processing parameters
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
GB            0.30 Hz
    
```

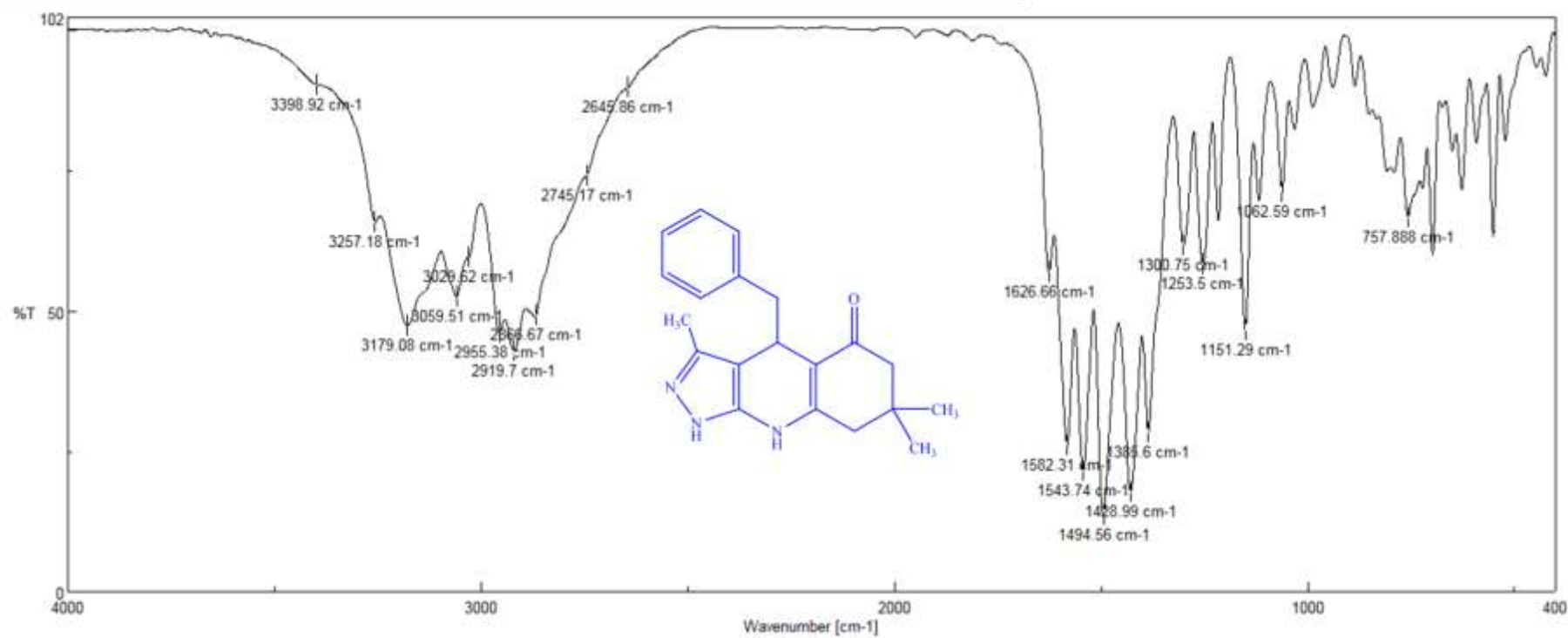




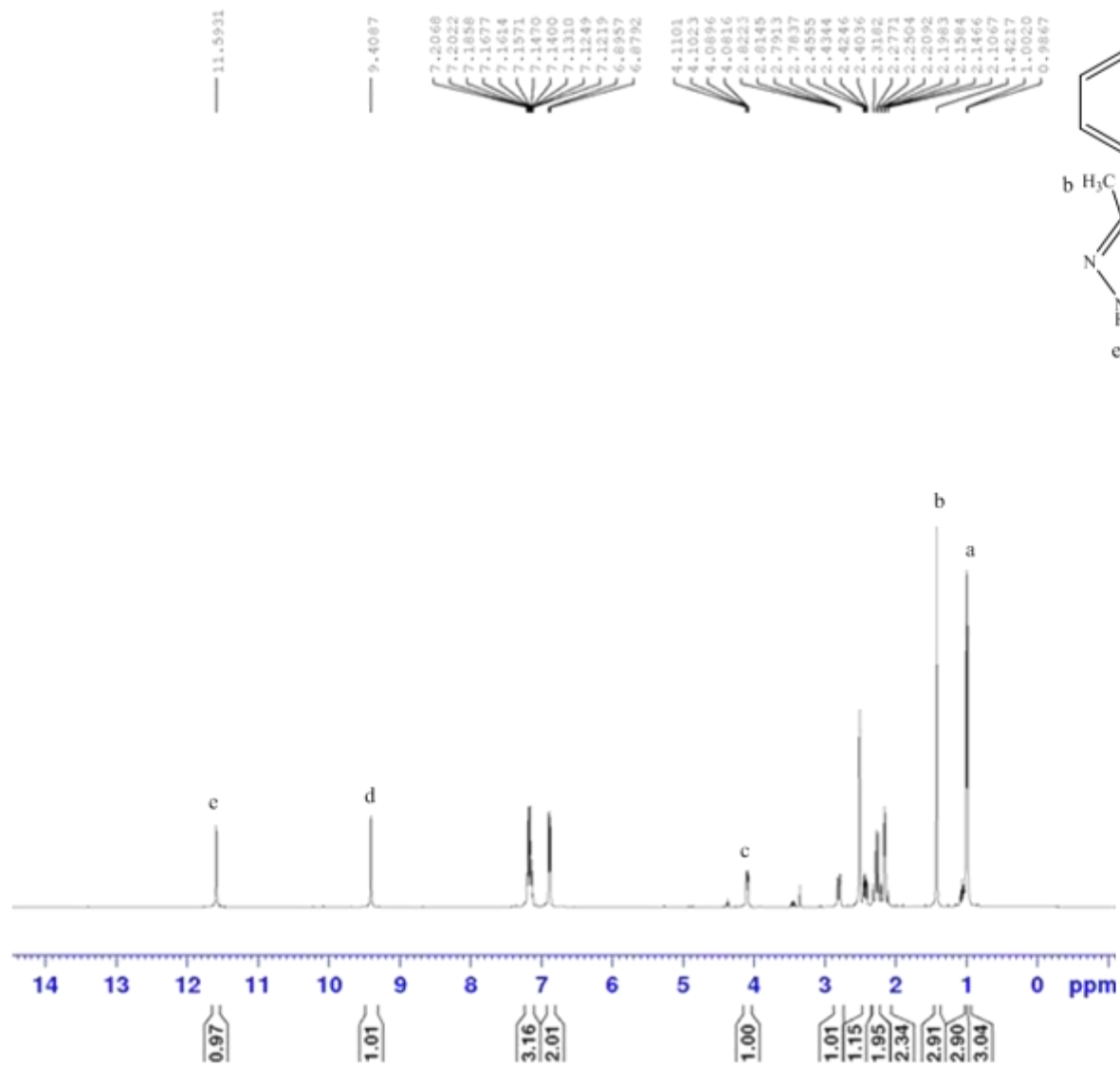
UV-Spectrum of compound **4p**

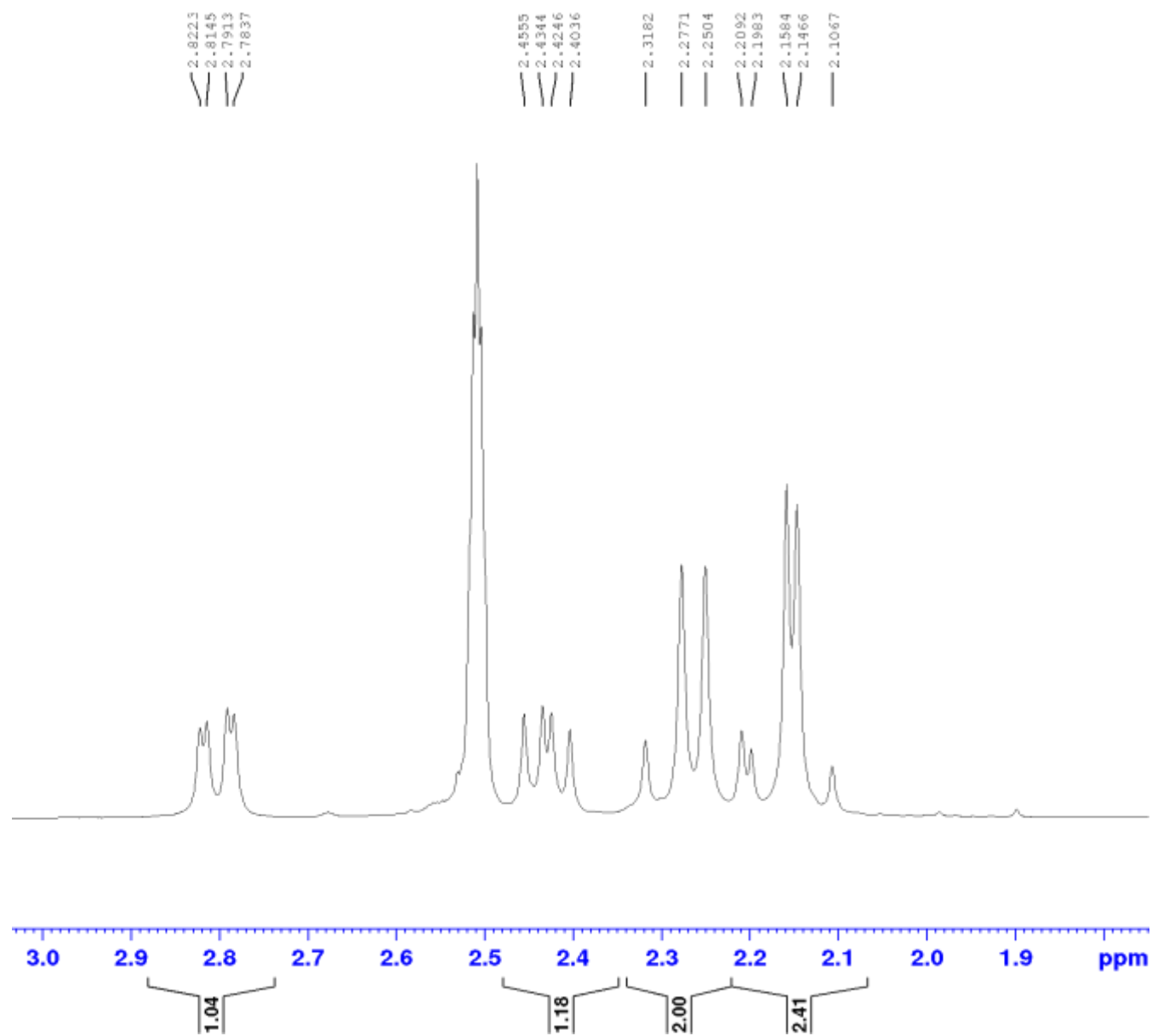


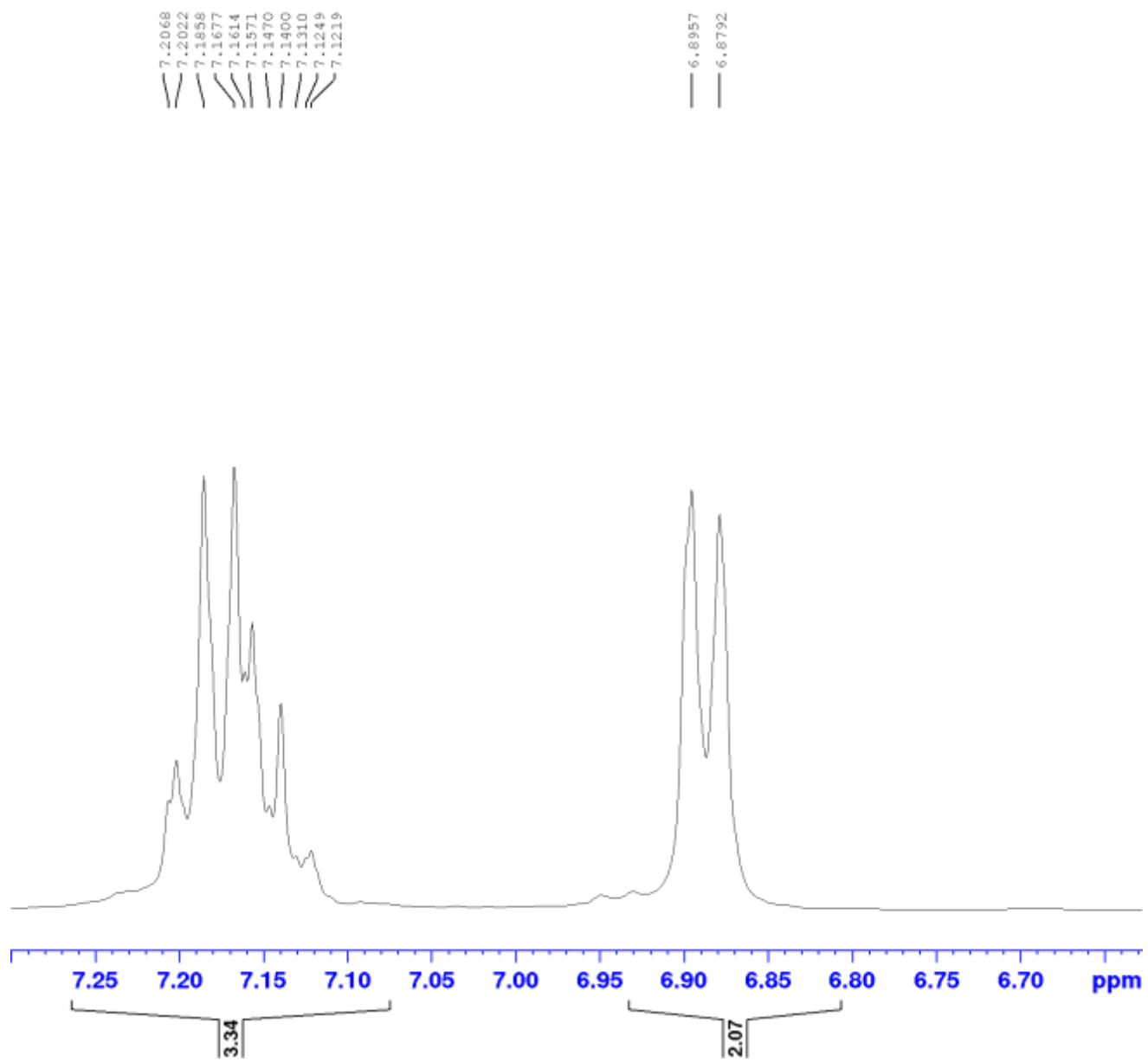
IR-Spectrum of compound 4q



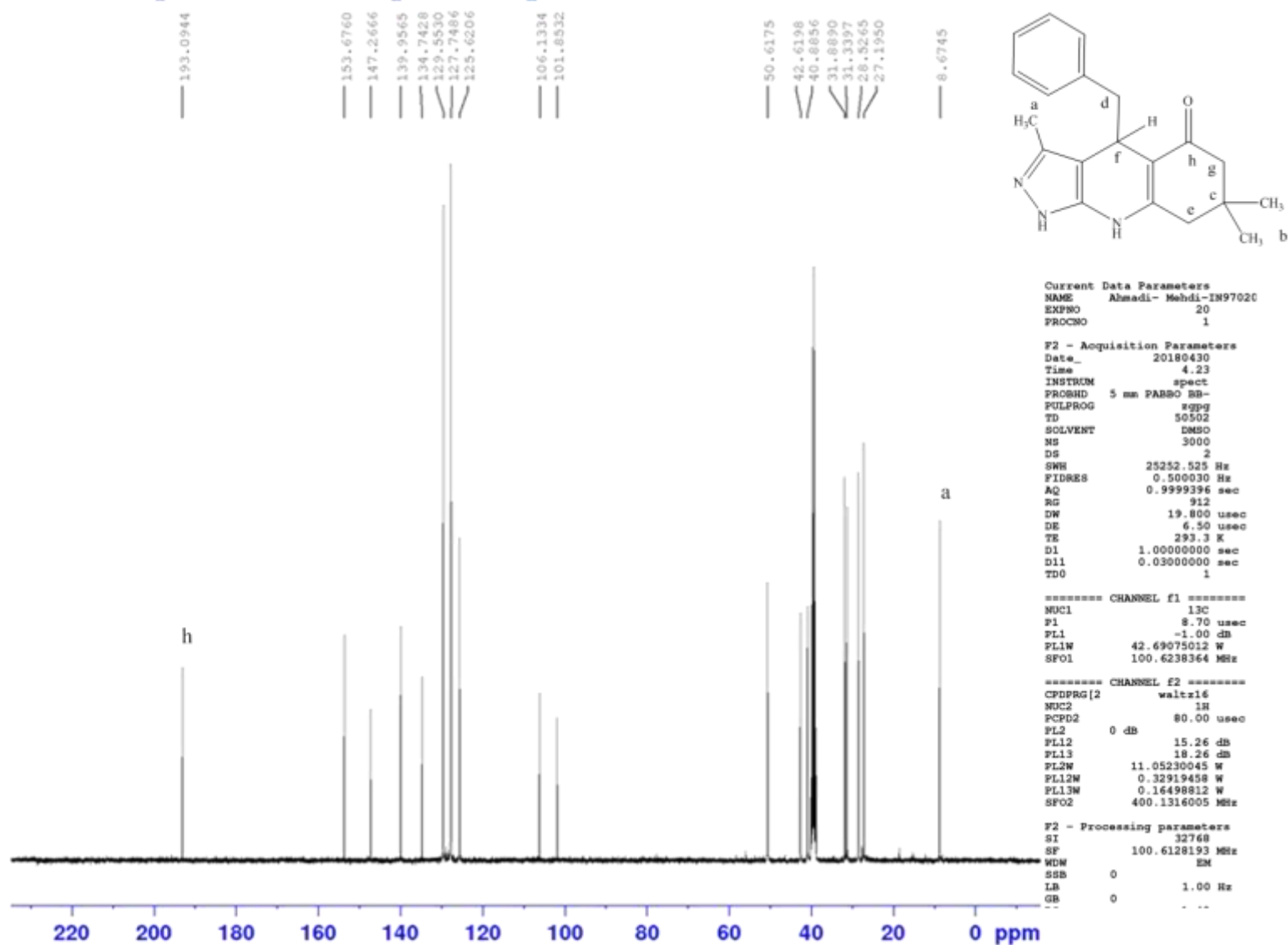
¹H NMR Spectrum of compound 4q

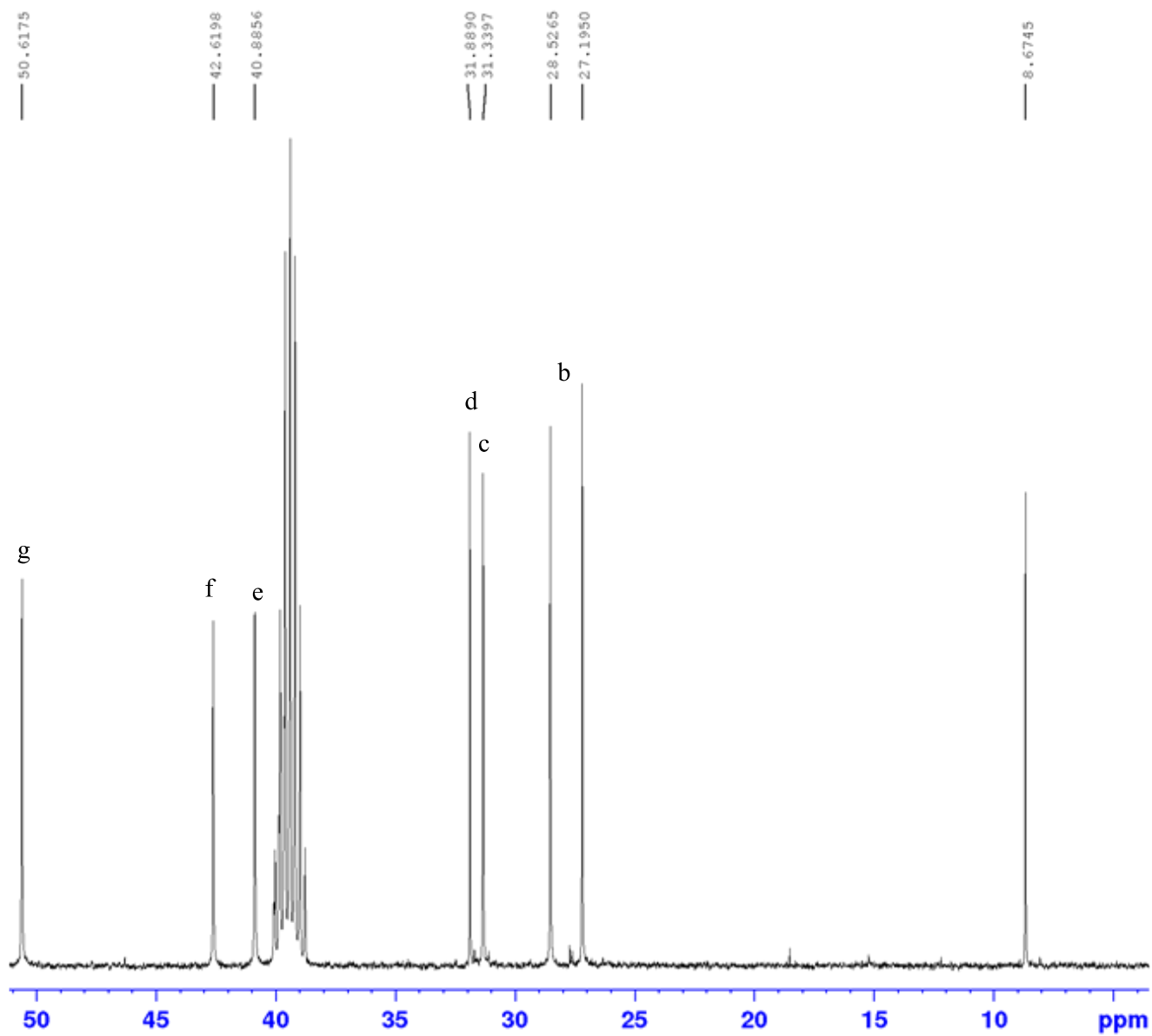




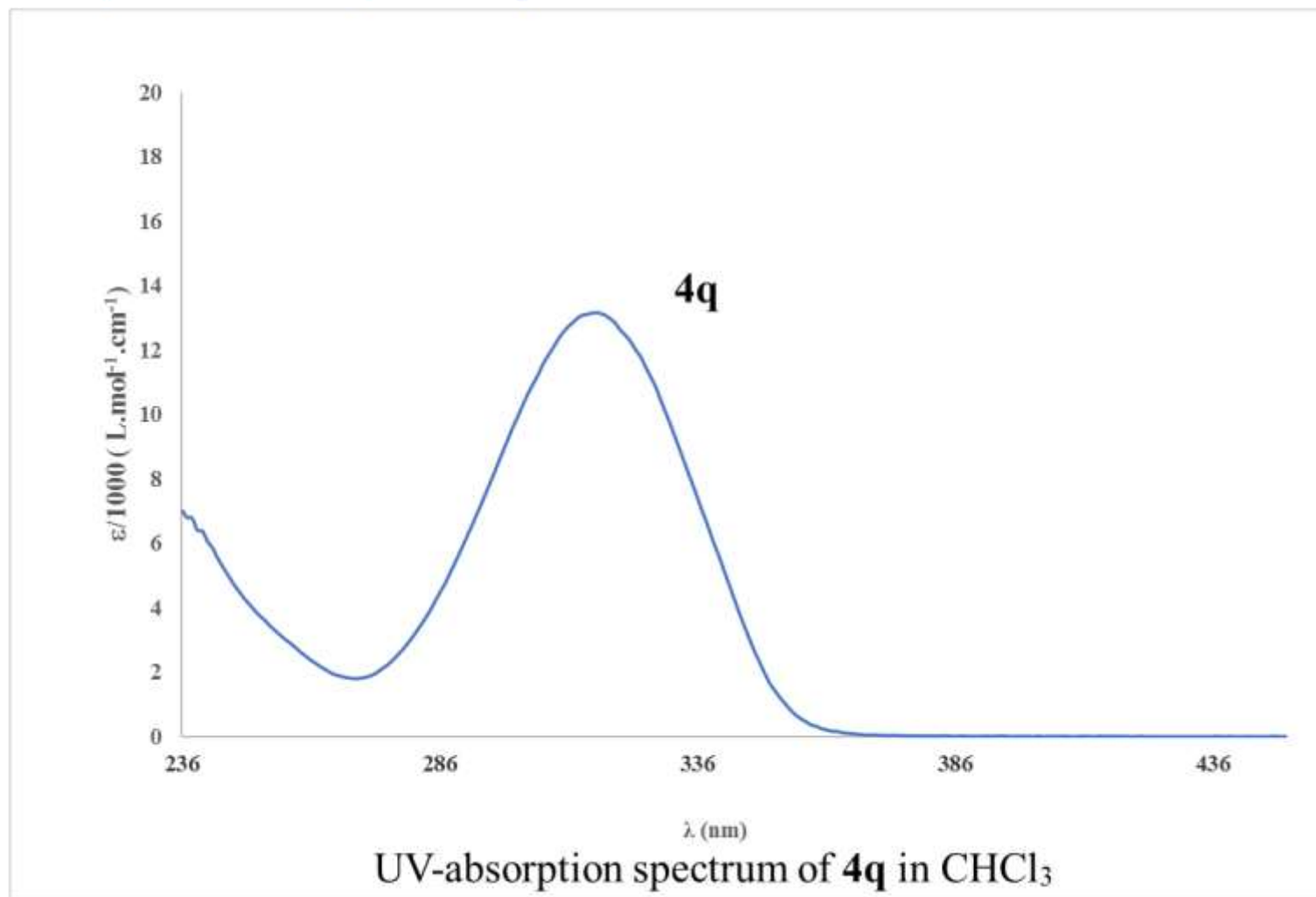


¹³C NMR Spectrum of compound 4q

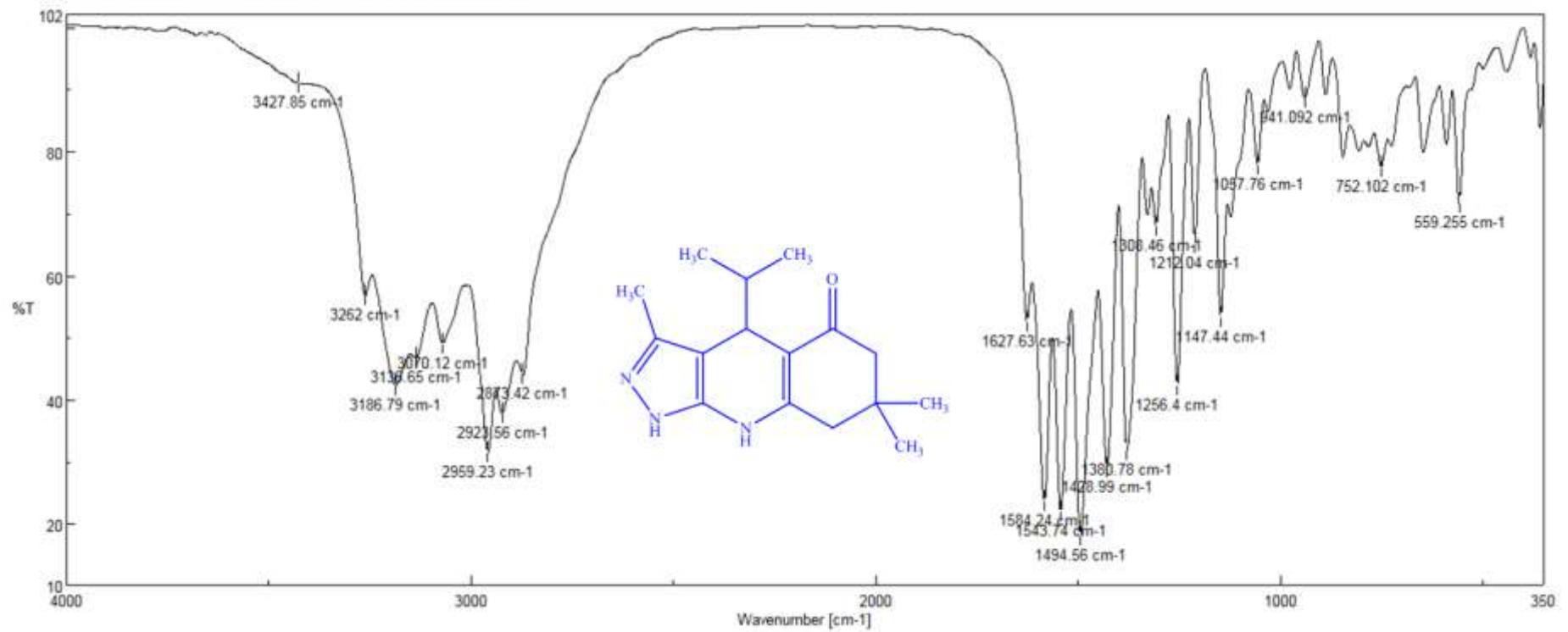




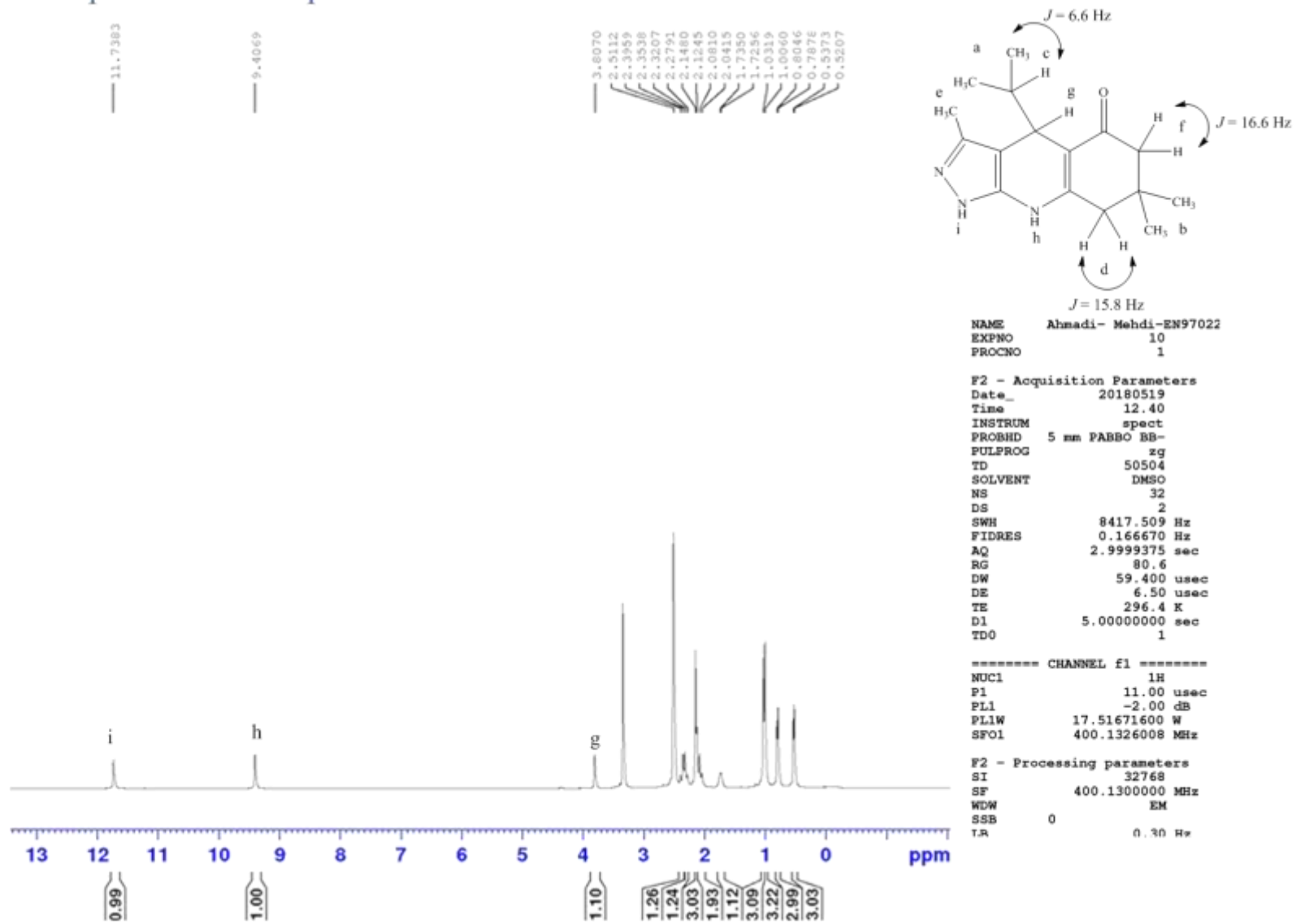
UV-Spectrum of compound **4q**

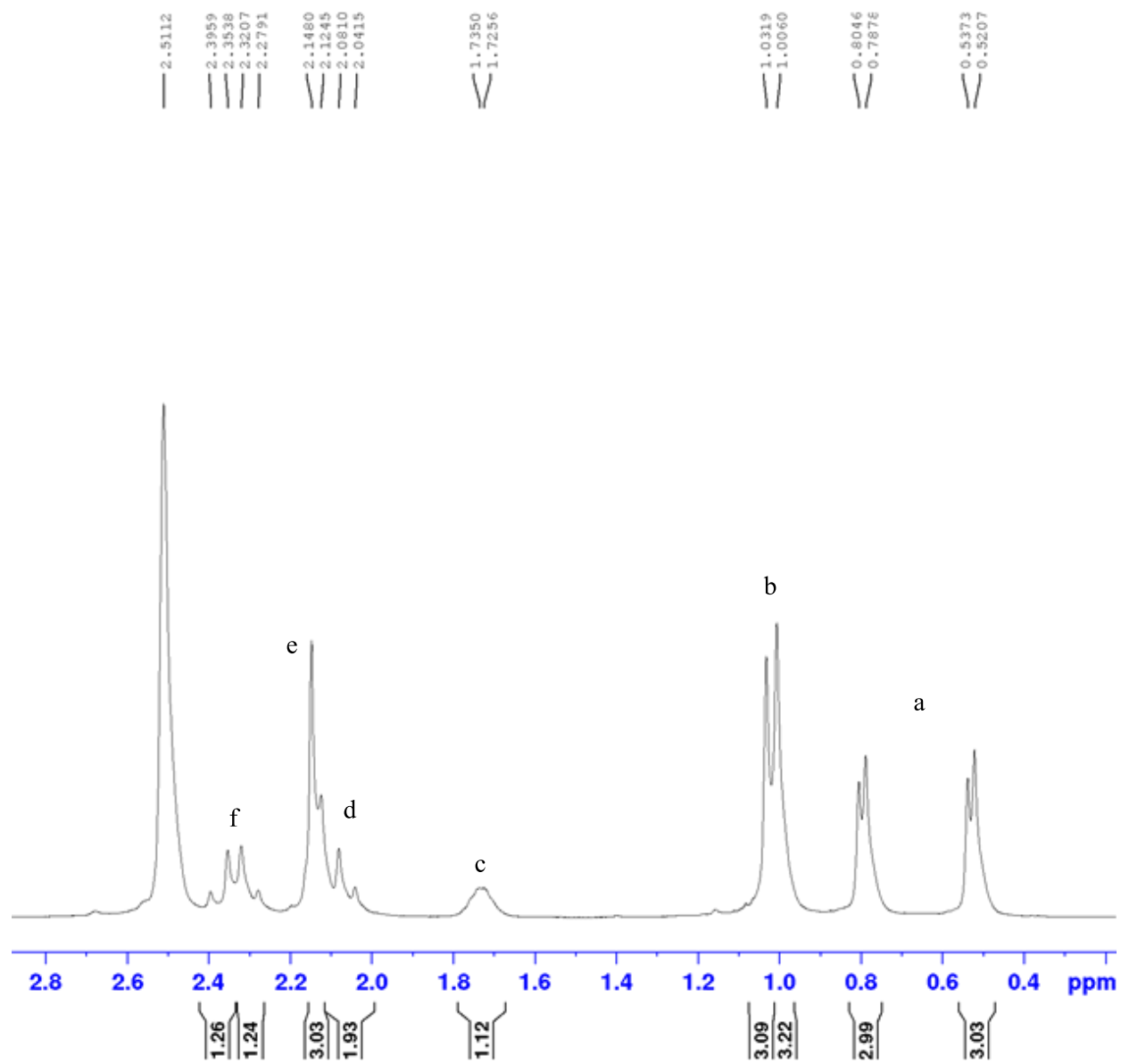


IR-Spectrum of compound **4r**

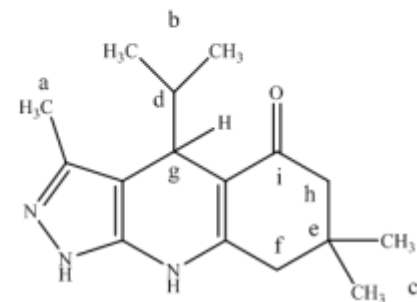
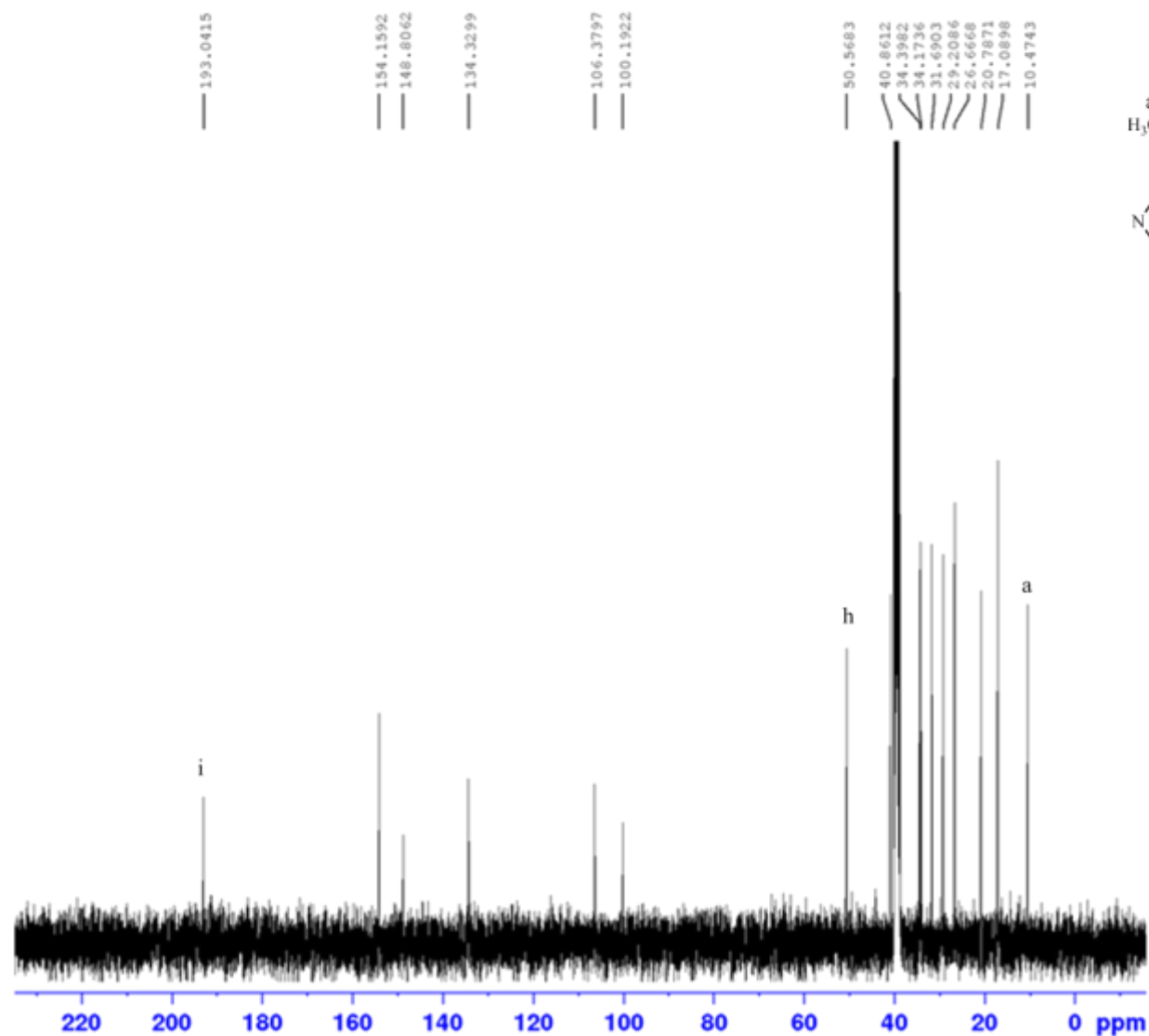


¹H NMR Spectrum of compound 4r





¹³C NMR Spectrum of compound 4r



```

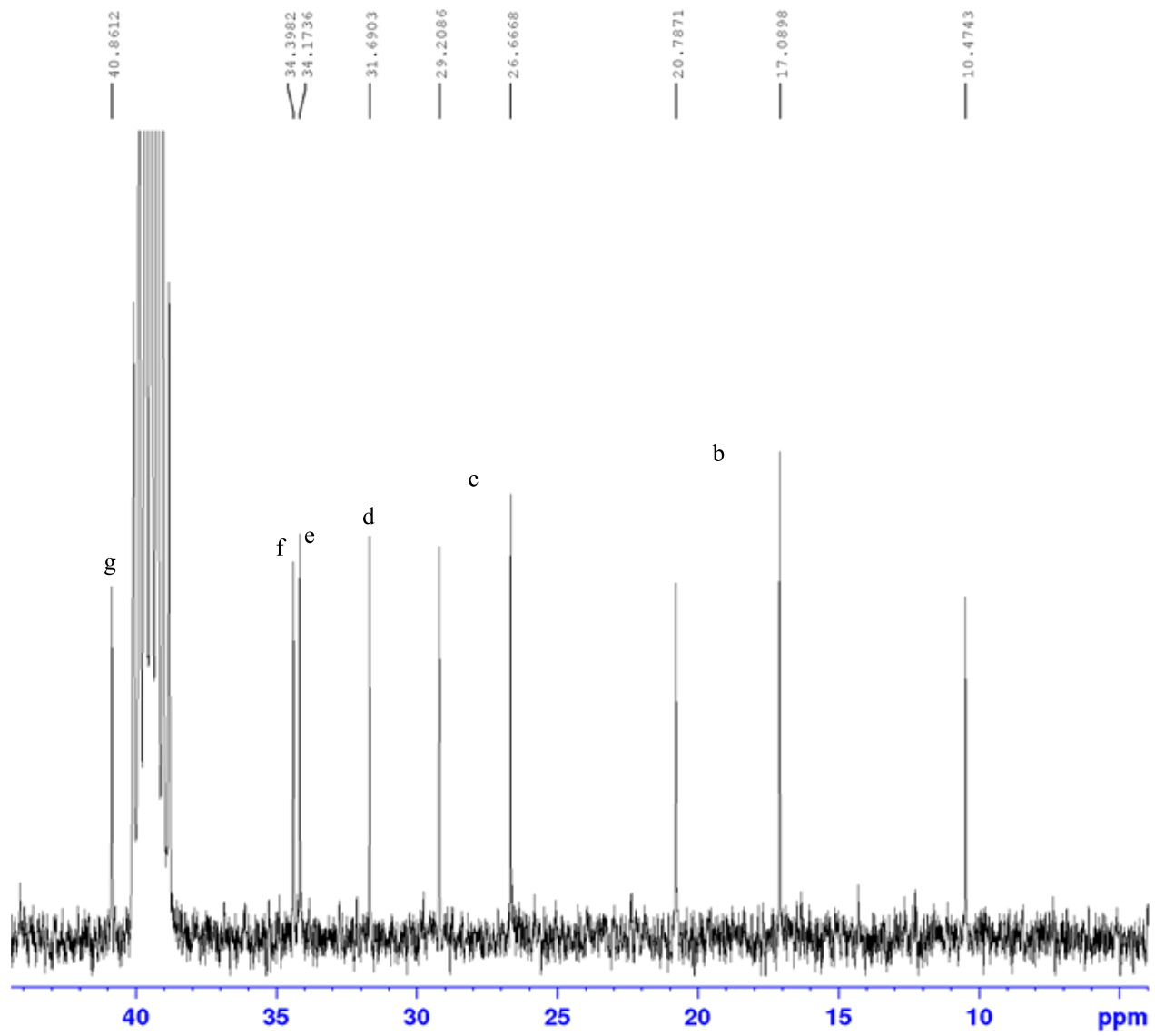
Current Data Parameters
NAME      Ahmadi- Mehdi-IN97030
EXPNO     31
PROCNO    1

