

Supporting information

***tert*-Butylphenylthiazoles with Oxadiazole Linker: A Novel Orally Bioavailable Class of Antibiotics Exhibiting Antibiofilm Activity**

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***In vitro* cytotoxicity analysis of compound 20 against fibroblast-like monkey kidney cells (Vero cells) and human colorectal adenocarcinoma (Caco-2)**

Method:

Compound **20** was assayed against a fibroblast-like monkey kidney cells (Vero cells) and human colorectal adenocarcinoma (Caco-2) (figure 1S & 2S) to determine its *in vitro* potential toxic effect, as described elsewhere [1, 2]. Briefly, Vero cells were cultured in Minimum Essential Medium (MEM) supplemented with 10% fetal bovine serum (FBS), 1 mM sodium pyruvate, and penicillin-streptomycin at 37 °C with CO₂ (5%). Caco-2 cells were cultured in Dulbecco's Modified Eagle Medium (DMEM) supplemented with 20% fetal bovine serum (FBS), non-essential amino acids (1X), penicillin-streptomycin at 37 °C with CO₂ (5%). Compound **20** and DMSO (in triplicates) were added to the cells. The cells were incubated with the compound at 37 °C with CO₂ (5%) for two hours. The assay reagent MTS 3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium) (Promega, Madison, WI, USA) was subsequently added and the plate was incubated for four hours. Absorbance readings (at OD₄₉₀) were measured using a kinetic microplate reader (Molecular Devices, Sunnyvale, CA, USA). The quantity of viable cells after treatment with the compound was expressed as a percentage of the viability relative to DMSO (average of triplicate wells ± standard deviation).

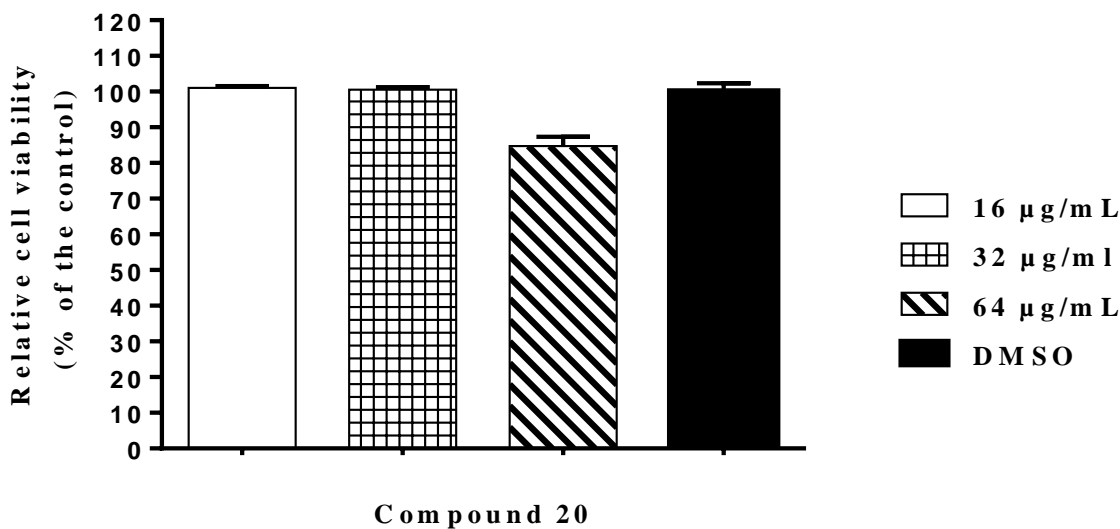


Figure 1S: *In vitro* cytotoxicity analysis of compound 20 against fibroblast-like monkey kidney cells (Vero cells) using the MTS 3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium) assay. Results are presented as percent viable mammalian cells (measured as average absorbance ratio relative to DMSO) which was used as a negative control to determine a baseline measurement for the cytotoxic impact of the compound. The absorbance values represent an average of a minimum of three samples analyzed for each compound. Error bars represent standard deviation values for the absorbance values.

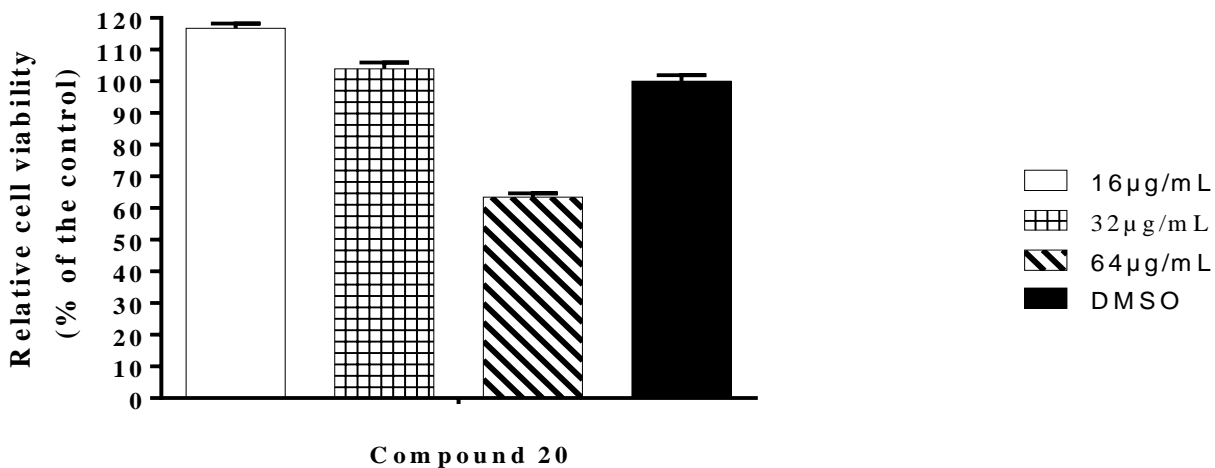


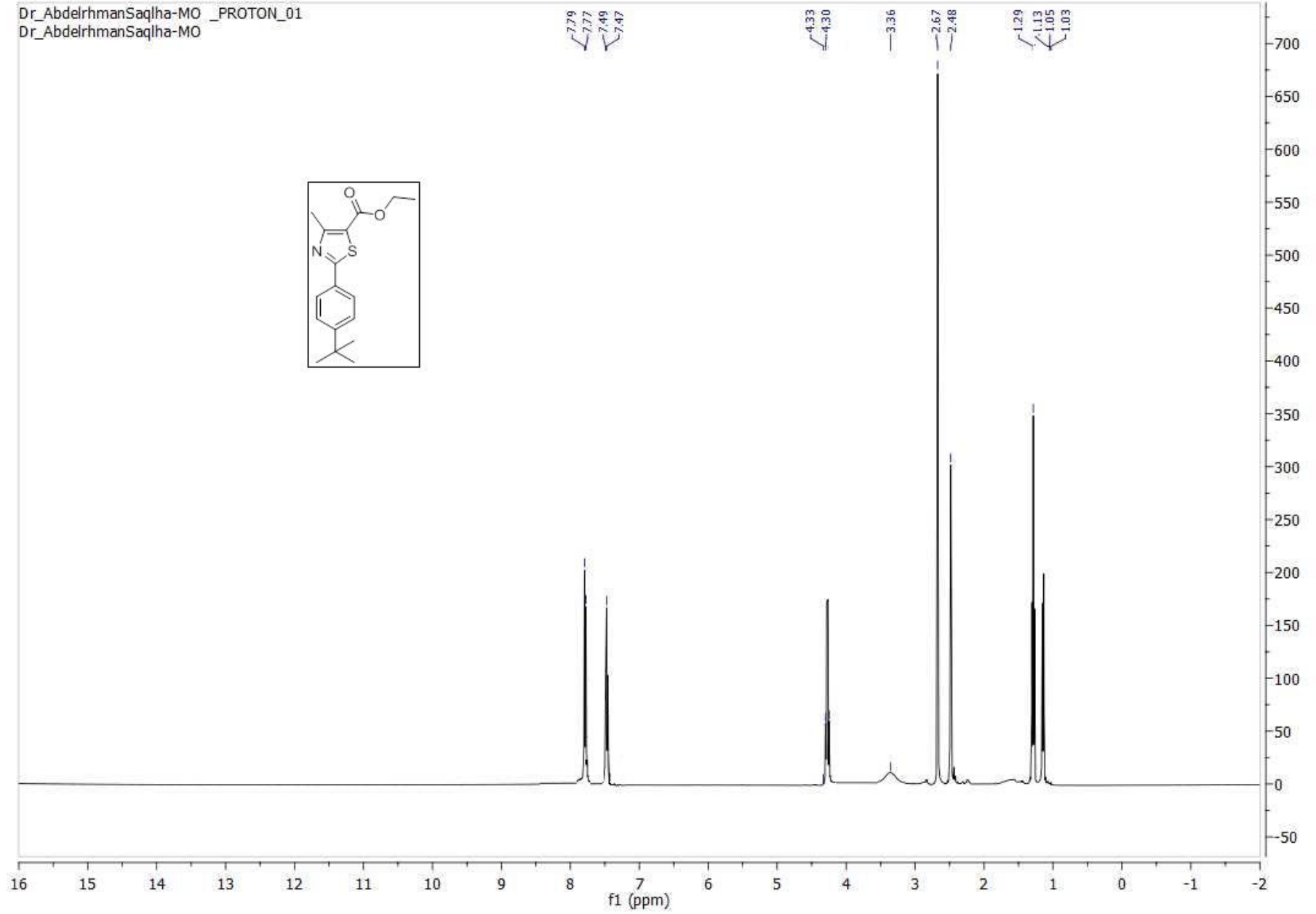
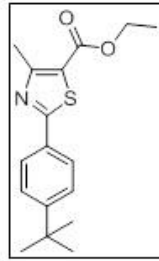
Figure 2S: *In vitro* cytotoxicity analysis of compound 20 against human colorectal adenocarcinoma (Caco-2) using the MTS 3-(4,5-dimethylthiazol-2-yl)-5-(3-

carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium) assay. Results are presented as percent viable mammalian cells (measured as average absorbance ratio relative to DMSO) which was used as a negative control to determine a baseline measurement for the cytotoxic impact of the compound. The absorbance values represent an average of a minimum of three samples analyzed for each compound. Error bars represent standard deviation values for the absorbance values.

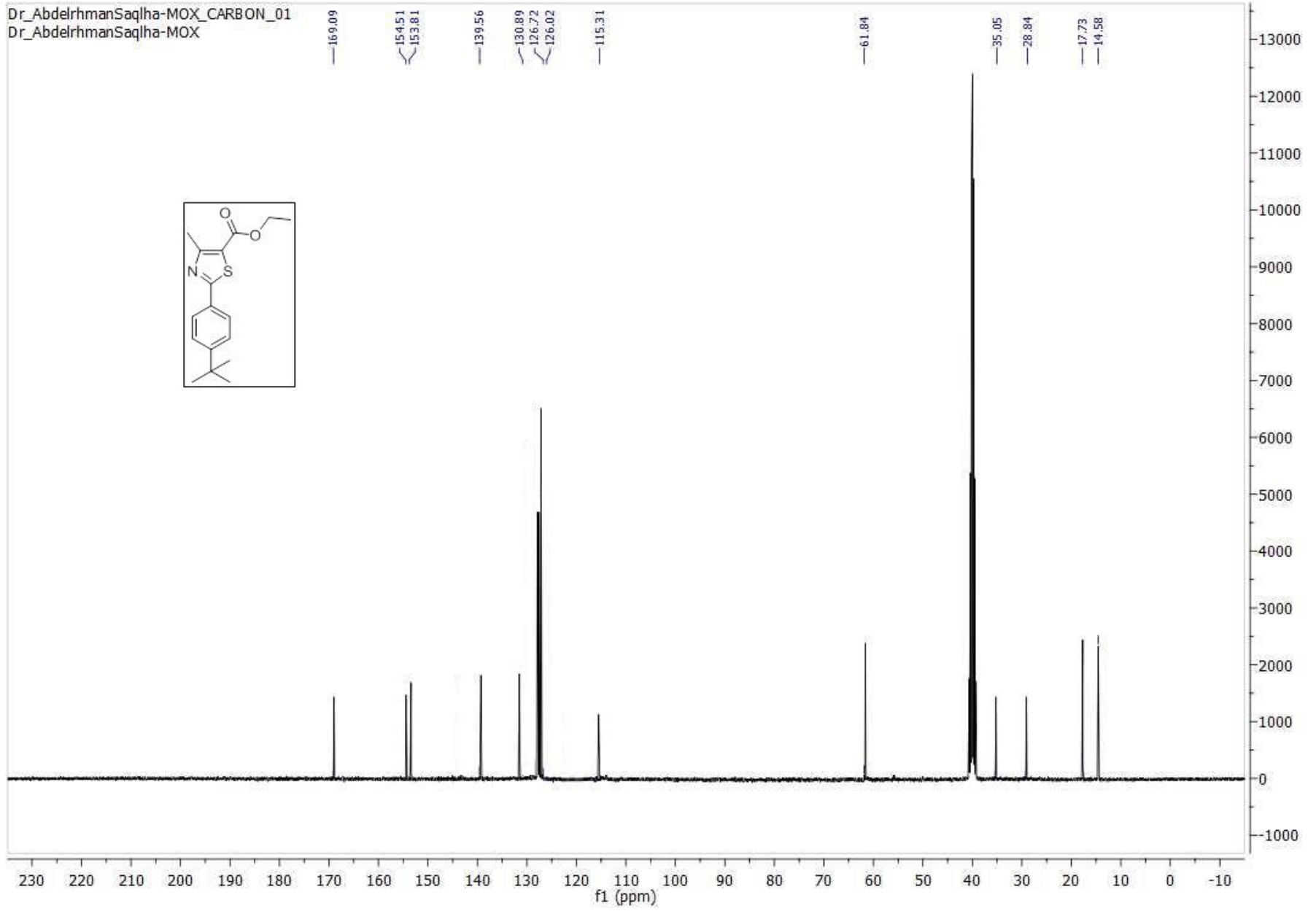
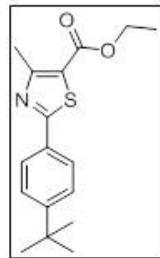
Results:

Compound **20** was highly tolerable to Vero cells and caco-2 cells at higher concentrations. Its 50% cytotoxic concentration (CC₅₀), the compound's concentration (µg/mL) required for the reduction of cell viability by 50%, is greater than 64 µg/mL at which about 85% and 65% of the cells were viable respectively.

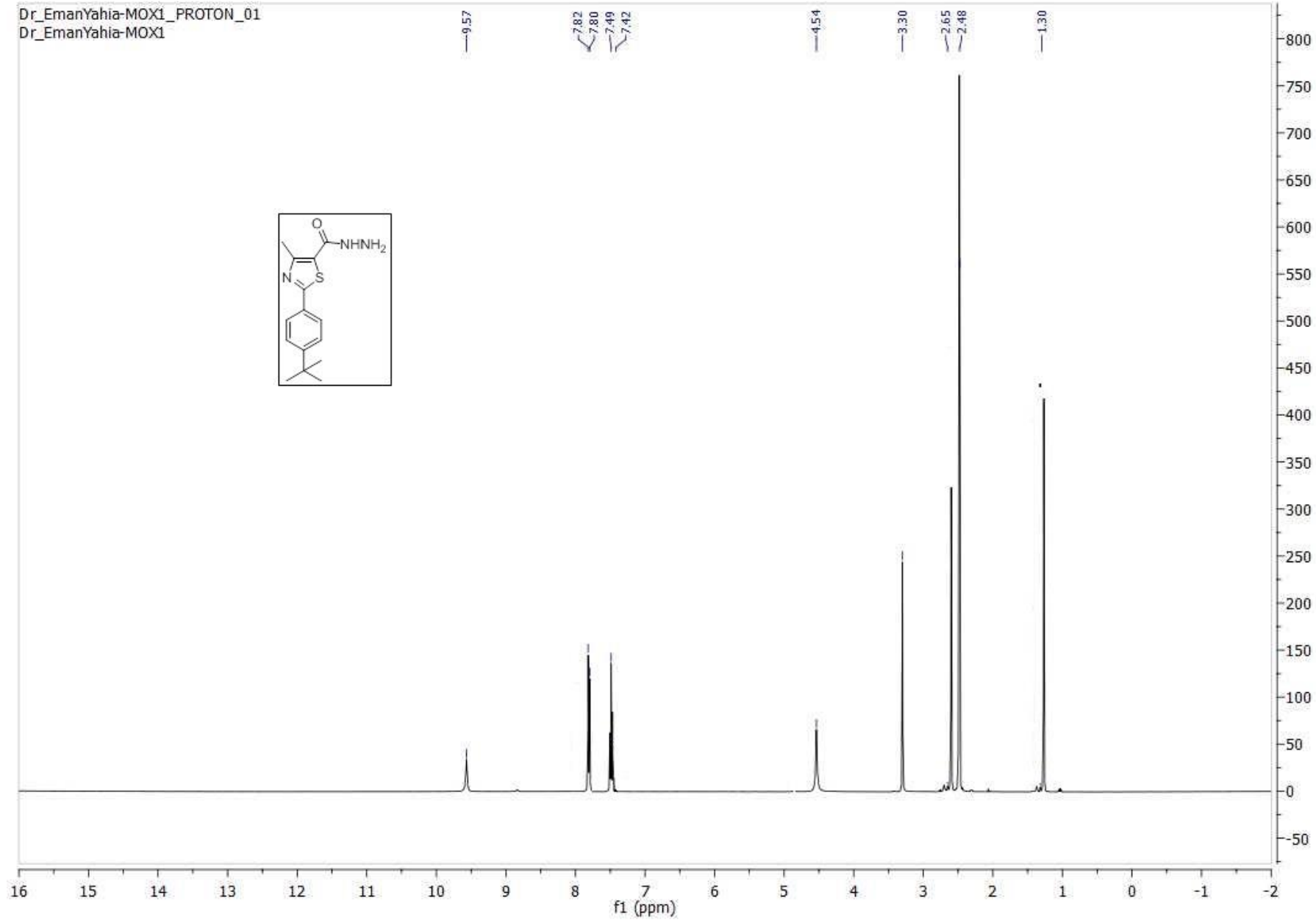
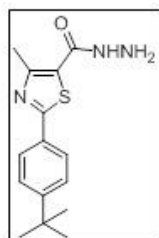
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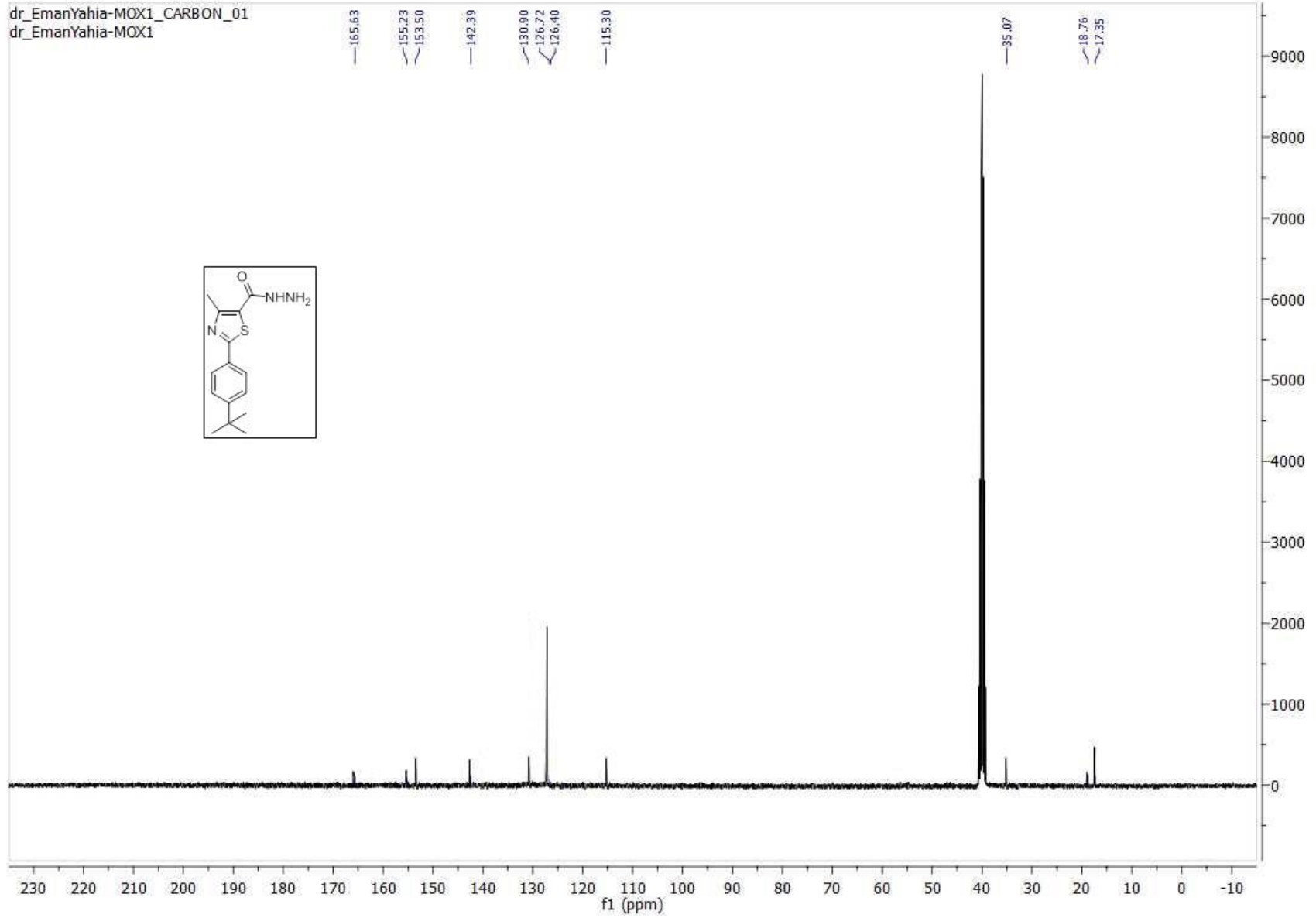
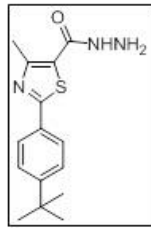
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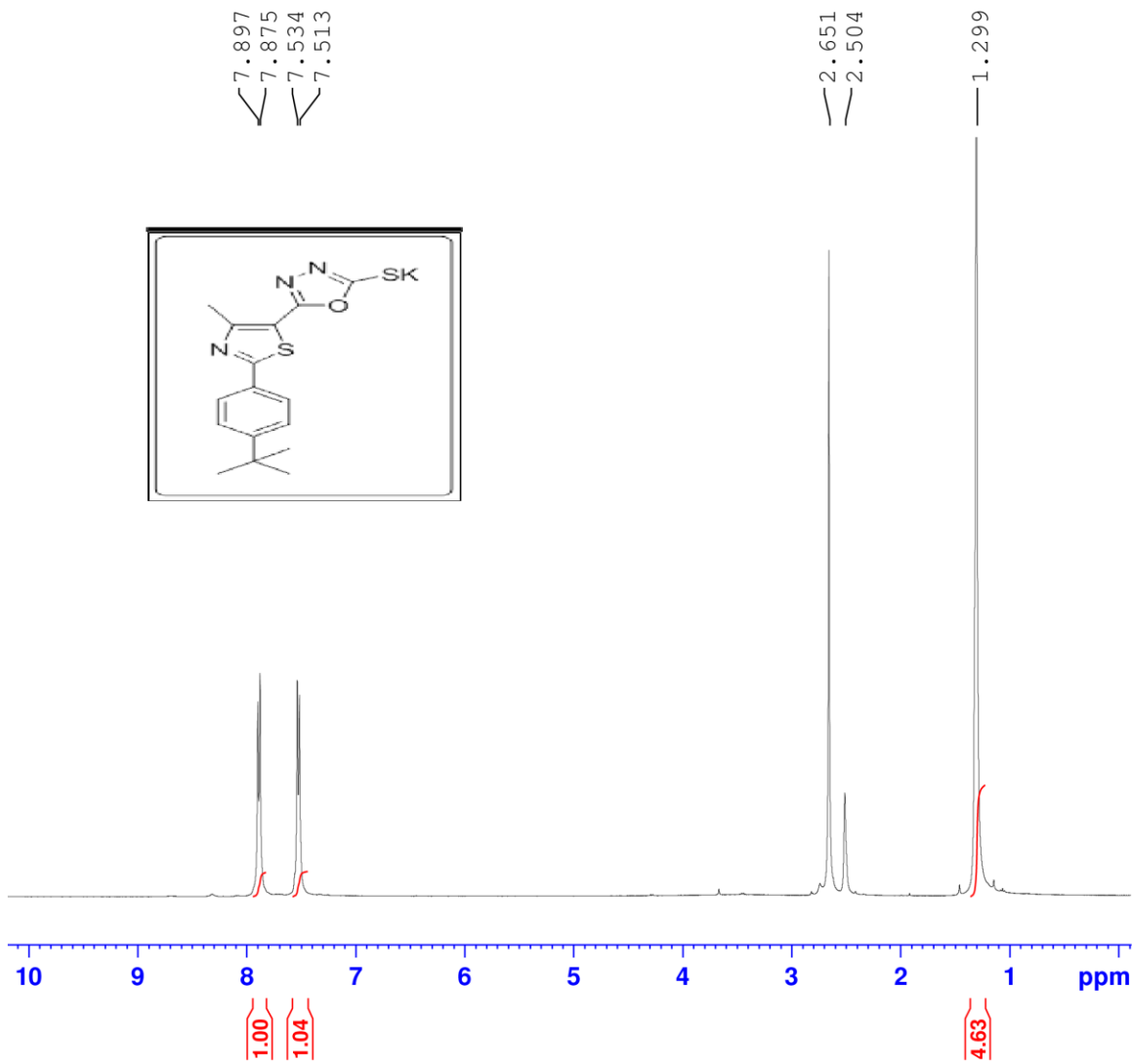


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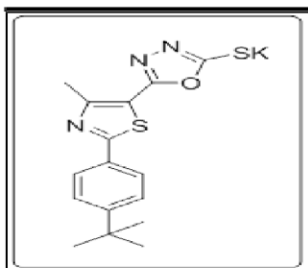
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg



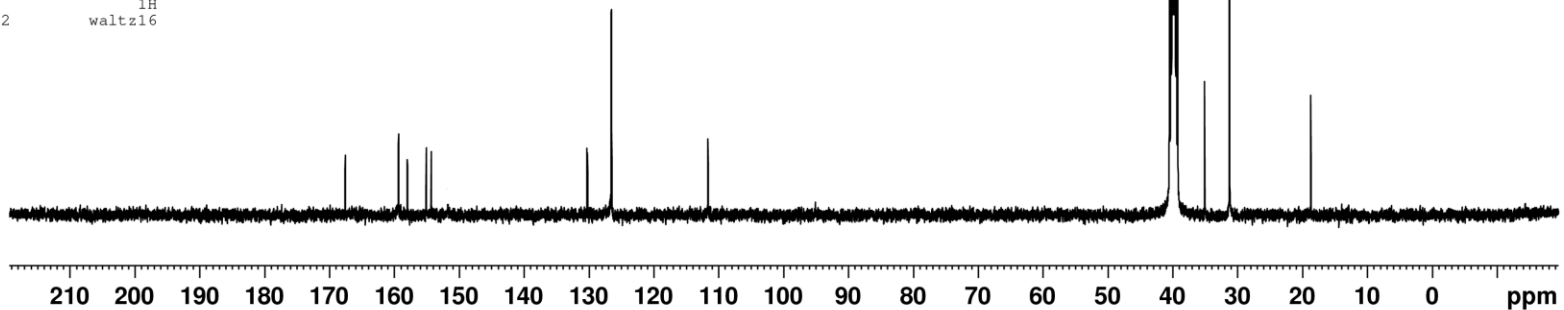
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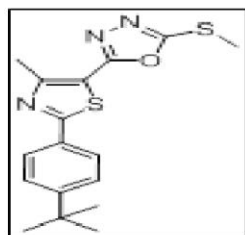
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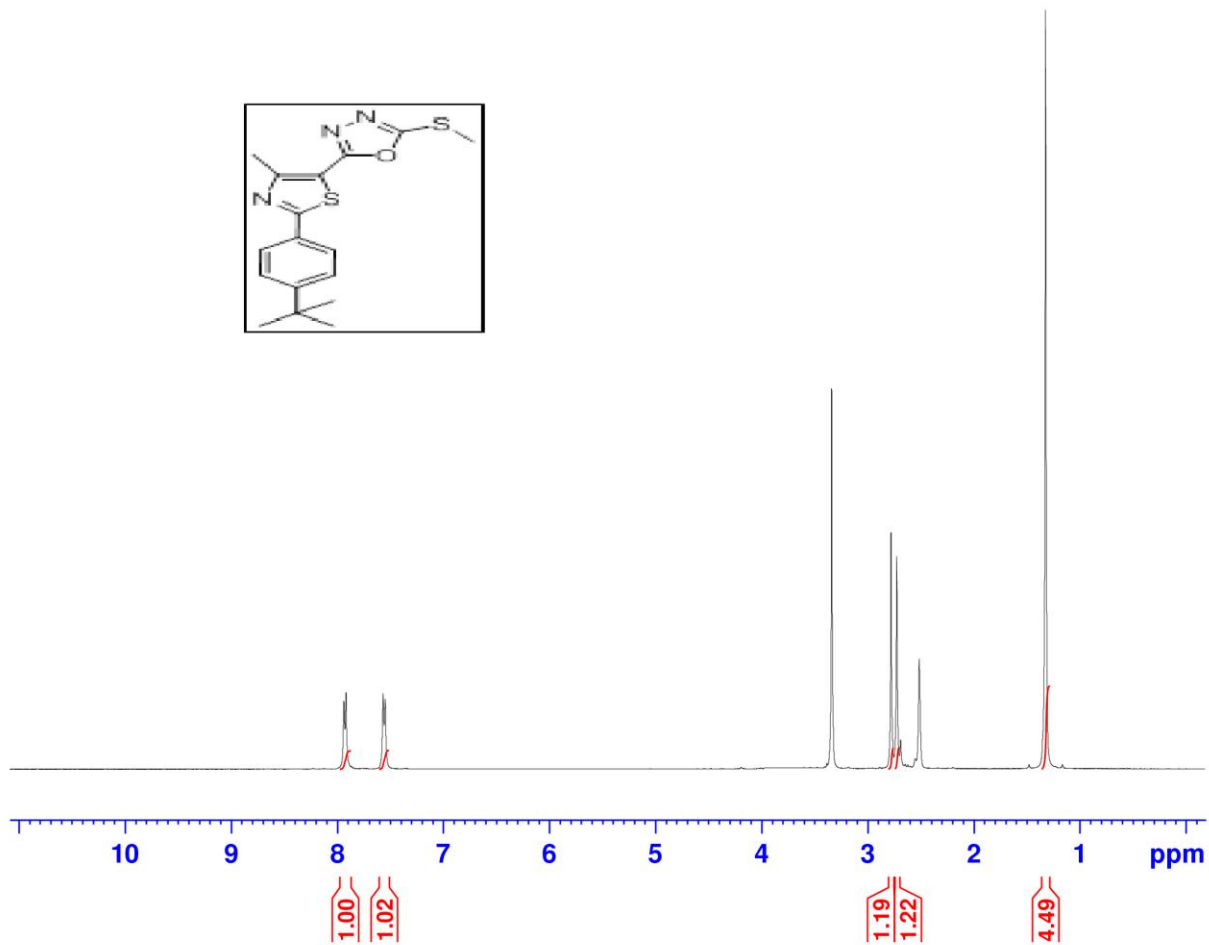


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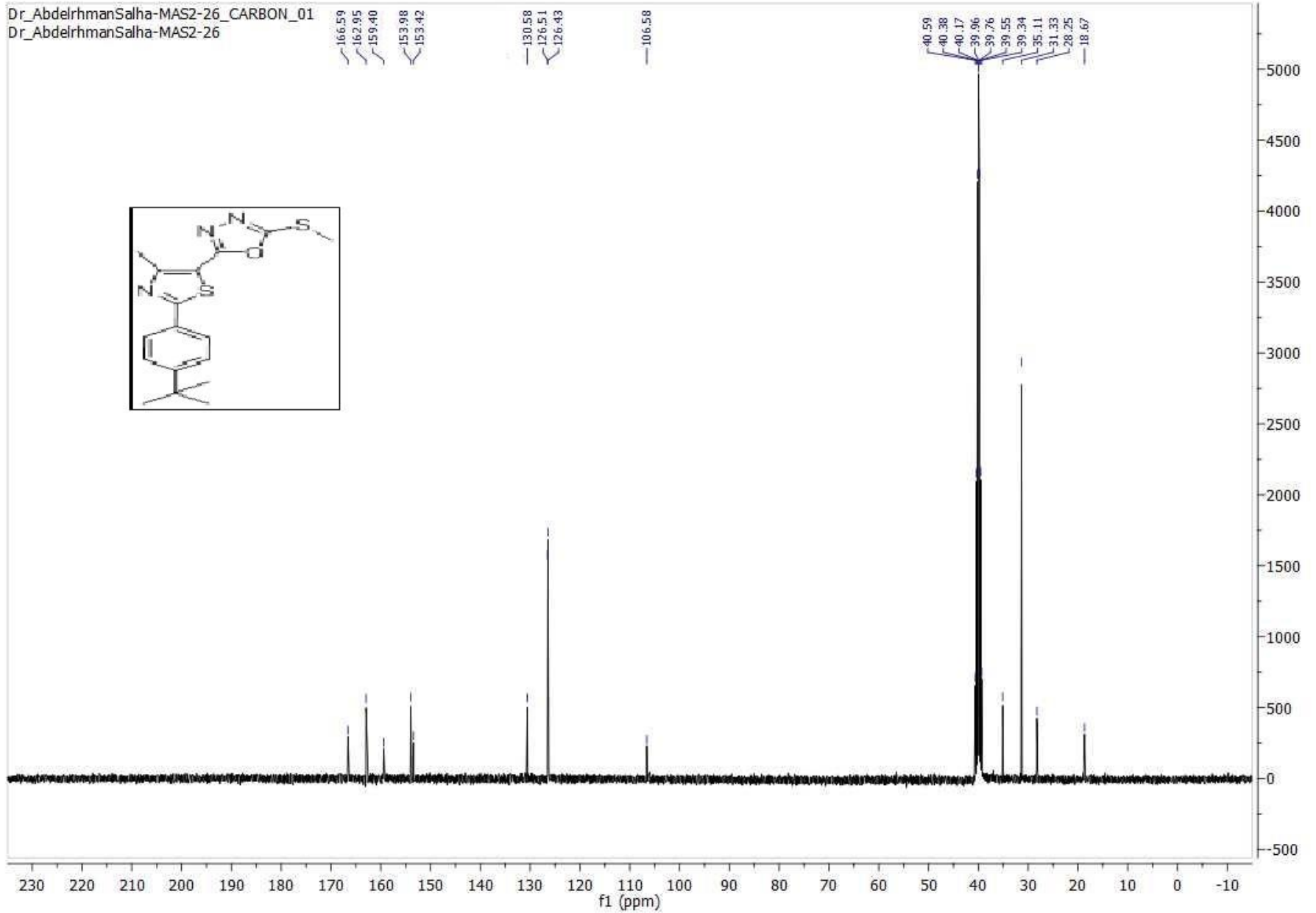
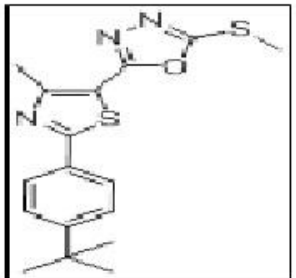
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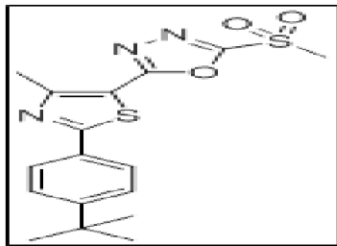
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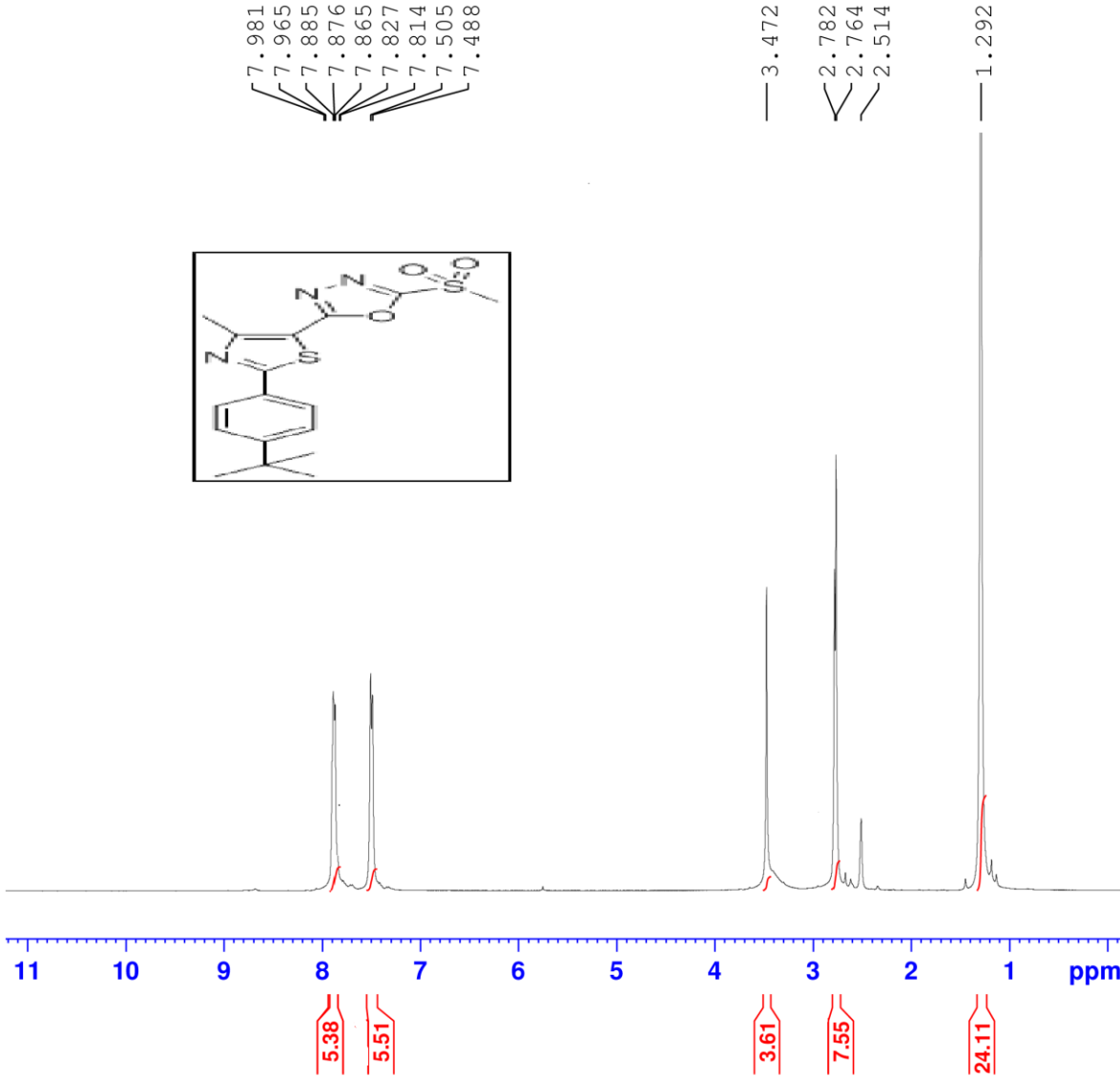




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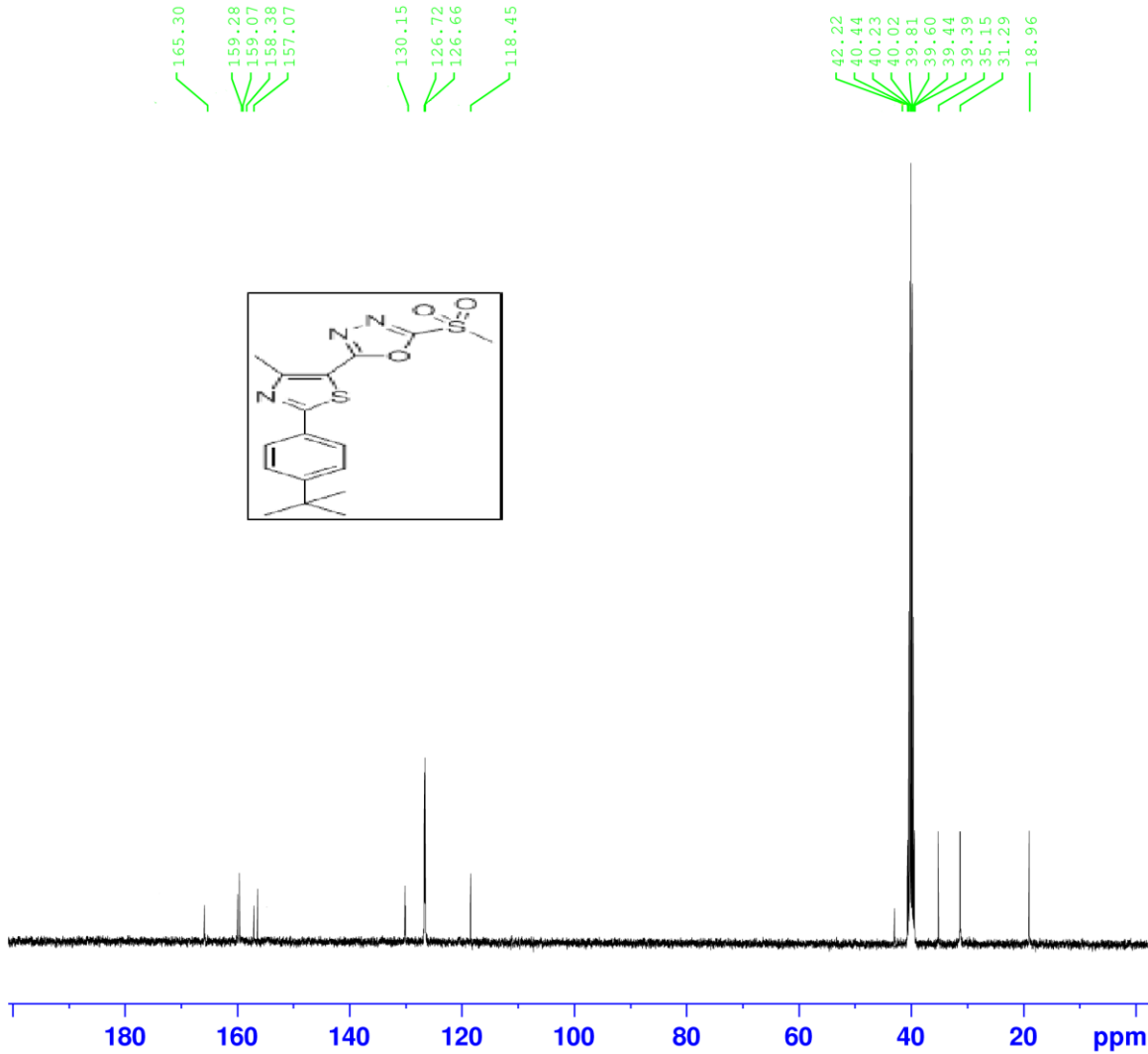
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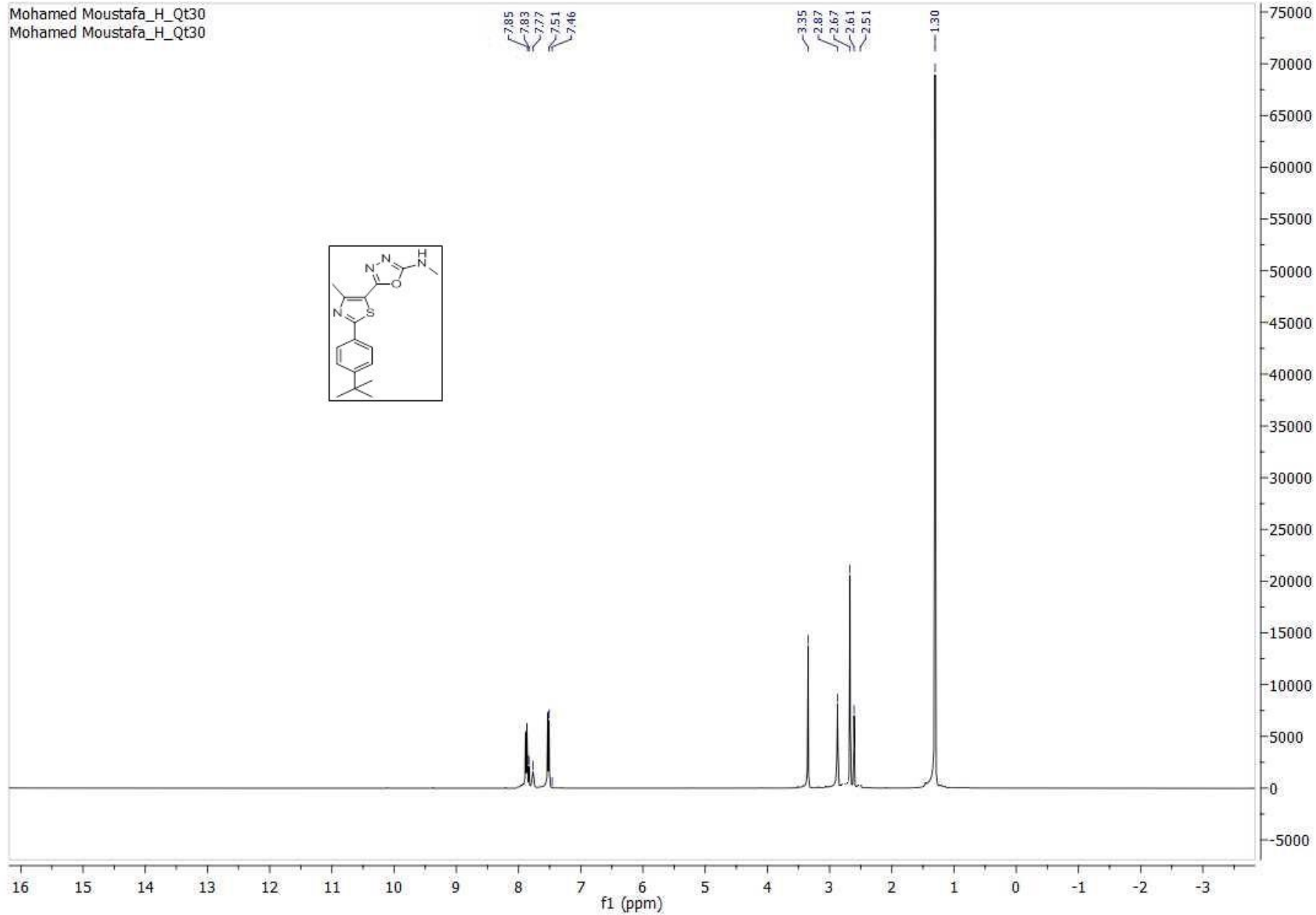
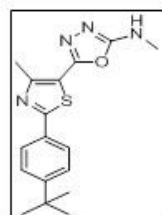
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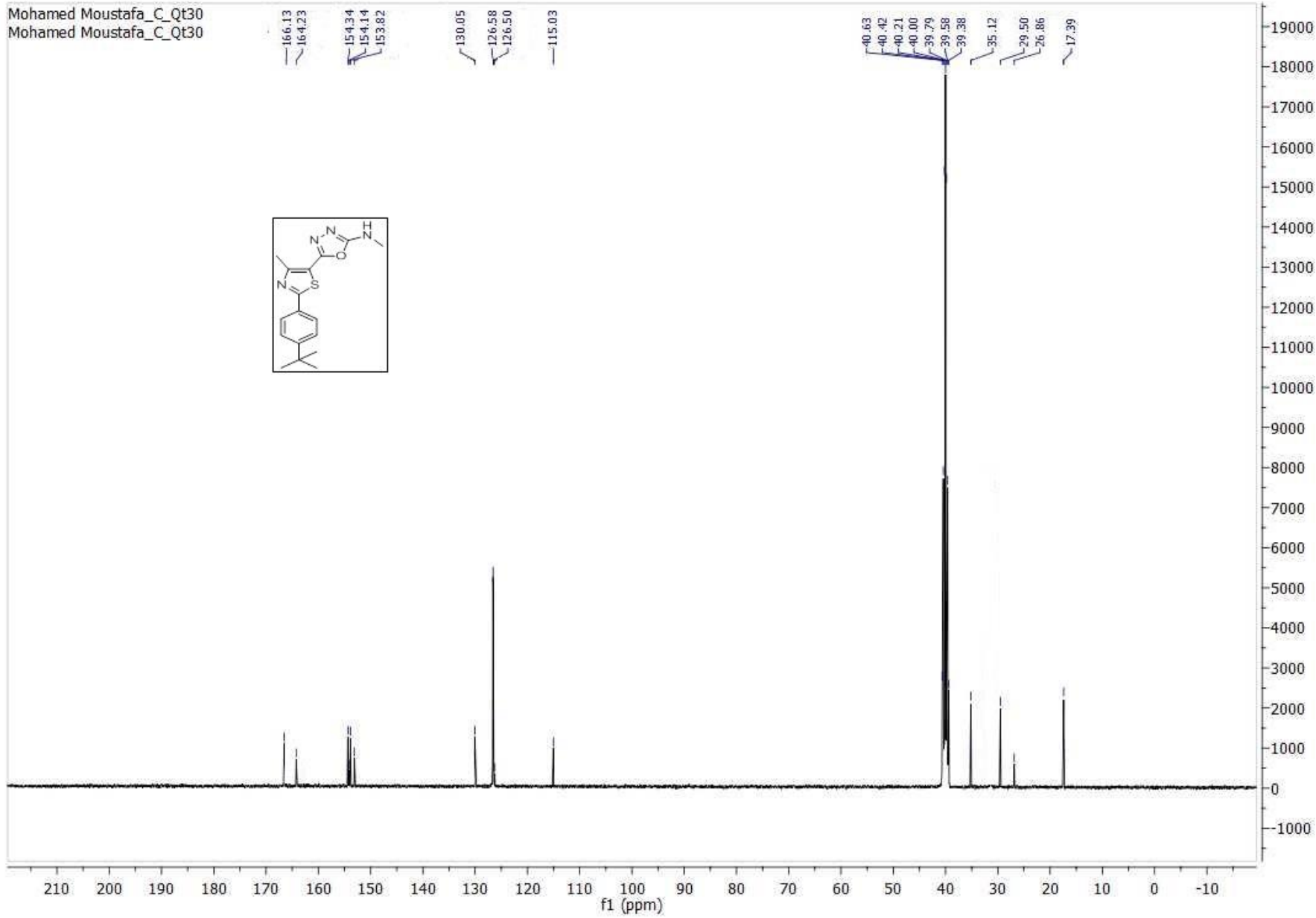
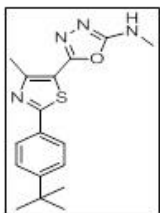


