Supporting Information

Design, Synthesis and Antifungal Activities of Novel Pyrazole Analogues Containing the Aryl Trifluoromethoxy Group

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songliyan@fafu.edu.cn (L.S.); linran@fafu.edu.cn (R.L.)

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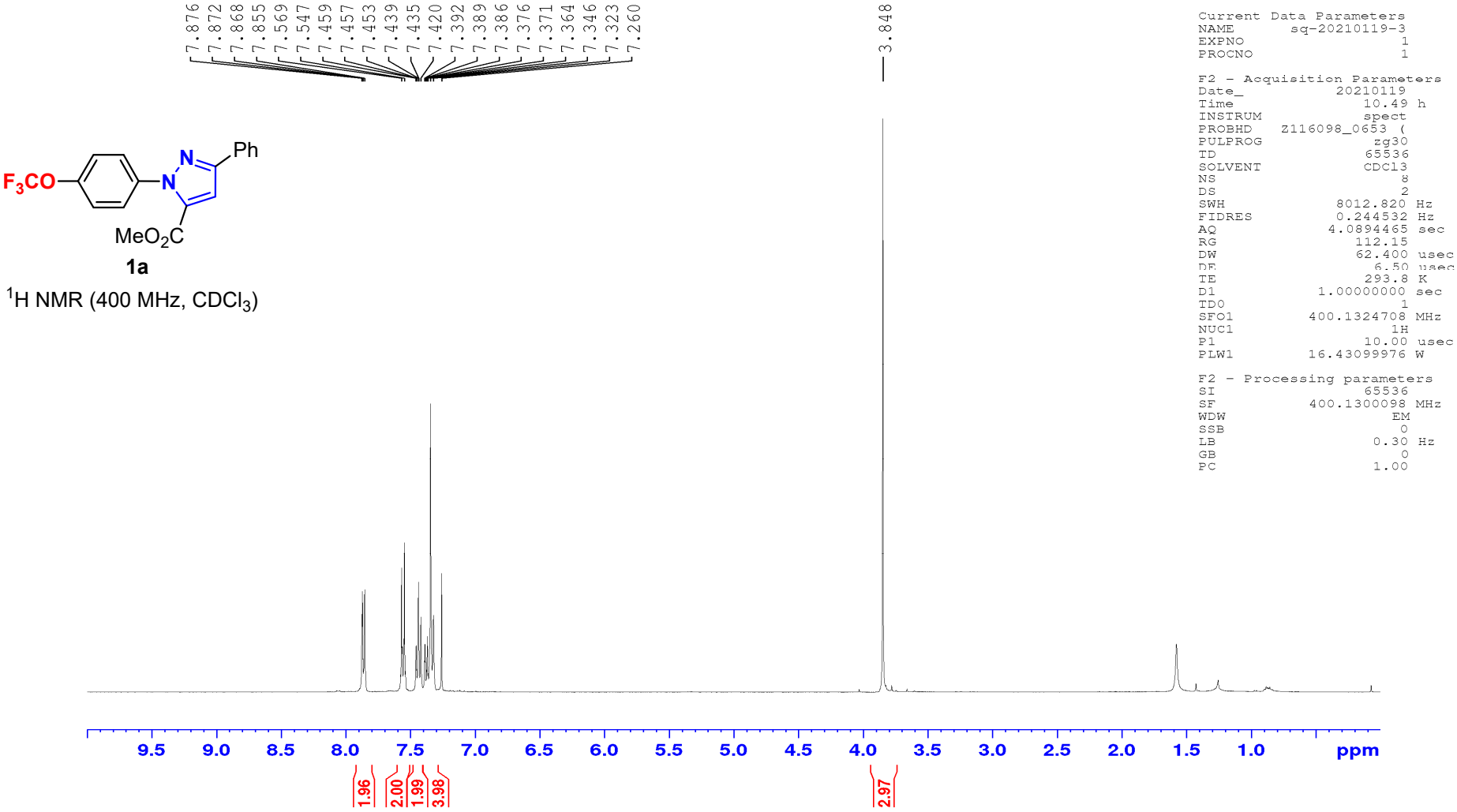
^{1}H and ^{13}C NMR Spectra of New Compounds **S-2**

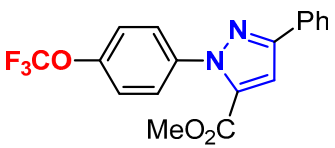
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7.876
7.872
7.868
7.855
7.569
7.547
7.459
7.457
7.453
7.439
7.435
7.420
7.392
7.389
7.386
7.376
7.371
7.364
7.346
7.323
7.260
3.848
F3CO
N
N
Ph
MeO2C
1a
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7.0
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6.0
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1.99
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2.97



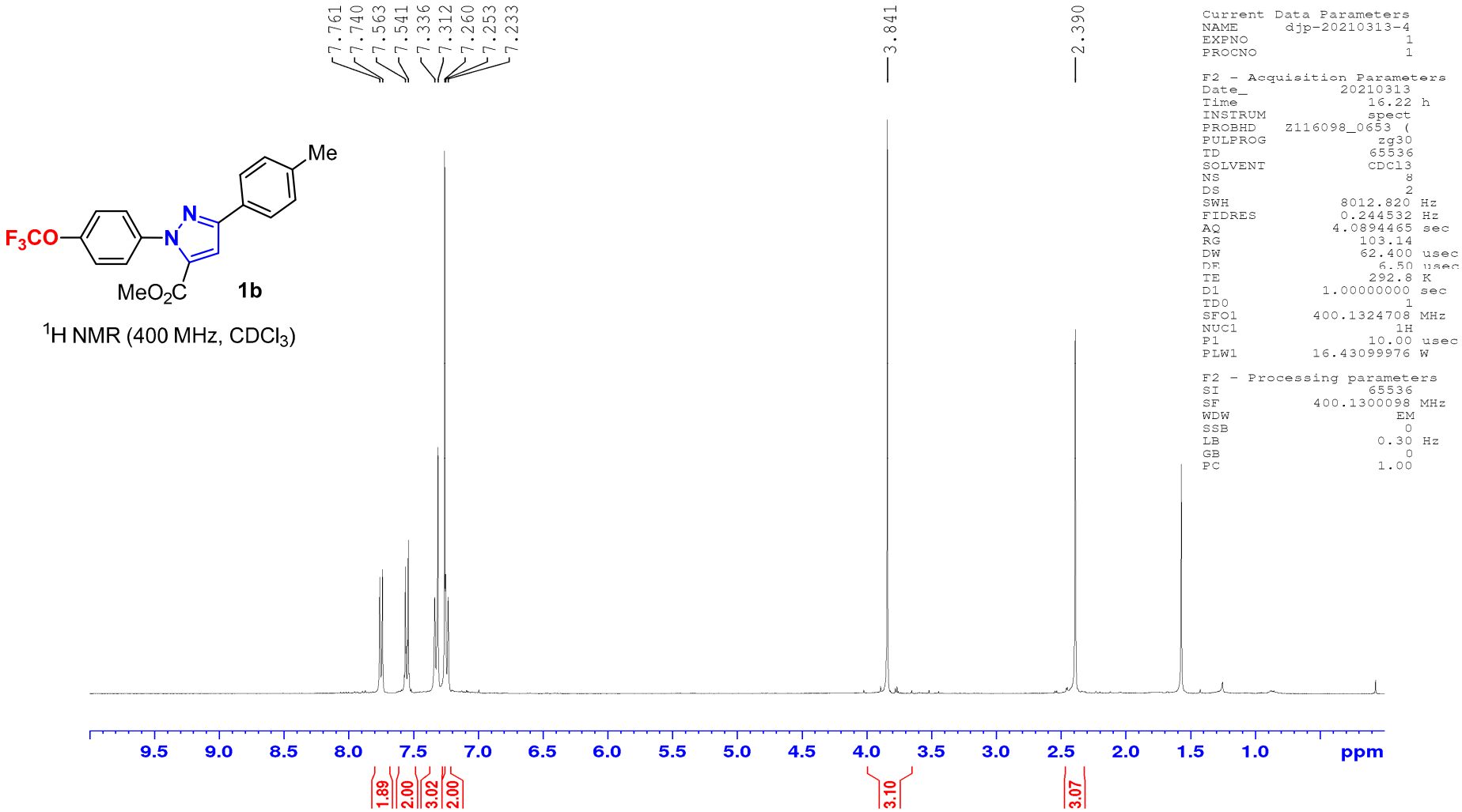
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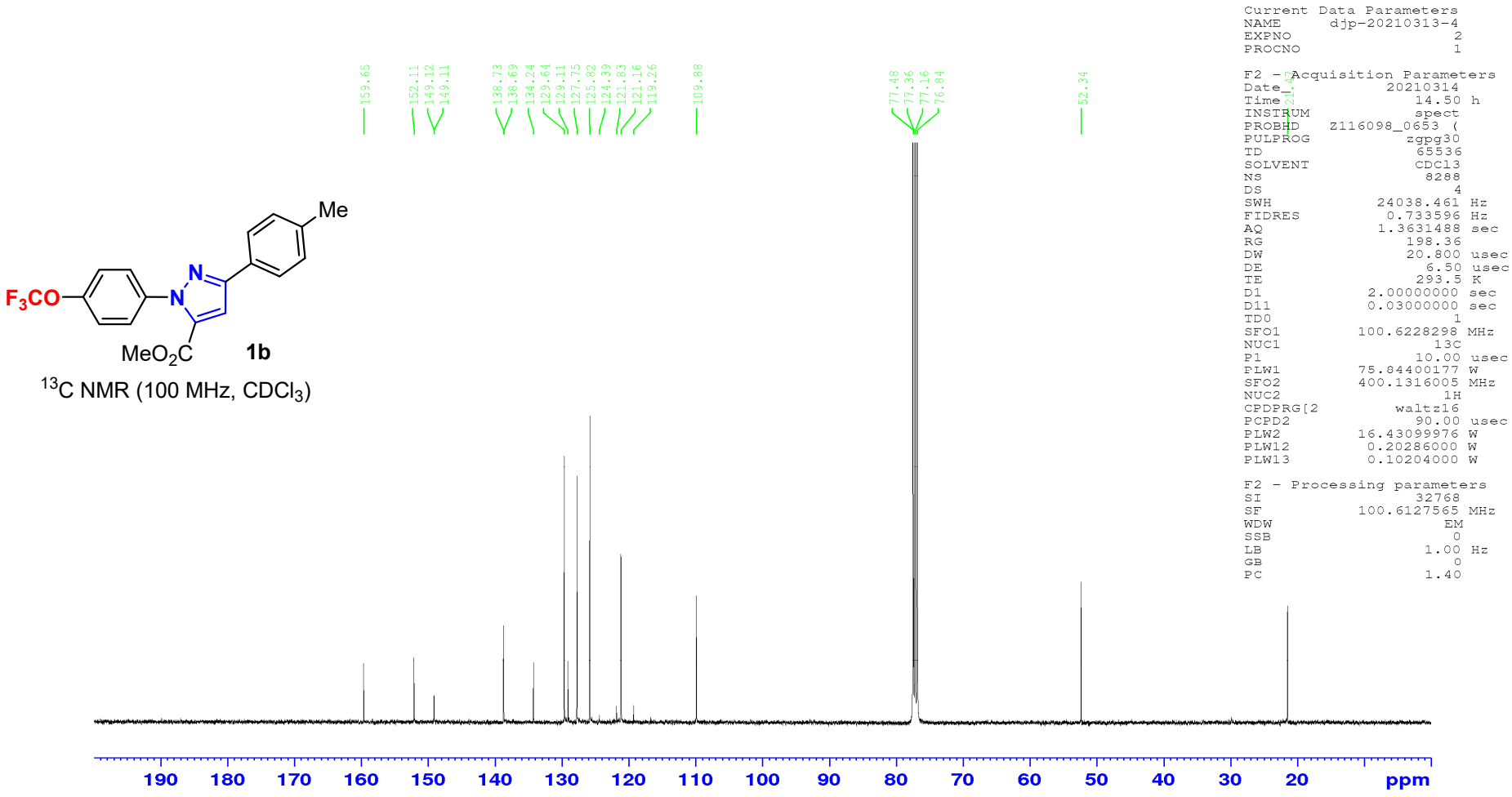
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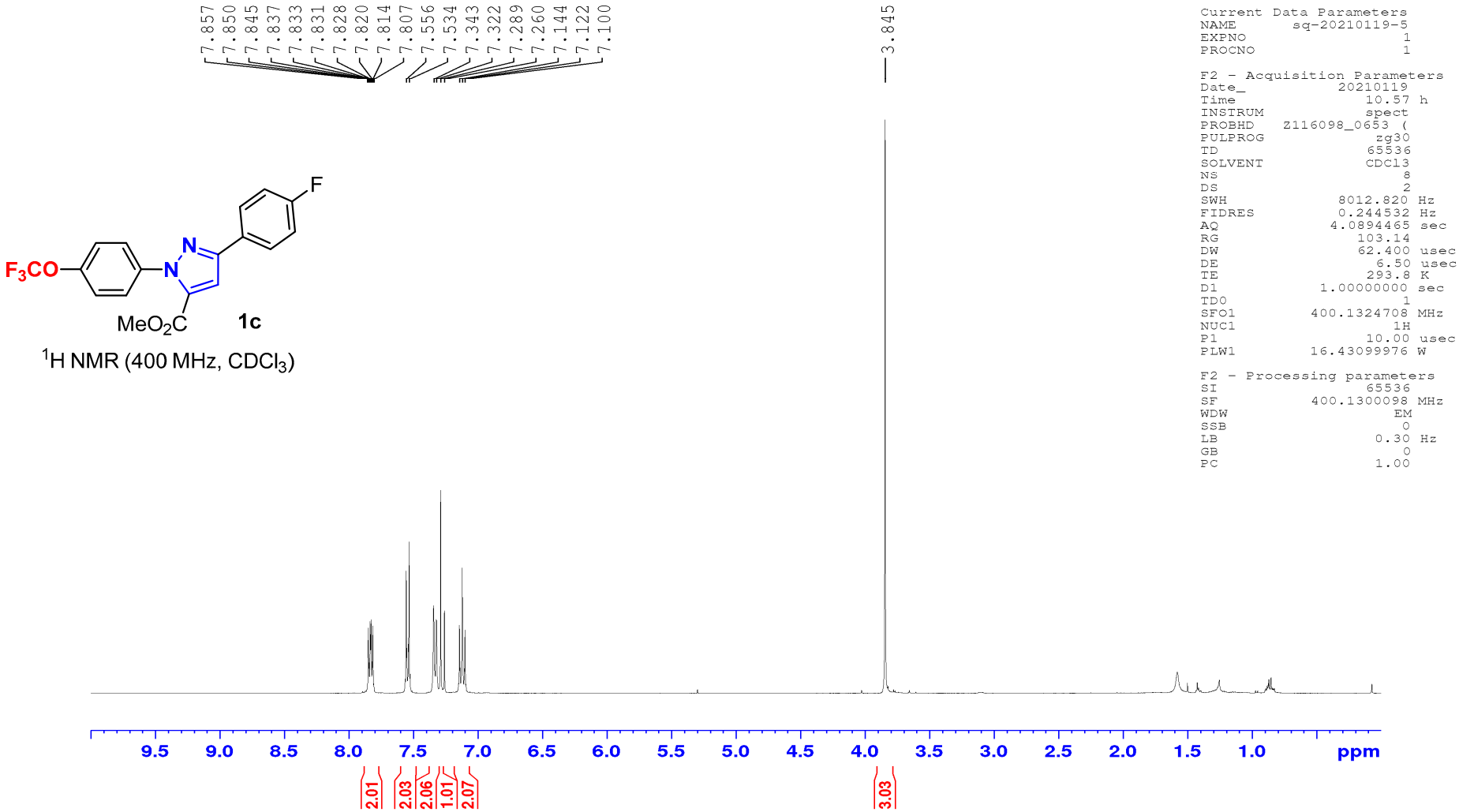

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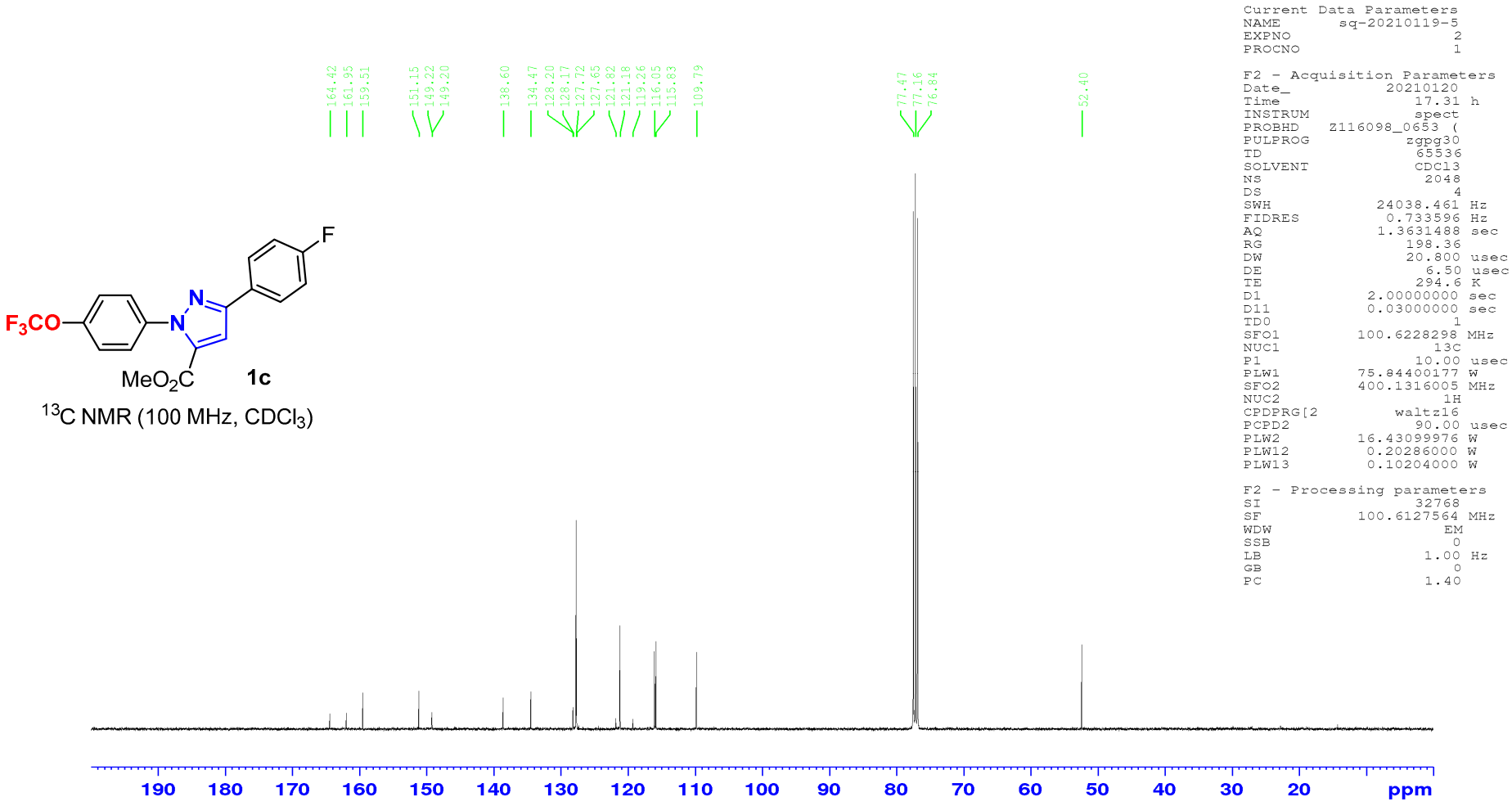
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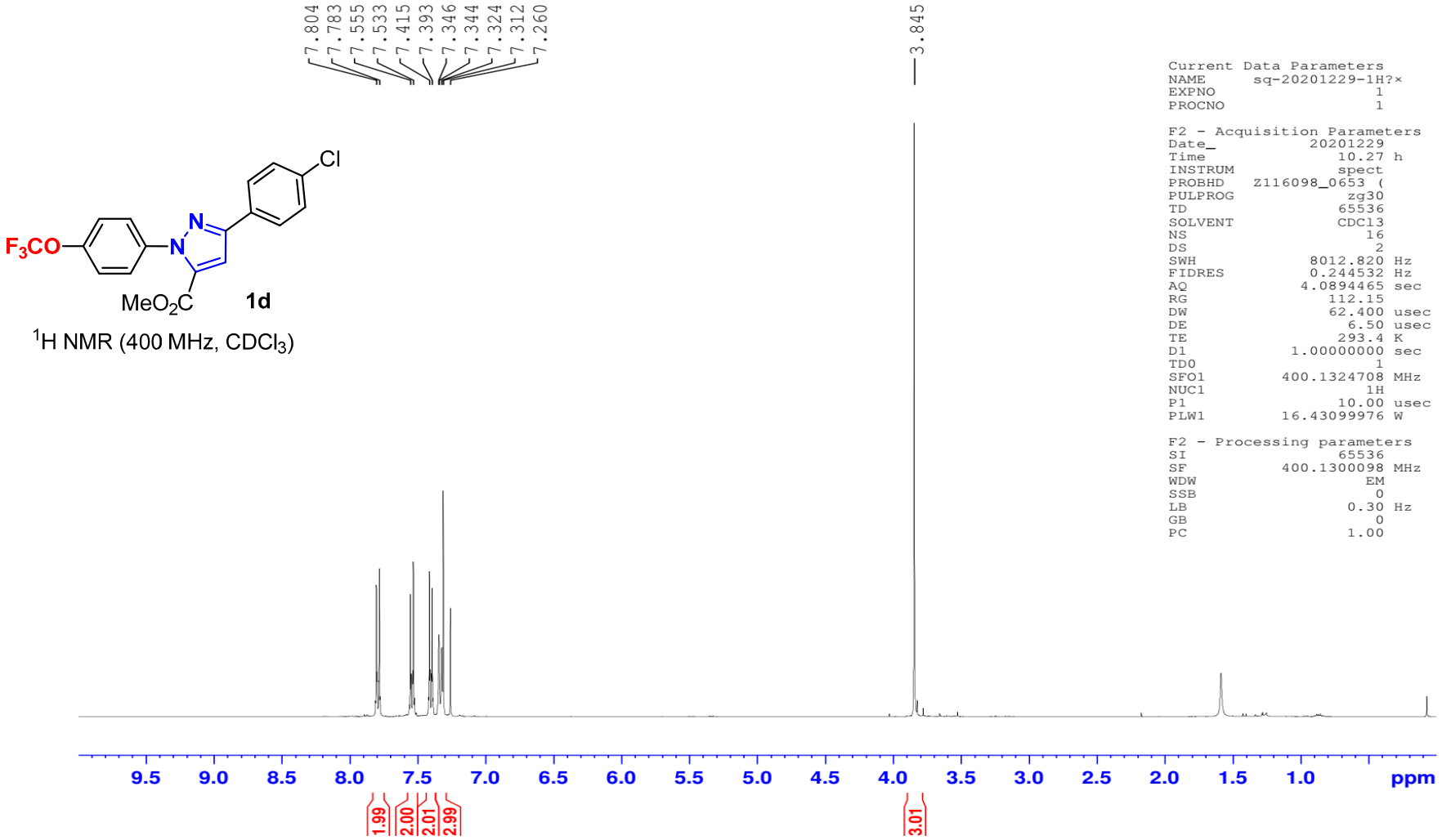
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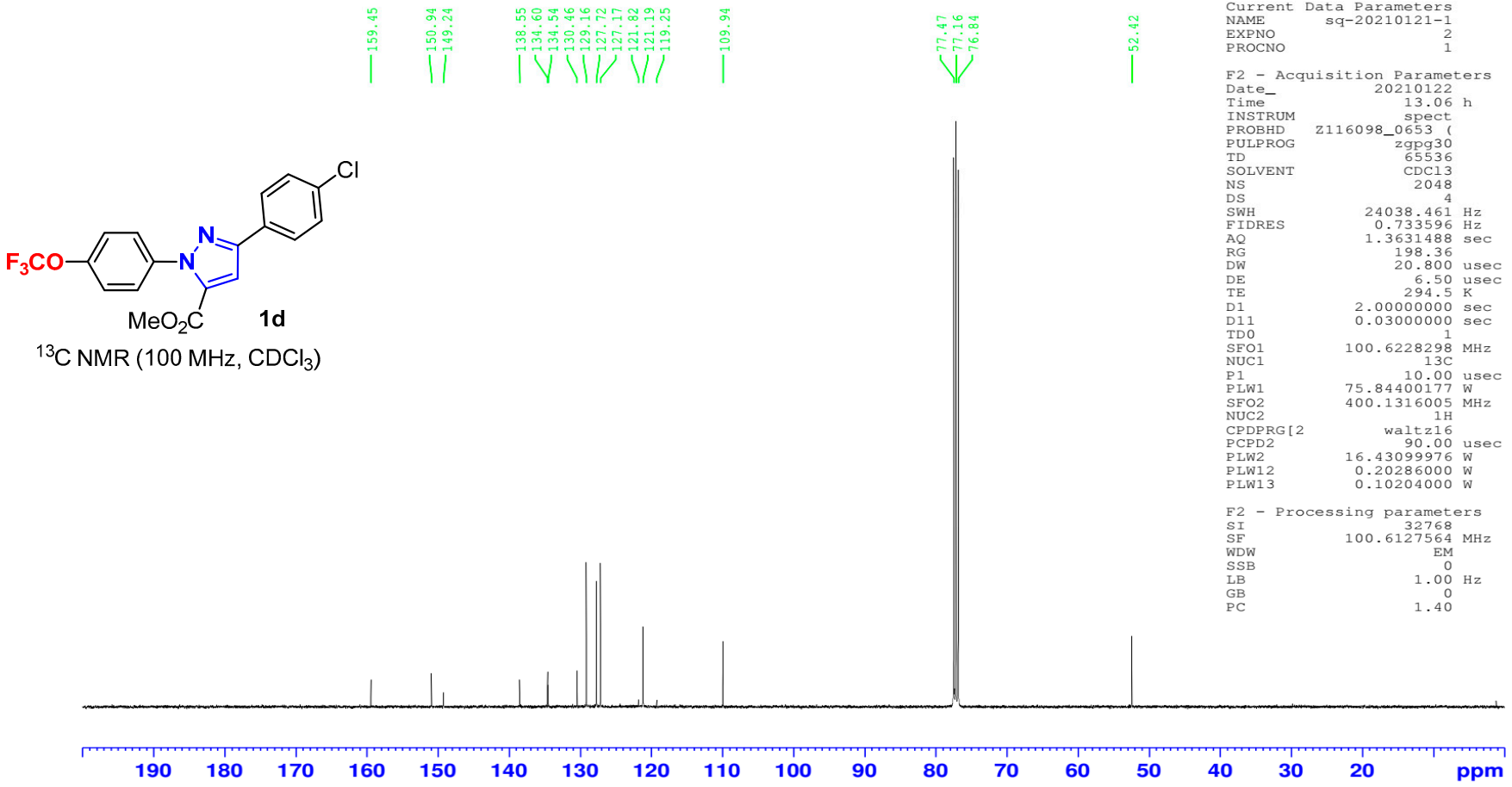

