Bio-Oriented Synthesis of Novel (S)-Flurbiprofen Clubbed Hydrazone Schiff's Bases for Diabetic Management: In Vitro and In Silico Studies

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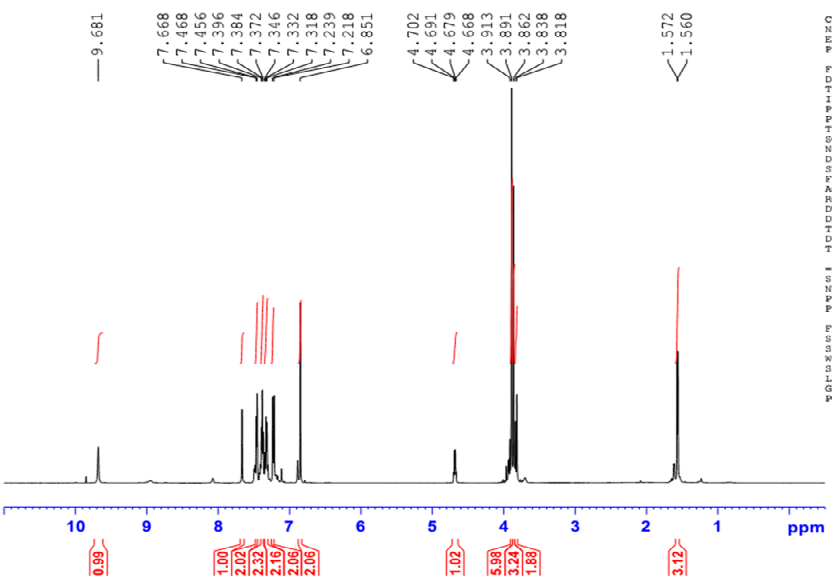
Abstract: A new series of flurbiprofen derivatives **(4a–4p)** and **(5a–5n)** were synthesized with different aromatic or aliphatic aldehydes and ketones to produce Schiff's bases and their structures were confirmed through HR-ESI-MS, ^{1}H and ^{13}C-NMR spectroscopy. The α-glucosidase inhibitory activities of the newly synthesized compounds were scrutinized, in which six compounds **5k**, **4h**, **5h**, **4d**, **4b** and **5i** showed potent inhibition in the range of 0.93 to 10.26μM, respectively, whereas fifteen compounds **4c, 4g, 4i, 4j, 4l, 4m, 4o, 4p, 5c, 5d, 5j, 5l, 5m, 5n** and **1** exhibited significant inhibitory activity with IC_{50} in range of = 11.42 to 48.39 μM. In addition, compounds **5g, 5f**, **4k**, **4n**, and **4f** displayed moderate-to-low activities. The modes of binding of all the active compounds were determined through molecular docking approach which revealed that two residues, specifically Glu277 and His351 are important in the stabilization of the active compounds in the active site of α-glucosidase. Furthermore, these compounds block the active site with high binding energies (–7.51 to –3.36 kcal/mol) thereby inhibiting the function of the enzyme.

Keywords: (S)-flurbiprofen; Schiff's bases; α-glucosidase inhibition; molecular docking

Dr. Najeeb/AFT-3o/CDCl3
PROTON



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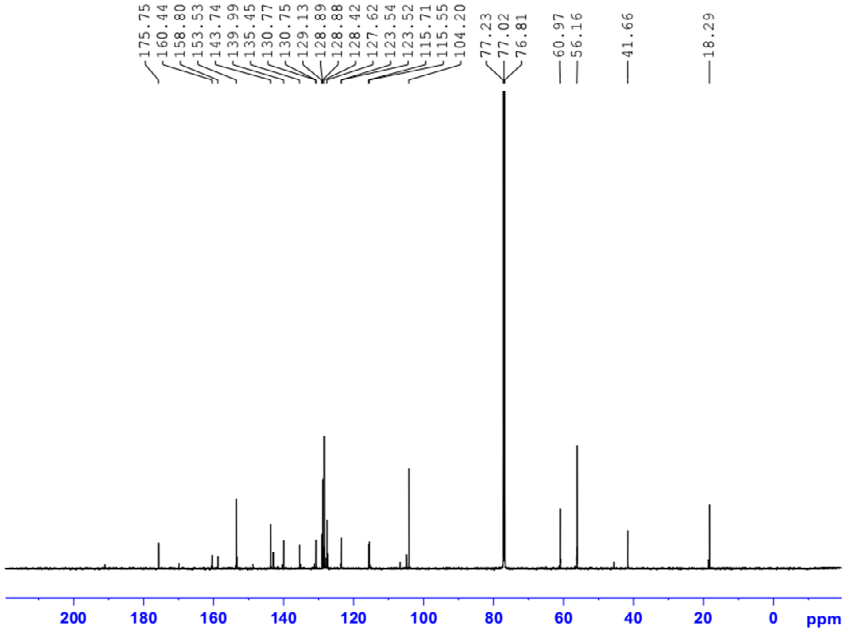
Dr. Najeeb/AFT-3o/CDCl3
C13CPD



BRUKER

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NUC2               1H
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PCPD2             70.00 usec
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PLW13         0.25874999 W

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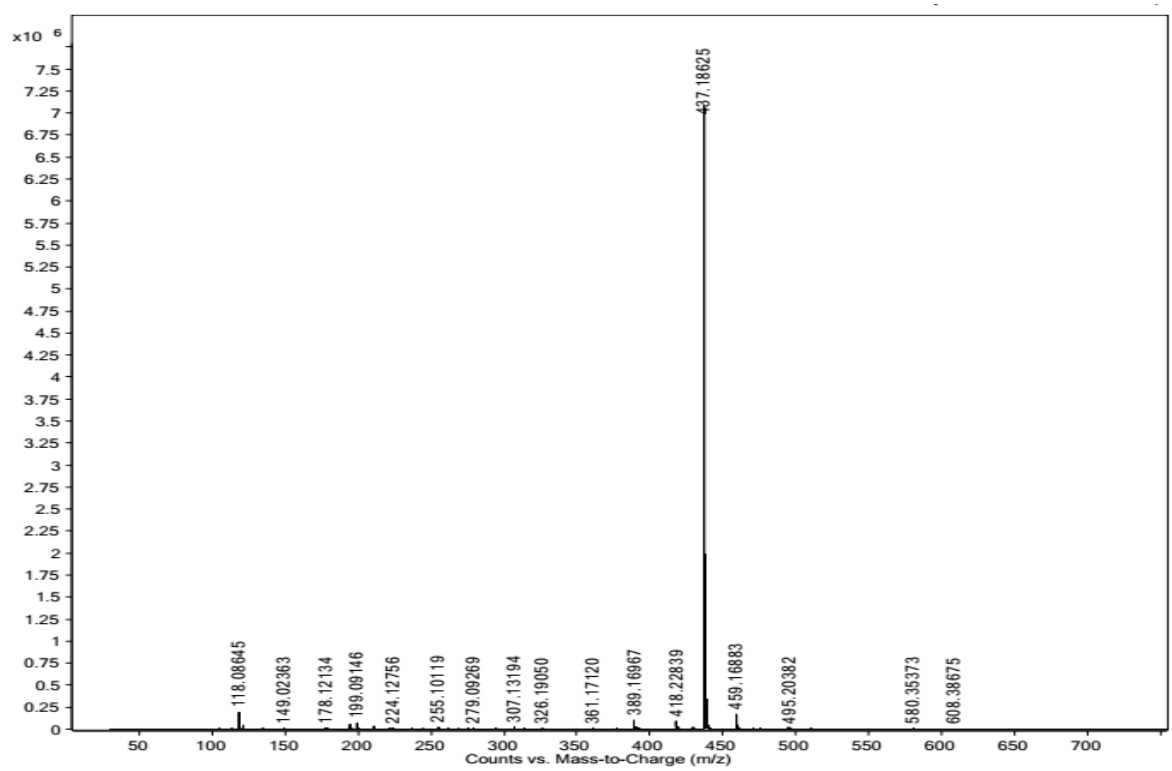
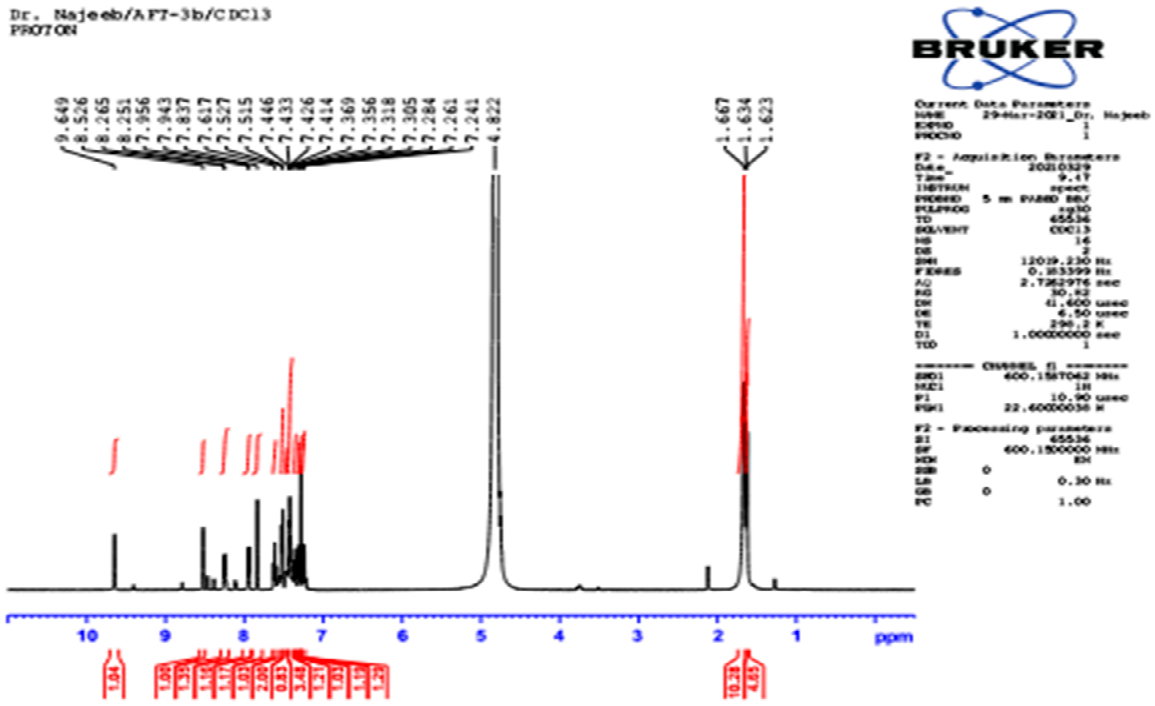


Figure S1: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4a**



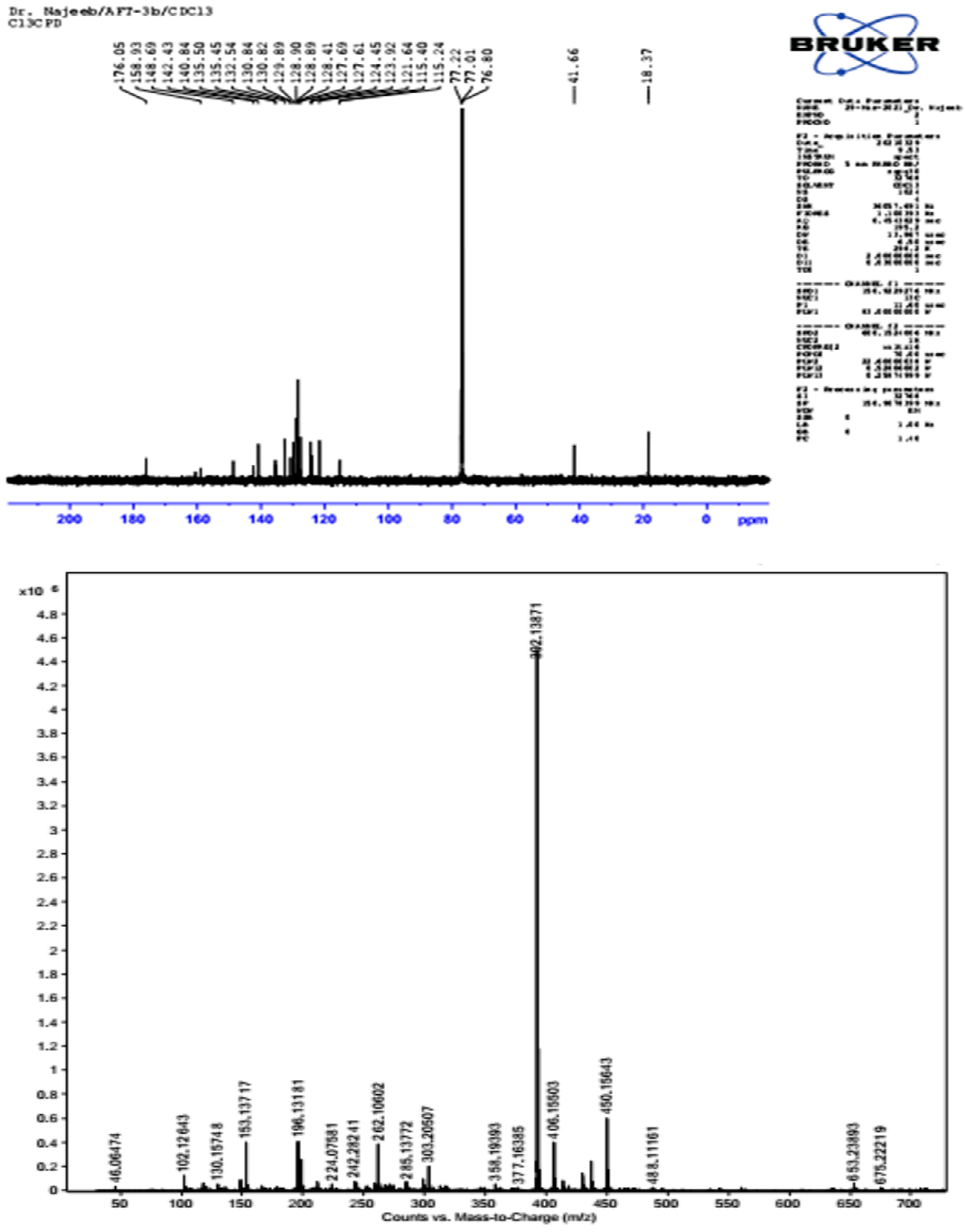
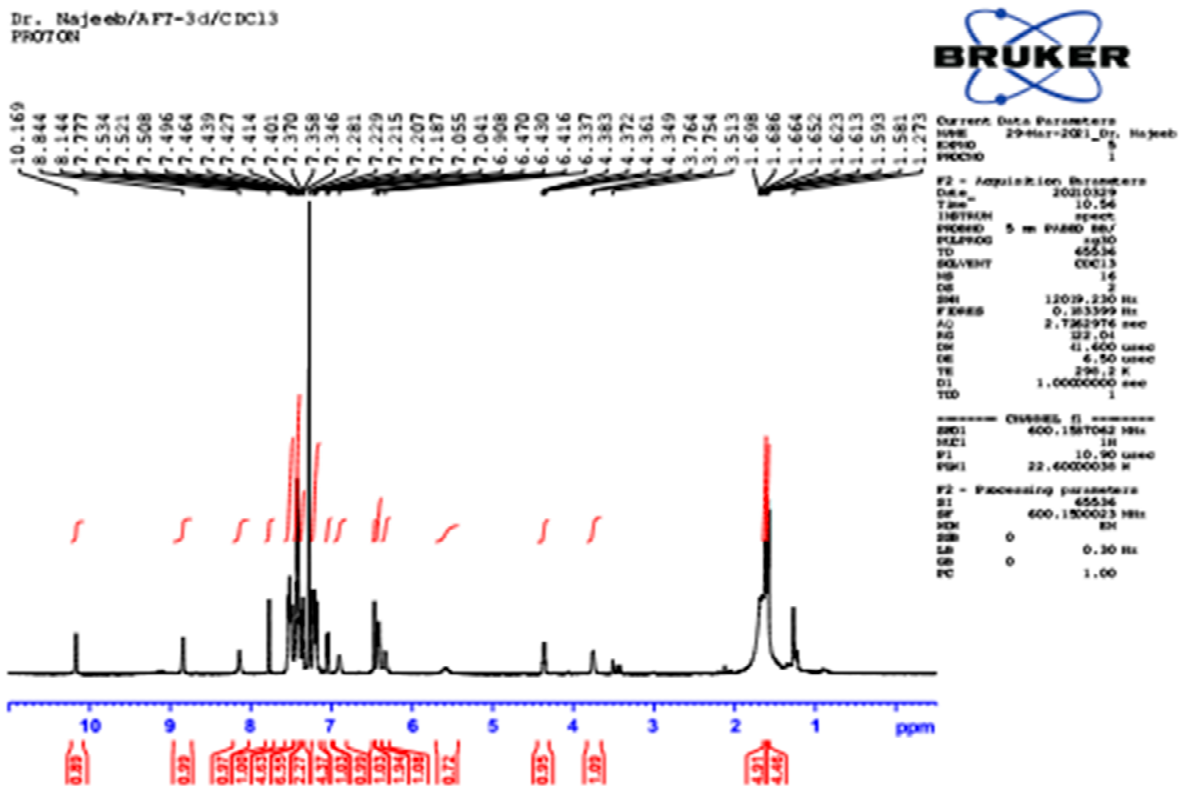


Figure S2: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4b**


Dr. Najeeb/AFT-3d/CDCl3
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7.508
7.496
7.464
7.439
7.427
7.414
7.401
7.370
7.358
7.346
7.281
7.229
7.215
7.207
7.187
7.055
7.041
6.908
6.470
6.430
6.416
6.337
4.383
4.372
4.361
4.349
3.764
3.754
3.513
1.698
1.686
1.664
1.652
1.623
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9
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7
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1
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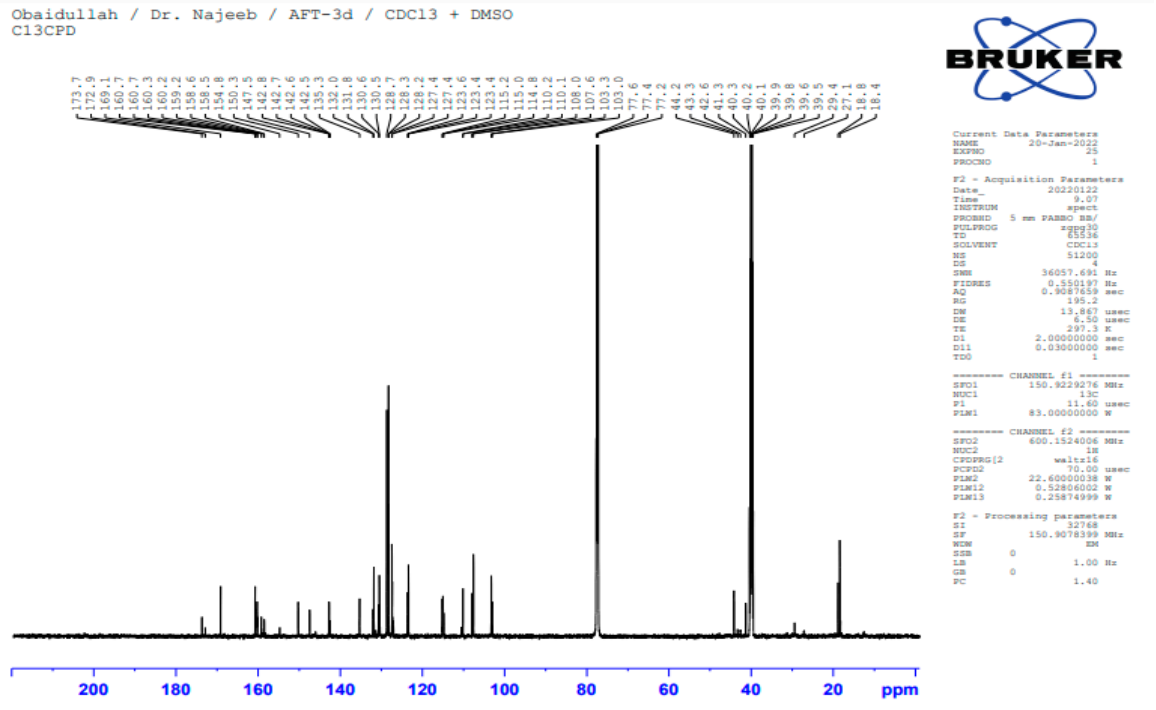
Obaidullah / Dr. Najeeb / AFT-3d / CDCl3 + DMSO
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160.7
160.3
160.2
159.2
158.6
158.5
154.8
150.3
147.5
142.8
142.7
142.6
142.5
135.3
132.0
131.8
130.6
130.5
128.7
128.3
128.2
127.4
127.4
123.6
123.4
123.4
115.2
115.0
114.8
110.2
110.1
108.0
107.6
103.3
103.0
77.6
77.4
77.2
44.2
43.3
42.6
41.3
40.3
40.2
40.1
39.9
39.8
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29.4
27.1
18.8
18.4
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140
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100
80
60
40
20
ppm

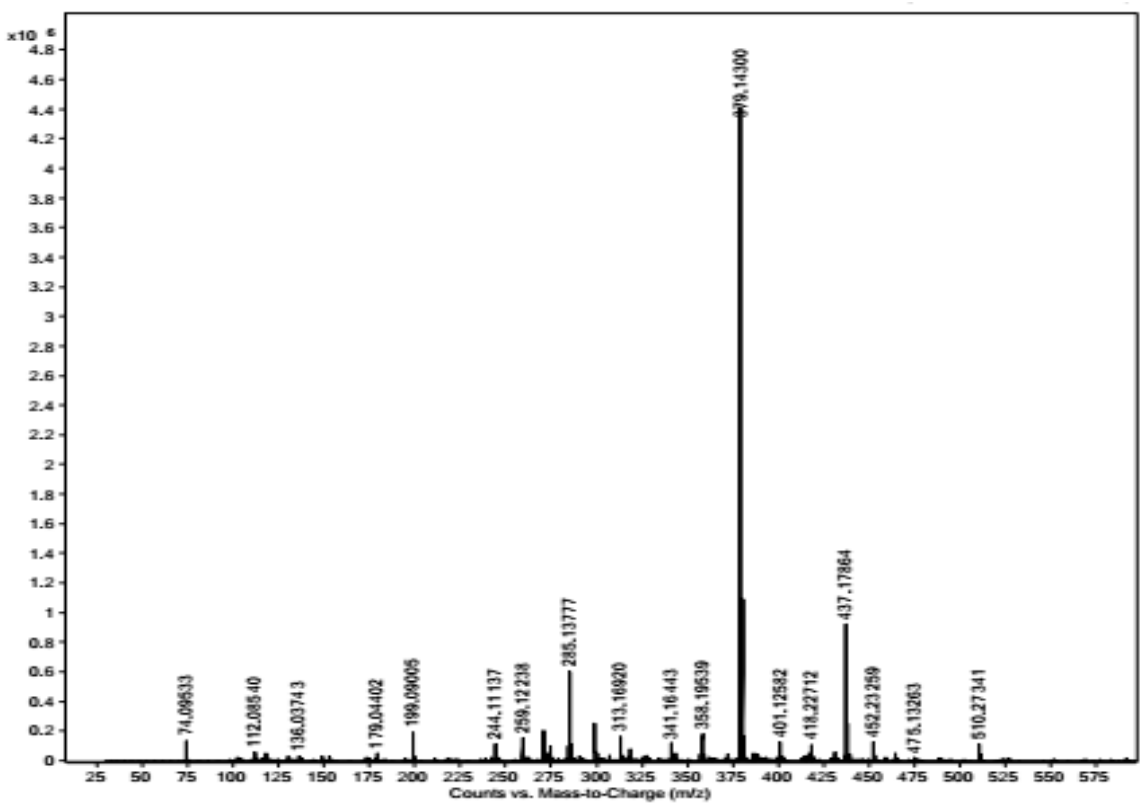
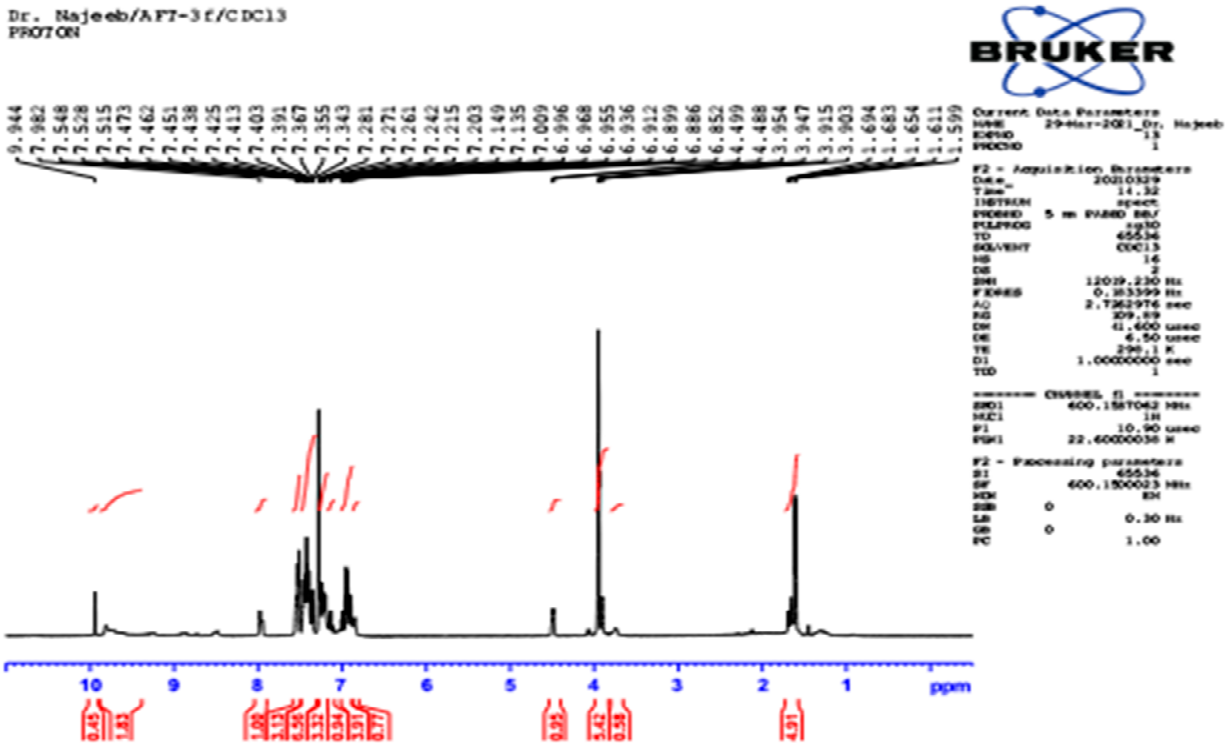