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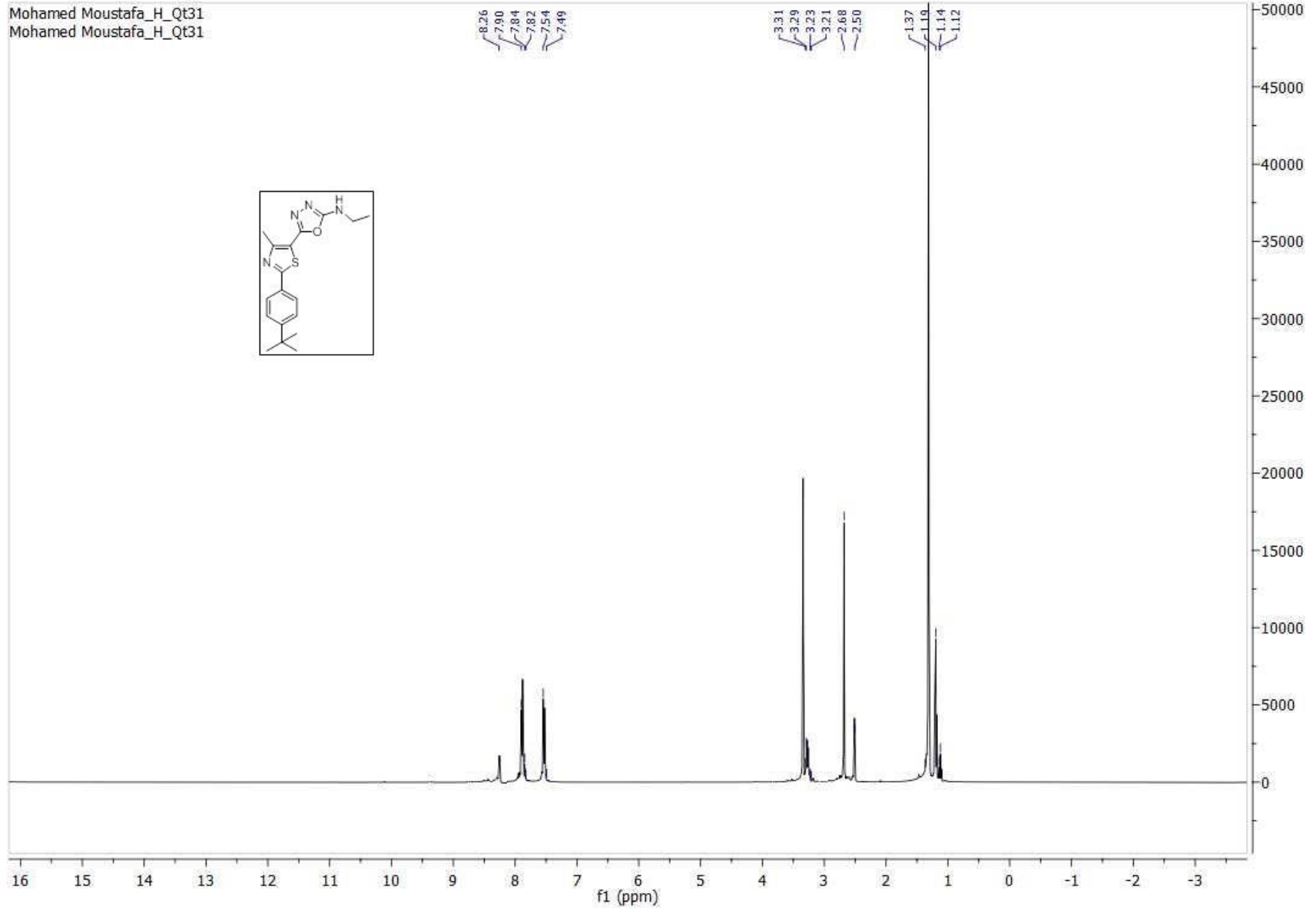
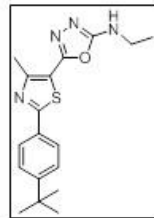
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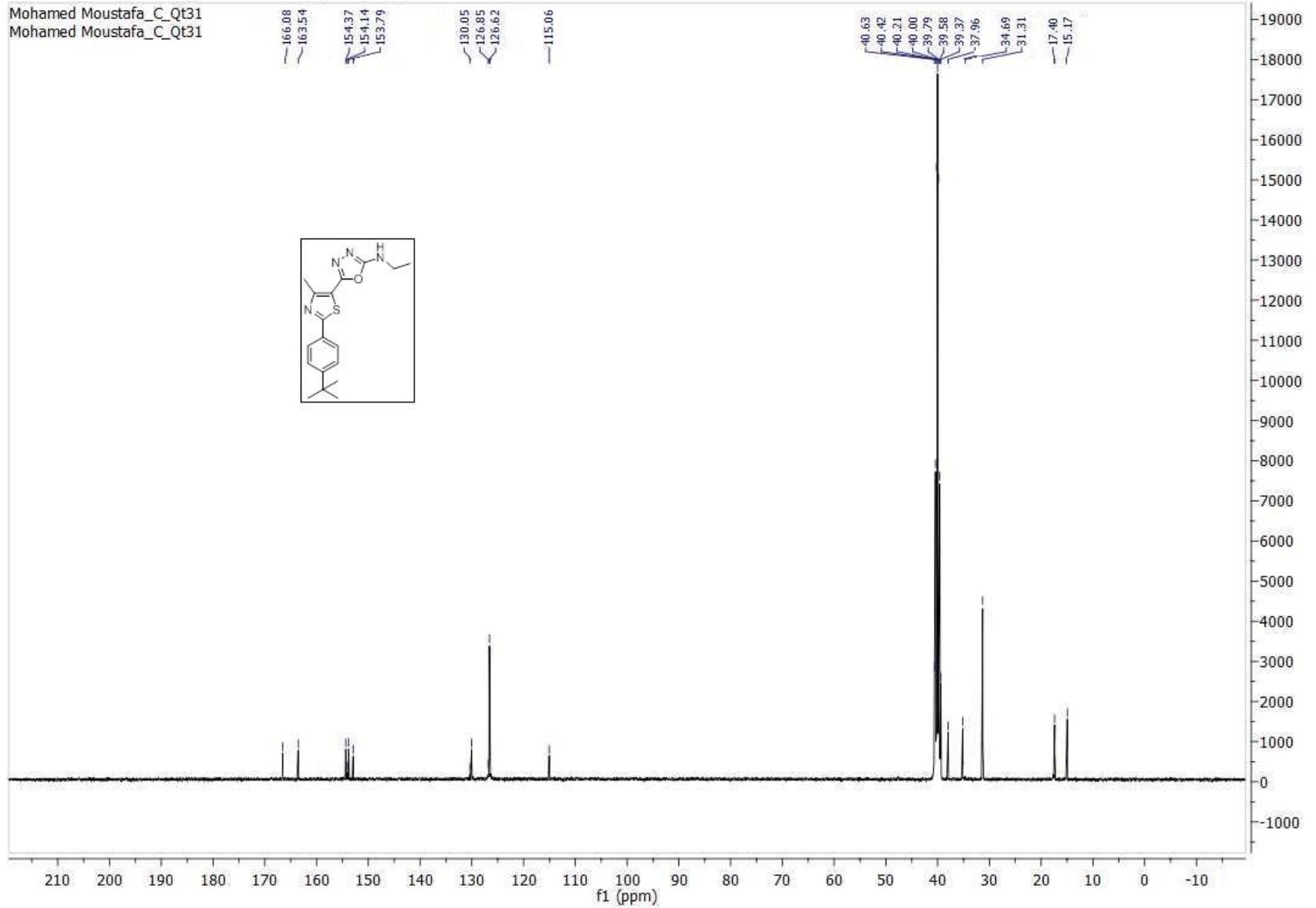
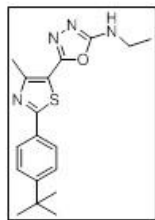
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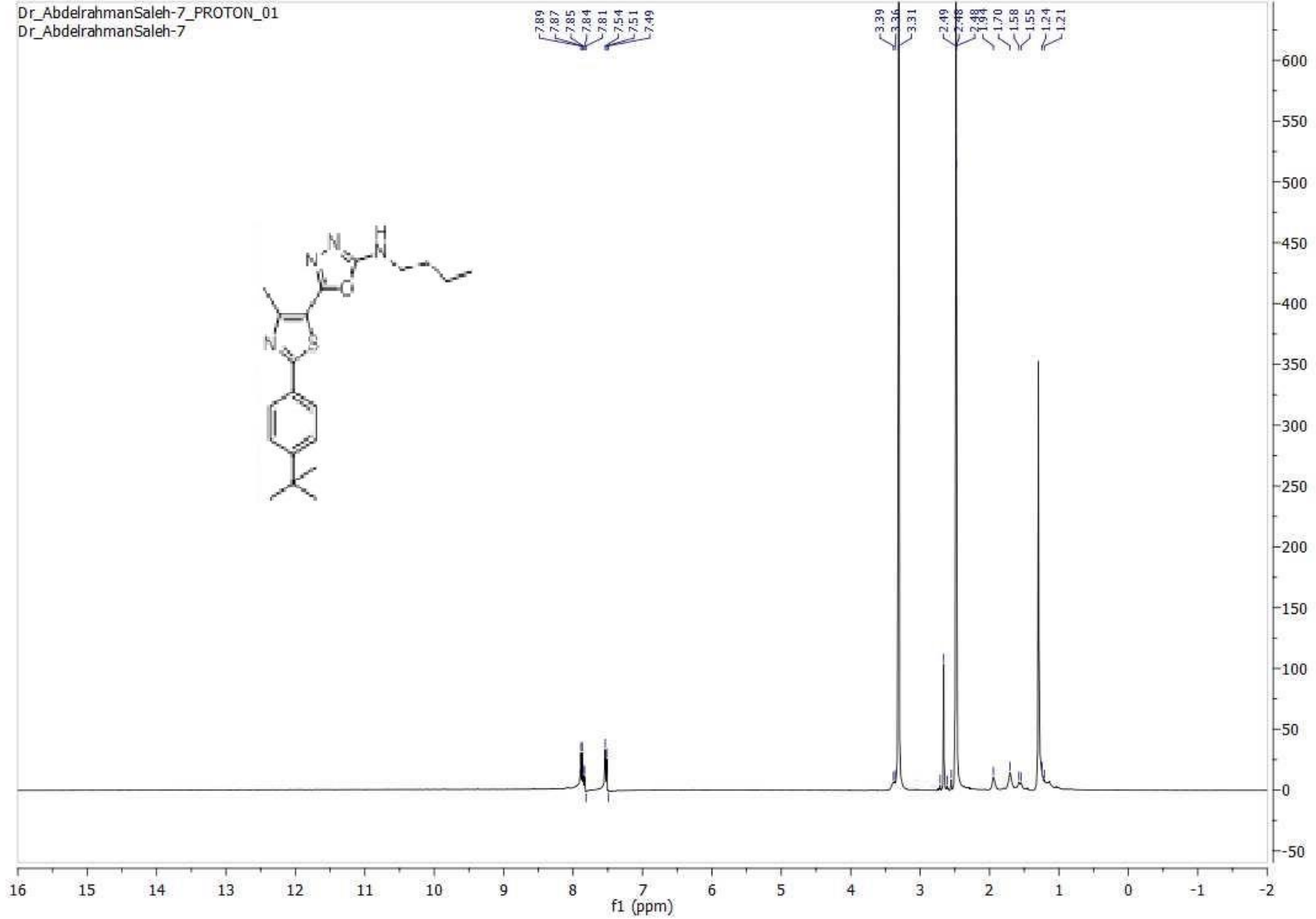
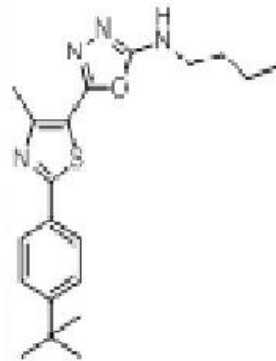
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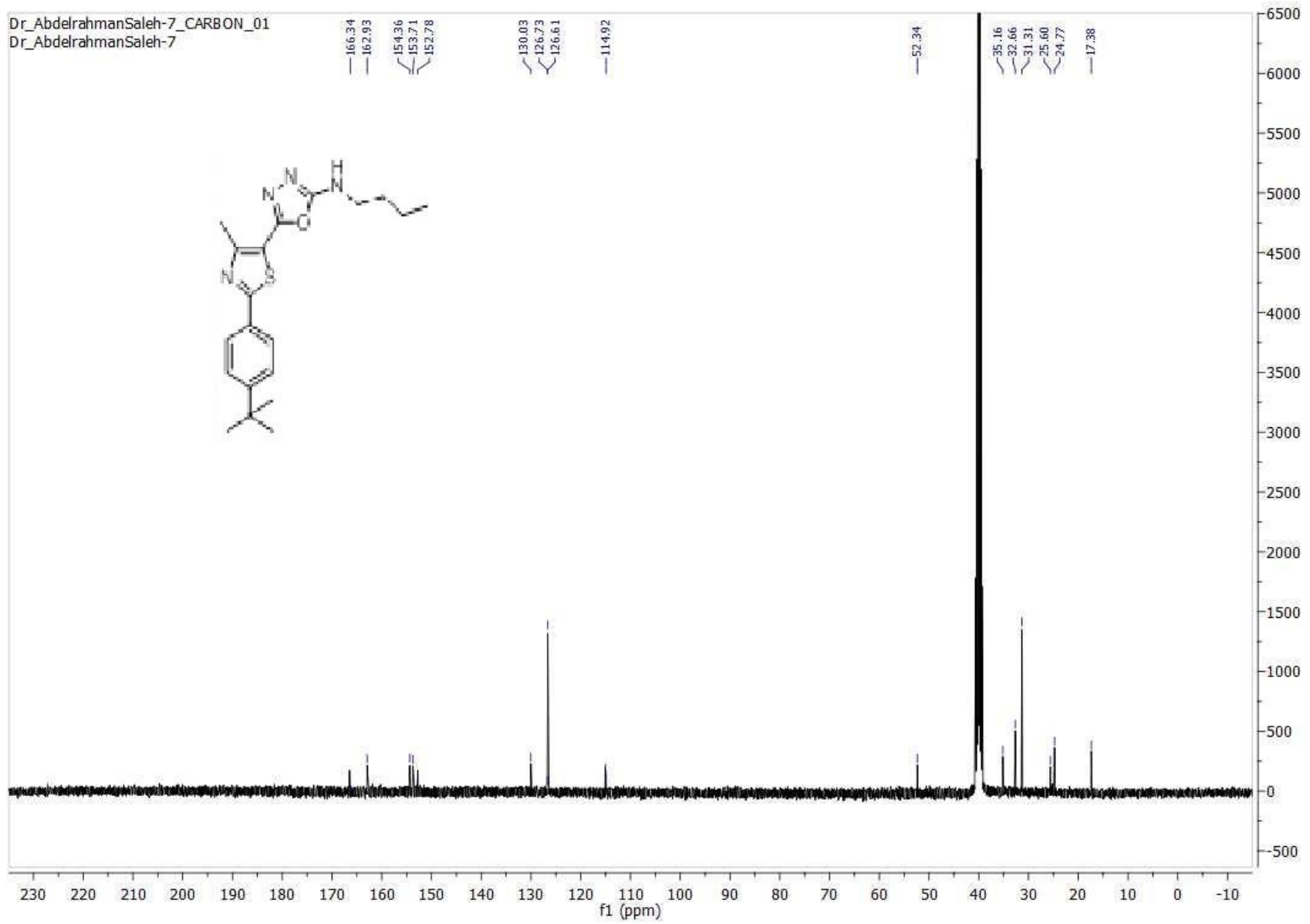
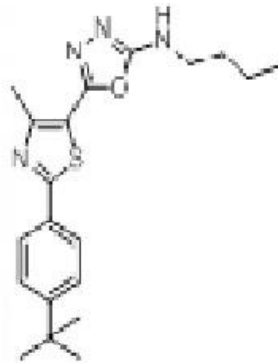
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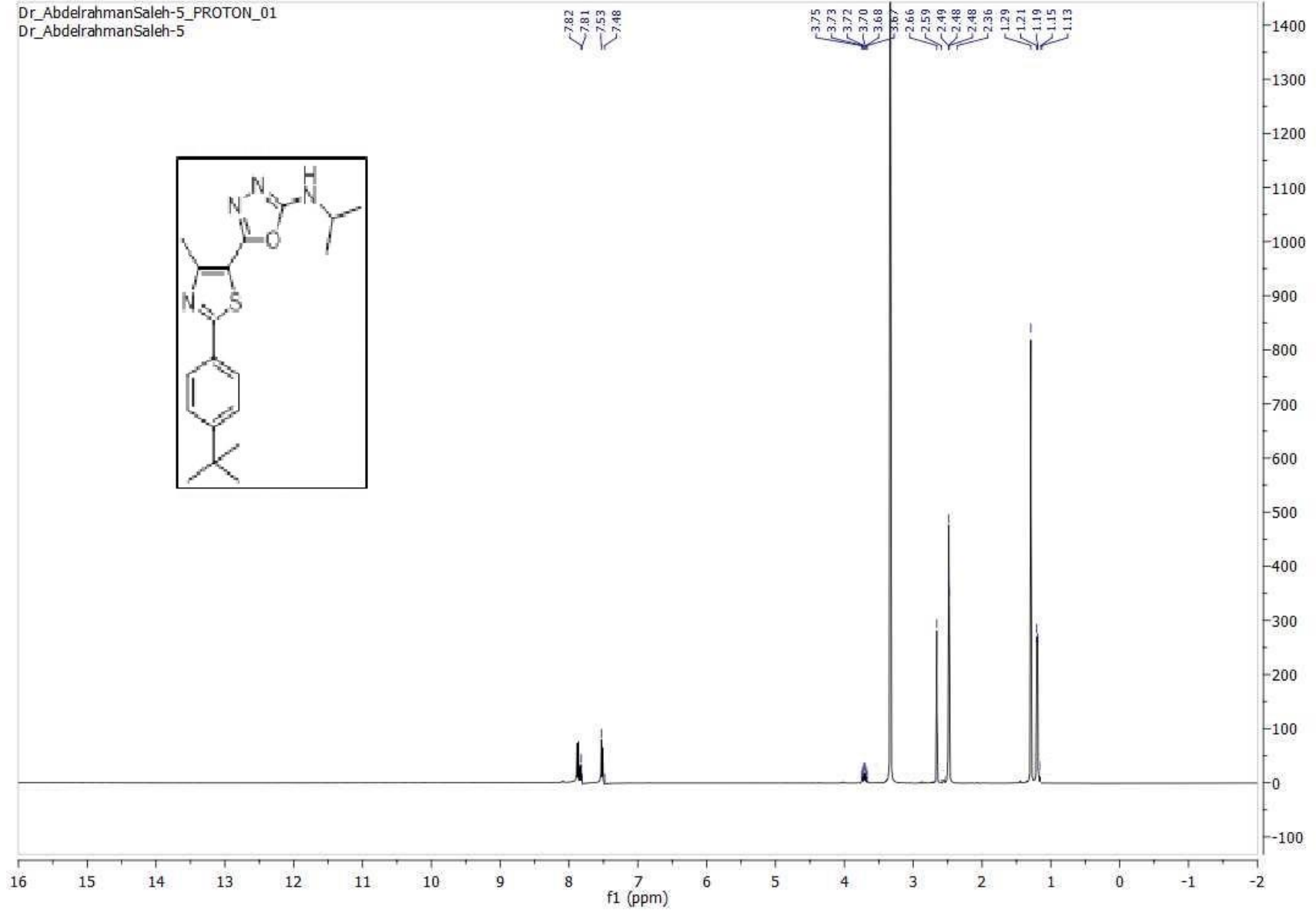
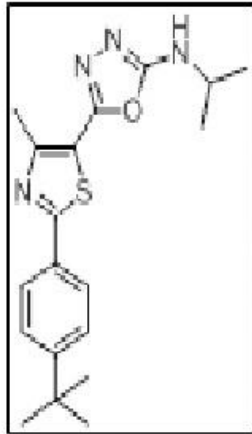
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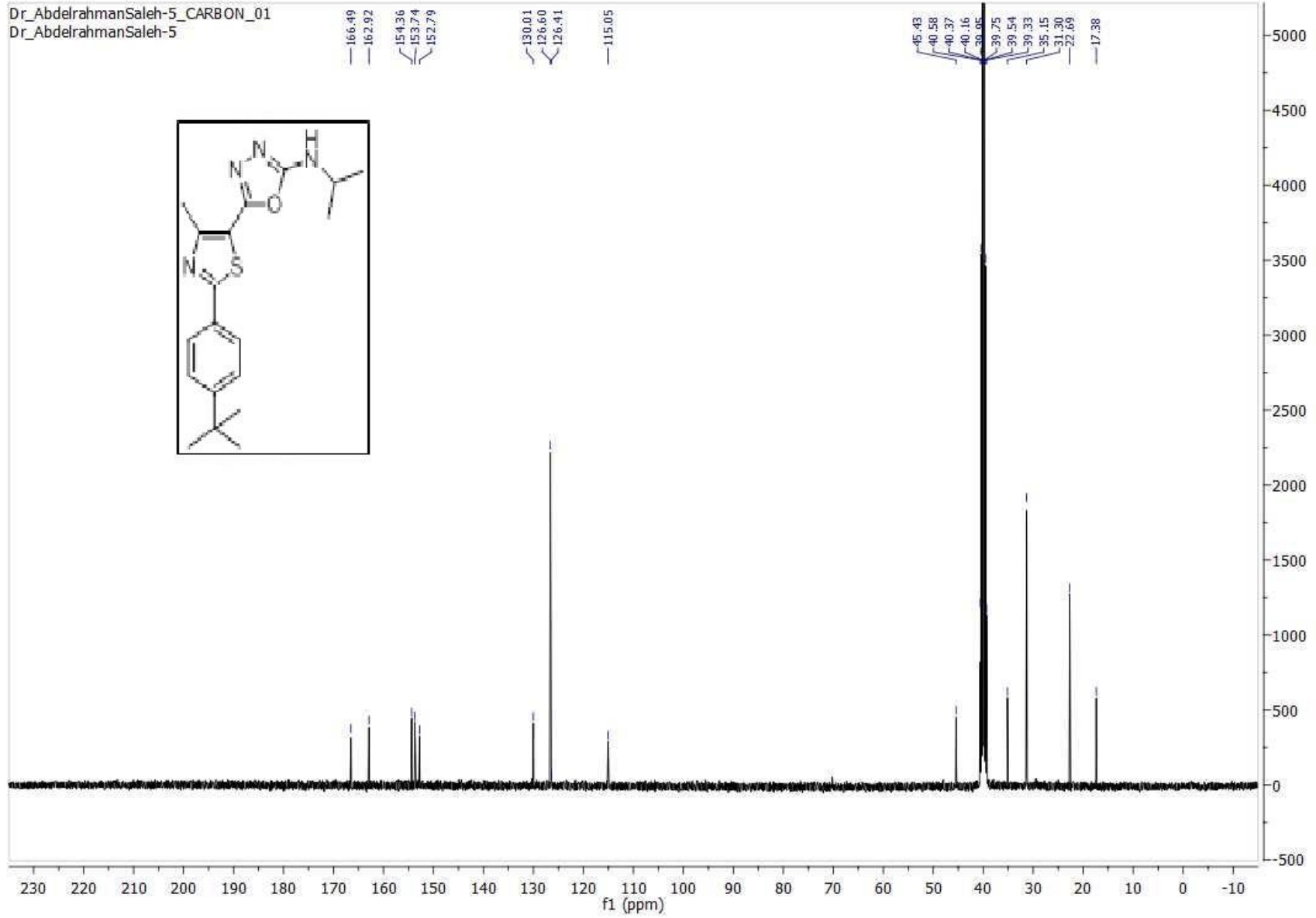
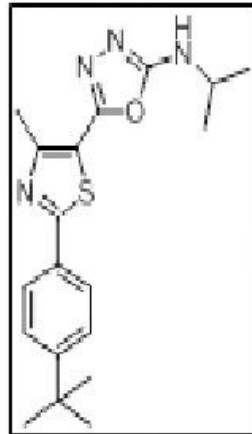
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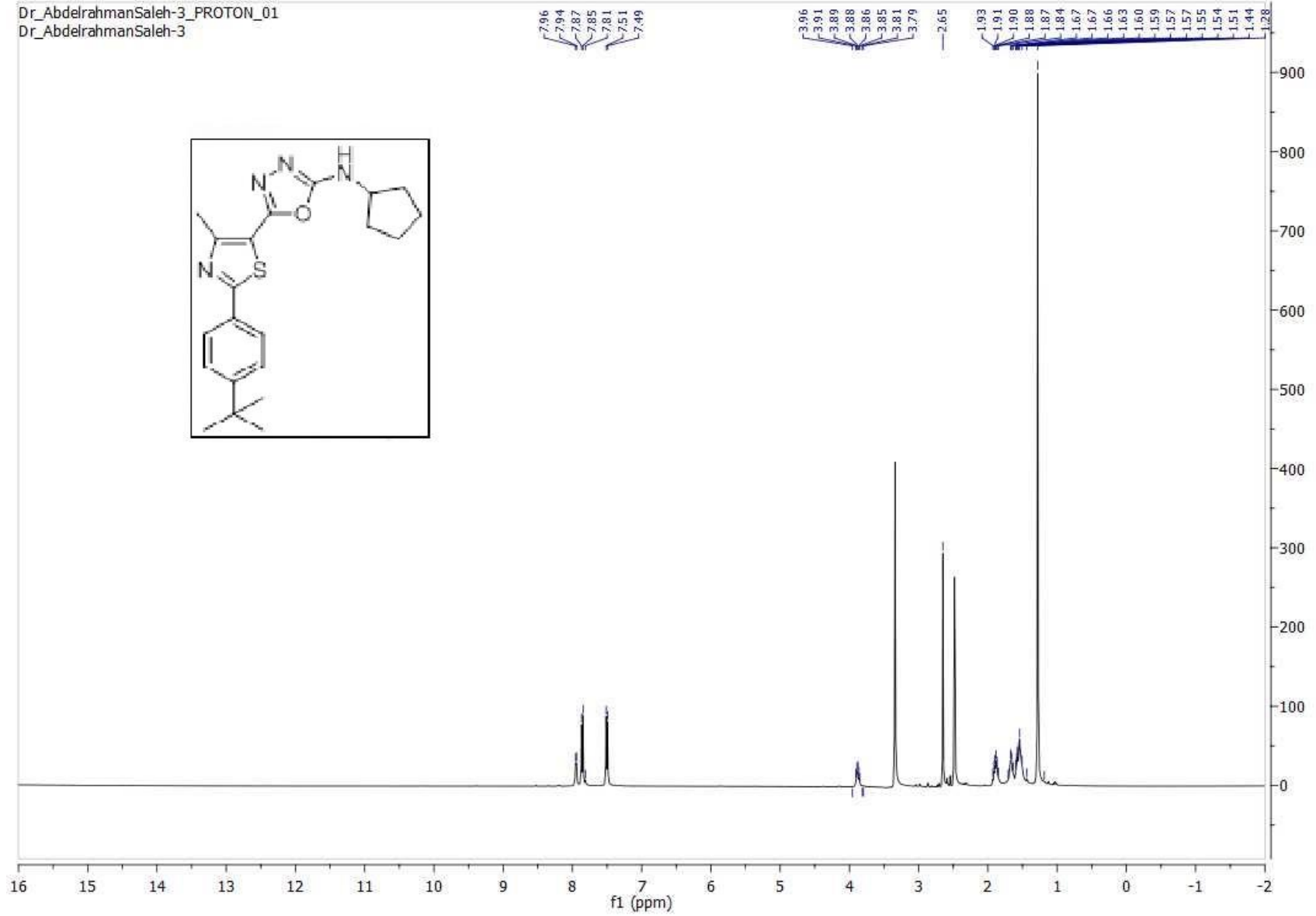
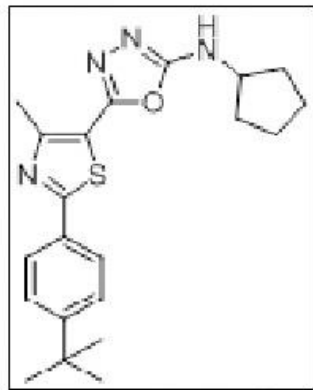
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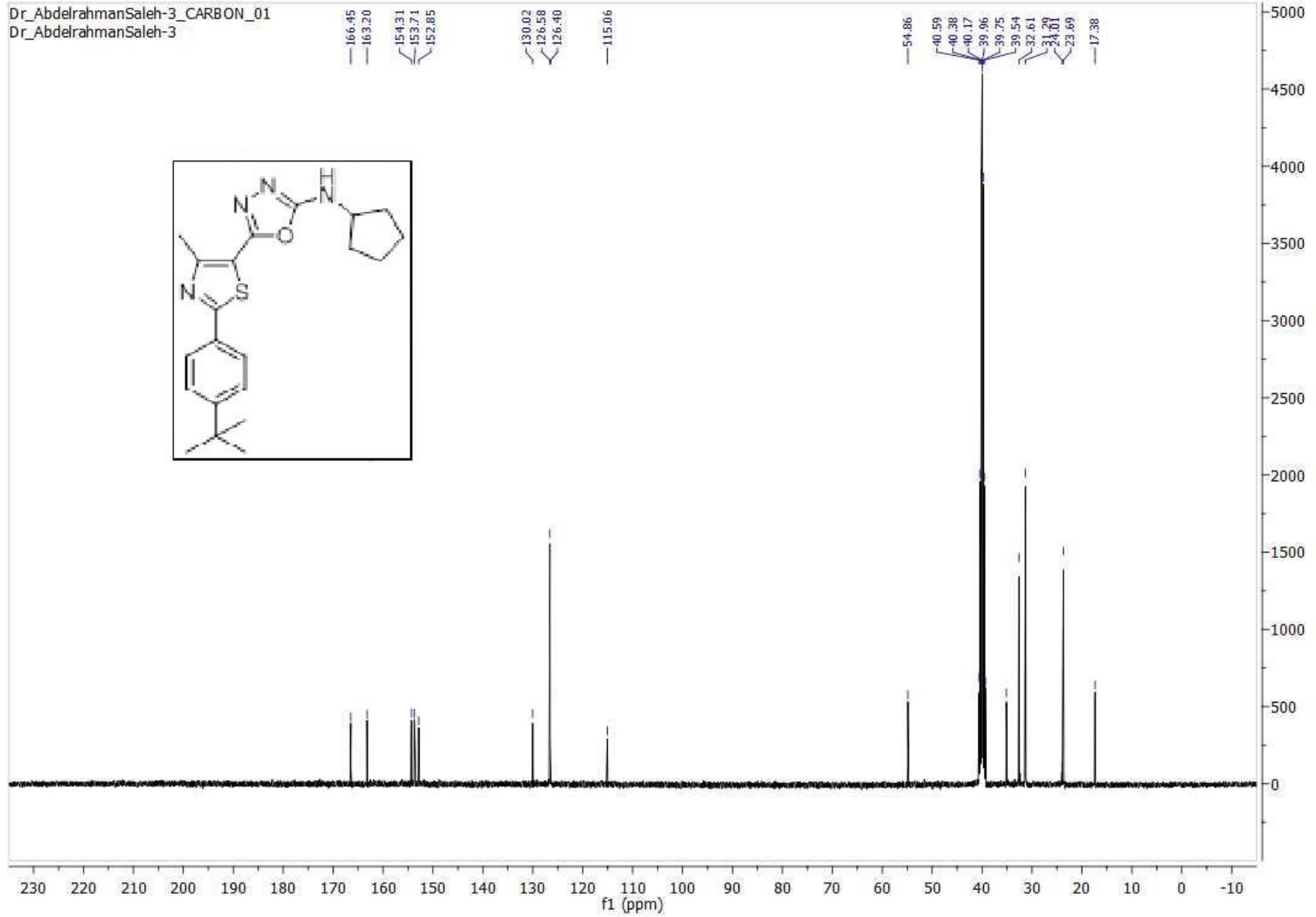
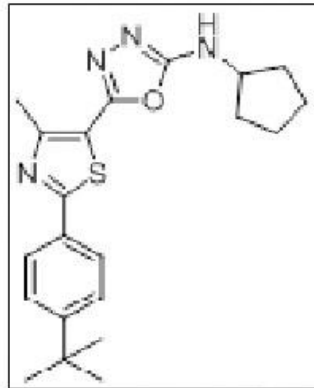
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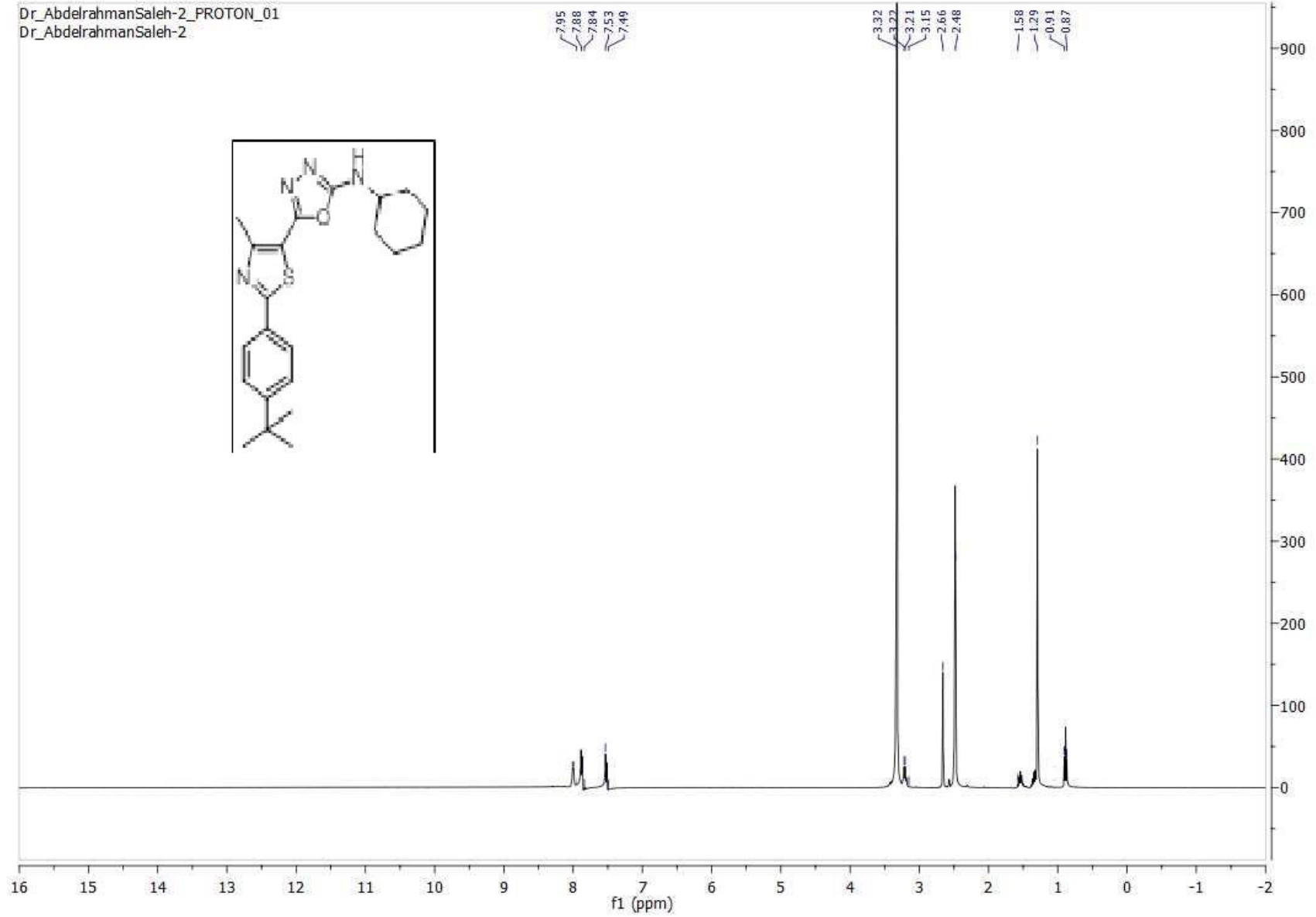
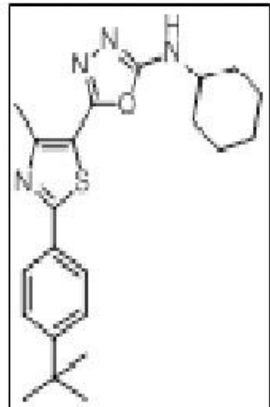
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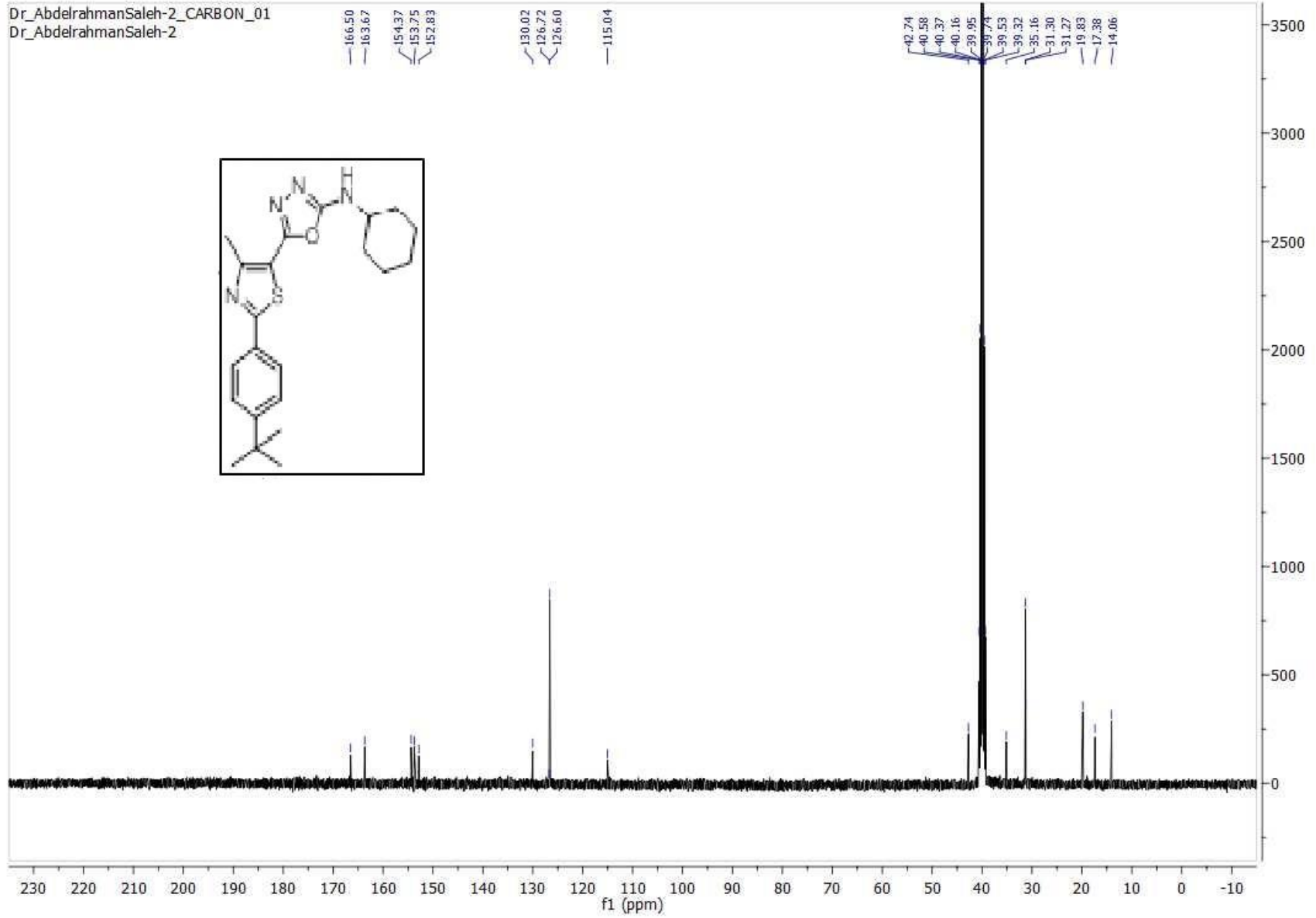
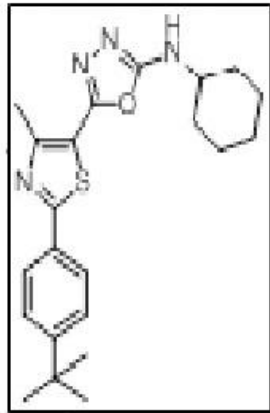
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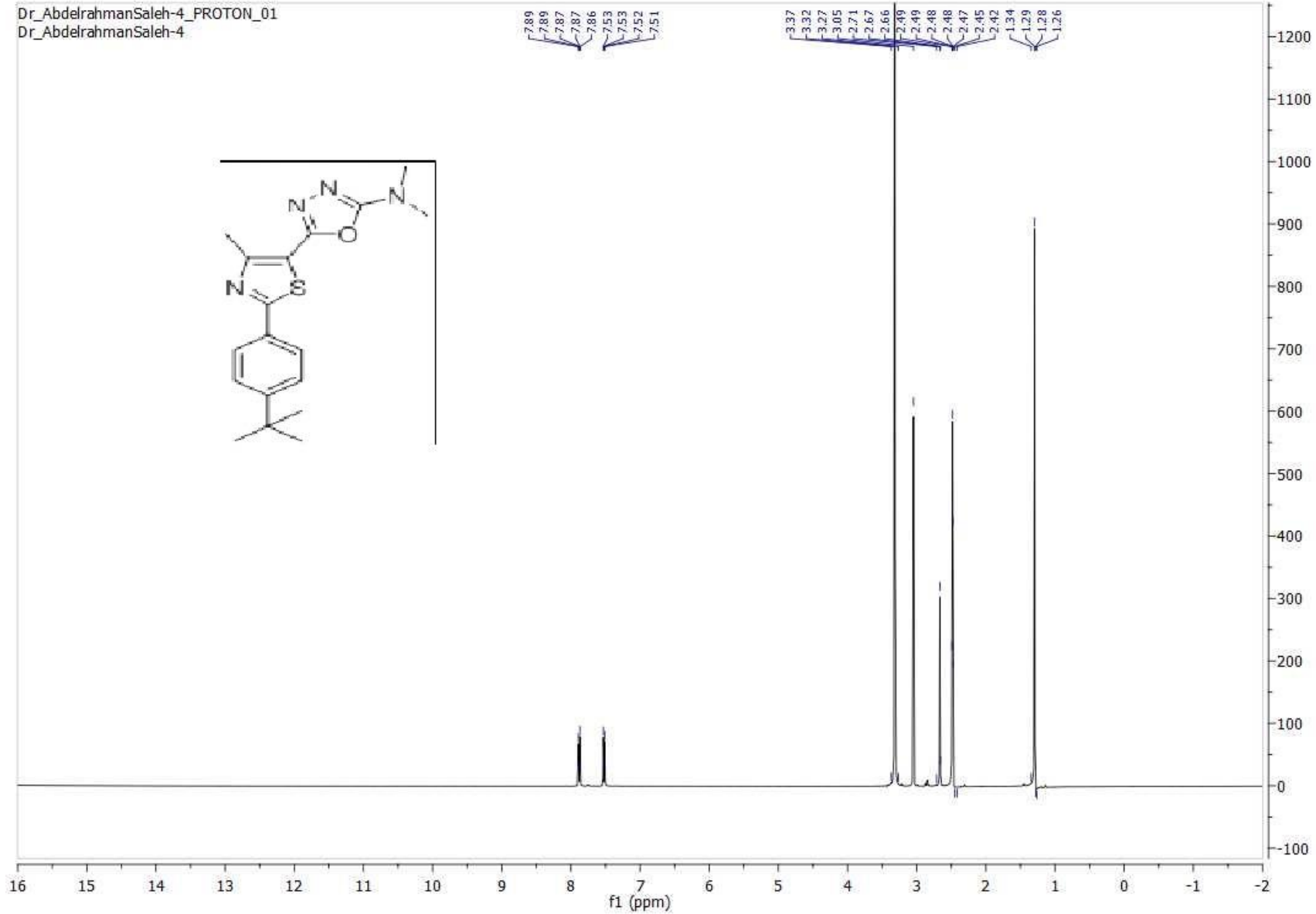
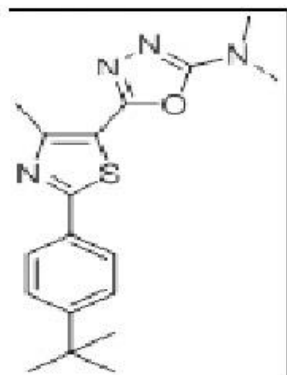
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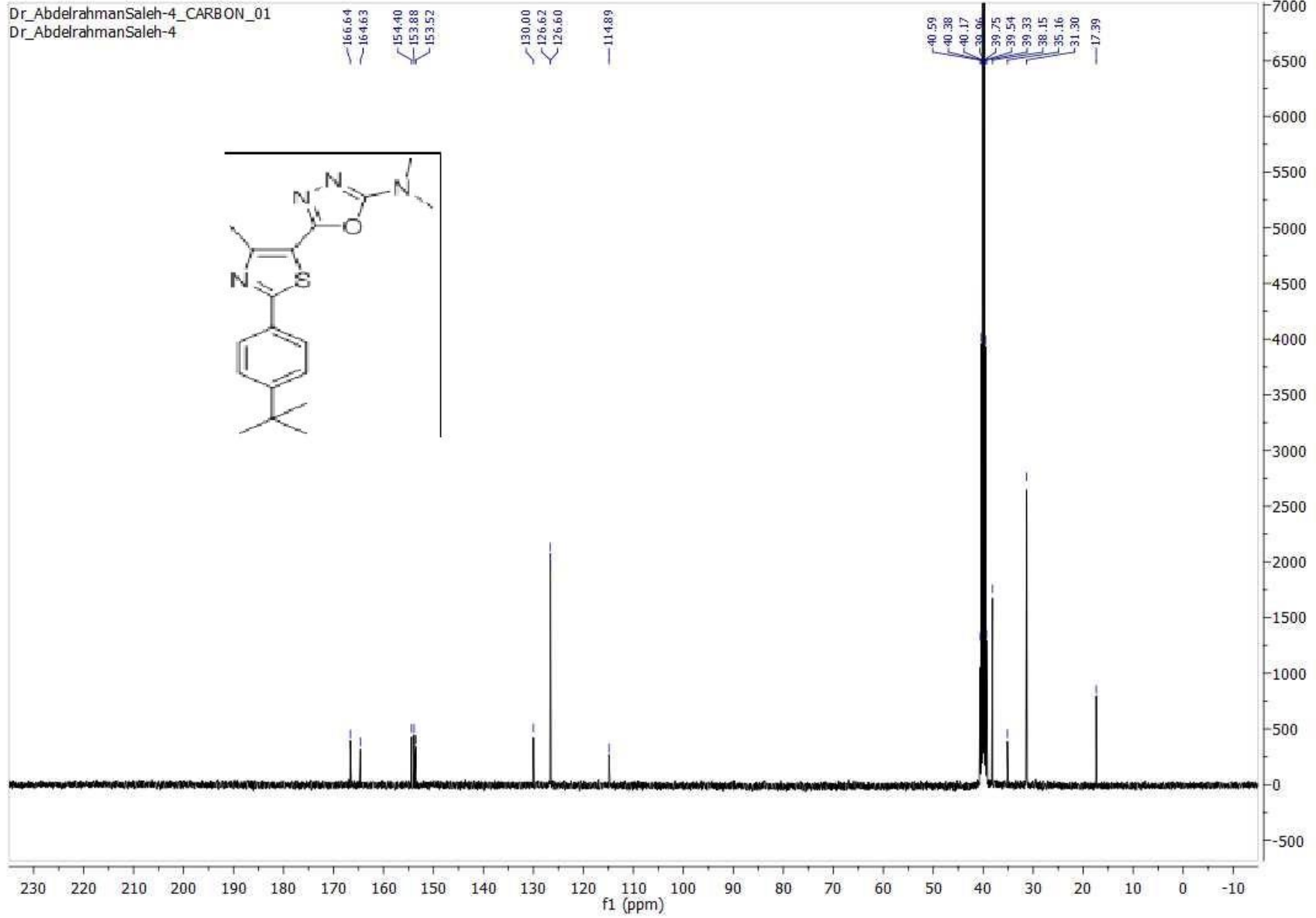
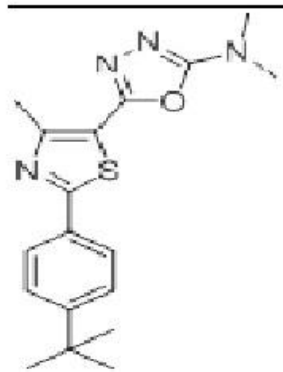
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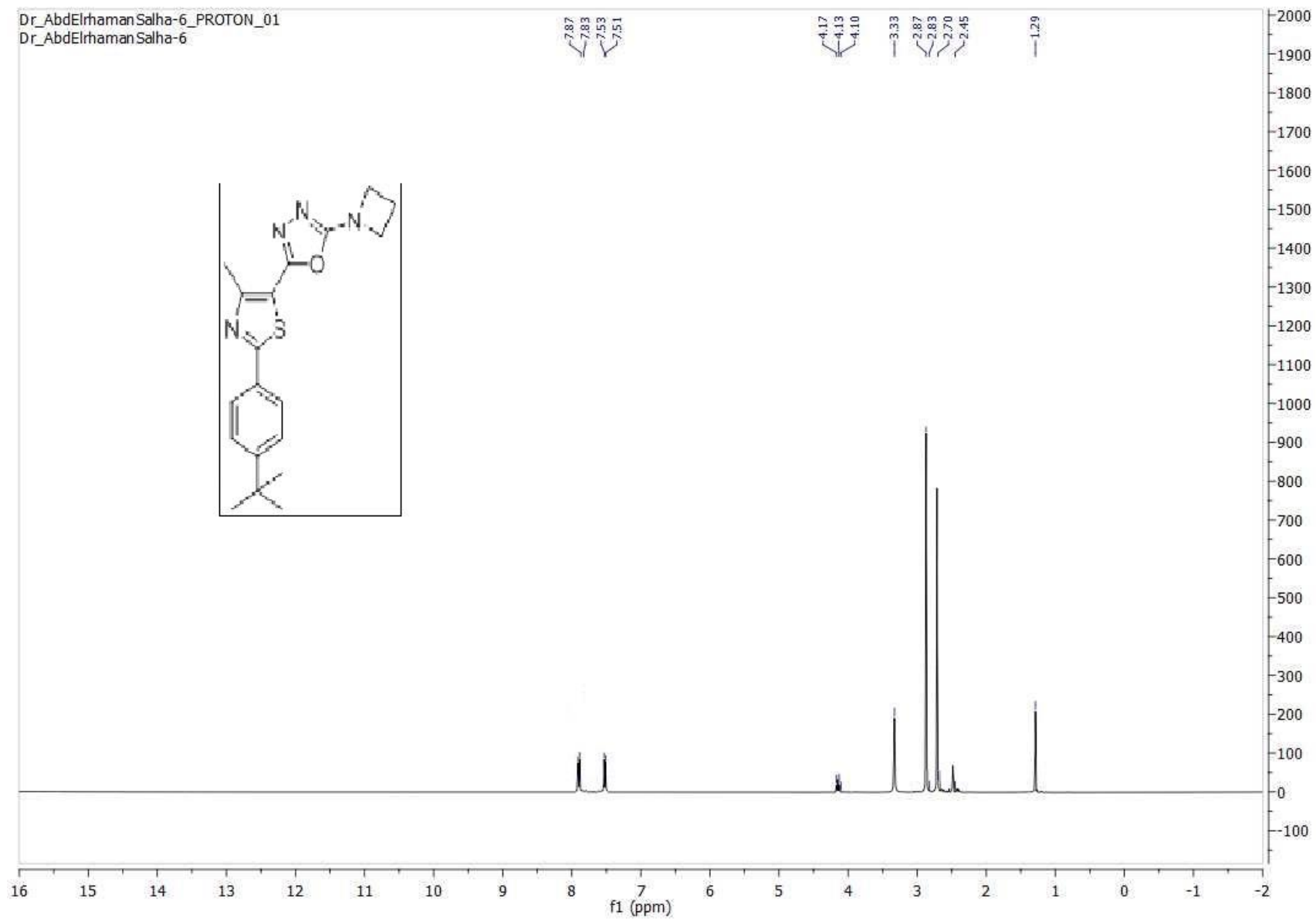
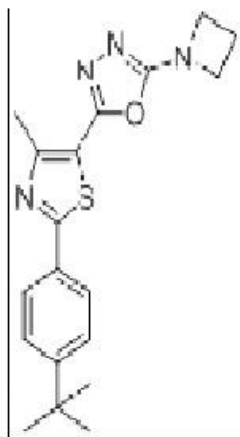
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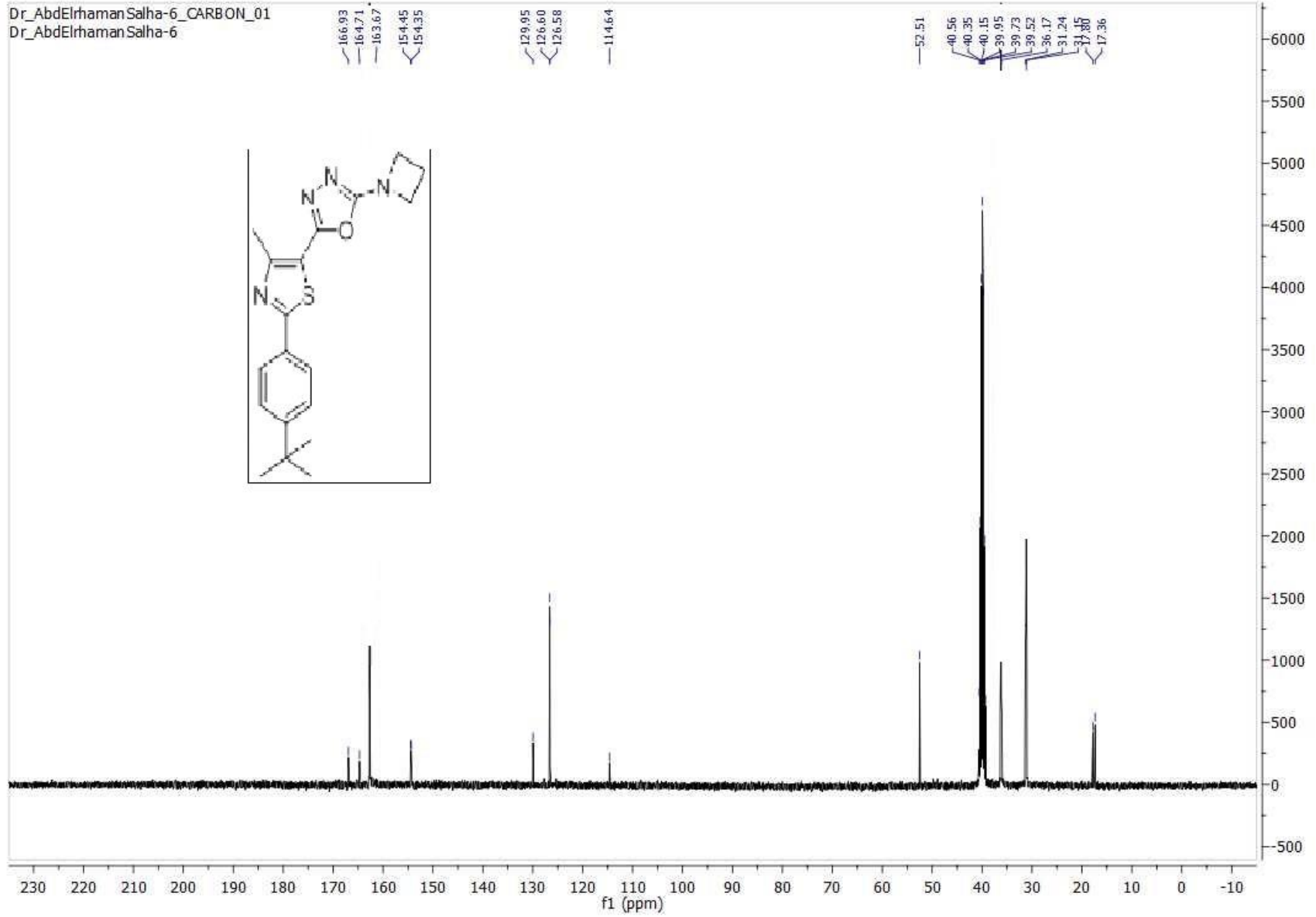
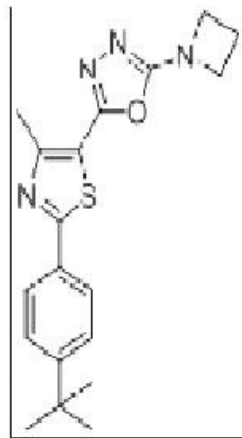
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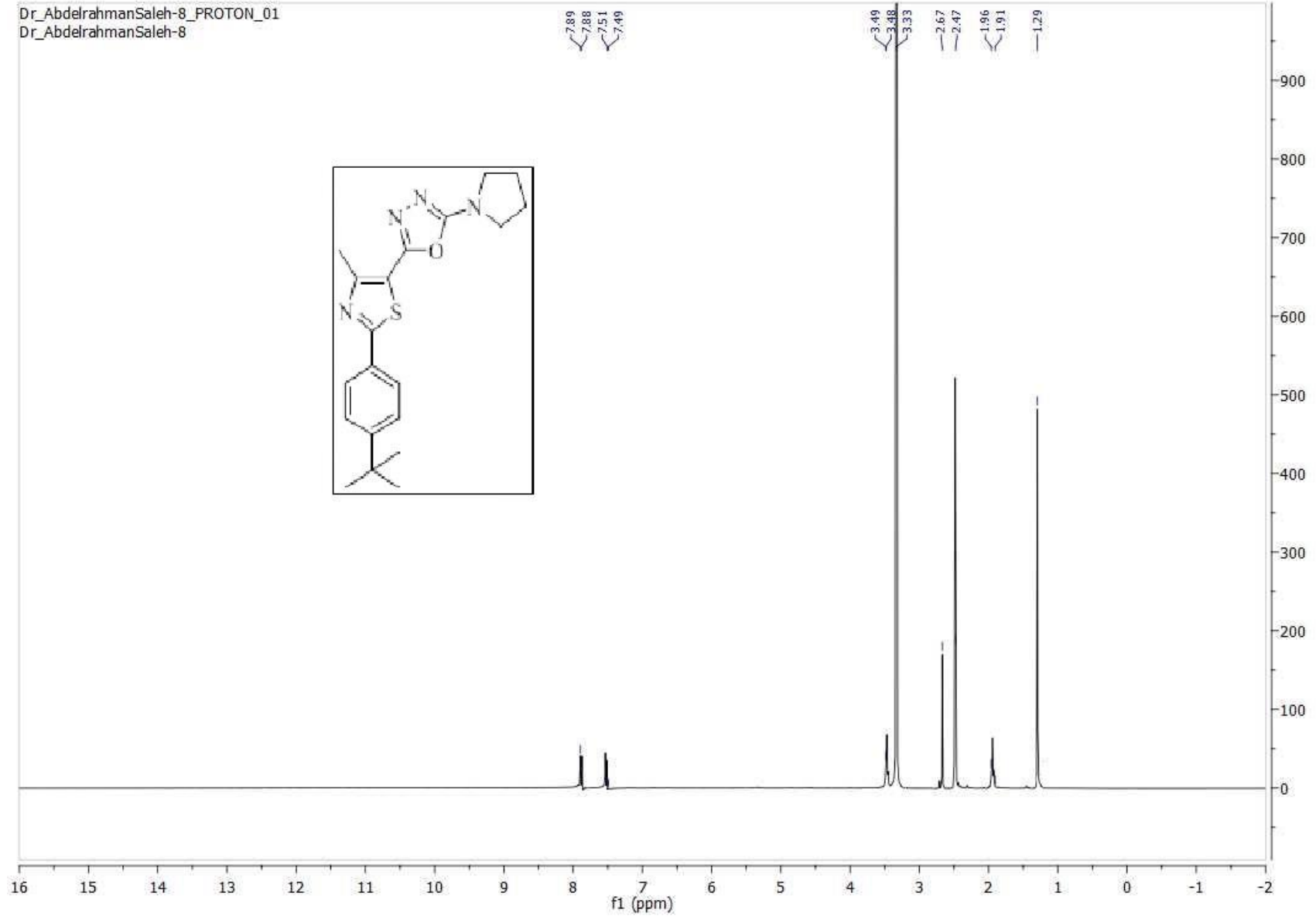
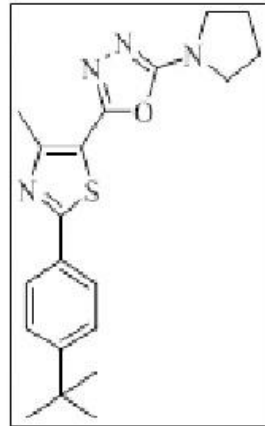
Dr_AbdElrhaman Salha-6_PROTON_01
Dr_AbdElrhaman Salha-6