F2 - Acquisition Parameters
Date_     20180523
Time      9.04
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         50502
SOLVENT   DMSO
NS         1500
DS         2
SWH        25252.525 Hz
FIDRES     0.500030 Hz
AQ         0.9999396 sec
RG         2050
DW         19.800 usec
DE         6.50 usec
TE         293.9 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

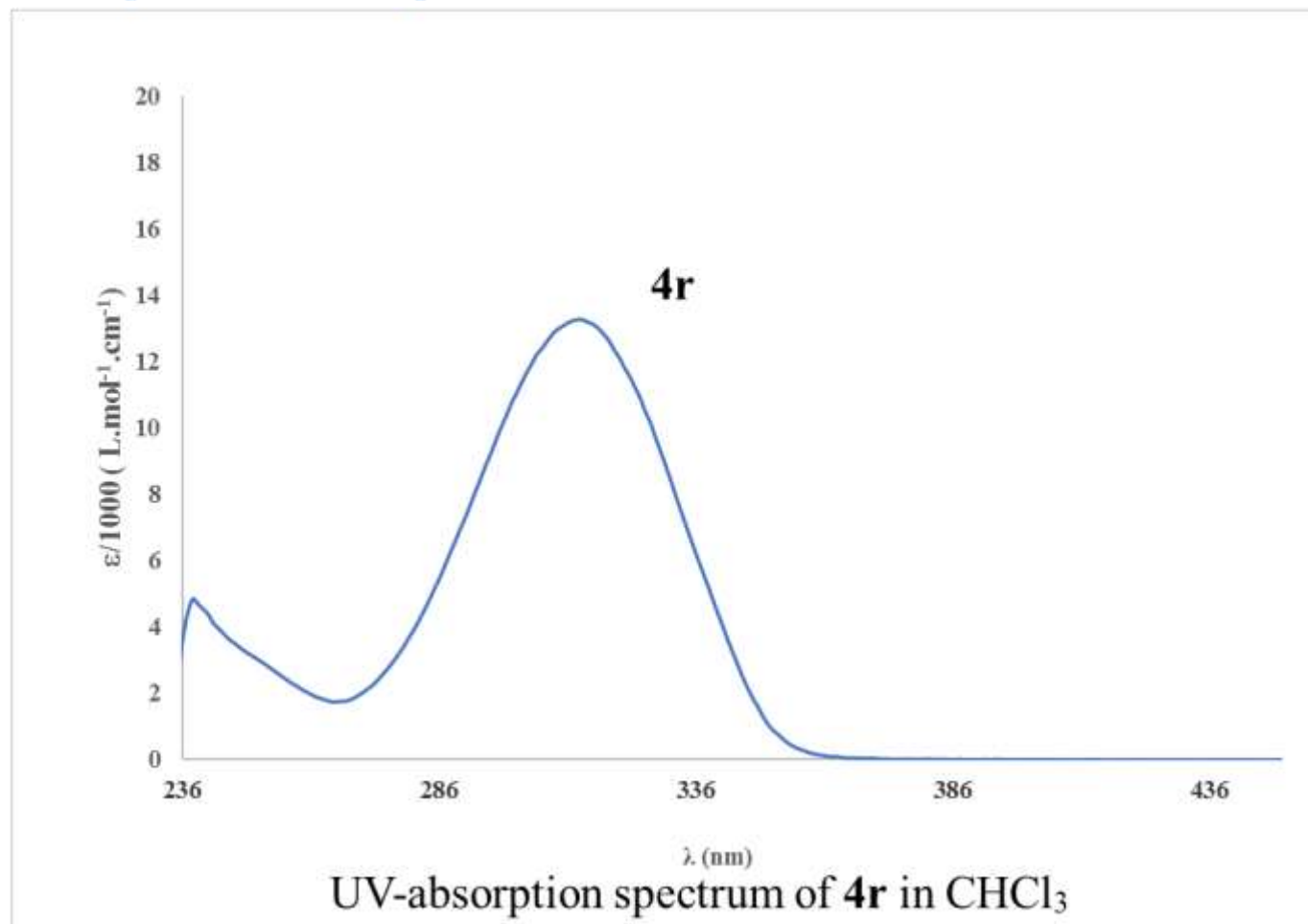
===== CHANNEL f1 =====
NUC1       13C
P1         8.70 usec
PL1        -1.00 dB
PL1W       42.69075012 W
SFO1       100.628364 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        0 dB
PL12       15.26 dB
PL13       18.26 dB
PL2W       11.05230045 W
PL12W      0.32919458 W
PL13W      0.14498812 W
SFO2       400.1316005 MHz

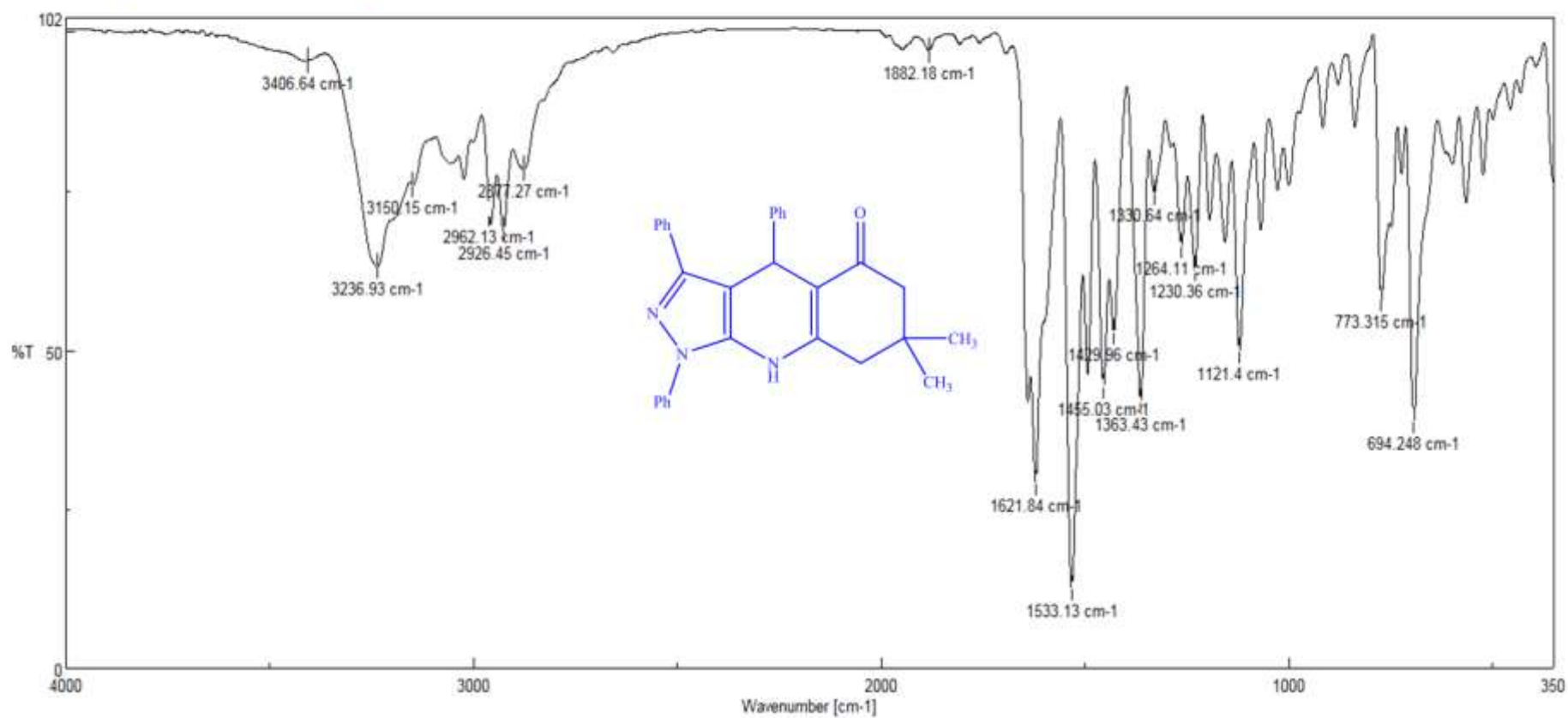
F2 - Processing parameters
SI         32768
SF         100.6128193 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
  
```



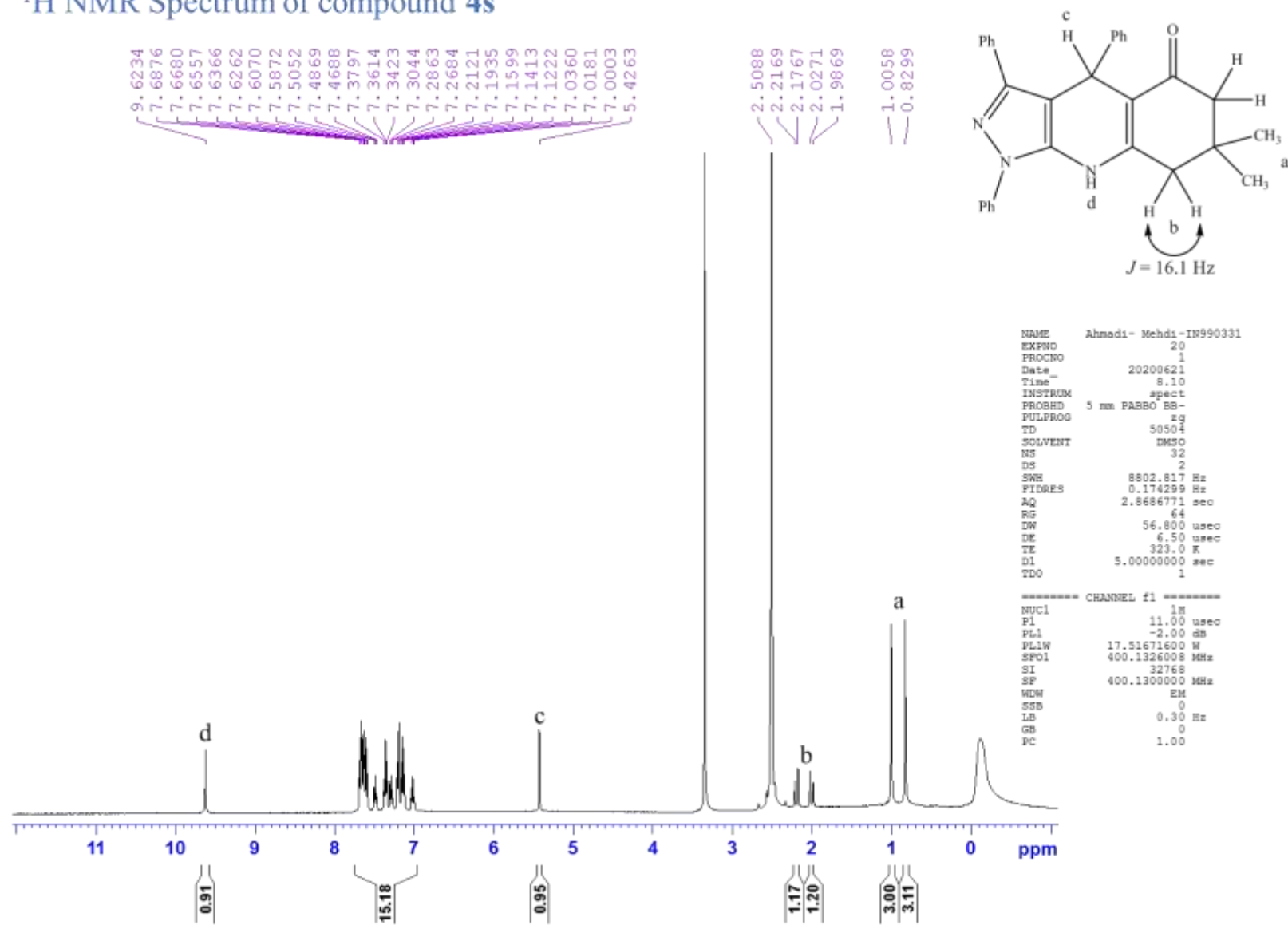
UV-Spectrum of compound **4r**

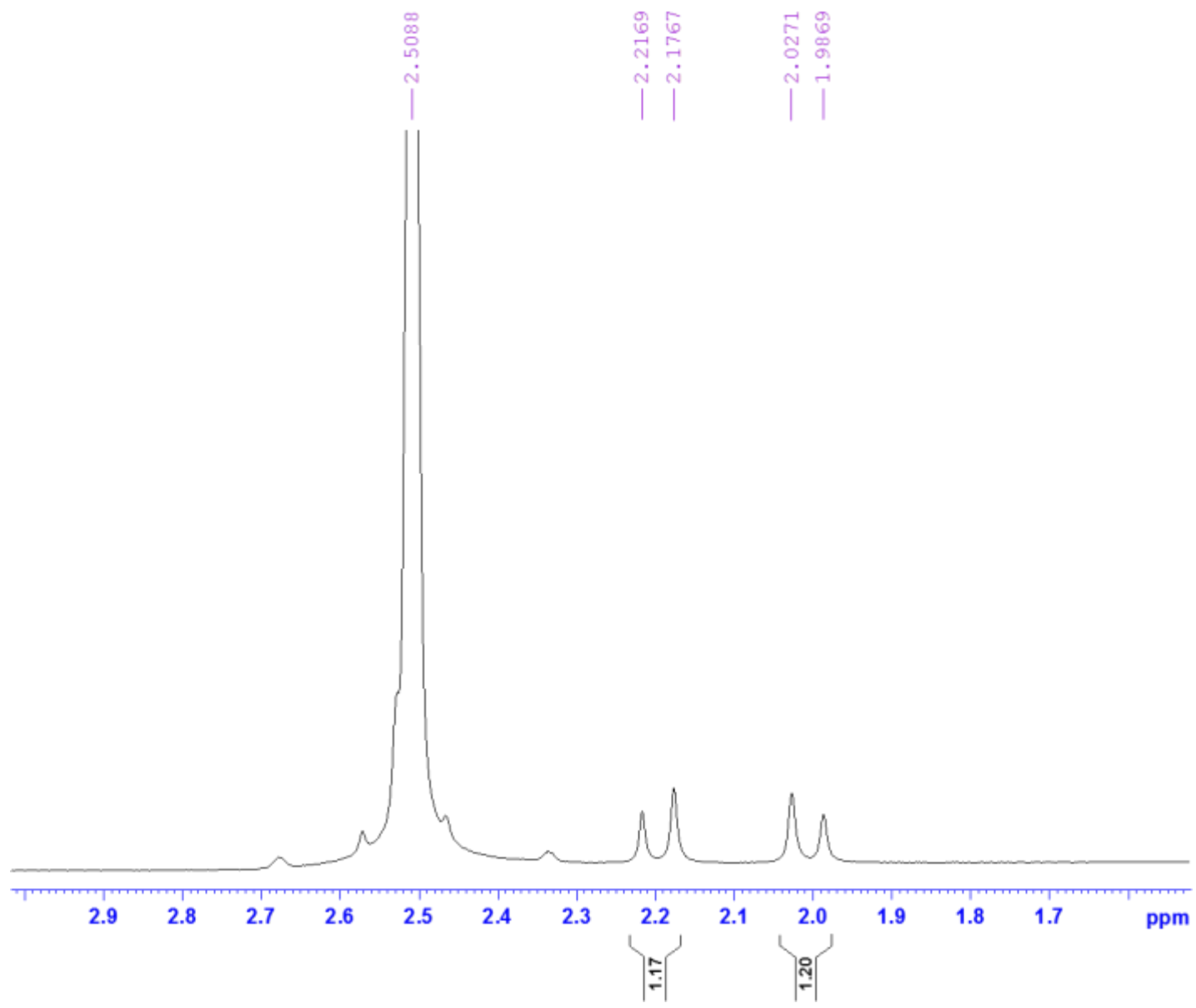


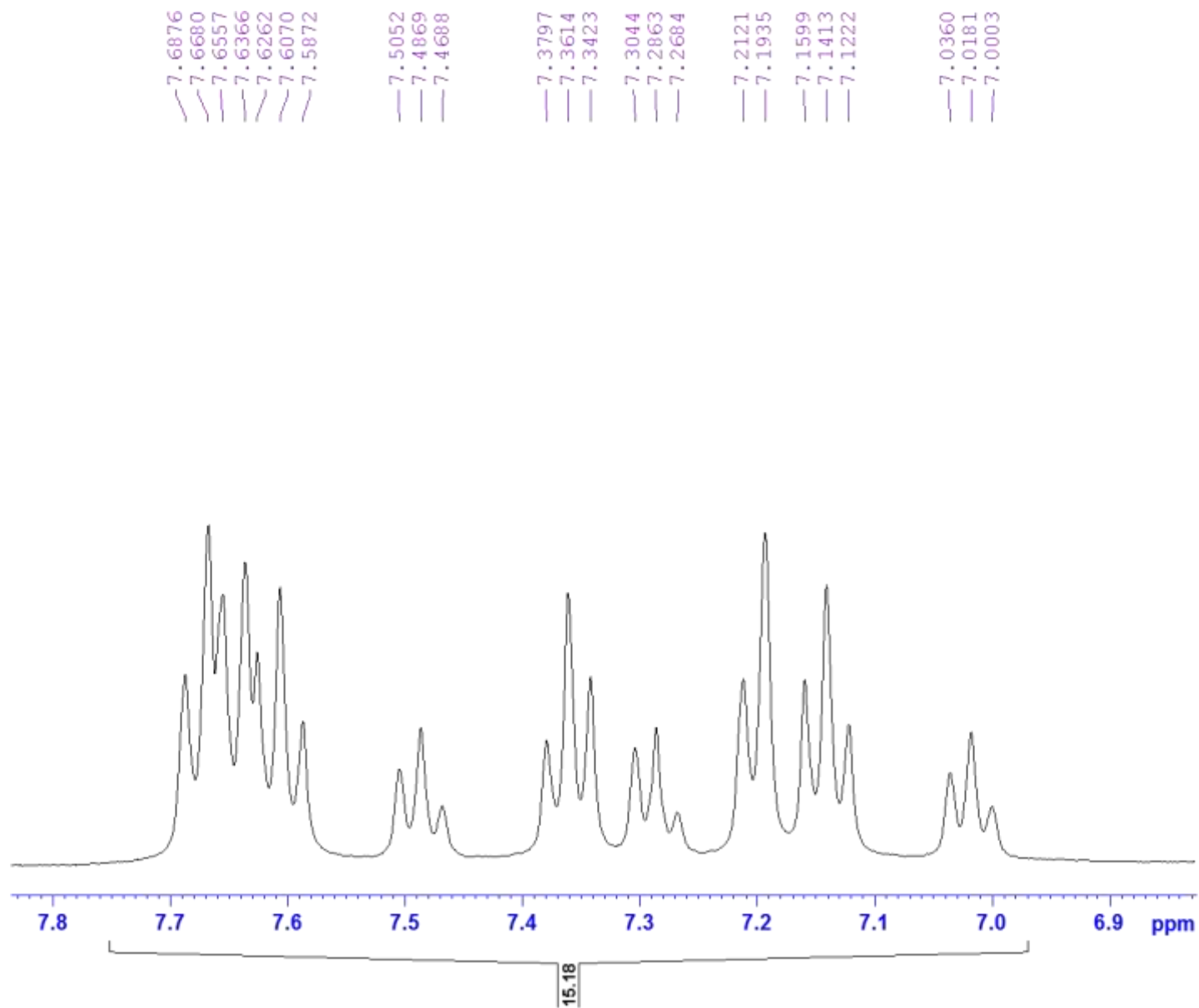
IR-Spectrum of compound 4s



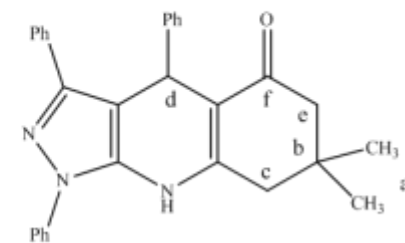
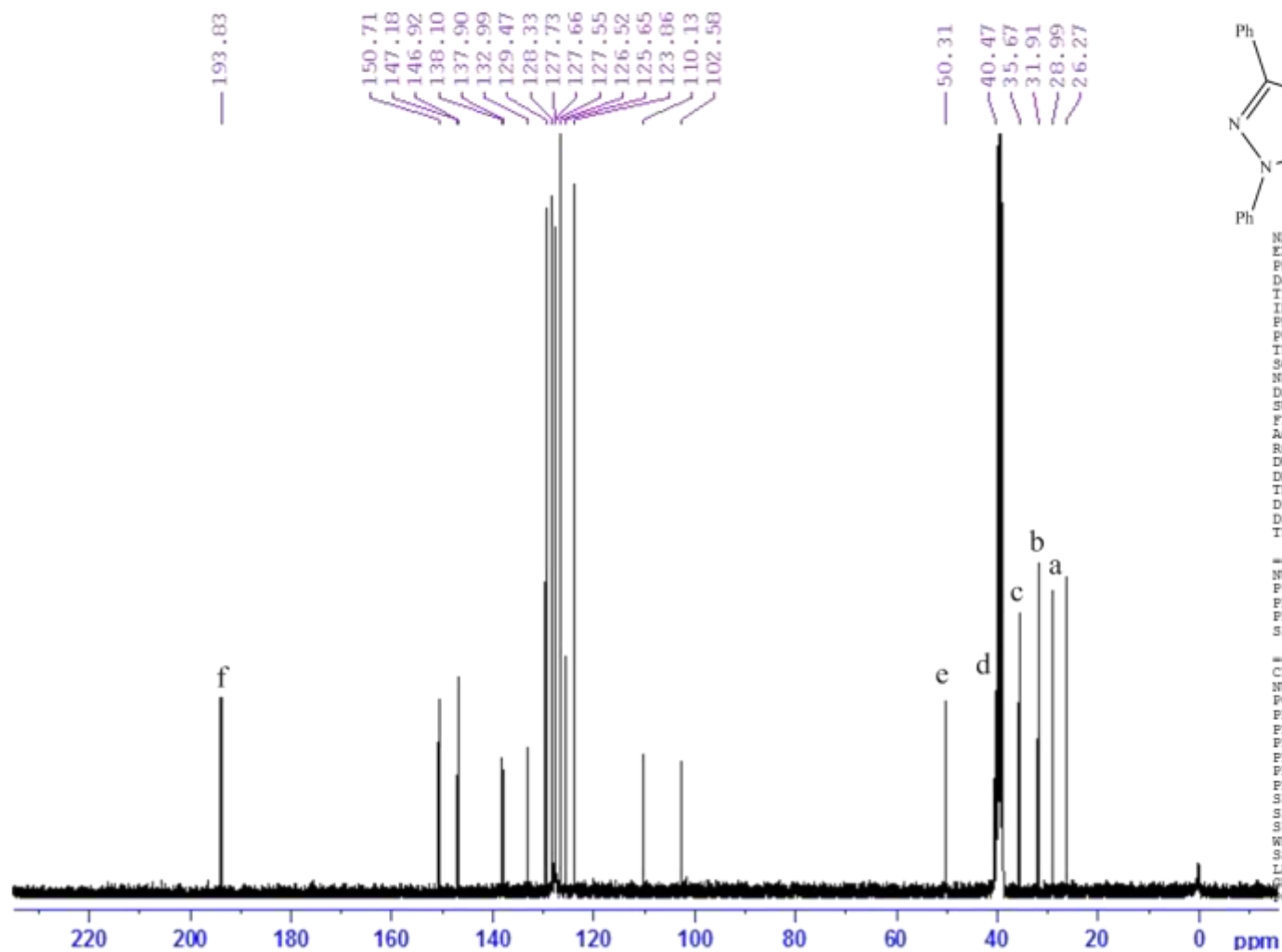
¹H NMR Spectrum of compound 4s







¹³C NMR Spectrum of compound 4s

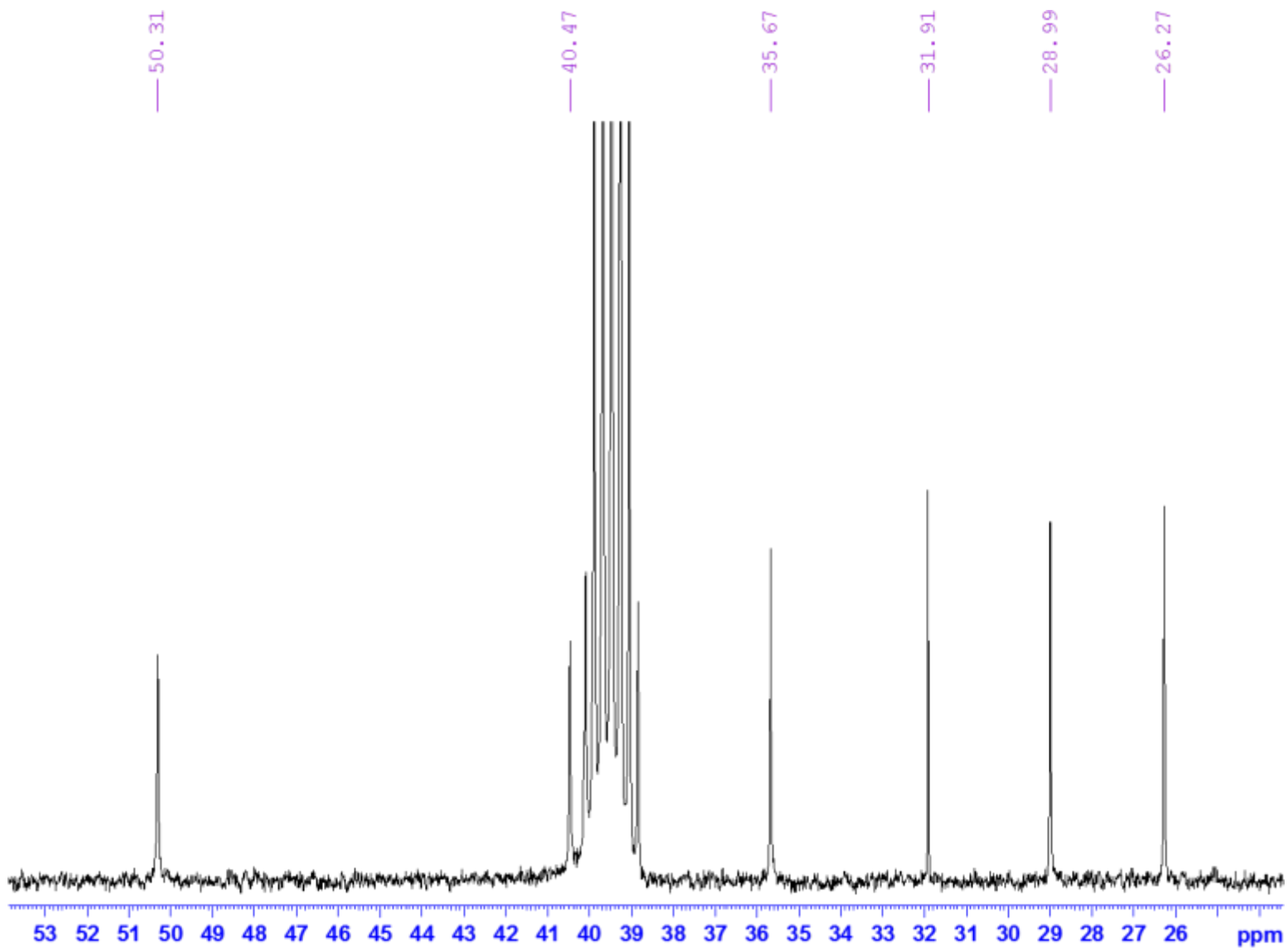


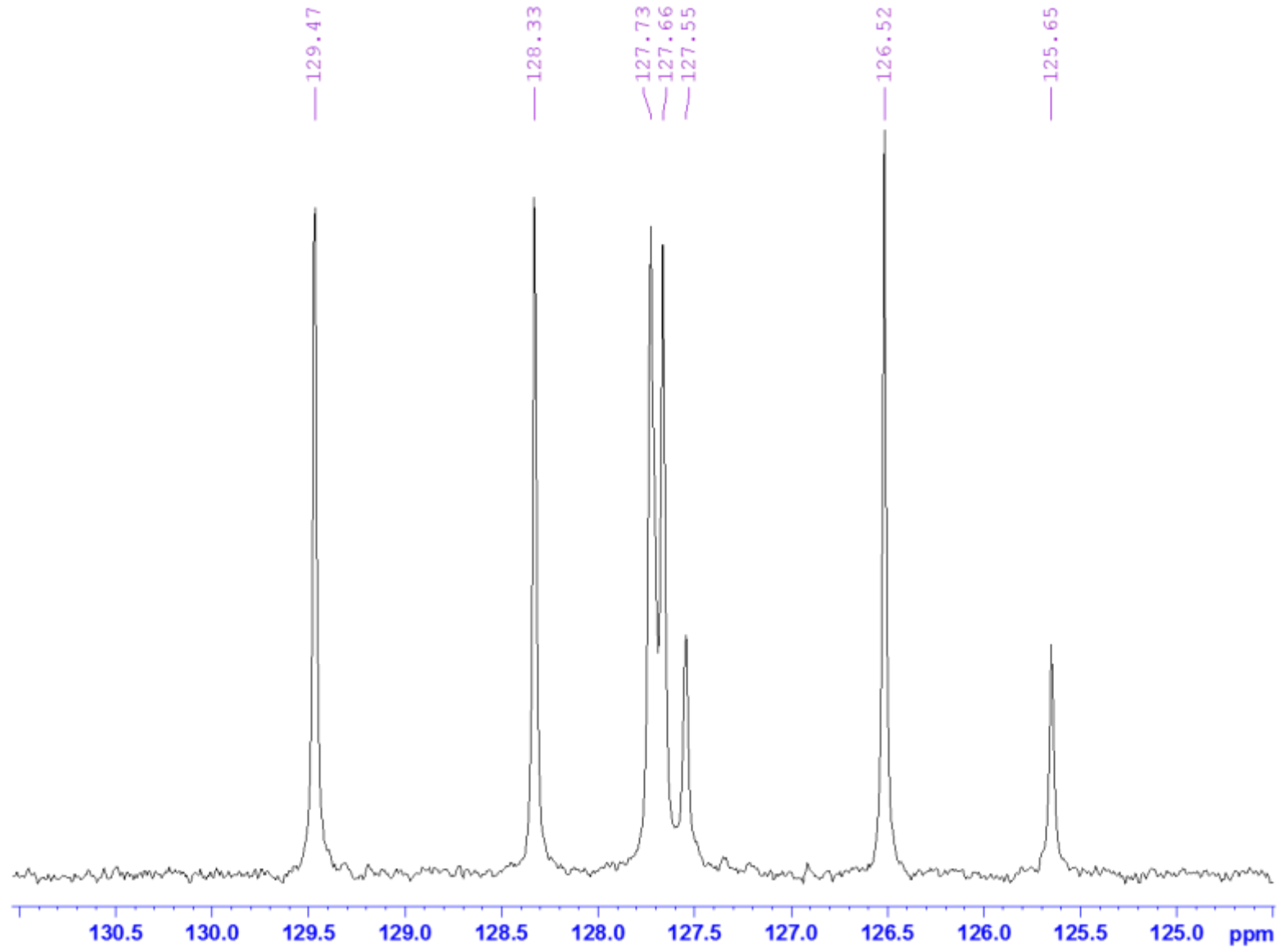
```

NAME      Ahmadi- Mehdi-IN990430
EXPNO     11
PROCNO    1
Date_     20200720
Time      9.58
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
ID        50502
SOLVENT   DMSO
NS        3000
DS        2
SWH       25252.525 Hz
FIDRES    0.500030 Hz
AQ        0.9999896 sec
RG        2080
DW        19.800 usec
DE        6.50 usec
TE        331.8 K
D1        1.00000000 sec
D11       0.03000000 sec
TD        1

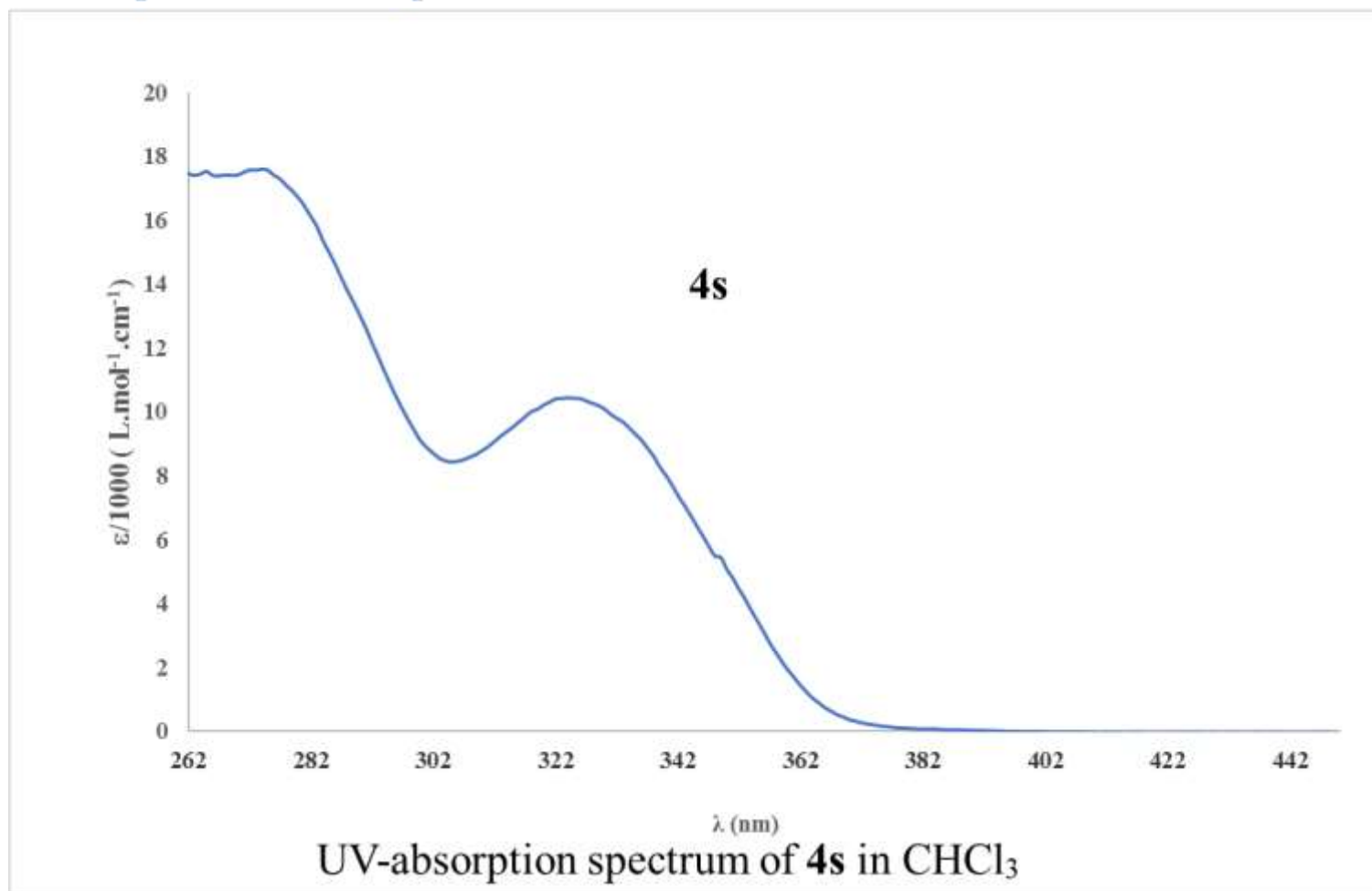
----- CHANNEL f1 -----
NUC1      13C
P1        9.50 usec
PL1       -1.00 dB
PL1W     42.69075012 W
SFO1     100.6238364 MHz

----- CHANNEL f2 -----
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       0.00 dB
PL12     15.26 dB
PL13     18.26 dB
PL2W     11.05230045 W
PL12W    0.32919458 W
PL13W    0.16498812 W
SFO2     400.1316005 MHz
SI        32768
SF        100.6128193 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
    
