

Synthesis of 2-Arylamino-3-Cyanoquinolines *via* A Cascade Reaction Through Nitrilium Intermediate

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Table S1. Crystal data and experimental details for **3i** (ic19402). **CCDC 1954817**

Crystal data	
Empirical formula	C ₂₅ H ₂₁ N ₃
Formula weight	363.45
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 11.6501(4) Å α = 90°. b = 10.8130(3) Å β = 106.886(4)°. c = 16.4196(5) Å γ = 90°.
Volume	1979.24(11) Å ³
Z	4
F(000)	768
Density (calculated)	1.220 Mg/m ³
Wavelength	0.71073 Å
Cell parameters reflections used	4543
Theta range for Cell parameters	3.8210 to 29.0090°.
Absorption coefficient	0.073 mm ⁻¹
Temperature	150(2) K
Crystal size	0.25 x 0.20 x 0.15 mm ³
Data collection	
Diffractometer	Xcalibur, Atlas, Gemini
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.89892
No. of measured reflections	10903
No. of independent reflections	4442 [R(int) = 0.0284]
No. of observed [I > 2σ(I)]	3276
Completeness to theta = 25.242°	99.8 %
Theta range for data collection	3.154 to 27.499°.
Refinement	
Final R indices [I > 2σ(I)]	R1 = 0.0599, wR2 = 0.1657
R indices (all data)	R1 = 0.0825, wR2 = 0.1887
Goodness-of-fit on F ²	1.003
No. of reflections	4442
No. of parameters	257
No. of restraints	0
Largest diff. peak and hole	0.492 and -0.449 e.Å ⁻³

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3i** (ic19402). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
N(1)	7941(2)	4179(2)	3512(1)	26(1)
N(2)	6675(2)	5462(2)	3974(1)	28(1)
N(3)	5184(2)	3649(2)	5135(1)	38(1)
C(1)	8541(2)	3080(2)	3568(1)	25(1)
C(2)	9407(2)	2971(2)	3121(1)	33(1)
C(3)	10114(2)	1934(2)	3214(2)	37(1)
C(4)	9972(2)	958(2)	3739(1)	35(1)
C(5)	9104(2)	1006(2)	4145(1)	29(1)
C(6)	8363(2)	2066(2)	4068(1)	24(1)
C(7)	7471(2)	2199(2)	4504(1)	23(1)
C(8)	6899(2)	3325(2)	4456(1)	24(1)
C(9)	7190(2)	4332(2)	3967(1)	24(1)
C(10)	7163(2)	1154(2)	4991(1)	26(1)
C(11)	6765(2)	39(2)	4582(1)	33(1)
C(12)	6459(2)	-932(2)	5027(2)	44(1)
C(13)	6559(2)	-806(2)	5880(2)	47(1)
C(14)	6969(2)	291(2)	6298(2)	44(1)
C(15)	7268(2)	1273(2)	5854(1)	33(1)
C(16)	5954(2)	3492(2)	4847(1)	27(1)
C(17)	6914(2)	6511(2)	3514(1)	25(1)
C(18)	8067(2)	7009(2)	3704(1)	29(1)
C(19)	8263(2)	7987(2)	3210(1)	31(1)
C(20)	7352(2)	8506(2)	2558(1)	30(1)
C(21)	6202(2)	8046(2)	2428(1)	29(1)
C(22)	5960(2)	7045(2)	2888(1)	27(1)
C(23)	9092(2)	6530(2)	4428(2)	44(1)
C(24)	7598(2)	9526(2)	2001(2)	44(1)
C(25)	4701(2)	6553(2)	2701(2)	40(1)

Table S3. Bond lengths [\AA] and angles [$^\circ$] for **3i** ic19402.

N(1)-C(9)	1.315(2)	C(10)-C(15)	1.392(3)
N(1)-C(1)	1.368(3)	C(10)-C(11)	1.393(3)
N(2)-C(9)	1.362(3)	C(11)-C(12)	1.383(3)
N(2)-C(17)	1.433(3)	C(12)-C(13)	1.379(4)
N(3)-C(16)	1.142(3)	C(13)-C(14)	1.384(4)
C(1)-C(2)	1.415(3)	C(14)-C(15)	1.389(3)
C(1)-C(6)	1.419(3)	C(17)-C(18)	1.396(3)
C(2)-C(3)	1.373(3)	C(17)-C(22)	1.401(3)
C(3)-C(4)	1.402(3)	C(18)-C(19)	1.391(3)
C(4)-C(5)	1.365(3)	C(18)-C(23)	1.511(3)
C(5)-C(6)	1.419(3)	C(19)-C(20)	1.388(3)
C(6)-C(7)	1.431(3)	C(20)-C(21)	1.387(3)
C(7)-C(8)	1.380(3)	C(20)-C(24)	1.514(3)
C(7)-C(10)	1.487(3)	C(21)-C(22)	1.395(3)
C(8)-C(16)	1.438(3)	C(22)-C(25)	1.506(3)
C(8)-C(9)	1.451(3)		
C(9)-N(1)-C(1)	118.85(16)	C(7)-C(8)-C(9)	120.49(17)
C(9)-N(2)-C(17)	123.47(17)	C(16)-C(8)-C(9)	119.06(17)
N(1)-C(1)-C(2)	117.68(17)	N(1)-C(9)-N(2)	119.05(17)
N(1)-C(1)-C(6)	123.53(17)	N(1)-C(9)-C(8)	121.38(17)
C(2)-C(1)-C(6)	118.76(18)	N(2)-C(9)-C(8)	119.57(17)
C(3)-C(2)-C(1)	120.36(19)	C(15)-C(10)-C(11)	119.32(18)
C(2)-C(3)-C(4)	120.6(2)	C(15)-C(10)-C(7)	120.92(18)
C(5)-C(4)-C(3)	120.51(19)	C(11)-C(10)-C(7)	119.77(17)
C(4)-C(5)-C(6)	120.33(19)	C(12)-C(11)-C(10)	120.2(2)
C(5)-C(6)-C(1)	119.26(18)	C(13)-C(12)-C(11)	120.2(2)
C(5)-C(6)-C(7)	123.20(17)	C(12)-C(13)-C(14)	120.2(2)
C(1)-C(6)-C(7)	117.46(17)	C(13)-C(14)-C(15)	119.9(2)
C(8)-C(7)-C(6)	117.95(17)	C(14)-C(15)-C(10)	120.1(2)
C(8)-C(7)-C(10)	120.87(17)	N(3)-C(16)-C(8)	177.7(2)
C(6)-C(7)-C(10)	121.18(17)	C(18)-C(17)-C(22)	120.75(18)
C(7)-C(8)-C(16)	120.34(17)	C(18)-C(17)-N(2)	120.62(17)

C(22)-C(17)-N(2)	118.61(18)	C(21)-C(20)-C(24)	120.8(2)
C(19)-C(18)-C(17)	118.28(18)	C(19)-C(20)-C(24)	121.6(2)
C(19)-C(18)-C(23)	119.53(19)	C(20)-C(21)-C(22)	122.18(19)
C(17)-C(18)-C(23)	122.19(19)	C(21)-C(22)-C(17)	118.43(19)
C(20)-C(19)-C(18)	122.57(19)	C(21)-C(22)-C(25)	120.11(18)
C(21)-C(20)-C(19)	117.54(19)	C(17)-C(22)-C(25)	121.46(18)

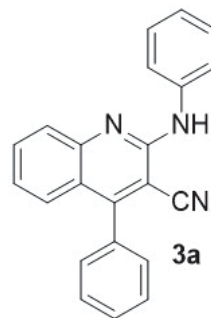
Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3i** (ic19402). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

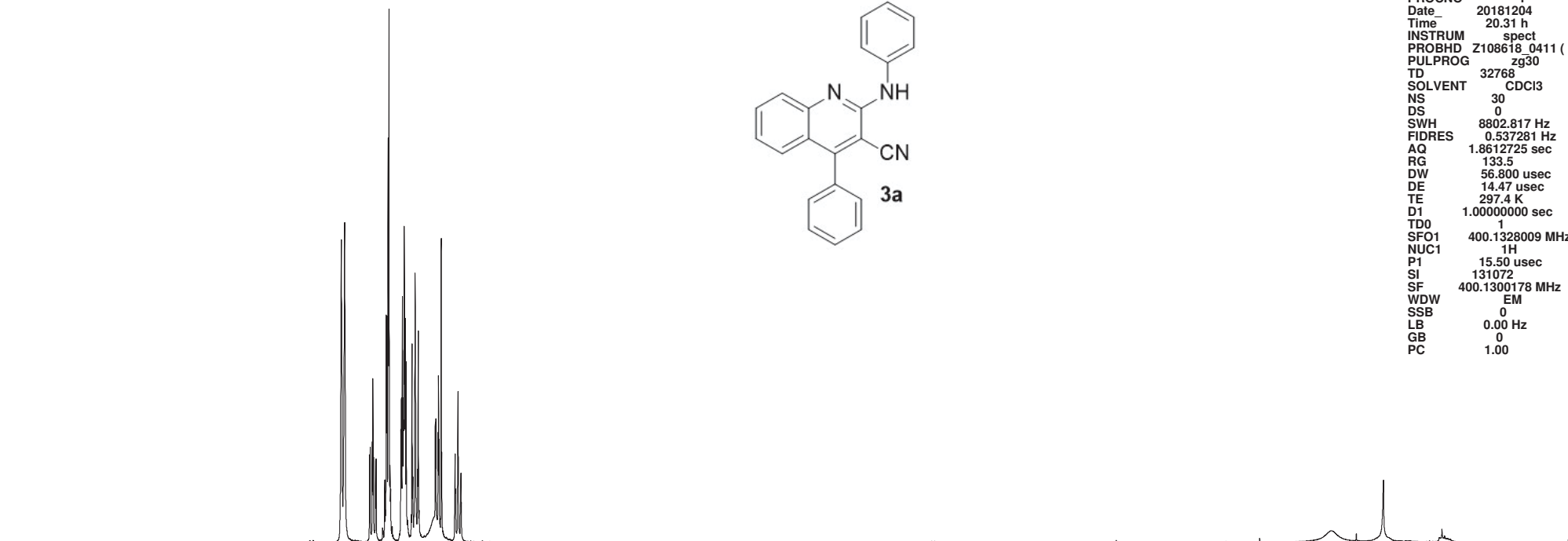
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	27(1)	26(1)	28(1)	4(1)	12(1)	2(1)
N(2)	32(1)	26(1)	30(1)	5(1)	15(1)	4(1)
N(3)	45(1)	29(1)	52(1)	4(1)	30(1)	5(1)
C(1)	24(1)	27(1)	25(1)	0(1)	7(1)	0(1)
C(2)	34(1)	32(1)	38(1)	6(1)	19(1)	2(1)
C(3)	32(1)	39(1)	46(1)	2(1)	22(1)	3(1)
C(4)	32(1)	30(1)	45(1)	2(1)	16(1)	7(1)
C(5)	29(1)	27(1)	32(1)	3(1)	11(1)	2(1)
C(6)	24(1)	25(1)	24(1)	1(1)	7(1)	0(1)
C(7)	23(1)	25(1)	21(1)	-1(1)	6(1)	-2(1)
C(8)	25(1)	26(1)	22(1)	0(1)	9(1)	0(1)
C(9)	22(1)	25(1)	22(1)	1(1)	4(1)	0(1)
C(10)	27(1)	26(1)	27(1)	4(1)	11(1)	3(1)
C(11)	40(1)	30(1)	33(1)	-1(1)	16(1)	-2(1)
C(12)	55(2)	28(1)	56(2)	2(1)	29(1)	-4(1)
C(13)	57(2)	38(1)	57(2)	19(1)	32(1)	3(1)
C(14)	54(2)	50(1)	31(1)	13(1)	21(1)	9(1)
C(15)	37(1)	34(1)	29(1)	3(1)	12(1)	3(1)
C(16)	33(1)	21(1)	30(1)	2(1)	12(1)	0(1)
C(17)	30(1)	22(1)	26(1)	-1(1)	11(1)	2(1)
C(18)	30(1)	25(1)	31(1)	-3(1)	7(1)	3(1)
C(19)	29(1)	26(1)	40(1)	-3(1)	12(1)	-2(1)
C(20)	38(1)	22(1)	35(1)	0(1)	18(1)	3(1)
C(21)	34(1)	26(1)	28(1)	1(1)	8(1)	6(1)
C(22)	28(1)	26(1)	26(1)	-2(1)	8(1)	1(1)
C(23)	36(1)	40(1)	47(1)	4(1)	-5(1)	-2(1)
C(24)	46(1)	38(1)	56(2)	16(1)	24(1)	4(1)
C(25)	30(1)	43(1)	43(1)	6(1)	4(1)	-4(1)

PD, 2-ABP, Malononitrile, 80deg, 5h, purified pale yellow solid

7.875
7.854
7.696
7.692
7.678
7.675
7.671
7.657
7.654
7.599
7.593
7.589
7.585
7.577
7.572
7.566
7.564
7.561
7.496
7.495
7.493
7.492
7.486
7.484
7.480
7.478
7.476
7.472
7.471
7.468
7.462
7.425
7.420
7.406
7.404
7.399
7.390
7.385
7.277
7.274
7.260
7.257
7.253
7.240
7.236
7.154
7.151
7.148
7.133
7.117
7.114
7.111



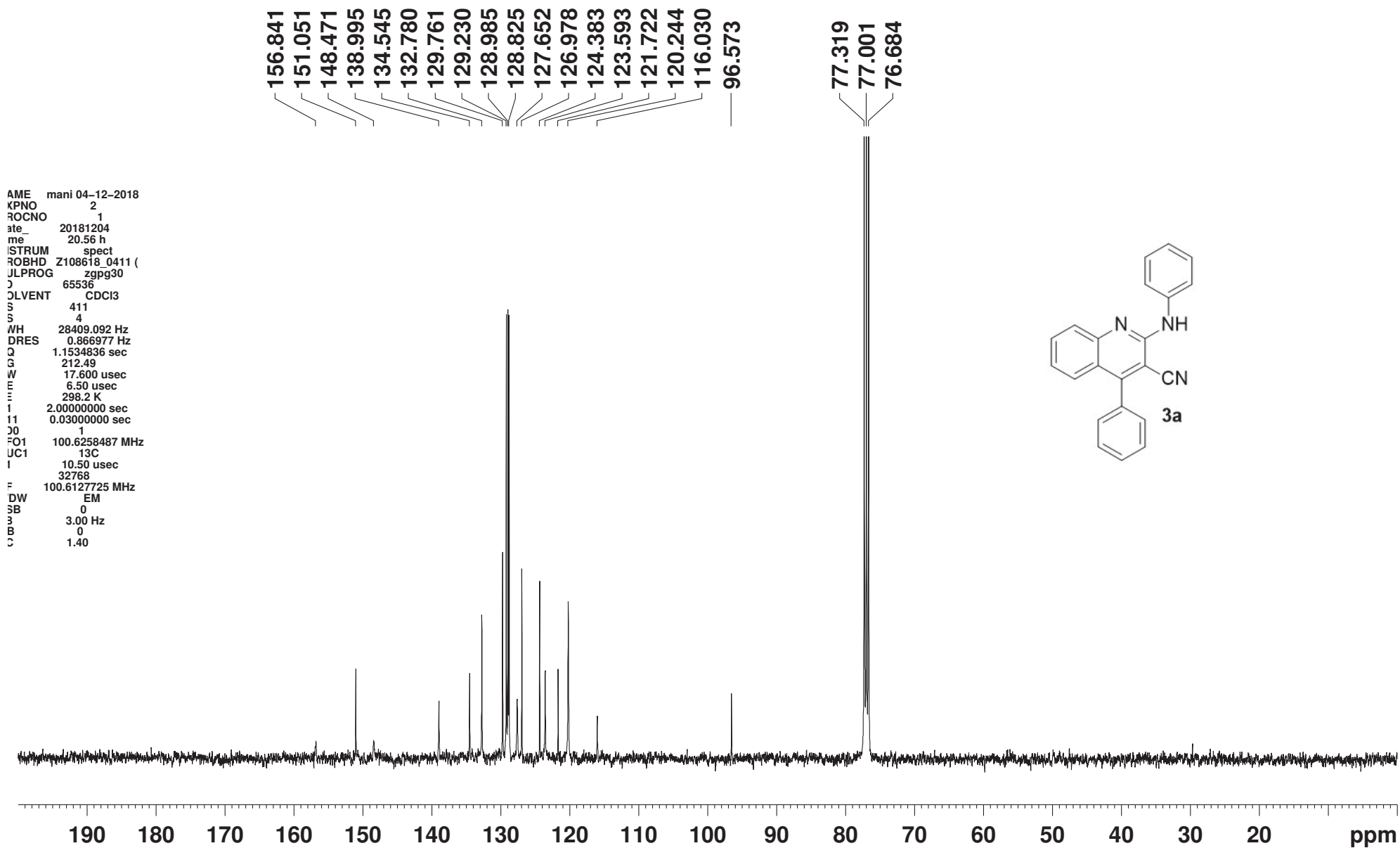
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FIDRES 0.537281 Hz
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RG 133.5
DW 56.800 usec
DE 14.47 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.1328009 MHz
NUC1 1H
P1 15.50 usec
SI 131072
SF 400.1300178 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 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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3.05
3.04
2.12
2.06
1.04

PD, 2-ABP, Malononitrile, 80deg, 5h, purified pale yellow solid



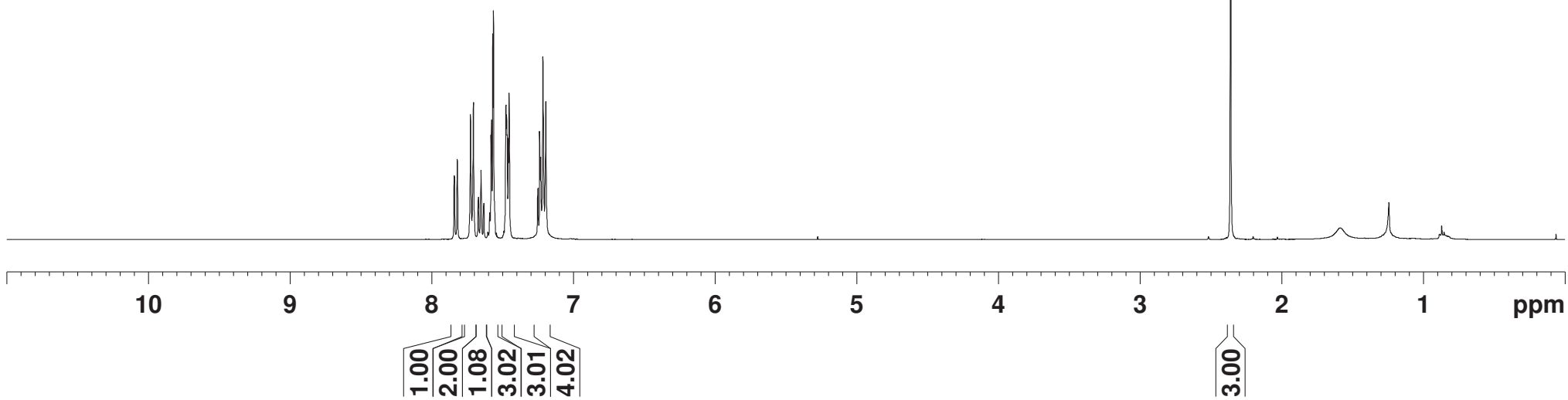
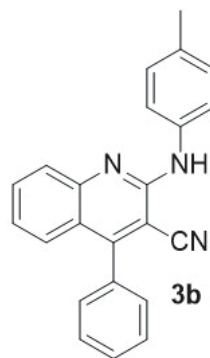
4MePD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid

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7.728
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7.674
7.671
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7.654
7.650
7.636
7.633
7.593
7.589
7.582
7.579
7.570
7.565
7.559
7.477
7.473
7.469
7.460
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7.251
7.239
7.233
7.230
7.216
7.196

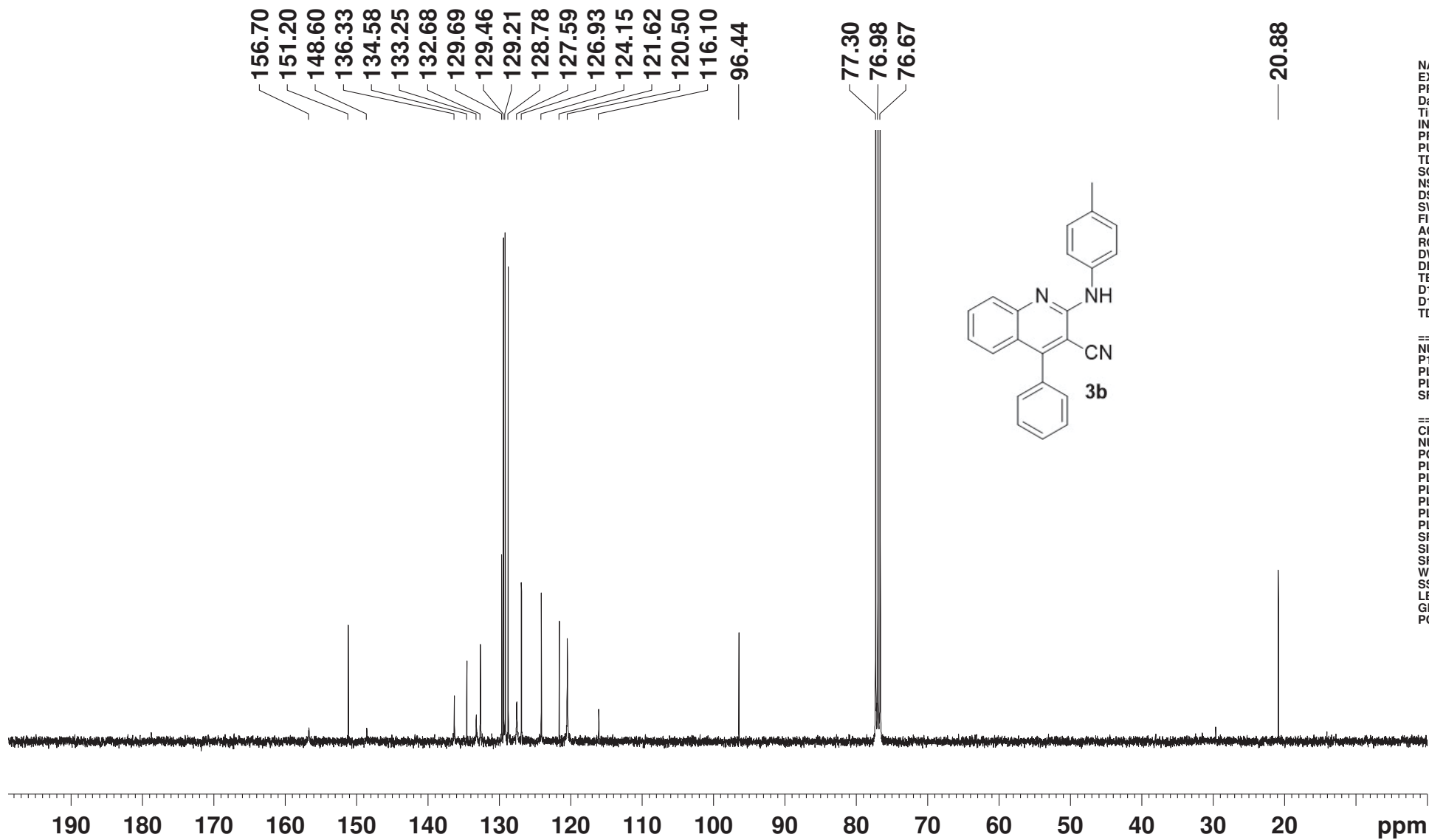
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SOLVENT CDCl3
NS 24
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FIDRES 0.250967 I
AQ 1.9923444 se
RG 161
DW 60.800 use
DE 6.50 usec
TE 295.5 K
D1 1.0000000 se
TD0 1

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NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.67551708
SFO1 400.1528010
SI 32768
SF 400.1500168 M
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



4MePD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid



NAME mani
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PROCNO
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Time 1
INSTRUM
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PULPROG
TD 65
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DW 17
DE 6
TE 29
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TD0

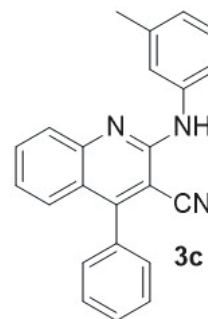
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P1 9.
PL1
PL1W 41.1
SFO1 100.