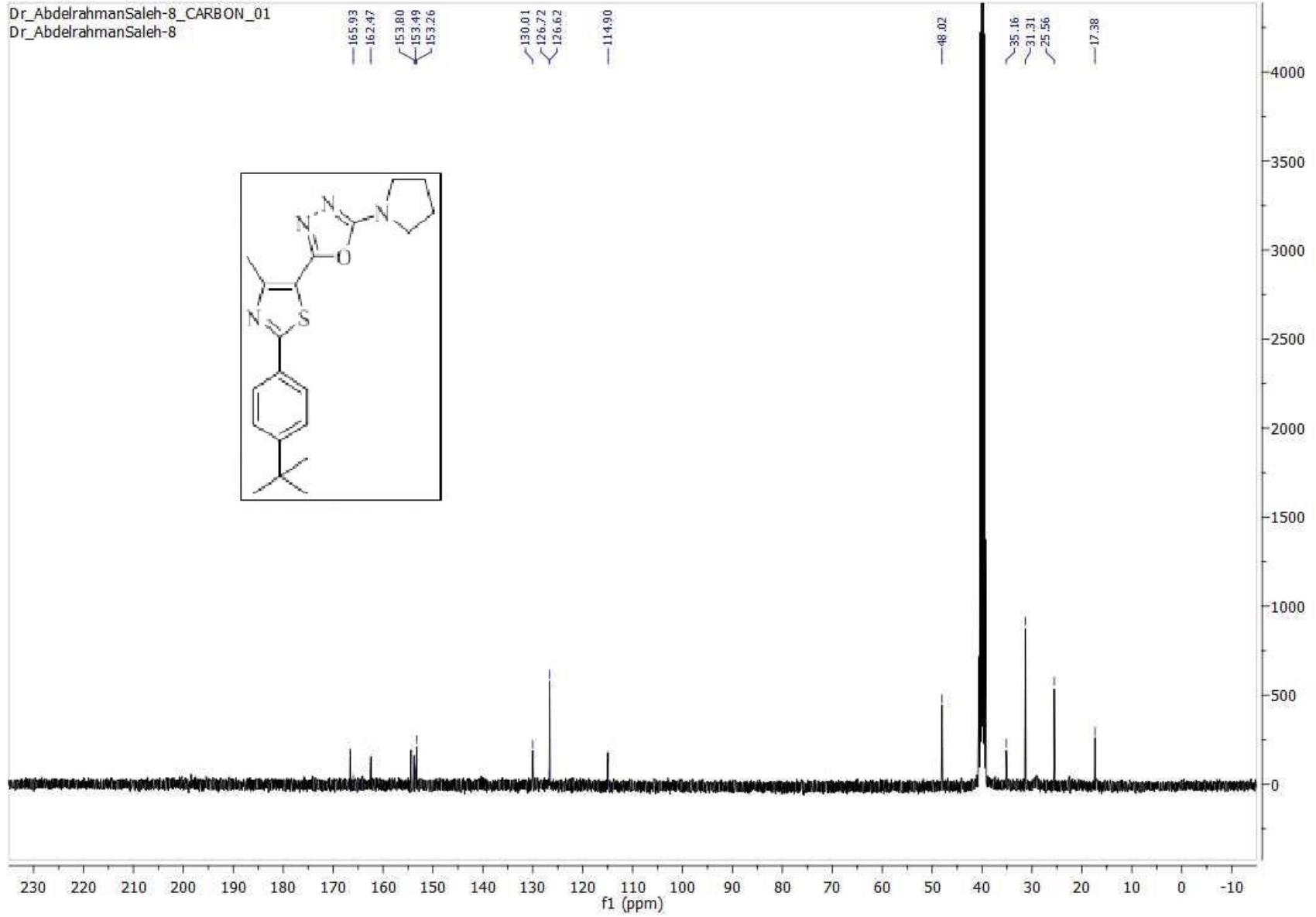
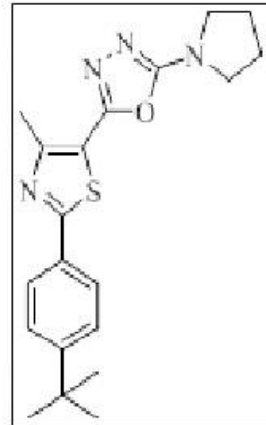
Dr_AbdElrhman Salha-6_CARBON_01
Dr_AbdElrhman Salha-6