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N
N
MeO2C
1b
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LB 0.30 Hz
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3.07

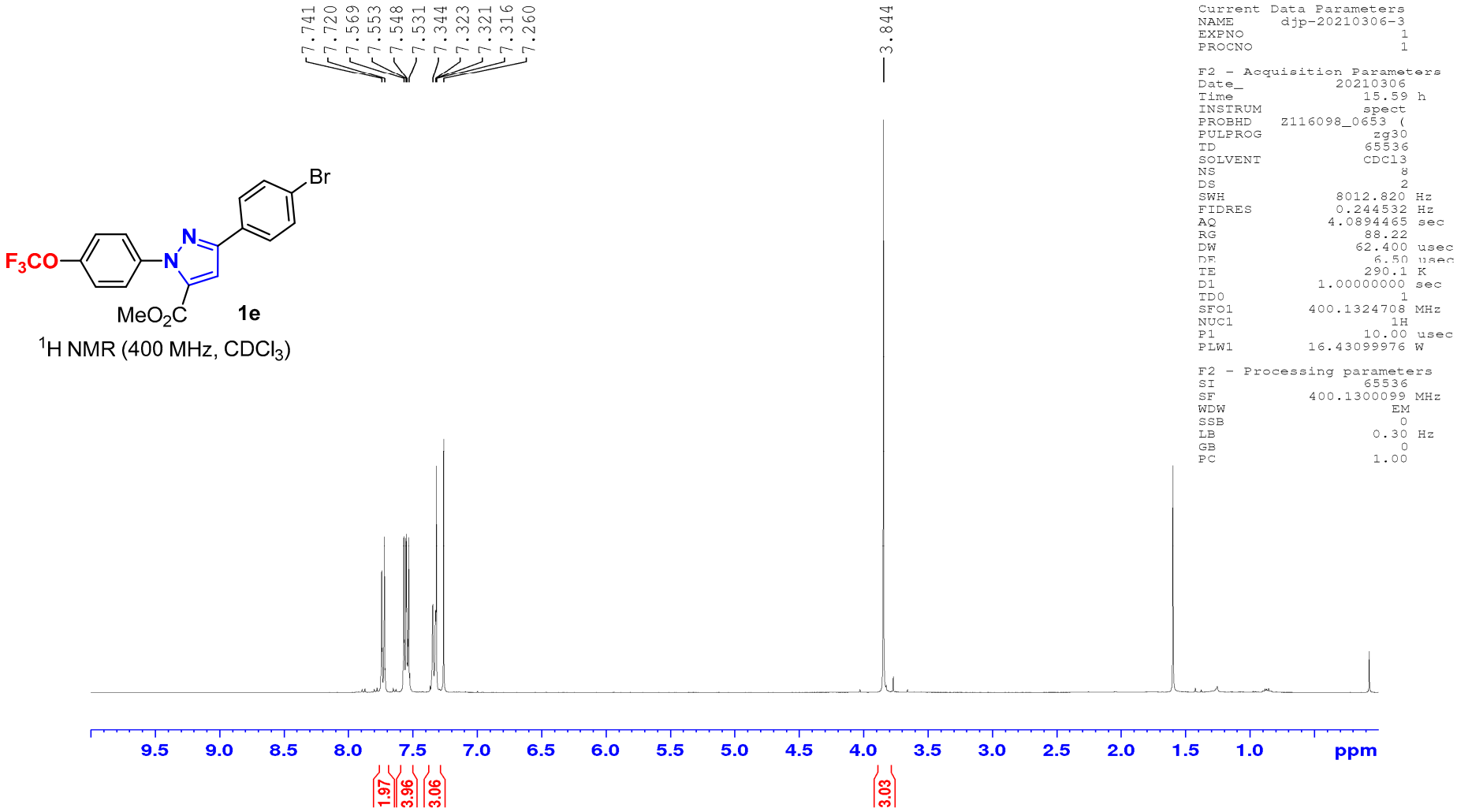

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149.12
149.11
138.73
138.69
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129.11
127.75
125.82
124.39
121.83
121.16
119.26
109.88
77.48
77.36
77.16
76.84
52.34
Me
F3CO
N
N
MeO2C
1b
13C NMR (100 MHz, CDCl3)
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PROCNO 1
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DE 6.50 usec
TE 293.5 K
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D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 75.84400177 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
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PLW12 0.20286000 W
PLW13 0.10204000 W
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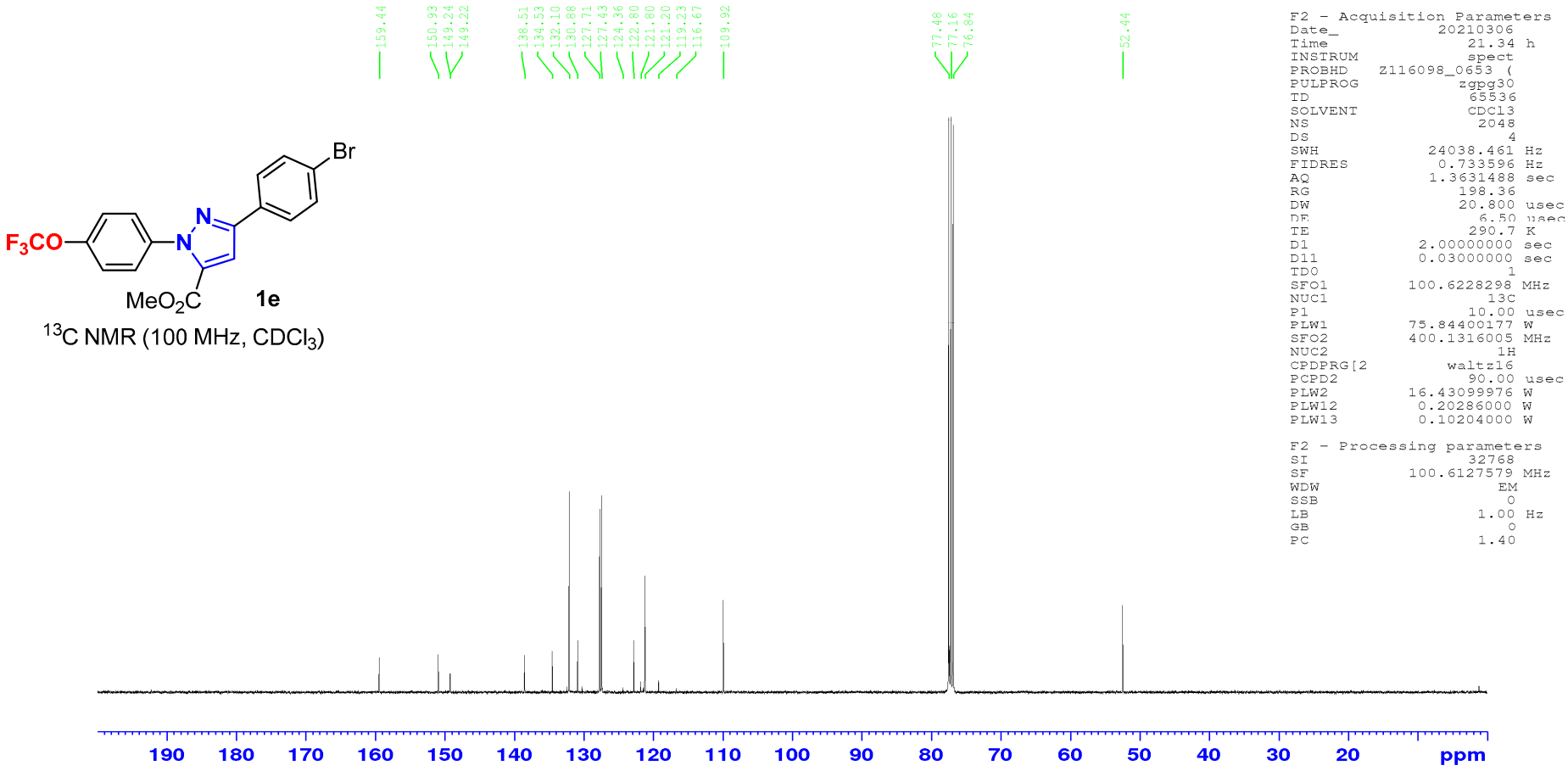

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7.122
7.100
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N
F3CO
MeO2C
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SOLVENT CDCl3
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DS 2
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RG 103.14
DW 62.400 usec
DE 6.50 usec
TE 293.8 K
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TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
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SSB 0
LB 0.30 Hz
GB 0
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2.01
2.03
2.06
1.01
2.07
3.03


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121.82
121.18
119.26
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115.83
109.79
77.47
77.16
76.84
52.40
F
F3CO
N
N
MeO2C
1c
13C NMR (100 MHz, CDCl3)
Current Data Parameters
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EXPNO 2
PROCNO 1
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TD 65536
SOLVENT CDCl3
NS 2048
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FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 198.36
DW 20.800 usec
DE 6.50 usec
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D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 75.84400177 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.43099976 W
PLW12 0.20286000 W
PLW13 0.10204000 W
F2 - Processing parameters
SI 32768
SF 100.6127564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
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30
20
ppm


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7.555
7.533
7.415
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7.344
7.324
7.312
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Cl
F3CO
N
N
MeO2C
1d
1H NMR (400 MHz, CDCl3)
Current Data Parameters
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PROCNO 1
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TD 65536
SOLVENT CDCl3
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LB 0.30 Hz
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3.0
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1.0
ppm
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2.00
2.01
2.99
3.01


159.45
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149.24
138.55
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134.54
130.46
129.16
127.72
127.17
121.82
121.19
119.25
109.94
77.47
77.16
76.84
52.42
Cl
F3CO
N
N
MeO2C
1d
13C NMR (100 MHz, CDCl3)
Current Data Parameters
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EXPNO 2
PROCNO 1
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RG 198.36
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NUC1 13C
P1 10.00 usec
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SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
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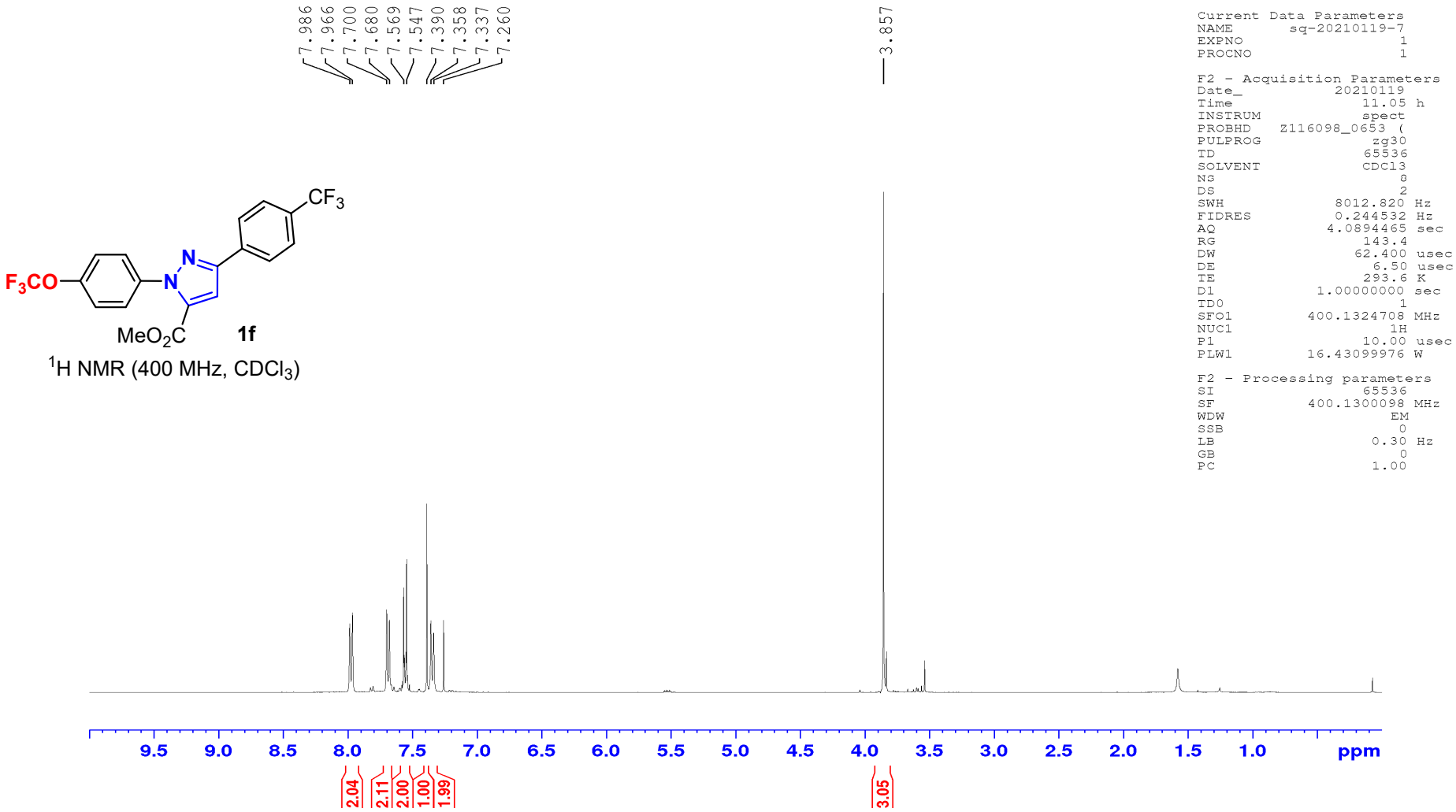

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N
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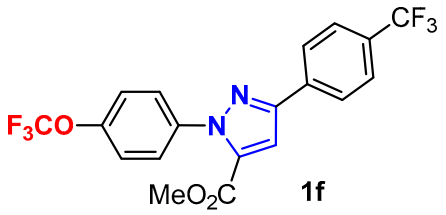



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7.547
7.390
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7.337
7.260
3.857
CF3
F3CO
N
N
MeO2C
1f
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PROCNO 1
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3.05



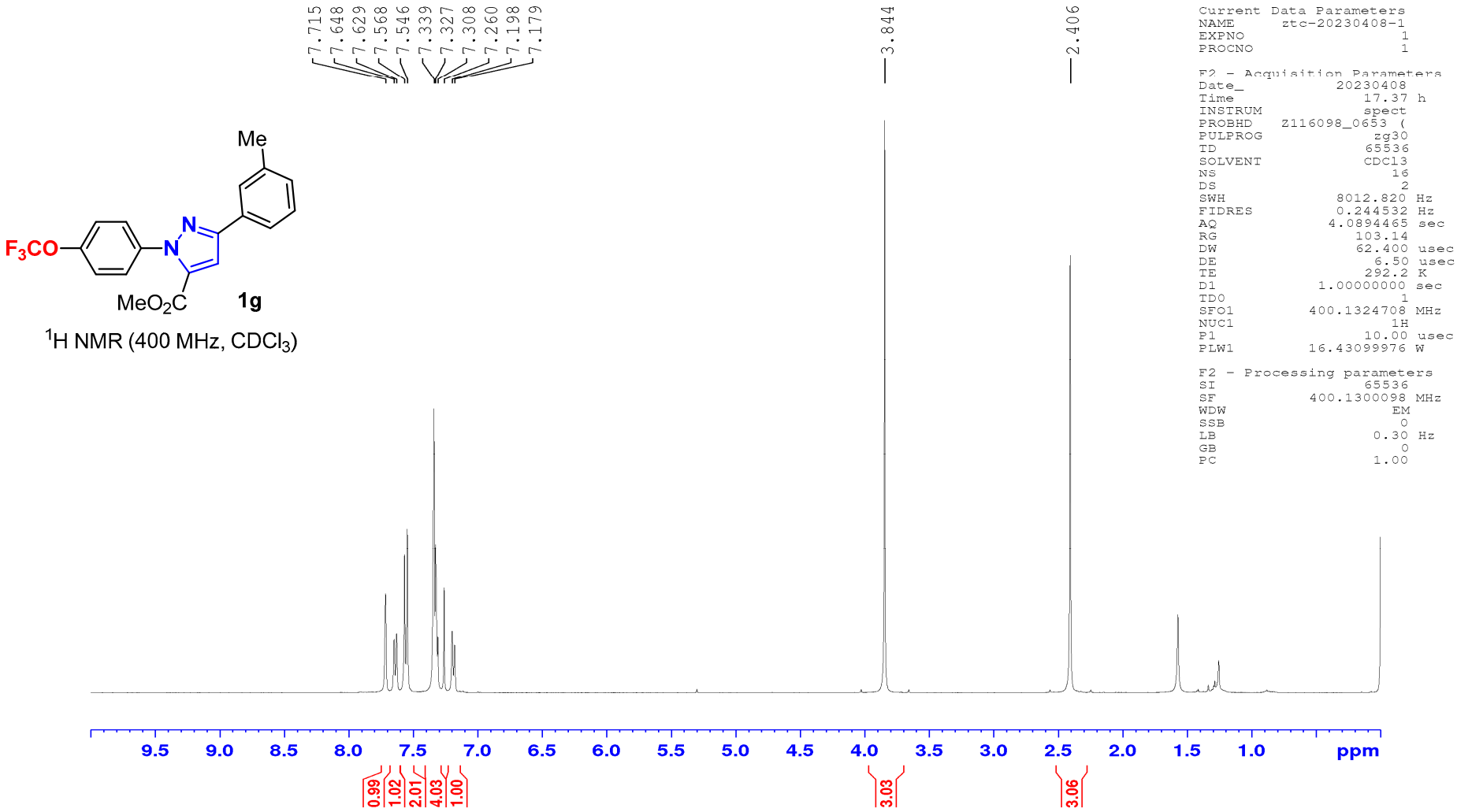
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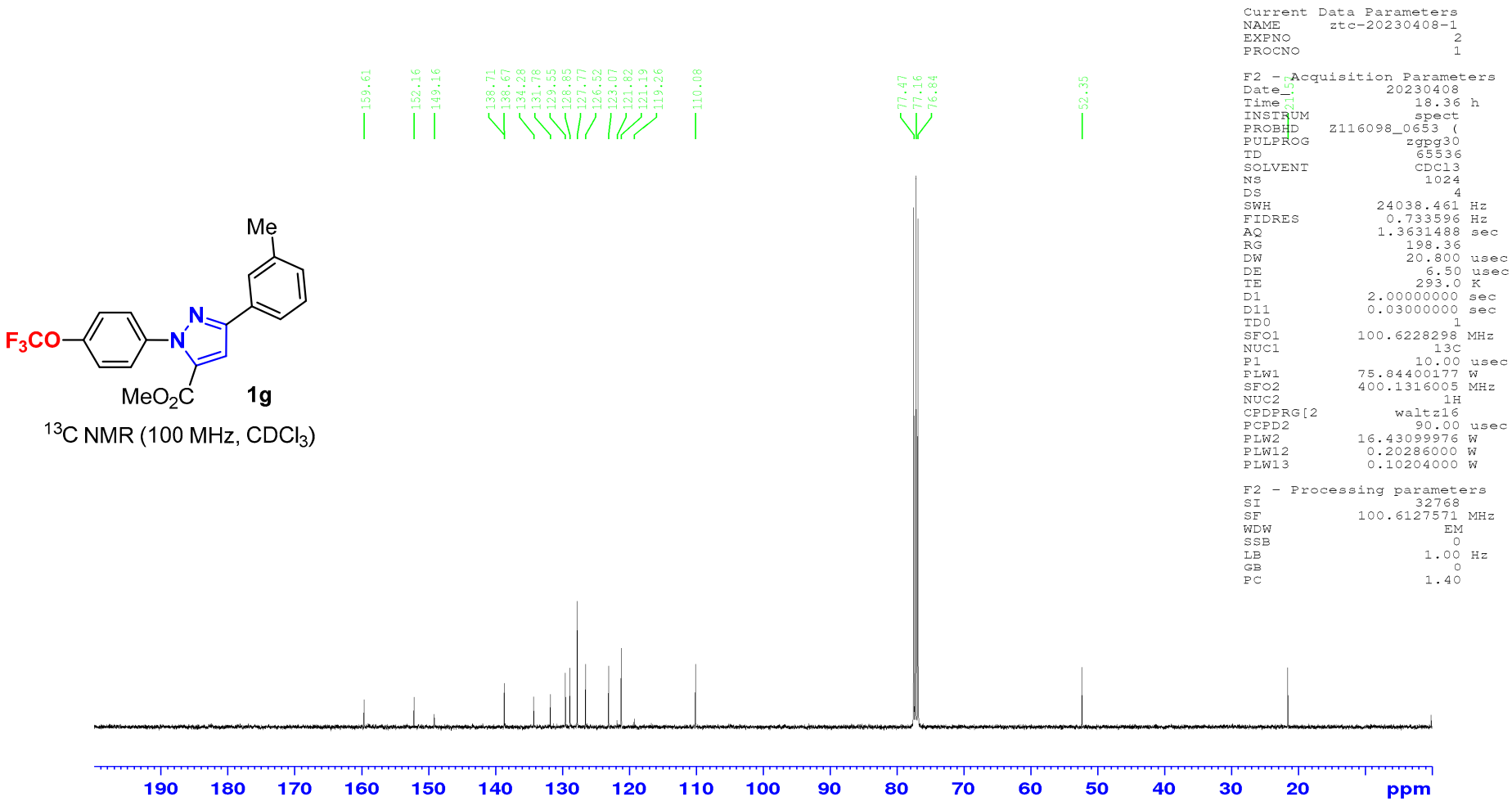
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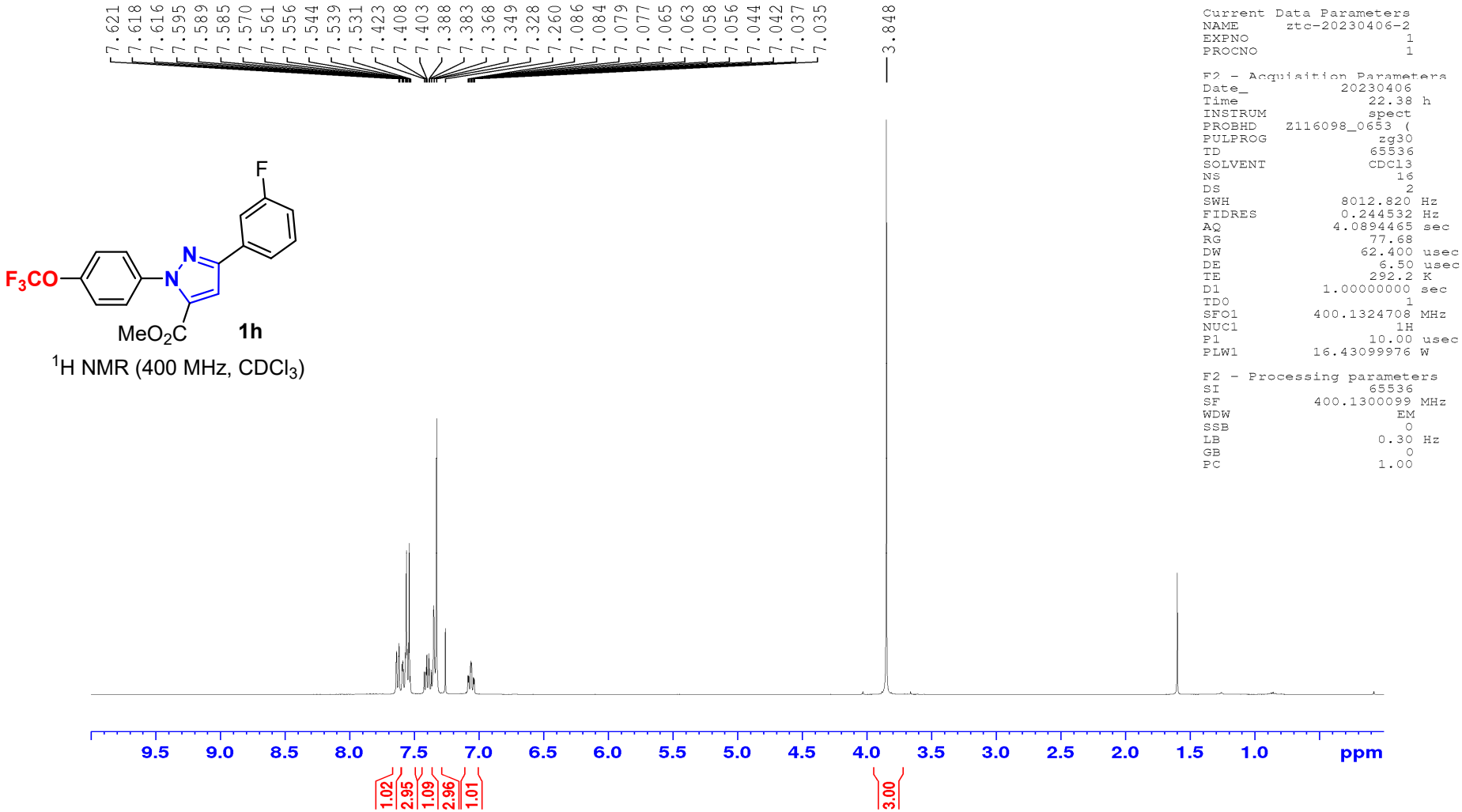

