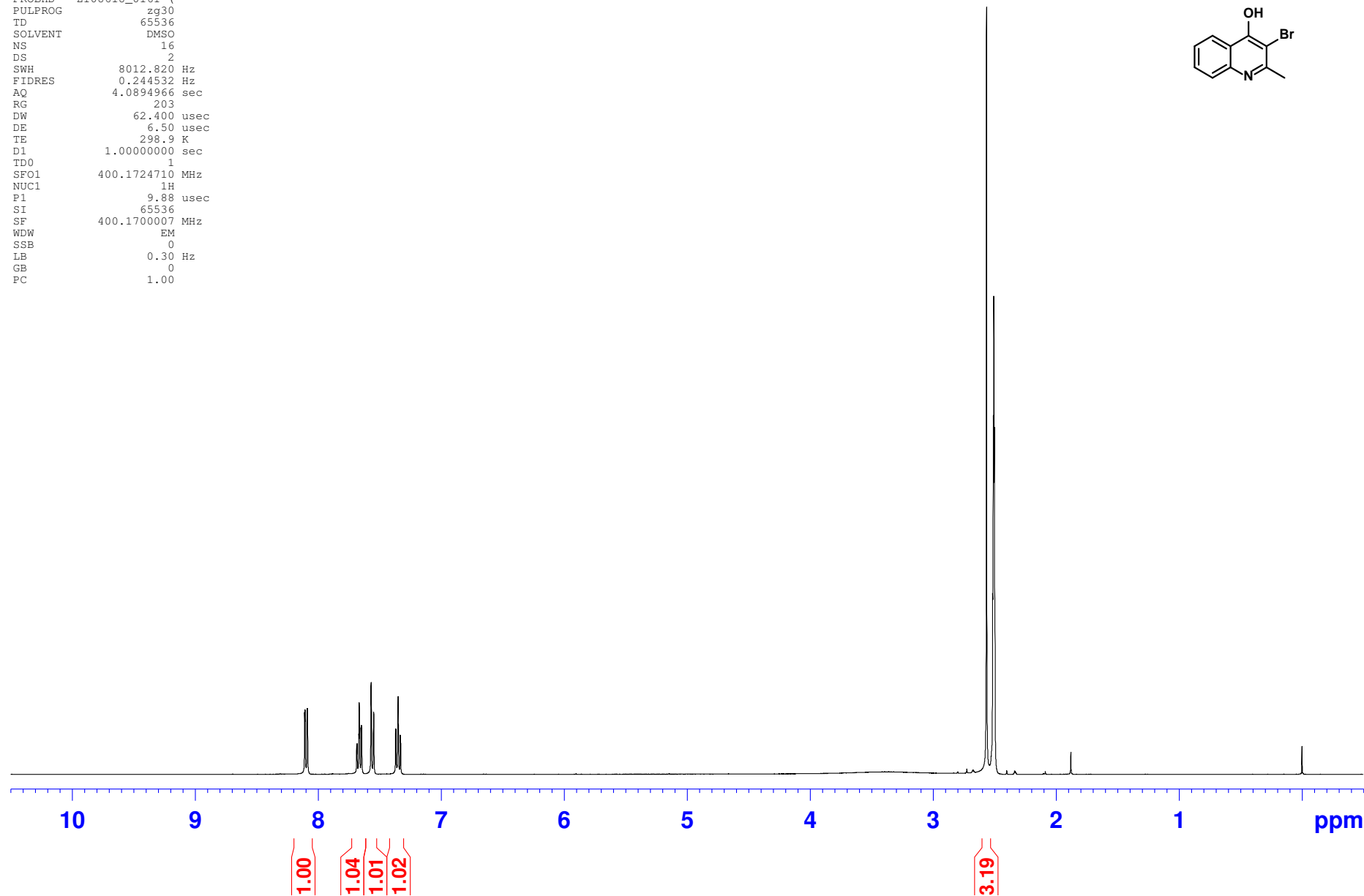
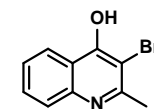


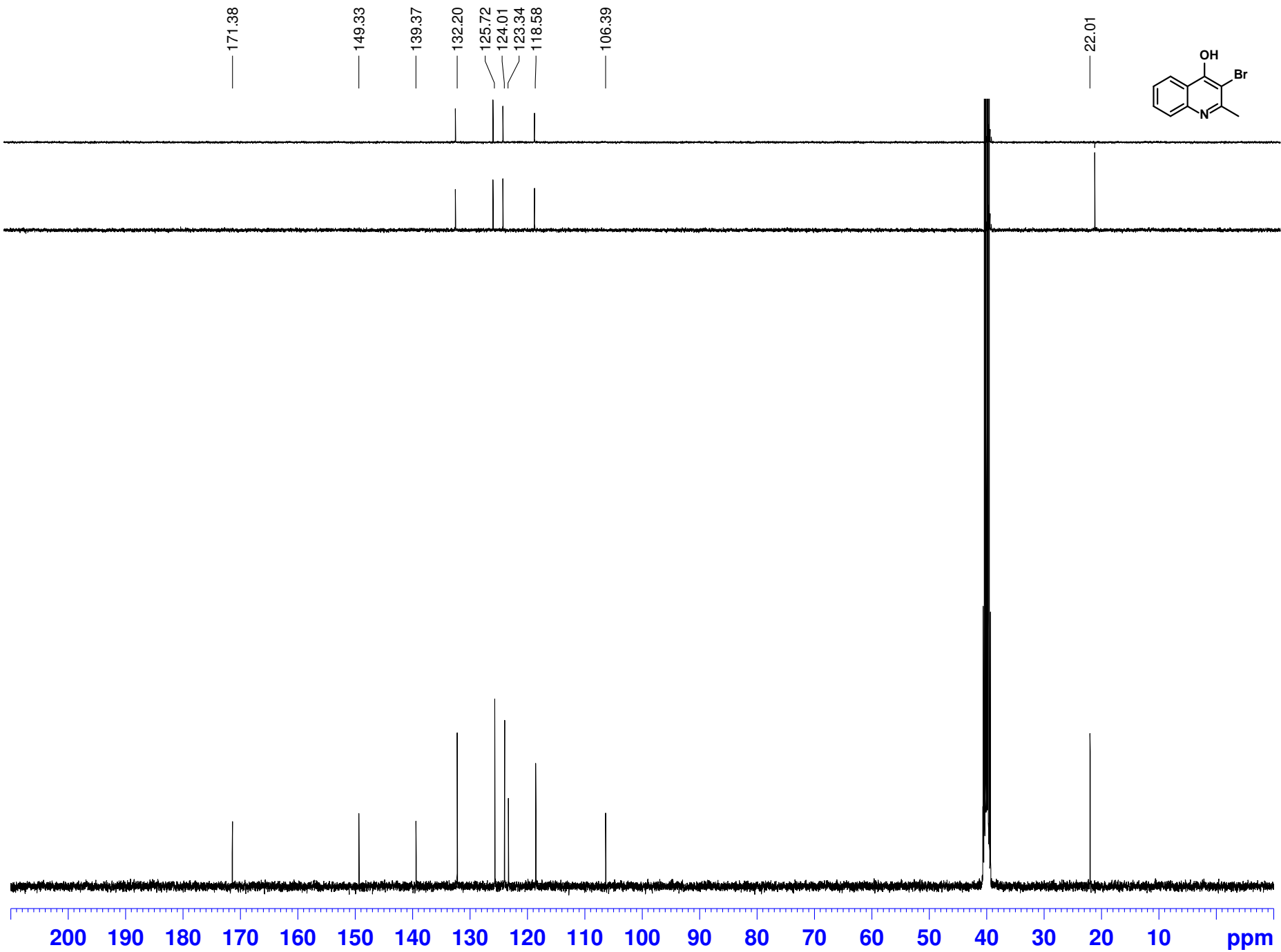
NGJ-7-011 (DMSO, 400 MHz) Crude Yellow Solid - bromination of 2-methyl quinolin-4-ol



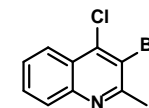
NAME NGJ-7-011
EXPNO 20
PROCNO 1
Date_ 20170329
Time_ 18.03 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700007 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



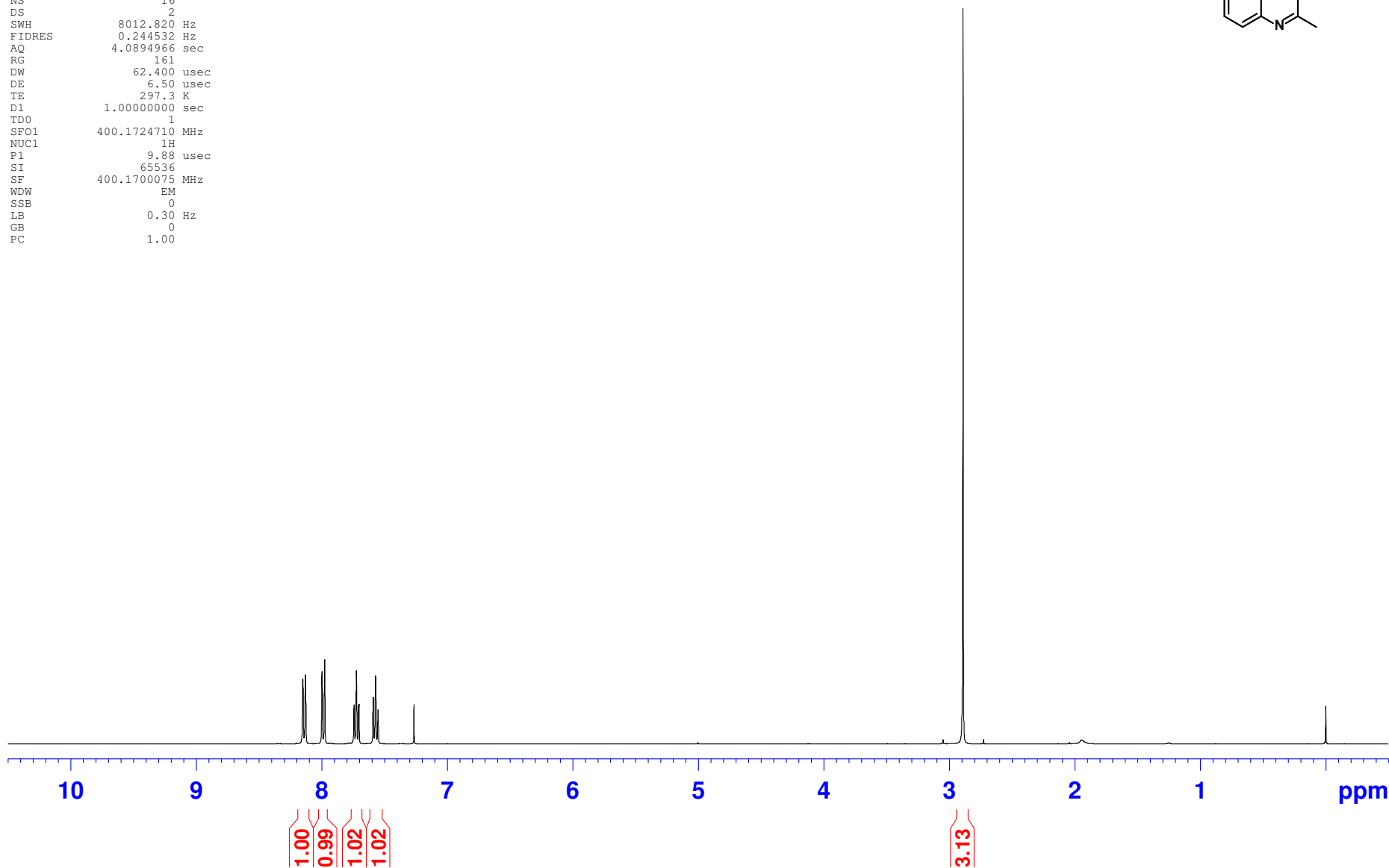
NGJ-7-011 (DMSO, 400 MHz) Crude Yellow Solid - bromination of



NGJ-7-012 (CDC13, 400 MHz) White Solid - chlorination of 3-bromo-2-methylquinolin-4-ol



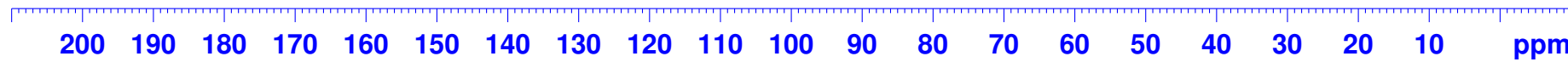
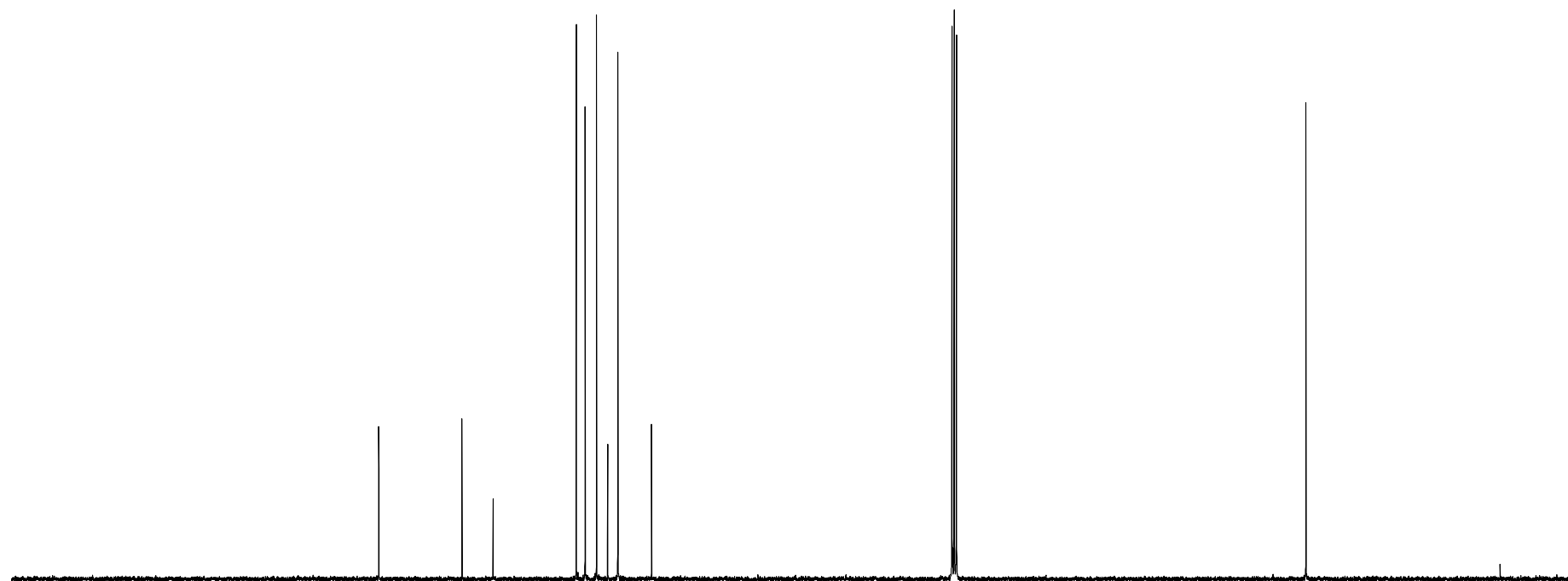
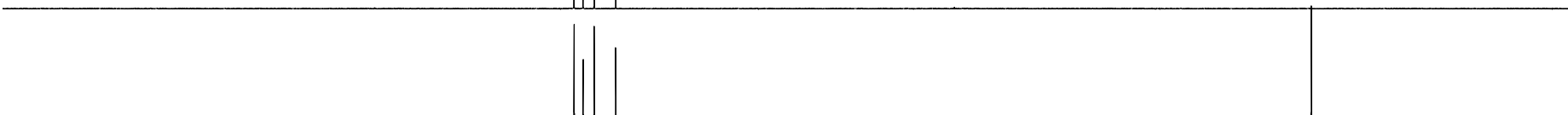
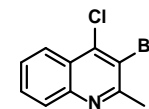
NAME NGJ-7-012
EXPNO 20
PROCNO 1
Date_ 20170330
Time_ 22.08 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NGJ-7-012 (CDCl₃, 400 MHz) White Solid - chlorination of 3-br

158.17
146.43
142.04
130.31
129.06
127.51
125.95
124.51
119.75

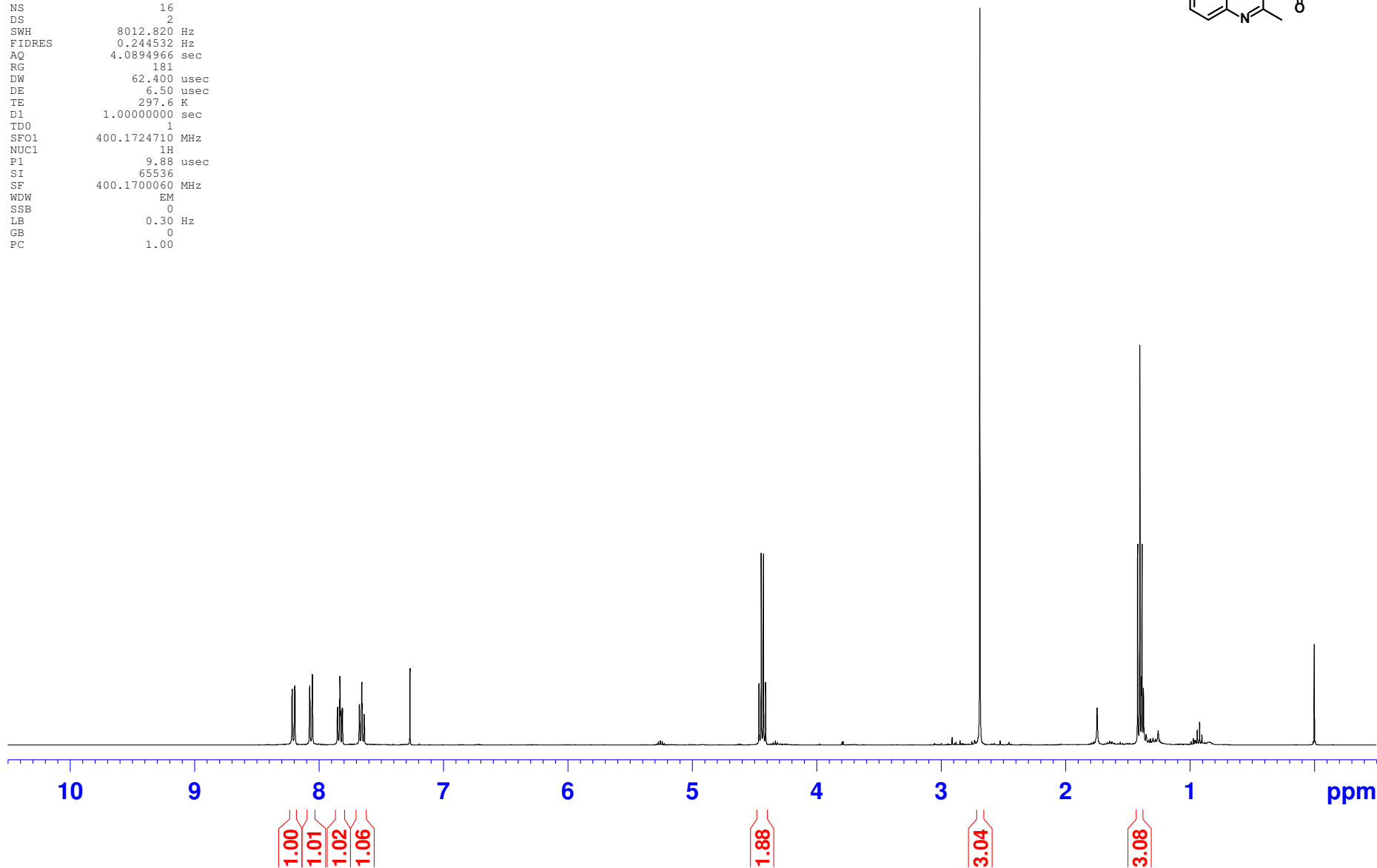
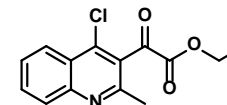
27.42



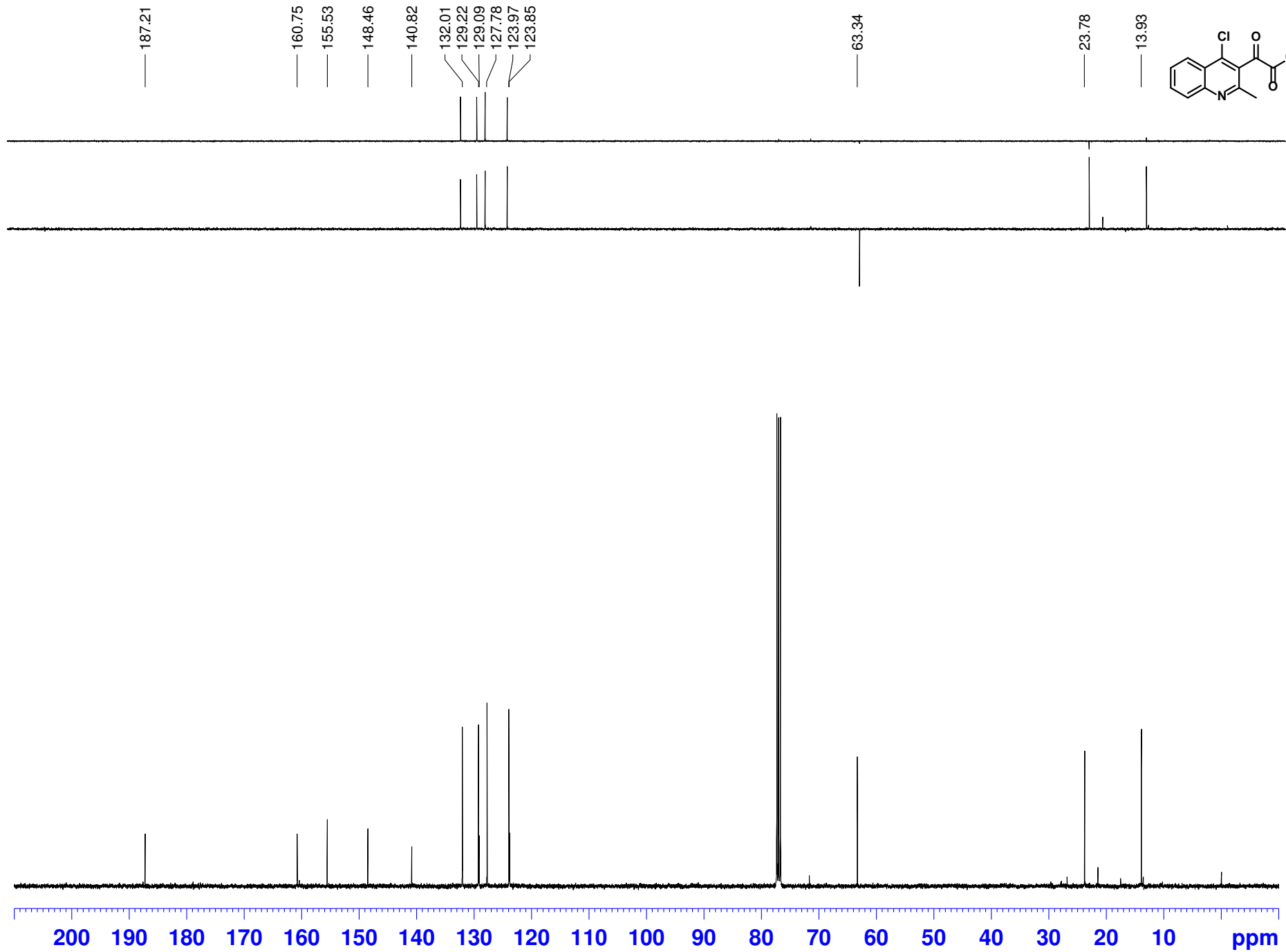
NGJ-7-018 (CDC13, 400 MHz) Pure Yellow Oil - grignard reaction with oxalyl chloride



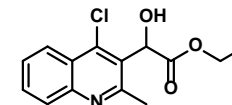
NAME NGJ-7-018
EXPNO 30
PROCNO 1
Date_ 20170410
Time_ 18.39 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



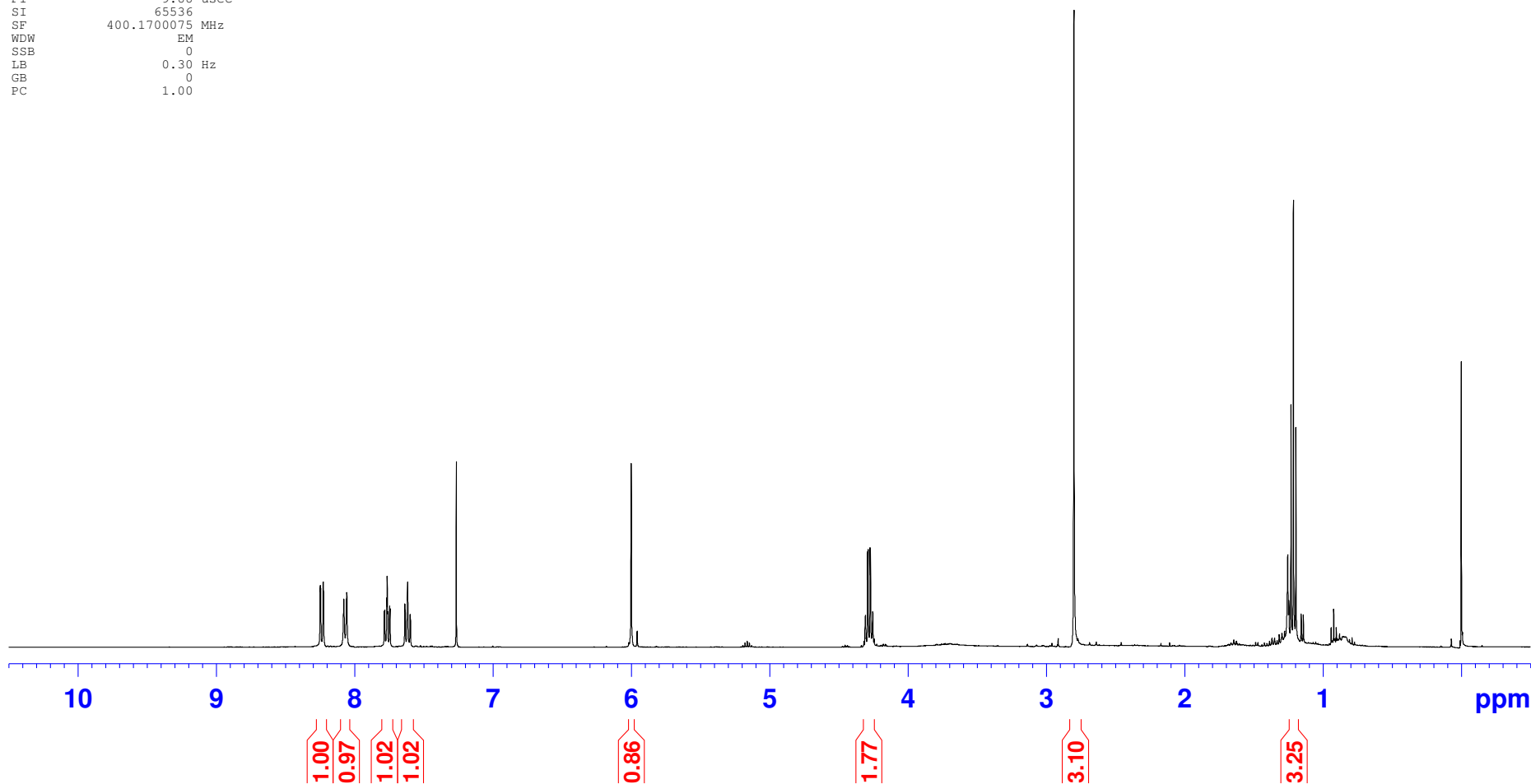
NGJ-7-018 (CDCl₃, 400 MHz) Pure Yellow Oil - grignard reactor



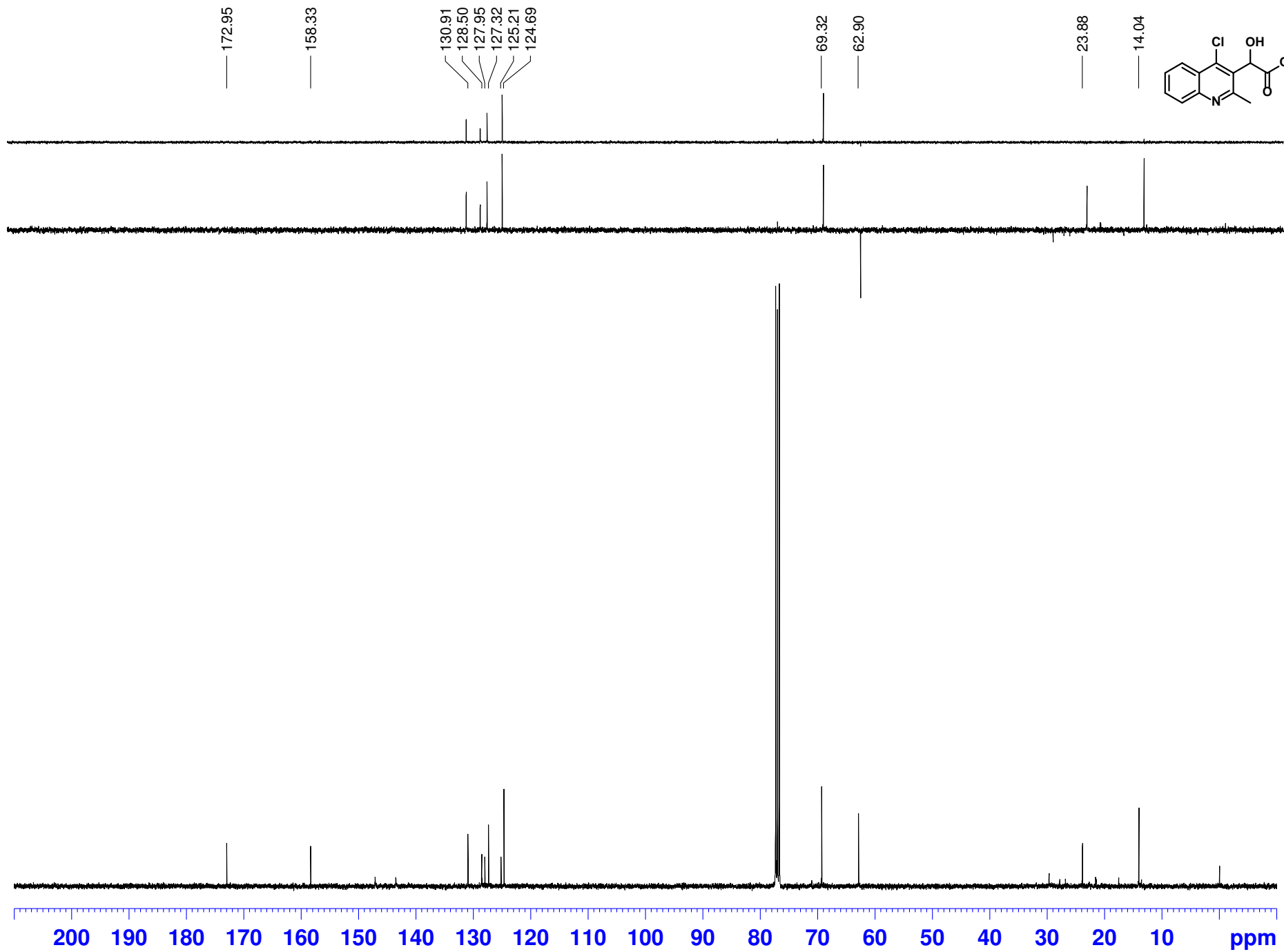
NGJ-7-027 (CDC13, 400 MHz) Pure Yellow Oil - NaBH4 reduction



NAME NGJ-7-027
EXPNO 20
PROCNO 1
Date_ 20170418
Time_ 17.52 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



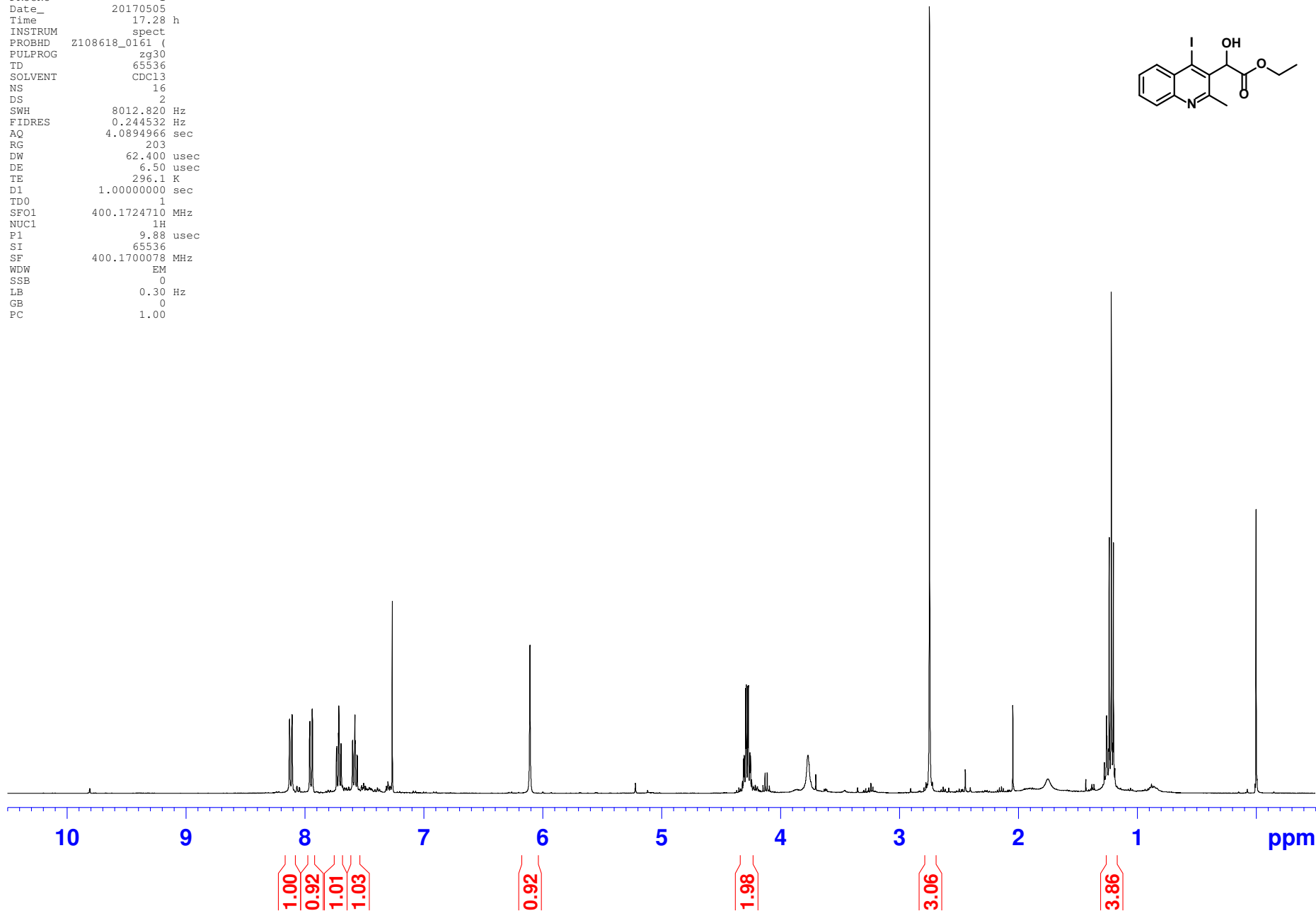
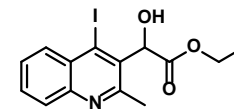
NGJ-7-027 (CDCl₃, 400 MHz) Pure Yellow Oil - NaBH₄ reduction



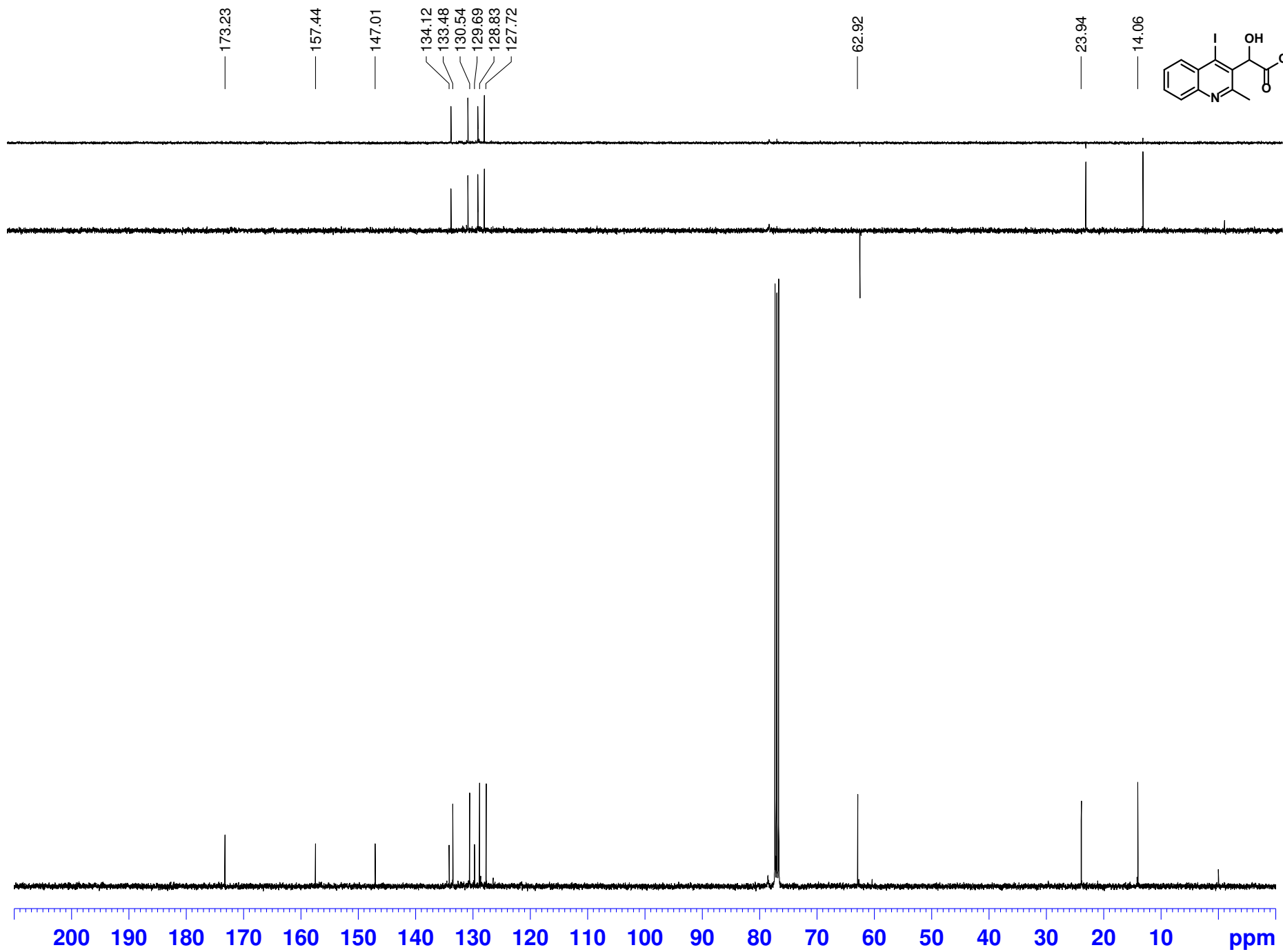
NGJ-7-046 (CDC13, 400 MHz) Brown Oil - transhalogenation of 4-chloroquinoline



NAME NGJ-7-046
EXPNO 20
PROCNO 1
Date_ 20170505
Time_ 17.28 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



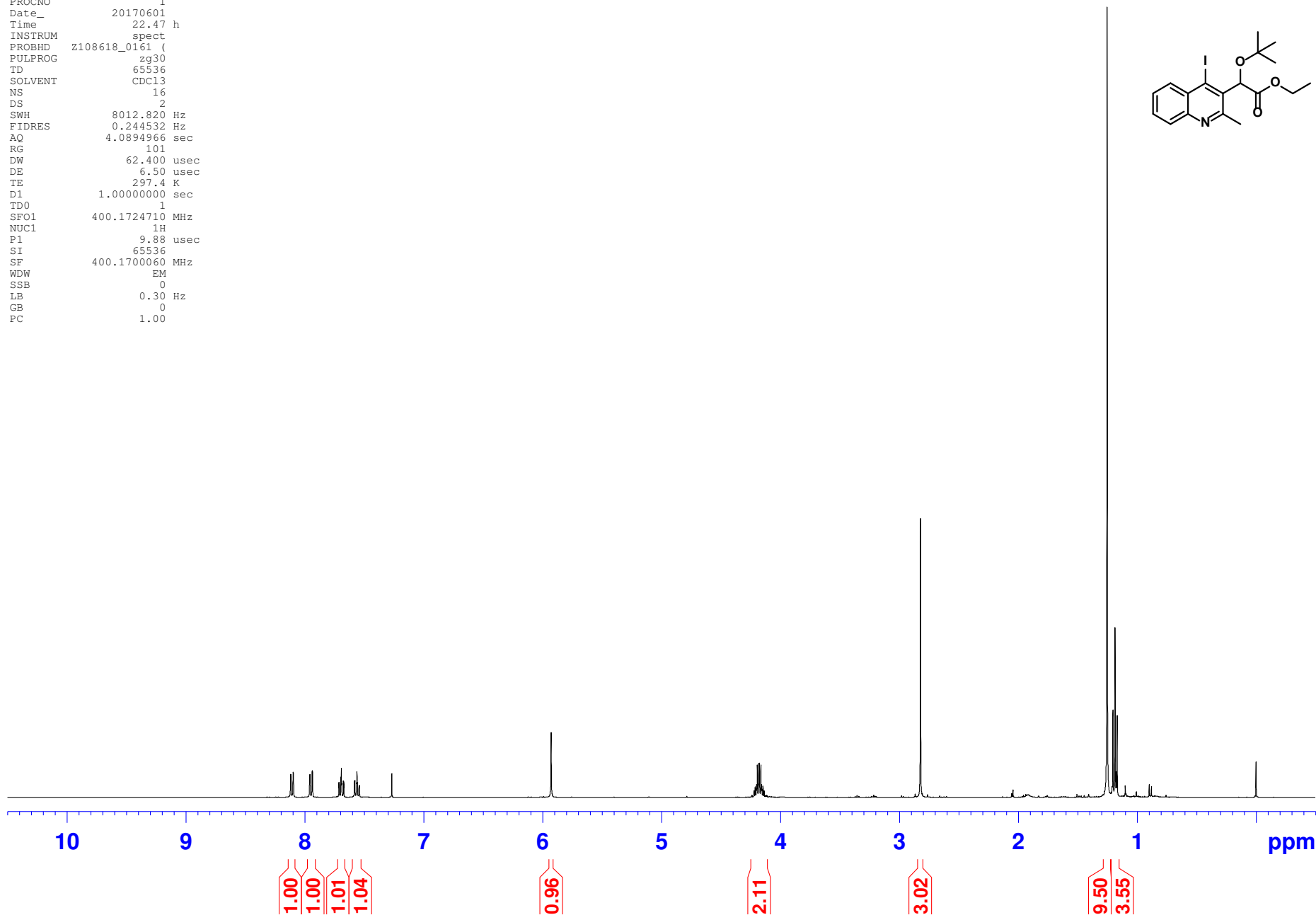
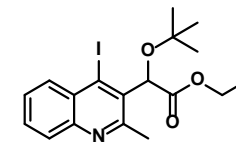
NGJ-7-046 (CDCl₃, 400 MHz) Brown Oil - transhalogenation of 4-



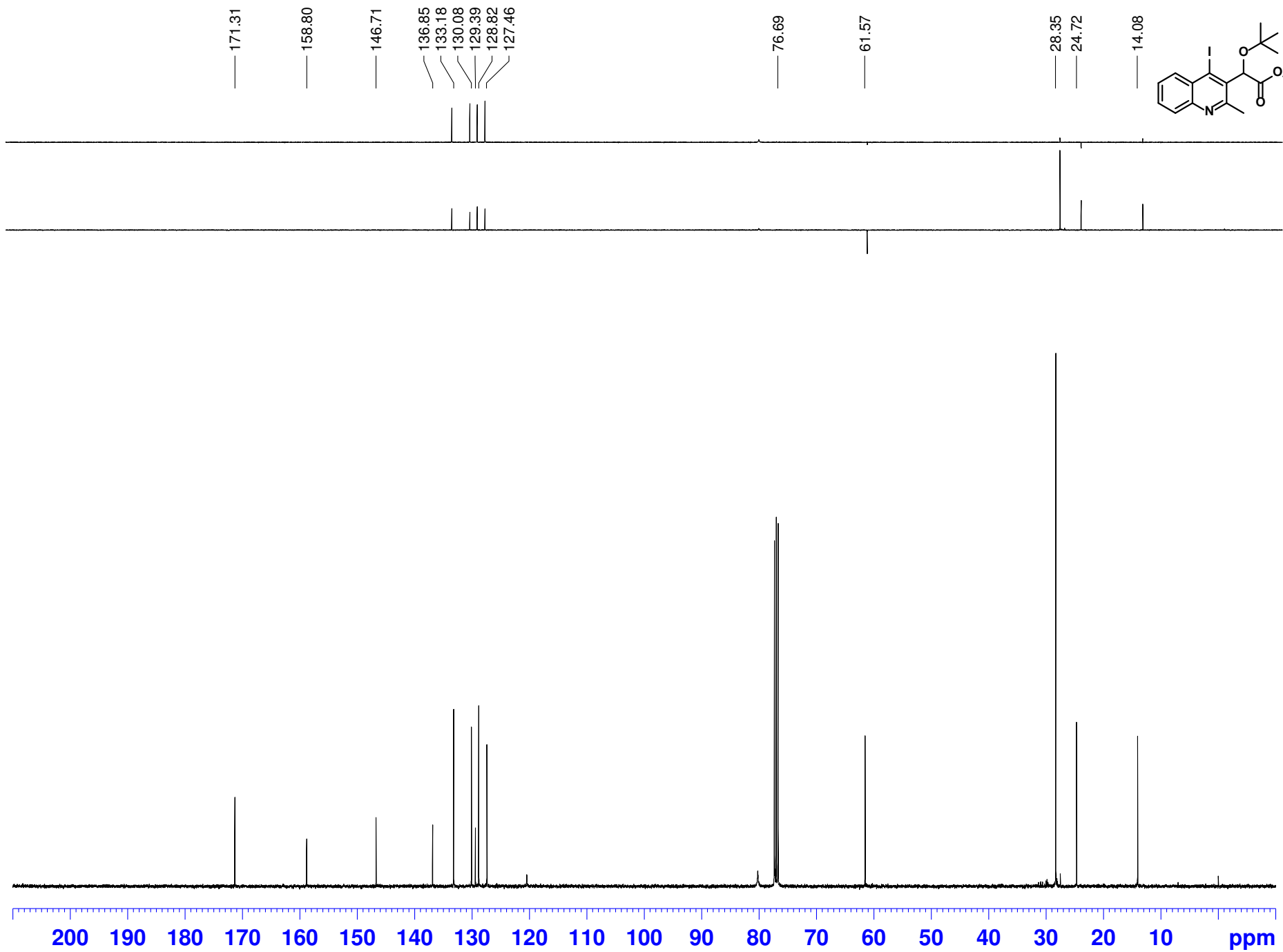
NGJ-7-070 (CDC13, 400 MHz) Pure Yellow Oil - t-butylation of iodo quinoline



NAME NGJ-7-070
EXPNO 20
PROCNO 1
Date_ 20170601
Time_ 22.47 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 101
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

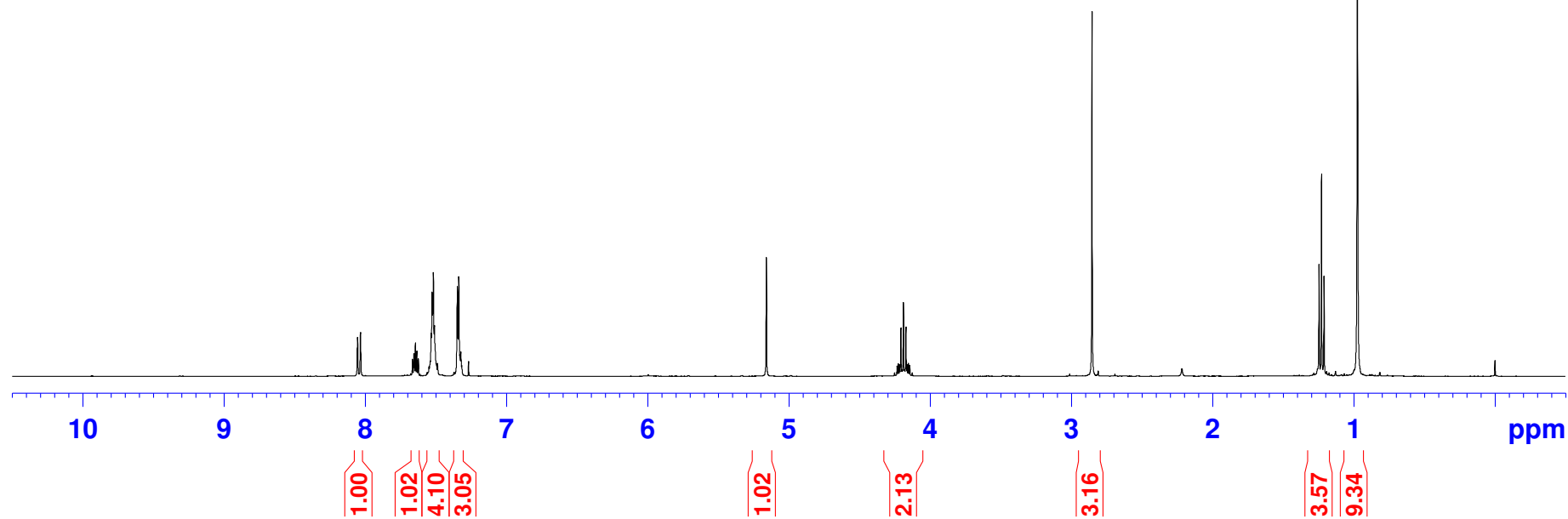
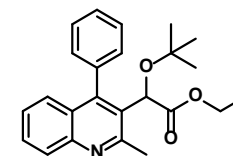
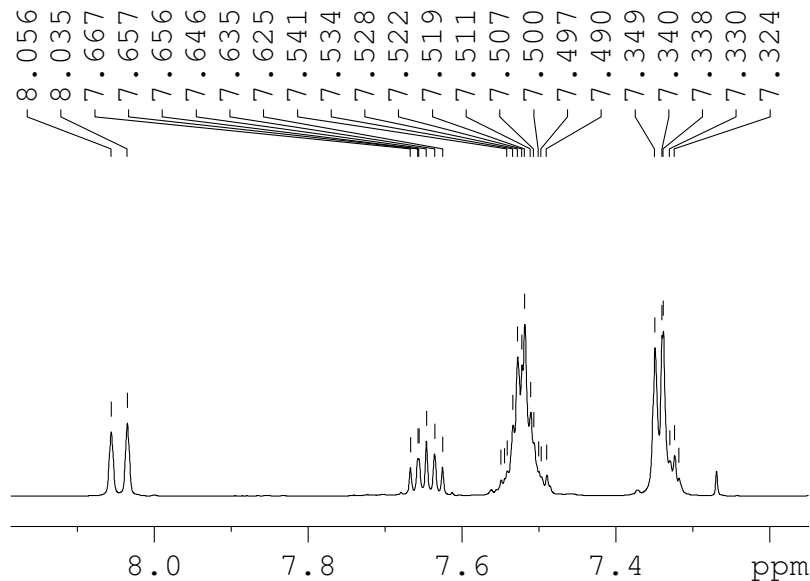


NGJ-7-070 (CDCl₃, 400 MHz) Pure Yellow Oil - t-butylation of i

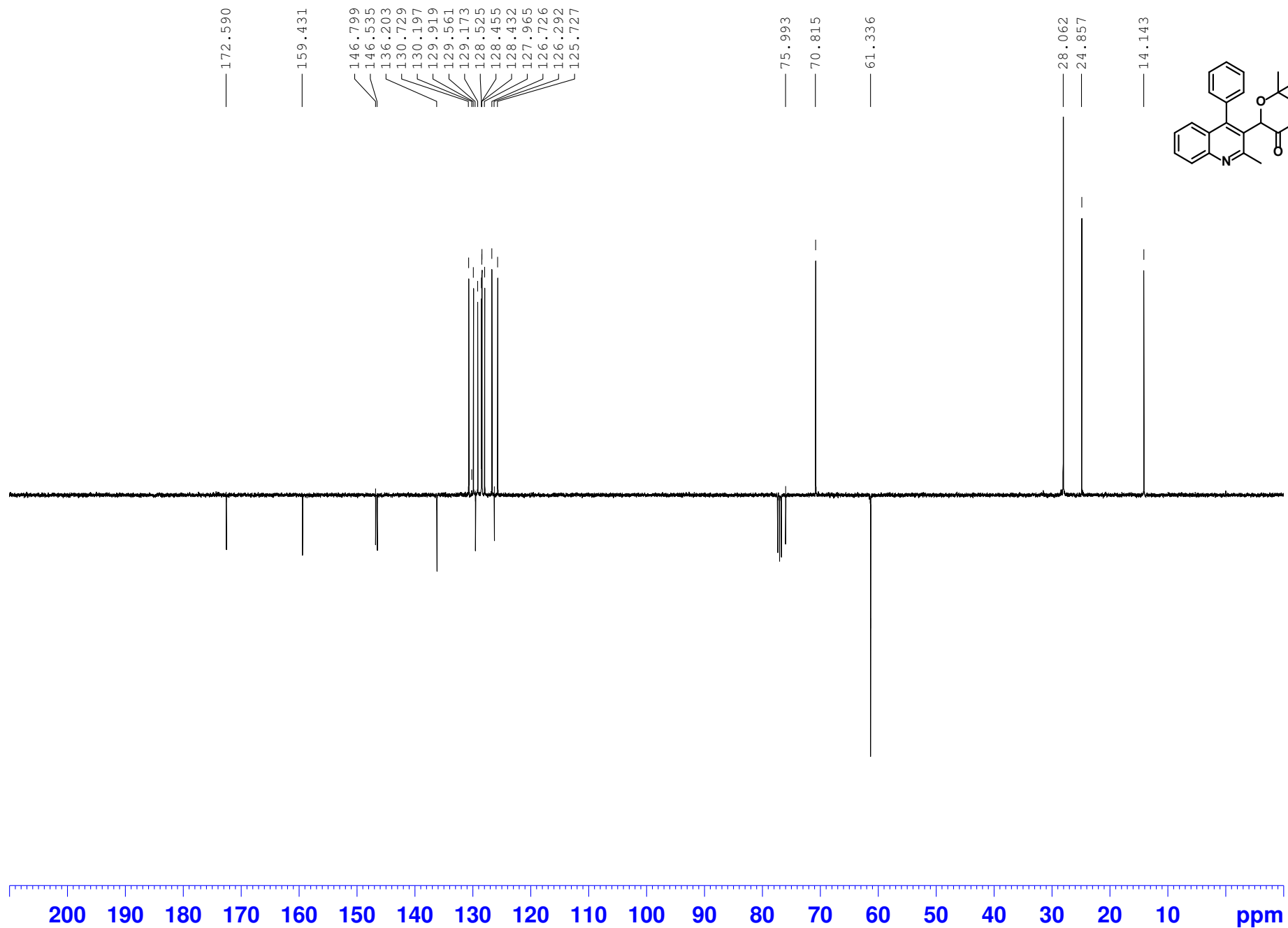


NGJ-9-018 (CDC13, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with phenylboronate

NAME NGJ-9-018
 EXPNO 30
 PROCNO 1
 Date_ 20171218
 Time_ 10.03 h
 INSTRUM spect
 PROBHD Z108618_0161 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 57
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700058 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



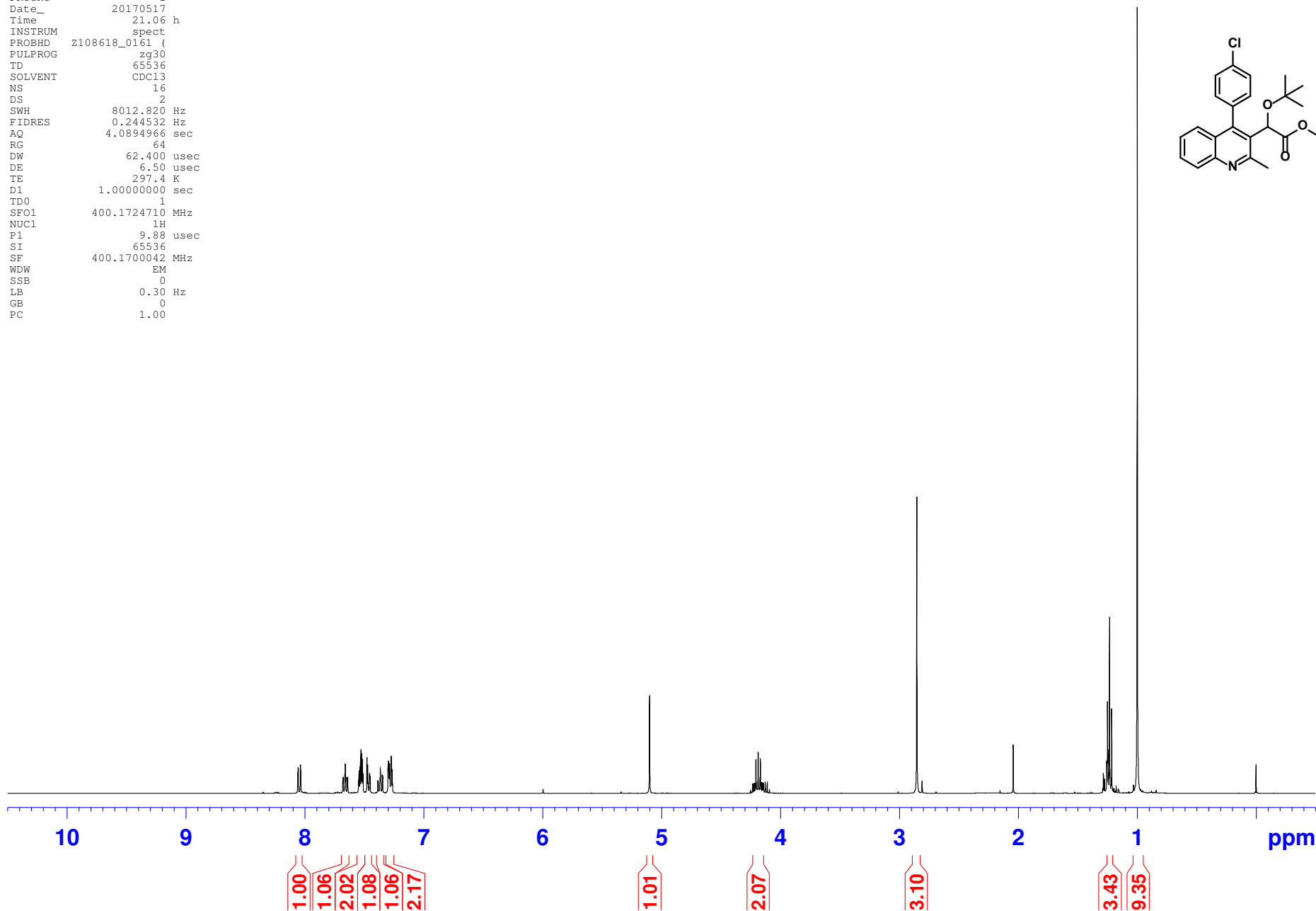
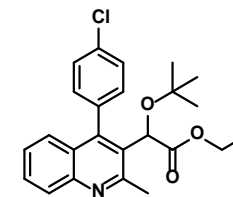
NGJ-9-018 (CDCl₃, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with phenylboronic acid



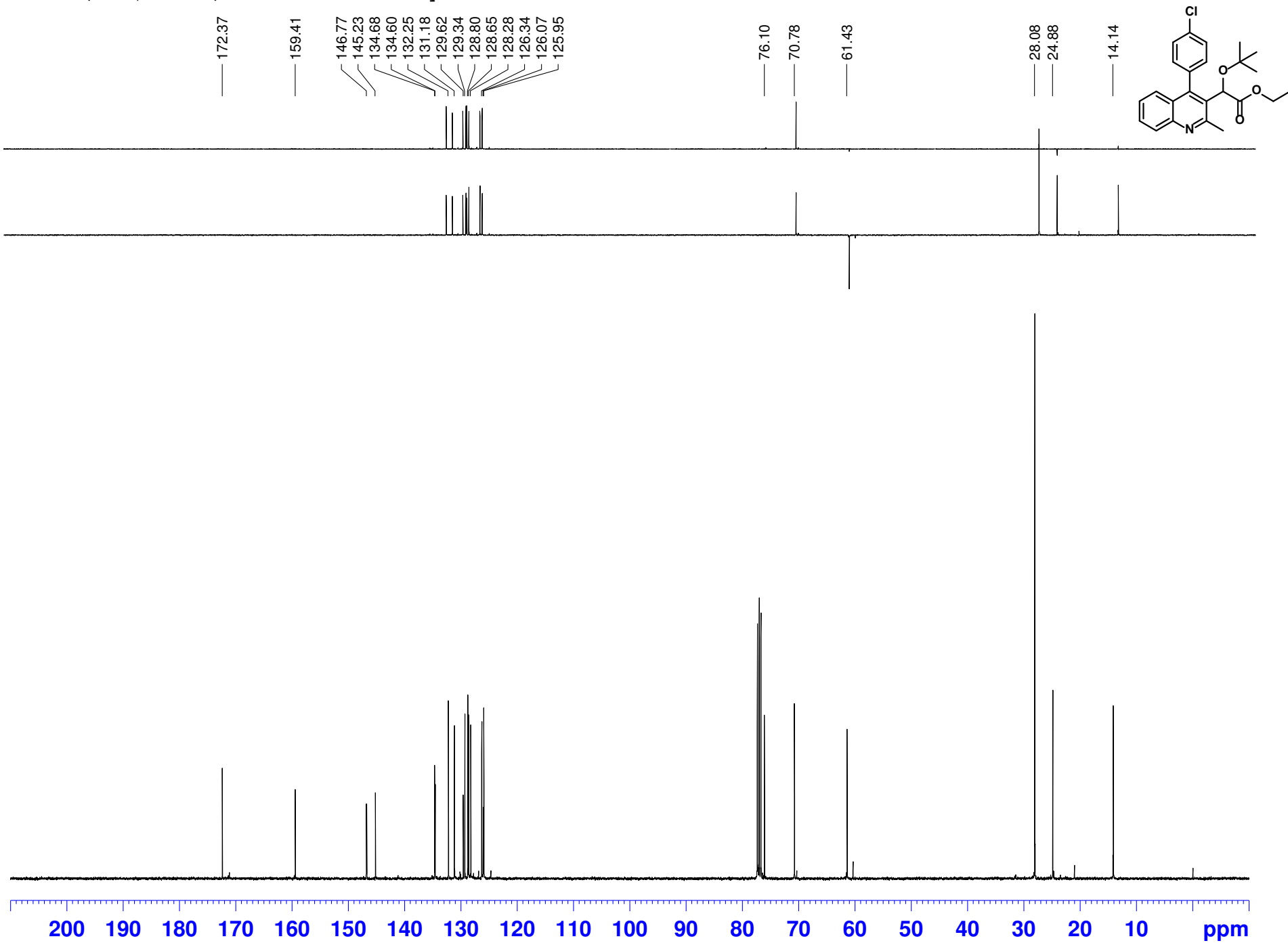
NGJ-7-059 (CDC13, 400 MHz) Pure Yellow Oil - t-butylation with HClO4



NAME NGJ-7-059
EXPNO 20
PROCNO 1
Date_ 20170517
Time_ 21.06 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700042 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

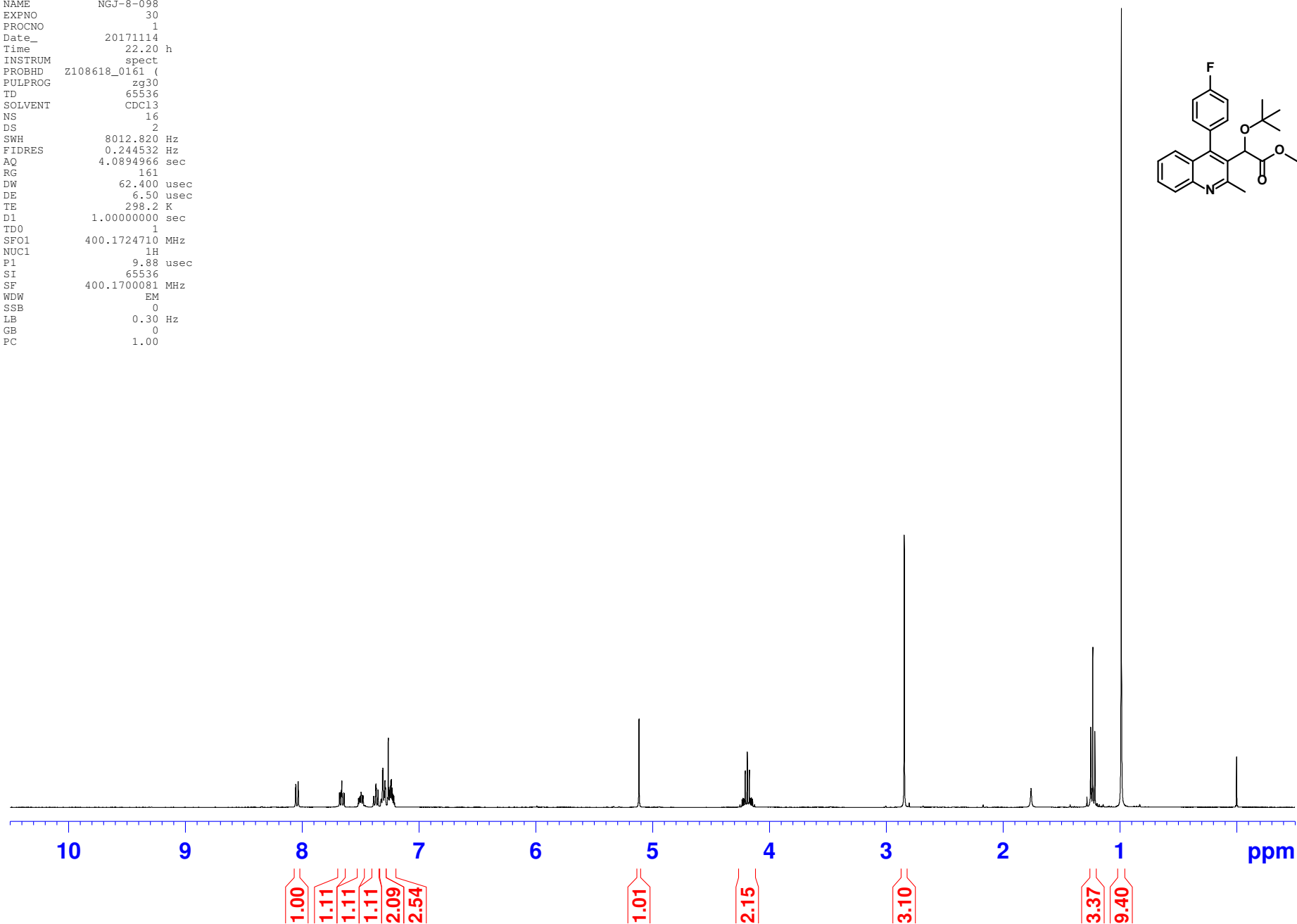
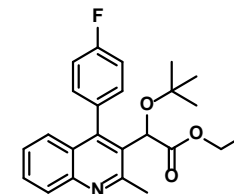


NGJ-7-059 (CDCl₃, 400 MHz) Pure Yellow Oil - t-butylation with

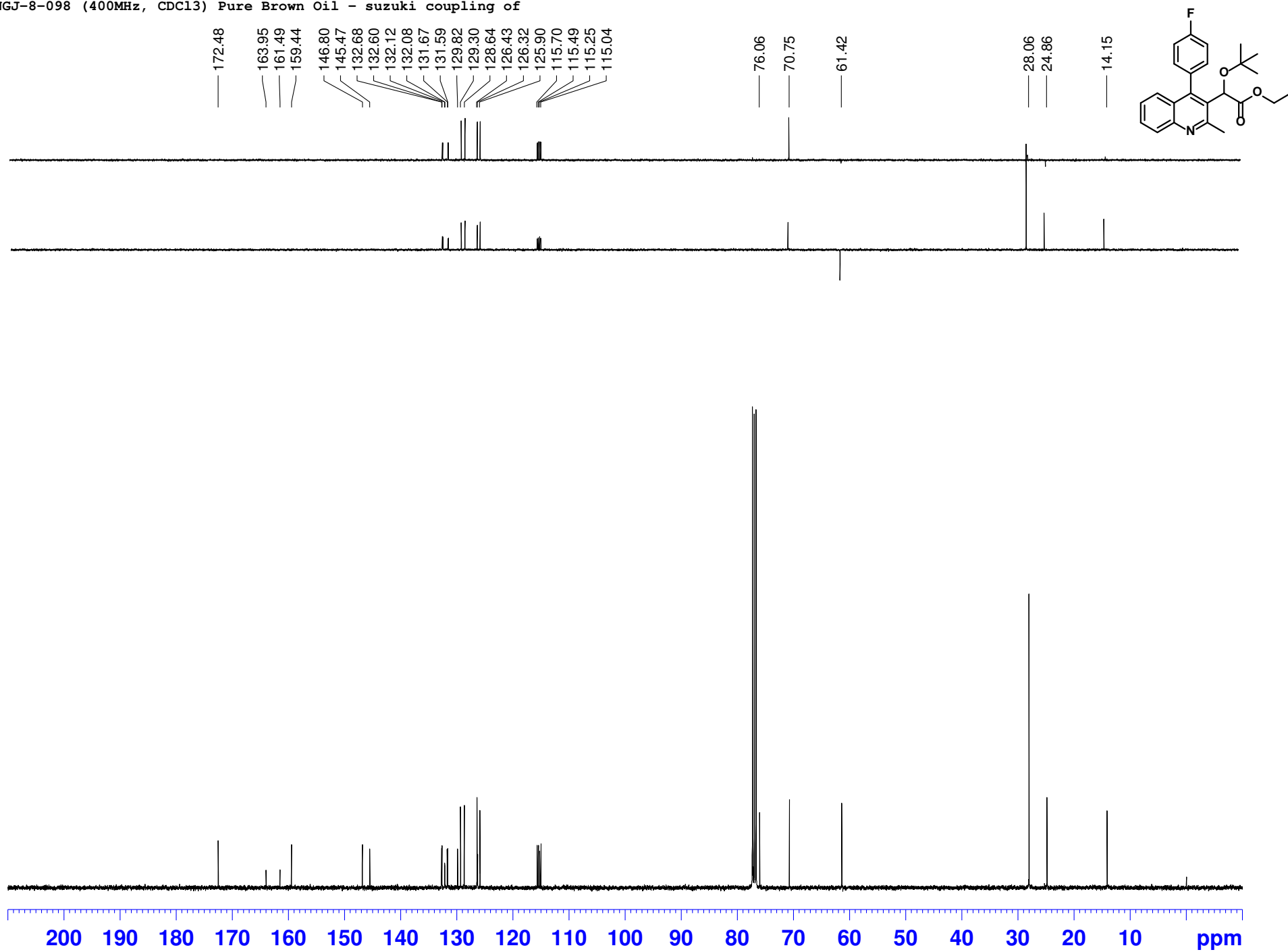


NGJ-8-098 (400MHz, CDCl3) Pure Brown Oil - suzuki coupling of iodoquinoline with 4-fluorophenyl

NAME NGJ-8-098
EXPNO 30
PROCNO 1
Date_ 20171114
Time_ 22.20 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



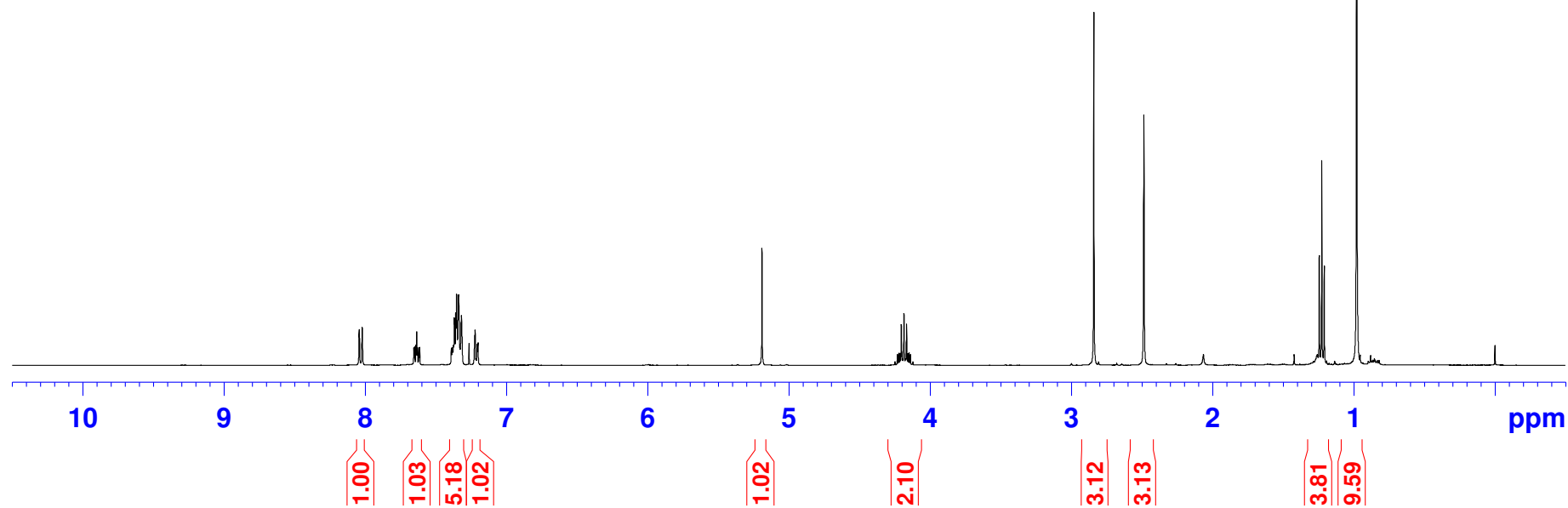
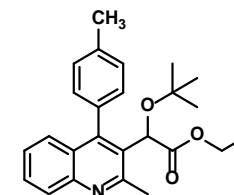
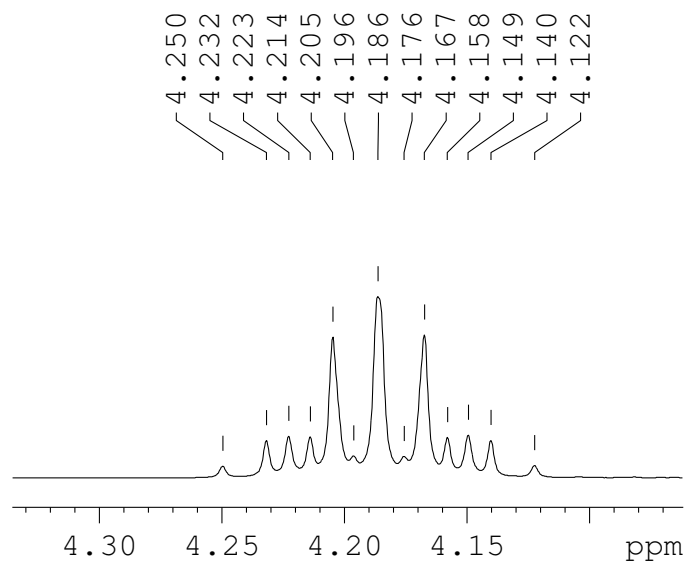
NGJ-8-098 (400MHz, CDC13) Pure Brown Oil - suzuki coupling of



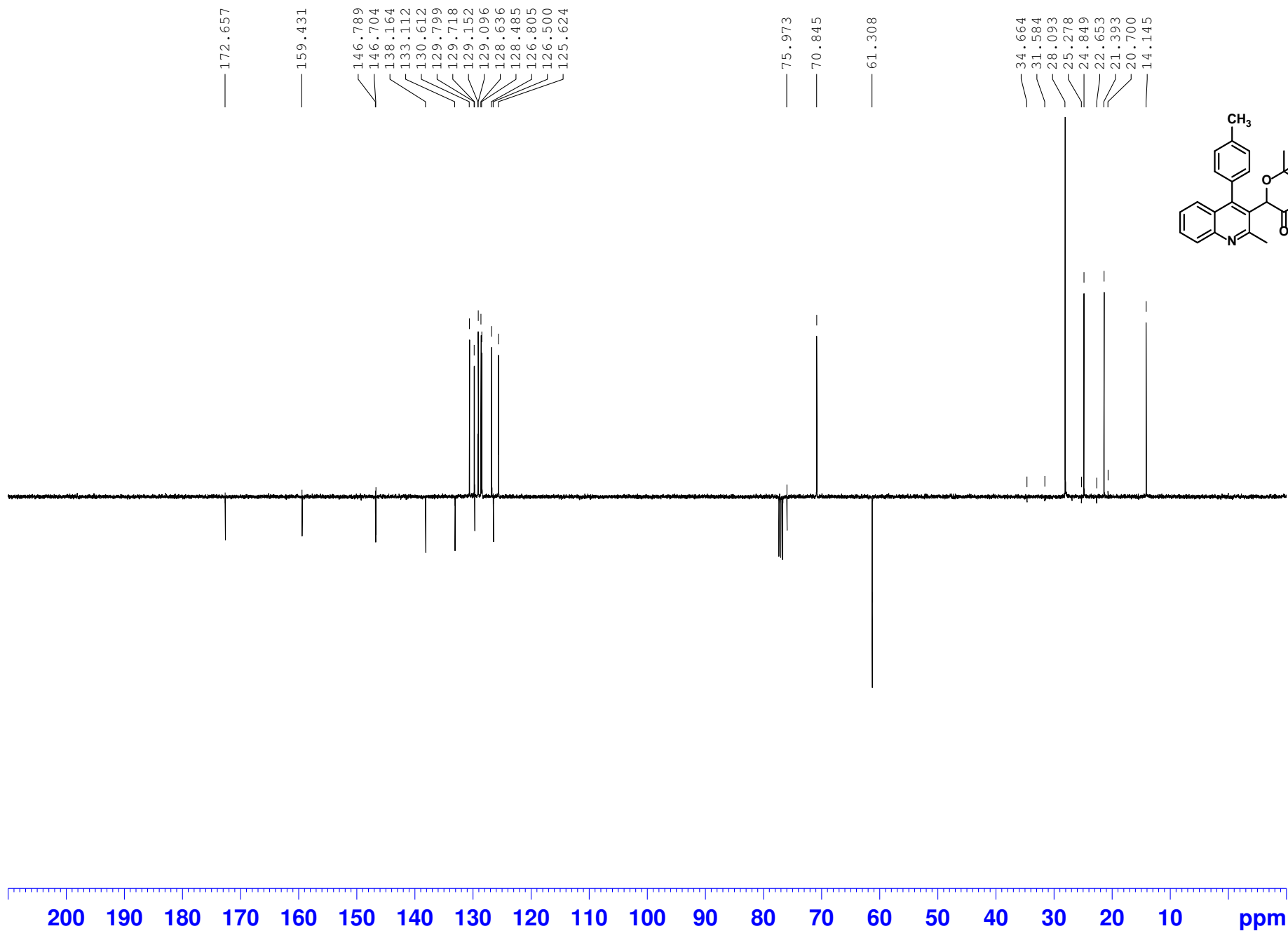
NGJ-9-019 (CDC13, 400MHz)

```

NAME      NGJ-9-019
EXPNO     30
PROCNO    1
Date_     20171219
Time      23.05 h
INSTRUM   spect
PROBHD    Z108618_0161 (
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         4.0894966 sec
RG          71.8
DW         62.400 usec
DE         6.50 usec
TE         298.3 K
D1         1.00000000 sec
TD0        1
SFO1      400.1724710 MHz
NUC1       1H
P1         9.88 usec
SI         65536
SF         400.1700073 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

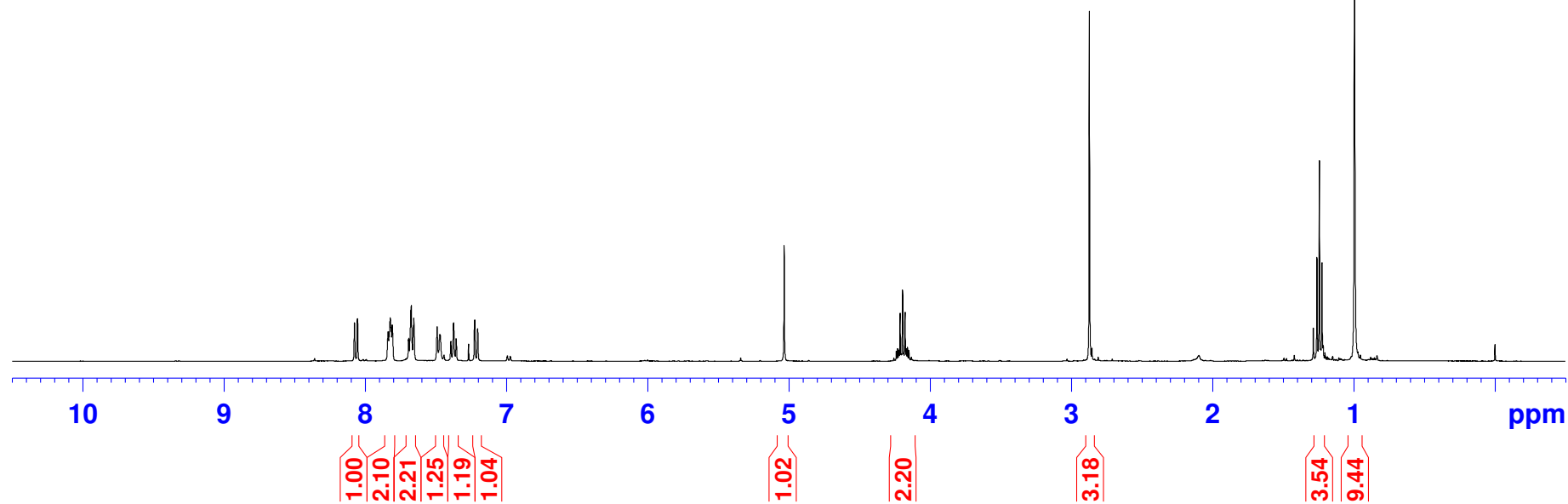
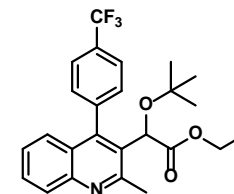
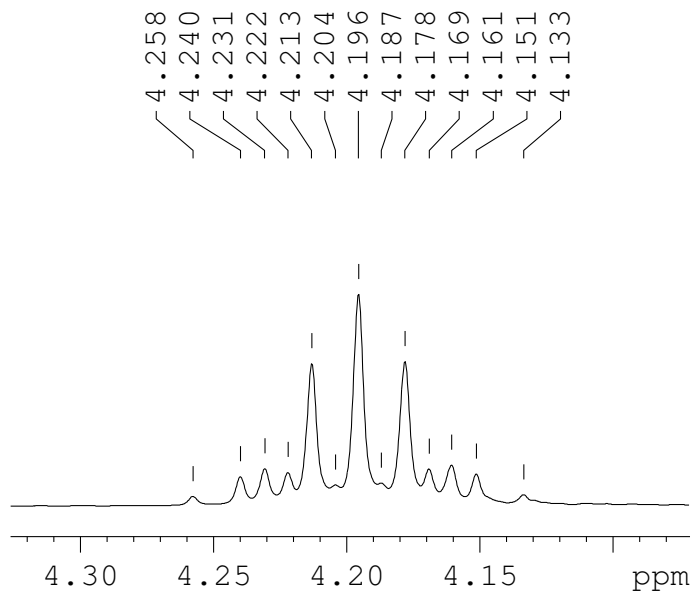


NGJ-9-019 (CDC13, 400MHz)



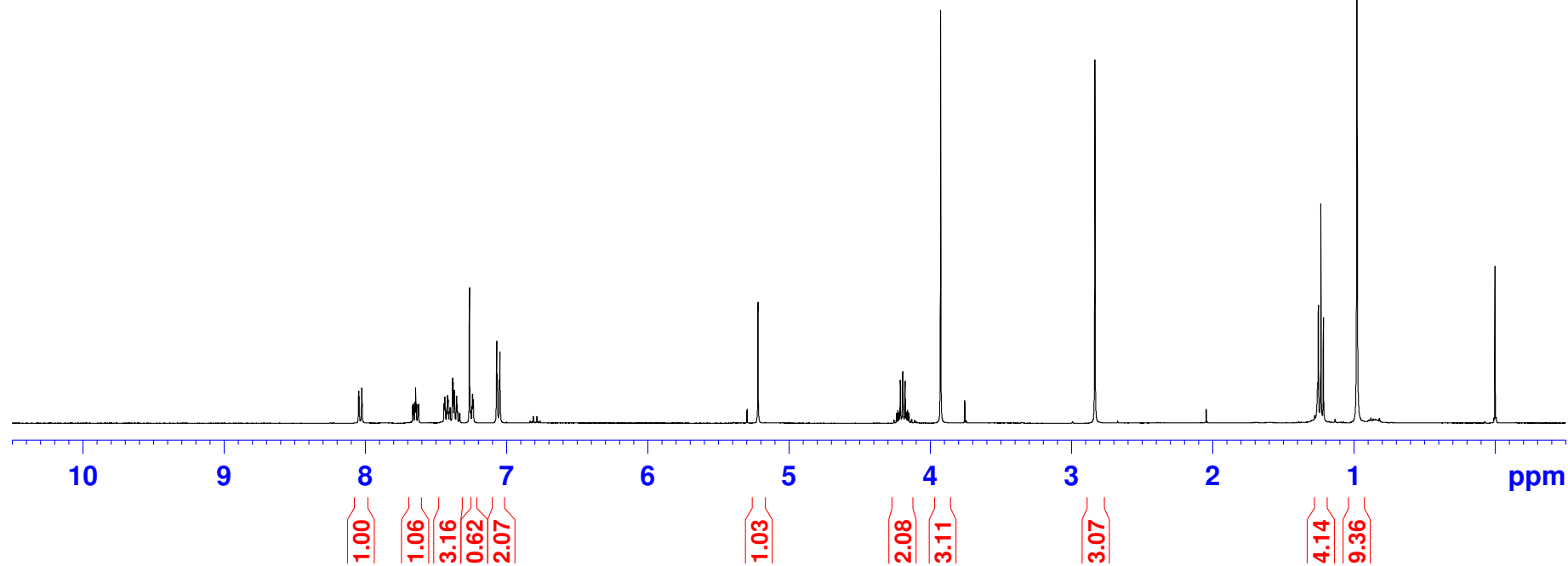
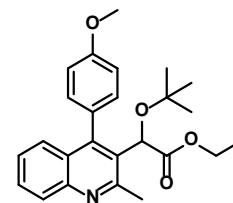
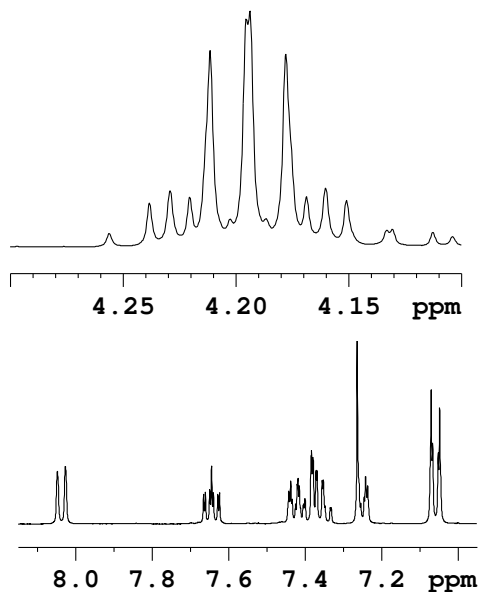
NGJ-9-020 (CDC13, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with 4-trifluor

NAME NGJ-9-020
 EXPNO 20
 PROCNO 1
 Date_ 20171220
 Time_ 17.02 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 64
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SF01 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700058 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

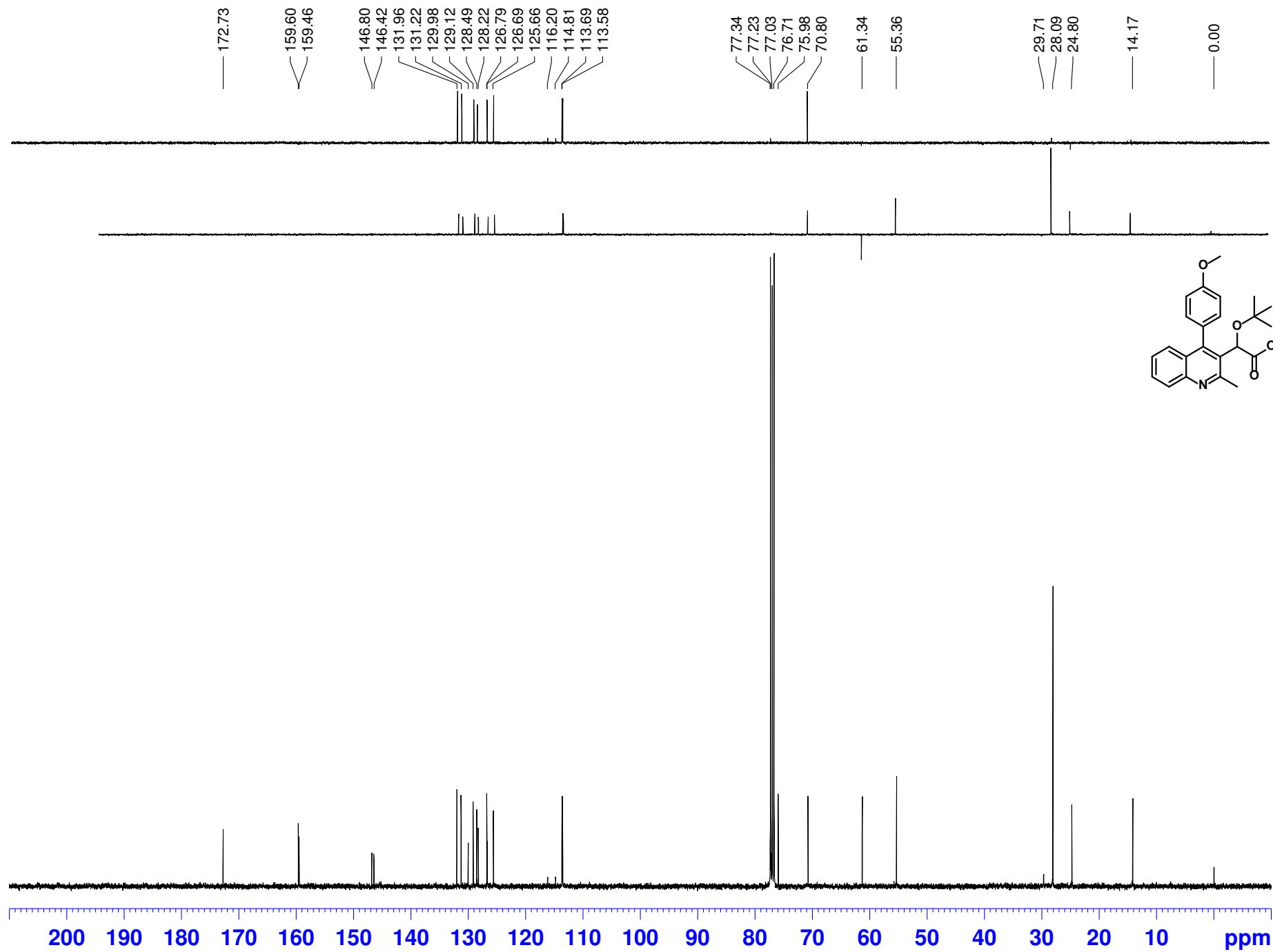


JDH-1-141 (CDC13, 400MHz) pure yellow oil - Suzuki Coupling of Iodoquinoline with 4 methoxyphenylboronic acid

NAME JDH-1-141
 EXPNO 50
 PROCNO 1
 Date_ 20170622
 Time_ 19.58 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 181
 DW 62.400 usec
 DE 6.50 usec
 TE 297.4 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700084 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

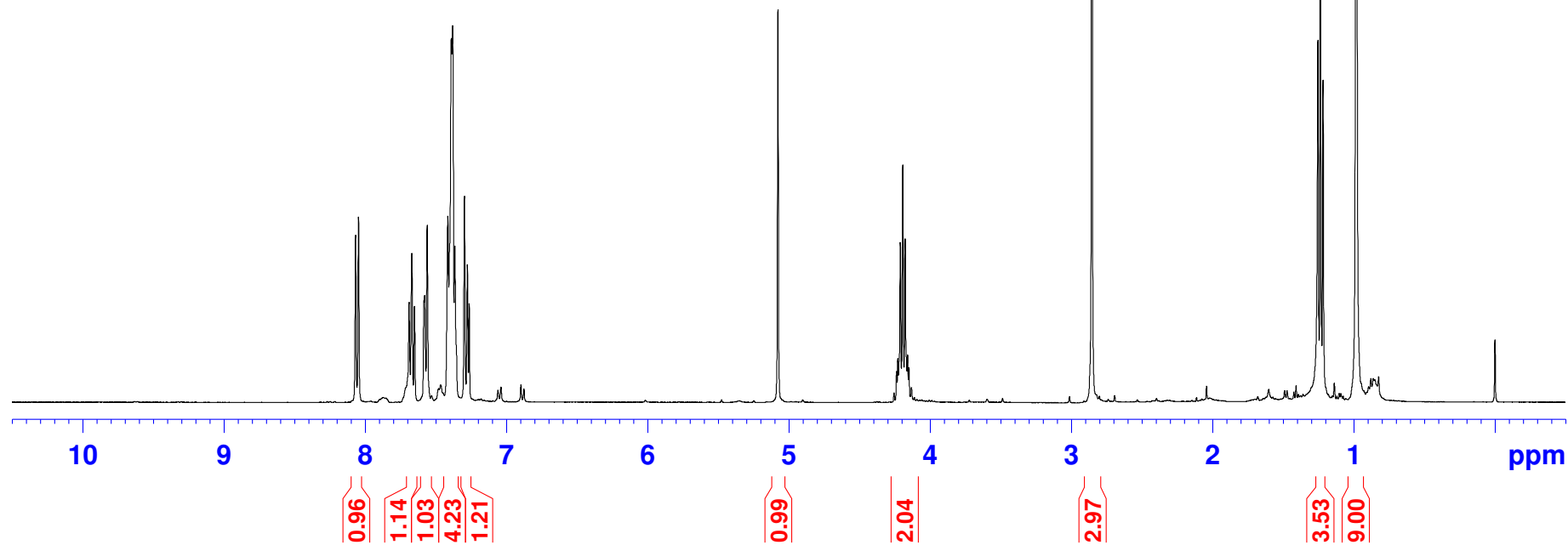
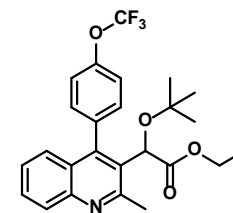
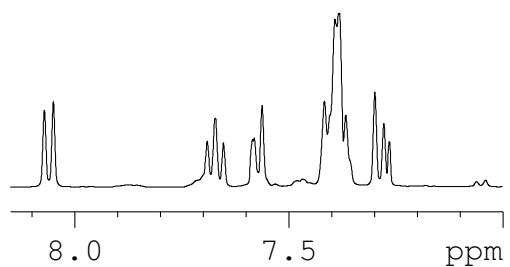
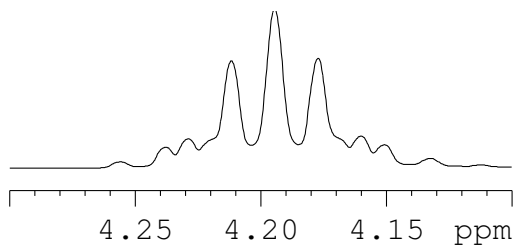


JDH-1-141 (CDCl₃, 400MHz) pure yellow oil - Suzuki Coupling of

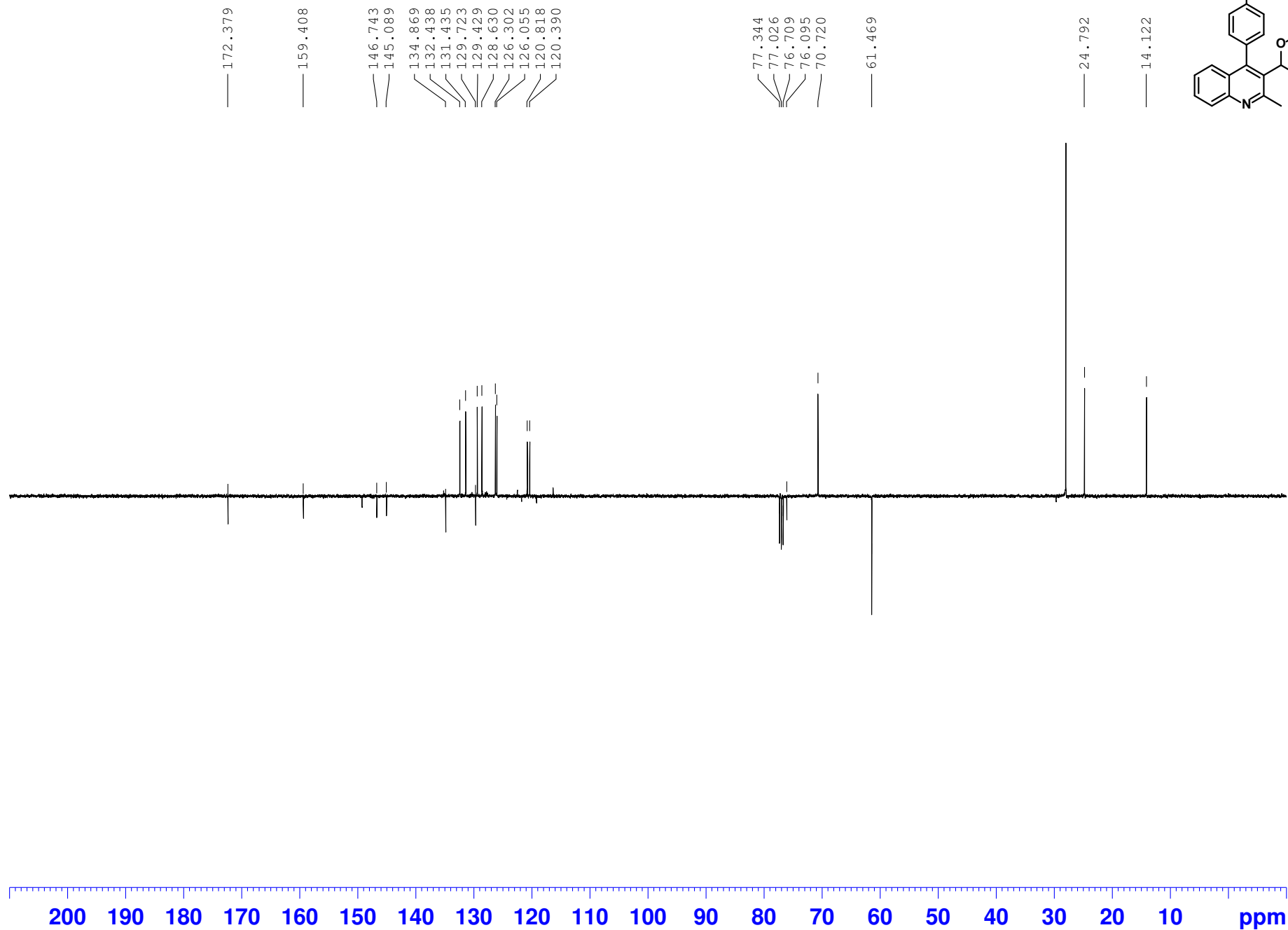
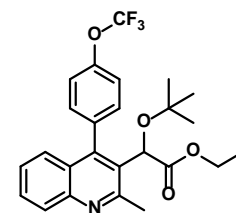


JDH-1-137 (CDC13, 400MHz) pure yellow oil - Suzuki Coupling of Iodoquinoline with 4 trifluoromethoxyphenylboronic ac

NAME JDH-1-137
EXPNO 11
PROCNO 1
Date_ 20171128
Time_ 19.06 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 101
DW 62.400 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

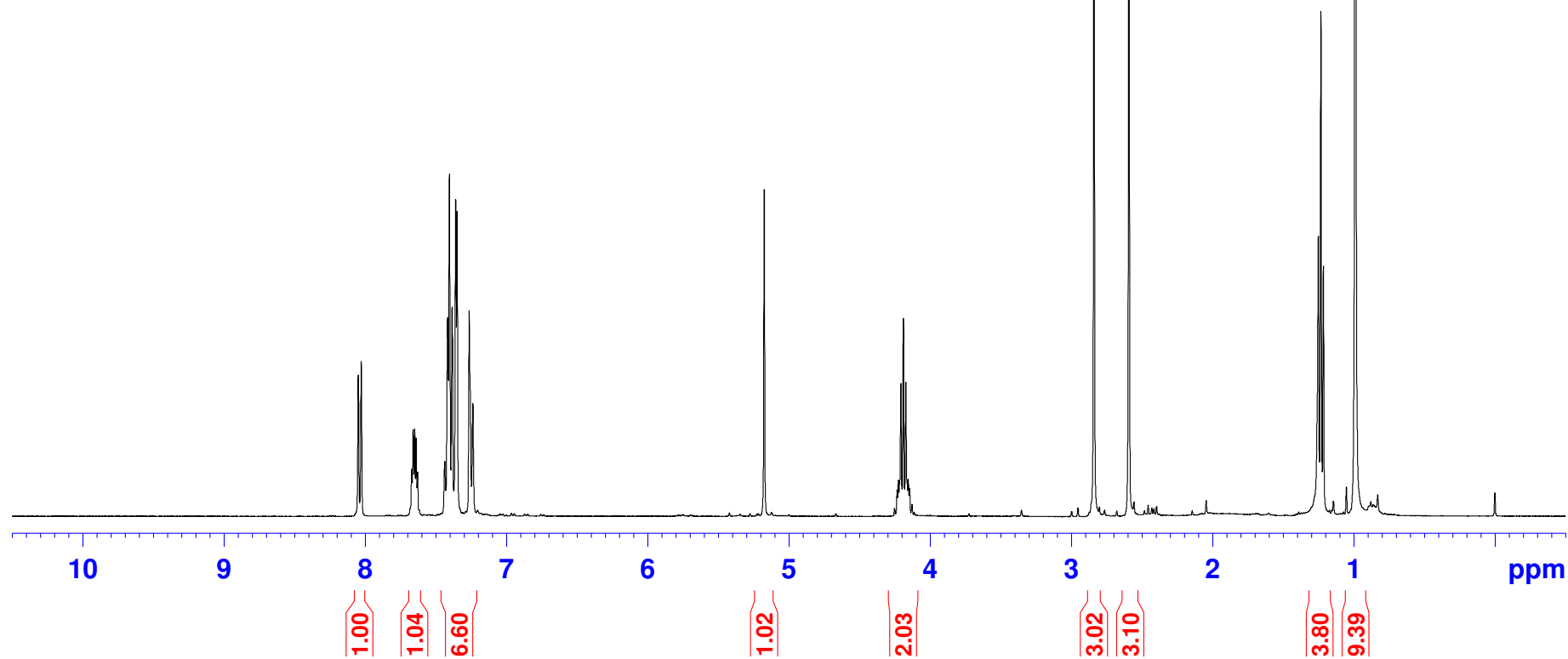
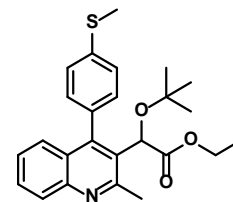
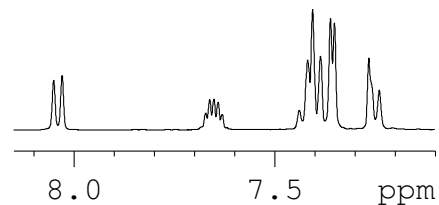
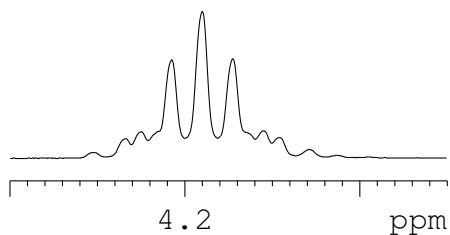


JDH-1-137 (CDCl₃, 400MHz) pure yellow oil - Suzuki Coupling of Iodoquinoline with 4 trifluoromethoxy

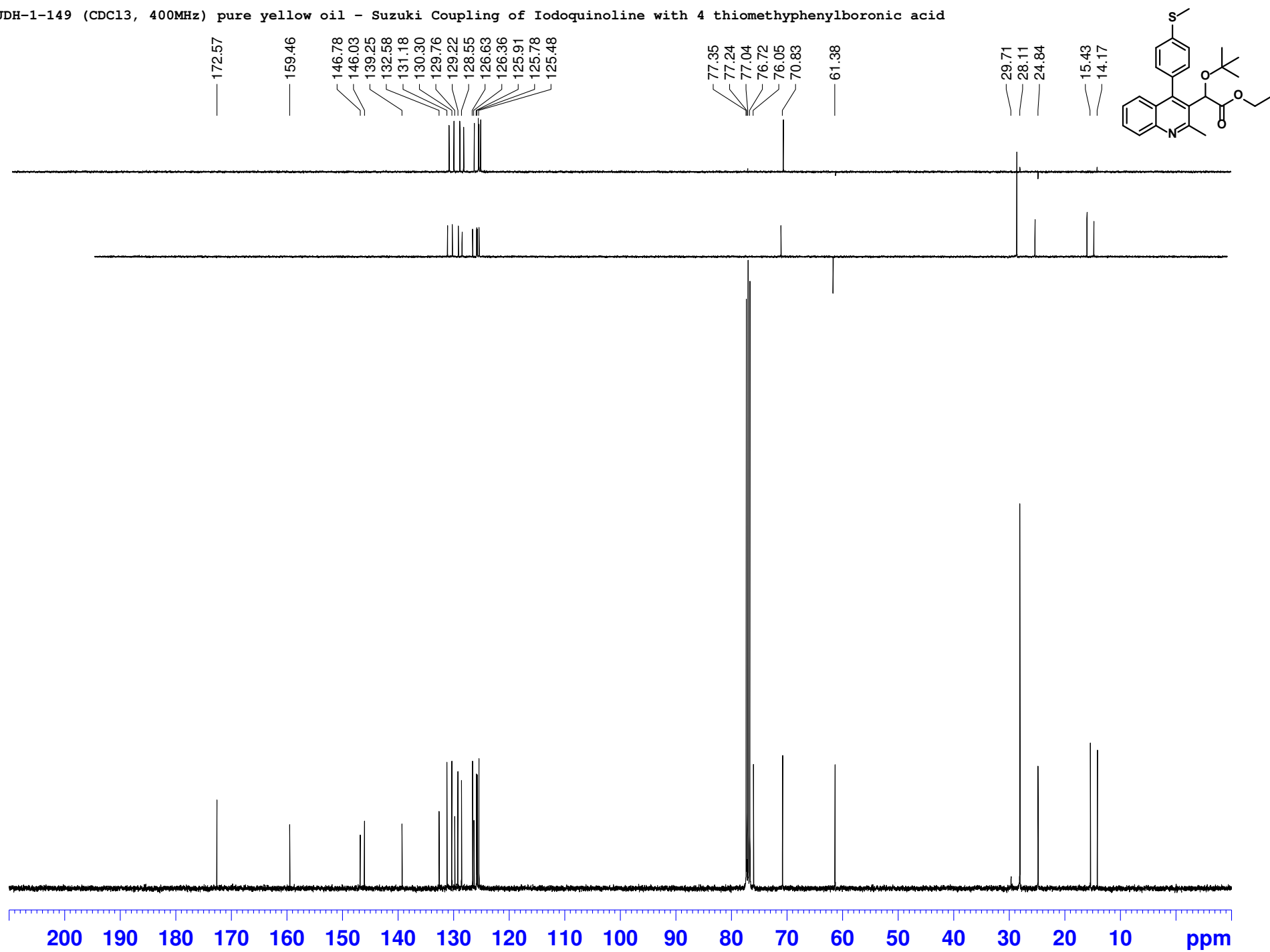


JDH-1-149 (CDC13, 400MHz) pure yellow oil - Suzuki Coupling of Iodoquinoline with 4 thiomethylphenylboronic acid

NAME JDH-1-149
EXPNO 50
PROCNO 1
Date_ 20170708
Time_ 15.48 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700071 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



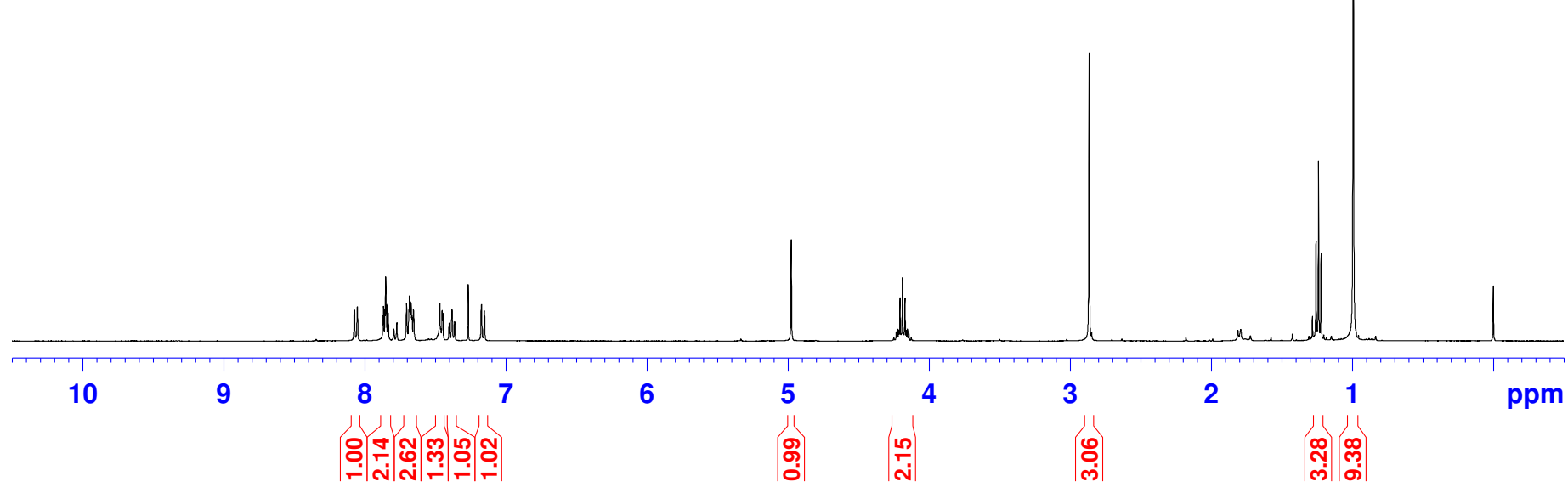
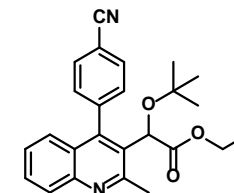
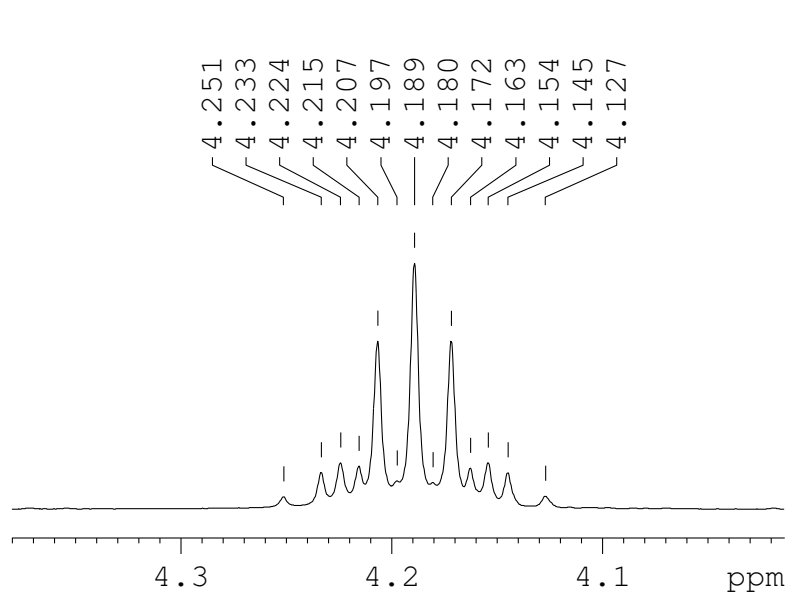
JDH-1-149 (CDCl₃, 400MHz) pure yellow oil - Suzuki Coupling of Iodoquinoline with 4 thiomethylphenylboronic acid



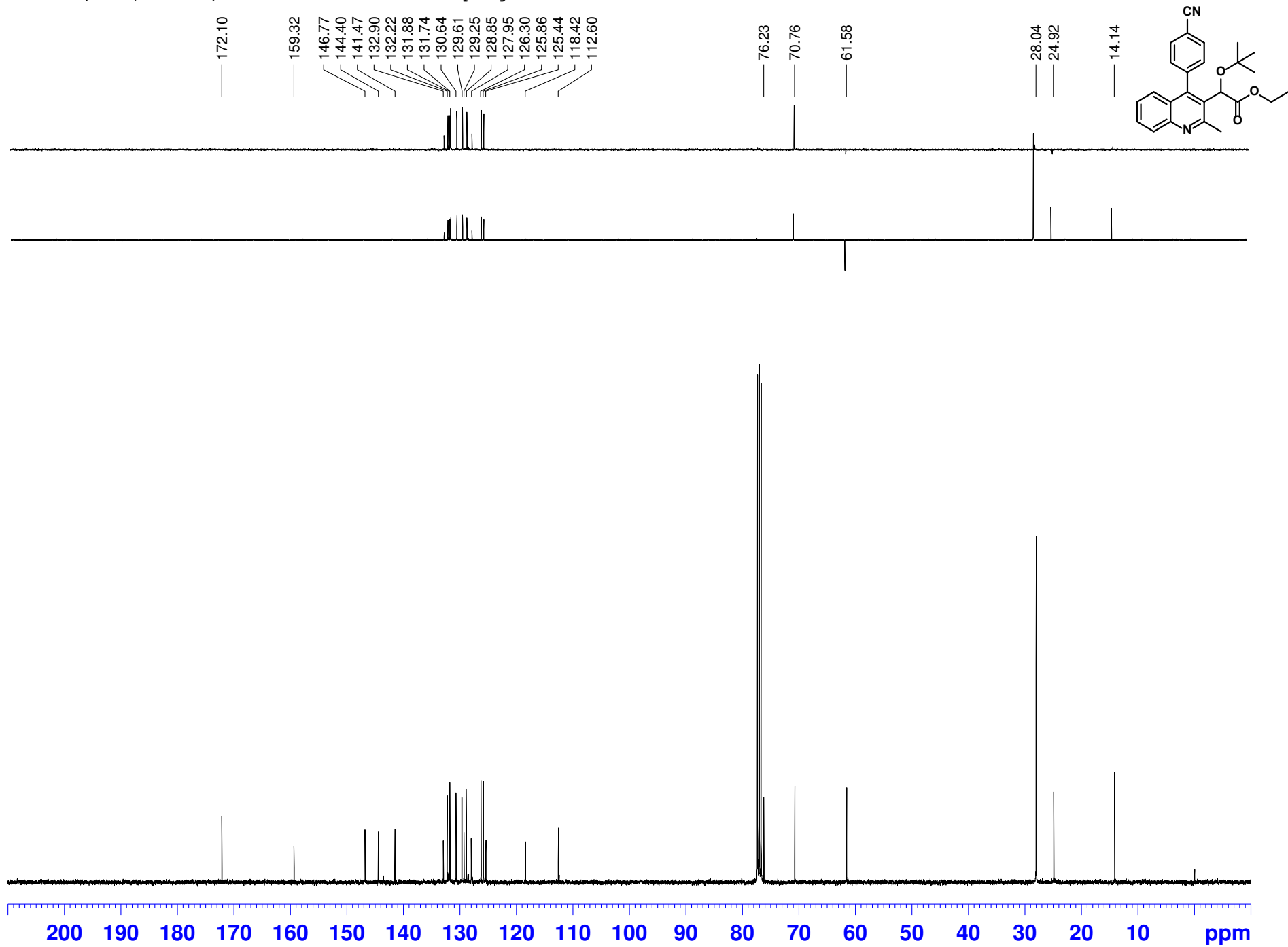
NGJ-8-078 (CDC13, 400 MHz) Pure Brown Oil - suzuki coupling of iodoquinoline with 4-cyanophenyl

```

NAME      NGJ-8-078
EXPNO     40
PROCNO    1
Date_     20171115
Time      18.42 h
INSTRUM   spect
PROBHD    Z108618_0161 (
PULPROG   zg30
TD         65536
SOLVENT   CDC13
NS         16
DS         2
SWH       8012.820 Hz
FIDRES    0.244532 Hz
AQ         4.0894966 sec
RG         144
DW         62.400 usec
DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec
TD0        1
SFO1      400.1724710 MHz
NUC1       1H
P1         9.88 usec
SI         65536
SF         400.1700061 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
```

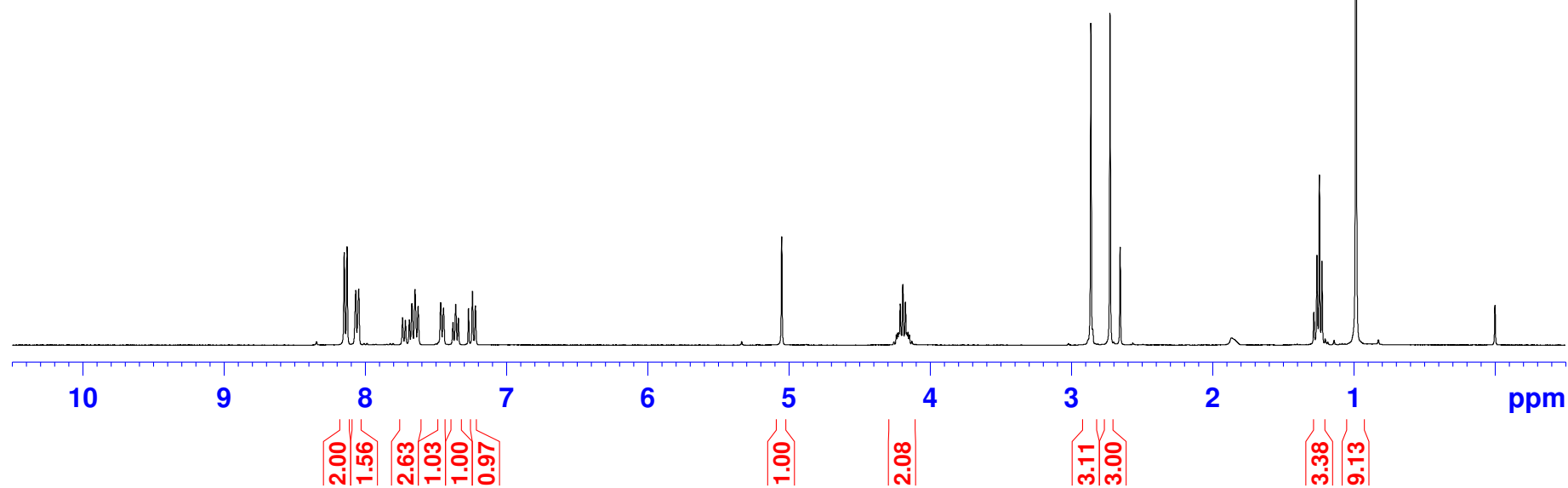
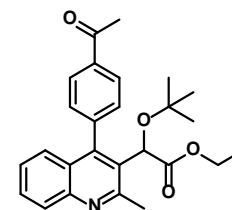
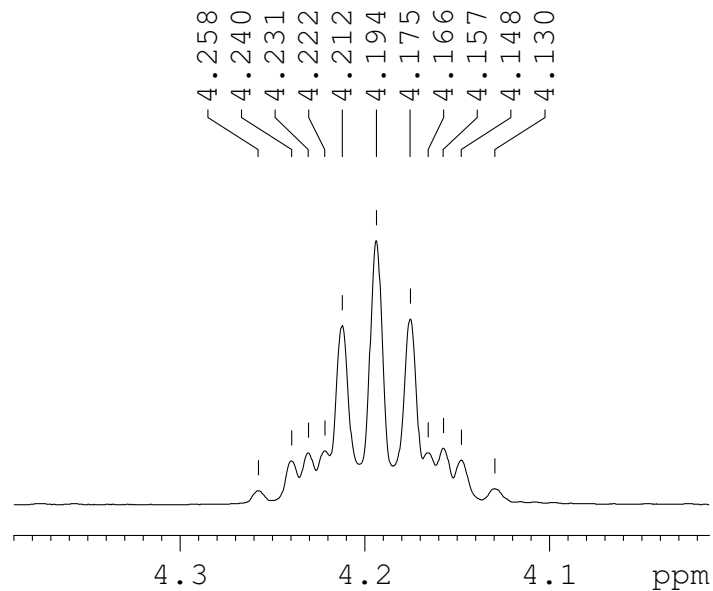


NGJ-8-078 (CDCl₃, 400 MHz) Pure Brown Oil - suzuki coupling of

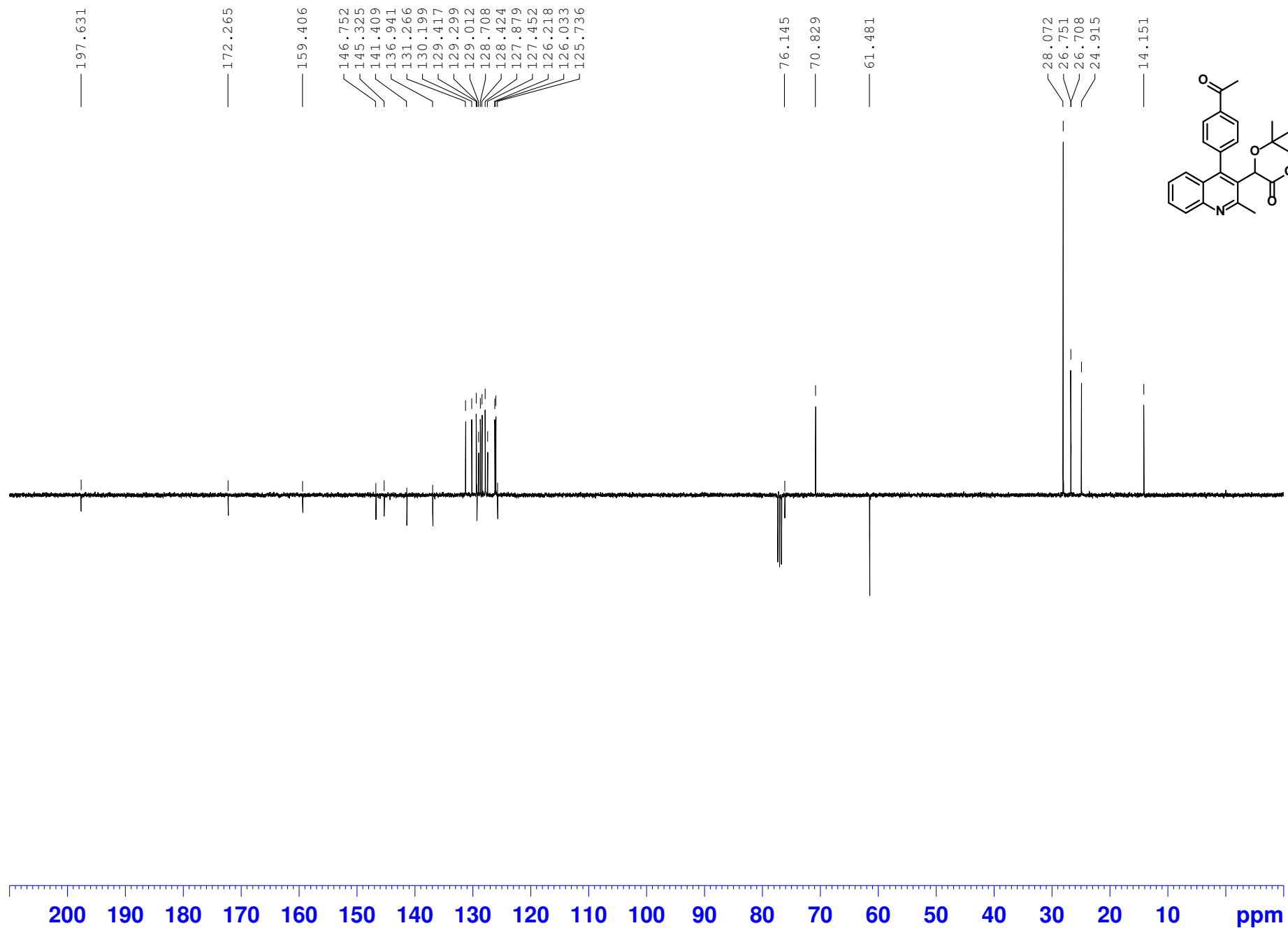


NGJ-8-072 (CDC13, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with 4-acetylph

NAME NGJ-8-072
 EXPNO 60
 PROCNO 1
 Date_ 20171127
 Time_ 19.44 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700053 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



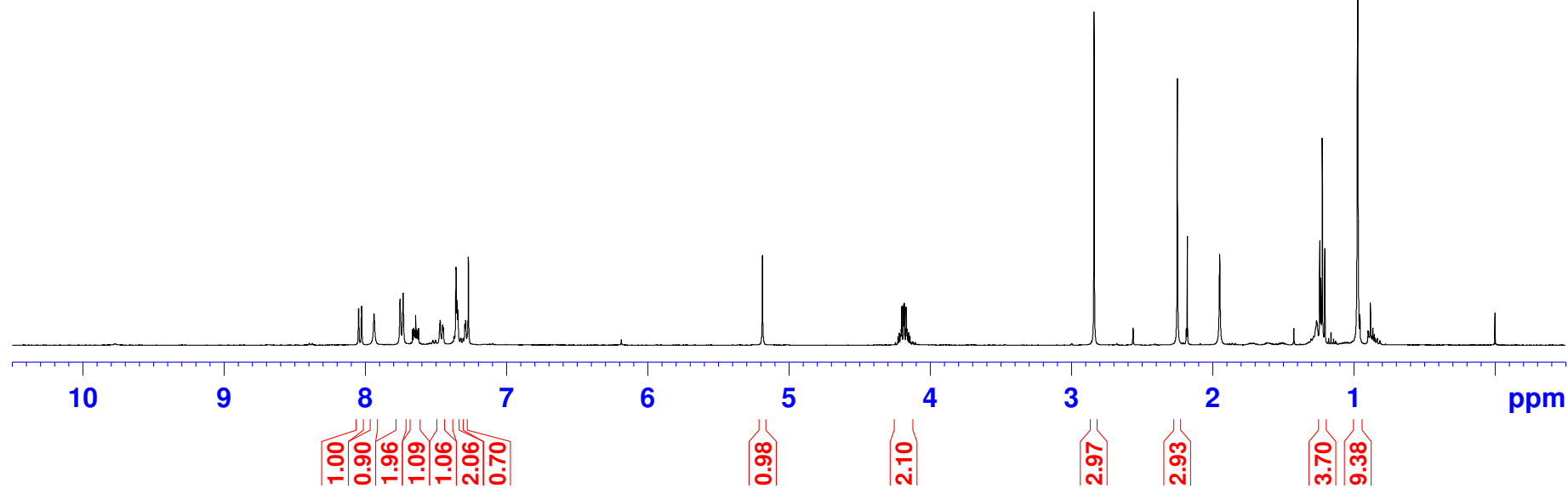
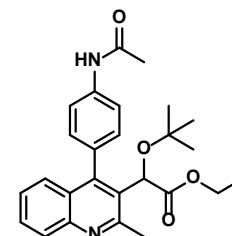
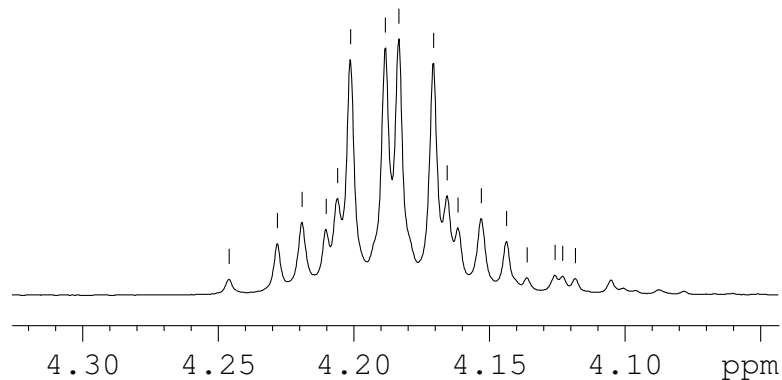
NGJ-8-072 (CDCl₃, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with 4-acetylphenylboro



NGJ-8-082 (CDC13, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with 4-acetamid

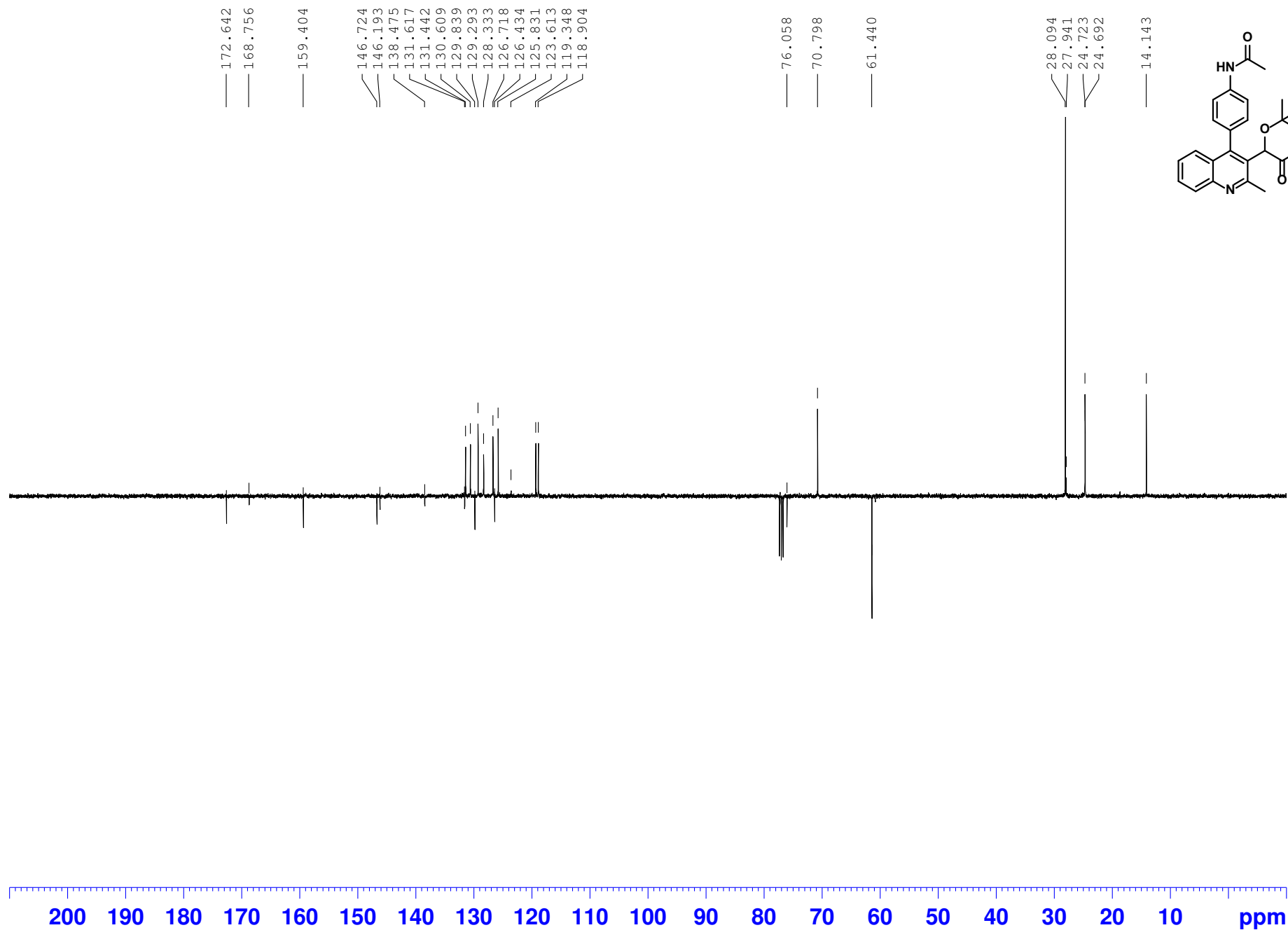
NAME NGJ-8-082
 EXPNO 20
 PROCNO 1
 Date_ 20171012
 Time_ 10.35 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 297.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700054 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

4.246
 4.228
 4.219
 4.210
 4.206
 4.201
 4.188
 4.183
 4.171
 4.166
 4.162
 4.153
 4.144
 4.136
 4.126
 4.123
 4.118



NGJ-8-082 (CDC13, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with 4-acetamido phenyl

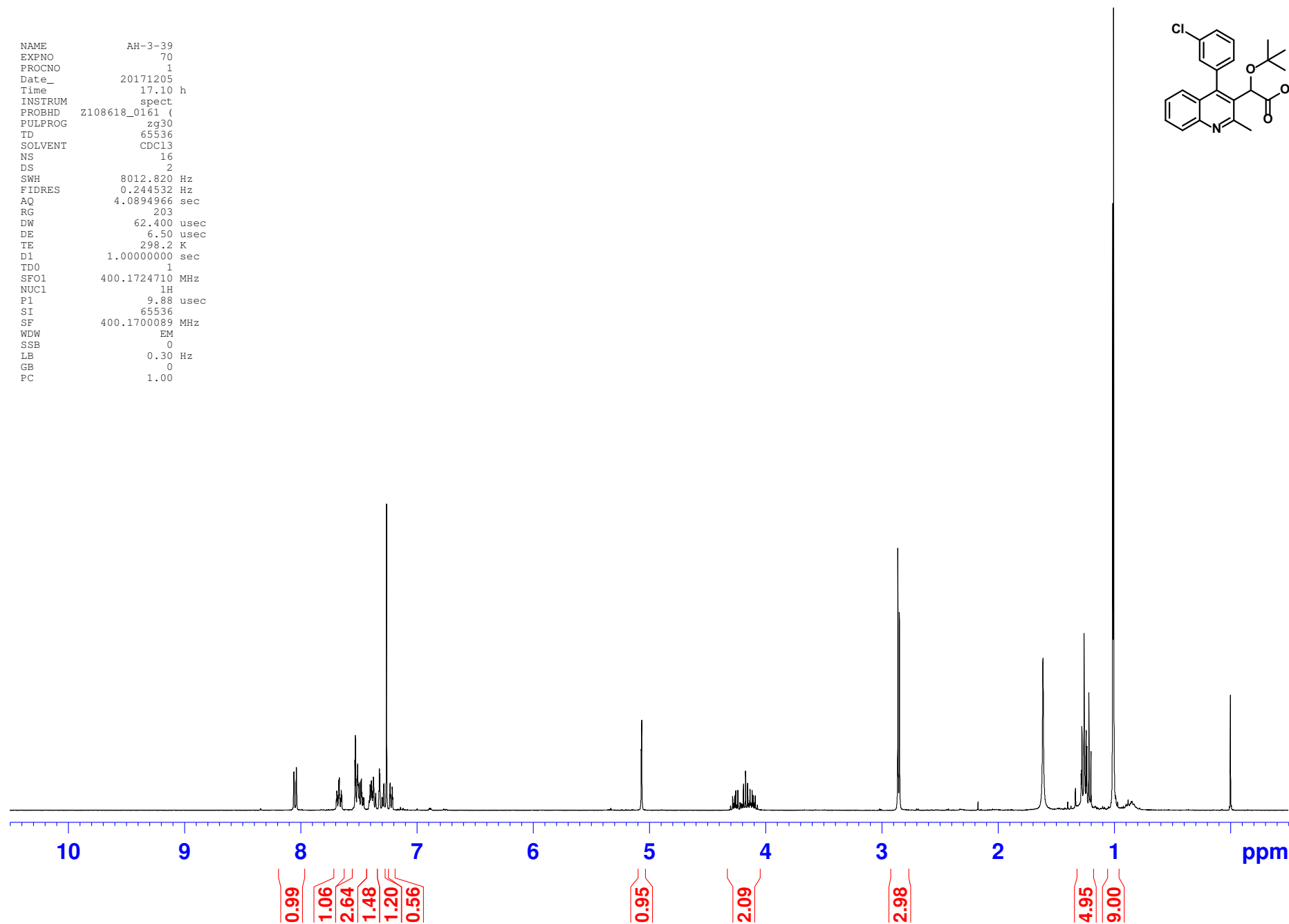
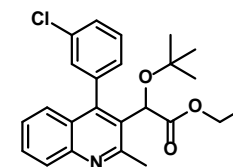
MISSISS



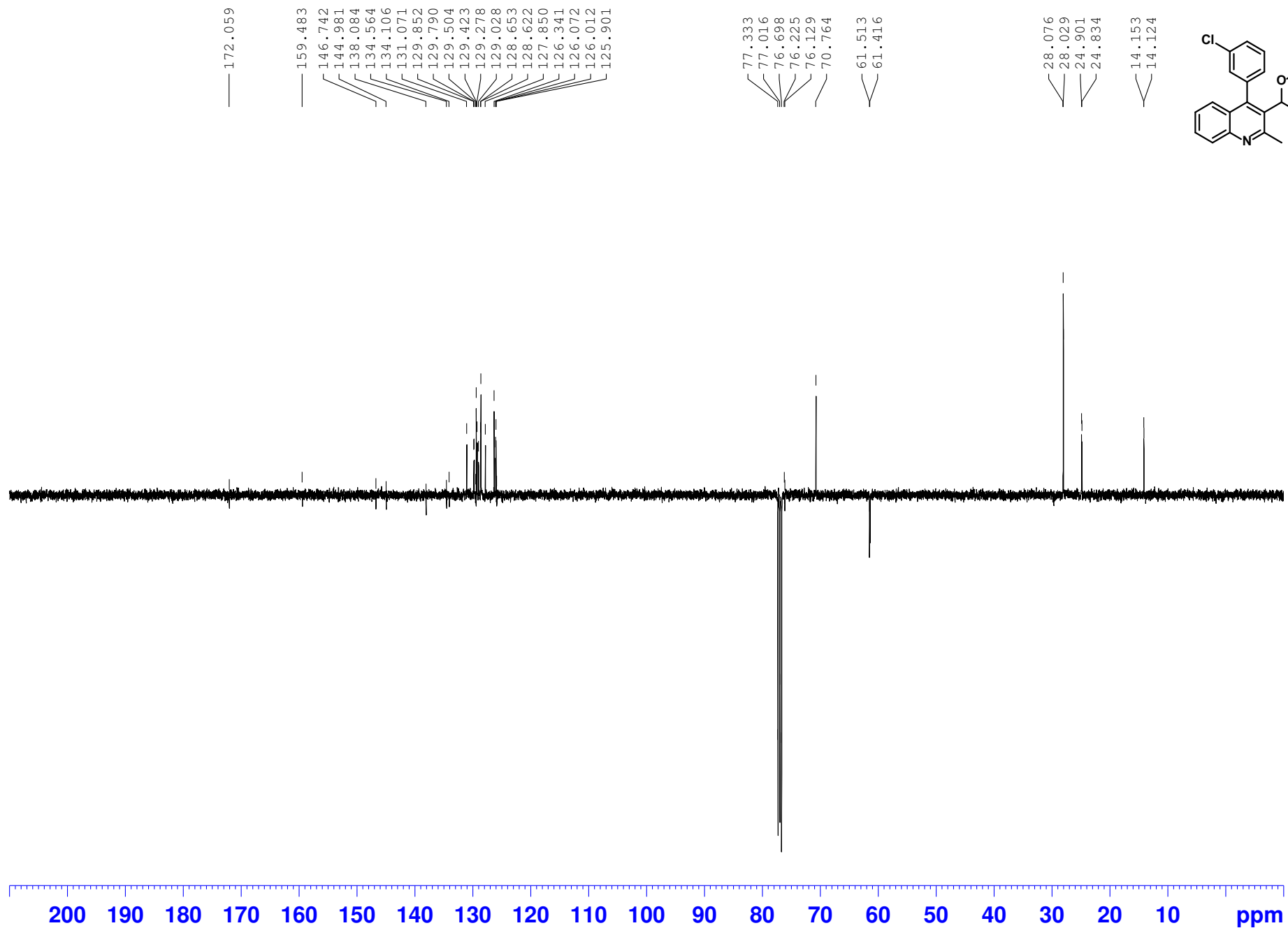
AH-3-39 Characterization

MISSISS

NAME AH-3-39
EXPNO 70
PROCNO 1
Date_ 20171205
Time 17.10 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

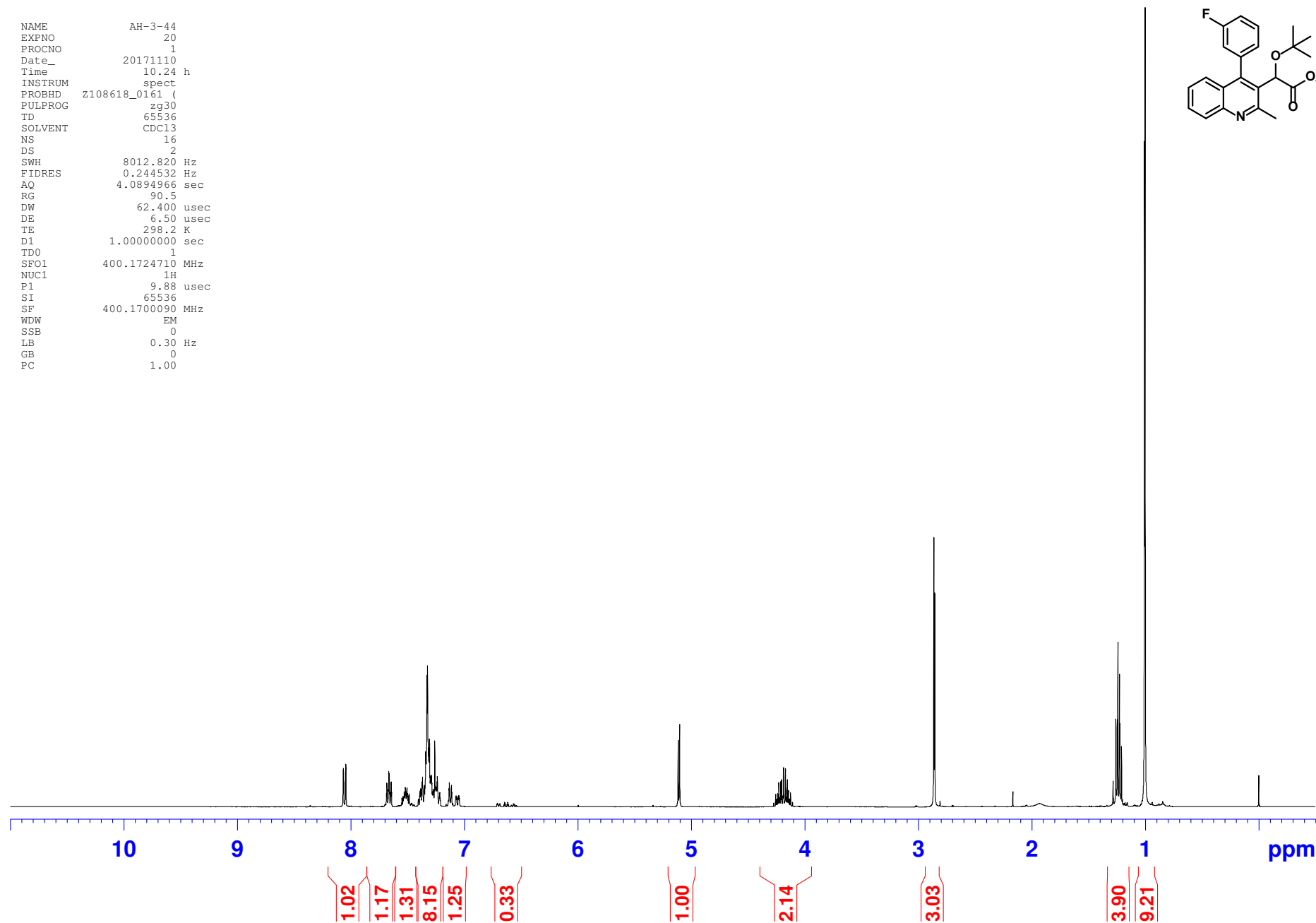
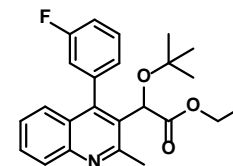


AH-3-39 Characterization



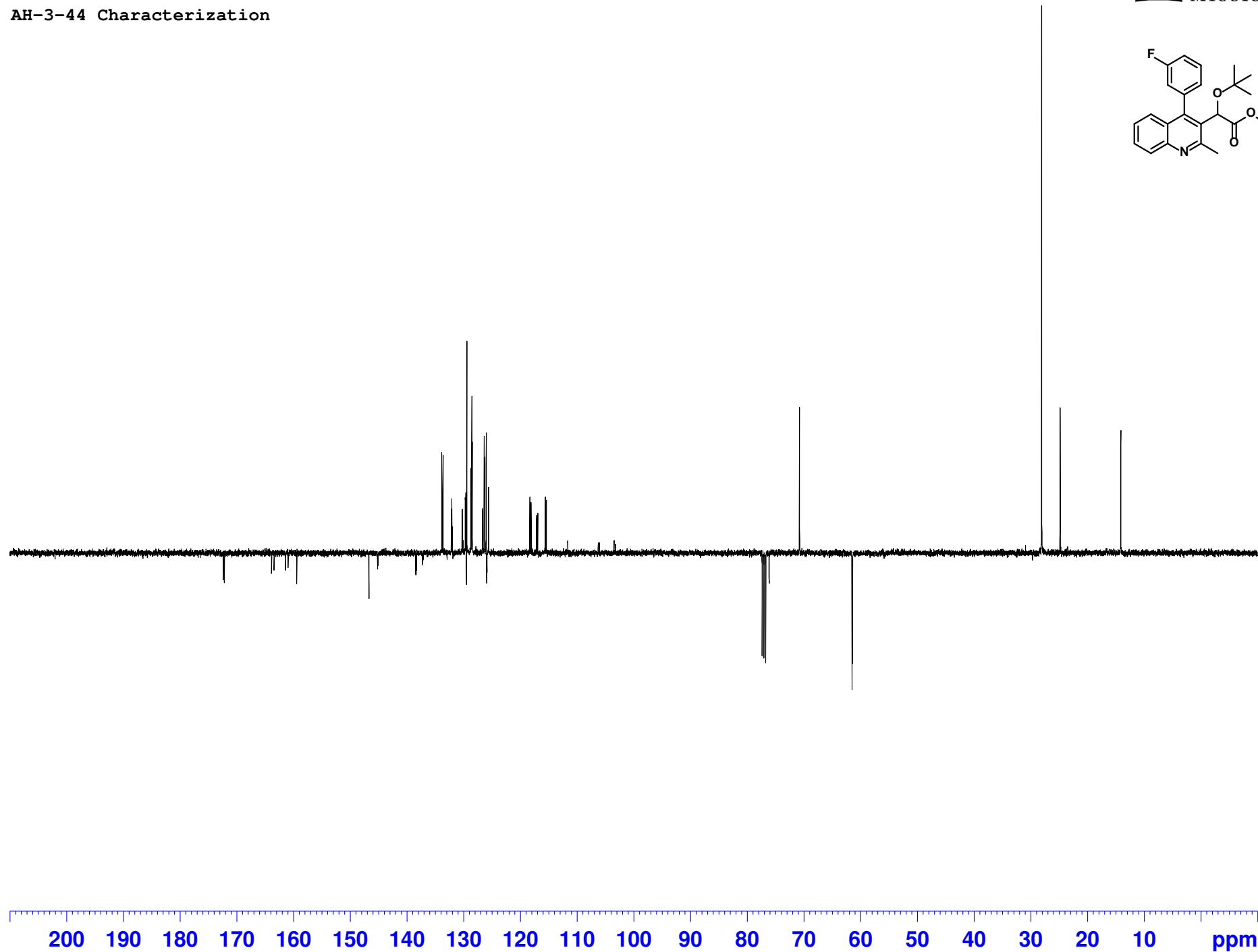
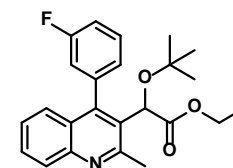
```

NAME      AH-3-44
EXPNO     20
PROCNO    1
Date_     20171110
Time      10.24 h
INSTRUM   spect
PROBHD    z108618_0161 (
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.244532 Hz
AQ        4.0894966 sec
RG        90.5
DW        62.400 usec
DE        6.50 usec
TE        298.2 K
D1        1.00000000 sec
TDO       1
SFO1      400.1724710 MHz
NUC1      1H
P1        9.88 usec
SI        65536
SF        400.1700090 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```



AH-3-44 Characterization

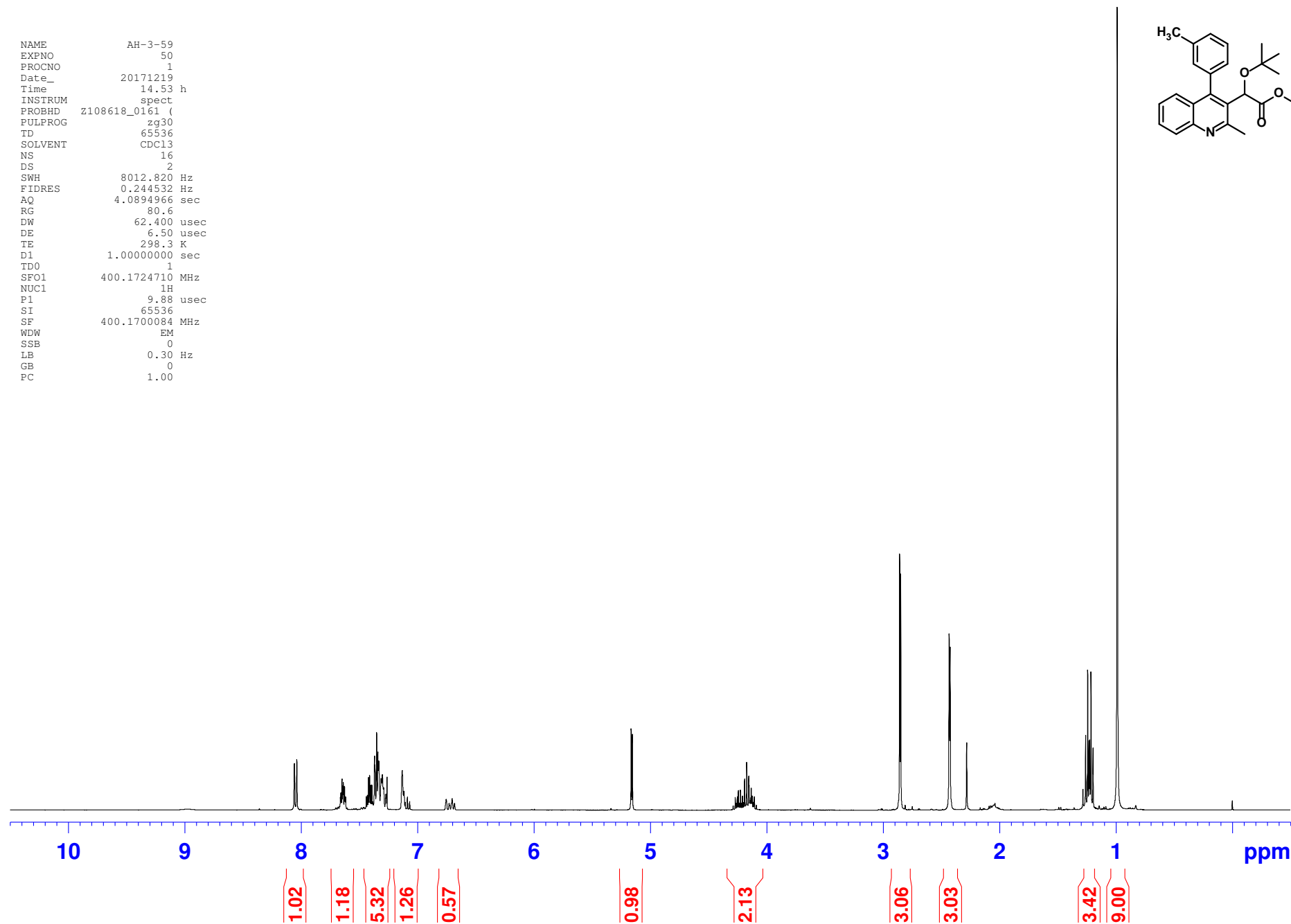
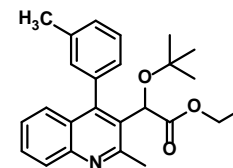
MISSISS



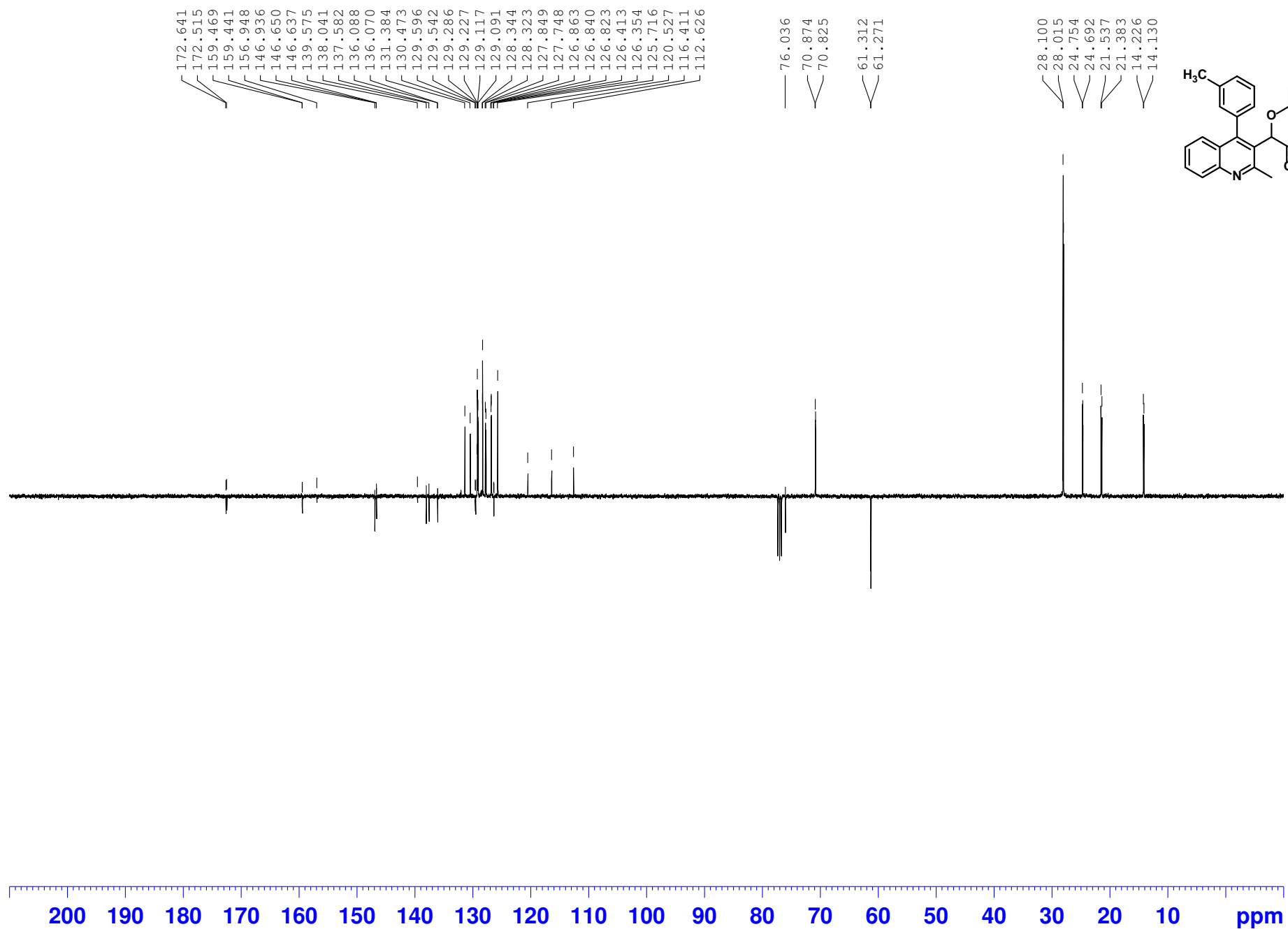
AH-3-59 Characterization

MISSISS

NAME AH-3-59
EXPNO 50
PROCNO 1
Date_ 20171219
Time 14.53 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 80.6
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



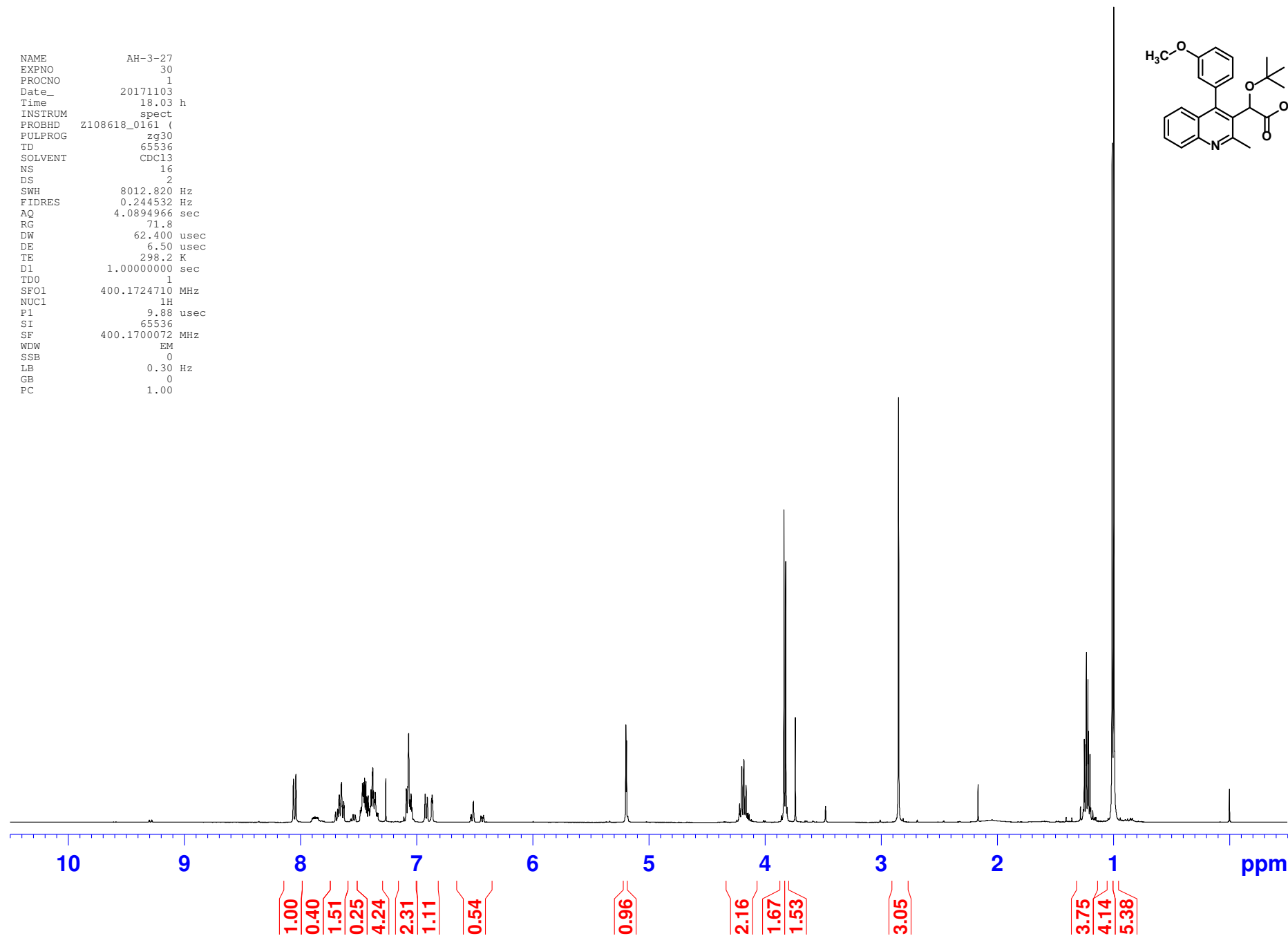
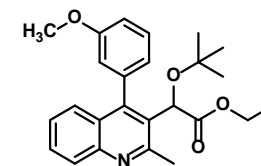
AH-3-59 Characterization

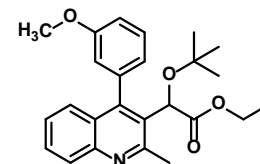
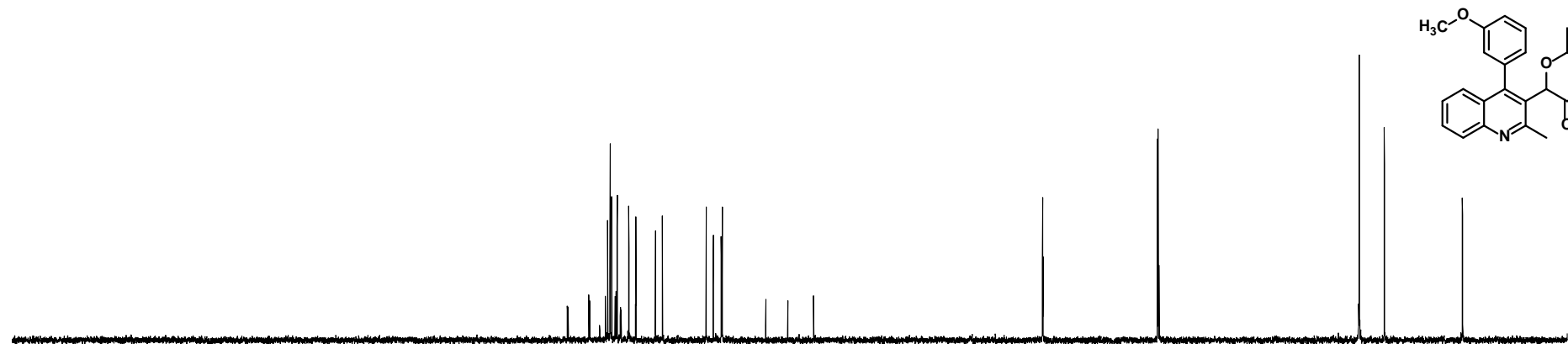
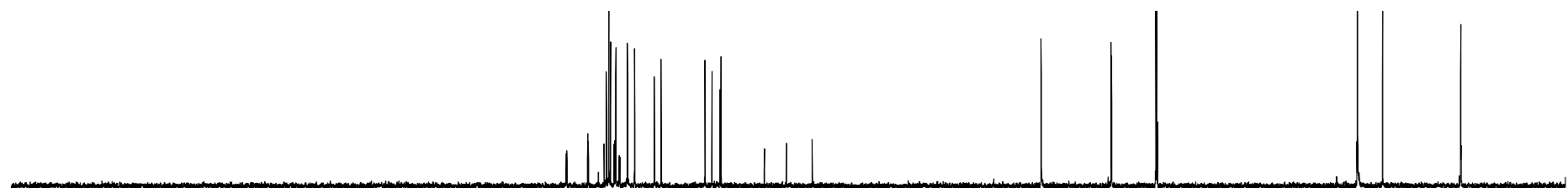


AH-3-27 Characterization

MISSISS

NAME AH-3-27
EXPNO 30
PROCNO 1
Date_ 20171103
Time 18.03 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

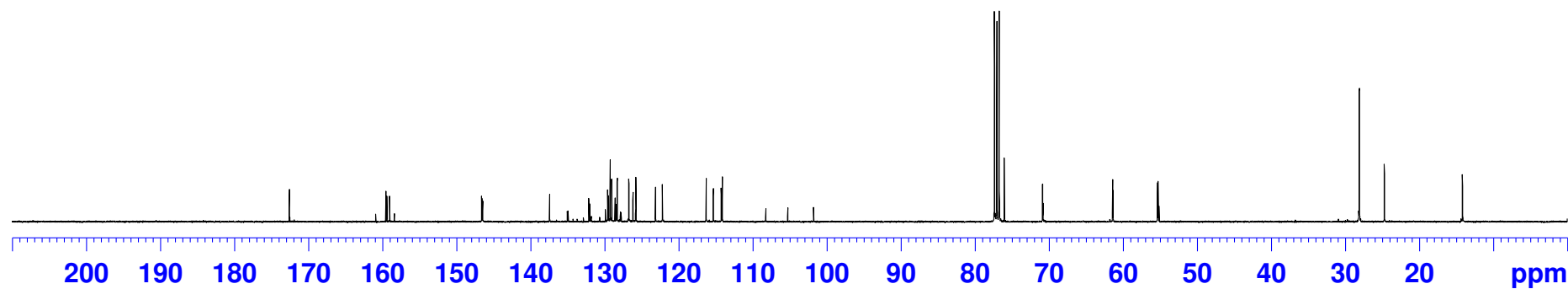




- 172.62
- 172.57
- 159.57
- 159.46
- 159.43
- 159.06
- 146.65
- 146.64
- 146.58
- 146.50
- 137.46
- 137.44
- 132.16
- 132.06
- 129.62
- 129.54
- 129.51
- 129.29
- 129.06
- 128.60
- 128.48
- 128.36
- 128.33
- 126.78
- 126.75
- 126.21
- 125.83
- 125.80
- 123.15
- 122.23
- 116.31
- 115.36
- 114.28
- 114.13

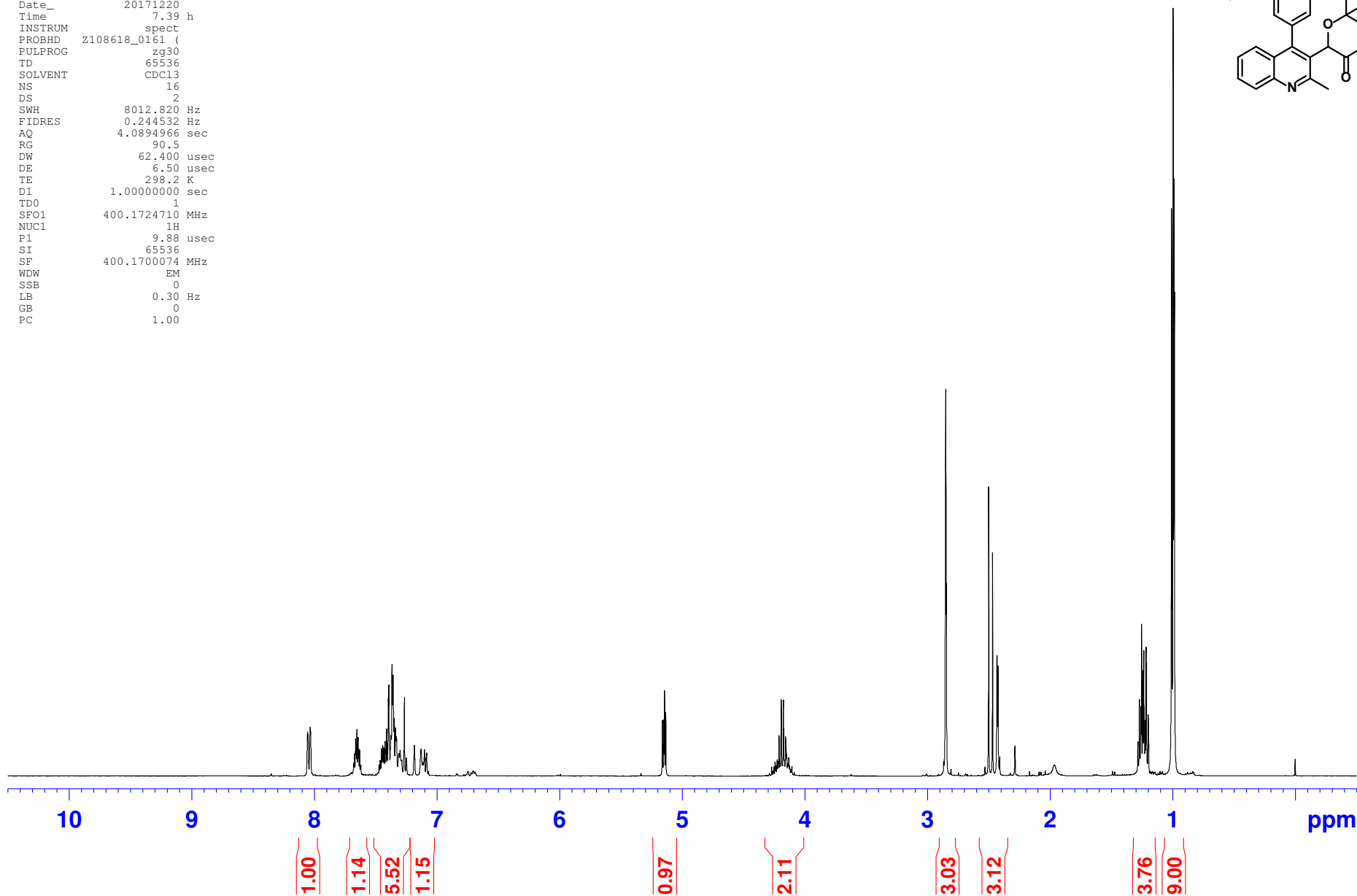
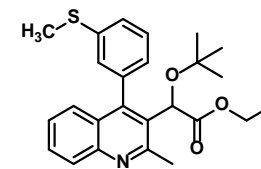
- 76.07
- 70.89
- 70.83
- 61.42
- 61.35
- 55.35
- 55.27

- 28.12
- 28.10
- 24.73
- 24.72
- 14.18
- 14.13

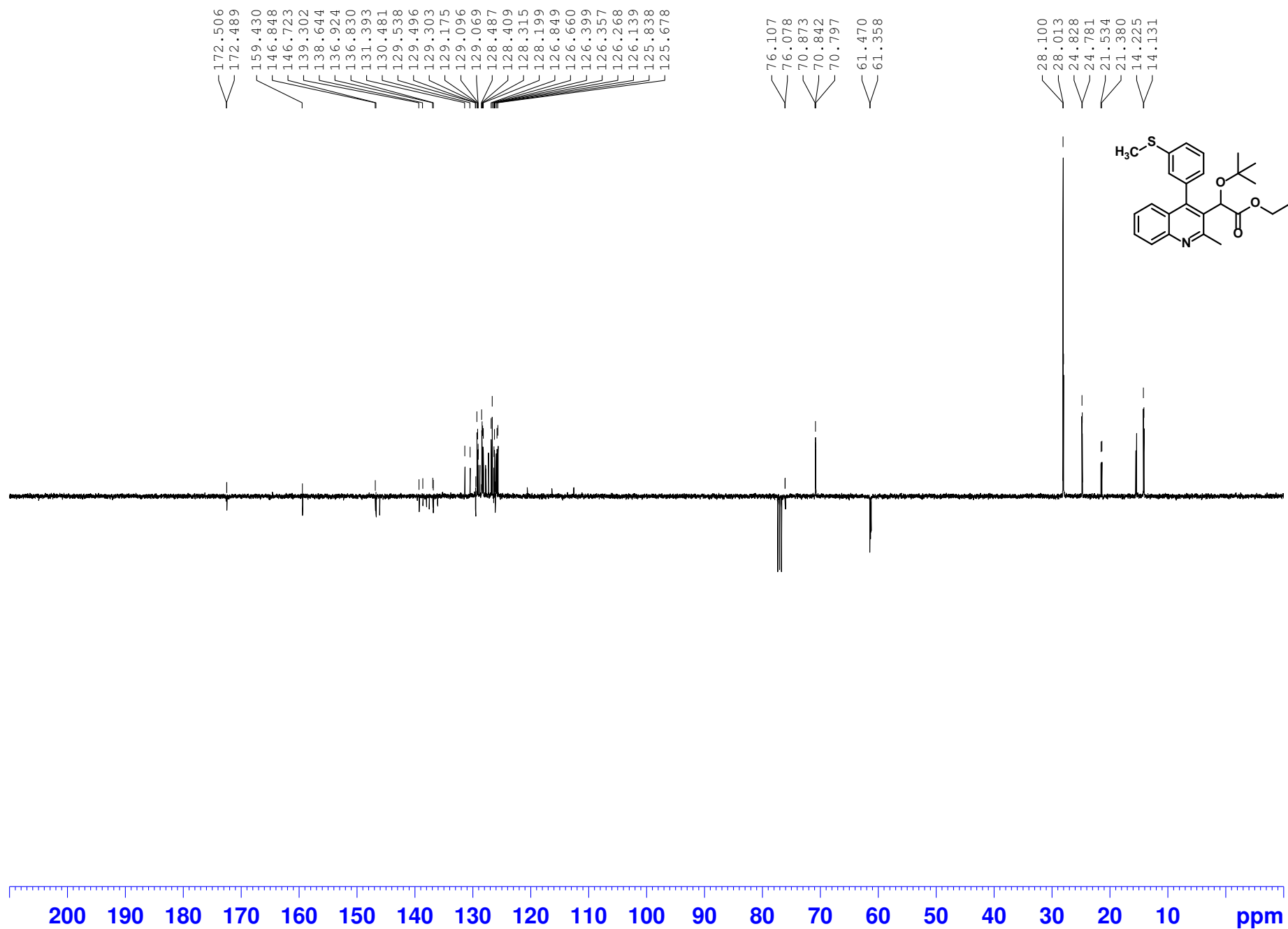


AH-3-60 Characterization

NAME AH-3-60
EXPNO 30
PROCNO 1
Date_ 20171220
Time 7.39 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 90.5
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



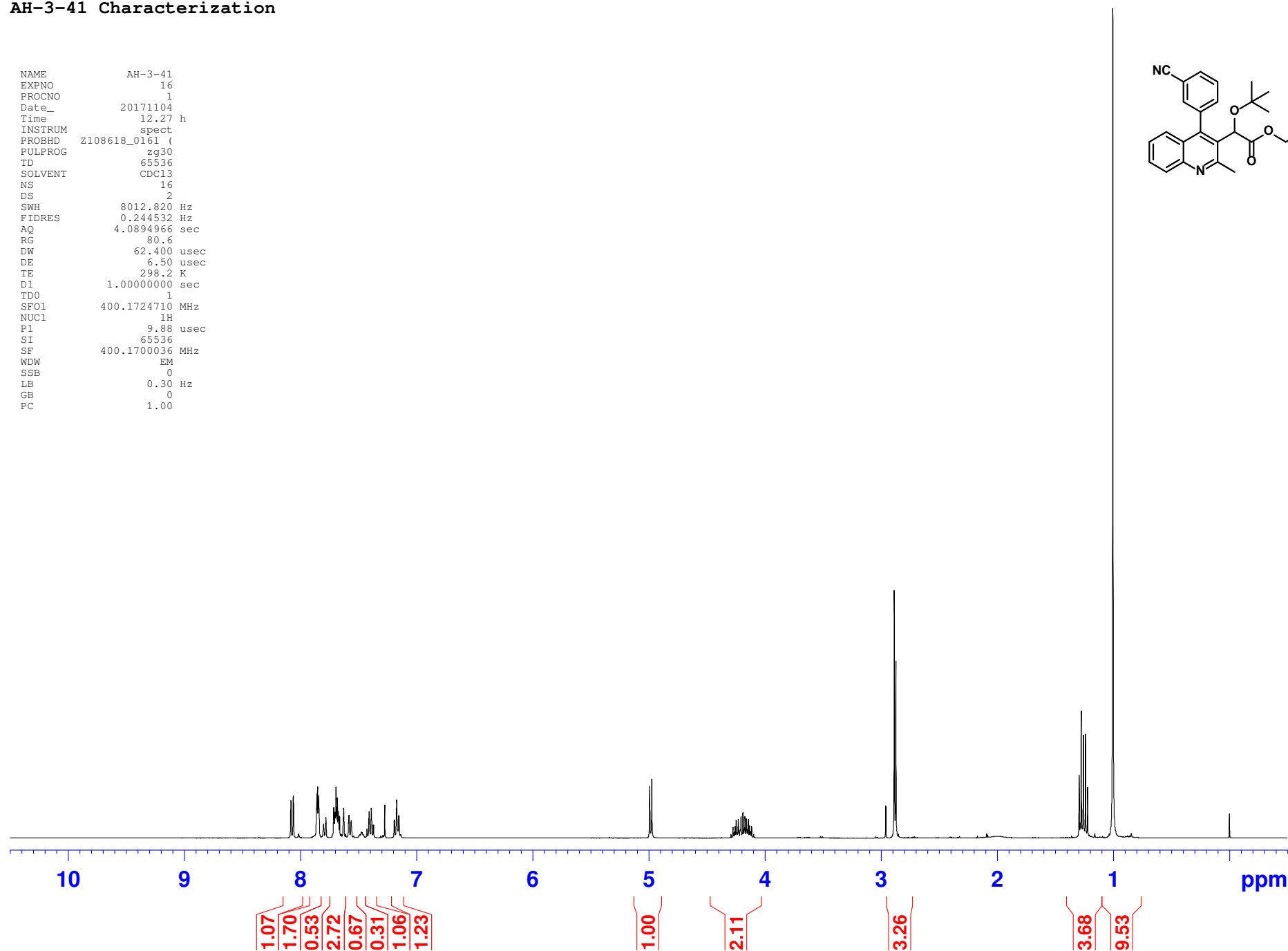
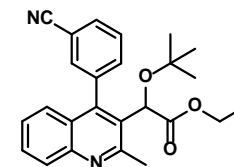
AH-3-60 Characterization



AH-3-41 Characterization

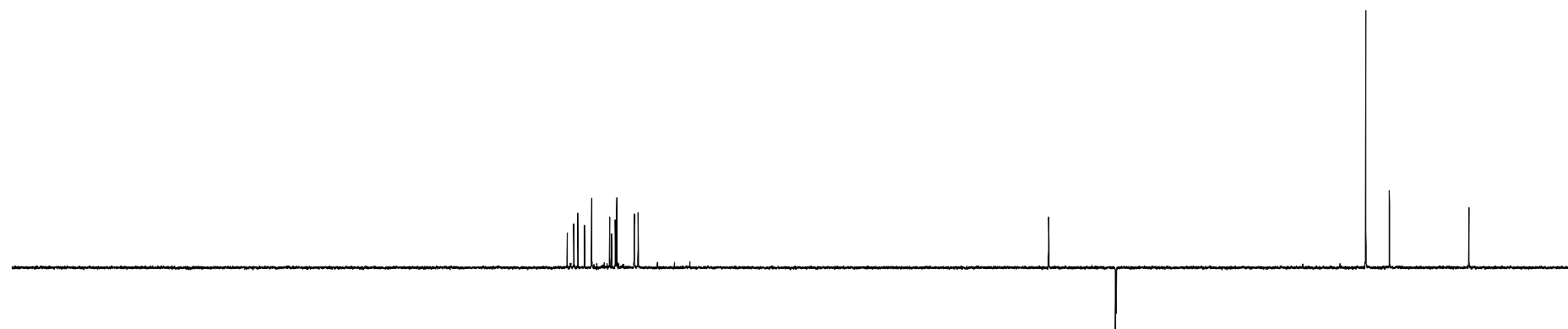
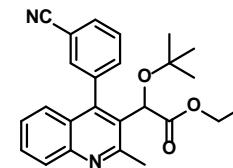
MISSISS

NAME AH-3-41
EXPNO 16
PROCNO 1
Date_ 20171104
Time 12.27 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 80.6
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700036 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-41 Characterization

MISSISS



172.14
171.79
159.34
159.26
146.73
146.72
144.04
143.98
137.81
137.78
135.40
134.52
133.98
133.08
132.12
129.70
129.68
129.66
129.58
129.43
128.94
128.75
126.42
126.36
125.88
125.85
125.76
125.69
118.28
118.19
112.91
112.44

76.26
76.22
70.70
70.66
61.69
61.58

28.03
28.01
24.85
24.81

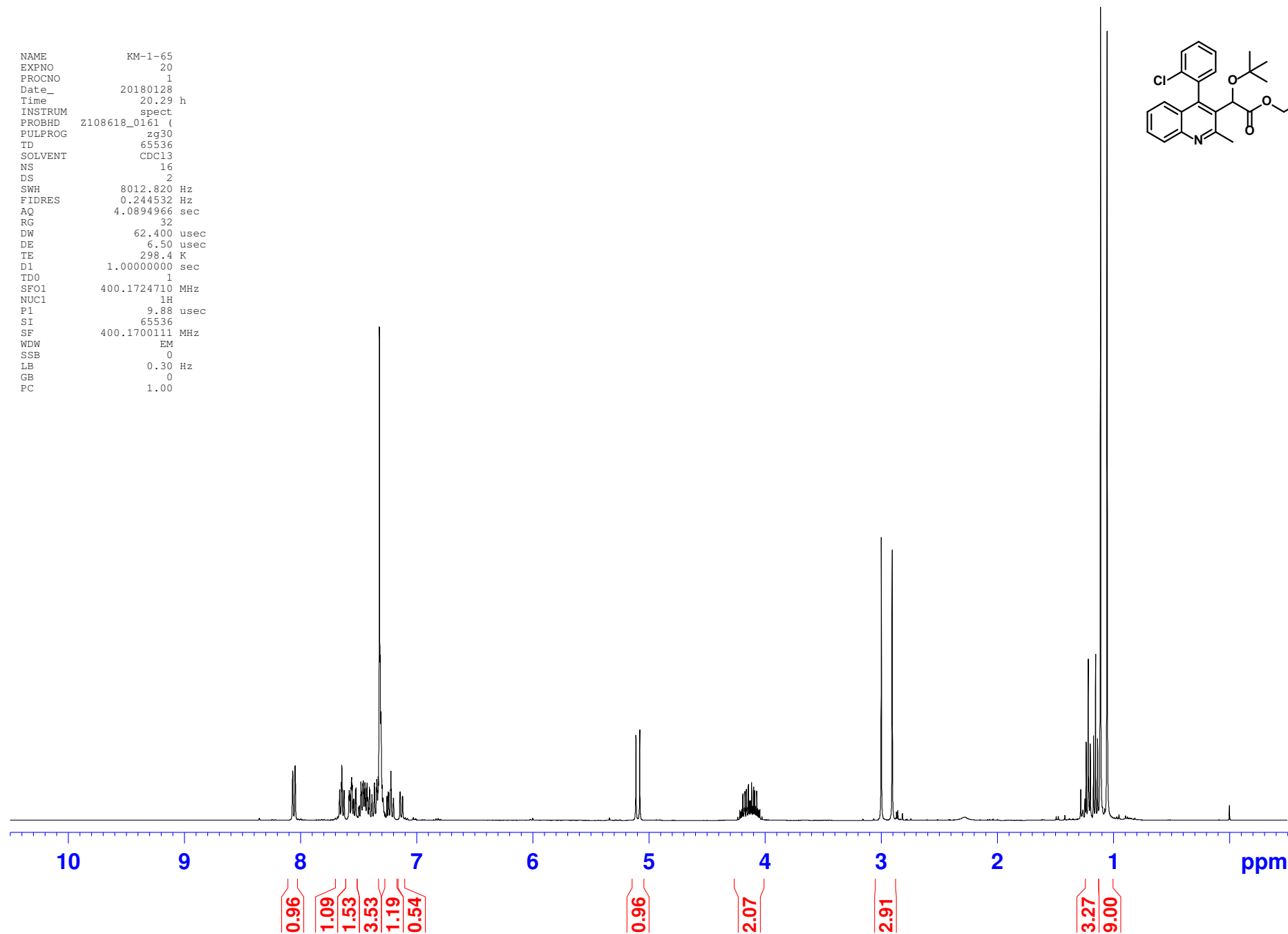
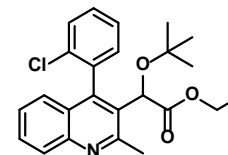
14.15
14.14

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

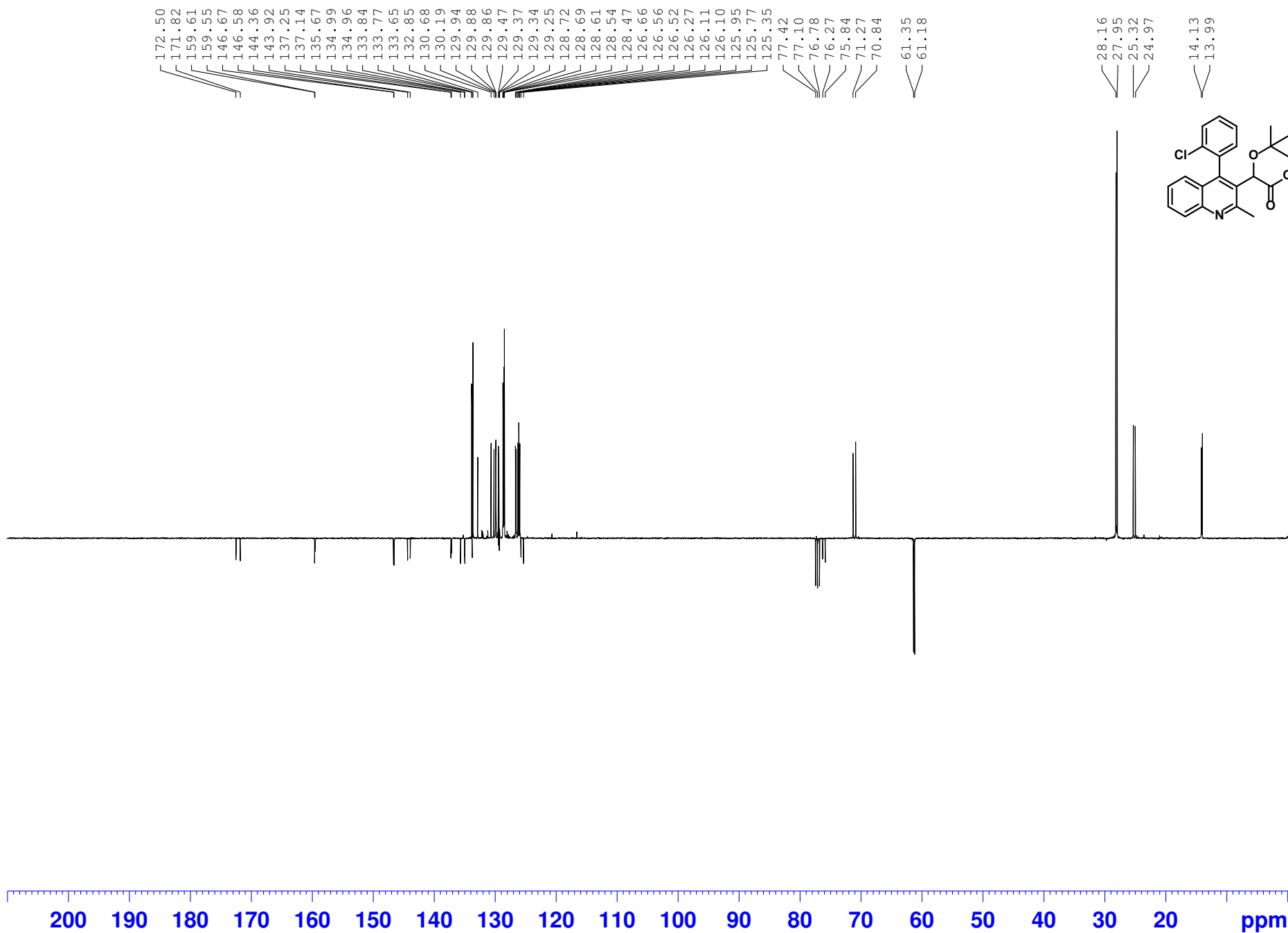
KM-1-65B1

MISSISS

NAME KM-1-65
EXPNO 20
PROCNO 1
Date_ 20180128
Time 20.29 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

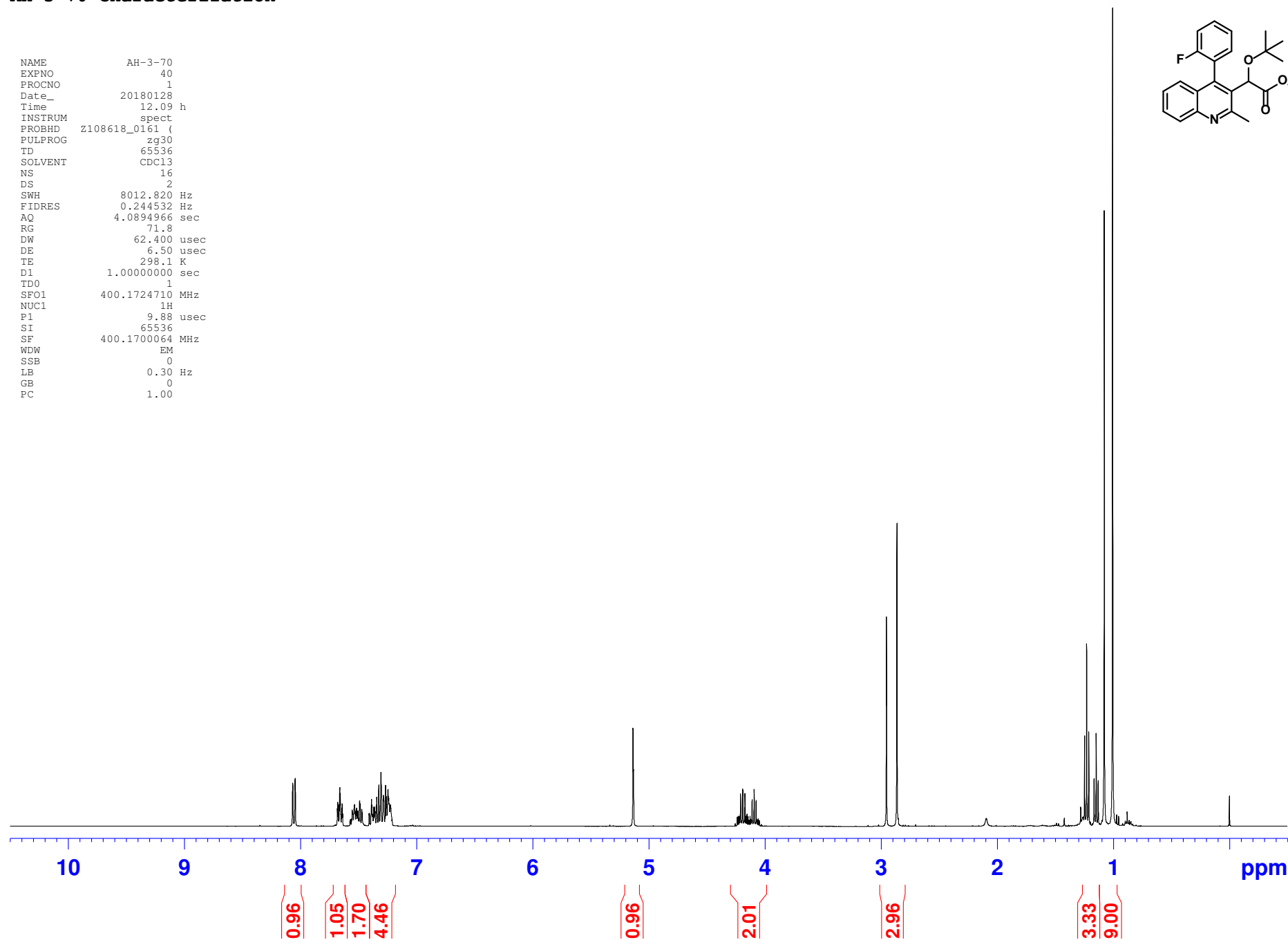
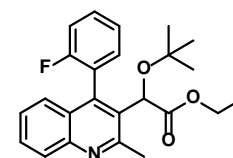


KM-1-65 Characterization

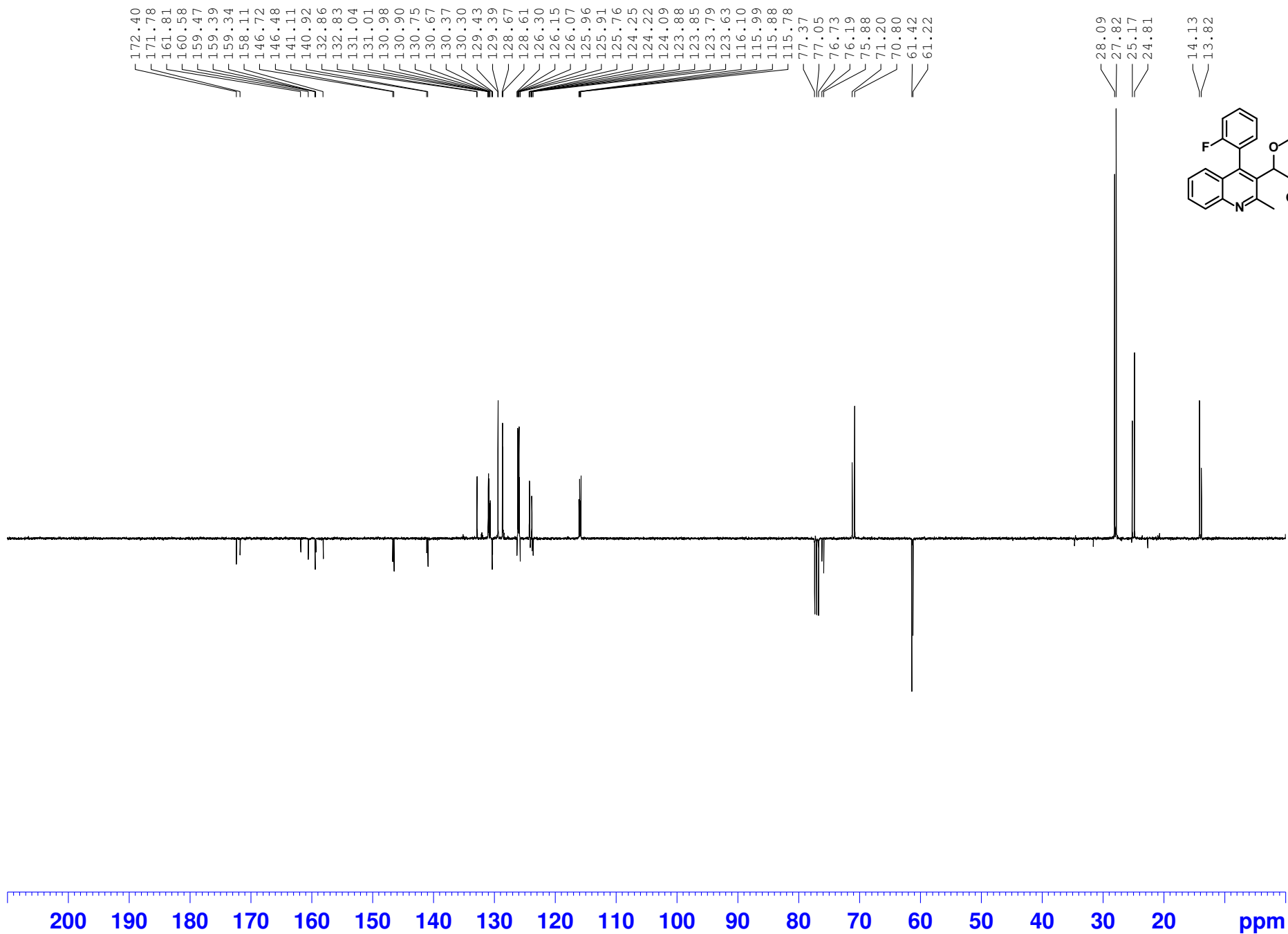


AH-3-70 Characterization

NAME AH-3-70
EXPNO 40
PROCNO 1
Date_ 20180128
Time 12.09 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700064 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

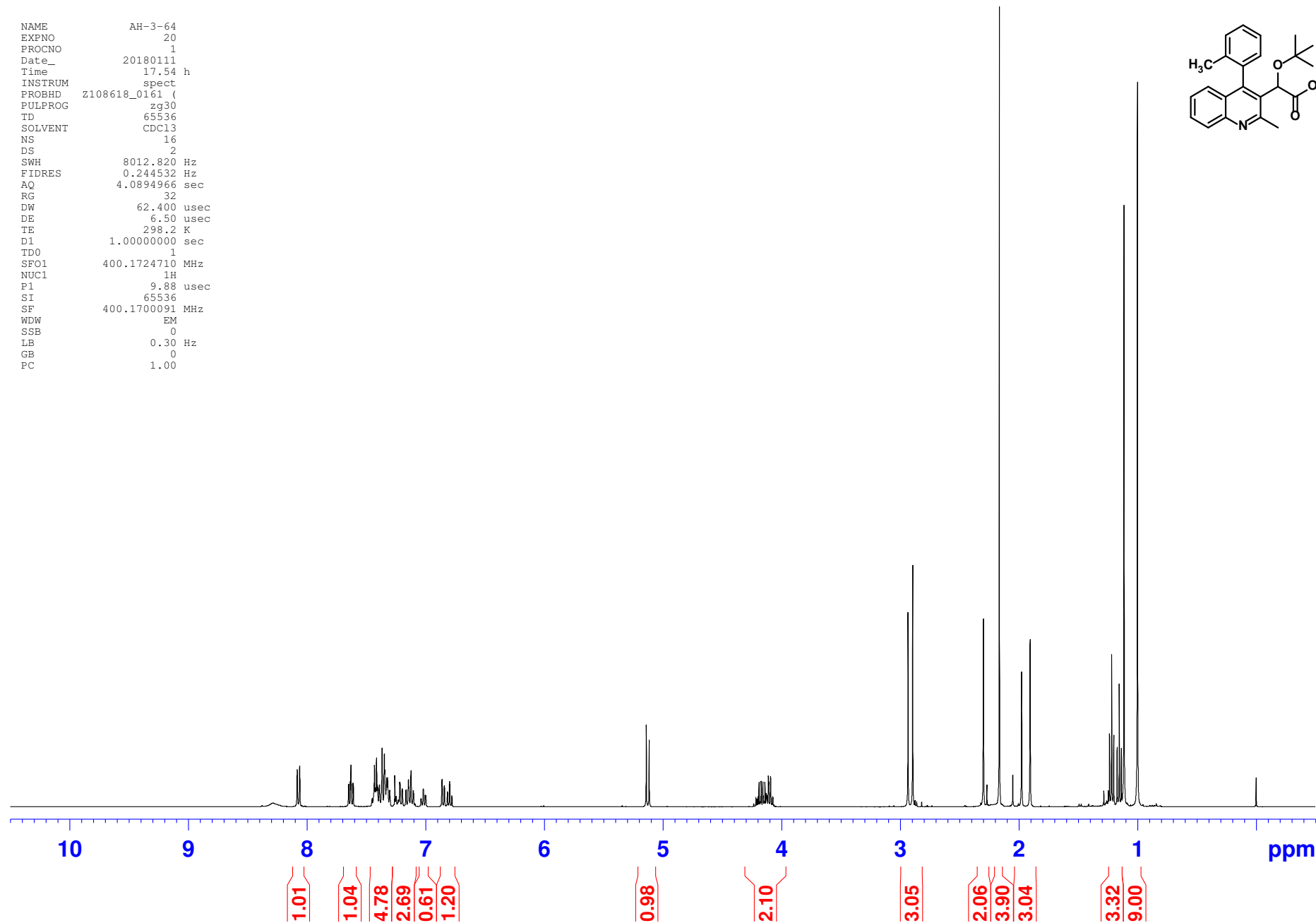
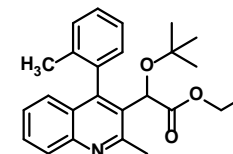


AH-3-70 Characterization

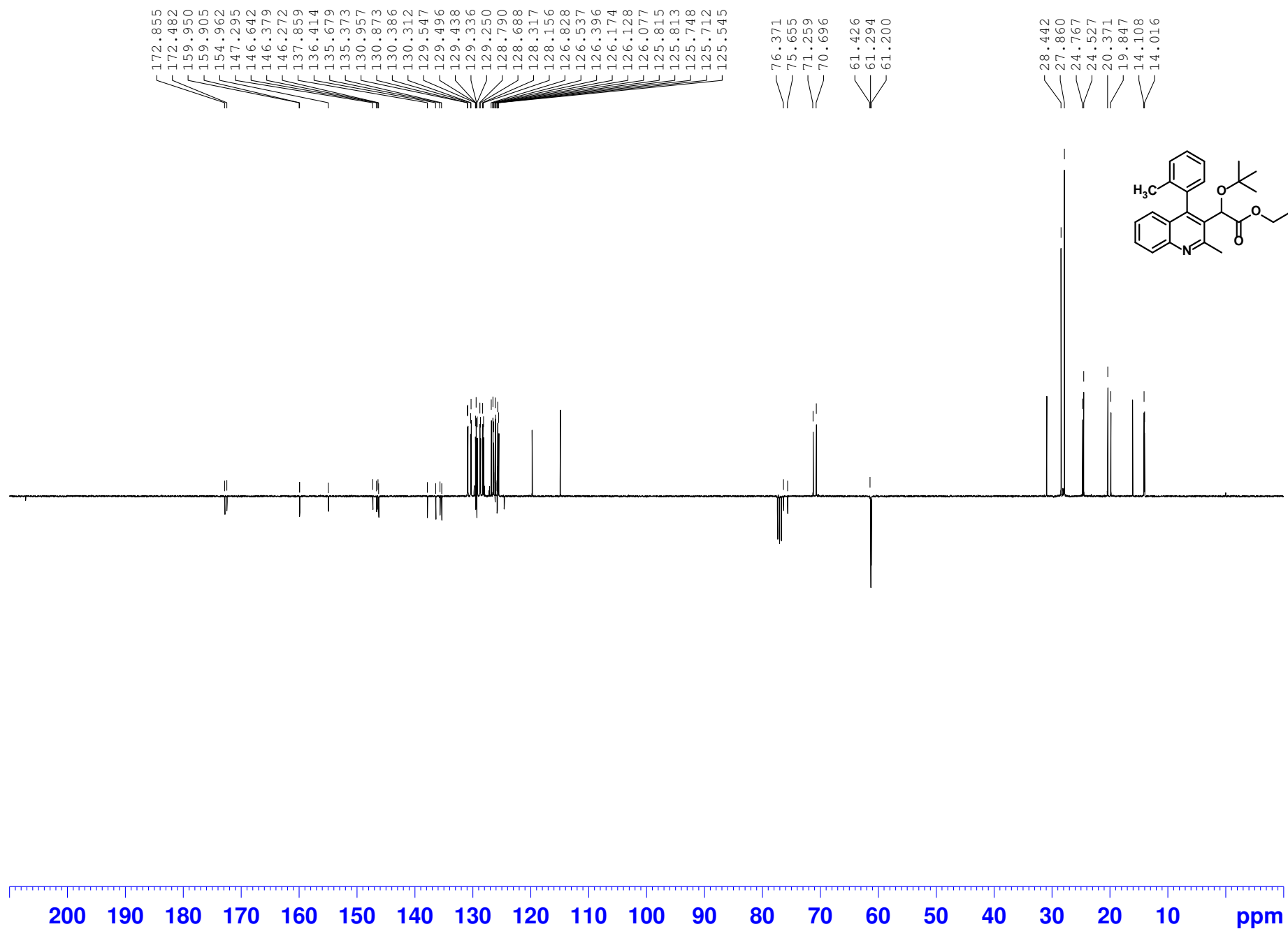


AH-3-64B Characterization

NAME AH-3-64
EXPNO 20
PROCNO 1
Date_ 20180111
Time 17.54 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



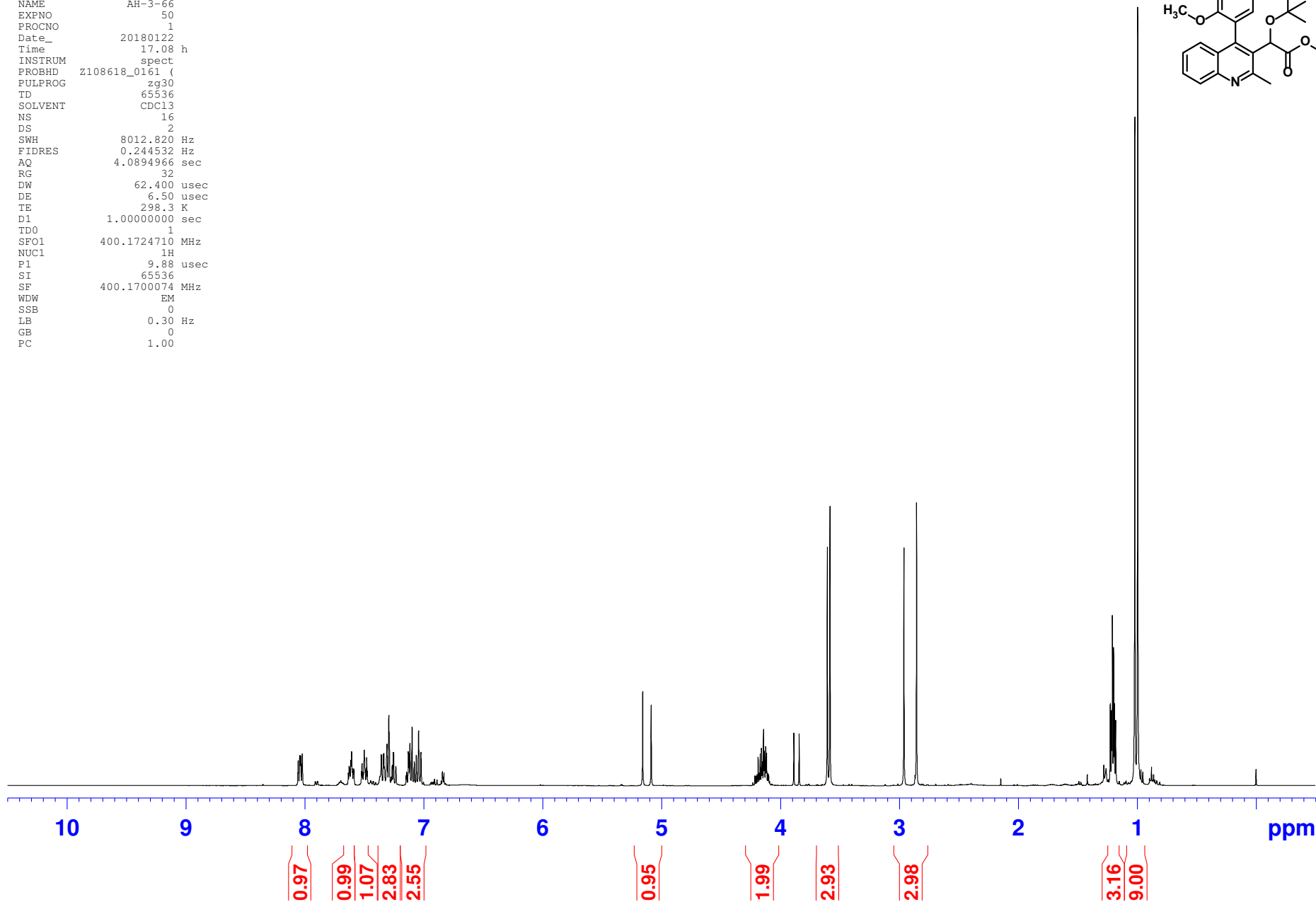
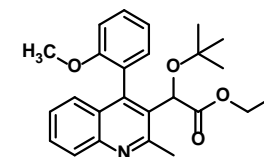
AH-3-64B Characterization



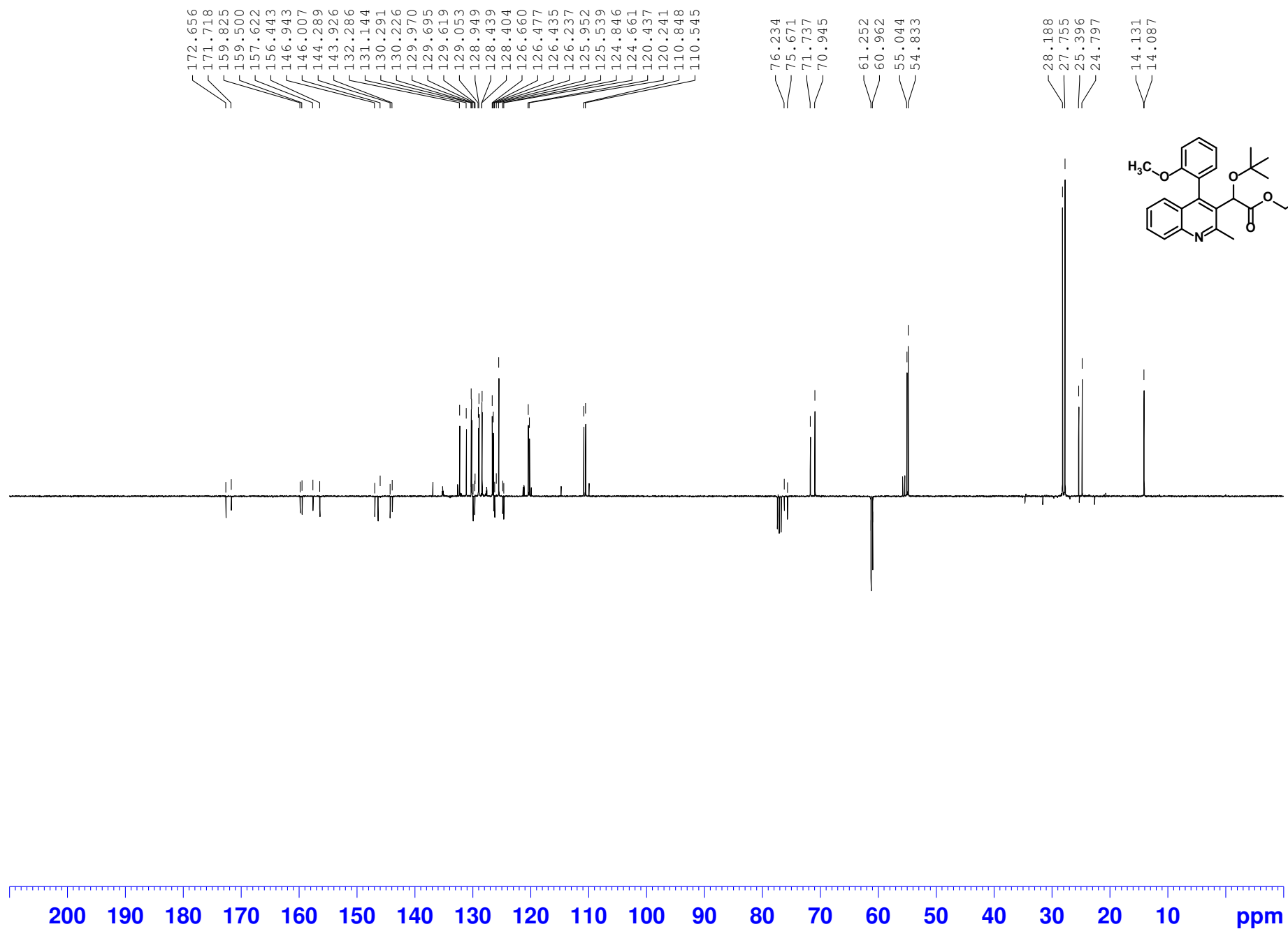
AH-3-66 characterizaion (400MHz, CDC13)

MISSISS

NAME AH-3-66
EXPNO 50
PROCNO 1
Date_ 20180122
Time 17.08 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 32
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



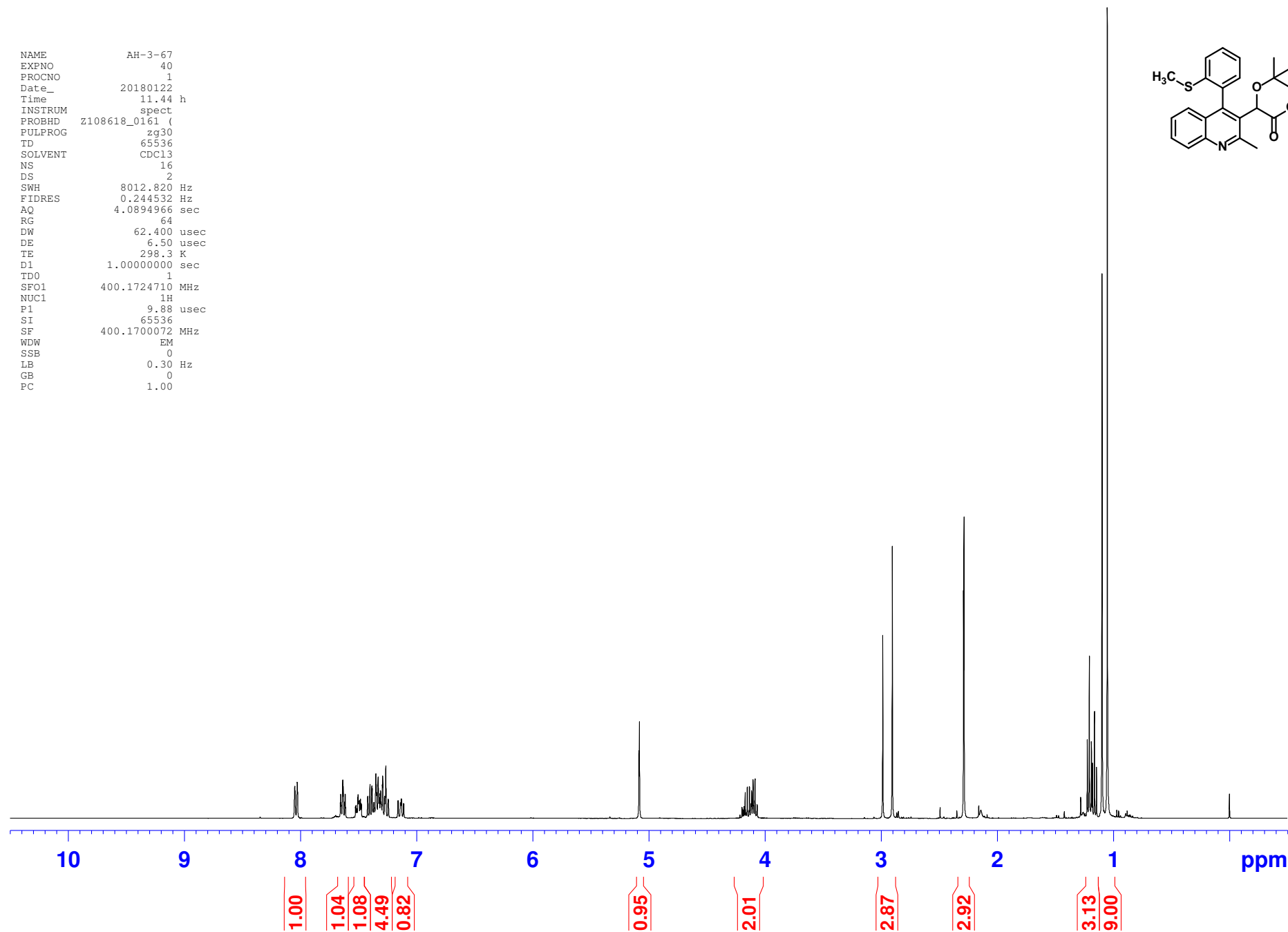
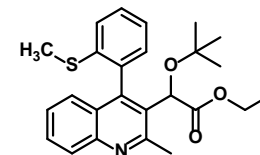
AH-3-66 characterizaion (400MHz, CDC13)



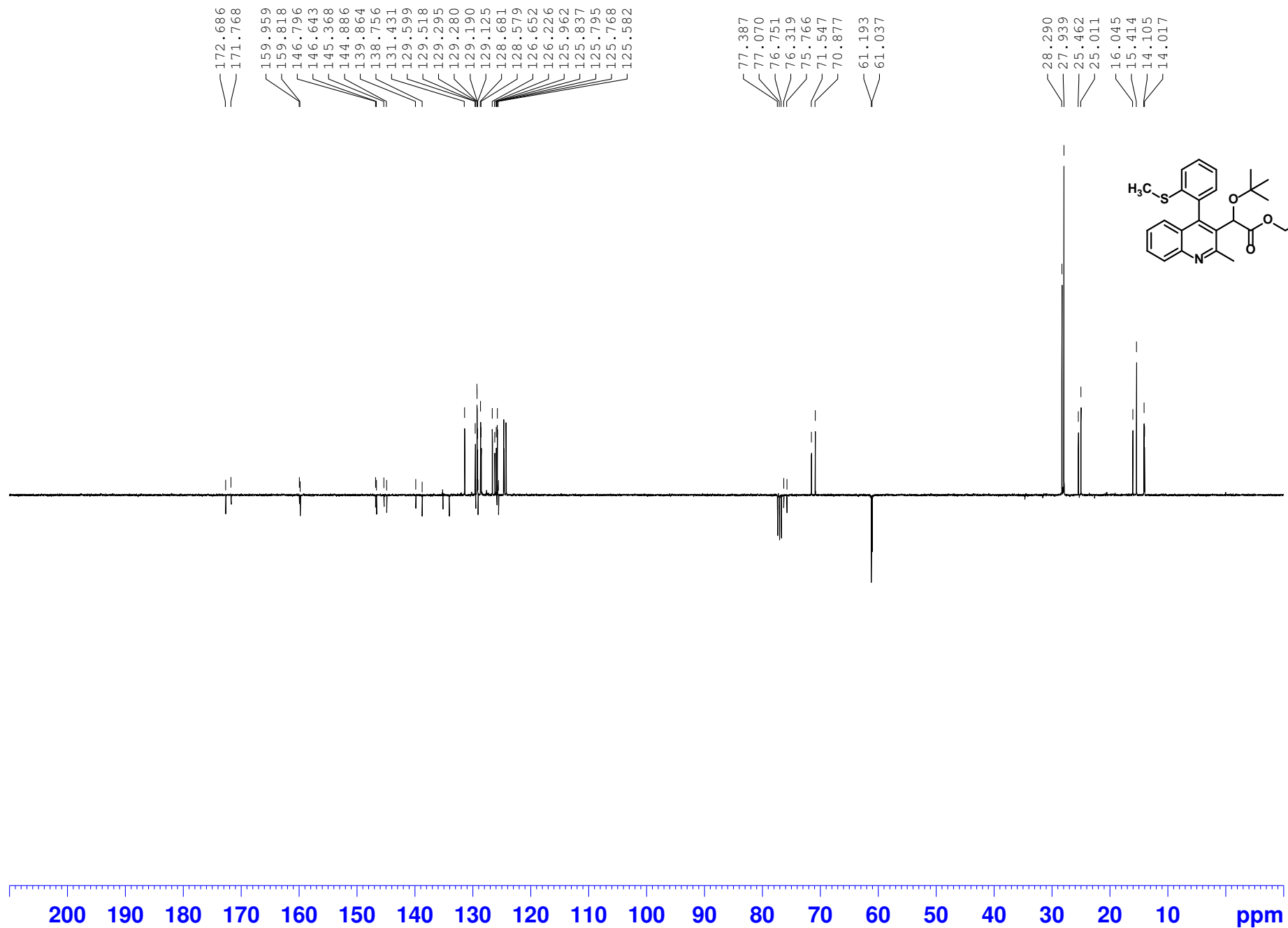
AH-3-67 Characterization

MISSISS

NAME AH-3-67
EXPNO 40
PROCNO 1
Date_ 20180122
Time 11.44 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



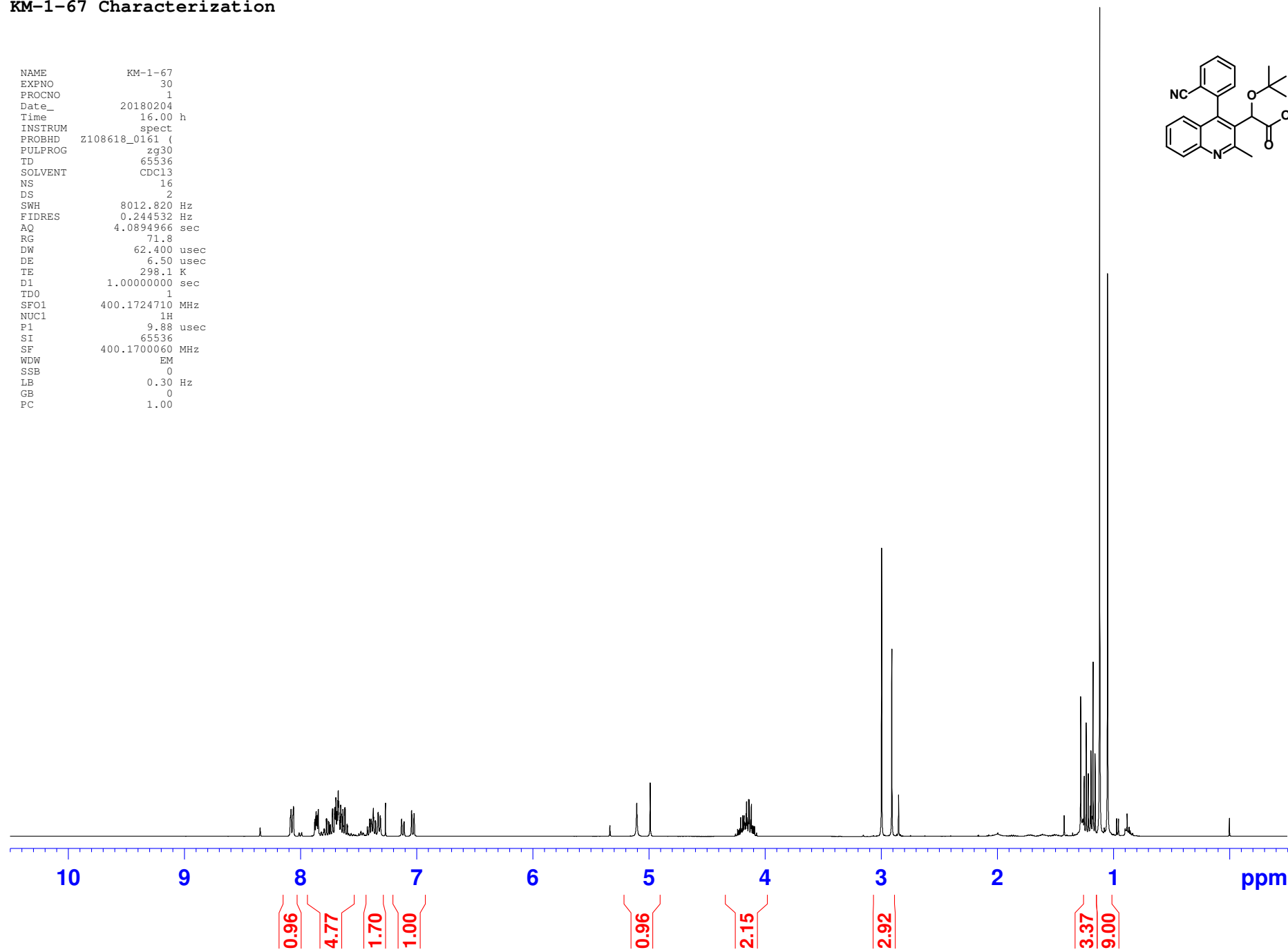
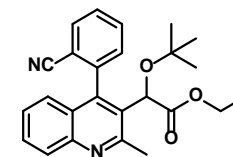
AH-3-67 Characterization



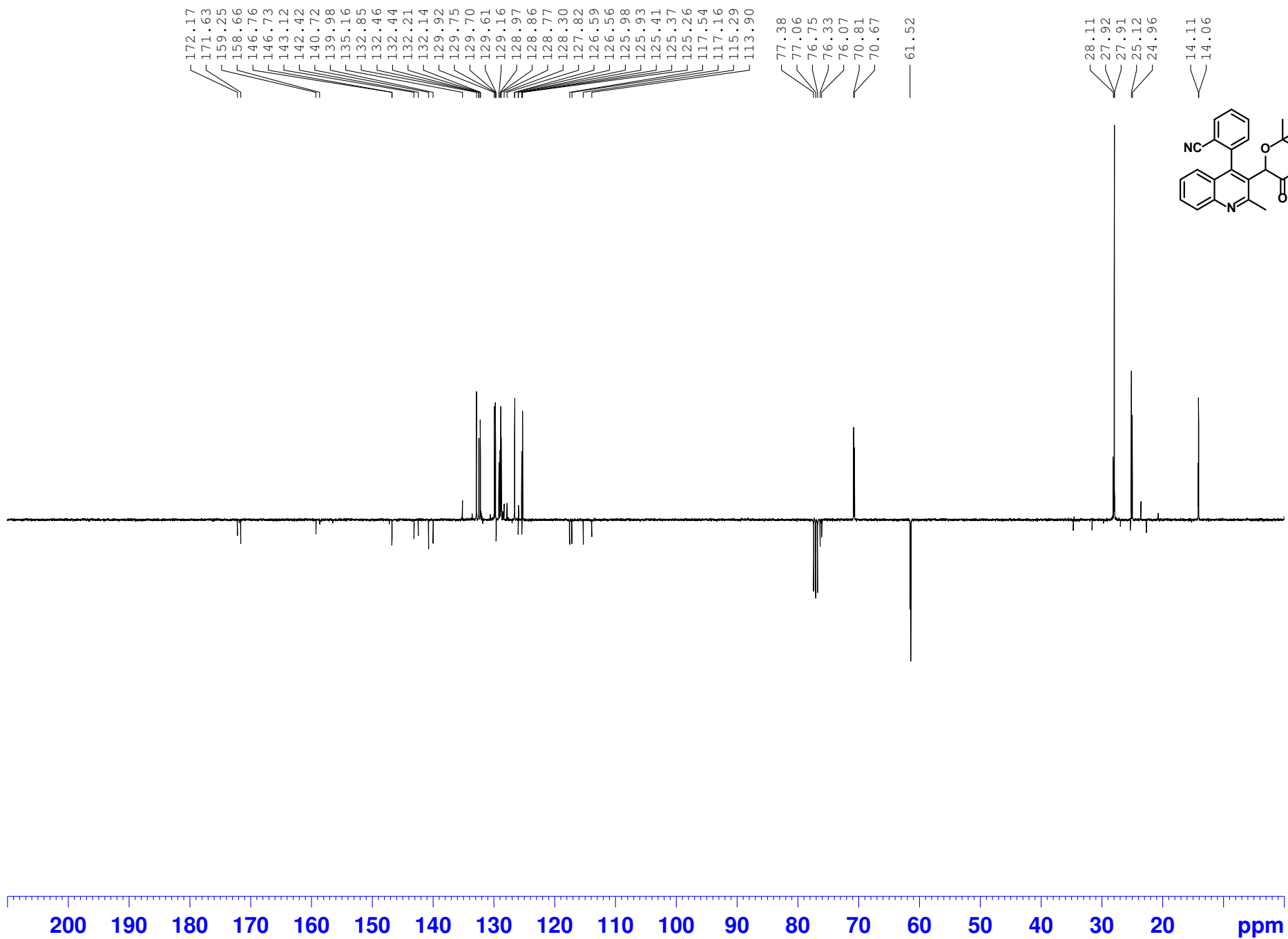
KM-1-67 Characterization

MISSISS

NAME KM-1-67
EXPNO 30
PROCNO 1
Date_ 20180204
Time 16.00 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700060 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

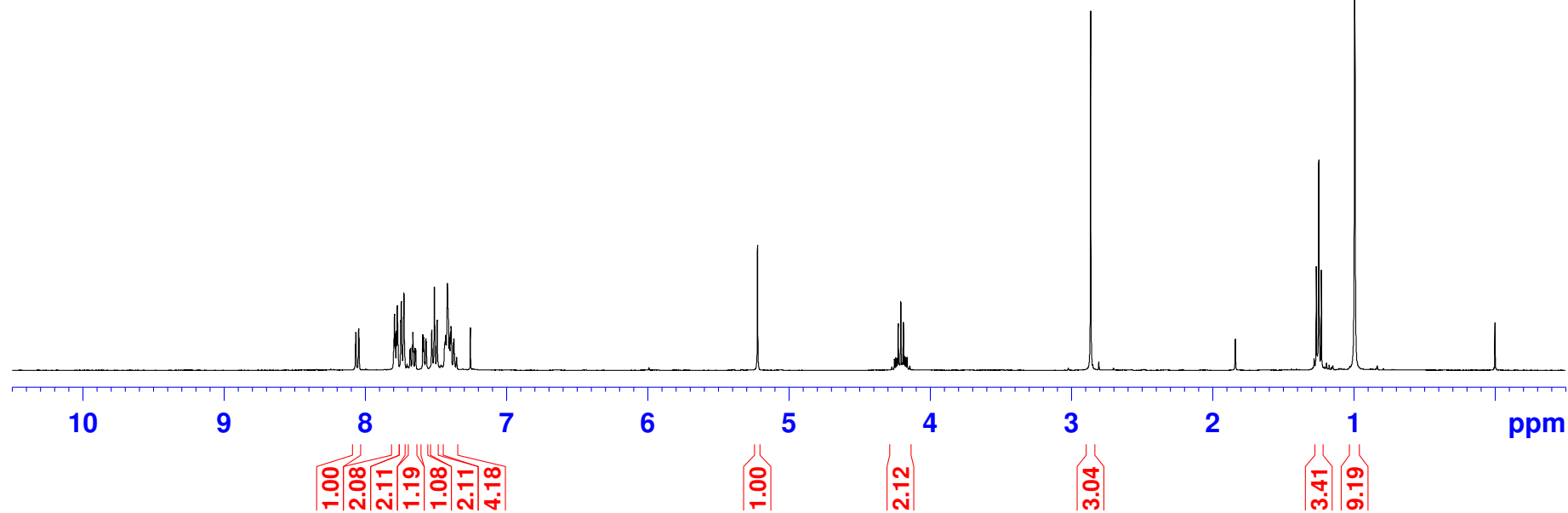
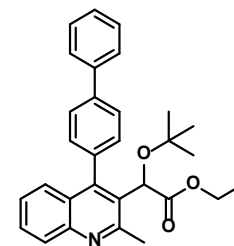
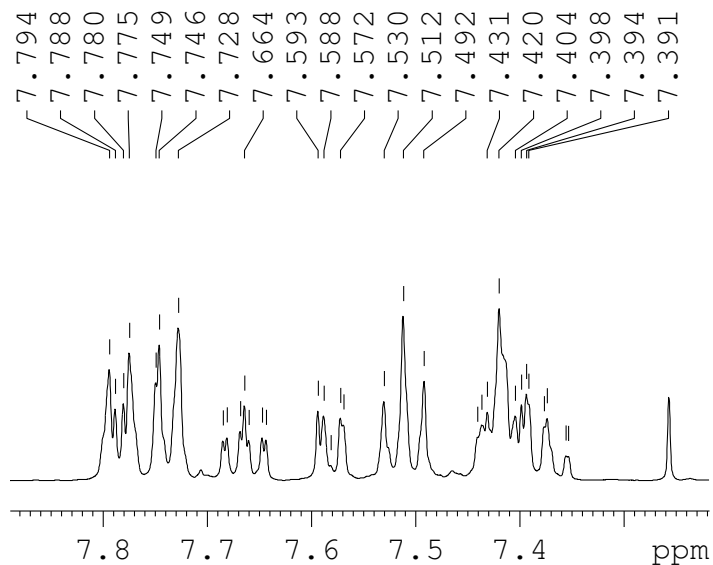


KM-1-67 Characterization

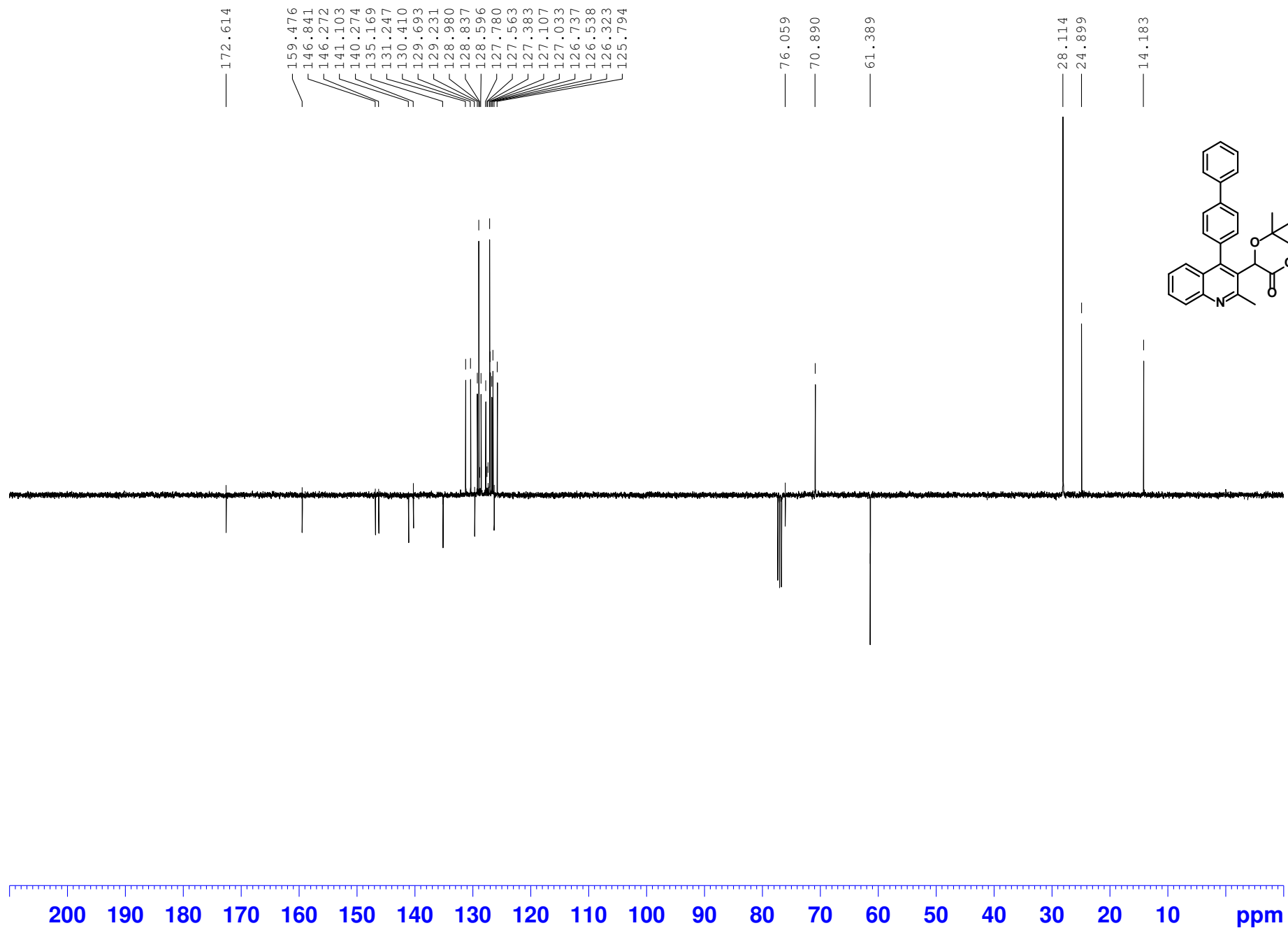


NGJ-8-084 (CDC13, 400 MHz) Pure Brown Oil - suzuki coupling of iodoquinoline with biphenylboron

NAME NGJ-8-084
 EXPNO 30
 PROCNO 1
 Date_ 20171206
 Time_ 17.16 h
 INSTRUM spect
 PROBHD Z108618_0161 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 114
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700108 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

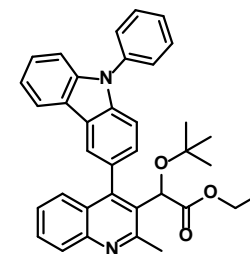


NGJ-8-084 (CDC13, 400 MHz) Pure Brown Oil - suzuki coupling of iodoquinoline with biphenylboronic aci

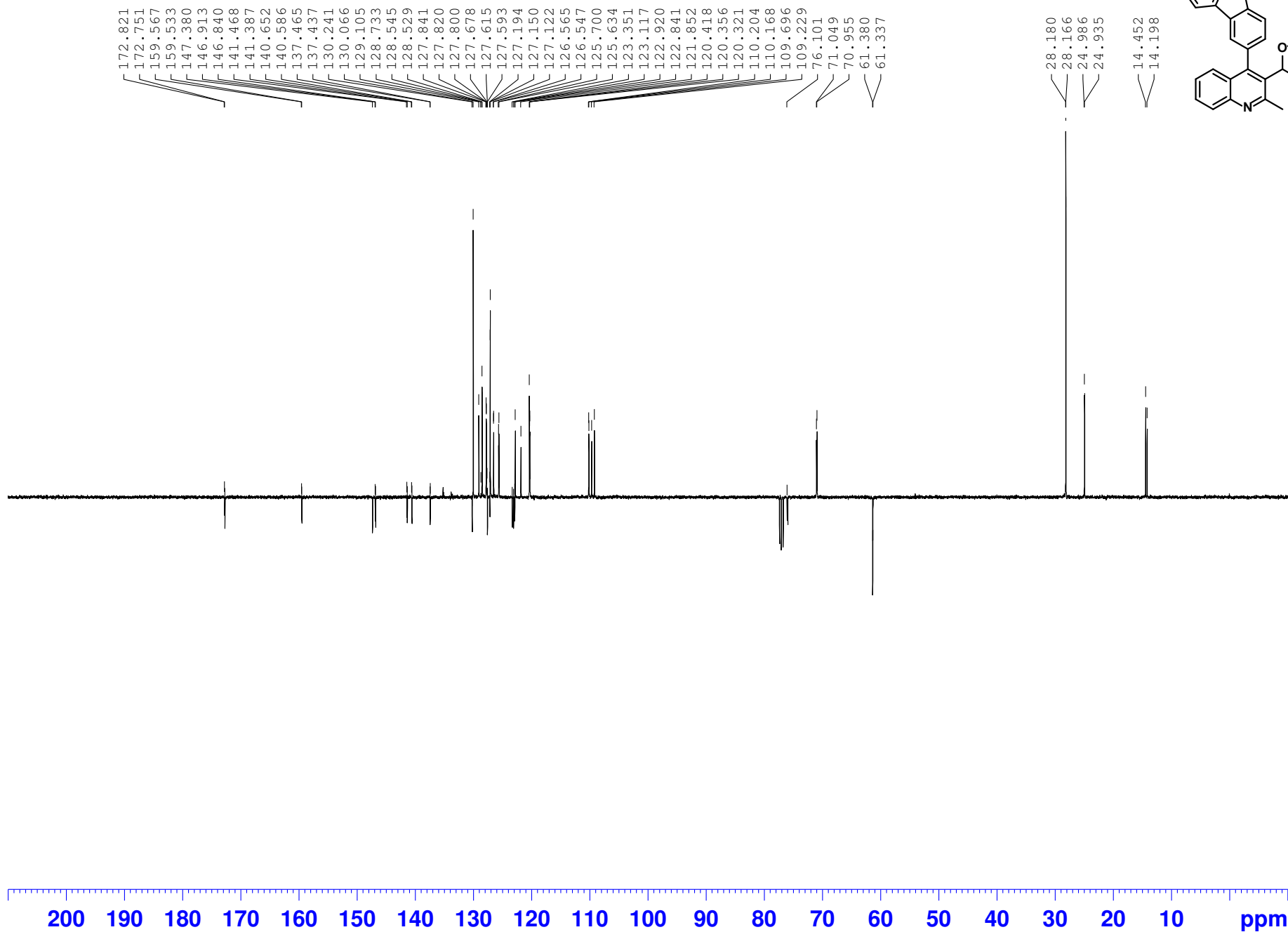
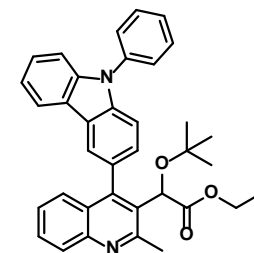


NGJ-9-025 (CDC13, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with carboxazole

NAME NGJ-9-025
EXPNO 30
PROCNO 1
Date_ 20180123
Time_ 16.59 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700173 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

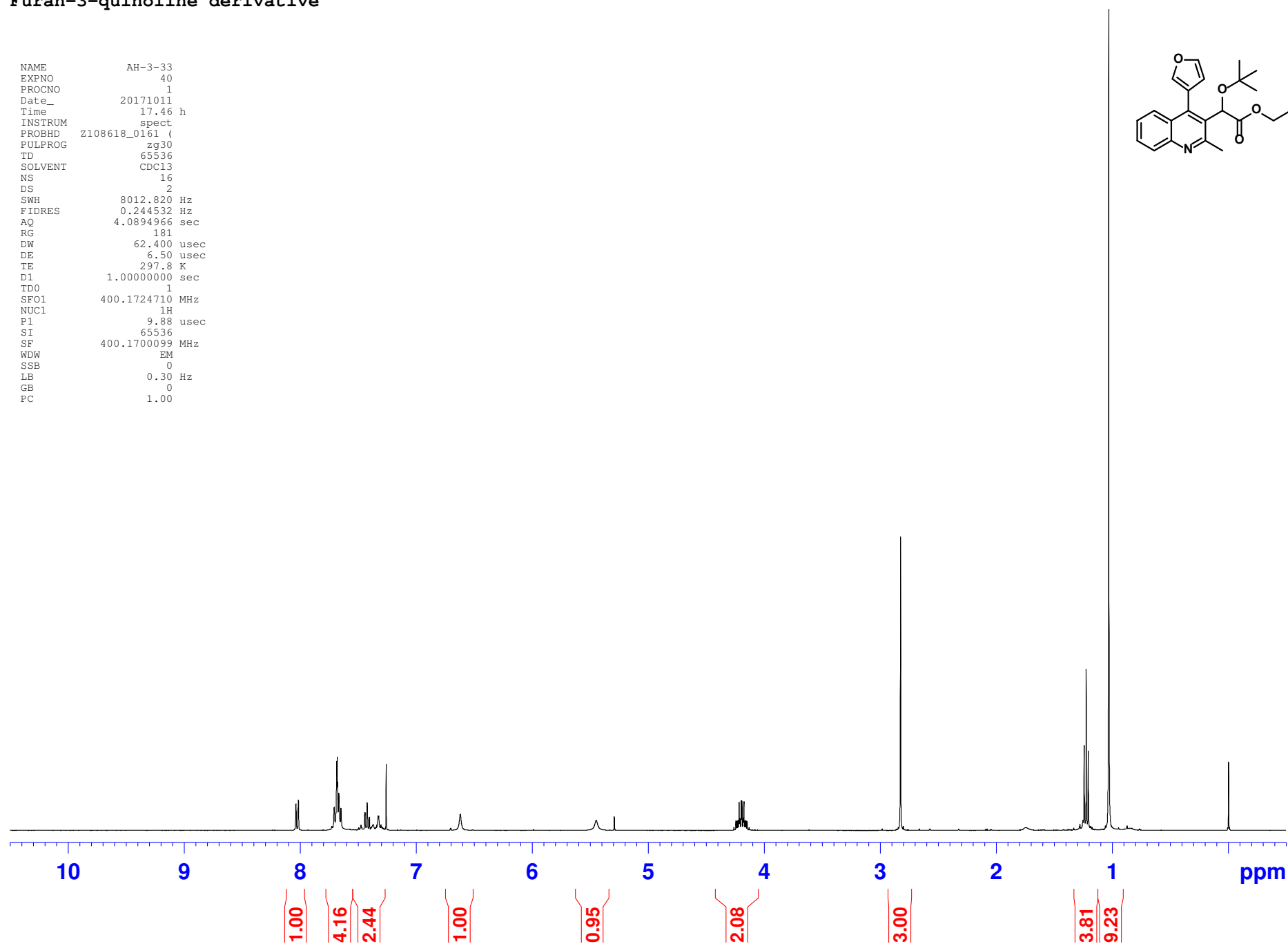
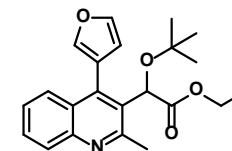


NGJ-9-025 (CDCl₃, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with carboxazole boroni



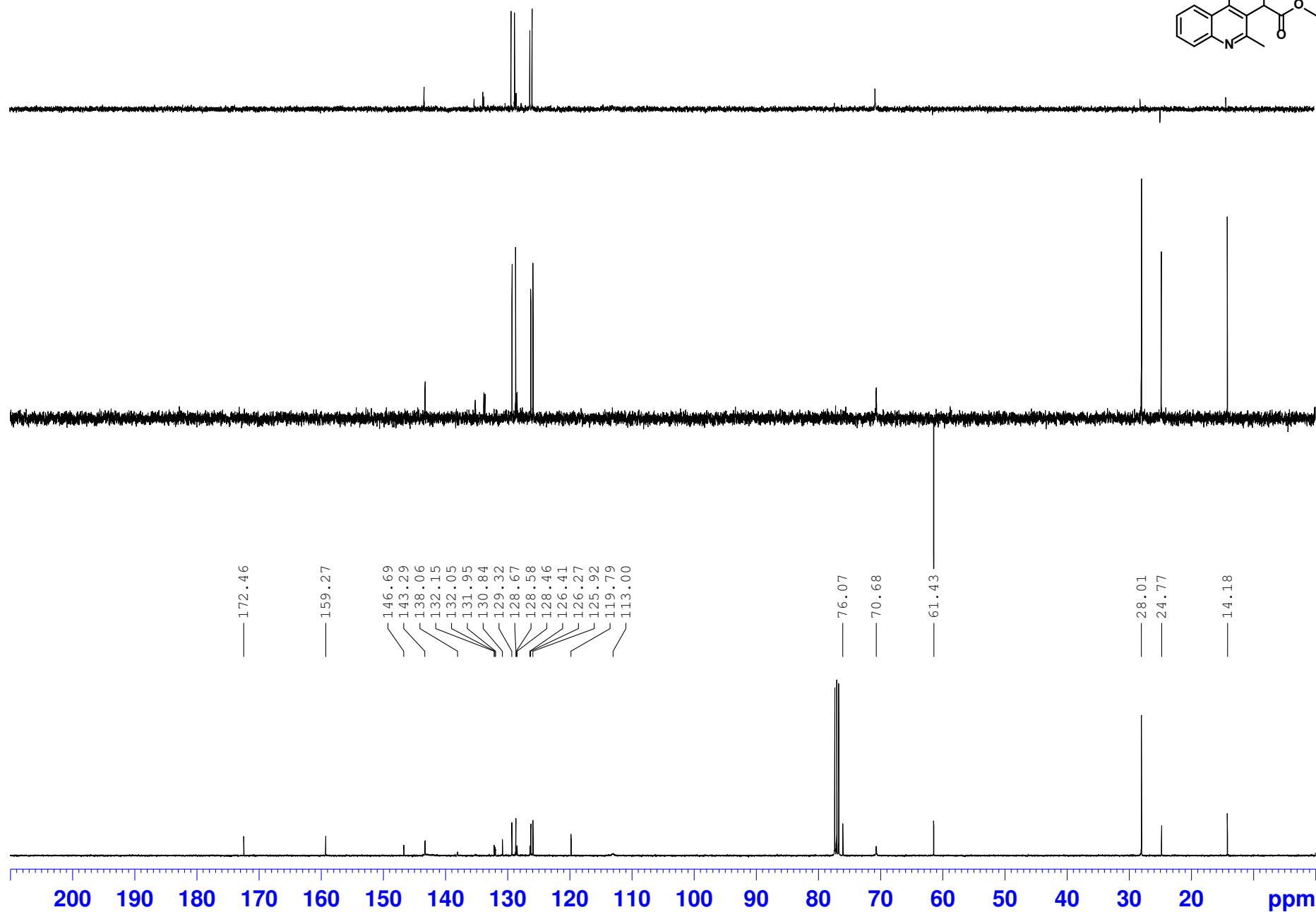
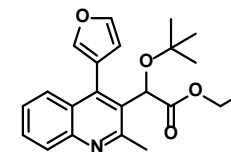
Furan-3-quinoline derivative

NAME AH-3-33
EXPNO 40
PROCNO 1
Date_ 20171011
Time 17.46 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 181
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Furan-3-quinoline derivative

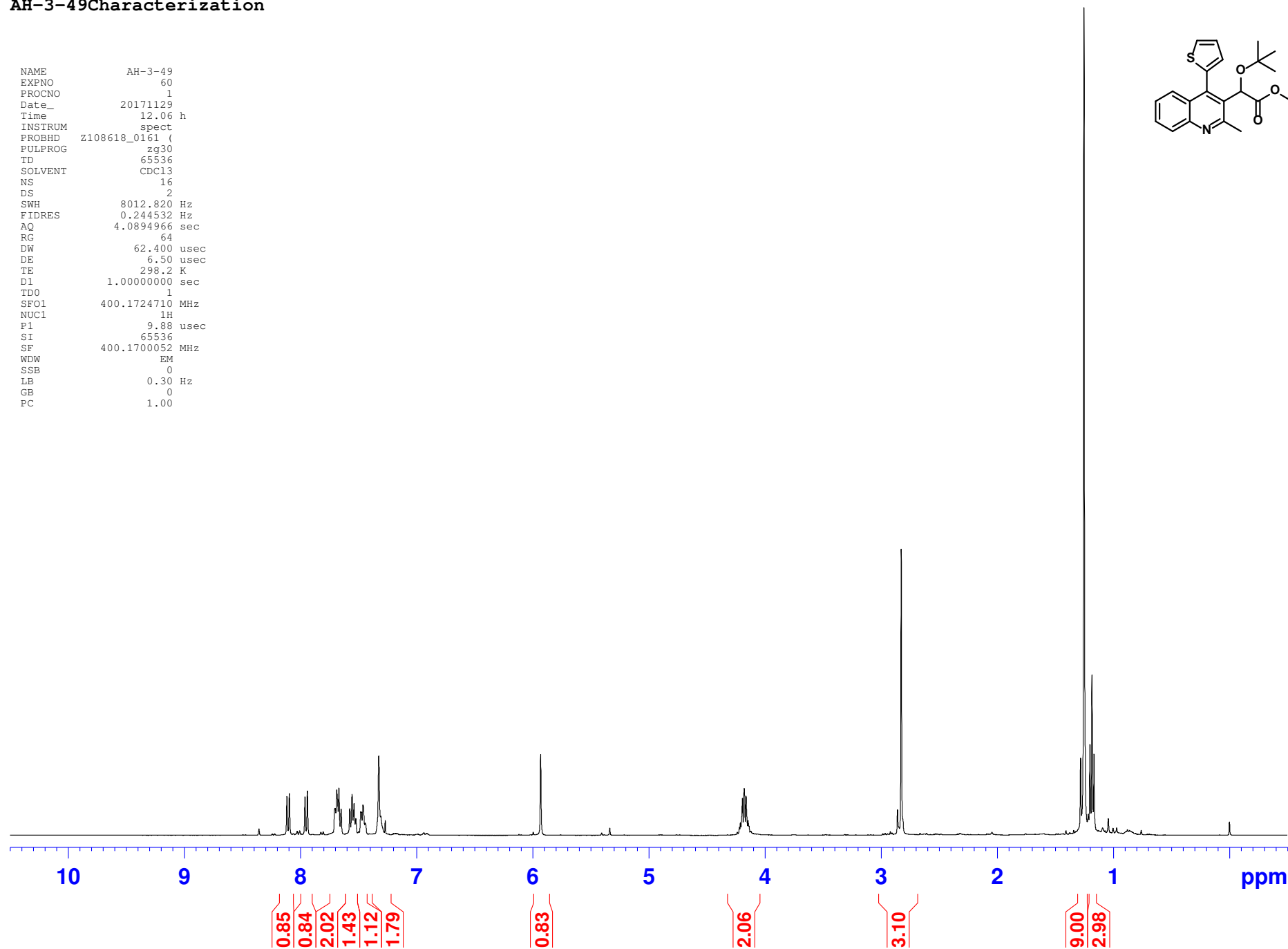
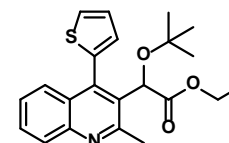
MISSISS



AH-3-49 Characterization

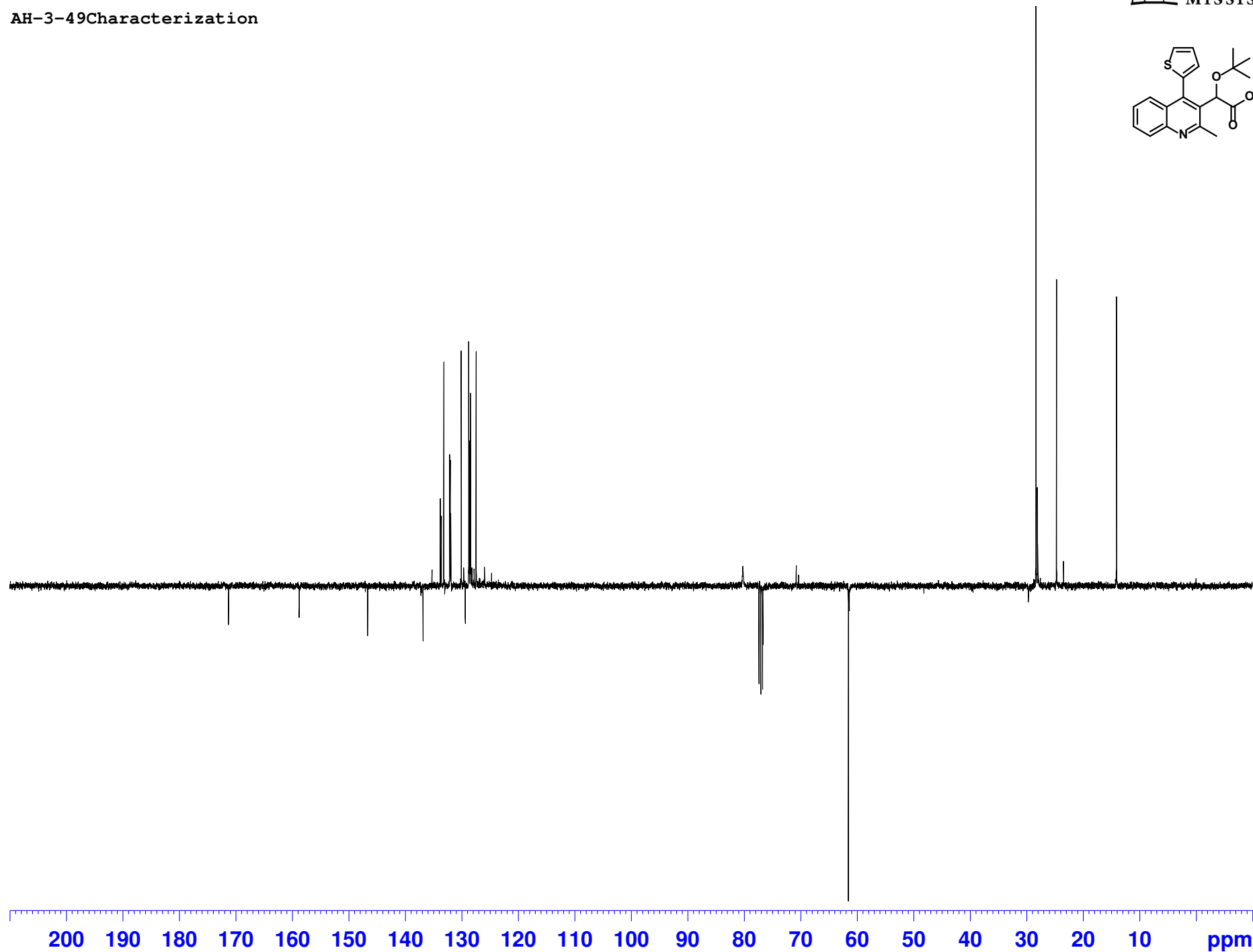
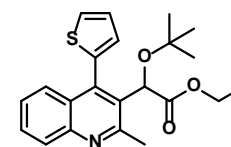
MISSISS

NAME AH-3-49
EXPNO 60
PROCNO 1
Date_ 20171129
Time 12.06 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



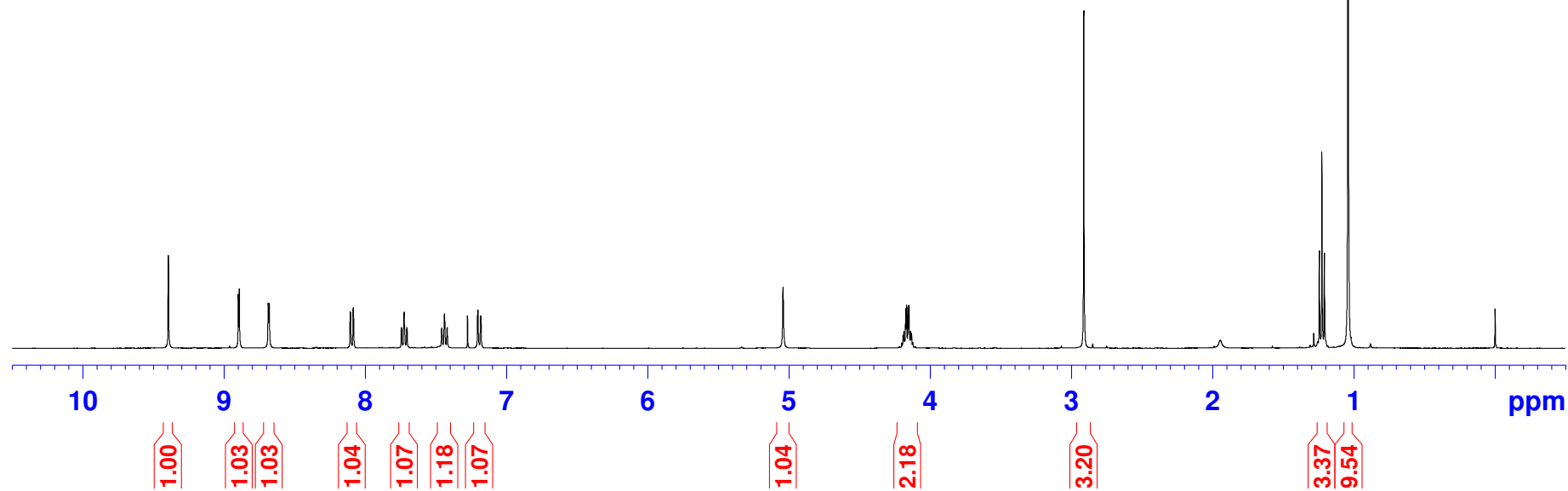
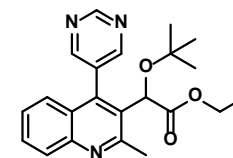
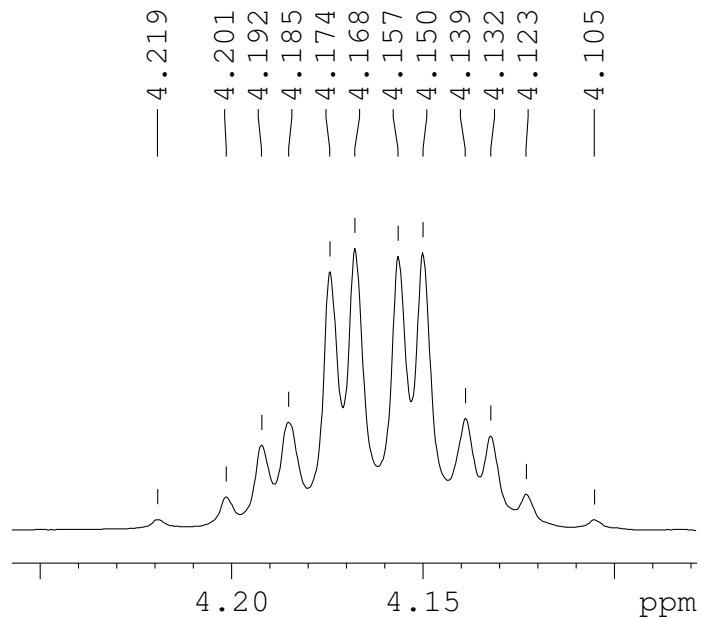
AH-3-49Characterization

MISSISS

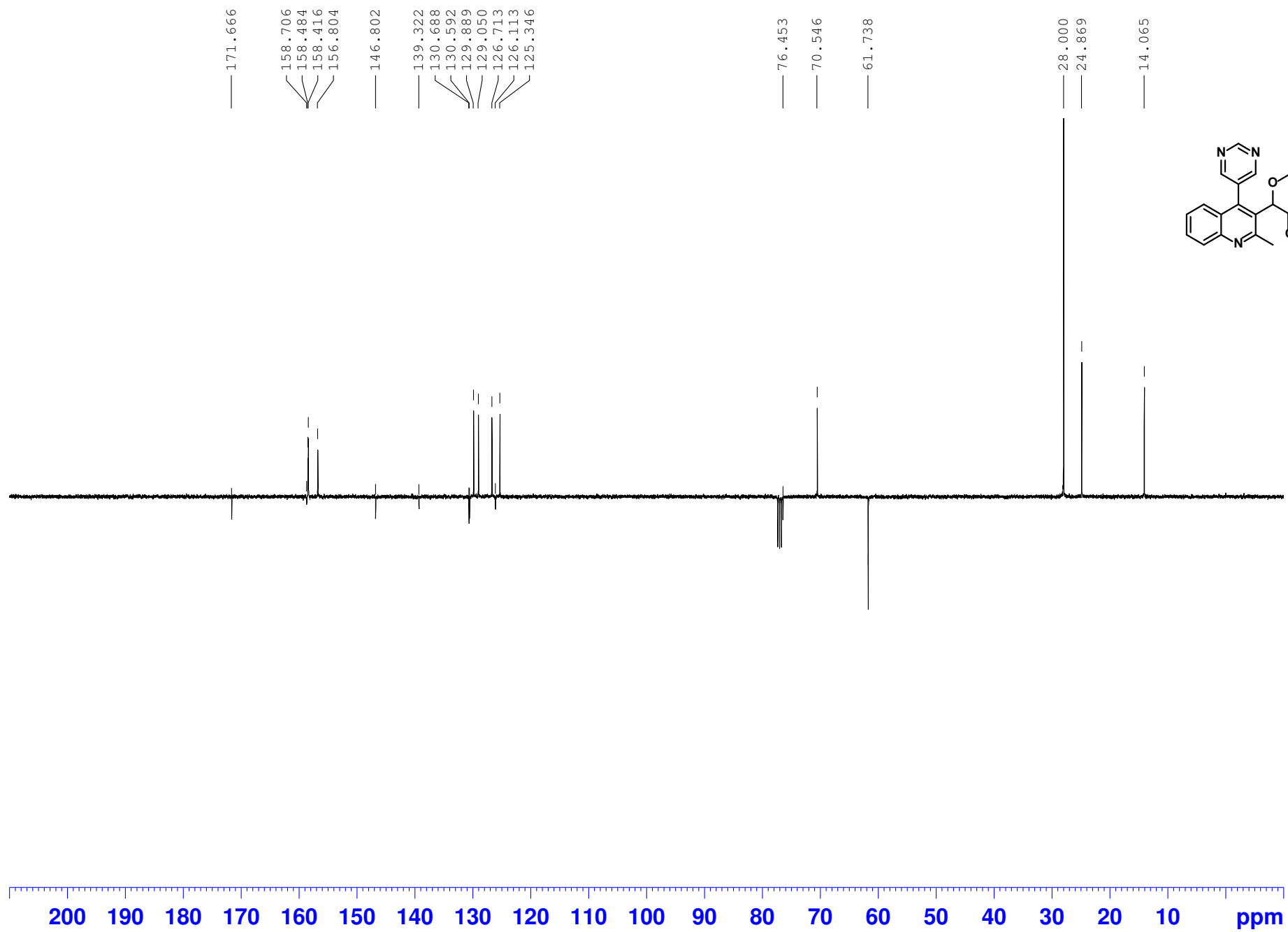


NGJ-9-003 (CDC13, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with pyrimidine

NAME NGJ-9-003
 EXPNO 30
 PROCNO 1
 Date_ 20171222
 Time_ 10.18 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 114
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700028 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

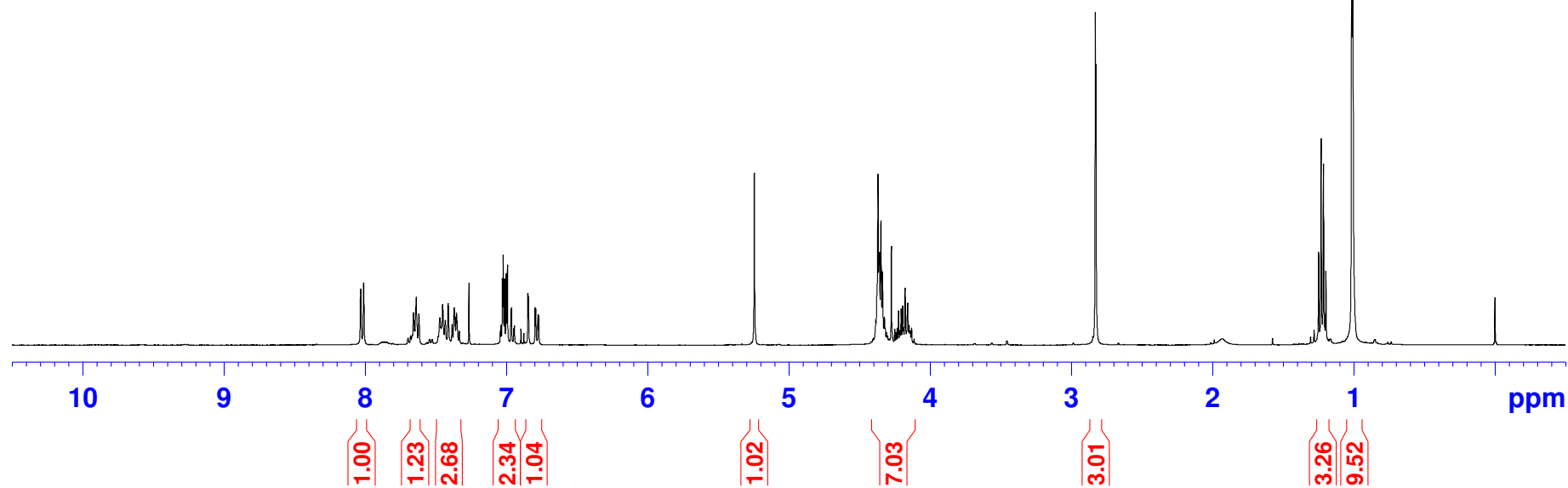
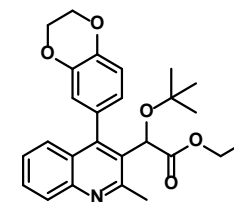
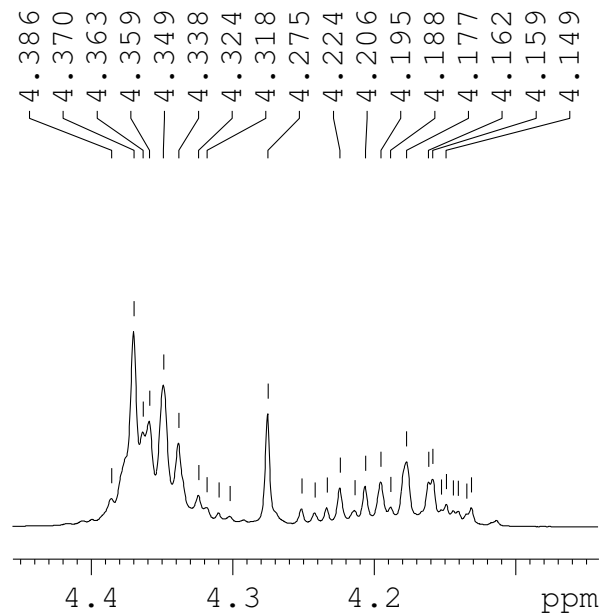
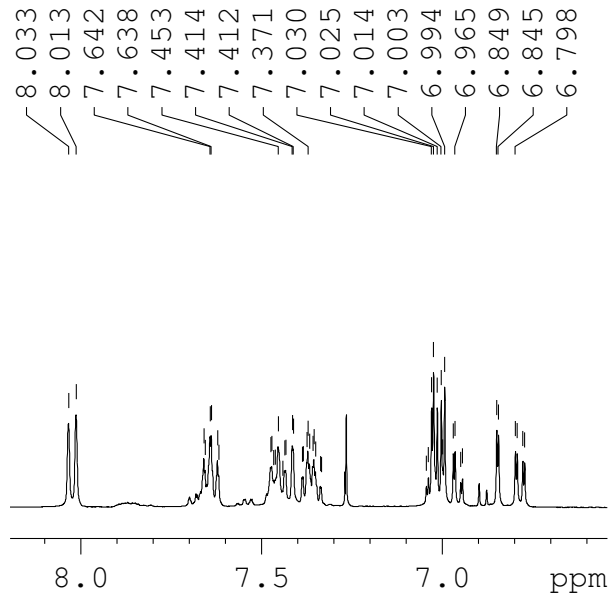


NGJ-9-003 CDC13

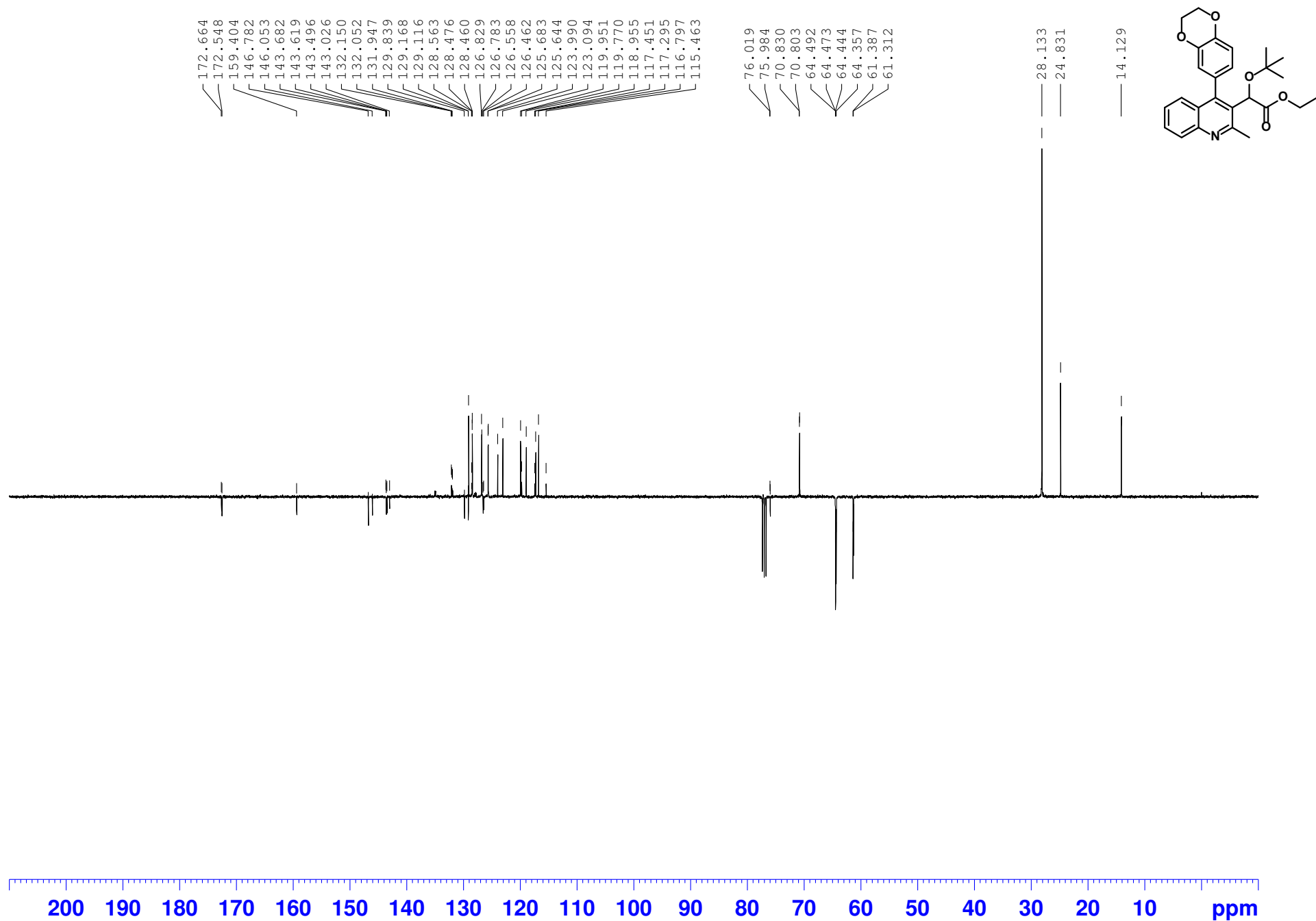


NGJ-8-099 (CDC13, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with benzodioxane

NAME NGJ-8-099
 EXPNO 40
 PROCNO 1
 Date_ 20180207
 Time_ 18.55 h
 INSTRUM spect
 PROBHD Z108618_0161 (zg30)
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 101
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700070 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NGJ-8-099 (CDCl₃, 400 MHz) Pure Yellow Oil - suzuki coupling of iodoquinoline with benzodioxaneboroni

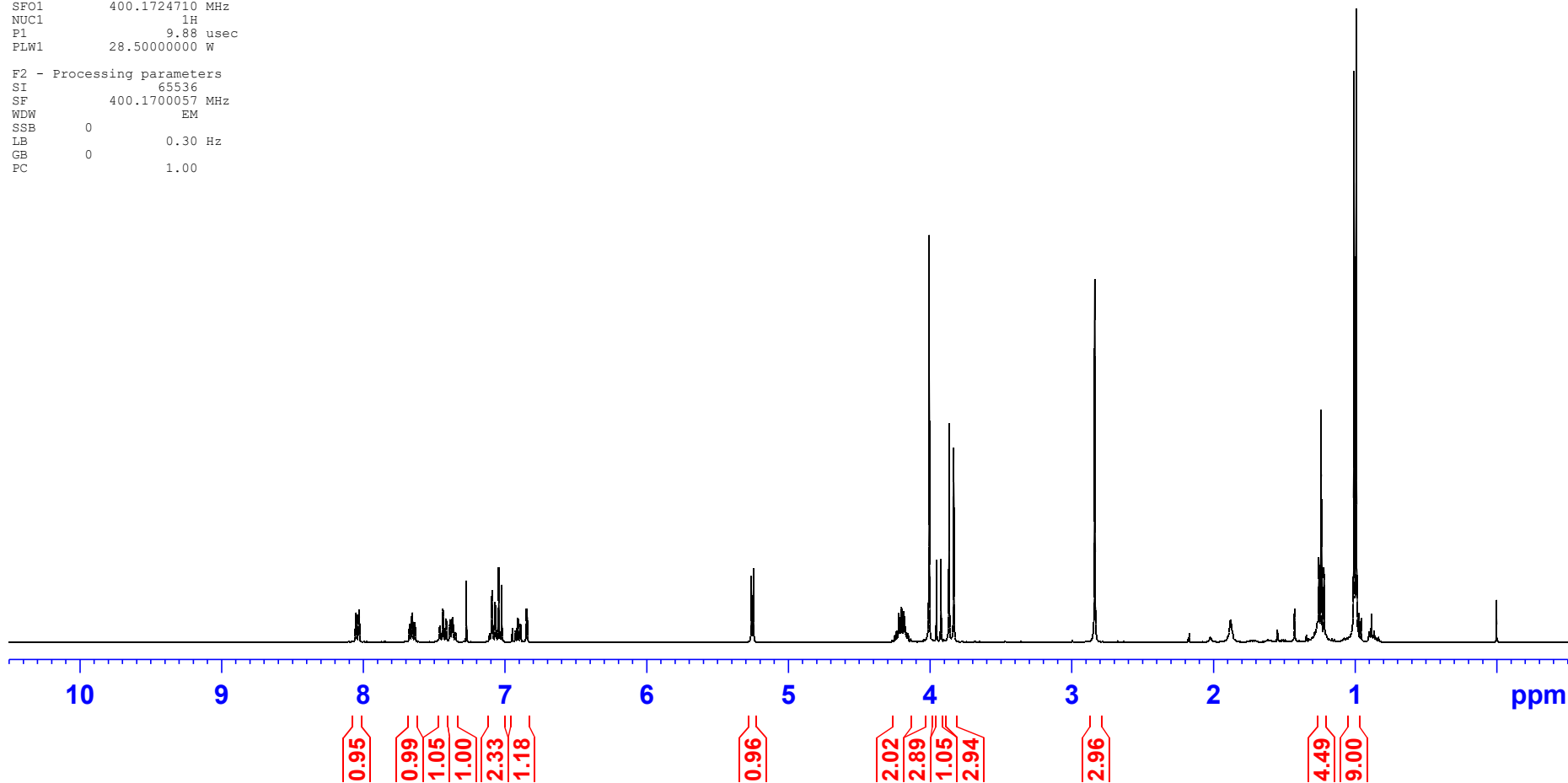
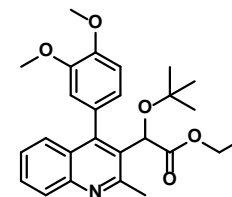


NGJ-9-091 (CDC13, 400 MHz) synthesis of 3,4-dimethoxy quinoline ester

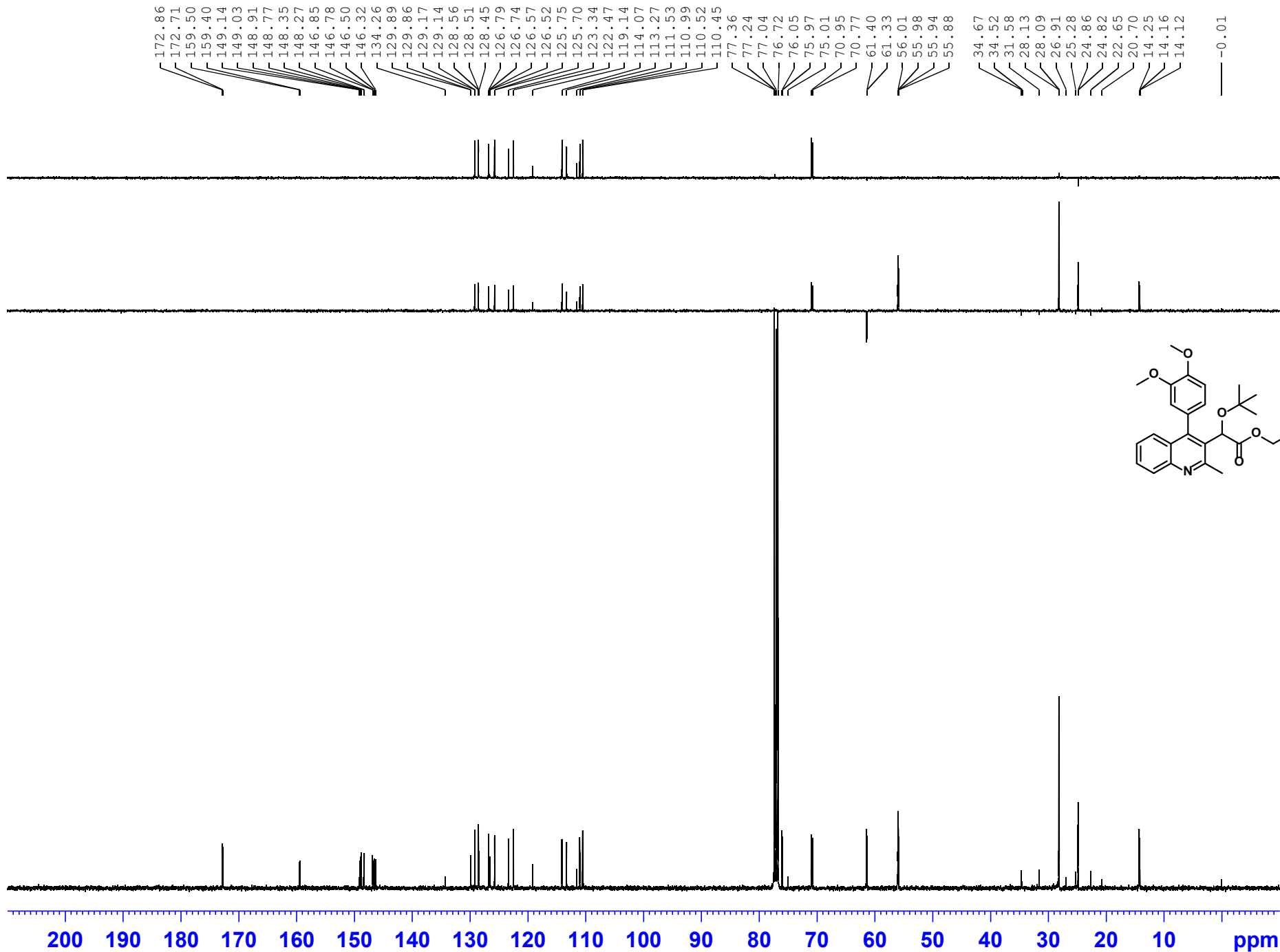
Current Data Parameters
NAME NGJ-9-091
EXPNO 40
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180705
Time_ 21.04 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
PLW1 28.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1700057 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



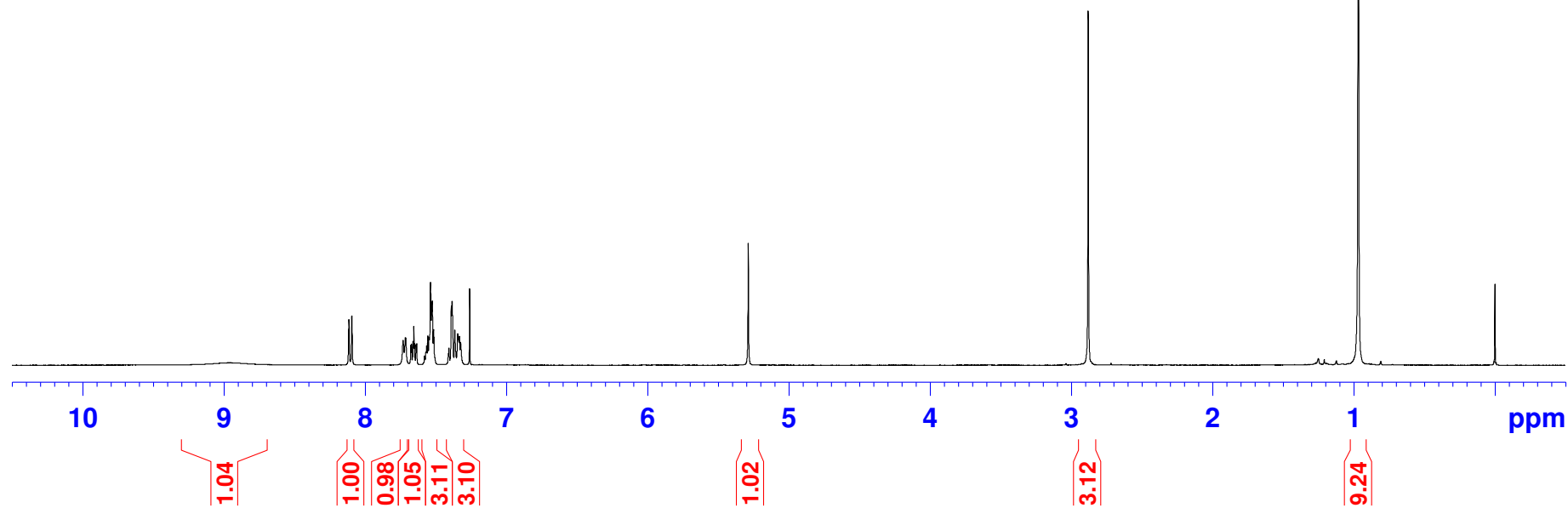
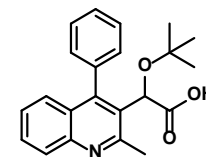
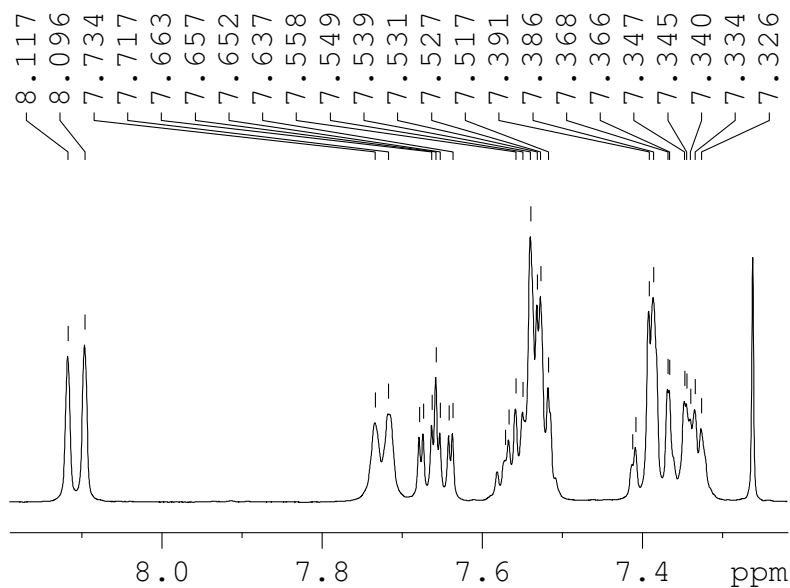
NGJ-9-091 (CDC13, 400 MHz) suzuki coupling of iodoquinoline wit



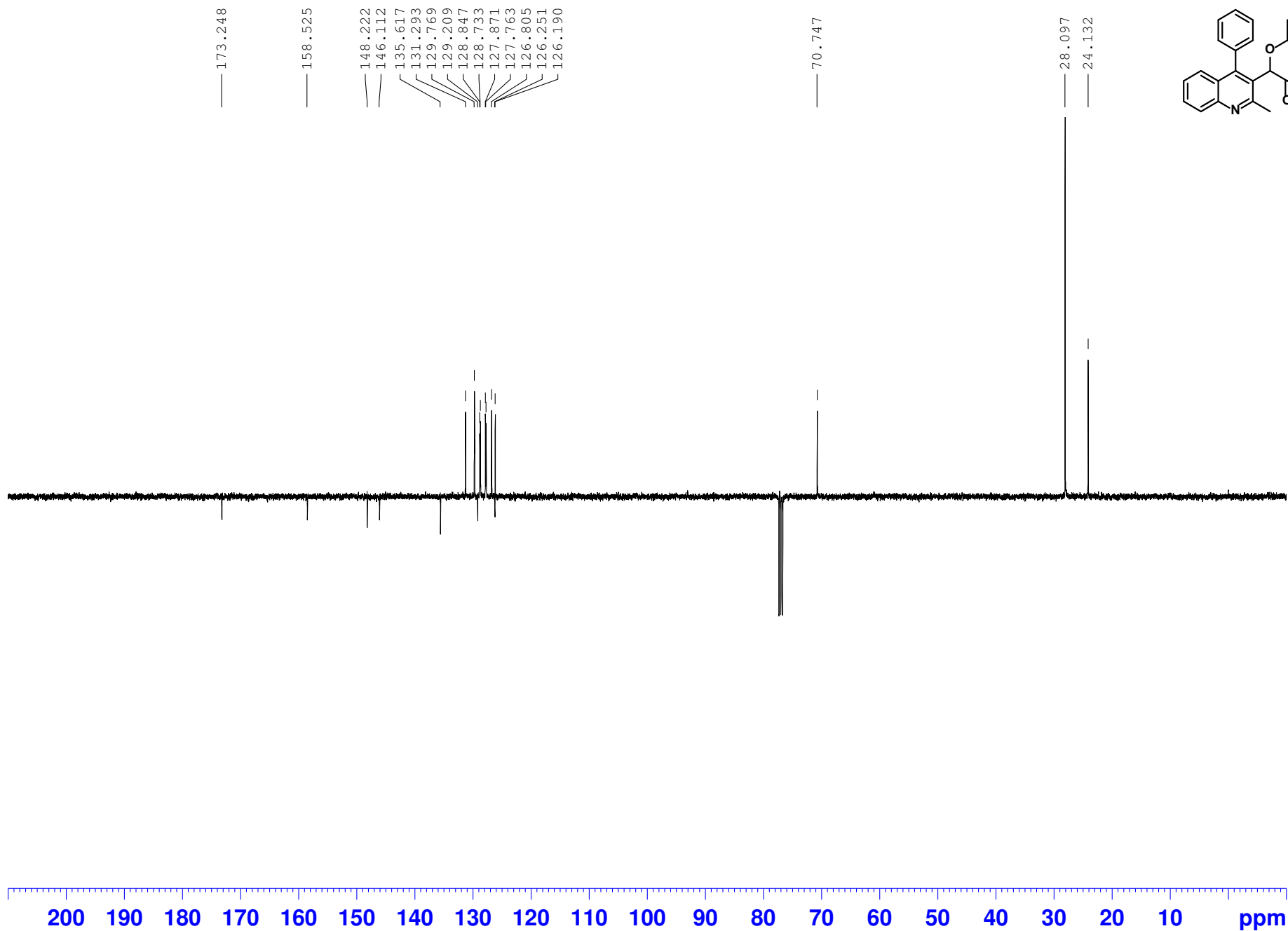
NGJ-9-021 (CDC13, 400 MHz) Pure Clear Oil - saponification of 4-phenylquinoline; post-neutral:

```

NAME      NGJ-9-021
EXPNO     30
PROCNO    1
Date_     20171219
Time      16.43 h
INSTRUM   spect
PROBHD    Z108618_0161 (
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.244532 Hz
AQ        4.0894966 sec
RG        161
DW        62.400 usec
DE        6.50 usec
TE        298.4 K
D1        1.00000000 sec
TD0       1
SF01      400.1724710 MHz
NUC1      1H
P1        9.88 usec
SI        65536
SF        400.1700089 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```



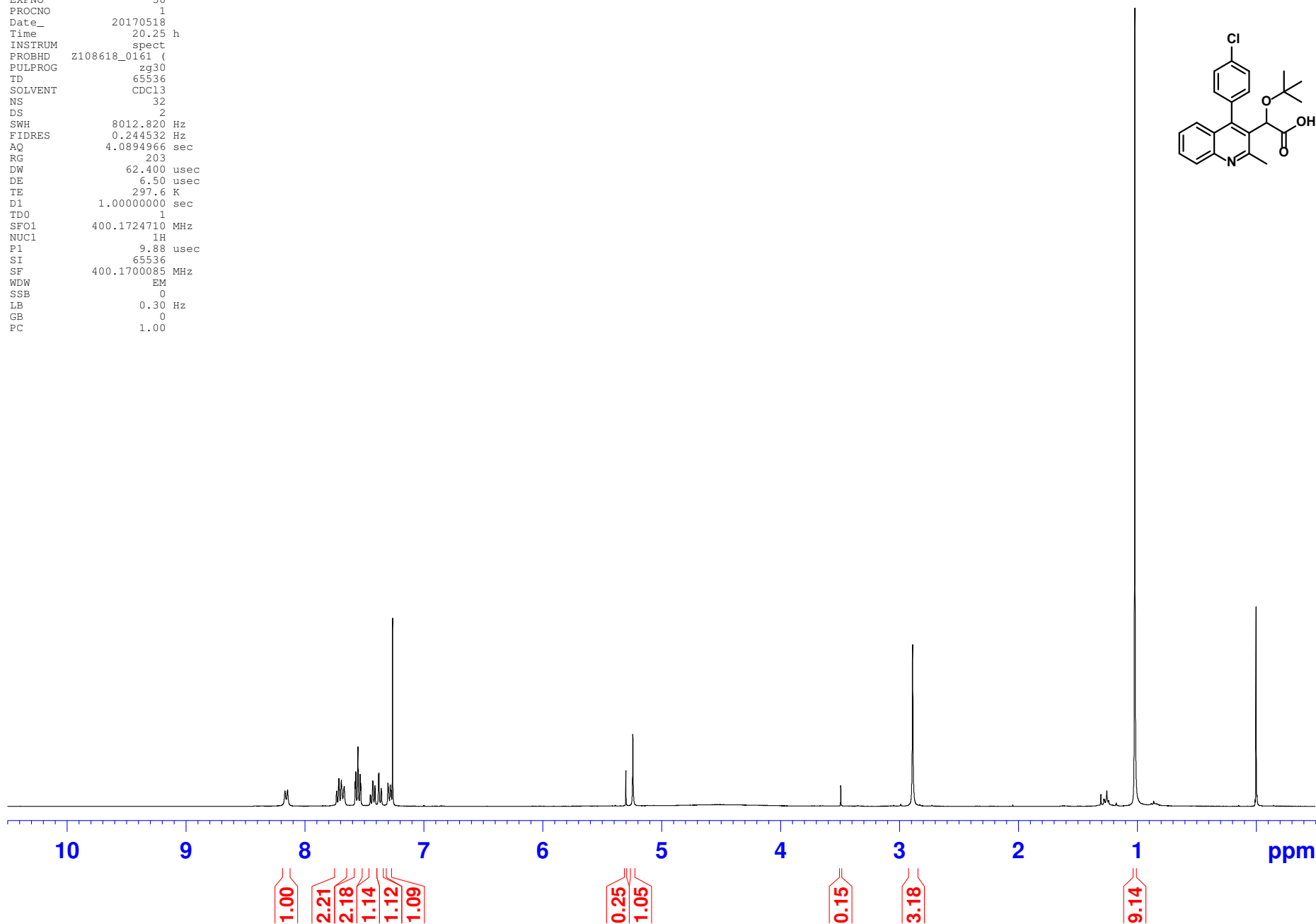
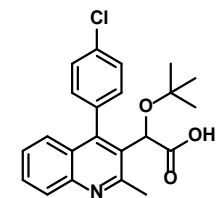
NGJ-9-021 (CDCl₃, 400 MHz) Pure Clear Oil - saponification of 4-phenylquinoline; post-neutralization



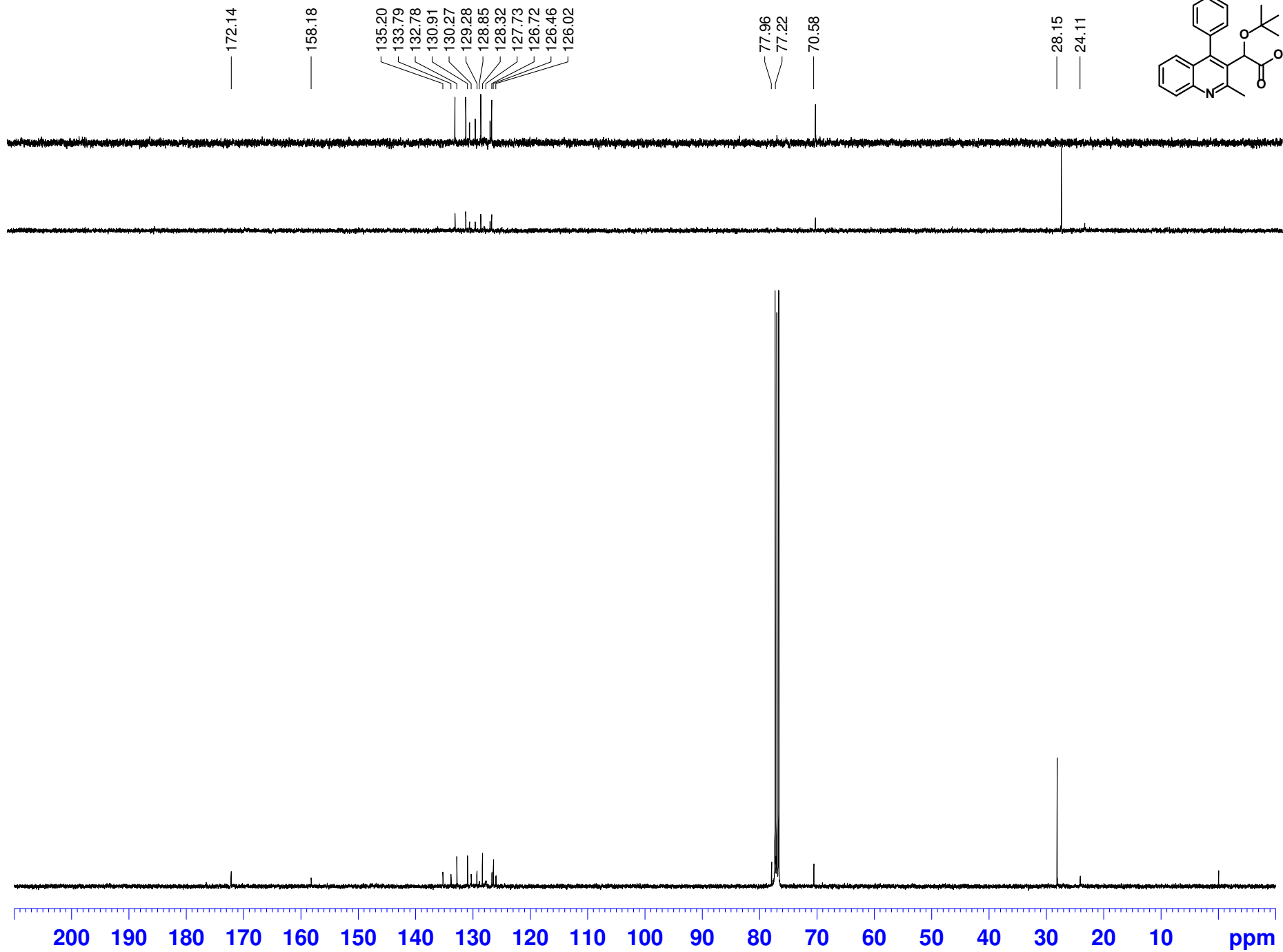
NGJ-7-060 (CDC13, 400 MHz) Pure White Solid - saponification of ester quinoline



NAME NGJ-7-060
EXPNO 30
PROCNO 1
Date_ 20170518
Time_ 20.25 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NGJ-7-060 (CDCl₃, 400 MHz) Pure White Solid - saponification c



Mass Spectrum List Report

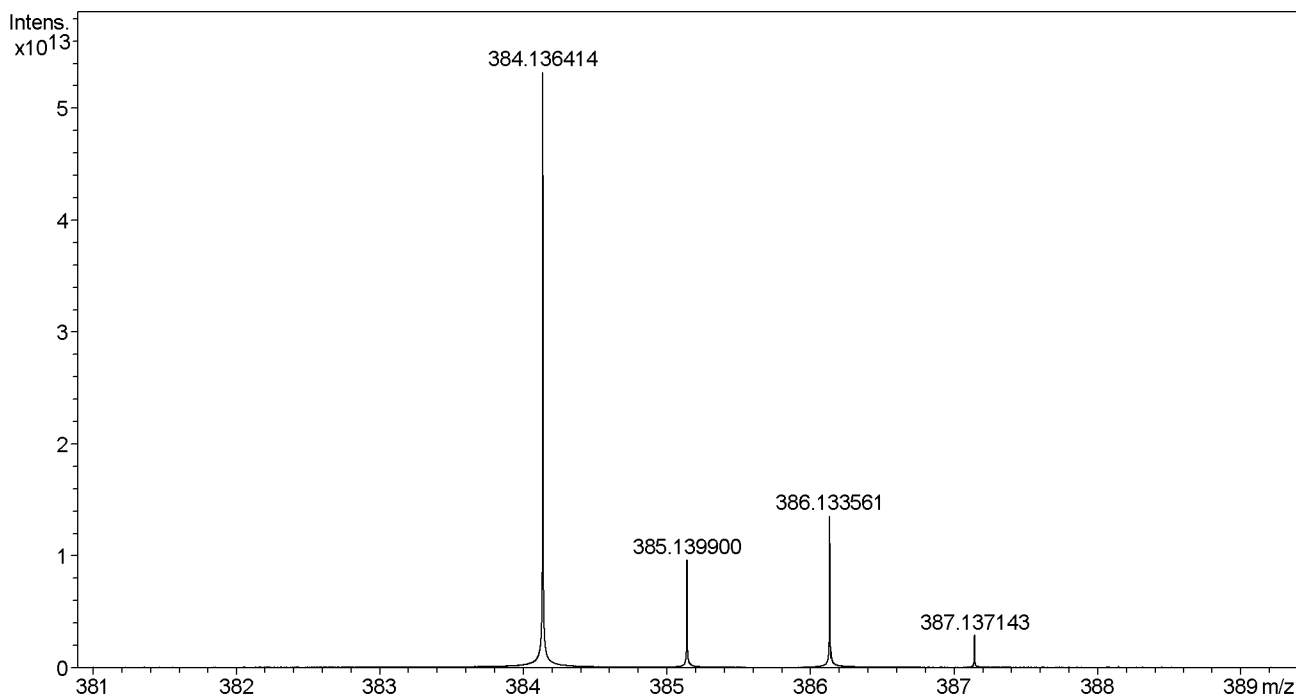
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-7-060_pos_000001.d
Method
Sample Name NGJ-7-060
Comment NGJ-7-060 in THF:MeOH C22H22ClNO3 H+

Acquisition Date 3/19/2018 12:08:06 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-7-060 in THF:MeOH
Exact Mass of C22H22ClNO3 H+ = 384.136098 m/z
Mass Observed = 384.136414 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.561401	21388630843
2	184.654214	22690279700
3	186.059464	21390935505
4	186.771490	21044178947
5	187.514591	22620291972
6	187.633819	25531528465
7	189.070049	22430880694
8	189.270012	21086502667
9	189.577568	22396779448
10	189.685336	35678851293
11	189.958190	21114067374
12	190.061543	100417214097
13	190.926723	21663734232
14	192.071089	456822191468
15	192.080898	26487592554
16	192.570059	25118277958
17	192.572886	73679980936
18	193.066904	30223676861
19	193.069715	69164080616
20	193.962032	24451331299

Mass Spectrum List Report

#	m/z	I
21	194.644604	22452094652
22	194.995028	21602038223
23	195.001061	21005657480
24	196.061242	21368354491
25	196.075727	24116008390
26	200.407328	21010639825
27	200.912673	23669856723
28	201.119355	21576610707
29	201.884797	25868850582
30	202.333255	21695291243
31	202.340491	195524968198
32	203.082521	22189958476
33	203.570082	21344203429
34	206.096392	20987577954
35	206.965657	21207010274
36	209.442007	65382977614
37	210.769443	21761440202
38	211.368721	21446125190
39	211.910236	22464042237
40	212.794578	21360998986
41	213.992894	23742464843
42	214.065060	28158915807
43	216.080893	24781486152
44	217.674438	21794583697
45	218.096365	22598418388
46	225.468756	21910446026
47	229.083621	22531440225
48	229.088599	24076344896
49	231.099751	22951691530
50	231.104350	39583931559
51	231.169345	24940002786
52	233.033156	21291683808
53	235.895778	24547286356
54	251.723888	24913544816
55	253.163471	21663127851
56	261.389462	22365499380
57	263.102950	21929882005
58	263.311315	21866752893
59	263.585336	22584677865
60	265.065698	26437511269
61	265.839187	22177191160
62	266.073080	50412517289
63	267.044770	27706514887
64	268.312735	43935383696
65	275.173360	21272900667
66	278.298220	22160023637
67	280.598549	24455725515
68	281.737666	21538040222
69	282.068201	83354423011
70	283.071645	24129505887
71	283.563502	31042149425
72	283.648494	22362103829
73	284.065120	83164101989
74	284.083624	25181322214
75	285.248655	22251175722
76	285.274220	22151559519
77	286.518468	22364818154
78	288.193251	24245226796
79	296.047384	21155976612
80	296.345477	25417870813
81	299.070948	21271835244
82	299.789605	23819953587
83	300.857501	22324817059
84	301.752660	21723616650

Mass Spectrum List Report

#	m/z	I
85	302.600388	22373633497
86	308.572788	22144187922
87	322.282123	33048958823
88	324.387700	125436472104
89	326.510815	149496060153
90	327.246376	22729245176
91	327.963457	29175803699
92	328.073920	45256836808
93	328.653064	30324105471
94	328.694657	1502022904019
95	329.076952	28992353670
96	330.070336	43308792433
97	340.146847	1685755825096
98	340.233694	23895542013
99	341.150306	158727601169
100	342.144054	334301085901
101	343.147525	37382501170
102	349.166594	24831556019
103	353.312694	24857767195
104	375.178460	27023369552
105	379.101704	25680473945
106	379.273018	26886876599
107	379.328266	27378409181
108	379.552354	26438805881
109	380.446709	26672269492
110	380.664650	25481213641
111	380.827973	26601957099
112	380.943276	25977709157
113	381.010736	29418599551
114	381.105719	26364148274
115	381.237897	31900070486
116	381.317545	27912362739
117	381.365910	36266601807
118	381.393019	25712413913
119	381.429669	25452953377
120	381.470601	30422917468
121	381.530378	25687990830
122	381.564267	29228416333
123	381.666445	28264146894
124	381.686875	28476457082
125	381.742860	25717684009
126	381.773940	29846075928
127	381.797210	26624628334
128	381.812706	26149695576
129	381.847947	28955605769
130	381.860693	30915130323
131	381.918798	27588352469
132	382.031865	28163192821
133	382.065494	30605131814
134	382.137117	34761195164
135	382.160251	39754801728
136	382.201437	35301260043
137	382.220031	34505376249
138	382.315806	32247266069
139	382.396603	33493015132
140	382.437325	35332227117
141	382.488177	36376908645
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143	382.547896	35593193990
144	382.616234	41308148778
145	382.661836	39622763884
146	382.718795	39003583095
147	382.743764	41505956093
148	382.822374	42755079728

Mass Spectrum List Report

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149	382.858395	42411877599
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151	382.972925	48282776841
152	383.051710	47502597045
153	383.067031	45647302959
154	383.106033	46217904593
155	383.128886	59893081276
156	383.165084	49669900825
157	383.183784	52540844777
158	383.268285	56143661859
159	383.339096	56111908828
160	383.352430	62778558598
161	383.380405	61207888941
162	383.473632	68032331156
163	383.509215	73984995450
164	383.576311	80346528176
165	383.604481	80930333821
166	383.629231	82549758491
167	383.661848	911111015483
168	383.718218	98571969151
169	383.743530	104635499346
170	384.136414	53256046967200
171	384.488540	95302642015
172	384.523124	87486101128
173	384.673463	60302209898
174	384.687672	57131578262
175	384.731899	50401373452
176	384.741993	49588181921
177	384.771232	47275652086
178	384.798090	48817154799
179	384.827401	43421605575
180	384.866927	41531616533
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182	385.036116	67313007338
183	385.139900	9681696952431
184	385.258098	71643651978
185	385.289485	66831344759
186	385.356578	53202093400
187	385.425853	40601023346
188	385.503977	35254652134
189	385.513204	33326834001
190	385.543202	30531161665
191	385.622155	26112140073
192	385.979156	58725946682
193	386.133561	13630889677465
194	386.143948	1354497091044
195	386.302402	93103984224
196	386.412732	60205108153
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199	386.567013	47445336506
200	386.626639	46642839507
201	386.655076	42953038035
202	386.764245	38129549260
203	386.828436	35414737395
204	386.855756	30837865463
205	386.931931	36143015989
206	386.953815	32046562934
207	387.005556	31143879865
208	387.023281	29214177040
209	387.066048	29131510311
210	387.137143	2947394813589
211	387.256634	46120778221
212	387.303975	45049650996

Mass Spectrum List Report

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215	387.455045	35305145143
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217	387.532752	36507719570
218	387.555065	31343649435
219	387.615706	35753472566
220	387.646090	30090253419
221	387.730214	33348584270
222	387.742246	29484430476
223	387.751906	29704822126
224	387.774640	27916742917
225	387.797613	29468632601
226	387.854126	36436966037
227	387.882080	31053264146
228	387.914978	26341398181
229	387.966408	25628943003
230	387.985390	25361417177
231	388.038398	28236078396
232	388.060627	31093656027
233	388.077820	30732543520
234	388.140917	107409943189
235	388.165358	27593842207
236	388.238048	26092081396
237	388.265965	29295938728
238	388.308575	29890674893
239	388.332429	28483429274
240	388.343197	27589924208
241	388.441677	30428322691
242	388.509350	30118145693
243	388.548305	26754887827
244	388.717519	26071543889
245	388.753912	25512777845
246	388.869405	26132609382
247	388.898563	25421790703
248	388.934854	26131926264
249	389.199278	28696304584
250	389.221085	27827800969
251	389.289840	26428277499
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253	389.969540	26313678231
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255	398.242419	202373015000
256	406.118954	231547817982
257	410.304991	25479231069
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259	428.100901	159702776245
260	428.419033	23487682140
261	429.104689	37477879508
262	435.343321	23089650784
263	447.038595	23291545451
264	462.076123	47271426644
265	480.551697	92704077078
266	481.102204	23467611819
267	481.554951	30653998143
268	484.379715	23953599208
269	497.622895	23245439874
270	503.725783	22740612068
271	508.582854	1412332414123
272	508.672849	26162004705
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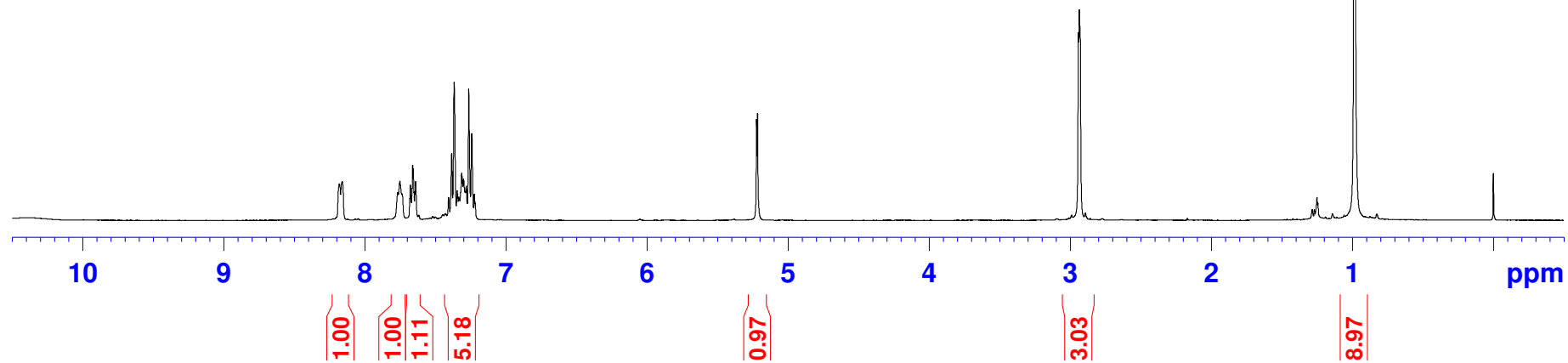
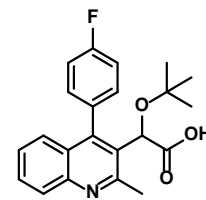
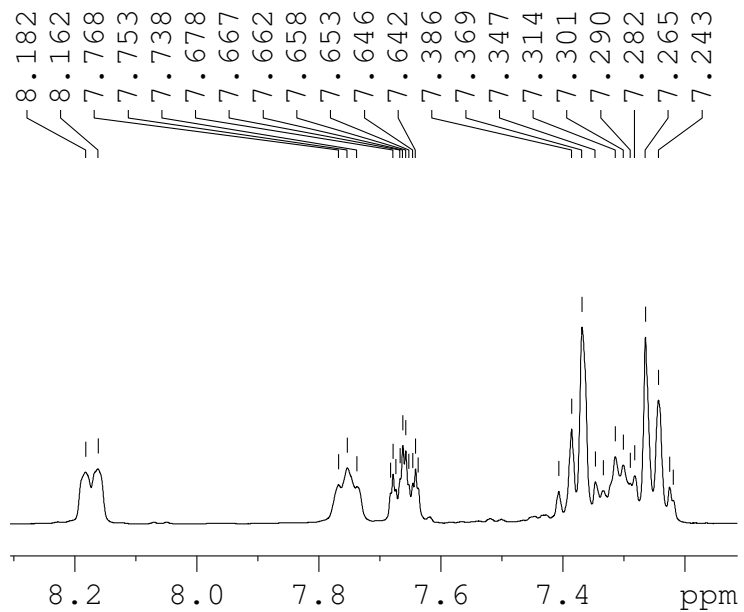
Mass Spectrum List Report

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280	534.976023	25405217050
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282	536.119361	25924784186
283	536.168641	24375691613
284	536.225197	24841425432
285	536.614088	5531971080102
286	536.955288	32065620331
287	536.984870	32452753823
288	537.049772	31265648193
289	537.073668	30686528693
290	537.286586	29318008365
291	537.510119	44483409120
292	537.617610	1838632918845
293	538.621220	198439987581
294	550.593807	29318398951
295	552.609648	68274040033
296	553.612897	29017400678
297	563.365113	26173222242
298	564.479092	25553066428
299	564.579009	45482244090
300	564.645727	1485695661014
301	565.649283	451024776649
302	566.652924	36955735618
303	568.592837	23097818940
304	569.404585	23660829732
305	572.560894	23983661699
306	574.210486	24233004236
307	592.476360	25883904556
308	592.677144	1817092120555
309	592.783197	36406401517
310	592.845787	35278667757
311	593.680633	678187817301
312	594.684179	65282981125
313	602.654392	25212504198
314	607.071775	23285591446
315	608.673265	28005737161
316	613.430983	26635658107
317	620.709216	43274532056
318	662.759933	23566555439
319	665.155105	26135944572
320	666.101271	22973552541
321	666.424280	23007900344
322	677.843898	23040739965
323	685.438383	72086164525
324	686.442240	25236573521
325	703.574240	28056164567
326	721.993936	23103373760
327	747.492421	23594531930
328	751.838450	23134526334
329	787.006136	25042004610
330	835.234466	27309963016
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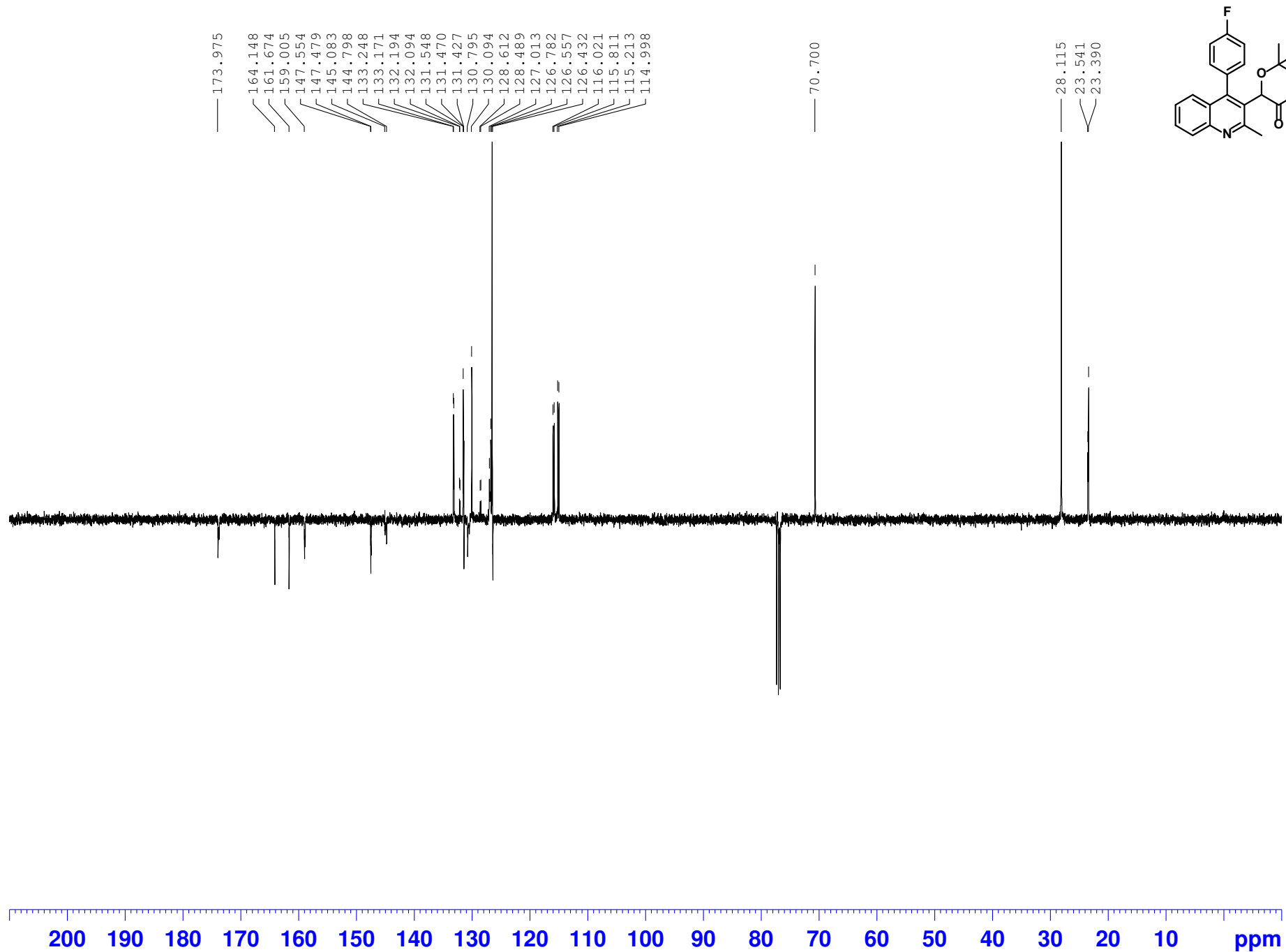
NGJ-8-100 characterization (400MHz, CDCl3)

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PROCNO    1
Date_     20171201
Time      18.47 h
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TD         65536
FIDRES    0.244532 Hz
AQ         4.0894966 sec
RG         90.5
DW         62.400 usec
DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec
TD0        1
SF01      400.1724710 MHz
NUC1       1H
P1         9.88 usec
SI         65536
SF         400.1700075 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
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NGJ-8-100 characterization (400MHz, CDC13)



Mass Spectrum List Report

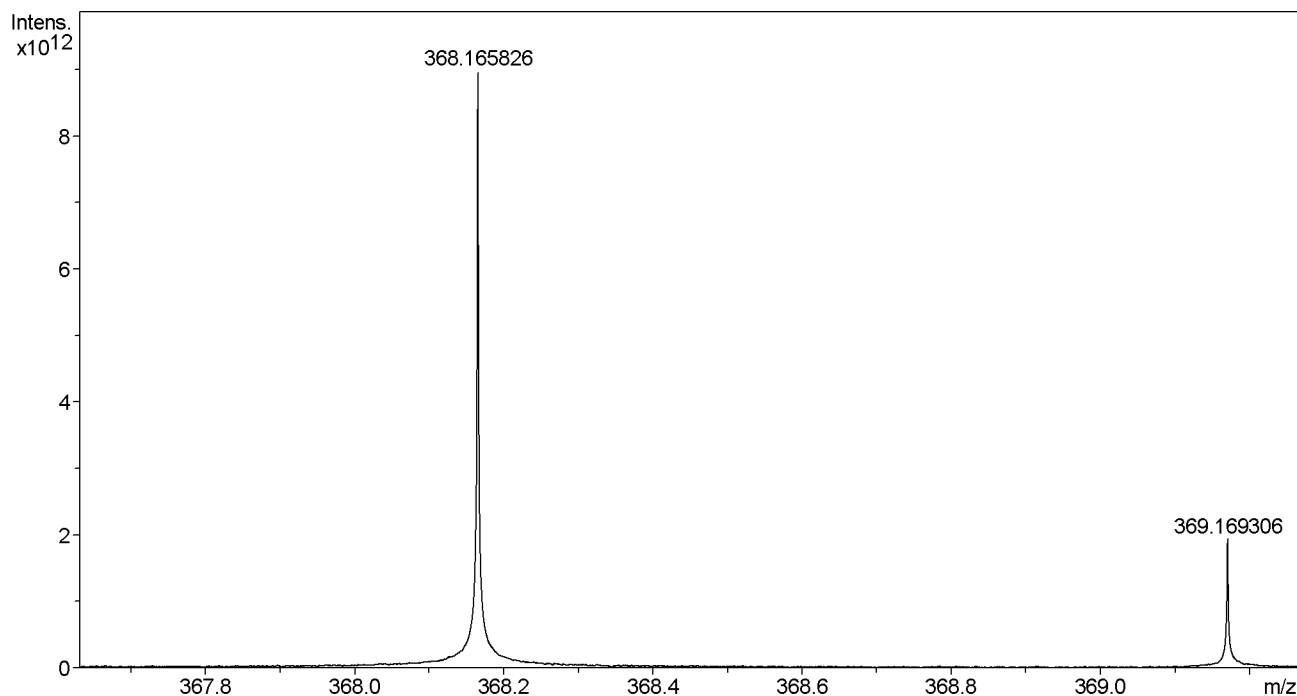
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-8-100_pos_000001.d
Method
Sample Name NGJ-8-100
Comment NGJ-8-100 in THF:MeOH C22H22FNO3 H+

Acquisition Date 3/19/2018 3:59:29 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-8-100 in THF:MeOH
Exact Mass of C22H22FNO3 H+ = 368.165648 m/z
Mass Observed = 368.165826 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.587286	29428104043
2	188.231366	21202293593
3	189.685592	23912711629
4	190.061808	75853387750
5	190.456284	21218081443
6	191.639829	21570365992
7	191.908687	21513637034
8	192.804667	21554919386
9	199.645191	21103024636
10	199.992880	21956606407
11	200.395320	21277755247
12	201.917945	22422443092
13	202.340548	81512240502
14	202.576100	21369689827
15	203.723946	22362429648
16	204.172700	21083402888
17	204.895441	21607673596
18	211.395570	23529712775
19	212.821155	21961818494
20	215.224766	21037800775

Mass Spectrum List Report

#	m/z	I
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23	225.664219	21048379591
24	228.294496	22255540082
25	230.914523	21300638718
26	230.969433	22049404968
27	231.649823	21399541736
28	234.244101	21869957666
29	239.949183	21914128764
30	245.170497	23807719984
31	245.715599	24180426662
32	246.393856	21188739722
33	246.684935	21887583257
34	249.152860	21518806174
35	255.212071	23418475510
36	255.254723	24084312304
37	256.207563	24472732120
38	256.986923	21168976854
39	258.706084	21845214515
40	260.187611	21394434868
41	261.856031	21566058180
42	262.945504	21916076789
43	263.954176	21637707313
44	267.953954	21500236923
45	270.054313	21409007901
46	272.236113	26922817202
47	272.437663	21312134992
48	278.220389	26153489451
49	283.115609	22777635133
50	283.184675	21804540940
51	283.218367	21278279257
52	283.562806	42574913004
53	285.374806	22055124499
54	289.965499	21459274567
55	291.628209	24048653305
56	294.443780	23529799711
57	296.011248	28581643140
58	298.347312	24329205924
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60	303.141719	33428311737
61	304.261355	52140151606
62	305.499451	22876753972
63	306.276946	21680759803
64	309.626456	22951122527
65	311.223910	24715028673
66	312.102744	34135525196
67	312.163012	22398968064
68	314.377988	23445295202
69	315.564510	21956640988
70	318.240769	39444096841
71	319.657451	21939176622
72	320.256386	54324095472
73	322.318986	25122932663
74	323.755605	26309094838
75	326.148845	21775535733
76	333.259135	22306231955
77	336.251394	31207746905
78	339.306527	22267727224
79	341.952986	22179617197
80	345.279460	25079947512
81	347.946088	24167717274
82	349.074646	22664770265
83	350.230690	23429183386
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Mass Spectrum List Report

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85	364.191202	23135689584
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88	366.826844	22621238447
89	367.509035	22837209830
90	367.572222	27611088877
91	367.606597	26746928355
92	367.654777	26530051411
93	367.668221	28072032185
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95	367.770567	23768921092
96	367.805670	29511969018
97	367.861038	32246462692
98	367.897439	34143205999
99	367.918000	33120524913
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101	367.972969	42043841622
102	368.036012	62228498823
103	368.165826	8976712369285
104	368.268222	63648690994
105	368.325391	50715750995
106	368.354500	37877610565
107	368.410409	33444684299
108	368.451236	33560952182
109	368.508999	27863971359
110	368.520315	31119575425
111	368.561800	24251410848
112	368.784498	25939171210
113	369.169306	1933774614521
114	369.229856	29979166319
115	369.569625	23389620523
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118	370.172849	105486679590
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121	383.177595	23435661312
122	384.136550	38441102863
123	387.482352	23611285449
124	390.148130	167984441468
125	391.151470	41577473475
126	391.164757	26261113984
127	398.241897	415760284509
128	399.245253	73466834112
129	405.516794	22976092972
130	408.181083	28317779985
131	412.130120	25289907273
132	424.179910	24561969433
133	424.228895	41694949574
134	425.287891	99766621964
135	435.345045	110485573132
136	437.952342	22404025911
137	452.519673	40161835580
138	453.447404	22233044806
139	480.550917	85435717979
140	481.554482	39253338015
141	484.235821	23606813704
142	493.175701	90344927228
143	495.212049	28829477673
144	505.426691	22458670635
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Mass Spectrum List Report

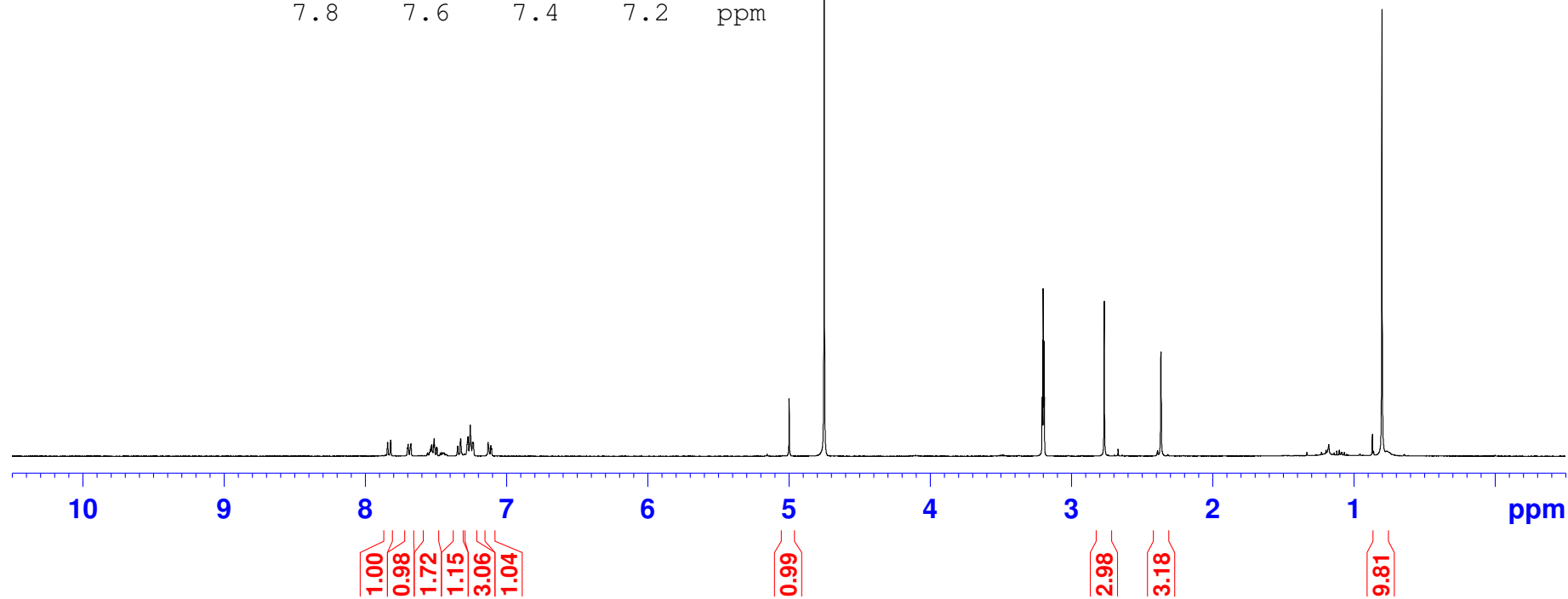
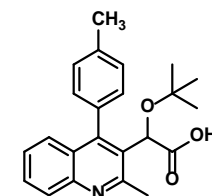
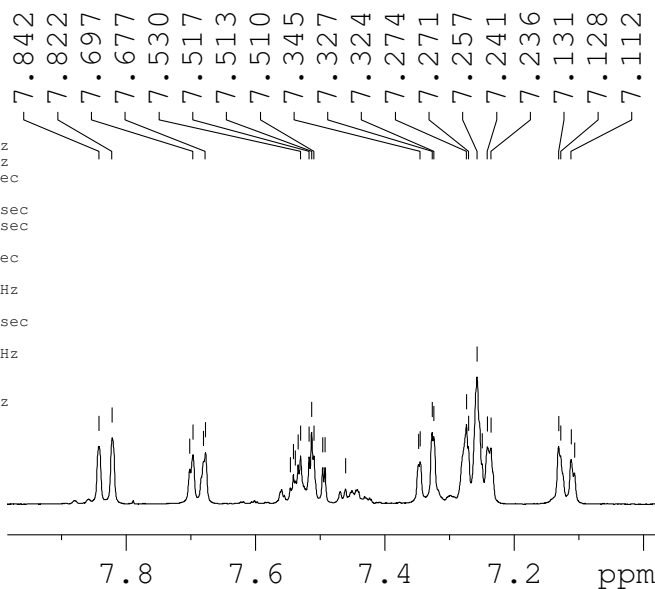
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154	536.254714	22686557462
155	536.613428	2905843622817
156	536.843366	28706842942
157	536.917089	25951370234
158	536.930710	26994213896
159	536.955538	24363399846
160	537.177998	22818626242
161	537.380482	24241015115
162	537.413155	22391148860
163	537.466211	23096453555
164	537.535504	32600926885
165	537.616885	1001934152788
166	538.620357	132134655521
167	539.344500	23587032199
168	550.593224	43466758503
169	550.629261	42151977956
170	552.608623	112216846025
171	553.302332	23196809930
172	553.612309	31367048143
173	554.864519	23762433445
174	558.123164	23997062637
175	561.889165	26598934701
176	564.644918	880897818422
177	564.832973	22955185682
178	565.534052	26378933388
179	565.648366	290175634190
180	566.651565	41198984503
181	578.848000	23803868520
182	580.640131	38671033189
183	587.248101	83099257280
184	588.235411	43608319033
185	589.244914	33601036311
186	592.385975	25629828794
187	592.676267	1134389213138
188	592.818144	27846535953
189	592.885783	24101766542
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191	594.683051	59611854440
192	599.549288	61829378317
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202	680.435994	24003212210
203	685.437006	51185341786
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208	883.691098	24567909324
209	909.351834	23515518842
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Mass Spectrum List Report

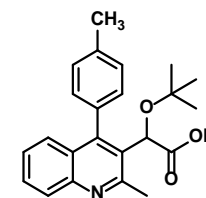
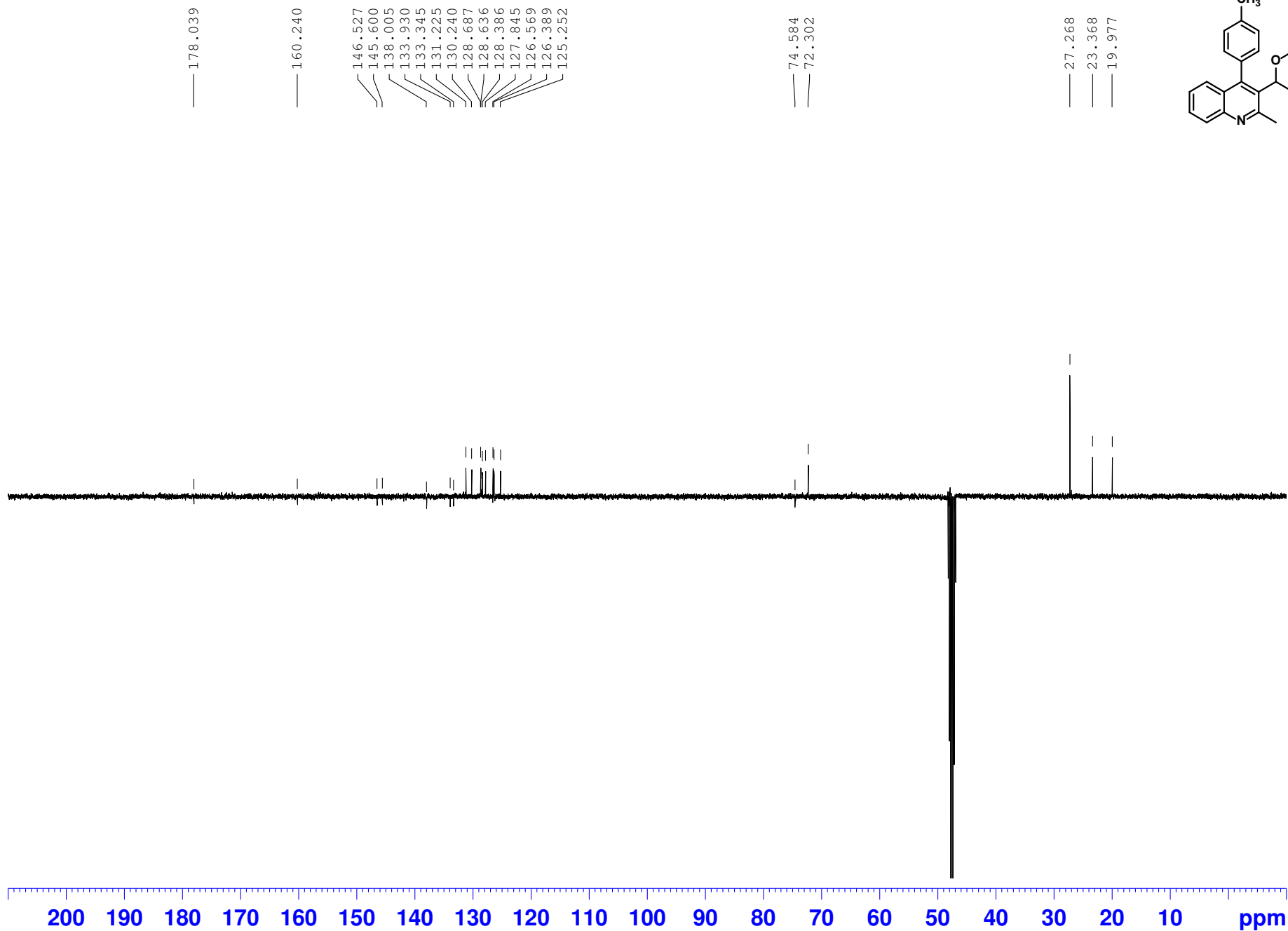
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NGJ-9-022 (CD3OD, 400MHz) Pure Yellow Oil - saponification of 4-methylphenyl quinoline

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 Date_ 20171221
 Time_ 16.50 h
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 PULPROG 65536
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700519 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NGJ-9-022 (CD3OD, 400MHz) Pure Yellow Oil - saponification of 4-methylphenyl quinoline



Mass Spectrum List Report

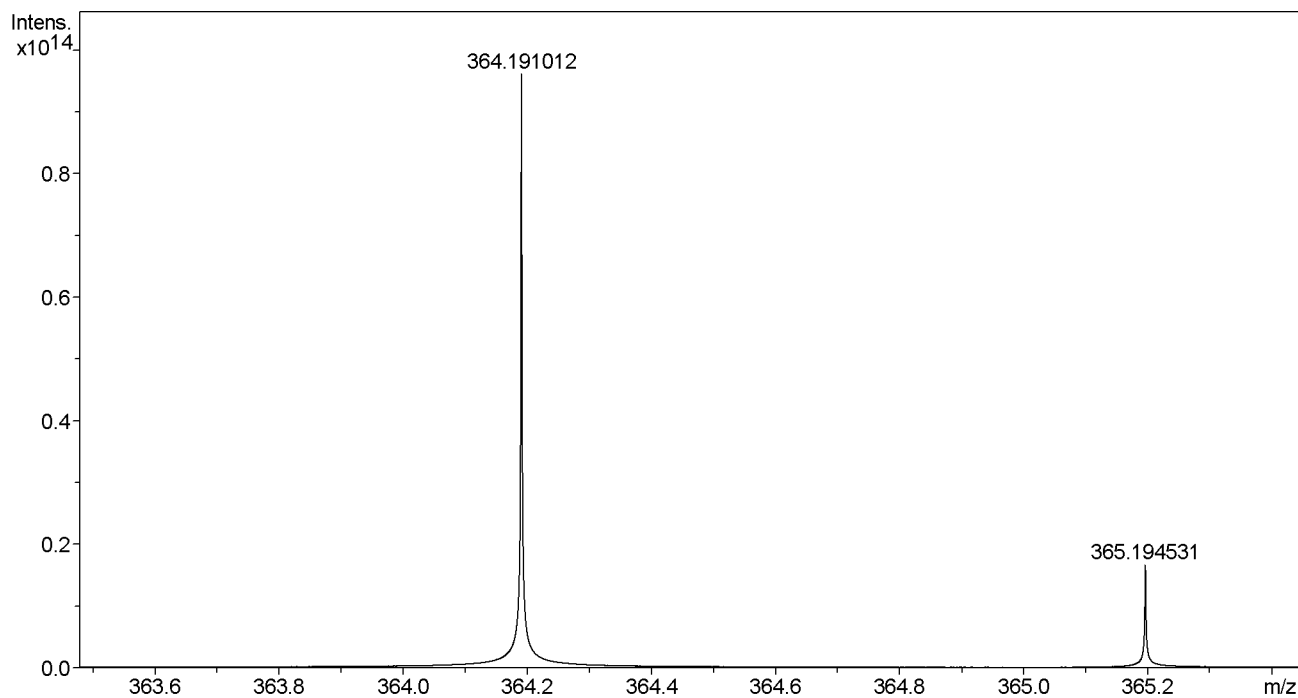
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-9-022_pos_000001.d
Method
Sample Name NGJ-9-022
Comment NGJ-9-022 in THF:MeOH C23H25NO3 H+

Acquisition Date 3/19/2018 2:54:39 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-9-022 in THF:MeOH
Exact Mass of C23H25NO3 H+ = 364.190720 m/z
Mass Observed = 364.191012 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.390484	26121340009
2	185.239329	27130217344
3	185.612710	26391942156
4	186.030889	117969552307
5	186.554601	680331019976
6	187.385720	27411029276
7	187.446888	30165753968
8	189.079212	27657244545
9	189.191218	26941872343
10	189.759607	26862098226
11	190.925524	27557996441
12	191.446331	27994216710
13	191.870158	28136291263
14	192.235430	26726095797
15	192.342017	27098959068
16	192.839923	27121706364
17	193.643766	47480269548
18	193.927230	25934989042
19	194.791813	29518261071
20	196.005217	27398920594

Mass Spectrum List Report

#	m/z	I
21	196.072295	30354712896
22	196.113298	36255918467
23	196.114220	86534104495
24	196.615942	39793569415
25	199.030982	30888572708
26	199.154736	27315693914
27	199.770558	28808296408
28	202.077832	34272316336
29	202.340539	83862114630
30	202.497369	26933006370
31	203.072938	27591224346
32	204.093494	27173366497
33	205.169101	28123315653
34	207.749166	28686423086
35	209.441854	29358358060
36	209.806335	26088464326
37	214.545251	26212148504
38	216.080968	27344366511
39	217.088121	27918221616
40	218.096602	32515625595
41	218.464172	27601850473
42	219.099944	30700106721
43	222.230976	29423067610
44	225.218543	28563888470
45	226.524058	26522856972
46	231.104320	34424479566
47	232.111982	38447115207
48	232.551938	26242094307
49	233.115305	27652658832
50	233.882704	35725973900
51	234.091479	28129749101
52	236.070050	32174840130
53	239.237478	26775330027
54	239.794487	26278653043
55	240.579593	27520294754
56	243.284116	27411499630
57	246.996805	29375506305
58	247.544663	27166093063
59	248.106995	47939064483
60	248.461275	26337203389
61	254.812095	27525424962
62	261.114966	44168657079
63	261.744470	27580645481
64	262.122007	41054476044
65	264.013042	29170032300
66	264.127068	29563436004
67	265.566023	26360542533
68	274.491454	28471594027
69	276.495993	27565009755
70	278.751943	26567475044
71	280.613466	26297930434
72	280.822738	28685898575
73	285.232936	27740897663
74	289.206140	26451128236
75	289.617284	25853076821
76	290.117085	29028692445
77	295.785125	26476626520
78	295.962963	26180606393
79	301.023701	27262530241
80	301.075841	813087137248
81	301.118453	31665341044
82	302.079243	63239449328
83	304.169794	31864817503
84	304.599081	25791021790

Mass Spectrum List Report

#	m/z	I
85	304.984789	26608947645
86	305.835487	26697681626
87	307.120385	32649596036
88	308.128318	101779901185
89	309.131690	41919386246
90	310.283603	48179556116
91	312.081496	26163451005
92	312.100157	149232909890
93	312.173995	333371732045
94	314.447876	26420554406
95	315.091581	140432102896
96	316.094965	37286525042
97	320.670327	31083670306
98	330.750217	30417787859
99	339.899024	67903351375
100	355.762535	37898782344
101	360.527247	38547812089
102	360.958773	37385817859
103	361.532243	35246336400
104	361.696052	38657263615
105	361.728644	35594714522
106	361.746228	35368683899
107	361.794131	40676427357
108	361.835760	36515734534
109	361.875236	35973647105
110	361.897776	37453329619
111	361.920485	38436521350
112	361.974037	41922199102
113	362.005991	41297900795
114	362.021084	40774140878
115	362.101467	43027353570
116	362.143438	45716982254
117	362.212987	47263192835
118	362.241732	51351730318
119	362.294153	41426366386
120	362.345131	41194185959
121	362.405410	54232885274
122	362.437690	47217354895
123	362.529023	55377920428
124	362.566785	48450428214
125	362.592202	49091252747
126	362.607357	50186459611
127	362.631835	47211459353
128	362.719069	51814769876
129	362.812865	56740272271
130	362.837873	55820101461
131	362.863754	59660912668
132	362.875584	58266176749
133	362.969789	58180235490
134	363.045807	65526805270
135	363.094967	65057633644
136	363.151451	71300851584
137	363.186963	59394995556
138	363.194260	73750213134
139	363.261174	72817886101
140	363.375847	78284178958
141	363.404920	81433014169
142	363.434919	88965788914
143	363.472118	89548146550
144	363.500054	91903570279
145	363.538530	100191322943
146	363.596249	103214335393
147	363.610666	112065218742
148	363.649926	110786586086

Mass Spectrum List Report

#	m/z	I
149	363.755428	136427169225
150	363.927256	210653626336
151	364.191012	95995498557340
152	364.588720	130698593891
153	364.721610	90574666050
154	364.784419	85206418296
155	364.829401	80555930791
156	364.891768	60041860567
157	364.938300	56023337177
158	365.194531	16711533920179
159	365.290133	161601114228
160	365.376104	118958510649
161	365.437195	100135956497
162	365.526632	75479320354
163	365.564802	80440344684
164	365.680969	68278315714
165	365.697104	69545920553
166	365.789735	60725645434
167	365.812969	67589264073
168	365.834808	56885096748
169	365.867476	56906591822
170	365.893409	59099725951
171	365.931775	56353912992
172	365.953410	58815251520
173	365.992857	61568746779
174	366.014529	53510240295
175	366.058674	56634363444
176	366.198121	1177730396501
177	366.280183	40062577476
178	366.351363	44799386555
179	366.518541	40940965163
180	366.546206	44161829340
181	366.650979	40997697407
182	366.686946	40594802027
183	366.739728	39647926631
184	366.785625	35970421463
185	366.854715	45603273853
186	366.867020	36333253787
187	366.903697	38116633456
188	366.949225	38494925889
189	367.051833	37643369380
190	367.188032	39105123566
191	367.339379	35075935140
192	367.909762	39601904859
193	369.333898	37146408755
194	370.682020	35044129076
195	370.787208	40668454509
196	372.233034	456085844096
197	373.236358	67374698958
198	379.180994	154510484111
199	381.225791	38224168488
200	382.463559	1436836473004
201	382.466769	304408845503
202	385.751891	35117891883
203	386.173593	291558851679
204	387.176920	100334368685
205	390.704030	33479478317
206	390.722208	35231198760
207	390.821627	32950439760
208	390.909991	32931571676
209	390.926584	33450808140
210	391.087341	33855239710
211	391.146441	38523534779
212	391.214398	48229998517

Mass Spectrum List Report

#	m/z	I
213	391.298525	44732976914
214	391.365223	37489271147
215	391.425181	42129108351
216	391.486039	50347916532
217	391.558605	51004316658
218	391.649737	50039033413
219	391.741714	62014537649
220	391.778536	63394826406
221	391.853916	71215565513
222	391.982551	105077099973
223	392.004145	109844947427
224	392.030377	118524353592
225	392.222462	28128044808847
226	392.452673	90672588132
227	392.519926	73218745509
228	392.542954	73233608490
229	392.586527	59689348967
230	392.641388	49846088754
231	392.657463	52792480821
232	392.713141	49875897869
233	392.738966	38906793671
234	392.806143	32696126059
235	392.843532	41506053813
236	393.225843	6872699187433
237	393.346659	71387307220
238	393.416059	53469227785
239	393.439840	49404610261
240	393.466245	50366102281
241	393.500884	48461214586
242	393.537608	44549951575
243	393.566498	42586605246
244	393.609470	37153000375
245	393.648649	42634122770
246	393.683909	36463027202
247	393.701358	37111278828
248	393.737282	32631343717
249	393.867437	34092847243
250	394.145586	33889826315
251	394.227387	62347623984
252	394.229727	214904196561
253	398.242381	103389787164
254	406.238619	708857403438
255	406.272580	33206951928
256	407.242215	99866746991
257	408.153399	136586897157
258	408.155655	296679022140
259	409.158886	48652408441
260	414.204870	674458262160
261	414.247422	28757933169
262	415.208419	75556148460
263	420.218020	27903822475
264	420.252949	597995293554
265	420.254269	580798517430
266	421.251768	58364958698
267	421.257520	458214509639
268	430.772803	27904261485
269	433.404688	28813235318
270	435.345963	29686421828
271	436.481777	28306915884
272	442.236072	34948343255
273	448.223200	30926942032
274	448.285605	1048581133215
275	448.340724	26891044798
276	448.360933	30504236565

Mass Spectrum List Report

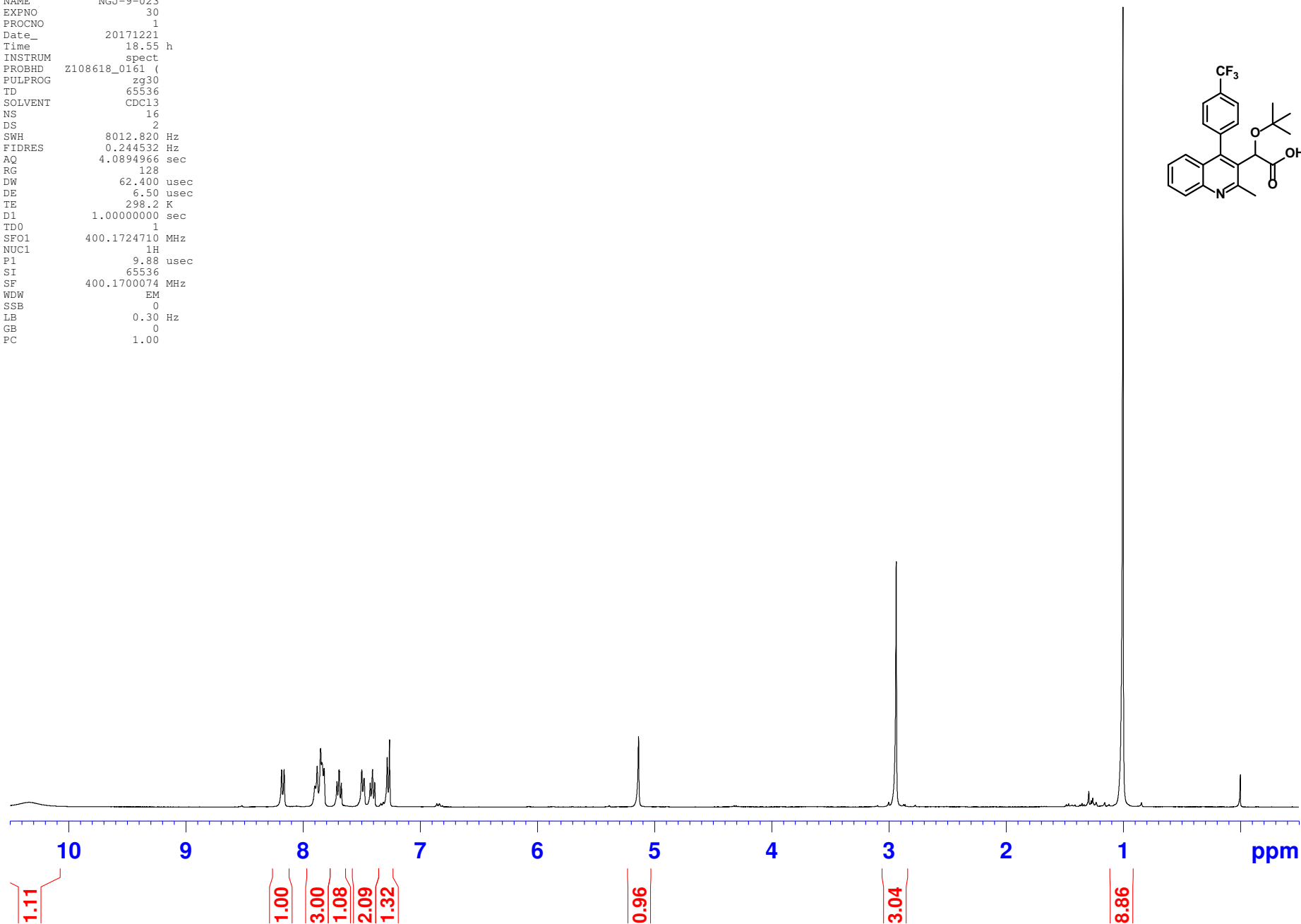
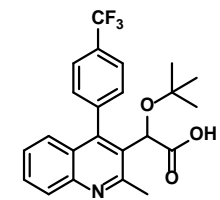
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277	449.289199	164627236181
278	453.211734	26520545324
279	458.216162	28187453580
280	481.263148	31103354752
281	482.801832	31290644137
282	484.503490	30512096024
283	487.082386	28647959636
284	490.069807	30503480955
285	501.053539	27614567894
286	508.583232	130361350485
287	509.586506	46448054571
288	511.053233	31183630971
289	524.578114	190837526270
290	525.289785	38338023179
291	525.581558	52269400586
292	536.542793	27758865112
293	536.581108	55536455165
294	536.614459	893055922157
295	537.396568	36886784842
296	537.617889	199219720844
297	538.621253	31233136291
298	548.601075	29710201694
299	552.537024	32143274461
300	552.609391	1034793338886
301	552.687797	35088691954
302	553.612909	227631243762
303	564.646086	250752466822
304	565.613003	27975479908
305	565.649377	52488328540
306	573.592519	29091981070
307	575.873561	30611754590
308	579.163246	36095610481
309	580.641086	214575743146
310	581.258679	73686667868
311	581.644660	62065392924
312	582.262086	33877333883
313	583.274278	130320099873
314	584.277560	28997313736
315	585.271178	54787170172
316	592.602975	33328604313
317	592.677423	736757717356
318	593.179325	32597916664
319	593.680889	195939735383
320	607.179358	27615866502
321	608.672457	406044815462
322	609.675945	117229213098
323	613.431145	50494195694
324	620.708981	40085695163
325	648.740306	42590791250
326	657.457275	58819479092
327	658.460467	38454801102
328	661.207172	29054915972
329	668.350638	28144604720
330	685.438179	179493095453
331	686.441337	64686173340
332	701.484102	45714049842
333	715.978104	27754199820
334	733.777938	27556887614
335	742.375526	28181272030
336	759.964561	28514714028
337	760.885232	28815545803
338	775.909068	31135494883
339	840.152161	30764128064
340	861.540272	28603245088

Mass Spectrum List Report

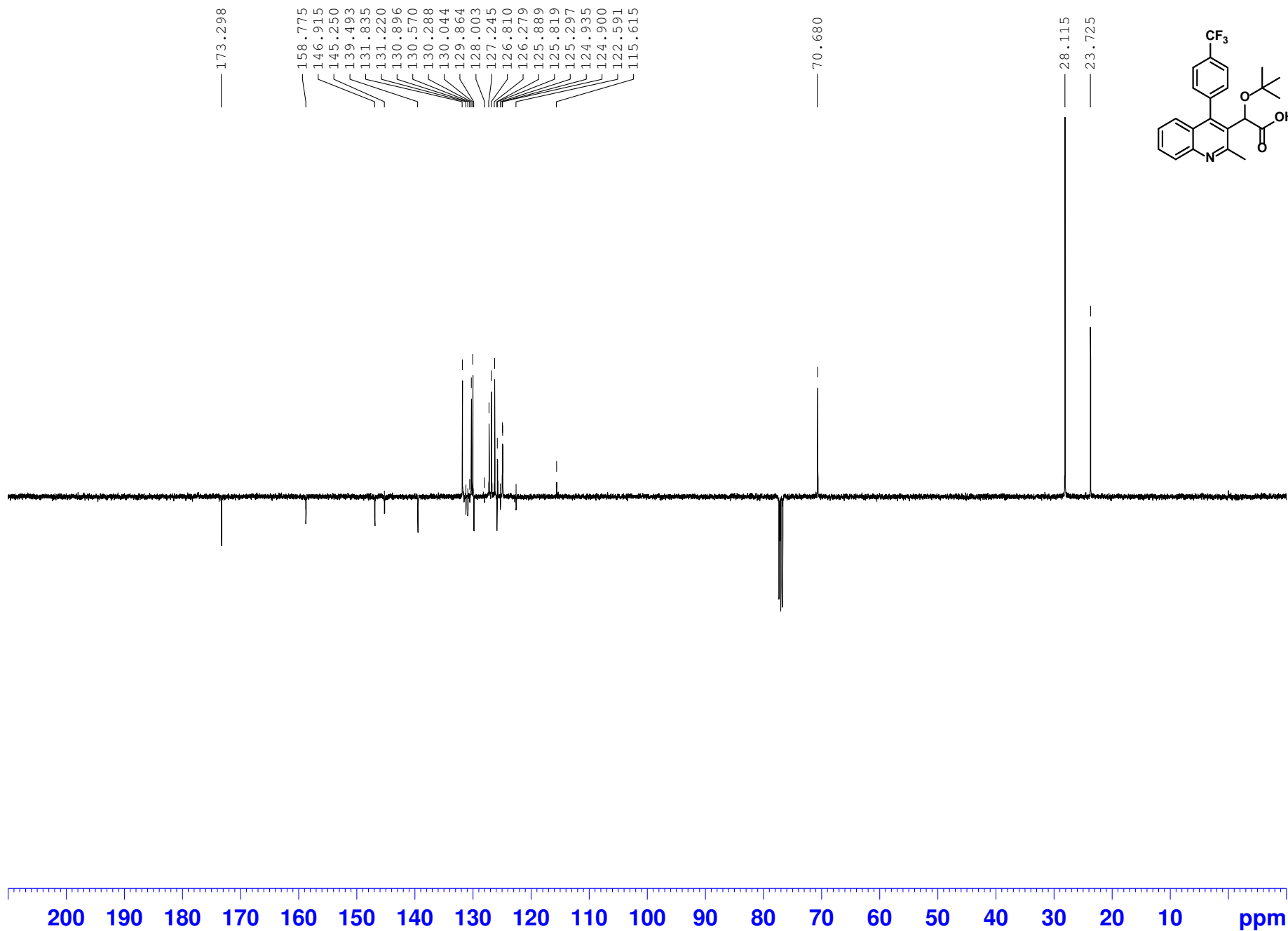
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341	964.855186	34389604639
342	986.982656	28939406768

NGJ-9-023 (CDC13, 400 MHz) Pure Yellow Oil - saponification of 4-trifluoromethylquinoline

NAME NGJ-9-023
EXPNO 30
PROCNO 1
Date_ 20171221
Time_ 18.55 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700074 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NGJ-9-023 (CDCl₃, 400 MHz) Pure Yellow Oil - saponification of 4-trifluoromethylquinoline



Mass Spectrum List Report

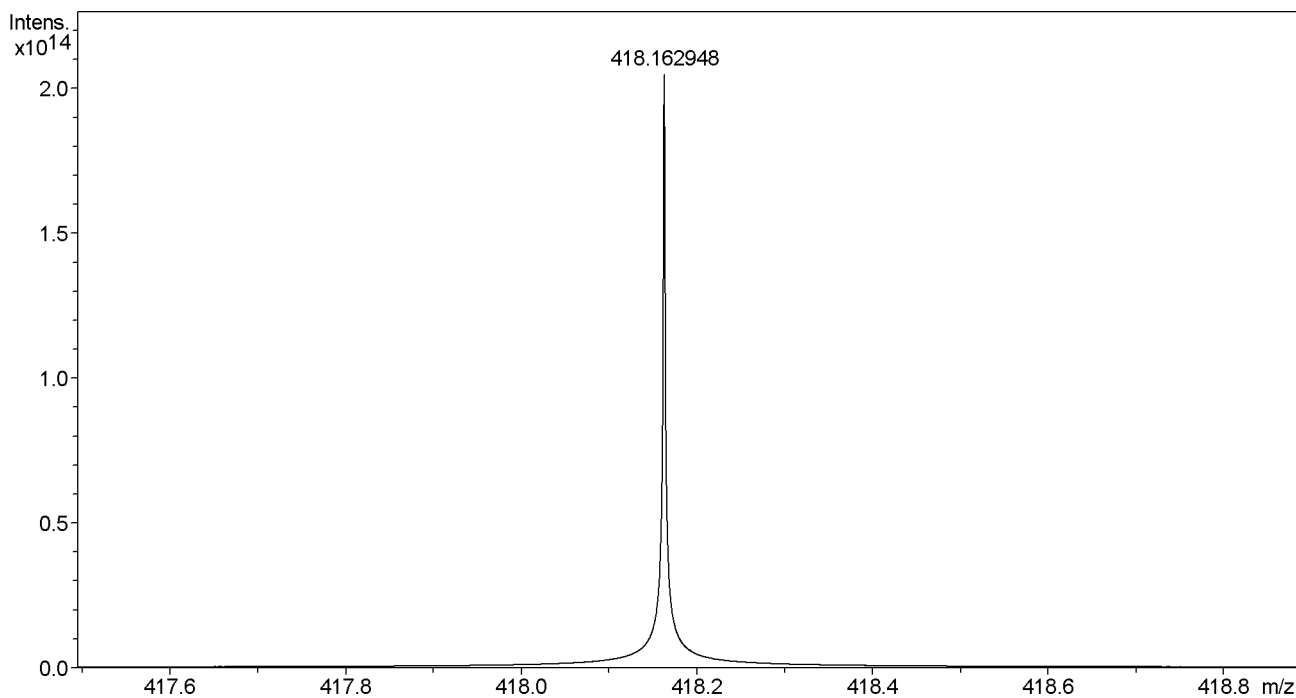
Analysis Info

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Method
Sample Name NGJ-9-023
Comment NGJ-9-023 in THF:MeOH C23H22F3NO3 H+

Acquisition Date 3/19/2018 3:01:42 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-9-023 in THF:MeOH
Exact Mass of C23H22F3NO3 H+ = 418.162455 m/z
Mass Observed = 418.162948 m/z

Difference < 2.0 ppm



#	m/z	I
1	202.340542	86751206538
2	208.834936	29843734451
3	209.080712	86335676380
4	209.084893	1673091714989
5	209.098245	37852187642
6	209.441923	48971971400
7	209.586633	436414815461
8	210.088373	27197991636
9	216.081010	36543265867
10	218.096591	43464272274
11	247.099391	27445481421
12	254.776910	27681524466
13	269.389760	41775973696
14	270.635987	431826604565
15	271.878647	78589768245
16	271.899725	4337416885871
17	271.928570	63779616472
18	271.948436	34638403230
19	272.021662	26814662402
20	283.563205	27634319208

Mass Spectrum List Report

#	m/z	I
21	284.068533	28094777763
22	285.076168	67437196183
23	288.099977	31532073034
24	294.519073	27153446276
25	299.091974	28404140765
26	300.099756	46285574461
27	315.086651	34637826822
28	316.094362	81583163239
29	316.191433	91259741997
30	316.228001	28505789768
31	317.097297	35431311719
32	317.102483	27728338574
33	330.073980	36218937019
34	339.085068	29355234851
35	361.092793	30660263878
36	362.099956	89811557175
37	363.103583	70458037502
38	364.191532	28778331519
39	366.072286	92061332578
40	374.173666	116217420162
41	409.562366	36346536963
42	409.692373	35889210817
43	409.804259	35296557243
44	410.662479	35355422133
45	410.739336	35986955457
46	411.012717	37511119970
47	411.100102	35768018816
48	411.229053	38556788610
49	411.397883	38343978952
50	411.541449	39606517838
51	411.655041	41034158527
52	411.707896	41892027621
53	411.830618	38849515275
54	411.848383	39861531827
55	412.140356	36949294799
56	412.182276	39092902939
57	412.398061	42836930940
58	412.582670	44111407937
59	412.729315	42595641933
60	412.812110	42073760110
61	412.886585	42932633532
62	412.945710	42680138671
63	412.994781	43349104804
64	413.035099	43131544528
65	413.116052	44688721618
66	413.317294	46310252717
67	413.384626	47957066644
68	413.493262	50862867674
69	413.557338	47550243873
70	413.717419	47830426373
71	413.879692	49908366039
72	413.927100	50782214612
73	414.496827	57284376779
74	414.684702	62414786182
75	414.705601	57879665753
76	414.783880	64563064762
77	414.911829	62278244140
78	415.063355	69306325025
79	415.158665	67722534428
80	415.360764	72349747664
81	415.463976	74317998524
82	415.528806	72846129803
83	415.628551	75486807055
84	415.732604	83395601948

Mass Spectrum List Report

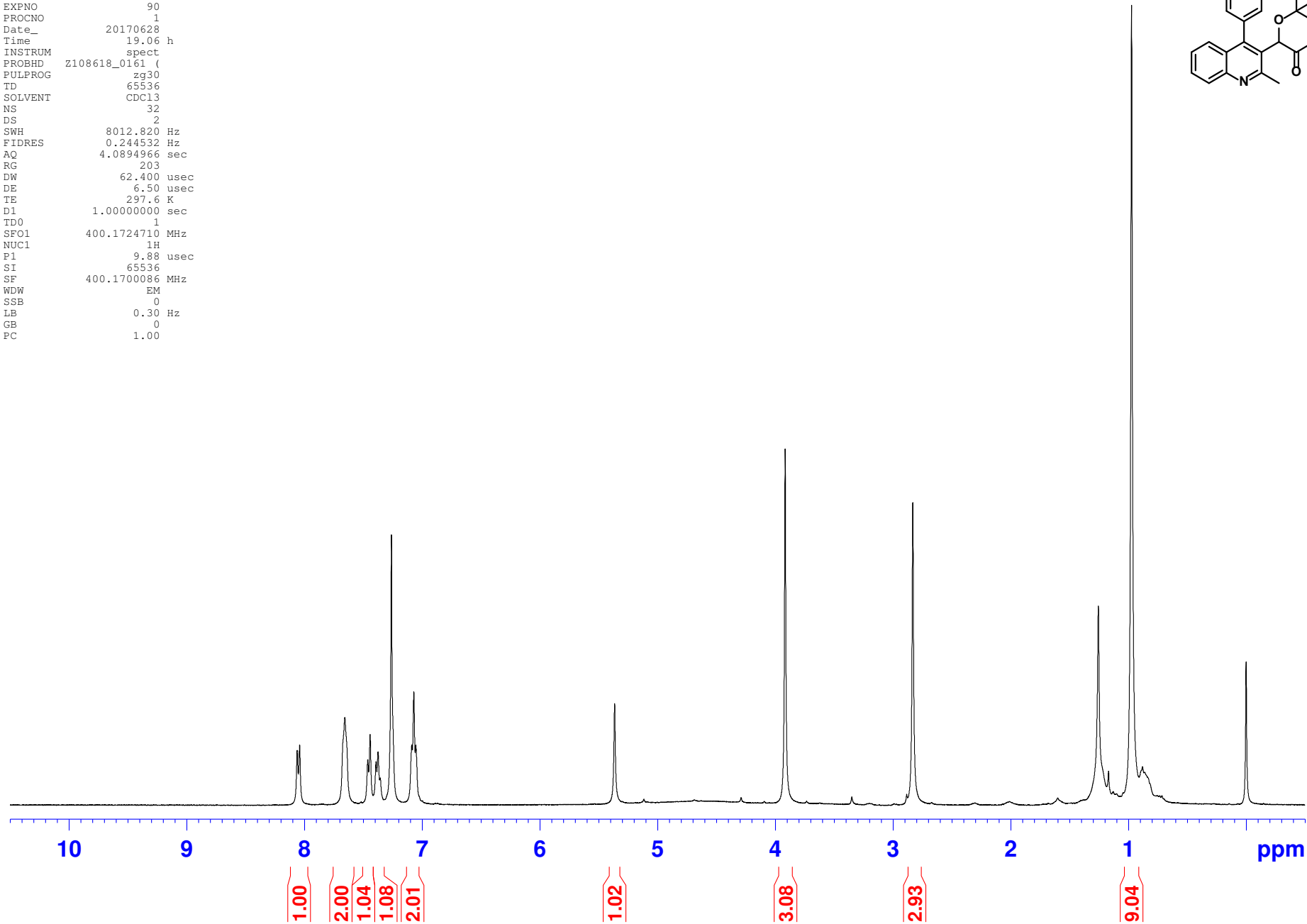
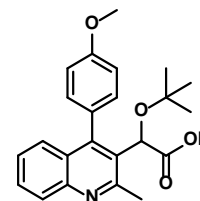
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89	416.226601	97169546209
90	416.547076	114140389986
91	416.878477	141520134633
92	416.948401	152223365519
93	417.155965	189777176546
94	417.274499	205331079785
95	417.657888	350077549111
96	418.162948	205852206981627
97	419.166354	34517495021950
98	419.224784	455137040550
99	419.416051	164131936423
100	419.641846	133220533012
101	419.668302	129703325624
102	419.845036	121106552736
103	419.922795	118197950380
104	419.965263	130168142166
105	420.048557	128768276958
106	420.169834	3855836010915
107	420.480617	75207368010
108	420.609448	78274521178
109	420.664913	75912706094
110	420.739781	74532176777
111	420.852334	71124497059
112	420.946679	68950742690
113	421.101786	69401839235
114	421.171016	105904139806
115	421.257920	66854719534
116	421.301926	62338965509
117	421.376474	65039440501
118	421.449494	62743743079
119	421.623754	57171163925
120	421.750383	55731991966
121	421.821300	54989003641
122	422.057817	49062319546
123	422.124398	48527344386
124	422.172936	51340547667
125	422.253376	50573737116
126	422.347393	52144966566
127	422.428755	51969572681
128	422.491105	56000014562
129	422.570584	51581292254
130	422.655323	46946337324
131	422.757996	50918591676
132	422.985439	47392397340
133	423.006881	43381835381
134	423.015233	43819435212
135	423.081484	43008966439
136	423.129266	43620813954
137	423.350418	46931920925
138	423.409232	47155866777
139	423.465909	43803183714
140	423.551347	45515147856
141	423.734359	44546575962
142	423.836323	37574711474
143	423.861170	37440200887
144	423.911430	42165355583
145	424.078623	42474973349
146	424.110852	42538859116
147	424.176539	39846395568
148	424.368799	43367370452

Mass Spectrum List Report

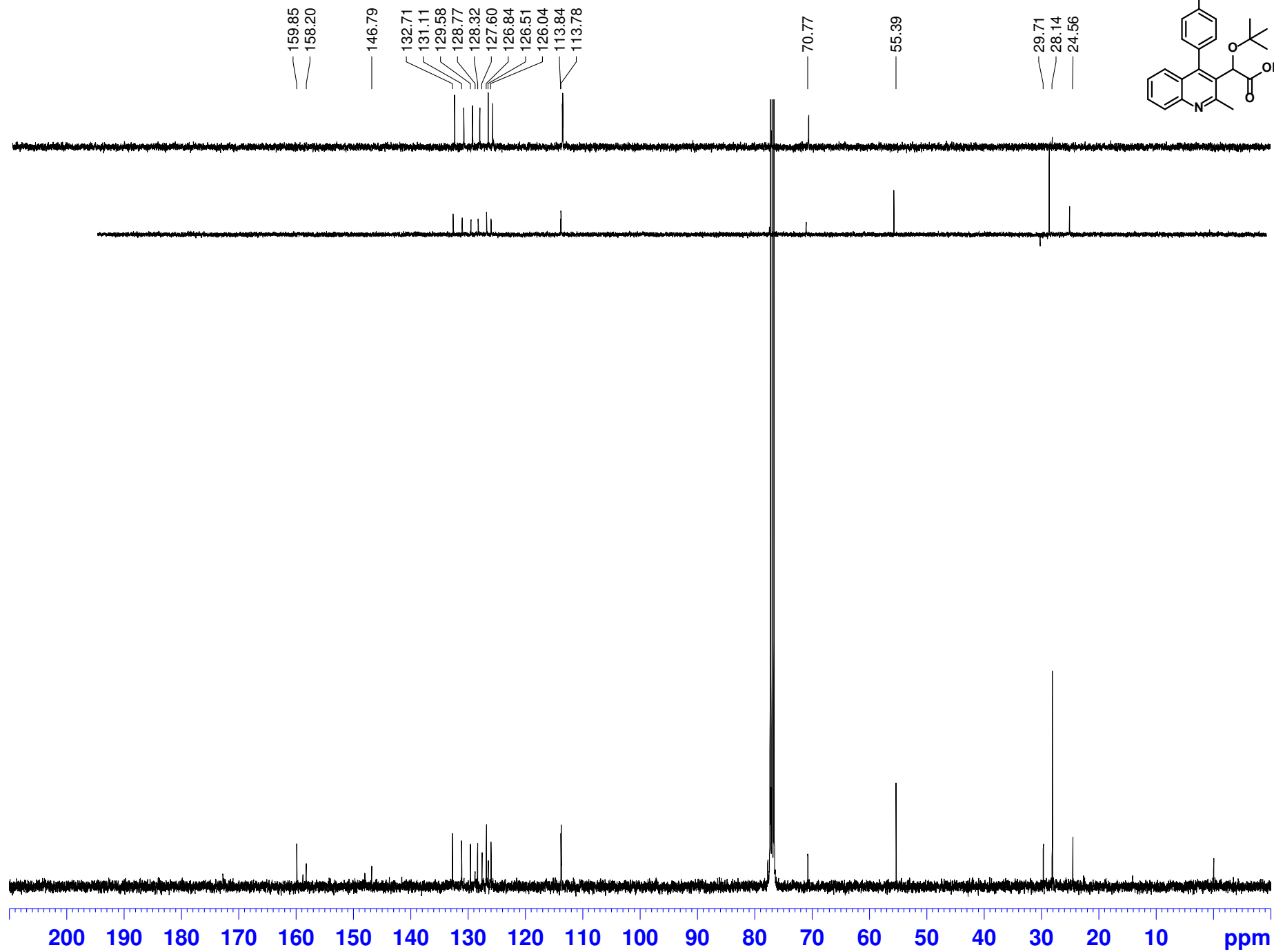
#	m/z	I
149	424.571478	37437591885
150	424.659163	40478563676
151	424.685072	39319378538
152	424.849941	37545554084
153	424.930998	42657082241
154	425.006177	37875198433
155	425.127254	37724915303
156	425.473872	38306884956
157	425.672495	39551176695
158	425.772375	37480002409
159	425.846748	37918609589
160	432.179354	123943179098
161	440.145738	81474585233
162	446.194411	139998442634
163	462.127052	343238650760
164	508.583648	61976618972
165	536.614454	756817591046
166	537.618185	132097051975
167	552.609796	28849186842
168	564.646275	151162331850
169	565.649327	29581177993
170	592.677831	247311187018
171	593.681009	41579293564
172	603.285468	28306381949
173	635.230930	155124151743
174	637.247062	34087056389
175	687.343917	37160958192
176	777.307835	121433546683
177	904.979703	213138073780
178	929.044077	29397931450

JDH-1-145 (CDC13, 400MHz) pure white solid - Saponification of 4 methoxyphenyl quinoline deriv

NAME JDH-1-145
EXPNO 90
PROCNO 1
Date_ 20170628
Time_ 19.06 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 32
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

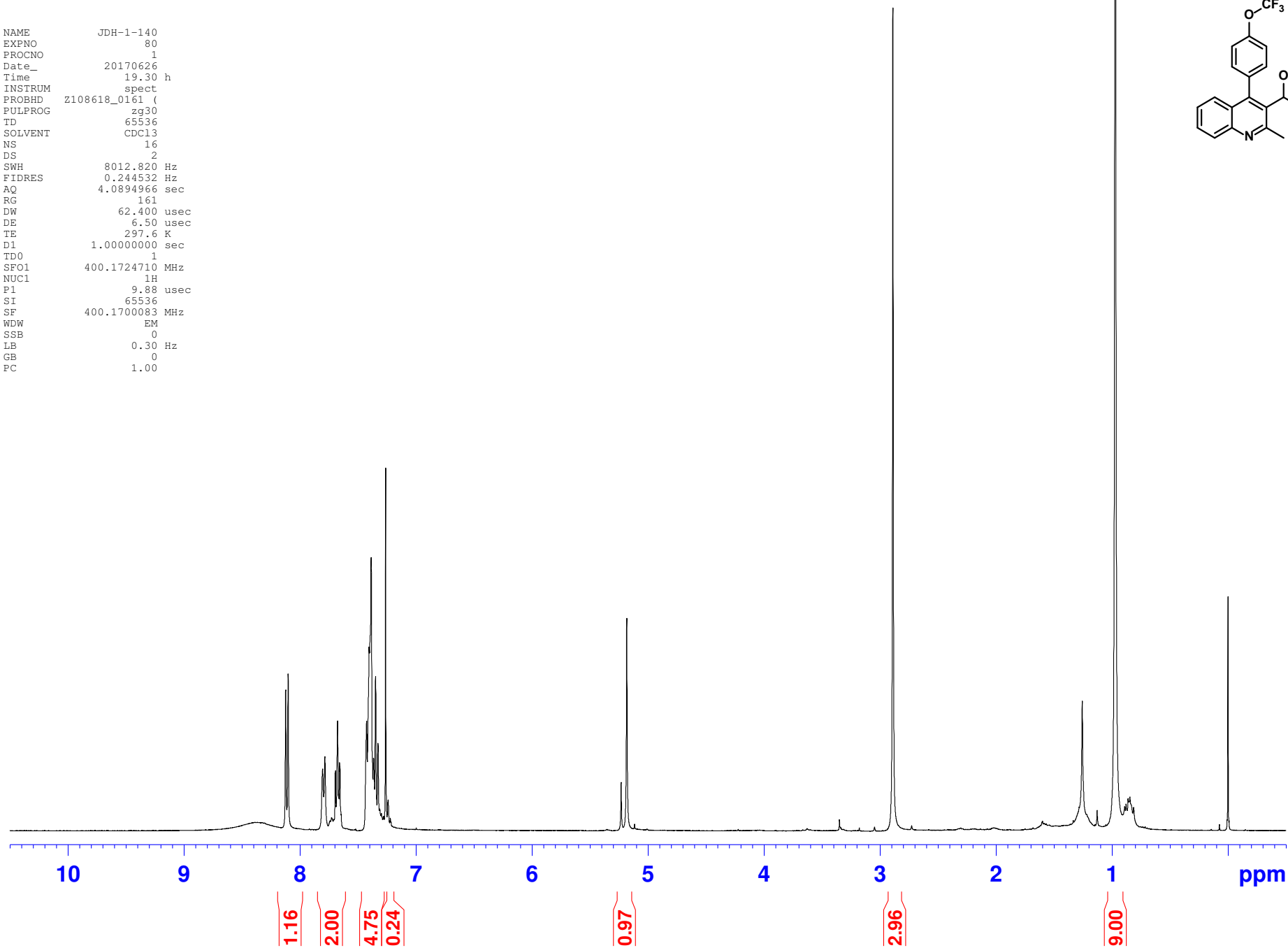
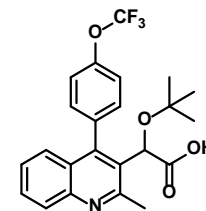


JDH-1-145 (CDCl₃, 400MHz) pure white solid - Saponification of 4 methoxyphenyl quinoline derivative

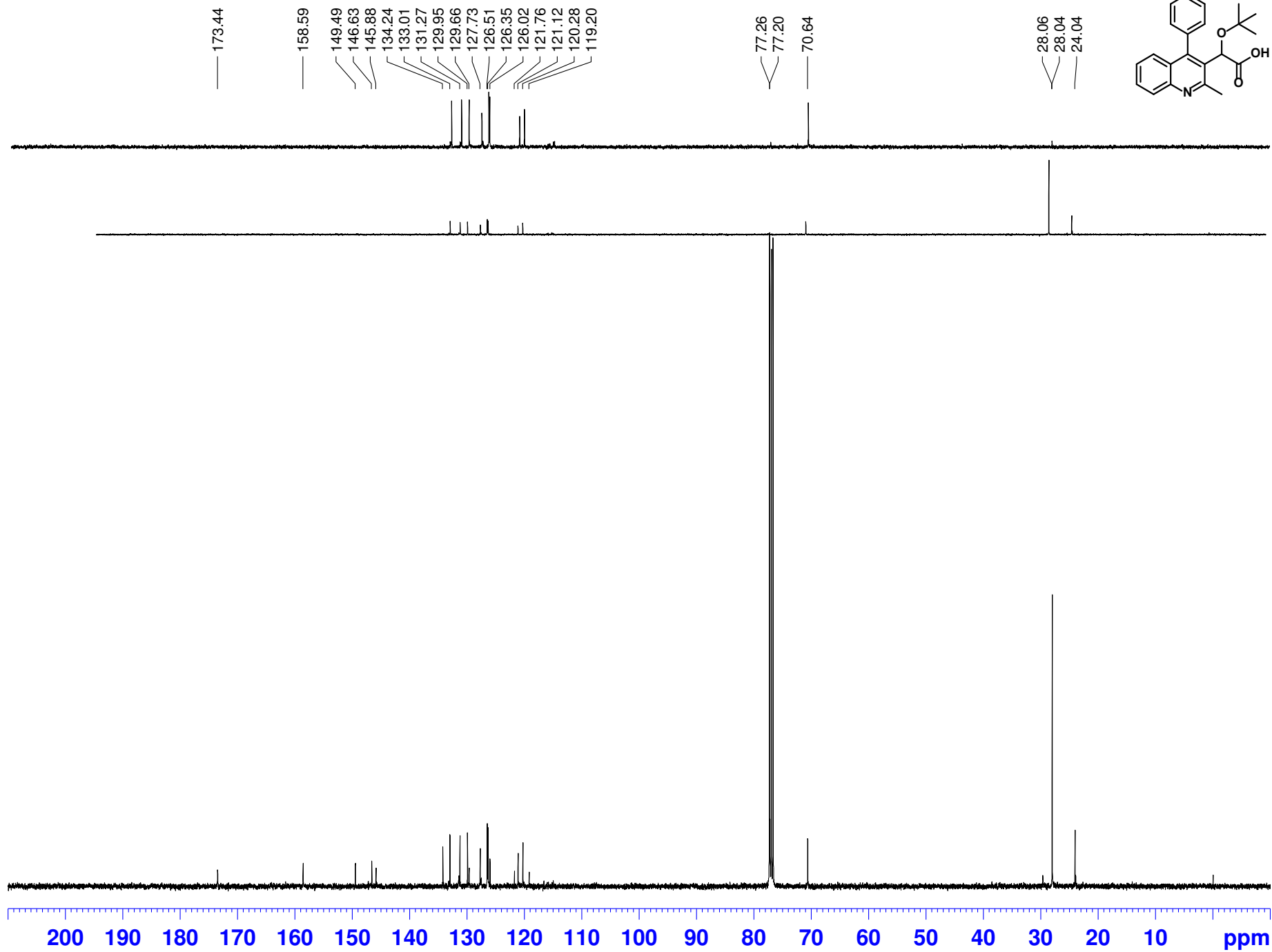
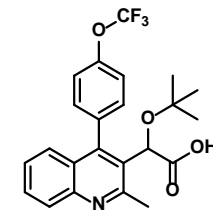


JDH-1-140 (CDC13, 400MHz) pure white solid - Saponification of 4 trifluoromethoxyphenyl quinoline derivative

NAME JDH-1-140
EXPNO 80
PROCNO 1
Date_ 20170626
Time_ 19.30 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700083 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

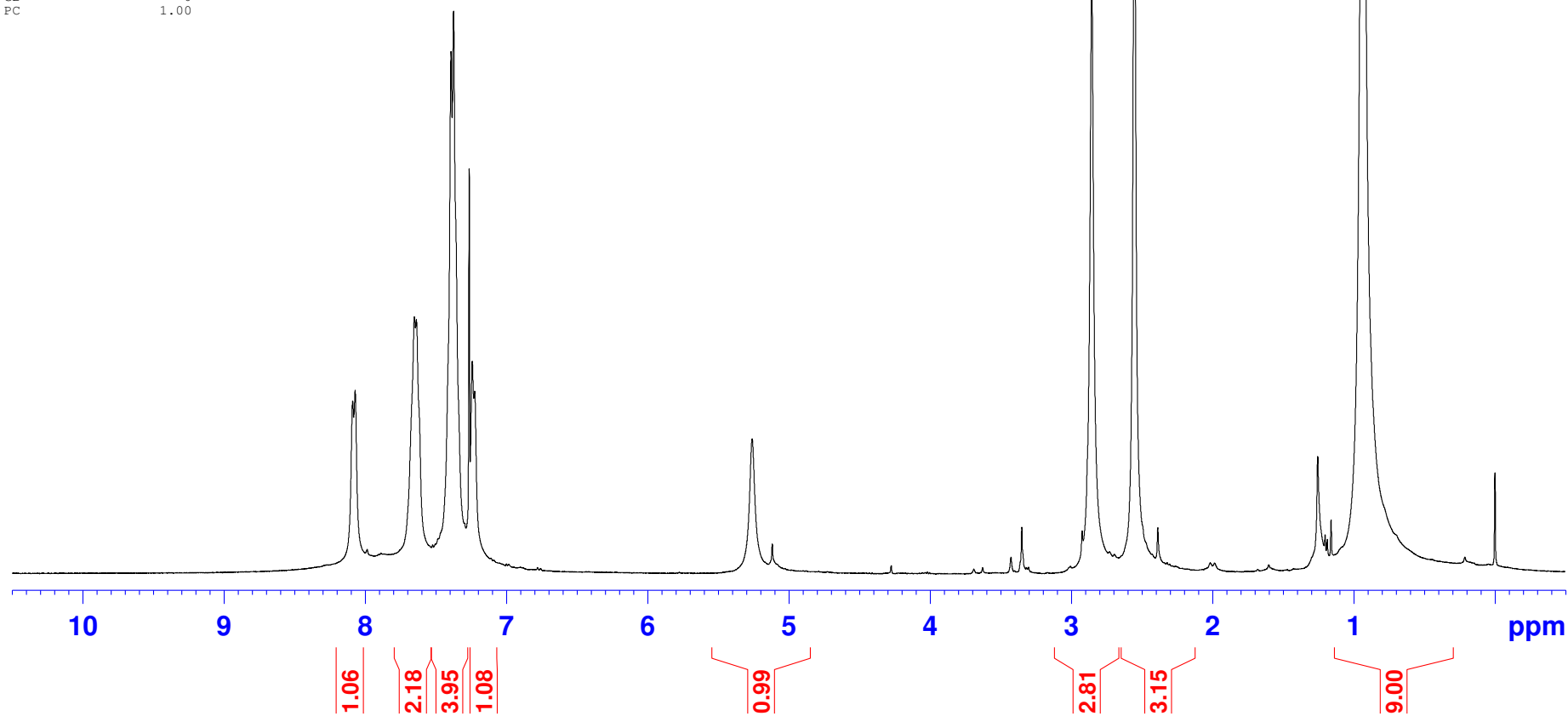
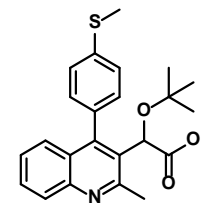


JDH-1-140 (CDCl₃, 400MHz) pure white solid - Saponification of 4 trifluoromethoxyphenyl quinoline derivative



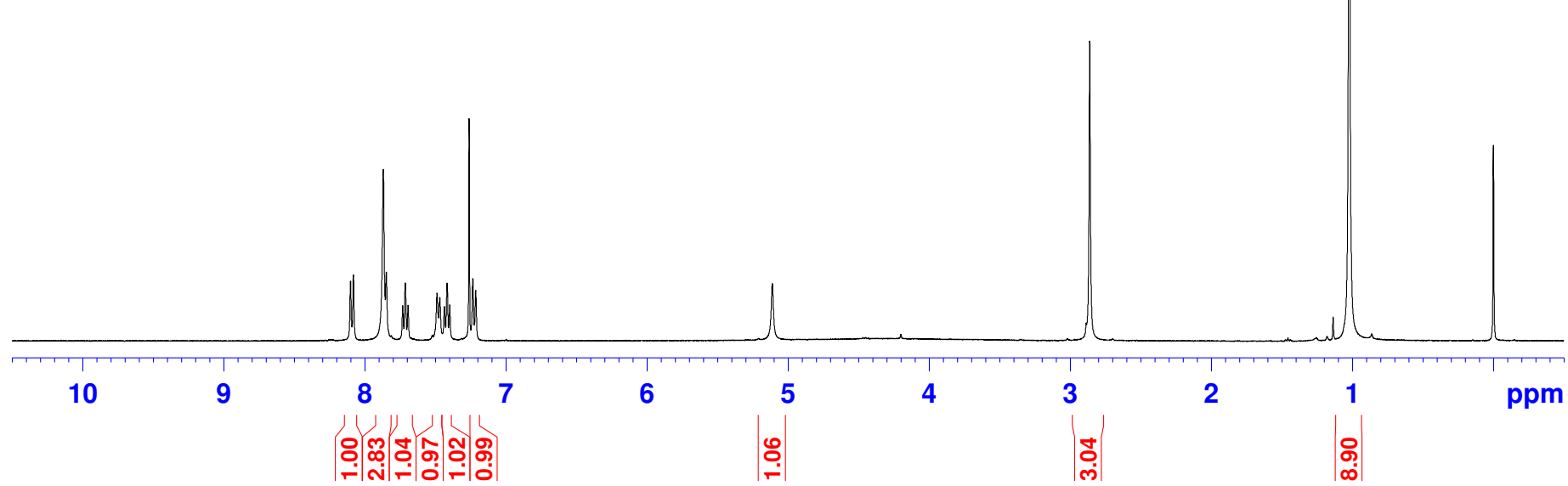
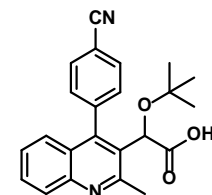
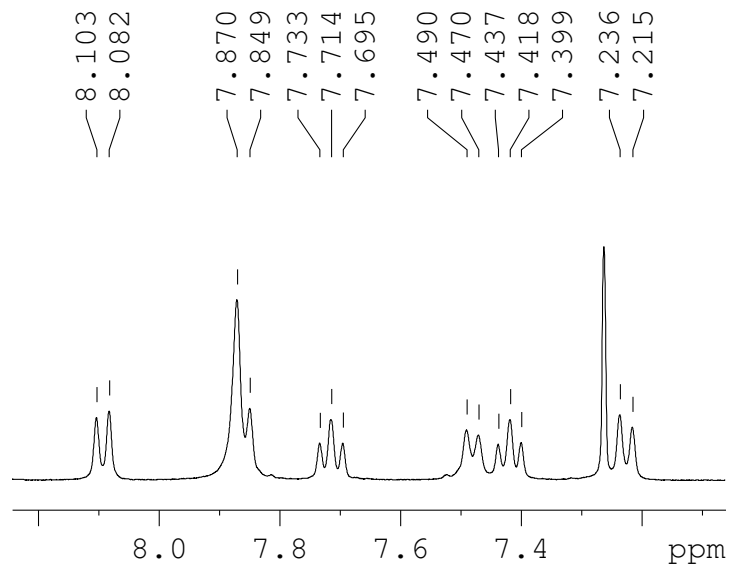
JDH-1-151 (CDC13, 400MHz) light yellow solid - Saponification of 4 thiomethylphenyl quinoline derivative

NAME JDH-1-151
EXPNO 60
PROCNO 1
Date_ 20170712
Time_ 22.51 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 48
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 297.6 K
D1 1.0000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700076 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

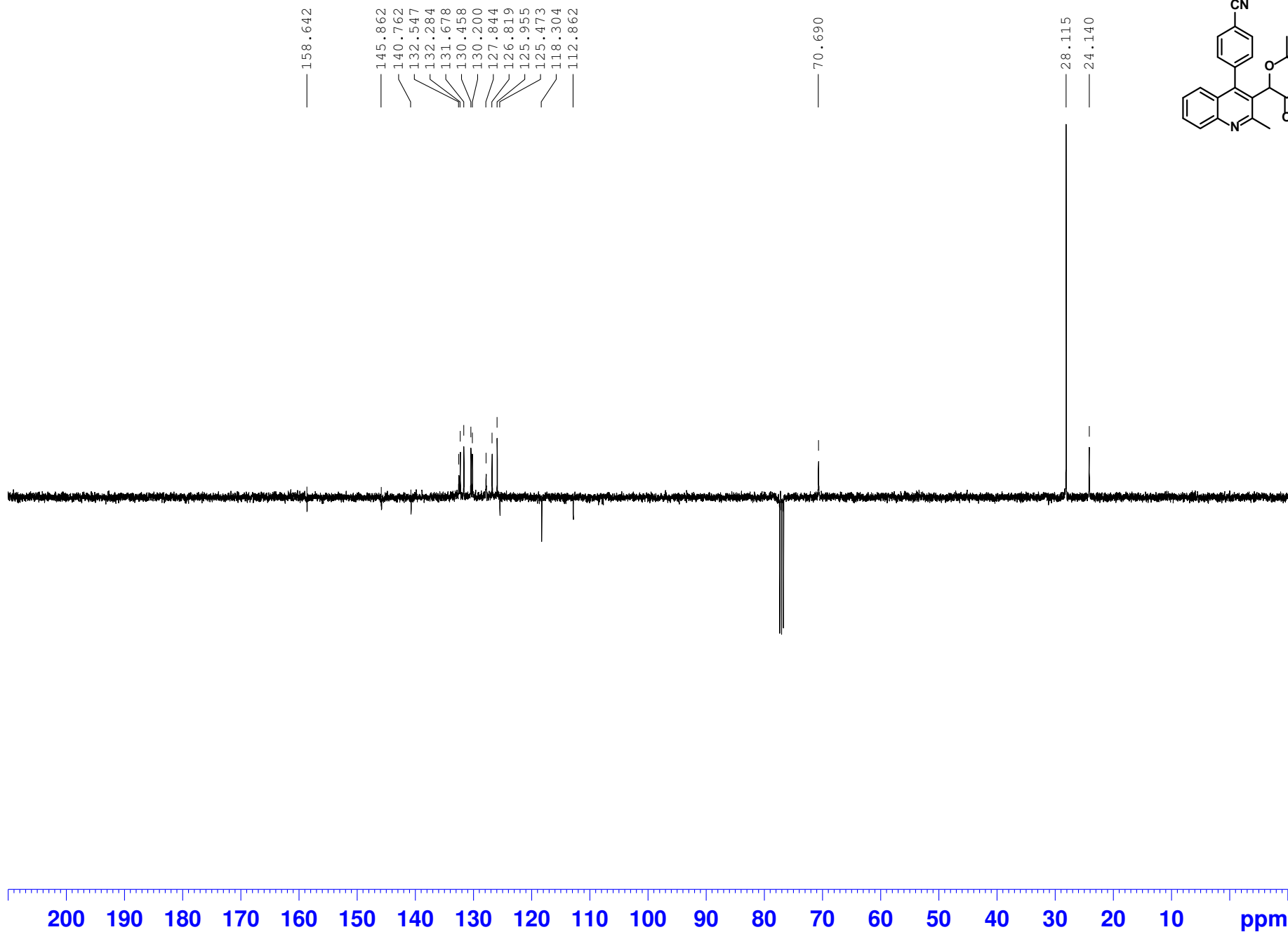


NGJ-8-094 (CDC13, 400 MHz) Sample Check

NAME NGJ-8-094
 EXPNO 50
 PROCNO 1
 Date_ 20171129
 Time_ 17.15 h
 INSTRUM spect
 PROBHD Z108618_0161 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SF01 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700084 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NGJ-8-094 (CDC13, 400 MHz) Black Oil - saponification of 4-cyanoquinoline



Mass Spectrum List Report

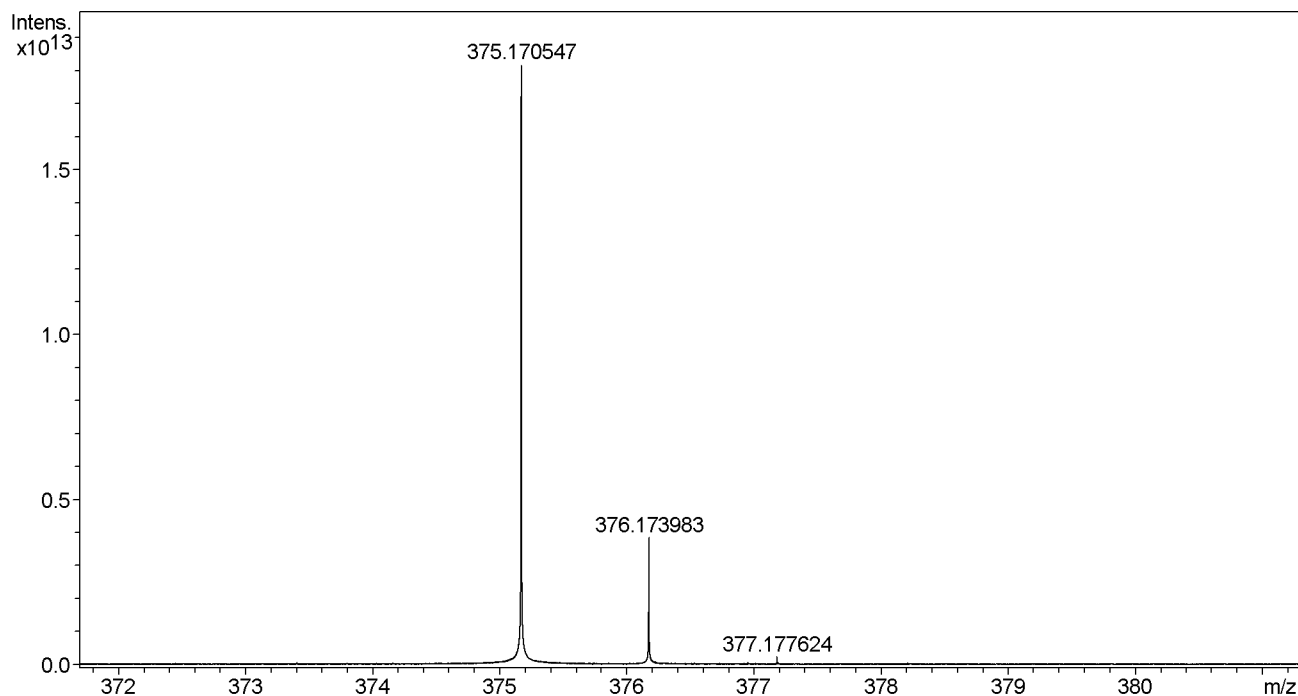
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-9-094_pos_000001.d
Method
Sample Name NGJ-9-094
Comment NGJ-9-094 in THF:MeOH C23H22N2O3 H+

Acquisition Date 3/19/2018 3:42:13 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-9-094 in THF:MeOH
Exact Mass of C23H22N2O3 H+ = 375.170319 m/z
Mass Observed = 375.170547 m/z

Difference < 1.0 ppm



#	m/z	I
1	185.385989	23073852109
2	187.588024	97957911094
3	187.838532	33807136073
4	187.961469	21830062061
5	188.089777	58595629357
6	190.061708	55949881016
7	190.213363	21448034084
8	191.251623	22319569734
9	192.397584	20942887410
10	193.254642	21427949610
11	193.370933	21480802824
12	194.814010	21941070037
13	196.658534	25972283640
14	198.871775	23482264301
15	199.892133	21664788799
16	201.839201	24319920694
17	202.340530	37456935998
18	202.452708	21320211202
19	204.734699	22266730938
20	204.760268	21675668191

Mass Spectrum List Report

#	m/z	I
21	206.444421	23563794021
22	206.454515	22609266981
23	206.903000	21094620796
24	207.611979	21120048614
25	209.442036	65341534790
26	210.294538	21793494921
27	211.016024	21330281874
28	214.563635	21058830270
29	215.256545	21608005730
30	218.533361	21300026015
31	224.638598	22510599324
32	226.685284	22485192860
33	228.319389	22748794637
34	229.259876	21793560113
35	231.120605	24551897993
36	231.249270	21721442831
37	234.240530	24444849946
38	236.077457	23733648508
39	238.285246	23742717950
40	239.160566	23188360231
41	240.532661	21296044015
42	241.725090	21592673813
43	244.540323	21487663043
44	244.979907	21181496375
45	247.498693	24061499203
46	252.377340	22209552497
47	256.473782	21518946123
48	257.107147	22737011479
49	258.078847	26808775224
50	259.312210	21701309682
51	260.127335	21412508466
52	265.729922	29496331472
53	266.925075	74852005161
54	268.071124	22083479378
55	276.440396	21801777371
56	278.406018	23574853270
57	281.969881	23365405164
58	282.598455	24623632058
59	286.856567	22041745677
60	293.618604	21492192500
61	294.196392	23835928686
62	295.260426	22845359353
63	302.918101	21349142018
64	304.162948	24418663766
65	305.301793	22515741415
66	306.396268	22812657202
67	310.336887	23333027295
68	311.877512	22869444938
69	313.434914	21862192741
70	313.743828	21733999027
71	313.926386	26022680994
72	320.128338	30132408932
73	327.986001	24400171433
74	330.434479	23654548878
75	331.180888	734083473148
76	331.202891	22784699100
77	331.235824	22433202809
78	332.184337	128317509935
79	335.831993	25332789767
80	337.300316	23289926700
81	341.131146	25400537205
82	347.580648	25358527939
83	349.166584	27315637167
84	350.176950	215904432368

Mass Spectrum List Report

#	m/z	I
85	355.753586	22782699597
86	361.740061	27258037167
87	363.170702	28249141146
88	368.350261	24975307290
89	372.457130	29347393833
90	373.109913	23414291211
91	373.336890	23087907789
92	373.407327	45298230059
93	373.563163	23833254613
94	373.802288	25349732754
95	373.895671	24353208340
96	373.943856	23131435477
97	373.994687	23129824430
98	374.033130	25922530474
99	374.085946	23626052945
100	374.162007	31812578262
101	374.266191	24754399307
102	374.290602	24517947535
103	374.314644	24375995260
104	374.361450	23718004998
105	374.366422	24455180234
106	374.418853	25707984678
107	374.449005	25776695420
108	374.518630	32915637328
109	374.530404	33453618655
110	374.542064	34308399947
111	374.560889	24077411381
112	374.619305	35371271412
113	374.659542	40859331568
114	374.695383	33073445551
115	374.715472	40306493505
116	374.733036	37244741071
117	374.767878	37003482847
118	374.779792	38901464907
119	374.832733	43397762576
120	374.932092	63606410502
121	374.964116	72163471641
122	375.004048	83376875965
123	375.170547	18171793133651
124	375.420893	53327949600
125	375.458710	49437509136
126	375.471654	48700024946
127	375.535686	39973797909
128	375.572058	35823170535
129	375.596625	35336672838
130	375.630364	34853229794
131	375.652196	33063274432
132	375.700436	33963553413
133	375.736419	30369975021
134	375.779049	31289363452
135	375.843961	32639284899
136	375.853031	32306399347
137	375.886239	24860599273
138	376.022204	30084635524
139	376.049187	26908214435
140	376.111172	43025467921
141	376.173983	3832243834652
142	376.232695	61291613062
143	376.290050	38945367992
144	376.315021	36503591528
145	376.379668	31337501669
146	376.456931	26584069299
147	376.505944	27053749484
148	376.533870	28791472417

Mass Spectrum List Report

#	m/z	I
149	376.731057	25720893756
150	376.921102	30094756866
151	376.950629	51510446905
152	377.013572	30996574383
153	377.062143	23317747322
154	377.177624	237426847412
155	378.200030	23469813417
156	378.206814	34535976344
157	384.136558	28565947903
158	393.209431	29330111033
159	395.146992	23798950804
160	397.152878	360384498065
161	398.156291	51879164699
162	398.242032	284769294792
163	399.245478	58358741021
164	405.111139	25329206997
165	413.212476	1182643216037
166	413.267280	33778752206
167	414.215955	81926005523
168	414.832789	23996945296
169	419.134895	93356956994
170	420.138030	29836704044
171	421.936056	28744959567
172	421.988508	26442530126
173	422.046095	34003616402
174	422.084958	39969791745
175	422.106716	49604436004
176	422.196675	4516590990858
177	422.284279	59860394758
178	422.331169	36223234575
179	422.357041	38595927259
180	422.398793	31001239744
181	422.434746	32506149007
182	422.461872	29558750429
183	422.863934	23798608278
184	423.200143	1238850902157
185	423.276175	28682118834
186	423.397676	24260519711
187	424.203562	58074321668
188	425.288086	59390625692
189	426.207087	110666944150
190	427.210196	38776102072
191	435.345471	46036630000
192	436.348877	23918602942
193	440.759043	22597850255
194	443.223357	118772419663
195	444.178947	138374370993
196	445.182445	25160675911
197	452.519534	22835473351
198	456.110542	25818617623
199	477.239487	35259352791
200	480.551182	56409975388
201	480.734298	23800837479
202	481.555025	28939240595
203	491.210466	35578169193
204	492.794925	22695716978
205	493.075577	23913301054
206	493.226084	883764332108
207	493.337101	27174149921
208	494.229537	182200506787
209	495.223275	192250629732
210	496.226670	41468025182
211	497.144981	22905524914
212	497.840467	23506929463

Mass Spectrum List Report

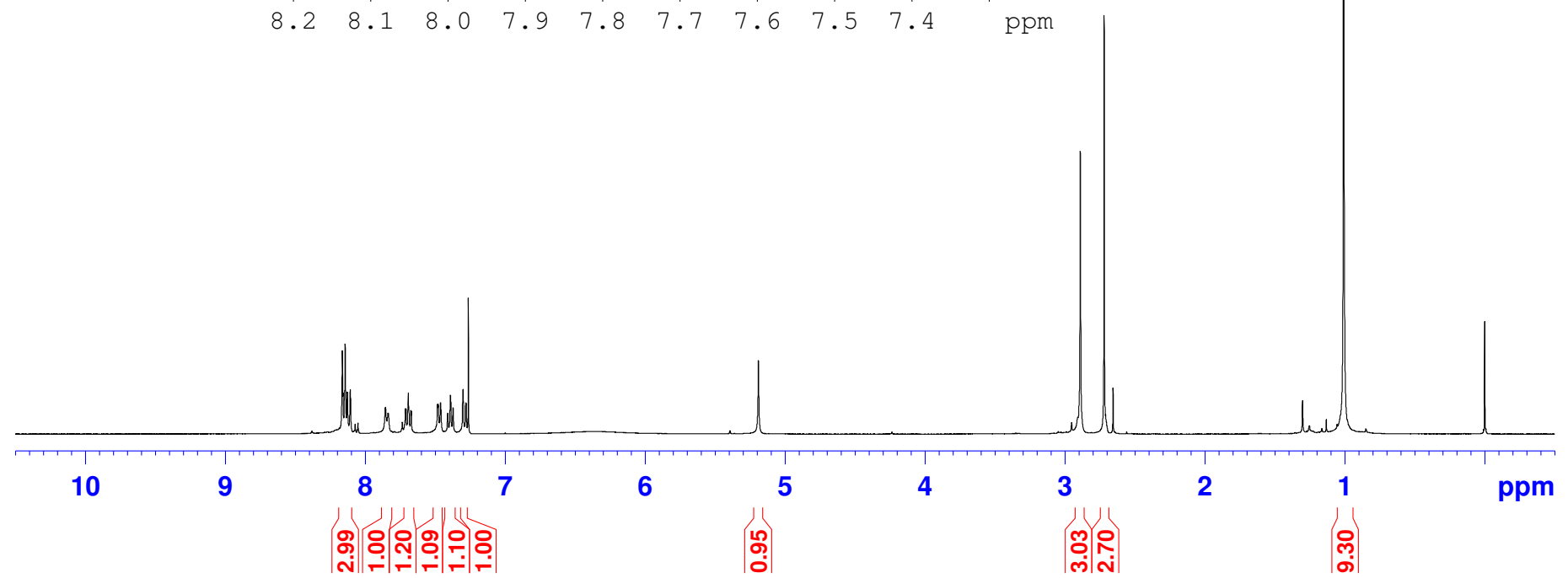
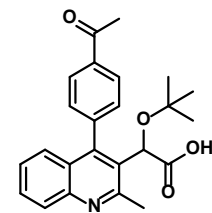
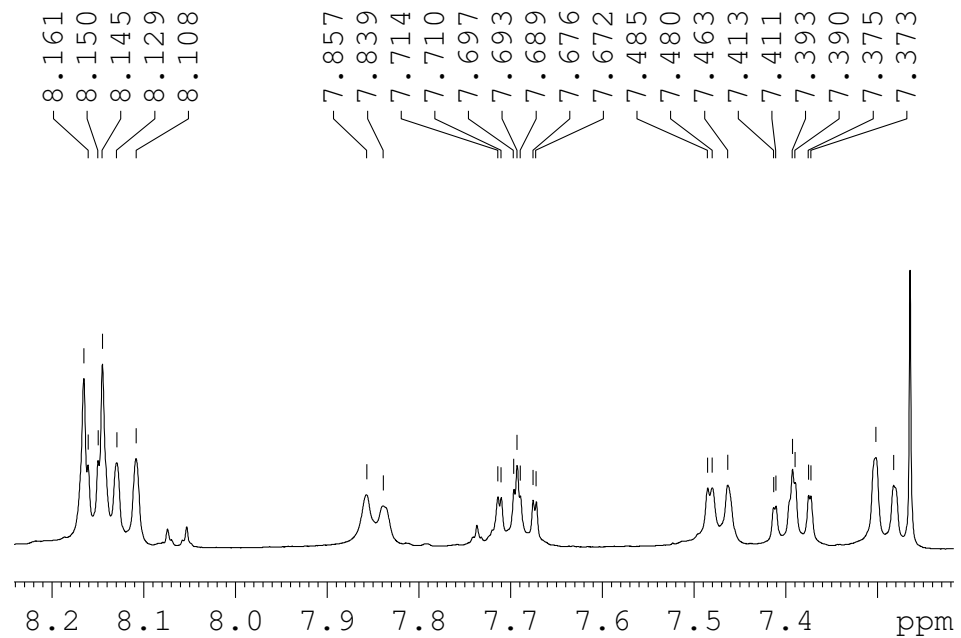
#	m/z	I
213	501.170555	28879718429
214	501.188144	25156230210
215	503.918186	22414351536
216	508.169413	23893183806
217	508.534582	25933743521
218	508.582456	661504758931
219	509.389963	22562632945
220	509.585880	181257020329
221	510.589027	29484083059
222	515.234149	25464932965
223	517.165823	40796121370
224	520.582822	23570545314
225	522.598305	36092075899
226	536.613717	2342851789251
227	536.945979	23419213228
228	537.032774	25870680565
229	537.262426	23764428126
230	537.617168	850988513076
231	538.620689	89563317749
232	539.623960	22573345022
233	547.332598	23193769348
234	550.291938	22934870338
235	550.593488	24414615354
236	551.596652	23579062195
237	552.119774	23011095849
238	552.608925	111809570398
239	553.612238	32915415382
240	554.443473	22748747099
241	556.304652	22919673697
242	564.645264	690849911653
243	565.648631	240583606845
244	580.640608	25836507415
245	589.223361	38834875180
246	592.676587	961166423399
247	592.779825	30008311282
248	593.680042	328060590334
249	594.252988	78926825448
250	594.683415	45816601678
251	595.240573	63222441330
252	596.243511	28528263106
253	603.290757	23601830882
254	608.671505	30099219676
255	620.708156	34171548854
256	627.197982	24625295383
257	627.222695	22965629072
258	632.098819	23008733986
259	632.169093	24498684965
260	642.515712	23681020691
261	648.739468	24242549750
262	649.249863	25162902514
263	649.853286	22575973560
264	651.053517	23689344034
265	658.799251	25699511299
266	661.874812	23821285737
267	680.153686	25599084783
268	685.437027	42281322526
269	686.440959	35130308826
270	702.872432	23490258182
271	708.447344	23394680504
272	751.128253	25175500151
273	752.060235	24457761679
274	765.394150	24960438776
275	801.777887	28727356878
276	819.469982	23760001991

Mass Spectrum List Report

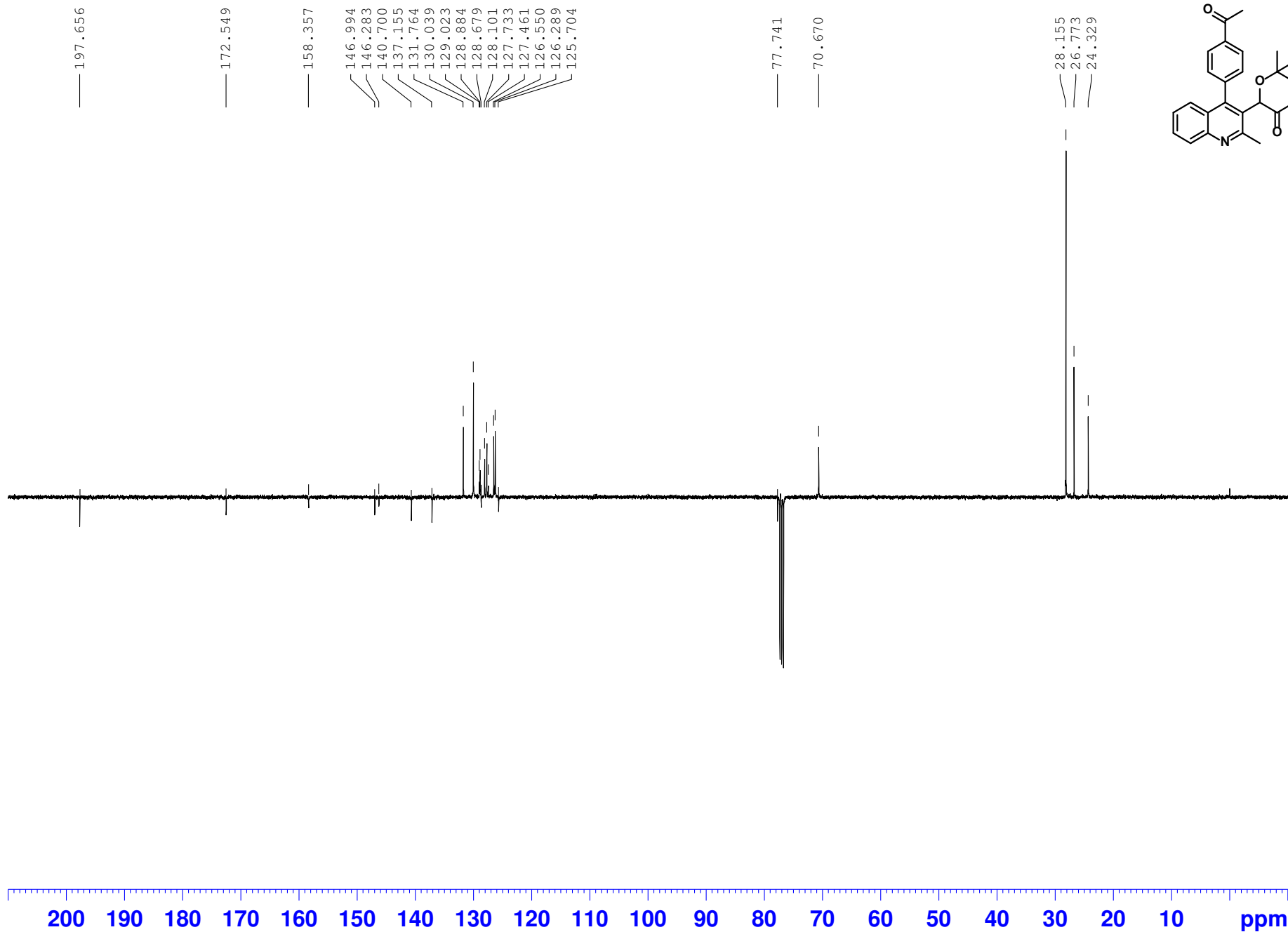
#	m/z	I
277	845.911570	23624316700
278	881.918607	23388219911
279	882.502587	24727641298
280	914.070428	23656622159
281	954.900816	23688409468
282	978.999930	24585977046

NGJ-8-092 (CDC13, 400MHz) Pure Yellow Oil - saponification of 4-acetylphenylquinoline

NAME NGJ-8-092
 EXPNO 60
 PROCNO 1
 Date_ 20180208
 Time_ 20.31 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 203
 DW 62.400 usec
 DE 6.50 usec
 TE 298.1 K
 D1 1.00000000 sec
 TD0 1
 SF01 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700077 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NGJ-8-092 (CDC13, 400MHz) Pure Yellow Oil - saponification of 4-acetylphenylquinoline



Mass Spectrum List Report

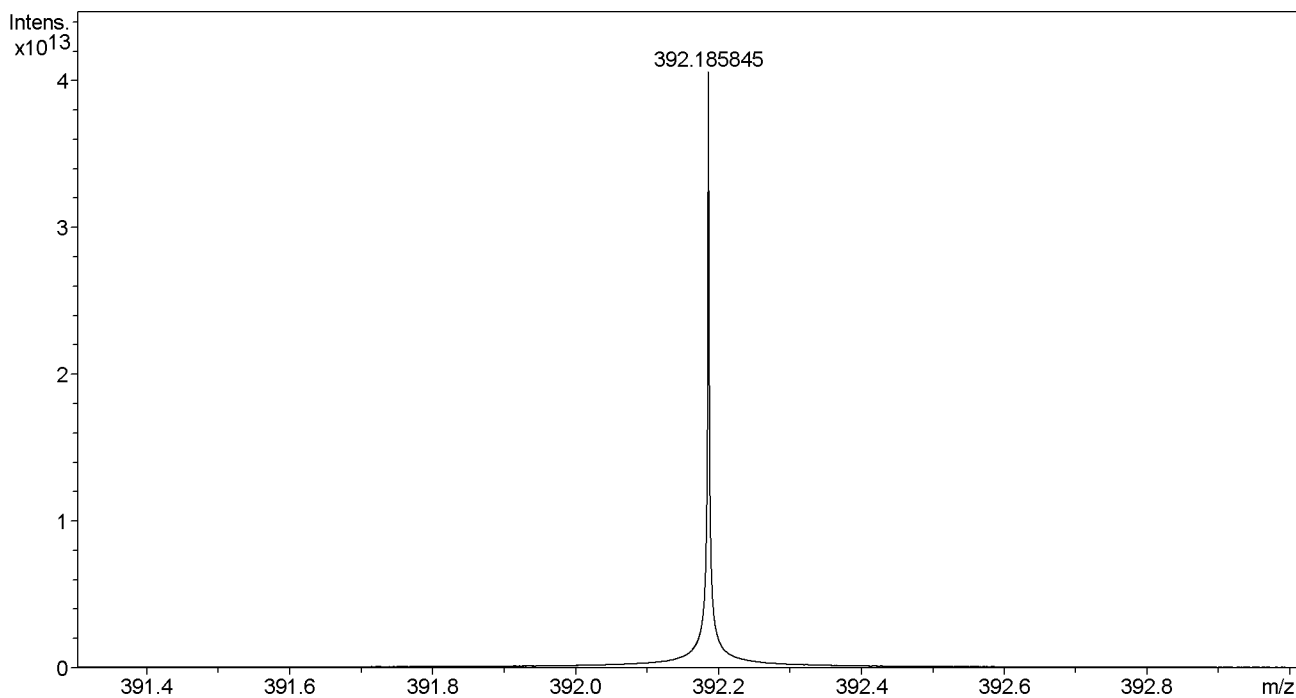
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-8-092_pos_000001.d
Method
Sample Name NGJ-8-092
Comment NGJ-8-092 in THF:MeOH C24H25NO4 H+

Acquisition Date 3/19/2018 12:25:11 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-8-092 in THF:MeOH
Exact Mass of C24H25NO4 H+ = 392.185635 m/z
Mass Observed = 392.185845 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.313288	23432782742
2	187.843246	21100986983
3	188.324667	21548011890
4	190.061649	68656043223
5	192.814914	24240196887
6	193.816811	22286902836
7	194.840653	22839239705
8	195.235908	22883549081
9	195.547281	21712112763
10	196.075794	22774449407
11	196.094871	28968895607
12	196.095937	186445922968
13	196.597725	28523682565
14	196.949359	21596644481
15	198.866946	21198384015
16	200.431067	21548896043
17	202.340456	29898630349
18	205.634116	22107066985
19	205.896325	23169490948
20	207.603198	21405889505

Mass Spectrum List Report

#	m/z	I
21	210.231727	23684986336
22	211.293206	22349782930
23	212.606347	21771070977
24	214.662199	22489199608
25	215.089343	21170593532
26	217.088663	23269230553
27	219.104417	25381377153
28	219.930807	22274232503
29	223.210256	22405160679
30	231.104424	34331752842
31	233.118921	22043407753
32	236.488428	22830809488
33	236.732215	22225214312
34	237.155793	23455280089
35	237.609365	21466958177
36	239.053783	21769335158
37	241.323809	21300537364
38	244.545741	21281482315
39	244.997899	21463008122
40	246.182707	23914111226
41	247.171413	22810367485
42	249.110450	21277270463
43	253.992631	21701673047
44	255.692790	23865725502
45	258.431449	24914727640
46	264.871238	23171348603
47	268.182320	21457653686
48	268.312572	24578150344
49	271.477985	22193884533
50	274.650003	21283235431
51	275.094249	22942622823
52	275.833598	21580077120
53	276.417495	23168689687
54	276.969955	21795748600
55	278.822432	22701743479
56	289.109612	31453386150
57	290.117699	64528311097
58	291.125372	30735719735
59	294.380356	21368311028
60	298.167230	21499811850
61	298.316799	24204359850
62	301.075790	27736454400
63	301.636002	22592615039
64	302.960067	24547587163
65	306.657405	21599639833
66	310.346212	25320558503
67	310.351750	37782926200
68	310.978278	23159863652
69	312.243571	604090848310
70	312.246810	105824340987
71	312.284992	23990846155
72	314.425771	22101649226
73	315.451566	21689028522
74	315.655705	22204739611
75	316.030027	27106990087
76	319.119428	23603906073
77	324.140575	23102592175
78	325.714436	22315369039
79	326.692202	23086361745
80	327.081756	22254273679
81	329.408815	22986106370
82	335.115515	25308912951
83	336.123220	104918094550
84	337.126698	32394830055

Mass Spectrum List Report

#	m/z	I
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87	348.158885	28665821009
88	348.196337	1280206863537
89	349.167060	34135761138
90	349.199795	204799796071
91	349.787053	24126654053
92	353.302479	23421961555
93	354.410104	23389411658
94	355.609154	23756613107
95	360.308409	39290004976
96	360.324246	695183548105
97	361.327702	72310817766
98	365.757389	24129624146
99	368.339580	24116222875
100	380.186506	43990371185
101	388.624743	25383906756
102	389.123325	23750988912
103	389.175525	24335225365
104	389.450636	26143075525
105	389.510689	24431962399
106	389.614572	24505693320
107	389.693714	23877291582
108	389.719403	24493937260
109	389.766261	34076594117
110	389.953387	24350960985
111	389.964482	26983088464
112	389.980227	30271017946
113	390.074972	27496403838
114	390.093437	30326583324
115	390.166977	27517991490
116	390.192978	30457872448
117	390.227152	25696999287
118	390.260066	26330148369
119	390.332423	26070001490
120	390.341625	27998434132
121	390.365911	29222999263
122	390.414801	28661141746
123	390.467593	31542214249
124	390.495602	29638810627
125	390.503779	27834063198
126	390.536777	30333540844
127	390.582816	31735186710
128	390.620943	27836945147
129	390.683745	27498955463
130	390.739929	27657063420
131	390.779021	29033331922
132	390.802549	33962326758
133	390.892152	33452659645
134	390.928416	31270568271
135	390.955129	34778746877
136	391.045094	35998688865
137	391.056476	34085875466
138	391.121807	37704096009
139	391.187922	42180557241
140	391.212296	45503044081
141	391.274272	42741256638
142	391.341002	45239820616
143	391.398055	49846723732
144	391.490865	50357086215
145	391.516290	55151354866
146	391.549694	56192878694
147	391.573479	56530010631
148	391.612318	62136210670

Mass Spectrum List Report

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152	391.783238	88360483463
153	391.933553	119125196238
154	391.955637	131649752343
155	392.014441	173809506273
156	392.030754	188449542476
157	392.185845	40550536590310
158	392.640674	61100311101
159	392.653957	57222938012
160	392.711247	56737628242
161	392.805531	41995668818
162	392.819971	45374940203
163	392.863829	41025365063
164	392.885253	39788730656
165	392.979186	28172242013
166	393.189448	6962530350913
167	393.337124	66635987894
168	393.361533	60442472391
169	393.390349	52461569247
170	393.434780	43884101608
171	393.450382	43655718867
172	393.489526	46987823113
173	393.518076	39603953836
174	393.555594	42243504082
175	393.649036	45465572669
176	393.705857	39248840044
177	393.759669	33977330853
178	393.832569	35611085787
179	393.871996	29456701968
180	393.914735	33079435201
181	393.977215	30731953976
182	393.996729	28620766717
183	394.047273	30250907305
184	394.130143	37269925914
185	394.147132	35229696403
186	394.166209	48858689112
187	394.193173	504372124324
188	394.195732	309898970496
189	394.277175	29090712151
190	394.306229	26862405721
191	394.346698	24729278396
192	394.486948	26735661124
193	394.503785	27105582794
194	394.531694	27589040878
195	394.619289	28141098106
196	394.703840	23865573735
197	394.747408	28246909598
198	394.910040	25727773966
199	395.129013	24396953572
200	395.196447	49197013080
201	395.449350	24085741842
202	396.527324	23984074695
203	397.766987	24475134543
204	398.242213	231191101496
205	398.260152	27833519756
206	399.245576	48196117147
207	413.213004	52453333467
208	414.168104	1404428337196
209	414.290483	25127325348
210	414.484752	22965497957
211	414.520605	23094094979
212	415.061182	23789874739

Mass Spectrum List Report

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215	427.213566	37914916672
216	432.254320	25942797476
217	435.345587	51455535266
218	436.150459	229290712556
219	437.153770	33131319044
220	448.249118	465084995910
221	449.252458	81365160146
222	458.536538	23893907132
223	462.228654	23412295257
224	464.244134	340468037584
225	465.247488	54297840796
226	466.259747	27460730228
227	479.619054	22507702347
228	480.551333	96997958963
229	481.554793	34386660622
230	484.272464	23126506878
231	486.226216	47606875684
232	486.781177	23468454072
233	494.567511	23236872212
234	508.467631	24075915820
235	508.582615	1122868734843
236	508.634544	37977371188
237	508.688281	28797327906
238	509.586102	265288949476
239	510.589090	27022089017
240	522.598571	37634179524
241	524.268805	22740178262
242	524.577931	49778965110
243	526.281351	51557490736
244	527.284220	24880665229
245	536.110179	26110597947
246	536.146487	23006255316
247	536.319460	27363450493
248	536.363459	28288514409
249	536.435656	29437159014
250	536.613887	3739964189713
251	536.940500	26790553509
252	537.056273	30194627241
253	537.149356	23135508766
254	537.187007	25182810331
255	537.207903	22944338695
256	537.283508	24050761066
257	537.394897	30403951273
258	537.538252	37582591842
259	537.617380	1224857049576
260	538.620951	129496427564
261	550.593683	29510807825
262	550.629844	34378167409
263	552.609163	184101105512
264	553.612564	48082155221
265	564.510709	23848065791
266	564.645466	882641354822
267	564.944924	23247658245
268	565.648918	297413405798
269	566.652319	23075602541
270	567.279381	26463973670
271	576.407043	24073910621
272	578.625762	25618634077
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274	592.581679	23272295935
275	592.676878	1005205620909
276	592.810473	31725415608

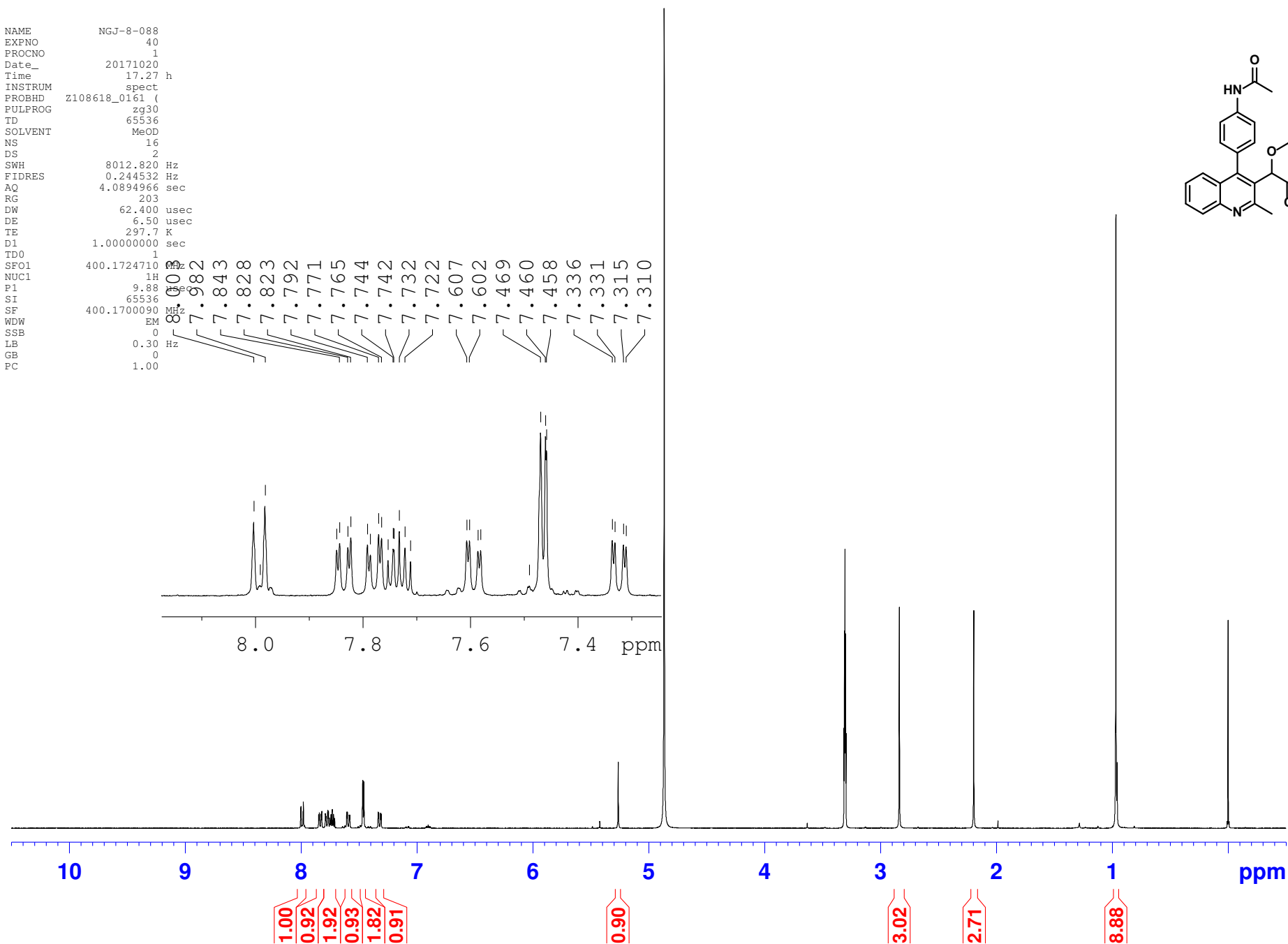
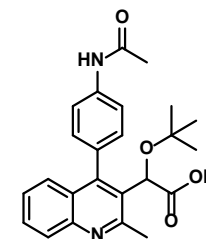
Mass Spectrum List Report

#	m/z	I
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280	593.680314	368338063515
281	594.683837	28662211176
282	608.671591	24180442952
283	609.252615	23873716104
284	611.269123	27840496519
285	612.255711	41415070760
286	617.681617	22541133470
287	620.708374	30479424322
288	621.711888	22341171184
289	626.266241	24434758284
290	643.312676	26766732558
291	656.302496	77988334334
292	657.305766	33120870943
293	671.886873	25355796336
294	672.230615	23140651961
295	673.317621	22433506952
296	678.283906	27135892983
297	685.437541	58109582952
298	733.900302	25665469129
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300	781.959889	22896996003
301	830.520487	26933614684
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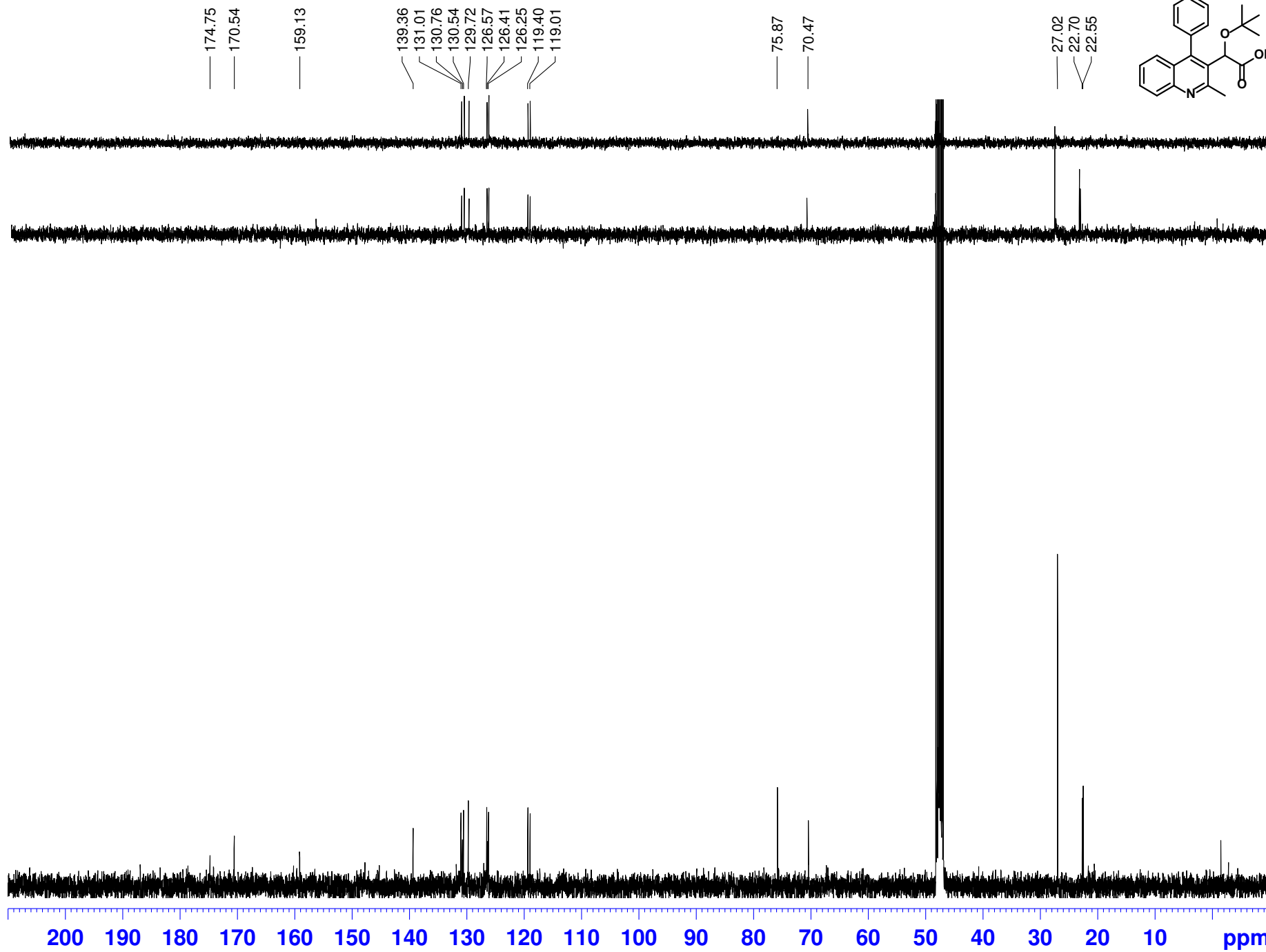
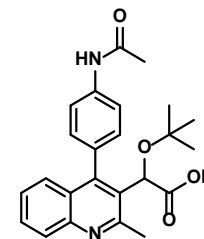
NGJ-8-088 (CD3OD, 400 MHz) Yellow Solid - saponification of 4-acetamidoquinoline; DCM extract:

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NAME      NGJ-8-088
EXPNO     40
PROCNO    1
Date_     20171020
Time      17.27 h
INSTRUM   spect
PROBHD    Z108618_0161 (
PULPROG   zg30
TD         65536
SOLVENT   MeOD
NS         16
DS         2
SWH        8012.820 Hz
FIDRES     0.244532 Hz
AQ         4.0894966 sec
RG          203
DW         62.400 usec
DE         6.50 usec
TE         297.7 K
D1         1.00000000 sec
TD0        1
SF01      400.1724710 MHz
NUC1       1H
P1         9.88 usec
SI         65536
SF         400.1700090 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
    
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NGJ-8-088 (CD3OD, 400 MHz) Yellow Solid - saponification of 4-



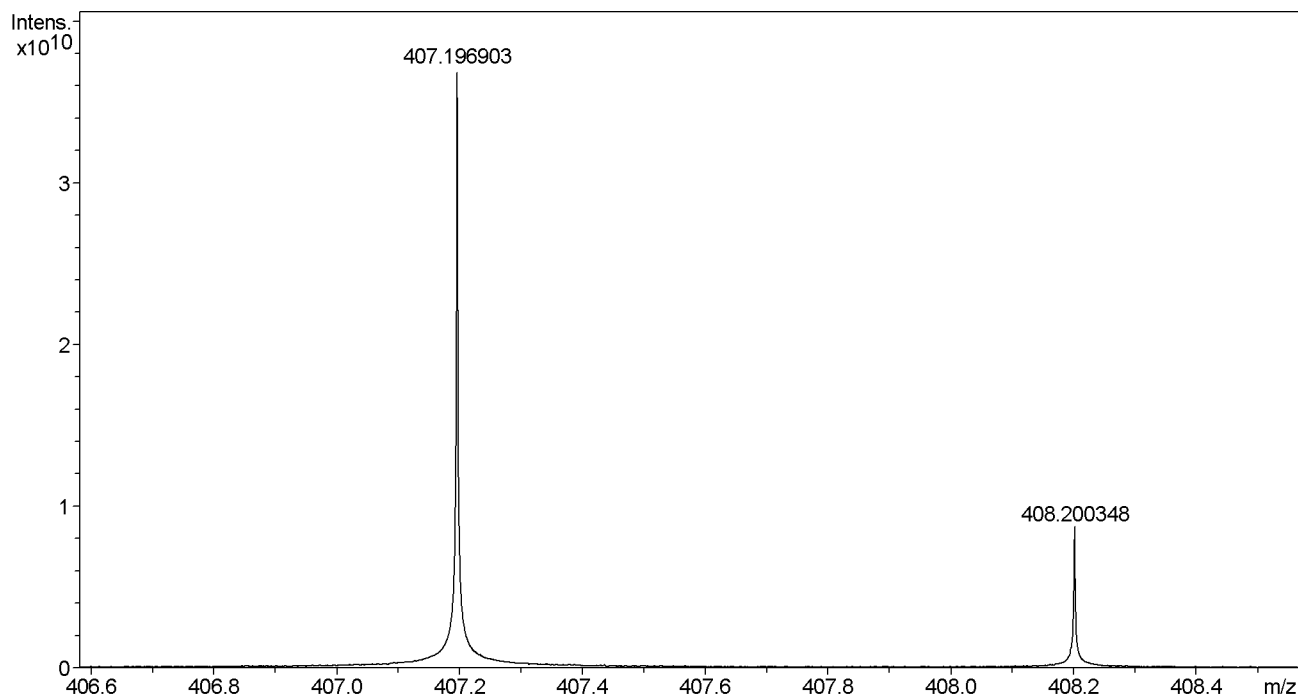
Mass Spectrum List Report

Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-8-088_pos_000003.d
Method
Sample Name NGJ-8-088
Comment NGJ-8-088 in THF:MeOH C24H26N2O4 H+

Acquisition Date 3/19/2018 12:01:38 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-8-088 in THF:MeOH
Exact Mass of C24H26N2O4 H+ = 407.196534 m/z
Mass Observed = 407.196903 m/z
Difference < 1.0 ppm



#	m/z	I
1	184.390826	305956616
2	189.312273	87482022
3	189.685646	766626834
4	190.061840	2074646750
5	199.094324	103824190
6	201.412837	179250526
7	201.885166	595341362
8	202.340474	220921121
9	203.601732	179599226
10	209.442000	311252522
11	215.089220	565125534
12	231.120584	229877215
13	233.071339	113891595
14	245.099849	217840813
15	251.573420	250108448
16	252.580927	1089144571
17	257.846464	123996933
18	258.935120	590323337
19	268.312306	102970778
20	285.131196	109887946

Mass Spectrum List Report

#	m/z	I
21	285.491572	216483917
22	286.975378	1119066599
23	298.347215	153823684
24	301.075649	119082723
25	301.126174	123610850
26	301.162629	121710305
27	301.299864	232877784
28	303.141819	247346105
29	311.115863	117987480
30	314.059987	218507549
31	314.342149	297241330
32	317.121110	219407881
33	321.196527	216650976
34	326.378575	94617917
35	334.308432	129441181
36	340.394197	265590490
37	341.397610	91354827
38	342.373565	119155461
39	351.251076	89637932
40	354.373403	194541994
41	354.409875	649219054
42	355.413202	203632237
43	356.389167	102510301
44	363.207121	3529637090
45	364.210559	727060549
46	365.186435	2271816147
47	365.222663	131608505
48	366.189815	463655546
49	368.166205	175247304
50	368.425608	115606289
51	370.404844	853759227
52	371.408205	209546033
53	375.199467	194250345
54	379.202198	143499059
55	384.420407	100966145
56	390.371105	132055043
57	391.238456	7855299527
58	392.241935	1703210858
59	393.210165	100515138
60	393.245281	169976688
61	393.298075	760207542
62	394.301455	169700505
63	396.456968	129223642
64	398.241895	7986302506
65	399.245339	1483167230
66	400.248766	195119415
67	405.217792	192784591
68	406.221185	116613349
69	407.196903	37023520276
70	407.436346	211080294
71	408.200348	8737741316
72	409.200833	198611397
73	409.203909	664294066
74	409.212680	254981464
75	410.436256	421528091
76	411.439558	127319786
77	412.451833	205533238
78	413.212521	1017410551
79	413.266822	252535200
80	414.215915	176527599
81	423.192104	263619002
82	423.228468	294446111
83	423.264839	940402293
84	424.268209	205077368

Mass Spectrum List Report

#	m/z	I
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89	429.178921	19246301500
90	430.182403	4651410119
91	431.185737	381856478
92	435.228203	34184600905
93	435.344827	763659129
94	435.355074	208709962
95	435.715221	105415644
96	436.231667	9253336794
97	436.349289	134861459
98	437.235151	833076665
99	441.298255	113653625
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101	451.161095	1930114966
102	452.164448	424030854
103	452.519678	735717543
104	453.523011	252085146
105	457.210408	4810875093
106	458.213867	975678322
107	459.217344	126368941
108	463.499196	109810916
109	465.239161	134831922
110	466.535242	220093928
111	467.254723	2226666583
112	468.258121	493829394
113	468.514697	308567727
114	469.517816	108295826
115	477.180890	229007941
116	479.192392	235654474
117	480.091722	102443829
118	480.550978	2417959996
119	481.262789	136575088
120	481.554346	780104339
121	482.557884	126616133
122	489.236745	285687472
123	493.175812	1212687705
124	493.226081	272849788
125	494.179147	292120819
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129	496.545969	670655511
130	497.549453	224078313
131	506.566777	108911112
132	507.322546	143499604
133	508.582178	18608936772
134	509.119622	272918891
135	509.585621	6327652089
136	510.562057	237696756
137	510.589086	950159352
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141	523.324937	166831312
142	523.564929	121282851
143	523.601392	376263619
144	524.577242	3342909794
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146	526.583959	150822734
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Mass Spectrum List Report

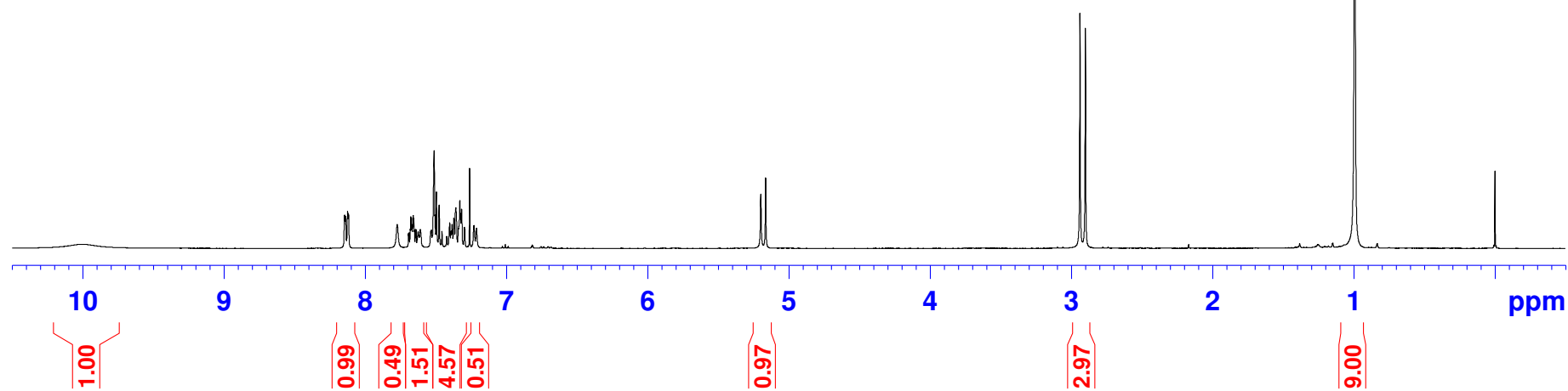
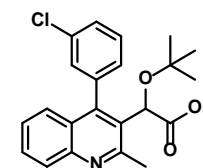
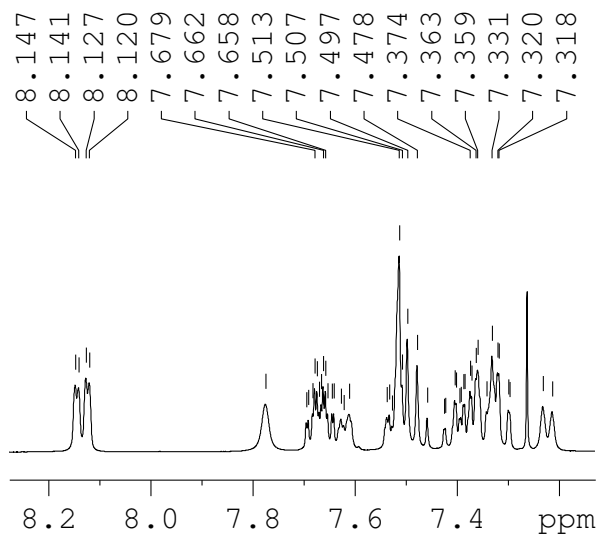
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153	537.616811	24354486009
154	538.593365	308228162
155	538.620444	3490738977
156	539.623925	319818700
157	540.572634	126455804
158	550.593245	748102704
159	550.629462	748231504
160	551.312399	138866052
161	551.596640	300638750
162	551.632772	311875680
163	552.608473	10064135906
164	553.612048	3359201305
165	554.615415	495129768
166	562.629596	157579605
167	563.263253	113226931
168	564.644777	21307840172
169	565.648301	7728918366
170	566.588149	213188407
171	566.651745	1072889690
172	567.654961	139061151
173	568.603728	185435294
174	569.403316	184879371
175	578.624252	387484303
176	578.660728	484145021
177	579.627703	172514880
178	579.664276	200780612
179	580.639948	2847634066
180	581.643368	958787857
181	582.646736	154506694
182	590.660825	404703124
183	591.664175	212677643
184	592.428130	305609721
185	592.676171	25856175504
186	593.679616	10826316652
187	594.618665	131690449
188	594.683105	1664555447
189	595.686671	186828743
190	599.549384	842711498
191	600.552529	286922879
192	606.655775	647661997
193	606.692287	213967619
194	607.659083	294443851
195	607.695242	99530035
196	608.671366	3502880484
197	609.674671	1309351698
198	610.678080	212013537
199	613.429694	271188692
200	614.536314	165982311
201	620.707816	1216285880
202	621.711095	498900415
203	622.650703	121886619
204	622.714435	117208380
205	626.279053	111358956
206	627.266371	622085222
207	628.269871	248912145
208	636.702903	175561161
209	648.739273	601055151
210	649.742529	295362680
211	651.667827	125205510
212	655.297714	118853562

Mass Spectrum List Report

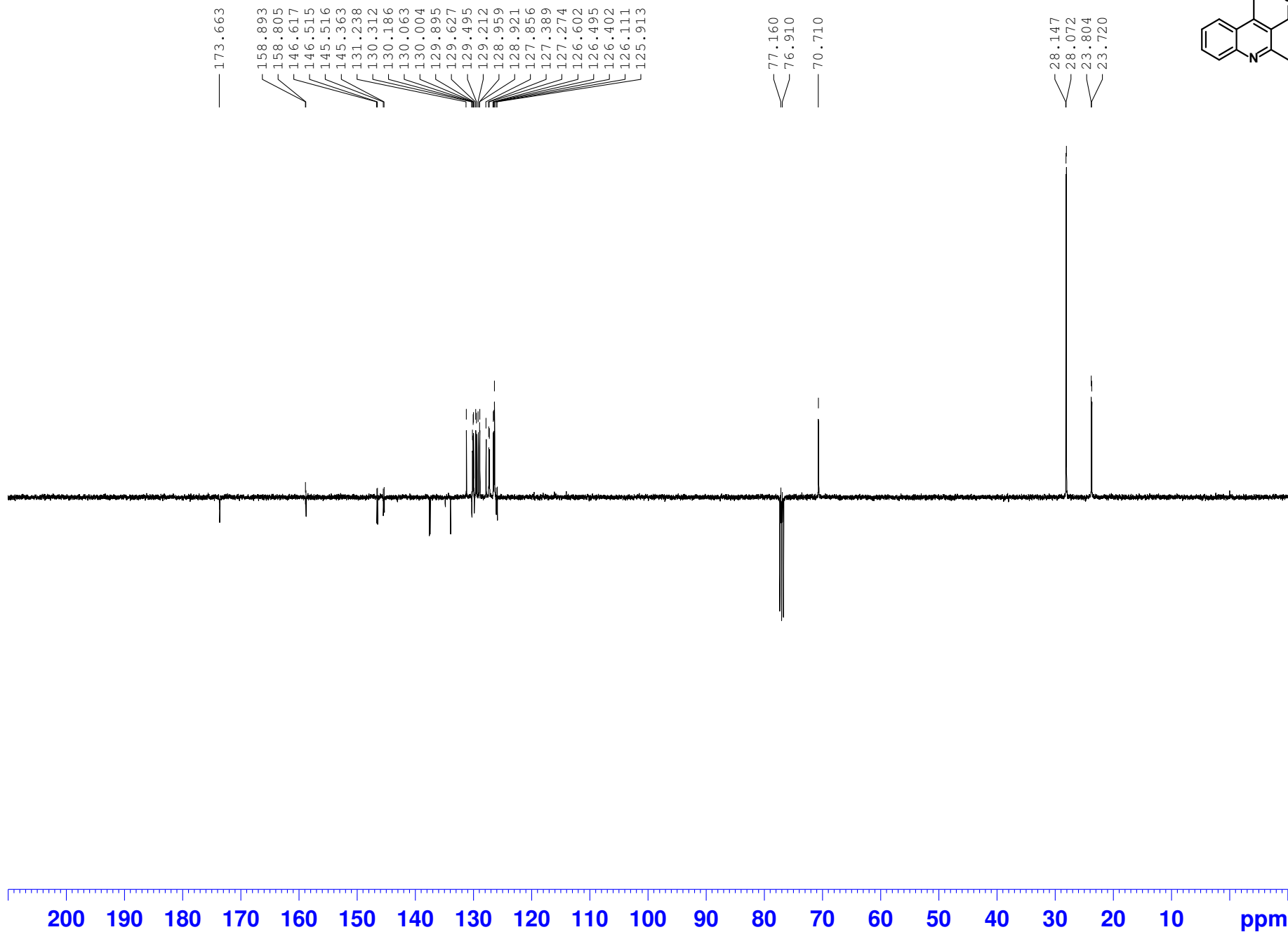
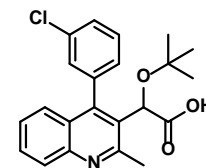
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214	658.459418	103777231
215	659.292723	126997889
216	664.734127	107114361
217	677.508086	94535730
218	685.436695	1726766683
219	686.440203	731199834
220	687.401143	114808342
221	687.443831	190960773
222	701.482130	147038993
223	814.700464	96684154
224	857.351074	149112909
225	861.541638	320329090
226	862.545623	187913263
227	877.537357	665343511
228	878.540953	384932460

NGJ-9-024 (CDC13, 400 MHz) Pure Yellow Oil - saponification of 3-chlorophenylquinoline

NAME NGJ-9-024
 EXPNO 30
 PROCNO 1
 Date_ 20171222
 Time_ 13.04 h
 INSTRUM spect
 PROBHD Z108618_0161 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 128
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SF01 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700086 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NGJ-9-024 (CDCl₃, 400 MHz) Pure Yellow Oil - saponification of 3-chlorophenylquinoline



Mass Spectrum List Report

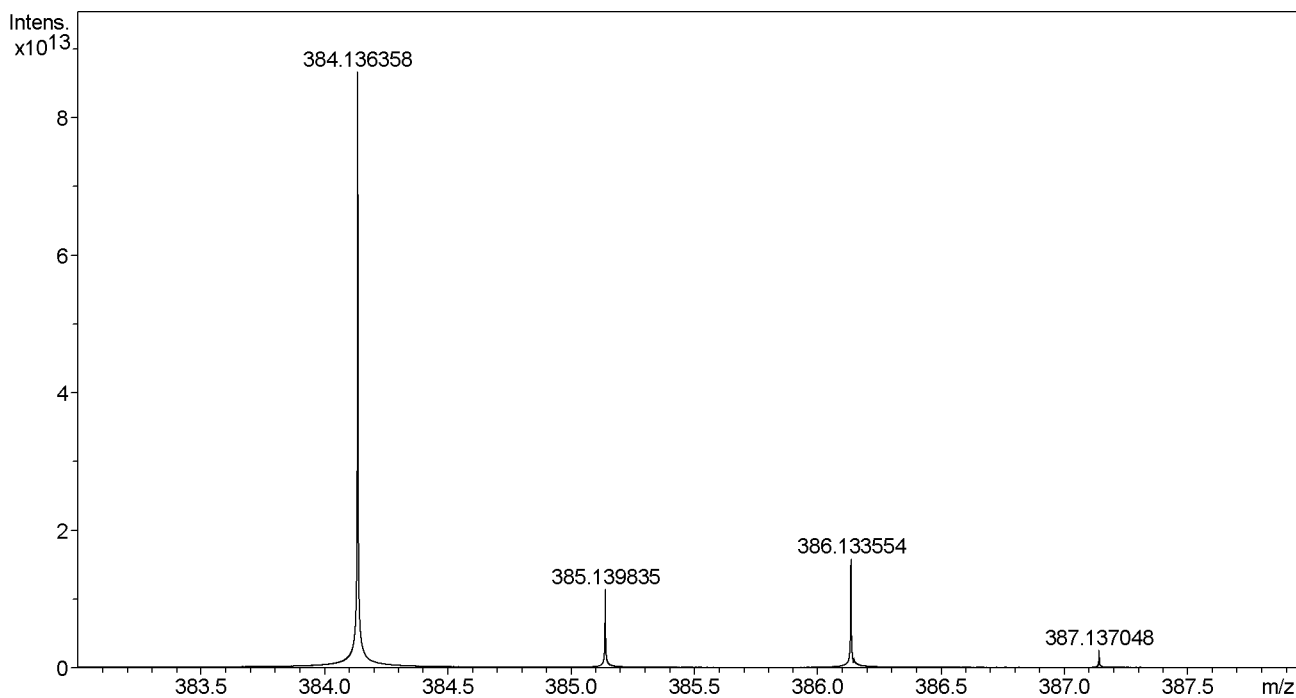
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-9-024_pos_000001.d
Method
Sample Name NGJ-9-024
Comment NGJ-9-024 in THF:MeOH C22H22ClNO3 H+

Acquisition Date 3/19/2018 3:27:38 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-9-024 in THF:MeOH
Exact Mass of C22H22ClNO3 H+ = 384.136098 m/z
Mass Observed = 384.136358 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.483553	24187905130
2	184.778135	22452626872
3	184.800287	23369493170
4	187.592456	23595124005
5	189.069833	22937675382
6	190.136791	21274825917
7	191.208246	21837192208
8	192.038736	22001977353
9	192.058483	26909852318
10	192.065090	28539603100
11	192.071087	715939544375
12	192.125164	22733230309
13	192.572834	93560618879
14	193.066949	27332398277
15	193.069710	89975538119
16	193.571448	41982626203
17	196.545325	22036765480
18	197.463070	22170216774
19	198.392450	25052346280
20	198.516274	22642828364

Mass Spectrum List Report

#	m/z	I
21	201.121307	23158512320
22	202.340551	122452898326
23	203.073104	43088210996
24	204.428826	21483797819
25	205.188064	24018509549
26	209.442020	93363947770
27	209.761852	29347239835
28	210.060692	23694671759
29	210.355983	25317709209
30	210.656328	22071636418
31	210.763696	22042249835
32	211.432105	27638799965
33	212.196074	24325195269
34	213.749027	22474268378
35	217.088639	46141440675
36	218.096563	37476259863
37	221.092112	22042516706
38	224.895402	22704439706
39	225.954432	21497645873
40	229.042883	21843527083
41	229.410910	21290958739
42	229.414216	25019488157
43	231.104317	22070563344
44	233.009318	23491728333
45	233.089460	22579605240
46	238.043303	22272144070
47	238.839187	23290955974
48	239.469242	22137750332
49	241.088708	21973943475
50	243.419709	21700184625
51	246.091360	24972157912
52	247.171365	28513342917
53	248.102188	22722331974
54	248.106984	25474980704
55	251.746972	22214071051
56	258.239532	23107421584
57	264.057525	40610662288
58	265.065509	27261870271
59	265.658198	22857362979
60	266.054486	23782930595
61	266.073300	42440386167
62	268.070257	26440856383
63	268.077002	23520403658
64	270.009377	21396384247
65	270.060589	22775453421
66	270.764580	22134282846
67	270.886941	21531925548
68	274.665823	21575779023
69	279.845182	22710963312
70	282.068389	85304592623
71	282.979207	21543839876
72	283.057495	29998321236
73	283.071573	36052793901
74	284.065150	35008230017
75	286.719746	21902116931
76	286.945331	21589817099
77	289.389527	23749963510
78	293.038574	23087845930
79	293.845540	22965638226
80	294.409375	24420951454
81	295.106284	22169826278
82	296.047087	24852781465
83	297.050776	21829430279
84	300.021535	22440625231

Mass Spectrum List Report

#	m/z	I
85	301.075772	24533100191
86	304.191326	130580997127
87	304.261719	88669858383
88	305.058381	27077003446
89	306.898047	21881175783
90	315.923179	21675026439
91	317.022530	21643837099
92	318.241076	31164981962
93	318.499382	22648277191
94	320.256666	35478380104
95	322.282346	29354493407
96	324.387805	88481510080
97	326.511075	84045544820
98	327.066002	25534088325
99	328.074062	44144564943
100	328.694784	544636715530
101	329.076365	26242242913
102	329.252438	22926197144
103	330.070361	46104444709
104	332.045553	125528823026
105	334.042551	24882944603
106	336.251617	24740485200
107	340.146935	349159635710
108	342.144108	51445545154
109	349.340891	25623736896
110	372.136990	62894504374
111	378.191555	28447867820
112	378.427914	27748851214
113	378.548164	27727159076
114	378.999598	33801946233
115	379.289079	28985722176
116	379.591326	28236832420
117	379.662206	32282678059
118	379.744657	28205212111
119	379.949920	29862573636
120	380.010583	28789248317
121	380.075942	29011977040
122	380.094839	30615758524
123	380.200289	29643646008
124	380.247052	29505373940
125	380.272983	32214840659
126	380.353090	31827542861
127	380.402631	32612581965
128	380.427672	27434135716
129	380.478294	28180859785
130	380.569518	28935002179
131	380.675335	31625738713
132	380.737975	28811808143
133	380.781084	31797490307
134	380.830466	33005543940
135	380.876652	28696453164
136	380.887711	32416131074
137	380.902915	32226744772
138	380.932928	33999132350
139	380.980547	33254486455
140	381.016913	30790327933
141	381.083071	32237889560
142	381.149682	30621357617
143	381.164965	33963160335
144	381.240015	37411790477
145	381.283238	38665395653
146	381.341051	36008202553
147	381.387706	35870106493
148	381.481476	35384816957

Mass Spectrum List Report

#	m/z	I
149	381.509431	34542039957
150	381.531317	37812470693
151	381.574486	34483882461
152	381.655414	39280033623
153	381.708875	39921043915
154	381.731792	41735345623
155	381.783758	39137325605
156	381.826661	37959332533
157	381.879770	41674997596
158	381.915438	39252799080
159	381.937136	43158111430
160	382.002507	44462982366
161	382.067221	44056576651
162	382.117699	45918129543
163	382.179311	42498182887
164	382.198995	42747543424
165	382.226129	46178052579
166	382.265678	49263857959
167	382.295459	44278014484
168	382.360341	53716742584
169	382.424118	53224818909
170	382.529306	52878506607
171	382.647985	59571203711
172	382.728766	60452034341
173	382.767525	60055731593
174	382.860466	62089028943
175	382.866645	61336476517
176	382.896745	62713706919
177	382.917102	63077417687
178	382.997187	68443077601
179	383.023841	68039793464
180	383.046541	68242454891
181	383.129061	84937729221
182	383.154652	76913157263
183	383.173080	77019748592
184	383.306368	84442769546
185	383.387212	94259557134
186	383.434365	101518317799
187	383.596862	126609990797
188	383.648941	139536292589
189	383.695776	155830008430
190	383.791938	192620279479
191	384.136358	86518544870037
192	384.185575	1167142019340
193	384.611753	127672492685
194	384.689217	104199162752
195	384.781288	84944176161
196	384.809104	84290853699
197	384.846633	78130277882
198	384.888411	74463040976
199	384.956483	71600042441
200	385.139835	11398185211197
201	385.337088	75214292074
202	385.474056	56668146433
203	385.552163	51435712008
204	385.626071	45658971562
205	385.708178	37089497318
206	385.775617	41681318082
207	385.798085	40524287228
208	386.002799	81806172244
209	386.133554	15810953139739
210	386.144138	1423701418542
211	386.265299	132047369560
212	386.311962	104665506637

Mass Spectrum List Report

#	m/z	I
213	386.360433	88987369510
214	386.417425	71608179044
215	386.474031	70966495976
216	386.585399	58587022714
217	386.613391	56821241572
218	386.630327	53605523396
219	386.664691	59872592583
220	386.721773	58216607504
221	386.756618	53801523962
222	386.812218	49183890043
223	386.871502	41830338193
224	386.911831	42181555043
225	386.962741	38253025174
226	387.011455	29101630218
227	387.064533	34508191590
228	387.137048	2529794230576
229	387.240541	63279791177
230	387.248839	56212512192
231	387.366154	45713548036
232	387.426070	41352959557
233	387.584297	39688600065
234	387.622612	30085954544
235	387.671204	37163148968
236	387.706951	36970800661
237	387.766322	35007545076
238	387.784384	34246558915
239	387.828518	36652282173
240	387.927573	39458556810
241	387.959015	40116536215
242	387.987164	35285898279
243	388.055205	34645981249
244	388.099690	35288343406
245	388.140798	186479380308
246	388.228215	35697226583
247	388.287757	37529255135
248	388.310421	34464941372
249	388.356331	27240637808
250	388.397505	32357270137
251	388.519316	32867122551
252	388.535271	32688435353
253	388.569041	31554344956
254	388.617529	30502836978
255	388.684088	33285293460
256	388.828571	28978521596
257	388.907176	30659415413
258	388.993709	35667265619
259	389.004548	32768547467
260	389.031973	29480976792
261	389.071575	27340812987
262	389.099577	27908163571
263	389.259111	27110251705
264	389.313662	29848013115
265	389.339021	31293270175
266	389.406920	27451918037
267	389.456454	30212084513
268	389.630418	29952041321
269	389.660247	27046765734
270	389.827175	29297309560
271	390.017789	28713396082
272	390.326232	29102570688
273	390.513346	26835174819
274	390.792076	27030962609
275	391.231182	27813162212
276	391.452691	27166327462

Mass Spectrum List Report

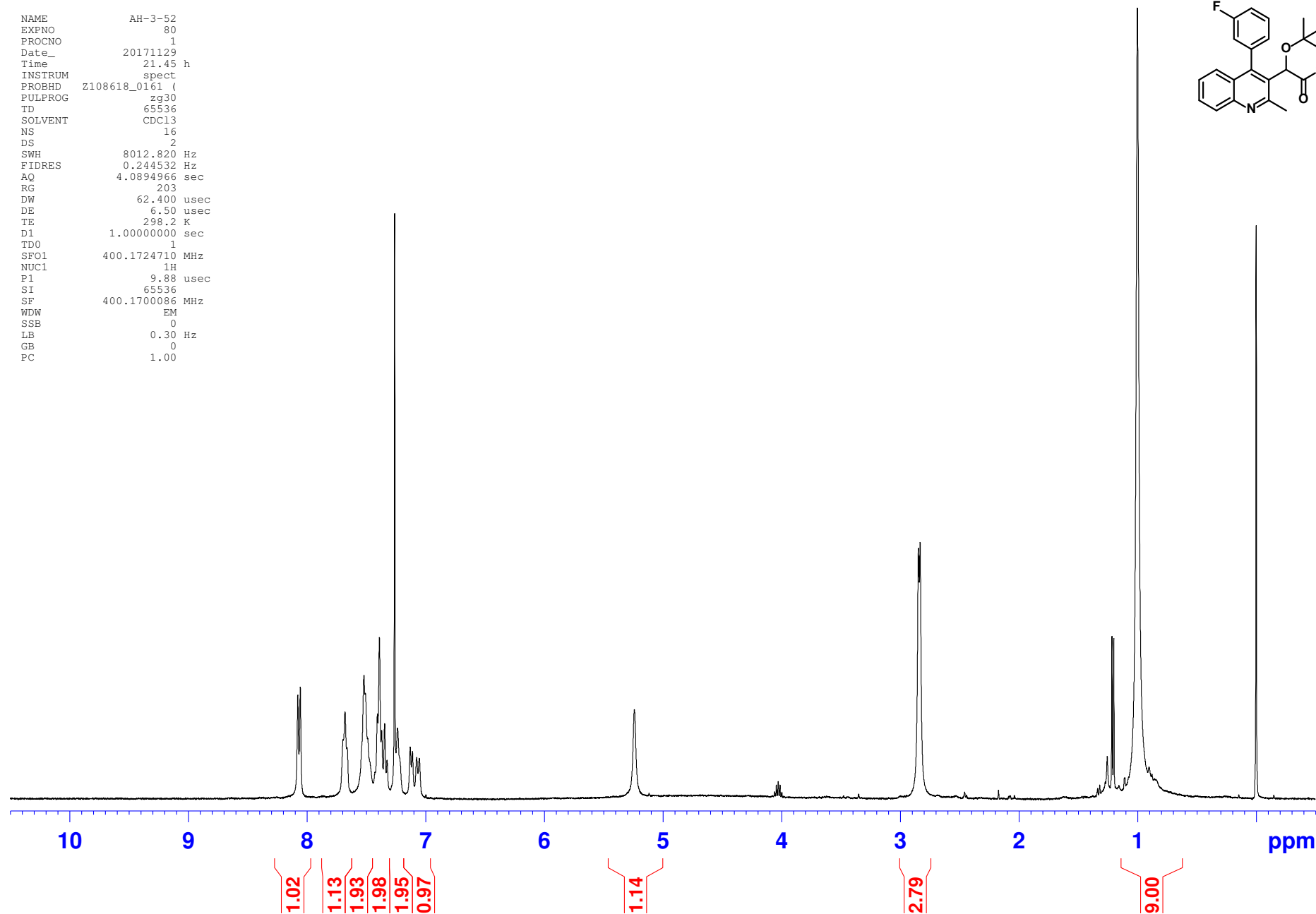
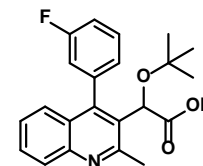
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280	396.652319	26583096093
281	398.152904	33675718645
282	405.210749	26282032315
283	406.118592	1006290938426
284	406.974780	24896762358
285	407.120178	62497633353
286	407.122323	209073704032
287	408.115880	293248173880
288	409.119457	47590104325
289	412.168533	105531296019
290	412.183933	25828849725
291	413.171770	26358154611
292	414.164410	31136104198
293	426.184282	54224934807
294	426.744082	23869509618
295	428.098863	95356586823
296	428.101167	137471482533
297	430.098512	24515644112
298	444.215742	22010664697
299	445.559825	22754929564
300	446.994330	22306294729
301	448.272300	22030609188
302	456.067236	36453747344
303	462.885960	25425163763
304	473.932199	26231840540
305	485.954114	23795872580
306	489.870565	22825087685
307	508.121190	40556130183
308	508.583110	72698670129
309	510.137040	42828791222
310	510.522837	23543229063
311	526.758526	22621993083
312	527.426856	22541459610
313	536.586485	23895101330
314	536.614410	427465426559
315	536.667415	22786202205
316	536.697056	24488459729
317	537.617795	94501274717
318	564.645951	101078201973
319	567.304372	22296984966
320	574.852860	23795096070
321	579.548360	23367030113
322	592.677418	117651539952
323	593.680602	31712345580
324	601.203987	55532239579
325	602.207156	23483176298
326	603.200436	27436947725
327	603.219626	94316165405
328	604.222646	29755953888
329	605.216840	38981923507
330	609.195610	25624823912
331	619.661113	25626502208
332	627.150233	24298787784
333	629.042565	22362078089
334	638.795277	22775448664
335	657.635404	22757322260
336	674.278511	23493933432
337	679.408142	23550999397
338	688.615604	23735227522
339	689.338622	23188931567
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Mass Spectrum List Report

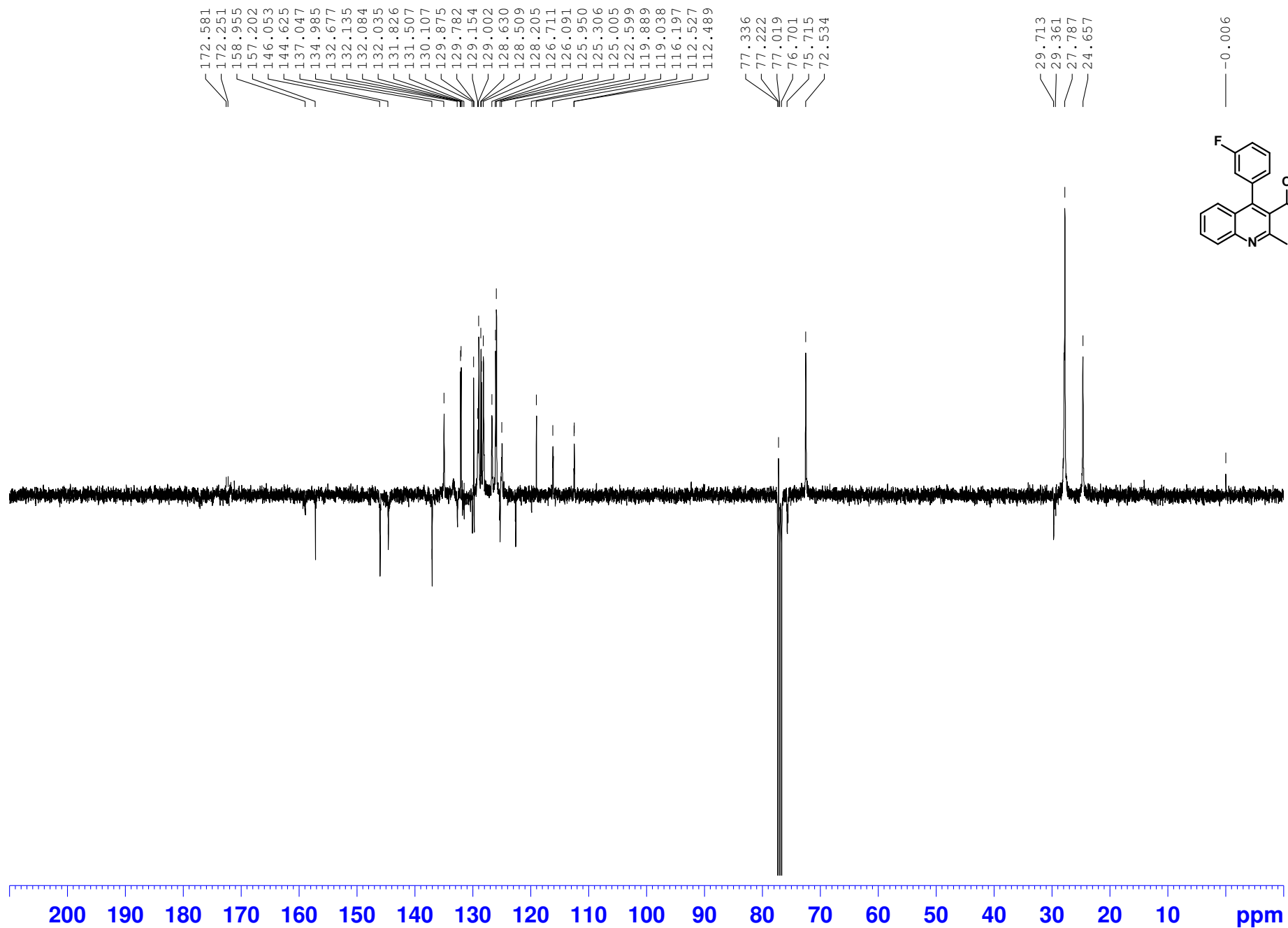
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344	753.000571	24460264107
345	795.014616	24005893701
346	796.844733	23192911128
347	901.554003	24888640558
348	923.823362	28157867087
349	944.019327	26604371520
350	958.655109	23753207748
351	998.024295	23697428003

AH-3-52B Characterization

NAME AH-3-52
EXPNO 80
PROCNO 1
Date_ 20171129
Time 21.45 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-52 Characterization



Mass Spectrum List Report

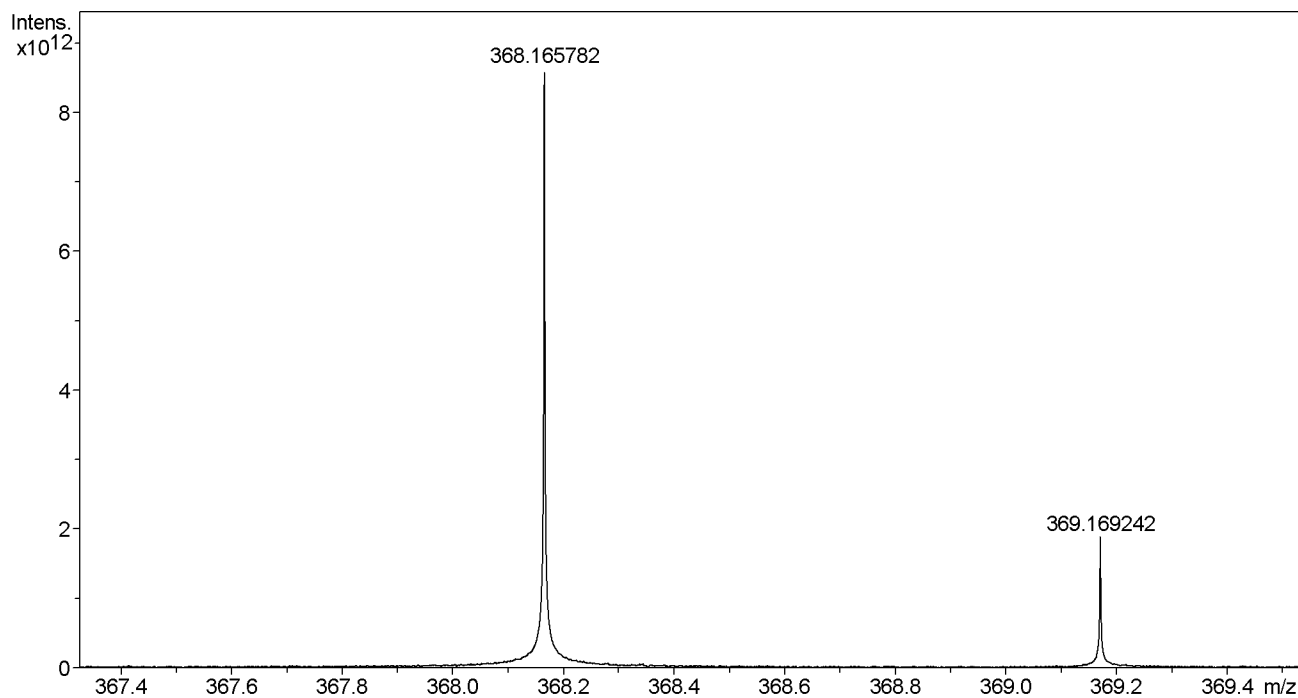
Analysis Info

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Method
Sample Name AH-3-52
Comment AH-3-52 in THF:MeOH C22H22FNO3 H+

Acquisition Date 3/19/2018 9:58:43 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-52 in THF:MeOH
Exact Mass of C22H22FNO3 H+ = 368.165648 m/z
Mass Observed = 368.165782 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.513752	25536860862
2	185.165457	21164275285
3	186.816818	21466734798
4	187.056136	21378278977
5	187.929062	23131997610
6	188.767568	21314475550
7	189.651783	22217139023
8	189.795054	22121851400
9	192.378645	21856081130
10	193.866375	21520593005
11	194.632279	22526132897
12	200.822657	21261306364
13	202.340442	74348764224
14	202.536504	21041884458
15	204.739139	21062310855
16	205.428614	21531596016
17	209.107420	21927788465
18	209.441662	27175144840
19	209.686007	36850880518
20	209.894465	21613473245

Mass Spectrum List Report

#	m/z	I
21	210.214569	22218379328
22	212.245527	21103490046
23	215.089246	21766151918
24	215.130312	21881230091
25	215.585643	21965468320
26	215.604474	21295236489
27	216.810598	21305985416
28	223.421531	21600507894
29	229.039886	23243392863
30	229.343516	21216028684
31	231.120515	27787390520
32	236.951075	23580721769
33	239.316215	21362539639
34	239.990984	21262080142
35	240.968833	21538308840
36	243.005772	22191492201
37	245.720365	22051796750
38	246.592526	28127129295
39	247.171974	27185630032
40	247.256760	22212171061
41	248.141922	23933054497
42	249.094794	31930512752
43	254.760681	23151472589
44	261.026292	21937226154
45	262.921819	22874659227
46	264.383888	24336059985
47	278.952404	21729115697
48	279.135219	25998571020
49	280.135999	22180172229
50	280.744885	24878055223
51	281.691801	21813160558
52	283.563822	26365980109
53	286.967933	23365636635
54	287.405941	21531108223
55	288.906632	21360650622
56	290.252129	24233879006
57	297.178858	22587170238
58	301.075617	159740273456
59	301.125980	24038498089
60	302.078964	28894372060
61	302.797851	23380147303
62	303.141689	28903553778
63	304.361163	22164050021
64	312.103372	24562198384
65	316.209614	22623013371
66	317.121183	26816702130
67	317.569137	26075066880
68	318.601975	22049306726
69	324.176116	35791154357
70	325.372969	22833963694
71	326.837166	21988882421
72	328.575152	21723204903
73	338.708972	22097960561
74	345.243207	22687803230
75	359.714796	22730851042
76	361.552250	24134585987
77	364.525314	22135271779
78	366.408975	28084947176
79	366.714016	22525262664
80	366.877151	40324143848
81	366.888742	32181469765
82	367.416958	24400588411
83	367.673149	25585317149
84	367.710196	25718874500

Mass Spectrum List Report

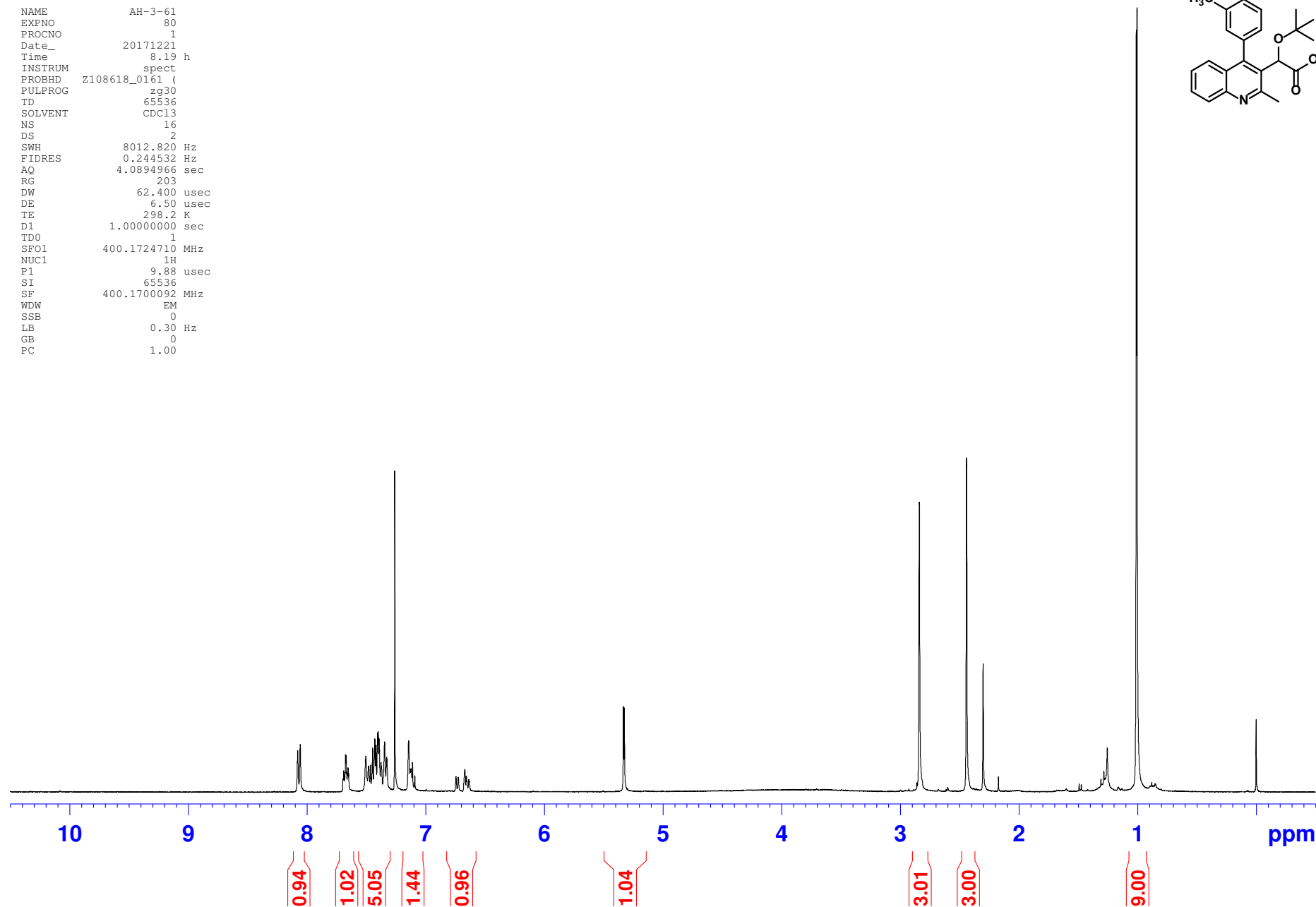
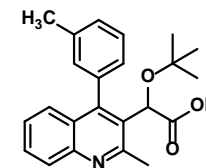
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87	367.827007	27876188969
88	367.846589	29230621414
89	367.883816	28863612248
90	367.938103	36789191410
91	368.004014	42628337601
92	368.032680	53792423453
93	368.094062	90015418278
94	368.165782	8626882596036
95	368.275282	62643183134
96	368.323477	45624028400
97	368.344343	53454204004
98	368.358014	37996467061
99	368.412211	30793770588
100	368.445227	29869946099
101	368.459939	30110115451
102	368.484220	24683809123
103	368.517886	25845734543
104	368.553724	24982865648
105	368.569125	25043729445
106	368.632727	22758812189
107	369.089846	26932161995
108	369.169242	1894591467481
109	369.253460	26386831482
110	369.288520	22865284715
111	369.426065	23365825160
112	369.451615	25249659866
113	369.882701	109480772953
114	370.172783	124394313774
115	372.980550	23366986522
116	377.834152	22780234100
117	380.871438	23410195605
118	390.022935	22893313439
119	390.100160	23763968318
120	390.147950	721318913164
121	391.151393	136283030663
122	393.107551	22194345451
123	393.297862	30376984735
124	395.688679	25144038605
125	398.241827	134071281599
126	398.547820	22332167375
127	412.130024	242737896944
128	413.133304	59882735233
129	424.228786	43999461353
130	425.243658	24198848112
131	425.287860	49034638077
132	428.850227	22909877194
133	430.890260	24507380547
134	435.345101	52632590222
135	439.082782	23259636133
136	440.598878	22283196704
137	445.705531	24349636446
138	456.443943	23659369657
139	459.170306	41841248706
140	460.173489	24672615607
141	461.185722	58974456000
142	465.380082	26024108259
143	470.088257	26602302887
144	477.180631	531327824969
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147	490.913441	22500777630
148	491.160095	38003696675

Mass Spectrum List Report

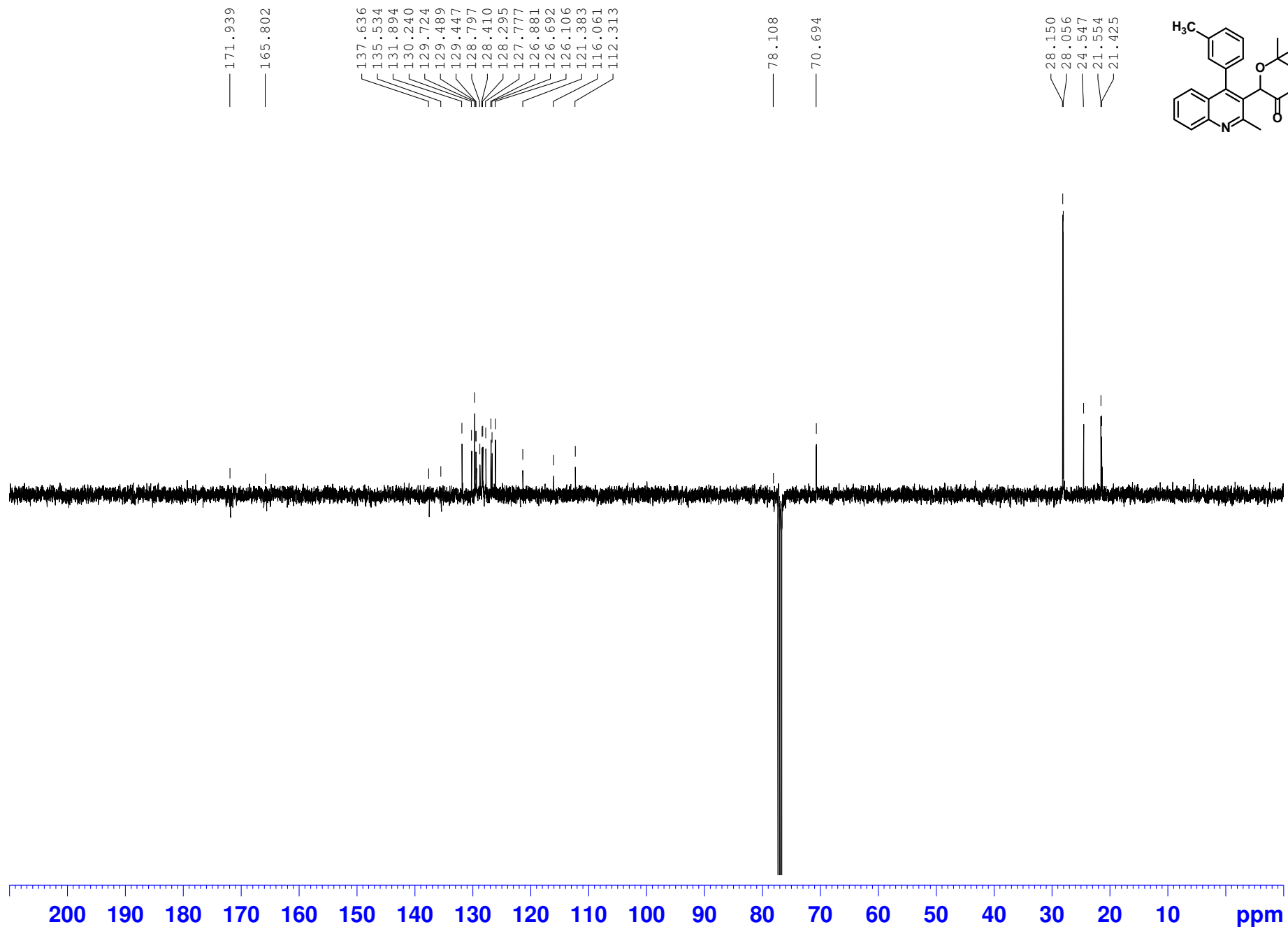
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150	492.894101	24280307115
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153	493.175478	2180530039904
154	493.324347	23883134976
155	493.820086	22898963228
156	493.890853	24235356701
157	494.178933	512186710438
158	495.182513	32849685734
159	500.511538	22443803184
160	503.550406	24978333039
161	505.413449	22231898342
162	508.582357	84708495208
163	509.207051	31806122525
164	509.585535	31107764164
165	516.797420	22539094905
166	519.441253	23977856732
167	523.186275	55795891090
168	524.576914	27330039985
169	536.613514	394423453273
170	537.616825	120697252873
171	538.620051	23506335111
172	552.608256	35046034097
173	554.367447	22769023858
174	554.707119	22333109033
175	557.825884	22962426010
176	564.645046	67858071615
177	572.908421	22312500884
178	579.058184	29722271657
179	579.162035	597201935235
180	580.165468	189870772834
181	581.169118	27401019185
182	588.235156	390718164364
183	589.238518	93894546971
184	592.676301	98862809952
185	593.679603	33015329109
186	599.549172	45452581601
187	600.552551	22950012419
188	613.429344	35106917774
189	630.441885	23195524934
190	646.194237	46983617326
191	646.252602	218230767064
192	647.255965	85577610341
193	657.455871	40310293881
194	668.234185	36792908122
195	681.936275	24602701001
196	685.436513	27180713062
197	697.259049	22795445474
198	704.290201	23931998135
199	712.747506	23421842116
200	743.514537	23698065842
201	744.711116	22706064918
202	762.575721	22777697581
203	767.865826	24617232976
204	801.686229	22810880372
205	815.047647	23032860180
206	824.203671	22834824121
207	837.024307	25847865437
208	861.541762	24591085278
209	955.290860	23828651378

AH-3-61 Characterization

NAME AH-3-61
EXPNO 80
PROCNO 1
Date_ 20171221
Time 8.19 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-61 Characterization



Mass Spectrum List Report

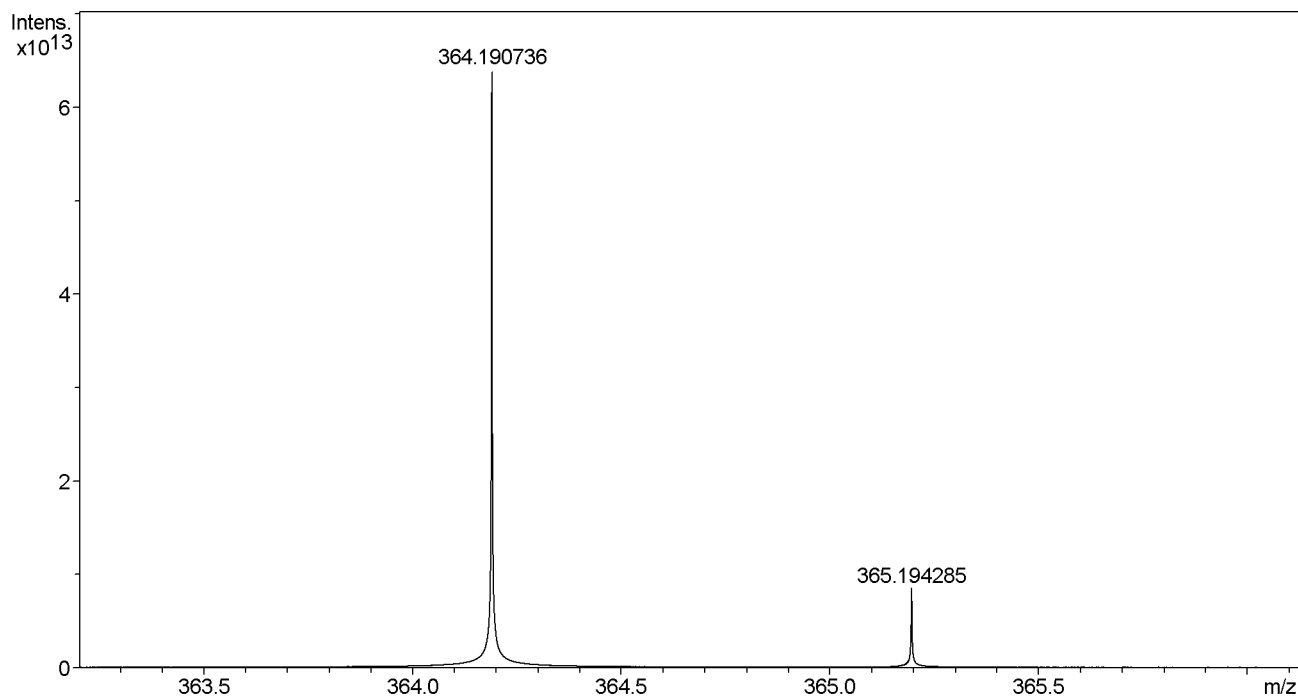
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-61_pos_000001.d
Method
Sample Name AH-3-61
Comment AH-3-61 in THF:MeOH C23H25NO3 H+

Acquisition Date 3/19/2018 9:52:39 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-61 in THF:MeOH
Exact Mass of C23H25NO3 H+ = 364.190720 m/z
Mass Observed = 364.190736 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.313478	23140322341
2	186.031022	27311889616
3	186.102546	29442334961
4	186.554781	313914080069
5	186.875101	24486097269
6	187.651594	22081109984
7	190.172477	21882455245
8	190.897225	21471860563
9	192.144313	23845132004
10	193.866735	22787421527
11	193.991547	21798788728
12	194.891295	23095550661
13	196.846687	21280090802
14	200.020657	21179973824
15	200.423340	21983580256
16	200.630591	21254788416
17	203.073077	22506996229
18	203.470548	22600768792
19	203.554973	23098838801
20	207.668154	23304951521

Mass Spectrum List Report

#	m/z	I
21	209.441585	45756103396
22	209.886788	21314831103
23	210.651286	23734631960
24	216.081071	23492578754
25	216.309527	21666868974
26	217.088552	26621441673
27	218.096310	27583870407
28	219.871073	22051149121
29	220.856163	24238483475
30	223.530788	21395230504
31	225.923812	21276165974
32	227.776849	21751235575
33	227.815699	22936034253
34	228.326920	21310082964
35	228.823449	23705216203
36	228.884447	22998148155
37	230.096655	24406905122
38	230.637053	21834576603
39	231.104355	21269955459
40	232.112307	35570069126
41	233.094644	22549669594
42	233.882760	24075758558
43	241.564126	21262059606
44	241.586047	21355452216
45	241.734790	22282345116
46	244.112385	30661770439
47	246.091379	23977459582
48	246.128012	36517346787
49	247.099051	24263988909
50	248.107262	27245670941
51	252.602547	21849607135
52	257.377987	21305768158
53	258.064977	22095801673
54	259.557982	21342712552
55	261.564940	23265441150
56	261.876045	22171233402
57	262.122858	34150283442
58	262.937759	21774548990
59	263.125984	35585175170
60	263.130608	29131170958
61	263.403269	21246853736
62	263.411515	22041836499
63	264.129166	22342762594
64	264.201211	22693156606
65	269.645884	21718822121
66	273.188965	21539465121
67	273.780784	22125931104
68	275.409600	23000017284
69	276.102098	26013201969
70	283.563705	36037233504
71	283.783055	25273132259
72	286.536348	21305827298
73	286.785237	23571820771
74	288.670642	23129099973
75	289.012660	22903575841
76	289.232092	24728441310
77	291.154092	24607979782
78	293.952600	22944448715
79	296.542348	21351650105
80	296.763227	22231350148
81	304.732740	23899903590
82	305.505650	24918981656
83	306.112750	25315752070
84	308.091902	21967191489

Mass Spectrum List Report

#	m/z	I
85	308.127737	44571068361
86	309.131287	27884773661
87	311.037095	22029160847
88	312.099989	21599652119
89	320.089924	24725615014
90	320.136192	26401316624
91	320.201235	2310475687170
92	320.263568	36419218475
93	320.274602	22367229409
94	320.327389	23011781444
95	321.204668	387180623599
96	332.697713	25547471614
97	343.869794	23578819519
98	352.191213	544971670944
99	353.194635	72196704371
100	360.137875	25951736782
101	361.009285	25340596287
102	361.044869	26090529792
103	361.247797	25910399392
104	361.509019	27716338087
105	361.550628	25042411165
106	361.568529	28061481793
107	361.611755	28162386284
108	361.714239	26702955073
109	361.745291	25348172502
110	361.765118	27330770040
111	361.783212	25697434280
112	361.857416	26382812868
113	361.909353	28467701038
114	361.964592	33201901380
115	362.025520	30741574674
116	362.083691	27217124694
117	362.157896	30798758456
118	362.253414	31033356307
119	362.307596	27476930827
120	362.316037	35297428544
121	362.379701	31394424414
122	362.400494	31031622008
123	362.445662	33688292185
124	362.467043	29082311059
125	362.528845	34698606451
126	362.625819	36777165391
127	362.697472	32916858982
128	362.787279	35508033599
129	362.806069	33216835898
130	362.822274	41457213741
131	362.854816	40545889181
132	362.902011	40962421512
133	362.939397	40781543315
134	362.985398	38952776649
135	363.010321	39327989786
136	363.058165	41651493481
137	363.104888	42758616297
138	363.140010	46788753354
139	363.181817	61129172756
140	363.196450	45792005997
141	363.300712	51117867841
142	363.331521	51844615118
143	363.344601	52008175323
144	363.379066	49872852081
145	363.417596	53227509445
146	363.444213	59717778609
147	363.528522	65249565729
148	363.554132	63708893379

Mass Spectrum List Report

#	m/z	I
149	363.615066	73357875392
150	363.638492	66416456741
151	363.724607	90793264198
152	363.733054	88343858016
153	363.748755	87822552276
154	363.762309	93699871521
155	363.880363	125664891863
156	364.190736	63966246025901
157	364.495218	124236447168
158	364.707531	73724047509
159	364.731722	72926599502
160	364.766648	65676965171
161	364.814248	72692947268
162	364.868140	63064619675
163	364.954186	58299995214
164	364.986290	58181127054
165	365.013858	65552666494
166	365.114193	82959008998
167	365.194285	8526829656527
168	365.331967	70927635148
169	365.342760	63495020264
170	365.418750	50522123758
171	365.536215	41852347024
172	365.600900	42956987317
173	365.626393	41299298338
174	365.653094	43752570671
175	365.705430	40162352161
176	365.785790	38616473168
177	365.804647	38970076241
178	365.817616	34590424386
179	365.827836	34150743276
180	365.868046	35205333034
181	365.903643	39414212629
182	365.950124	37166687191
183	365.979045	37617205958
184	366.017510	35499416053
185	366.069630	30531457567
186	366.127541	32143808245
187	366.197951	433369221643
188	366.239031	37807526354
189	366.275531	36408612447
190	366.289054	31381200779
191	366.307144	33380903334
192	366.378425	28231200763
193	366.479974	29175833978
194	366.587831	27307097750
195	366.621648	28885014445
196	366.770104	26878393869
197	366.818838	29325711753
198	366.872129	29021753843
199	366.913084	26283048400
200	366.963424	25340054487
201	367.063323	27348841598
202	367.110807	26209309450
203	367.163881	32192314698
204	367.471475	27233865618
205	367.601183	25452053809
206	368.311559	27894879192
207	368.502988	25554497285
208	379.181837	94582257712
209	382.464476	1171241100993
210	386.173133	739041673730
211	386.858522	25129165048
212	387.174587	41284558019

Mass Spectrum List Report

#	m/z	I
213	387.176721	88108659345
214	398.242334	33669782936
215	408.155379	93043637848
216	425.288109	33801132903
217	425.936132	22179968114
218	425.946678	23086661542
219	426.792346	21905675464
220	435.345365	40580702148
221	441.736088	22690669959
222	449.442535	22323518375
223	453.268834	21587080302
224	453.407341	32392979740
225	454.692361	22146049940
226	458.365175	21892214848
227	478.892532	22280460616
228	478.989841	21920434853
229	481.351499	23667373129
230	489.724914	23713961452
231	500.343813	24016406913
232	502.570624	22705582113
233	508.582708	75817914978
234	509.585680	24125043582
235	525.001907	24690669694
236	536.614020	324203879885
237	537.267861	84423406707
238	537.395878	63321762922
239	537.617325	104824225939
240	539.264672	29081080882
241	542.609184	23875800037
242	552.609077	36982596295
243	558.563258	24839459529
244	563.219348	24723575293
245	564.645669	53908498398
246	569.403802	28047202044
247	581.257929	47997717176
248	583.273763	38963668460
249	592.676964	79475362125
250	593.680013	35959609374
251	596.124523	22231100371
252	596.583173	22772850407
253	597.213562	22482749549
254	599.549961	26272022078
255	601.031927	22917979301
256	613.429856	32156382329
257	645.409771	24602474691
258	652.187686	22657222987
259	652.257507	23854661454
260	657.456615	36307318888
261	658.459425	22433251977
262	662.105160	24536553680
263	674.280158	25323176794
264	674.328499	36033005711
265	675.730244	23564585967
266	698.940997	23557995899
267	699.436291	25389366740
268	701.482715	22982164105
269	704.901406	22881829862
270	710.740435	23463416095
271	727.204241	24309522437
272	728.421216	22961739442
273	773.047098	24272637729
274	778.063458	22665608210
275	798.426342	22574840968
276	826.750832	23373796530

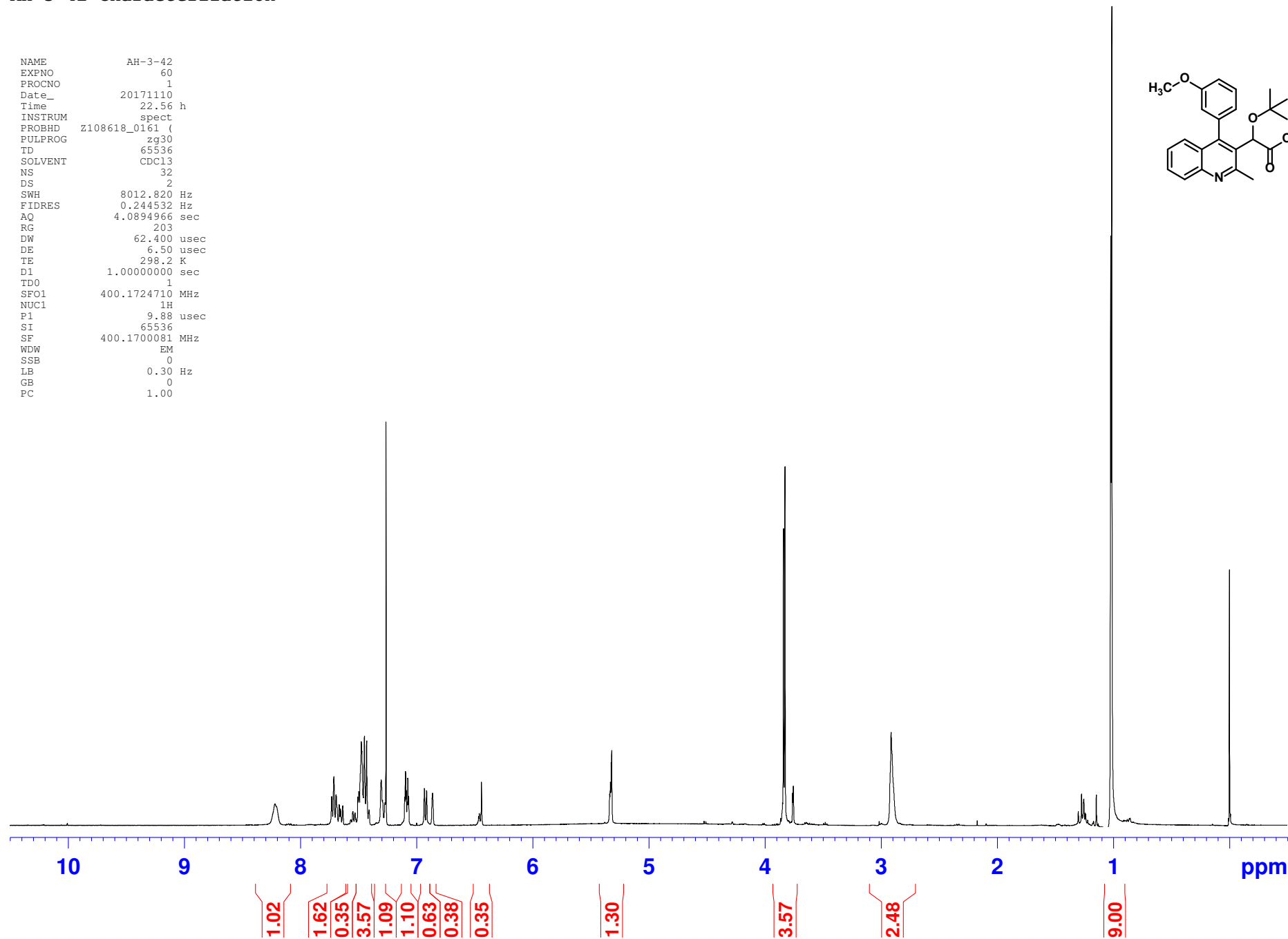
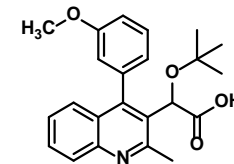
Mass Spectrum List Report

#	m/z	I
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279	860.514501	22951530967
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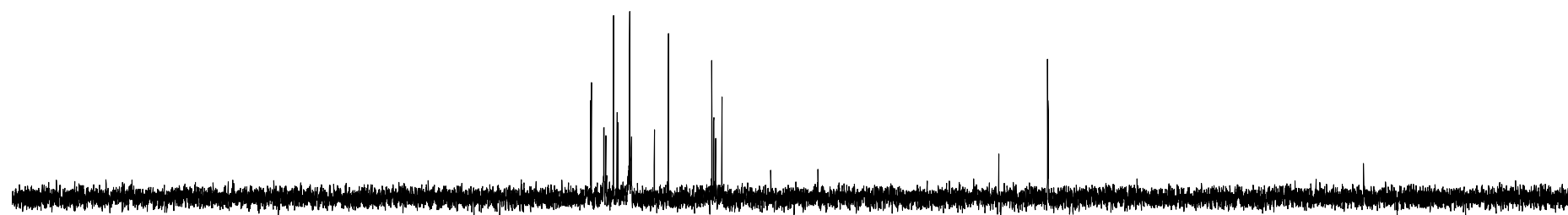
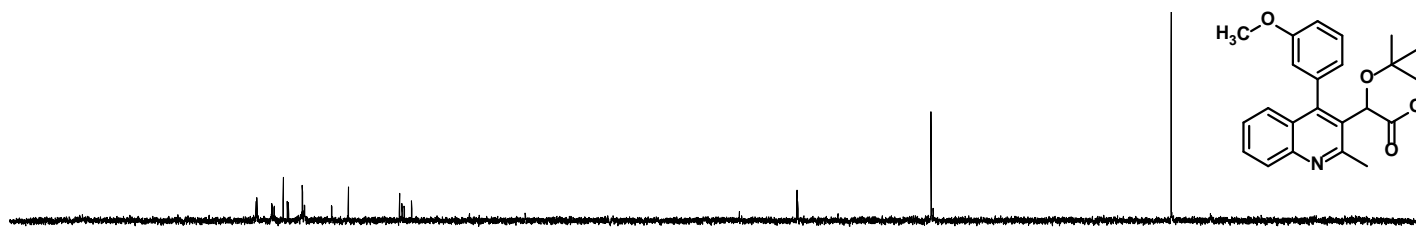
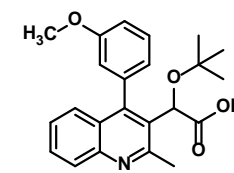
AH-3-42 Characterization

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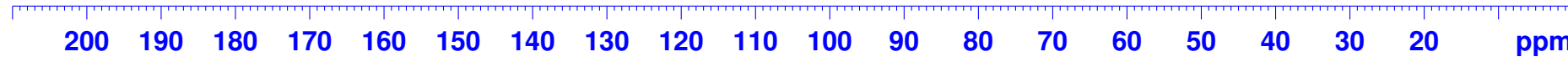
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EXPNO     60
PROCNO    1
Date_     20171110
Time      22.56 h
INSTRUM   spect
PROBHD    z108618_0161 (
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        32
DS        2
SWH       8012.820 Hz
FIDRES    0.244532 Hz
AQ        4.0894966 sec
RG        203
DW        62.400 usec
DE        6.50 usec
TE        298.2 K
D1        1.00000000 sec
TDO       1
SFO1      400.1724710 MHz
NUC1      1H
P1        9.88 usec
SI        65536
SF        400.1700081 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
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AH-3-42 Characterization

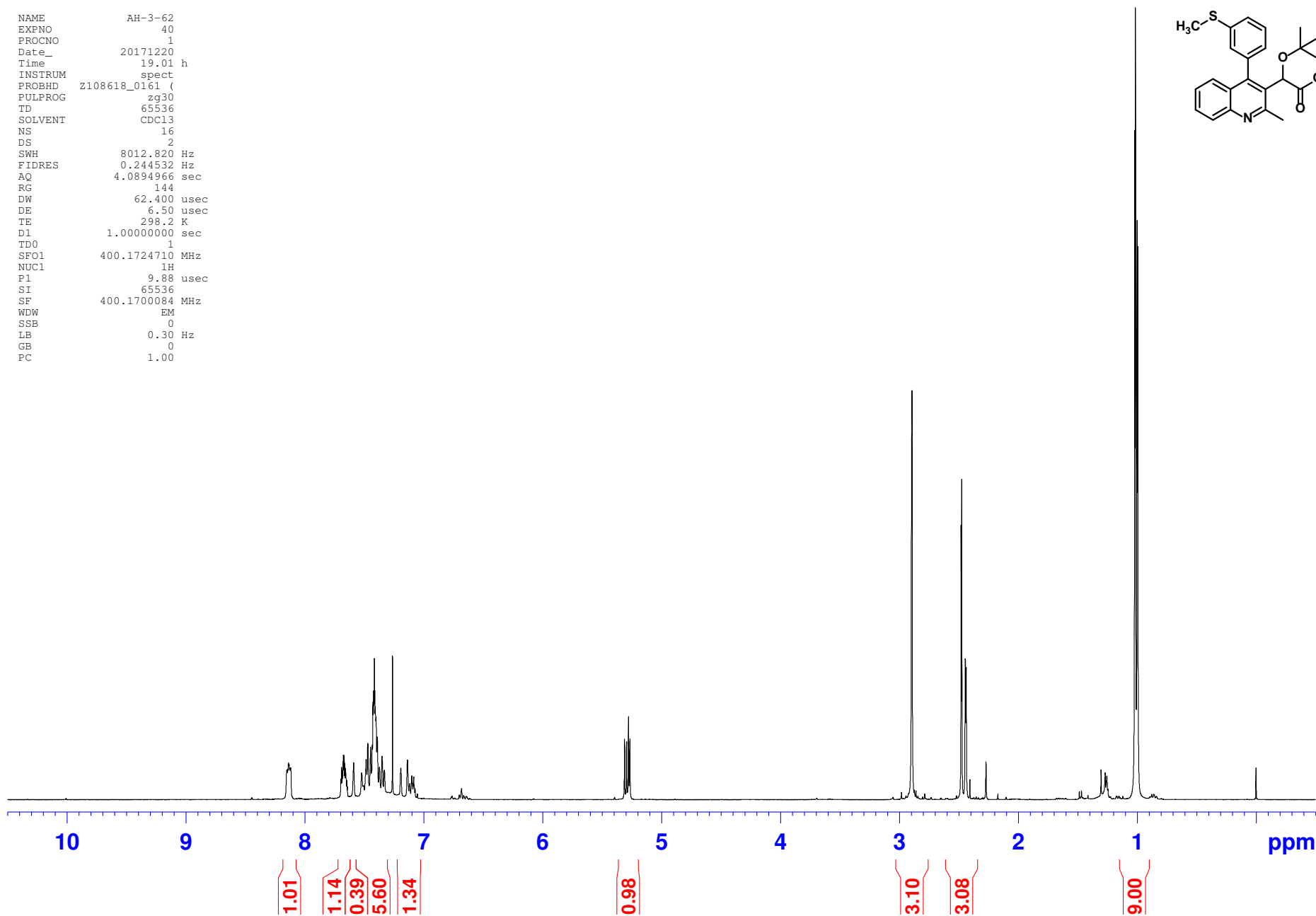
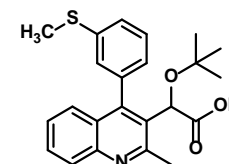


- 172.35
- 159.82
- 159.04
- 136.52
- 136.45
- 132.18
- 132.08
- 130.37
- 130.13
- 130.02
- 129.09
- 128.62
- 128.50
- 126.93
- 126.68
- 126.15
- 123.59
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- 115.60
- 115.34
- 114.49
- 77.23
- 70.68
- 70.59
- 55.43
- 28.13

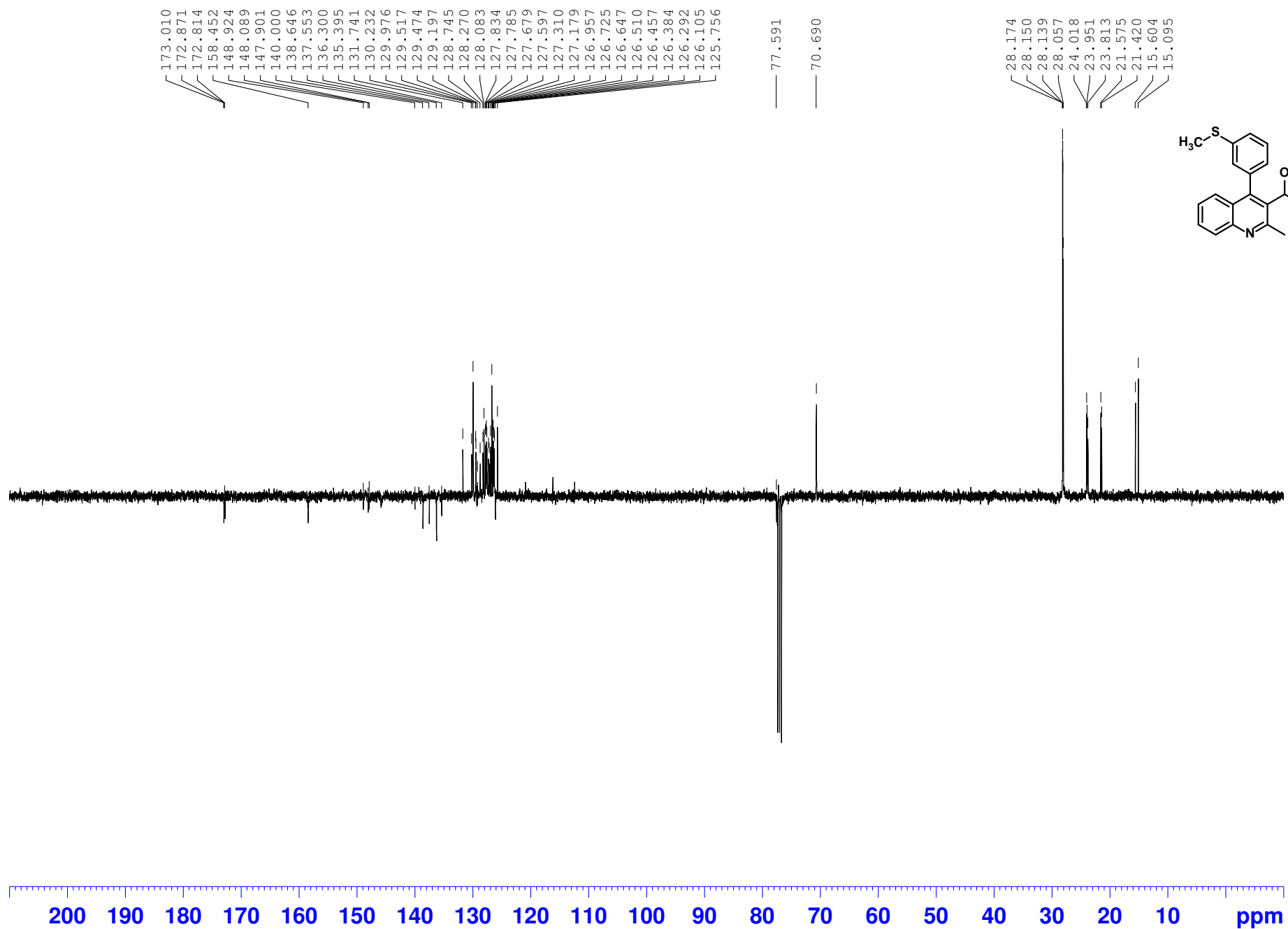


AH-3-62 Characterization

NAME AH-3-62
EXPNO 40
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Date_ 20171220
Time 19.01 h
INSTRUM spect
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PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700084 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-62 Characterization



Mass Spectrum List Report

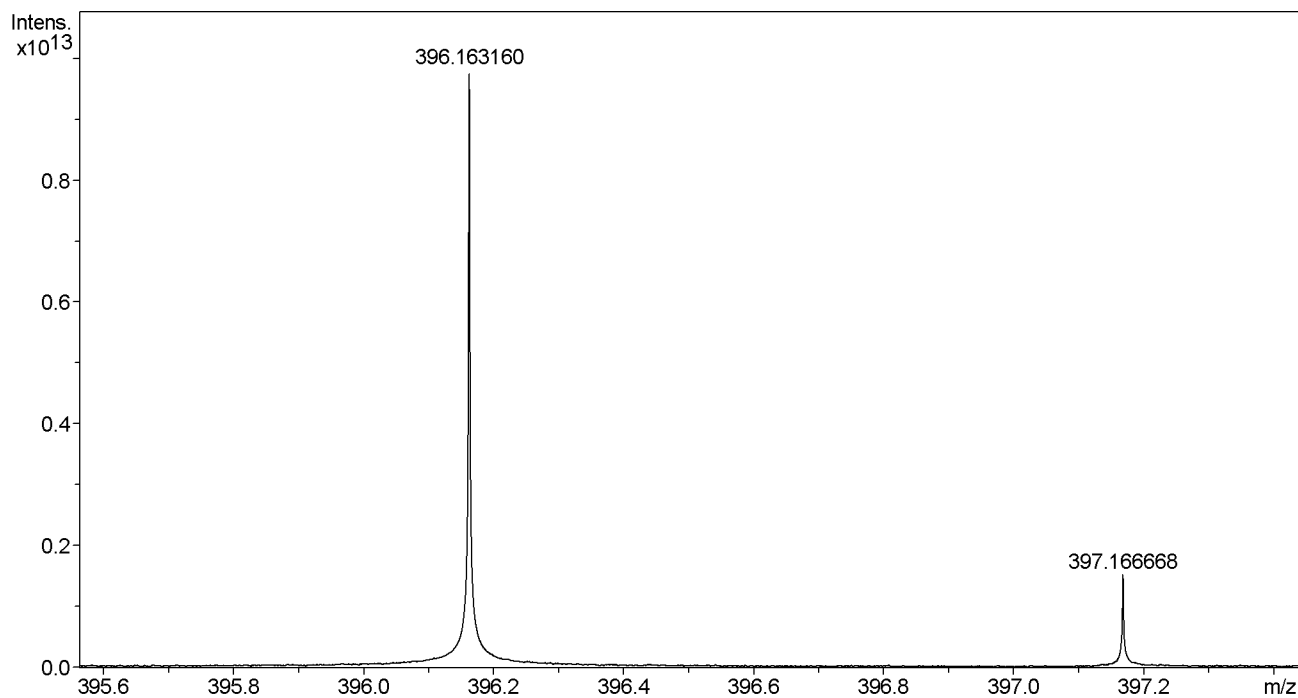
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-62_pos_000001.d
Method
Sample Name AH-3-62
Comment AH-3-62 in THF:MeOH C23H25NO3S H+

Acquisition Date 3/19/2018 10:05:39 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-62 in THF:MeOH
Exact Mass of C23H25NO3S H+ = 396.162791 m/z
Mass Observed = 396.163160 m/z

Difference < 1.0 ppm



#	m/z	I
1	185.843550	22403615856
2	186.030937	36260878547
3	186.554598	63714776266
4	187.958183	22043541232
5	188.001011	21388588655
6	188.720466	22640774754
7	189.455895	22088414249
8	189.873588	22888885067
9	190.193407	21840571523
10	192.145763	20959642258
11	193.312809	54521564719
12	194.050658	23455884941
13	195.206251	22127287894
14	196.645087	21258939202
15	197.999885	22135380859
16	198.084694	24348307216
17	199.750758	21007737635
18	201.512333	21547967800
19	202.340459	42299566455
20	202.593965	21043138152

Mass Spectrum List Report

#	m/z	I
21	203.081141	21519134453
22	204.080826	21065863665
23	205.084282	22602736989
24	205.169144	21562360074
25	205.486354	24815081113
26	206.805223	20929868928
27	207.122694	21190025905
28	209.441733	59814311080
29	210.238752	21734825041
30	210.600164	23329030048
31	214.252293	23051256357
32	216.080973	28493892750
33	217.641879	21824519552
34	218.096317	39918139896
35	224.938084	21305837042
36	225.154269	21749280950
37	227.024572	21717257688
38	227.953540	21784325610
39	230.096418	27856425584
40	231.104429	63866835924
41	234.117784	22322977746
42	234.196346	23018753901
43	238.967557	22194879218
44	239.789335	22012350403
45	243.780880	21202364100
46	245.119694	46831445456
47	246.091349	29221836310
48	246.424636	25375070364
49	246.718275	21272693272
50	248.102589	21286375636
51	248.107038	32359085822
52	249.114791	23372135634
53	250.068712	23926054967
54	252.980799	26454370752
55	257.529838	22201099496
56	259.516350	21462362110
57	259.770127	21641139406
58	260.106994	23762477698
59	262.122501	42909949489
60	263.130665	24419412856
61	267.666115	22346824138
62	267.717550	23035915303
63	270.950074	23310164941
64	271.830353	26265732334
65	275.273283	21466033947
66	276.499696	27686665790
67	277.356226	23359035845
68	287.472778	22712560612
69	291.746096	24266055562
70	294.094568	60732125931
71	294.160419	22136397448
72	295.098276	27520326307
73	297.595649	21486511741
74	298.155431	22604311274
75	304.209566	22306438865
76	304.931322	68217180864
77	307.414982	27071536242
78	308.128055	66699533318
79	312.100037	35554881717
80	315.232140	22623205553
81	316.227593	34877394735
82	319.658304	25295396965
83	319.934868	25022219424
84	320.109307	32345940767

Mass Spectrum List Report

#	m/z	I
85	320.138473	28898438342
86	320.201300	2819355994281
87	320.262051	32671923007
88	320.282068	24991702256
89	320.308834	22911950580
90	320.340313	22344033948
91	321.204750	644515938061
92	326.731857	23143624074
93	332.072226	69508502943
94	340.099608	31752489840
95	341.103235	27961215670
96	342.377538	25516749583
97	351.886510	25701656662
98	351.960404	26544731058
99	352.173340	6181465784931
100	352.245867	56703705423
101	352.389344	27365053392
102	352.407762	24685514256
103	353.176886	1257822616189
104	354.169470	122297476784
105	354.180358	33867217870
106	355.173000	24939636653
107	360.067331	74427696115
108	362.471917	41577112973
109	362.529859	28179574103
110	362.748069	28879879138
111	362.855002	26415710382
112	362.897385	26742611584
113	362.986928	37384716939
114	363.050696	29707765240
115	363.108223	26795008637
116	363.133048	26751764695
117	363.155224	30237312956
118	363.182235	36133769872
119	363.196391	30141525858
120	363.233512	29837248418
121	363.250772	28585222038
122	363.280620	29395487967
123	363.304516	26513491763
124	363.319231	35545023721
125	363.377251	30551357385
126	363.415586	37818662760
127	363.429976	29384087602
128	363.441909	28802116605
129	363.481532	35667187118
130	363.519026	32421839305
131	363.615063	40502589110
132	363.646469	36145488979
133	363.718329	48112003960
134	363.731778	42351536031
135	363.840621	58846026370
136	363.886870	64953741294
137	363.965521	82504954448
138	364.191043	24777126998133
139	364.340508	111170771133
140	364.428329	69464847739
141	364.468268	57827086008
142	364.495616	56033107782
143	364.520034	54481686381
144	364.527792	52030658009
145	364.552306	55973645913
146	364.584841	44051174417
147	364.623616	38124839444
148	364.686771	37519441851

Mass Spectrum List Report

#	m/z	I
149	364.775981	27980140727
150	364.805253	28032858955
151	364.832281	25667910815
152	364.878958	26142086492
153	365.111339	37310838859
154	365.194423	5693264192023
155	365.272600	71908131116
156	365.369566	40289542331
157	365.386763	39811173227
158	365.405697	39346469061
159	365.449309	46850854078
160	365.483962	39428600737
161	365.559589	33839188754
162	365.605946	31824114523
163	365.628278	30392415063
164	365.644383	27859860545
165	365.675617	28608824009
166	365.712656	26420171190
167	365.777668	28246210792
168	365.812926	30289050725
169	365.832546	27057019566
170	365.920879	33162483391
171	365.982975	25081177979
172	366.198186	253739087209
173	366.581517	24963306992
174	367.005012	26152789551
175	368.168497	753813136134
176	368.224075	28971016560
177	369.172045	71854493161
178	379.181422	65995222259
179	382.463683	383012316258
180	382.469288	62460969021
181	386.173307	819400666103
182	386.214770	29700327204
183	387.176796	123706378329
184	390.150648	156493018479
185	391.154106	32081837066
186	394.941084	25062464449
187	395.516733	27726500389
188	395.627900	24611192500
189	395.653762	25605444571
190	395.678110	30415248623
191	395.714241	298666565729
192	395.820195	33350695667
193	395.840209	32877458634
194	395.891337	37475863797
195	395.969059	51563266679
196	396.026606	57343988026
197	396.163160	9812343688296
198	396.299365	60259900608
199	396.380200	39288294596
200	396.437683	41023856137
201	396.508993	29687408314
202	396.541071	34858166902
203	396.749983	24188676010
204	396.807198	24582061227
205	397.166668	1521546567360
206	397.224434	38522850947
207	397.310657	25466447042
208	397.346758	26177193638
209	398.159449	122040907708
210	398.167597	31531743583
211	398.170604	59157419900
212	398.241998	64775303167

Mass Spectrum List Report

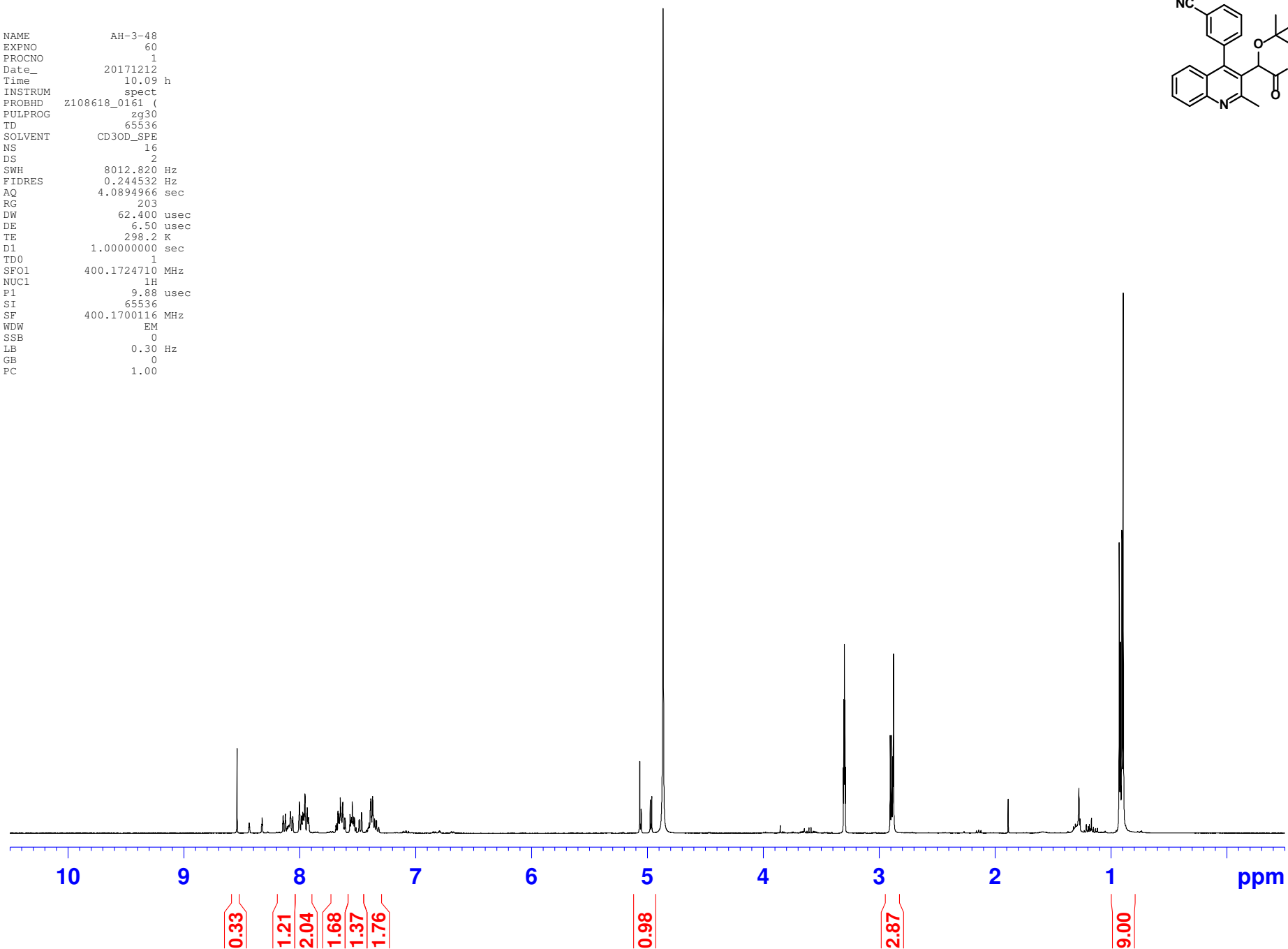
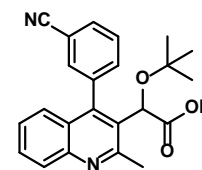
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213	399.163071	30226991154
214	408.155474	86453027265
215	412.158583	250673544532
216	413.162083	31820781745
217	418.061098	25917870633
218	418.145625	120197718007
219	419.149011	31718875892
220	421.474584	23378425186
221	422.521750	23902284527
222	433.167968	22826684690
223	434.010729	24017387145
224	434.087736	30062222561
225	434.140467	1026357557195
226	434.193863	32766539557
227	435.143992	150908573105
228	440.127693	79328579115
229	441.130409	25891731287
230	449.457395	22098718388
231	451.619976	23217920934
232	453.407707	28284249012
233	456.122666	164815957776
234	457.126082	29462745355
235	479.439874	21924777303
236	479.711218	23715721397
237	493.146673	22819456270
238	498.172744	22667427829
239	508.582889	104442810112
240	509.585948	33938258019
241	512.883274	22826977557
242	513.696638	22468501680
243	521.546221	24985676761
244	532.781832	23196747271
245	536.614171	500337961583
246	537.268173	60987328828
247	537.617626	113826377778
248	538.620846	27779003917
249	541.853404	22619281650
250	552.609431	24759614222
251	564.645625	100340919552
252	565.121841	23840990036
253	565.648803	39327353135
254	567.360665	22322971043
255	568.368879	22239762969
256	569.404172	23890971683
257	572.809741	22642366306
258	581.258113	35967012904
259	583.273760	29230273460
260	583.788985	23351551307
261	587.510170	23801316937
262	592.677148	134089437561
263	592.705543	24889747902
264	593.680402	50516038295
265	608.051069	23219221910
266	628.154577	22618164560
267	643.202706	24009198371
268	657.456645	24136701668
269	685.438211	25851636742
270	707.918582	24715394207
271	716.264265	26238341351
272	741.069595	23627864027
273	746.726960	26519199382
274	746.757549	22984016372
275	771.860760	23138437209
276	777.134719	23359618958

Mass Spectrum List Report

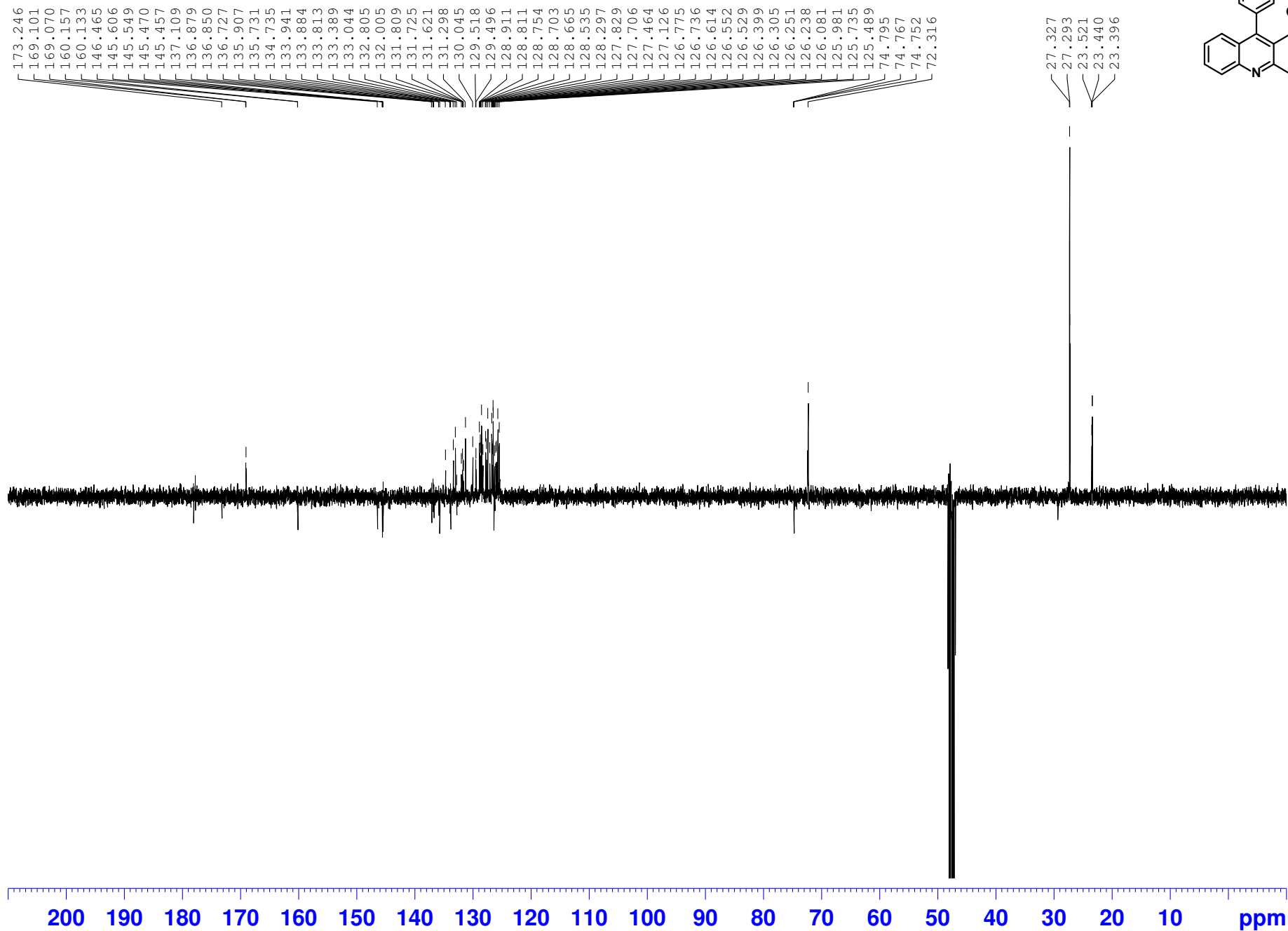
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277	801.093755	23136634610
278	837.044034	25221957861
279	849.280141	25003640961
280	866.242147	22632262106
281	868.618166	24904662726
282	895.803363	24696973487
283	943.110906	24110205972
284	968.066334	23894135413

AH-3-47 Characterization

NAME AH-3-48
EXPNO 60
PROCNO 1
Date_ 20171212
Time_ 10.09 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CD3OD_SPE
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700116 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-47 Characterization



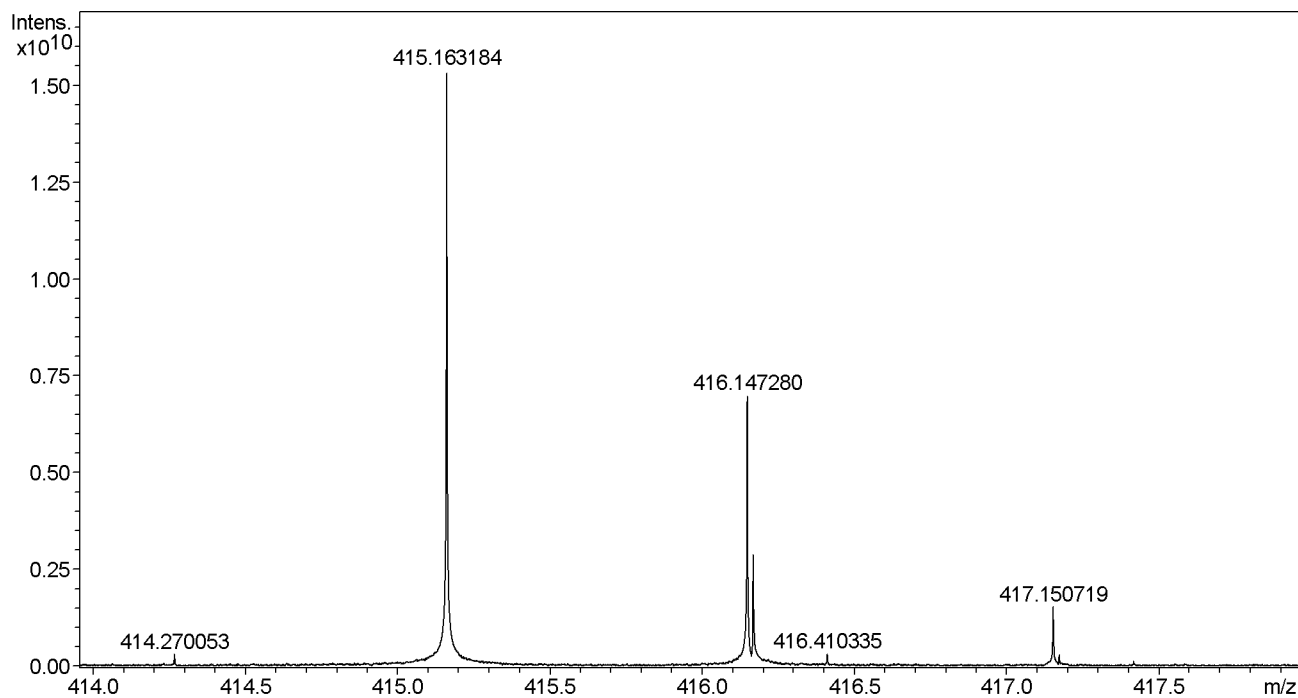
Mass Spectrum List Report

Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-47_pos_000003.d
Method
Sample Name AH-3-47
Comment AH-3-47 in THF:MeOH C23H22N2O3.H2O Na+

Acquisition Date 3/19/2018 4:52:40 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-47 in THF:MeOH
Exact Mass of C23H22N2O3.H2O Na+= 415.162828 m/z
Mass Observed = 415.163184 m/z
Difference < 1.0 ppm



#	m/z	I
1	189.685652	432859212
2	190.061850	1144490704
3	201.412870	102817951
4	201.885187	321514768
5	209.144336	236171421
6	209.686029	994414455
7	215.089252	334112004
8	216.092269	103680918
9	219.051533	102584090
10	231.120532	247736272
11	245.099828	153398078
12	246.592565	104369466
13	249.702339	297522670
14	250.667120	351729114
15	268.312283	96459033
16	269.136281	140863290
17	273.047954	132401583
18	274.493234	221778696
19	275.786834	499946697
20	283.115515	94095977

Mass Spectrum List Report

#	m/z	I
21	285.131160	118158165
22	298.347182	107186994
23	301.075591	3489383241
24	301.162426	99861758
25	301.299942	183699377
26	302.078986	662542010
27	303.141787	231910033
28	314.342165	105814830
29	317.121045	121867783
30	322.199229	107041057
31	324.214889	91129227
32	325.123778	326400705
33	334.191427	99127729
34	334.308350	99117310
35	335.200777	142611394
36	341.090052	110109287
37	349.183723	142814838
38	354.409806	454353955
39	355.413105	116414501
40	360.324109	1522843248
41	361.327457	330408448
42	362.303349	108588923
43	366.225513	119887010
44	368.425588	119437646
45	370.404764	247224521
46	374.303219	109453687
47	375.199361	119926449
48	376.319030	179184634
49	384.384013	337851655
50	385.387483	112221857
51	390.371208	199314539
52	393.181371	692430665
53	393.210070	202455865
54	393.298025	197310275
55	394.165358	1057353292
56	394.184668	190705909
57	395.168725	194599158
58	396.456870	116948003
59	398.241850	7038281205
60	399.245275	1298543314
61	400.248719	128016334
62	401.077579	315675709
63	401.184031	138691364
64	408.308893	146426626
65	409.220044	99075265
66	411.199888	96860317
67	413.266772	1255841708
68	414.270053	296901605
69	415.163184	15380416608
70	416.147280	6984498557
71	416.166724	2873753538
72	416.410335	317635674
73	417.150719	1532588563
74	417.170115	283079756
75	417.413905	127795240
76	418.154227	120826802
77	421.329307	108361045
78	424.488320	171049027
79	425.287940	1466344812
80	426.291230	318650425
81	427.105118	197105674
82	432.197895	192052925
83	433.181866	396537803
84	434.185307	97455492

Mass Spectrum List Report

#	m/z	I
85	435.345024	1771834648
86	436.348333	365711851
87	437.145195	11734961261
88	437.236706	299233105
89	438.129237	9269504492
90	438.148609	2148231800
91	439.132680	1788052602
92	439.151590	263595250
93	440.135829	205855649
94	440.446802	437789221
95	441.298188	114909806
96	441.450200	121099546
97	449.376060	173346392
98	452.175598	114746596
99	452.519572	496411389
100	453.522870	160140457
101	455.163928	179613740
102	456.140051	123865021
103	459.036170	152697853
104	459.170129	657992358
105	460.111301	2069602616
106	460.173485	186744985
107	461.114690	422811451
108	461.185847	1000117895
109	462.189213	245214408
110	466.535307	127527244
111	471.226099	231004893
112	472.473033	407248197
113	473.476561	103821706
114	475.165031	168496615
115	477.180721	3376252448
116	478.184120	781620840
117	479.187512	114379195
118	480.091499	110734815
119	480.270307	267625002
120	480.550879	1253230881
121	481.262636	222903300
122	481.554289	401171521
123	491.160083	501538767
124	491.196451	640852496
125	492.199982	157590044
126	493.175424	30362575653
127	494.178949	7429974230
128	494.566607	279970936
129	495.104140	425356138
130	495.182625	702361902
131	495.300645	189716955
132	496.107619	106407454
133	496.165399	174422658
134	496.545938	141899659
135	497.101105	127951489
136	497.360792	188888795
137	501.200245	131880156
138	506.566717	111218213
139	508.302033	114533652
140	508.582145	10657022043
141	509.207128	319307135
142	509.585573	3357778599
143	510.210262	113983584
144	510.588972	533186036
145	513.355760	224009132
146	518.070021	183983283
147	522.561516	147244800
148	522.597959	458492600

Mass Spectrum List Report

#	m/z	I
149	523.186511	325715513
150	523.601271	168611846
151	524.577178	710775284
152	525.288854	141297920
153	525.377052	174678460
154	525.580557	236287476
155	527.107193	234908776
156	529.350852	111871258
157	534.597876	272270532
158	536.613369	34790699107
159	537.336126	176696300
160	537.395565	236032188
161	537.616809	13573309109
162	538.620329	1918866147
163	539.623879	206971065
164	550.593012	423529111
165	550.629263	375999555
166	551.596396	183359386
167	551.632655	129399083
168	552.608515	1849287099
169	553.390720	115650564
170	553.611932	657000501
171	554.615145	133307213
172	558.142124	228371164
173	561.159429	140961916
174	561.202014	181745889
175	563.174889	2578891609
176	564.158774	838484667
177	564.178072	596591278
178	564.397061	151241213
179	564.644779	11250483448
180	565.161858	228662787
181	565.181466	125484514
182	565.648277	3928275511
183	566.651583	671067960
184	568.603552	103239018
185	569.403187	296204983
186	574.590521	147290672
187	576.433759	222803664
188	577.154266	164776803
189	577.437164	109758881
190	578.624185	257665704
191	578.660466	222398495
192	579.162054	5943239811
193	580.123104	114240651
194	580.165521	1910135100
195	580.639923	541995994
196	581.168863	268323003
197	581.643106	228737236
198	585.065976	144133224
199	586.140844	1059334439
200	587.144330	273905556
201	590.660526	209902419
202	591.664174	111095556
203	592.252617	258521578
204	592.428461	659947528
205	592.676154	13709400900
206	593.432485	199821544
207	593.679573	5490885333
208	594.572255	107914863
209	594.682933	902767798
210	595.686679	136016137
211	599.136083	127322302
212	599.549190	1337482596

Mass Spectrum List Report

#	m/z	I
213	600.552366	447636312
214	601.556027	125351269
215	605.366982	167696033
216	606.655622	369225748
217	606.692414	109004917
218	607.658888	153272631
219	608.247562	1075816170
220	608.671266	636767913
221	609.250793	347837807
222	609.674573	308264061
223	611.413579	100556157
224	613.250614	517424980
225	613.342124	114439135
226	613.429353	426795377
227	614.234524	946681371
228	614.254766	184046014
229	614.432861	116575160
230	614.536273	121452005
231	615.237994	282083460
232	620.707665	651485800
233	621.133667	355601050
234	621.711099	321410082
235	622.136984	115862871
236	622.650737	132371703
237	623.130954	125654050
238	632.496570	223096226
239	633.499608	105966282
240	634.201007	127507468
241	634.245101	109749566
242	636.216614	1009741232
243	637.220032	309289060
244	638.410755	183910739
245	642.630411	95530651
246	644.099654	145151713
247	648.491417	231993413
248	648.739152	366945456
249	649.494685	158844064
250	649.742394	172178211
251	655.440172	203490077
252	657.455813	579582430
253	658.459295	186740341
254	671.209142	169781942
255	676.328123	105609782
256	685.436523	2283427649
257	686.439930	946578043
258	687.401150	156199070
259	687.443367	223882138
260	688.404235	93036380
261	689.204265	504423911
262	690.207888	151947167
263	693.249601	171350560
264	694.175180	218589548
265	694.233805	103197771
266	699.466530	163727902
267	701.481890	431352616
268	702.485049	203903597
269	712.170253	186631995
270	713.431784	159649269
271	745.508173	190432607
272	786.669010	323597500
273	787.672206	171295235
274	808.322127	110873316
275	814.700282	728805358
276	815.703622	405533815

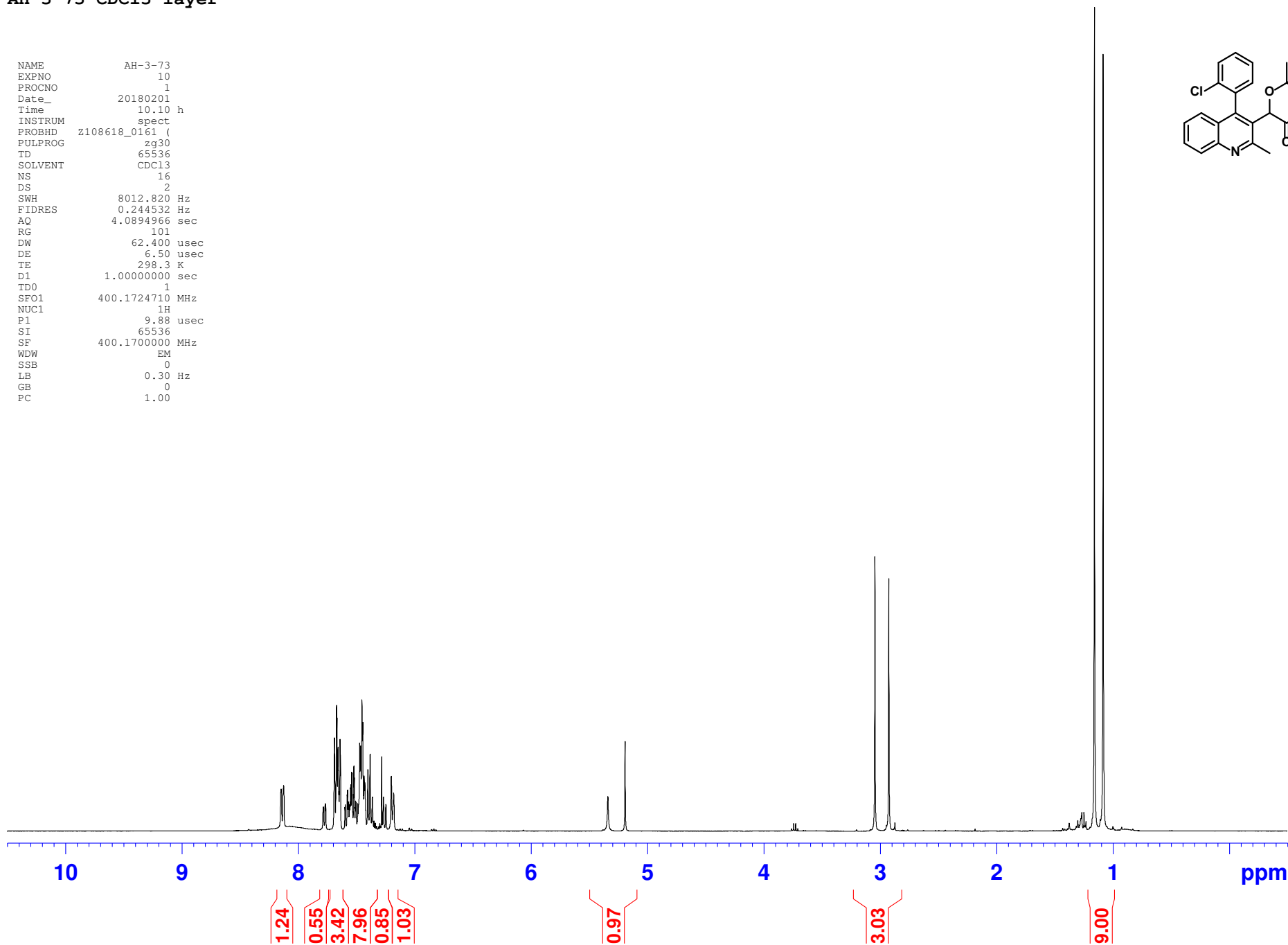
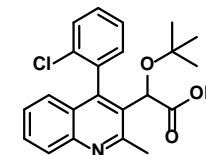
Mass Spectrum List Report

#	m/z	I
277	816.707026	127022949
278	829.319572	99069990
279	830.303976	210508344
280	831.288246	149561932
281	842.731711	180493193
282	843.734856	102647983
283	852.285412	161739127
284	853.269781	117786136
285	861.541738	324909586
286	862.545227	152572828
287	870.763657	184625777
288	871.766454	111143650
289	877.537055	926128546
290	878.540429	475451091
291	893.567605	111436618

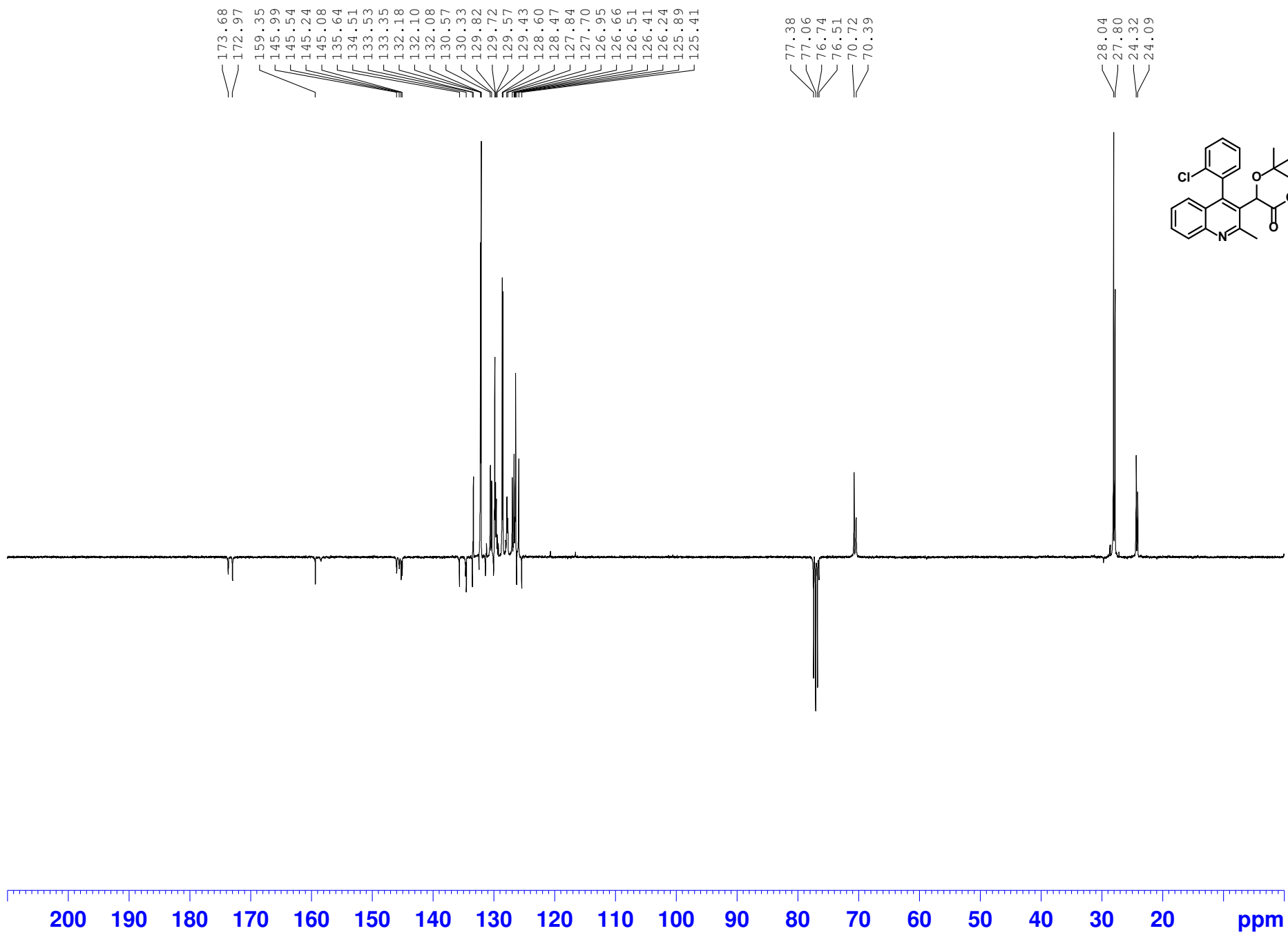
AH-3-73 CDCl3 layer

MISSISS

NAME AH-3-73
EXPNO 10
PROCNO 1
Date_ 20180201
Time 10.10 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 101
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-73 Characterization



Mass Spectrum List Report

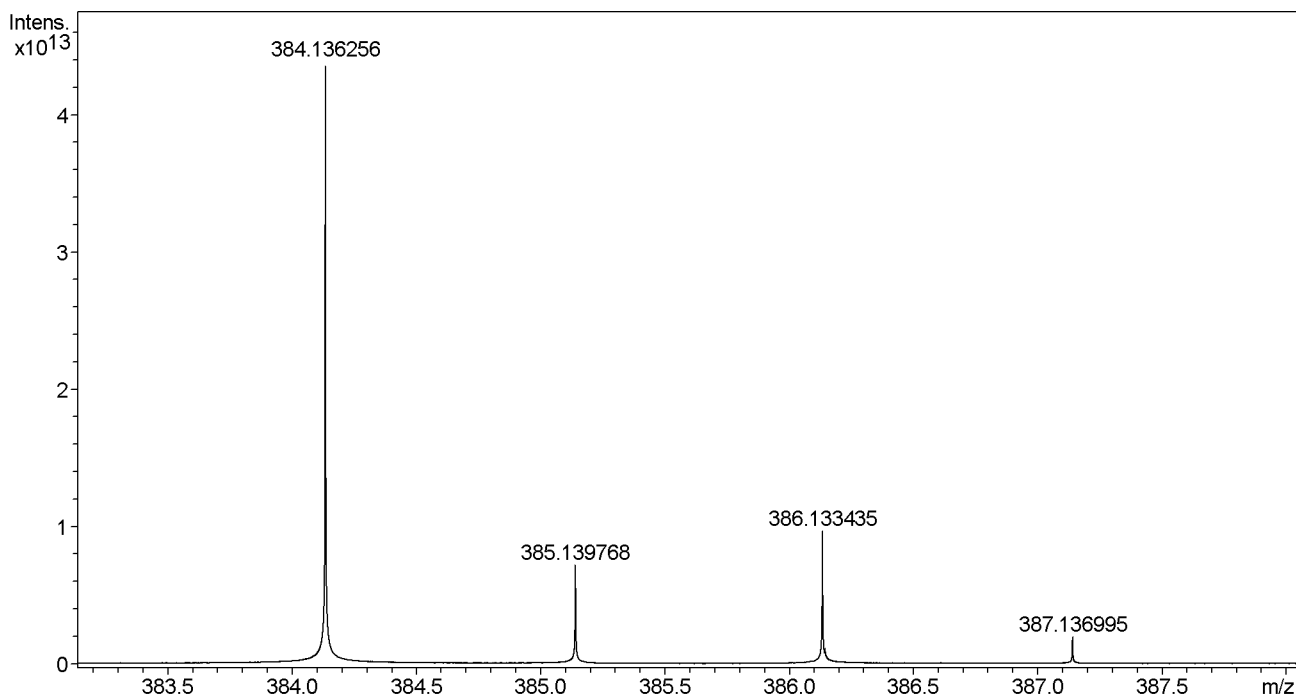
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-73_pos_000001.d
Method
Sample Name AH-3-73
Comment AH-3-73 in THF:MeOH C22H22ClNO3 H+

Acquisition Date 3/19/2018 10:55:47 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-73 in THF:MeOH
Exact Mass of C22H22ClNO3 H+ = 384.136098 m/z
Mass Observed = 384.136256 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.479504	22062649394
2	185.647052	21818182739
3	188.775655	21806568082
4	190.107631	22326049022
5	191.575980	28687588259
6	191.592467	21422141607
7	192.067895	21950563977
8	192.070589	147874204245
9	192.071045	237184780715
10	193.069660	52310397052
11	194.864873	21993979726
12	195.904712	21933335277
13	198.110760	21240119271
14	200.931044	21972953482
15	202.340500	26170411851
16	204.236051	22078179834
17	204.339714	22979413011
18	205.341361	22356610912
19	206.603213	22425925732
20	206.983821	21125391950

Mass Spectrum List Report

#	m/z	I
21	207.572488	22002111159
22	209.441964	21335801995
23	215.020414	21594396237
24	215.959384	21100176929
25	217.088502	21597524602
26	218.096572	22752796159
27	218.774472	22482370684
28	218.908207	21515631333
29	222.322984	21234561413
30	224.531564	21277973431
31	230.933393	22183350068
32	231.099666	23054591689
33	237.562220	23122077881
34	238.381939	21541413048
35	239.284702	24662310473
36	239.664124	23387417683
37	241.654462	21476850756
38	244.889329	22063658900
39	246.091348	42979244332
40	247.171659	35888872133
41	248.106826	22921518847
42	249.110340	22751421375
43	261.555805	22113316899
44	263.129971	21931730891
45	266.120417	24786134136
46	268.219313	23138008891
47	269.828938	23886052207
48	270.849108	22085063828
49	276.102394	24726608192
50	276.472076	22311259312
51	279.621081	22065084061
52	282.067860	44075457091
53	282.498751	21733672921
54	285.407409	22382849180
55	286.942611	22656727064
56	288.906029	23522131879
57	289.783412	22920291758
58	300.998580	21340849108
59	301.021141	23643425477
60	301.075680	1754447959368
61	301.145988	23953214026
62	302.079123	200900634718
63	302.090129	21411711048
64	303.079815	25977666408
65	304.406291	21305917635
66	304.609407	23592682352
67	310.888041	22360338398
68	311.821669	22250793360
69	312.595415	22047227842
70	313.937356	22840564365
71	322.282499	28012046013
72	324.388082	86718017305
73	325.525726	22082078501
74	326.025999	23553645133
75	328.694961	261233508360
76	328.695794	155109251427
77	328.697229	127130139957
78	329.062863	24493876975
79	329.077004	22412450102
80	330.069978	29675575119
81	332.045491	25496523543
82	340.002719	23586076164
83	340.100145	24185592202
84	340.146755	1300311277749

Mass Spectrum List Report

#	m/z	I
85	340.186398	34012450801
86	340.211842	22778360819
87	340.239488	22849695902
88	341.150222	180019559077
89	342.143923	272829325204
90	343.147206	39874072356
91	368.338731	29752692459
92	369.015042	25039391708
93	370.157569	27414656919
94	372.136704	1113905323910
95	372.223079	26735700211
96	373.140321	101888014551
97	374.133860	260373333153
98	375.137220	37326212303
99	377.436748	25261612878
100	380.552108	28748919506
101	381.345718	27664857016
102	381.489734	26420678771
103	381.509739	24108116529
104	382.026410	26926548410
105	382.104112	24505894943
106	382.123690	27992992172
107	382.162502	26391149898
108	382.257658	24256752416
109	382.273978	24817895592
110	382.398619	28242191878
111	382.476931	27785800214
112	382.505583	27704485124
113	382.538268	31311226962
114	382.583181	29894892048
115	382.600267	29618892884
116	382.626857	27052274113
117	382.661162	31608446032
118	382.722759	28546699775
119	382.761930	28337328176
120	382.783541	29019968467
121	382.798421	27565687796
122	382.836386	36662174755
123	382.853545	29265062441
124	382.876010	28664756260
125	382.908557	27414169536
126	382.962924	34109795867
127	383.030851	35022052645
128	383.039642	33088507485
129	383.094667	33184330365
130	383.117498	36205926699
131	383.127753	49751048200
132	383.143013	32264550712
133	383.154780	35615660096
134	383.199687	41220028104
135	383.209578	37550156454
136	383.262100	40094420583
137	383.313327	48013437560
138	383.360630	43522600024
139	383.417599	41127220050
140	383.481997	48394636567
141	383.500986	52112390656
142	383.588843	53867404385
143	383.617856	57390783392
144	383.657044	66500845326
145	383.736609	76619387947
146	383.812918	91690389862
147	383.832892	98720836663
148	384.136256	43809523131870

Mass Spectrum List Report

#	m/z	I
149	384.308898	155307304829
150	384.325145	141381997805
151	384.345354	131831295550
152	384.394055	111059527883
153	384.456746	93823627841
154	384.477486	86296144120
155	384.505951	80660118373
156	384.545066	75948133476
157	384.584037	65037953476
158	384.643488	62956757917
159	384.747317	52870898481
160	384.751022	53619266116
161	384.776689	54546110581
162	384.822081	56380481698
163	384.882670	55034043049
164	384.927909	56558556201
165	384.981612	64576515374
166	385.139768	7190618095718
167	385.256293	46262577644
168	385.328049	30330119785
169	385.337653	30093721308
170	385.370691	26470076899
171	385.390269	24953677800
172	385.429195	26834245920
173	385.681500	25933672368
174	385.858340	29428763169
175	385.885971	30479537349
176	385.915550	28970310639
177	385.949810	36627665672
178	386.133435	9642492570481
179	386.143651	1102486812912
180	386.314095	57705309753
181	386.336989	51318182423
182	386.347870	53465870622
183	386.393291	46829757108
184	386.414539	48675172943
185	386.447278	47288953071
186	386.464070	48404105721
187	386.534310	40647444773
188	386.559472	42055406962
189	386.608167	51349849824
190	386.631385	35393029368
191	386.652275	30105113648
192	386.699371	31599809083
193	386.730770	27699969478
194	386.760998	32367341313
195	386.797784	32311948423
196	386.828254	24283284200
197	386.866412	30184563895
198	386.894572	29565963241
199	386.959105	32833827069
200	386.978764	31101250167
201	387.001535	30368310376
202	387.024585	32819888775
203	387.047770	38429774179
204	387.136995	1948713415193
205	387.193565	30758820185
206	387.243575	24633763545
207	387.298980	24426905234
208	387.340513	24382418216
209	387.374986	23922291795
210	387.533203	25027386319
211	387.660335	24898167996
212	388.140638	122953137212

Mass Spectrum List Report

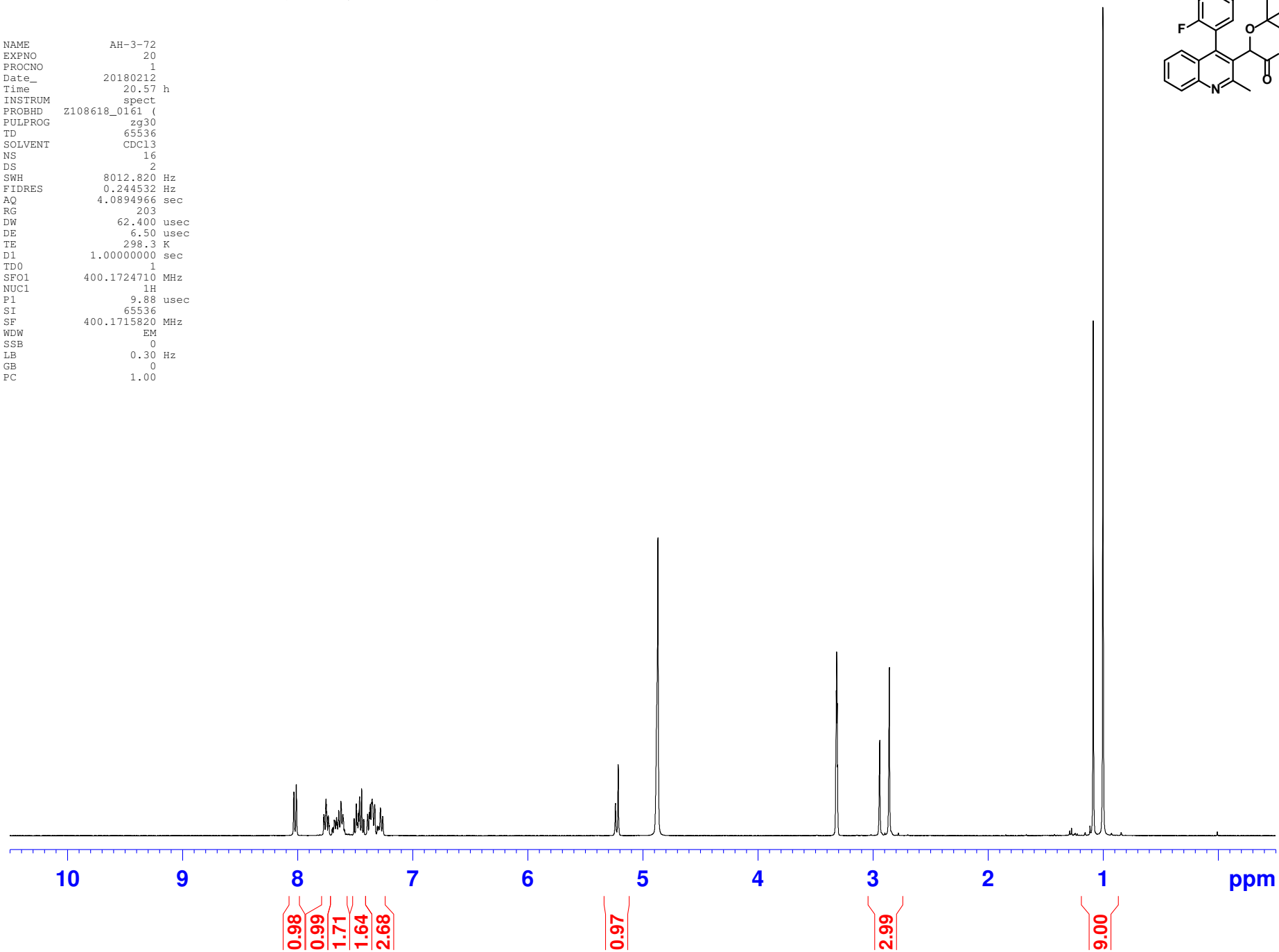
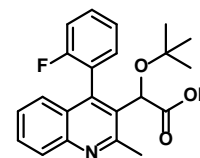
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216	392.151583	25782777435
217	398.152550	27852265445
218	398.242225	90022083972
219	399.810352	23335967761
220	406.116755	145499338955
221	406.118836	321118980299
222	407.122085	52078917104
223	408.116037	69598116242
224	409.315439	24391595903
225	410.550647	22847630260
226	415.550137	23239468397
227	421.477331	23920729753
228	422.275335	23786982105
229	426.289858	24070973363
230	428.086558	78461426834
231	428.100835	202184750322
232	428.217522	26059640361
233	429.104262	35776082241
234	430.084553	42701673099
235	430.097988	51845041044
236	435.345467	30824461234
237	435.828772	22737967835
238	440.199595	68501658030
239	443.096616	22526209917
240	443.707688	22281919540
241	447.555876	22737892923
242	447.613116	22646637444
243	451.889152	25786965241
244	459.120763	22600197120
245	460.168188	29915893867
246	463.262980	24387003614
247	471.891652	22639936798
248	474.607711	24563711534
249	476.704869	24128059212
250	486.059568	22462047733
251	490.798303	22673395335
252	492.043420	33718061538
253	498.432620	22487881767
254	505.485008	25257459258
255	508.582793	184131290153
256	509.586116	52735223055
257	519.388859	22985665695
258	524.577593	33707348929
259	525.581088	22167932755
260	536.551885	33666243803
261	536.614056	835112933982
262	537.593783	28434609104
263	537.617533	223677943818
264	537.957610	22978708353
265	552.609036	158854968155
266	553.612771	55527626071
267	556.442785	22484009235
268	564.645513	161200296327
269	565.648904	56166379197
270	578.835894	22758630028
271	579.162643	1517693425318
272	579.313713	31567526709
273	580.166196	466101965787
274	581.169844	56687597716
275	592.677048	183263461441
276	593.660148	22683545920

Mass Spectrum List Report

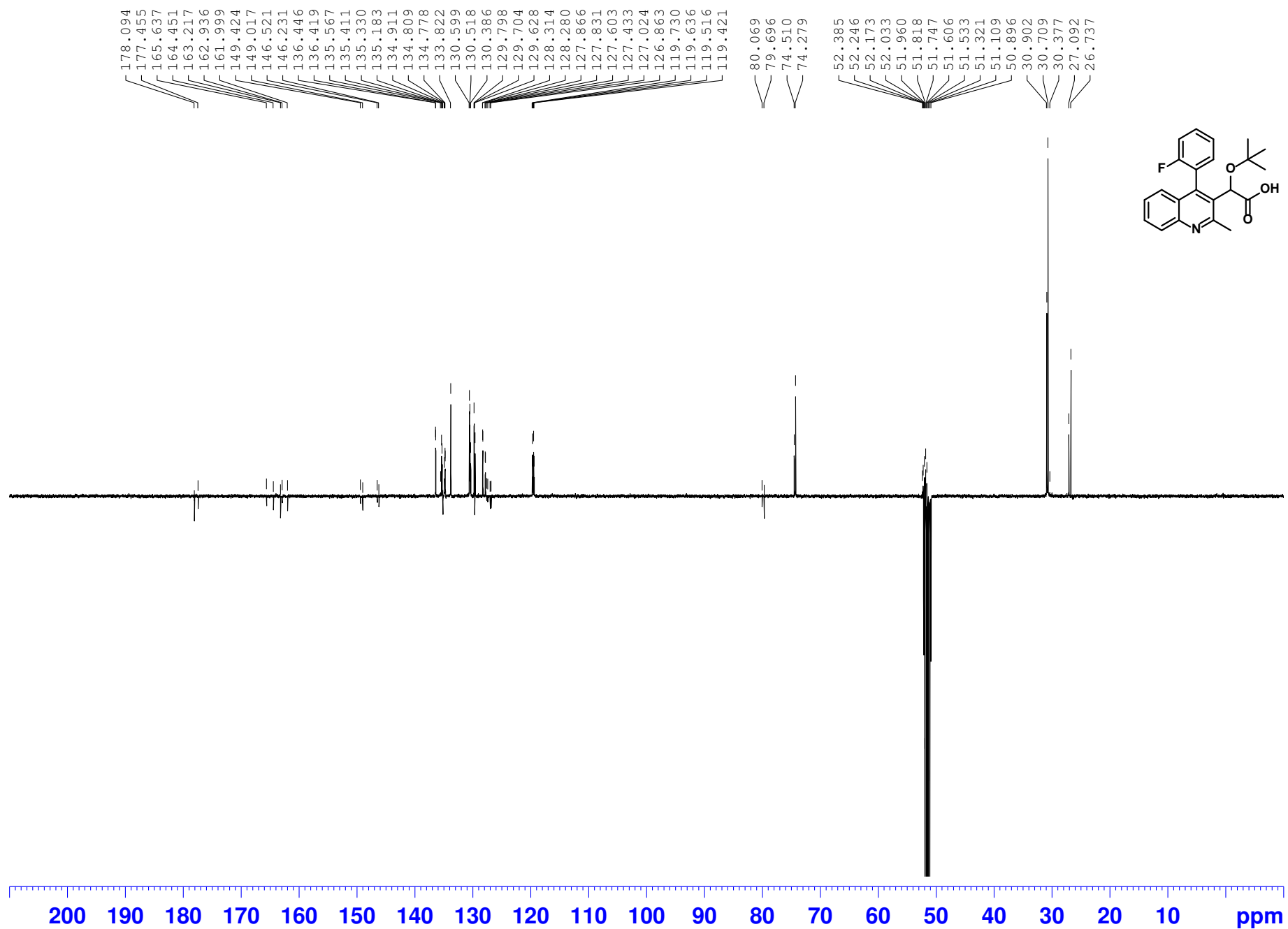
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279	596.548946	25214414867
280	599.549962	35676078935
281	601.203475	34341721036
282	603.218917	26813973903
283	608.672153	34048785283
284	608.796888	23772301498
285	614.804732	23360632676
286	617.383802	23898960831
287	624.180892	23314044717
288	624.418689	22813716211
289	633.018042	22919904174
290	655.747976	23836211484
291	677.408884	27971694839
292	685.437426	57297344681
293	685.470320	25595828742
294	686.440628	26710853117
295	691.140768	24342978324
296	721.652543	24039062530
297	739.971373	24710606370
298	763.765281	23721178332
299	787.909603	22882471763
300	861.976459	23113953855
301	960.820125	26620464776
302	965.663837	25389804042
303	977.101886	23571501632

AH-3-72 Characterization (CDC13, 400MHz)

NAME AH-3-72
EXPNO 20
PROCNO 1
Date_ 20180212
Time_ 20.57 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1715820 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-72 Characterization (CDCl₃, 400MHz)



Mass Spectrum List Report

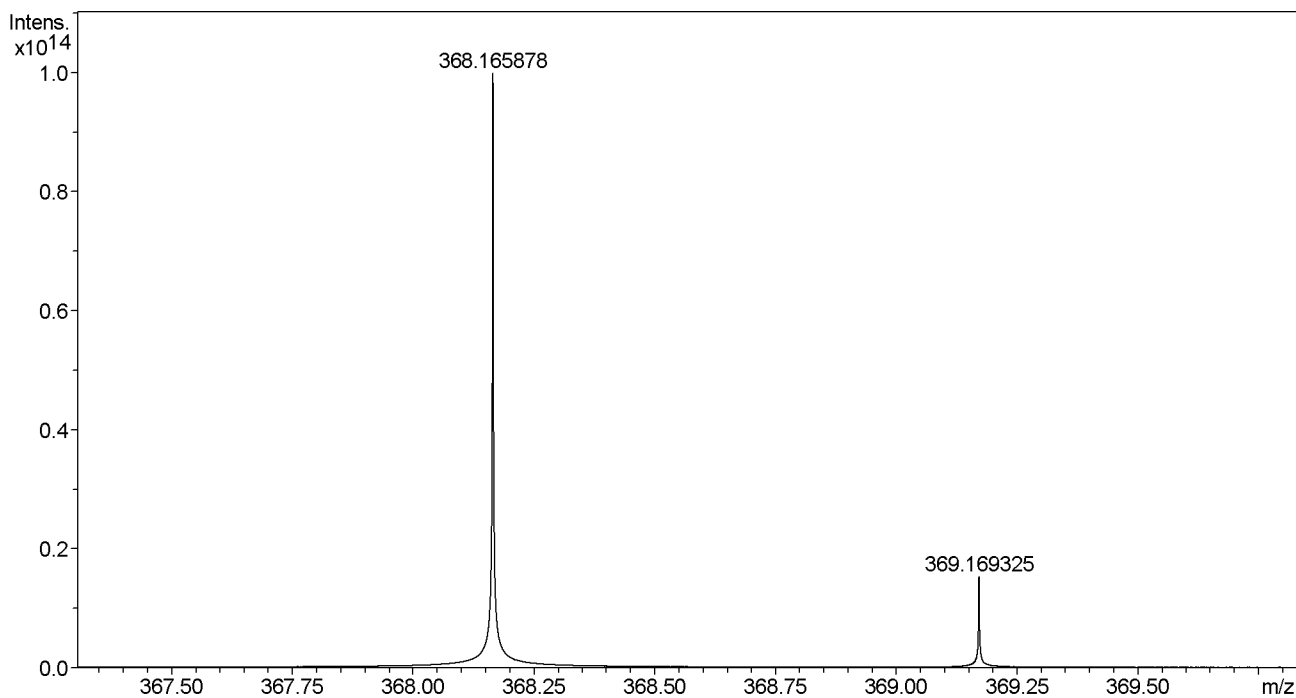
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-72_pos_000001.d
Method
Sample Name AH-3-72
Comment AH-3-72 in THF:MeOH C22H22FNO3 H+

Acquisition Date 3/19/2018 11:46:34 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-72 in THF:MeOH
Exact Mass of C22H22FNO3 H+ = 368.165648 m/z
Mass Observed = 368.165878 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.513784	356447518873
2	184.587349	135771809014
3	184.601590	21567838472
4	184.691540	24447821410
5	184.814763	21106696160
6	184.943833	51479874577
7	185.095518	22213033661
8	185.296864	21174478623
9	187.638660	22015557561
10	188.617117	22480510277
11	188.720321	24082826237
12	189.226961	21182058490
13	190.061603	25153355807
14	190.352916	21669688146
15	190.965227	21349011319
16	191.270649	25094959156
17	193.735686	23791456210
18	194.839092	23439826295
19	194.850347	23564777334
20	200.681086	22692333499

Mass Spectrum List Report

#	m/z	I
21	200.721600	21438347074
22	202.077824	22944887299
23	202.340491	21169694452
24	206.083787	21296577194
25	206.327134	23323291199
26	206.369290	21764958275
27	207.845665	22703643258
28	208.846072	21322465485
29	208.983973	21754831876
30	210.238525	21113288267
31	210.411017	21236912349
32	210.442540	22705002424
33	213.830053	23688091350
34	214.089215	22160820803
35	215.670402	21471103881
36	217.088737	55423810364
37	217.673459	21352075879
38	222.071139	22309282116
39	222.239692	23724315814
40	226.771631	23875286601
41	227.664028	21680622869
42	228.080626	27327133595
43	228.421089	23536348974
44	230.147251	21648418391
45	230.152403	21336790835
46	232.697610	24084939145
47	234.071494	22521746513
48	236.086863	43883726319
49	239.246988	23412020861
50	242.532655	22948232751
51	246.091373	44940770476
52	246.328125	22500932826
53	247.171674	31069094130
54	247.857235	22324301660
55	248.169147	23091616989
56	250.102678	25114691300
57	251.832274	21876522006
58	252.965691	24332670590
59	257.695301	22224988055
60	258.394027	28009424677
61	263.312602	22123394773
62	264.240740	21364606517
63	266.097941	43860876163
64	266.725018	23143640056
65	267.100717	34110536187
66	267.105625	44630567581
67	268.104472	25366069687
68	270.337180	22678313949
69	270.960298	26403410766
70	277.530090	22813797710
71	278.319165	22633230092
72	279.503743	22470947123
73	282.273512	22105407518
74	293.475598	21979552323
75	294.087875	23227947716
76	296.093599	21515312654
77	296.272696	21618513936
78	300.602904	24435210167
79	300.653929	21897047166
80	301.075895	71304765989
81	303.104438	21333085069
82	306.634420	22060668861
83	309.148649	23233386522
84	311.059503	21406855276

Mass Spectrum List Report

#	m/z	I
85	312.102907	67742698464
86	312.428128	22464262984
87	312.488366	23150316122
88	313.034968	21549348812
89	313.106727	34857119720
90	313.720915	22445602682
91	316.075041	215045737680
92	316.188417	26963594595
93	321.470225	22359966447
94	324.143296	23156156716
95	324.176337	895808459029
96	325.179955	67501365493
97	328.215616	23867047084
98	328.771344	24274390996
99	328.873791	23309118207
100	333.538363	24915212761
101	334.085878	32759140751
102	337.975666	26028545211
103	340.304062	27738988701
104	354.187184	48509376041
105	356.166327	28042618560
106	359.725634	27431111889
107	362.250754	28710036456
108	362.323359	28764475887
109	363.062126	31023129050
110	363.200503	28152478850
111	363.908277	27968470629
112	364.058813	28448413187
113	364.204527	28019857242
114	364.352569	31106407908
115	364.396820	28505192526
116	364.463726	28301240440
117	364.525857	33477963725
118	364.585943	30868503631
119	364.674330	28509975982
120	364.743900	34640648404
121	364.815401	30968649307
122	364.896467	29585288633
123	364.937071	31618134785
124	364.989684	32116508028
125	365.037347	29358821818
126	365.069336	32801942433
127	365.116311	35843952297
128	365.179157	39255262887
129	365.199477	32048601280
130	365.239713	30952363533
131	365.251327	30494299301
132	365.276394	31728339202
133	365.298956	35072273180
134	365.359433	32980251612
135	365.387278	35593928223
136	365.410358	32211652263
137	365.456209	34977514726
138	365.524522	36248105658
139	365.568948	35594289207
140	365.680298	34864377494
141	365.743036	39316323999
142	365.769263	43730892790
143	365.812013	37206775530
144	365.825073	38447885434
145	365.846190	34228069740
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147	365.901720	37077663411
148	365.944142	38950376241

Mass Spectrum List Report

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152	366.248024	46153569491
153	366.262728	47652410284
154	366.320915	45504851571
155	366.346469	45607026899
156	366.364419	48237005289
157	366.400178	49395374729
158	366.464628	64529563288
159	366.486600	45286771672
160	366.534376	49843931970
161	366.557641	50256348902
162	366.675935	51214575153
163	366.754637	54776133866
164	366.863823	64261682493
165	366.876969	118531395267
166	366.919512	60922808111
167	366.973698	70980277020
168	367.018123	68112911542
169	367.053631	69815844274
170	367.083321	71712031164
171	367.167752	82140111167
172	367.211029	76702347232
173	367.256422	84591659336
174	367.331494	87689426956
175	367.507756	107463485845
176	367.605236	127052191185
177	368.165878	99805271535965
178	368.211361	1352843793395
179	368.342576	376201293781
180	368.454089	236017196856
181	368.543886	181637157540
182	368.661836	134867756356
183	368.722791	126837184457
184	368.897634	99332446032
185	368.916793	96061915173
186	368.956623	95587028309
187	369.169325	15283026844985
188	369.365296	88219589954
189	369.448822	84081802892
190	369.500767	68669612594
191	369.528999	68599624407
192	369.594313	71025312443
193	369.606325	65687287671
194	369.635078	68425908719
195	369.653263	64415515363
196	369.743675	59297091302
197	369.790793	58437776884
198	369.837738	55717754136
199	369.882447	550684867369
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201	369.957930	50359497074
202	369.983108	54942306892
203	370.067531	54694903209
204	370.096539	55842514429
205	370.135517	56892413595
206	370.170643	288949548902
207	370.172955	966749121907
208	370.199330	29745810710
209	370.280066	41081998441
210	370.304220	43201910082
211	370.410346	43382481345
212	370.470292	44537571701

Mass Spectrum List Report

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217	370.823423	42696048755
218	370.874521	35077701258
219	370.915948	36863329659
220	370.988460	33764801224
221	371.046551	34366963584
222	371.107374	36529039327
223	371.123987	32192128492
224	371.140209	32330661445
225	371.228305	34676229739
226	371.262281	34107491482
227	371.299525	38045970340
228	371.341372	38561040124
229	371.379367	31094284628
230	371.471384	31650409059
231	371.509095	31298998904
232	371.540756	30752464707
233	371.595033	31354810898
234	371.653230	34593837704
235	371.678112	34322576283
236	371.733335	35247071573
237	371.836730	35114908466
238	371.928882	34363115783
239	371.952000	28369720438
240	372.005870	28947962811
241	372.046710	28465939597
242	372.140658	32702666533
243	372.202523	30205071005
244	372.301019	33793486658
245	372.318120	32055897480
246	372.533134	35596774584
247	372.616048	30224684309
248	372.690266	34274209138
249	372.814270	31045237791
250	372.916169	29321014007
251	373.304820	28786902186
252	373.342308	30641862753
253	373.910343	29073265217
254	375.227320	28001910213
255	376.113524	30226175581
256	379.377240	27549370683
257	389.723743	27041660666
258	389.946395	27762683002
259	389.967912	30803403040
260	389.983729	30918207126
261	390.147936	3777879637060
262	390.273029	29226842326
263	391.151643	628474791006
264	392.155360	28788273311
265	398.242374	56492786803
266	409.360374	24182548625
267	410.424402	23785322862
268	412.129160	417778669413
269	412.130454	564193314685
270	413.133922	94731409737
271	418.574693	22875032063
272	422.274506	25267144096
273	424.229277	61013120944
274	433.012725	22236915614
275	445.303554	21353122364
276	449.327323	21546692113

Mass Spectrum List Report

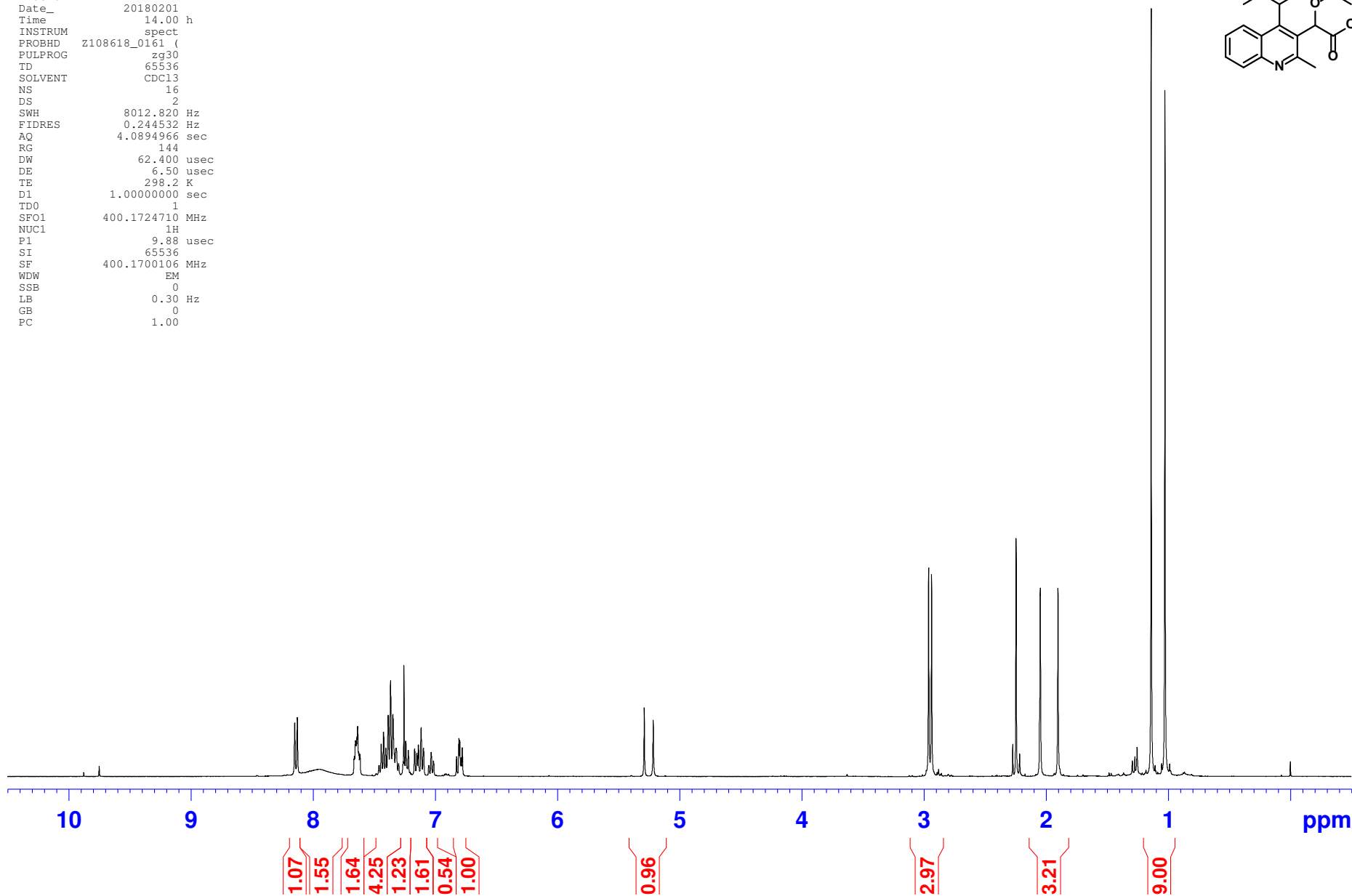
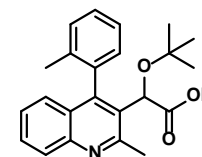
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281	468.928538	25115880988
282	472.229437	24117636325
283	480.551723	28144606328
284	480.761296	22188814784
285	489.263481	22896441239
286	499.258640	26651676825
287	508.582848	489872883902
288	508.615834	30292461914
289	509.586303	67752260479
290	524.577897	23101257980
291	536.416610	23087918794
292	536.478999	34740434509
293	536.614118	2069444349700
294	536.772668	29292429510
295	536.827986	24694942137
296	536.845519	26601954765
297	536.943546	23163199930
298	537.170693	22677406703
299	537.617662	671327038809
300	538.621260	47029730447
301	541.243282	94632951955
302	541.826795	22649520767
303	542.246766	26295798578
304	543.240474	23225442726
305	543.258778	69927911144
306	546.511990	22346536215
307	547.826755	22549070928
308	550.542076	23786602894
309	550.630188	31845294758
310	552.609432	55892699131
311	556.591754	22636547506
312	557.238443	32396631643
313	557.281437	22348108523
314	564.645729	501764596220
315	565.649176	121022942598
316	578.377223	22799100949
317	585.233142	41586701405
318	586.236780	25544390849
319	587.248855	65326121778
320	588.252329	24031886724
321	589.246441	25787912976
322	592.039784	25077243354
323	592.677157	676070448349
324	593.680568	177007328804
325	603.141541	23466551194
326	611.746857	22605457205
327	612.389760	22290717105
328	613.429889	24178758561
329	616.168424	22282608655
330	620.709672	22682178868
331	625.408234	25882295396
332	637.345712	43486194089
333	640.628931	23309709516
334	659.618838	22374214284
335	676.714240	22743738262
336	685.437844	58142730452
337	686.441019	32294814588
338	688.832643	23065422669
339	705.384853	25136520726
340	706.895481	22829968305

Mass Spectrum List Report

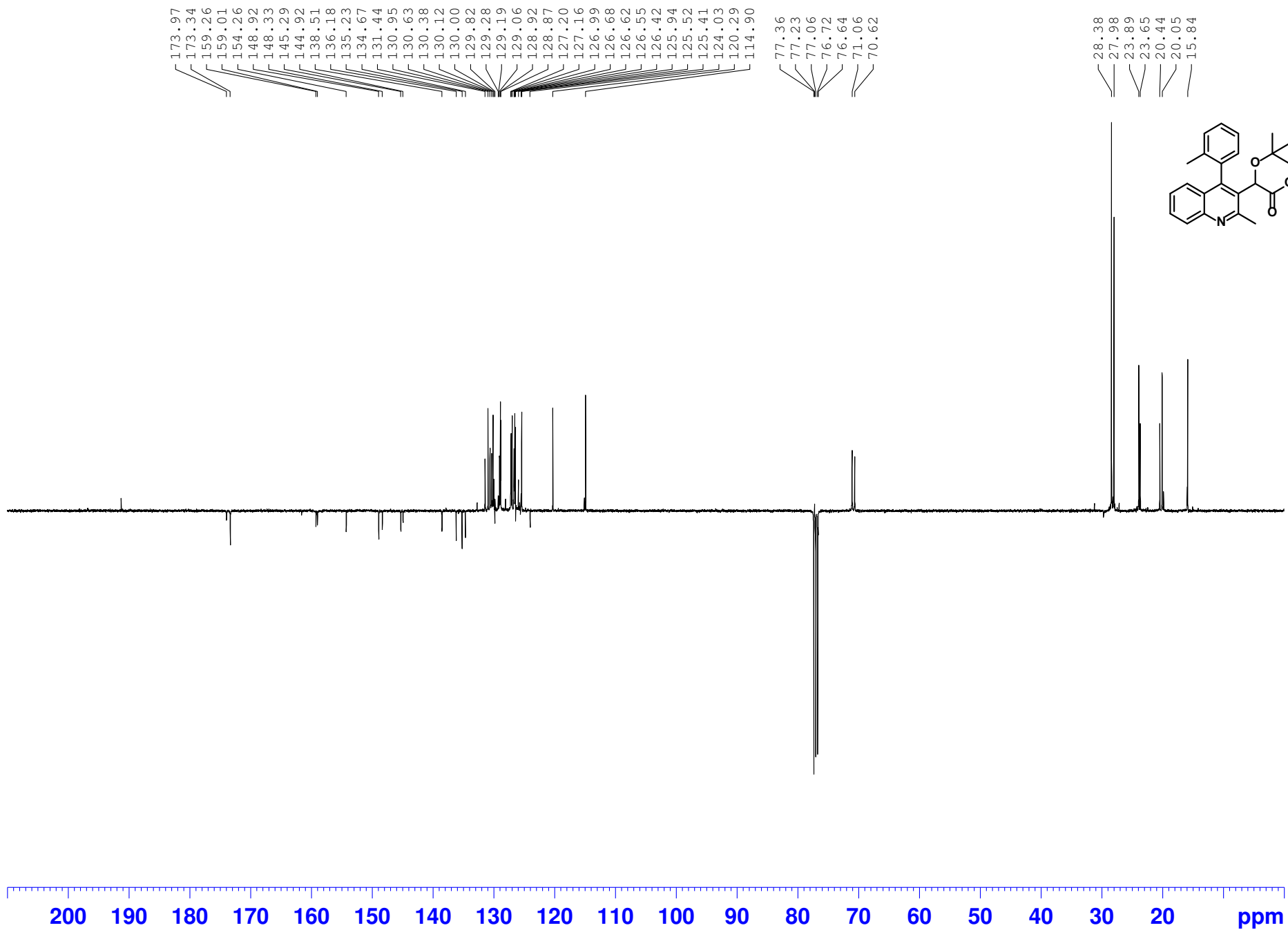
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345	754.022182	22882374832
346	788.564730	26616008388
347	801.272237	23597487927
348	838.491935	23002232872
349	882.401377	25475472226
350	908.887024	23331609920
351	944.924240	24054107493
352	977.164569	24921078109

AH-3-65 check

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EXPNO 50
PROCNO 1
Date_ 20180201
Time 14.00 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-65 Characterization (400MHz, CDCl3)



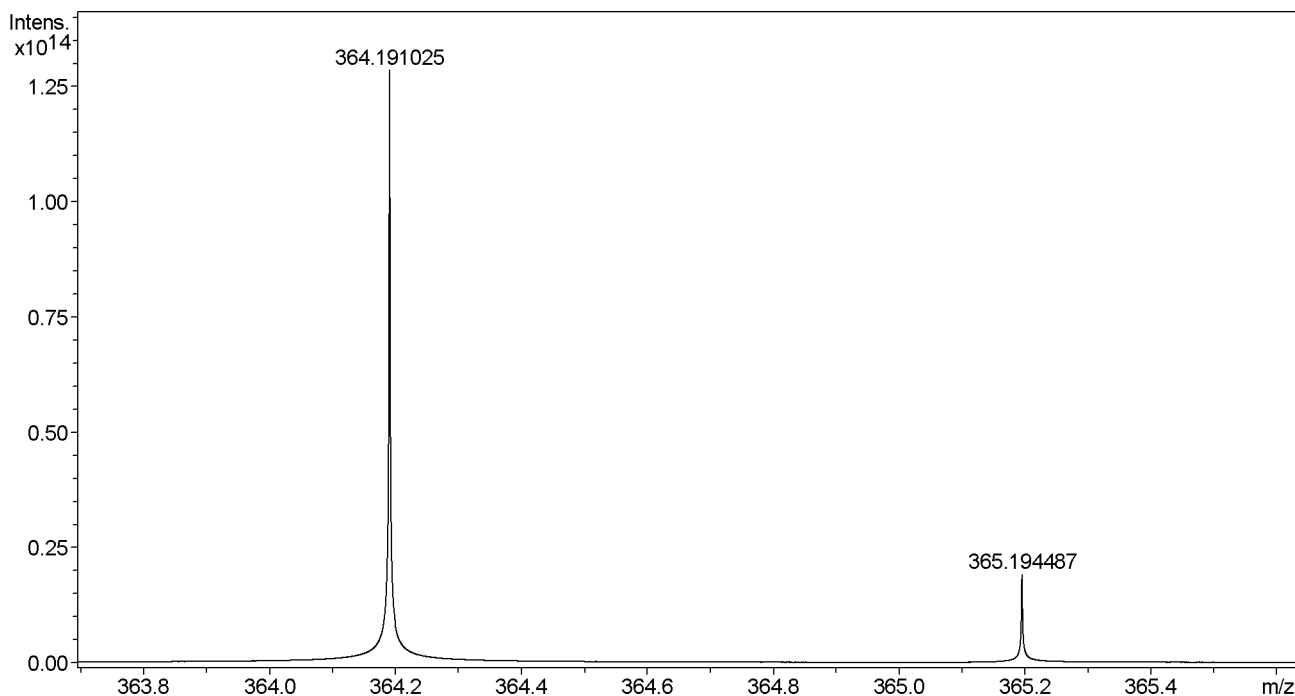
Mass Spectrum List Report

Analysis Info

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Method
Sample Name AH-3-65
Comment AH-3-65 in THF:MeOH C23H25NO3 H+

Acquisition Date 3/19/2018 9:43:41 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-65 in THF:MeOH
Exact Mass of C23H25NO3 H+ = 364.190720 m/z
Mass Observed = 364.191025 m/z
Difference < 1.0 ppm



#	m/z	I
1	184.306043	21978299799
2	186.030892	58676003351
3	186.324250	22225608798
4	186.471797	21060399132
5	186.548566	22931871479
6	186.554612	375957479719
7	187.452079	22726901060
8	188.699159	22465502741
9	189.842582	24587087968
10	191.008613	23002706449
11	191.207568	21051216541
12	191.234748	24264376989
13	191.932762	22204137916
14	192.062276	23390771120
15	192.689408	21546576588
16	193.084083	25108646277
17	194.893525	23737982197
18	196.958319	21292823939
19	197.075428	22366146284
20	197.288018	21236938168

Mass Spectrum List Report

#	m/z	I
21	200.570062	21199376818
22	202.077770	42214876964
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24	202.626419	21031585650
25	202.709231	21896531930
26	202.727682	21898012273
27	203.822469	21227520059
28	207.258682	22077685604
29	209.441361	33237718843
30	212.831718	21476894183
31	214.089470	22744264885
32	214.660126	21673543570
33	217.084346	21237009247
34	217.088867	25278269365
35	218.096574	33120672560
36	218.550833	22668399095
37	221.272203	22301831202
38	224.351322	25112785773
39	228.081047	21395704151
40	230.096252	23580011495
41	231.099917	24735346966
42	231.104447	45042569667
43	232.075695	24192675982
44	232.112147	30463293063
45	233.083643	34398646343
46	233.882912	24692978073
47	241.088754	26707296570
48	242.096765	22535864882
49	243.104317	44268781090
50	244.112285	44585087259
51	245.120178	40208941040
52	246.127909	24482042992
53	247.648080	21523498488
54	248.106963	24597394405
55	249.280902	22037871744
56	252.270150	23399986519
57	253.387017	23765683621
58	255.102814	21563385538
59	257.144379	23936369822
60	259.742591	21965147771
61	260.107452	25811360601
62	261.110596	26521900641
63	261.115163	35489651065
64	261.409972	21657086209
65	262.122561	58454524920
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67	267.465317	21658886328
68	269.320592	21917002785
69	275.798744	22661196141
70	276.101639	33080412891
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72	281.356805	22651841384
73	282.467113	21571169848
74	286.224528	21737879689
75	286.898483	21459797812
76	287.180993	21421304642
77	287.783269	21895737254
78	296.045926	21671880461
79	296.921903	23882823491
80	300.136208	22917205089
81	304.215061	21548910948
82	304.902652	22195623980
83	306.112611	31556956519
84	308.128547	102610553518

Mass Spectrum List Report

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89	320.201446	705427166352
90	320.227856	23842999117
91	321.204960	66253828389
92	332.446694	26884838818
93	345.775562	27635760323
94	347.584901	75006576194
95	352.191551	52576972402
96	356.217875	32895088671
97	358.708055	29513609926
98	358.774101	30461096236
99	358.852229	30264342350
100	358.886314	31044795623
101	358.916648	29355780414
102	359.050717	30945402137
103	359.199163	30468672565
104	359.296659	33644010030
105	359.334797	31341306608
106	359.417358	31183946909
107	359.430047	31521393320
108	359.551728	34395185670
109	359.595207	32981826990
110	359.685968	30832524948
111	359.775487	33854928798
112	359.858308	33341699243
113	359.916924	32717717450
114	359.965212	29901834432
115	360.030415	35995169720
116	360.090002	32273856787
117	360.129653	31530119301
118	360.149690	30458855102
119	360.214981	33887841883
120	360.231711	36120692690
121	360.375941	39607458573
122	360.495970	37897404498
123	360.550707	37156925309
124	360.607325	33094973962
125	360.709855	36368940897
126	360.770909	36634128340
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132	360.965526	37729604047
133	360.975179	40255890363
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136	361.103639	43838861168
137	361.162221	40516173098
138	361.200152	42149926584
139	361.281829	36851622136
140	361.305110	43252931539
141	361.333059	45812630761
142	361.454018	42904383676
143	361.483650	47607735729
144	361.614273	46982897218
145	361.631329	47633426475
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148	361.788985	46602433367

Mass Spectrum List Report

#	m/z	I
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152	362.053079	53796821860
153	362.103380	51670578924
154	362.127915	57789420344
155	362.161627	57976904391
156	362.233874	56096201457
157	362.261958	58761547564
158	362.310071	57508294247
159	362.385794	62284404123
160	362.399653	60133495546
161	362.502702	59805284603
162	362.536833	64831258585
163	362.626163	63822763597
164	362.649180	67389606658
165	362.695279	67913574147
166	362.736316	67592534542
167	362.811044	70445267676
168	362.919686	84495244912
169	363.007134	79582214944
170	363.038026	83653400431
171	363.058861	84907133416
172	363.101696	92951158592
173	363.193798	105503576085
174	363.262342	108165980448
175	363.307295	115503890077
176	363.423550	120500263067
177	363.530545	142198434119
178	363.567103	146981897021
179	363.726058	186383457705
180	364.191025	128318775074238
181	364.634721	175777213199
182	364.680190	161816672737
183	364.737369	137436357773
184	364.785148	122390796080
185	364.851709	107088681908
186	364.966784	84013891784
187	365.020598	74328814328
188	365.194487	19162243389994
189	365.433805	121601749677
190	365.539107	100611768048
191	365.760125	76829062007
192	365.890805	70000390748
193	366.065853	64378116328
194	366.198030	1141288170574
195	366.315494	63703906651
196	366.333143	56780173323
197	366.354198	61487285141
198	366.380363	60774151549
199	366.423648	57345891895
200	366.444506	56899757221
201	366.491294	54149467381
202	366.523510	58181531062
203	366.590731	54130386642
204	366.614245	57204771088
205	366.737178	52405022586
206	366.778950	50077437846
207	366.795809	51850372742
208	366.830037	46444045912
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Mass Spectrum List Report

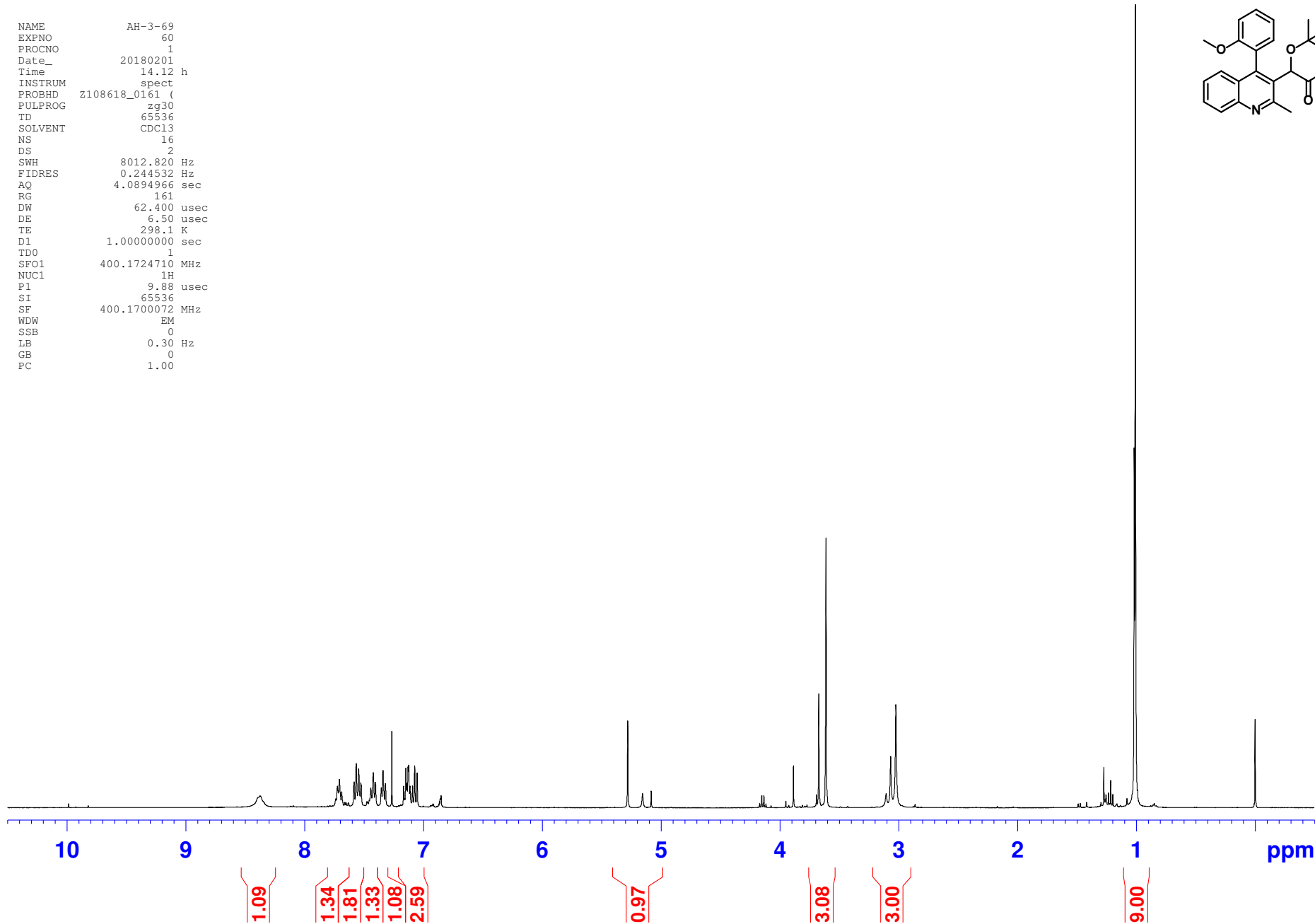
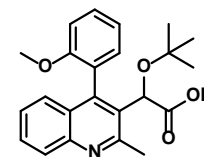
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214	367.238058	41882674006
215	367.344111	40693506405
216	367.373125	43599077980
217	367.403464	41260190589
218	367.656271	39482121119
219	367.728965	39779789689
220	367.816770	37490335545
221	367.867219	41921444553
222	367.897575	36487726353
223	367.953774	38029706242
224	368.003512	36242425926
225	368.047567	34305989590
226	368.113985	38434654775
227	368.129898	32596060846
228	368.154627	33701236629
229	368.235037	37577194390
230	368.277579	32670940513
231	368.336532	39151033416
232	368.340530	34254345876
233	368.362935	32680279531
234	368.399026	32705645069
235	368.458083	33519385657
236	368.572632	32812404721
237	368.582046	31693417050
238	368.612132	30674704943
239	368.710719	33529677284
240	368.736090	32767532214
241	368.913231	38288960038
242	368.935045	32143259008
243	369.065041	31740560839
244	369.185352	31958830918
245	369.426516	32759216254
246	369.509759	32022310628
247	369.550938	32005165234
248	369.689440	30565427605
249	369.740384	30968491036
250	369.883020	31732674570
251	369.937802	31183616556
252	370.168989	32271715657
253	370.877876	30637389183
254	379.181149	171554237522
255	382.463635	2776691373759
256	382.522911	32750815820
257	382.541690	30849754856
258	386.173437	271239973958
259	392.221723	266378659756
260	392.222997	298406218384
261	393.226319	37652155298
262	393.297077	28131758741
263	398.242655	28350173488
264	408.155040	613581661928
265	409.157872	136338880414
266	413.962374	25704931185
267	433.812050	24154213368
268	434.240225	21981792238
269	435.345850	30139801308
270	446.823763	23298748488
271	453.407813	24040718472
272	459.169281	25219786330
273	466.002927	21561398751
274	466.917375	23375145794
275	469.002188	21773708847
276	470.622951	21683821093

Mass Spectrum List Report

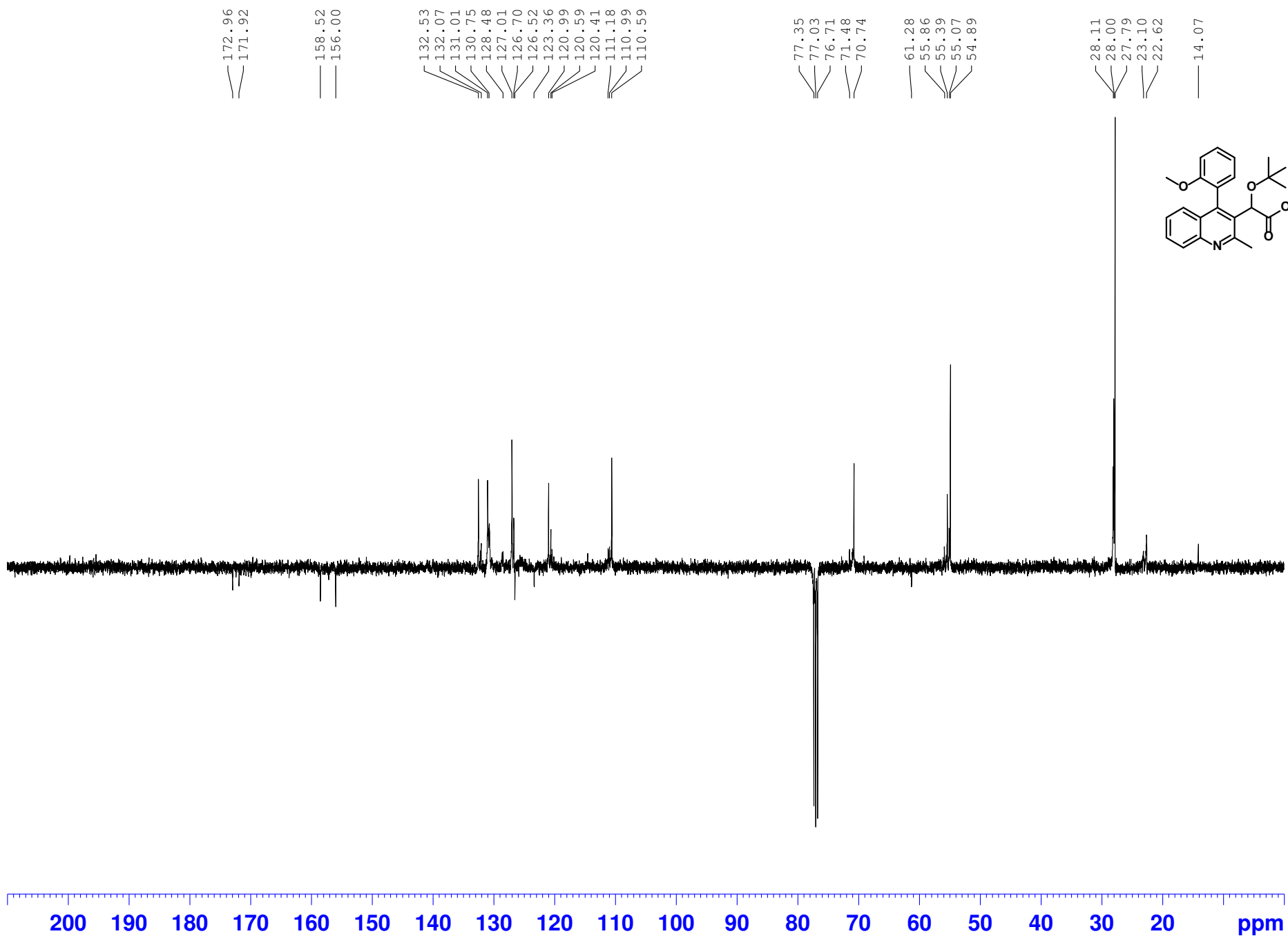
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278	482.841934	24070889624
279	492.150487	22553747177
280	495.104376	24056871073
281	508.583041	56419807690
282	512.056631	22611367787
283	536.614493	276463409995
284	537.617868	66792221494
285	547.409132	22477178982
286	552.609381	101273217836
287	564.646179	44737410131
288	580.640942	23563708494
289	586.507549	22622412217
290	590.056753	23422650138
291	592.677569	57575363290
292	599.550605	26296640843
293	608.671496	22837182384
294	617.864250	22681847634
295	622.116809	22316707050
296	651.318567	22726769408
297	662.696942	22841617637
298	685.438189	46853537652
299	698.811431	23071045328
300	703.985657	22826293235
301	708.531530	23802700574
302	735.765403	22594866131
303	752.557990	22941643724
304	768.703325	22662436896
305	789.240335	23579255079
306	801.922828	23629654236
307	834.657505	23122858899
308	903.276854	23472525880
309	940.284723	25498285499
310	995.321400	23921244015

AH-3-69 check

NAME AH-3-69
EXPNO 60
PROCNO 1
Date_ 20180201
Time 14.12 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 161
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700072 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-69 Characterization



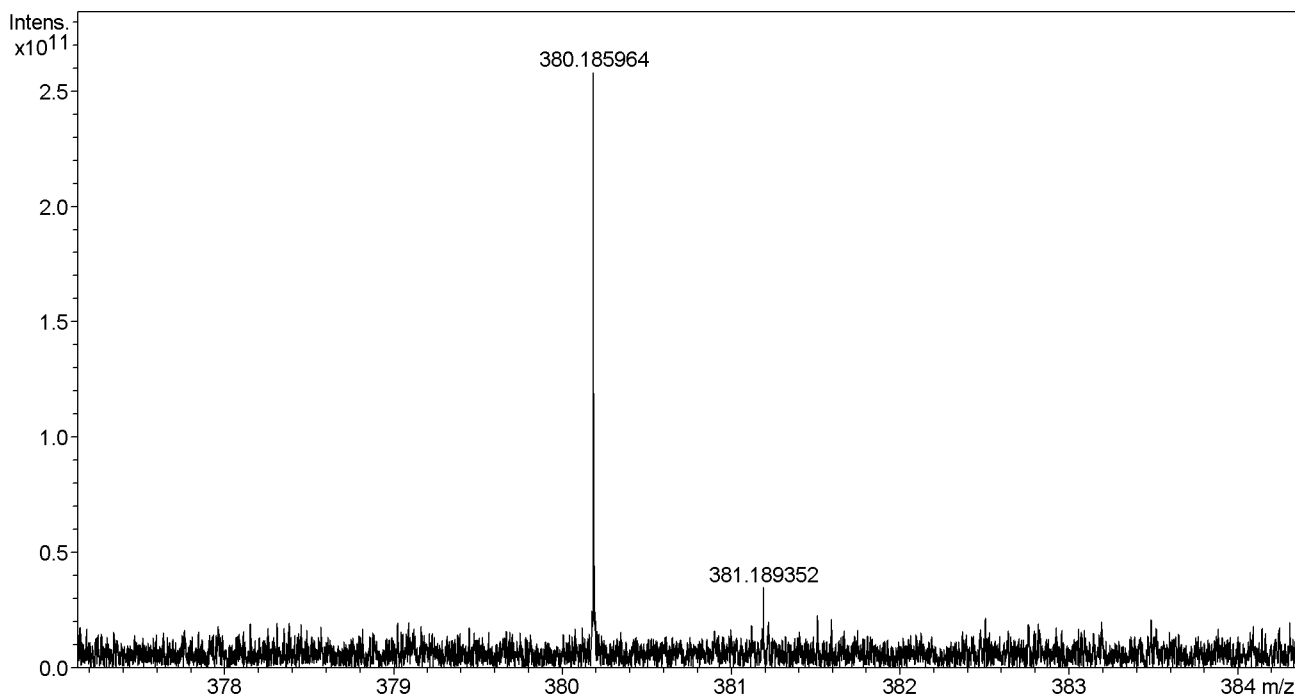
Mass Spectrum List Report

Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-69_pos_000001.d
Method
Sample Name AH-3-69
Comment AH-3-69 in THF:MeOH C23H25NO4 H+

Acquisition Date 3/19/2018 11:03:36 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-69 in THF:MeOH
Exact Mass of C23H25NO4 H+ = 380.185635 m/z
Mass Observed = 380.185964 m/z
Difference < 1.0 ppm



#	m/z	I
1	184.752971	21702234487
2	185.245744	23768222291
3	186.670138	21197396856
4	190.061872	42694681854
5	190.827591	21169879643
6	194.402918	21195028048
7	195.516466	21714454504
8	196.168145	22064962784
9	200.887880	21979833241
10	202.340499	73287724334
11	205.007992	21493470887
12	209.441961	78756666634
13	210.175949	21242427072
14	211.315724	21447708080
15	212.164690	23097491192
16	212.818399	21146873138
17	215.089118	43547569299
18	215.260669	24411469706
19	217.979644	21423186154
20	218.110773	22485773696

Mass Spectrum List Report

#	m/z	I
21	219.258142	21974602777
22	219.358867	21827253764
23	219.431224	21159683513
24	219.557001	21858646364
25	220.578842	22568043269
26	222.594386	21082504079
27	229.291309	24271262722
28	231.120459	30195849628
29	231.633470	21162924561
30	233.753430	21547281708
31	234.217144	22497463089
32	238.967491	25199307974
33	239.676444	24229581990
34	242.309649	25352909386
35	245.302515	22739119191
36	247.171777	28768850135
37	248.435296	21329401768
38	250.869054	22768638939
39	251.318680	23575205342
40	254.296837	21955632261
41	255.592993	21805814701
42	256.091987	21915431051
43	257.142145	23587418587
44	258.167653	21586976011
45	258.184467	21656070252
46	258.196846	22201212859
47	263.343427	21576629867
48	270.997670	22350395722
49	279.632880	21950132502
50	279.854338	21566345852
51	280.138346	23679491289
52	281.800682	21407326196
53	283.563640	42914152583
54	284.850162	23613717002
55	286.676534	21612446912
56	287.310616	23904593053
57	292.082232	23695839839
58	293.319920	21958695314
59	294.611302	21960783834
60	296.331211	21970262709
61	296.596886	23844130773
62	298.012916	22224754993
63	302.466868	23583058826
64	304.732129	24653331443
65	313.380143	22048862023
66	315.670593	22324397333
67	317.412359	24917329056
68	317.641074	21877786160
69	319.431644	21977473240
70	326.762210	22565083474
71	331.980930	22209478091
72	333.326203	23409986654
73	335.995047	24192906083
74	336.196084	48361979973
75	342.764055	22419801682
76	343.138638	25365030373
77	351.989907	22757175885
78	354.409720	27378943456
79	358.907673	24596716252
80	359.146369	25703028106
81	360.323985	39725428268
82	362.580200	22879089047
83	363.469046	22054375226
84	368.345731	24896099448

Mass Spectrum List Report

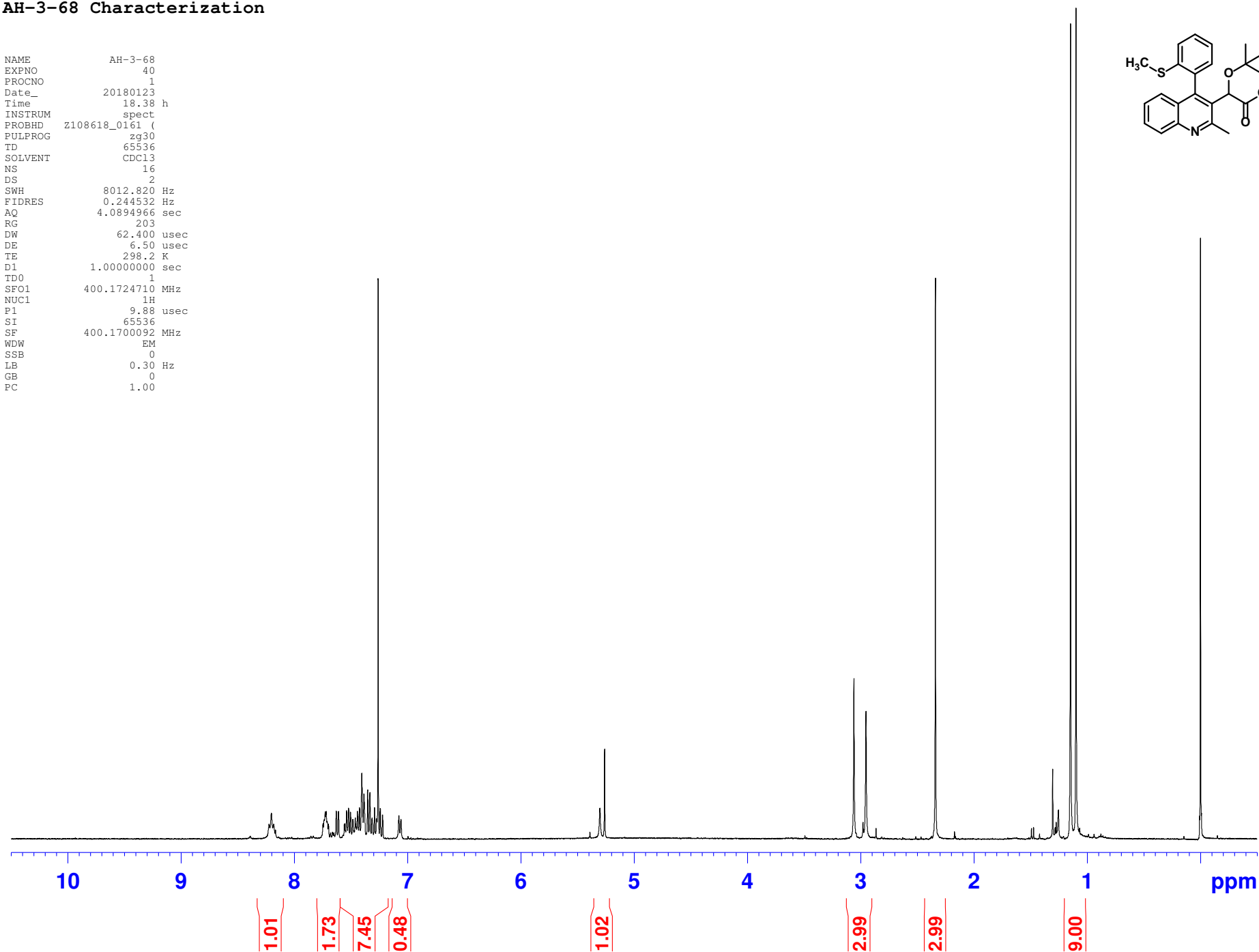
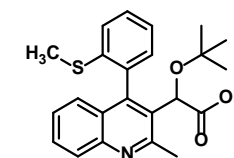
#	m/z	I
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87	381.189352	34687247938
88	381.510631	22542159256
89	389.676419	22607178194
90	398.241769	311775984046
91	398.271802	23433622384
92	399.245120	60381481962
93	407.864135	27626846076
94	408.217250	50715203800
95	412.655017	22038708995
96	414.688173	22375428924
97	416.847809	22590357030
98	419.926361	22393563900
99	420.245824	22587194714
100	425.287760	47241188421
101	431.330408	23392072230
102	432.878693	23418351633
103	435.344998	64743947254
104	440.149355	23460172041
105	454.562292	22399354027
106	462.637926	23355735284
107	466.384572	25633955282
108	474.376013	22627548924
109	480.550666	38947195367
110	480.966115	24215788109
111	481.350651	23174539154
112	488.996439	22965870866
113	493.175509	52466219896
114	502.480420	22642356998
115	508.582025	343430014521
116	509.585343	100569868536
117	510.589176	28594536926
118	511.054899	23211811541
119	512.443497	25075984451
120	516.164517	22755045207
121	522.597721	26293165106
122	523.142832	29665219662
123	523.432893	23320022456
124	525.139939	28392062196
125	526.380428	23269804197
126	536.513291	29290333902
127	536.613246	1335173227924
128	536.702238	34956790097
129	536.793268	24490403251
130	537.518891	23030269455
131	537.616719	418600019250
132	538.620268	65636237648
133	548.940299	22380363229
134	550.592862	33722296854
135	550.629273	26895989322
136	552.608160	93624029437
137	553.611775	41616515601
138	564.644714	392139349086
139	565.648225	135478791597
140	566.651371	33822945170
141	569.403036	56655760733
142	580.549903	23753149920
143	580.640148	23917094012
144	580.871731	22443706203
145	592.676031	504346981882
146	592.743789	27181208187
147	593.679393	188130209747
148	599.548940	74003614636

Mass Spectrum List Report

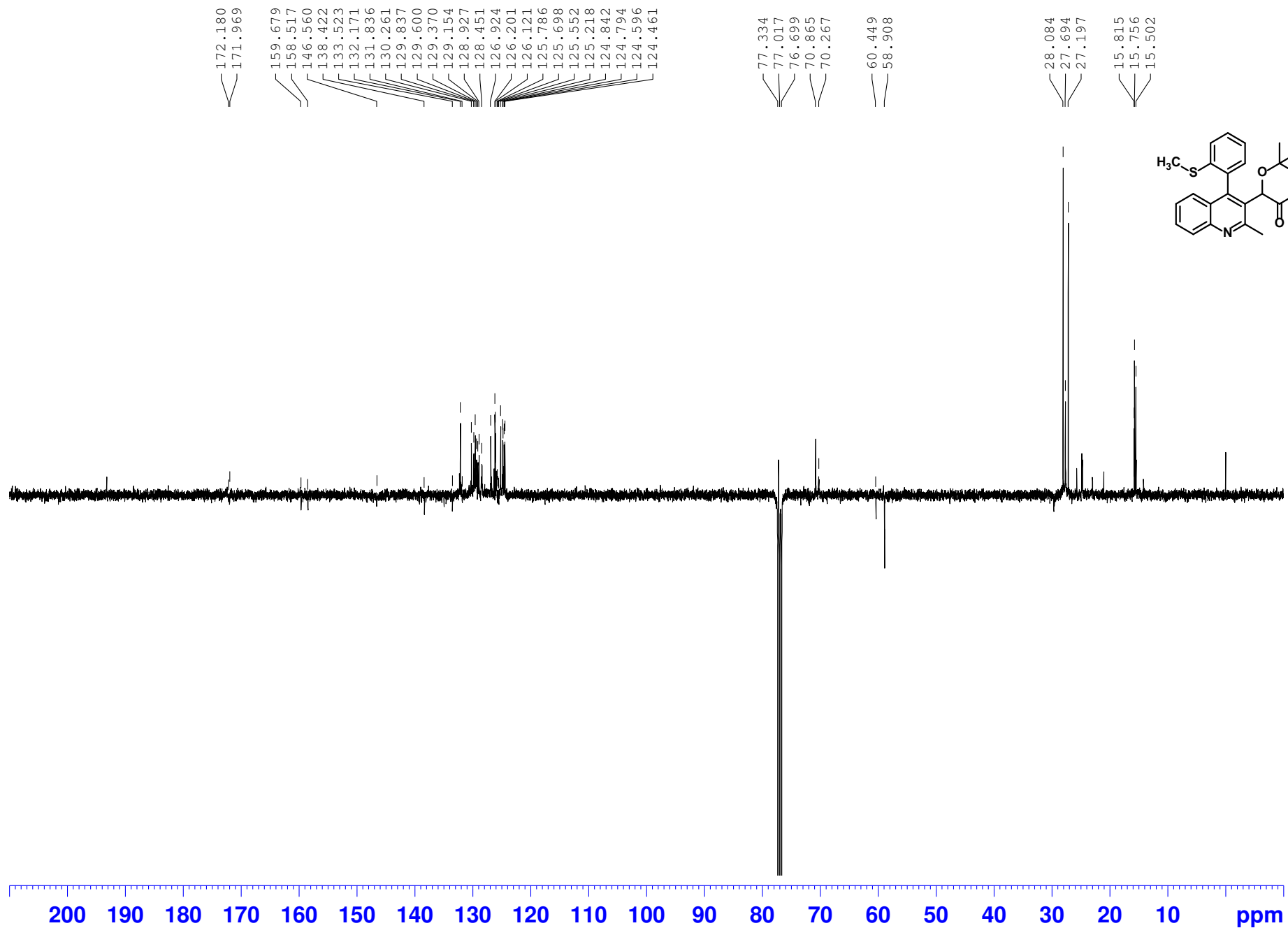
#	m/z	I
149	600.551933	33198559760
150	606.654957	24476955996
151	608.671060	27161662521
152	609.674135	23338339935
153	610.041402	23032666200
154	613.429131	27985422320
155	620.707548	24229764582
156	630.794954	23724352093
157	637.135188	22451756524
158	637.622212	22554241861
159	653.447346	22581780360
160	657.455394	61772398617
161	658.459009	28154601936
162	677.381019	25725699585
163	685.436066	35274515176
164	701.481400	29031077802
165	715.173181	23590959712
166	715.852644	23304615715
167	717.757824	25370842126
168	732.889120	24693909911
169	756.797061	23073824187
170	771.841263	26251503103
171	795.347345	24491839658
172	837.362994	23791603508
173	857.775843	23408919615
174	866.448985	23432749952
175	877.536018	36394563048
176	878.540573	23304382275
177	923.046175	24066128695

AH-3-68 Characterization

NAME AH-3-68
EXPNO 40
PROCNO 1
Date_ 20180123
Time_ 18.38 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-68 Characterization



Mass Spectrum List Report

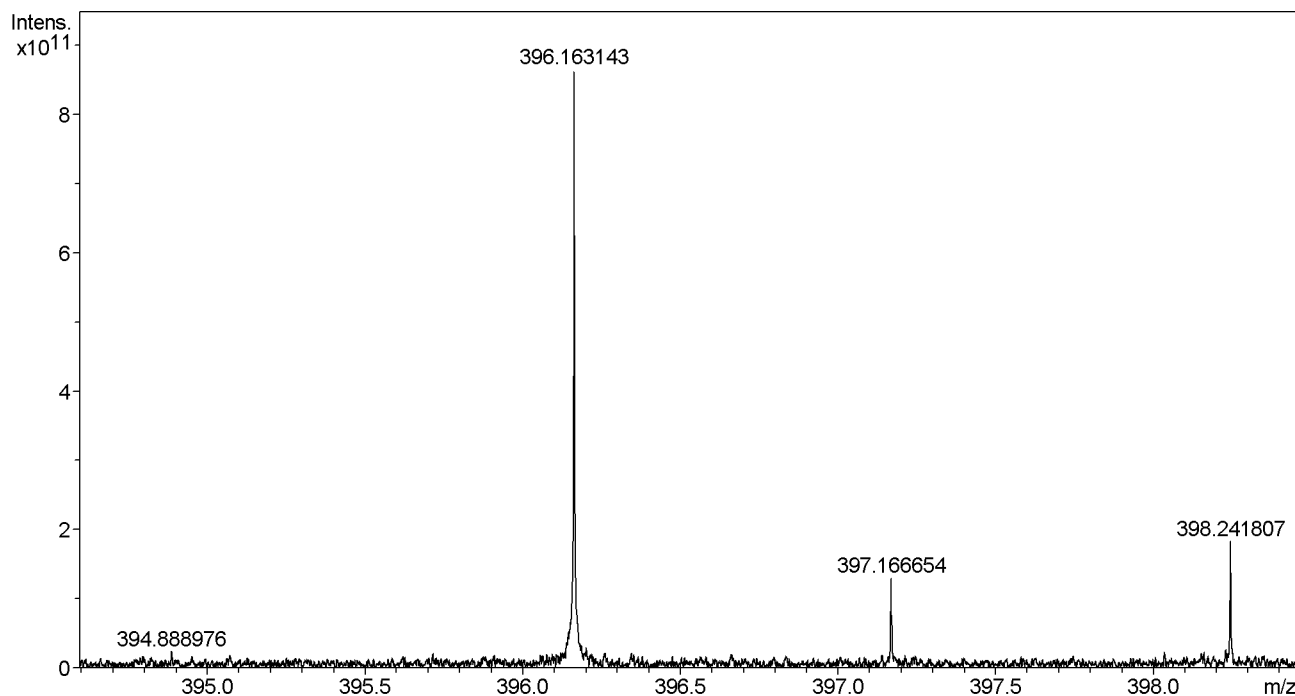
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-68_pos_000002.d
Method
Sample Name AH-3-68
Comment AH-3-68 in THF:MeOH C23H25NO3S H+

Acquisition Date 3/19/2018 10:36:56 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-68 in THF:MeOH
Exact Mass of C23H25NO3S H+ = 396.162791 m/z
Mass Observed = 396.163143 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.364001	22762458289
2	184.878384	21241342333
3	187.343157	21017350075
4	187.384622	24685059974
5	189.577846	21260231704
6	189.858746	21575374142
7	190.308343	23723229279
8	191.050071	24852381984
9	194.871909	21265921149
10	195.825594	23528541146
11	196.136598	22843993004
12	196.270055	21433605743
13	198.489568	22199415308
14	202.370411	22999981502
15	202.668439	28846841770
16	204.709005	22815448704
17	209.441901	26444619663
18	212.946072	21831298705
19	217.487644	24530435932
20	217.969529	25690661529

Mass Spectrum List Report

#	m/z	I
21	218.053567	21060645137
22	219.446103	21234781170
23	222.121596	21240470973
24	229.501778	21162683038
25	230.908060	21129262035
26	231.120541	34001978291
27	235.150701	21242356141
28	237.549981	21702182660
29	237.864993	21838912751
30	240.558713	23361251609
31	242.376620	25477906007
32	246.256235	24447650142
33	246.518926	22842564091
34	247.432059	24116011970
35	249.724005	21451010258
36	250.068624	22901684403
37	250.623625	21137323541
38	254.143797	21259062333
39	257.931354	22297626738
40	267.232699	23960109483
41	270.178636	22211686703
42	271.130873	21494832411
43	273.047857	55883701960
44	277.235362	22765915263
45	280.965398	21578340146
46	281.606337	23316786097
47	282.618576	21192919352
48	287.244641	22918493936
49	289.853077	21477666536
50	291.293112	23004931587
51	294.094888	44068813778
52	296.393401	22406344703
53	301.075573	70870106424
54	302.063945	21358051566
55	304.931454	23175440368
56	310.573513	22446442828
57	313.405142	21467227899
58	326.820948	21633659553
59	330.769015	21773651988
60	332.206950	24654211243
61	332.654519	21982838321
62	332.679223	21958095027
63	340.146612	81639749893
64	341.150053	21951617321
65	342.143742	29396908379
66	344.069915	22450396999
67	351.356680	21912267560
68	351.931879	26252213719
69	351.960104	28176058898
70	351.997444	27770546441
71	352.057501	35219723454
72	352.084375	33886027330
73	352.096696	34818743010
74	352.173172	4193072757933
75	352.228123	59338107484
76	352.241609	43279376398
77	352.288976	34138431250
78	352.340115	31944324471
79	352.390142	23267126615
80	352.443116	26538207728
81	353.156062	33250476436
82	353.176589	849144565106
83	353.179467	364039769756
84	354.169089	52424319335

Mass Spectrum List Report

#	m/z	I
85	354.180078	46508314293
86	355.172358	28276942887
87	356.418548	22567510073
88	361.607795	23171425353
89	365.107209	22590738186
90	366.152607	24103033917
91	368.168256	98441701868
92	369.171493	29331077604
93	372.970622	27216633152
94	374.155445	36058628828
95	374.967327	23940724709
96	377.327751	24148259426
97	382.182752	22118605458
98	382.596283	22478062851
99	384.136514	127509451743
100	386.133601	46992887507
101	386.811707	22946605637
102	389.586757	23771674094
103	390.150387	28808588623
104	390.360696	22623648459
105	393.297782	23915393931
106	394.888976	23533305017
107	396.163143	864260531360
108	396.201462	28432003826
109	397.166654	129635243670
110	398.031668	22171288247
111	398.158884	22639283950
112	398.227084	25973764373
113	398.241807	182527781662
114	399.245281	36916809819
115	400.040863	29937106789
116	400.255696	22578597080
117	406.232422	23840783291
118	409.844347	21952549544
119	416.129695	23136531046
120	418.145542	30619373805
121	421.179126	24976824446
122	422.022811	46206617783
123	425.287941	40430215530
124	428.536022	112075231033
125	432.936330	21772787393
126	435.345060	67226819896
127	439.603504	23998717997
128	455.354180	21911599674
129	459.179522	22262073031
130	461.185606	22147437736
131	464.054605	22273316275
132	477.180676	33345949814
133	479.182045	28329901838
134	480.551023	23971358987
135	487.479361	23853373209
136	490.885063	36733260714
137	493.143064	22493795734
138	493.175597	399524301639
139	494.179036	59504457568
140	508.582218	196347035284
141	509.585638	59286346704
142	511.436561	26346917757
143	524.576973	80706771110
144	525.580721	28848920987
145	536.193366	25494882228
146	536.547736	27406230545
147	536.613411	739468037766
148	537.395290	27288531733

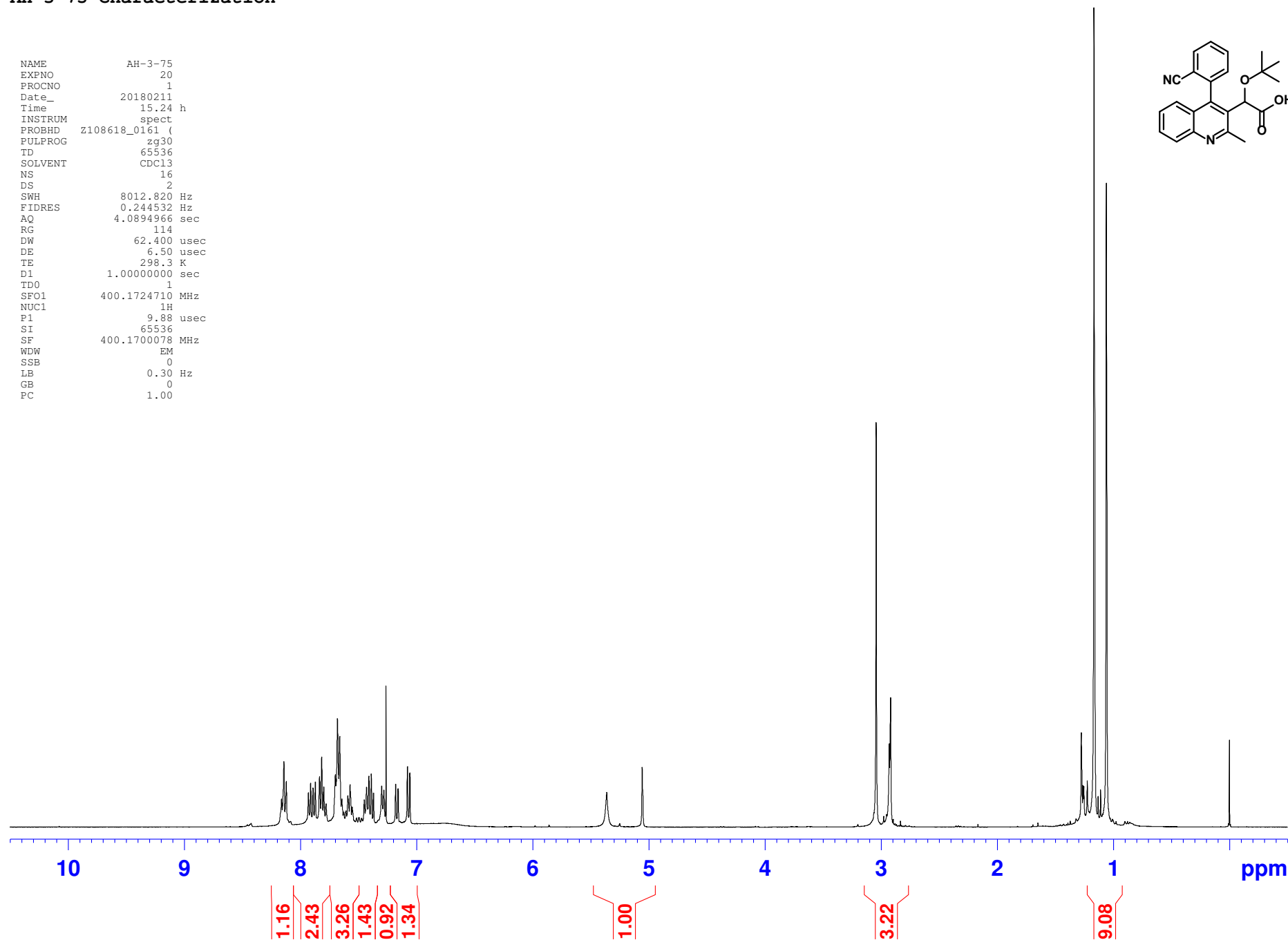
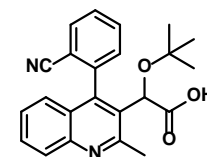
Mass Spectrum List Report

#	m/z	I
149	537.616897	229005406938
150	538.620396	39400798882
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152	545.023414	22620677394
153	552.608495	250675779816
154	553.611811	79075726262
155	556.141831	22530372775
156	558.857306	22354908055
157	564.644871	229671811401
158	565.648104	72667817955
159	569.403172	34653445266
160	580.639771	69218601882
161	581.642681	30364128875
162	585.235666	22741325804
163	592.676253	262043319321
164	593.679668	103091093315
165	599.549195	30664111375
166	608.670998	72909453790
167	613.429565	40963108996
168	615.226096	22924191615
169	618.284811	23945482779
170	632.701866	23812440410
171	657.456011	36874118527
172	667.994095	22915574141
173	685.436785	49450802655
174	686.439961	24679519489
175	716.411481	23087344457
176	727.725250	23642289216
177	741.031525	24267356353
178	745.507752	22975457003
179	759.772411	23342313433
180	770.375636	24198511463
181	937.930416	27764977923
182	964.671285	26713493822
183	965.781709	26314823463

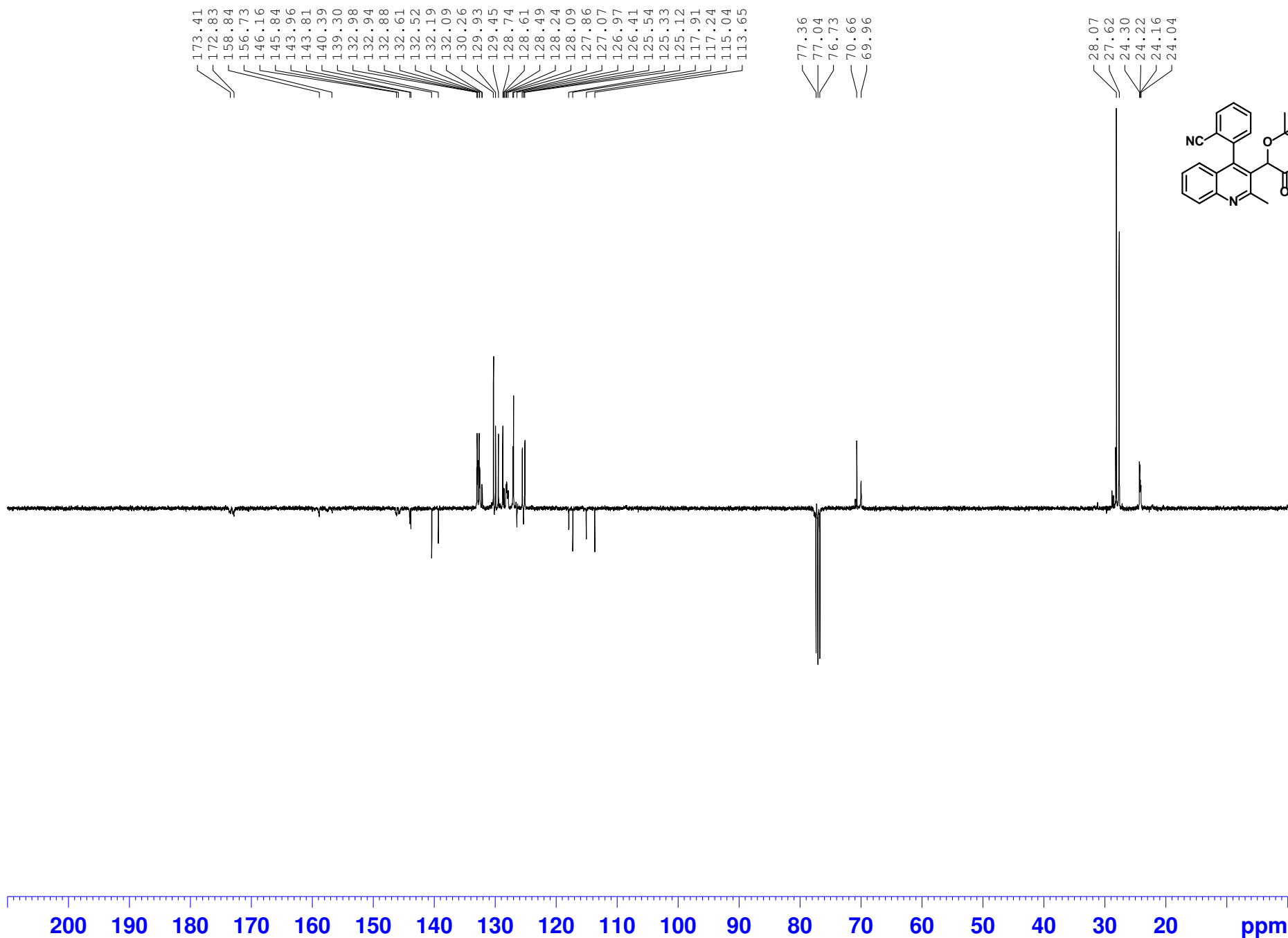
AH-3-75 Characterization

MISSISS

NAME AH-3-75
EXPNO 20
PROCNO 1
Date_ 20180211
Time 15.24 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700078 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-75 Characterization



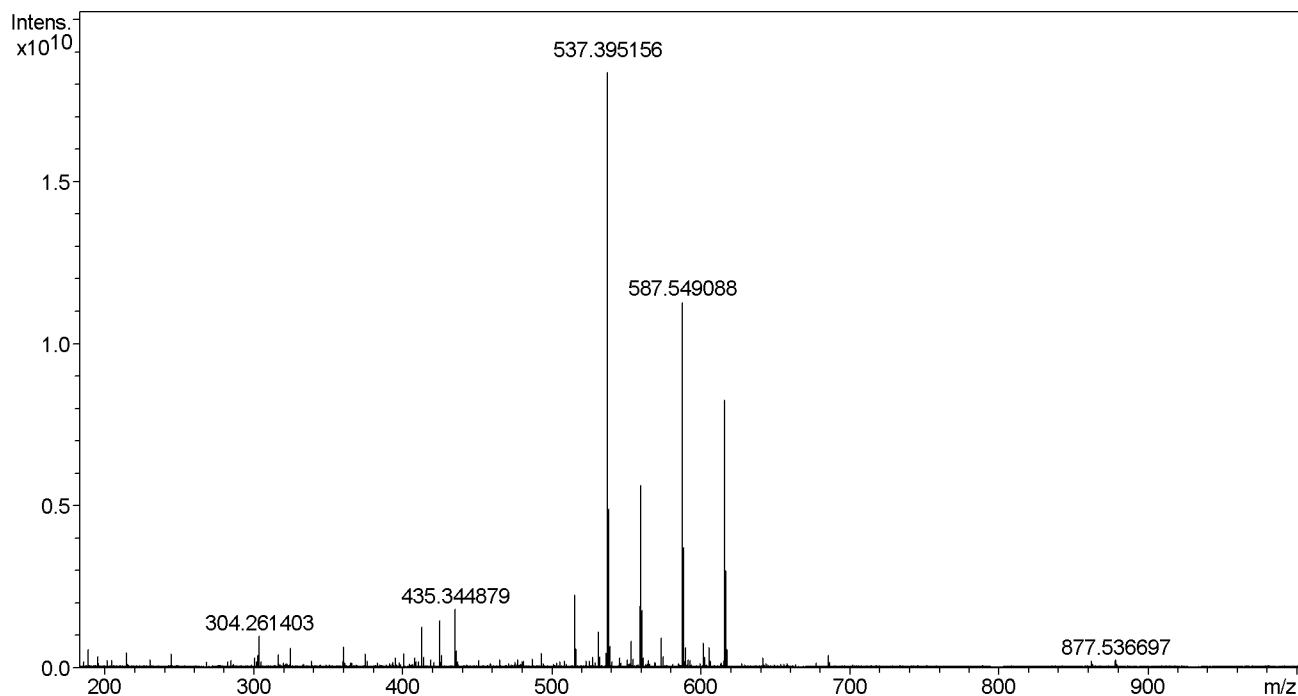
Mass Spectrum List Report

Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-75_pos_000003.d
Method
Sample Name AH-3-75
Comment AH-3-75 in THF:MeOH C23H22N2O3 H+

Acquisition Date 3/19/2018 11:34:16 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-75 in THF:MeOH
Exact Mass of C23H22N2O3 H+ = 375.170319 m/z
Mass Not Observed = m/z
Difference = N/A



#	m/z	I
1	189.394538	139196720
2	189.768514	557014958
3	202.340515	210169631
4	215.089195	454344571
5	216.092530	108243493
6	231.120546	234538242
7	245.099787	419395313
8	269.136172	168792193
9	283.115525	181324552
10	285.131103	215789866
11	287.146789	104514300
12	301.126061	300737935
13	301.141316	125404668
14	301.162456	233539219
15	302.245683	183706730
16	303.141741	374967393
17	304.261403	981797212
18	305.264705	178629215
19	317.120972	405206612
20	317.157374	100662963

Mass Spectrum List Report

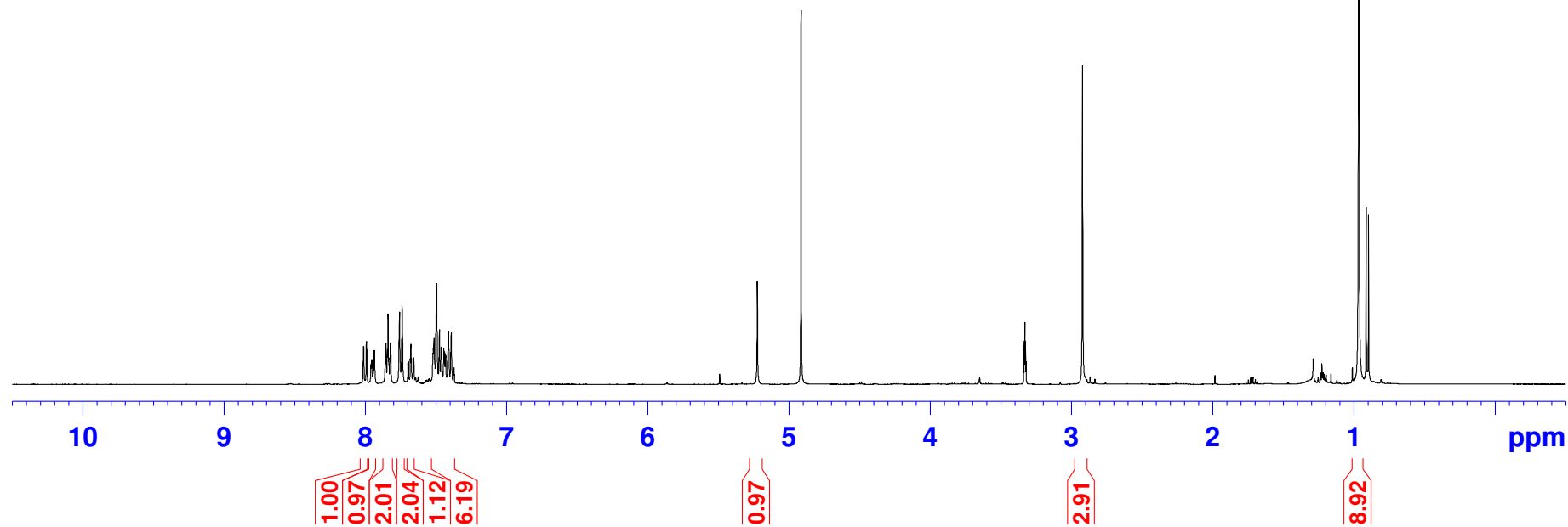
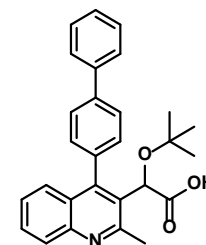
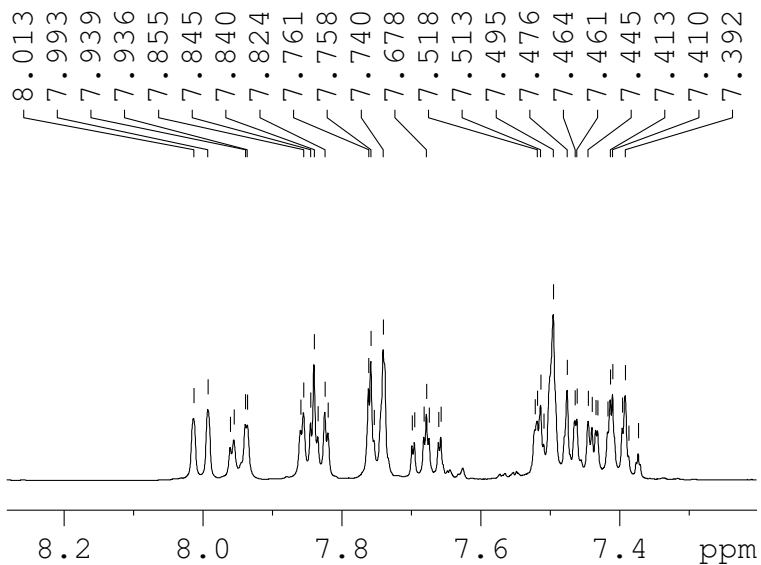
#	m/z	I
21	317.172640	103358171
22	320.256317	135905083
23	322.199215	112953104
24	323.107976	100942031
25	325.123728	601905317
26	334.235600	104728518
27	339.102937	169404334
28	339.154653	200926983
29	360.323964	625407957
30	361.084949	155542606
31	361.327463	144274256
32	365.136322	151080195
33	366.225345	137682614
34	375.199251	429278660
35	375.214506	103415307
36	376.318989	196647689
37	383.082418	148826092
38	391.194133	102378984
39	391.209368	110210679
40	393.209852	106377619
41	393.297868	154148072
42	395.165630	310244368
43	398.241836	163785129
44	399.061896	108509388
45	401.077417	446256243
46	405.188818	114206764
47	407.189168	98769737
48	407.204309	88855494
49	407.313598	106671957
50	408.308869	304852763
51	409.220004	183028531
52	411.160546	181404571
53	413.266645	1243503321
54	414.270023	324342458
55	419.043557	235604859
56	421.329321	163890538
57	425.139768	234403042
58	425.287784	1459319994
59	426.291169	385487382
60	435.344879	1827363439
61	436.348219	509410678
62	437.038552	90124406
63	437.236224	183595596
64	451.153080	227719960
65	459.036127	122611249
66	465.184039	243744787
67	471.119596	110829012
68	475.325973	163299977
69	477.180603	108872315
70	477.316666	233617366
71	479.313666	100413977
72	480.091576	170560301
73	481.262443	196648824
74	487.114331	264728568
75	493.175476	438170934
76	494.178716	128660854
77	501.093725	98870205
78	503.332161	99596080
79	503.455266	142351014
80	505.348043	173025570
81	508.582146	192723762
82	515.259694	2264390335
83	516.263097	577389311
84	523.075635	202571405

Mass Spectrum List Report

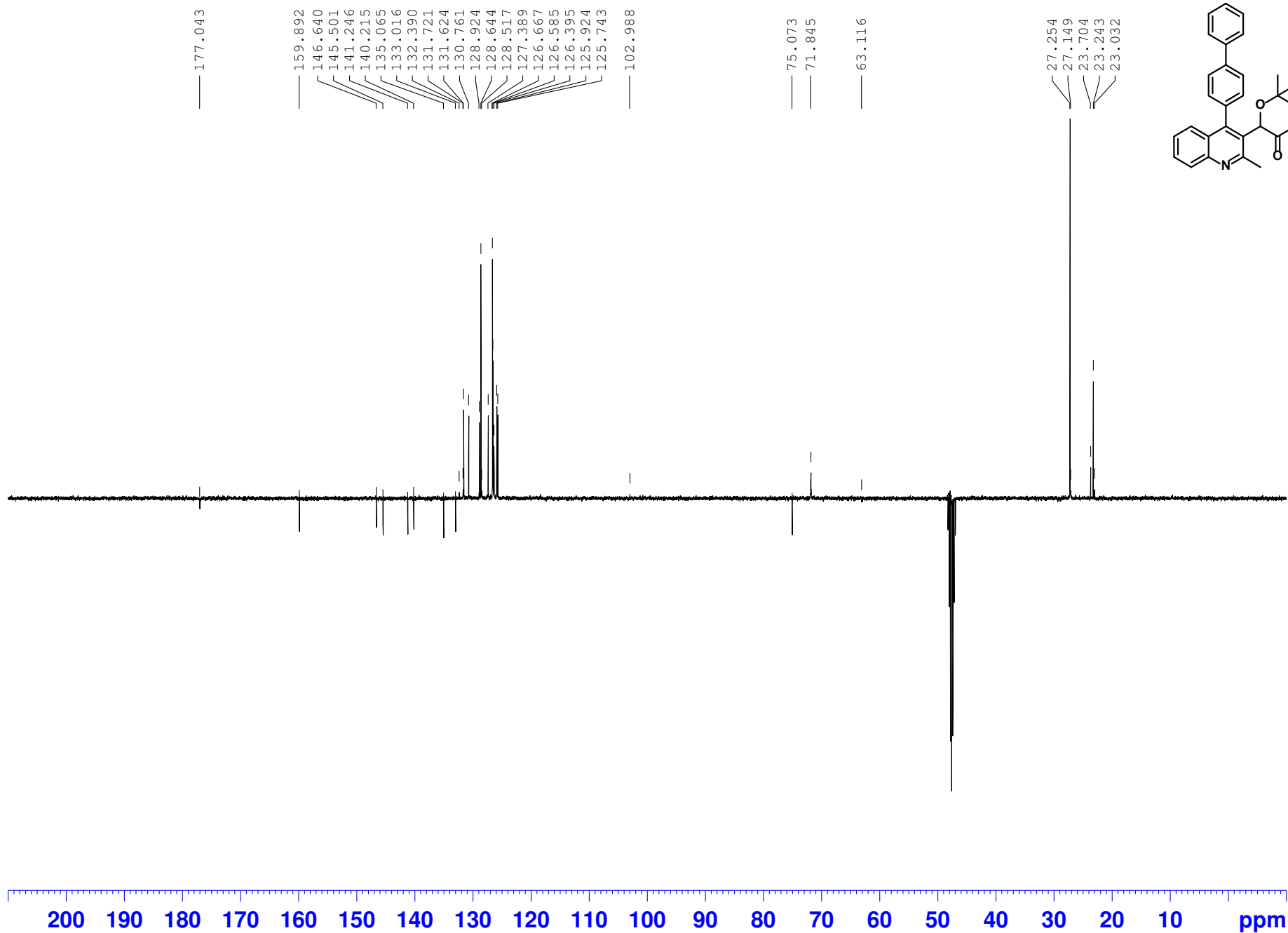
#	m/z	I
85	523.142663	132704565
86	525.091310	106768824
87	525.288640	190371842
88	527.106990	316795638
89	529.239019	163324197
90	531.486535	1112553426
91	532.489896	328383617
92	536.613420	455995807
93	537.190520	245481868
94	537.210910	219657152
95	537.395156	18653611985
96	537.616564	265207720
97	538.398655	4897632747
98	539.391321	640538089
99	539.402190	659085061
100	540.394644	175846920
101	545.502187	311849717
102	546.505505	142738813
103	550.628964	237950547
104	552.608228	112572201
105	553.390303	803758687
106	554.393497	249651569
107	559.517800	5604400700
108	560.521226	1796105180
109	561.524444	307471742
110	564.644829	220680603
111	565.426617	99960529
112	565.648114	106918743
113	569.314801	158506964
114	569.402905	126565690
115	573.218310	131105455
116	573.533519	922178827
117	574.536928	344090461
118	581.034288	97403332
119	585.065588	123341367
120	587.549088	11299437943
121	588.552471	3741279776
122	589.371720	205372627
123	589.555831	614665242
124	591.213578	232837589
125	592.676124	226075671
126	599.548964	128592973
127	601.564809	777201439
128	602.568278	316142367
129	605.366595	619112758
130	606.369956	204583222
131	613.429277	133133771
132	615.580374	8263536301
133	616.583824	2985628767
134	617.587068	555981464
135	627.444564	113683980
136	641.289098	293028893
137	643.611944	124084029
138	653.135964	103955707
139	655.268509	92881173
140	657.455318	125682373
141	663.424643	105589512
142	677.250793	131588312
143	685.436324	371904705
144	686.439484	159551969
145	861.541194	193453587
146	862.544876	103385238
147	877.536697	228947574
148	878.540283	104834344

NGJ-8-090 (CD3OD, 400MHz) Pure Yellow Oil - saponification of biphenylquinoline

NAME NGJ-8-090
 EXPNO 30
 PROCNO 1
 Date_ 20171207
 Time_ 17.09 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT MeOD
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 90.5
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NGJ-8-090 (CD3OD, 400MHz) Pure Yellow Oil - saponification of biphenylquinoline



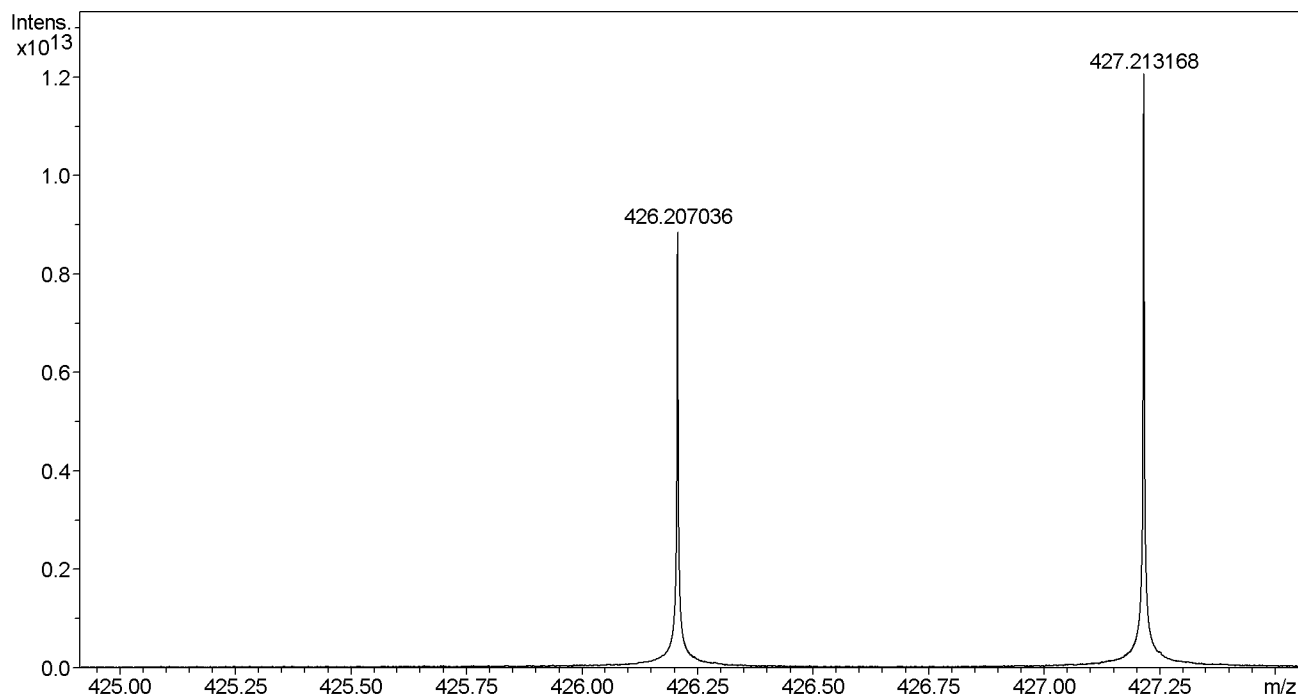
Mass Spectrum List Report

Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-8-090_pos_000001.d
Method
Sample Name NGJ-8-090
Comment NGJ-8-090 in THF:MeOH C28H27NO3 H+

Acquisition Date 3/19/2018 12:13:19 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-8-090 in THF:MeOH
Exact Mass of C28H27NO3 H+ = 426.206370 m/z
Mass Observed = 426.207036 m/z
Difference < 2.0 ppm



#	m/z	I
1	184.313270	33310053773
2	184.917264	22295500552
3	186.740640	21508528502
4	188.104573	21980134048
5	190.831216	24572204461
6	193.465473	21497786750
7	194.838837	22326081671
8	195.066385	25011980163
9	195.276287	21442156534
10	196.909851	21298449841
11	197.399873	21844493955
12	200.664623	21582837734
13	201.178828	23078591444
14	202.075183	25013248059
15	202.340487	106158526274
16	202.359516	22062305083
17	202.629790	24593510285
18	209.153386	21655678932
19	210.429918	21410099490
20	212.155292	21591127437

Mass Spectrum List Report

#	m/z	I
21	213.107016	36608268683
22	213.358317	31281259568
23	213.610158	133545095591
24	214.113210	37793895562
25	214.902986	21176593238
26	217.913017	21215311291
27	218.291318	21629011015
28	222.329046	22025999591
29	223.507053	21151435438
30	223.520231	21296142087
31	224.408916	21604075758
32	228.050127	23866130468
33	228.837690	21353860041
34	233.453948	21487114017
35	239.045270	21237434596
36	239.609881	25583902927
37	240.080913	24292301457
38	241.088552	22557833473
39	242.816701	21113706283
40	243.978037	22415426017
41	251.199288	22868201618
42	255.692332	24629633706
43	255.879542	21197625072
44	256.185395	23260153117
45	258.886669	27862350672
46	260.178675	22497260744
47	260.378821	21793815838
48	261.109703	35367409355
49	262.137067	22741301856
50	262.244809	74830529404
51	262.388396	21559497486
52	263.106683	21604265708
53	271.247141	22343773631
54	271.284799	26430818534
55	275.478351	22176215147
56	278.622238	22554890104
57	278.863296	21873784663
58	285.577418	23300115193
59	285.764296	21428256534
60	285.853722	24355074507
61	286.666453	21473020615
62	289.646349	21354084688
63	290.888788	22954974980
64	291.104175	25765015096
65	291.250817	22504901031
66	292.111612	28144574501
67	293.595946	24040245095
68	294.769659	22880656109
69	295.134681	21423633176
70	296.140396	28551275417
71	297.068742	22174353768
72	301.059114	22747461034
73	301.075731	258778005274
74	302.581251	25350831390
75	305.993703	24393067160
76	306.127335	29833077614
77	308.143055	24288386816
78	309.114807	38264677426
79	309.149885	32387933418
80	310.069757	21512298446
81	310.153418	22883560715
82	311.180000	21766833788
83	312.443399	21756766689
84	323.131461	23753857272

Mass Spectrum List Report

#	m/z	I
85	324.138228	37389259998
86	325.144822	82026318559
87	326.147829	39482027529
88	326.150667	27213679832
89	326.648665	22838780353
90	327.154437	26052376153
91	330.495486	27462019449
92	332.716359	23012425812
93	335.489877	24037116980
94	337.631768	21532975704
95	343.631701	21950188194
96	353.139682	22145244558
97	363.075916	22440306250
98	369.587775	23476889994
99	371.577753	24180275251
100	372.156019	22058503248
101	374.116150	37832805181
102	375.122323	77509805568
103	376.128704	37782079504
104	377.107213	51808870520
105	381.740605	22171561128
106	382.217461	255734612591
107	382.730942	22610613244
108	383.174749	23152659979
109	383.223605	387821578633
110	383.248450	24745335930
111	384.229847	380972710282
112	385.236252	76602379903
113	386.332095	23353411947
114	386.769506	23510941080
115	398.242513	36361531474
116	423.971766	24928654086
117	424.732675	27340731718
118	425.197709	24579542046
119	425.248825	24675292003
120	425.373416	25372597717
121	425.451411	30327342837
122	425.520828	28097973736
123	425.568946	26315293601
124	425.610564	29115898688
125	425.659384	34688323464
126	425.695307	34897072131
127	425.743325	31194964751
128	425.765872	34224170541
129	425.797417	35622893311
130	425.836639	36514802917
131	425.885177	42012634648
132	425.937871	46252064162
133	426.030516	58337684539
134	426.076084	70170592334
135	426.207036	8895704146425
136	426.244145	225996186502
137	426.460320	33466961058
138	426.600130	25474889412
139	426.685871	24449537605
140	426.719724	25727914741
141	426.757445	27310395535
142	426.849661	32037022008
143	426.910807	41904403331
144	427.213168	12052241498134
145	427.519144	42916751380
146	427.580141	41135192752
147	427.624805	37229415975
148	427.704137	37639178519

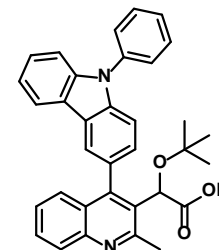
Mass Spectrum List Report

#	m/z	I
149	427.758142	30927701400
150	427.834064	26932503490
151	427.894802	29240236498
152	427.927786	30626829407
153	427.955638	27870478952
154	428.050459	24623877000
155	428.211863	123981157211
156	428.218842	2068191029342
157	428.253537	62103765707
158	428.354165	29769649044
159	428.398498	40403123397
160	428.553449	26330086227
161	428.608515	26615181362
162	428.696602	26631329772
163	428.723241	24958720183
164	428.858993	25027723918
165	428.910631	25597217278
166	428.967739	25765638953
167	429.049587	27681559961
168	429.132759	29783073192
169	429.223223	1570715484885
170	429.226236	969151633271
171	429.336266	32959124692
172	429.456033	24494625888
173	429.498487	27345048711
174	429.565359	23719106185
175	429.602877	23701333484
176	430.226798	138680690864
177	430.229890	171928940716
178	447.496175	24609072563
179	448.138414	23193284132
180	448.188974	595970383380
181	448.553891	23841711501
182	449.069507	23844486713
183	449.136847	39154794105
184	449.195262	1325781317994
185	449.284958	29381560967
186	450.201556	719689172682
187	450.300929	23225563262
188	451.205442	73296706542
189	454.238846	269046778414
190	455.244603	570541477840
191	455.280889	30170325372
192	456.152910	23047043638
193	456.204430	24075594220
194	456.250806	1096422797435
195	457.254766	491796403068
196	457.257785	425350182304
197	457.295262	34298838404
198	458.261154	93124793317
199	462.404221	24255449616
200	470.170991	134205807911
201	470.303877	24708403373
202	471.177194	386635922340
203	471.307279	24810589560
204	472.180256	83006574261
205	472.183773	147535885804
206	473.186836	40159446745
207	477.180868	36939163183
208	477.227178	32829160024
209	478.232917	56357256290
210	478.445726	25736649915
211	479.239592	26711607497
212	482.268183	24947854797

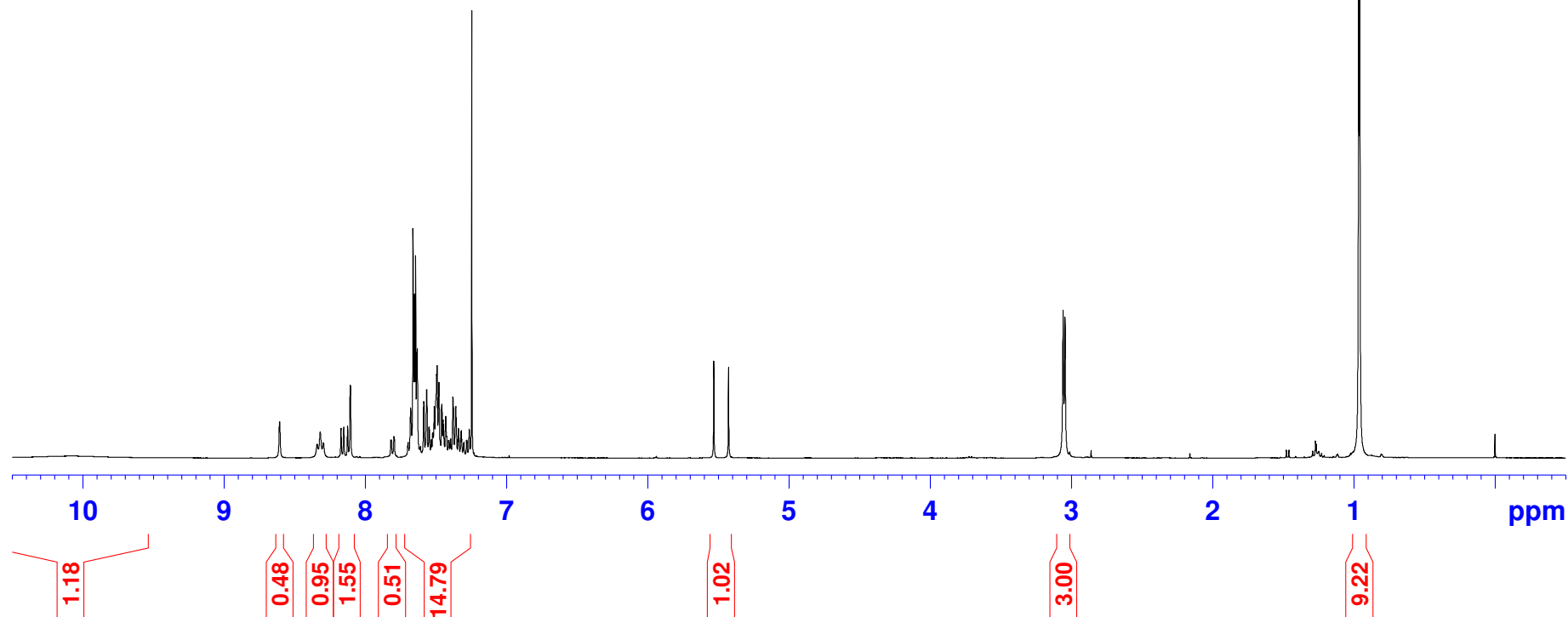
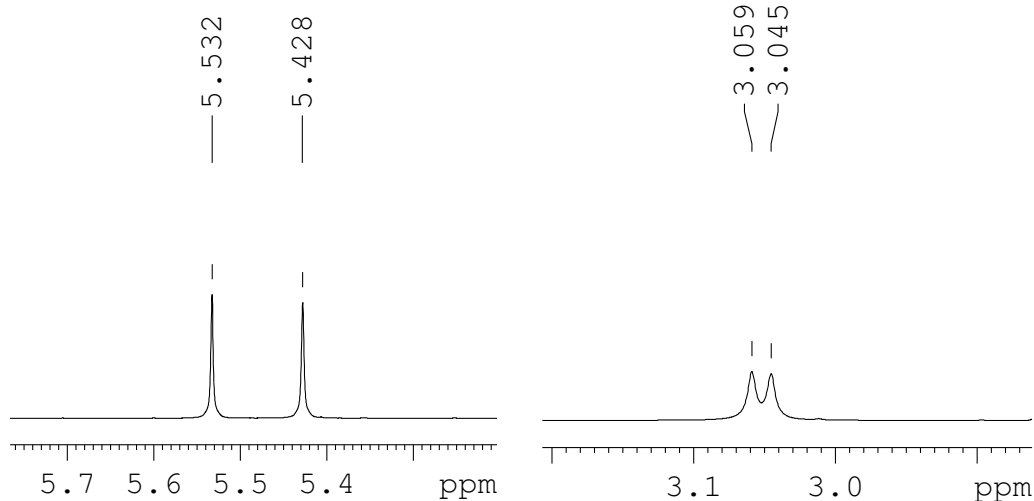
Mass Spectrum List Report

#	m/z	I
213	483.276358	83438711670
214	484.283209	49083281952
215	485.282330	29199564758
216	489.521523	23049177724
217	493.175608	665769889904
218	493.225942	24334832503
219	493.271518	22574141696
220	494.179036	112433681227
221	494.801205	22523346570
222	499.176857	22815681852
223	503.841413	22919789863
224	508.582455	62917606380
225	523.325386	37238911593
226	525.376480	27829206965
227	529.248308	24150834932
228	536.614141	405304917340
229	537.617249	88361679588
230	549.196694	24752704605
231	552.609508	33419898184
232	559.134806	22358699198
233	561.243866	23336033234
234	564.645897	78018079988
235	565.649326	31115187964
236	569.207352	91925868904
237	572.527287	22990152929
238	579.110940	36812813294
239	579.162373	539689257142
240	580.165915	143299381984
241	587.577291	22704439049
242	588.027381	22945434029
243	592.677540	83738805755
244	592.978760	23007331302
245	593.681128	22836245011
246	597.207716	32738273916
247	621.596572	24770493434
248	626.780552	23483740915
249	647.283094	31782664271
250	647.302564	30553764847
251	648.309205	32899858310
252	655.194194	40808717726
253	659.568554	24786671625
254	674.358716	23366675812
255	674.986986	26308459525
256	685.437710	24833175182
257	711.362407	27692166399
258	717.266780	25940194985
259	747.811329	23240858521
260	757.487345	25756800702
261	836.397524	24041956398
262	836.604609	24429191817
263	871.489501	23275150855
264	883.562371	23140730157
265	953.529998	24268779150

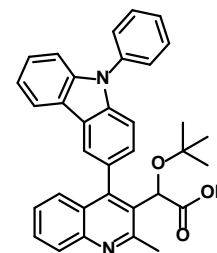
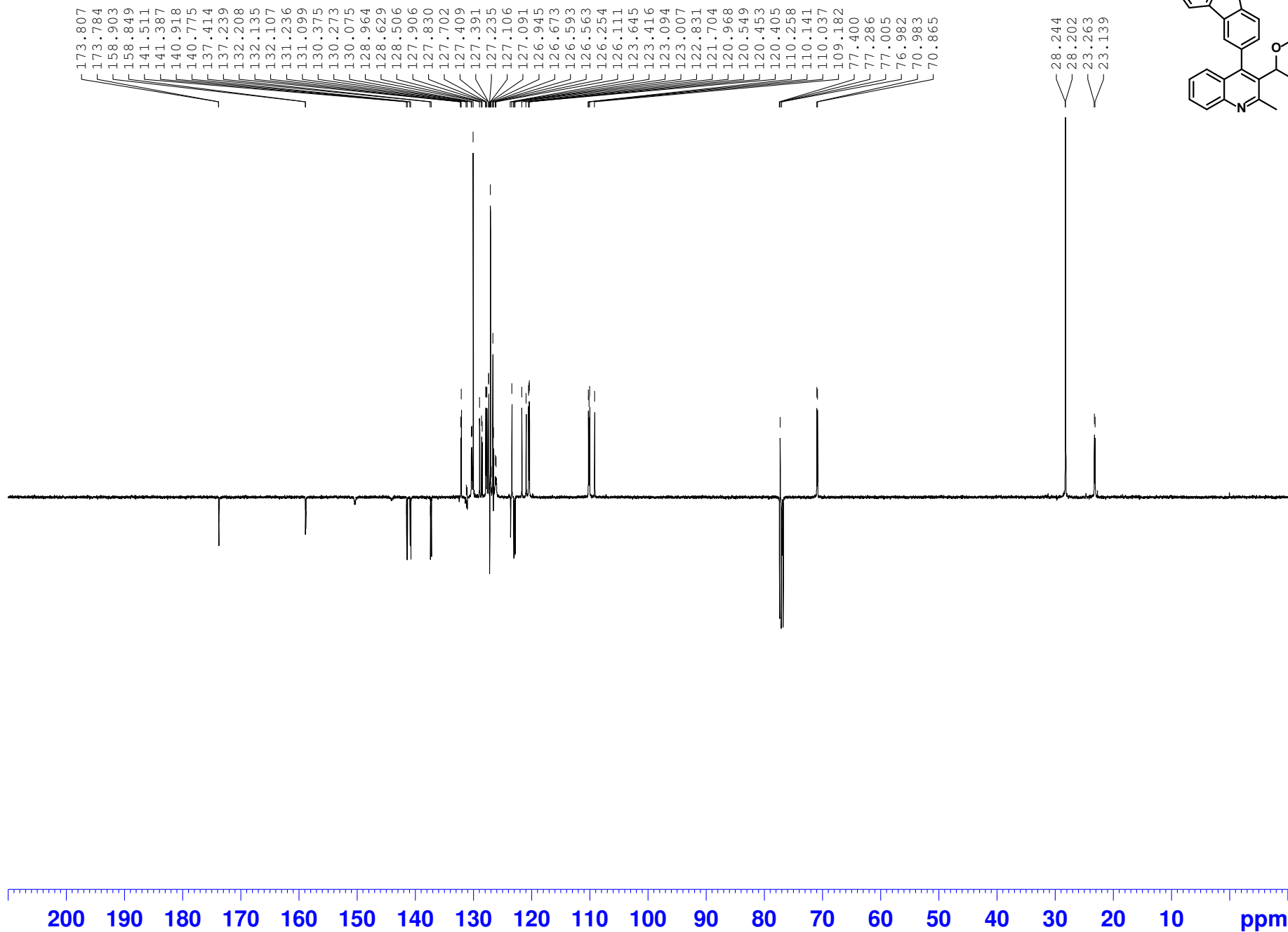
NGJ-9-028-1 (400MHz, CDC13) Pure Yellow Oil - saponification of carboxazole quinoline



NAME NGJ-9-028-1
 EXPNO 10
 PROCNO 1
 Date_ 20180219
 Time_ 21.59 h
 INSTRUM spect
 PROBHD Z108618_0161 ()
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 71.8
 DW 62.400 usec
 DE 6.50 usec
 TE 298.3 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700149 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NGJ-9-028-1 (400MHz, CDCl3) Pure Yellow Oil - saponification of carboxazole quinoline



Mass Spectrum List Report

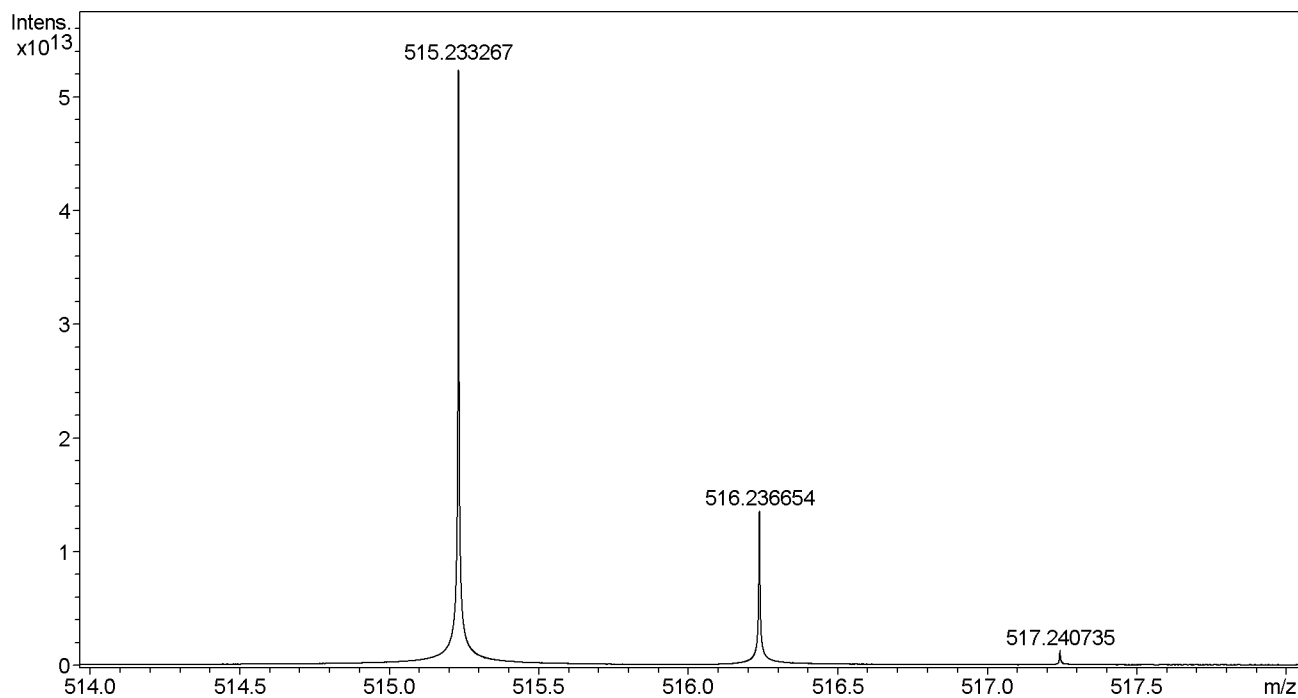
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-9-028_pos_000001.d
Method
Sample Name NGJ-9-028
Comment NGJ-9-028 in THF:MeOH C34H30N2O3 H+

Acquisition Date 3/19/2018 3:36:15 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-9-028 in THF:MeOH
Exact Mass of C34H30N2O3 H+ = 515.232919 m/z
Mass Observed = 515.233267 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.313315	23790647788
2	186.149630	21225329637
3	186.640907	24021462437
4	188.587707	21645158821
5	189.006973	23781227672
6	190.448227	21340957900
7	192.165680	22460859905
8	193.279608	22087961660
9	194.789516	21783952854
10	197.069244	23195469943
11	198.073902	21734427815
12	198.382199	120156427615
13	198.679509	28014348369
14	198.828596	1066124637173
15	198.829708	188027696017
16	198.830488	83723342669
17	201.720161	21995204486
18	202.161876	22307935887
19	202.340550	421670441690
20	202.350521	21061190337

Mass Spectrum List Report

#	m/z	I
21	202.572712	22590813110
22	206.098154	27238754410
23	206.258583	50812370841
24	207.077786	22167323219
25	208.019252	22341503177
26	210.036066	28180410408
27	210.998146	21423732534
28	212.648915	21965184292
29	220.009219	21978025534
30	222.248945	98889877273
31	222.783272	21548977111
32	222.918941	24904546712
33	222.919450	38863715192
34	224.453389	26809210482
35	230.987447	22806416798
36	231.120686	59036466595
37	231.923360	25221443918
38	233.285310	22944524442
39	234.056187	22412451906
40	235.626188	93823380977
41	236.128039	51602219309
42	236.896411	22612762160
43	237.536396	23340528257
44	238.911542	23339441235
45	241.088869	21685455512
46	241.227297	23162167762
47	242.223489	21792766220
48	244.618032	21220341076
49	245.285979	22399480954
50	246.062083	21298338933
51	253.680223	21212525734
52	255.078308	21608748103
53	257.620733	70700238417
54	257.621808	252111750992
55	258.123581	96081651046
56	259.617447	23769699183
57	266.571663	22680802676
58	267.138147	24274042833
59	267.383338	21622710942
60	269.262101	21919775893
61	269.417638	23169368681
62	269.959467	24883514079
63	270.235019	22478652217
64	270.265866	22087115738
65	270.521004	21351335708
66	273.798146	22525797969
67	275.697920	22218192110
68	277.746818	21821960232
69	279.555611	23022375099
70	281.474884	22415708587
71	283.562933	38851434101
72	285.965673	22460726845
73	286.865820	21599944855
74	290.849776	21486577747
75	292.887769	22547651828
76	295.117461	22461587058
77	295.521311	21331079625
78	295.671420	22528676397
79	296.438476	22246593074
80	298.208600	25058428732
81	300.060596	23443112066
82	301.075863	81449844484
83	312.205204	21365002074
84	317.121303	22265981007

Mass Spectrum List Report

#	m/z	I
85	318.115502	26368479270
86	319.122698	21614448947
87	323.764223	23072298374
88	330.759791	21534093484
89	338.623164	21777821479
90	341.415139	23011082745
91	344.894285	22785443709
92	345.889823	21749062993
93	347.858121	22107724772
94	351.554147	22358588270
95	360.324478	28800364155
96	365.107126	22218175179
97	366.116143	24128829446
98	366.377858	22121250942
99	367.123298	25140003734
100	368.130216	22570079146
101	369.051023	23620627584
102	369.138869	30314503196
103	380.130082	37727631995
104	381.135475	24649463203
105	381.139174	22263135746
106	382.146654	32123011119
107	383.150025	28734143120
108	383.154046	24035175463
109	386.497443	22618616532
110	386.573855	22014679044
111	389.394804	26451821192
112	394.204214	22910641889
113	395.154721	25021293698
114	396.160801	37645479853
115	397.170334	90025107158
116	397.942827	21618144121
117	398.172745	39249098097
118	398.242357	72549990378
119	402.123474	23620457490
120	404.693354	21775615656
121	406.589516	23876759648
122	411.149382	39405608382
123	412.157154	34701739257
124	413.165909	76517048034
125	416.183199	26212955152
126	417.998101	21884743672
127	419.152918	37729794593
128	419.607111	22414731072
129	425.288423	29069600311
130	425.550924	22617328137
131	427.757017	23071209786
132	429.160468	24913312018
133	435.257987	23481826874
134	435.345650	37646493526
135	442.010871	23547666342
136	459.170644	39937665955
137	463.635575	25703205599
138	469.238904	26624945926
139	469.467015	26810619559
140	469.760339	27389932187
141	469.966786	29198133248
142	470.029077	35974106412
143	470.062391	27724983781
144	470.121421	28664012811
145	470.210955	31084557279
146	470.235266	36886011601
147	470.314087	34084101357
148	470.365339	33891449798

Mass Spectrum List Report

#	m/z	I
149	470.471385	38084931613
150	470.507860	35415052175
151	470.547408	41733976257
152	470.631841	46939784083
153	470.679814	50563263058
154	470.717630	47495508526
155	470.764850	49974422610
156	470.994890	89952756505
157	471.243709	17691328221541
158	471.640492	50886805039
159	471.765698	36588041192
160	471.805195	34391728009
161	471.900346	26762597368
162	472.038952	30228177491
163	472.112601	34934943428
164	472.247258	5989204513329
165	472.370495	72115334432
166	472.561627	42237299635
167	472.692847	40966584447
168	472.805935	36558990403
169	472.854642	29880929031
170	473.250984	660812038856
171	473.410152	30978163899
172	473.515780	27573177963
173	473.543863	30881294957
174	473.668325	26585846945
175	473.908534	26855349587
176	474.154072	27415305405
177	474.198107	27195234631
178	474.254487	46082949685
179	475.156253	29297164381
180	476.843585	30239736463
181	485.223575	187131574178
182	486.226963	53893484525
183	487.239268	82961950418
184	488.242707	33718401625
185	493.176511	30700200803
186	493.226599	42287794131
187	501.254985	177652906388
188	502.258389	45403141187
189	503.233986	1998043445465
190	504.237589	548467256486
191	504.388525	30998207381
192	505.241169	43839177724
193	505.732639	29303159805
194	507.138653	33422392207
195	507.718611	27852222889
196	508.054936	27908469677
197	508.582946	52951062807
198	509.586650	41201184200
199	509.621091	29778858122
200	509.800176	29567788619
201	509.900333	28786217320
202	510.212525	30847201293
203	510.516617	28799323870
204	510.741464	28092506403
205	510.908186	29268210067
206	511.004559	33902052265
207	511.103259	30708292222
208	511.260353	31403781796
209	511.323676	30479623053
210	511.372503	29942953498
211	511.477685	33286058565
212	511.651404	30732947488

Mass Spectrum List Report

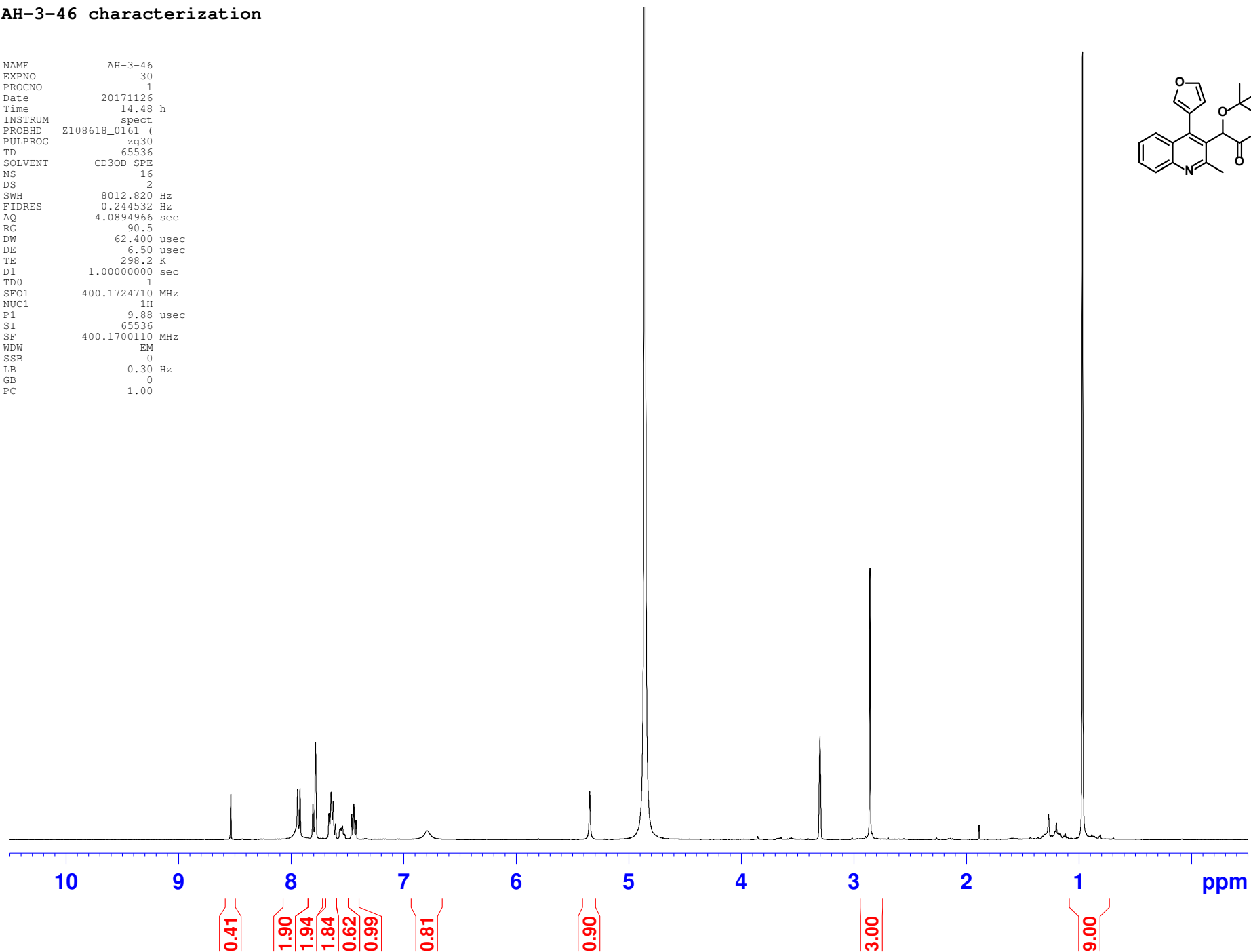
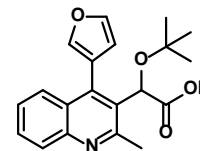
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214	511.743147	31445463399
215	511.850428	43657396371
216	511.955130	36378081747
217	512.084887	32405515143
218	512.205835	43911101039
219	512.290646	36087251268
220	512.408020	39443213552
221	512.485641	39035822558
222	512.578141	40843336783
223	512.795392	41166864942
224	512.893877	40877650355
225	512.911178	43010933577
226	513.086114	43518776160
227	513.402412	53290056971
228	513.462383	52426995266
229	513.682342	60568833115
230	513.722211	63741746781
231	513.861982	65471622846
232	513.904032	64758791386
233	513.942741	65150594770
234	514.017114	67286828225
235	514.057754	71642264206
236	514.118578	71437655437
237	514.208580	84337925190
238	514.294861	81629827617
239	514.337651	88938712707
240	514.583974	112335058526
241	515.233267	52738732711001
242	515.927500	66272738995
243	516.003948	66925539691
244	516.236654	13601925041960
245	516.752268	79825376743
246	516.830390	75105442801
247	516.992000	70991293630
248	517.240735	1287723358418
249	517.416987	57432714631
250	517.451914	56451955307
251	517.471732	45329027719
252	517.548391	56404741552
253	517.590851	47525350071
254	517.676268	49866978745
255	517.837215	45475251103
256	517.934820	43095159060
257	517.967290	41740803867
258	518.032301	42043859093
259	518.238615	40890478212
260	518.244584	71593855034
261	518.356630	37270193464
262	518.517726	35917447574
263	518.664480	37174780666
264	518.743721	32958702712
265	518.801044	32265764421
266	518.839915	32884013193
267	518.877004	33282052560
268	518.974447	33204723543
269	519.137250	32683988165
270	519.247702	31806580444
271	519.322980	31852089975
272	519.393035	28249058875
273	519.514794	32306744773
274	519.875775	29141073643
275	520.243836	28234073994
276	520.319132	28453778934

Mass Spectrum List Report

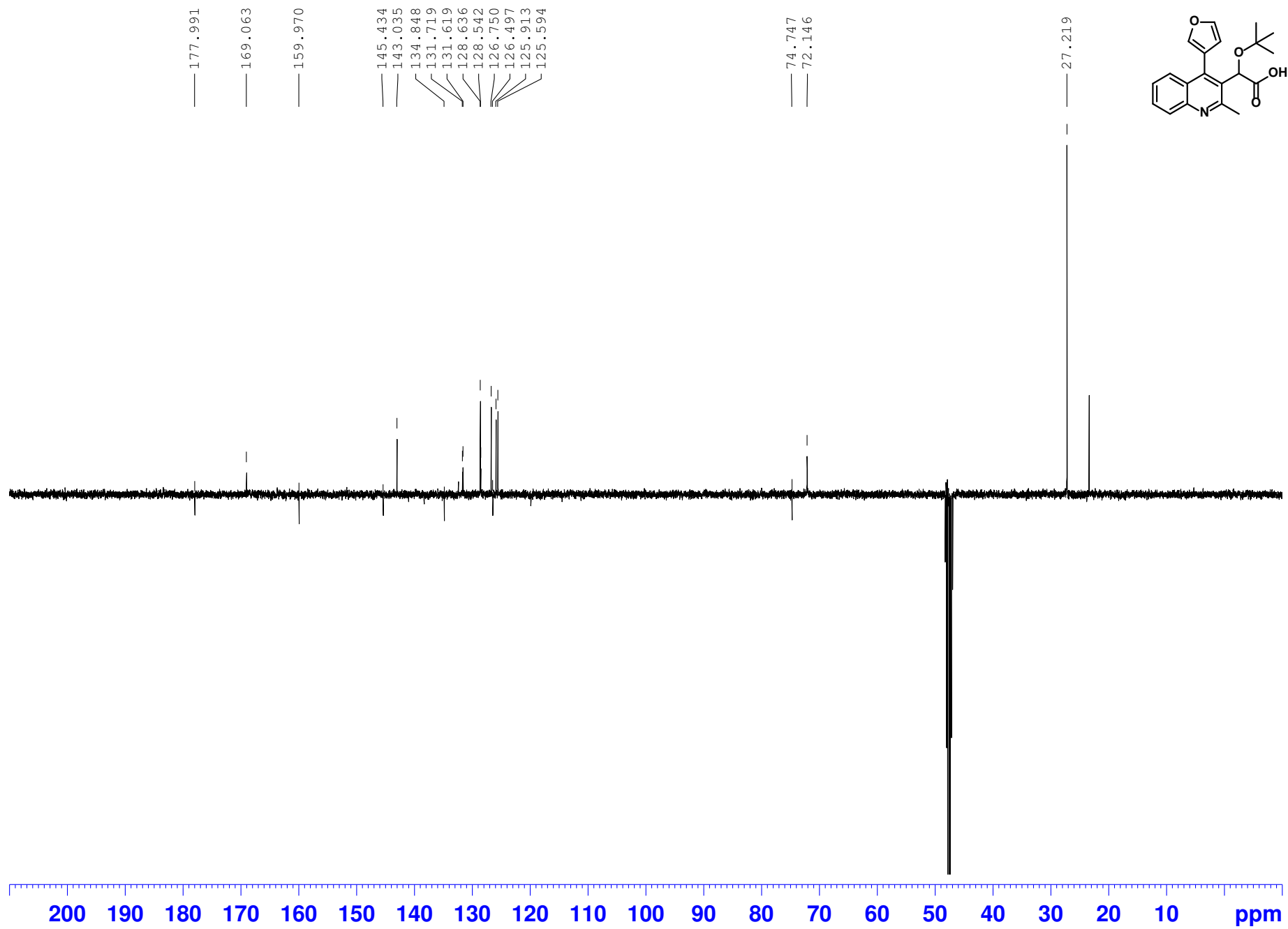
#	m/z	I
277	520.507841	28441485356
278	520.677622	27982966490
279	520.845643	28990831448
280	520.873677	27948004603
281	521.772879	29231717105
282	523.213276	28113777983
283	524.577832	39247308360
284	530.385010	29310251018
285	530.774117	27752618792
286	531.229171	53172661421
287	536.614352	263336375105
288	537.215928	1440272010599
289	537.618178	59105585990
290	538.219610	342957211051
291	539.223151	33338888412
292	543.265834	80515404013
293	544.268956	30373084603
294	552.609600	95407561608
295	553.613031	38653830484
296	557.317948	41782751401
297	559.198525	96857121958
298	564.645988	45480790623
299	565.649459	27531293522
300	568.281159	29504655239
301	571.297476	90220043505
302	572.301017	25842658270
303	579.163299	74547520954
304	592.677437	73628729944
305	599.550457	25190186729
306	606.907324	23459957465
307	622.040045	22798040659
308	631.306158	23032579177
309	677.673357	23022897393
310	685.437685	22956327685
311	715.830148	22516639822
312	732.918915	25485224119
313	794.170158	24406180476
314	852.979823	24539643413
315	871.215513	24515290086
316	878.112390	24148209665

AH-3-46 characterization

NAME AH-3-46
EXPNO 30
PROCNO 1
Date_ 20171126
Time_ 14.48 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CD3OD_SPE
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 90.5
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SF01 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700110 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



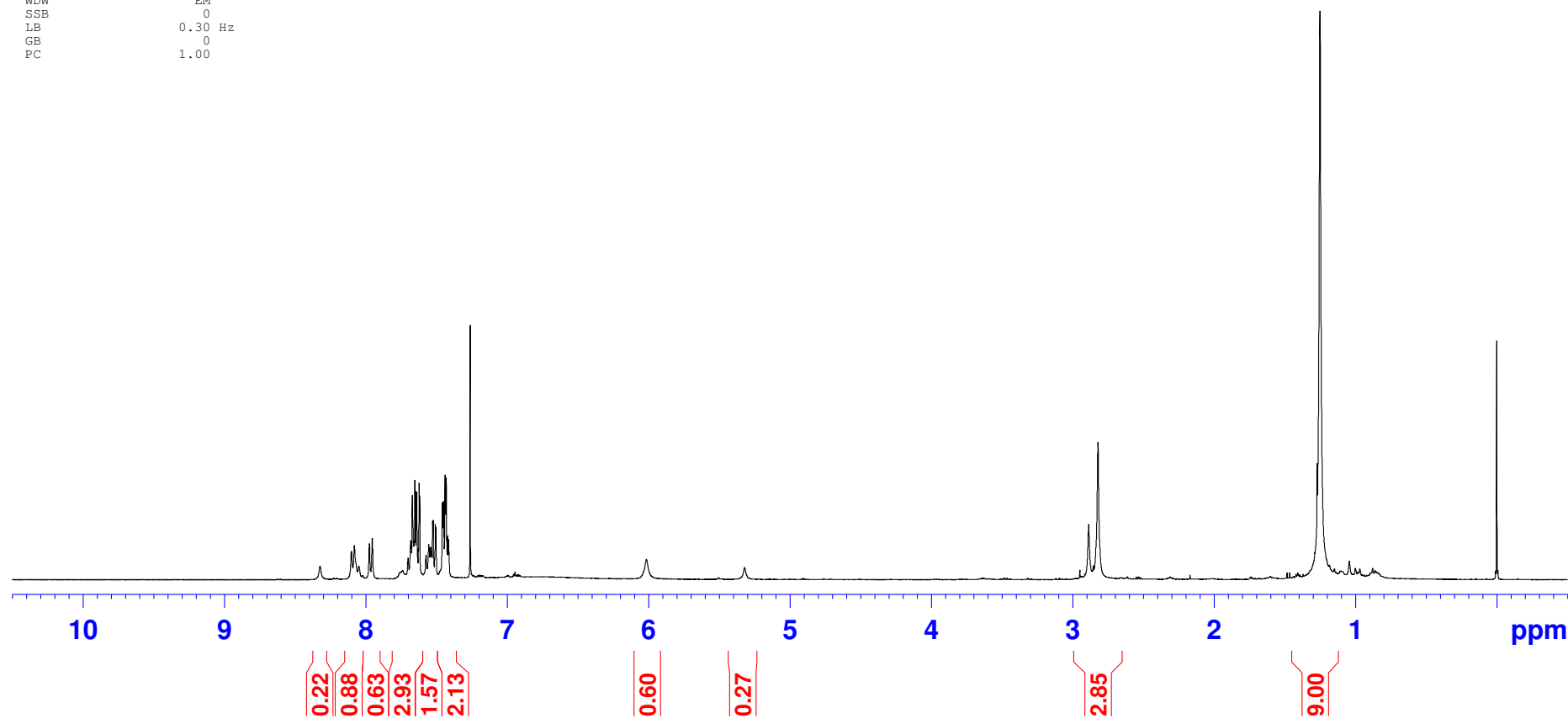
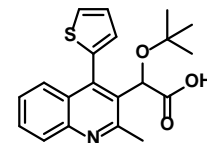
AH-3-46 Characterization



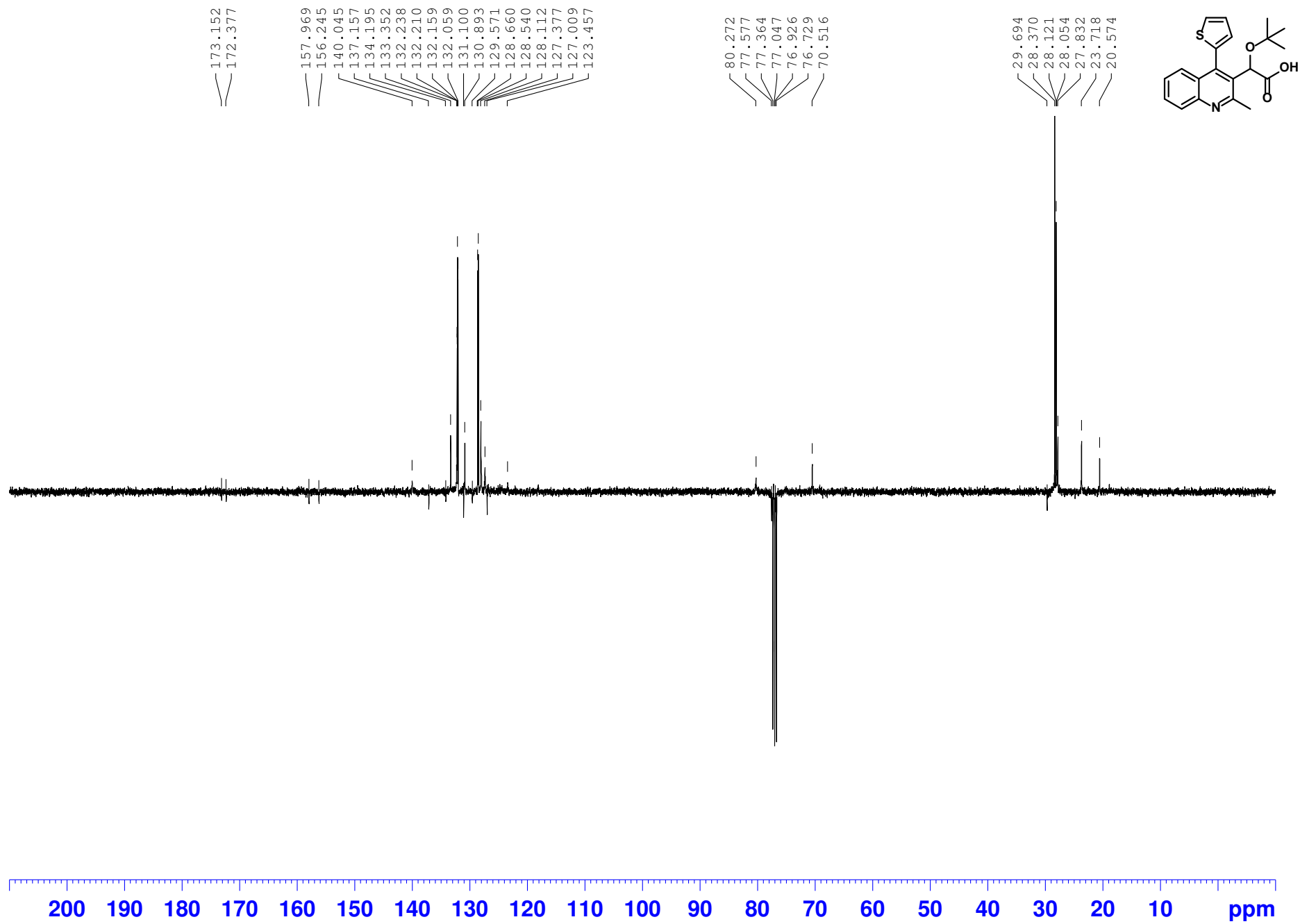
AH-3-55A characterization (CDC13, 400MHz)

MISSISS

NAME AH-3-55
EXPNO 20
PROCNO 1
Date_ 20171130
Time 22.52 h
INSTRUM spect
PROBHD z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894966 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
SI 65536
SF 400.1700087 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



AH-3-55 Characterization



Mass Spectrum List Report

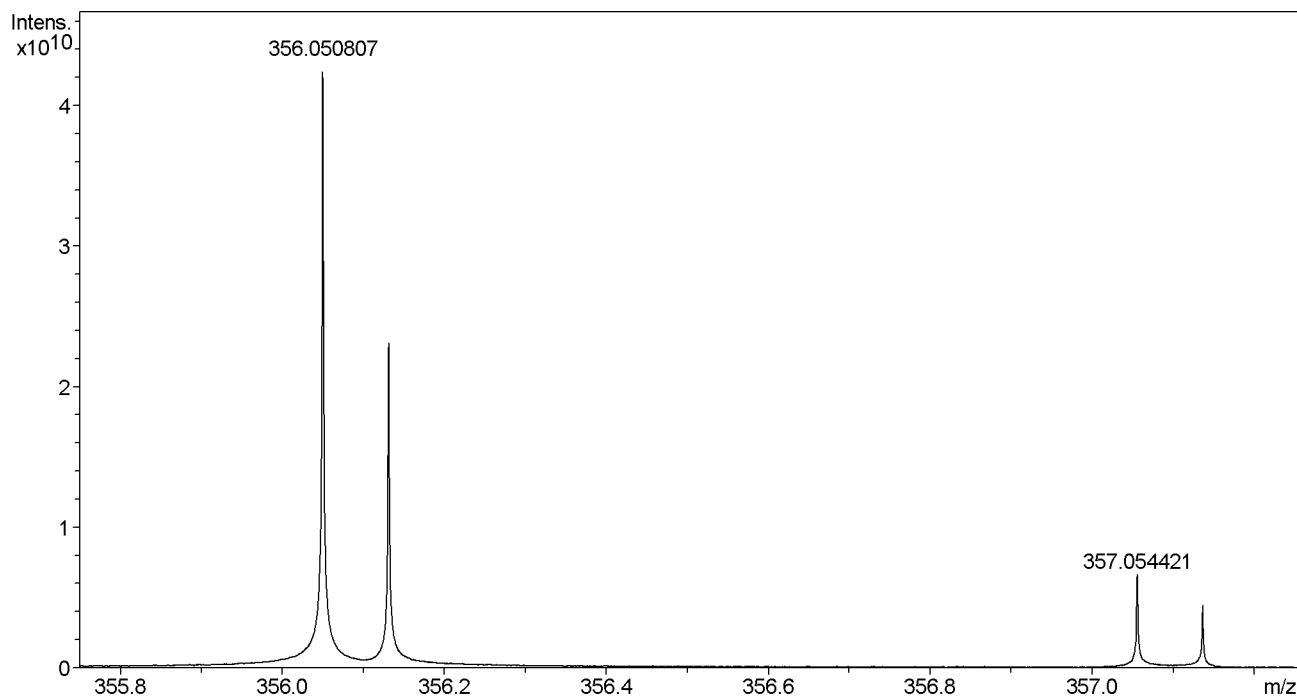
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\AH-3-55_pos_000003.d
Method
Sample Name AH-3-55
Comment AH-3-55 in THF:MeOH C20H21NO3S H+

Acquisition Date 3/19/2018 10:24:26 AM
Operator FTMS_USER
Instrument apex-Qe

Sample Name AH-3-55 in THF:MeOH
Exact Mass of C20H21NO3S H+ = 356.131491 m/z
Mass Observed = 356.131781 m/z

Difference < 1.0 ppm



#	m/z	I
1	190.982384	100791272
2	191.028985	118010564
3	200.023558	121617396
4	209.441826	91227211
5	222.259533	149105122
6	224.990068	105241373
7	230.154239	545323291
8	231.157628	134842810
9	237.578652	103007233
10	264.115328	103691225
11	269.165240	552915918
12	270.168589	146631266
13	272.201258	970610822
14	273.204571	122169049
15	274.144034	19338379718
16	275.147502	3942053969
17	276.150928	133119766
18	279.092649	376951231
19	279.093746	1090015694
20	280.097040	177519169

Mass Spectrum List Report

#	m/z	I
21	281.977268	89399750
22	286.216969	253481730
23	290.139146	207253201
24	296.595648	166842105
25	298.255695	1389347443
26	300.196331	128576342
27	301.075540	26715696880
28	302.078990	6187550558
29	302.175535	546942977
30	302.211879	212734788
31	303.082416	410616365
32	303.178937	95245067
33	308.105306	501501766
34	310.092920	115150235
35	310.102332	152475303
36	311.137091	105388774
37	312.107338	990497510
38	312.108530	1330137867
39	312.119662	2488929367
40	312.120995	5675650173
41	312.141848	32055332592
42	313.111887	207892986
43	313.123215	455082841
44	313.124508	559448960
45	313.144040	1271465433
46	313.145453	3439724032
47	314.136643	363437778
48	314.137977	651869946
49	314.148950	285020245
50	314.248417	163638432
51	315.141416	96408731
52	316.191282	289498031
53	316.226453	216877126
54	316.227756	201910386
55	322.253435	237436161
56	323.041724	354407953
57	324.045083	105138914
58	324.174956	664962917
59	324.176356	1397917596
60	324.232745	103981187
61	325.179805	208844687
62	326.136845	294027889
63	326.248430	99359903
64	330.206874	685254886
65	331.050665	155957378
66	331.210186	177918903
67	334.103023	333358087
68	334.253435	915512813
69	335.256731	182975103
70	336.173010	203773929
71	336.196360	166804460
72	336.269127	554661996
73	337.272403	137258049
74	338.248383	704678577
75	339.251801	166835395
76	340.152463	661539905
77	341.155810	145613715
78	342.035531	136291527
79	343.144690	220785041
80	346.165482	98969120
81	346.201889	129616816
82	356.050807	43103255635
83	356.131781	23206004002
84	357.054421	6663169716

Mass Spectrum List Report

#	m/z	I
85	357.135328	4429836033
86	358.057871	291506913
87	358.127885	566415778
88	358.138963	204169912
89	358.274698	174055353
90	364.173625	195066126
91	365.960428	177441354
92	368.164382	730802432
93	368.166231	2649336072
94	368.425688	102858128
95	369.169610	465401631
96	370.126786	103349196
97	370.238234	141425606
98	374.173243	219310973
99	378.206936	109627934
100	378.316147	888760605
101	379.319562	234074416
102	380.186263	238329333
103	380.222662	211786314
104	380.295401	827863806
105	381.298755	224627072
106	382.150562	1289578860
107	383.153841	244584671
108	383.958472	390138534
109	384.148130	139452893
110	384.163476	160284635
111	384.254010	130495456
112	385.228212	150999002
113	386.269613	115186579
114	388.249032	119985912
115	389.115855	220042308
116	390.168142	288712320
117	390.316157	1307987351
118	391.319588	326689319
119	392.331908	122933401
120	392.942795	98818935
121	393.215564	210526772
122	398.098217	199113085
123	398.145583	475050062
124	398.215455	273531576
125	398.233317	98160435
126	398.269657	239360041
127	399.149202	130165749
128	399.207442	121270409
129	400.040805	43318525001
130	400.161741	444335201
131	400.284986	315960307
132	400.306742	131830959
133	401.044389	5589661041
134	401.164645	116237709
135	401.223035	633098743
136	402.047890	311438824
137	402.226470	188475987
138	406.310991	101086833
139	407.849418	124395688
140	408.166318	165376759
141	408.253969	112867831
142	411.825159	644938793
143	412.114021	143267573
144	412.150434	1138491459
145	412.194745	489994270
146	412.285340	105162630
147	413.198086	115110387
148	416.184076	155577443

Mass Spectrum List Report

#	m/z	I
149	416.280232	157113458
150	418.163169	508951890
151	418.257025	167665327
152	419.166610	116896754
153	420.236305	352847690
154	422.023158	200643212
155	424.246550	1270825588
156	425.249957	306762872
157	425.288077	114839675
158	426.183282	141571542
159	426.225753	179249583
160	426.264586	97689075
161	426.646947	94357922
162	428.072488	1403342346
163	428.108814	127097641
164	428.205068	186393480
165	429.075803	256352925
166	430.199701	172644811
167	434.158161	592582190
168	434.378943	142713106
169	435.161693	126497320
170	435.184207	156877261
171	435.345206	176701281
172	436.267775	99603819
173	436.285421	98661707
174	438.225843	290157985
175	438.262327	211555814
176	440.243944	517509684
177	440.316672	556569533
178	441.247261	168647262
179	441.320060	192793692
180	442.088223	158720869
181	442.124596	416138387
182	442.220800	1163642810
183	443.127871	93218837
184	443.197343	447261378
185	443.224140	199257037
186	443.270061	185626005
187	445.213293	93416326
188	446.378971	285155372
189	447.257043	93690370
190	447.382331	99023205
191	452.277885	867567786
192	453.281222	238581458
193	456.103835	3389570831
194	456.236443	2085866067
195	457.107191	606967058
196	457.239824	427925641
197	457.285772	386606213
198	458.254584	667482378
199	458.289353	140569623
200	458.327330	247340910
201	459.257892	170090889
202	459.301354	384865626
203	460.304840	103480973
204	462.189548	224884409
205	466.293616	137551680
206	468.348107	327756709
207	469.351445	95337665
208	470.203143	213139386
209	470.215800	310706356
210	472.231328	5368846075
211	473.234759	1014357245
212	474.238275	112619350

Mass Spectrum List Report

#	m/z	I
213	476.265113	992549134
214	476.278155	438507974
215	477.268578	239038098
216	477.281631	139468603
217	479.133744	807675105
218	480.137111	226700204
219	480.309299	882201028
220	481.131741	825486450
221	481.312681	267022791
222	482.135073	233801596
223	483.190047	152186122
224	483.210927	104840550
225	484.231516	114694949
226	484.267994	115579779
227	486.358895	133018311
228	488.213793	124662884
229	489.257913	240358544
230	493.185990	117575380
231	493.226198	319040893
232	494.251644	164620698
233	494.288536	1894484035
234	494.325017	1907197674
235	494.364568	125822329
236	495.291948	531079702
237	495.328448	536289443
238	496.231624	122256383
239	496.331799	97699794
240	496.379503	101864913
241	498.247376	101962767
242	498.283453	457777773
243	498.395025	105327958
244	499.172296	654424436
245	499.286769	116786207
246	500.175758	206760478
247	501.275744	678745405
248	502.279013	227632262
249	503.291382	259322687
250	504.309386	570687990
251	505.312685	158536185
252	508.162150	98050073
253	508.340730	428968039
254	509.344124	161144419
255	512.299348	207729092
256	515.150052	97449187
257	516.332996	228445945
258	520.304438	110725574
259	522.319942	995726059
260	522.356807	115491744
261	523.324353	462129587
262	524.328269	126502858
263	527.120059	538051758
264	527.146943	174827054
265	528.123269	175391093
266	529.145154	149817488
267	529.182816	119896926
268	530.642575	401670742
269	531.122292	308833778
270	531.144183	206196733
271	532.125584	98717844
272	532.327786	520070581
273	532.340899	327509786
274	535.236857	280274420
275	536.372046	1947625768
276	537.175466	108004780

Mass Spectrum List Report

#	m/z	I
277	537.190649	420046894
278	537.375420	614368747
279	538.193862	159026912
280	539.173794	109198681
281	539.272207	130641795
282	540.294322	99418717
283	543.322645	108778309
284	548.335741	151225806
285	550.387817	171028255
286	554.309696	13353936129
287	555.313238	3494250650
288	556.316446	395931143
289	557.250910	130523285
290	557.490889	125507350
291	560.372156	143800281
292	563.188737	612748606
293	564.191986	272370986
294	564.403486	897542538
295	565.406832	286573929
296	568.325739	190957112
297	569.121664	113223853
298	569.166999	266609799
299	569.250876	139328115
300	571.136878	738982721
301	571.354237	152064299
302	572.140256	215167135
303	573.135035	506027007
304	574.138315	156205208
305	575.132079	204790266
306	576.153966	279342976
307	576.655515	181589112
308	578.419860	131854706
309	579.162295	18023850741
310	579.187602	1600071483
311	580.165770	6287968053
312	580.192130	455066449
313	581.169098	855465637
314	581.184492	721248490
315	582.187718	270379709
316	583.182763	151471519
317	585.198059	268349903
318	585.245747	1747596775
319	585.320251	182262835
320	586.248787	499909460
321	587.243234	201088989
322	587.252019	129323093
323	590.195091	14163250935
324	590.419832	257134215
325	591.198336	4572972449
326	592.192732	1371203909
327	592.201878	819783916
328	592.434844	210493291
329	593.196133	437369096
330	594.377898	208865159
331	596.356983	135292448
332	601.240711	1086567491
333	602.243651	409693572
334	603.238287	148306744
335	605.030734	224387265
336	606.173079	365520738
337	606.450474	111567052
338	607.028701	223890232
339	607.176184	149365931
340	607.227676	316806935

Mass Spectrum List Report

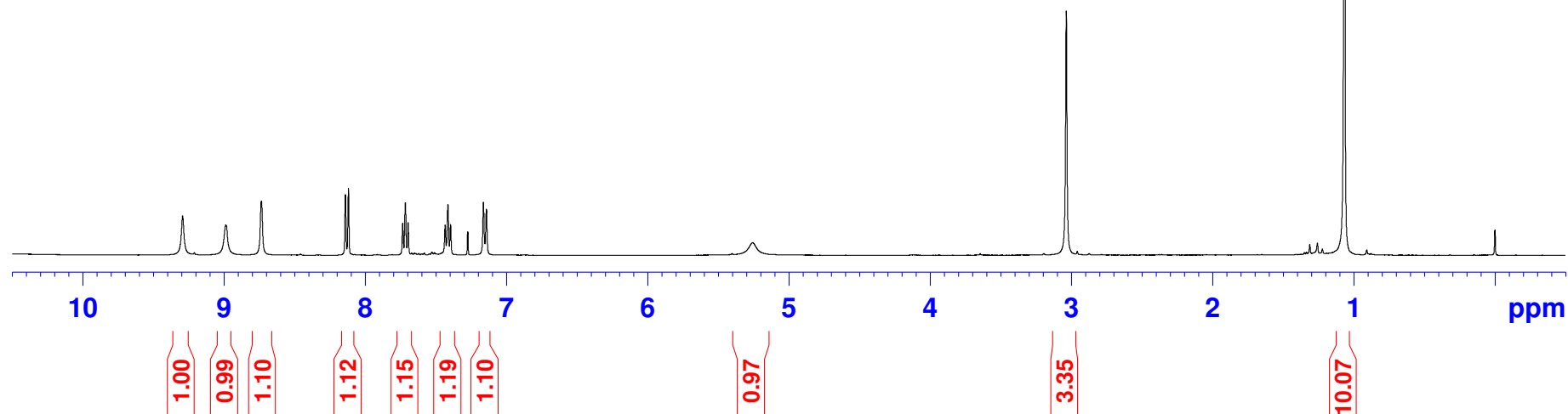
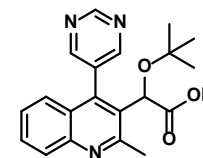
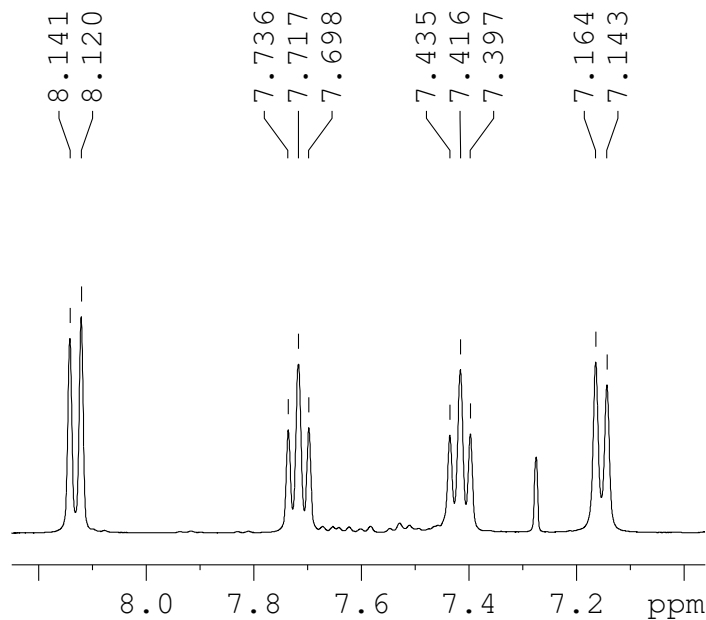
#	m/z	I
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342	610.559469	488354581
343	610.893662	415453270
344	611.226609	281959650
345	611.559957	251529411
346	611.893148	114762599
347	612.225358	380059139
348	612.727785	107258563
349	615.891206	211725815
350	616.225482	185483253
351	616.557513	147948025
352	616.891925	131072701
353	617.218238	257750499
354	618.221816	96105525
355	622.145167	421061425
356	623.148175	146237389
357	623.222739	1914662320
358	624.225720	702091865
359	625.220898	229194219
360	627.172976	139803283
361	627.269105	161184222
362	629.188437	291761933
363	630.139716	272527721
364	630.191561	111034372
365	631.142824	98551421
366	632.136297	114619258
367	639.200443	143232585
368	645.217428	151704053
369	652.524987	150819323
370	652.859581	136475250
371	653.163956	314414841
372	653.525306	109193173
373	654.167290	146031700
374	657.279719	143854721
375	661.133676	221410110
376	661.174737	121783051
377	662.252991	281932553
378	663.171997	100039371
379	663.256072	105946074
380	667.233723	101427850
381	669.219722	736823715
382	670.223230	277807724
383	671.295485	99398896
384	691.360584	230003890
385	692.363718	126387681
386	695.147867	195711907
387	700.097515	163054664
388	703.255202	110682845
389	703.589424	95521036
390	703.923441	113258116
391	705.083550	404061242
392	705.376219	261602917
393	706.087174	152019348
394	707.081677	387776808
395	708.084712	127998763
396	713.342455	360958155
397	714.345638	135587020
398	721.371820	96817938
399	727.358109	786165824
400	728.361555	332637970
401	733.124169	110125268
402	782.191769	178602920
403	783.195040	114726241
404	805.771521	563351161

Mass Spectrum List Report

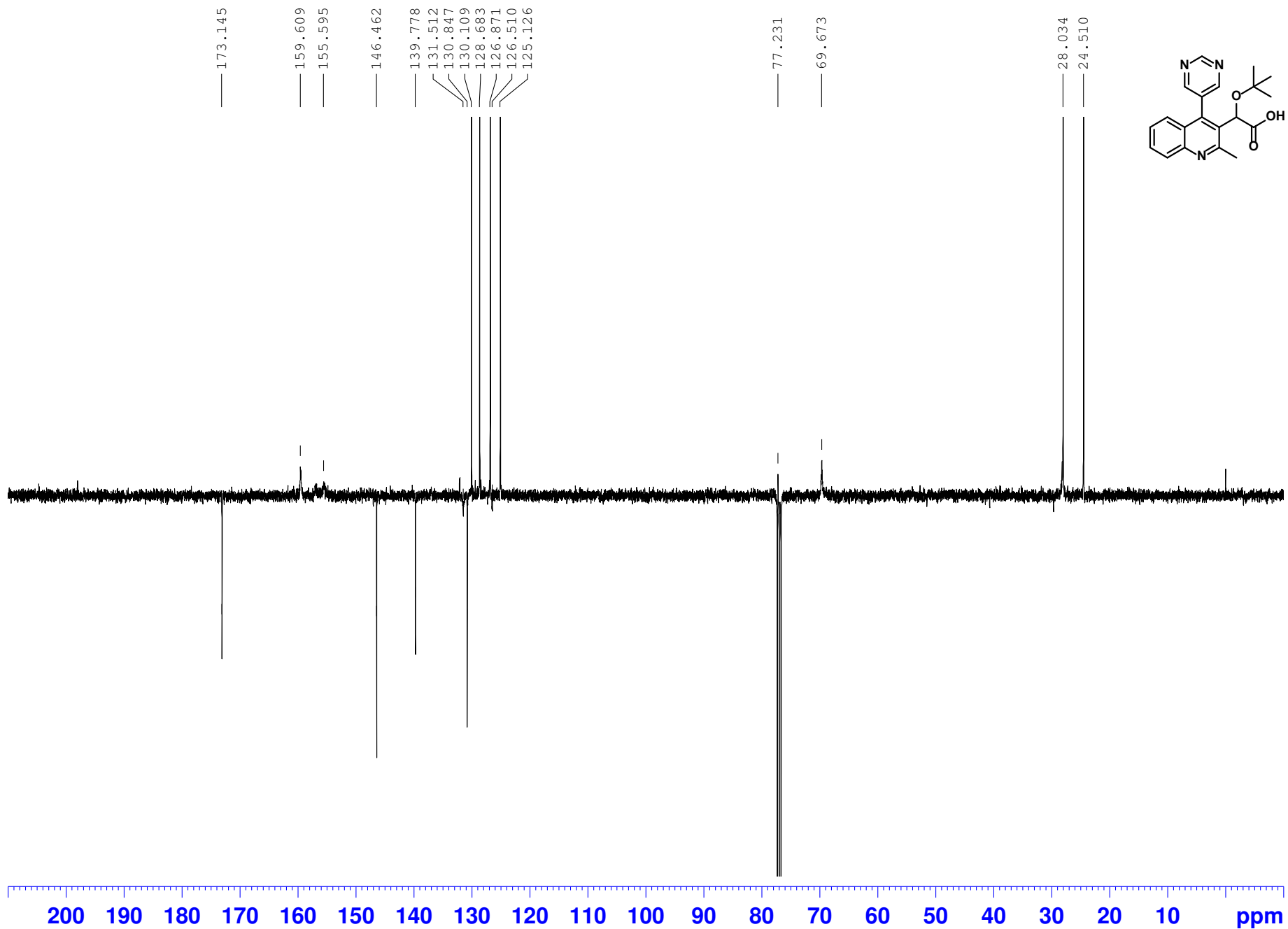
#	m/z	I
405	806.187689	150788924
406	868.282562	93489251
407	884.259874	219215513
408	885.263210	125074969

NGJ-9-005 (CDC13, 400 MHz) Pure Yellow Oil - saponification of pyrimidine quinoline

NAME NGJ-9-005
 EXPNO 20
 PROCNO 1
 Date_ 20171128
 Time_ 17.09 h
 INSTRUM spect
 PROBHD Z108618_0161 (
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.244532 Hz
 AQ 4.0894966 sec
 RG 101
 DW 62.400 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1
 SFO1 400.1724710 MHz
 NUC1 1H
 P1 9.88 usec
 SI 65536
 SF 400.1700033 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



NGJ-9-005 (CDC13, 400 MHz) Pure Yellow Oil - saponification of pyrimidine quinoline



Mass Spectrum List Report

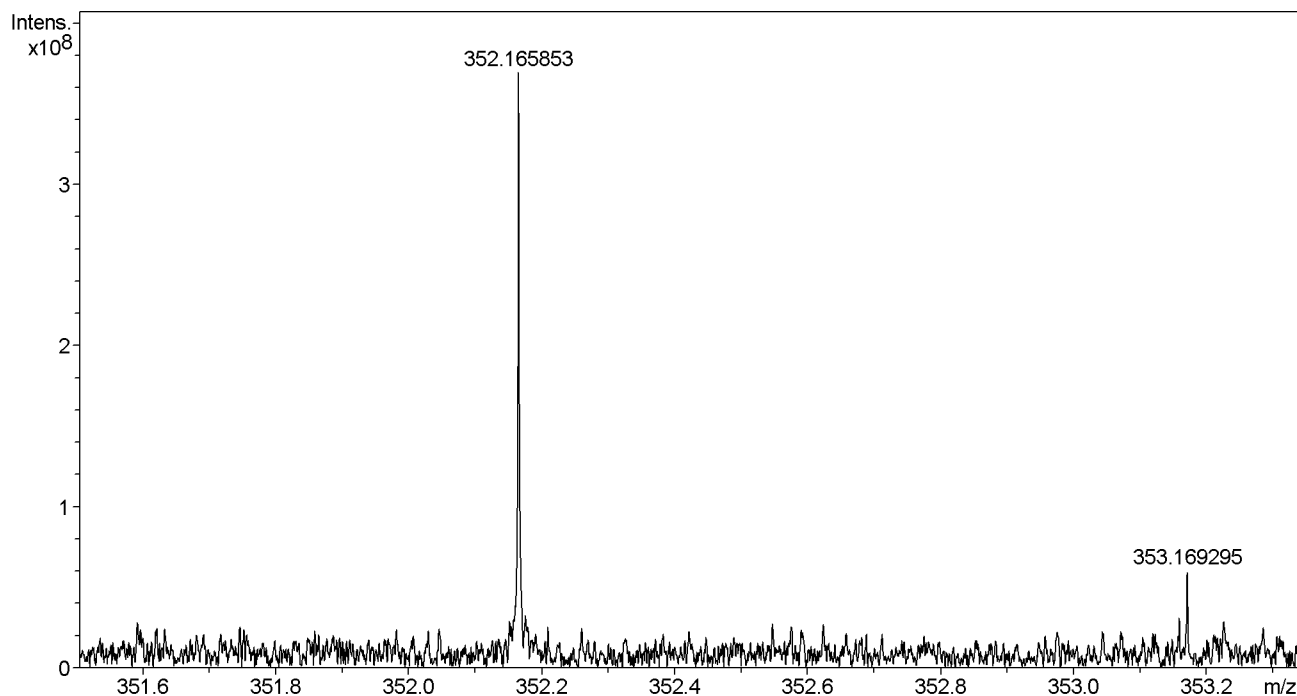
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-9-005_pos_000002.d
Method
Sample Name NGJ-9-005
Comment NGJ-9-005 in THF:MeOH C20H21N3O3 H+

Acquisition Date 3/19/2018 2:46:37 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-9-005 in THF:MeOH
Exact Mass of C20H21N3O3 H+ = 352.165568 m/z
Mass Observed = 352.165853 m/z

Difference < 1.0 ppm



#	m/z	I
1	184.390863	67087584
2	190.061855	122585753
3	202.340528	111540498
4	215.089214	127729295
5	231.120554	93255337
6	245.099778	155489750
7	269.136194	79859806
8	283.115540	54971893
9	285.131084	87659990
10	301.126046	99162811
11	301.162414	103285459
12	303.141754	151939195
13	304.097121	69602208
14	314.342045	60310319
15	317.120971	163943113
16	340.394067	66492255
17	352.165853	369545031
18	353.169295	60633698
19	354.409702	74856905
20	360.323956	394454146

Mass Spectrum List Report

#	m/z	I
21	361.327363	102415768
22	364.191048	601908299
23	365.194430	148341724
24	370.404645	216014035
25	371.408042	54846767
26	374.303289	62136669
27	375.199250	123830838
28	376.318952	101866627
29	378.170348	86801343
30	386.172994	59256300
31	392.313881	79370098
32	393.209804	89026406
33	393.297706	63301472
34	396.180929	185945316
35	398.241788	1139341613
36	399.245155	215201491
37	400.152146	62235753
38	405.188663	53179004
39	408.180920	967759029
40	408.308892	56347667
41	409.184335	221548455
42	409.219931	53949304
43	410.436010	62994706
44	412.451626	56790503
45	413.266645	88594742
46	425.139710	53741156
47	425.287816	392711535
48	426.291171	80455418
49	426.467405	66108890
50	433.157776	53062908
51	435.344870	487715148
52	436.348226	127183970
53	437.236067	89296974
54	452.519338	88392021
55	468.514316	84484640
56	469.517507	58220955
57	480.091626	55860748
58	480.550782	227176706
59	481.262297	58406691
60	481.553909	67453892
61	491.116757	121829877
62	493.113875	69468497
63	493.175454	150758674
64	494.178881	52517549
65	494.566419	89696950
66	496.545740	126023516
67	497.548983	64524183
68	508.582062	1154969094
69	509.585464	418918274
70	510.588924	73189514
71	520.582141	85141940
72	522.597750	173724685
73	523.143037	93671338
74	523.601260	78173829
75	524.576995	669062636
76	525.140052	63897725
77	525.376642	72668031
78	525.580407	248382685
79	536.613330	3982996837
80	537.395430	144827258
81	537.616778	1385023266
82	538.592967	58412419
83	538.620187	238548447
84	550.592855	138658589

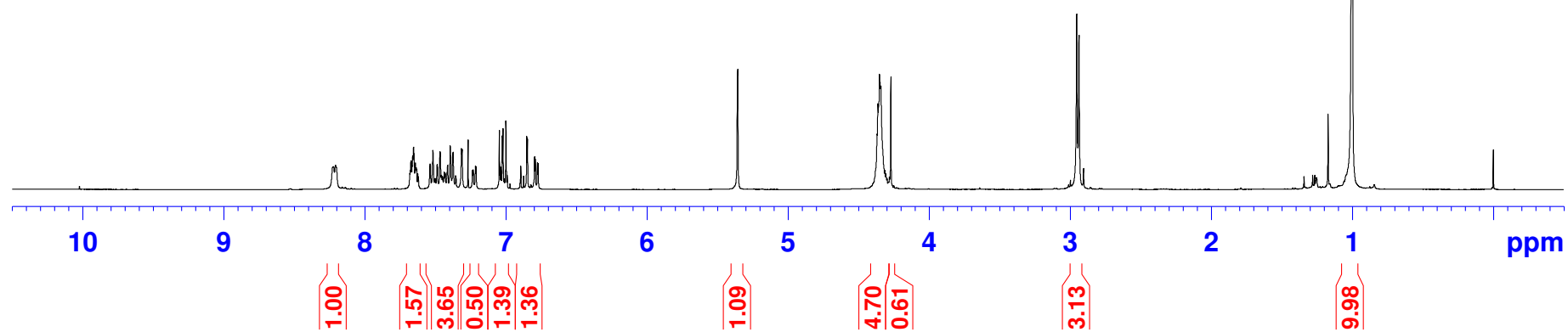
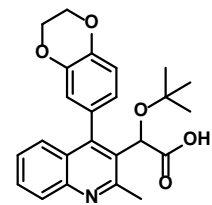
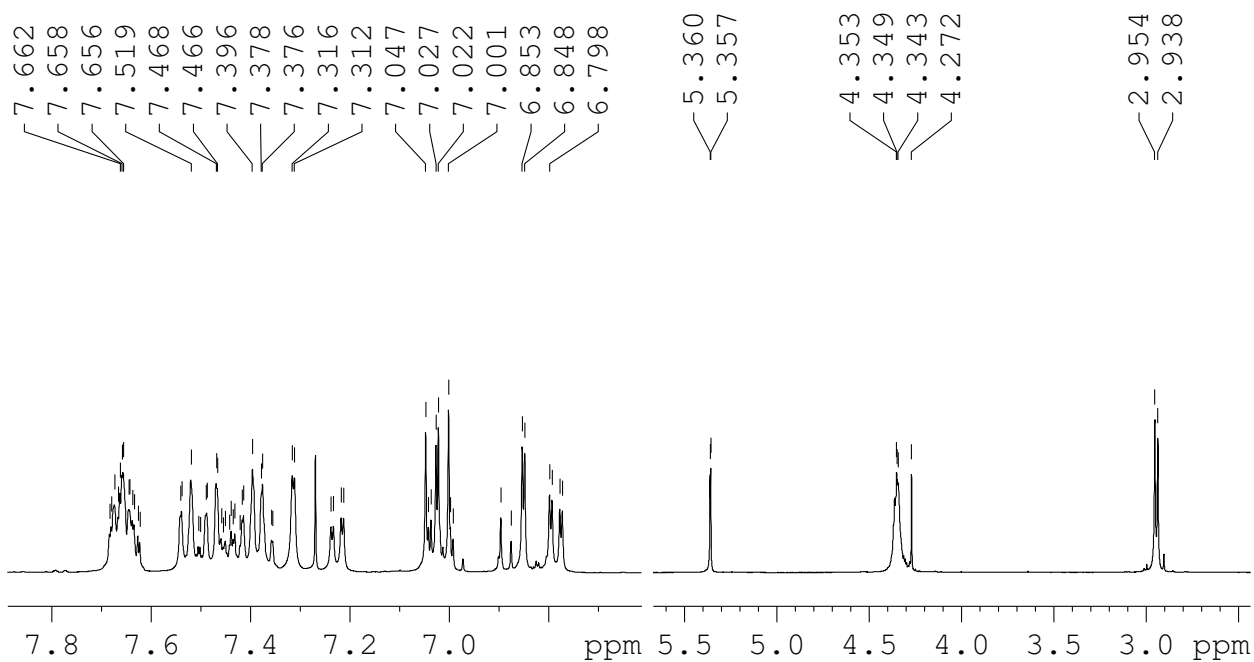
Mass Spectrum List Report

#	m/z	I
85	550.629251	142877305
86	551.632271	65390563
87	552.608284	2073660361
88	553.390342	100002381
89	553.611674	735704355
90	554.615041	109063301
91	564.644699	1413089722
92	565.648116	509583368
93	566.587883	77279227
94	566.651390	113583425
95	568.603424	68931313
96	569.402843	107559567
97	572.234969	114697549
98	578.624000	64558791
99	578.660330	107099371
100	580.639647	499978052
101	581.642930	204487561
102	592.676007	1847766520
103	593.679413	747142656
104	594.682694	145174211
105	599.548926	430502774
106	600.552204	154396761
107	606.655277	82821742
108	608.671047	529991582
109	609.674280	229172126
110	610.677766	52805751
111	613.429095	156730459
112	614.432682	52517985
113	620.707510	145625281
114	621.710913	63367009
115	642.630407	57961890
116	648.738848	81113449
117	655.439650	80696225
118	657.455470	277961339
119	658.458799	93361917
120	685.436297	211850411
121	686.439605	103433439
122	699.466319	67497285
123	700.469196	53375762
124	701.481739	190982106
125	702.484923	70531976
126	745.507782	88578639
127	861.540920	71021492
128	877.536500	110838930
129	878.540620	75853257

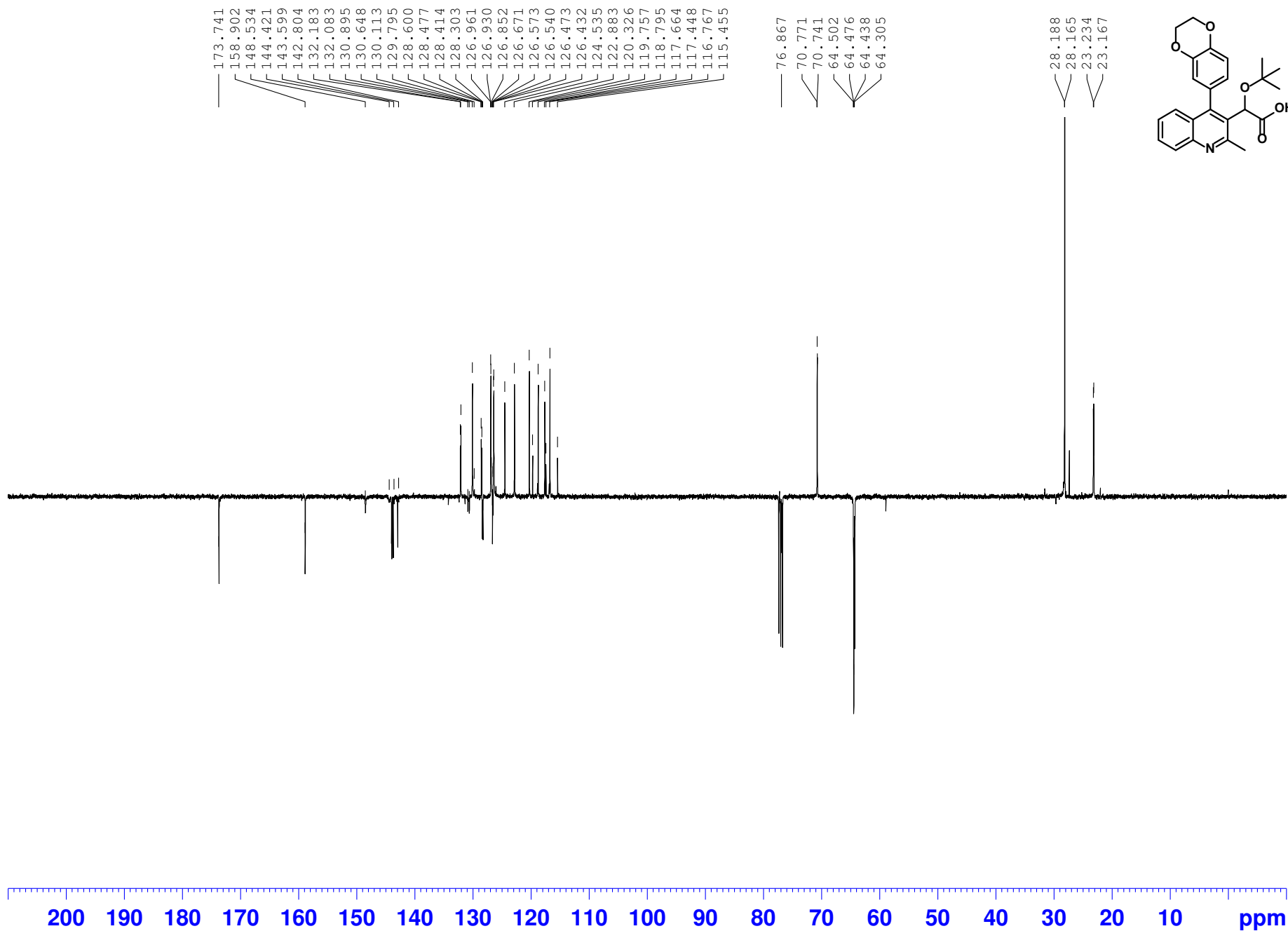
NGJ-9-002 (CDC13, 400 MHz) Pure Red/Brown Oil - saponification of benzodioxane

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NAME      NGJ-9-002
EXPNO     50
PROCNO    1
Date_     20180208
Time      18.07 h
INSTRUM   spect
PROBHD    Z108618_0161 (
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS        16
DS        2
SWH       8012.820 Hz
FIDRES    0.244532 Hz
AQ        4.0894966 sec
RG        80.6
DW        62.400 usec
DE        6.50 usec
TE        298.2 K
D1        1.00000000 sec
TD0       1
SF01      400.1724710 MHz
NUC1      1H
P1        9.88 usec
SI        65536
SF        400.1700057 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
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NGJ-9-002 (CDC13, 400 MHz) Pure Red/Brown Oil - saponification of benzodioxane



Mass Spectrum List Report

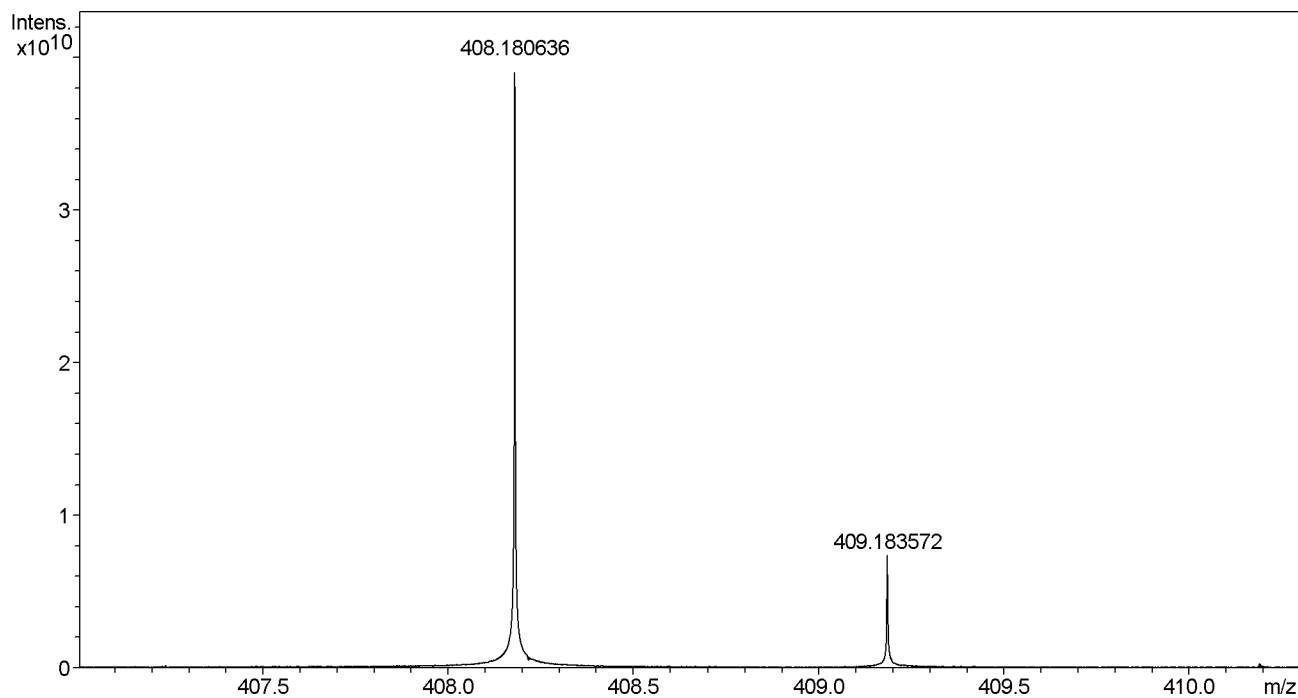
Analysis Info

Analysis Name F:\MS1-091514 - 080917\Data\apexdata031918\NGJ-9-002_pos_000003.d
Method
Sample Name NGJ-9-002
Comment NGJ-9-002 in THF:MeOH C24H25NO5 H+

Acquisition Date 3/19/2018 2:31:18 PM
Operator FTMS_USER
Instrument apex-Qe

Sample Name NGJ-9-002 in THF:MeOH
Exact Mass of C24H25NO5 H+ = 408.180549 m/z
Mass Observed = 408.180636 m/z

Difference < 1.0 ppm



#	m/z	I
1	186.031046	431823987
2	186.554638	1560984987
3	186.557349	174630460
4	198.093353	282319933
5	204.093554	167354969
6	209.441469	98643343
7	227.793384	258517694
8	251.592600	240919932
9	251.593399	178228601
10	285.520706	355783736
11	289.109995	100862974
12	290.117864	154048873
13	293.109512	188282766
14	294.112968	168555969
15	301.075763	2984045873
16	302.079189	394280523
17	303.131719	152713886
18	304.097339	176703571
19	304.900352	1960503372
20	304.901583	446712117

Mass Spectrum List Report

#	m/z	I
21	306.113068	267996819
22	308.475828	174068456
23	336.981422	193057935
24	338.139381	163777228
25	339.130423	210976504
26	347.584107	1062231701
27	352.567557	225634449
28	359.081428	273667731
29	363.193235	805248396
30	364.190861	828503970120
31	365.194247	152982509087
32	366.198004	9210665141
33	367.198775	318819003
34	367.201891	396914683
35	375.972059	300841881
36	378.170620	5222592751
37	378.207383	499076032
38	379.171787	262510169
39	379.174201	940671770
40	379.181762	3242260944
41	380.186538	341622416
42	381.363988	253483122
43	382.464167	23935140382
44	386.173395	843710261
45	387.176863	229682489
46	394.200048	2218677619
47	394.201589	7342936280
48	395.204414	3299222680
49	396.180589	107272862894
50	397.182548	1735266749
51	397.184137	6689786631
52	398.186591	605964121
53	400.151494	514886736
54	406.237453	801640883
55	408.180636	39770927228
56	408.217188	712313147
57	408.221373	639597966
58	409.183572	7446352322
59	410.186220	244949004
60	410.188394	217093673
61	416.220822	135718632
62	416.223114	195362133
63	418.163576	251995396
64	430.162295	5592433234
65	431.166910	456353301
66	436.211253	10020935516
67	436.212970	6027826434
68	436.248181	299351220
69	436.256008	239453238
70	437.215147	4214055375
71	438.219759	271660737
72	450.225713	172753722
73	450.228625	506004289
74	450.262273	169591724
75	450.265048	477905845
76	451.231964	178628689
77	451.268499	140368858
78	452.145649	151515126
79	452.244315	222585051
80	458.195045	258700545
81	459.170738	181792964
82	464.243811	10665443503
83	465.243519	246219183
84	465.247516	1632761071

Mass Spectrum List Report

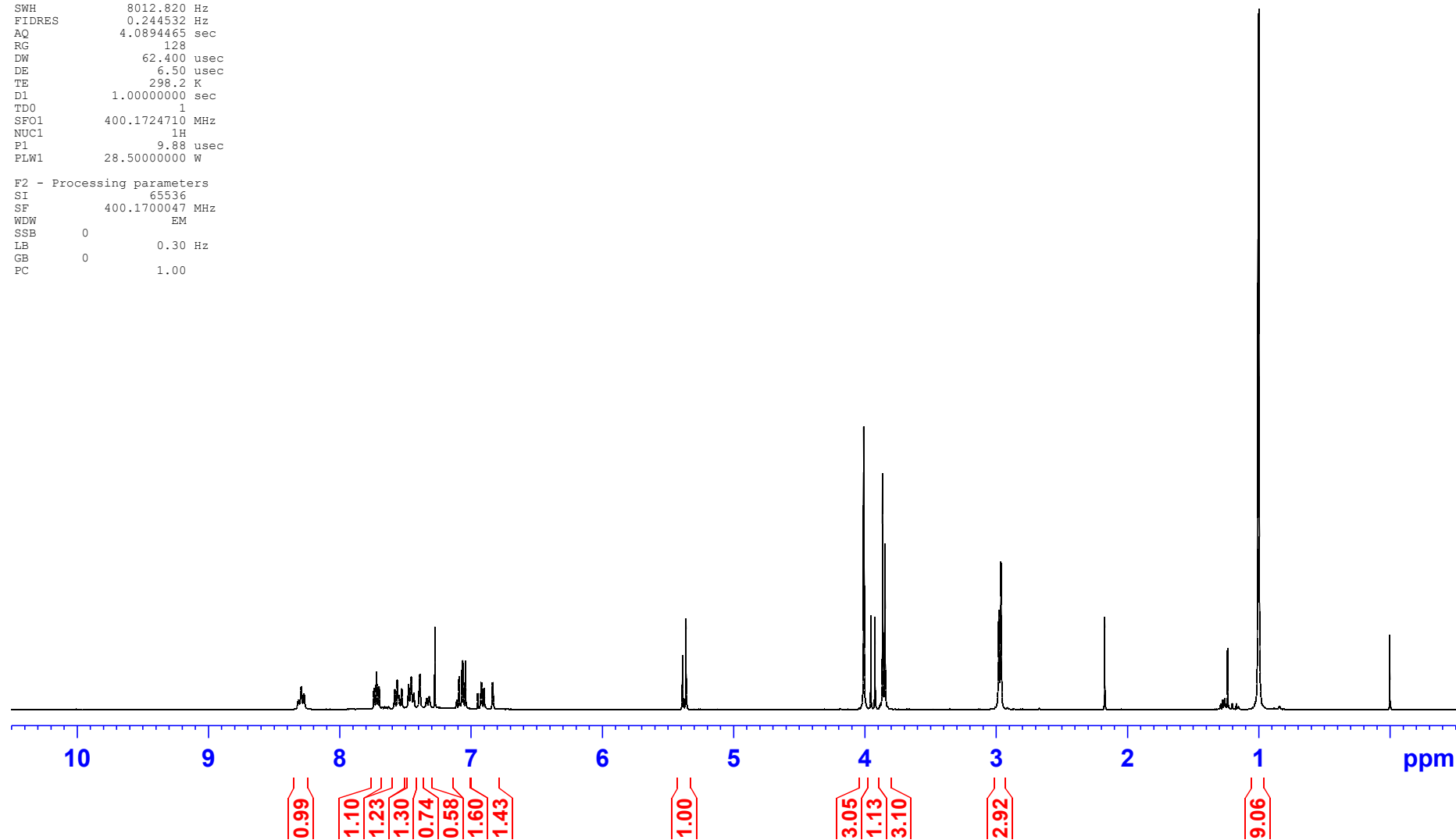
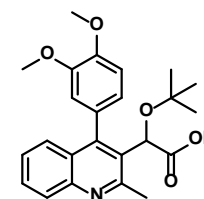
#	m/z	I
85	466.251049	194781406
86	477.181275	112294413
87	486.226423	164978972
88	492.275703	587294778
89	493.176251	605617278
90	493.279092	191998828
91	494.179652	180018600
92	533.244942	98082210
93	549.312481	124335330
94	563.189112	190115923
95	579.162691	1119242044
96	580.166250	3325924464
97	581.169683	475339683
98	581.258112	326429931
99	582.261749	115740241
100	583.255264	124708829
101	637.168663	341085528
102	638.171943	116643415
103	642.277851	457200313
104	643.281587	168439508
105	667.282248	1204743469
106	668.285748	534247766
107	669.288117	105113651
108	669.298185	119089246
109	700.284431	162486363
110	701.287765	299667724
111	702.291180	102434736
112	708.250565	281970586
113	709.254073	121598409
114	741.356057	117752908
115	769.350719	191238890

NGJ-9-092 (CDC13, 400 MHz) Pure Yellow Oil - saponification of 3,4-dimethoxyquinoline

Current Data Parameters
NAME NGJ-9-092
EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180708
Time_ 19.35 h
INSTRUM spect
PROBHD Z108618_0161 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1
SFO1 400.1724710 MHz
NUC1 1H
P1 9.88 usec
PLW1 28.50000000 W

F2 - Processing parameters
SI 65536
SF 400.1700047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NGJ-9-092 (CDC13, 400 MHz) Pure Yellow Oil- saponification of

