Electronic Supplementary Material (ESI) for ChemComm.

CuI-catalyzed Intramolecular Aminocyanation of Terminal Alkynes in *N*-(2-Ethynylphenyl)-*N*-sulfonylcyanamides *via* Cu-vinylidene Intermediates

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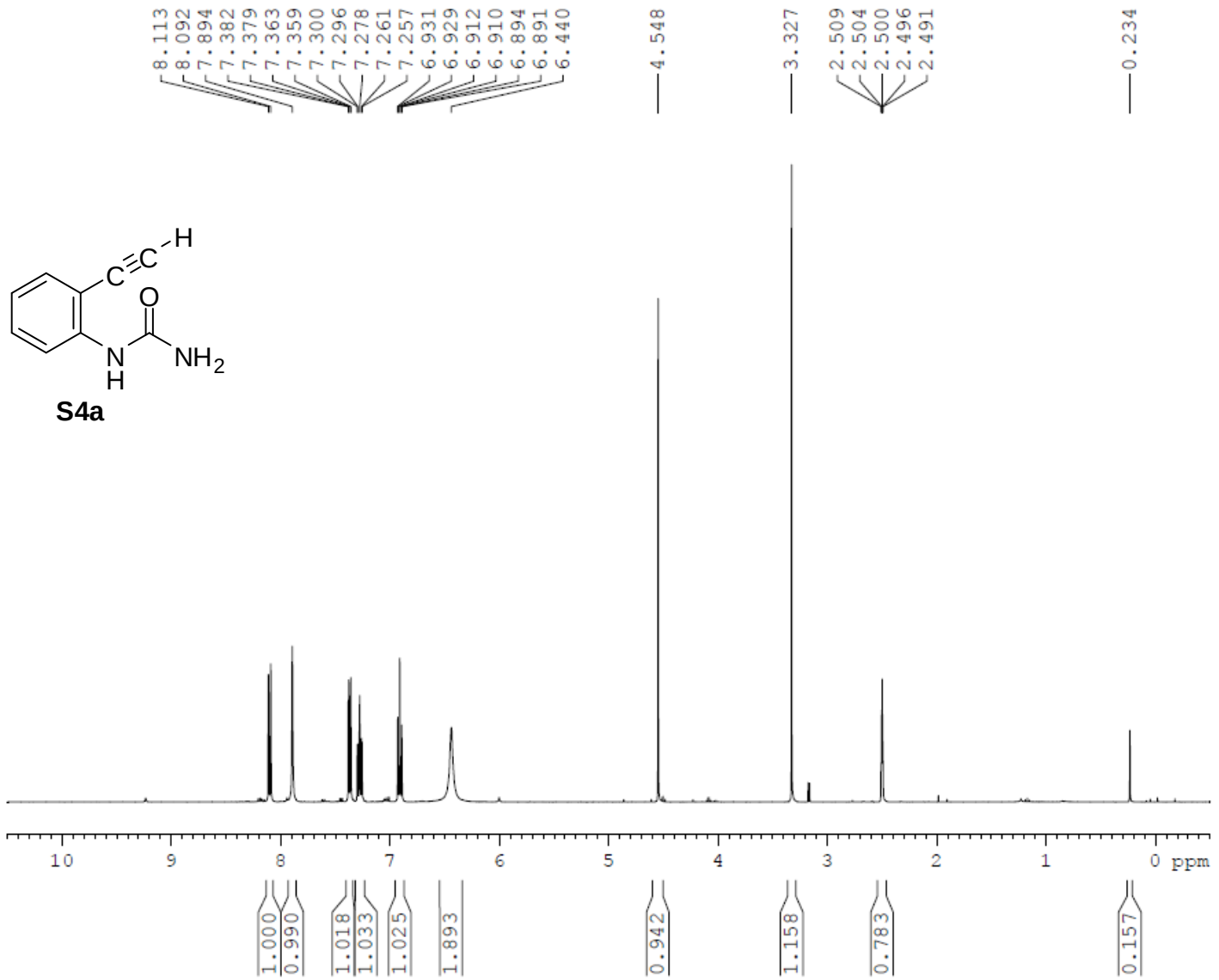


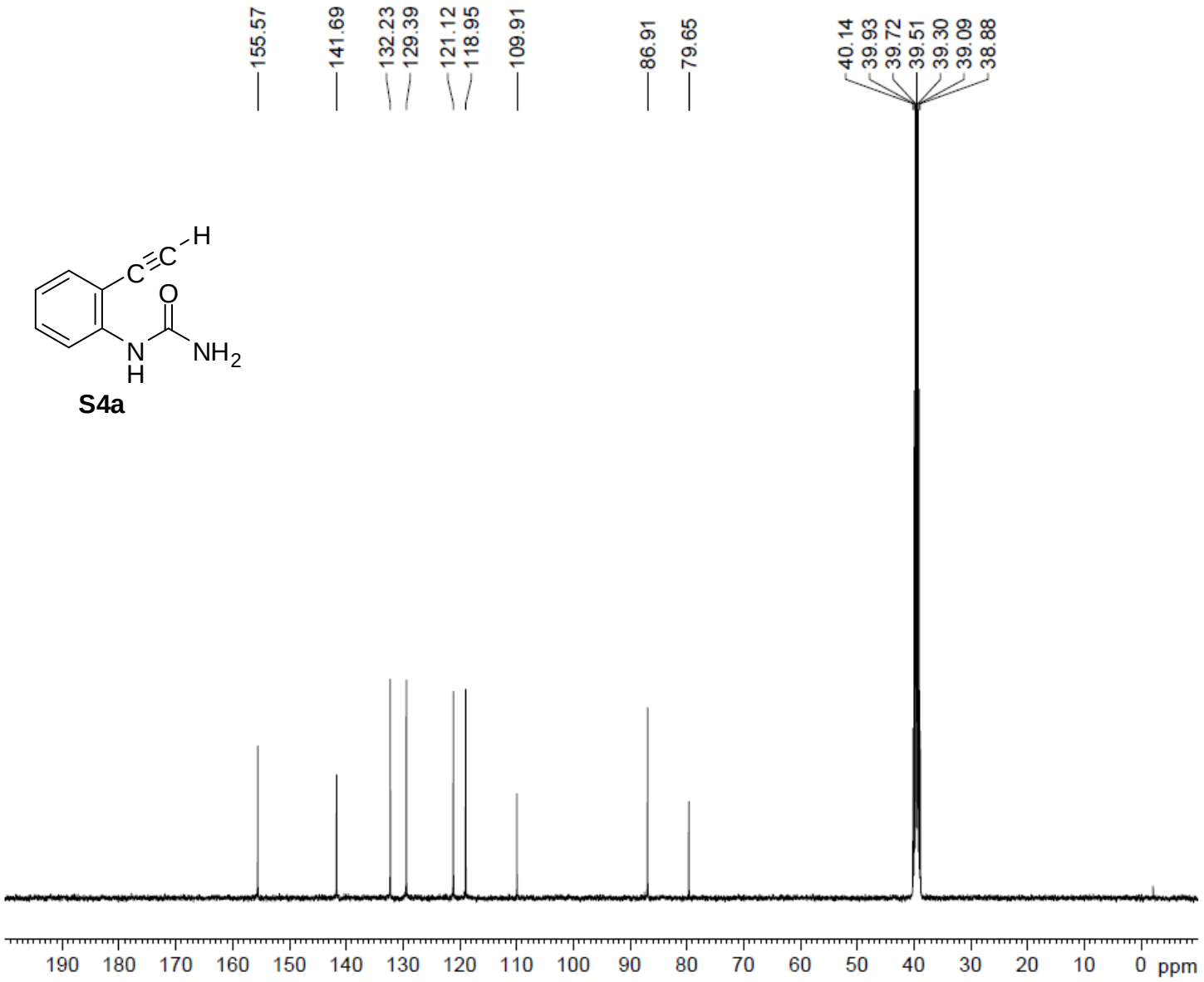
S4a

Current Data Parameters
NAME SO001
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141030
Time 8.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 298.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300032 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SO001
EXPNO 3
PROCNO 1

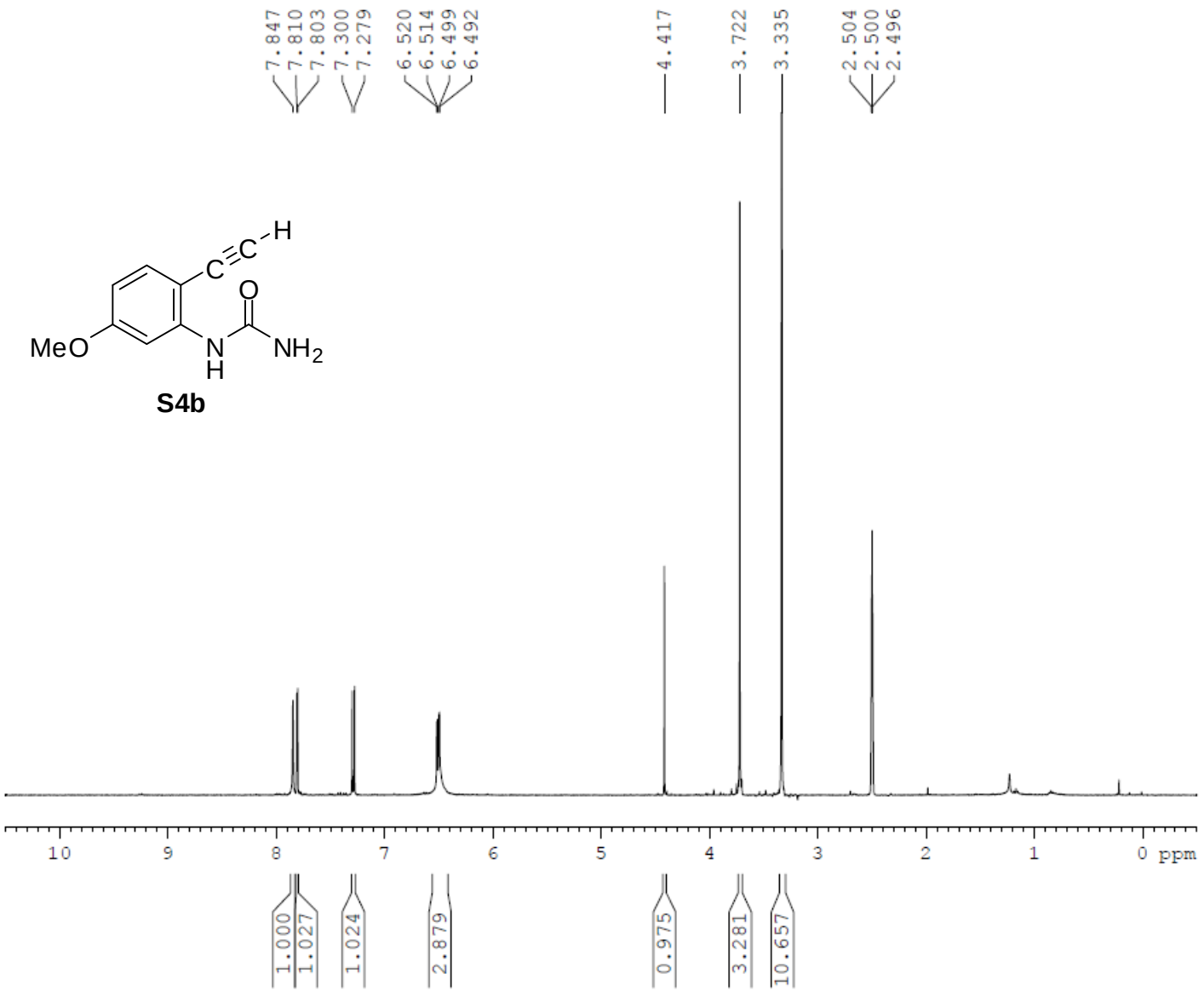
F2 - Acquisition Parameters
Date_ 20141030
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6128201 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

down point



S4b

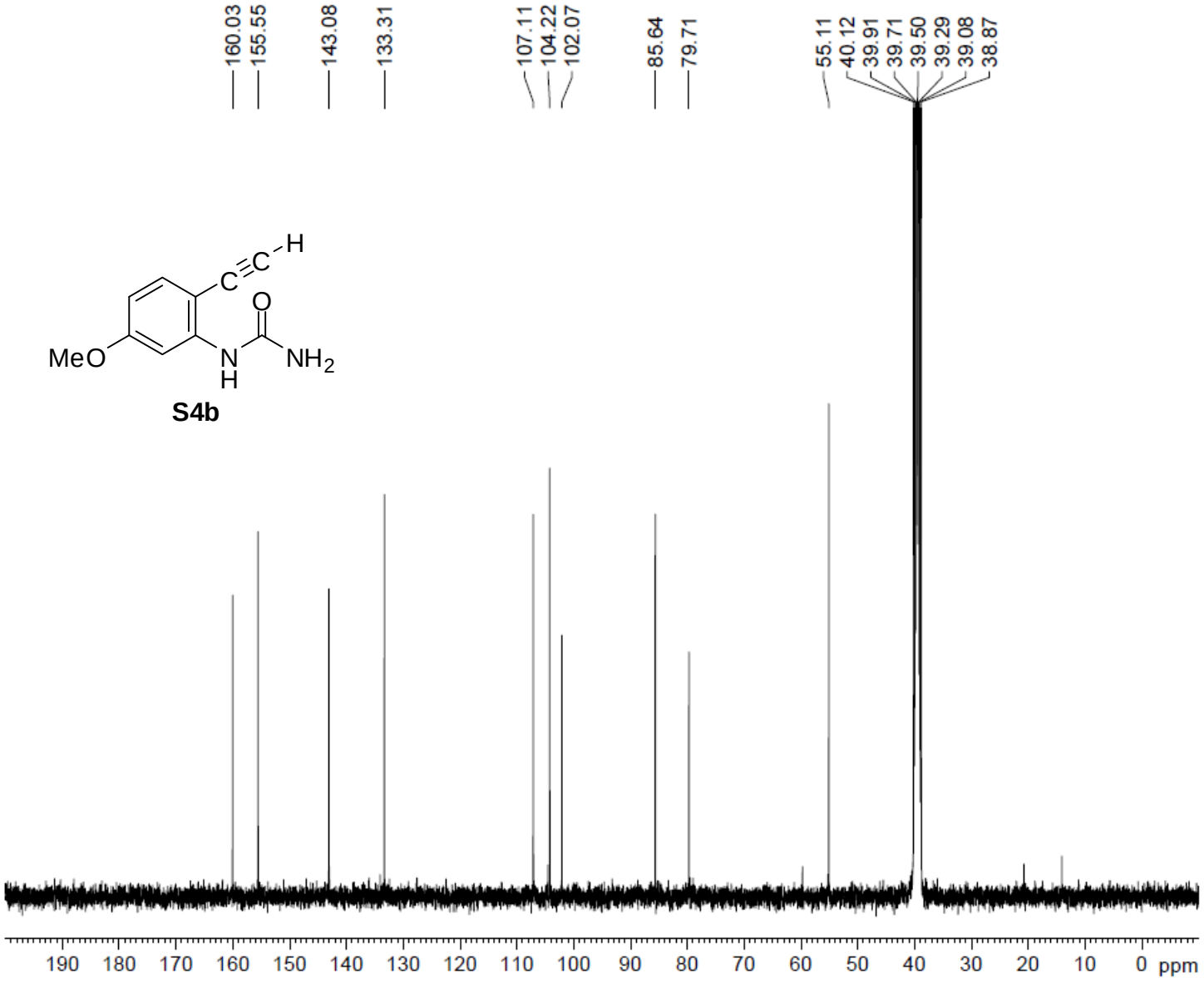
Current Data Parameters
NAME SD-086
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140613
Time 19.36
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 574.7
DW 69.000 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300044 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

down point pure



S4b

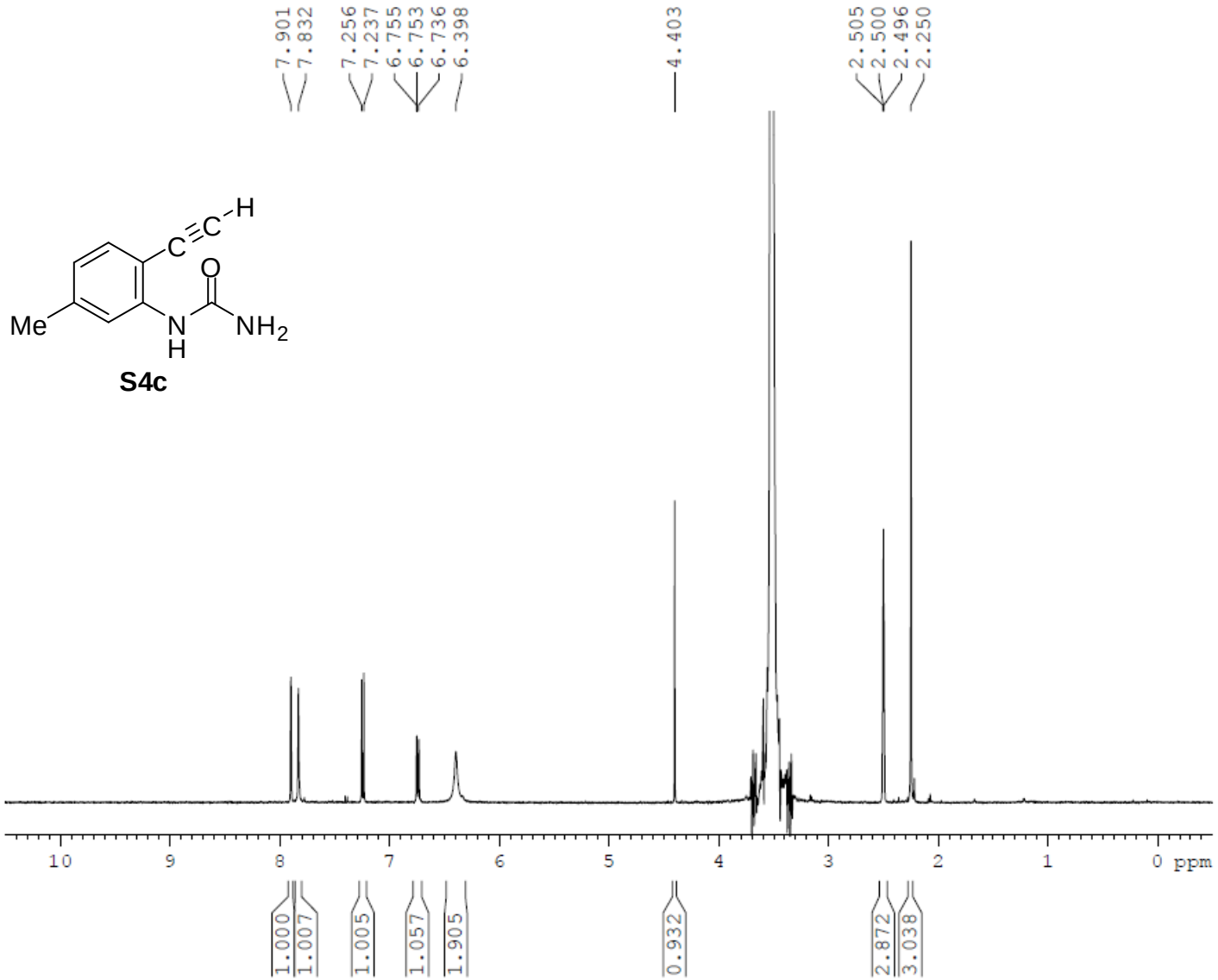
Current Data Parameters
NAME SD-086
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140615
Time 10.53
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 18965
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128186 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

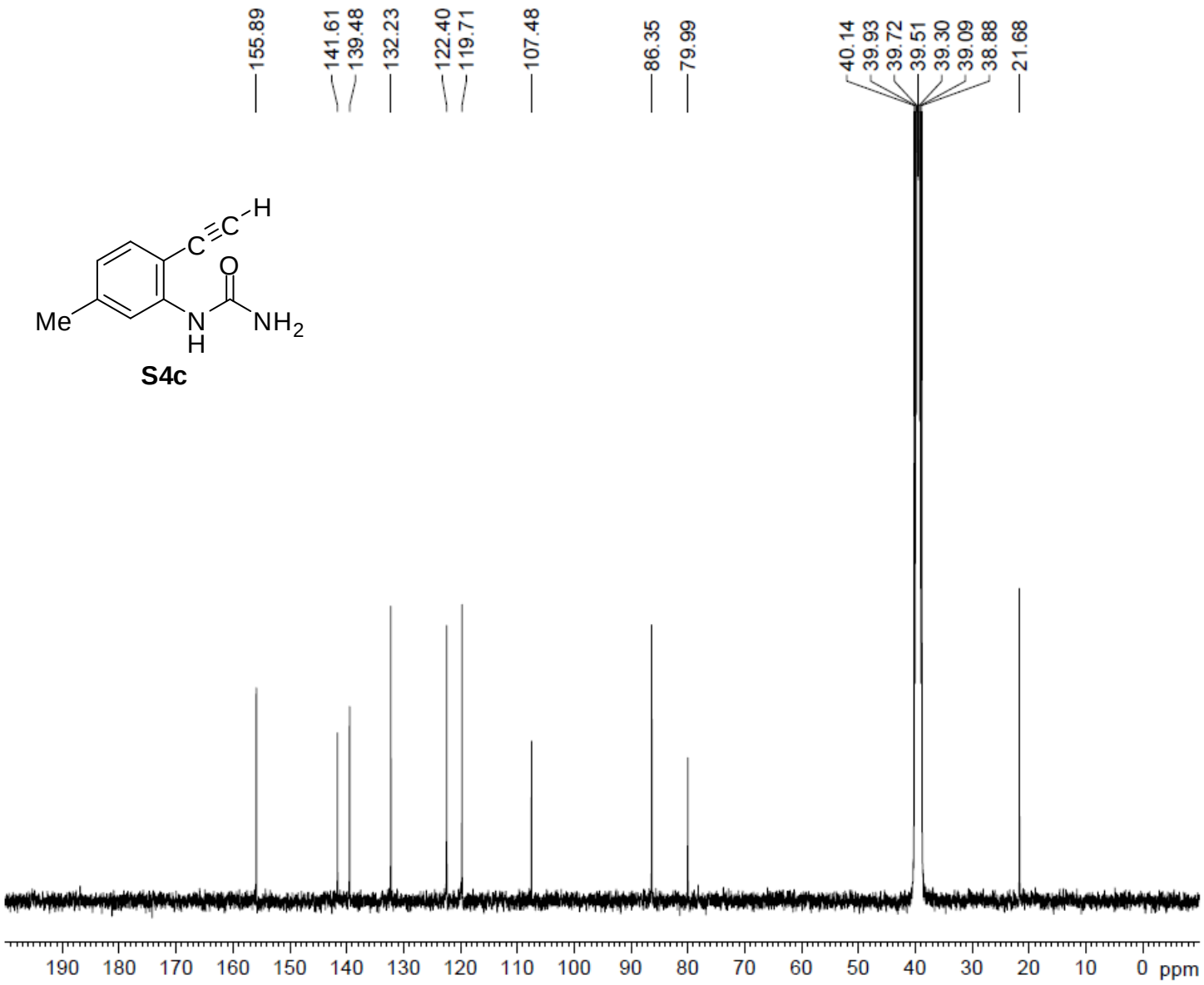


Current Data Parameters
NAME SC156
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140703
Time 11.40
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



S4c

Current Data Parameters
NAME SC156
EXPNO 5
PROCNO 1

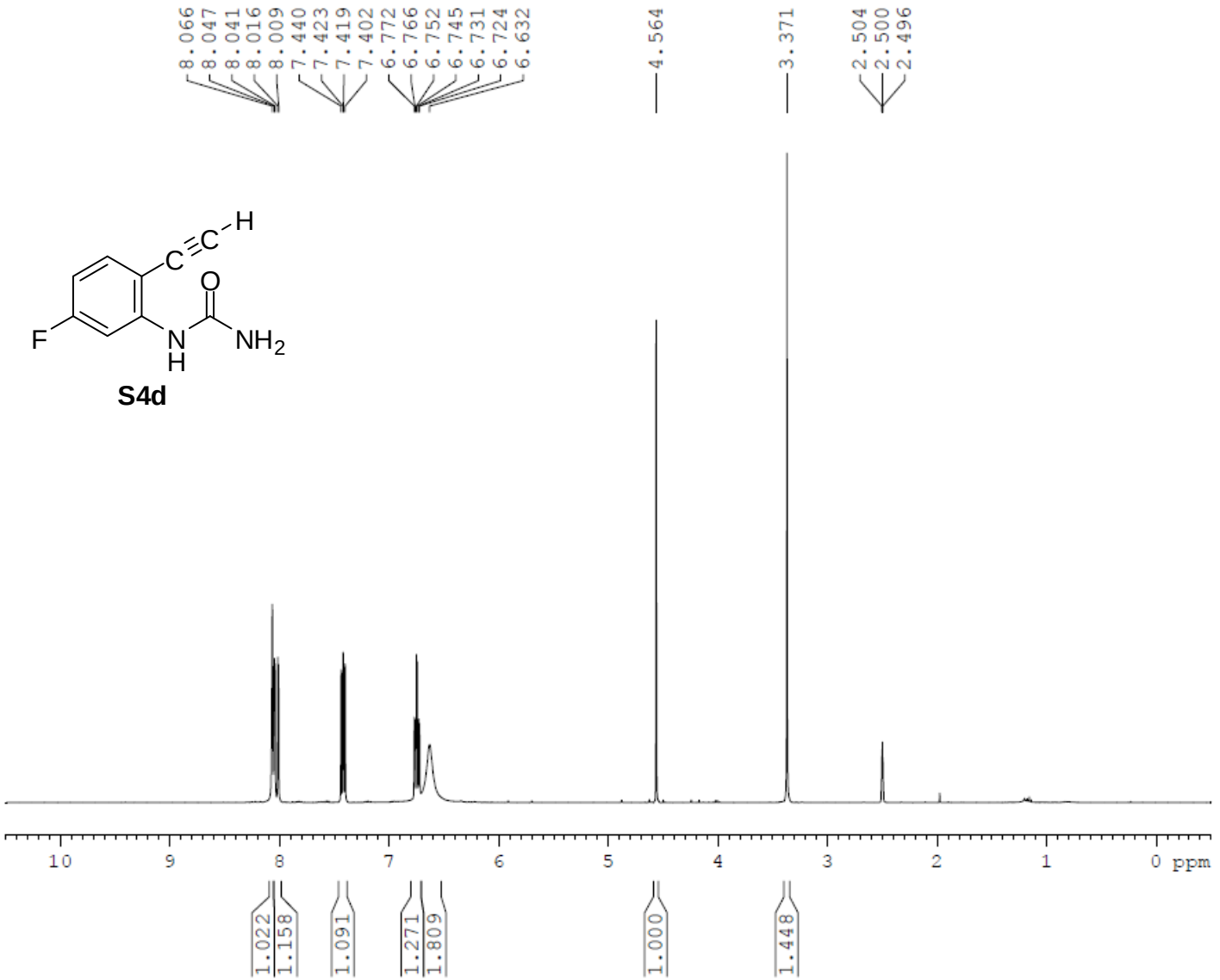
F2 - Acquisition Parameters
Date_ 20140709
Time 6.34
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 10000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127986 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

pure DMSO



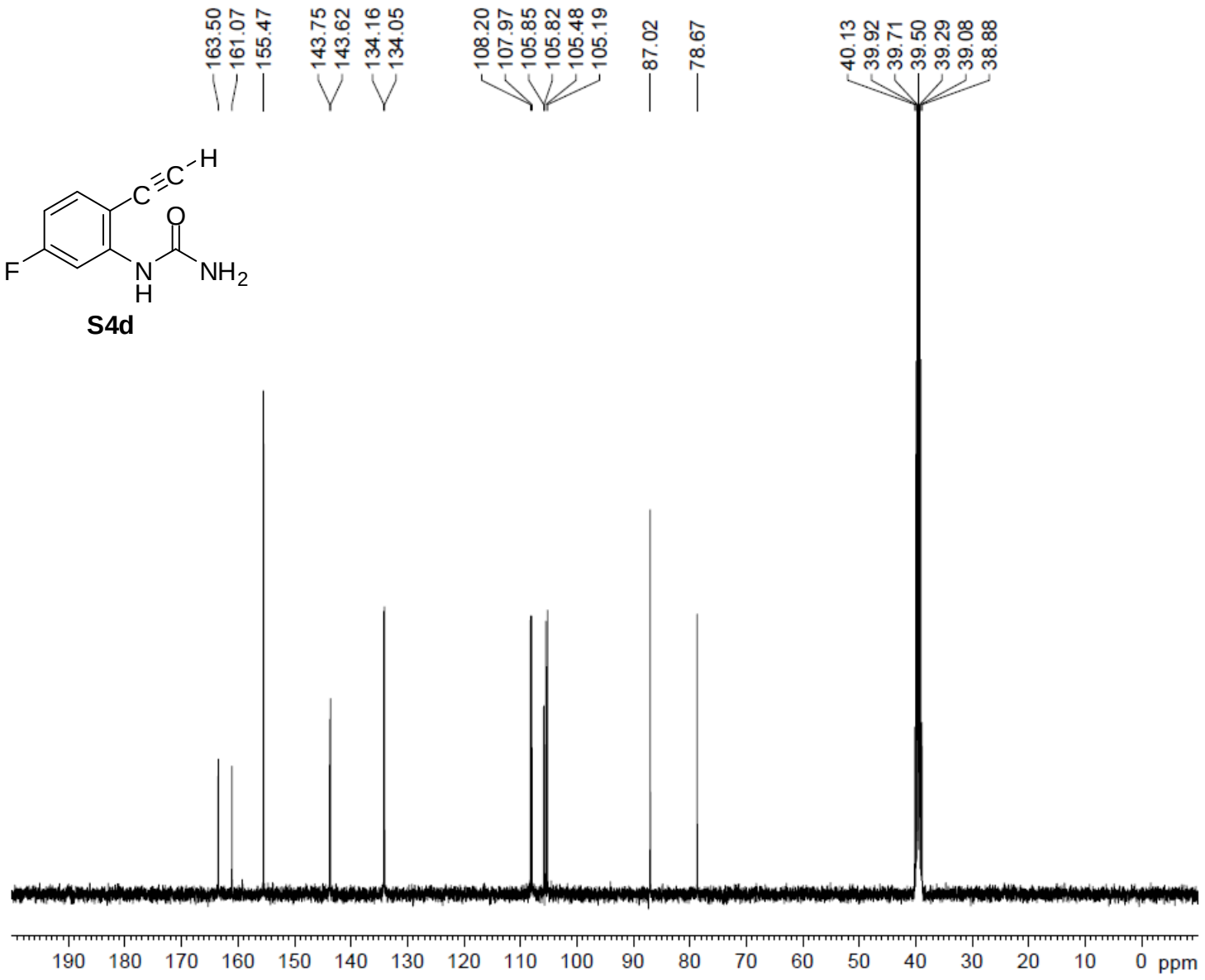
Current Data Parameters
NAME SD-078
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140529
Time 21.32
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300022 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure DMSO



S4d

Current Data Parameters
NAME SD-078
EXPNO 5
PROCNO 1

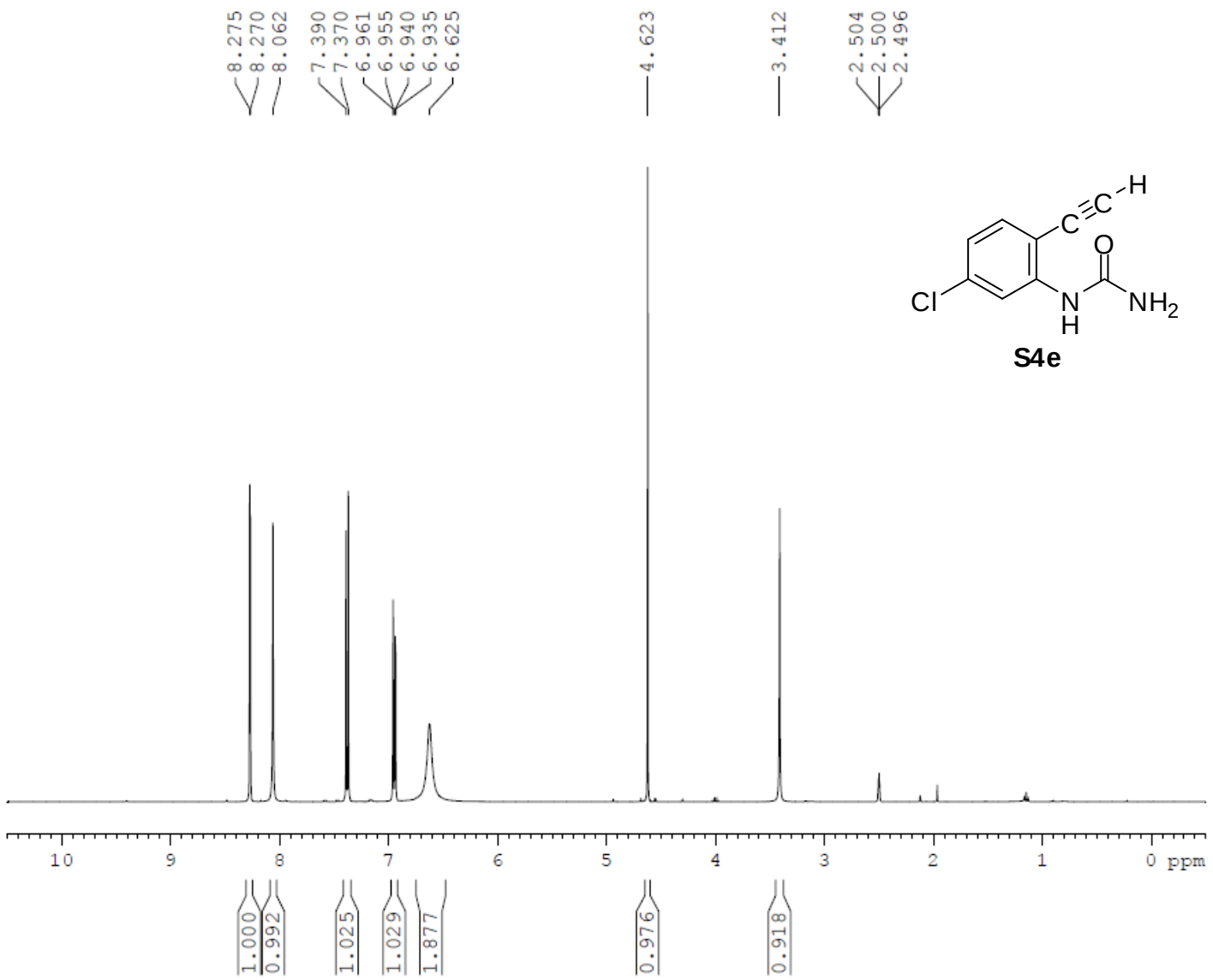
F2 - Acquisition Parameters
Date_ 20140529
Time 21.46
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 700
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

pure



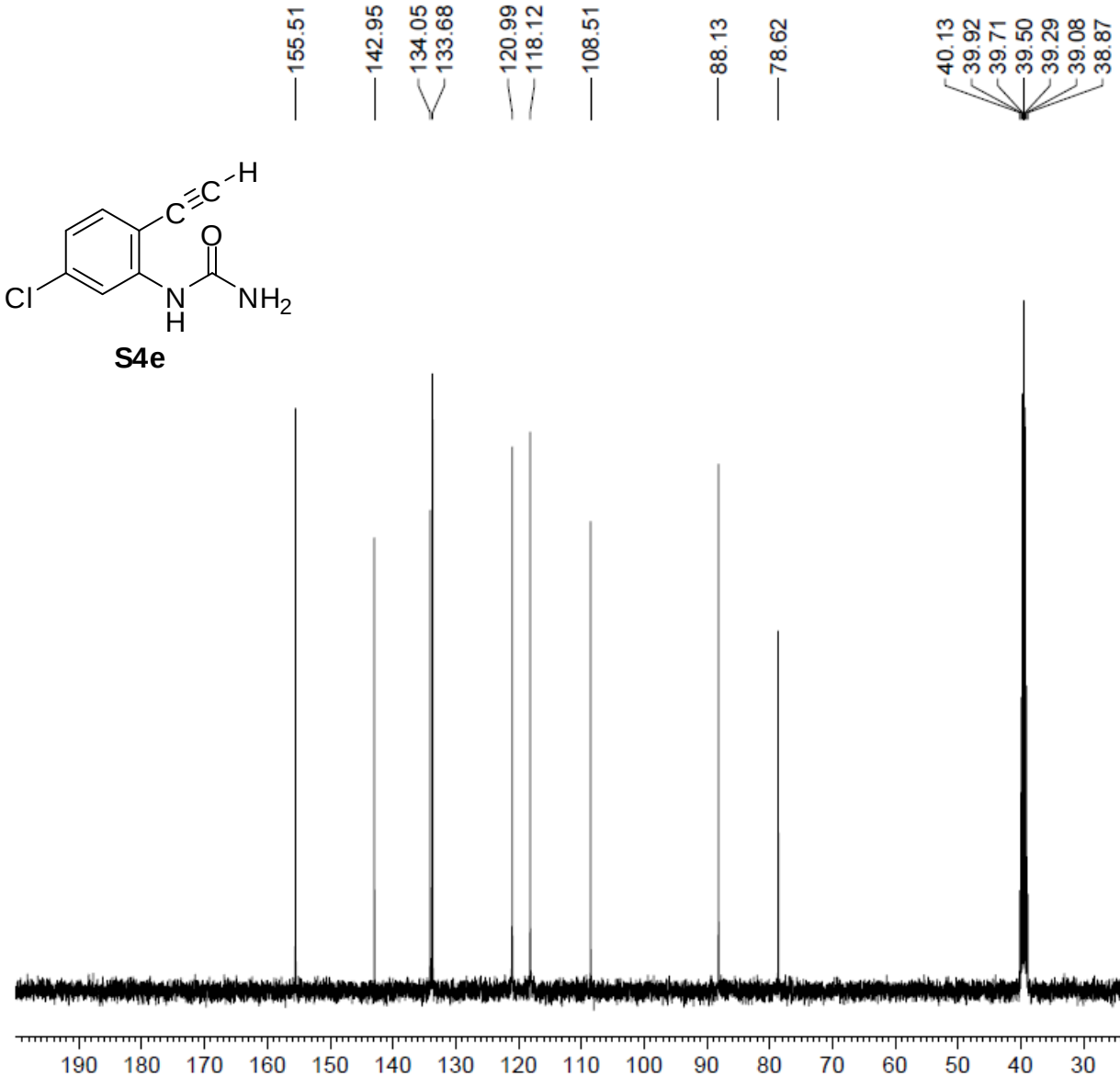
Current Data Parameters
NAME SD-062(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140424
Time 15.35
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300024 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



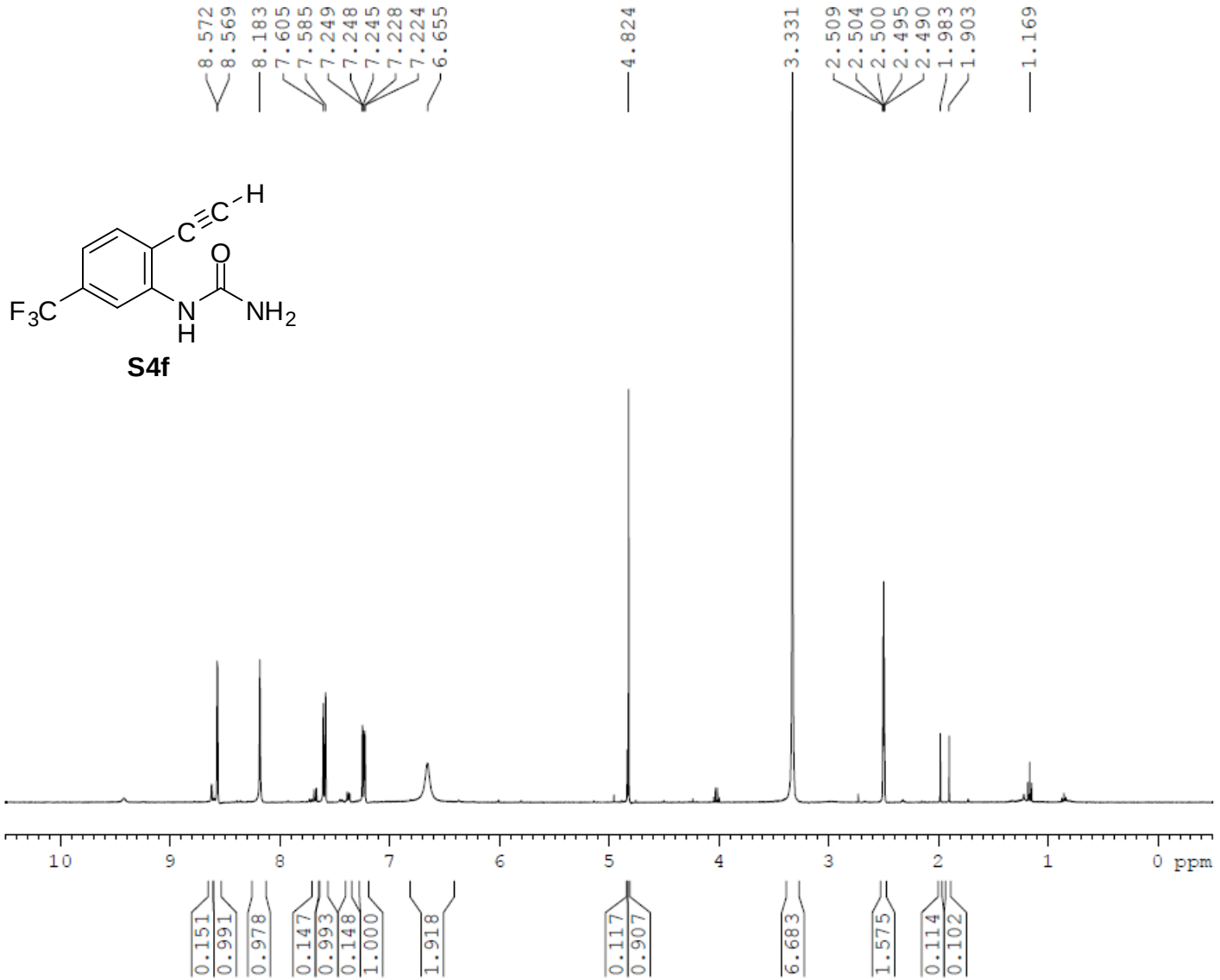
Current Data Parameters
NAME SD-062(old)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140424
Time 15.45
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 704
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128121 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

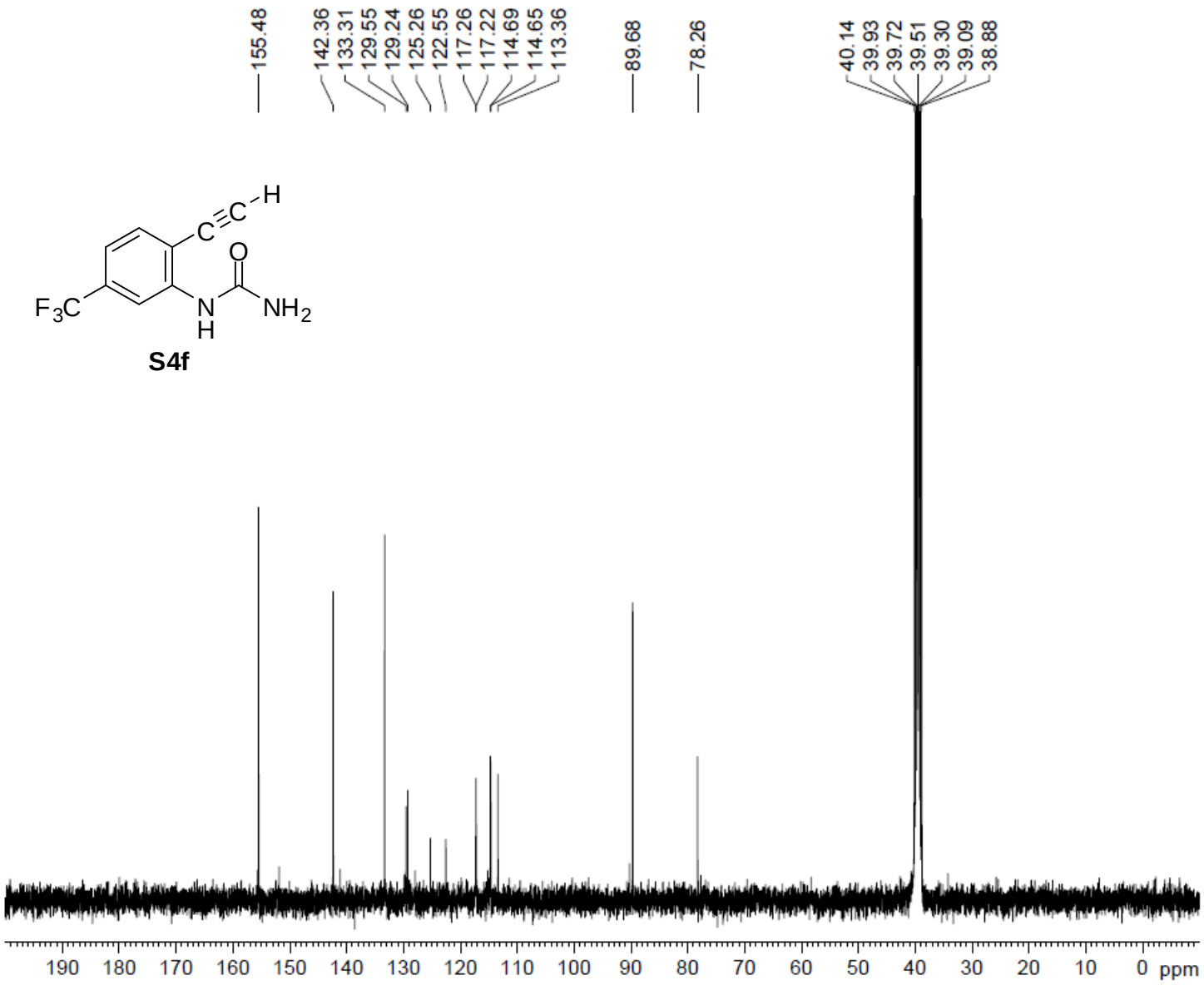


Current Data Parameters
NAME SO150
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150906
Time 10.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 5.30 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SO150
EXPNO 2
PROCNO 1

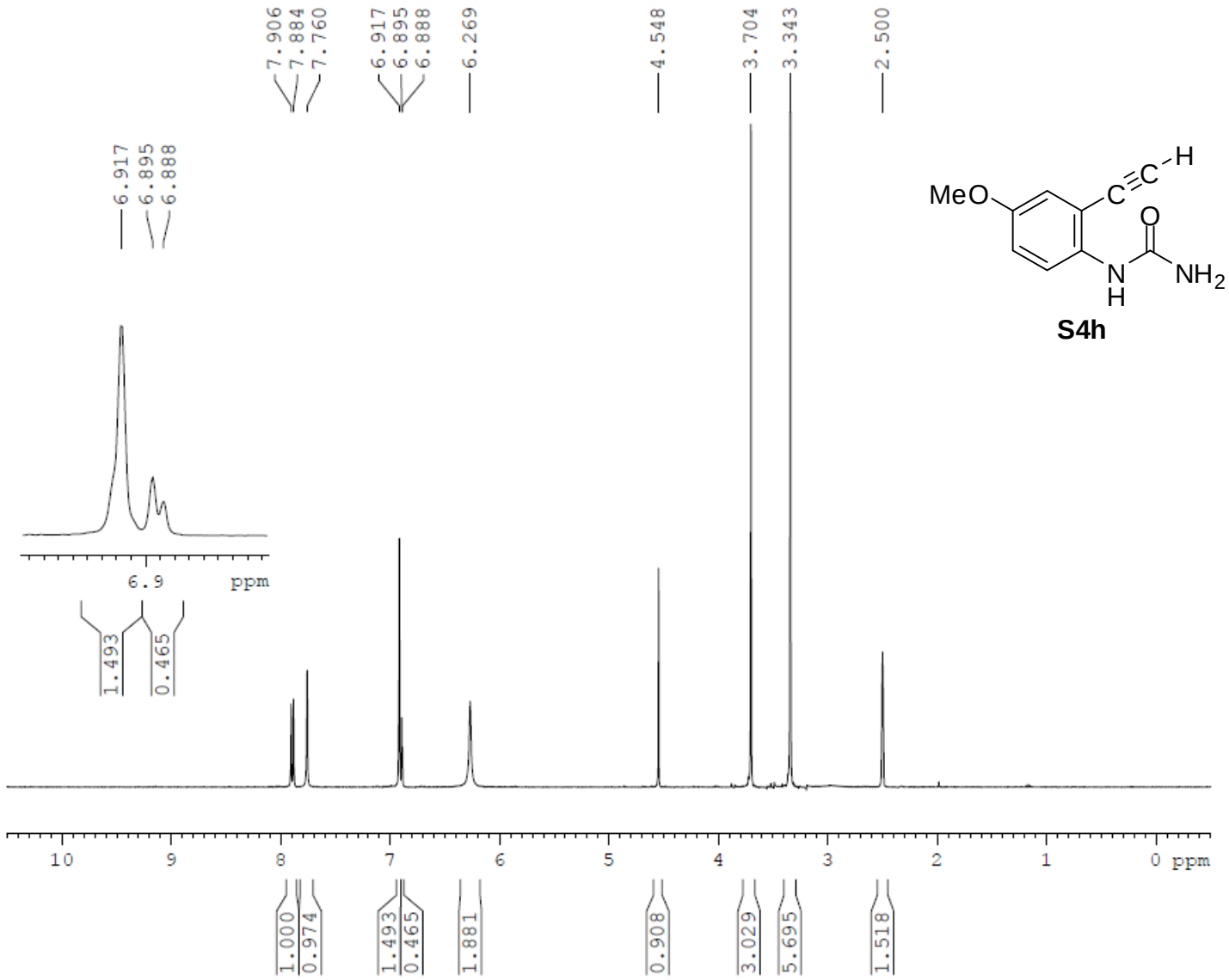
F2 - Acquisition Parameters
Date_ 20150906
Time 10.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1100
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 6502
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 4.60 dB
PL12 20.40 dB
PL13 23.40 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128173 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

recrystallized from EtOAc



S4h

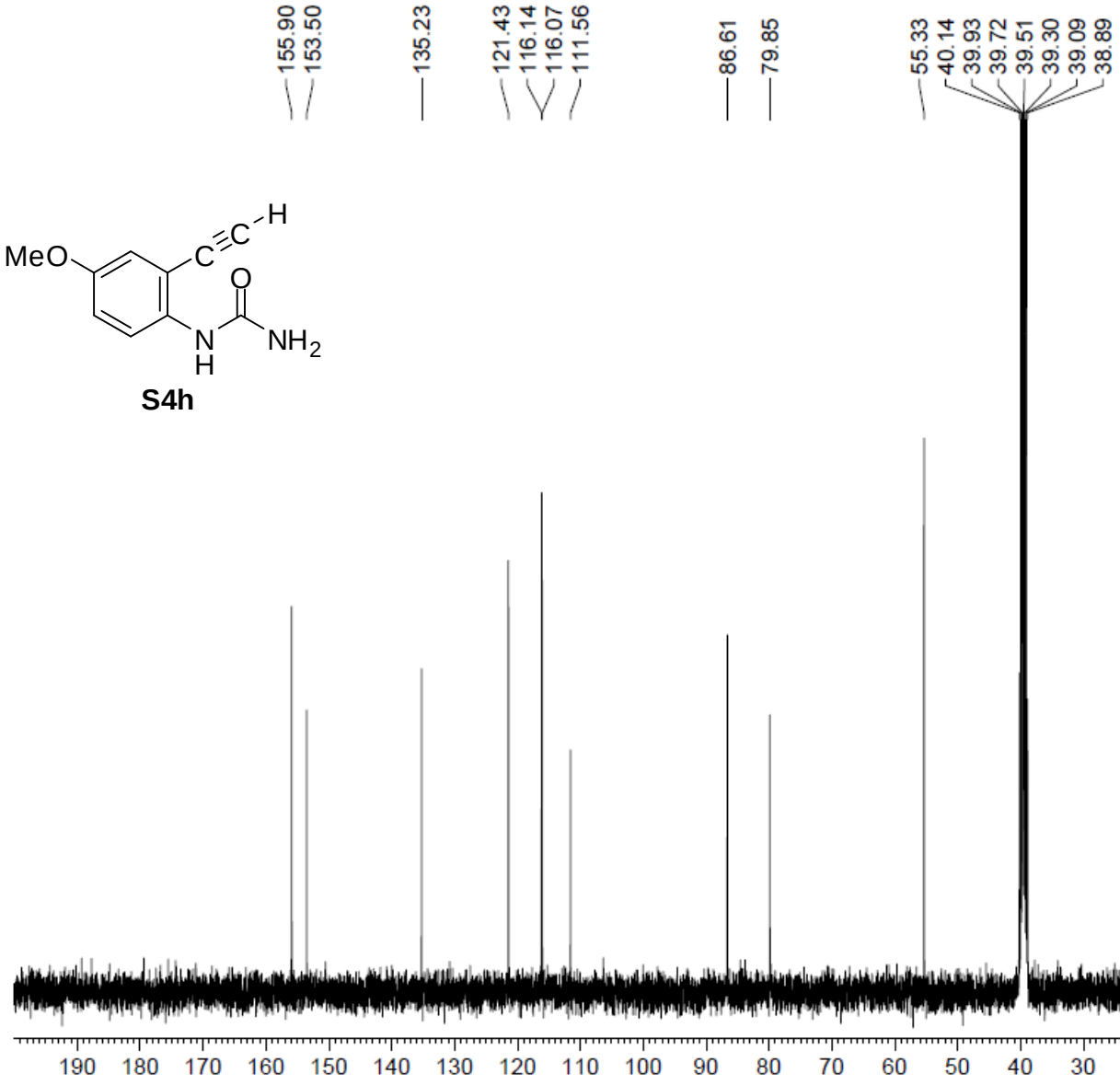
Current Data Parameters
NAME SO067
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150129
Time 9.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 295.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

recrystallized from EtOAc



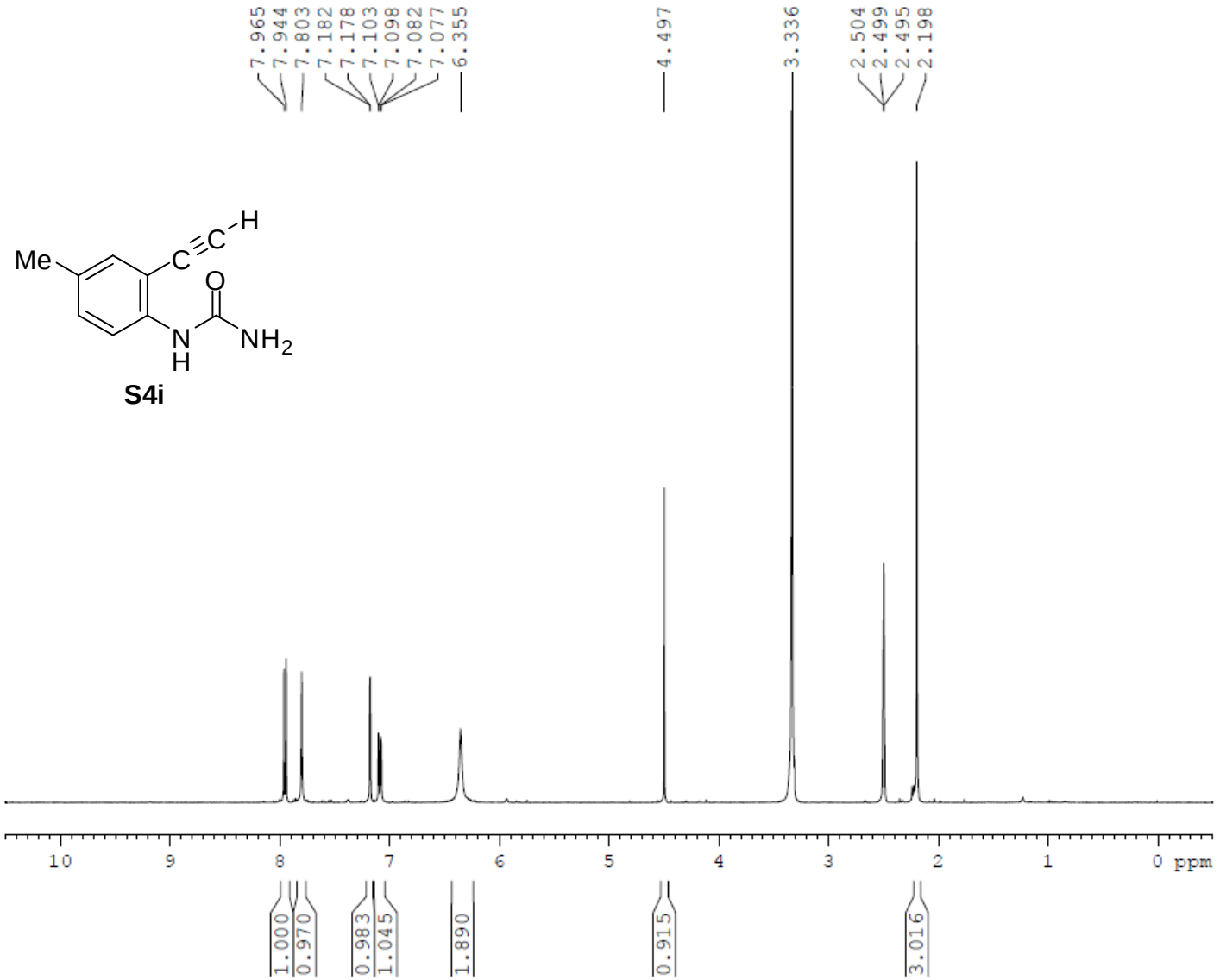
Current Data Parameters
NAME SO067
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150129
Time 10.12
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 151
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4597.6
DW 20.800 usec
DE 6.50 usec
TE 295.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128141 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

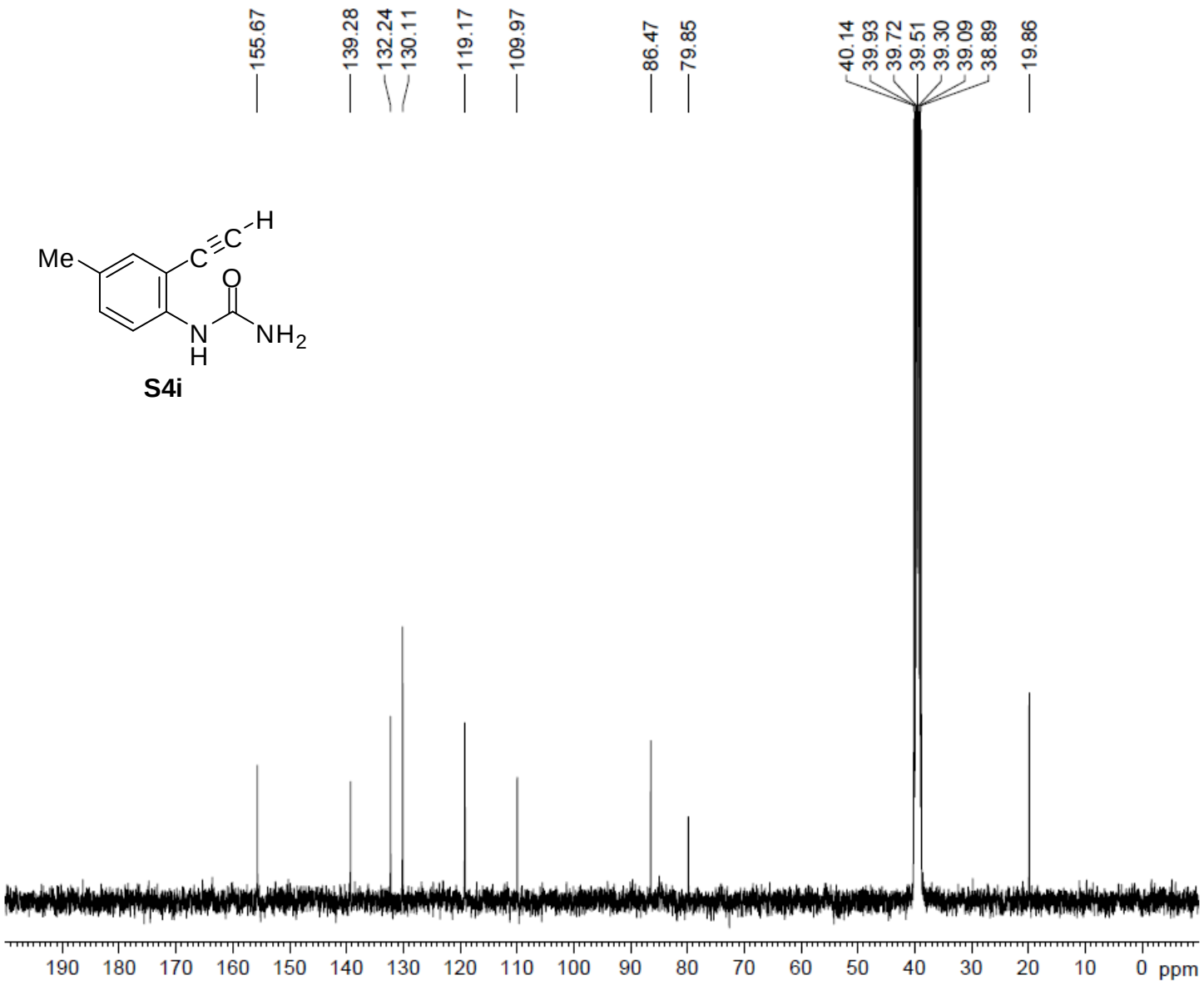


Current Data Parameters
NAME SC111
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140420
Time 21.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 113.31
DW 69.333 usec
DE 10.52 usec
TE 298.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300033 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



S4i

Current Data Parameters
NAME SC111
EXPNO 3
PROCNO 1

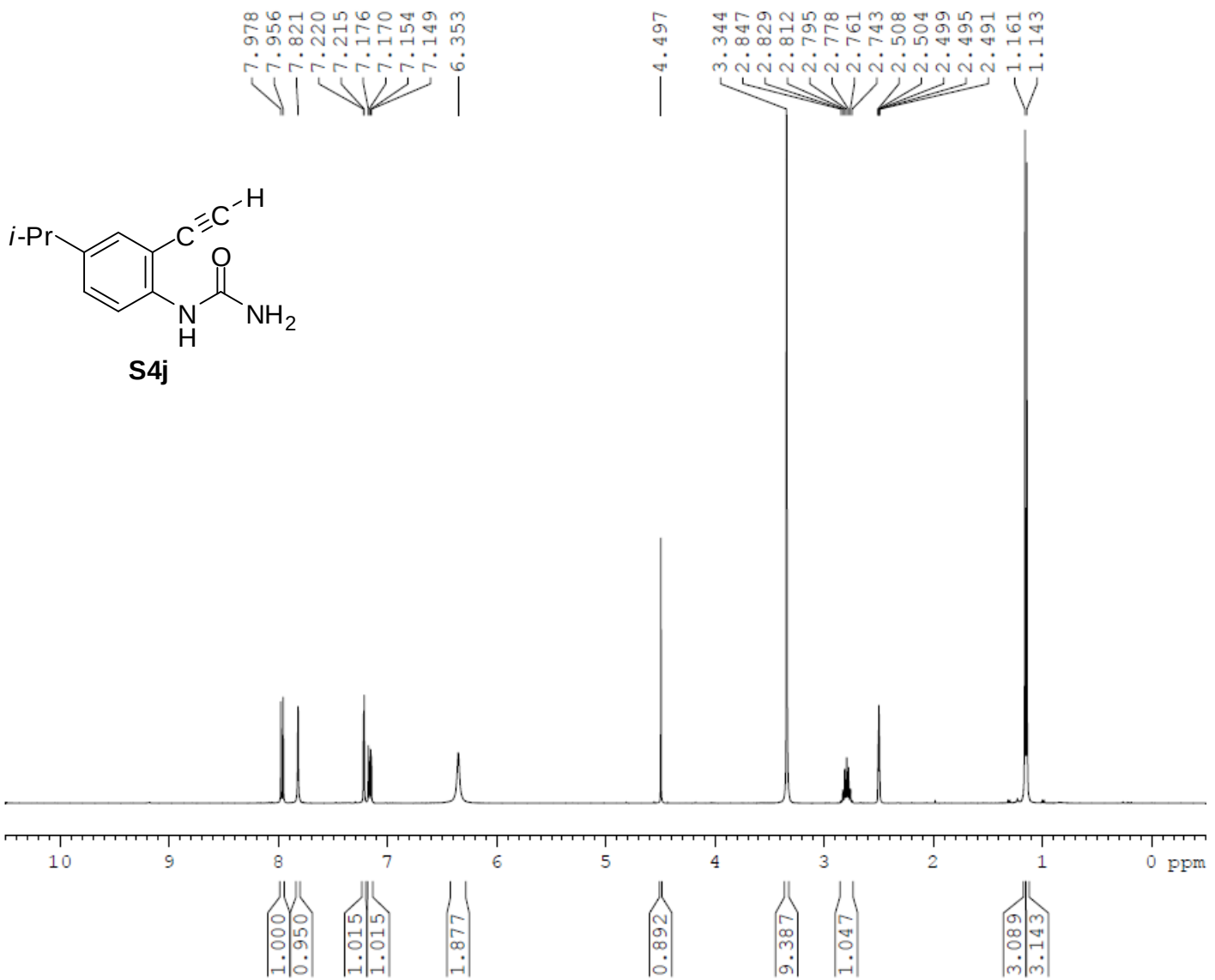
F2 - Acquisition Parameters
Date_ 20140420
Time 22.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 908
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6128187 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

pure



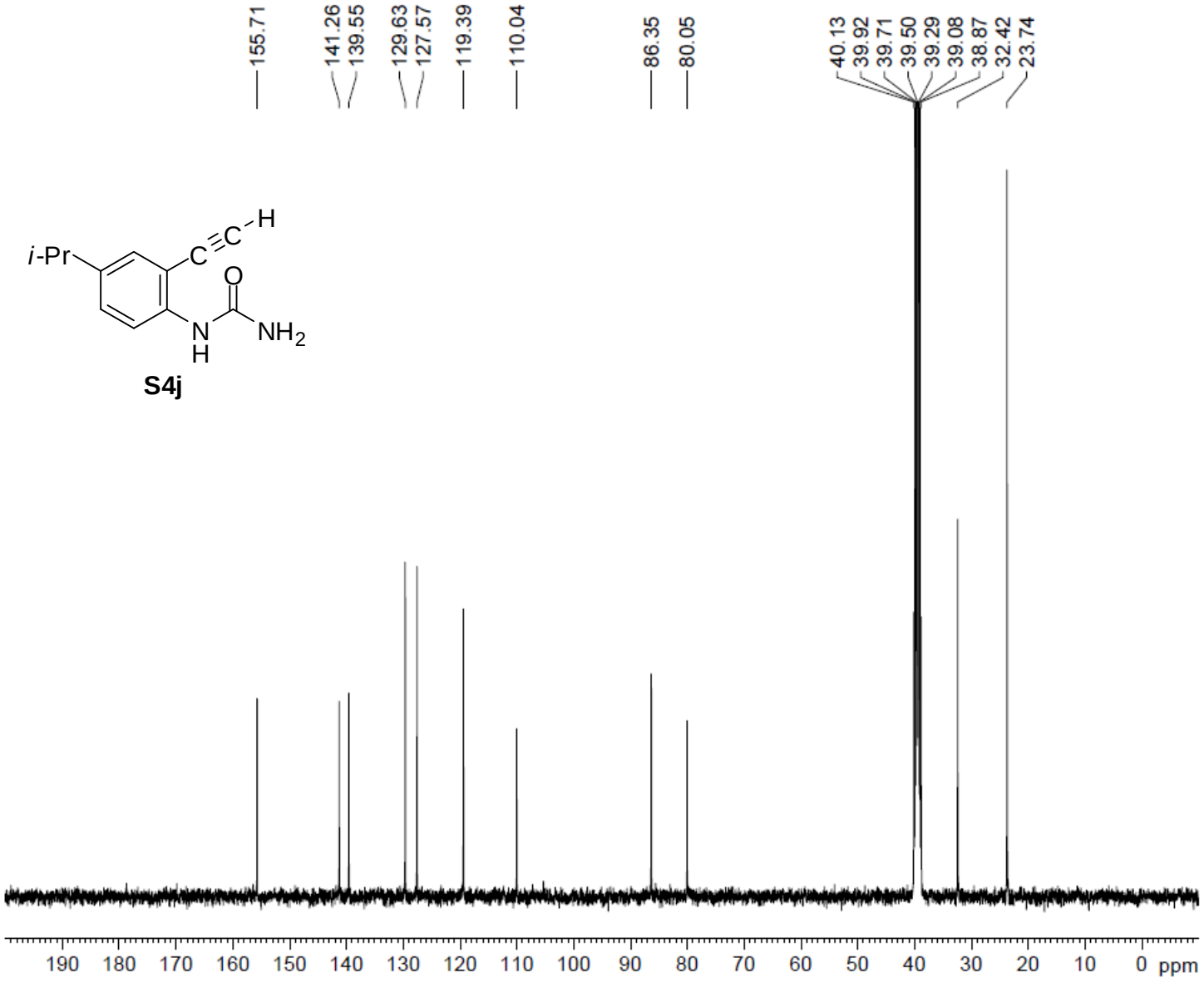
Current Data Parameters
NAME SD-090(new)
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140619
Time 19.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 89.08
DW 69.333 usec
DE 10.52 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300034 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



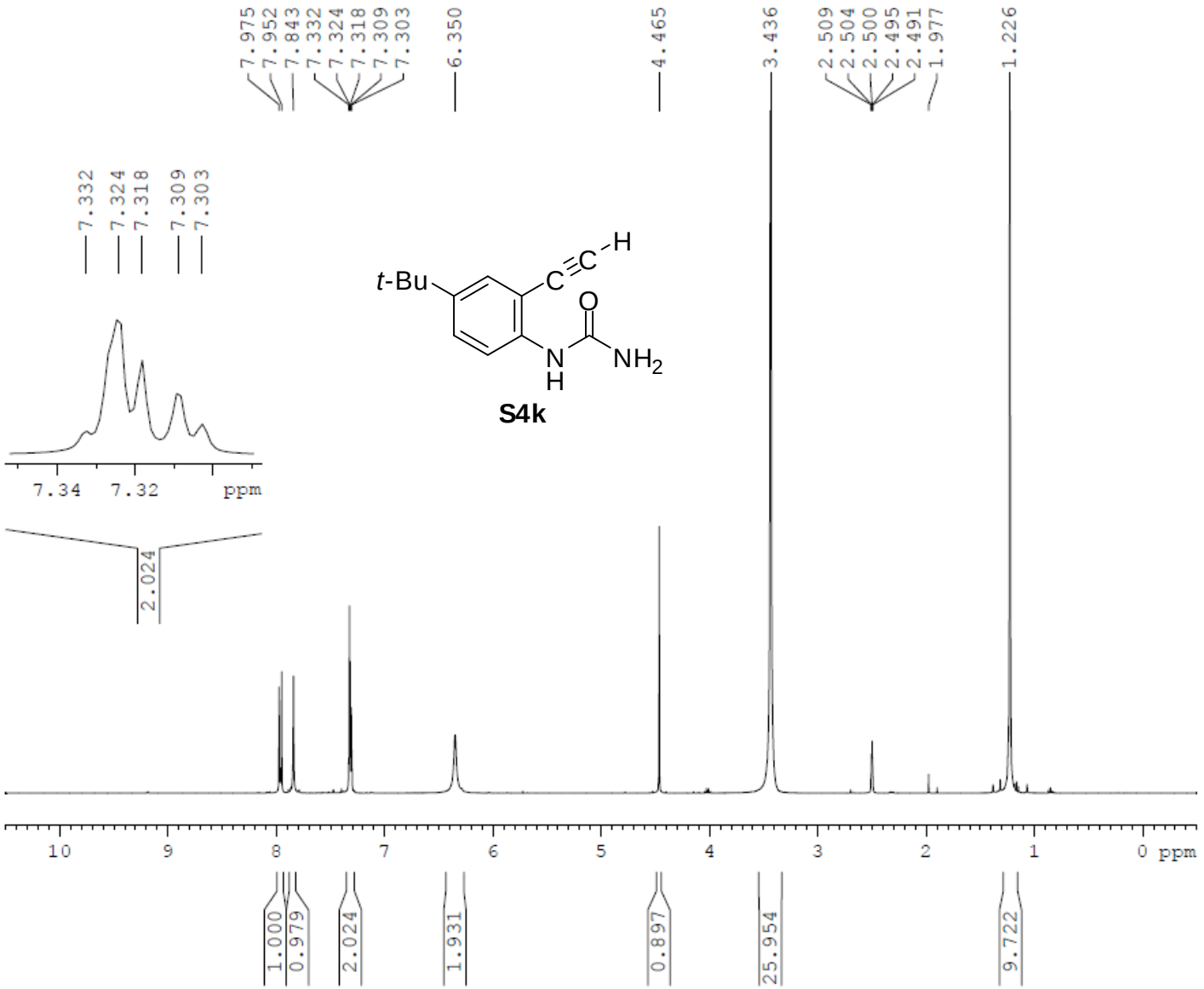
Current Data Parameters
NAME SD-090(new)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140619
Time 20.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 447
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6128177 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

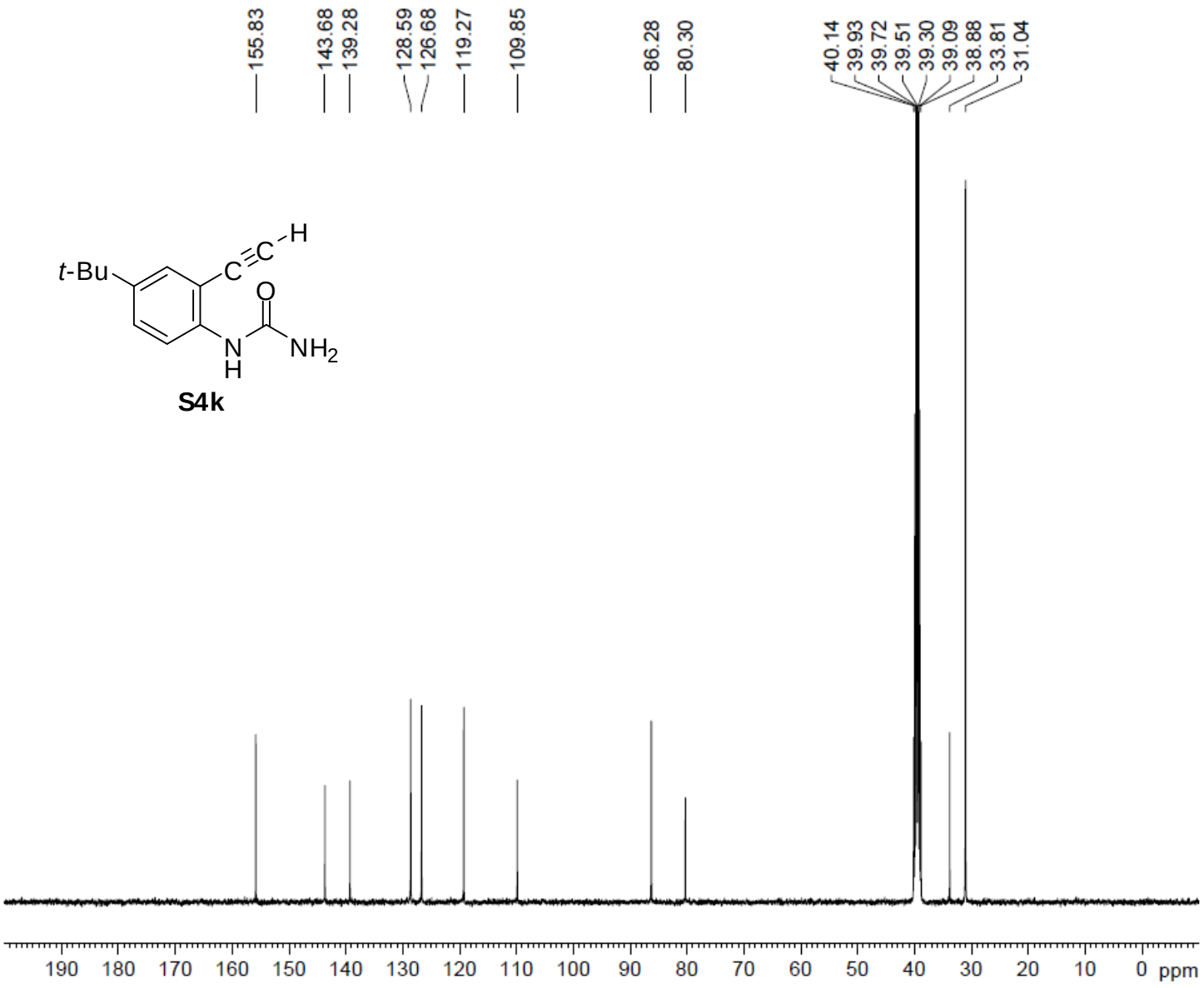


Current Data Parameters
NAME SC155
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140702
Time 8.12
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 45.15
DW 69.333 usec
DE 10.52 usec
TE 298.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300032 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



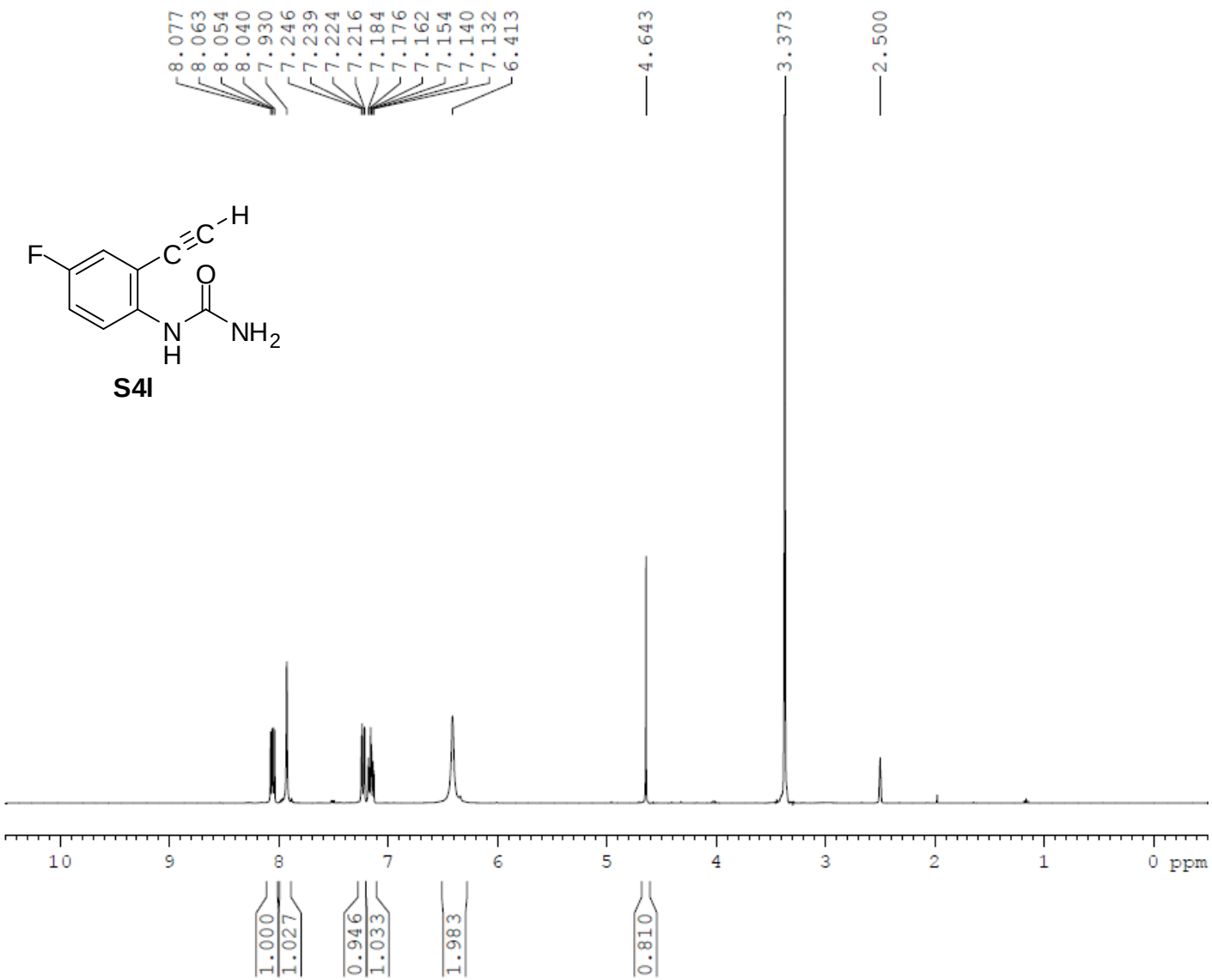
Current Data Parameters
NAME SC155
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140702
Time 9.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

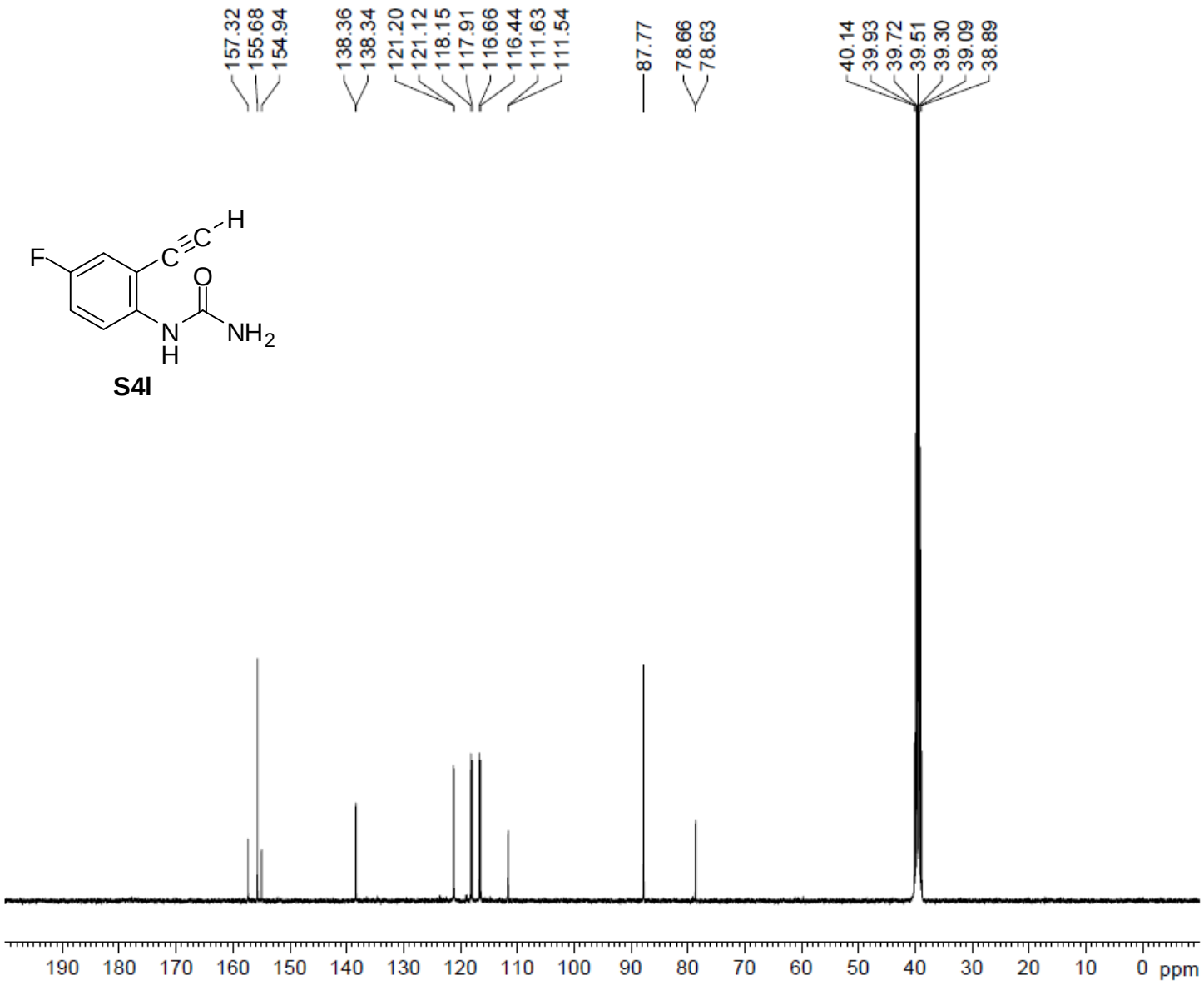
F2 - Processing parameters
SI 32768
SF 100.6128096 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



S4l

NAME SC165
EXPNO 2
PROCNO 1
Date_ 20140801
Time 22.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz
SI 16384
SF 400.1300035 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



S4l

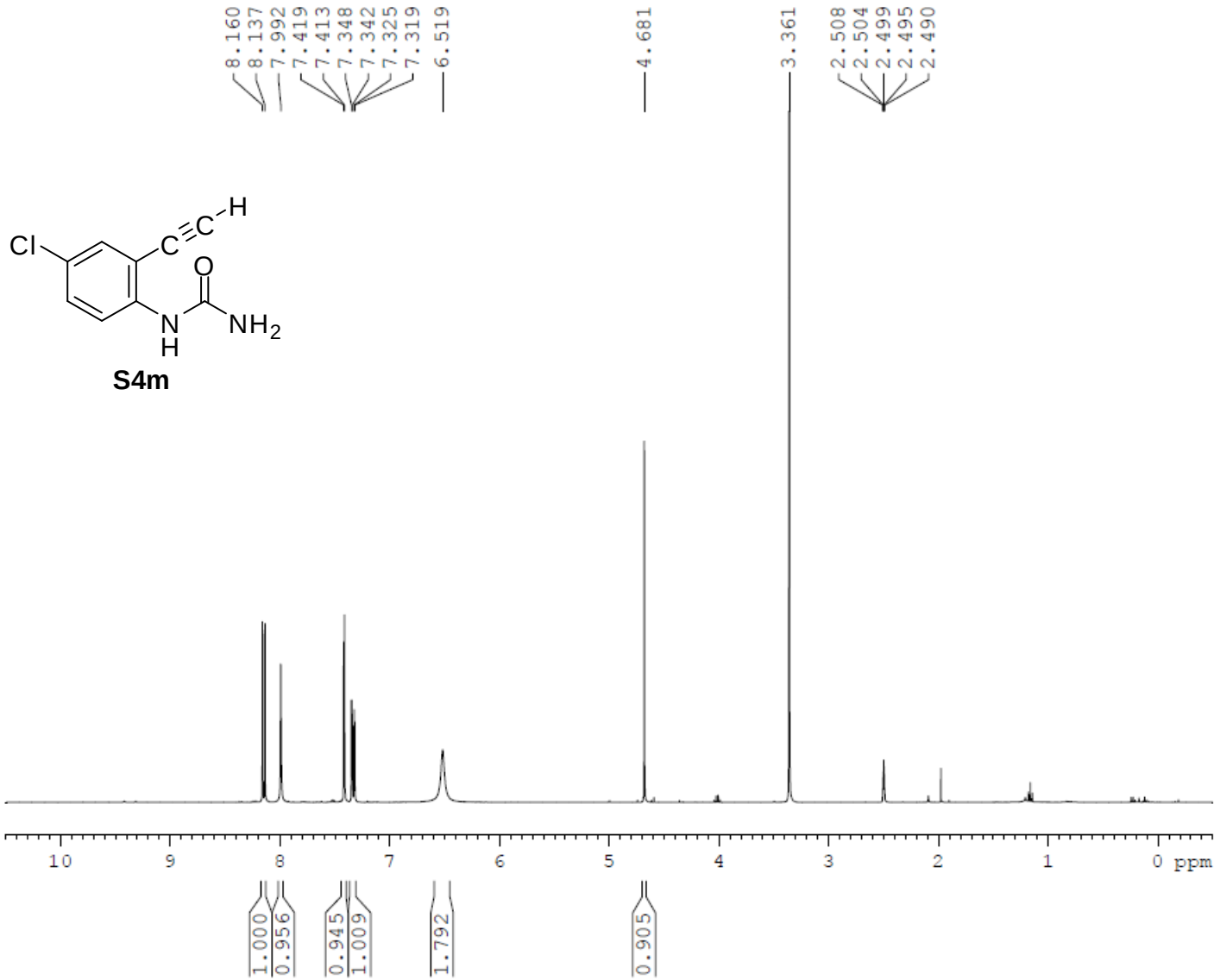
Current Data Parameters
NAME SC165
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140801
Time 23.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1964
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 301.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128174 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



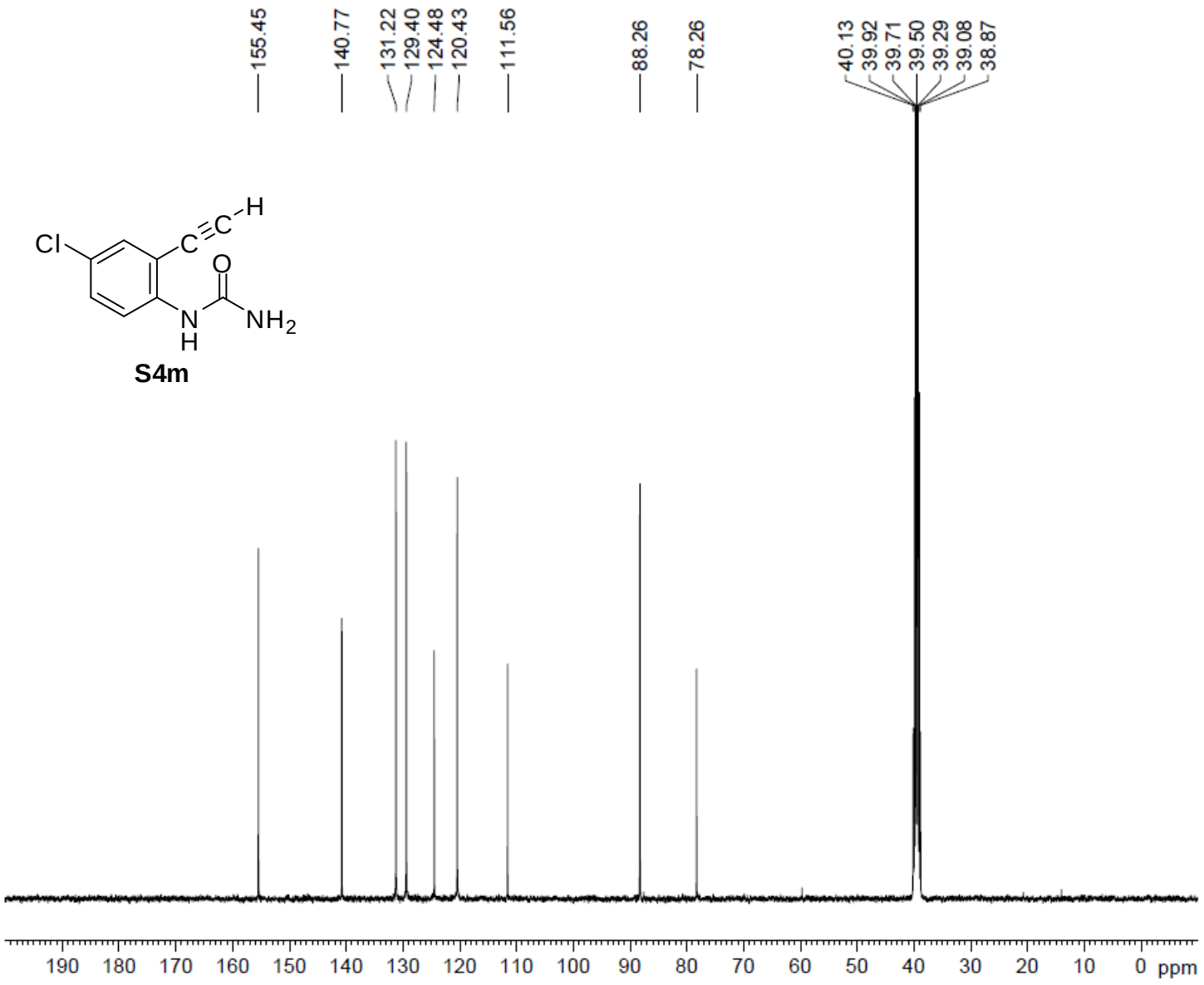
S4m

Current Data Parameters
NAME SD-096(new)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140627
Time 13.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 71.42
DW 69.333 usec
DE 10.52 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300034 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



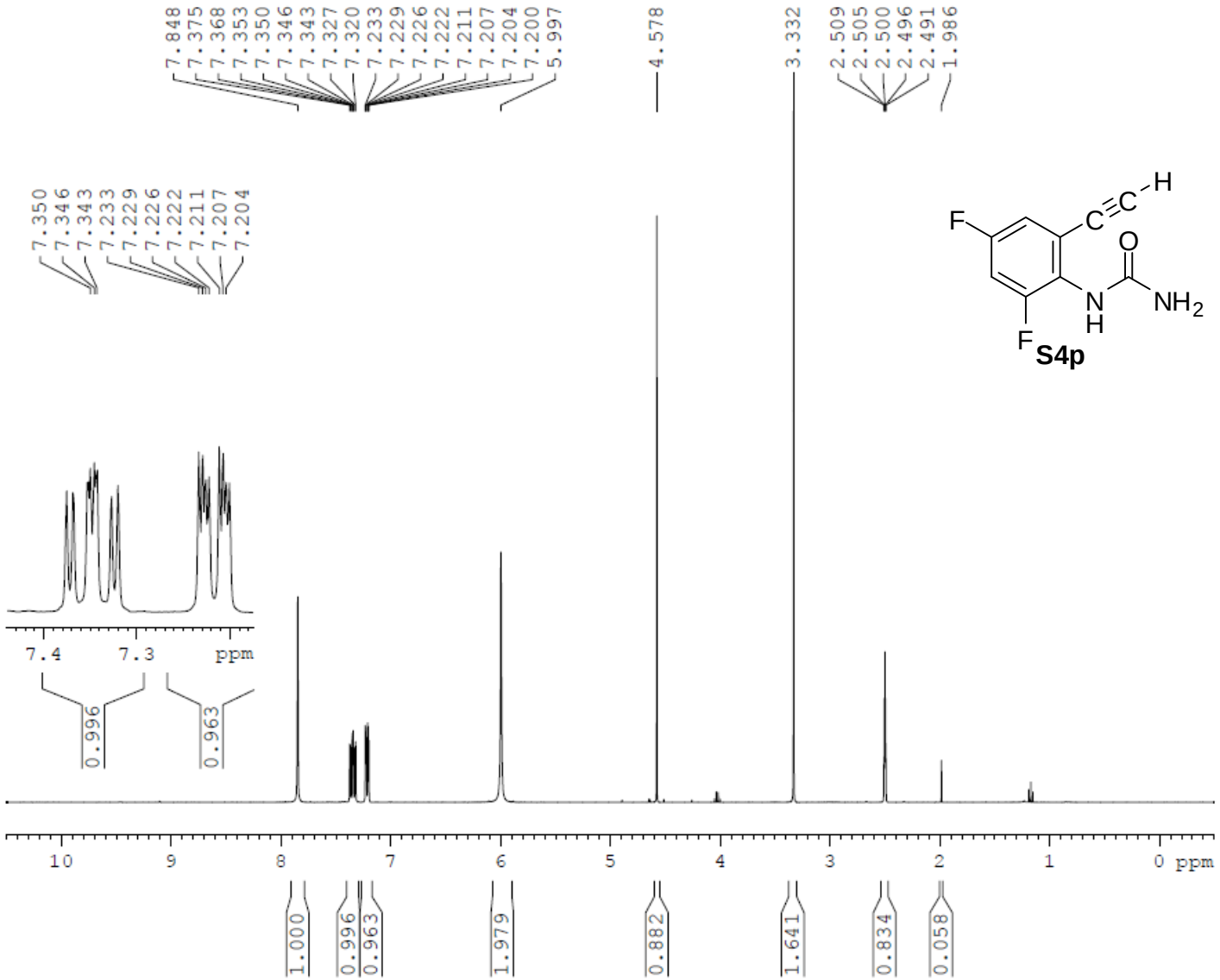
Current Data Parameters
NAME SD-096(new)
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140627
Time 17.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6128182 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

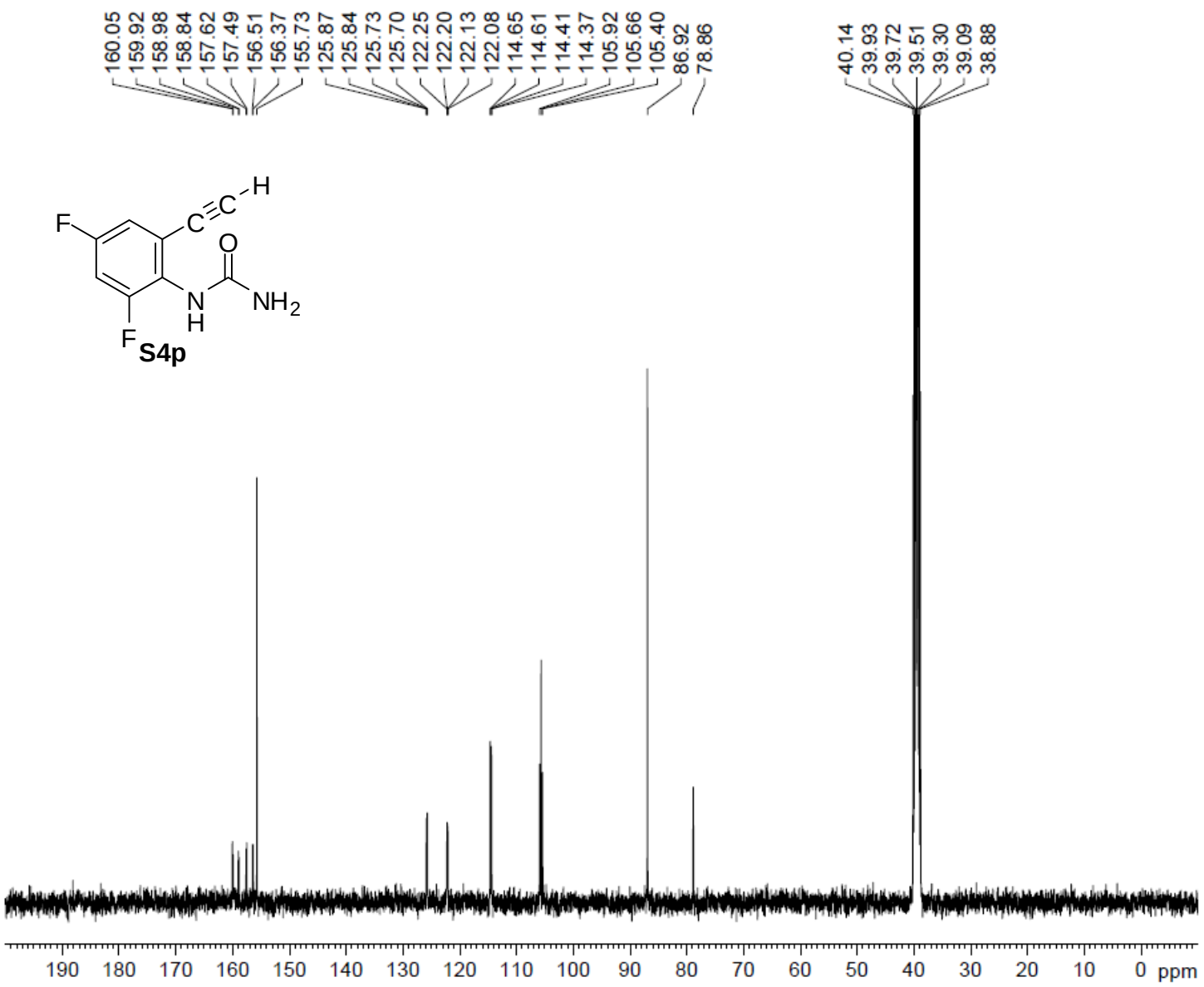


Current Data Parameters
NAME SO151
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150909
Time 16.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 177.16
DW 69.333 usec
DE 10.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300036 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



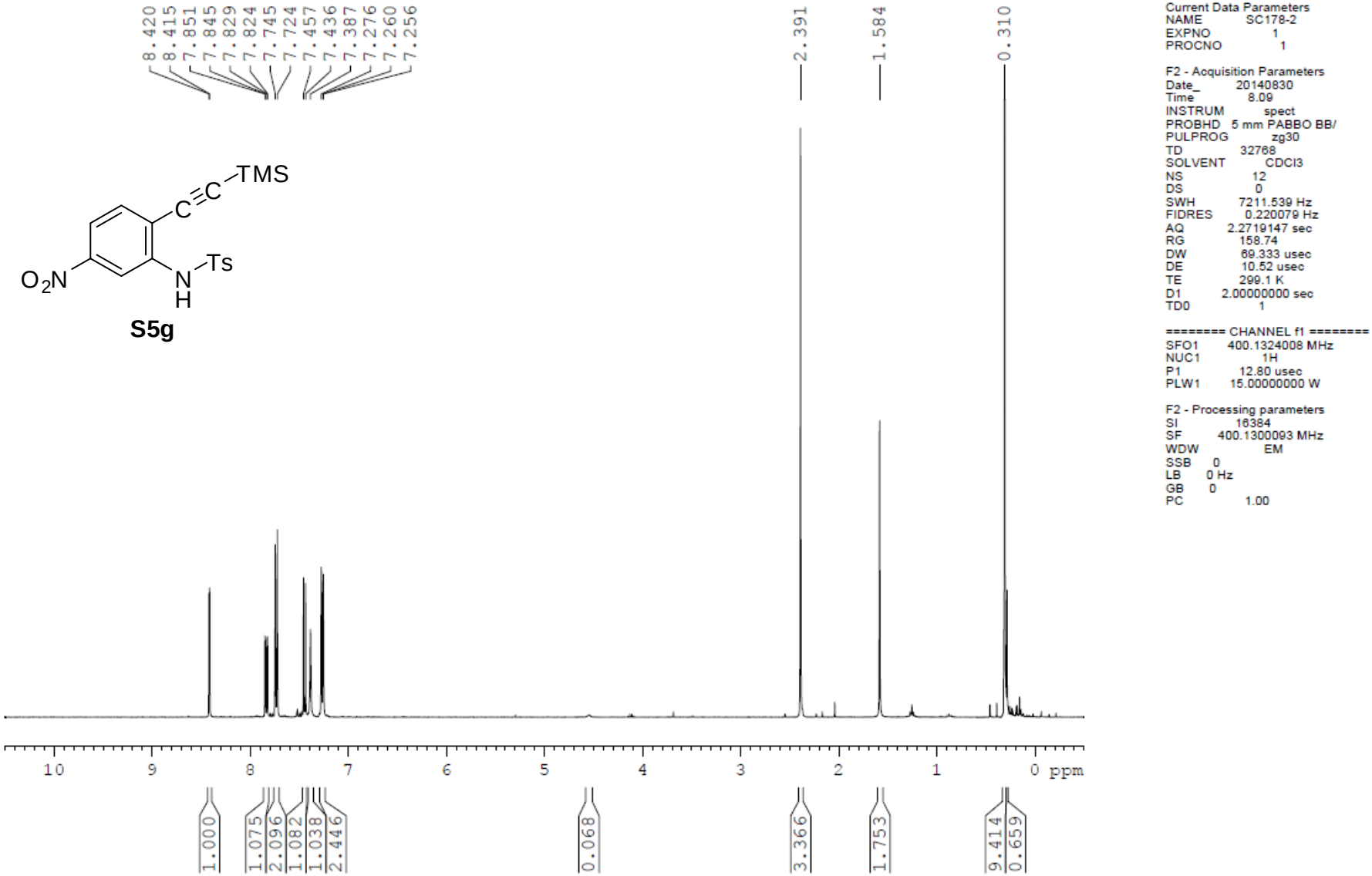
Current Data Parameters
NAME SO151
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150911
Time 8.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 558
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.50000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W
PLW13 0.27338001 W

F2 - Processing parameters
SI 32768
SF 100.6128190 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

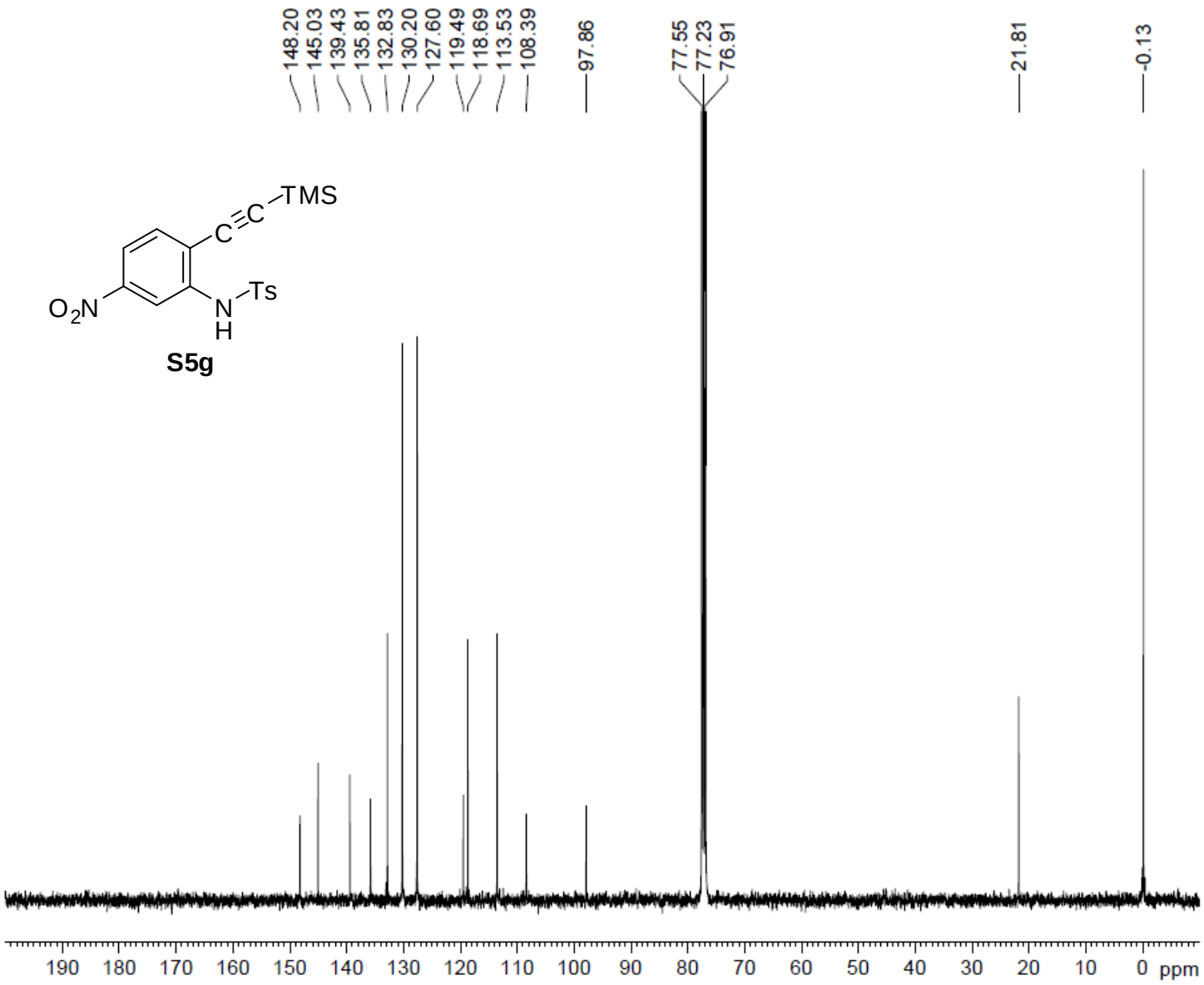


Current Data Parameters
NAME SC178-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140830
Time 8.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 158.74
DW 69.333 usec
DE 10.52 usec
TE 299.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



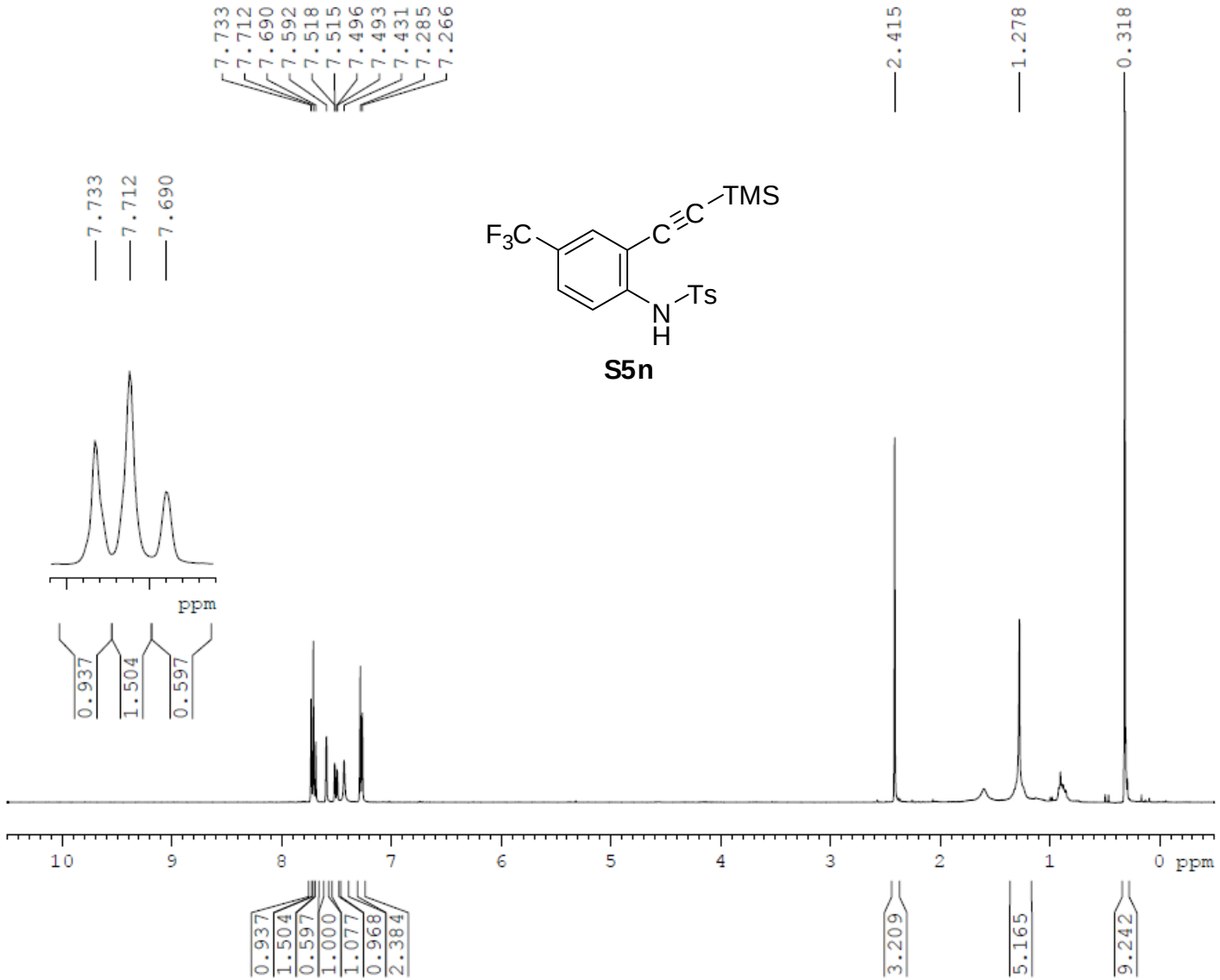
Current Data Parameters
NAME SC178-2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140830
Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1195
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 300.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127464 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

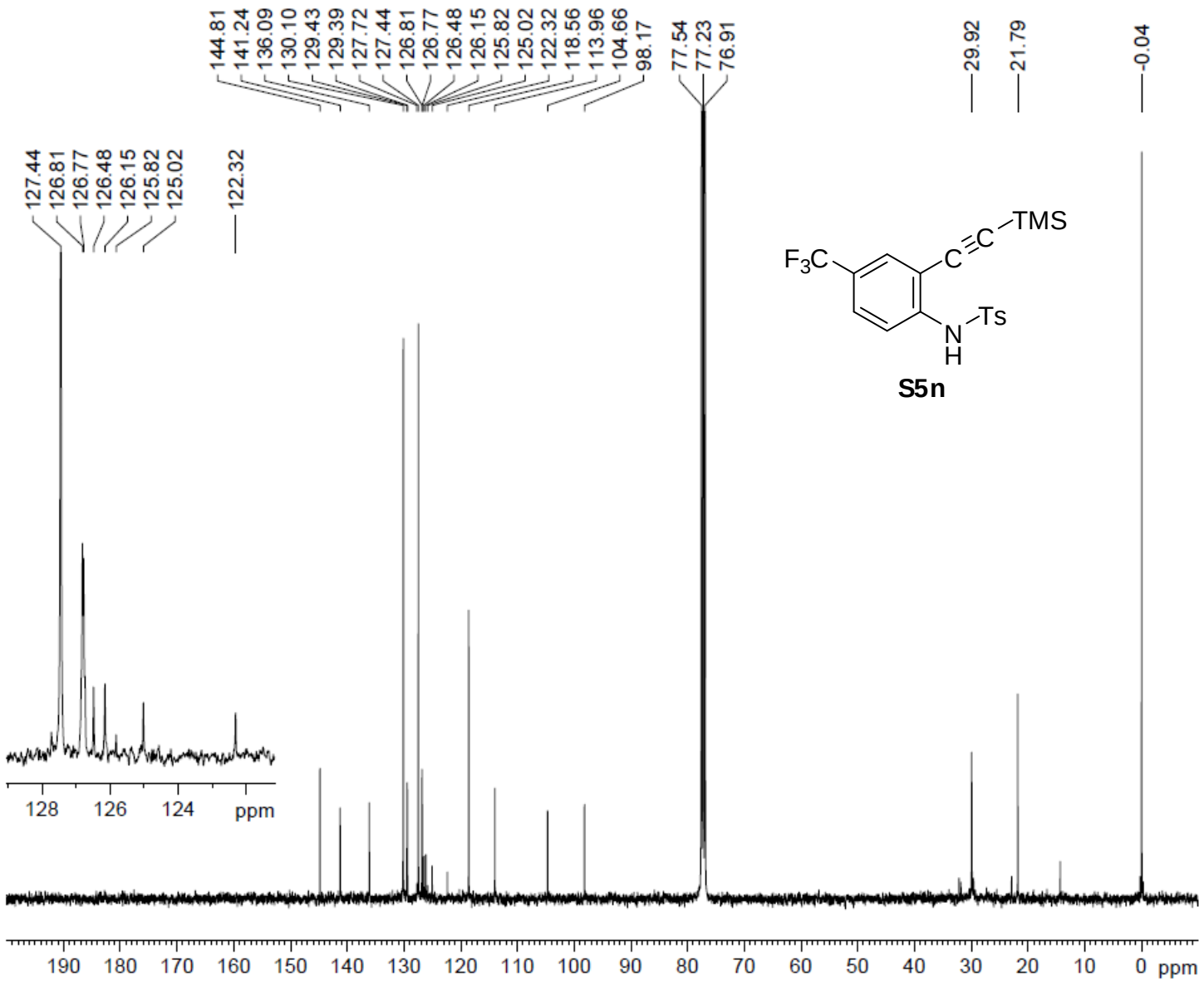


Current Data Parameters
NAME SC174
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140823
Time 14.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 89.08
DW 69.333 usec
DE 10.52 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



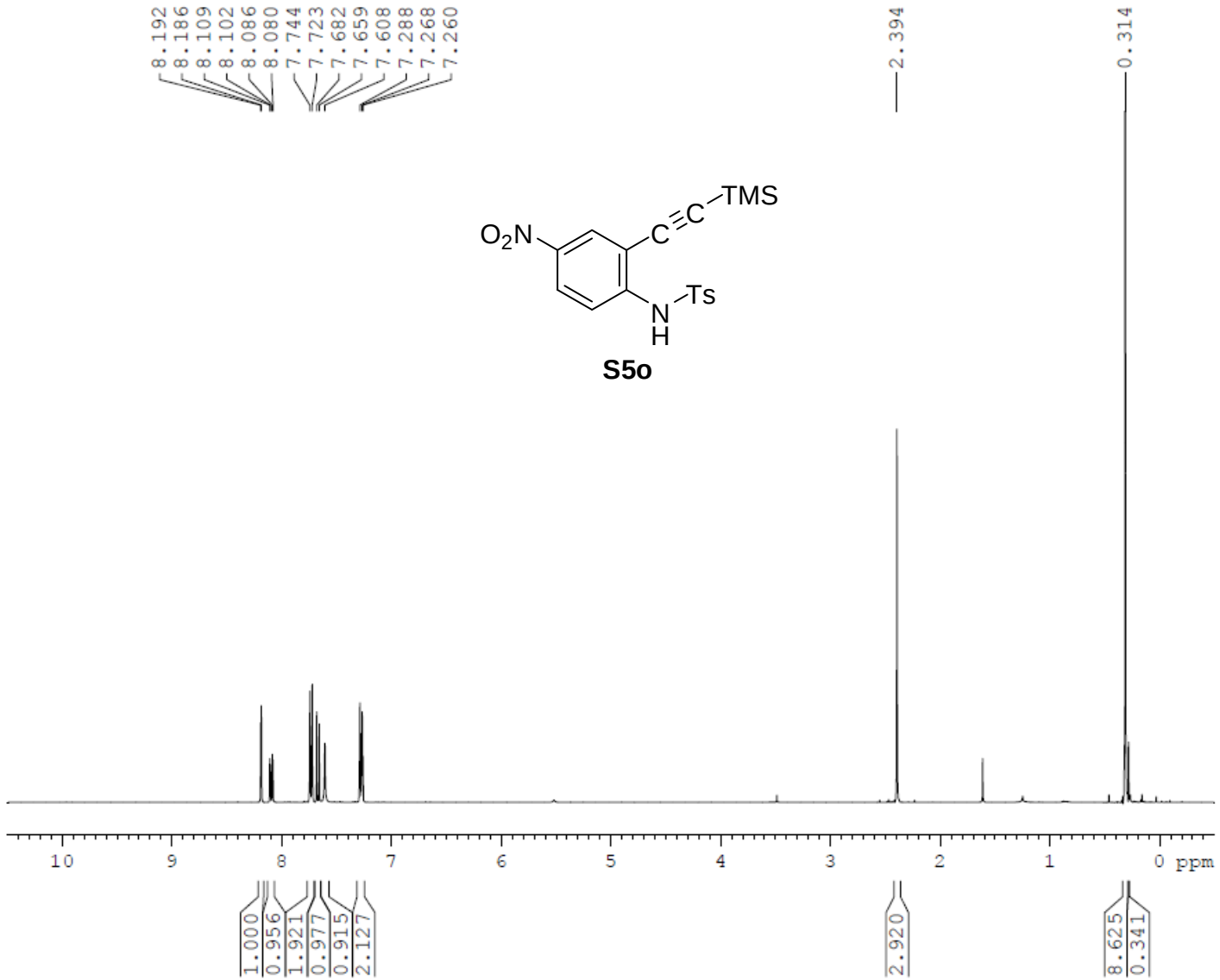
Current Data Parameters
NAME SC174
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140824
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2192
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127460 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



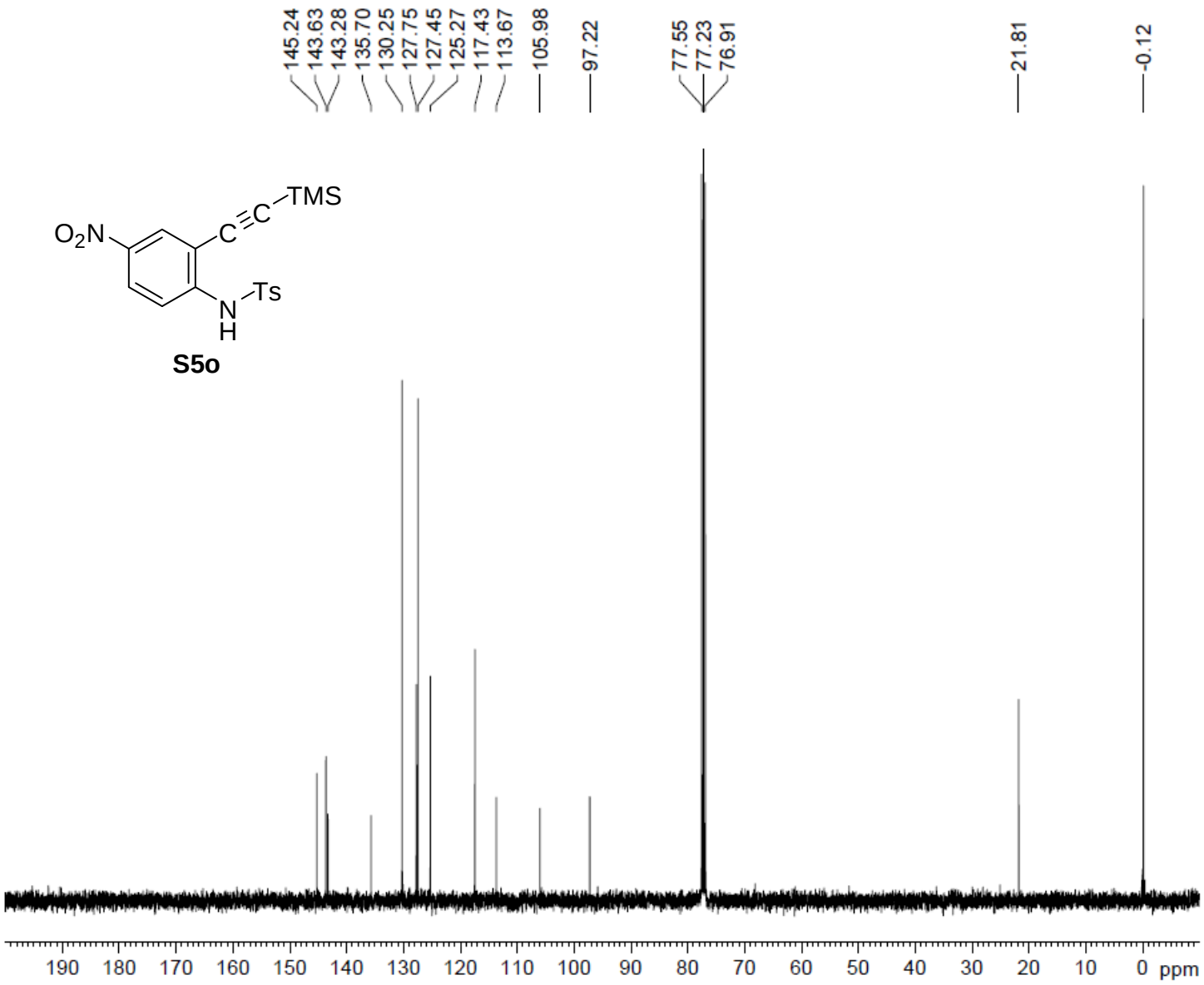
S5o

Current Data Parameters
NAME SO066-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150122
Time 8.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



S5o

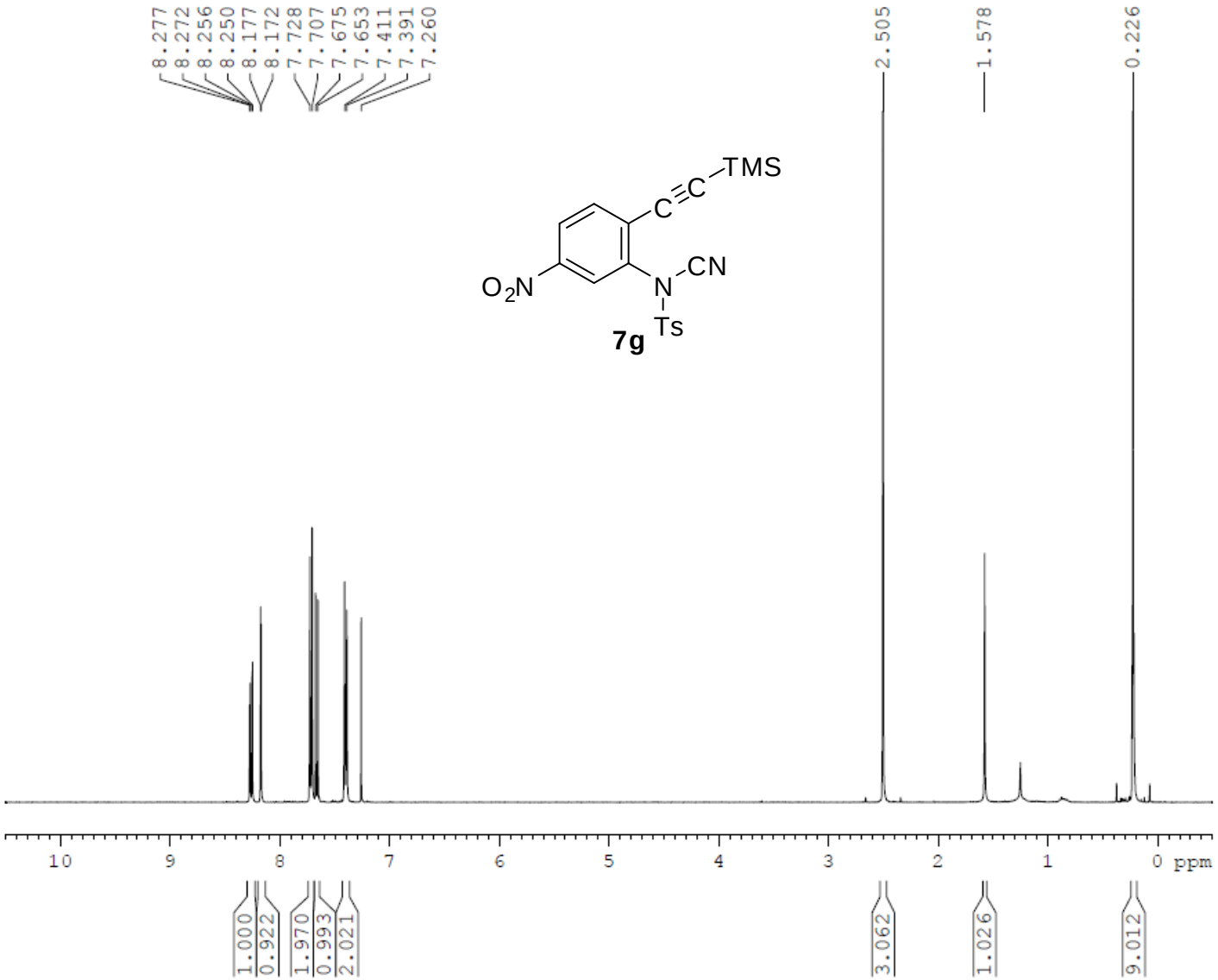
Current Data Parameters
NAME SO066-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150122
Time 8.44
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 108
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127506 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

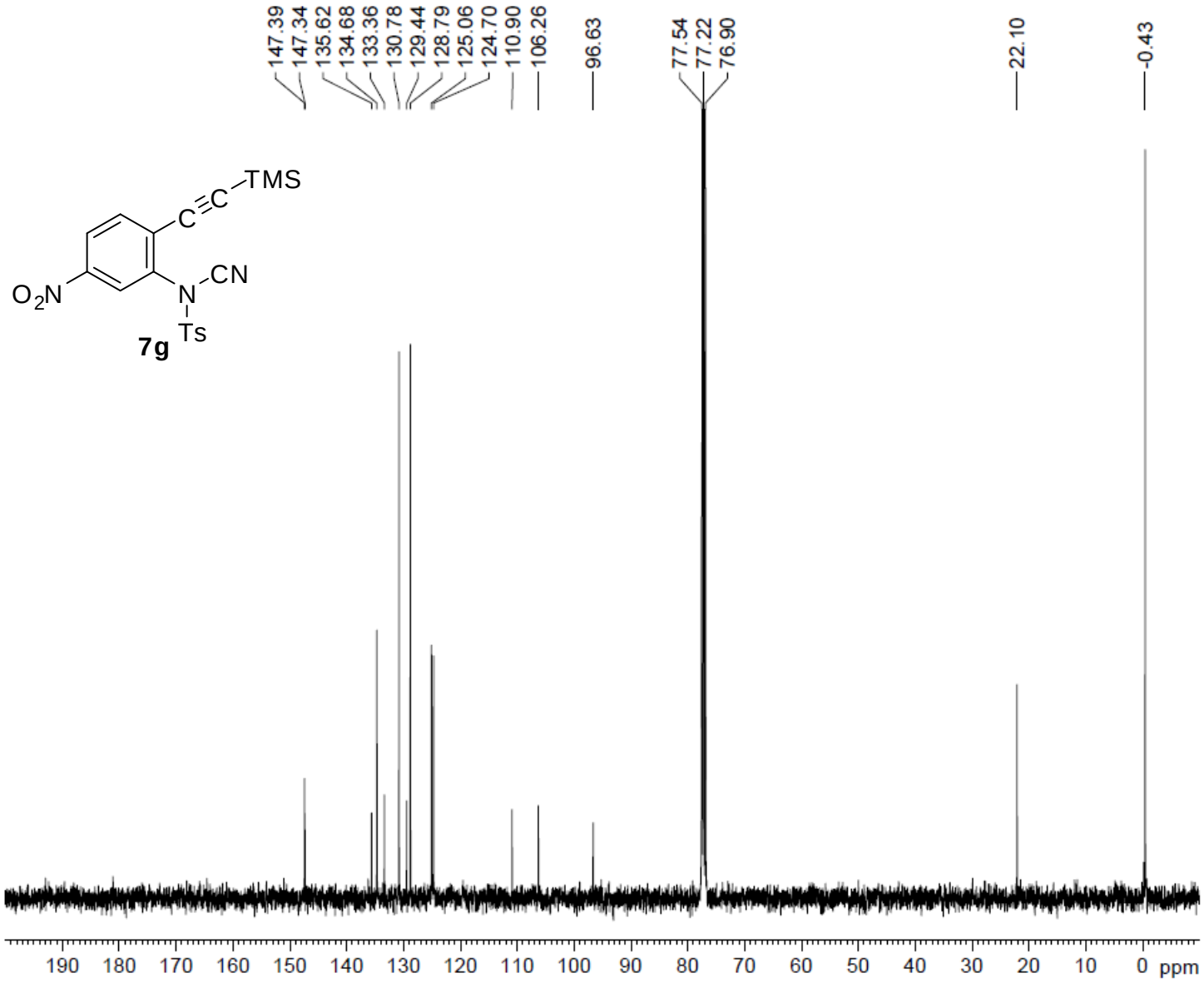


Current Data Parameters
NAME SC181-2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140831
Time 14.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



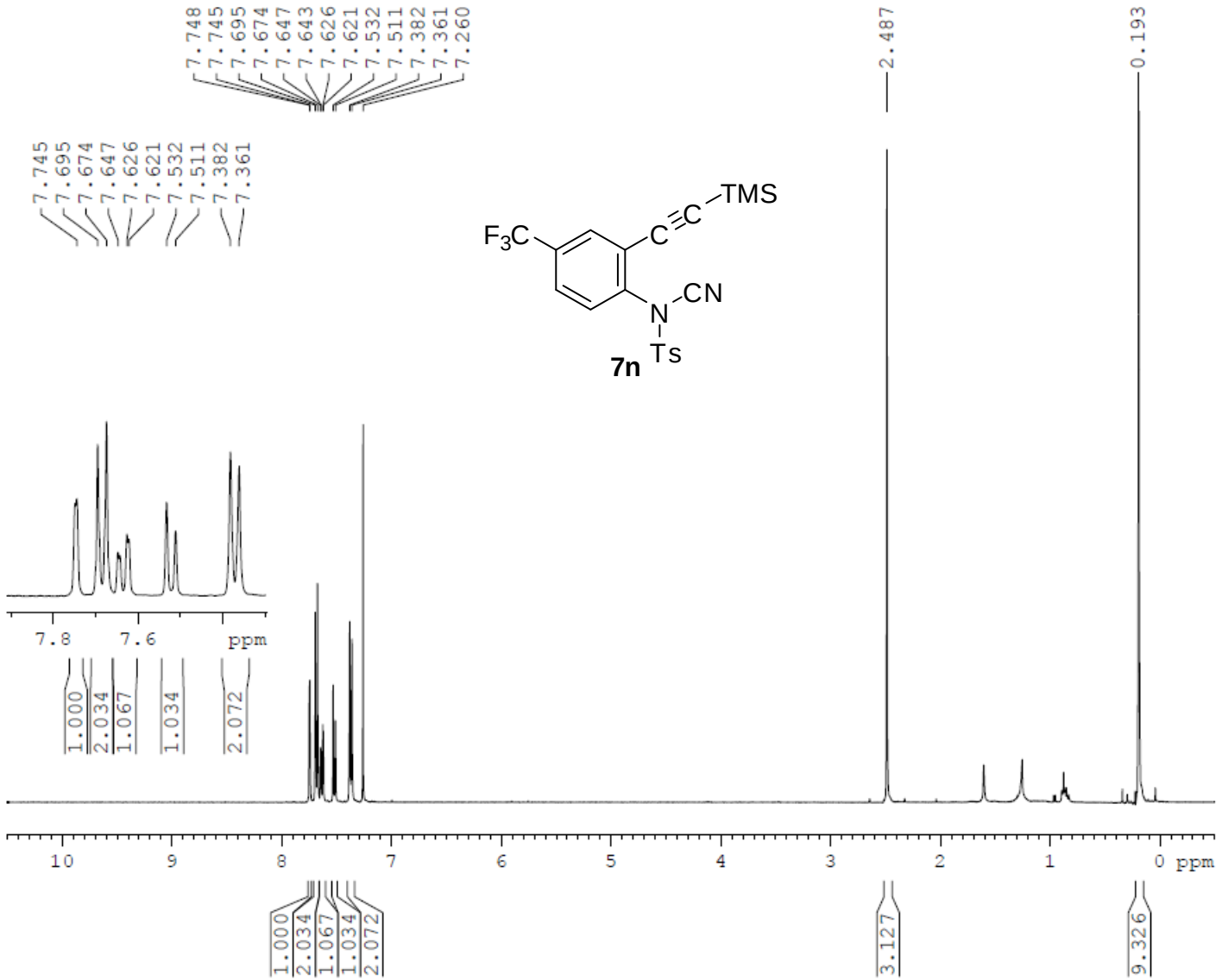
Current Data Parameters
NAME SC181-2
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140831
Time 14.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 251
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127485 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

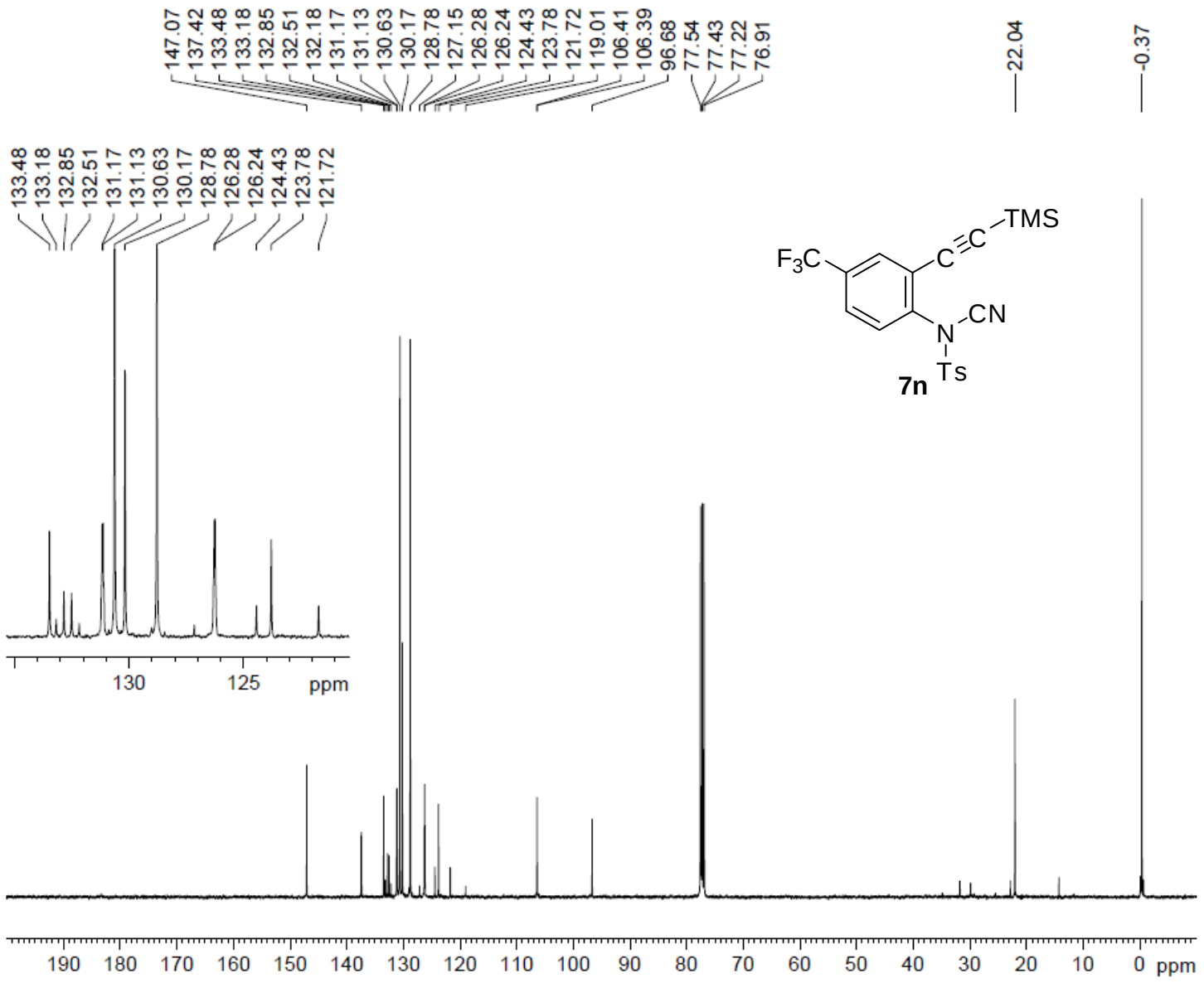


Current Data Parameters
NAME SC176
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140825
Time 8.41
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 57.42
DW 69.333 usec
DE 10.52 usec
TE 298.7 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



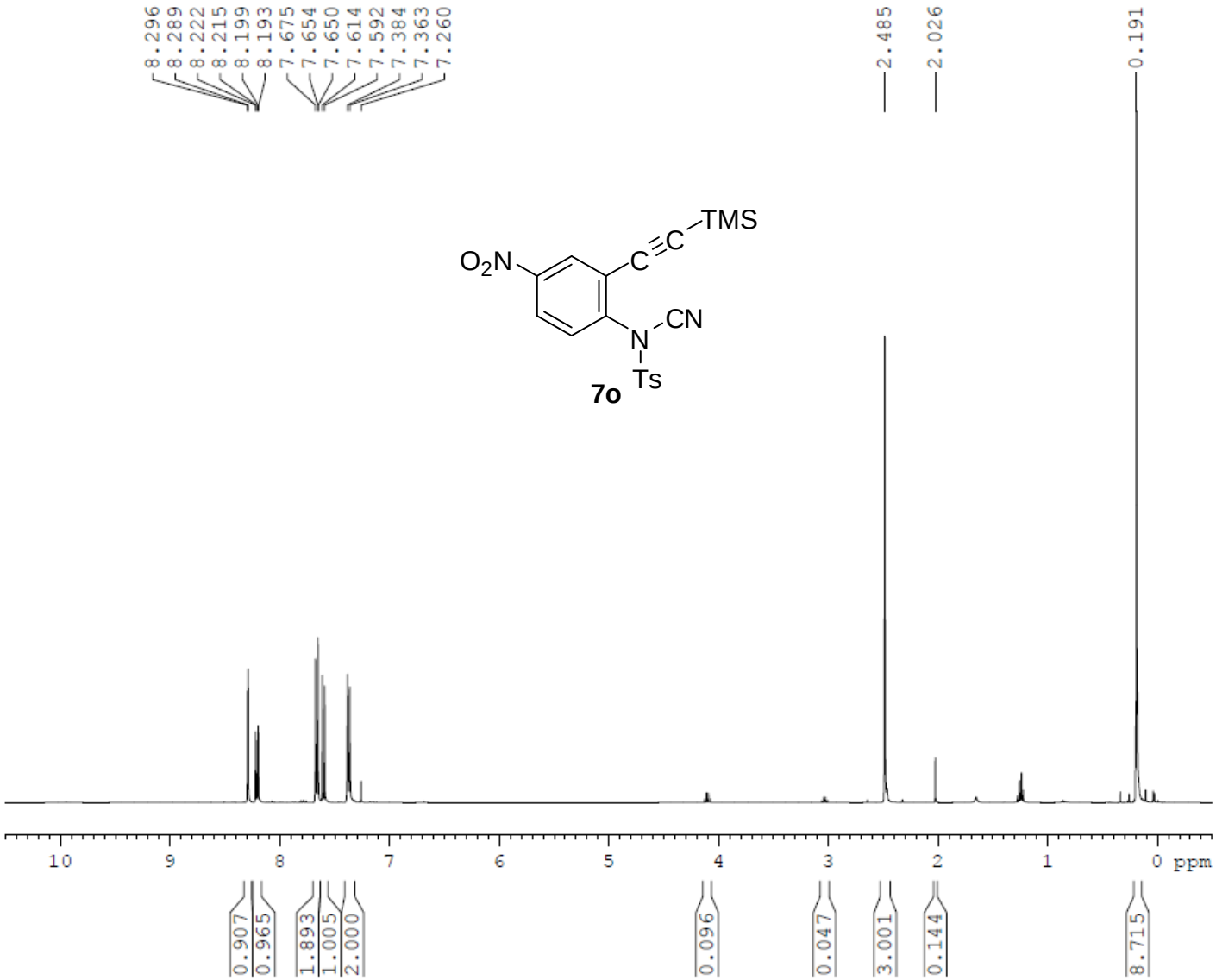
Current Data Parameters
NAME SC176
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140826
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1744
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

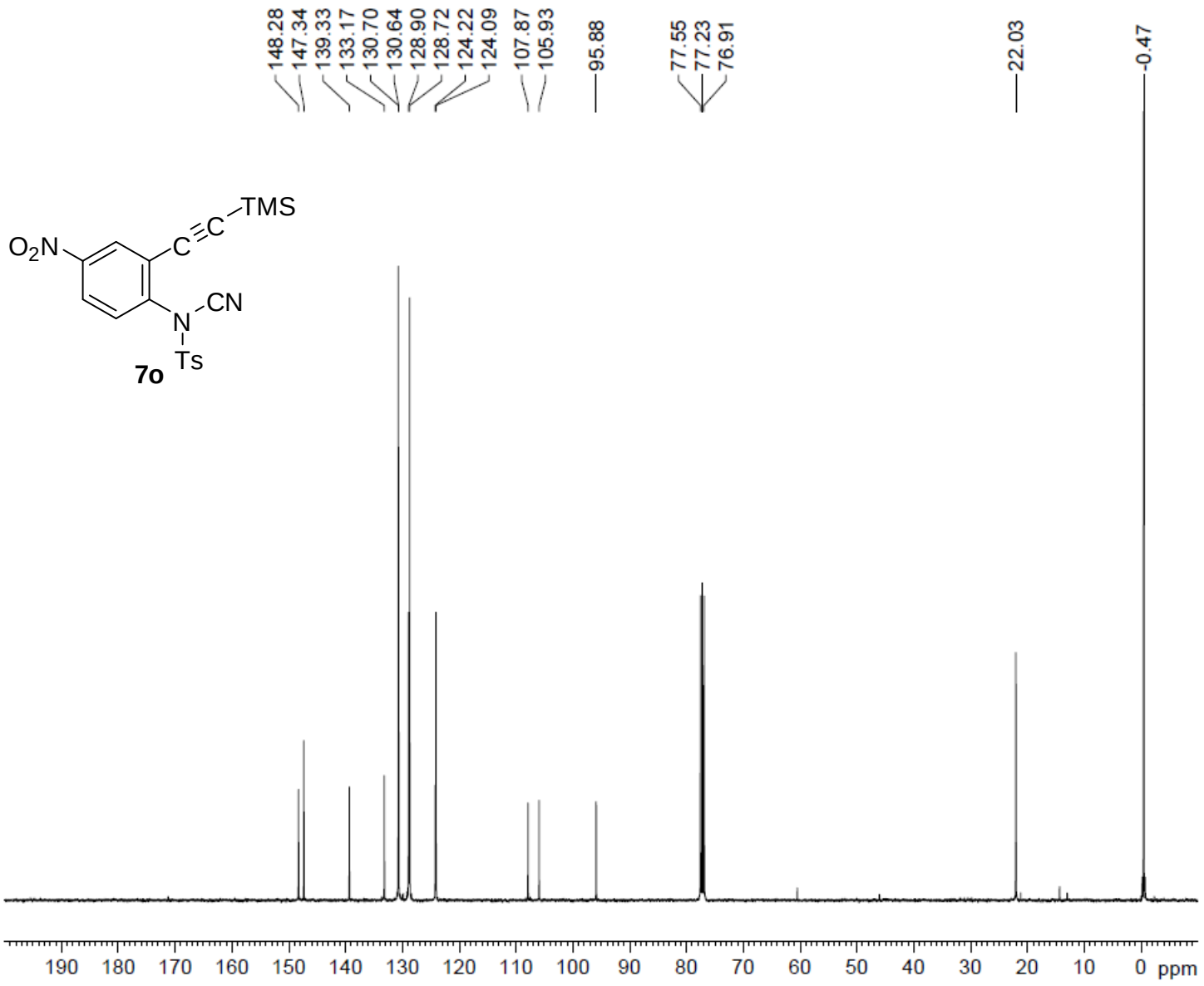


Current Data Parameters
NAME SO071
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150203
Time 8.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 38.89
DW 69.333 usec
DE 10.52 usec
TE 297.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



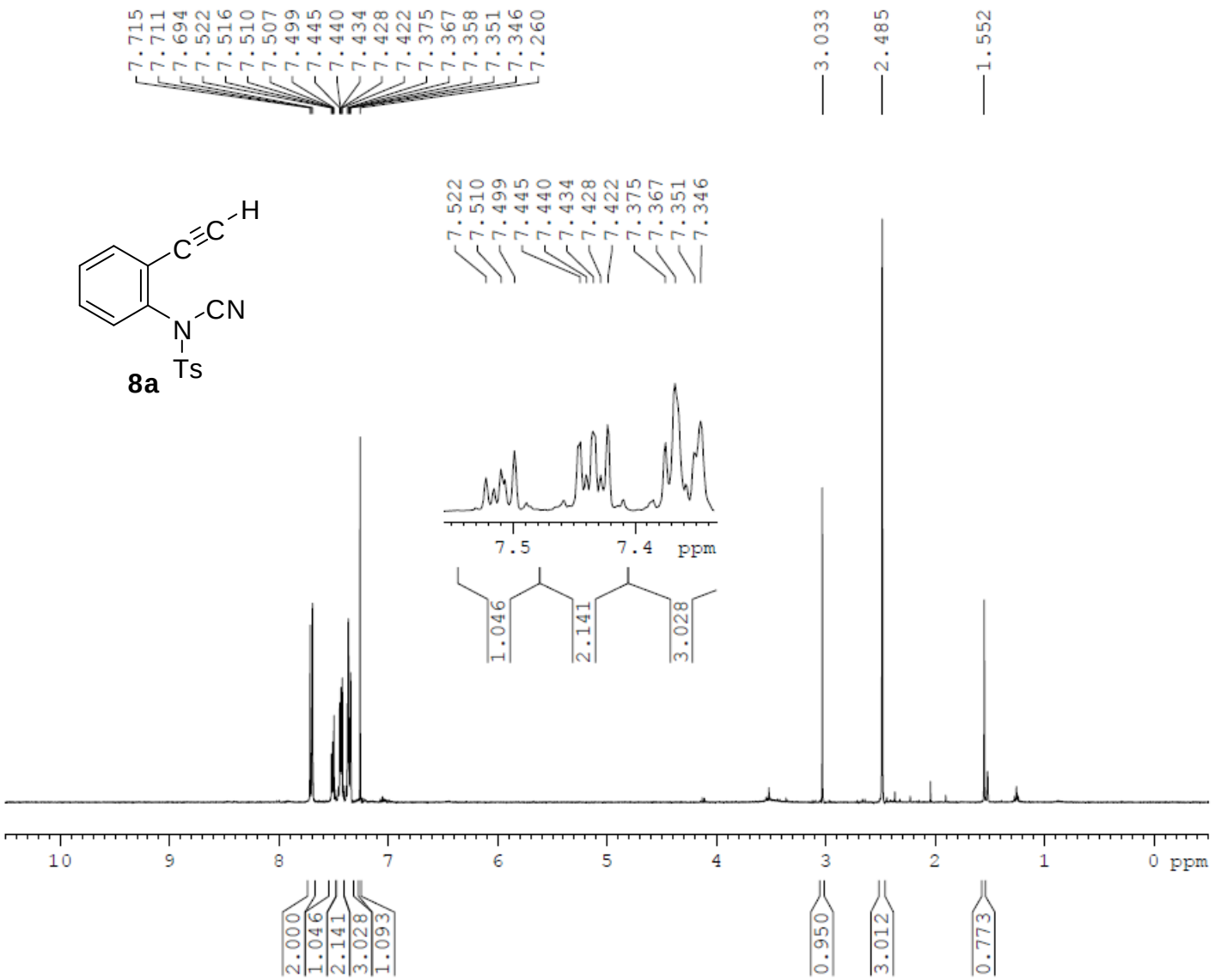
Current Data Parameters
NAME SO071
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150203
Time 9.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

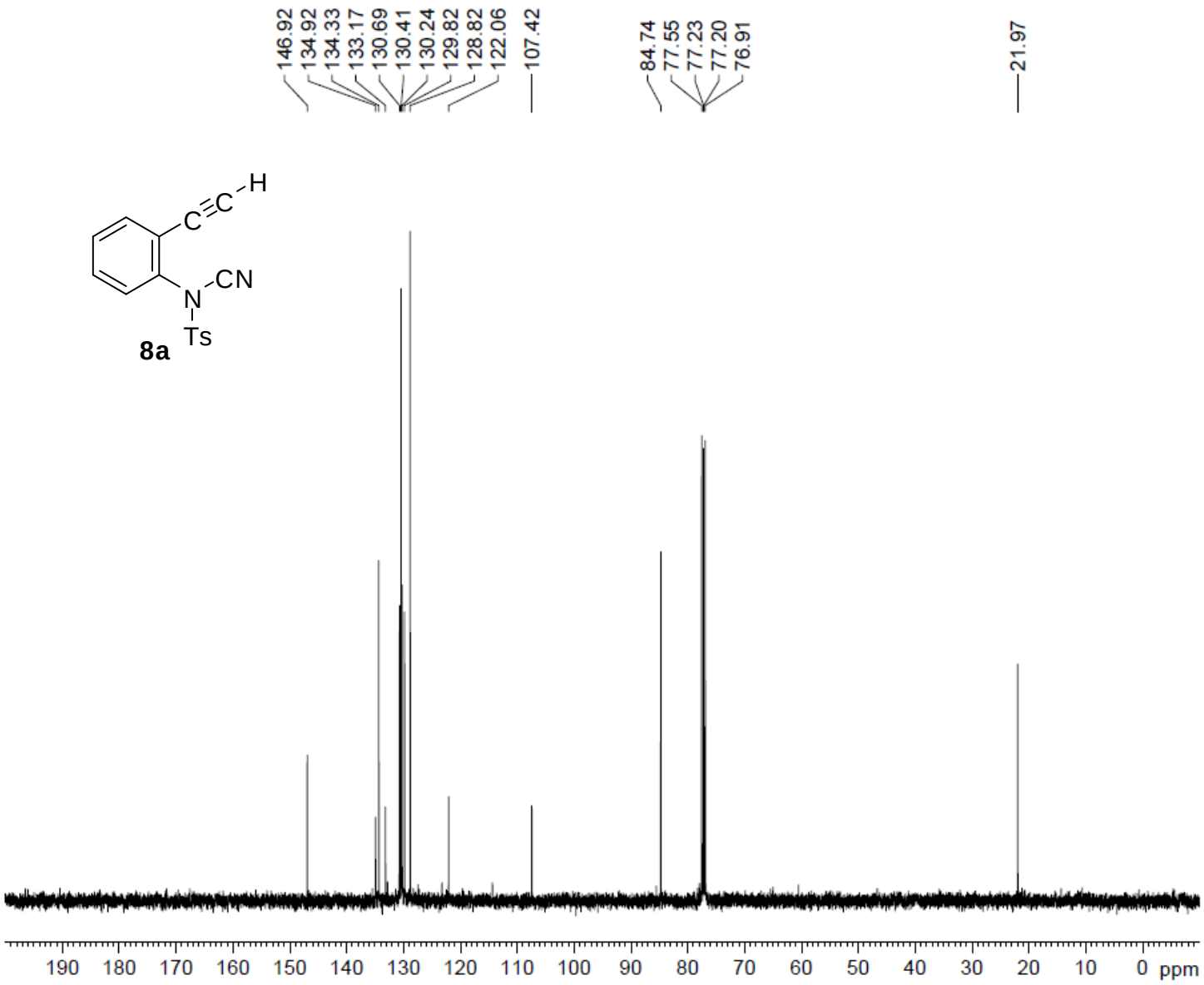
======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127537 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



NAME SO103
EXPNO 1
PROCNO 1
Date_ 20150406
Time 11.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2611110 sec
RG 574.7
DW 69.000 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



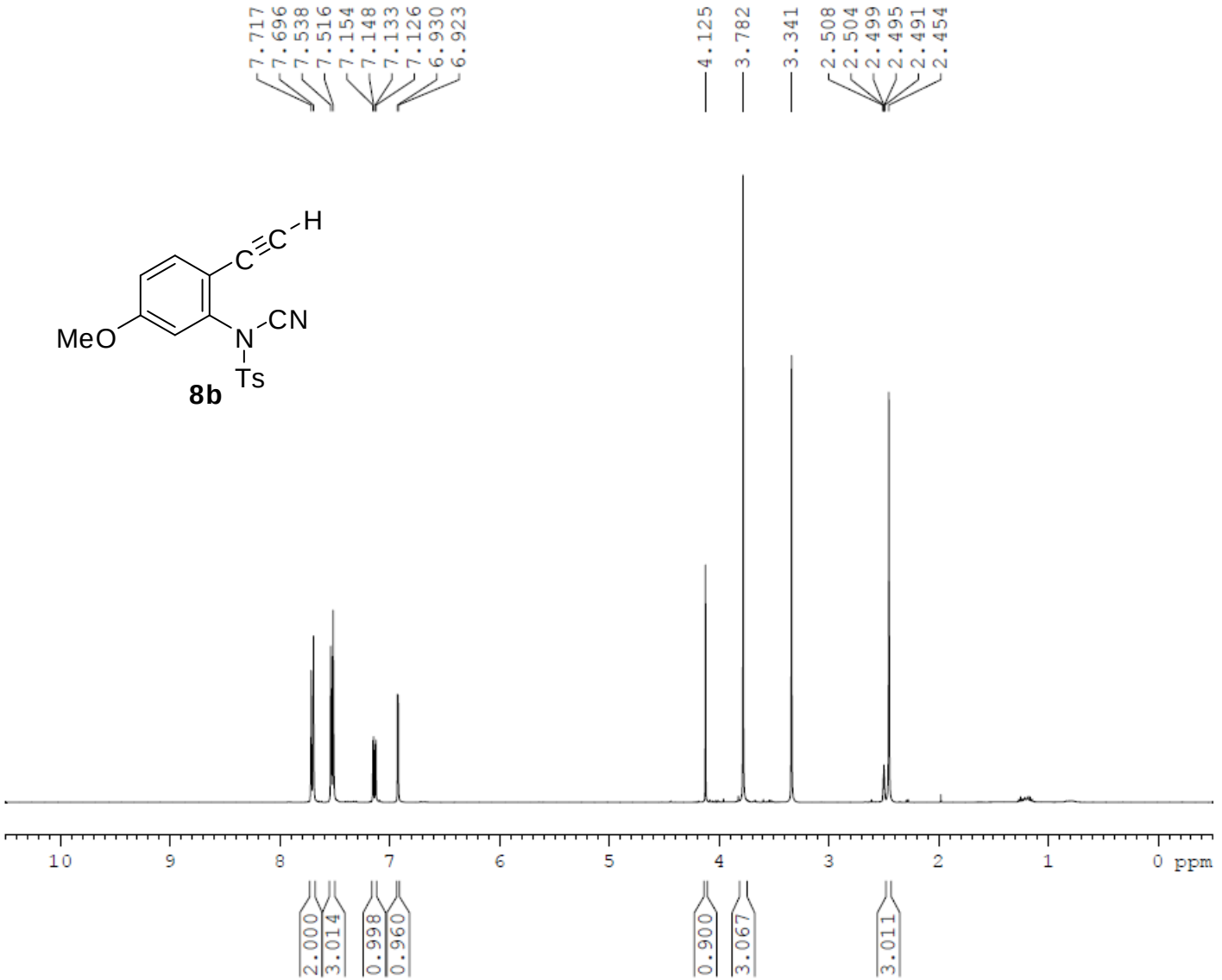
Current Data Parameters
NAME SO103
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150409
Time 13.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 53
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 294.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127581 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

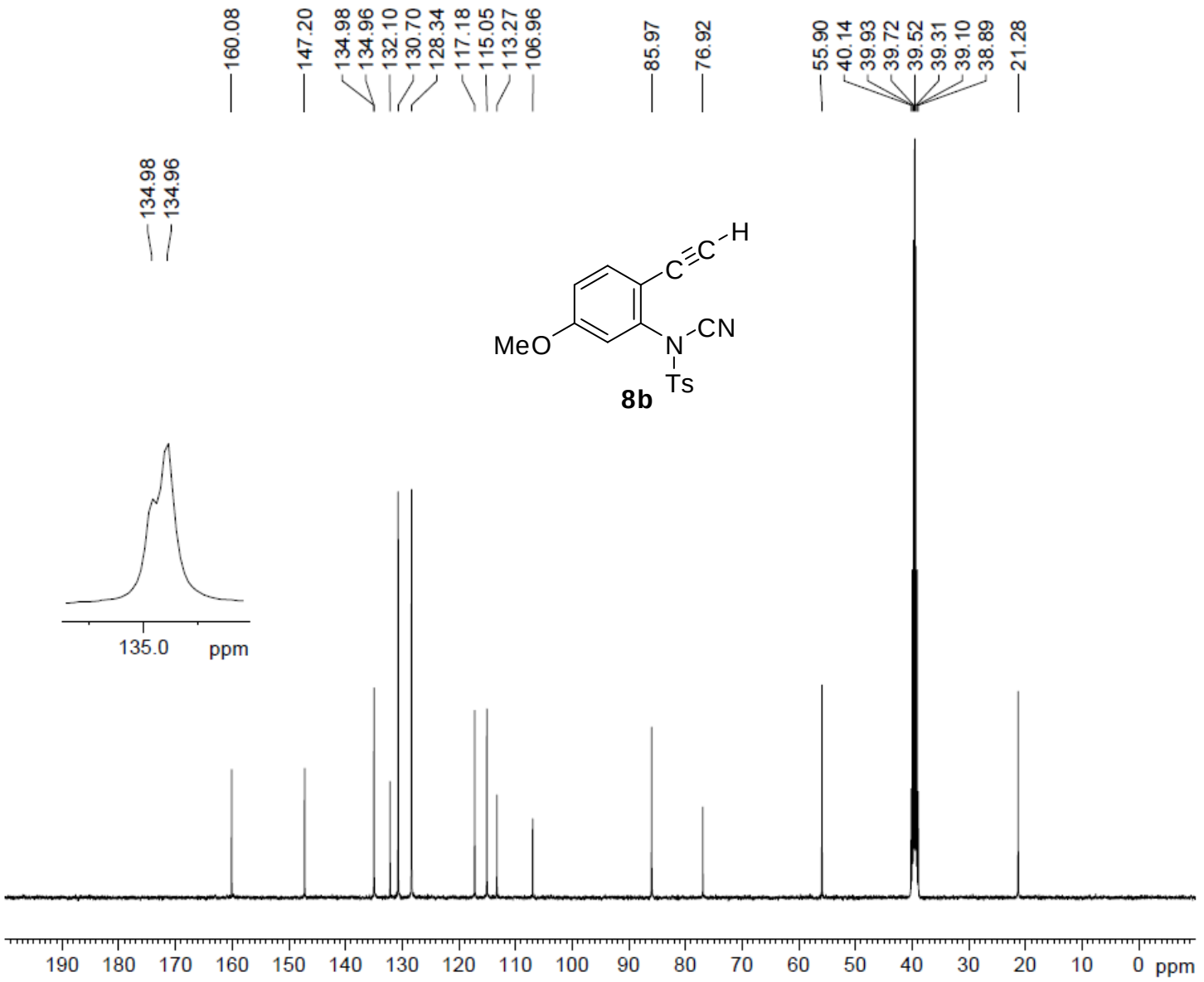


Current Data Parameters
NAME SD-102-DMSO(new)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140707
Time 13.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 63.58
DW 69.333 usec
DE 10.52 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300034 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



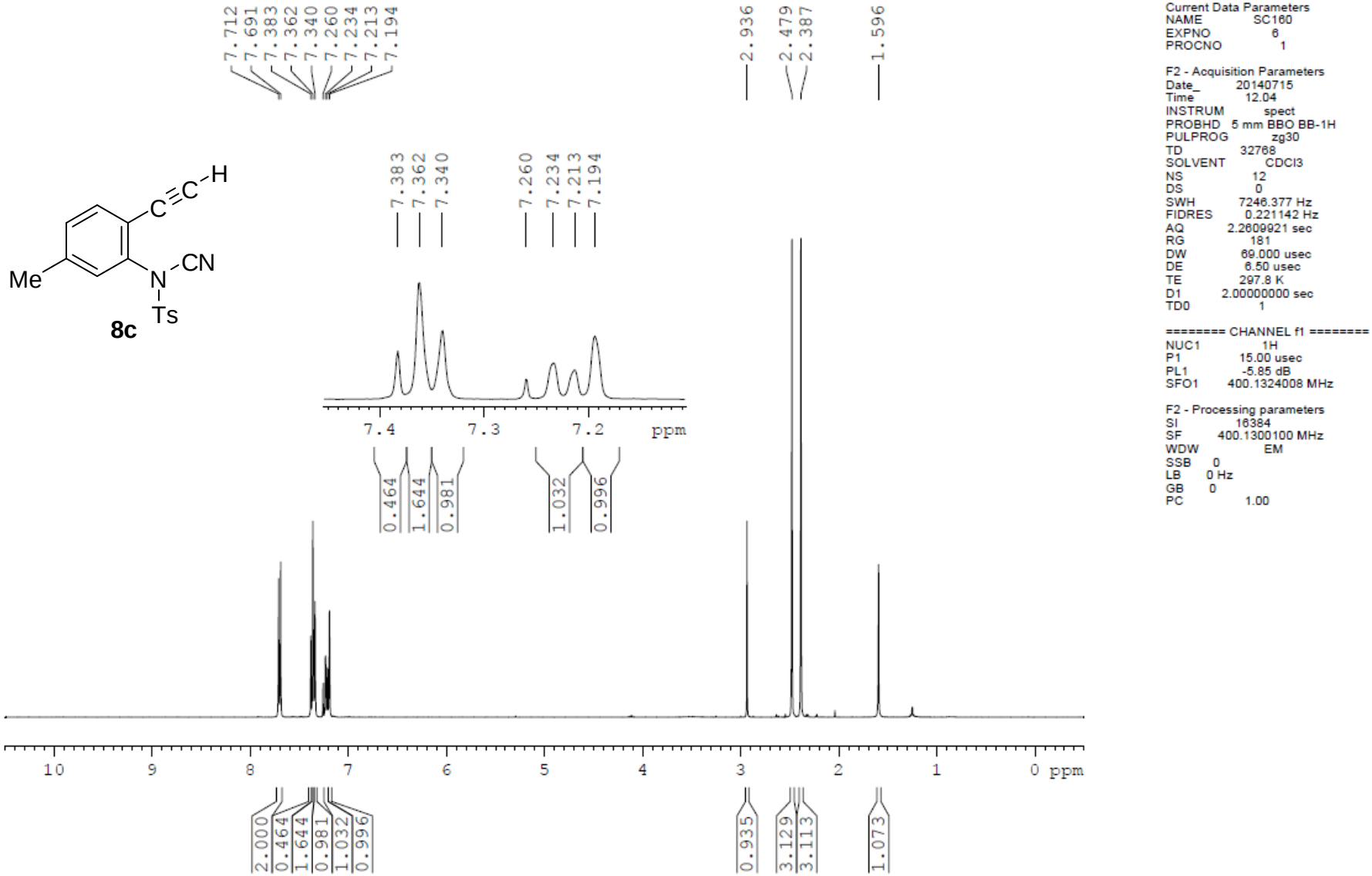
Current Data Parameters
NAME SD-102-DMSO(new)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140707
Time 14.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1046
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6128192 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

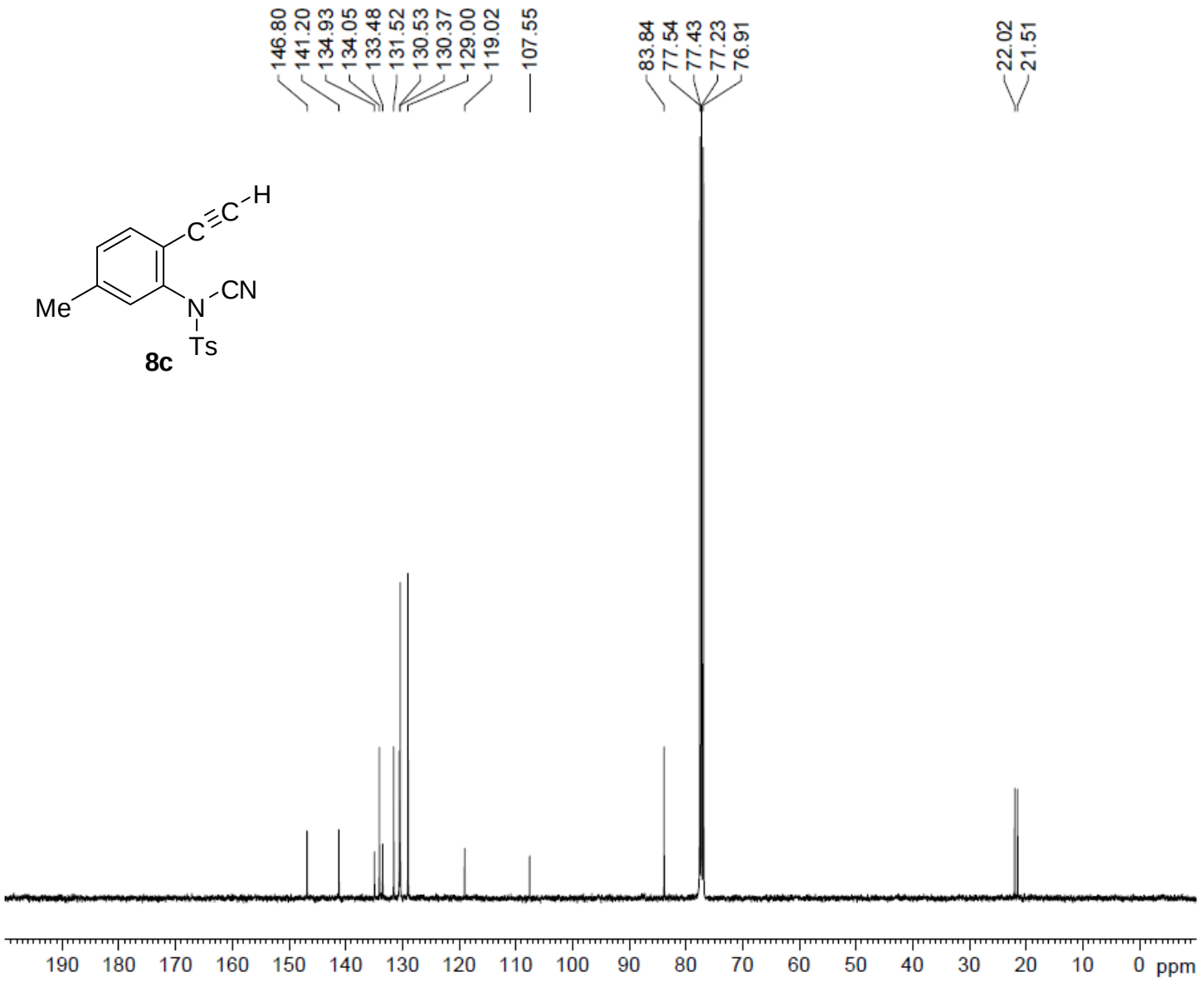


Current Data Parameters
NAME SC160
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140715
Time 12.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300100 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SC160
EXPNO 1
PROCNO 1

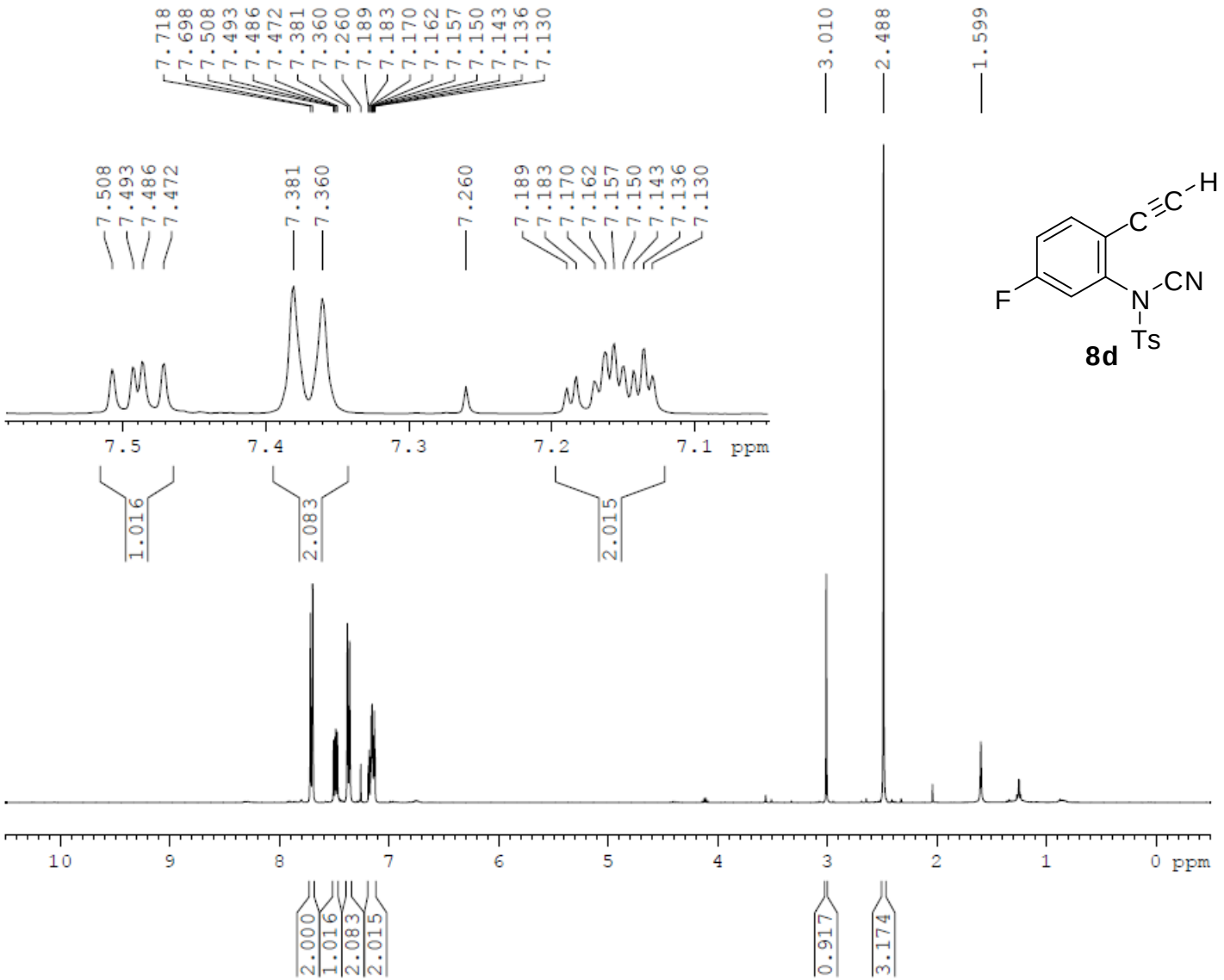
F2 - Acquisition Parameters
Date_ 20140716
Time 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 963
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127484 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

first point



8d

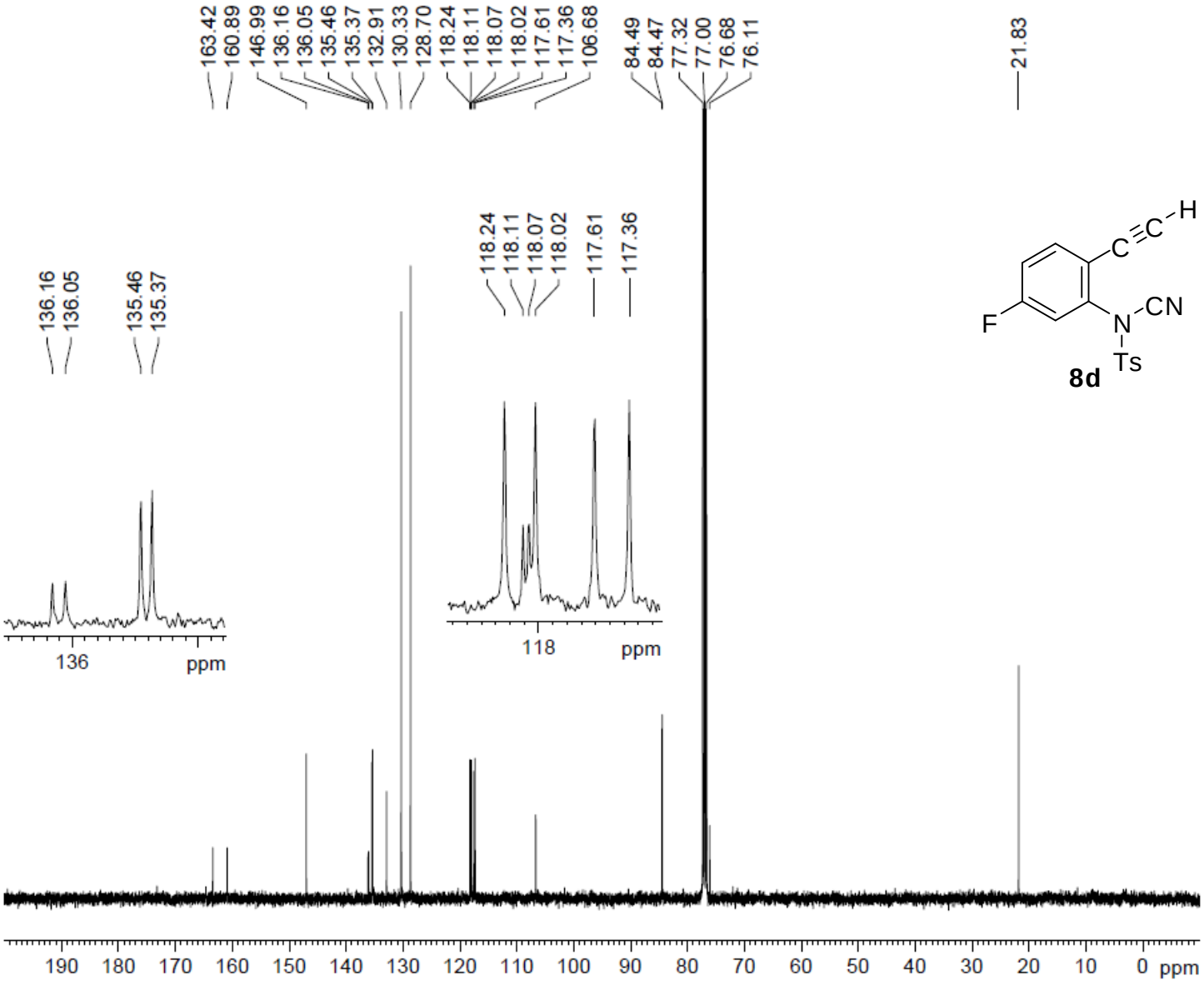
Current Data Parameters
NAME SD-083(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140604
Time 14.48
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

first point



8d

Current Data Parameters
NAME SD-083(old)
EXPNO 4
PROCNO 1

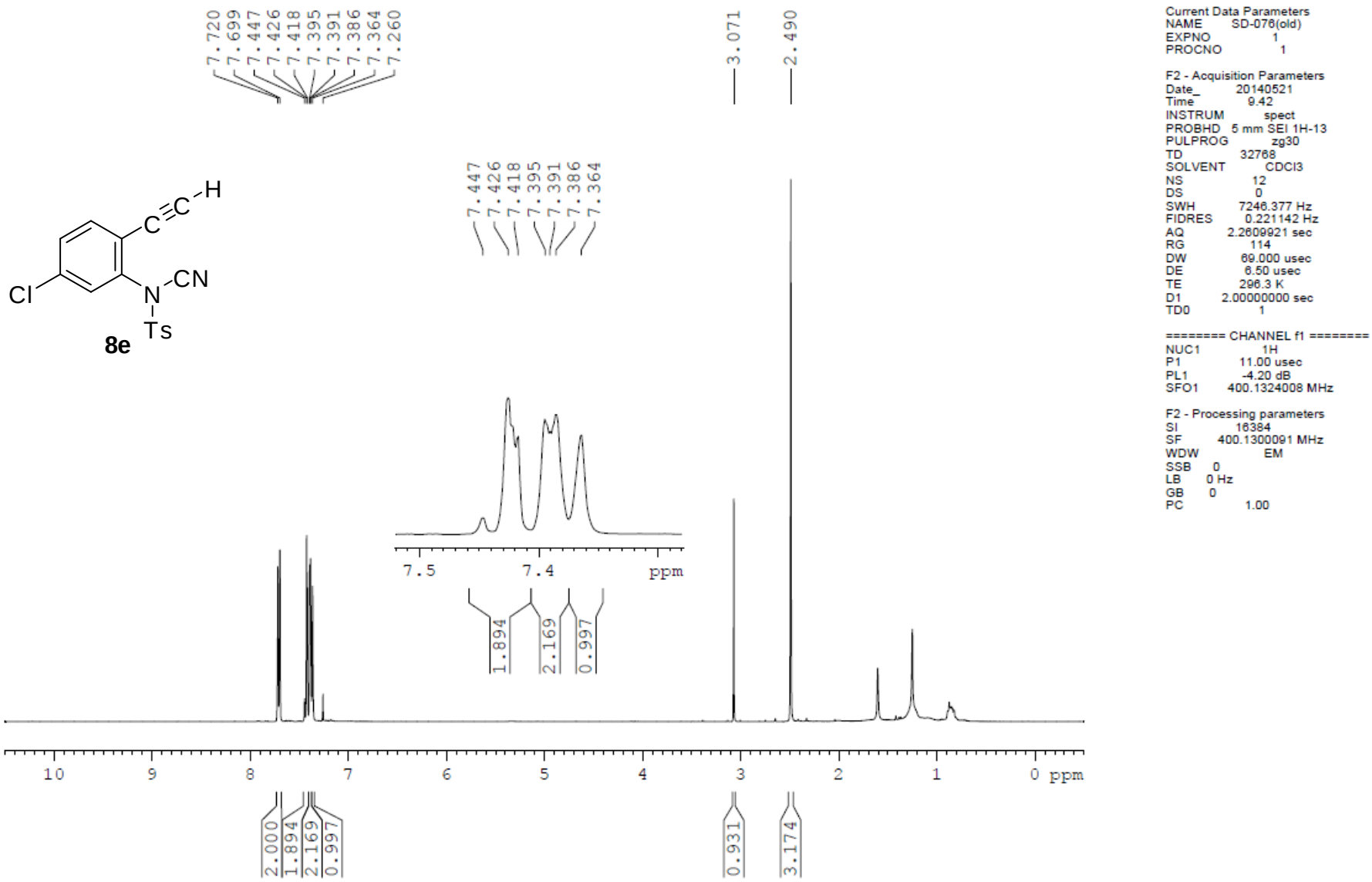
F2 - Acquisition Parameters
Date_ 20140604
Time 18.46
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1047
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127723 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

pure



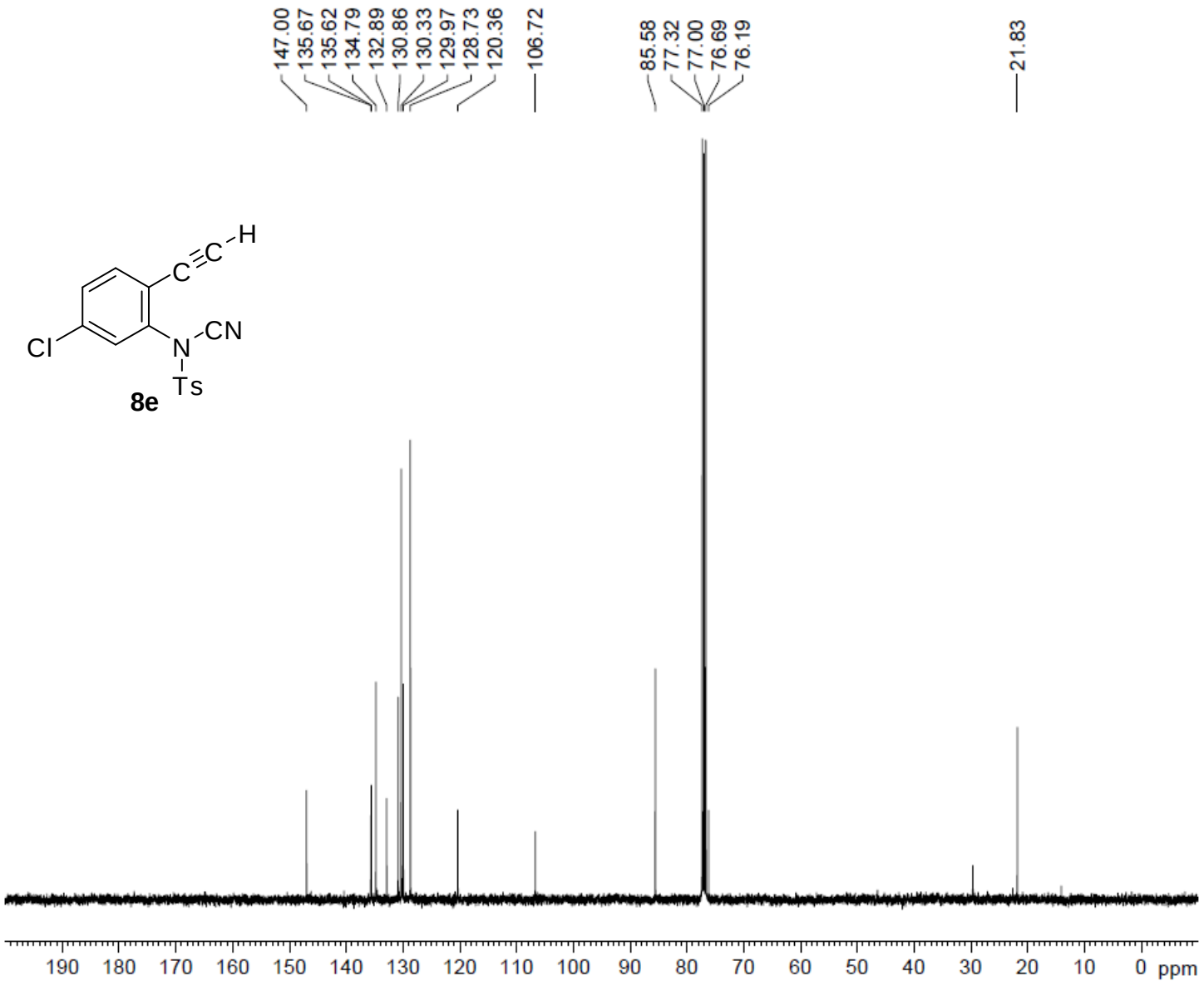
Current Data Parameters
NAME SD-076(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140521
Time 9.42
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



Current Data Parameters
NAME SD-076(old)
EXPNO 4
PROCNO 1

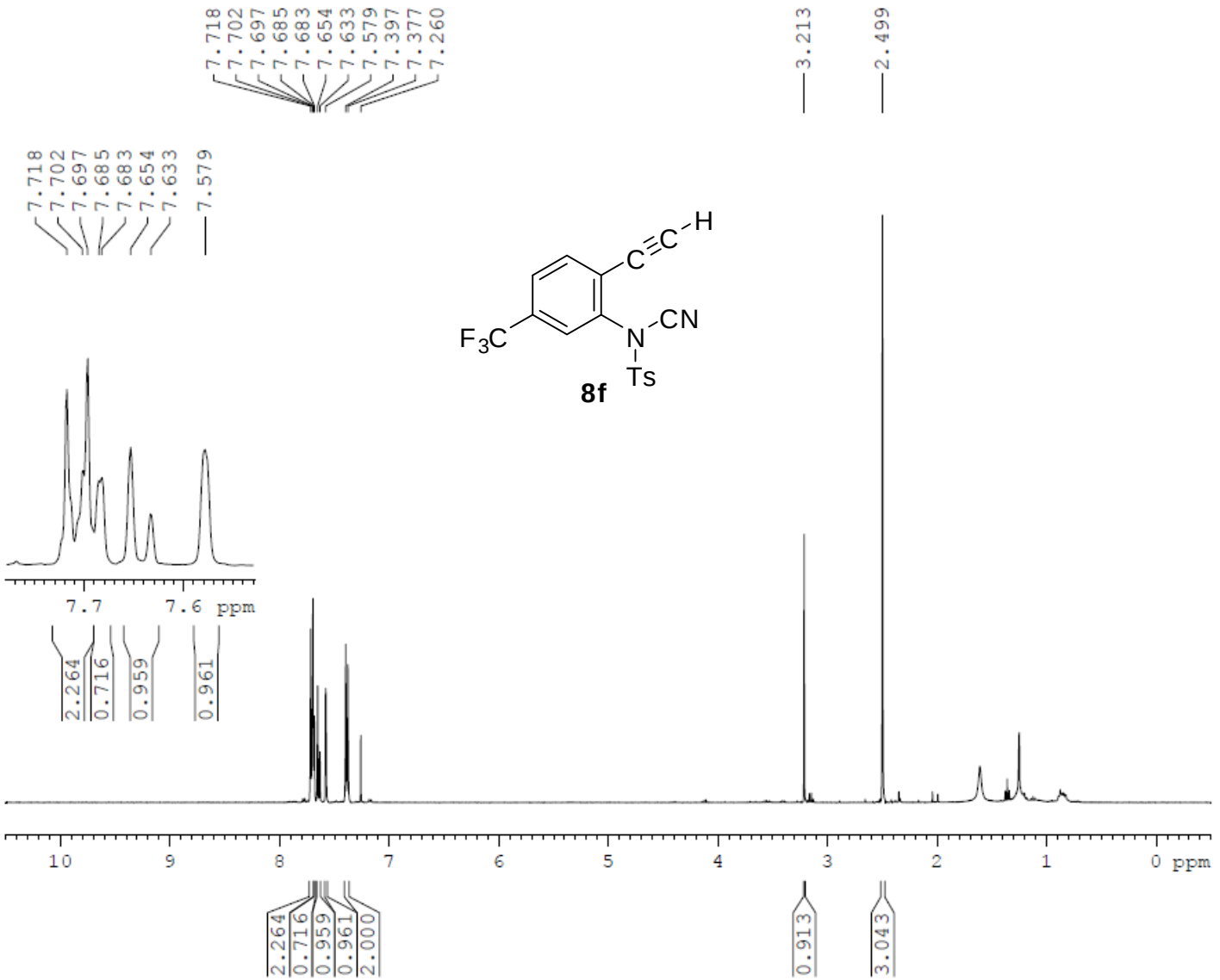
F2 - Acquisition Parameters
Date_ 20140521
Time 19.03
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1129
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 7298.2
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127723 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

pure



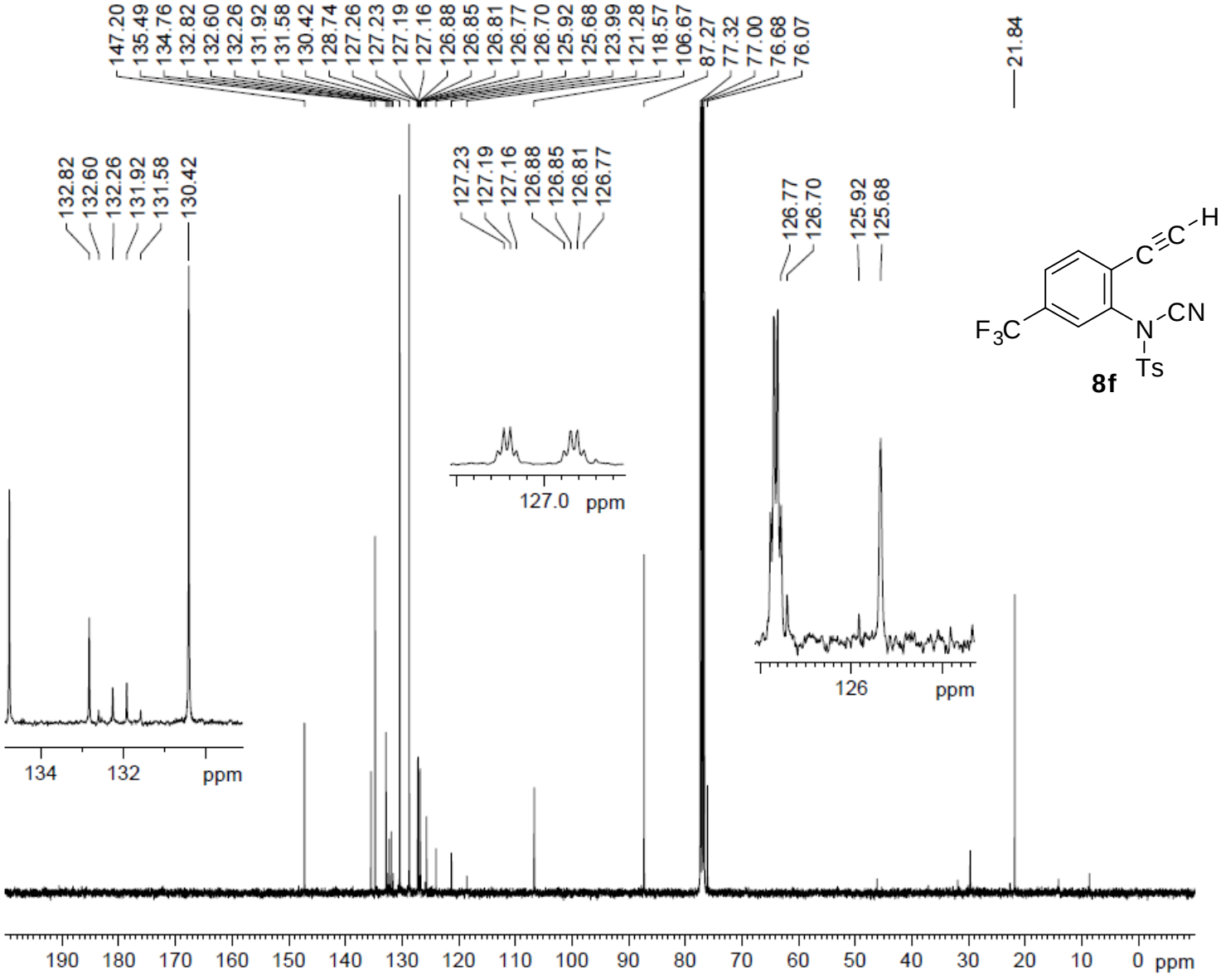
Current Data Parameters
NAME SD-073-pure(old)
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140521
Time 21.59
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



8f

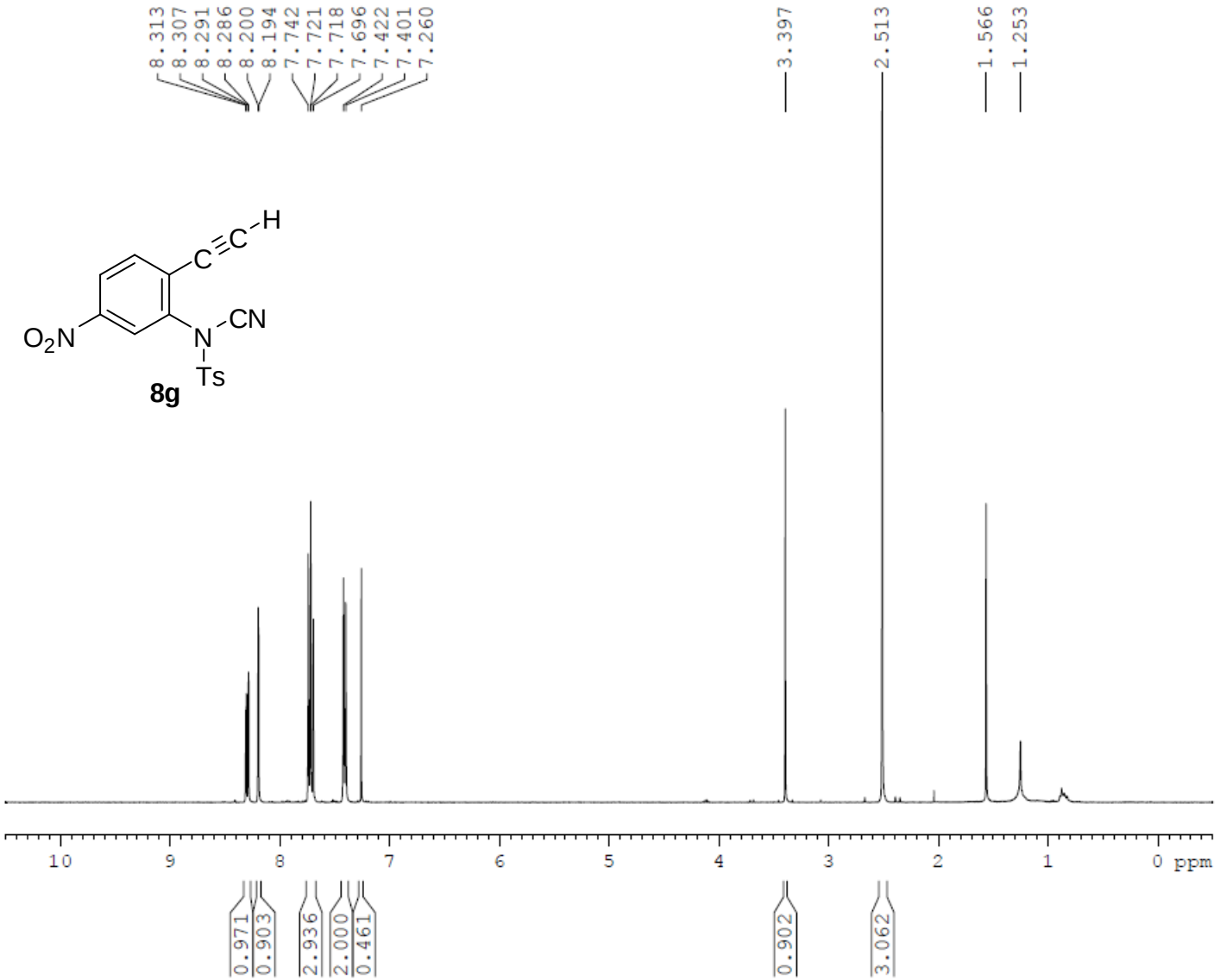
Current Data Parameters
NAME SD-073-pure(old)
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140521
Time 22.59
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 12000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127701 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

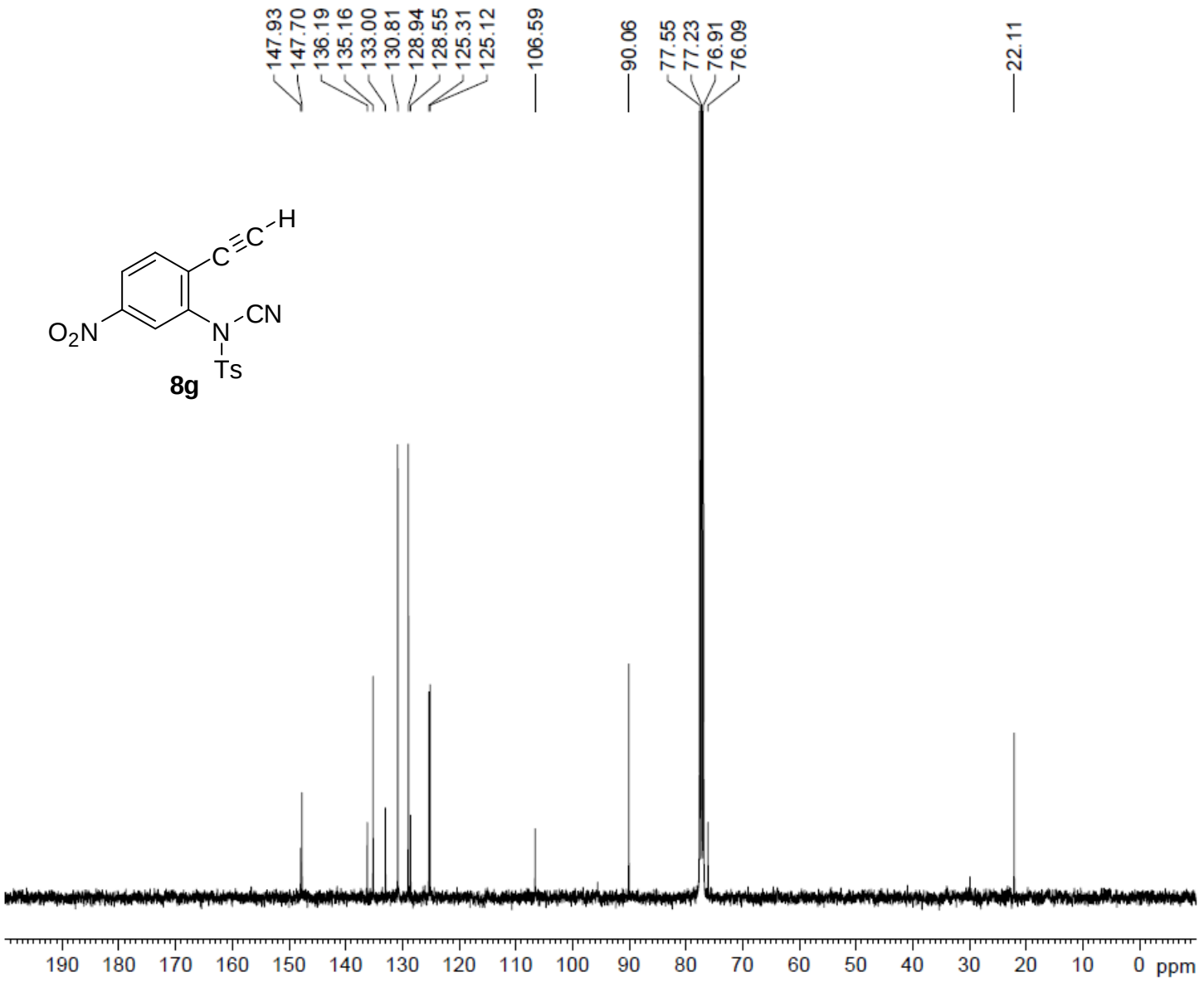


Current Data Parameters
NAME SC183
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 18.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 198.09
DW 69.333 usec
DE 10.52 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



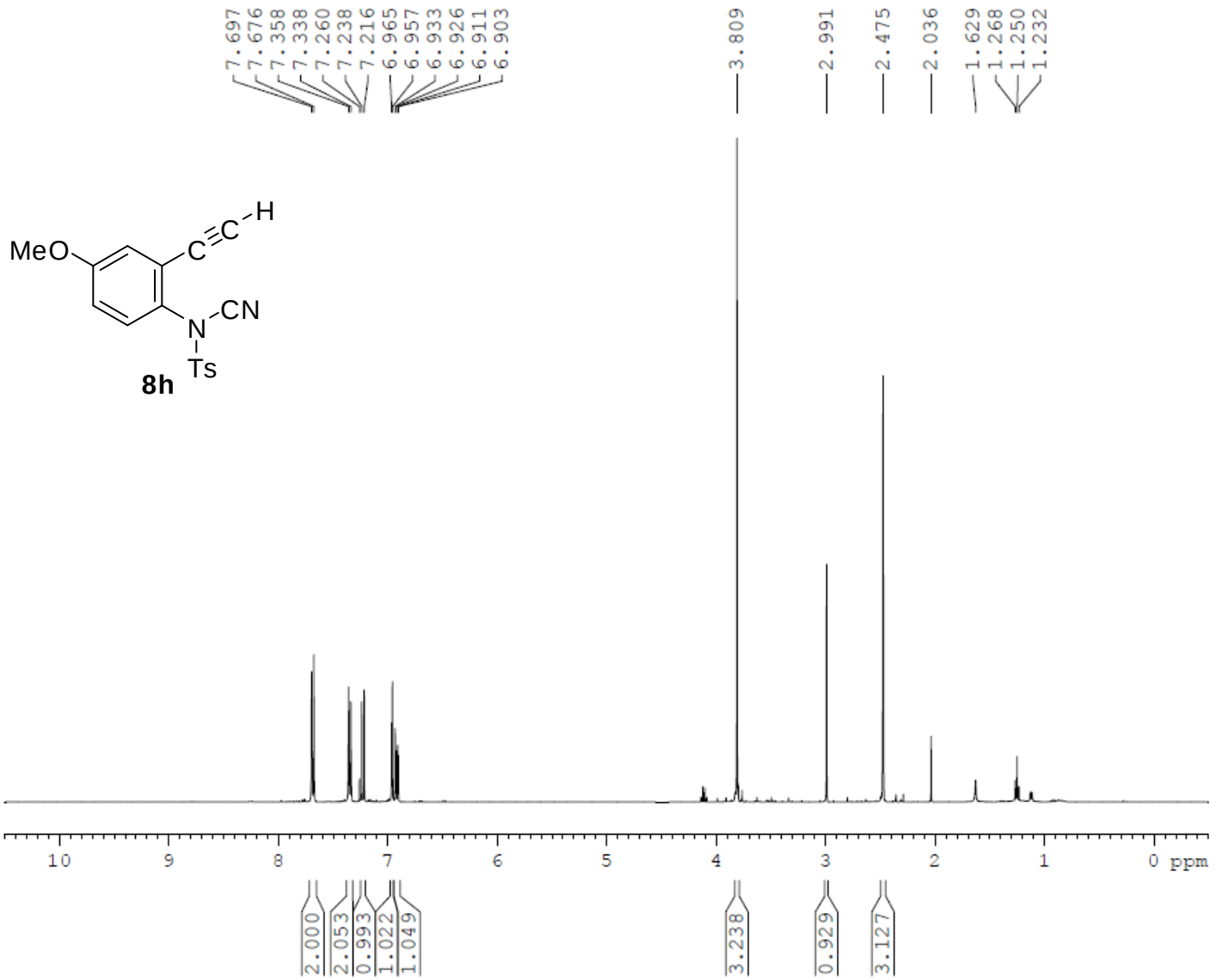
Current Data Parameters
NAME SC183
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140904
Time 19.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 619
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127471 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

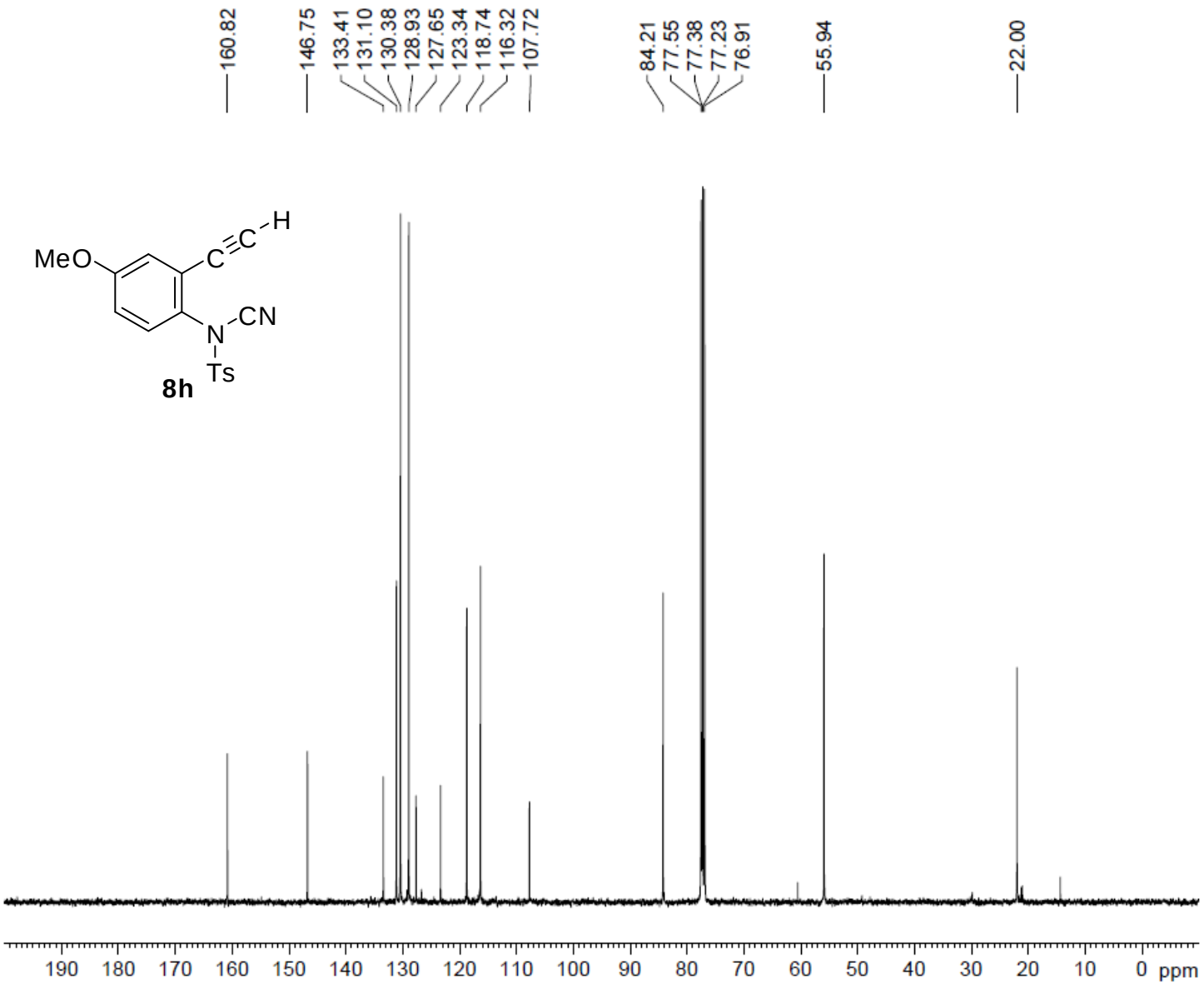


Current Data Parameters
NAME SC106
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140416
Time 8.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 71.42
DW 69.333 usec
DE 10.52 usec
TE 298.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SC106
EXPNO 3
PROCNO 1

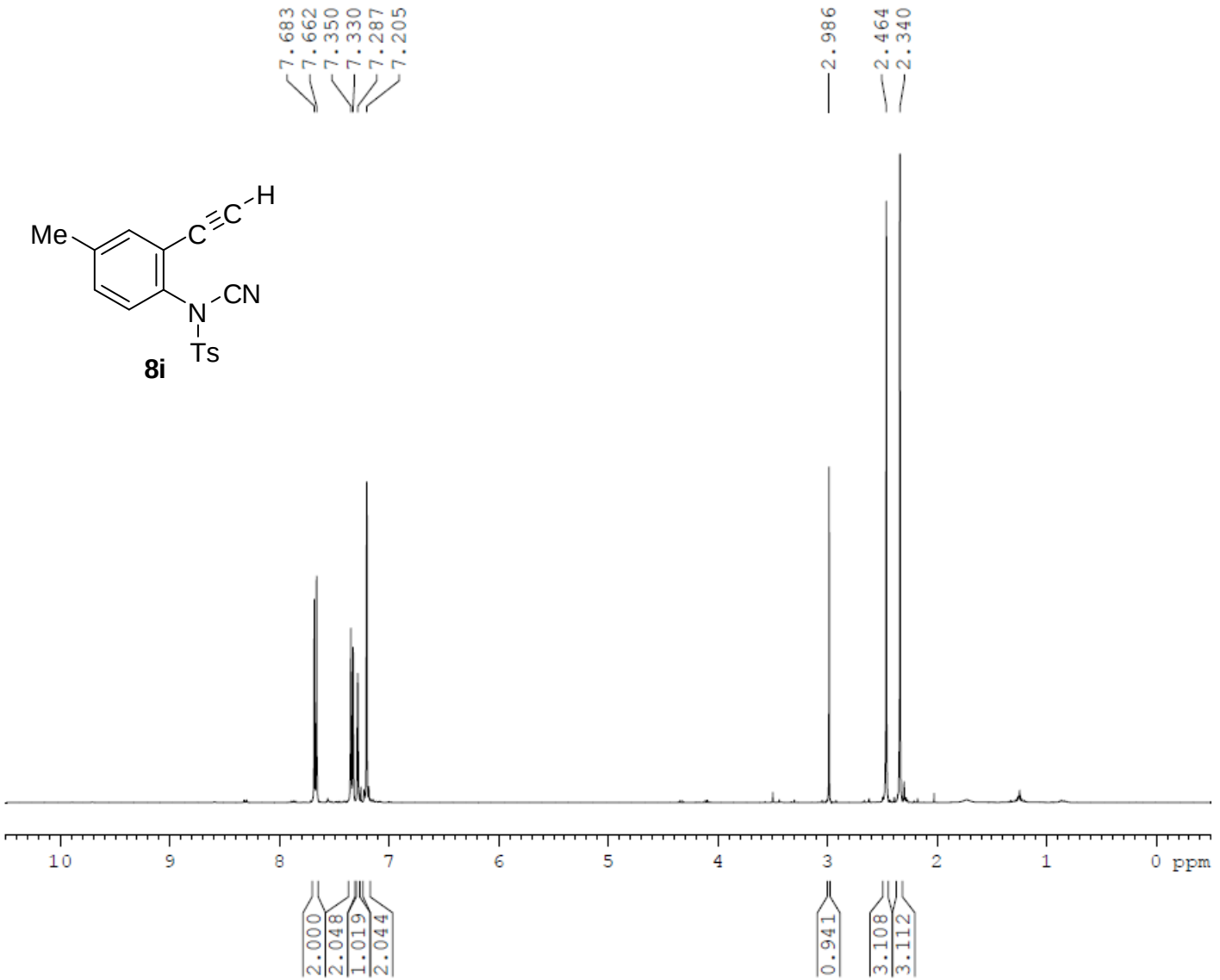
F2 - Acquisition Parameters
Date_ 20140416
Time 9.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1092
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127507 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

pure



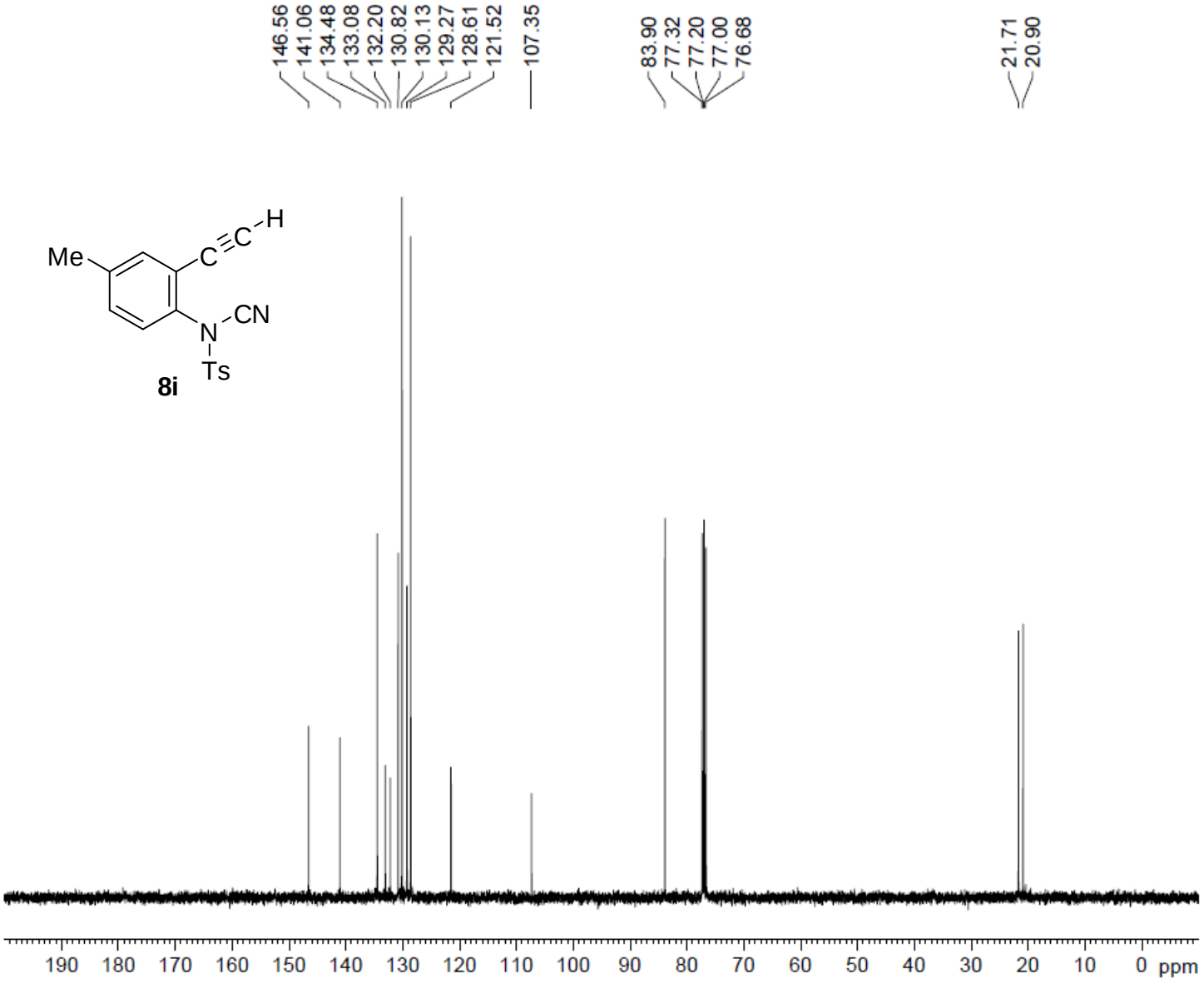
Current Data Parameters
NAME SD-061(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140423
Time 14.18
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 45.3
DW 69.000 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



Current Data Parameters
NAME SD-061(old)
EXPNO 4
PROCNO 1

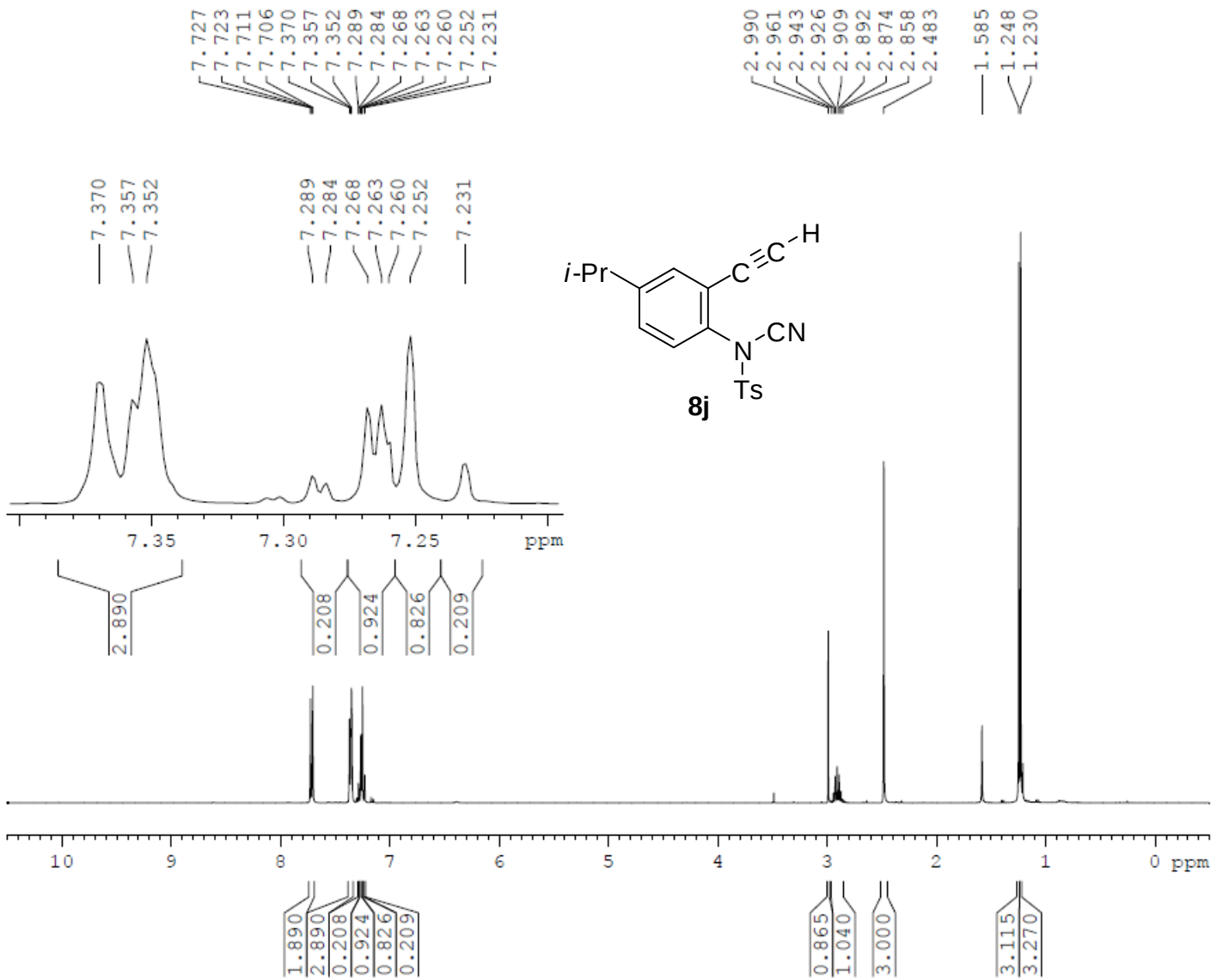
F2 - Acquisition Parameters
Date_ 20140423
Time 19.38
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 206
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127797 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

pure



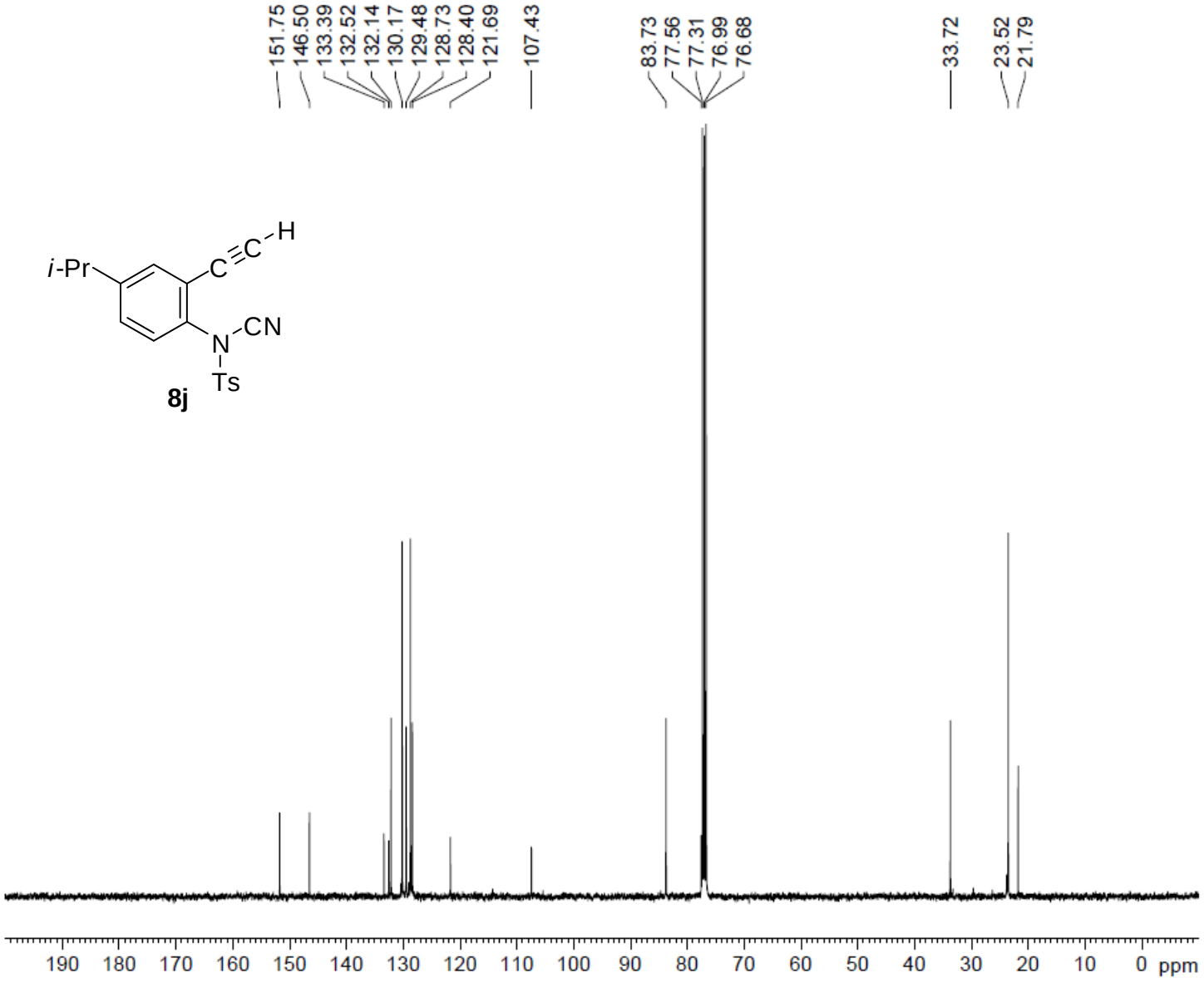
Current Data Parameters
NAME SD-091(new)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140622
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 89.08
DW 69.333 usec
DE 10.52 usec
TE 299.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



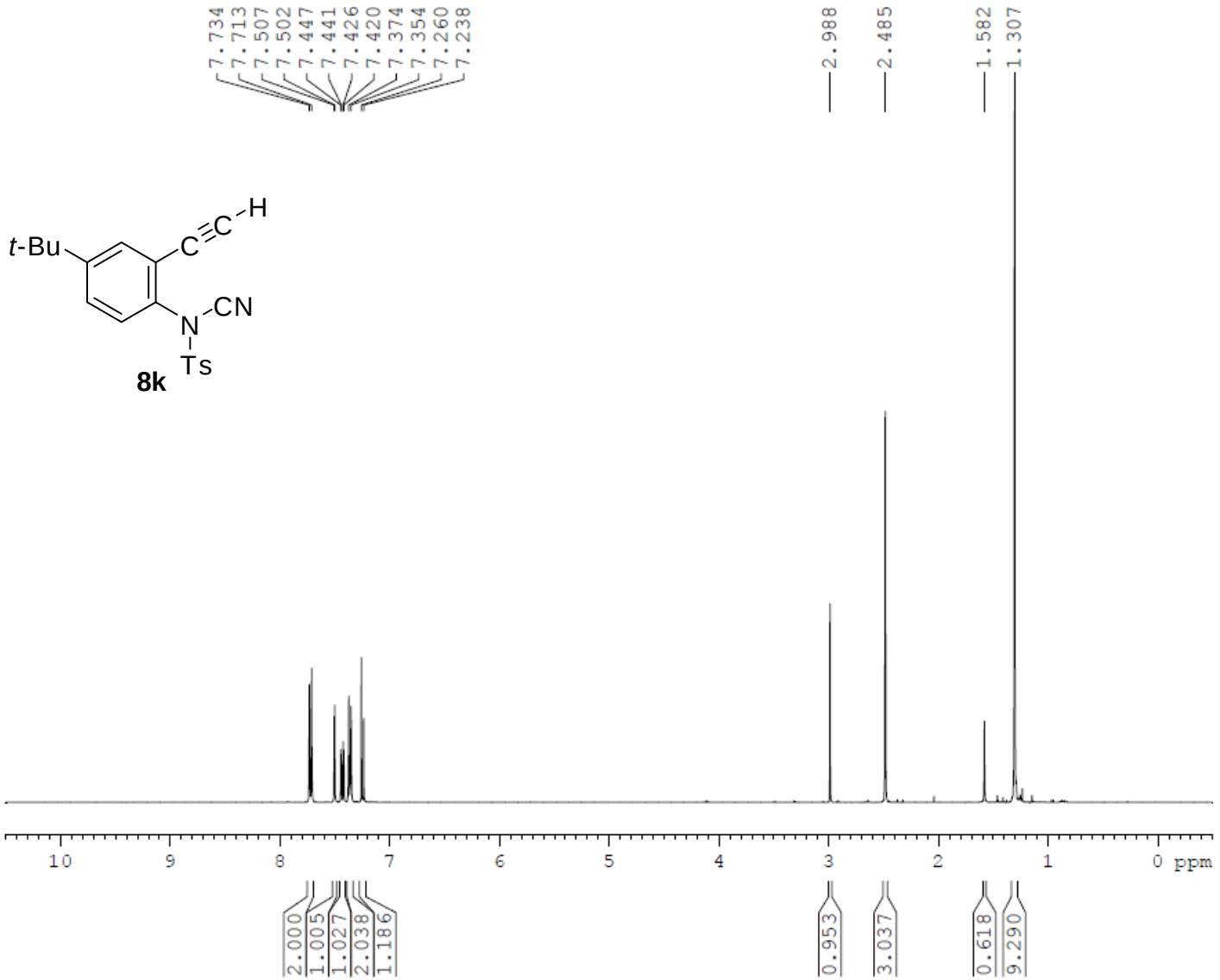
Current Data Parameters
NAME SD-091(new)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140622
Time 10.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 988
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127713 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

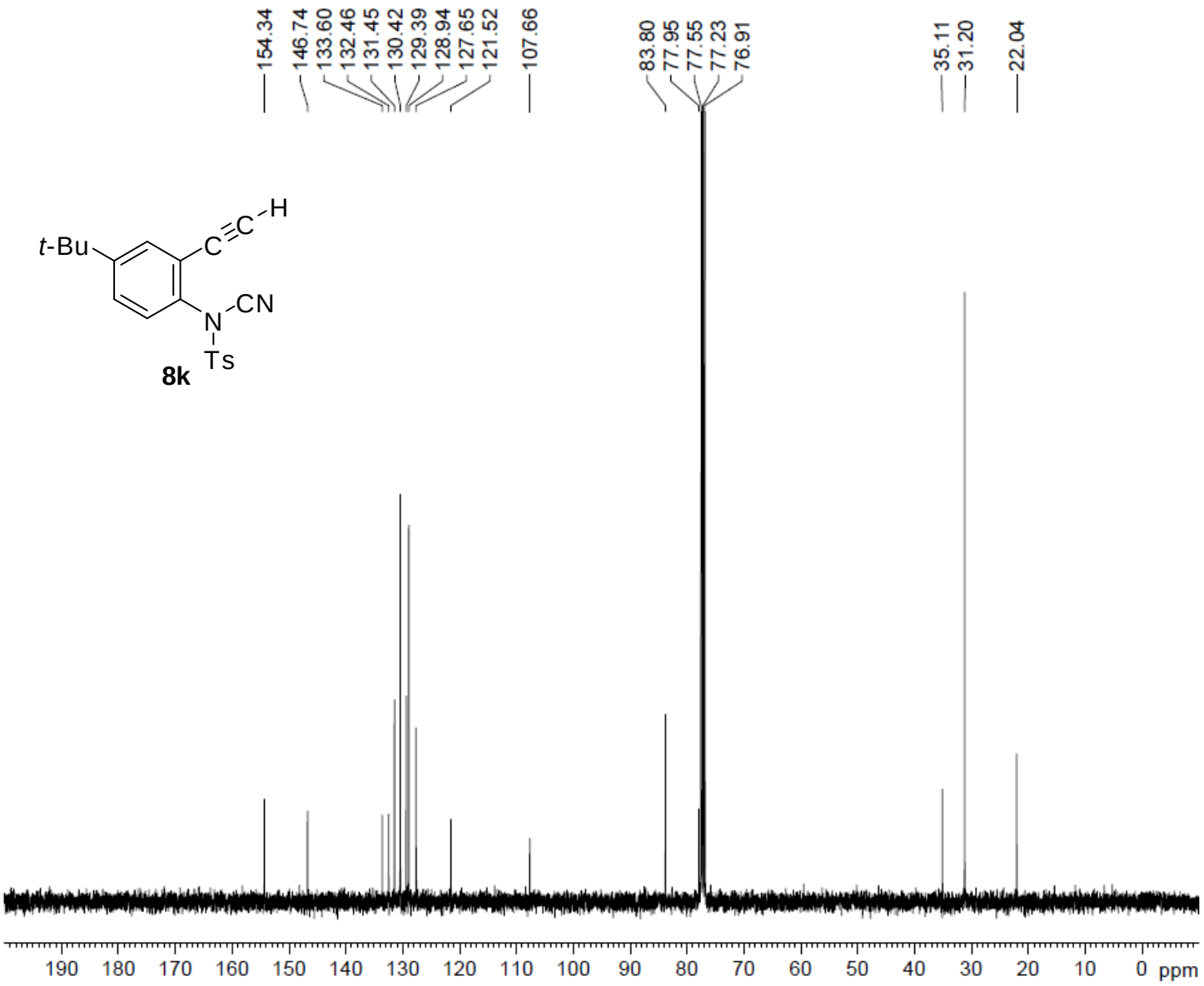


Current Data Parameters
NAME SC157
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140707
Time 9.58
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



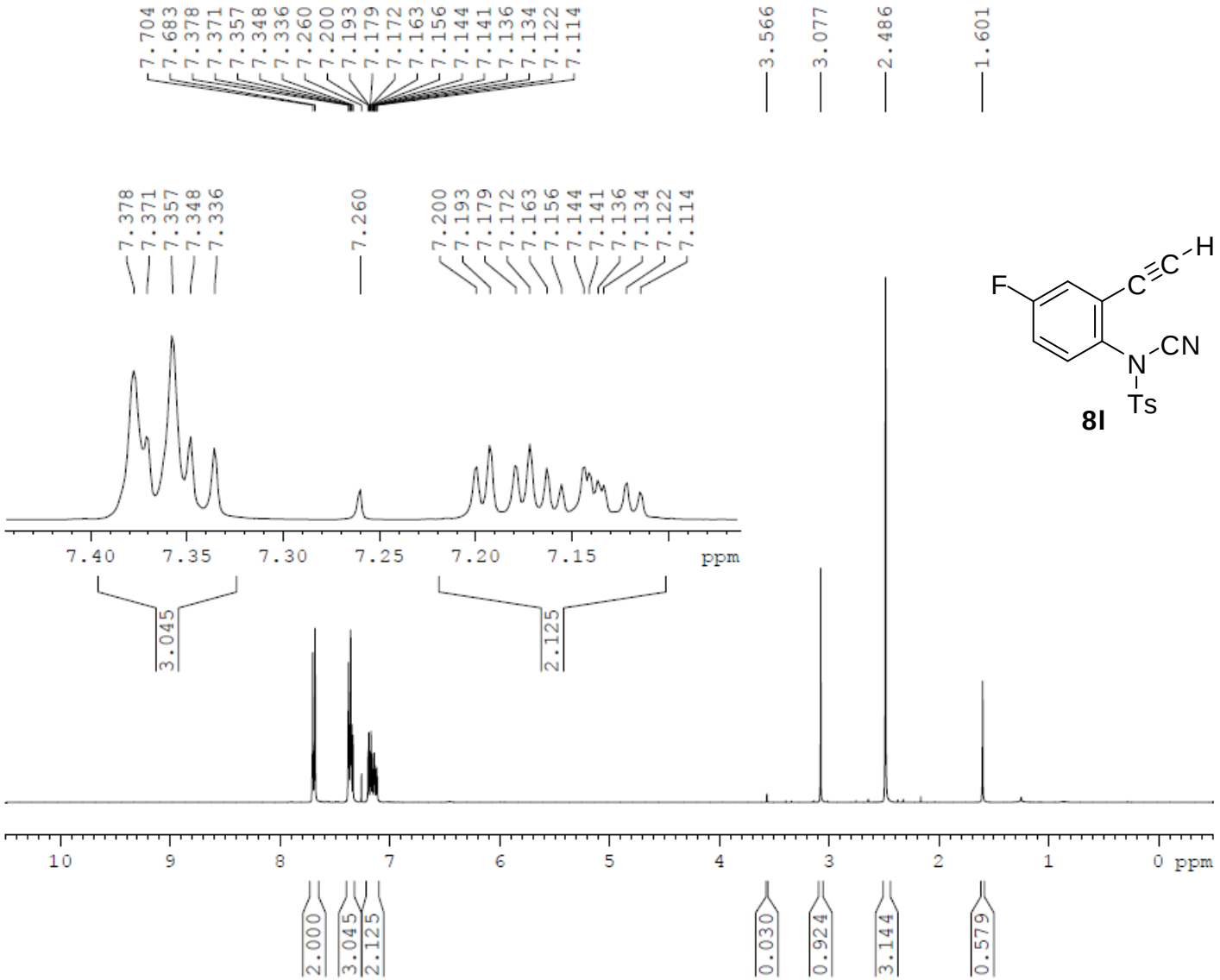
Current Data Parameters
NAME SC157
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140707
Time 10.21
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 472
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4597.6
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127491 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



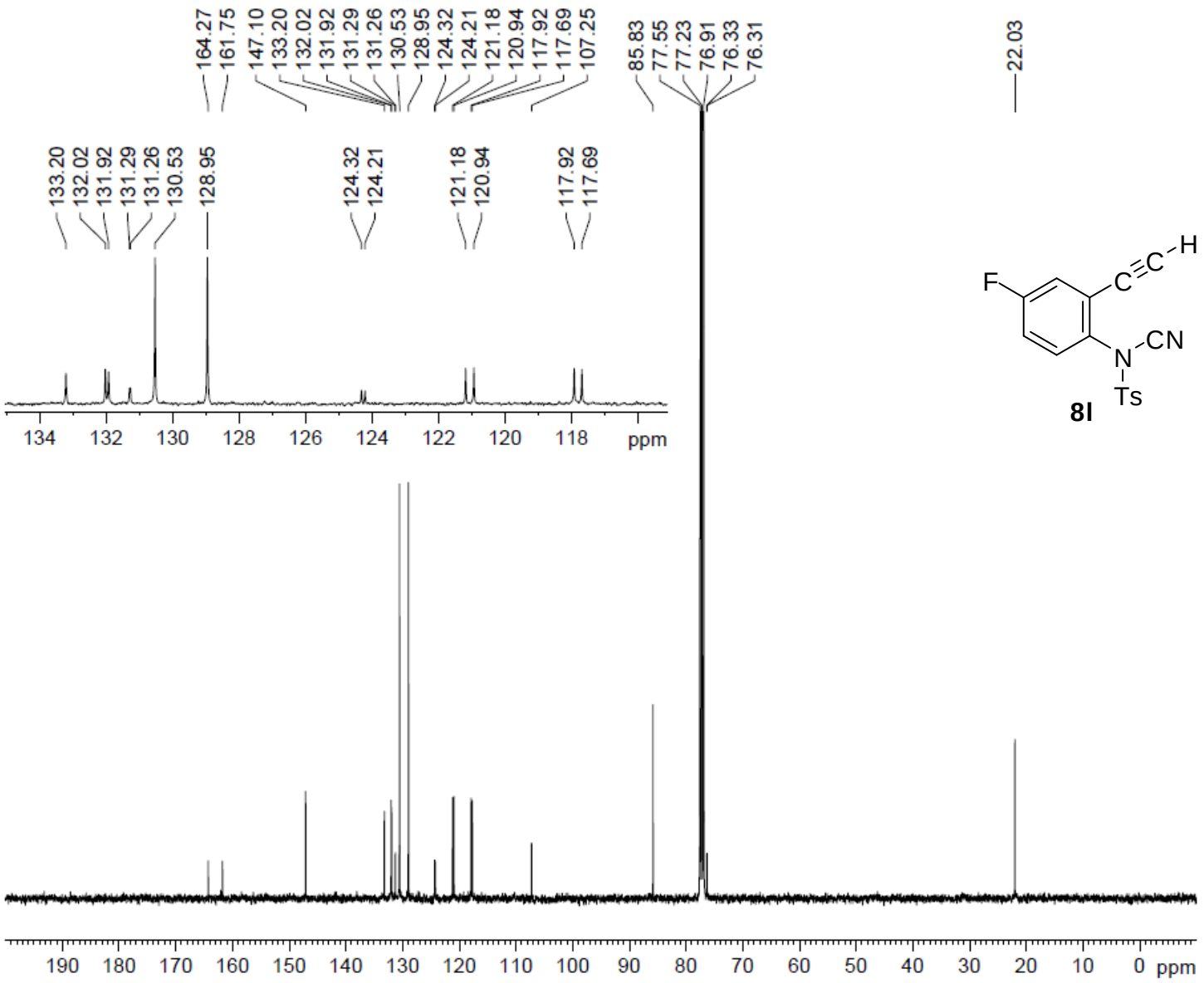
8l

Current Data Parameters
NAME SC169
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140815
Time 8.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



8l

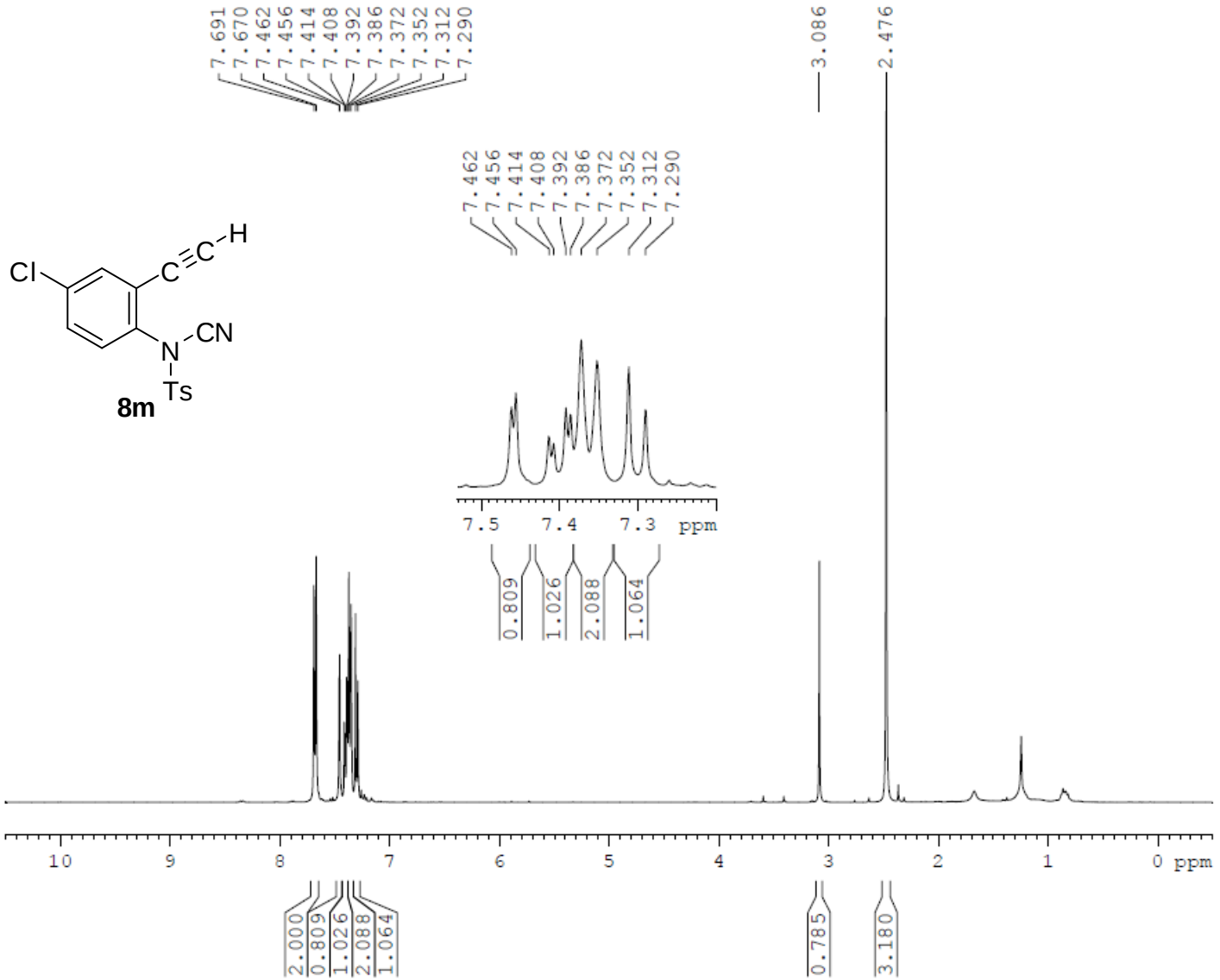
Current Data Parameters
NAME SC169
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140815
Time 9.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127492 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

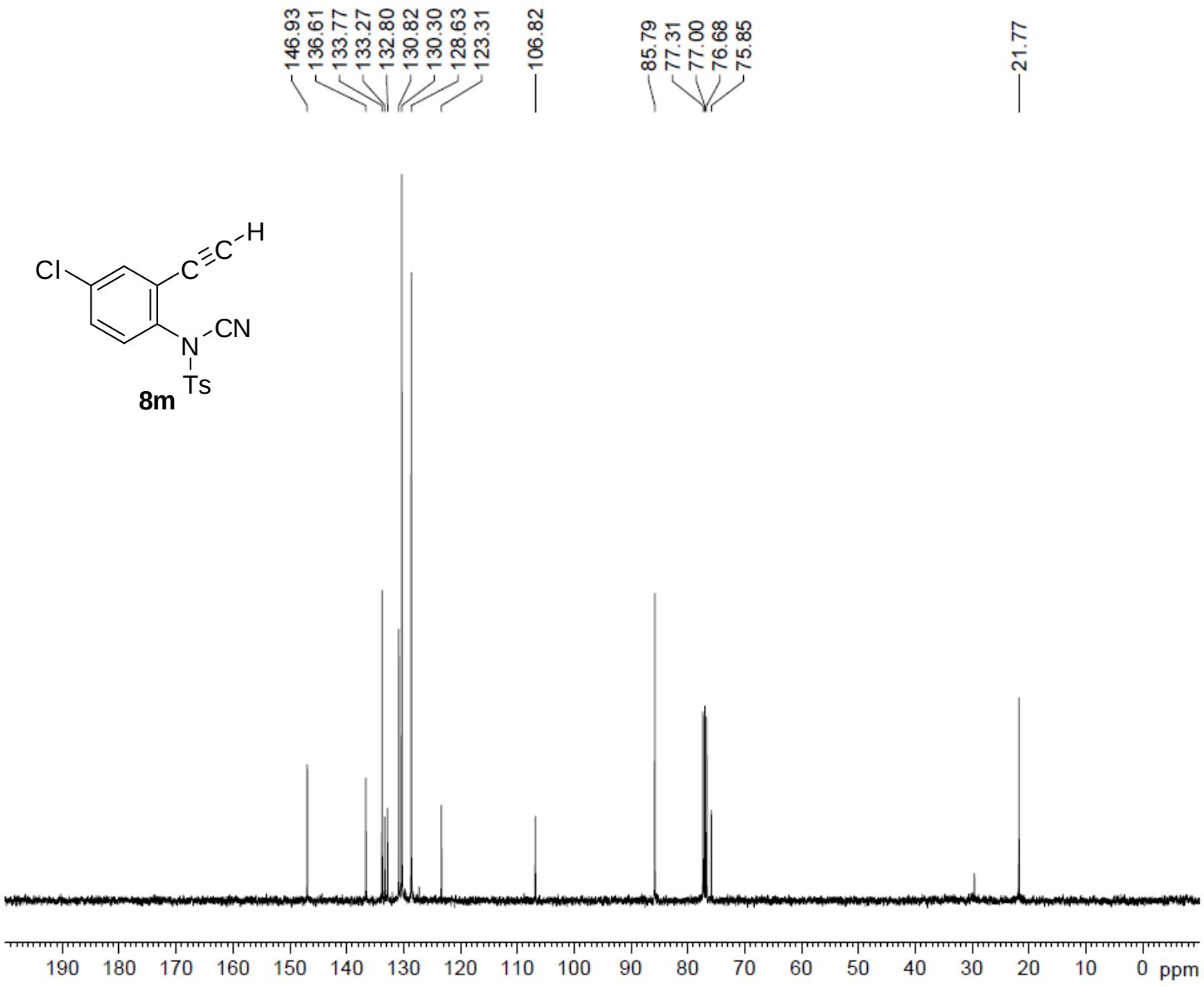


Current Data Parameters
NAME SD-098(new)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140629
Time 10.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 51.8
DW 69.333 usec
DE 10.52 usec
TE 298.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SD-098(new)
EXPNO 3
PROCNO 1

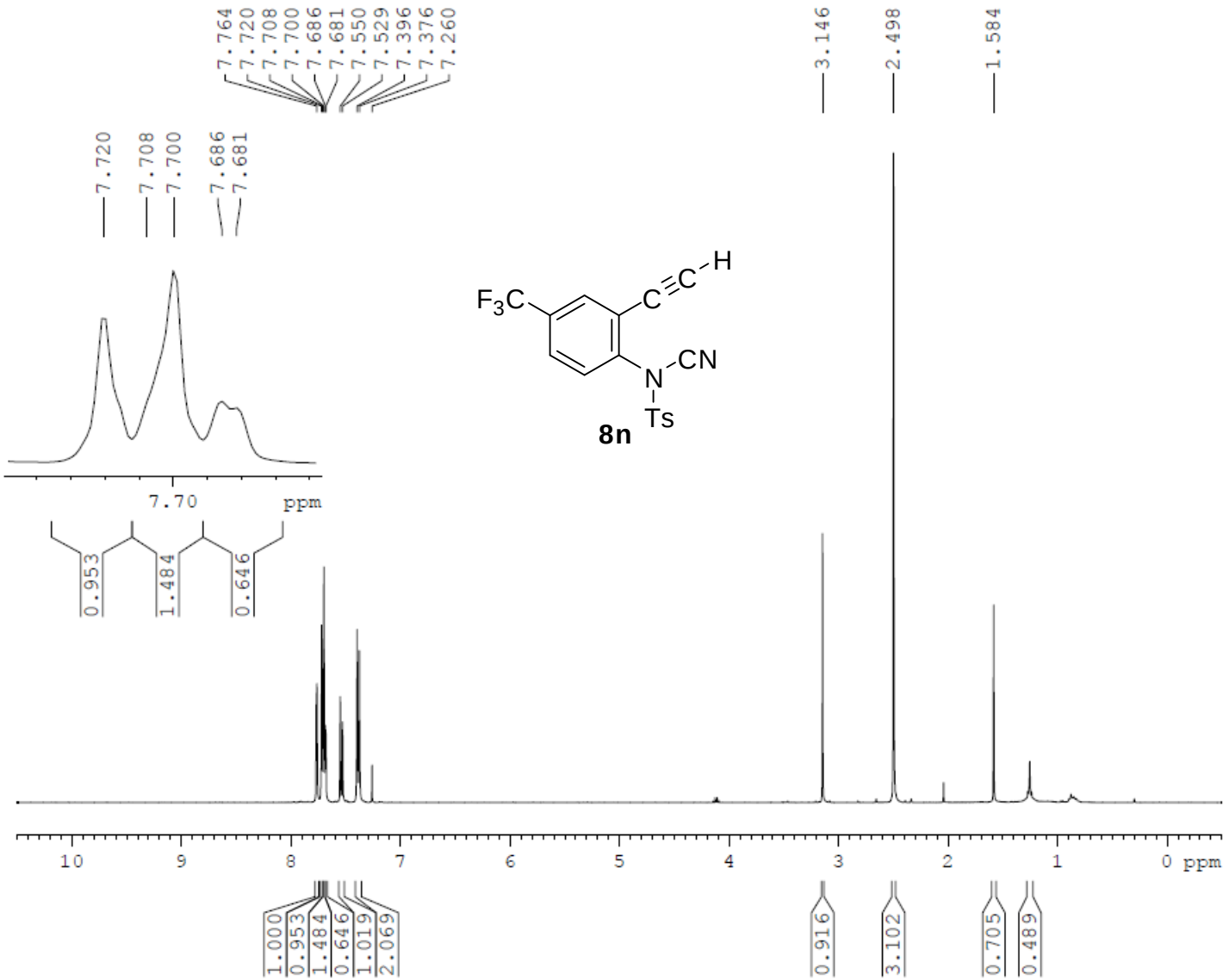
F2 - Acquisition Parameters
Date_ 20140629
Time 10.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 150
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127779 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

solid

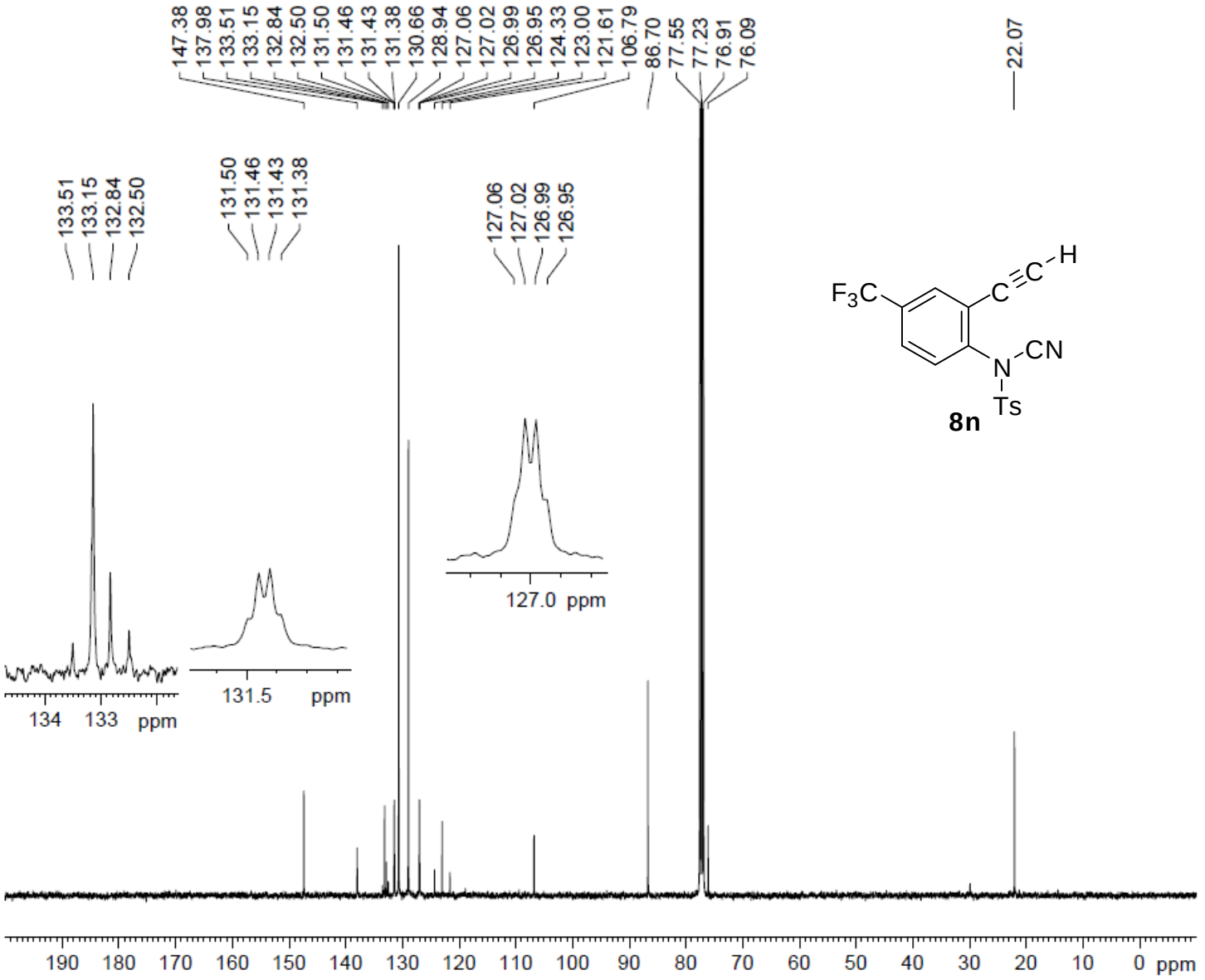


Current Data Parameters
NAME SC177-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140827
Time 8.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SC177-1
EXPNO 4
PROCNO 1

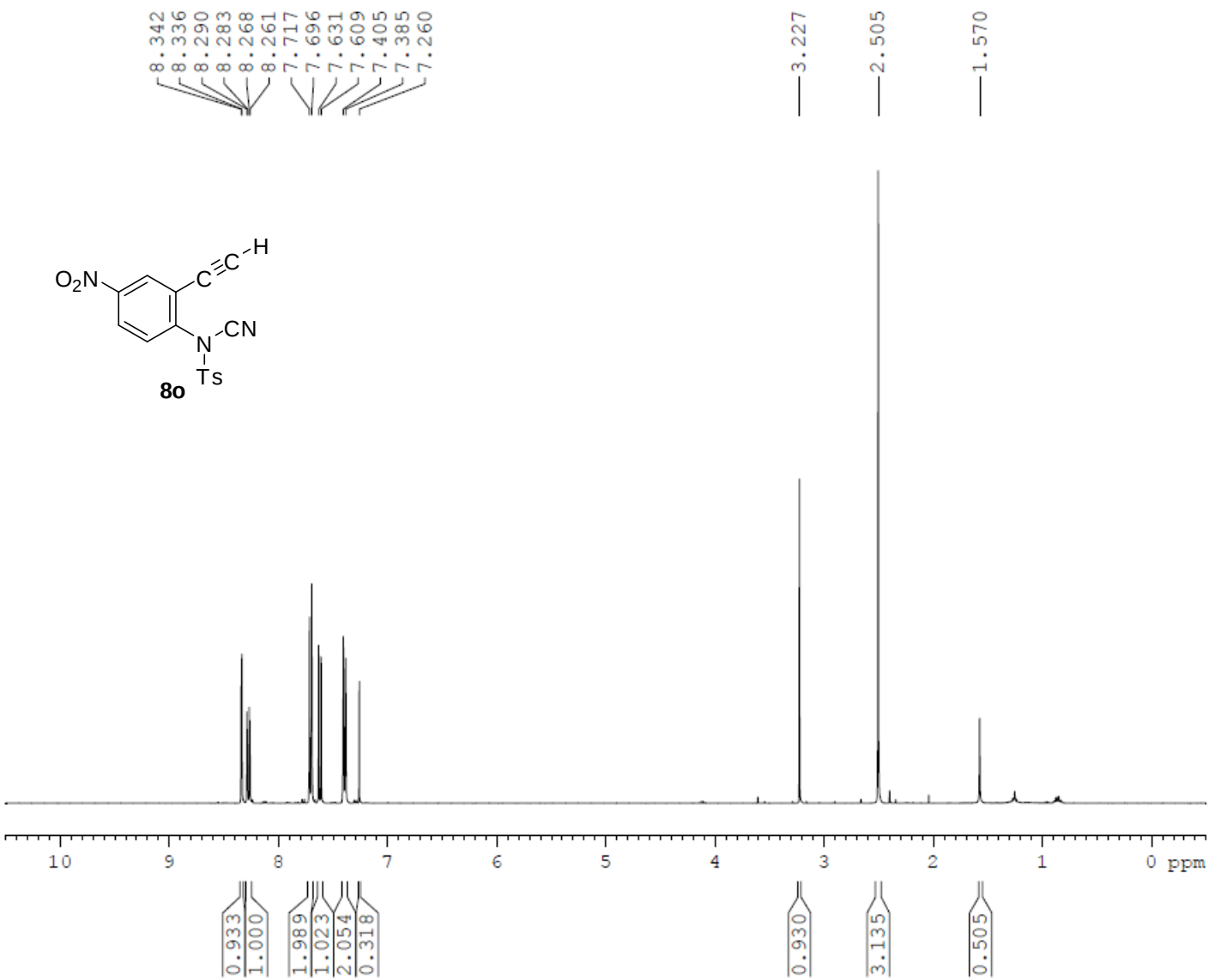
F2 - Acquisition Parameters
Date_ 20140827
Time 9.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127475 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

1H



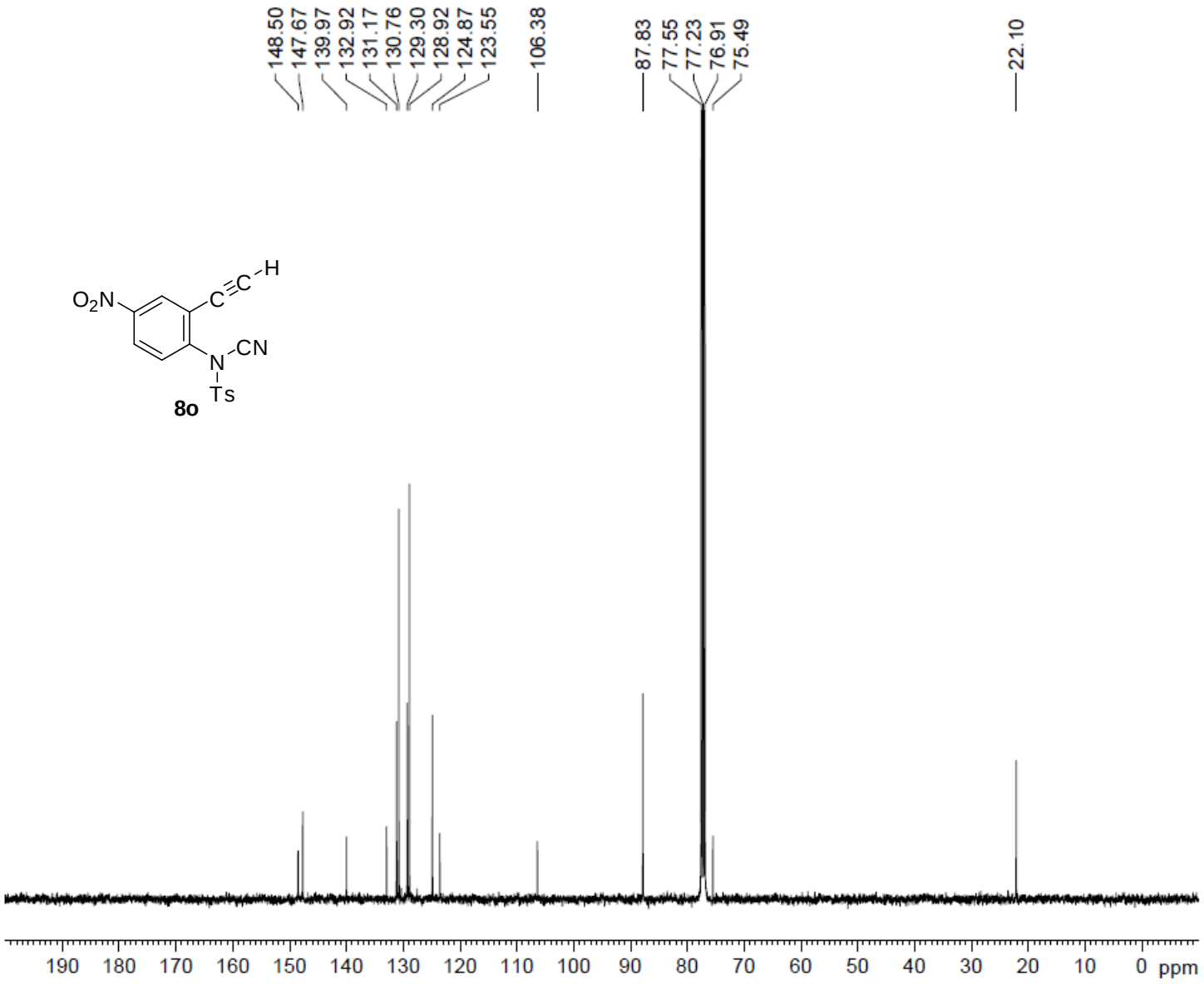
Current Data Parameters
NAME SC195
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141022
Time 2.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 177.16
DW 69.333 usec
DE 10.52 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

13C



Current Data Parameters
NAME SC195
EXPNO 3
PROCNO 1

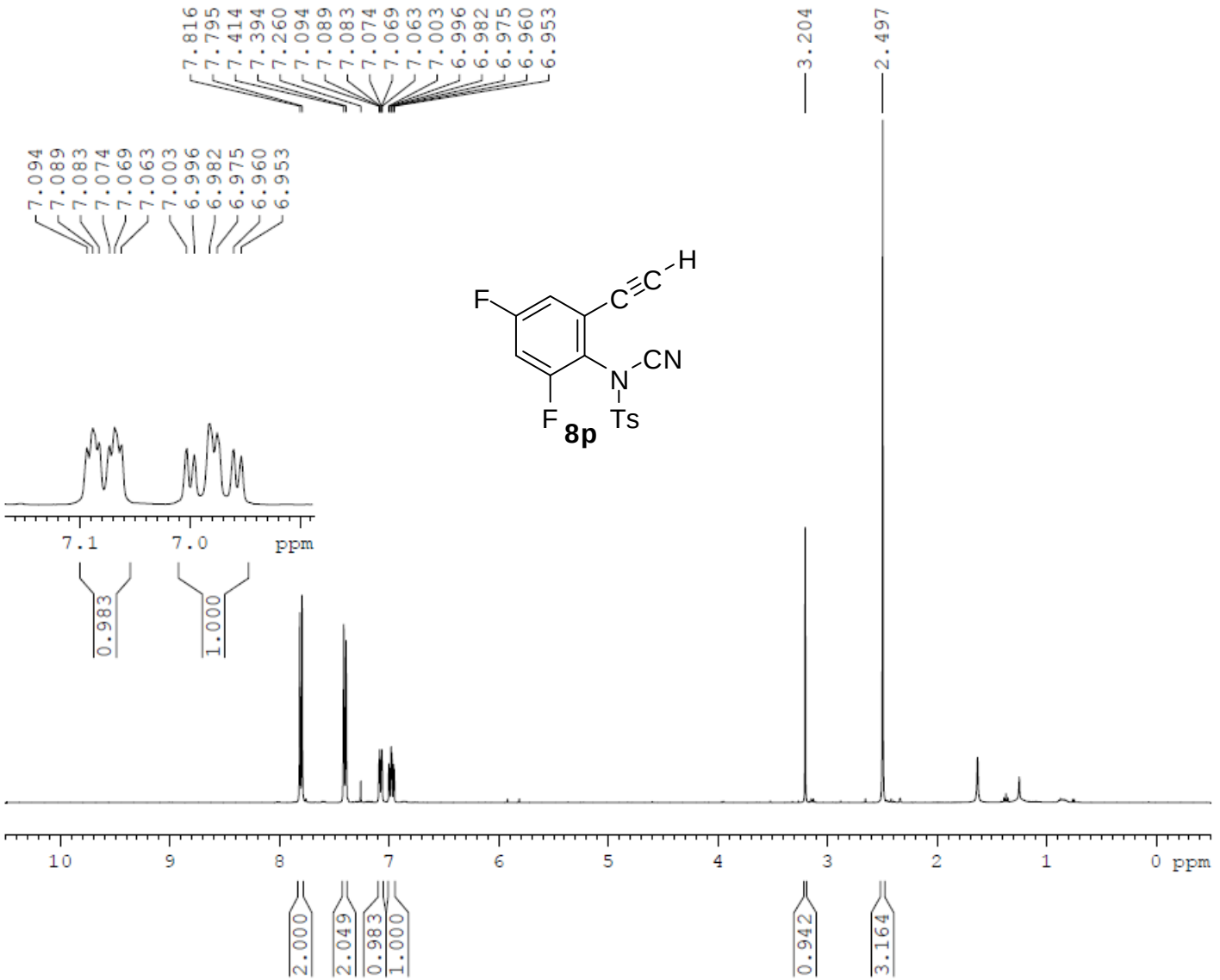
F2 - Acquisition Parameters
Date_ 20141022
Time 3.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127481 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

pure

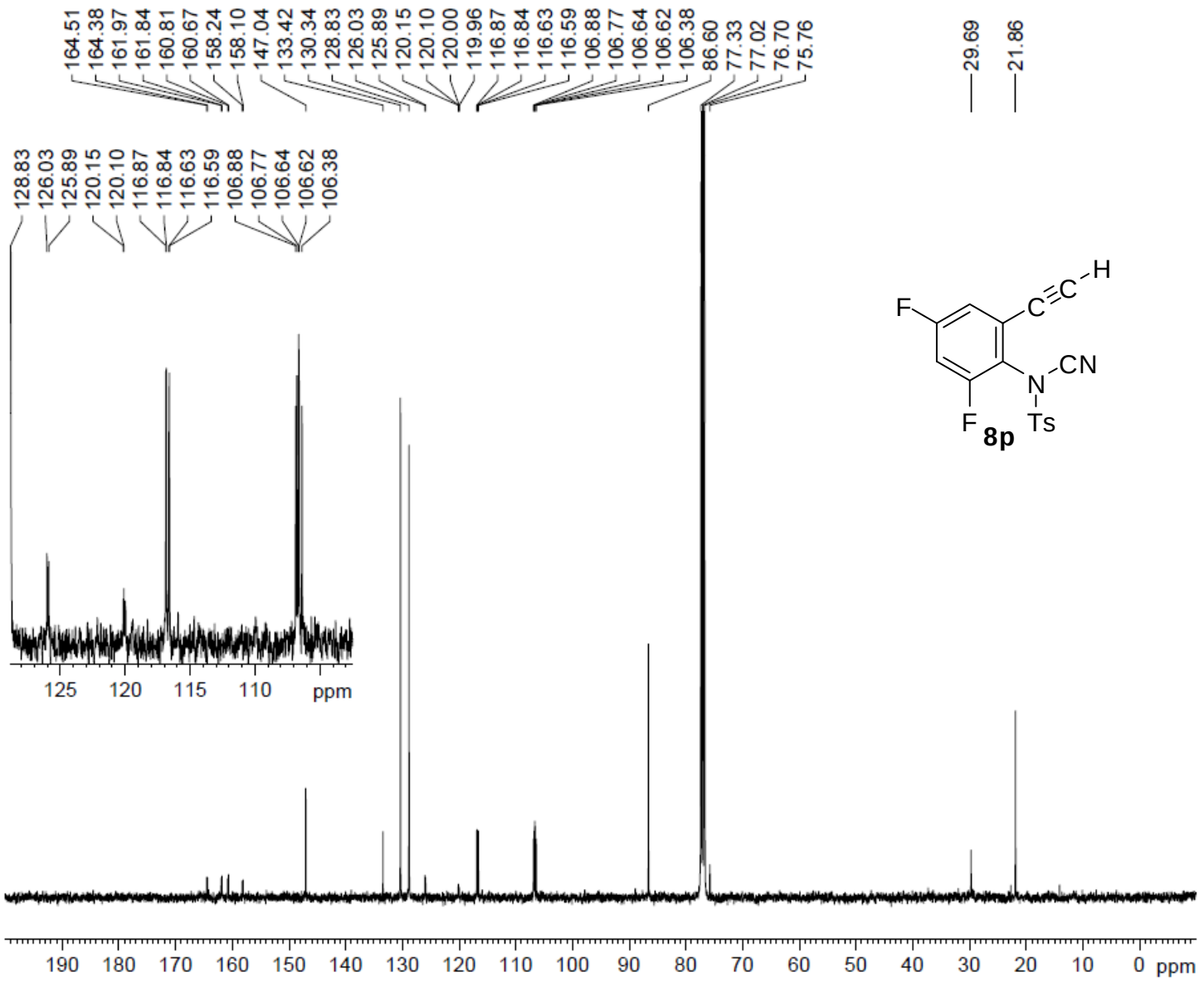


Current Data Parameters
NAME SD-071(new)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140512
Time 15.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 78.51
DW 69.333 usec
DE 10.52 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



8p

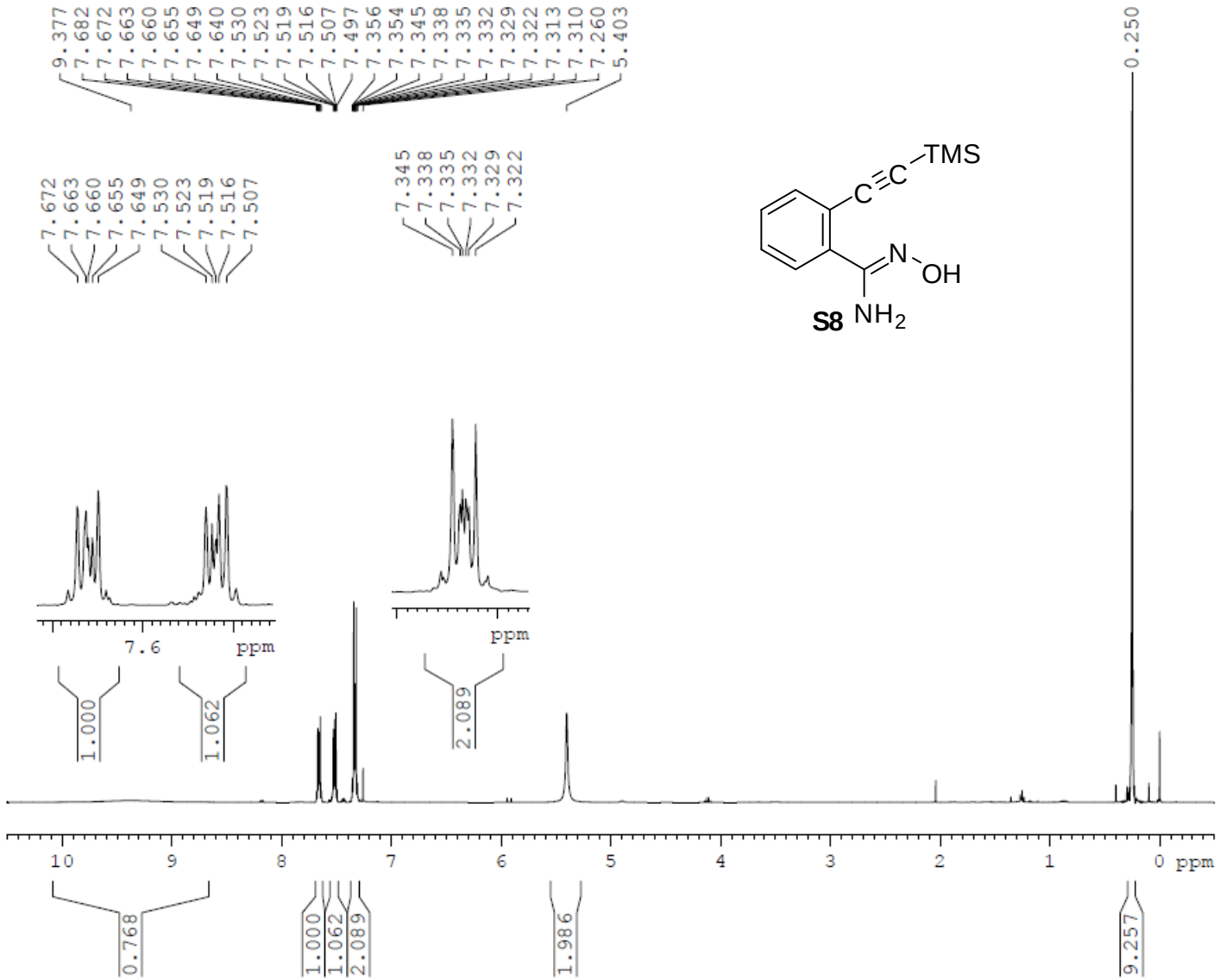
Current Data Parameters
NAME SD-071(new)
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140522
Time 14.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2813
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

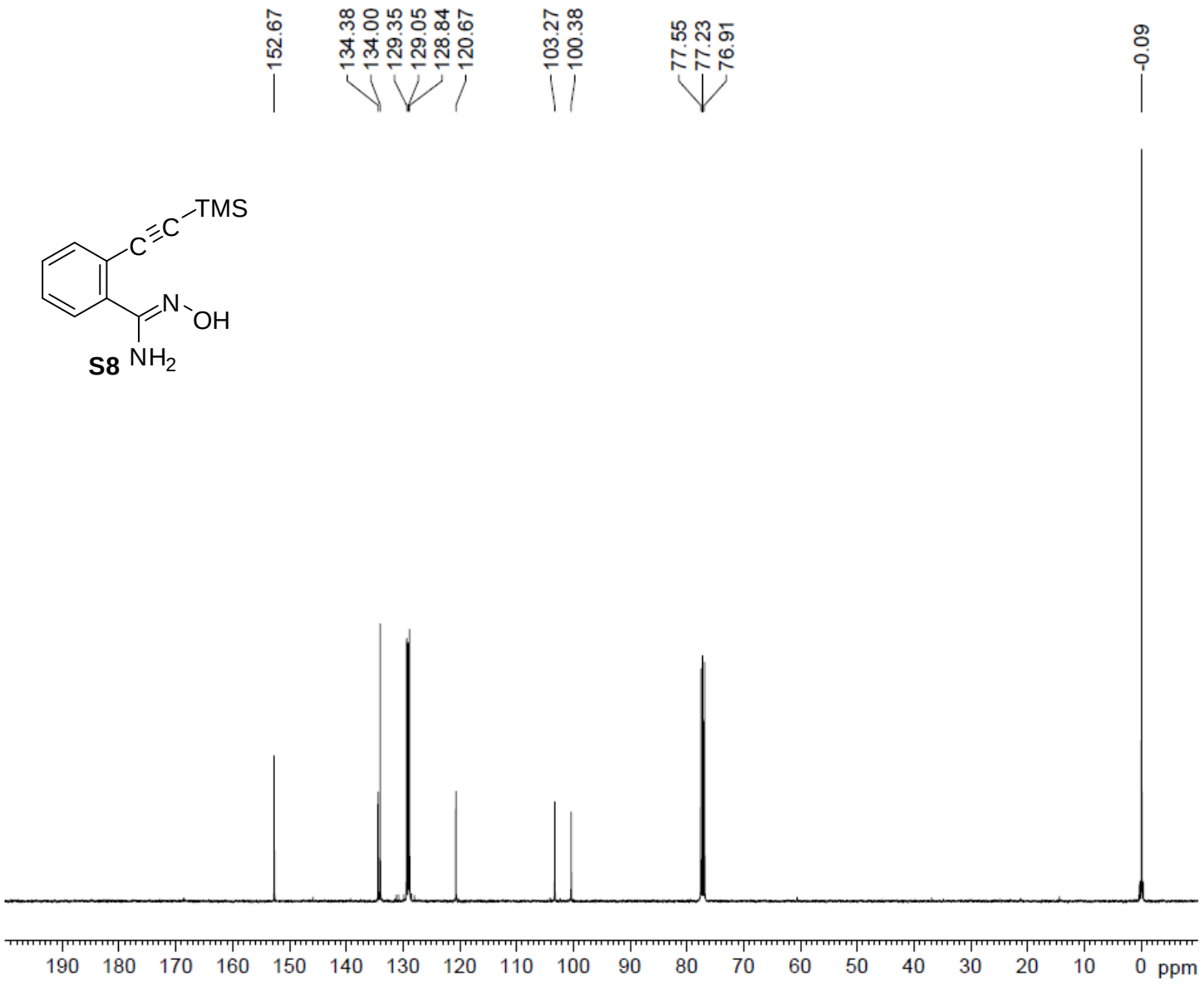


Current Data Parameters
NAME SO012
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141114
Time 19.34
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 35.9
DW 69.000 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



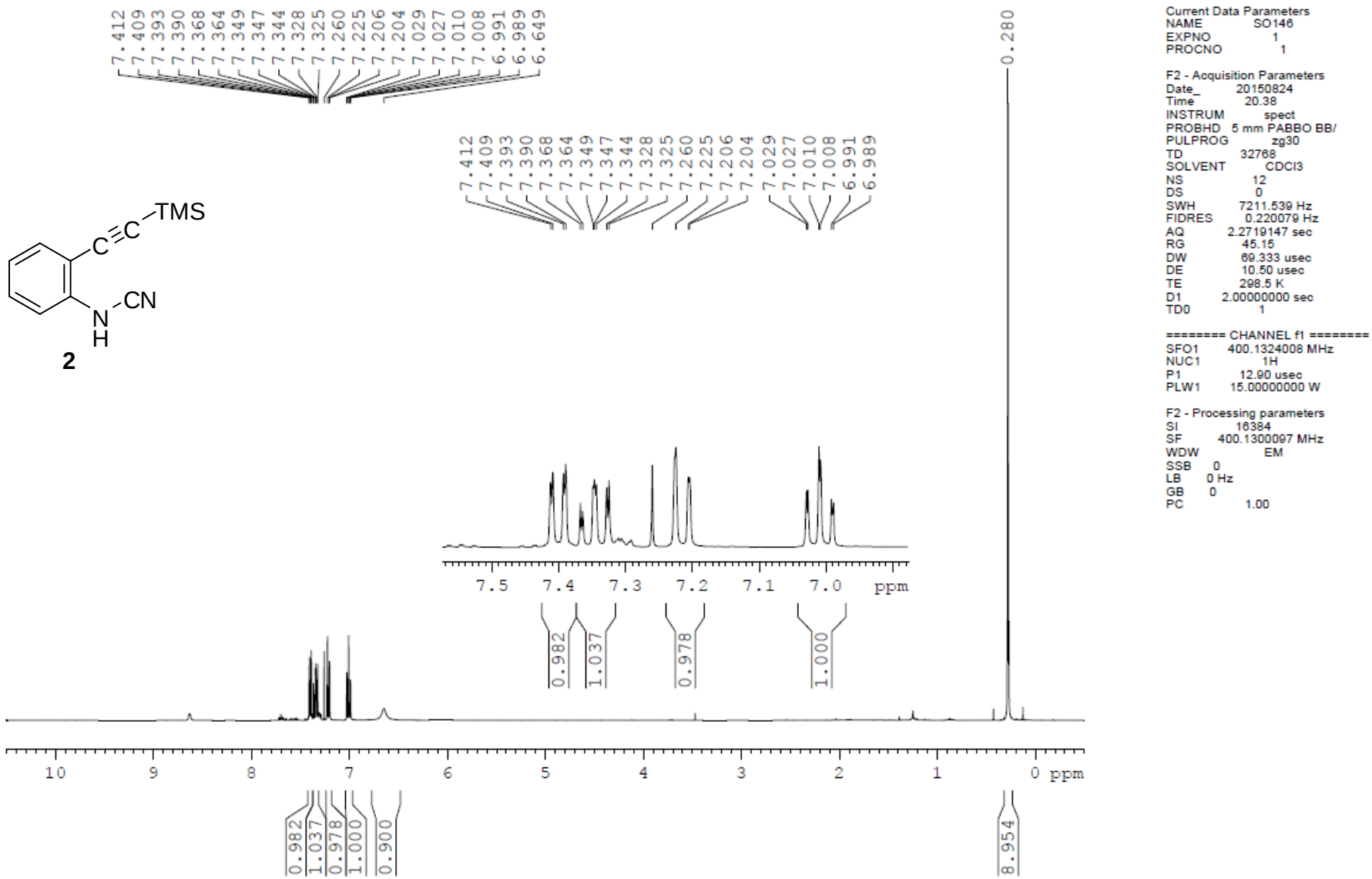
Current Data Parameters
NAME SO012
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141115
Time 9.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127516 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

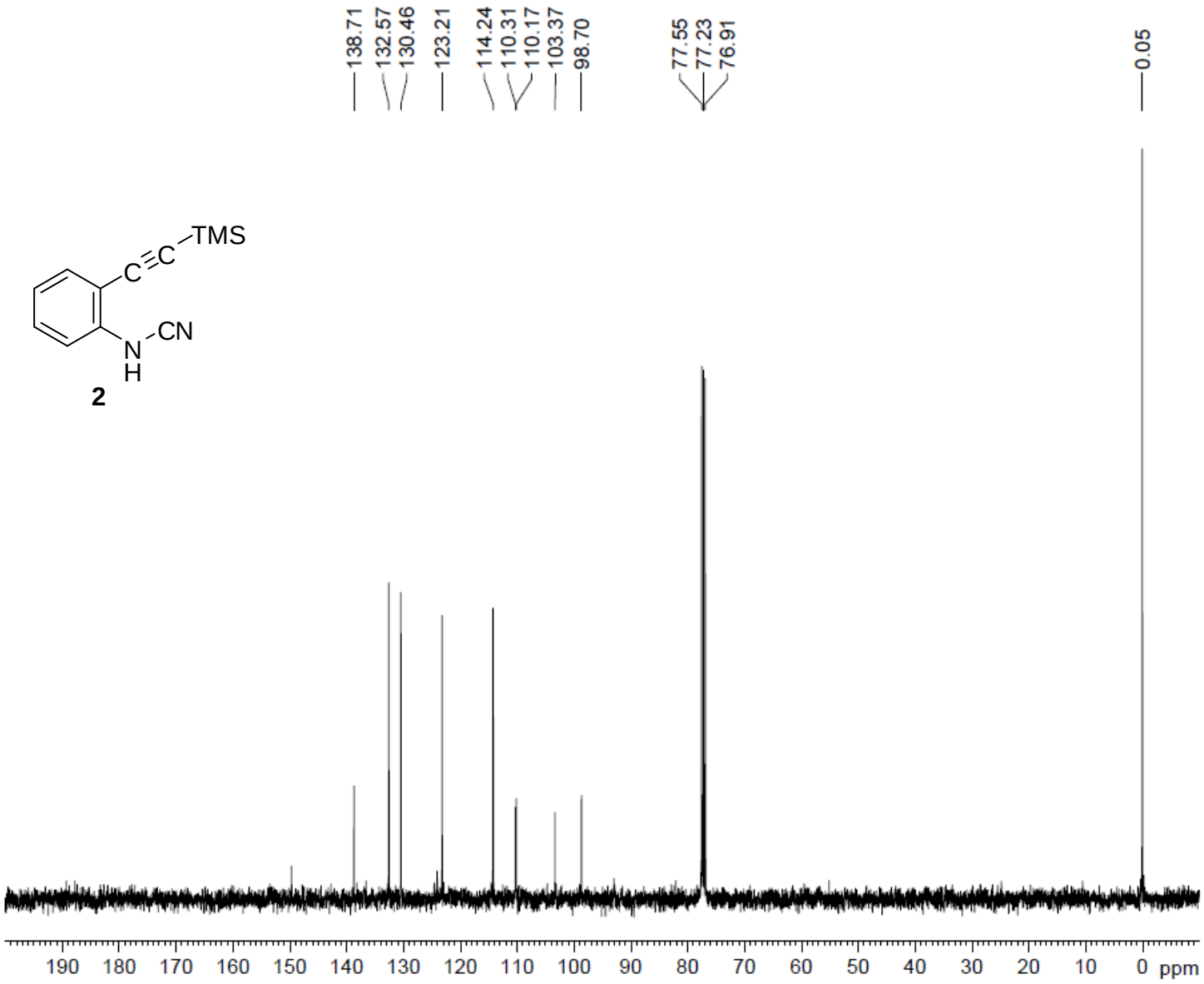


Current Data Parameters
NAME SO146
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150824
Time 20.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 45.15
DW 69.333 usec
DE 10.50 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



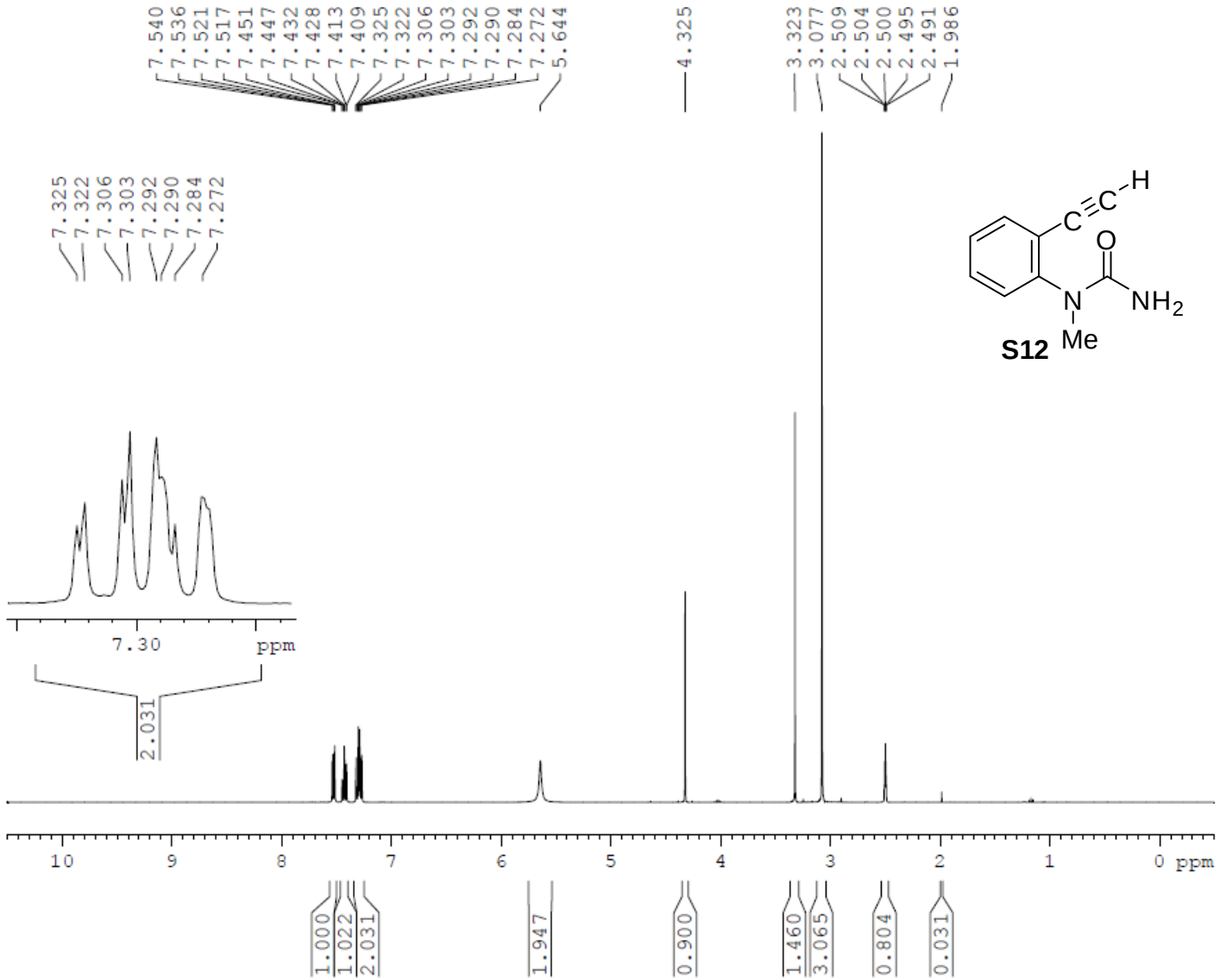
Current Data Parameters
NAME SO146
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150824
Time 20.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 13
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.50000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W
PLW13 0.27338001 W

F2 - Processing parameters
SI 32768
SF 100.6127540 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

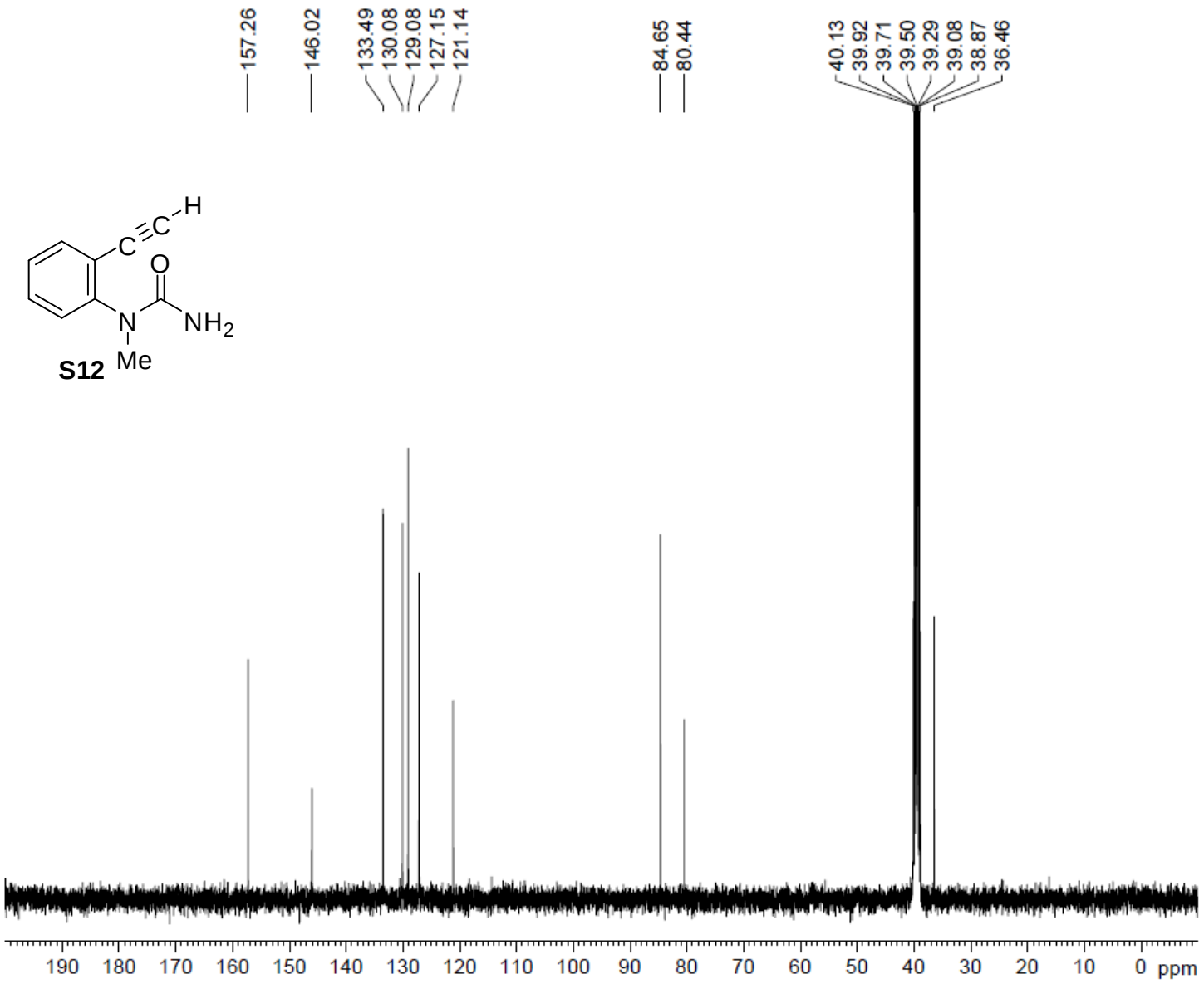


Current Data Parameters
NAME SO015
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141121
Time 8.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 181
DW 69.000 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



S12

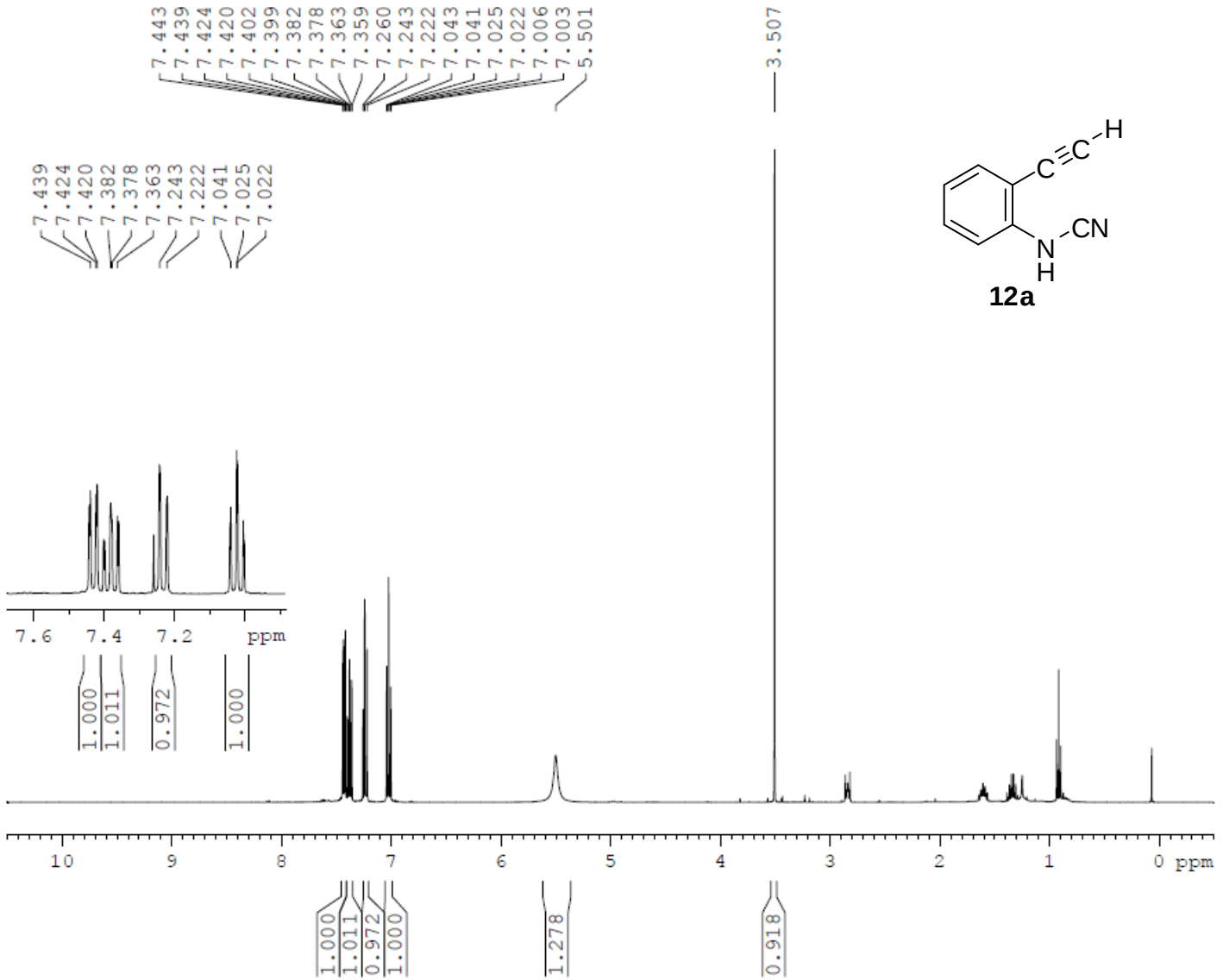
Current Data Parameters
NAME SO015
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141121
Time 10.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 261
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4597.6
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128203 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



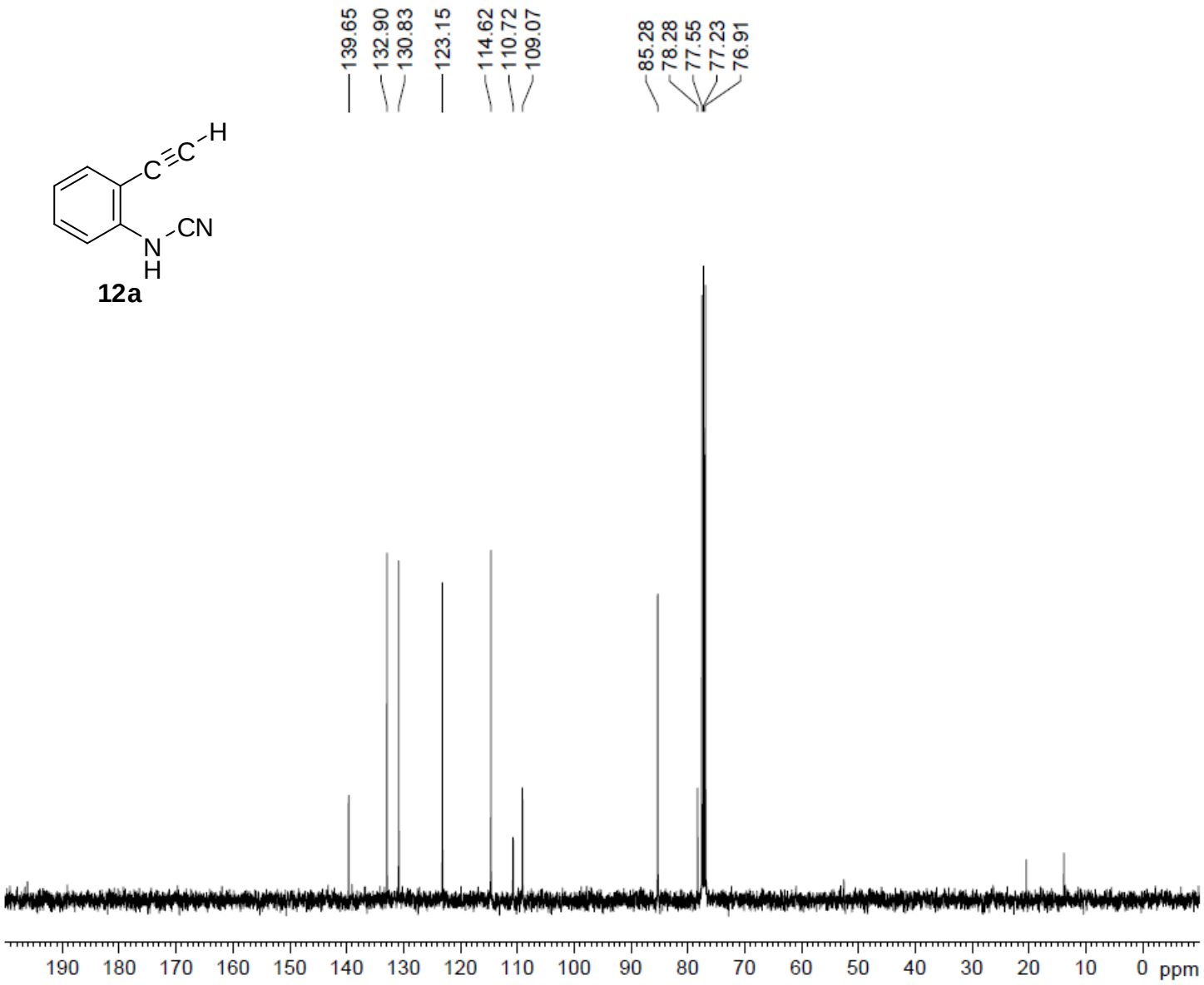
12a

Current Data Parameters
NAME SO147
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150826
Time 16.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 71.42
DW 69.333 usec
DE 10.50 usec
TE 298.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



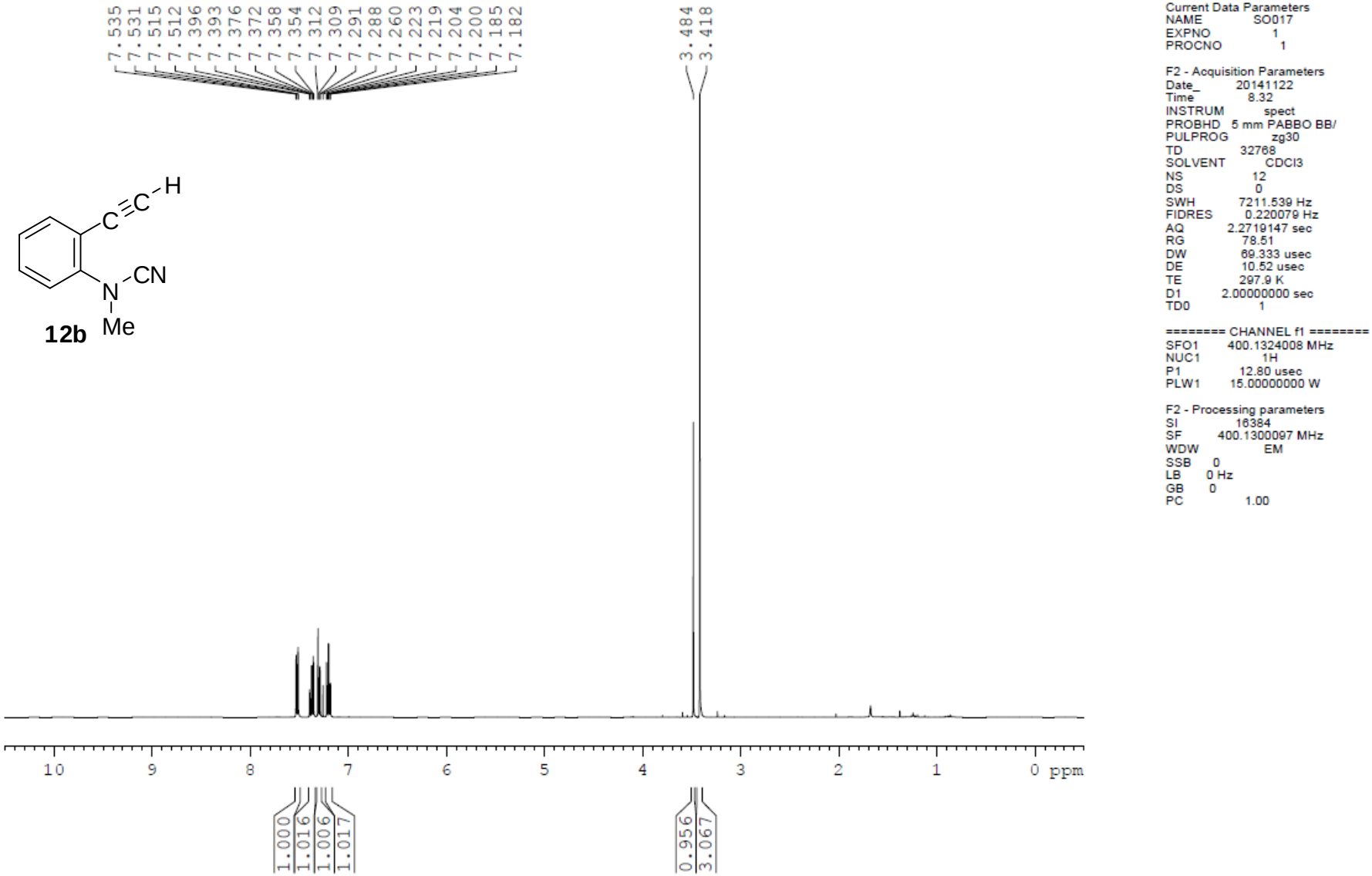
Current Data Parameters
NAME SO147
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150826
Time 16.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 36
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.50000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W
PLW13 0.27338001 W

F2 - Processing parameters
SI 32768
SF 100.6127530 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

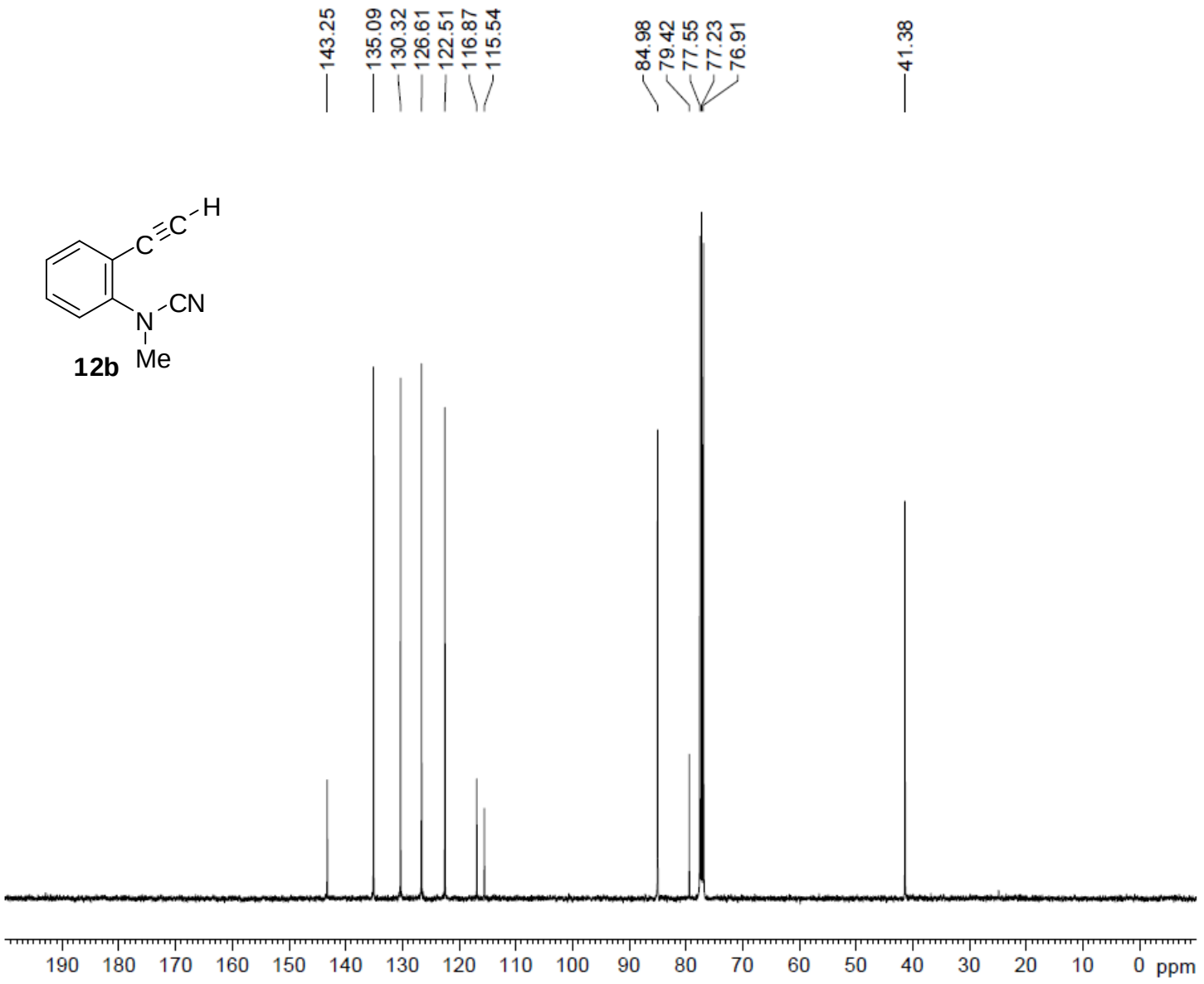


Current Data Parameters
NAME SO017
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141122
Time 8.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 78.51
DW 69.333 usec
DE 10.52 usec
TE 297.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



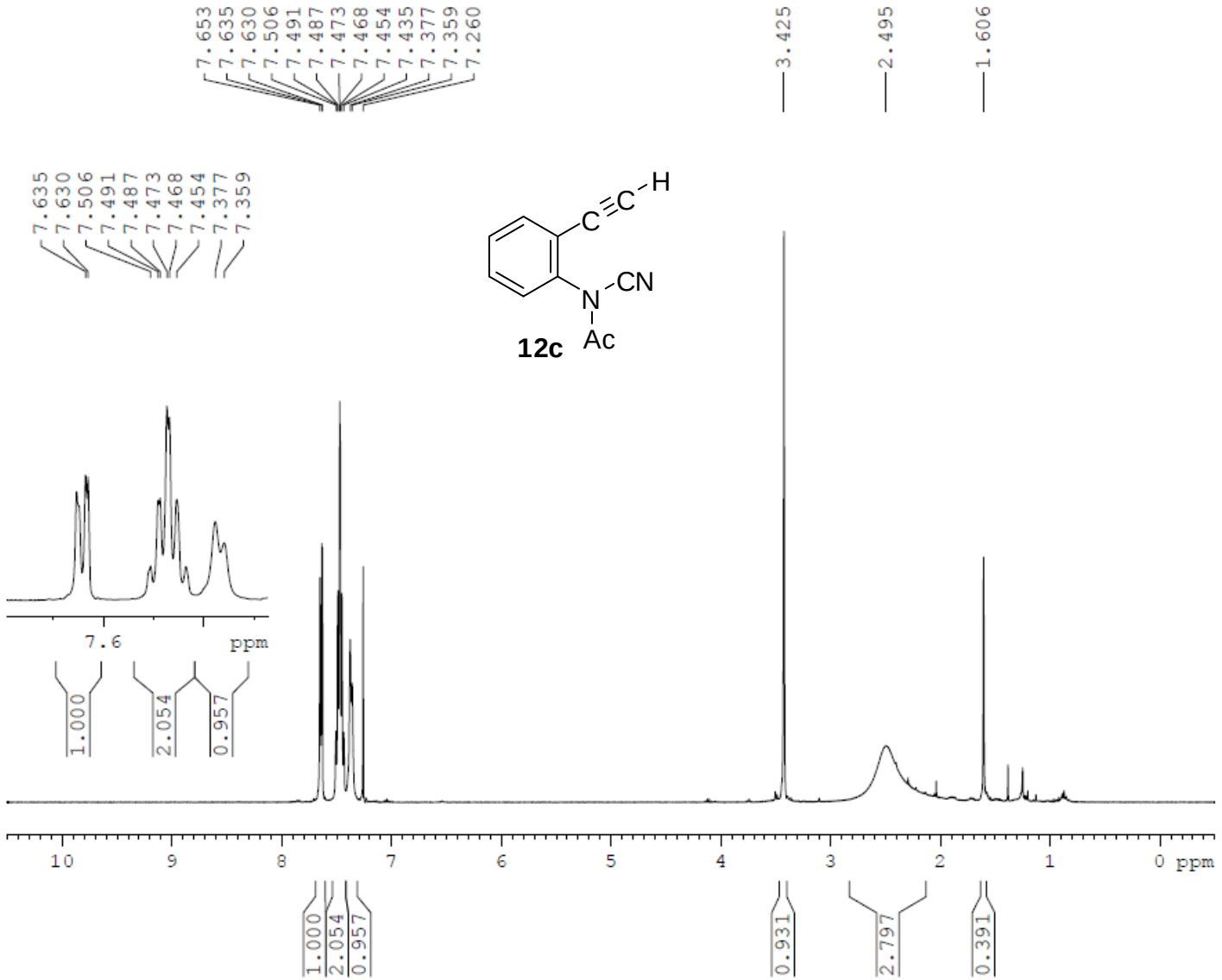
Current Data Parameters
NAME SO017
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141122
Time 9.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127523 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

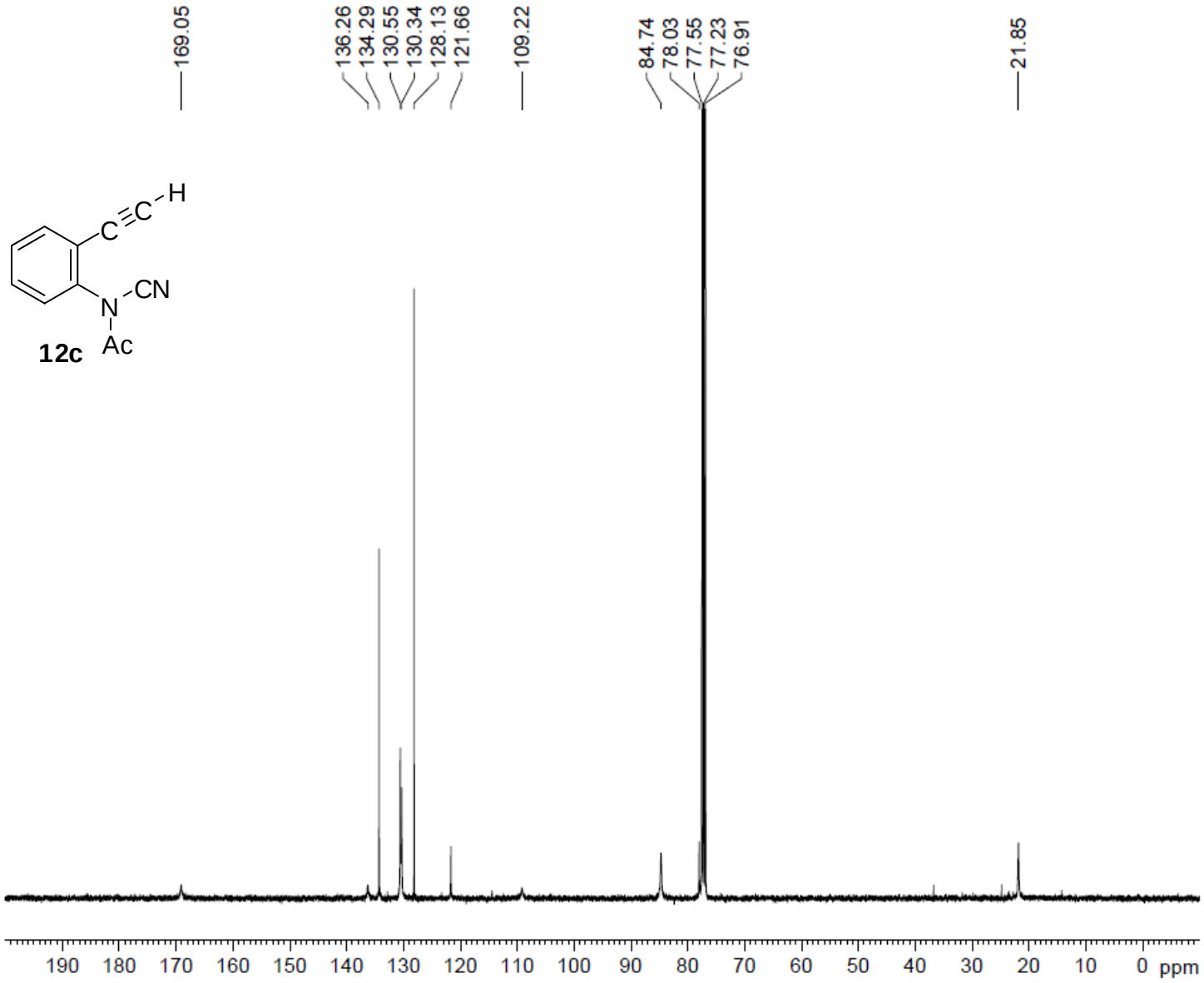


Current Data Parameters
NAME SO180
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160106
Time 20.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.40 usec
PL1 1.80 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SO180
EXPNO 4
PROCNO 1

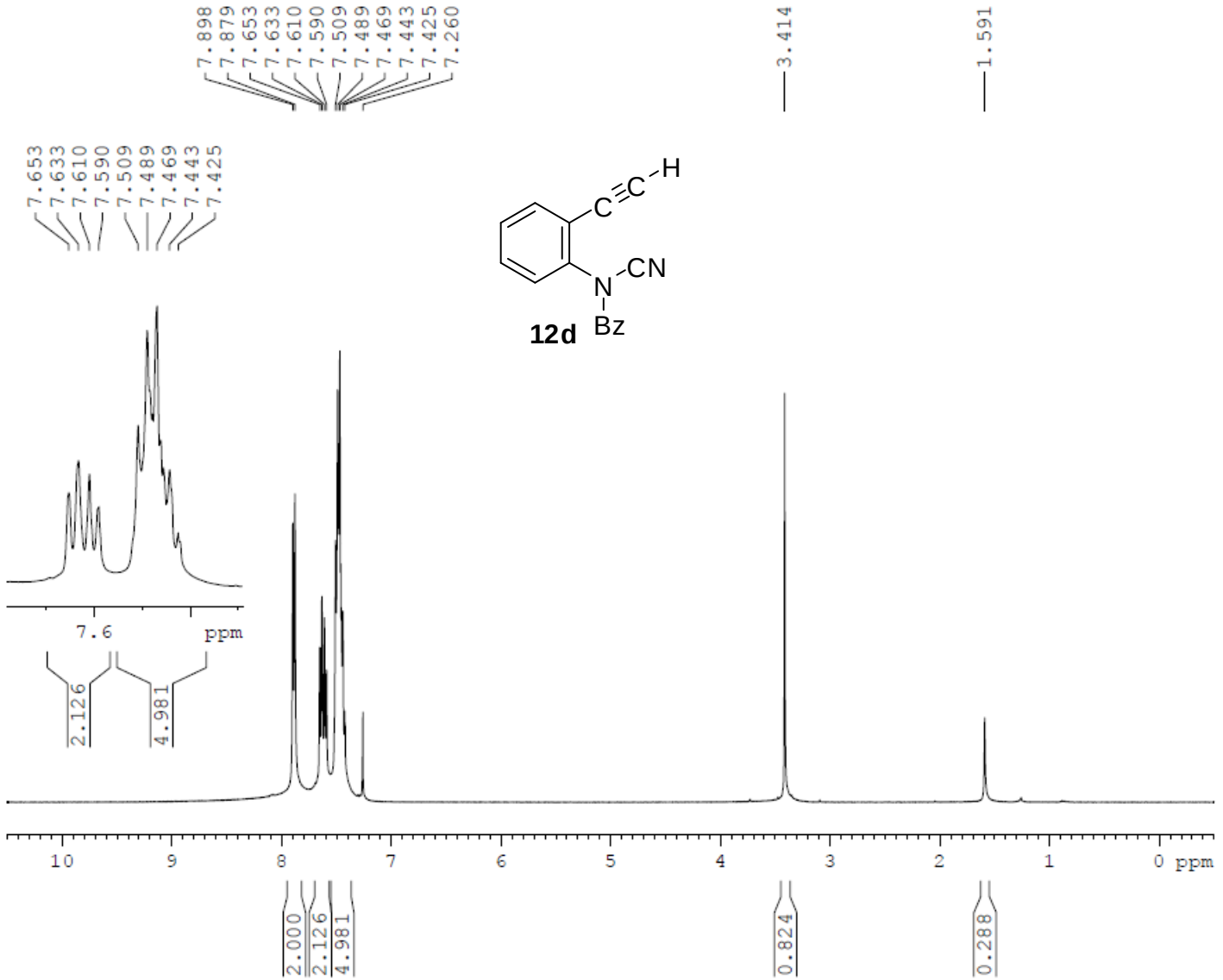
F2 - Acquisition Parameters
Date_ 20160106
Time 21.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2195
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 1.80 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127536 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

recrystallized



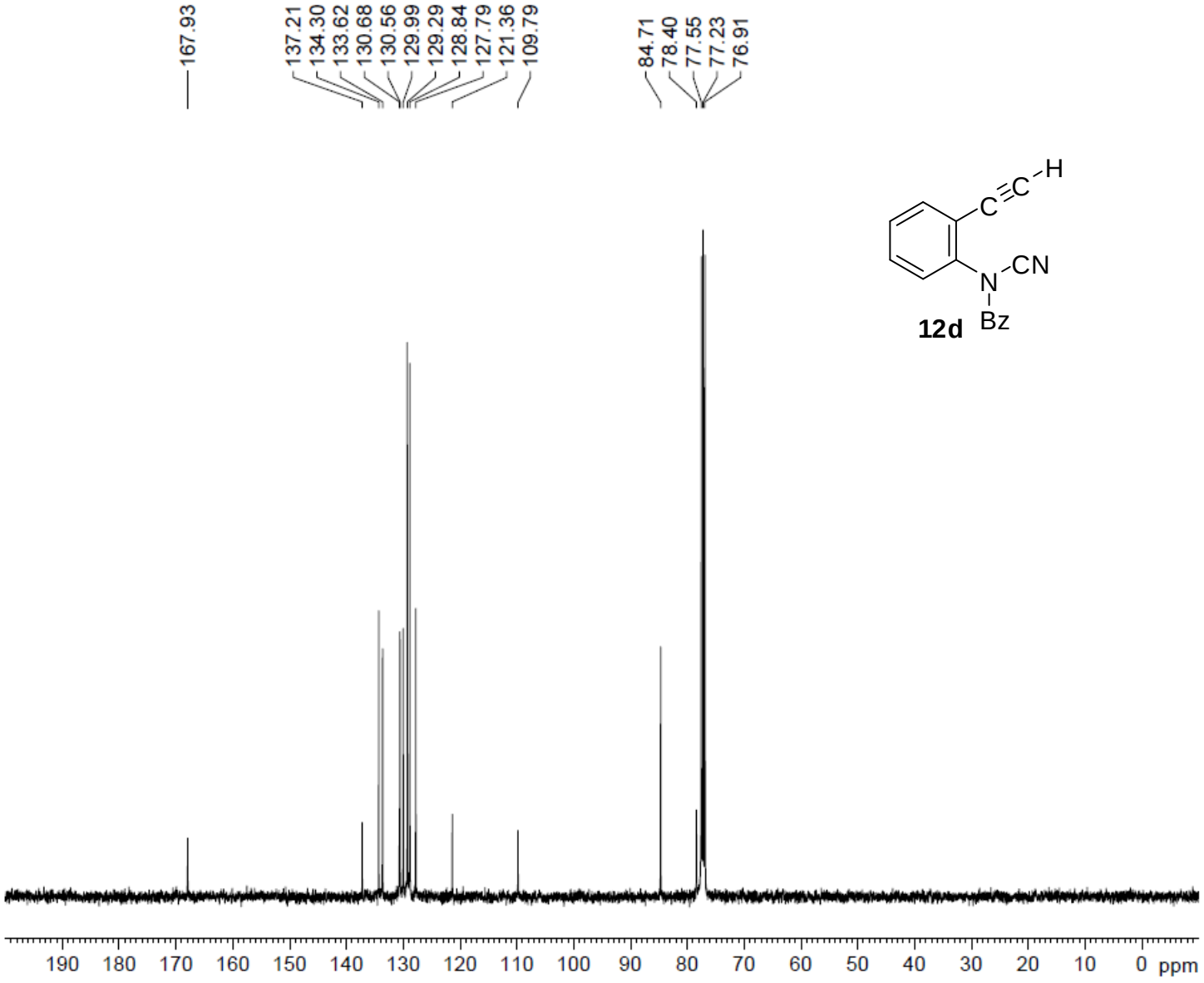
Current Data Parameters
NAME SO181-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160107
Time 8.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.50 usec
TE 297.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

recrystallized



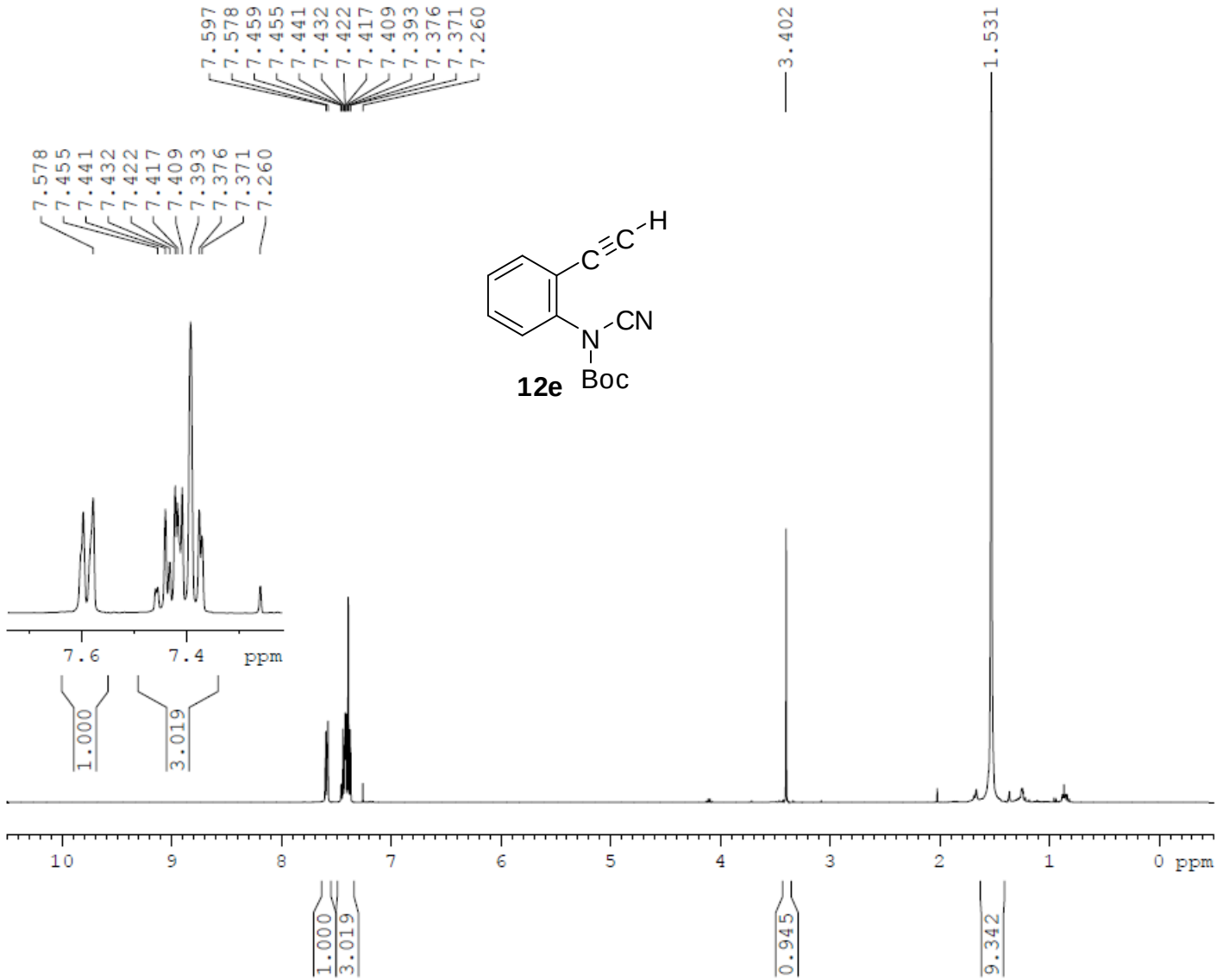
Current Data Parameters
NAME SO181-1
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160107
Time 10.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 293
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.50000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W
PLW13 0.27338001 W

F2 - Processing parameters
SI 32768
SF 100.6127516 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

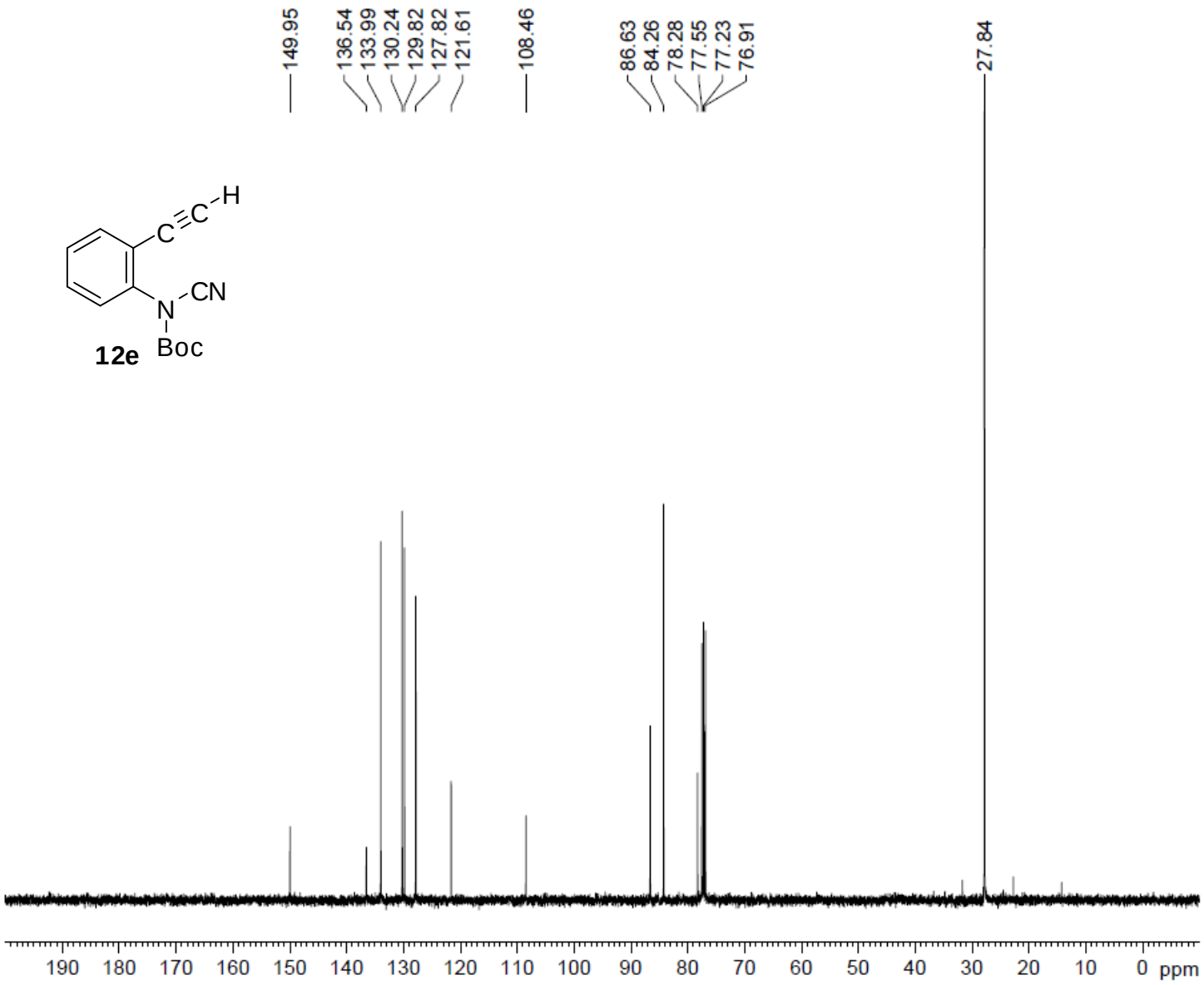


Current Data Parameters
NAME SO182
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160109
Time 21.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 35.9
DW 69.000 usec
DE 6.50 usec
TE 297.9 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 14.40 usec
PL1 1.80 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



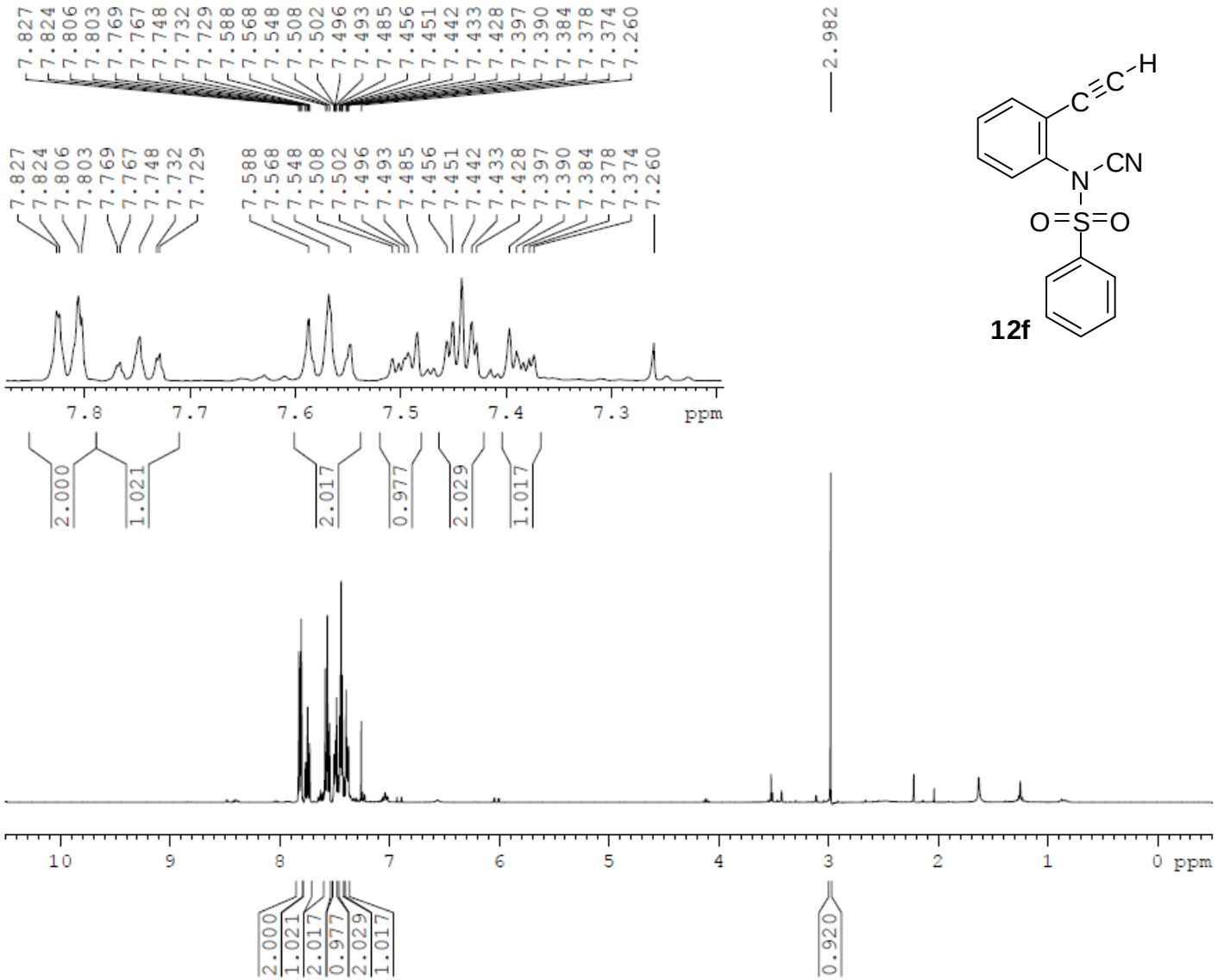
Current Data Parameters
NAME SO182
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160109
Time 21.13
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 135
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 1024
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 1.80 dB
PL12 17.00 dB
PL13 20.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127558 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



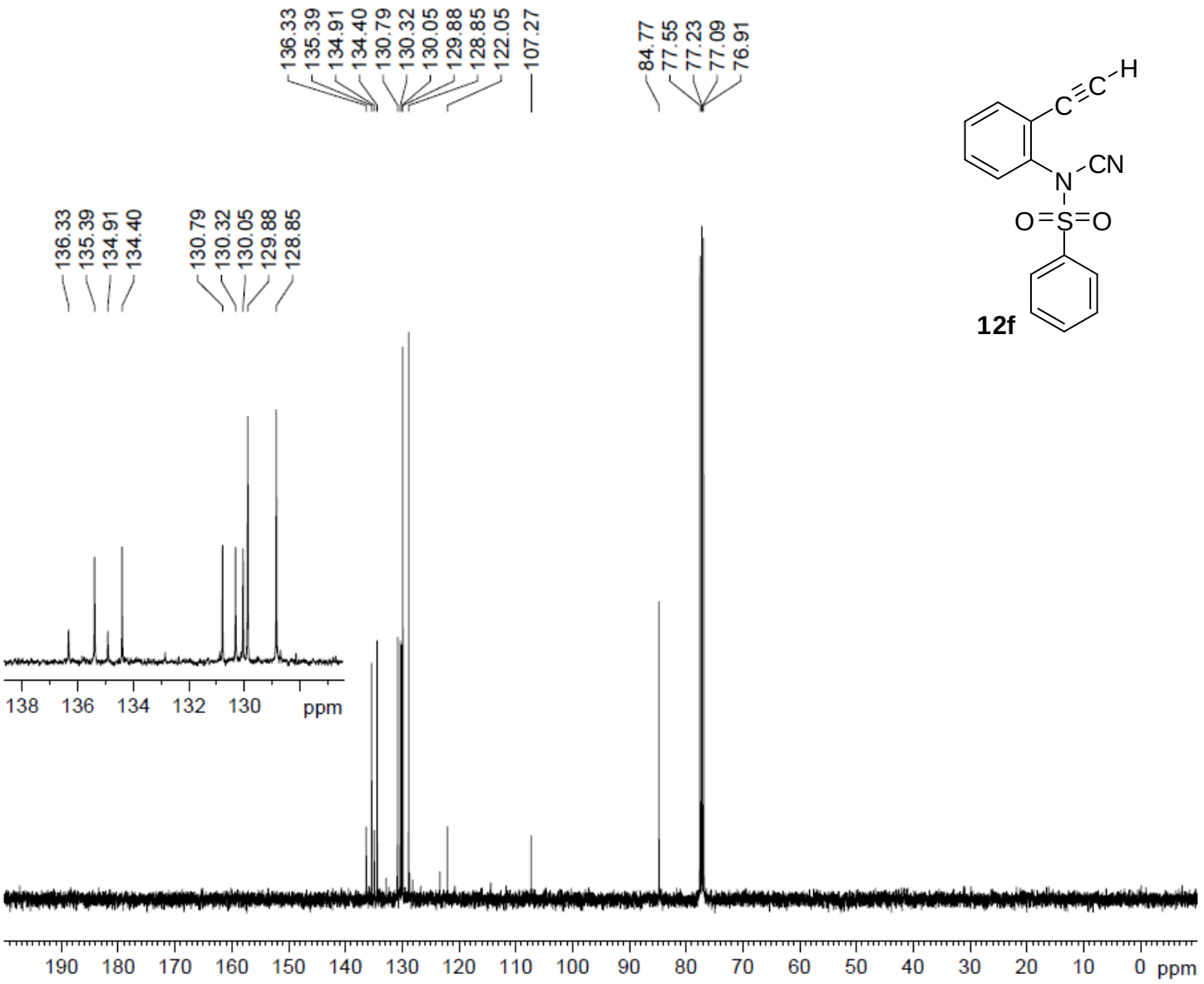
12f

```
Current Data Parameters
NAME          SO124-2
EXPNO               1
PROCNO              1

F2 - Acquisition Parameters
Date_        20150606
Time            10.31
INSTRUM          spect
PROBHD  5 mm BBO BB-1H
PULPROG          zg30
TD              32768
SOLVENT         CDCl3
NS                 12
DS                  0
SWH          7246.377 Hz
FIDRES       0.221142 Hz
AQ           2.2609921 sec
RG               228.1
DW              69.000 usec
DE               6.50 usec
TE               297.4 K
D1           2.00000000 sec
TD0                 1

======== CHANNEL f1 ========
NUC1               1H
P1             21.45 usec
PL1            -5.85 dB
SFO1       400.1324008 MHz

F2 - Processing parameters
SI              16384
SF         400.1300091 MHz
WDW                EM
SSB     0
LB      0 Hz
GB      0
PC              1.00
```



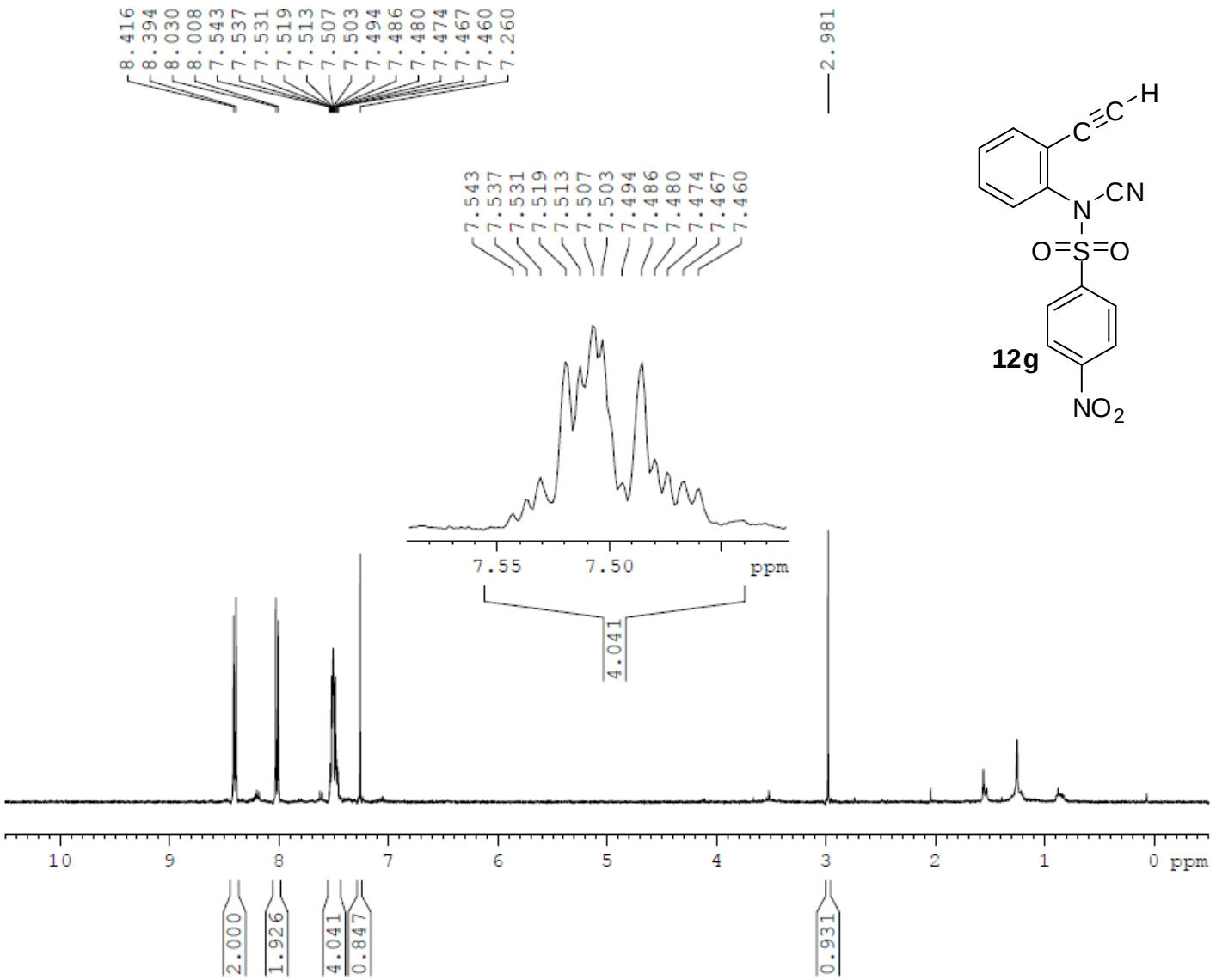
Current Data Parameters
NAME SO124-2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150606
Time 10.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 144
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4597.6
DW 20.800 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127520 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



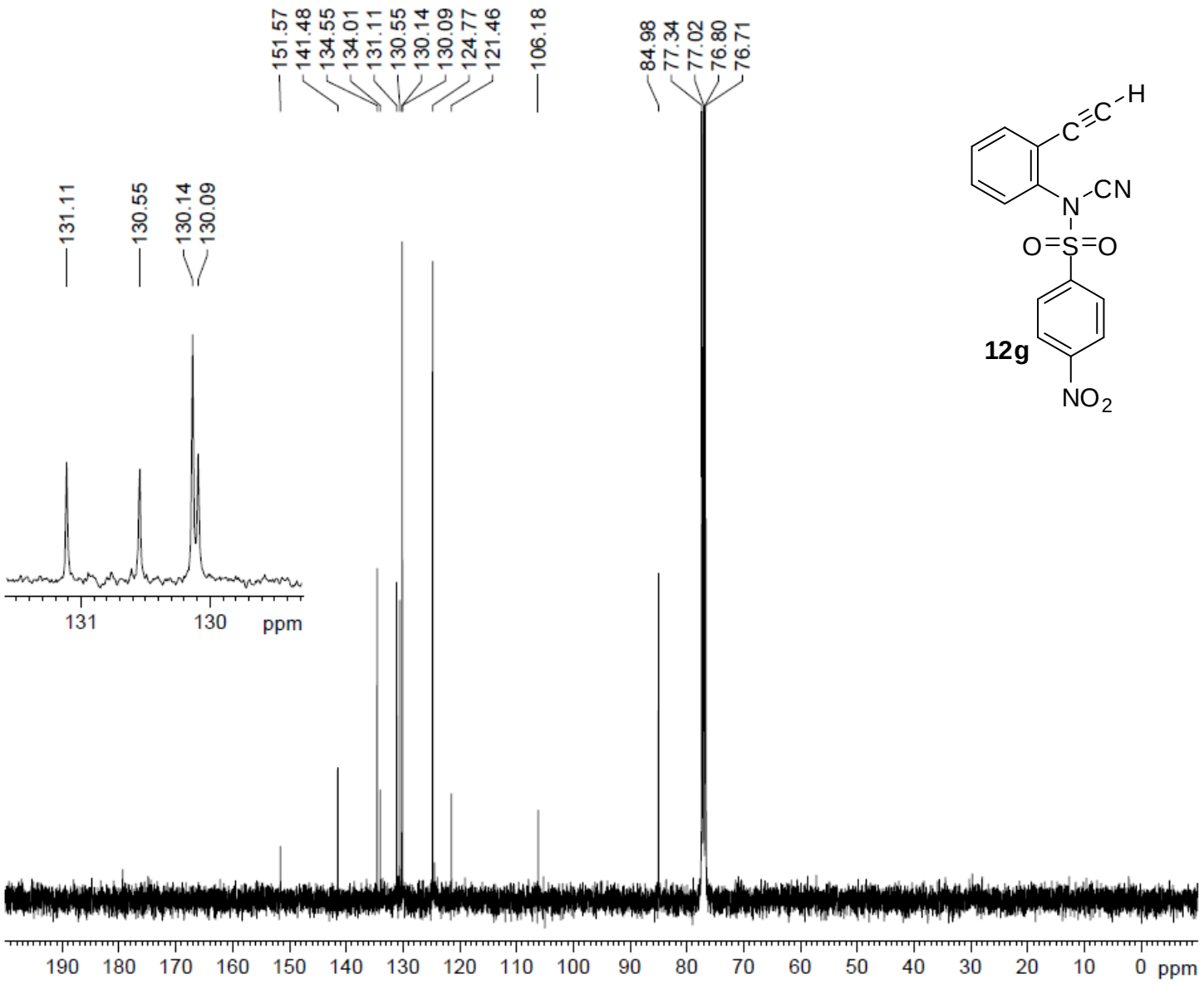
12g

Current Data Parameters
NAME SO028
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141205
Time 18.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 1
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 322.5
DW 69.000 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



12g

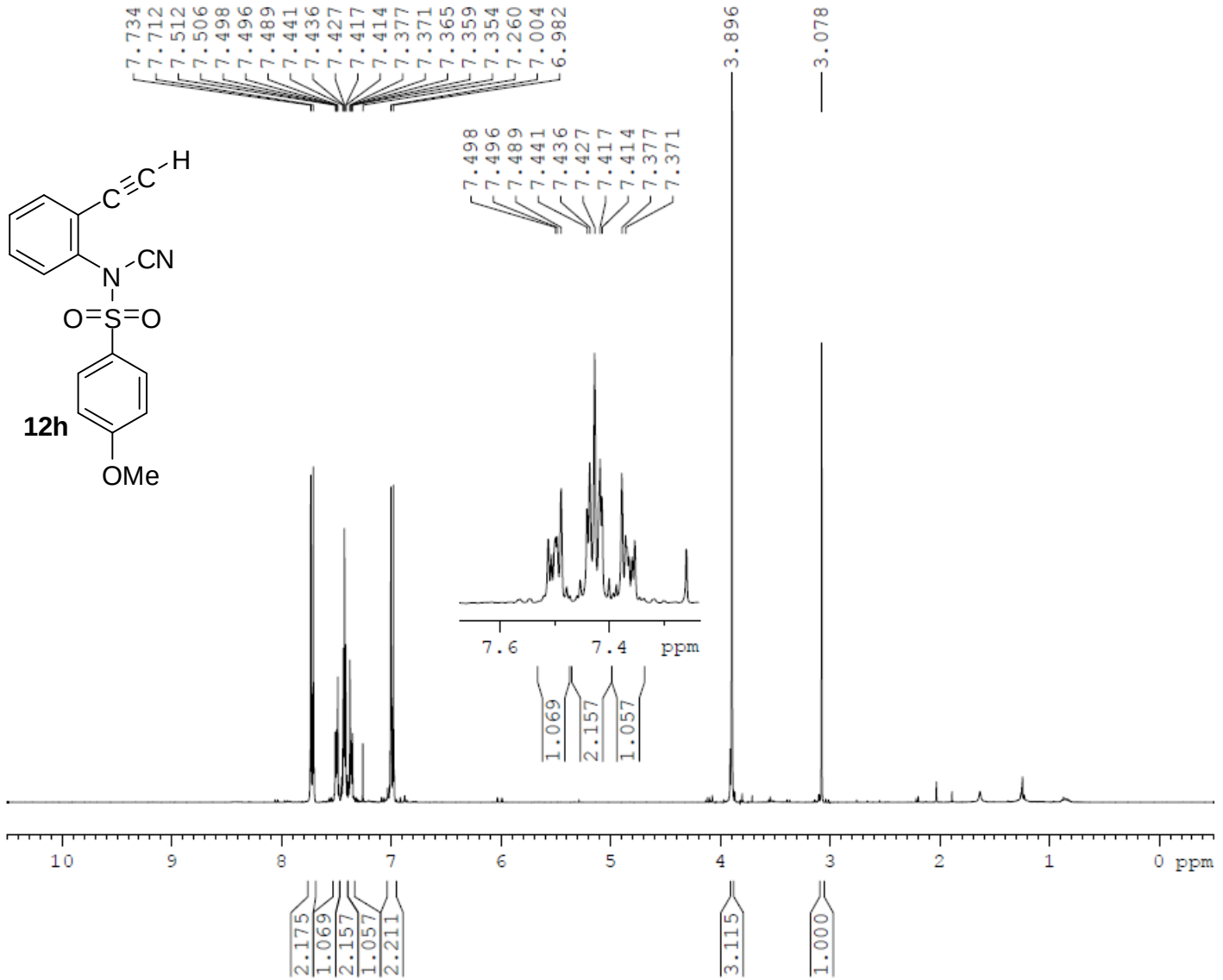
Current Data Parameters
NAME SO028
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141205
Time 18.25
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

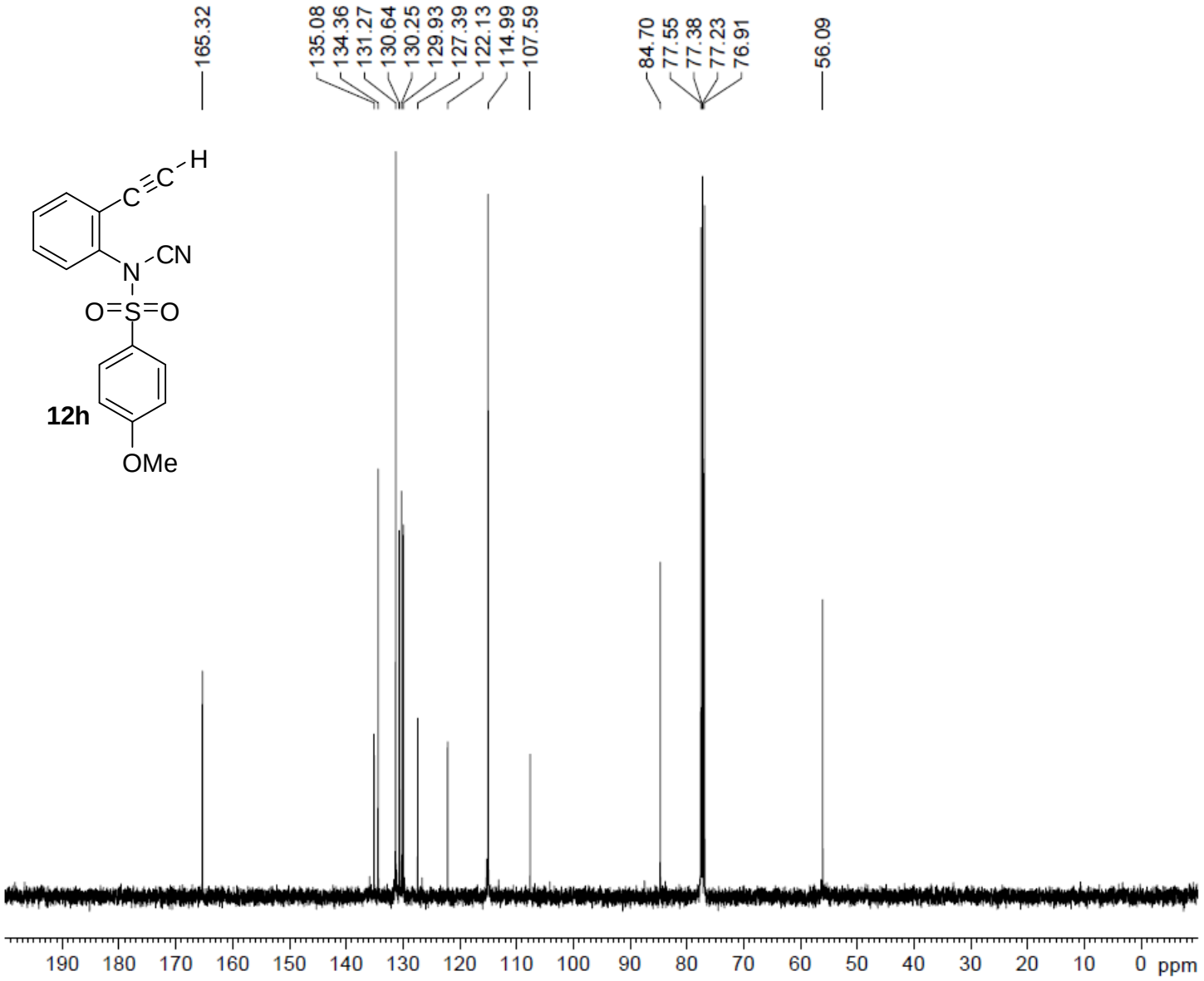


Current Data Parameters
NAME SO126
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150609
Time 16.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 21.45 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



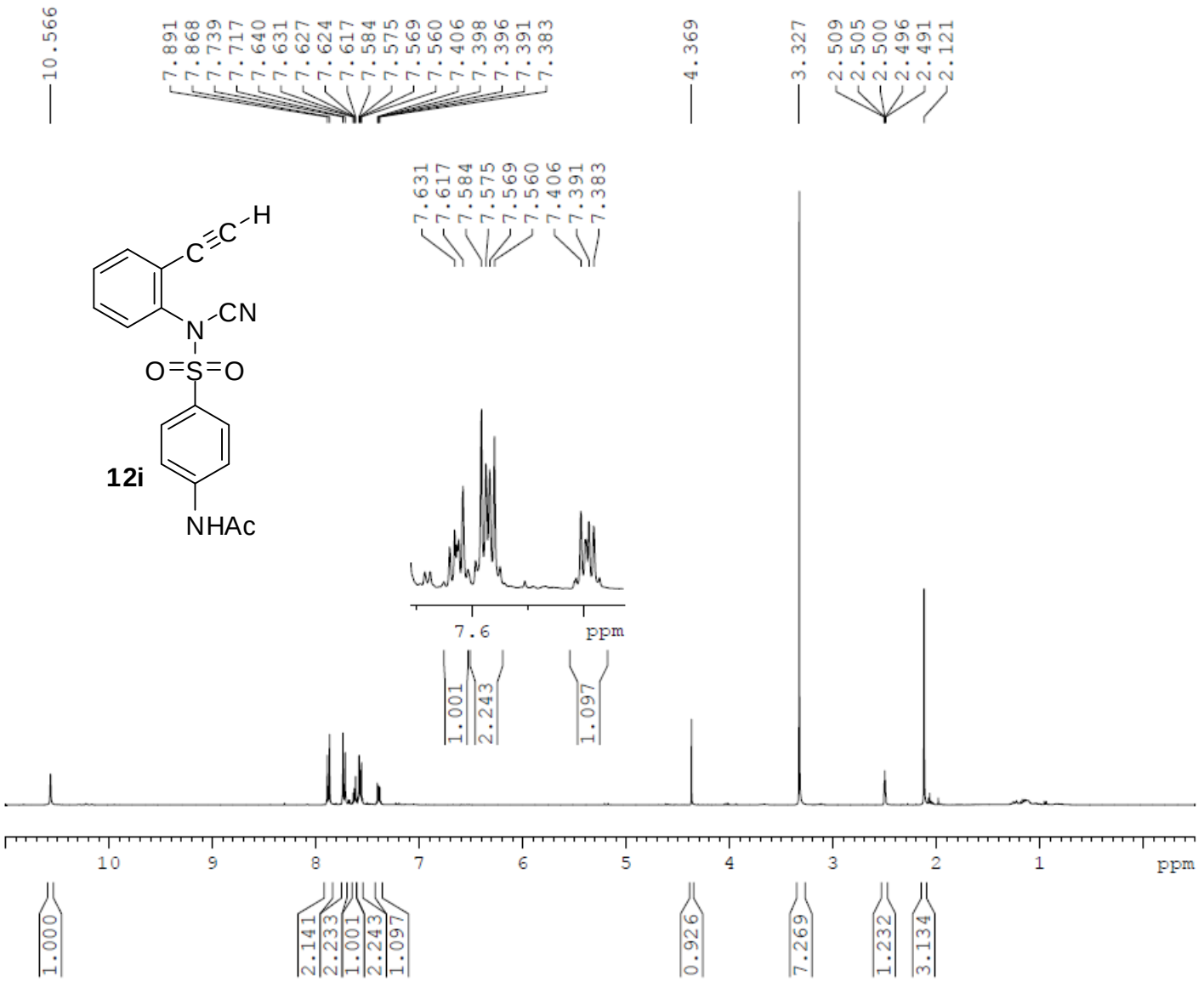
Current Data Parameters
NAME SO126
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150609
Time 16.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 195
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127536 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

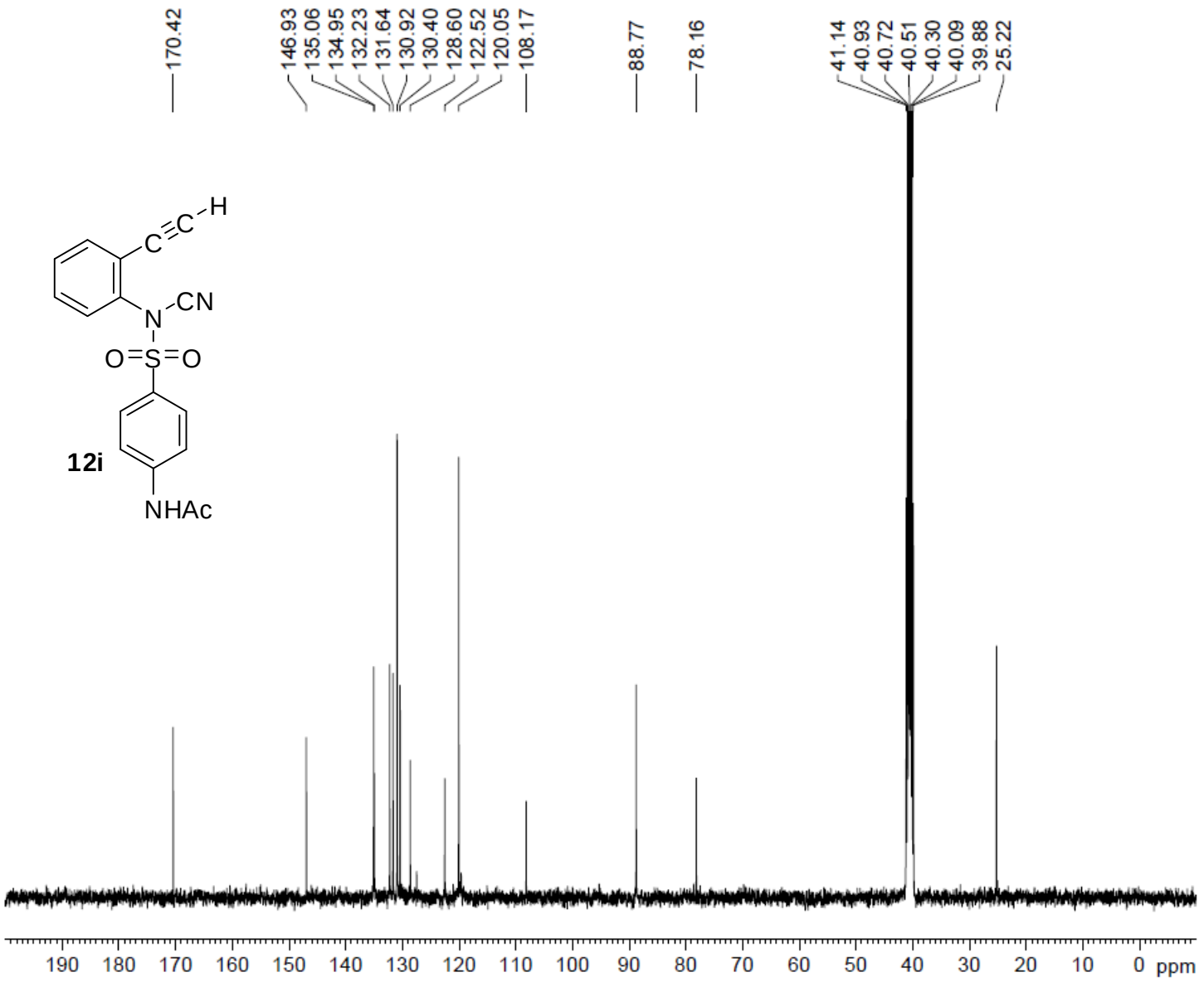


Current Data Parameters
NAME SO130
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150618
Time 9.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 301.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



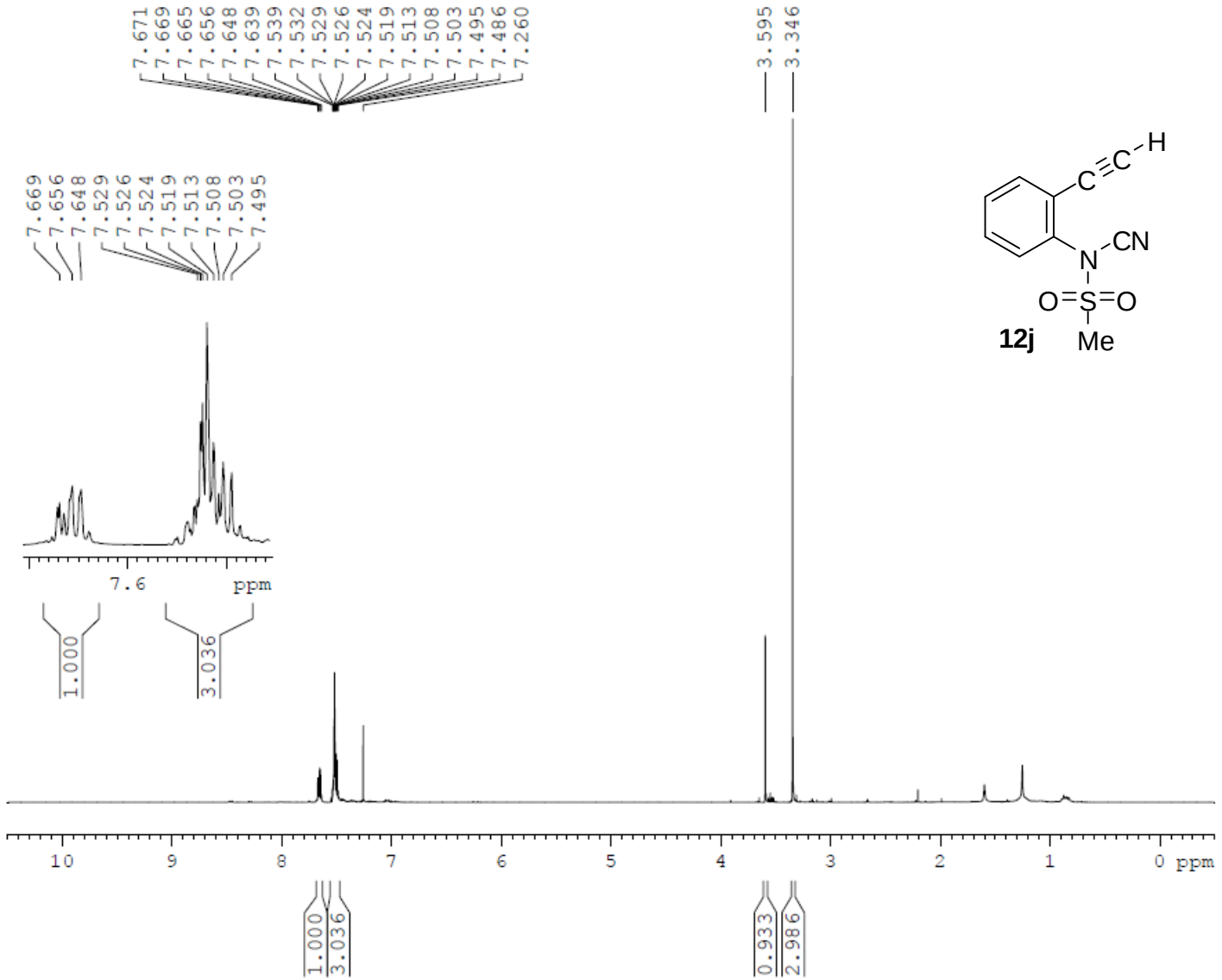
Current Data Parameters
NAME SO130
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150618
Time 9.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 769
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 301.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127202 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

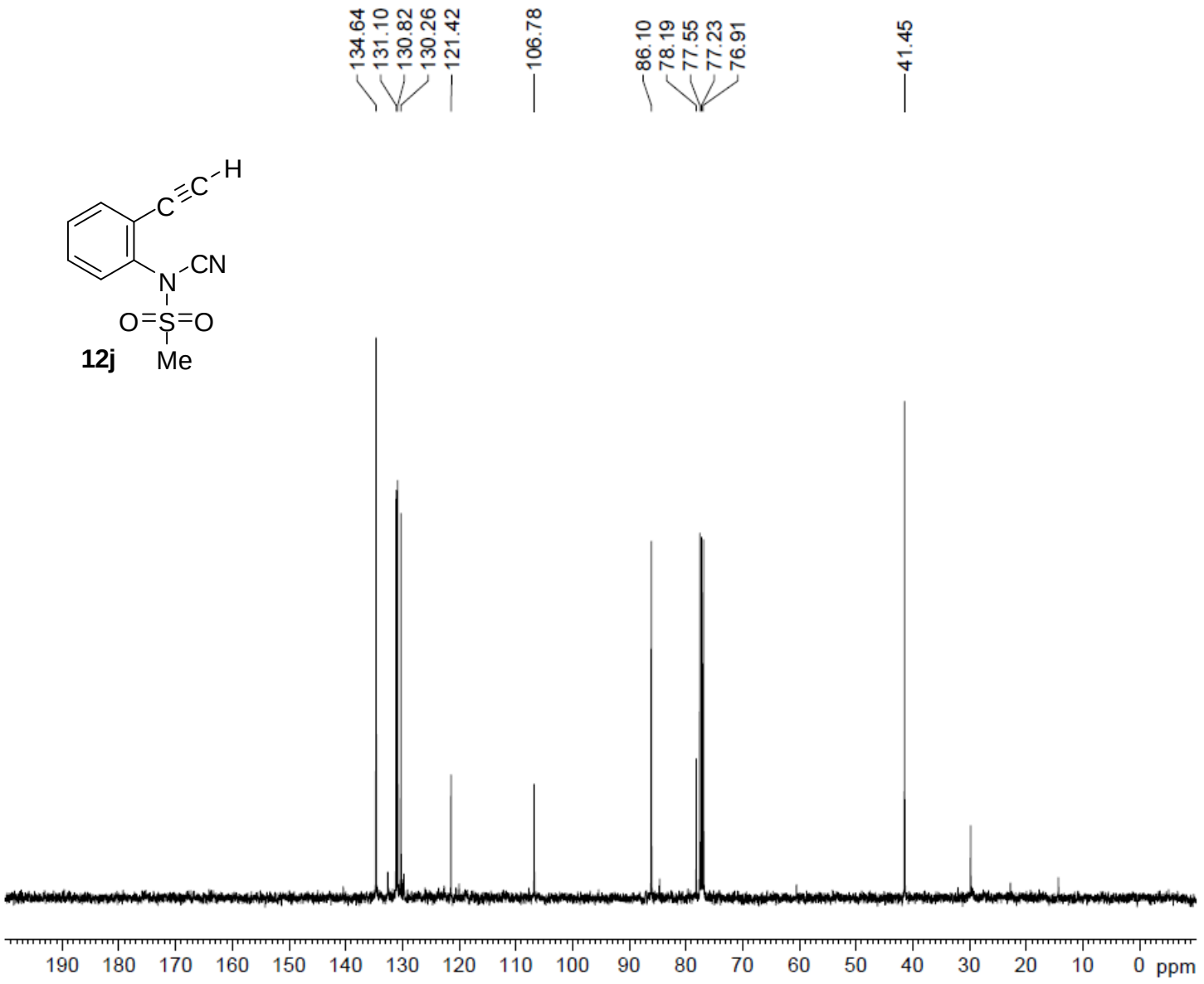


Current Data Parameters
NAME SO136
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150624
Time 10.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 298.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



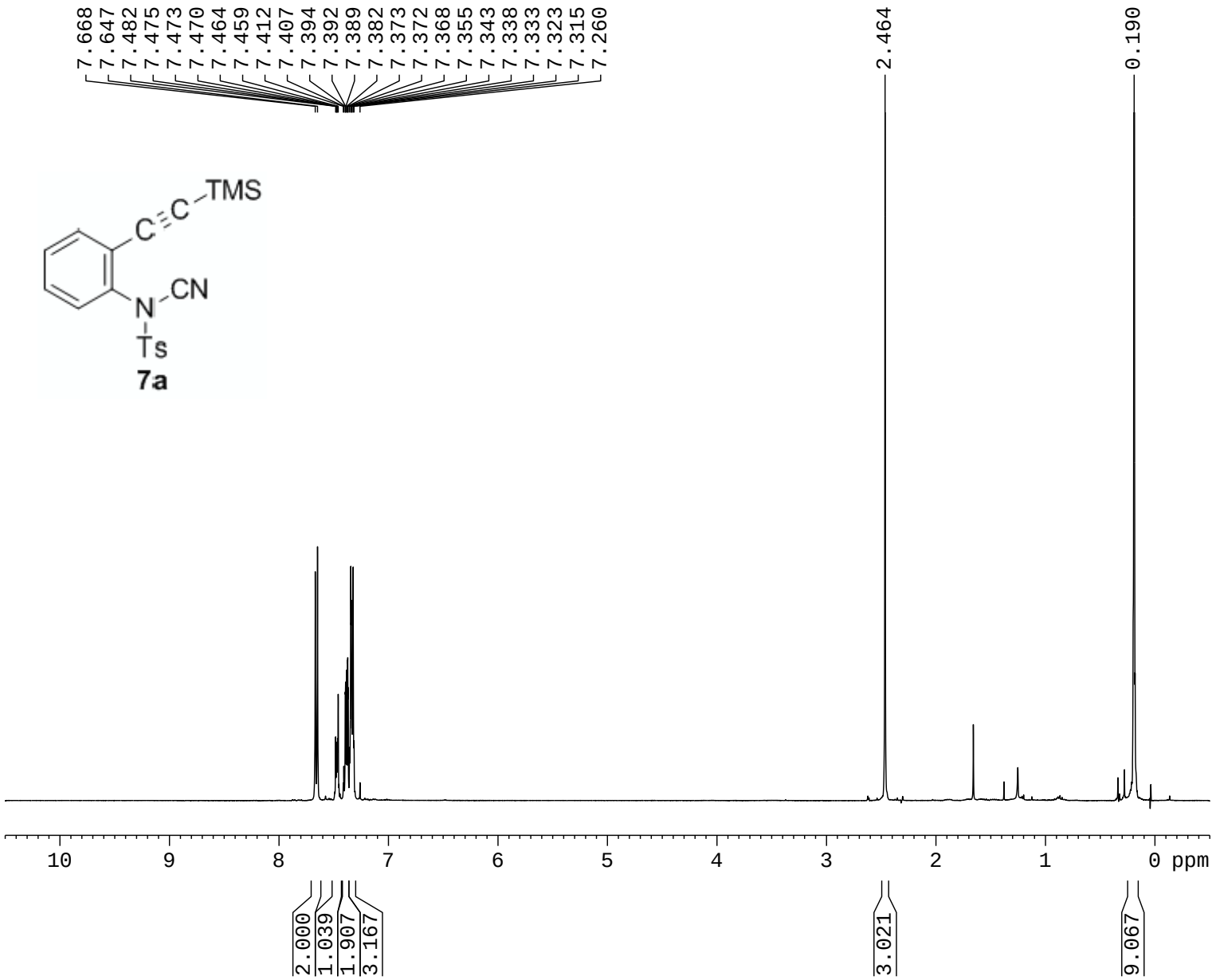
Current Data Parameters
NAME SO136
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150626
Time 11.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 112
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127575 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

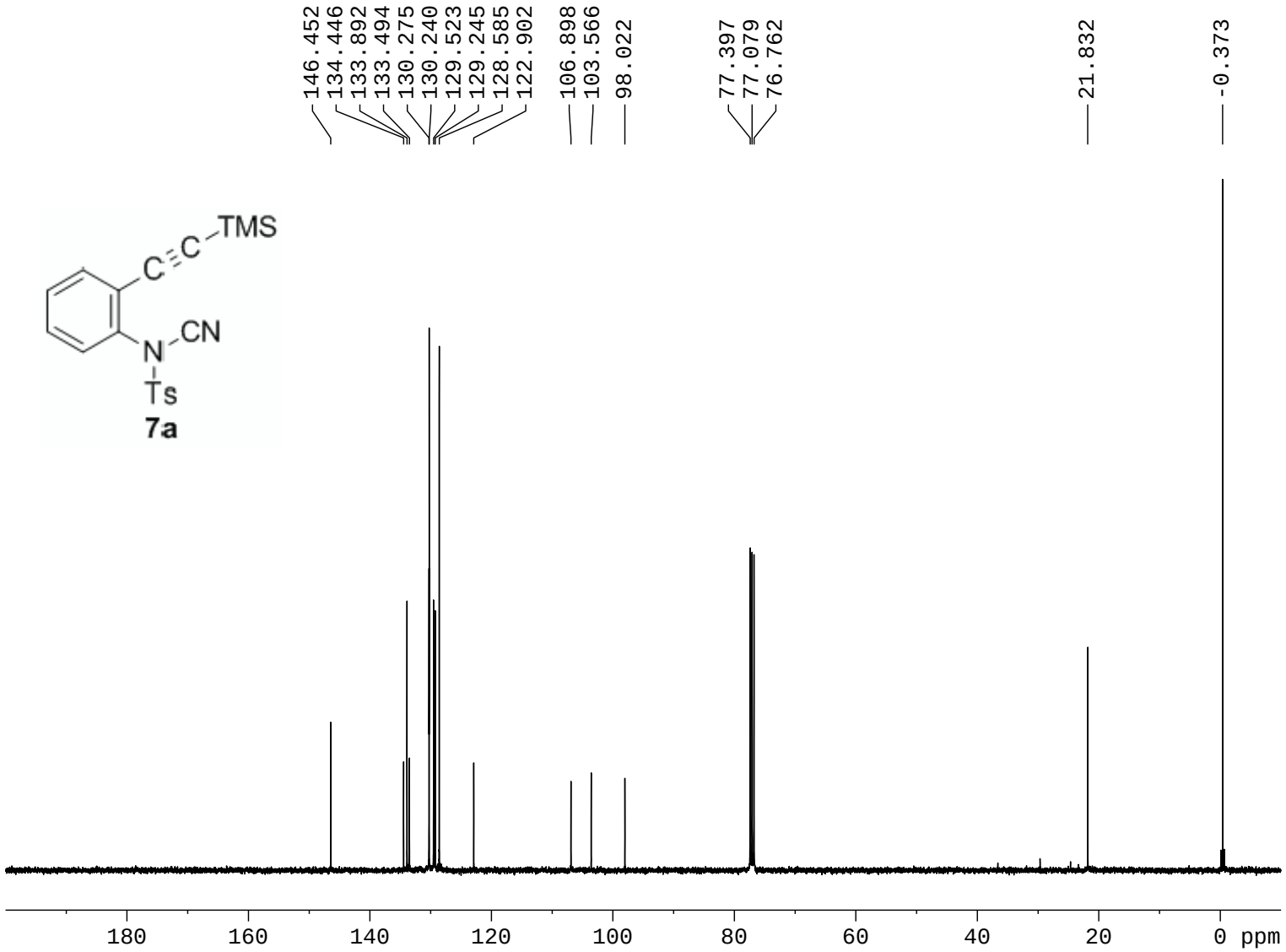


Current Data Parameters
NAME RV086
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130719
Time 10.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 45.3
DW 69.000 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.90 usec
PL1 3.00 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



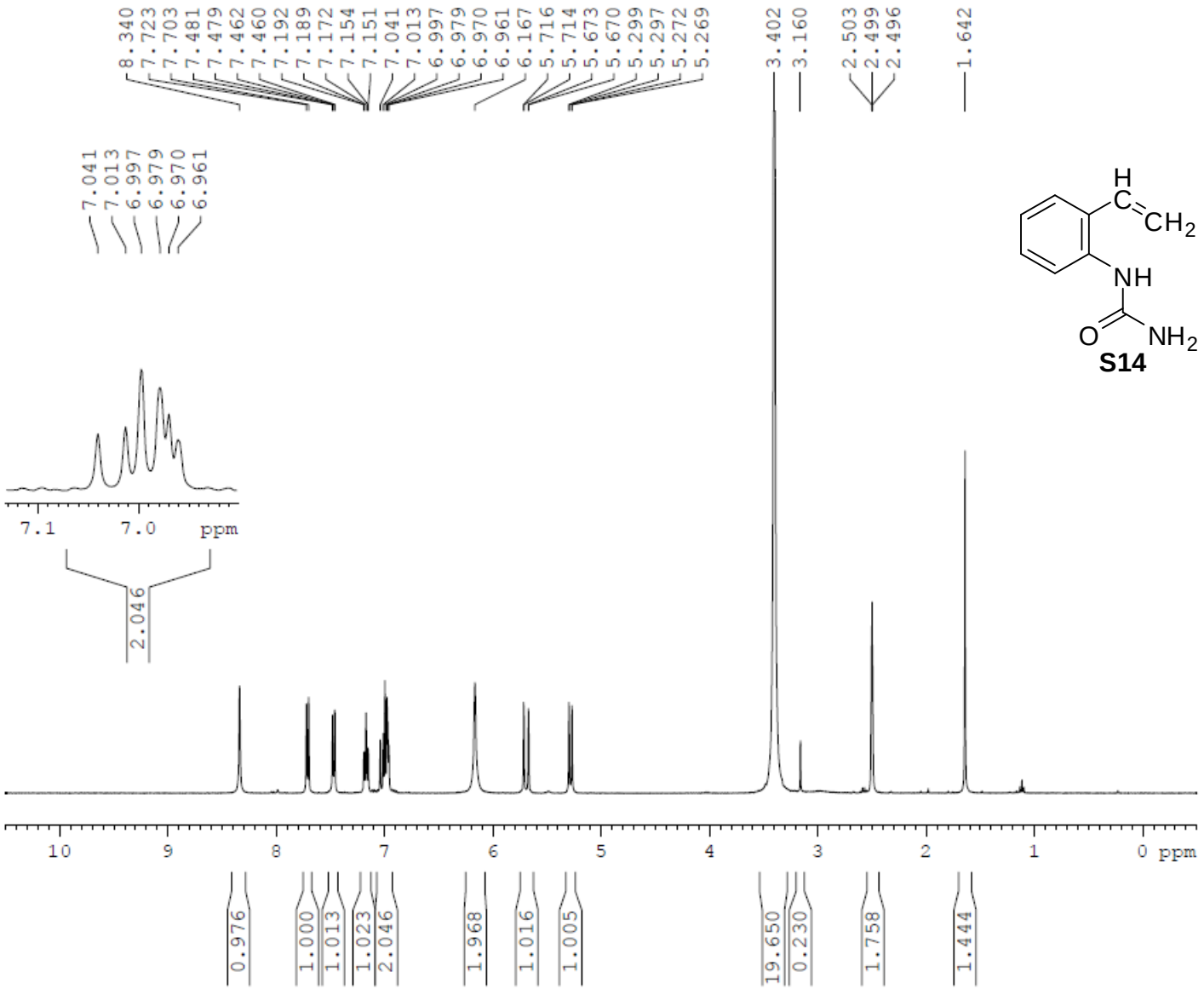
Current Data Parameters
NAME RV086
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130719
Time 10.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 345
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 1024
DW 20.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.40 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 3.00 dB
PL12 20.70 dB
PL13 23.70 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



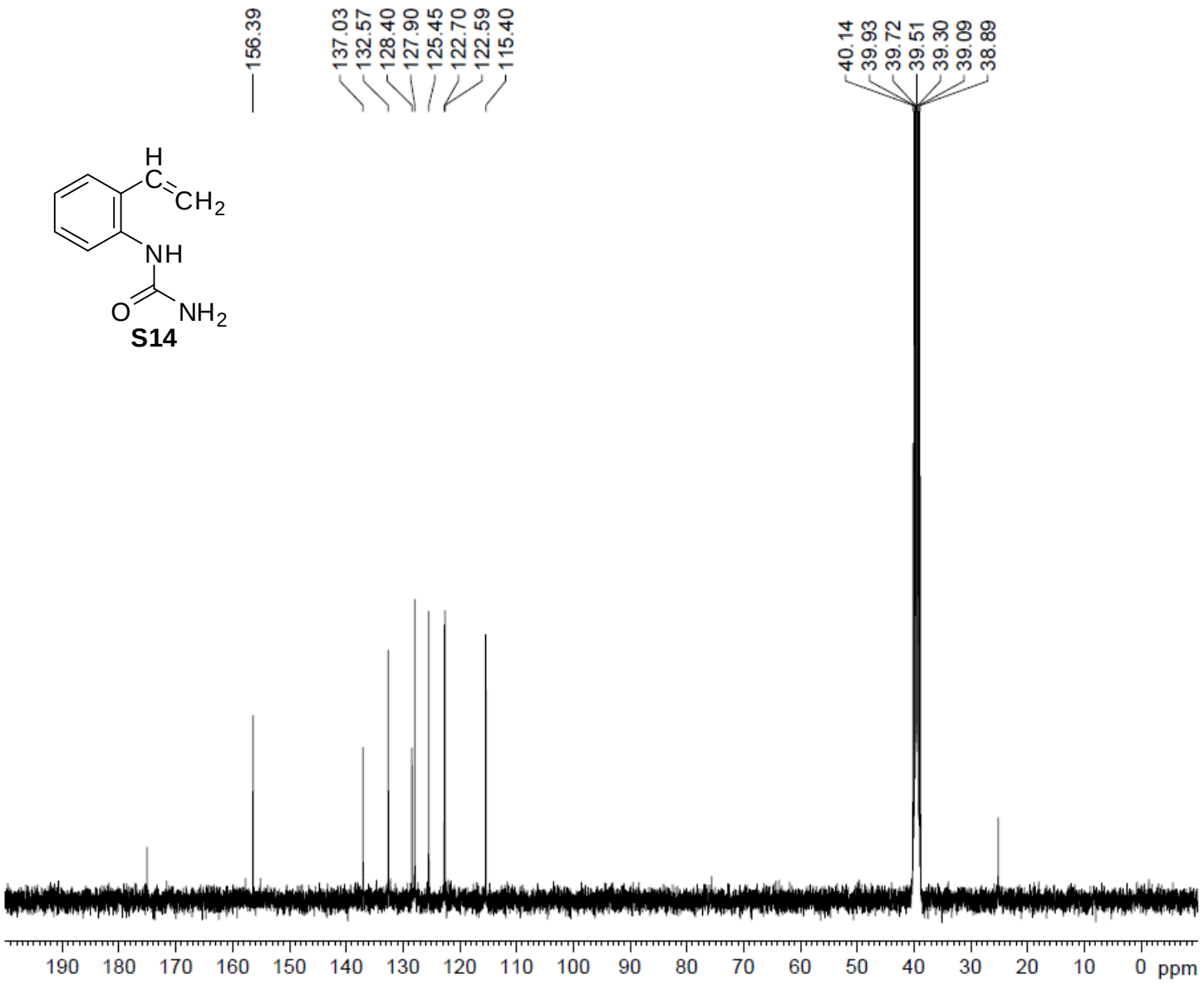
S14

Current Data Parameters
NAME SO020
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141128
Time 8.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



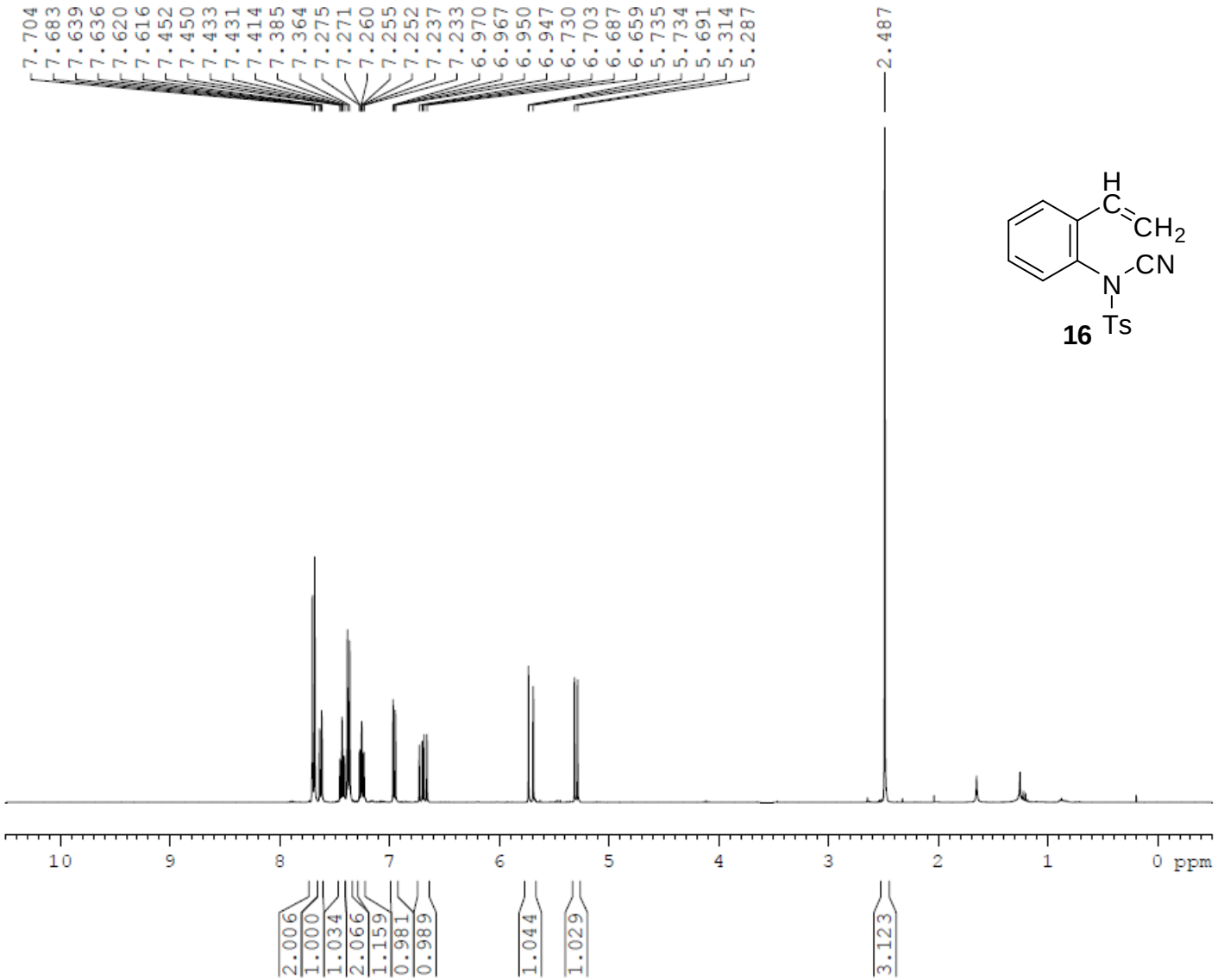
Current Data Parameters
NAME SO020
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141129
Time 9.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 919
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128156 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



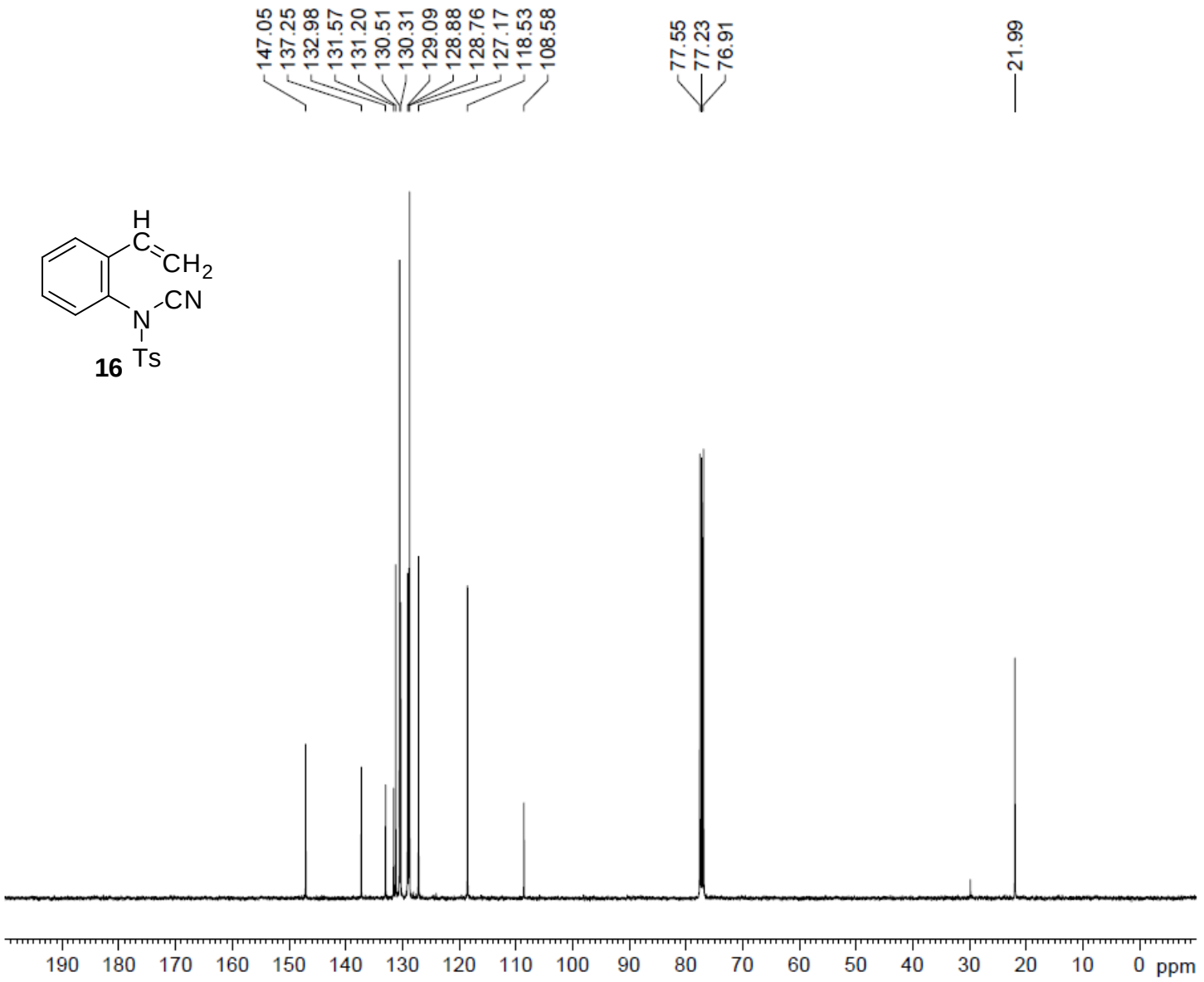
16

Current Data Parameters
NAME SO021
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141129
Time 18.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 51.8
DW 69.333 usec
DE 10.52 usec
TE 297.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



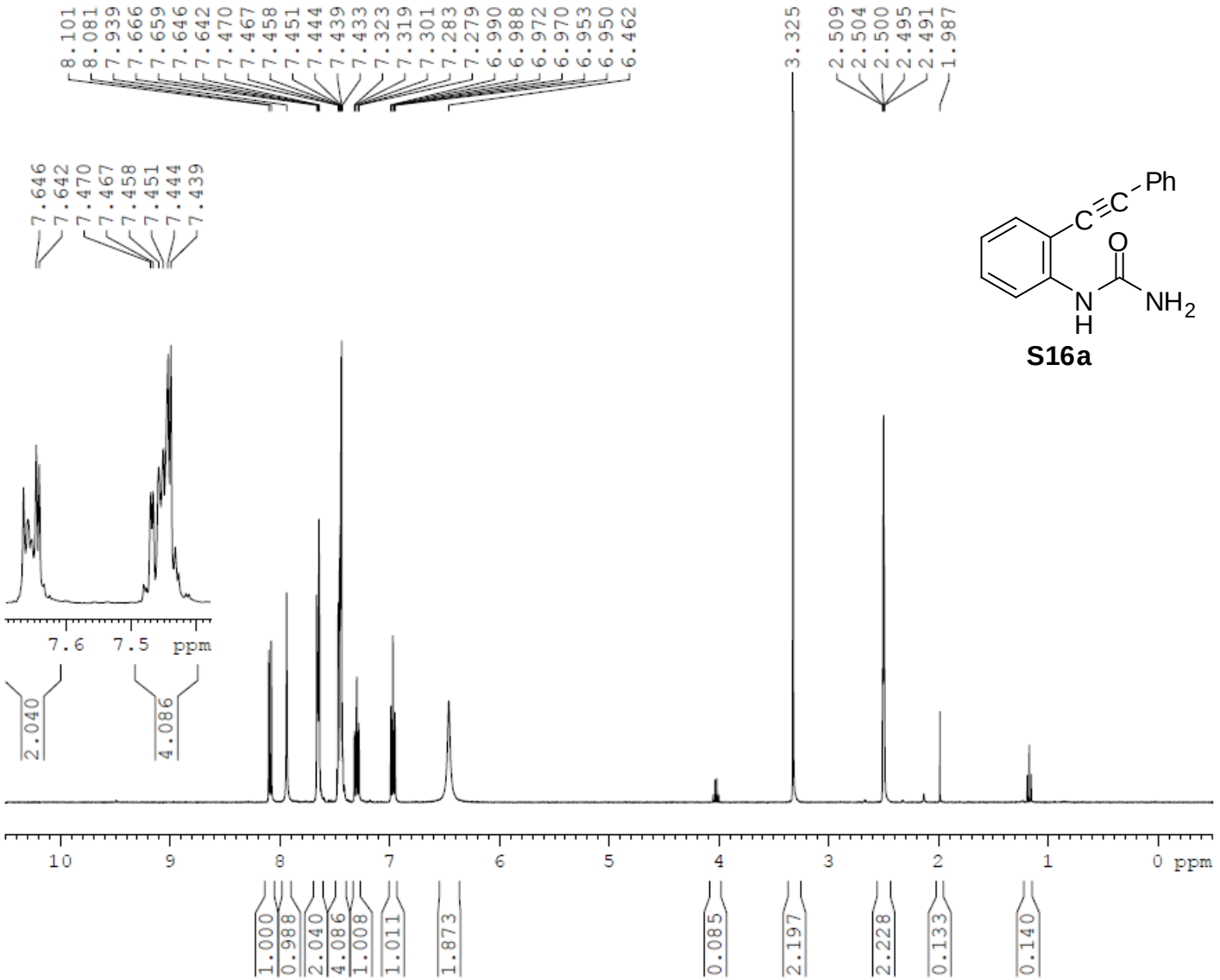
Current Data Parameters
NAME SO021
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141129
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127534 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



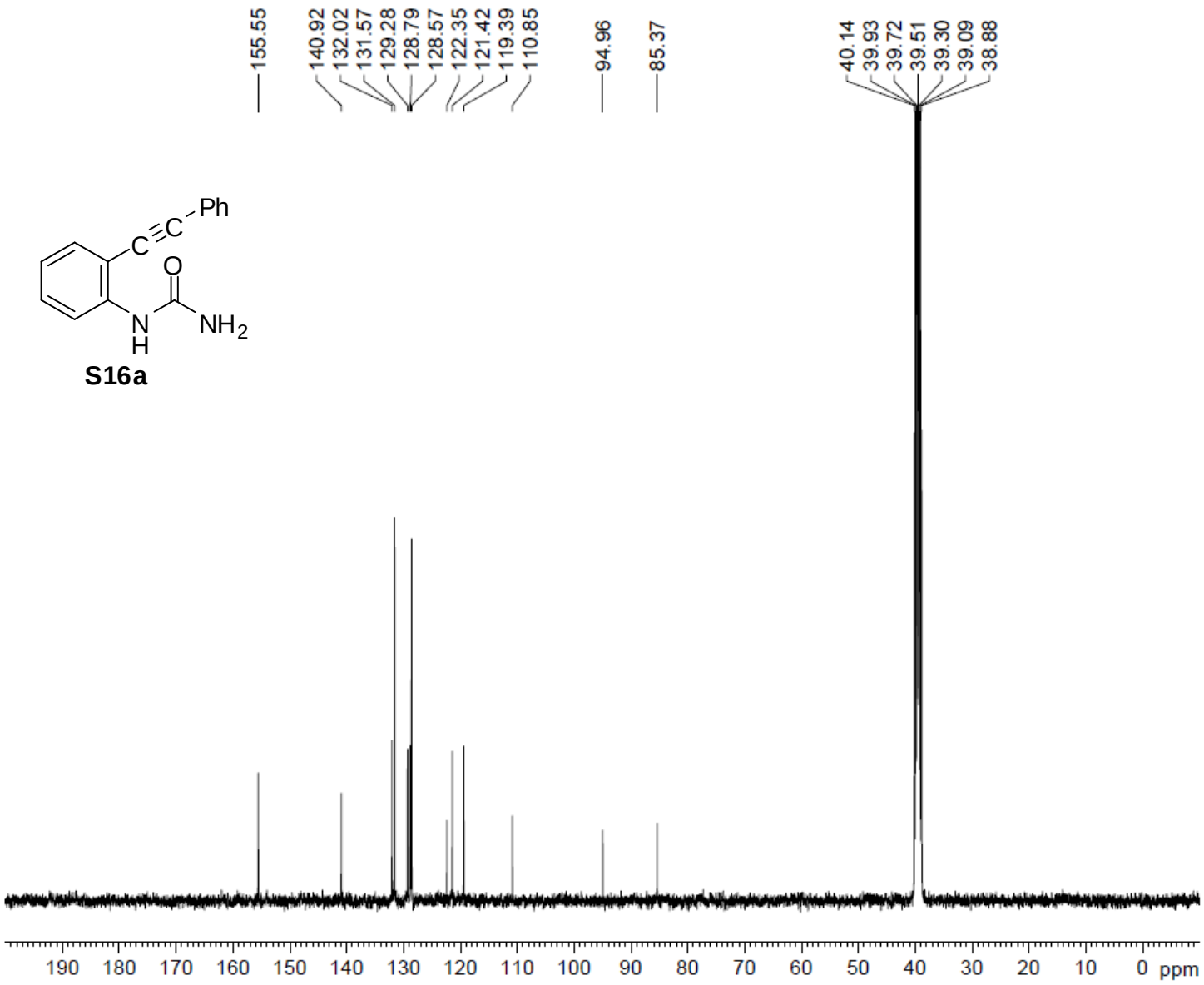
S16a

Current Data Parameters
NAME SO038
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141220
Time 9.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 198.09
DW 69.333 usec
DE 10.52 usec
TE 297.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300027 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



S16a

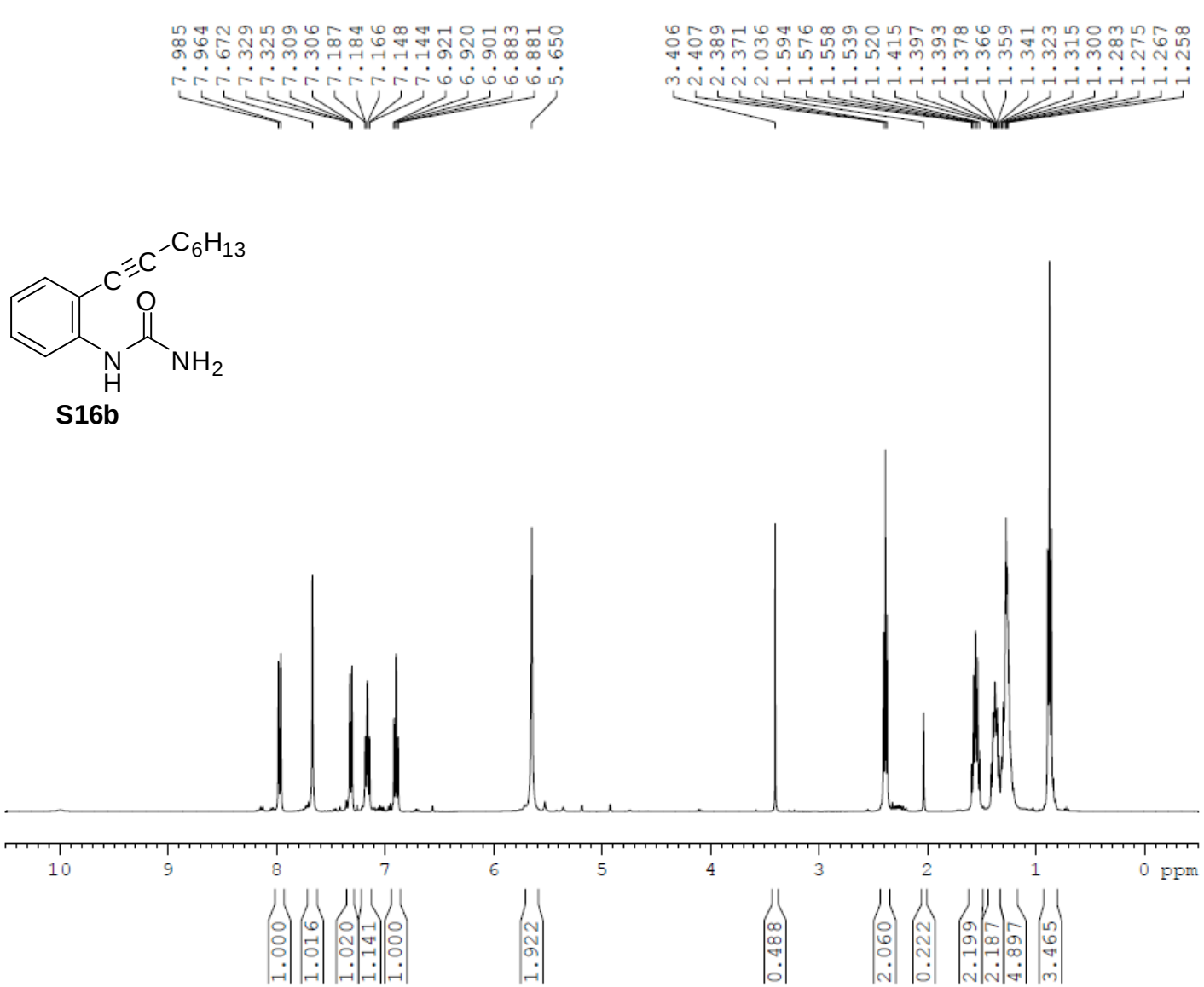
Current Data Parameters
NAME SO038
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141220
Time 10.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1408
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

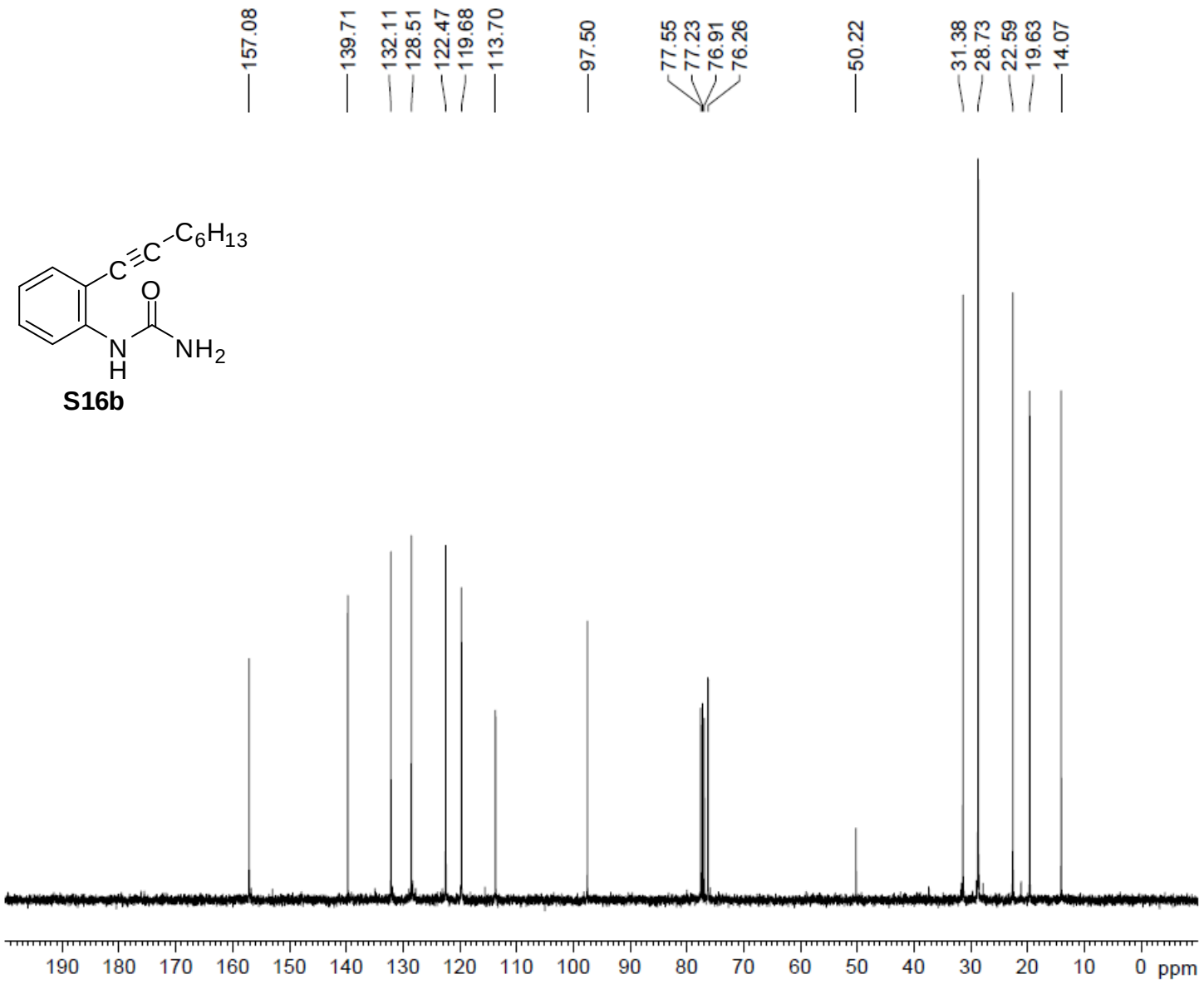
F2 - Processing parameters
SI 32768
SF 100.6128202 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



S16b

```
NAME          SC127
EXPNO             1
PROCNO            1
Date_      20140513
Time          16.03
INSTRUM        spect
PROBHD  5 mm SEI 1H-13
PULPROG         zg30
TD             32768
SOLVENT         CDCl3
NS                12
DS                 0
SWH        7246.377 Hz
FIDRES     0.221142 Hz
AQ         2.2611110 sec
RG                11.3
DW           69.000 usec
DE            6.50 usec
TE            299.1 K
D1         2.00000000 sec
TD0               1

======== CHANNEL f1 ========
NUC1              1H
P1           11.00 usec
PL1           -4.20 dB
SFO1     400.1324008 MHz
SI            16384
SF       400.1300087 MHz
WDW              EM
SSB               0
LB            0.00 Hz
GB                0
PC             1.00
```



S16b

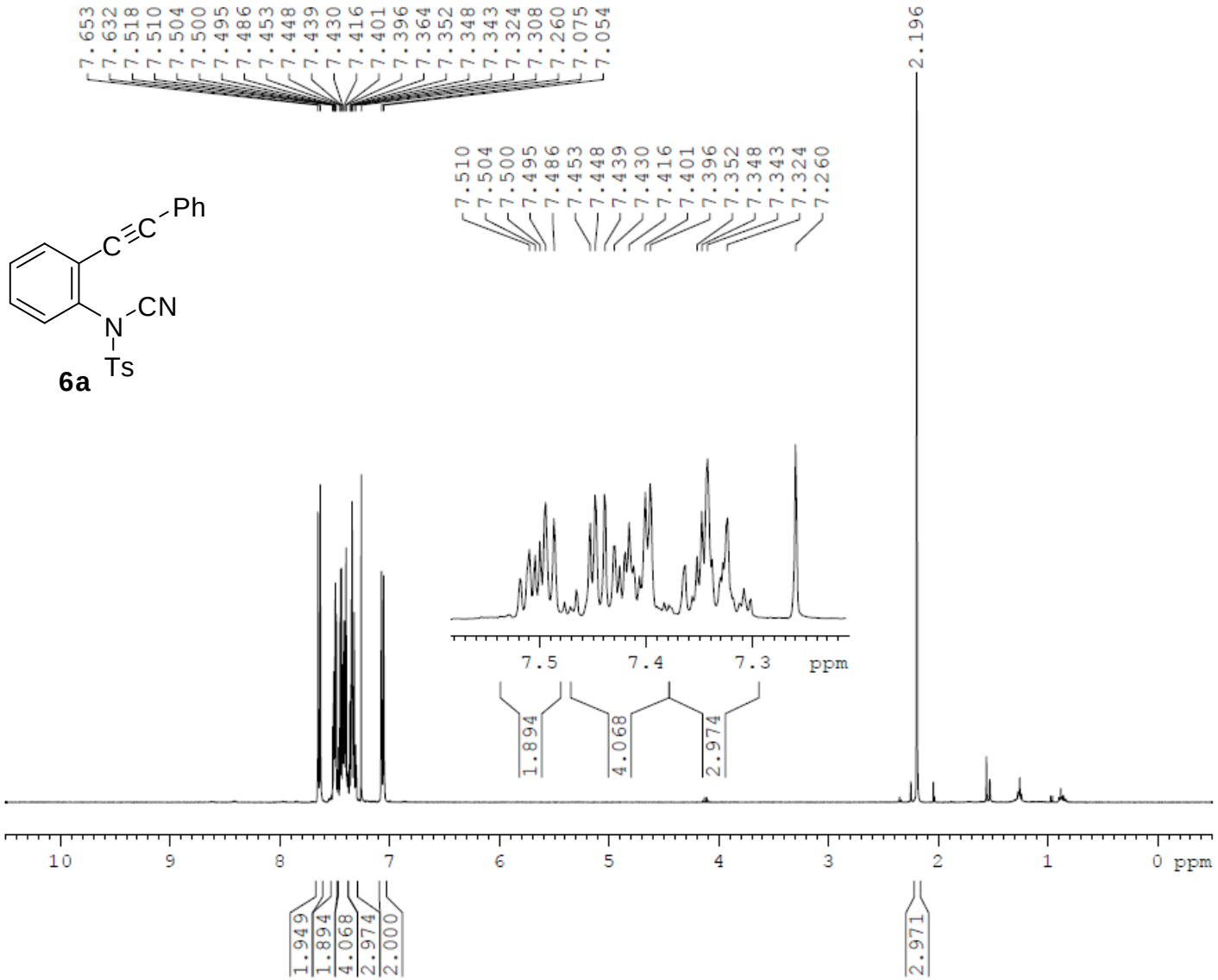
Current Data Parameters
NAME SC127
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140514
Time 8.46
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 32768
DW 20.800 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127675 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

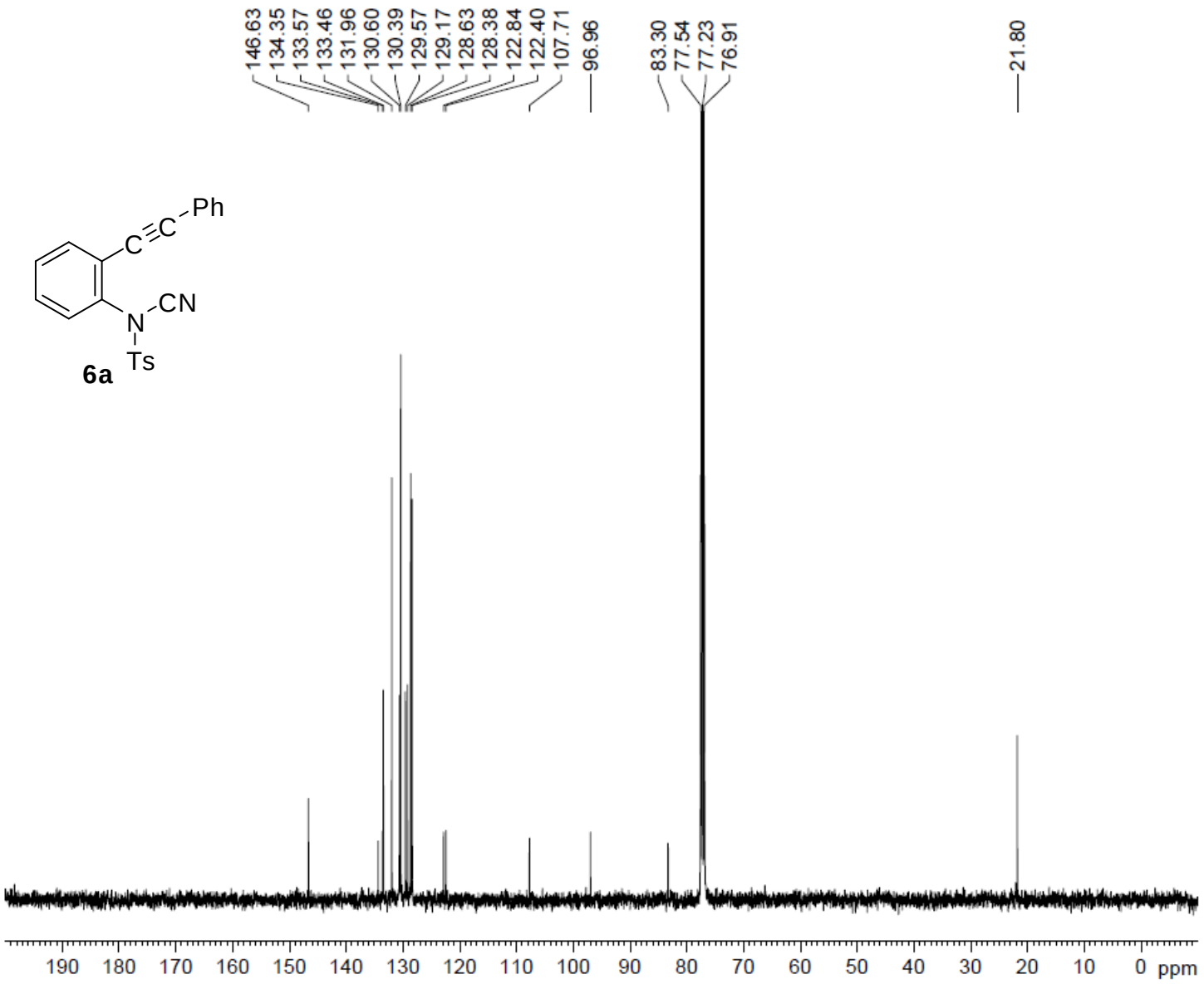


Current Data Parameters
NAME SO041
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141220
Time 22.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 177.16
DW 69.333 usec
DE 10.52 usec
TE 297.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



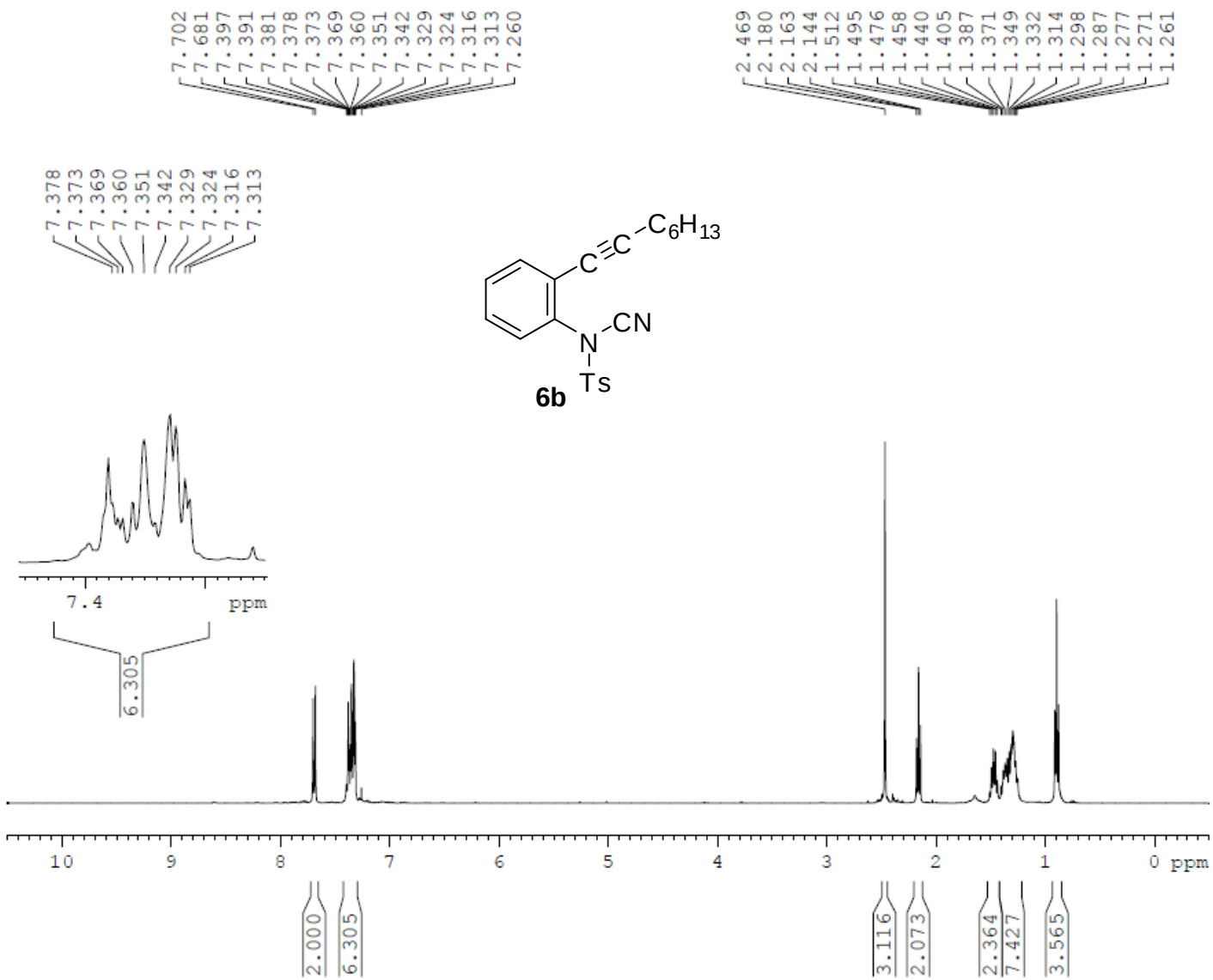
Current Data Parameters
NAME SO041
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141220
Time 23.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 480
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127481 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

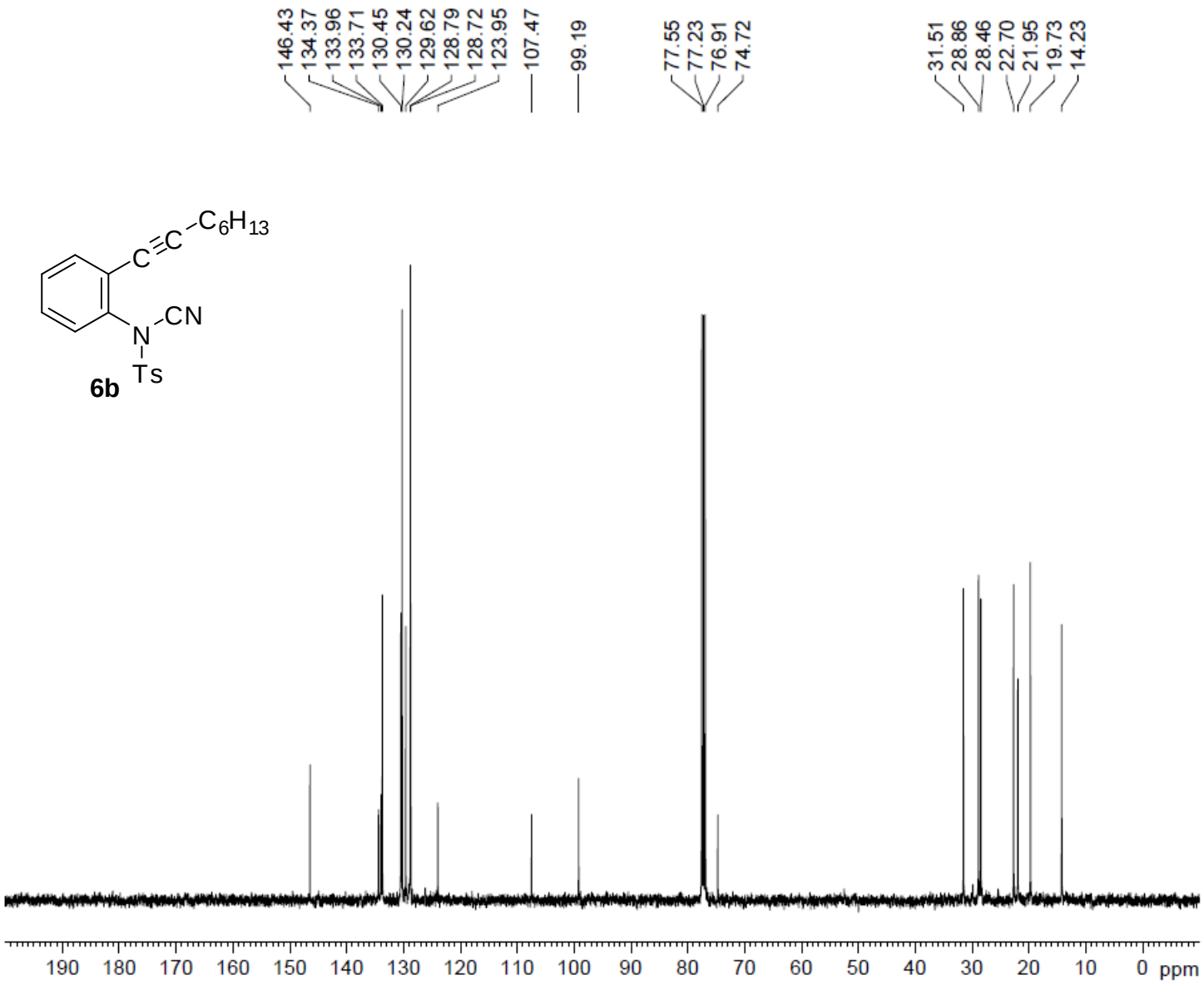


Current Data Parameters
NAME SC131
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140516
Time 10.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 45.15
DW 69.333 usec
DE 10.52 usec
TE 298.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



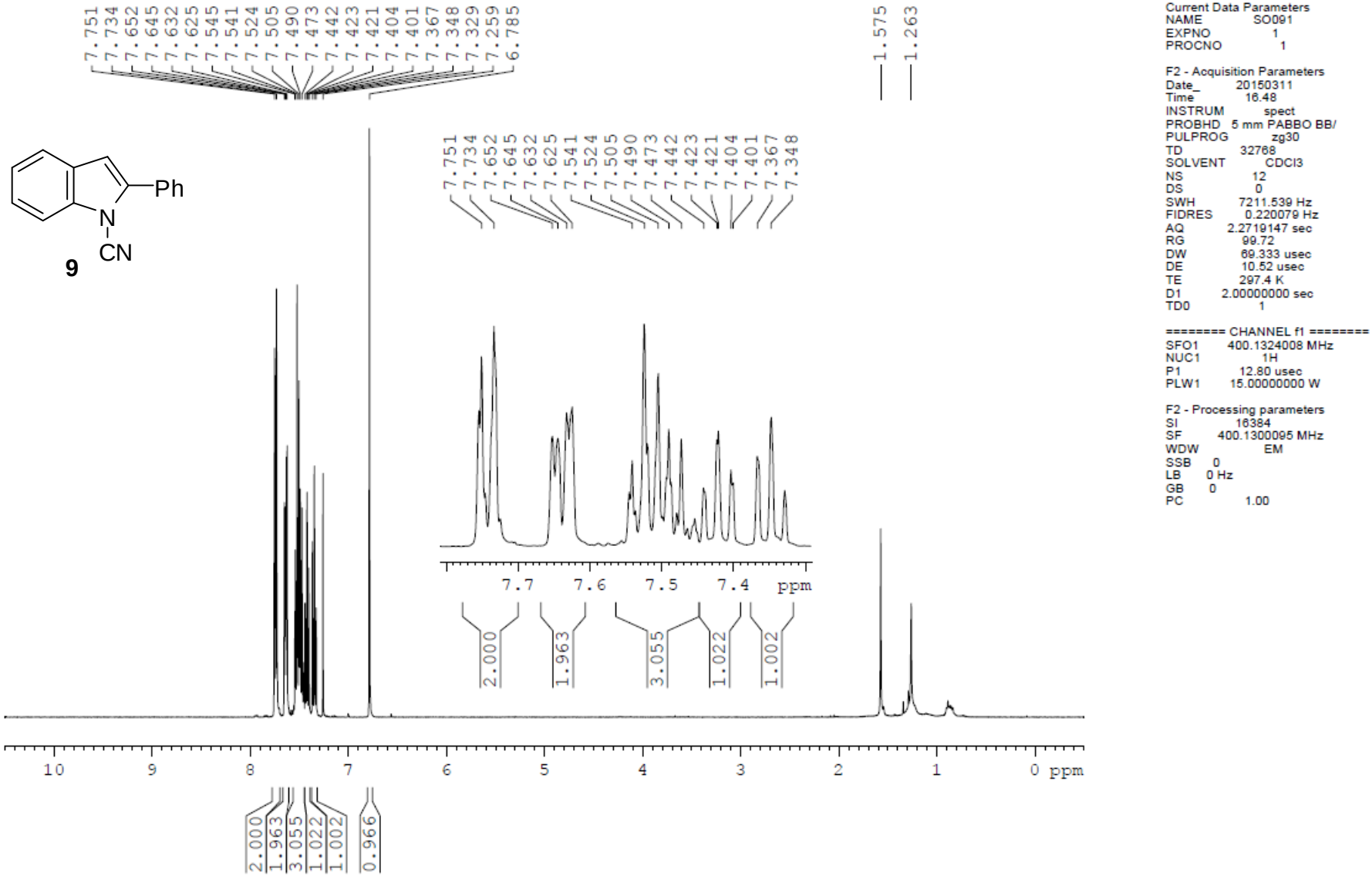
Current Data Parameters
NAME SC131
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140516
Time 10.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 173
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127519 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

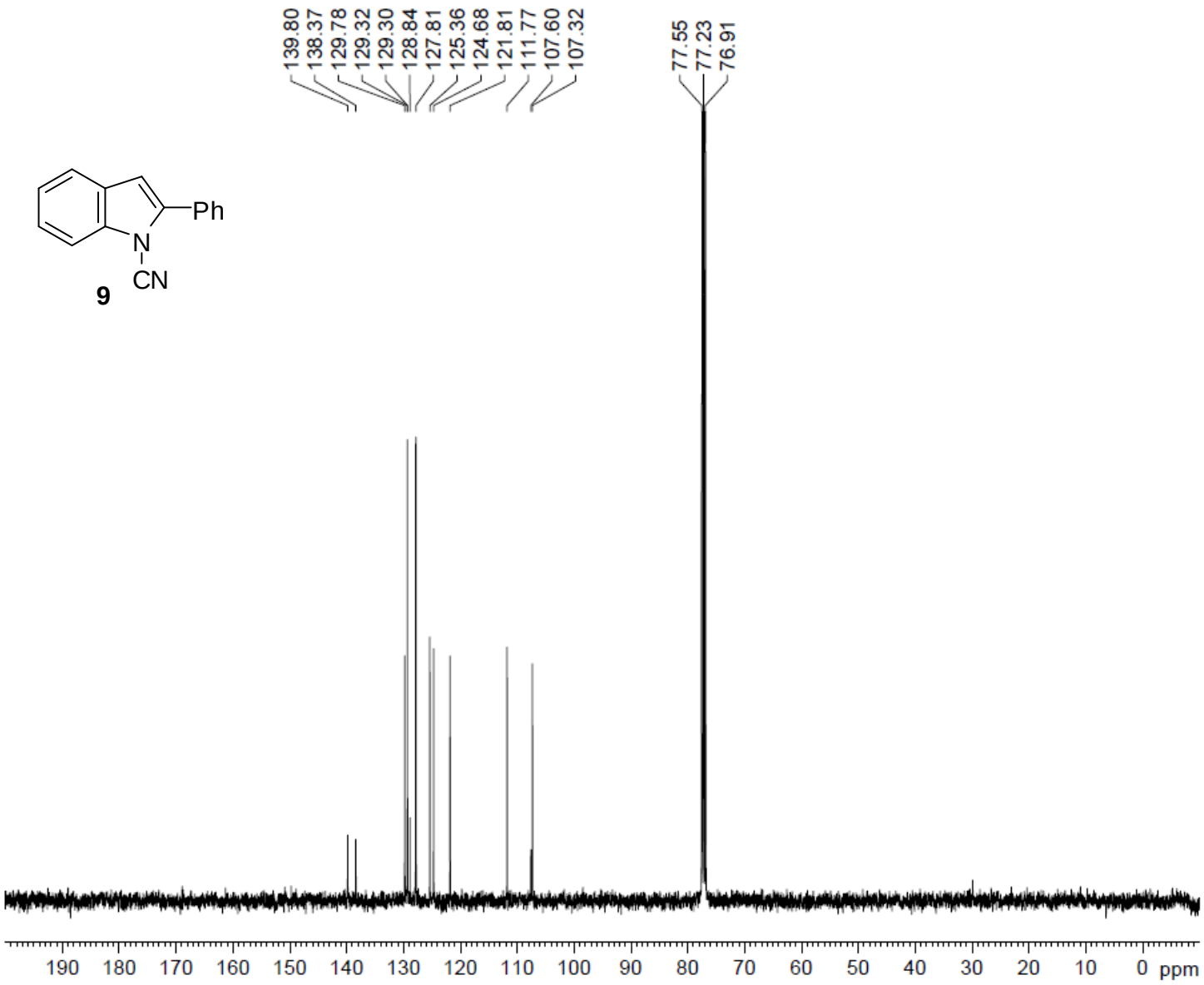


Current Data Parameters
NAME SO091
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150311
Time 16.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 297.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SO091
EXPNO 2
PROCNO 1

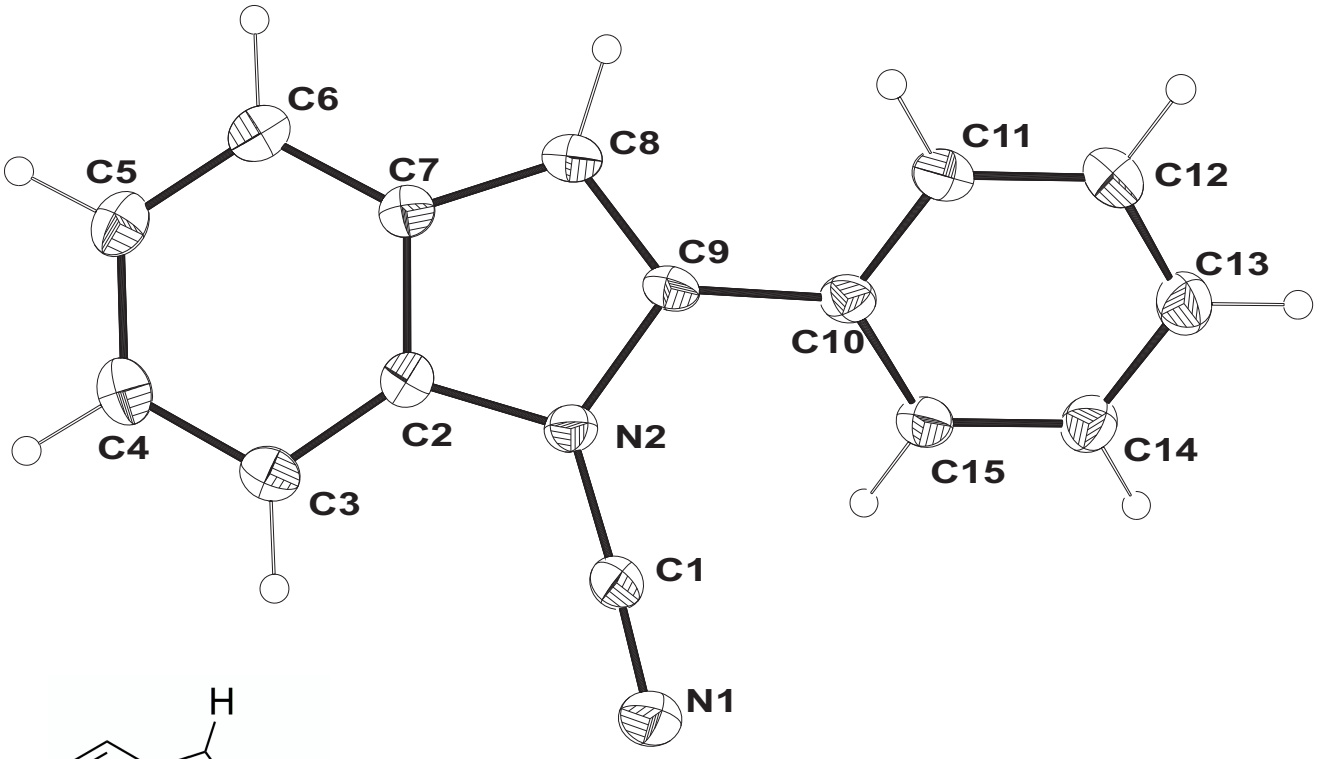
F2 - Acquisition Parameters
Date_ 20150312
Time 10.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 150
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

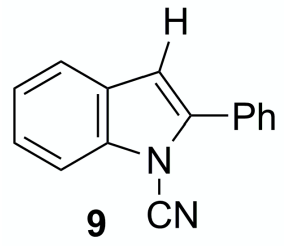
======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127494 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

a15780





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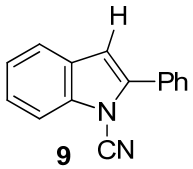


9

Table 1. Crystal data and structure refinement for a15780.

Identification code	a15780	
Empirical formula	C15 H10 N2	
Formula weight	218.25	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P b c a	
Unit cell dimensions	a = 13.936(7) Å	α= 90°.
	b = 7.077(3) Å	β= 90°.
	c = 22.807(10) Å	γ = 90°.
Volume	2249.2(17) $Å^3$	
Z	8	
Density (calculated)	1.289 Mg/m^3	
Absorption coefficient	0.078 mm^{-1}	
F(000)	912	
Crystal size	0.21 x 0.18 x 0.03 mm^3	
Theta range for data collection	3.43 to 25.19°.	
Index ranges	-16<=h<=16, -8<=k<=5, -26<=l<=27	
Reflections collected	15611	
Independent reflections	2016 [R(int) = 0.1822]	
Completeness to theta = 25.19°	99.3 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9977 and 0.9839	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2016 / 0 / 154	
Goodness-of-fit on F^2	0.976	
Final R indices [I>2sigma(I)]	R1 = 0.0582, wR2 = 0.1137	
R indices (all data)	R1 = 0.1301, wR2 = 0.1461	
Largest diff. peak and hole	0.213 and -0.222 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for a15780. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	725(2)	6898(4)	4090(1)	36(1)
C(2)	1117(2)	9035(4)	4881(1)	33(1)
C(3)	852(2)	7998(4)	5364(1)	37(1)
C(4)	1048(2)	8802(4)	5905(1)	43(1)
C(5)	1485(2)	10561(4)	5949(1)	44(1)
C(6)	1728(2)	11584(4)	5459(1)	42(1)
C(7)	1551(2)	10809(4)	4908(1)	34(1)
C(8)	1705(2)	11441(4)	4316(1)	35(1)
C(9)	1374(2)	10114(4)	3938(1)	33(1)
C(10)	1338(2)	10111(4)	3296(1)	33(1)
C(11)	2066(2)	10992(4)	2984(1)	45(1)
C(12)	2036(3)	11077(4)	2377(1)	53(1)
C(13)	1290(2)	10281(4)	2074(1)	48(1)
C(14)	560(2)	9386(4)	2376(1)	43(1)
C(15)	583(2)	9297(4)	2984(1)	38(1)
N(1)	481(2)	5417(4)	3949(1)	52(1)
N(2)	998(2)	8602(3)	4280(1)	33(1)

Table 3. Bond lengths [Å] and angles [°] for a15780.

C(1)-N(1)	1.148(3)
C(1)-N(2)	1.337(4)
C(2)-C(3)	1.374(4)
C(2)-C(7)	1.395(4)
C(2)-N(2)	1.413(3)
C(3)-C(4)	1.386(4)
C(3)-H(3)	0.9500
C(4)-C(5)	1.389(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.374(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.392(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.438(4)
C(8)-C(9)	1.356(4)
C(8)-H(8)	0.9500
C(9)-N(2)	1.425(3)
C(9)-C(10)	1.465(3)
C(10)-C(11)	1.386(4)
C(10)-C(15)	1.394(4)
C(11)-C(12)	1.388(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.370(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.382(4)
C(13)-H(13)	0.9500
C(14)-C(15)	1.387(3)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500

N(1)-C(1)-N(2)	177.3(3)
C(3)-C(2)-C(7)	124.1(3)
C(3)-C(2)-N(2)	129.0(3)
C(7)-C(2)-N(2)	106.8(2)

C(2)-C(3)-C(4)	116.2(3)
C(2)-C(3)-H(3)	121.9
C(4)-C(3)-H(3)	121.9
C(3)-C(4)-C(5)	121.2(3)
C(3)-C(4)-H(4)	119.4
C(5)-C(4)-H(4)	119.4
C(6)-C(5)-C(4)	121.4(3)
C(6)-C(5)-H(5)	119.3
C(4)-C(5)-H(5)	119.3
C(5)-C(6)-C(7)	118.9(3)
C(5)-C(6)-H(6)	120.6
C(7)-C(6)-H(6)	120.6
C(6)-C(7)-C(2)	118.1(3)
C(6)-C(7)-C(8)	134.3(3)
C(2)-C(7)-C(8)	107.6(2)
C(9)-C(8)-C(7)	109.4(3)
C(9)-C(8)-H(8)	125.3
C(7)-C(8)-H(8)	125.3
C(8)-C(9)-N(2)	107.2(2)
C(8)-C(9)-C(10)	130.5(3)
N(2)-C(9)-C(10)	122.3(2)
C(11)-C(10)-C(15)	118.5(3)
C(11)-C(10)-C(9)	119.1(3)
C(15)-C(10)-C(9)	122.4(3)
C(10)-C(11)-C(12)	120.6(3)
C(10)-C(11)-H(11)	119.7
C(12)-C(11)-H(11)	119.7
C(13)-C(12)-C(11)	120.6(3)
C(13)-C(12)-H(12)	119.7
C(11)-C(12)-H(12)	119.7
C(12)-C(13)-C(14)	119.7(3)
C(12)-C(13)-H(13)	120.2
C(14)-C(13)-H(13)	120.2
C(13)-C(14)-C(15)	120.2(3)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9

C(14)-C(15)-C(10)	120.6(3)
C(14)-C(15)-H(15)	119.7
C(10)-C(15)-H(15)	119.7
C(1)-N(2)-C(2)	122.9(2)
C(1)-N(2)-C(9)	127.2(2)
C(2)-N(2)-C(9)	109.0(2)

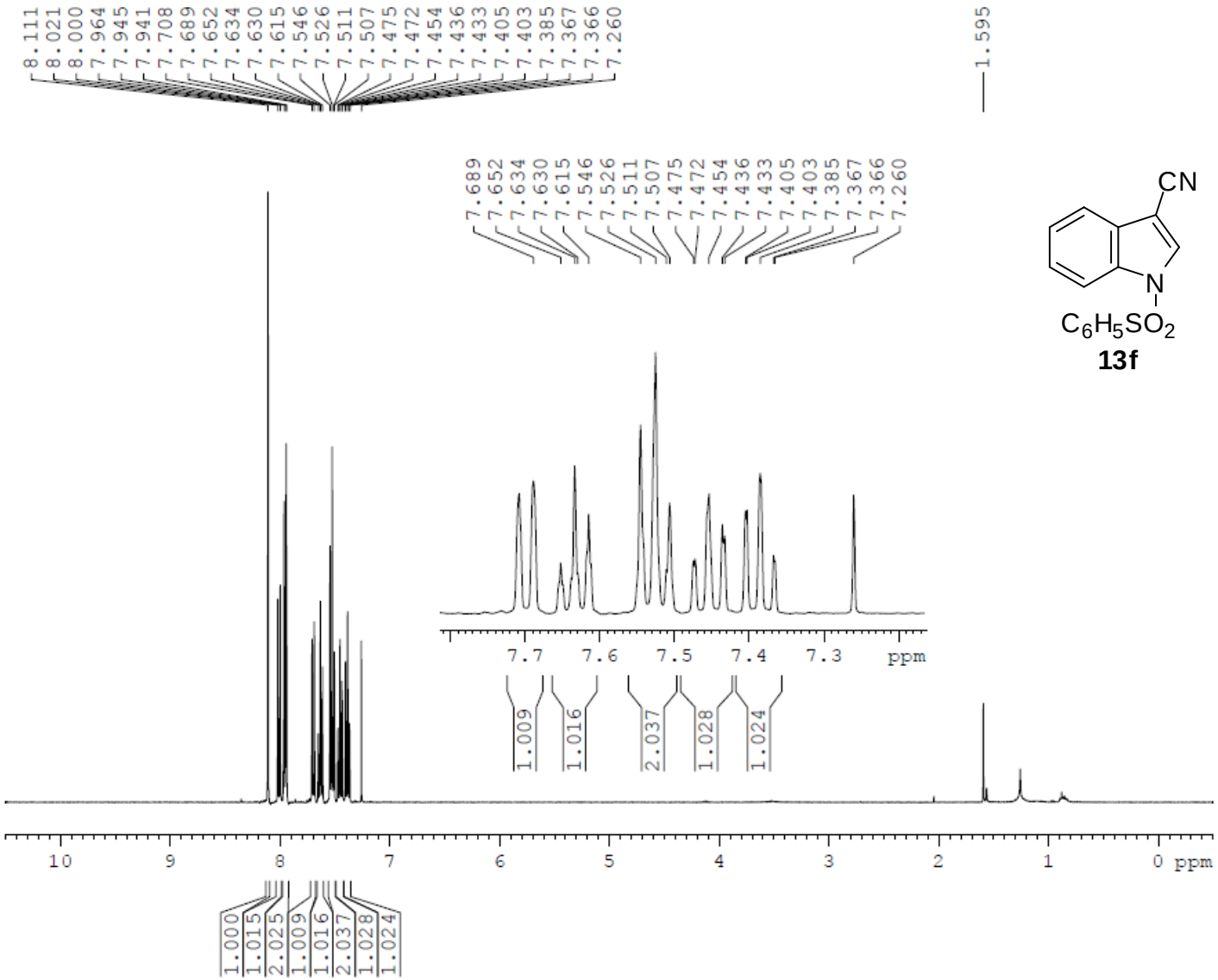
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for a15780. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	44(2)	31(2)	35(2)	4(1)	-2(1)	0(2)
C(2)	30(2)	34(2)	34(2)	-2(1)	-1(1)	5(1)
C(3)	34(2)	34(2)	44(2)	3(1)	2(1)	2(1)
C(4)	40(2)	50(2)	37(2)	6(2)	4(1)	7(2)
C(5)	41(2)	53(2)	39(2)	-9(2)	-1(1)	2(2)
C(6)	39(2)	41(2)	46(2)	-7(2)	-3(1)	-2(2)
C(7)	30(2)	33(2)	38(2)	0(1)	-2(1)	1(1)
C(8)	32(2)	29(2)	45(2)	2(1)	-1(1)	-3(1)
C(9)	34(2)	24(2)	39(2)	5(1)	0(1)	-2(1)
C(10)	38(2)	23(2)	38(2)	4(1)	-5(1)	2(1)
C(11)	51(2)	41(2)	44(2)	5(1)	-2(2)	-14(2)
C(12)	70(3)	47(2)	43(2)	8(2)	8(2)	-14(2)
C(13)	68(3)	40(2)	36(2)	3(1)	2(2)	2(2)
C(14)	49(2)	41(2)	39(2)	-1(1)	-7(2)	-1(2)
C(15)	40(2)	32(2)	41(2)	2(1)	0(1)	-3(2)
N(1)	74(2)	34(2)	47(2)	4(1)	-9(1)	-7(2)
N(2)	36(2)	27(1)	35(1)	1(1)	-4(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for a15780.

	x	y	z	U(eq)
H(3)	552	6798	5329	45
H(4)	880	8138	6252	51
H(5)	1619	11067	6326	53
H(6)	2011	12800	5495	50
H(8)	1993	12606	4207	42
H(11)	2590	11542	3189	55
H(12)	2537	11694	2169	64
H(13)	1273	10343	1658	58
H(14)	41	8831	2168	51
H(15)	81	8677	3189	45

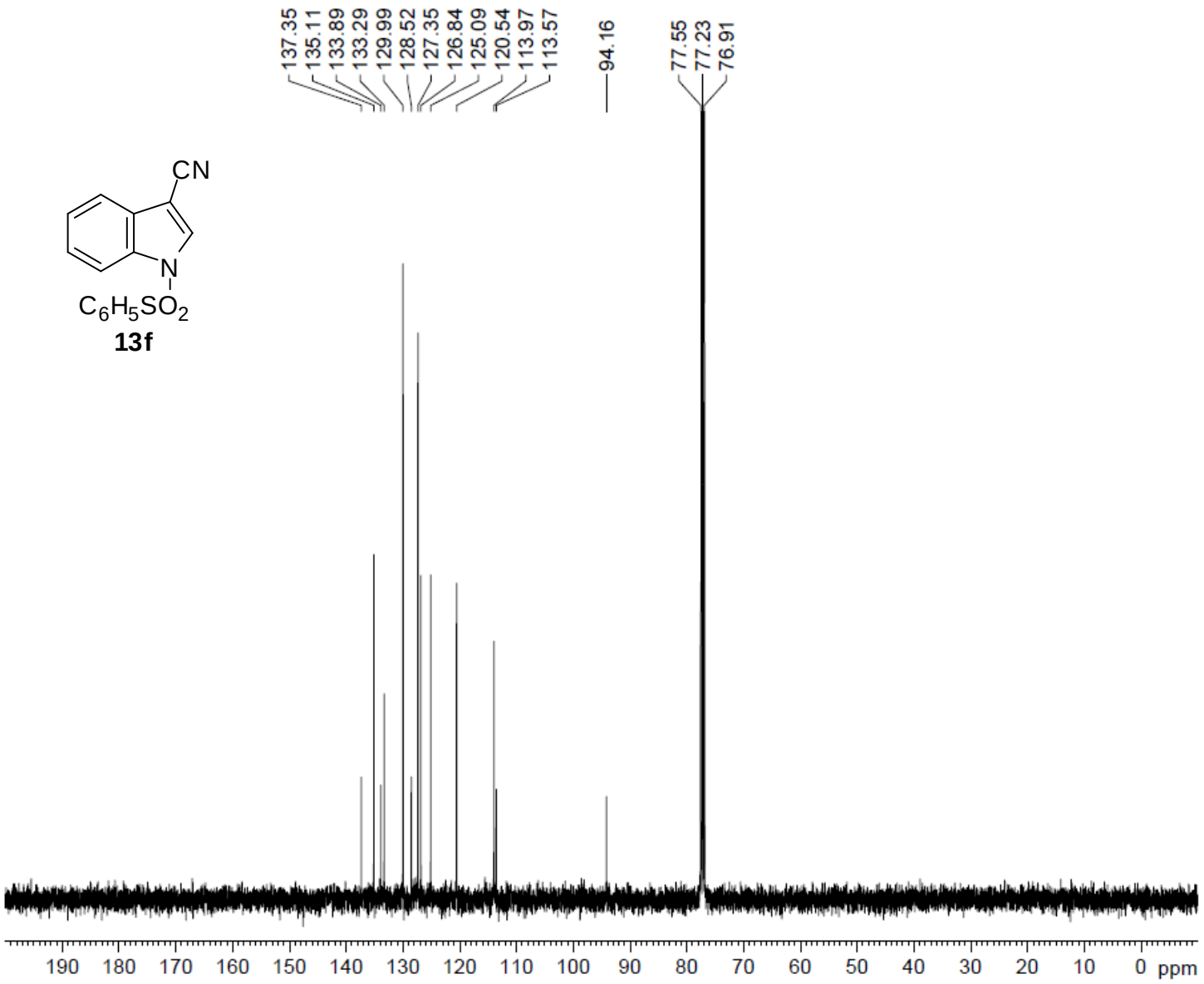


Current Data Parameters
NAME SO125
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150609
Time 9.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 456.1
DW 69.000 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 21.45 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



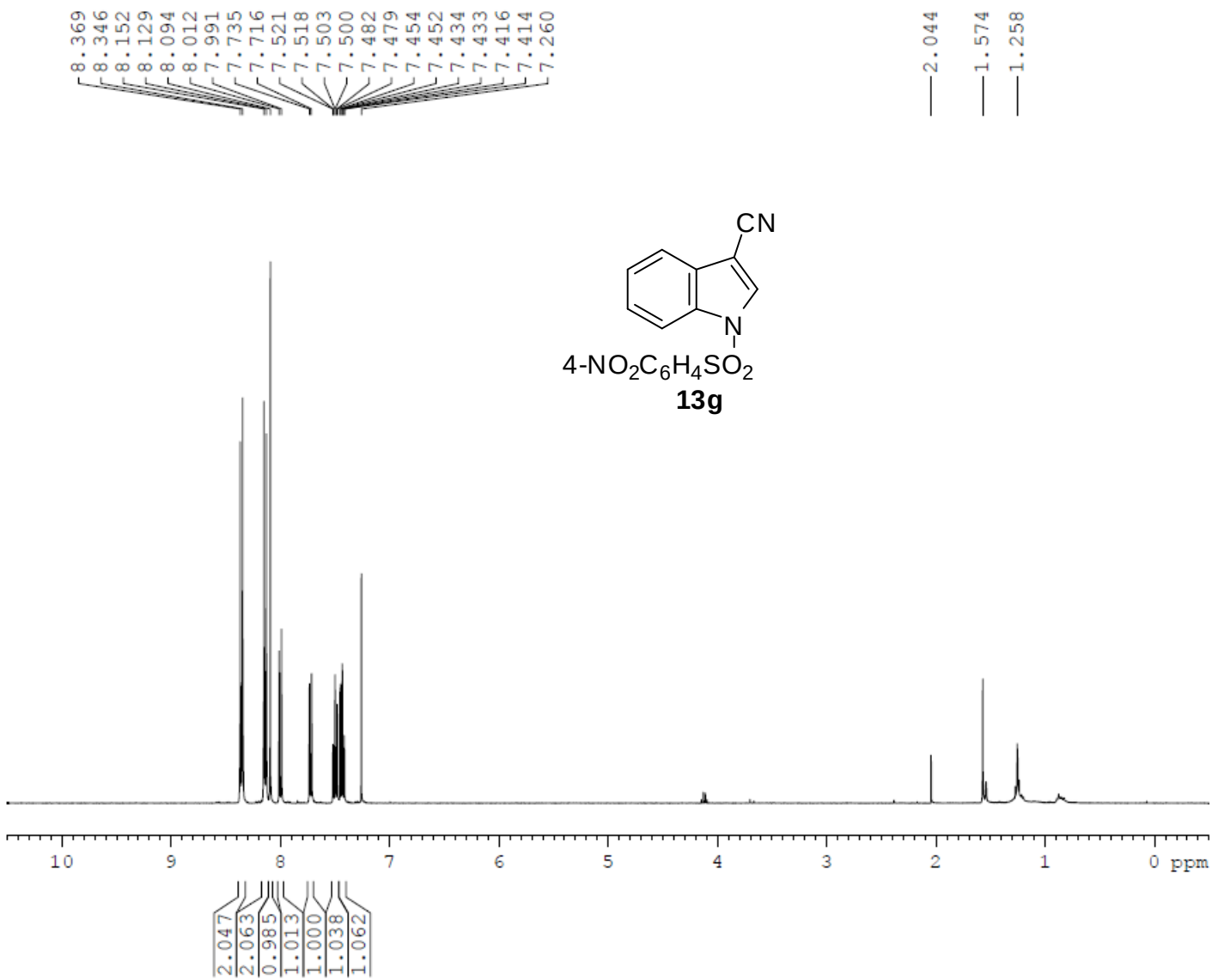
Current Data Parameters
NAME SO125
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150609
Time 9.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 131
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 9195.2
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127506 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

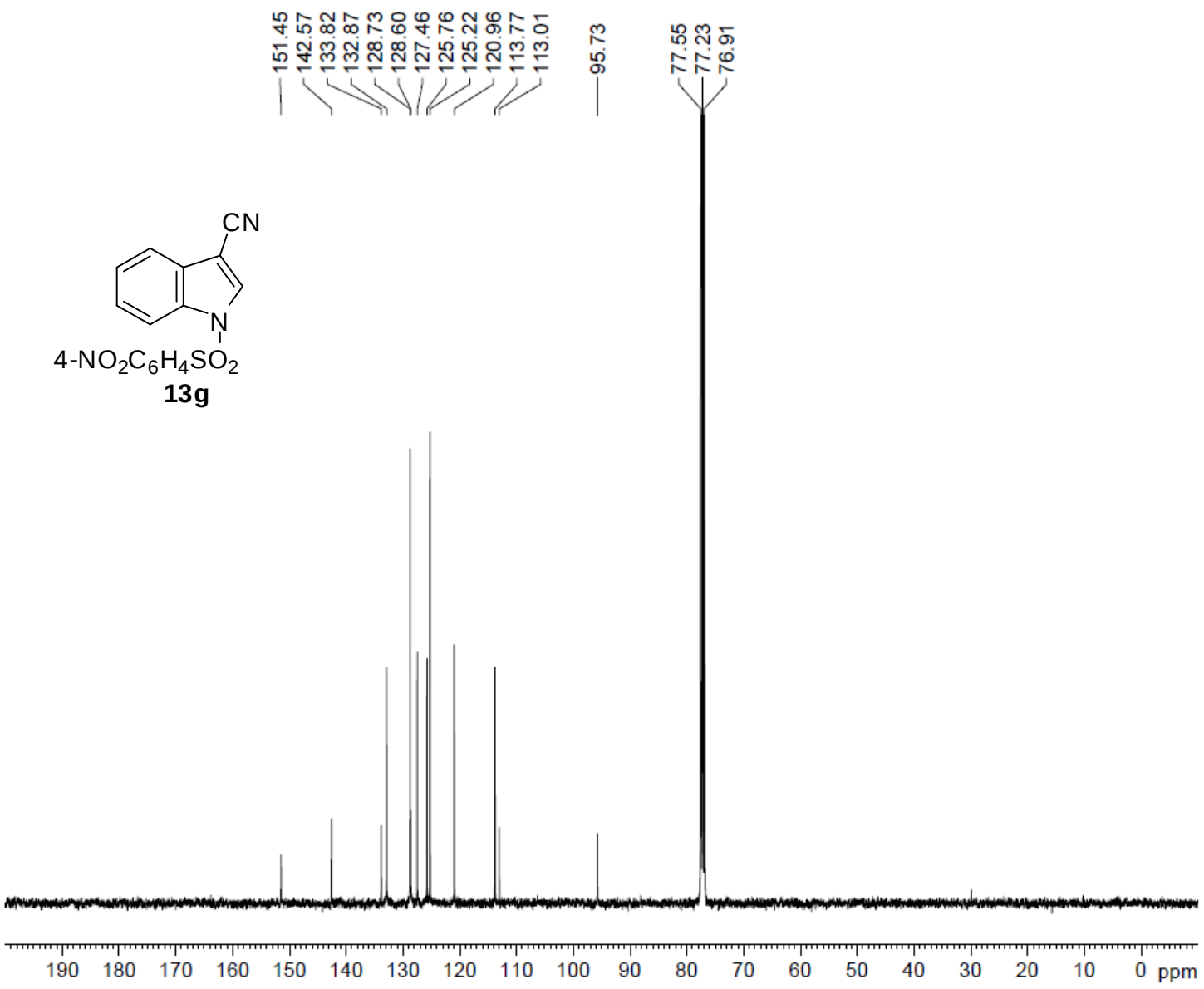


Current Data Parameters
NAME SO030
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141210
Time 8.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 198.09
DW 69.333 usec
DE 10.52 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



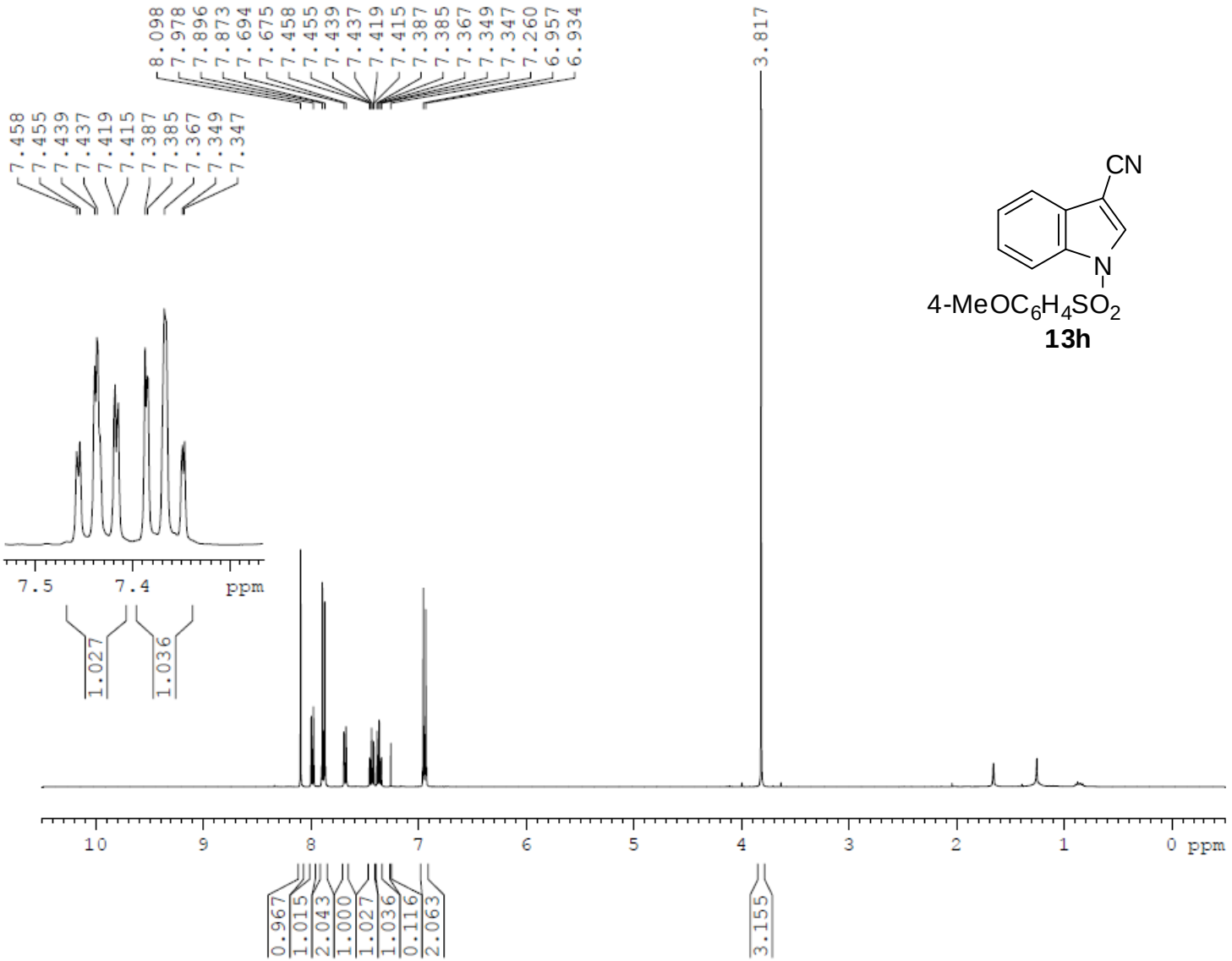
Current Data Parameters
NAME SO030
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141210
Time 9.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1229
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127479 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



4-MeOC$_6$H$_4$SO$_2$

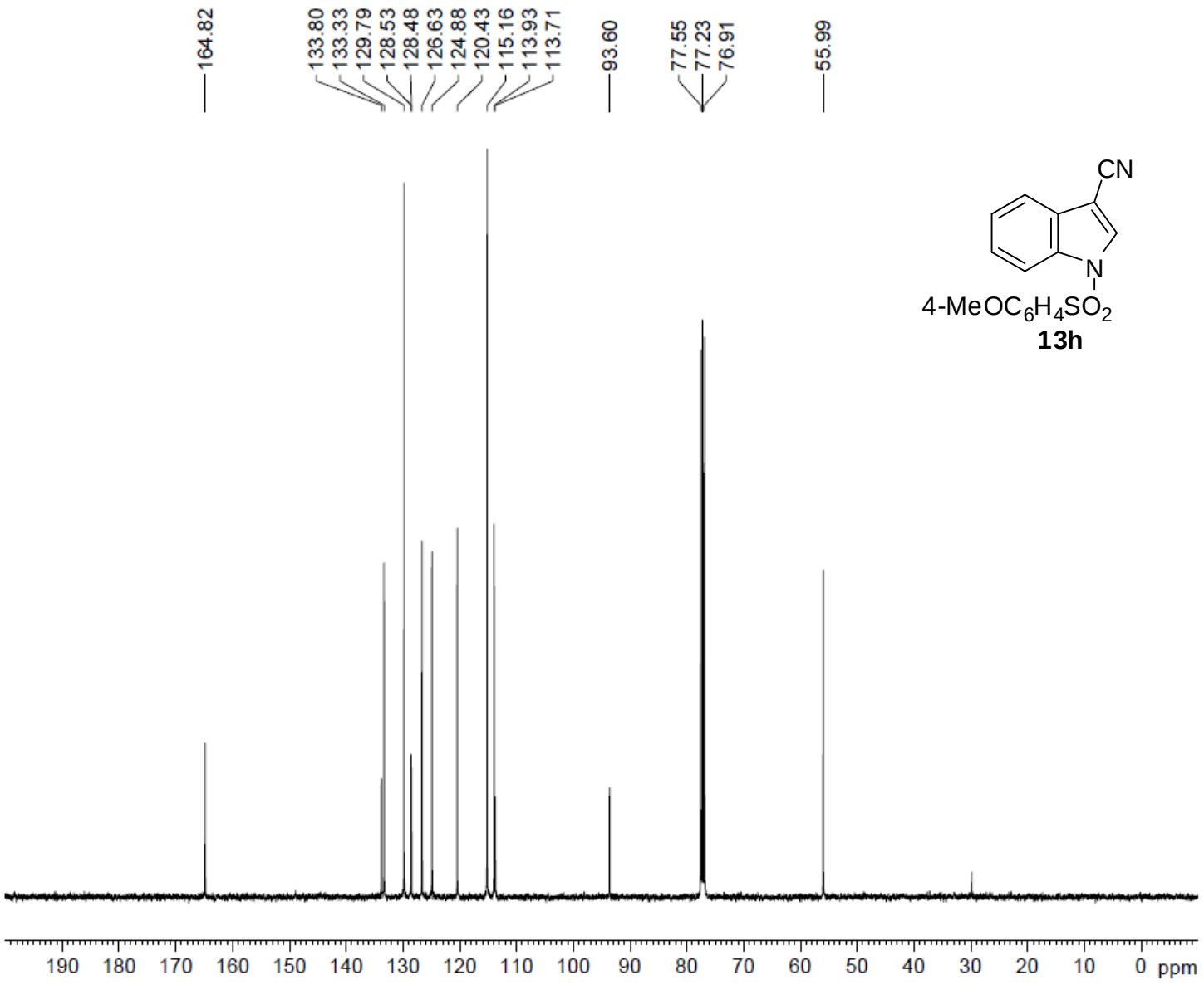
13h

Current Data Parameters
NAME SO128
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150612
Time 8.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 63.58
DW 69.333 usec
DE 10.52 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



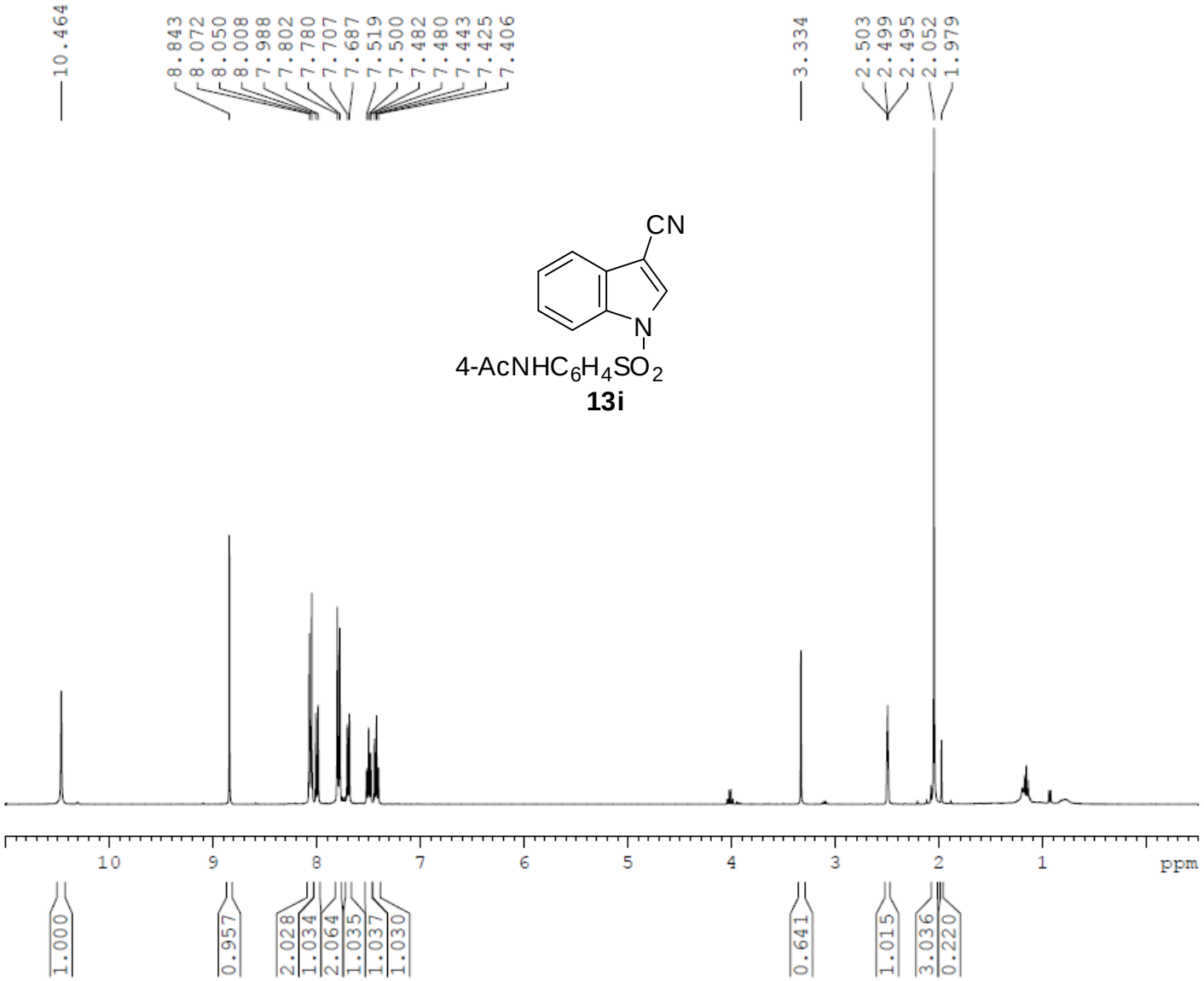
Current Data Parameters
NAME SO128
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150612
Time 8.40
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127522 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

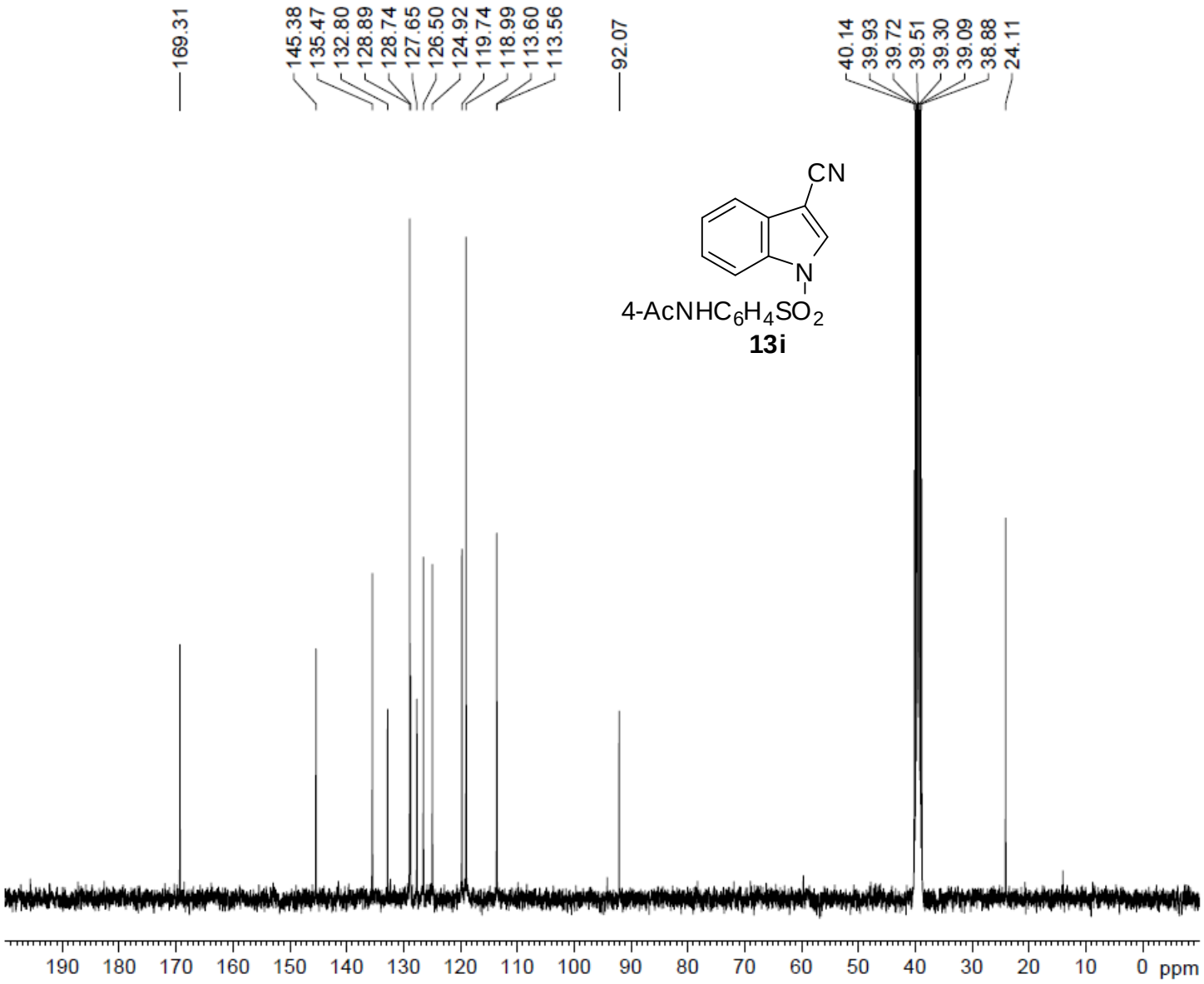


Current Data Parameters
NAME SO133
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150622
Time 14.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 89.08
DW 69.333 usec
DE 10.52 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300030 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



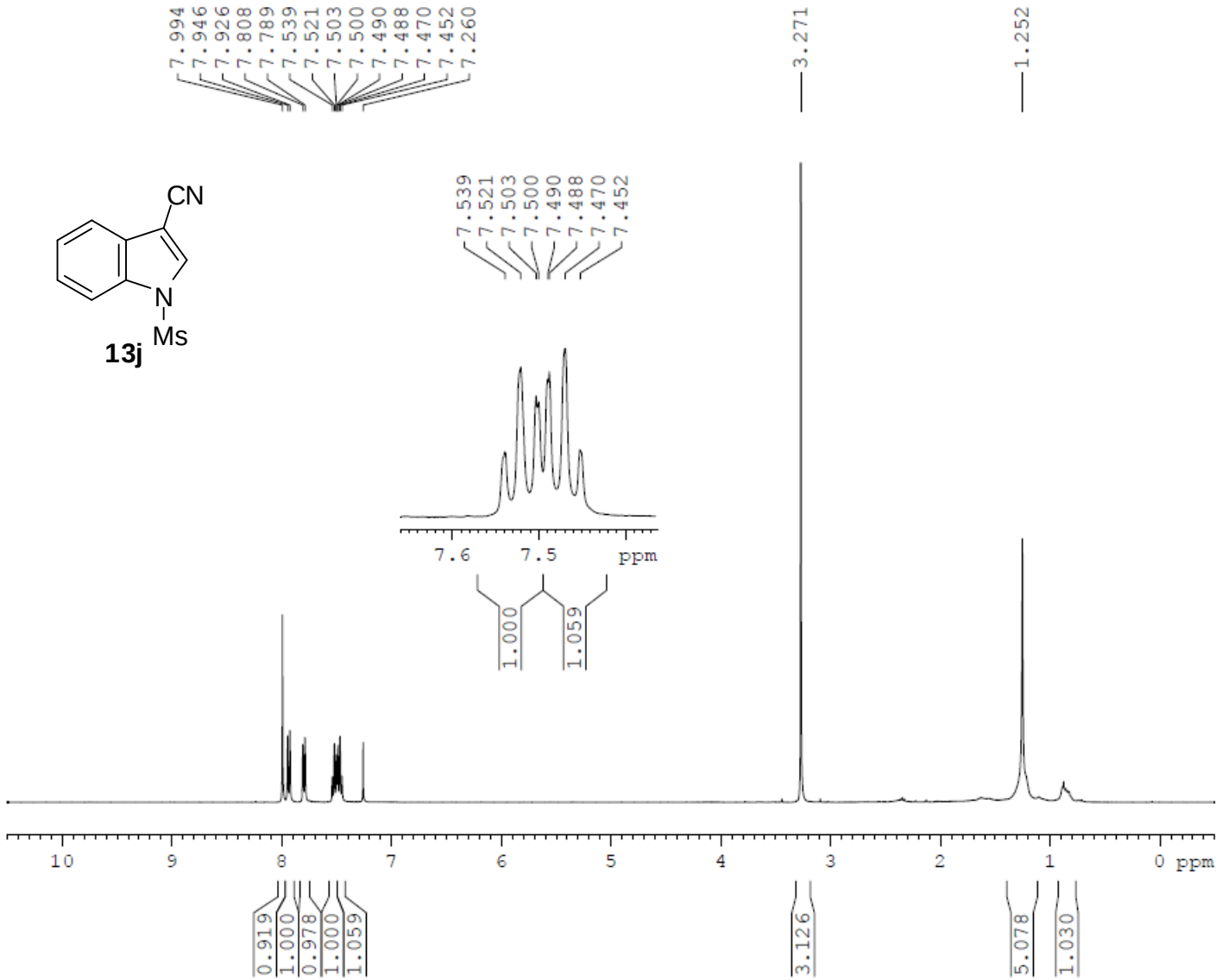
Current Data Parameters
NAME SO133
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150622
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 428
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6128204 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



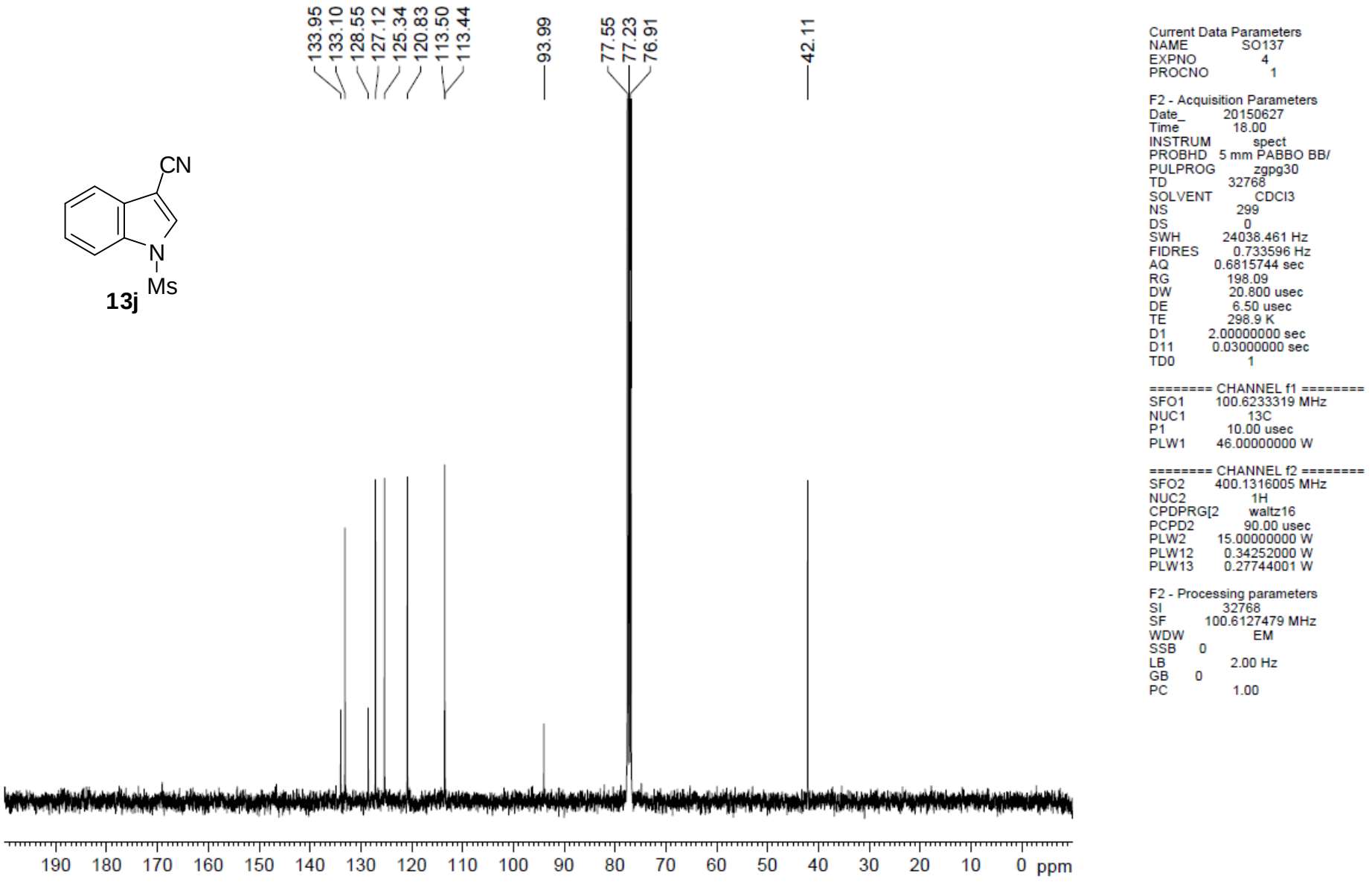
Current Data Parameters
NAME SO137
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150627
Time 8.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 89.08
DW 69.333 usec
DE 10.52 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

recrystallized



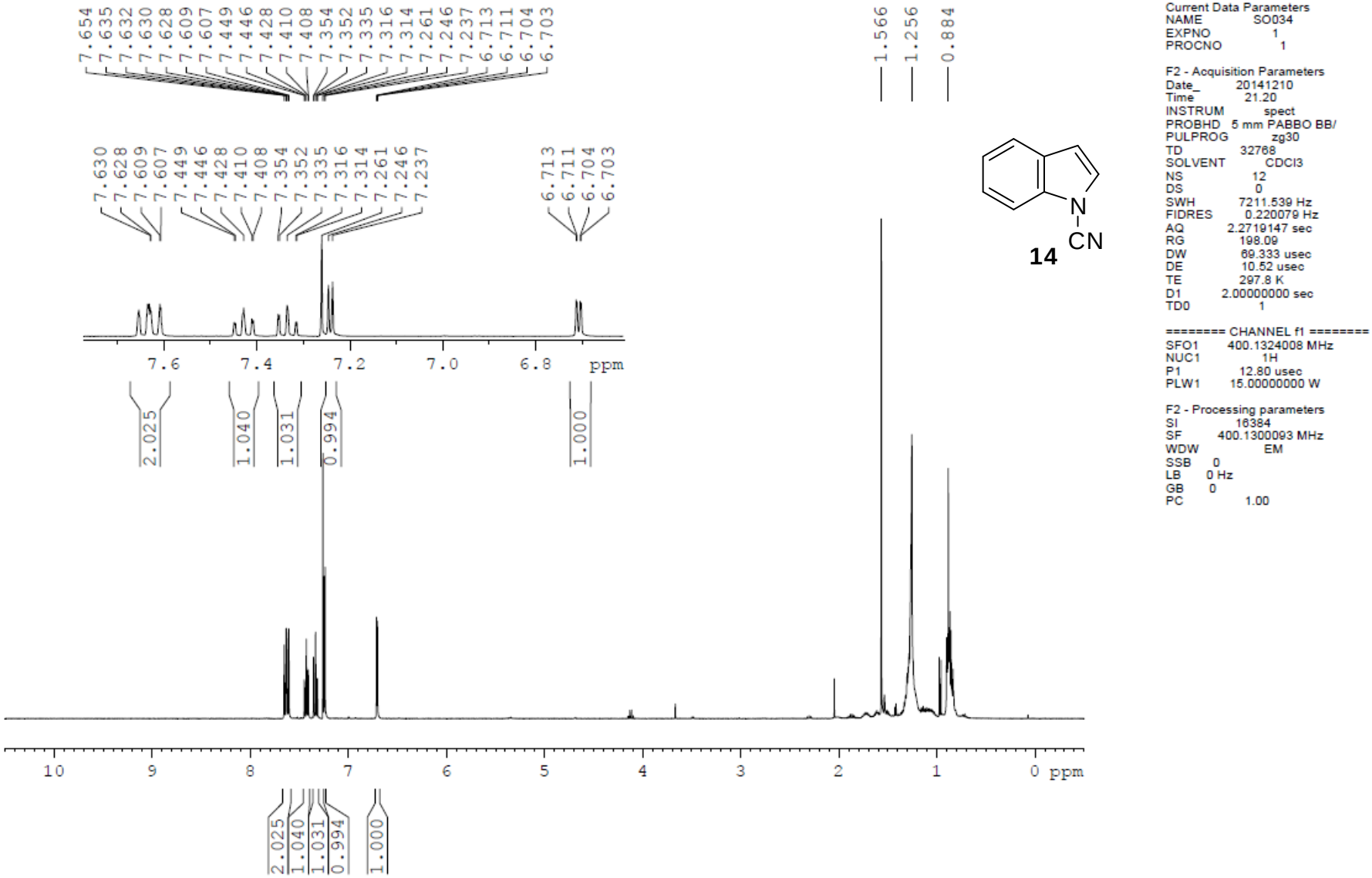
Current Data Parameters
NAME SO137
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150627
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 299
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127479 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

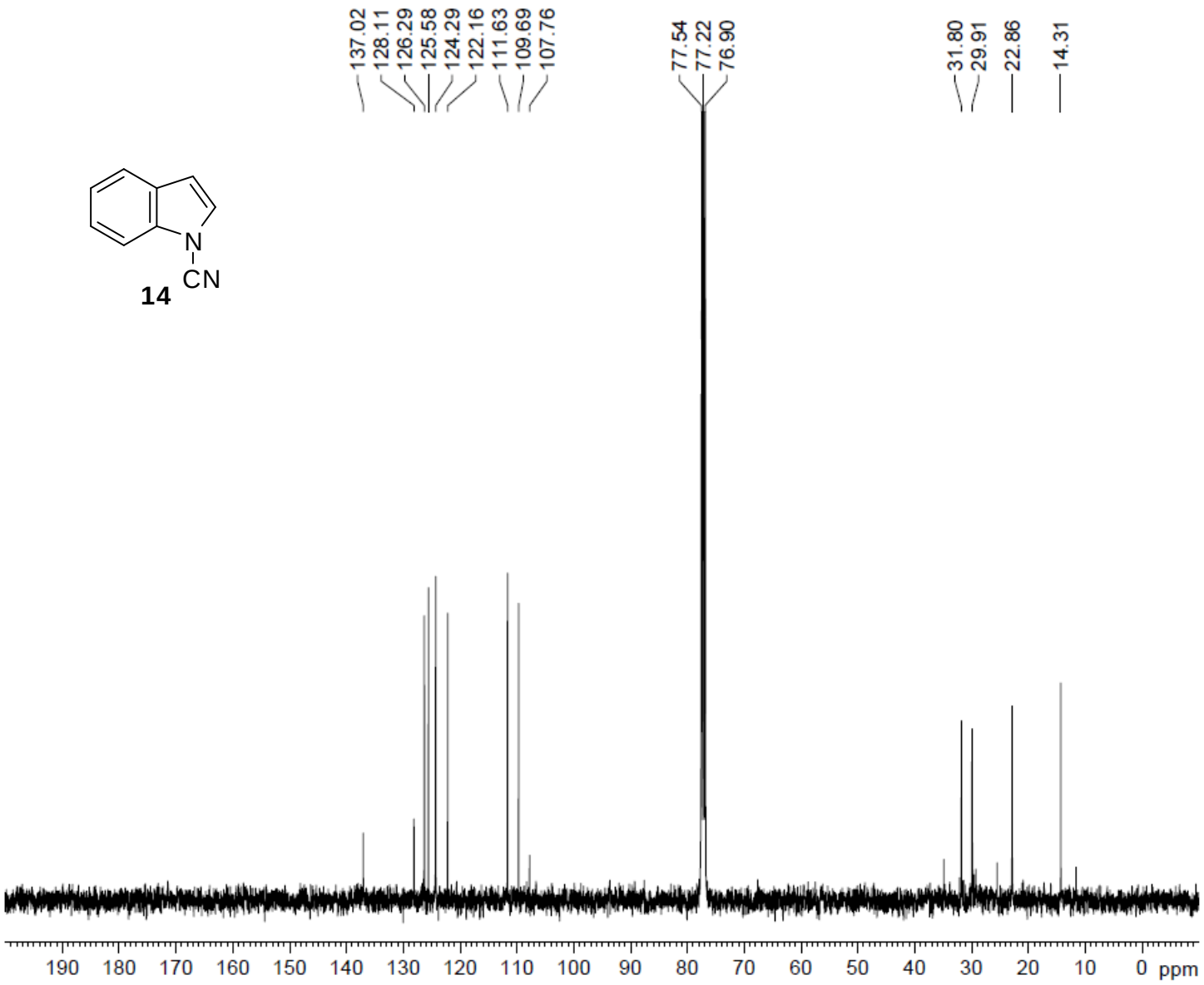


Current Data Parameters
NAME SO034
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141210
Time 21.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 198.09
DW 69.333 usec
DE 10.52 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



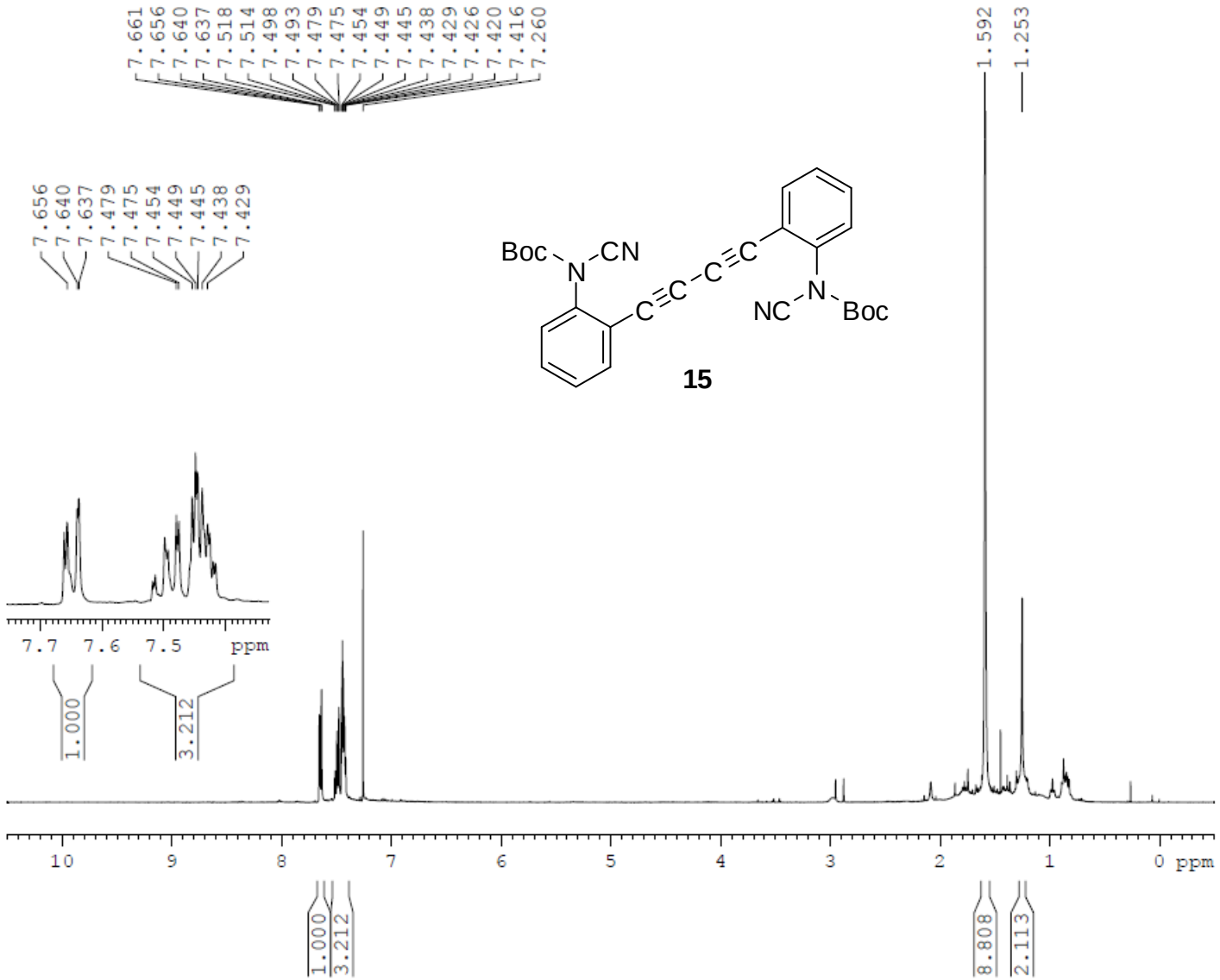
Current Data Parameters
NAME SO034
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141211
Time 9.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1004
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127464 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

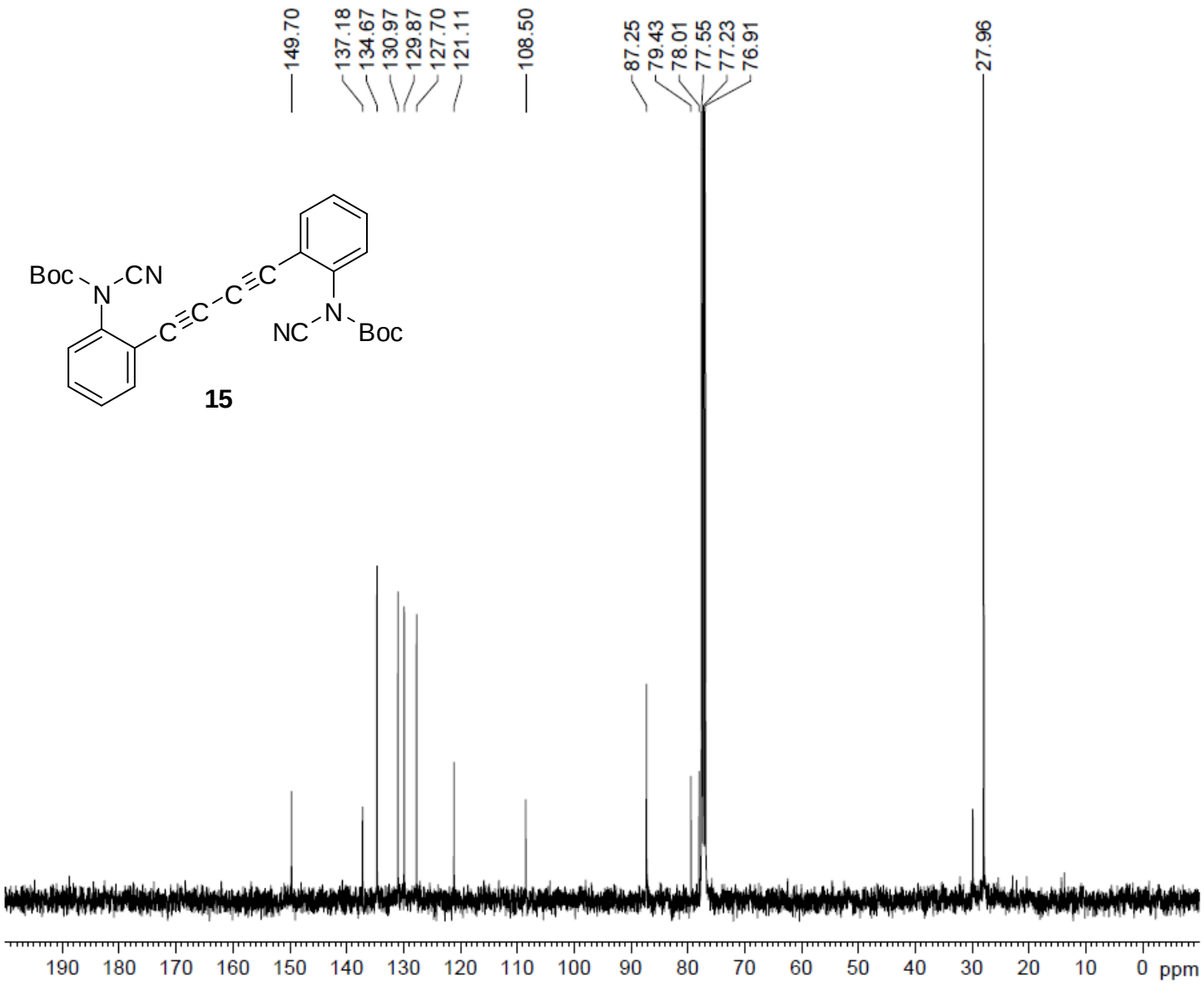


Current Data Parameters
NAME SO155
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150917
Time 14.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 89.08
DW 69.333 usec
DE 10.50 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.90 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



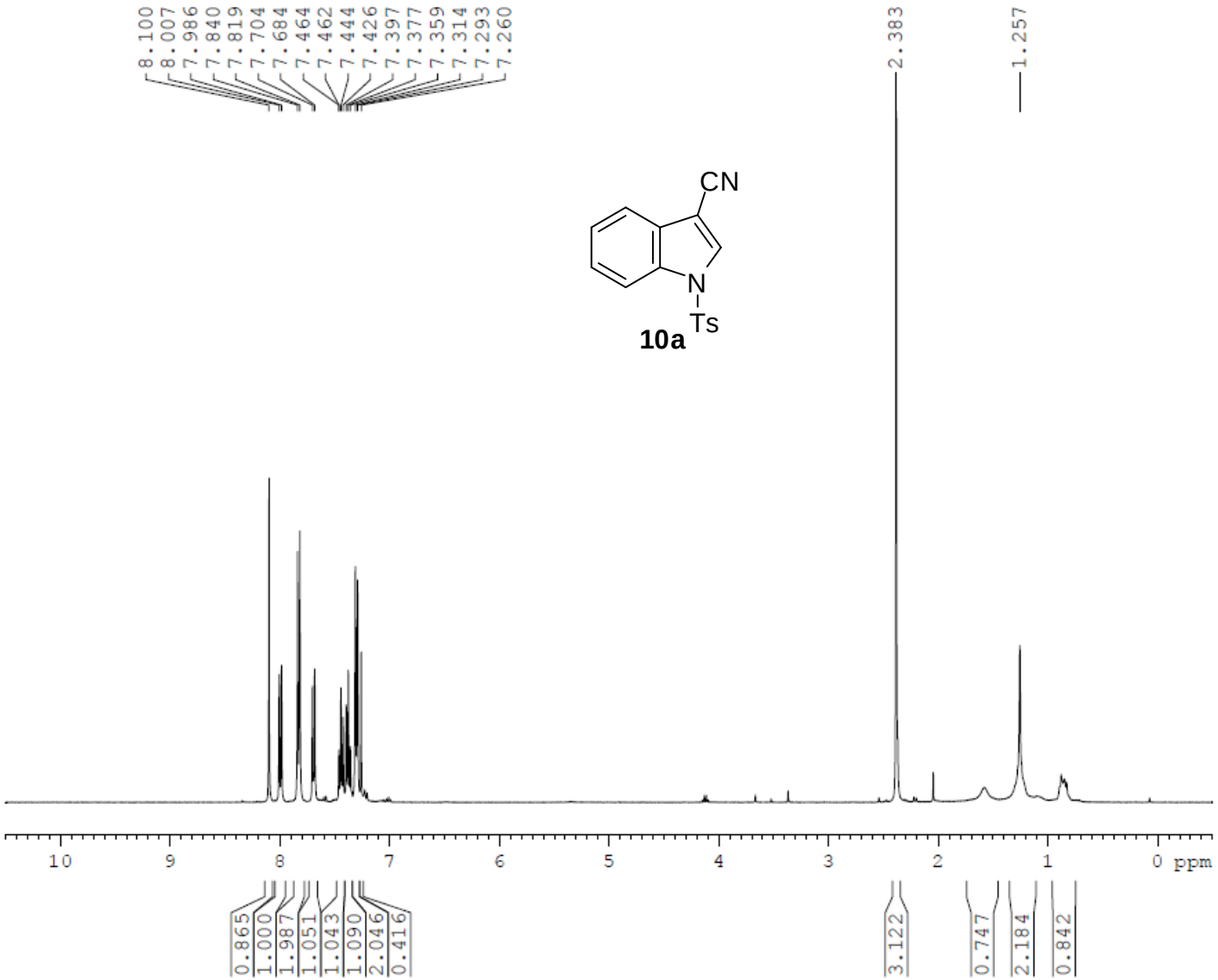
Current Data Parameters
NAME SO155
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150917
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 271
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 47.50000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W
PLW13 0.27338001 W

F2 - Processing parameters
SI 32768
SF 100.6127493 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

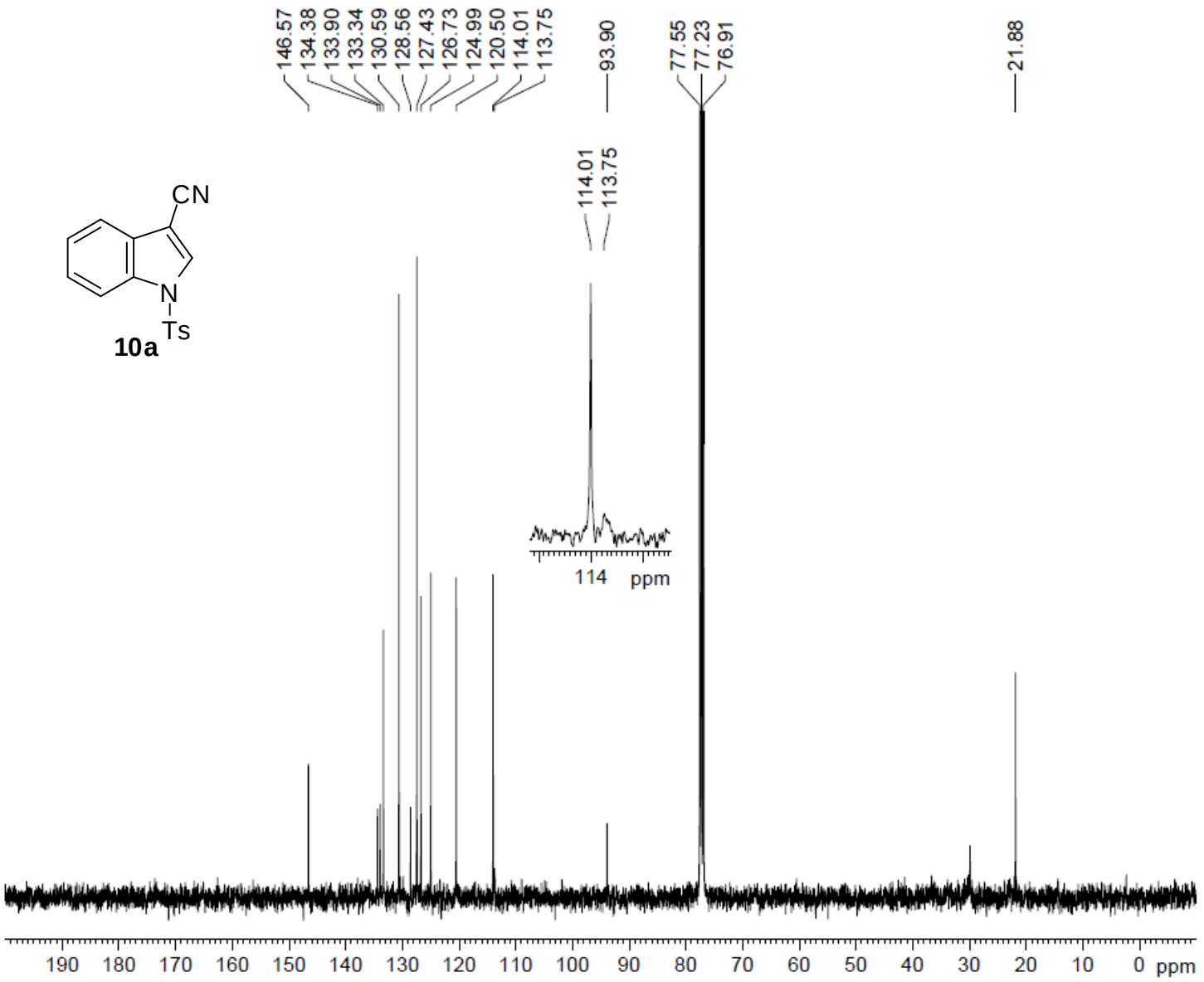


Current Data Parameters
NAME SO050indole
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150209
Time 9.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 99.72
DW 69.333 usec
DE 10.52 usec
TE 297.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SO050indole
EXPNO 3
PROCNO 1

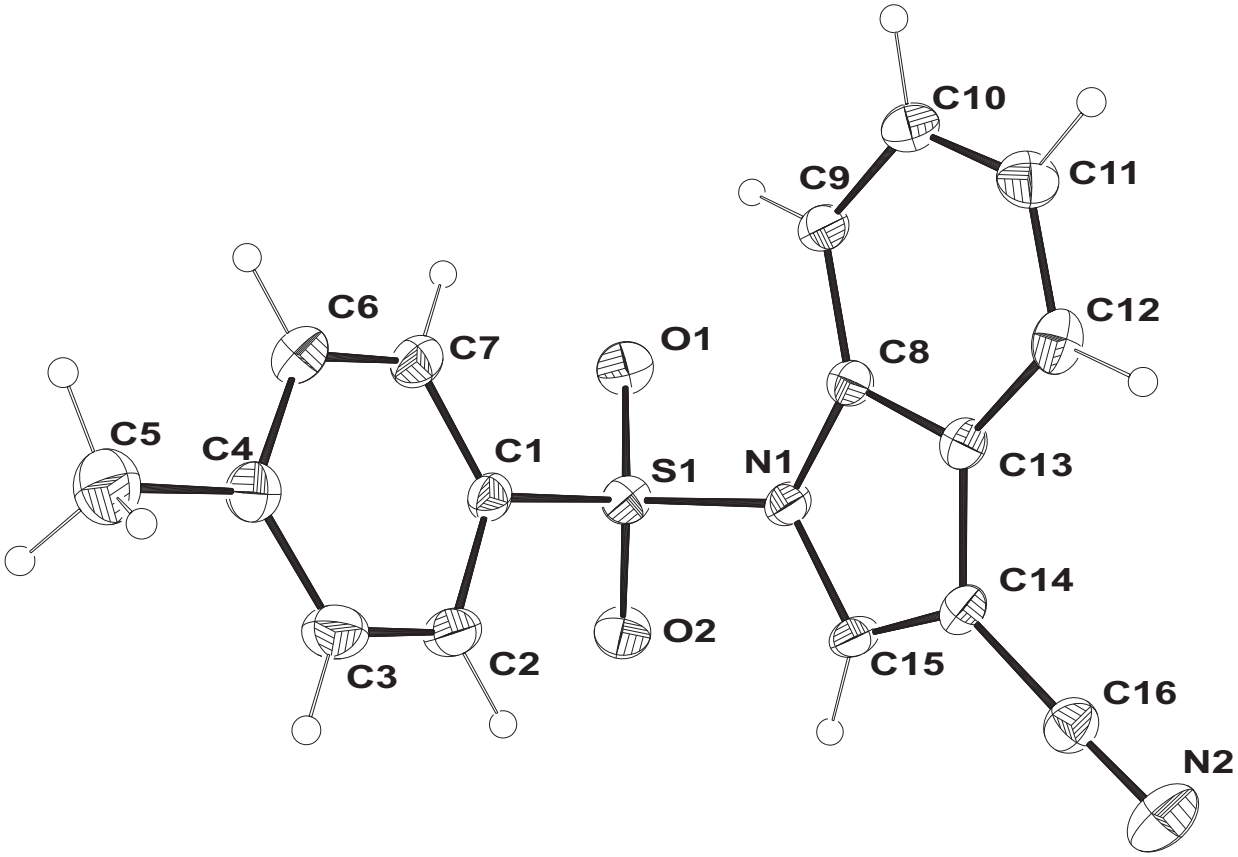
F2 - Acquisition Parameters
Date_ 20150209
Time 9.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 262
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

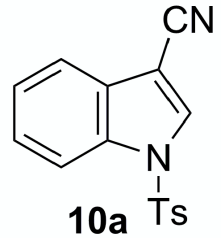
======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

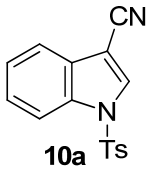
F2 - Processing parameters
SI 32768
SF 100.6127486 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

a15781


C10
C9
C11
C6
C12
C7
O1
C8
C5
C4
C1
S1
N1
C13
C14
O2
C3
C2
C15
C16
N2


CN
N
Ts

10a



10a

Table 1. Crystal data and structure refinement for a15781.

Identification code	a15781	
Empirical formula	C16 H12 N2 O2 S	
Formula weight	296.34	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 9.0829(15) Å	α= 90°.
	b = 10.2351(14) Å	β= 97.384(10)°.
	c = 15.664(2) Å	γ = 90°.
Volume	1444.1(4) $Å^3$	
Z	4	
Density (calculated)	1.363 Mg/m^3	
Absorption coefficient	0.229 mm^{-1}	
F(000)	616	
Crystal size	0.23 x 0.07 x 0.03 mm^3	
Theta range for data collection	2.26 to 25.02°.	
Index ranges	-10<=h<=10, -12<=k<=12, -18<=l<=18	
Reflections collected	9899	
Independent reflections	2547 [R(int) = 0.0797]	
Completeness to theta = 25.02°	99.6 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9932 and 0.9492	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2547 / 0 / 190	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0529, wR2 = 0.1059	
R indices (all data)	R1 = 0.1015, wR2 = 0.1274	
Largest diff. peak and hole	0.314 and -0.317 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for a15781. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3412(3)	1652(3)	1185(2)	31(1)
C(2)	4047(4)	408(3)	1177(2)	41(1)
C(3)	3516(4)	-459(3)	534(2)	49(1)
C(4)	2373(4)	-122(3)	-108(2)	40(1)
C(5)	1822(4)	-1052(4)	-832(3)	60(1)
C(6)	1744(4)	1120(3)	-82(2)	42(1)
C(7)	2260(4)	2008(3)	557(2)	39(1)
C(8)	1717(3)	2233(3)	2932(2)	29(1)
C(9)	604(4)	3057(3)	2540(2)	35(1)
C(10)	-799(4)	2891(4)	2770(2)	43(1)
C(11)	-1103(4)	1951(3)	3373(2)	44(1)
C(12)	6(4)	1152(3)	3768(2)	38(1)
C(13)	1437(3)	1292(3)	3541(2)	29(1)
C(14)	2853(4)	676(3)	3832(2)	31(1)
C(15)	3899(4)	1223(3)	3401(2)	34(1)
C(16)	3119(4)	-298(3)	4498(2)	38(1)
N(1)	3255(3)	2196(2)	2859(2)	31(1)
N(2)	3305(3)	-1058(3)	5036(2)	57(1)
O(1)	3419(2)	4015(2)	1814(2)	42(1)
O(2)	5603(2)	2584(2)	2260(2)	45(1)
S(1)	4043(1)	2747(1)	2009(1)	34(1)

Table 3. Bond lengths [Å] and angles [°] for a15781.

C(1)-C(7)	1.390(4)
C(1)-C(2)	1.398(4)
C(1)-S(1)	1.751(3)
C(2)-C(3)	1.381(4)
C(2)-H(2)	0.9500
C(3)-C(4)	1.393(5)
C(3)-H(3)	0.9500
C(4)-C(6)	1.396(4)
C(4)-C(5)	1.516(4)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-C(7)	1.388(4)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(8)-C(9)	1.397(4)
C(8)-C(13)	1.402(4)
C(8)-N(1)	1.417(4)
C(9)-C(10)	1.378(5)
C(9)-H(9)	0.9500
C(10)-C(11)	1.400(5)
C(10)-H(10)	0.9500
C(11)-C(12)	1.381(4)
C(11)-H(11)	0.9500
C(12)-C(13)	1.398(4)
C(12)-H(12)	0.9500
C(13)-C(14)	1.452(4)
C(14)-C(15)	1.355(4)
C(14)-C(16)	1.441(4)
C(15)-N(1)	1.389(4)
C(15)-H(15)	0.9500
C(16)-N(2)	1.143(4)
N(1)-S(1)	1.687(3)
O(1)-S(1)	1.434(2)

O(2)-S(1)	1.431(2)

C(7)-C(1)-C(2)	120.5(3)
C(7)-C(1)-S(1)	120.0(3)
C(2)-C(1)-S(1)	119.5(3)
C(3)-C(2)-C(1)	119.0(3)
C(3)-C(2)-H(2)	120.5
C(1)-C(2)-H(2)	120.5
C(2)-C(3)-C(4)	121.7(3)
C(2)-C(3)-H(3)	119.2
C(4)-C(3)-H(3)	119.2
C(3)-C(4)-C(6)	118.4(3)
C(3)-C(4)-C(5)	121.9(3)
C(6)-C(4)-C(5)	119.8(3)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-C(4)	121.0(3)
C(7)-C(6)-H(6)	119.5
C(4)-C(6)-H(6)	119.5
C(6)-C(7)-C(1)	119.5(3)
C(6)-C(7)-H(7)	120.2
C(1)-C(7)-H(7)	120.2
C(9)-C(8)-C(13)	122.0(3)
C(9)-C(8)-N(1)	130.3(3)
C(13)-C(8)-N(1)	107.6(3)
C(10)-C(9)-C(8)	116.9(3)
C(10)-C(9)-H(9)	121.6
C(8)-C(9)-H(9)	121.6
C(9)-C(10)-C(11)	122.0(3)
C(9)-C(10)-H(10)	119.0
C(11)-C(10)-H(10)	119.0
C(12)-C(11)-C(10)	120.9(3)

C(12)-C(11)-H(11)	119.5
C(10)-C(11)-H(11)	119.5
C(11)-C(12)-C(13)	118.3(3)
C(11)-C(12)-H(12)	120.9
C(13)-C(12)-H(12)	120.9
C(12)-C(13)-C(8)	120.0(3)
C(12)-C(13)-C(14)	133.7(3)
C(8)-C(13)-C(14)	106.3(3)
C(15)-C(14)-C(16)	125.7(3)
C(15)-C(14)-C(13)	108.3(3)
C(16)-C(14)-C(13)	126.0(3)
C(14)-C(15)-N(1)	109.5(3)
C(14)-C(15)-H(15)	125.3
N(1)-C(15)-H(15)	125.3
N(2)-C(16)-C(14)	178.4(4)
C(15)-N(1)-C(8)	108.2(3)
C(15)-N(1)-S(1)	122.3(2)
C(8)-N(1)-S(1)	125.3(2)
O(2)-S(1)-O(1)	120.96(13)
O(2)-S(1)-N(1)	104.49(13)
O(1)-S(1)-N(1)	105.95(14)
O(2)-S(1)-C(1)	110.28(15)
O(1)-S(1)-C(1)	109.86(15)
N(1)-S(1)-C(1)	103.67(14)

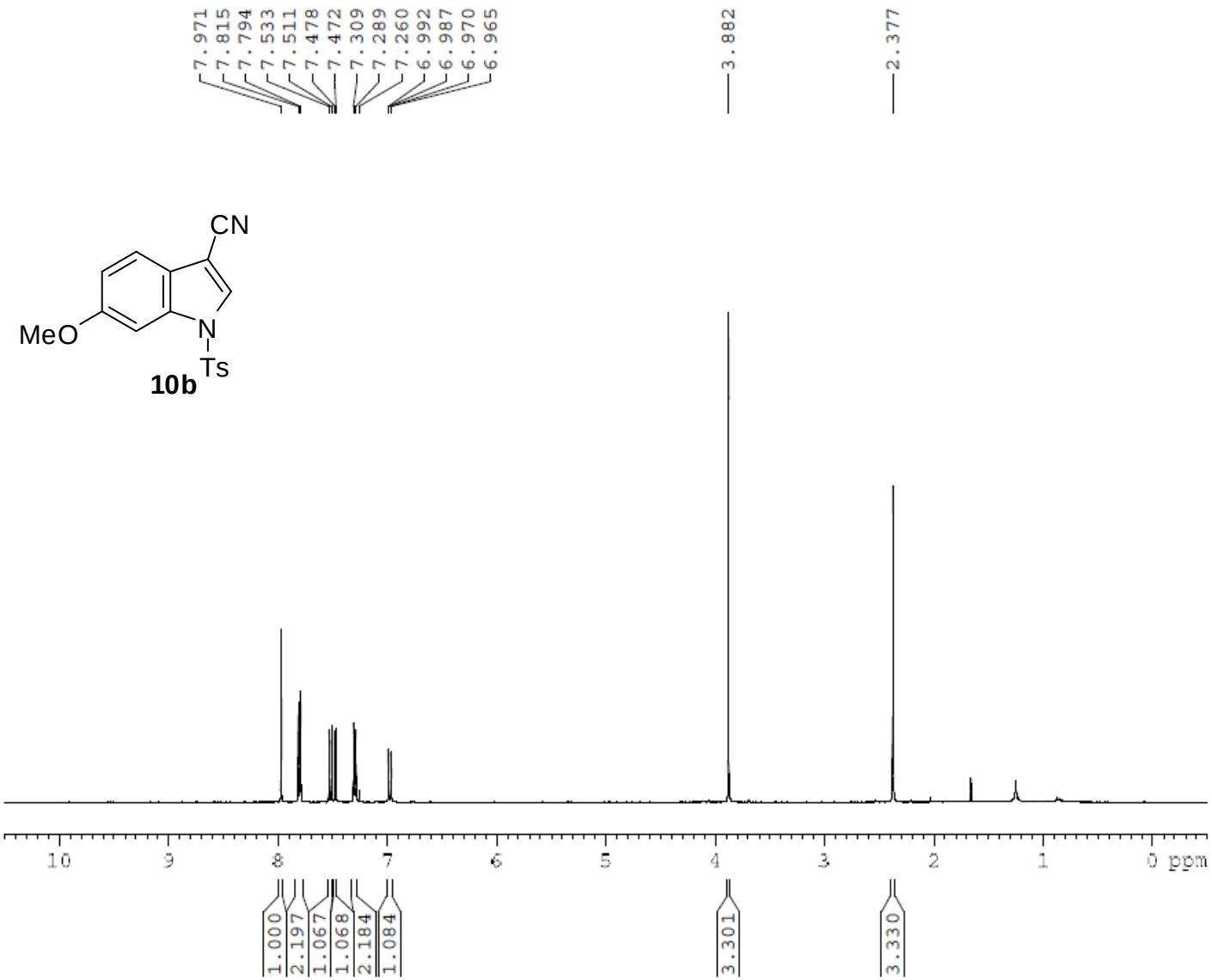
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for a15781. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(2)	35(2)	27(2)	5(2)	5(2)	-1(2)
C(2)	40(2)	39(2)	41(2)	1(2)	-4(2)	6(2)
C(3)	49(3)	40(2)	55(3)	-2(2)	0(2)	9(2)
C(4)	43(2)	40(2)	38(2)	-2(2)	6(2)	-3(2)
C(5)	70(3)	56(3)	53(3)	-13(2)	2(2)	0(2)
C(6)	46(2)	42(2)	36(2)	6(2)	-1(2)	-2(2)
C(7)	42(2)	39(2)	34(2)	7(2)	3(2)	1(2)
C(8)	28(2)	32(2)	27(2)	-6(2)	-2(2)	0(2)
C(9)	32(2)	38(2)	33(2)	5(2)	1(2)	3(2)
C(10)	31(2)	57(2)	39(2)	1(2)	-4(2)	5(2)
C(11)	25(2)	59(2)	47(3)	-3(2)	1(2)	-7(2)
C(12)	41(2)	40(2)	32(2)	1(2)	5(2)	-14(2)
C(13)	32(2)	29(2)	26(2)	-3(2)	0(2)	-5(1)
C(14)	38(2)	28(2)	25(2)	2(2)	-1(2)	-1(2)
C(15)	37(2)	35(2)	29(2)	2(2)	-5(2)	10(2)
C(16)	41(2)	37(2)	35(2)	0(2)	1(2)	-1(2)
N(1)	27(2)	37(2)	29(2)	6(1)	2(1)	1(1)
N(2)	72(2)	45(2)	50(2)	15(2)	-6(2)	-5(2)
O(1)	45(2)	31(1)	49(2)	5(1)	6(1)	-6(1)
O(2)	23(1)	63(2)	49(2)	0(1)	1(1)	-5(1)
S(1)	30(1)	36(1)	36(1)	4(1)	3(1)	-5(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for a15781.

	x	y	z	U(eq)
H(2)	4831	162	1608	49
H(3)	3942	-1306	530	59
H(5A)	1019	-636	-1215	90
H(5B)	1451	-1852	-590	90
H(5C)	2640	-1269	-1158	90
H(6)	950	1361	-509	50
H(7)	1829	2853	564	46
H(9)	804	3702	2135	42
H(10)	-1583	3431	2512	52
H(11)	-2086	1862	3511	53
H(12)	-198	523	4183	45
H(15)	4916	978	3461	41



Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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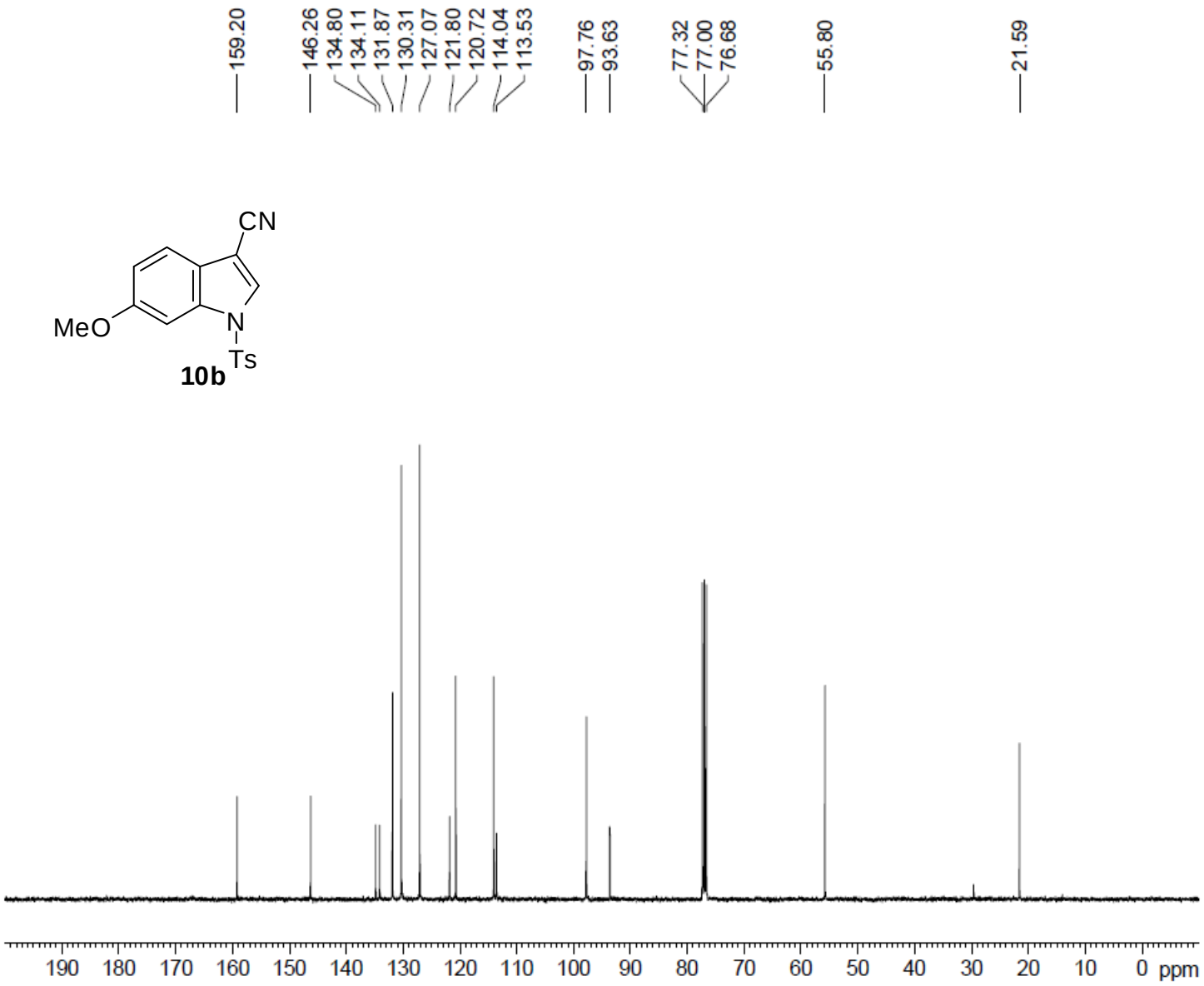
Time 9.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 57.42
DW 69.333 usec
DE 10.52 usec
TE 298.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.60 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



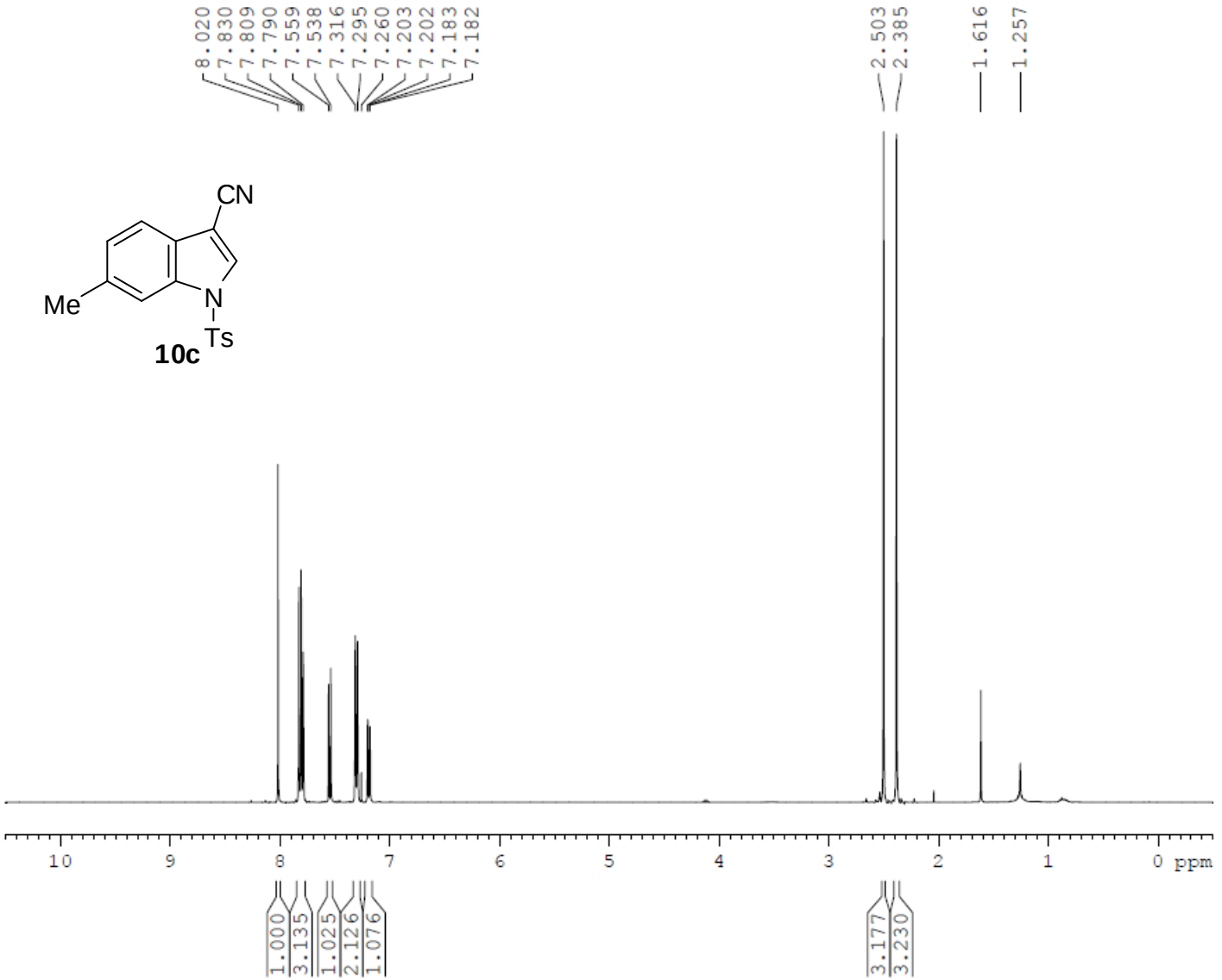
Current Data Parameters
NAME SD-103(new)
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140707
Time 13.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 456
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127756 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

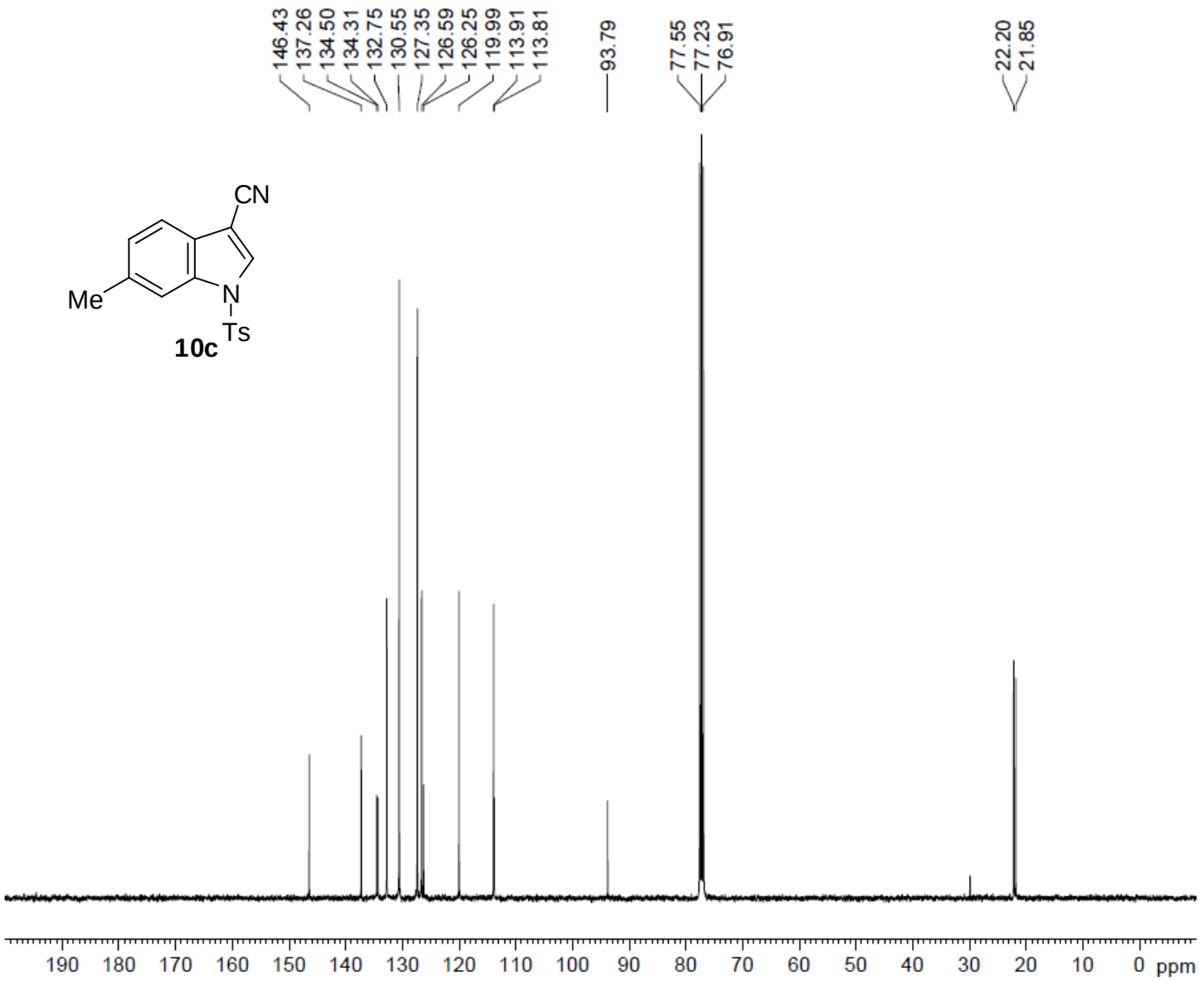


Current Data Parameters
NAME SC163-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140718
Time 9.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 298.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SC163-1
EXPNO 2
PROCNO 1

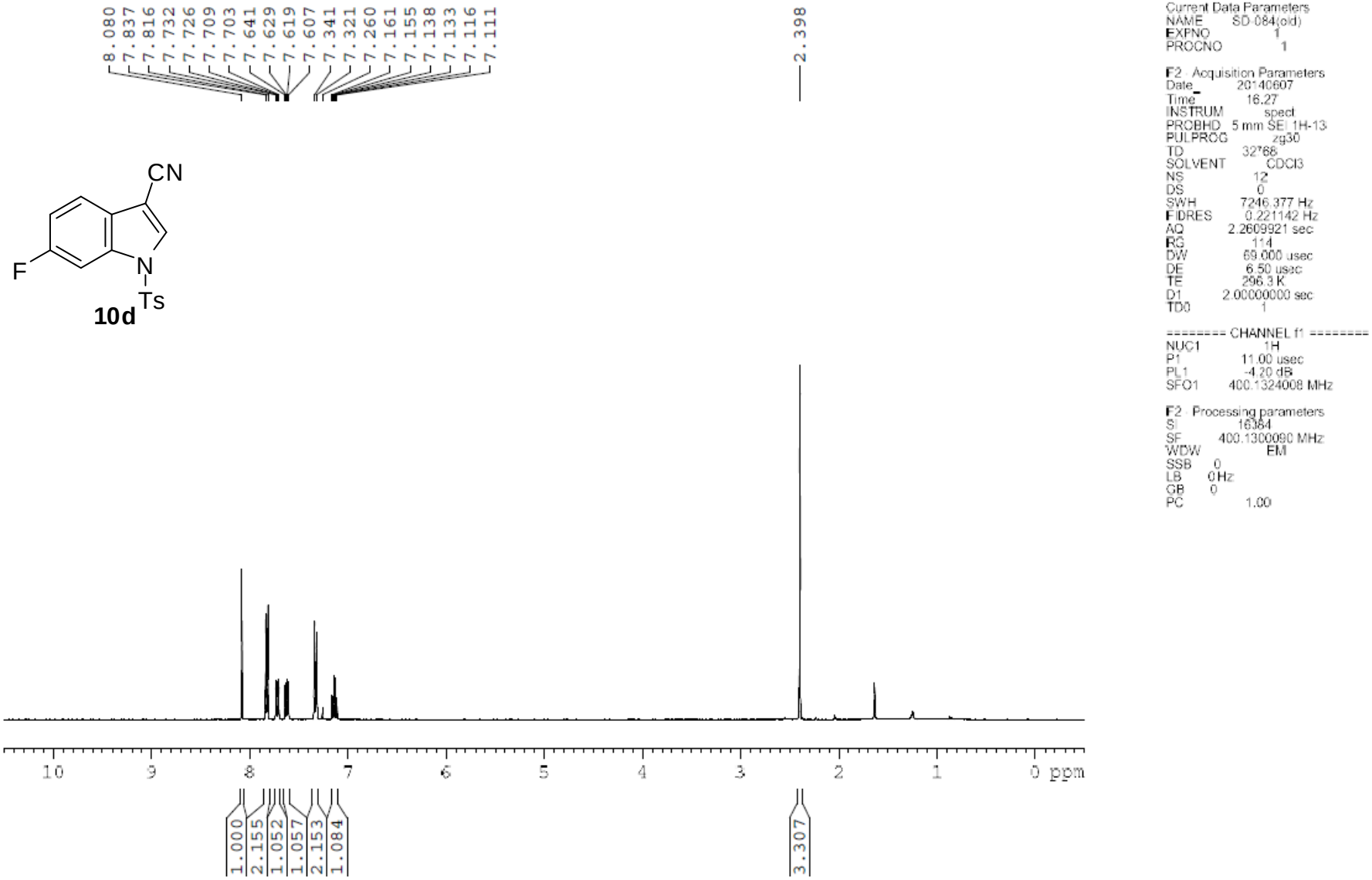
F2 - Acquisition Parameters
Date_ 20140718
Time 18.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127500 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

pure



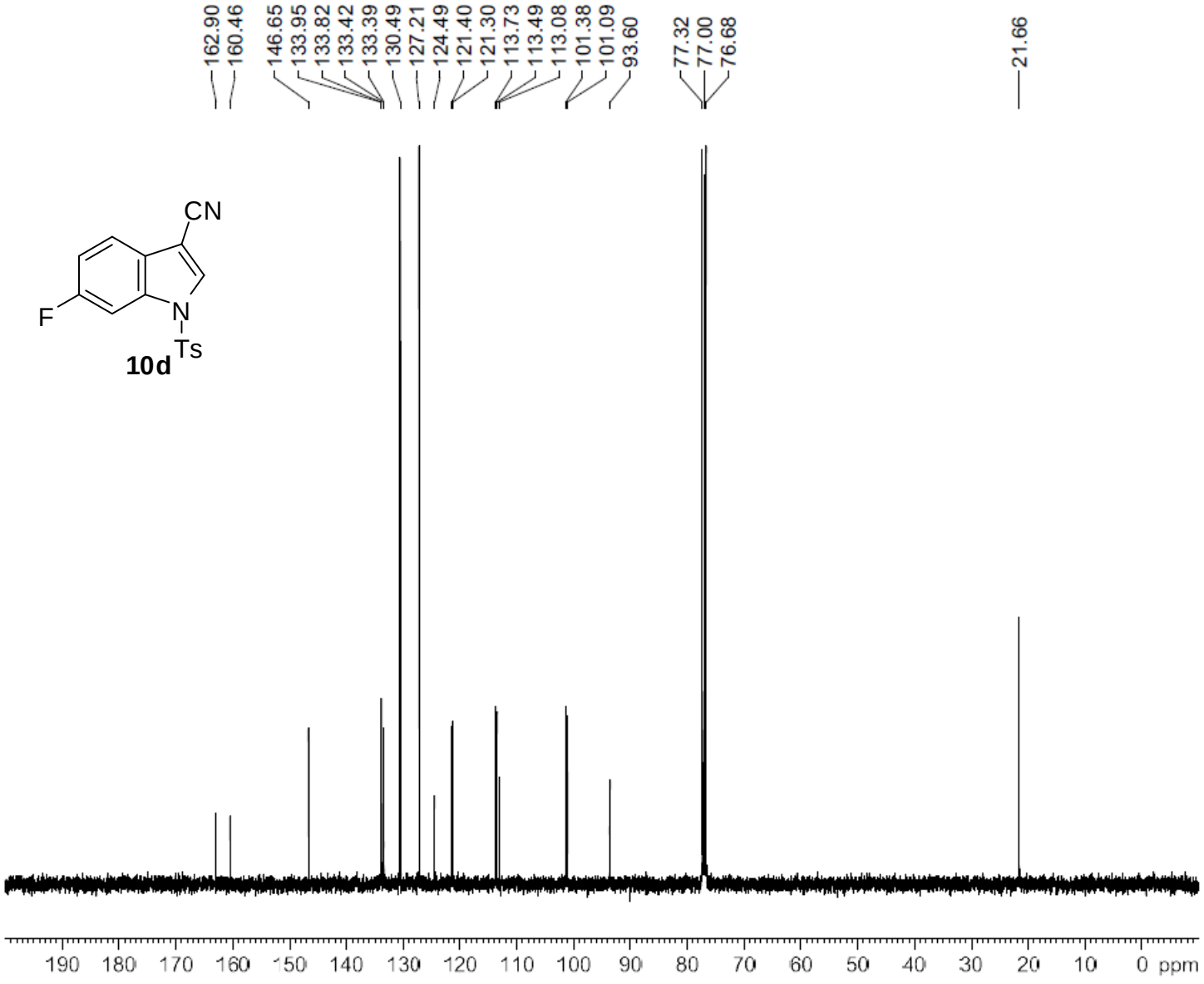
Current Data Parameters
NAME SD-084(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140607
Time 16.27
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



Current Data Parameters
NAME SD-084(old)
EXPNO 3
PROCNO 1

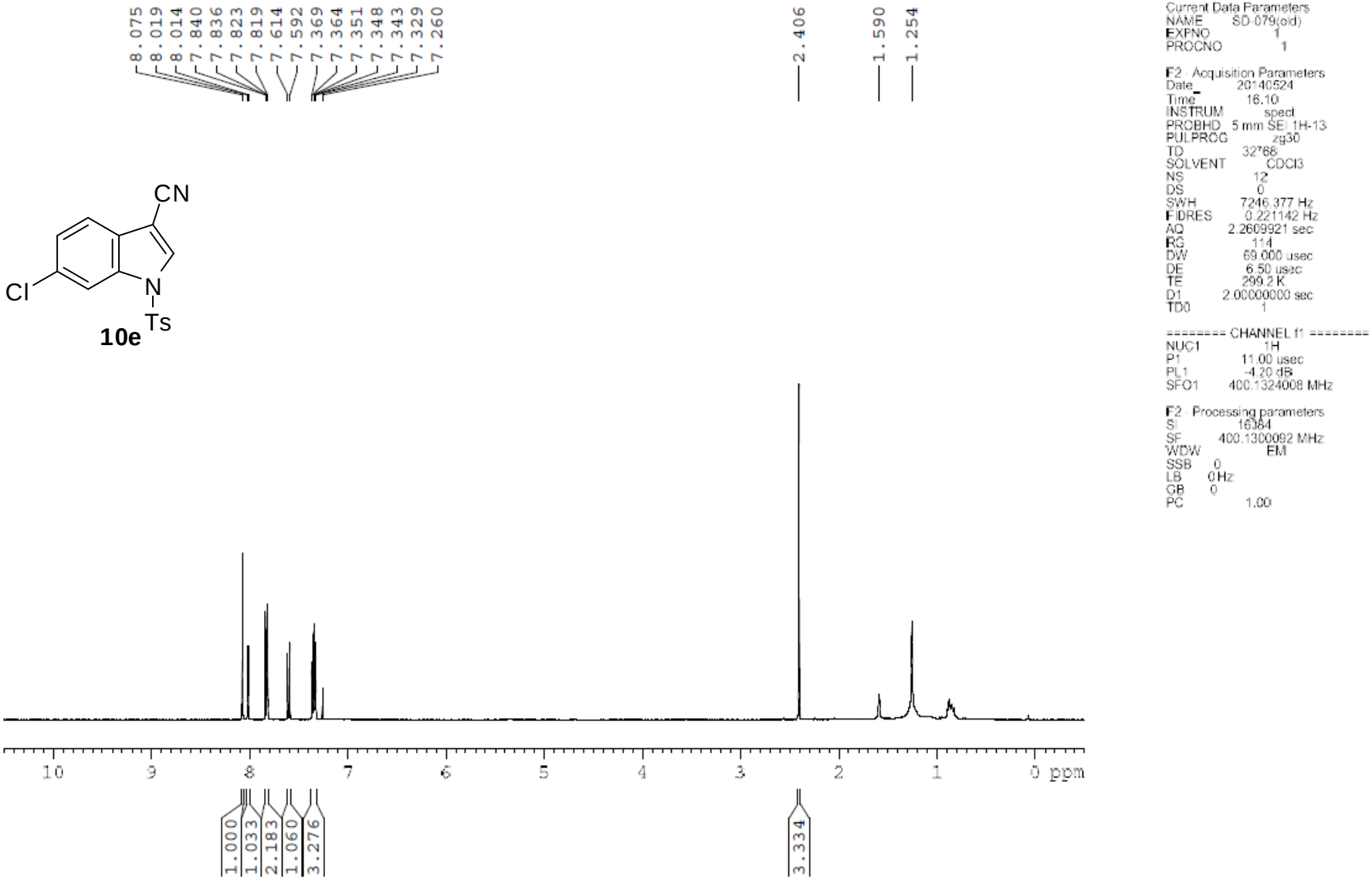
F2 - Acquisition Parameters
Date_ 20140607
Time 16.54
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 381
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

pure



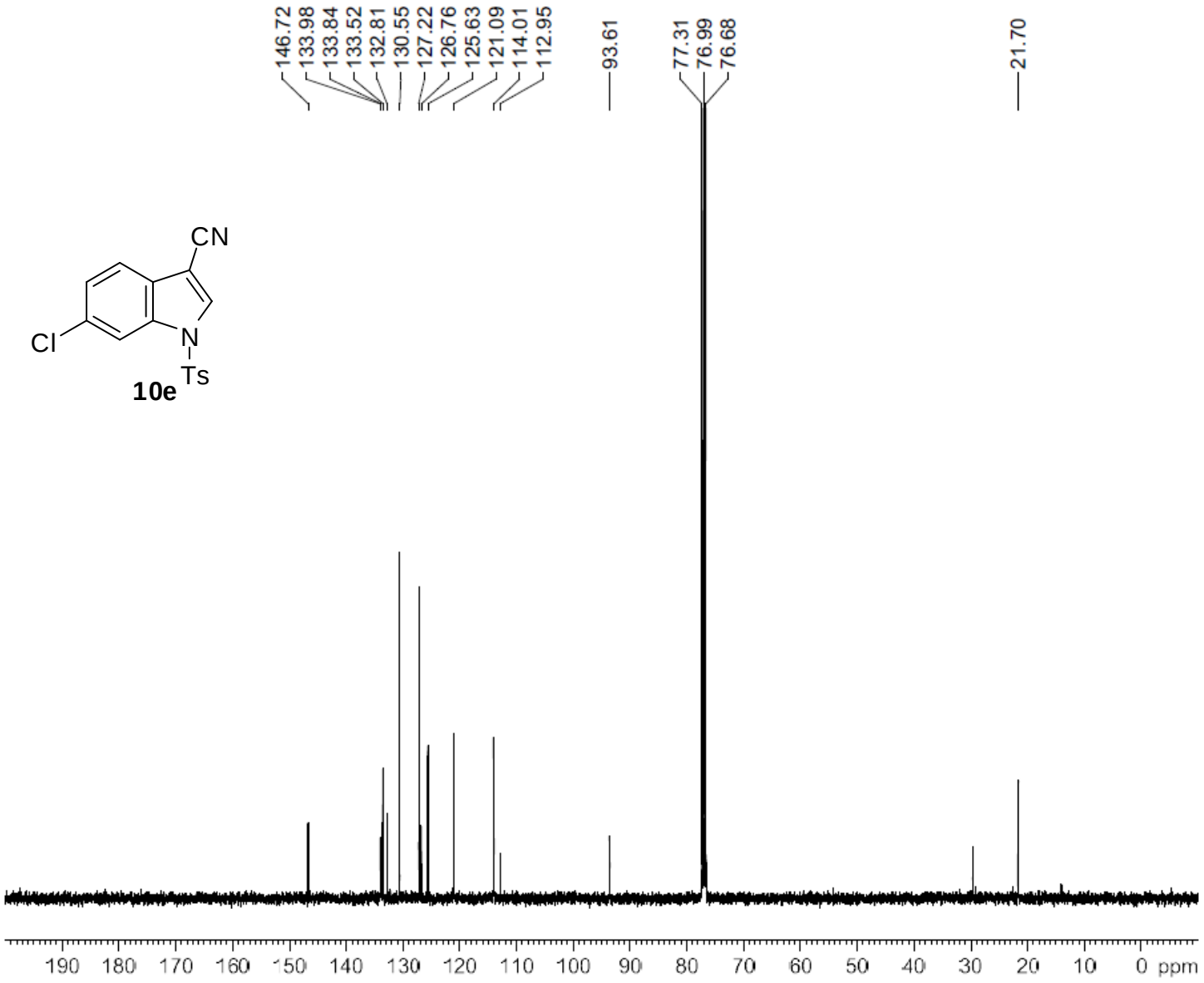
Current Data Parameters
NAME SD-079(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140524
Time 16.10
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



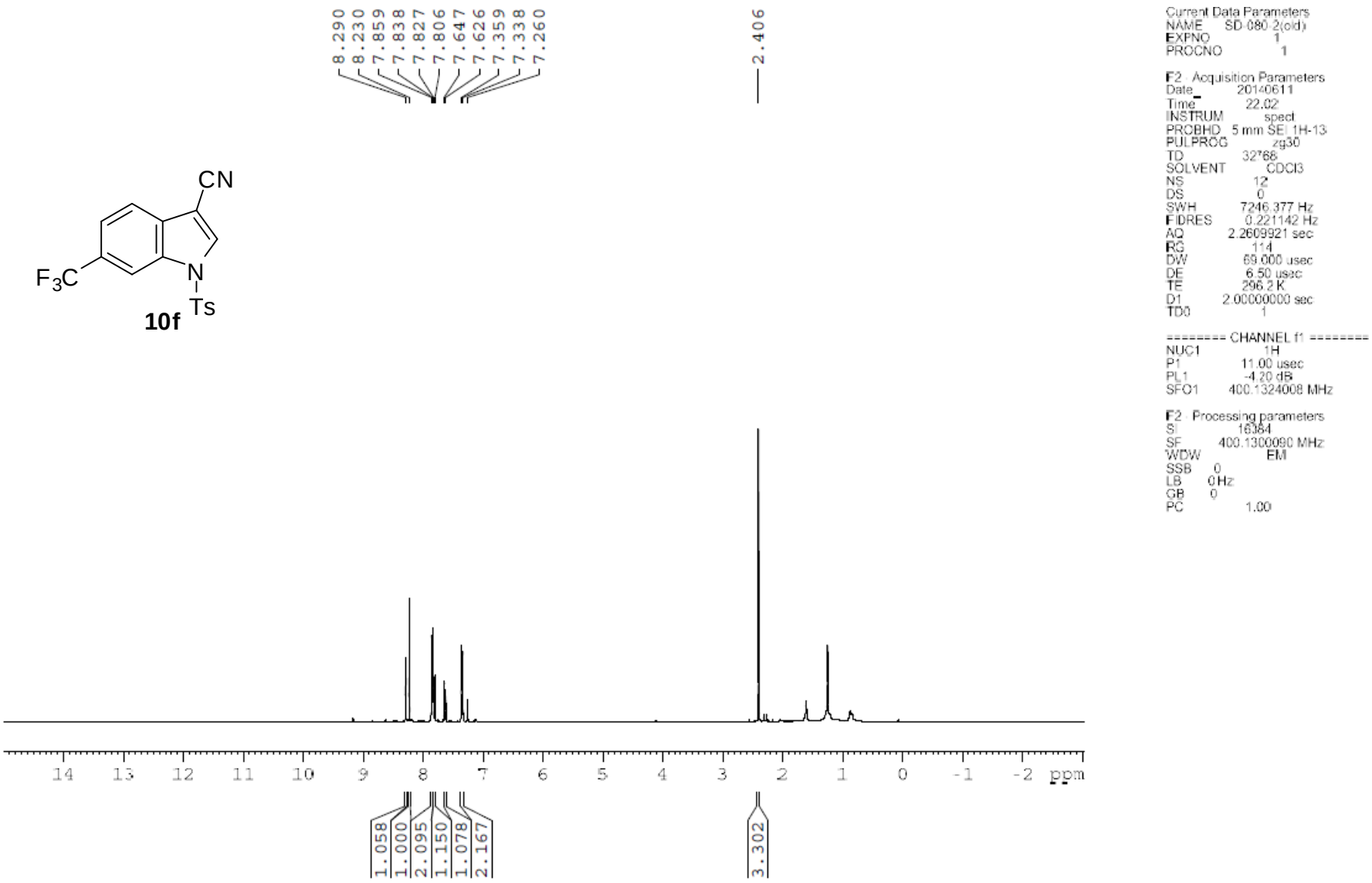
Current Data Parameters
NAME SD-079(old)
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140528
Time 12.05
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1331
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127723 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

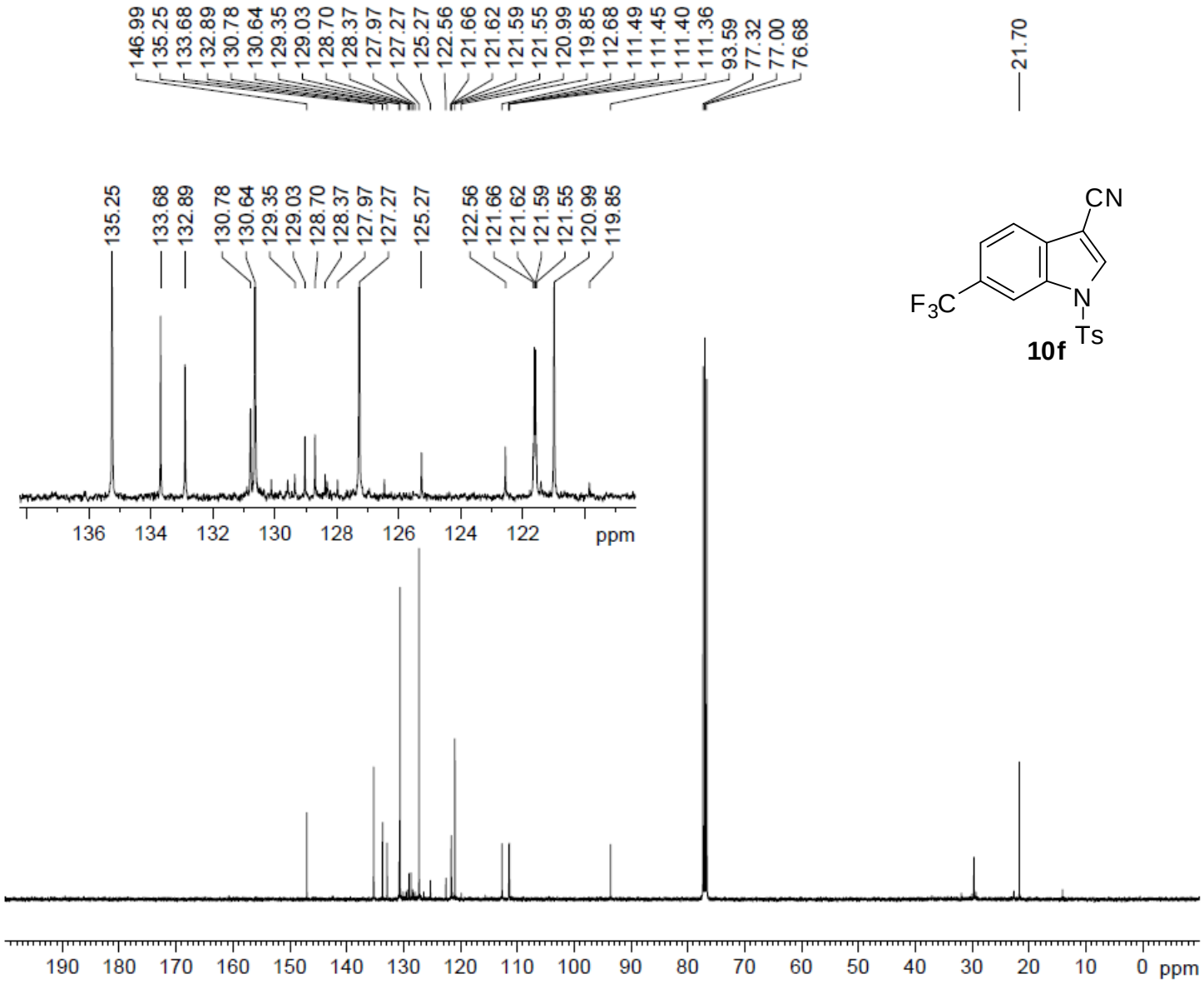


Current Data Parameters
NAME SD-080-2(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140611
Time 22.02
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 296.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



10f

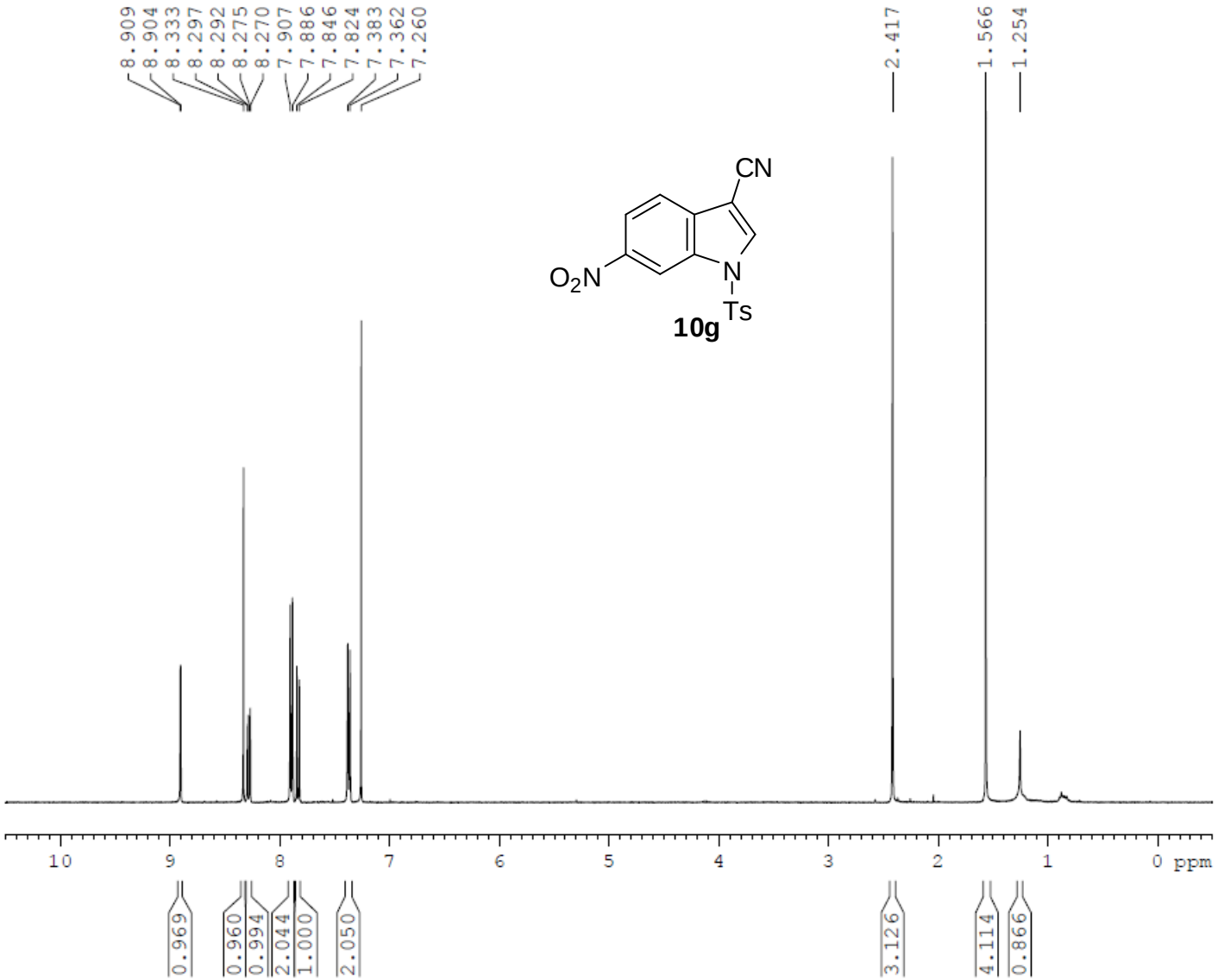
Current Data Parameters
NAME SD-080-2(old)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140611
Time 22.59
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 6000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 7298.2
DW 20.800 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127709 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

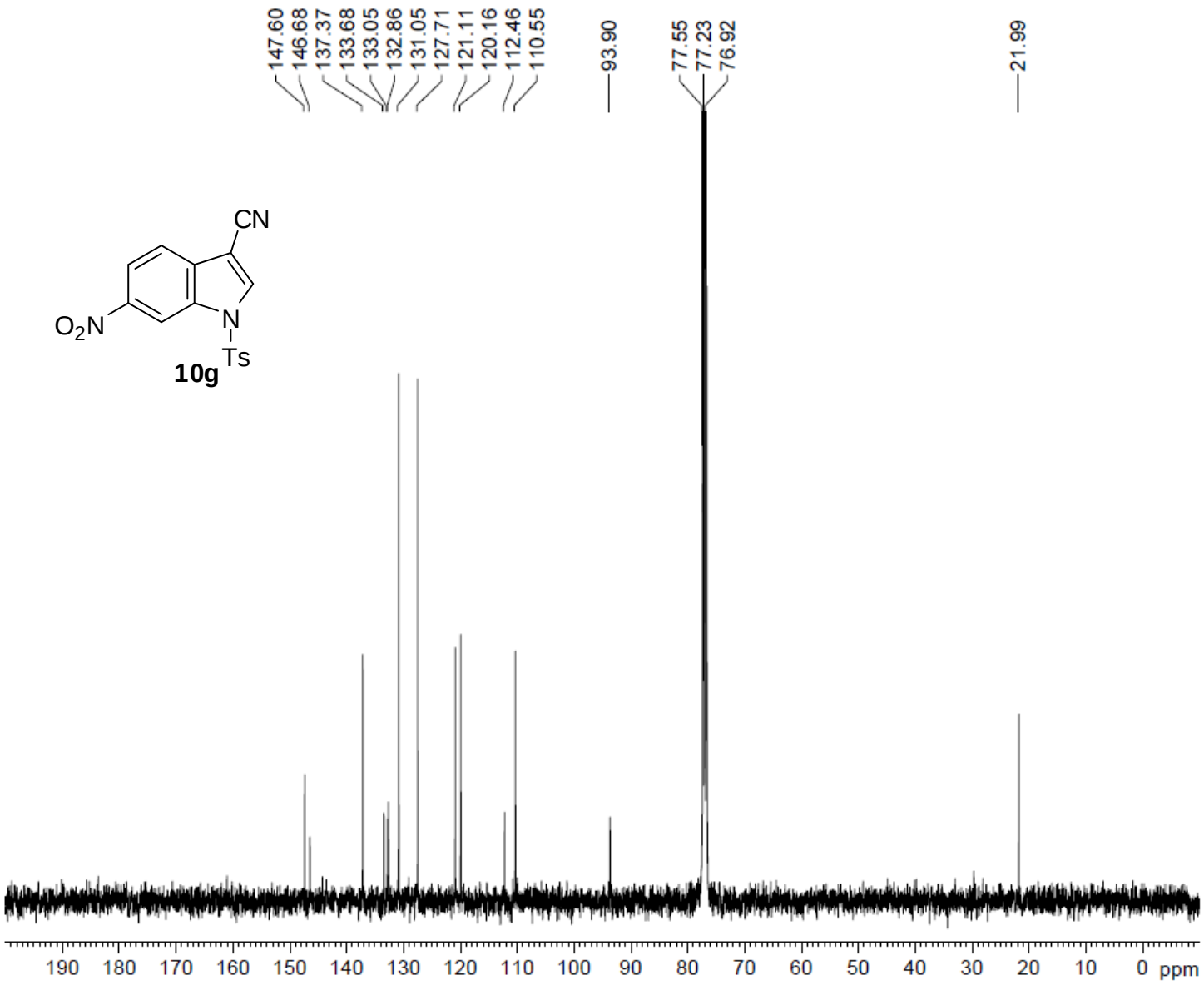


Current Data Parameters
NAME SC184
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140916
Time 8.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 198.09
DW 69.333 usec
DE 10.52 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



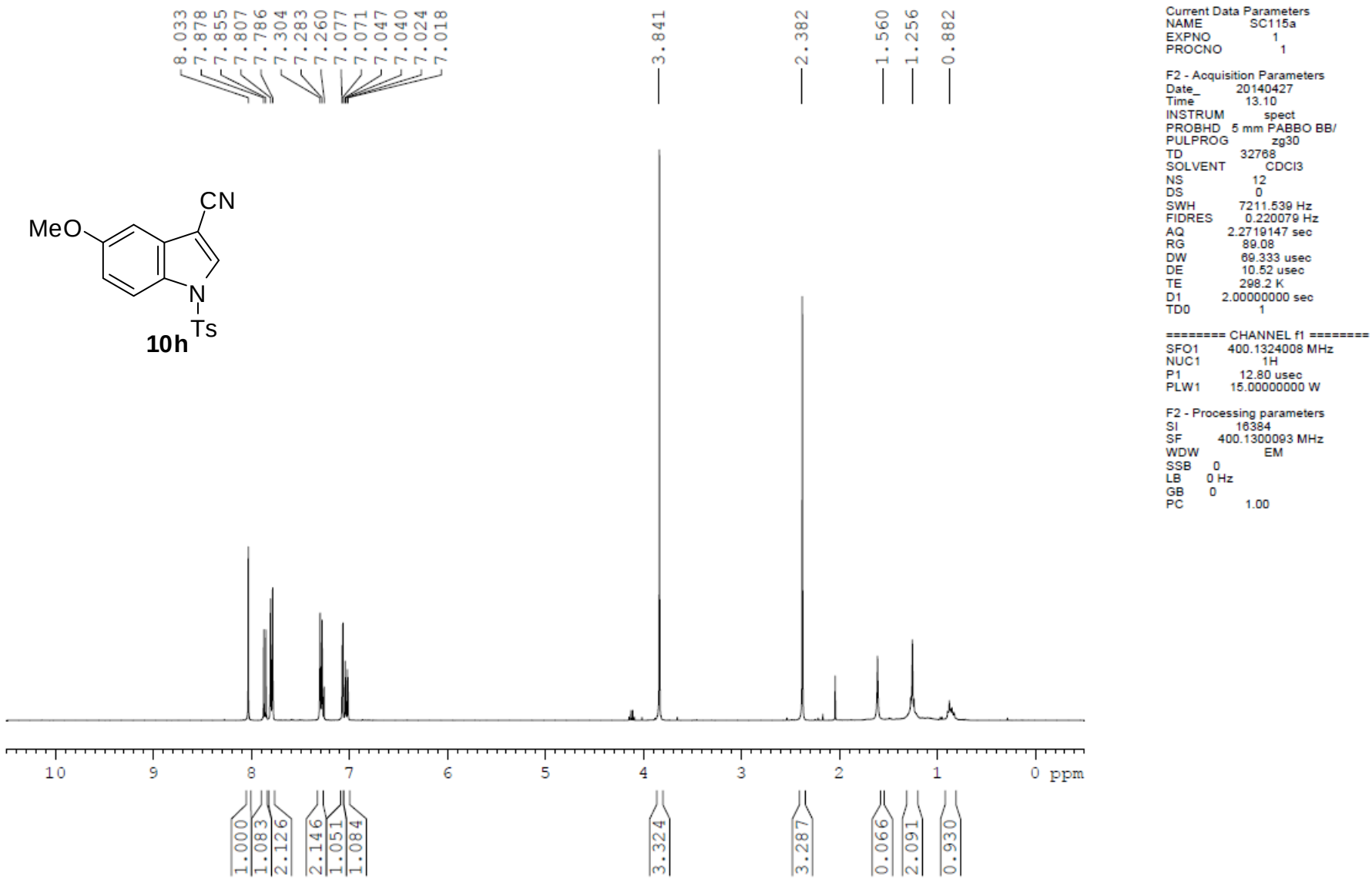
Current Data Parameters
NAME SC184
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140916
Time 9.29
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1645
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127685 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

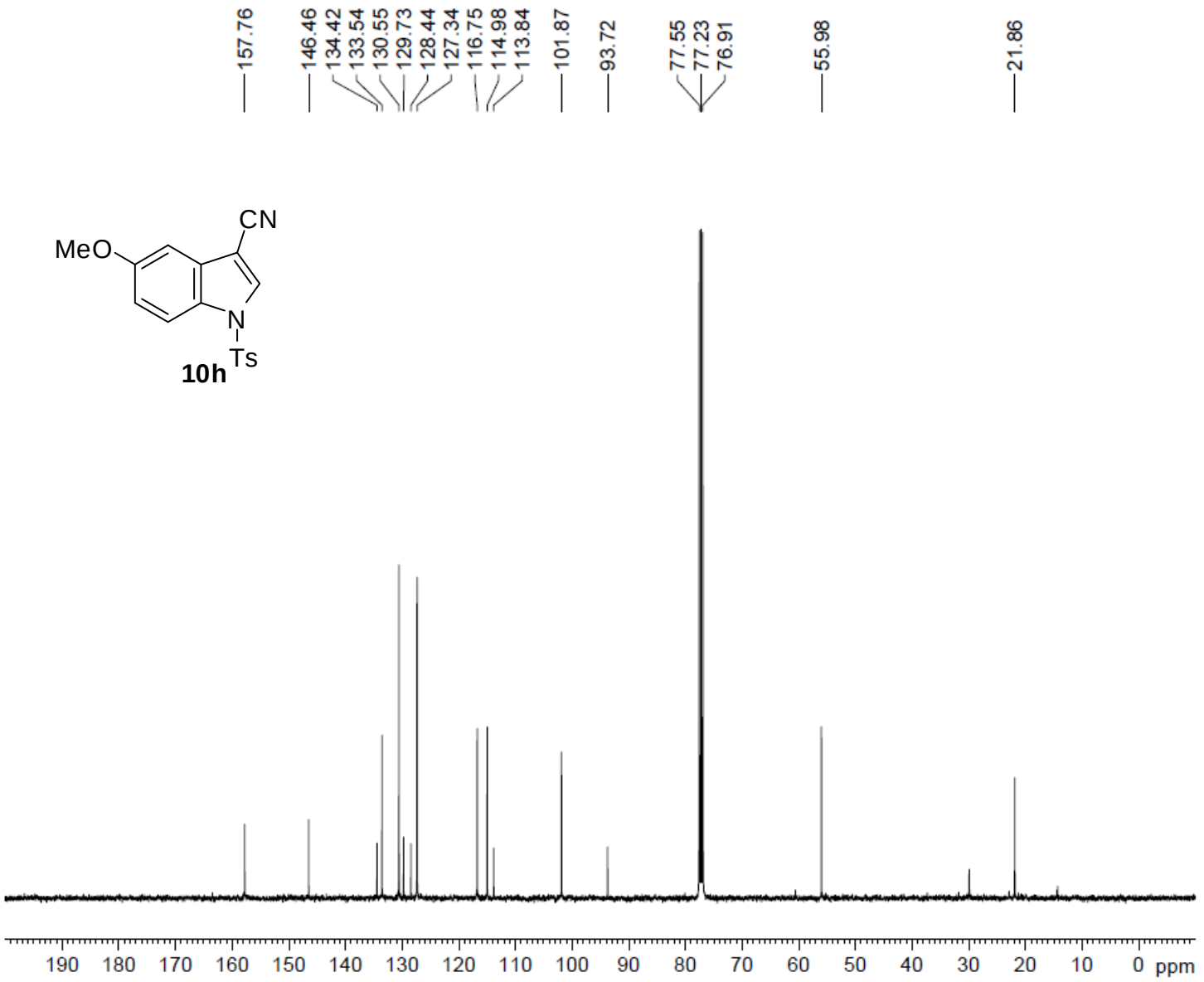


Current Data Parameters
NAME SC115a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140427
Time 13.10
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 89.08
DW 69.333 usec
DE 10.52 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SC115a
EXPNO 3
PROCNO 1

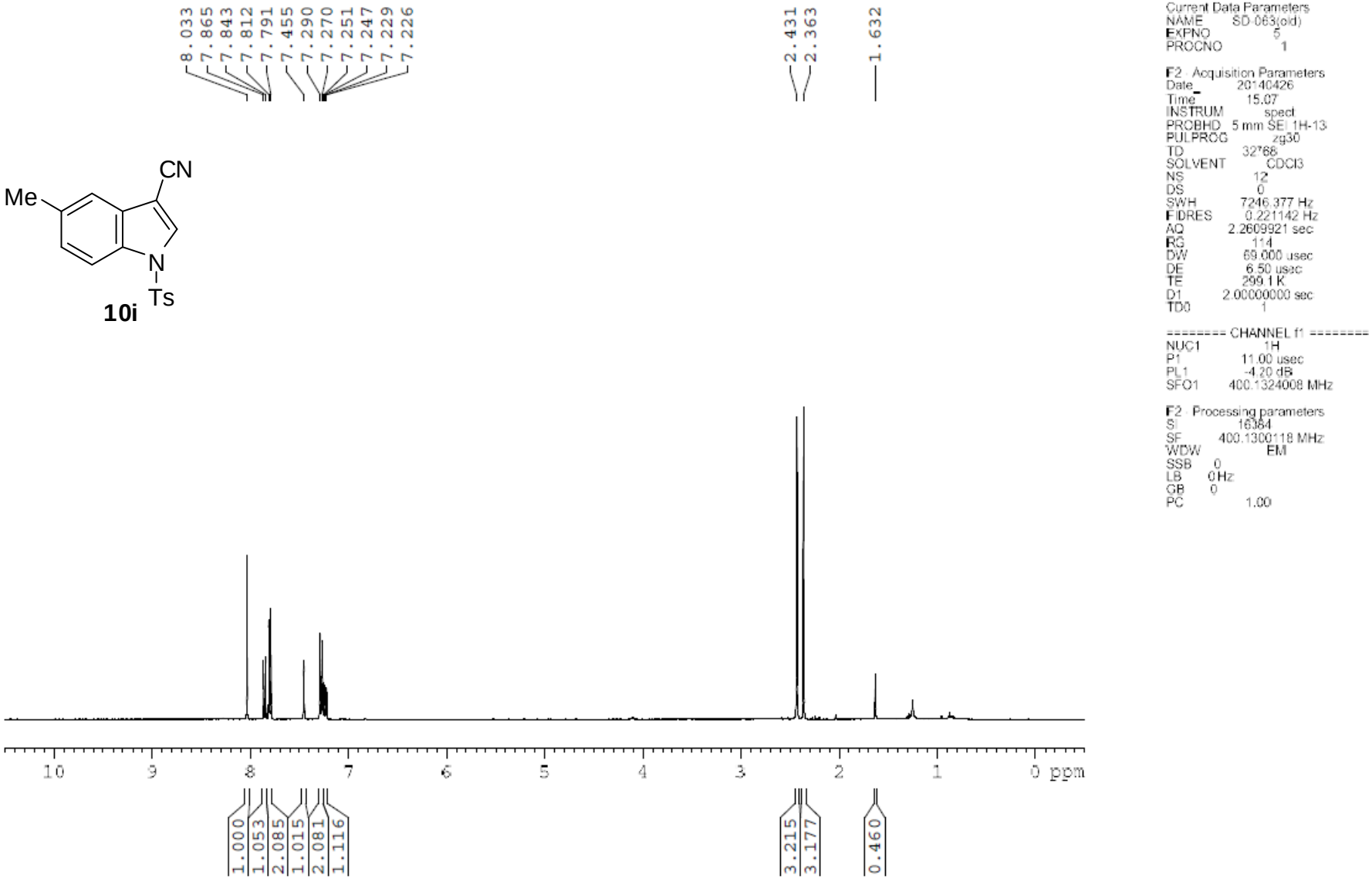
F2 - Acquisition Parameters
Date_ 20140427
Time 14.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1040
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127481 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

pure



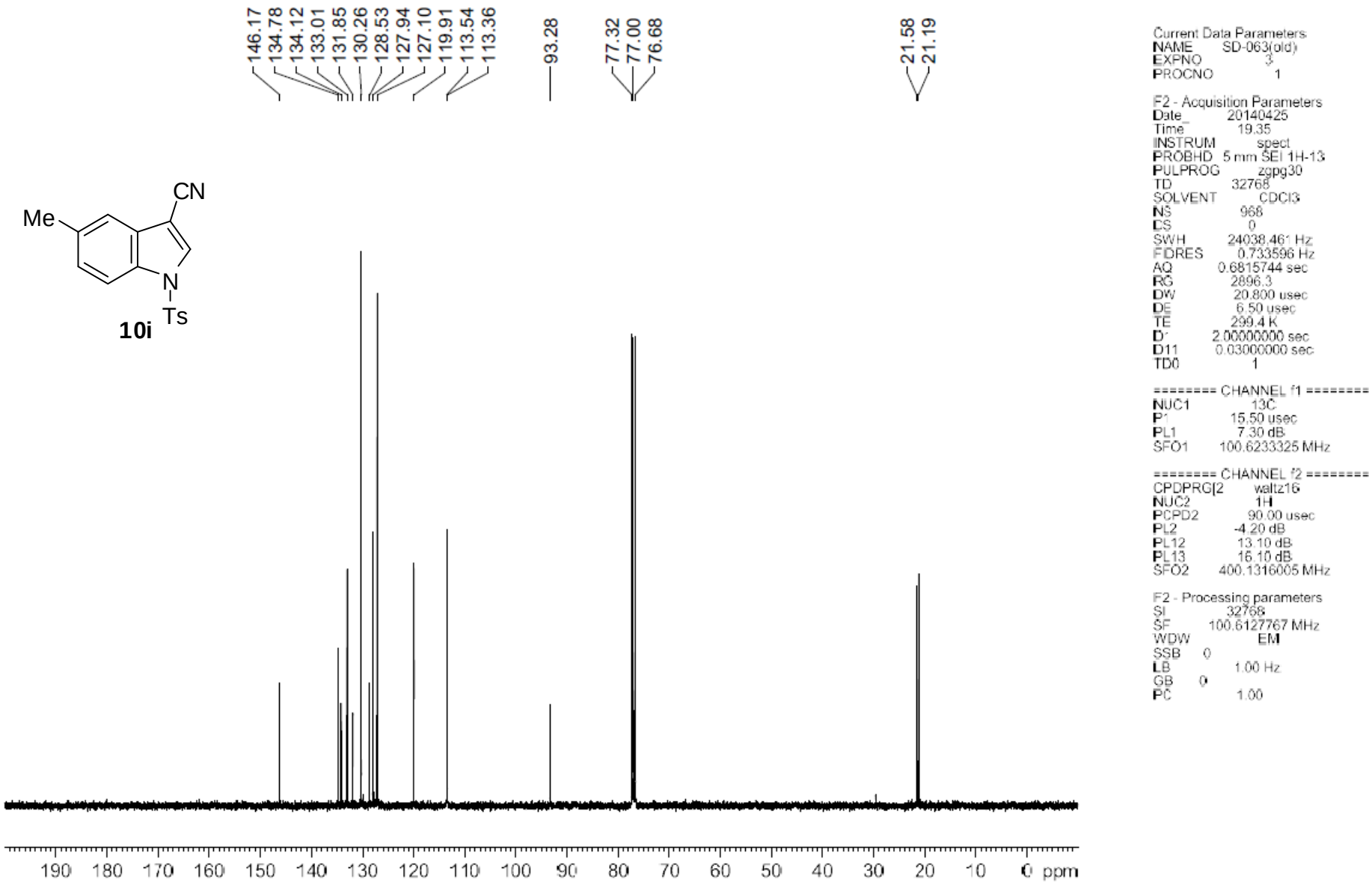
Current Data Parameters
NAME SD-063(old)
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140426
Time 15.07
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300118 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



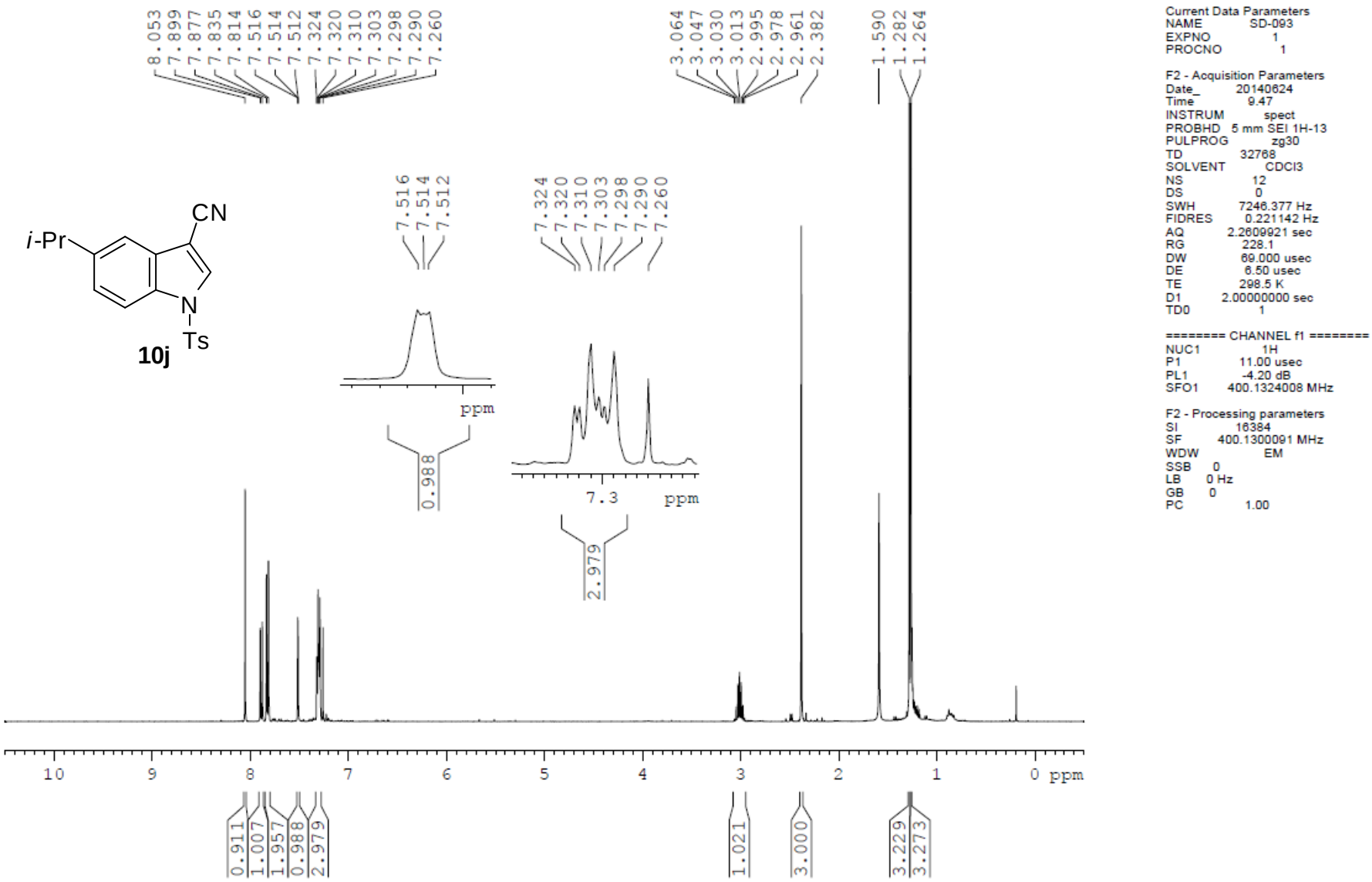
Current Data Parameters
NAME SD-063(old)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140425
Time 19.35
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 968
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127767 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00



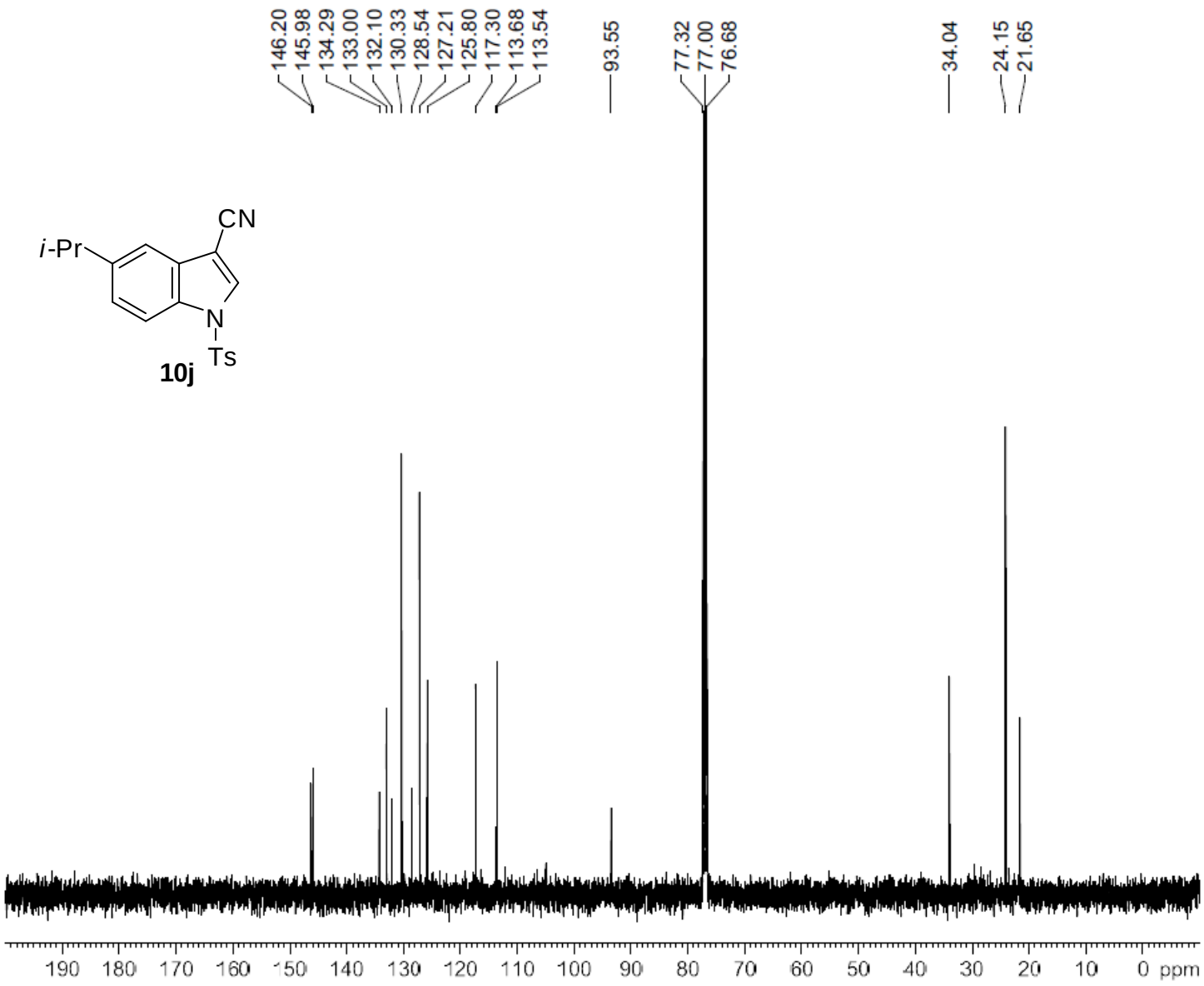
Current Data Parameters
NAME SD-093
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140624
Time 9.47
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 228.1
DW 69.000 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



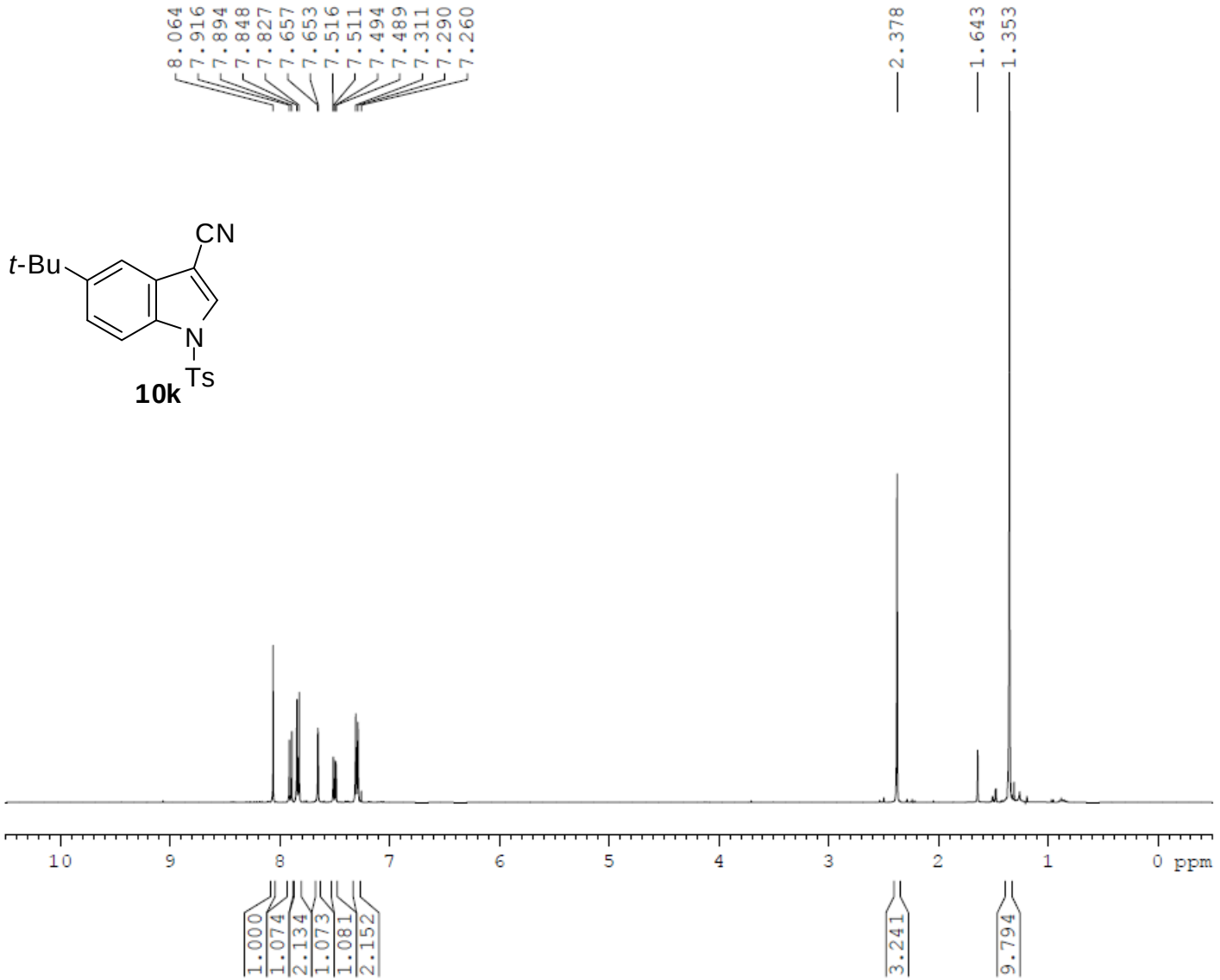
Current Data Parameters
NAME SD-093(OLD)
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140624
Time 12.56
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 822
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127701 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

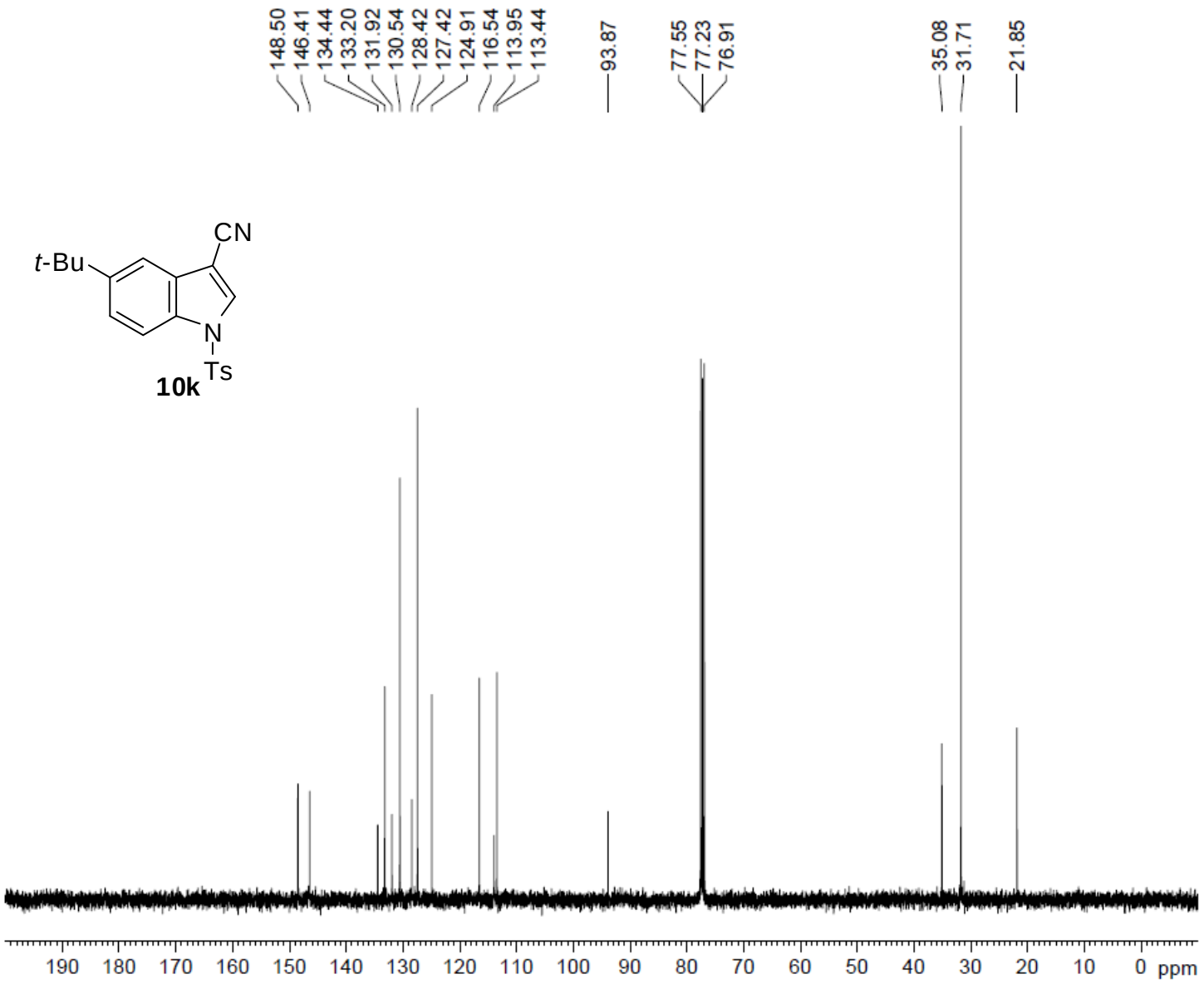


Current Data Parameters
NAME SC159-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140711
Time 9.36
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 57
DW 69.000 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



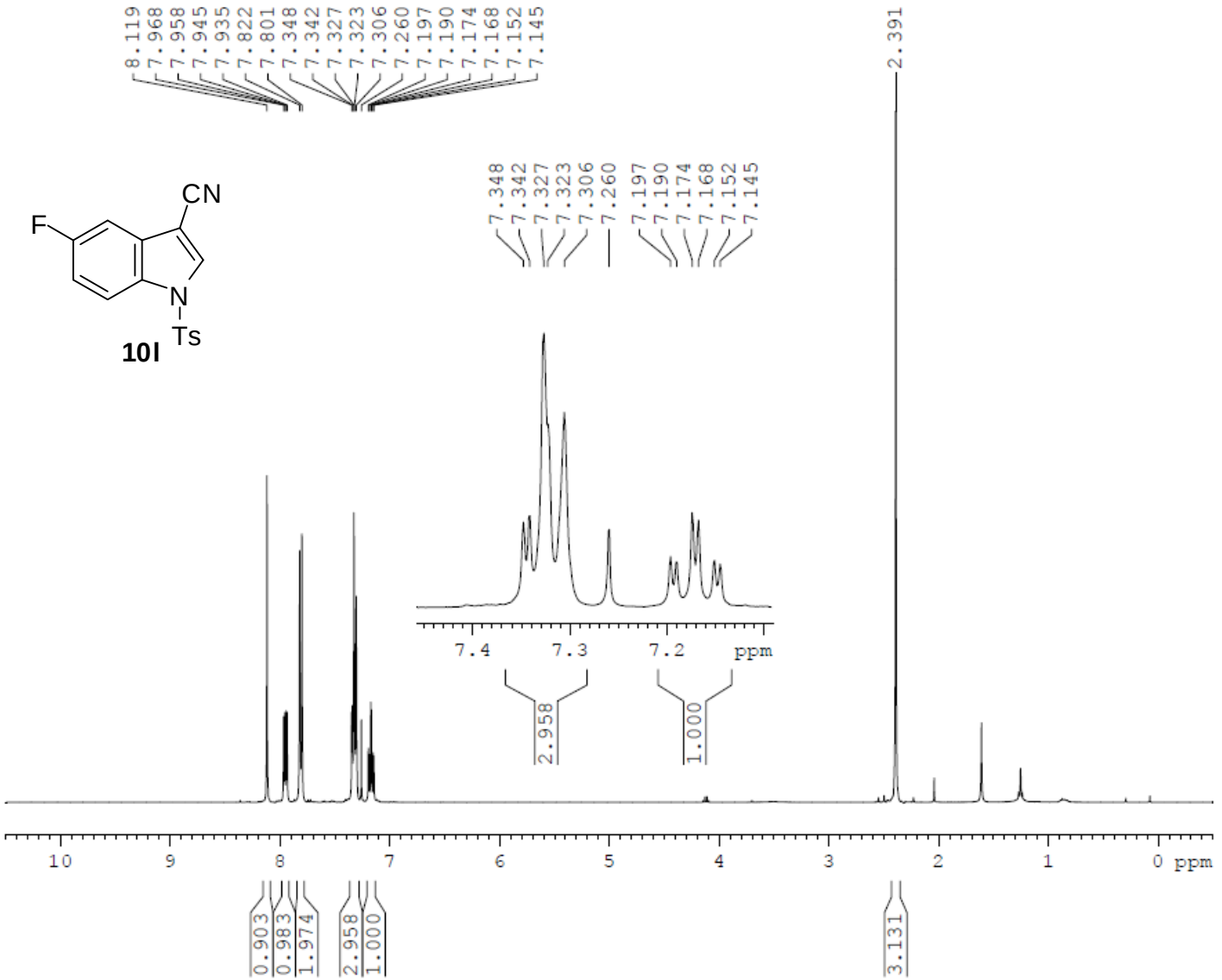
Current Data Parameters
NAME SC159-1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140711
Time 9.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 68
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2048
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

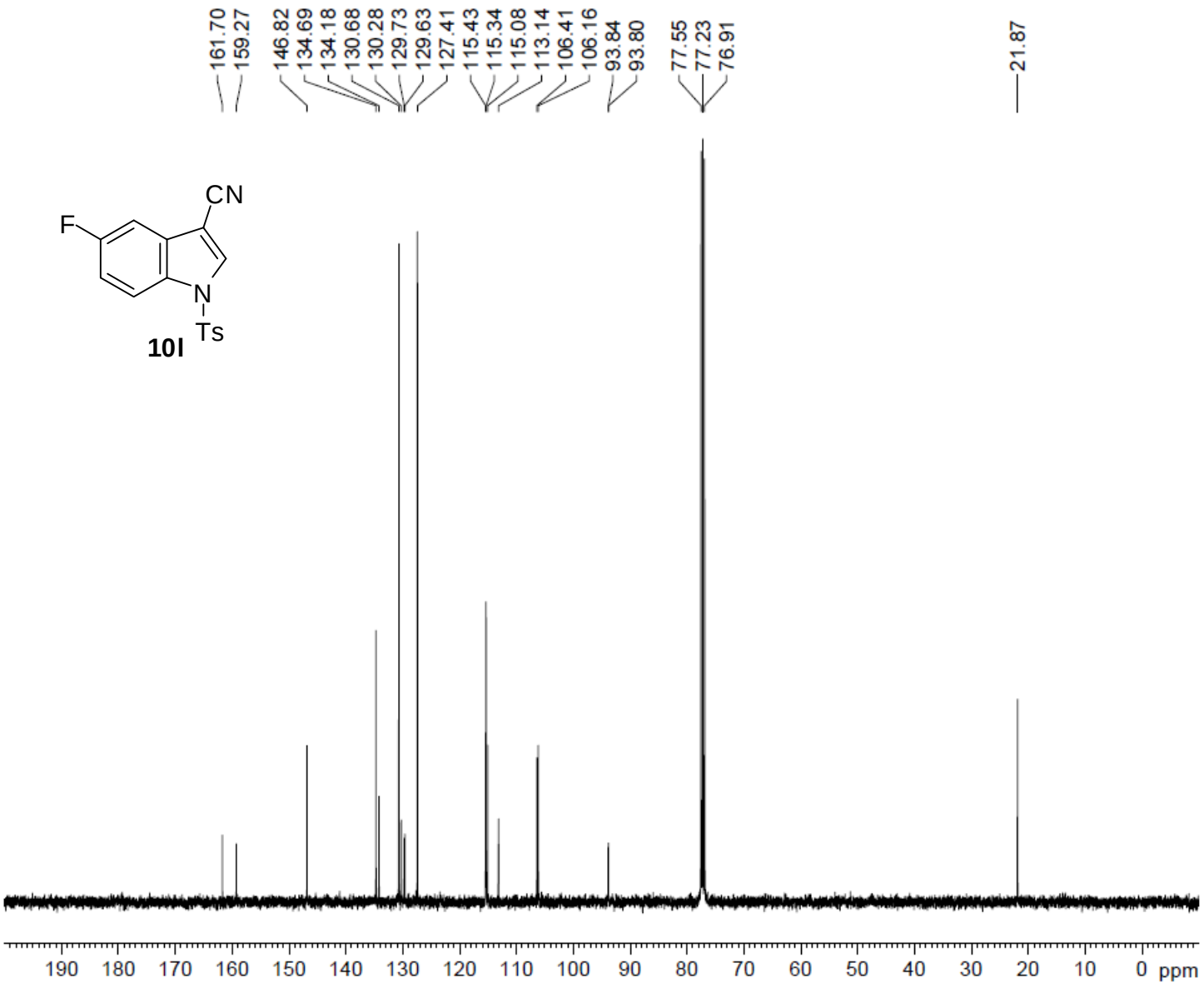


Current Data Parameters
NAME SC172
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140818
Time 10.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



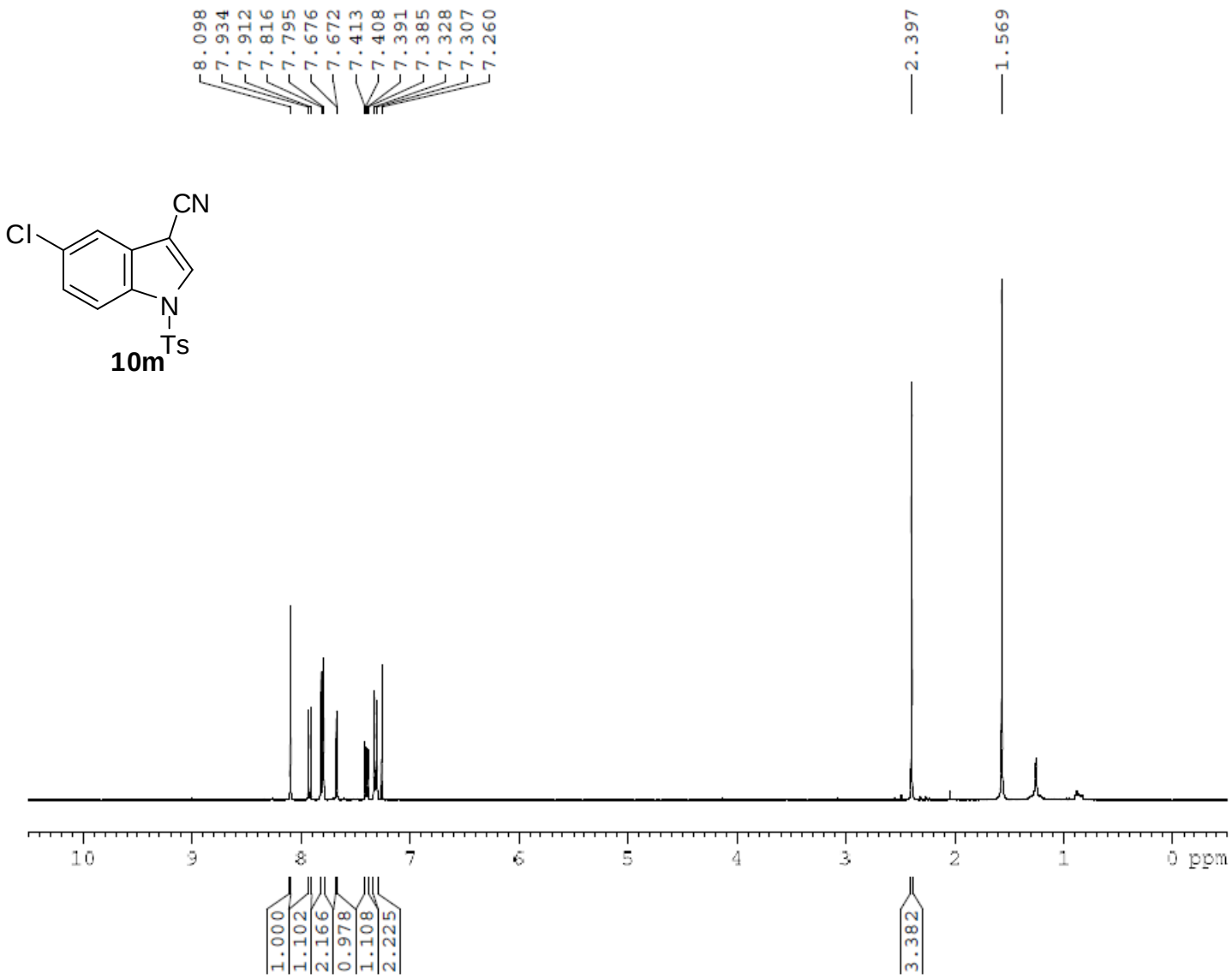
Current Data Parameters
NAME SC172
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140818
Time 10.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 382
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 302.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127487 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

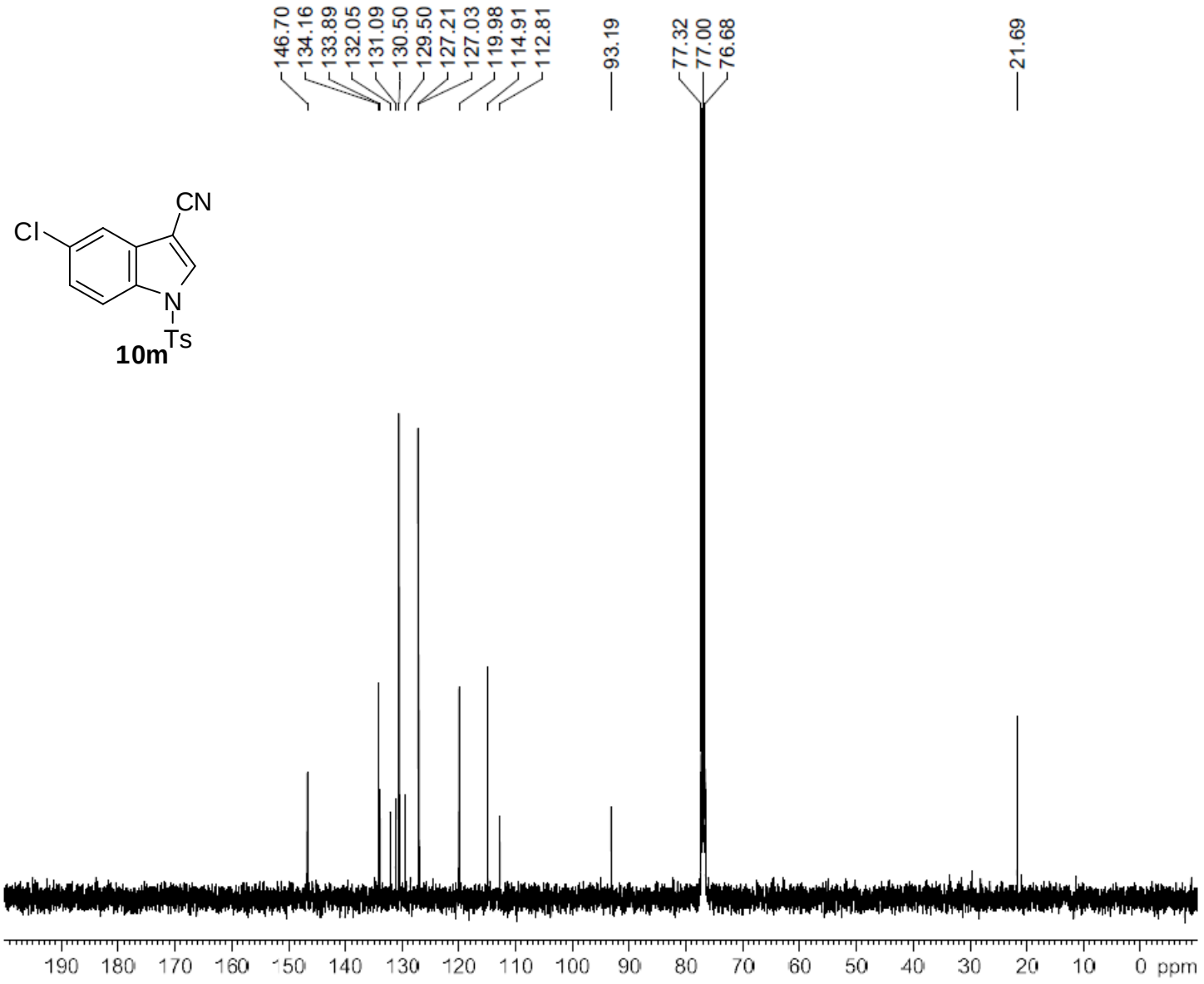


Current Data Parameters
NAME SD-099(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140630
Time 21.09
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 512
DW 69.000 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



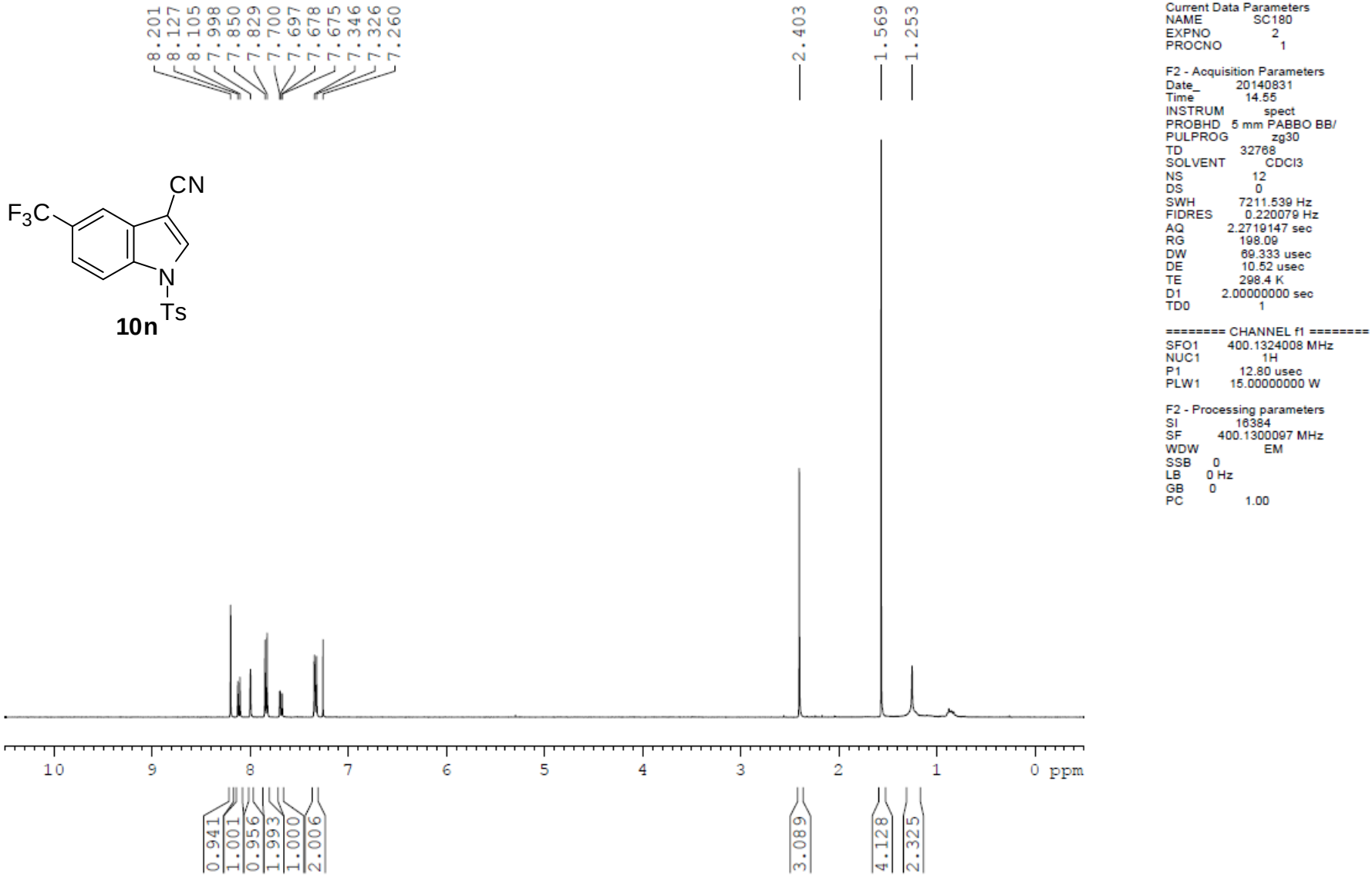
Current Data Parameters
NAME SD-099(old)
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140701
Time 1.44
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4210
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127693 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

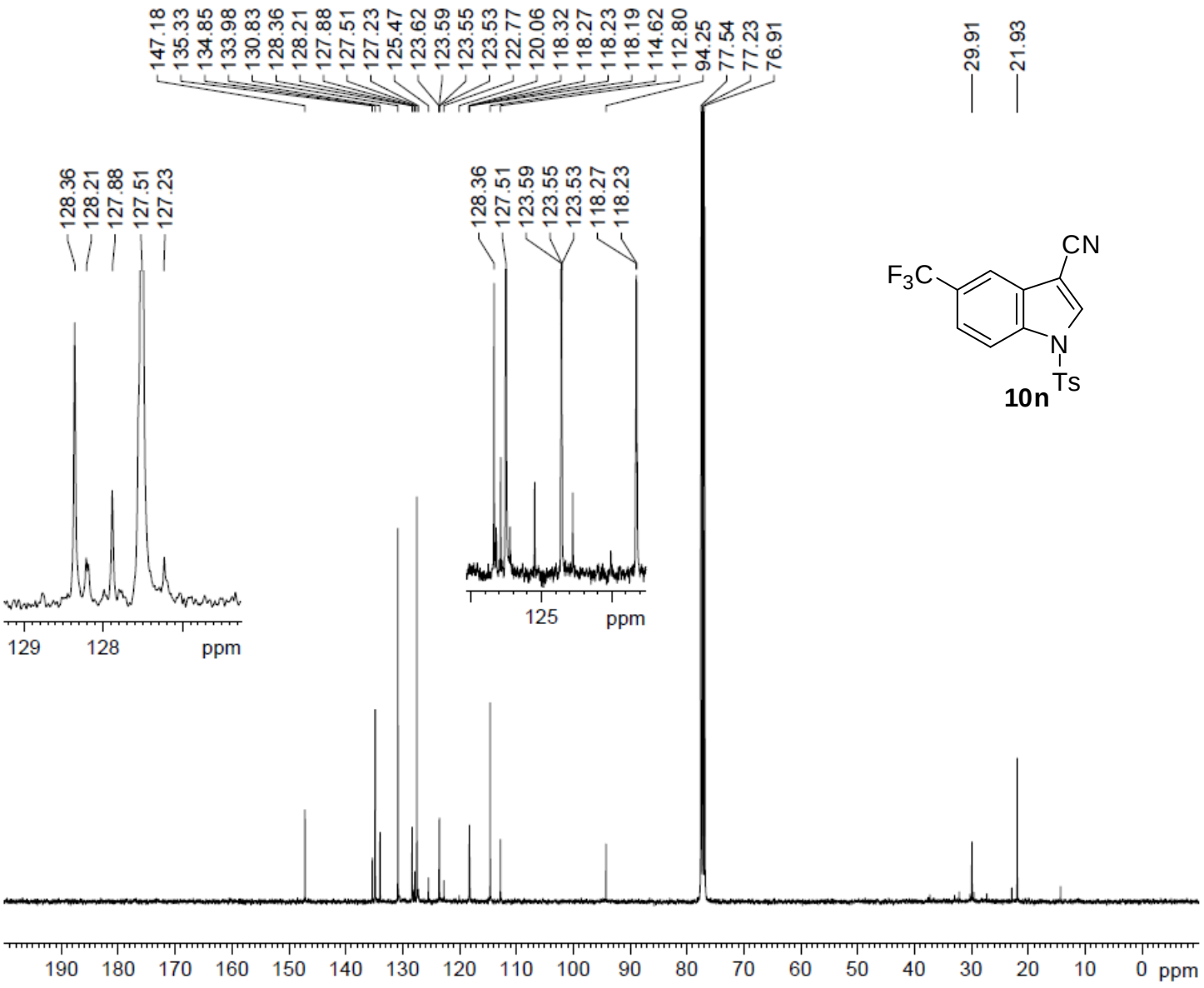


Current Data Parameters
NAME SC180
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140831
Time 14.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 198.09
DW 69.333 usec
DE 10.52 usec
TE 298.4 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



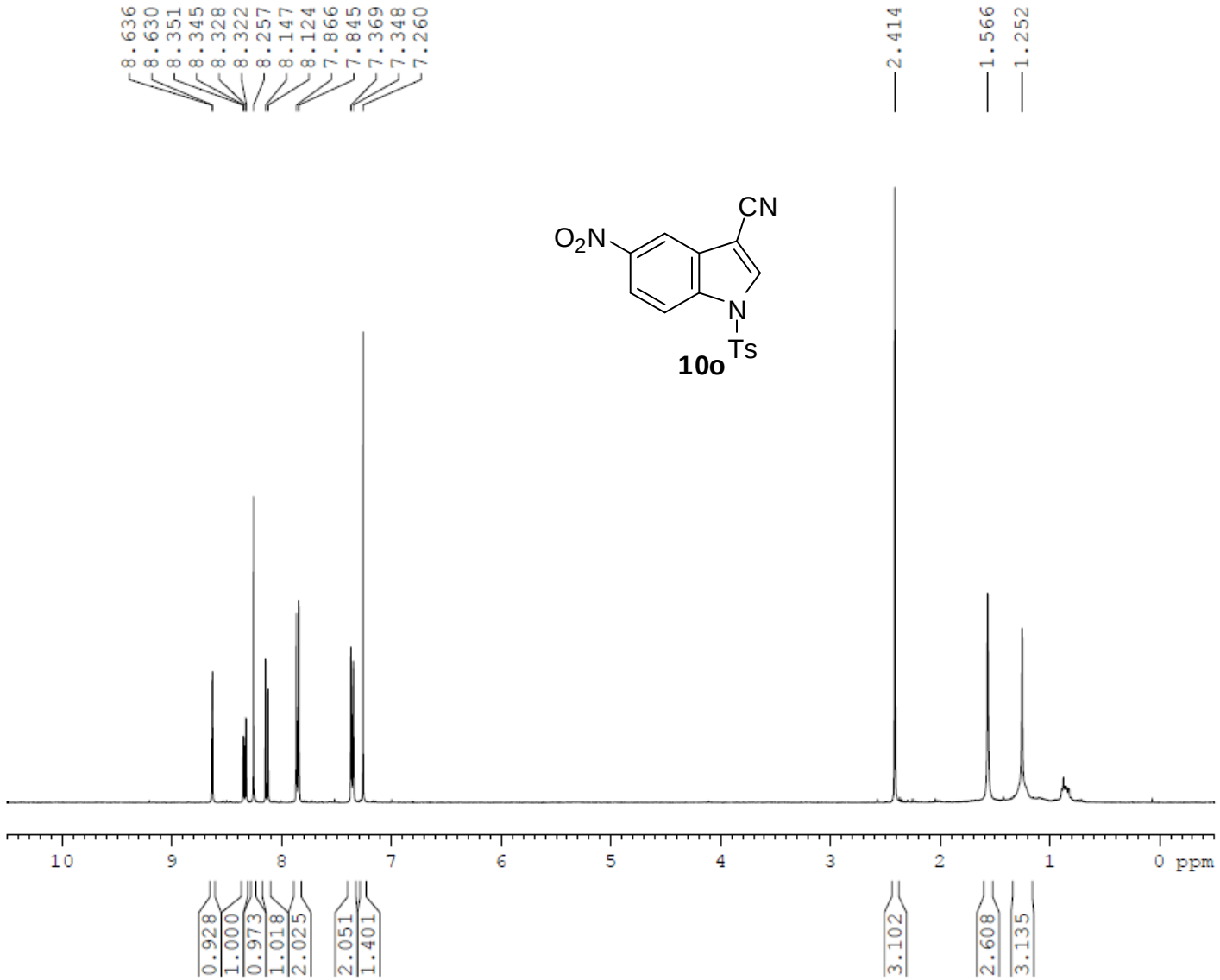
Current Data Parameters
NAME SC180
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140831
Time 19.30
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 3136
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127468 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

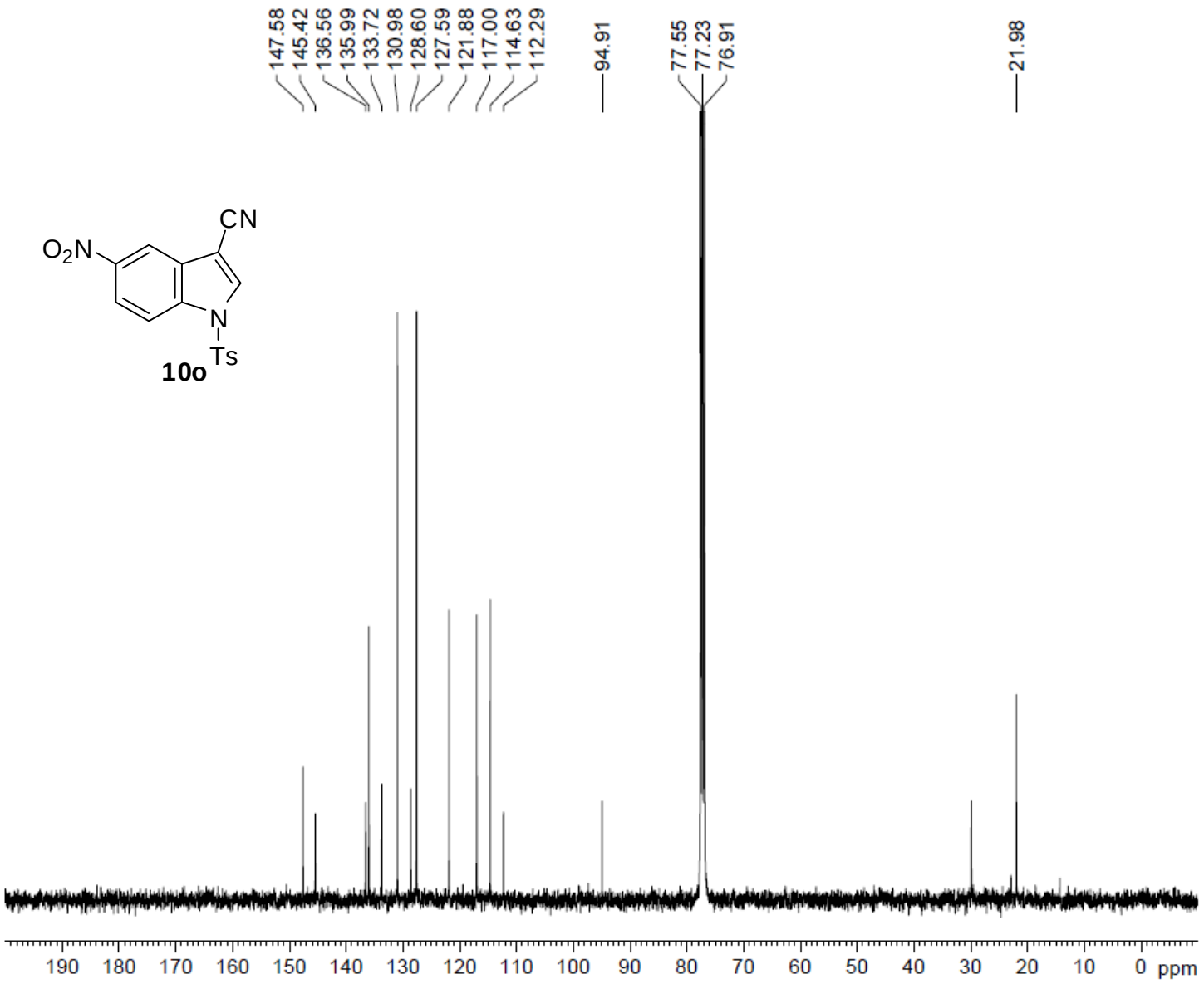


Current Data Parameters
NAME SC196
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141024
Time 8.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 198.09
DW 69.333 usec
DE 10.52 usec
TE 298.7 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 400.1324008 MHz
NUC1 1H
P1 12.80 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 16384
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SC196
EXPNO 2
PROCNO 1

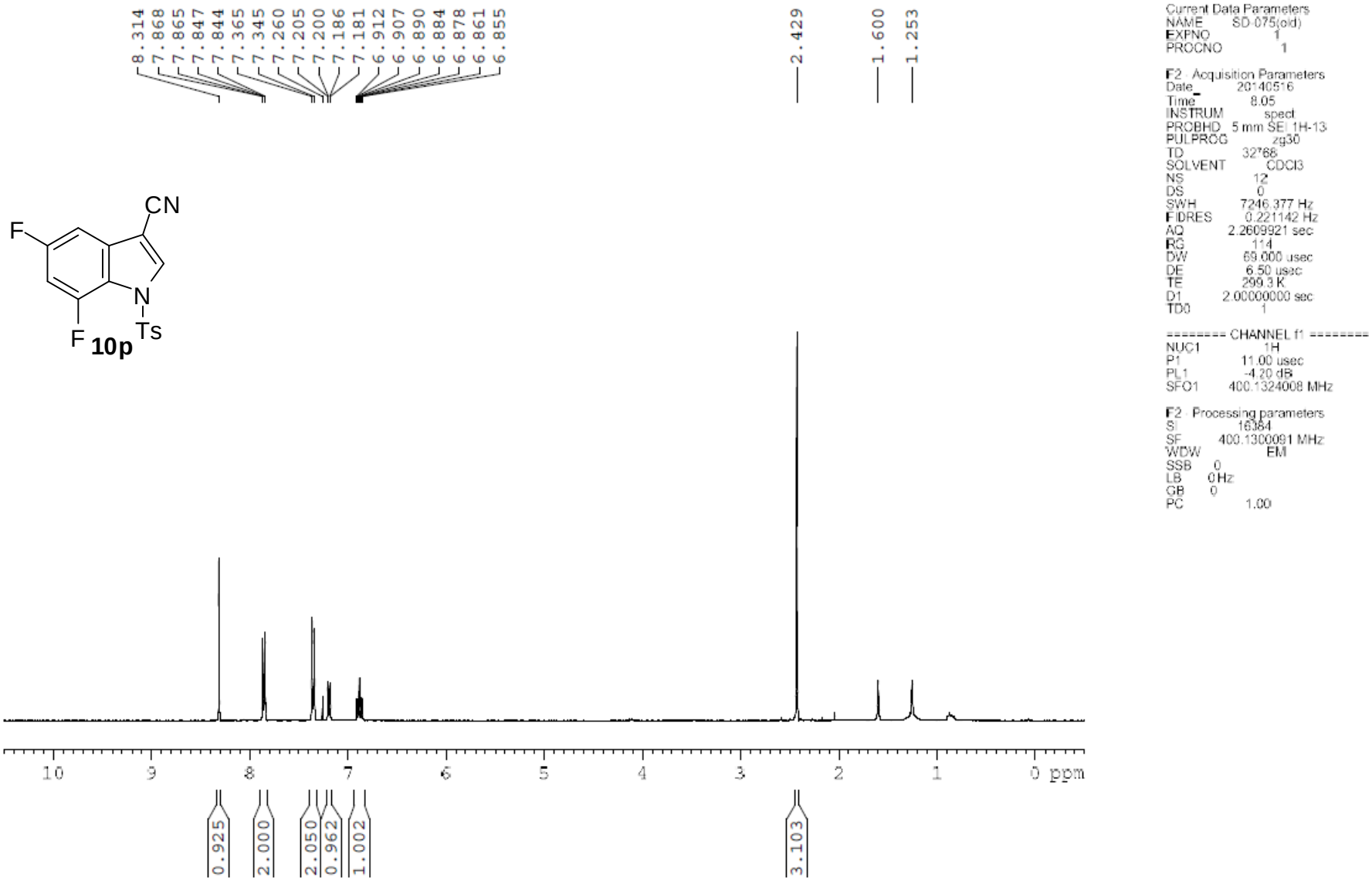
F2 - Acquisition Parameters
Date_ 20141024
Time 10.33
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2921
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

======== CHANNEL f2 ========
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

F2 - Processing parameters
SI 32768
SF 100.6127463 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

product



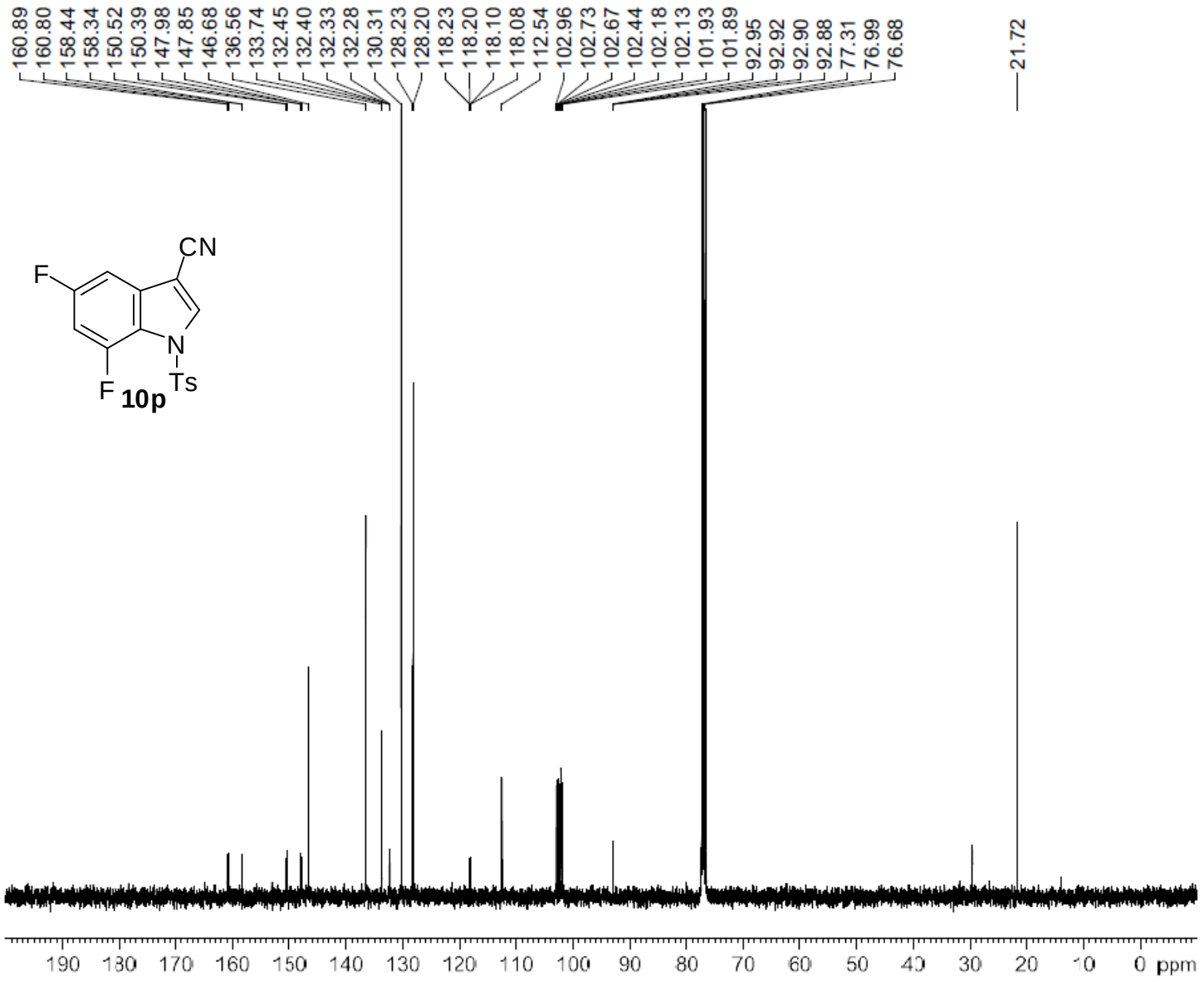
Current Data Parameters
NAME SD-075(old)
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140516
Time 8.05
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 11.00 usec
PL1 -4.20 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

product



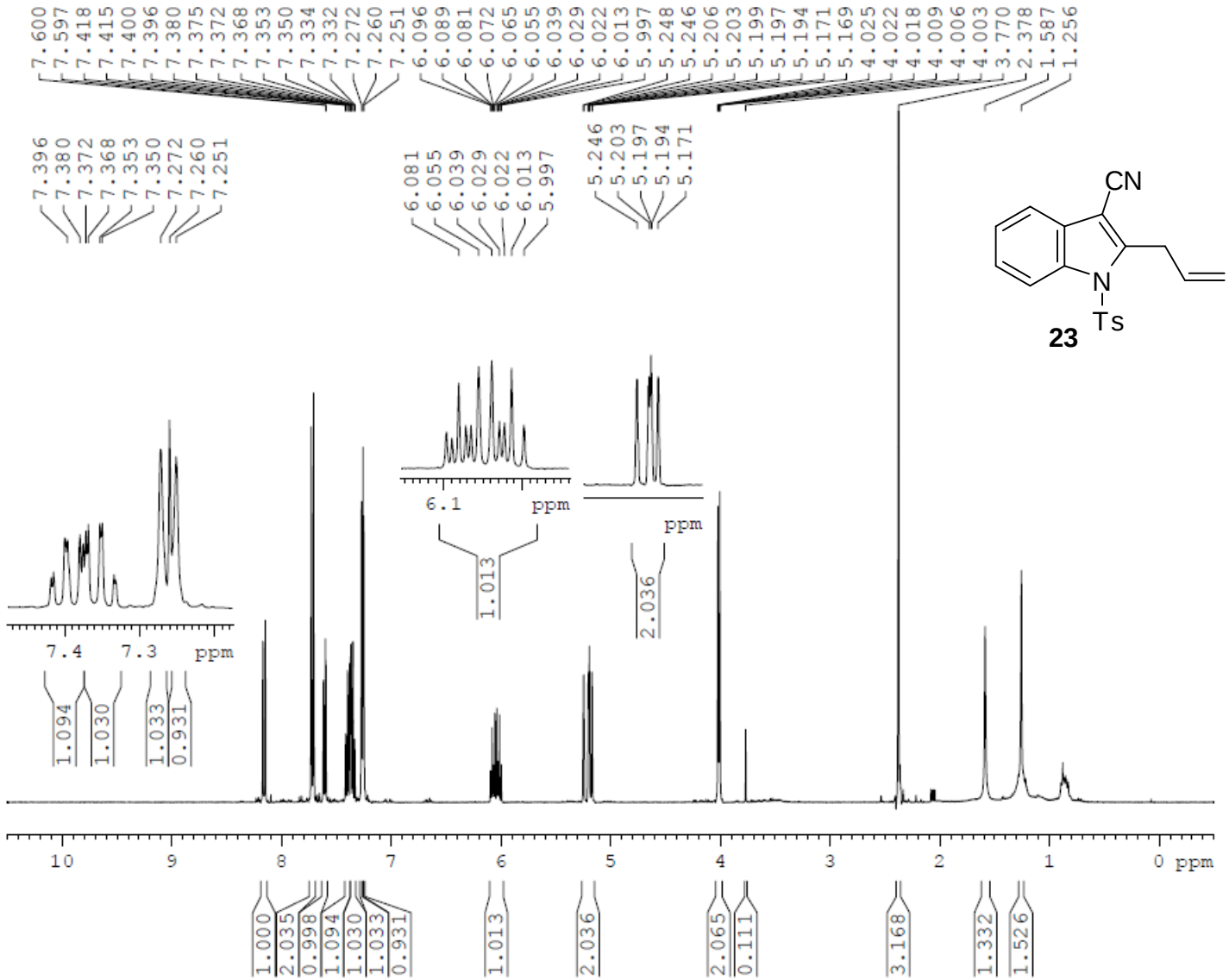
Current Data Parameters
NAME SD-075(old)
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140516
Time 8.10
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1487
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4597.6
DW 20.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.20 dB
PL12 13.10 dB
PL13 16.10 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

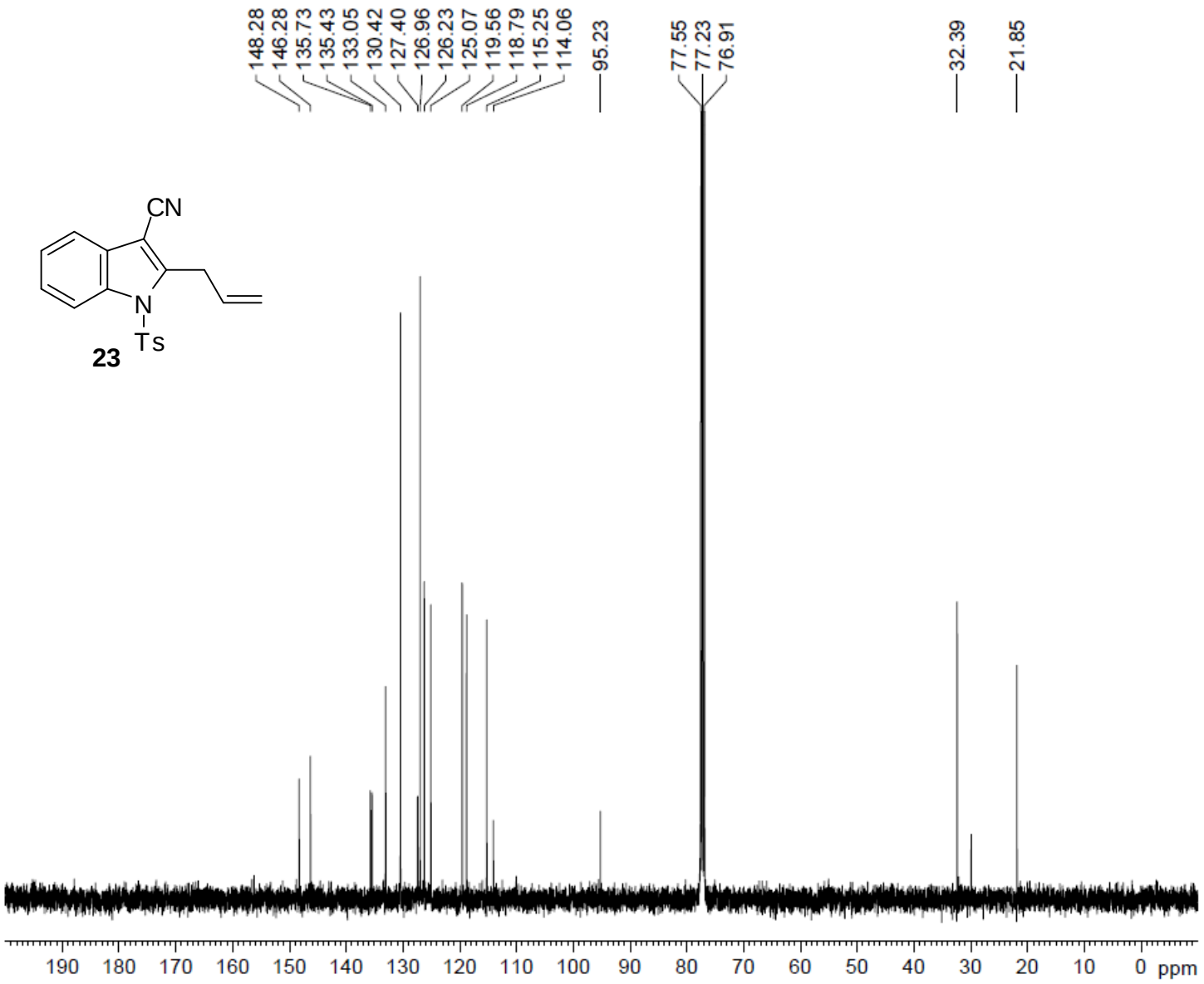


Current Data Parameters
NAME SO119a-1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150504
Time 21.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 256
DW 69.000 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 21.45 usec
PL1 -5.85 dB
SFO1 400.1324008 MHz

F2 - Processing parameters
SI 16384
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



Current Data Parameters
NAME SO119a-1
EXPNO 3
PROCNO 1

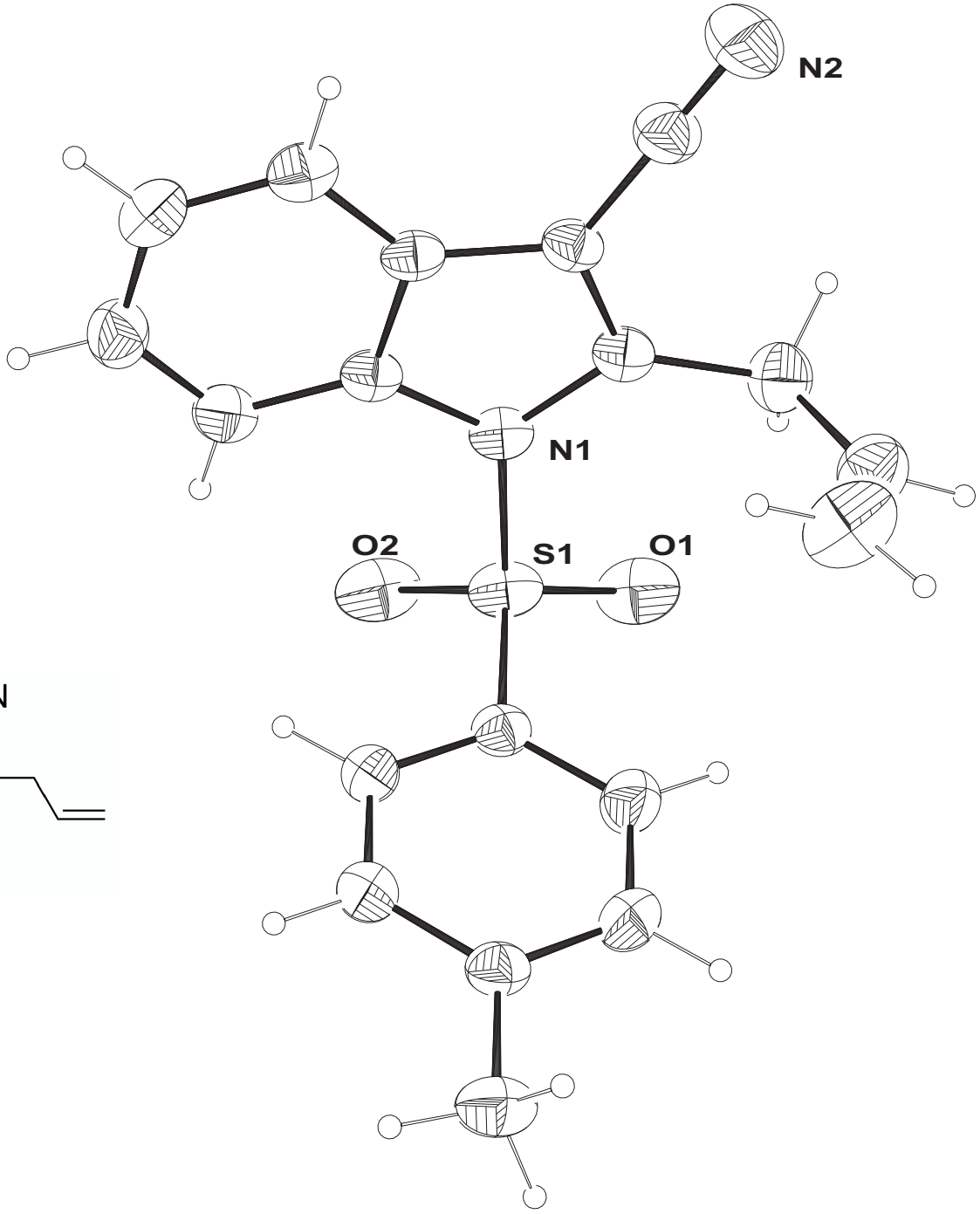
F2 - Acquisition Parameters
Date_ 20150505
Time 9.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 342
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 6502
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

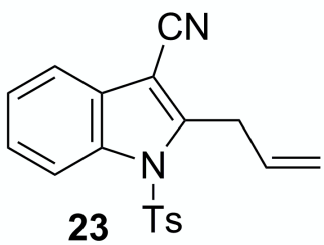
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 6.00 dB
PL13 9.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127482 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00

a17991





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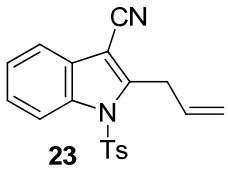

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Table 1. Crystal data and structure refinement for a17991.

Identification code	a17991	
Empirical formula	C19 H16 N2 O2 S	
Formula weight	336.40	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 9.3811(4) Å	α= 90°.
	b = 20.8484(10) Å	β= 99.098(2)°.
	c = 8.6963(4) Å	γ = 90°.
Volume	1679.43(13) $Å^3$	
Z	4	
Density (calculated)	1.330 Mg/m^3	
Absorption coefficient	0.206 mm^{-1}	
F(000)	704	
Crystal size	0.52 x 0.28 x 0.20 mm^3	
Theta range for data collection	1.95 to 25.05°.	
Index ranges	-9<=h<=11, -13<=k<=24, -10<=l<=9	
Reflections collected	11240	
Independent reflections	2958 [R(int) = 0.0313]	
Completeness to theta = 25.05°	99.4 %	
Absorption correction	multi-scan	
Max. and min. transmission	0.9600 and 0.9005	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2958 / 0 / 217	
Goodness-of-fit on F^2	1.026	
Final R indices [I>2sigma(I)]	R1 = 0.0536, wR2 = 0.1392	
R indices (all data)	R1 = 0.0786, wR2 = 0.1575	
Largest diff. peak and hole	0.296 and -0.228 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for a17991. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	2001(3)	6776(1)	11365(3)	64(1)
C(2)	2547(4)	7363(2)	11887(4)	88(1)
C(3)	1815(4)	7914(1)	11372(4)	89(1)
C(4)	552(3)	7896(1)	10344(3)	70(1)
C(5)	-229(4)	8503(2)	9781(4)	97(1)
C(6)	29(3)	7302(2)	9856(4)	90(1)
C(7)	734(3)	6744(1)	10354(4)	83(1)
C(8)	3163(3)	5570(1)	9156(3)	61(1)
C(9)	1814(3)	5295(1)	8741(4)	78(1)
C(10)	1479(4)	5050(2)	7268(5)	90(1)
C(11)	2449(4)	5067(2)	6214(4)	89(1)
C(12)	3788(4)	5331(1)	6630(4)	78(1)
C(13)	4159(3)	5583(1)	8119(3)	62(1)
C(14)	5429(3)	5890(1)	8910(3)	63(1)
C(15)	6733(4)	5990(2)	8308(4)	84(1)
C(16)	5233(3)	6064(1)	10365(3)	66(1)
C(17)	6328(4)	6392(2)	11555(4)	92(1)
C(18)	6367(4)	7099(2)	11461(5)	108(1)
C(19)	5768(6)	7460(2)	10493(6)	136(2)
N(1)	3836(2)	5865(1)	10553(2)	66(1)
N(2)	7768(4)	6072(2)	7822(4)	123(1)
O(1)	4006(3)	6219(1)	13329(2)	107(1)
O(2)	1931(3)	5574(1)	12085(3)	107(1)
S(1)	2934(1)	6075(1)	12016(1)	81(1)

Table 3. Bond lengths [Å] and angles [°] for a17991.

C(1)-C(7)	1.364(4)
C(1)-C(2)	1.376(4)
C(1)-S(1)	1.750(3)
C(2)-C(3)	1.376(4)
C(2)-H(2)	0.9300
C(3)-C(4)	1.368(4)
C(3)-H(3)	0.9300
C(4)-C(6)	1.374(4)
C(4)-C(5)	1.507(4)
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(6)-C(7)	1.374(4)
C(6)-H(6)	0.9300
C(7)-H(7)	0.9300
C(8)-C(9)	1.384(4)
C(8)-C(13)	1.397(3)
C(8)-N(1)	1.418(3)
C(9)-C(10)	1.368(5)
C(9)-H(9)	0.9300
C(10)-C(11)	1.390(5)
C(10)-H(10)	0.9300
C(11)-C(12)	1.367(4)
C(11)-H(11)	0.9300
C(12)-C(13)	1.390(4)
C(12)-H(12)	0.9300
C(13)-C(14)	1.429(4)
C(14)-C(16)	1.357(4)
C(14)-C(15)	1.421(4)
C(15)-N(2)	1.131(4)
C(16)-N(1)	1.409(3)
C(16)-C(17)	1.502(4)
C(17)-C(18)	1.478(5)
C(17)-H(17A)	0.9700

C(17)-H(17B)	0.9700
C(18)-C(19)	1.200(5)
C(18)-H(18)	0.9300
C(19)-H(19A)	0.9300
C(19)-H(19B)	0.9300
N(1)-S(1)	1.693(2)
O(1)-S(1)	1.429(2)
O(2)-S(1)	1.414(2)

C(7)-C(1)-C(2)	119.8(3)
C(7)-C(1)-S(1)	120.5(2)
C(2)-C(1)-S(1)	119.7(2)
C(3)-C(2)-C(1)	119.6(3)
C(3)-C(2)-H(2)	120.2
C(1)-C(2)-H(2)	120.2
C(4)-C(3)-C(2)	121.7(3)
C(4)-C(3)-H(3)	119.1
C(2)-C(3)-H(3)	119.1
C(3)-C(4)-C(6)	117.2(3)
C(3)-C(4)-C(5)	121.1(3)
C(6)-C(4)-C(5)	121.7(3)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(7)-C(6)-C(4)	122.4(3)
C(7)-C(6)-H(6)	118.8
C(4)-C(6)-H(6)	118.8
C(1)-C(7)-C(6)	119.2(3)
C(1)-C(7)-H(7)	120.4
C(6)-C(7)-H(7)	120.4
C(9)-C(8)-C(13)	121.1(3)
C(9)-C(8)-N(1)	131.9(2)
C(13)-C(8)-N(1)	107.0(2)

C(10)-C(9)-C(8)	117.6(3)
C(10)-C(9)-H(9)	121.2
C(8)-C(9)-H(9)	121.2
C(9)-C(10)-C(11)	122.1(3)
C(9)-C(10)-H(10)	119.0
C(11)-C(10)-H(10)	119.0
C(12)-C(11)-C(10)	120.3(3)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	118.9(3)
C(11)-C(12)-H(12)	120.6
C(13)-C(12)-H(12)	120.6
C(12)-C(13)-C(8)	119.9(3)
C(12)-C(13)-C(14)	133.2(3)
C(8)-C(13)-C(14)	106.8(2)
C(16)-C(14)-C(15)	123.8(3)
C(16)-C(14)-C(13)	110.1(2)
C(15)-C(14)-C(13)	126.1(3)
N(2)-C(15)-C(14)	179.7(4)
C(14)-C(16)-N(1)	107.1(3)
C(14)-C(16)-C(17)	125.9(3)
N(1)-C(16)-C(17)	127.0(3)
C(18)-C(17)-C(16)	115.8(3)
C(18)-C(17)-H(17A)	108.3
C(16)-C(17)-H(17A)	108.3
C(18)-C(17)-H(17B)	108.3
C(16)-C(17)-H(17B)	108.3
H(17A)-C(17)-H(17B)	107.4
C(19)-C(18)-C(17)	130.6(4)
C(19)-C(18)-H(18)	114.7
C(17)-C(18)-H(18)	114.7
C(18)-C(19)-H(19A)	120.0
C(18)-C(19)-H(19B)	120.0
H(19A)-C(19)-H(19B)	120.0
C(16)-N(1)-C(8)	108.9(2)
C(16)-N(1)-S(1)	126.6(2)

C(8)-N(1)-S(1)	123.25(18)
O(2)-S(1)-O(1)	120.66(15)
O(2)-S(1)-N(1)	104.81(13)
O(1)-S(1)-N(1)	106.39(14)
O(2)-S(1)-C(1)	109.19(14)
O(1)-S(1)-C(1)	109.66(14)
N(1)-S(1)-C(1)	104.88(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for a17991. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	68(2)	68(2)	60(2)	0(1)	25(1)	1(1)
C(2)	86(2)	85(2)	88(2)	-14(2)	-5(2)	3(2)
C(3)	94(2)	63(2)	106(2)	-14(2)	10(2)	-2(2)
C(4)	70(2)	72(2)	73(2)	-3(1)	25(2)	7(1)
C(5)	102(2)	81(2)	113(3)	5(2)	30(2)	24(2)
C(6)	71(2)	84(2)	111(3)	-16(2)	-1(2)	10(2)
C(7)	70(2)	65(2)	116(3)	-14(2)	15(2)	-3(1)
C(8)	70(2)	51(1)	67(2)	12(1)	20(1)	9(1)
C(9)	78(2)	66(2)	93(2)	7(2)	28(2)	1(1)
C(10)	85(2)	72(2)	112(3)	-3(2)	7(2)	-8(2)
C(11)	112(3)	74(2)	79(2)	-9(2)	8(2)	1(2)
C(12)	95(2)	70(2)	75(2)	2(2)	27(2)	7(2)
C(13)	75(2)	51(1)	63(2)	7(1)	22(1)	12(1)
C(14)	64(2)	57(1)	72(2)	9(1)	20(1)	7(1)
C(15)	81(2)	80(2)	96(2)	0(2)	32(2)	-1(2)
C(16)	71(2)	61(2)	66(2)	11(1)	12(1)	10(1)
C(17)	92(2)	98(2)	81(2)	5(2)	2(2)	-1(2)
C(18)	116(3)	107(3)	96(3)	-8(2)	5(2)	-2(2)
C(19)	195(5)	108(3)	104(3)	13(3)	17(3)	14(3)
N(1)	79(2)	63(1)	59(1)	9(1)	21(1)	11(1)
N(2)	98(2)	135(3)	149(3)	-6(2)	58(2)	-17(2)
O(1)	142(2)	128(2)	50(1)	14(1)	10(1)	39(2)
O(2)	150(2)	79(1)	112(2)	26(1)	78(2)	4(1)
S(1)	109(1)	78(1)	63(1)	18(1)	37(1)	17(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for a17991.

	x	y	z	U(eq)
H(2)	3406	7388	12584	106
H(3)	2189	8309	11733	106
H(5A)	-1089	8398	9072	146
H(5B)	387	8765	9258	146
H(5C)	-483	8734	10654	146
H(6)	-832	7277	9163	108
H(7)	351	6348	10005	100
H(9)	1158	5278	9438	93
H(10)	575	4867	6964	109
H(11)	2184	4898	5220	107
H(12)	4441	5341	5929	94
H(17A)	6138	6273	12583	110
H(17B)	7276	6228	11453	110
H(18)	6952	7297	12289	129
H(19A)	5164	7299	9628	164
H(19B)	5909	7900	10608	164