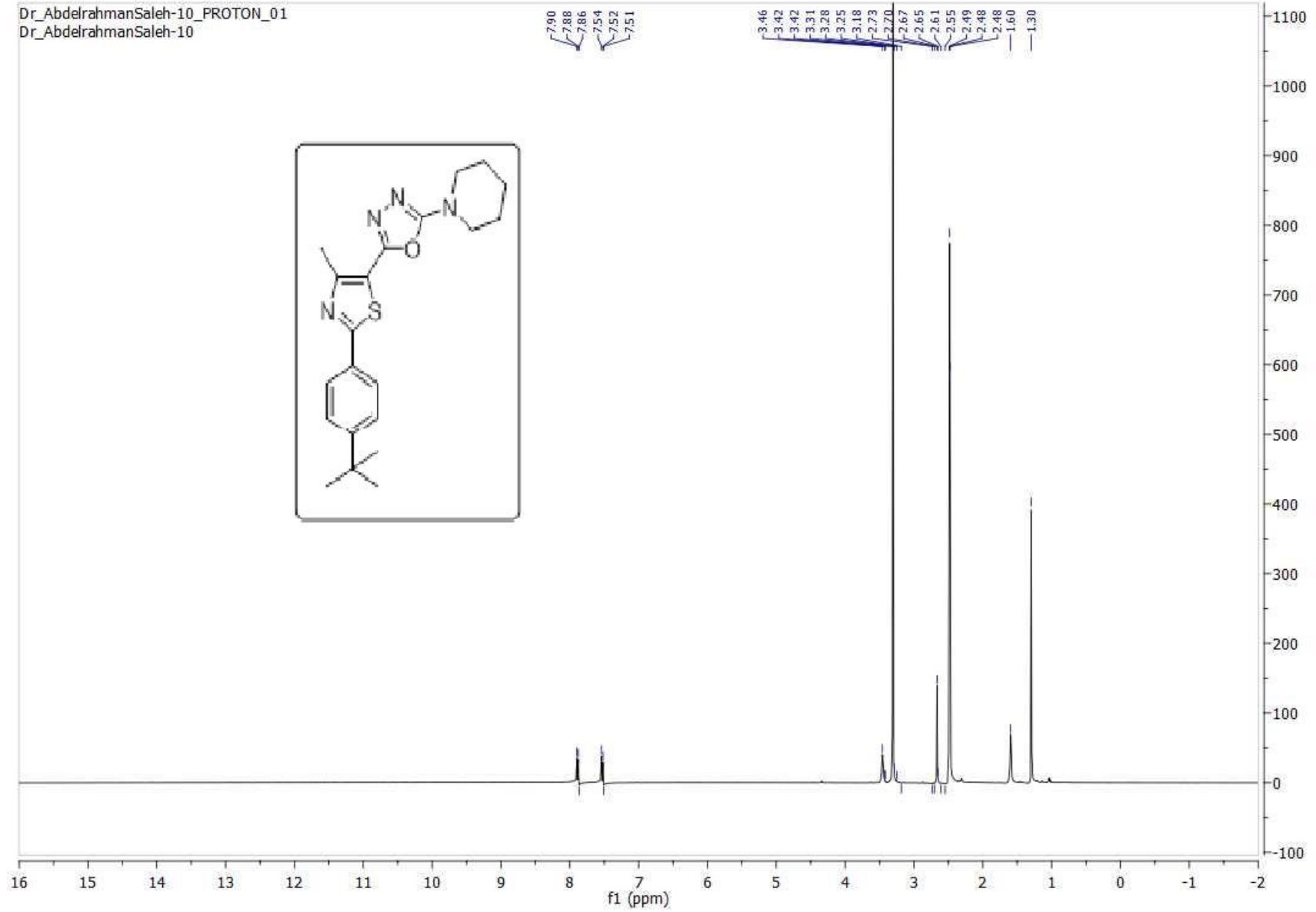
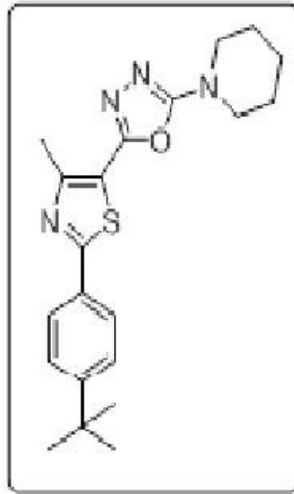
Dr_AbdelrahmanSaleh-8_PROTON_01
Dr_AbdelrahmanSaleh-8



Dr_AbdelrahmanSaleh-8_CARBON_01
Dr_AbdelrahmanSaleh-8



Dr_AbdelrahmanSaleh-10_PROTON_01
Dr_AbdelrahmanSaleh-10



Dr_AbdelrahmanSaleh-10_CARBON_01
Dr_AbdelrahmanSaleh-10

166.73
164.03

154.43
154.04
153.50

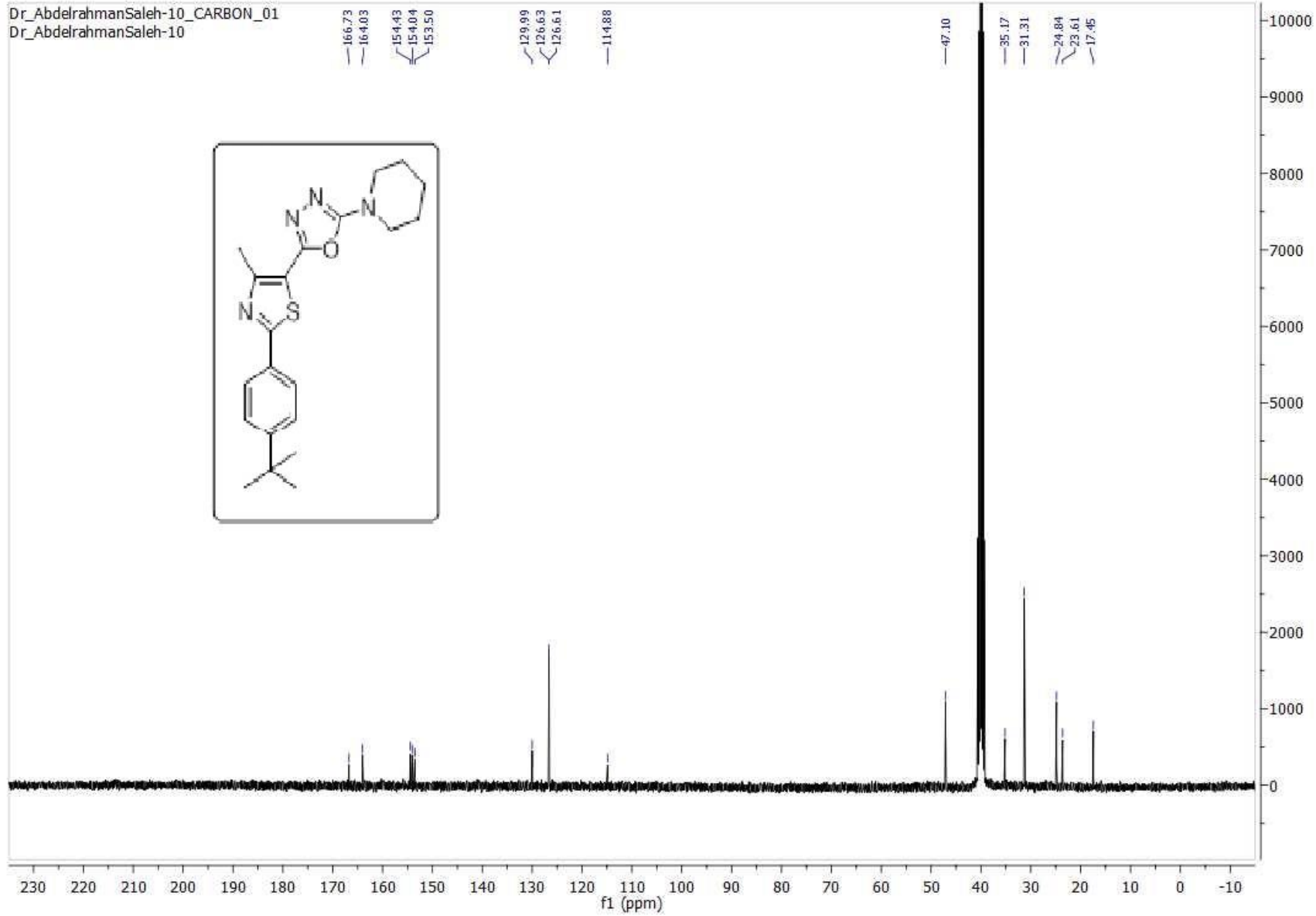
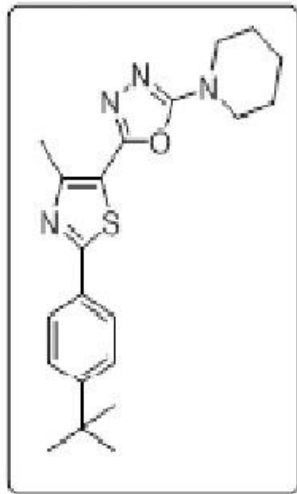
129.99
126.63
126.61

114.88

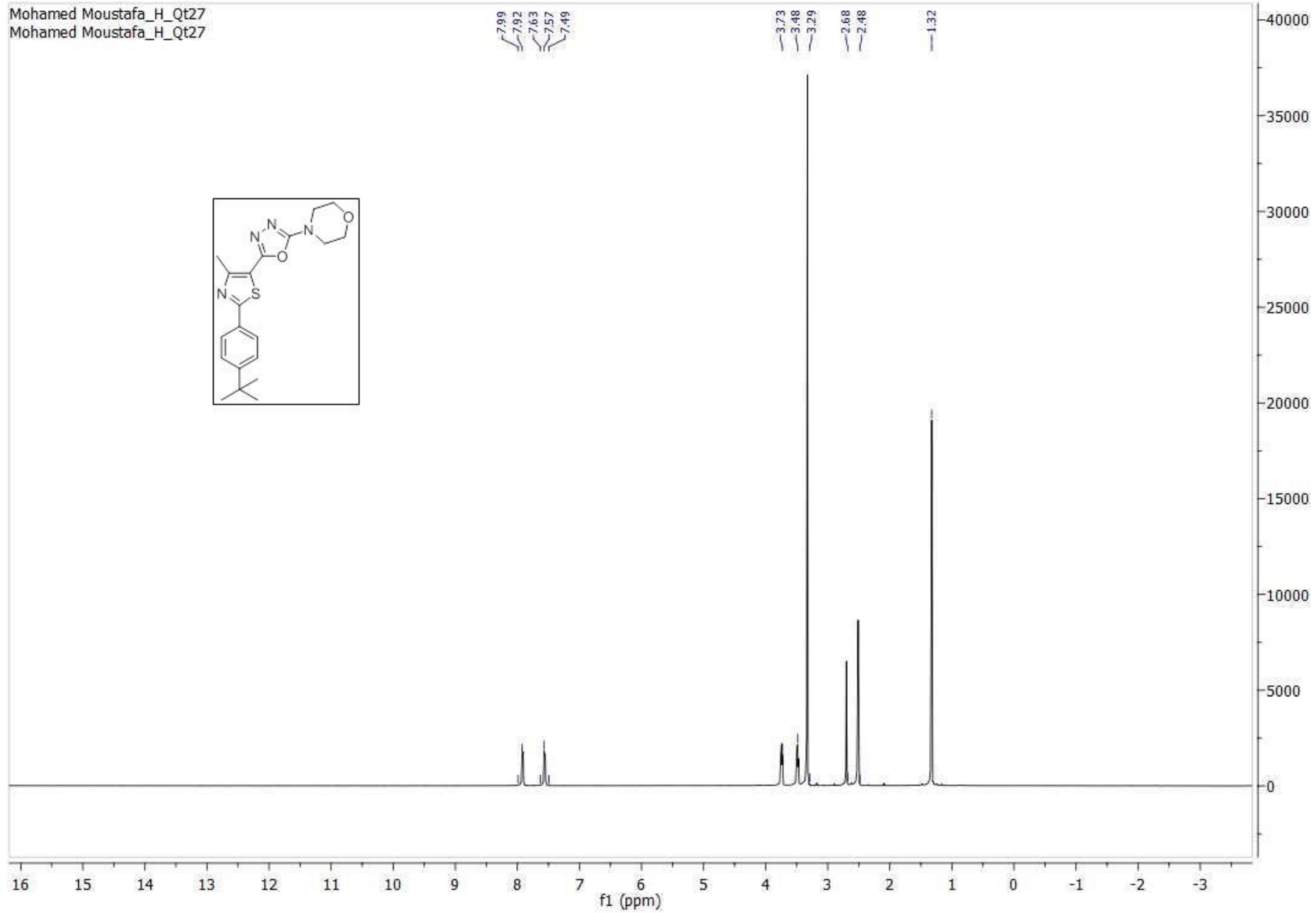
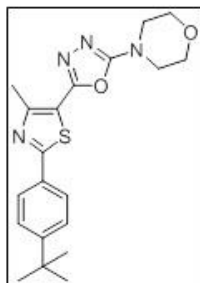
47.10

35.17
31.31

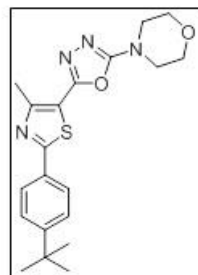
24.84
23.61
17.45



Mohamed Moustafa_H_Qt27
Mohamed Moustafa_H_Qt27



Mohamed Moustafa_C_Qt27
Mohamed Moustafa_C_Qt27



167.02
164.01

154.53
154.00
153.18

130.00
126.68
126.31

114.73

65.61

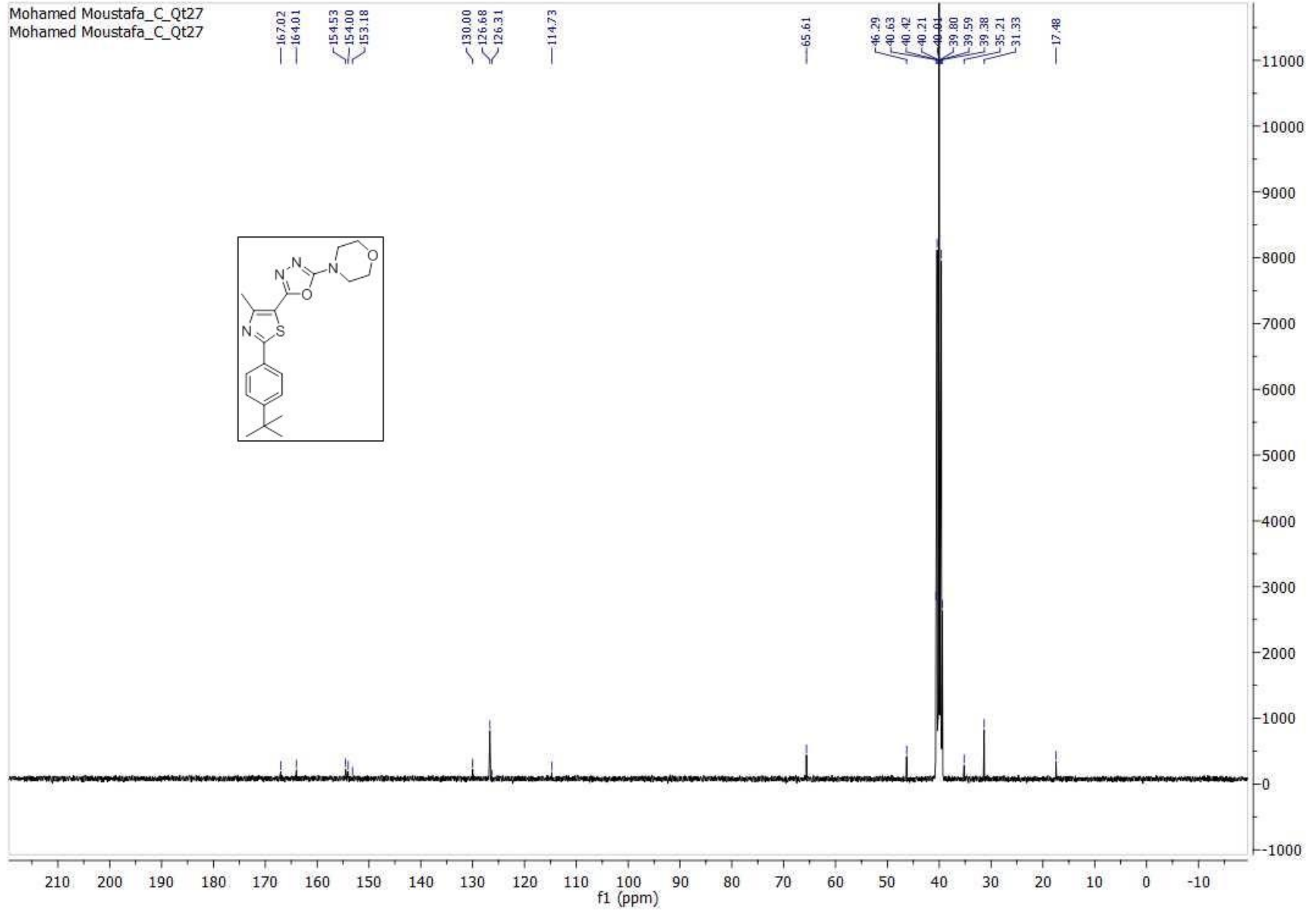
46.29
40.63
40.42

40.21
40.04

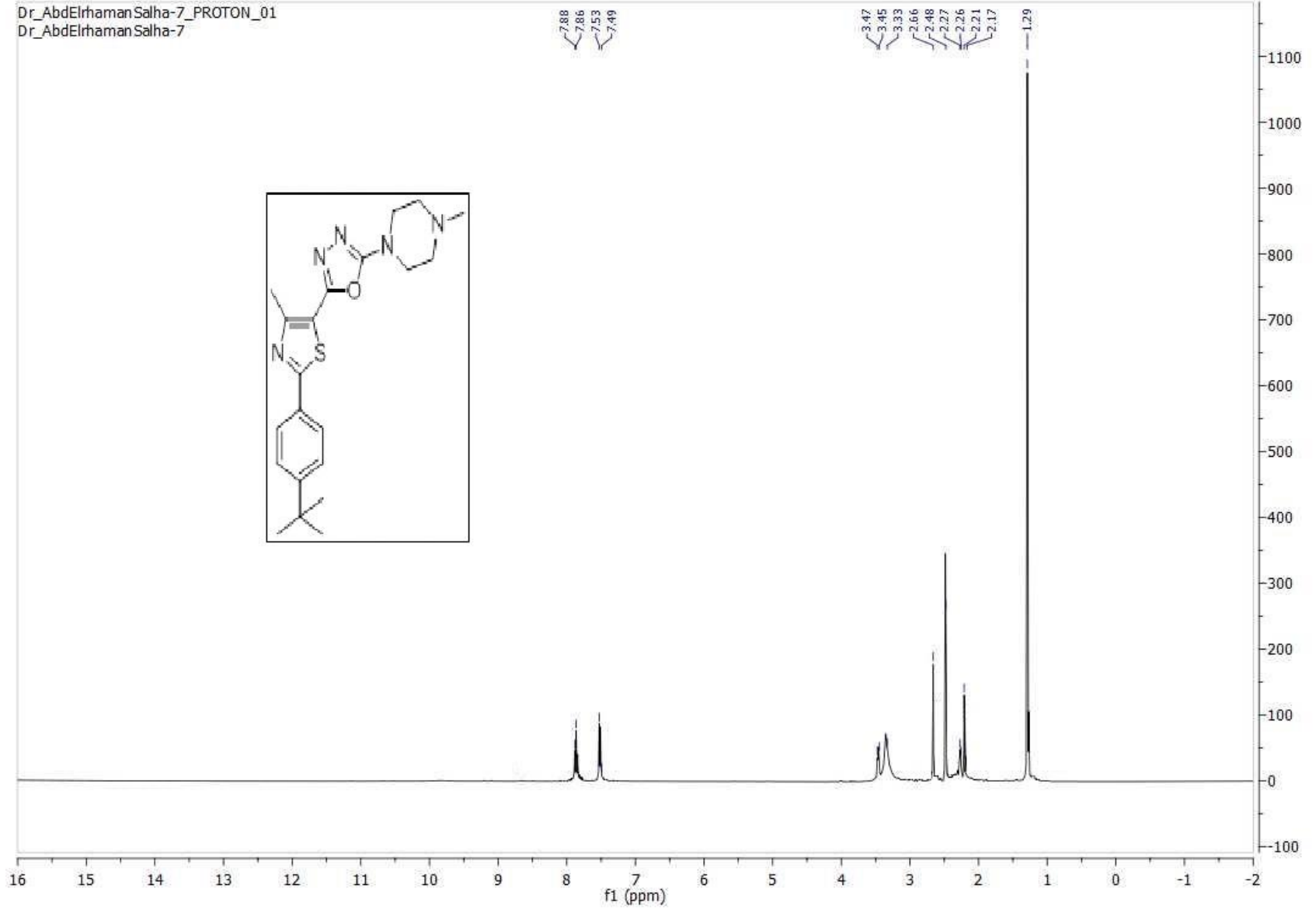
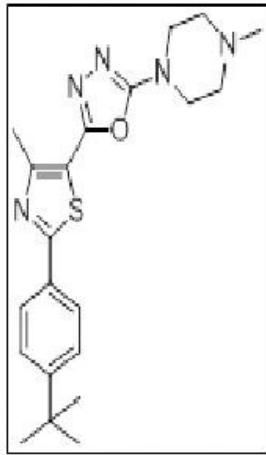
39.80
39.59
39.38

35.21
31.33

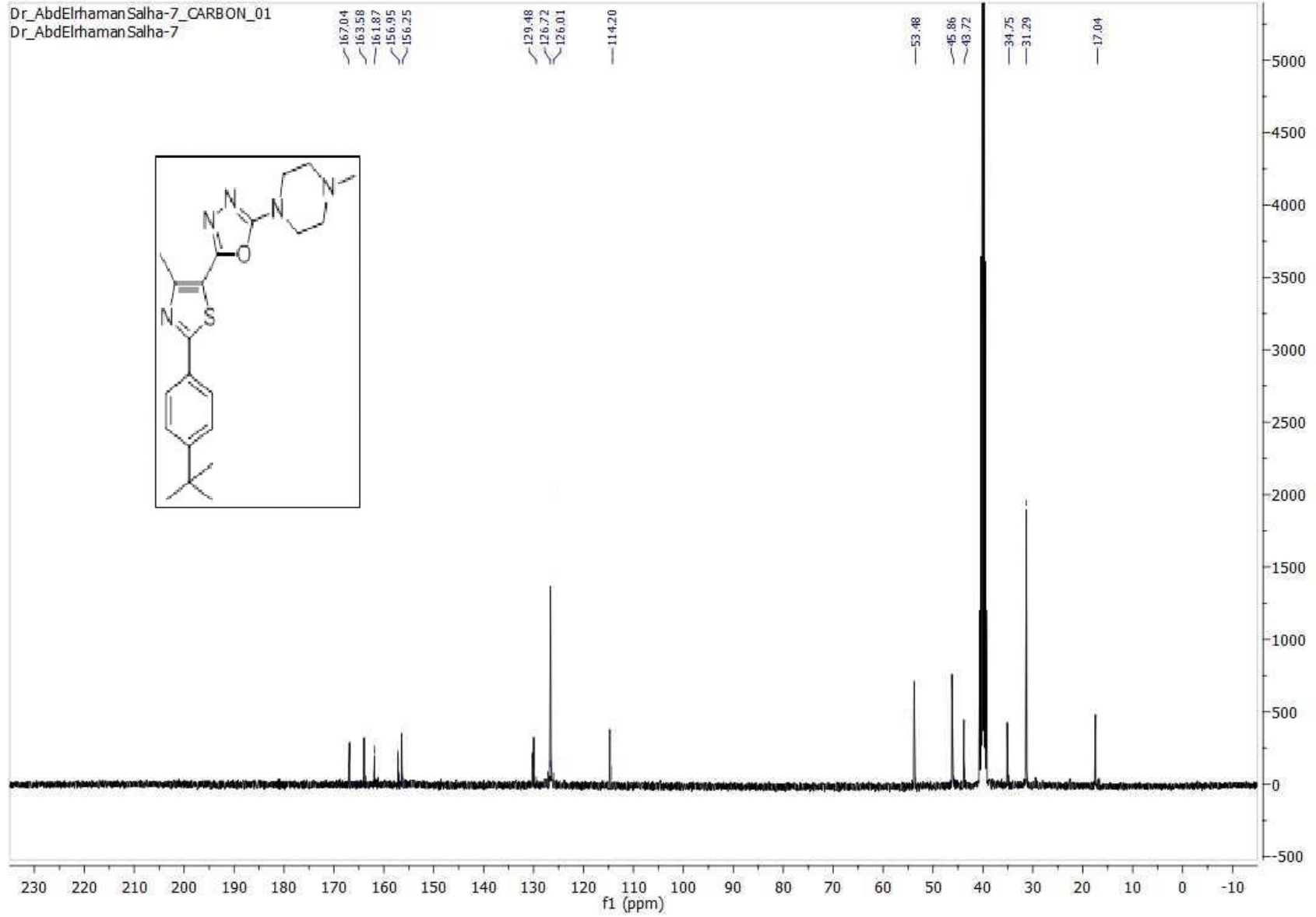
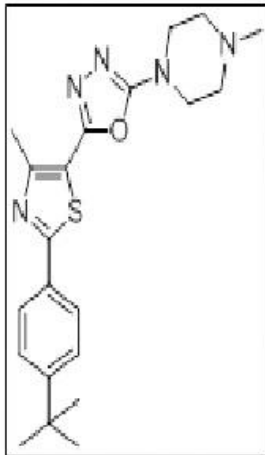
17.48