Figure S3: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4c**



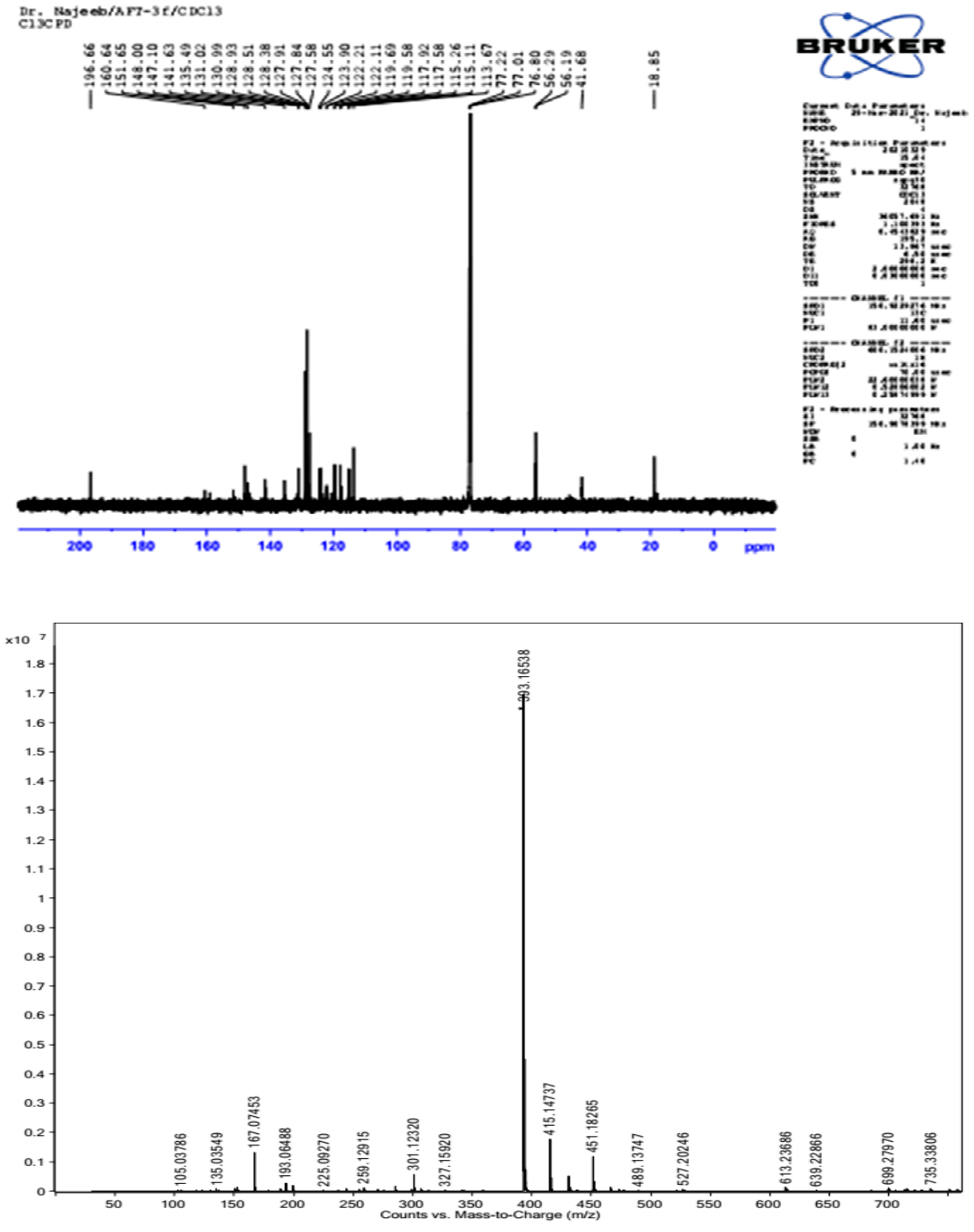
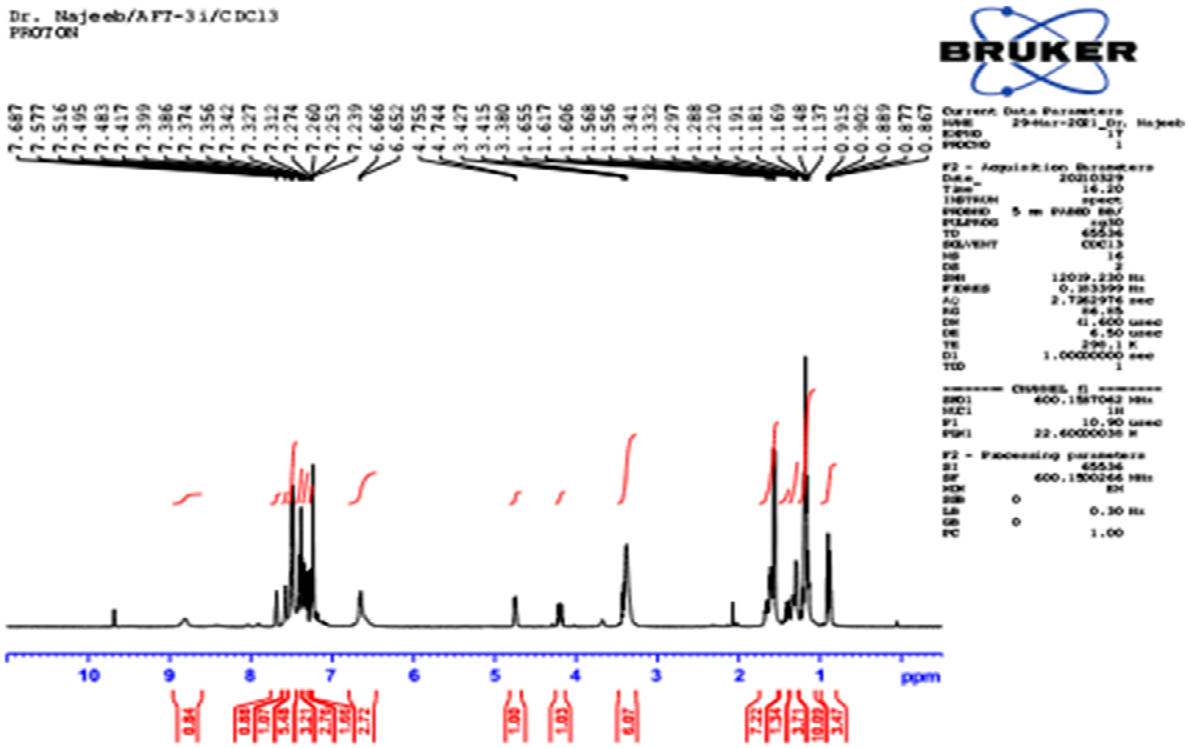


Figure S4: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4d**


Dr. Najeeb/AF7-3i/CDCl3
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7.253
7.239
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6.652
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3.415
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1.606
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1.181
1.169
1.148
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0.889
0.877
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8
7
6
5
4
3
2
1
ppm
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0.88
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4.43
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5.07
7.22
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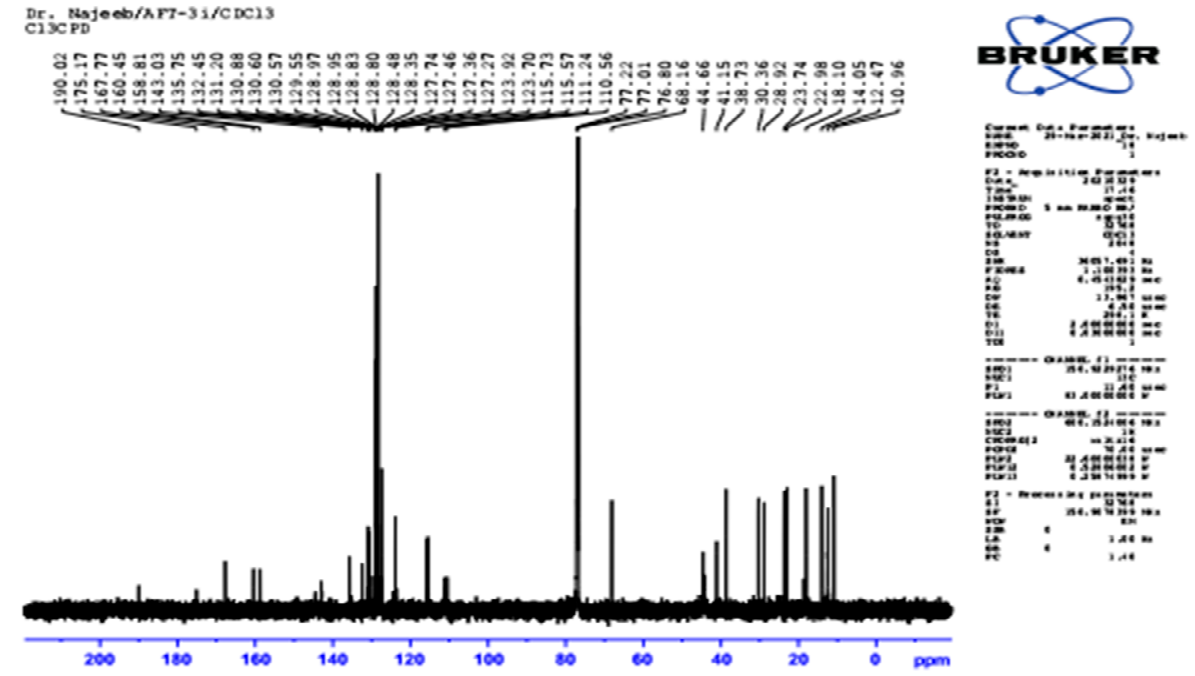
3.72
10.00
3.47


Dr. Najeeb/AF7-3i/CDCl3
C13CPD
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132.45
131.20
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130.60
130.57
129.55
128.97
128.95
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128.48
128.35
127.74
127.46
127.36
127.27
123.92
123.70
115.73
115.57
111.24
110.56
77.22
77.01
76.80
68.16
44.66
41.15
38.73
30.36
28.92
23.74
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20
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ppm

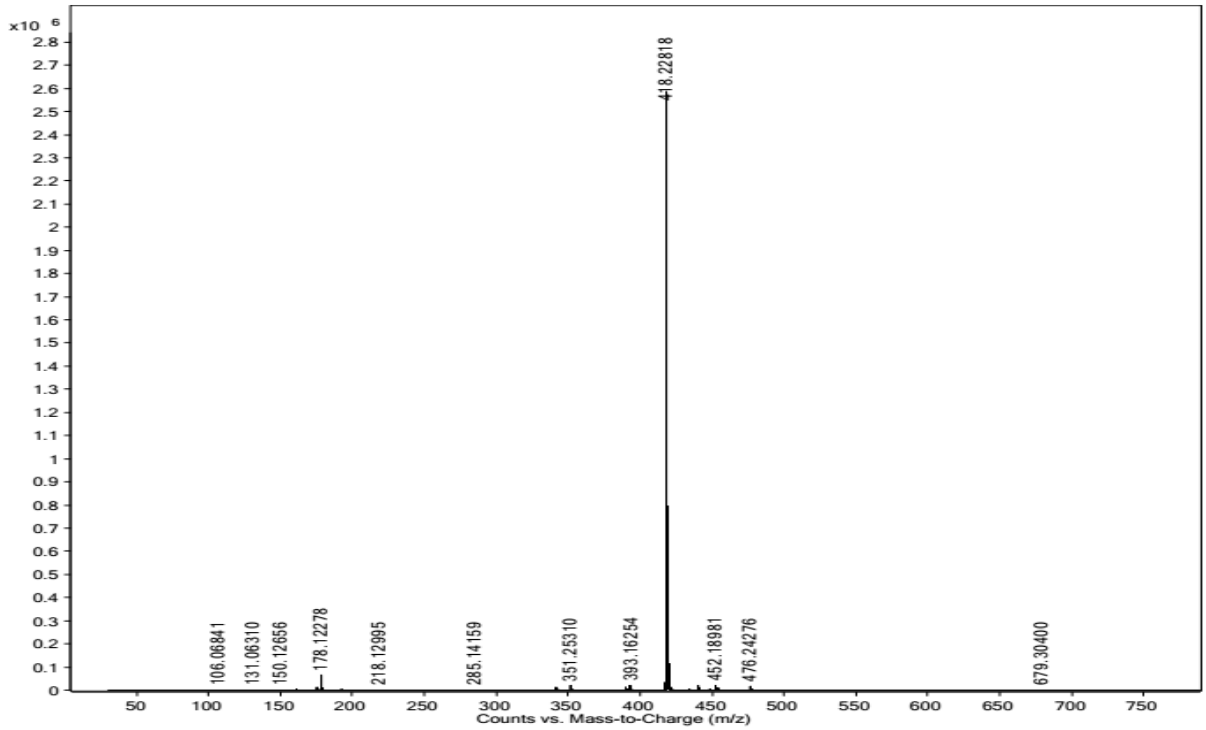
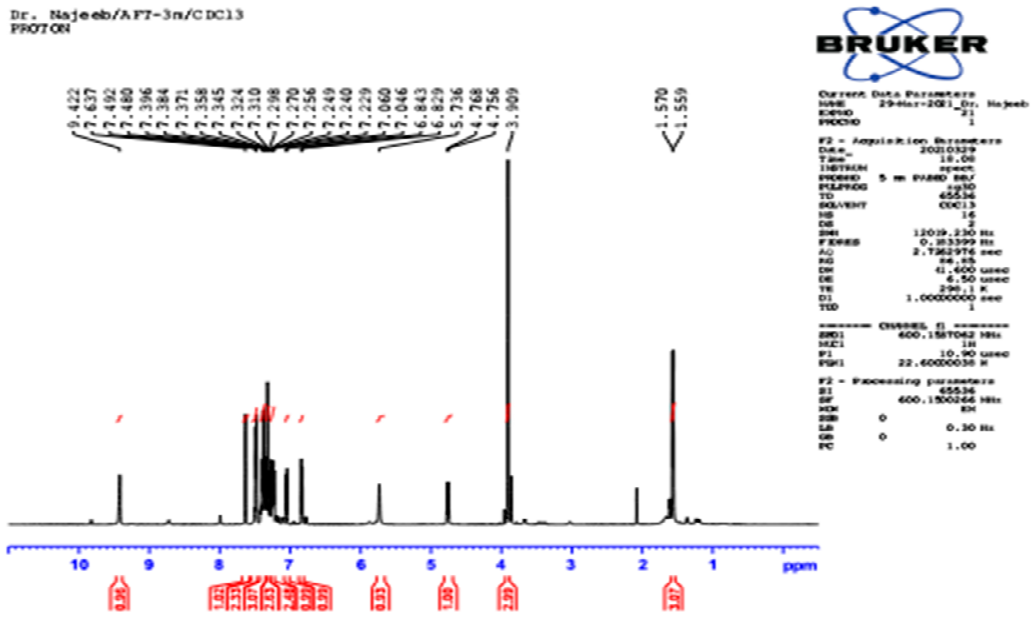


Figure S5: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4e**



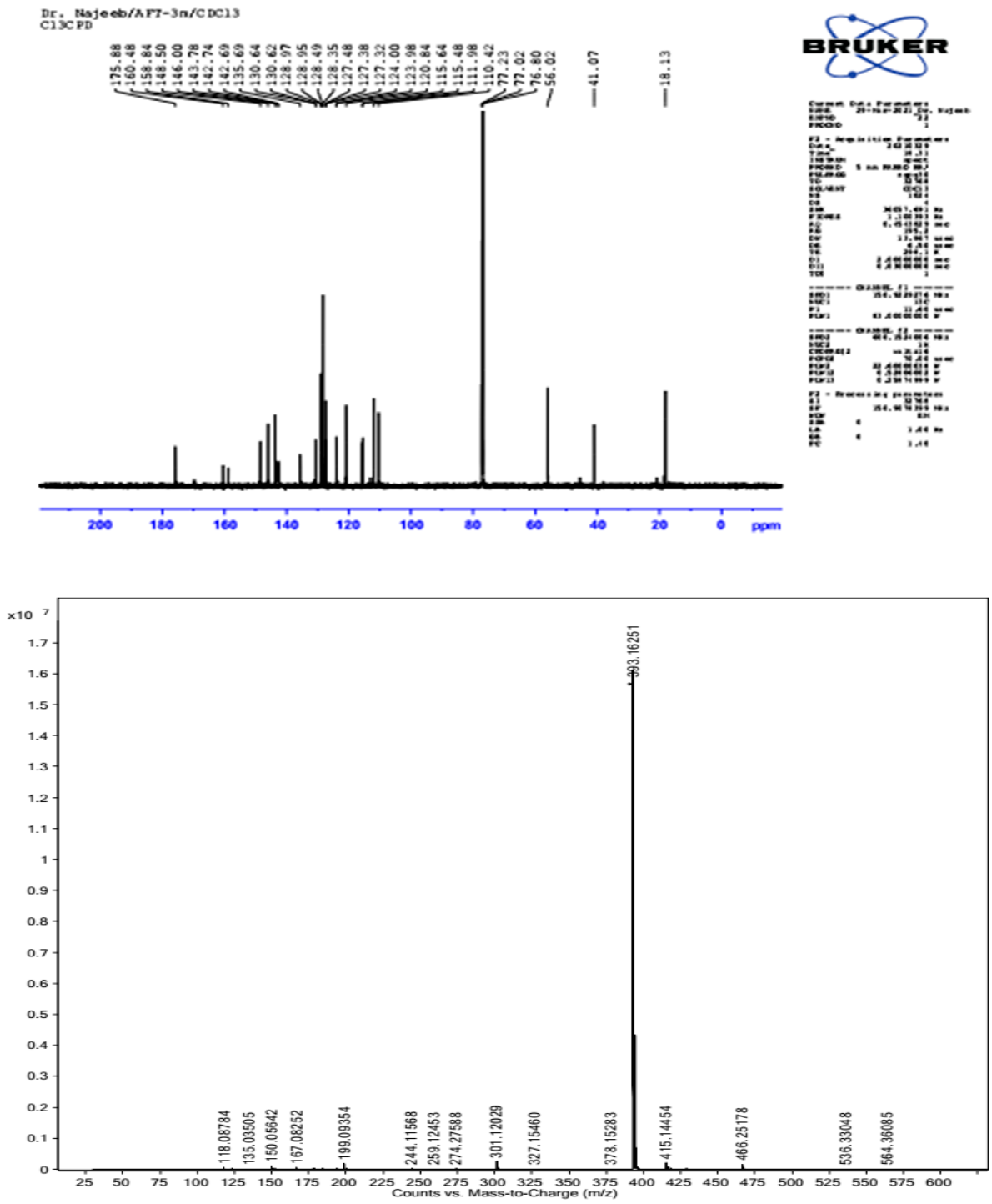
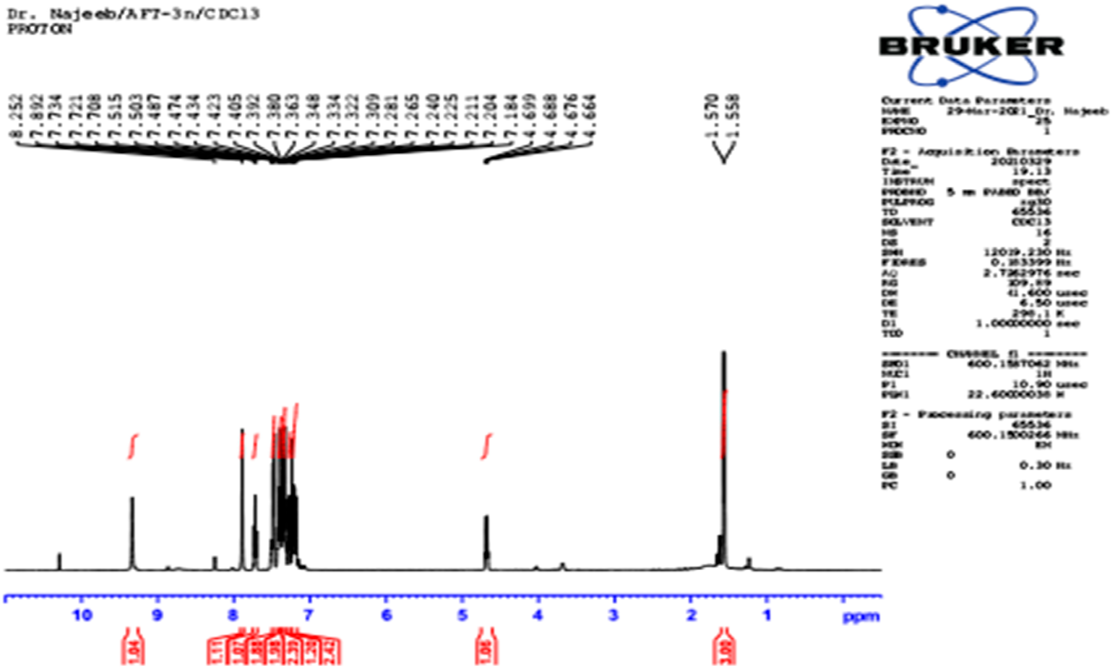


Figure S6: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4f**


Dr. Najeeb/AF7-3n/CDCl3
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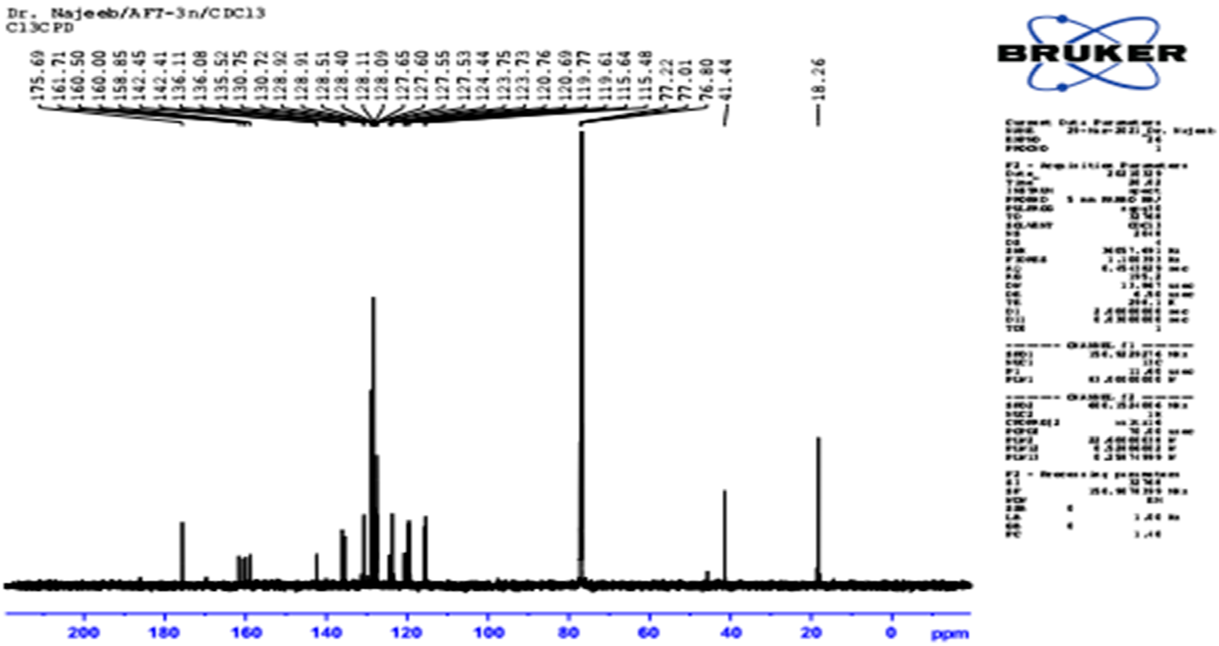
1.570 1.558
BRUKER
10 9 8 7 6 5 4 3 2 1 ppm


Dr. Najeeb/AF7-3n/CDCl3
C13CPD
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18.26
BRUKER
200 180 160 140 120 100 80 60 40 20 0 ppm

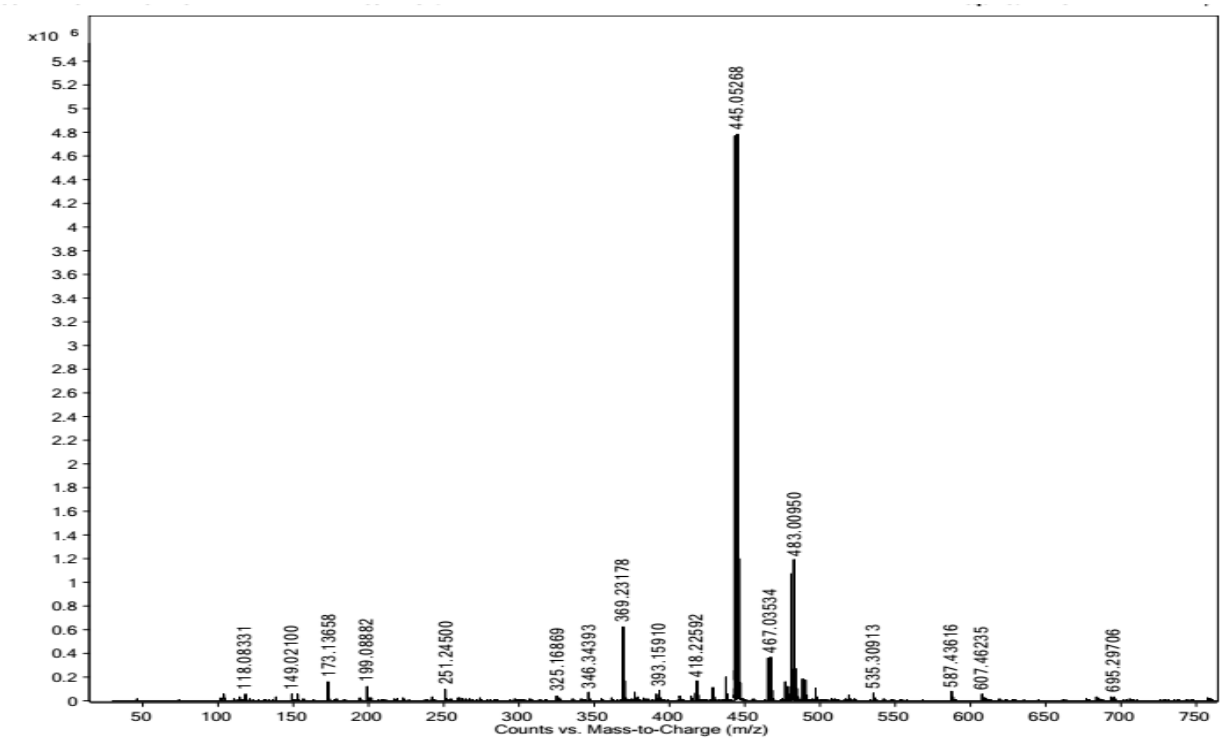
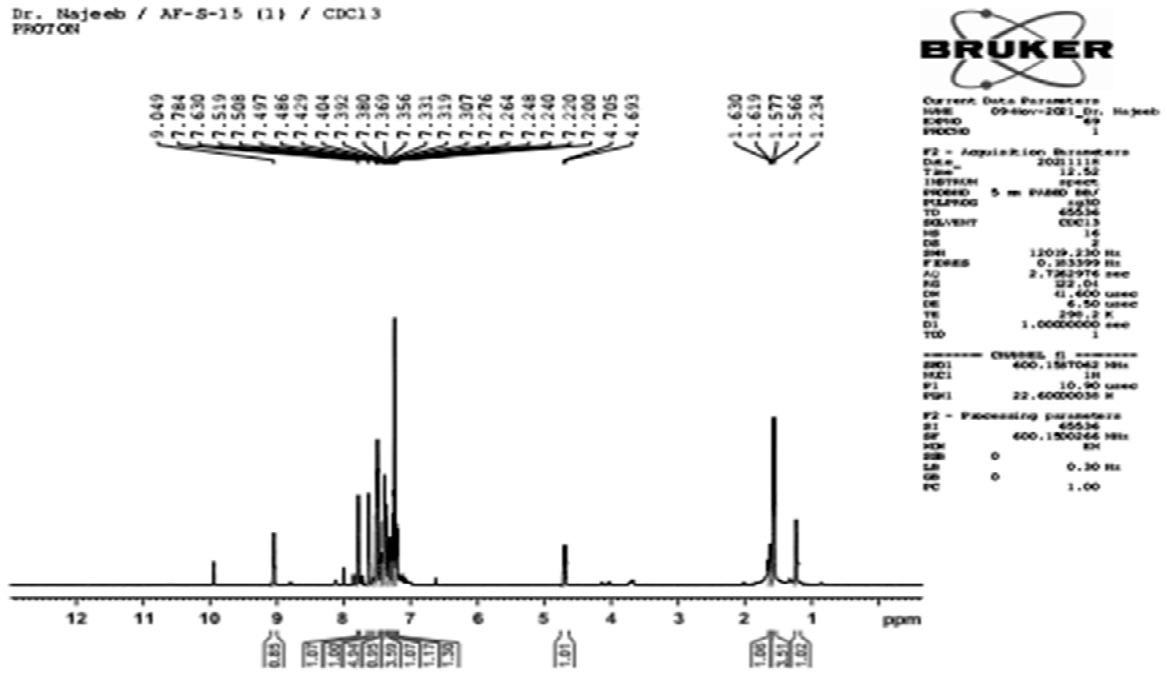