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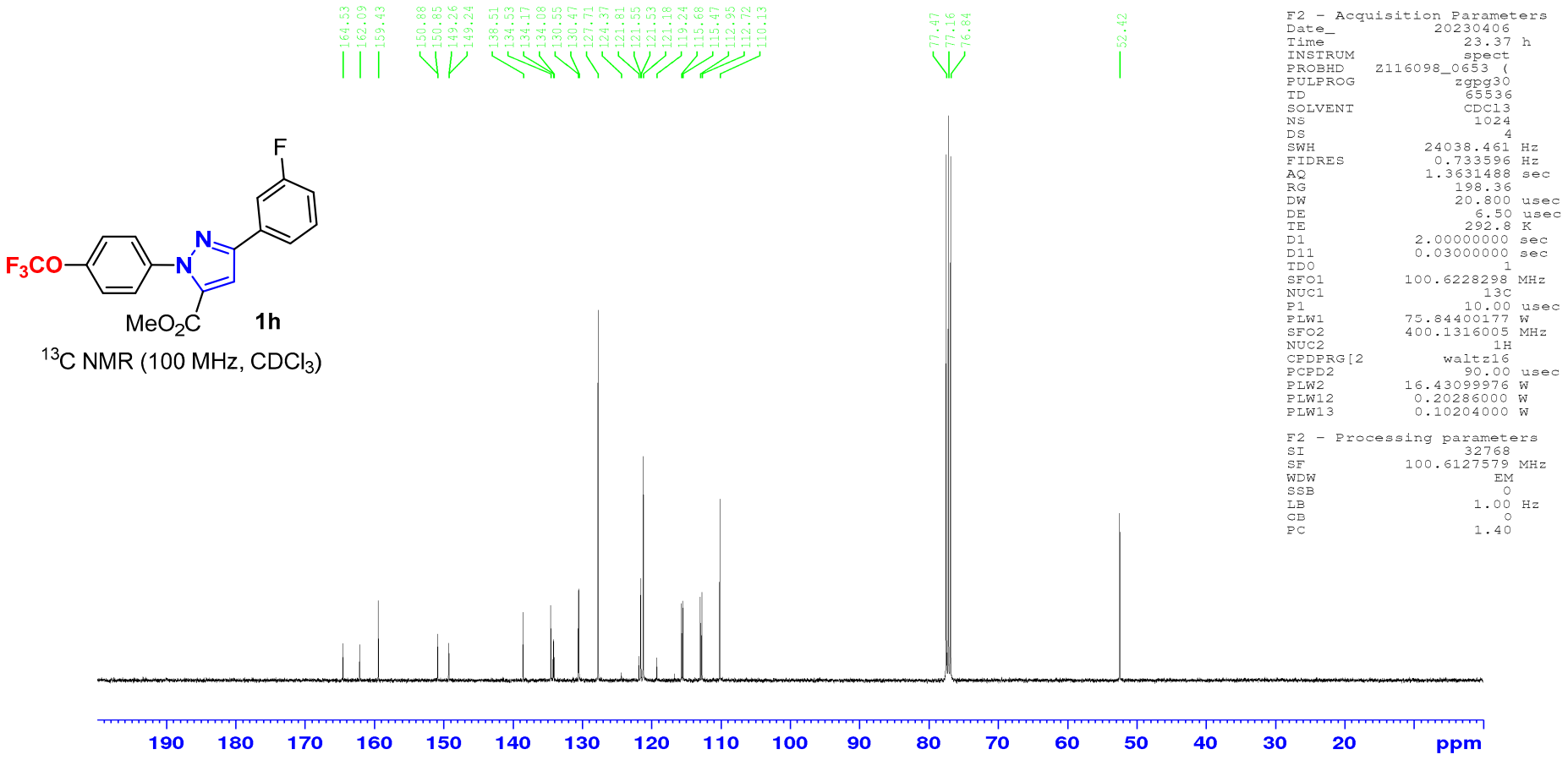
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RG                 198.36
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DE                   6.50 usec
TE                  294.7 K
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NUC1                  13C
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PLW1          75.84400177 W
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NUC2                  1H
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PCPD2               90.00 usec
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PLW12          0.20286000 W
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F3CO
N
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MeO2C
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Current Data Parameters
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INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 103.14
DW 62.400 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
0.99
1.02
2.01
4.03
1.00
3.03
3.06


159.61
152.16
149.16
138.71
138.67
134.28
131.78
129.55
128.85
127.77
126.52
123.07
121.82
121.19
119.26
110.08
77.47
77.16
76.84
52.35
Me
F3CO
N
N
MeO2C
1g
13C NMR (100 MHz, CDCl3)
Current Data Parameters
NAME ztc-20230408-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230408
Time 18.36 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 198.36
DW 20.800 usec
DE 6.50 usec
TE 293.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 75.84400177 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.43099976 W
PLW12 0.20286000 W
PLW13 0.10204000 W
F2 - Processing parameters
SI 32768
SF 100.6127571 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

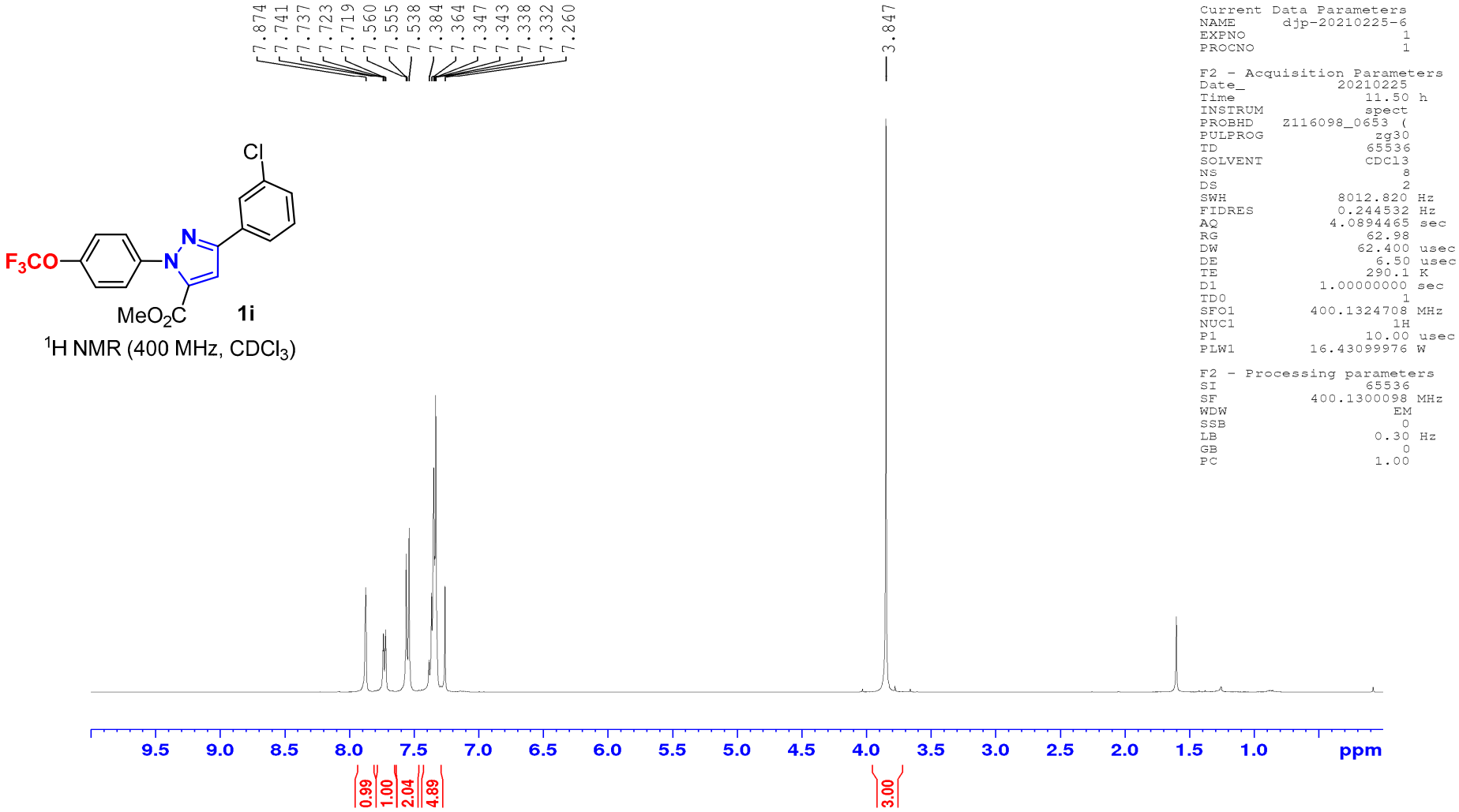

7.621
7.618
7.616
7.595
7.589
7.585
7.570
7.561
7.556
7.544
7.539
7.531
7.423
7.408
7.403
7.388
7.383
7.368
7.349
7.328
7.260
7.086
7.084
7.079
7.077
7.065
7.063
7.058
7.056
7.044
7.042
7.037
7.035
3.848
F
F3CO
N
N
MeO2C
1h
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME ztc-20230406-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230406
Time 22.38 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 77.68
DW 62.400 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
1.02
2.95
1.09
2.96
1.01
3.00

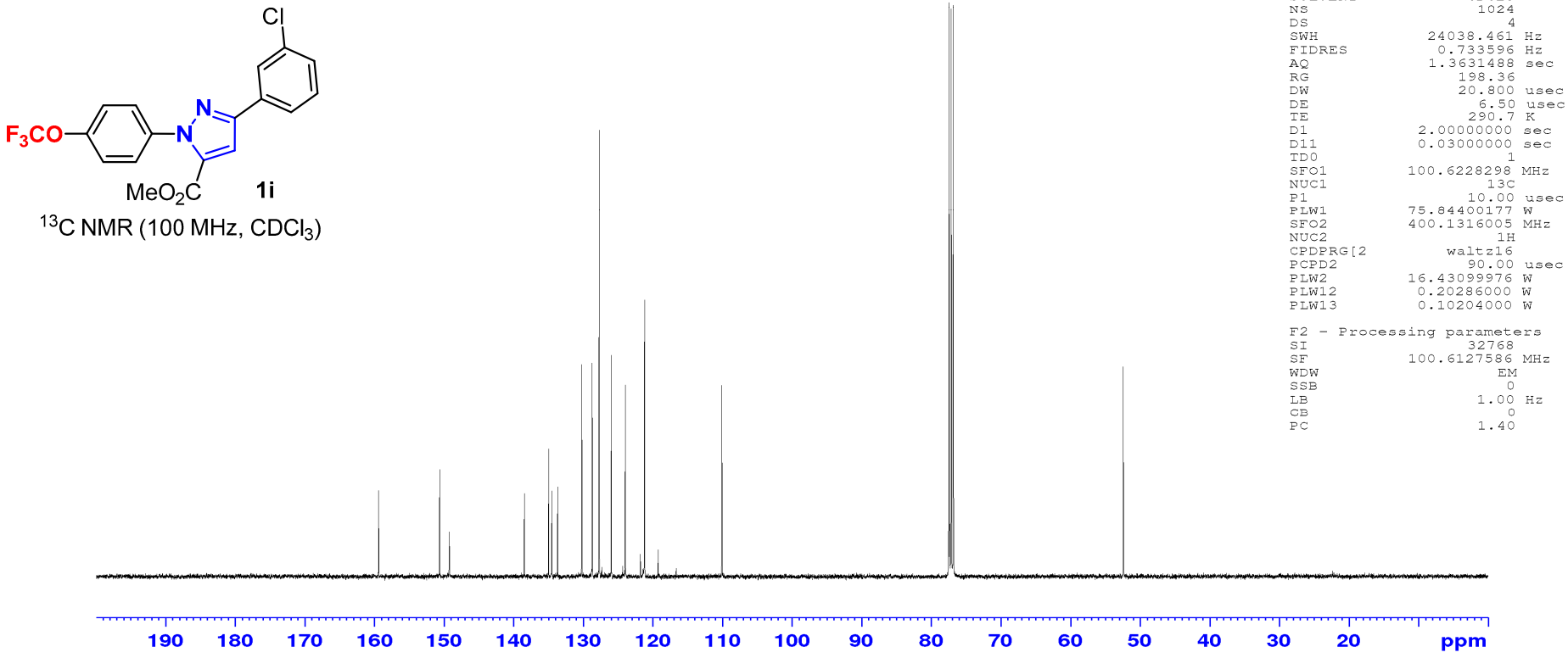



```
Current Data Parameters
NAME      ztc-20230406-2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230406
Time               23.37 h
INSTRUM            spect
PROBHD    Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                198.36
DW                20.800 usec
DE                 6.50 usec
TE                292.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1               13C
P1                10.00 usec
PLW1        75.84400177 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2             90.00 usec
PLW2        16.43099976 W
PLW12        0.20286000 W
PLW13        0.10204000 W

F2 - Processing parameters
SI                32768
SF          100.6127579 MHz
WDW                EM
SSB                0
LB              1.00 Hz
GB                 0
PC              1.40
```

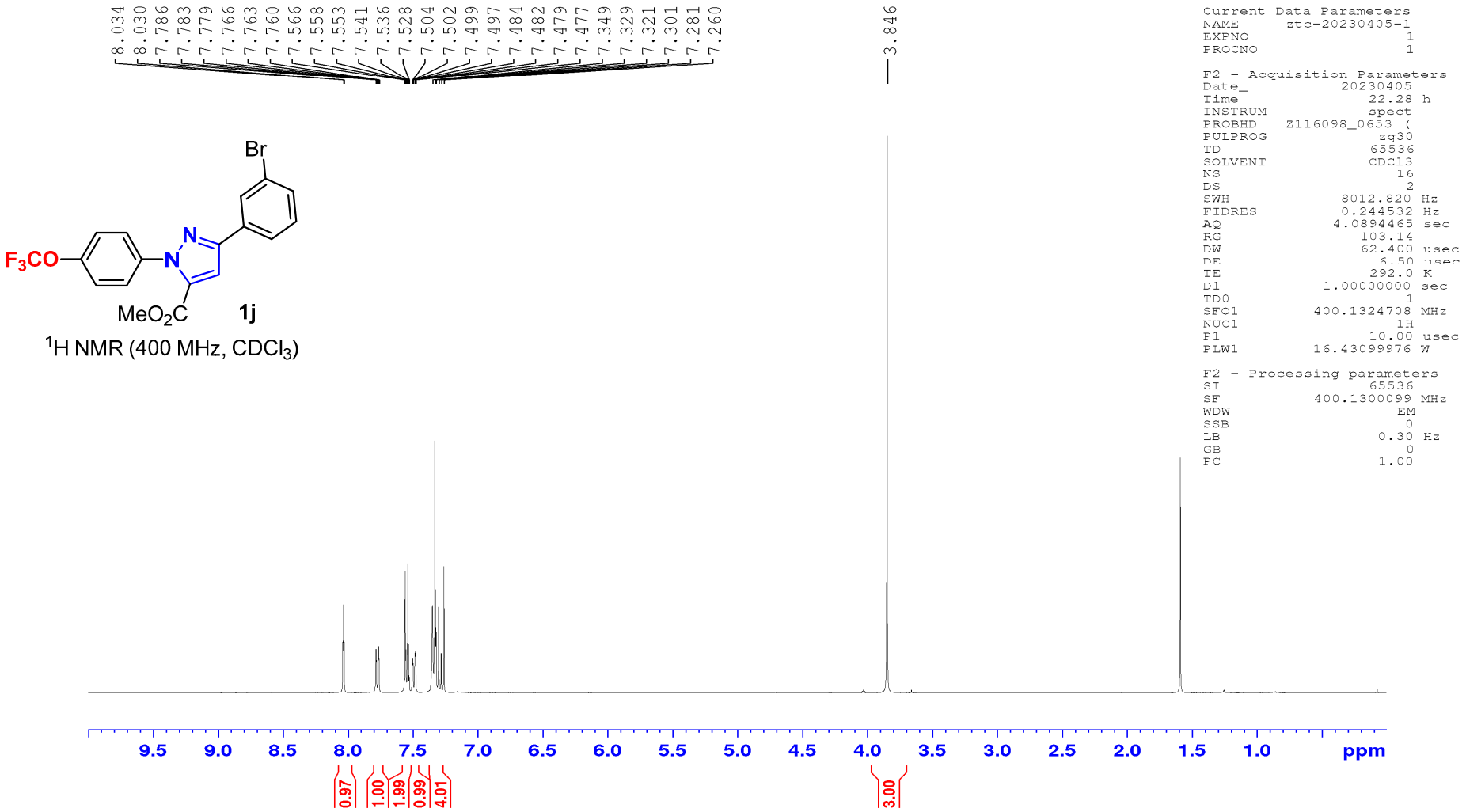

7.874
7.741
7.737
7.723
7.719
7.560
7.555
7.538
7.384
7.364
7.347
7.343
7.338
7.332
7.260
3.847
Cl
N
N
F3CO
MeO2C
1i
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME djp-20210225-6
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210225
Time 11.50 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 62.98
DW 62.400 usec
DE 6.50 usec
TE 290.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
0.99
1.00
2.04
4.89
3.00

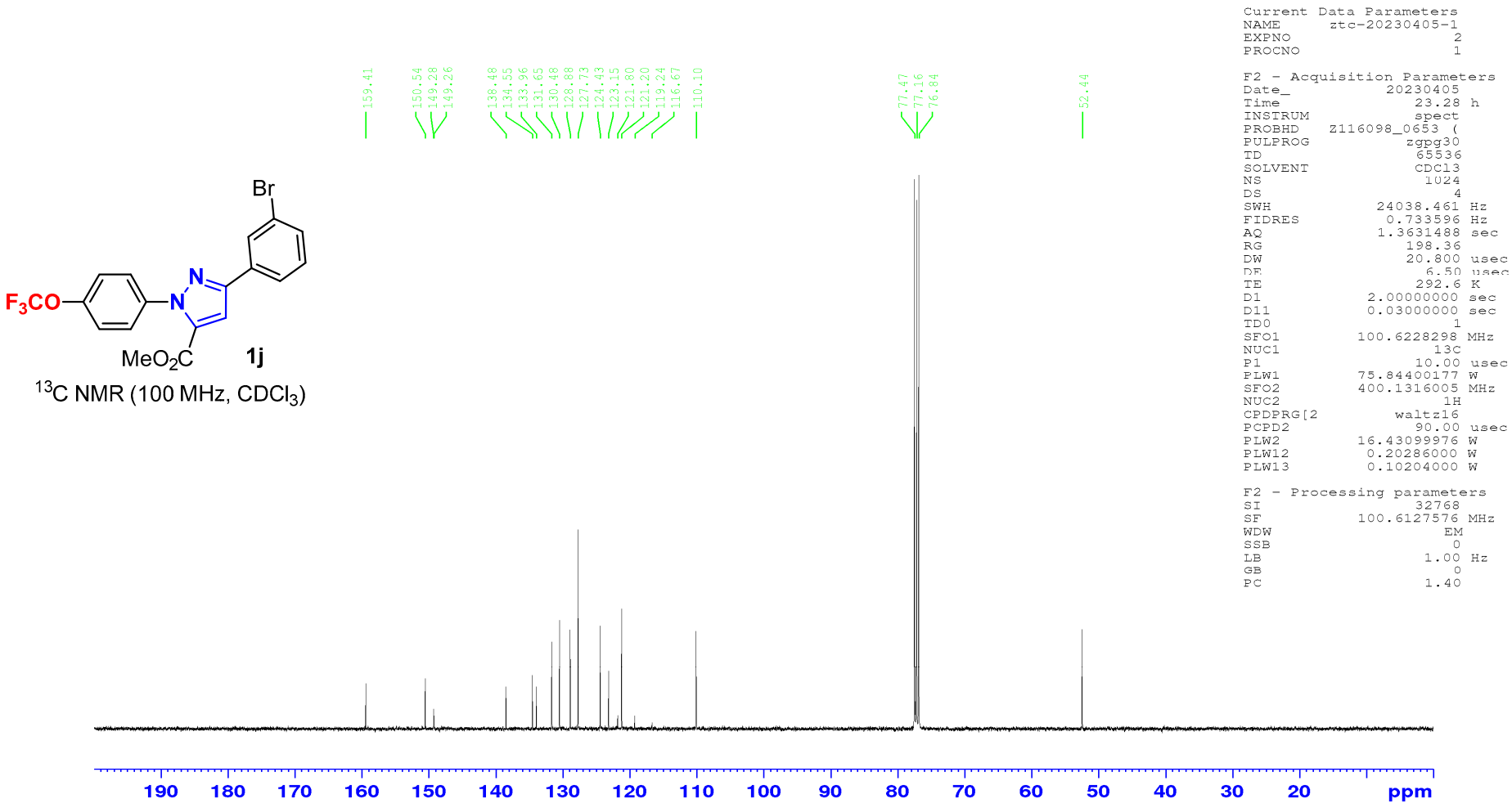



```
Current Data Parameters
NAME      djp-20210225-6
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210225
Time              23.39 h
INSTRUM             spect
PROBHD   Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                198.36
DW                20.800 usec
DE                 6.50 usec
TE                290.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         75.84400177 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         16.43099976 W
PLW12         0.20286000 W
PLW13         0.10204000 W

F2 - Processing parameters
SI                 32768
SF          100.6127586 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

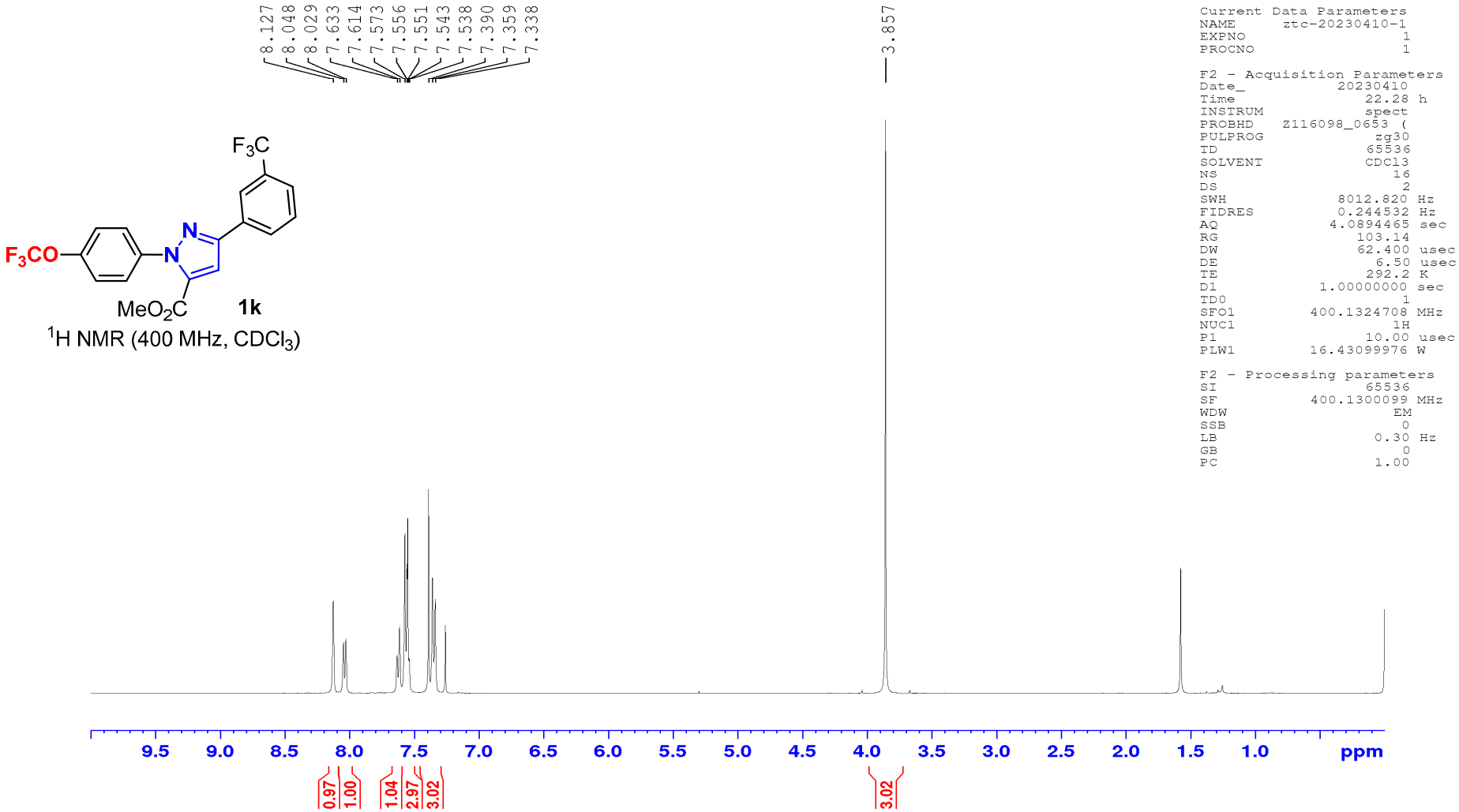

8.034
8.030
7.786
7.783
7.779
7.766
7.763
7.760
7.566
7.558
7.553
7.541
7.536
7.528
7.504
7.502
7.499
7.497
7.484
7.482
7.479
7.477
7.349
7.329
7.321
7.301
7.281
7.260
3.846
Br
F3CO
N
N
MeO2C
1j
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME ztc-20230405-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230405
Time 22.28 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 103.14
DW 62.400 usec
DE 6.50 usec
TE 292.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
0.97
1.00
1.99
0.99
4.01
3.00

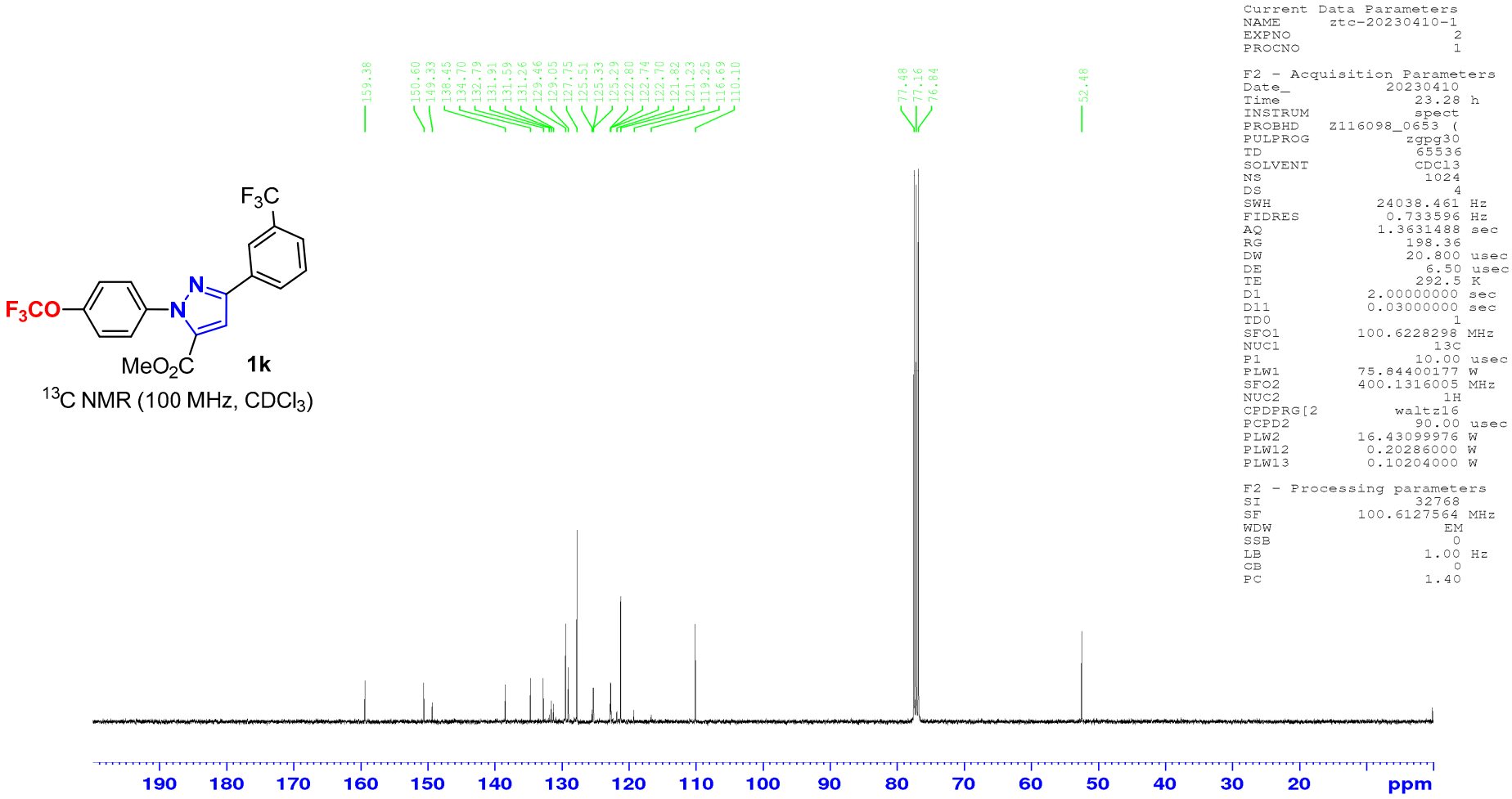



