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 ºC with CO_2 (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 OD_{490}) 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).

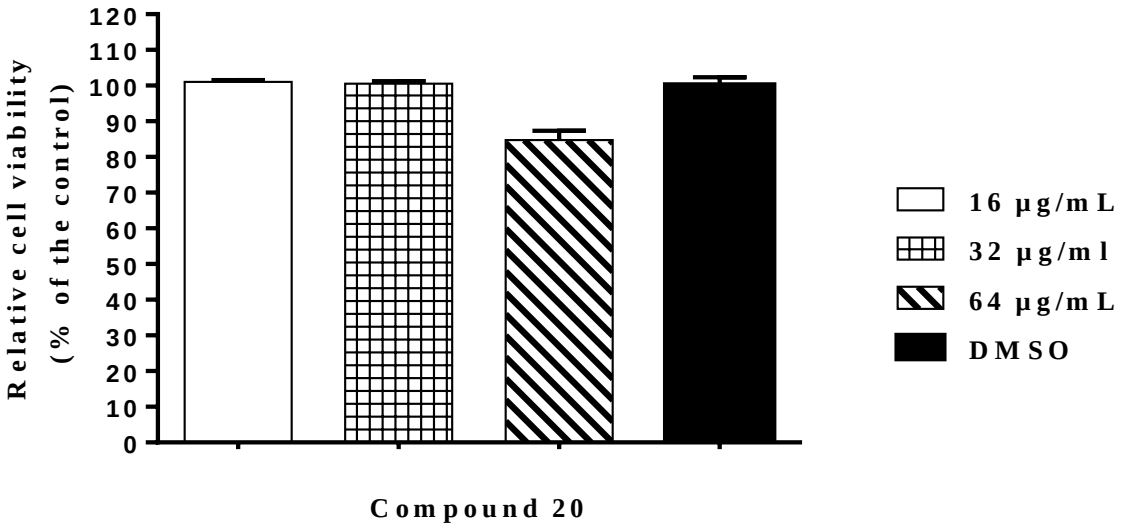


Figure 1S: *In vitro* cytotoxicity analysis of compound 20 against fibroblast-like monkey kidney cells (Vero cells) using the MTS 3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2*H*-tetrazolium) assay. Results are presented as percent viable mammalian cells (measured as average 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.

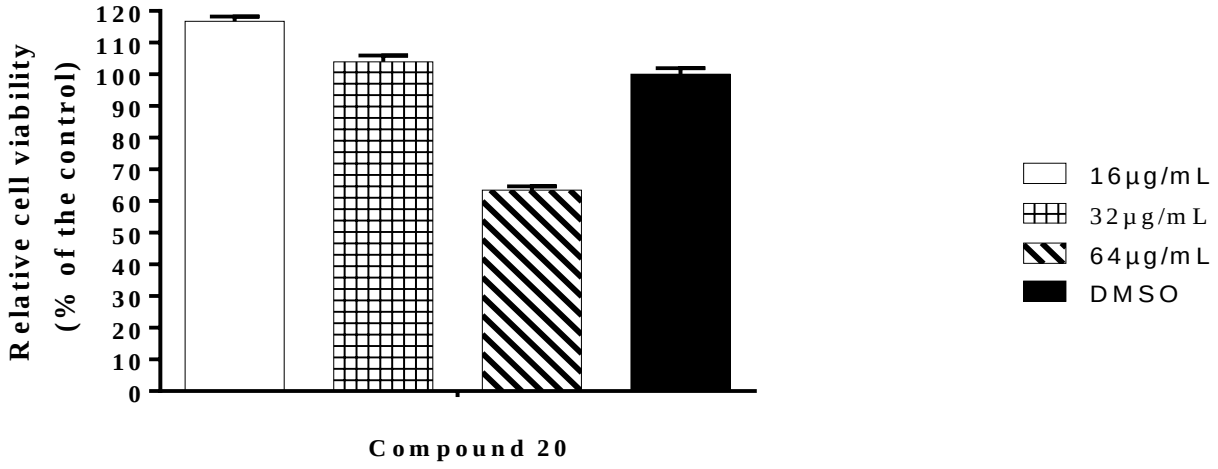
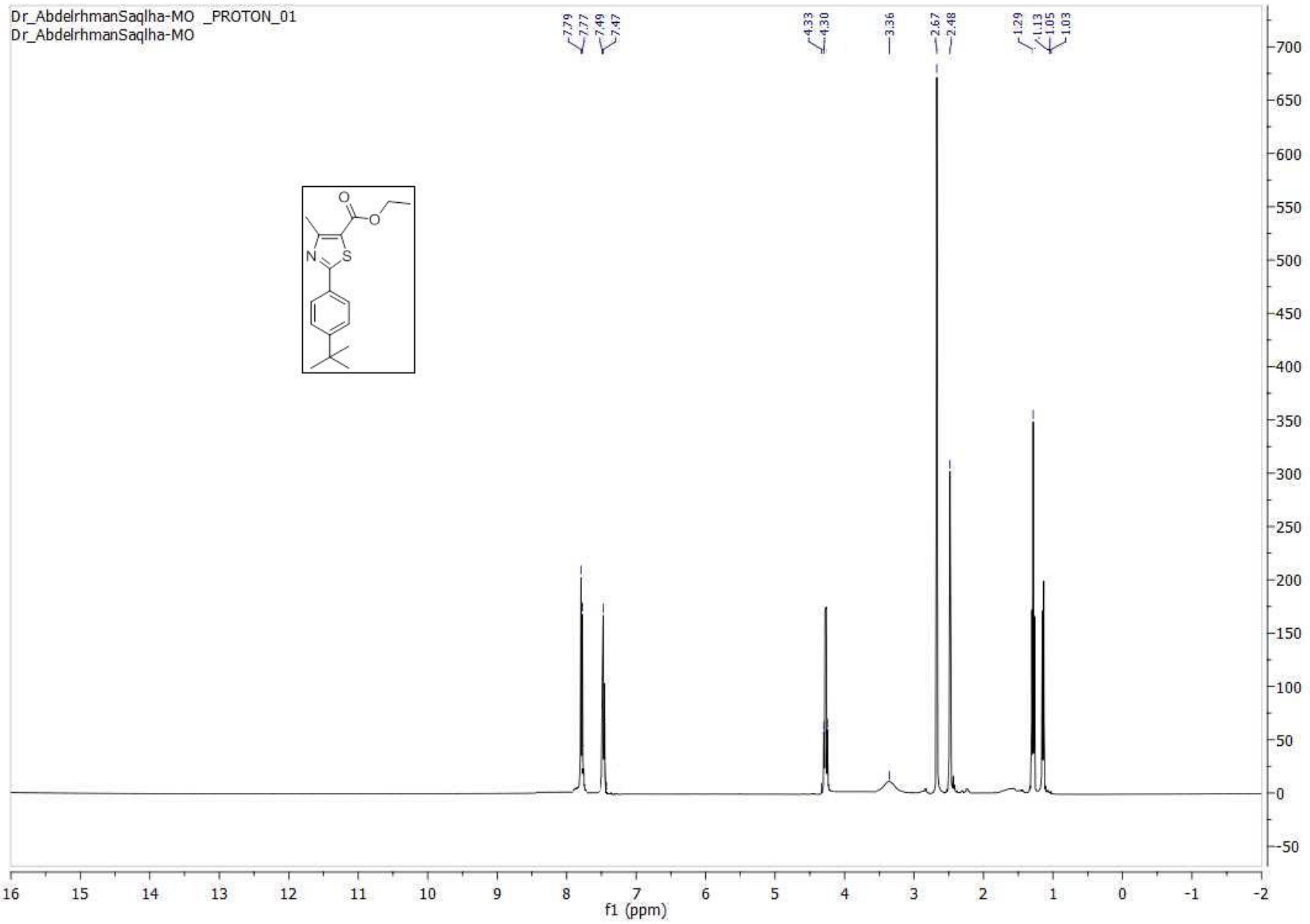


Figure 2S: *In vitro* cytotoxicity analysis of compound 20 against human colorectal adenocarcinoma (Caco-2) using the MTS 3-(4,5-dimethylthiazol-2-yl)-5-(3-

carboxymethoxyphenyl)-2-(4-sulfophenyl)-2*H*-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 (CC_{50}), 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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1.03
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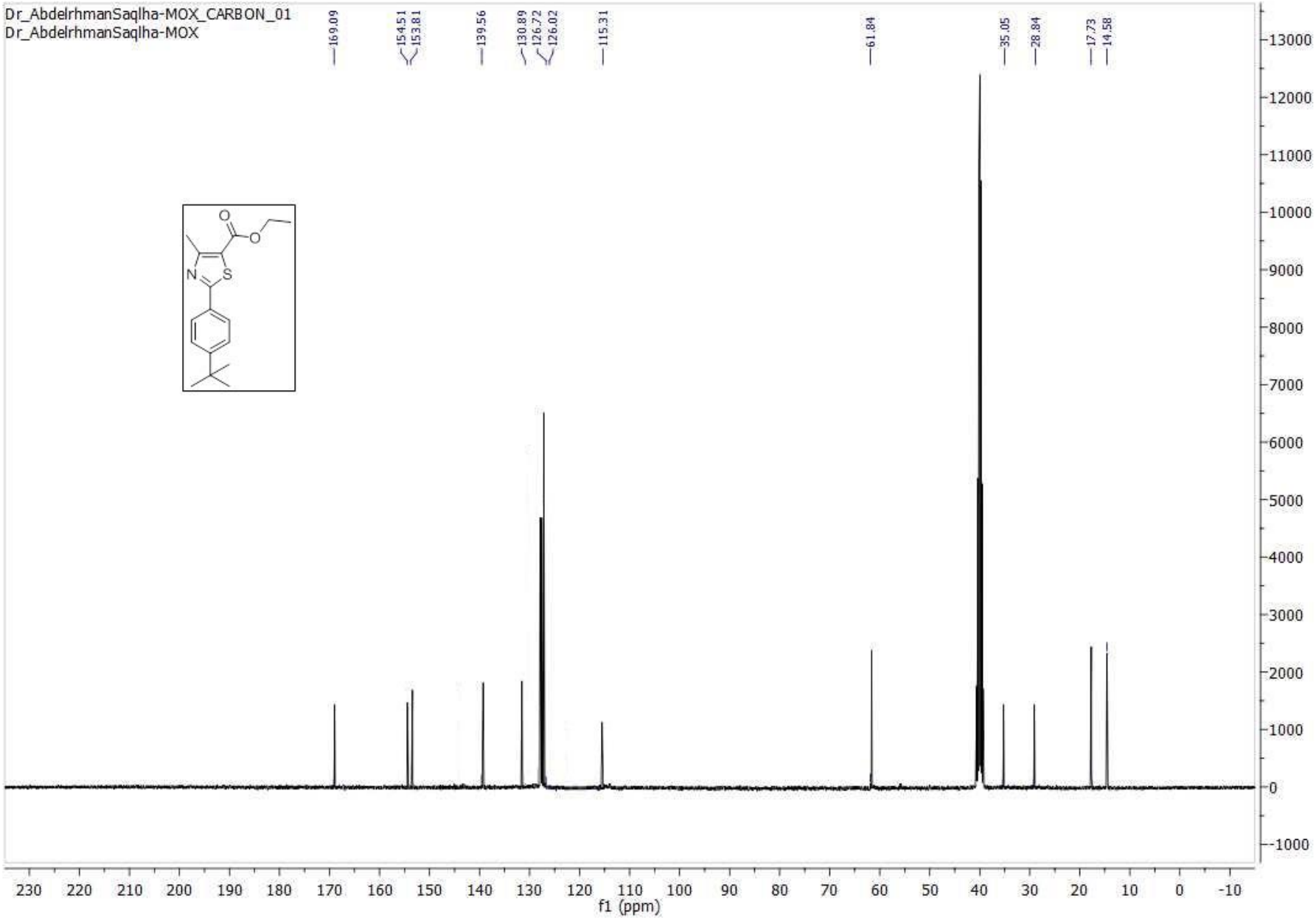
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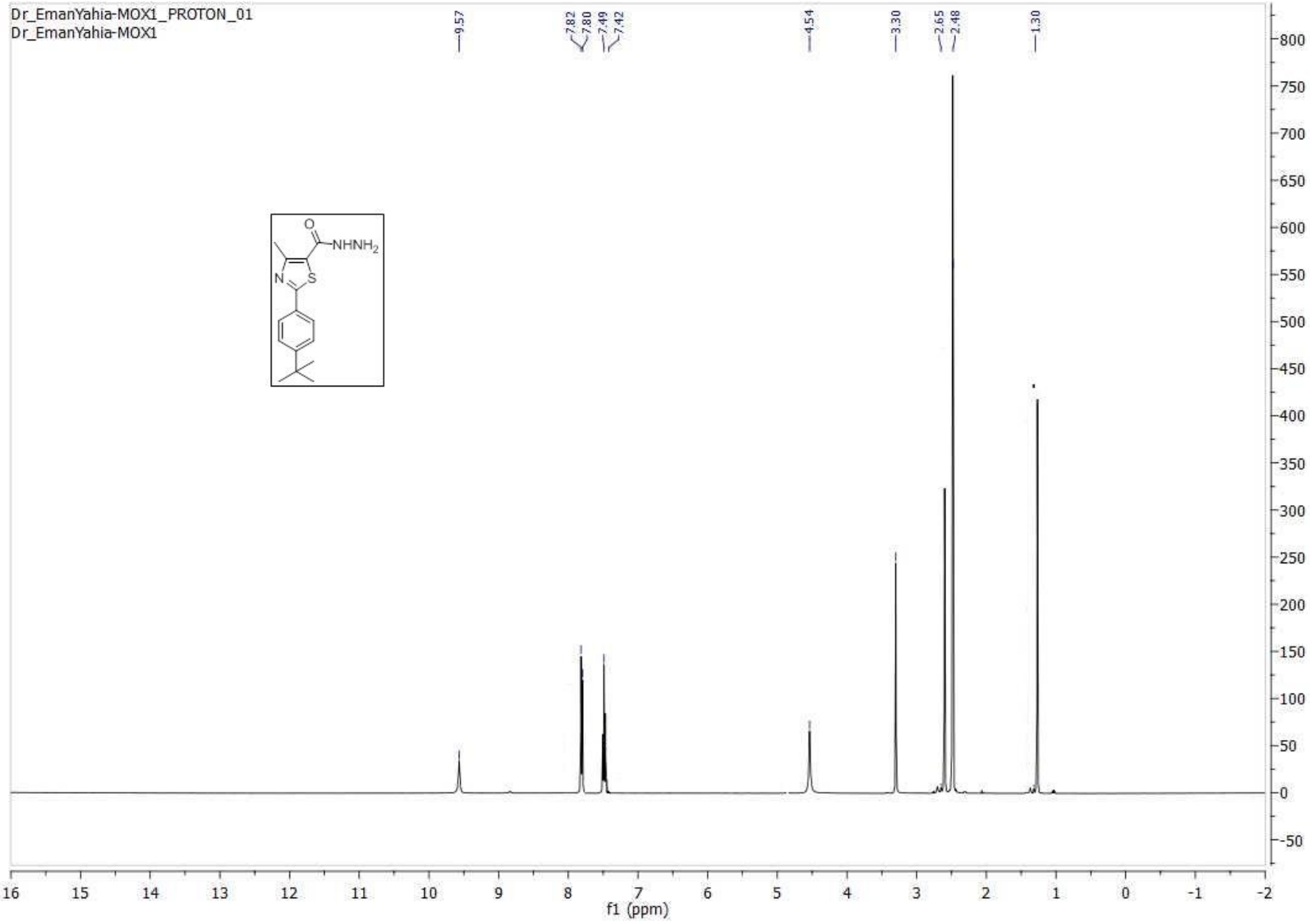
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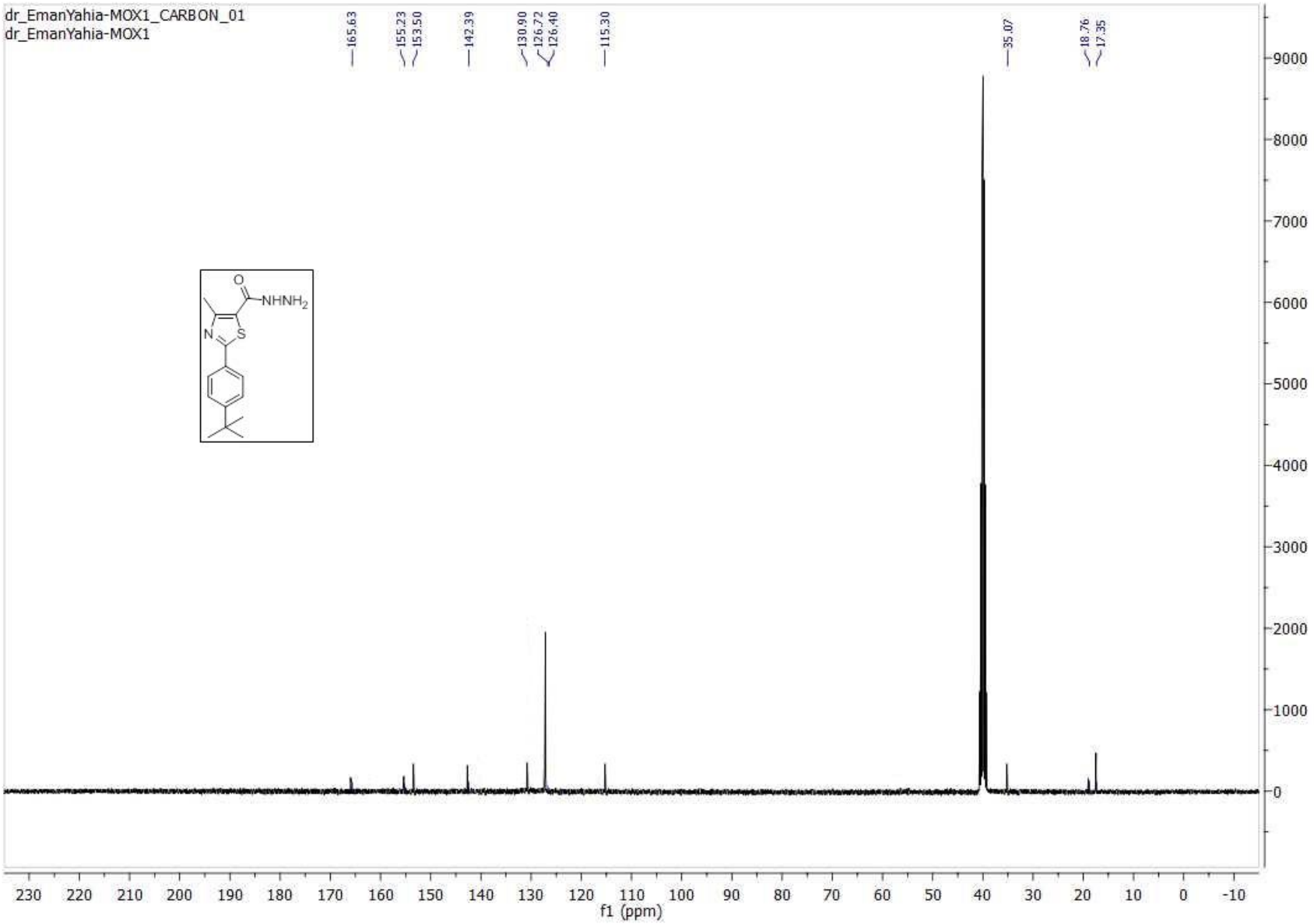
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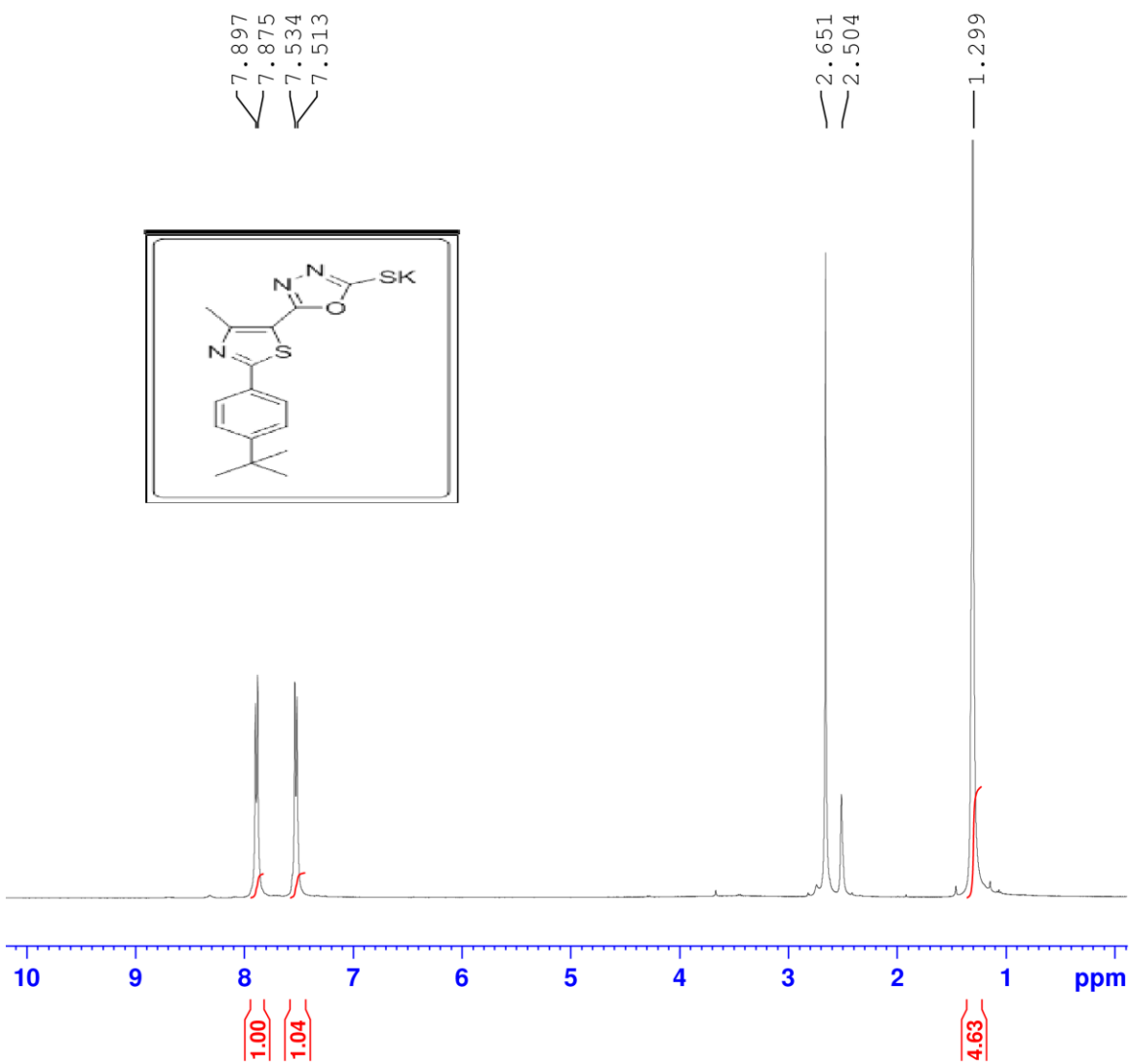

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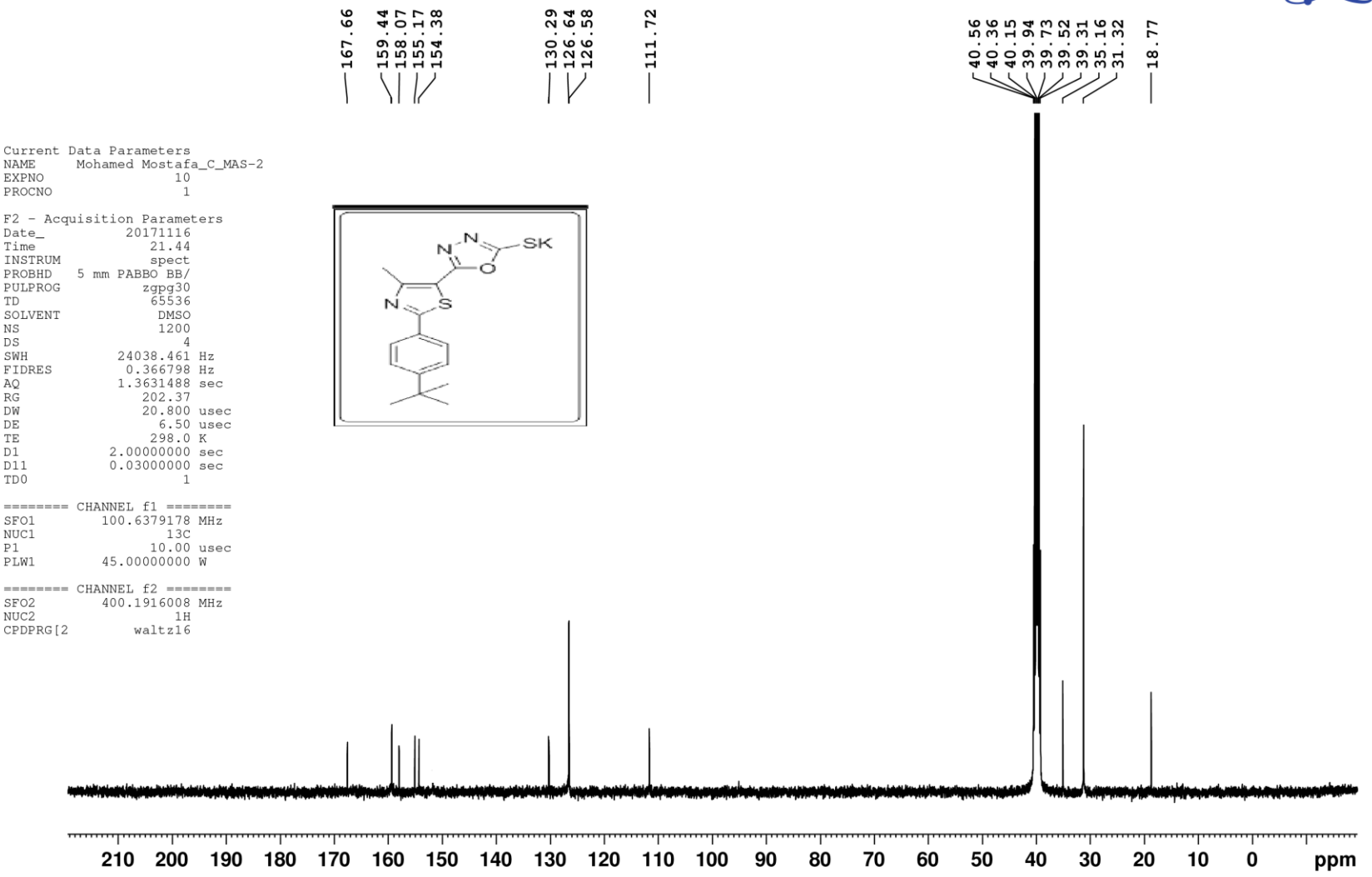
PC 1.00

Mohamed Mostafa_C_MAS-2-21

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

BRUKER

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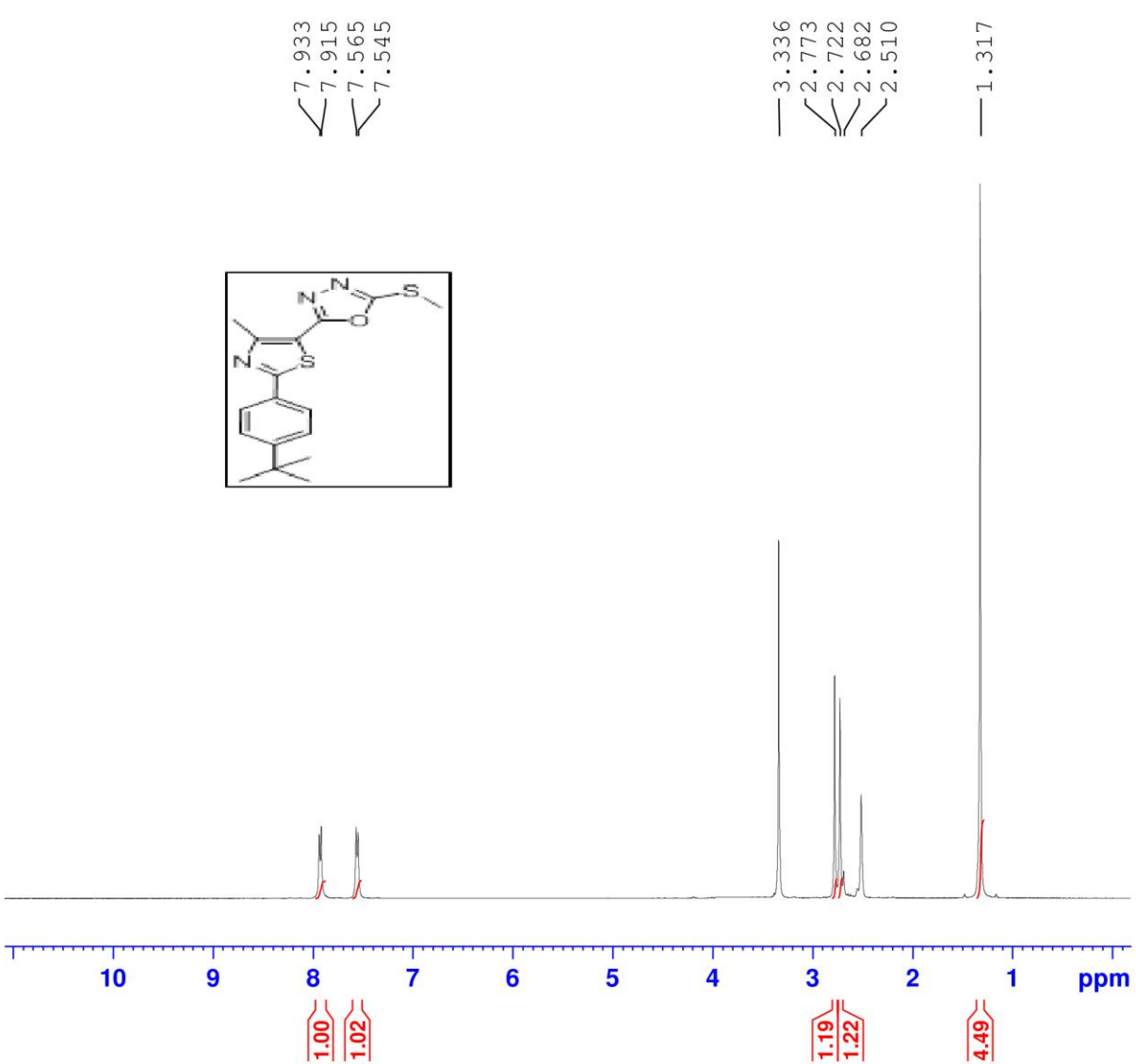

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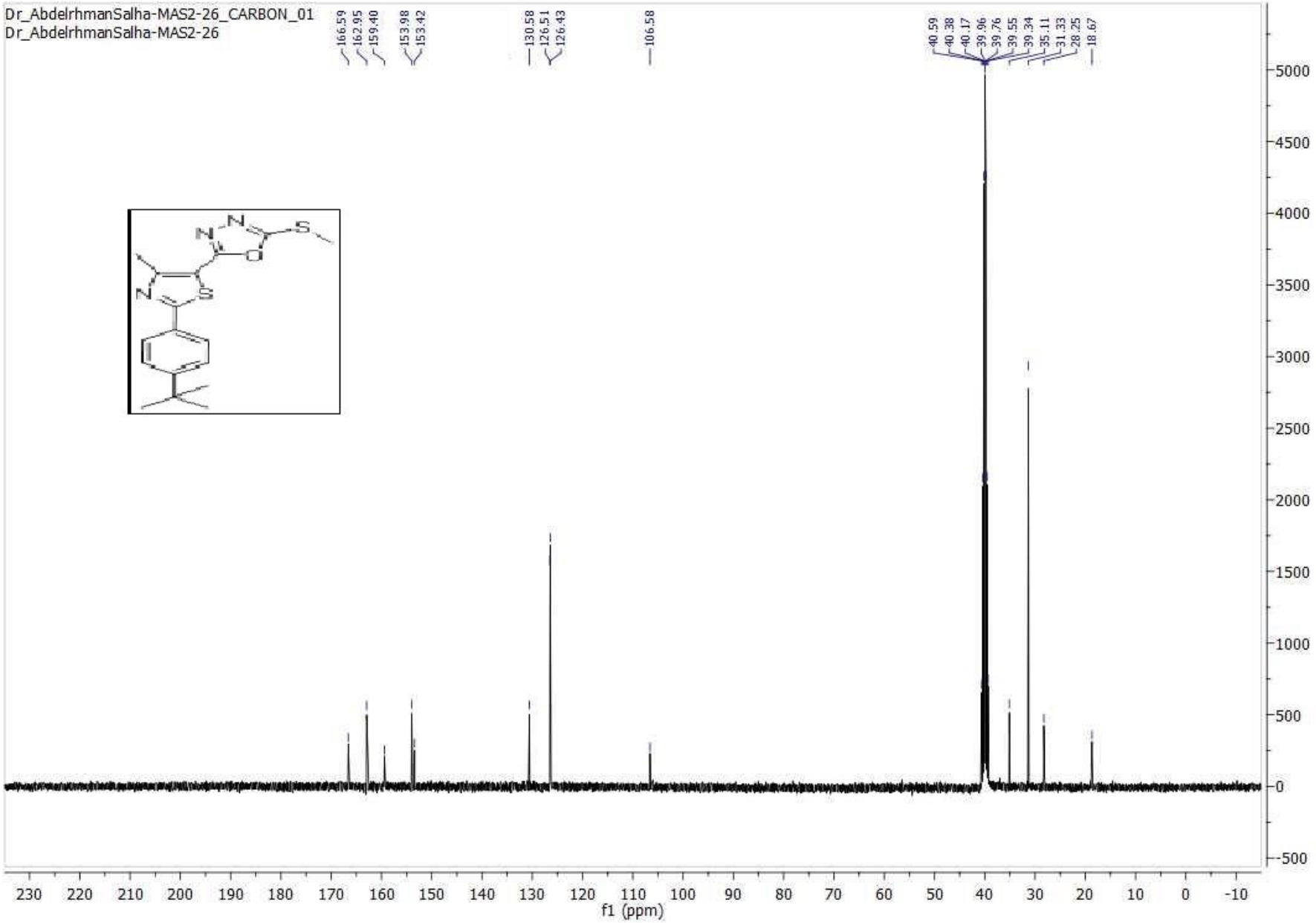
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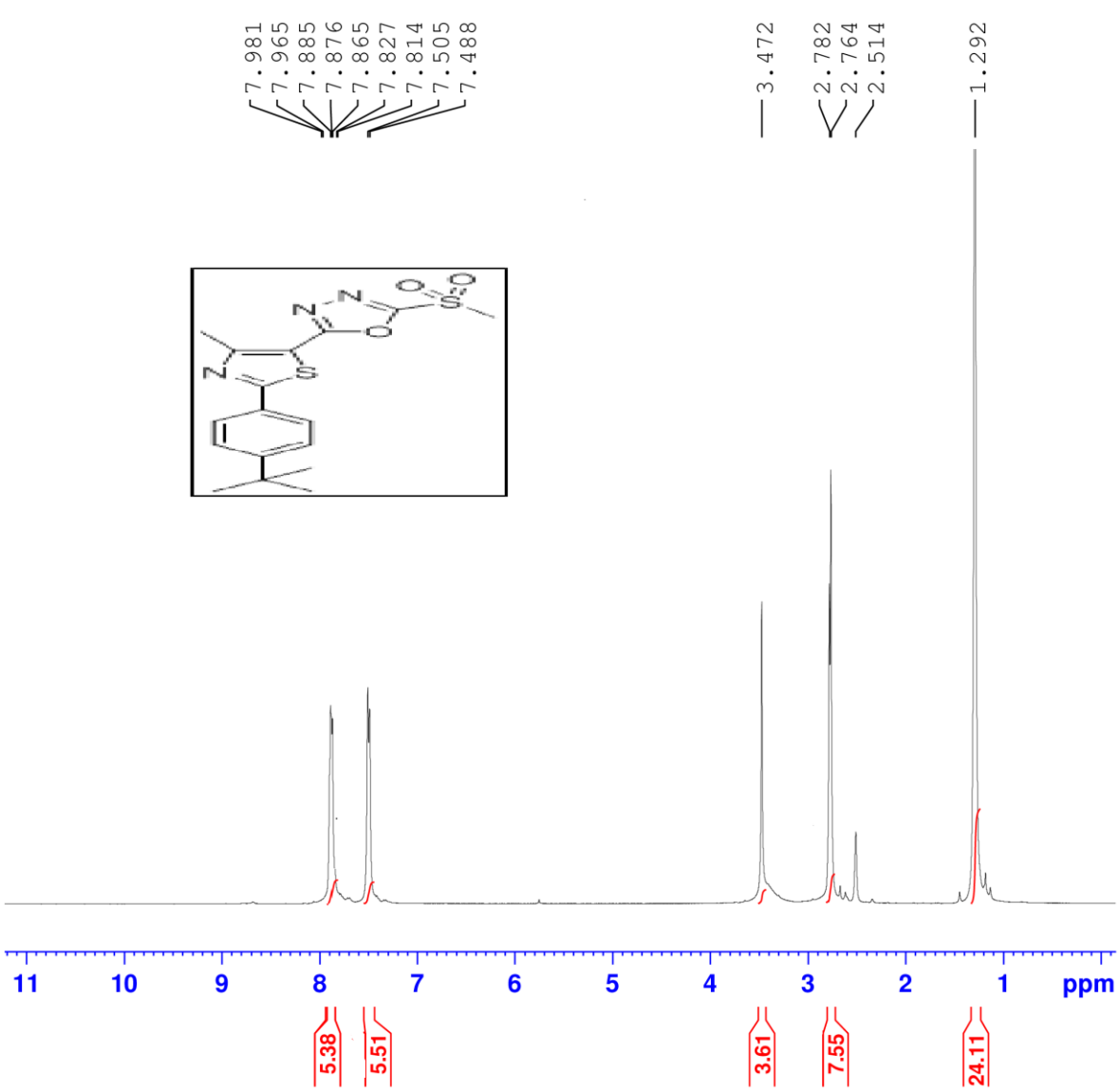

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NUC1 1H
P1 12.00 usec
PLW1 18.00000000 W

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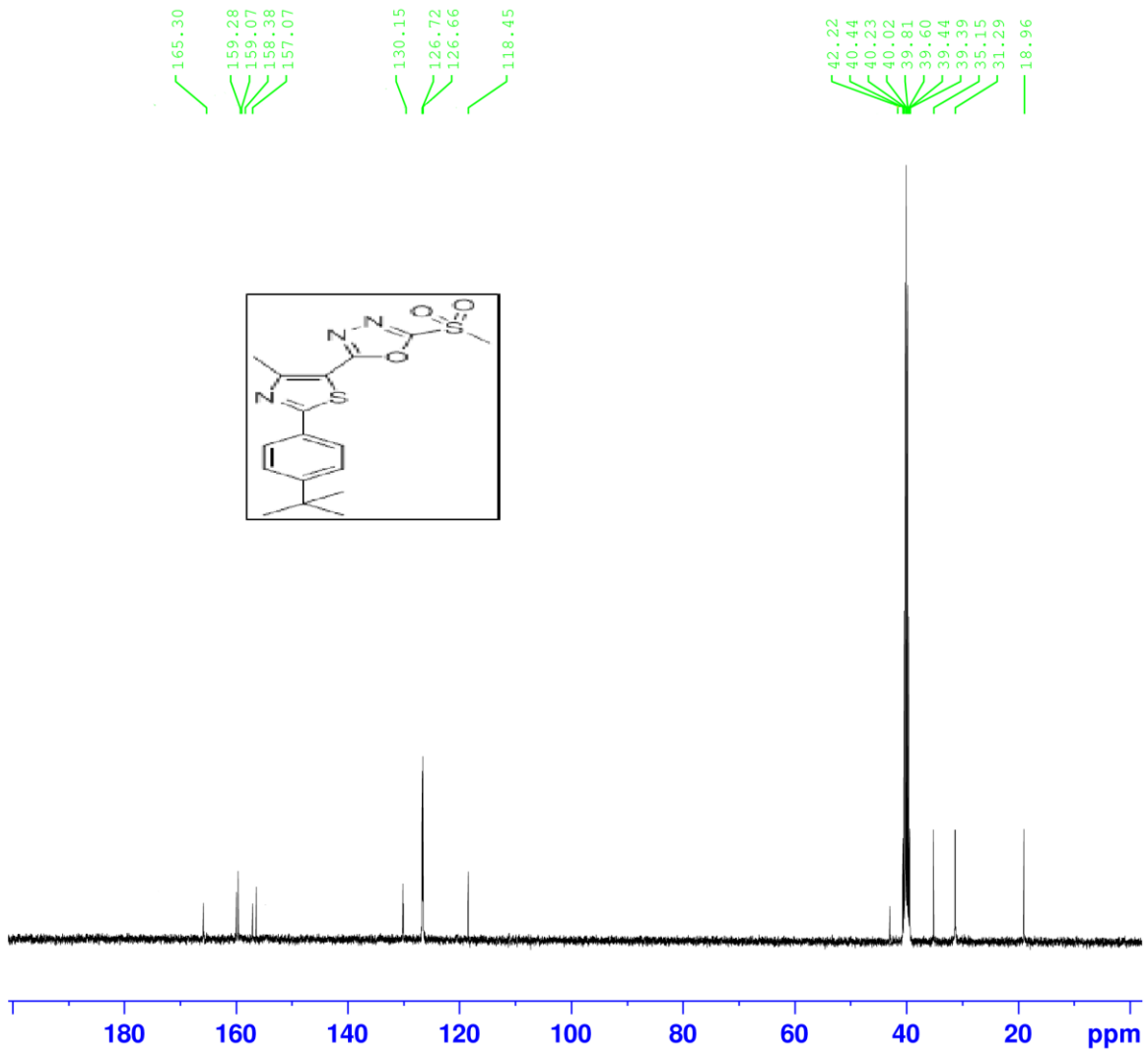

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FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG               205.37
DW               20.800 usec
DE                6.50 usec
TE               300.0 K
D1           2.00000000 sec
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TD0                   1

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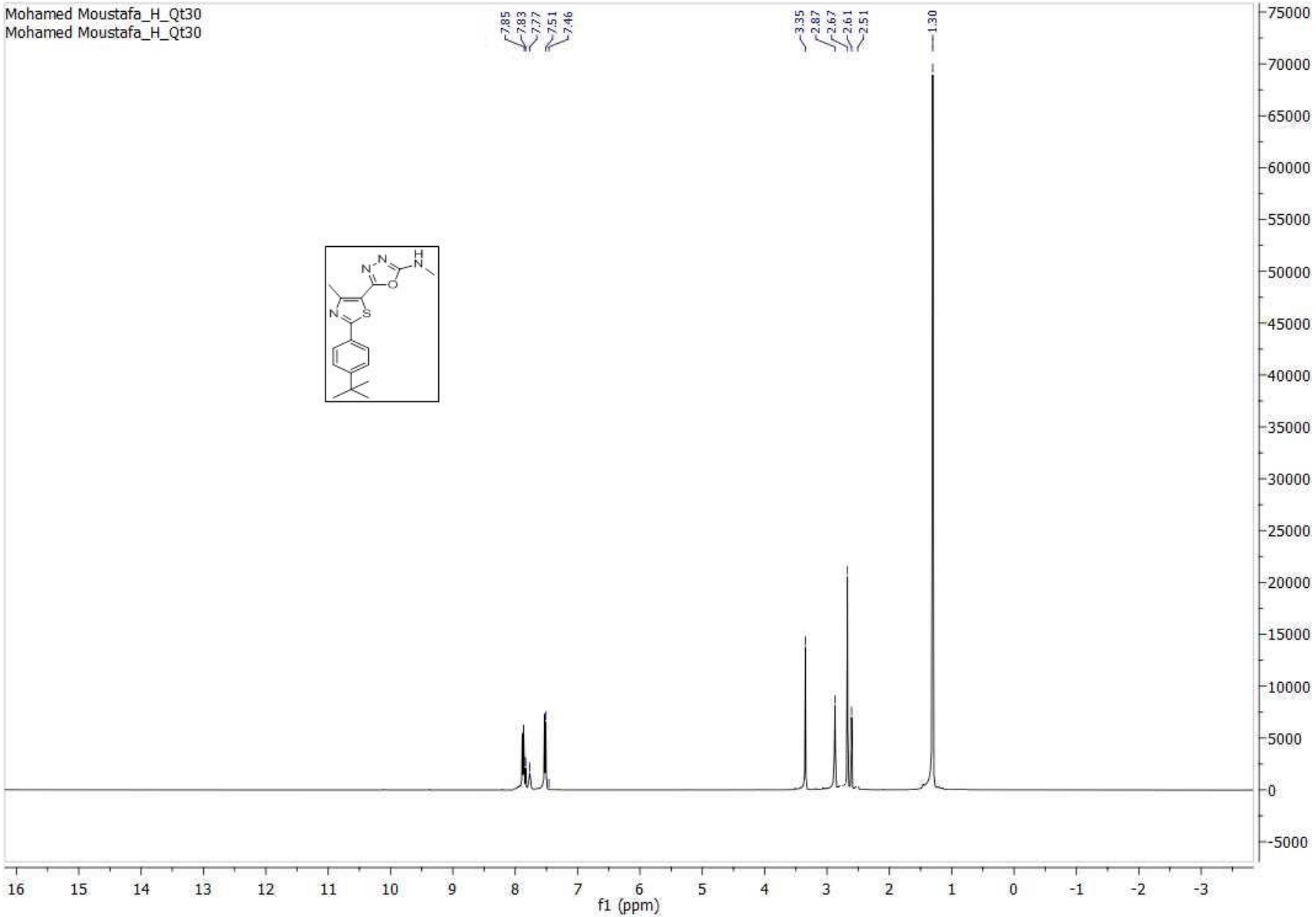
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Mohamed Moustafa_H_Qt30
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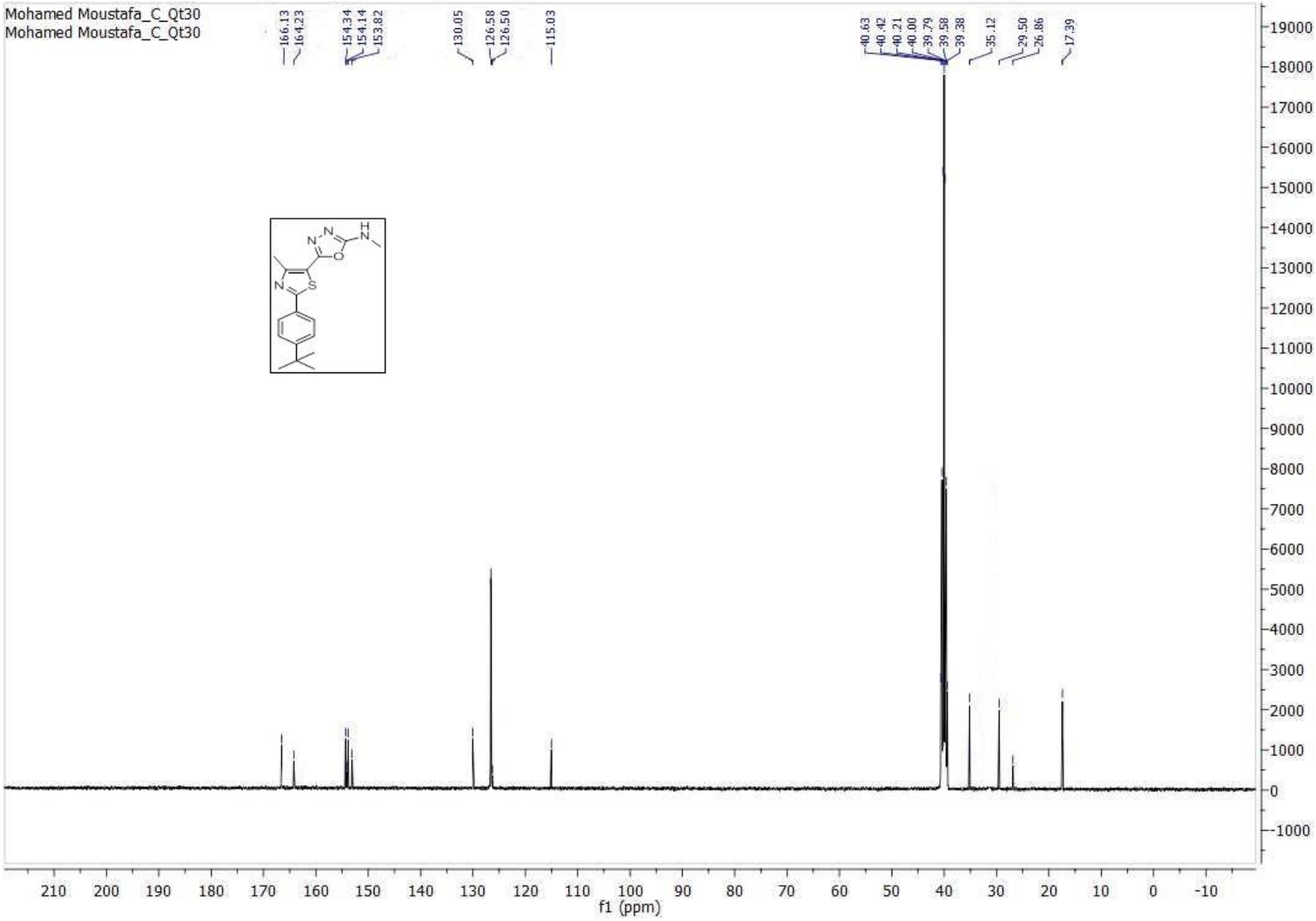
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Mohamed Moustafa_C_Qt30
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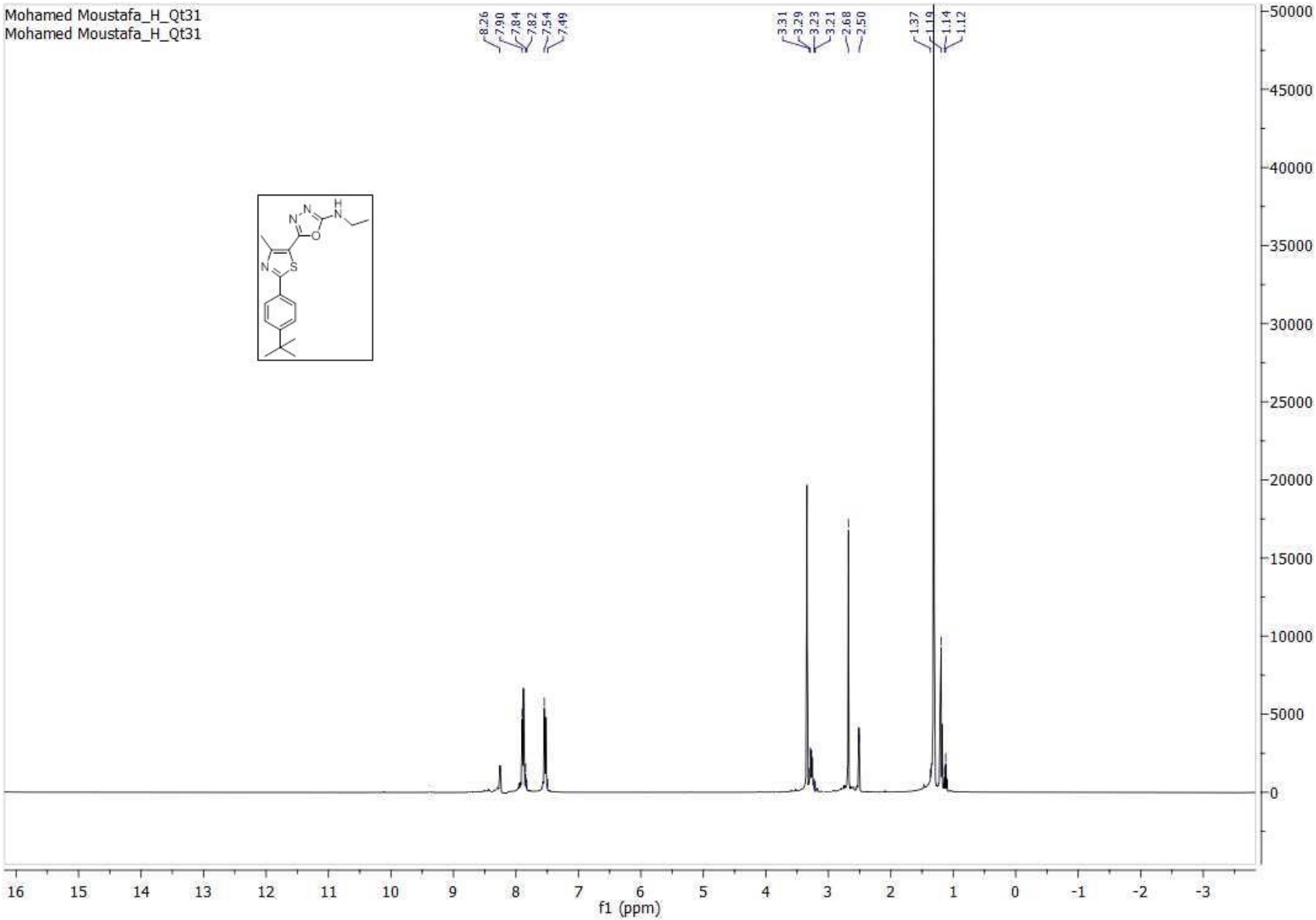
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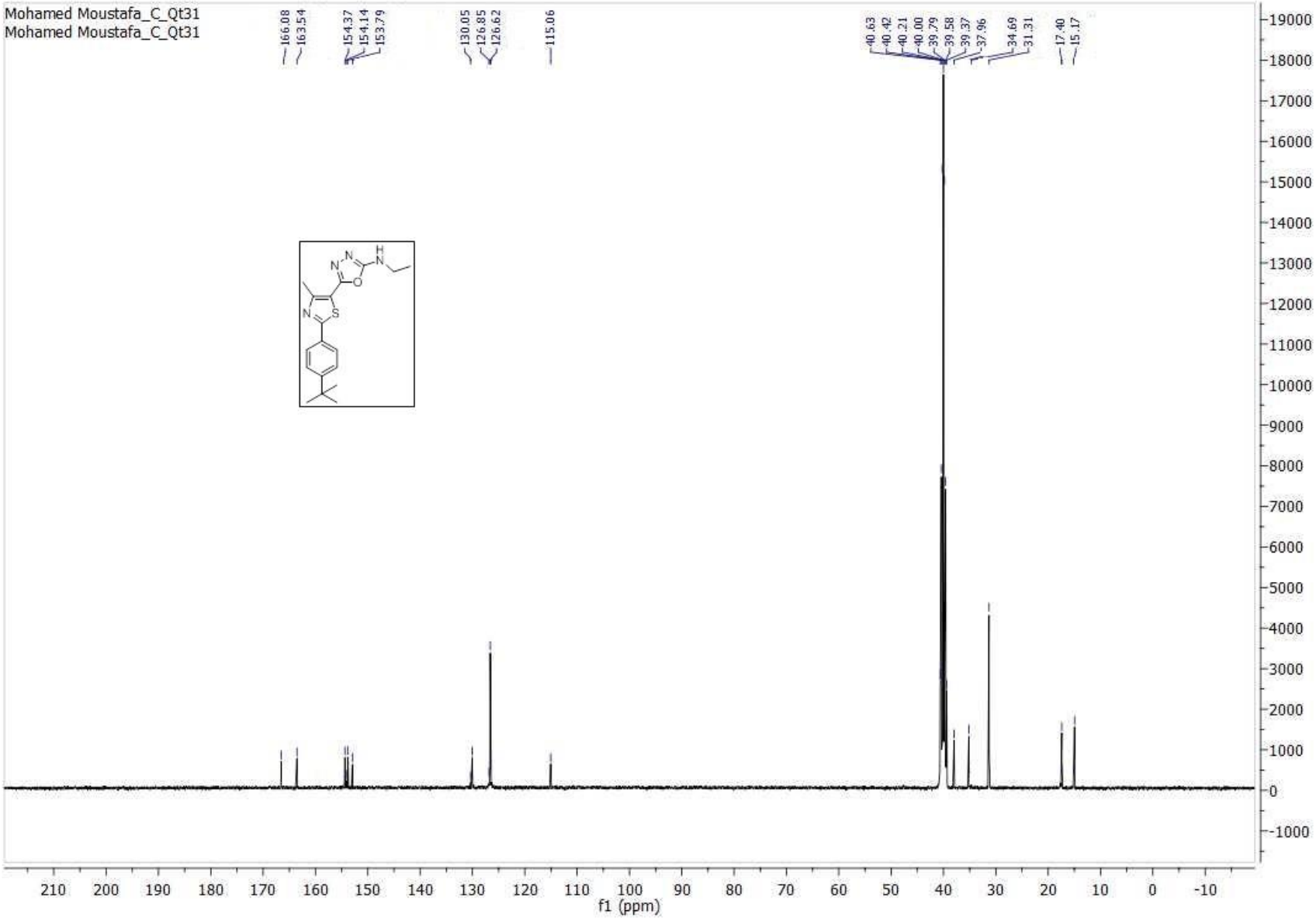
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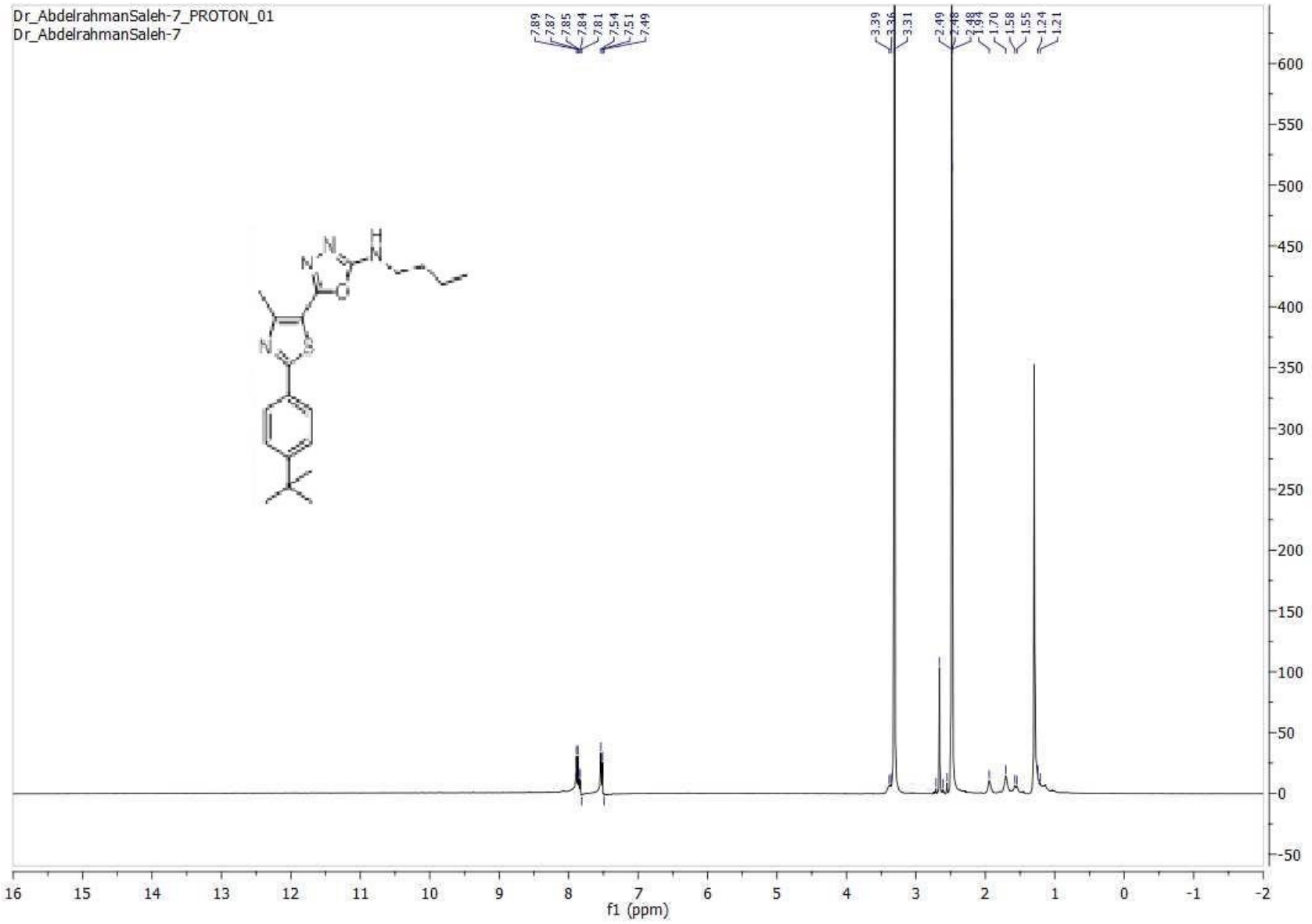
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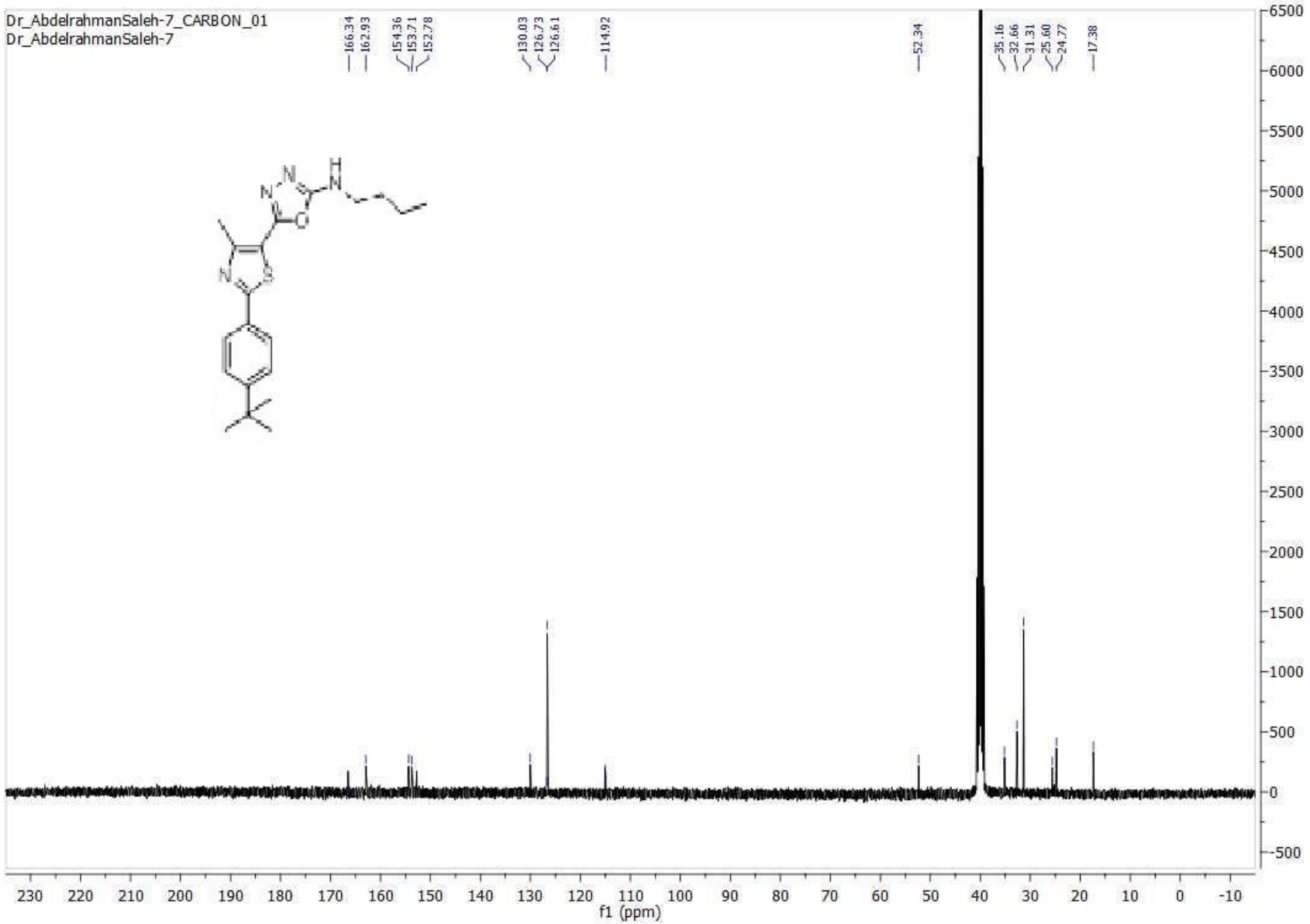
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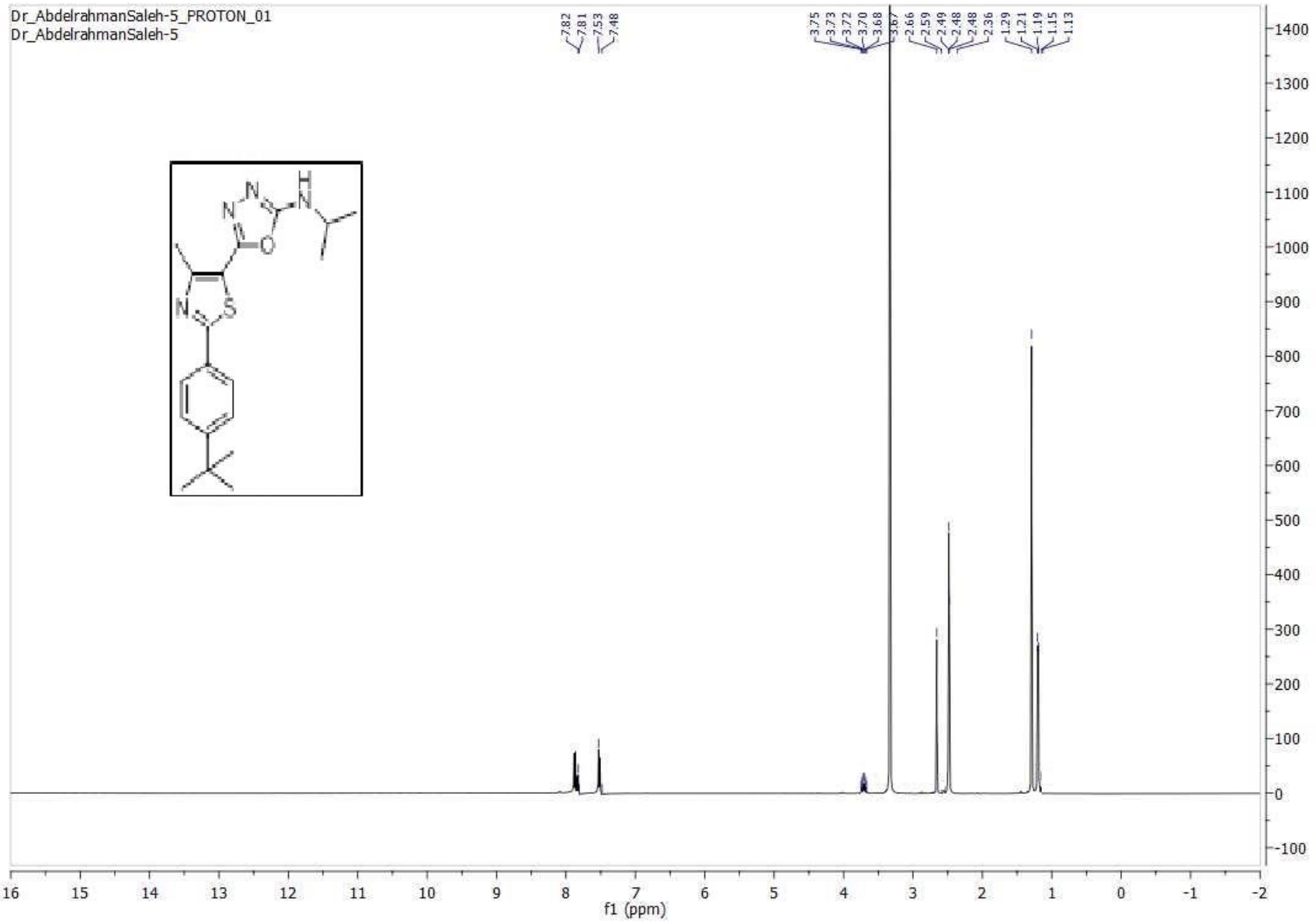
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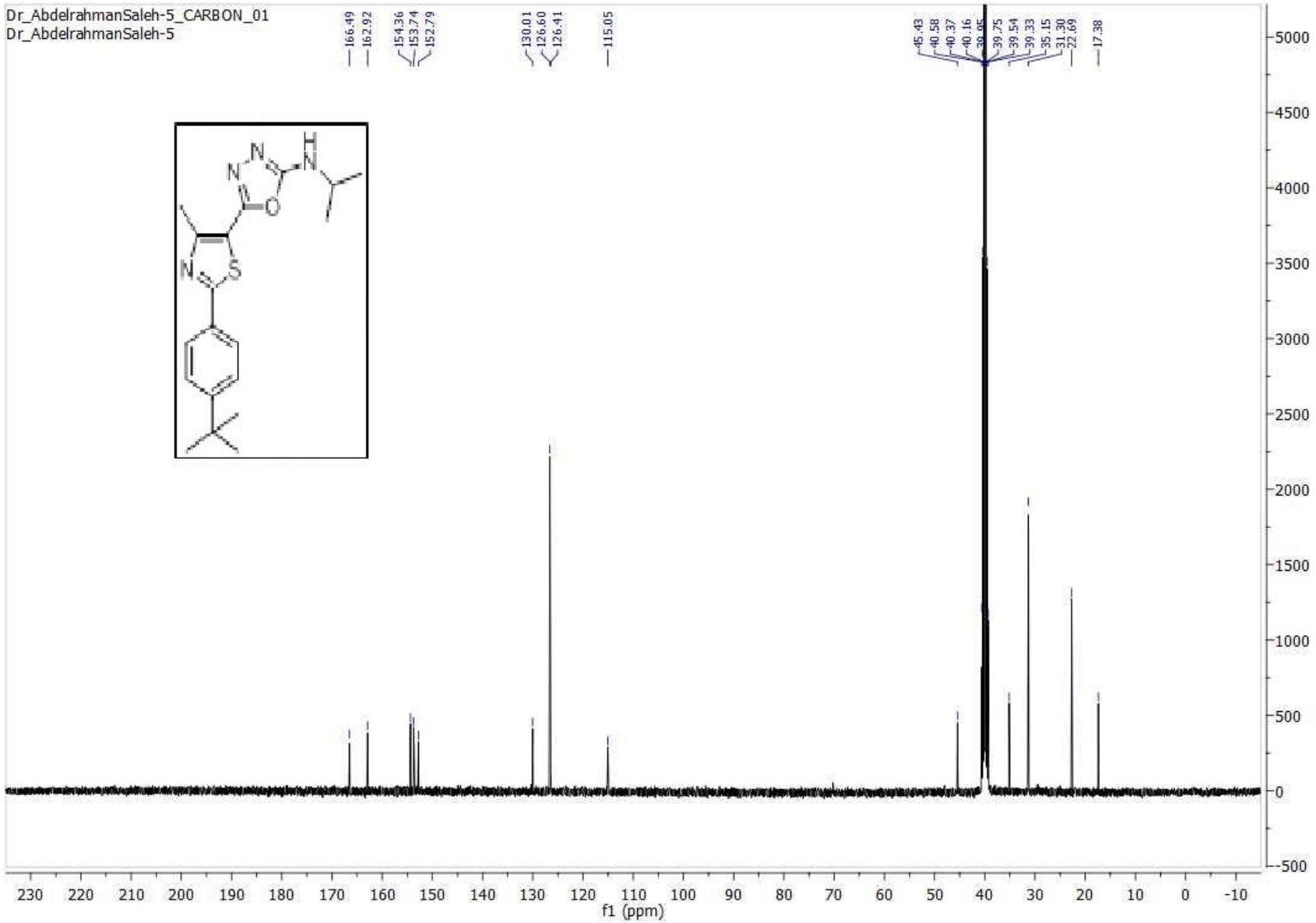
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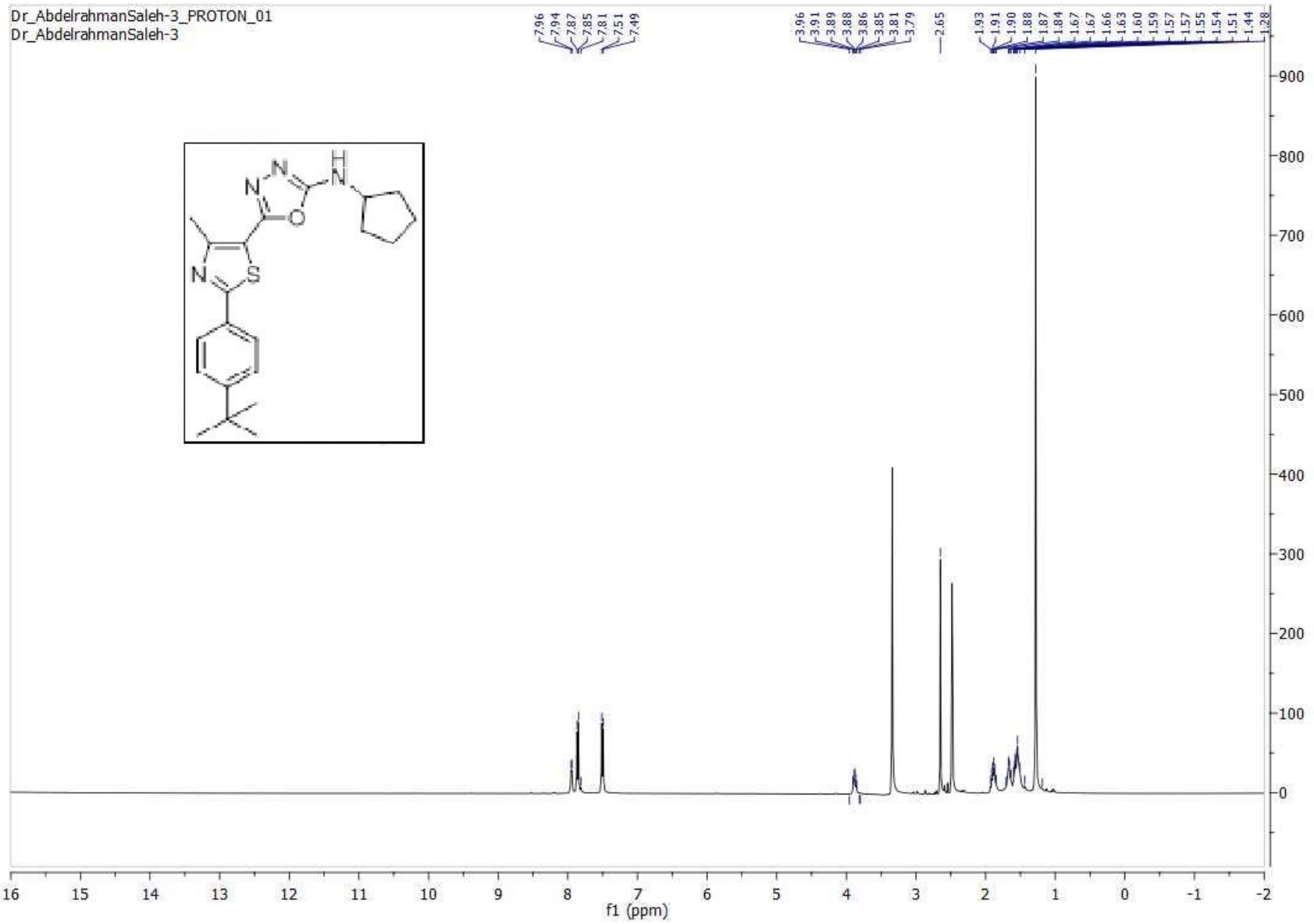
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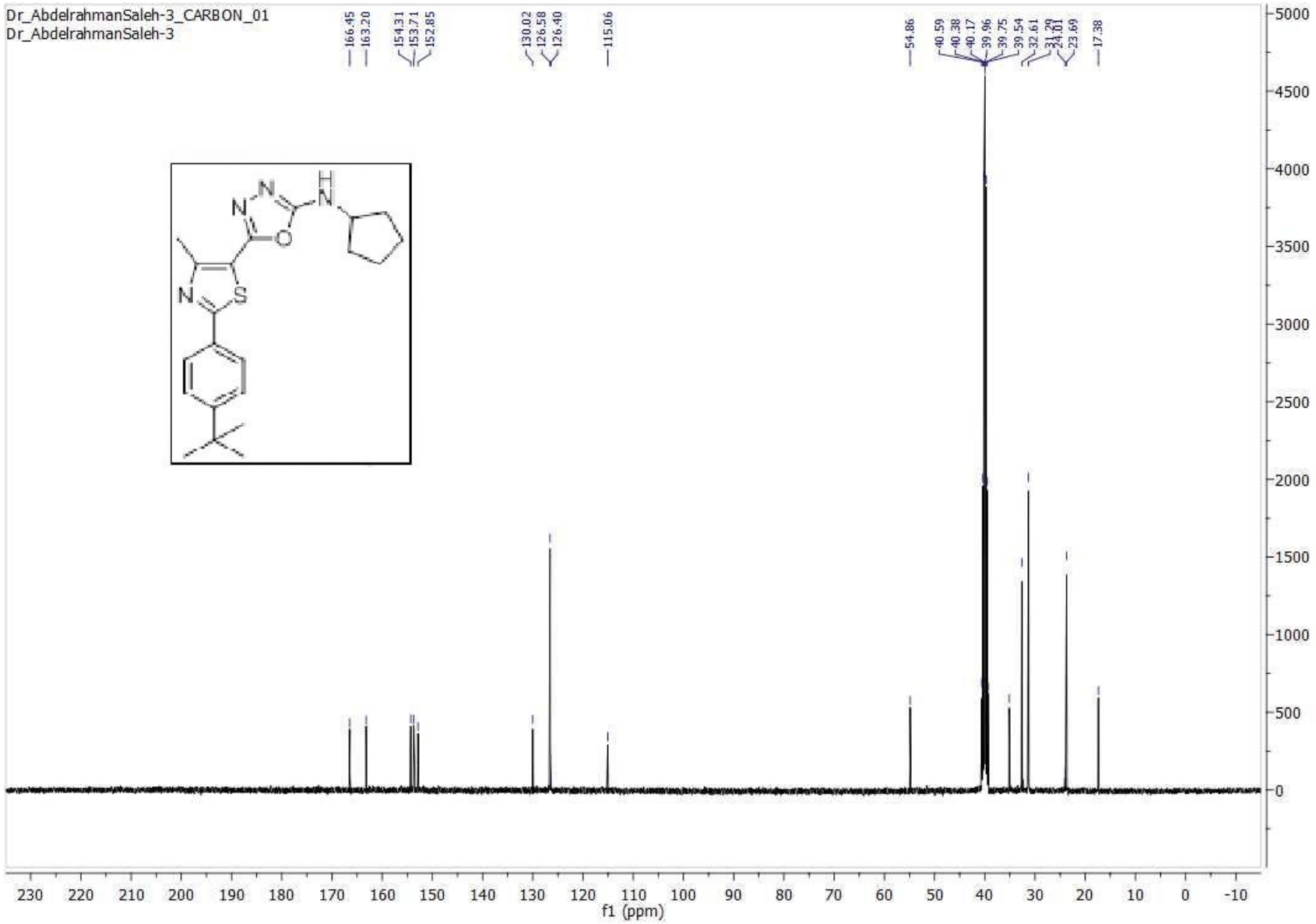
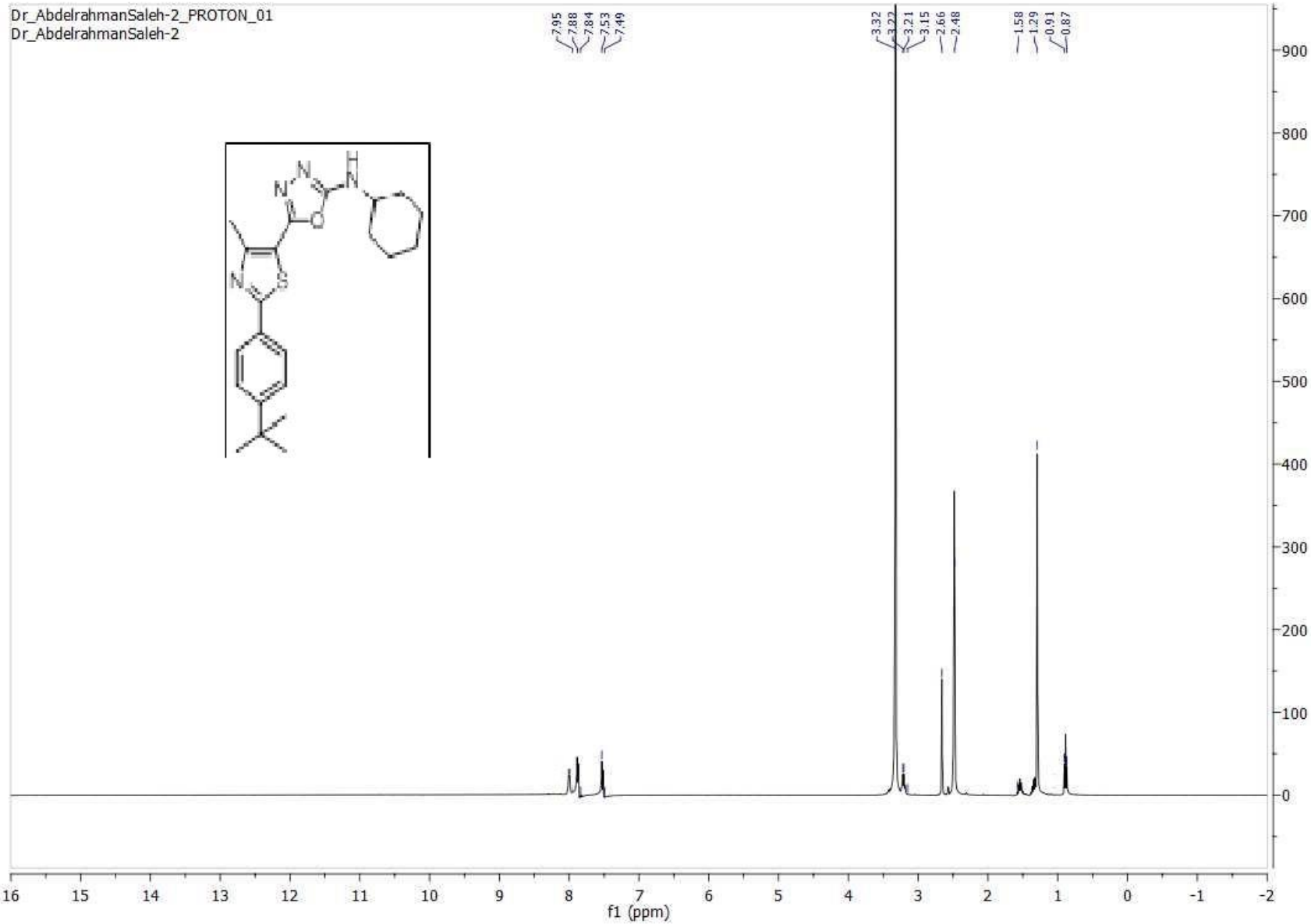
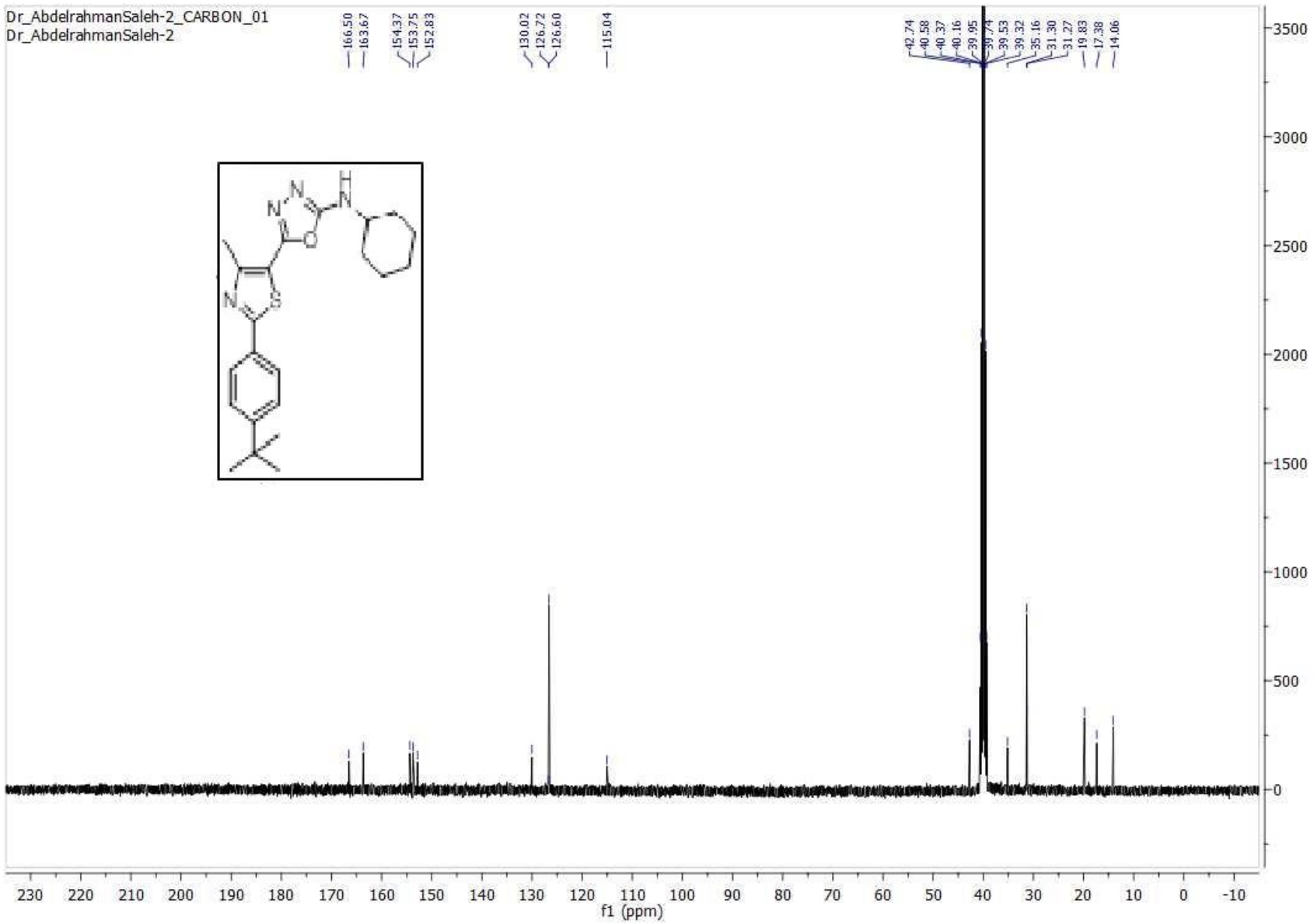
f1 (ppm)


Dr_AbdelrahmanSaleh-3_CARBON_01
Dr_AbdelrahmanSaleh-3
166.45
163.20
154.31
153.71
152.85
130.02
126.58
126.40
115.06
54.86
40.59
40.38
40.17
39.96
39.75
39.54
32.61
31.20
24.01
23.69
17.38
N
N
O
N
H
S
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Dr_AbdelrahmanSaleh-2_PROTON_01
Dr_AbdelrahmanSaleh-2
7.95
7.88
7.84
7.53
7.49
3.32
3.22
3.21
3.15
2.66
2.48
1.58
1.29
0.91
0.87
900
800
700
600
500
400
300
200
100
0
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


Dr_AbdelrahmanSaleh-2_CARBON_01
Dr_AbdelrahmanSaleh-2
166.50
163.67
154.37
153.75
152.83
130.02
126.72
126.60
115.04
42.74
40.58
40.37
40.16
39.95
39.74
39.53
39.32
35.16
31.30
31.27
19.83
17.38
14.06
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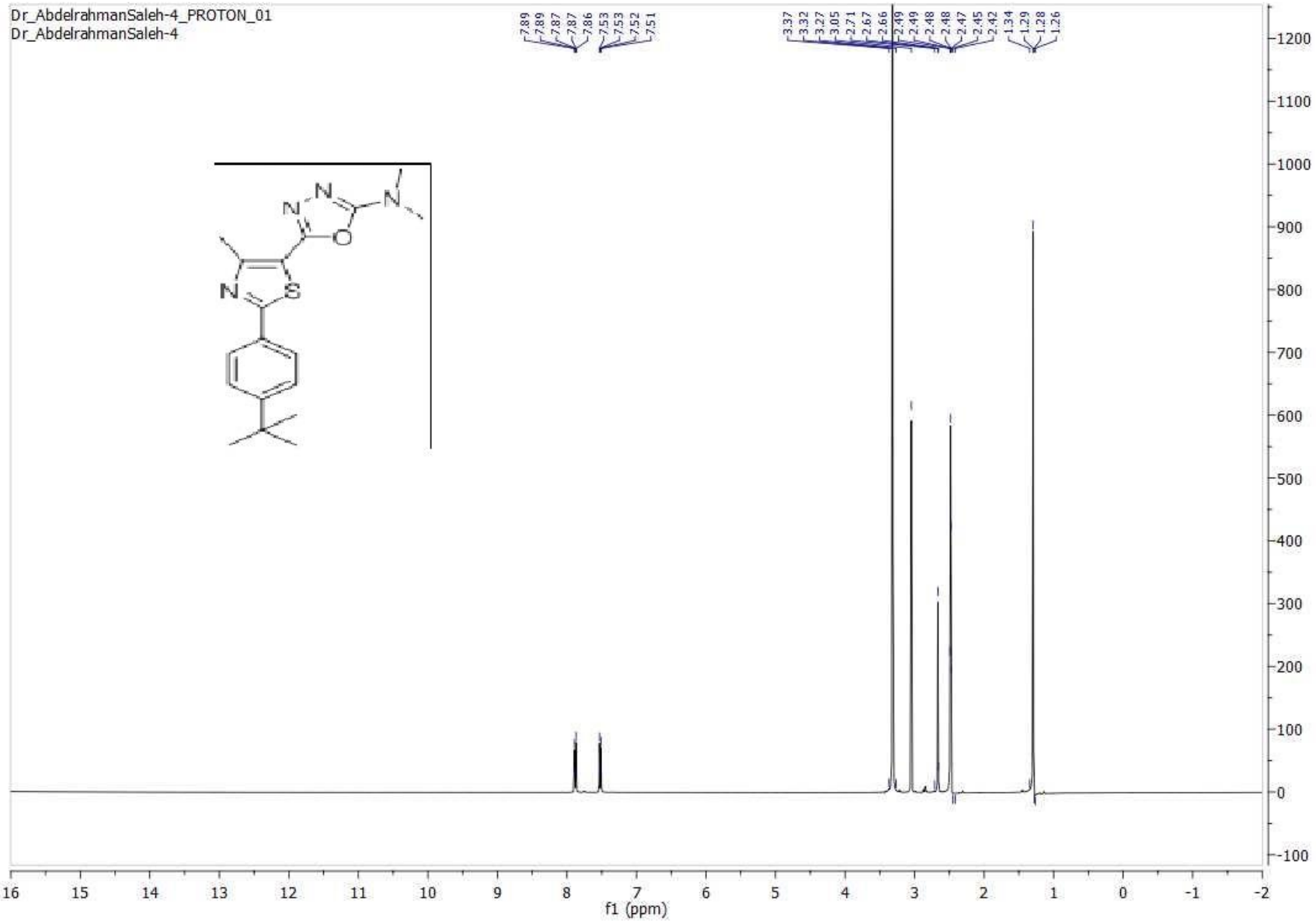
3000
2500
2000
1500
1000
500
0
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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Dr_AbdelrahmanSaleh-4
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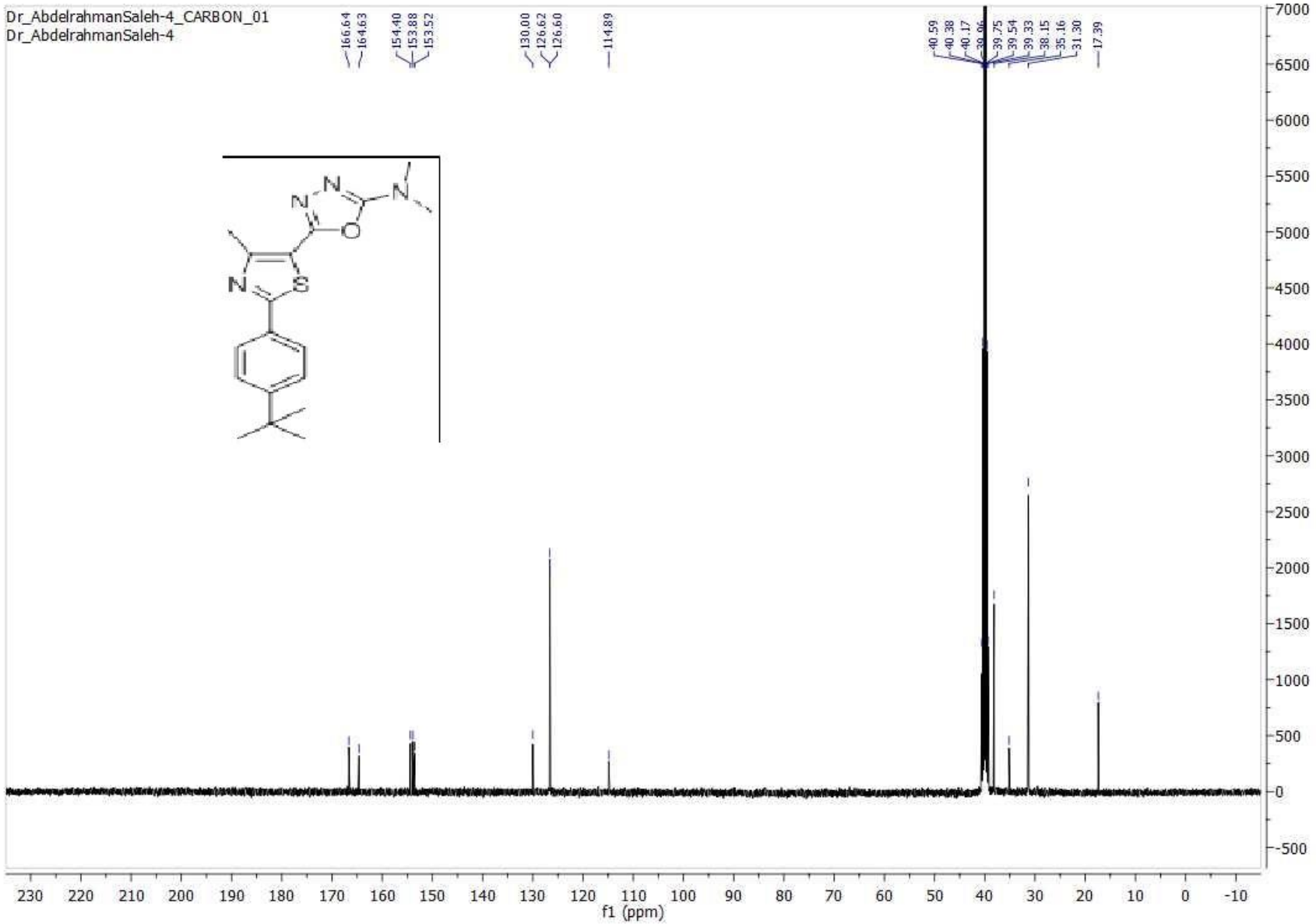
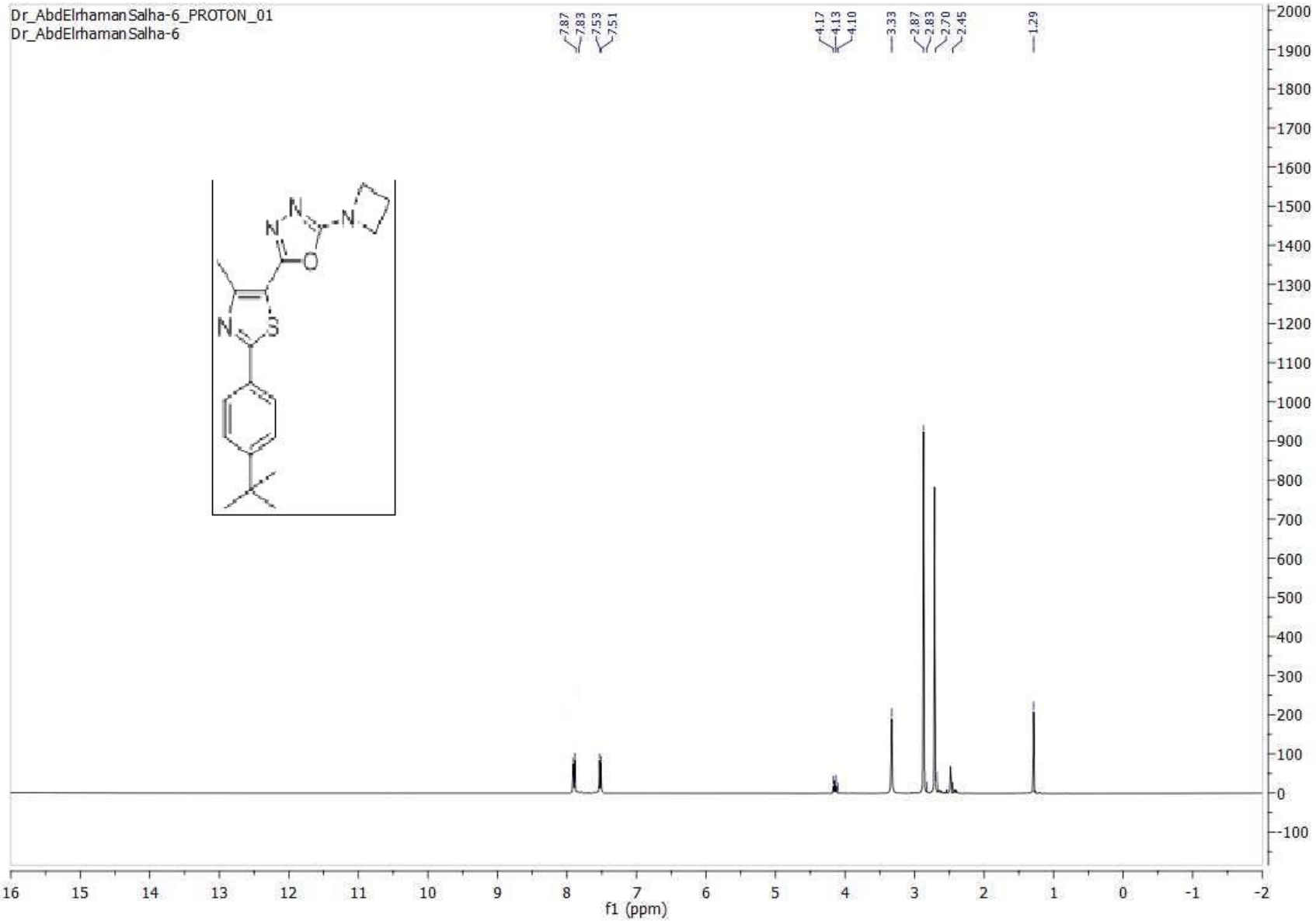
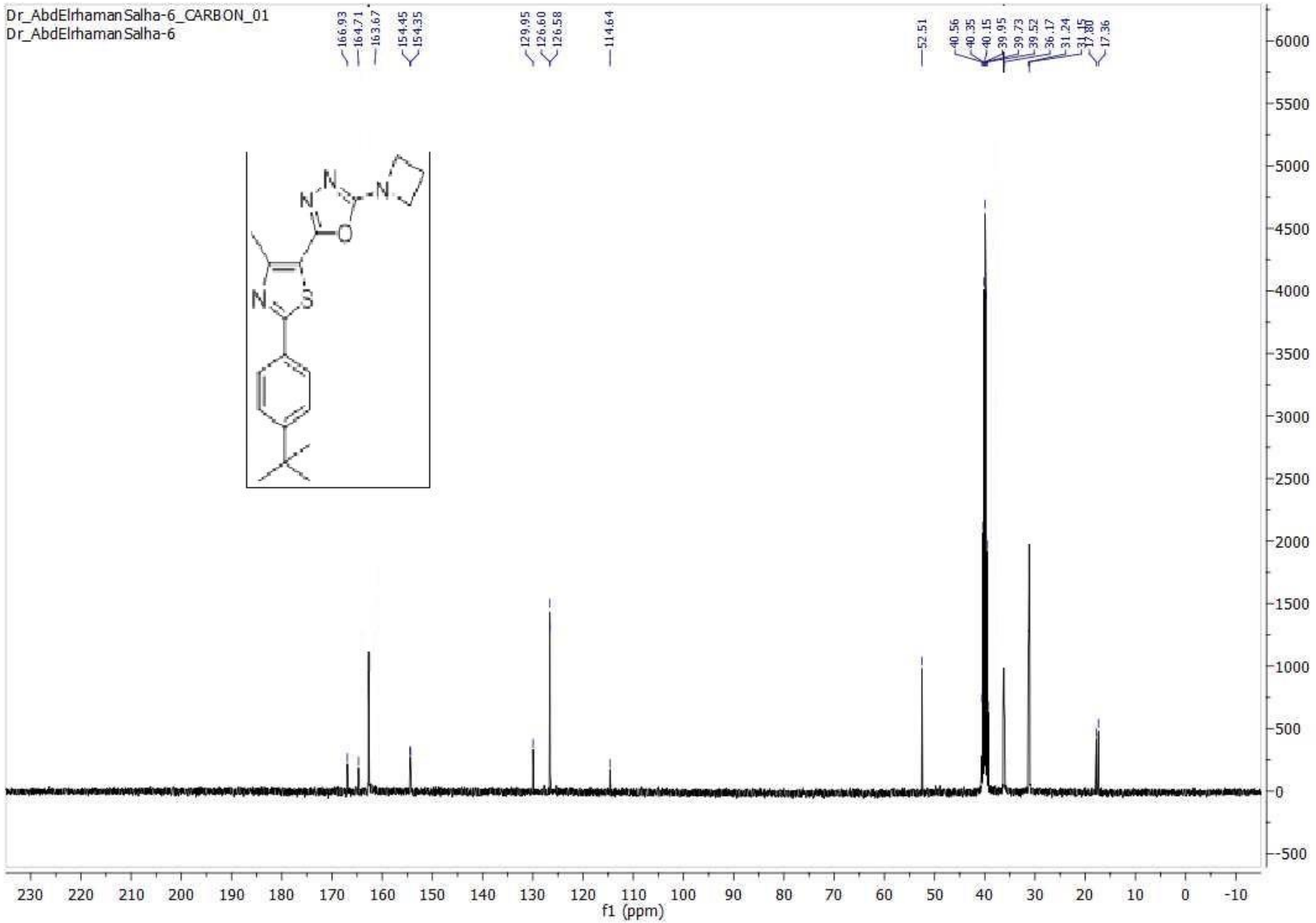
7.89
7.87
7.87
7.86
7.53
7.53
7.52
7.51
3.37
3.32
3.27
3.05
2.71
2.67
2.66
2.49
2.49
2.48
2.48
2.47
2.45
2.42
1.34
1.29
1.28
1.26
N
N
N
O
N
S
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


Dr_AbdelrahmanSaleh-4_CARBON_01
Dr_AbdelrahmanSaleh-4
166.64
164.63
154.40
153.88
153.52
130.00
126.62
126.60
114.89
40.59
40.38
40.17
39.96
39.75
39.54
39.33
38.15
35.16
31.30
17.39
N
N
O
N
S
7000
6500
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Dr_AbdElrhaman Salha-6_PROTON_01
Dr_AbdElrhaman Salha-6
7.87
7.83
7.53
7.51
4.17
4.13
4.10
3.33
2.87
2.83
2.70
2.45
1.29
N
N
N
O
N
S
2000
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


Dr_AbdElrhamanSalha-6_CARBON_01
Dr_AbdElrhamanSalha-6
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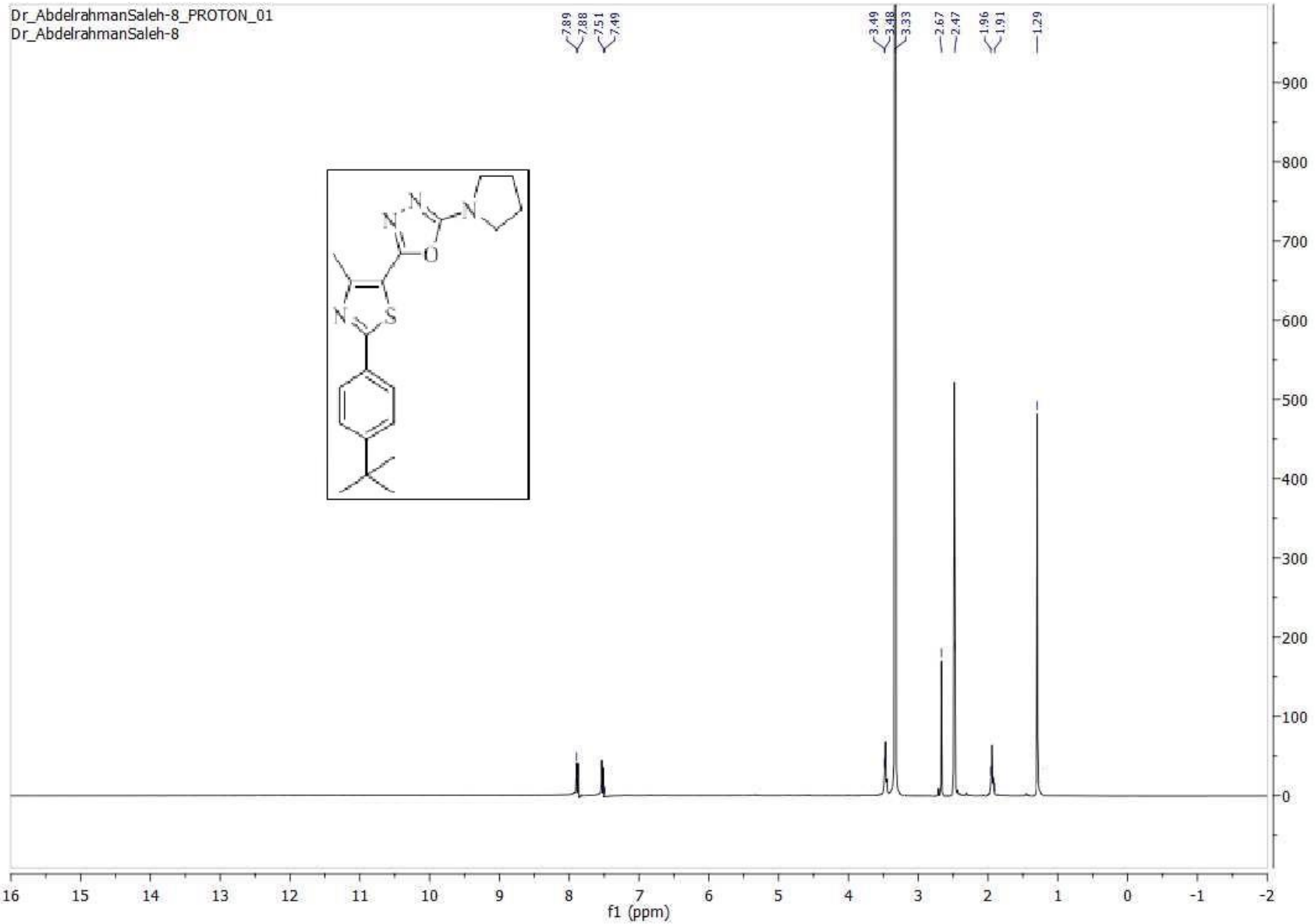
164.71
163.67
154.45
154.35
129.95
126.60
126.58
114.64
52.51
40.56
40.35
40.15
39.95
39.73
39.52
36.17
31.24
17.36
N
N
O
N
S
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Dr_AbdelrahmanSaleh-8_PROTON_01
Dr_AbdelrahmanSaleh-8
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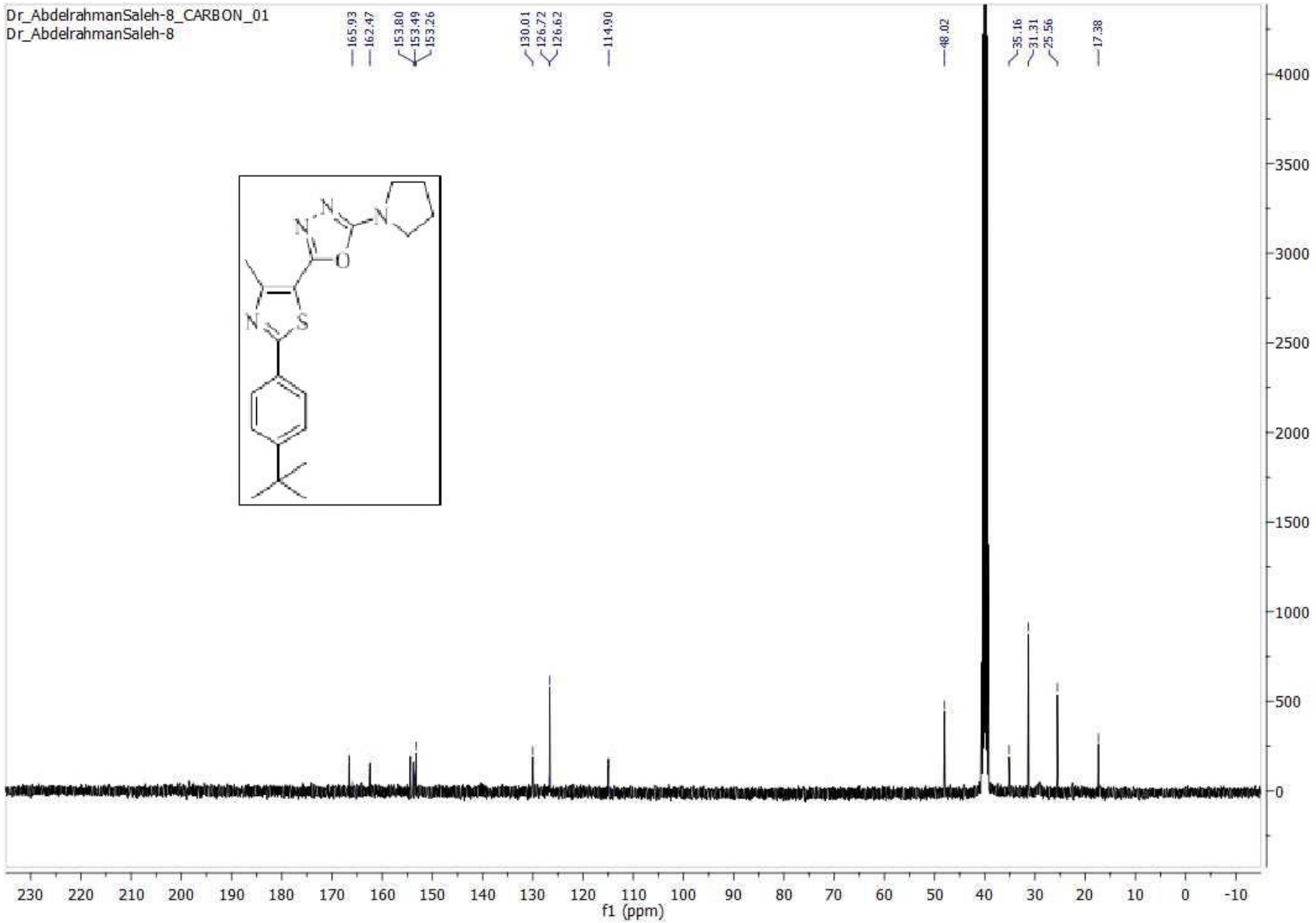
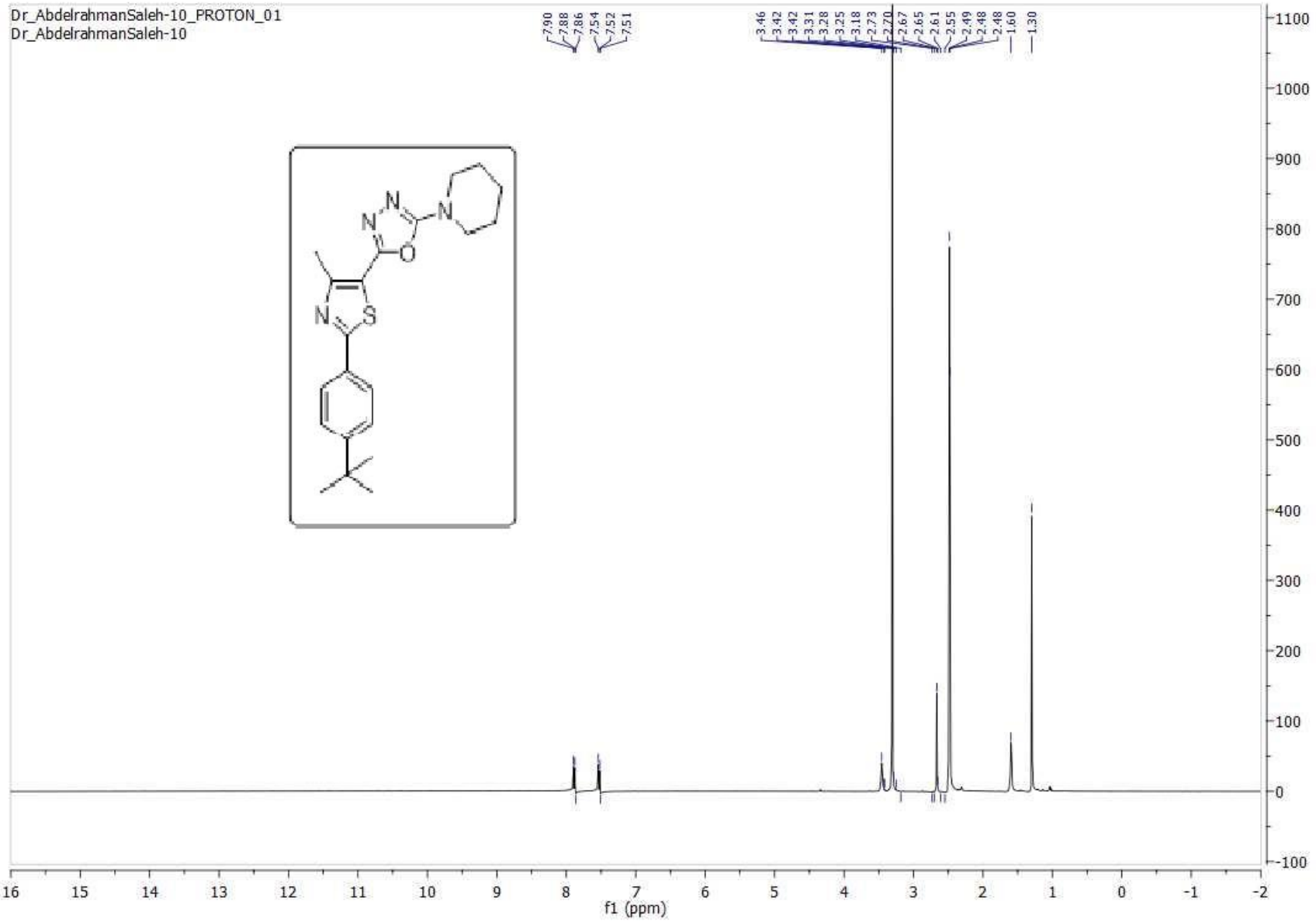
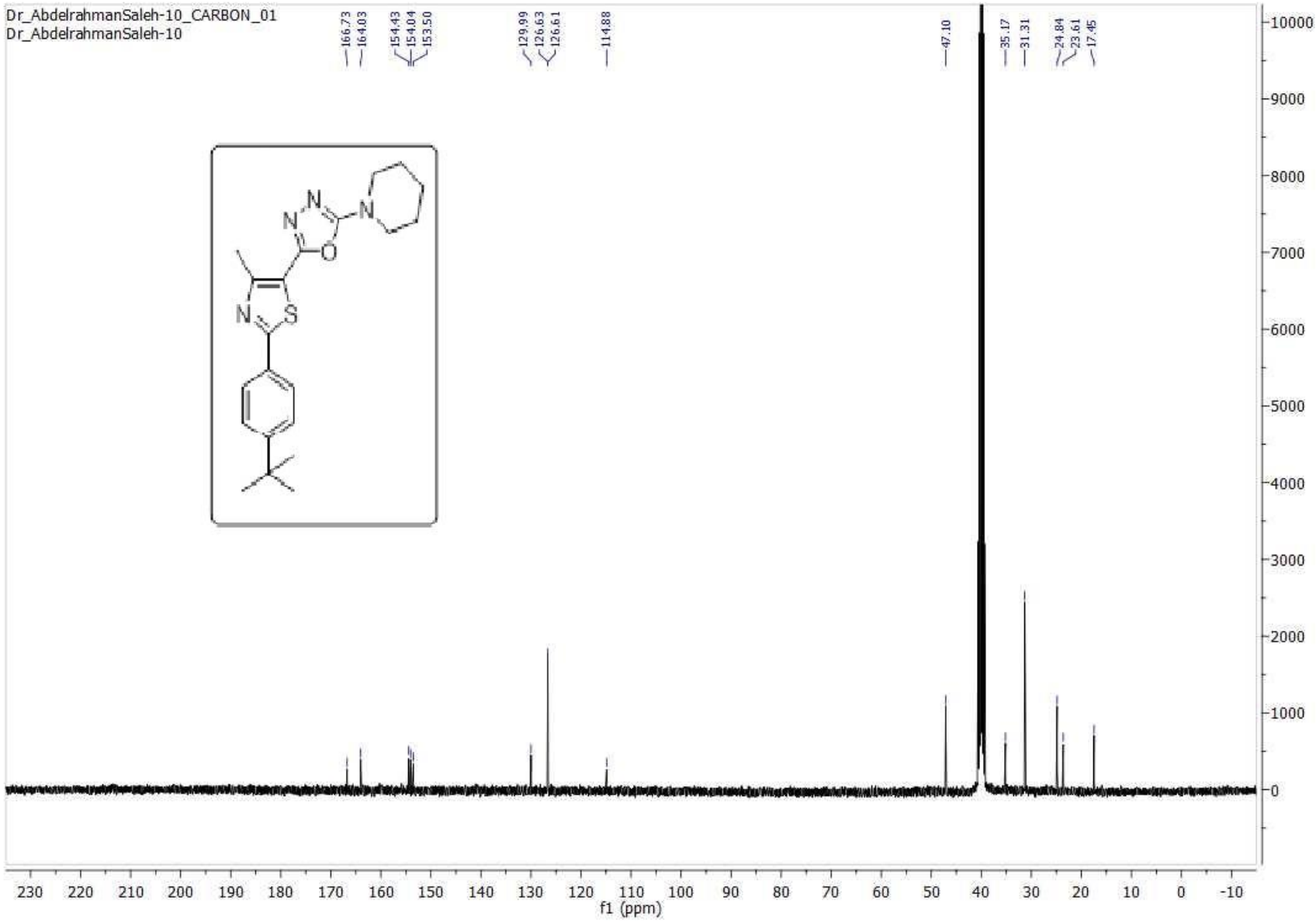
7.88
7.51
7.49
3.49
3.48
3.33
2.67
2.47
1.96
1.91
1.29
900
800
700
600
500
400
300
200
100
0
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


Dr_AbdelrahmanSaleh-8_CARBON_01
Dr_AbdelrahmanSaleh-8
165.93
162.47
153.80
153.49
153.26
130.01
126.72
126.62
114.90
48.02
35.16
31.31
25.56
17.38
4000
3500
3000
2500
2000
1500
1000
500
0
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Dr_AbdelrahmanSaleh-10_PROTON_01
Dr_AbdelrahmanSaleh-10
7.90
7.88
7.86
7.54
7.52
7.51
3.46
3.42
3.42
3.31
3.28
3.25
3.18
2.73
2.70
2.67
2.65
2.61
2.55
2.49
2.48
1.60
1.30
N
N
O
N
S
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


Dr_AbdelrahmanSaleh-10_CARBON_01
Dr_AbdelrahmanSaleh-10
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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
N
N
O
N
N
S
10000
9000
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7000
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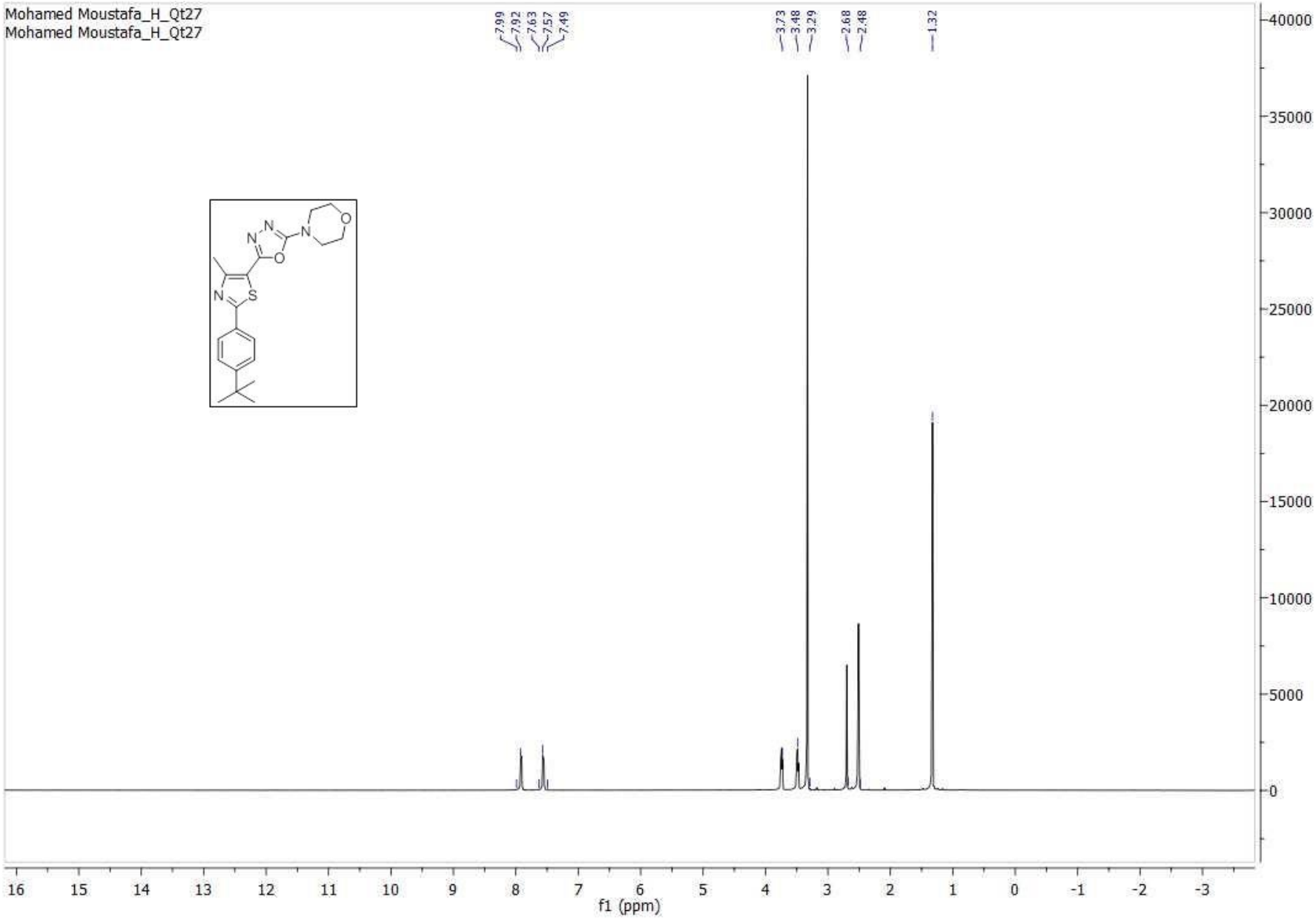
5000
4000
3000
2000
1000
0
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Mohamed Moustafa_H_Qt27
Mohamed Moustafa_H_Qt27
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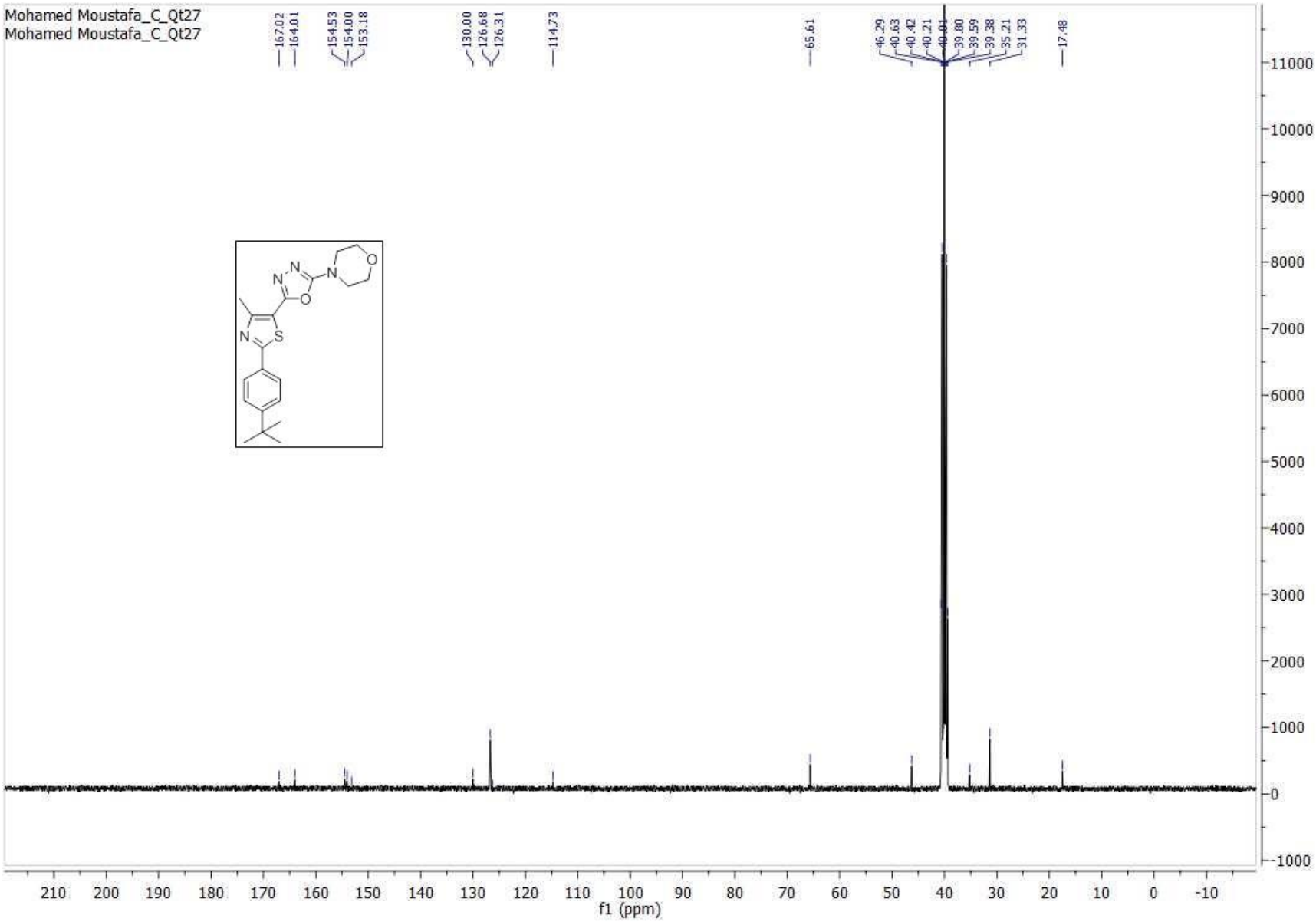
7.92
7.63
7.57
7.49
3.73
3.48
3.29
2.68
2.48
1.32
40000
35000
30000
25000
20000
15000
10000
5000
0
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


Mohamed Moustafa_C_Qt27
Mohamed Moustafa_C_Qt27
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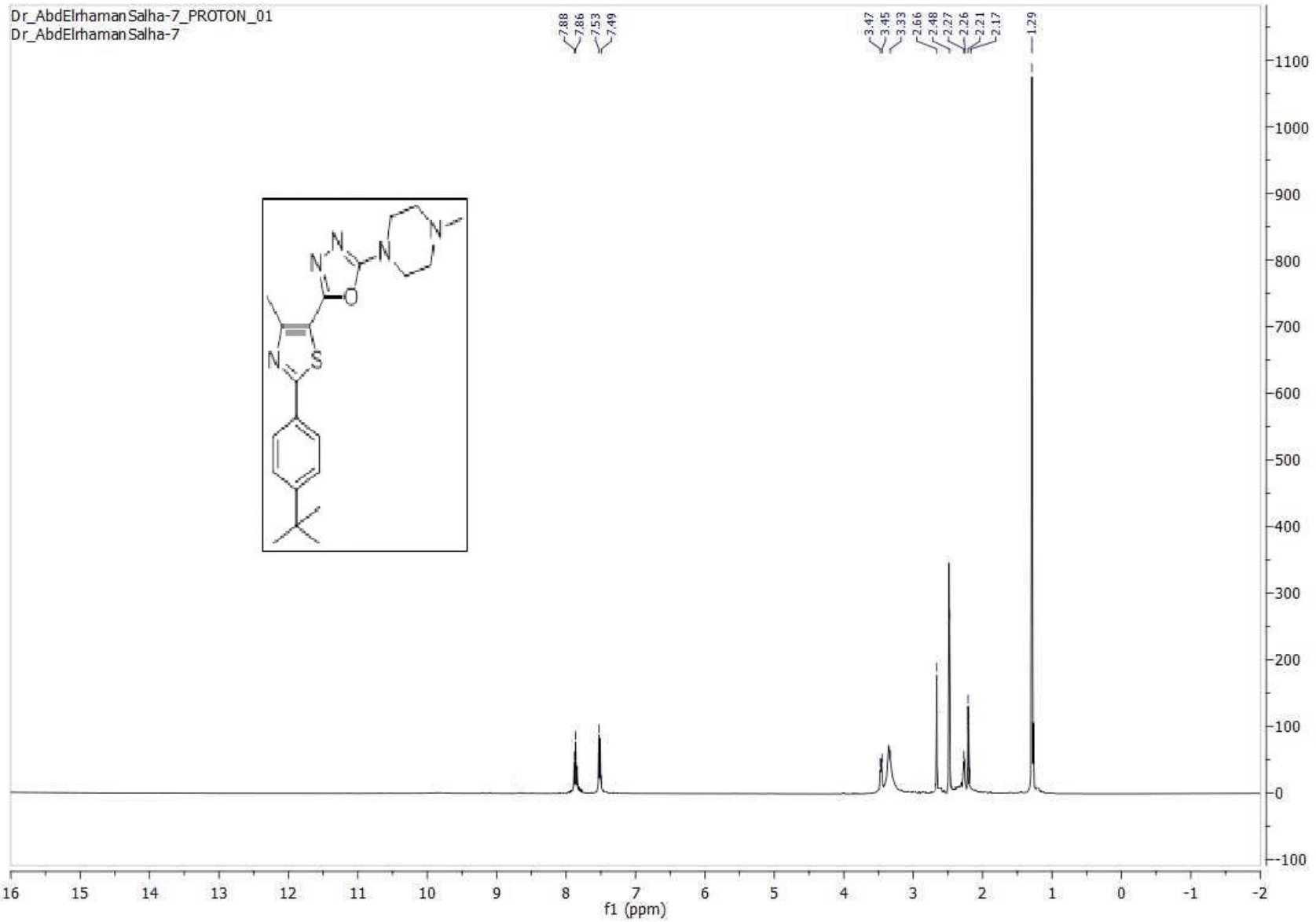
164.01
154.53
154.00
153.18
130.00
126.68
126.31
114.73
65.61
46.29
40.63
40.42
40.21
40.01
39.80
39.59
39.38
35.21
31.33
17.48
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Dr_AbdElrhamanSalha-7_PROTON_01
Dr_AbdElrhamanSalha-7
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7.86
7.53
7.49
3.47
3.45
3.33
2.66
2.48
2.27
2.26
2.21
2.17
1.29
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
16
15
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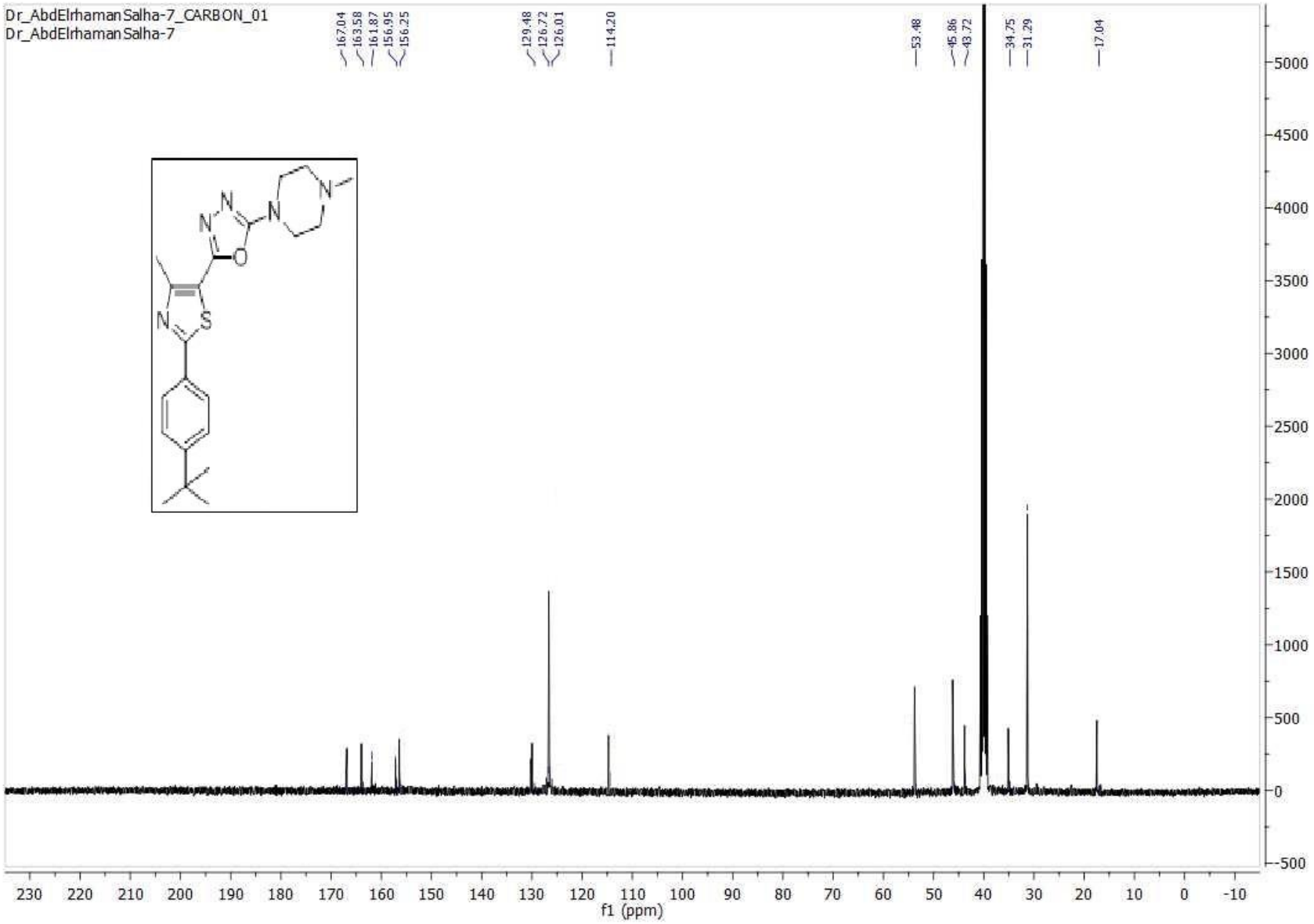
10
9
8
7
6
5
4
3
2
1
0
-1
-2
f1 (ppm)


Dr_AbdElrhamanSalha-7_CARBON_01
Dr_AbdElrhamanSalha-7
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163.58
161.87
156.95
156.25
129.48
126.72
126.01
114.20
53.48
45.86
43.72
34.75
31.29
17.04
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

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 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                 64.21
DW                62.400 usec
DE                 6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    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
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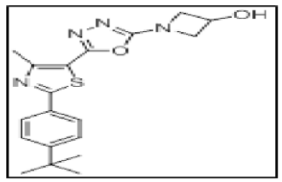

Mohamed Mostafa_C_Qt-16

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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 ========
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NUC2                 1H
CPDPRG[2         waltz16
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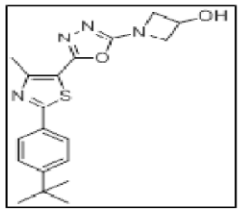

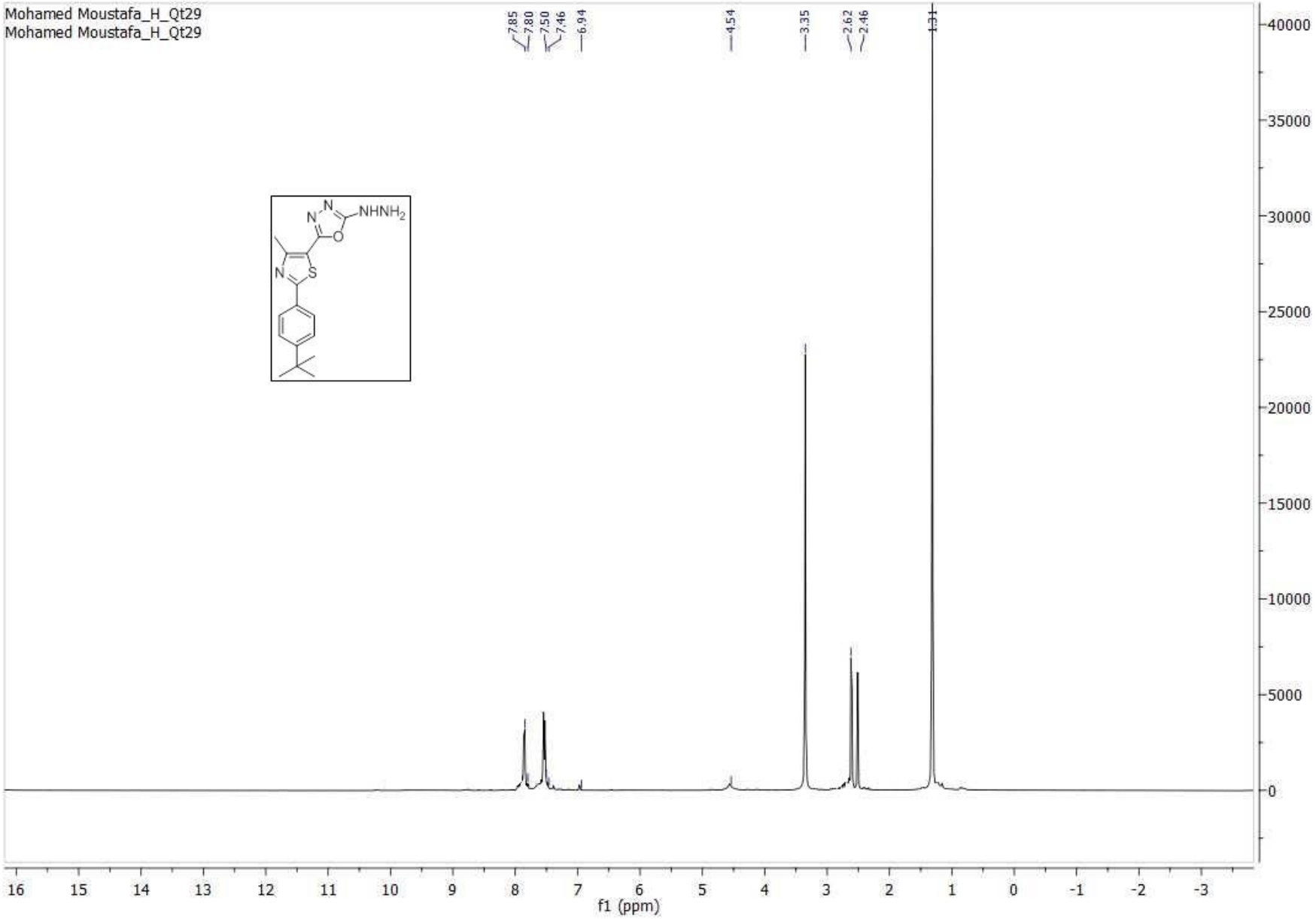
Mohamed Moustafa_H_Qt29
Mohamed Moustafa_H_Qt29
7.85
7.80
7.50
7.46
6.94
4.54
3.35
2.62
2.46
1.31
NHNH2
N
N
O
N
S
40000
35000
30000
25000
20000
15000
10000
5000
0
16
15
14
13
12
11
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9
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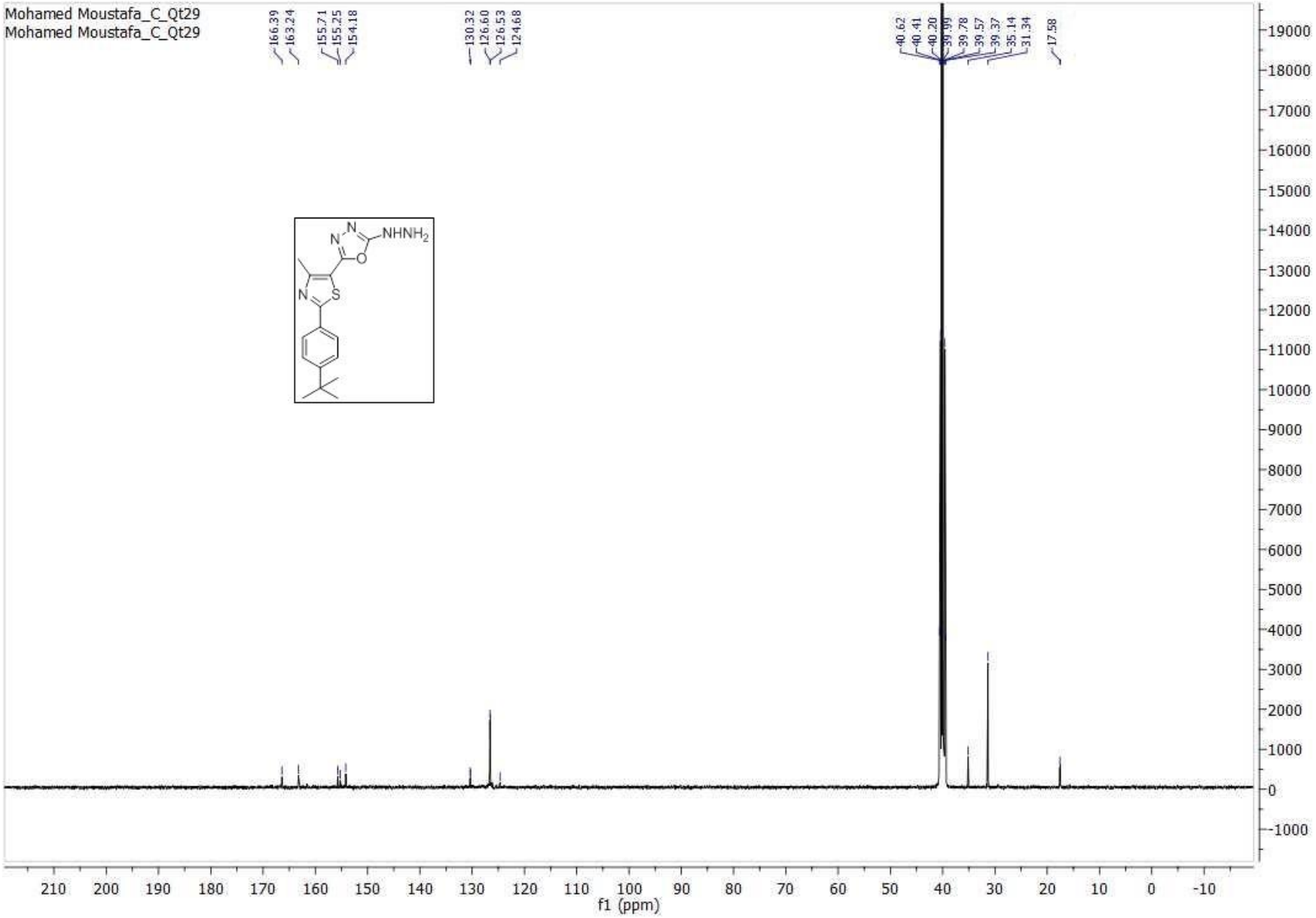
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


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
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39.57
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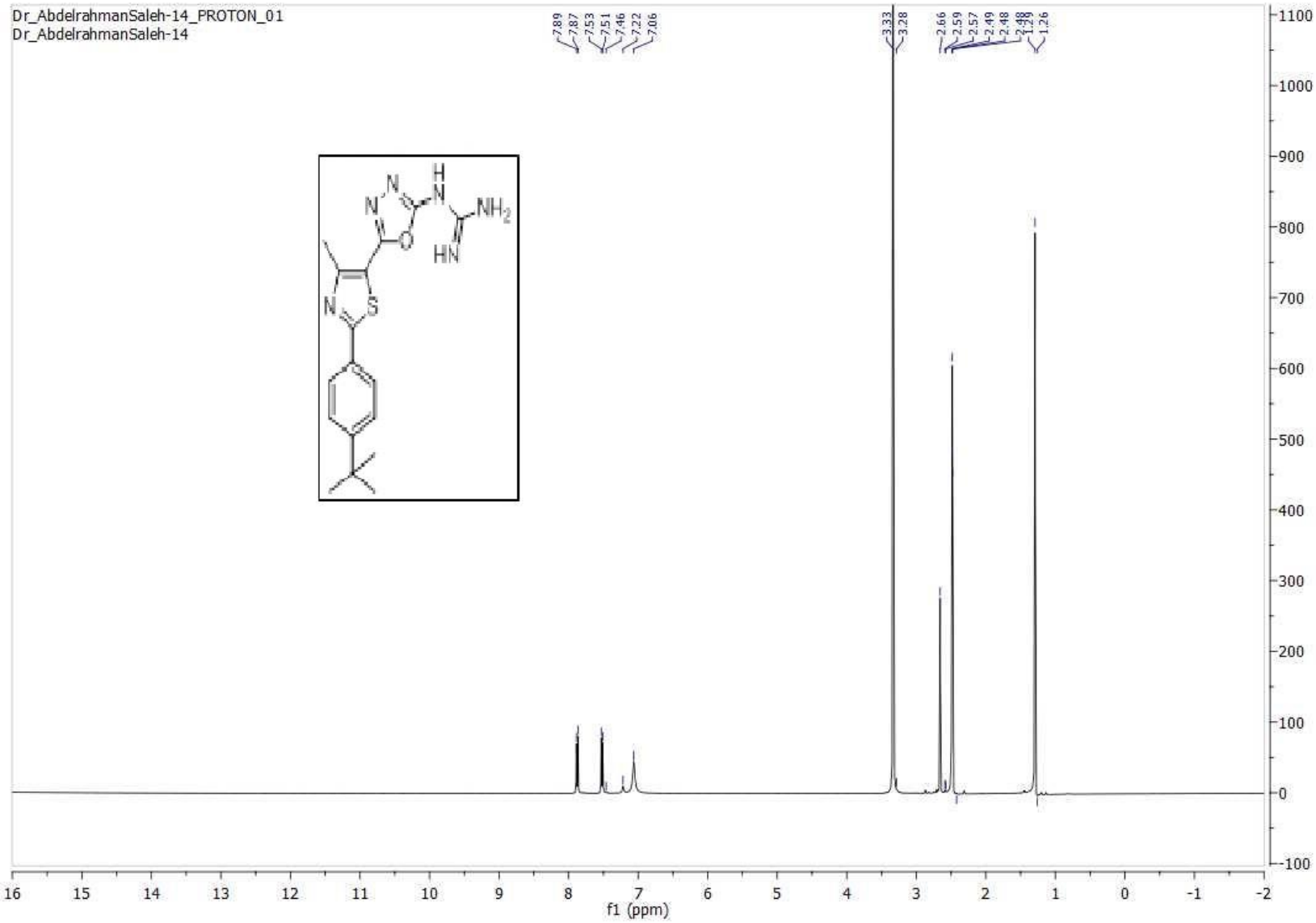
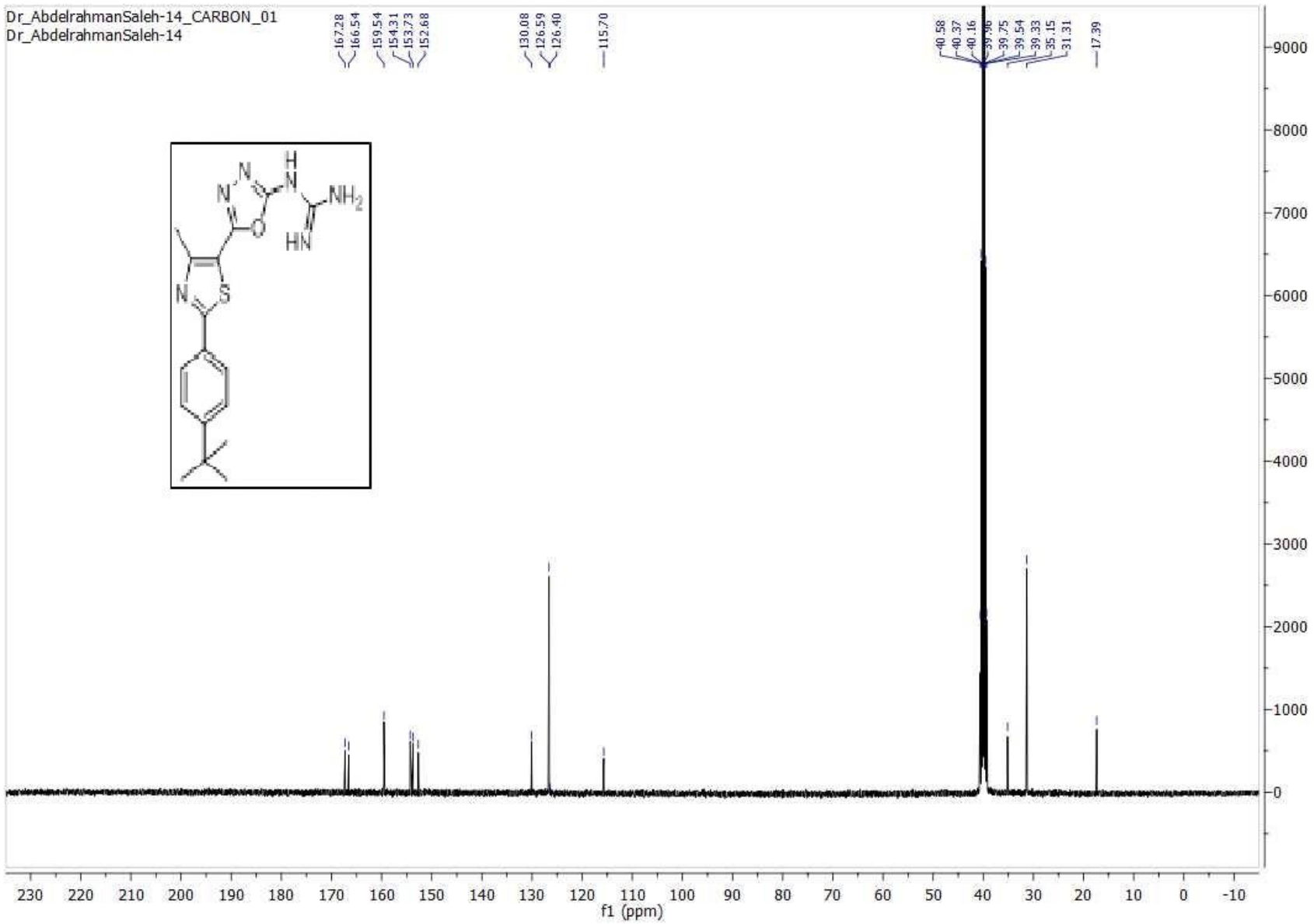
31.34
17.58
NHNH2
N
O
S
f1 (ppm)


Dr_AbdelrahmanSaleh-14_PROTON_01
Dr_AbdelrahmanSaleh-14
7.89
7.87
7.53
7.51
7.46
7.22
7.06
3.33
3.28
2.66
2.59
2.57
2.49
2.48
1.29
1.26
f1 (ppm)


Dr_AbdelrahmanSaleh-14_CARBON_01
Dr_AbdelrahmanSaleh-14
167.28
166.54
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154.31
153.73
152.68
130.08
126.59
126.40
115.70
40.58
40.37
40.16
39.96
39.75
39.54
39.33
35.15
31.31
17.39
NH2
HN
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

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
TD0                    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
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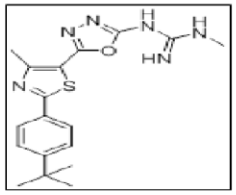

Mohamed Mostafa_C_Qt-20

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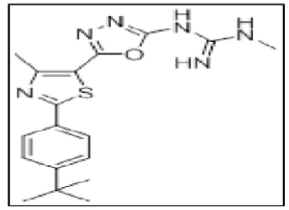
166.58
164.24
154.39
153.85
153.08
130.10
130.03
126.62
126.58
115.01
40.58
40.37
40.16
39.96
39.75
39.54
39.33
35.16
31.31
29.50
17.40

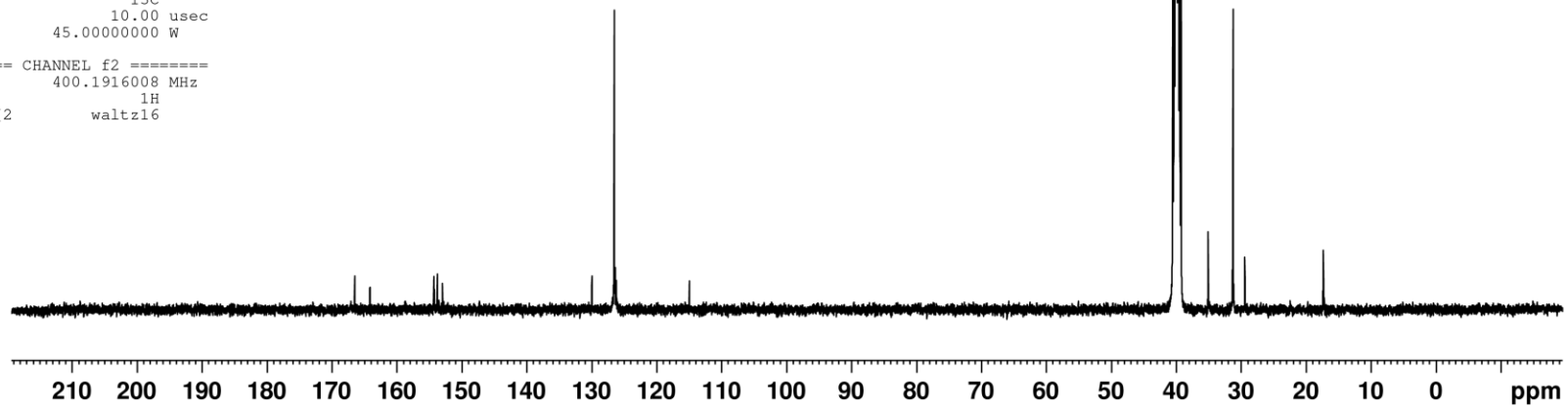
```
Current Data Parameters
NAME      Mohamed Mostafa_C_Qt-20
EXPNO                 10
PROCNO                 1

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

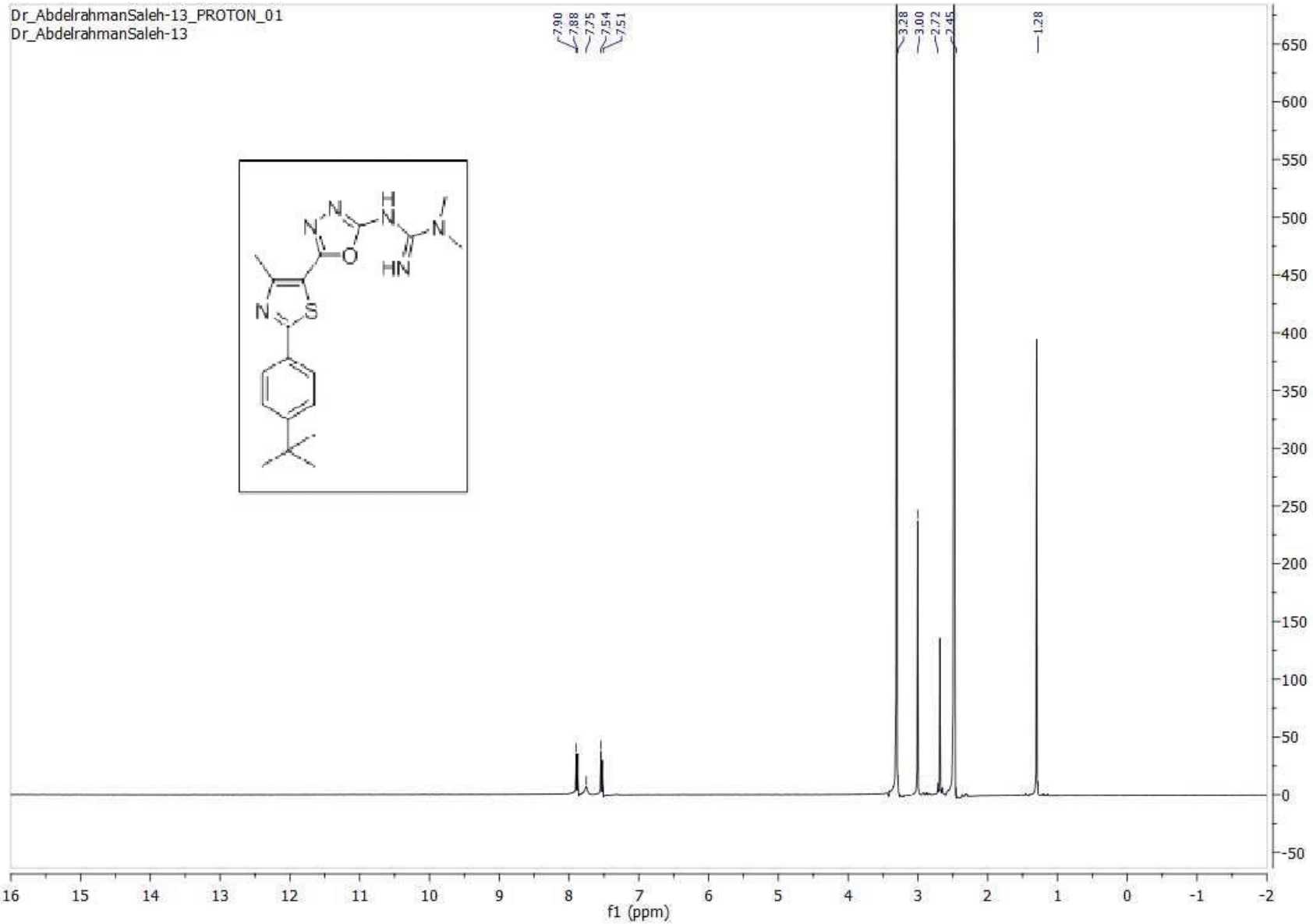
======== CHANNEL f1 ========
SFO1         100.6379178 MHz
NUC1                 13C
P1                 10.00 usec
PLW1         45.00000000 W

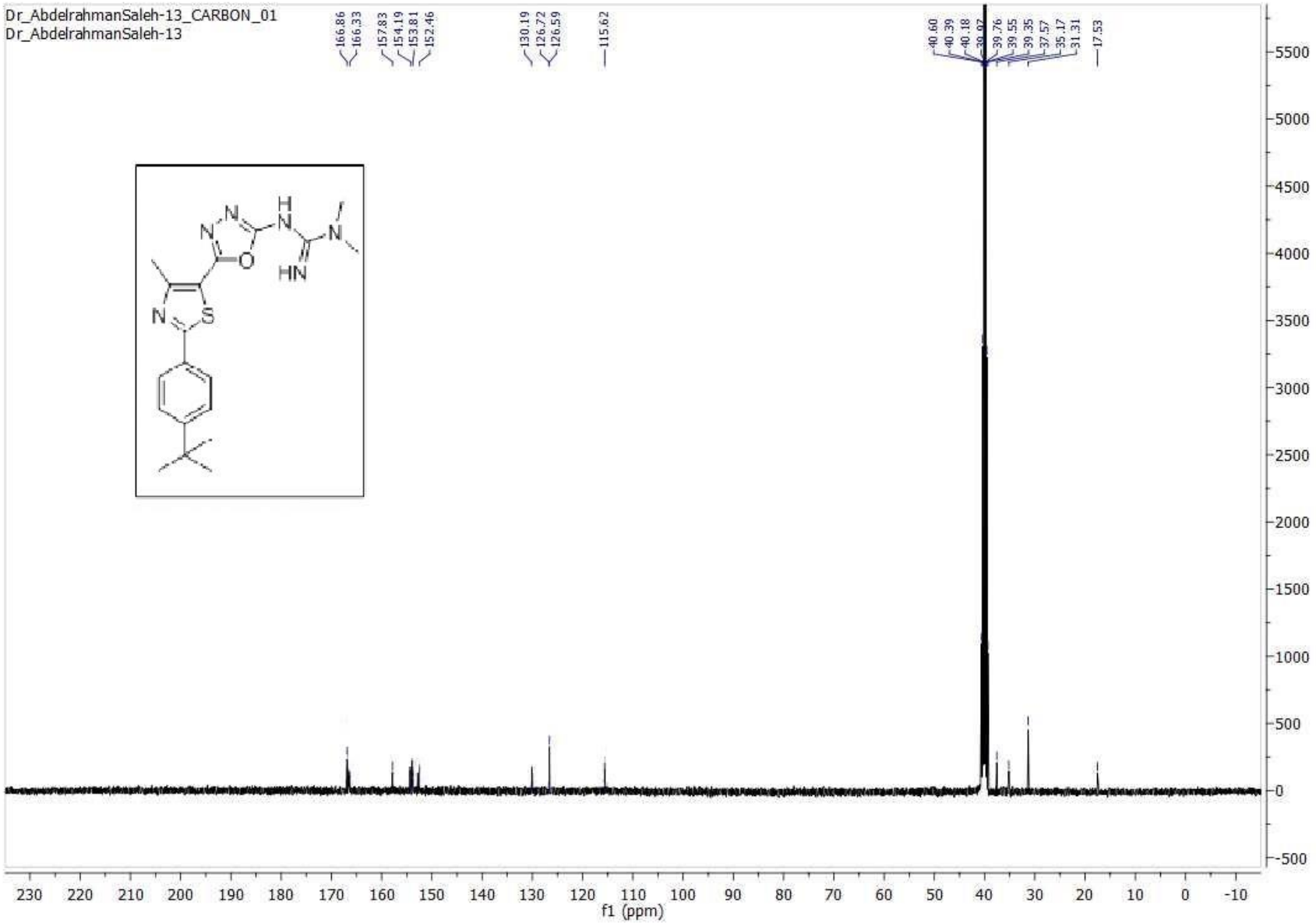
======== CHANNEL f2 ========
SFO2         400.1916008 MHz
NUC2                 1H
CPDPRG[2          waltz16
```





210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Dr_AbdelrahmanSaleh-13_PROTON_01
Dr_AbdelrahmanSaleh-13
7.90
7.88
7.75
7.54
7.51
3.28
3.00
2.72
2.45
1.28
f1 (ppm)


Dr_AbdelrahmanSaleh-13_CARBON_01
Dr_AbdelrahmanSaleh-13
166.86
166.33
157.83
154.19
153.81
152.46
130.19
126.72
126.59
115.62
40.60
40.39
40.18
39.97
39.76
39.55
39.35
37.57
35.17
31.31
17.53
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Mohamed Mostafa_H_Qt-15

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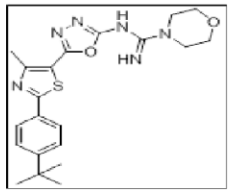
```
Current Data Parameters
NAME      Mohamed Mostafa_H_Qt-15
EXPNO                 10
PROCNO                 1

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
TD0                    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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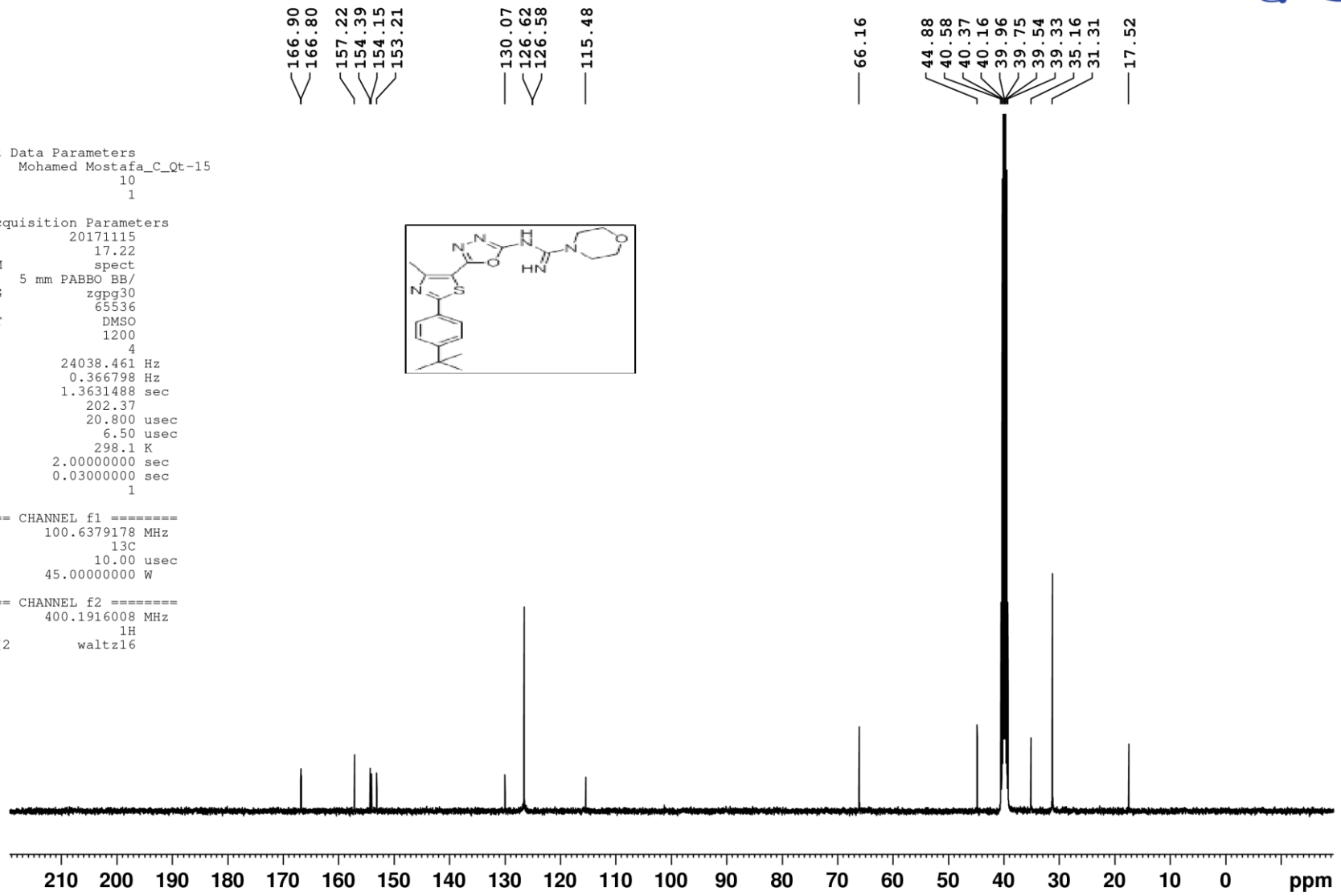
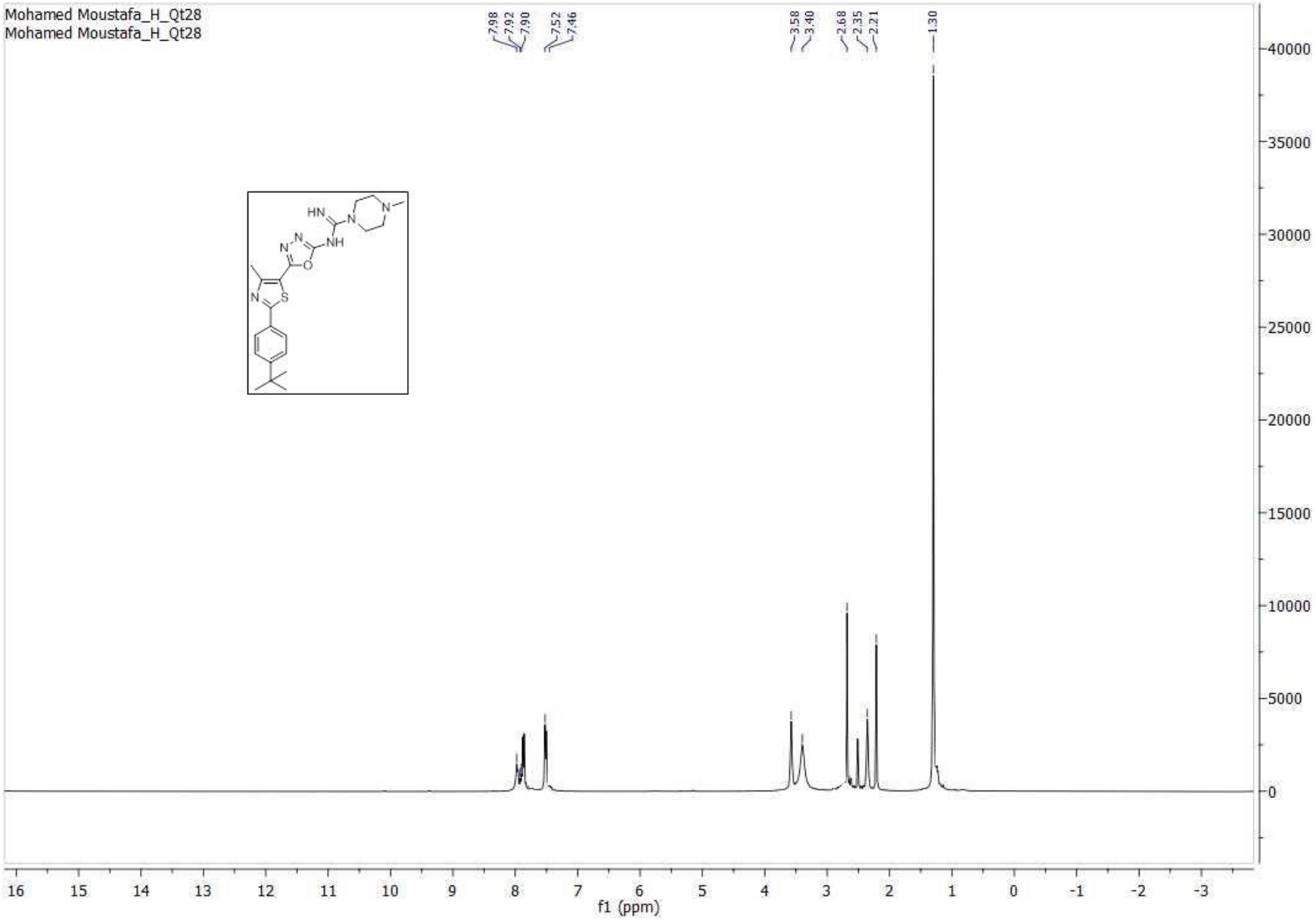


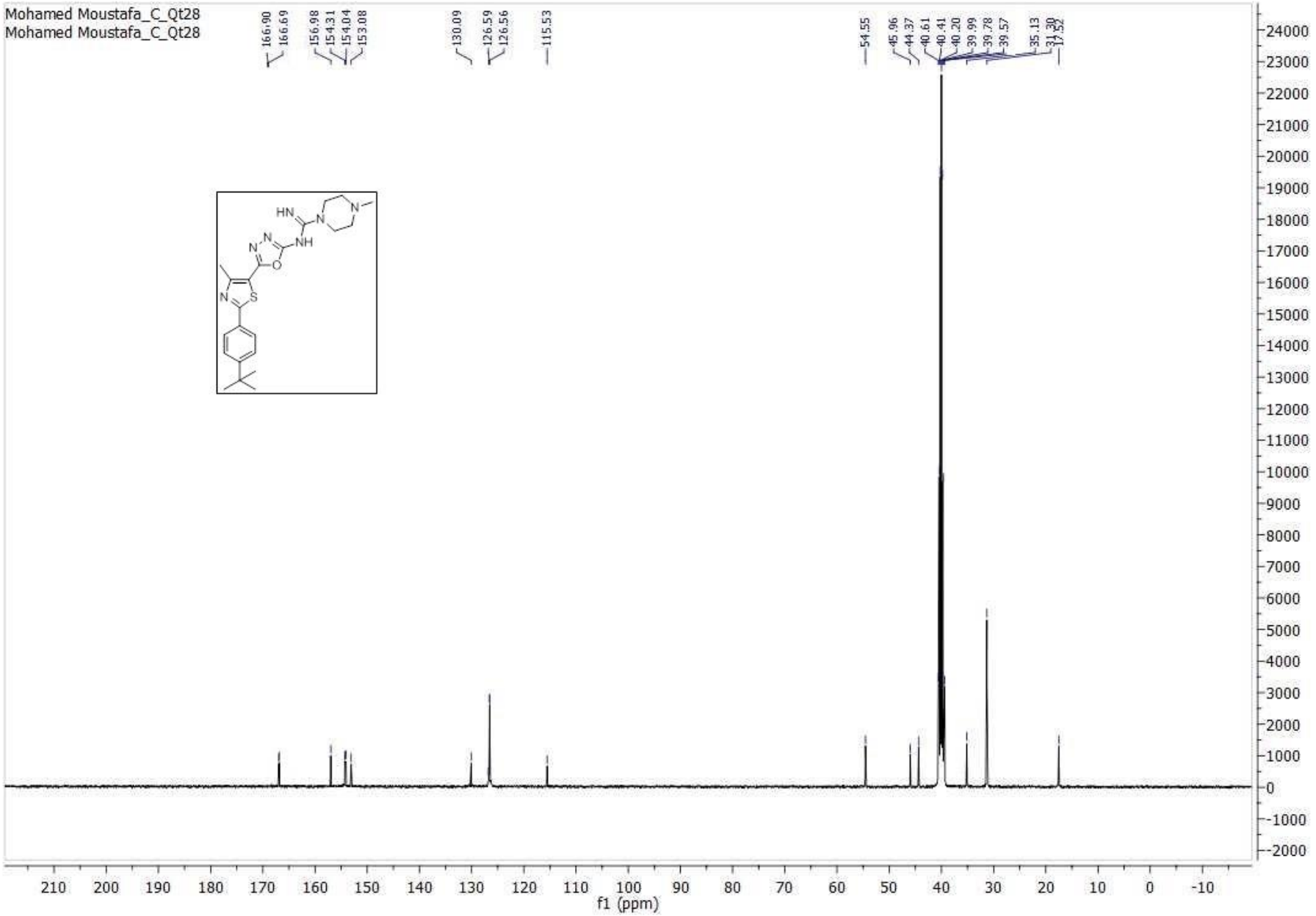

```
Current Data Parameters
NAME      Mohamed Mostafa_C_Qt-15
EXPNO                 10
PROCNO                 1

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
CPDPRG[2         waltz16
```


Mohamed Moustafa_H_Qt28
Mohamed Moustafa_H_Qt28
7.98
7.92
7.90
7.52
7.46
3.58
3.40
2.68
2.35
2.21
1.30
HN
NH
N
O
S
40000
35000
30000
25000
20000
15000
10000
5000
0
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
f1 (ppm)


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
17.52
HN
NH
N
O
S
f1 (ppm)

Mohamed Mostafa_H_Qt-17

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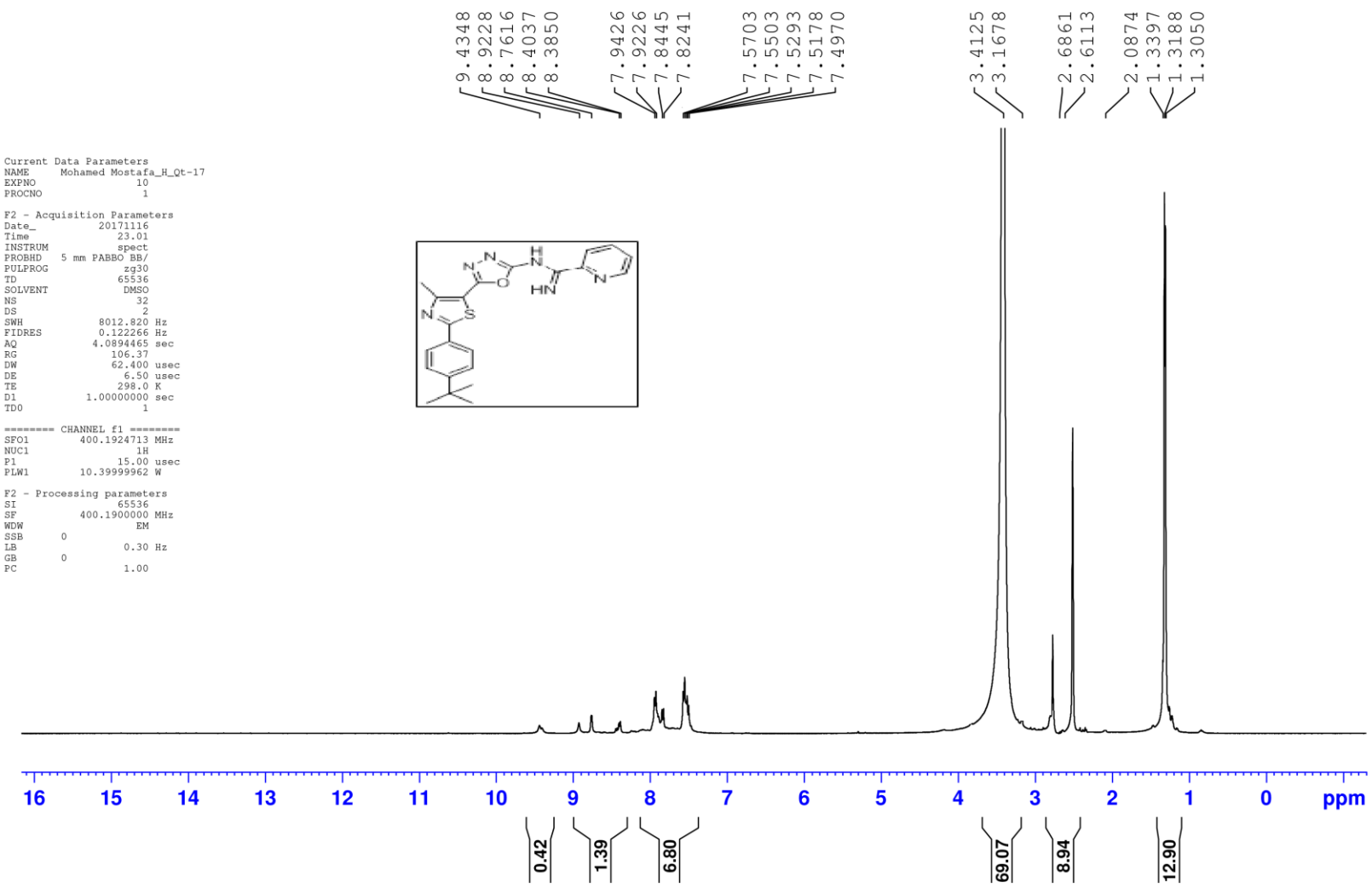


```
Current Data Parameters
NAME      Mohamed Mostafa_H_Qt-17
EXPNO                 10
PROCNO                 1

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
TD0                    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_MAS-85

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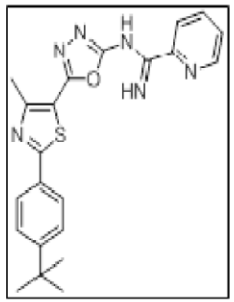
167.27
166.95
162.82
158.48
158.09
154.22
153.91
149.00
138.01
131.72
130.50
126.56
126.48
122.69
111.43
40.58
40.38
40.17
39.75
39.54
39.33
35.15
31.34
18.70

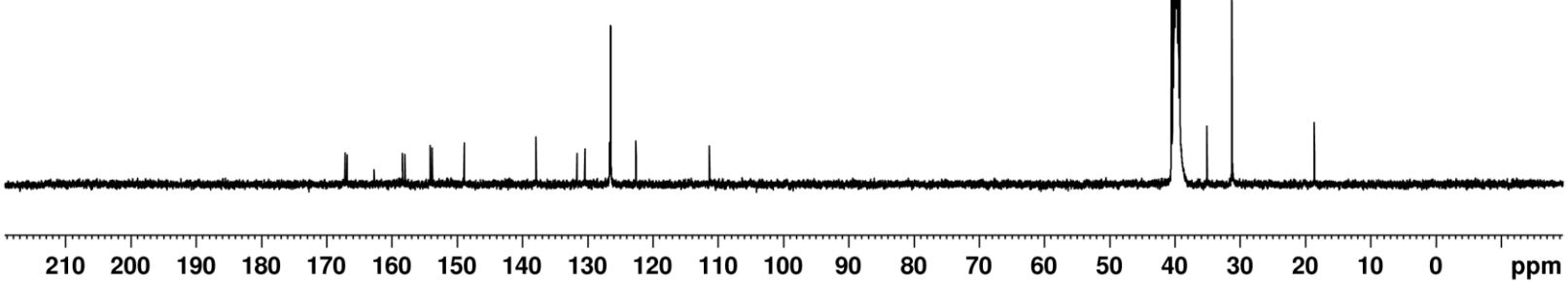
```
Current Data Parameters
NAME      Mohamed Mostafa_C_MAS-8
EXPNO                  10
PROCNO                  1

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
```





210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Mohamed Mostafa_H_Qt-18

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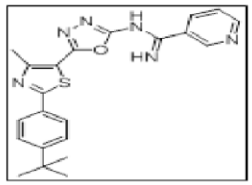
```
Current Data Parameters
NAME      Mohamed Mostafa_H_Qt-18
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171117
Time              1.31
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                64.21
DW               62.400 usec
DE                6.50 usec
TE               298.0 K
D1            1.00000000 sec
TD0                  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-18

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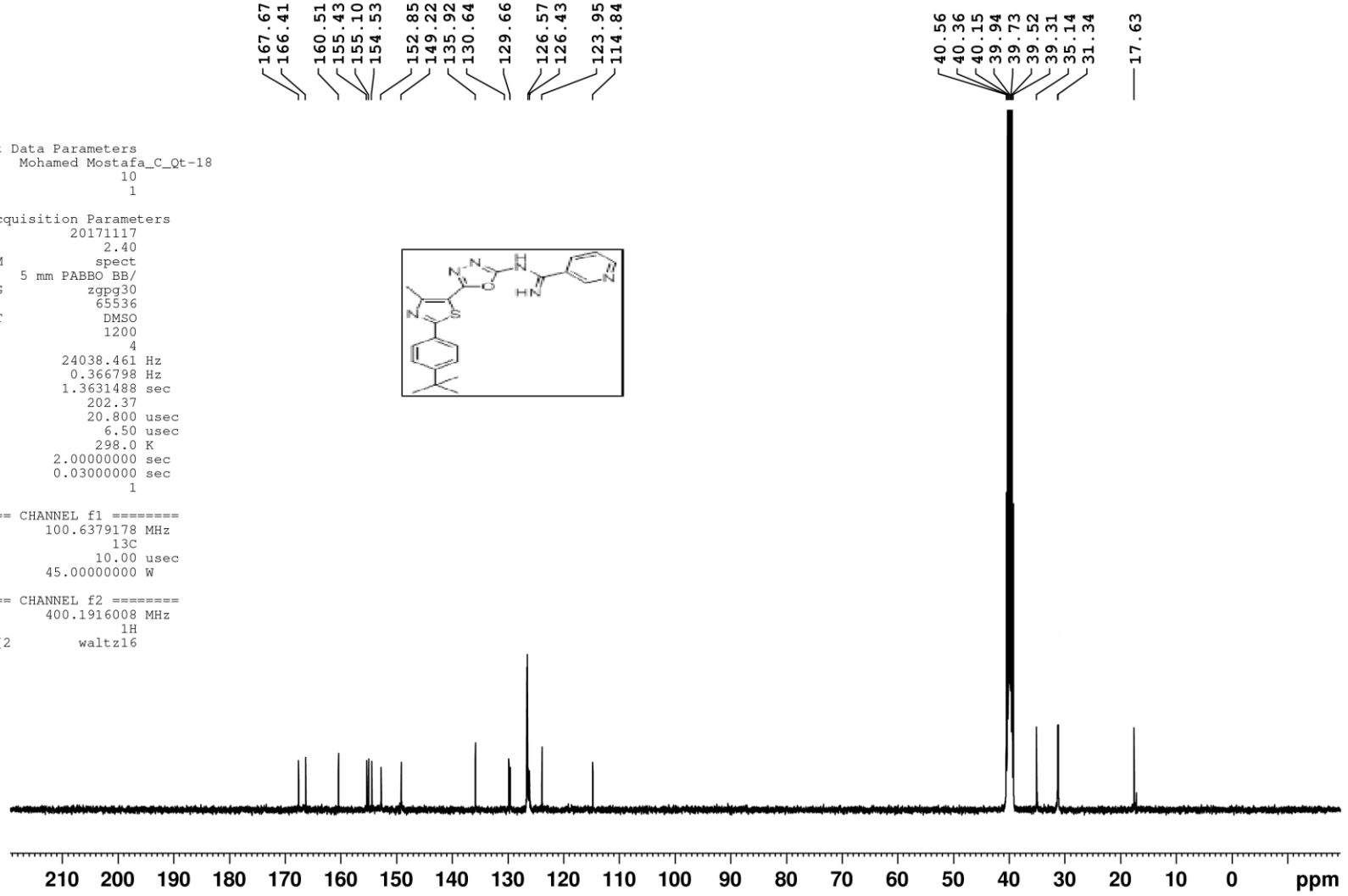

Mohamed Mostafa_H_Qt-19

Microanalytical Unit - FOPCU - NMR laboratory
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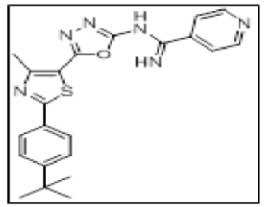
BRUKER

```
Current Data Parameters
NAME      Mohamed Mostafa_H_Qt-19
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171117
Time               0.16
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                    72.66
DW                 62.400 usec
DE                  6.50 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                    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-19

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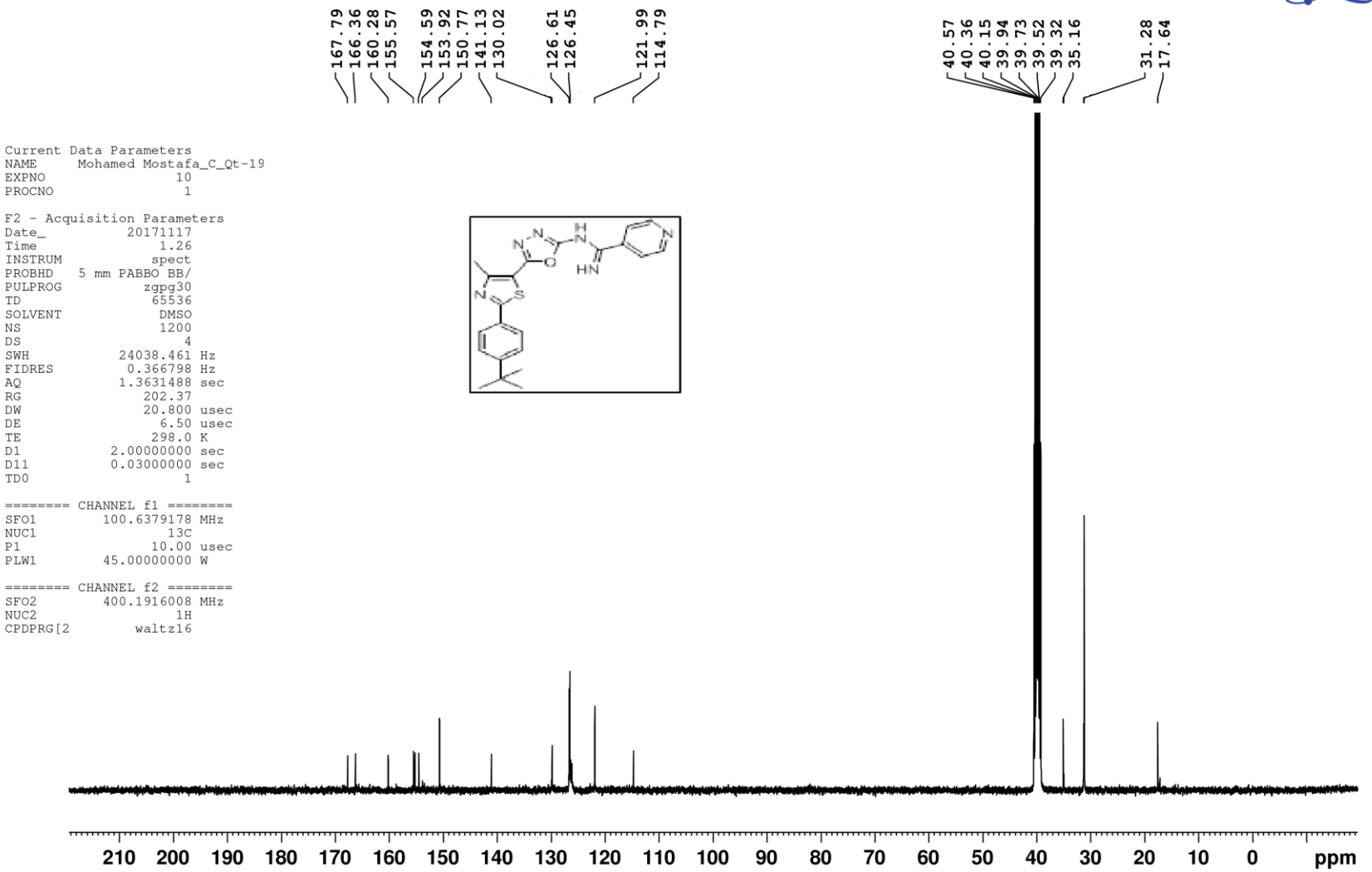
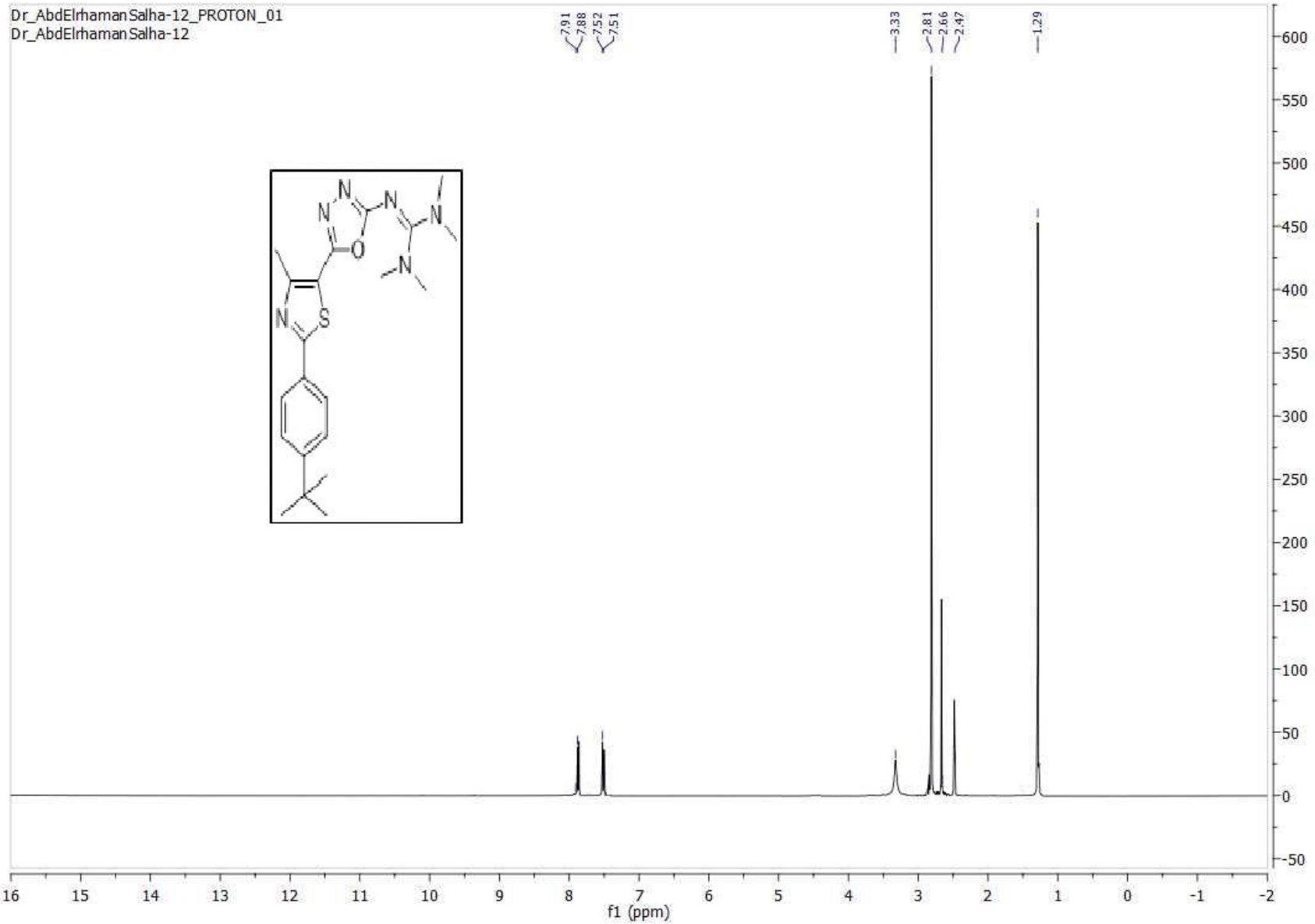


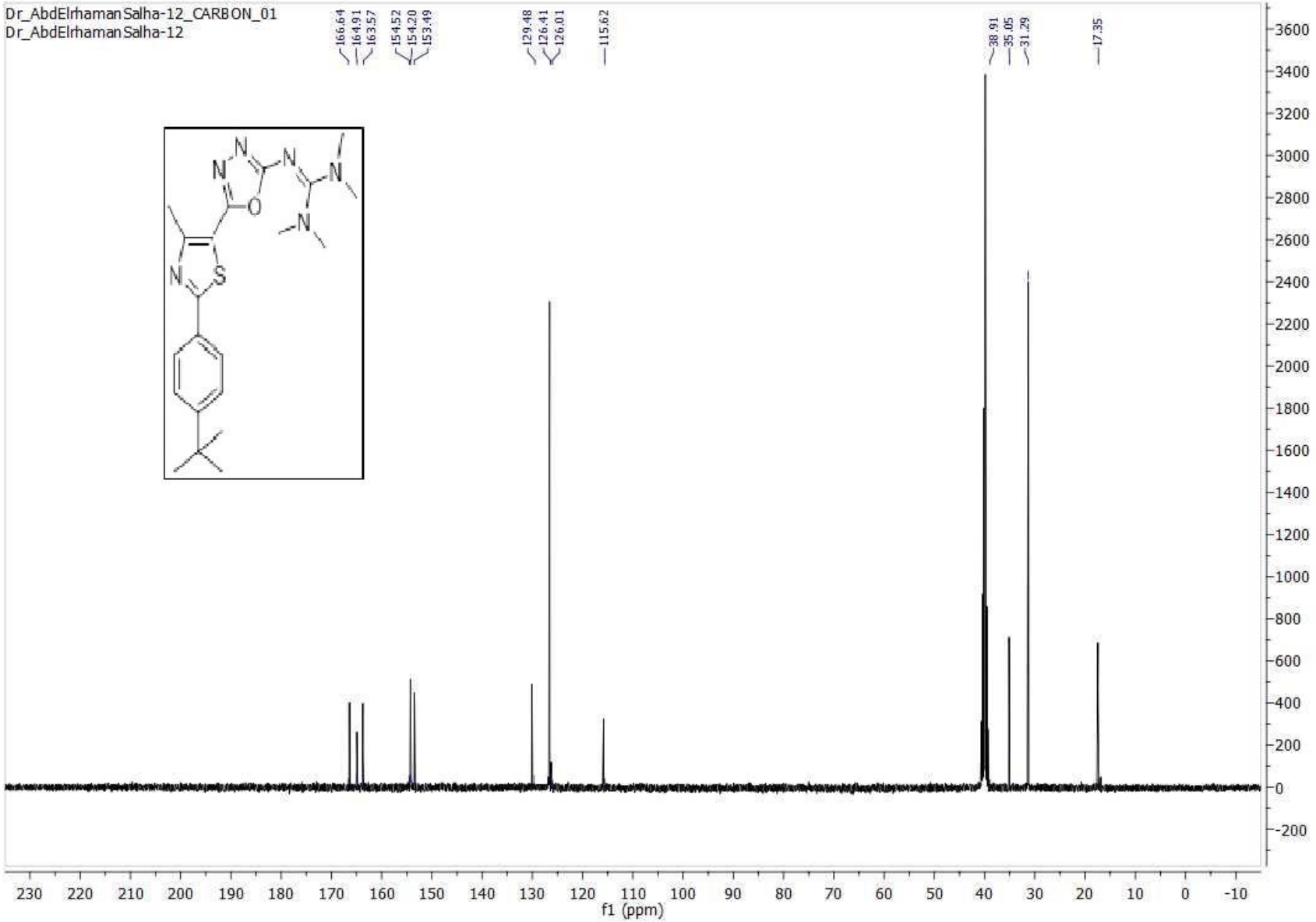

```
Current Data Parameters
NAME      Mohamed Mostafa_C_Qt-19
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171117
Time                1.26
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
```


Dr_AbdElrhaman Salha-12_PROTON_01
Dr_AbdElrhaman Salha-12
7.91
7.88
7.52
7.51
3.33
2.81
2.66
2.47
1.29
f1 (ppm)


Dr_AbdElrhamanSalha-12_CARBON_01
Dr_AbdElrhamanSalha-12
166.64
164.91
163.57
154.52
154.20
153.49
129.48
126.41
126.01
115.62
38.91
35.05
31.29
17.35
f1 (ppm)

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. Hagras, 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.