Figure S7: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4g**



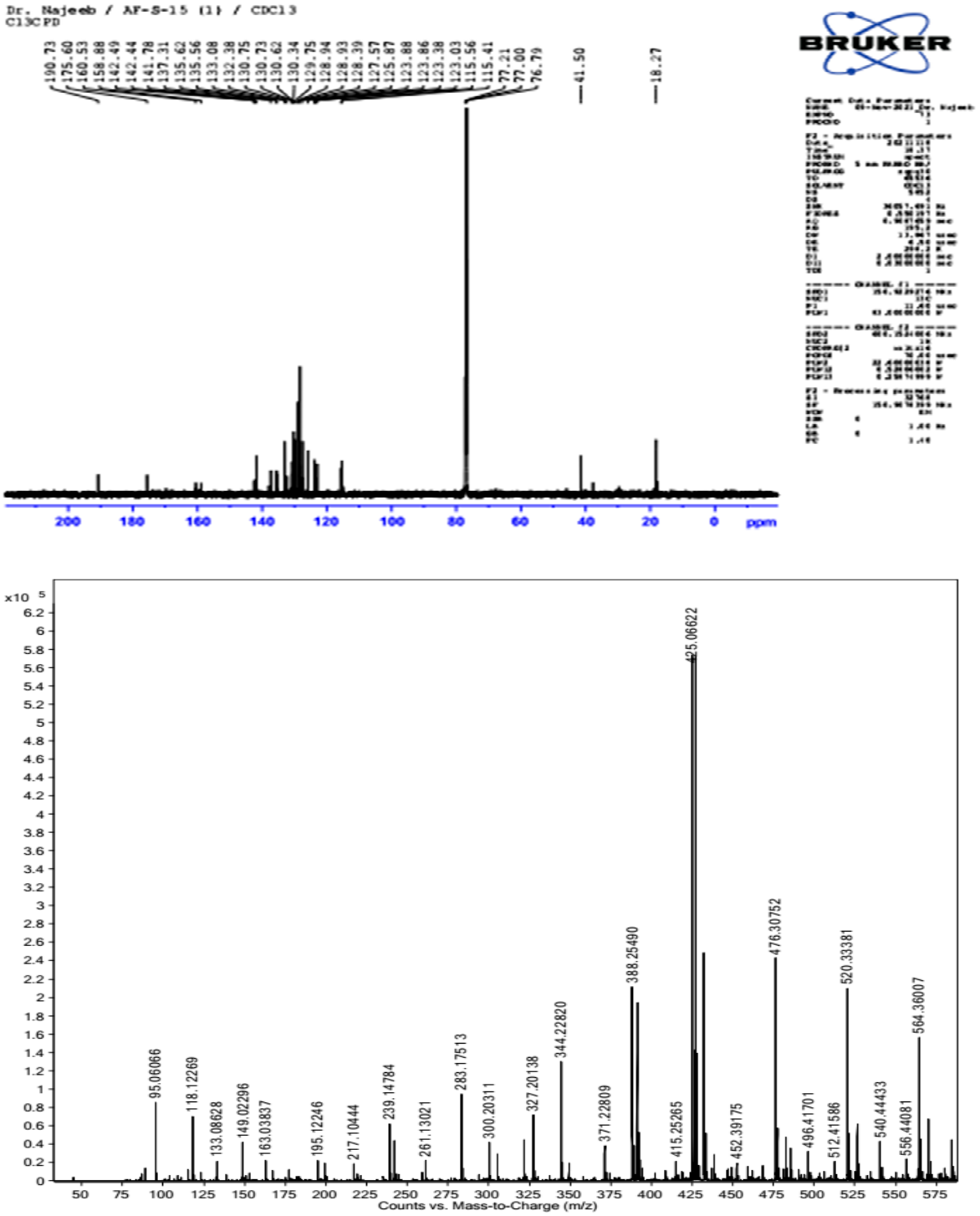
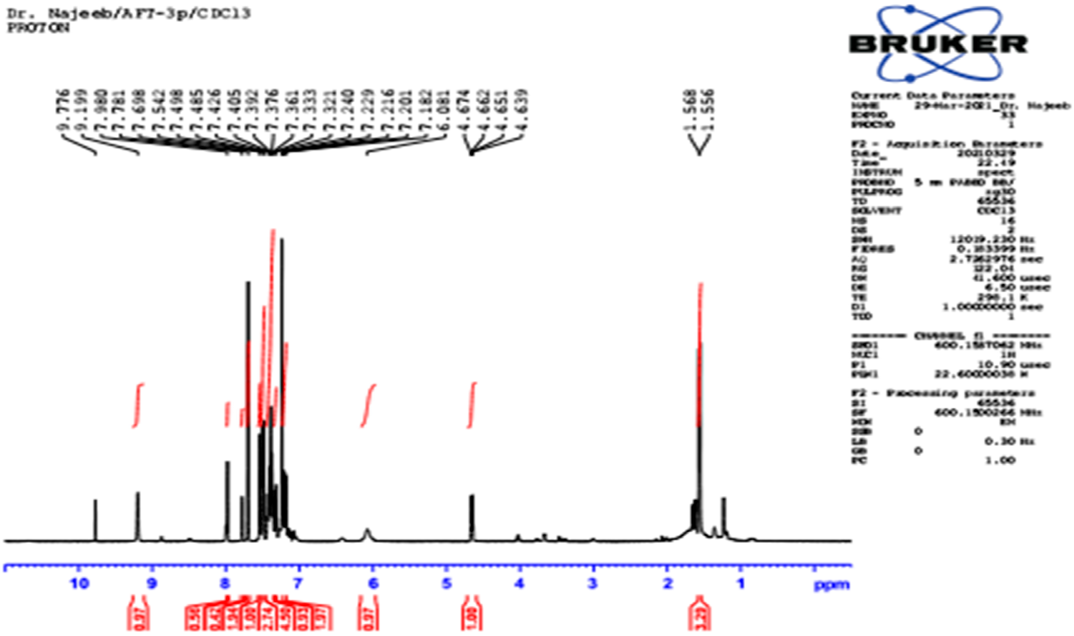


Figure S8: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4h**


Dr. Najeeb/AF7-3p/CDCl3
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9.776
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7.542
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7.485
7.426
7.405
7.392
7.376
7.361
7.333
7.321
7.240
7.229
7.216
7.201
7.182
6.081
4.674
4.662
4.651
4.639
1.568
1.556
BRUKER
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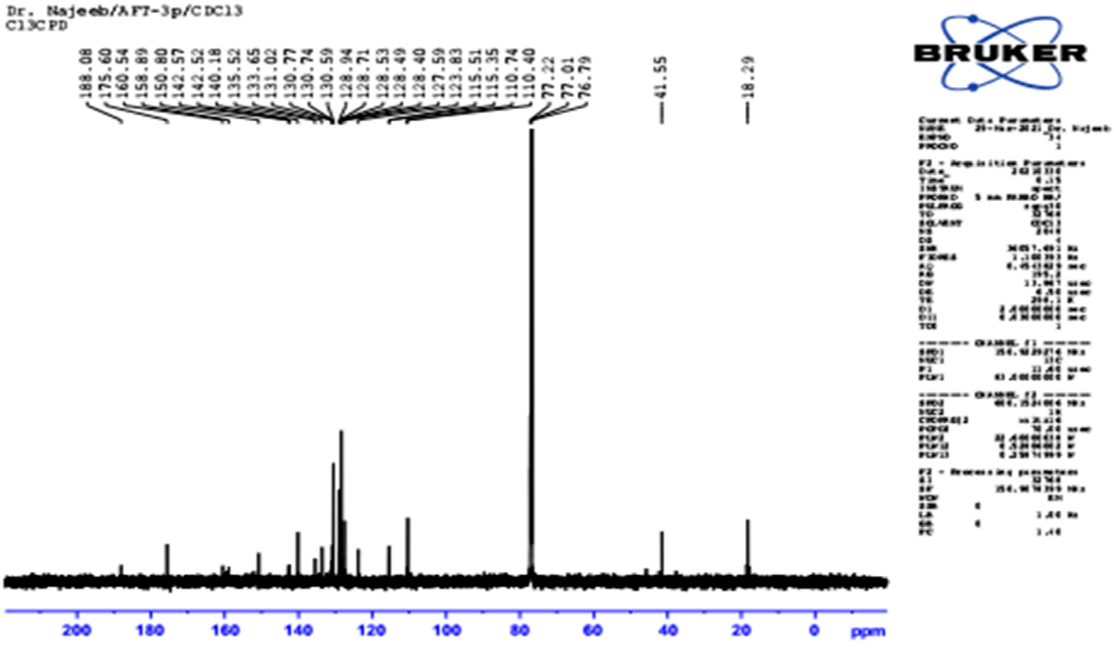
9
8
7
6
5
4
3
2
1
ppm


Dr. Najeeb/AF7-3p/CDCl3
C13CPD
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140.18
135.52
133.65
131.02
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130.74
130.59
128.94
128.71
128.53
128.49
128.40
127.59
123.83
115.51
115.35
110.74
110.40
77.22
77.01
76.79
41.55
18.29
BRUKER
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140
120
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80
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ppm

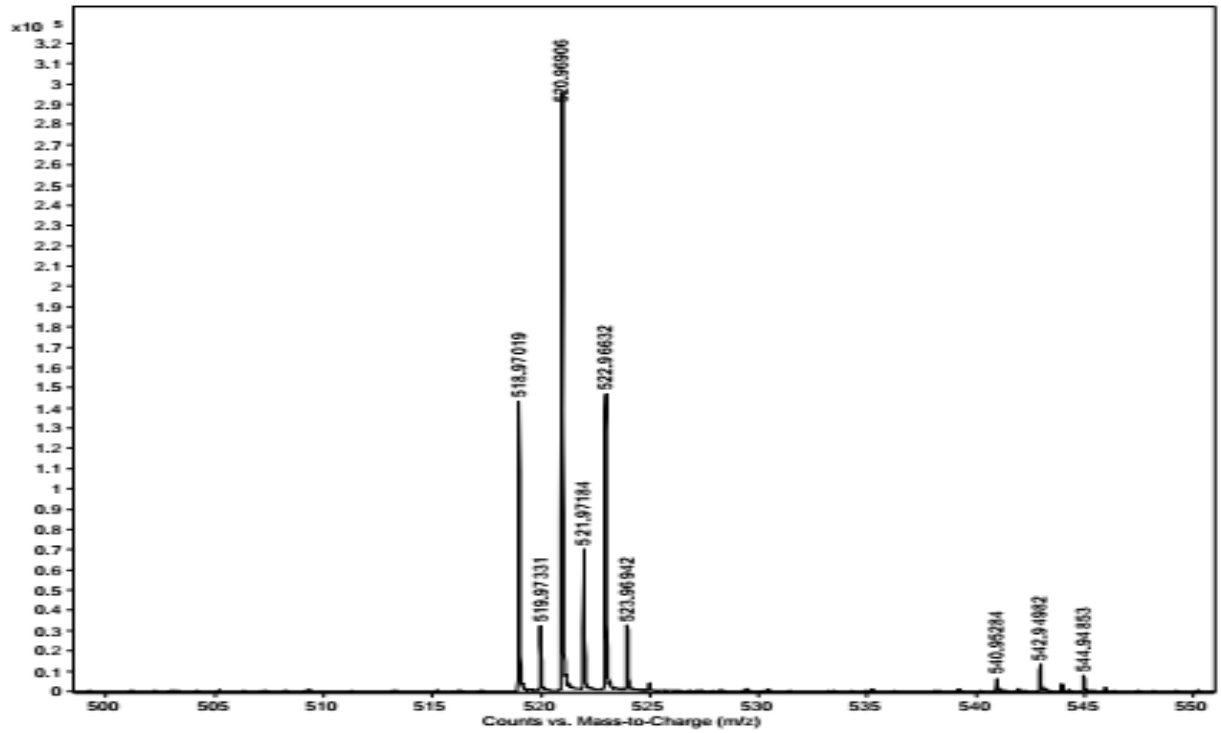
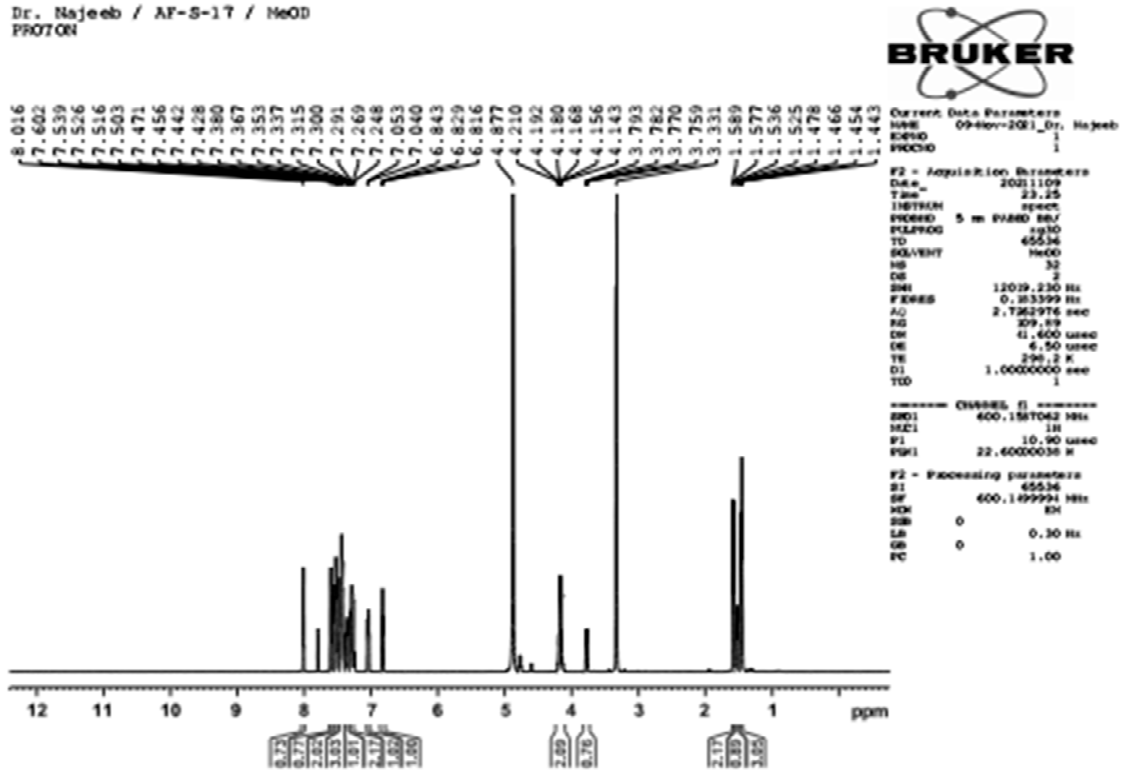


Figure S9. ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4i**



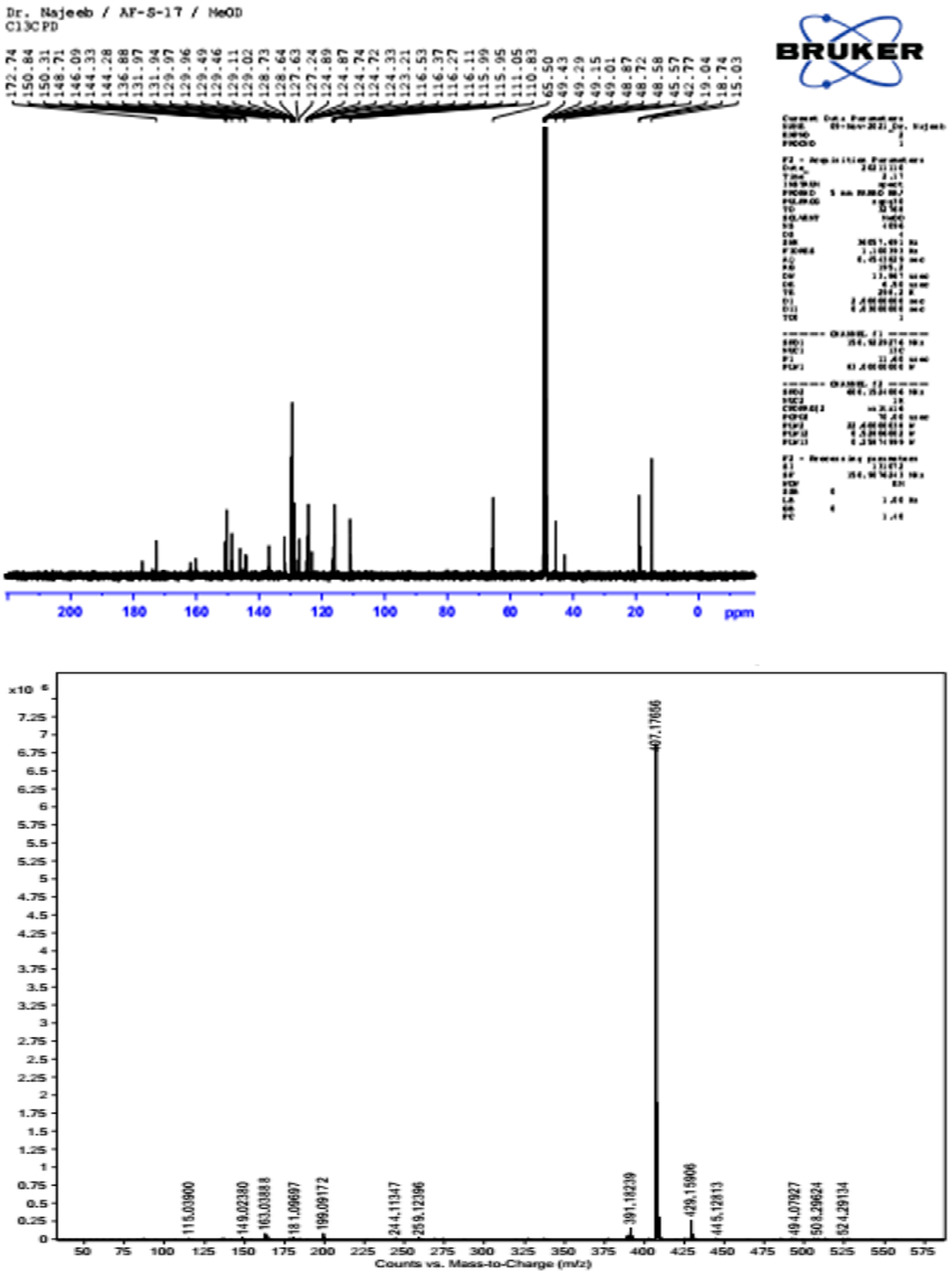
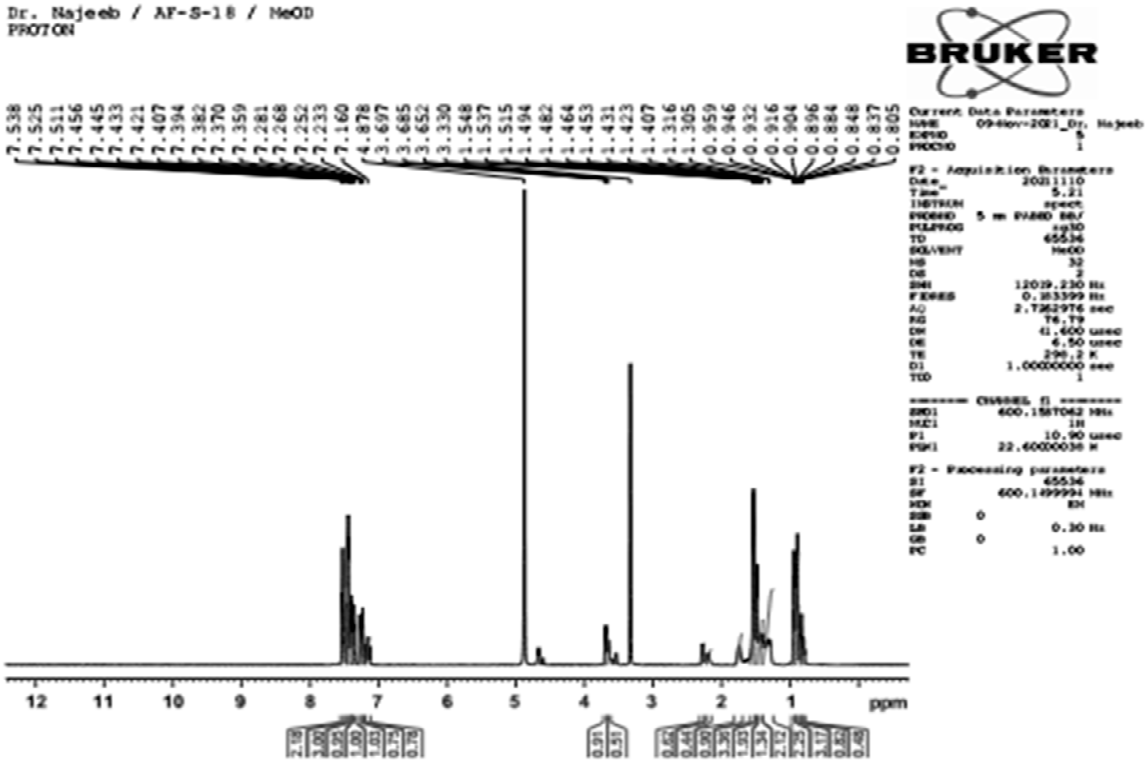


Figure S10: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4j**


Dr. Najeeb / AF-S-18 / MeOD
PROTON
BRUKER
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7.433
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7.394
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1.407
1.316
1.305
0.959
0.946
0.932
0.916
0.904
0.896
0.884
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7
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4
3
2
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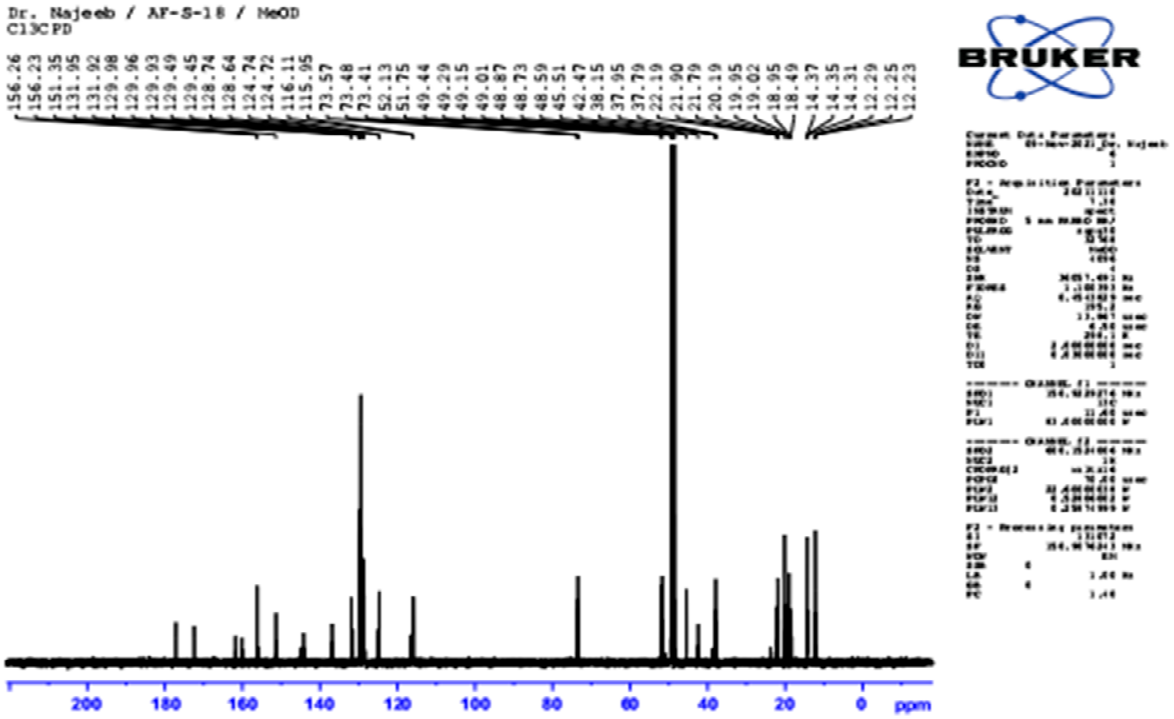
ppm


Dr. Najeeb / AF-S-18 / MeOD
C13CPD
BRUKER
156.26
156.23
151.35
151.95
131.92
129.98
129.96
129.93
129.49
129.45
128.74
128.64
124.74
124.72
116.11
115.95
73.57
73.48
73.41
52.13
51.75
49.44
49.29
49.15
49.01
48.87
48.73
48.59
48.51
42.47
38.15
37.95
37.79
22.19
21.90
21.79
20.19
19.95
19.02
18.95
18.49
14.37
14.35
14.31
12.29
12.25
12.23
200
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40
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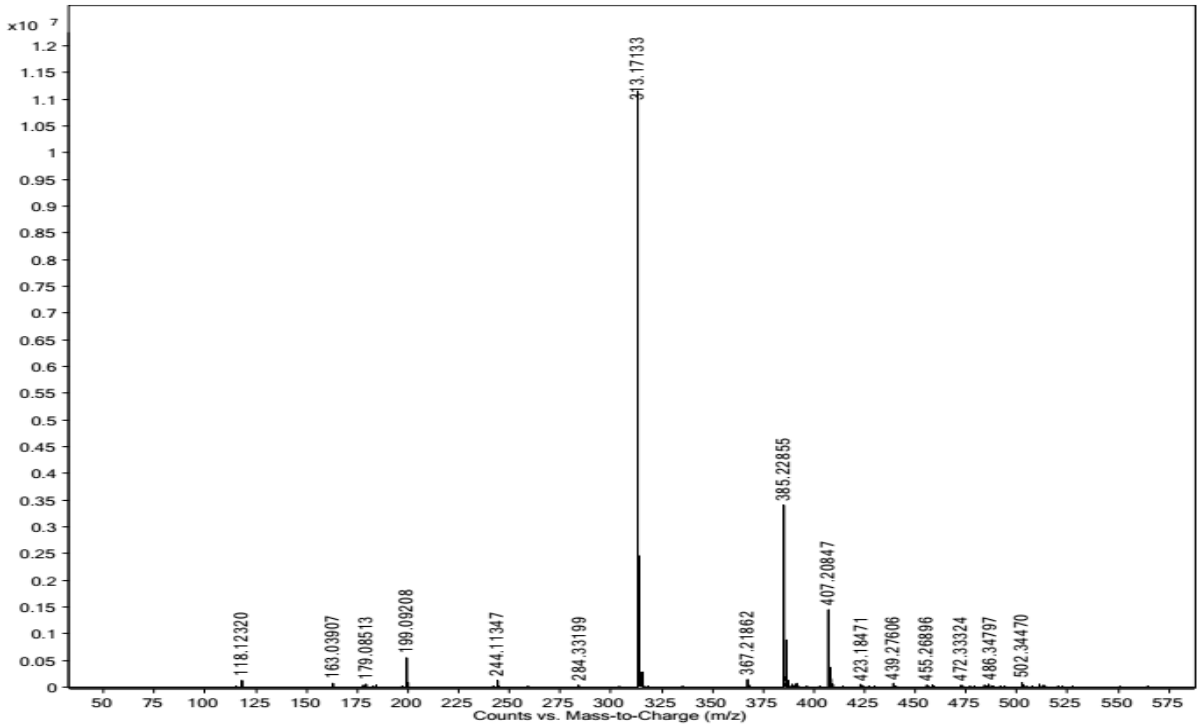
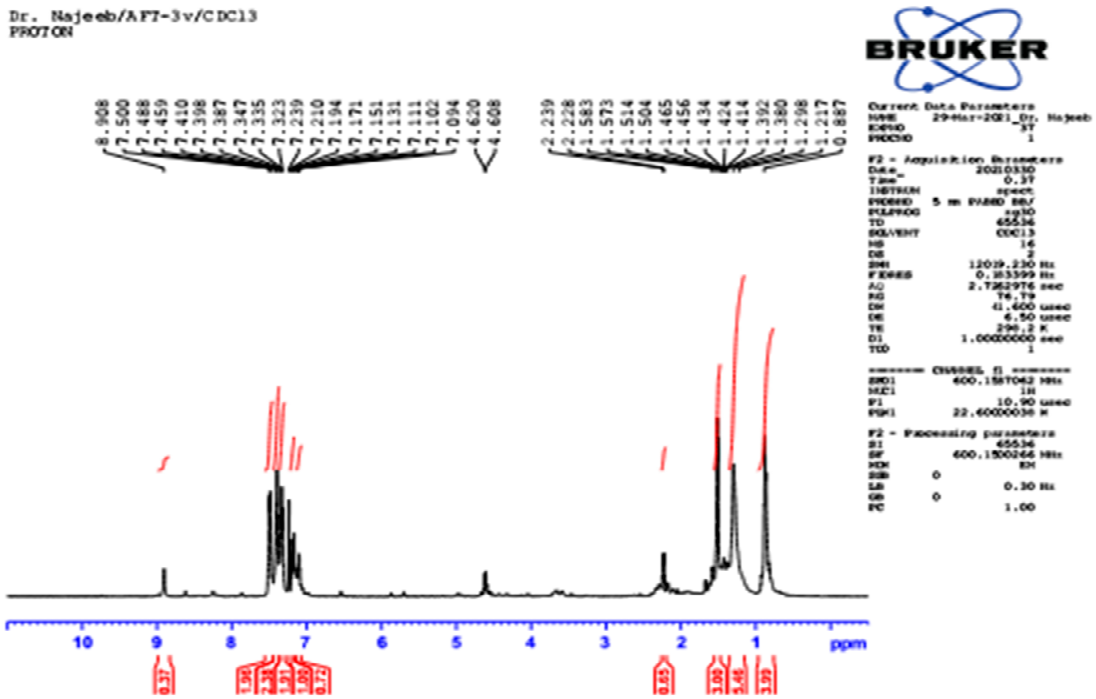