```

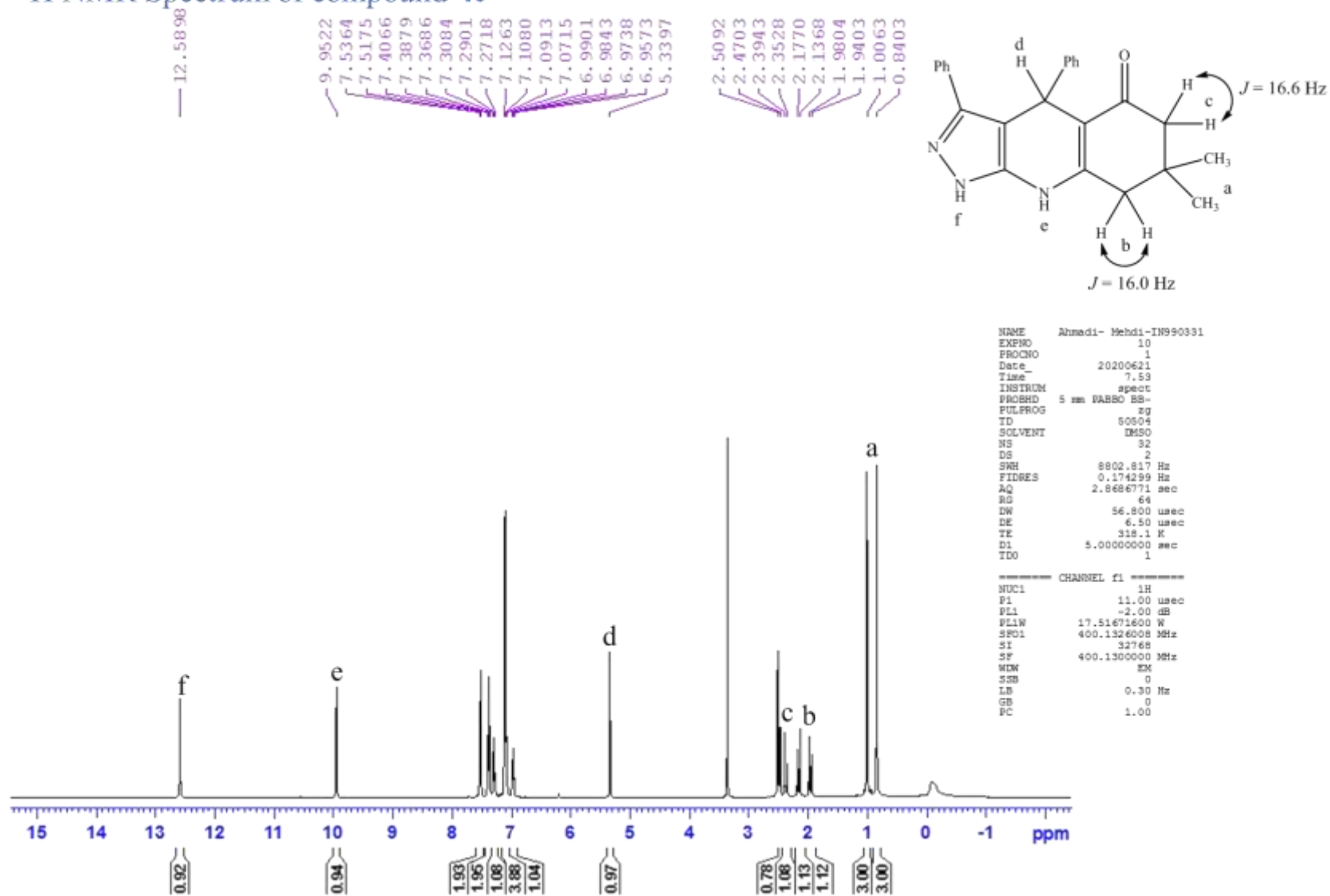


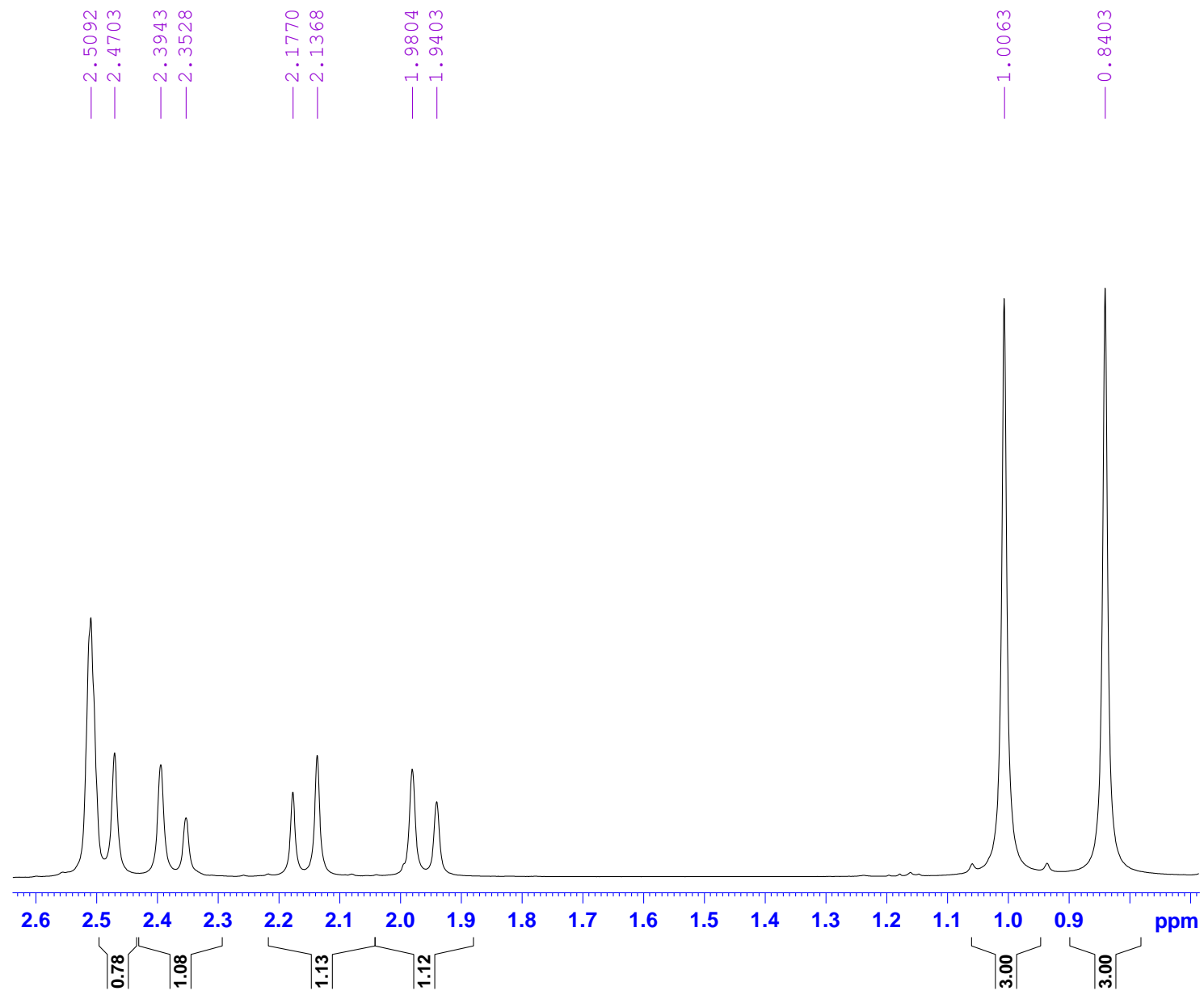


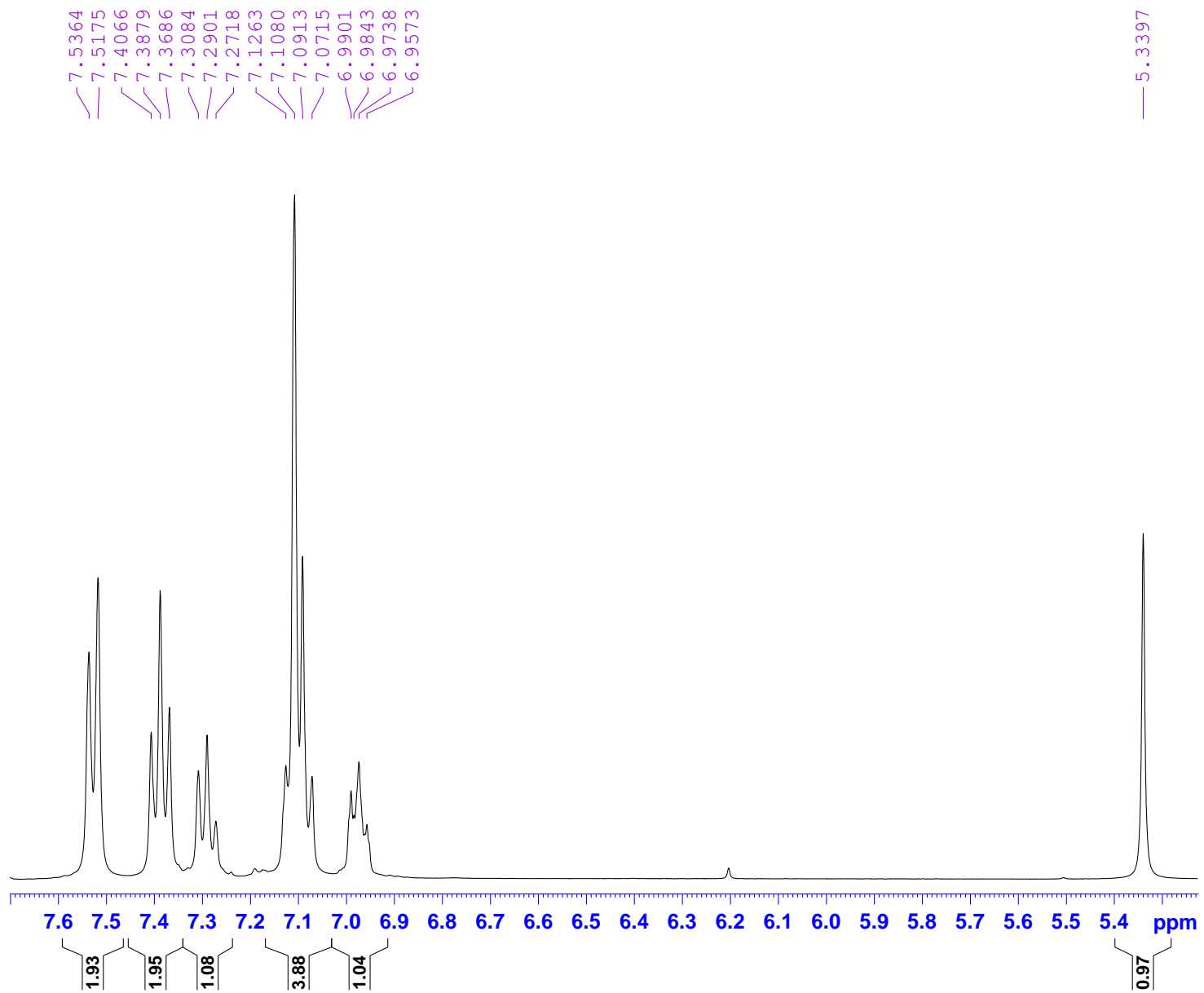
UV-Spectrum of compound **4s**



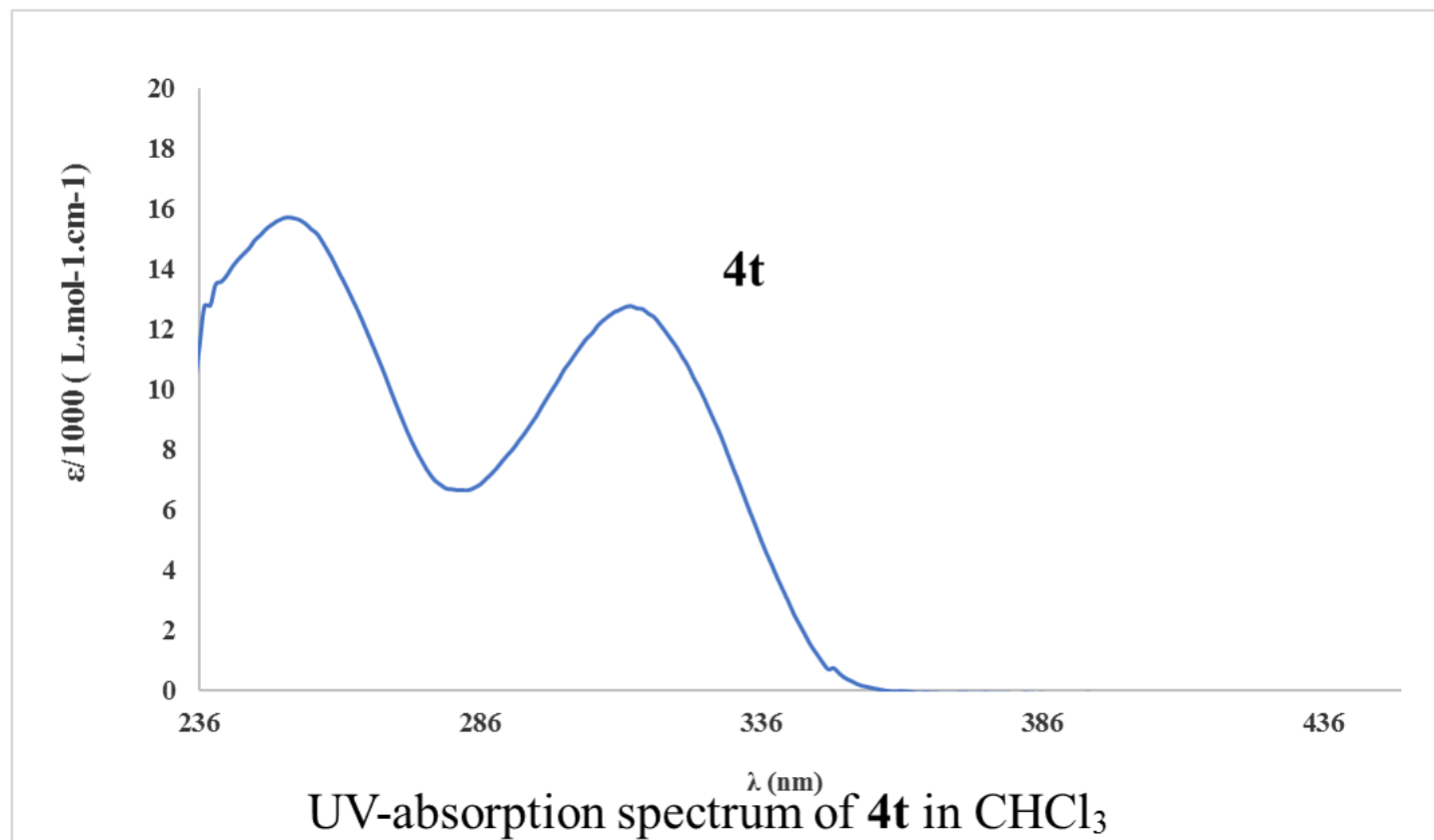
¹H NMR Spectrum of compound 4t



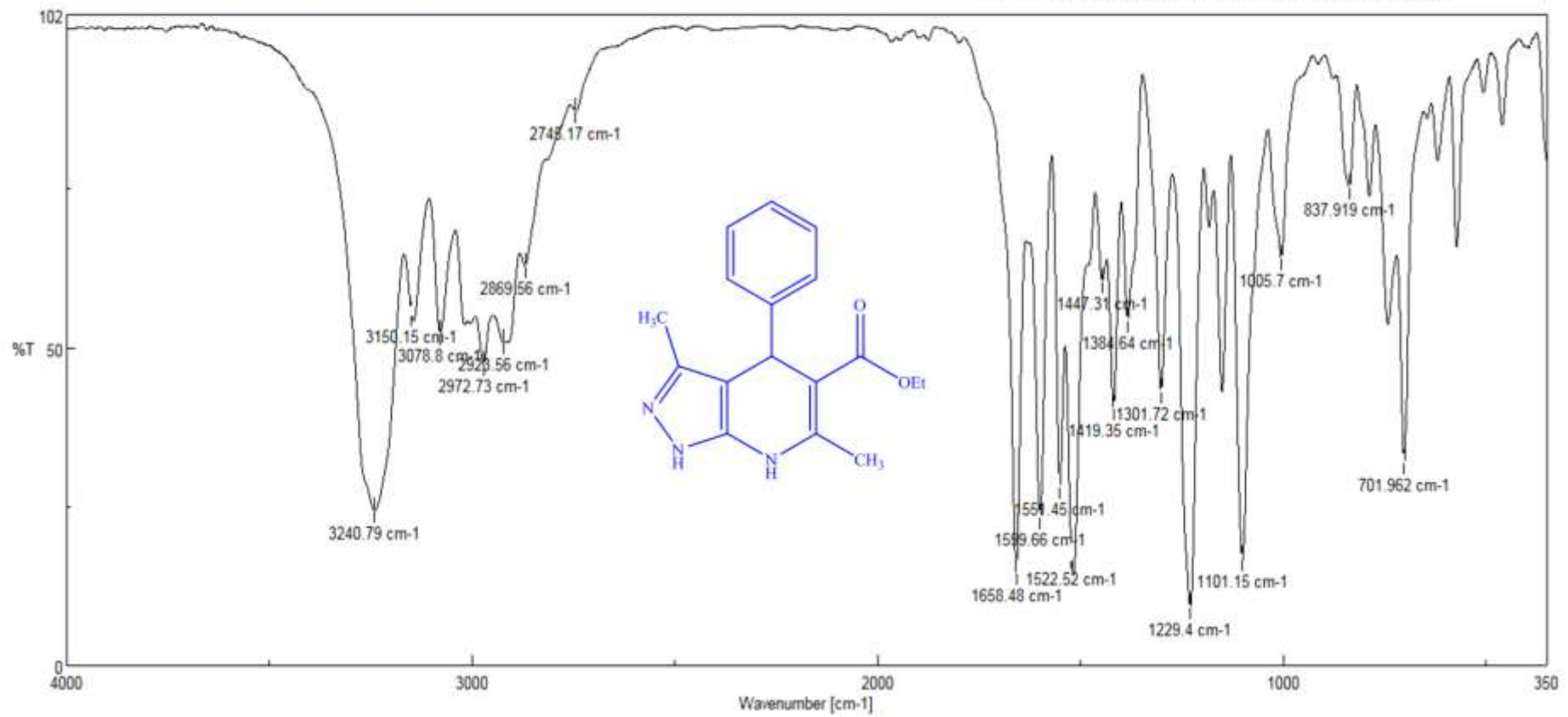




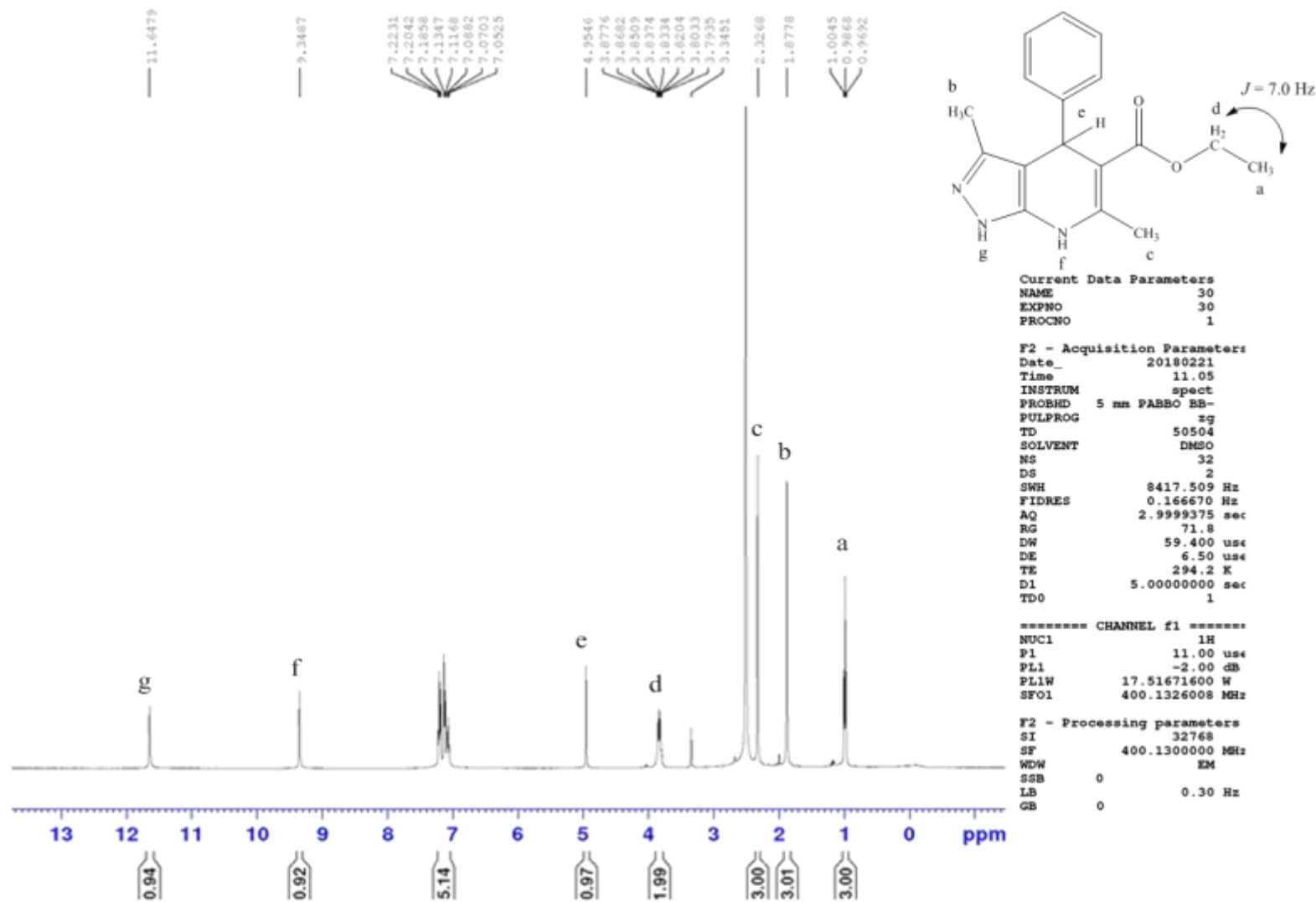
UV-Spectrum of compound **4t**

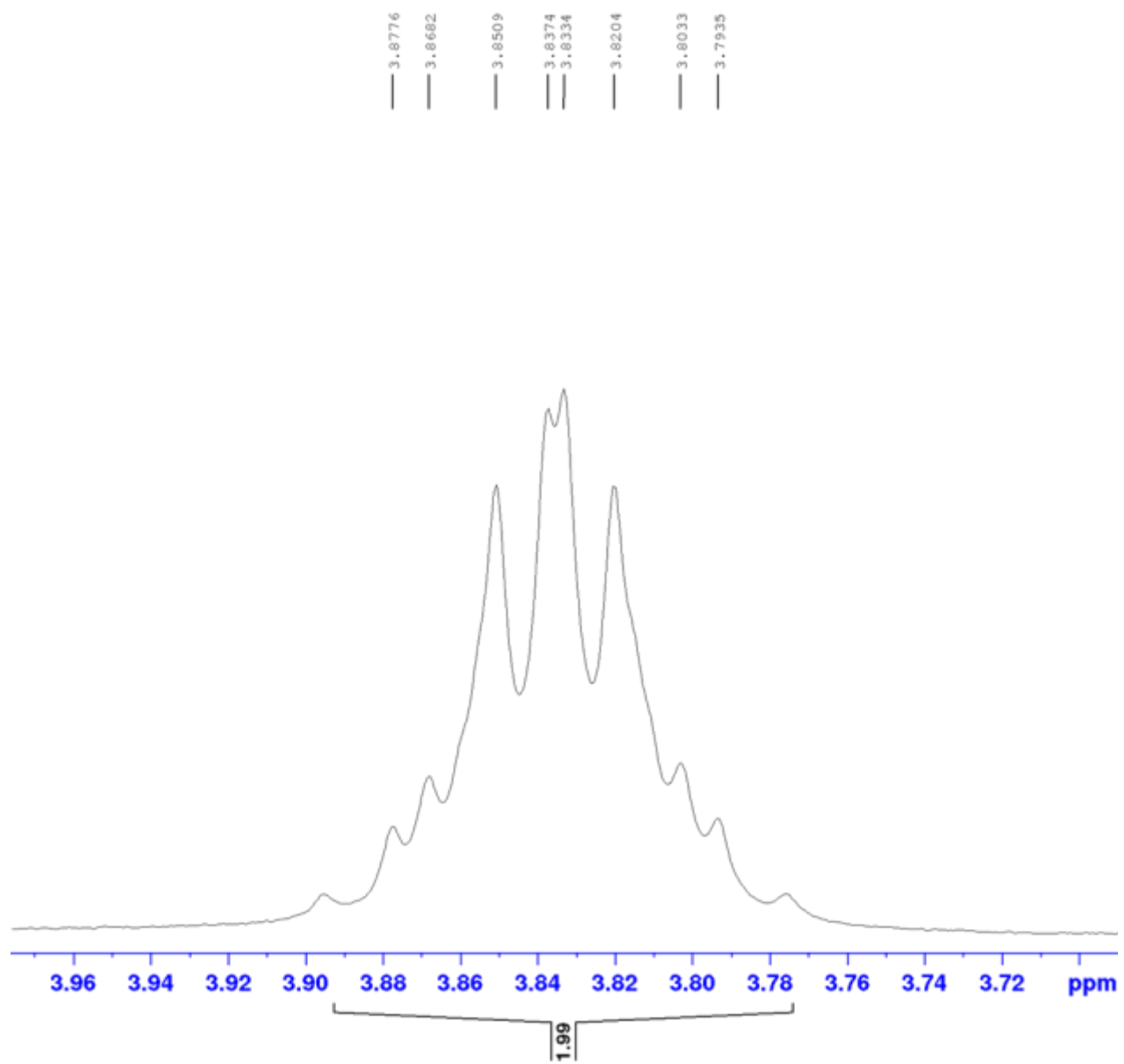


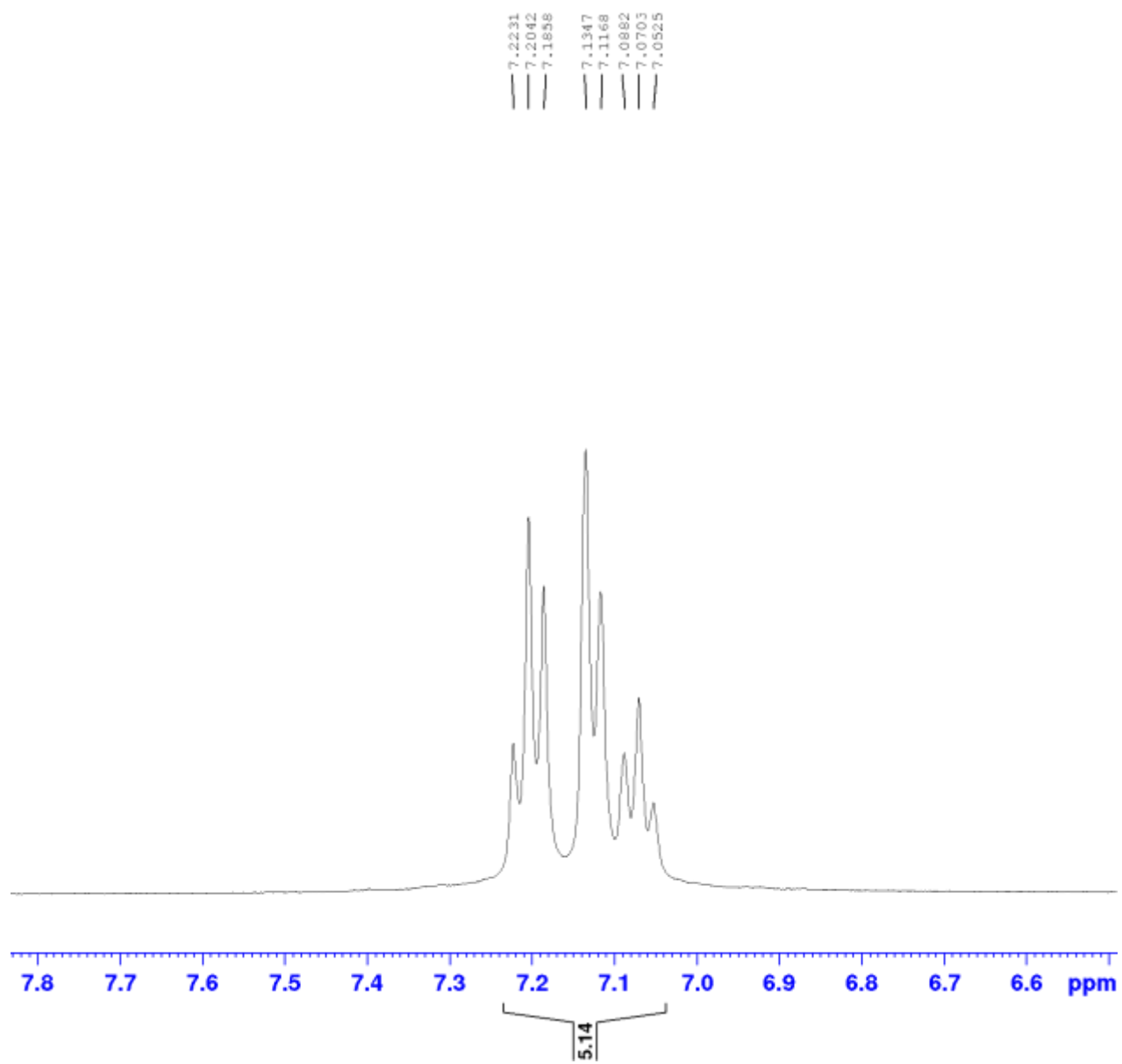
IR-Spectrum of compound 4u



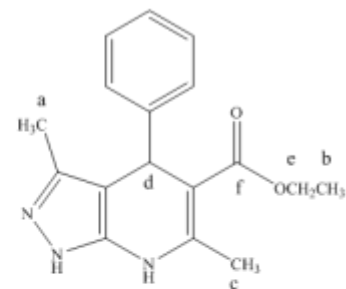
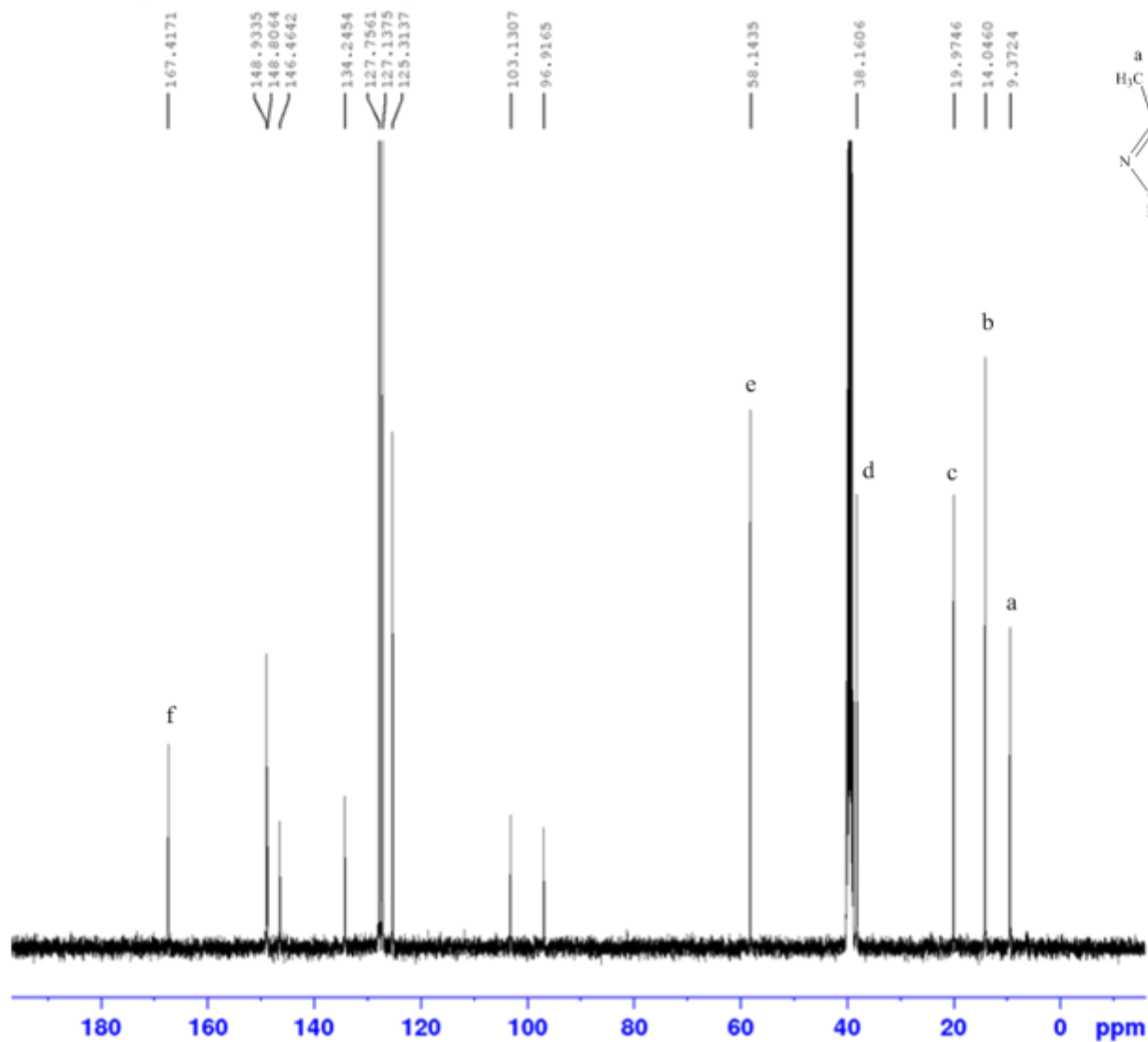
¹H NMR Spectrum of compound 4u







¹³C NMR Spectrum of compound 4u



```

Current Data Parameters
NAME      Abmadi- Mehdi- IN9612
EXPNO     10
PROCNO    1

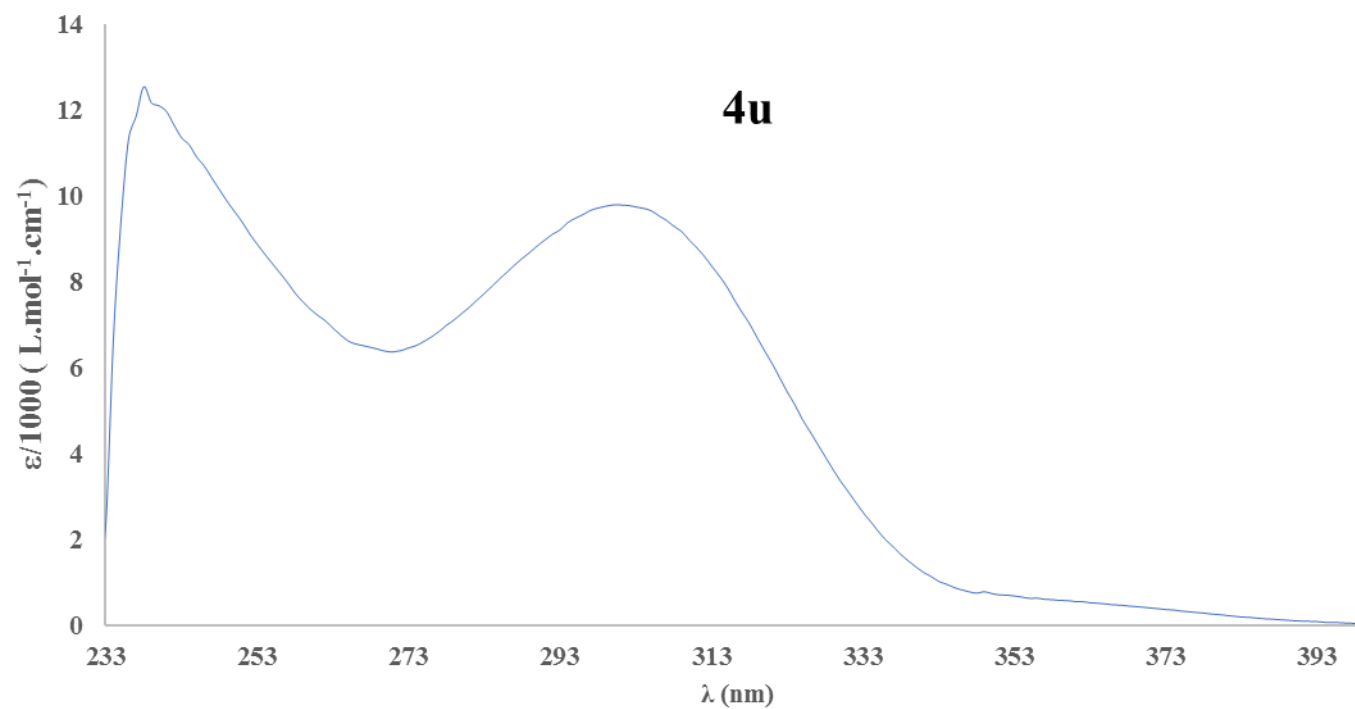
F2 - Acquisition Parameters
Date_     20180303
Time      14.22
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         50502
SOLVENT   DMSO
NS         3000
DS         2
SWH        25252.525 Hz
FIDRES     0.500030 Hz
AQ         0.9999396 sec
RG         1820
DW         19.800 usec
DE         6.50 usec
TE         294.7 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

***** CHANNEL f1 *****
NUC1       13C
P1         8.70 usec
PL1        -1.00 dB
PL1W       42.69075012 W
SFO1       100.6238364 MHz

***** CHANNEL f2 *****
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2         0 dB
PL12       15.26 dB
PL13       18.26 dB
PL1W       11.05230045 W
PL12W      0.32919458 W
PL13W      0.16498812 W
SFO2       400.1316005 MHz

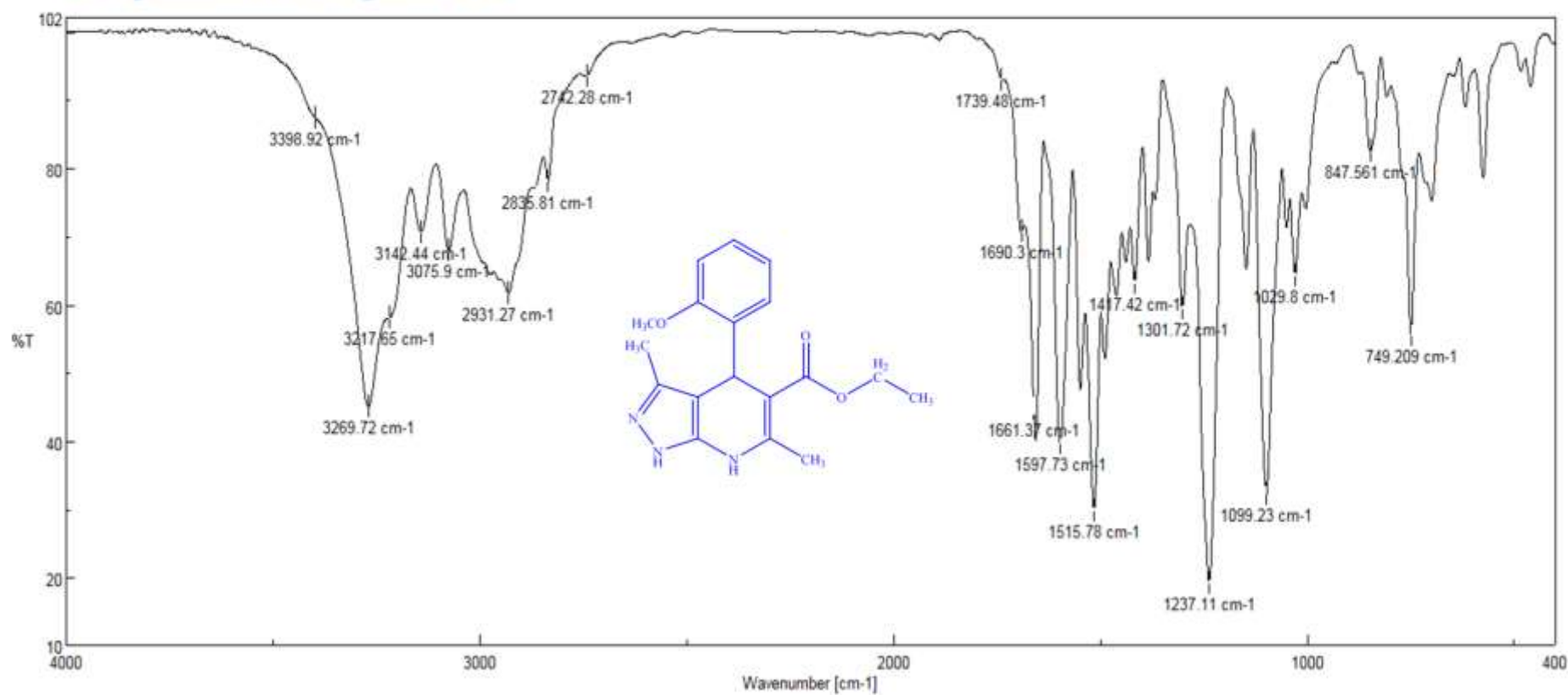
F2 - Processing parameters
SI         32768
SF         100.6128193 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
  
```

UV-Spectrum of compound **4u**

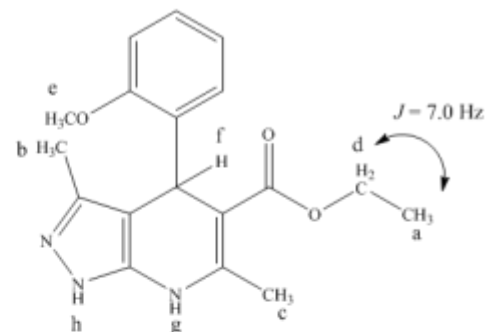
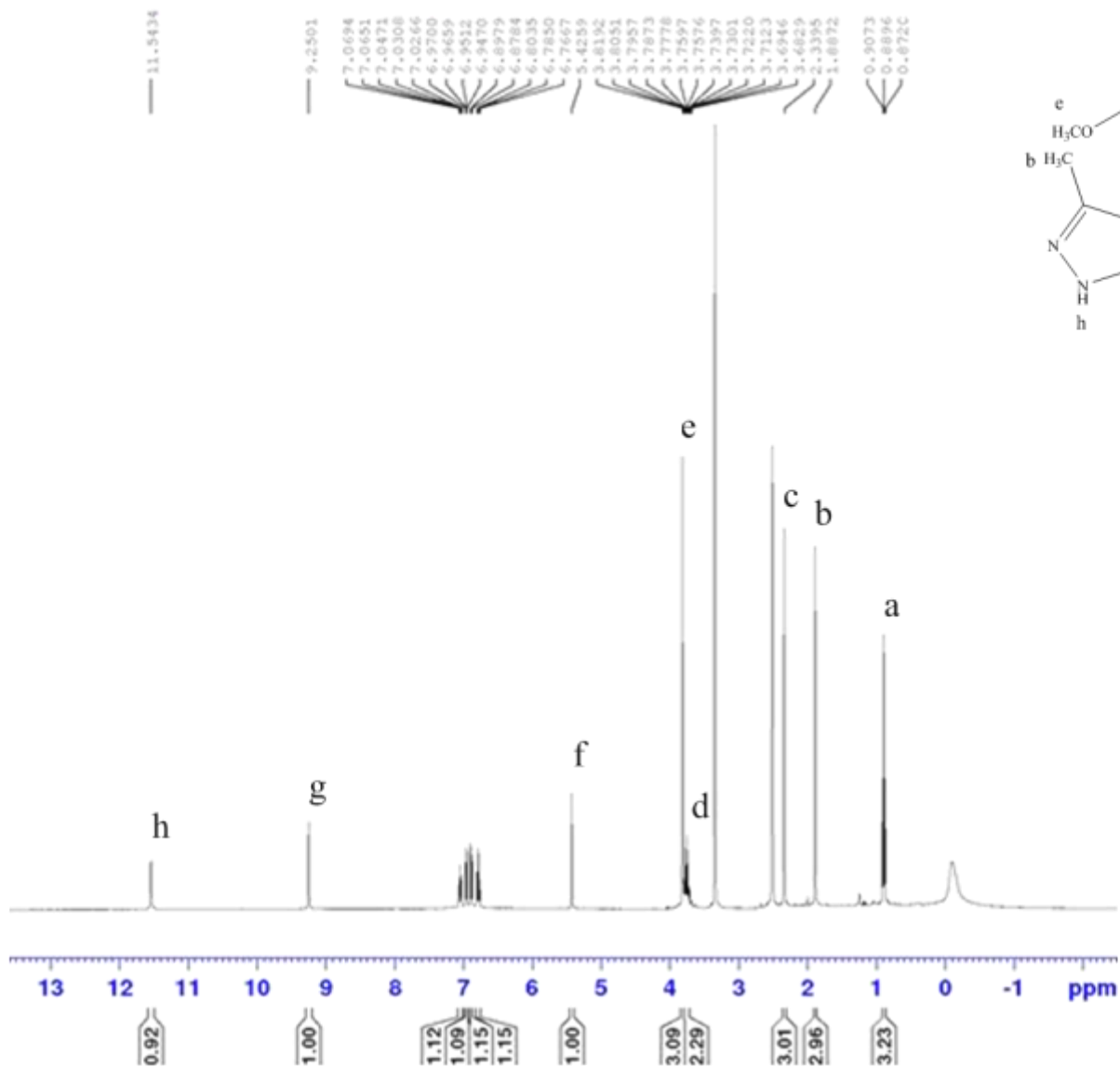


UV-absorption spectrum of **4u** in CHCl_3

IR-Spectrum of compound 4v



¹H NMR Spectrum of compound 4v



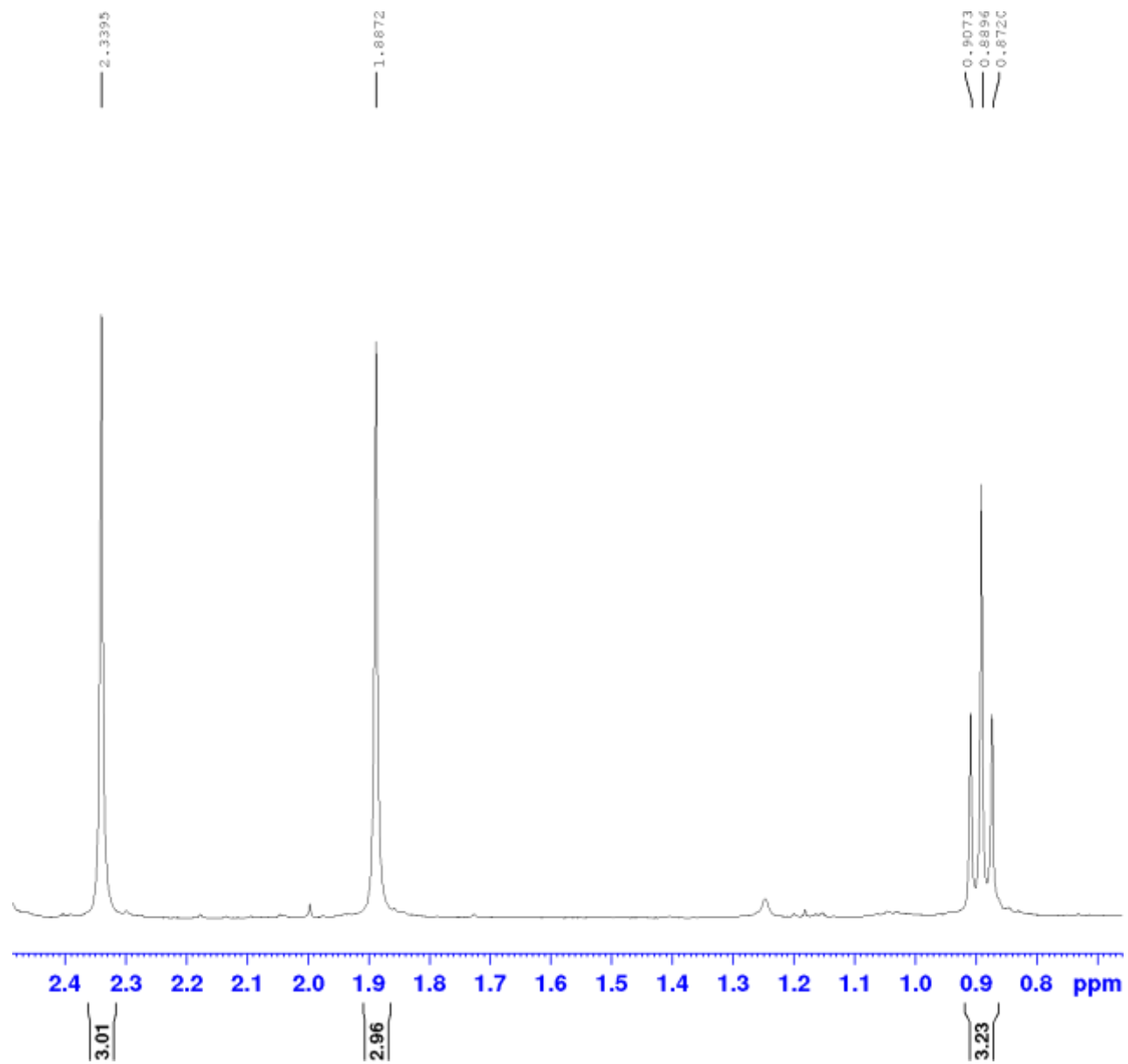
```

