Supplementary Material

Synthesis and antimicrobial activity of novel pyrido[2,3-*d*]pyrimidin-4(1*H*)-ones, and 2-pyrazoline derivatives

Ahmed Abdou O. Abeed, [a] * Mohamed Mohany, [b] Sinisa Djurasevic, [c] Salim S. Al-Rejaie, [b] and Talaat I. El-Emary [a]

[a] Department of Chemistry, Faculty of Science, Assiut University, Assiut 71516, Egypt
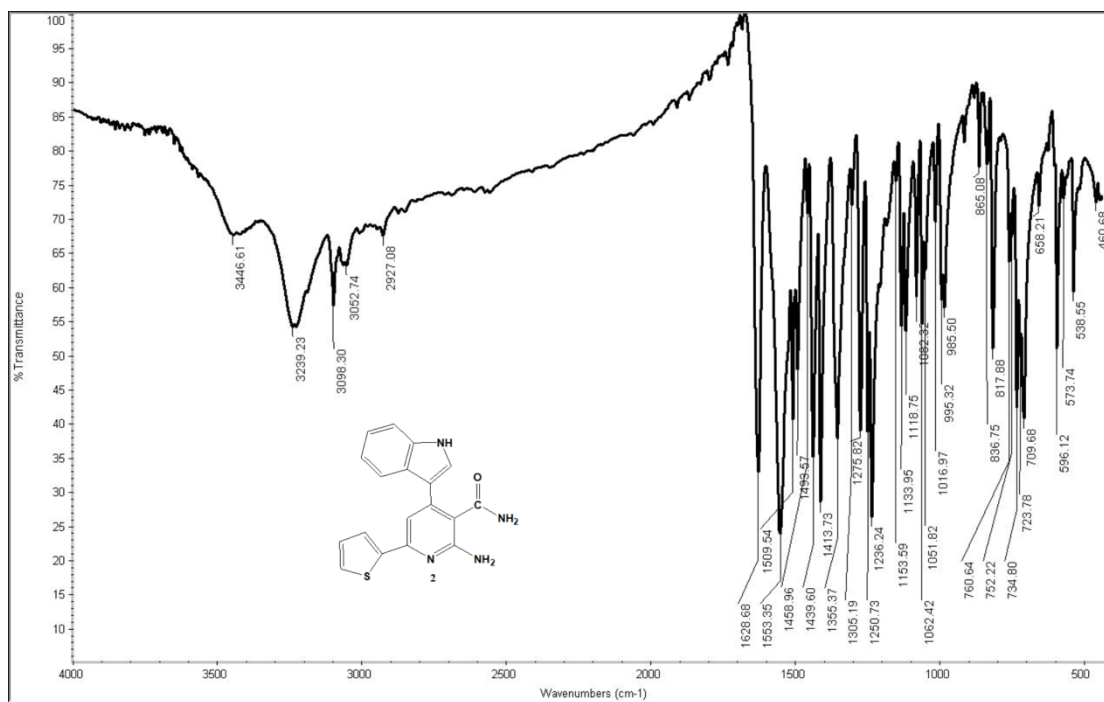*[b] Department of Pharmacology and Toxicology, College of Pharmacy, King Saud University, P.O. Box 55760, Riyadh 11451, Saudi Arabia*
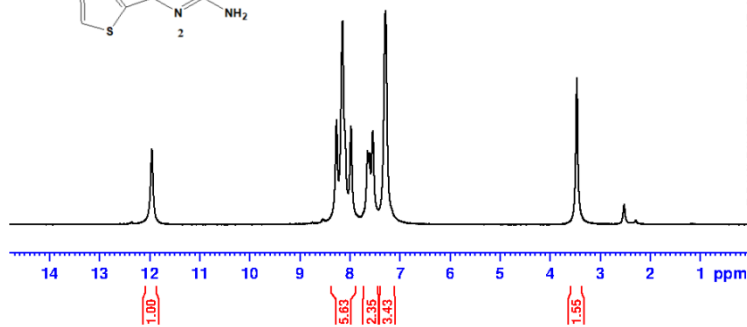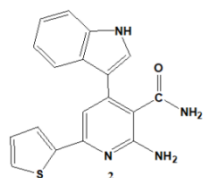*[c] Faculty of Biology, University of Belgrade, 11158 Belgrade 118, Serbia*
Email: ahmed.abeed76@aun.edu.eg

Table of Contents

AHMED ABDO-2
C13-BSU DMSO {C:\data} abeer 12

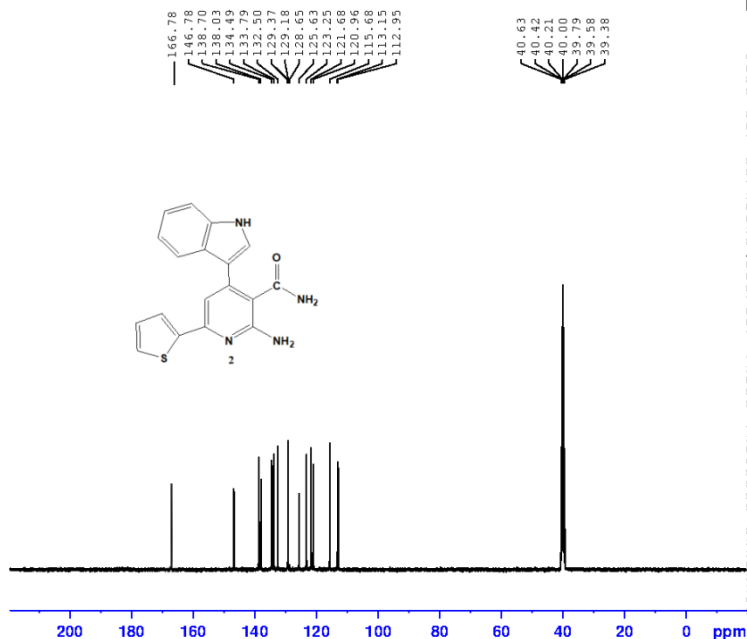Current Data Parameters
NAME   Nov22-2023-abeer
EXPNO   21
PROCNO   1

F2 - Acquisition Parameters
Date_   20231122
Time   17.36
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.44
DW   20.800 usec
DE   6.50 usec
TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

AHMEDABDO-3
PROTON_BSU DMSO {C:\data} abeer 16

12.572

8.556
8.529
8.221
8.212
8.125
8.113
8.109
8.101
8.095
8.084
8.045
7.953
7.941
7.916
7.897
7.597
7.579
7.559
7.526
7.520
7.516
7.504
7.311
7.293
7.276
7.269
7.266
7.248
7.240
7.230
4.296
4.278
4.261
4.243
3.507
1.383
1.347
1.311

Current Data Parameters
NAME   Nov15-2023-abeer
EXPNO   40
PROCNO   1

F2 - Acquisition Parameters
Date_   20231115
Time   20.03
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   65536
SOLVENT   DMSO
NS   16
DS   2
SWH   8012.820 Hz
FIDRES   0.122266 Hz
AQ   4.0894465 sec
RG   56.51
DW   62.400 usec
DE   6.50 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   400.1324710 MHz
NUC1   1H
P1   10.00 usec
PLW1   16.00000000 W

F2 - Processing parameters
SI   65536
SF   400.1300000 MHz
WDW   EM
SSB   0
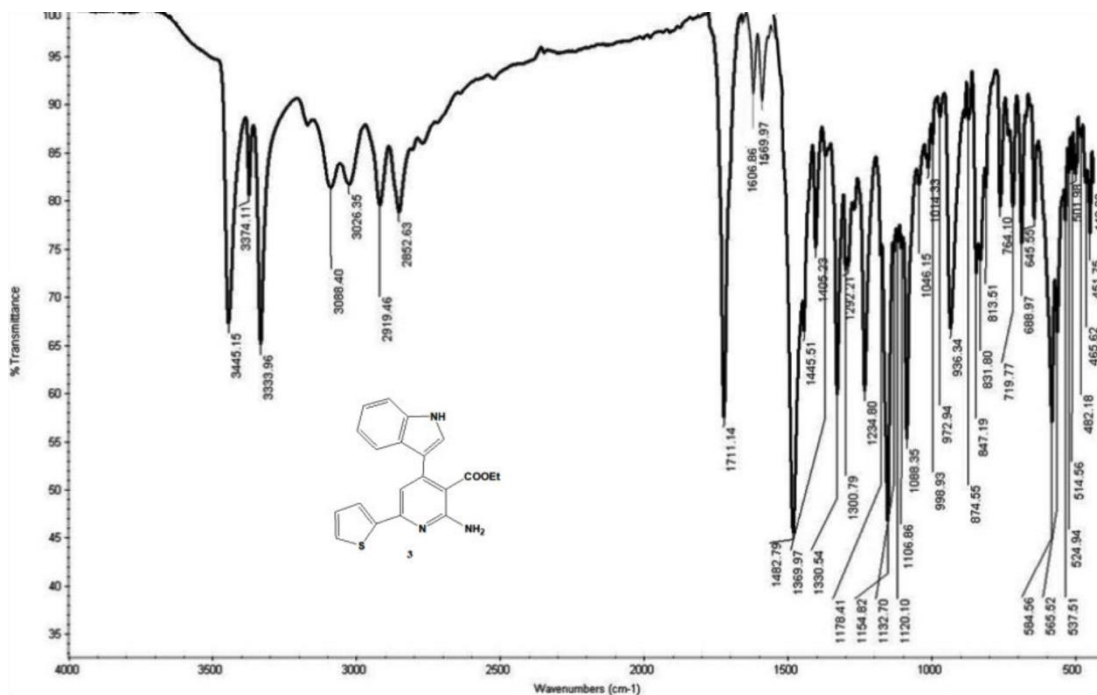LB   0.10 Hz
GB   0
PC   1.00

0.42   1.00 0.09 0.22 0.03 0.60 0.59 0.10 1.30   1.02 3.49   1.54

AHMEDABDO-3
C13-BSU DMSO {C:\data} abeer 16

176.94
146.96
146.71
146.66
138.01
136.71
134.42
133.71
133.01
132.42
129.32
129.14
128.61
127.40
125.73
125.59
124.08
123.20
122.65
122.61
121.65
120.89
118.93
118.50
115.63
115.38
113.38
113.10
110.92
110.45
92.83
61.88
40.53
40.32
40.11
39.90
39.69
39.48
39.27
14.58