Figure S11: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4k**



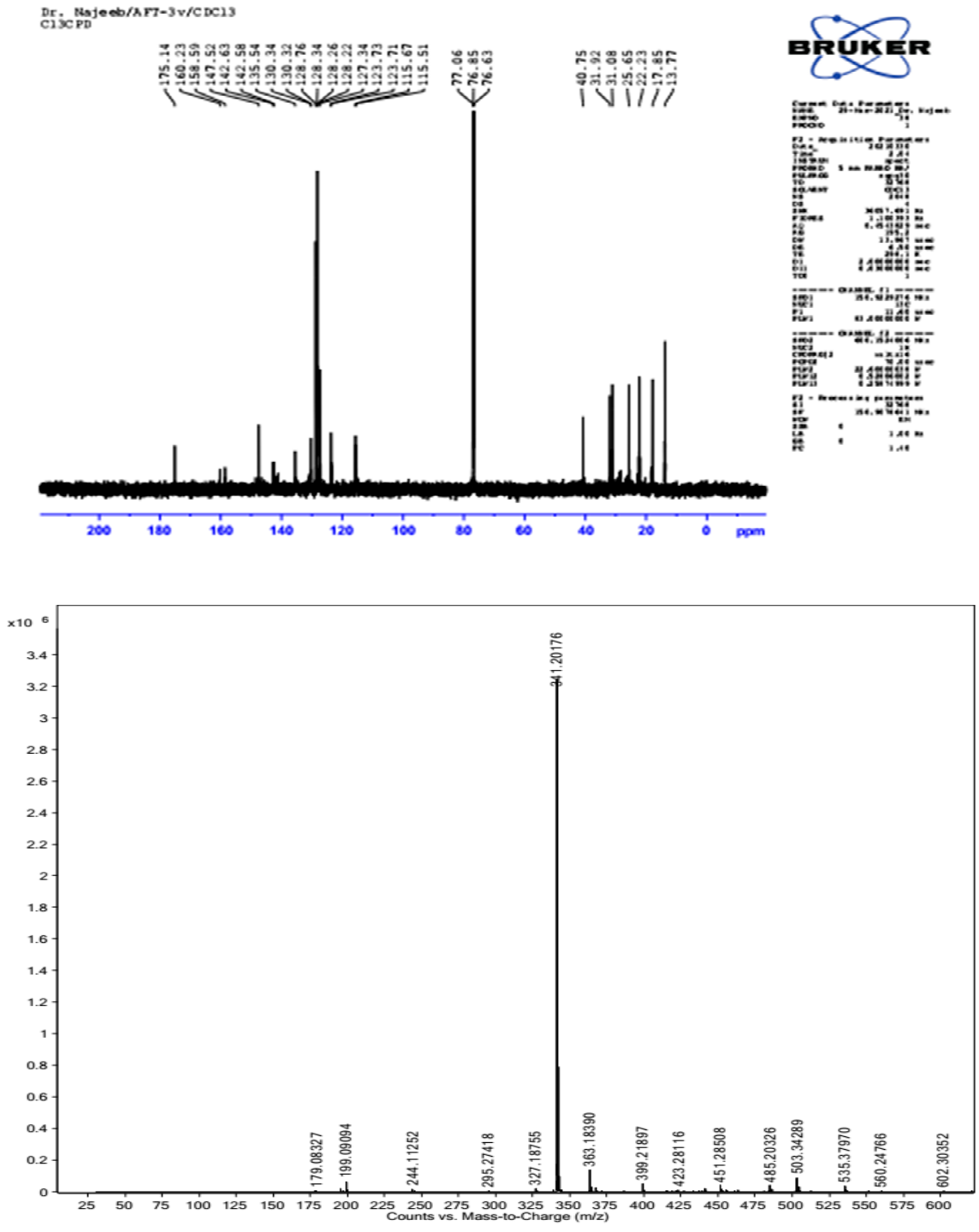
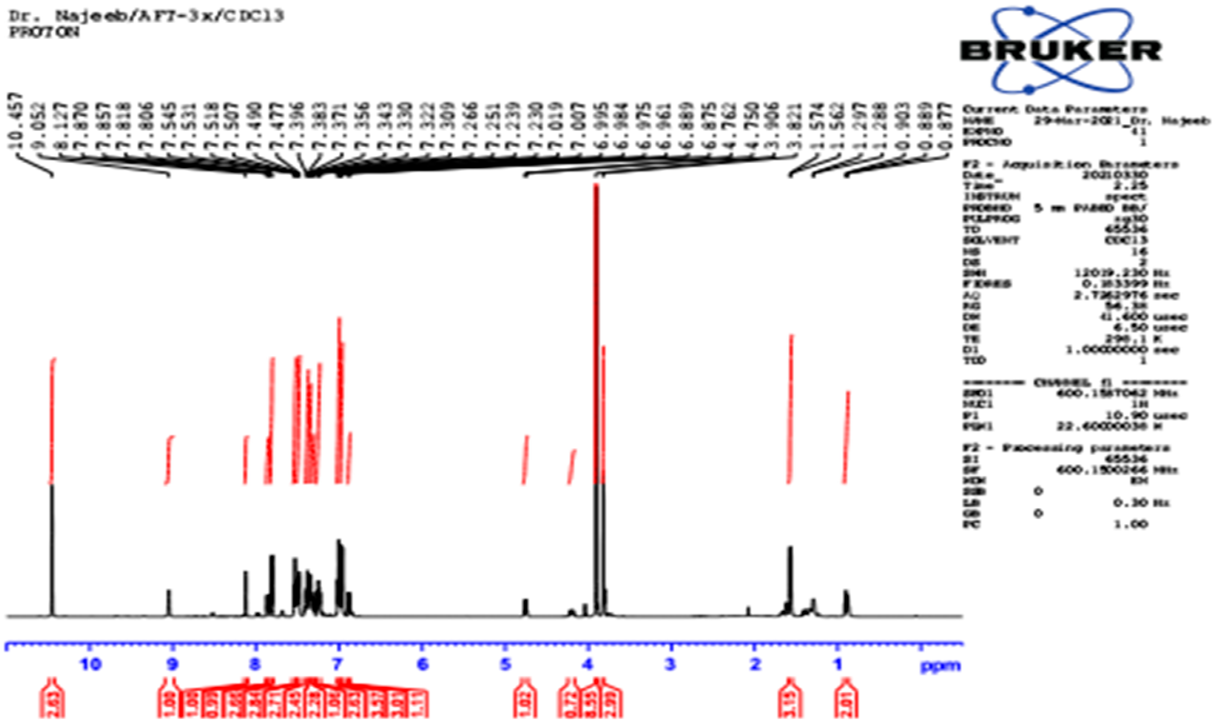
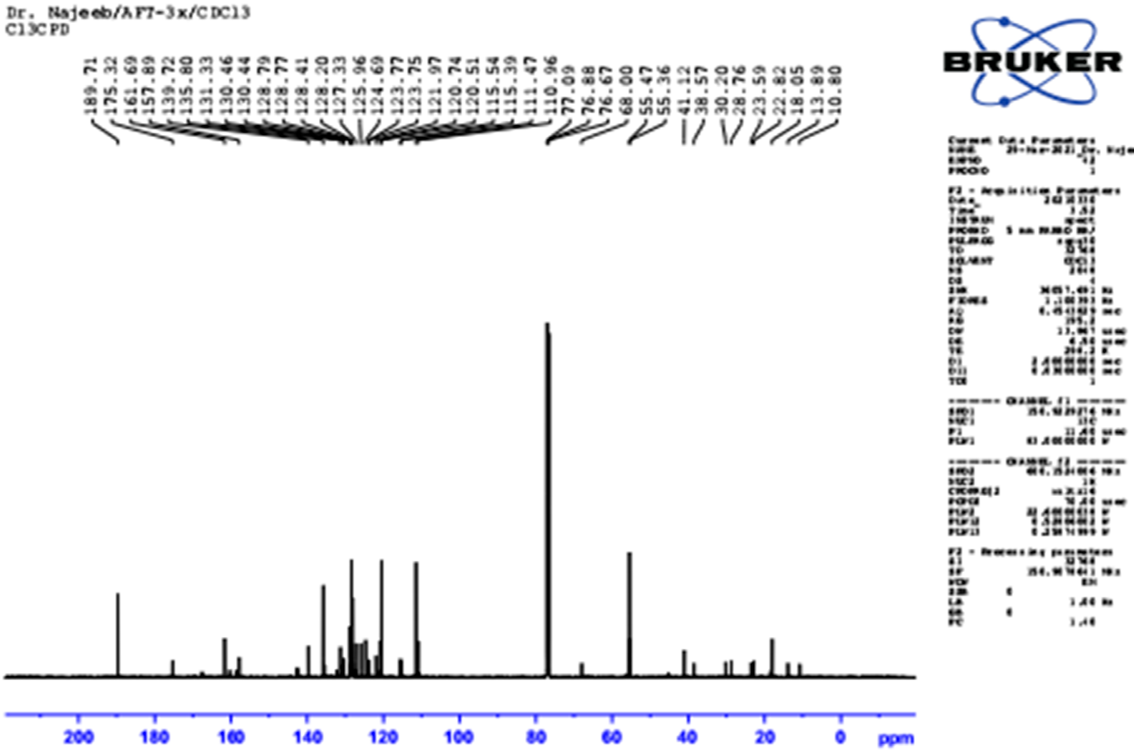


Figure S12: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4l**


Dr. Najeeb/AF7-3x/CDCl3
PROTON
BRUKER
10.457 9.052 8.127 7.870 7.857 7.818 7.806 7.545 7.531 7.518 7.507 7.490 7.477 7.396 7.383 7.371 7.356 7.343 7.330 7.322 7.309 7.266 7.251 7.239 7.230 7.019 7.007 6.995 6.984 6.975 6.961 6.889 6.875 4.762 4.750 3.906 3.821 1.574 1.562 1.297 1.288 0.903 0.889 0.877
10 9 8 7 6 5 4 3 2 1 ppm


Dr. Najeeb/AF7-3x/CDCl3
C13CPD
BRUKER
189.71 175.32 161.69 157.89 139.72 135.80 131.33 130.46 130.44 128.79 128.77 128.41 128.20 127.33 125.96 124.69 123.77 123.75 121.97 120.74 120.51 115.54 115.39 111.47 110.96 77.09 76.88 76.67 68.00 55.47 55.36 41.12 38.57 30.20 28.76 23.59 22.82 18.05 13.89 10.80
200 180 160 140 120 100 80 60 40 20 0 ppm

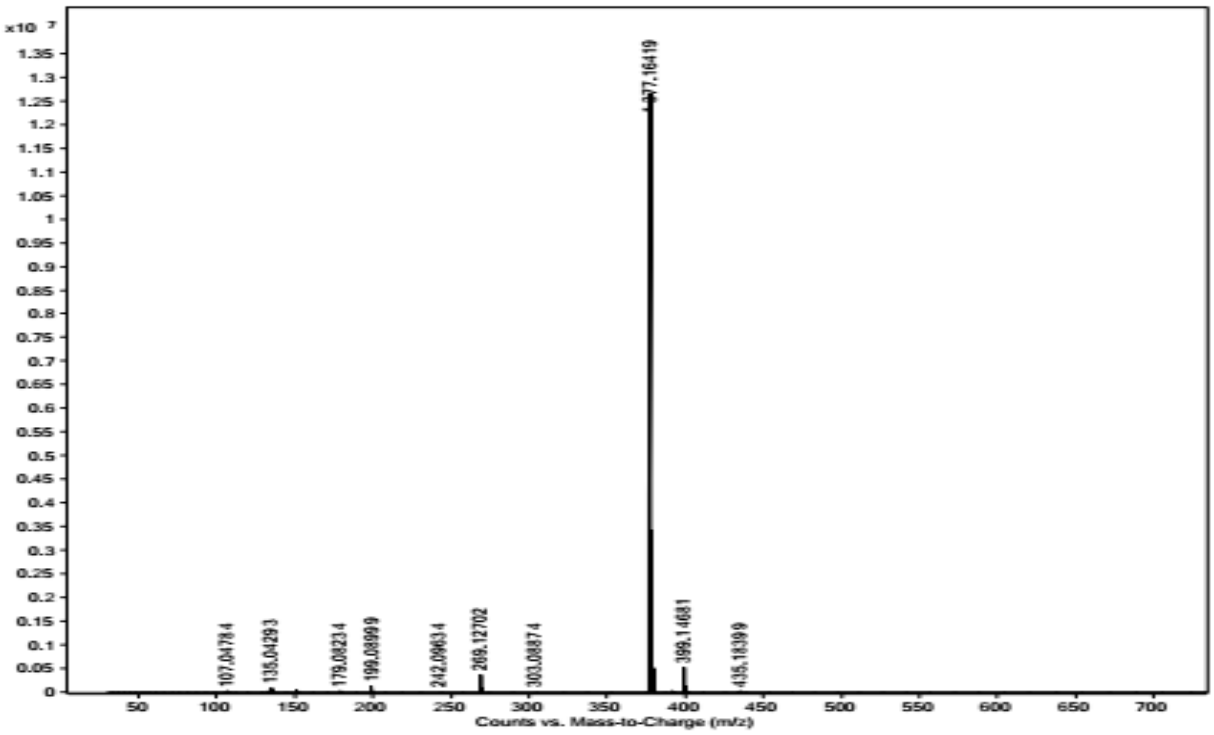
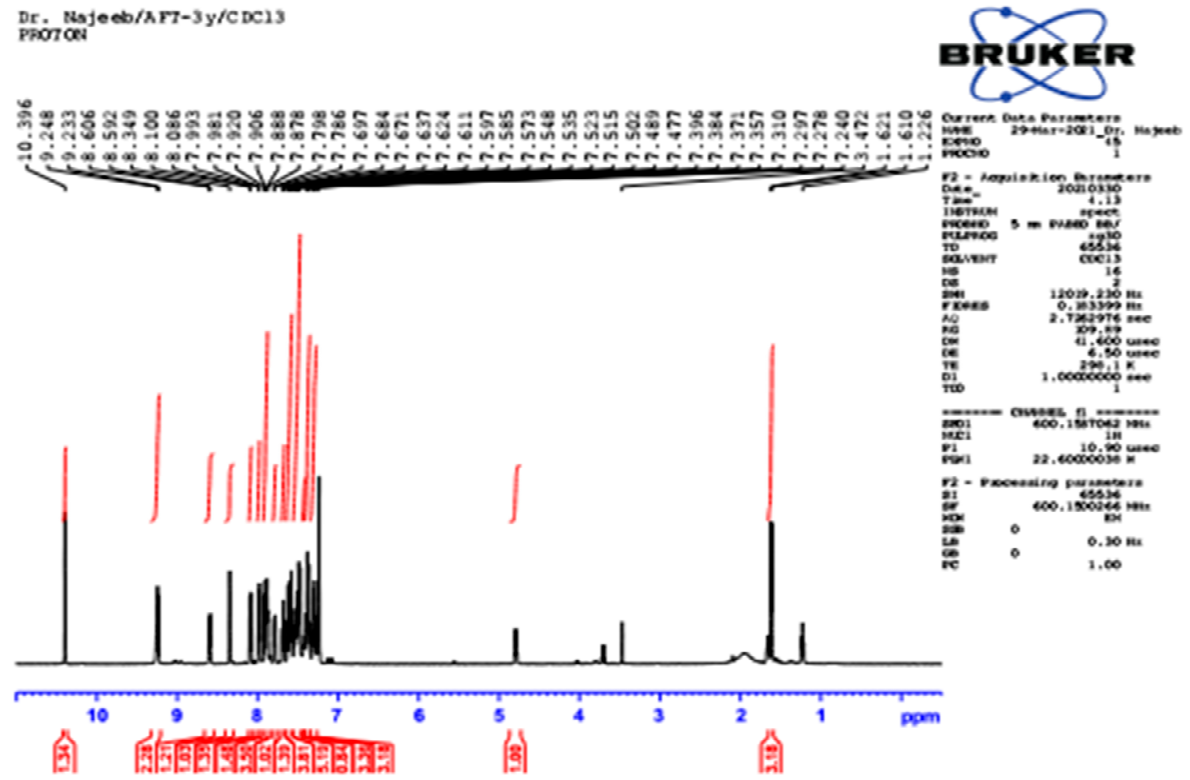


Figure S13: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4m**



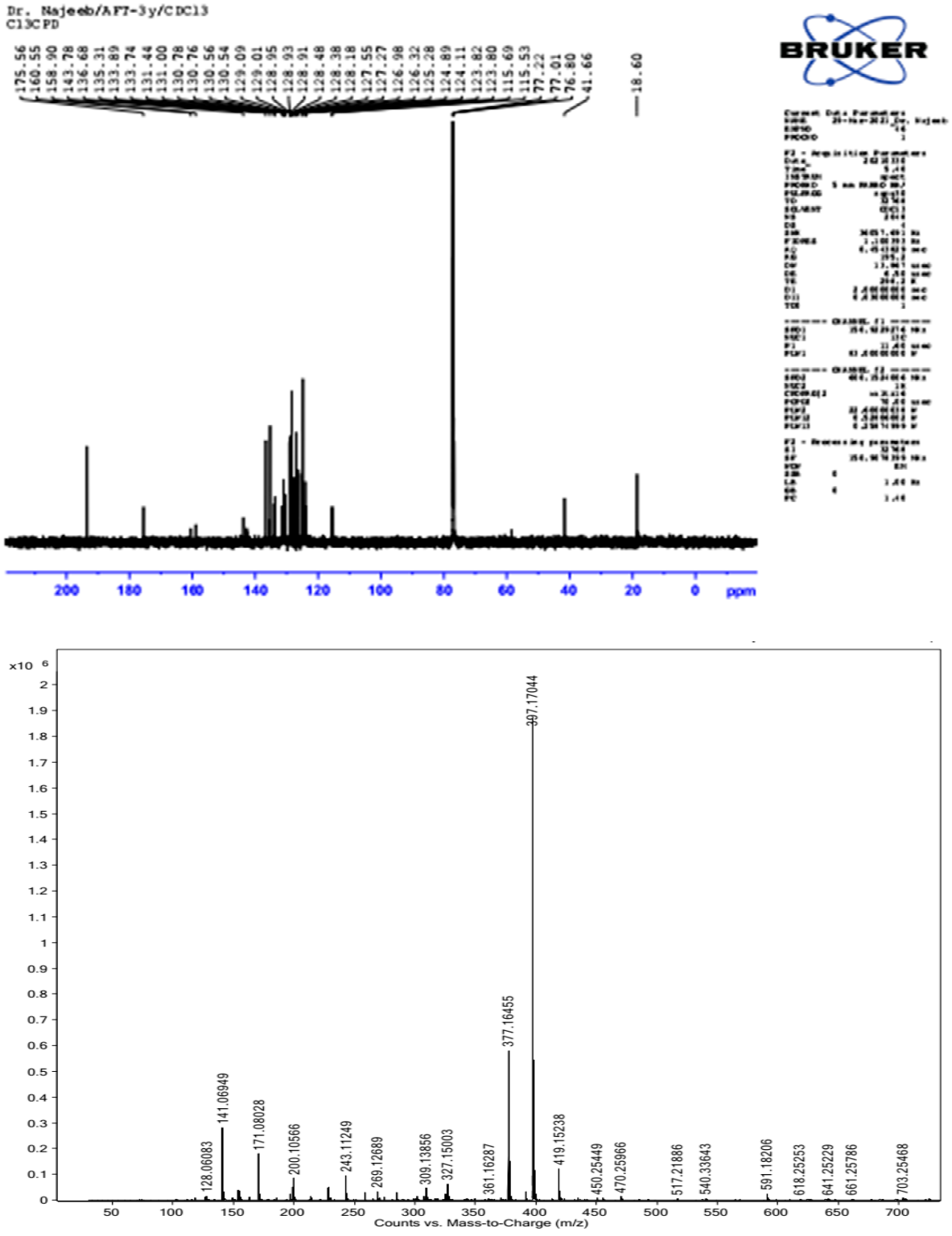
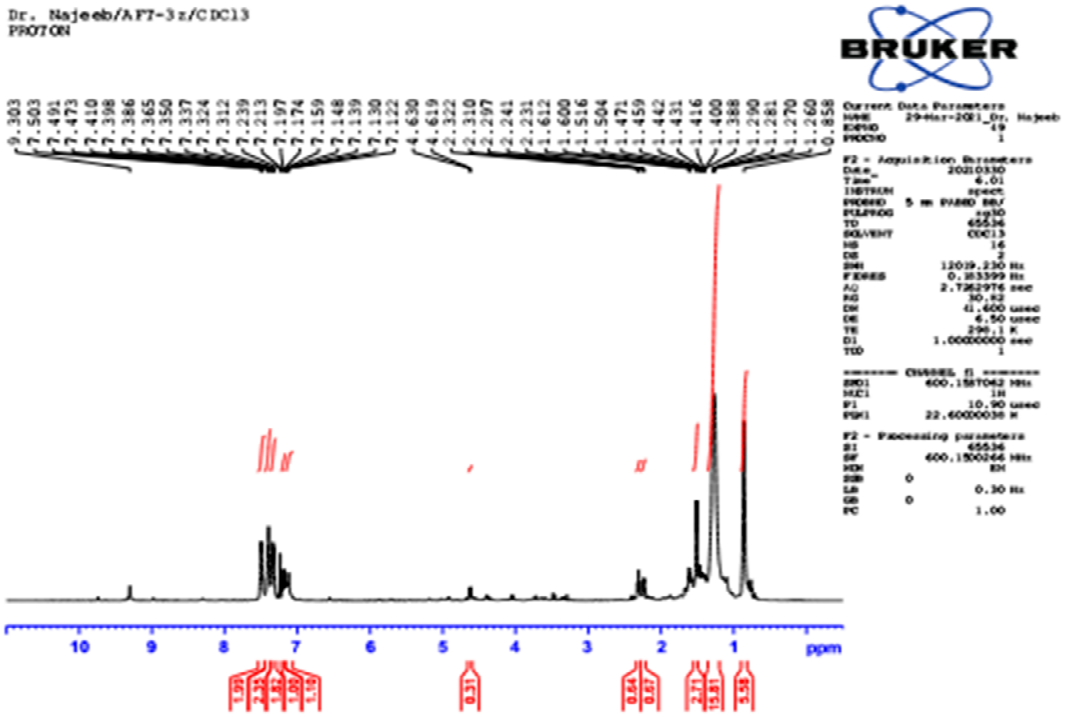


Figure S14: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4n**


Dr. Najeeb/AF7-3z/CDCl3
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BRUKER
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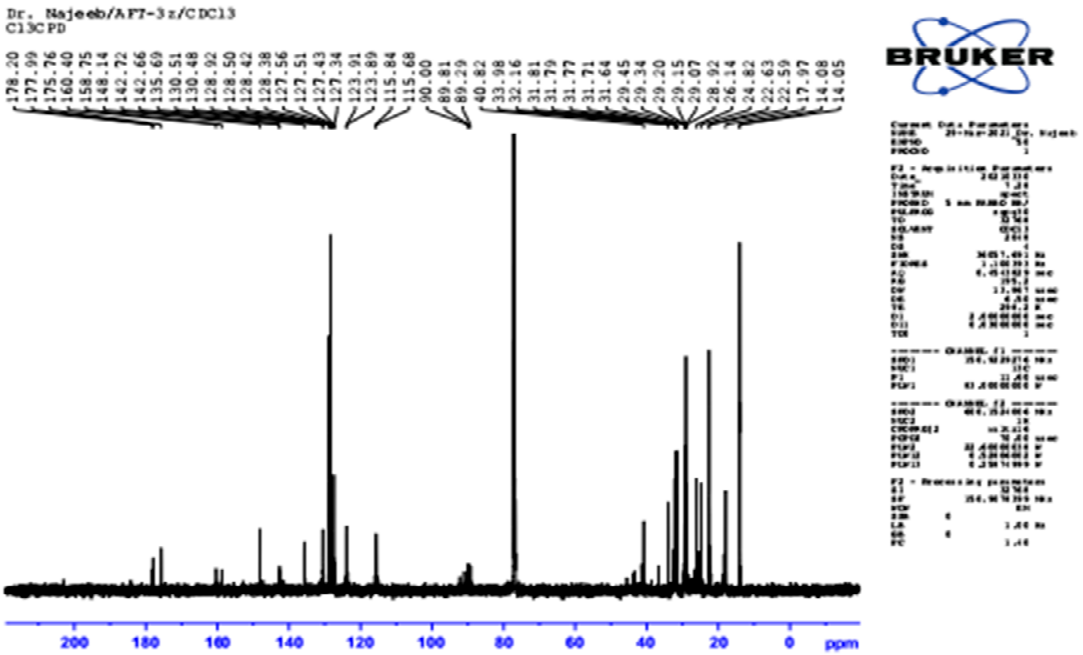
7.473
7.410
7.398
7.386
7.365
7.350
7.337
7.324
7.312
7.239
7.213
7.197
7.174
7.159
7.148
7.139
7.130
7.122
4.630
4.619
2.322
2.310
2.297
2.241
2.231
1.612
1.600
1.516
1.504
1.471
1.459
1.442
1.431
1.416
1.400
1.388
1.290
1.281
1.270
1.260
0.858
10
9
8
7
6
5
4
3
2
1
ppm


Dr. Najeeb/AF7-3z/CDCl3
C13CPD
BRUKER
178.20
177.99
175.76
160.40
158.75
148.14
142.72
142.66
135.69
130.51
130.48
128.92
128.50
128.42
128.38
127.56
127.51
127.43
127.34
123.91
123.89
115.84
115.68
90.00
89.81
89.29
40.82
33.98
32.16
31.81
31.79
31.77
31.71
31.64
29.45
29.34
29.20
29.15
29.07
28.92
26.14
24.82
22.63
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14.08
14.05
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120
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0
ppm