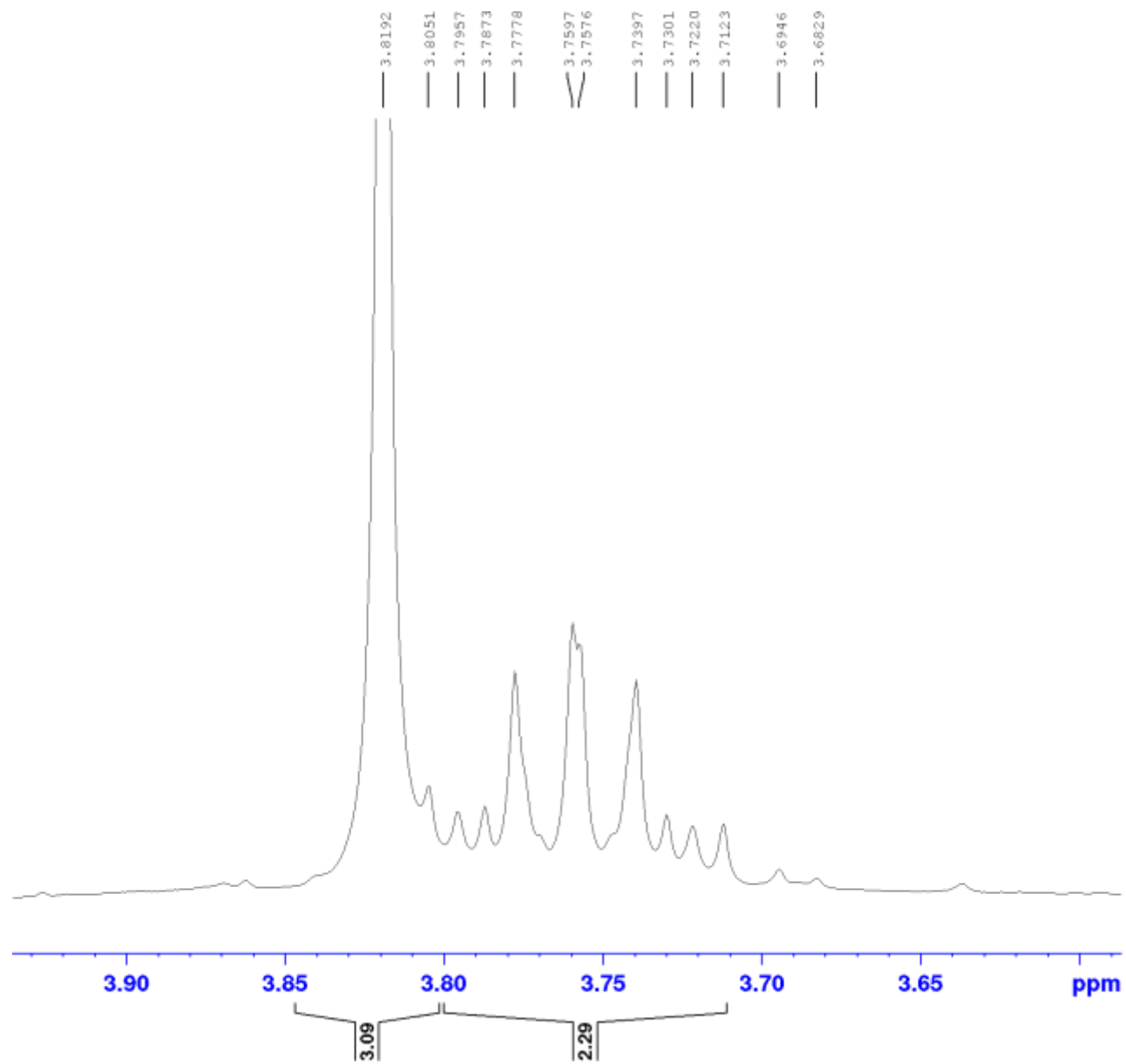
NAME      Ahnadi- Mehdi-IN97082
EXPNO     30
PROCNO    1

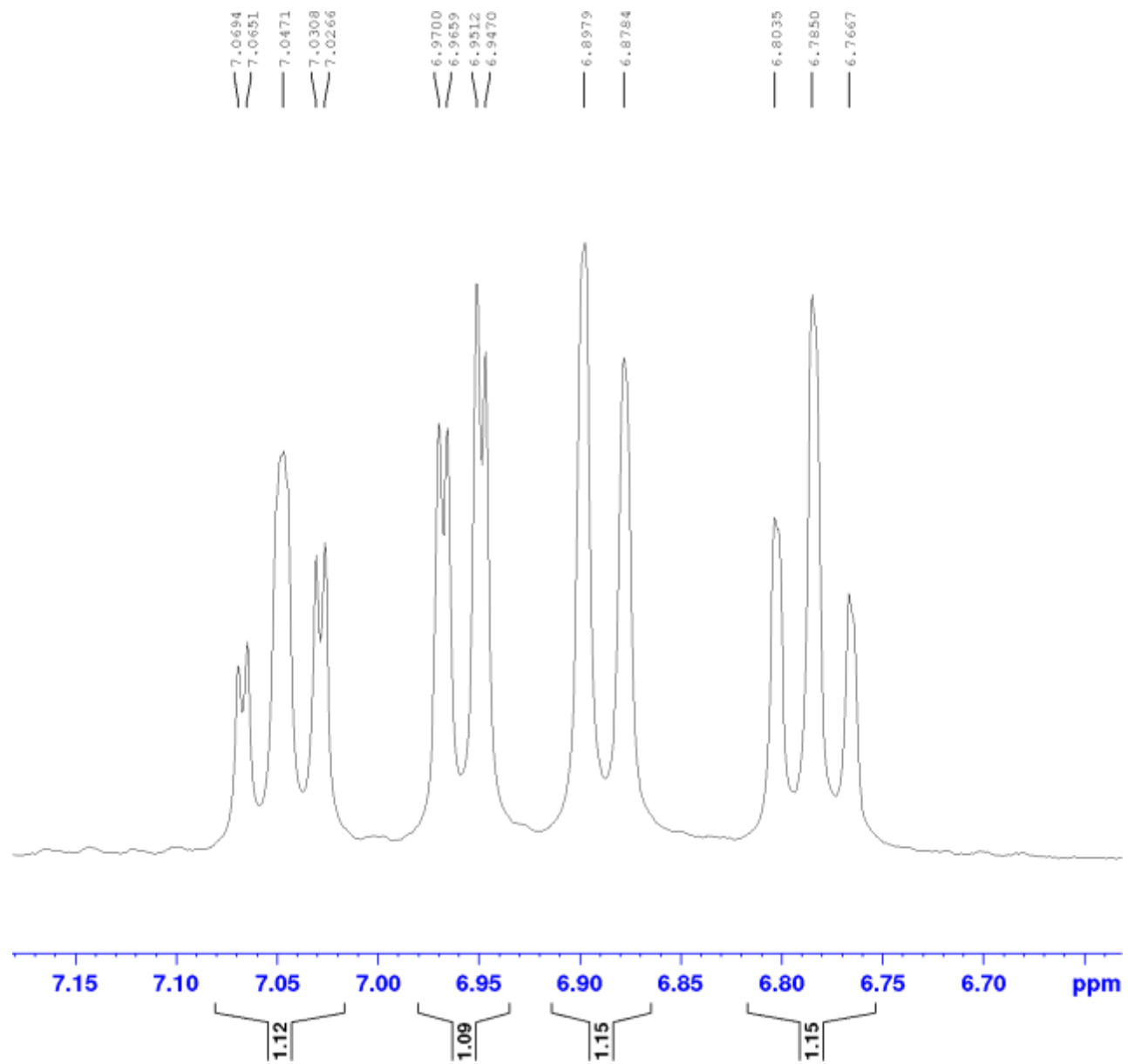
F2 - Acquisition Parameters
Date_     20181119
Time      17.41
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg
TD         50504
SOLVENT   DMSO
NS         32
DS         2
SWH        8802.817 Hz
FIDRES     0.174299 Hz
AQ         2.8686273 sec
RG         71.8
DW         56.800 usec
DE         6.50 usec
TE         294.8 K
D1         5.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         11.00 usec
PL1        -2.00 dB
PL1W       17.51671600 W
SFO1       400.1326008 MHz

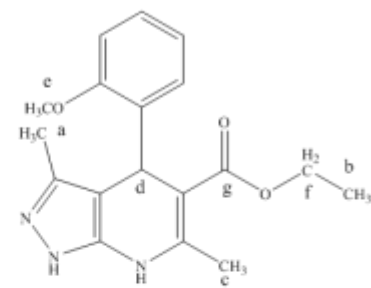
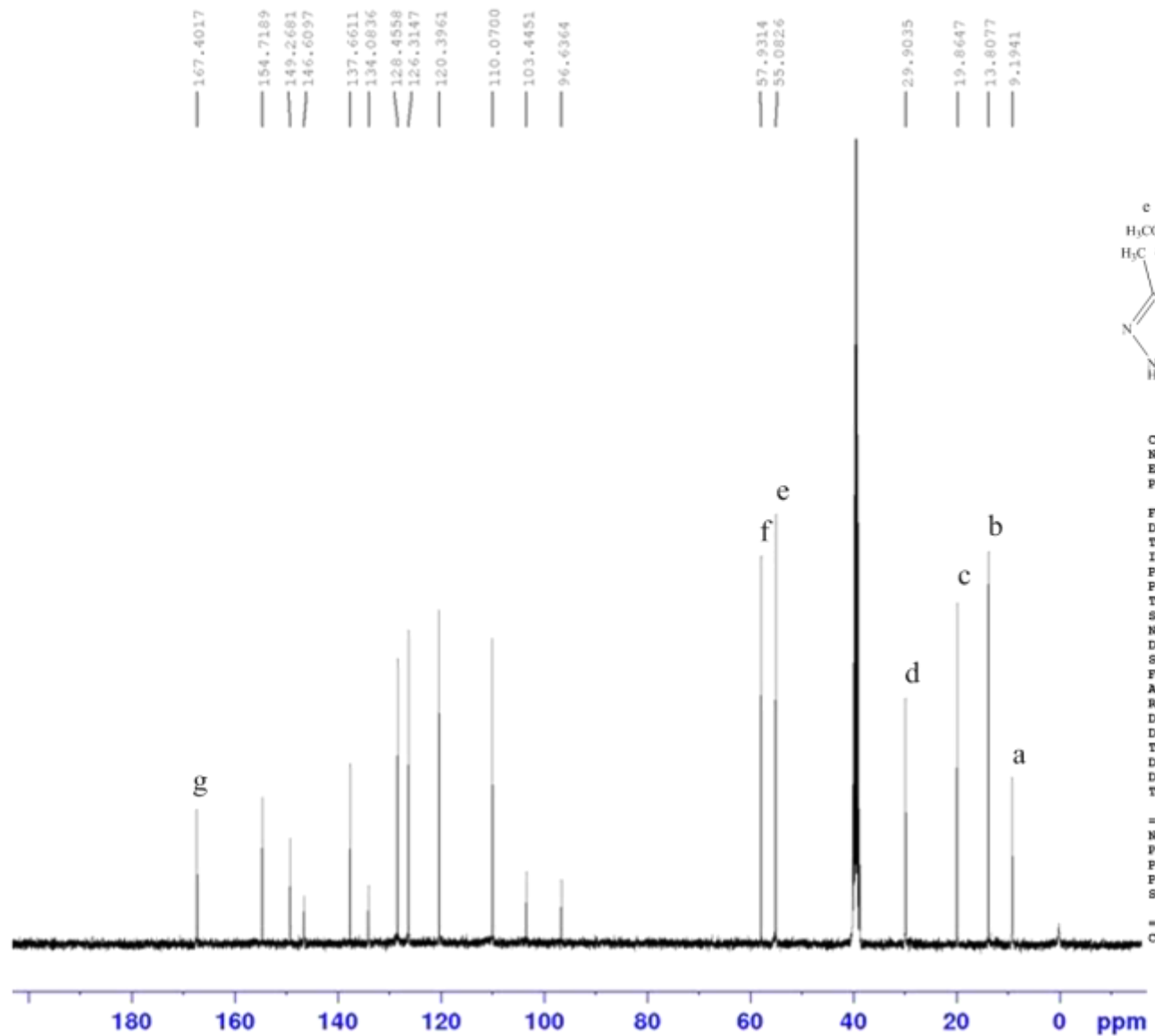
F2 - Processing parameters
SI         32768
SF         400.1300000 MHz
WDW        EM
SSB        0
TA         0.90 Hz
    
```





¹³C NMR Spectrum of compound 4v



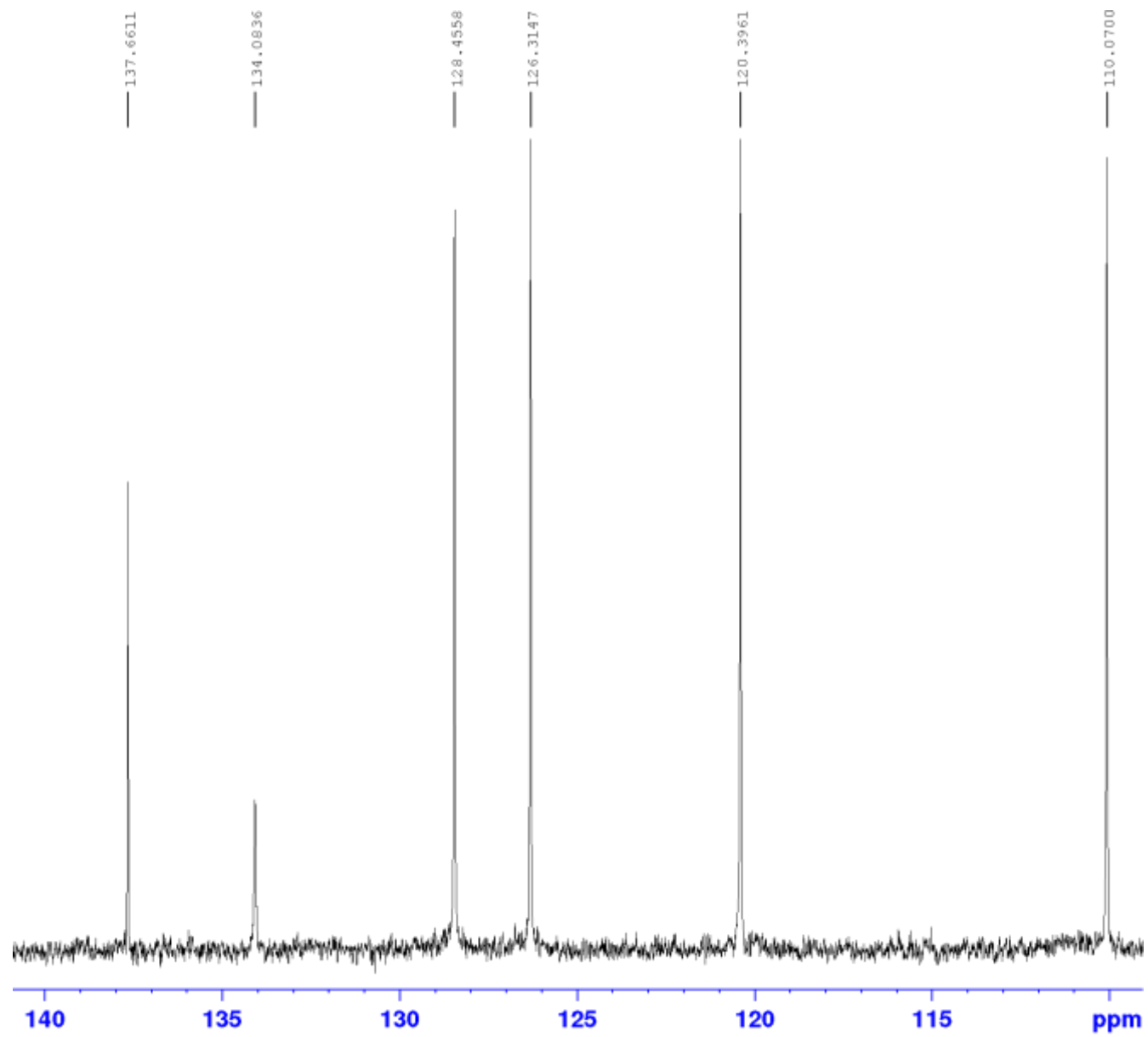
```

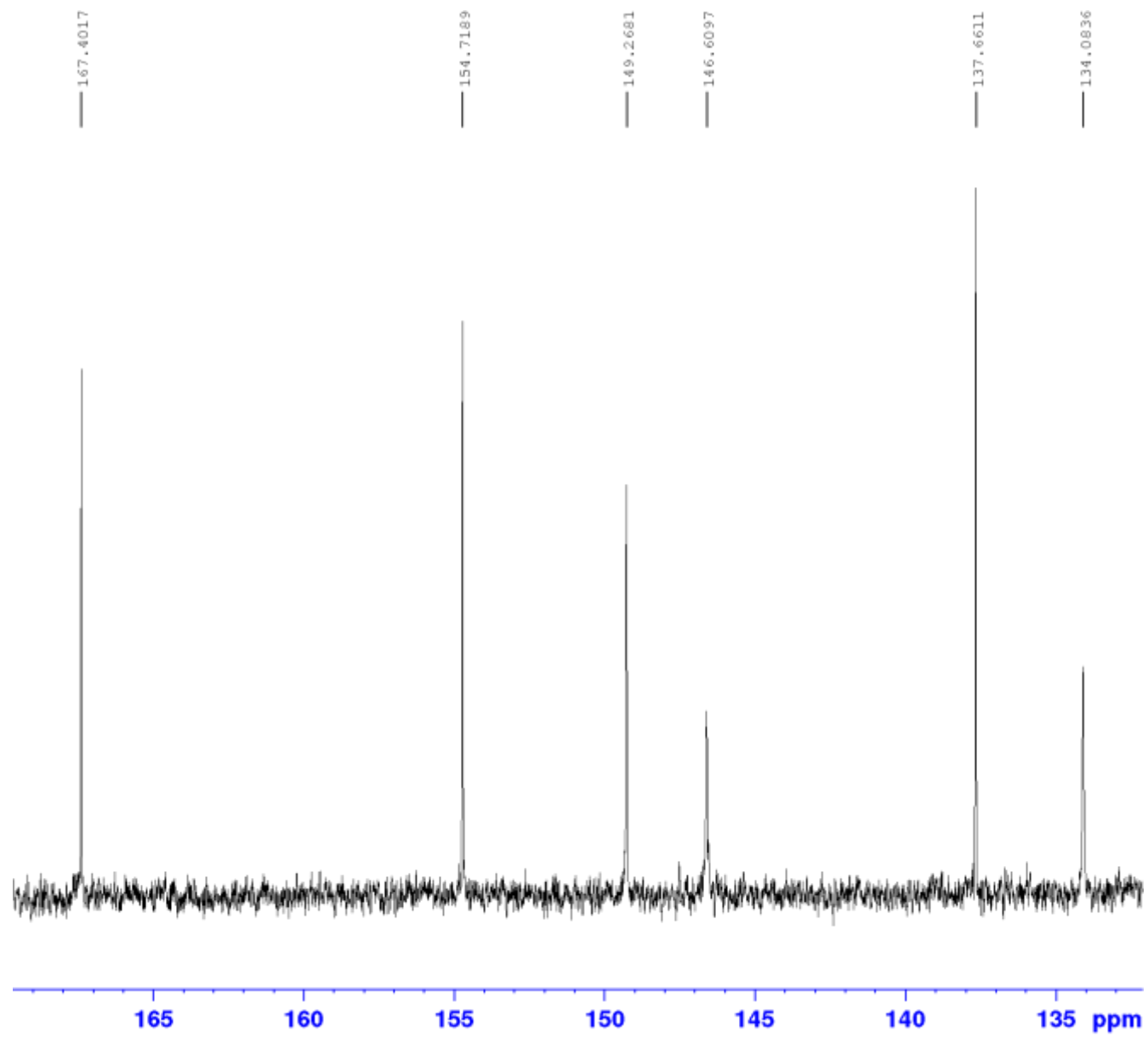
Current Data Parameters
NAME      Ahmadi-Mehdi-IN970830
EXPNO     31
PROCNO    1

F2 - Acquisition Parameters
Date_     20181124
Time      12.02
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         50502
SOLVENT   DMSO
NS         3000
DS         2
SWH        25252.525 Hz
FIDRES     0.500030 Hz
AQ         0.9999396 sec
RG         2050
DW         19.800 usec
DE         6.50 usec
TE         294.7 K
D1         1.00000000 sec
D11        0.03000000 sec
TD0        1

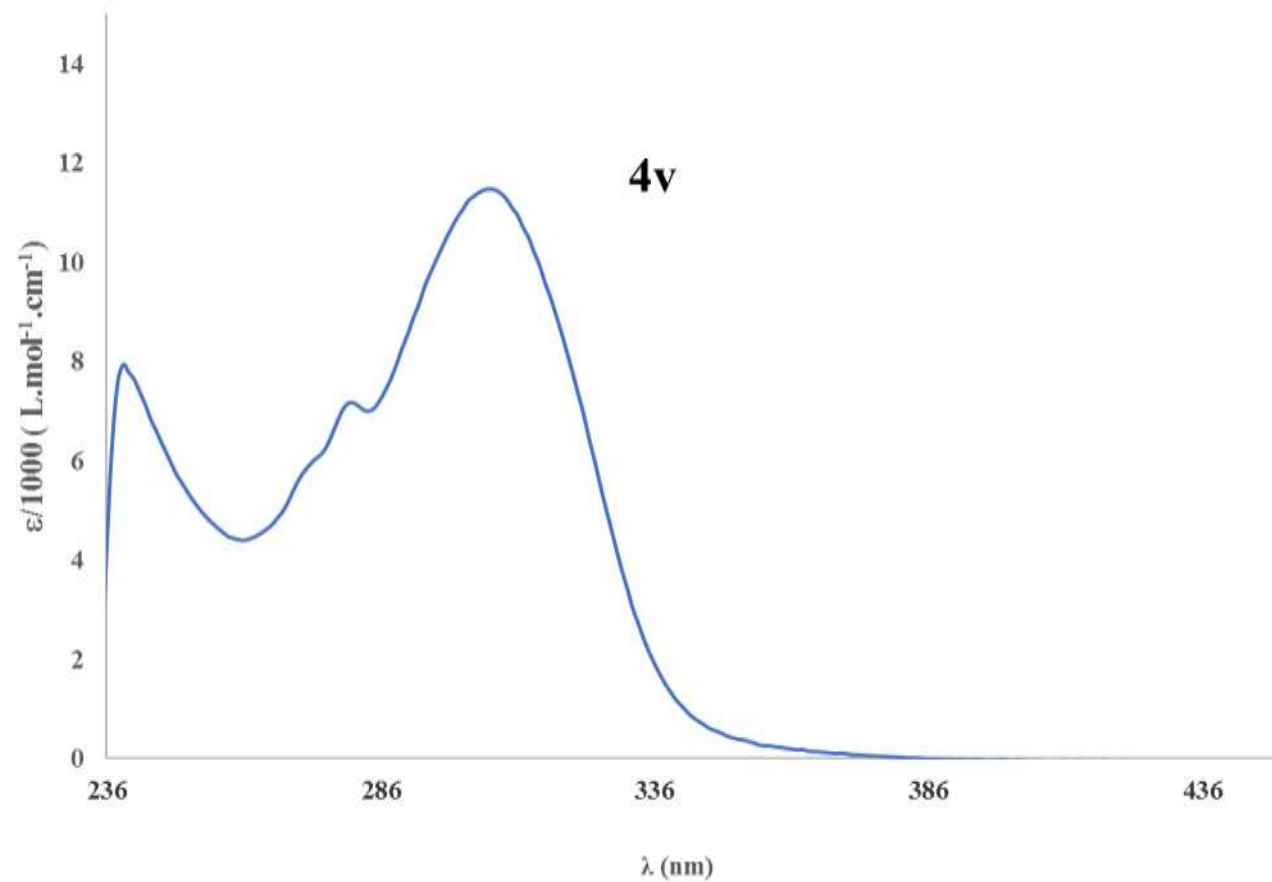
===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -1.00 dB
PL1W       42.69075012 W
SFO1       100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
    
```



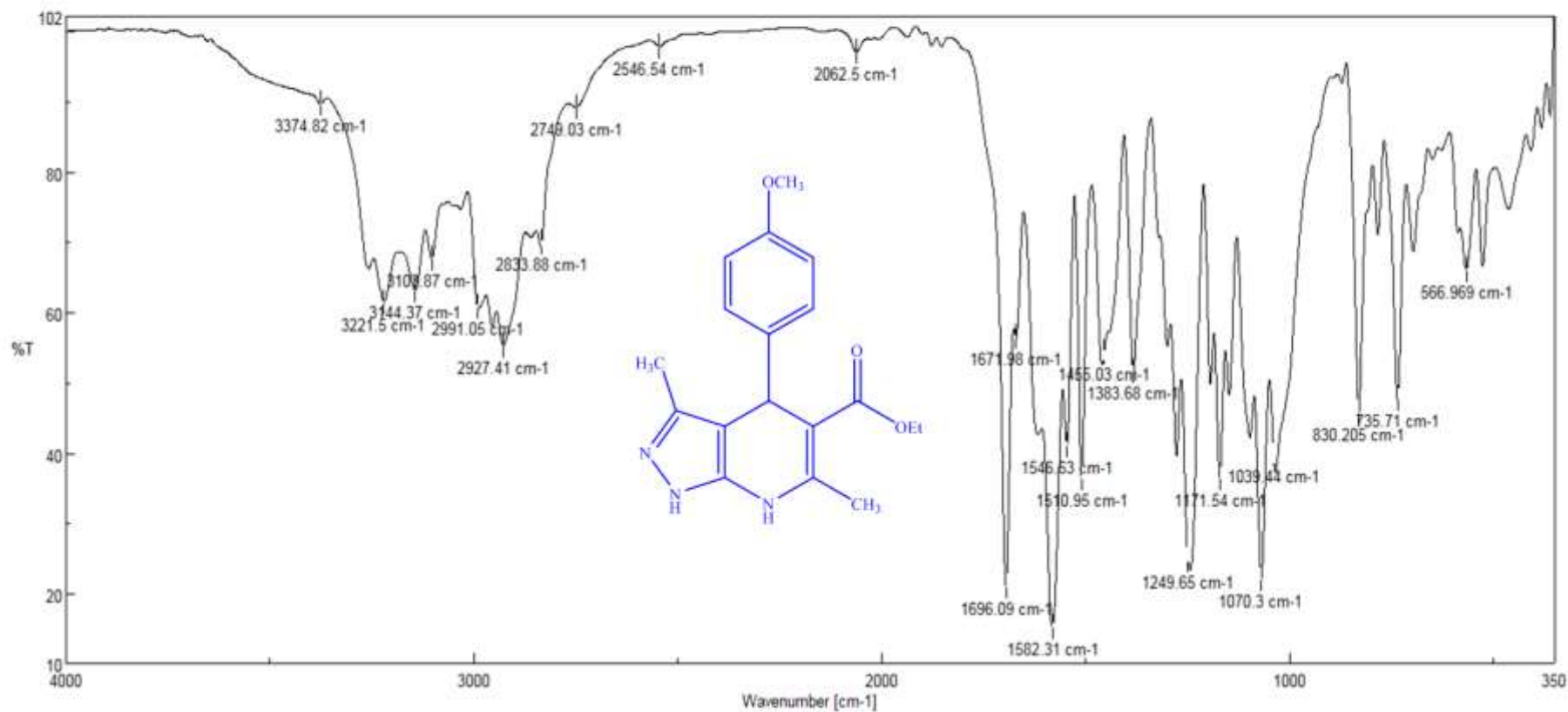


UV-Spectrum of compound **4v**

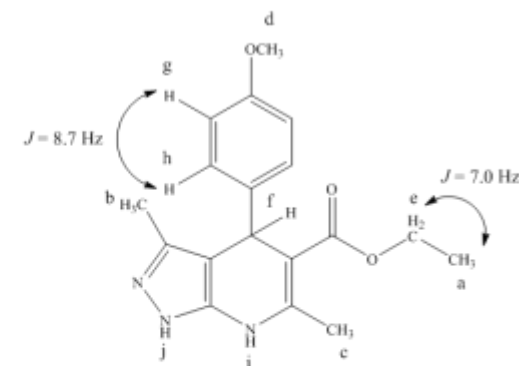
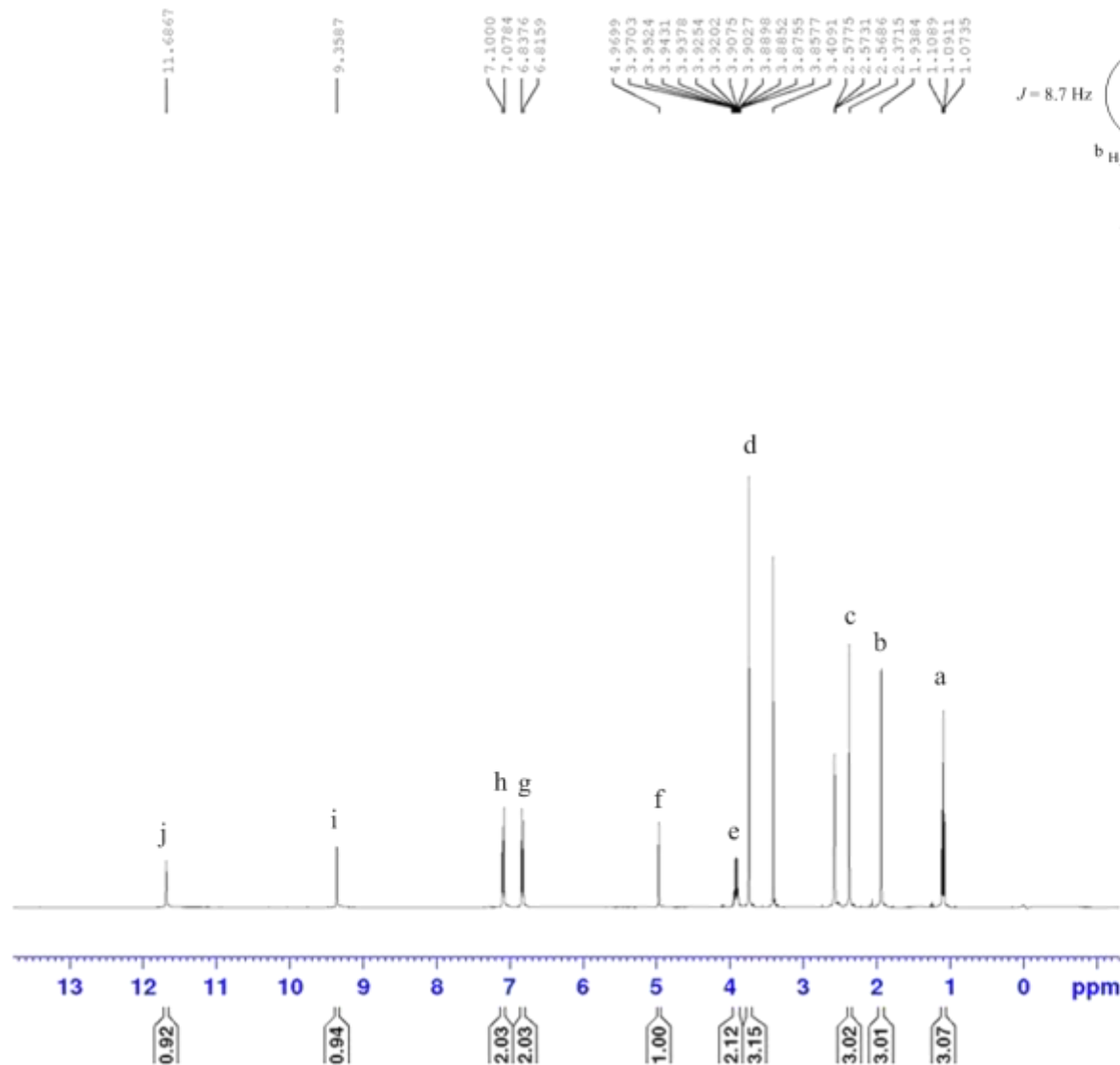


UV-absorption spectrum of **4v** in CHCl_3

IR-Spectrum of compound 4w



¹H NMR Spectrum of compound 4w



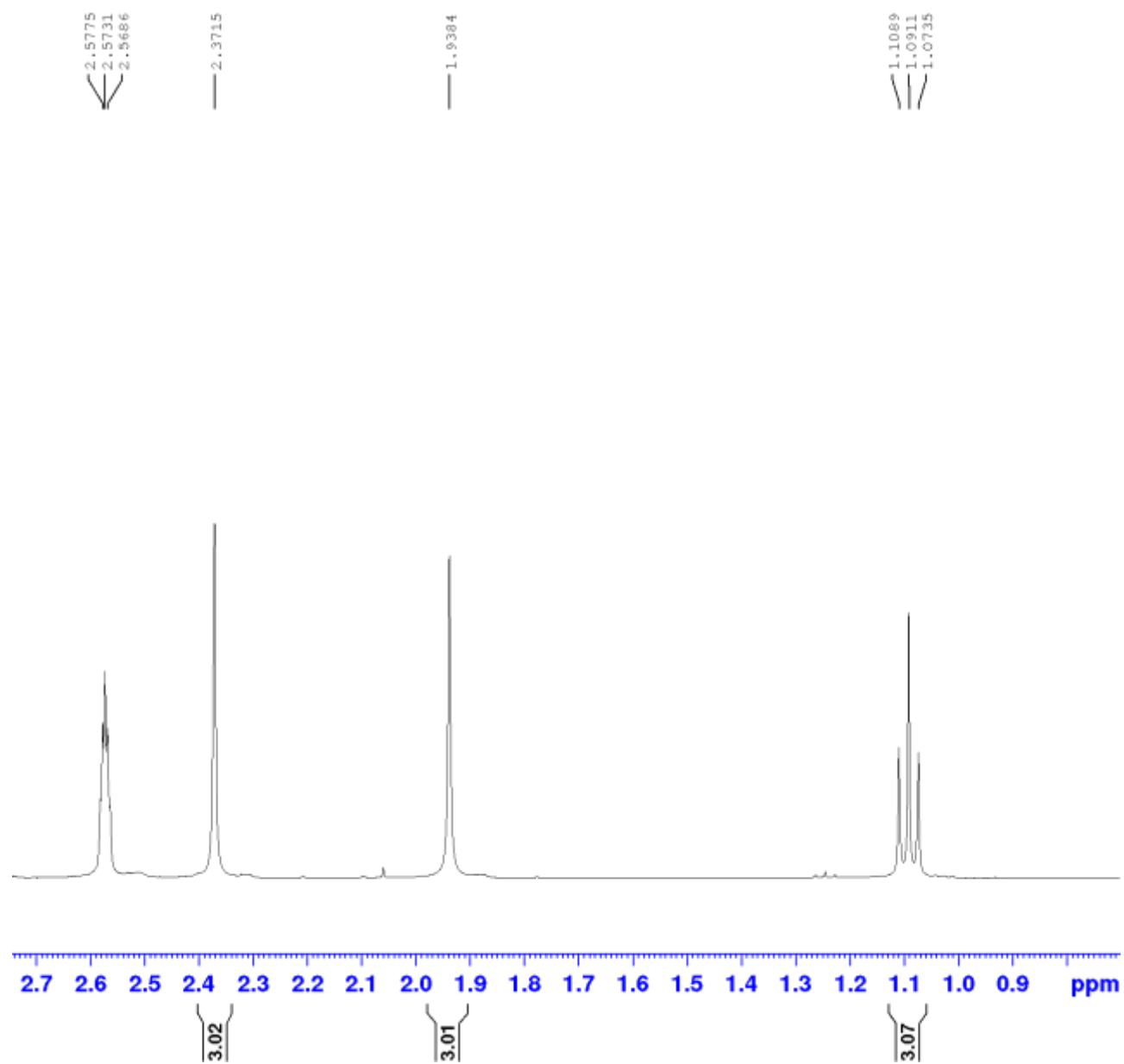
```

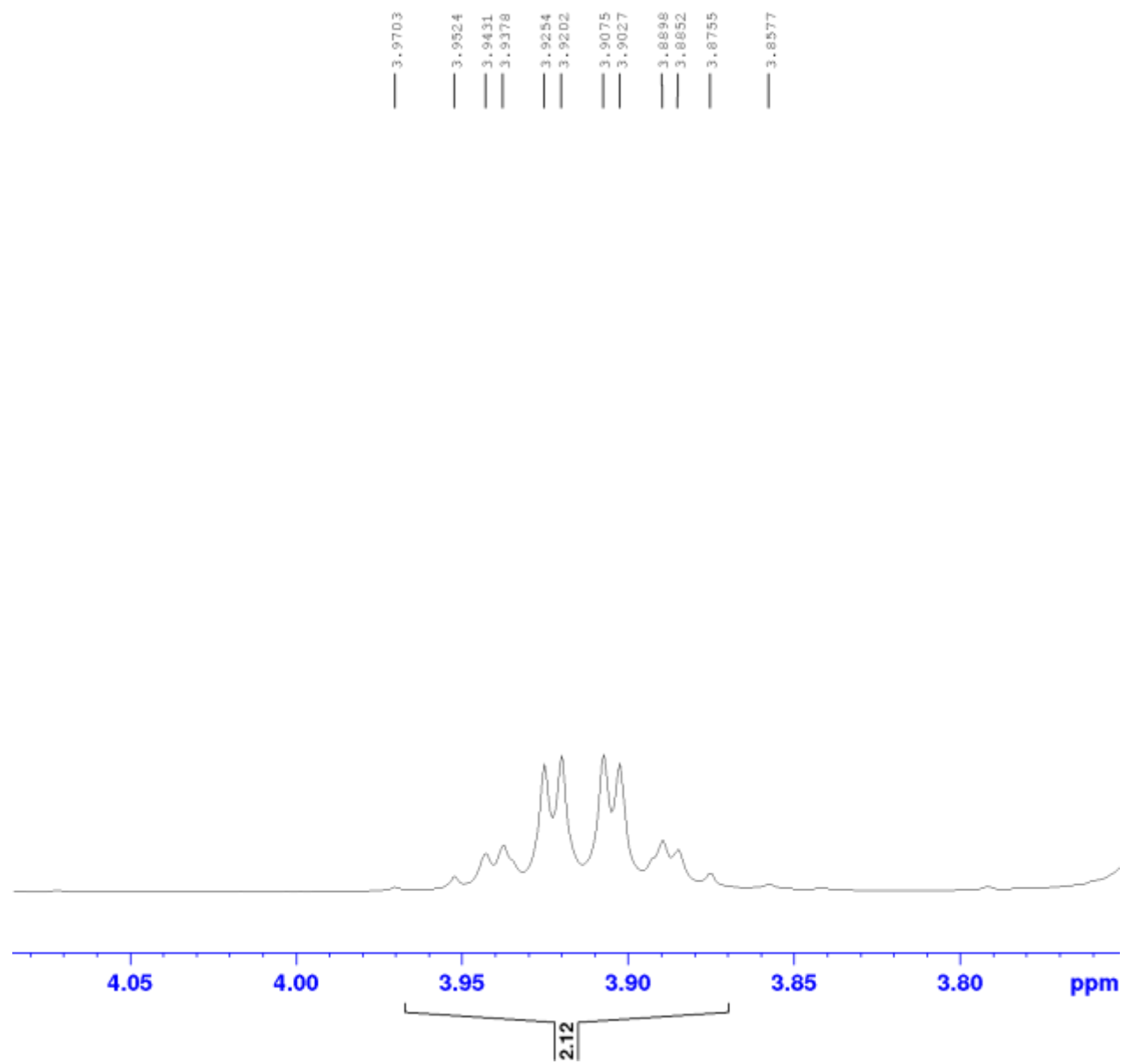
NAME      Ahmadi- Mehdi-EN97041
EXPNO     10
PROCNO    1

F2 - Acquisition Parameters
Date_     20180711
Time      11.57
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zg
TD         50504
SOLVENT   DMSO
NS         32
DS         2
SWH        8802.817 Hz
FIDRES     0.174299 Hz
AQ         2.8686273 sec
RG         80.6
DW         56.800 usec
DE         6.50 usec
TE         295.3 K
D1         5.00000000 sec
TD0        1