Current Data Parameters
NAME   Nov15-2023-abeer
EXPNO   41
PROCNO   1

F2 - Acquisition Parameters
Date_   20231115
Time   23.53
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.444
DW   20.800 usec
DE   6.50 usec
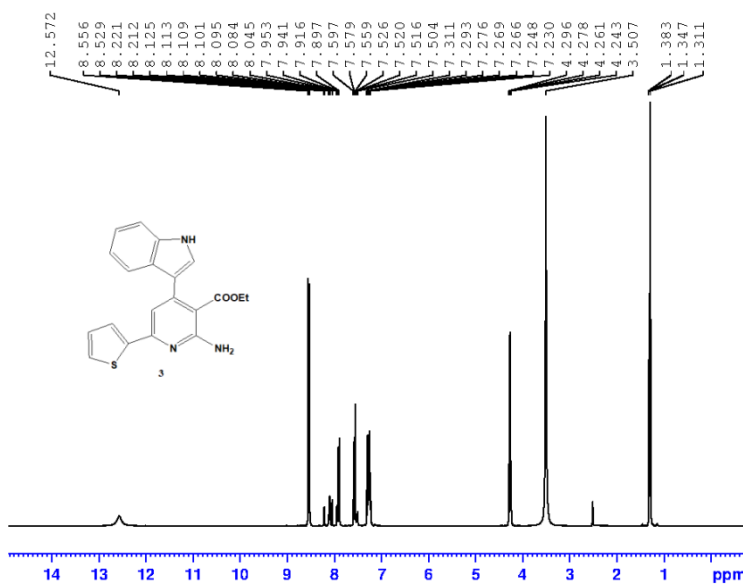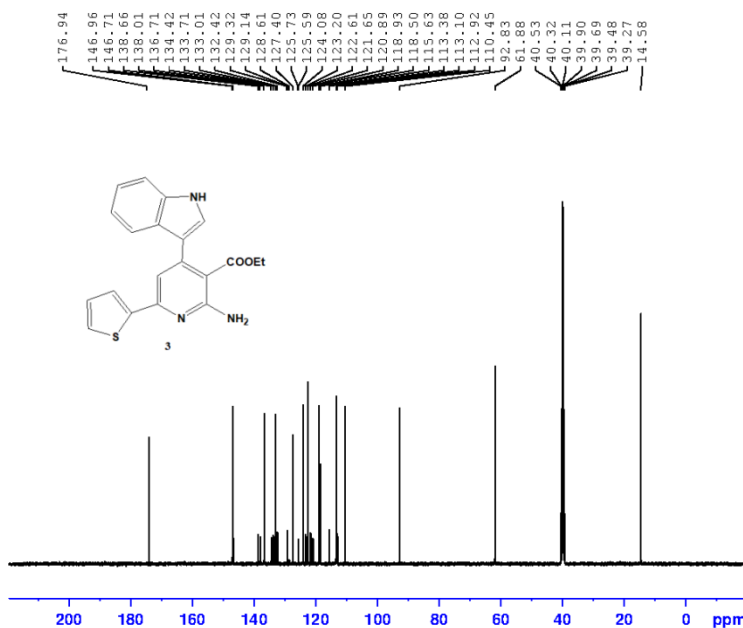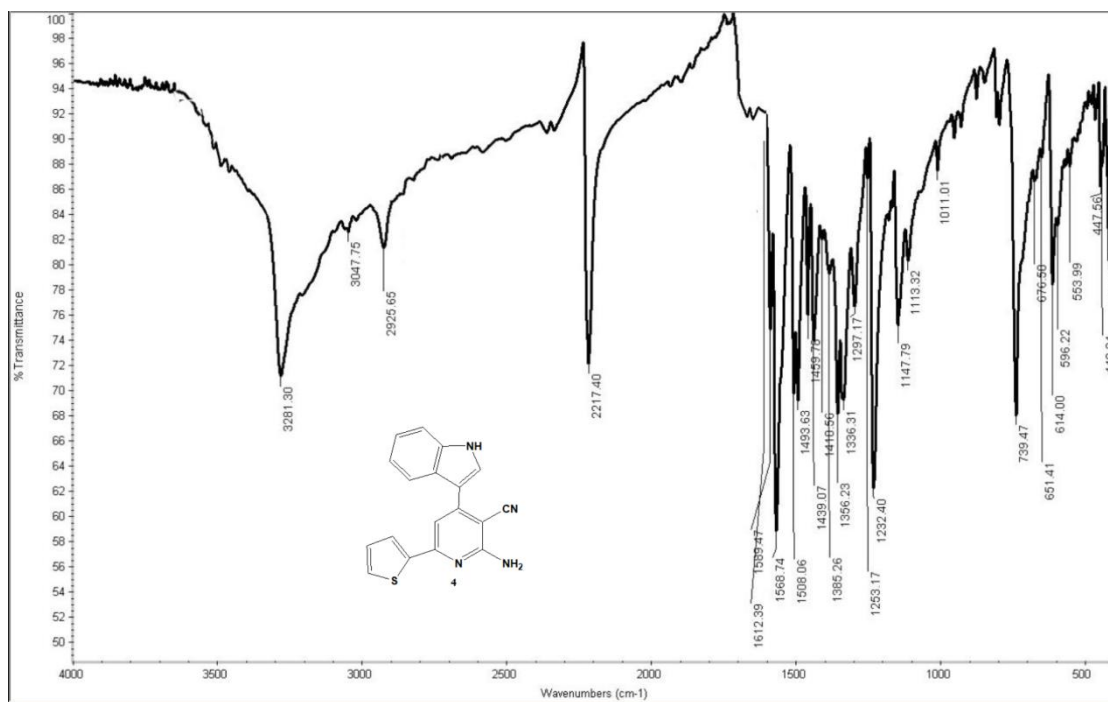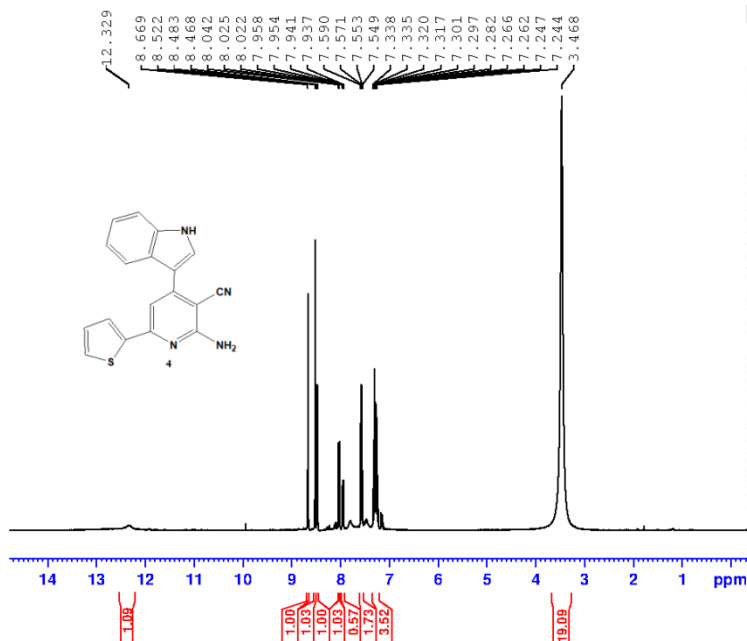TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
SSB   0
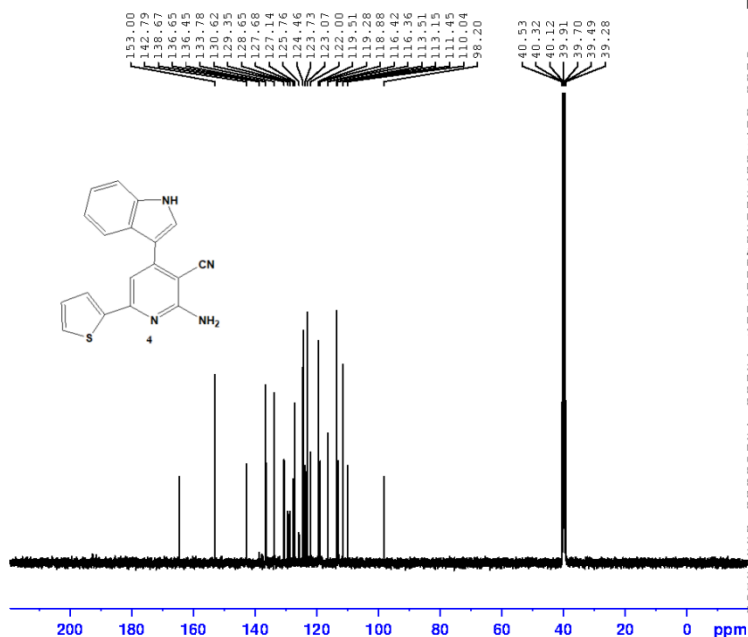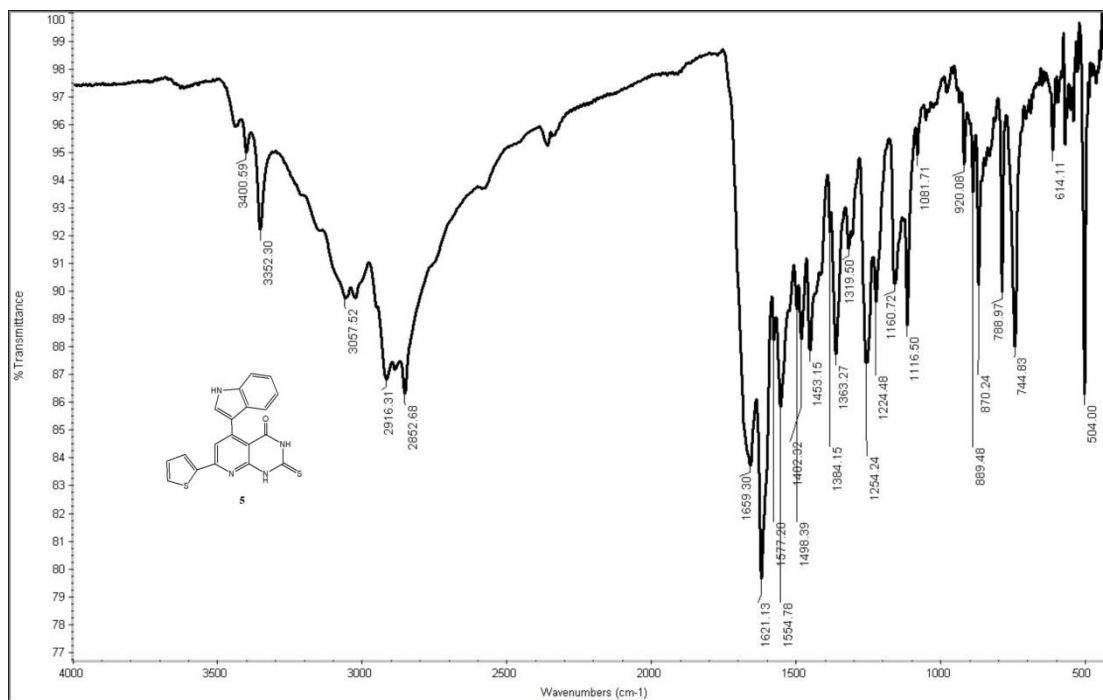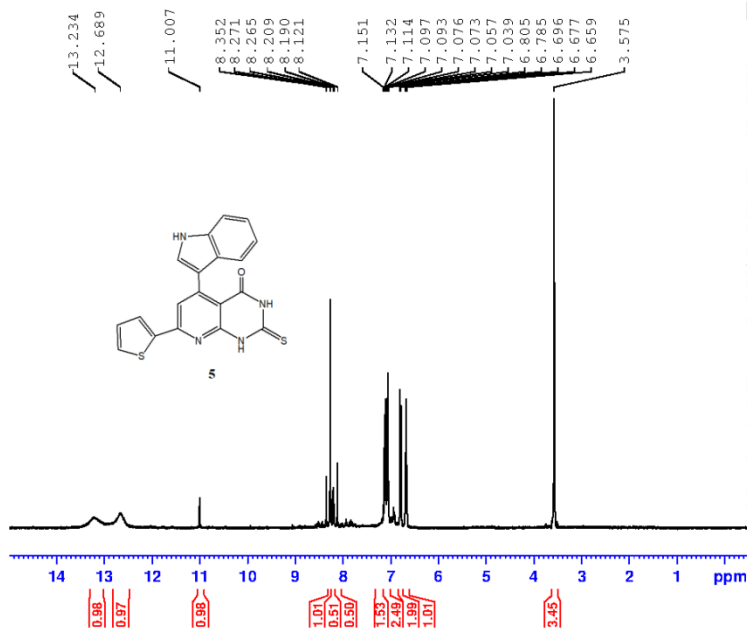LB   1.00 Hz
GB   0
PC   1.40