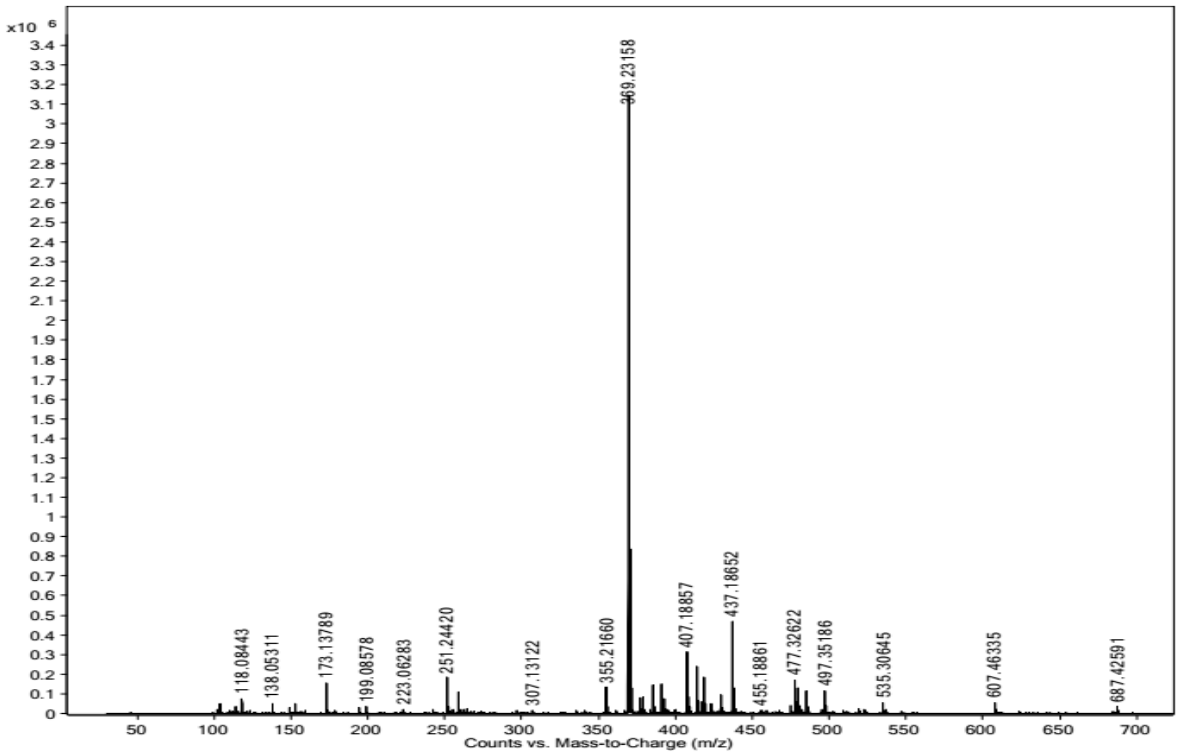
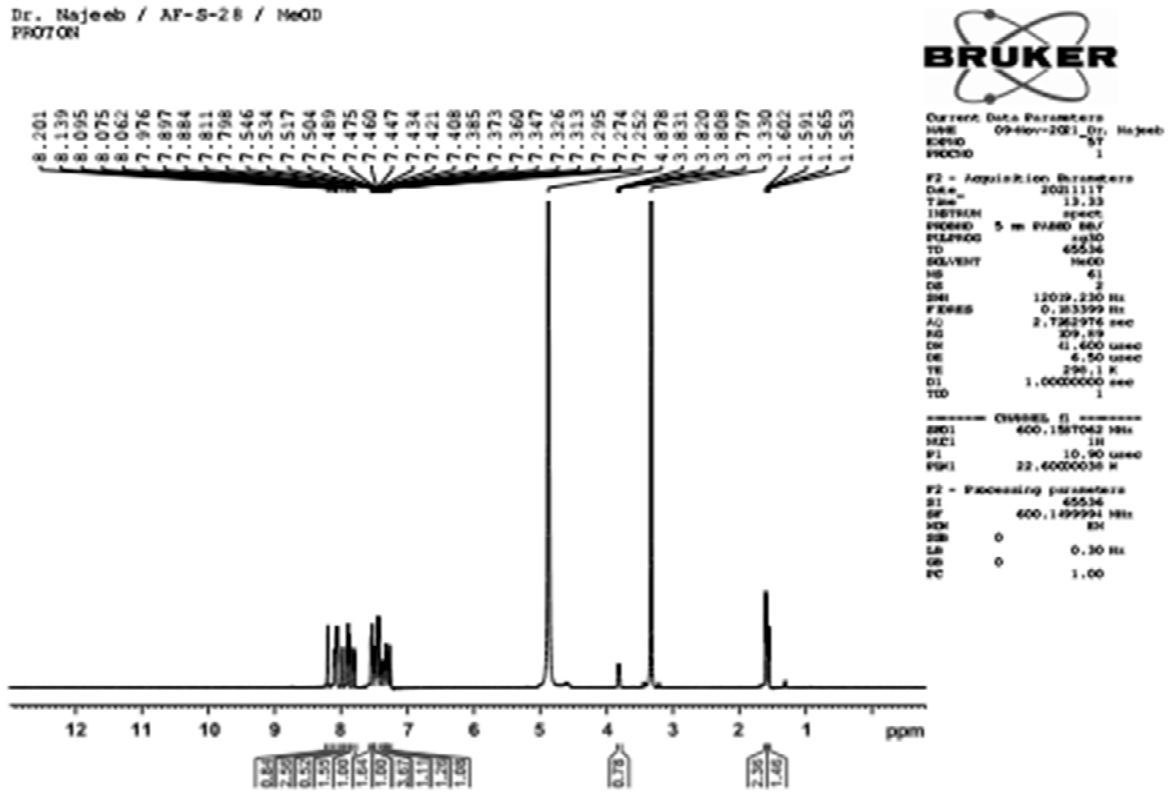


Figure S15: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4o**



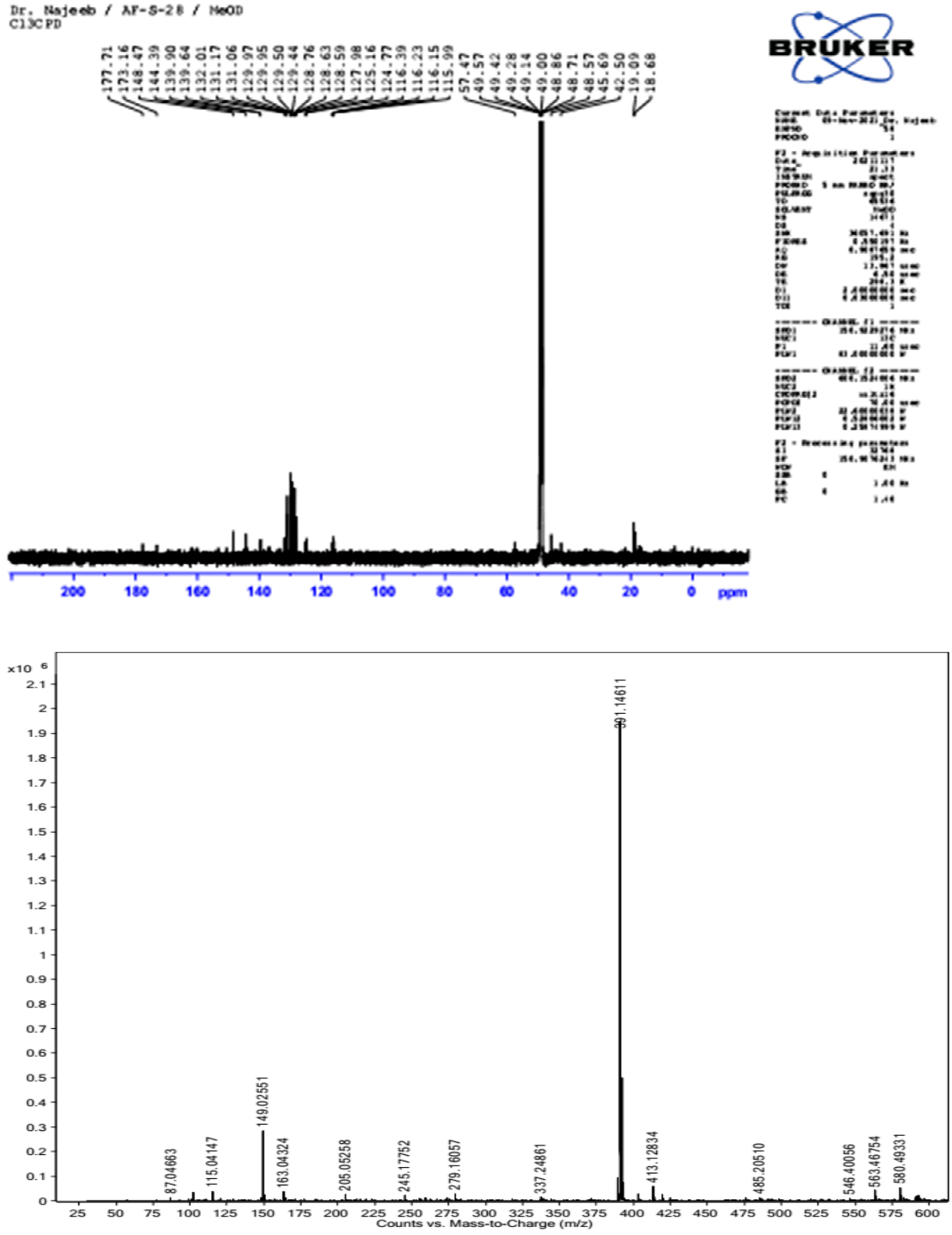
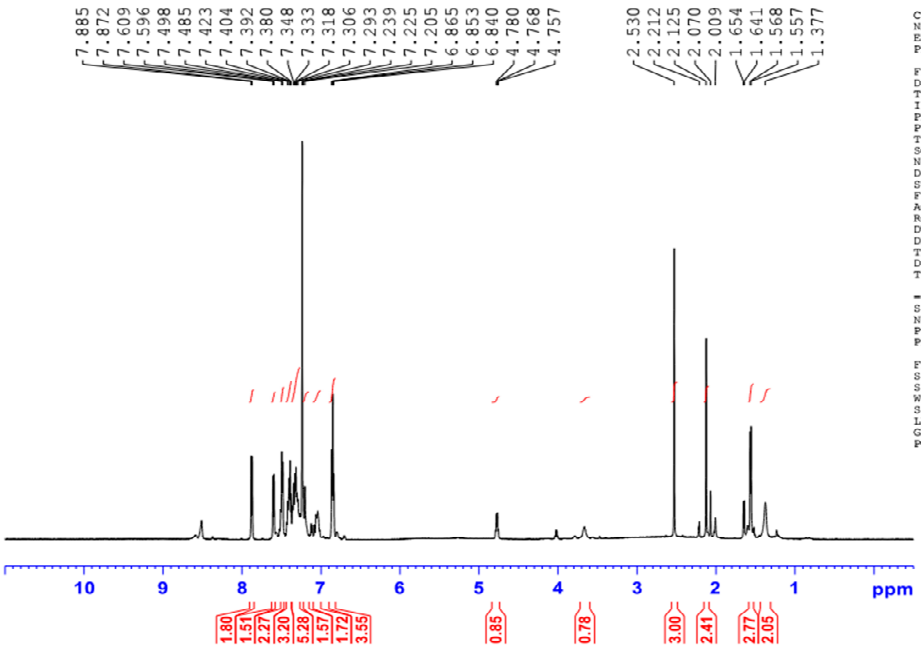


Figure S16: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **4p**

Dr. Najeeb/AF-K-I/CDCl3
PROTON



BRUKER

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PROCNO                   1

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TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH              12019.230 Hz
FIDRES               0.183399 Hz
AQ                2.7262976 sec
RG                   122.04
DW                  41.600 usec
DE                   6.50 usec
TE                  298.2 K
D1                1.00000000 sec
TD0                      1

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NUC1                     1H
P1                   10.90 usec
PLW1            22.60000038 W

F2 - Processing parameters
SI                   65536
SF               600.1500266 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
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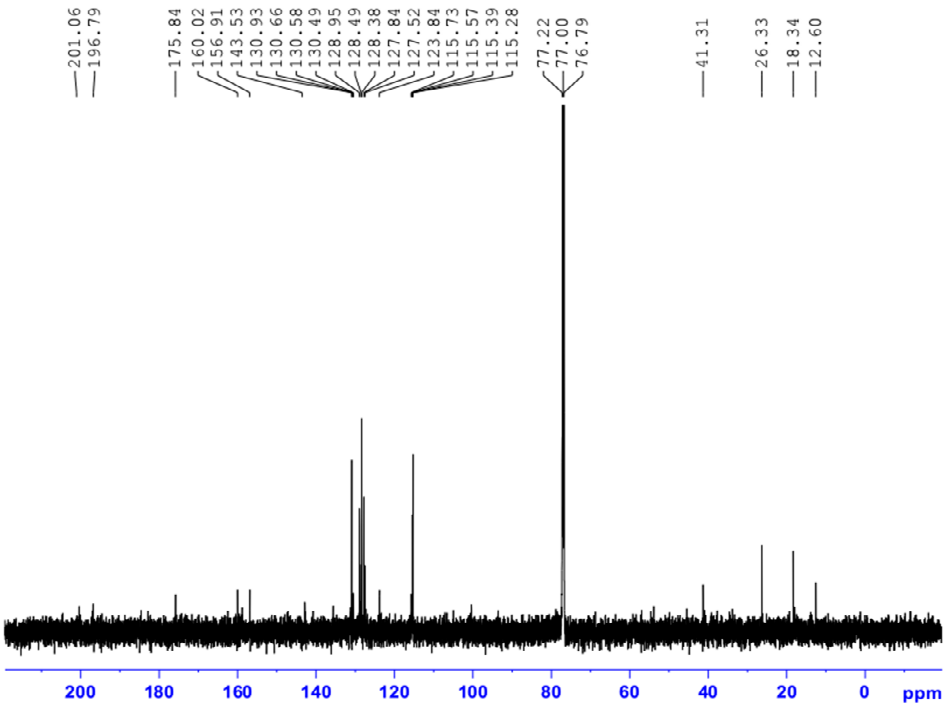
Dr. Najeeb/AF-K-I/CDCl3
C13CPD



BRUKER

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PROCNO                   1

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PULPROG             zgpg30
TD                   32768
SOLVENT              CDCl3
NS                    2048
DS                       4
SWH              36057.691 Hz
FIDRES               1.100393 Hz
AQ                0.4543829 sec
RG                   195.2
DW                  13.867 usec
DE                   6.50 usec
TE                  298.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1             150.9229276 MHz
NUC1                    13C
P1                   11.60 usec
PLW1            83.00000000 W

======== CHANNEL f2 ========
SFO2             600.1524006 MHz
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                70.00 usec
PLW2            22.60000038 W
PLW12            0.52806002 W
PLW13            0.25874999 W

F2 - Processing parameters
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SF               150.9078399 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
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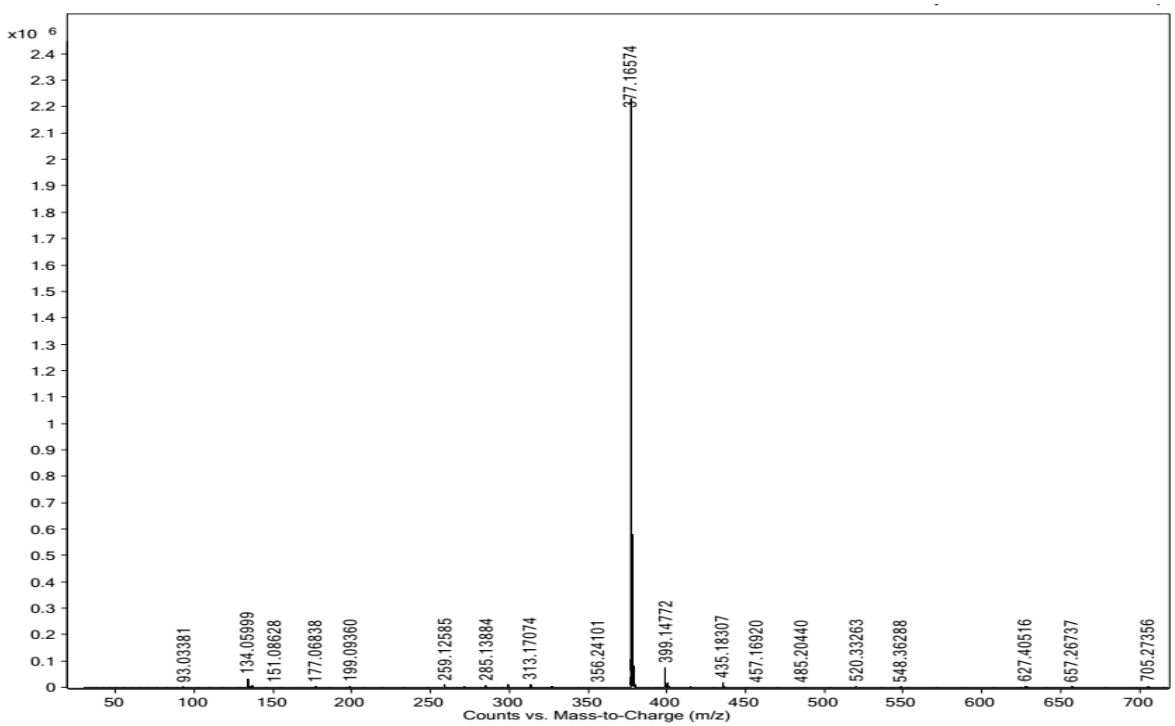
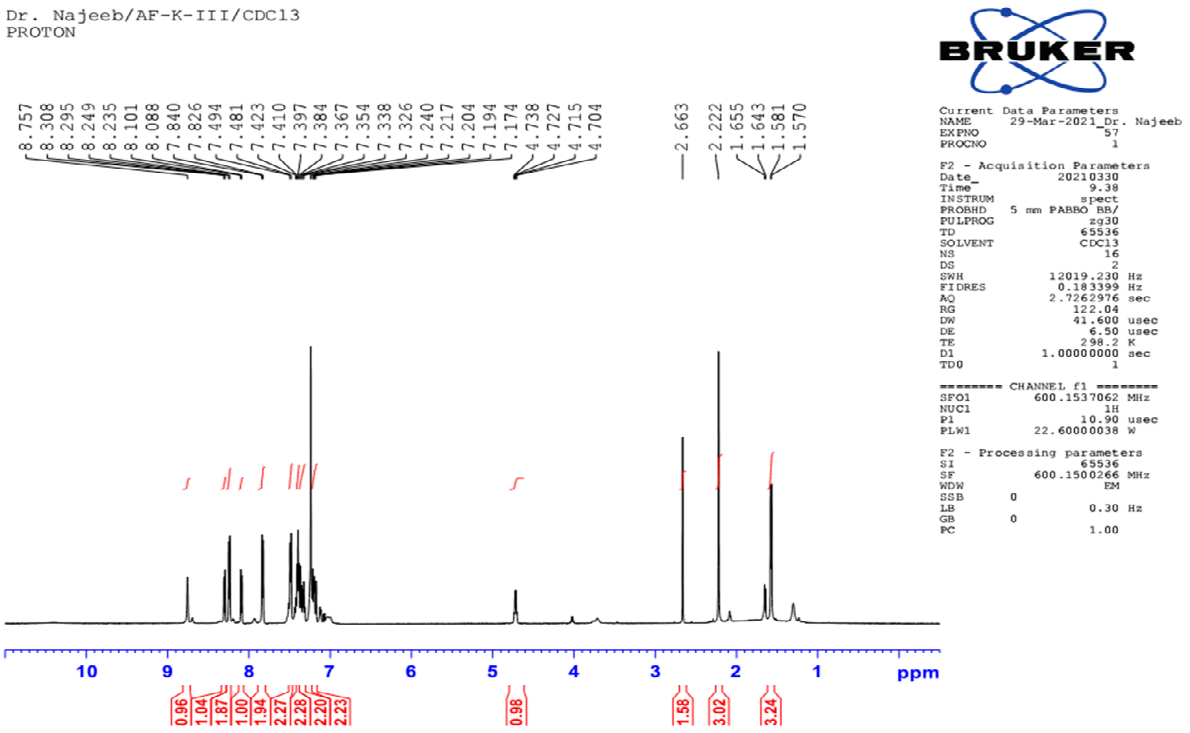


Figure S17. ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5a**



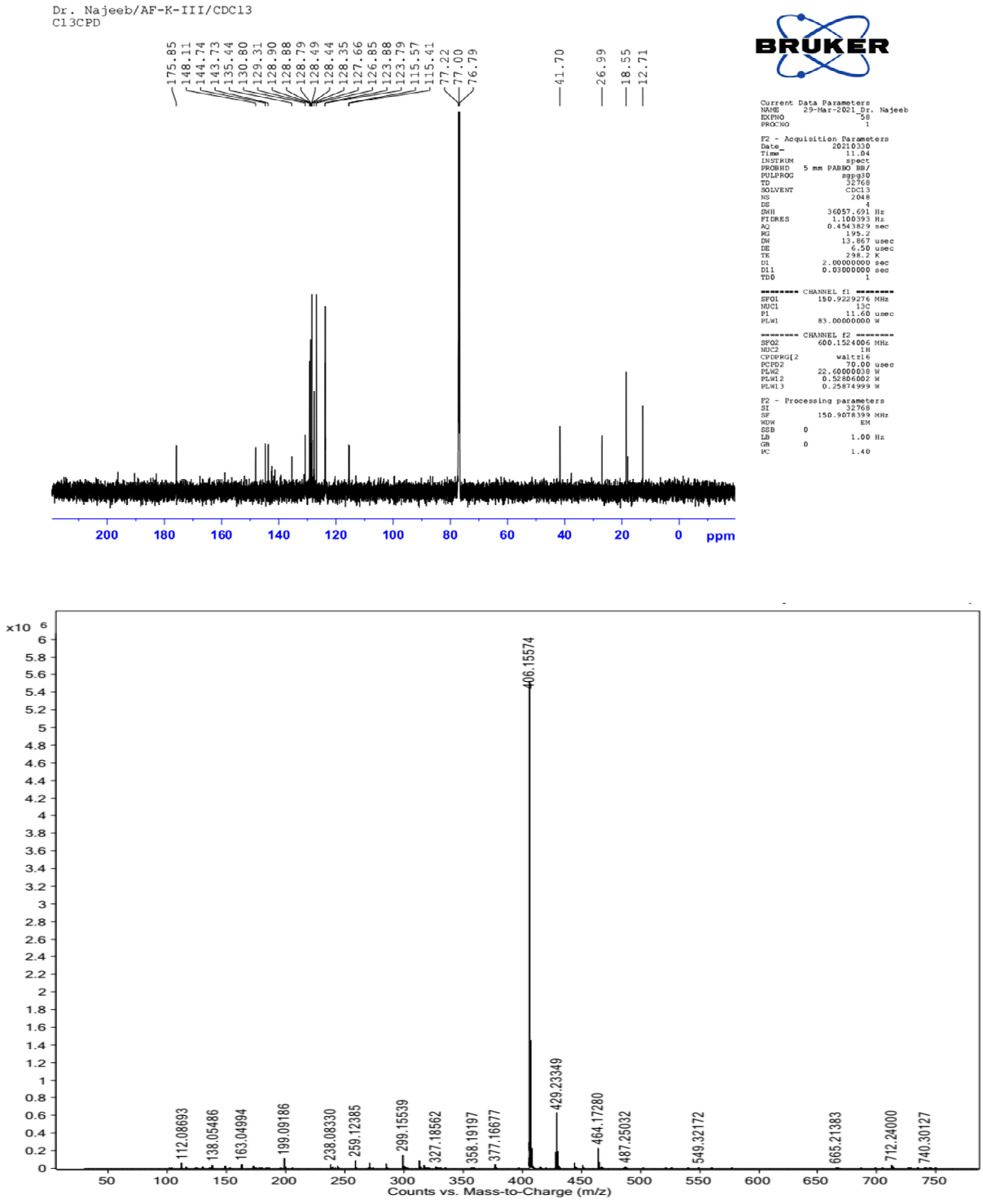
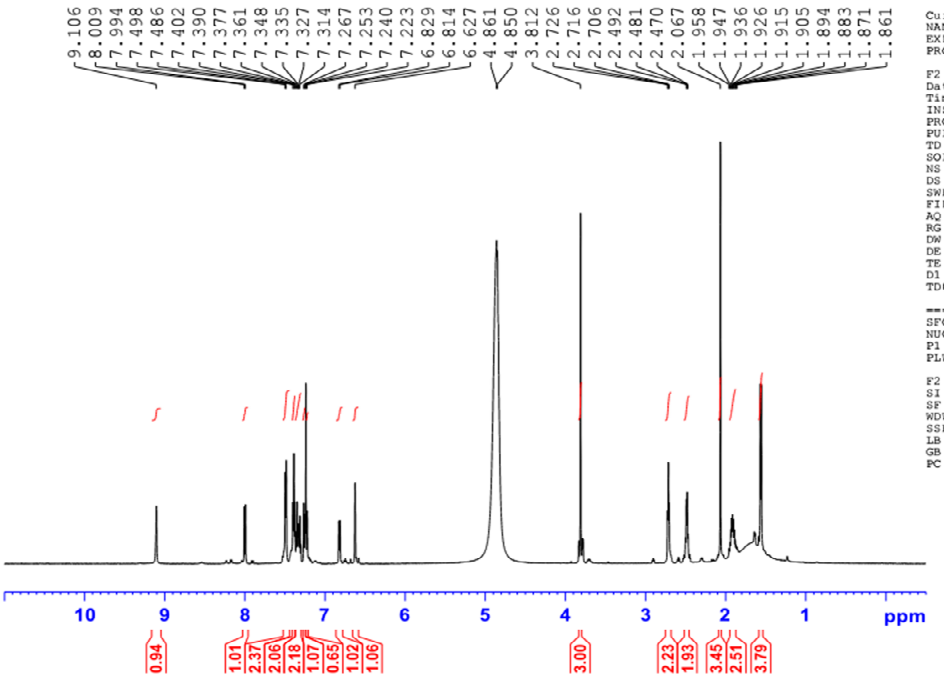


Figure S18: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5b**

Dr. Najeeb/AF-K-IV/CDCl3
PROTON

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EXPNO                      61
PROCNO                      1

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PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 12019.230 Hz
FIDRES                0.183399 Hz
AQ                    2.7262976 sec
RG                        76.79
DW                       41.600 usec
DE                        6.50 usec
TE                      298.1 K
D1                  1.00000000 sec
TD0                         1

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SFO1                600.1537062 MHz
NUC1                        1H
P1                       10.90 usec
PLW1                22.60000038 W

F2 - Processing parameters
SI                         65536
SF                  600.1500266 MHz
WDW                           EM
SSB          0
LB                        0.30 Hz
GB           0
PC                        1.00
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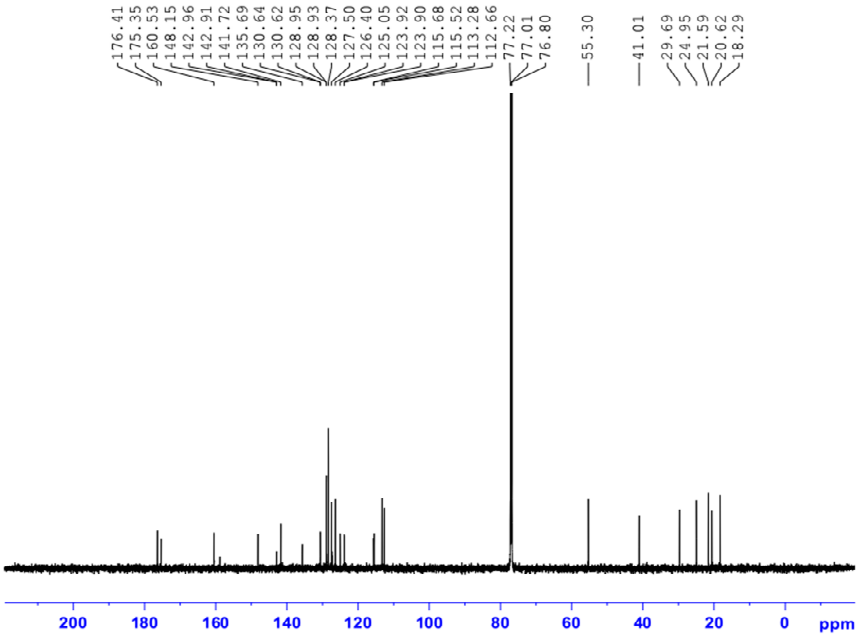
Dr. Najeeb/AF-K-IV/CDCl3
C13CPD

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PROCNO                      1