Dr_AbdElrhaman Salha-7_PROTON_01
Dr_AbdElrhaman Salha-7



Dr_AbdElrhamanSalha-7_CARBON_01
Dr_AbdElrhamanSalha-7



Mohamed Mostafa_H_Qt-16

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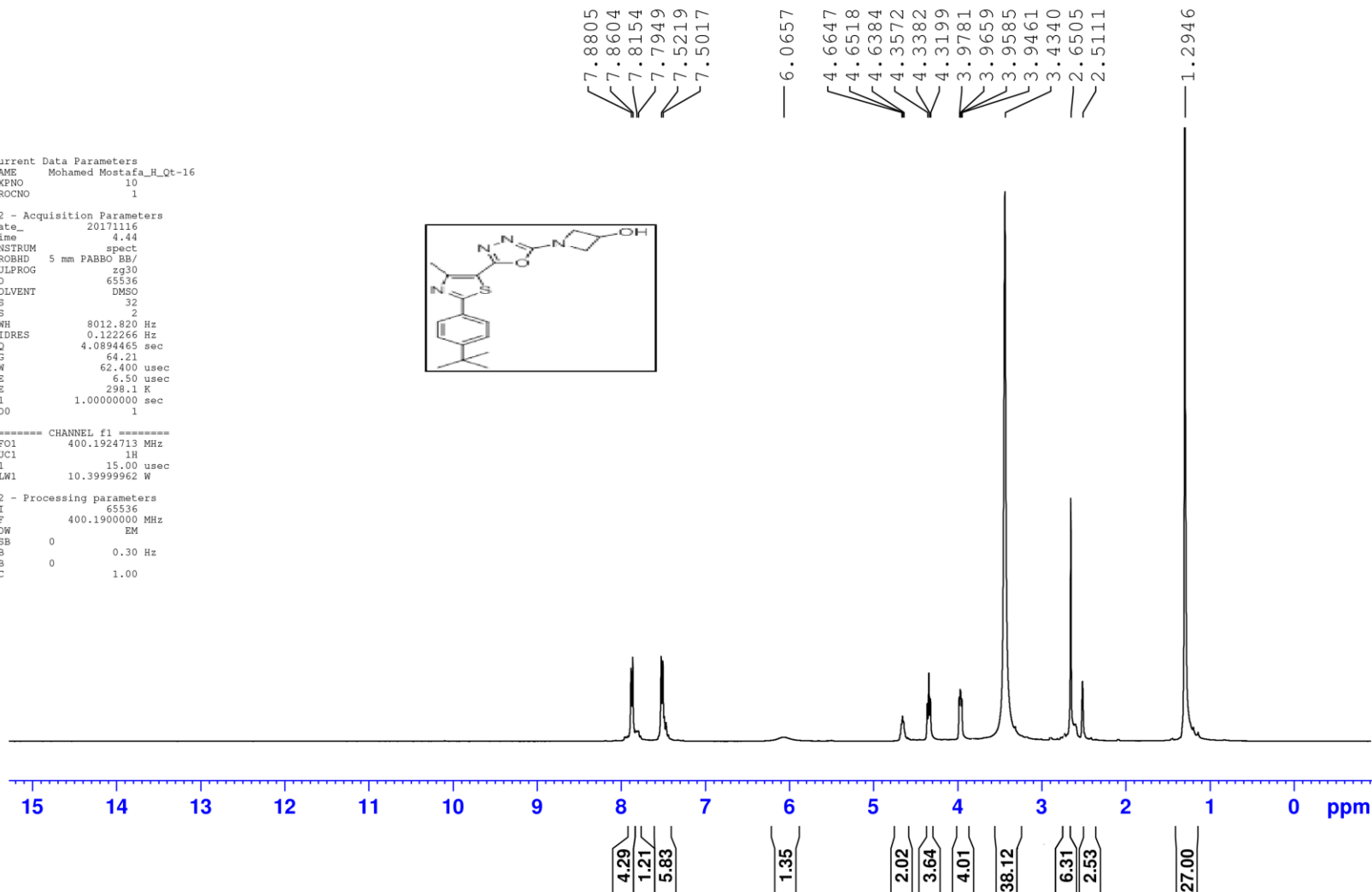
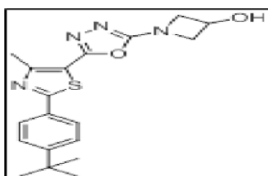


Current Data Parameters
NAME Mohamed Mostafa_H_Qt-16
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 4.44
INSTRUM spect
PROBHD 5 mm FAPBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 64.21
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Mohamed Mostafa_C_Qt-16

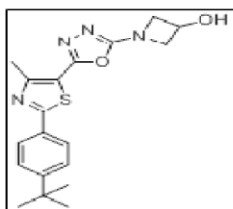
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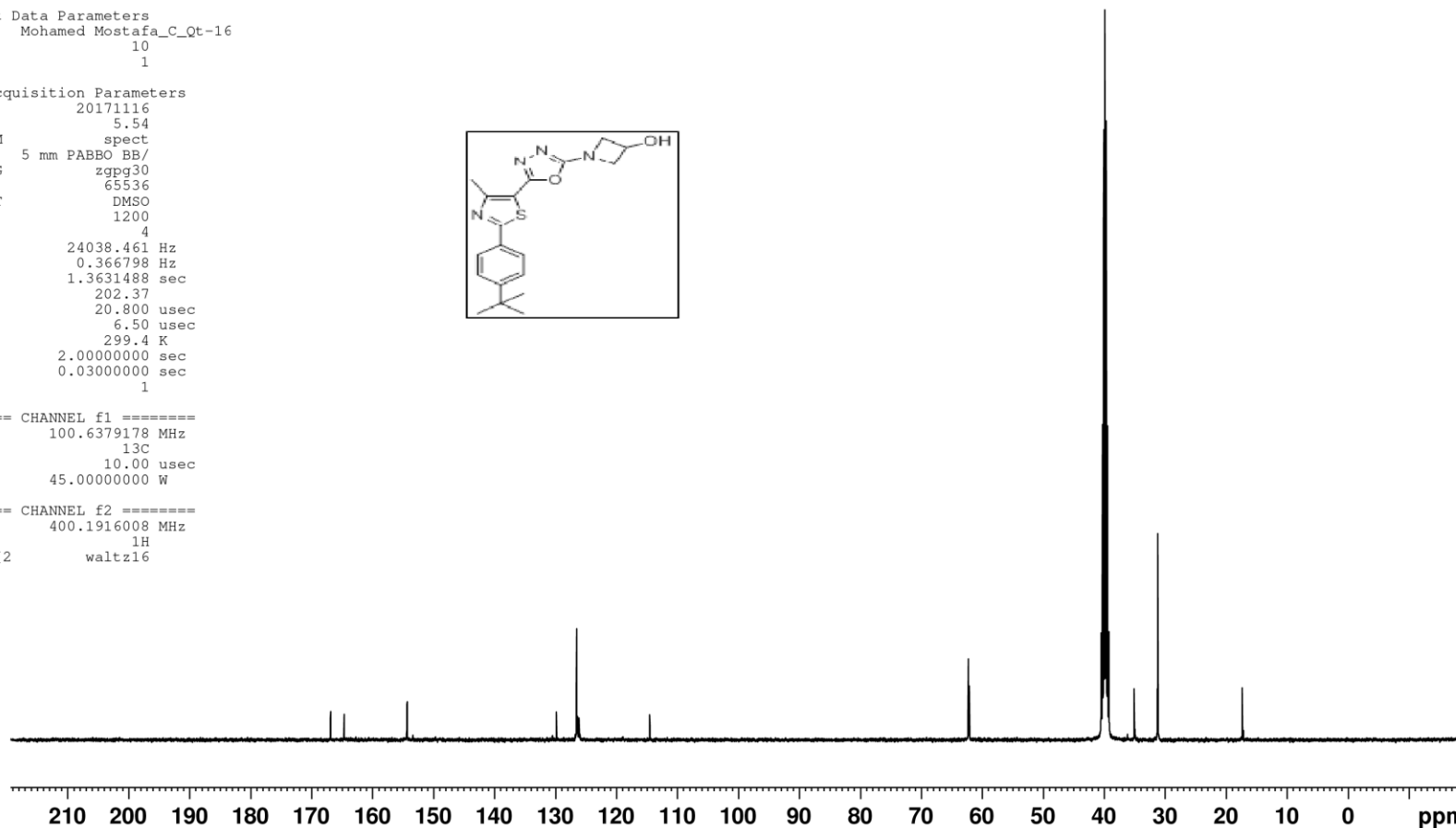
166.98
164.76
154.49
154.45
154.42
129.95
126.63
126.42
114.61
62.36
62.18
40.56
40.35
40.15
39.94
39.73
39.52
39.31
35.14
31.33
31.29
17.42

Current Data Parameters
NAME Mohamed Mostafa_C_Qt-16
EXPNO 10
PROCNO 1

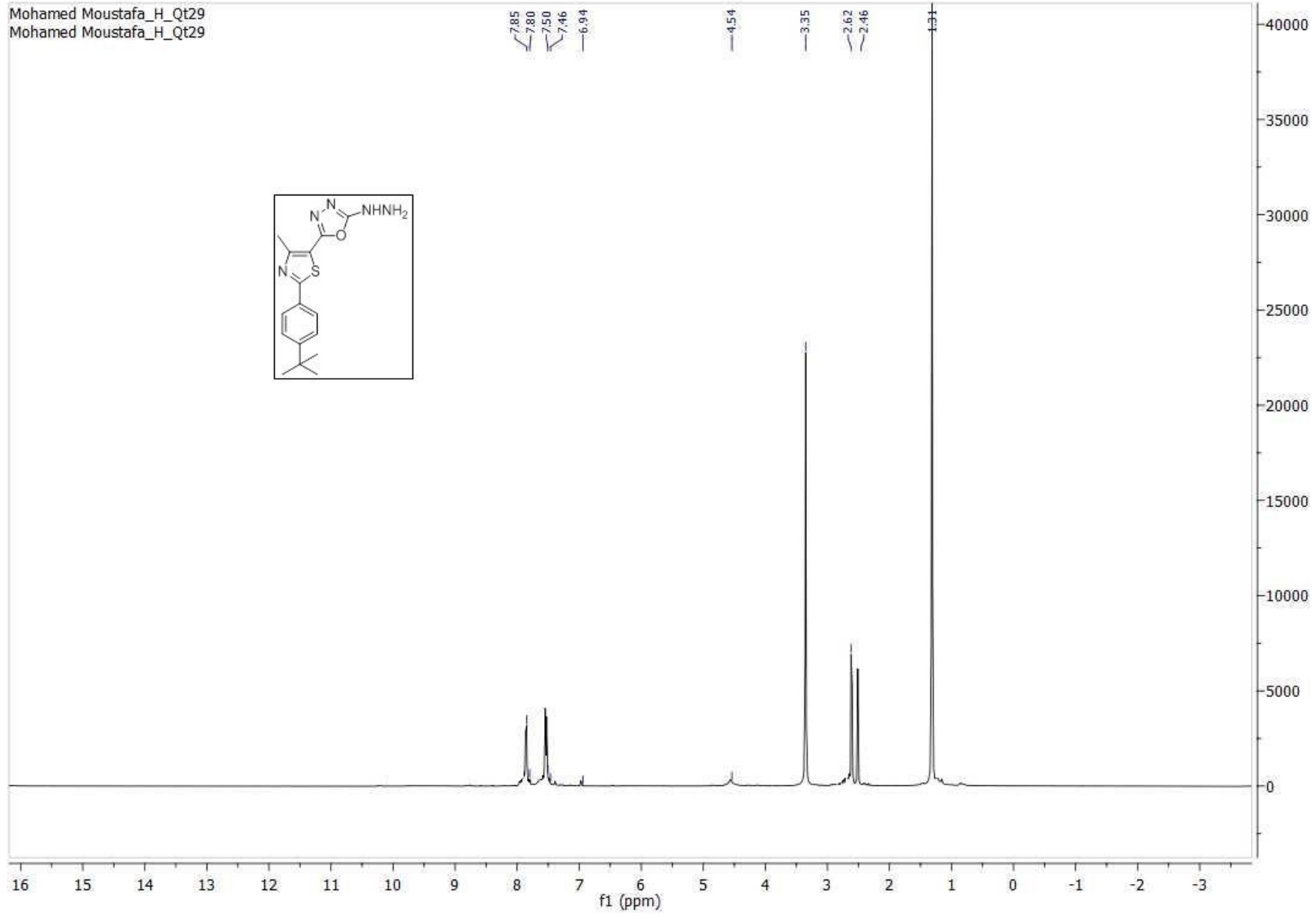
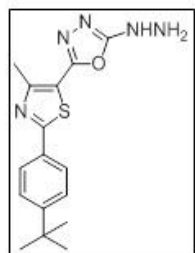
F2 - Acquisition Parameters
Date_ 20171116
Time 5.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



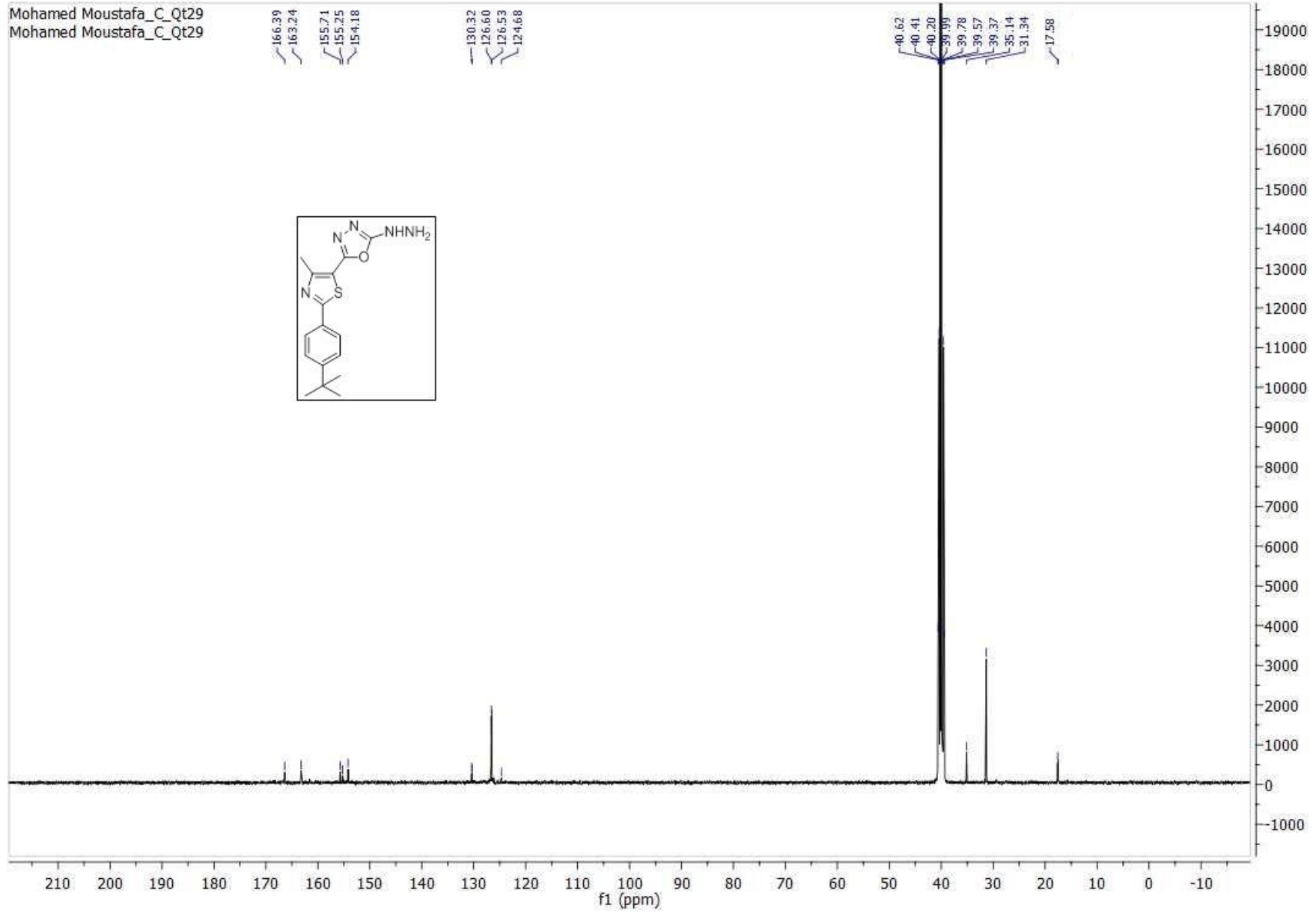
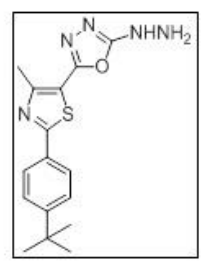
Mohamed Moustafa_H_Qt29
Mohamed Moustafa_H_Qt29



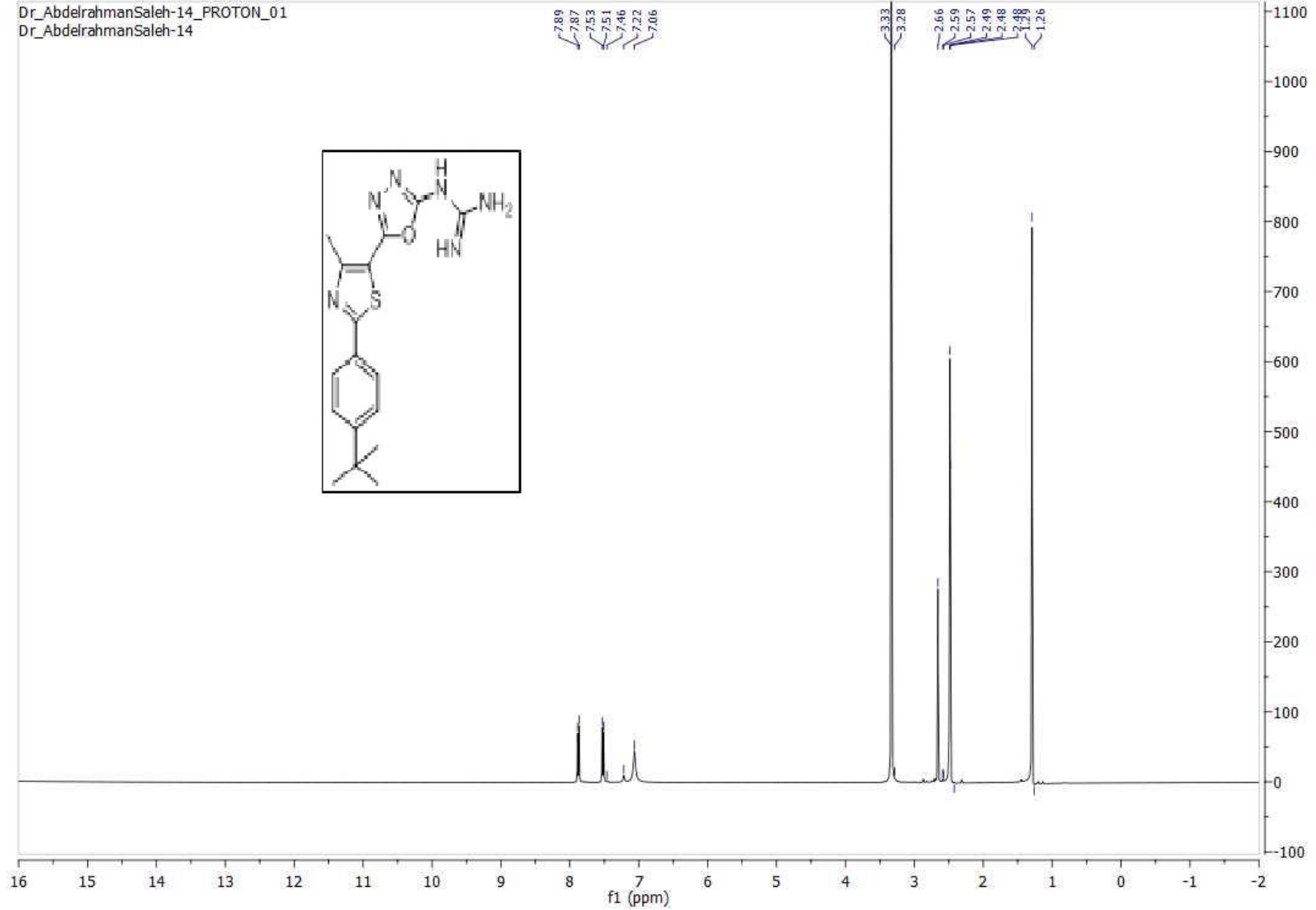
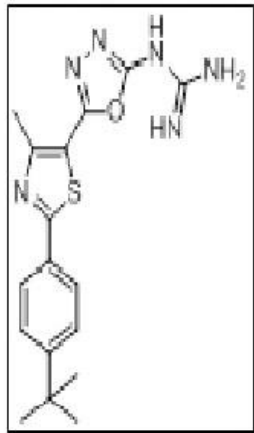
Mohamed Moustafa_C_Qt29
Mohamed Moustafa_C_Qt29

166.39
163.24
155.71
155.25
154.18
130.32
126.60
126.53
124.68

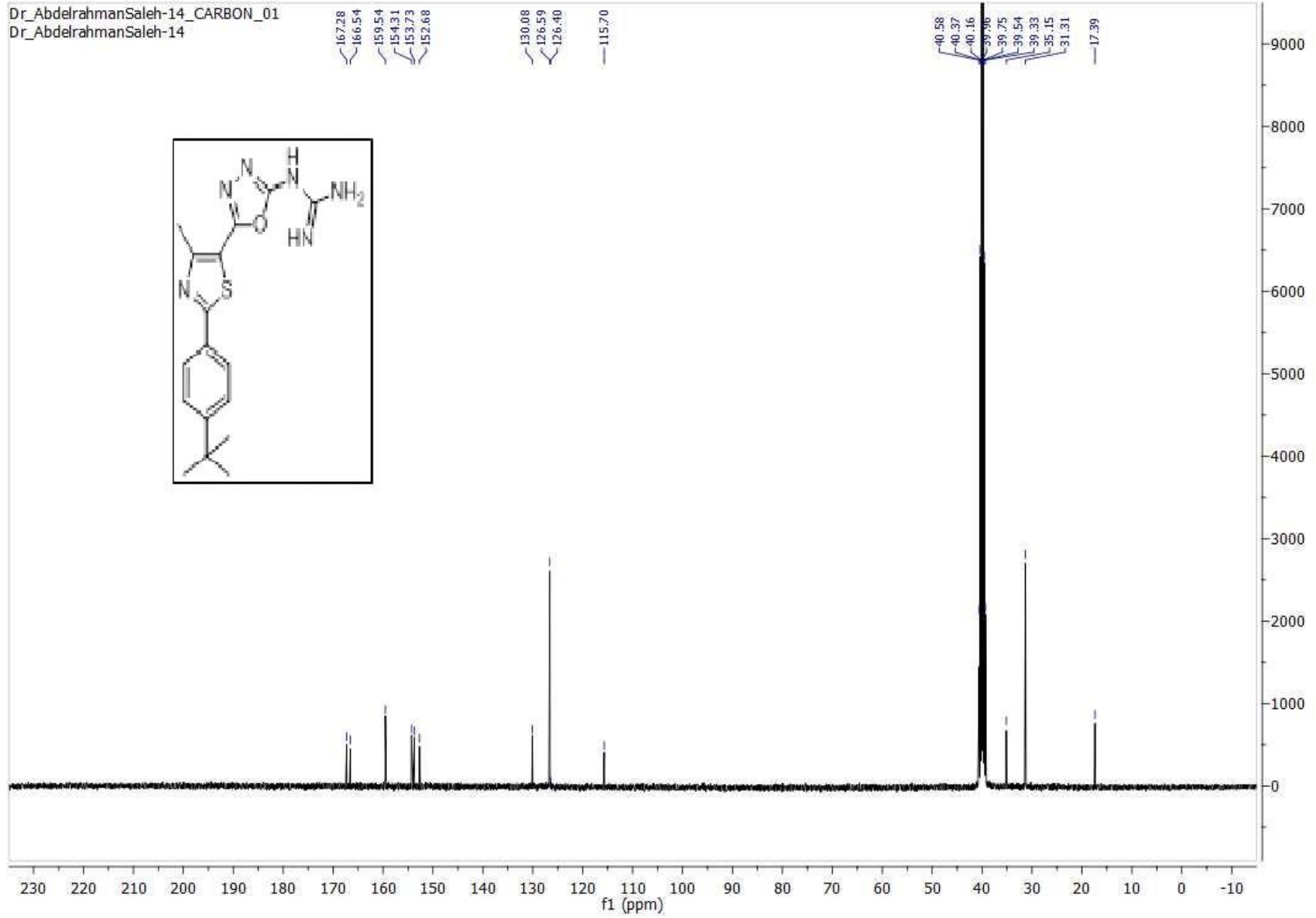
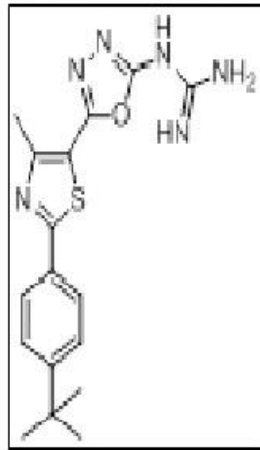
40.62
40.41
40.20
39.99
39.78
39.57
39.37
35.14
31.34
17.58



Dr_AbdelrahmanSaleh-14_PROTON_01
Dr_AbdelrahmanSaleh-14



Dr_AbdelrahmanSaleh-14_CARBON_01
Dr_AbdelrahmanSaleh-14



Mohamed Mostafa_H_Qt-20

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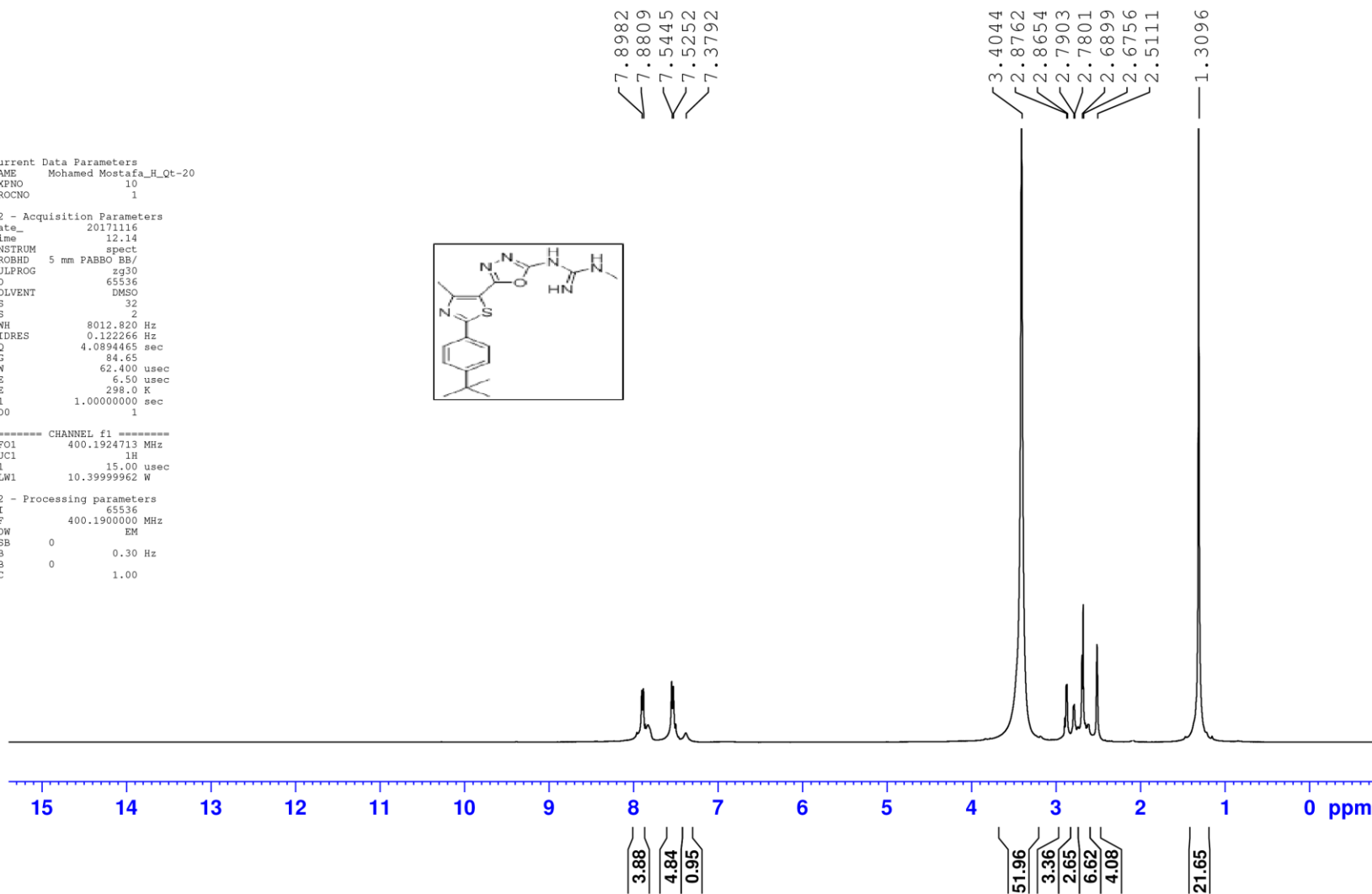
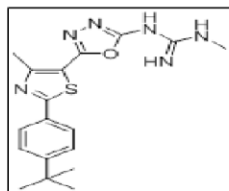


Current Data Parameters
NAME Mohamed Mostafa_H_Qt-20
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 12.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 84.65
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SF01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Mohamed Mostafa_C_Qt-20

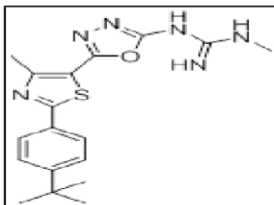
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166.58
164.24
154.39
153.85
153.08
130.10
130.03
126.62
126.58
115.01
40.58
40.37
40.16
39.96
39.75
39.54
39.33
35.16
31.31
29.50
17.40

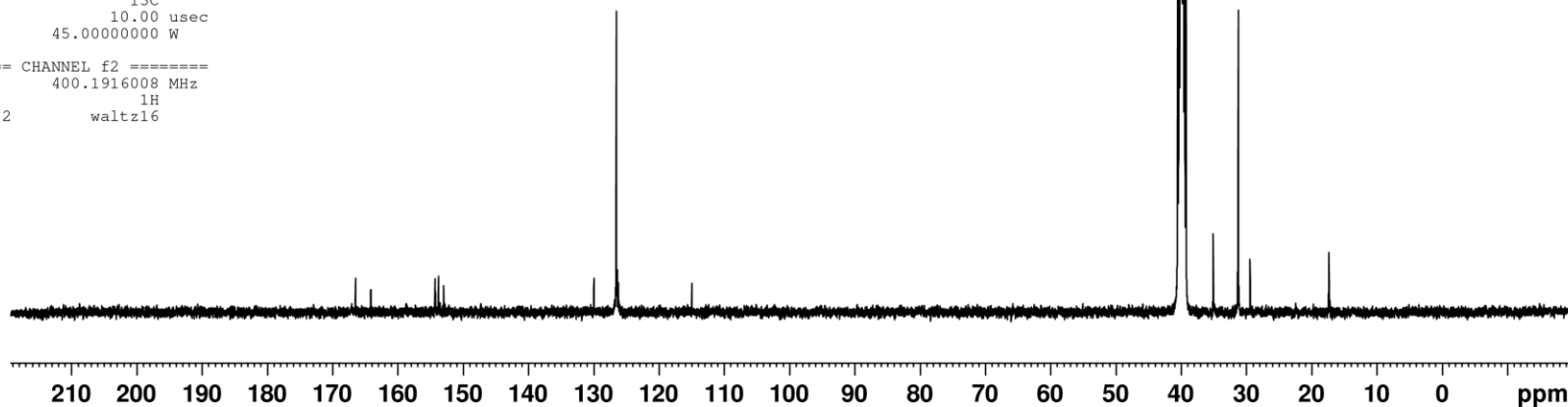
Current Data Parameters
NAME Mohamed Mostafa_C_Qt-20
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 13.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

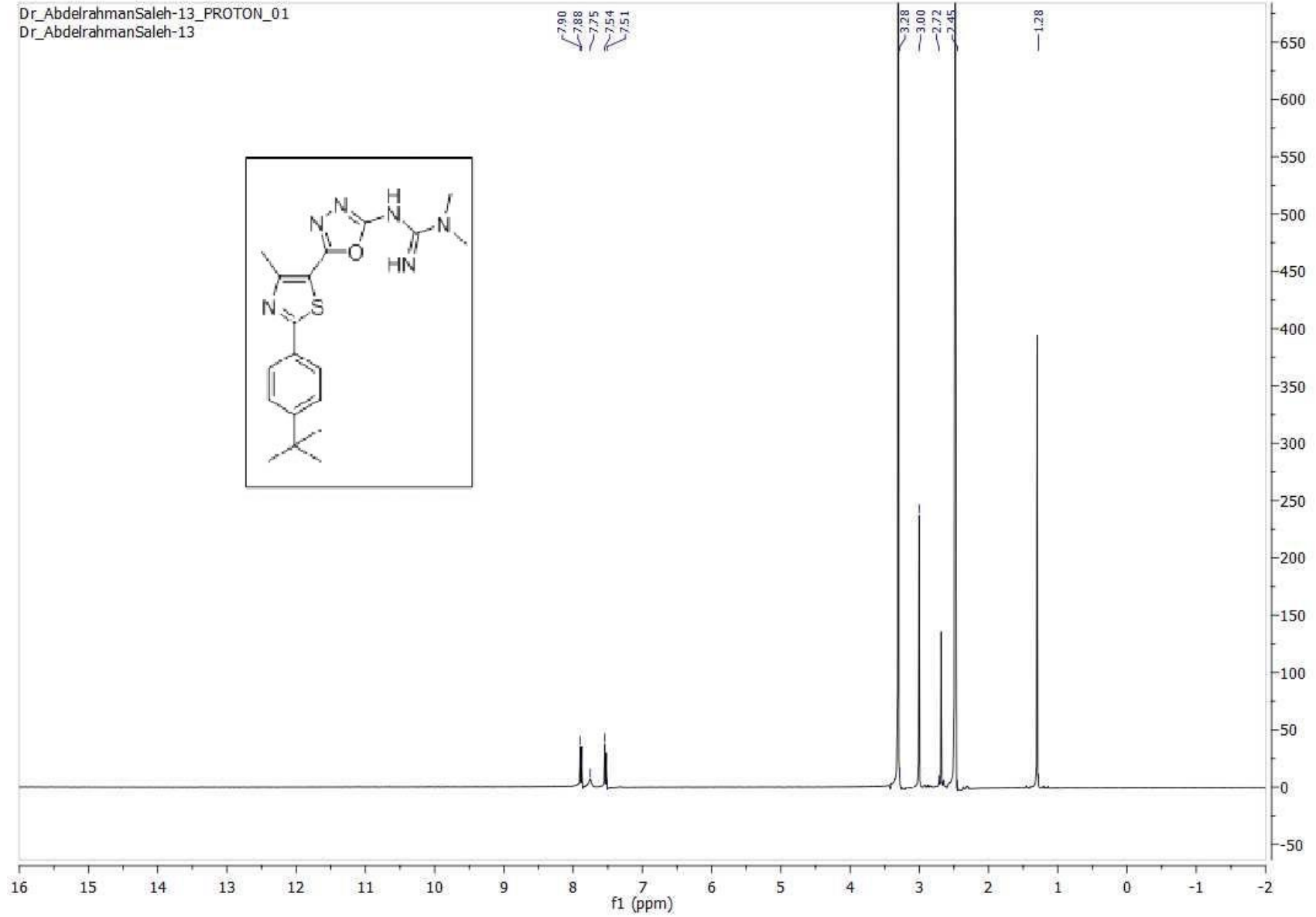
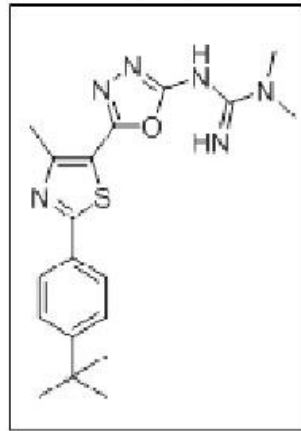


==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

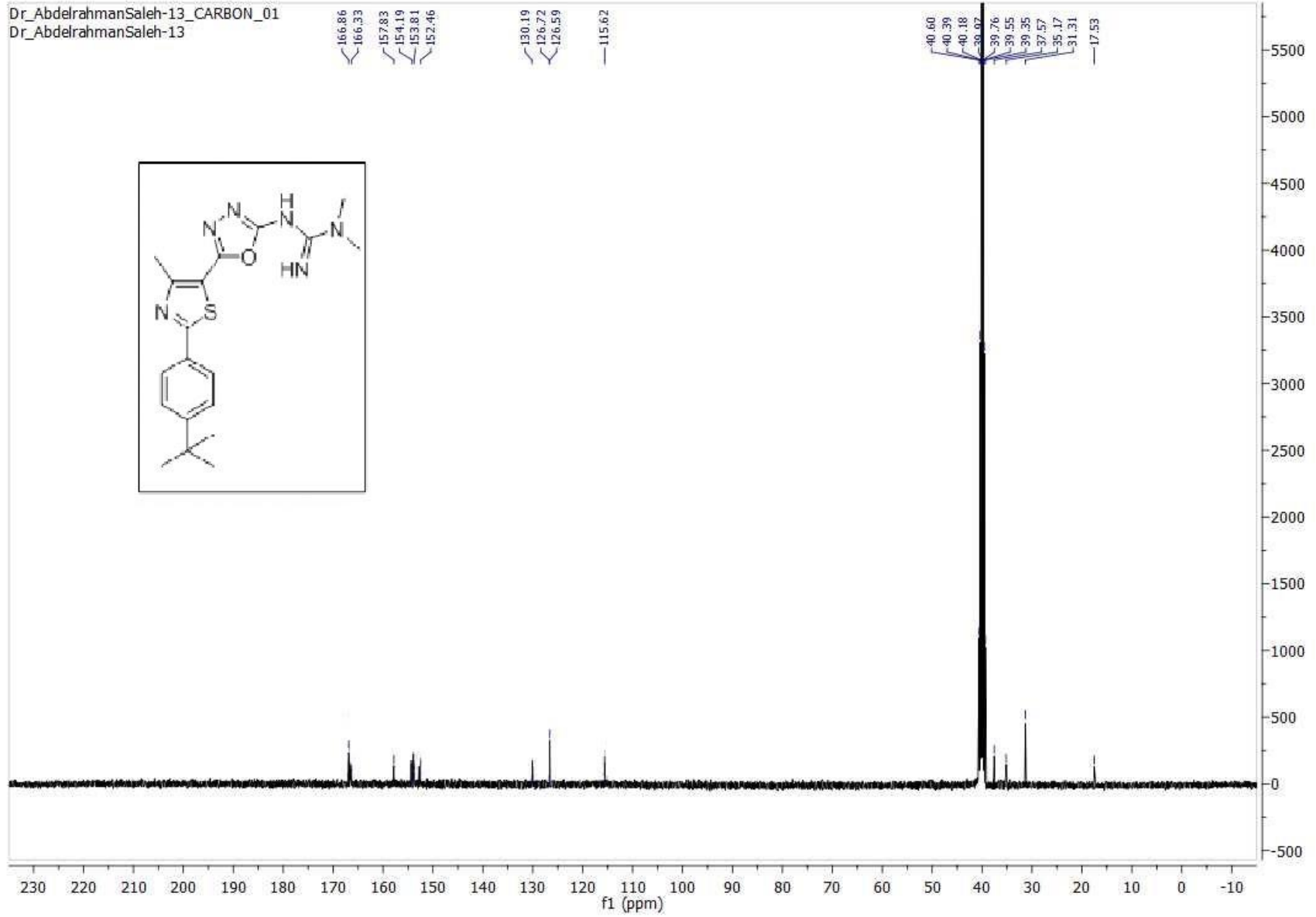
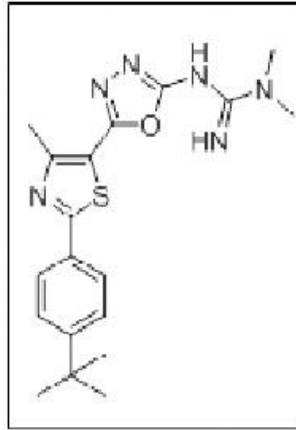
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2 waltz16



Dr_AbdelrahmanSaleh-13_PROTON_01
Dr_AbdelrahmanSaleh-13



Dr_AbdelrahmanSaleh-13_CARBON_01
Dr_AbdelrahmanSaleh-13



Mohamed Mostafa_H_Qt-15

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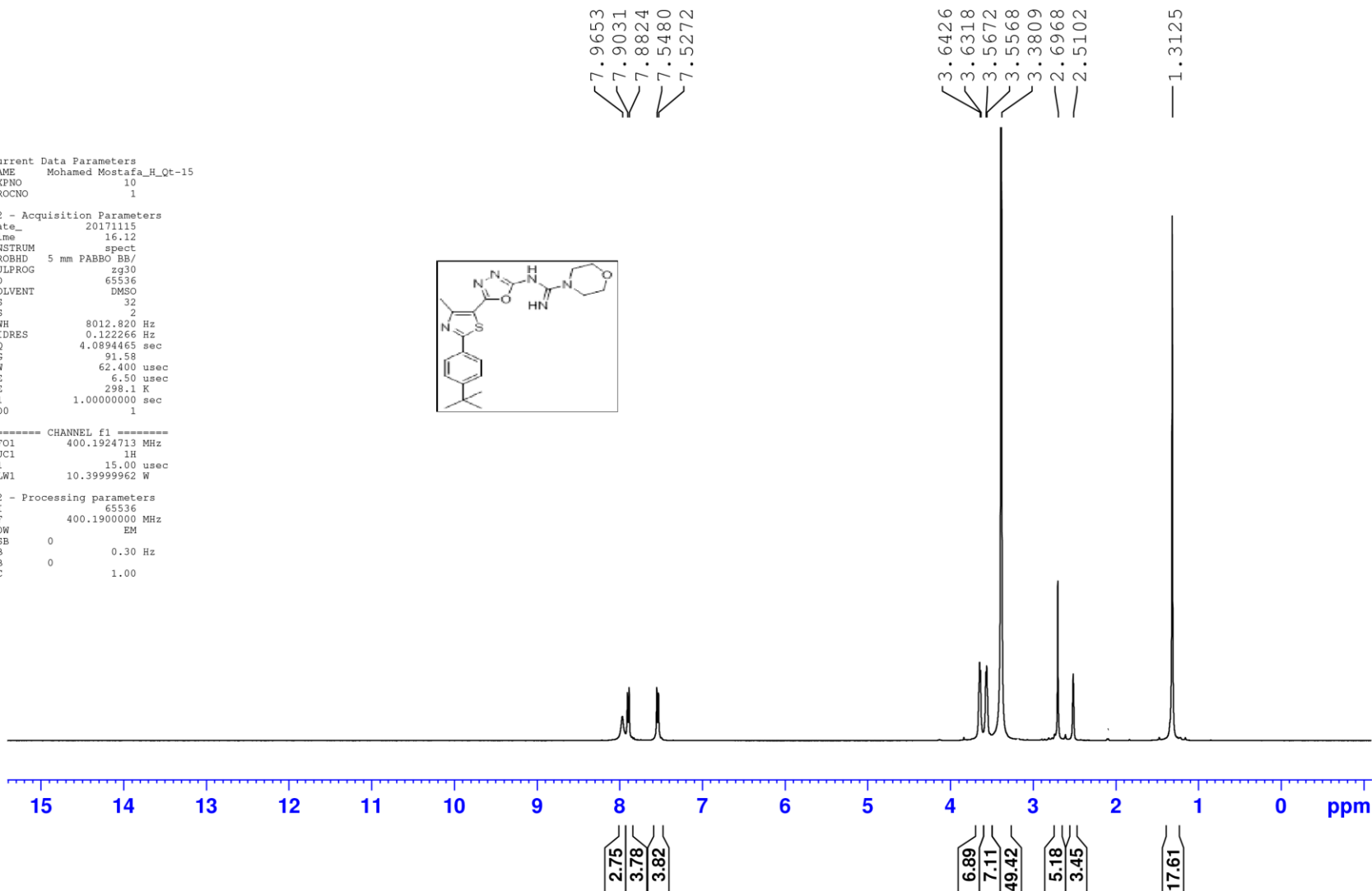
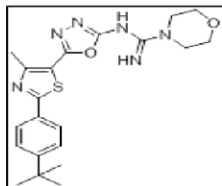


Current Data Parameters
NAME Mohamed Mostafa_H_Qt-15
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171115
Time 16.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 91.58
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Mohamed Mostafa_C_Qt-15

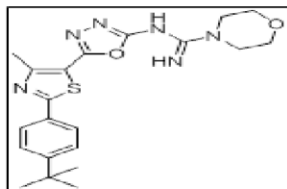
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166.90
166.80
157.22
154.39
154.15
153.21
130.07
126.62
126.58
115.48
66.16
44.88
40.58
40.37
40.16
39.96
39.75
39.54
39.33
35.16
31.31
17.52

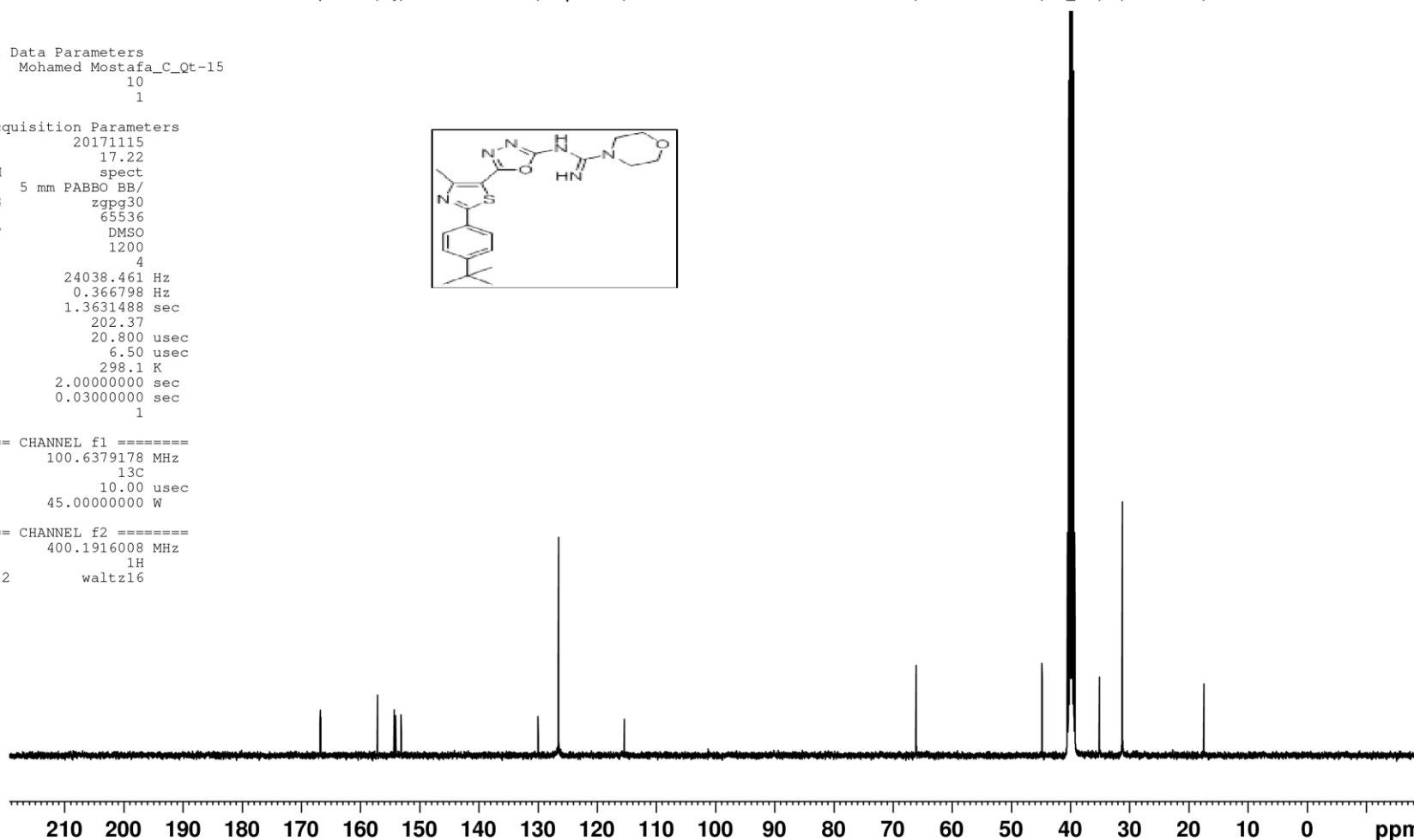
Current Data Parameters
NAME Mohamed Mostafa_C_Qt-15
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171115
Time 17.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

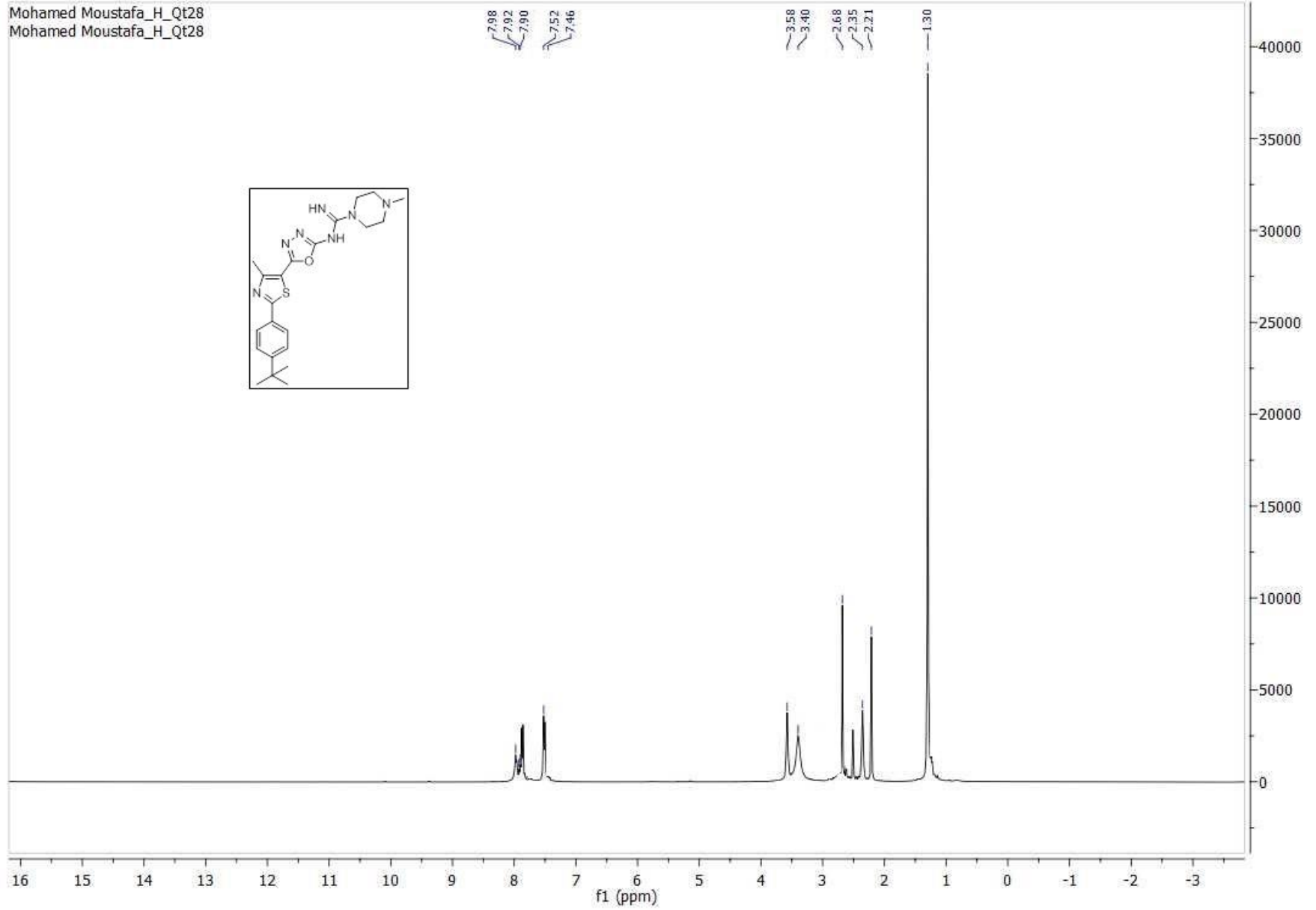
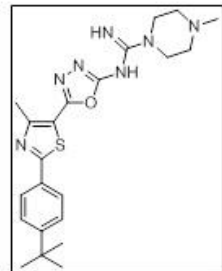


==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

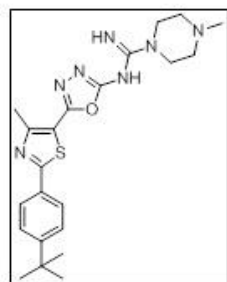
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG2 waltz16



Mohamed Moustafa_H_Qt28
Mohamed Moustafa_H_Qt28



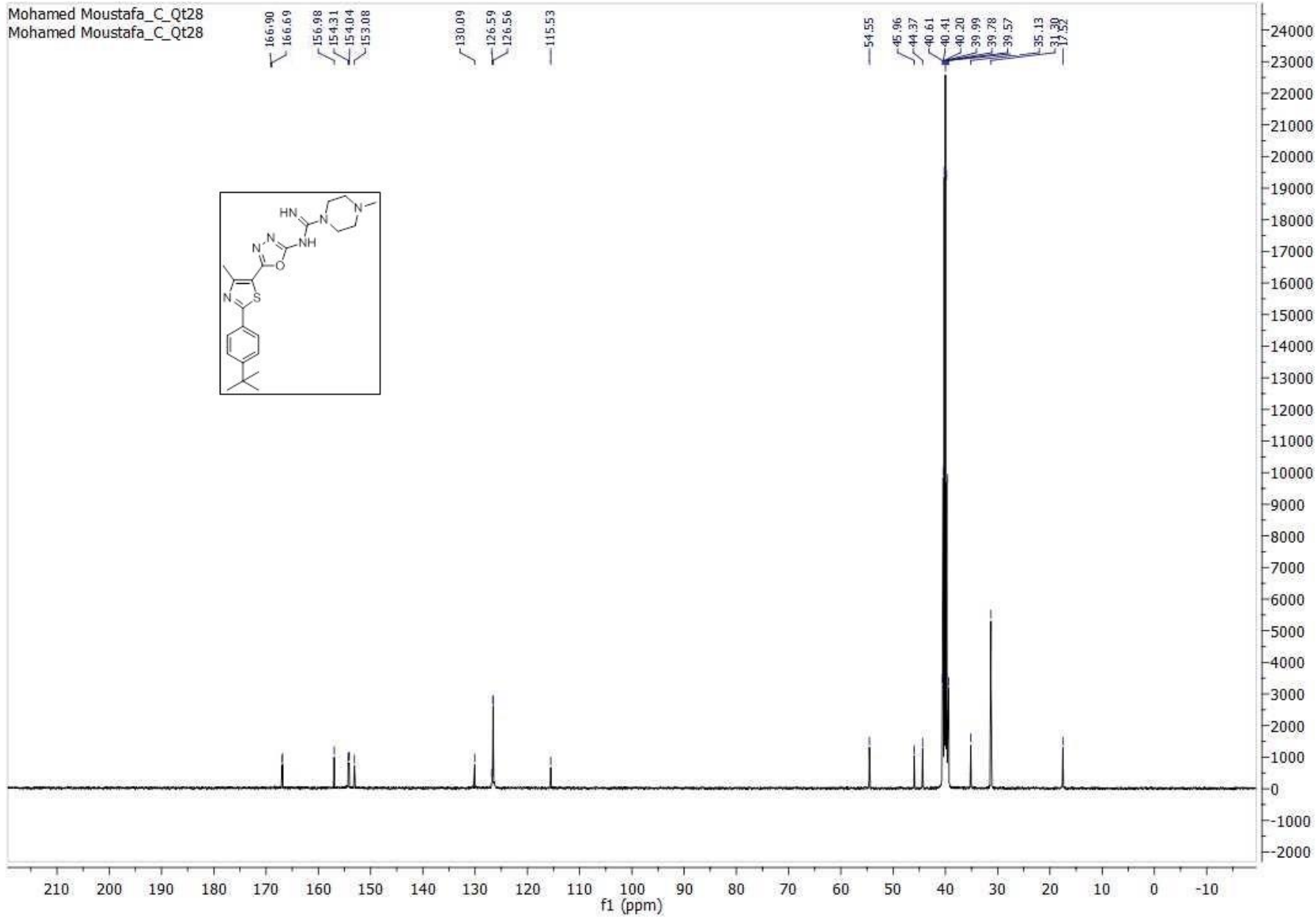
Mohamed Moustafa_C_Qt28
Mohamed Moustafa_C_Qt28



166.90
166.69
156.98
154.31
154.04
153.08

130.09
126.59
126.56
115.53

54.55
45.96
44.37
40.61
40.41
40.20
39.99
39.78
39.57
35.13
31.30
31.29



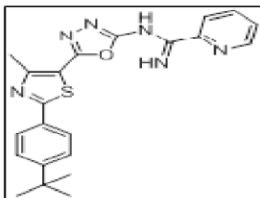
Mohamed Mostafa_H_Qt-17

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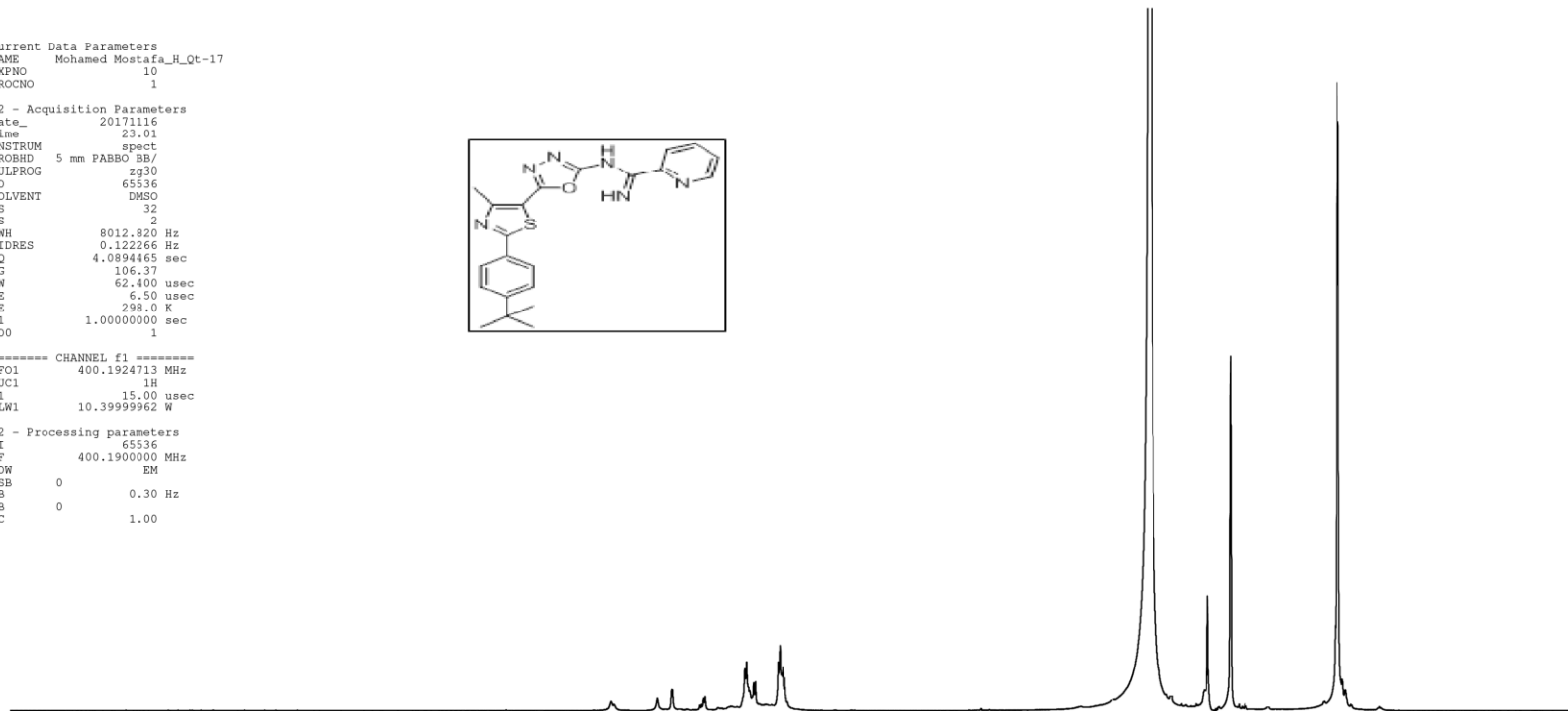
Current Data Parameters
NAME Mohamed Mostafa_H_Qt-17
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 23.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 106.37
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1



9.4348
8.9228
8.7616
8.4037
8.3850
7.9426
7.9226
7.8445
7.8241
7.5703
7.5503
7.5293
7.5178
7.4970
3.4125
3.1678
2.6861
2.6113
2.0874
1.3397
1.3188
1.3050

==== CHANNEL f1 =====
SP01 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W
F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm

0.42
1.39
6.80
69.07
8.94
12.90

Mohamed Mostafa_C_MAS-85

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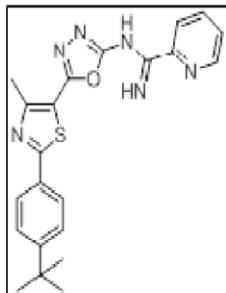


167.27
166.95
162.82
158.48
158.09
154.22
153.91
149.00
138.01
131.72
130.50
126.56
126.48
122.69
111.43

40.58
40.38
40.17
39.75
39.54
39.33
35.15
31.34
18.70

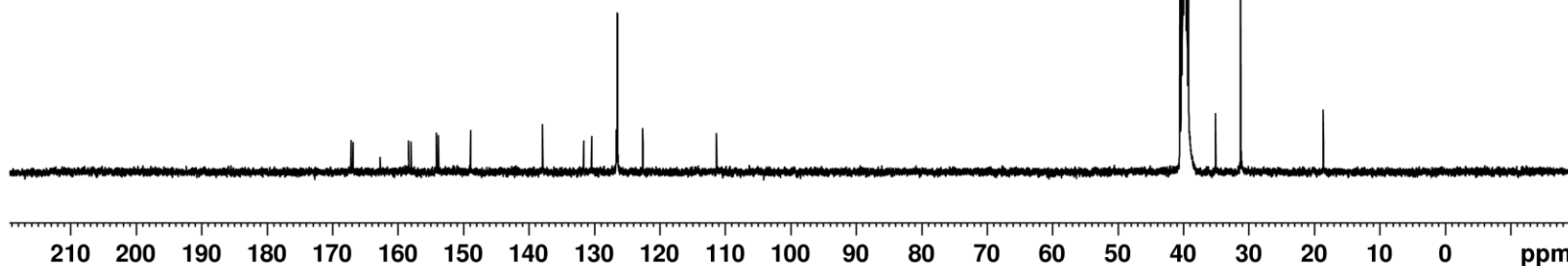
Current Data Parameters
NAME Mohamed Mostafa_C_MAS-8
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171115
Time 18.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



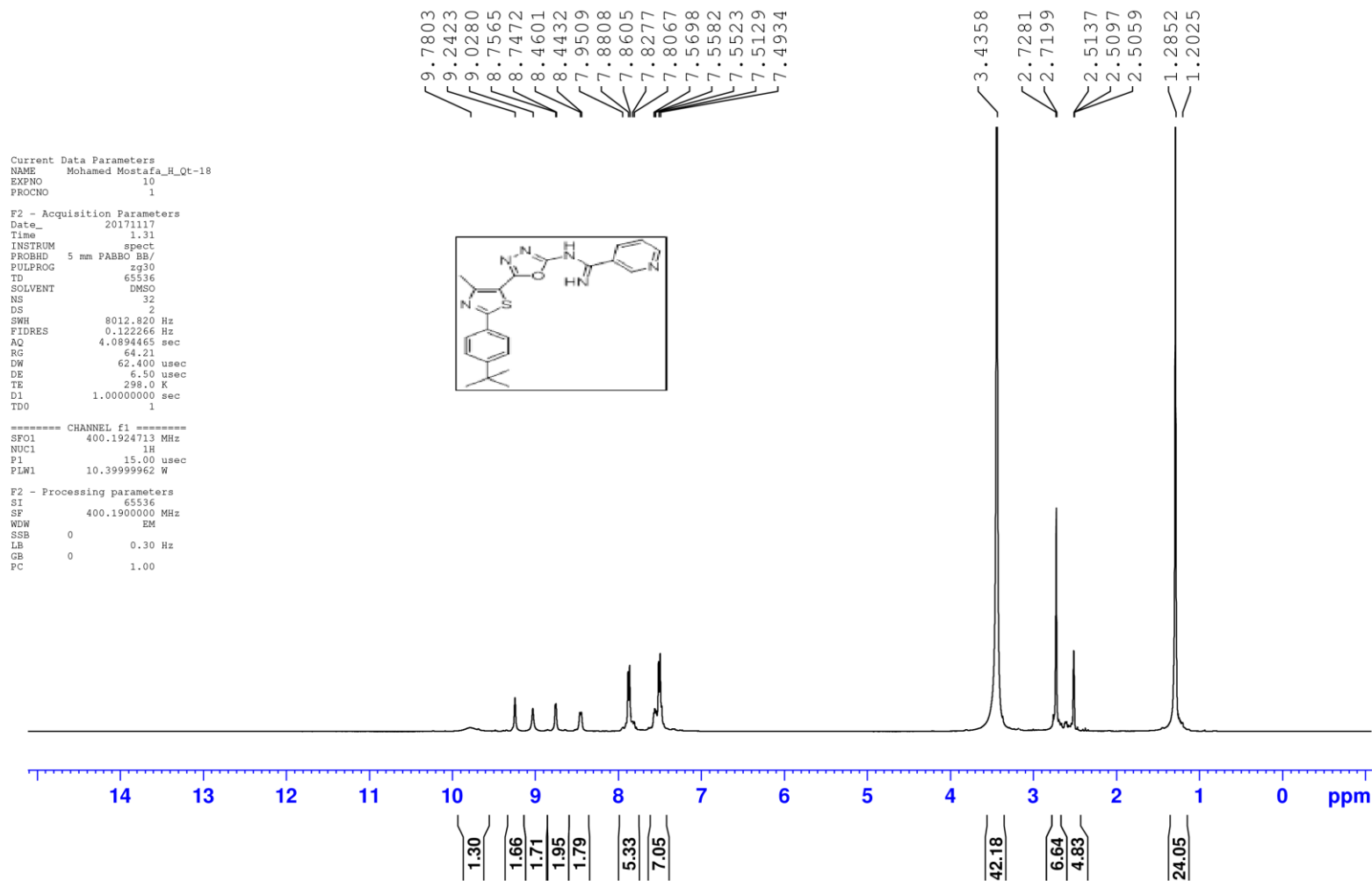
===== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

===== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



Mohamed Mostafa_H_Qt-18

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Mohamed Mostafa_C_Qt-18

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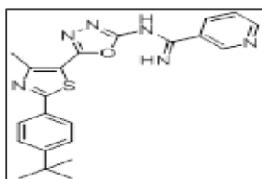


167.67
166.41
160.51
155.43
155.10
154.53
152.85
149.22
135.92
130.64
129.66
126.57
126.43
123.95
114.84

40.56
40.36
40.15
39.94
39.73
39.52
39.31
35.14
31.34
17.63

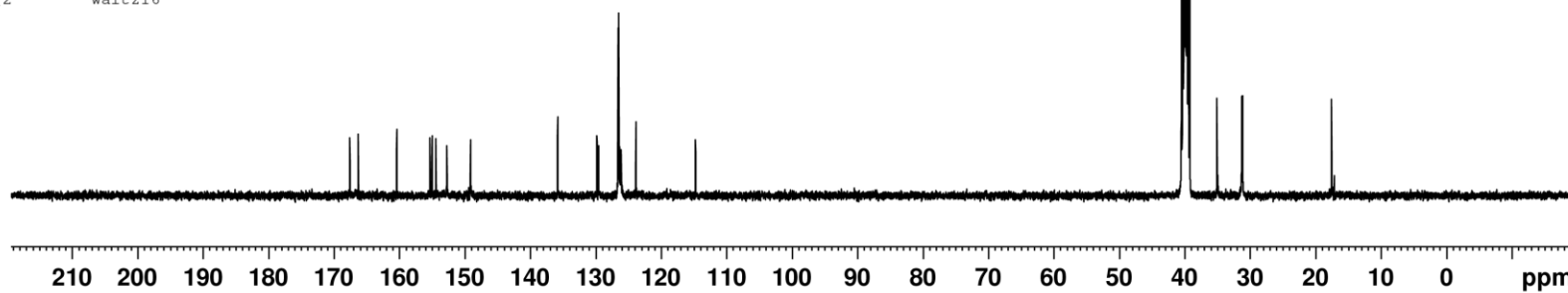
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NAME Mohamed Mostafa_C_Qt-18
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171117
Time 2.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1



==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.00000000 W

==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



Mohamed Mostafa_H_Qt-19

Microanalytical Unit - FOPCU - NMR laboratory
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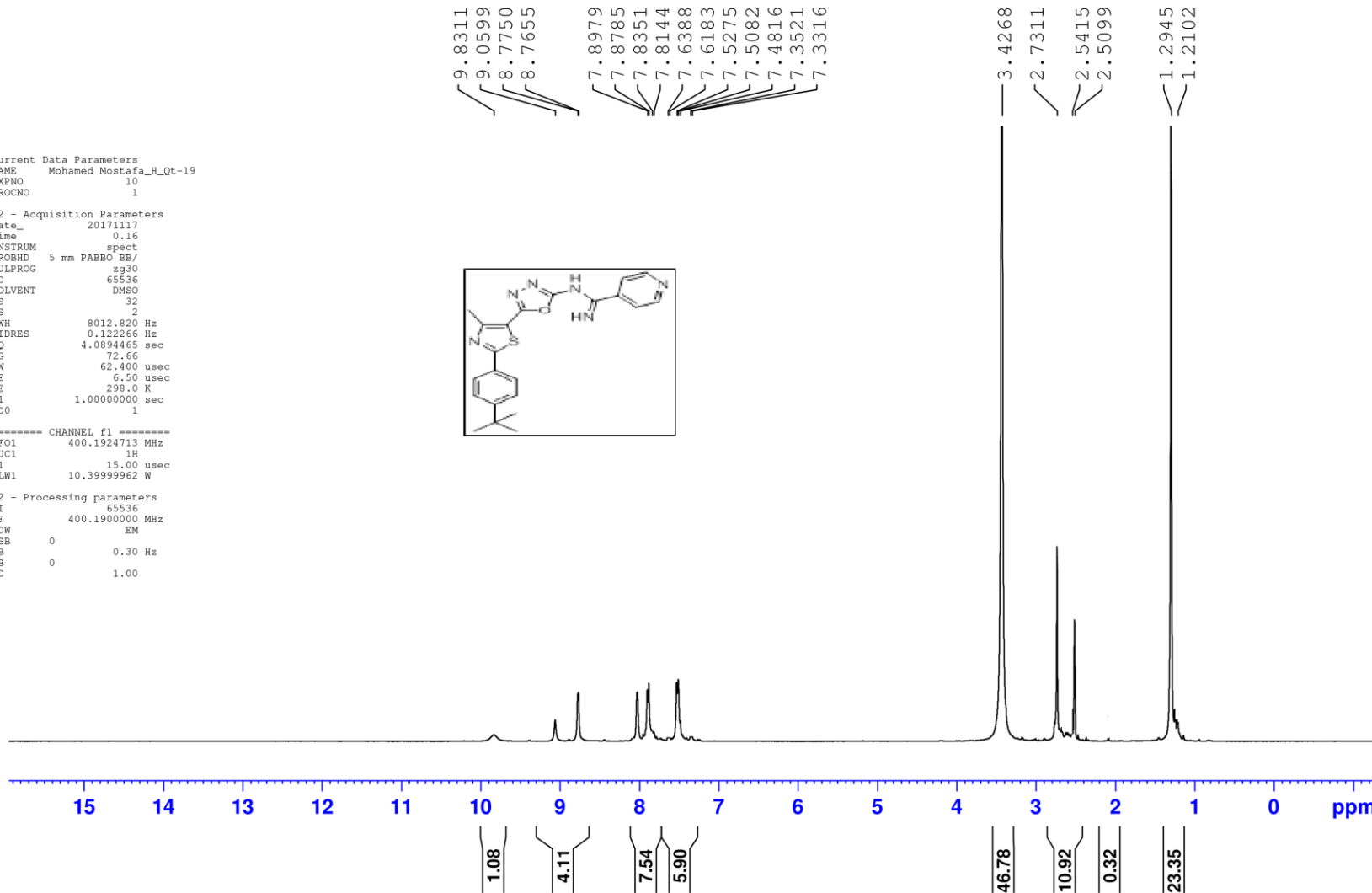
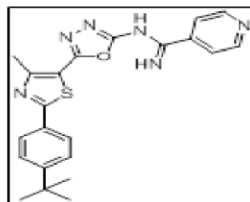
Current Data Parameters
NAME Mohamed Mostafa_H_Qt-19
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171117
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INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT DMSO
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 72.66
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TDO 1

----- CHANNEL f1 -----
SFO1 400.1924713 MHz
NUC1 1H
P1 15.00 usec
PLW1 10.39999962 W

F2 - Processing parameters
SI 65536
SF 400.1900000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

9.8311
9.0599
8.7750
8.7655
7.8979
7.8785
7.8351
7.8144
7.6388
7.6183
7.5275
7.5082
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2.5415
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1.2945
1.2102



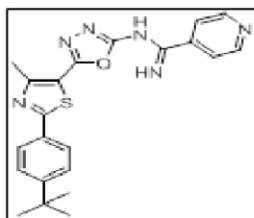
Mohamed Mostafa_C_Qt-19

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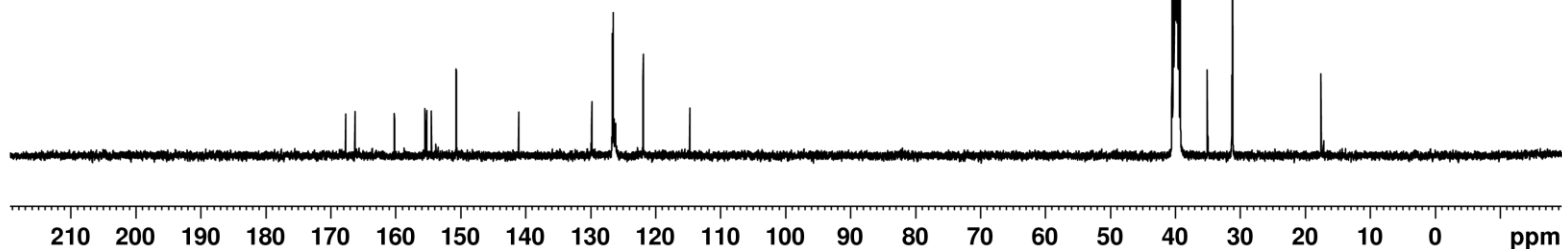
Current Data Parameters
NAME Mohamed Mostafa_C_Qt-19
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 202.37
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

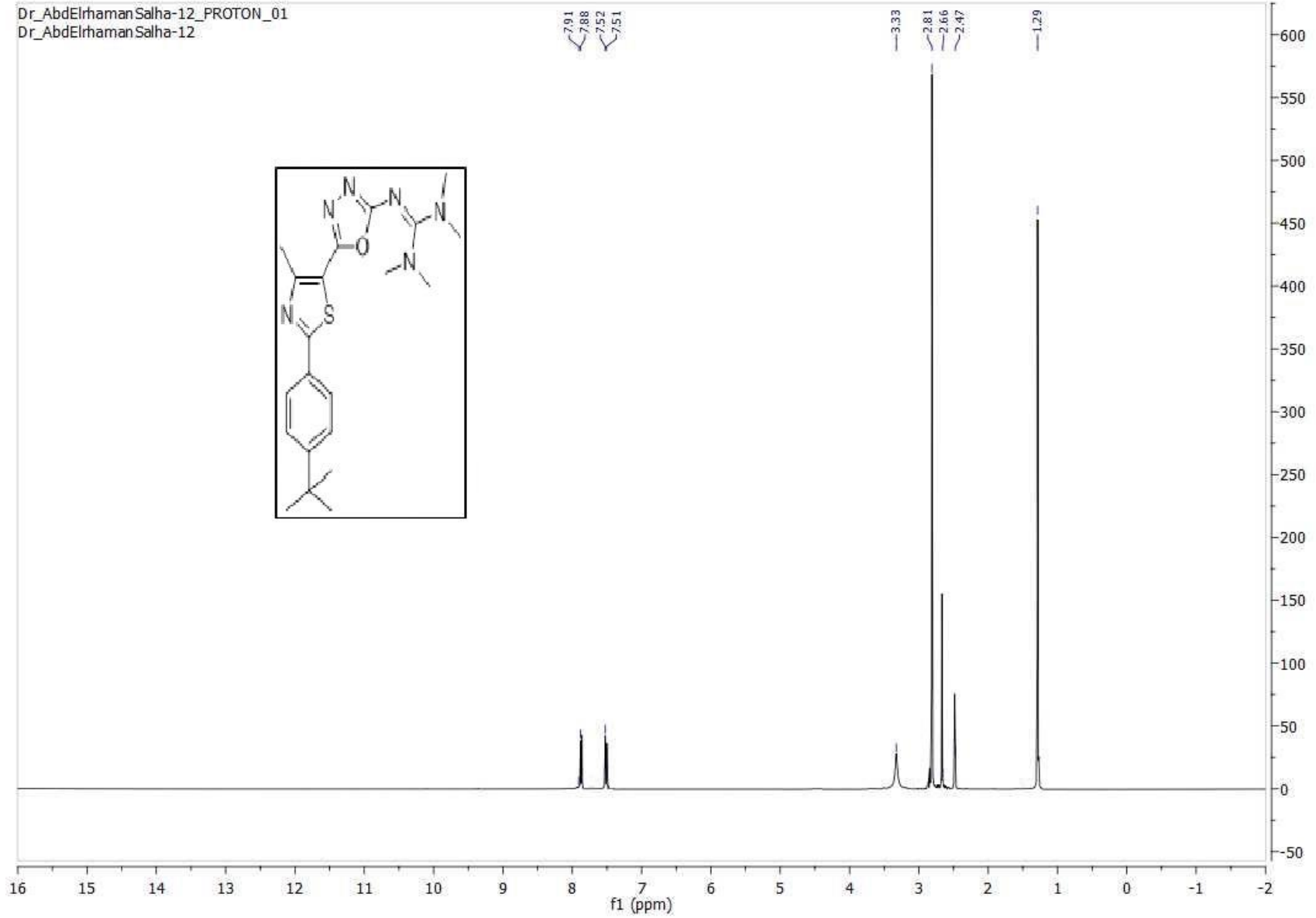
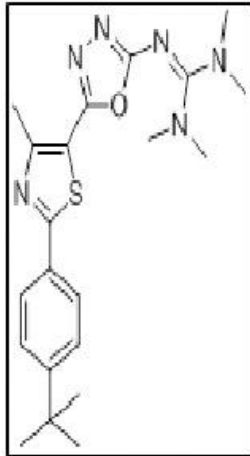


==== CHANNEL f1 =====
SFO1 100.6379178 MHz
NUC1 13C
P1 10.00 usec
PLW1 45.0000000 W

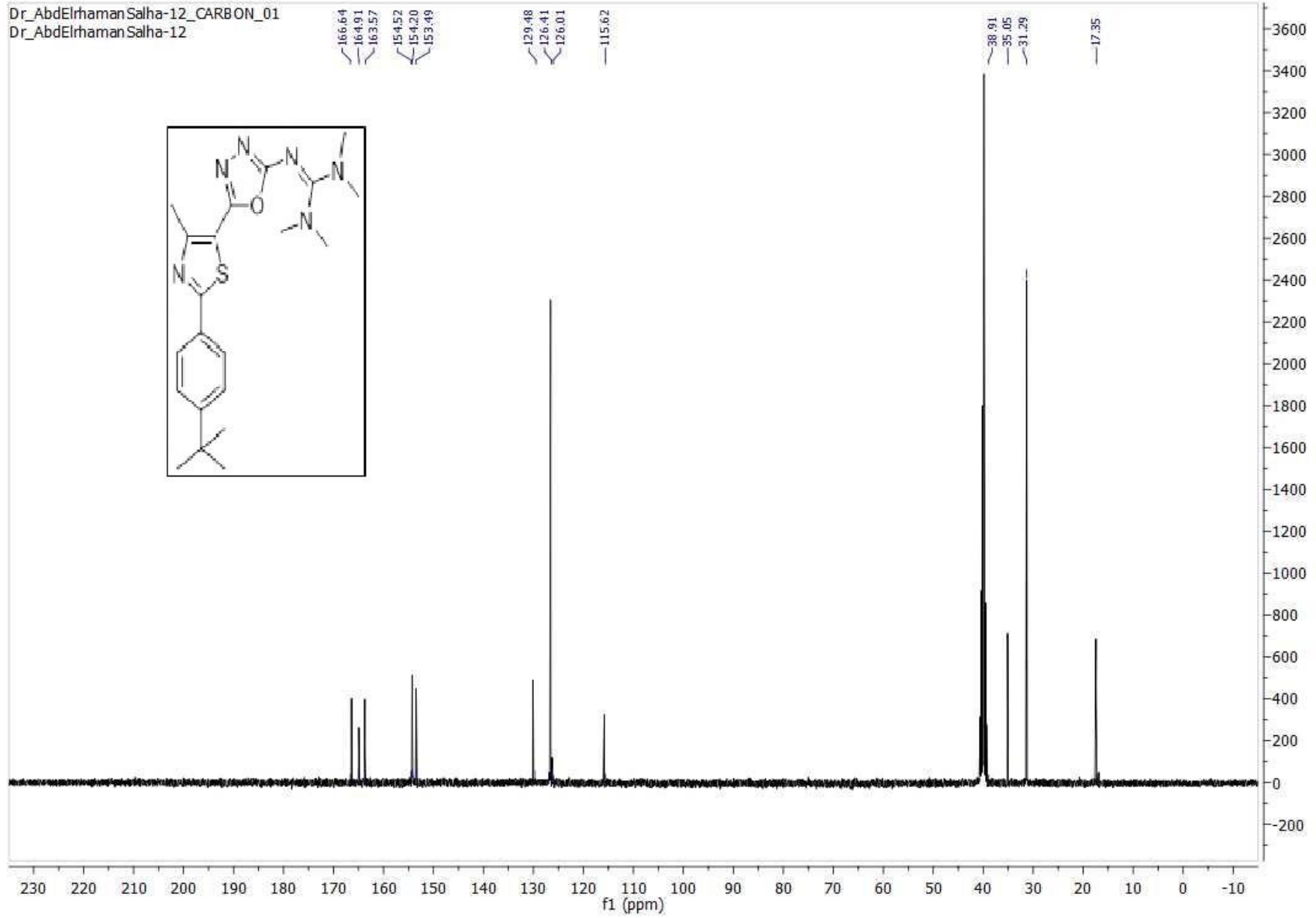
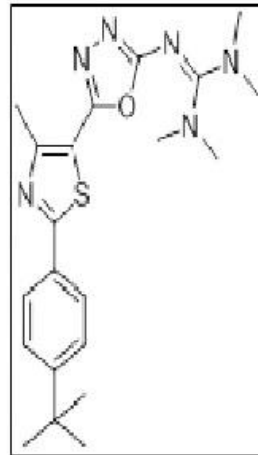
==== CHANNEL f2 =====
SFO2 400.1916008 MHz
NUC2 1H
CPDPRG[2] waltz16



Dr_AbdElrhman Salha-12_PROTON_01
Dr_AbdElrhman Salha-12



Dr_AbdElrhman Salha-12_CARBON_01
Dr_AbdElrhman Salha-12



References:

- [1] H. Mohammad, K. Kyei-Baffour, W. Younis, D.C. Davis, H. Eldesouky, M.N. Seleem, M.J. Dai, Investigation of aryl isonitrile compounds with potent, broad-spectrum antifungal activity, *Bioorgan Med Chem*, 25 (2017) 2926-2931.
- [2] A. Kotb, N.S. Abutaleb, M.A. Seleem, M. Hagra, H. Mohammad, A. Bayoumi, A. Ghiaty, M.N. Seleem, A.S. Mayhoub, Phenylthiazoles with tert-Butyl side chain: Metabolically stable with anti-biofilm activity, *European journal of medicinal chemistry*, 151 (2018) 110-120.