```
Current Data Parameters
NAME      ztc-20230405-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230405
Time              23.28 h
INSTRUM             spect
PROBHD    Z116098_0653 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                198.36
DW                20.800 usec
DE                 6.50 usec
TE                292.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        75.84400177 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        16.43099976 W
PLW12        0.20286000 W
PLW13        0.10204000 W

F2 - Processing parameters
SI                32768
SF          100.6127576 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

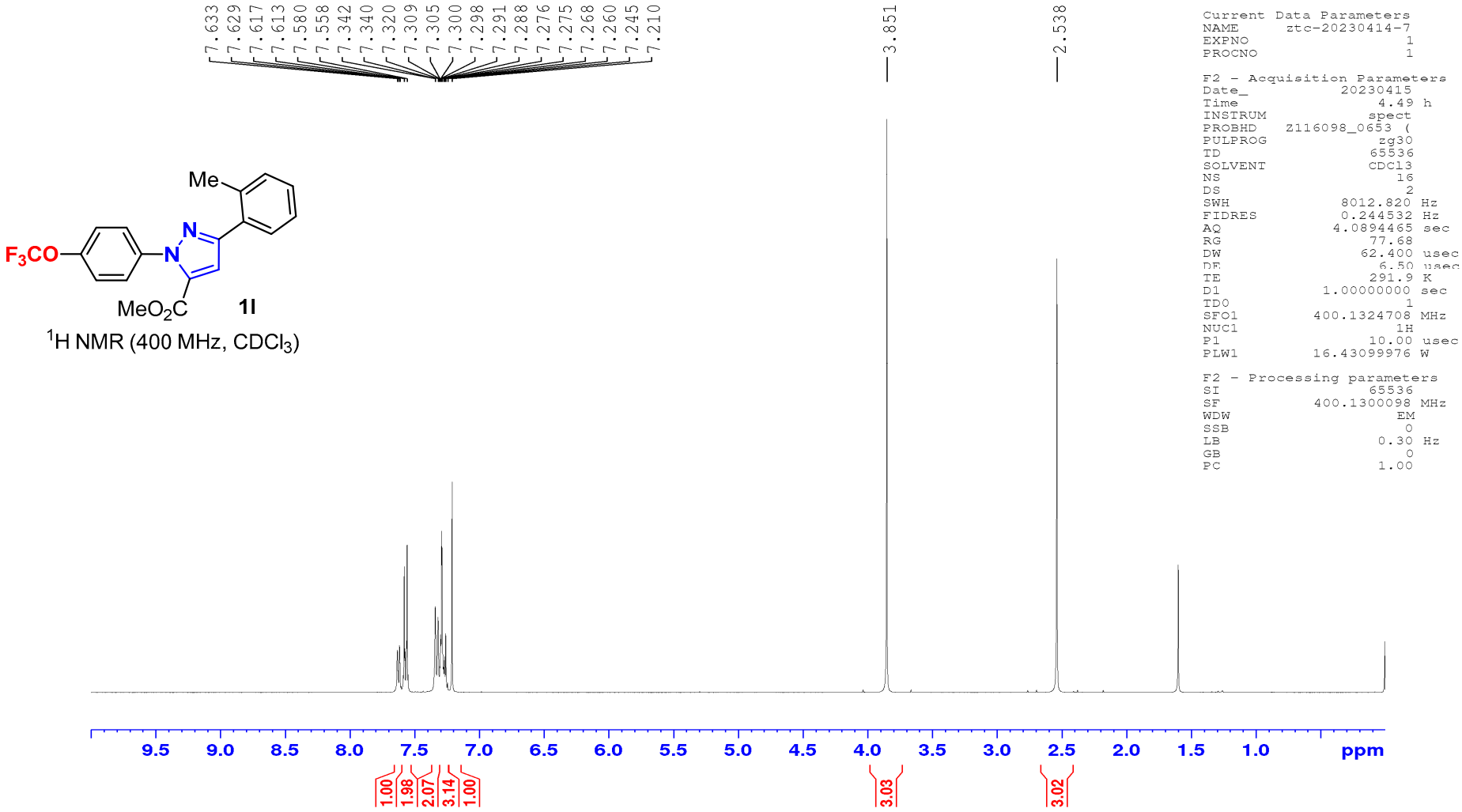

8.127
8.048
8.029
7.633
7.614
7.573
7.556
7.551
7.543
7.538
7.390
7.359
7.338
3.857
F3C
F3CO
N
N
MeO2C
1k
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME ztc-20230410-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230410
Time 22.28 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 103.14
DW 62.400 usec
DE 6.50 usec
TE 292.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
0.97
1.00
1.04
2.97
3.02
3.02

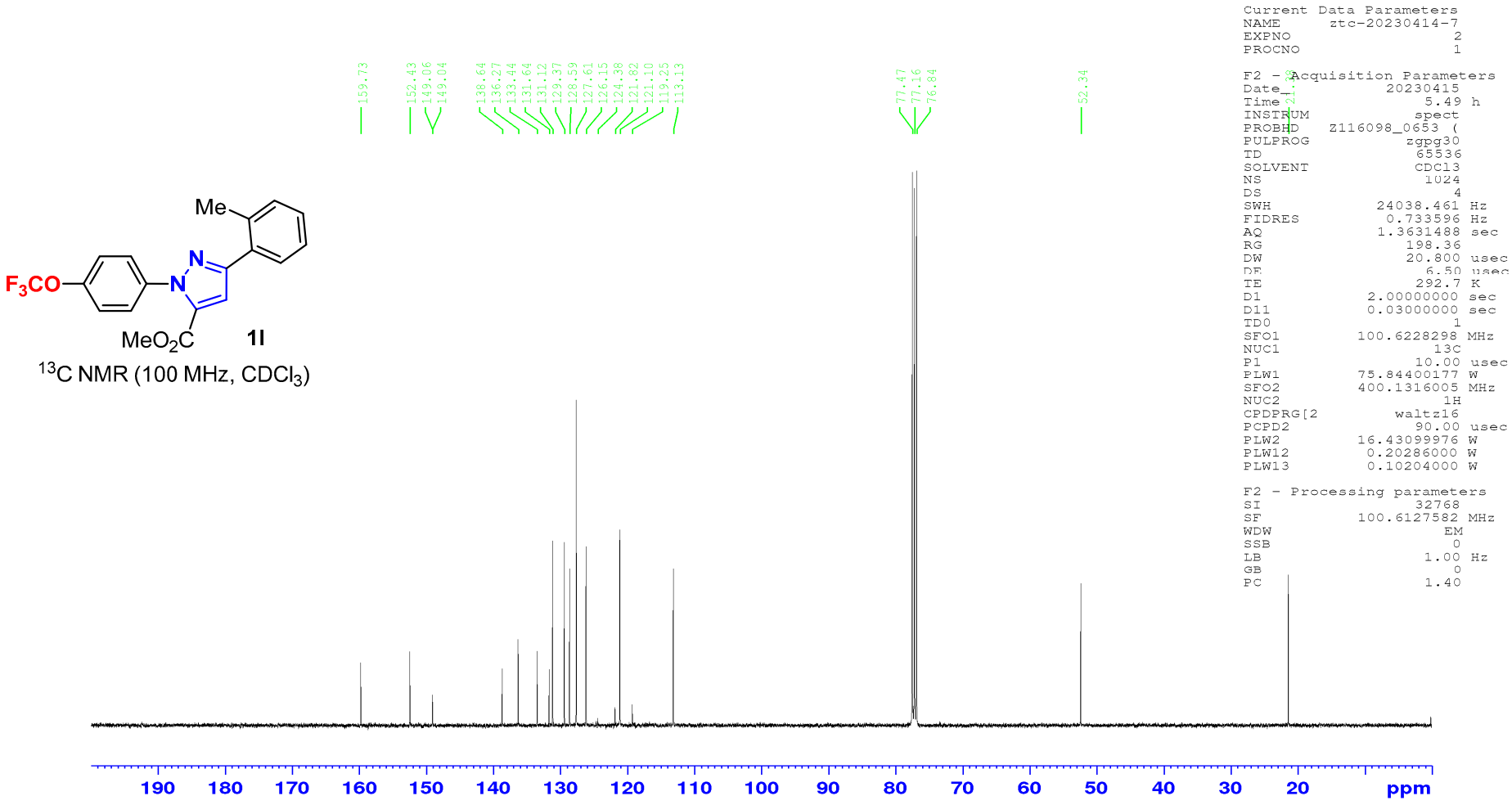



```
Current Data Parameters
NAME      ztc-20230410-1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230410
Time              23.28 h
INSTRUM             spect
PROBHD   Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                198.36
DW                20.800 usec
DE                 6.50 usec
TE                292.5 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        75.84400177 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        16.43099976 W
PLW12        0.20286000 W
PLW13        0.10204000 W

F2 - Processing parameters
SI                32768
SF          100.6127564 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

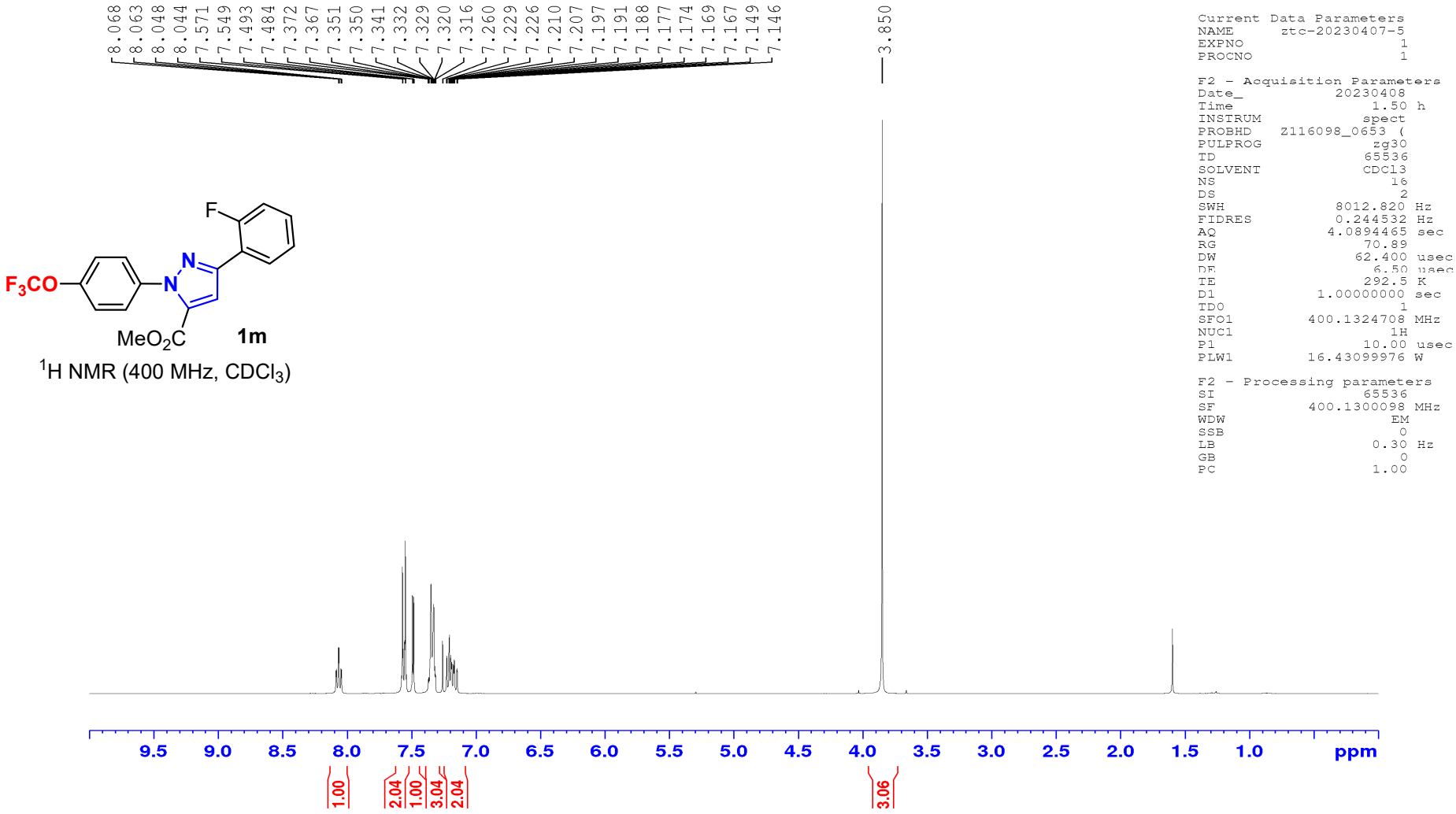

7.633
7.629
7.617
7.613
7.580
7.558
7.342
7.340
7.320
7.309
7.305
7.300
7.298
7.291
7.288
7.276
7.275
7.268
7.260
7.245
7.210
3.851
2.538
Me
F3CO
N
N
MeO2C
1l
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME ztc-20230414-7
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230415
Time 4.49 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 77.68
DW 62.400 usec
DE 6.50 usec
TE 291.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
1.00
1.98
2.07
3.14
1.00
3.03
3.02

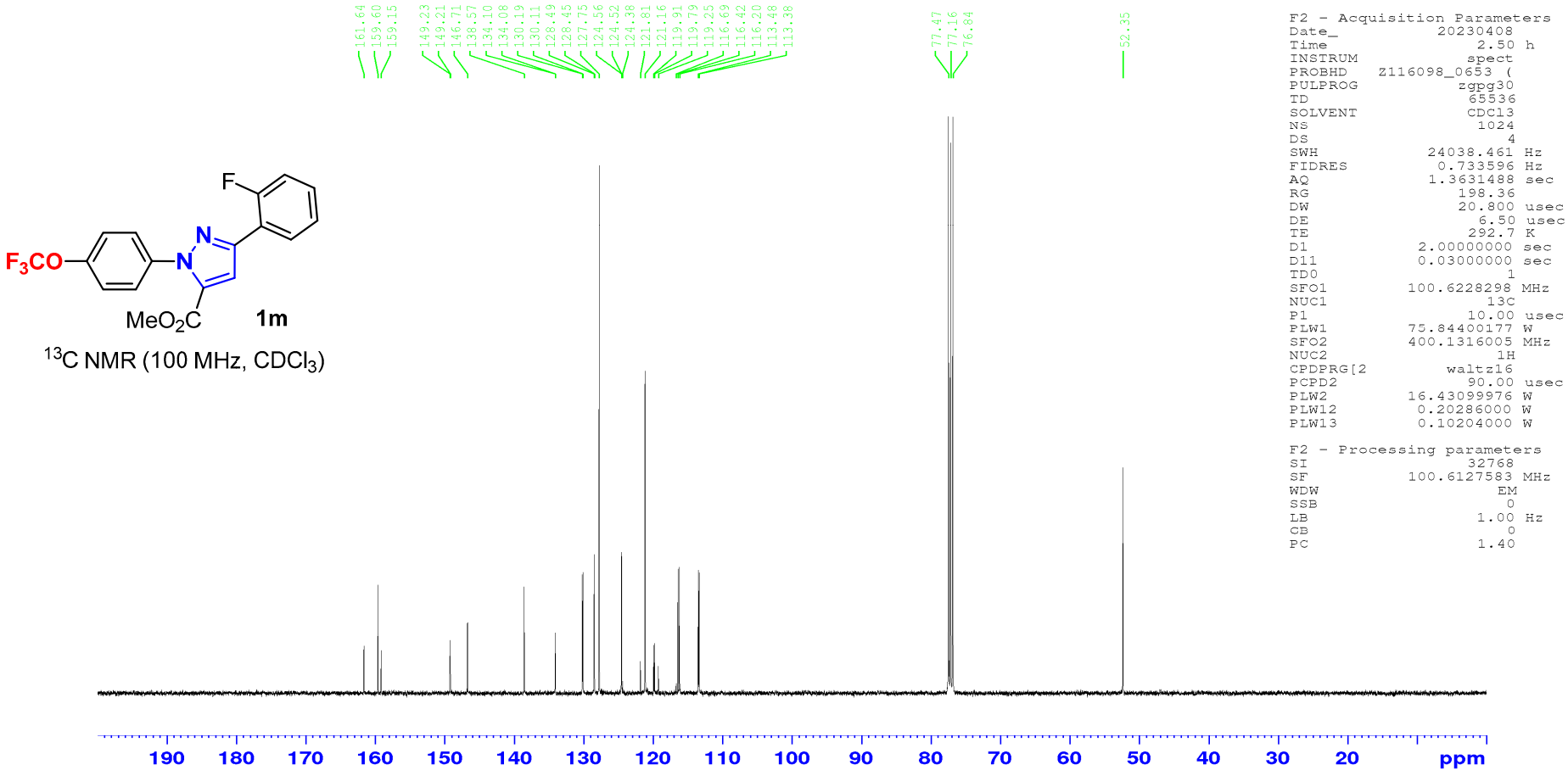



```
Current Data Parameters
NAME      ztc-20230414-7
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230415
Time              5.49 h
INSTRUM            spect
PROBHD   Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG               198.36
DW               20.800 usec
DE                6.50 usec
TE               292.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        75.84400177 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        16.43099976 W
PLW12        0.20286000 W
PLW13        0.10204000 W

F2 - Processing parameters
SI                32768
SF          100.6127582 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

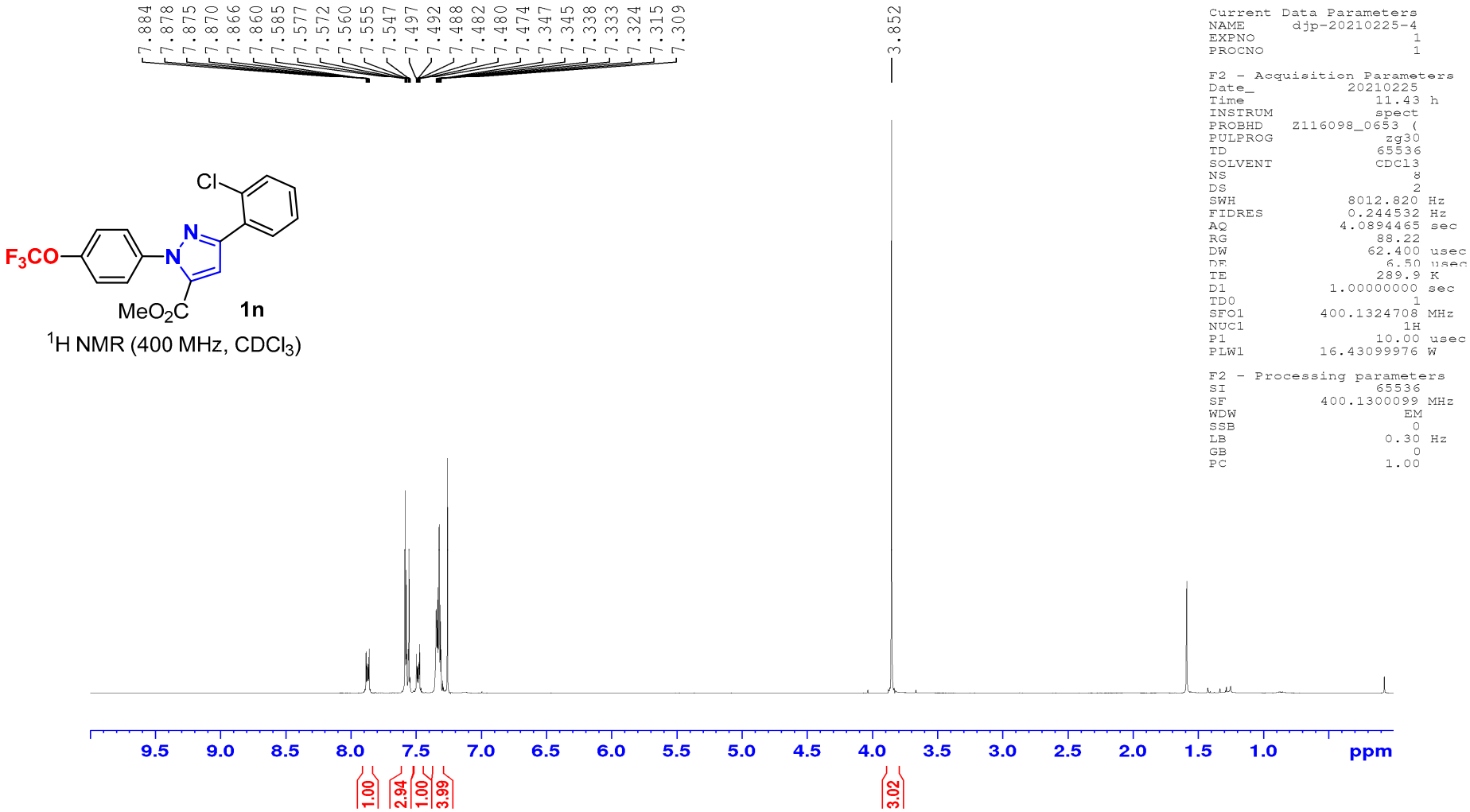

8.068
8.063
8.048
8.044
7.571
7.549
7.493
7.484
7.372
7.367
7.351
7.350
7.341
7.332
7.329
7.320
7.316
7.260
7.229
7.226
7.210
7.207
7.197
7.191
7.188
7.177
7.174
7.169
7.167
7.149
7.146
3.850
F
F3CO
N
N
MeO2C
1m
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME ztc-20230407-5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230408
Time 1.50 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 70.89
DW 62.400 usec
DE 6.50 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
1.00
2.04
1.00
3.04
2.04
3.06