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PULPROG                 zgpg30
TD                     32768
SOLVENT                CDCl3
NS                      2048
DS                         4
SWH                 36057.691 Hz
FIDRES                1.100393 Hz
AQ                    0.4543829 sec
RG                        195.2
DW                       13.867 usec
DE                        6.50 usec
TE                      298.1 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
SFO1                150.9229276 MHz
NUC1                        13C
P1                       11.60 usec
PLW1                83.00000000 W

======== CHANNEL f2 ========
SFO2                600.1524006 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                    70.00 usec
PLW2                22.60000038 W
PLW12               0.52806002 W
PLW13               0.25874999 W

F2 - Processing parameters
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SF                  150.9078399 MHz
WDW                           EM
SSB          0
LB                        1.00 Hz
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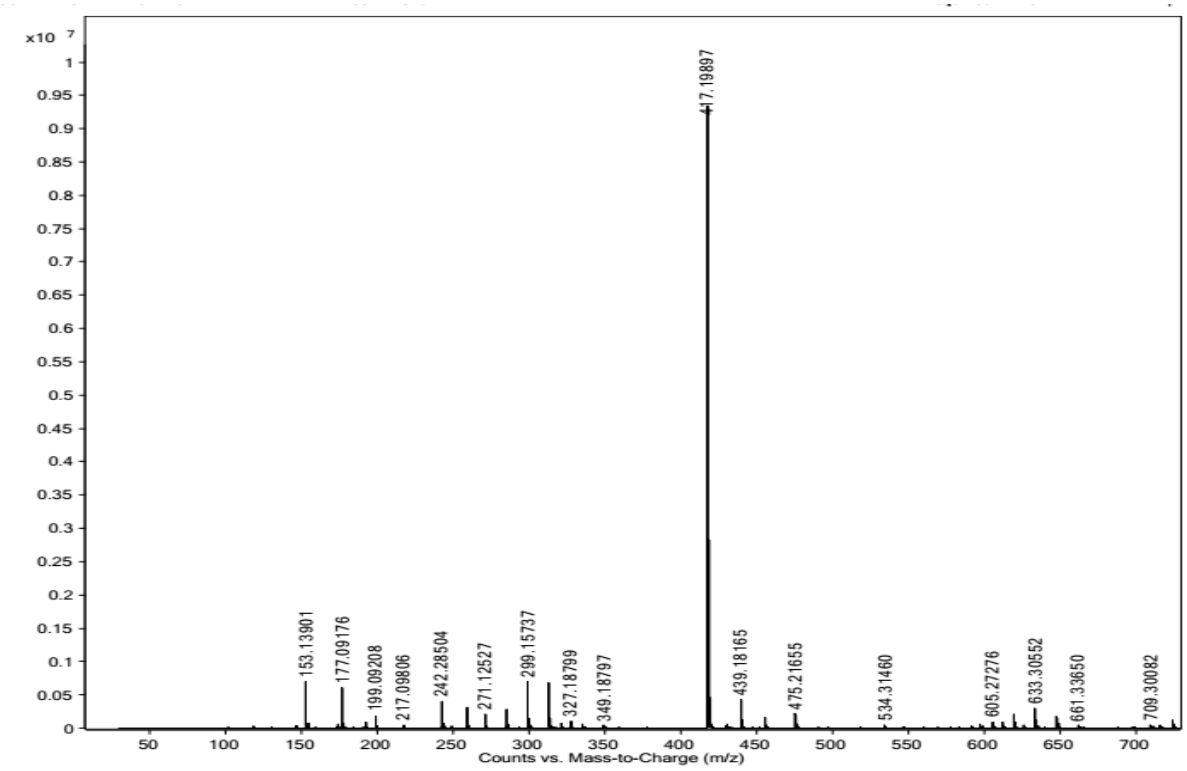
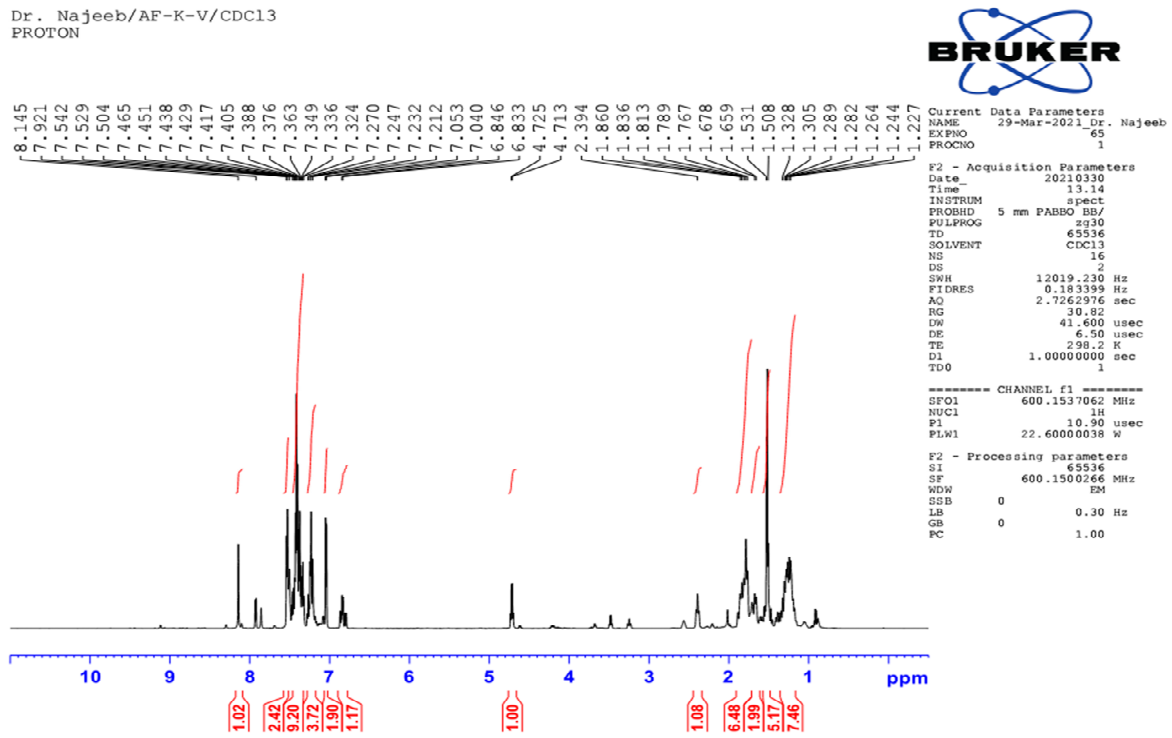


Figure S19: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5c**



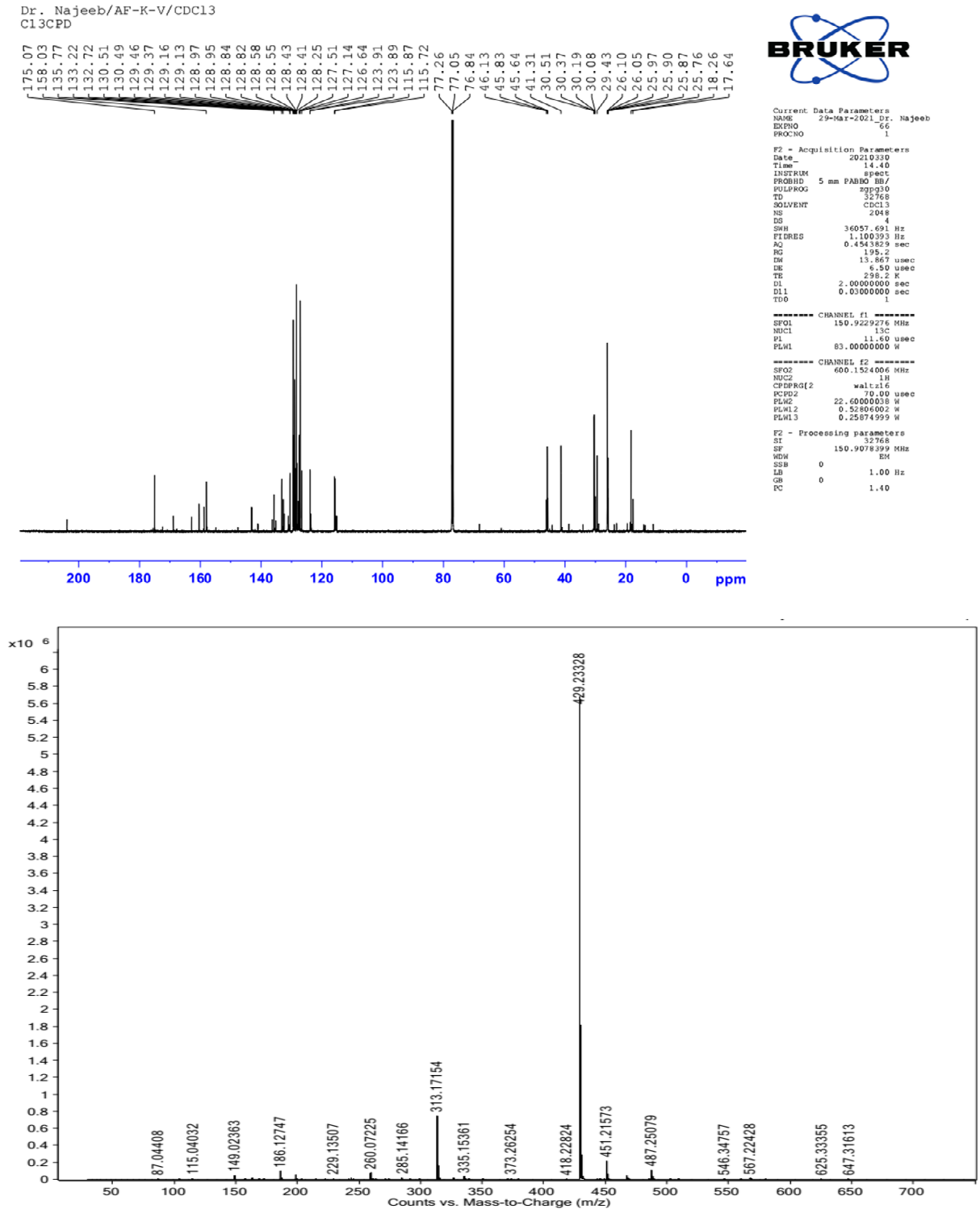
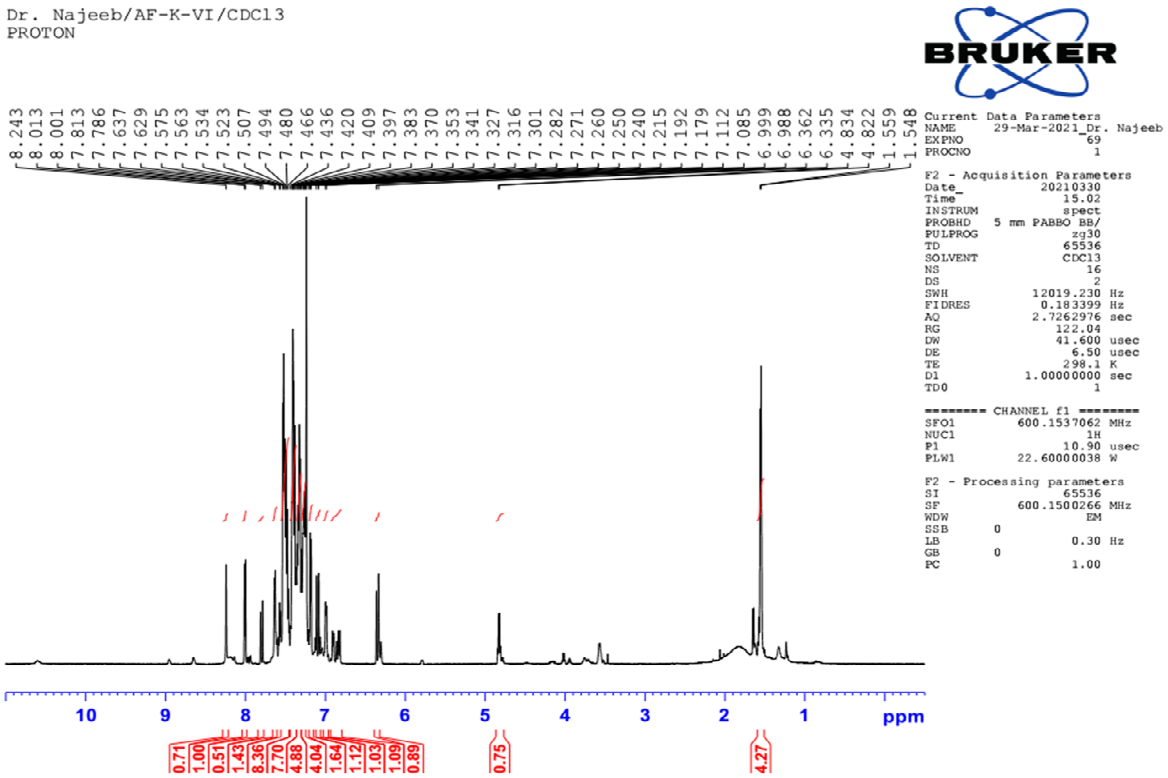


Figure S20: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5d**


Dr. Najeeb/AF-K-VI/CDCl3
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7.629
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7.563
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7.523
7.507
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7.480
7.466
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7.409
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7.383
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7.240
7.215
7.192
7.179
7.112
7.085
6.999
6.988
6.362
6.335
4.834
4.822
1.559
1.548
10
9
8
7
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5
4
3
2
1
ppm
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0.51
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7.70
4.88
4.04
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1.12
1.03
1.09
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0.75
4.27
BRUKER
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RG 122.04
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
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NUC1 1H
P1 10.90 usec
PLW1 22.60000038 W
F2 - Processing parameters
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SSB 0
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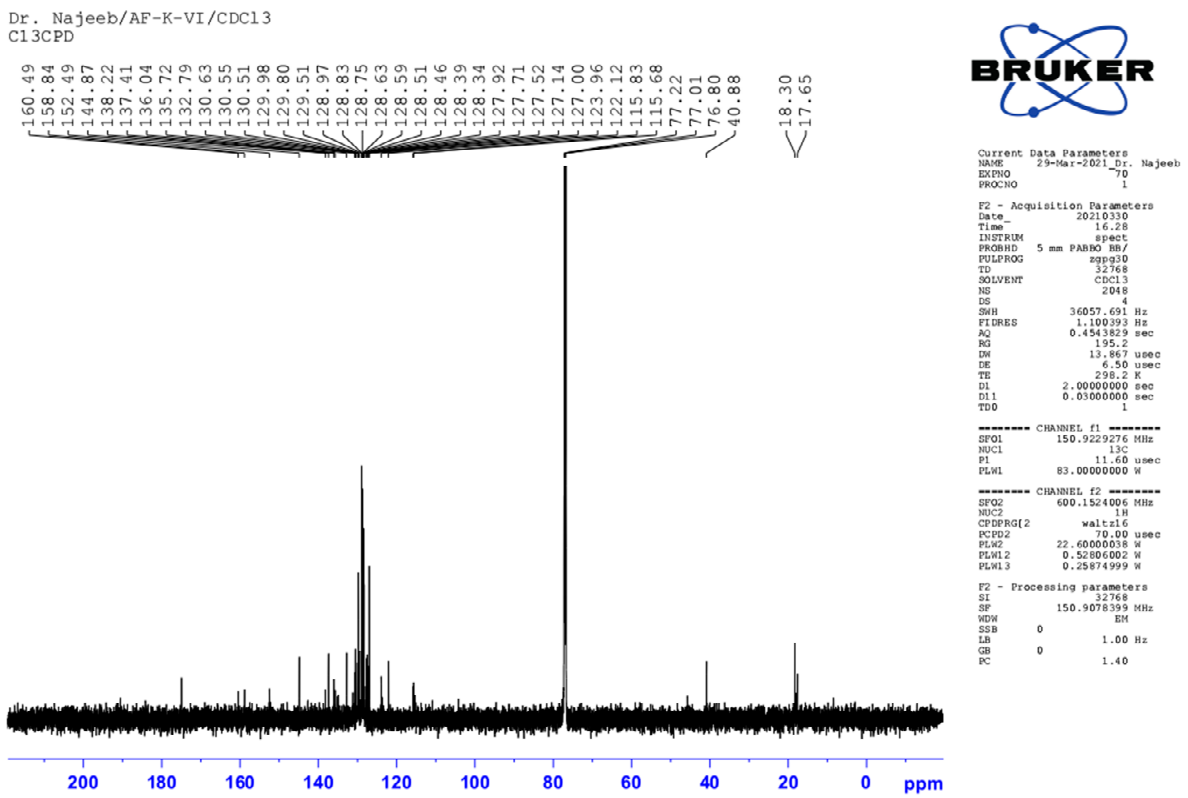
GB 0
PC 1.00


Dr. Najeeb/AF-K-VI/CDCl3
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120
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ppm
BRUKER
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EXPNO 70
PROCNO 1
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
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SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DW 13.867 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W
======== CHANNEL f2 ========
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.52806002 W
PLW13 0.25874999 W
F2 - Processing parameters
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SF 150.9078399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

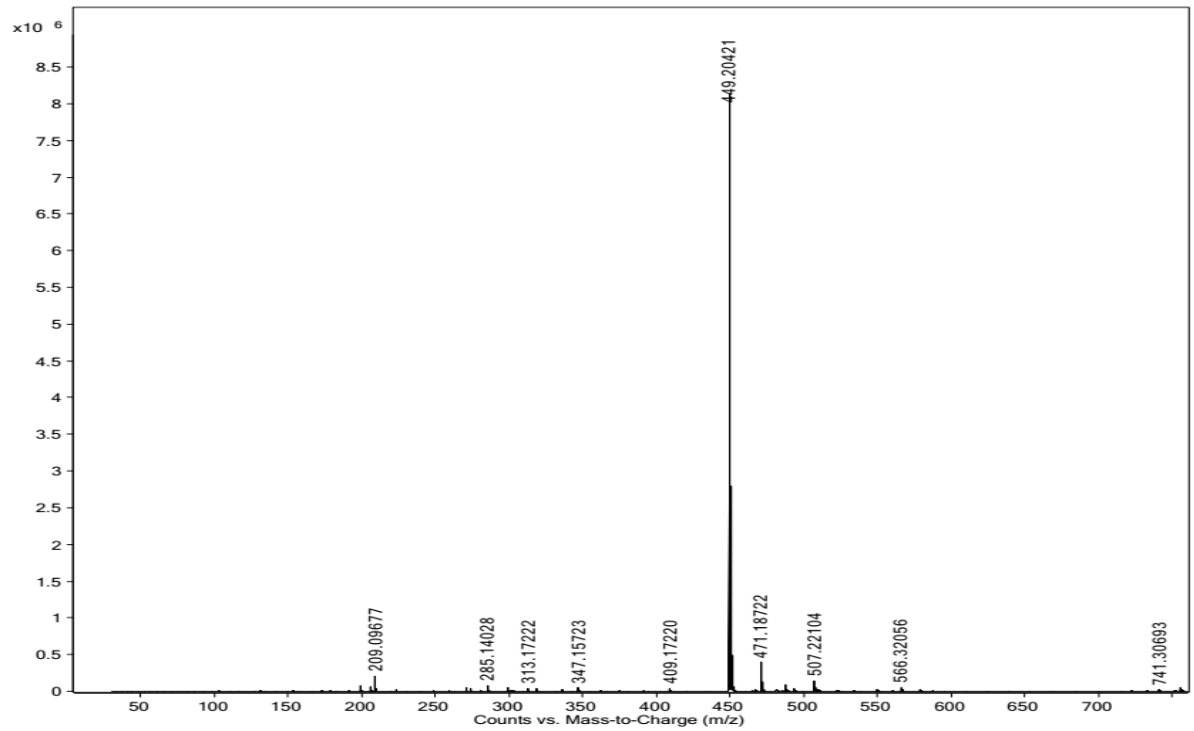
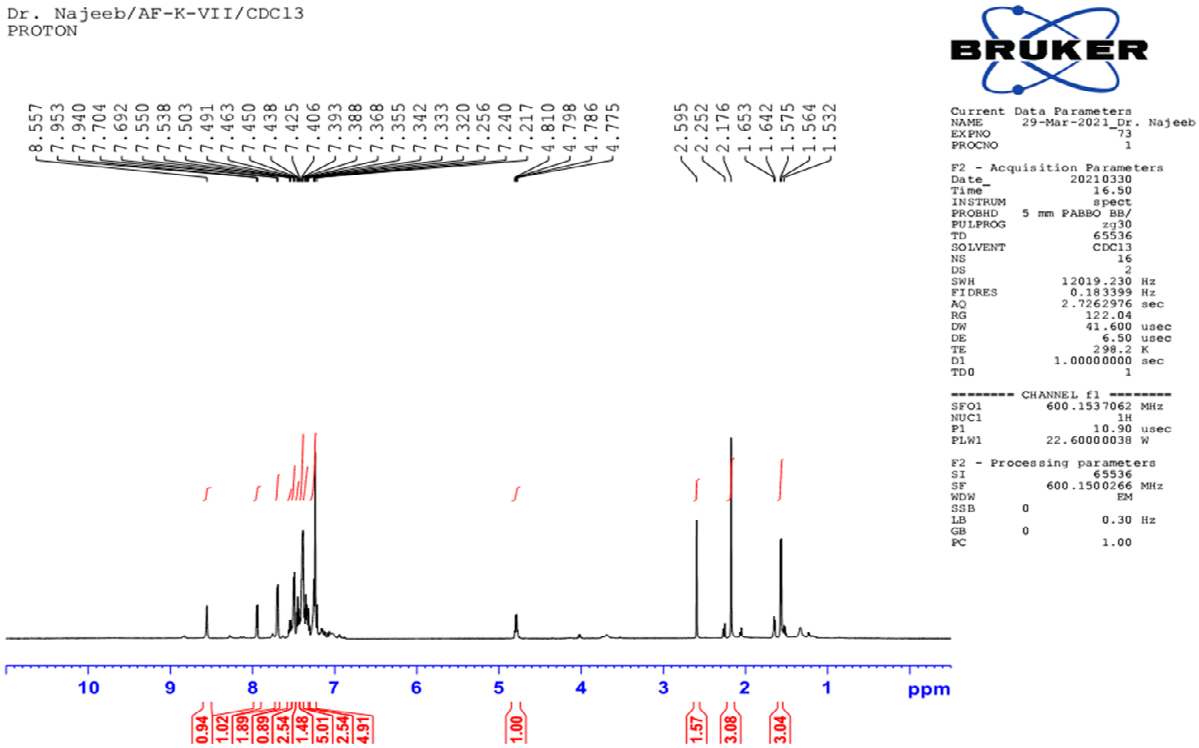


Figure S21: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5e**



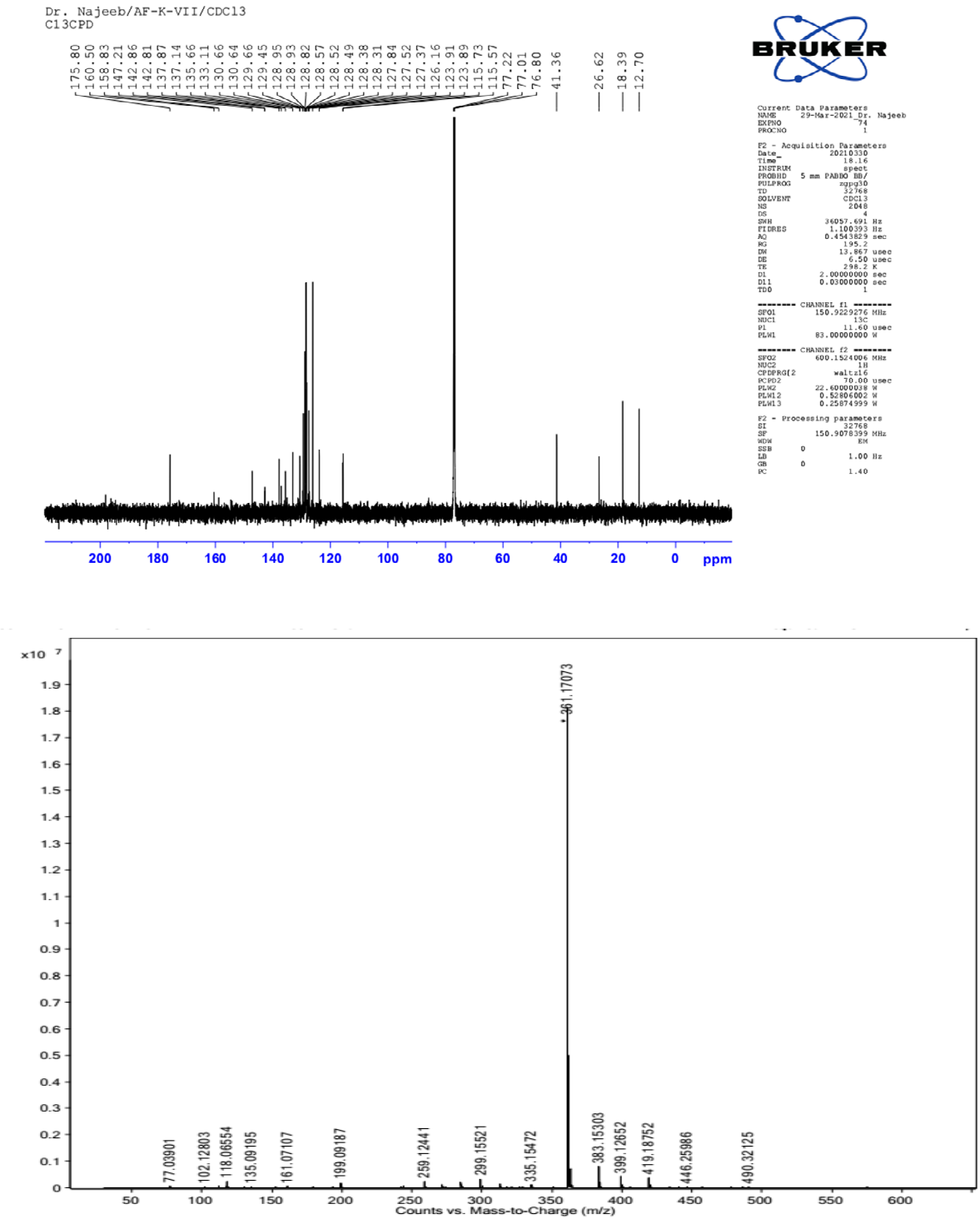
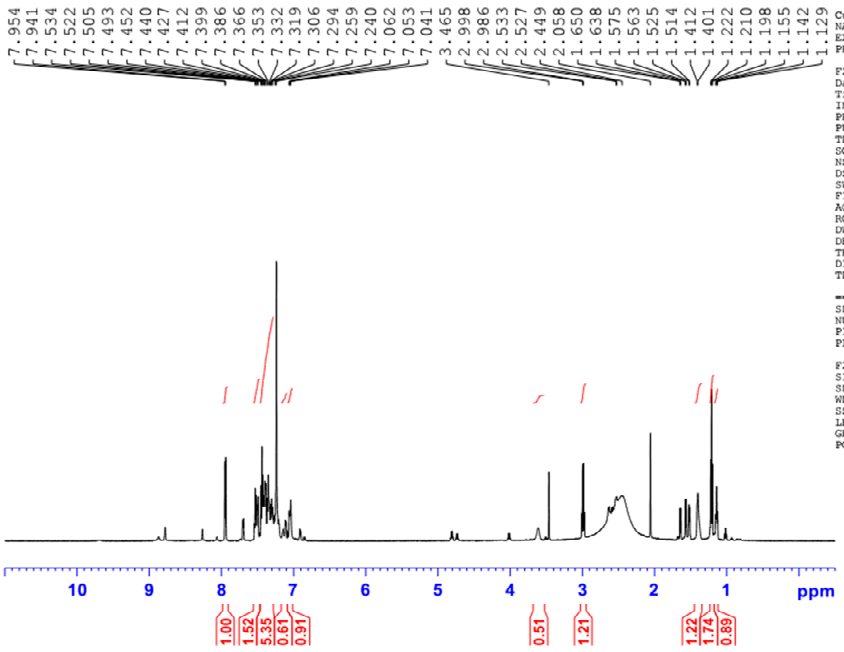