=====
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NUC2 CH/
PCPD2
PL2
PL12 1
PL13 1
PL2W 13.4
PL12W 0.3
PL13W 0.1
SFO2 400.
SI 32.
SF 100.6
WDW
SSB
LB 1
GB
PC 1

3-MePD, MCN, 2-ABP, 80deg, 5h, purified pale yellow solid

7.690
7.687
7.673
7.669
7.666
7.652
7.648
7.604
7.586
7.582
7.574
7.569
7.563
7.559
7.498
7.490
7.486
7.477
7.475
7.466
7.461
7.453
7.312
7.293
7.273
7.269
7.266
7.252
7.248
7.245
7.239
7.231
7.228
6.960
6.941

2.404



NAME mani 31-12-2018
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TD 32768
SOLVENT CDCl3
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FIDRES 0.537281 Hz
AQ 1.8612725 sec
RG 118.08
DW 56.800 usec
DE 14.47 usec
TE 296.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.1328009 MH:
NUC1 1H
P1 15.50 usec
SI 131072
SF 400.1300180 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0

1.00
1.04
1.08
4.01
3.01
1.09
2.08
1.01

3.01

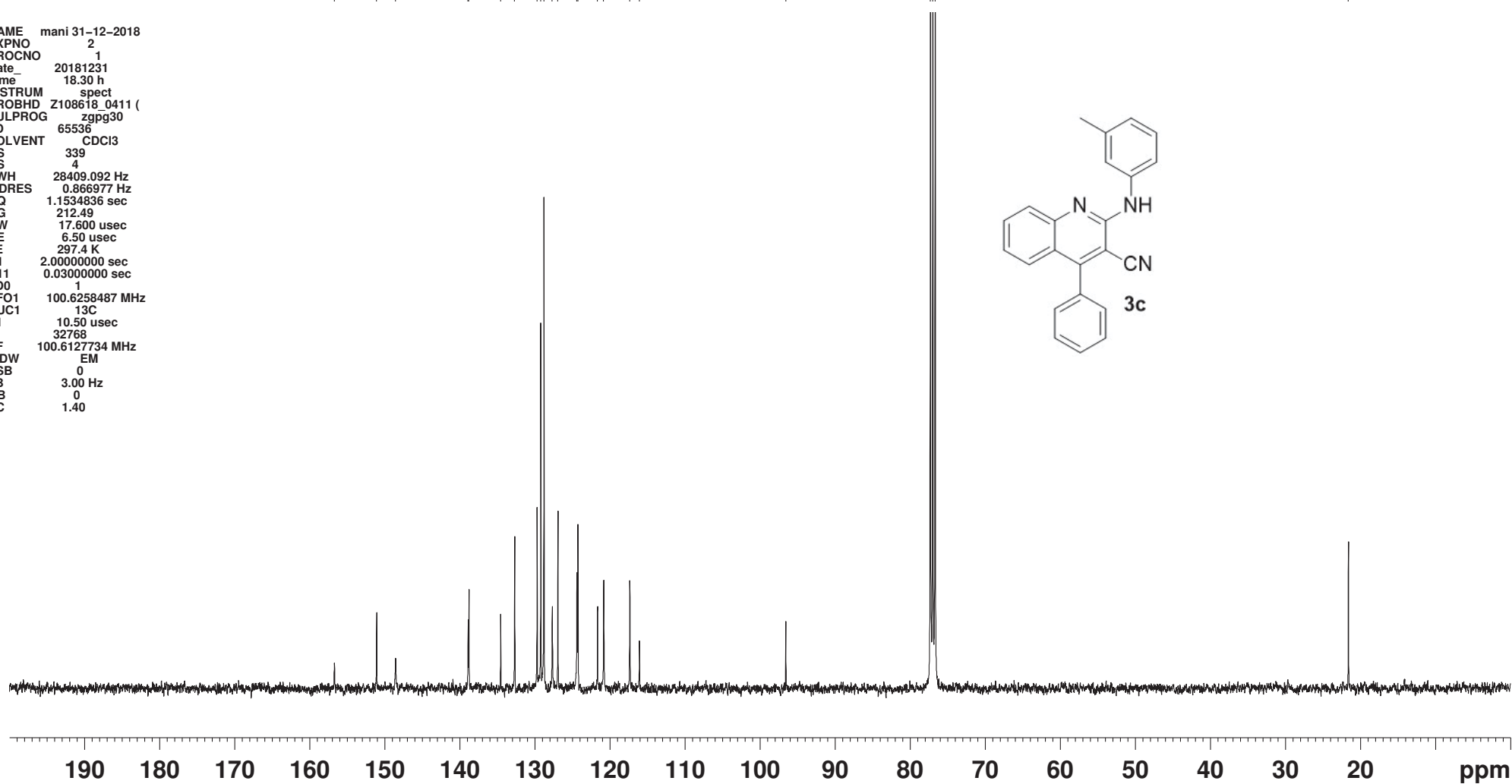
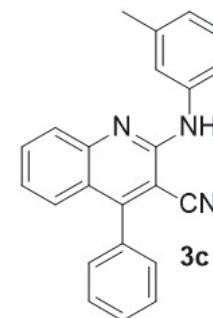
3-MePD, MCN, 2-ABP, 80deg, 5h, purified pale yellow solid

156.728
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148.571
138.911
138.799
134.577
132.702
129.725
129.233
128.809
127.692
126.946
124.414
124.285
121.674
120.837
117.368
116.085
96.576

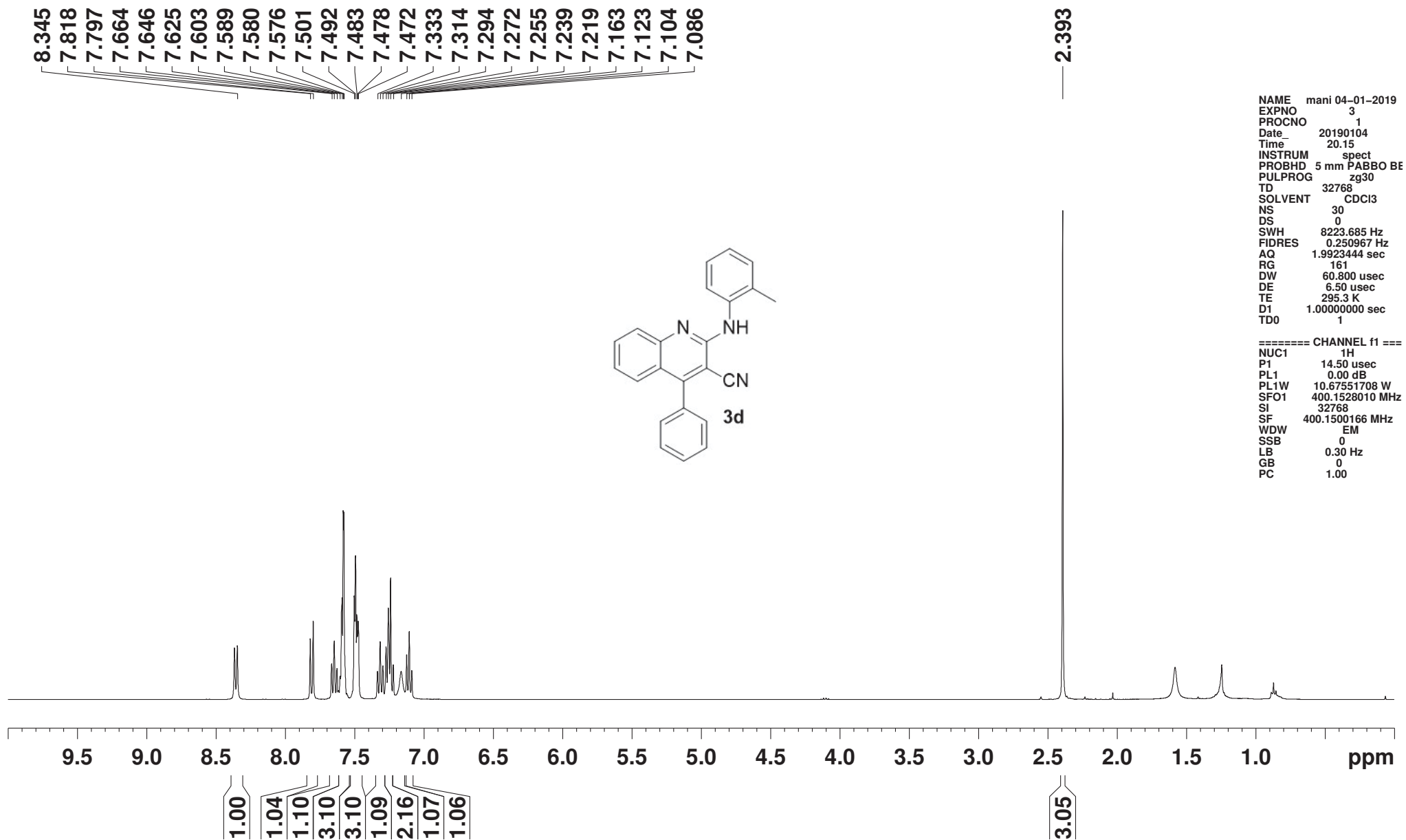
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77.002
76.684

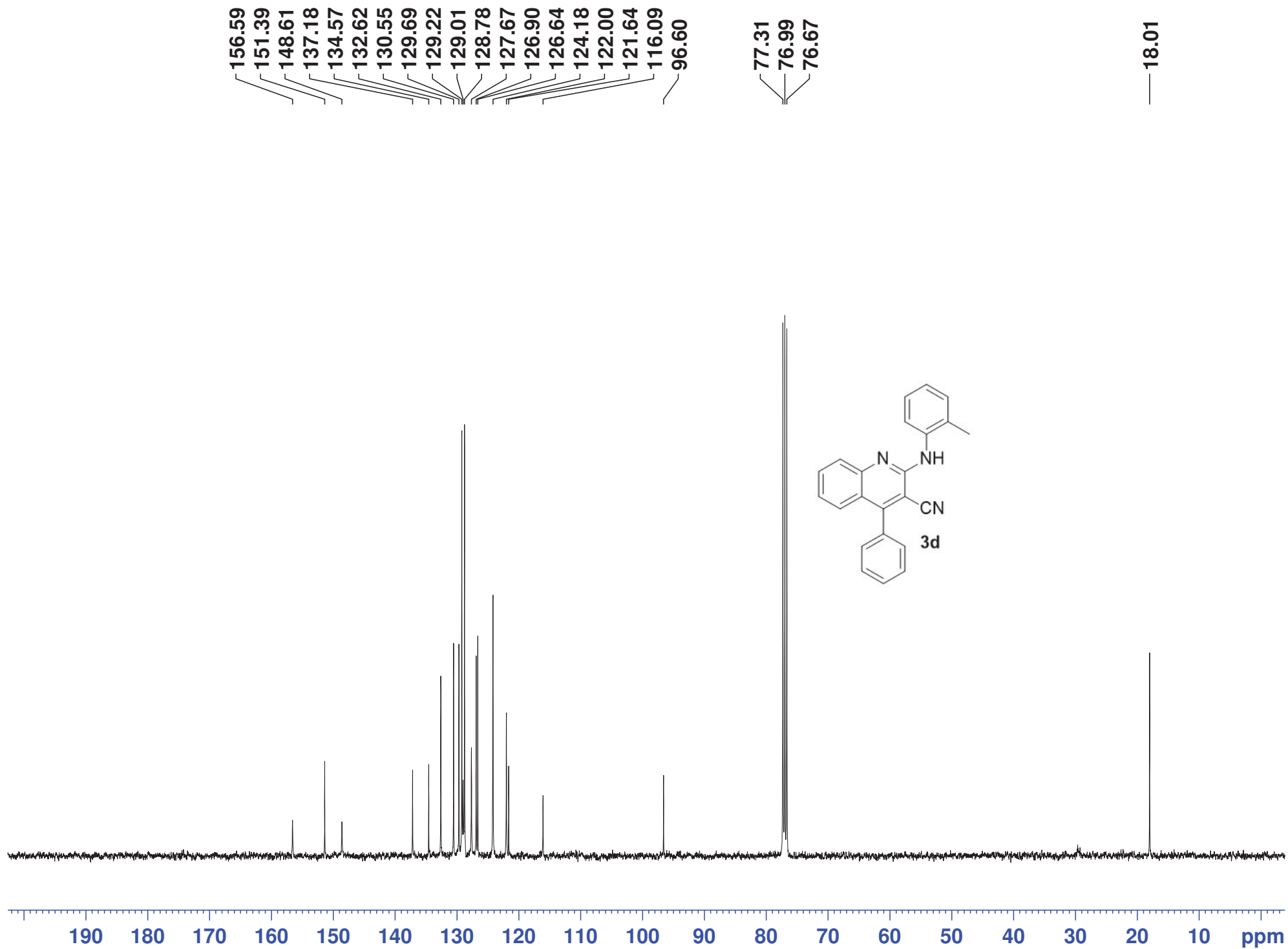
21.611

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SOLVENT CDCl3
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FIDRES 0.866977 Hz
AQ 1.1534836 sec
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JW 17.600 usec
JE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6258487 MHz
NUC1 13C
P1 10.50 usec
SI 32768
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WDW EM
SSB 0
LB 3.00 Hz
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2MePD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid



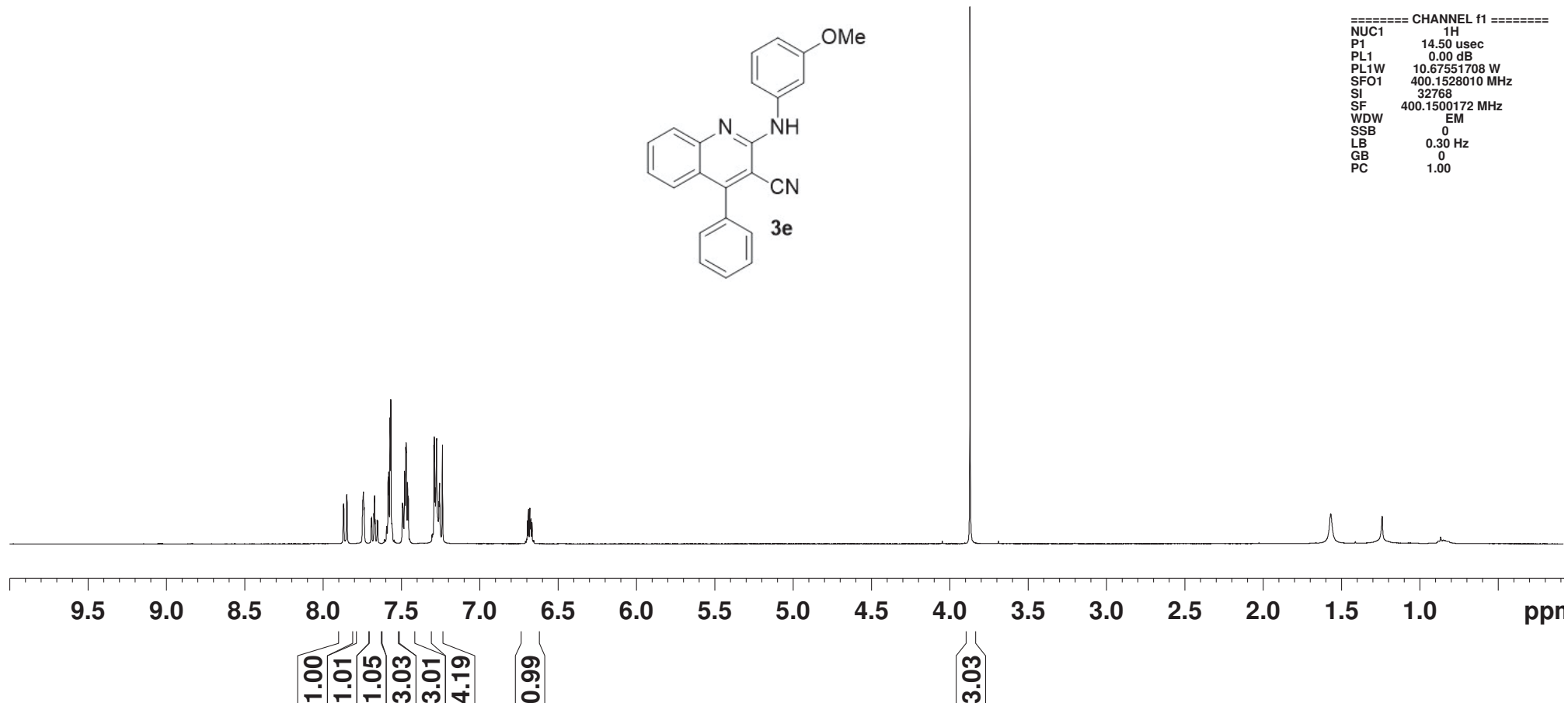
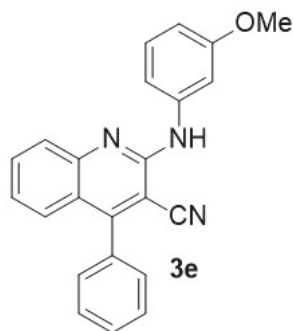


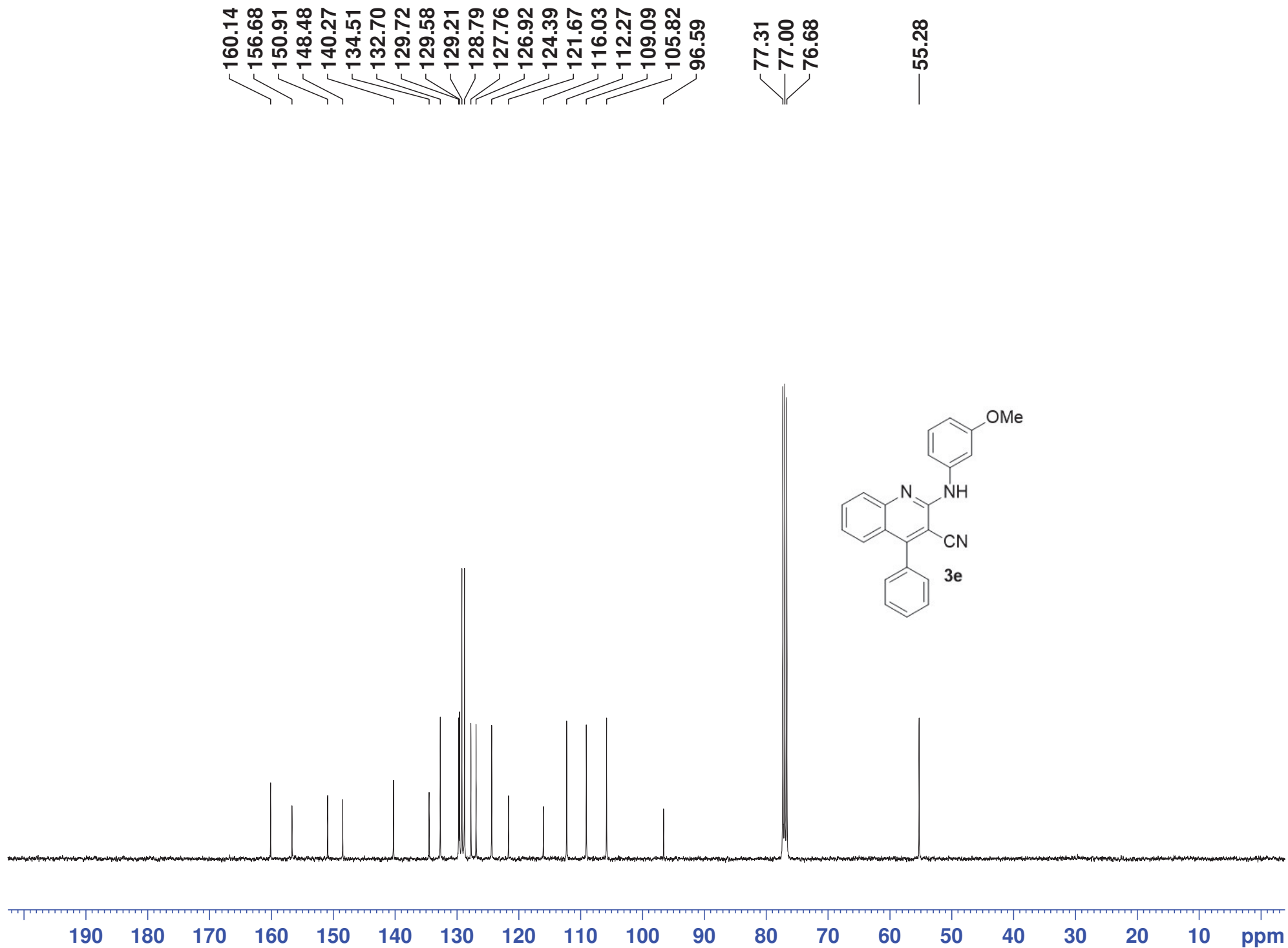
3OMePD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid

7.668
7.654
7.651
7.595
7.591
7.585
7.580
7.572
7.567
7.561
7.557
7.493
7.490
7.486
7.480
7.472
7.469
7.461
7.456
7.305
7.300
7.292
7.289
7.285
7.280
7.275
7.260
7.257
7.238
6.695
6.689
6.680
6.675
6.673
6.666
3.870

NAME mani 08-01-2019
EXPNO 2
PROCNO 1
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PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 8223.685 Hz
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D1 1.0000000 sec
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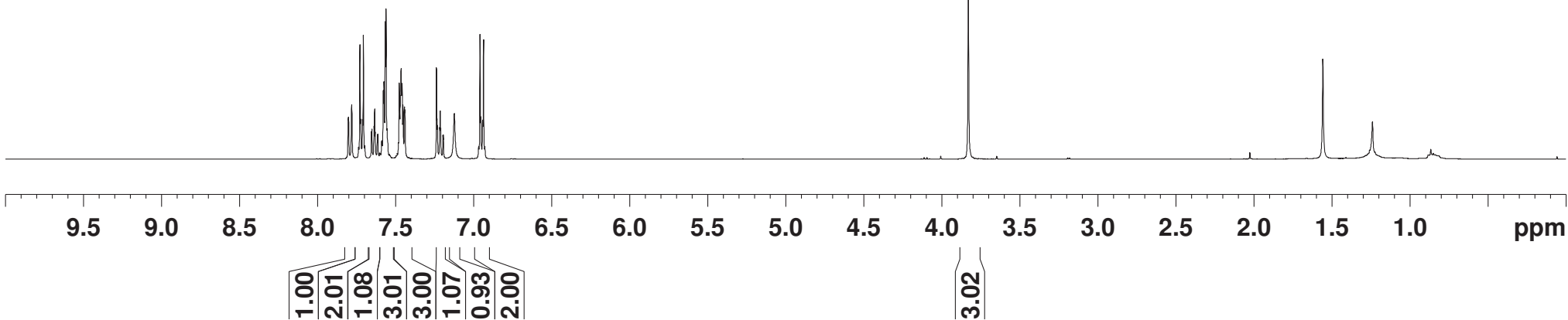
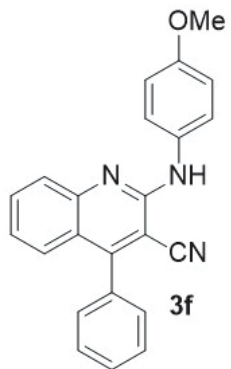
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SFO1 400.1528010 MHz
SI 32768
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





4OMePD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid

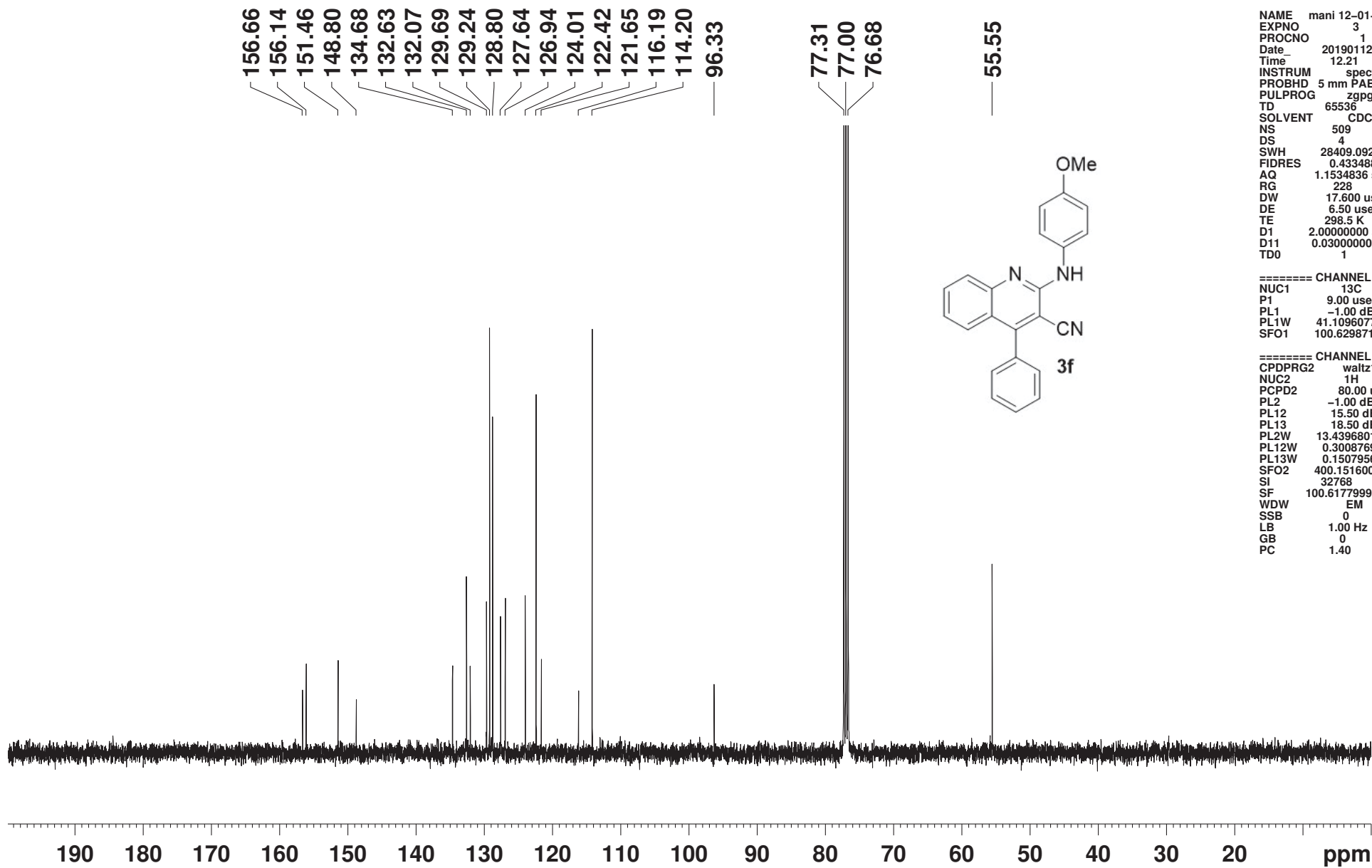
7.632
7.618
7.615
7.590
7.587
7.580
7.575
7.567
7.563
7.556
7.552
7.483
7.478
7.470
7.466
7.463
7.459
7.454
7.444
7.442
7.239
7.236
7.233
7.219
7.215
7.212
7.198
7.195
7.125
6.969
6.960
6.955
6.943
6.938
6.929
3.831