AHMED ABDO-4
C13-BSU DMSO {C:\data} abeer 18

Current Data Parameters
NAME   Nov15-2023-abeer
EXPNO   61
PROCNO   1

F2 - Acquisition Parameters
Date_   20231116
Time   7.41
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.44
DW   20.800 usec
DE   6.50 usec
TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

AHMED ABDO-5
PROTON_BSU DMSO {C:\data} abeer 15

13.234
12.689
11.007
8.352
8.271
8.265
8.209
8.190
8.121
7.151
7.132
7.114
7.097
7.093
7.076
7.073
7.057
7.039
7.037
6.805
6.785
6.696
6.677
6.659
3.575
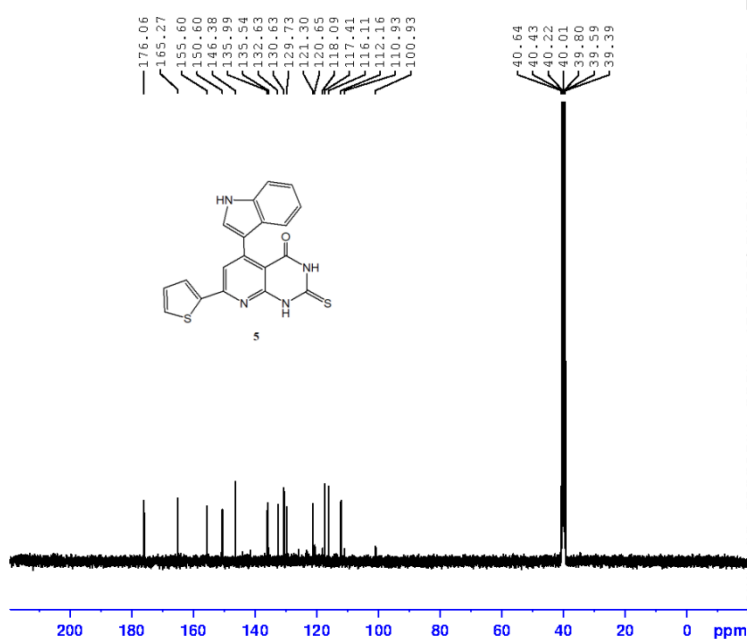

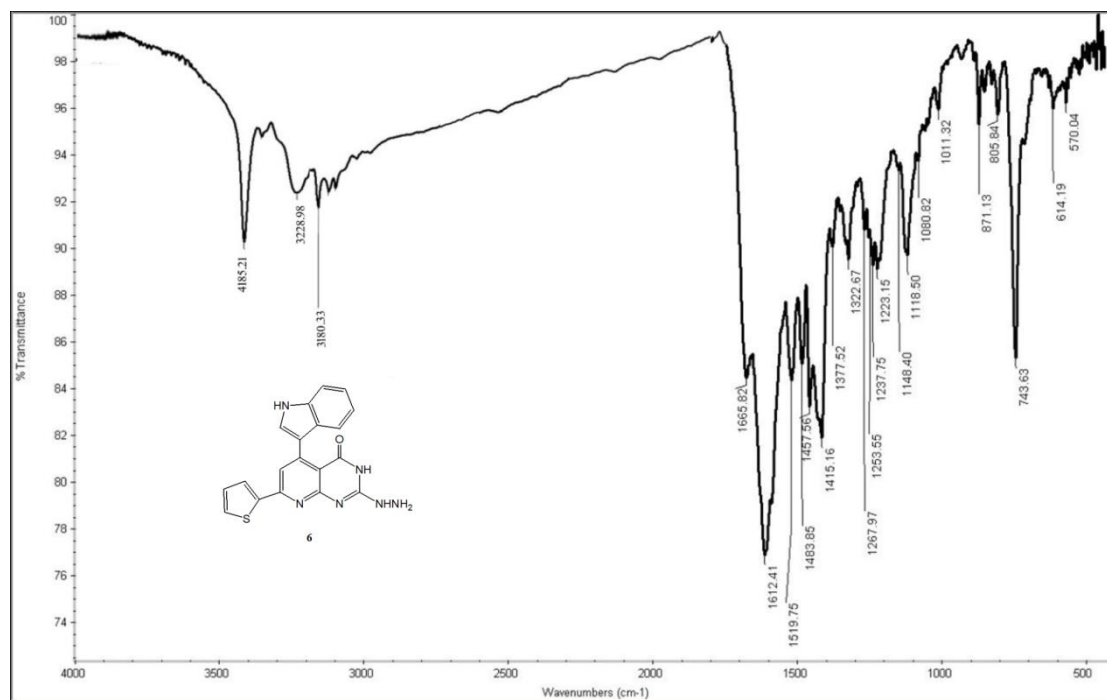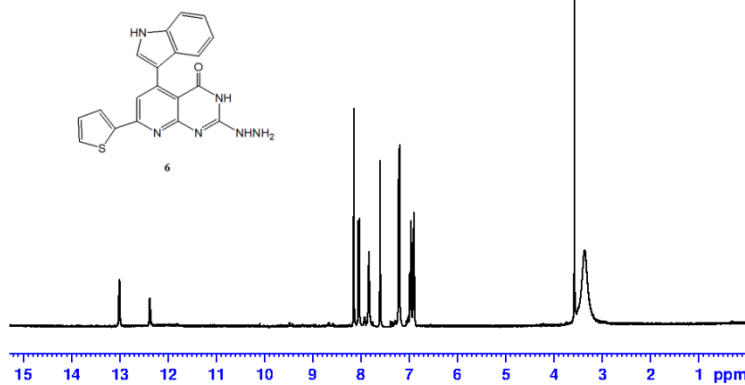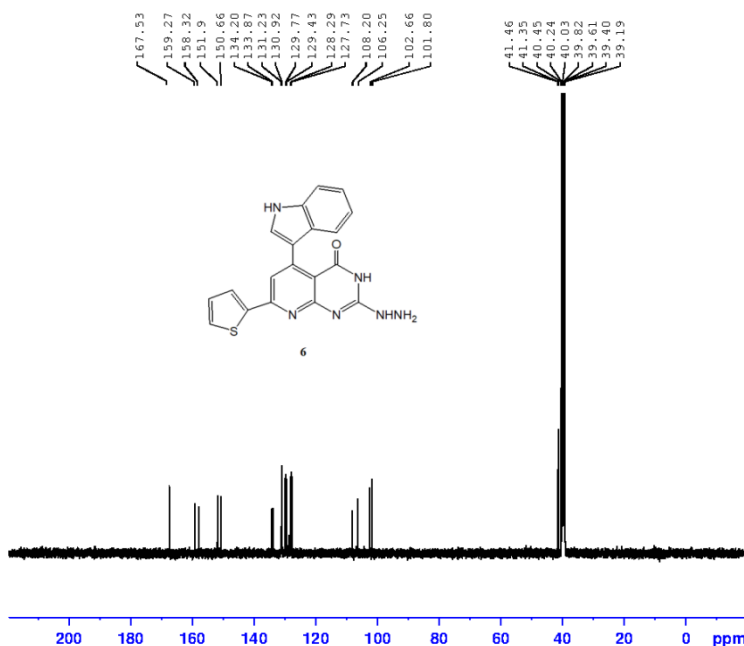Current Data Parameters
NAME   Nov22-2023-abeer
EXPNO   50
PROCNO   1

F2 - Acquisition Parameters
Date_   20231123
Time   1.27
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   65536
SOLVENT   DMSO
NS   16
DS   2
SWH   8012.820 Hz
FIDRES   0.122266 Hz
AQ   4.0894465 sec
RG   147.93
DW   62.400 usec
DE   6.50 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   400.1324710 MHz
NUC1   1H
P1   10.00 usec
PLW1   16.00000000 W

F2 - Processing parameters
SI   65536
SF   400.1300000 MHz
WDW   EM
SSB   0
LB   0.10 Hz
GB   0
PC   1.00

5

14 13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

0.98 0.97 | 0.98 | 1.01 0.51 0.50 | 1.53 2.49 1.99 1.01 | 3.45

AHMED ABDO 5
C13-BSU DMSO {C:\data} abeer 15

176.06
165.27
155.60
150.60
146.38
135.99
135.54
132.63
130.63
129.73
121.30
120.65
118.09
117.41
116.16
112.16
110.93
100.93

40.64
40.43
40.22
40.01
39.80
39.59
39.39

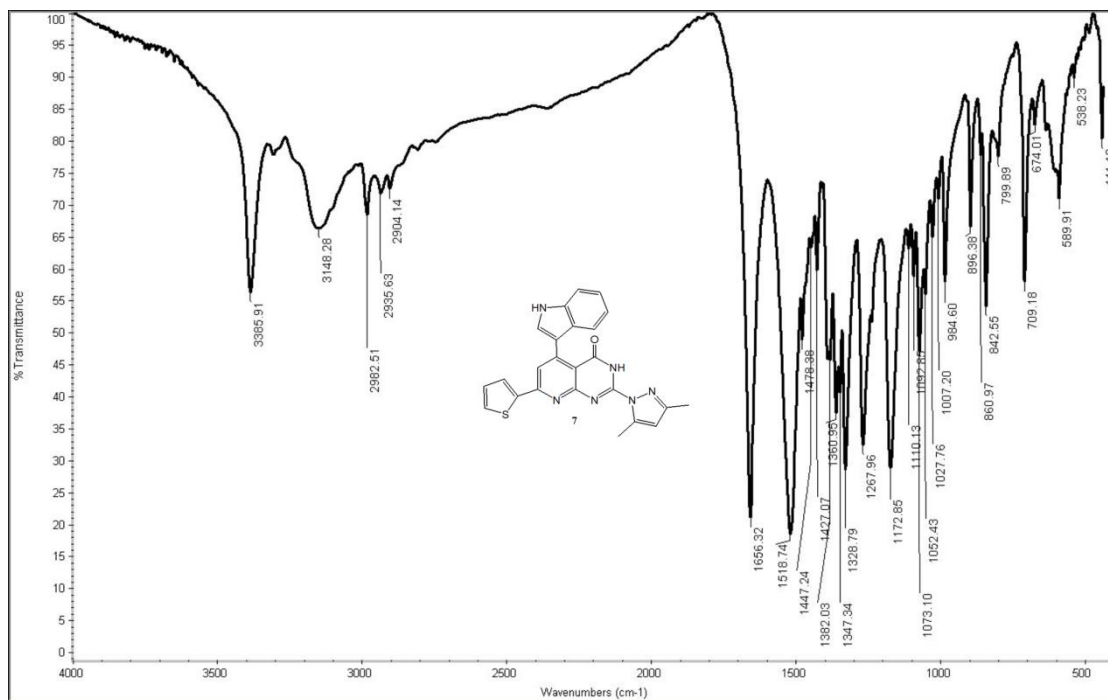Current Data Parameters
NAME   Nov22-2023-abeer
EXPNO   51
PROCNO   1