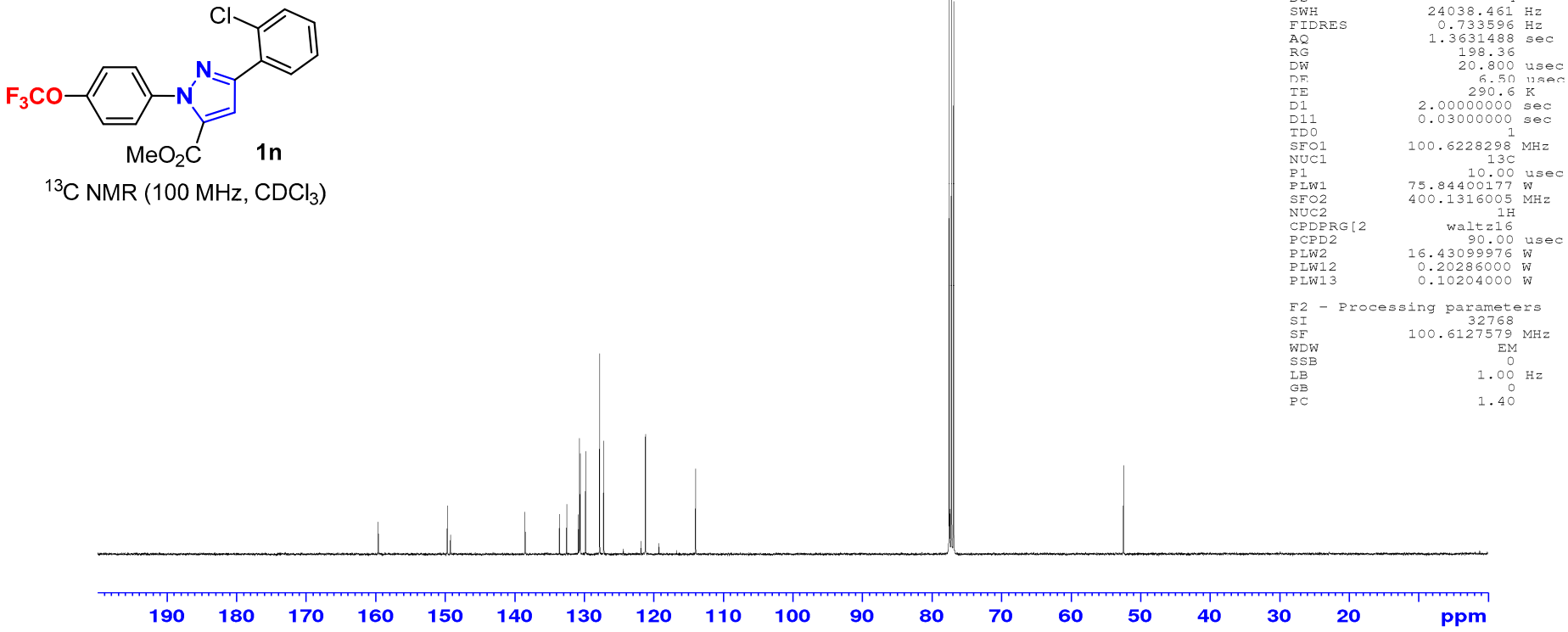



```
Current Data Parameters
NAME       ztc-20230407-5
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_              20230408
Time                 2.50 h
INSTRUM              spect
PROBHD    Z116098_0653 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES          0.733596 Hz
AQ              1.3631488 sec
RG                 198.36
DW                 20.800 usec
DE                   6.50 usec
TE                  292.7 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1          100.6228298 MHz
NUC1                  13C
P1                  10.00 usec
PLW1          75.84400177 W
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          16.43099976 W
PLW12          0.20286000 W
PLW13          0.10204000 W

F2 - Processing parameters
SI                  32768
SF            100.6127583 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

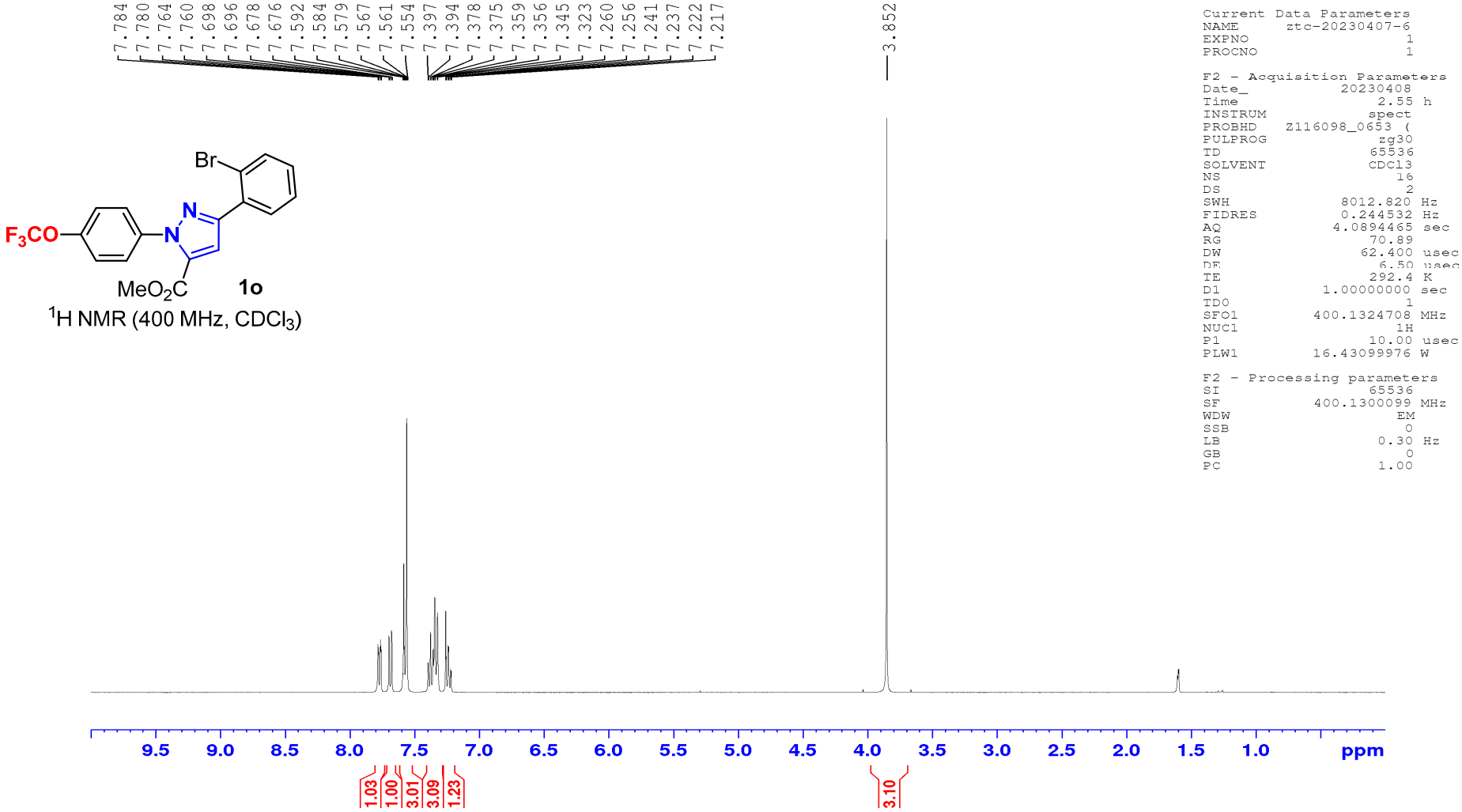

7.884
7.878
7.875
7.870
7.866
7.860
7.585
7.577
7.572
7.560
7.555
7.547
7.497
7.492
7.488
7.482
7.480
7.474
7.347
7.345
7.338
7.333
7.324
7.315
7.309
3.852
Cl
N
N
F3CO
MeO2C
1n
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME djp-20210225-4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210225
Time 11.43 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 88.22
DW 62.400 usec
DE 6.50 usec
TE 289.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
1.00
2.94
1.00
3.99
3.02

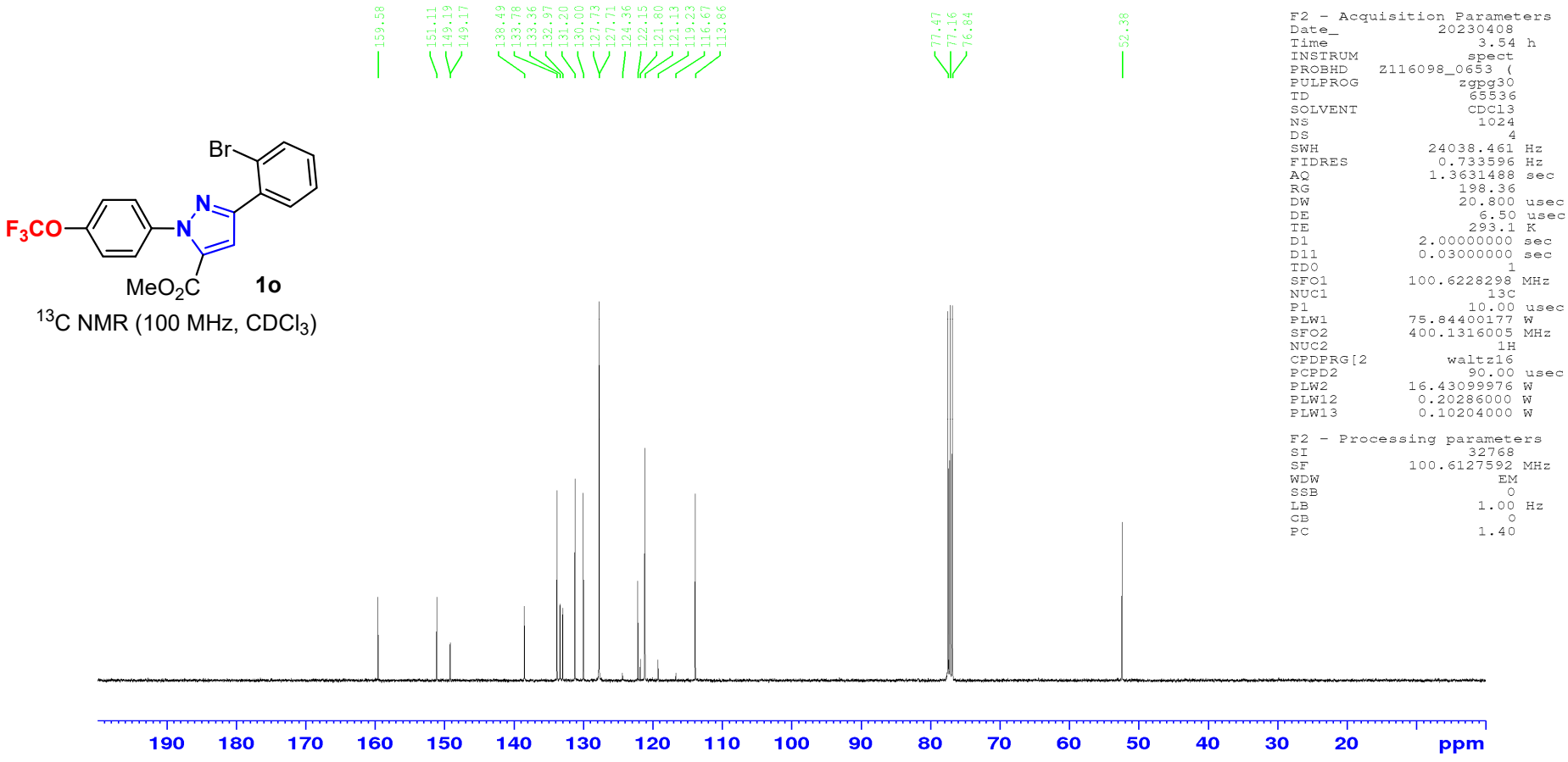



```
Current Data Parameters
NAME      djp-20210225-4
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210225
Time               22.37 h
INSTRUM             spect
PROBHD    Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3000
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                198.36
DW                20.800 usec
DE                 6.50 usec
TE                290.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         75.84400177 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         16.43099976 W
PLW12         0.20286000 W
PLW13         0.10204000 W

F2 - Processing parameters
SI                32768
SF           100.6127579 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

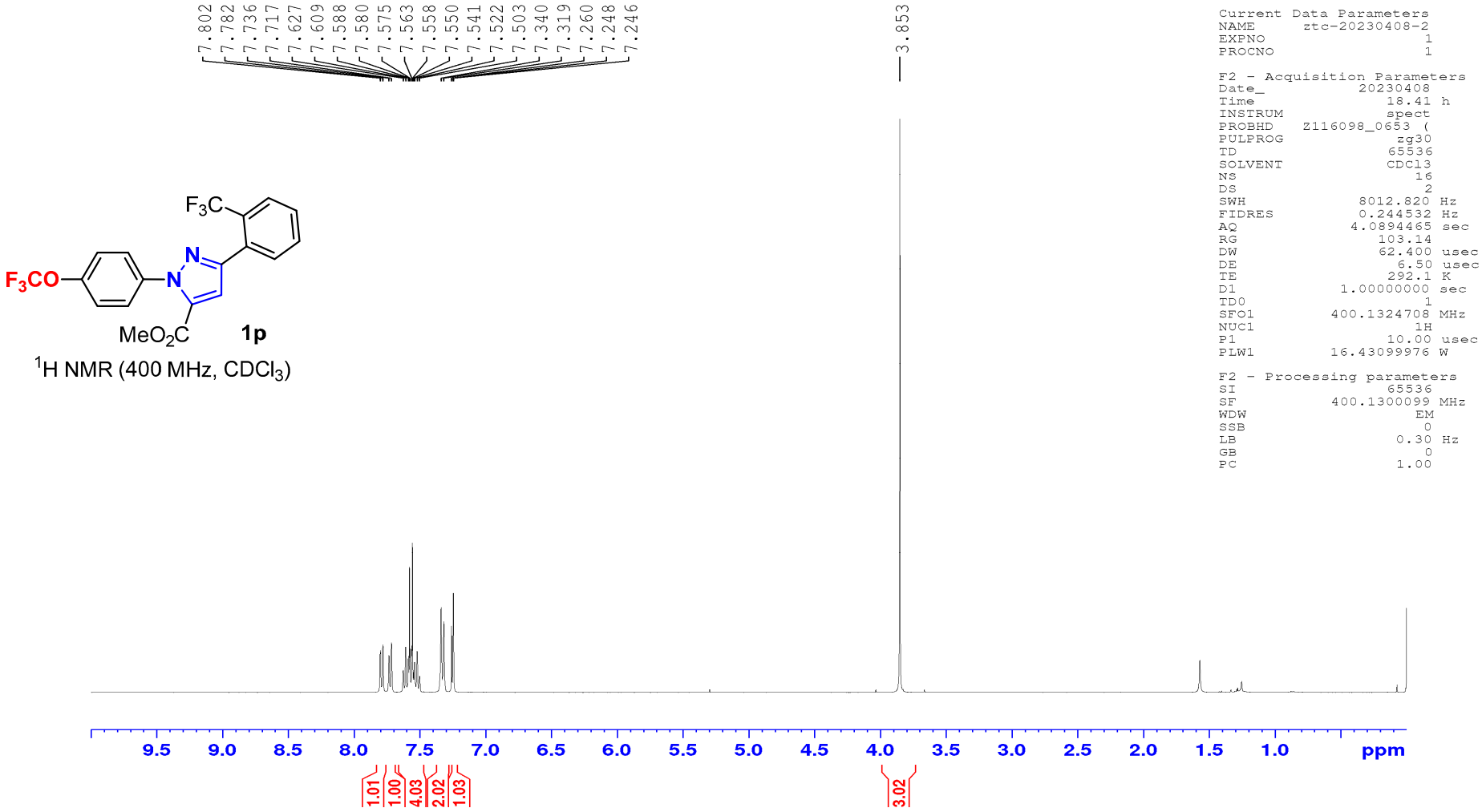

7.784
7.780
7.764
7.760
7.698
7.696
7.678
7.676
7.592
7.584
7.579
7.567
7.561
7.554
7.397
7.394
7.378
7.375
7.359
7.356
7.345
7.323
7.260
7.256
7.241
7.237
7.222
7.217
3.852
Br
N
N
F3CO
MeO2C
1o
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME ztc-20230407-6
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230408
Time 2.55 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 70.89
DW 62.400 usec
DE 6.50 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
1.03
1.00
3.01
3.09
1.23
3.10