Figure S22: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5f**

Dr. Najeeb/AF-K-VIII/CDCl3
PROTON



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PROCNO 1

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PULPROG zg30
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FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 109.89
DW 41.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

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NUC1 1H
P1 10.90 usec
PLW1 22.60000038 W

F2 - Processing parameters
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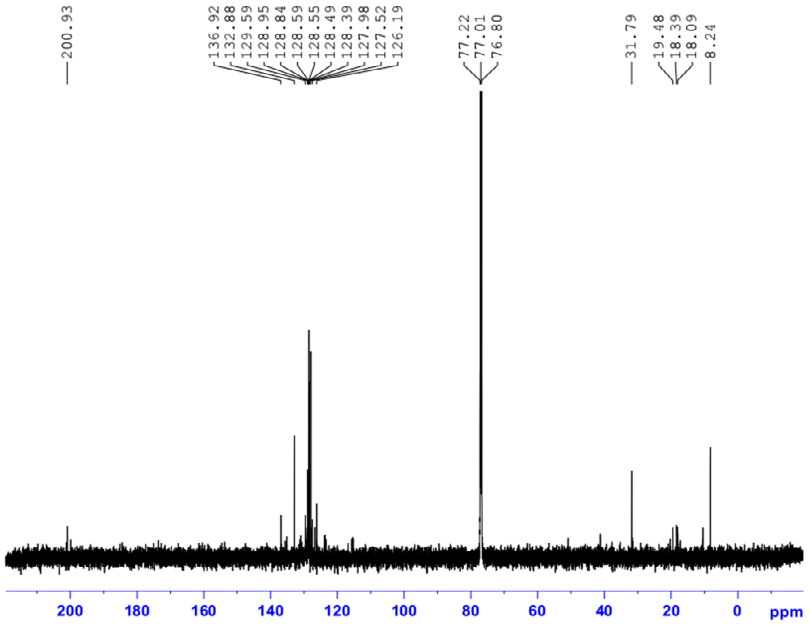
SF 600.1500266 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dr. Najeeb/AF-K-VIII/CDCl3
C13CPD



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PROCNO 1

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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
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SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W

======== CHANNEL f2 ========
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.52806002 W
PLW13 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9078399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

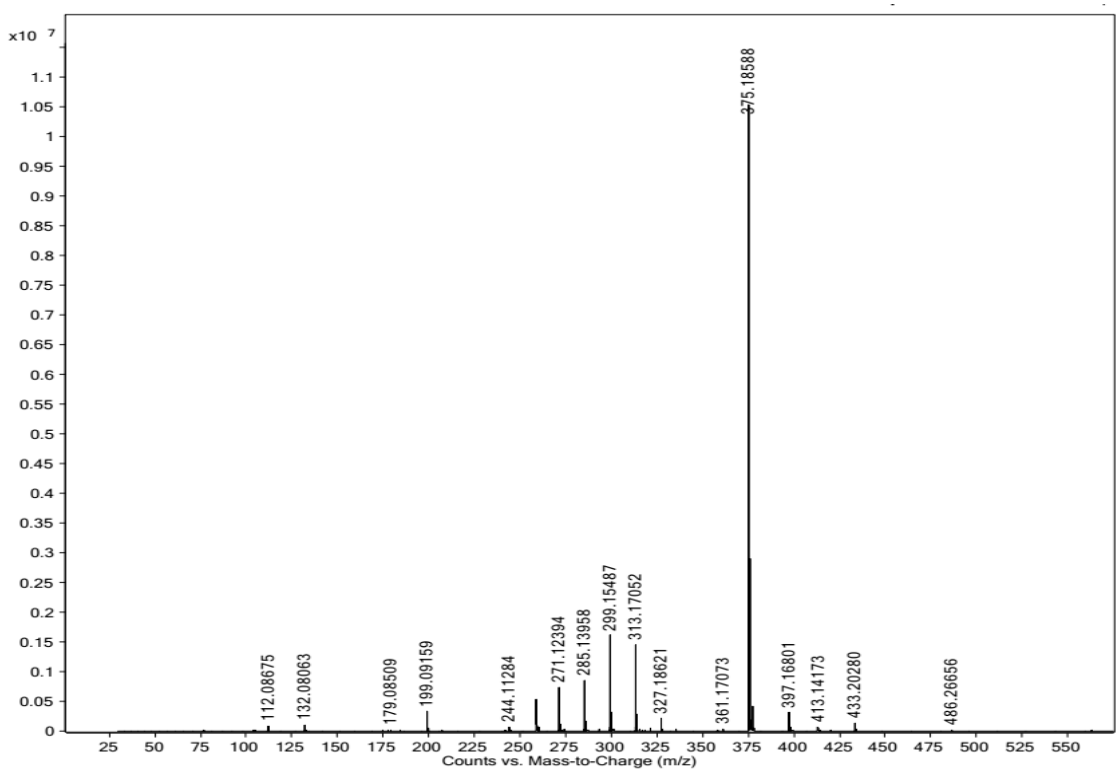
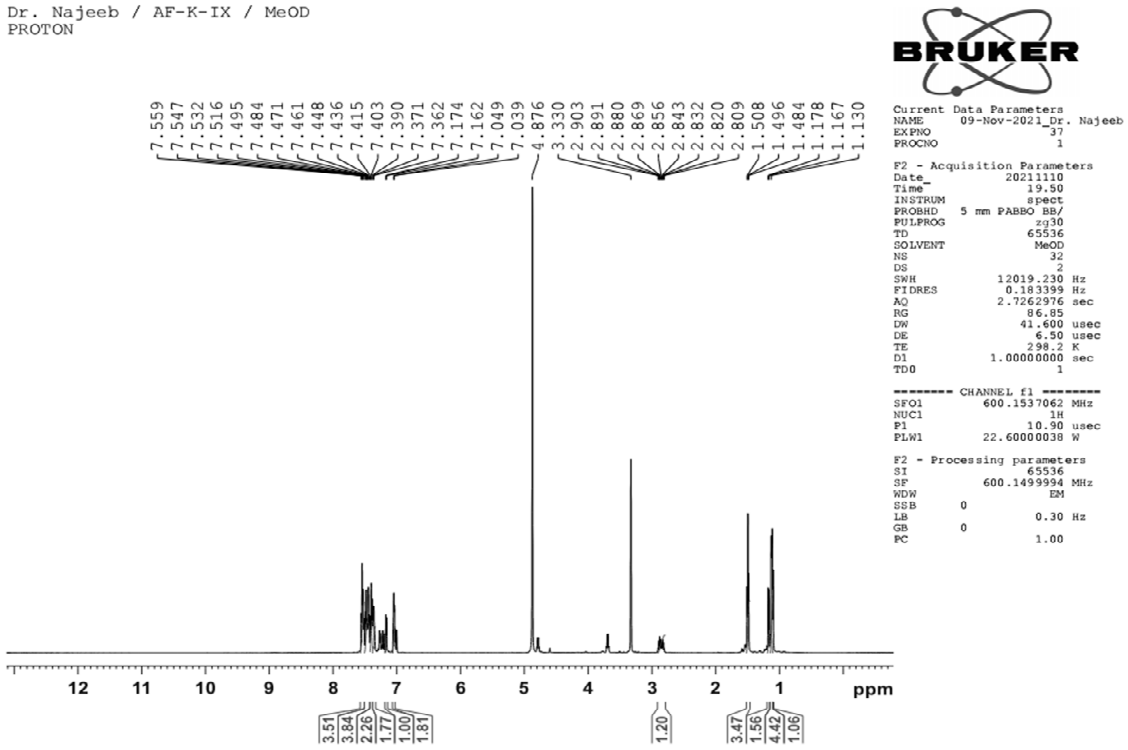


Figure S23: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5g**



Current Data Parameters
NAME 09-Nov-2021_Dr. Najeeb
EXPNO 37
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211110
Time 19.50
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 86.85
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 600.1537062 MHz
NUC1 1H
P1 10.90 usec
PLW1 22.60000038 W

F2 - Processing parameters
SI 65536
SF 600.1499994 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

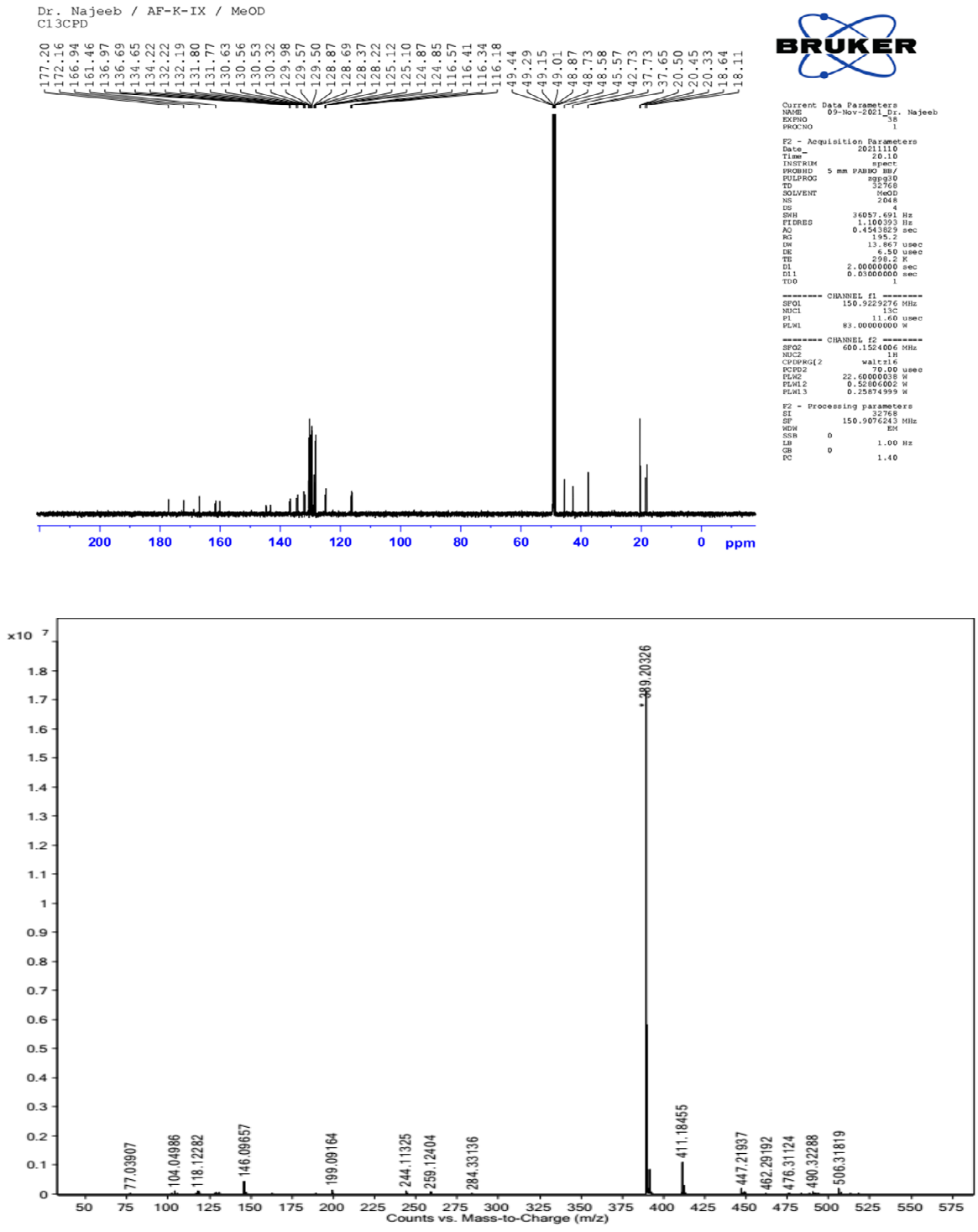


Figure S24: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5h**

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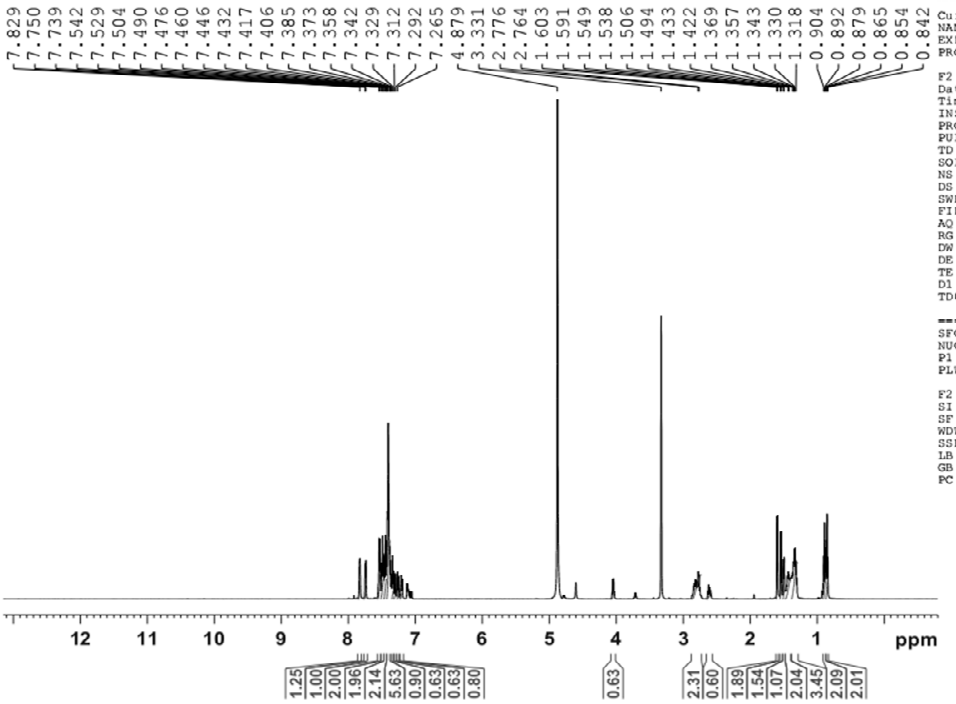


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Current Data Parameters
NAME      09-Nov-2021_Dr. Najeeb
EXPNO                 45
PROCNO                 1

F2 - Acquisition Parameters
Date_              20211111
Time                  2.48
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT               MeOD
NS                      32
DS                       2
SWH              12019.230 Hz
FIDRES               0.183399 Hz
AQ                2.7262976 sec
RG                   76.79
DW                  41.600 usec
DE                   6.50 usec
TE                  298.1 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            600.1537062 MHz
NUC1                    1H
P1                   10.90 usec
PLW1            22.60000038 W

F2 - Processing parameters
SI                   65536
SF              600.1499994 MHz
WDW                     EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

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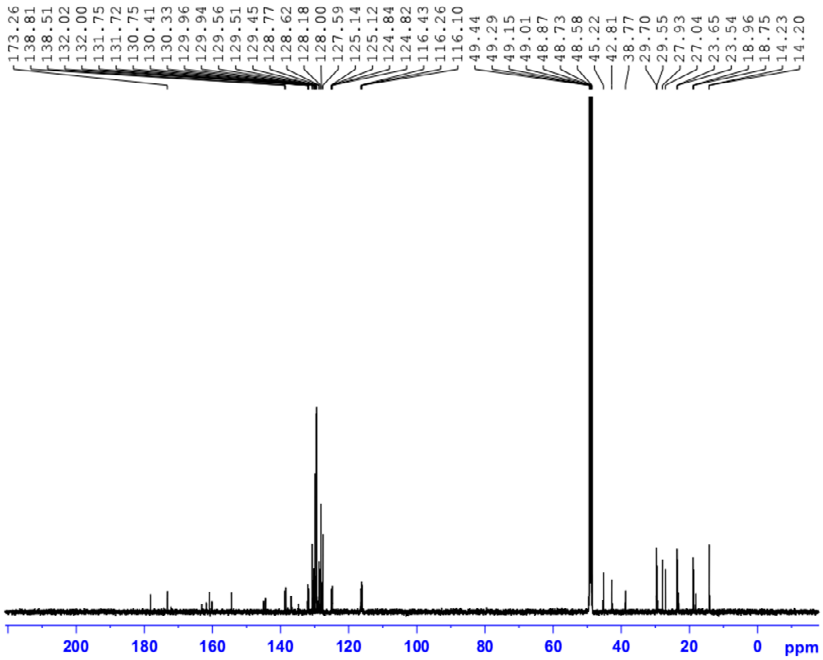
C13CPD

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Current Data Parameters
NAME      09-Nov-2021_Dr. Najeeb
EXPNO                 46
PROCNO                 1

F2 - Acquisition Parameters
Date_              20211111
Time                  4.56
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                   32768
SOLVENT               MeOD
NS                    4096
DS                       4
SWH              36057.691 Hz
FIDRES               1.100393 Hz
AQ                0.4543829 sec
RG                   195.2
DW                  13.867 usec
DE                   6.50 usec
TE                  298.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            150.9229276 MHz
NUC1                    13C
P1                   11.60 usec
PLW1            83.00000000 W

======== CHANNEL f2 ========
SFO2            600.1524006 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                70.00 usec
PLW2            22.60000038 W
PLW12            0.52806002 W
PLW13            0.25874999 W

F2 - Processing parameters
SI                   32768
SF              150.9076243 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

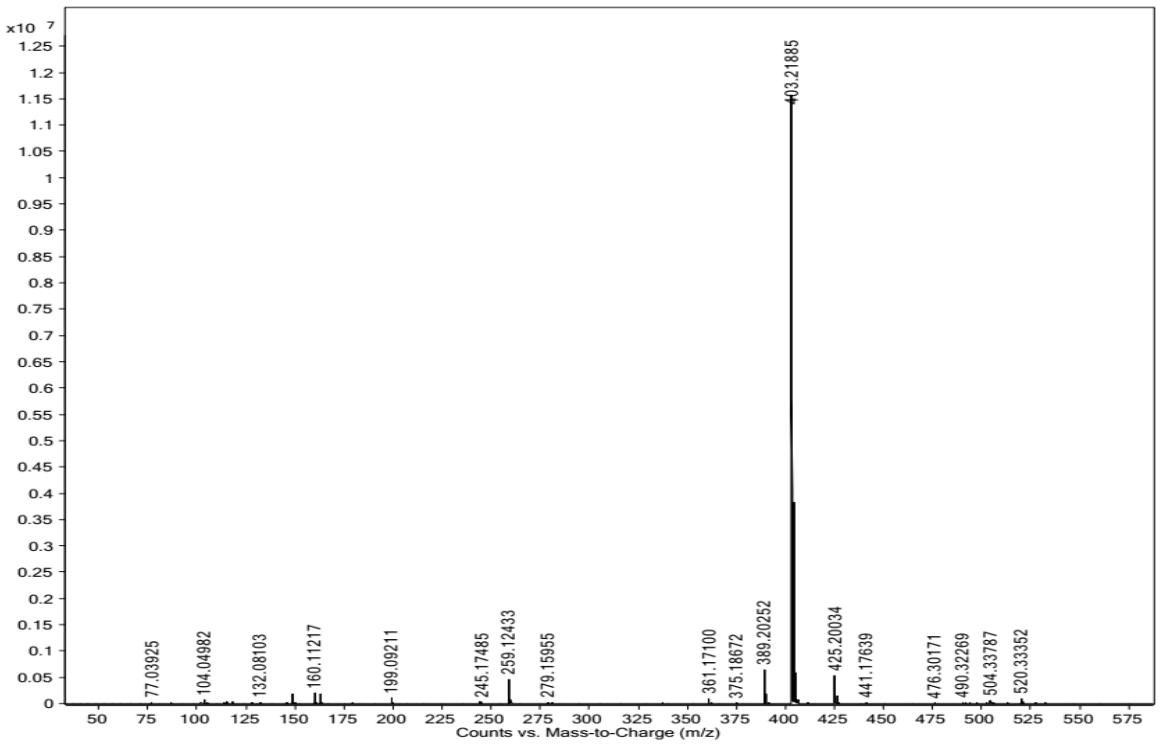
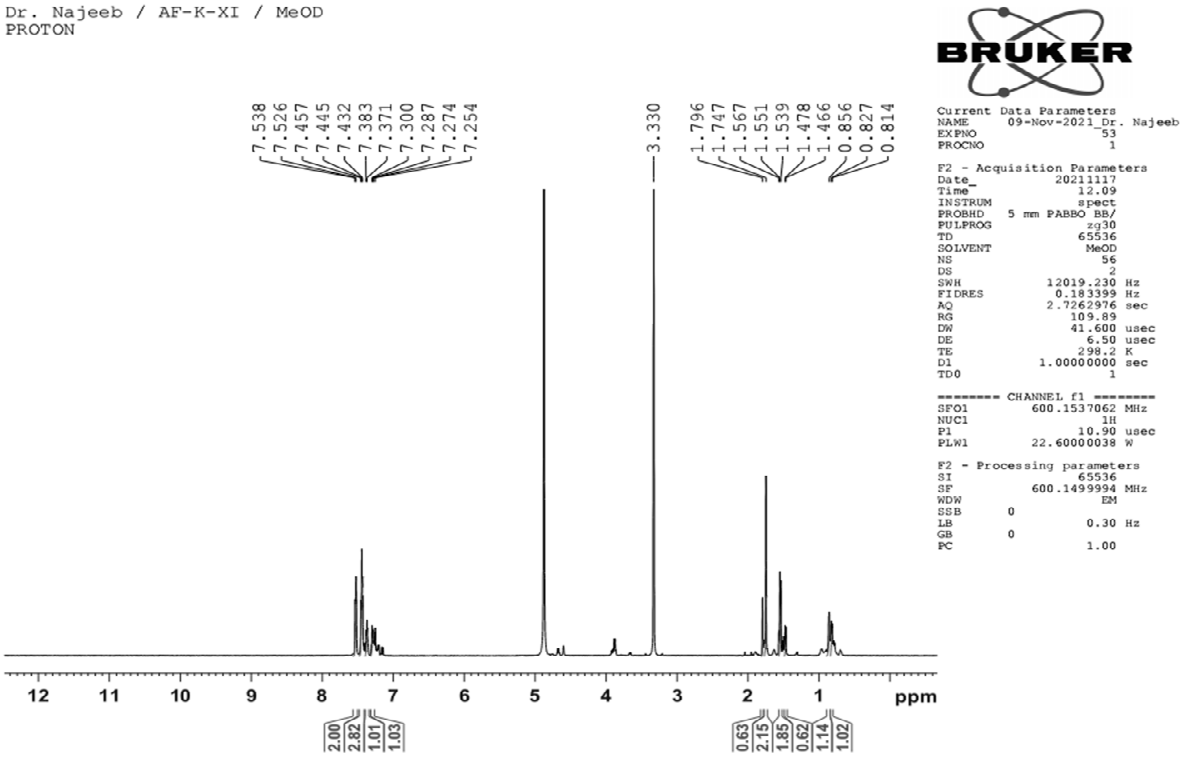


Figure S25: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5i**



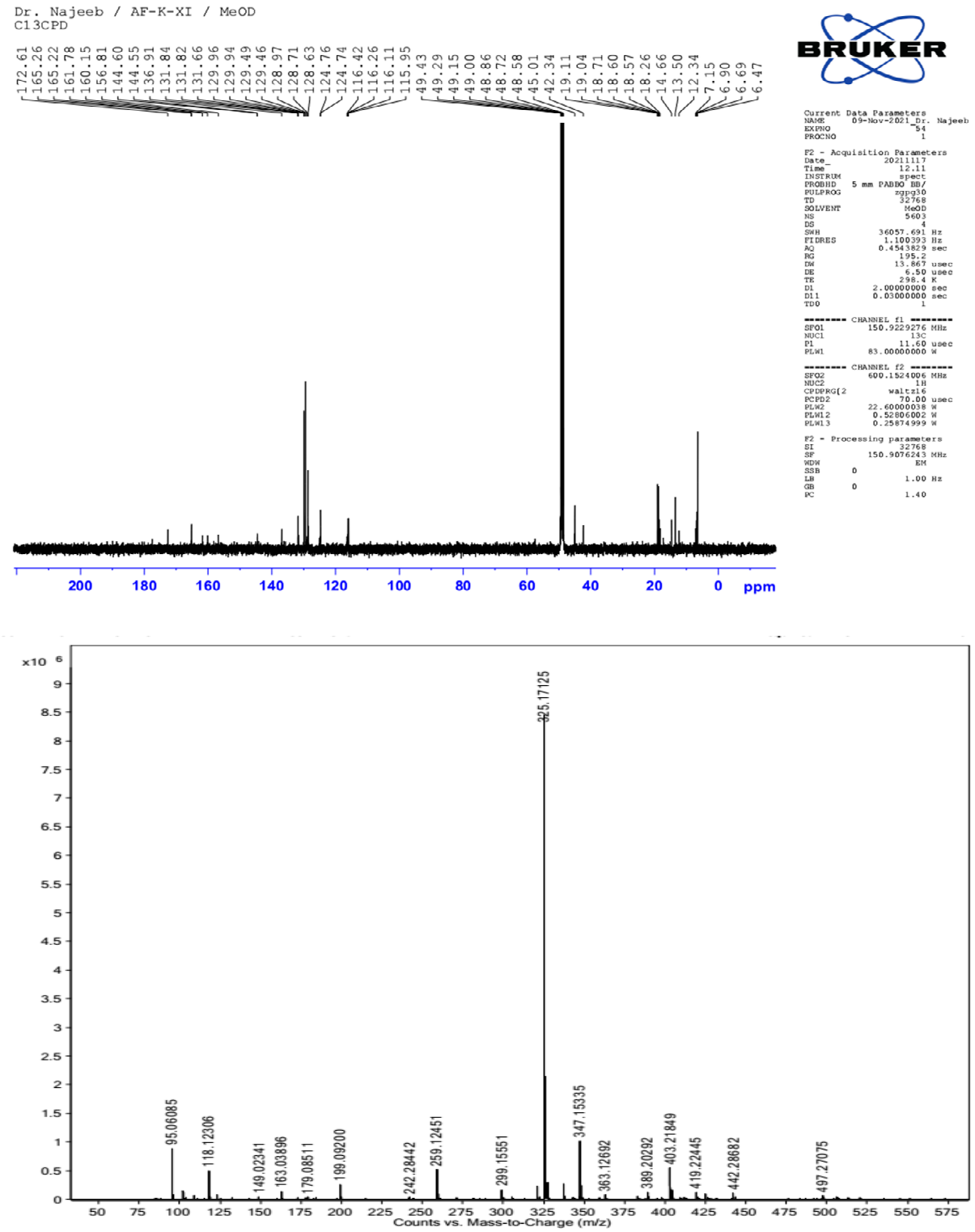


Figure S26: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5j**

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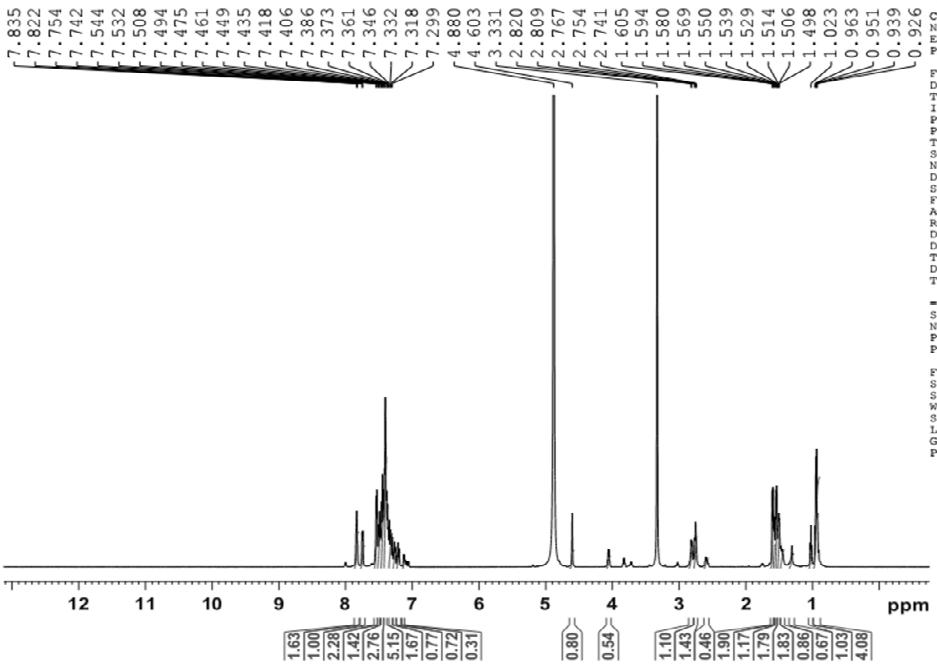