F2 - Acquisition Parameters
Date_   20231123
Time   5.17
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.444
DW   20.800 usec
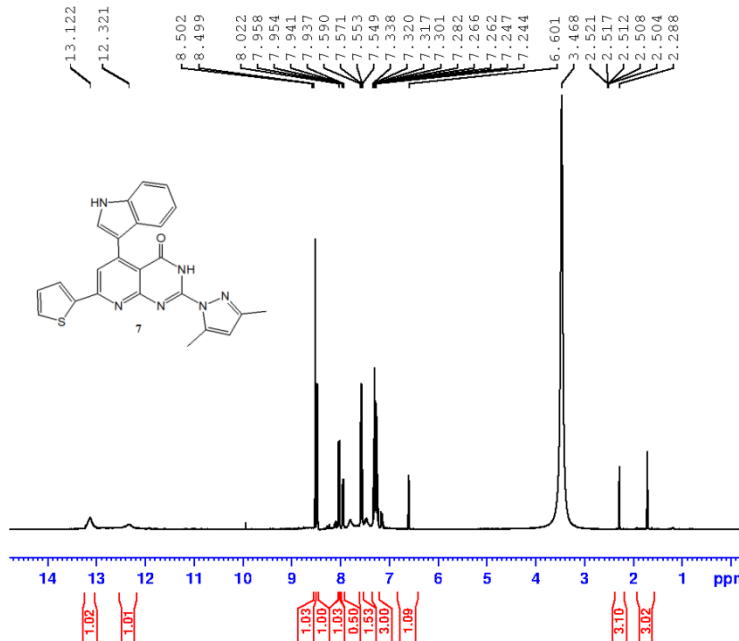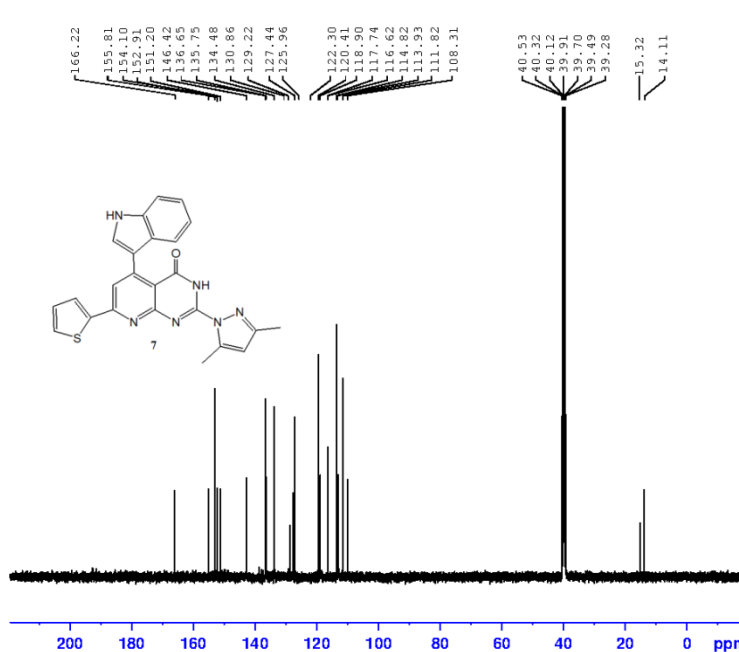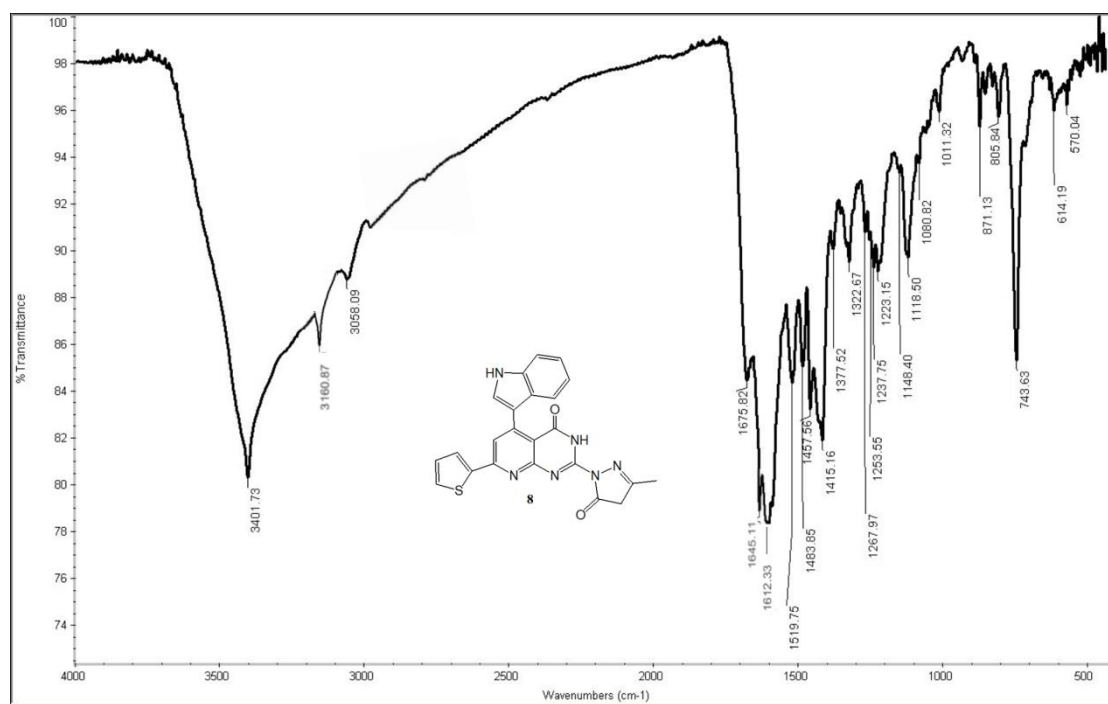DE   6.50 usec
TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

5

200 180 160 140 120 100 80 60 40 20 0 ppm

AHMED ABDO-6
C13-BSU DMSO {C:\data} abeer 21

167.53
159.27
158.32
151.9
150.66
134.20
133.87
131.23
130.92
129.77
129.43
128.29
127.73
108.20
106.25
102.66
101.80

41.46
41.35
40.45
40.24
40.03
39.82
39.61
39.40
39.19

BRUKER

Current Data Parameters
NAME   Nov23-2023-abeer
EXPNO   51
PROCNO   1

F2 - Acquisition Parameters
Date_   20231123
Time   20.33
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.44
DW   20.800 usec
DE   6.50 usec
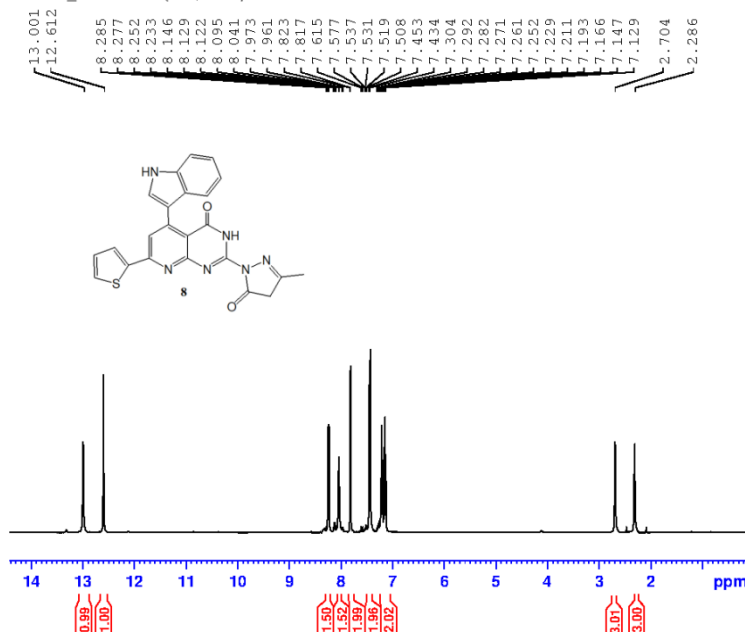TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
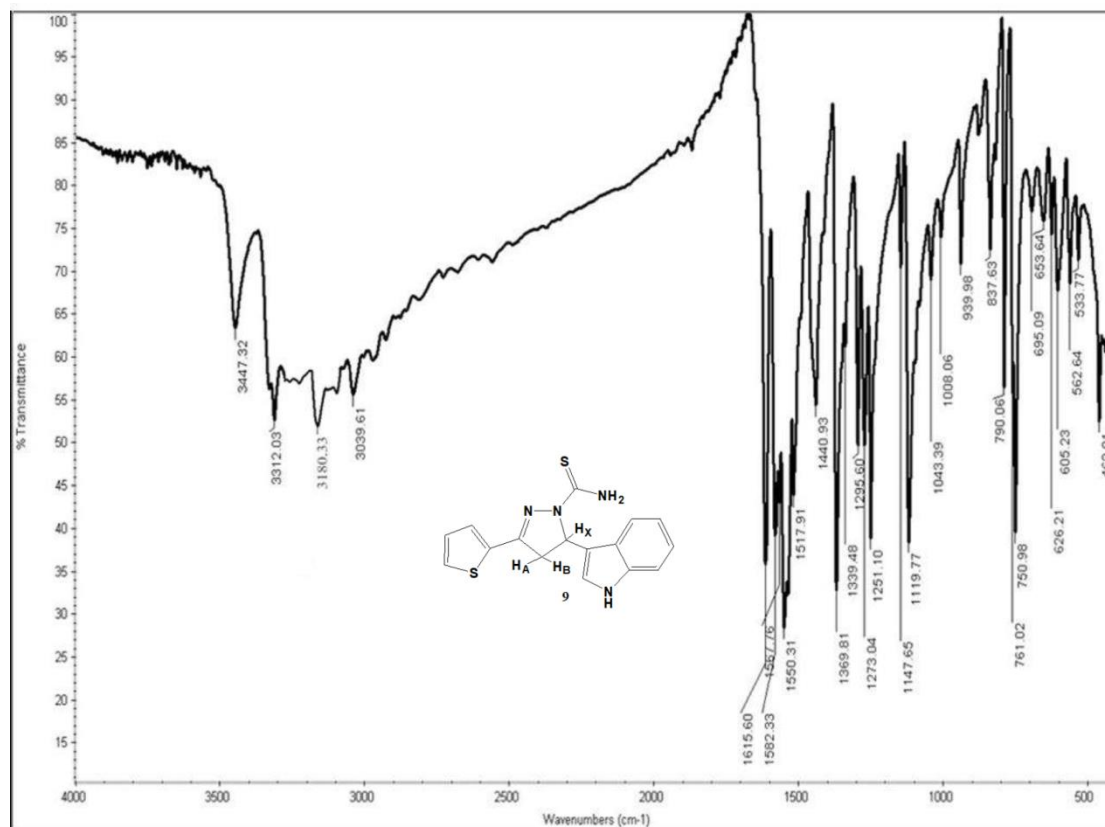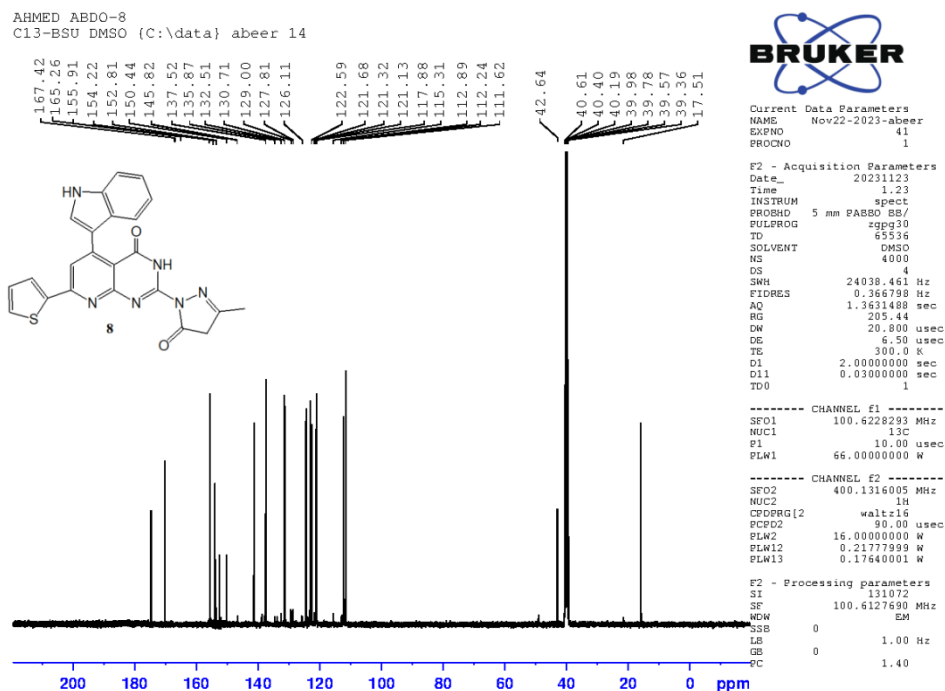SSB   0
LB   1.00 Hz
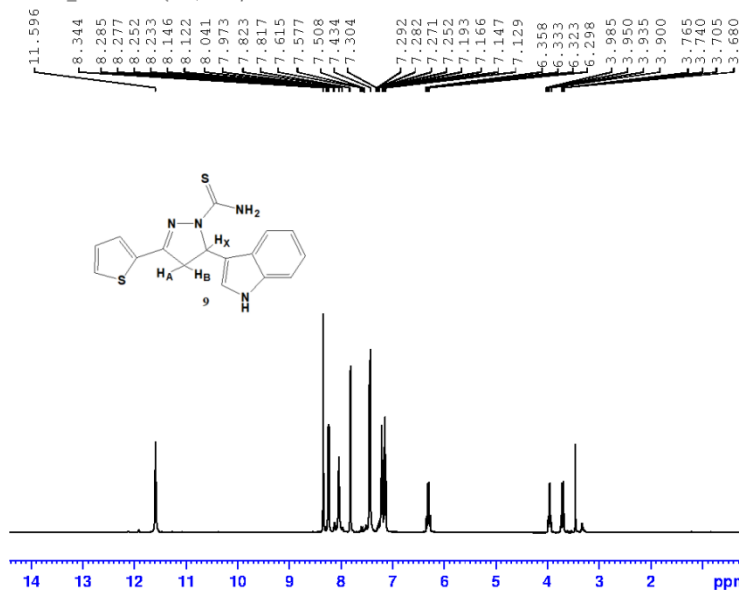GB   0
PC   1.40