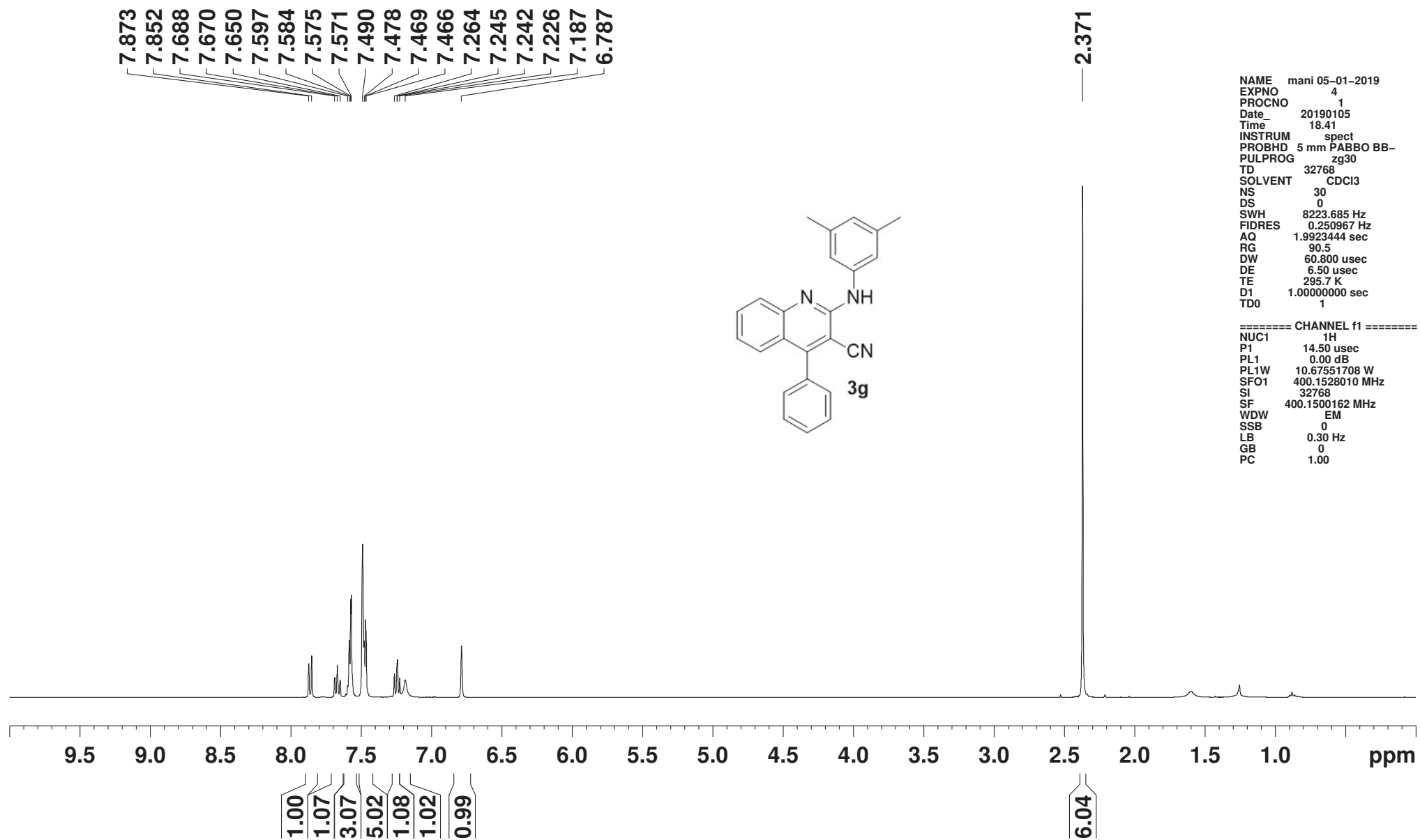
NAME mani 12-01-2018
EXPNO 2
PROCNO 1
Date_ 20190112
Time 12.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.67551708 W
SFO1 400.1528010 MHz
SI 32768
SF 400.1500167 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

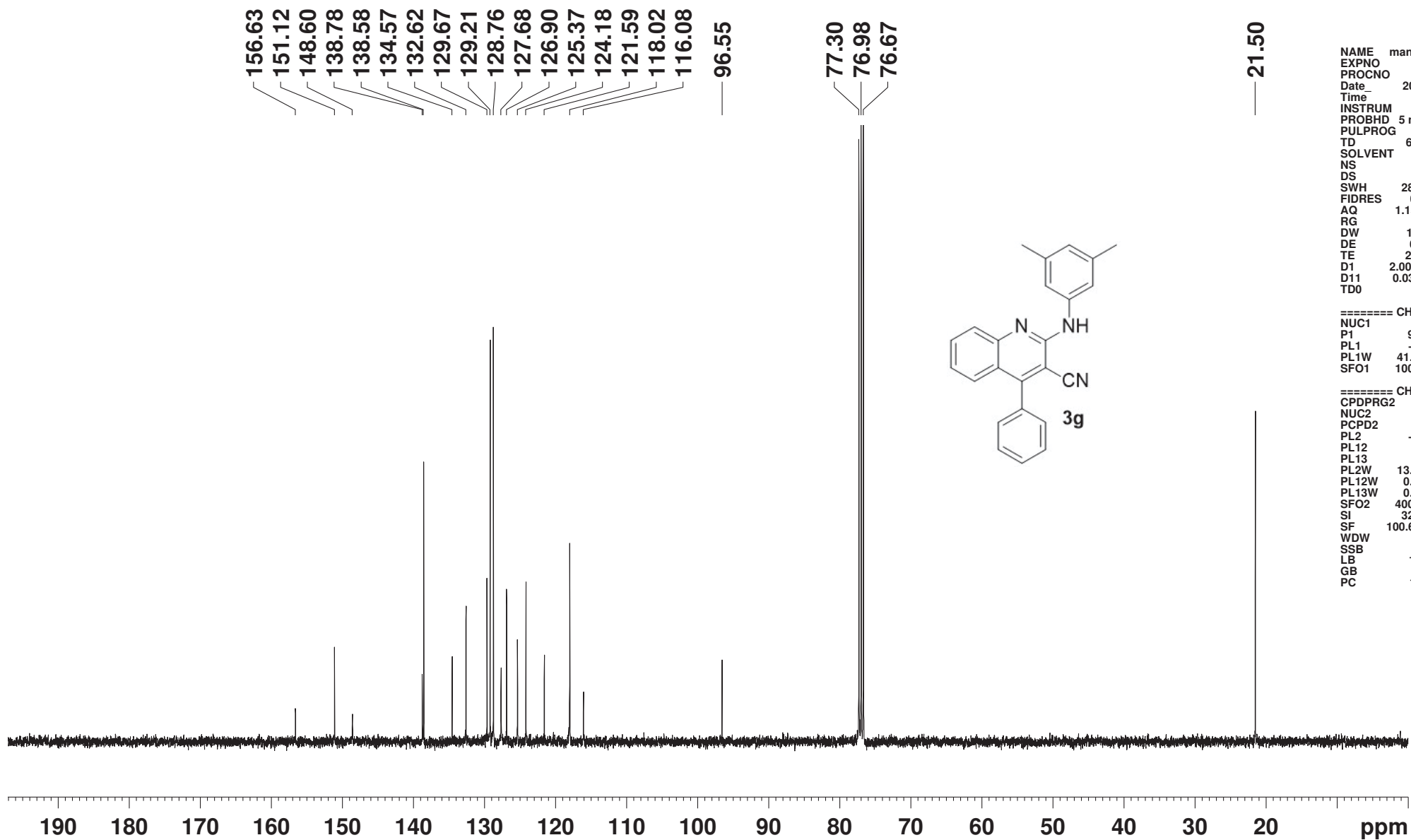
4OMePD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid



35diMePD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid



35diMePD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid



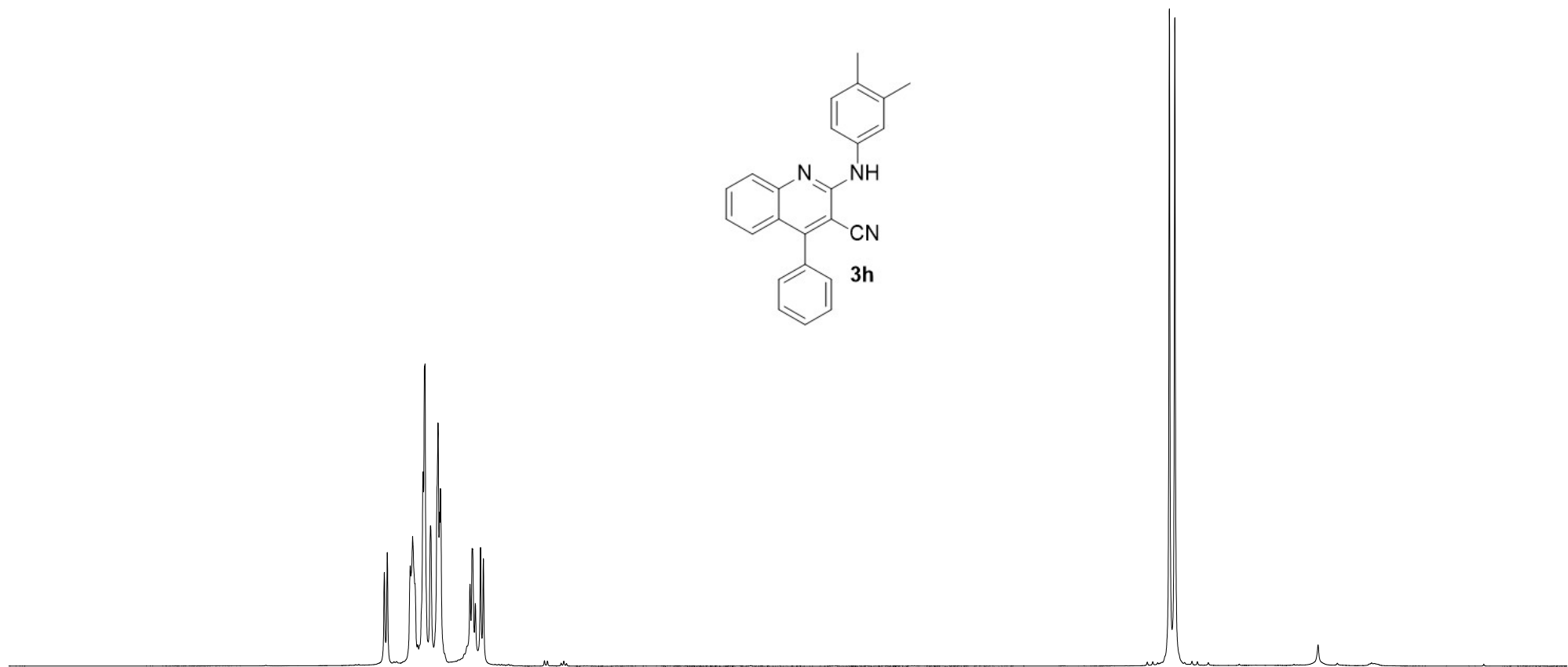
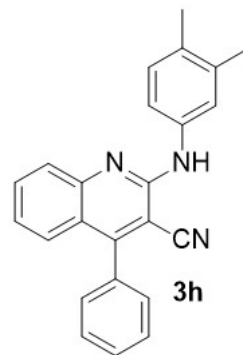
```
NAME mani 05-
EXPNO
PROCNO
Date_ 20190
Time 18.4
INSTRUM s
PROBHD 5 mm l
PULPROG z
TD 65536
SOLVENT C
NS 244
DS 4
SWH 28409
FIDRES 0.43
AQ 1.15348
RG 144
DW 17.60
DE 6.50
TE 295.9
D1 2.00000
D11 0.03000
TD0 1

===== CHANN
NUC1 13
P1 9.00
PL1 -1.00
PL1W 41.109
SFO1 100.625

===== CHANN
CPDPRG2 w
NUC2 11
PCPD2 80.
PL2 -1.00
PL12 15.5
PL13 18.5
PL2W 13.439
PL12W 0.300
PL13W 0.150
SFO2 400.151
SI 32768
SF 100.6178
WDW E
SSB 0
LB 1.00
GB 0
PC 1.40
```

7.848
7.827
7.665
7.648
7.631
7.574
7.565
7.561
7.522
7.468
7.458
7.452
7.243
7.228
7.225
7.169
7.149

2.308
2.270



1.02
2.08
3.07
1.04
3.07
2.00
1.03

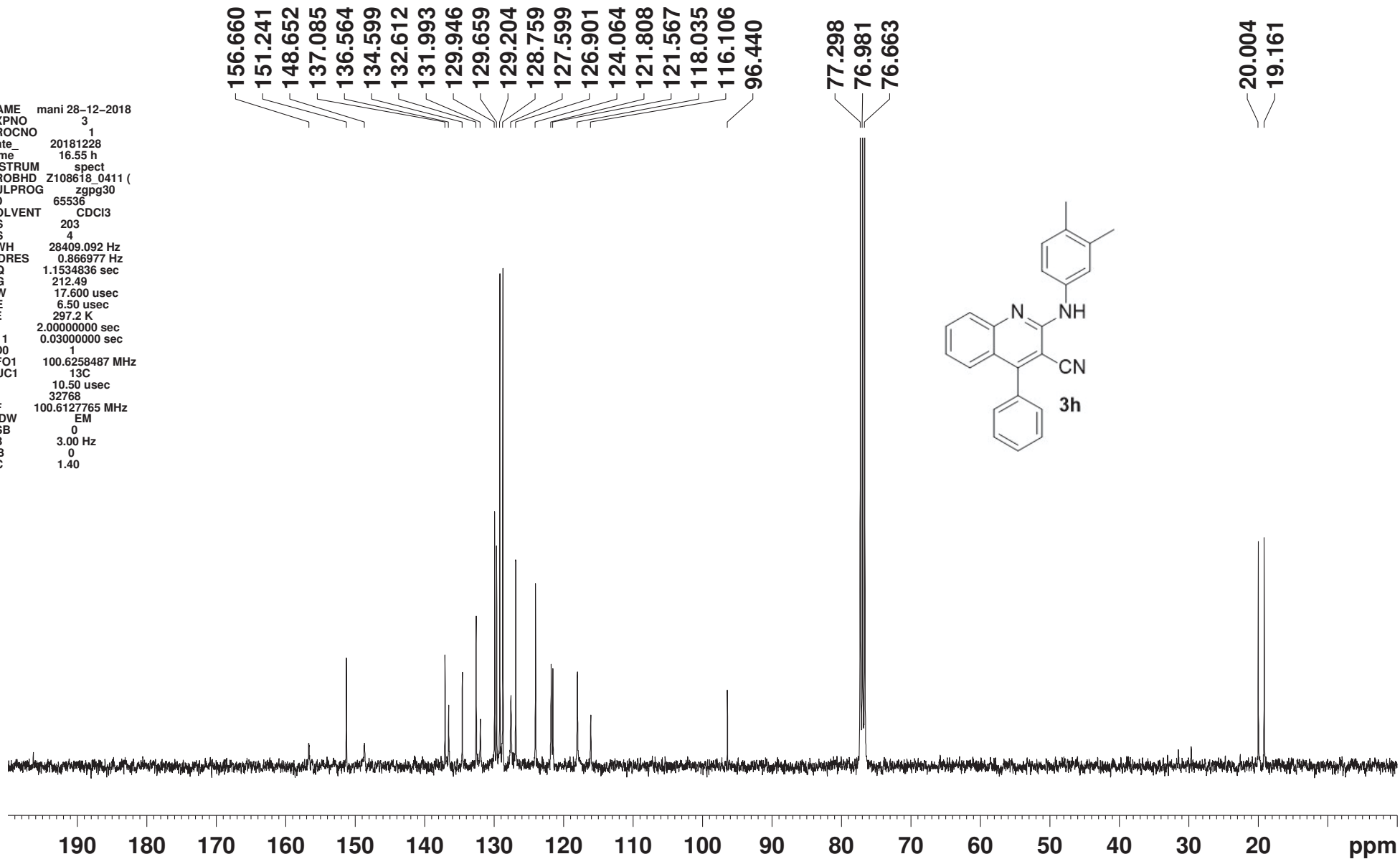
3.00
3.03

S20

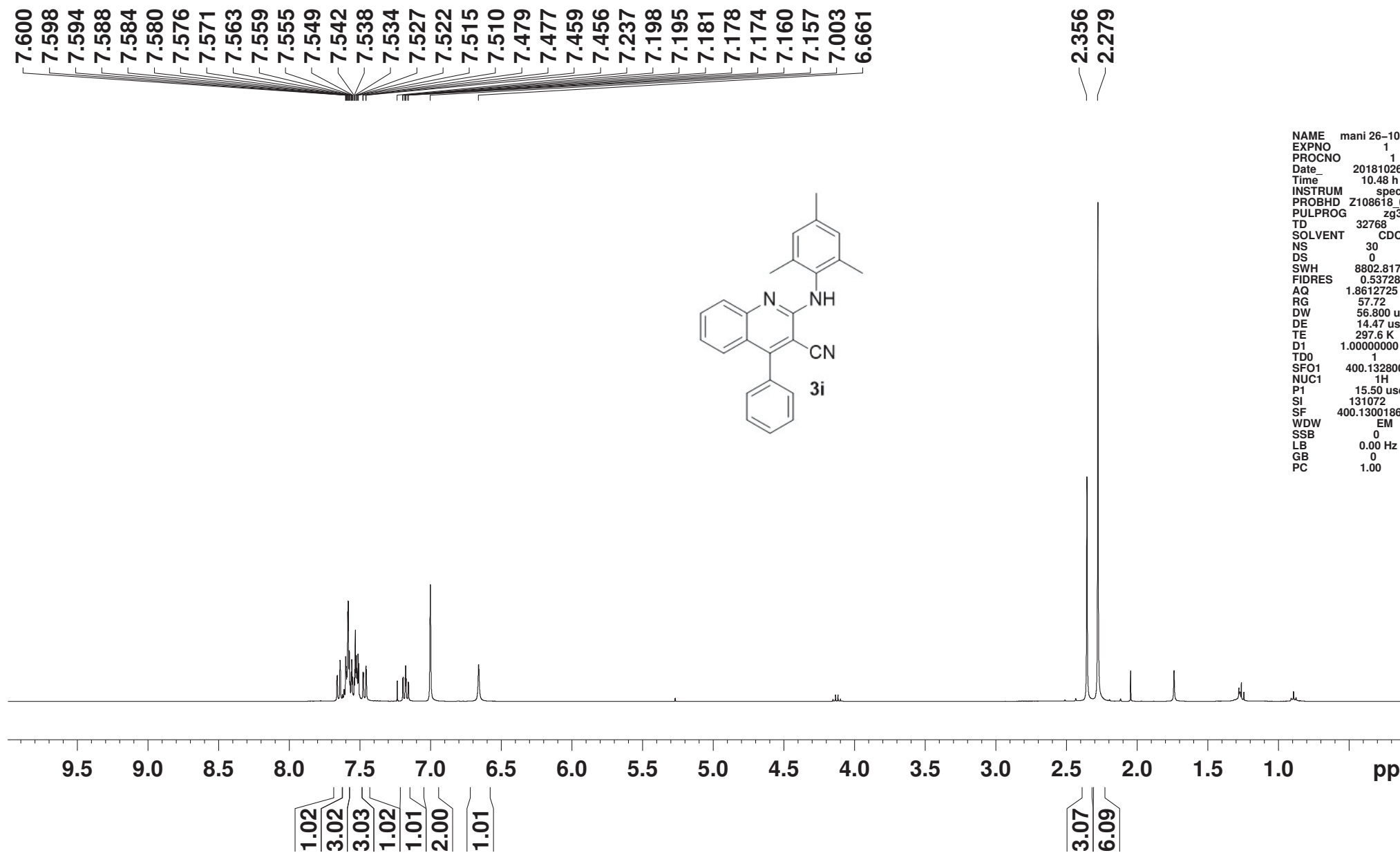
ppm

34-diMePD, MCN, 2-ABP, 80deg, 5h, purified pale yellow solid

NAME mani 28-12-2018
EXPNO 3
PROCNO 1
Date_ 20181228
Time 16.55 h
INSTRUM spect
PROBHD Z108618_0411 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 203
DS 4
SWH 28409.092 Hz
FIDRES 0.866977 Hz
AQ 1.1534836 sec
RG 212.49
DW 17.600 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6258487 MHz
NUC1 13C
P1 10.50 usec
SI 32768
SF 100.6127765 MHz
WDB EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



246triMePD, 2-ABP, malononitrile, 120deg, 5h, purified pale yellow solid



246triMePD, 2-ABP, malononitrile, 120deg, 5h, purified pale yellow solid

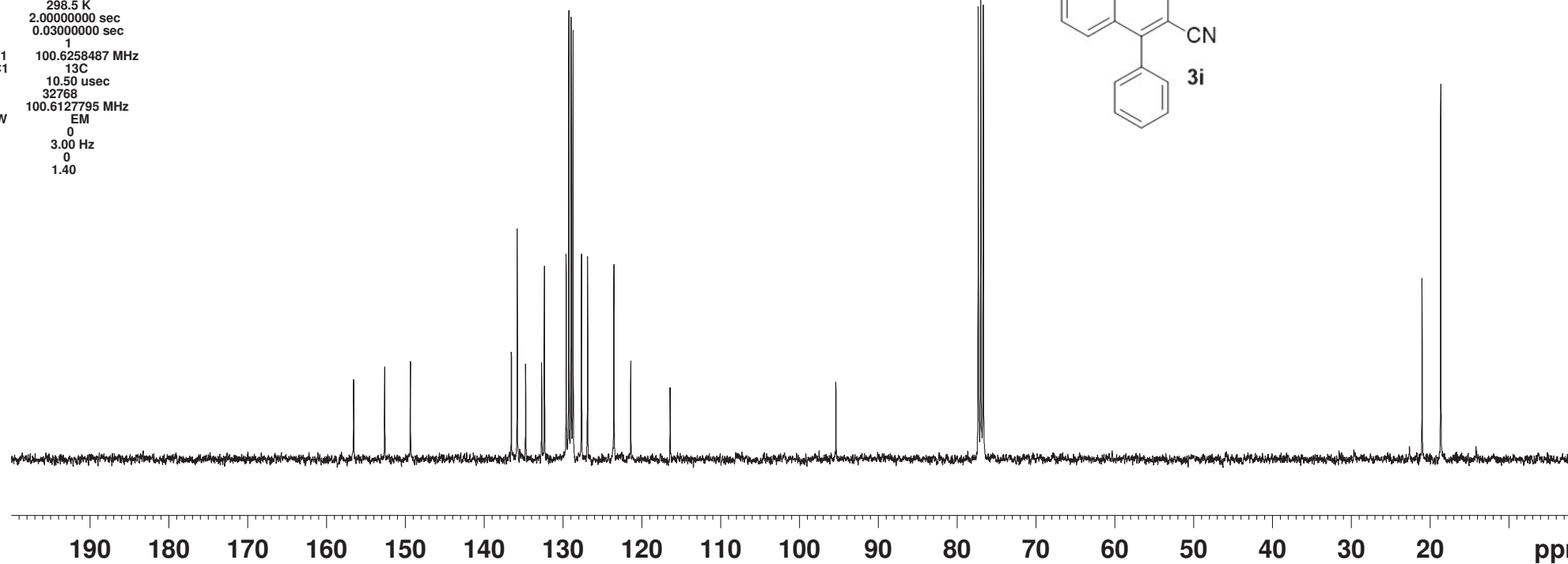
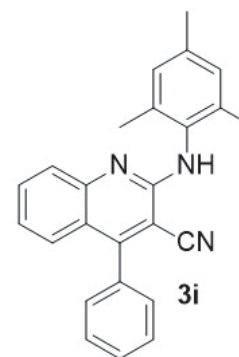
NAME mani 26-10-2018
EXPNO 2
PROCNO 1
Date_ 20181026
Time 10.57 h
INSTRUM spect
PROBHD Z108618_0411 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 124
DS 4
SWH 28409.092 Hz
FIDRES 0.866977 Hz
AQ 1.1534836 sec
RG 212.49
DW 17.600 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6258487 MHz
NUC1 13C
P1 10.50 usec
SI 32768
SF 100.6127795 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

156.554
152.609
149.340
136.532
135.793
134.725
132.691
132.340
129.579
129.252
128.953
128.713
127.639
126.866
123.527
121.393
116.391