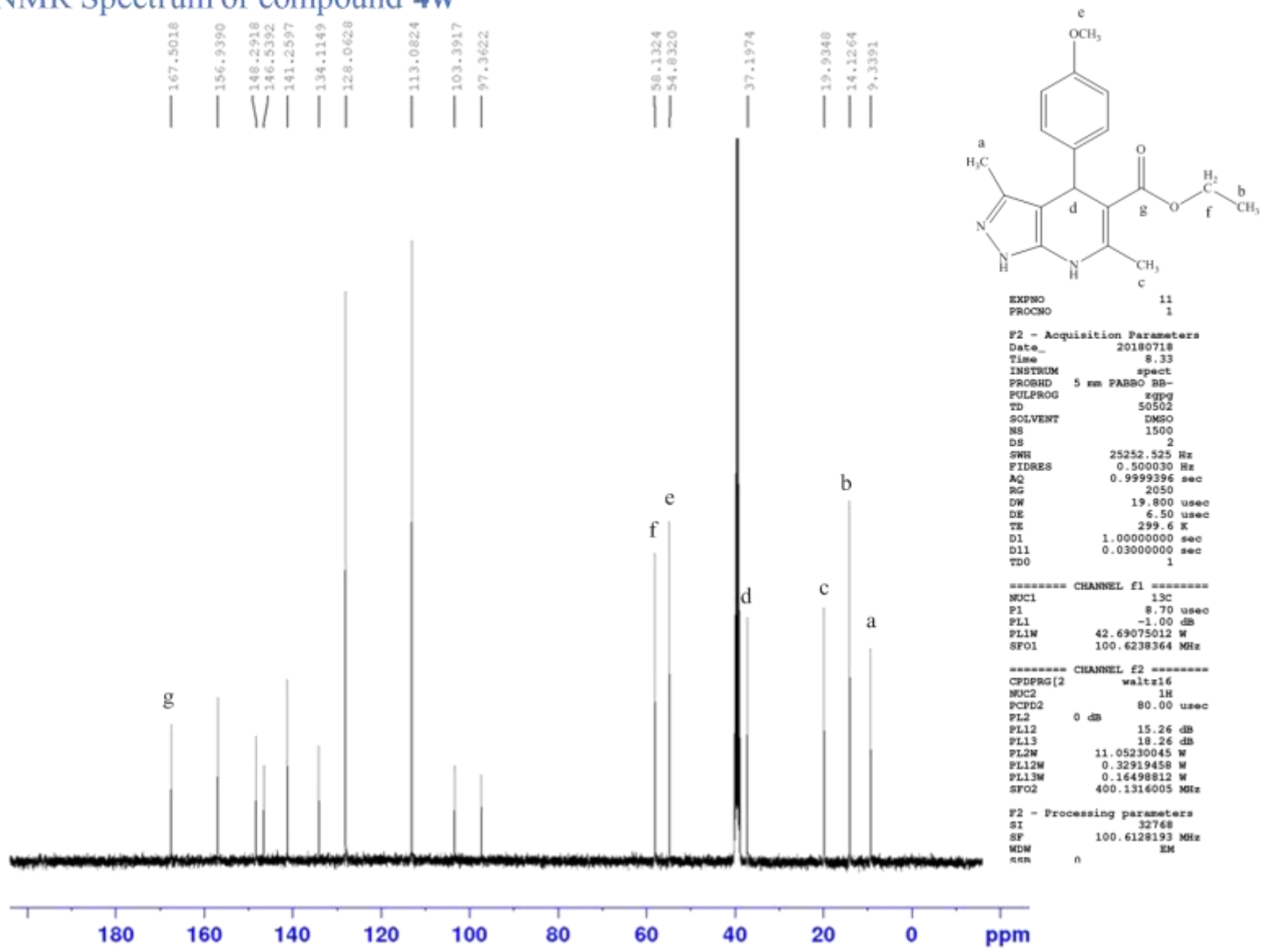
----- CHANNEL f1 -----
NUC1      1H
P1         11.00 usec
PL1        -2.00 dB
PL1W       17.51671600 W
SFO1       400.1326008 MHz

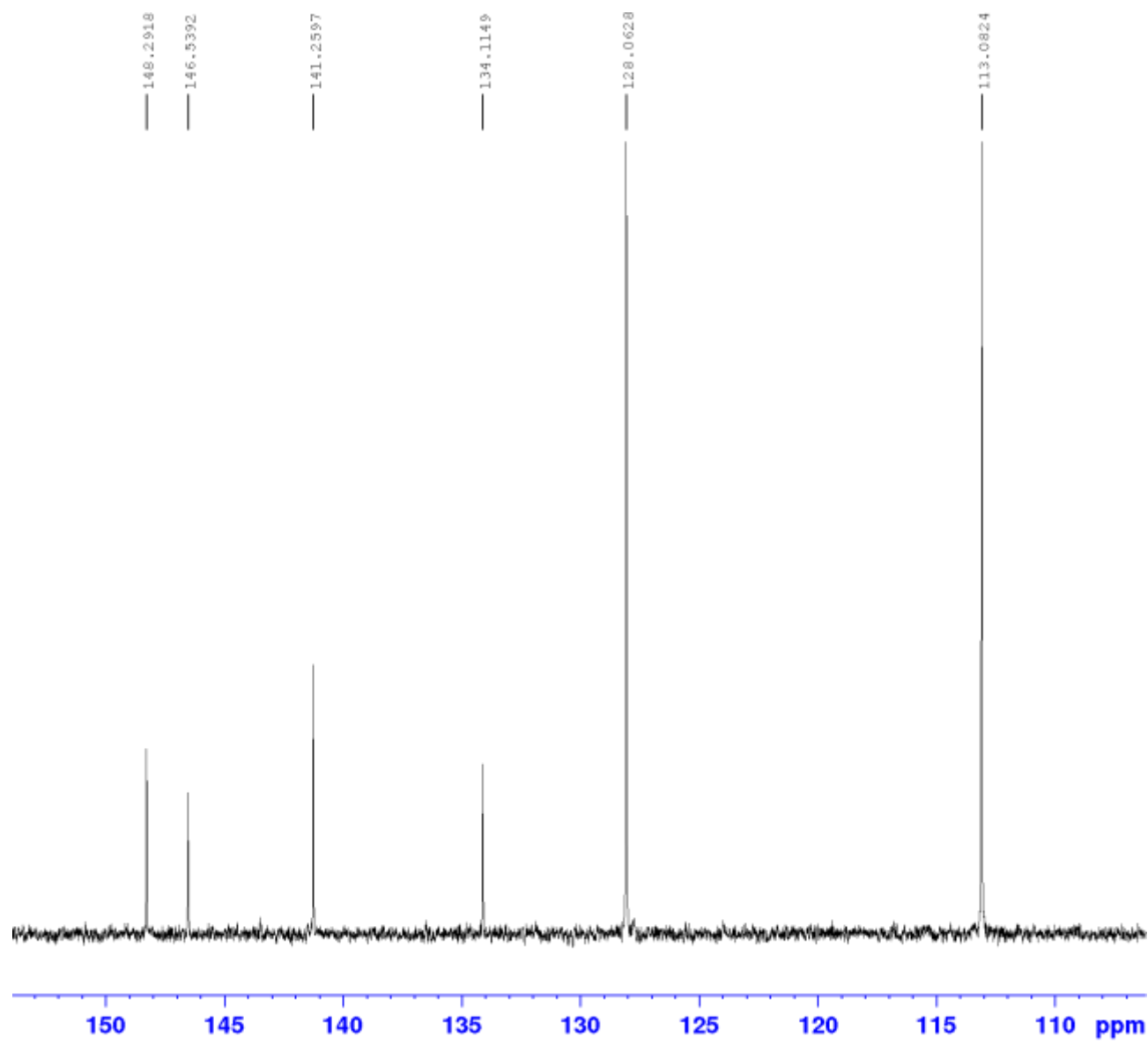
F2 - Processing parameters
SI         32768
SF         400.1299745 MHz
WDW        EM
SSB        0
LR         0.30 Hz
    
```



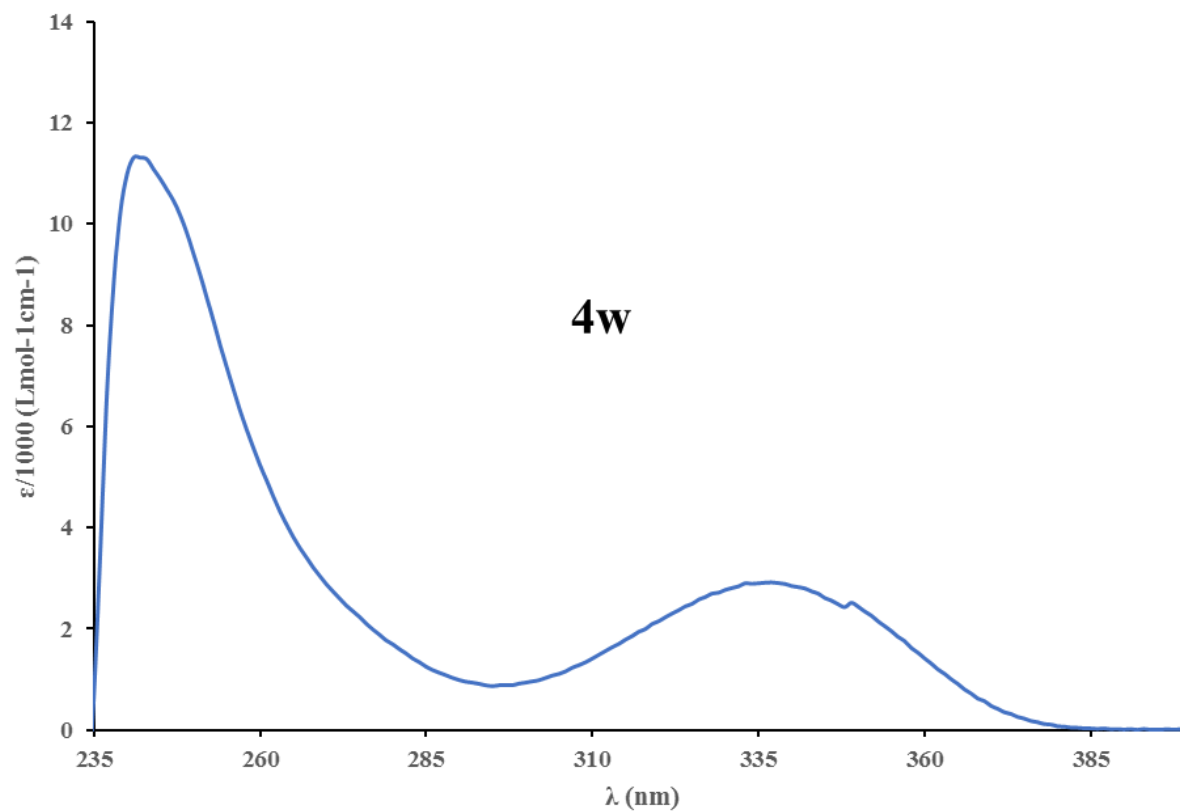


¹³C NMR Spectrum of compound 4w





UV-Spectrum of compound **4w**

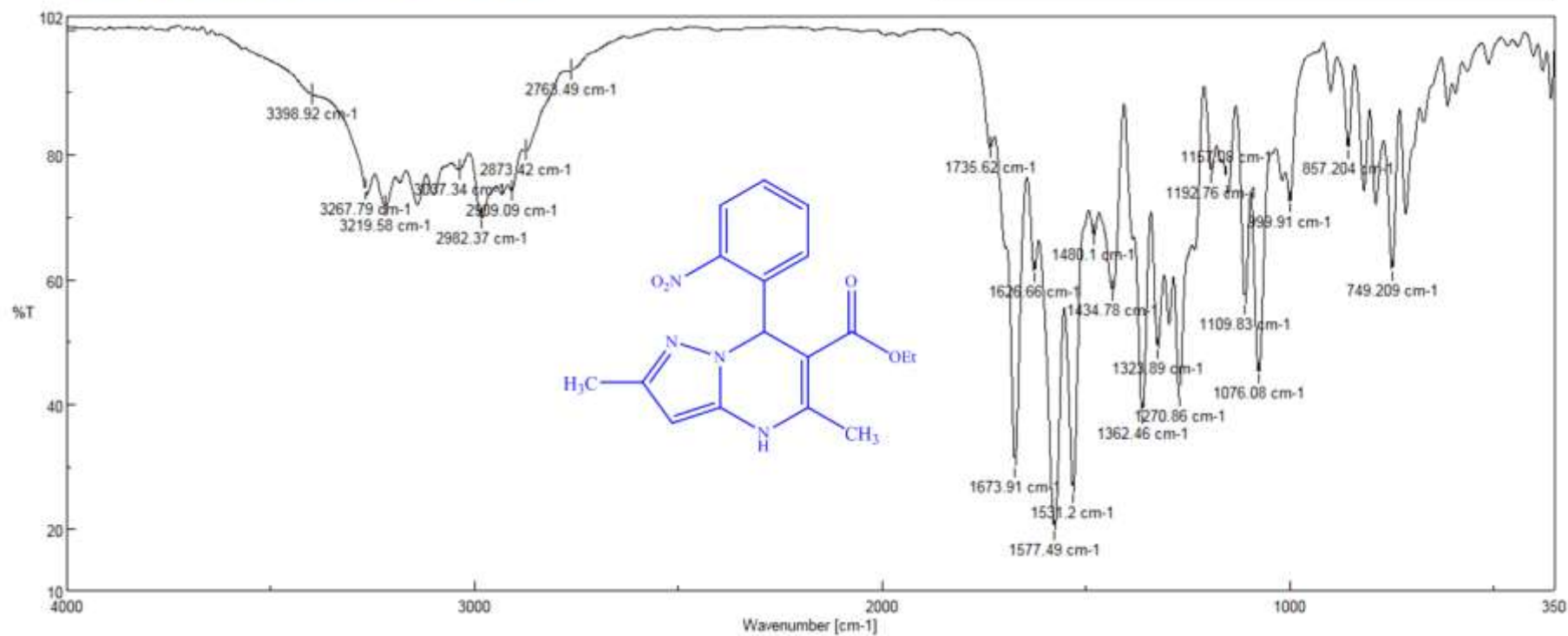


UV-absorption spectrum of **4w** in CHCl_3

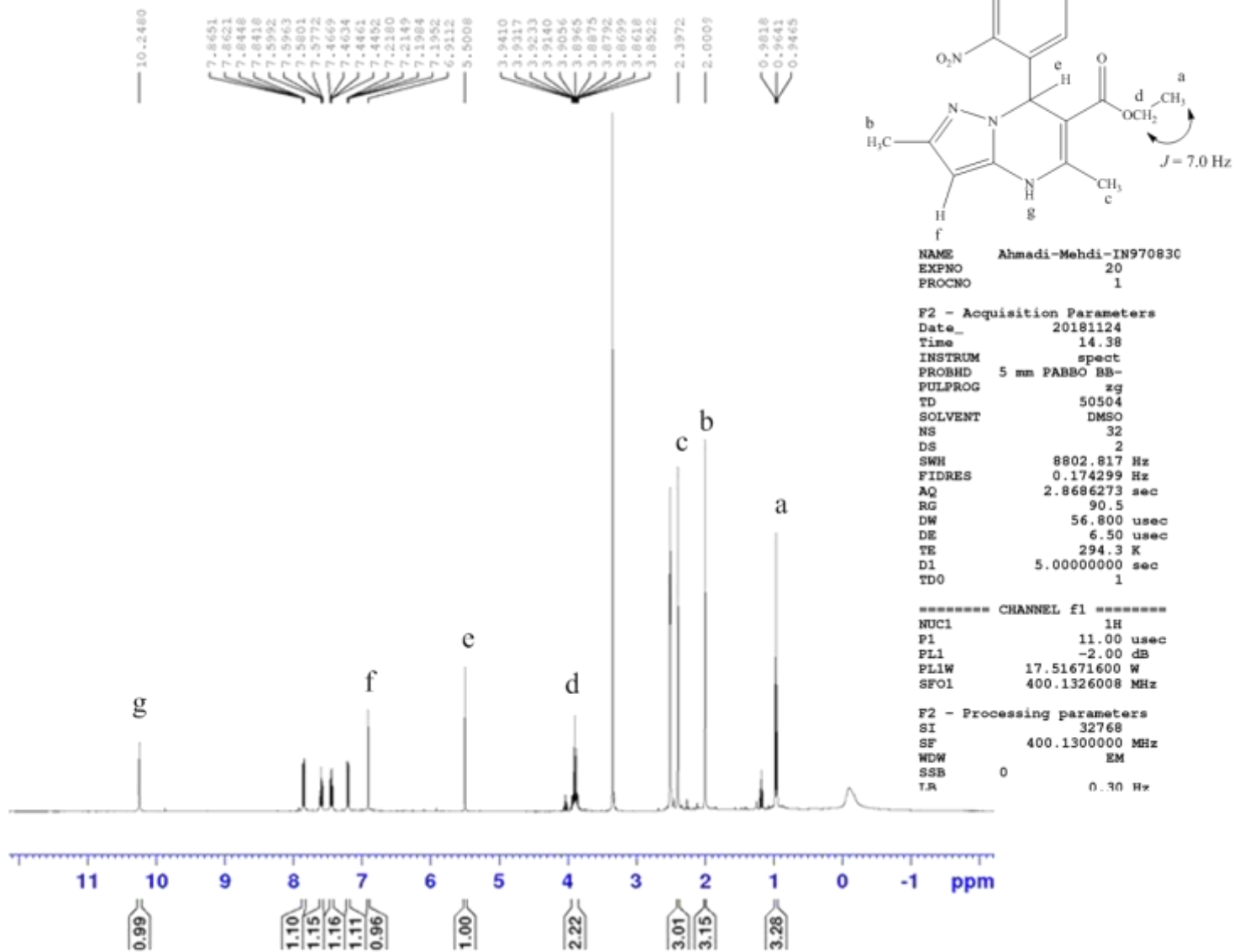
Instrument Specifications

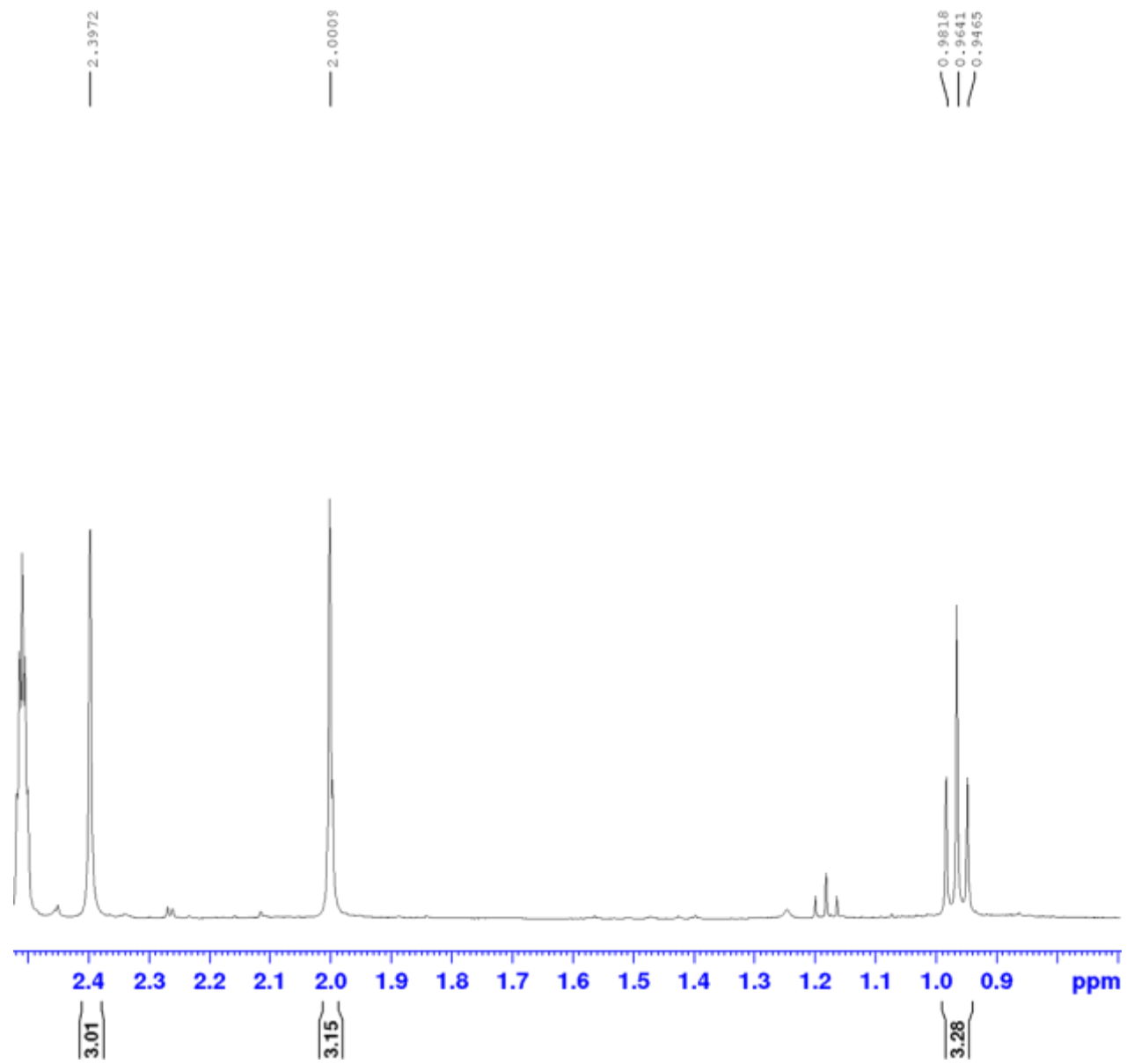
FT Infrared Spectroscopy, JASCO, FT/IR-6300 (400-4000 cm^{-1}), Japan

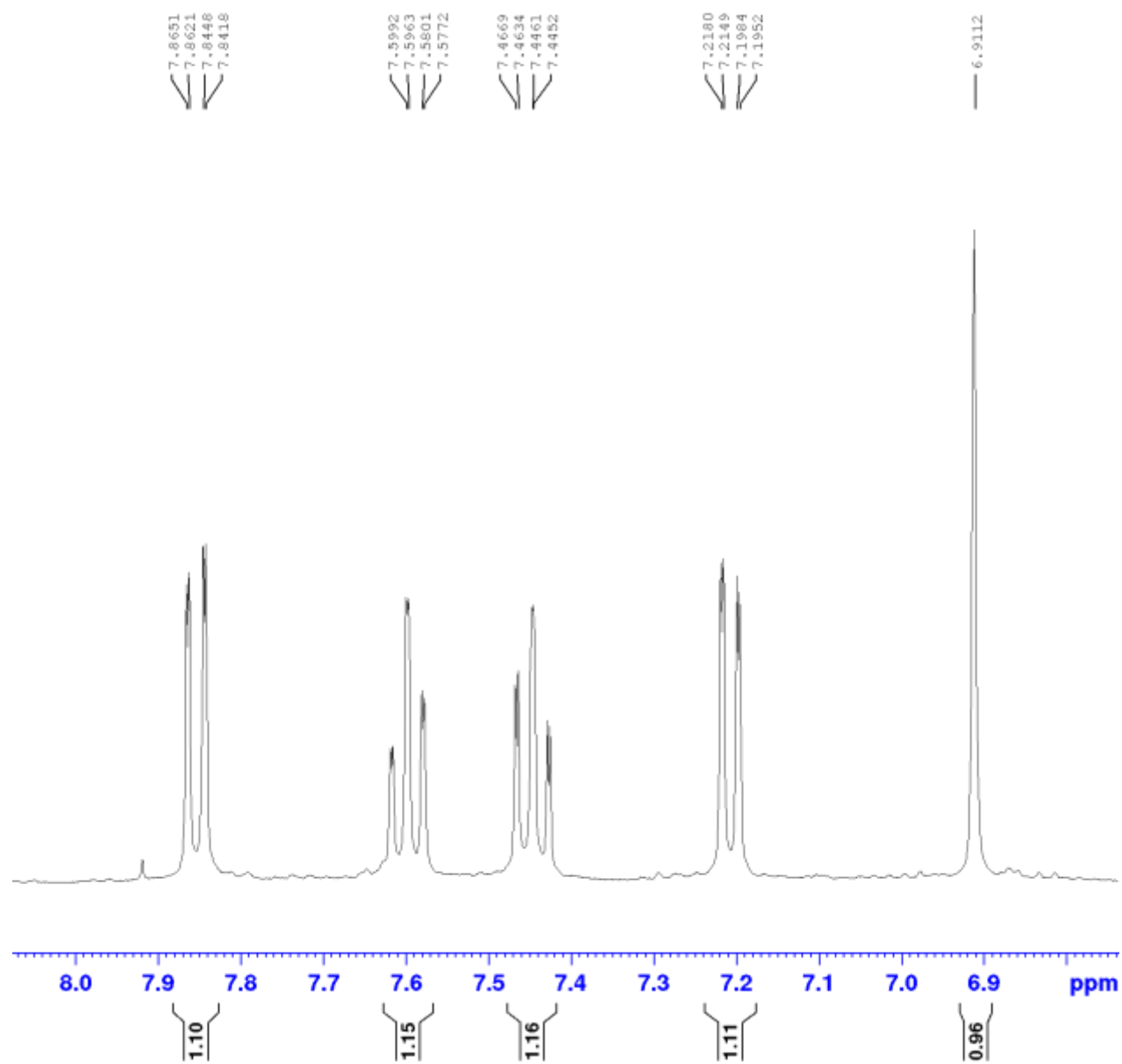
IR-Spectrum of compound 5a



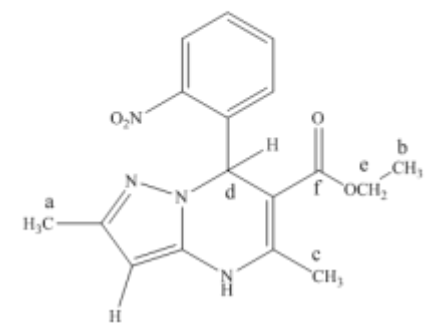
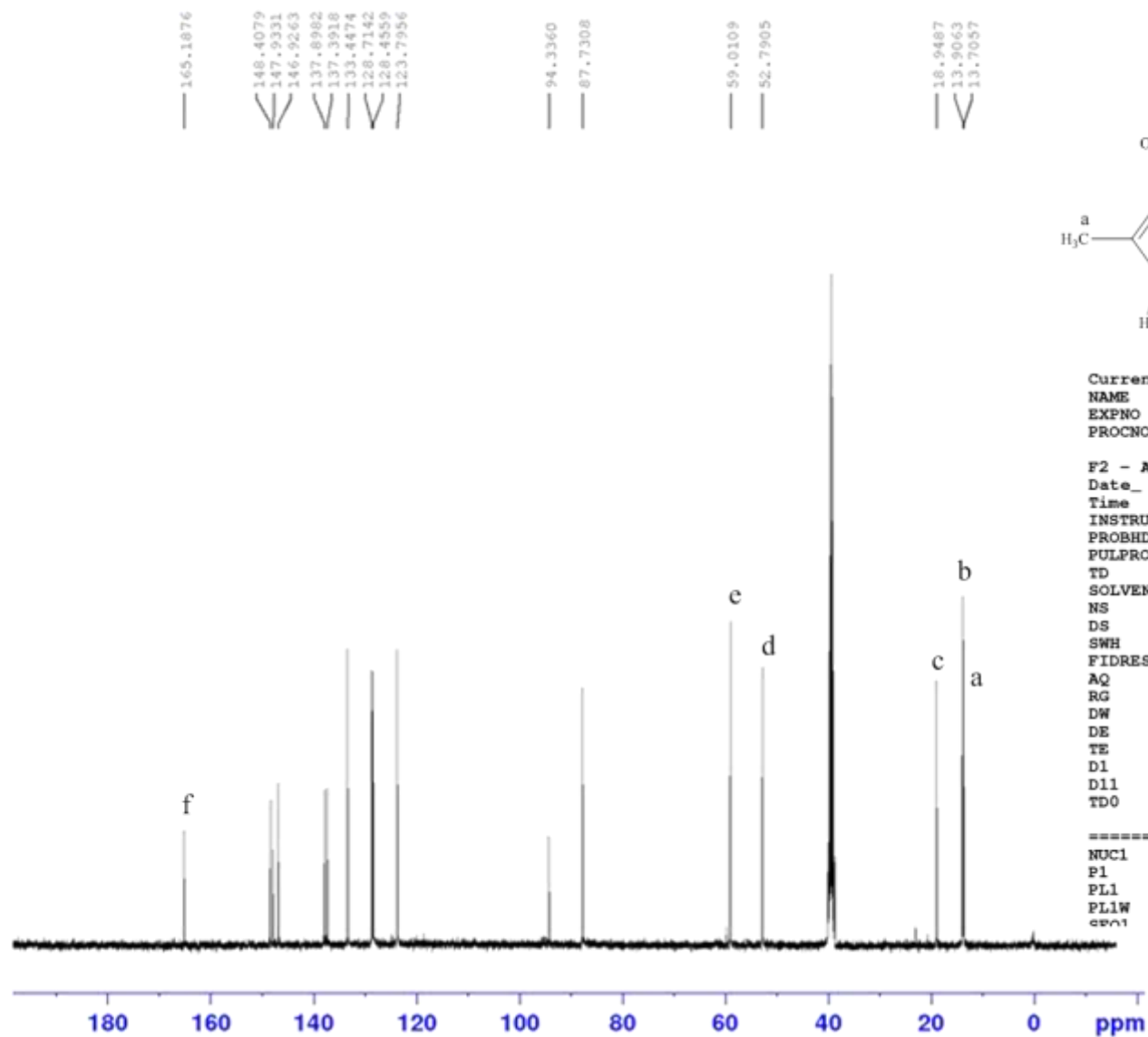
¹H NMR Spectrum of compound 5a







¹³C NMR Spectrum of compound 5a

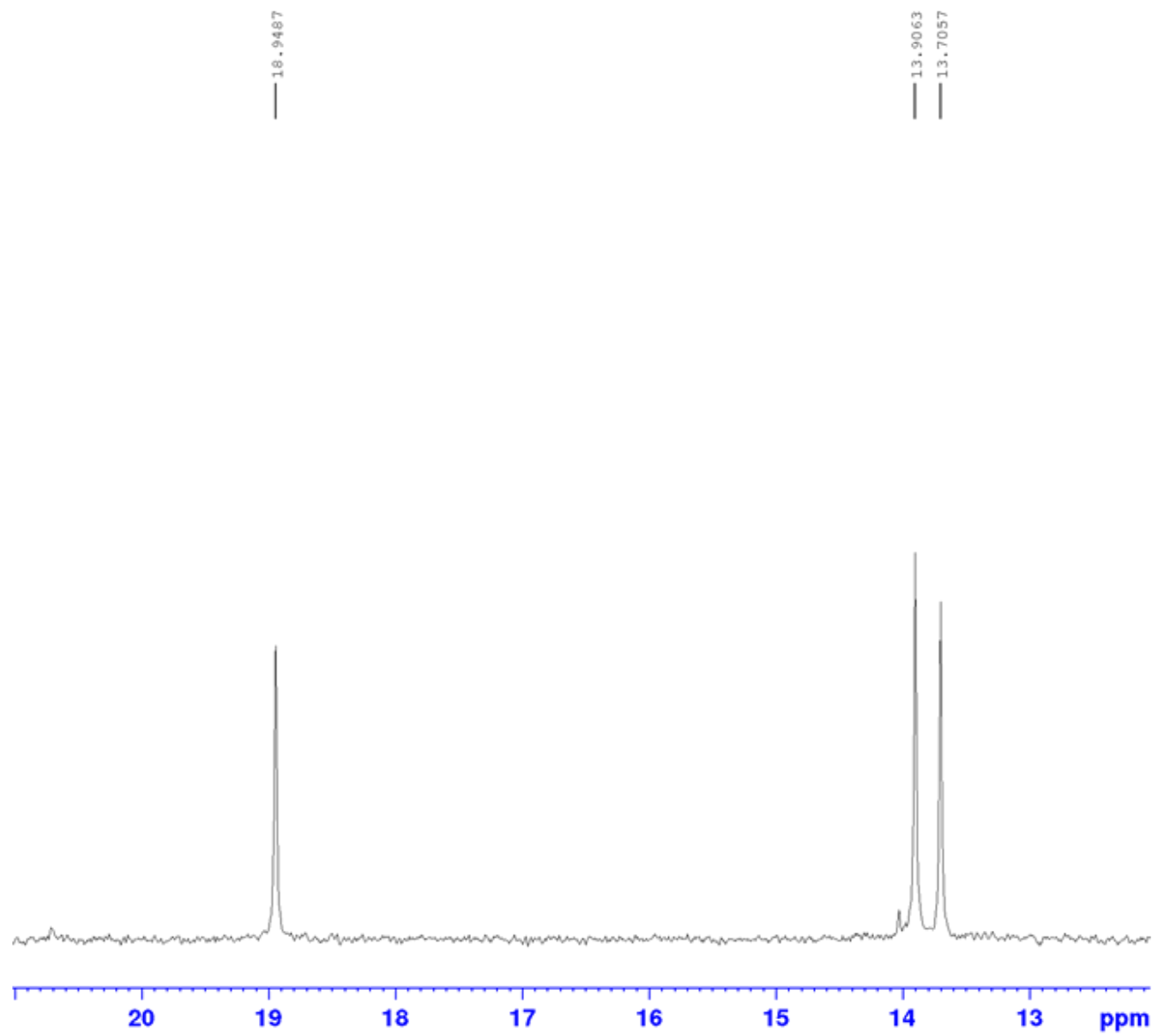


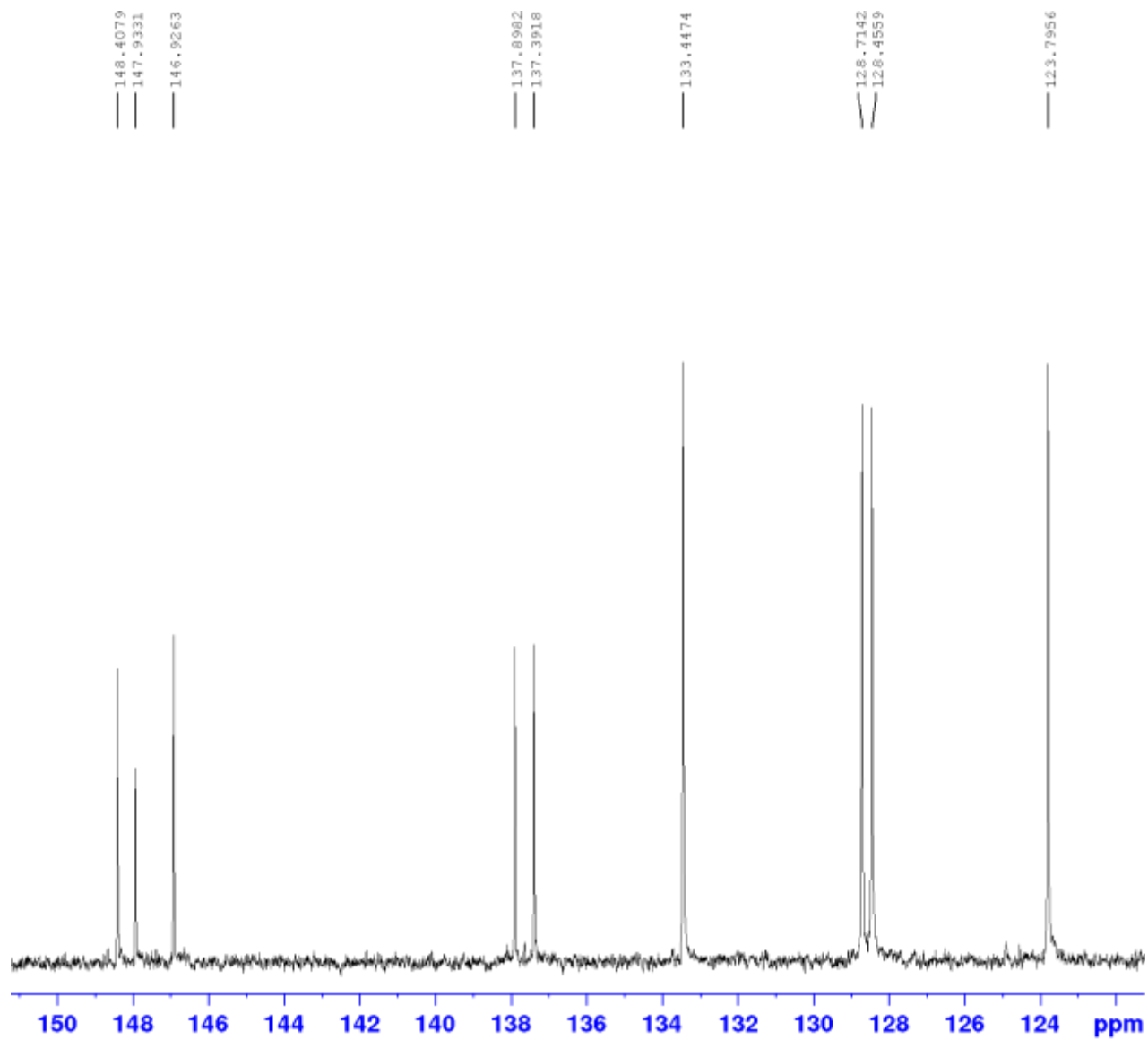
```

Current Data Parameters
NAME      Ahmadi- Mehdi-IN97091
EXPNO     21
PROCNO    1

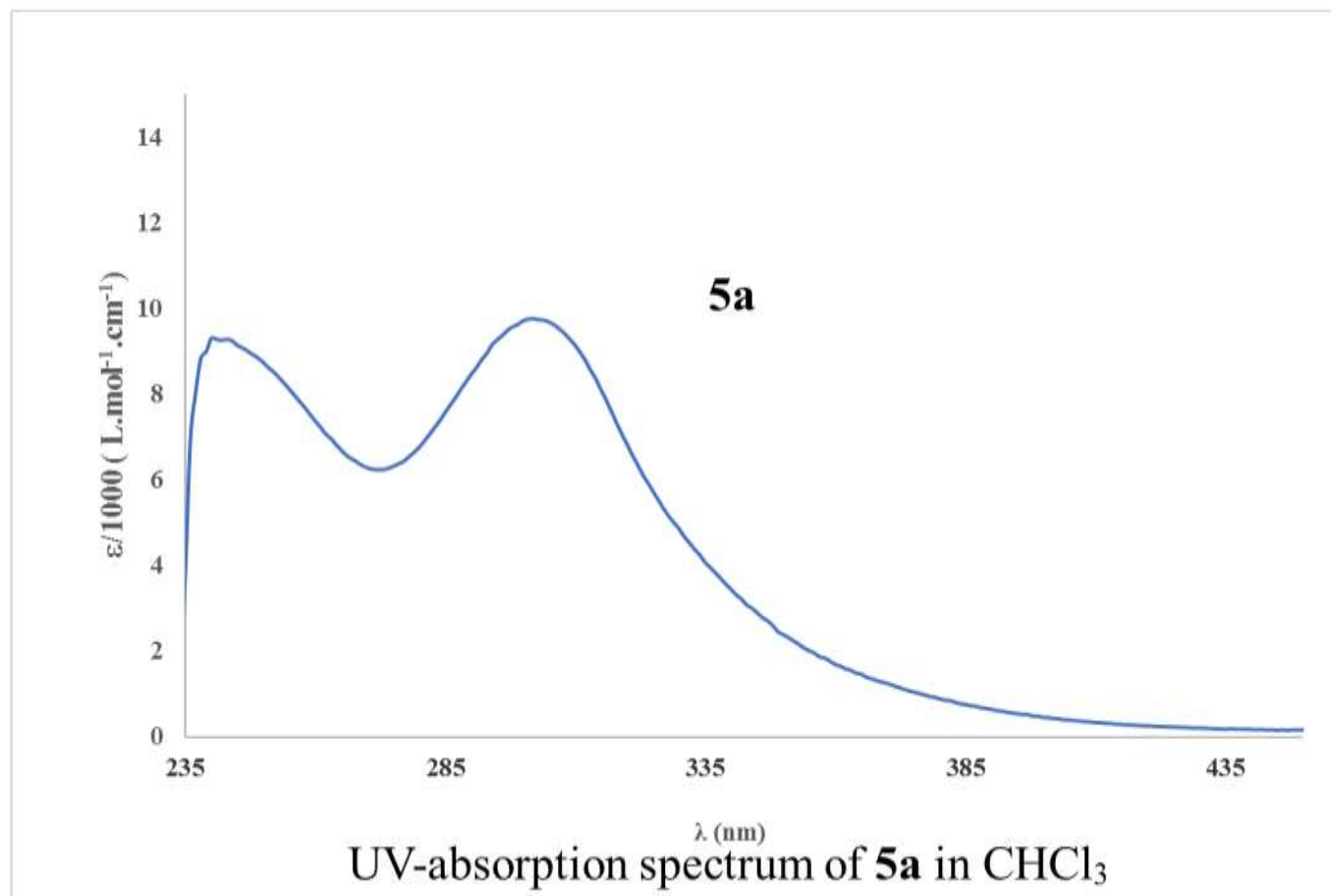
F2 - Acquisition Parameters
Date_     20181211
Time      9.17
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         50502
SOLVENT   DMSO
NS         1339
DS         2
SWH       25252.525 Hz
FIDRES    0.500030 Hz
AQ         0.9999396 sec
RG         2050
DW         19.800 usec
DE         6.50 usec
TE         294.8 K
D1         1.00000000 sec
D11        0.03000000 sec
TDO        1

===== CHANNEL f1 =====
NUC1       13C
P1         9.50 usec
PL1        -1.00 dB
PL1W       42.69075012 W
CP01      100.6230364 MHz
    