AHMED ABDO-7
PROTON_BSU DMSO {C:\data} abeer 18

AHMED ABDO-7
C13-BSU DMSO {C:\data} abeer 18

AHMED ABDO-8
C13-BSU DMSO {C:\data} abeer 14

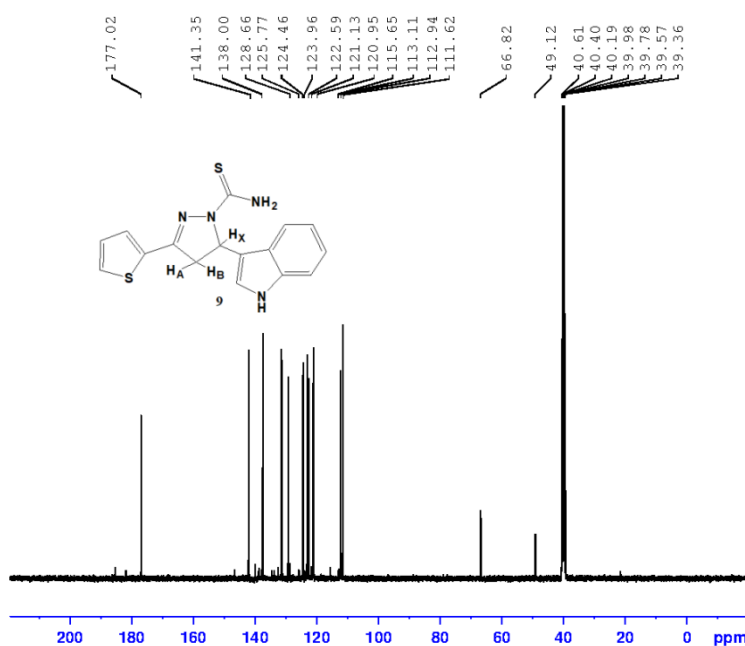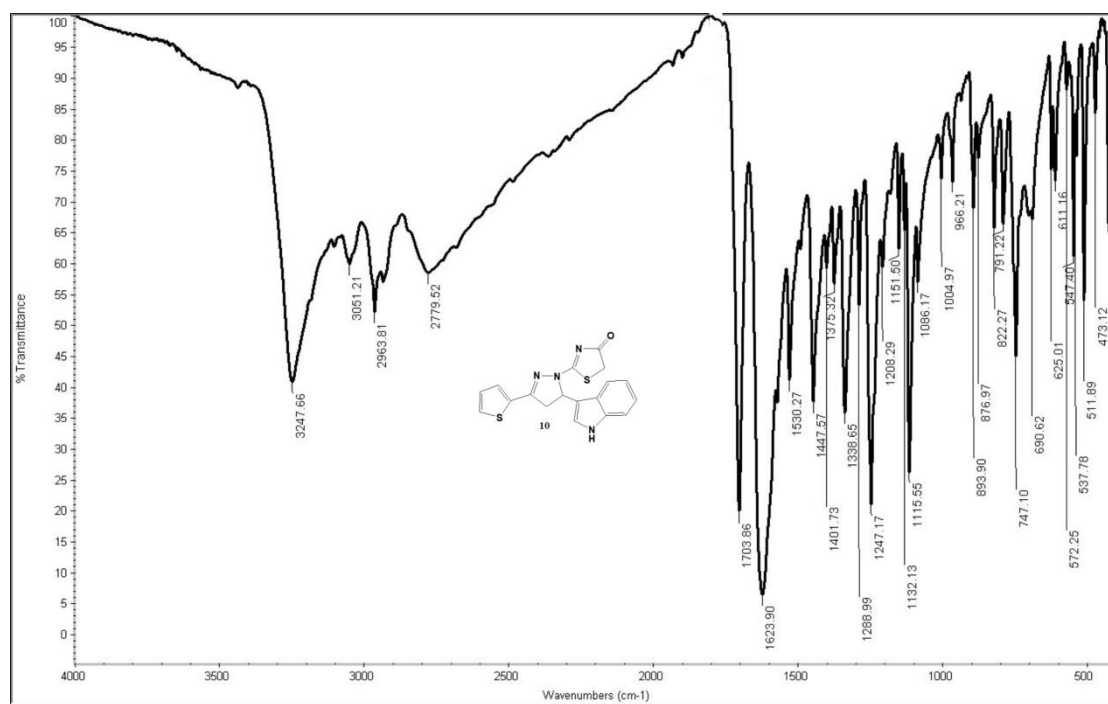Current Data Parameters
NAME   Nov22-2023-abeer
EXPNO   41
PROCNO   1

F2 - Acquisition Parameters
Date_   20231123
Time   1.23
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.44
DW   20.800 usec
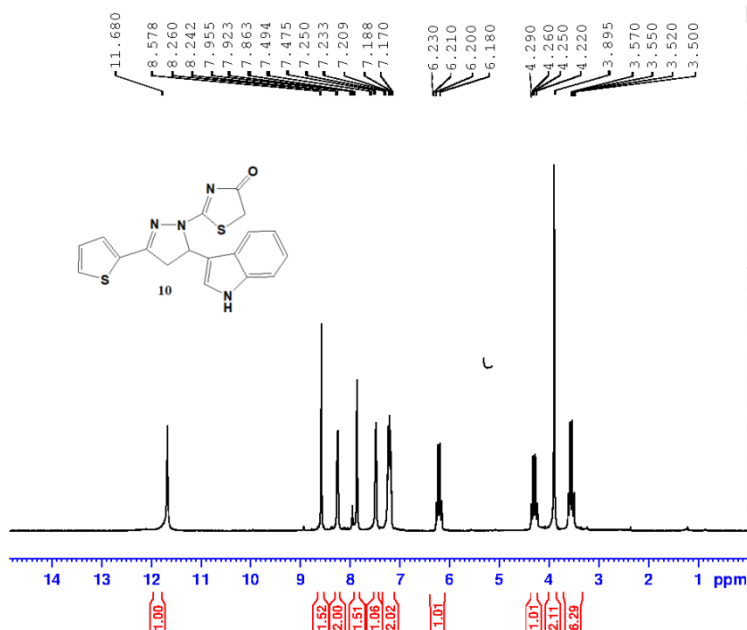DE   6.50 usec
TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
SSB   0
LB   1.00 Hz
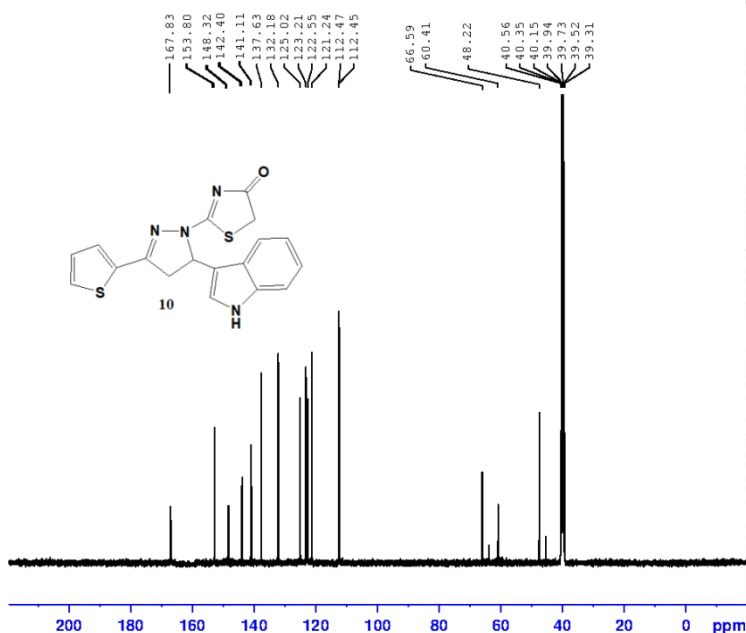GB   0
PC   1.40

AHMED ABDO-9
PROTON_BSU DMSO {C:\data} abeer 14

AHMED ABDO-9
C13-BSU DMSO {C:\data} abeer 14

AHMED ABDO-10
C13-BSU DMSO {C:\data} abeer 19

AHMED ABDO-11
PROTON_BSU DMSO {C:\data} abeer 21

11.701
9.001
8.157
7.857
7.846
7.834
7.814
7.767
7.734
7.407
7.376
7.365
7.238
7.230
7.224
7.218
7.210
7.148
7.140
7.131
6.180
6.155
6.150
6.125
4.235
4.205
4.195
4.165
3.980
3.955
3.935
3.910
3.521

BRUKER

Current Data Parameters
NAME   Nov23-2023-abeer
EXPNO   50
PROCNO   1

F2 - Acquisition Parameters
Date_   20231123
Time   16.43
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   65536
SOLVENT   DMSO
NS   16
DS   2
SWH   8012.820 Hz
FIDRES   0.122266 Hz
AQ   4.0894465 sec
RG   56.51
DW   62.400 usec
DE   6.50 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   400.1324710 MHz
NUC1   1H
P1   10.00 usec
PLW1   16.00000000 W