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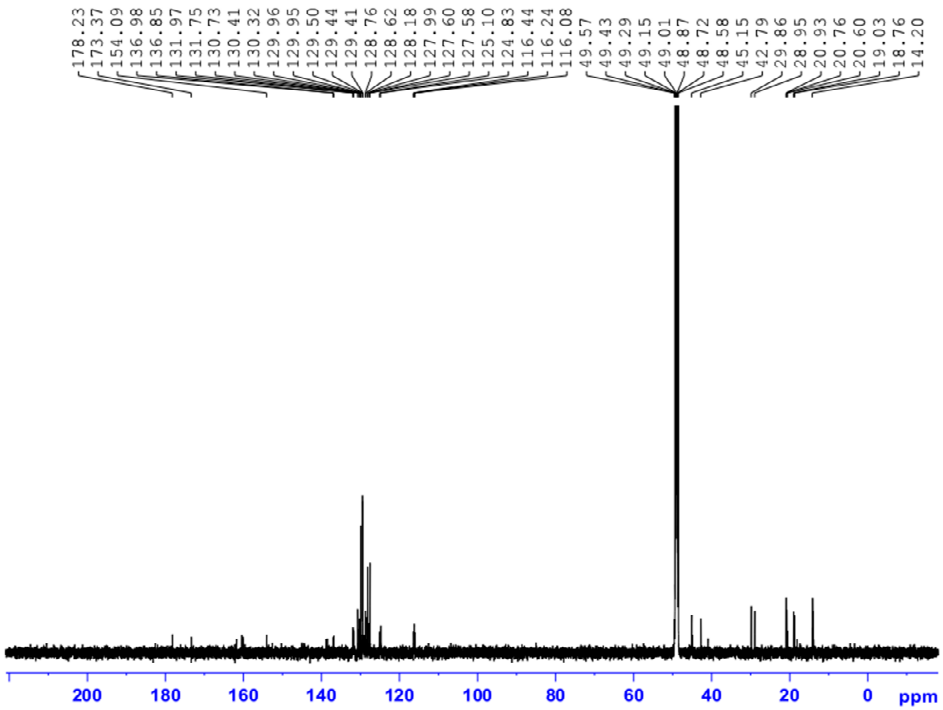
Current Data Parameters
NAME      09-Nov-2021_Dr. Najeeb
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211115
Time              13.02
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT           MeOD
NS                   32
DS                    2
SWH           12019.230 Hz
FIDRES            0.183399 Hz
AQ            2.7262976 sec
RG                76.79
DW               41.600 usec
DE                6.50 usec
TE              298.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          600.1537062 MHz
NUC1                  1H
P1                10.90 usec
PLW1          22.60000038 W

F2 - Processing parameters
SI                65536
SF            600.1499994 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

Dr. Najeeb / AF-K-XII / MeOD
C13CPD

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Current Data Parameters
NAME      09-Nov-2021_Dr. Najeeb
EXPNO                 22
PROCNO                 1

F2 - Acquisition Parameters
Date_           20211115
Time              13.03
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           MeOD
NS                 2808
DS                    4
SWH           36057.691 Hz
FIDRES            0.550197 Hz
AQ            0.9087659 sec
RG                195.2
DW               13.867 usec
DE                6.50 usec
TE              298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1          150.9229276 MHz
NUC1                 13C
P1                11.60 usec
PLW1          83.00000000 W

======== CHANNEL f2 ========
SFO2          600.1524006 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             70.00 usec
PLW2          22.60000038 W
PLW12          0.52806002 W
PLW13          0.25874999 W

F2 - Processing parameters
SI                32768
SF            150.9076243 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

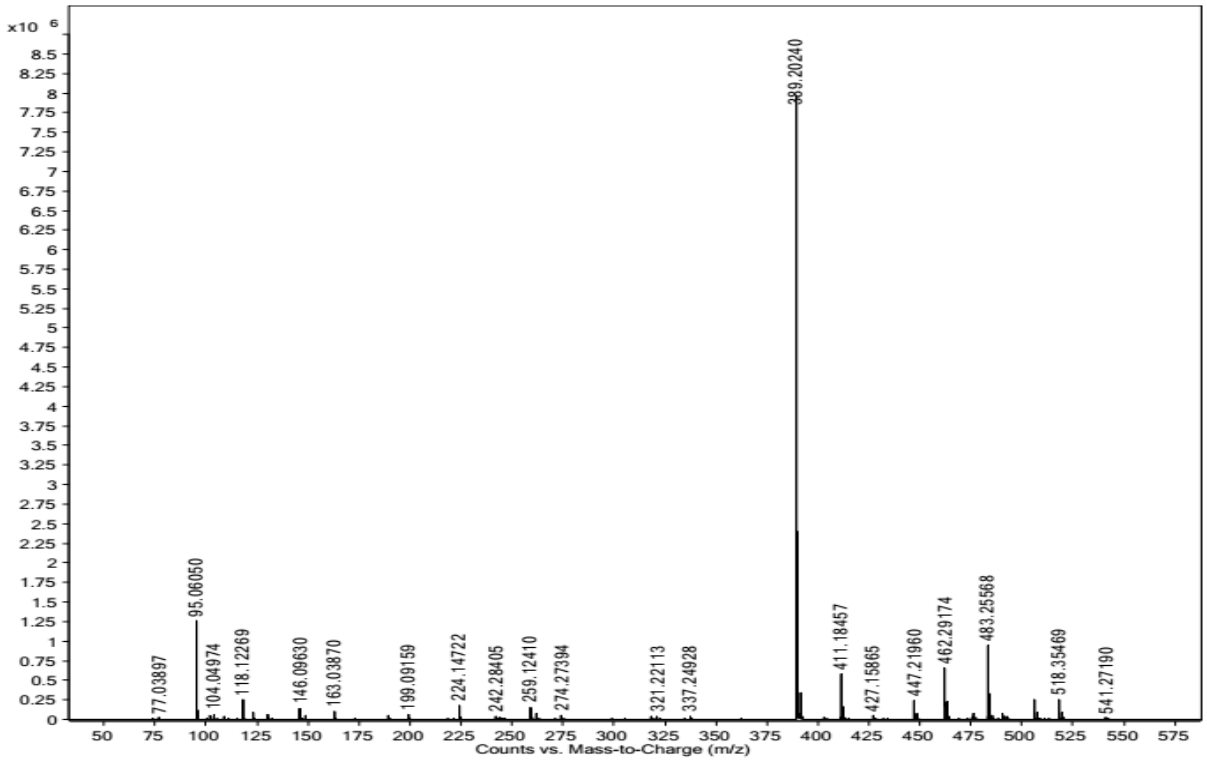
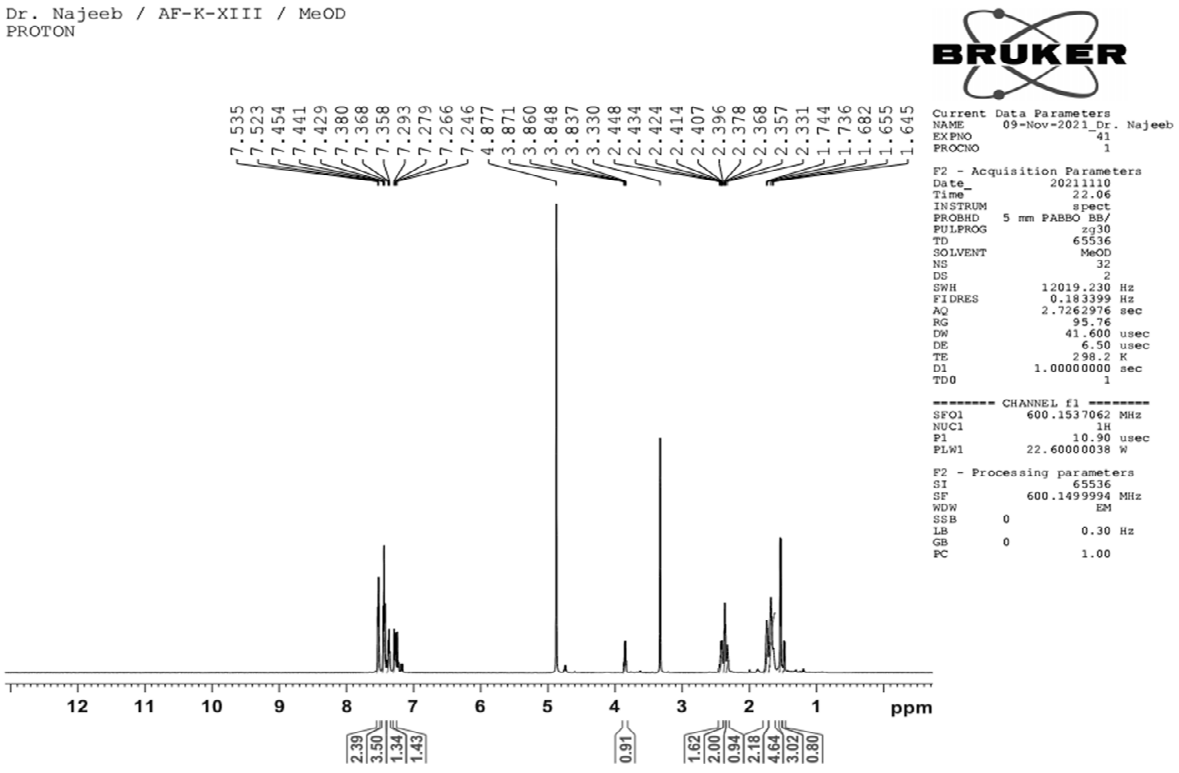


Figure S27: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5k**



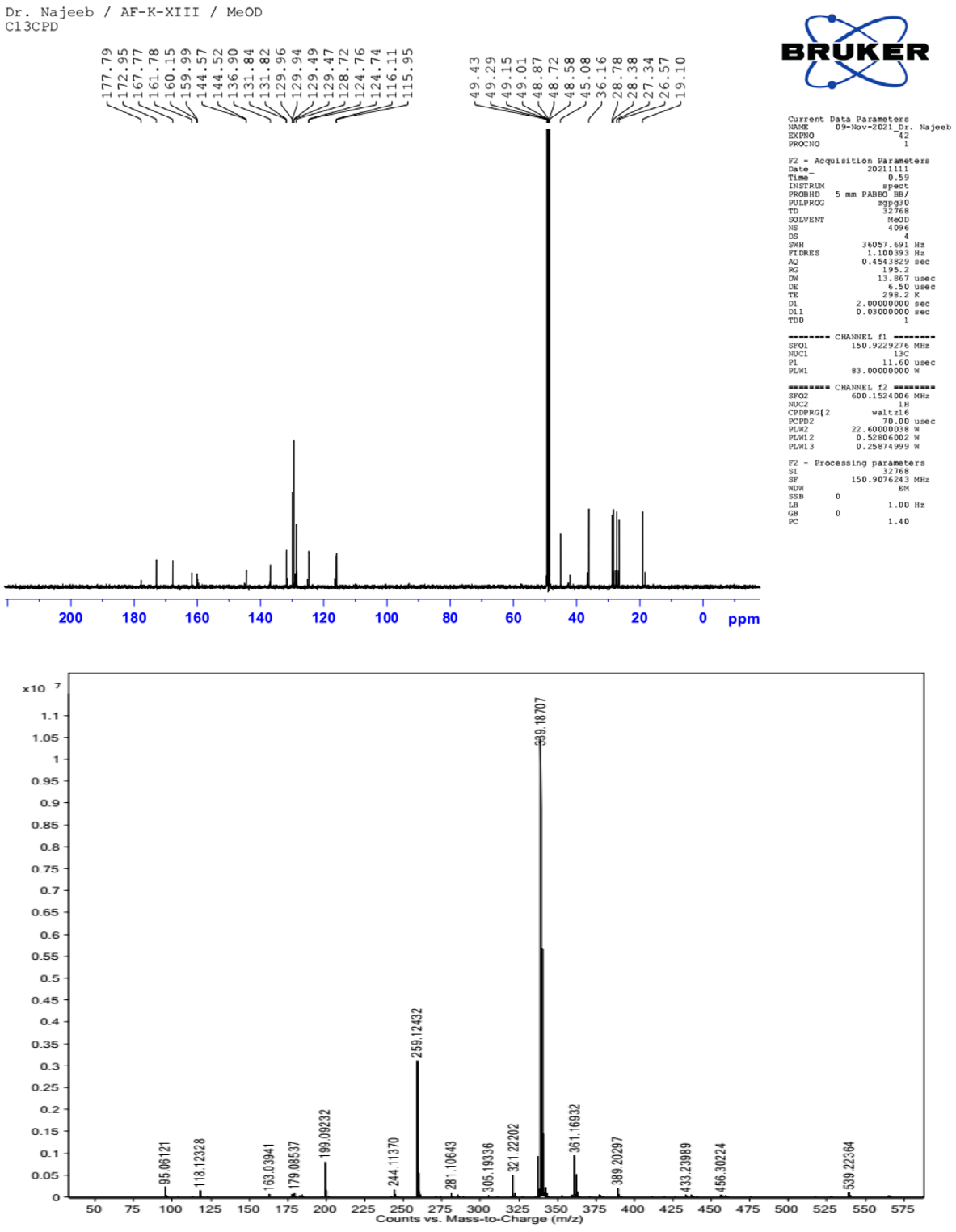


Figure S28: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5l**

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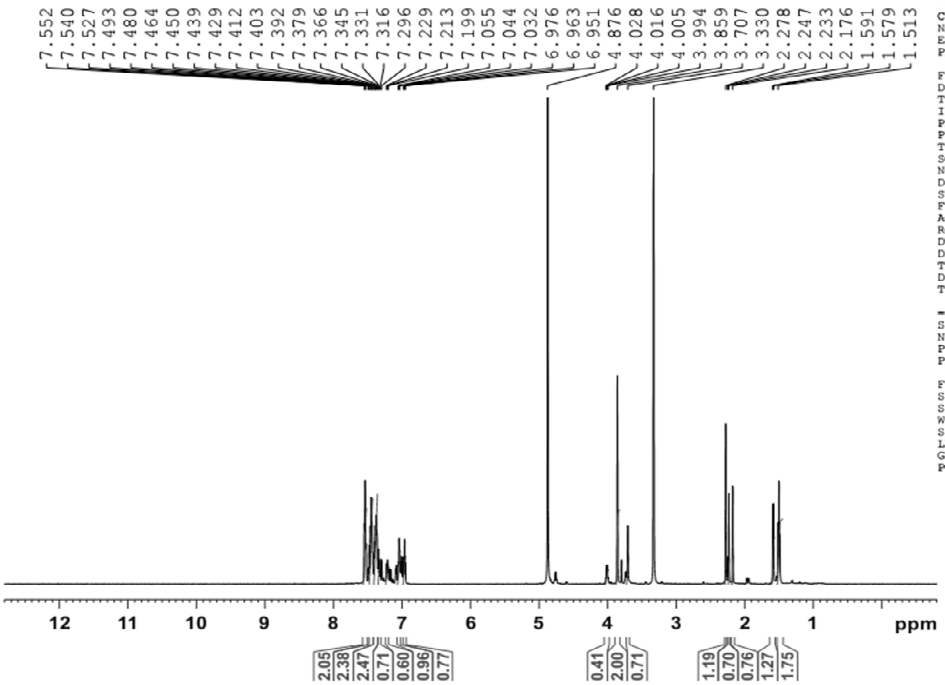


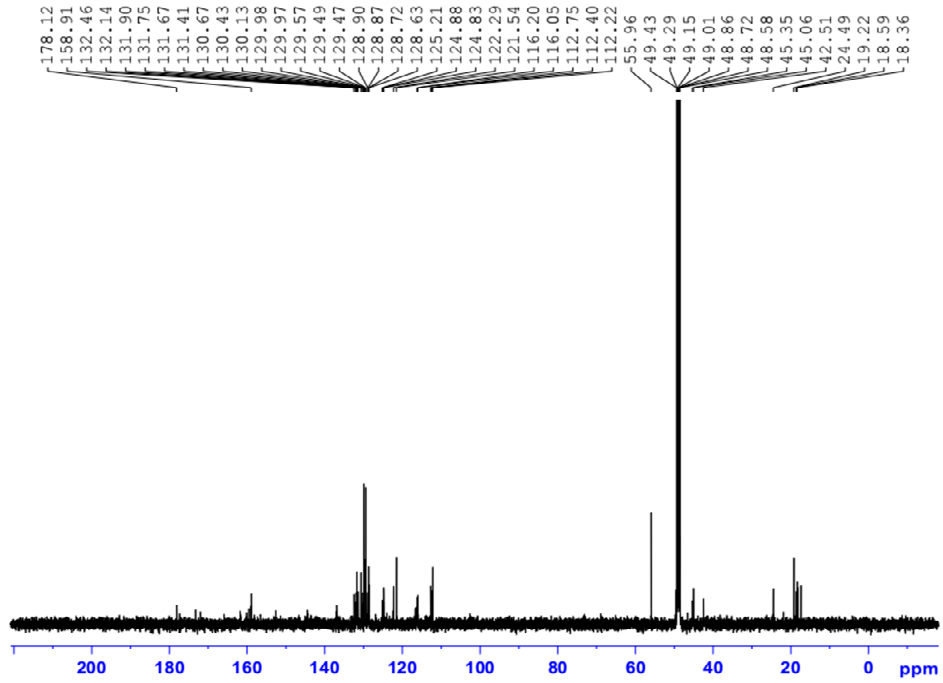
Current Data Parameters
NAME 09-Nov-2021_Dr. Najeeb
EXPNO 49
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211111
Time 6.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT MeOD
NS 32
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7262976 sec
RG 109.89
DW 41.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 600.1537062 MHz
NUC1 1H
P1 10.90 usec
PLW1 22.60000038 W

F2 - Processing parameters
SI 65536
SF 600.1499994 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Dr. Najeeb / AF-K-XIV / MeOD
C13CPD



Current Data Parameters
NAME 09-Nov-2021_Dr. Najeeb
EXPNO 50
PROCNO 1

F2 - Acquisition Parameters
Date_ 20211111
Time 7.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT MeOD
NS 4096
DS 4
SWH 36057.691 Hz
FIDRES 1.100393 Hz
AQ 0.4543829 sec
RG 195.2
DW 13.867 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 150.9229276 MHz
NUC1 13C
P1 11.60 usec
PLW1 83.00000000 W

======== CHANNEL f2 ========
SFO2 600.1524006 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 70.00 usec
PLW2 22.60000038 W
PLW12 0.52806002 W
PLW13 0.25874999 W

F2 - Processing parameters
SI 32768
SF 150.9076243 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

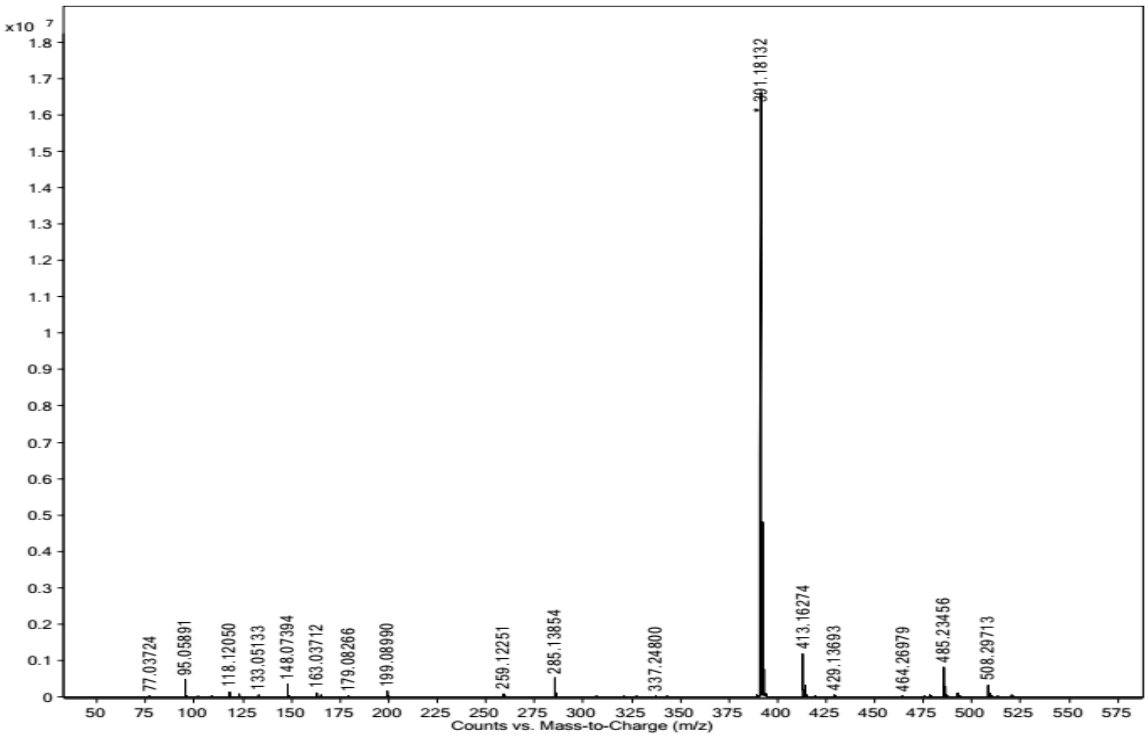
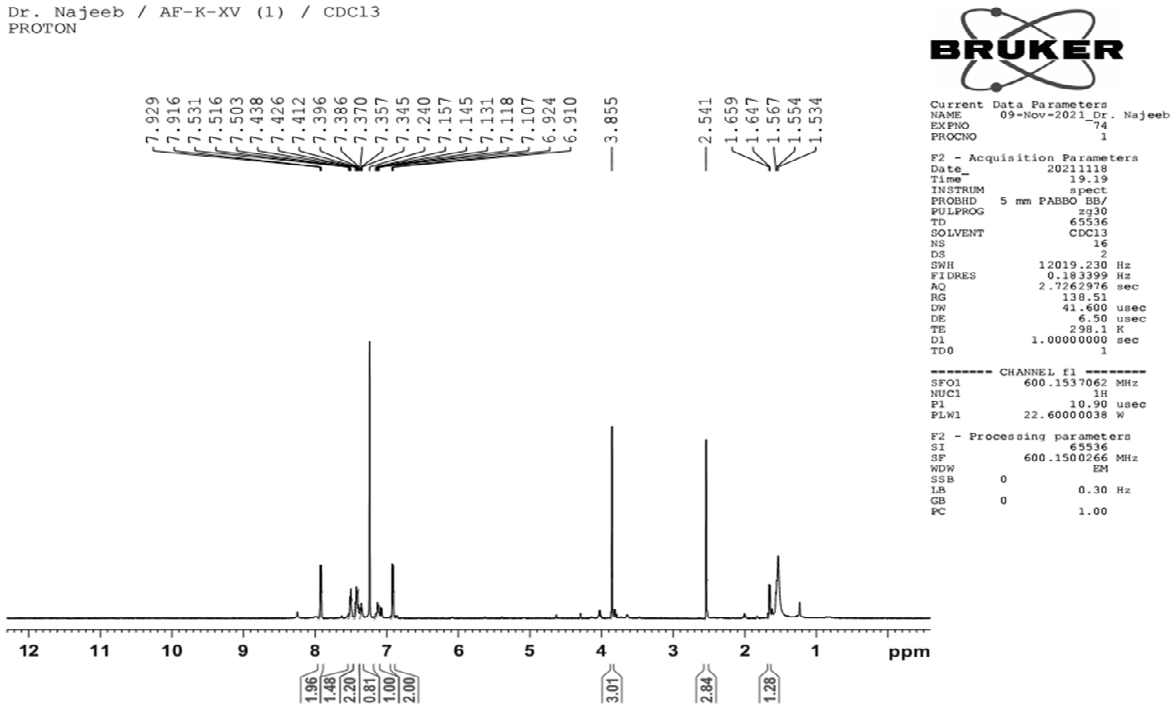


Figure S29: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5m**



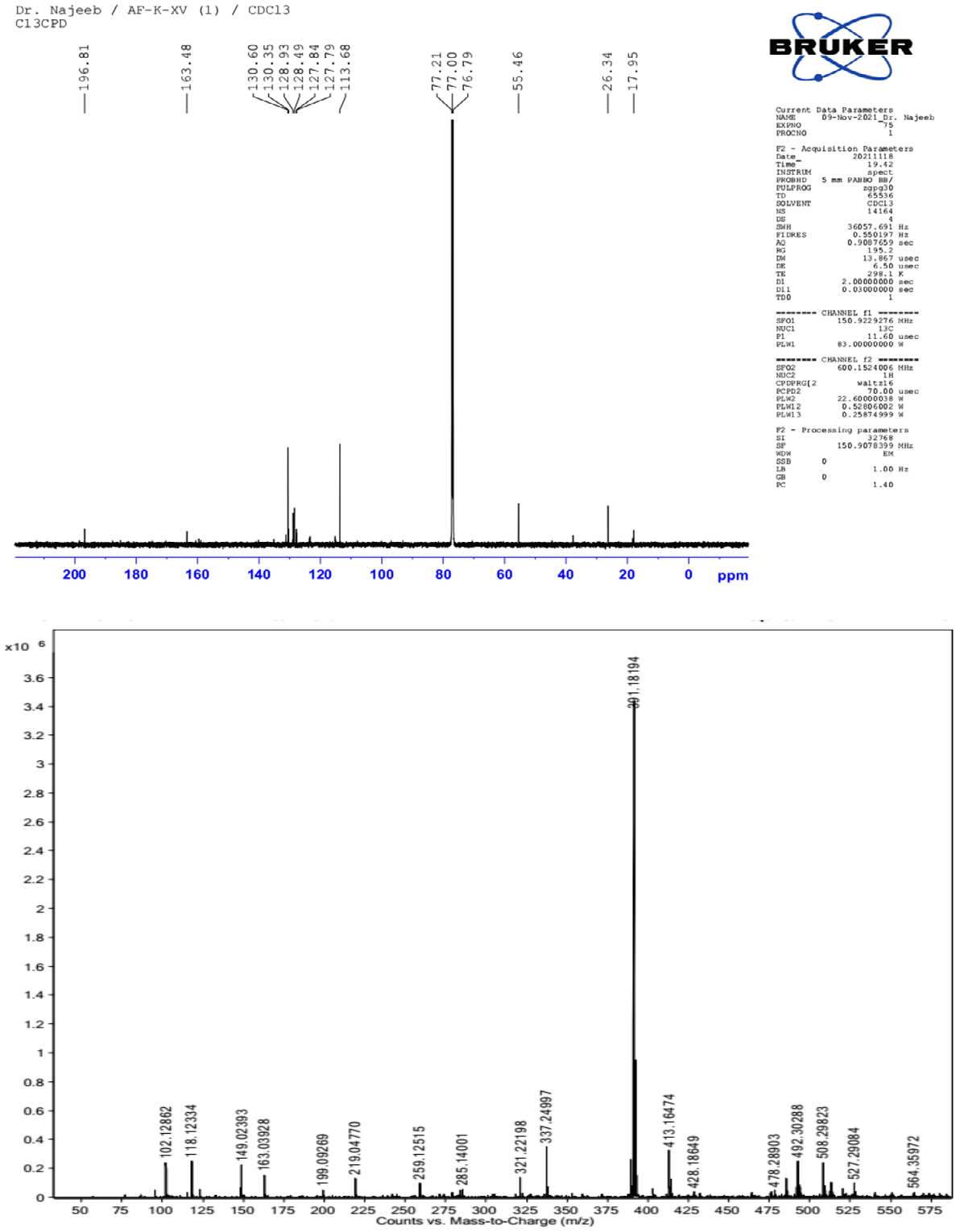


Figure S30: ^{1}H, ^{13}C NMR and HRMS (ESI^{+}) of compound **5n**