95.362

77.300
76.982
76.664

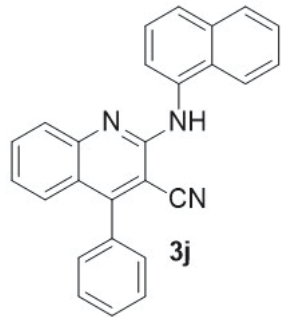
20.989
18.621



1-naphthylPD, 2-ABP, MCN, 80deg, 5h, purified pale yellow solid

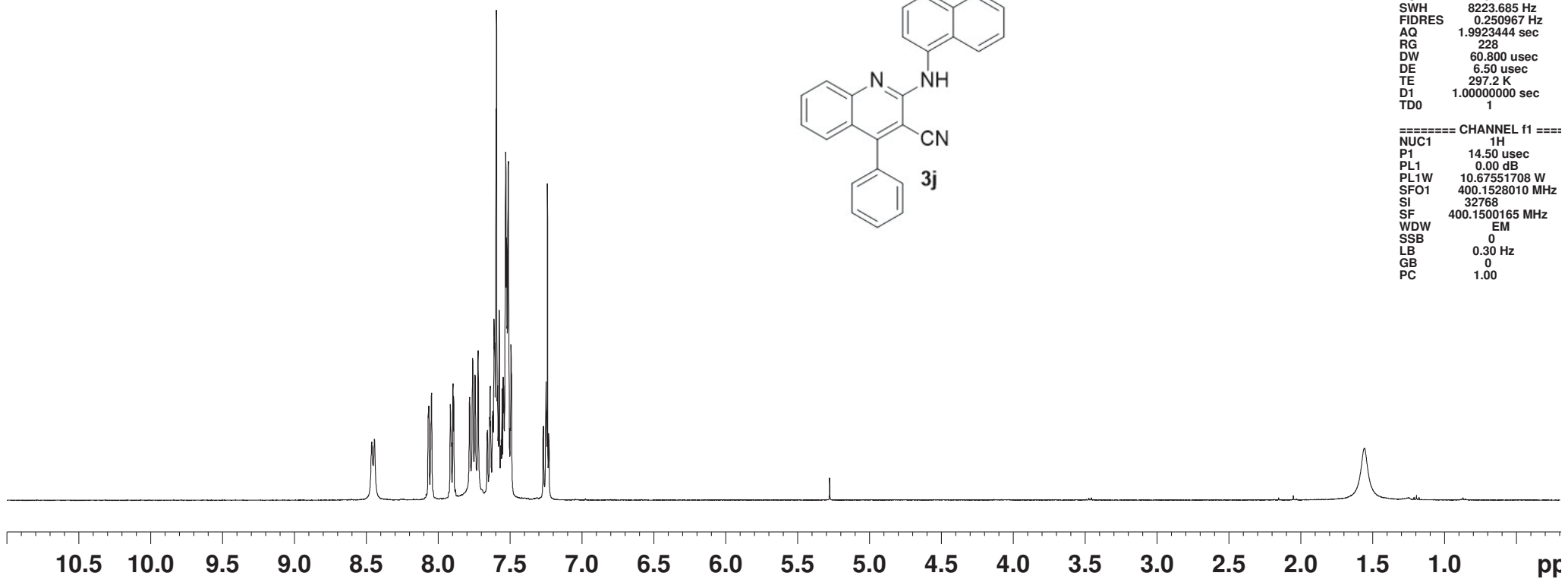
7.892
7.781
7.760
7.743
7.723
7.660
7.657
7.642
7.639
7.635
7.620
7.612
7.609
7.607
7.598
7.594
7.587
7.582
7.576
7.566
7.561
7.556
7.548
7.544
7.541
7.530
7.524
7.521
7.512
7.498
7.494
7.490
7.270
7.267
7.252
7.250
7.246
7.240
7.232
7.229

1.556

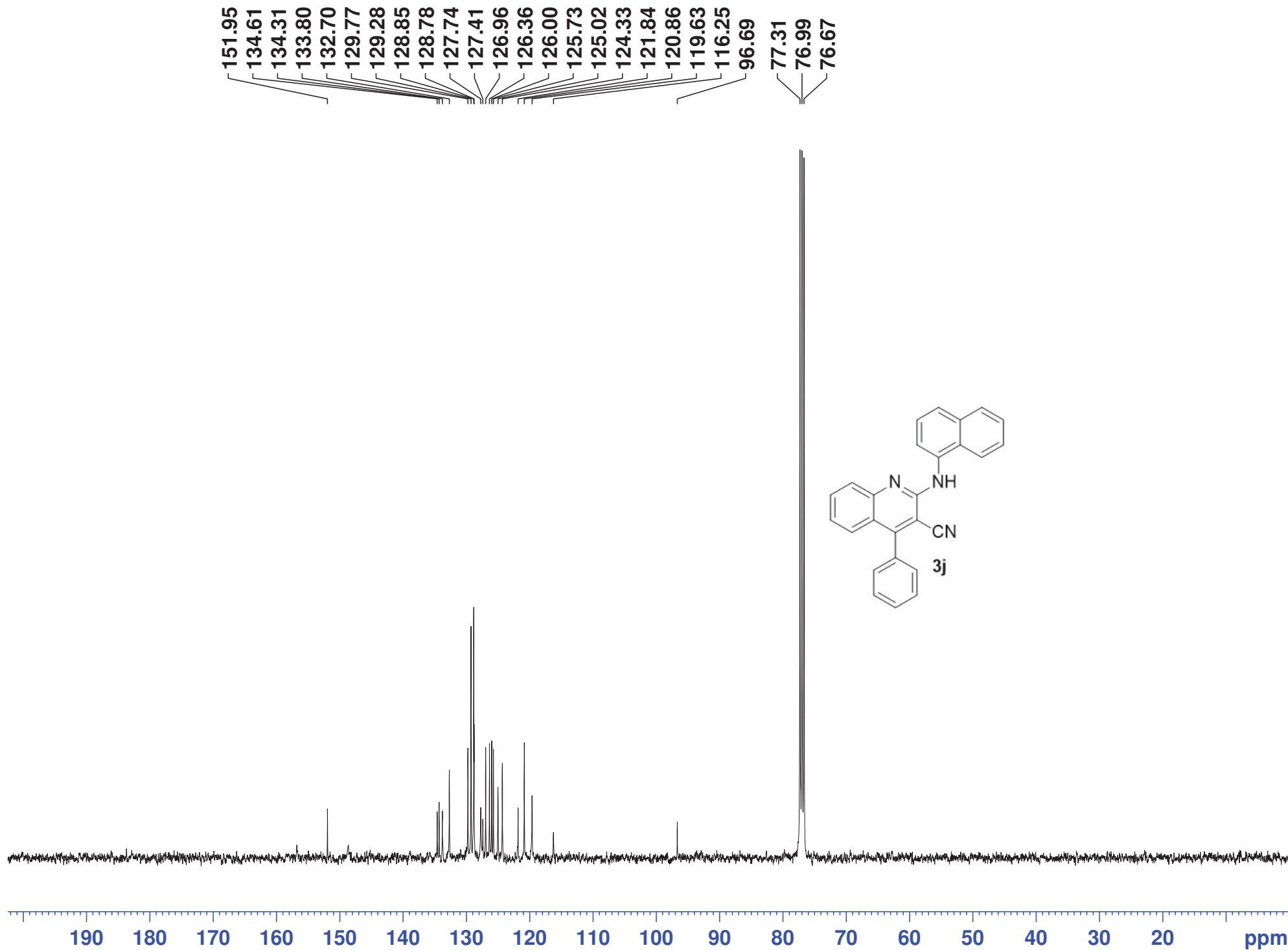


NAME mani 08-01-2019
EXPNO 4
PROCNO 1
Date_ 20190108
Time 20.39
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 15
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 228
DW 60.800 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.67551708 W
SFO1 400.1528010 MHz
SI 32768
SF 400.1500165 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

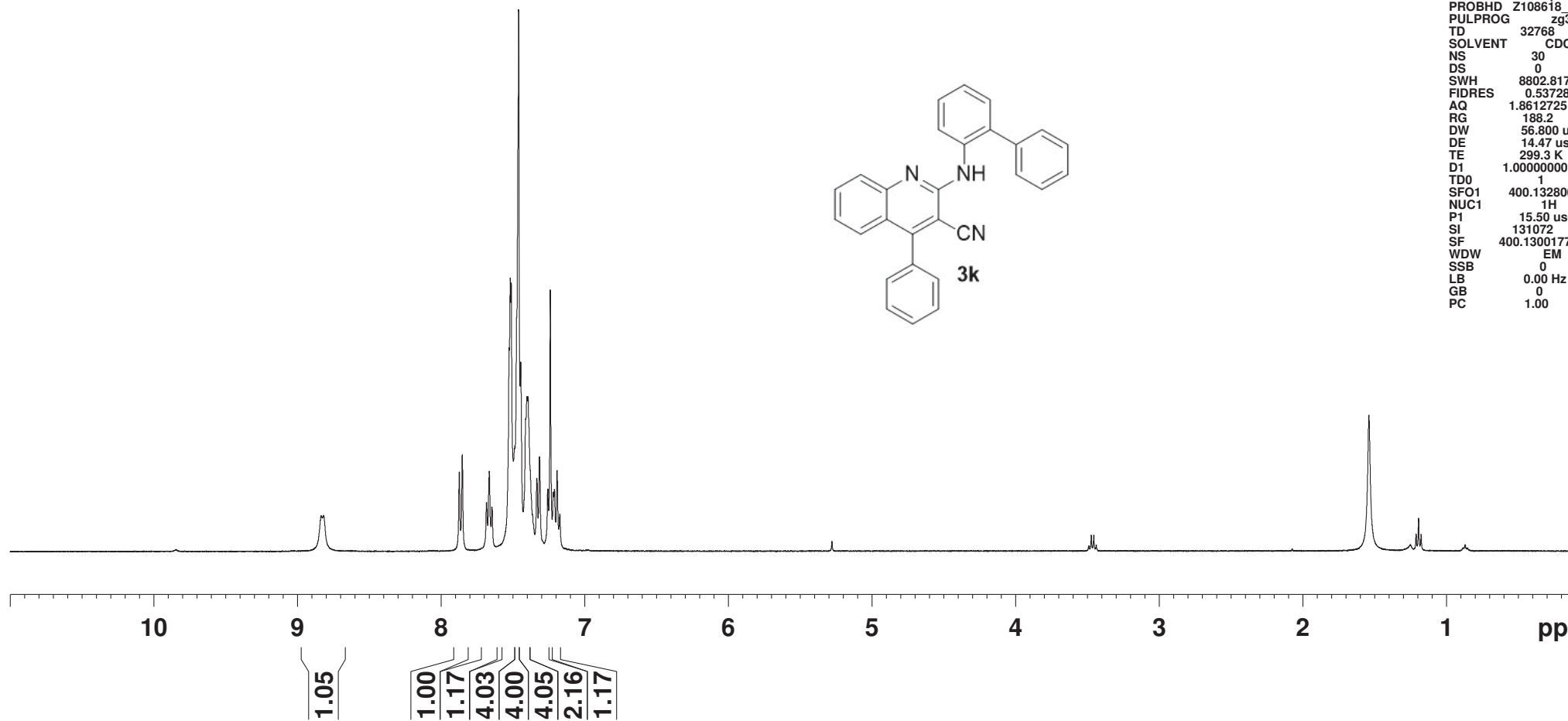


1.00
1.07
1.10
2.89
2.13
3.13
5.19
1.27



2PhPD, ABP, MCN, 80deg, 5h, purified pale yellow solid

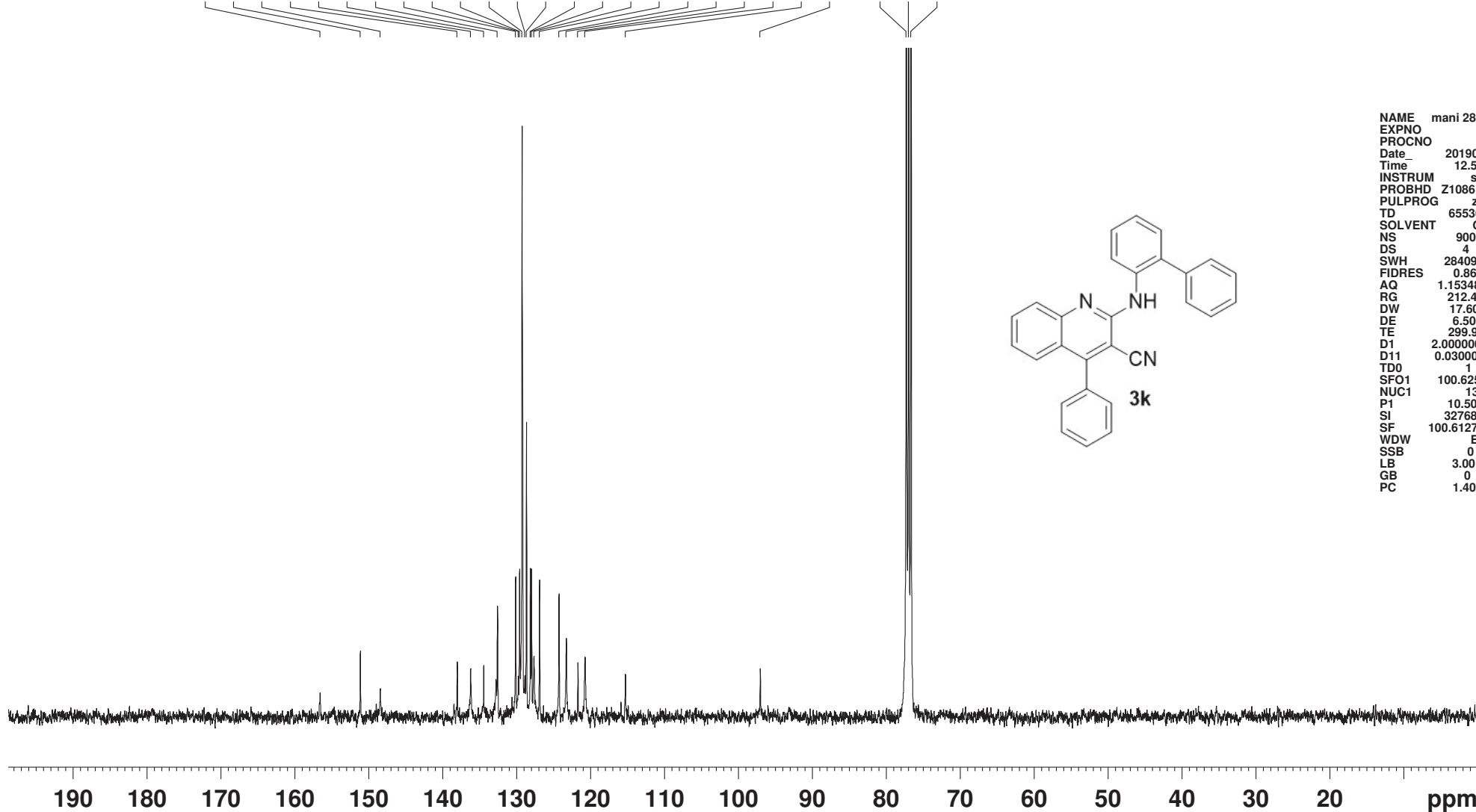
8.836
8.819
7.873
7.853
7.683
7.665
7.646
7.527
7.518
7.512
7.486
7.460
7.446
7.411
7.402
7.395
7.363
7.334
7.315
7.256
7.240
7.219
7.211
7.192
7.174



NAME mani 28-01
EXPNO 5
PROCNO 1
Date_ 20190126
Time 19.51 h
INSTRUM spec
PROBHD Z108618_1
PULPROG zg3
TD 32768
SOLVENT CDC
NS 30
DS 0
SWH 8802.817
FIDRES 0.53728
AQ 1.8612725
RG 188.2
DW 56.800 u
DE 14.47 us
TE 299.3 K
D1 1.0000000
TD0 1
SFO1 400.132801
NUC1 1H
P1 15.50 us
SI 131072
SF 400.1300177
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

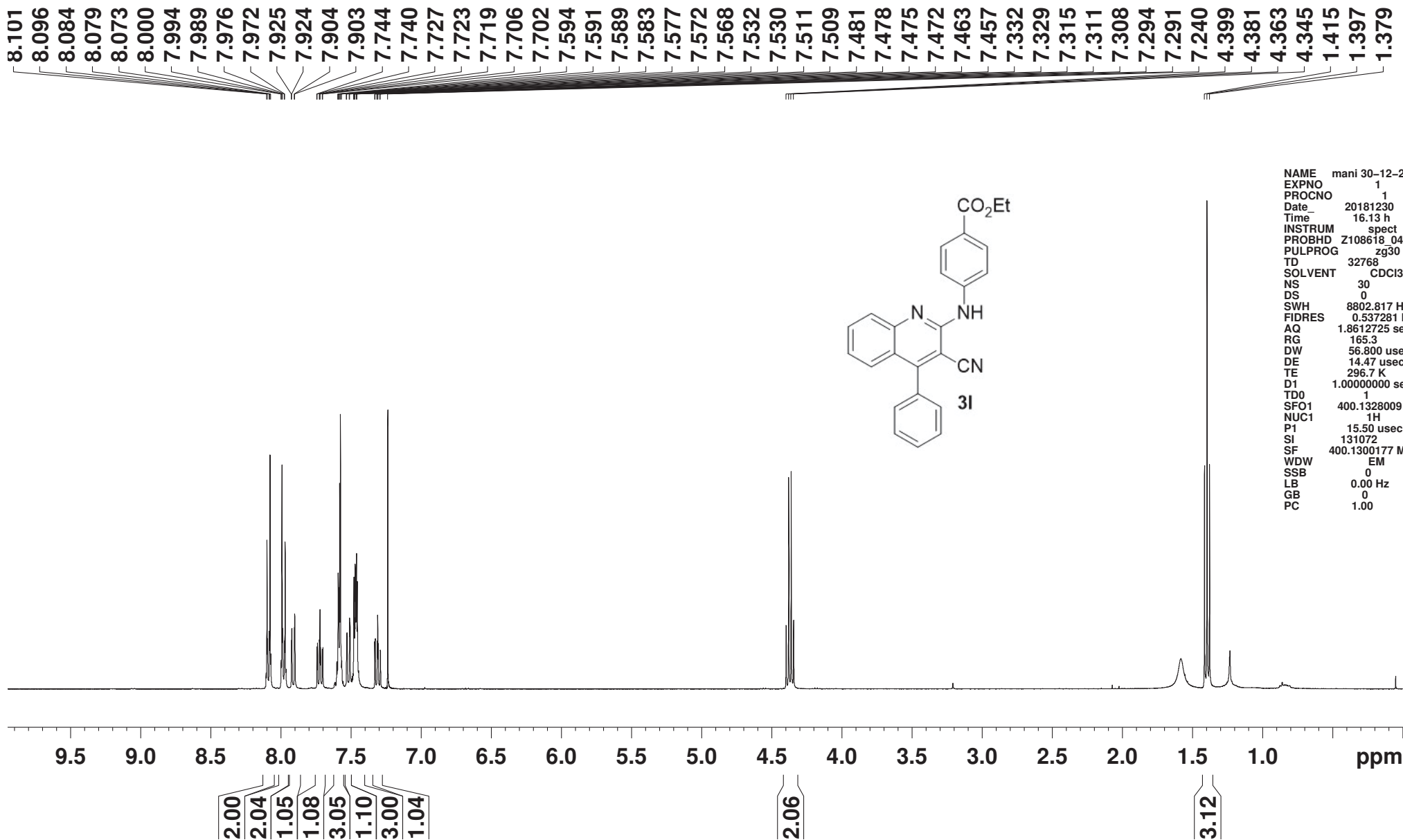
2PhPD, ABP, MCN, 80deg, 5h, purified pale yellow solid

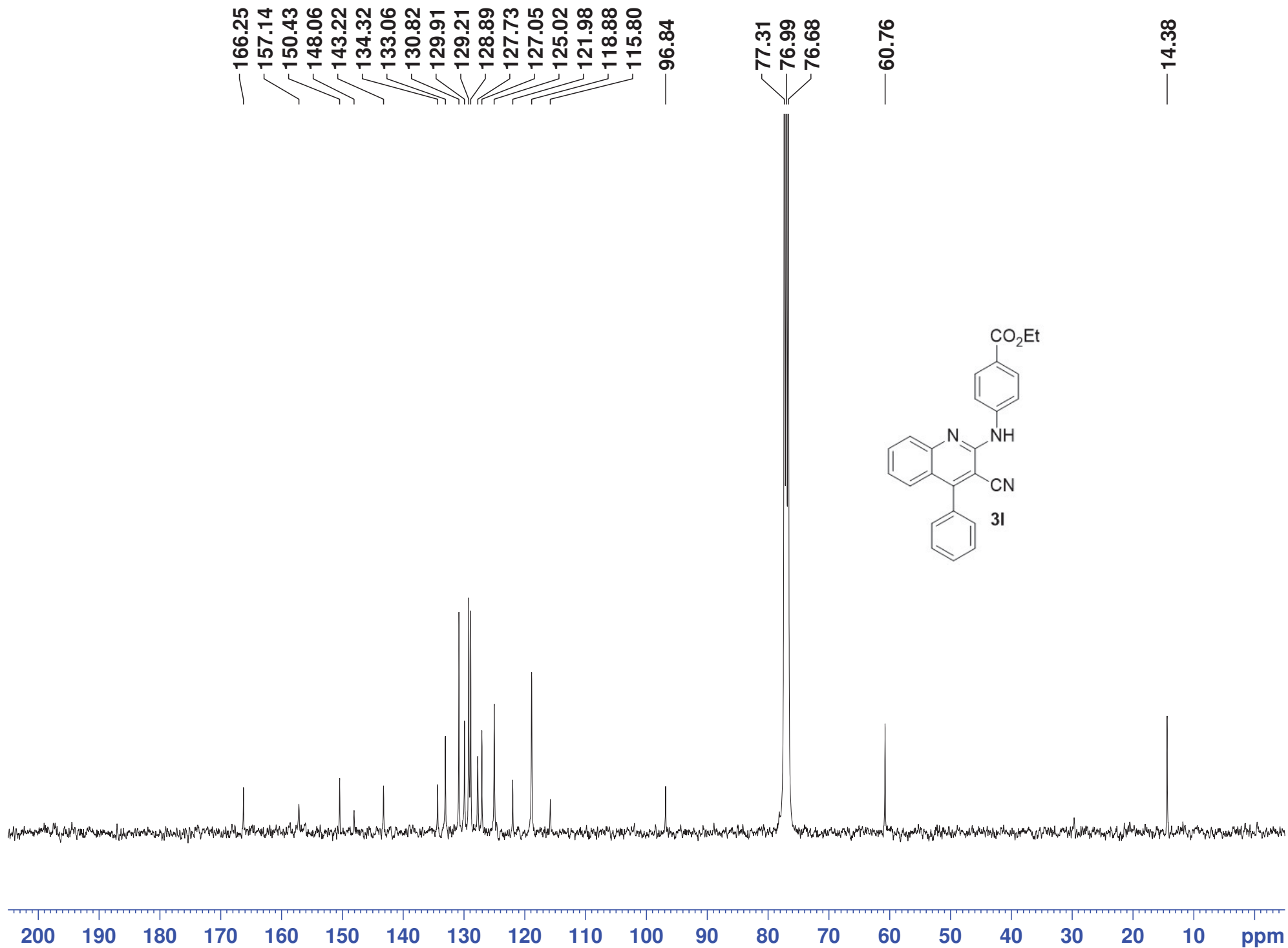
156.610
151.161
148.473
138.046
136.249
134.476
132.612
130.164
129.794
129.621
129.286
128.899
128.688
128.151
127.995
127.677
126.924
124.290
123.295
121.733
120.765
115.310
97.065
77.303
76.986
76.668



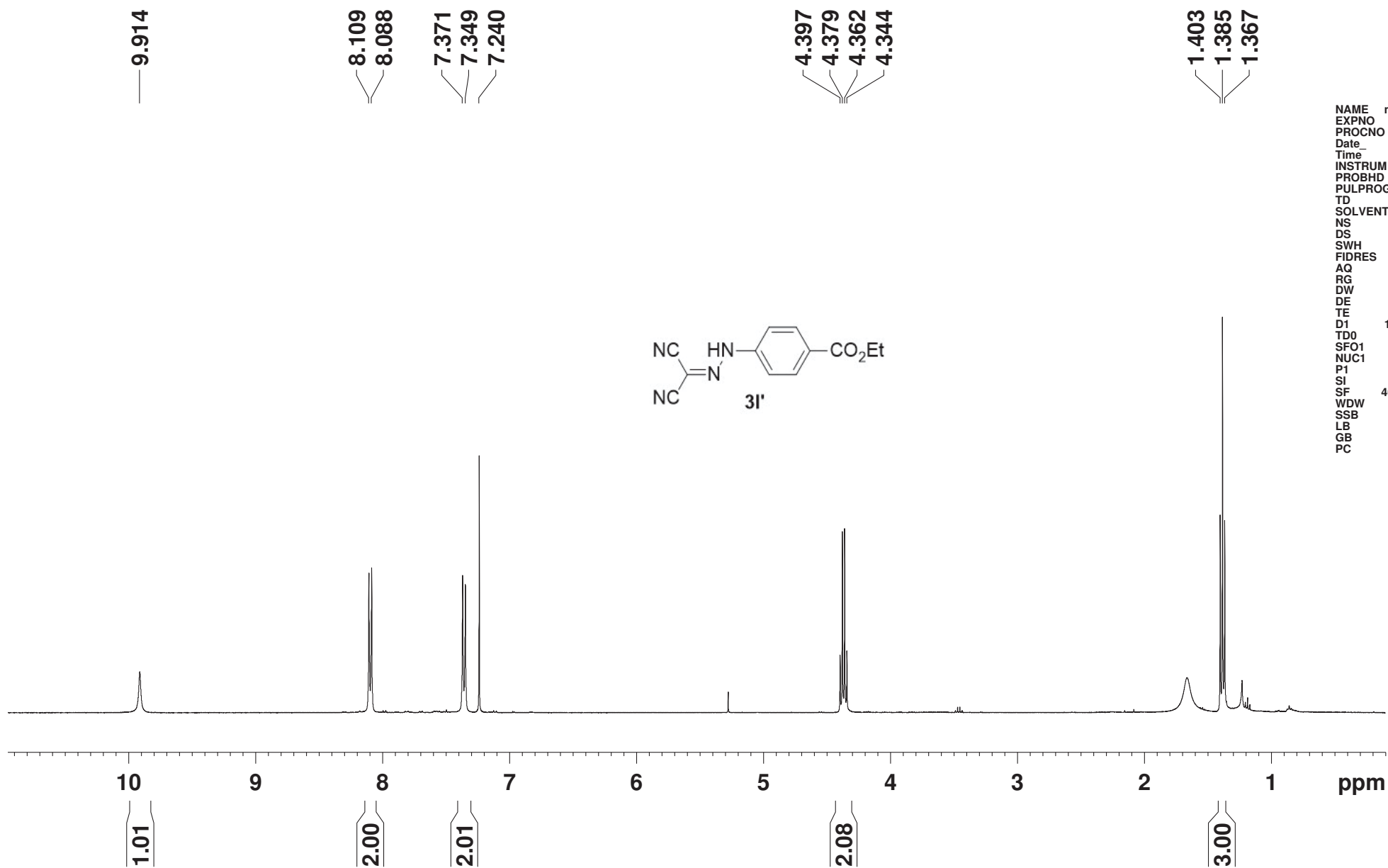
NAME mani 28-01-20
EXPNO 2
PROCNO 1
Date_ 20190128
Time_ 12.56 h
INSTRUM spect
PROBHD Z108618_041
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 900
DS 4
SWH 28409.092 Hz
FIDRES 0.866977 H
AQ 1.1534836 sec
RG 212.49
DW 17.600 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 se
TD0 1
SFO1 100.6258487 M
NUC1 13C
P1 10.50 usec
SI 32768
SF 100.6127708 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

4-CO₂EtPD, MCN, 2-ABP, 80deg, 5h, purified pale yellow solid (midspot)



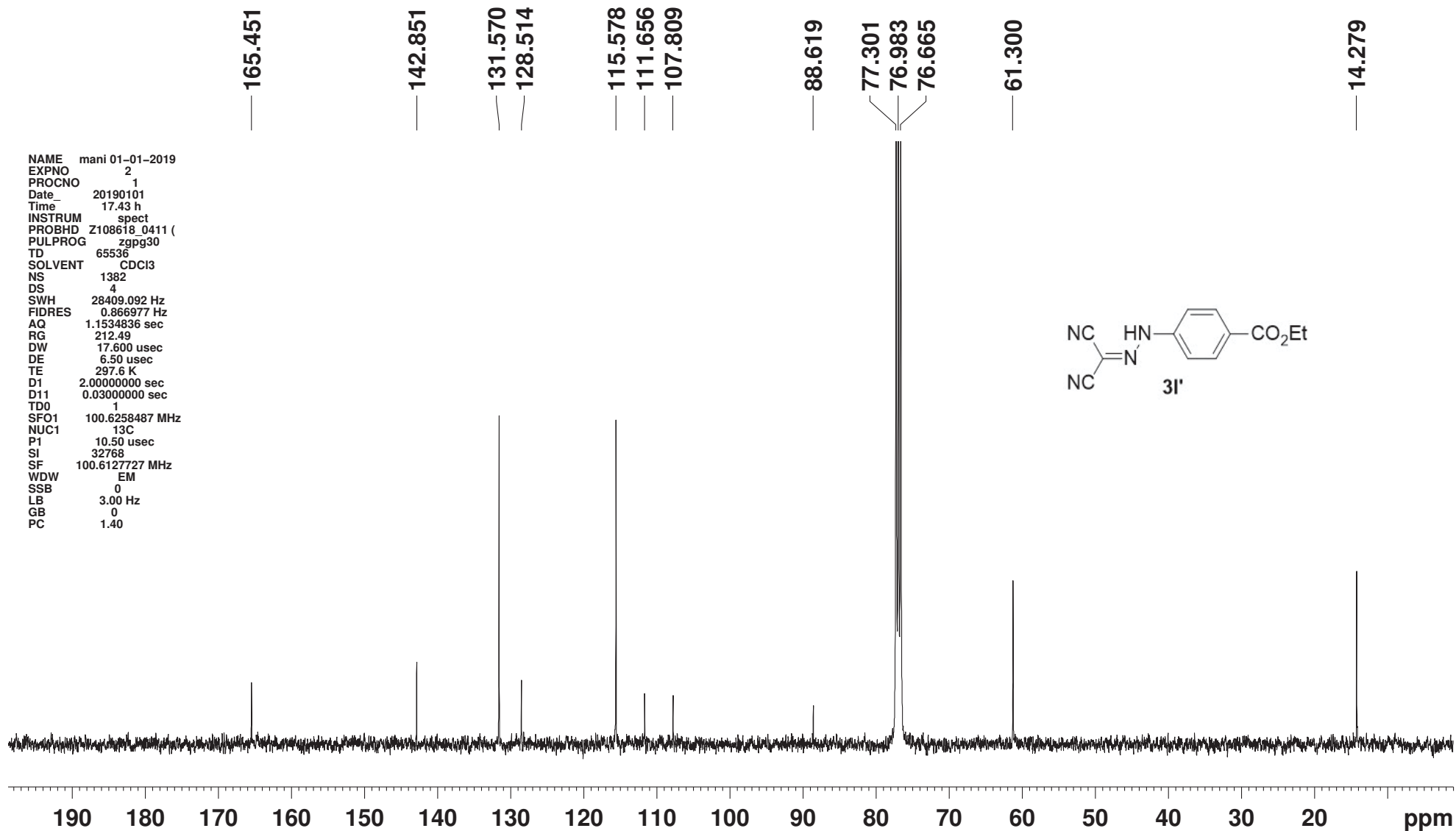


4-CO₂EtPD, MCN, 2-ABP, 80deg, 5h, purified orange solid (bottom spot)



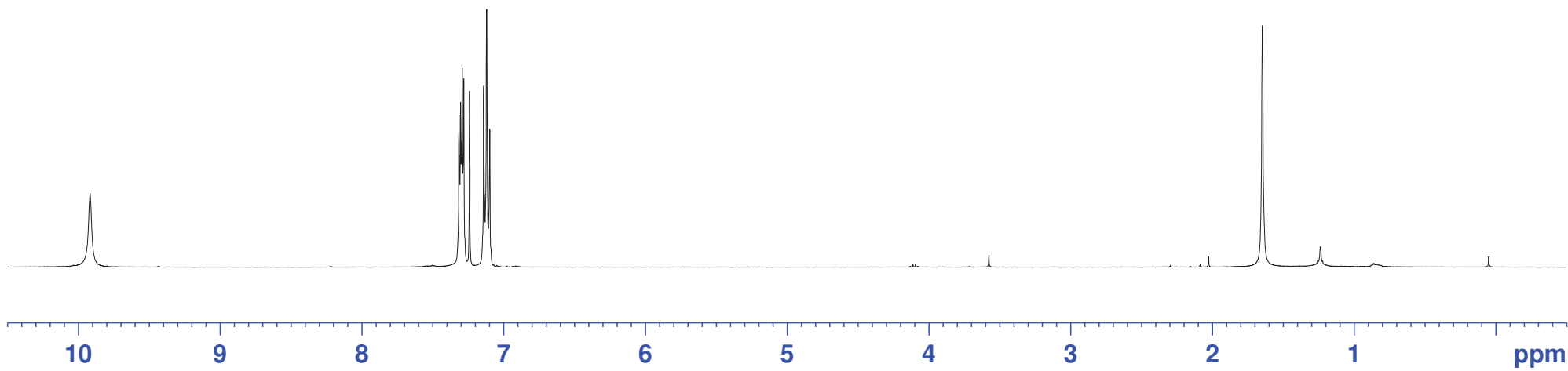
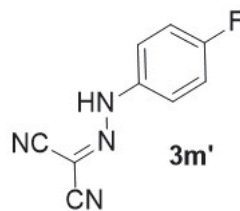
NAME	mani 01-C
EXPNO	1
PROCNO	1
Date_	201901
Time	16.28
INSTRUM	spt
PROBHD	Z108618
PULPROG	z1
TD	32768
SOLVENT	CC
NS	30
DS	0
SWH	8802.8
FIDRES	0.5372
AQ	1.861272
RG	212.49
DW	56.800
DE	14.47
TE	296.7
D1	1.0000000
TD0	1
SFO1	400.1328
NUC1	1H
P1	15.50
SI	131072
SF	400.13001
WDW	EM
SSB	0
LB	0.00
GB	0
PC	1.00

4-CO₂EtPD, MCN, 2-ABP, 80deg, 5h, purified orange solid



— 9.918

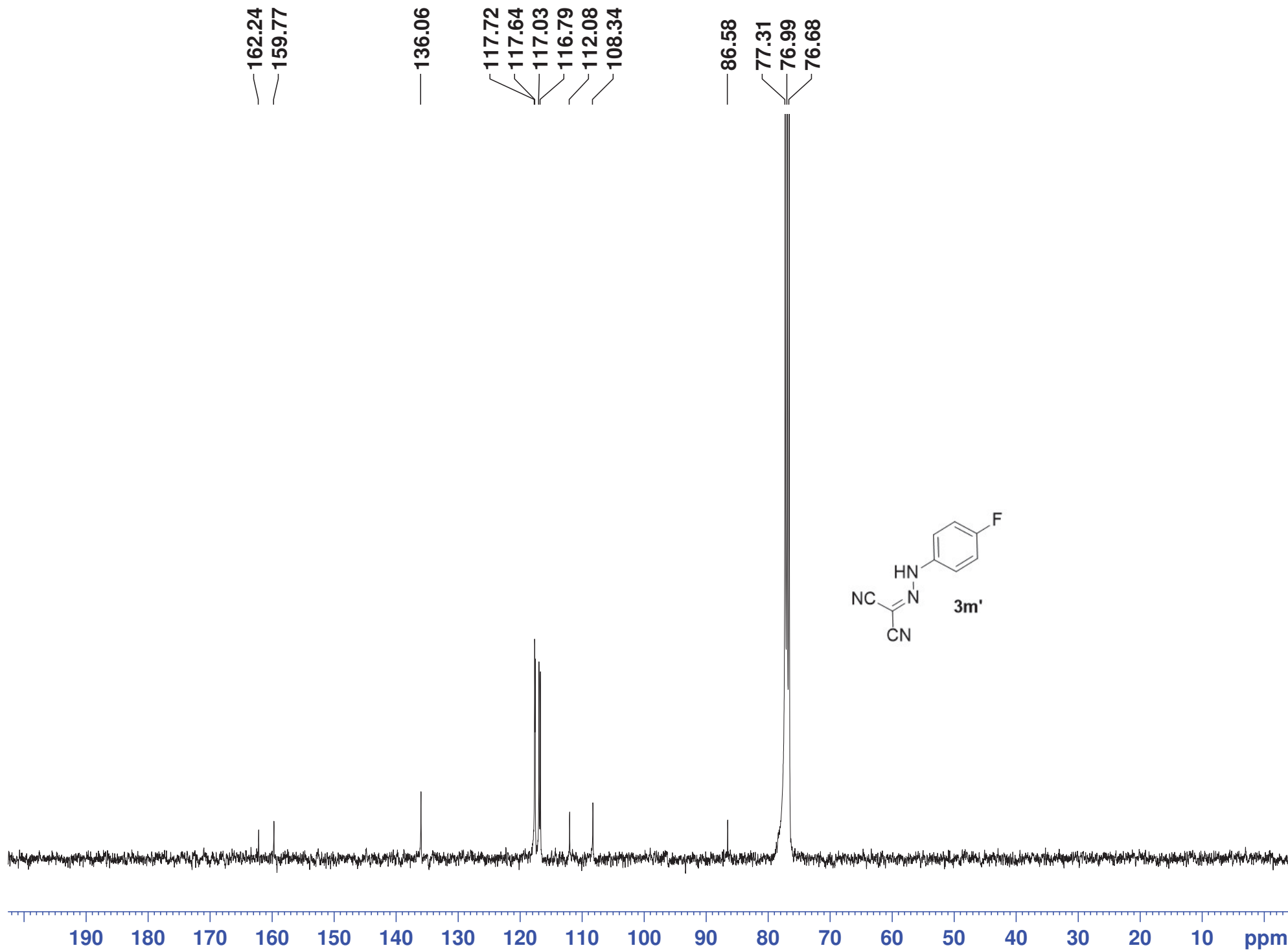
7.315
7.309
7.303
7.298
7.292
7.281
7.240
7.140
7.120
7.098



1.00

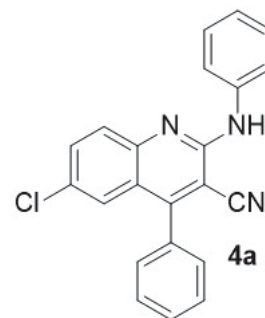
2.01
1.99

S32



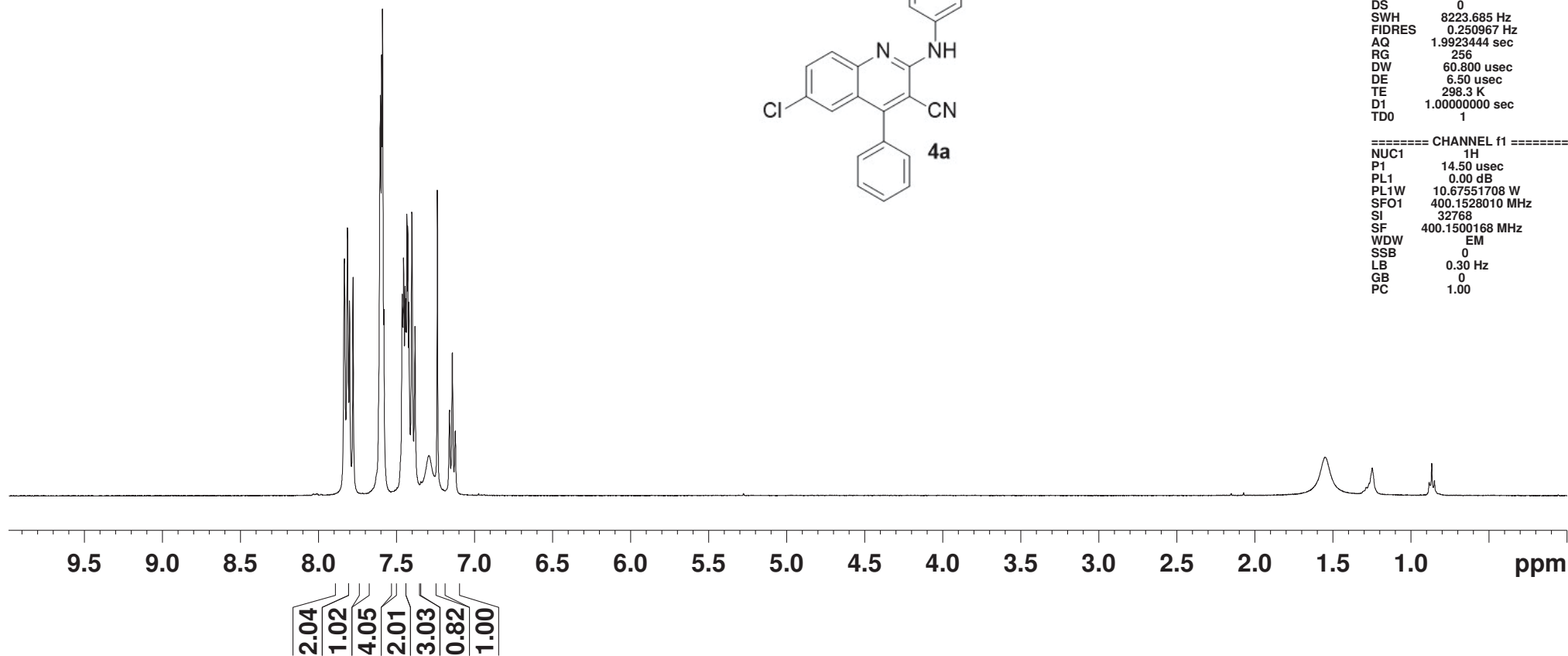
PD, 5-ClABP, MCN, 80deg, 5h, purified pale yellow solid

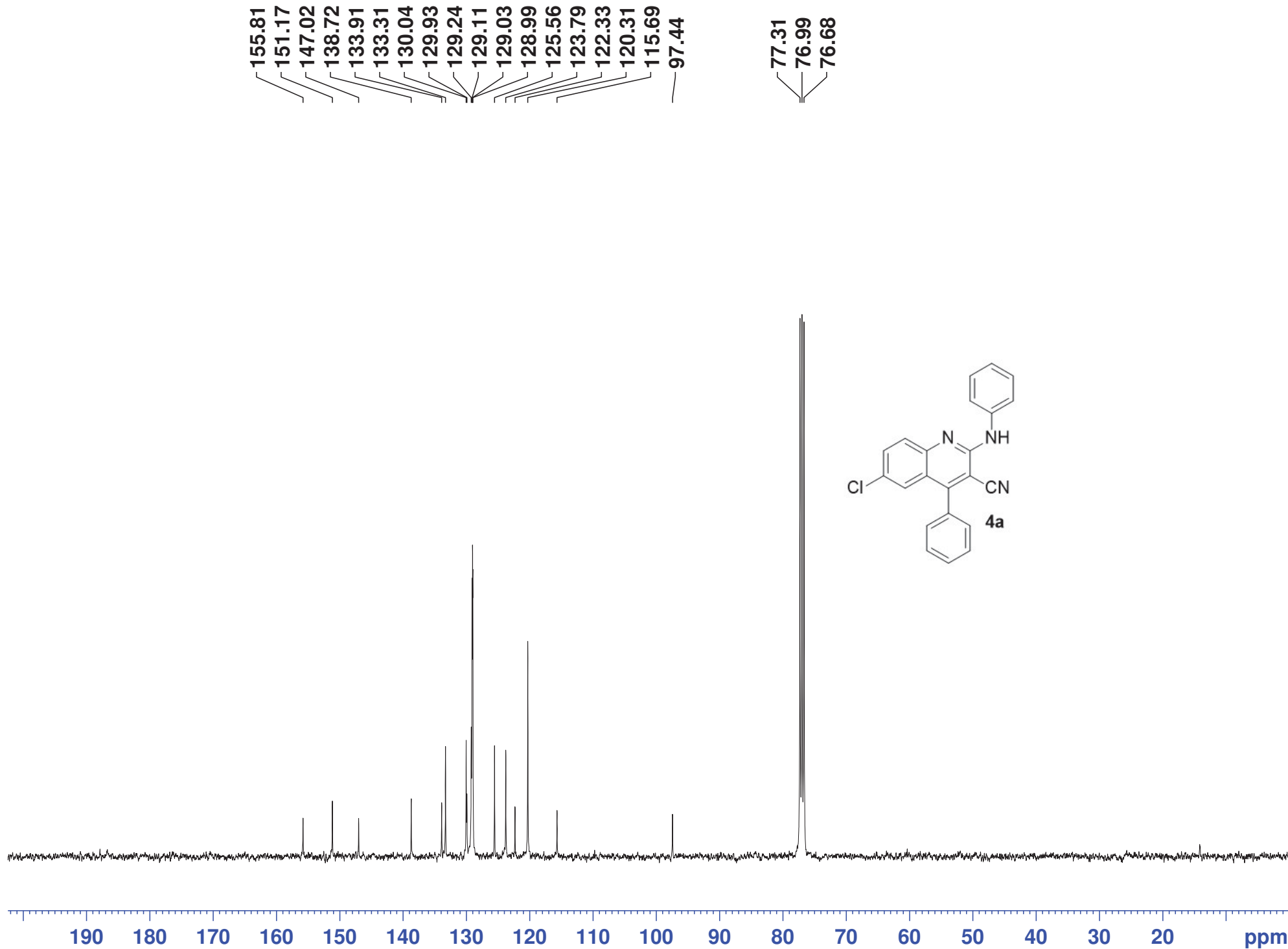
7.835
7.816
7.802
7.780
7.605
7.597
7.591
7.582
7.465
7.456
7.447
7.441
7.435
7.429
7.422
7.403
7.383
7.293
7.239
7.162
7.144
7.125



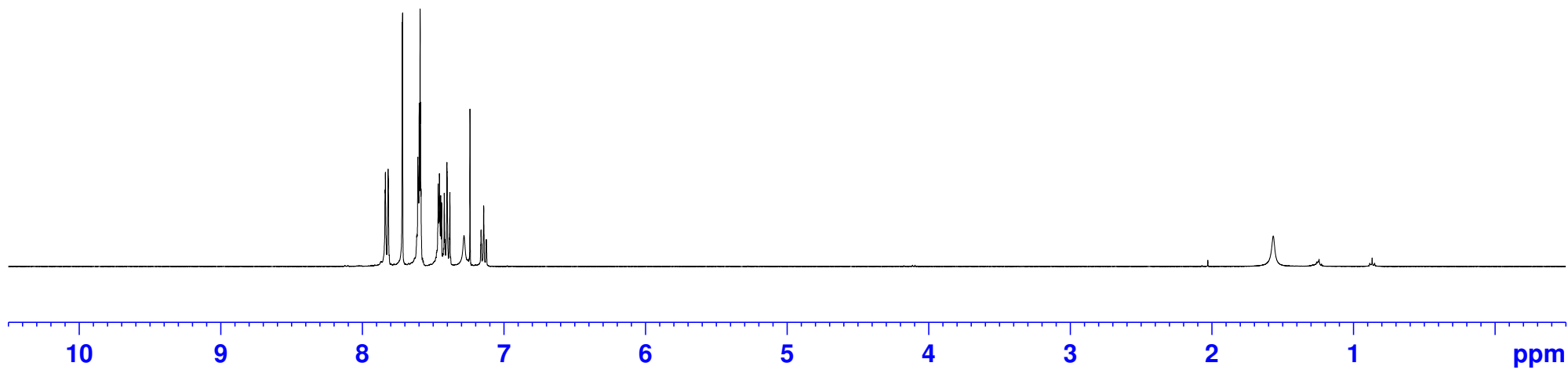
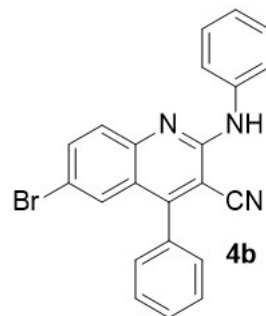
NAME mani 15-01-2019
EXPNO 2
PROCNO 1
Date_ 20190115
Time 19.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 30
DS 0
SWH 8223.685 Hz
FIDRES 0.250967 Hz
AQ 1.9923444 sec
RG 256
DW 60.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.67551708 W
SFO1 400.1528010 MHz
SI 32768
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

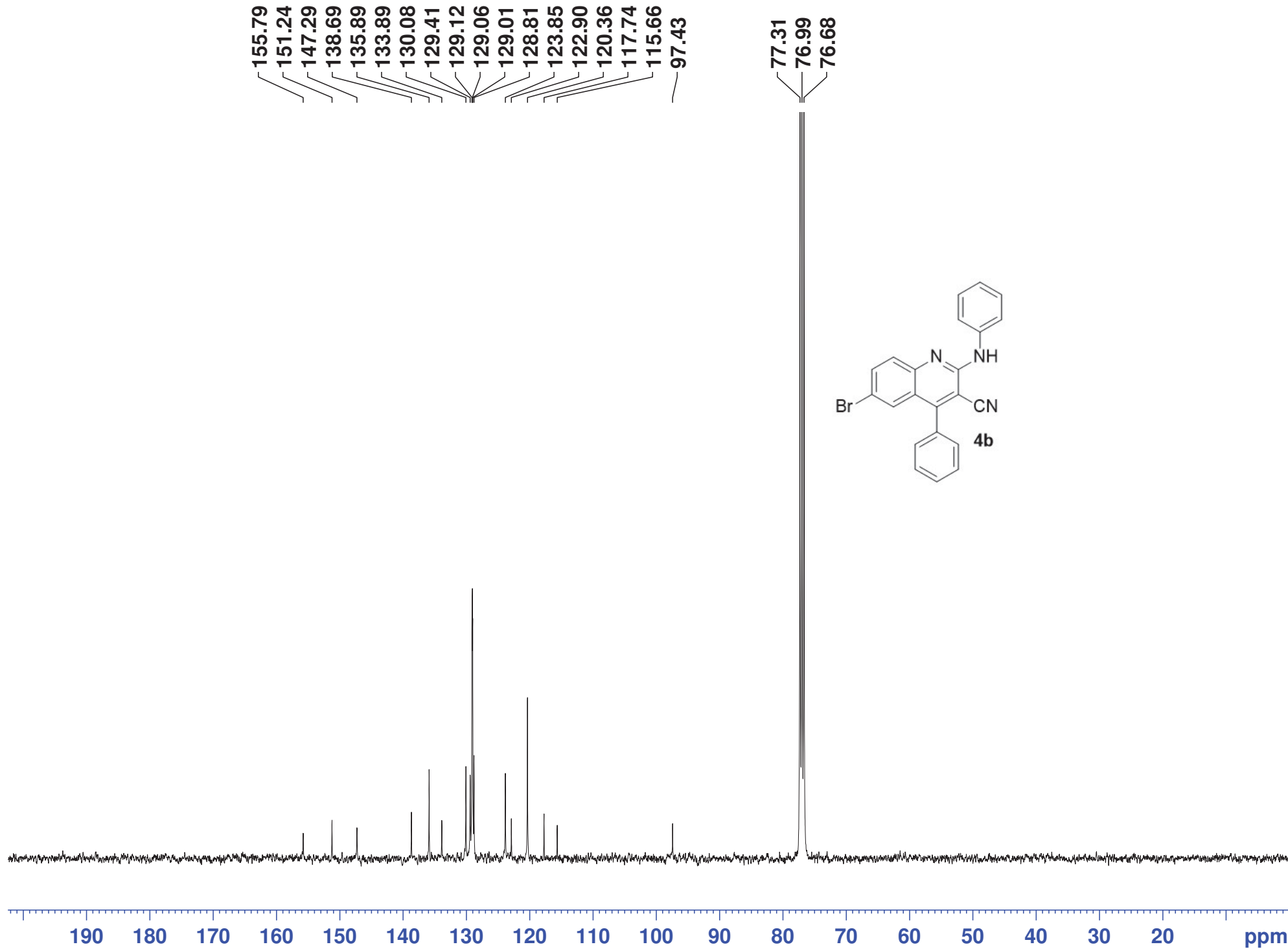




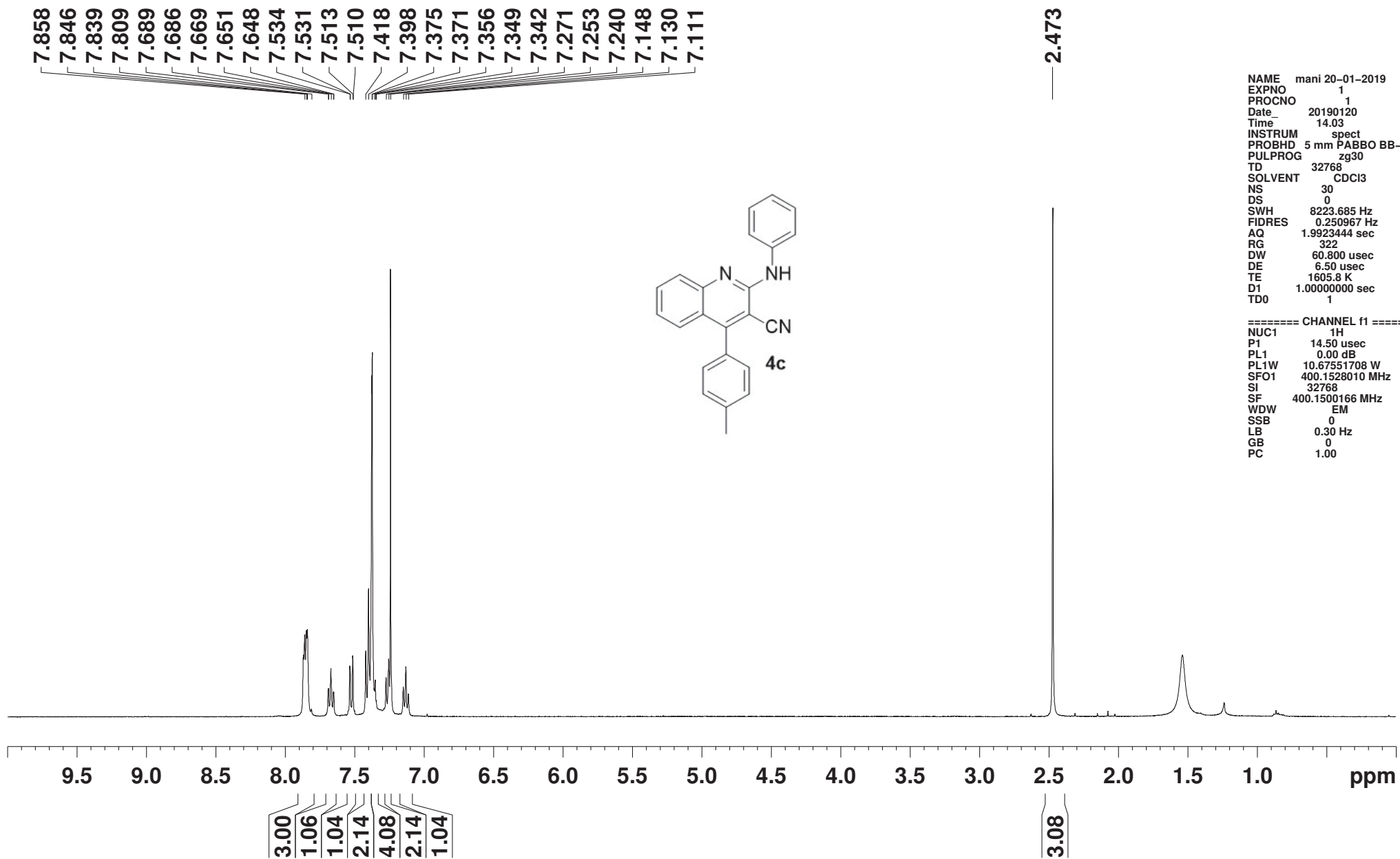
7.837
7.818
7.719
7.715
7.616
7.614
7.608
7.603
7.598
7.592
7.589
7.585
7.464
7.459
7.455
7.452
7.446
7.440
7.421
7.416
7.402
7.386
7.381
7.281
7.239
7.161
7.143
7.124



2.01
1.99
4.02
2.04
2.03
1.01
1.00



PD, 4'-Me2-ABP, MCN, 80deg, 5h, purified pale yellow solid



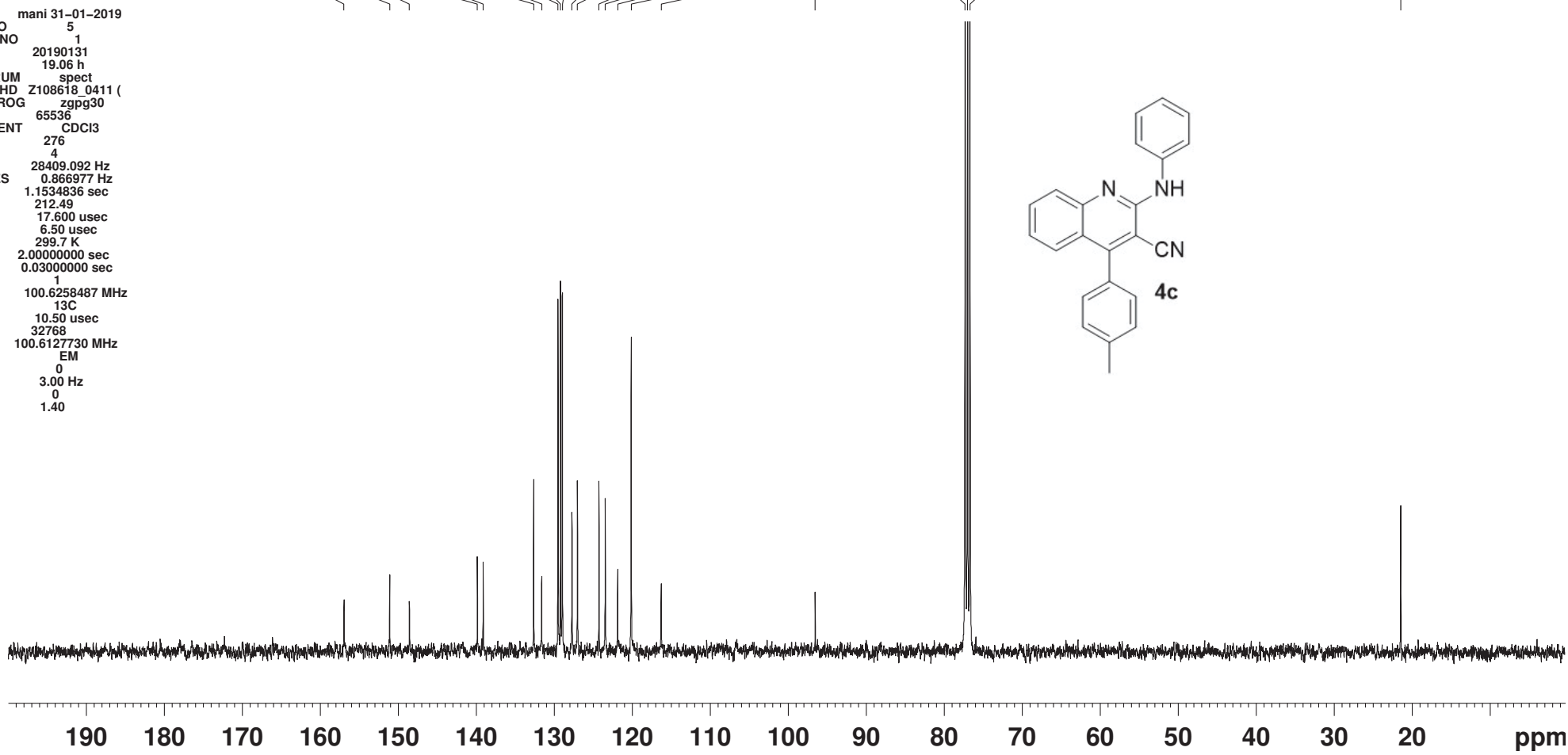
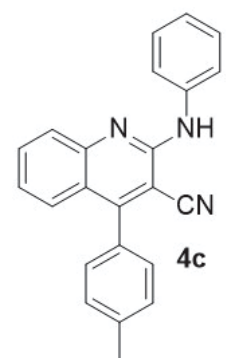
PD, 4'-MeABP, MCN, 80deg, 5h, pale yellow solid

NAME mani 31-01-2019
EXPNO 5
PROCNO 1
Date_ 20190131
Time 19.06 h
NSTRUM spect
PROBHD Z108618_0411 (
PULPROG zgpg30
ID 65536
SOLVENT CDCl3
NS 276
DS 4
SWH 28409.092 Hz
FIDRES 0.866977 Hz
AQ 1.1534836 sec
RG 212.49
JW 17.600 usec
JE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
FO1 100.6258487 MHz
UC1 13C
P1 10.50 usec
PI 32768
PF 100.6127730 MHz
NDW EM
SBS 0
B 3.00 Hz
B 0
C 1.40

156.949
151.090
148.562
139.855
139.108
132.629
131.604
129.504
129.191
128.952
127.716
127.014
124.246
123.447
121.854
120.123
116.275
96.534

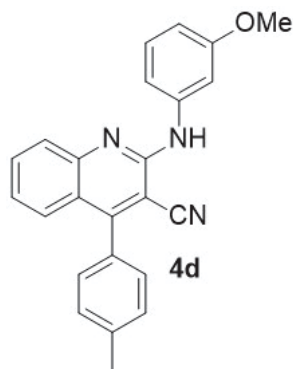
77.309
76.991
76.674

21.430

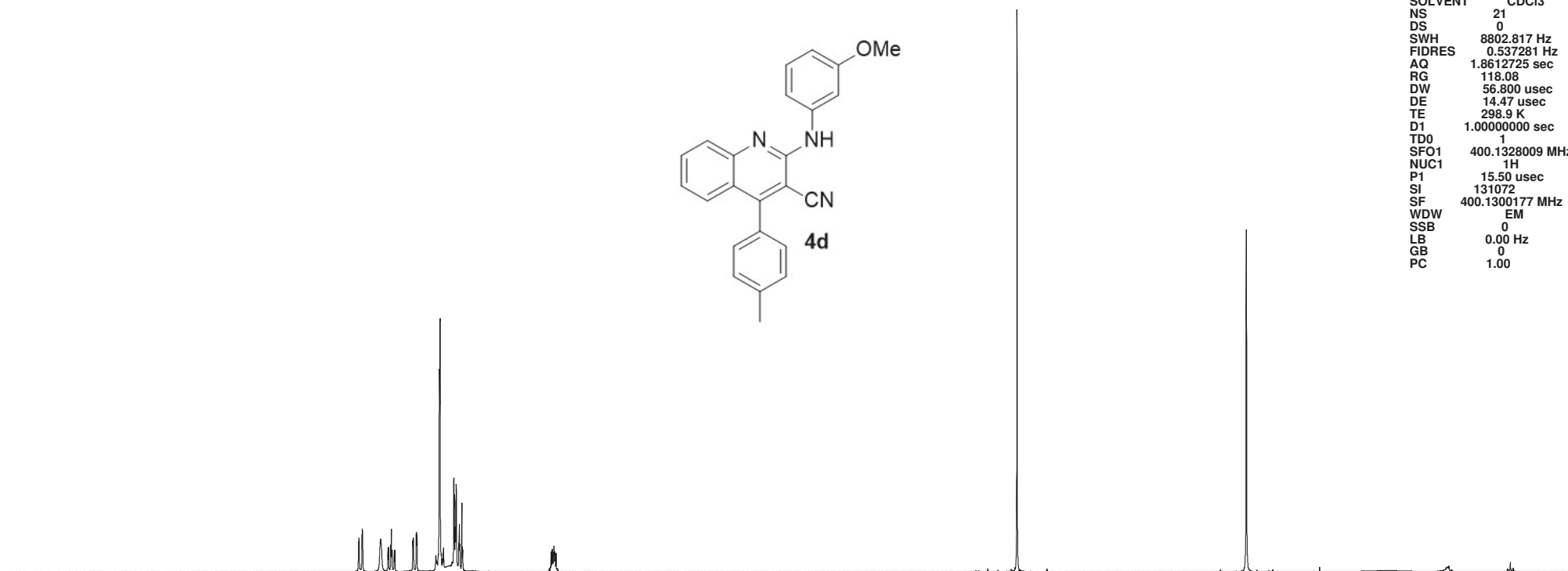


3OMePD, 4'MeABP, MCN, 80deg, 5h, purified pale yellow solid

7.650
7.646
7.538
7.537
7.535
7.533
7.517
7.516
7.514
7.398
7.383
7.376
7.372
7.365
7.358
7.353
7.351
7.289
7.286
7.280
7.275
7.273
7.258
7.255
7.252
7.240
7.238
7.234
6.709
6.702
6.697
6.691
6.689
6.680
6.674
6.668
6.663
6.657
3.868
2.476



NAME mani 25-01-2019
EXPNO 4
PROCNO 1
Date_ 20190125
Time 22.26 h
INSTRUM spect
PROBHD Z108618_0411 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 21
DS 0
SWH 8802.817 Hz
FIDRES 0.537281 Hz
AQ 1.8612725 sec
RG 118.08
DW 56.800 usec
DE 14.47 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.1328009 MHz
NUC1 1H
P1 15.50 usec
SI 131072
SF 400.1300177 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

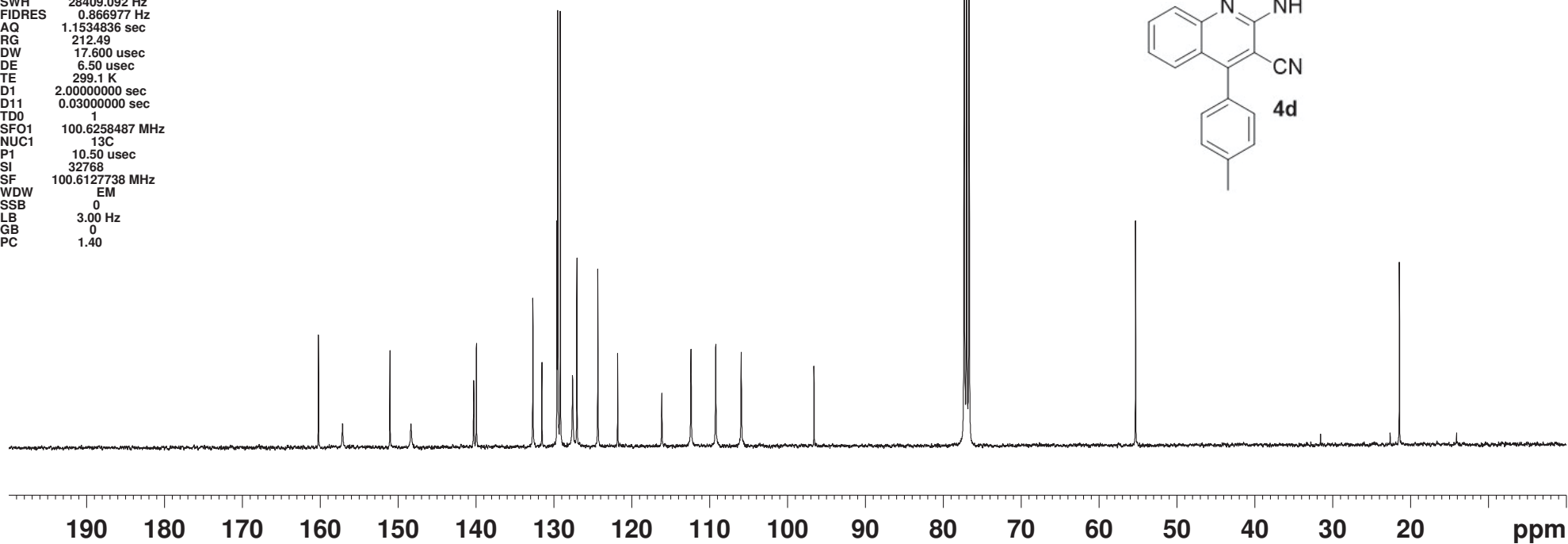


1.04
1.00
1.06
1.05
4.20
2.33
1.08
1.00
3.01
3.06

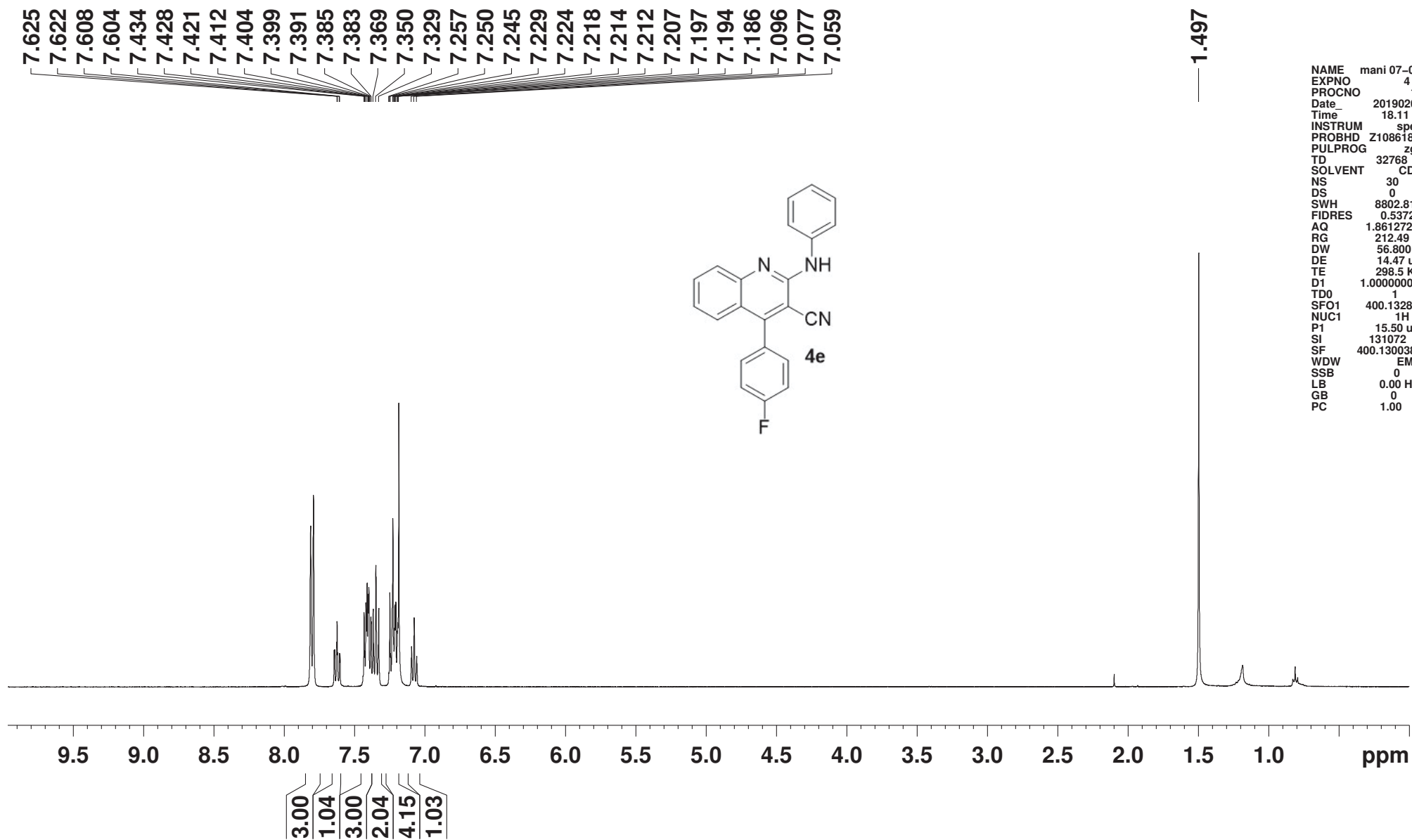
3OMePD, 4'MeABP, MCN, 80deg, 5h, purified pale yellow solid

160.183
157.083
150.996
148.295
140.240
139.895
132.701
131.536
129.601
129.505
129.179
127.602
127.041
124.358
121.810
116.134
112.393
109.217
105.939
96.591
77.310
76.992
76.675
55.299
21.421

NAME mani 25-01-2019
EXPNO 6
PROCNO 1
Date_ 20190126
Time_ 1.10 h
INSTRUM spect
PROBHD Z108618_0411 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2999
DS 4
SWH 28409.092 Hz
FIDRES 0.866977 Hz
AQ 1.1534836 sec
RG 212.49
DW 17.600 usec
DE 6.50 usec
TE 299.1 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1
SFO1 100.6258487 MHz
NUC1 13C
P1 10.50 usec
Sf 32768
SF 100.6127738 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



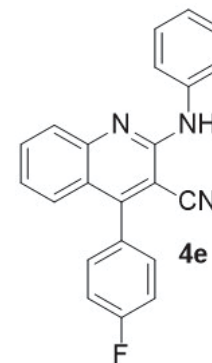
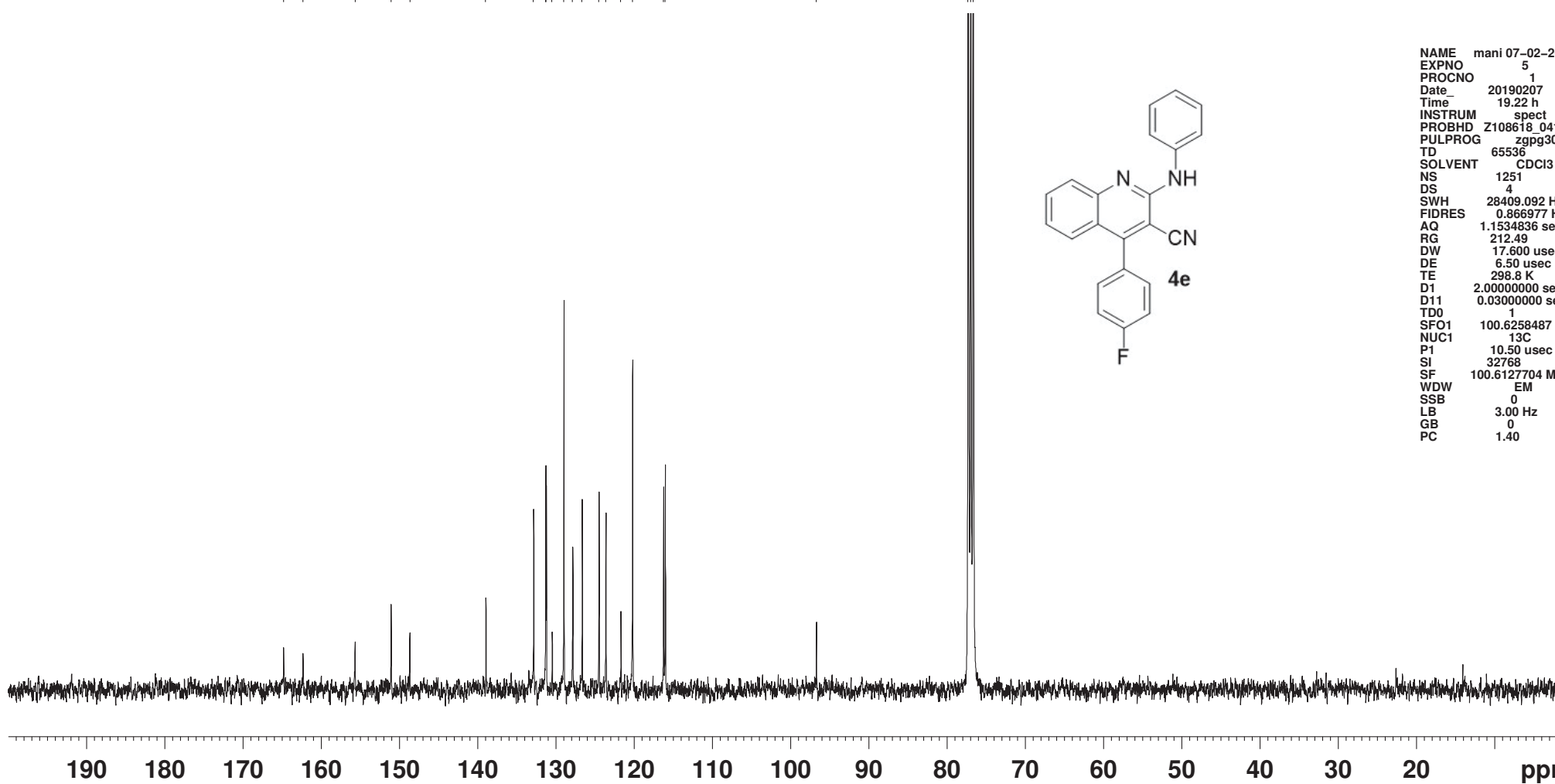
PD, MCN, 2-amino-4'-F-ABP, 80deg, 5h, purified topspot



PD, MCN, 2-amino-4'-F-ABP, 80deg, 5h, purified topspot

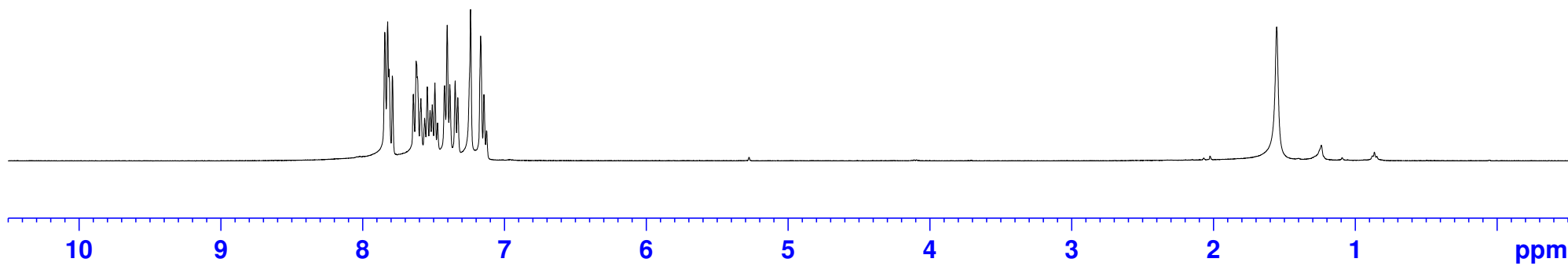
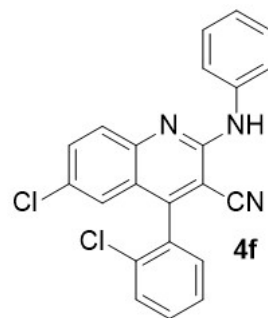
164.795
162.306
155.650
151.041
148.653
138.977
132.869
131.329
131.245
130.515
129.004
127.867
126.663
124.510
123.632
121.718
120.222
116.260
116.040
96.717

77.316
76.998
76.680

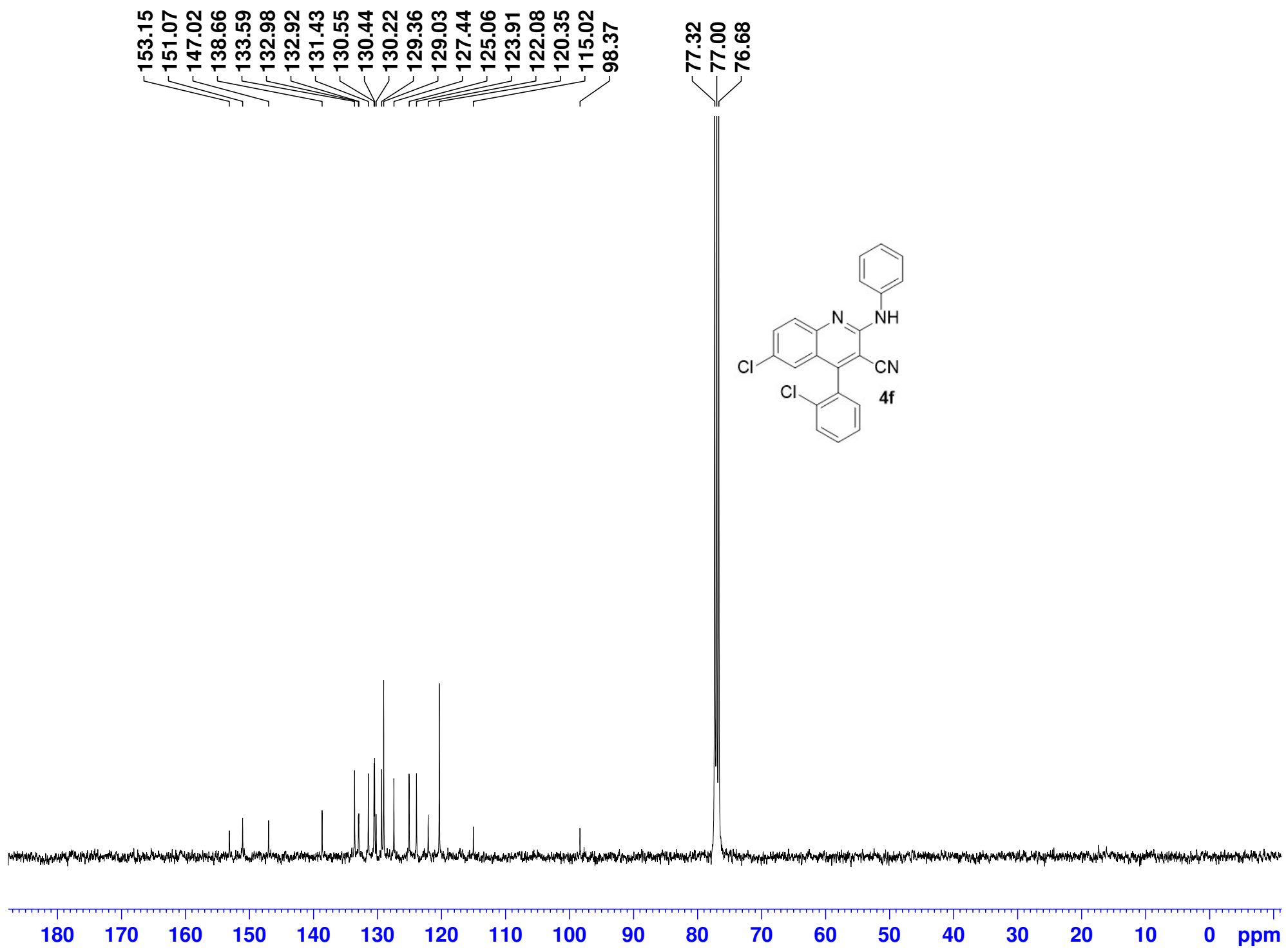


NAME mani 07-02-21
EXPNO 5
PROCNO 1
Date_ 20190207
Time 19.22 h
INSTRUM spect
PROBHD Z108618_041
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1251
DS 4
SWH 28409.092 H
FIDRES 0.866977 Hz
AQ 1.1534836 sec
RG 212.49
DW 17.600 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6258487 MHz
NUC1 13C
P1 10.50 usec
SI 32768
SF 100.6127704 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

7.844
7.823
7.814
7.790
7.643
7.622
7.614
7.589
7.544
7.509
7.490
7.422
7.404
7.385
7.348
7.329
7.239
7.168
7.145

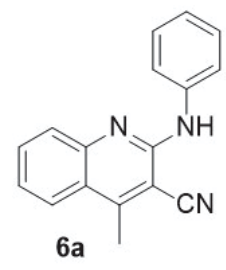


2.99
1.99
1.07
1.09
3.04
0.94
2.01



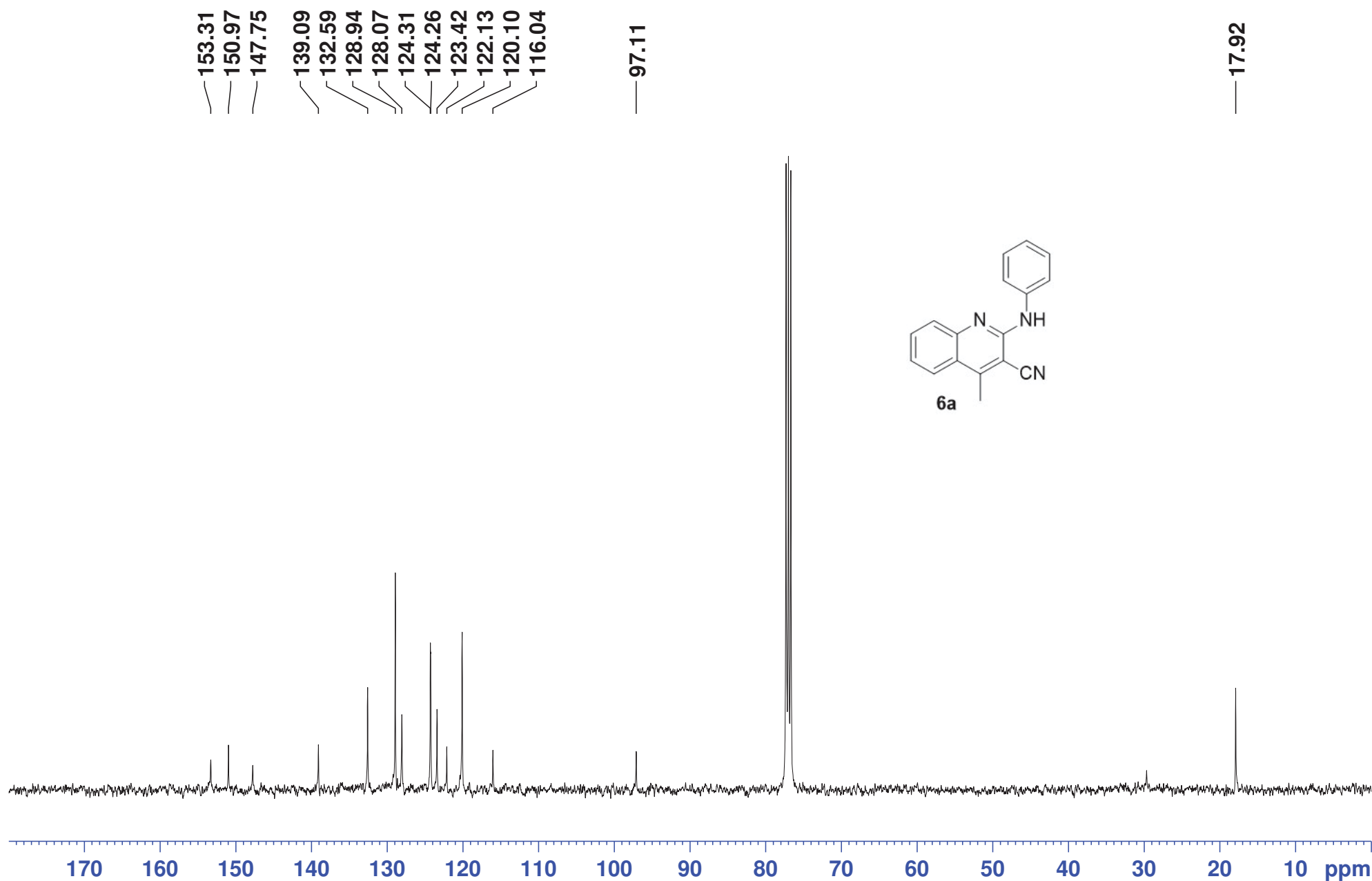
7.798
7.778
7.776
7.680
7.676
7.662
7.659
7.655
7.641
7.638
7.403
7.399
7.393
7.380
7.377
7.369
7.366
7.363
7.359
7.352
7.349
7.345
7.331
7.328
7.240
7.135
7.128
7.125
7.122
7.107
7.091
7.088
7.085

— 2.831



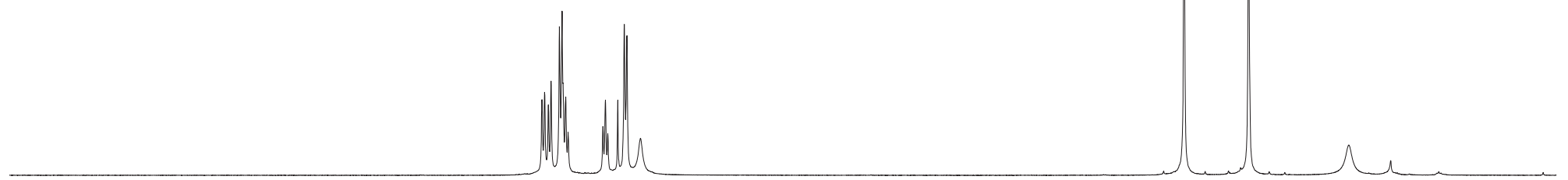
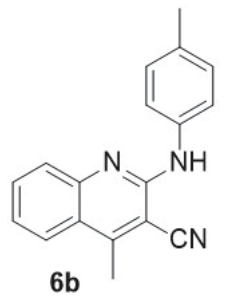
4.01
1.04
3.02
1.93

3.00



7.870
7.849
7.820
7.799
7.734
7.713
7.706
7.685
7.667
7.397
7.377
7.359
7.281
7.231
7.210
7.105

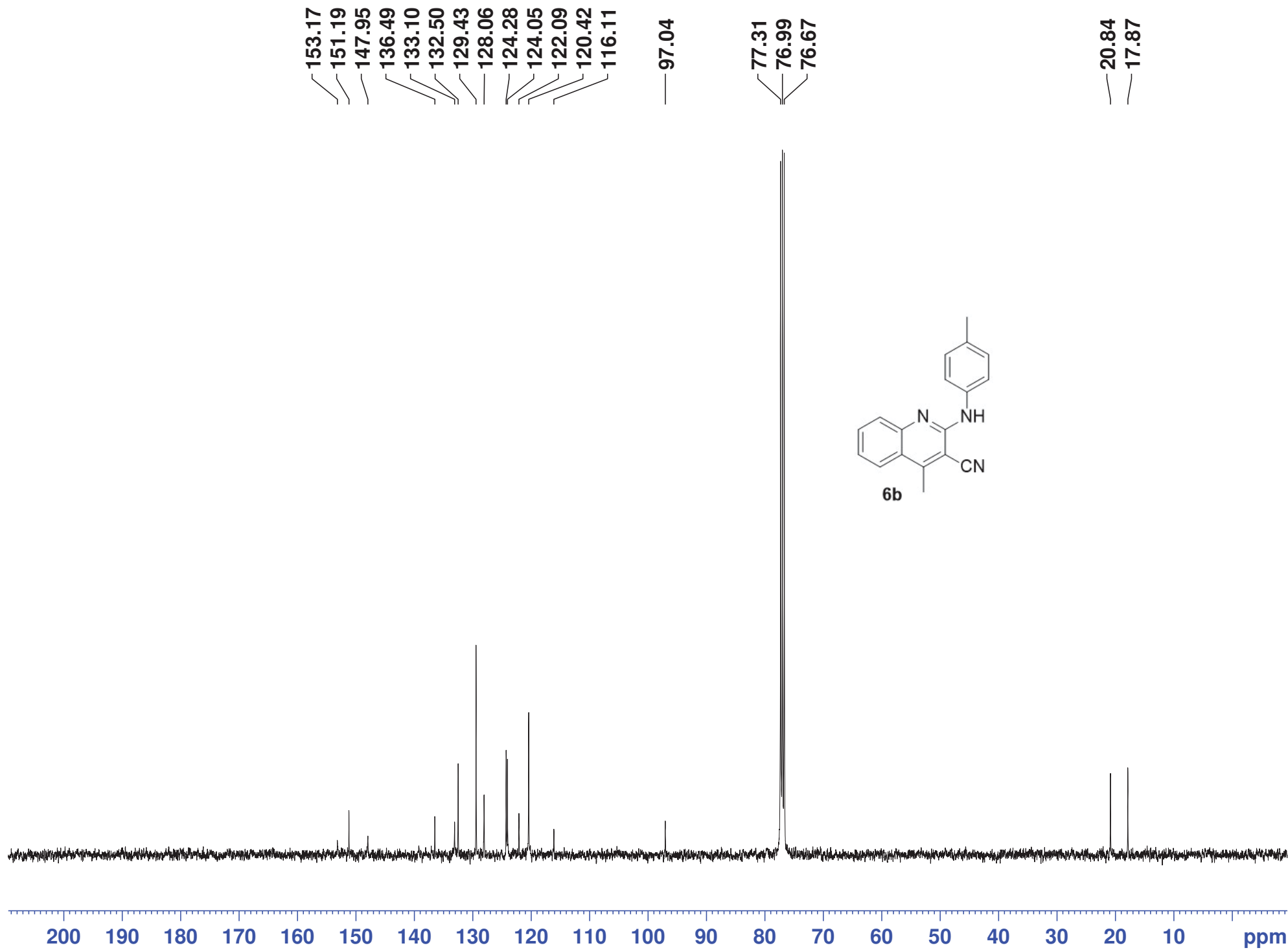
— 2.886
— 2.386



11 10 9 8 7 6 5 4 3 2 1 ppm

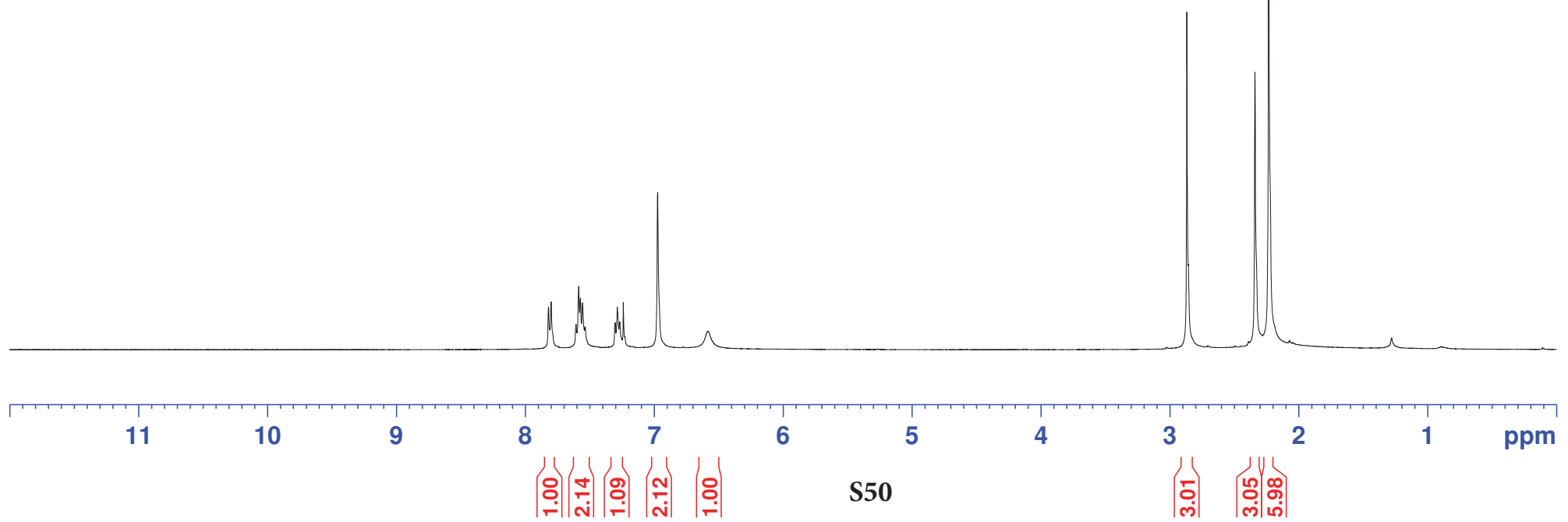
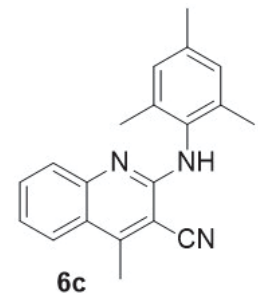
1.00
0.99
2.93
1.01
1.97
0.97

3.00
3.06



7.821
7.800
7.607
7.586
7.572
7.556
7.538
7.535
7.303
7.287
7.270
7.266
7.240
6.974
6.584

2.868
2.339
2.233

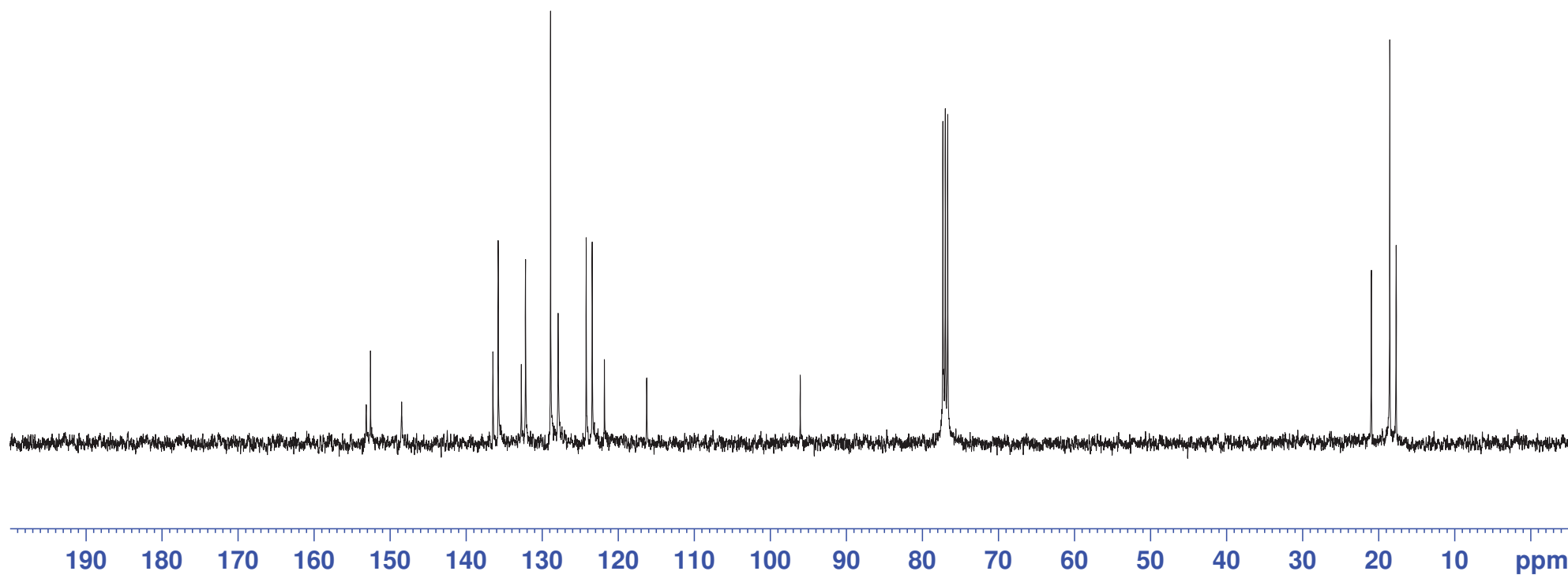
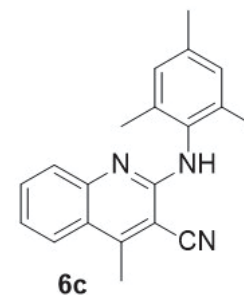


153.15
152.60
148.50
136.49
135.80
132.76
132.20
128.91
127.91
124.22
123.43
121.83
116.26

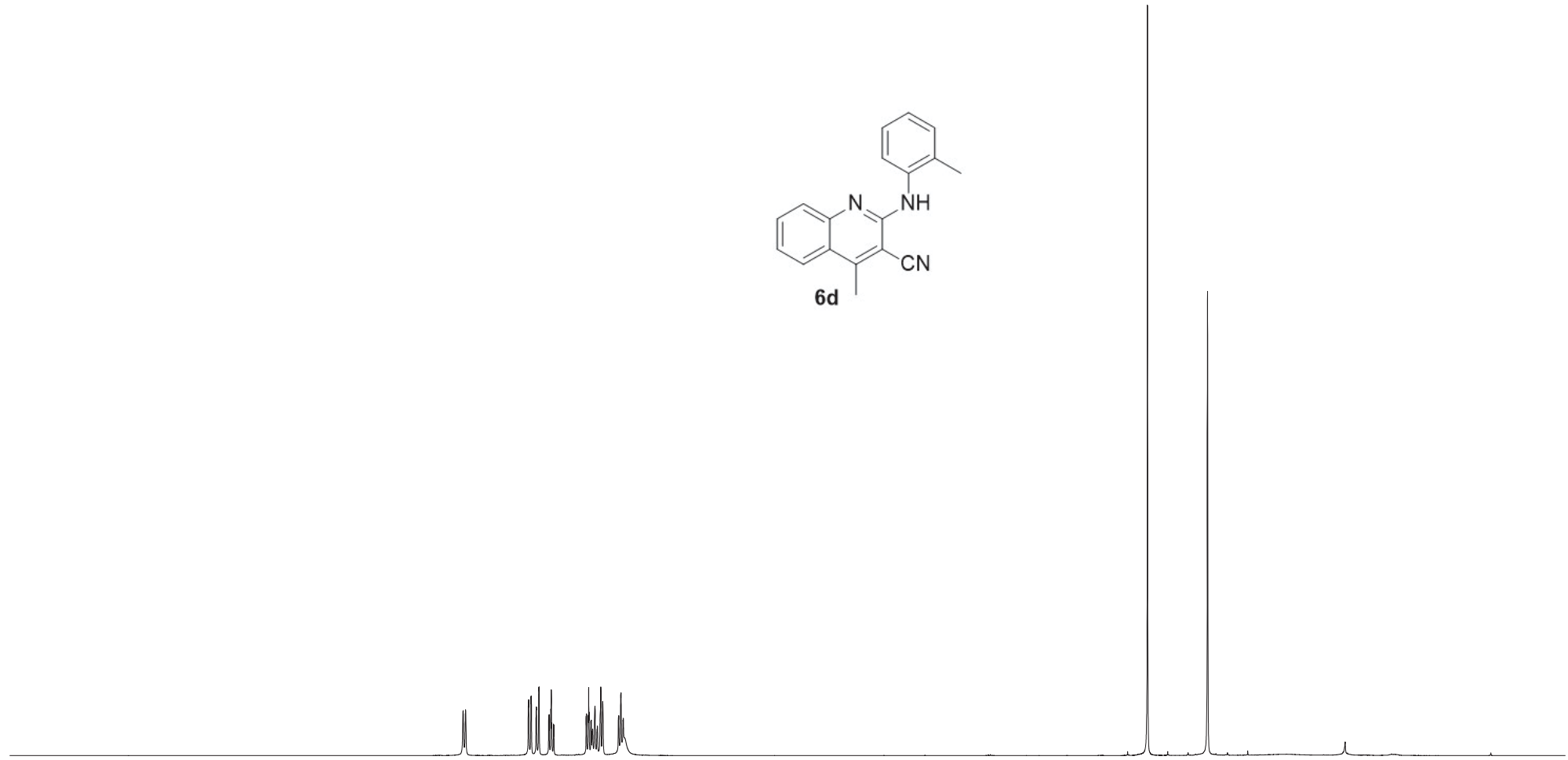
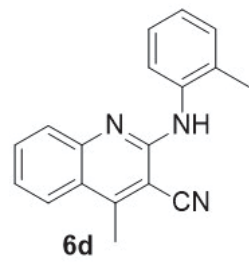
96.07

77.31
76.99
76.68

20.95
18.53
17.70



8.393
8.373
7.868
7.865
7.847
7.844
7.805
7.803
7.784
7.782
7.704
7.701
7.687
7.683
7.680
7.666
7.663
7.403
7.400
7.386
7.383
7.379
7.365
7.362
7.354
7.351
7.332
7.315
7.312
7.285
7.270
7.144
7.141
7.125
7.122
7.106
7.104
— 2.887
— 2.403



11 10 9 8 7 6 5 4 3 2 1 ppm

0.96
1.03
0.98
1.01
2.06
1.10
1.88

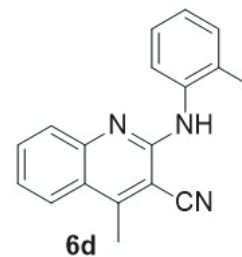
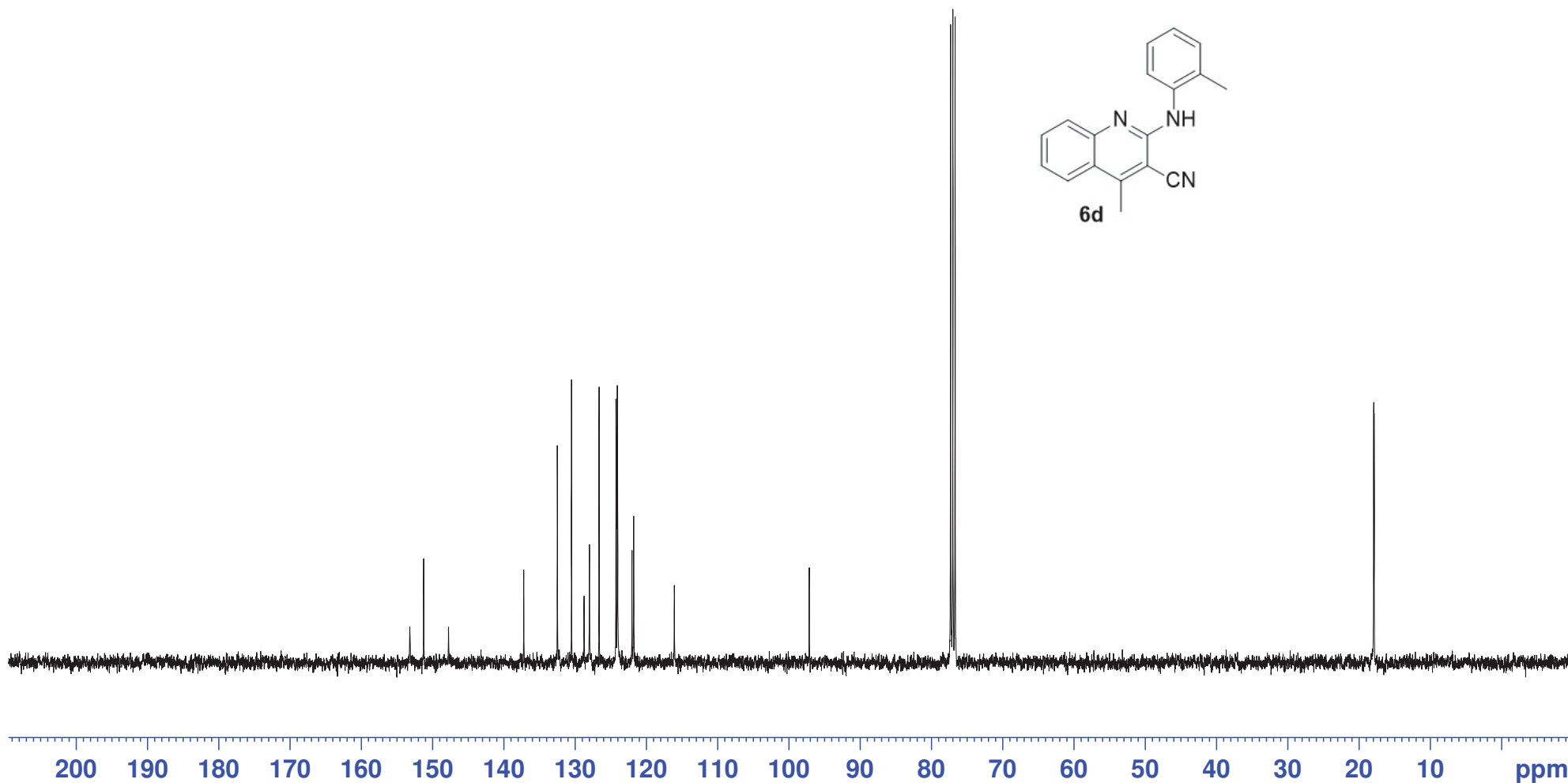
S52

3.03
3.00

153.21
151.25
147.76
137.20
132.49
130.50
128.73
127.98
126.64
124.26
124.08
124.02
122.01
121.77
116.07
97.14

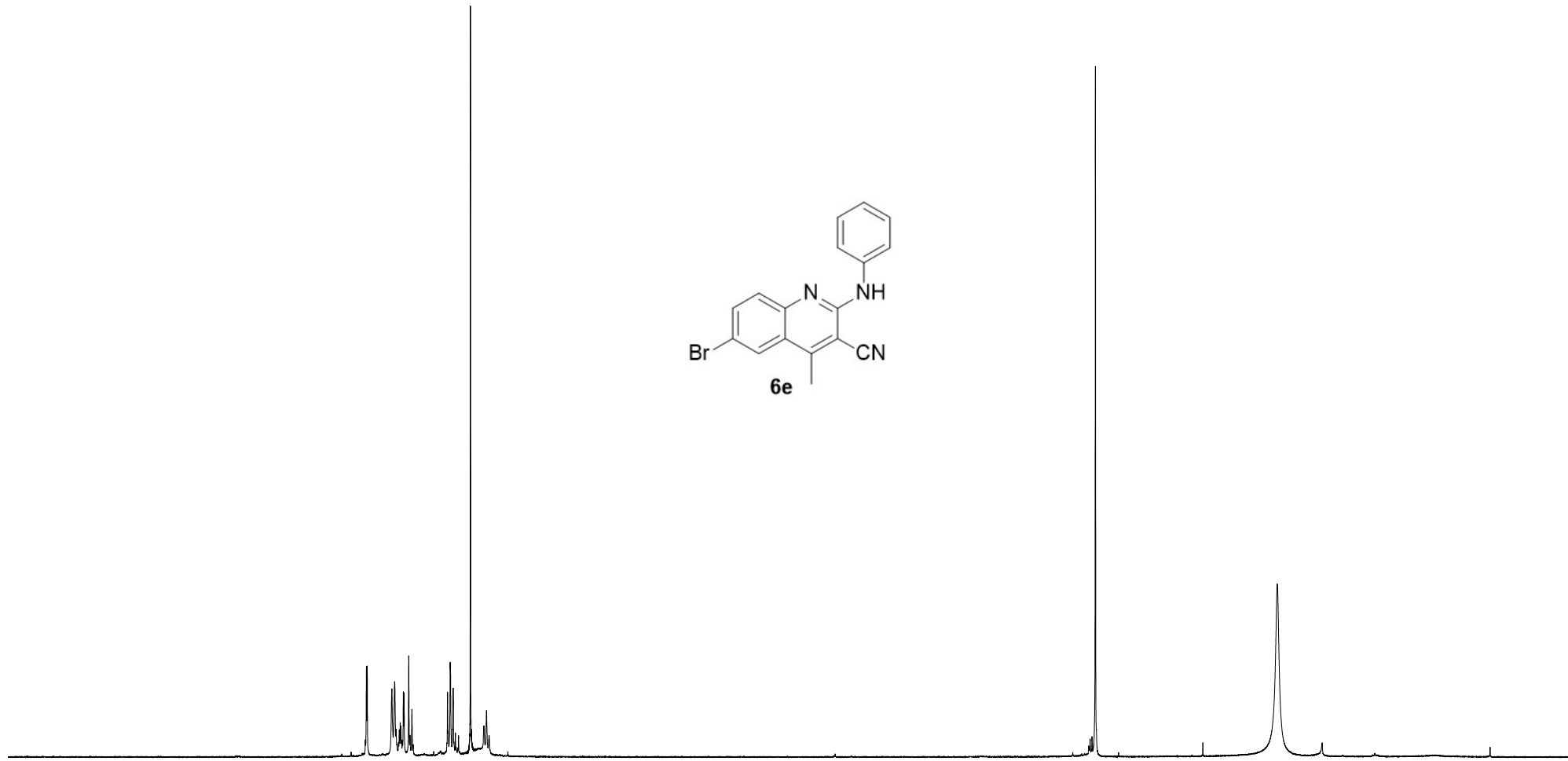
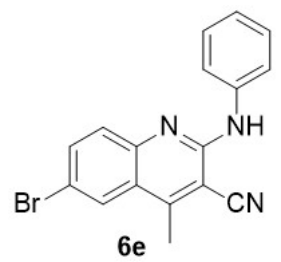
77.31
76.99
76.67

17.94
17.87



7.973
7.968
7.794
7.774
7.764
7.741
7.735
7.730
7.713
7.708
7.675
7.653
7.401
7.397
7.383
7.362
7.346
7.240
7.145
7.126

2.833

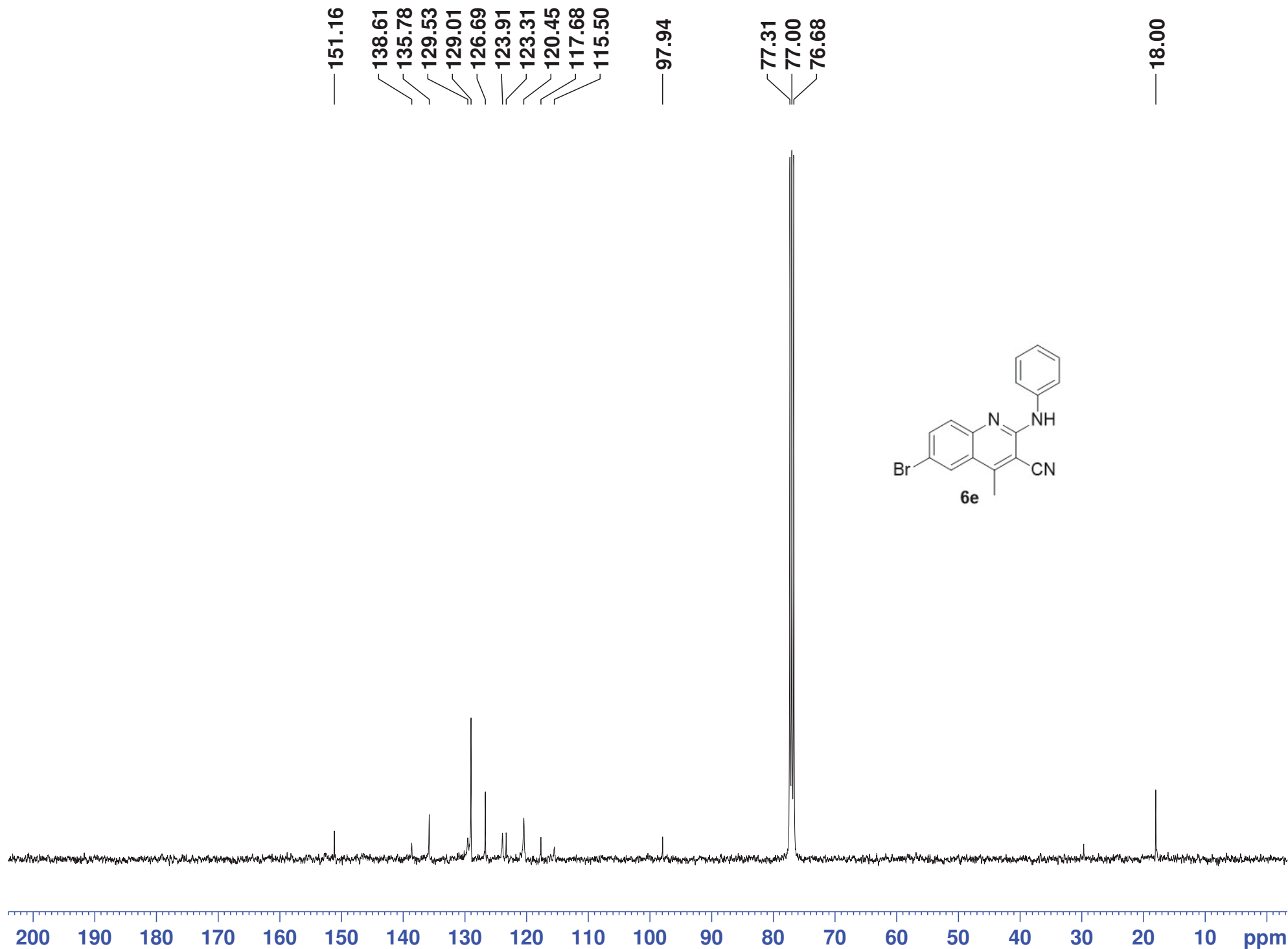


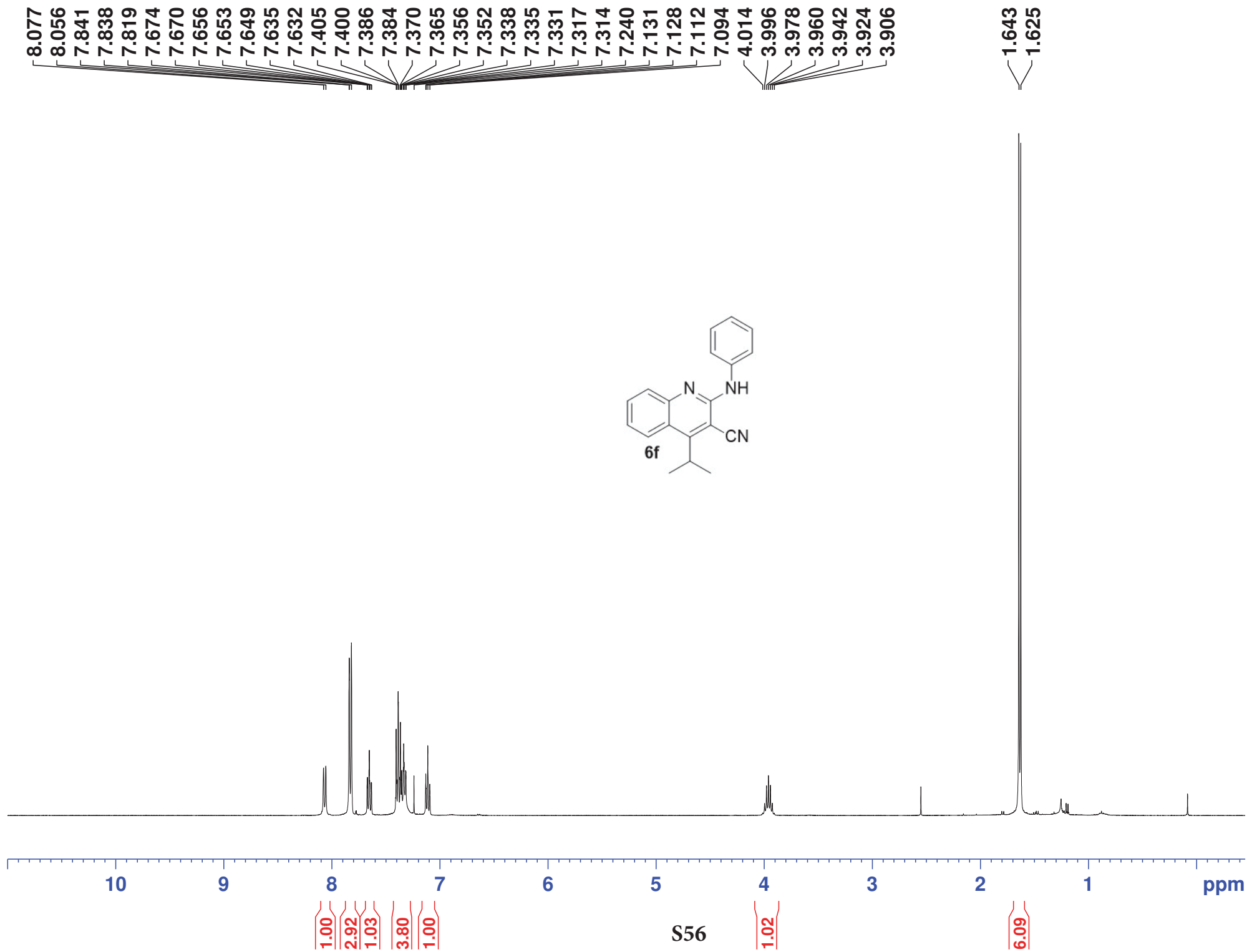
10 9 8 7 6 5 4 3 2 1 ppm

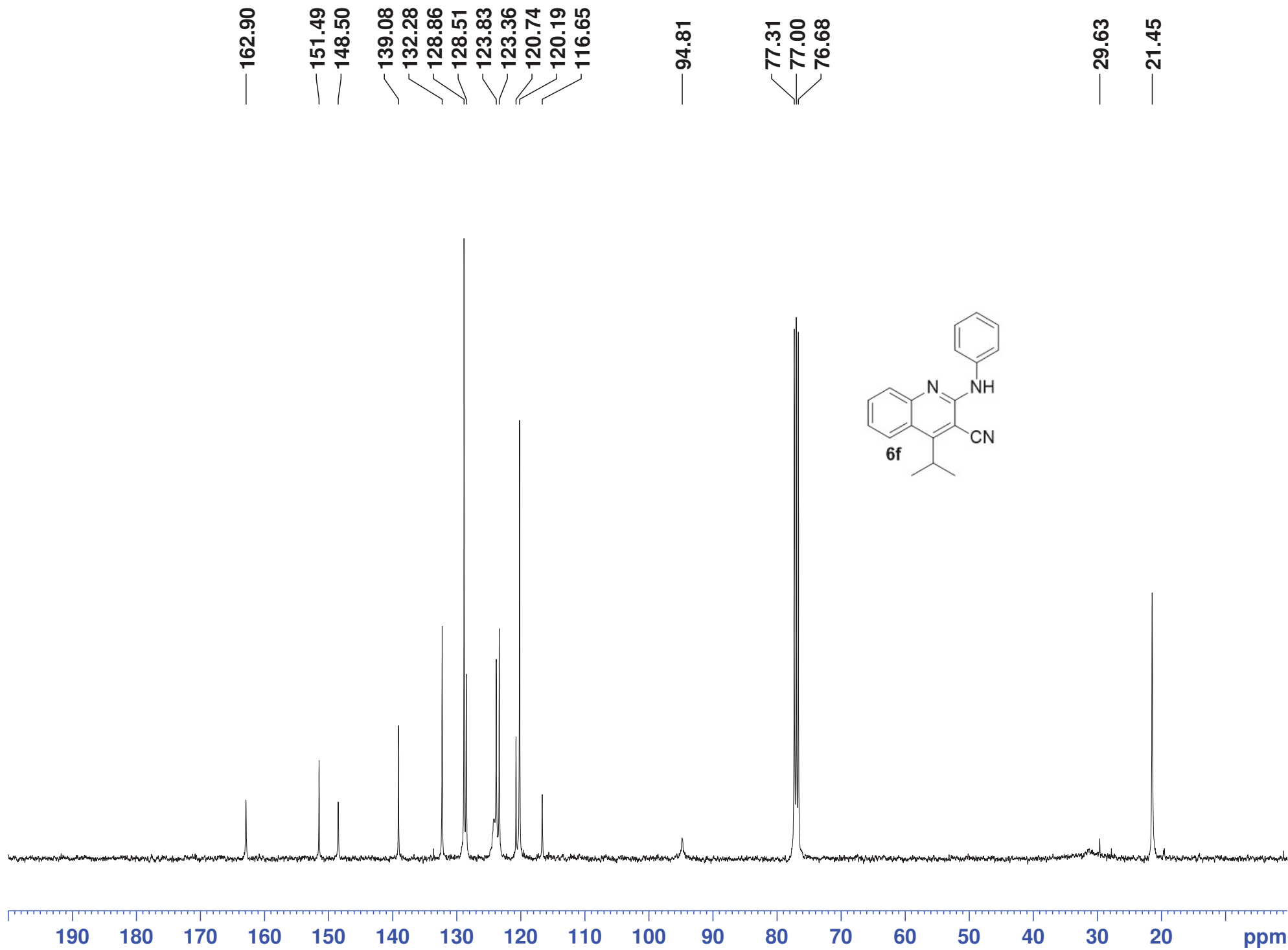
1.04
2.02
2.00
2.04
2.00

3.00

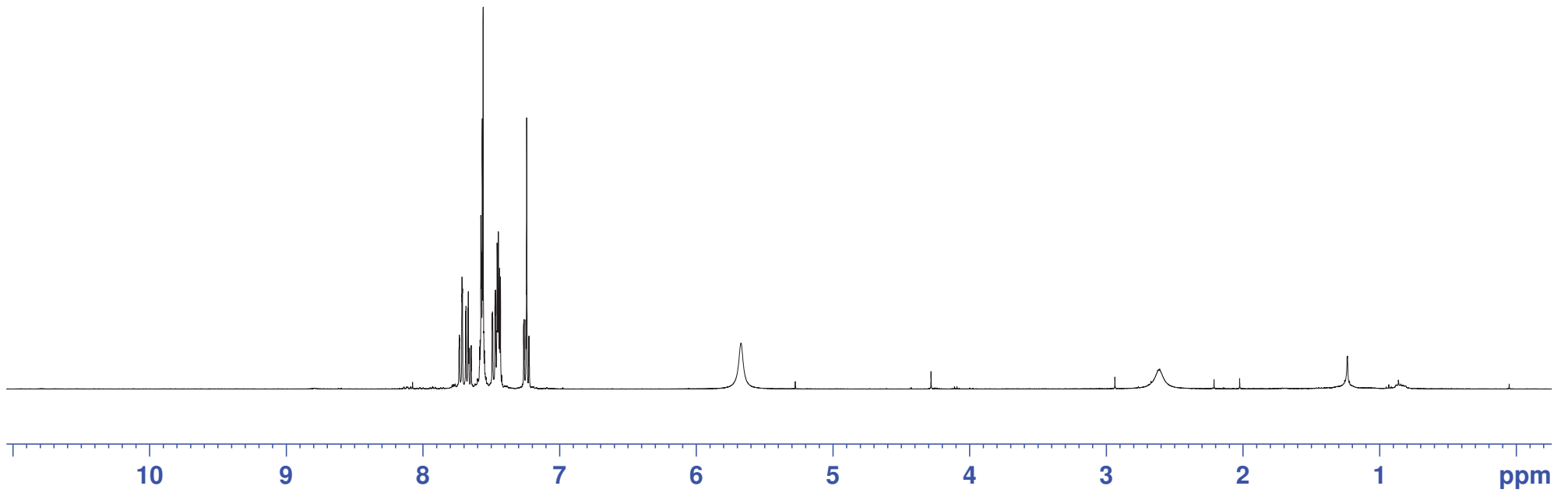
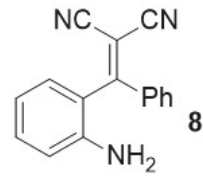
S54







7.710
7.688
7.684
7.671
7.667
7.581
7.576
7.573
7.571
7.565
7.559
7.555
7.494
7.492
7.490
7.489
7.473
7.471
7.469
7.468
7.459
7.457
7.454
7.451
7.448
7.445
7.439
7.437
7.433
7.263
7.259
7.246
7.240
7.238
7.225
7.221
5.673



1.00
1.04
2.99
1.08
1.91
1.44

1.96

S58