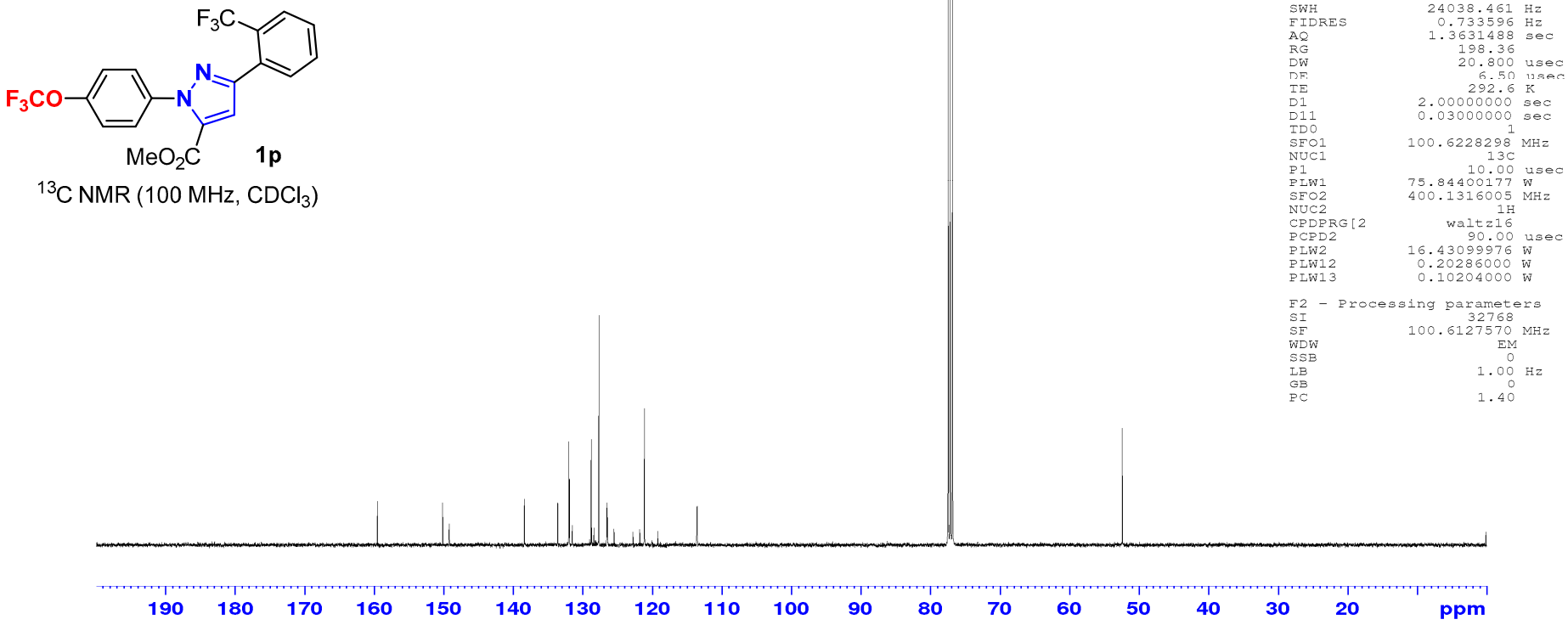



```
Current Data Parameters
NAME      ztc-20230407-6
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20230408
Time                3.54 h
INSTRUM            spect
PROBHD   Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                198.36
DW                20.800 usec
DE                 6.50 usec
TE                293.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1               13C
P1                10.00 usec
PLW1         75.84400177 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2             90.00 usec
PLW2         16.43099976 W
PLW12         0.20286000 W
PLW13         0.10204000 W

F2 - Processing parameters
SI                32768
SF          100.6127592 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

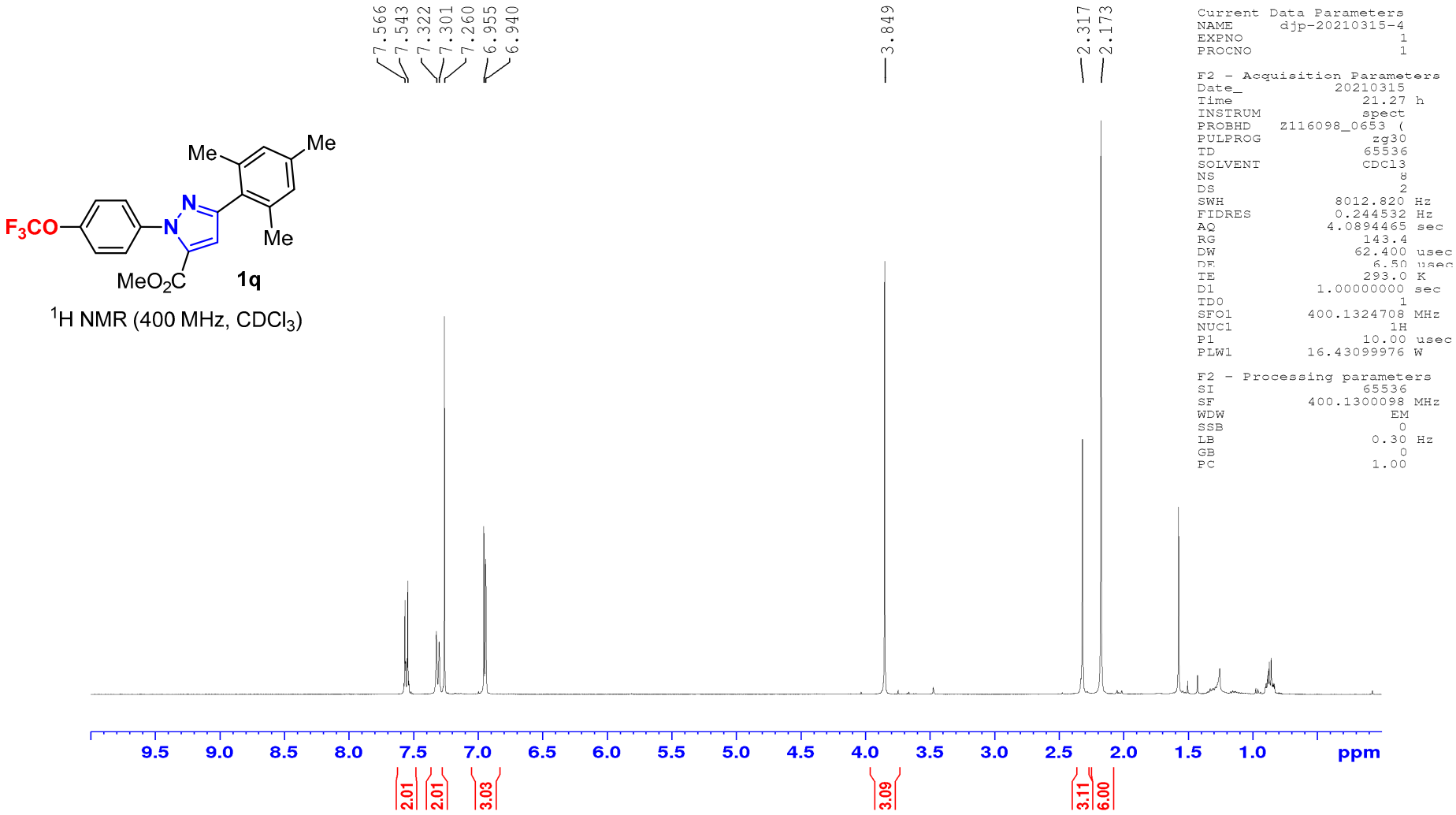

7.802
7.782
7.736
7.717
7.627
7.609
7.588
7.580
7.575
7.563
7.558
7.550
7.541
7.522
7.503
7.340
7.319
7.260
7.248
7.246
3.853
F3C
F3CO
N
N
MeO2C
1p
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME ztc-20230408-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20230408
Time 18.41 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 103.14
DW 62.400 usec
DE 6.50 usec
TE 292.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
1.01
1.00
4.03
2.02
1.03
3.02

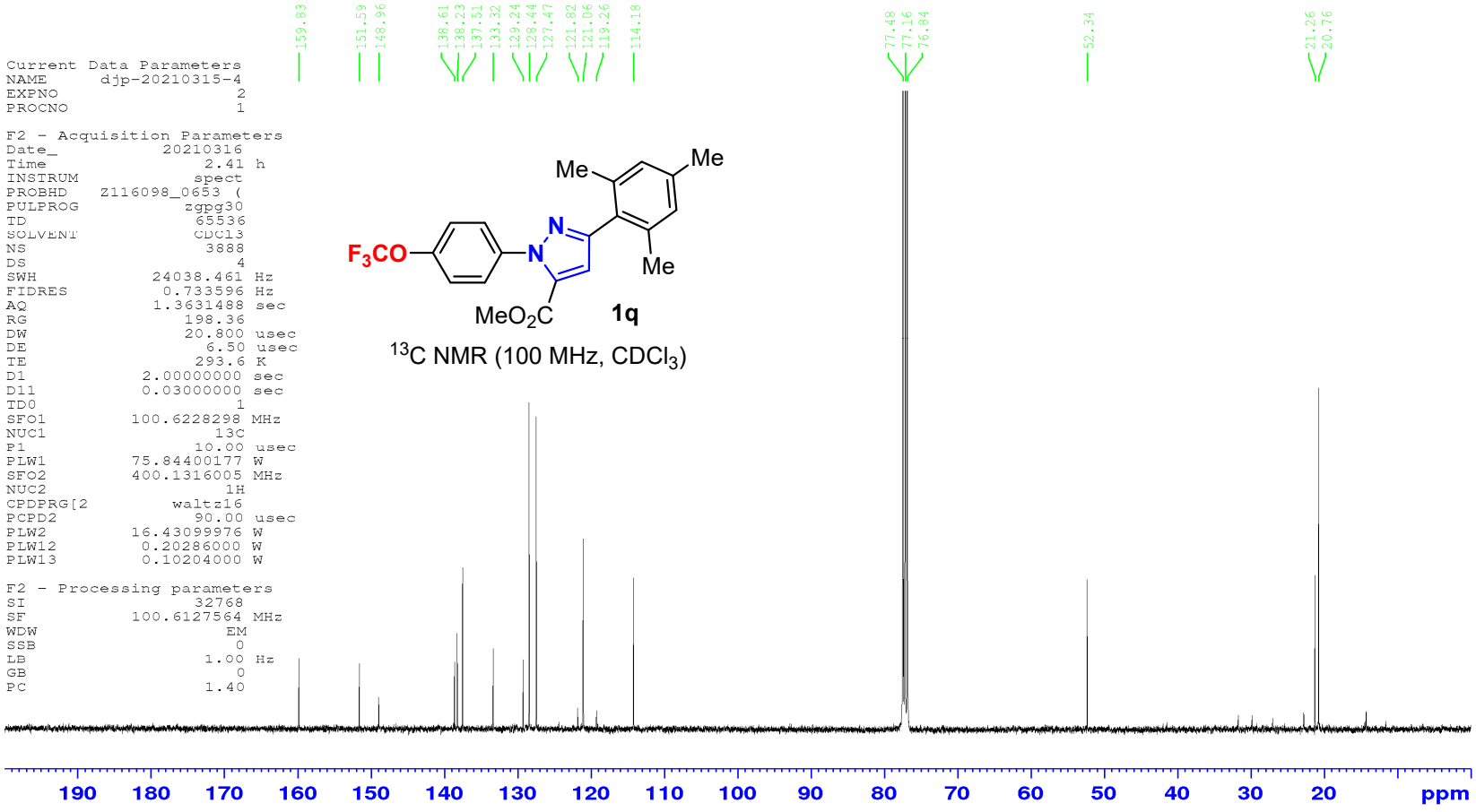


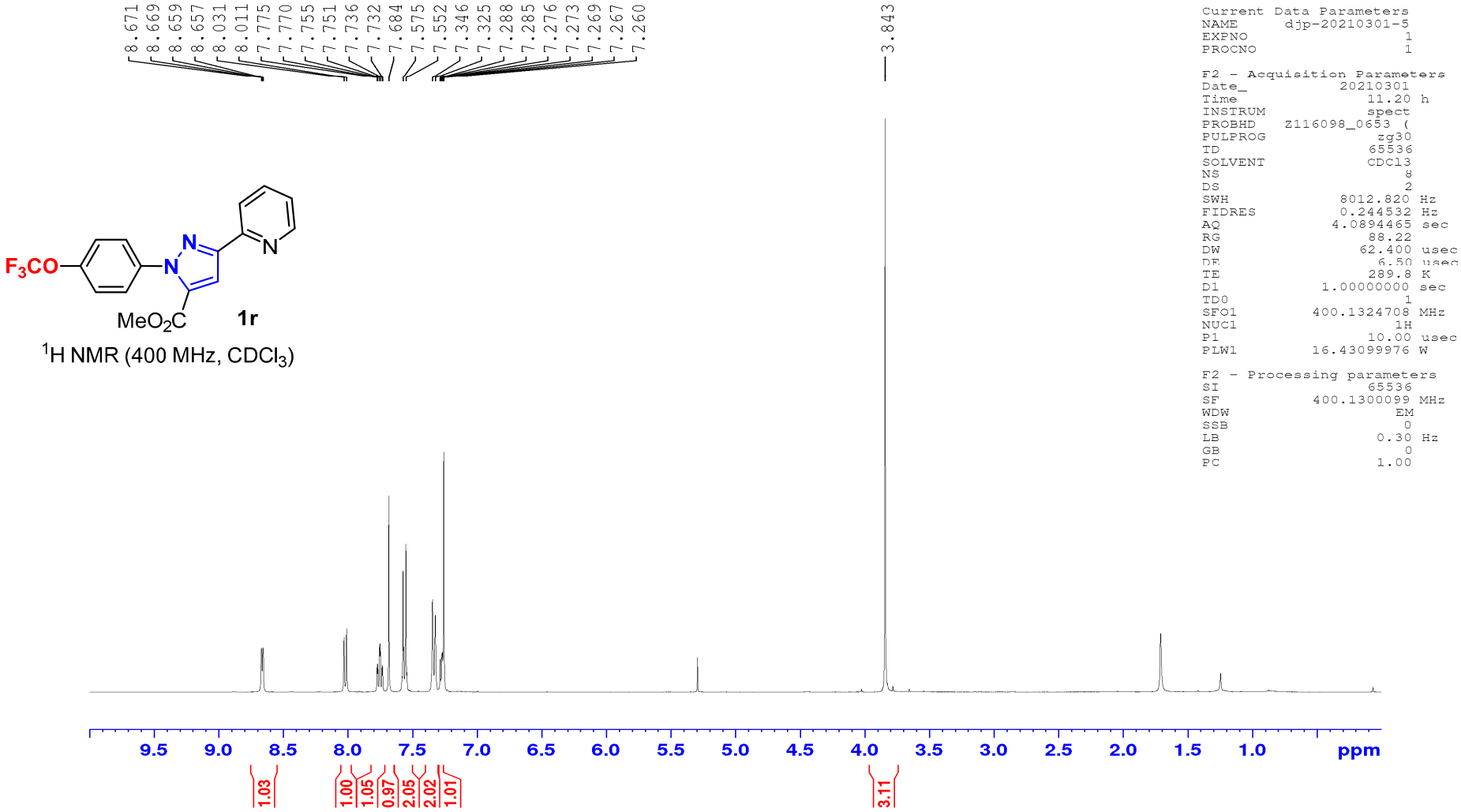

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Current Data Parameters
NAME      ztc-20230408-2
EXPNO                  2
PROCNO                 1

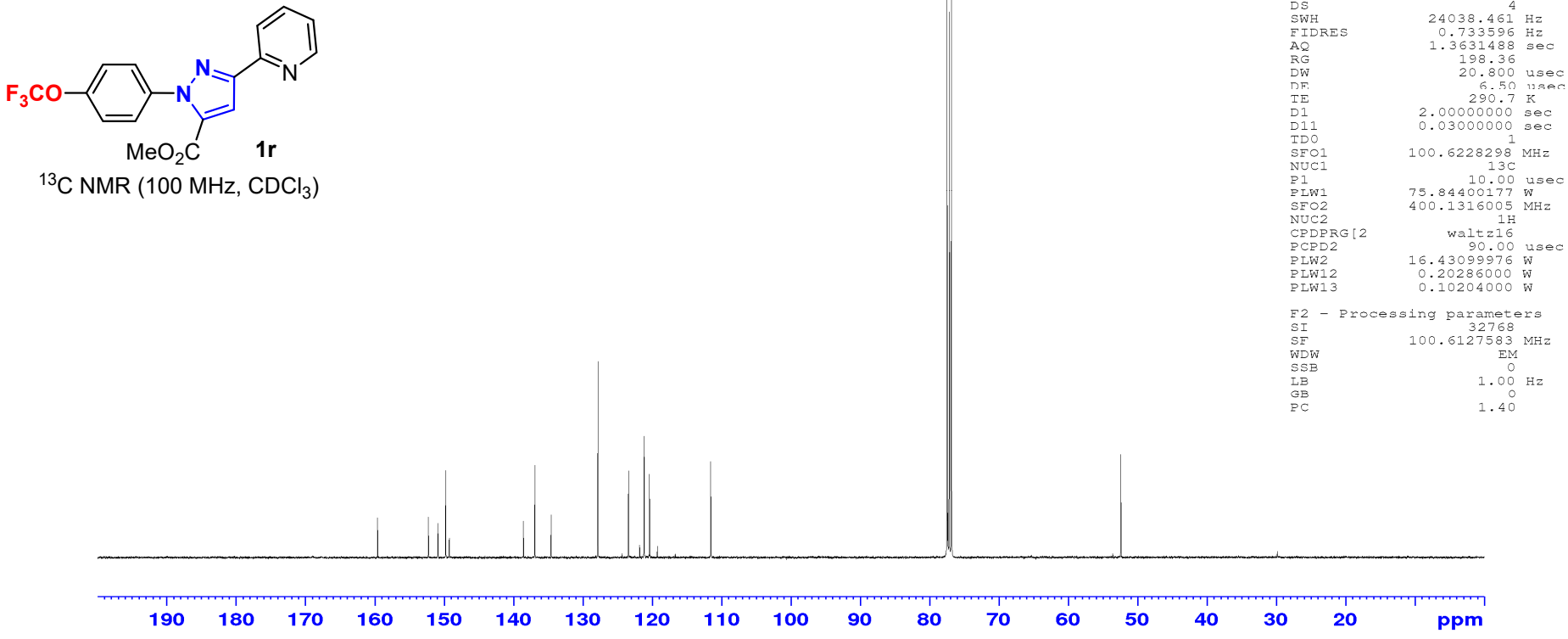
F2 - Acquisition Parameters
Date_           20230408
Time               19.40 h
INSTRUM            spect
PROBHD    Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                198.36
DW                20.800 usec
DE                 6.50 usec
TE                292.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1               13C
P1                10.00 usec
PLW1        75.84400177 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2             90.00 usec
PLW2        16.43099976 W
PLW12        0.20286000 W
PLW13        0.10204000 W

F2 - Processing parameters
SI                32768
SF          100.6127570 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


7.566
7.543
7.322
7.301
7.260
6.955
6.940
3.849
2.317
2.173
Me
Me
Me
F3CO
N
N
MeO2C
1q
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME djp-20210315-4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210315
Time 21.27 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.4
DW 62.400 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
2.01
2.01
3.03
3.09
3.11
6.00


159.83
151.59
148.96
138.61
138.23
137.51
133.32
129.24
128.44
127.47
121.82
121.06
119.26
114.18
77.48
77.16
76.84
52.34
21.26
20.76
Current Data Parameters
NAME djp-20210315-4
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210316
Time 2.41 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3888
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 198.36
DW 20.800 usec
DE 6.50 usec
TE 293.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 75.84400177 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.43099976 W
PLW12 0.20286000 W
PLW13 0.10204000 W
F2 - Processing parameters
SI 32768
SF 100.6127564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
Me
Me
N
N
F3CO
MeO2C
1q
13C NMR (100 MHz, CDCl3)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

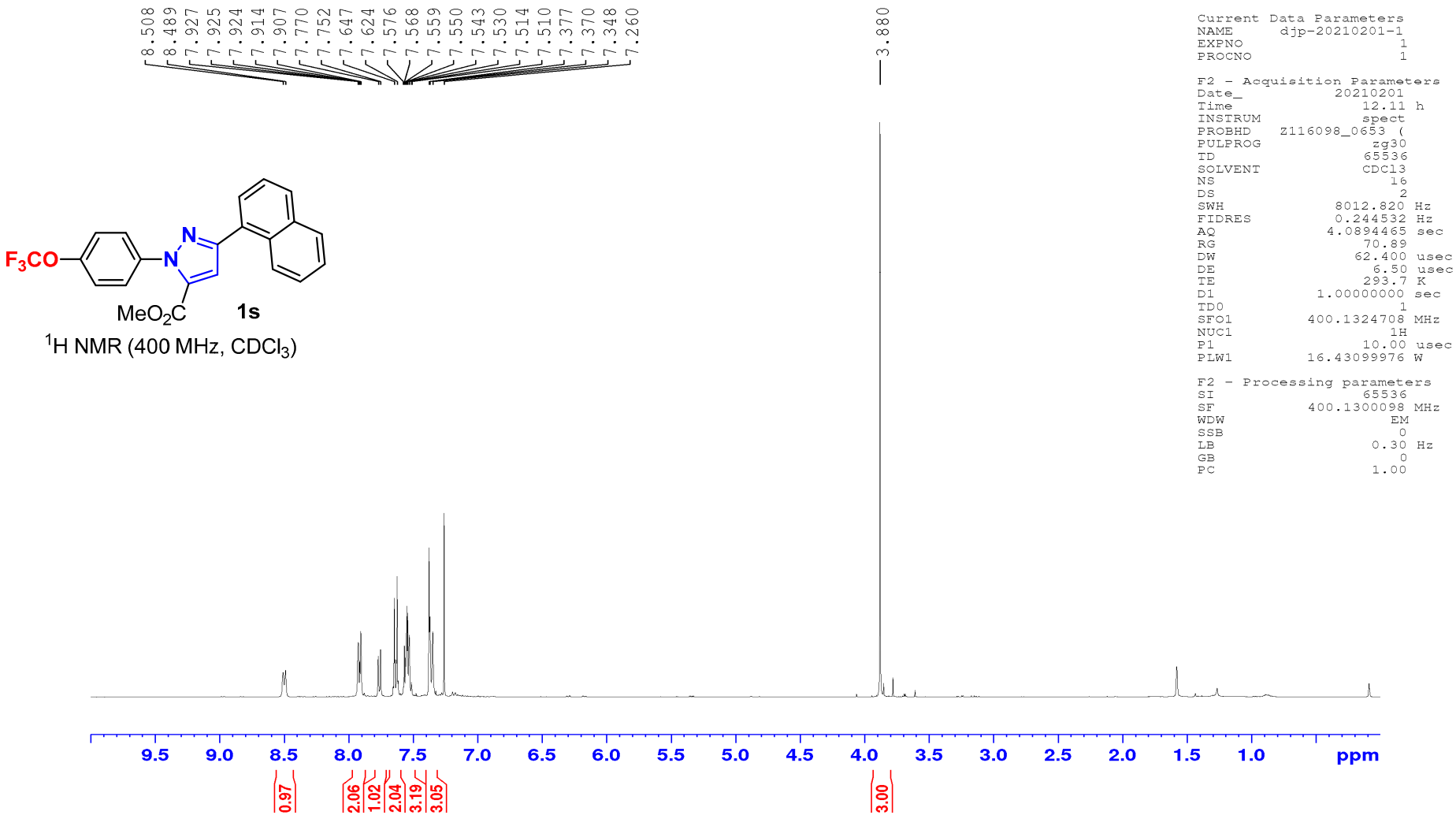

8.671
8.669
8.659
8.657
8.031
8.011
7.775
7.770
7.755
7.751
7.736
7.732
7.684
7.575
7.552
7.346
7.325
7.288
7.285
7.276
7.273
7.269
7.267
7.260
3.843
F3CO
N
N
N
MeO2C
1r
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME djp-20210301-5
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210301
Time 11.20 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 88.22
DW 62.400 usec
DE 6.50 usec
TE 289.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
1.03
1.00
1.05
0.97
2.05
2.02
1.01
3.11

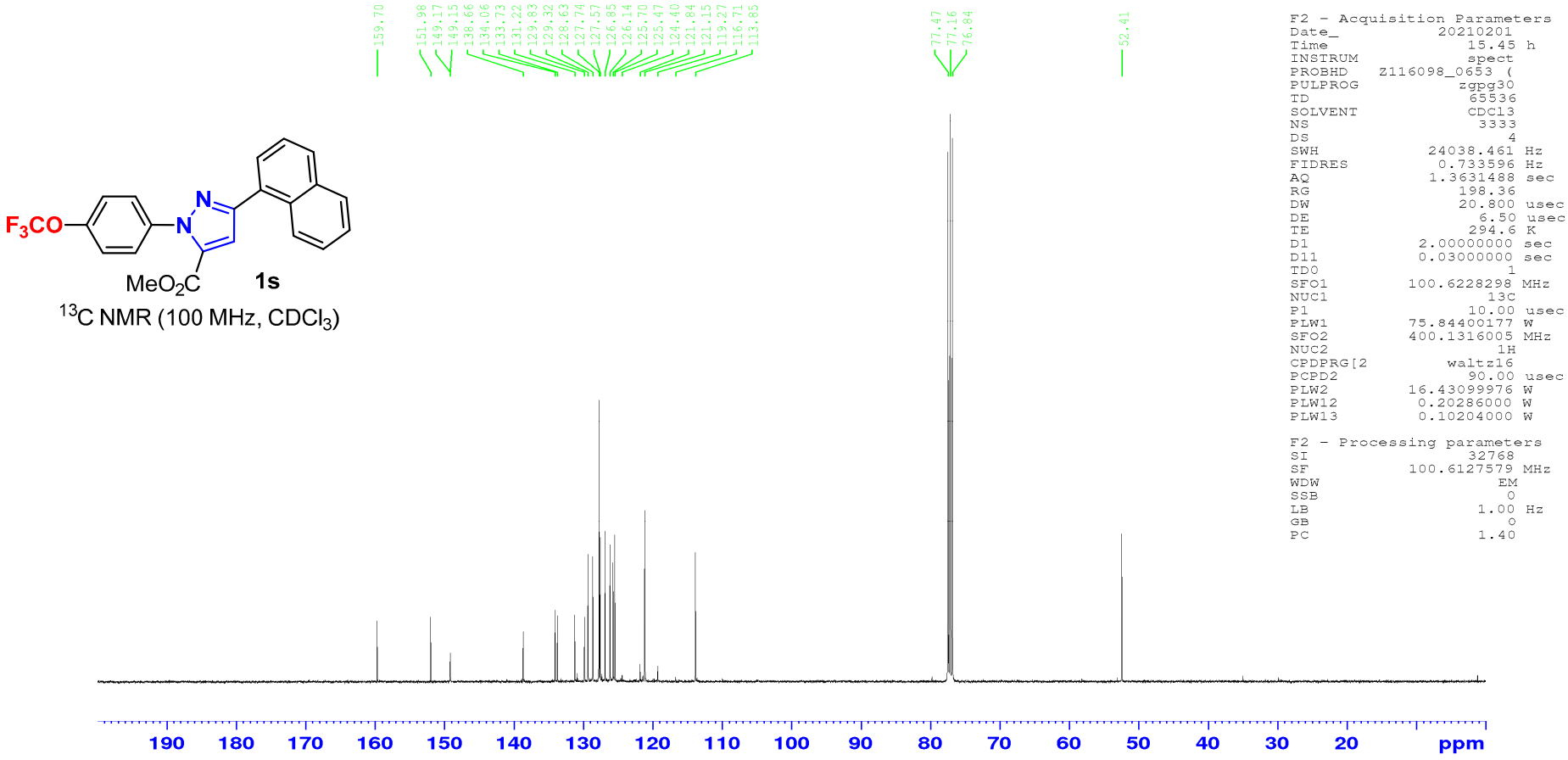



```
Current Data Parameters
NAME      djp-20210301-5
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210301
Time              22.32 h
INSTRUM           spect
PROBHD    Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3333
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG               198.36
DW               20.800 usec
DE                6.50 usec
TE                290.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1               13C
P1               10.00 usec
PLW1        75.84400177 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2       waltz16
PCPD2            90.00 usec
PLW2        16.43099976 W
PLW12        0.20286000 W
PLW13        0.10204000 W

