Supporting information

Aryl and Heteroaryl Phenylthiazoles for Enhanced Antimicrobial Activity Against Multidrug-Resistant Pathogens

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1.Result

1.1.Chemistry

1-(4-Methyl-2-(2'-methyl-[1,1'-biphenyl]-4-yl)thiazol-5-yl)ethan-1-one (3c).

Following the general procedure (method A), compound **3c** was obtained as light-brown oil (241 mg, 77%). ^{1}H NMR (DMSO-d_6) δ: 8.03 (d, *J* = 8.2 Hz, 2H), 7.65 (d, *J* = 8.2 Hz, 2H), 7.41-7.35 (m, 2H), 7.16 (d, *J* = 8 Hz, 1H), 7.08 (t, *J* = 8 Hz, 1H), 2.72 (s, 3H), 2.57 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (DMSO-d_6); δ 192.6, 168.8, 158.6, 156.6, 141.7, 132.5, 131.0, 130.7, 130.6, 130.0, 129.0, 126.7, 121.3, 112.3, 30.8, 25.0, 18.6; MS (*m*\z); 307.

1-(2-(4-benzylphenyl)-4-methylthiazol-5-yl)ethan-1-one (4c)

Following the general procedure (method A), compound 4c was obtained as light-brown oil (198 mg, 66%). 1H NMR (DMSO-d6) δ: 8.21-8.16 (m, 2H), 7.83-7.73 (m, 4H), 7.54-7.48 (m, 2H), 7.43-7.38 (m, 1H), 3.94 (s, 2H), 2.67 (s, 3H), 2.26 (s, 3H); 13C NMR (DMSO-d6); δ 190.8, 155.6, 152.9, 148.6, 140.79, 140.75, 140.0, 138.0, 137.0, 135.5, 135.4, 129.4, 128.1, 127.3, 127.0, 117.4, 42.3, 25.3, 17.5; MS (m\z); 307.

Methyl 4'-(5-acetyl-4-methylthiazol-2-yl)-[1,1'-biphenyl]-3-carboxylate (5c)

Following the general procedure (method B), compound 5c was obtained as yellow oil (288 mg, 59%). 1H NMR (DMSO-d6) δ: 8.22 (s, 1H), 8.07 (d, J = 8 Hz, 2H), 8.01-7.97 (m, 2H), 7.85 (d, J = 8 Hz, 2H), 7.66 (t, J = 8 Hz, 1H), 3.90 (s, 3H), 2.71 (s, 3H), 2.56 (s, 3H); 13C NMR (DMSO-d6); δ: 191.0, 168.3, 166.4, 165.9, 158.7, 141.7, 139.7, 132.5, 131.9, 130.9, 130.5, 129.2, 128.0, 127.5, 52.7, 30.8, 18.6; MS (m\z); 351.

1-(2-(3'-hydroxy-[1,1'-biphenyl]-4-yl)-4-methylthiazol-5-yl)ethan-1-one (6c)

Following the general procedure (method B), compound 6c was obtained as yellow oil (271 mg, 63%). 1H NMR (DMSO-d6) δ: 9.63 (brs, 1H), 8.07 (d, J = 8 Hz, 2H), 7.32 (d, J = 8 Hz, 2H), 7.32 (t, J = 8 Hz, 1H), 7.16 (d, J = 8 Hz, 1H), 7.10 (s, 1H), 6.84 (d, J = 8 Hz, 1H), 2.73 (s, 3H), 2.58 (s, 3H); 13C NMR (DMSO-d6); δ: 181.1, 168.6, 158.7, 158.4, 143.4, 140.7, 132.5, 131.5, 130.6, 127.8, 127.6, 117.9, 115.7, 113.9, 30.9, 18.6; MS (m\z); 309.

1-(4-Methyl-2-(4-(1-methyl-1H-pyrrol-2-yl)phenyl)thiazol-5-yl)ethan-1-one (7c)

Following the general procedure (method A), compound 7c was obtained as light-brown oil (203 mg, 67%). 1H NMR (DMSO-d6) δ: 8.02 (d, J = 8.2 Hz, 2H), 7.99 (d, J = 8.2 Hz, 2H), 7.66-7.61 (m, 2H), 7.20-7.18 (m, 1H), 2.99 (s, 3H), 2.71 (s, 3H), 2.56 (s, 3H); 13C NMR (DMSO-d6); δ 191.0, 188.3, 158.7, 142.9, 136.8, 132.4, 131.3, 129.3, 127.7, 127.5, 126.4, 125.4, 30.8, 28.7, 18.6; MS (m\z); 296.

1-(4-methyl-2-(4-(4-methylthiophen-3-yl)phenyl)thiazol-5-yl)ethan-1-one (8c)

Following the general procedure (method B), compound 8c was obtained as yellow oil (296 mg, 68%). 1H NMR (DMSO-d6) δ: 8.01 (d, J = 8 Hz, 2H), 7.63-7.58 (m, 3H), 7.33 (s, 1H), 2.72 (s, 1H), 2.58 (s, 3H), 2.23 (s, 3H); 13C NMR (DMSO-d6); δ: 190.1, 168.4, 158.5, 141.2, 139.5, 135.5, 132.2, 131.2, 129.3, 127.1, 124.6, 123.6, 30.9, 18.4, 15.7; MS (m\z); 313.

5-(4-(5-acetyl-4-methylthiazol-2-yl)phenyl)-N-propylthiophene-2-sulfonamide (9c)

Following the general procedure (method B), compound 9c was obtained as yellow oil (345 mg, 59%). 1H NMR (DMSO-d6) δ: 8.07 (d, J = 8 Hz, 2H), 7.92 (brs, 1H), 7.89 (d, J = 8 Hz, 2H), 7.71 (d, J = 8 Hz, 1H), 7.61 (d, J = 8 Hz, 1H), 2.91 (t, J = 8 Hz, 2H), 2.72 (s, 3H), 2.58 (s, 3H) 1.43-1.38 (m, 2H), 0.84 (t, J = 8 Hz, 3H); 13C NMR (DMSO-d6); δ: 191.1, 167.9, 158.7, 147.7, 141.5, 135.29, 135.28, 132.9, 132.6, 127.8, 127.1, 125.6, 42.9, 31.4, 19.7, 18.6, 13.9; MS (m\z); 420.

5-(4-(5-acetyl-4-methylthiazol-2-yl)phenyl)-N-(3-hydroxypropyl)thiophene-2-sulfonamide (10c)

Following the general procedure (method B), compound 10c was obtained as yellow oil (383 mg, 63%). 1H NMR (DMSO-d6) δ: 8.06 (d, J = 8 Hz, 2H), 7.88 (d, J = 8 Hz, 2H), 7.72 (brs, 1H), 7.62 (d, J = 8 Hz, 1H), 7.57 (d, J = 8 Hz, 1H), 5.33 (brs, 1H), 3.87 (t, J = 8 Hz, 2H), 2.71 (s, 3H), 2.57 (s, 3H) 2.22-2.21 (m, 2H), 1.62 (t, J = 8 Hz, 2H); 13C NMR (DMSO-d6); δ: 191.1, 167.9, 158.7, 148.0, 140.1, 135.2, 133.2, 132.9, 132.7, 127.8, 127.1, 125.6, 58.7, 39.3, 30.9, 29.3, 18.6; MS (m\z); 436.

5-(4-(5-acetyl-4-methylthiazol-2-yl)phenyl)-N-cyclohexylthiophene-2-sulfonamide (11c)

Following the general procedure (method B), compound 11c was obtained as yellow oil (378 mg, 59%). 1H NMR (DMSO-d6) δ: 8.08 (d, J = 8 Hz, 2H), 7.89 (brs, 1H), 7.87 (d, J = 8 Hz, 2H), 7.70 (d, J = 8 Hz, 1H), 7.61 (d, J = 8 Hz, 1H), 3.30-3.20 (m, 1H), 2.72 (s, 3H), 2.58 (s, 3H) 1.33-1.25 (m, 4H), 1.23-1.21 (m, 3H), 0.99-0.79 (m, 3H); 13C NMR (DMSO-d6); δ: 191.1, 167.9, 158.7, 147.5, 143.2, 135.3, 132.9, 132.7, 132.6, 127.9, 127.0, 125.5, 49.8, 30.9, 21.5, 18.8, 18.6, 14.1; MS (m\z); 460.

2-(1-(4-Methyl-2-(2'-methyl-[1,1'-biphenyl]-4-yl)thiazol-5-yl)ethylidene)hydrazine-1-carboximidamide (3d).

Light-brown solid (100 mg, 74%); mp 130-131 oC; 1H NMR (DMSO-d6) δ: 7.94 (d, J = 8.2 Hz, 2H), 7.60 (d, J = 8.2 Hz, 2H), 7.40-7.34 (m, 2H), 7.15 (d, J = 8 Hz, 1H), 7.06 (t, J = 8 Hz, 1H), 5.98 (brs, 4H), 2.61 (s, 3H), 2.33 (s, 3H), 2.23 (s, 3H); 13C NMR (DMSO-d6); δ 162.7, 159.7, 158.6, 156.6, 141.7, 132.5, 131.0, 130.7, 130.6, 130.0, 129.0, 126.7, 121.3, 112.3, 30.8, 25.0, 18.6, 16.7; MS (m\z); 363; HPLC purity 96.1 % (acetonitrile-3%TEA, 1:4).

2-(1-(2-(4-Benzylphenyl)-4-methylthiazol-5-yl)ethylidene)hydrazine-1-carboximidamide (4d)

Yellow solid (101 mg, 78%); mp 117-118 oC; 1H NMR (DMSO-d6) δ: 8.21-8.16 (m, 2H), 7.83-7.75 (m, 4H), 7.73-7.48 (m, 2H), 7.41-7.38 (m, 1H), 5.78 (brs, 2H), 3.95 (s, 2H), 2.67 (s, 3H), 2.26 (s, 3H); 13C NMR (DMSO-d6); δ 190.8, 155.6, 152.9, 148.6, 140.79, 140.75, 140.0, 138.0, 137.0, 135.5, 135.4, 129.4, 128.1, 127.3, 127.0, 117.4, 42.4, 25.3, 17.5; MS (m\z); 363; HPLC purity 95.9 % (acetonitrile-3%TEA, 1:4).

Methyl-4'-(5-(1-(2-carbamimidoylhydrazono)ethyl)-4-methylthiazol-2-yl)-[1,1'-biphenyl]-3-carboxylate (5d)

Brown solid (113 mg, 75%); mp 134-135 oC; 1H NMR (DMSO-d6) δ: 8.22 (s, 1H), 8.07 (d, J = 8 Hz, 2H), 7.99-7.97 (m, 2H), 7.85 (d, J = 8 Hz, 2H), 7.66 (t, J = 8 Hz, 1H), 5.79 (brs, 2H), 5.65 (brs, 2H), 3.90 (s, 3H), 2.71 (s, 3H), 2.34 (s, 3H); MS (m\z); 407; HPLC purity 96.9 % (acetonitrile-3%TEA, 1:4).

2-(1-(2-(3'-Hydroxy-[1,1'-biphenyl]-4-yl)-4-methylthiazol-5-yl)ethylidene)hydrazine-1-carboximidamide (6d)

Light-brown solid (107 mg, 79%); mp 127-128 oC; 1H NMR (DMSO-d6) δ: 9.61 (brs, 1H), 7.97 (d, J = 8 Hz, 2H), 7.73 (d, J = 8 Hz, 2H), 7.29 (t, J = 8 Hz, 1H), 7.15 (d, J = 8 Hz, 1H), 7.0 (s, 1H), 6.82 (d, J = 8 Hz, 1H), 5.78 (brs, 4H), 2.61 (s, 3H), 2.33 (s, 3H); 13C NMR (DMSO-d6); δ: 162.3, 160.0, 158.3, 148.5, 143.2, 141.8, 141.0, 135.7, 132.6, 130.5, 127.6, 126.7, 117.8, 115.4, 113.8, 18.6, 16.5; MS (m\z); 365; HPLC purity 97.5 % (acetonitrile-3%TEA, 1:4).

2-(1-(4-Methyl-2-(4-(1-methyl-1H-pyrrol-2-yl)phenyl)thiazol-5-yl)ethylidene)hydrazine-1-carboximidamide (7d)

Light-yellow solid (109 mg, 83%); mp 120-121 oC; 1H NMR (DMSO-d6) δ: 7.94 (d, J = 8.2 Hz, 2H), 7.64 (d, J = 8.2 Hz, 2H), 7.61-7.57 (m, 2H), 7.56-7.37 (m, 1H), 5.79 (brs, 2H), 5.67 (brs, 2H), 2.94 (s, 3H), 2.60 (s, 3H), 2.33 (s, 3H); 13C NMR (DMSO-d6); δ 160.3, 155.7, 152.1, 148.3, 145.7, 138.1, 137.1, 135.9, 132.0, 129.1, 128.8, 127.4, 126.0, 29.1, 25.2, 17.4; MS (m\z); 352; HPLC purity 97.3 % (acetonitrile-3%TEA, 1:4).

2-(1-(4-Methyl-2-(4-(4-methylthiophen-3-yl)phenyl)thiazol-5-yl)ethylidene)hydrazine-1-carboximidamide (8d)

Brown solid (102 mg, 74%); mp 123-124 oC; 1H NMR (DMSO-d6) δ: 7.98 (d, J = 8 Hz, 2H), 7.58-7.53 (m, 3H), 7.31 (s, 1H), 5.79 (brs, 2H), 5.69 (brs, 2H), 2.61 (s, 1H), 2.32 (s, 3H), 2.28 (s, 3H); 13C NMR (DMSO-d6); δ: 161.8, 160.1, 148.1, 143.2, 141.8, 138.2, 135.9, 132.2, 128.9, 128.6, 126.2, 124.6, 18.4, 16.3, 15.4; MS (m\z); 369; HPLC purity 98.4 % (acetonitrile-3%TEA, 1:4).

2-(1-(4-methyl-2-(4-(5-(N-propylsulfamoyl)thiophen-2-yl)phenyl)thiazol-5-yl)ethylidene)hydrazine-1-carboximidamide (9d)

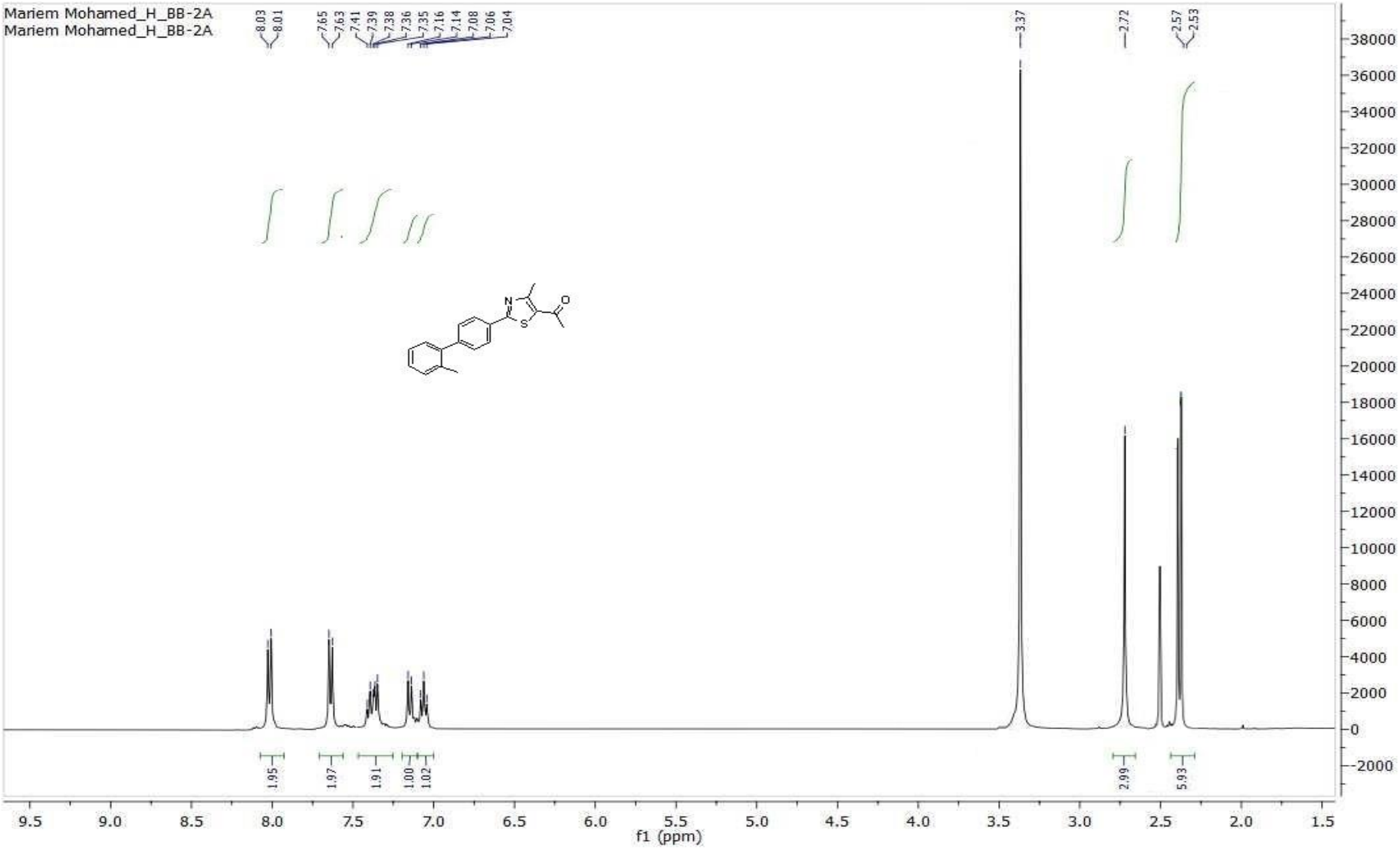
Yellow solid (120 mg, 68%); mp 139-140 oC; 1H NMR (DMSO-d6) δ: 7.97 (d, J = 8 Hz, 2H), 7.90 (brs, 1H), 7.88 (d, J = 8 Hz, 2H), 7.67 (d, J = 8 Hz, 1H), 7.60 (d, J = 8 Hz, 1H), 5.86 (brs, 4H), 2.90 (t, J = 8 Hz, 2H), 2.60 (s, 3H), 2.33 (s, 3H) 1.43-1.39 (m, 2H), 0.85 (t, J = 8 Hz, 3H); 13C NMR (DMSO-d6); δ: 161.6, 159.9, 148.8, 148.2, 143.2, 141.0, 136.1, 133.8, 133.7, 132.9, 126.9, 125.0, 42.9, 31.4, 19.7, 18.6, 13.9; MS (m\z); 476; HPLC purity 99.2 % (acetonitrile-3%TEA, 1:4).

2-(1-(2-(4-(5-(N-(3-Hydroxypropyl)sulfamoyl)thiophen-2-yl)phenyl)-4-methylthiazol-5-yl)ethylidene)hydrazine-1-carboximidamide (10d)

Light-brown solid (148 mg, 81%); mp 148-149 oC; 1H NMR (DMSO-d6) δ: 7.97 (d, J = 8 Hz, 2H), 7.84 (brs, 1H), 7.82 (d, J = 8 Hz, 2H), 7.68 (d, J = 8 Hz, 1H), 7.60 (d, J = 8 Hz, 1H), 5.78 (brs, 1H), 5.67 (brs, 1H), 5.34 (brs, 1H), 3.88 (t, J = 8 Hz, 2H), 2.56 (s, 3H), 2.32 (s, 3H) 2.22-2.21 (m, 2H), 1.68 (t, J = 8 Hz, 2H); 13C NMR (DMSO-d6); δ: 161.5, 160.2, 148.5, 148.4, 142.9, 139.6, 136.4, 133.9, 133.6, 133.2, 126.9, 125.0, 59.0, 39.3, 29.3, 18.6, 16.4; MS (m\z); 492; HPLC purity 96.7 % (acetonitrile-3%TEA, 1:4).

2-(1-(2-(4-(5-(N-Cyclohexylsulfamoyl)thiophen-2-yl)phenyl)-4-methylthiazol-5-yl)ethylidene)hydrazine-1-carboximidamide (11d)

Light-yellow solid (136 mg, 71%); mp 136-137 oC; 1H NMR (DMSO-d6) δ: 7.97 (d, J = 8 Hz, 2H), 7.83 (brs, 1H), 7.81 (d, J = 8 Hz, 2H), 7.65 (d, J = 8 Hz, 1H), 7.59 (d, J = 8 Hz, 1H), 5.83 (brs,4H), 3.30-3.28 (m, 1H), 2.60 (s, 3H), 2.32 (s, 3H) 1.33-1.21 (m, 4H), 0.98-0.97 (m, 3H), 0.79-0.76 (m, 3H); 13C NMR (DMSO-d6); δ: 161.6, 160.0, 148.7, 148.0, 143.2, 142.6, 136.2, 133.8, 133.7, 132.7, 126.9, 124.9, 49.8, 30.9, 21.5, 18.8, 18.6, 14.1; MS (m\z); 516; HPLC purity 97.1 % (acetonitrile-3%TEA, 1:4).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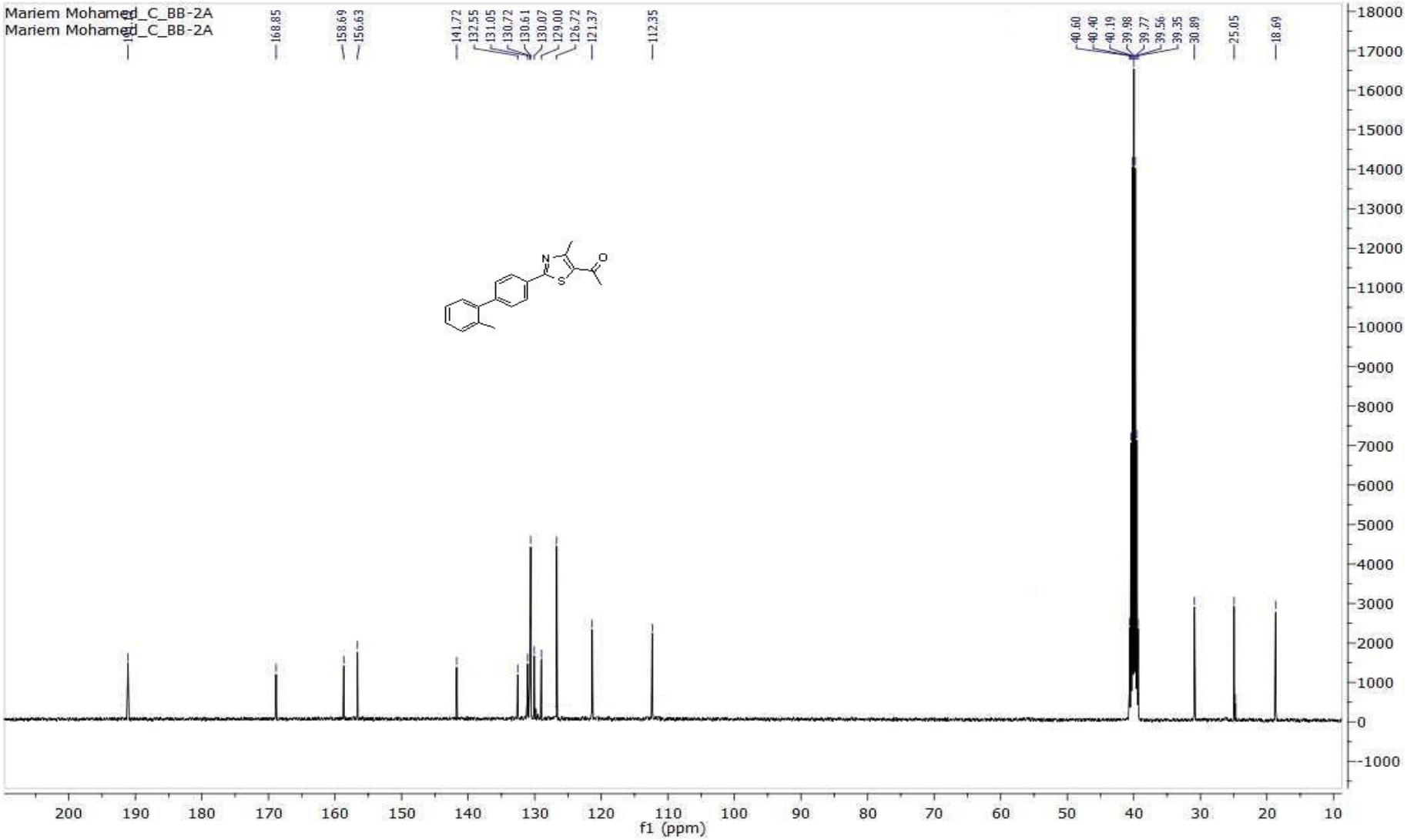
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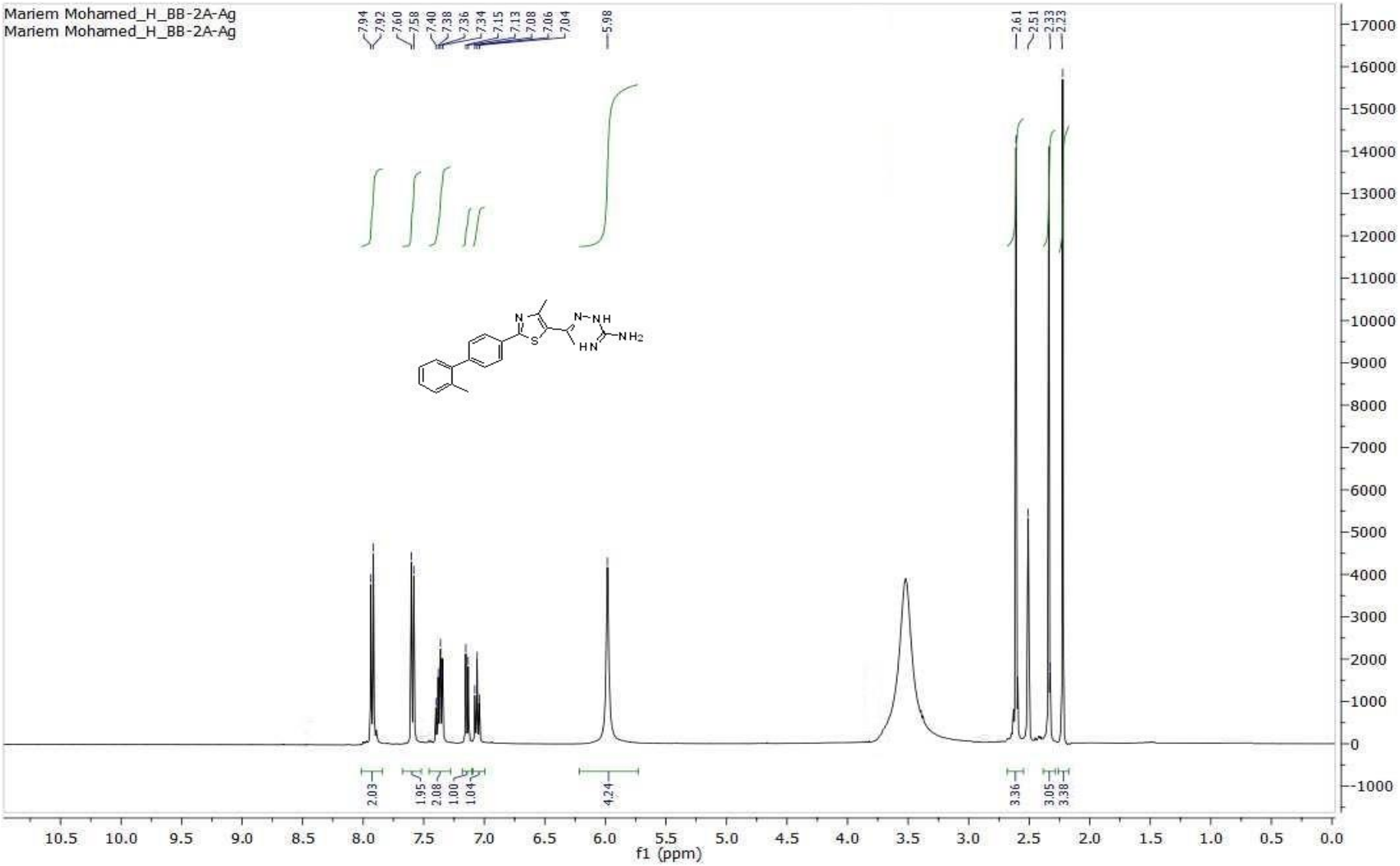
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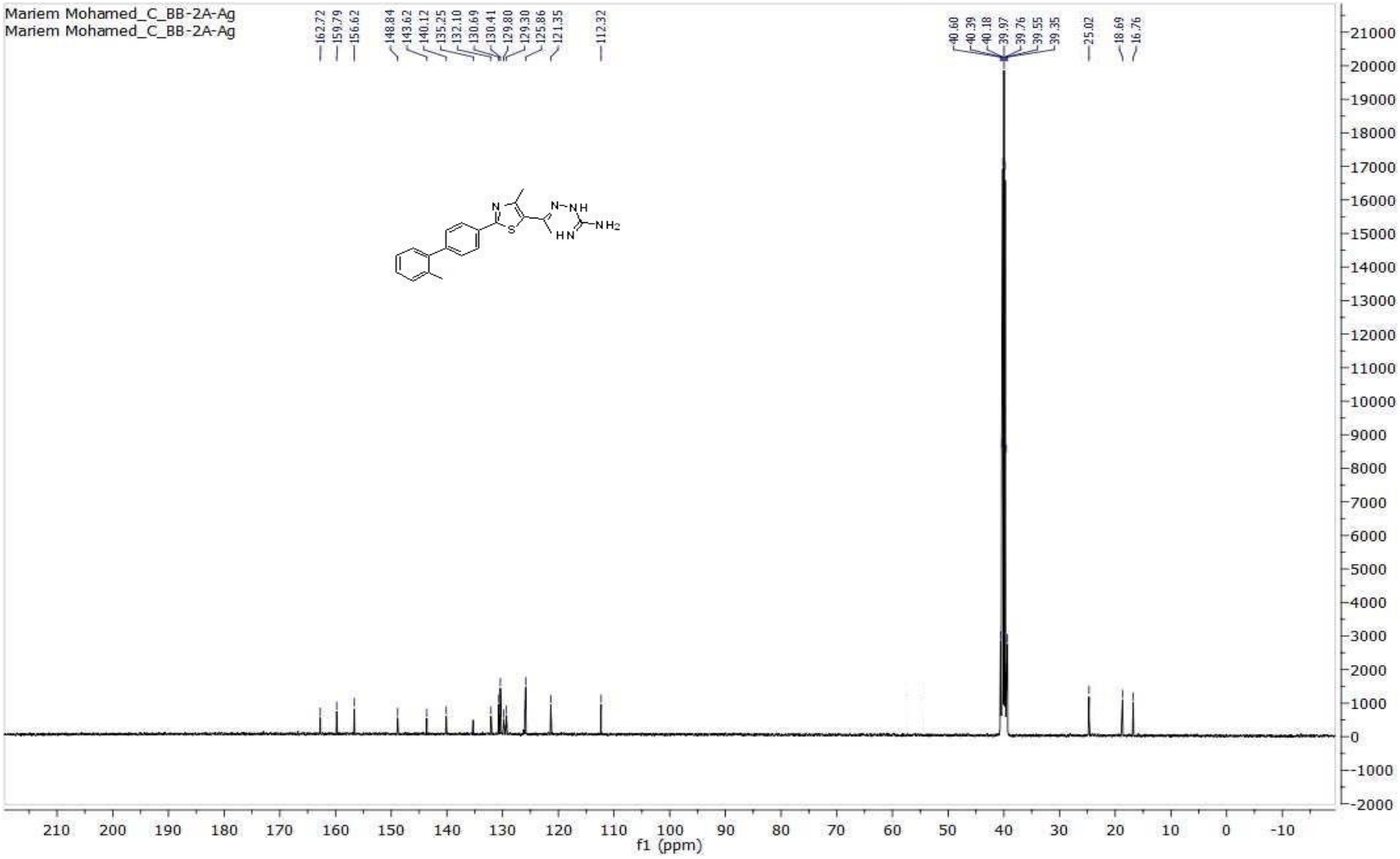
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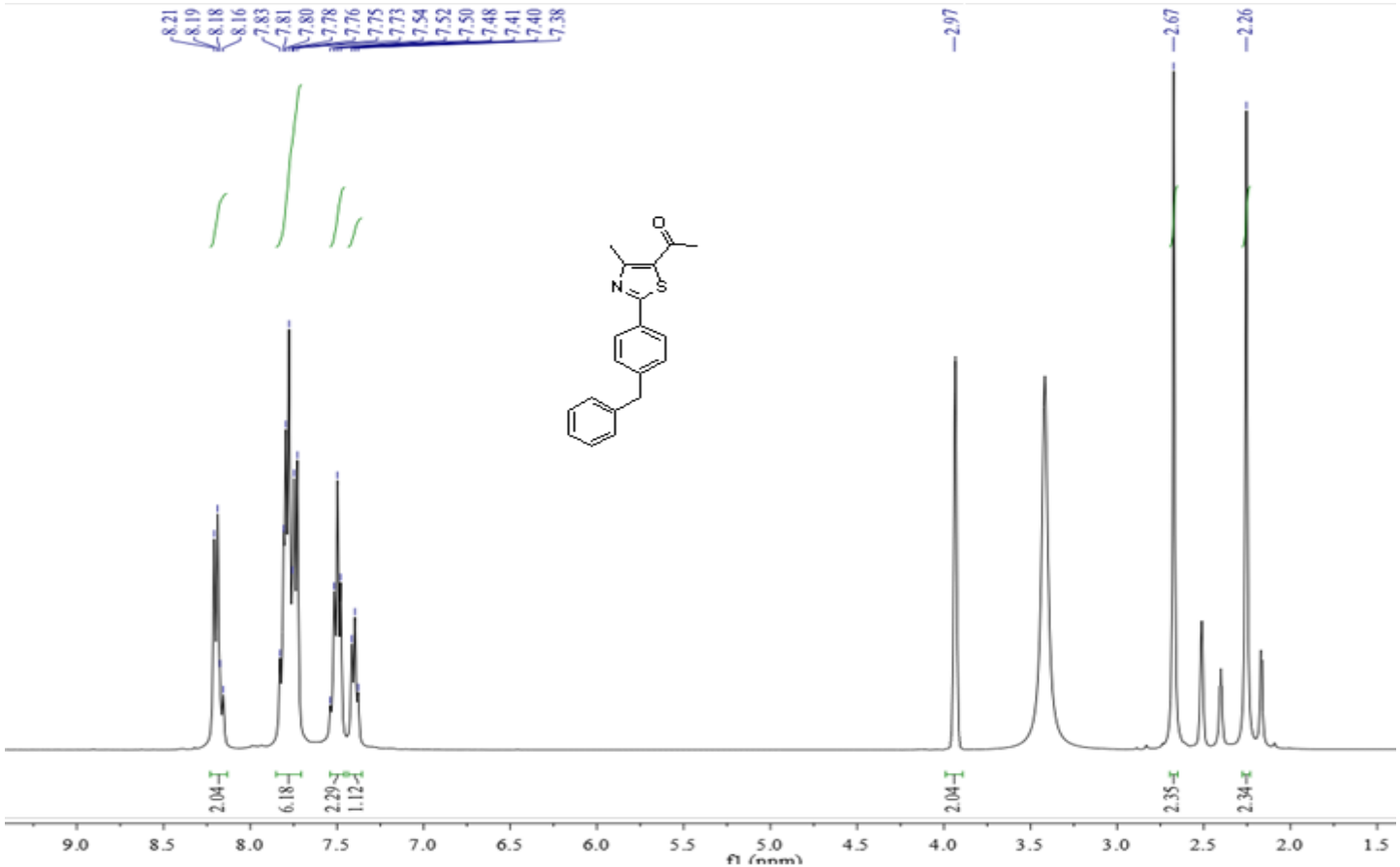
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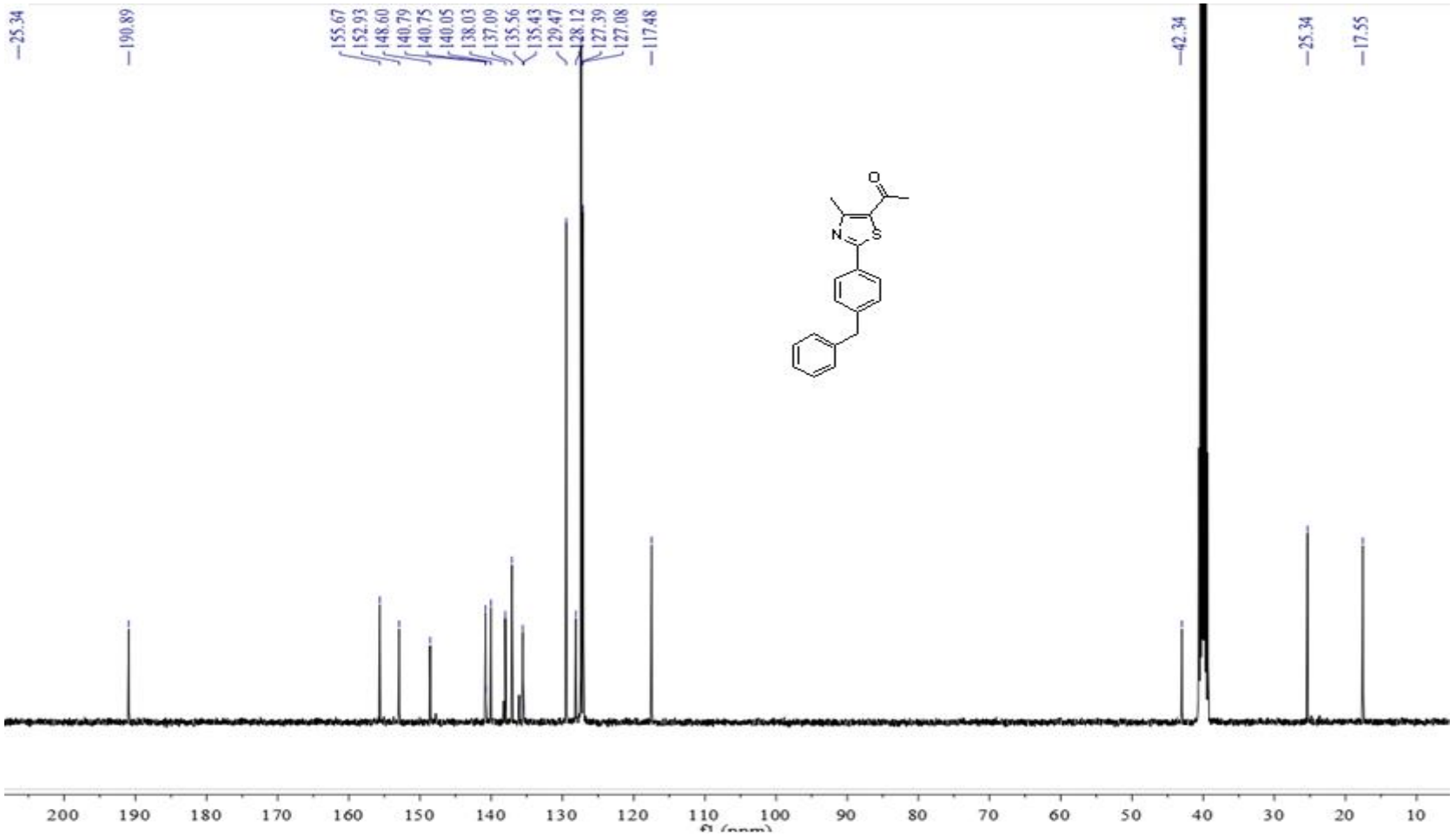
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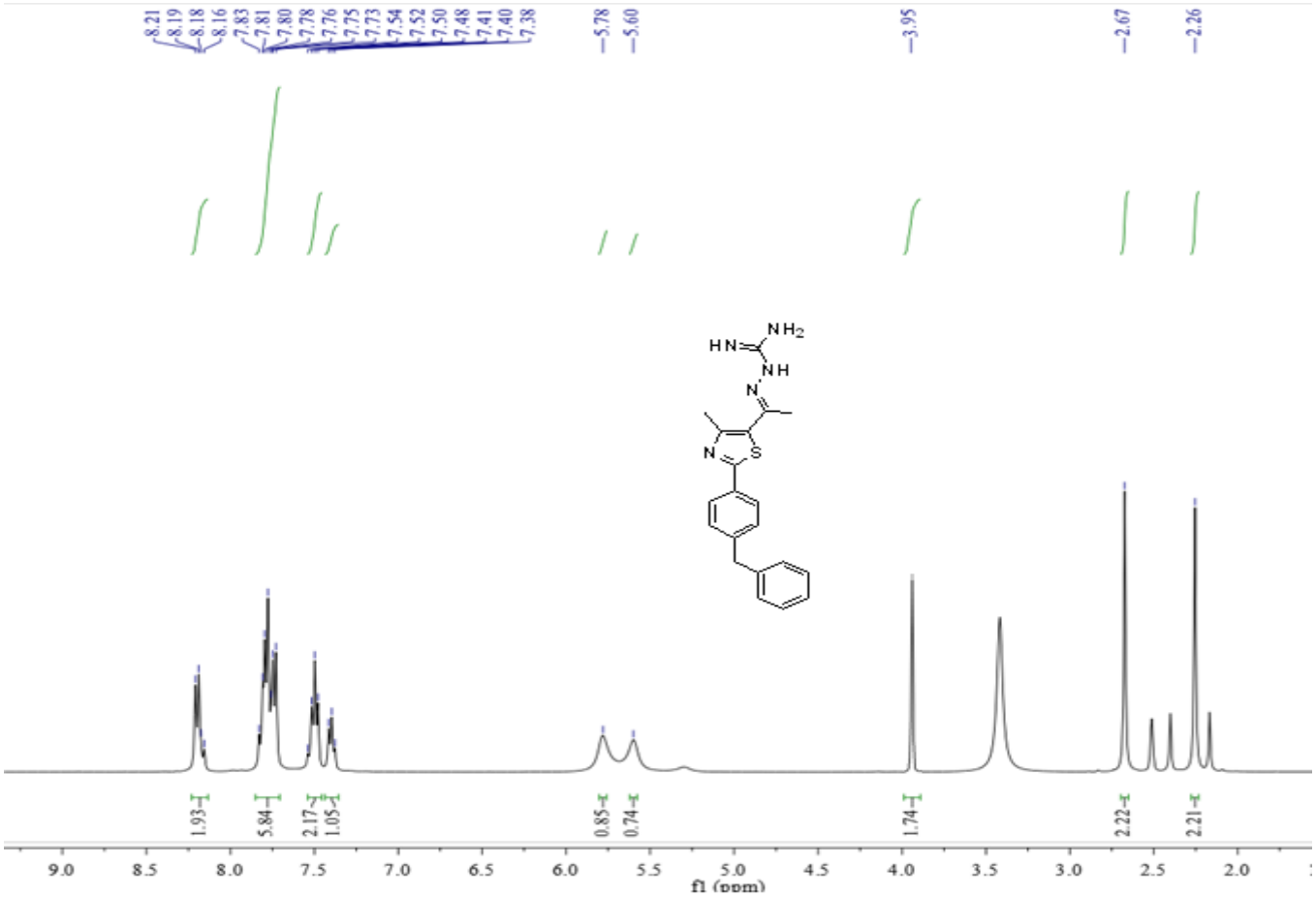
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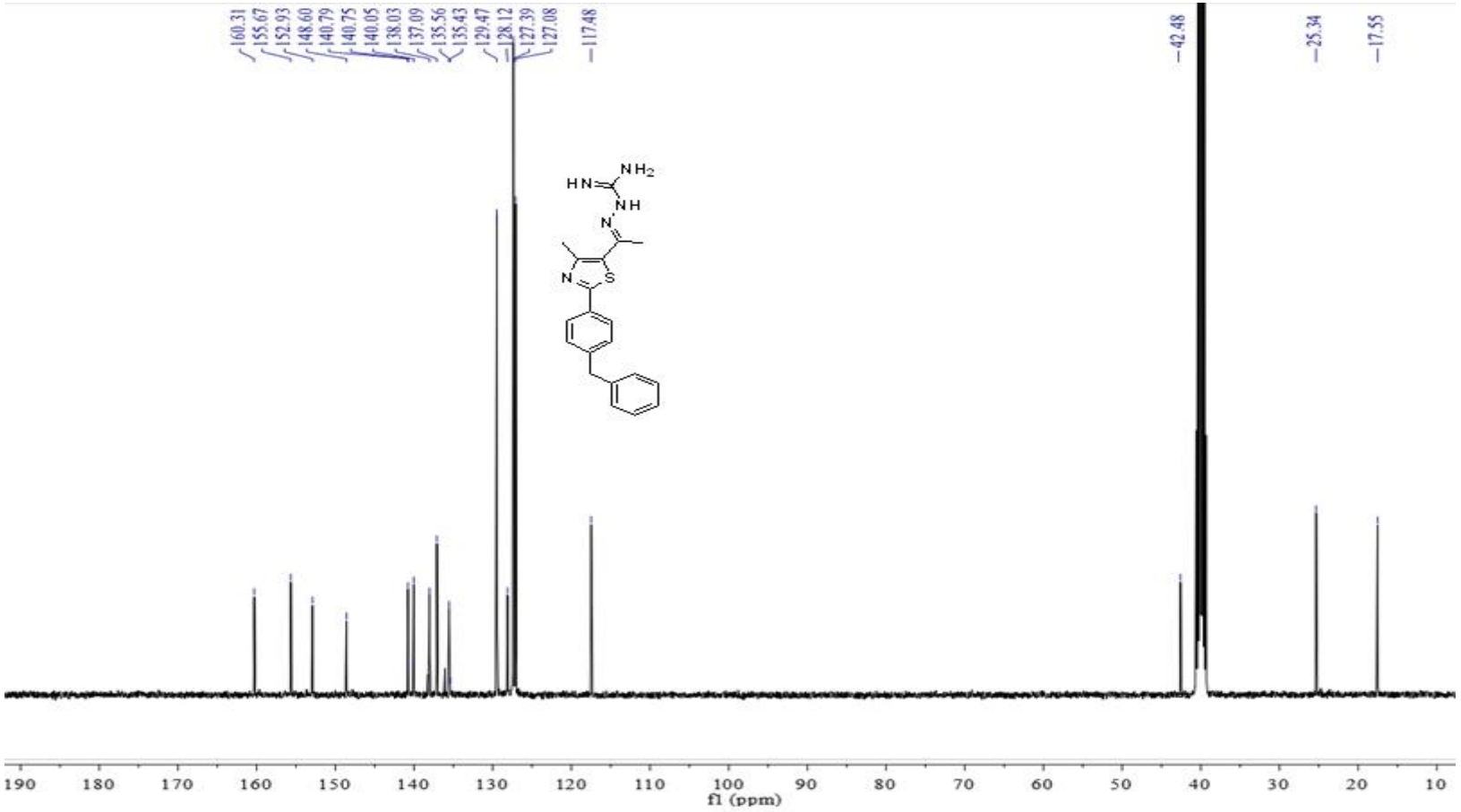
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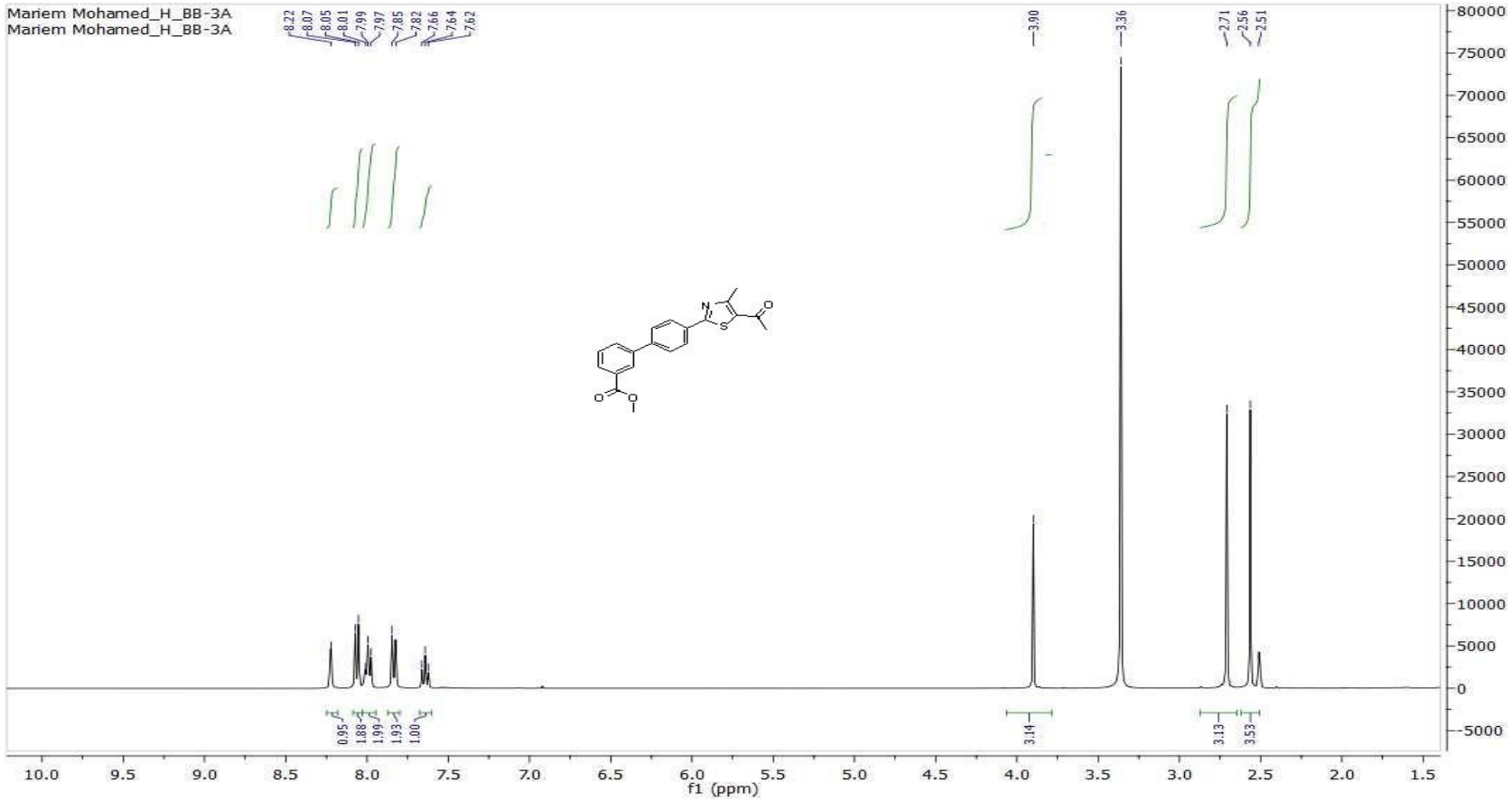
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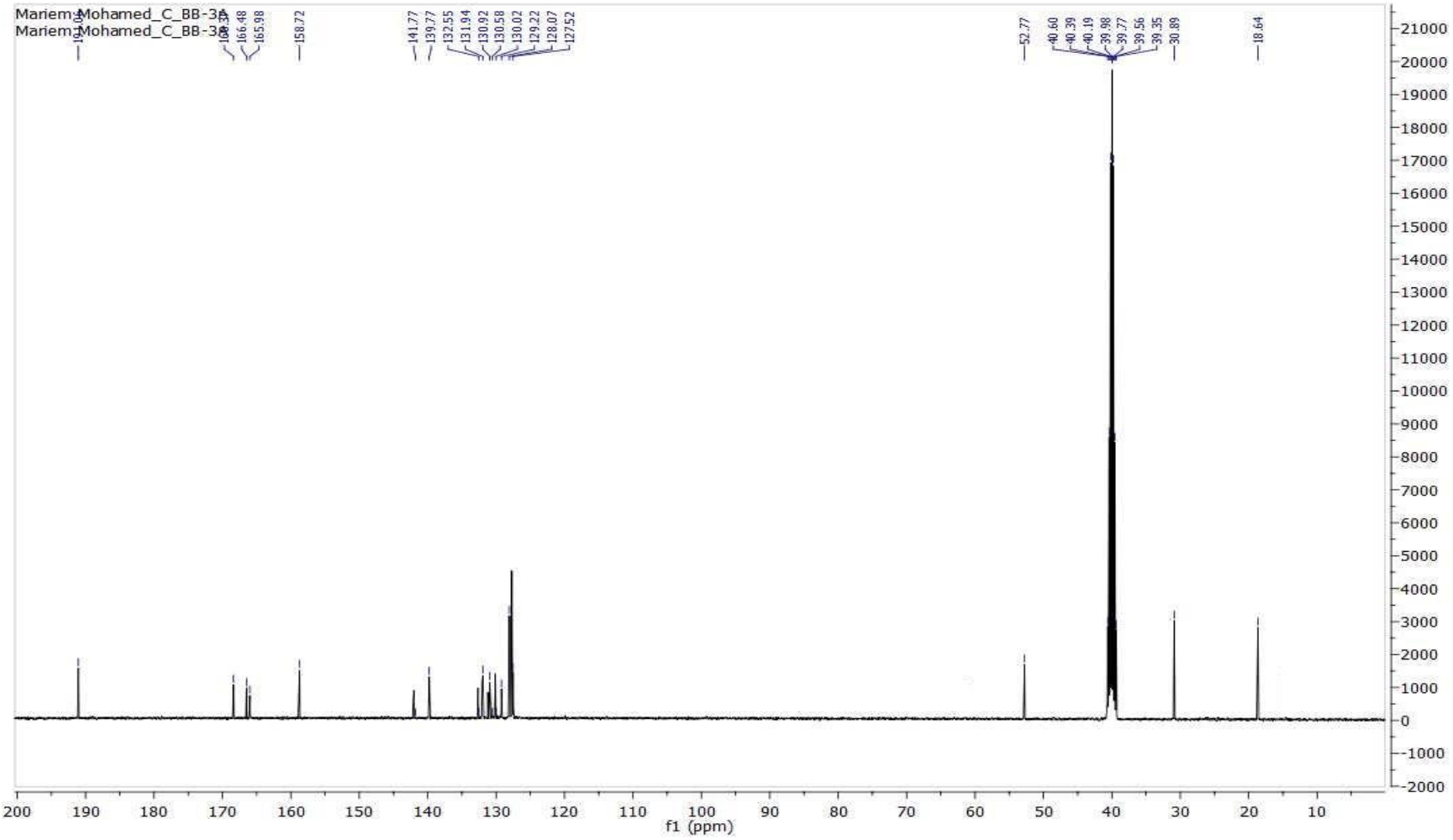
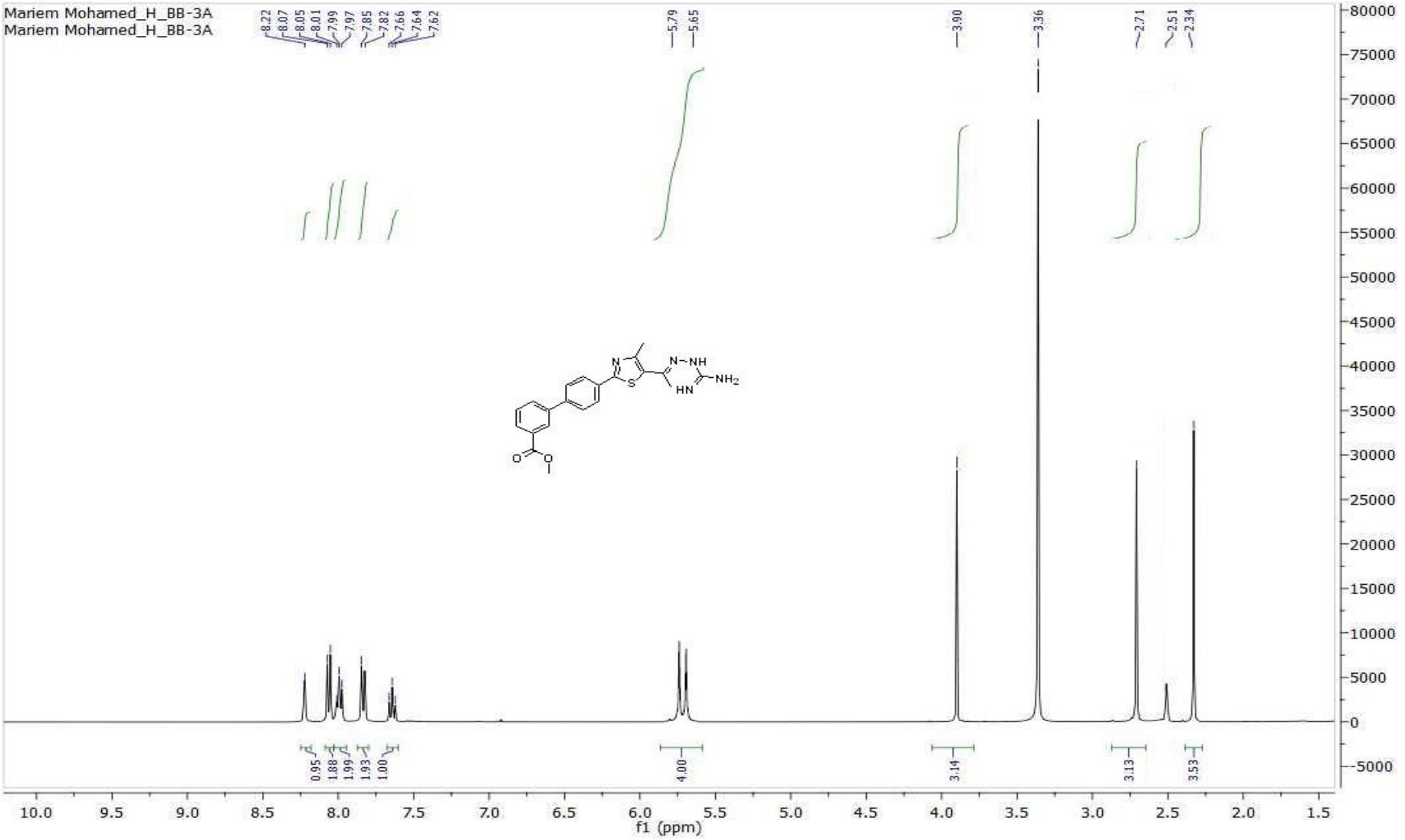
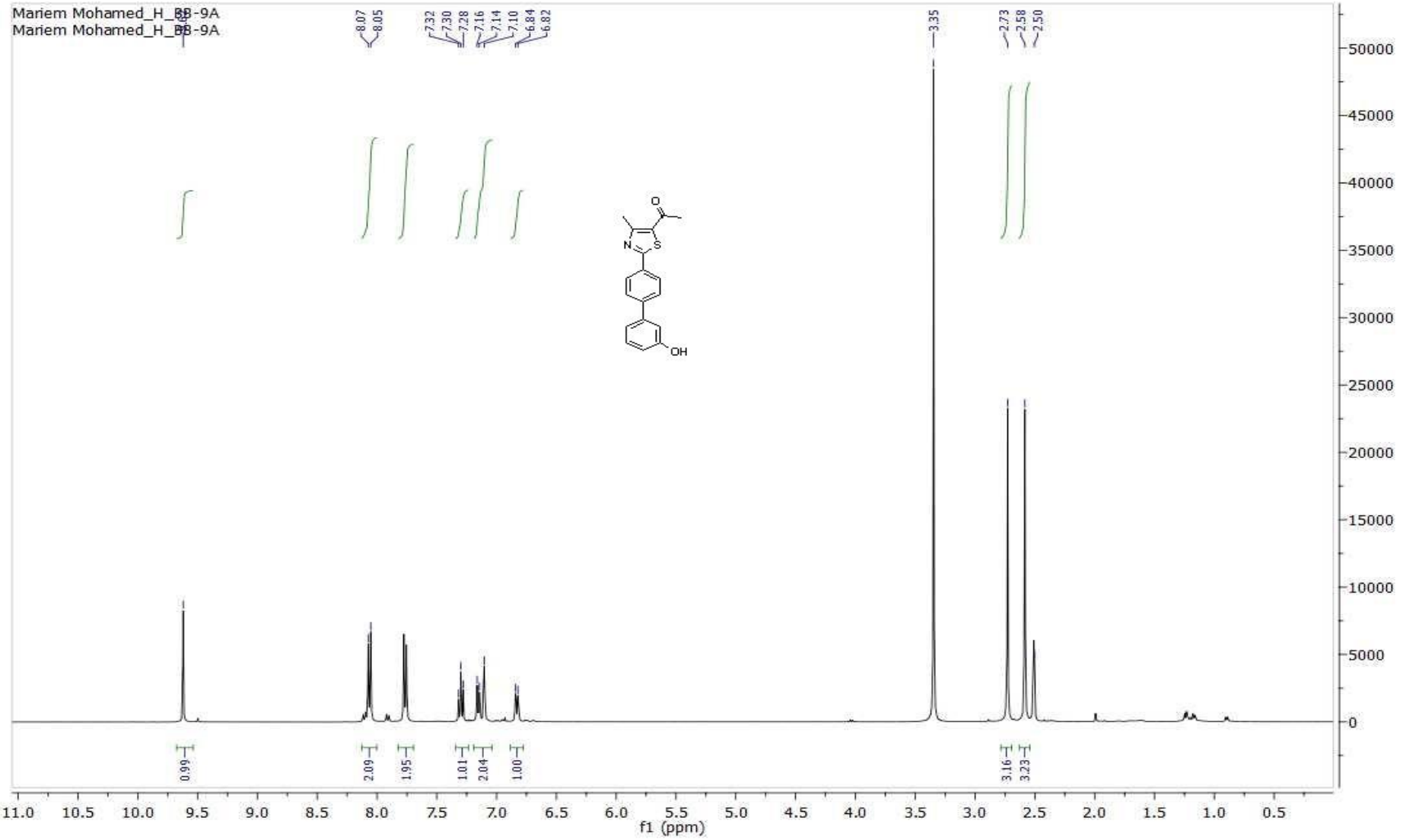
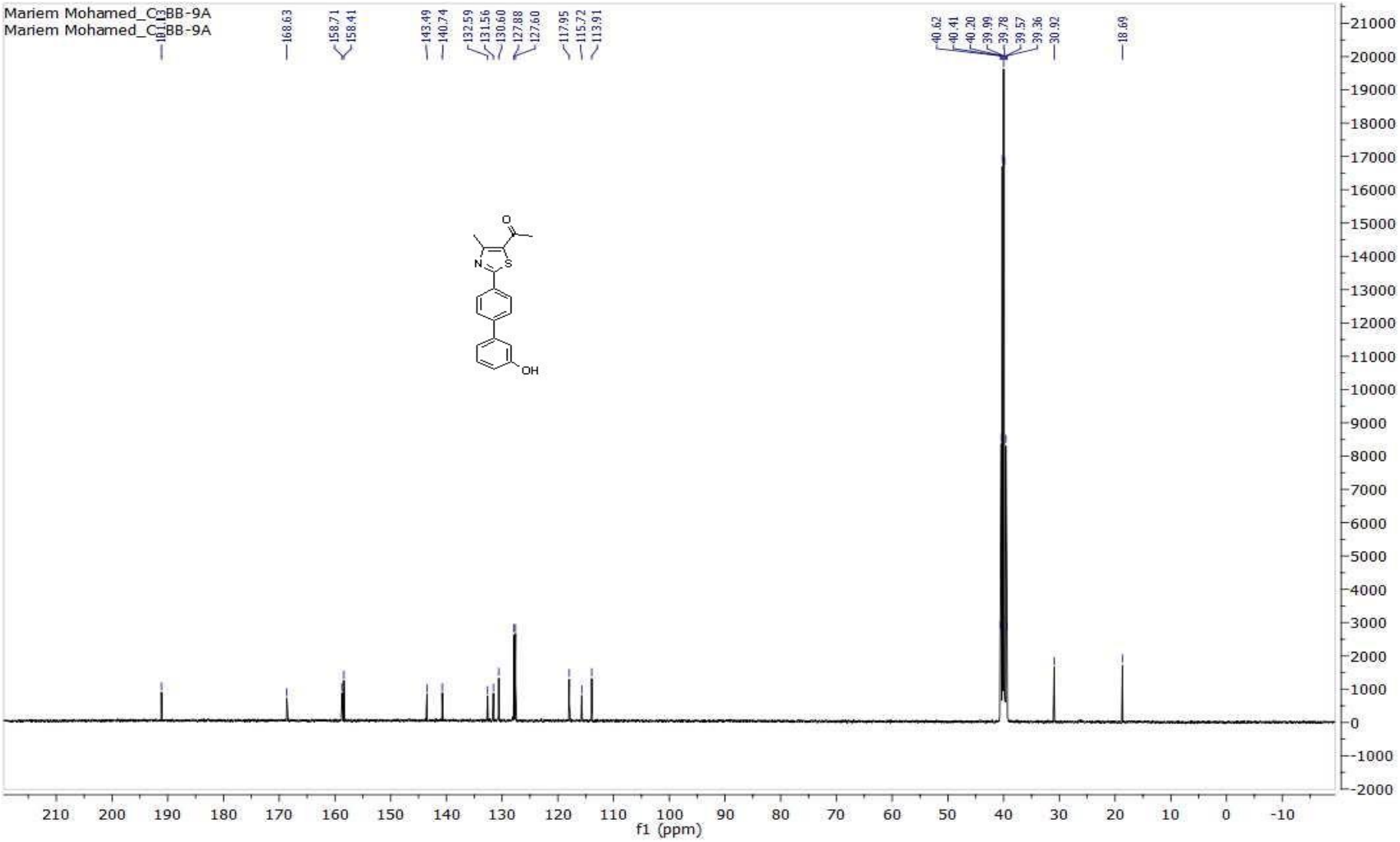
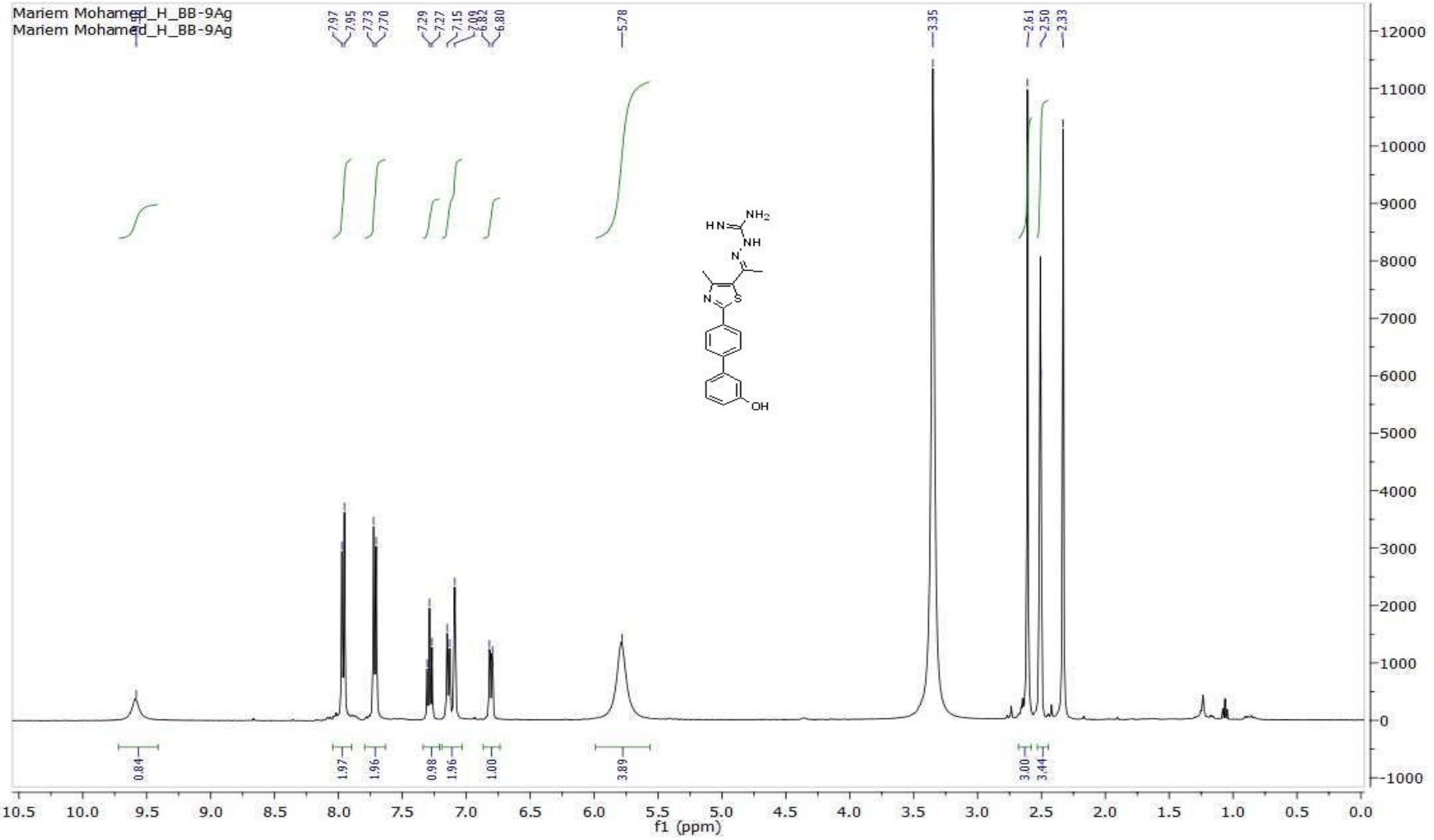
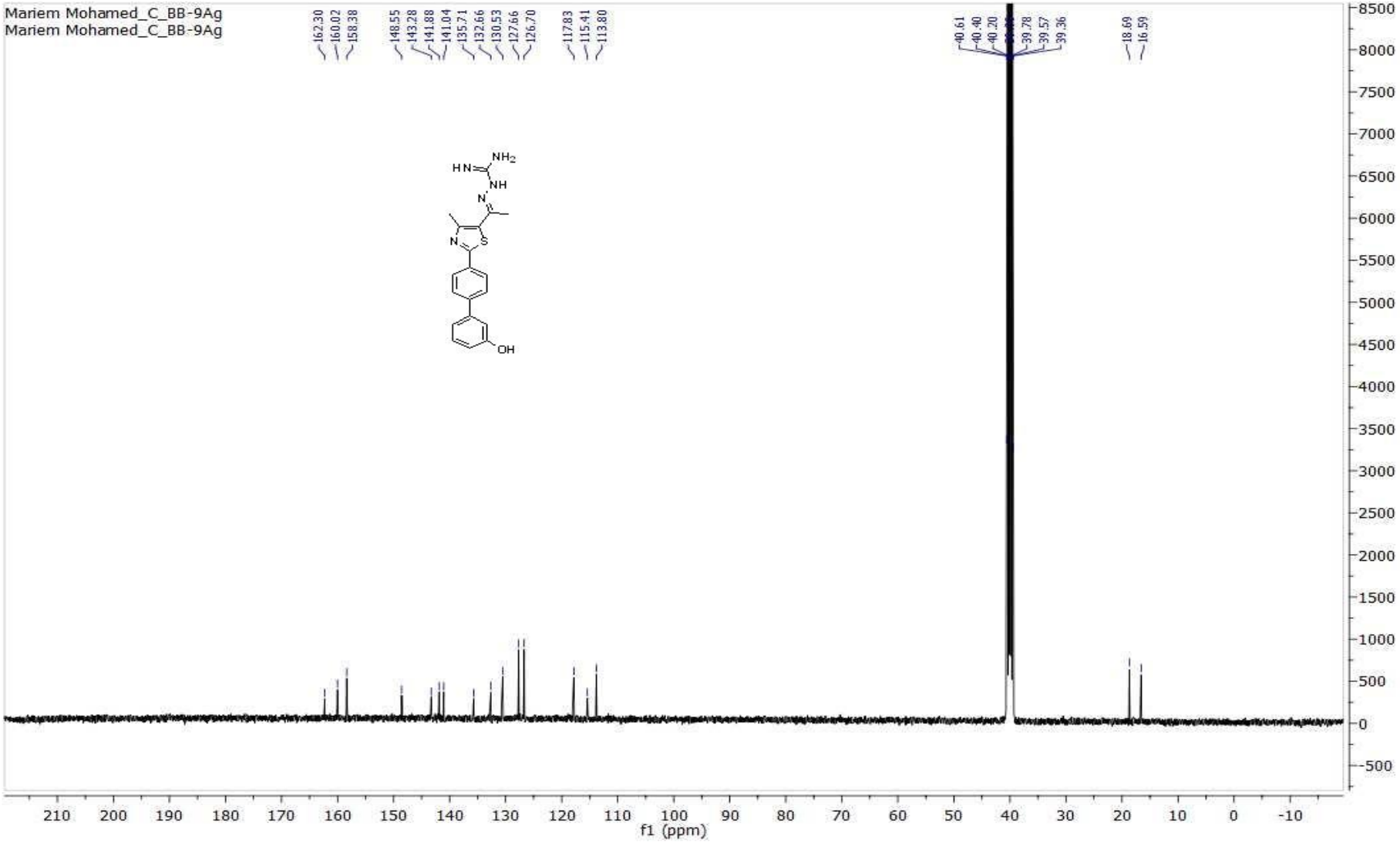

Mariem_Mohamed_C_BB-3A
Mariem_Mohamed_C_BB-3A
166.48
165.98
158.72
141.77
139.77
132.55
131.94
130.92
130.58
130.02
129.22
128.07
127.52
52.77
40.60
40.39
40.19
39.98
39.77
39.56
39.35
30.89
18.64
f1 (ppm)

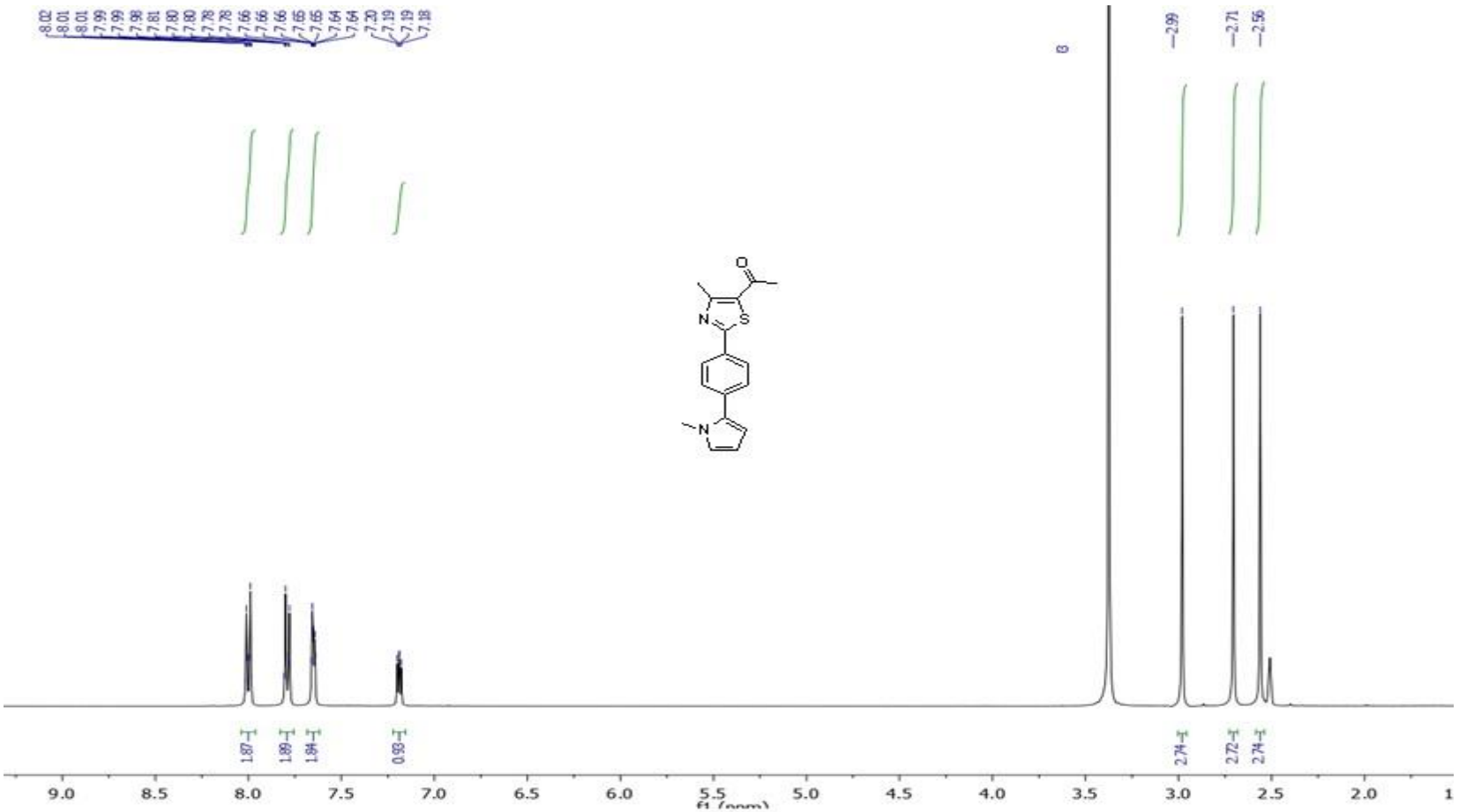

Mariem Mohamed_H_BB-3A
Mariem Mohamed_H_BB-3A
8.22
8.07
8.05
8.01
7.99
7.97
7.85
7.82
7.66
7.64
7.62
5.79
5.65
3.90
3.36
2.71
2.51
2.34
0.95
1.88
1.99
1.93
1.00
4.00
3.14
3.13
3.53
f1 (ppm)

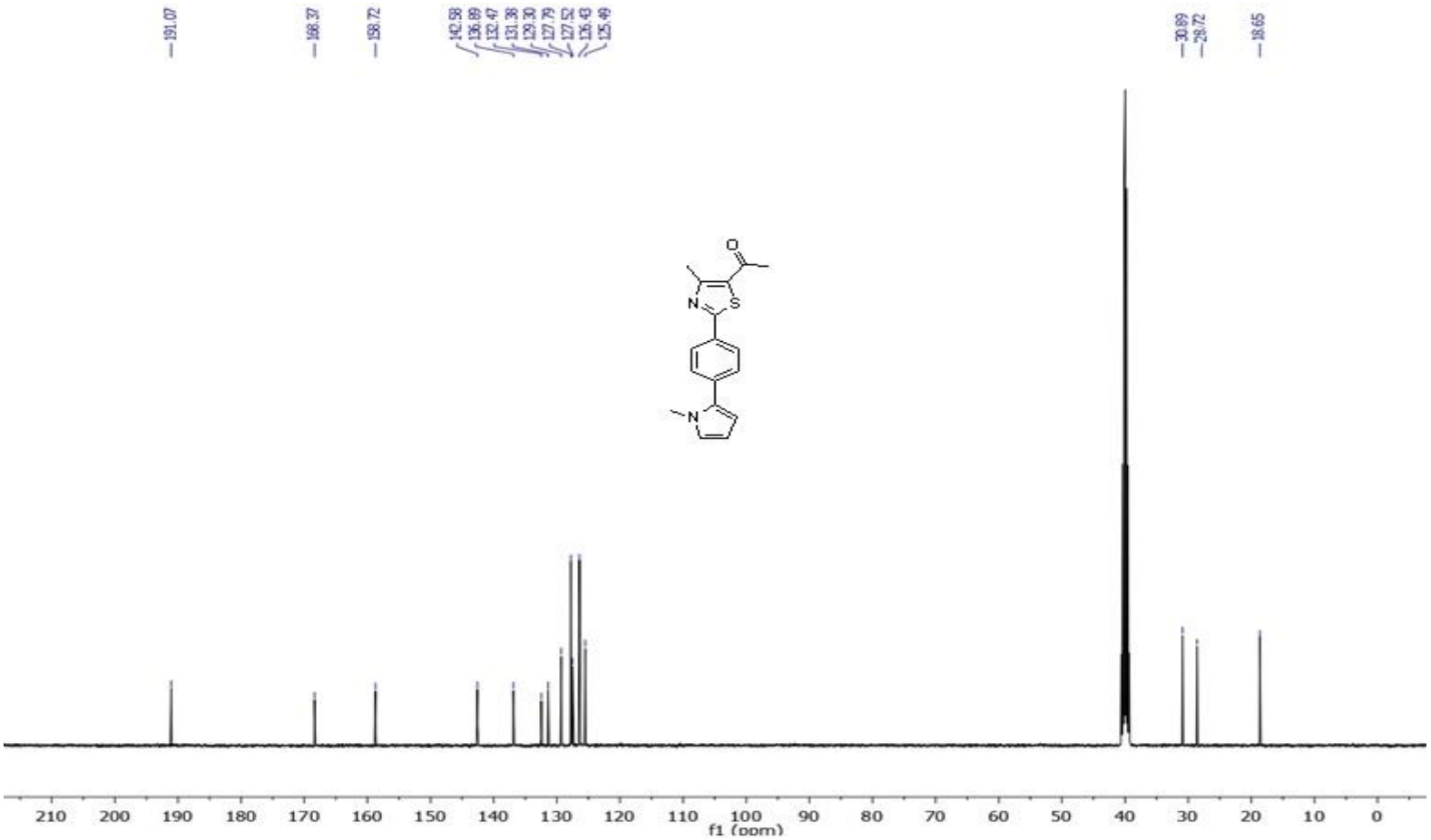

Mariem Mohamed_H_BB-9A
Mariem Mohamed_H_BB-9A
8.07
8.05
7.32
7.30
7.28
7.16
7.14
7.10
6.84
6.82
3.35
2.73
2.58
2.50
O
N
S
OH
0.99
2.09
1.95
1.01
2.04
1.00
3.16
3.23
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

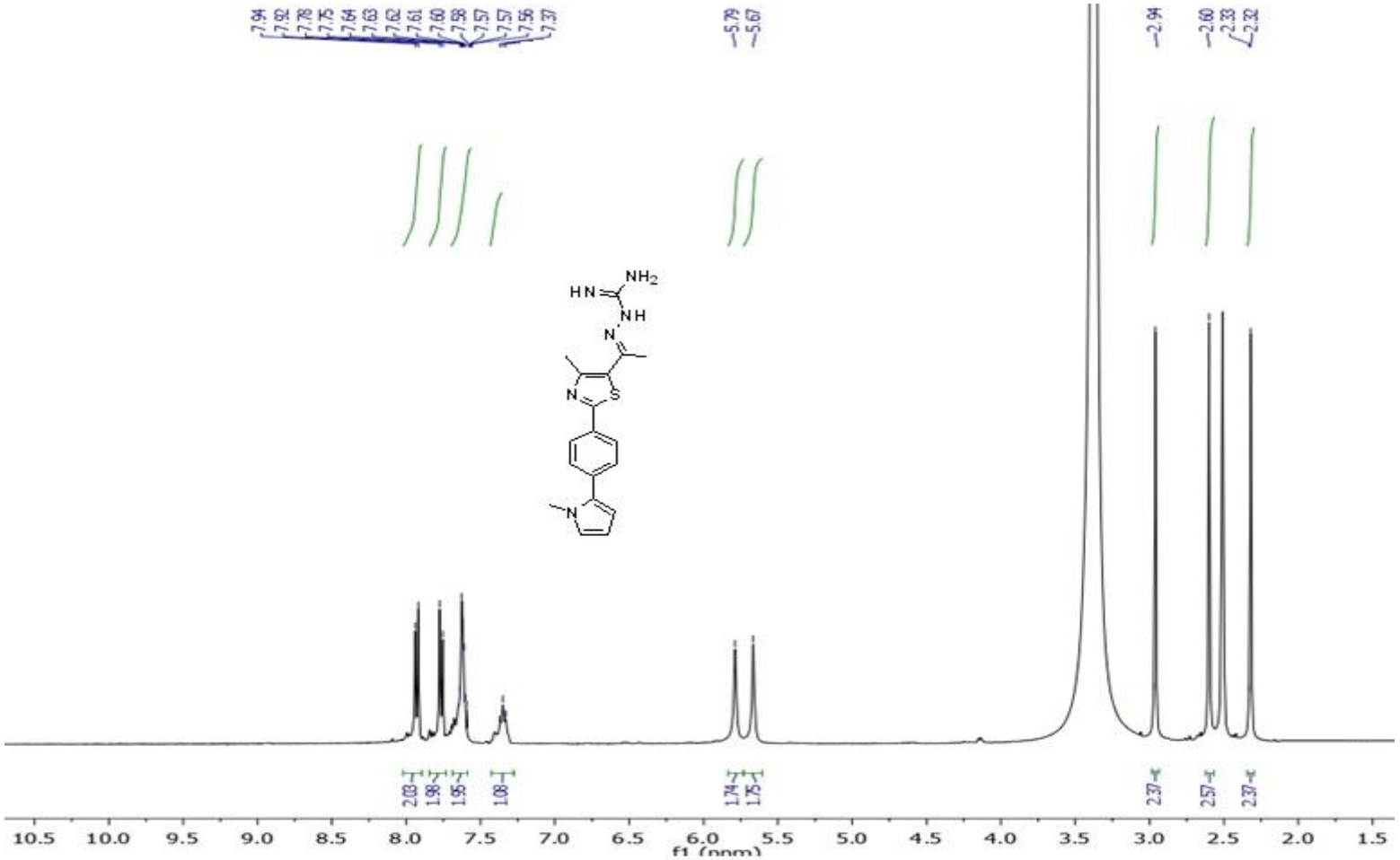

Mariem Mohamed_C13BB-9A
Mariem Mohamed_C13BB-9A
168.63
158.71
158.41
143.49
140.74
132.59
131.56
130.60
127.88
127.60
117.95
115.72
113.91
40.62
40.41
40.20
39.99
39.78
39.57
39.36
30.92
18.69
O
N
S
OH
f1 (ppm)

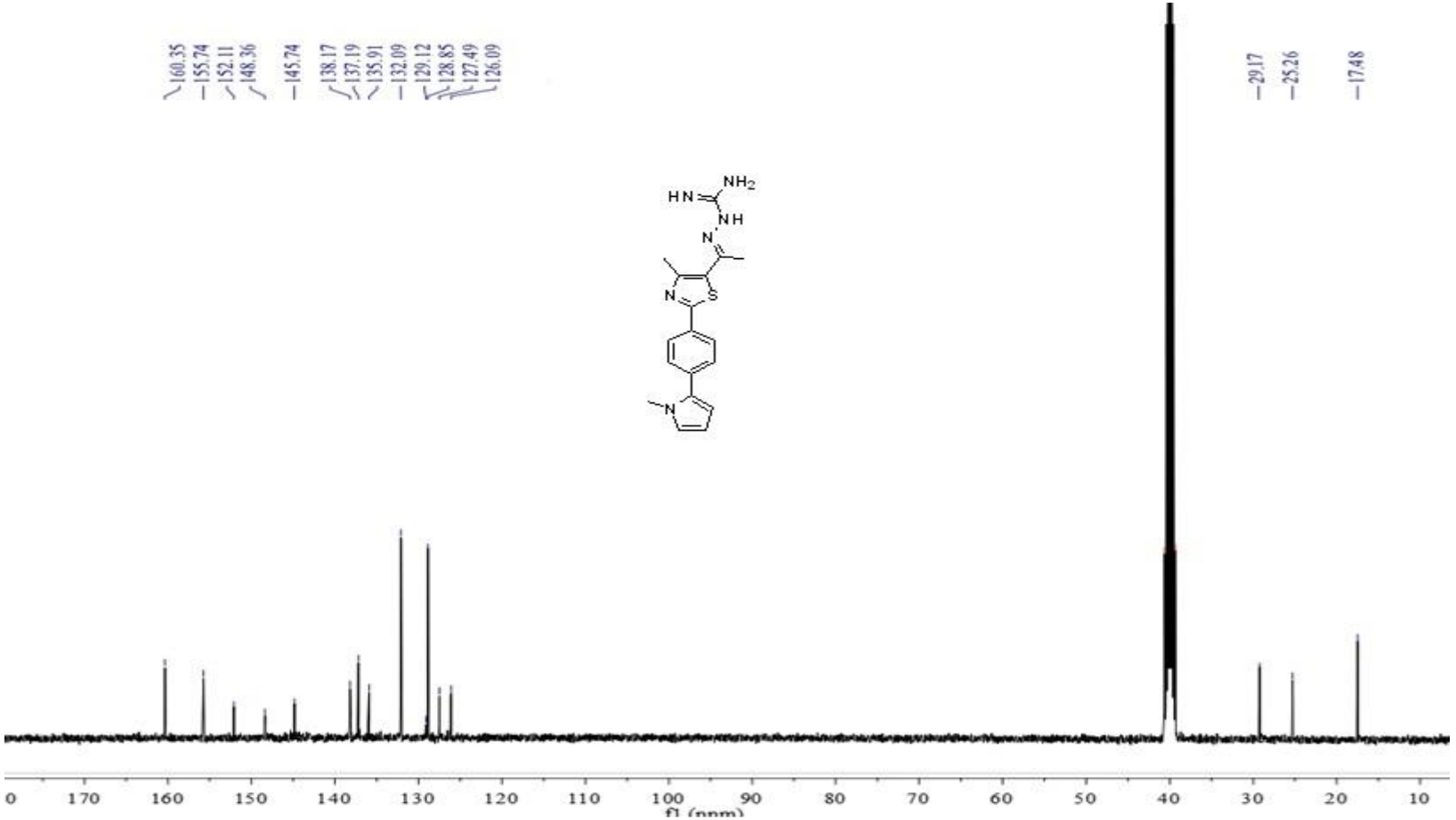

Mariem Mohamed_H_BB-9Ag
Mariem Mohamed_H_BB-9Ag
9.48
7.97
7.95
7.73
7.70
7.29
7.27
7.15
7.09
6.82
6.80
5.78
3.35
2.61
2.50
2.33
0.84
1.97
1.96
0.98
1.96
1.00
3.89
3.00
3.44
f1 (ppm)

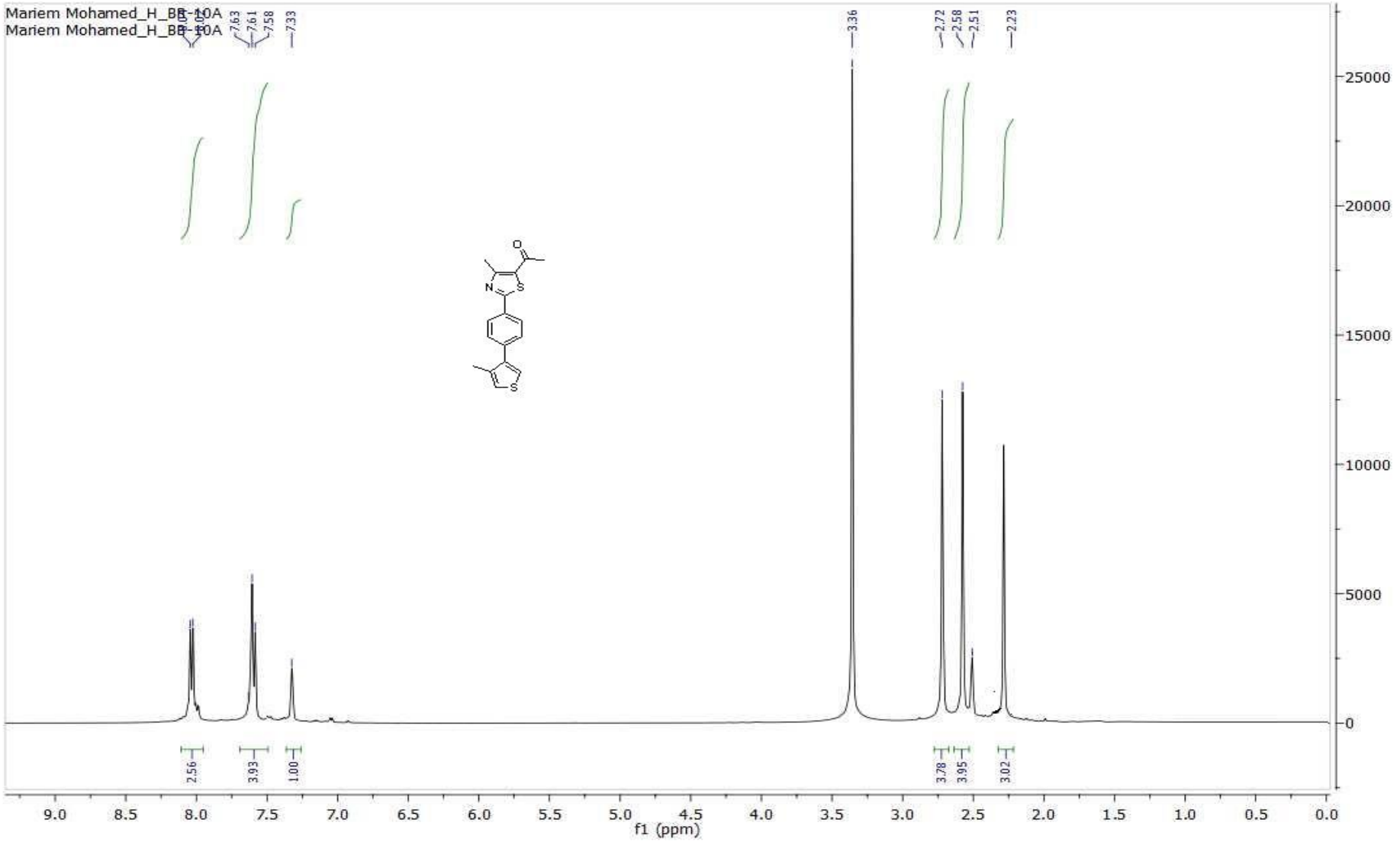

Mariem Mohamed_C_BB-9Ag
Mariem Mohamed_C_BB-9Ag
162.30
160.02
158.38
148.55
143.28
141.88
141.04
135.71
132.66
130.53
127.66
126.70
117.83
115.41
113.80
40.61
40.40
40.20
39.78
39.57
39.36
18.69
16.59
HN
NH2
NH
N
N
S
OH
f1 (ppm)

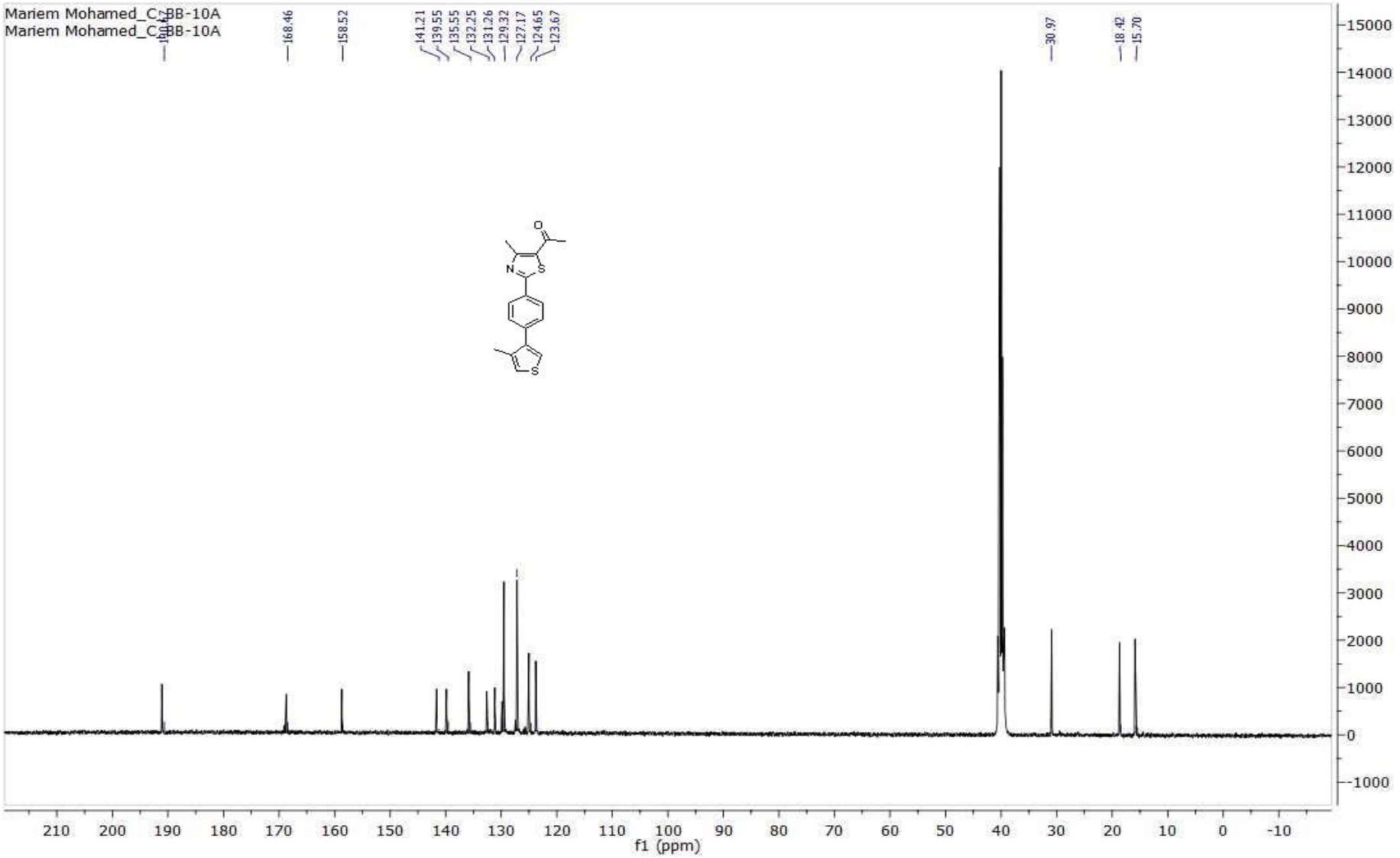

8.02
8.01
8.01
7.99
7.99
7.98
7.81
7.80
7.80
7.78
7.78
7.66
7.66
7.66
7.65
7.65
7.64
7.64
7.20
7.19
7.19
7.18
2.99
2.71
2.56
1.87
1.99
1.94
0.93
2.74
2.72
2.74
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1
f1 (ppm)

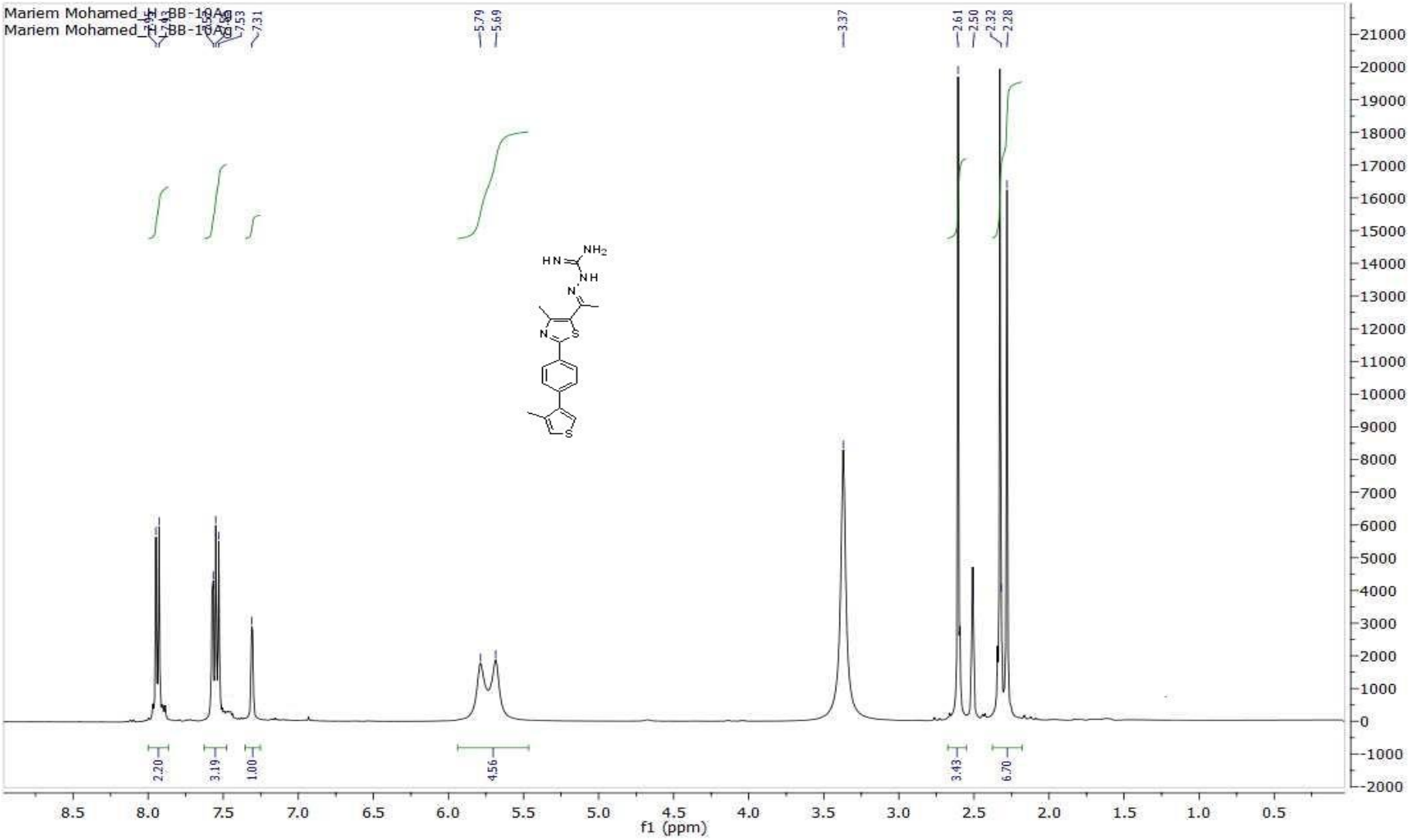

191.07
168.37
158.72
140.58
136.89
132.47
131.38
129.30
127.79
127.52
126.43
125.49
30.89
28.72
18.65
O
N
S
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

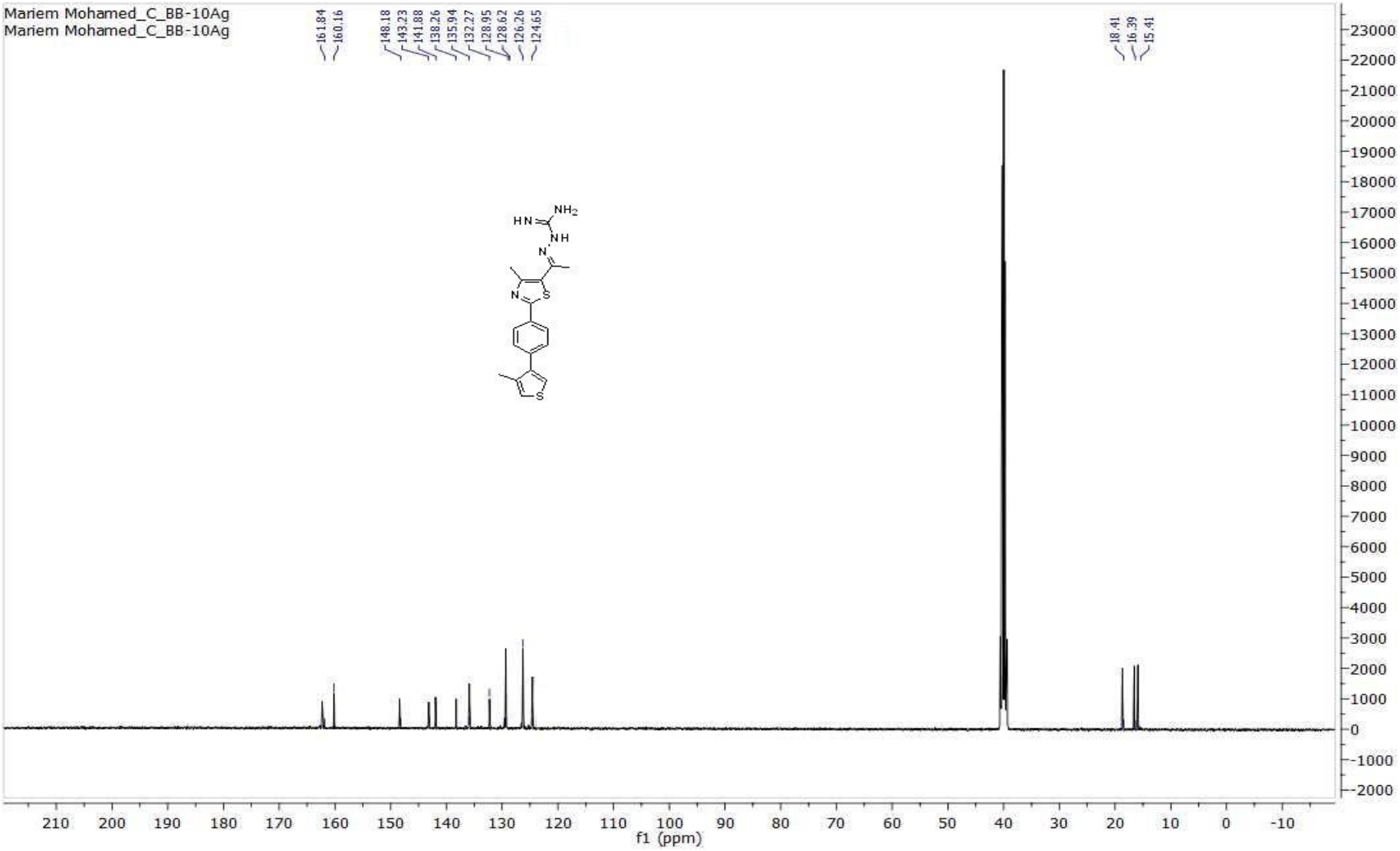

7.94
7.92
7.78
7.75
7.64
7.63
7.62
7.61
7.60
7.58
7.57
7.57
7.56
7.37
5.79
5.67
2.94
2.60
2.33
2.32
NH2
HN
NH
N
N
S
N
2.03
1.98
1.95
1.08
1.74
1.75
2.37
2.57
2.37
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

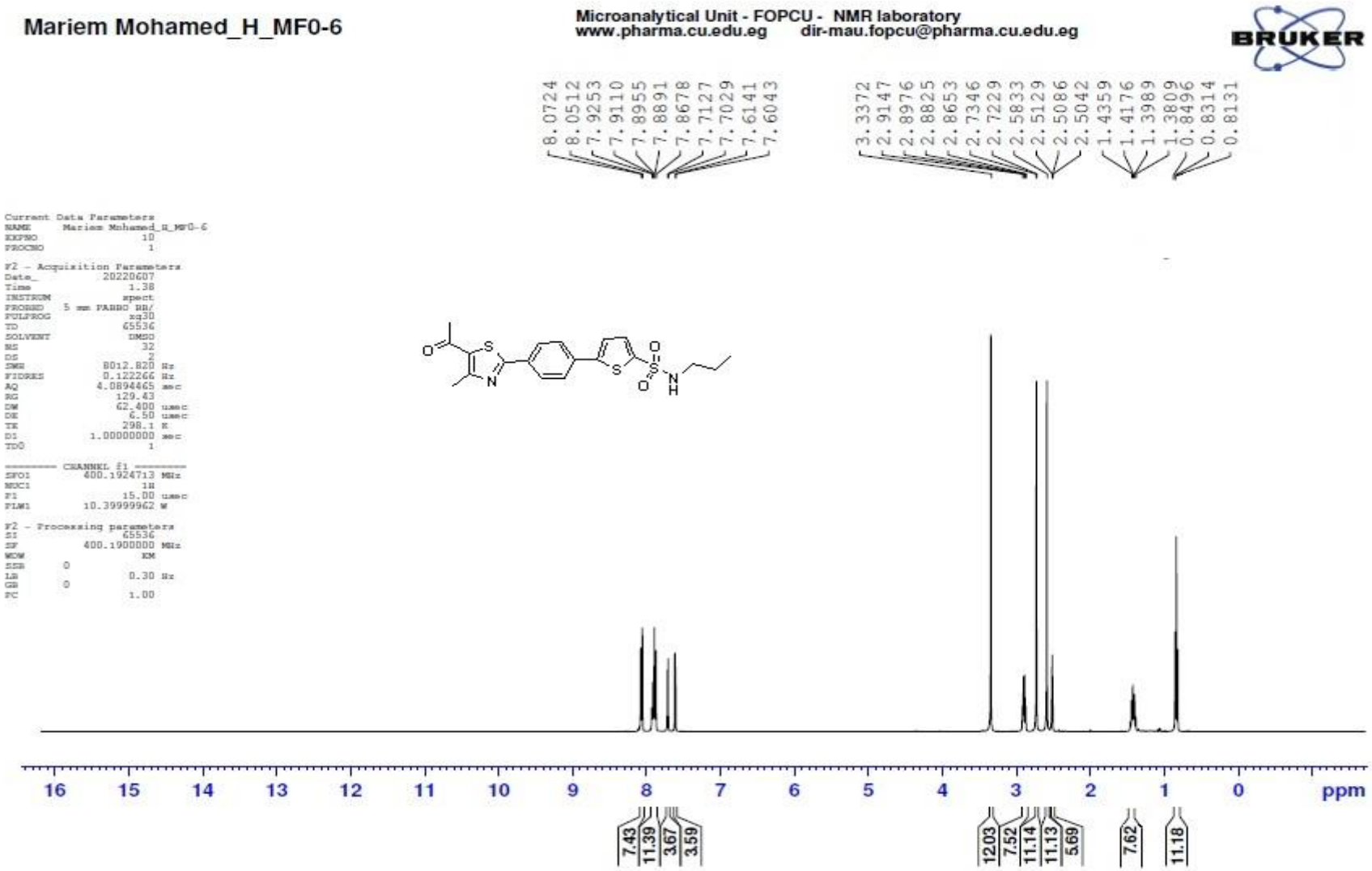

160.35
155.74
152.11
148.36
145.74
138.17
137.19
135.91
132.09
129.12
128.85
127.49
126.09
29.17
25.26
17.48
NH2
HN
NH
N
N
S
N
0
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

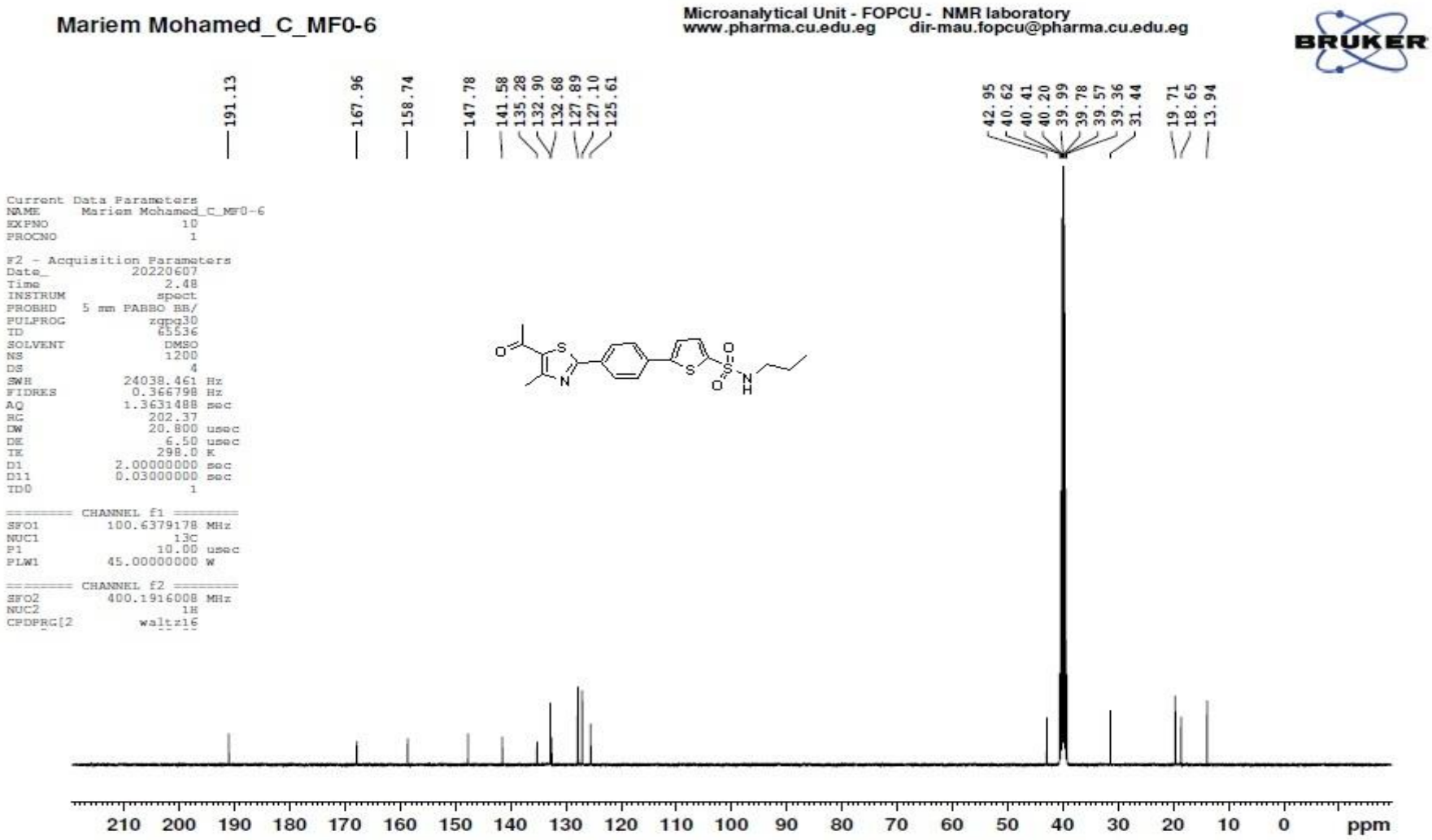

Mariem Mohamed_H_BB-10A
Mariem Mohamed_H_BB-10A
8.03
8.01
7.63
7.61
7.58
7.33
3.36
2.72
2.58
2.51
2.23
O
N
S
S
25000
20000
15000
10000
5000
0
2.56
3.93
1.00
3.78
3.95
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

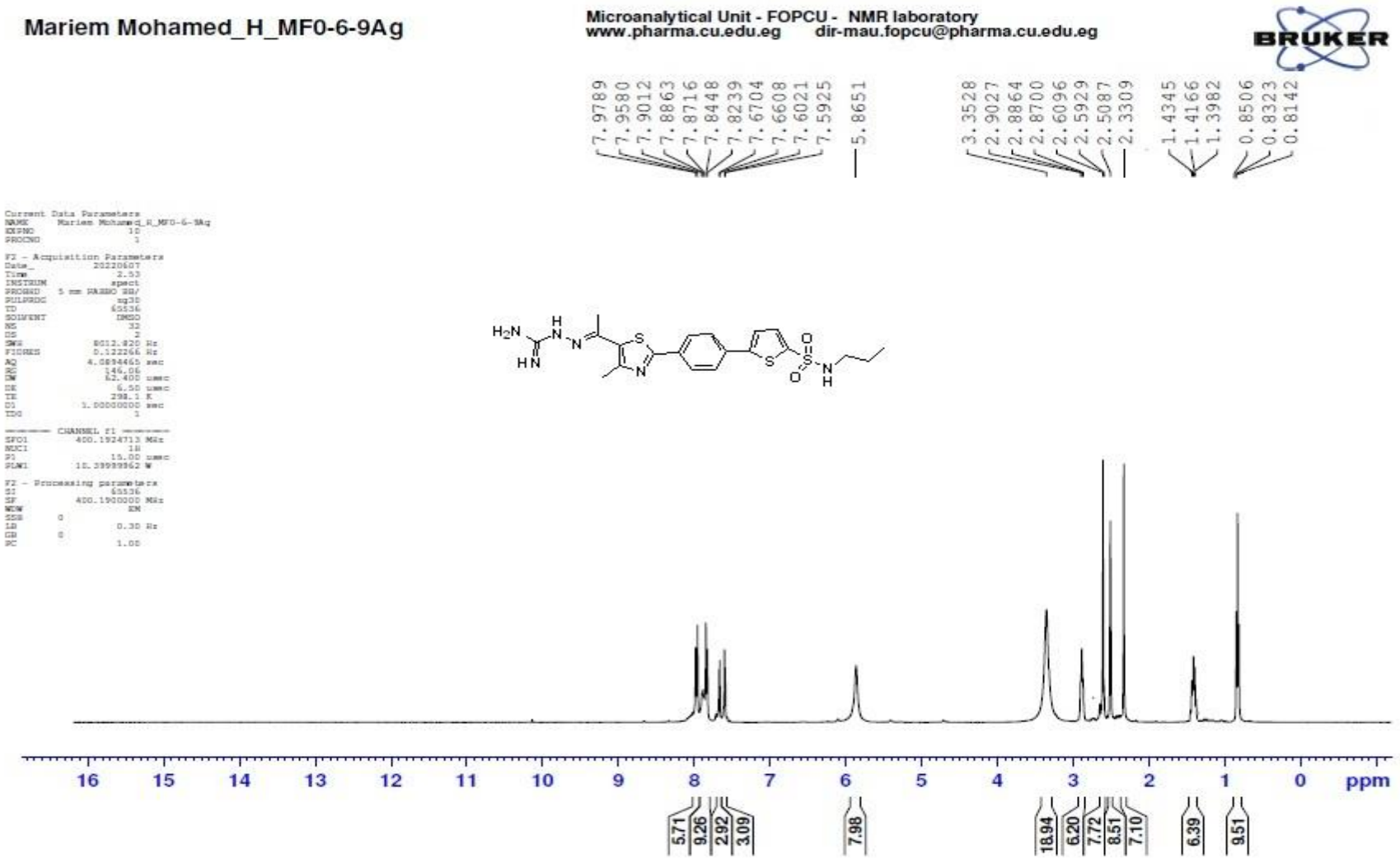

Mariem Mohamed_C_BB-10A
Mariem Mohamed_C_BB-10A
168.46
158.52
141.21
139.55
135.55
132.25
131.26
129.32
127.17
124.65
123.67
30.97
18.42
15.70
O
N
S
S
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

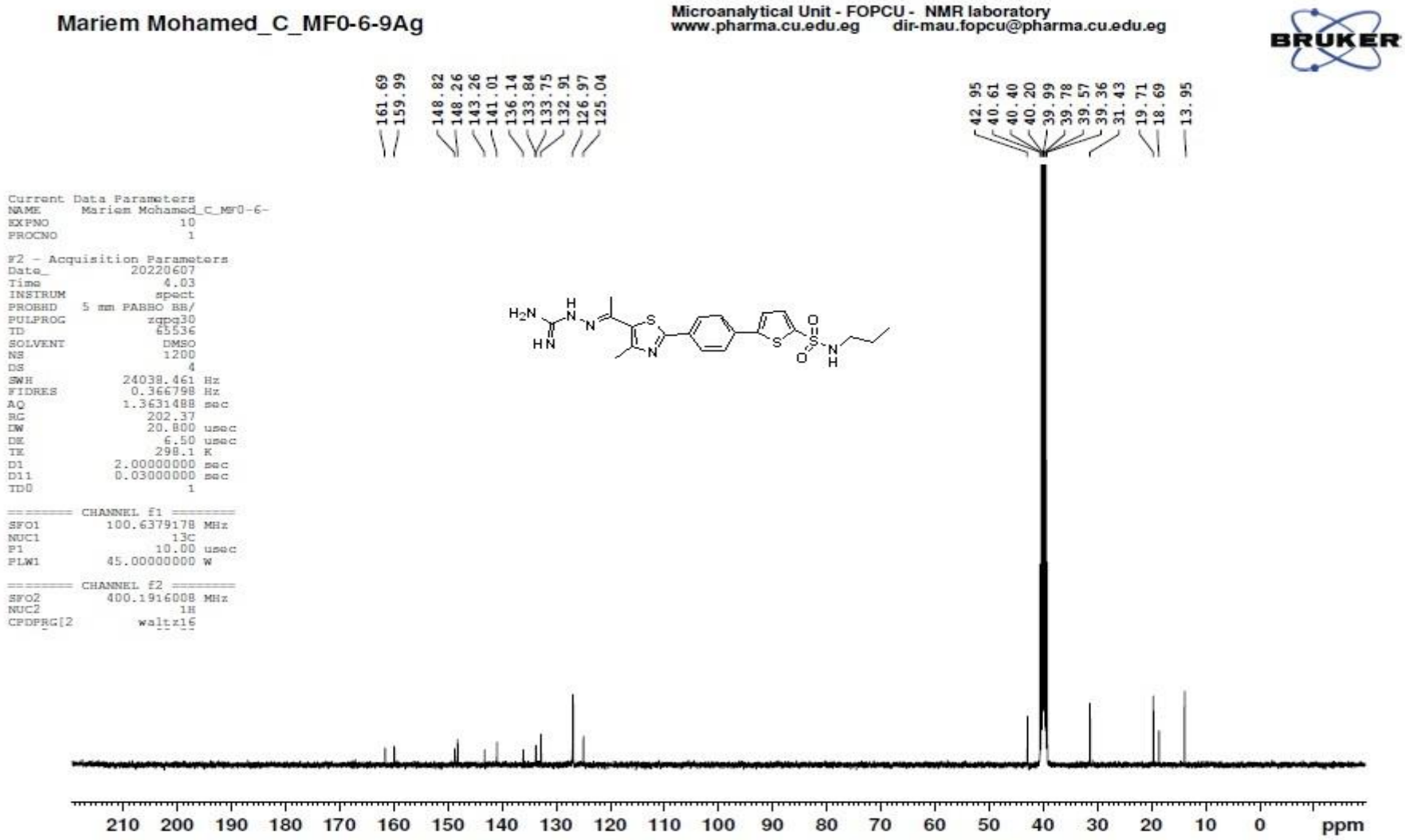

Mariem Mohamed_1H_BB-10Ag
Mariem Mohamed_1H_BB-10Ag
7.93
7.43
7.53
7.31
5.79
5.69
3.37
2.61
2.50
2.32
2.28
HN
NH2
NH
N
N
S
S
2.20
3.19
1.00
4.56
3.43
6.70
f1 (ppm)

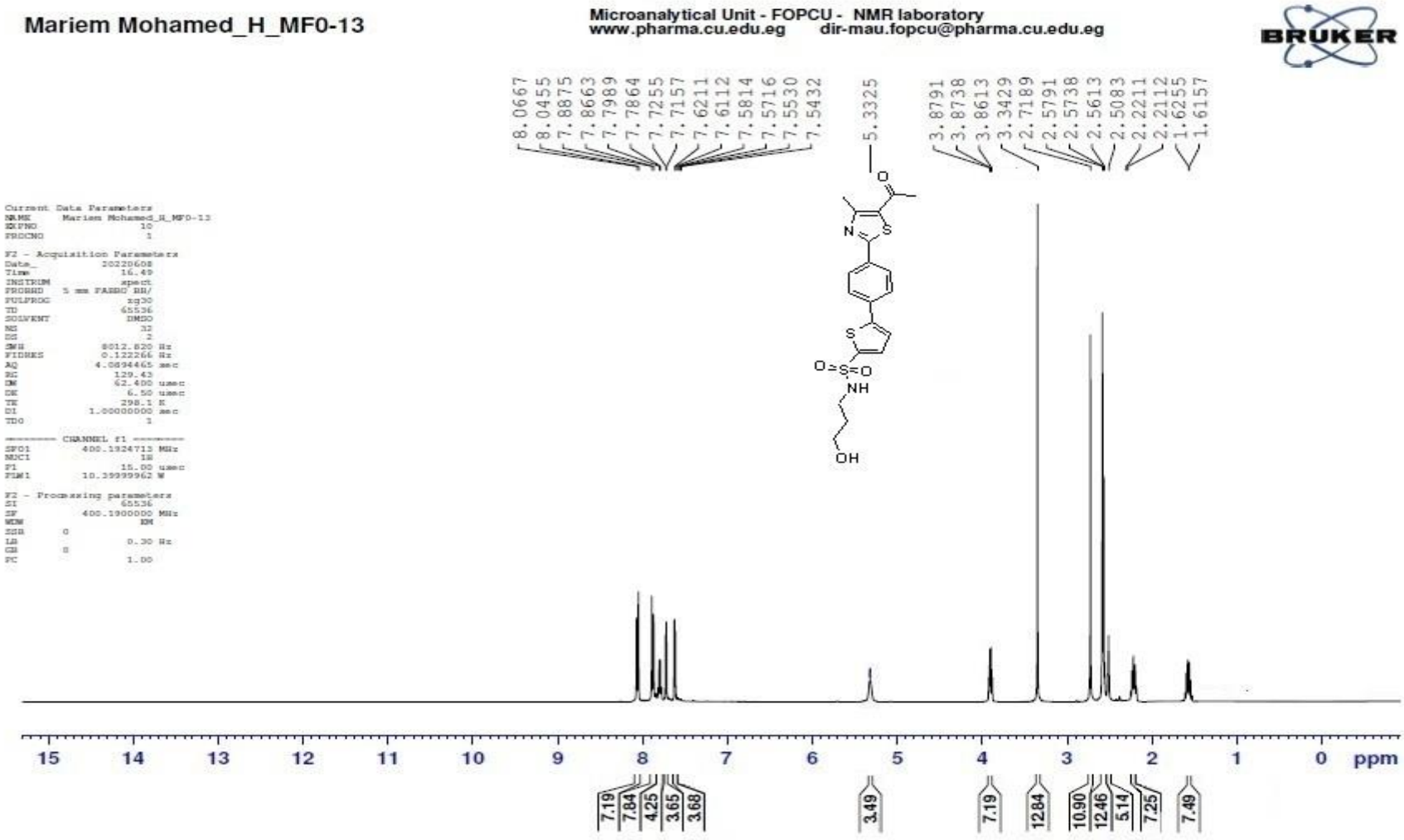

Mariem Mohamed_C_BB-10Ag
Mariem Mohamed_C_BB-10Ag
161.84
160.16
148.18
143.23
141.88
138.26
135.94
132.27
128.95
128.62
126.26
124.65
18.41
16.39
15.41
HN
NH2
NH
N
N
S
S
23000
22000
21000
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
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)

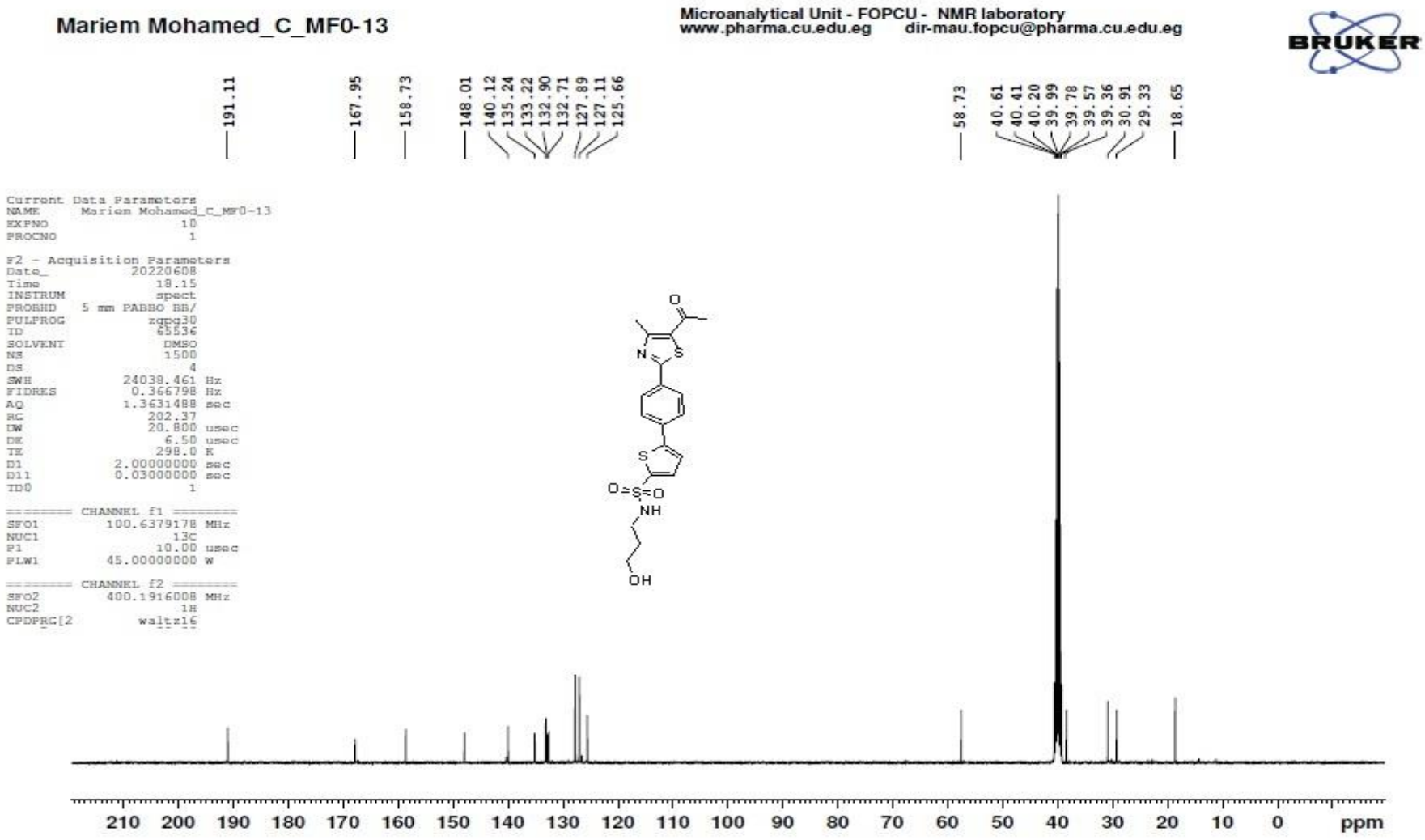

Mariem Mohamed_H_MF0-6
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.0724
8.0512
7.9253
7.9110
7.8955
7.8891
7.8678
7.7127
7.7029
7.6141
7.6043
3.3372
2.9147
2.8976
2.8825
2.8653
2.7346
2.7229
2.5833
2.5129
2.5086
2.5042
1.4359
1.4176
1.3989
1.3809
0.8496
0.8314
0.8131
Current Data Parameters
NAME Mariem Mohamed_H_MF0-6
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220607
Time 1.38
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 129.43
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
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
7.43
11.39
3.67
3.59
12.03
7.52
11.14
11.13
5.69
7.62
11.18

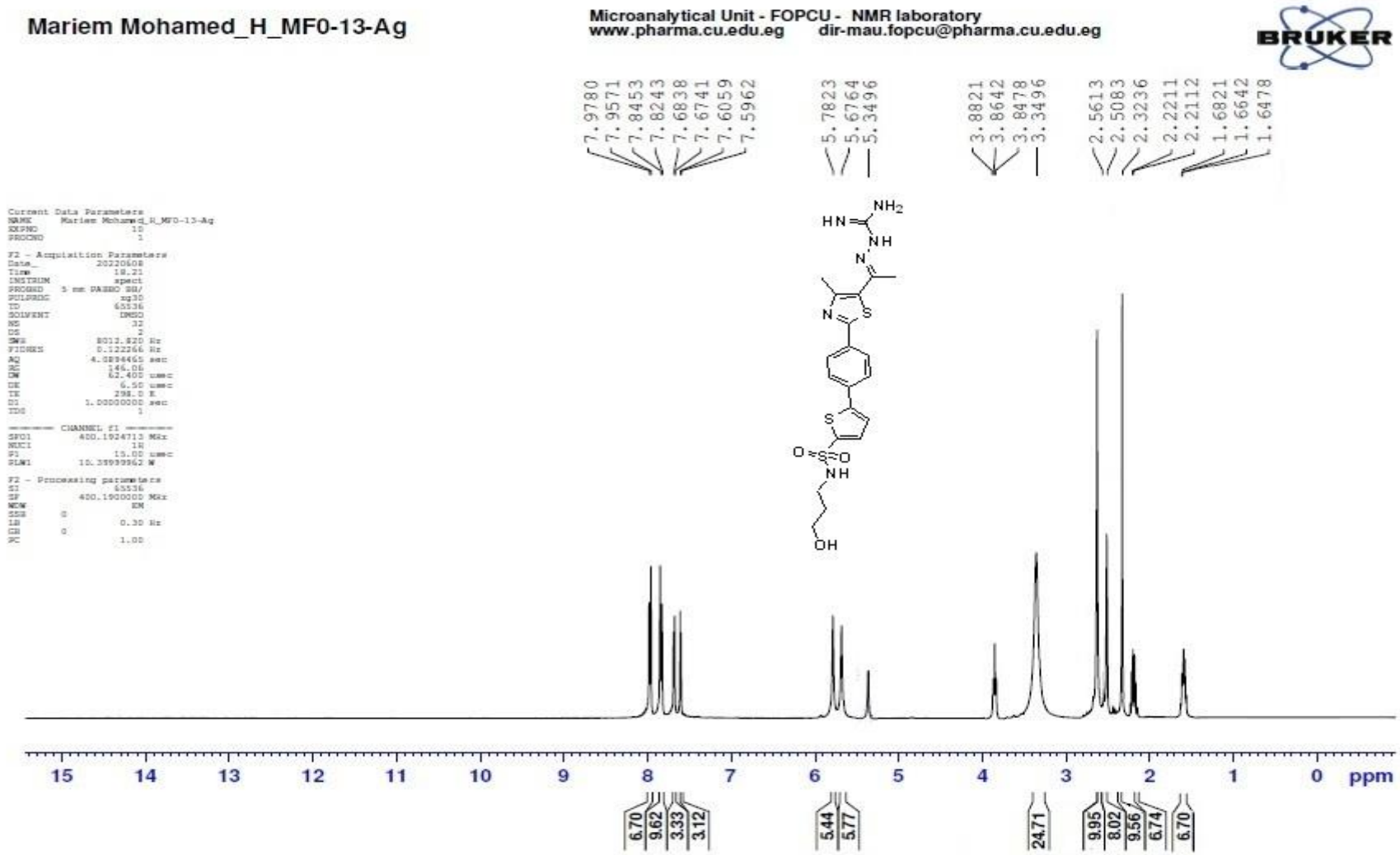

Mariem Mohamed_C_MF0-6
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
191.13
167.96
158.74
147.78
141.58
135.28
132.90
132.68
127.89
127.10
125.61
42.95
40.62
40.41
40.20
39.99
39.78
39.57
39.36
31.44
19.71
18.65
13.94
Current Data Parameters
NAME Mariem Mohamed_C_MF0-6
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220607
Time 2.48
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

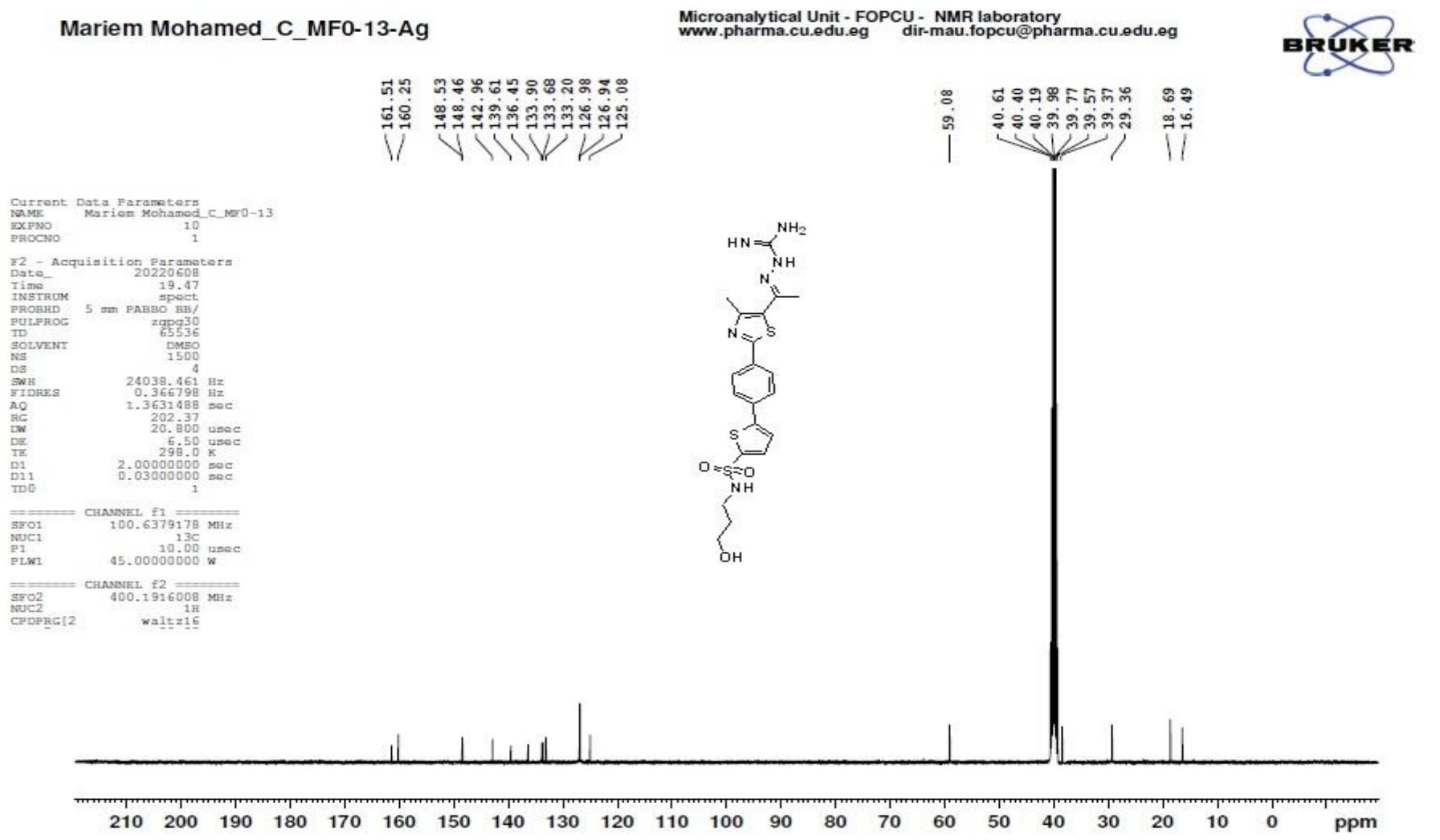

Mariem Mohamed_H_MF0-6-9Ag
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
7.9789
7.9580
7.9012
7.8863
7.8716
7.8448
7.8239
7.6704
7.6608
7.6021
7.5925
5.8651
3.3528
2.9027
2.8864
2.8700
2.6096
2.5929
2.5087
2.3309
1.4345
1.4166
1.3982
0.8506
0.8323
0.8142
Current Data Parameters
NAME Mariem Mohamed_H_MF0-6-9Ag
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220607
Time 2.53
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 146.06
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 16.39999962 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
5.71
9.26
2.92
3.09
7.98
18.94
6.20
7.72
8.51
7.10
6.39
9.51

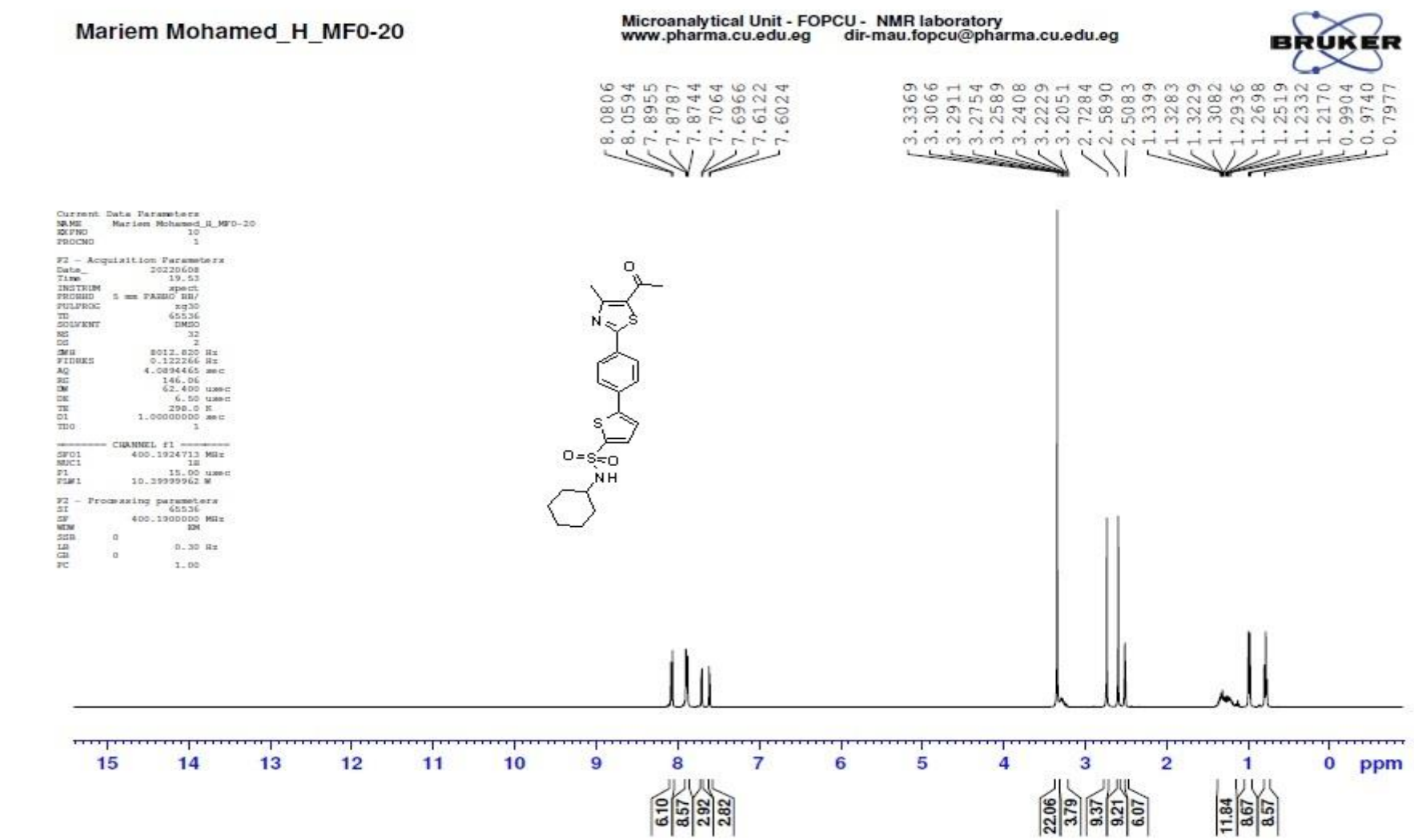

Mariem Mohamed_C_MF0-6-9Ag
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
161.69
159.99
148.82
148.26
143.26
141.01
136.14
133.84
133.75
132.91
126.97
125.04
42.95
40.61
40.40
40.20
39.99
39.78
39.57
39.36
31.43
19.71
18.69
13.95
Current Data Parameters
NAME Mariem Mohamed_C_MF0-6-
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220607
Time 4.03
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

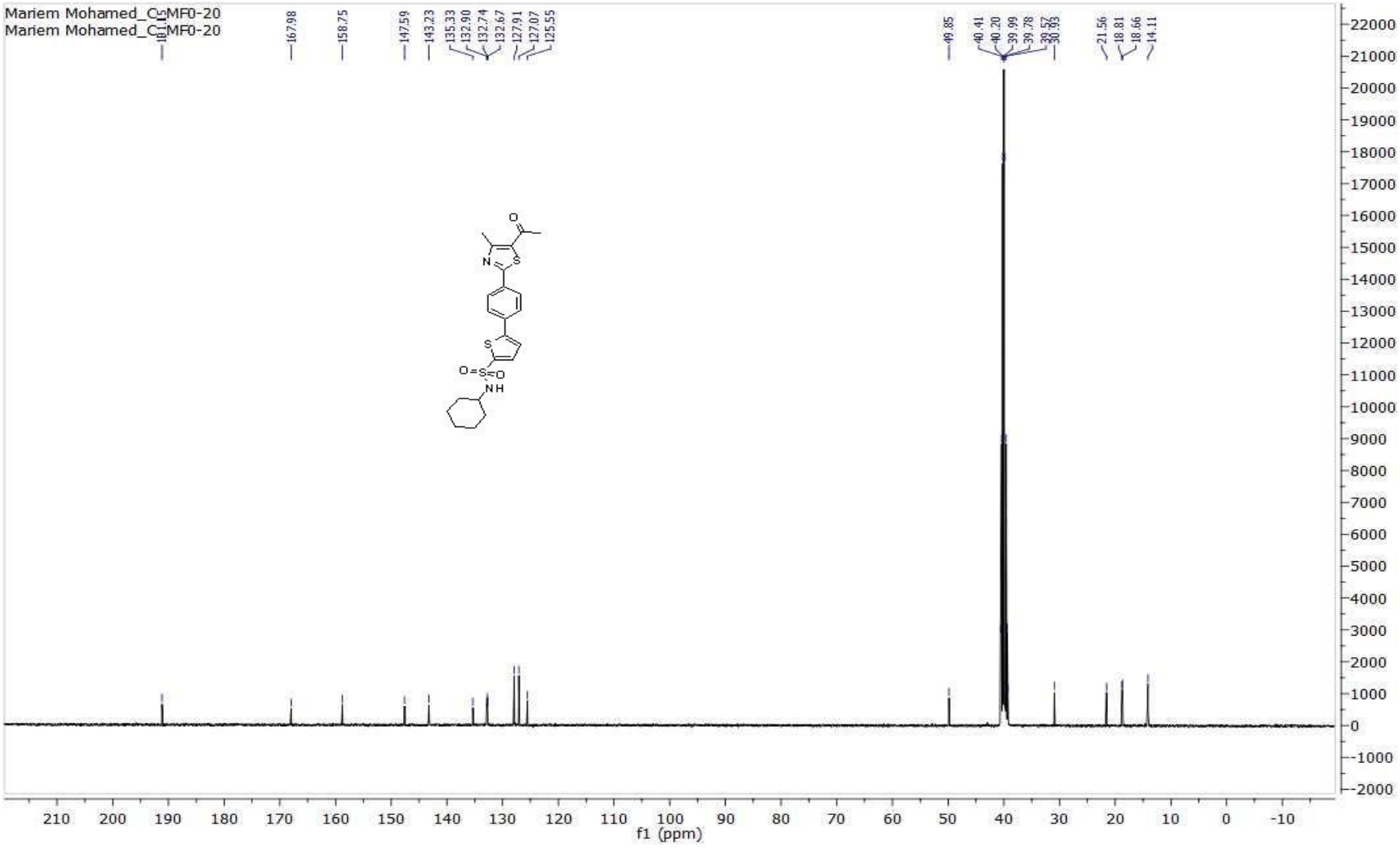

Mariem Mohamed_H_MF0-13
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.0667
8.0455
7.8875
7.8663
7.7989
7.7864
7.7255
7.7157
7.6211
7.6112
7.5814
7.5716
7.5530
7.5432
5.3325
3.8791
3.8738
3.8613
3.3429
2.7189
2.5791
2.5738
2.5613
2.5083
2.2211
2.2112
1.6255
1.6157
Current Data Parameters
NAME Mariem Mohamed_H_MF0-13
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220608
Time 16.49
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 129.43
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
O
N
S
S
O=S=O
NH
OH
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
7.19
7.84
4.25
3.65
3.68
3.49
7.19
12.84
10.90
12.46
5.14
7.25
7.49

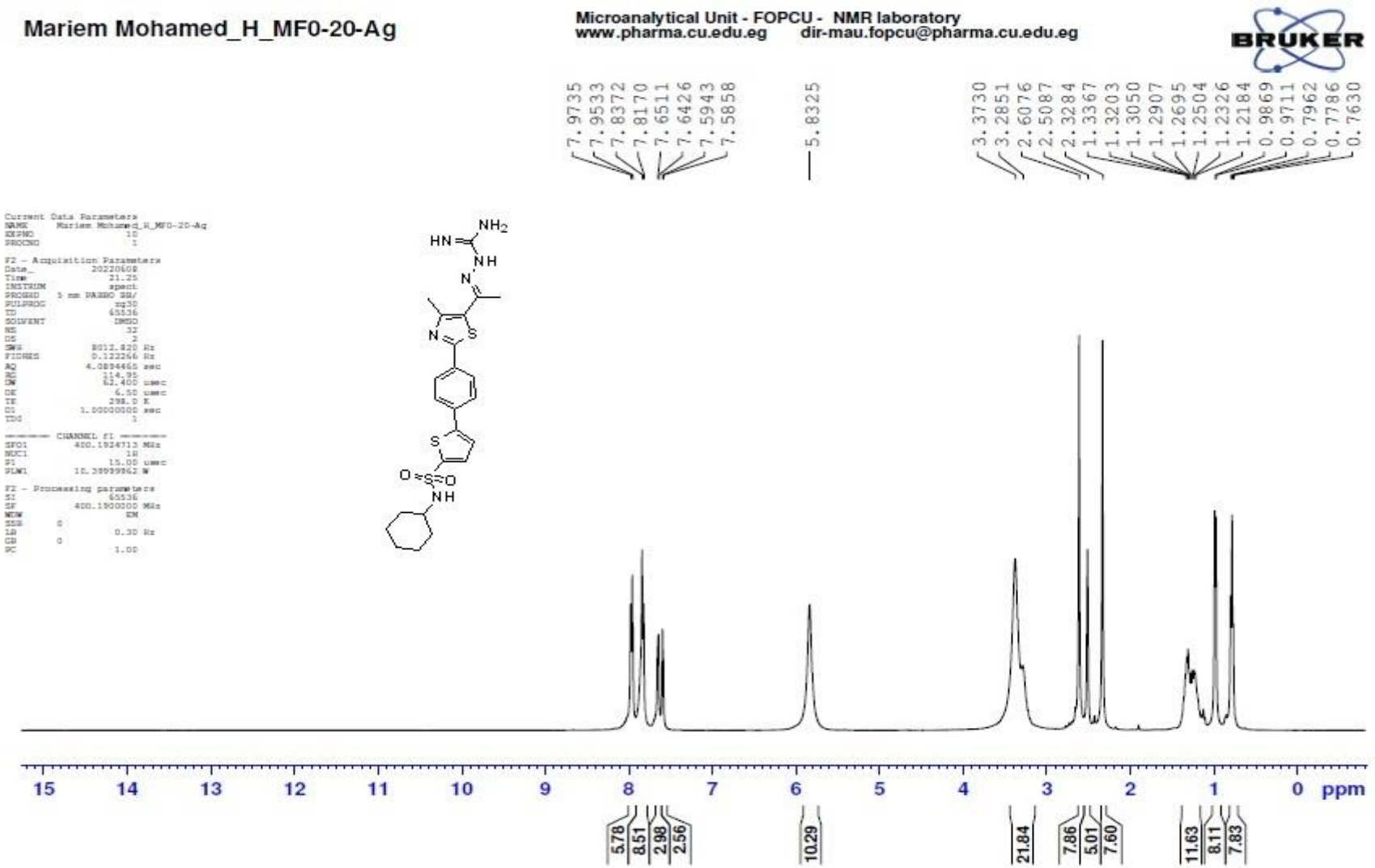

Mariem Mohamed_C_MF0-13
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
191.11
167.95
158.73
148.01
140.12
135.24
133.22
132.90
132.71
127.89
127.11
125.66
58.73
40.61
40.41
40.20
39.99
39.78
39.57
39.36
30.91
29.33
18.65
Current Data Parameters
NAME Mariem Mohamed_C_MF0-13
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220608
Time 18.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULFROG zgpg30
TD 65536
SOLVENT DMSO
NS 1500
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
O
N
S
S
O=S=O
NH
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

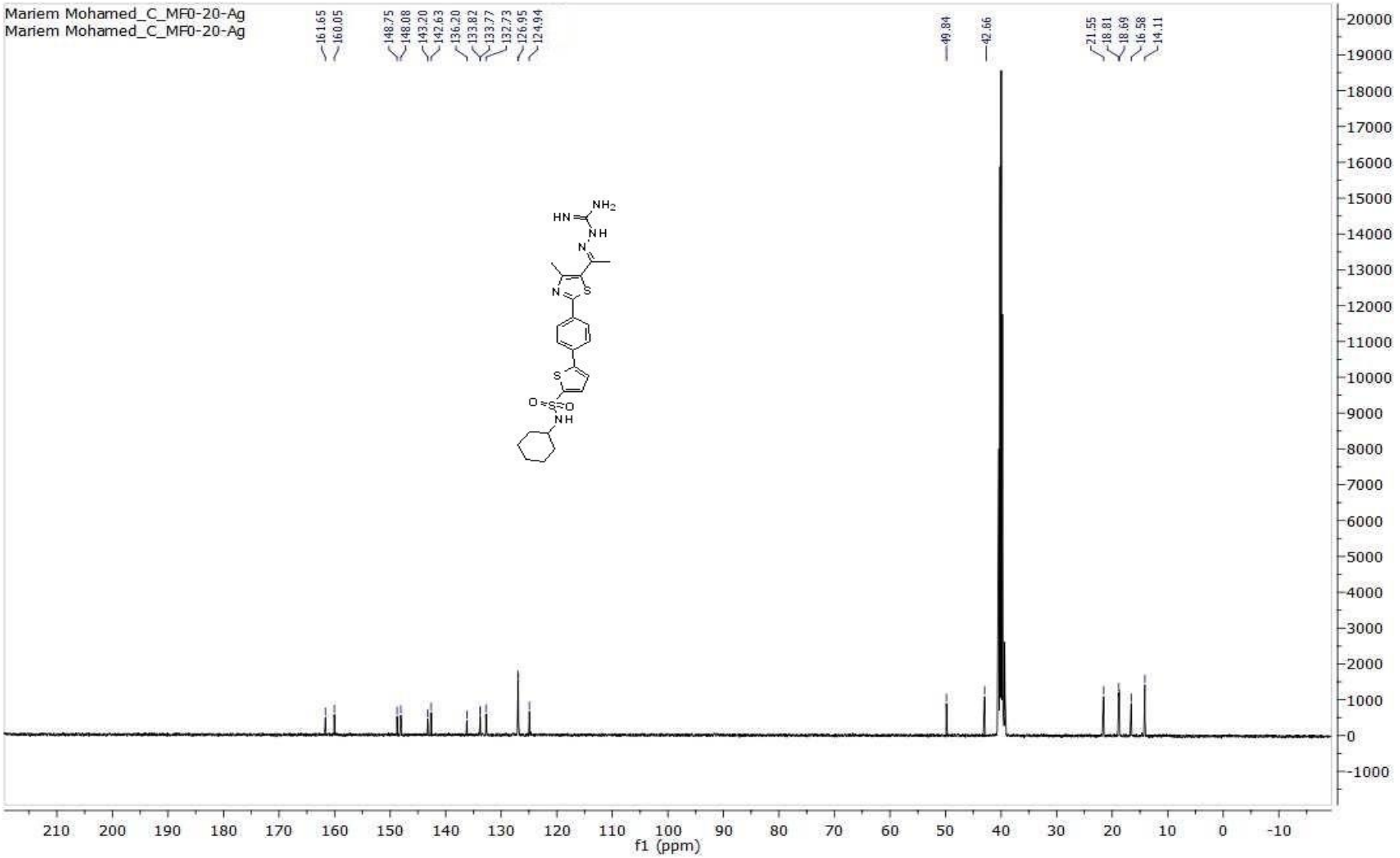

Mariem Mohamed_H_MF0-13-Ag
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
7.9780
7.9571
7.8453
7.8243
7.6838
7.6741
7.6059
7.5962
5.7823
5.6764
5.3496
3.8821
3.8642
3.8478
3.3496
2.5613
2.5083
2.3236
2.2211
2.2112
1.6821
1.6642
1.6478
Current Data Parameters
NAME Mariem Mohamed_H_MF0-13-Ag
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220608
Time 18.21
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 146.05
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
NH2
HN
NH
N
N
S
S
O
S
O
NH
OH
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.70
9.62
3.33
3.12
5.44
5.77
24.71
9.95
8.02
9.56
6.74
6.70


Mariem Mohamed_C_MF0-13-Ag
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
161.51
160.25
148.53
148.46
142.96
139.61
136.45
133.90
133.68
133.20
126.98
126.94
125.08
59.08
40.61
40.40
40.19
39.98
39.77
39.57
39.37
29.36
18.69
16.49
Current Data Parameters
NAME Mariem Mohamed_C_MF0-13
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220608
Time 19.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1500
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
NH2
HN
NH
N
N
S
S
O
S
O
NH
OH
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


Mariem Mohamed_H_MF0-20
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
8.0806
8.0594
7.8955
7.8787
7.8744
7.7064
7.6966
7.6122
7.6024
3.3369
3.3066
3.2911
3.2754
3.2589
3.2408
3.2229
3.2051
2.7284
2.5890
2.5083
1.3399
1.3283
1.3229
1.3082
1.2936
1.2698
1.2519
1.2332
1.2170
0.9904
0.9740
0.7977
Current Data Parameters
NAME Mariem Mohamed_H_MF0-20
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220608
Time 19.53
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 146.06
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
O
N
S
S
O=S=O
NH
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
6.10
8.57
2.92
2.82
22.06
3.79
9.37
9.21
6.07
11.84
8.67
8.57


Mariem Mohamed_C_MF0-20
Mariem Mohamed_C_MF0-20
167.98
158.75
147.59
143.23
135.33
132.90
132.74
132.67
127.91
127.07
125.55
49.85
40.41
40.20
39.99
39.78
39.57
30.93
21.56
18.81
18.66
14.11
f1 (ppm)


Mariem Mohamed_H_MF0-20-Ag
Microanalytical Unit - FOPCU - NMR laboratory
www.pharma.cu.edu.eg dir-mau.fopcu@pharma.cu.edu.eg
BRUKER
7.9735
7.9533
7.8372
7.8170
7.6511
7.6426
7.5943
7.5858
5.8325
3.3730
3.2851
2.6076
2.5087
2.3284
1.3367
1.3203
1.3050
1.2907
1.2695
1.2504
1.2326
1.2184
0.9869
0.9711
0.7962
0.7786
0.7630
Current Data Parameters
NAME Mariem Mohamed_H_MF0-20-Ag
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220608
Time 21.25
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 114.95
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
NH2
HN
NH
N
N
S
S
O
S
O
NH
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
5.78
8.51
2.98
2.56
10.29
21.84
7.86
5.01
7.60
11.63
8.11
7.83


Mariem Mohamed_C_MF0-20-Ag
Mariem Mohamed_C_MF0-20-Ag
161.65
160.05
148.75
148.08
143.20
142.63
136.20
133.82
133.77
132.73
126.95
124.94
49.84
42.66
21.55
18.81
18.69
16.58
14.11
f1 (ppm)