F2 - Processing parameters
SI   65536
SF   400.1300000 MHz
WDW   EM
SSB   0
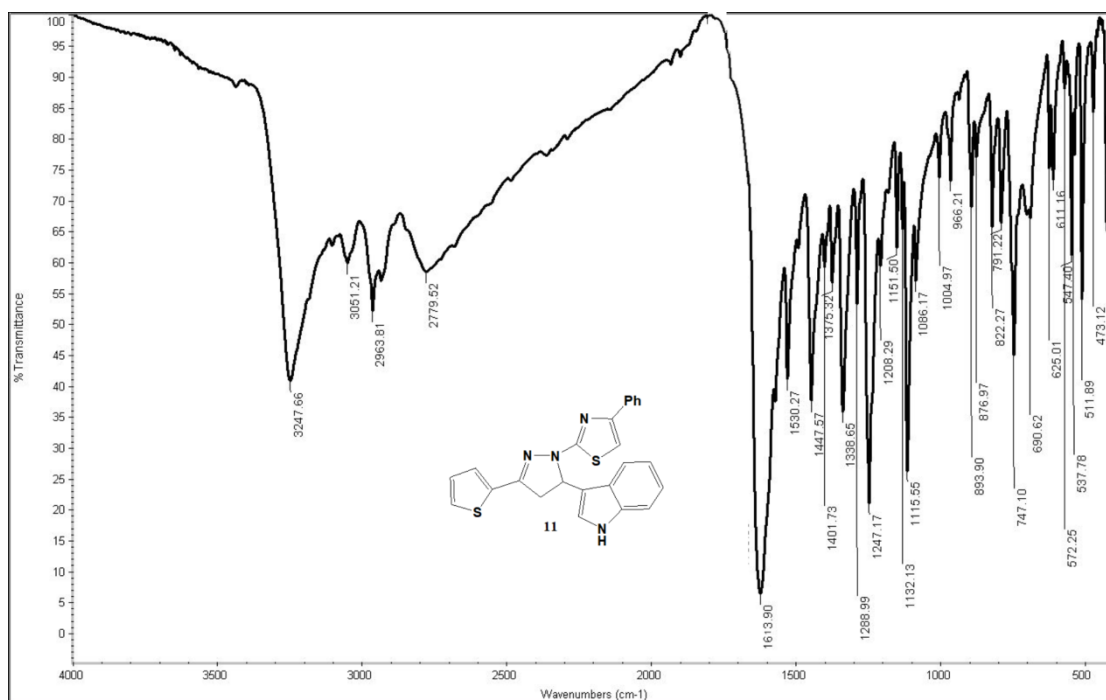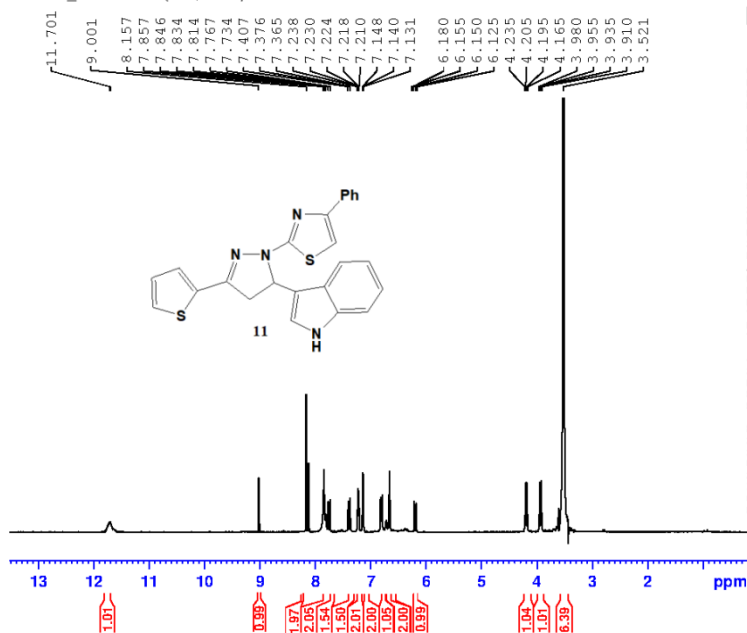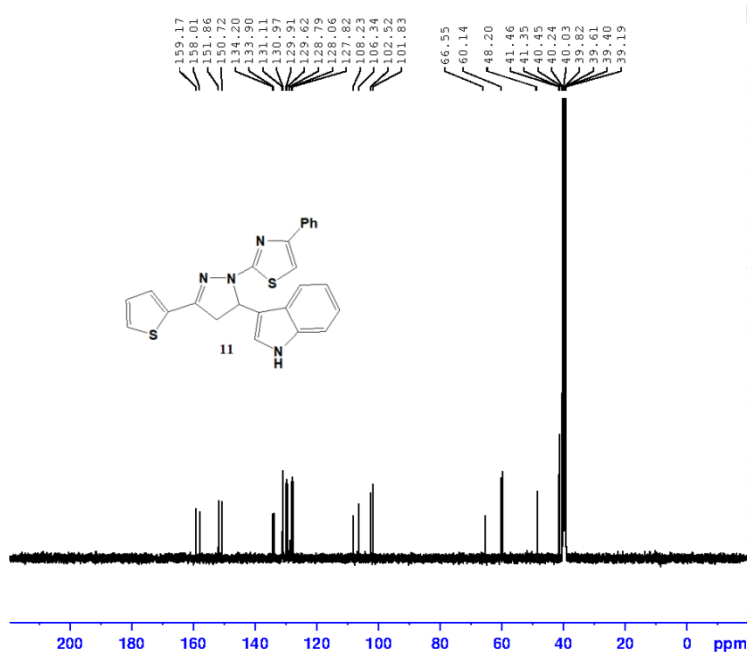LB   0.10 Hz
GB   0
PC   1.00

13 12 11 10 9 8 7 6 5 4 3 2 ppm

1.01 | 0.99 | 1.97 2.05 1.54 1.50 2.01 2.00 1.05 2.00 0.99 | 1.04 1.01 6.39

AHMED ABDO-11
C13-BSU DMSO {C:\data} abeer 21

159.17
158.01
151.86
150.72
134.20
133.90
131.11
130.97
129.91
129.62
128.06
127.82
108.23
106.34
102.52
101.83

66.55
60.14
48.20
41.46
41.35
40.45
40.24
40.03
39.82
39.61
39.40
39.19

BRUKER

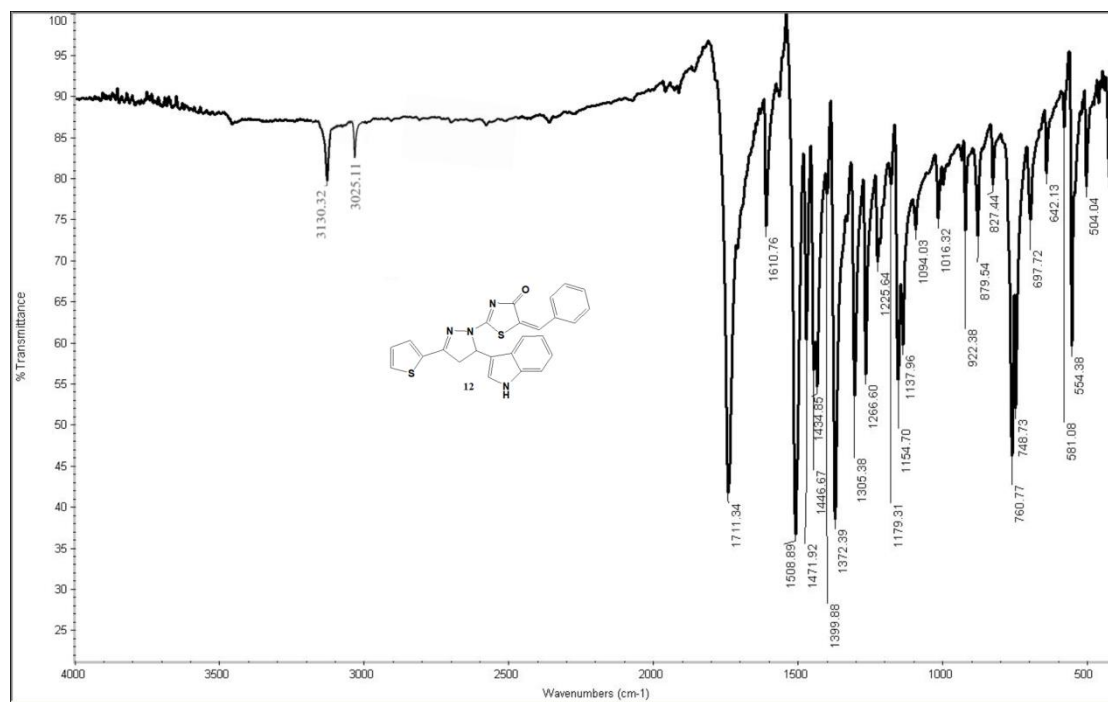Current Data Parameters
NAME   Nov23-2023-abeer
EXPNO   51
PROCNO   1

F2 - Acquisition Parameters
Date_   20231123
Time   20.33
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.444
DW   20.800 usec
DE   6.50 usec
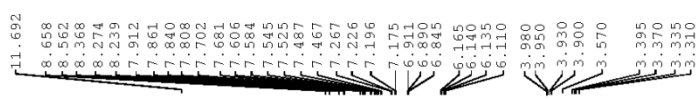TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
SSB   0
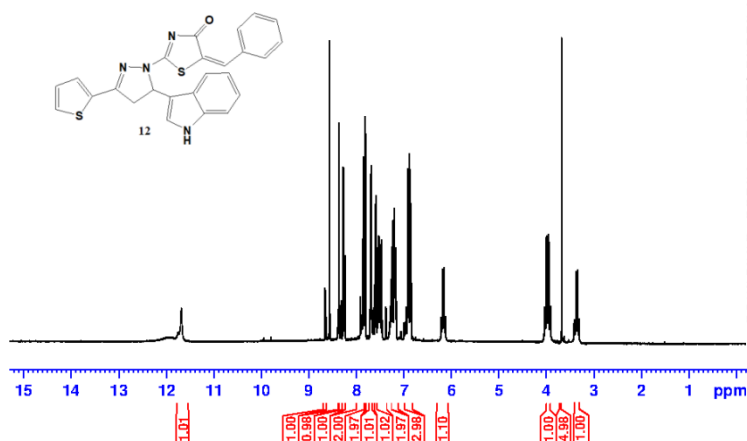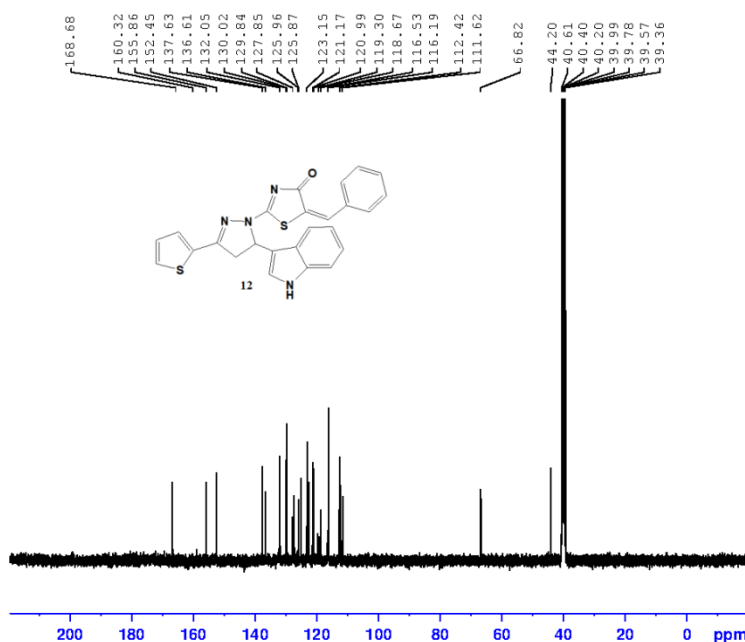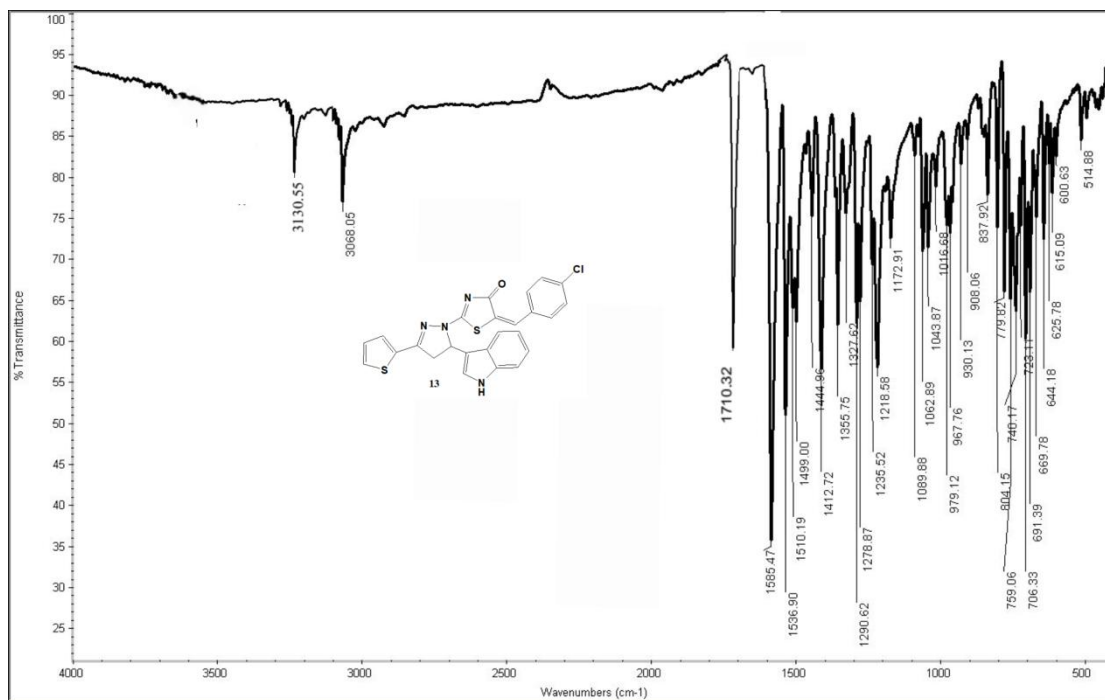LB   1.00 Hz
GB   0
PC   1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

AHMED ABDO-12
PROTON_BSU DMSO {C:\data} abeer 13

AHMED ABDO-14
PROTON_BSU DMSO {C:\data} abeer 13

AHMED ABDO-15
PROTON_BSU DMSO {C:\data} abeer 17

12.483

8.563
8.550
7.949
7.931
7.585
7.566
7.320
7.305
7.303
7.286
7.282
7.260
7.244
5.563
5.533
5.530
5.500
4.251
3.881
3.848
3.843
3.810
3.612
3.519
3.511
3.200
3.170
3.130

15

H_A H_B H_z

BRUKER

Current Data Parameters
NAME   Nov15-2023-abeer
EXPNO   50
PROCNO   1

F2 - Acquisition Parameters
Date_   20231115
Time   23.57
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zg30
TD   65536
SOLVENT   DMSO
NS   16
DS   2
SWH   8012.820 Hz
FIDRES   0.122266 Hz
AQ   4.0894465 sec
RG   74.78
DW   62.400 usec
DE   6.50 usec
TE   300.0 K
D1   1.00000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   400.1324710 MHz
NUC1   1H
P1   10.00 usec
PLW1   16.00000000 W

F2 - Processing parameters
SI   65536
SF   400.1300000 MHz
WDW   EM
SSB   0
LB   0.10 Hz
GB   0
PC   1.00

13 12 11 10 9 8 7 6 5 4 3 2 1 ppm

1.00   2.01 1.53 1.53 1.54 3.50 2.02   1.00   1.02 1.03 3.07 1.01

AHMED ABDO-15
C13-BSU DMSO {C:\data} abeer 14

158.00
155.94
155.22
153.31
150.45
145.52
137.52
133.66
132.87
125.38
123.11
122.04
121.68
120.99
118.40
116.22

68.66
60.21

46.28

40.61
40.40
40.19
39.98
39.78
39.57
39.36
18.50

15

H_A H_B H_z

BRUKER

Current Data Parameters
NAME   Nov22-2023-abeer
EXPNO   41
PROCNO   1

F2 - Acquisition Parameters
Date_   20231123
Time   1.23
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.444
DW   20.800 usec
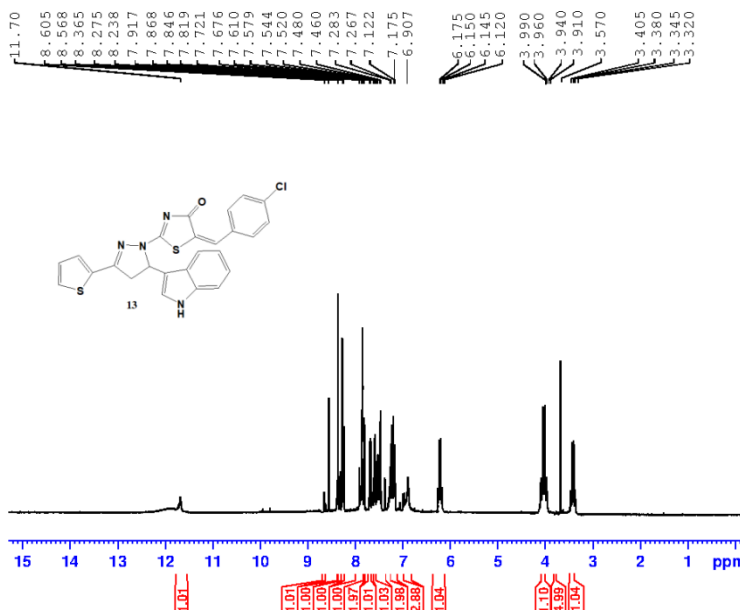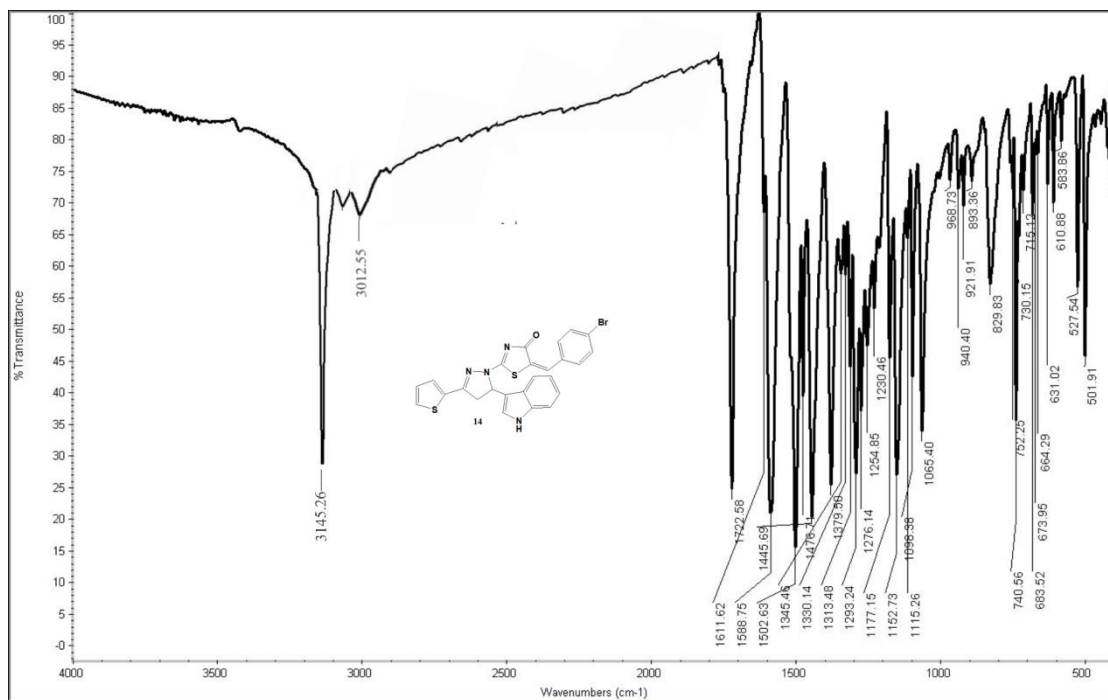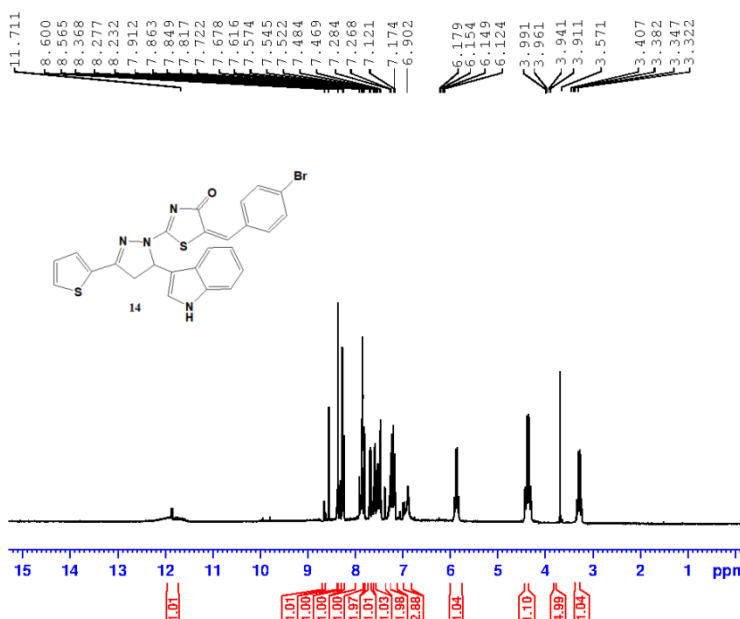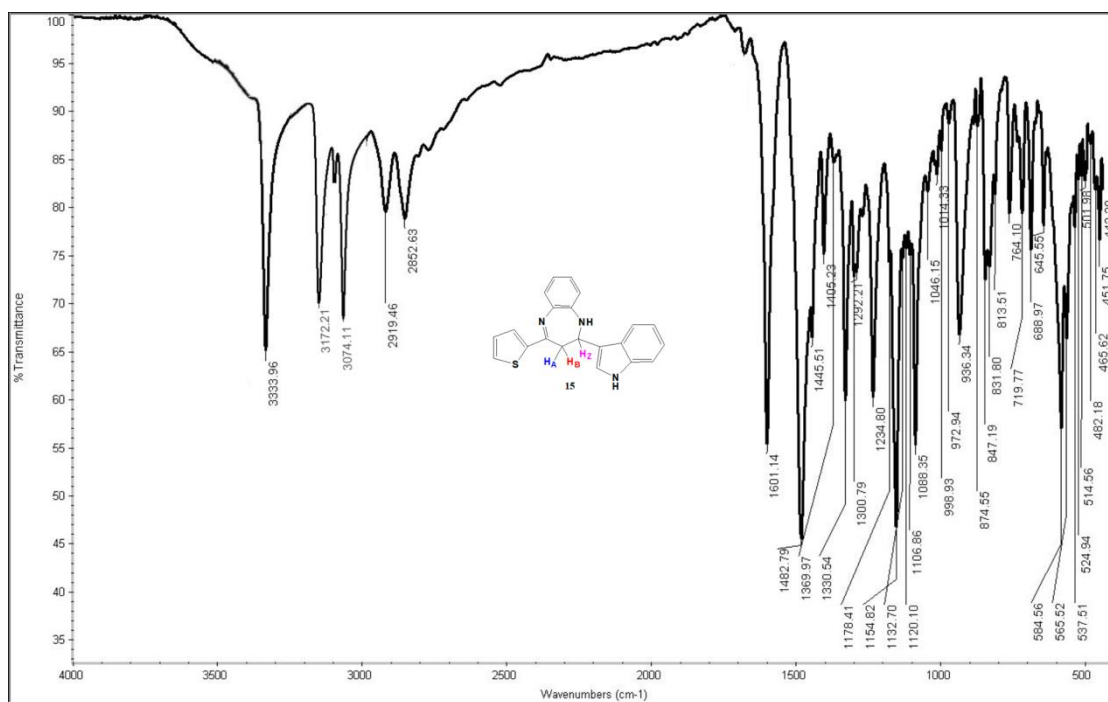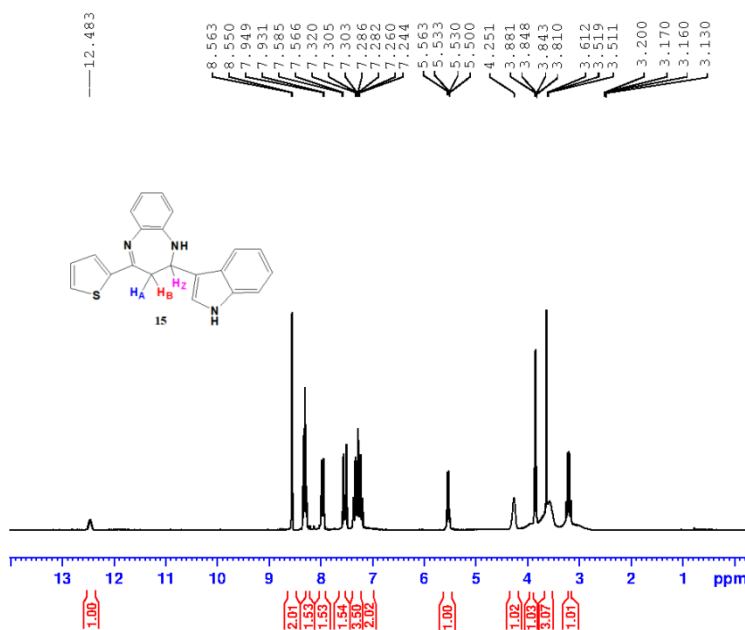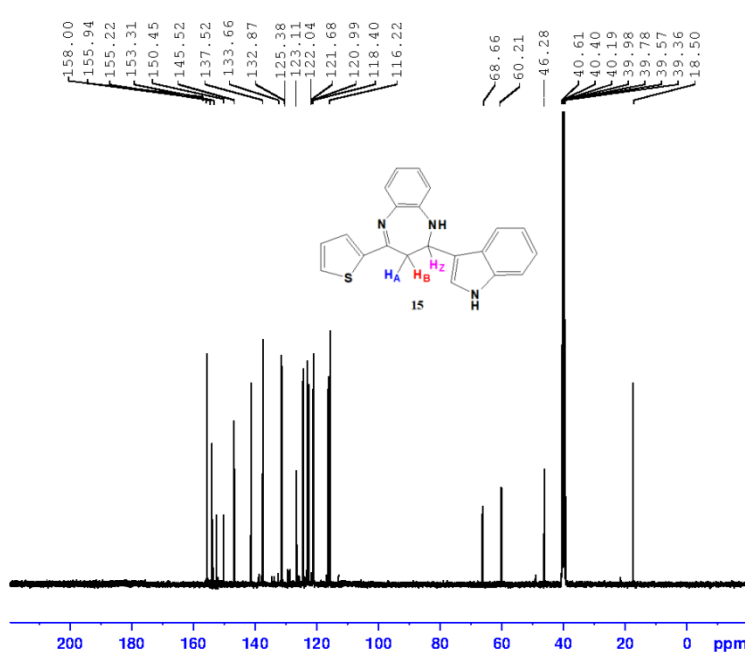DE   6.50 usec
TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
PC   1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

AHMED ABDO-8
C13-BSU DMSO {C:\data} abeer 14

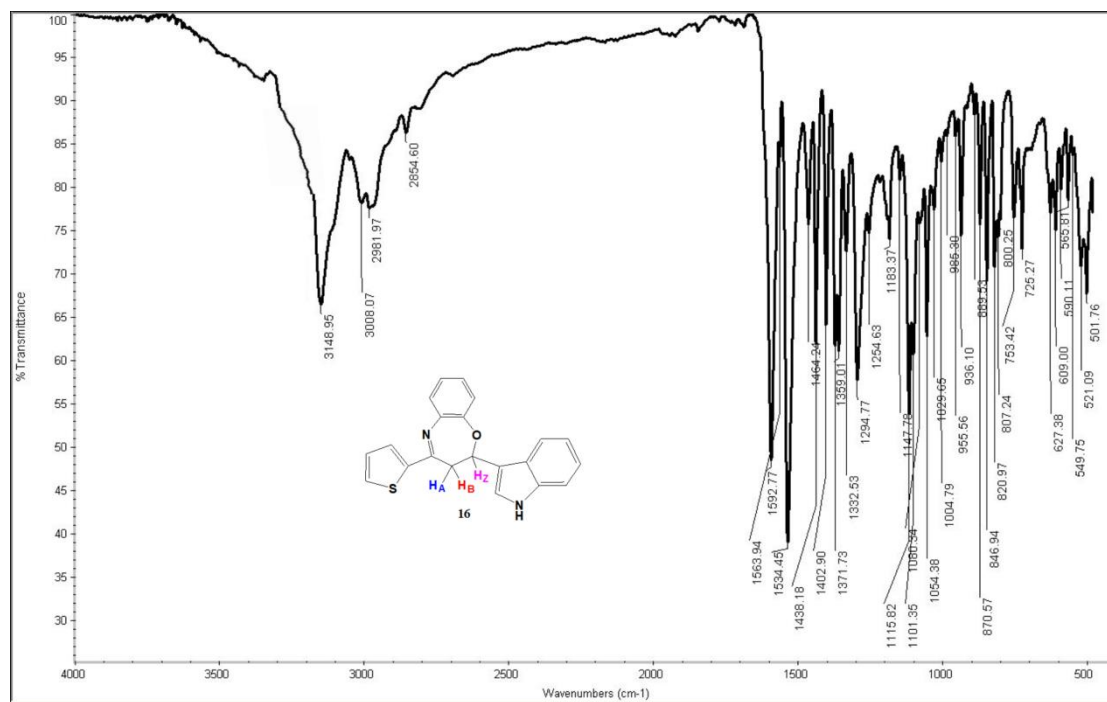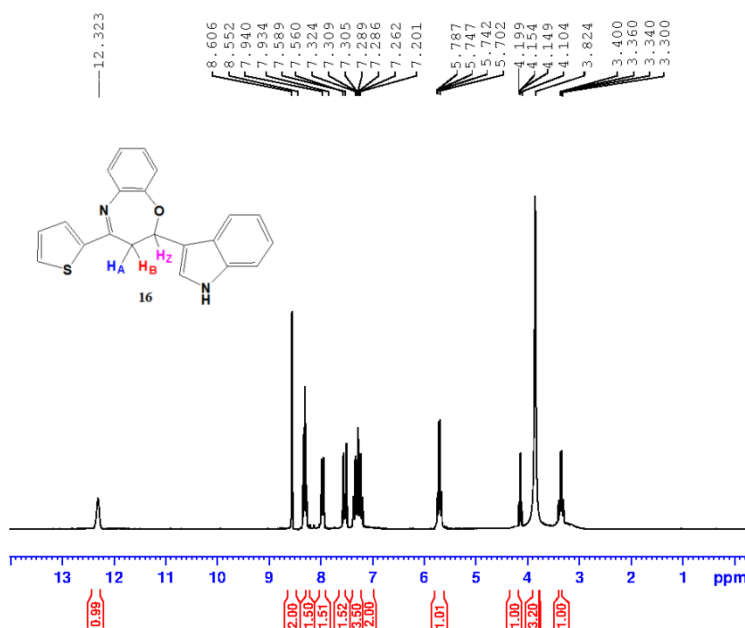Current Data Parameters
NAME   Nov23-2023-abeer
EXPNO   41
PROCNO   1

F2 - Acquisition Parameters
Date_   20231124
Time   1.33
INSTRUM   spect
PROBHD   5 mm PABBO BB/
PULPROG   zgpg30
TD   65536
SOLVENT   DMSO
NS   4000
DS   4
SWH   24038.461 Hz
FIDRES   0.366798 Hz
AQ   1.3631488 sec
RG   205.44
DW   20.800 usec
DE   6.50 usec
TE   300.0 K
D1   2.00000000 sec
D11   0.03000000 sec
TD0   1

-------- CHANNEL f1 --------
SFO1   100.6228293 MHz
NUC1   13C
P1   10.00 usec
PLW1   66.00000000 W

-------- CHANNEL f2 --------
SFO2   400.1316005 MHz
NUC2   1H
CPDPRG[2   waltz16
PCPD2   90.00 usec
PLW2   16.00000000 W
PLW12   0.21777999 W
PLW13   0.17640001 W

F2 - Processing parameters
SI   131072
SF   100.6127690 MHz
WDW   EM
SSB   0
LB   1.00 Hz
GB   0
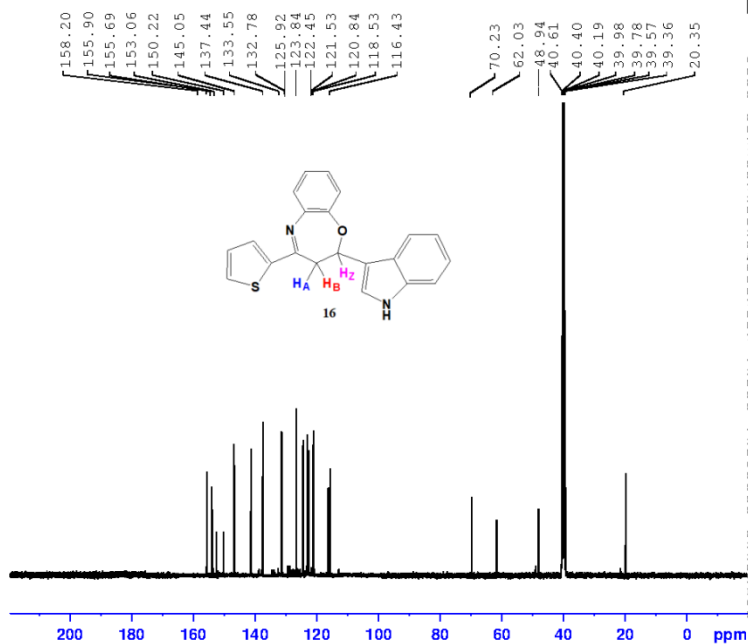PC   1.40