F2 - Processing parameters
SI                32768
SF          100.6127583 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC              1.40
```

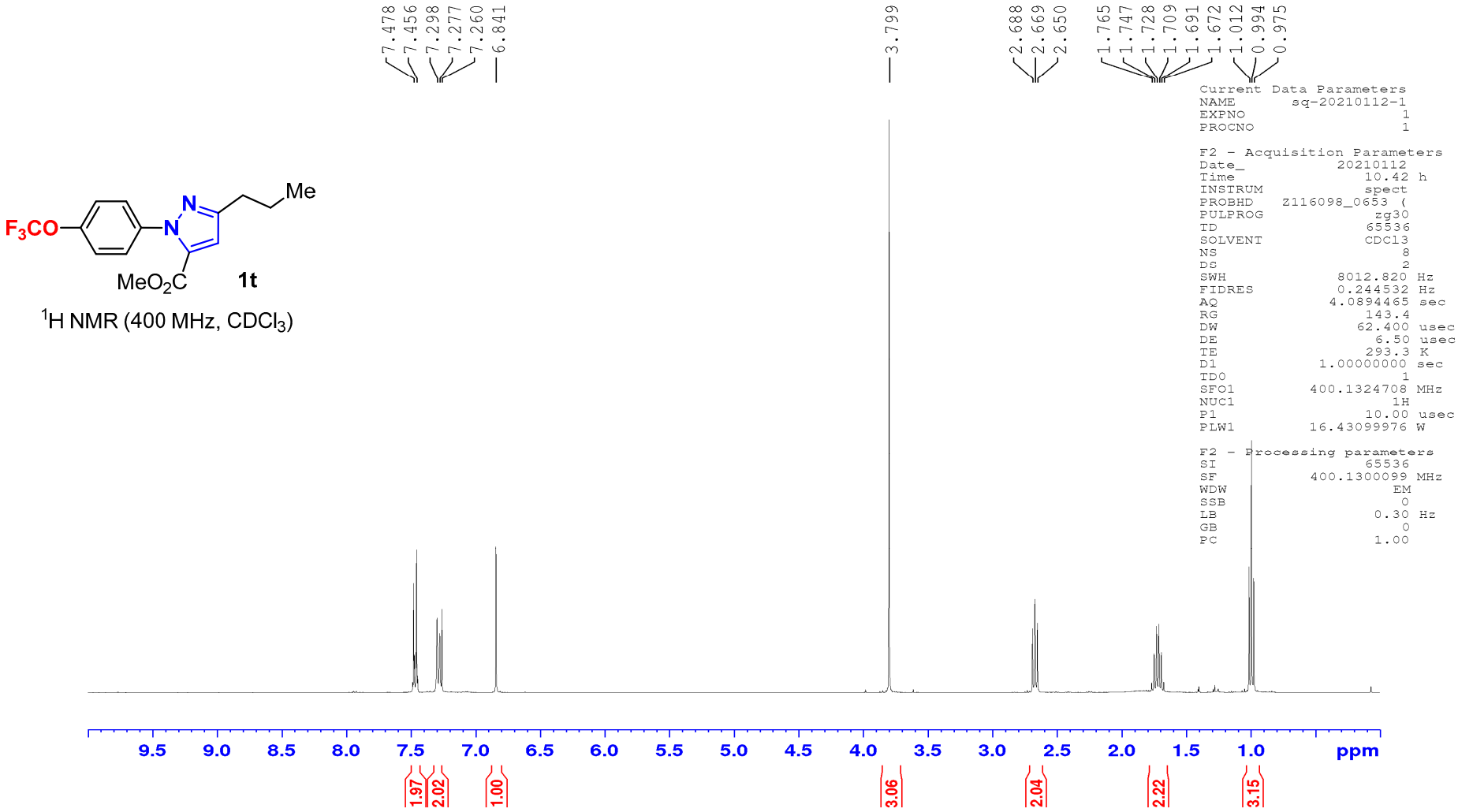

8.508
8.489
7.927
7.925
7.924
7.914
7.907
7.770
7.752
7.647
7.624
7.576
7.568
7.559
7.550
7.543
7.530
7.514
7.510
7.377
7.370
7.348
7.260
3.880
F3CO
N
N
MeO2C
1s
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME djp-20210201-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210201
Time 12.11 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 70.89
DW 62.400 usec
DE 6.50 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
0.97
2.06
1.02
2.04
3.19
3.05
3.00

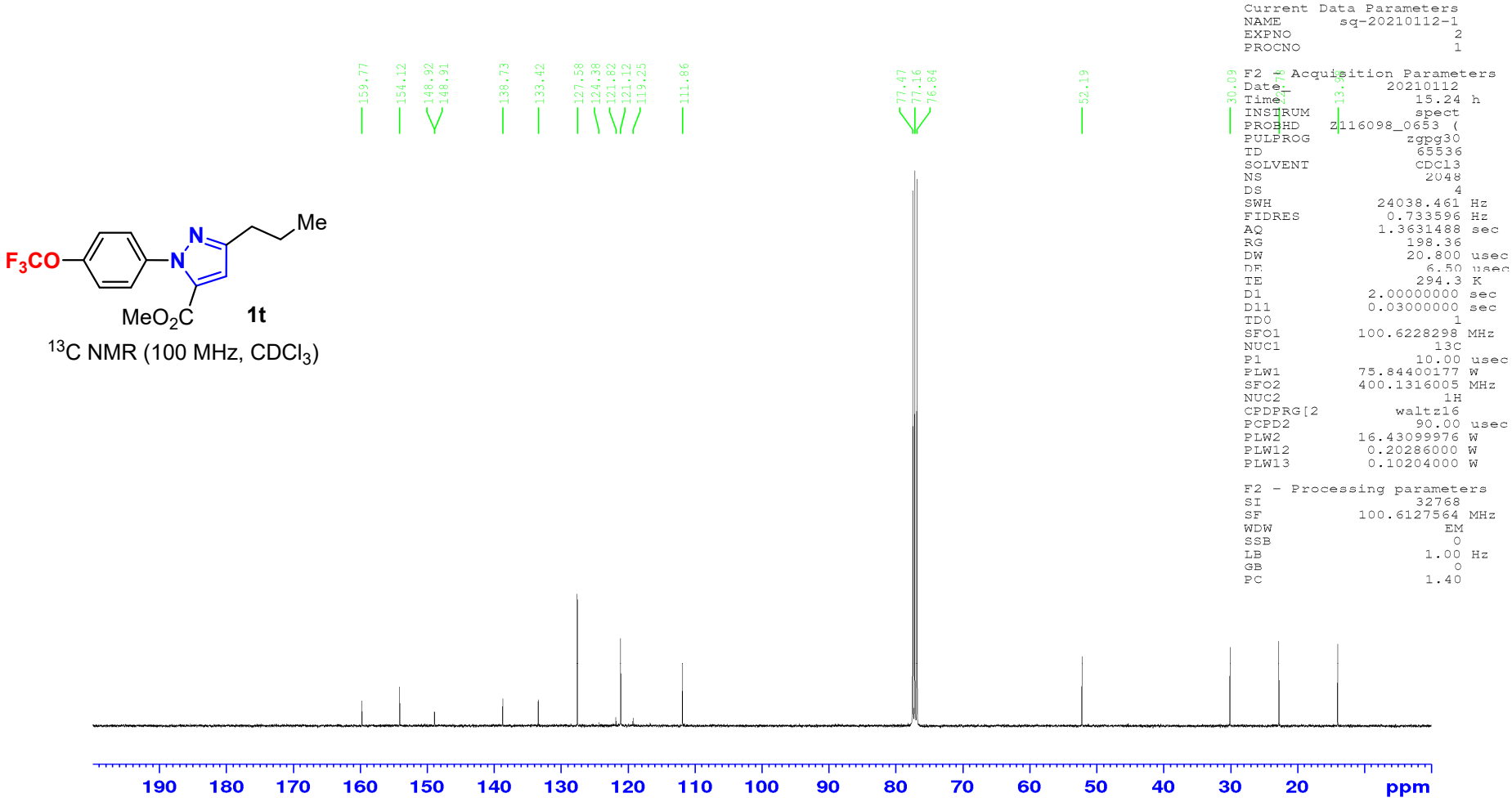


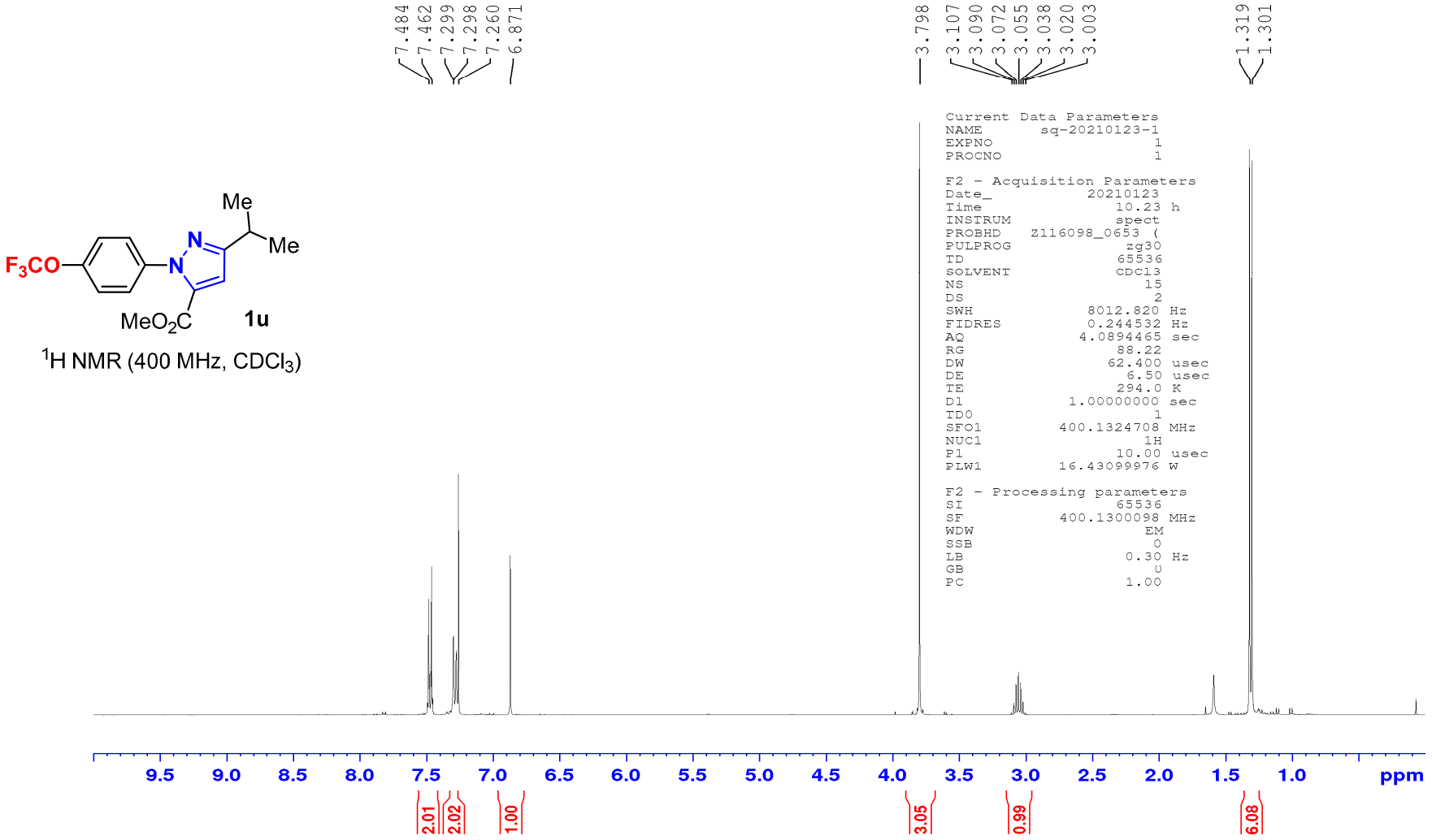

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Current Data Parameters
NAME      djp-20210201-1
EXPNO                  2
PROCNO                 1

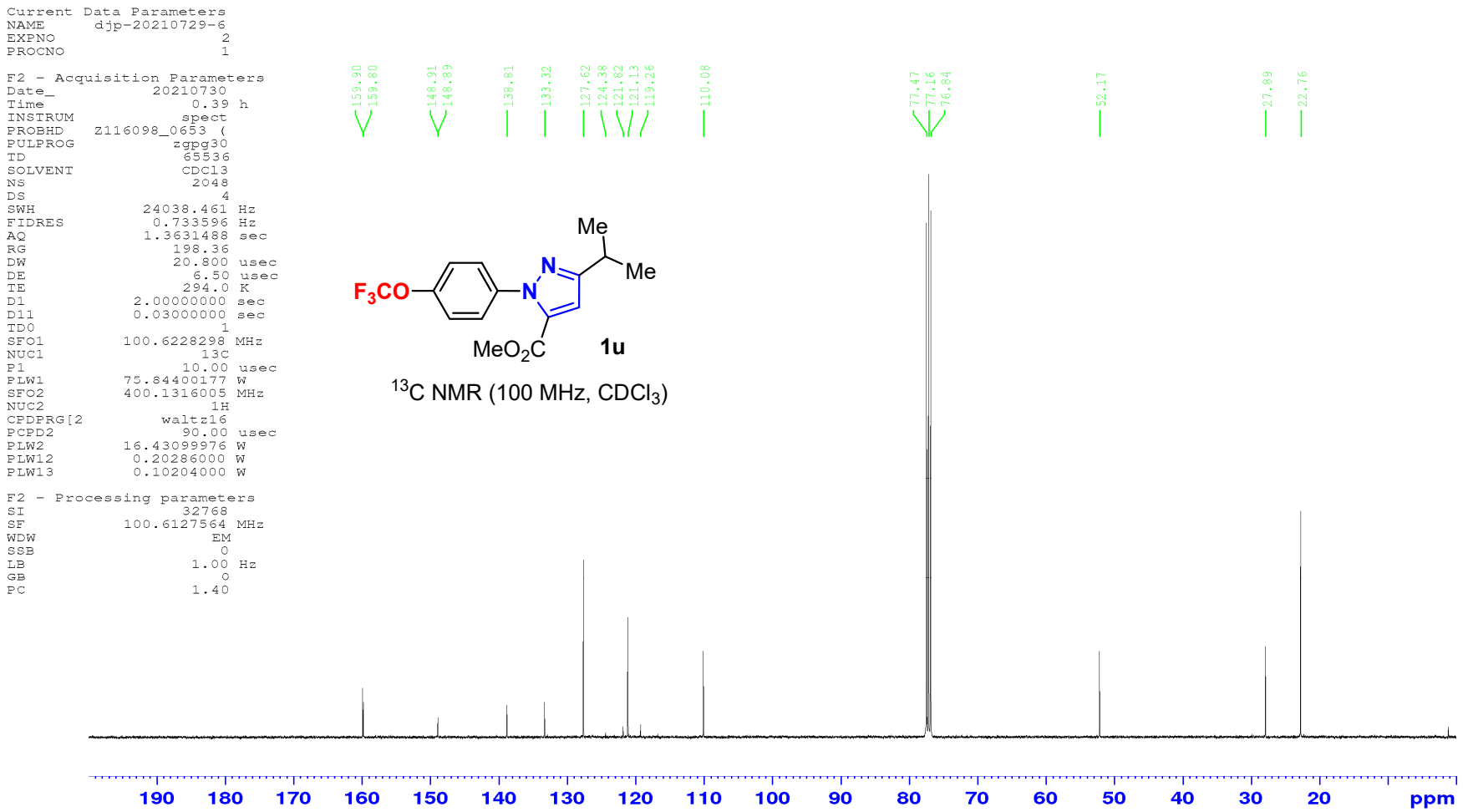
F2 - Acquisition Parameters
Date_           20210201
Time              15.45 h
INSTRUM             spect
PROBHD    Z116098_0653 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3333
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ             1.3631488 sec
RG                198.36
DW                20.800 usec
DE                 6.50 usec
TE                294.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1        75.84400177 W
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        16.43099976 W
PLW12        0.20286000 W
PLW13        0.10204000 W

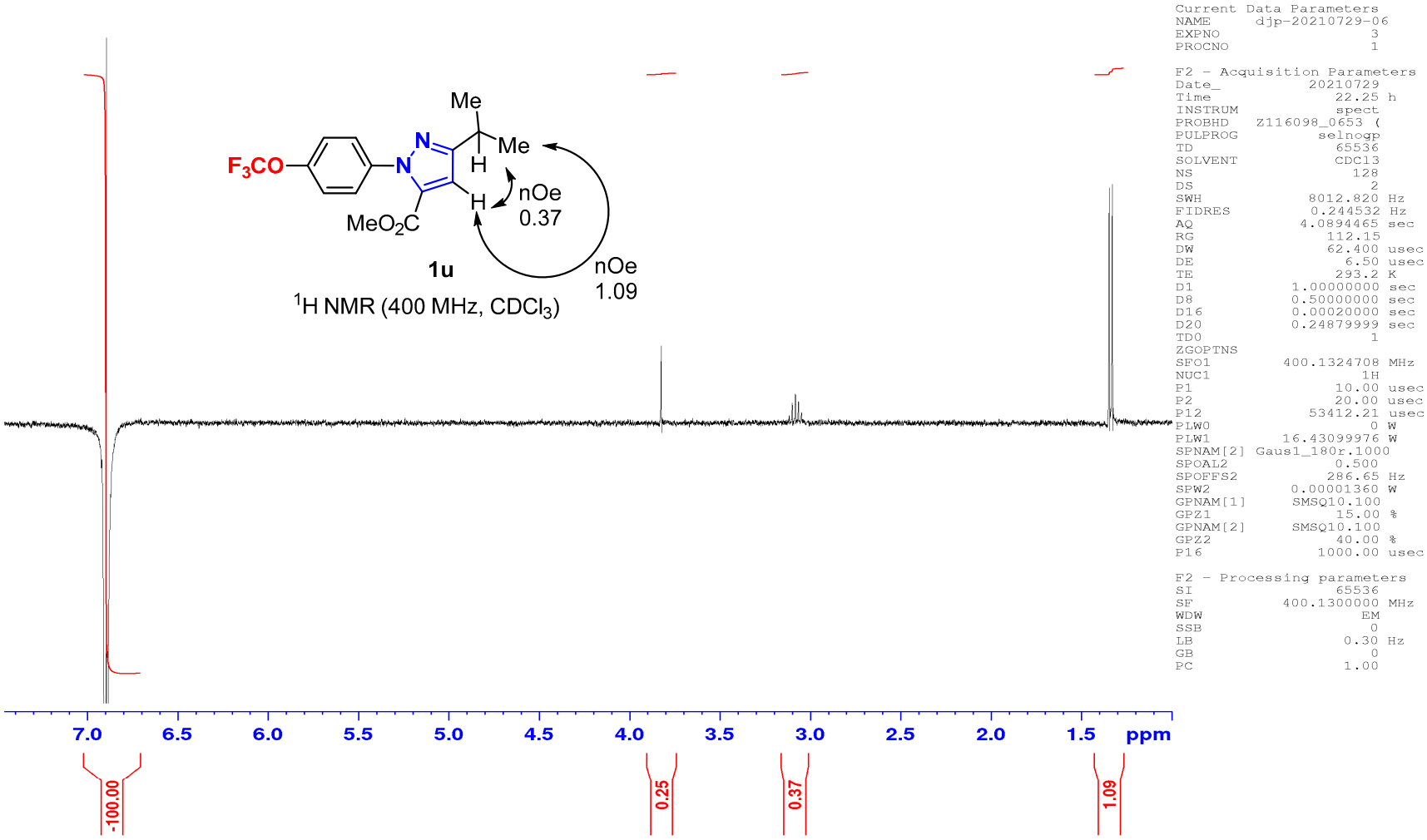
F2 - Processing parameters
SI                32768
SF          100.6127579 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


7.478
7.456
7.298
7.277
7.260
6.841
3.799
2.688
2.669
2.650
1.765
1.747
1.728
1.709
1.691
1.672
1.012
0.994
0.975
Me
F3CO
N
N
MeO2C
1t
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME sq-20210112-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210112
Time 10.42 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 143.4
DW 62.400 usec
DE 6.50 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
1.97
2.02
1.00
3.06
2.04
2.22
3.15


F3CO
N
N
Me
MeO2C
1t
13C NMR (100 MHz, CDCl3)
159.77
154.12
148.92
148.91
138.73
133.42
127.58
124.38
121.82
121.12
119.25
111.86
77.47
77.16
76.84
52.19
30.09
Current Data Parameters
NAME sq-20210112-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210112
Time 15.24 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 198.36
DW 20.800 usec
DE 6.50 usec
TE 294.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 75.84400177 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.43099976 W
PLW12 0.20286000 W
PLW13 0.10204000 W
F2 - Processing parameters
SI 32768
SF 100.6127564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.484
7.462
7.299
7.298
7.260
6.871
3.798
3.107
3.090
3.072
3.055
3.038
3.020
3.003
1.319
1.301
Me
Me
F3CO
N
N
MeO2C
1u
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME sq-20210123-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210123
Time 10.23 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 15
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 88.22
DW 62.400 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
2.01
2.02
1.00
3.05
0.99
6.08

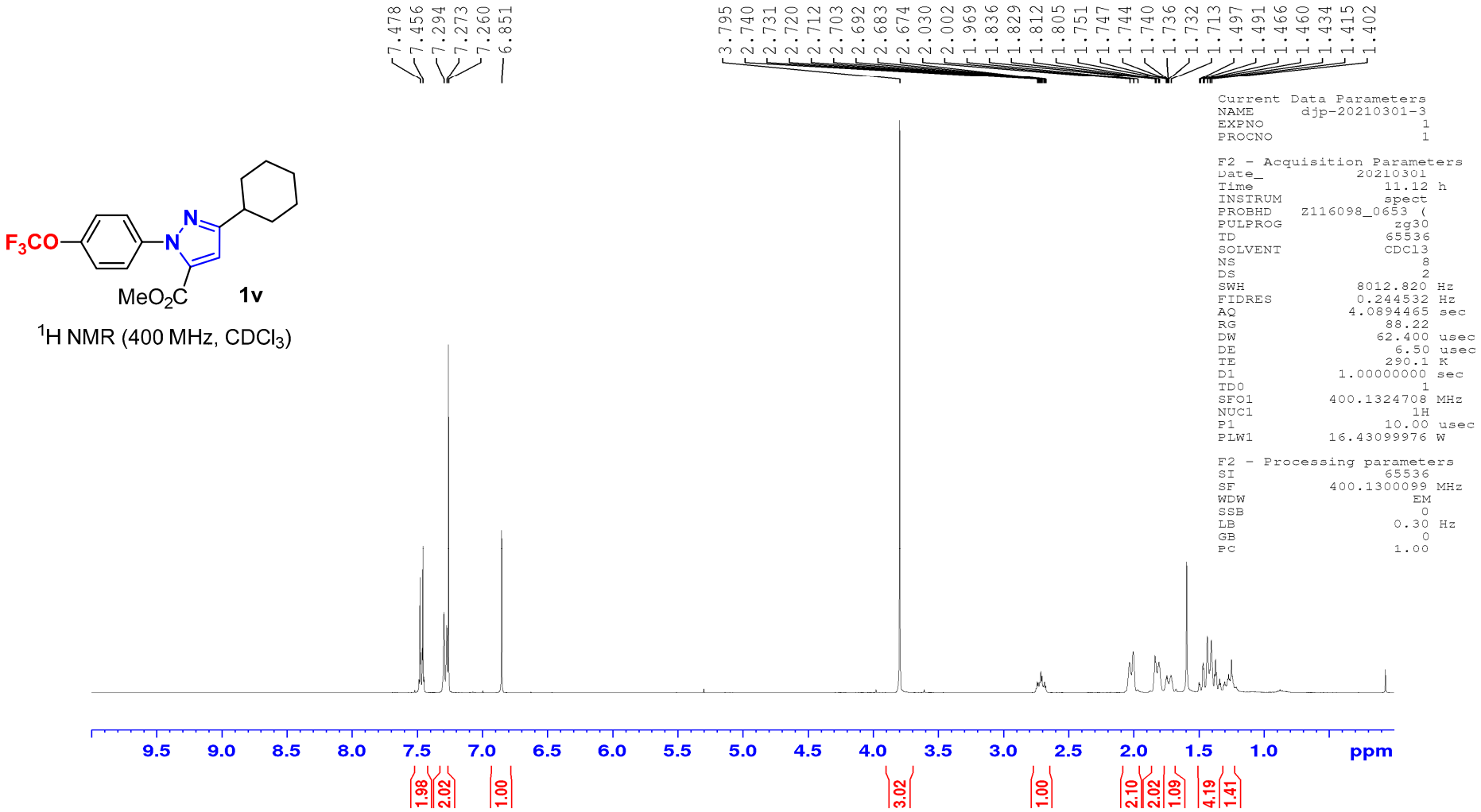

Current Data Parameters
NAME djp-20210729-6
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210730
Time 0.39 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 198.36
DW 20.800 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 75.84400177 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.43099976 W
PLW12 0.20286000 W
PLW13 0.10204000 W
F2 - Processing parameters
SI 32768
SF 100.6127564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
159.90
159.80
148.91
148.89
138.81
133.32
127.62
124.38
121.82
121.13
119.26
110.08
77.47
77.16
76.84
52.17
27.89
22.76
Me
Me
N
N
F3CO
MeO2C
1u
13C NMR (100 MHz, CDCl3)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

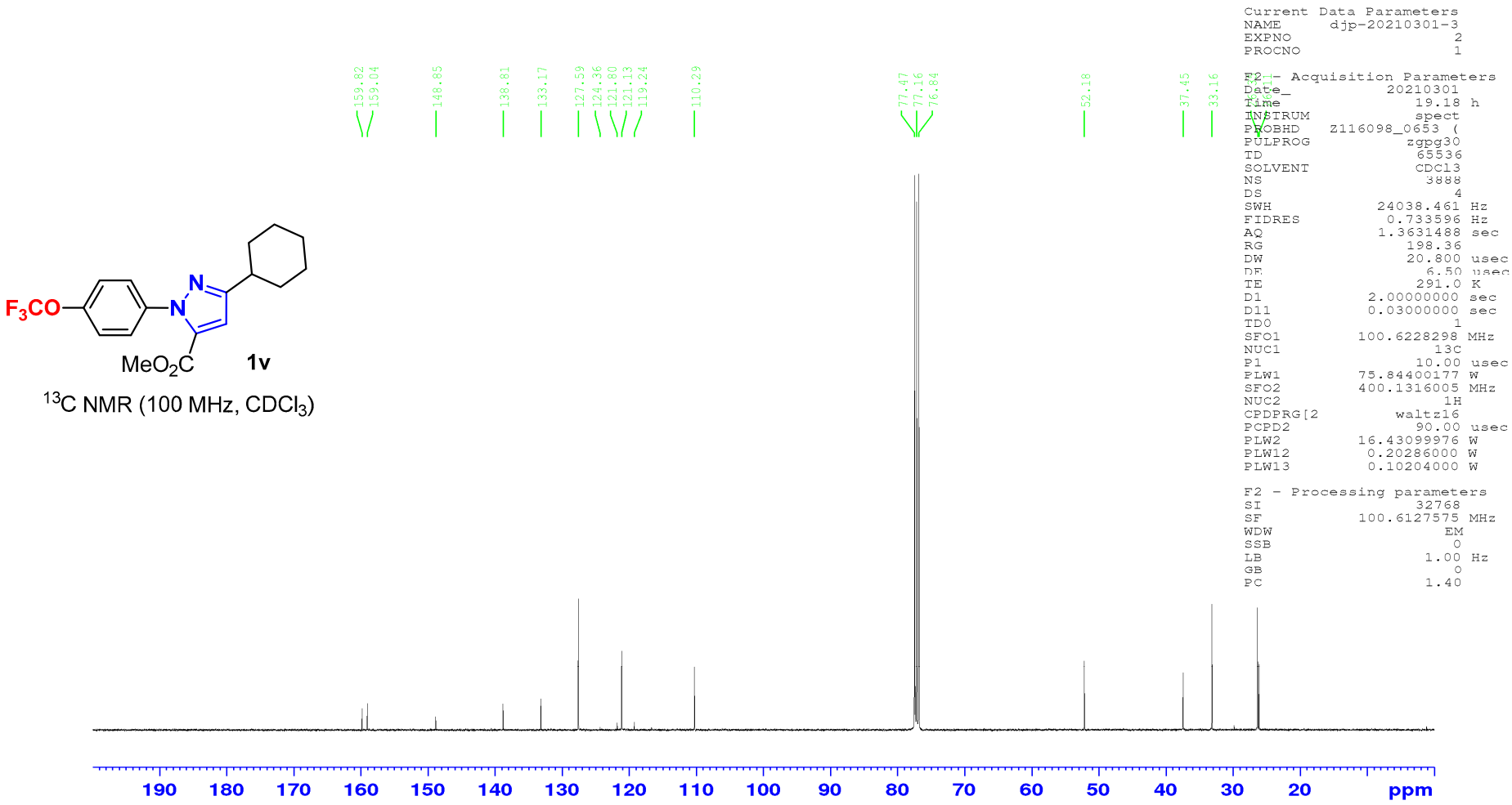


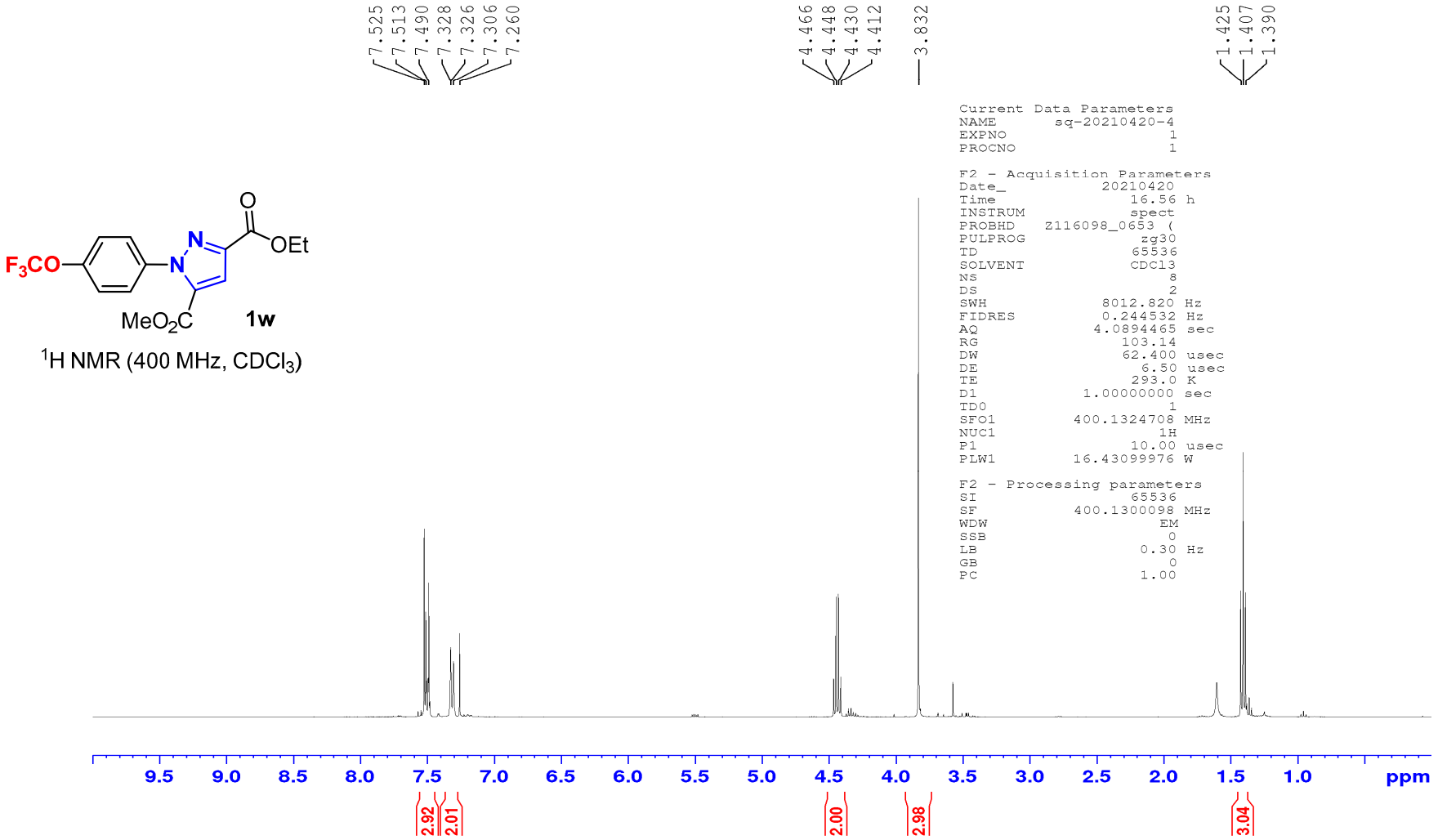

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Current Data Parameters
NAME      djp-20210729-06
EXPNO                  3
PROCNO                 1

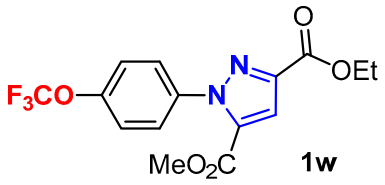
F2 - Acquisition Parameters
Date_           20210729
Time              22.25 h
INSTRUM             spect
PROBHD    Z116098_0653 (
PULPROG          selnogp
TD                 65536
SOLVENT            CDCl3
NS                   128
DS                     2
SWH           8012.820 Hz
FIDRES         0.244532 Hz
AQ            4.0894465 sec
RG                112.15
DW                62.400 usec
DE                 6.50 usec
TE                293.2 K
D1           1.00000000 sec
D8           0.50000000 sec
D16          0.00020000 sec
D20          0.24879999 sec
TD0                    1
ZGOPTNS
SFO1        400.1324708 MHz
NUC1                  1H
P1                10.00 usec
P2                20.00 usec
P12            53412.21 usec
PLW0                 0 W
PLW1         16.43099976 W
SPNAM[2] Gaus1_180r.1000
SPOAL2              0.500
SPOFFS2           286.65 Hz
SPW2         0.00001360 W
GPNAM[1]      SMSQ10.100
GPZ1              15.00 %
GPNAM[2]      SMSQ10.100
GPZ2              40.00 %
P16             1000.00 usec

F2 - Processing parameters
SI                 65536
SF          400.1300000 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```


7.478
7.456
7.294
7.273
7.260
6.851
3.795
2.740
2.731
2.720
2.712
2.703
2.692
2.683
2.674
2.030
2.002
1.969
1.836
1.829
1.812
1.805
1.751
1.747
1.744
1.740
1.736
1.732
1.713
1.497
1.491
1.466
1.460
1.434
1.415
1.402
F3CO
N
N
MeO2C
1v
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME djp-20210301-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210301
Time 11.12 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 88.22
DW 62.400 usec
DE 6.50 usec
TE 290.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
1.98
2.02
1.00
3.02
1.00
2.10
2.02
1.09
4.19
1.41


159.82
159.04
148.85
138.81
133.17
127.59
124.36
121.80
121.13
119.24
110.29
77.47
77.16
76.84
52.18
37.45
33.16
Current Data Parameters
NAME djp-20210301-3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210301
Time 19.18 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3888
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 198.36
DW 20.800 usec
DE 6.50 usec
TE 291.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 75.84400177 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.43099976 W
PLW12 0.20286000 W
PLW13 0.10204000 W
F2 - Processing parameters
SI 32768
SF 100.6127575 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
F3CO
N
N
MeO2C
1v
13C NMR (100 MHz, CDCl3)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.525
7.513
7.490
7.328
7.326
7.306
7.260
4.466
4.448
4.430
4.412
3.832
1.425
1.407
1.390
Current Data Parameters
NAME sq-20210420-4
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210420
Time 16.56 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 103.14
DW 62.400 usec
DE 6.50 usec
TE 293.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F2O
OEt
N
N
MeO2C
1w
1H NMR (400 MHz, CDCl3)
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 ppm
2.92
2.01
2.00
2.98
3.04

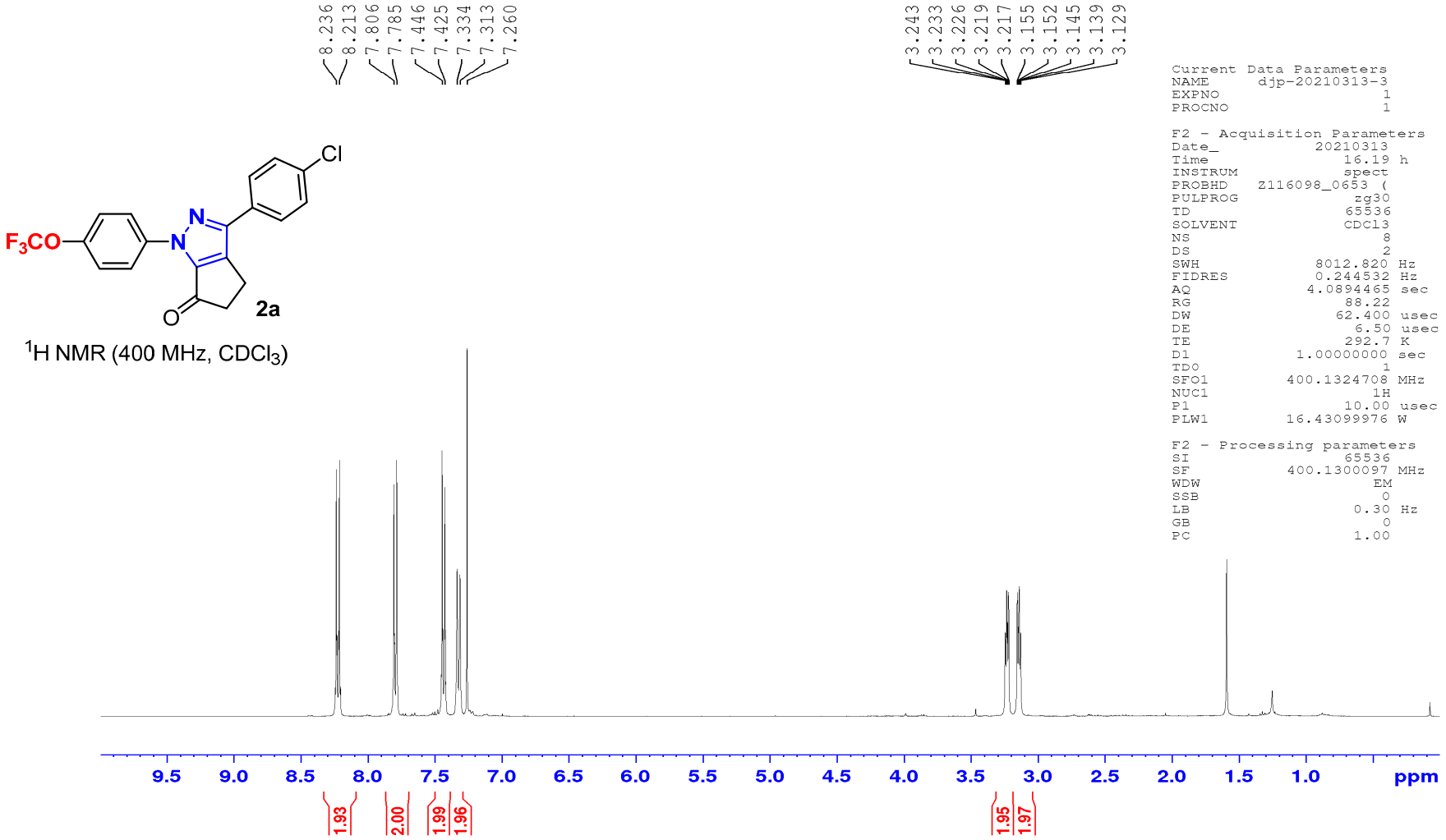


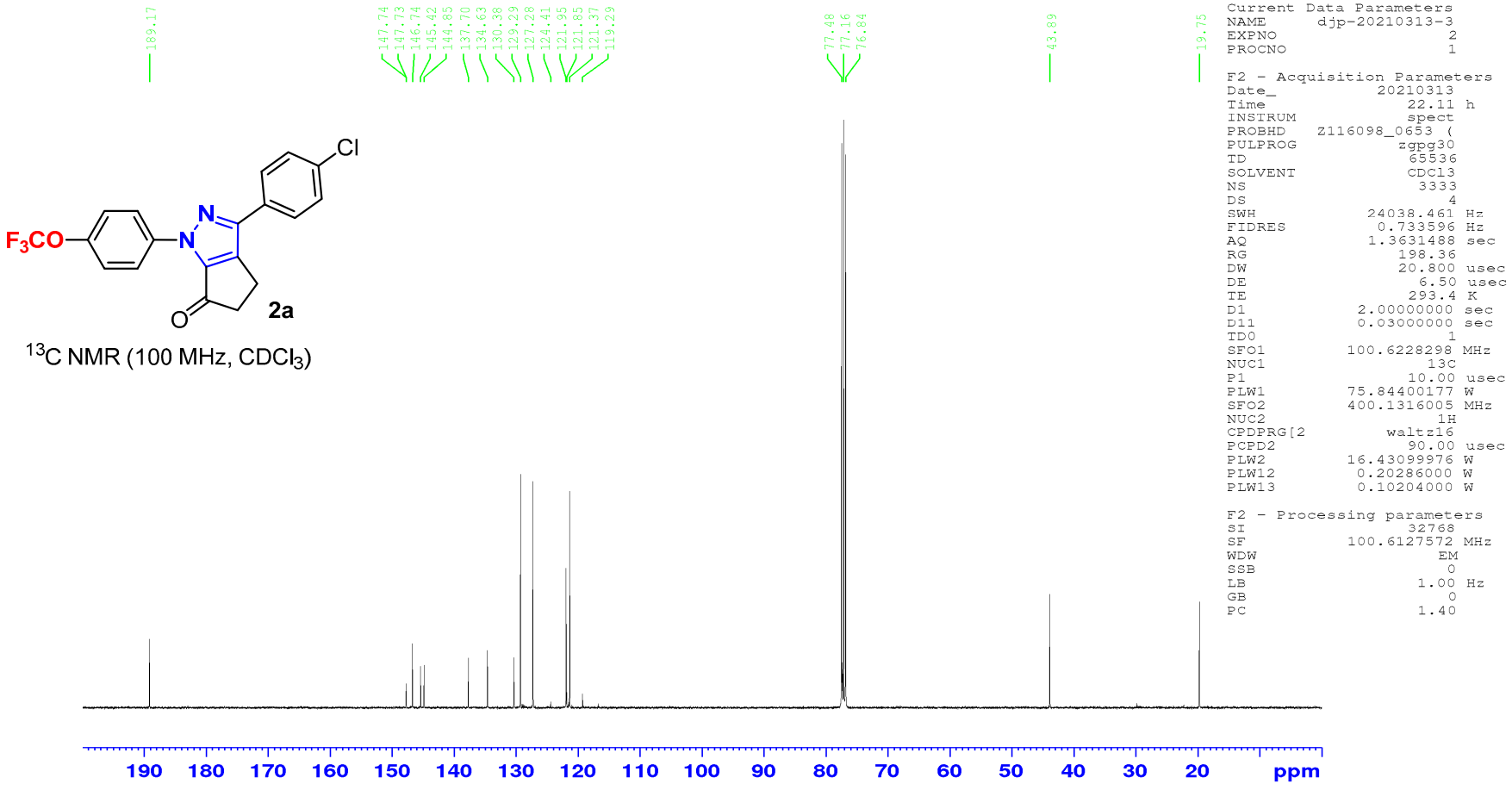
^{13}C NMR (100 MHz, $CDCl_3$)