```



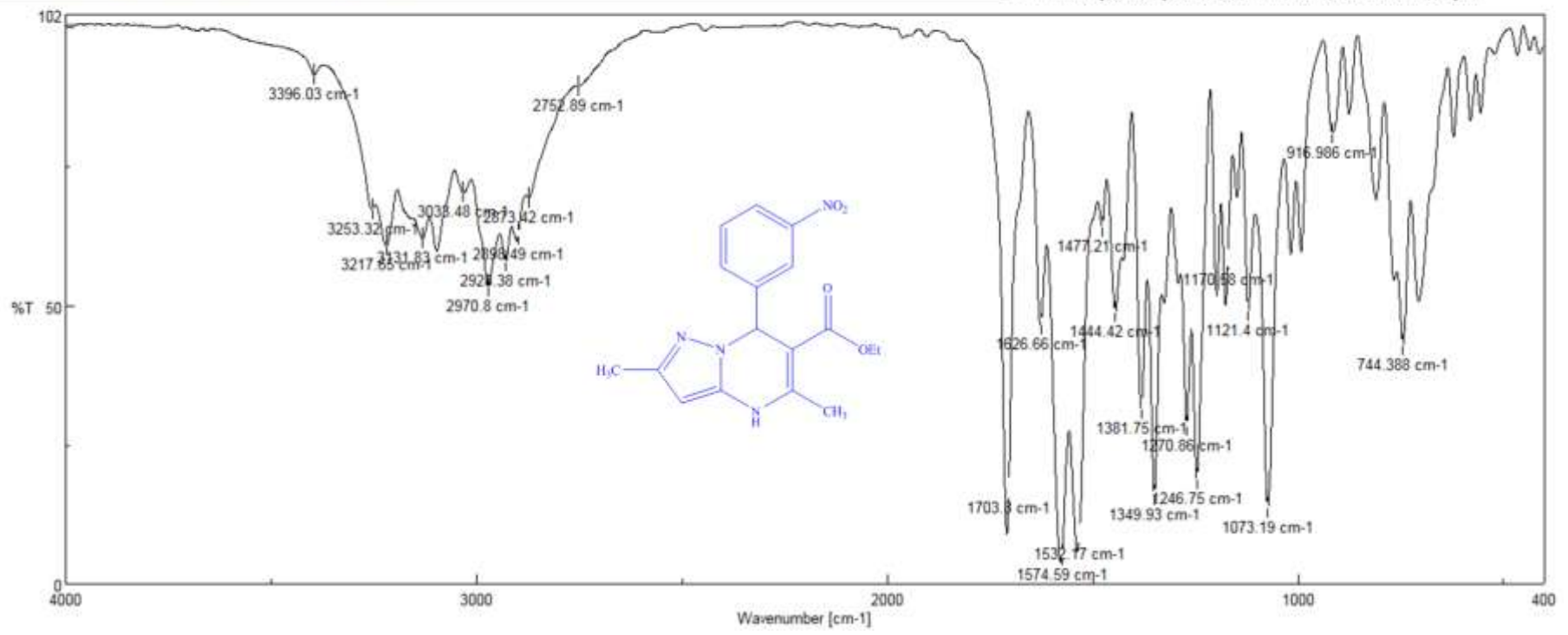


UV-Spectrum of compound **5a**

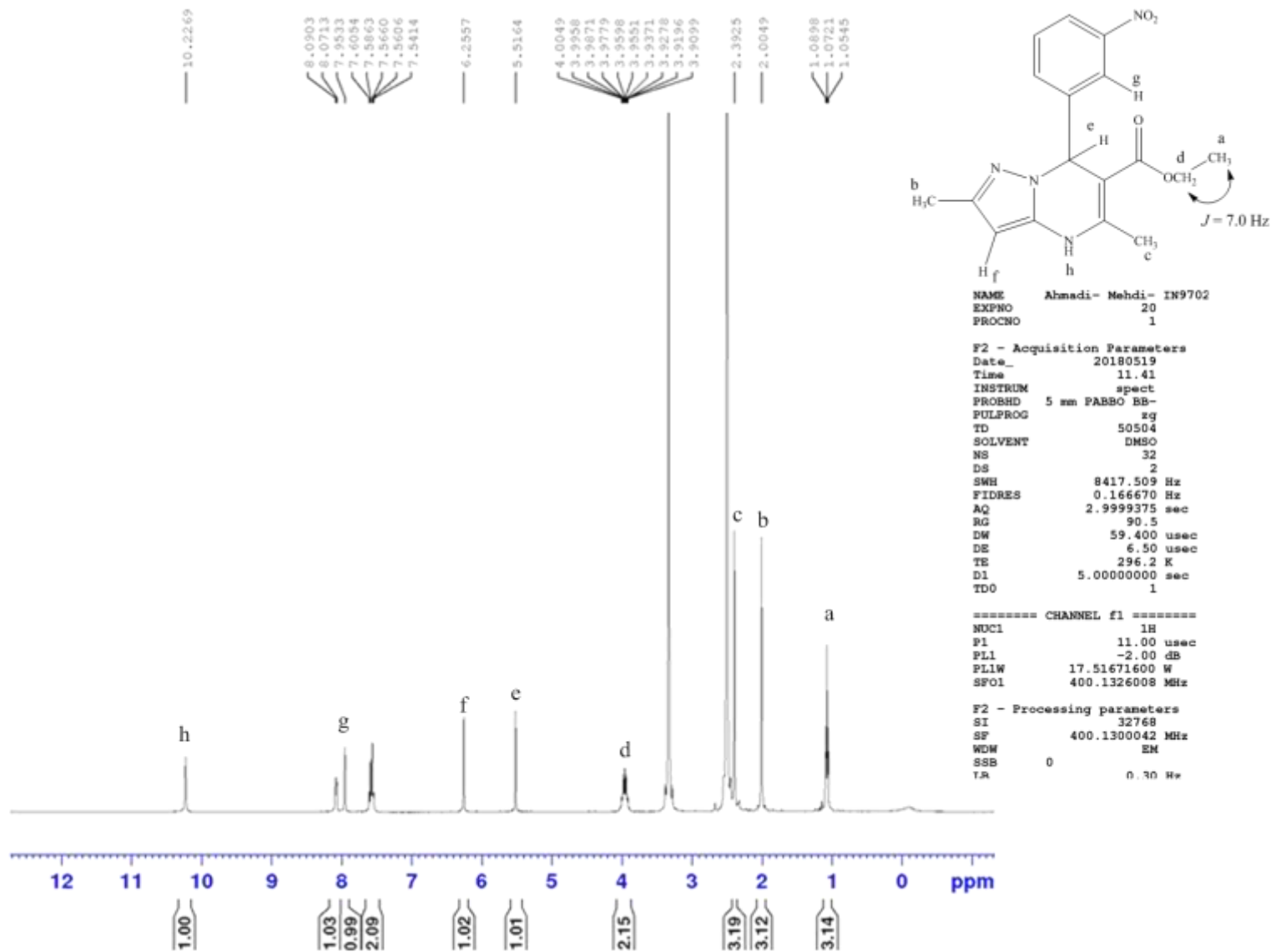


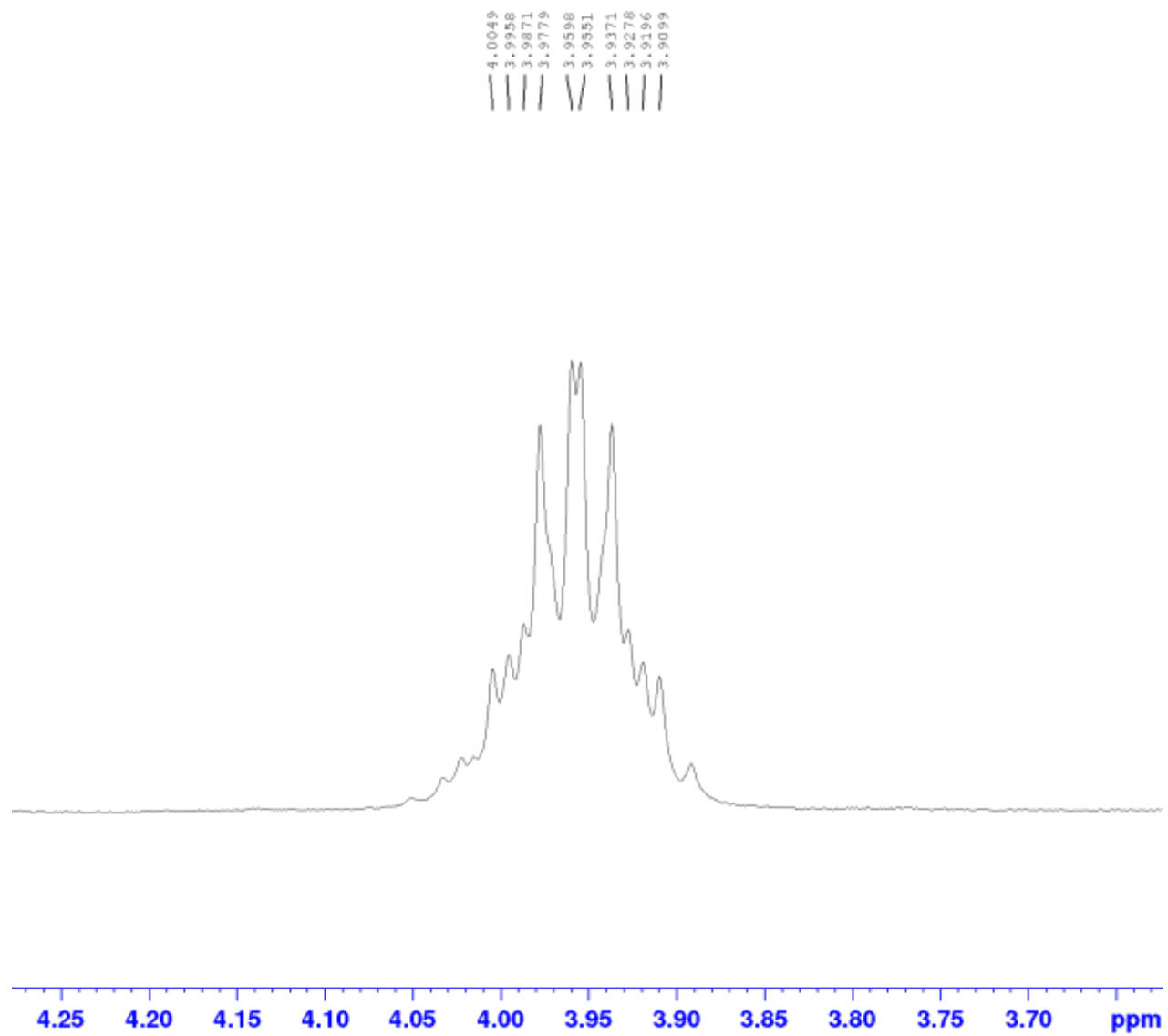
IR-Spectrum of compound 5b

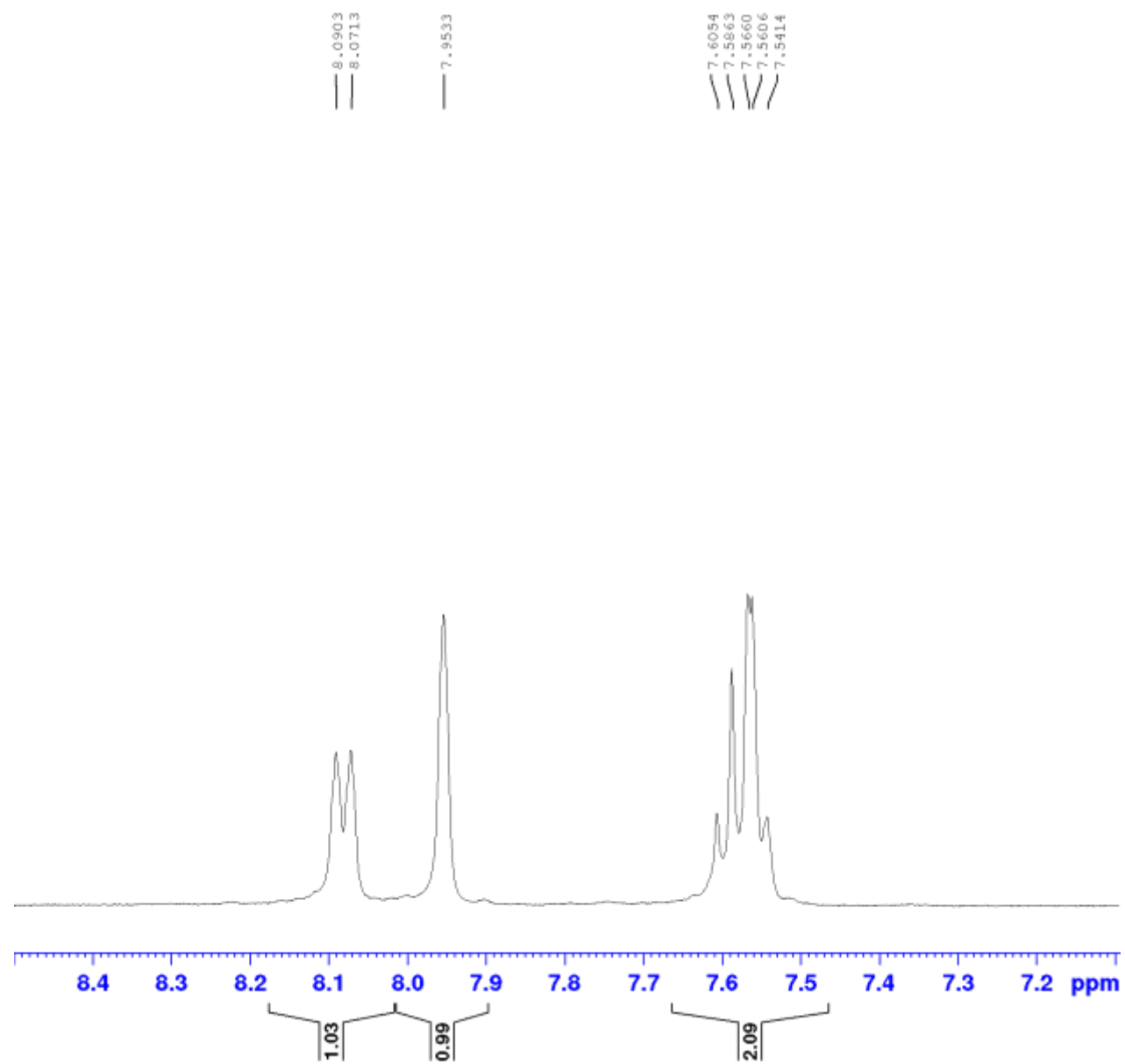
Instrument Specifications
FT Infrared Spectroscopy, JASCO, FT/IR-6300 (400-4000 cm⁻¹), Japan



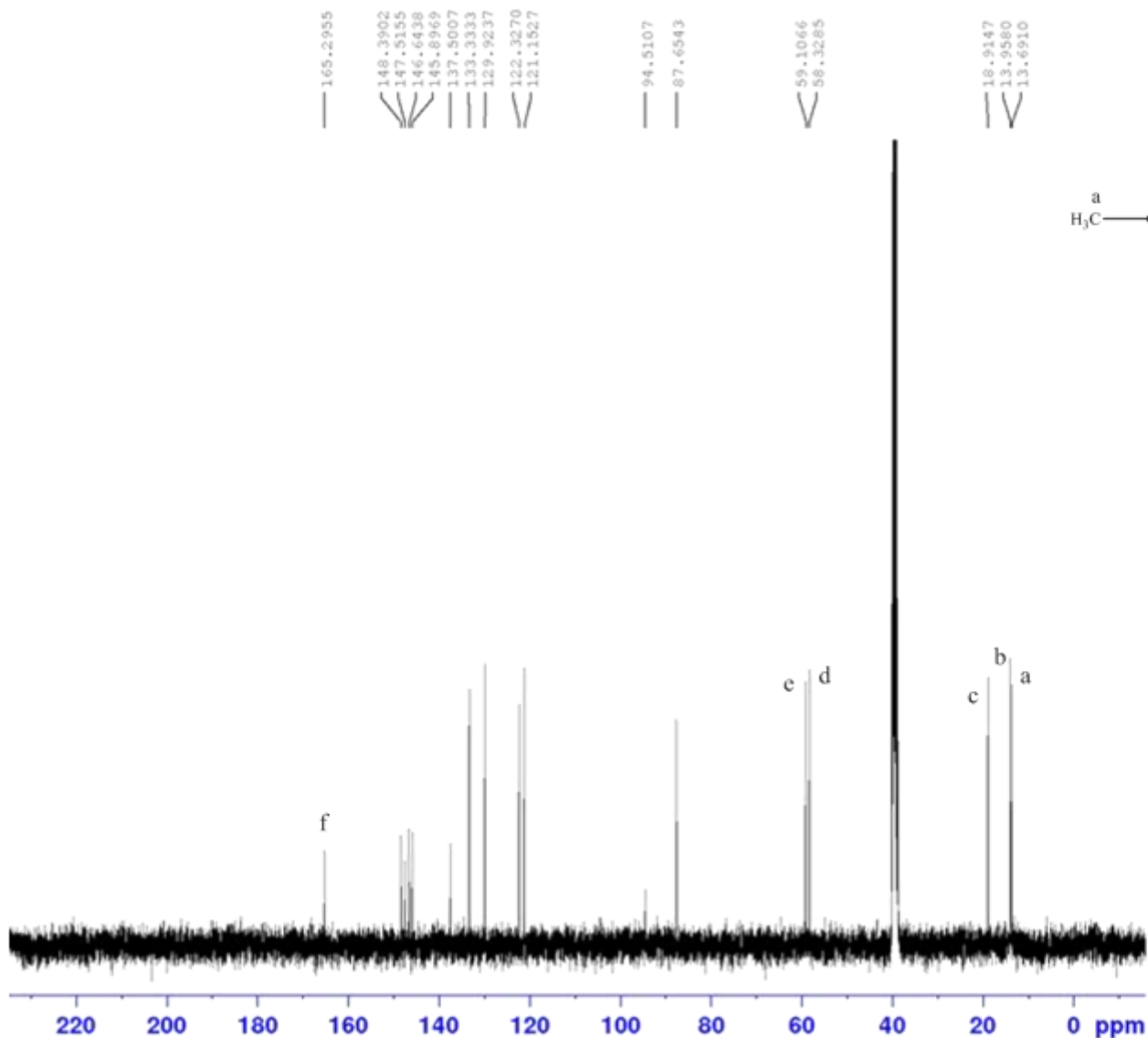
¹H NMR Spectrum of compound **5b**



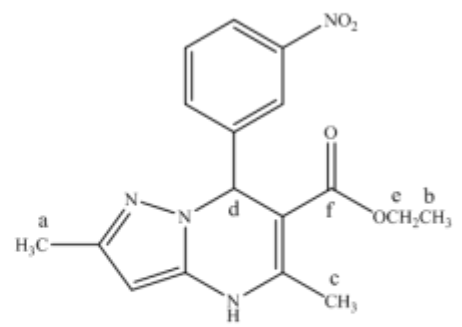




¹³C NMR Spectrum of compound **5b**



165.2955
 148.3902
 147.5155
 146.6438
 145.8969
 137.5007
 133.3333
 129.9237
 122.3270
 121.1527
 94.5107
 87.6543
 59.1066
 56.3285
 18.9147
 13.9580
 13.6910



```

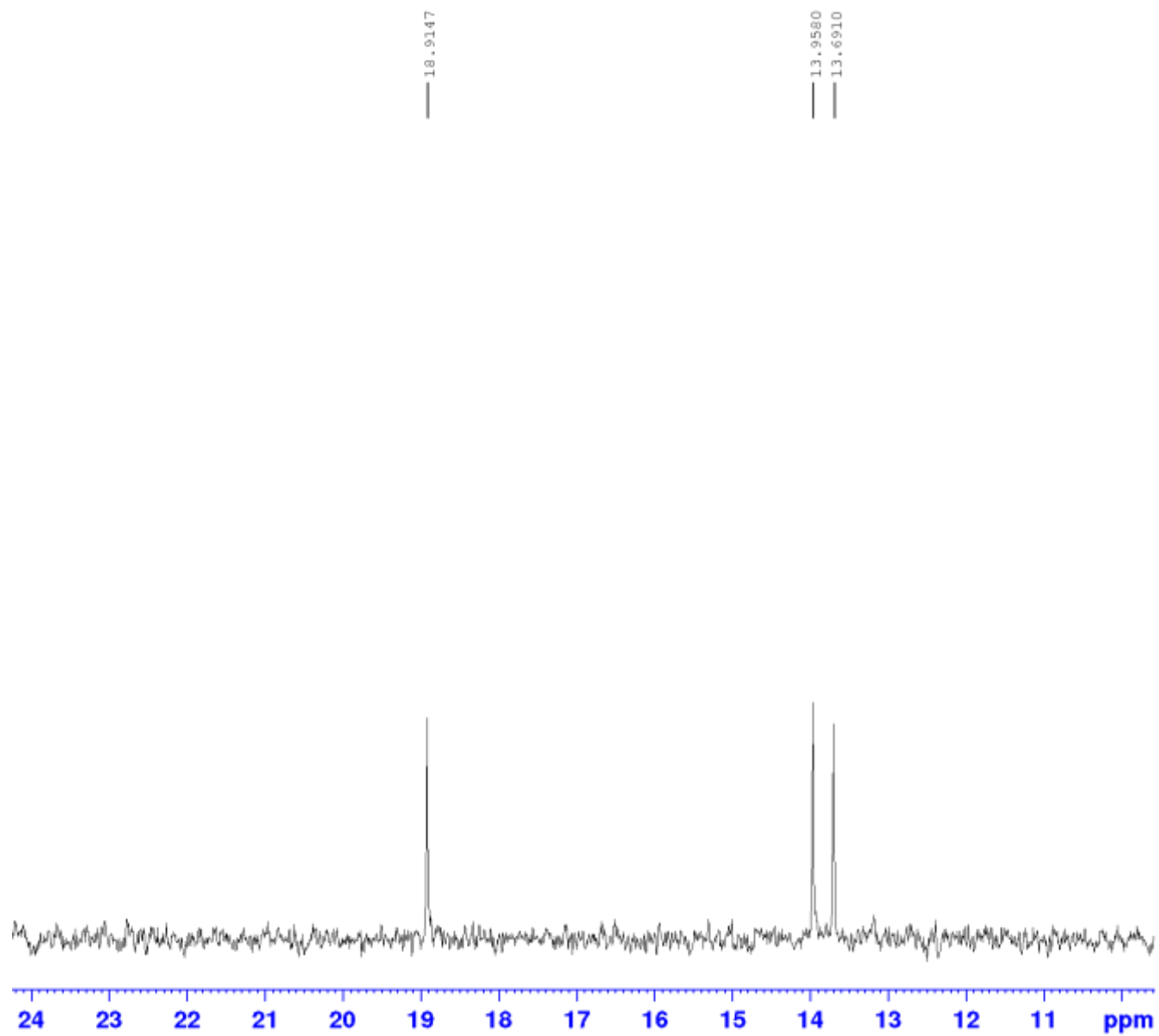
Current Data Parameters
NAME          cmer
EXPNO         20
PROCNO        1

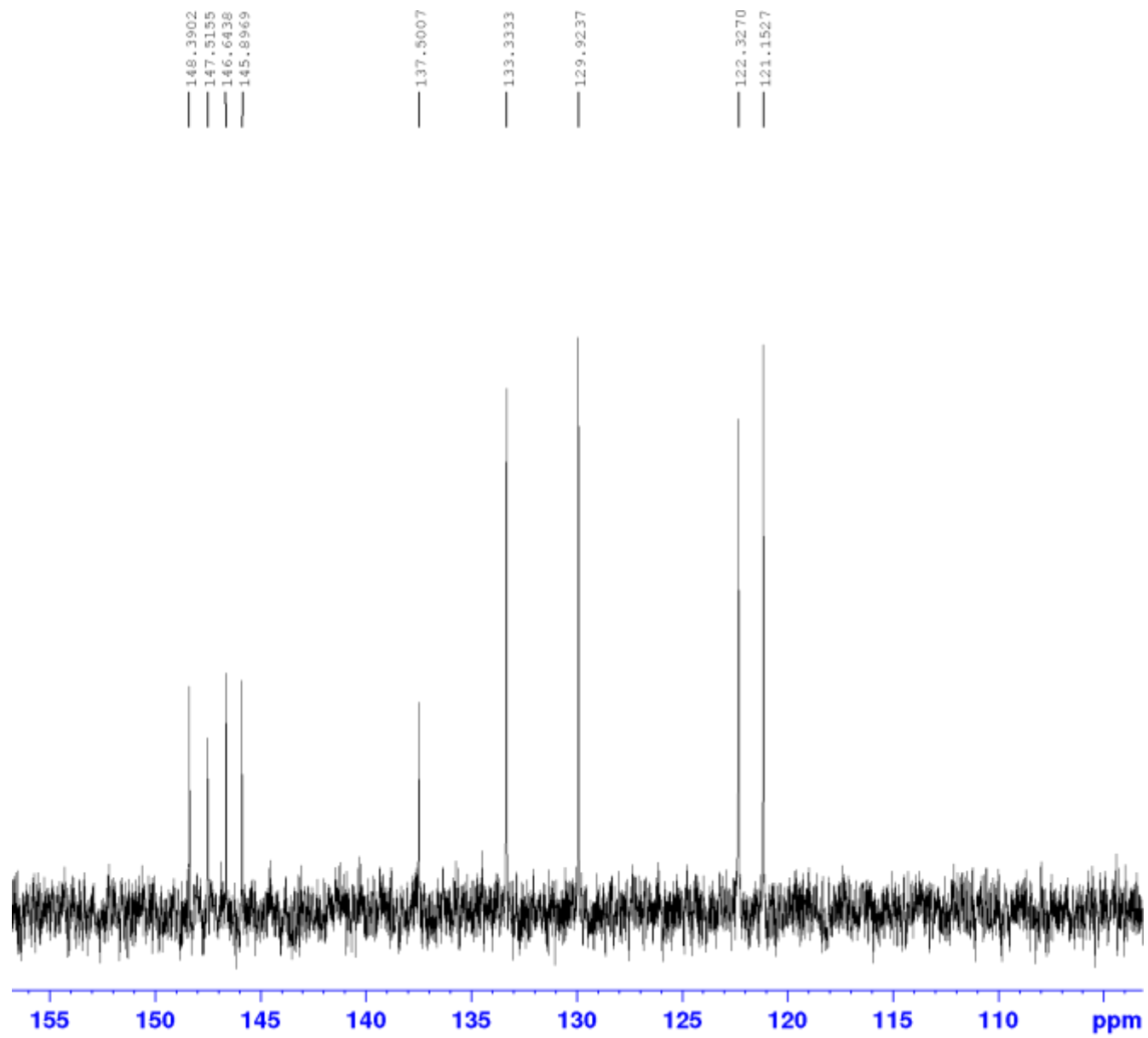
F2 - Acquisition Parameters
Date_         20180522
Time          15.04
INSTRUM       spect
PROBHD        5 mm F4BBO BB-
PULPROG       zgpg
TD             50532
SOLVENT       DMSO
NS             1500
DS             2
SWH            25252.525 Hz
FIDRES         0.500030 Hz
AQ             0.9999396 sec
RG             2050
DN             19.800 usec
DE             6.50 usec
TE             297.2 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0            1

===== CHANNEL f1 =====
NUC1           13C
P1              8.70 usec
PL1             -1.00 dB
PL1W           42.69075012 W
SFO1           100.6238364 MHz

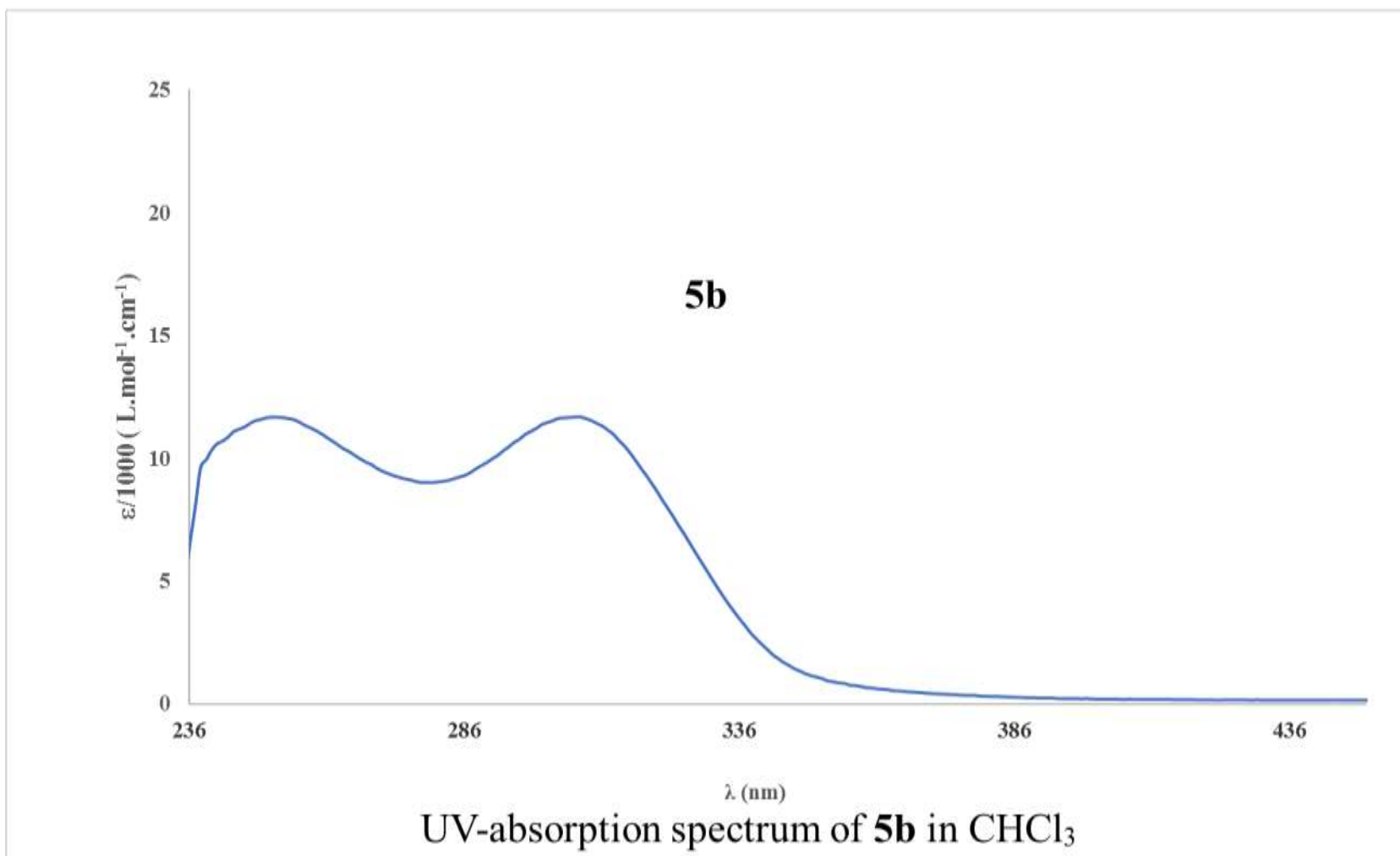
===== CHANNEL f2 =====
CPDPRG[2]     waltz16
NUC2           1H
PCPD2          80.00 usec
PL2             0 dB
PL12           15.26 dB
PL13           18.26 dB
PL2W           11.05230045 W
PL12W          0.32919458 W
PL13W          0.16498812 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI             32768
SF             100.6128193 MHz
WDW            EM
SSB            0
LB             1.00 Hz
GB             0
  
```

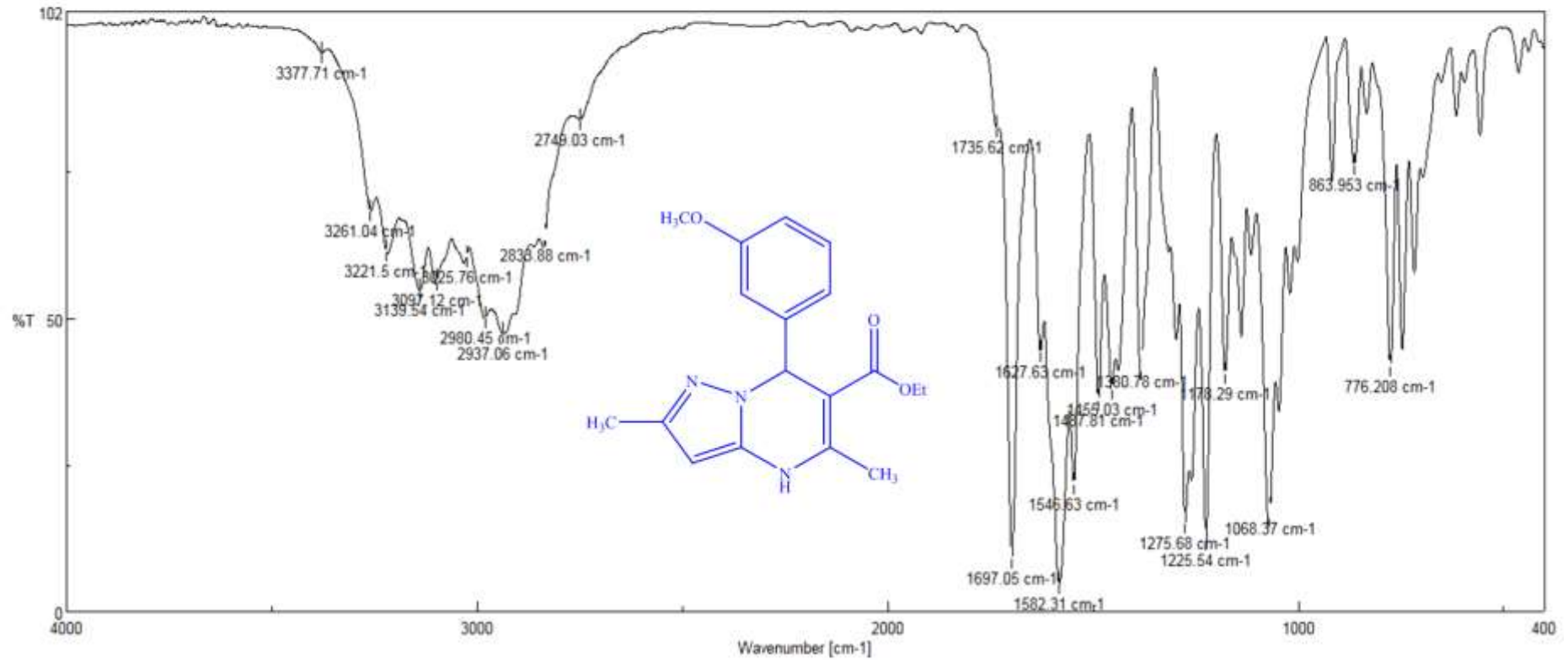




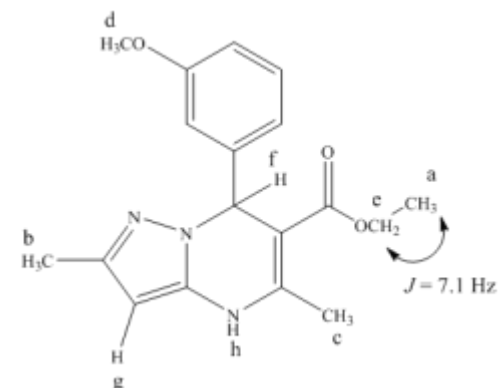
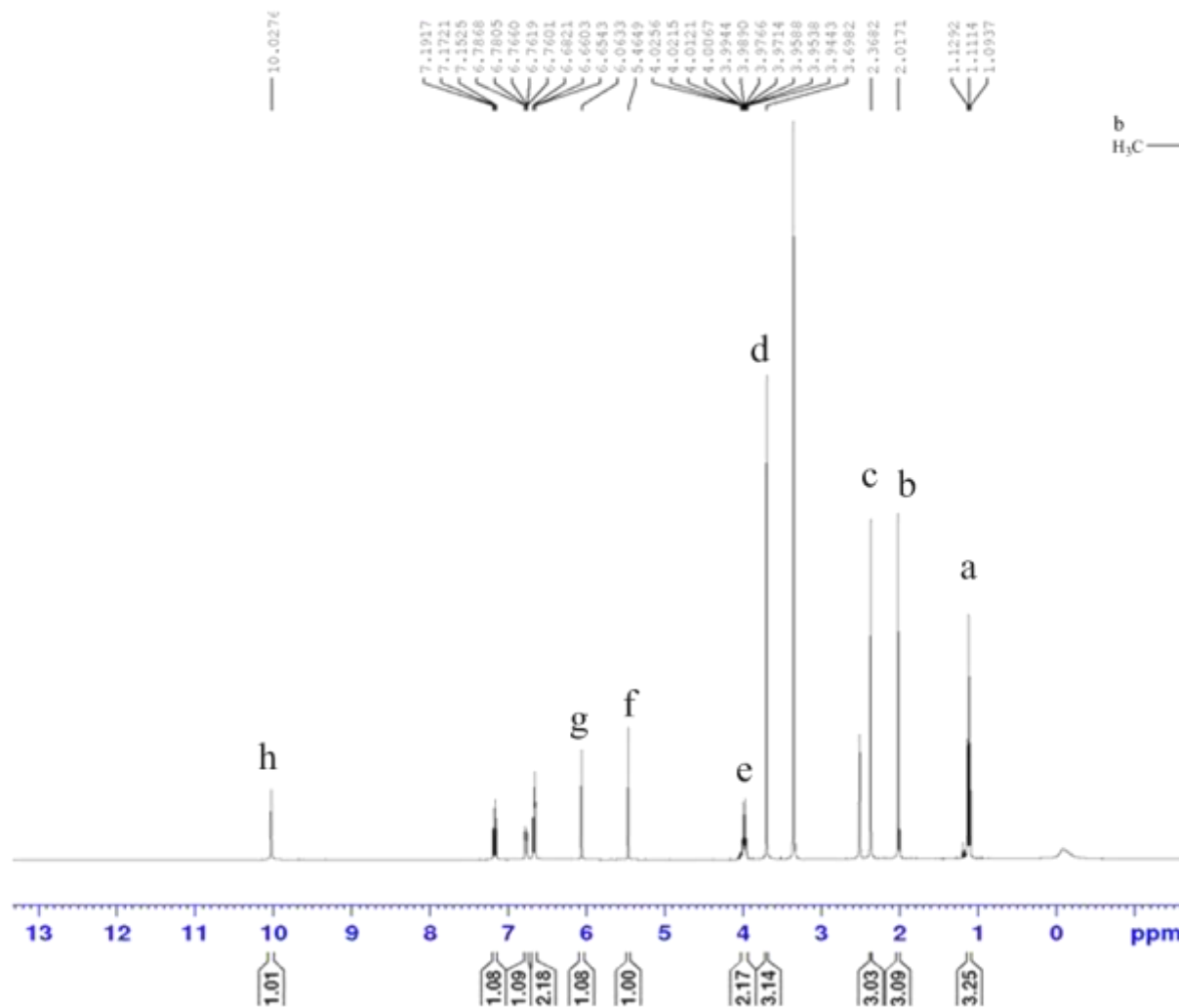
UV-Spectrum of compound **5b**



IR-Spectrum of compound 5c



¹H NMR Spectrum of compound 5c



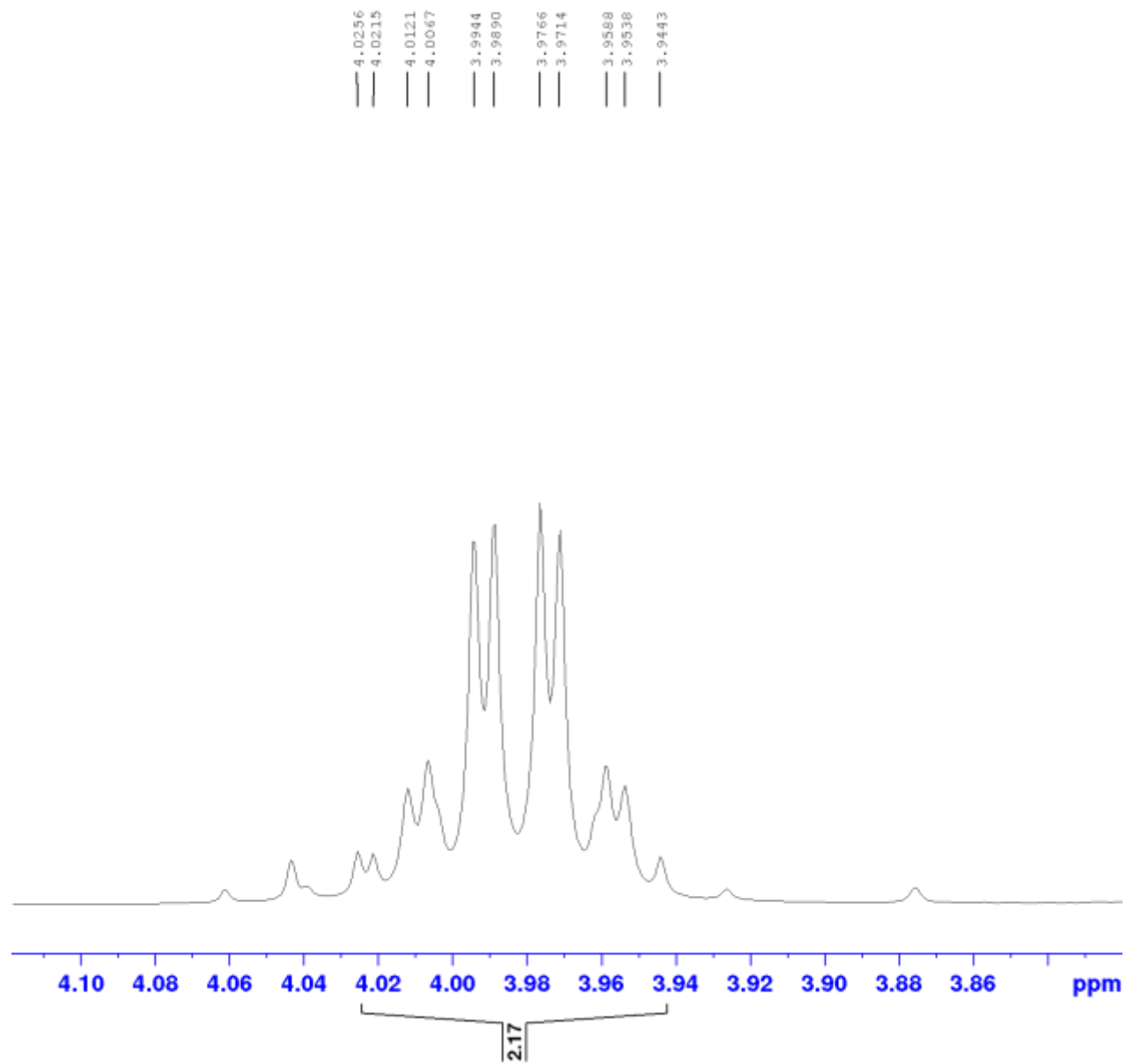
```

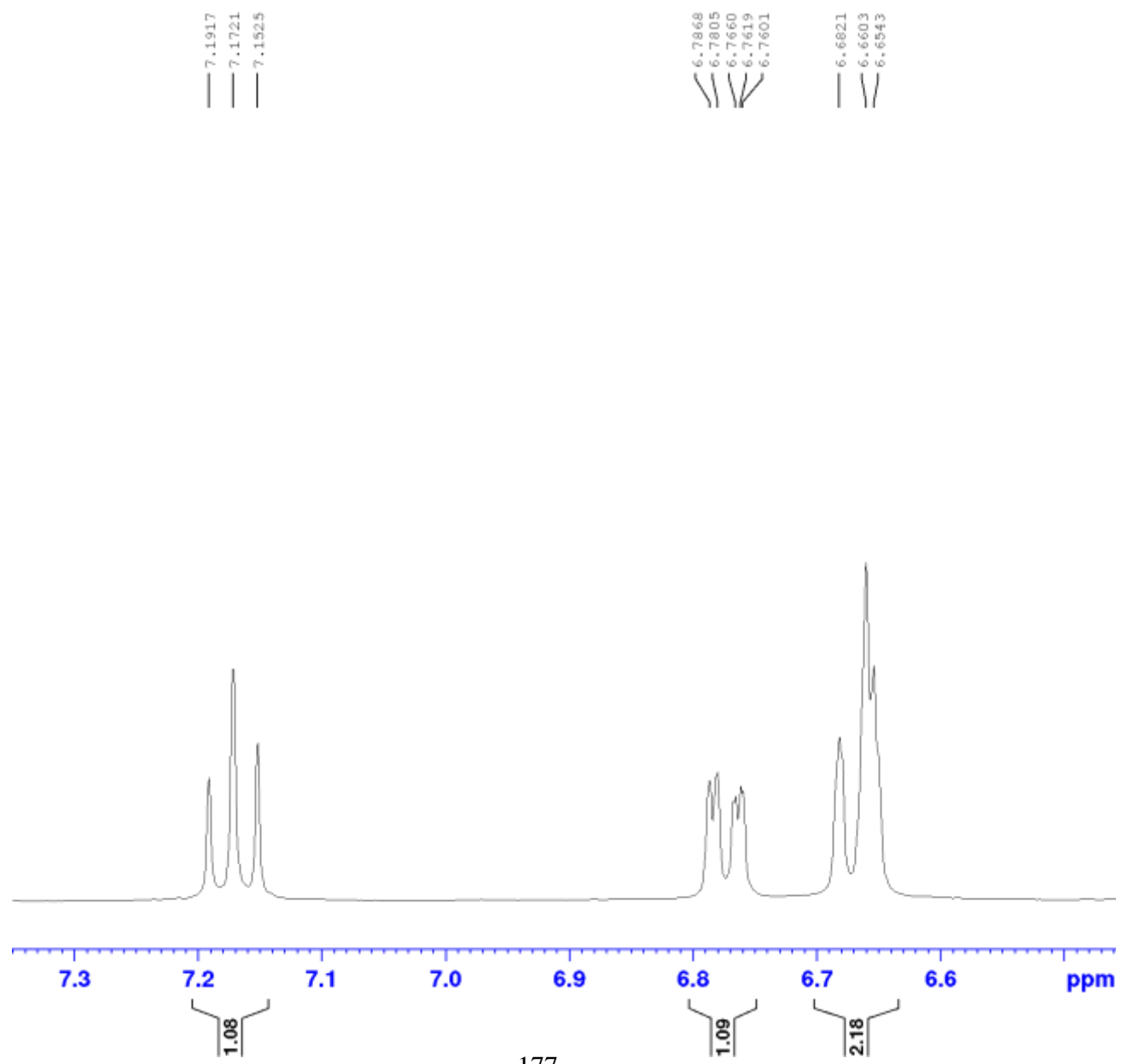
NAME          Desktop
EXPNO         30
PROCNO        1

F2 - Acquisition Parameters
Date_         20181211
Time          13.16
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg
TD            50504
SOLVENT       DMSO
NS            32
DS            2
SWH           8802.817 Hz
FIDRES        0.174299 Hz
AQ            2.8686273 sec
RG            50.8
DW            56.800 usec
DE            6.50 usec
TE            295.1 K
D1            5.00000000 sec
TD0           1

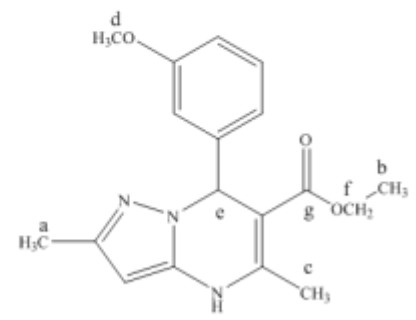
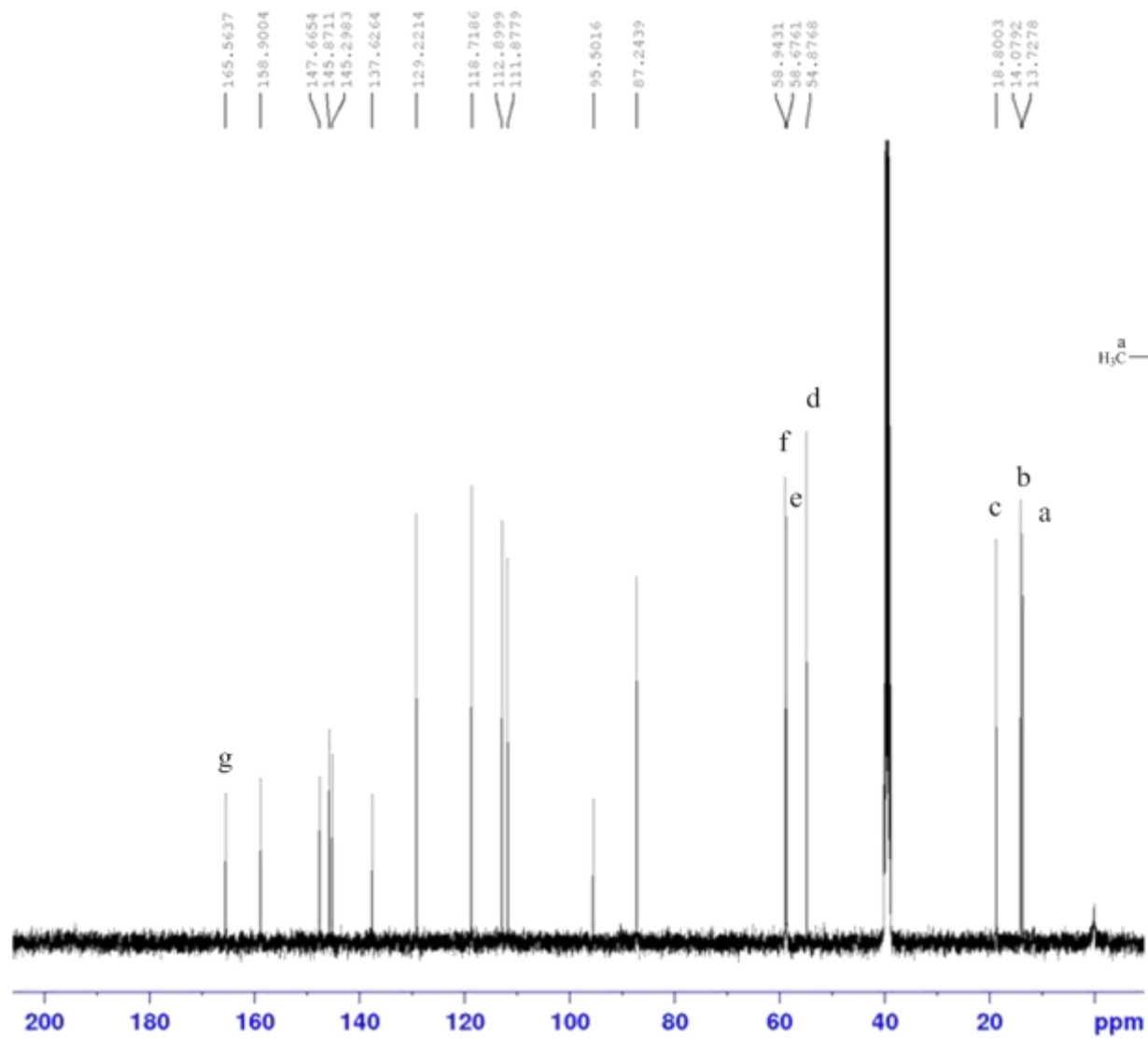
===== CHANNEL f1 =====
NUC1          1H
P1            11.00 usec
PL1           -2.00 dB
PL1W          17.51671600 W
SFO1          400.1326008 MHz

F2 - Processing parameters
SI            32768
SF            400.1300000 MHz
WDW           EM
SSB           0
GB            0.30 Hz
    
```



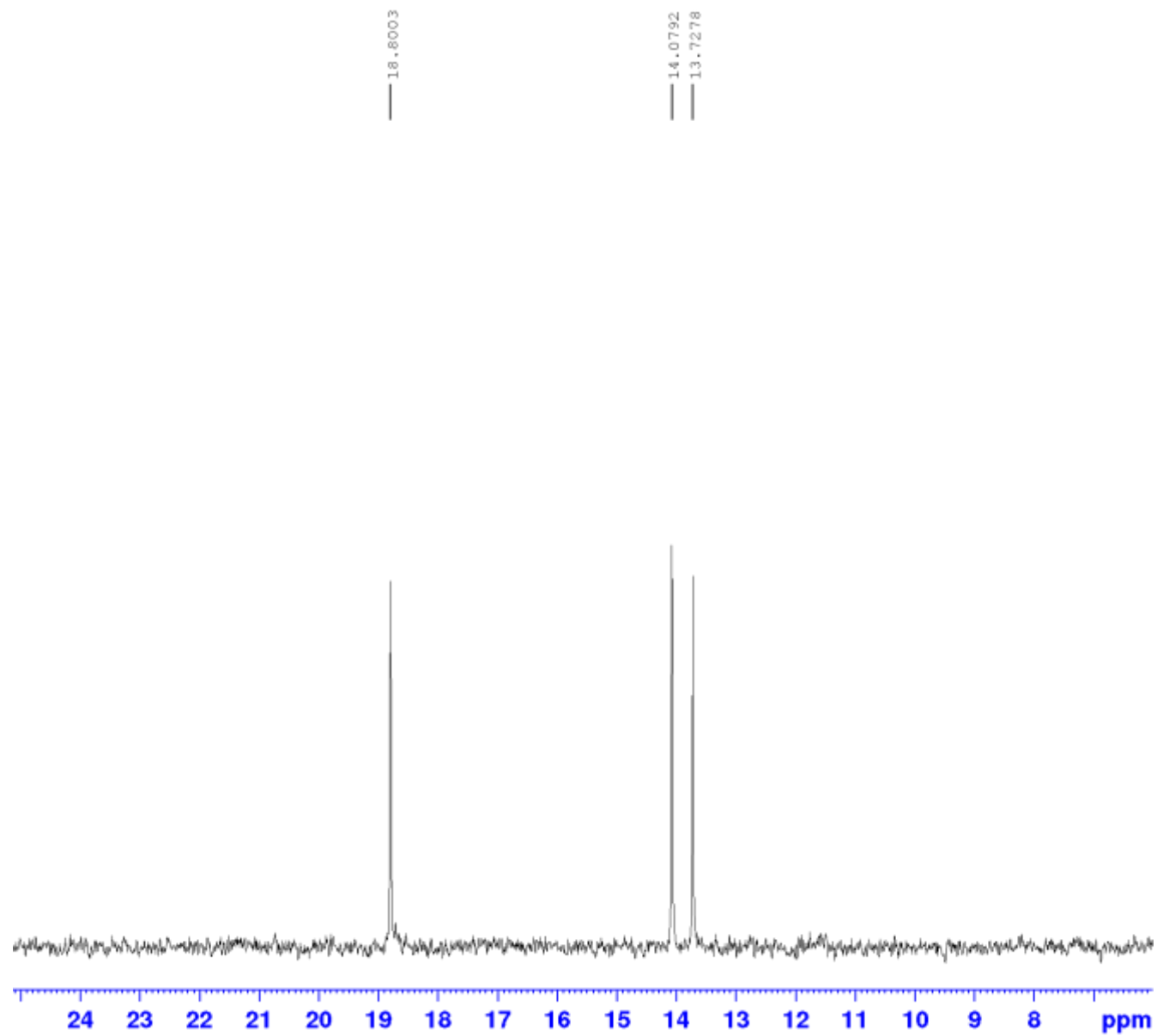
¹³C NMR Spectrum of compound 5c

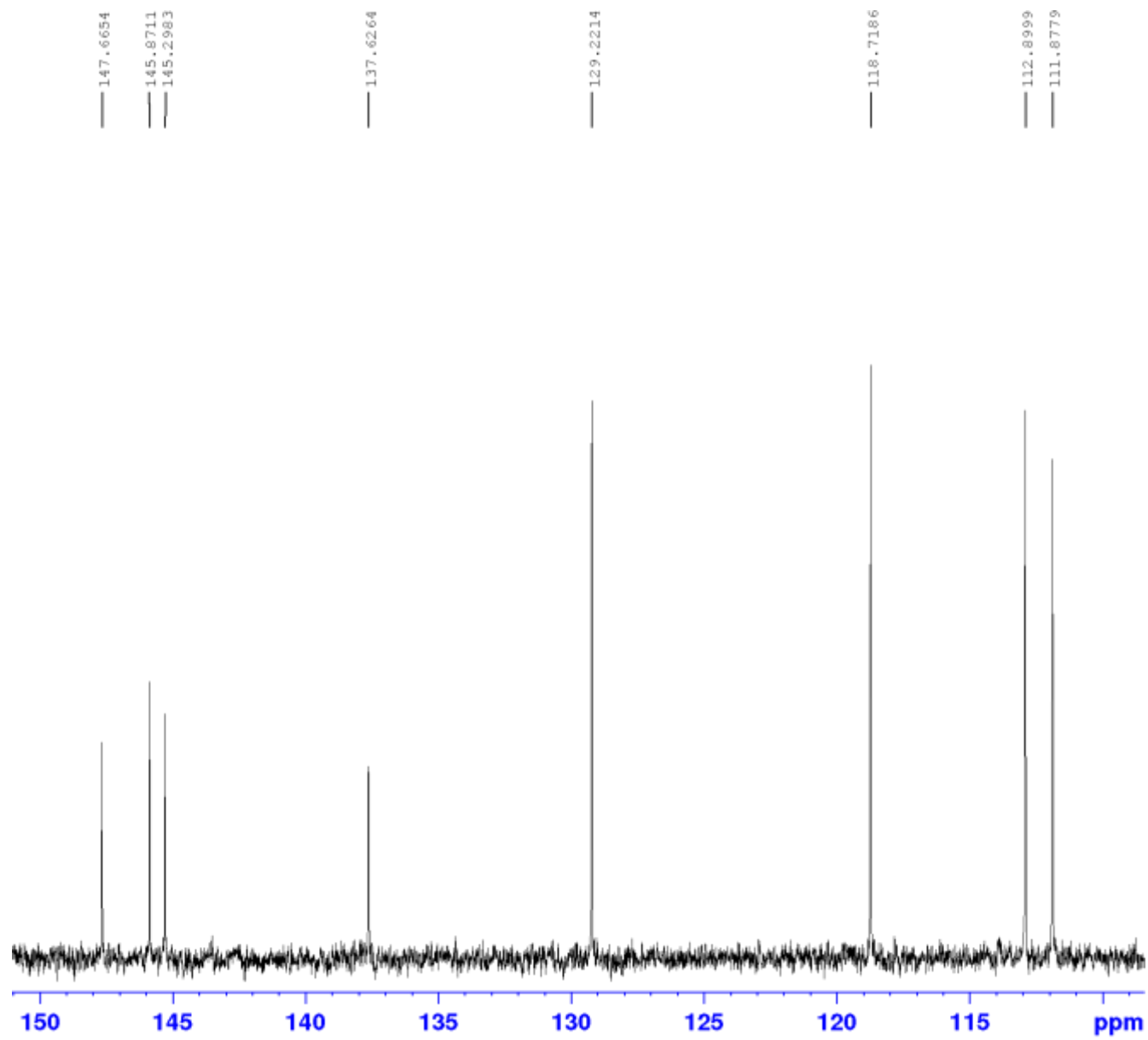


Current Data Parameters
 NAME Ahmadi-mahdi-IN971124-
 EXPNO 10
 PROCNO 1

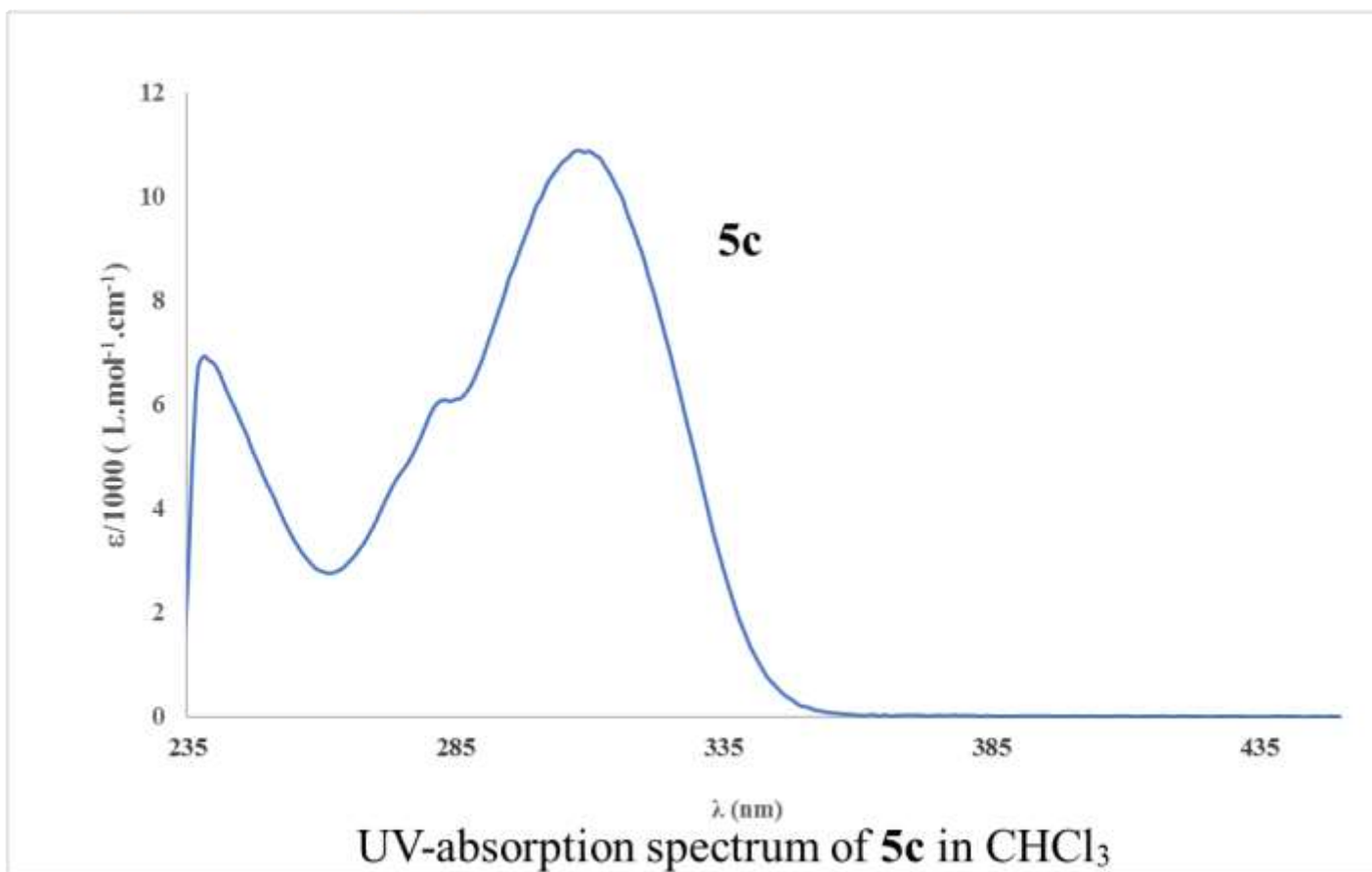
F2 - Acquisition Parameters
 Date_ 20190217
 Time 17.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 50502
 SOLVENT DMSO
 NS 2000
 DS 2
 SWH 25252.525 Hz
 FIDRES 0.500030 Hz
 AQ 0.9999396 sec
 RG 2050
 DW 19.800 usec
 DE 6.50 usec
 TE 294.5 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

***** CHANNEL f1 *****
 NUC1 13C
 P1 9.50 usec
 PL1 -1.00 dB
 PL1W 42.69075012 W
 SFO1 100.6238364 MHz

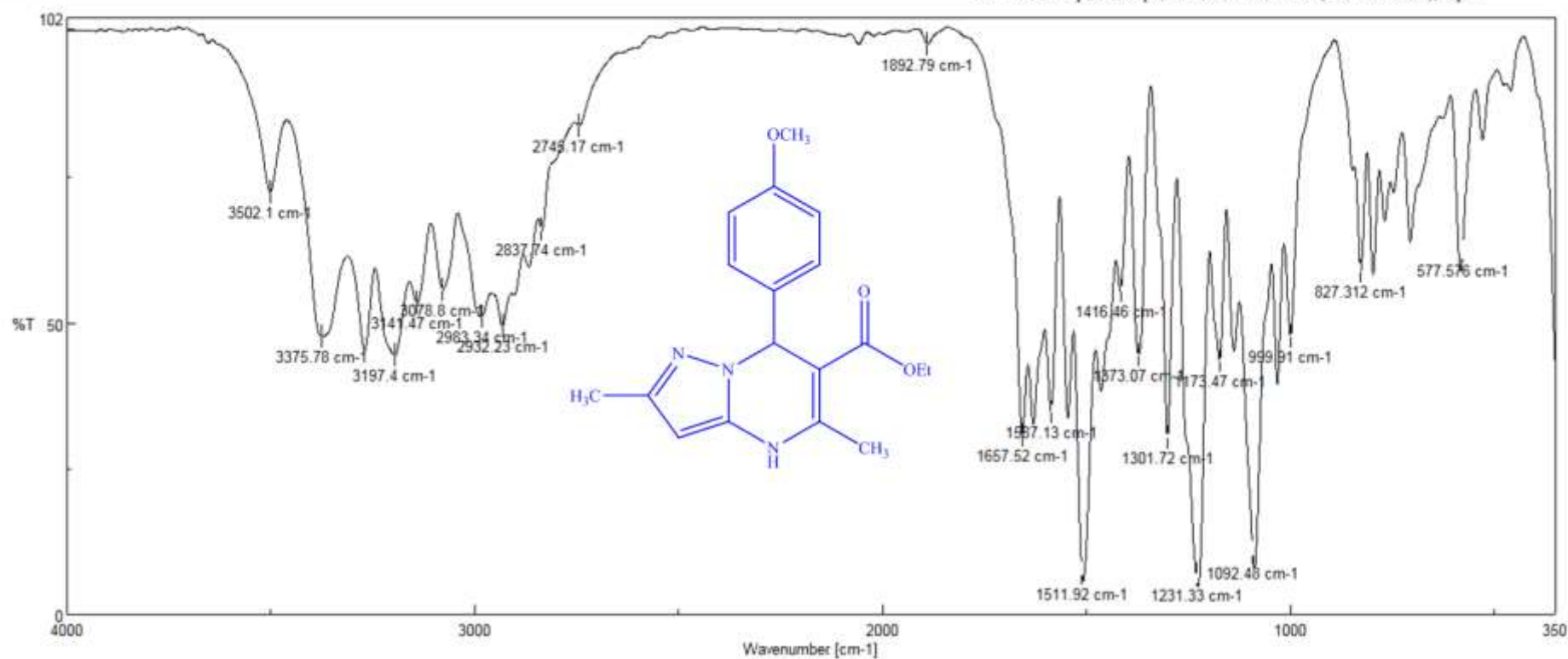




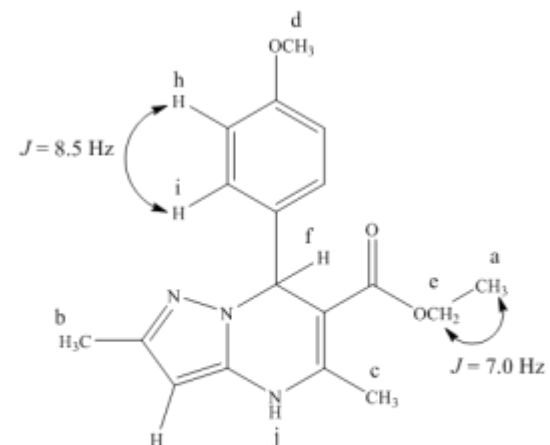
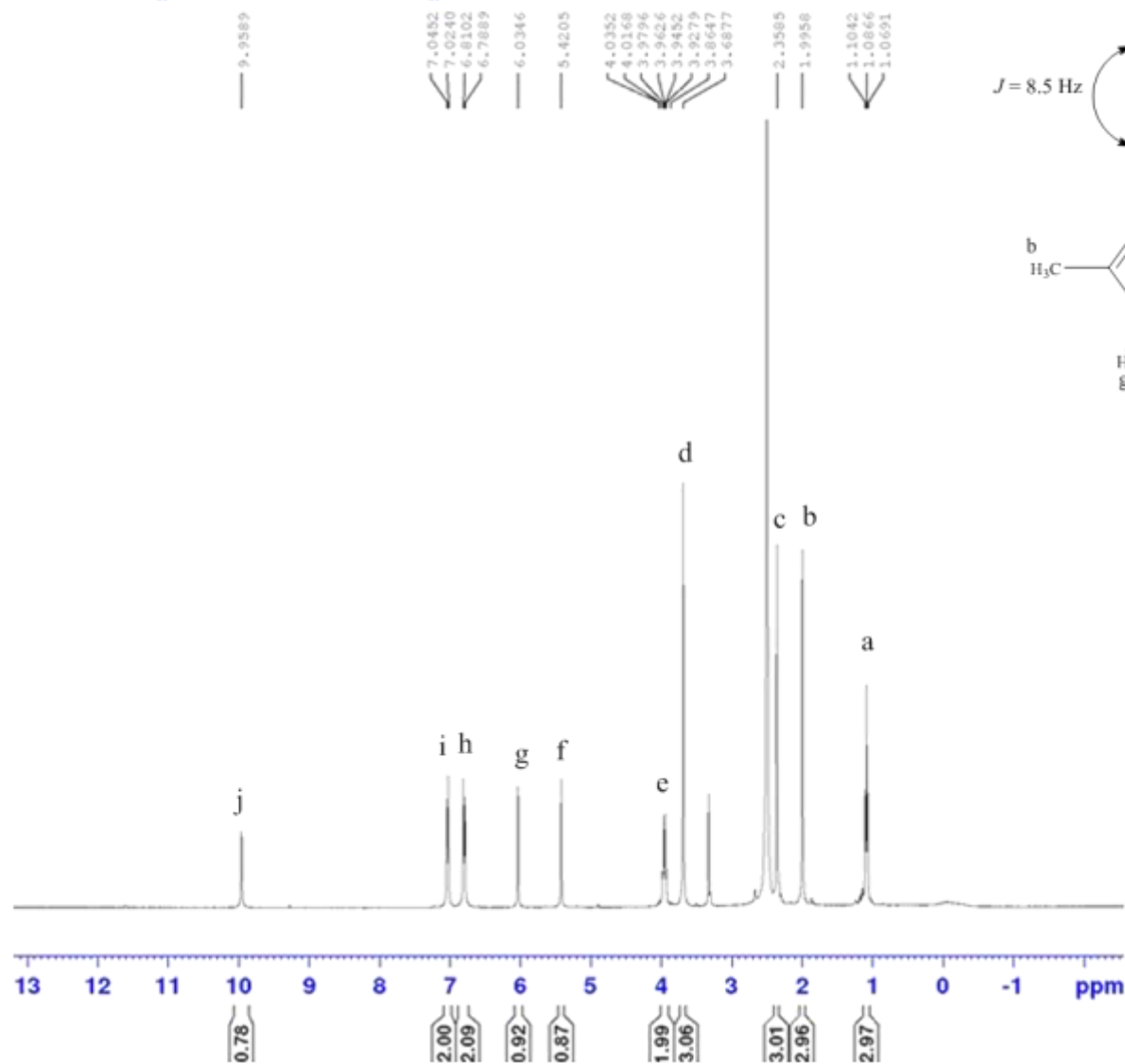
UV-Spectrum of compound **5c**



IR-Spectrum of compound 5d



¹H NMR Spectrum of compound 5d

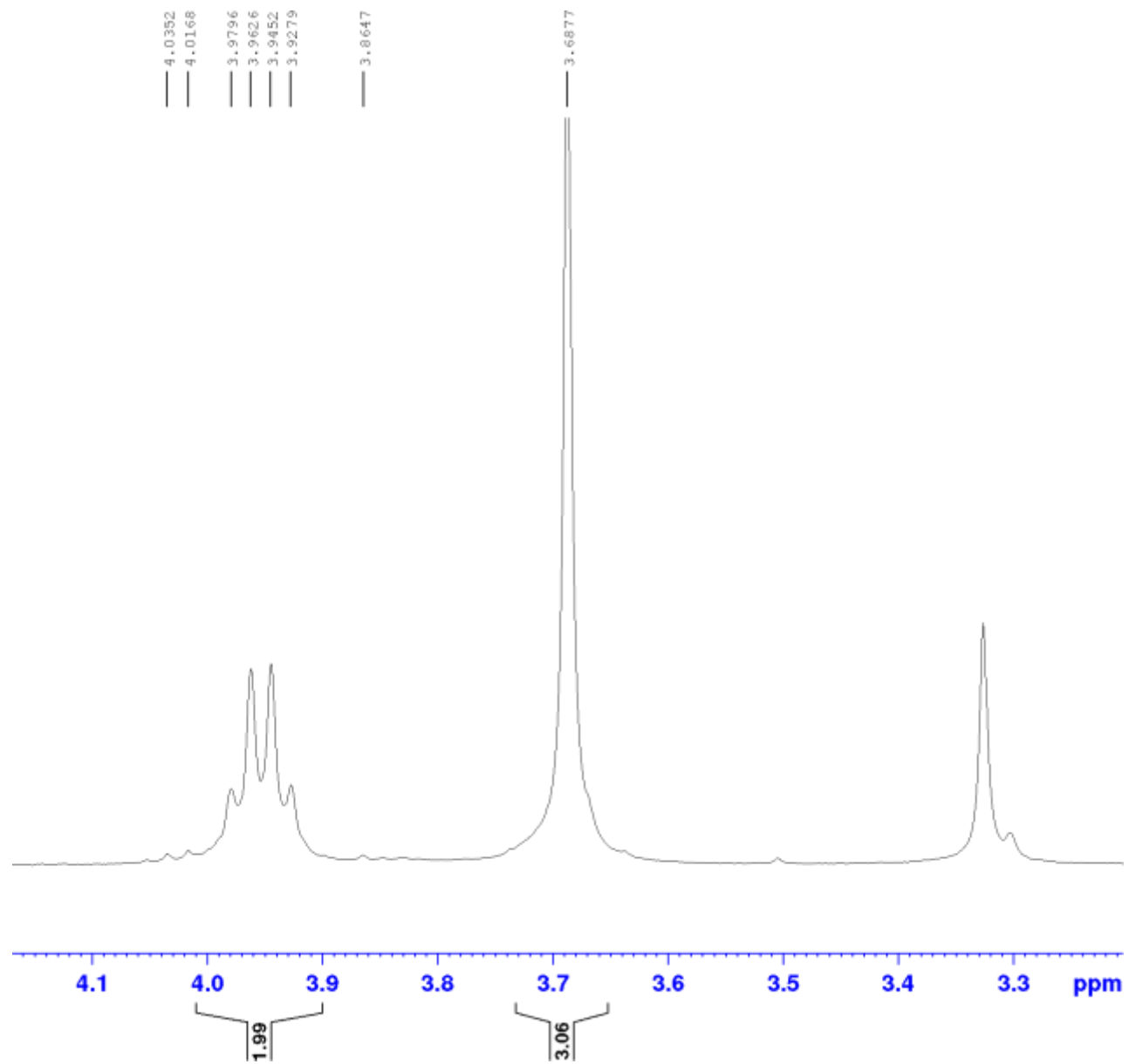


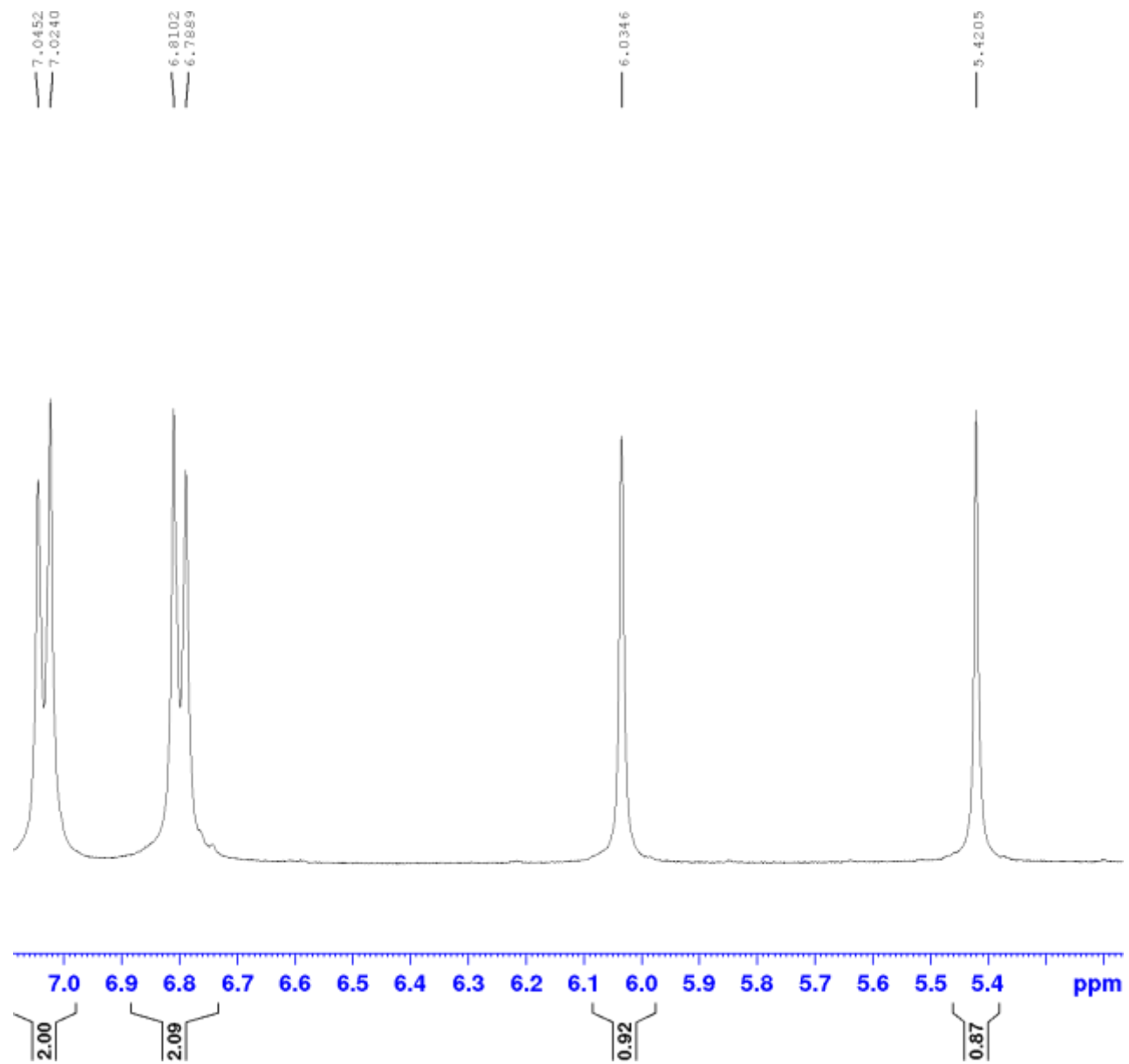
Current Data Parameters
 NAME Ahmadi- Mehdi- IN9702
 EXPNO 10
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180519
 Time 11.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg
 TD 50504
 SOLVENT DMSO
 NS 32
 DS 2
 SWH 8417.509 Hz
 FIDRES 0.166670 Hz
 AQ 2.9999375 sec
 RG 114
 DW 59.400 usec
 DE 6.50 usec
 TE 296.2 K
 D1 5.00000000 sec
 TDO 1

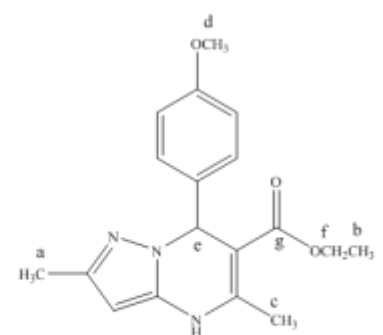
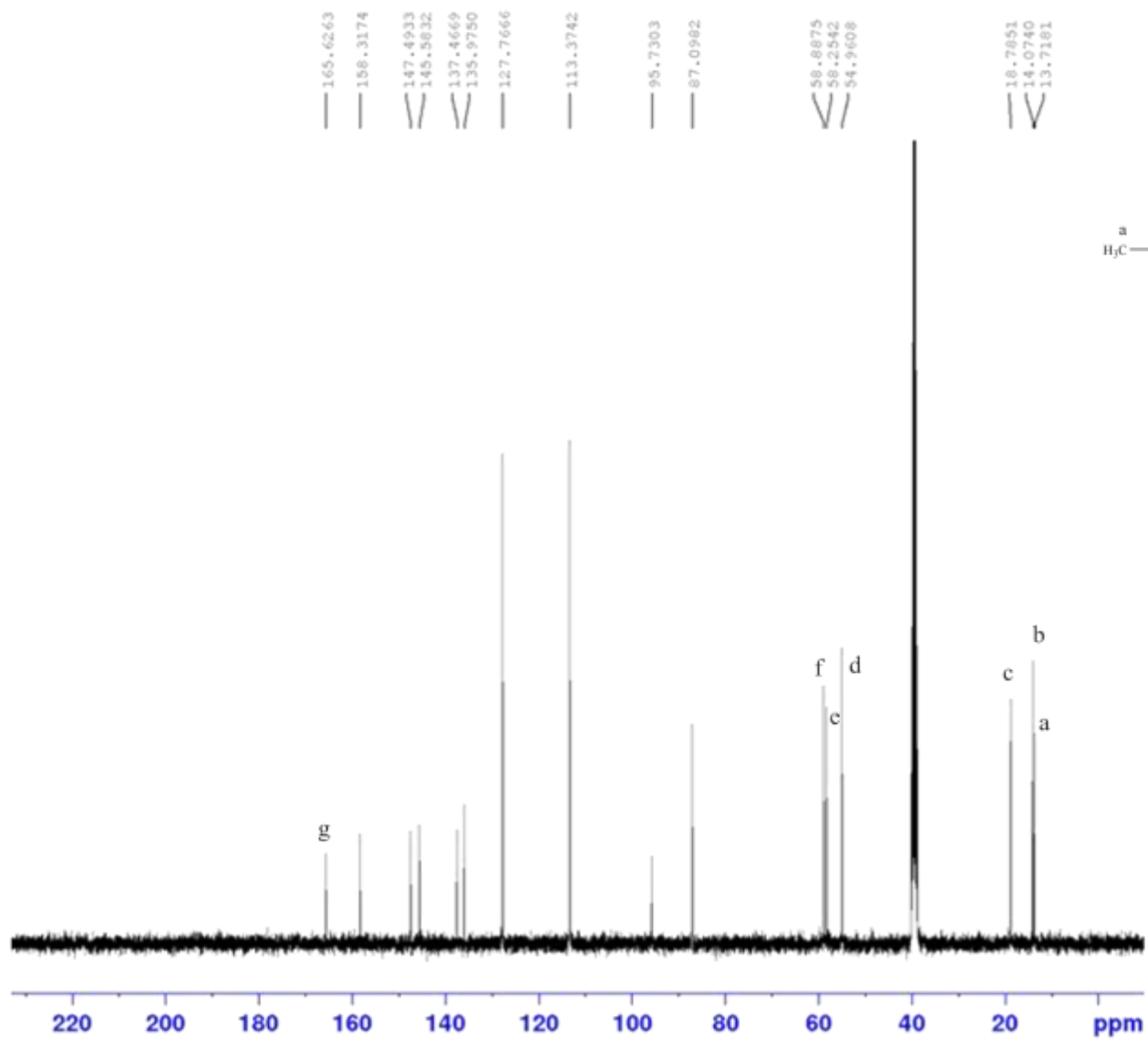
----- CHANNEL f1 -----
 NUC1 1H
 P1 11.00 usec
 PL1 -2.00 dB
 PL1W 17.51671600 W
 SFO1 400.1326008 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300040 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





¹³C NMR Spectrum of compound **5d**



```

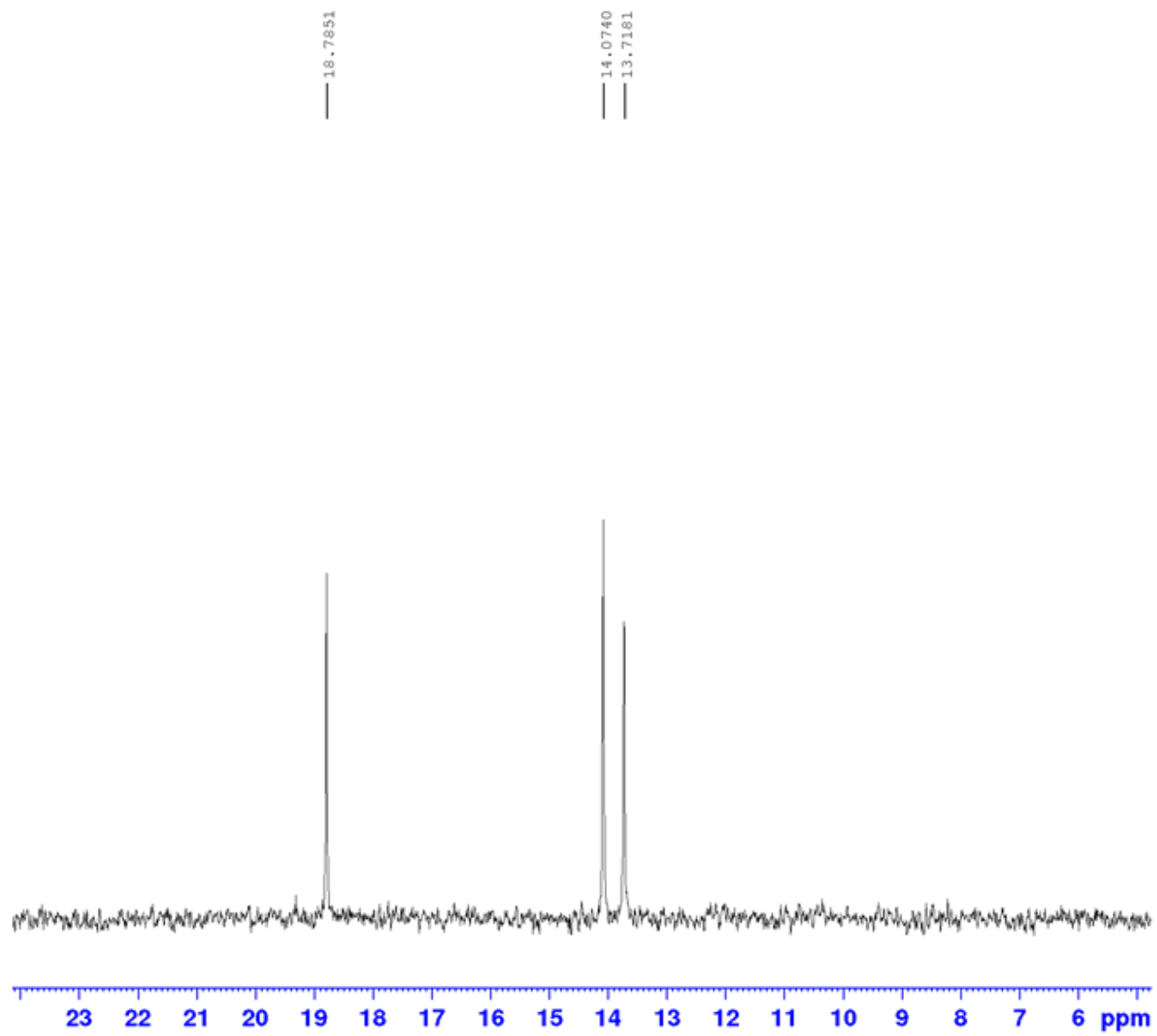
Current Data Parameters
NAME      Ahmadi-Mehdi-1897031
EXPNO     10
PROCNO    1

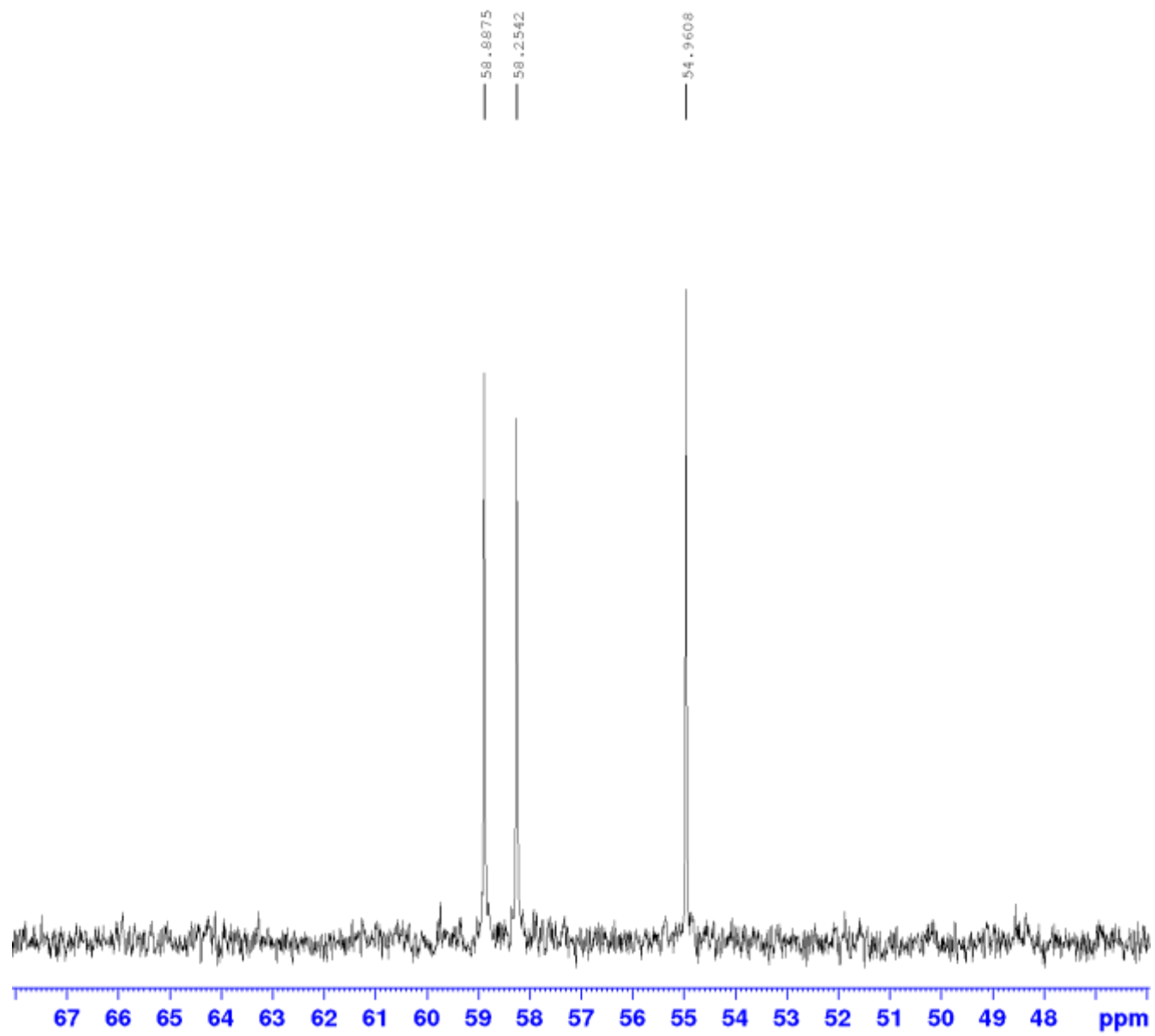
F2 - Acquisition Parameters
Date_     20180527
Time      11.27
INSTRUM   spect
PROBHD    5 mm PABBO BB-
PULPROG   zgpg
TD         65536
SOLVENT   DMSO
MS         1500
DS         2
SWH        25252.525 Hz
FIDRES     0.506030 Hz
AQ         0.9999396 sec
RG         2030
DW         19.800 usec
DE         6.50 usec
TE         294.7 K
D1         1.0000000 sec
D11        0.0300000 sec
TSD        1

----- CHANNEL f1 -----
NUC1       13C
P1         8.70 usec
PL1        -1.00 dB
PL1W       42.69075012 W
SFO1       100.628364 MHz

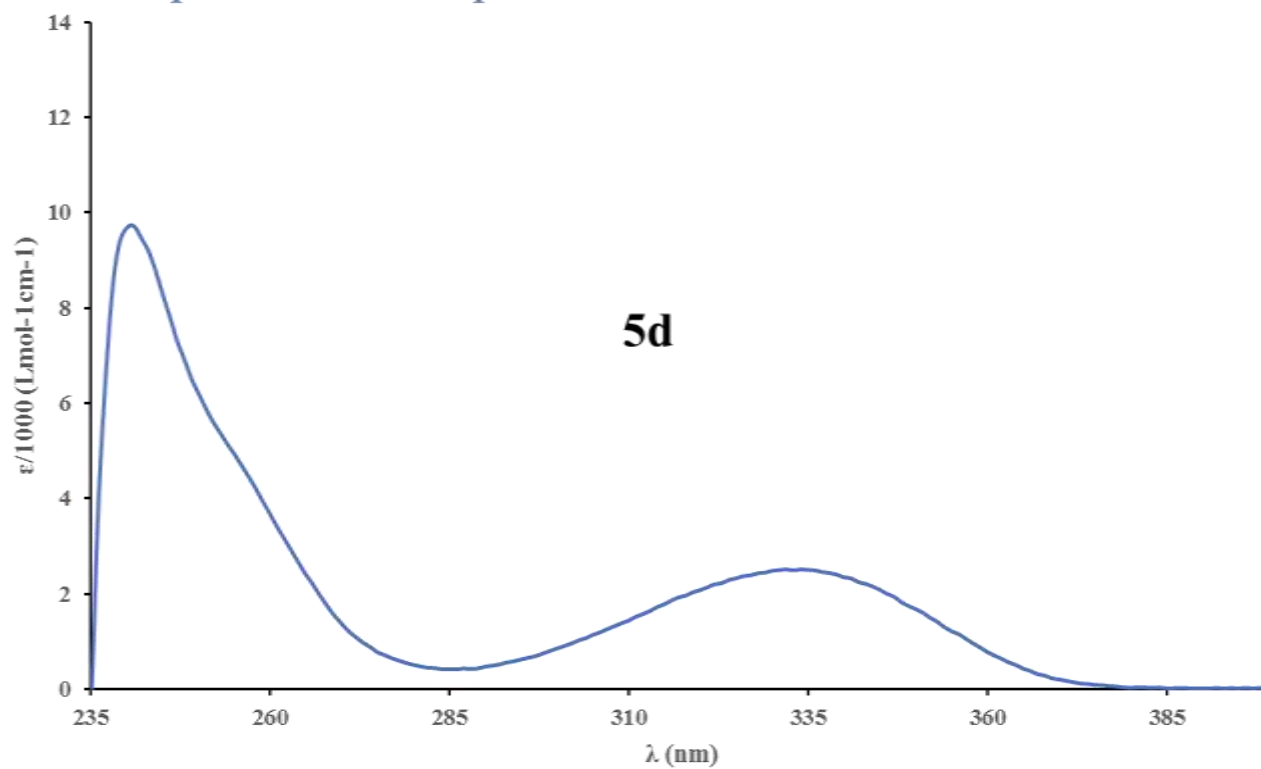
----- CHANNEL f2 -----
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2         0 dB
PL12        15.26 dB
PL13        18.26 dB
PL1W       11.05230045 W
PL12W      0.32819458 W
PL13W      0.16498812 W
SFO2       400.1314005 MHz

F2 - Processing parameters
SI         32768
SF         100.6128193 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
  
```



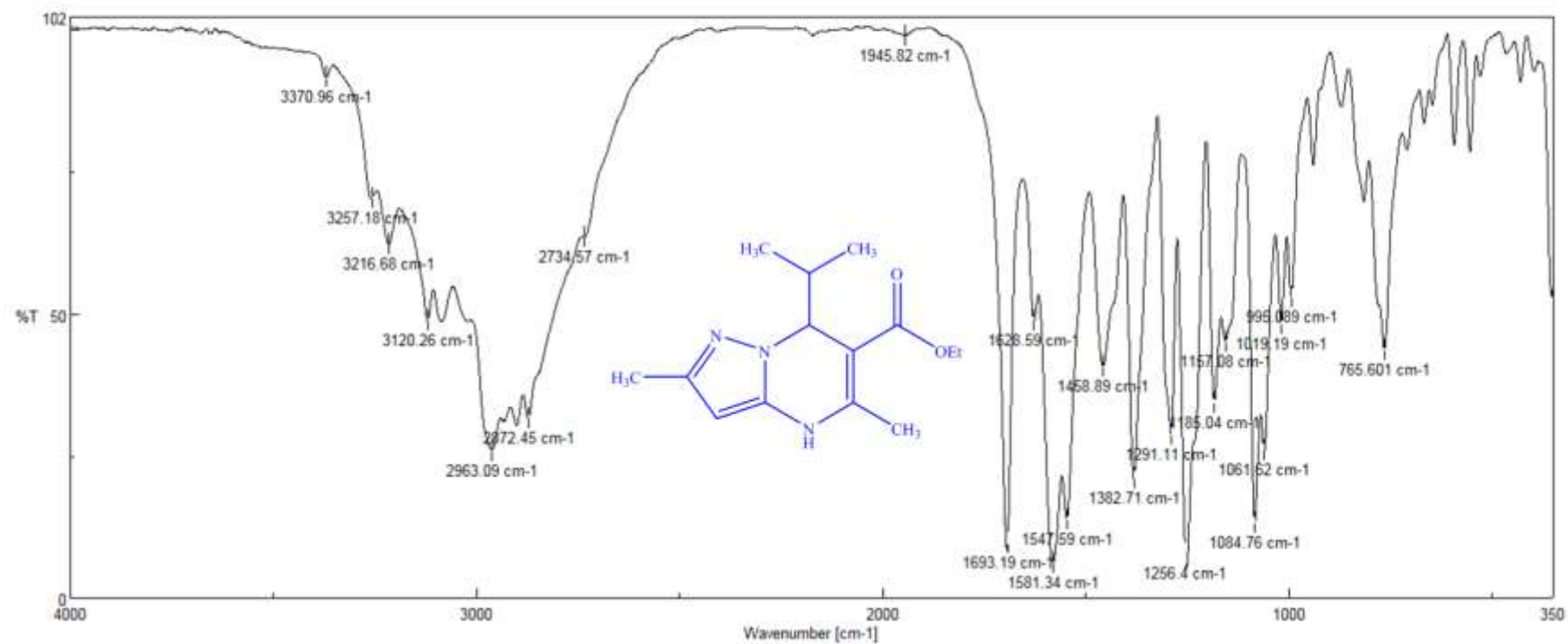


UV-Spectrum of compound **5d**

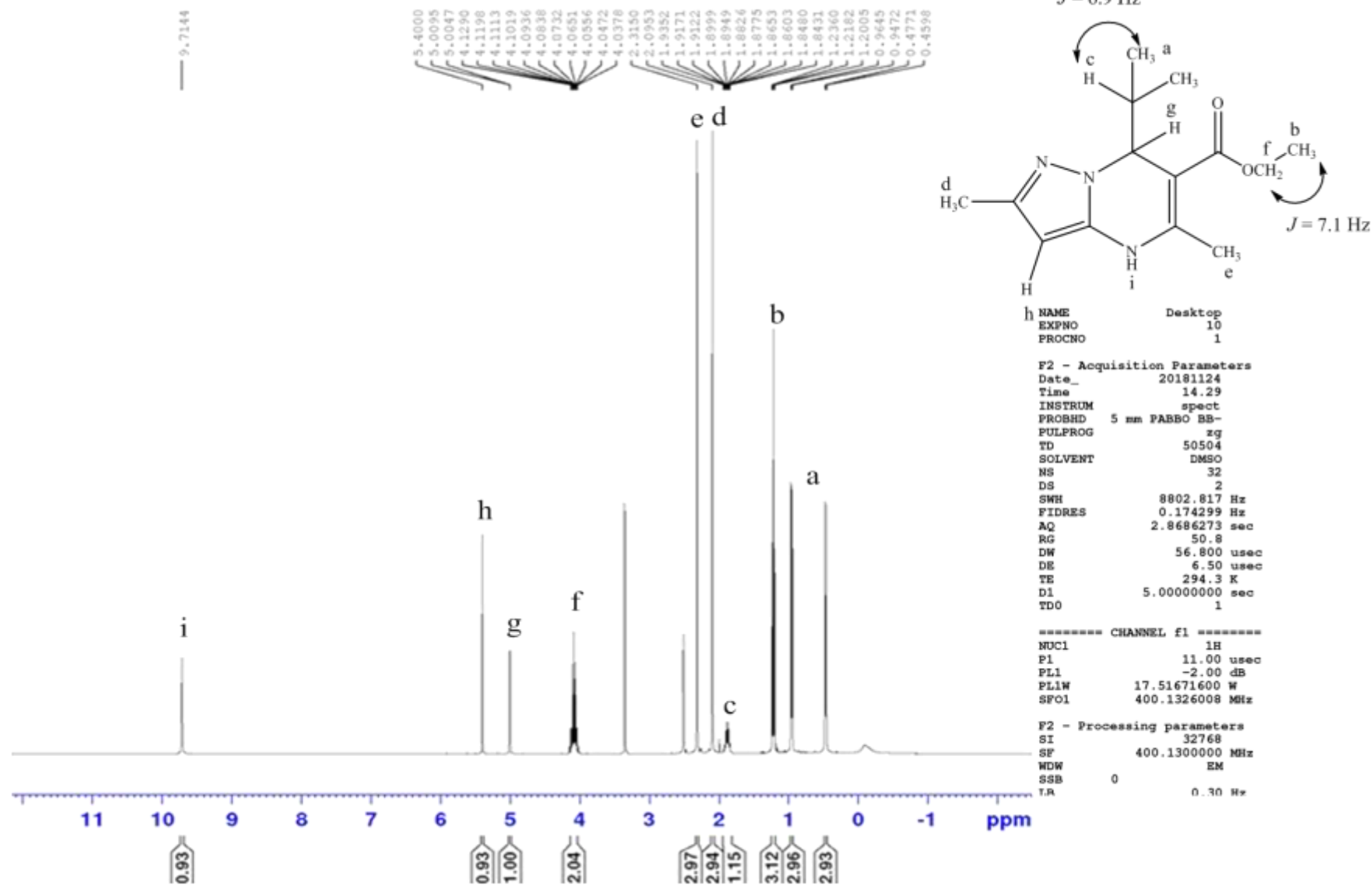


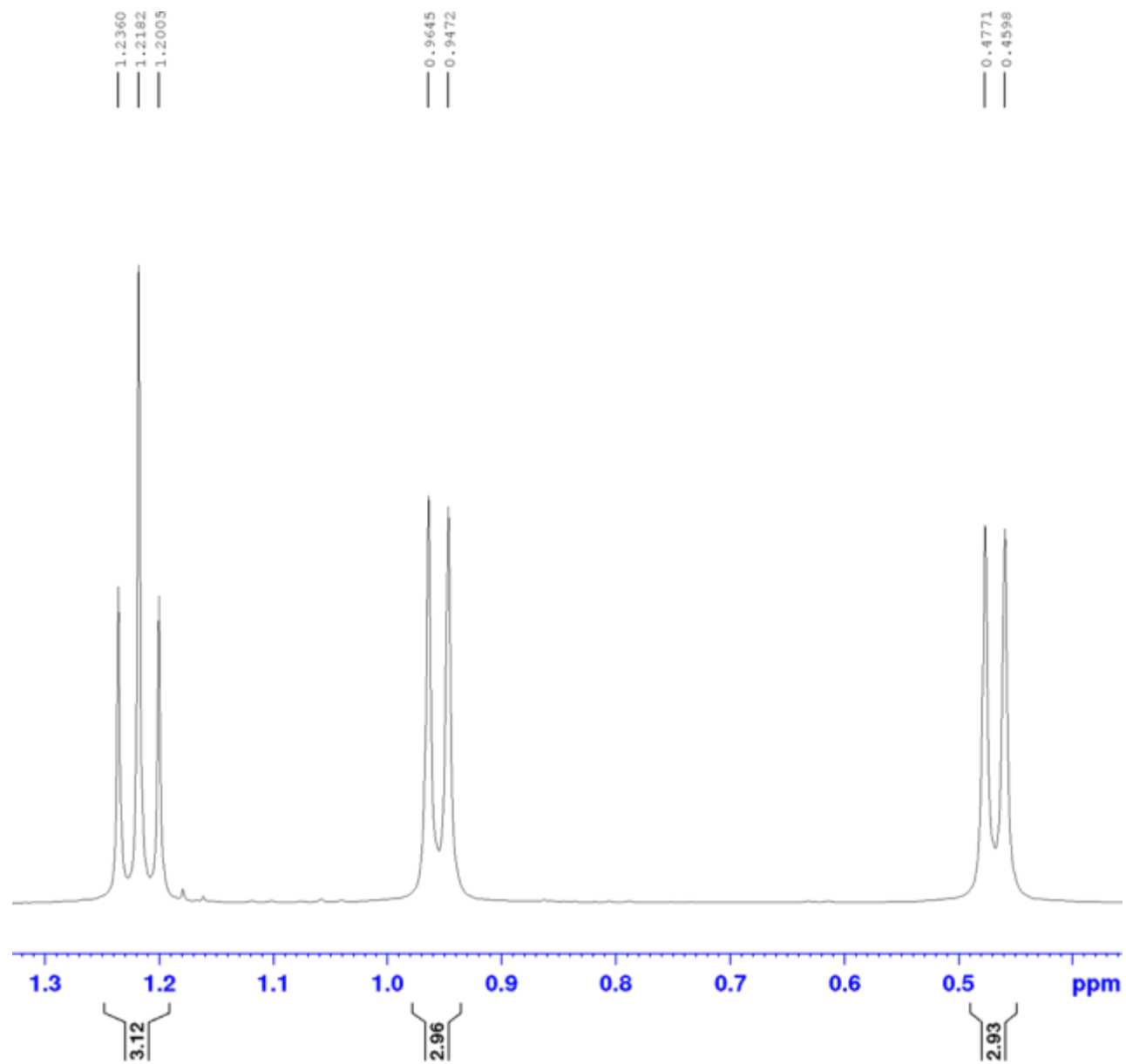
UV-absorption spectrum of **5d** in CHCl_3

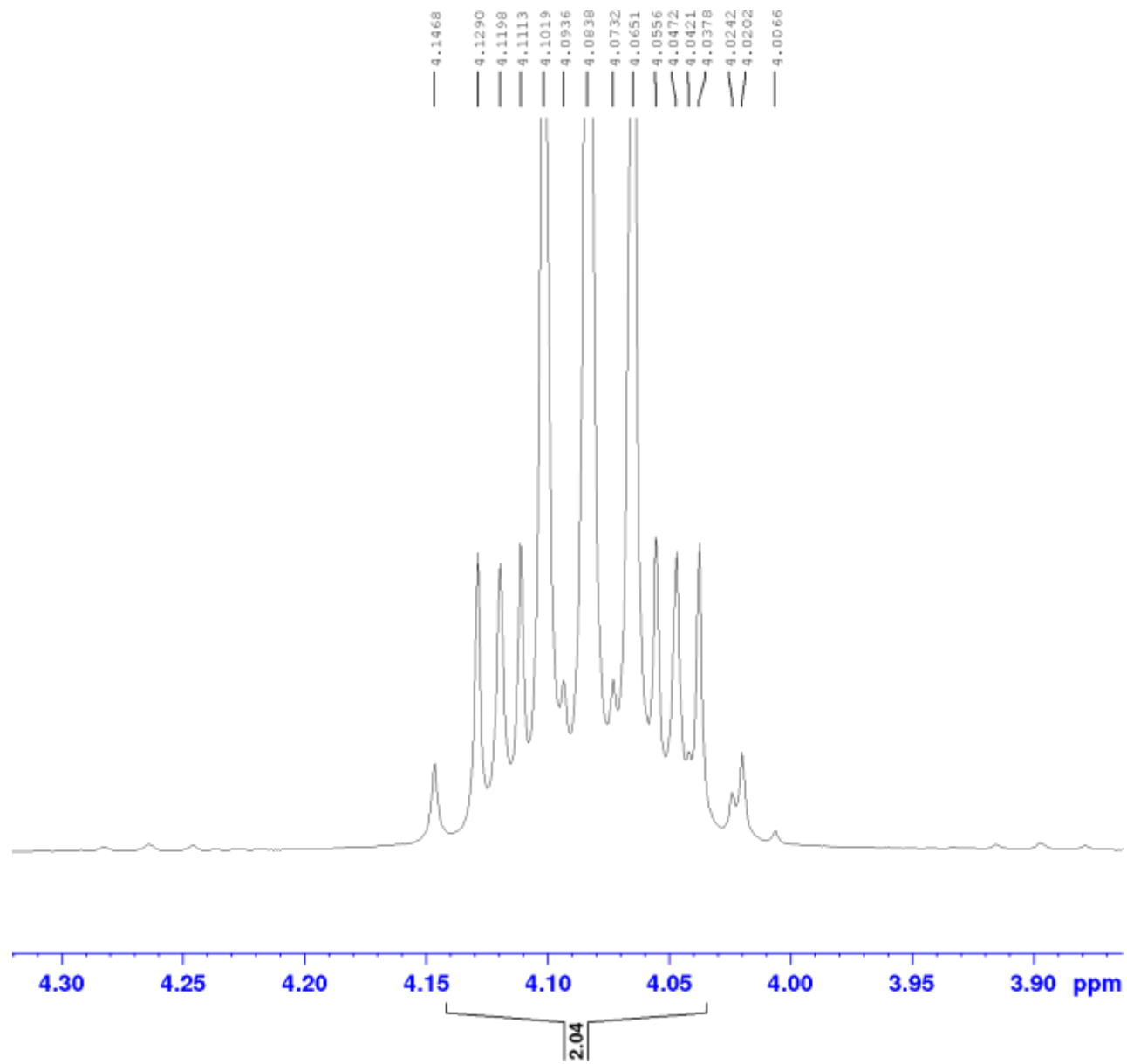
IR-Spectrum of compound 5e



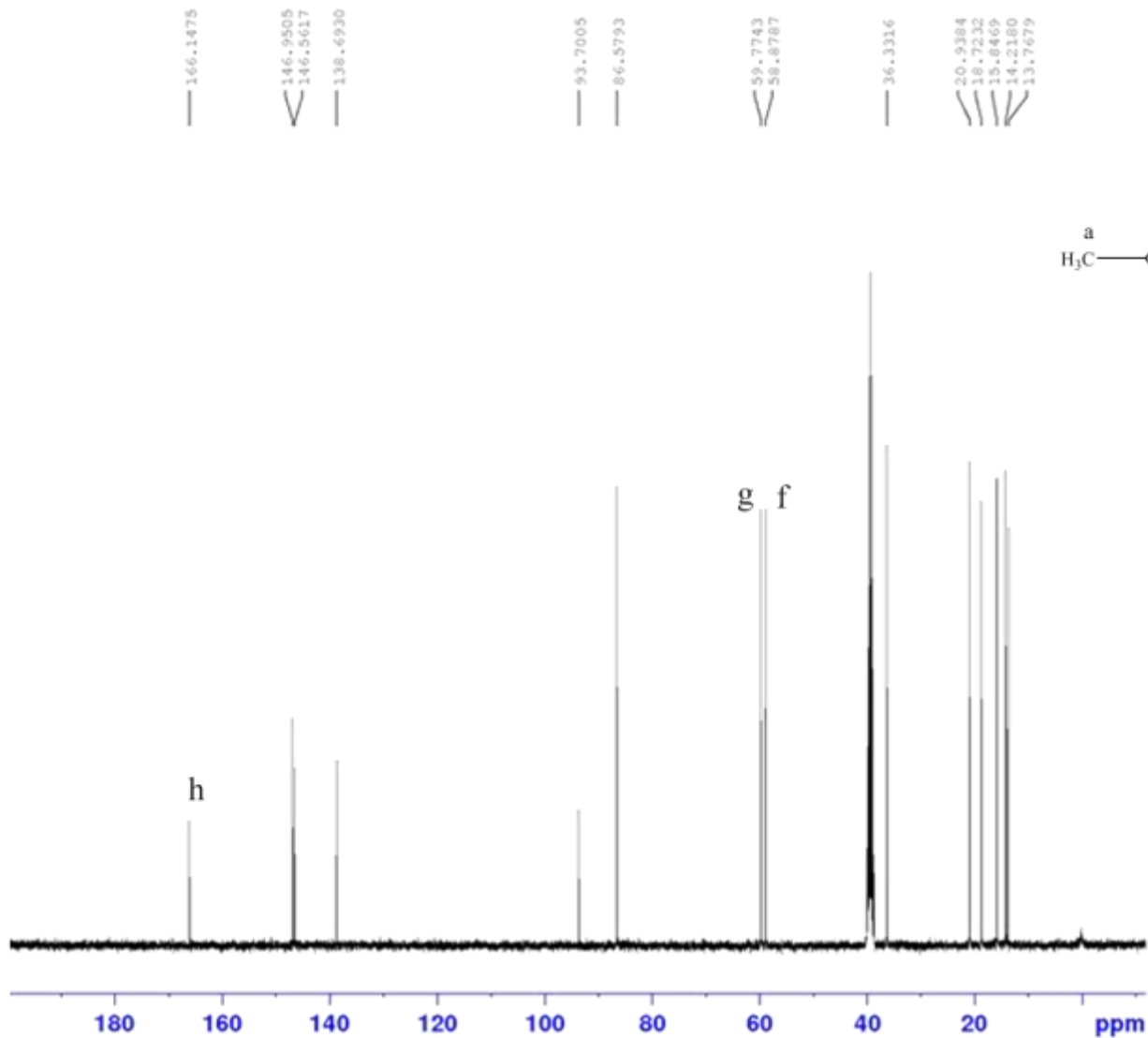
¹H NMR Spectrum of compound 5e

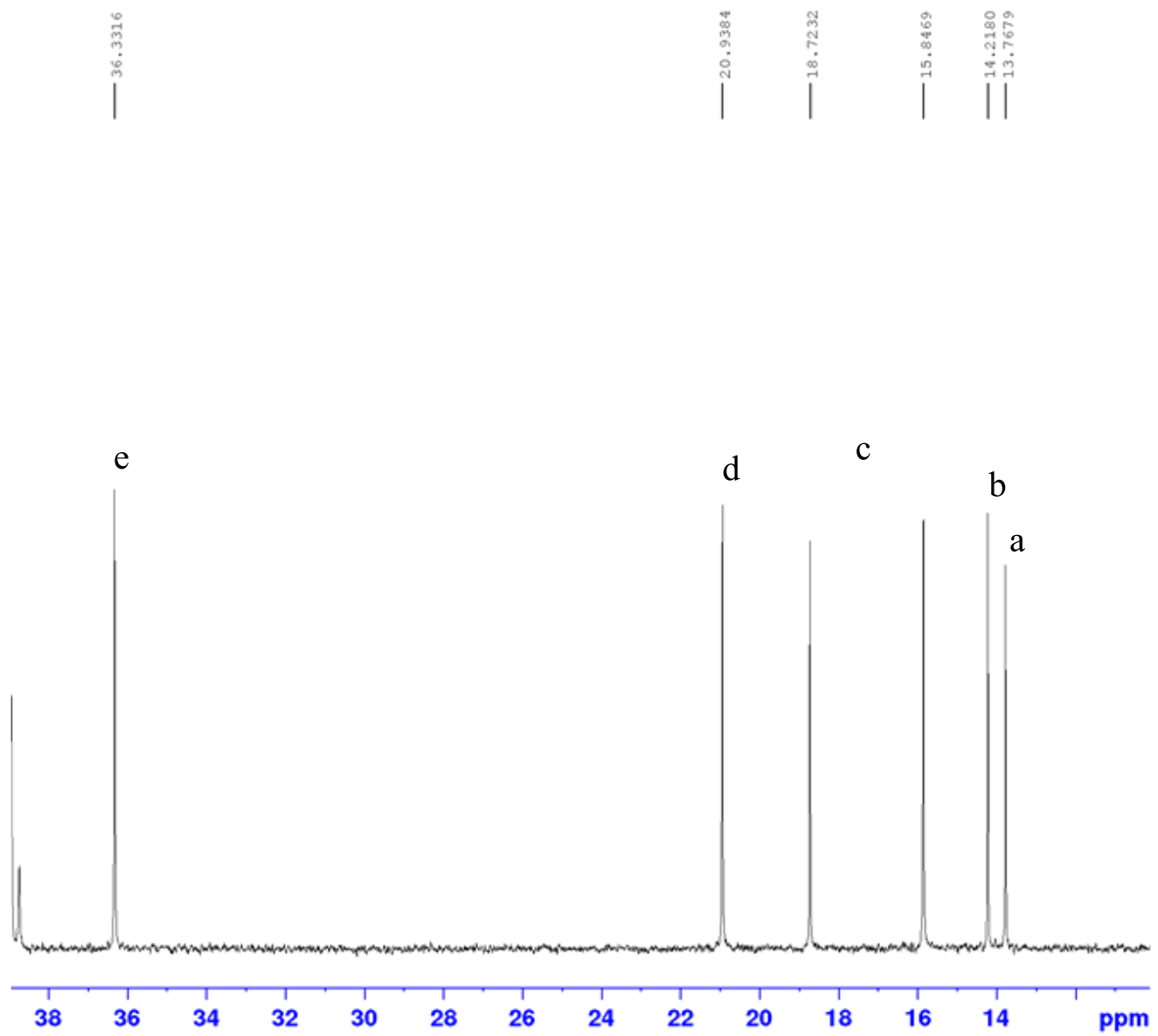


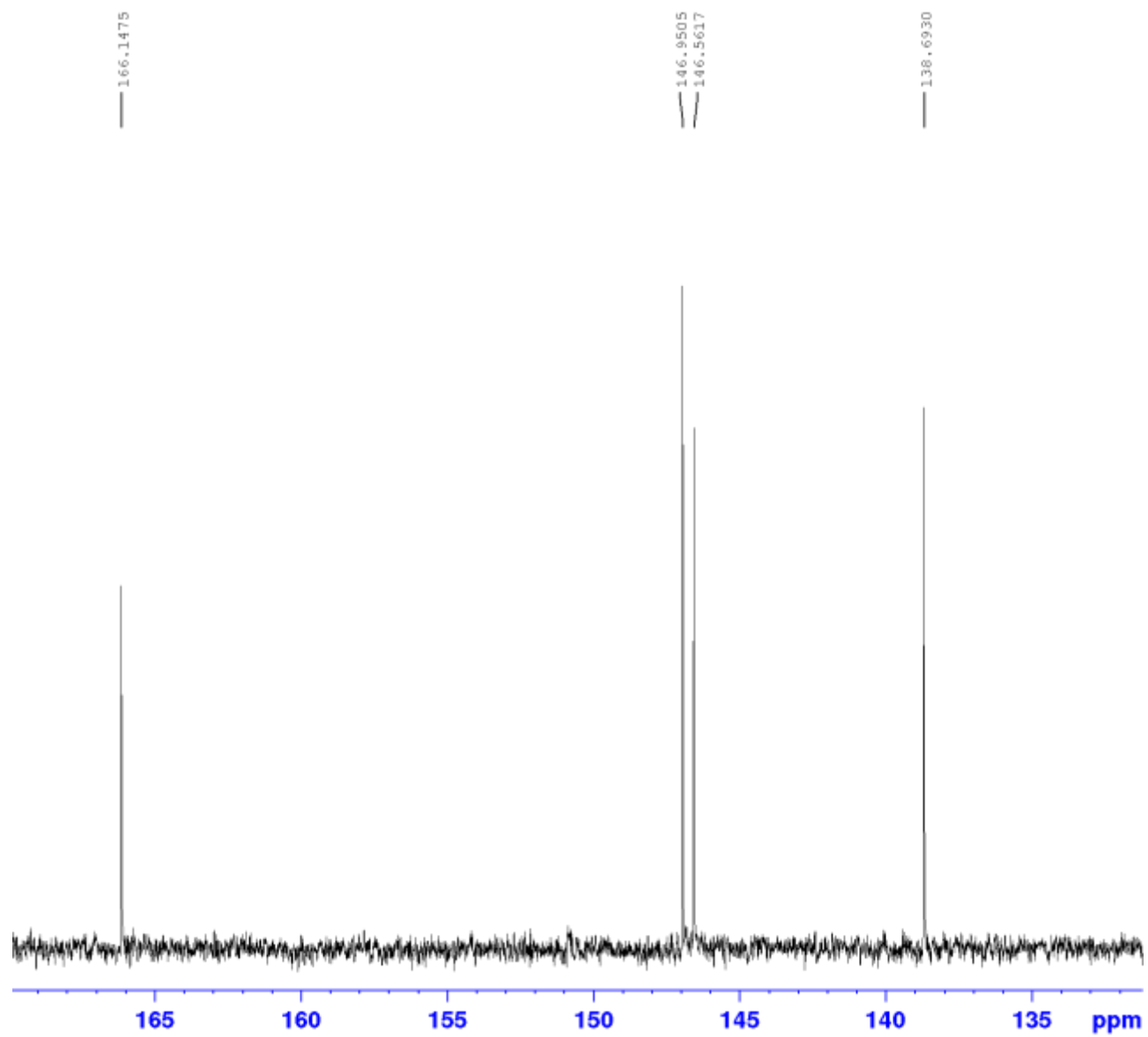




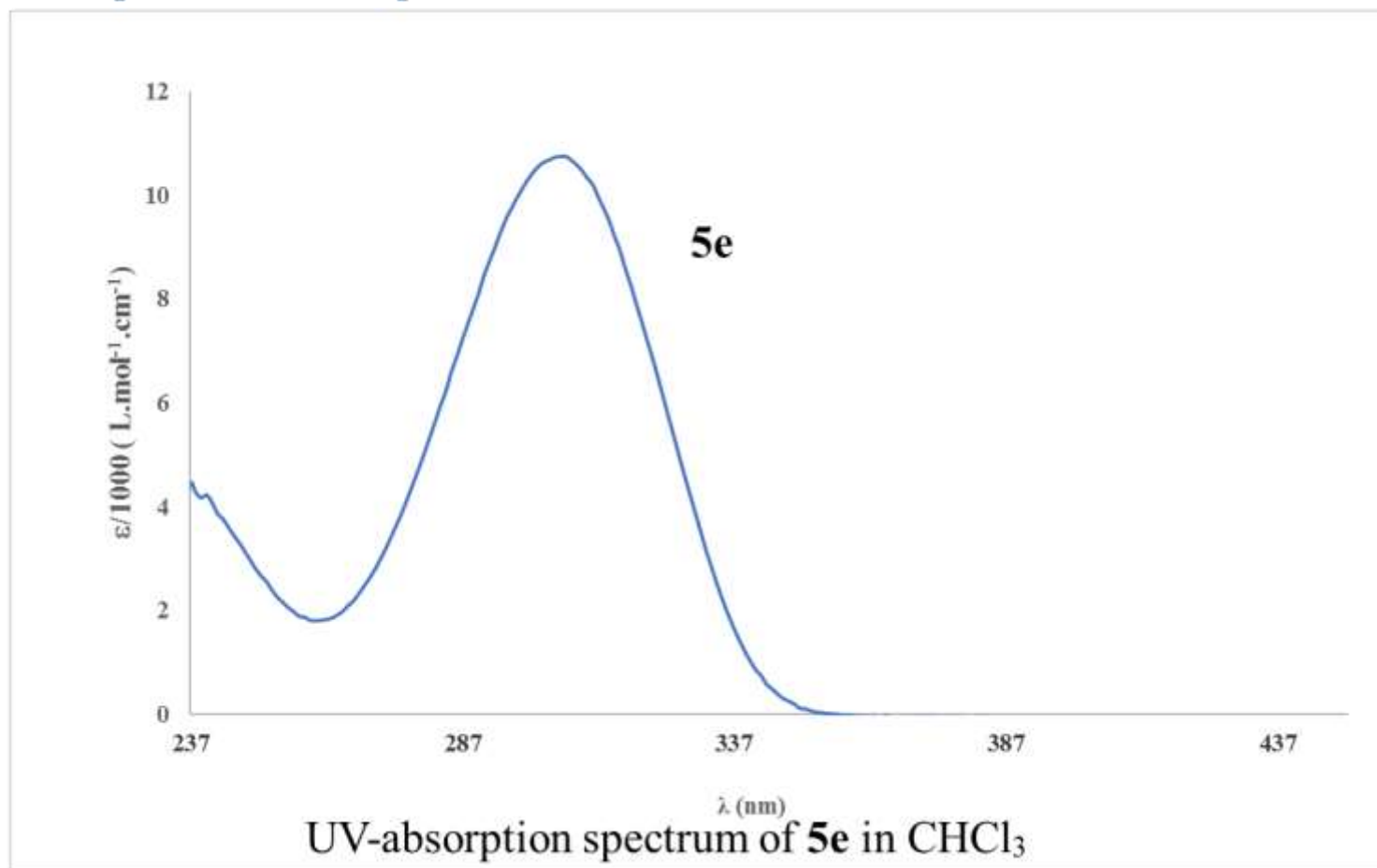
¹³C NMR Spectrum of compound 5e

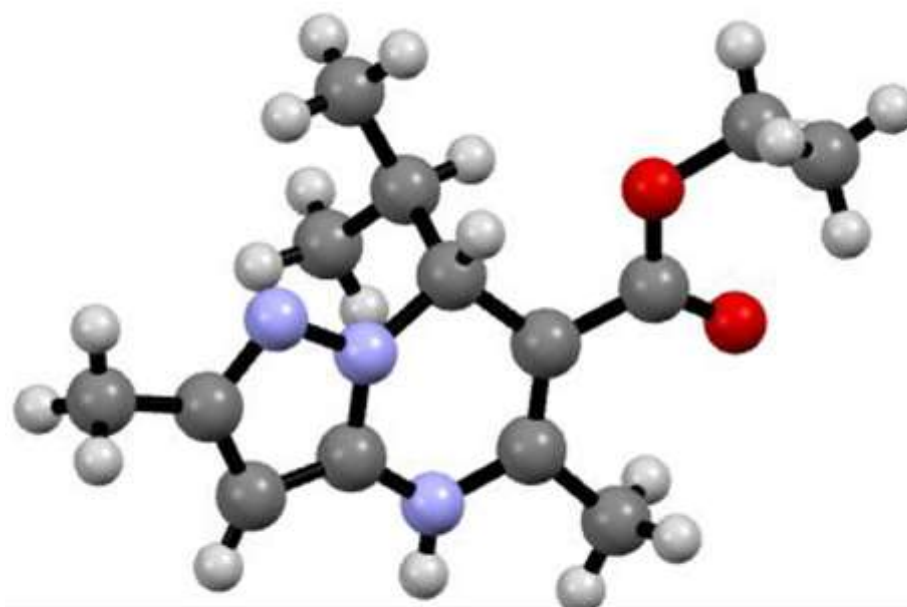




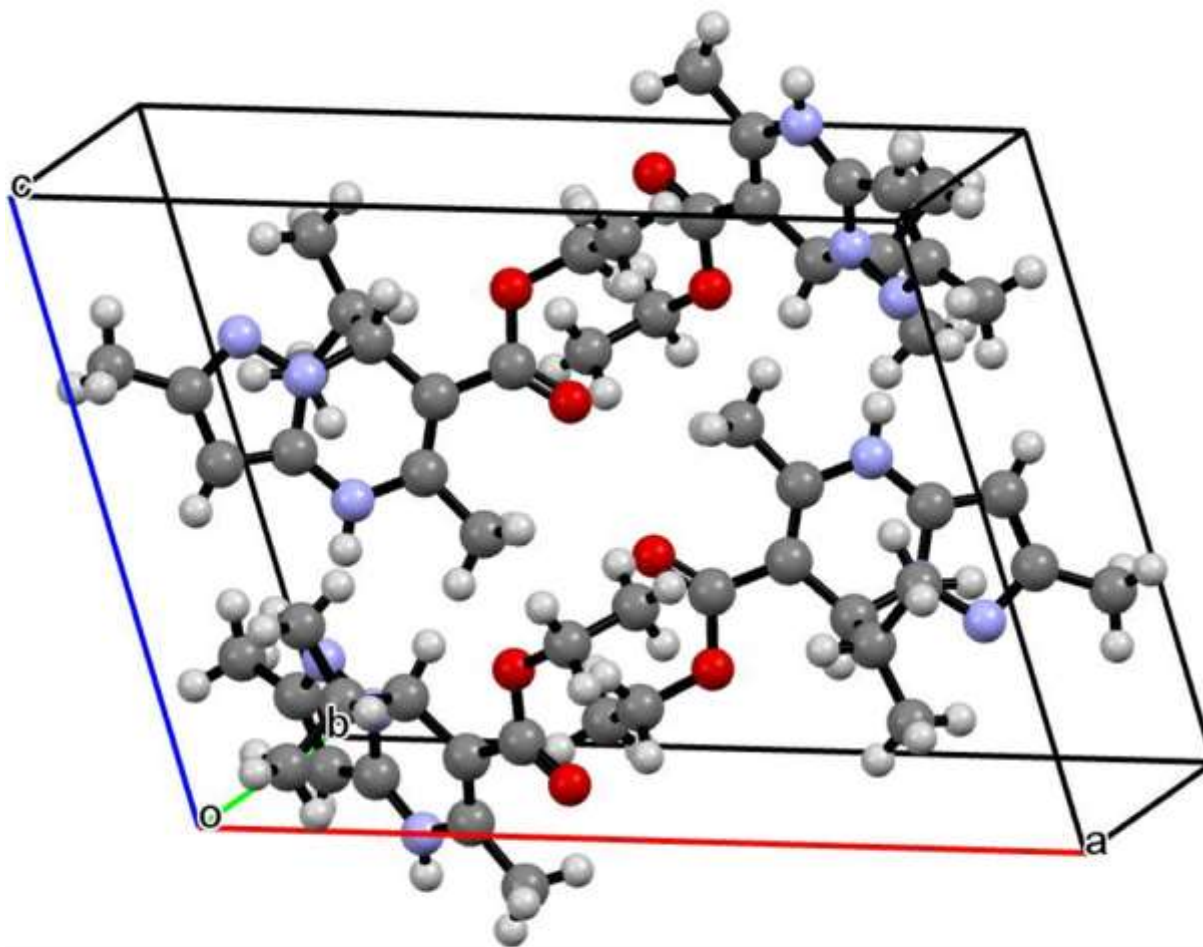


UV-Spectrum of compound **5e**





X-ray structure of compound **5e**



X-ray Crystal Packing Structure **5e**