```
Current Data Parameters
NAME       sq-20210420-4
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210420
Time              20.15 h
INSTRUM             spect
PROBHD    Z116098_0653 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1333
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG               198.36
DW               20.800 usec
DE                6.50 usec
TE               293.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6228298 MHz
NUC1               13C
P1                10.00 usec
PLW1        75.84400177 W
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        16.43099976 W
PLW12        0.20286000 W
PLW13        0.10204000 W

F2 - Processing parameters
SI                32768
SF          100.6127564 MHz
WDW                EM
SSB                 0
LB              1.00 Hz
GB                  0
PC              1.40
```

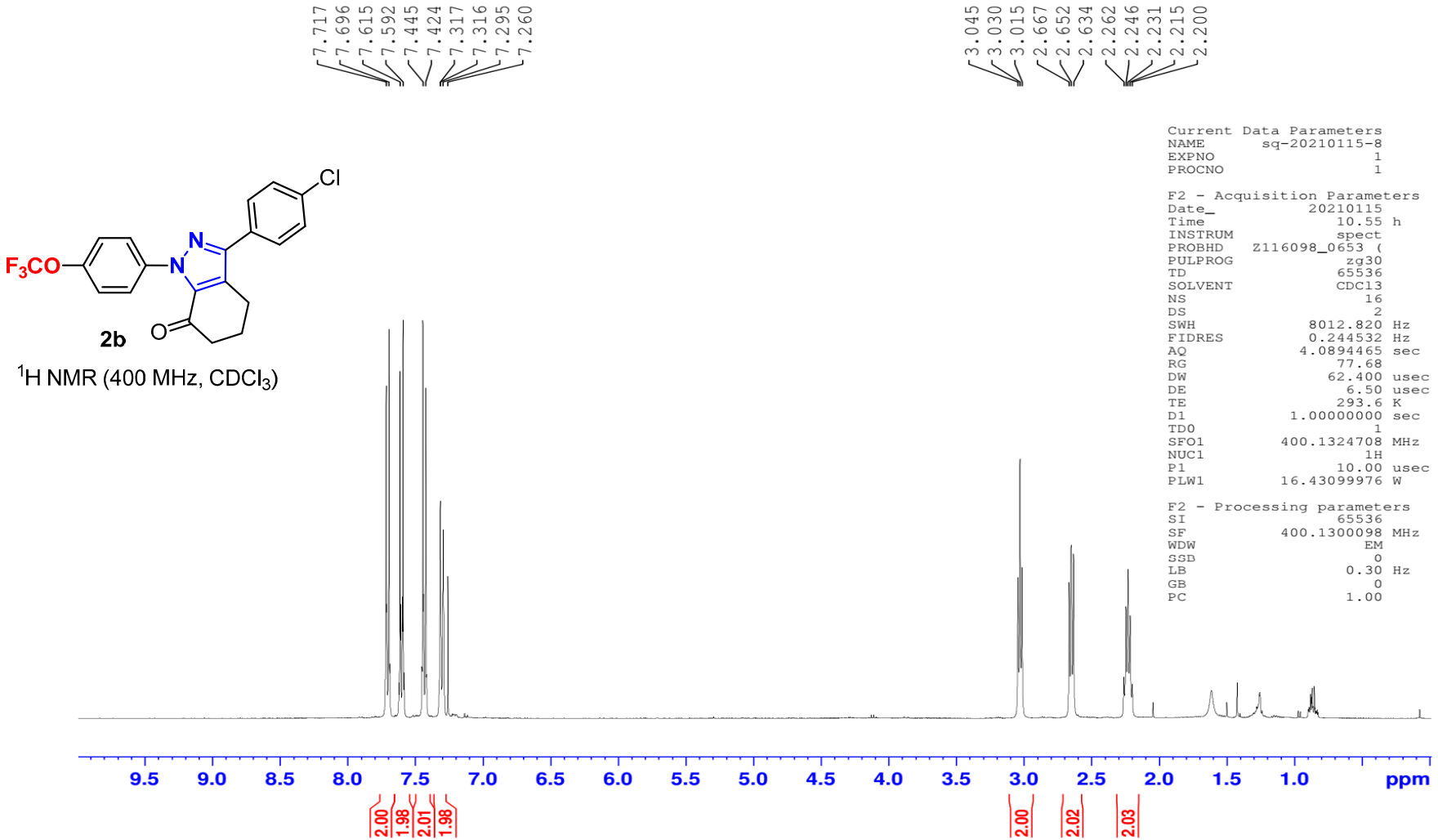

8.236
8.213
7.806
7.785
7.446
7.425
7.334
7.313
7.260
3.243
3.233
3.226
3.219
3.217
3.155
3.152
3.145
3.139
3.129
Cl
F3CO
N
N
O
2a
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME djp-20210313-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210313
Time 16.19 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 88.22
DW 62.400 usec
DE 6.50 usec
TE 292.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
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1.96
1.95
1.97

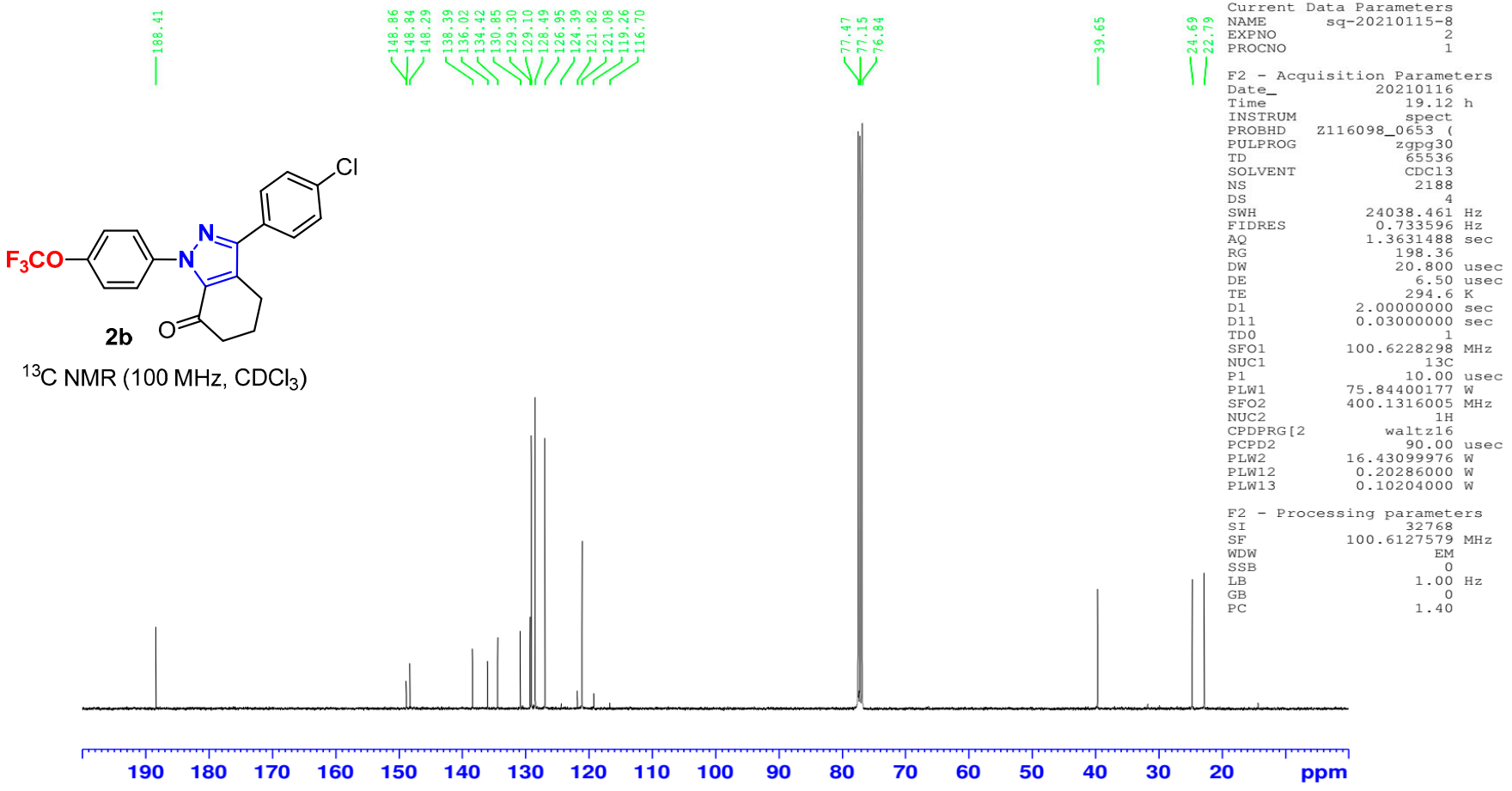



```
Current Data Parameters
NAME      djp-20210313-3
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210313
Time              22.11 h
INSTRUM            spect
PROBHD   Z116098_0653 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                3333
DS                   4
SWH          24038.461 Hz
FIDRES        0.733596 Hz
AQ            1.3631488 sec
RG               198.36
DW               20.800 usec
DE                6.50 usec
TE               293.4 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1
SFO1       100.6228298 MHz
NUC1              13C
P1              10.00 usec
PLW1       75.84400177 W
SFO2       400.1316005 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2           90.00 usec
PLW2       16.43099976 W
PLW12       0.20286000 W
PLW13       0.10204000 W

F2 - Processing parameters
SI               32768
SF         100.6127572 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

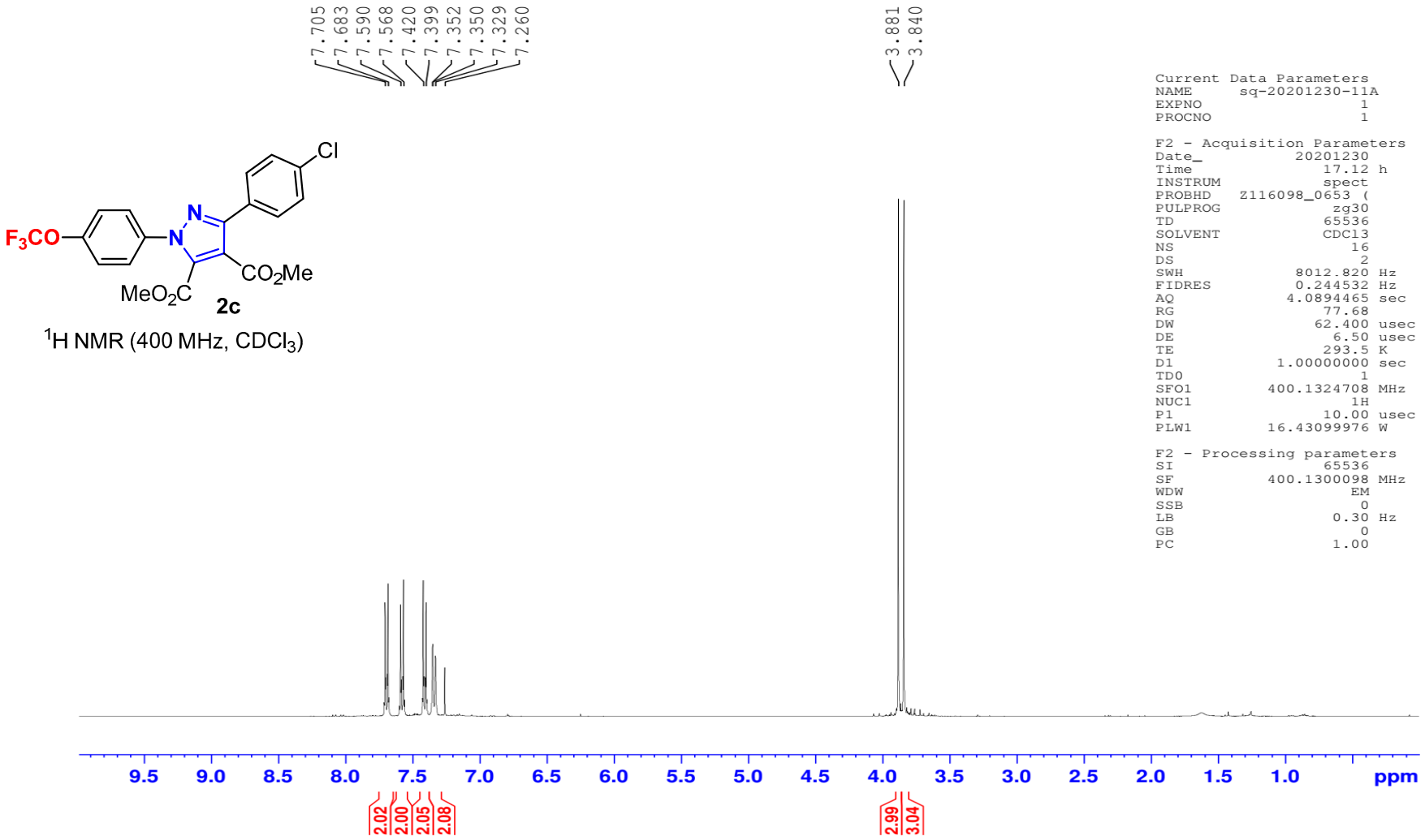

7.717
7.696
7.615
7.592
7.445
7.424
7.317
7.316
7.295
7.260
3.045
3.030
3.015
2.667
2.652
2.634
2.262
2.246
2.231
2.215
2.200
Cl
F3CO
N
N
O
2b
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME sq-20210115-8
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210115
Time 10.55 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 77.68
DW 62.400 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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
ppm
2.00
1.98
2.01
1.98
2.00
2.02
2.03

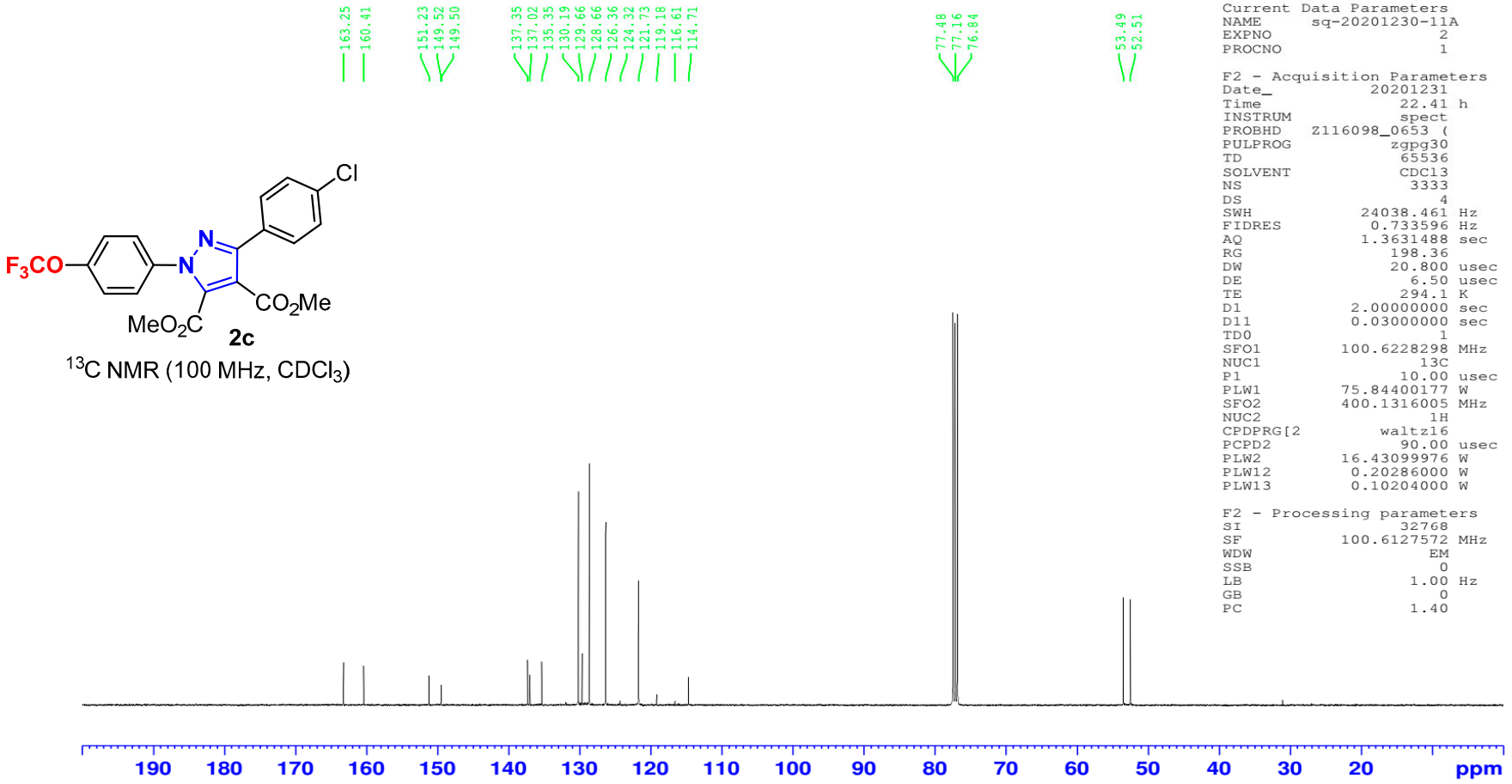



```
Current Data Parameters
NAME       sq-20210115-8
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210116
Time               19.12 h
INSTRUM            spect
PROBHD   Z116098_0653 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2188
DS                    4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG               198.36
DW               20.800 usec
DE                6.50 usec
TE               294.6 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6228298 MHz
NUC1                13C
P1                10.00 usec
PLW1         75.84400177 W
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         16.43099976 W
PLW12         0.20286000 W
PLW13         0.10204000 W

F2 - Processing parameters
SI                32768
SF           100.6127579 MHz
WDW                EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


7.705
7.683
7.590
7.568
7.420
7.399
7.352
7.350
7.329
7.260
3.881
3.840
Cl
F3CO
N
N
CO2Me
MeO2C
2c
1H NMR (400 MHz, CDCl3)
Current Data Parameters
NAME sq-20201230-11A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201230
Time 17.12 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 77.68
DW 62.400 usec
DE 6.50 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
SFO1 400.1324708 MHz
NUC1 1H
P1 10.00 usec
PLW1 16.43099976 W
F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
2.02
2.00
2.05
2.08
2.99
3.04


163.25
160.41
151.23
149.52
149.50
137.35
137.02
135.35
130.19
129.66
128.66
126.36
124.32
121.73
119.18
116.61
114.71
77.48
77.16
76.84
53.49
52.51
Cl
F3CO
N
N
CO2Me
MeO2C
2c
13C NMR (100 MHz, CDCl3)
Current Data Parameters
NAME sq-20201230-11A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201231
Time 22.41 h
INSTRUM spect
PROBHD Z116098_0653 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3333
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 198.36
DW 20.800 usec
DE 6.50 usec
TE 294.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
PLW1 75.84400177 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.43099976 W
PLW12 0.20286000 W
PLW13 0.10204000 W
F2 - Processing parameters
SI 32768
SF 100.6127572 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm