

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

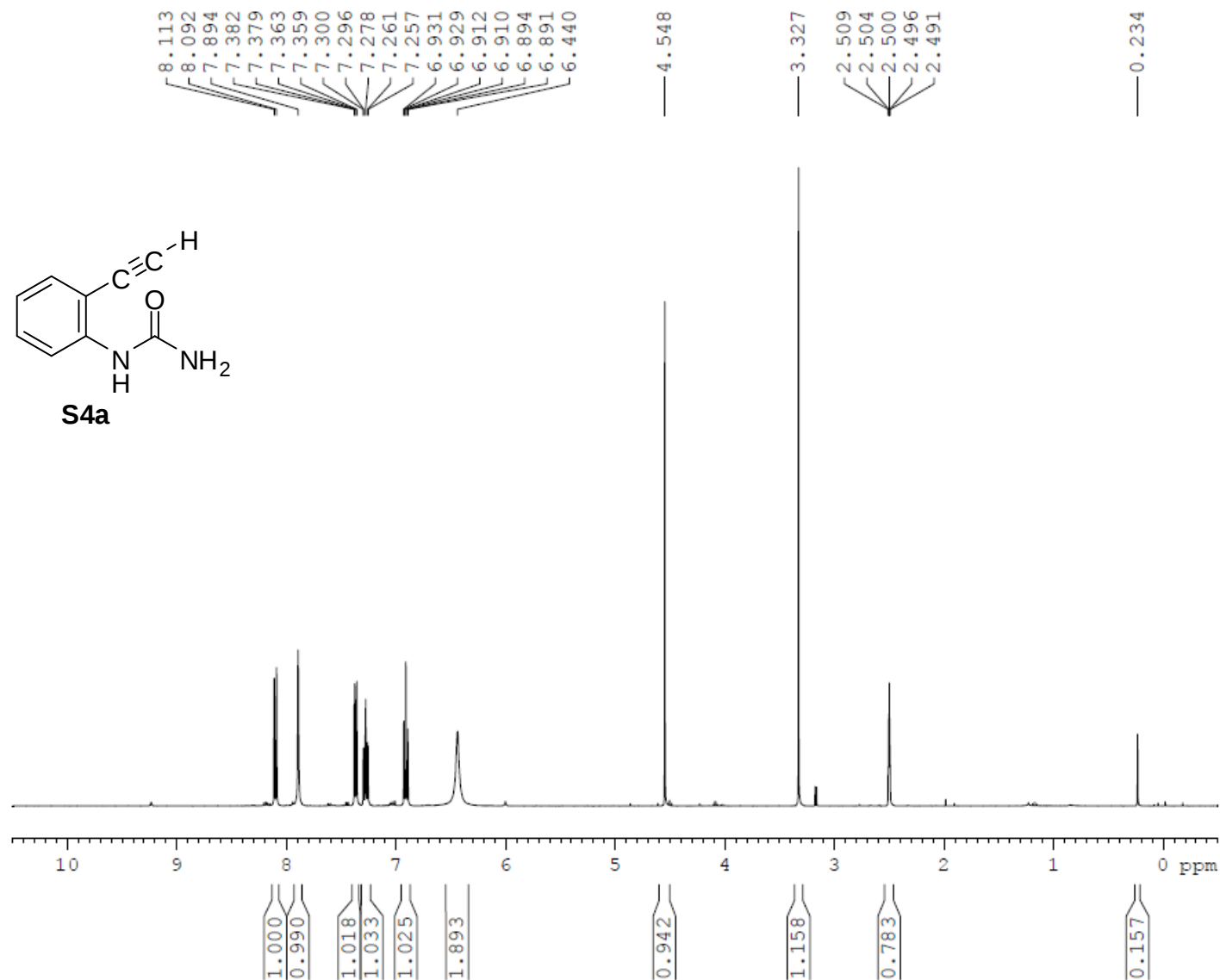
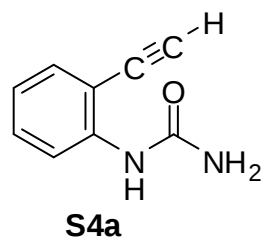
Zhen-Yuan Liao, Pen-Yuan Liao, and Tun-Cheng Chien*

Department of Chemistry, National Taiwan Normal University, Taipei 11677, Taiwan

tcchien@ntnu.edu.tw

compound #	content	page #	compound #	content	page #
Schemes S1 & S2:			8b	¹ H NMR	43
S4a	¹ H NMR	3		¹³ C NMR	44
	¹³ C NMR	4	8c	¹ H NMR	45
S4b	¹ H NMR	5		¹³ C NMR	46
	¹³ C NMR	6	8d	¹ H NMR	47
S4c	¹ H NMR	7		¹³ C NMR	48
	¹³ C NMR	8	8e	¹ H NMR	49
S4d	¹ H NMR	9		¹³ C NMR	50
	¹³ C NMR	10	8f	¹ H NMR	51
S4e	¹ H NMR	11		¹³ C NMR	52
	¹³ C NMR	12	8g	¹ H NMR	53
S4f	¹ H NMR	13		¹³ C NMR	54
	¹³ C NMR	14	8h	¹ H NMR	55
S4h	¹ H NMR	15		¹³ C NMR	56
	¹³ C NMR	16	8i	¹ H NMR	57
S4i	¹ H NMR	17		¹³ C NMR	58
	¹³ C NMR	18	8j	¹ H NMR	59
S4j	¹ H NMR	19		¹³ C NMR	60
	¹³ C NMR	20	8k	¹ H NMR	61
S4k	¹ H NMR	21		¹³ C NMR	62
	¹³ C NMR	22	8l	¹ H NMR	63
S4l	¹ H NMR	23		¹³ C NMR	64
	¹³ C NMR	24	8m	¹ H NMR	65
S4m	¹ H NMR	25		¹³ C NMR	66
	¹³ C NMR	26	8n	¹ H NMR	67
S4p	¹ H NMR	27		¹³ C NMR	68
	¹³ C NMR	28	8o	¹ H NMR	69
S5g	¹ H NMR	29		¹³ C NMR	70
	¹³ C NMR	30	8p	¹ H NMR	71
S5n	¹ H NMR	31		¹³ C NMR	72
	¹³ C NMR	32	Schemes S3-S6:		
S5o	¹ H NMR	33	S8	¹ H NMR	73
	¹³ C NMR	34		¹³ C NMR	74
7g	¹ H NMR	35	2	¹ H NMR	75
	¹³ C NMR	36		¹³ C NMR	76
7n	¹ H NMR	37	S12	¹ H NMR	77
	¹³ C NMR	38		¹³ C NMR	78
7o	¹ H NMR	39	12a	¹ H NMR	79
	¹³ C NMR	40		¹³ C NMR	80
8a	¹ H NMR	41	12b	¹ H NMR	81
	¹³ C NMR	42			

12c	¹³ C NMR	82	13j	¹ H NMR	131
	¹ H NMR	83		¹³ C NMR	132
12d	¹³ C NMR	84	14	¹ H NMR	133
	¹ H NMR	85		¹³ C NMR	134
12e	¹³ C NMR	86	15	¹ H NMR	135
	¹ H NMR	87		¹³ C NMR	136
	¹³ C NMR	88			
12f	¹ H NMR	89	Scheme 5:		
	¹³ C NMR	90	10a	¹ H NMR	137
12g	¹ H NMR	91		¹³ C NMR	138
	¹³ C NMR	92		ORTEP projection	139
12h	¹ H NMR	93		Crystal data	140~146
	¹³ C NMR	94	10b	¹ H NMR	147
12i	¹ H NMR	95		¹³ C NMR	148
	¹³ C NMR	96	10c	¹ H NMR	149
12j	¹ H NMR	97		¹³ C NMR	150
	¹³ C NMR	98	10d	¹ H NMR	151
7a	¹ H NMR	99		¹³ C NMR	152
	¹³ C NMR	100	10e	¹ H NMR	153
Scheme S7:				¹³ C NMR	154
S14	¹ H NMR	101	10f	¹ H NMR	155
	¹³ C NMR	102		¹³ C NMR	156
16	¹ H NMR	103	10g	¹ H NMR	157
	¹³ C NMR	104		¹³ C NMR	158
Scheme S8:			10h	¹ H NMR	159
S16a	¹ H NMR	105		¹³ C NMR	160
	¹³ C NMR	106	10i	¹ H NMR	161
S16b	¹ H NMR	107		¹³ C NMR	162
	¹³ C NMR	108	10j	¹ H NMR	163
6a	¹ H NMR	109		¹³ C NMR	164
	¹³ C NMR	110	10k	¹ H NMR	165
6b	¹ H NMR	111		¹³ C NMR	166
	¹³ C NMR	112	10l	¹ H NMR	167
Scheme 3(A):				¹³ C NMR	168
9	¹ H NMR	113	10m	¹ H NMR	169
	¹³ C NMR	114		¹³ C NMR	170
	ORTEP projection	115	10n	¹ H NMR	171
	Crystal data	116~122		¹³ C NMR	172
Scheme 4:			10o	¹ H NMR	173
13f	¹ H NMR	123		¹³ C NMR	174
	¹³ C NMR	124	10p	¹ H NMR	175
13g	¹ H NMR	125		¹³ C NMR	176
	¹³ C NMR	126	Scheme 7(E):		
13h	¹ H NMR	127	23	¹ H NMR	177
	¹³ C NMR	128		¹³ C NMR	178
13i	¹ H NMR	129		ORTEP projection	179
	¹³ C NMR	130		Crystal data	180~187

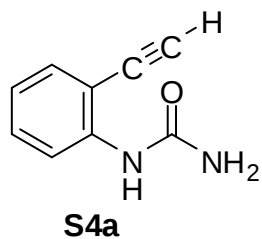


Current Data Parameters
 NAME S0001
 EXPNO 1
 PROCNO 1

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



155.57
141.69
132.23
129.39
121.12
118.95
109.91
86.91
79.65
40.14
39.93
39.72
39.51
39.30
39.09
38.88

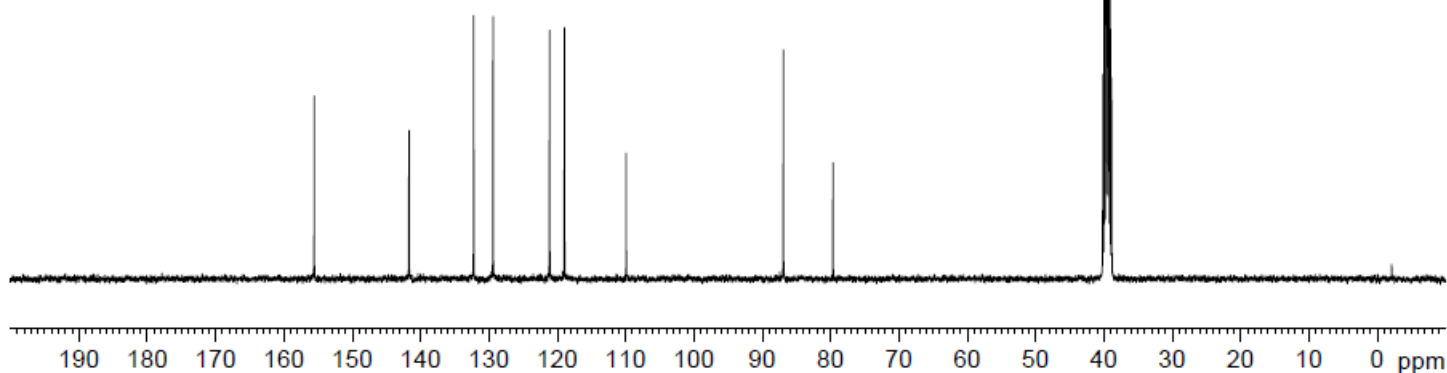
Current Data Parameters
NAME SO001
EXPNO 3
PROCNO 1

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

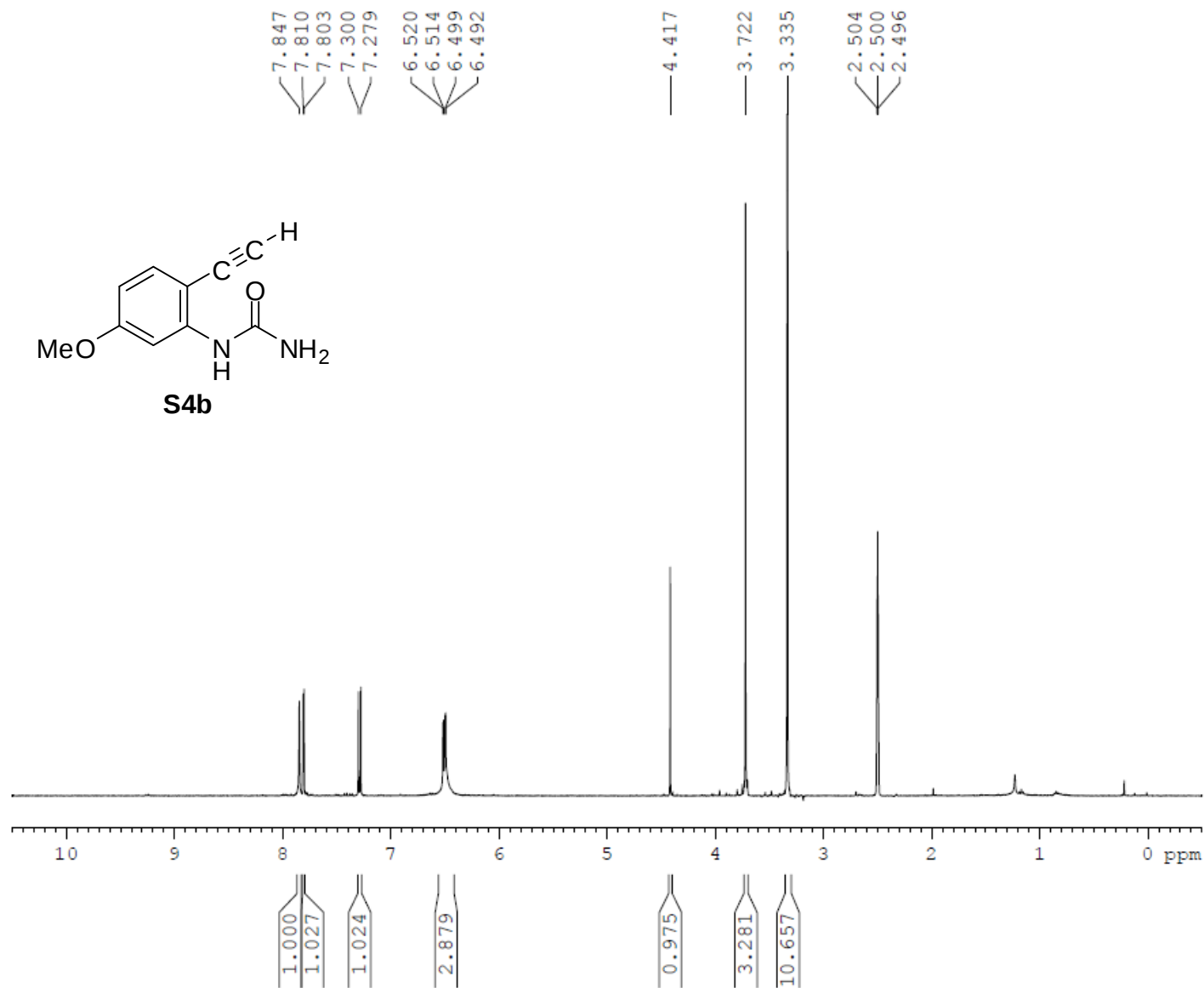
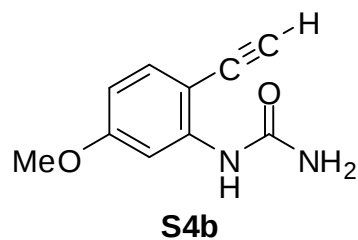
===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 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



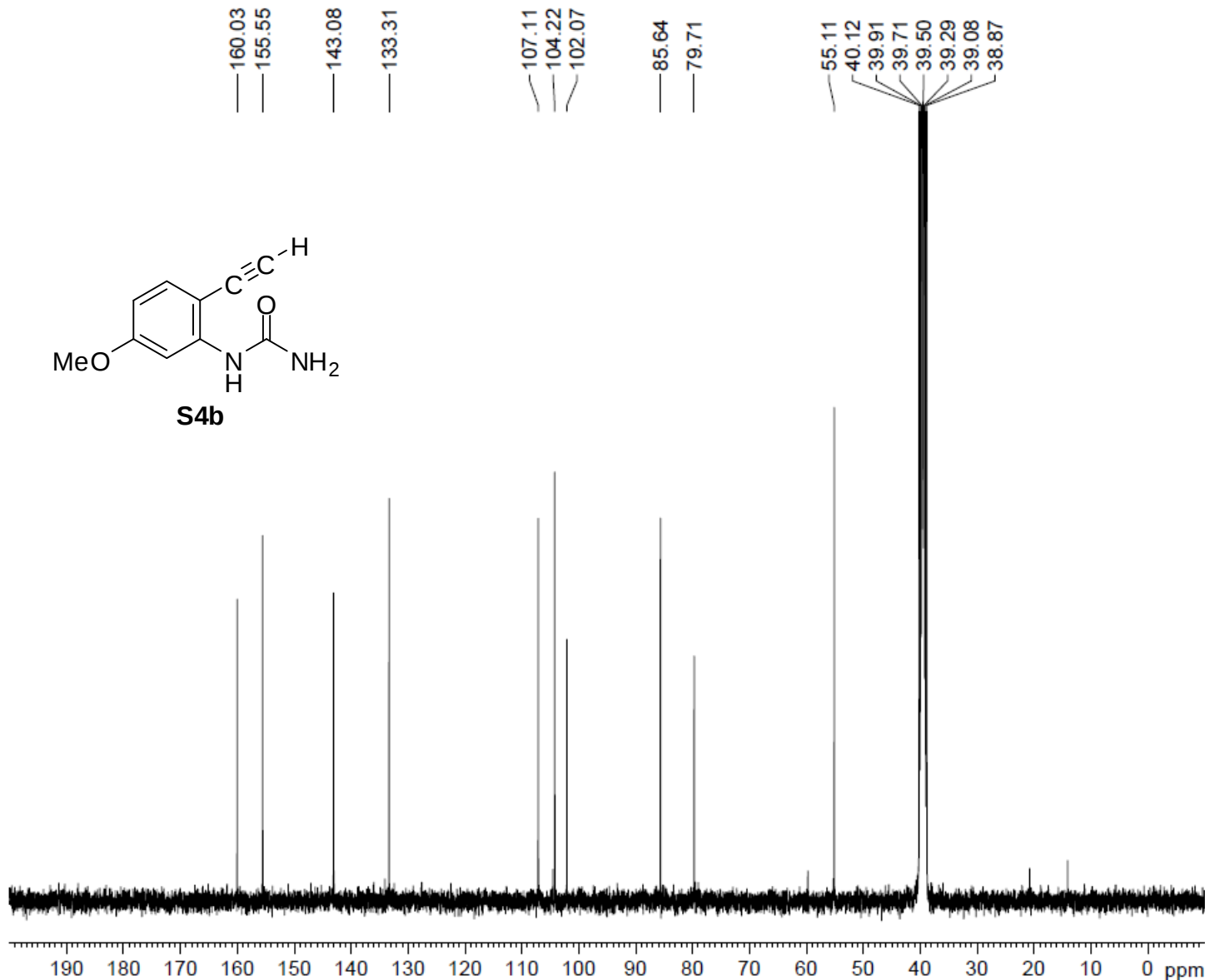
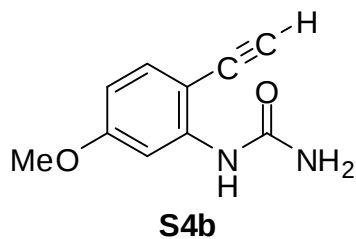
Current Data Parameters
 NAME SD-086
 EXPNO 3
 PROCNO 1

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



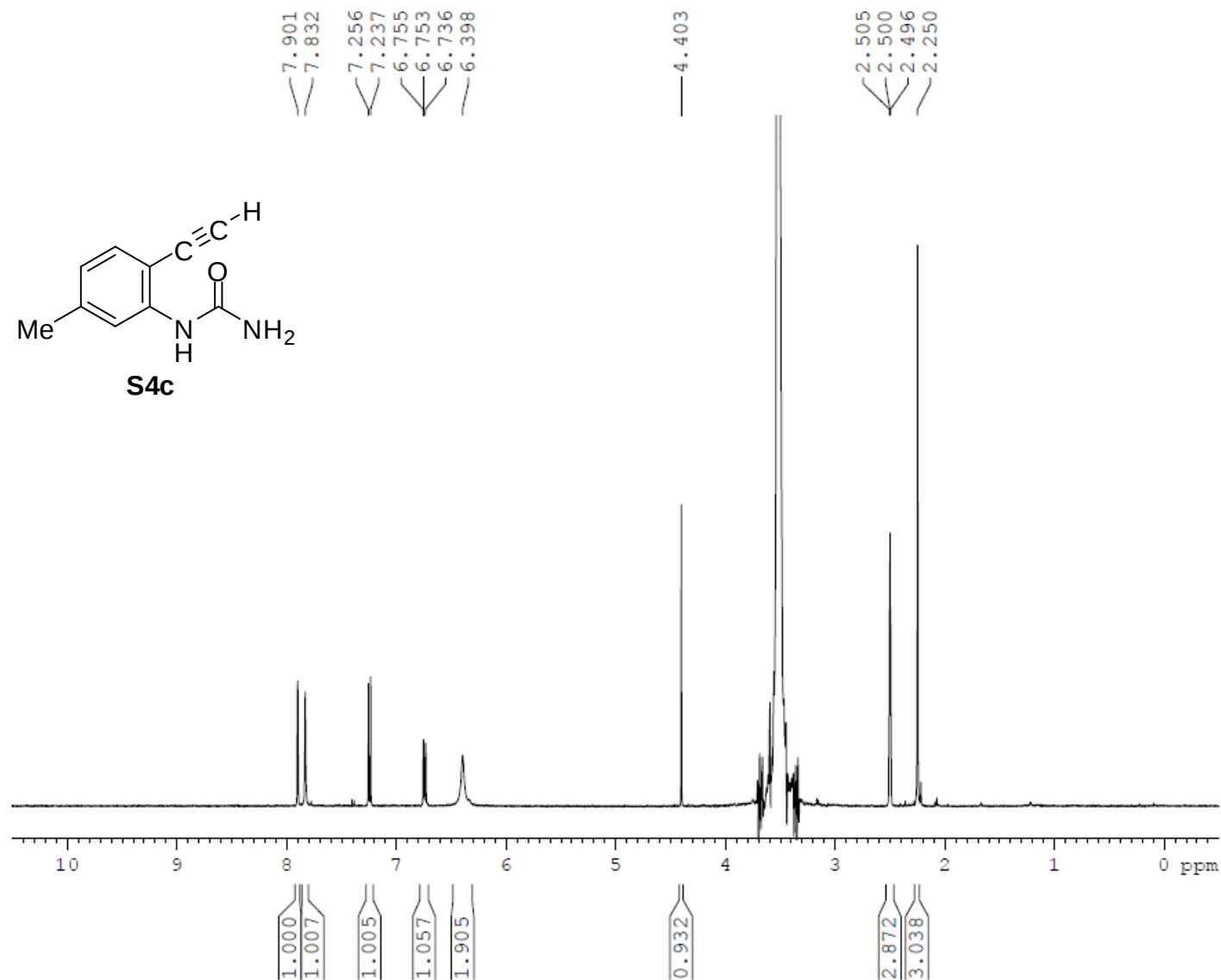
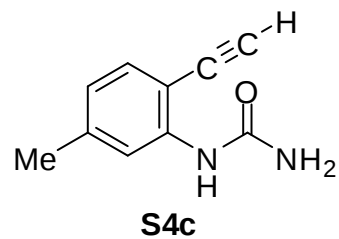
Current Data Parameters
NAME SD-086
EXPNO 7
PROCNO 1

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 =====
CPDPRG2 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

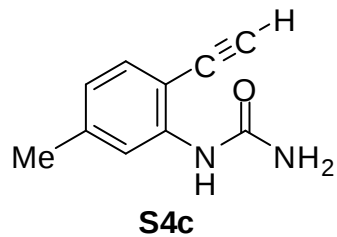


Current Data Parameters
 NAME SC156
 EXPNO 2
 PROCNO 1

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
 TDO 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



—155.89
 —141.61
 —139.48
 —132.23
 —122.40
 —119.71
 —107.48
 —86.35
 —79.99

40.14
 39.93
 39.72
 39.51
 39.30
 39.09
 38.88
 21.68

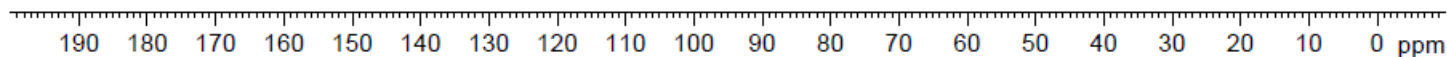
Current Data Parameters
 NAME SC156
 EXPNO 5
 PROCNO 1

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

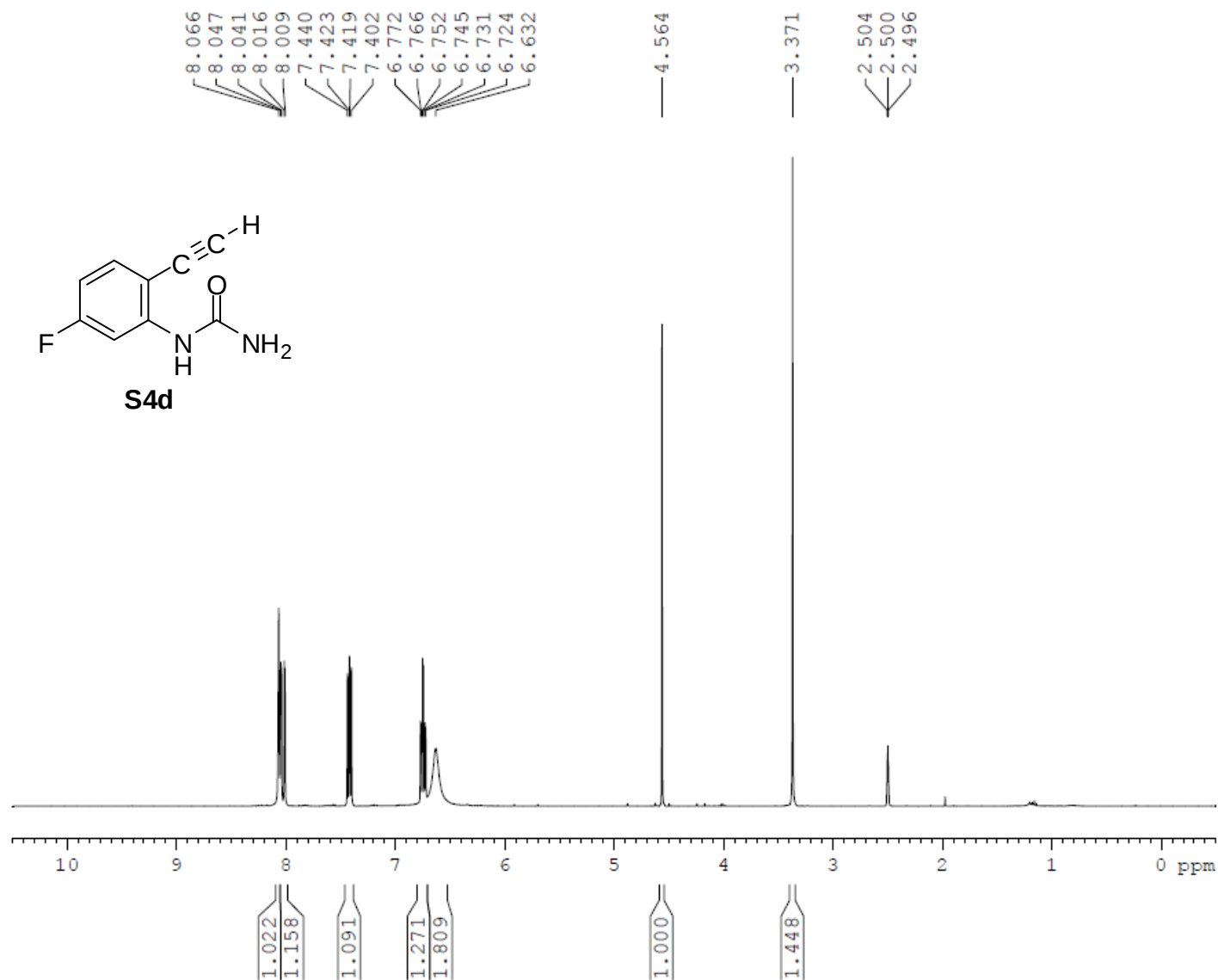
===== CHANNEL f1 =====
 SFO1 100.623319 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 46.00000000 W

===== 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

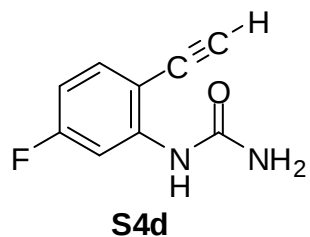
F2 - Acquisition Parameters
Date_ 20140529
Time 21.32
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 0
SWH 7246.377 Hz
FIDRES 0.221142 Hz
AQ 2.2609921 sec
RG 114
DW 69.000 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
TD0 1

===== 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

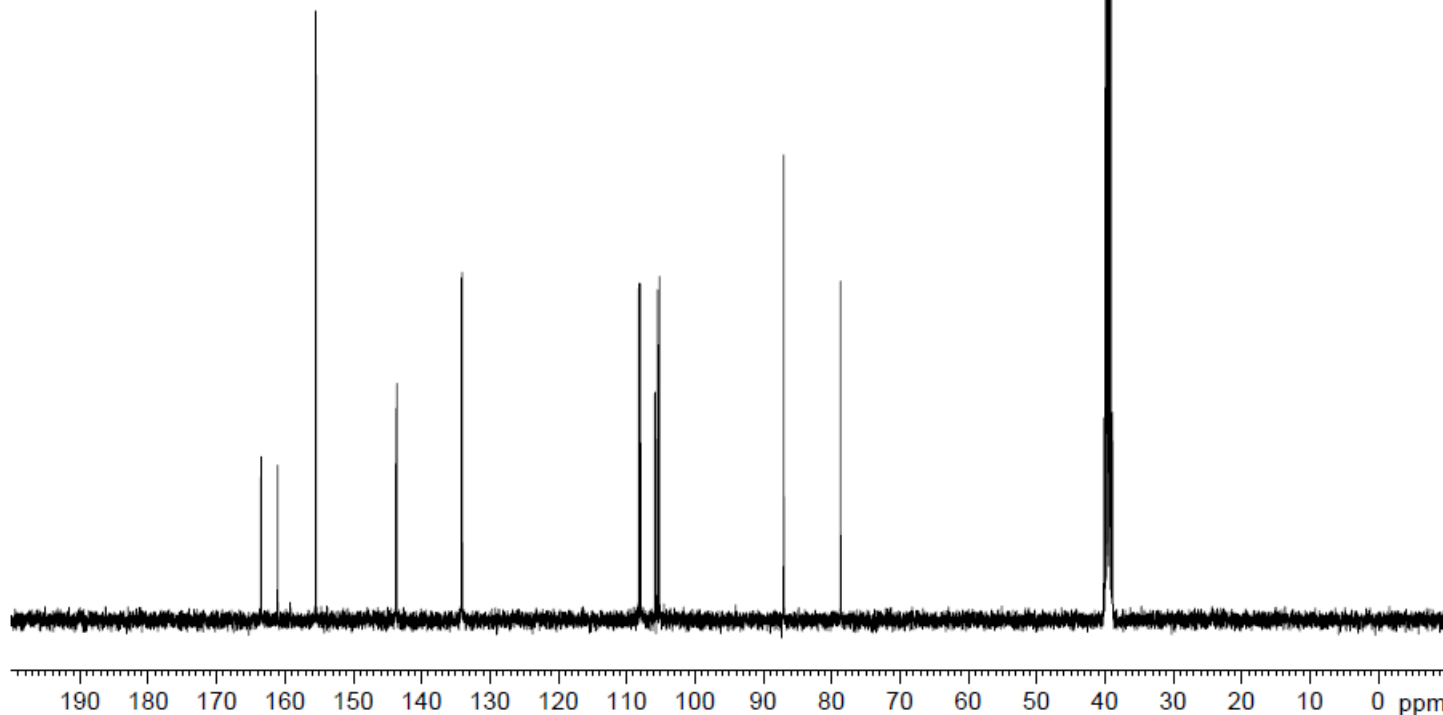


163.50
161.07
155.47
143.75
143.62
134.16
134.05

108.20
107.97
105.85
105.82
105.48
105.19

87.02
78.67

40.13
39.92
39.71
39.50
39.29
39.08
38.88



Current Data Parameters
NAME SD-078
EXPNO 5
PROCNO 1

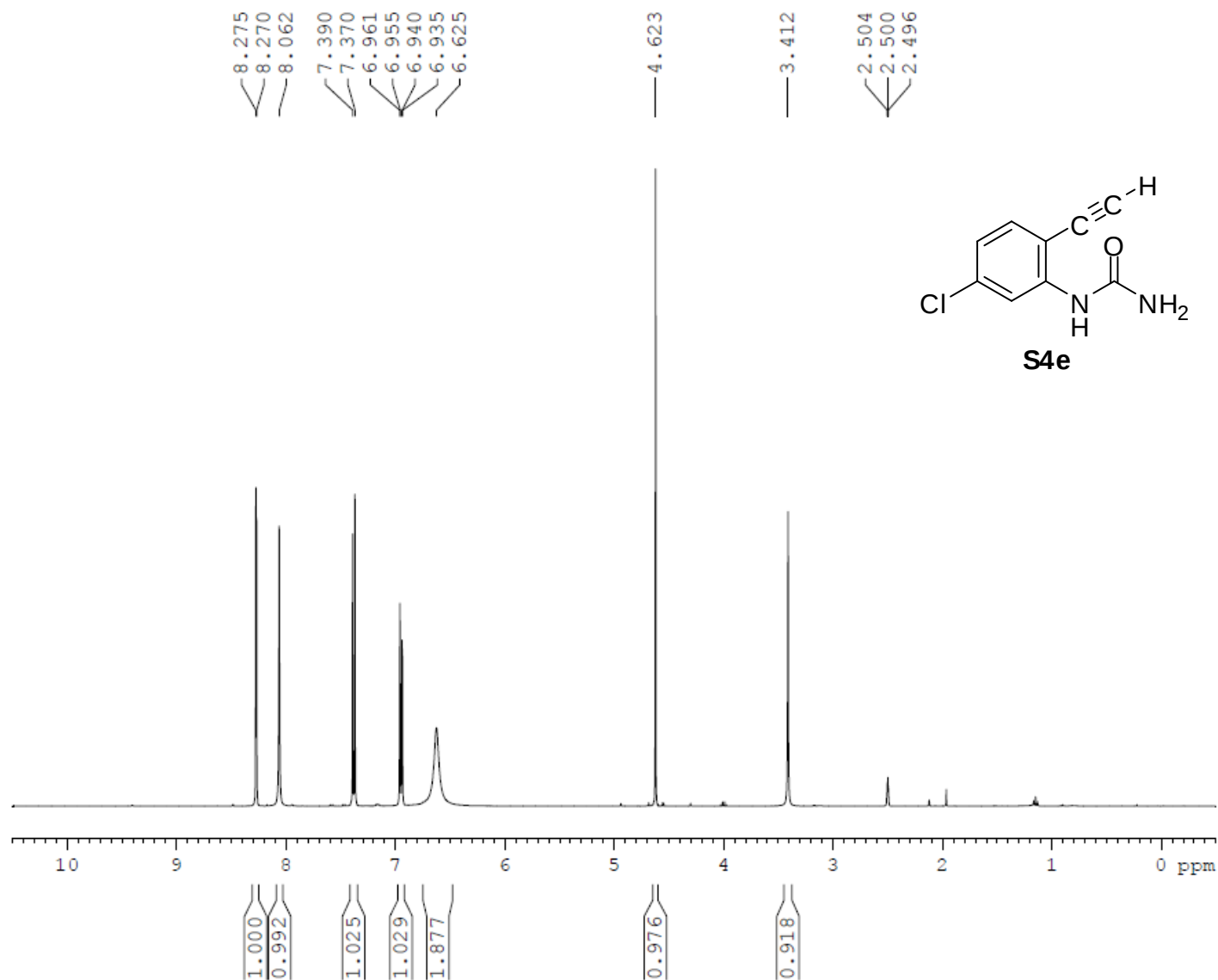
F2 - Acquisition Parameters
Date_ 20140529
Time 21.46
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 700
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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



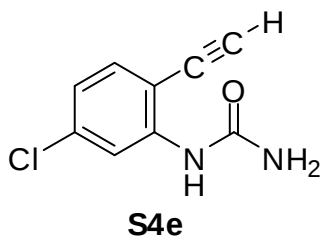
Current Data Parameters
 NAME SD-062(old)
 EXPNO 1
 PROCNO 1

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

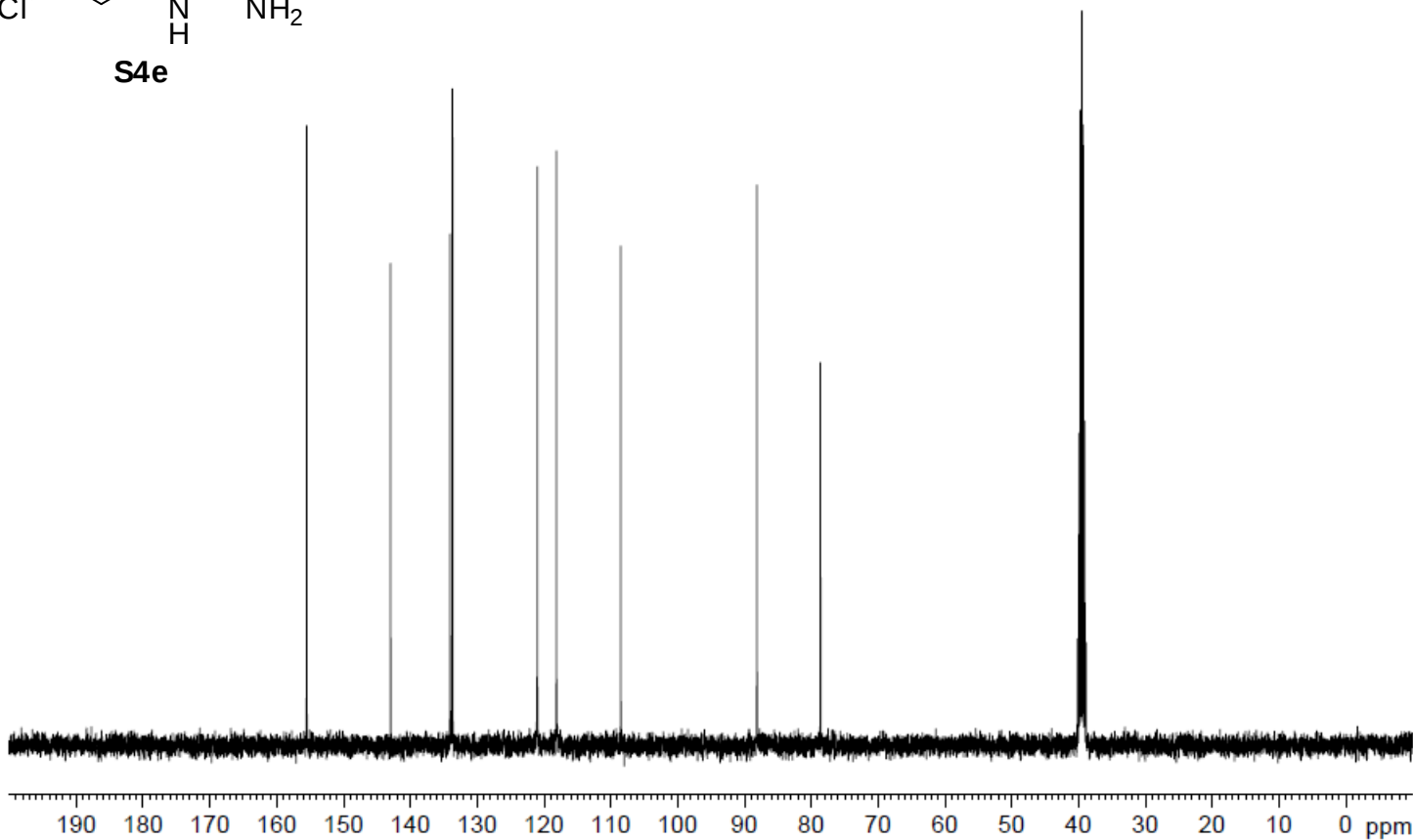
===== CHANNEL f1 =====
 NUC1 1H
 P1 11.00 usec
 PL1 -4.20 dB
 SFO1 400.1324008 MHz

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

pure



155.51
142.95
134.05
133.68
120.99
118.12
108.51
88.13
78.62
40.13
39.92
39.71
39.50
39.29
39.08
38.87



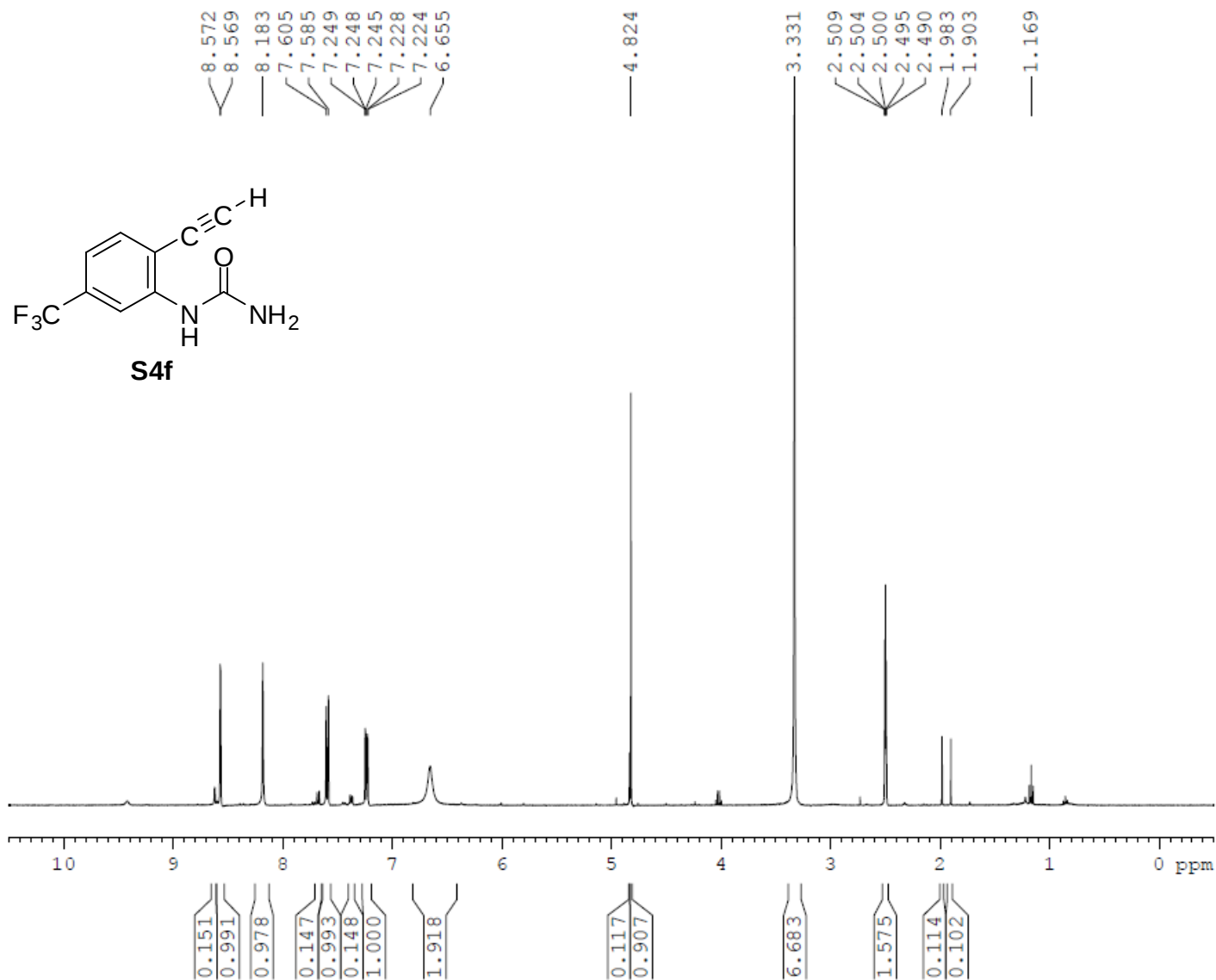
Current Data Parameters
NAME SD-062(old)
EXPNO 3
PROCNO 1

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 =====
CPDPRG2 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

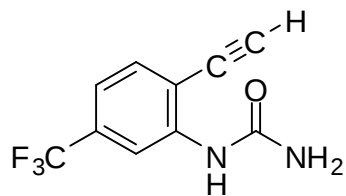


Current Data Parameters
 NAME SO150
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150908
 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
 TDO 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



S4f

155.48
142.36
133.31
129.55
129.24
125.26
122.55
117.26
117.22
114.69
114.65
113.36

89.68

78.26

40.14
39.93
39.72
39.51
39.30
39.09
38.88

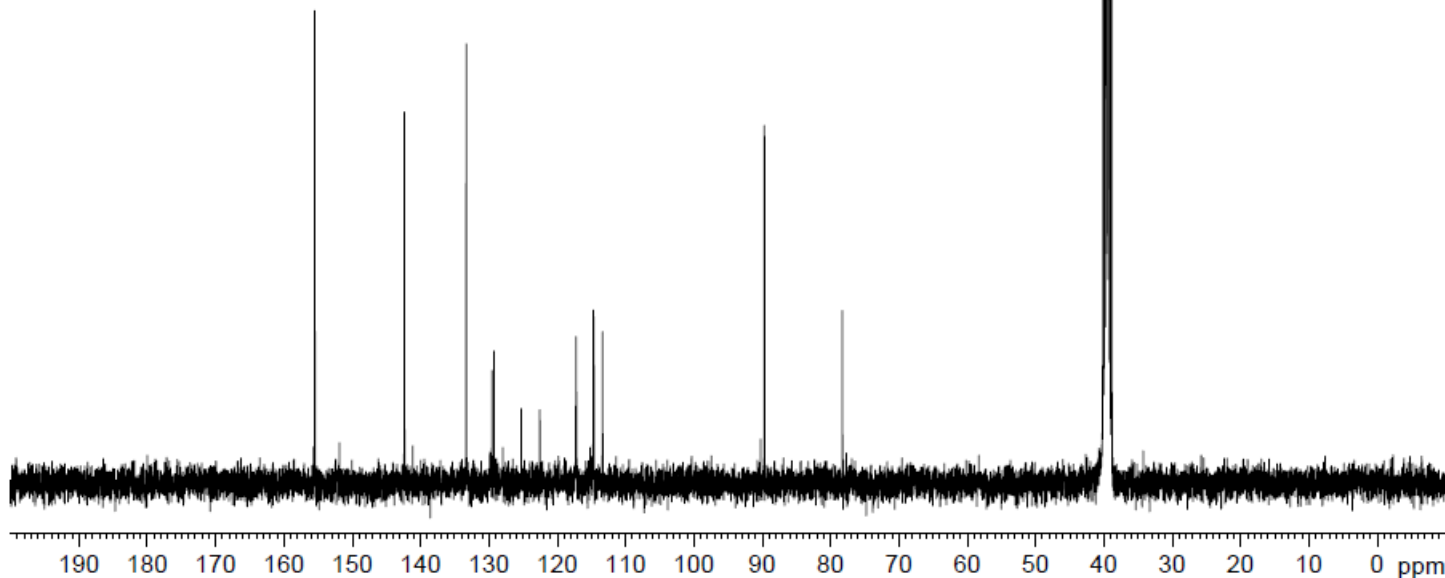
Current Data Parameters
NAME SO150
EXPNO 2
PROCNO 1

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

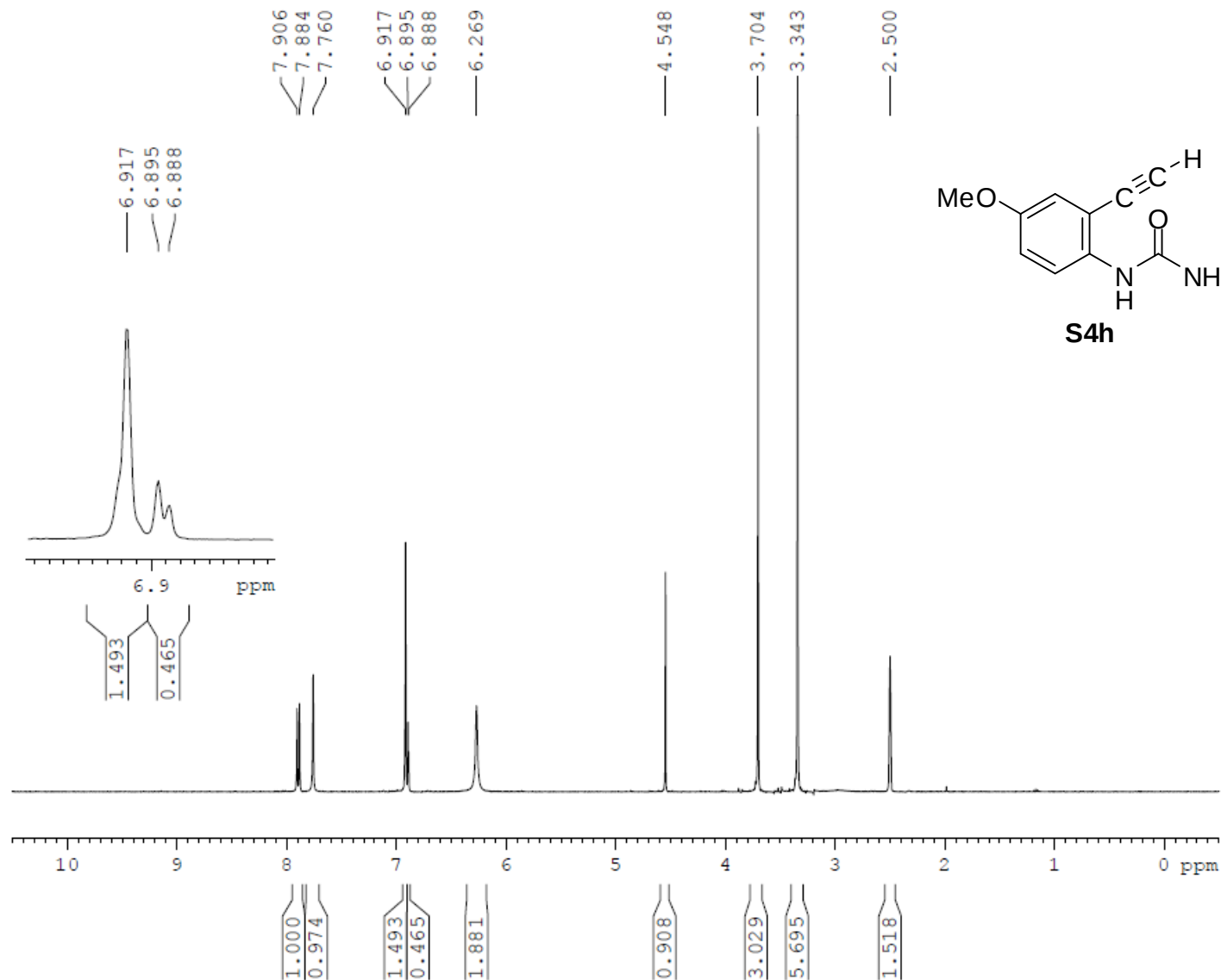
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 7.00 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG2 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



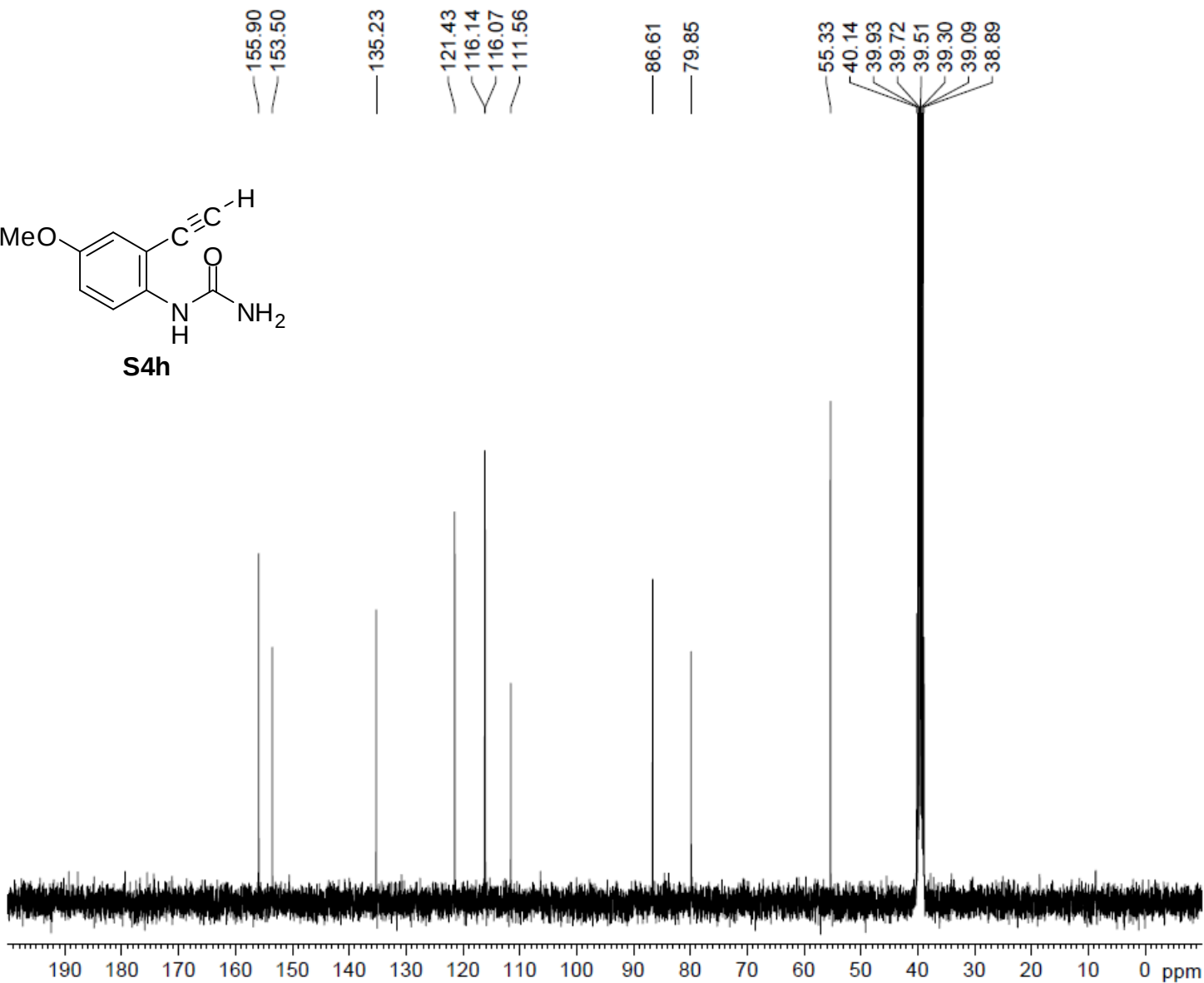
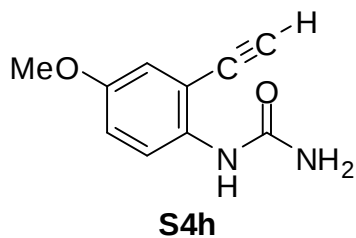
Current Data Parameters
 NAME SO067
 EXPNO 1
 PROCNO 1

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



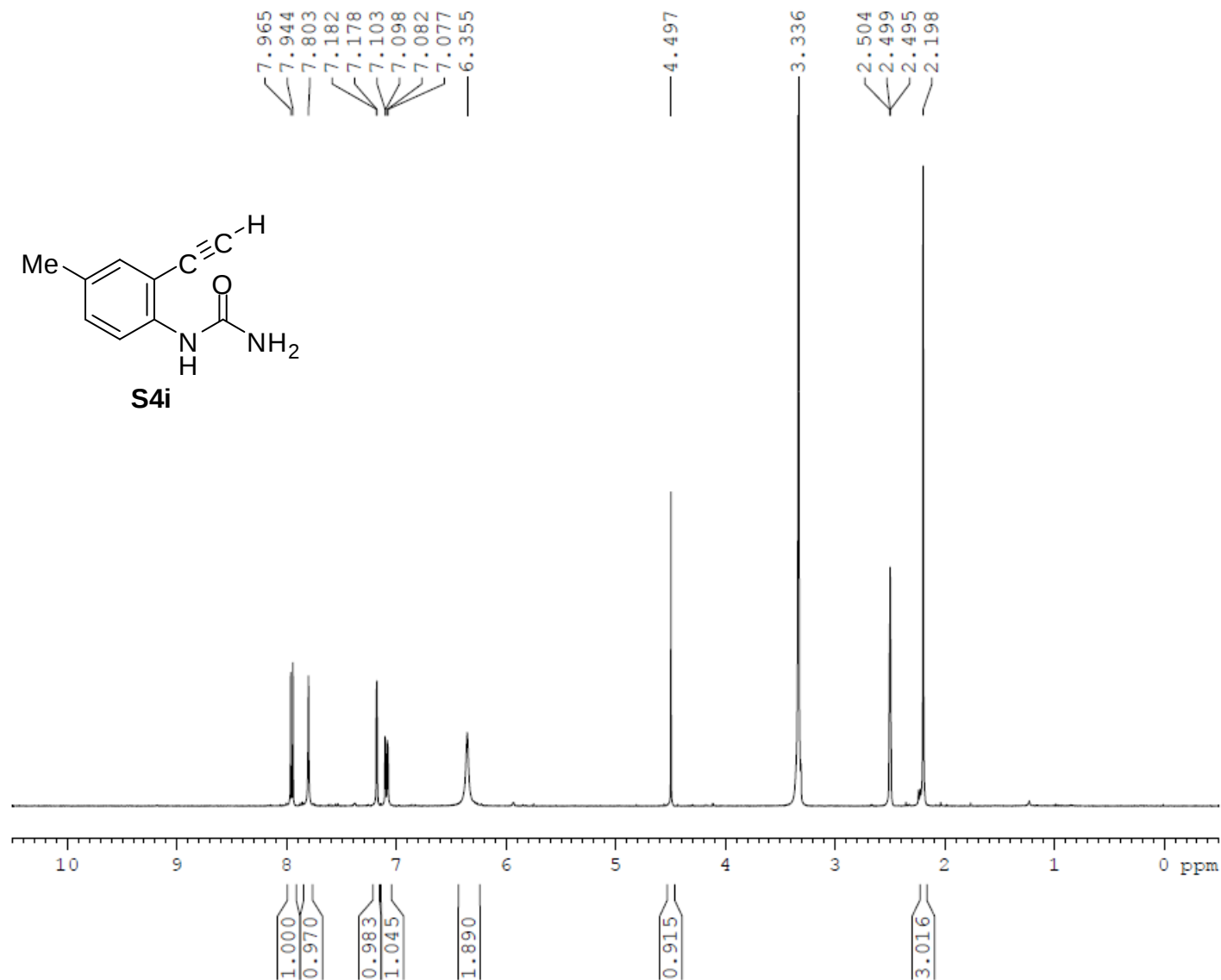
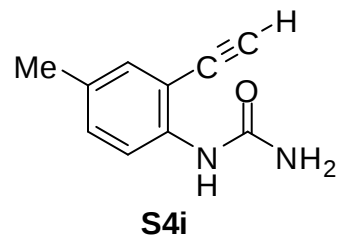
Current Data Parameters
NAME SO067
EXPNO 3
PROCNO 1

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 =====
CPDPRG2 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

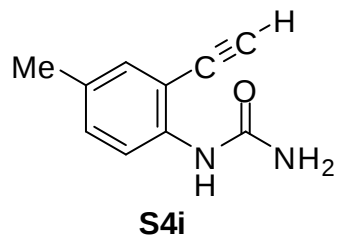


Current Data Parameters
 NAME SC111
 EXPNO 1
 PROCNO 1

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
 TDO 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



— 155.67
 — 139.28
 — 132.24
 — 130.11
 — 119.17
 — 109.97
 — 86.47
 — 79.85

40.14
 39.93
 39.72
 39.51
 39.30
 39.09
 38.89
 — 19.86

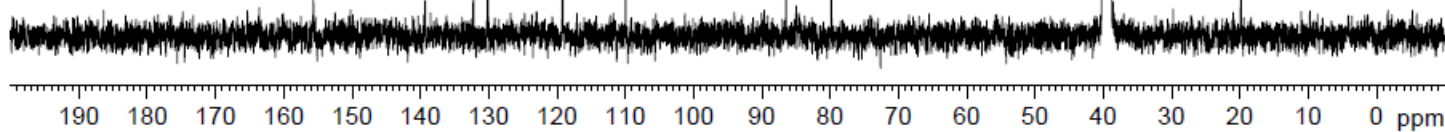
Current Data Parameters
 NAME SC111
 EXPNO 3
 PROCNO 1

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 100.623319 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



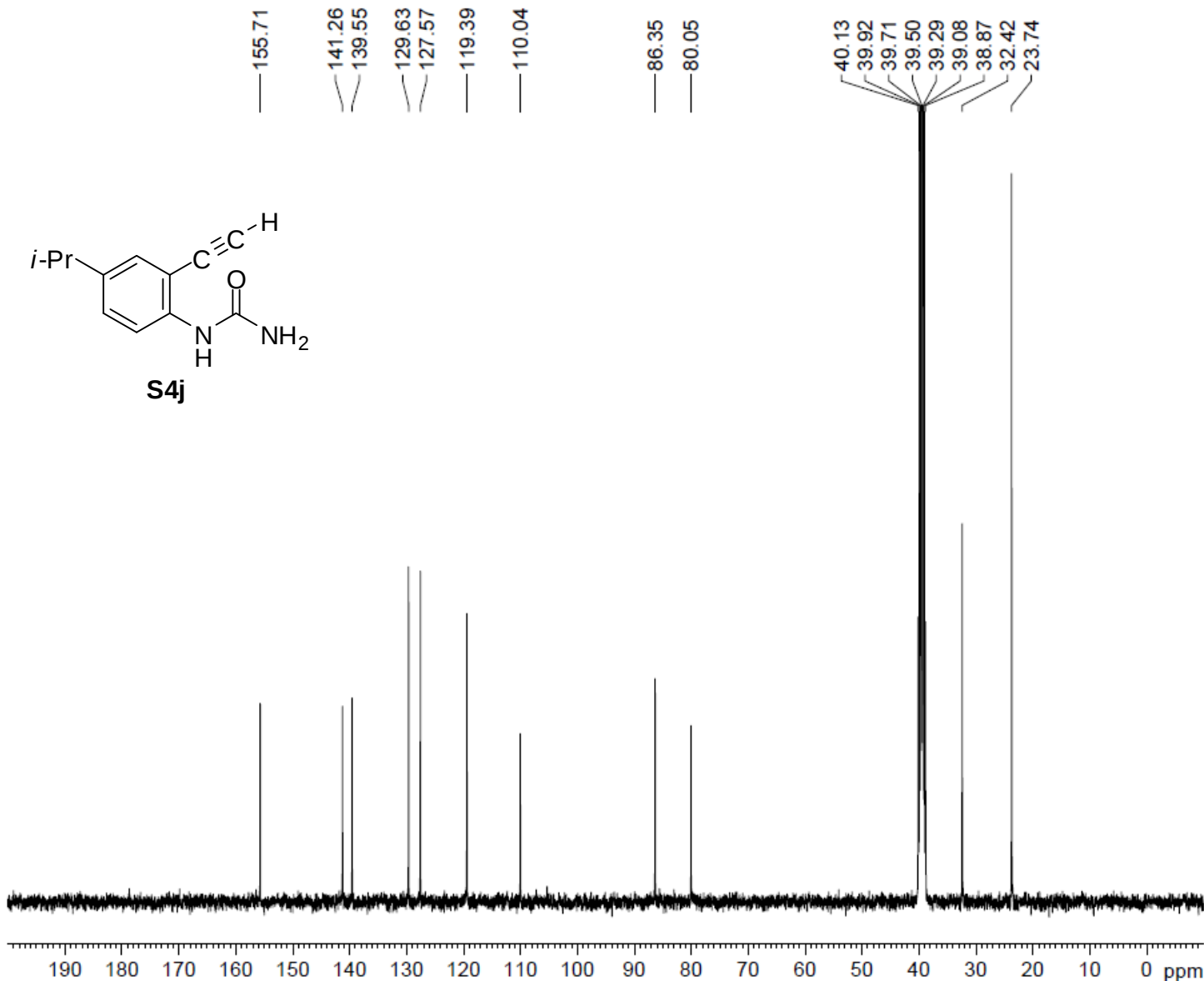
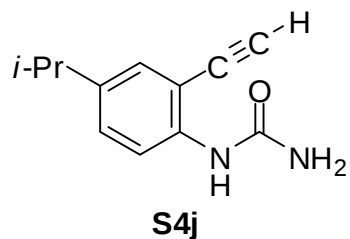
Current Data Parameters
 NAME SD-090(new)
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140819
 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



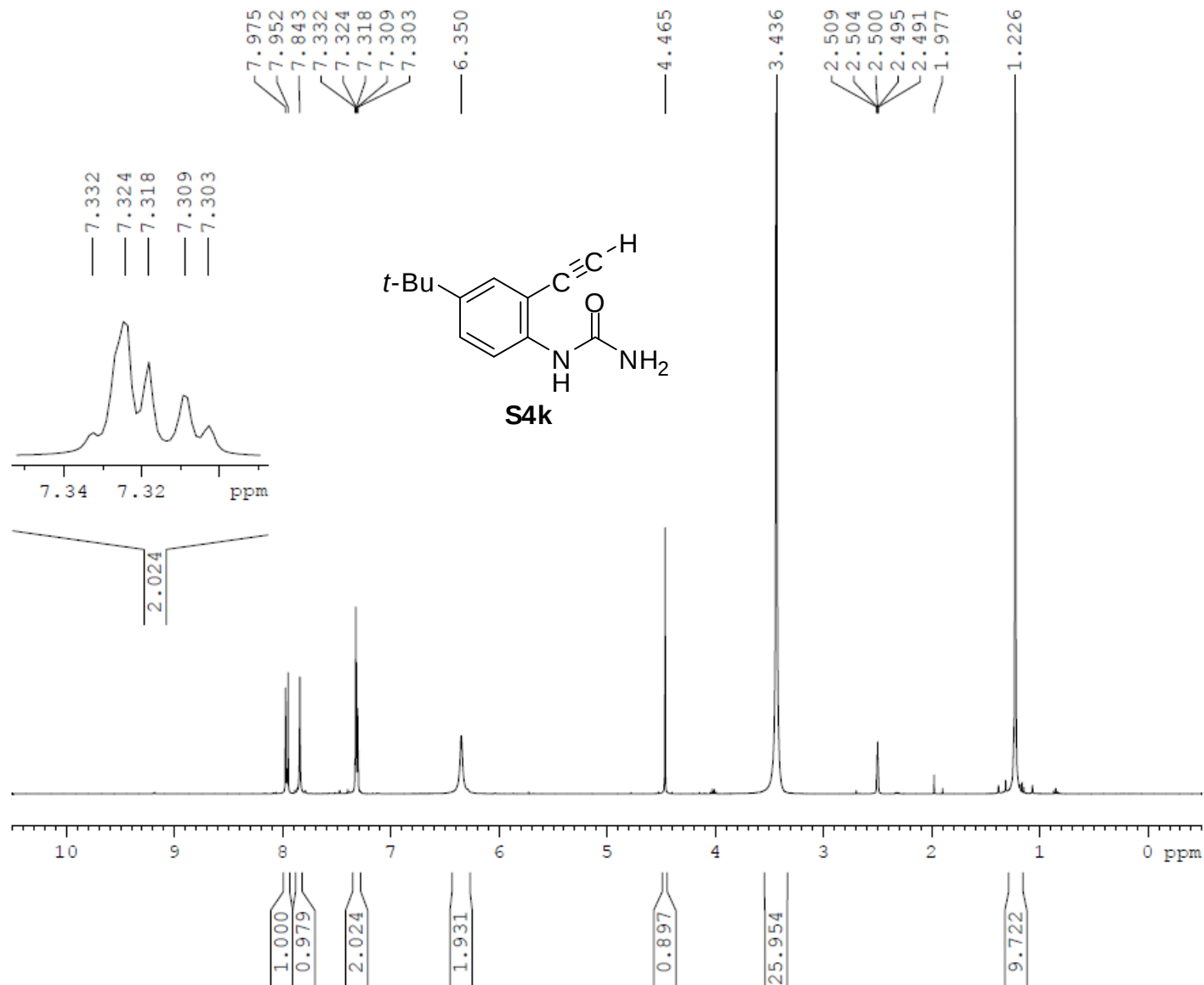
Current Data Parameters
NAME SD-090(new)
EXPNO 3
PROCNO 1

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
CPDPRG2 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

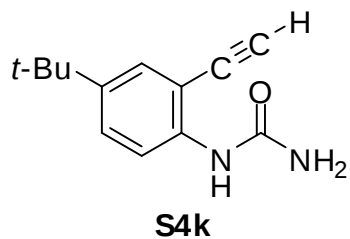


Current Data Parameters
 NAME SC155
 EXPNO 1
 PROCNO 1

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
 TDO 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



— 155.83
 — 143.68
 — 139.28
 — 128.59
 — 126.68
 — 119.27
 — 109.85

— 86.28
 — 80.30

40.14
 39.93
 39.72
 39.51
 39.30
 39.09
 38.88
 33.81
 31.04

Current Data Parameters
 NAME SC155
 EXPNO 3
 PROCNO 1

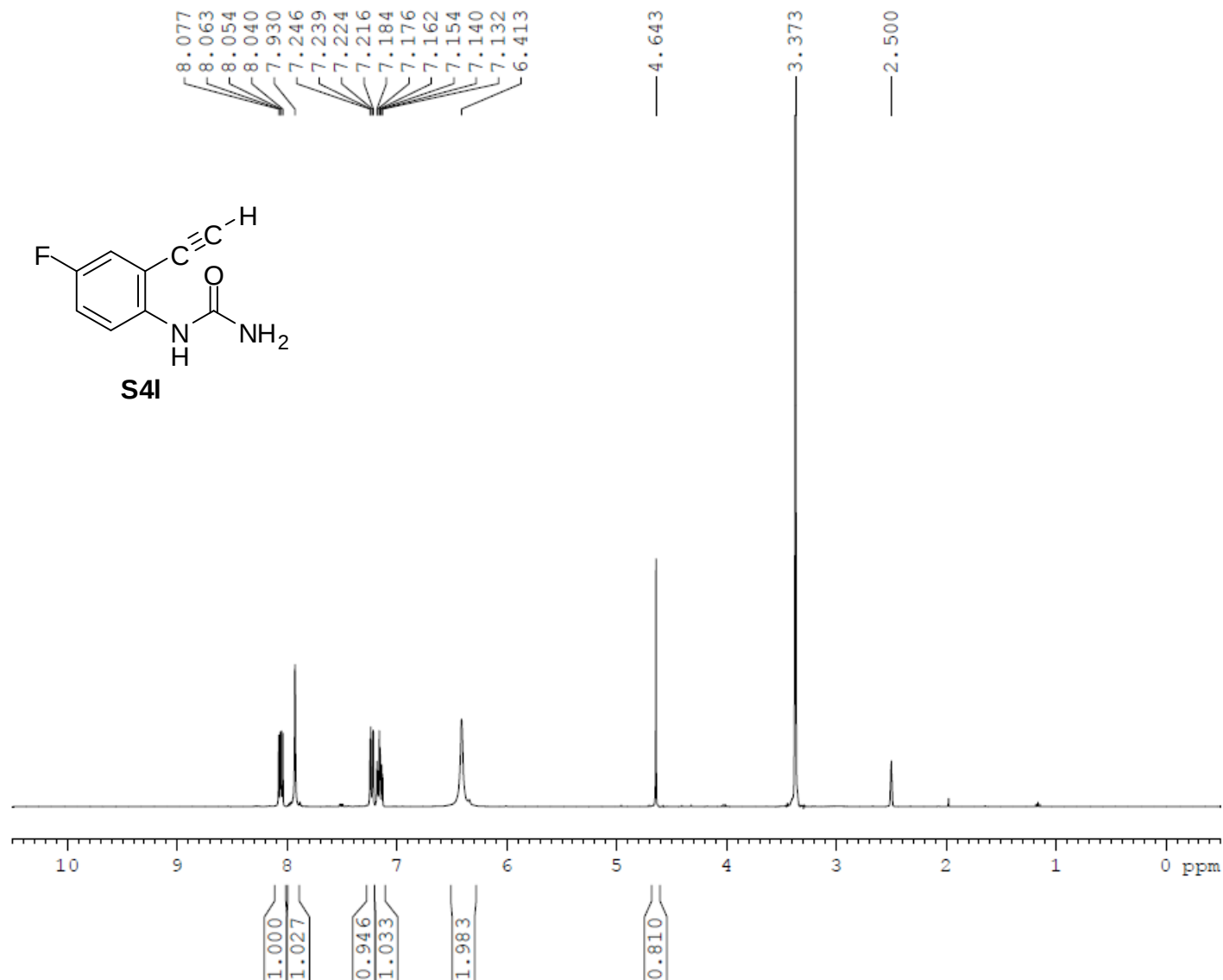
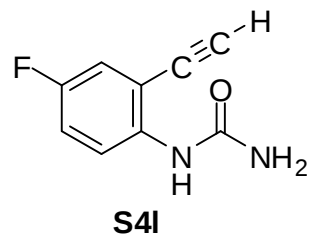
F2 - Acquisition Parameters
 Date_ 20140702
 Time 9.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT DMSO
 NS 1000
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

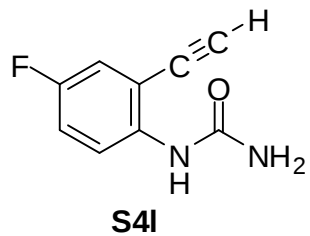


```

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
  
```



157.32
155.68
154.94

138.36
138.34

121.20
121.12

118.15
117.91

116.66
116.44

111.63
111.54

87.77

78.66
78.63

40.14
39.93
39.72
39.51
39.30
39.09
38.89

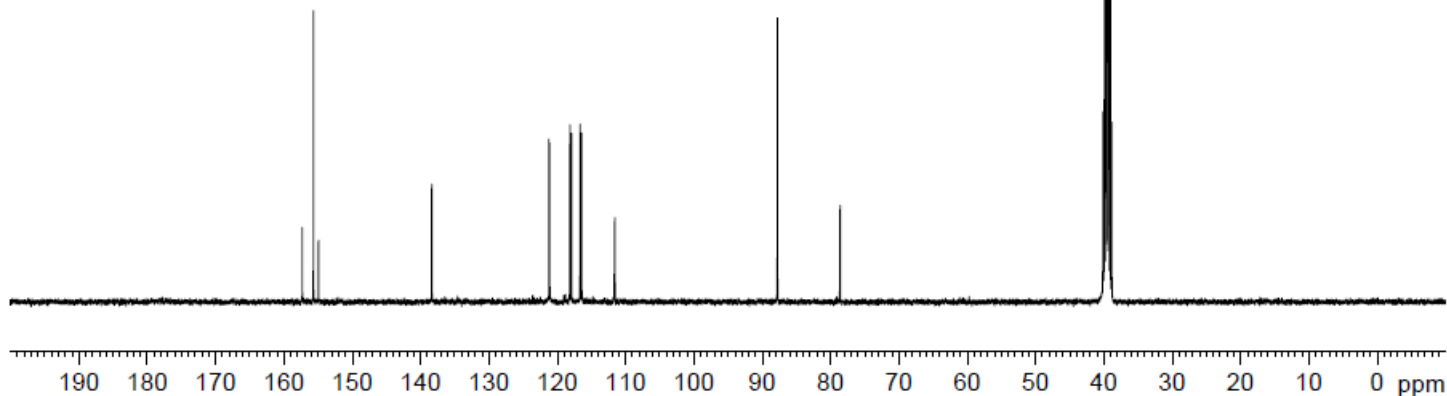
Current Data Parameters
NAME SC165
EXPNO 4
PROCNO 1

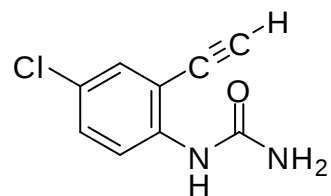
F2 - Acquisition Parameters
Date_ 20140801
Time 23.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1964
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 301.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

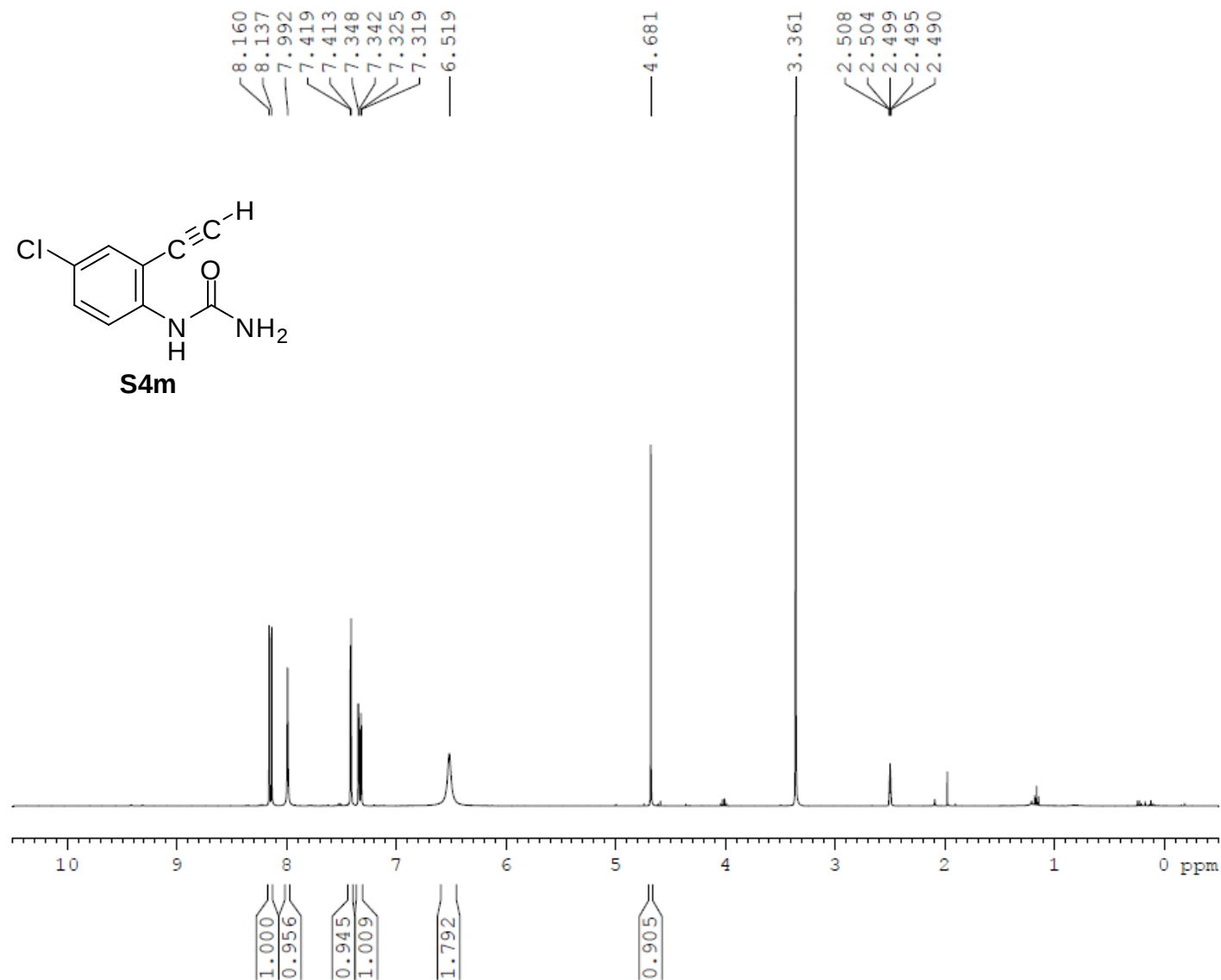
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -5.85 dB
PL12 9.10 dB
PL13 12.10 dB
SFO2 400.1316005 MHz

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





S4m

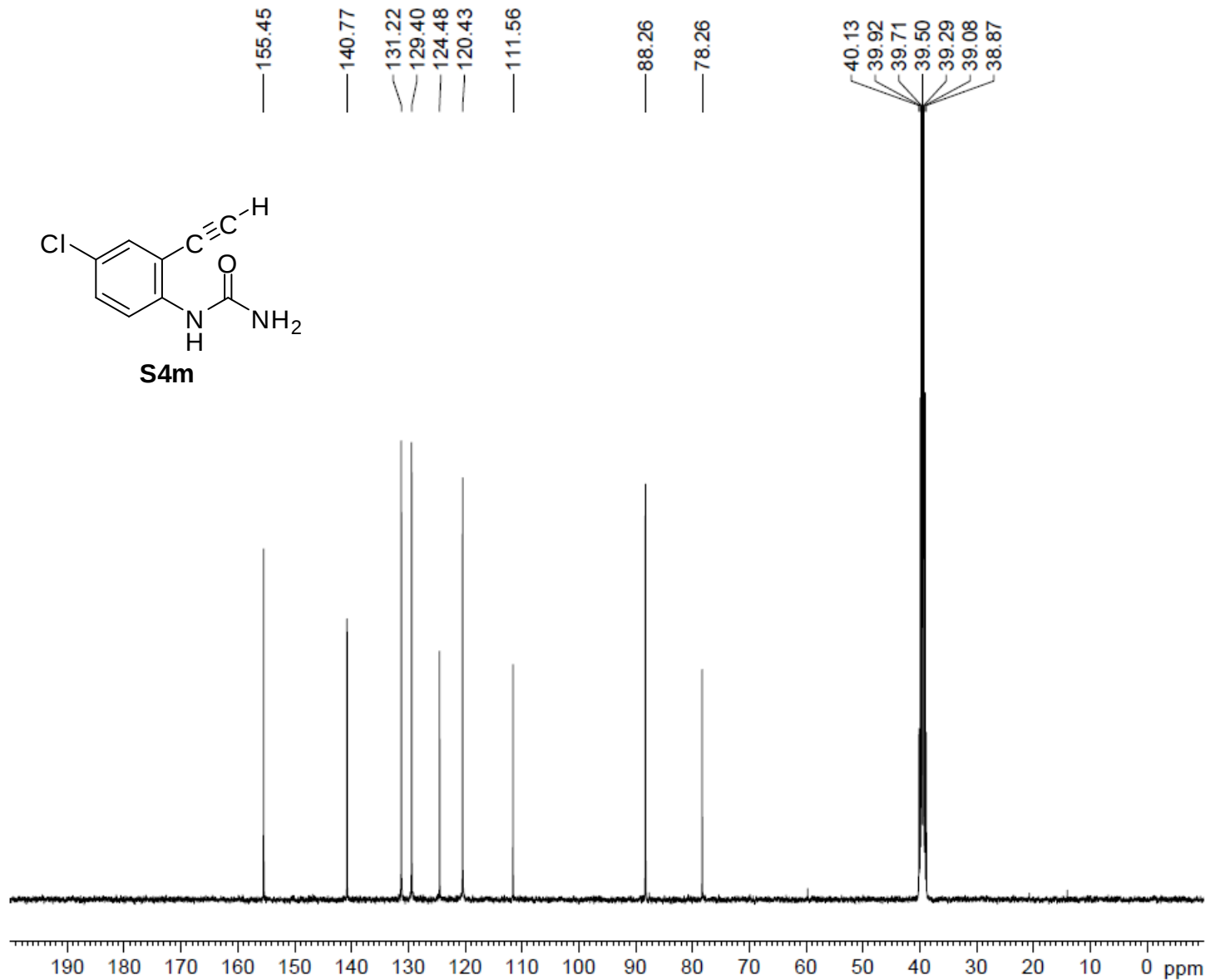
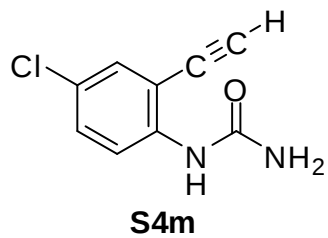


Current Data Parameters
 NAME SD-096(new)
 EXPNO 1
 PROCNO 1

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
 TDO 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



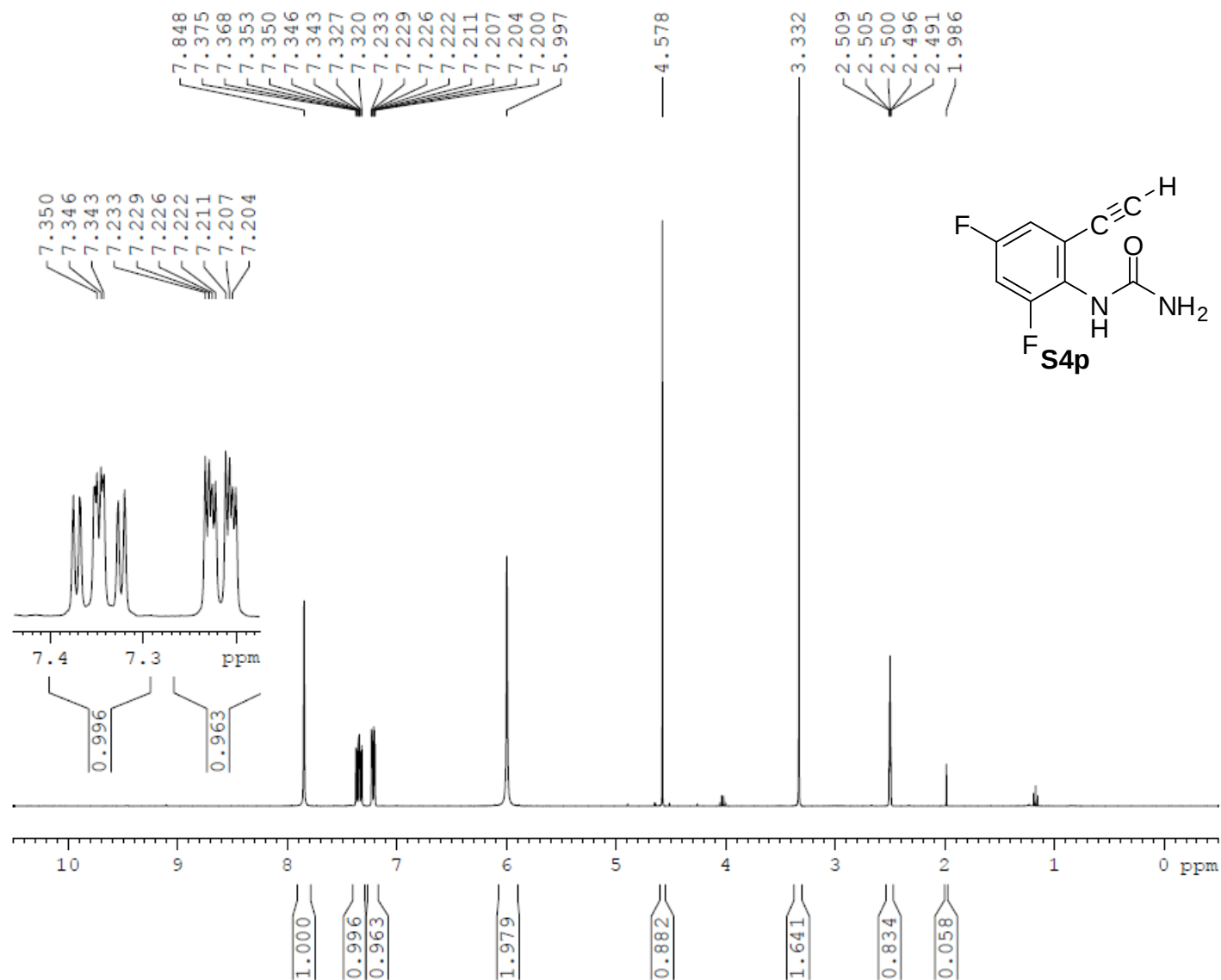
Current Data Parameters
 NAME SD-096(new)
 EXPNO 4
 PROCNO 1

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 100.623319 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

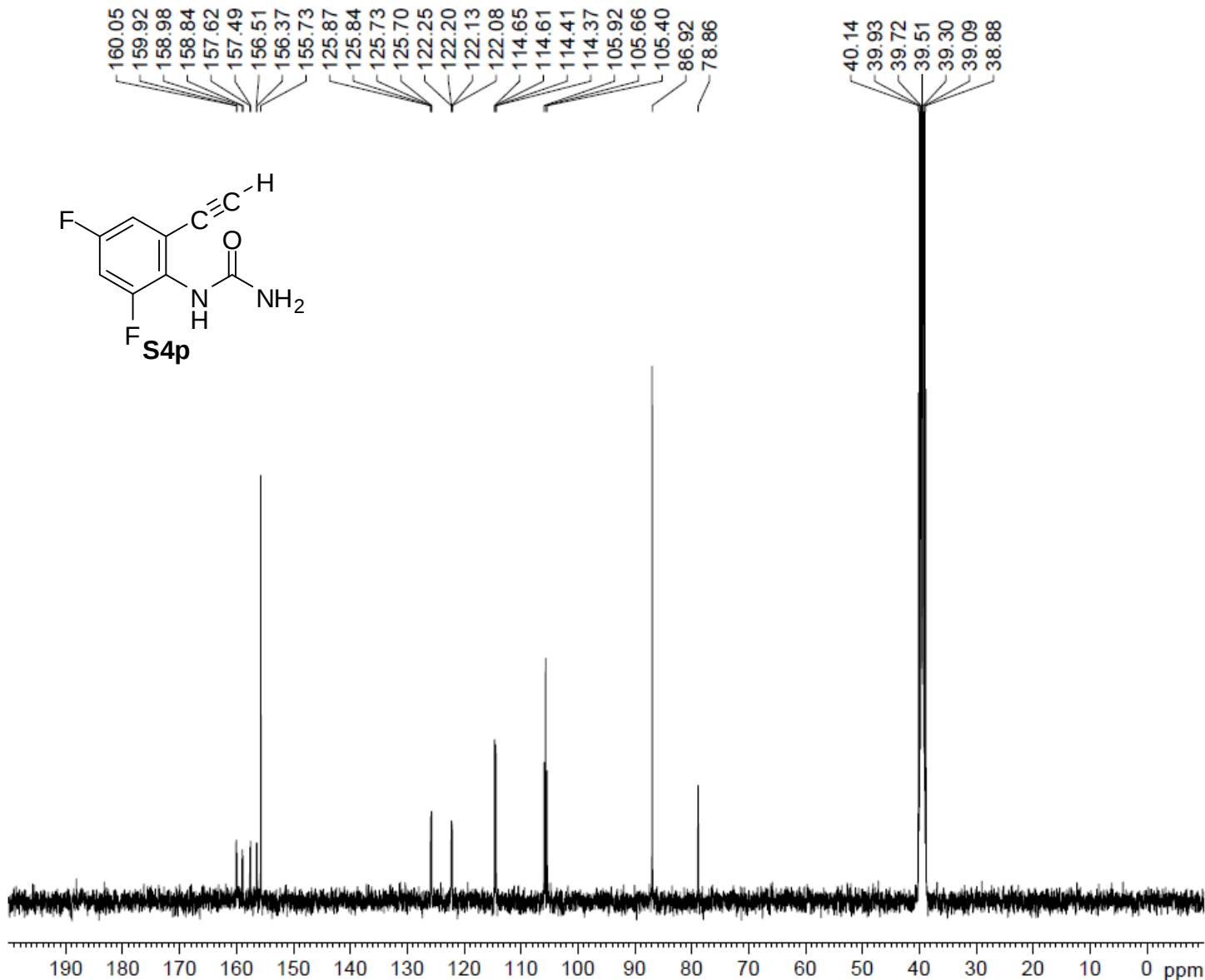
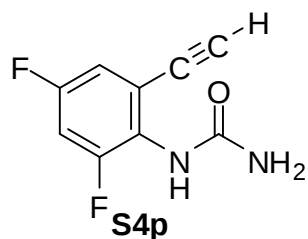


Current Data Parameters
 NAME SO151
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150909
 Time 18.55
 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 12.00 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 18384
 SF 400.1300036 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



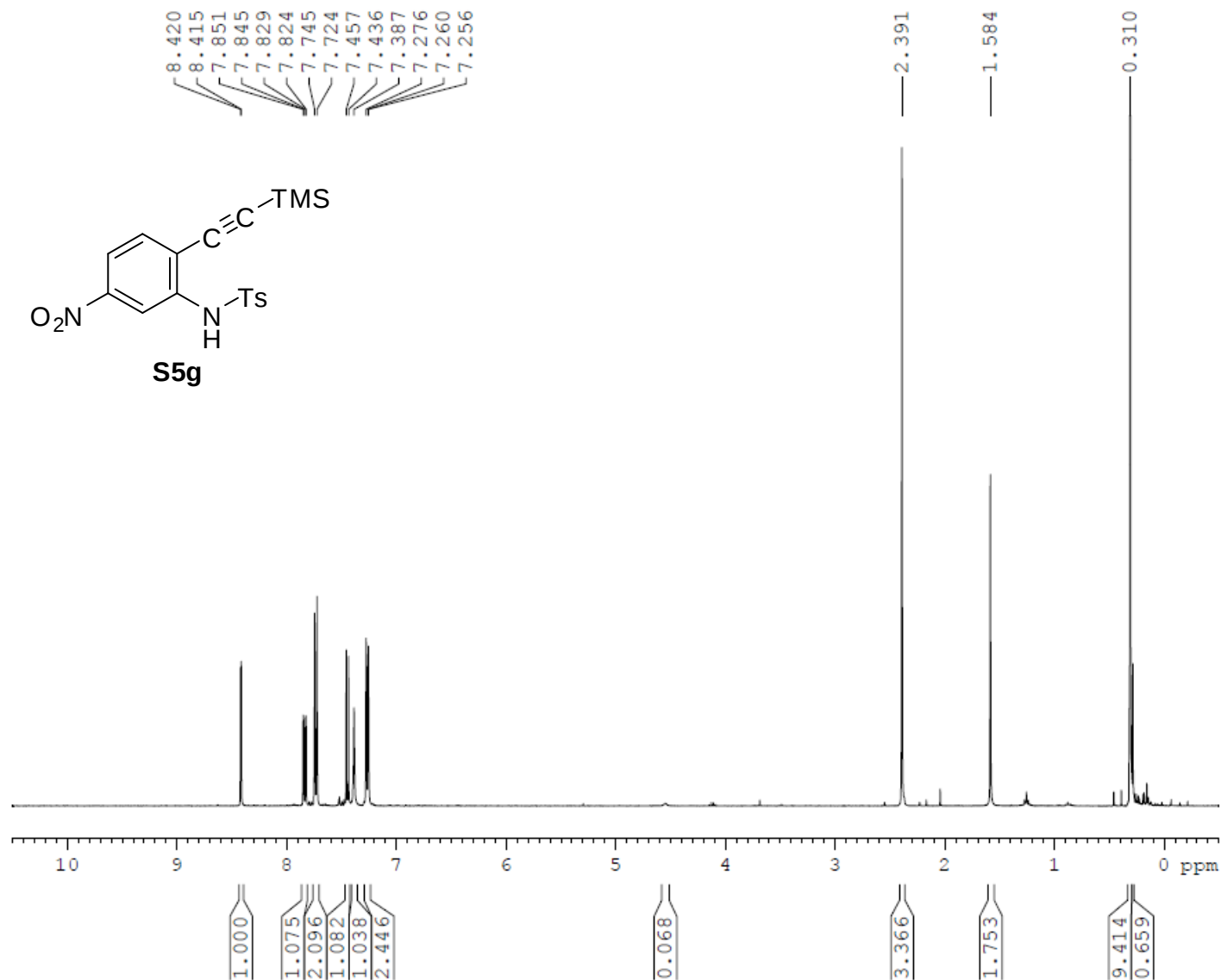
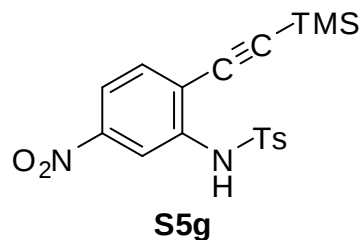
Current Data Parameters
 NAME SO151
 EXPNO 3
 PROCNO 1

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

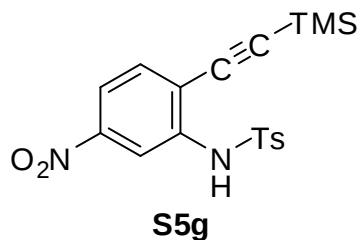


Current Data Parameters
 NAME SC178-2
 EXPNO 1
 PROCNO 1

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
 TDO 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



148.20
 145.03
 139.43
 135.81
 132.83
 130.20
 127.60
 119.49
 118.69
 113.53
 108.39
 97.86

77.55
 77.23
 76.91

21.81

-0.13

Current Data Parameters
 NAME SC178-2
 EXPNO 3
 PROCNO 1

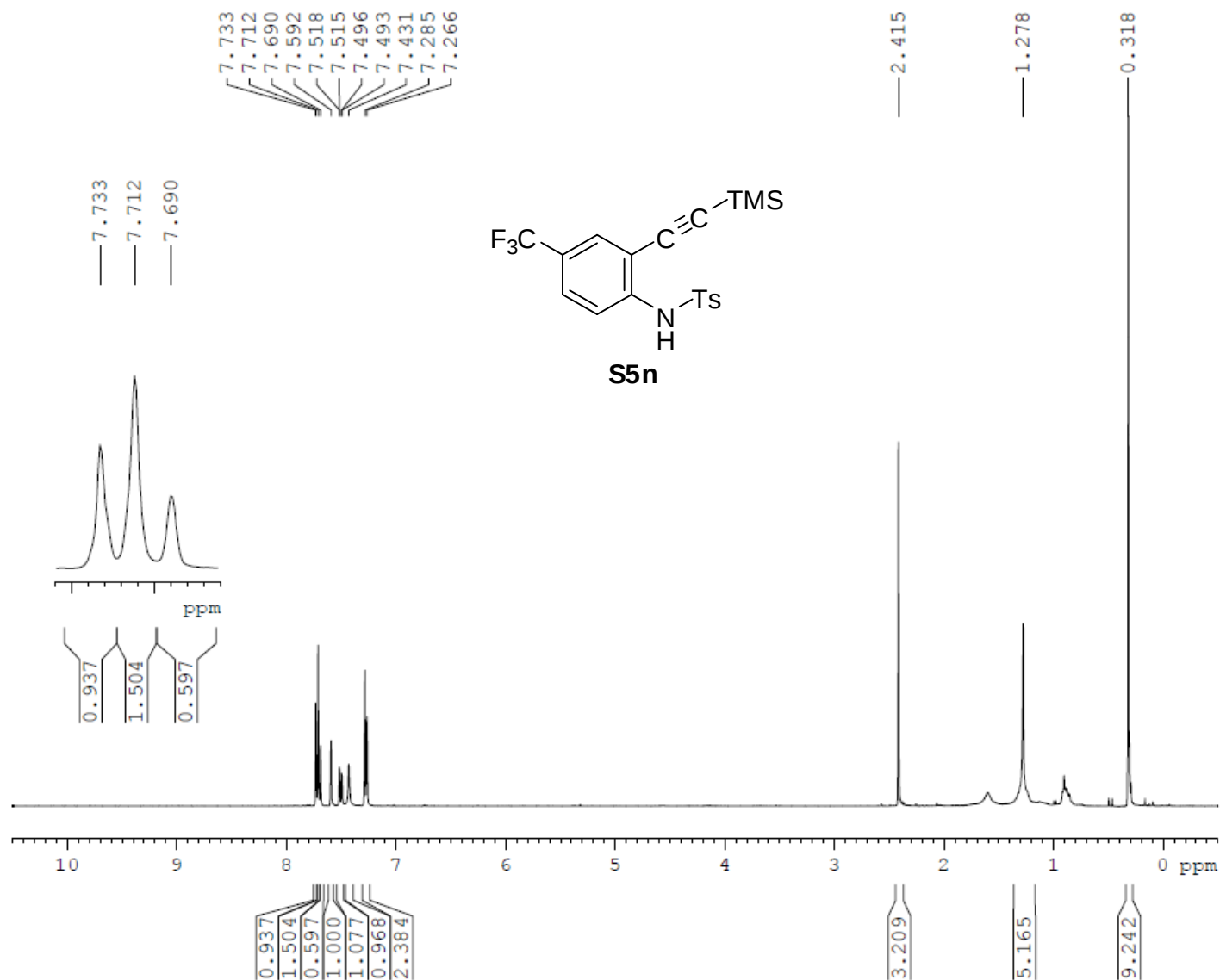
F2 - Acquisition Parameters
 Date_ 20140830
 Time 9.14
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1195
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 300.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

===== CHANNEL f1 =====
 SFO1 100.623319 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

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

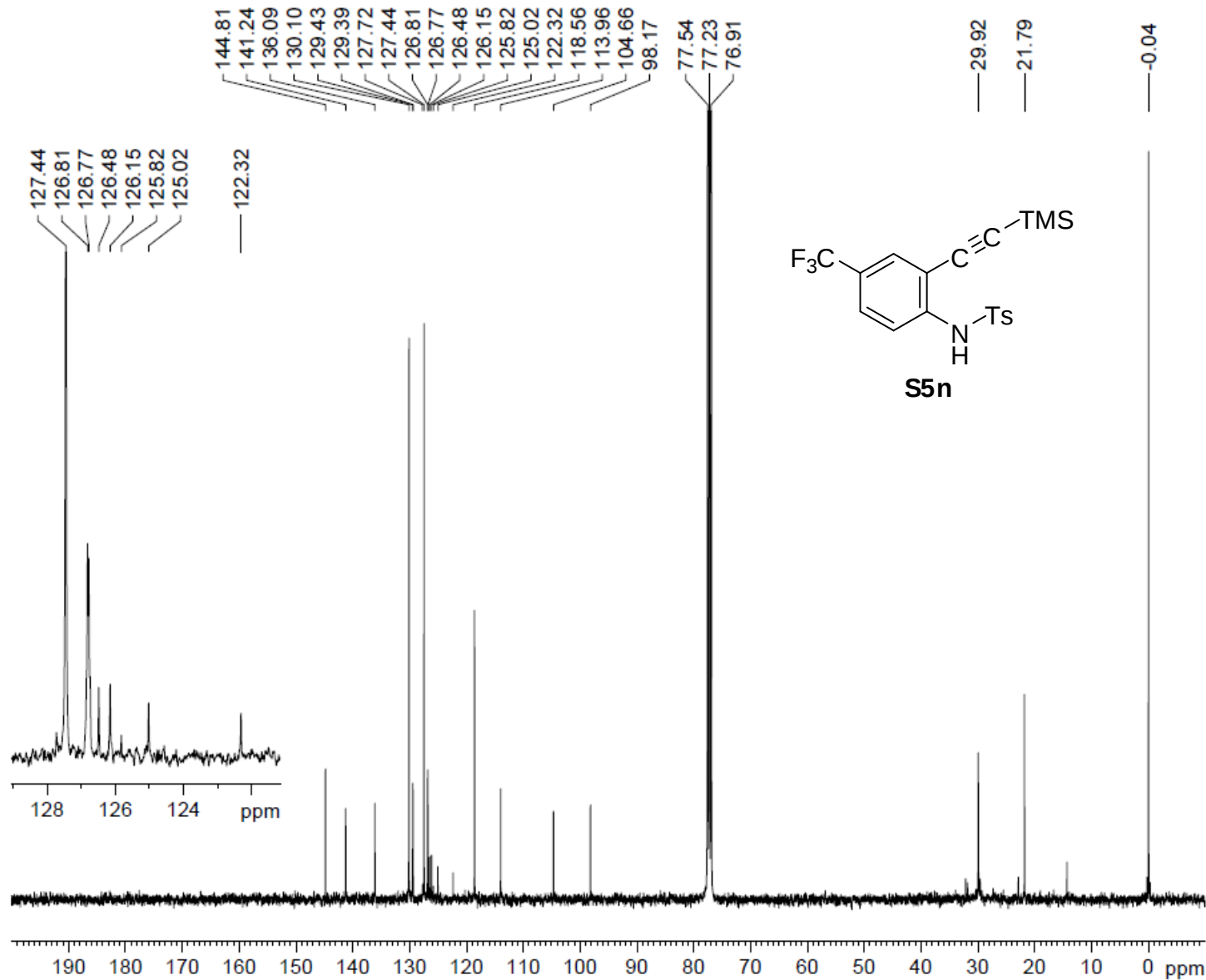


Current Data Parameters
 NAME SC174
 EXPNO 7
 PROCNO 1

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
 TDO 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



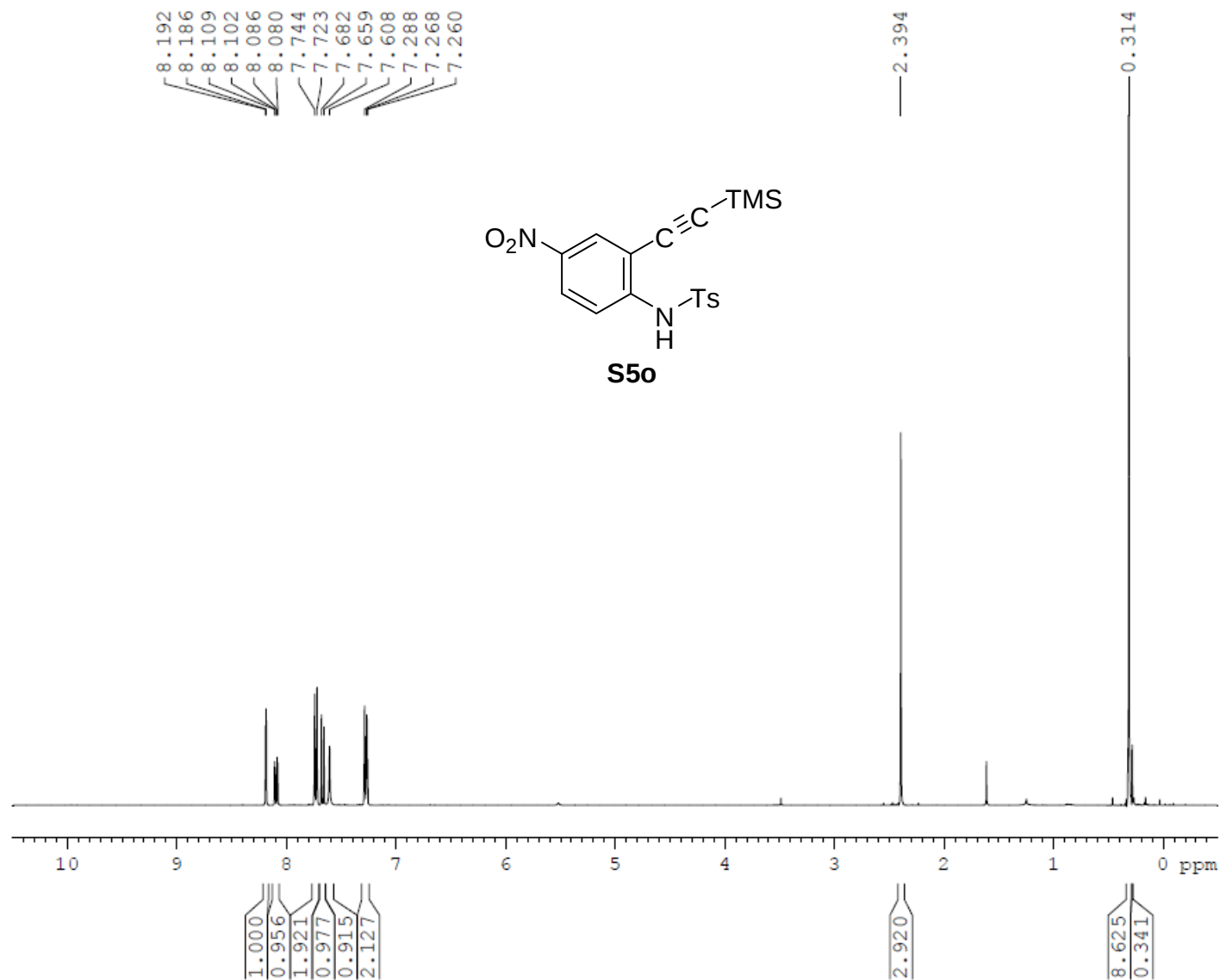
Current Data Parameters
 NAME SC174
 EXPNO 5
 PROCNO 1

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
 CPDPRG2 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

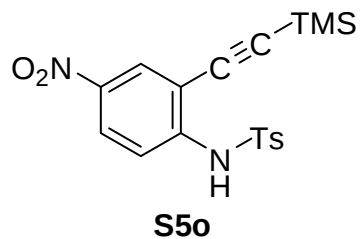


Current Data Parameters
 NAME SO086-1
 EXPNO 1
 PROCNO 1

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
 TDO 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



145.24
 143.63
 143.28
 135.70
 130.25
 127.75
 127.45
 125.27
 117.43
 113.67
 105.98
 97.22

77.55
 77.23
 76.91

21.81

-0.12

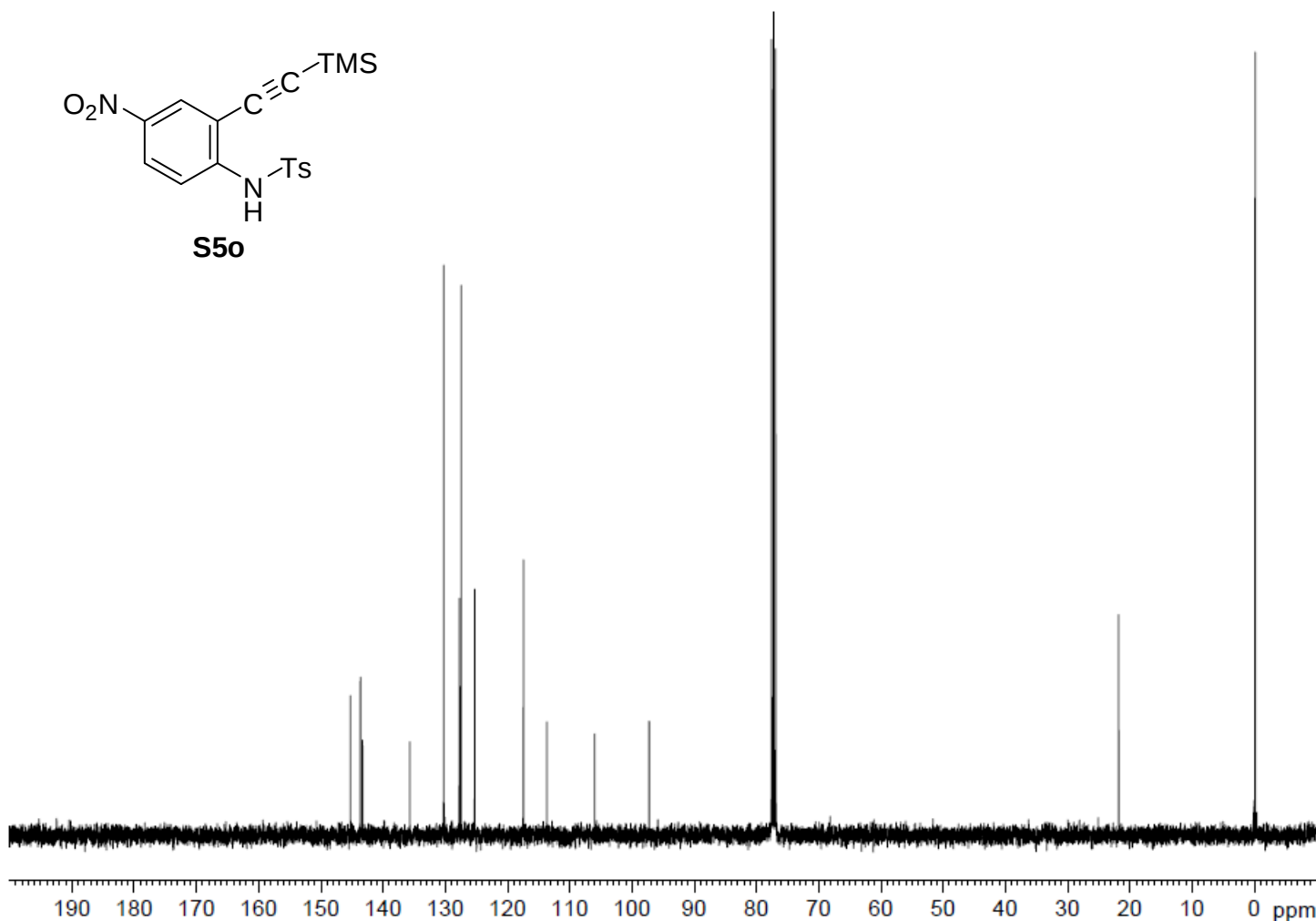
Current Data Parameters
 NAME SO066-1
 EXPNO 2
 PROCNO 1

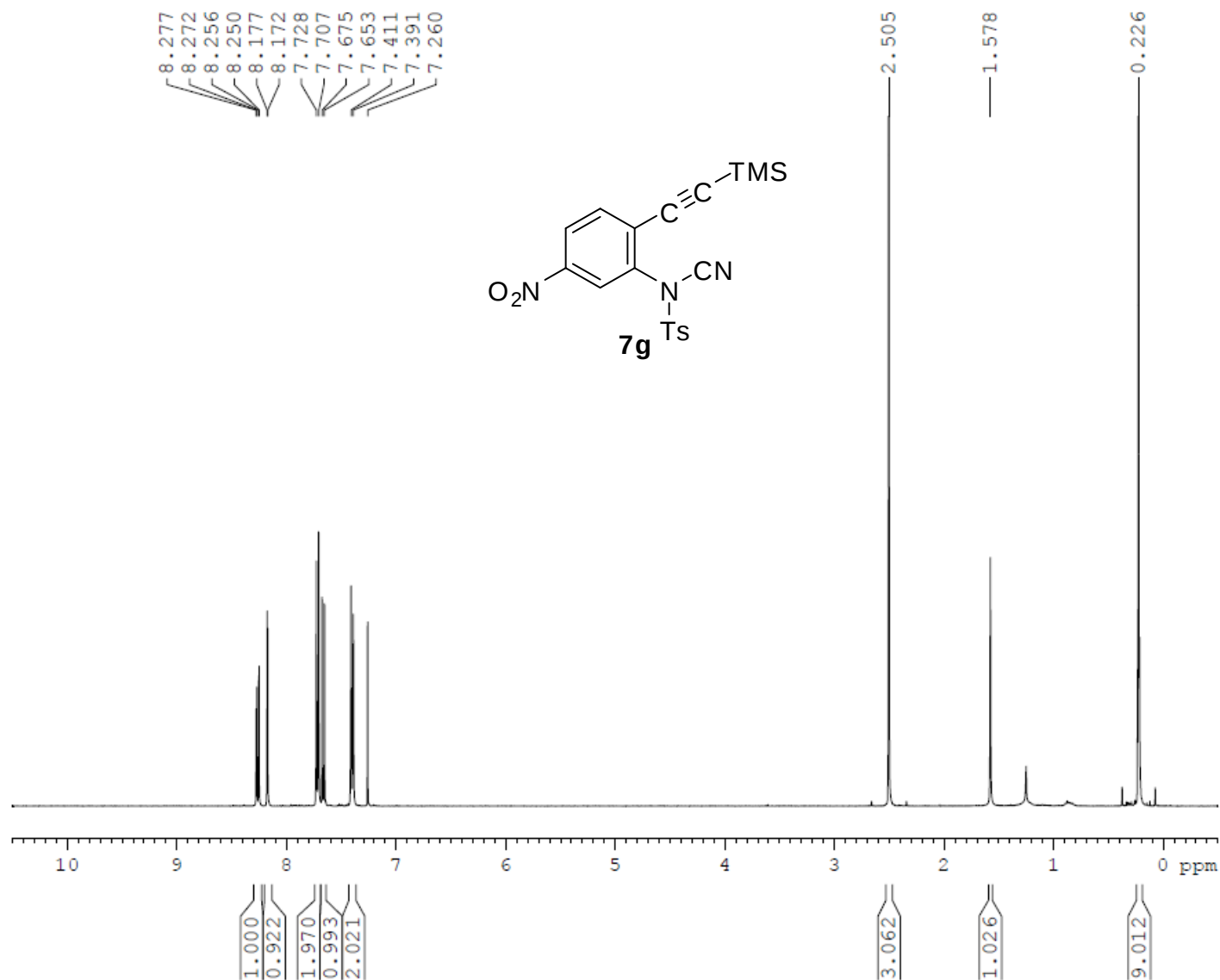
F2 - Acquisition Parameters
 Date_ 20150122
 Time 8.44
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 108
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 2896.3
 DW 20.800 usec
 DE 6.50 usec
 TE 295.9 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

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

===== CHANNEL f2 =====
 CPDPRG2 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



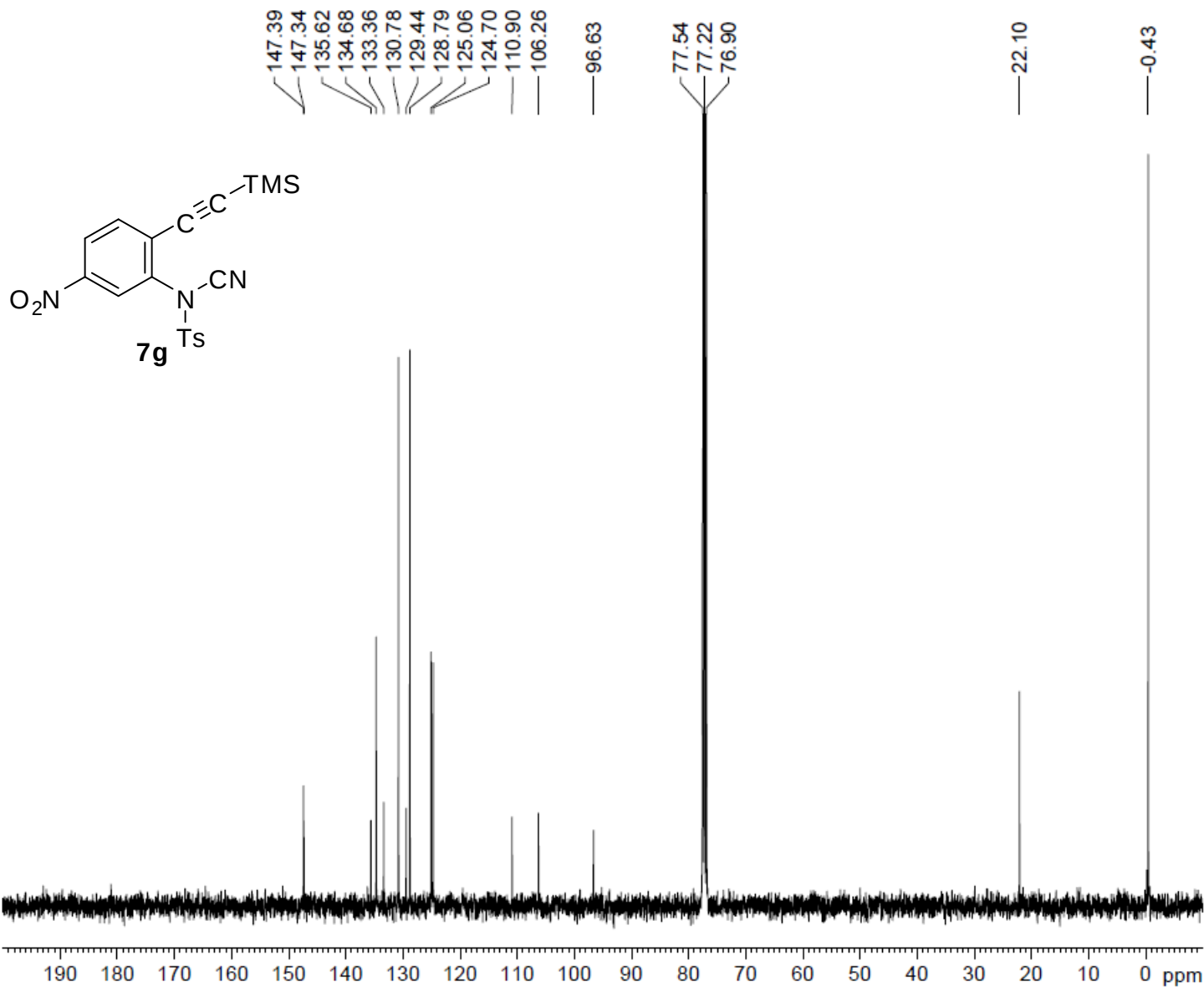


Current Data Parameters
 NAME SC181-2
 EXPNO 1
 PROCNO 1

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
 TDO 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



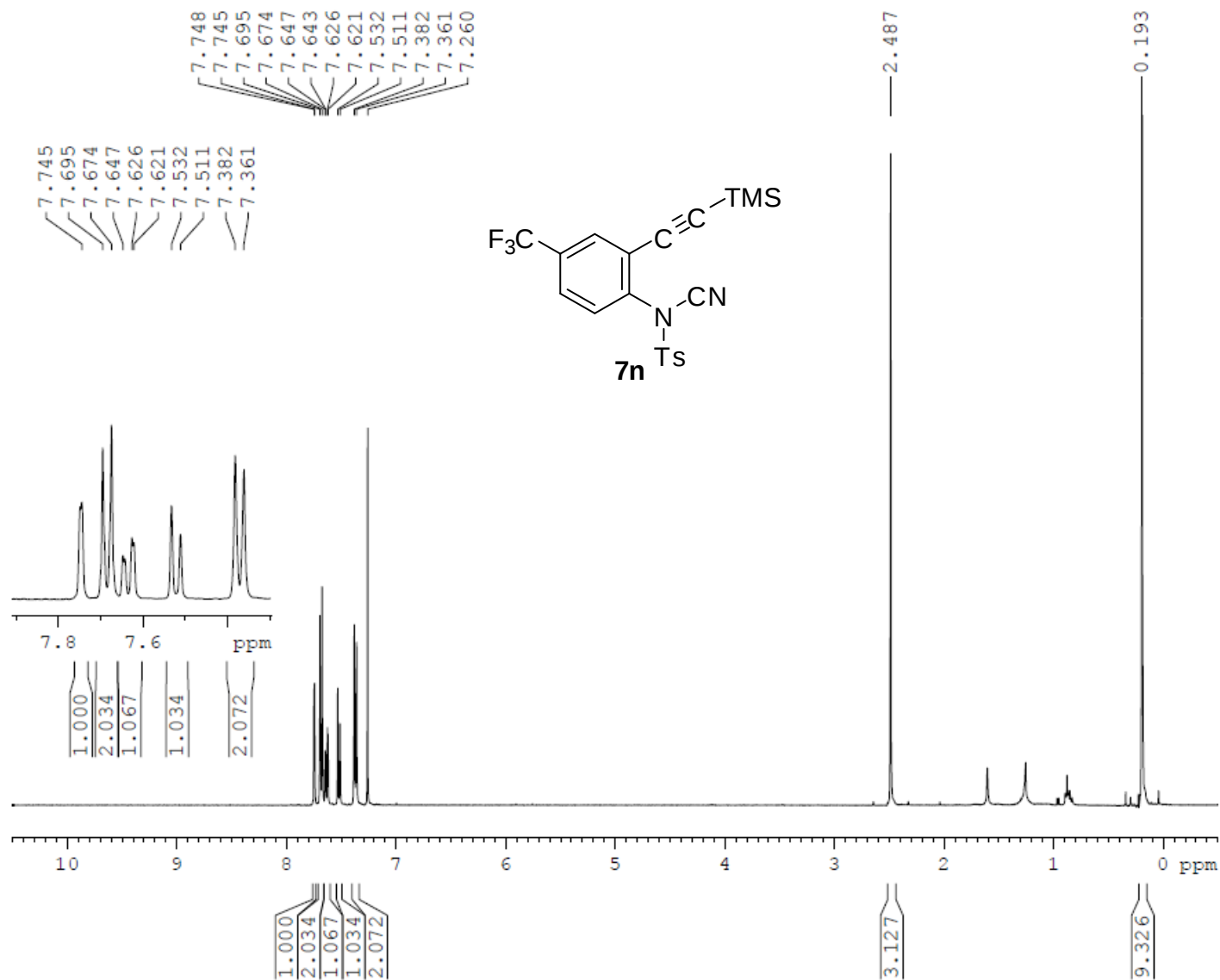
Current Data Parameters
 NAME SC181-2
 EXPNO 3
 PROCNO 1

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
 CPDPRG2 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

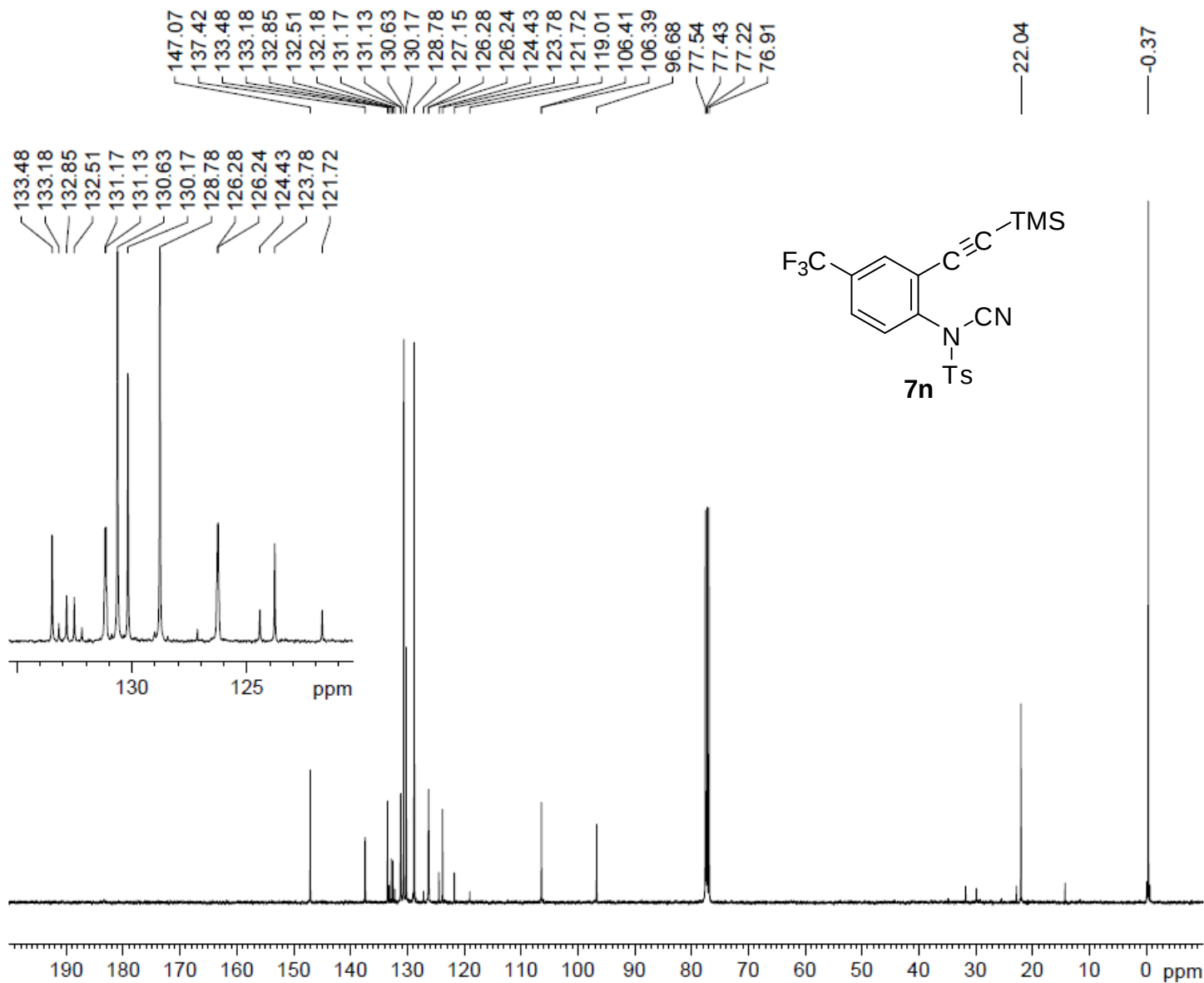


Current Data Parameters
 NAME SC176
 EXPNO 2
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130093 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



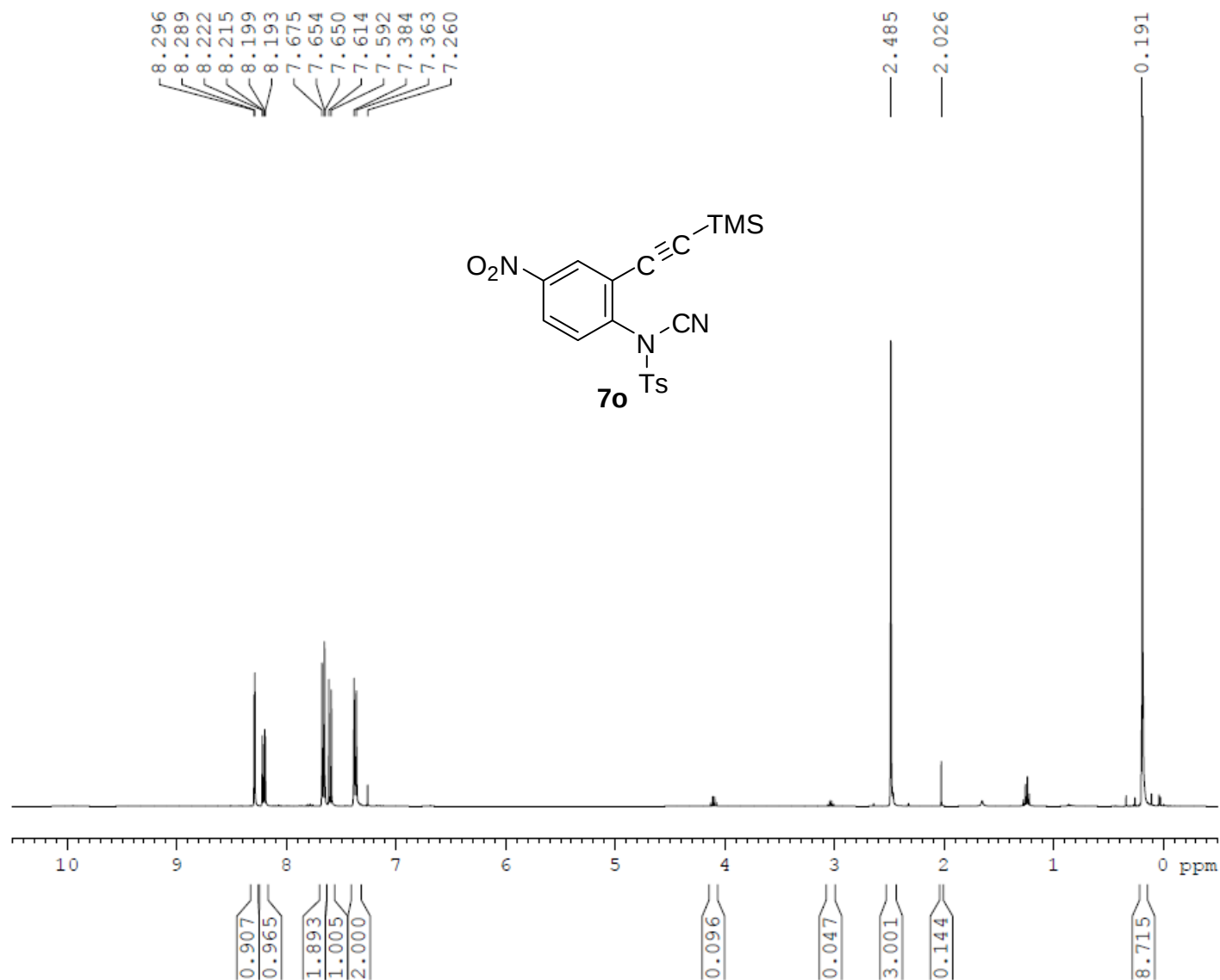
Current Data Parameters
 NAME SC176
 EXPNO 4
 PROCNO 1

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
 TDO 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

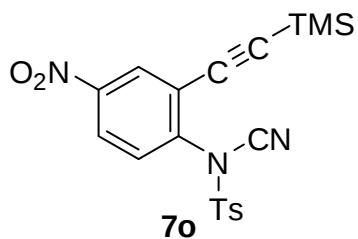


Current Data Parameters
 NAME S0071
 EXPNO 1
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130090 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



148.28
147.34
139.33
133.17
130.70
130.64
128.90
128.72
124.22
124.09
107.87
105.93
95.88
77.55
77.23
76.91

22.03

-0.47

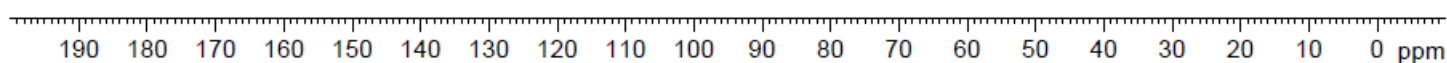
Current Data Parameters
NAME SO071
EXPNO 3
PROCNO 1

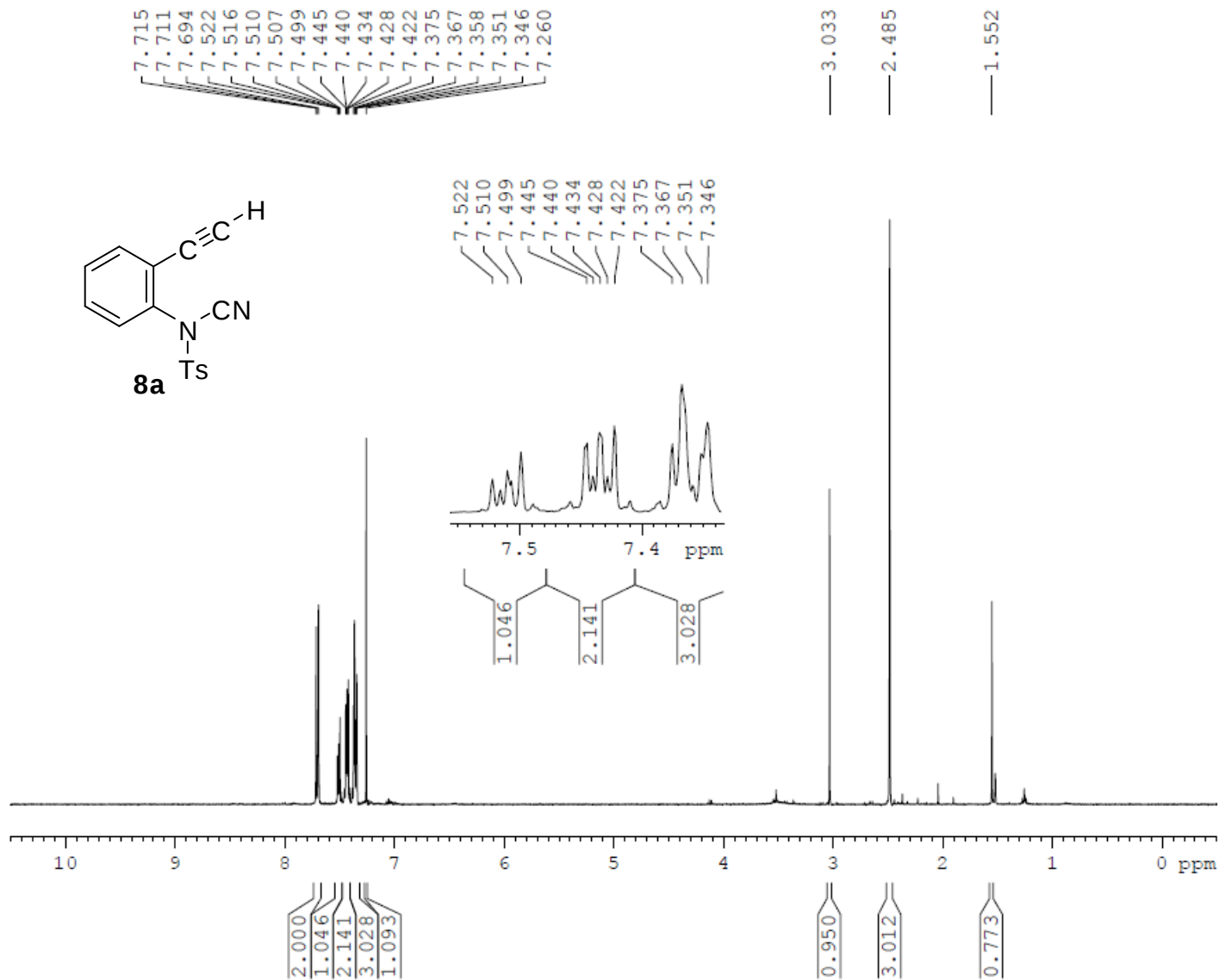
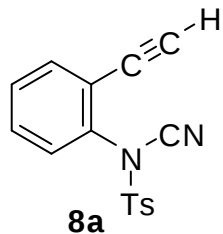
F2 - Acquisition Parameters
Date_ 20150203
Time 9.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.623319 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

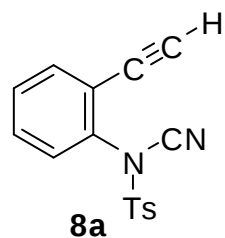
F2 - Processing parameters
SI 32768
SF 100.6127537 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00





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



146.92
 134.92
 134.33
 133.17
 130.69
 130.41
 130.24
 129.82
 128.82
 122.06
 107.42

84.74
 77.55
 77.23
 77.20
 76.91

21.97

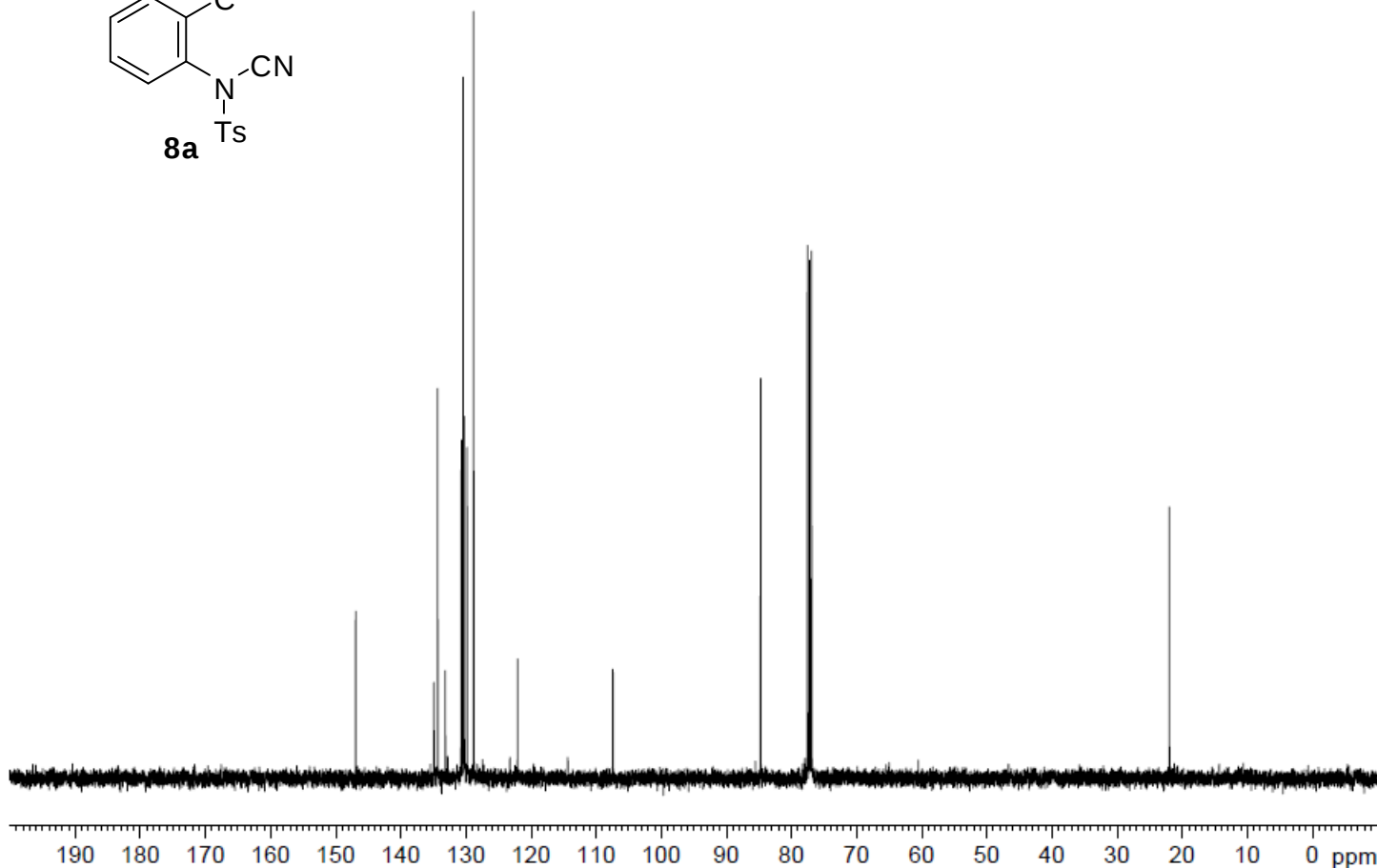
Current Data Parameters
 NAME SO103
 EXPNO 3
 PROCNO 1

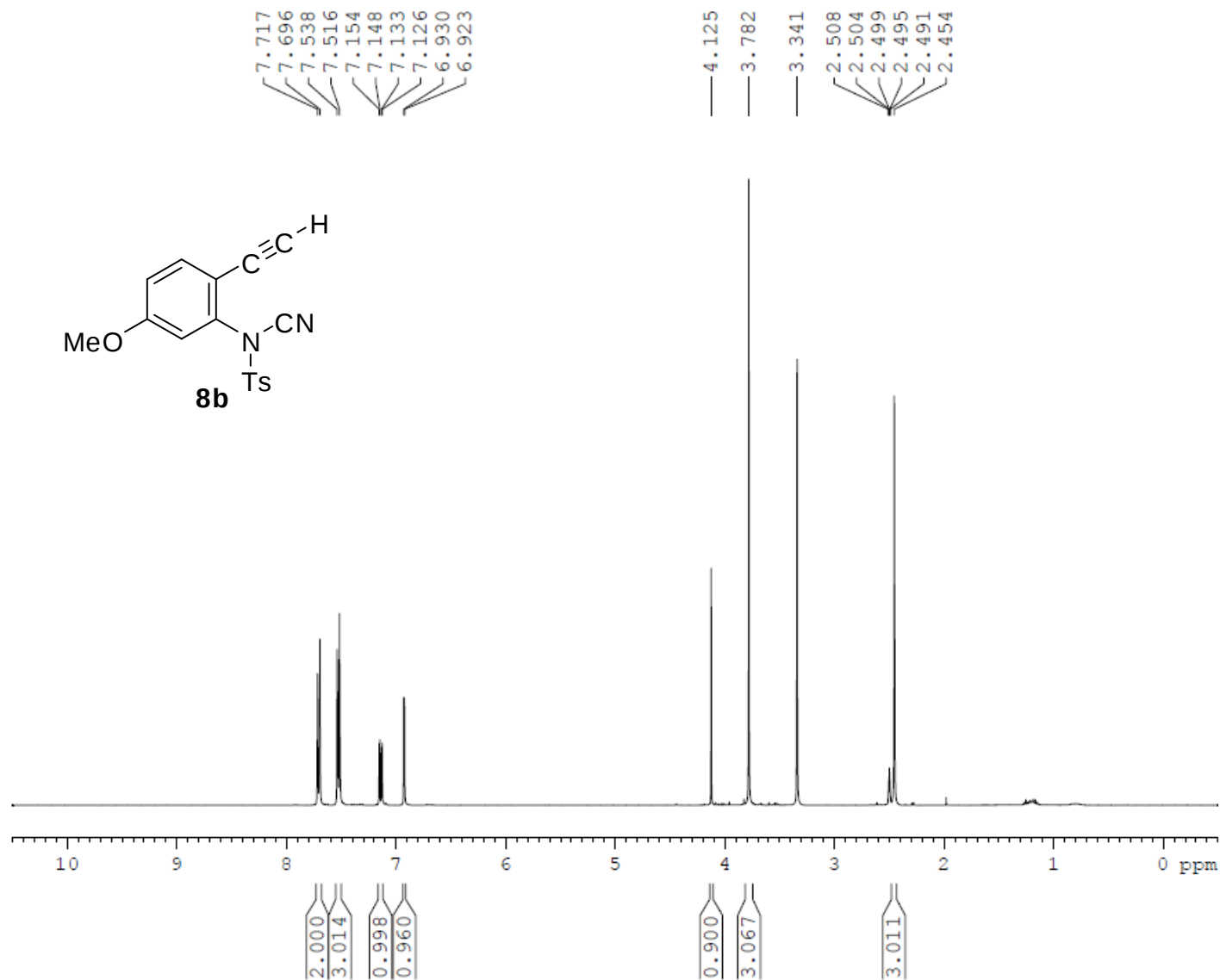
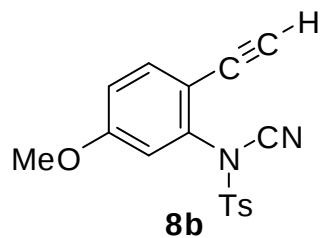
F2 - Acquisition Parameters
 Date_ 20150409
 Time 13.53
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 53
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 2896.3
 DW 20.800 usec
 DE 6.50 usec
 TE 294.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

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

===== CHANNEL f2 =====
 CPDPRG2 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



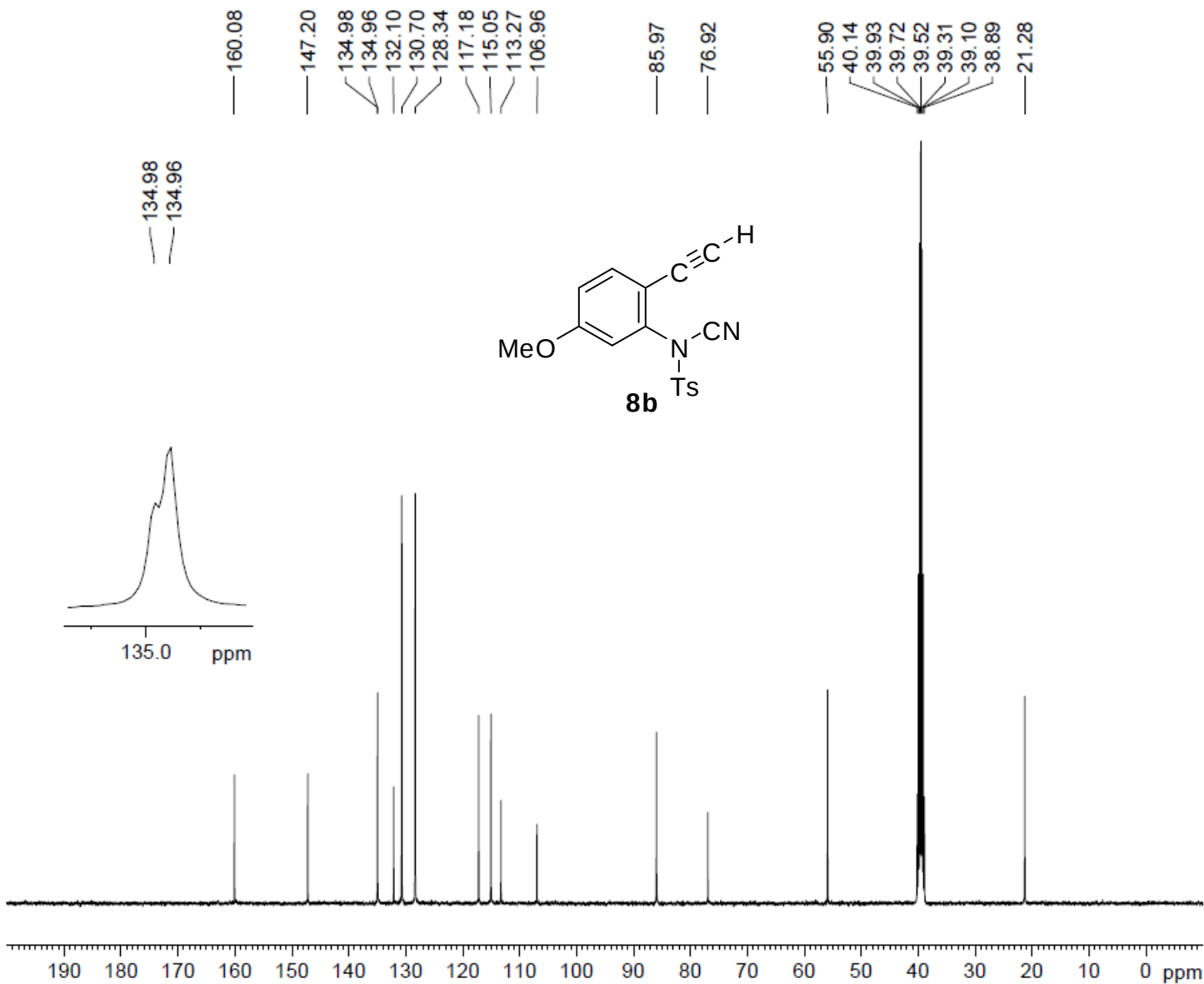


Current Data Parameters
 NAME SD-102-DMSO(new)
 EXPNO 1
 PROCNO 1

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 63.68
 DW 69.333 usec
 DE 10.52 usec
 TE 299.0 K
 D1 2.00000000 sec
 TDO 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



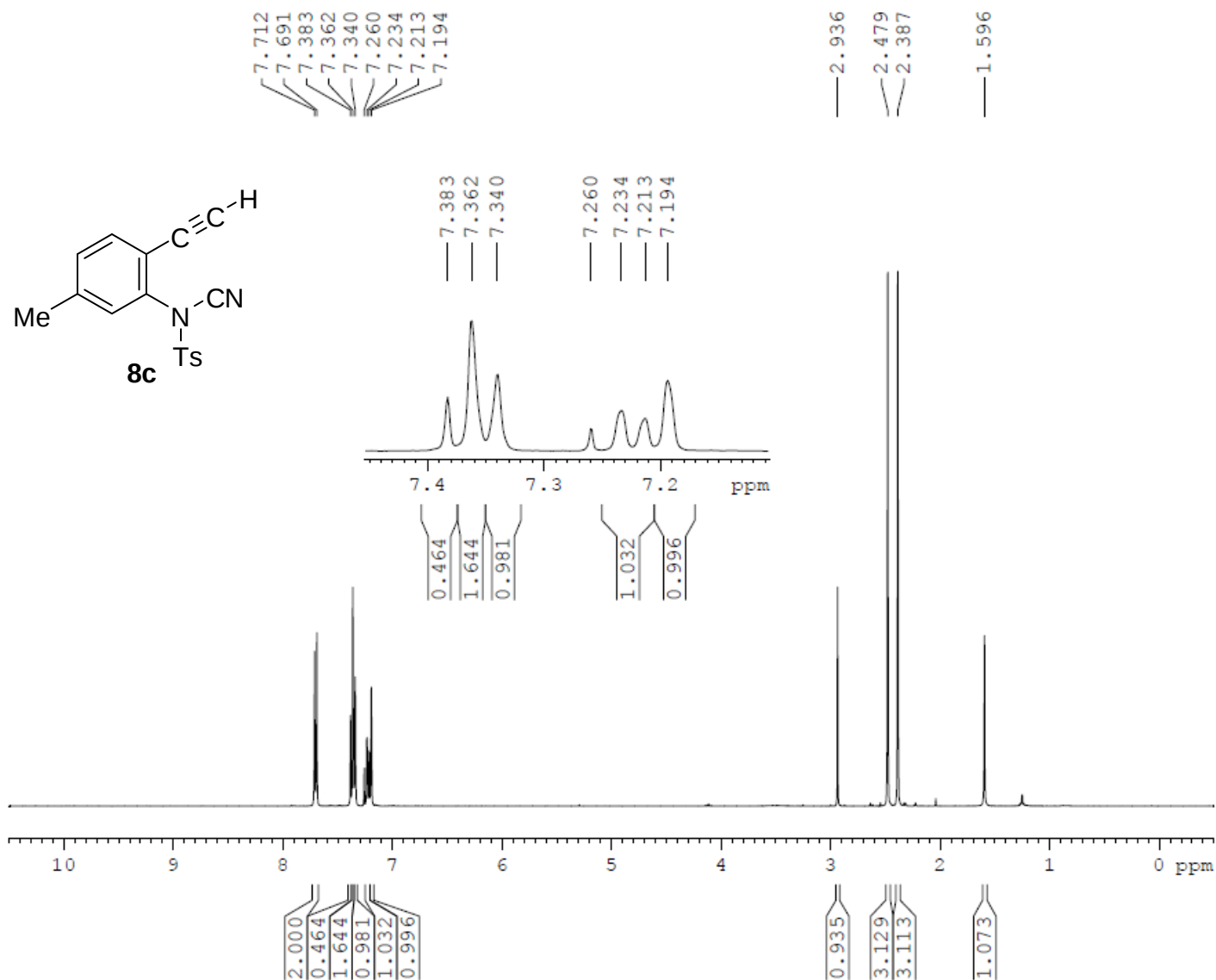
Current Data Parameters
 NAME SD-102-DMSO(new)
 EXPNO 3
 PROCNO 1

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 100.623319 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

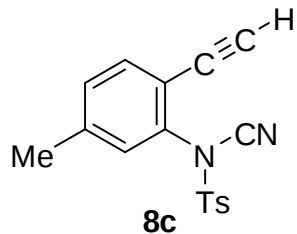


Current Data Parameters
 NAME SC180
 EXPNO 6
 PROCNO 1

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
 TDO 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



146.80
141.20
134.93
134.05
133.48
131.52
130.53
130.37
129.00
119.02
— 107.55

83.84
77.54
77.43
77.23
76.91

22.02
21.51

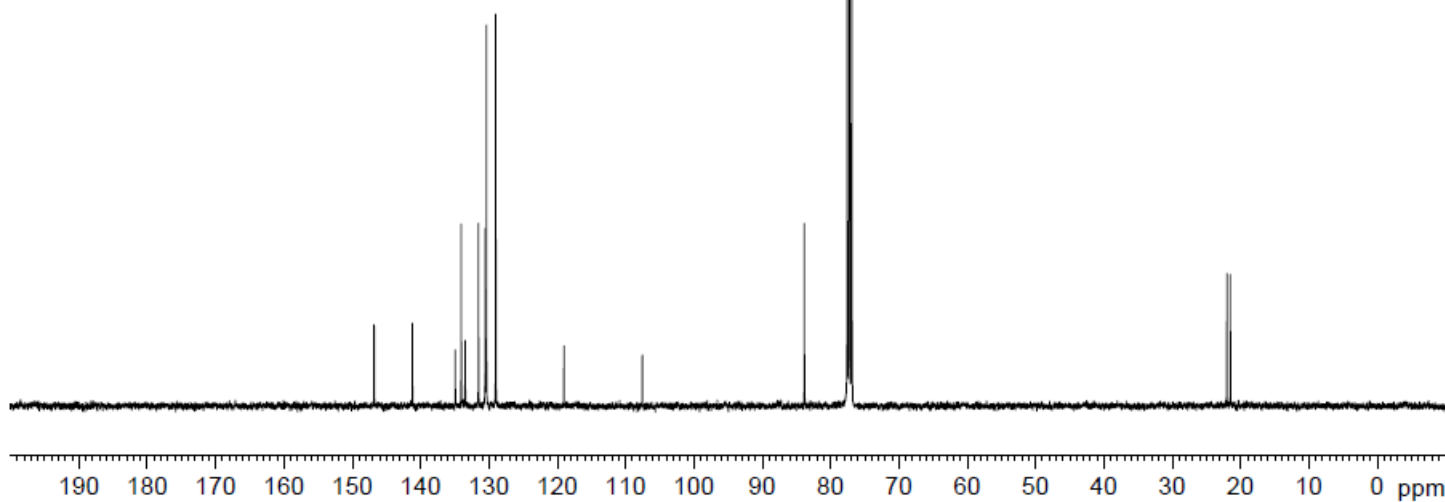
Current Data Parameters
NAME SC160
EXPNO 1
PROCNO 1

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

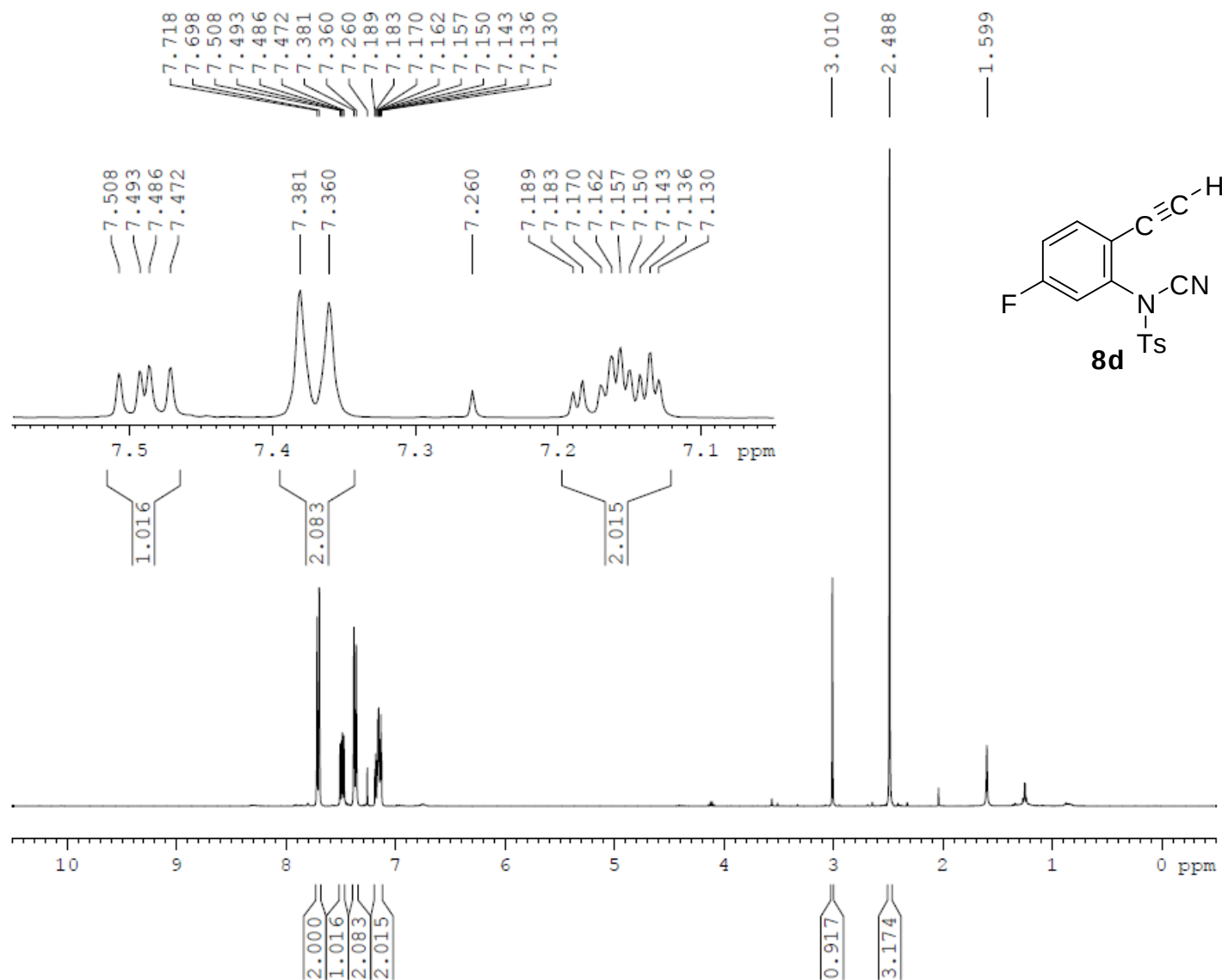
===== CHANNEL f1 =====
SFO1 100.623319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== 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



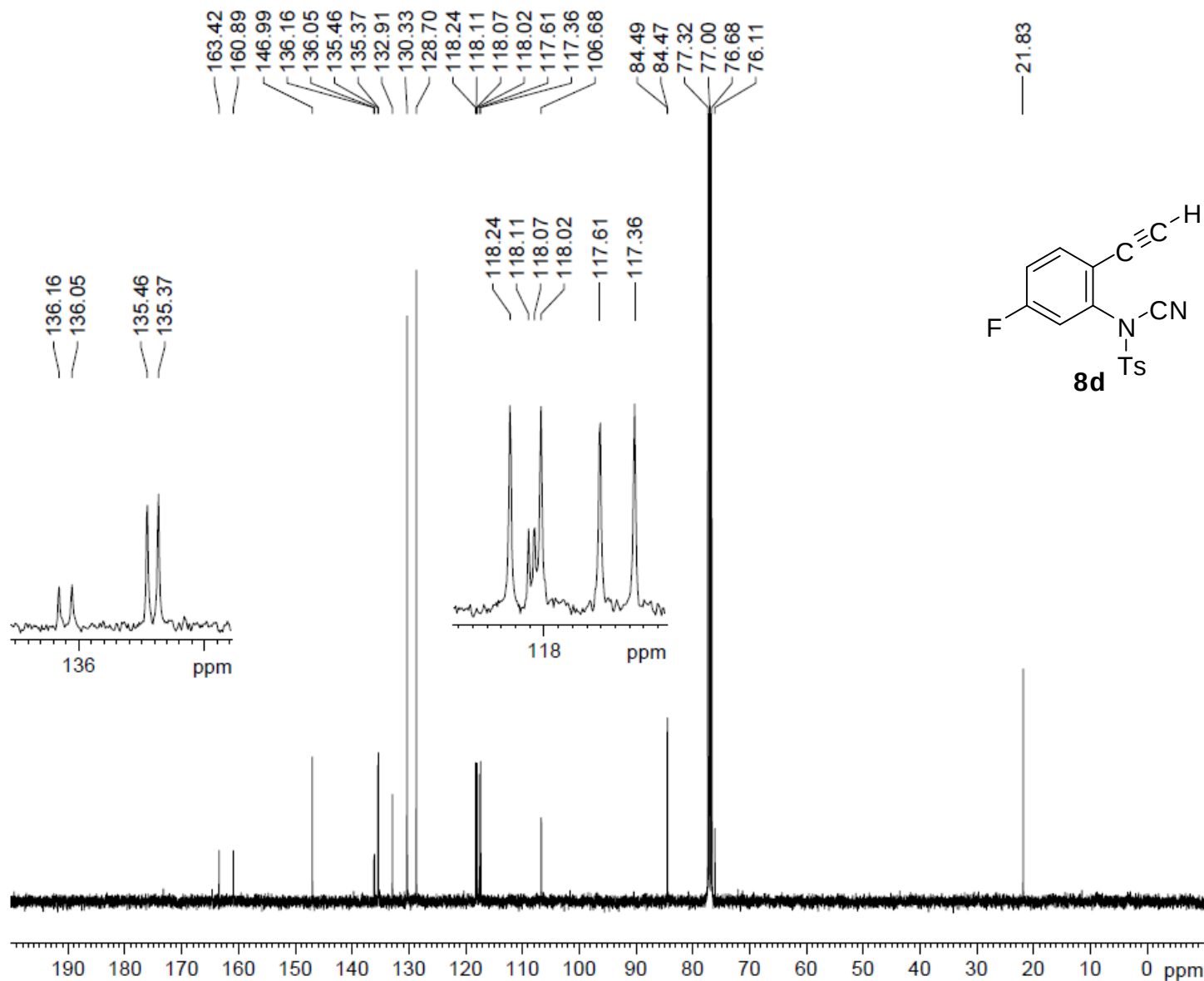
Current Data Parameters
 NAME SD-083(old)
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140804
 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
 TDO 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



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

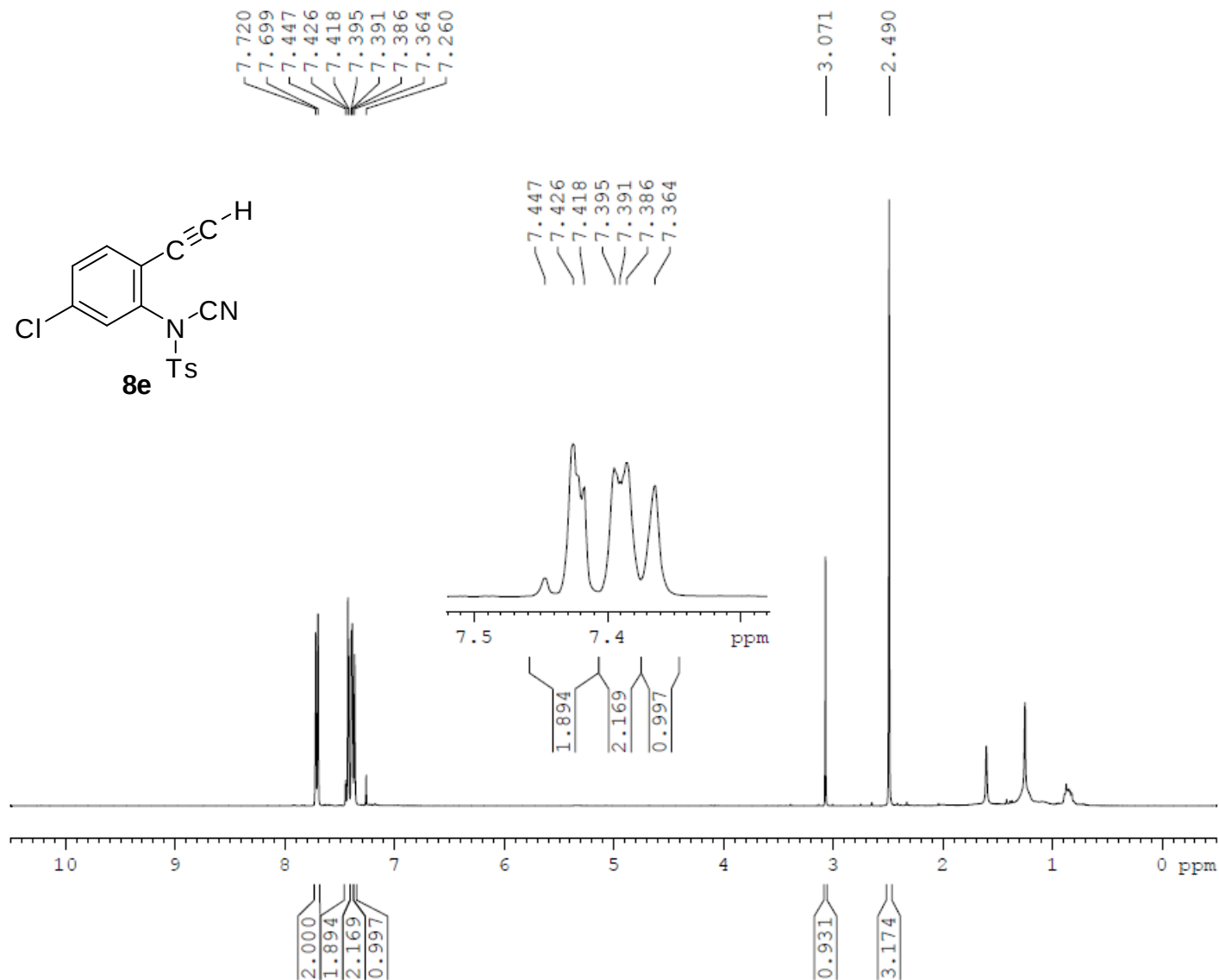
F2 - Acquisition Parameters
 Date_ 20140604
 Time 18.46
 INSTRUM spect
 PROBHD 5 mm SEI 1H-13
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1047
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 8192
 DW 20.800 usec
 DE 6.50 usec
 TE 297.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

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

===== CHANNEL f2 =====
 CPDPRG2 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



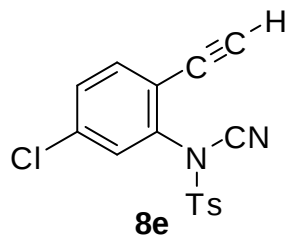
Current Data Parameters
 NAME SD-076(old)
 EXPNO 1
 PROCNO 1

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



147.00
135.67
135.62
134.79
132.89
130.86
130.33
129.97
128.73
120.36
— 106.72

85.58
77.32
77.00
76.69
76.19

— 21.83

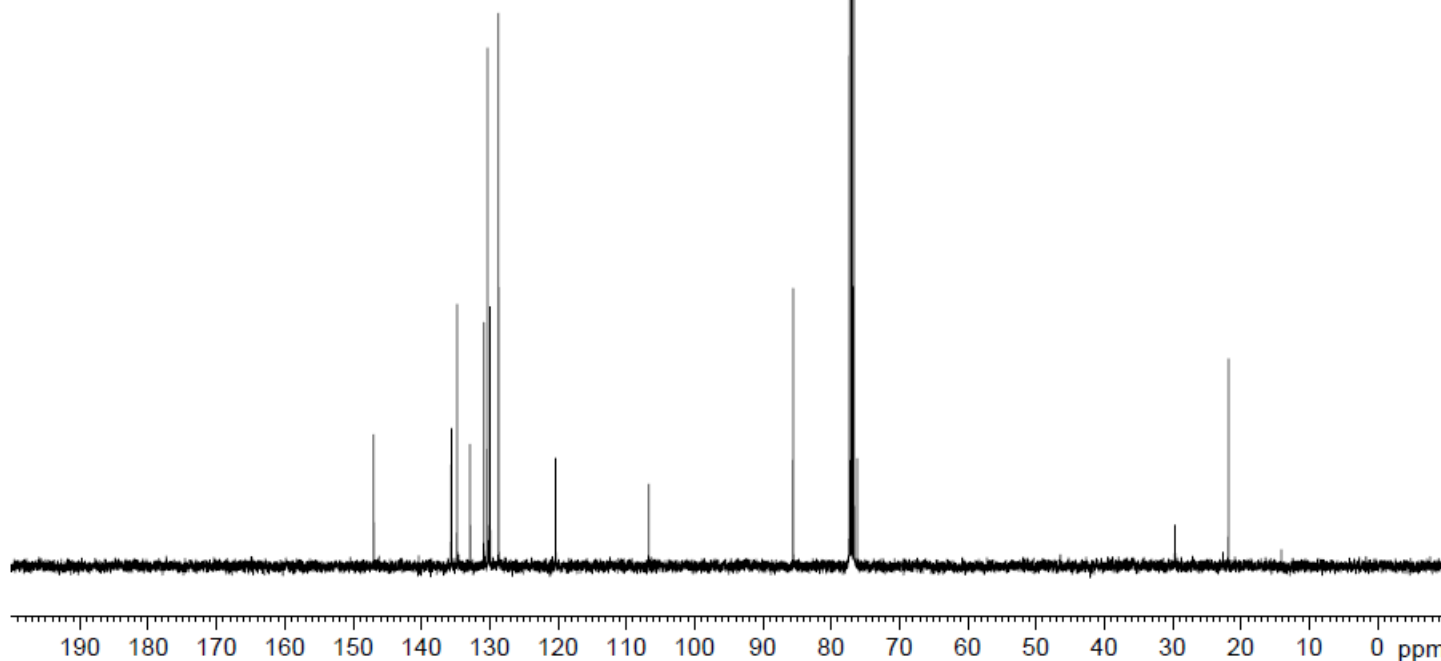
Current Data Parameters
NAME SD-076(old)
EXPNO 4
PROCNO 1

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

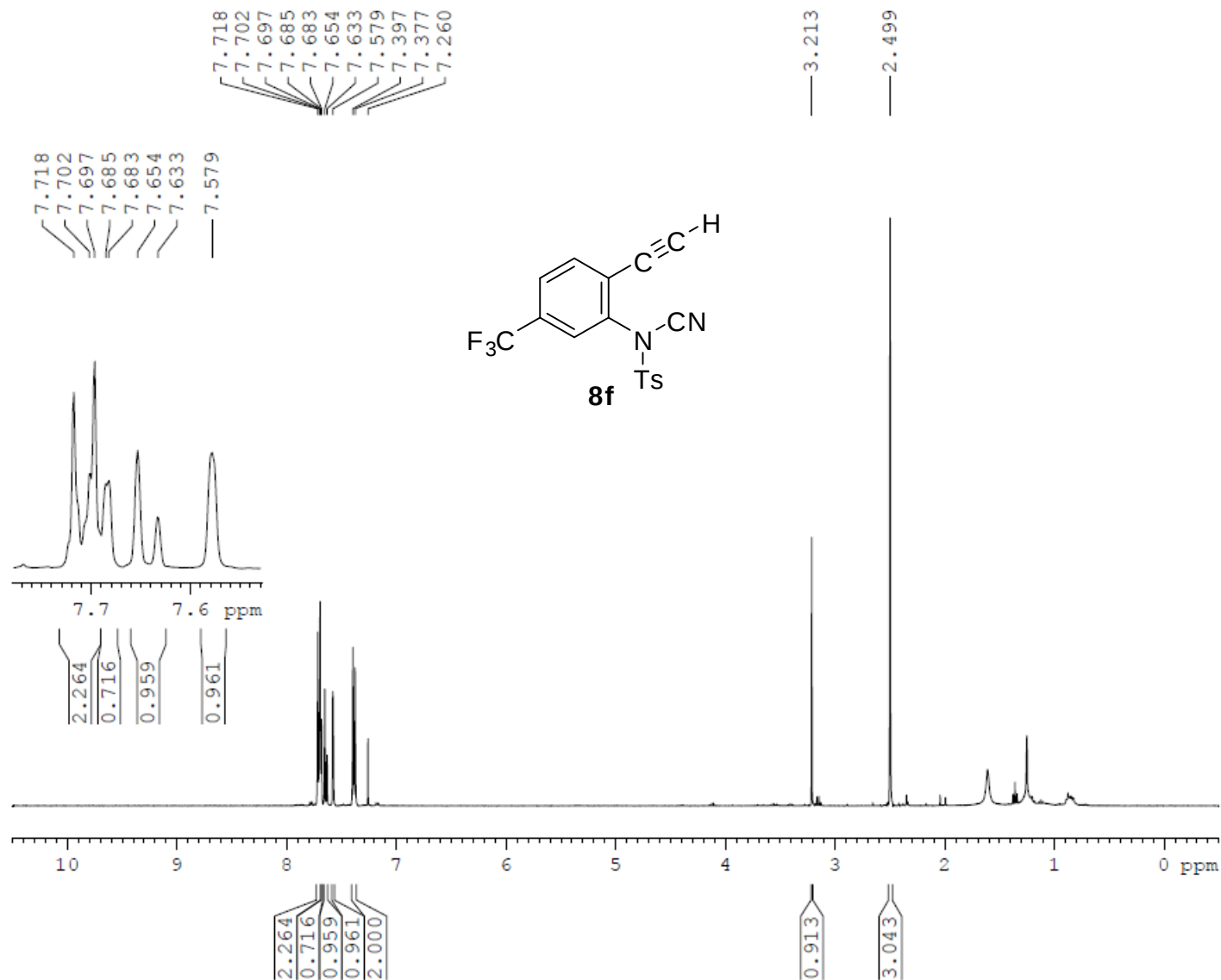
===== CHANNEL f1 =====
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG2 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



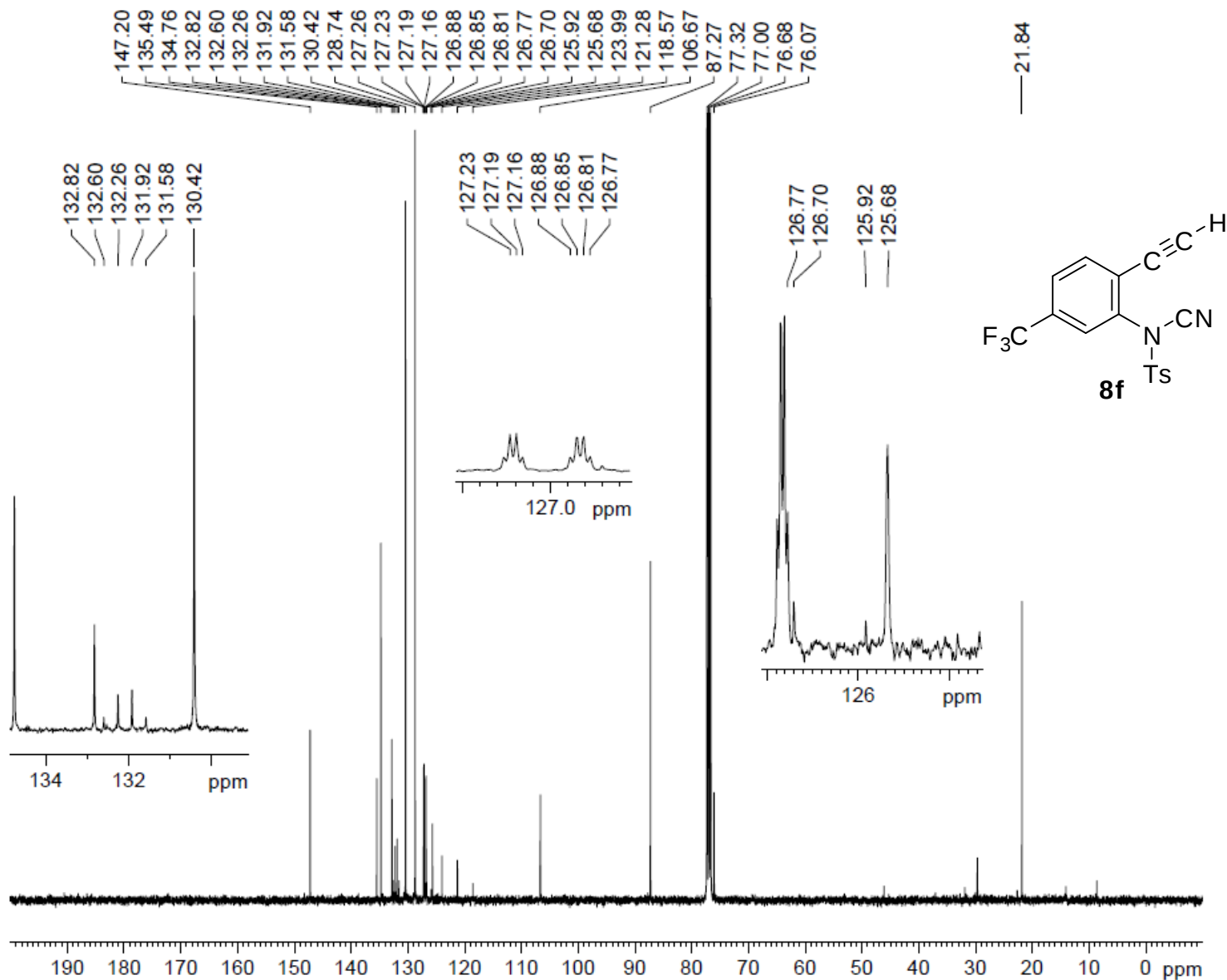
Current Data Parameters
 NAME SD-073-pure(old)
 EXPNO 5
 PROCNO 1

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



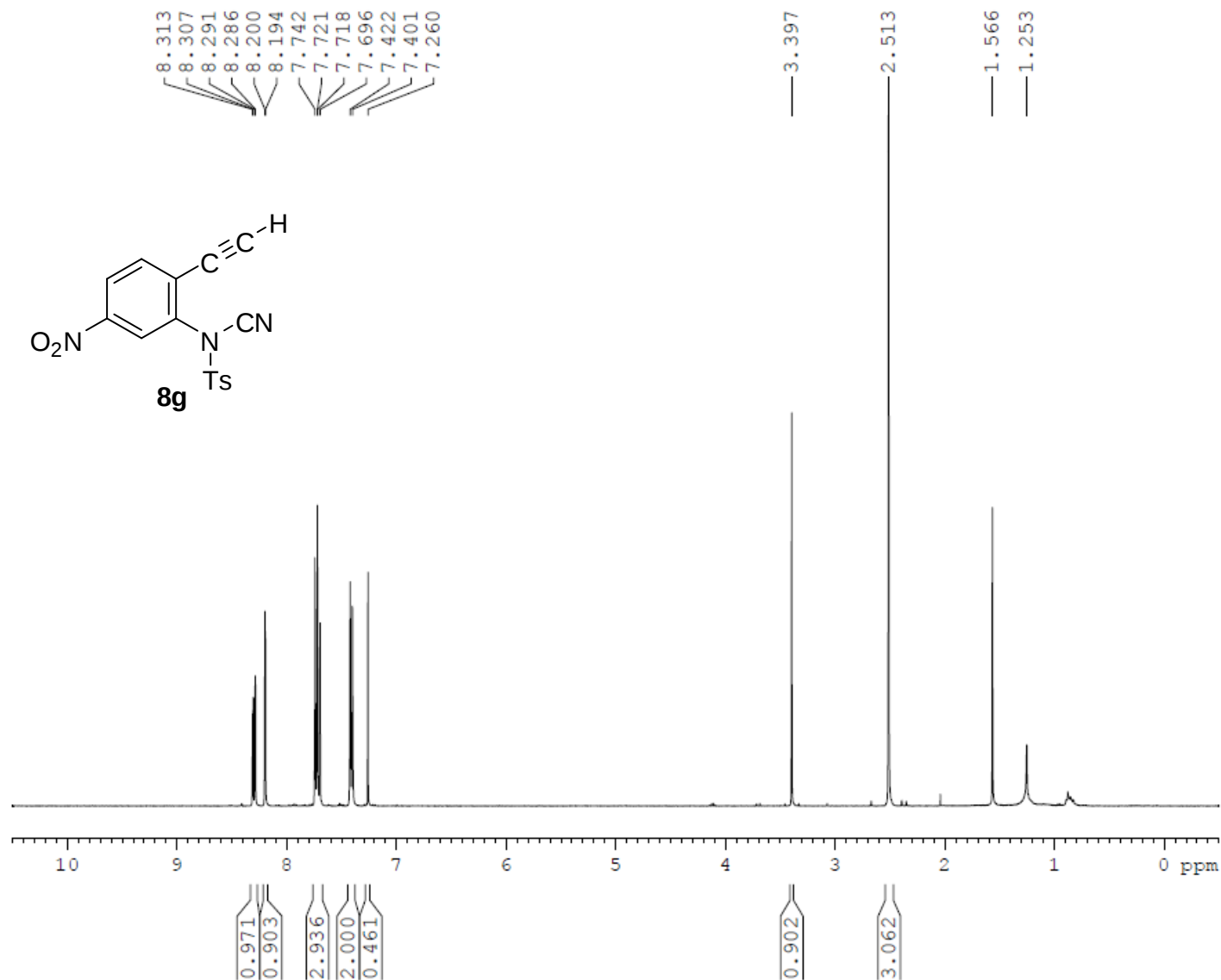
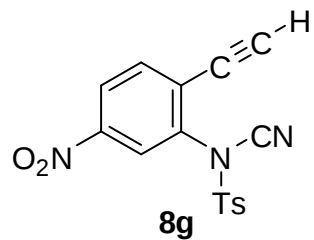
Current Data Parameters
NAME SD-073-pure(old)
EXPNO 7
PROCNO 1

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 =====
CPDPRG2 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

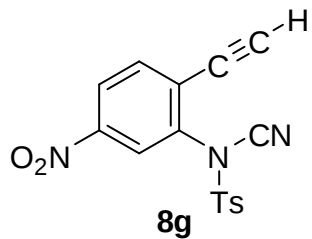


Current Data Parameters
 NAME SC183
 EXPNO 1
 PROCNO 1

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
 TDO 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



147.93
147.70
136.19
135.16
133.00
130.81
128.94
128.55
125.31
125.12
— 106.59

— 90.06
77.55
77.23
76.91
76.09

— 22.11

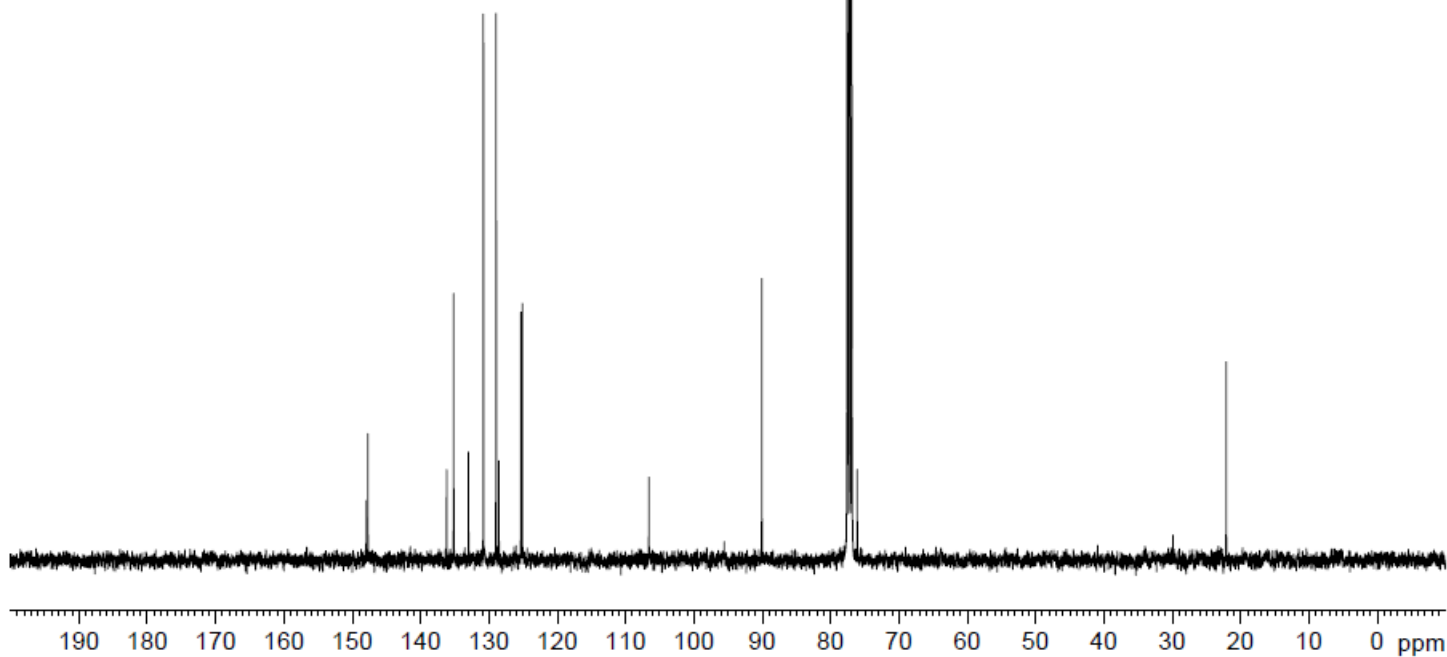
Current Data Parameters
NAME SC183
EXPNO 2
PROCNO 1

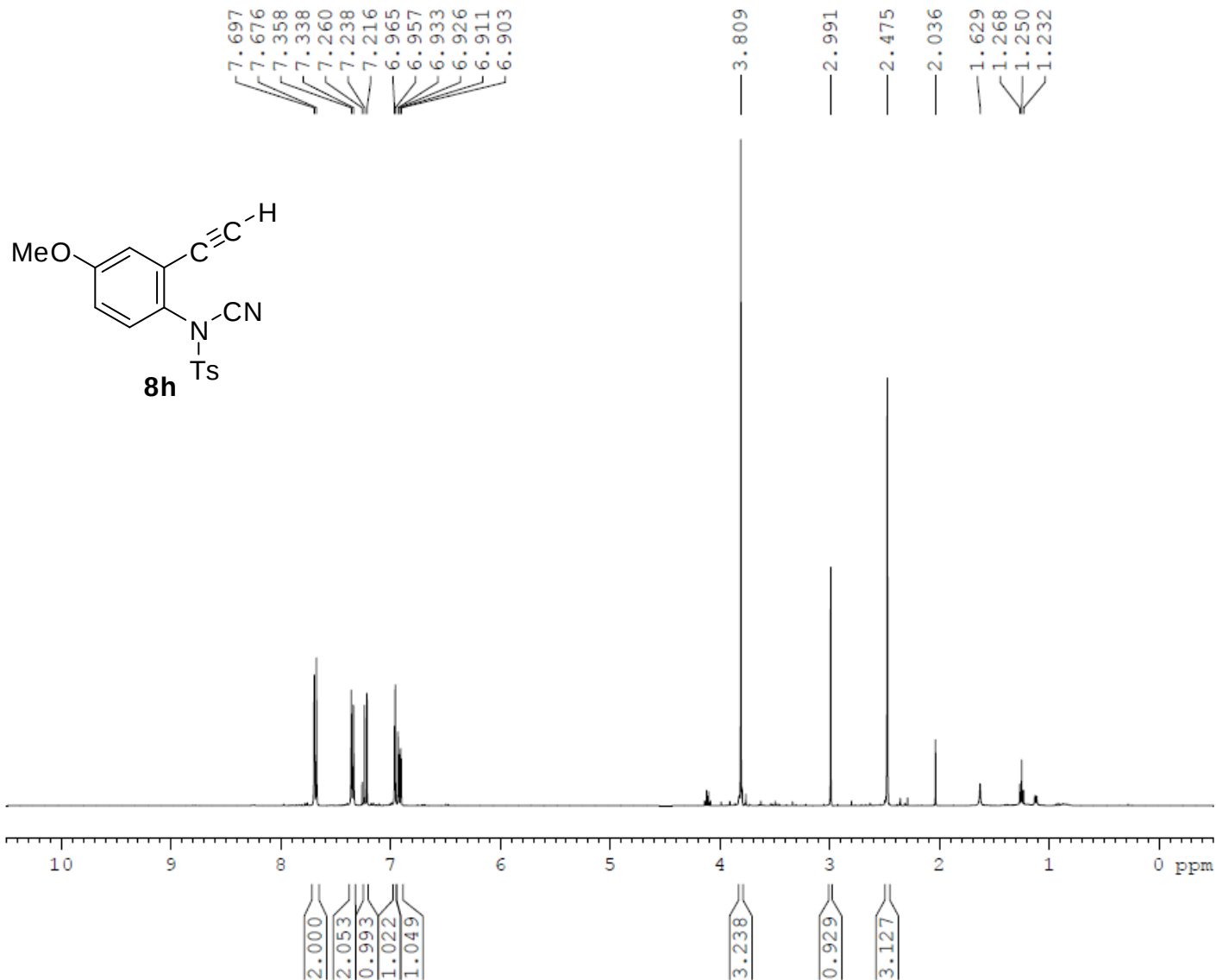
F2 - Acquisition Parameters
Date_ 20140904
Time 19.27
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 619
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.623319 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



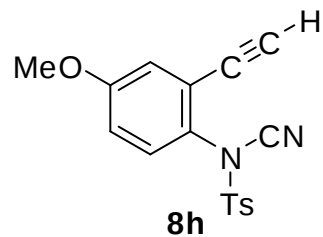


Current Data Parameters
 NAME SC106
 EXPNO 1
 PROCNO 1

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 7211.530 Hz
 FIDRES 0.220070 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



—160.82
 —146.75
 133.41
 131.10
 130.38
 128.93
 127.65
 123.34
 118.74
 116.32
 107.72

84.21
 77.55
 77.38
 77.23
 76.91

—55.94

—22.00

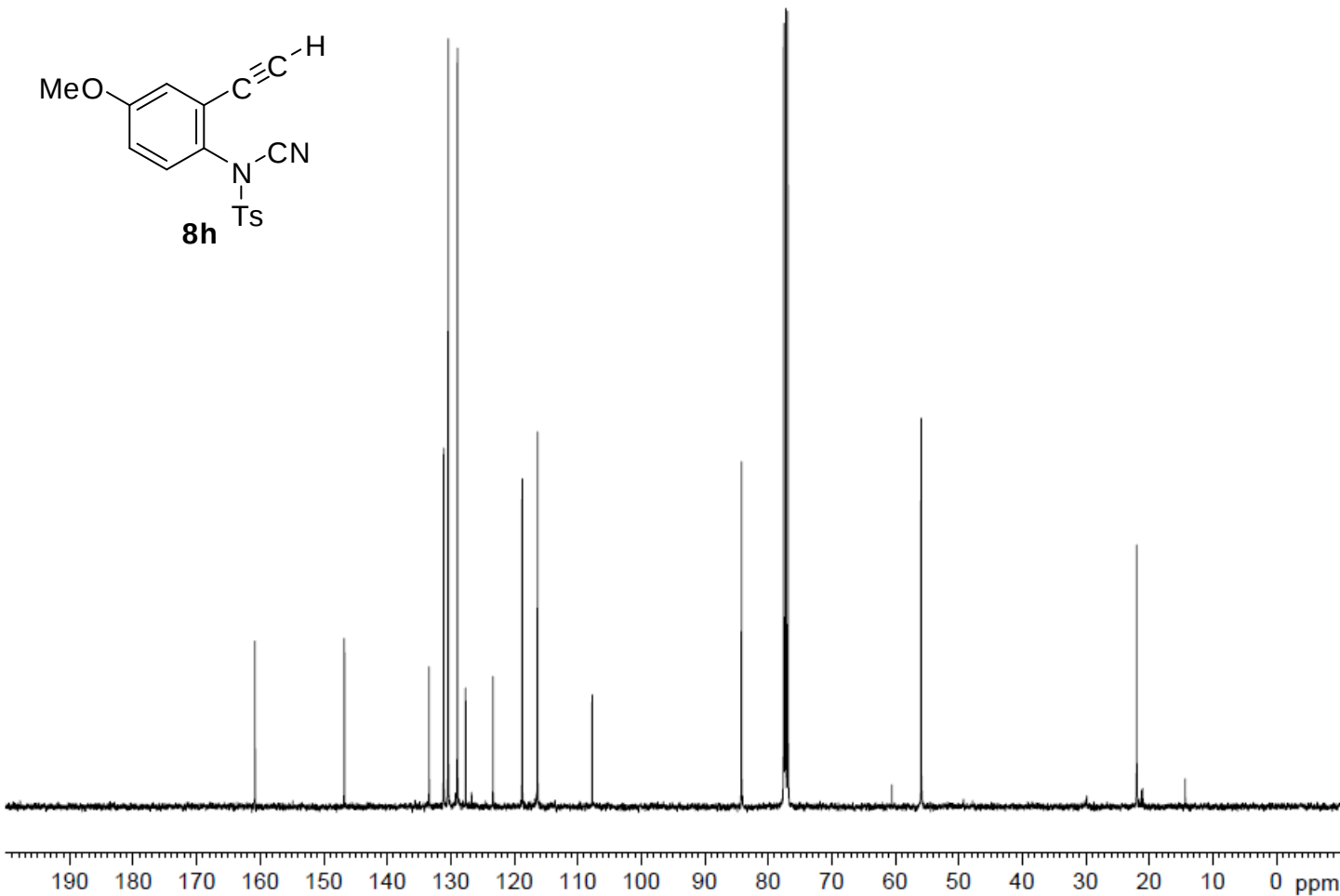
Current Data Parameters
 NAME SC106
 EXPNO 3
 PROCNO 1

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

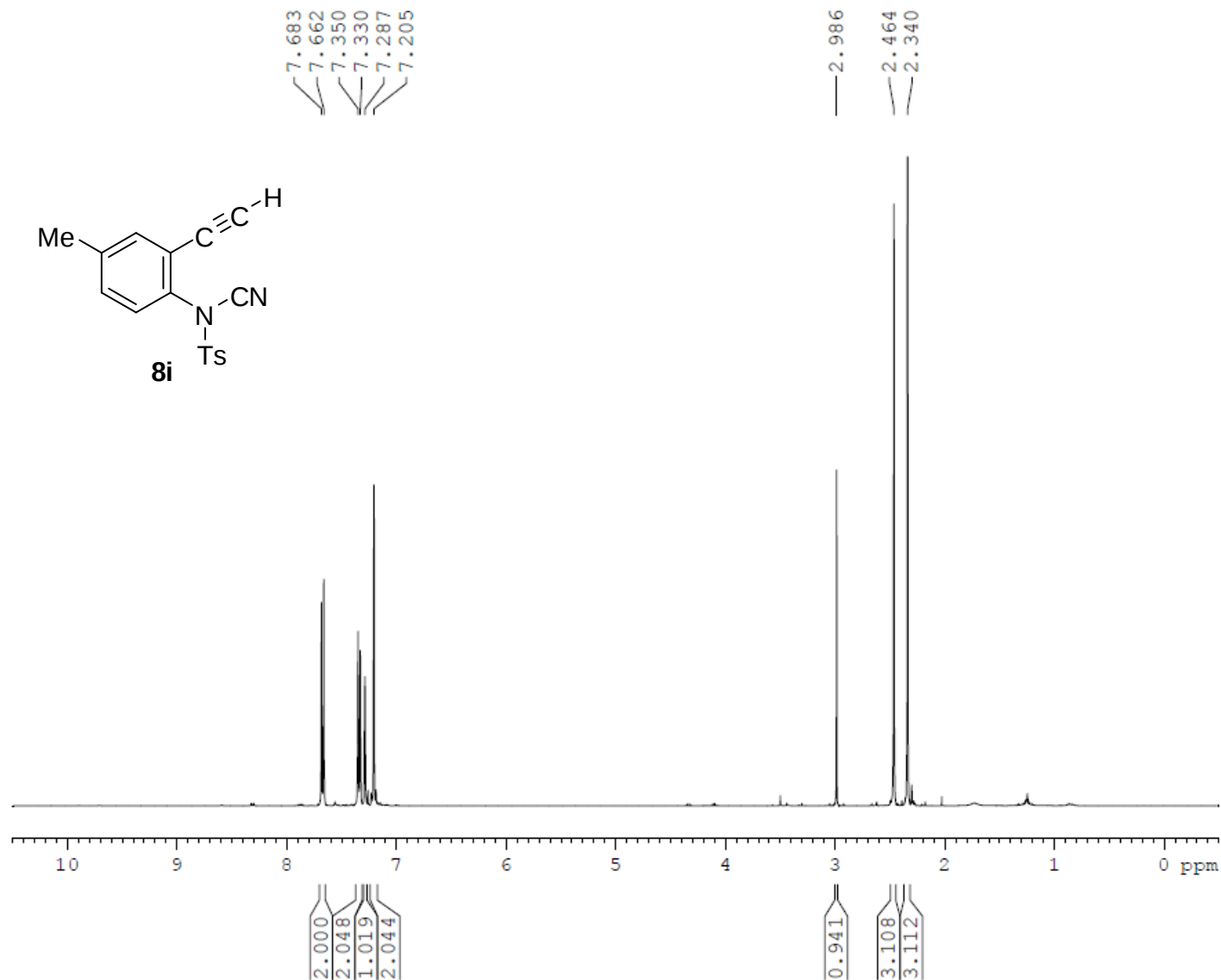
===== CHANNEL f1 =====
 SFO1 100.6233319 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 46.00000000 W

===== 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



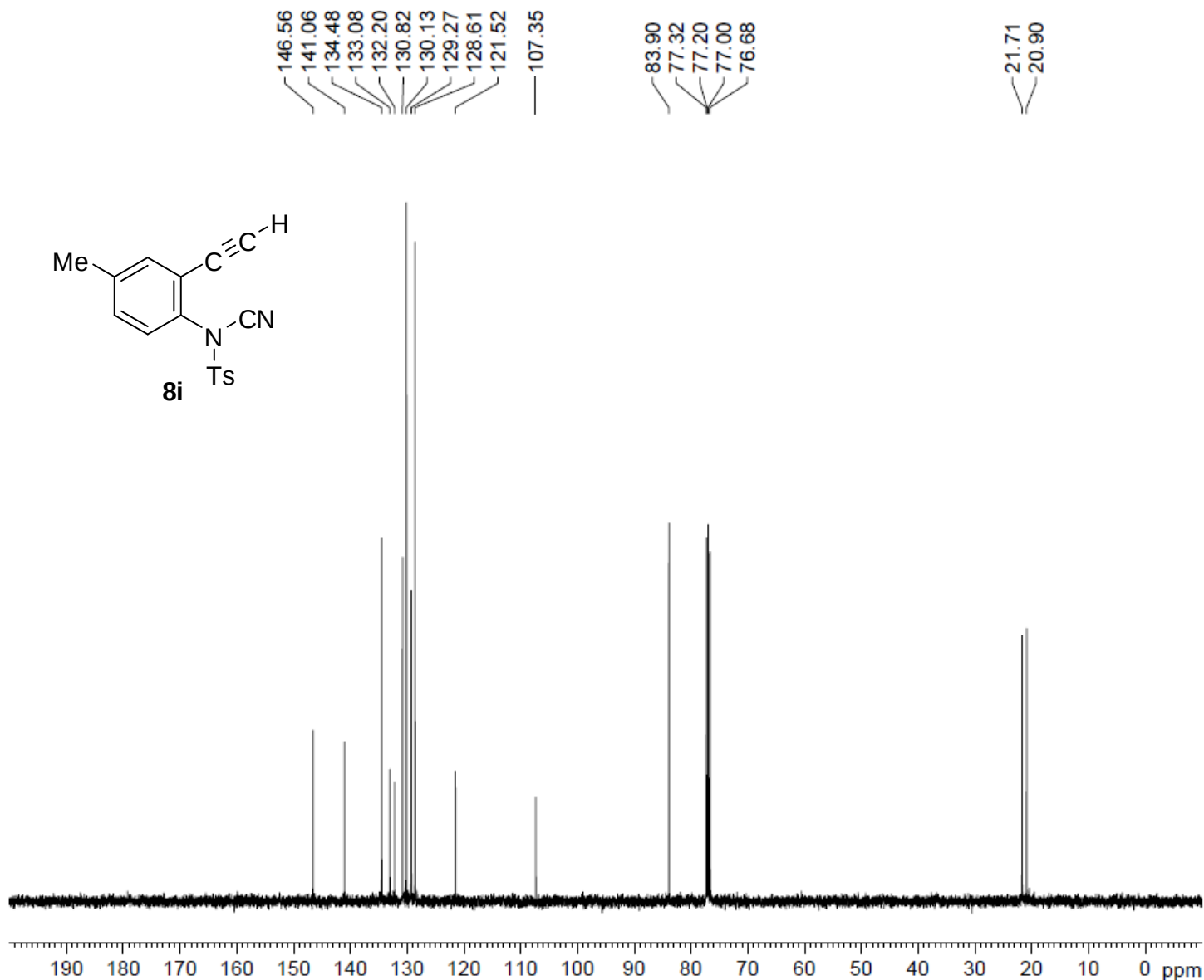
Current Data Parameters
 NAME SD-081(old)
 EXPNO 1
 PROCNO 1

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
 TDO 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

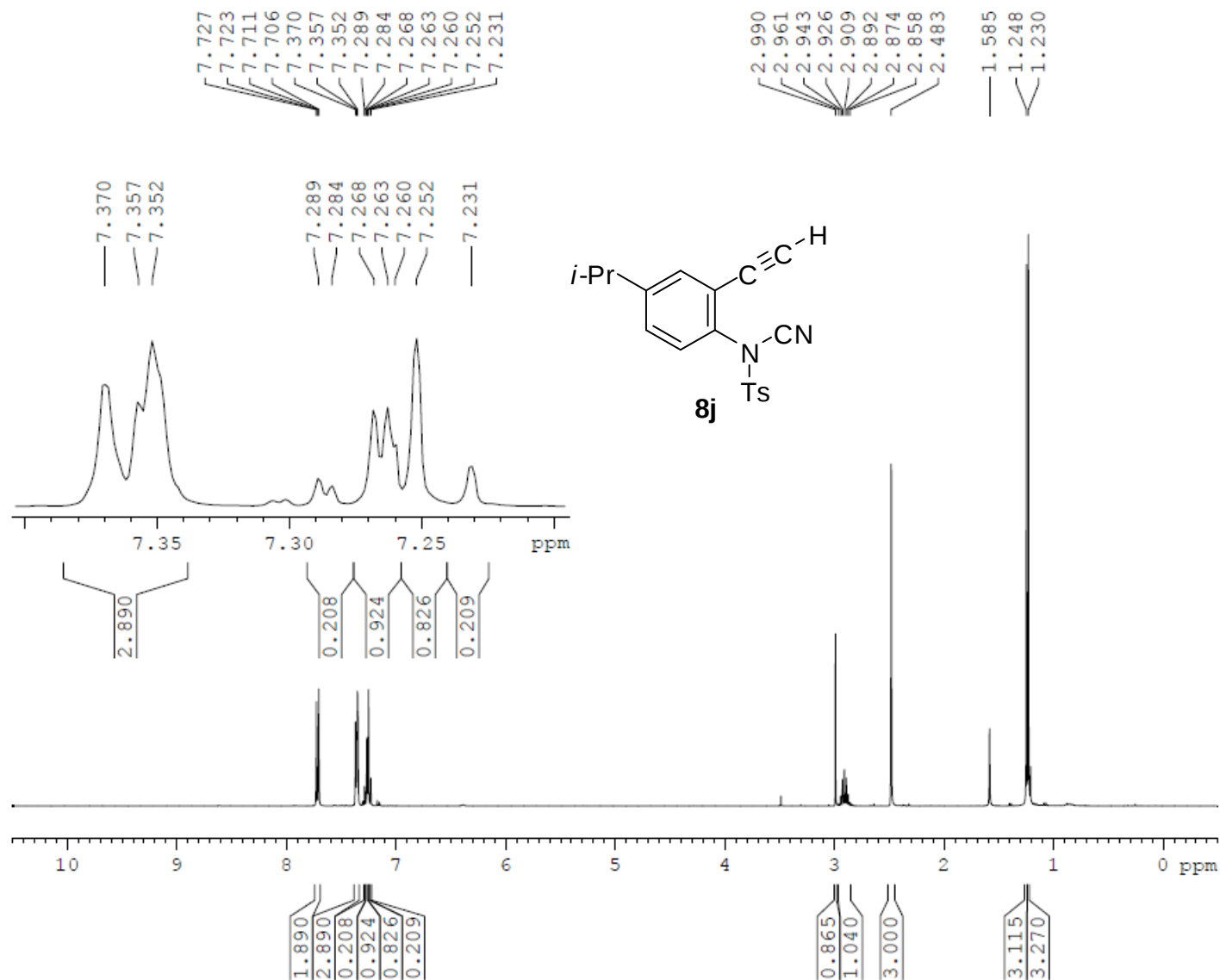
F2 - Acquisition Parameters
Date_ 20140423
Time 19.38
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 206
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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



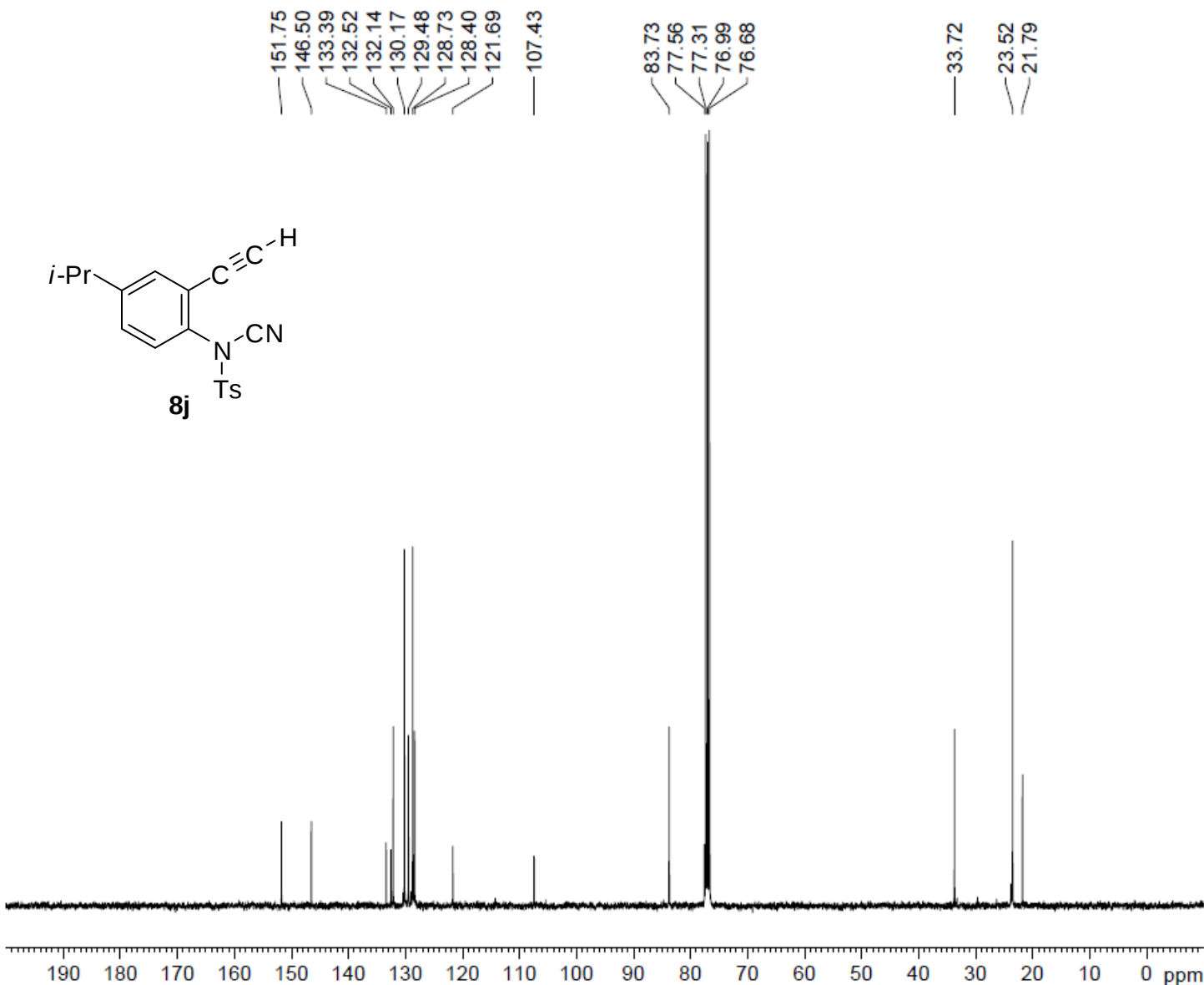
Current Data Parameters
 NAME SD-091(new)
 EXPNO 1
 PROCNO 1

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
 TDO 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



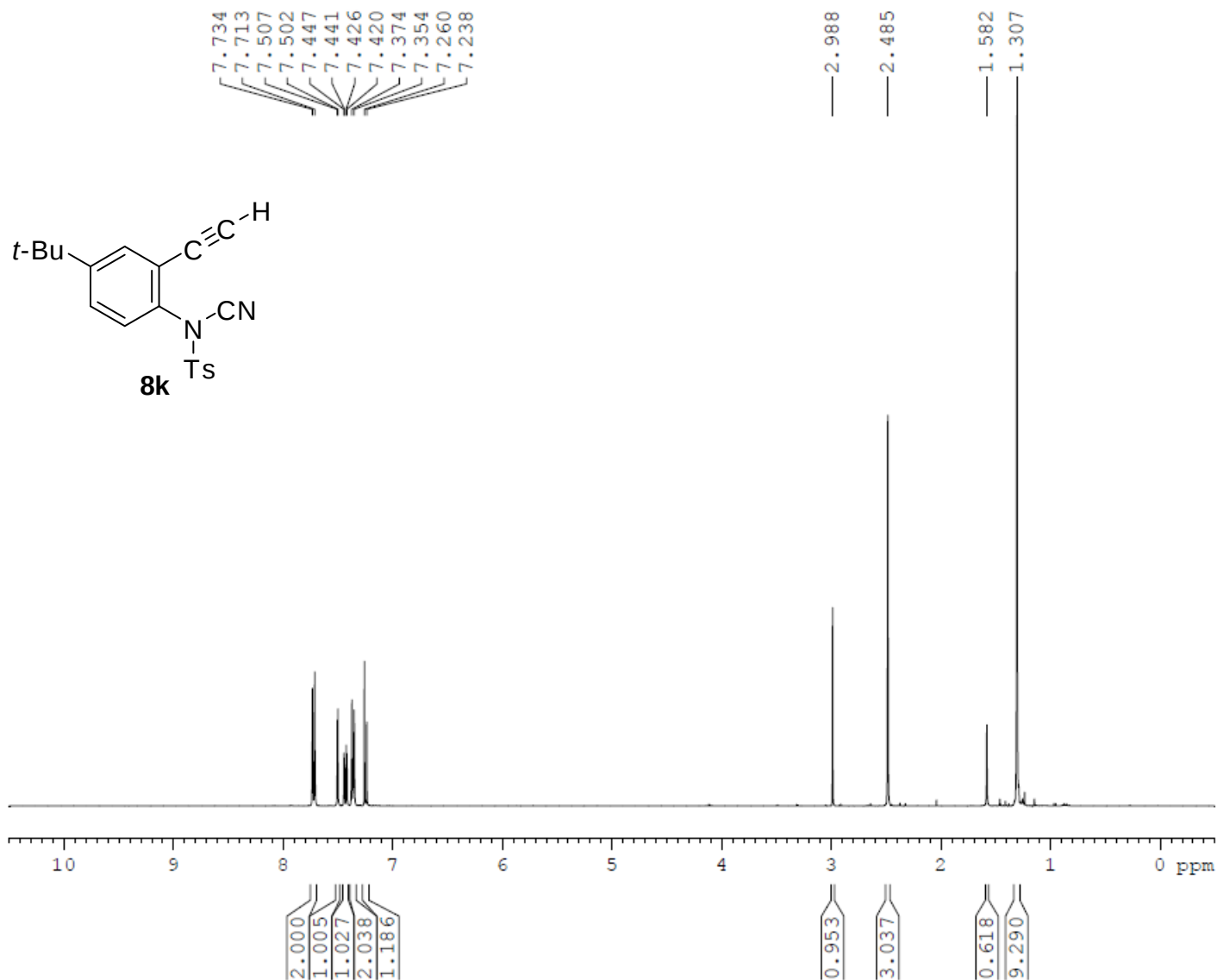
Current Data Parameters
NAME SD-091(new)
EXPNO 3
PROCNO 1

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
CPDPRG2 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

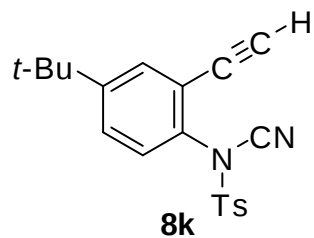


Current Data Parameters
 NAME SC157
 EXPNO 2
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130091 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



154.34
146.74
133.60
132.46
131.45
130.42
129.39
128.94
127.65
121.52
107.66

83.80
77.95
77.55
77.23
76.91

35.11
31.20
22.04

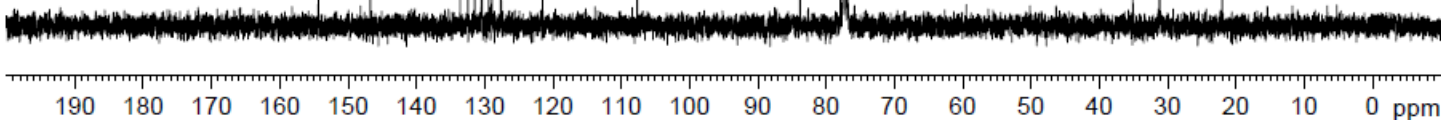
Current Data Parameters
NAME SC157
EXPNO 4
PROCNO 1

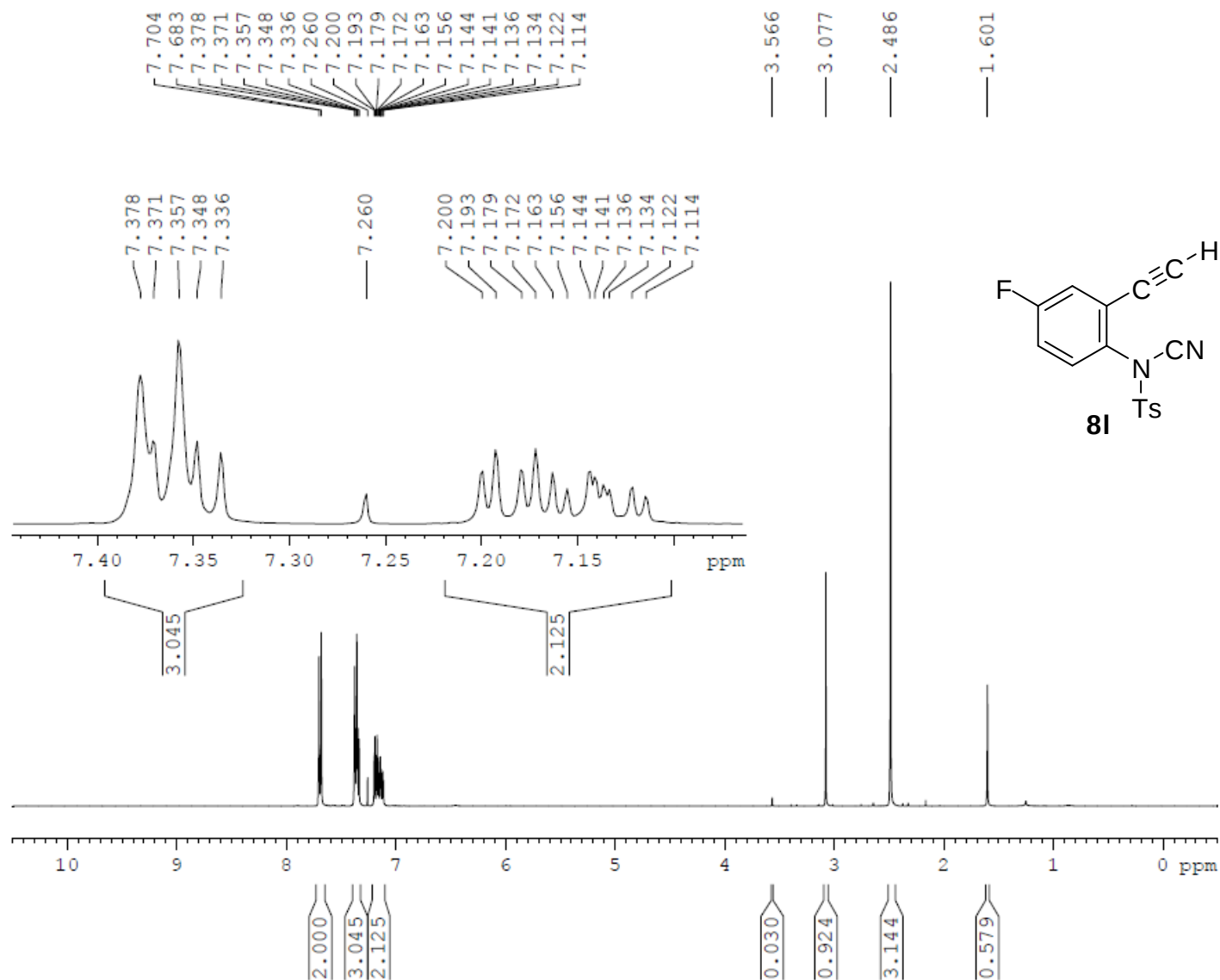
F2 - Acquisition Parameters
Date_ 20140707
Time 10.21
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 472
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4597.6
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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



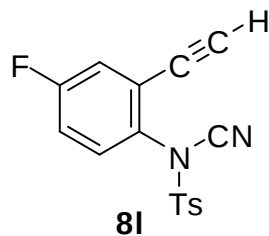
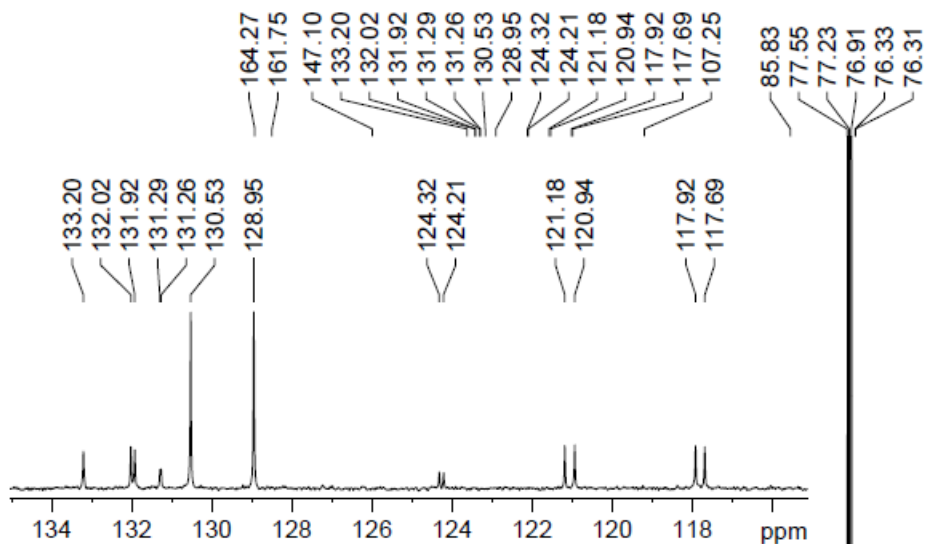


Current Data Parameters
NAME SC169
EXPNO 3
PROCNO 1

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



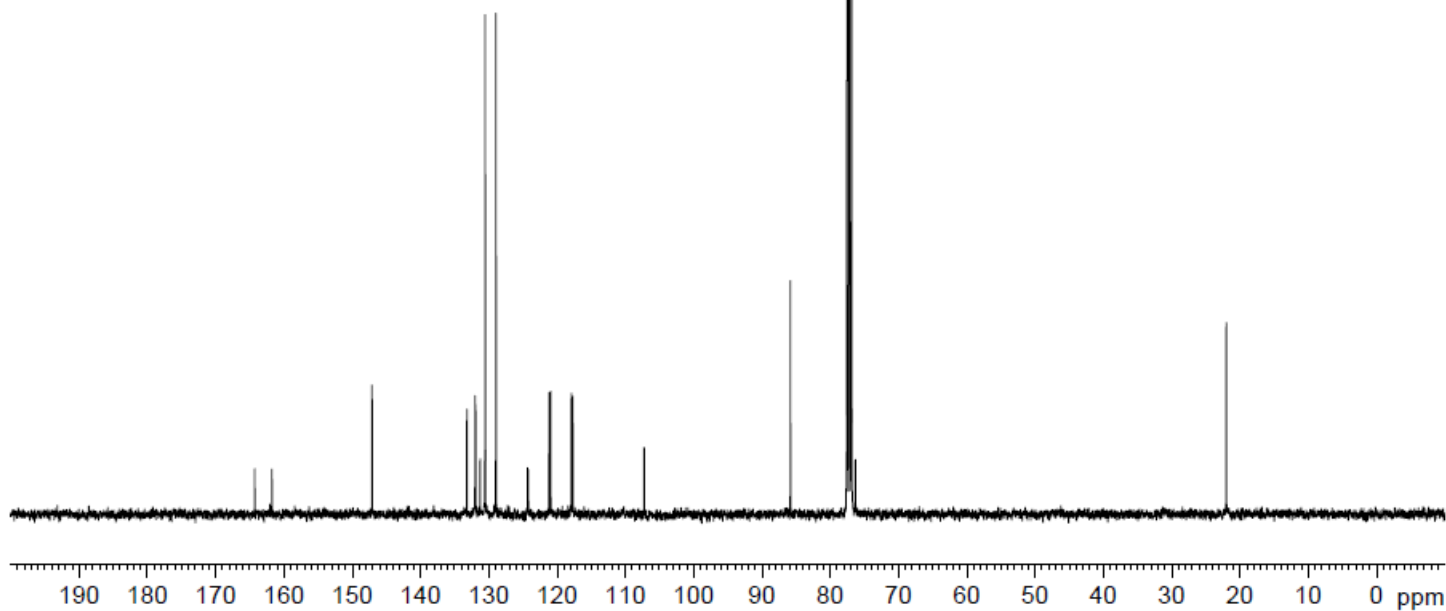
Current Data Parameters
 NAME SC169
 EXPNO 5
 PROCNO 1

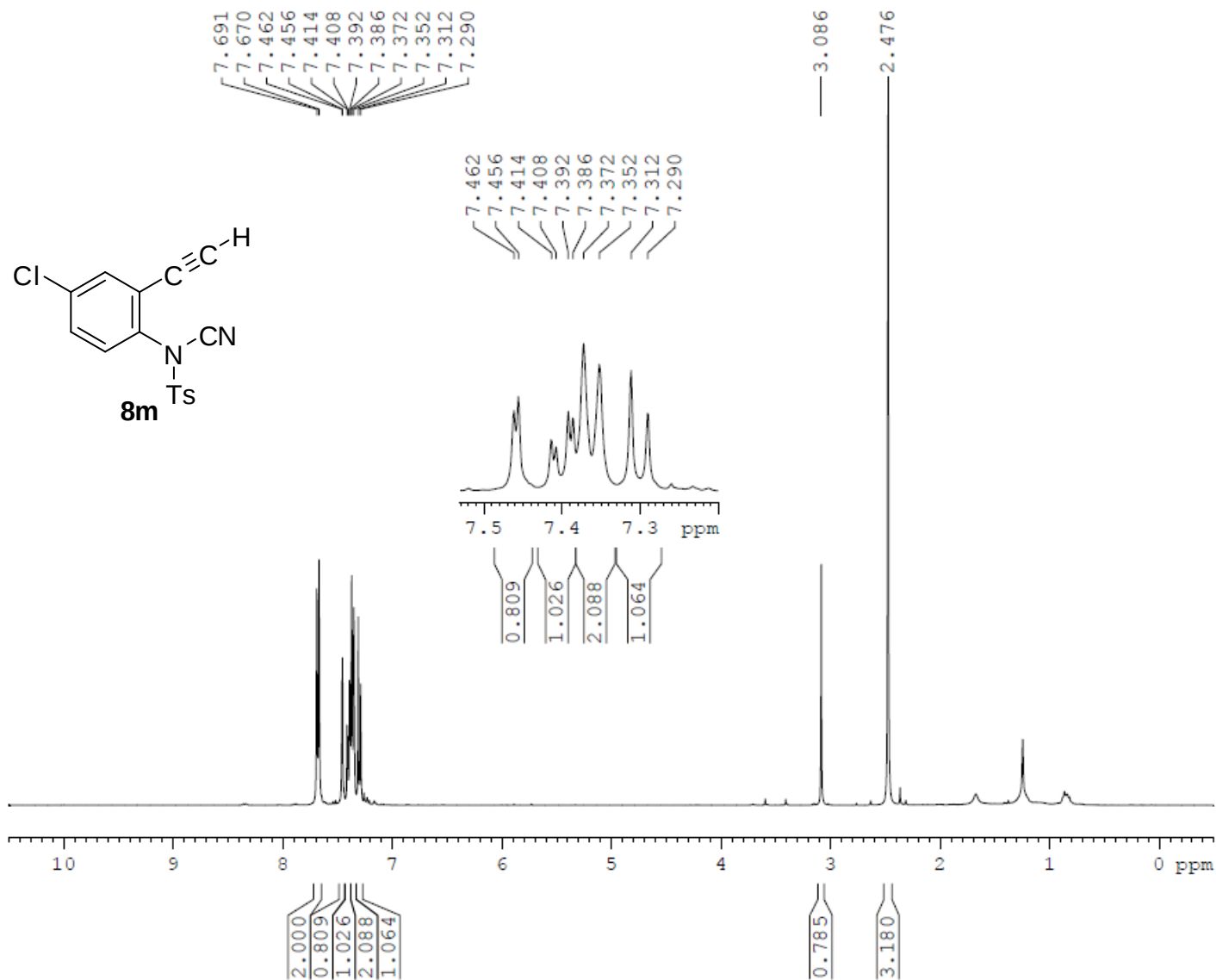
F2 - Acquisition Parameters
 Date_ 20140815
 Time 9.19
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 299.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO 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
 CPDPRG2 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



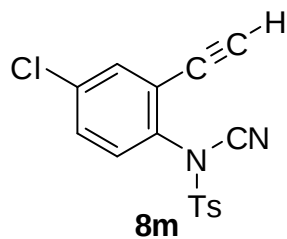


Current Data Parameters
 NAME SD-098(new)
 EXPNO 1
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130093 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



146.93
136.61
133.77
133.27
132.80
130.82
130.30
128.63
123.31
— 106.82

85.79
77.31
77.00
76.68
75.85

— 21.77

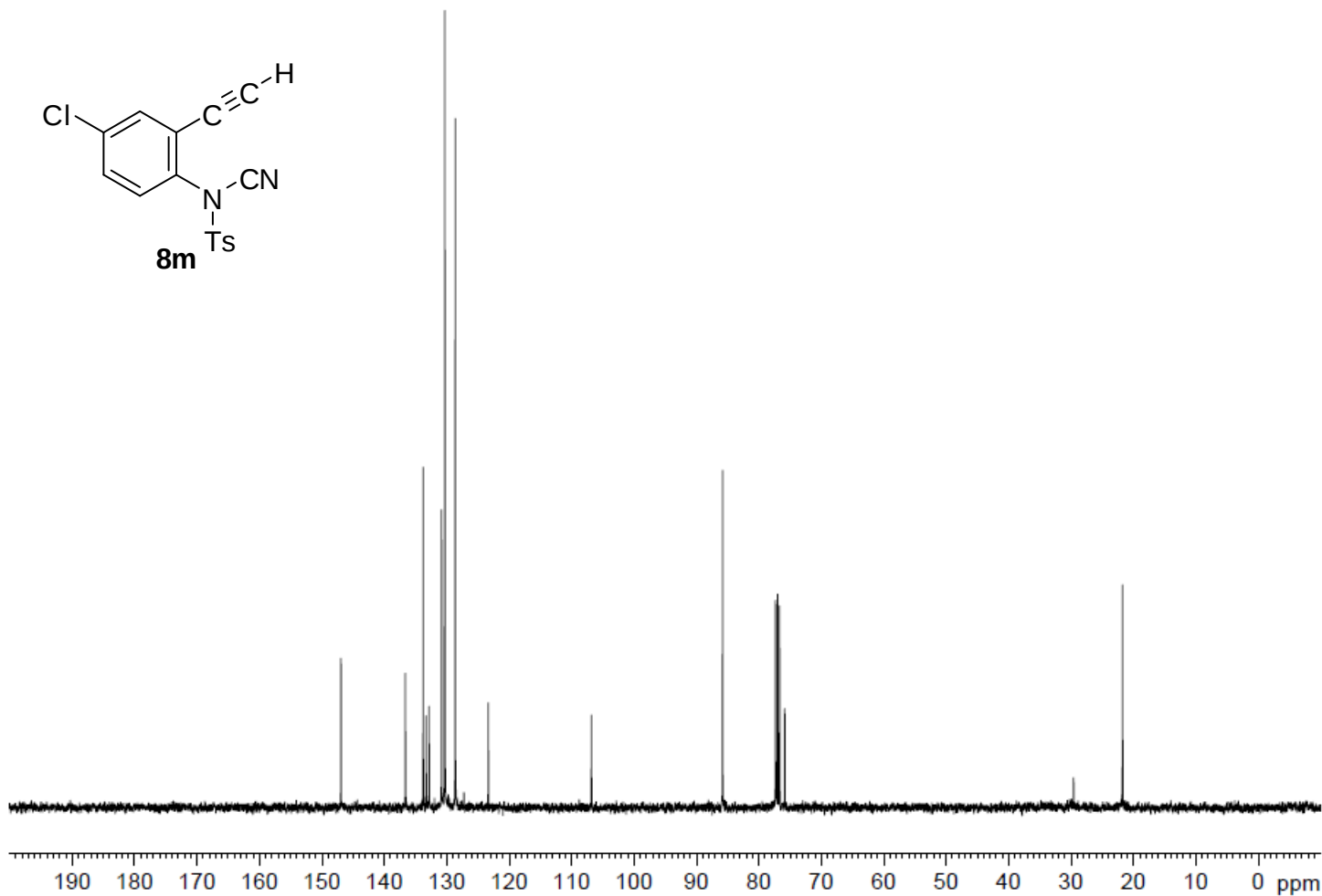
Current Data Parameters
NAME SD-098(new)
EXPNO 3
PROCNO 1

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

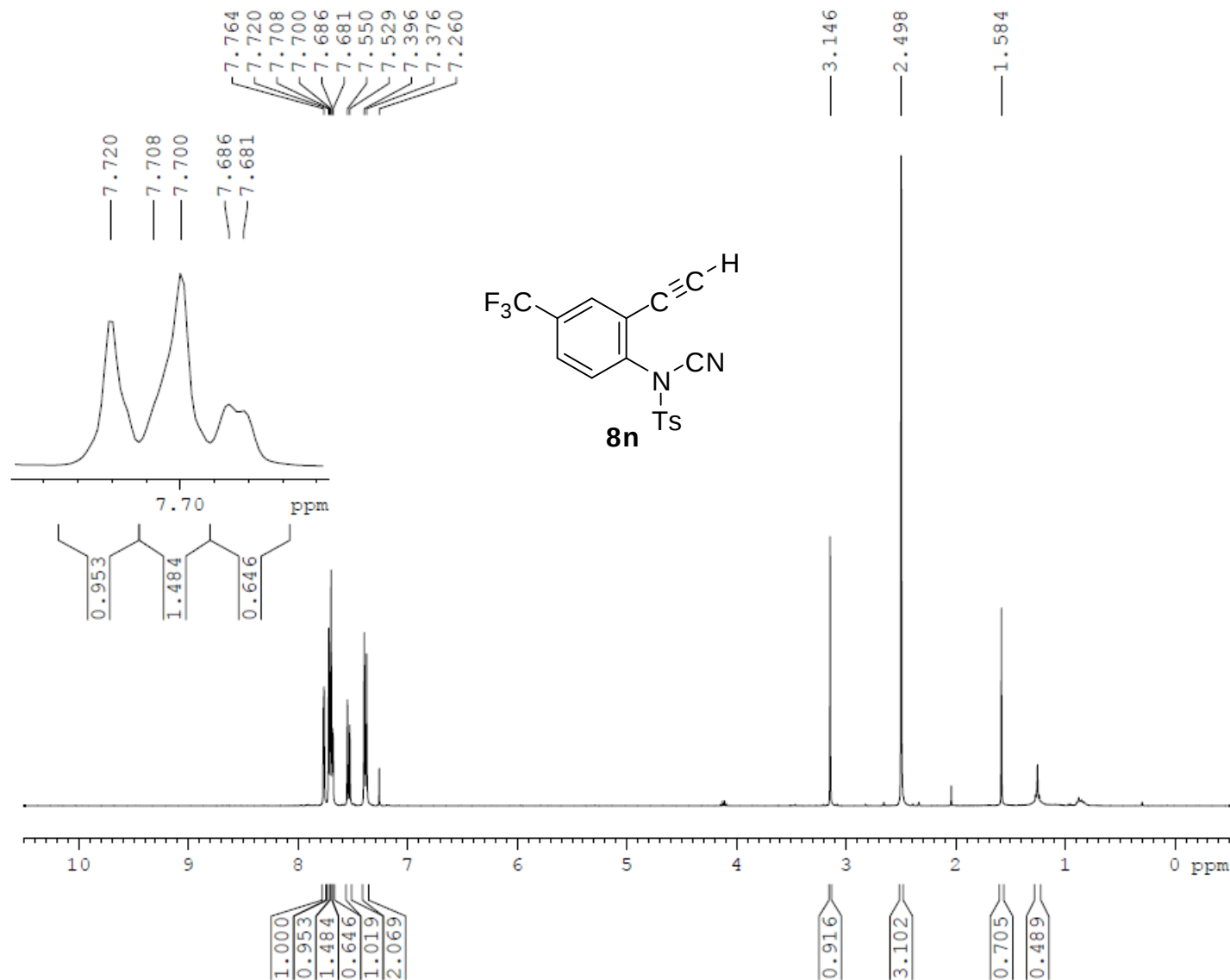
===== CHANNEL f1 =====
SFO1 100.623319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 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

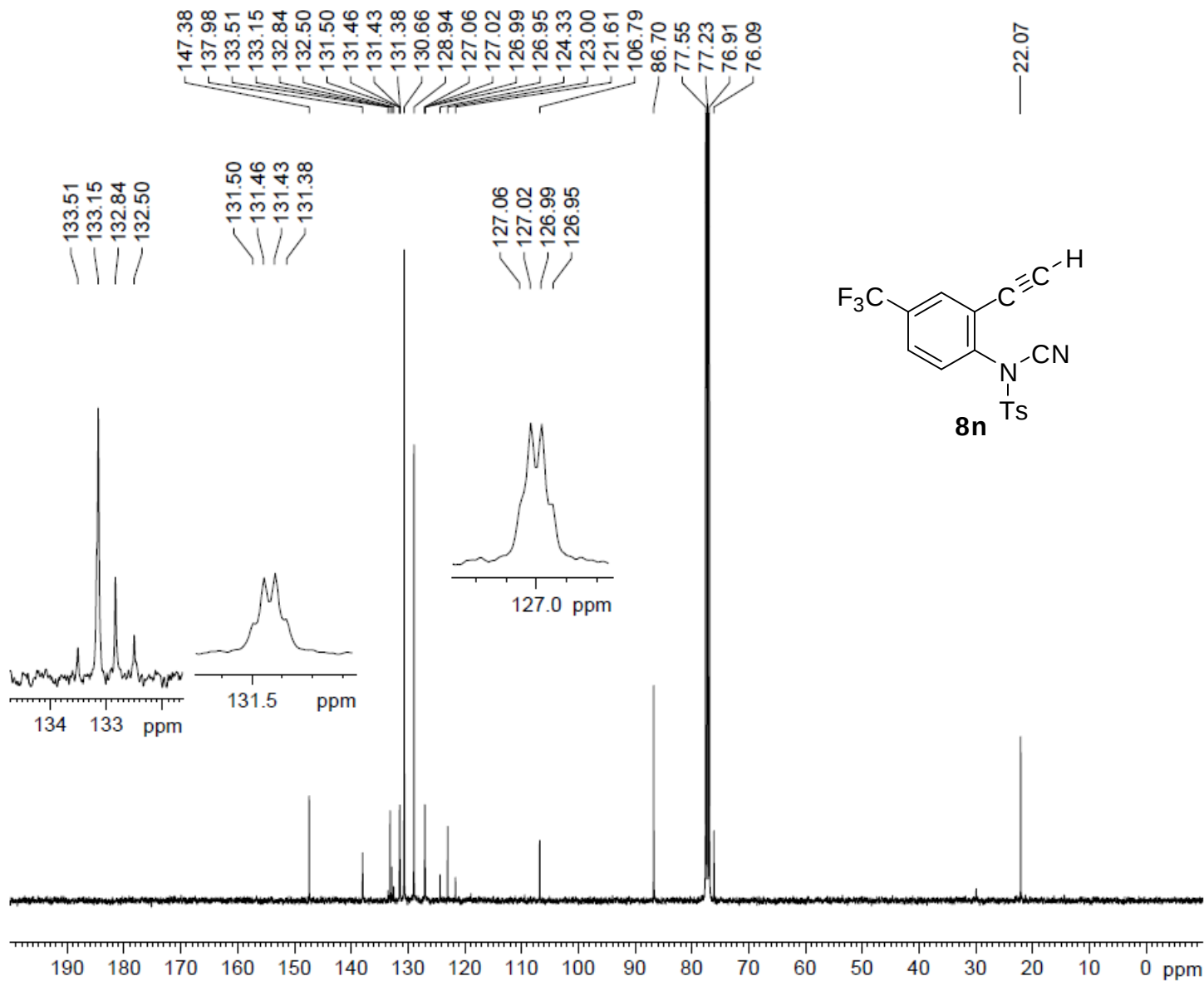


Current Data Parameters
 NAME SC177-1
 EXPNO 2
 PROCNO 1

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

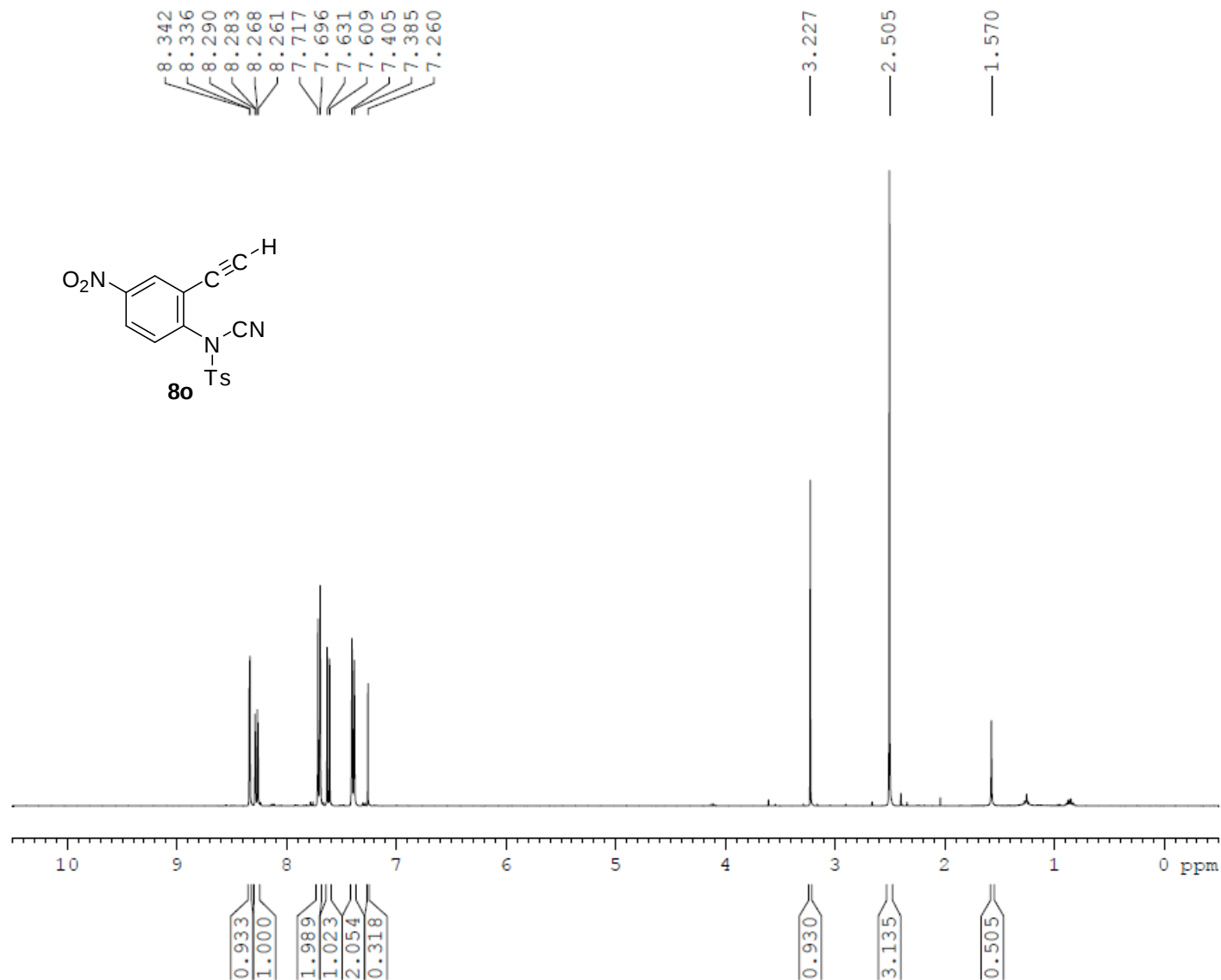
F2 - Acquisition Parameters
 Date_ 20140827
 Time 9.05
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1000
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 299.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

===== CHANNEL f1 =====
 SFO1 100.623319 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

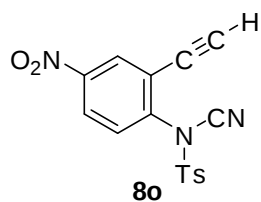


Current Data Parameters
NAME SC195
EXPNO 1
PROCNO 1

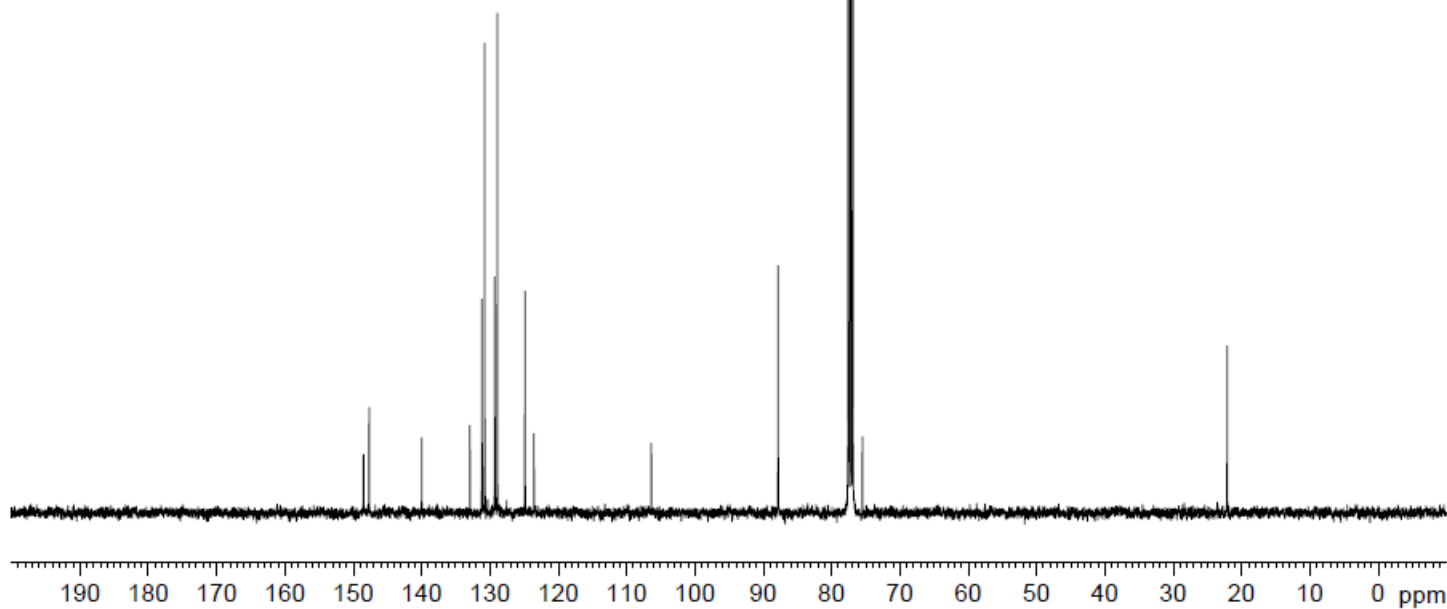
F2 - Acquisition Parameters
Date_ 20141022
Time 2.53
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 12
DS 0
SWH 7211.539 Hz
FIDRES 0.220079 Hz
AQ 2.2719147 sec
RG 177.16
DW 69.333 usec
DE 10.52 usec
TE 297.8 K
D1 2.00000000 sec
TD0 1

===== 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



148.50
147.67
139.97
132.92
131.17
130.76
129.30
128.92
124.87
123.55
106.38
87.83
77.55
77.23
76.91
75.49
22.10



Current Data Parameters
NAME SC195
EXPNO 3
PROCNO 1

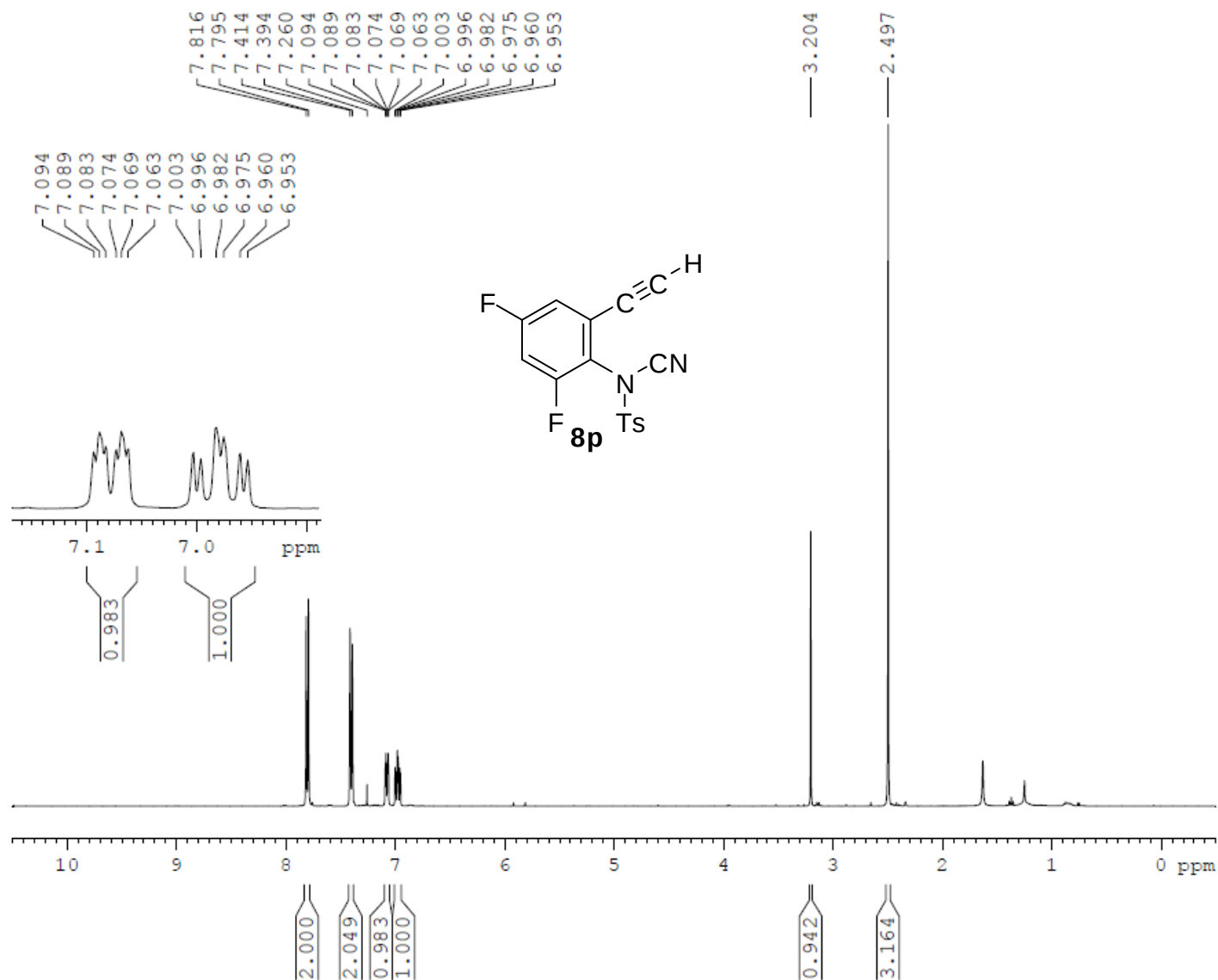
F2 - Acquisition Parameters
Date_ 20141022
Time 3.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 500
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 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

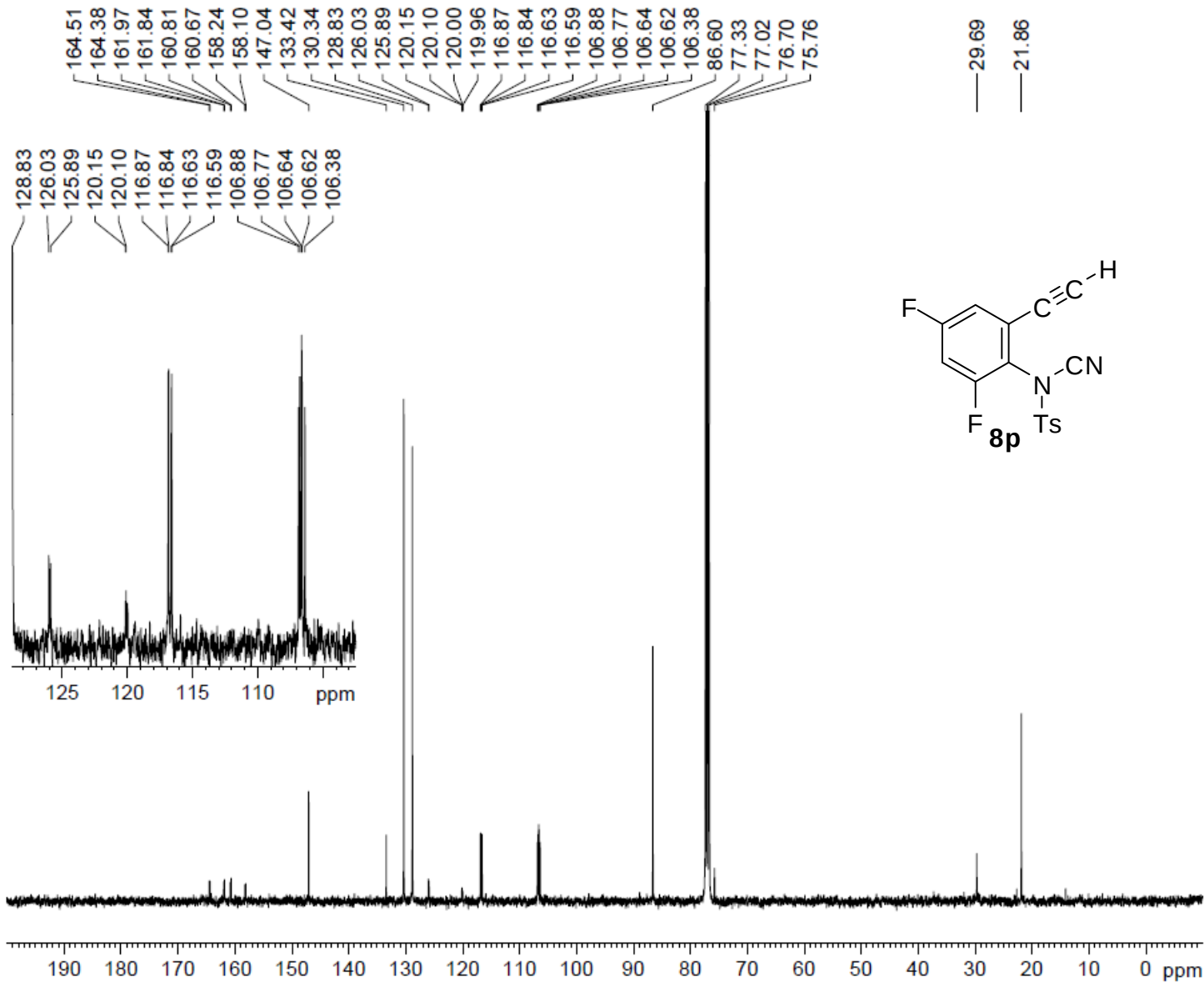


Current Data Parameters
 NAME SD-071(new)
 EXPNO 1
 PROCNO 1

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
 TDO 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



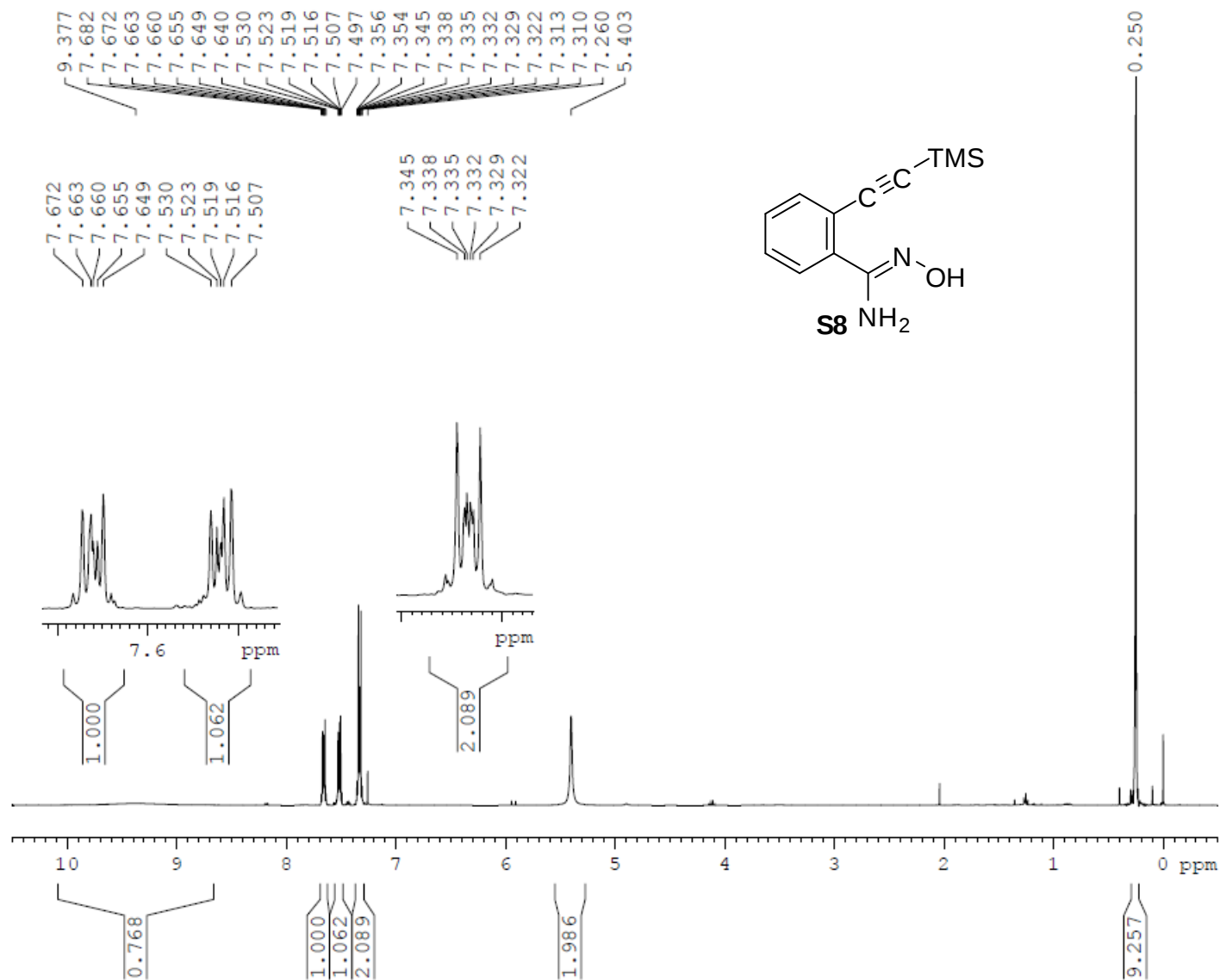
Current Data Parameters
 NAME SD-071(new)
 EXPNO 4
 PROCNO 1

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 100.623319 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

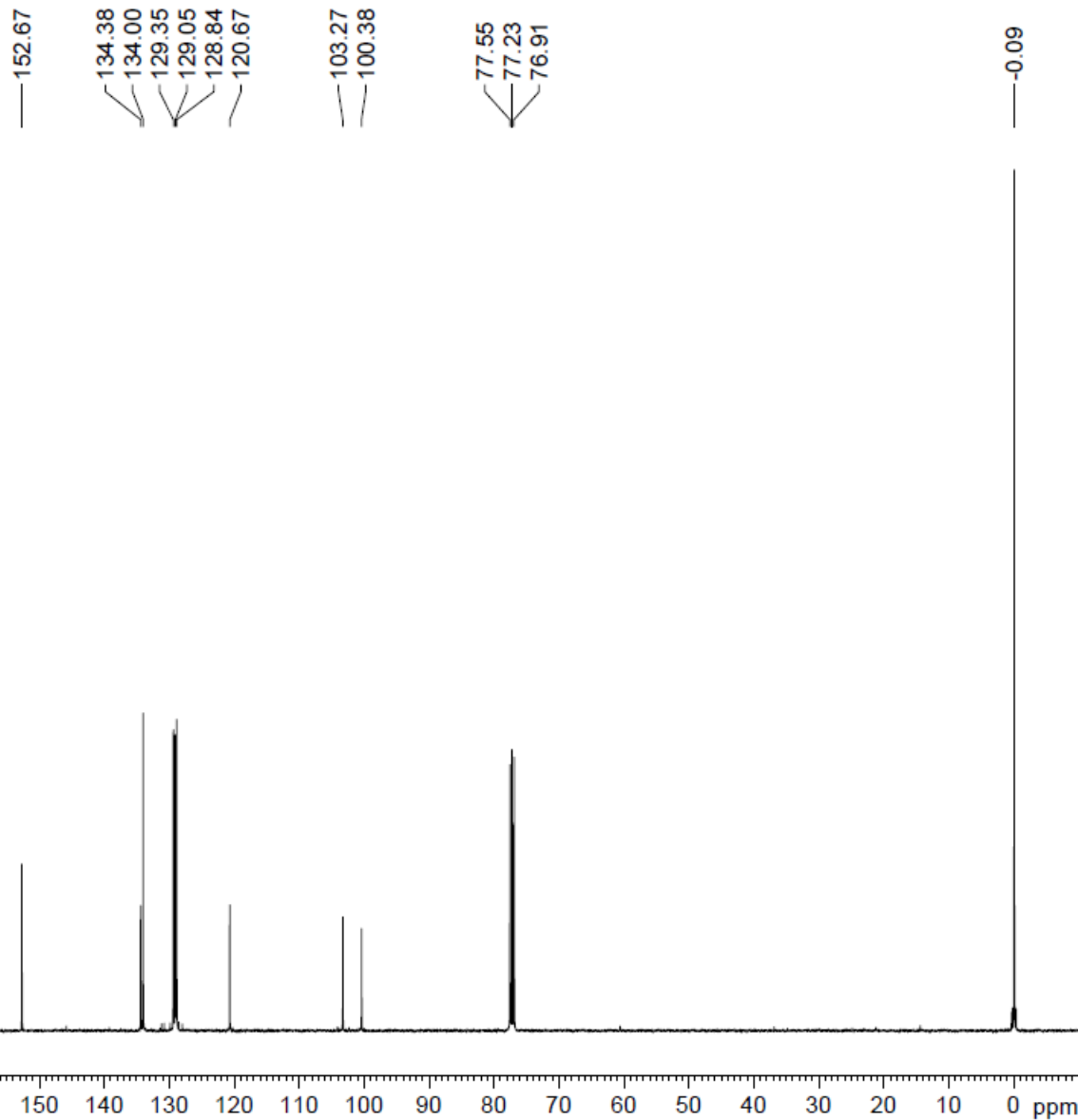
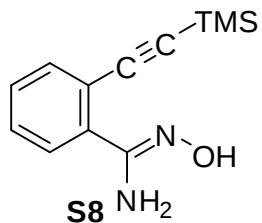


Current Data Parameters
 NAME S0012
 EXPNO 1
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130091 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



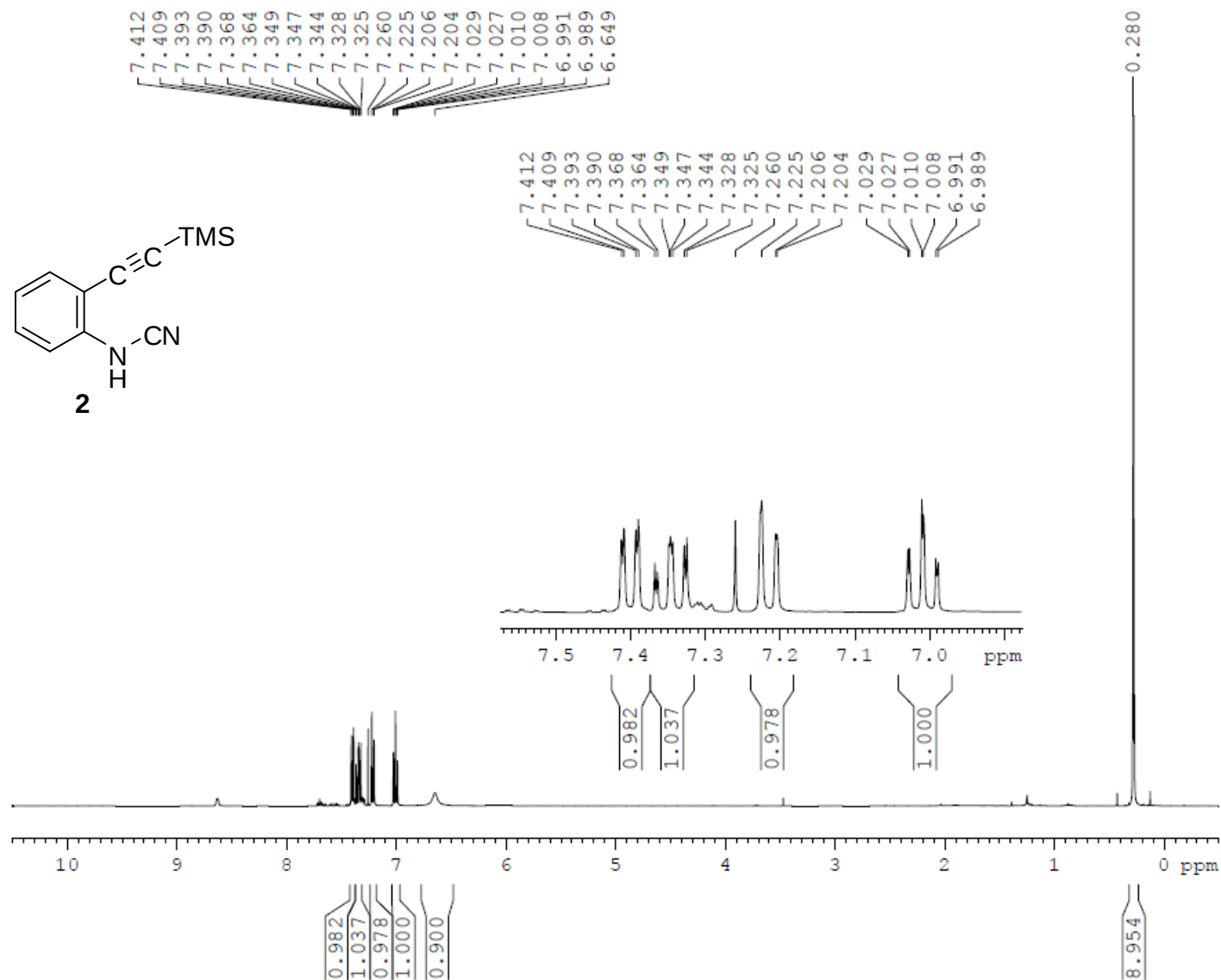
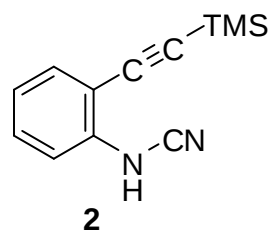
Current Data Parameters
 NAME SO012
 EXPNO 3
 PROCNO 1

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 100.623319 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

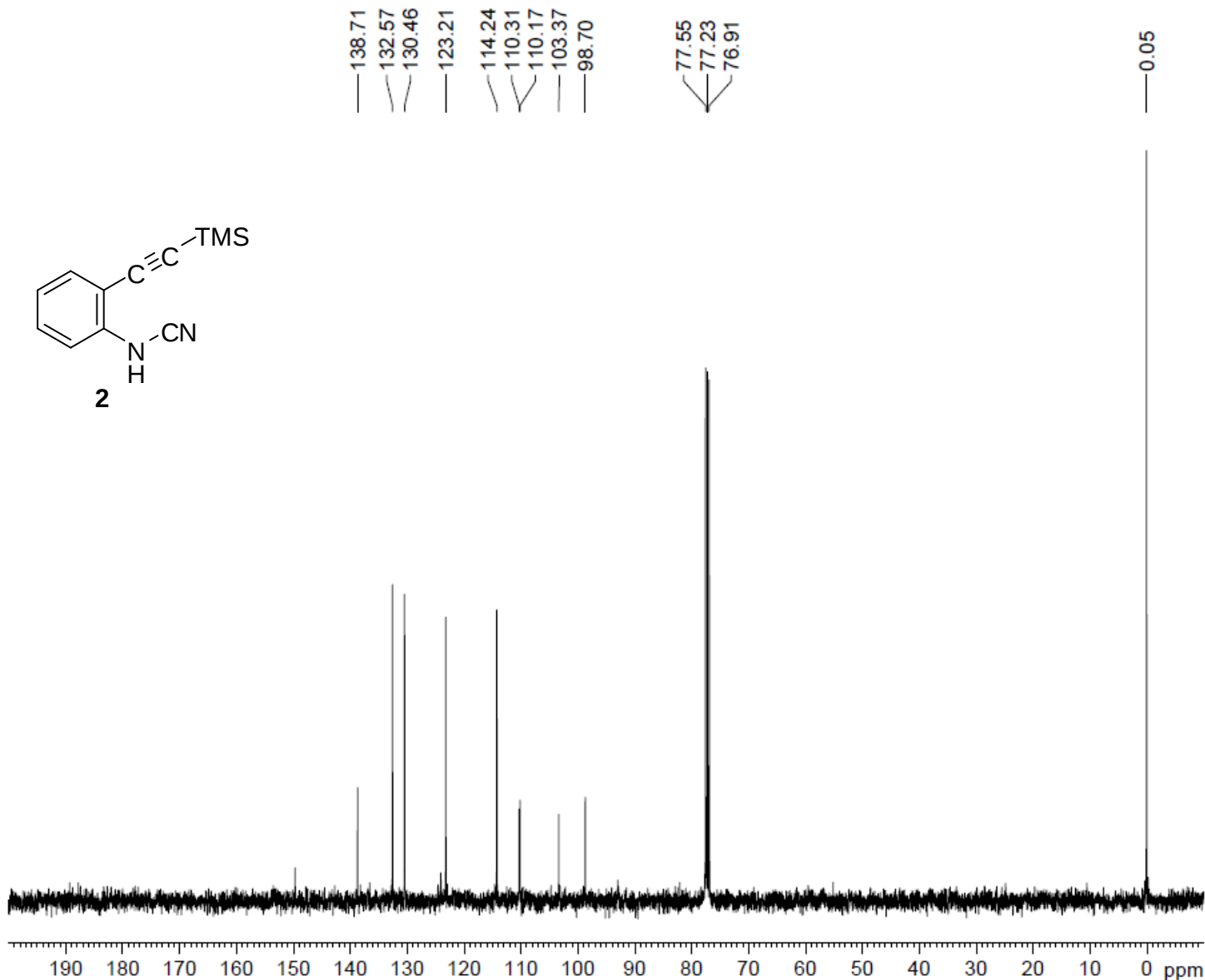
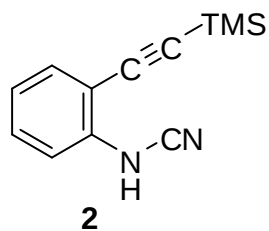


Current Data Parameters
NAME SO146
EXPNO 1
PROCNO 1

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
TDO 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



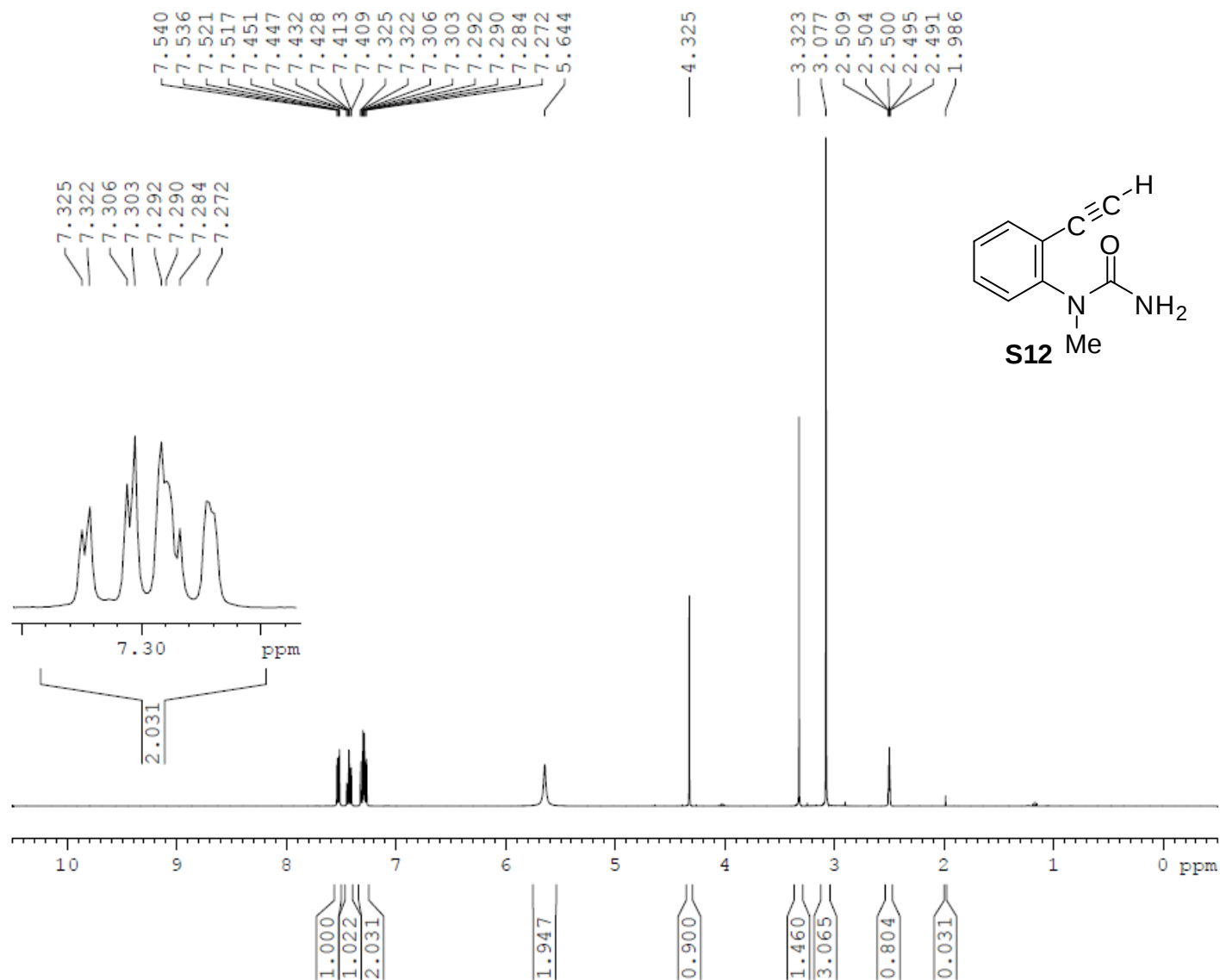
Current Data Parameters
 NAME SO146
 EXPNO 2
 PROCNO 1

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

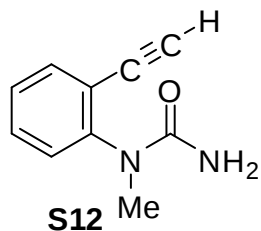


Current Data Parameters
 NAME S0015
 EXPNO 1
 PROCNO 1

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
 TDO 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



157.26
146.02
133.49
130.08
129.08
127.15
121.14
84.65
80.44
40.13
39.92
39.71
39.50
39.29
39.08
38.87
36.46

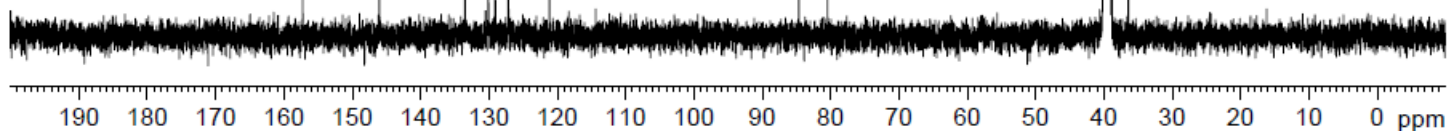
Current Data Parameters
NAME SO015
EXPNO 3
PROCNO 1

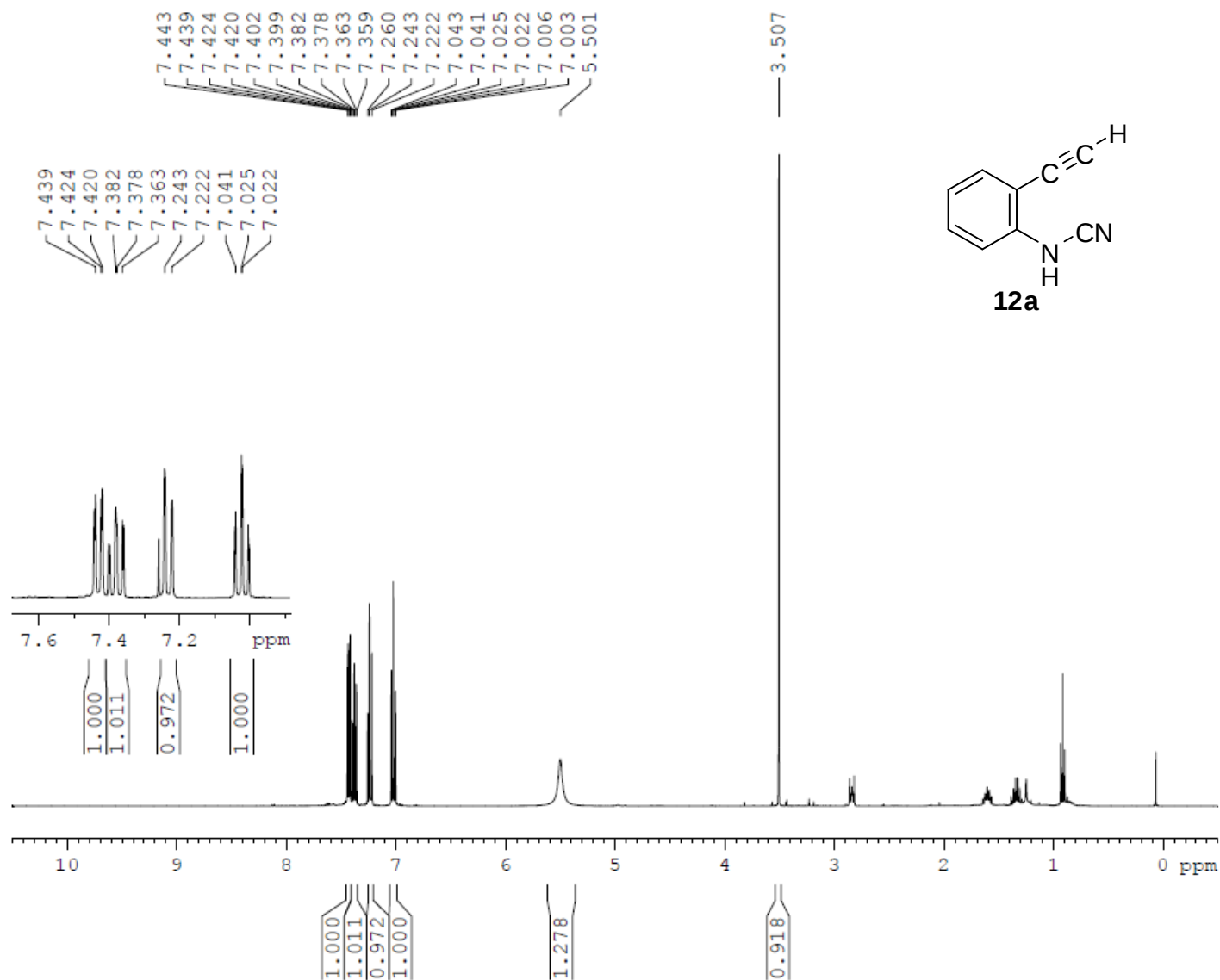
F2 - Acquisition Parameters
Date_ 20141121
Time 10.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 261
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 4597.6
DW 20.800 usec
DE 6.50 usec
TE 299.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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



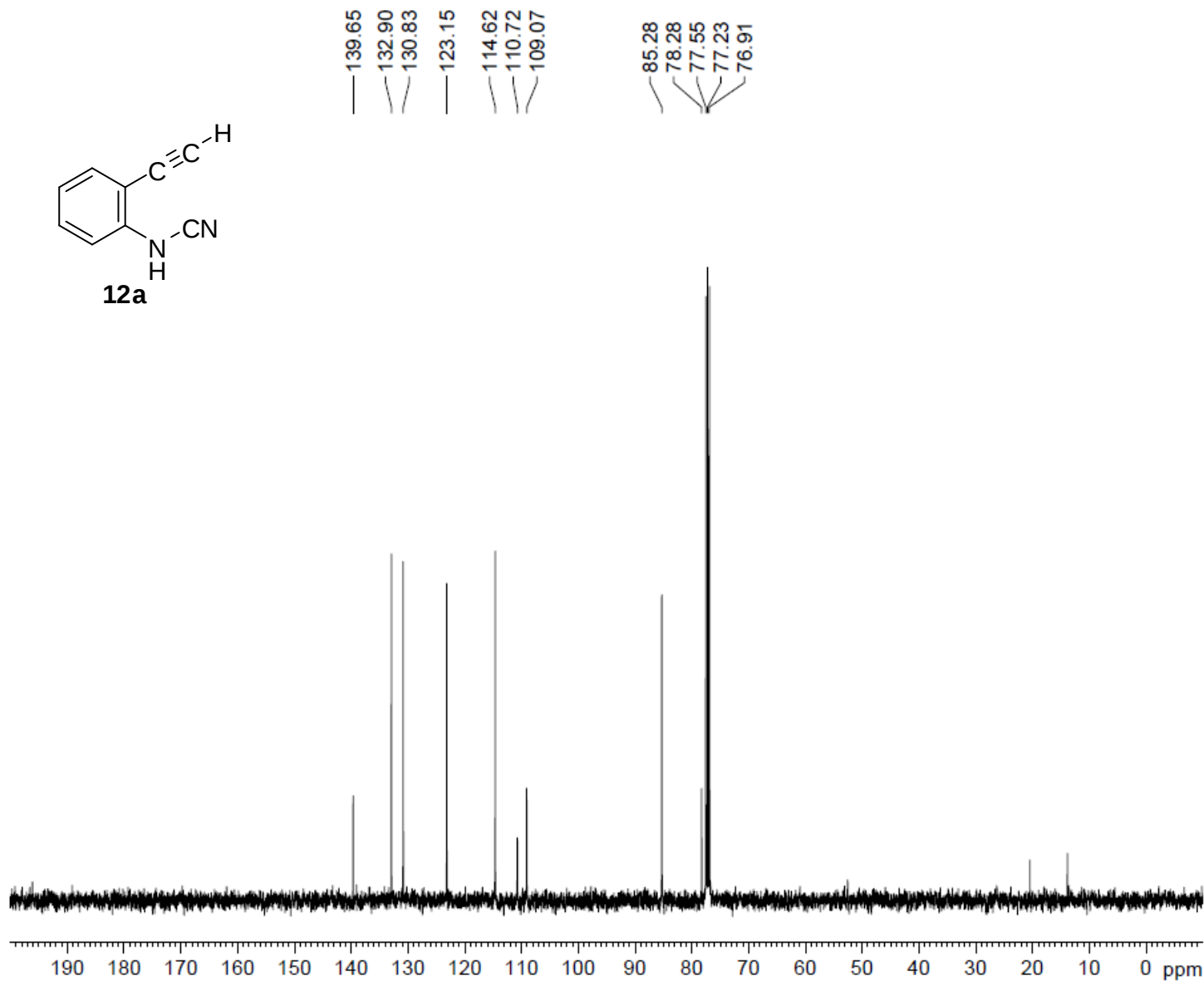
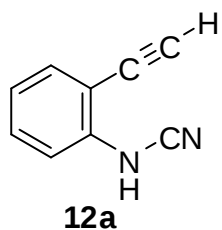


Current Data Parameters
 NAME SO147
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150828
 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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130097 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



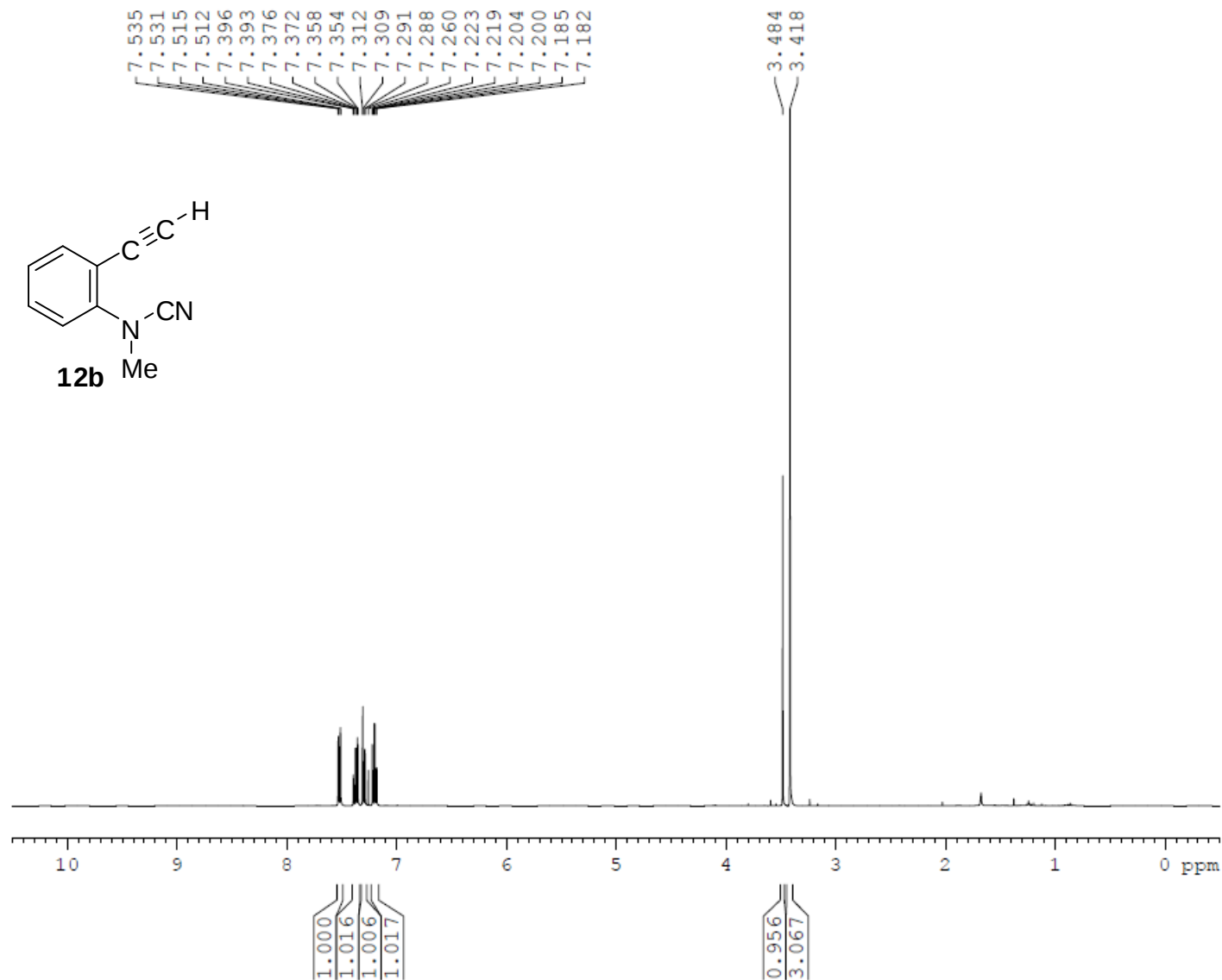
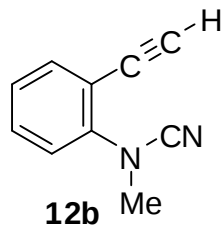
Current Data Parameters
 NAME SO147
 EXPNO 2
 PROCNO 1

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

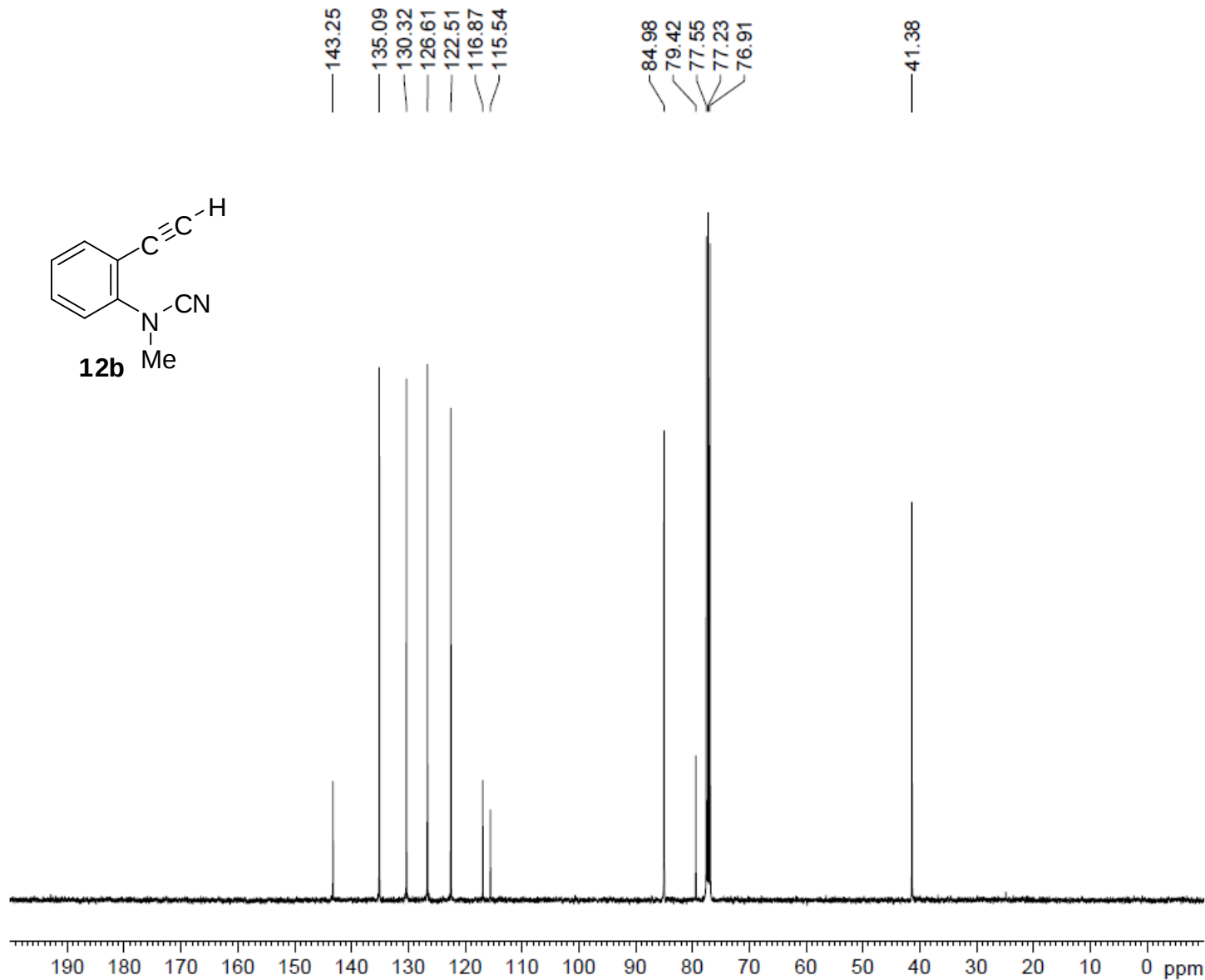
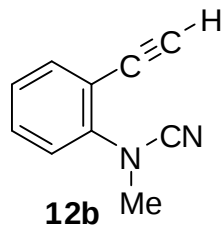


Current Data Parameters
 NAME S0017
 EXPNO 1
 PROCNO 1

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
 TDO 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



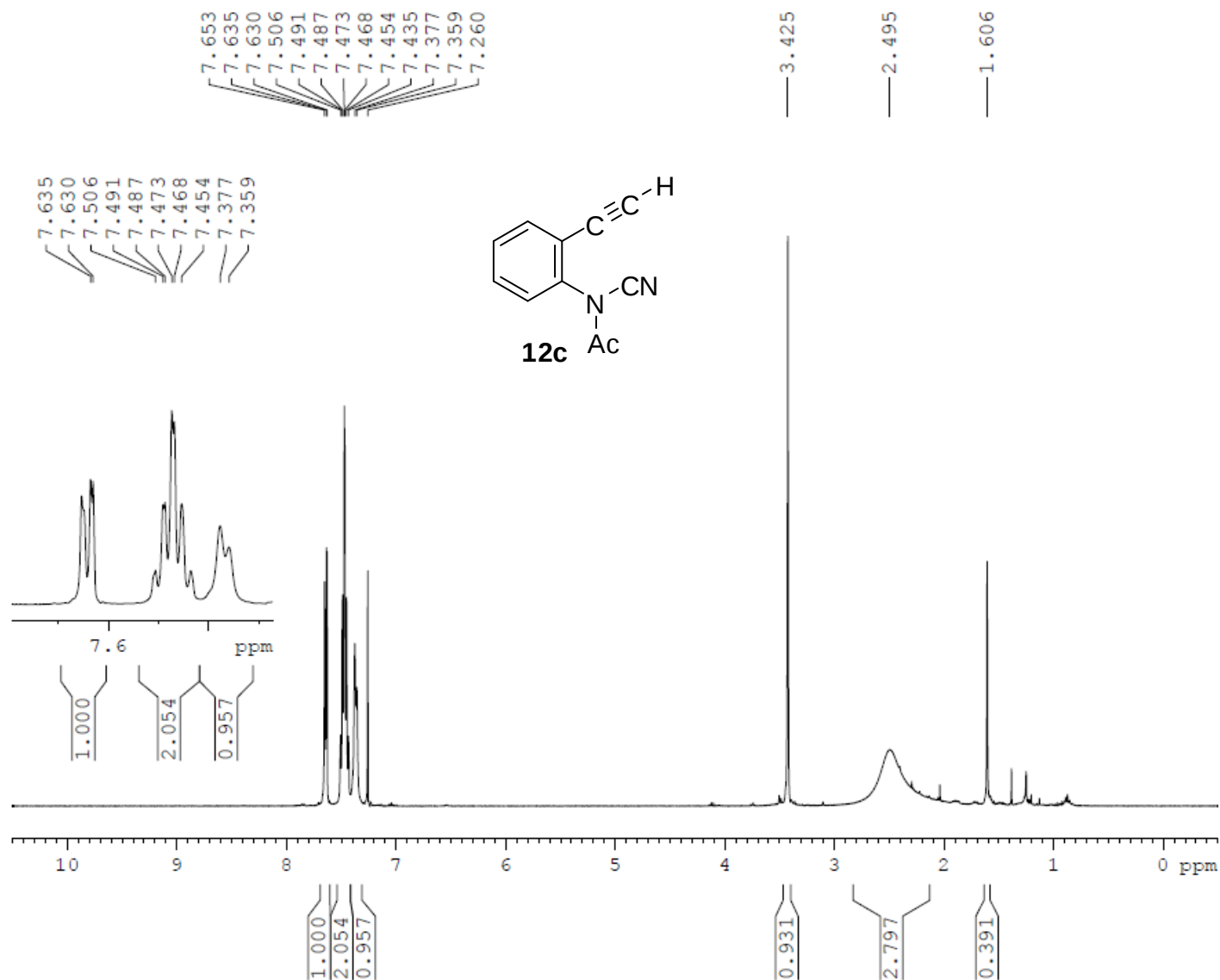
Current Data Parameters
 NAME SO017
 EXPNO 3
 PROCNO 1

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 100.623319 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

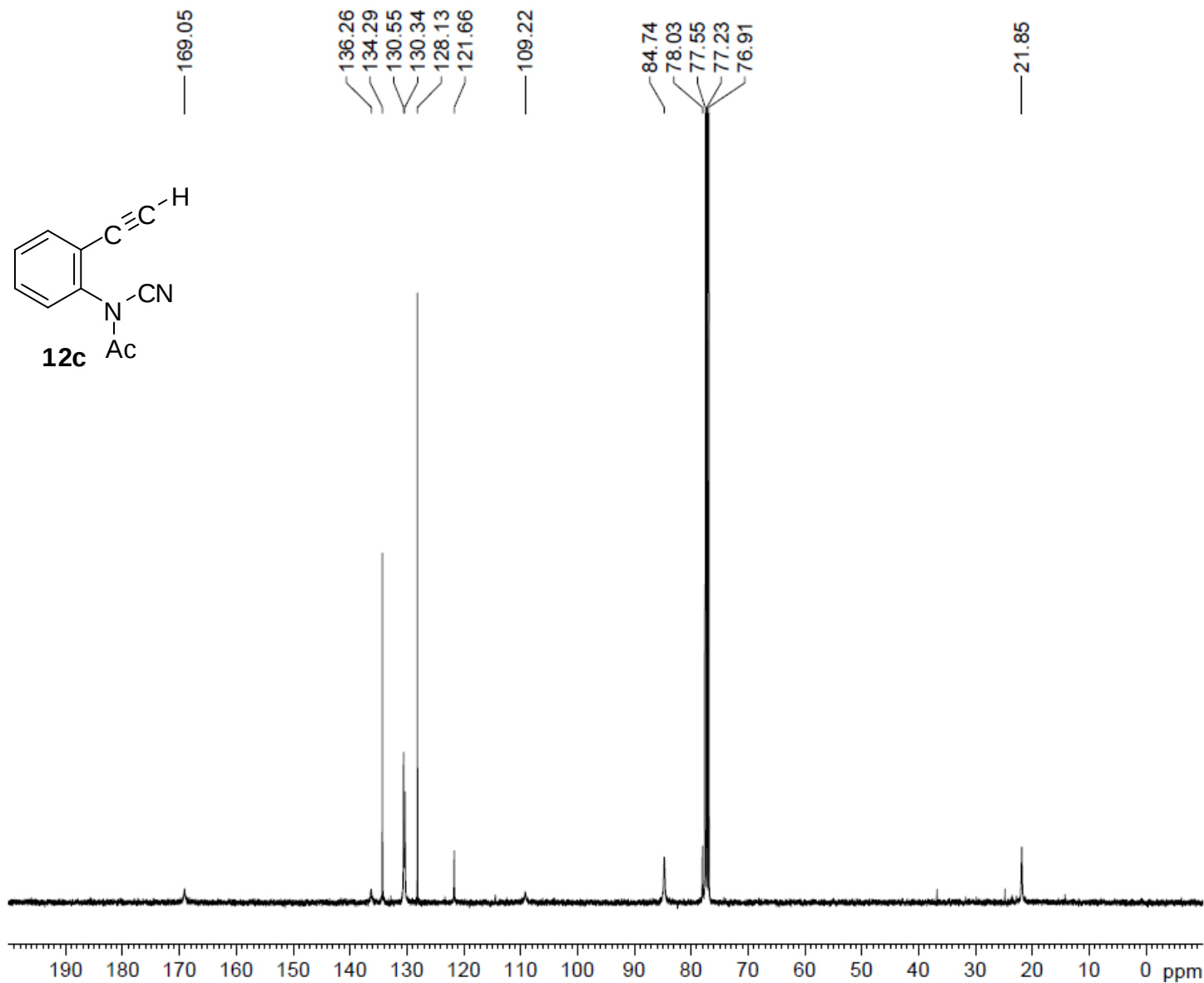
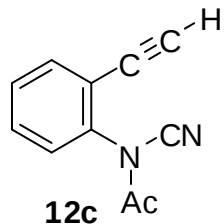


Current Data Parameters
 NAME SO180
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20160108
 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
 TDO 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

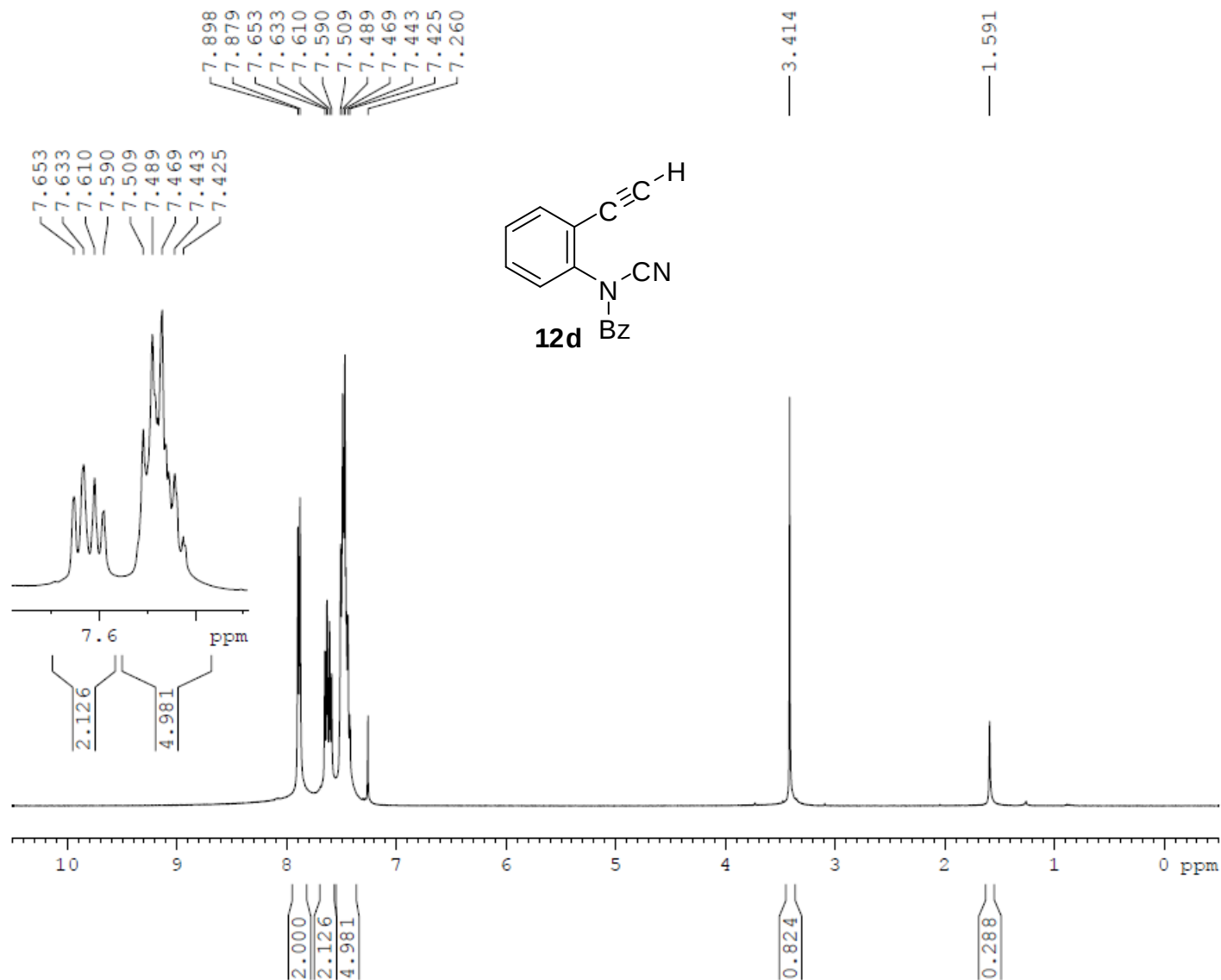
F2 - Acquisition Parameters
 Date_ 20160106
 Time 21.56
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 2195
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 2896.3
 DW 20.800 usec
 DE 6.50 usec
 TE 297.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

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

===== CHANNEL f2 =====
 CPDPRG2 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

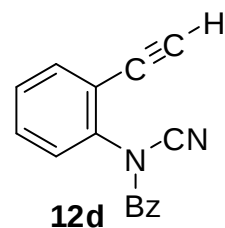
F2 - Acquisition Parameters
 Date_ 20180107
 Time 8.53
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 12
 DS 0
 SWH 7211.539 Hz
 FIDRES 0.220079 Hz
 AQ 2.2719147 sec
 RG 99.72
 DW 69.333 usec
 DE 10.50 usec
 TE 297.2 K
 D1 2.0000000 sec
 TDO 1

===== 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

167.93
137.21
134.30
133.62
130.68
130.56
129.99
129.29
128.84
127.79
121.36
109.79
84.71
78.40
77.55
77.23
76.91



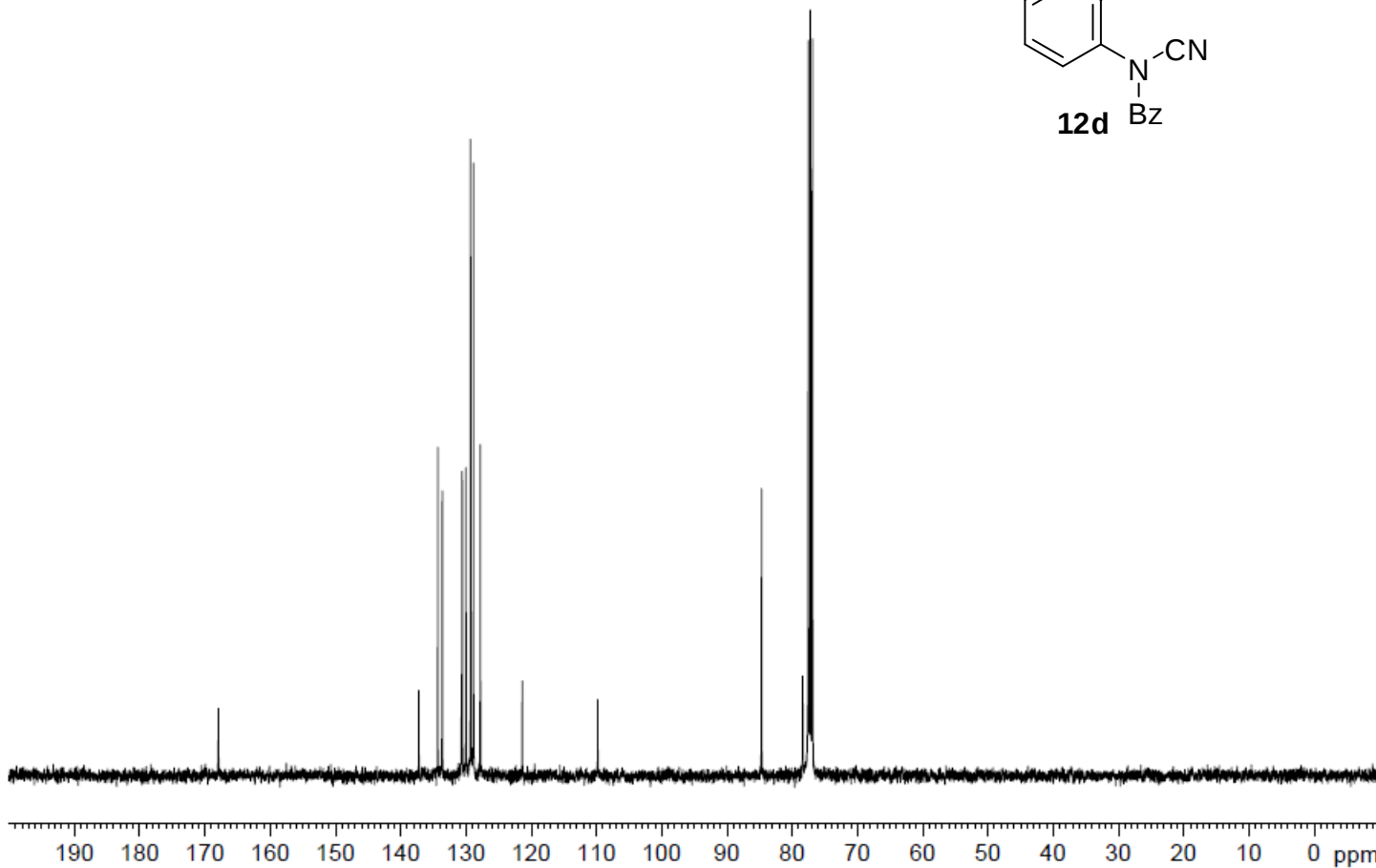
Current Data Parameters
NAME SO181-1
EXPNO 4
PROCNO 1

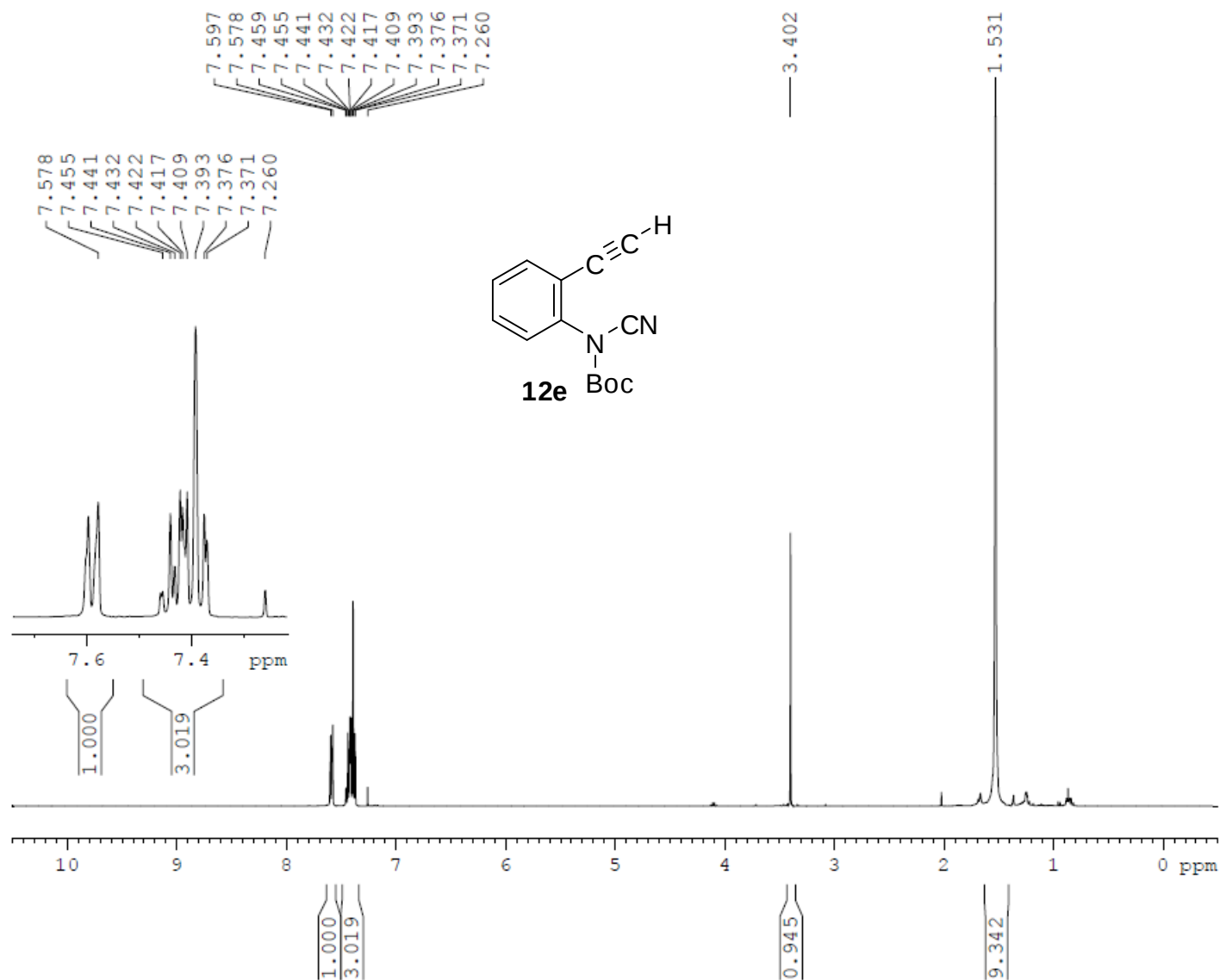
F2 - Acquisition Parameters
Date_ 20160107
Time 10.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 293
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 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



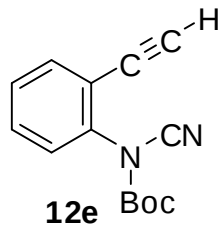


Current Data Parameters
 NAME SO182
 EXPNO 1
 PROCNO 1

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
 TDO 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



— 149.95
 136.54
 133.99
 130.24
 129.82
 127.82
 121.61
 — 108.46
 86.63
 84.26
 78.28
 77.55
 77.23
 76.91
 27.84

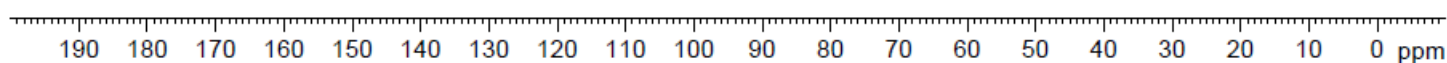
Current Data Parameters
 NAME SO182
 EXPNO 3
 PROCNO 1

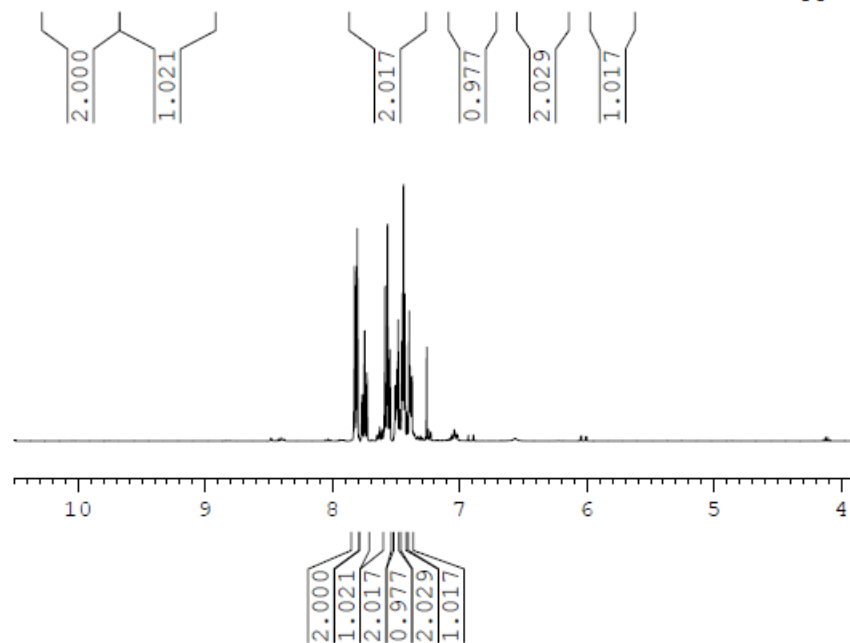
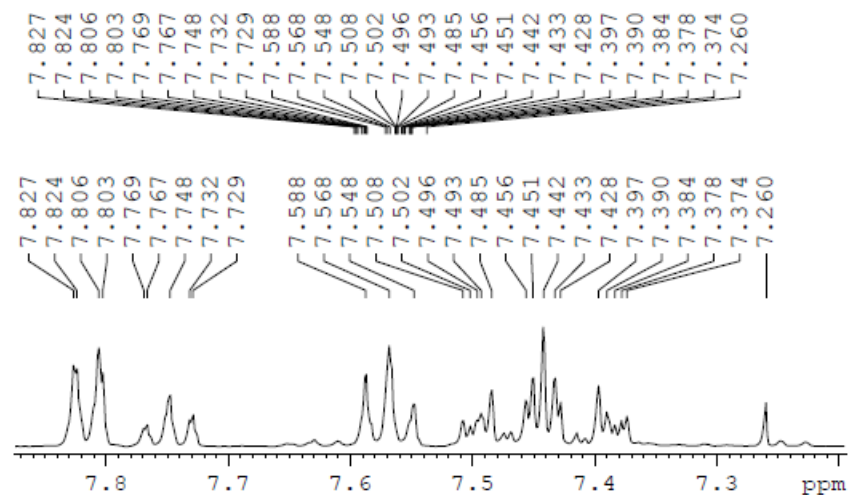
F2 - Acquisition Parameters
 Date_ 20160109
 Time 21.13
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 135
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 1024
 DW 20.800 usec
 DE 6.50 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

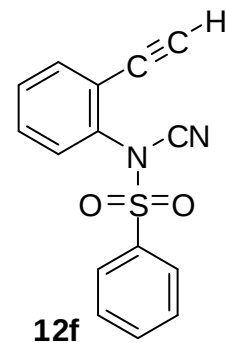
===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 1.80 dB
 PL12 17.00 dB
 PL13 20.00 dB
 SFO2 400.1316005 MHz

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





— 2.982

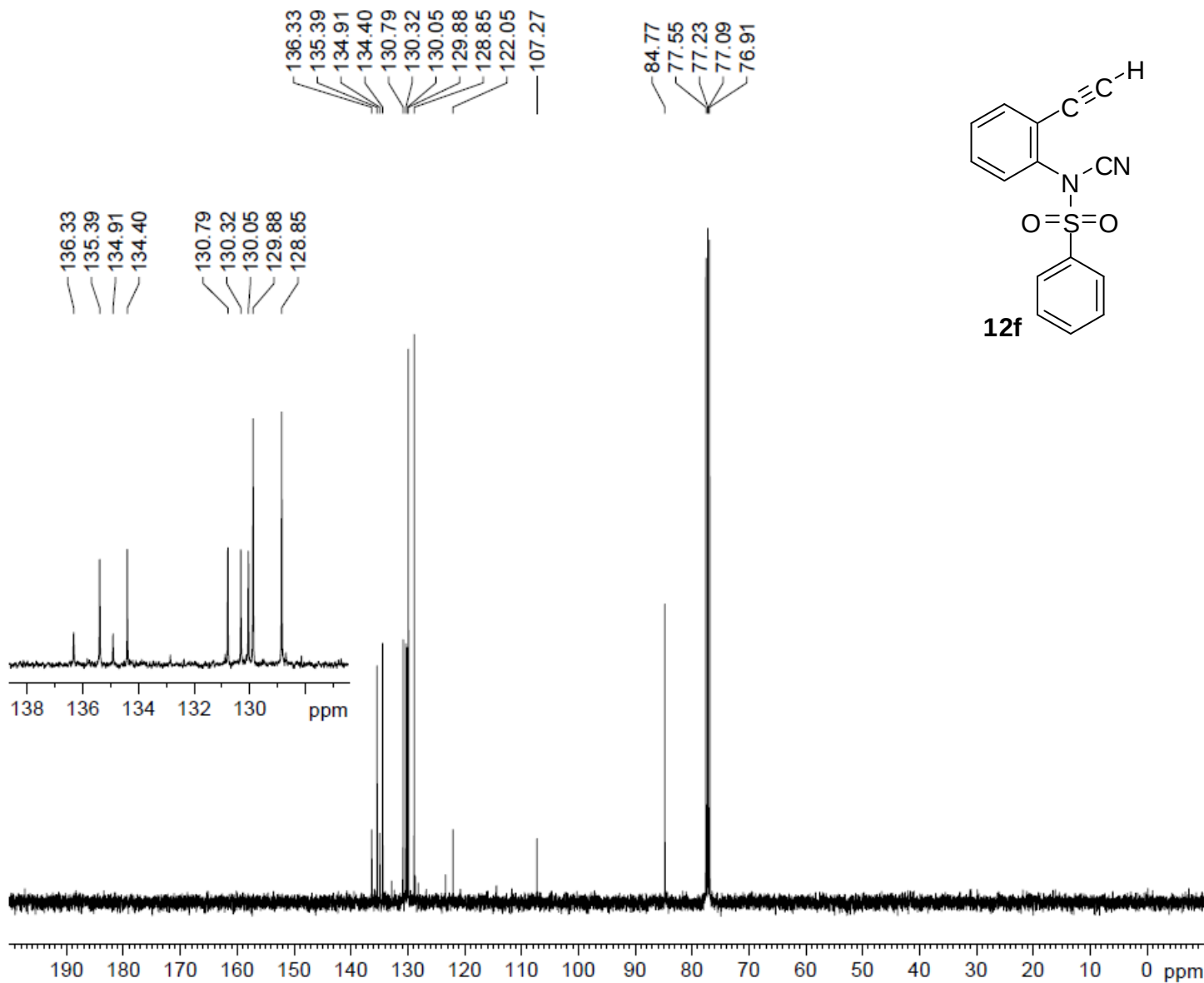


Current Data Parameters
NAME SO124-2
EXPNO 1
PROCNO 1

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



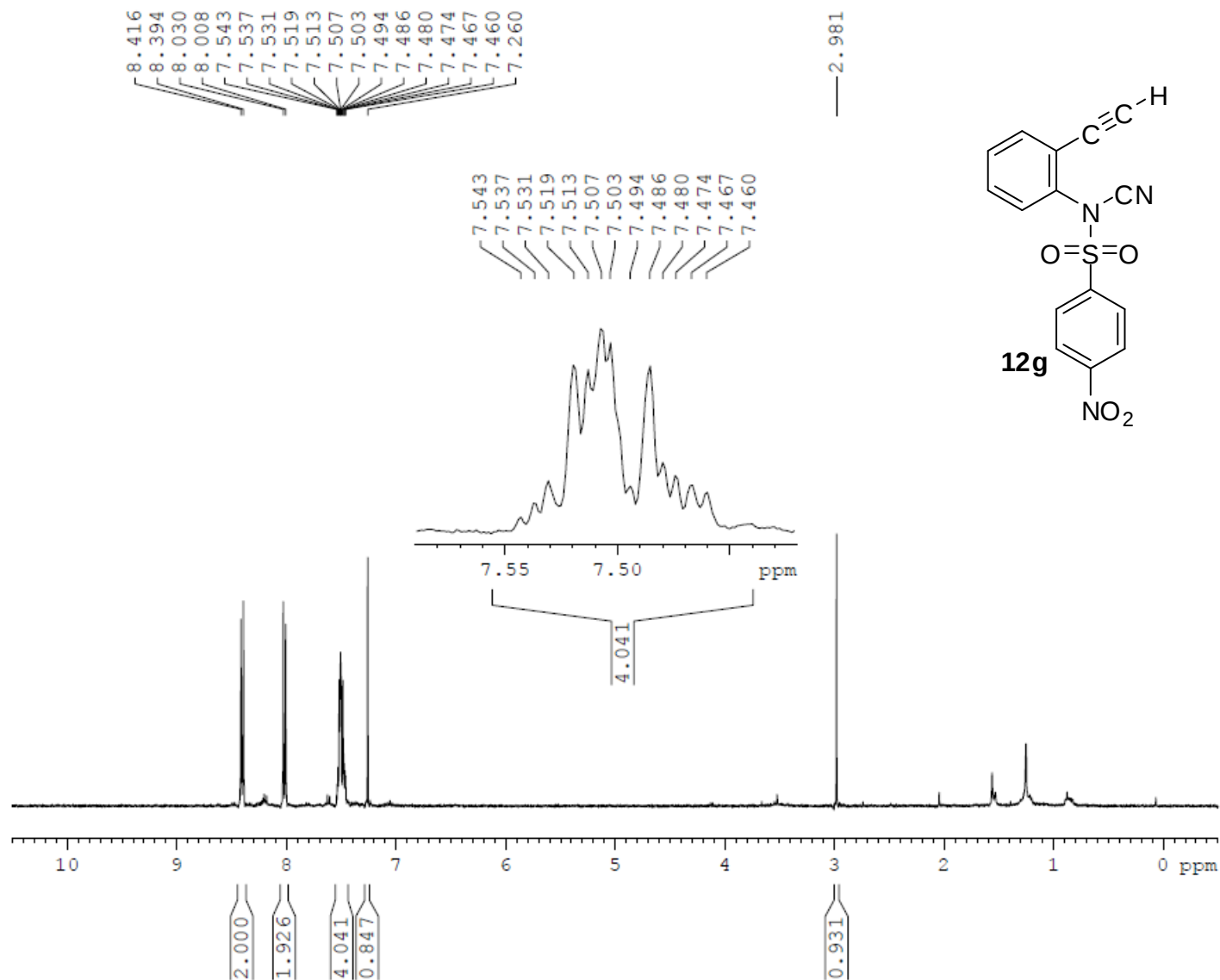
Current Data Parameters
 NAME SO124-2
 EXPNO 2
 PROCNO 1

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 =====
 CPDPRG2 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

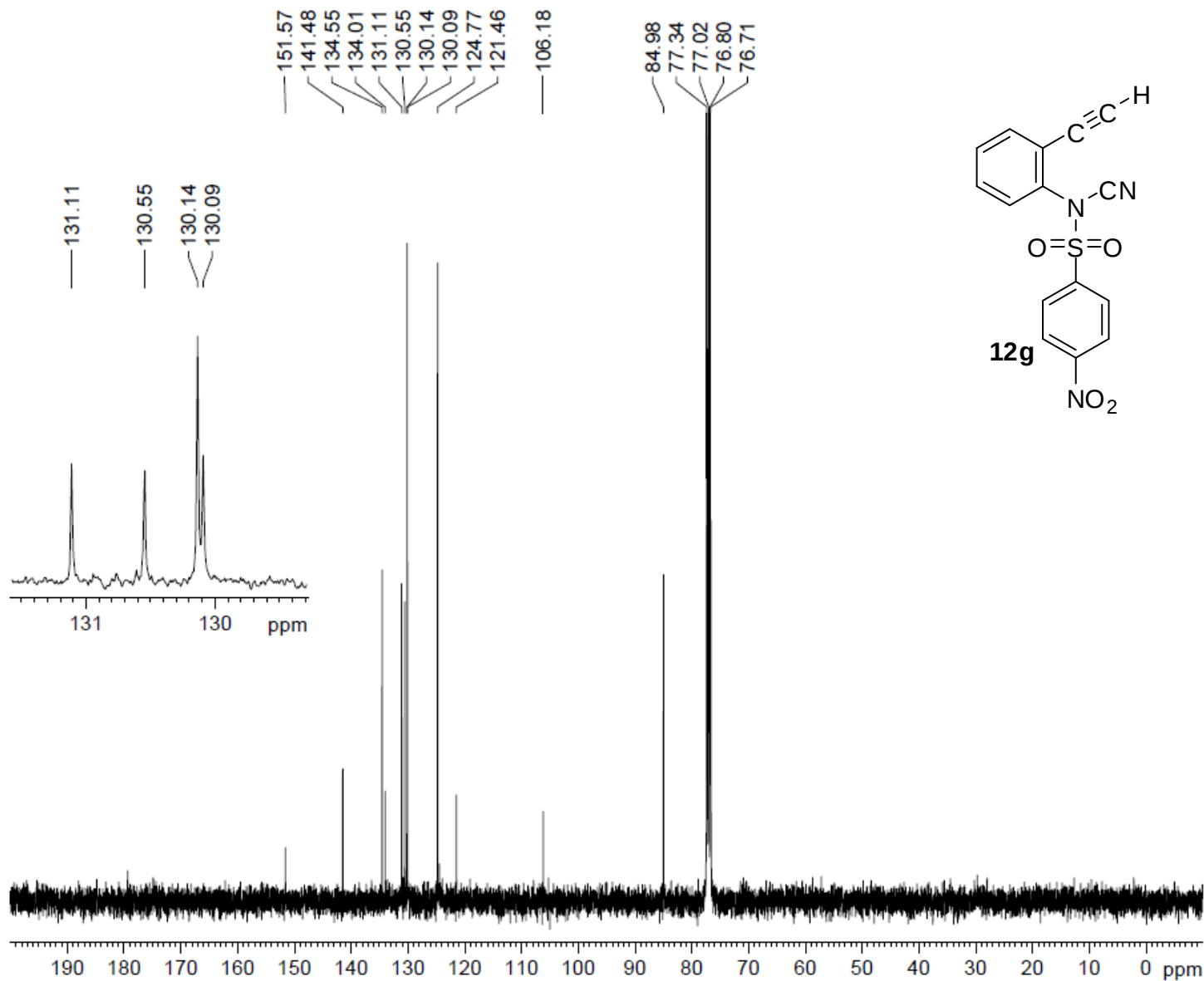


Current Data Parameters
 NAME SO028
 EXPNO 3
 PROCNO 1

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



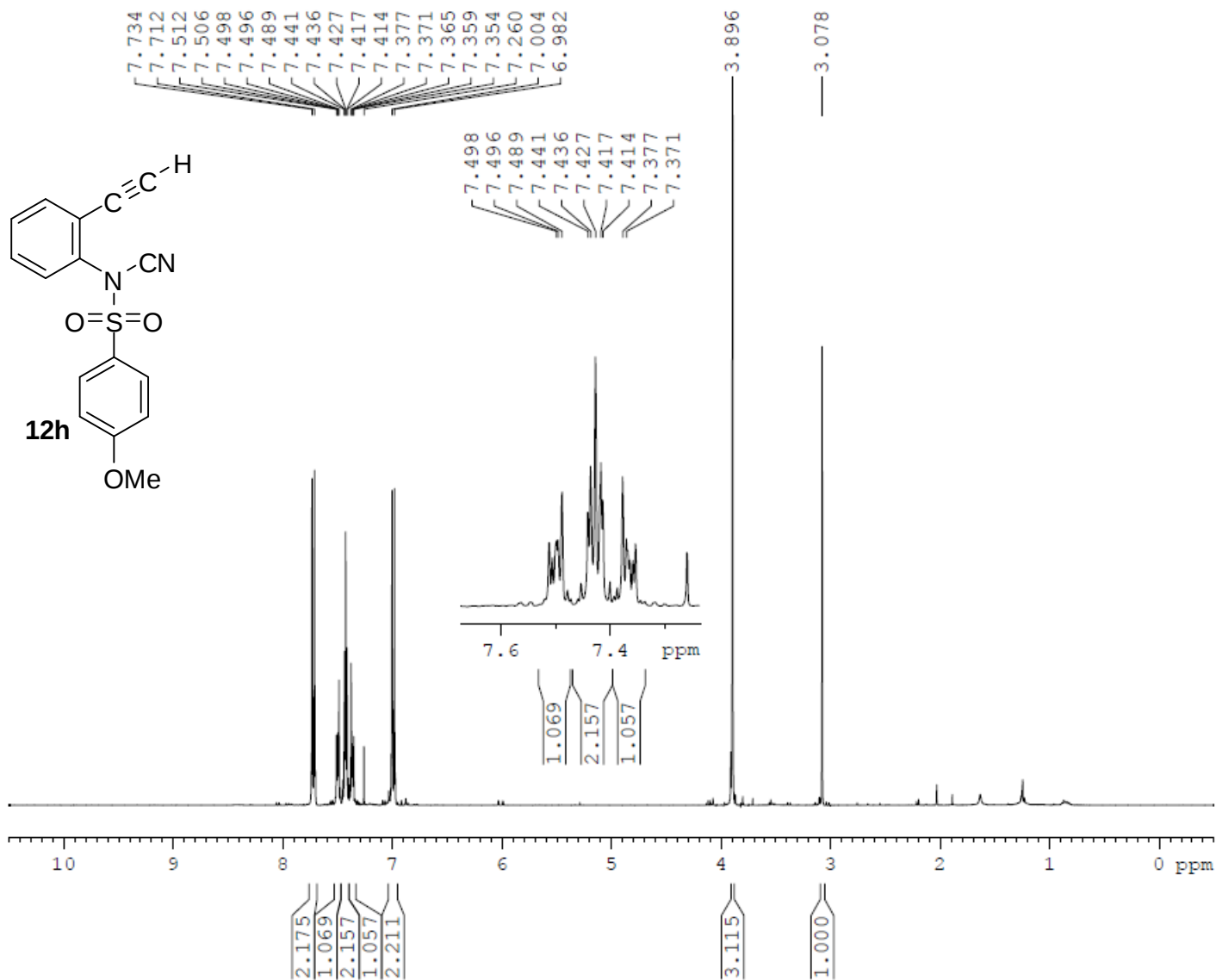
Current Data Parameters
 NAME SO028
 EXPNO 5
 PROCNO 1

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 =====
 CPDPRG2 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

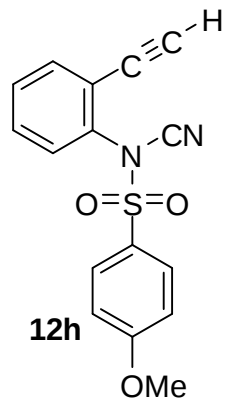


Current Data Parameters
NAME SO126
EXPNO 1
PROCNO 1

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
TDO 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



165.32

135.08
134.36
131.27
130.64
130.25
129.93
127.39
122.13
114.99
107.59

84.70
77.55
77.38
77.23
76.91

56.09

Current Data Parameters
NAME SO126
EXPNO 2
PROCNO 1

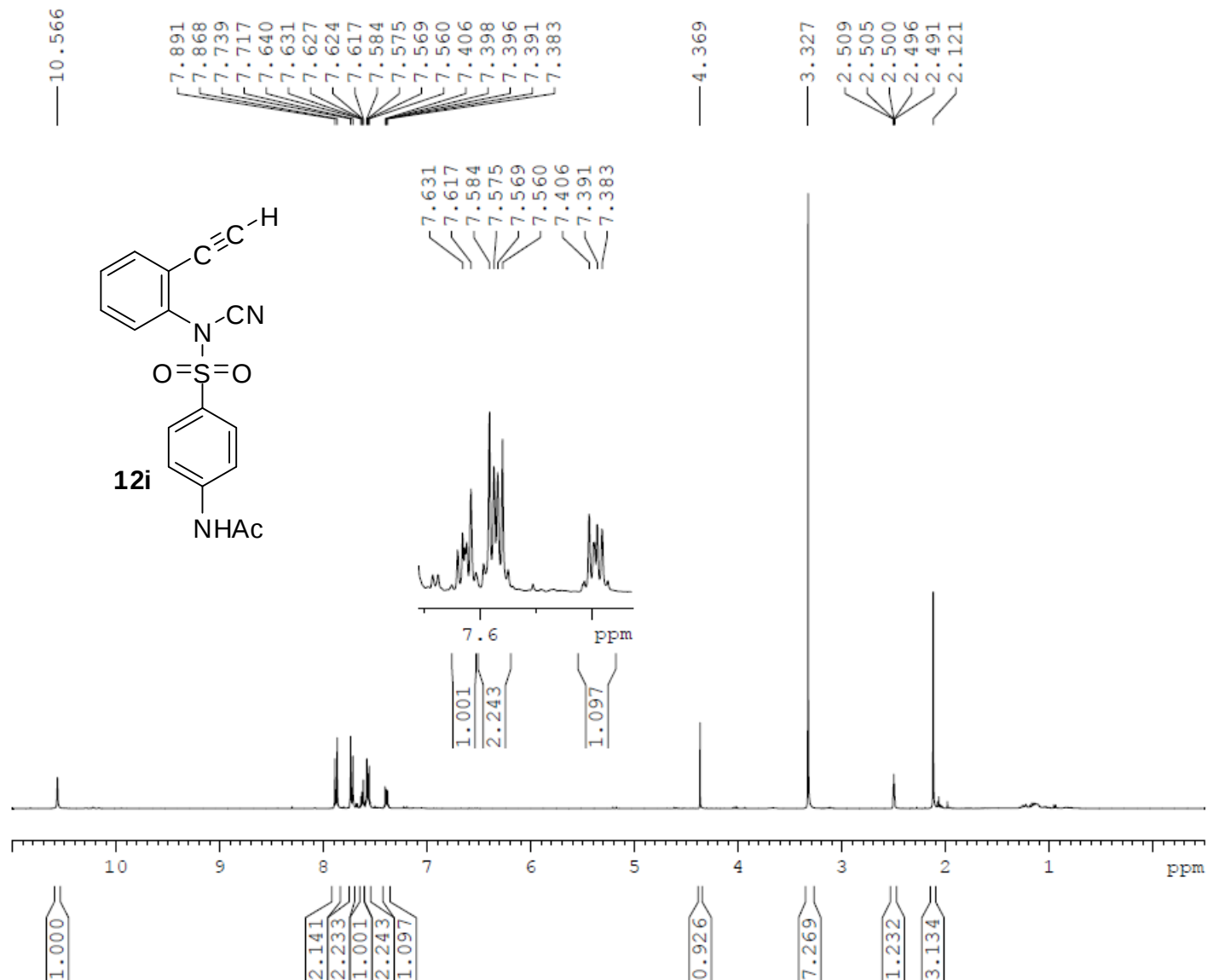
F2 - Acquisition Parameters
Date_ 20150609
Time 16.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 195
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 5792.6
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

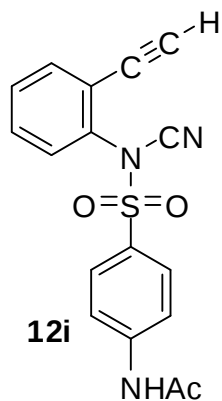


Current Data Parameters
 NAME SO130
 EXPNO 2
 PROCNO 1

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 89.333 usec
 DE 10.52 usec
 TE 301.2 K
 D1 2.00000000 sec
 TDO 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



170.42
146.93
135.06
134.95
132.23
131.64
130.92
130.40
128.60
122.52
120.05
108.17
88.77
78.16

41.14
40.93
40.72
40.51
40.30
40.09
39.88
25.22

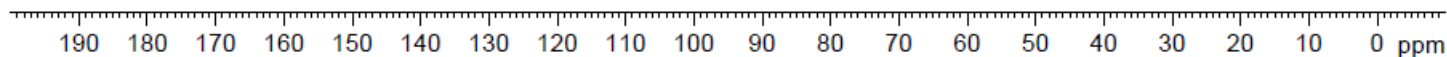
Current Data Parameters
NAME SO130
EXPNO 3
PROCNO 1

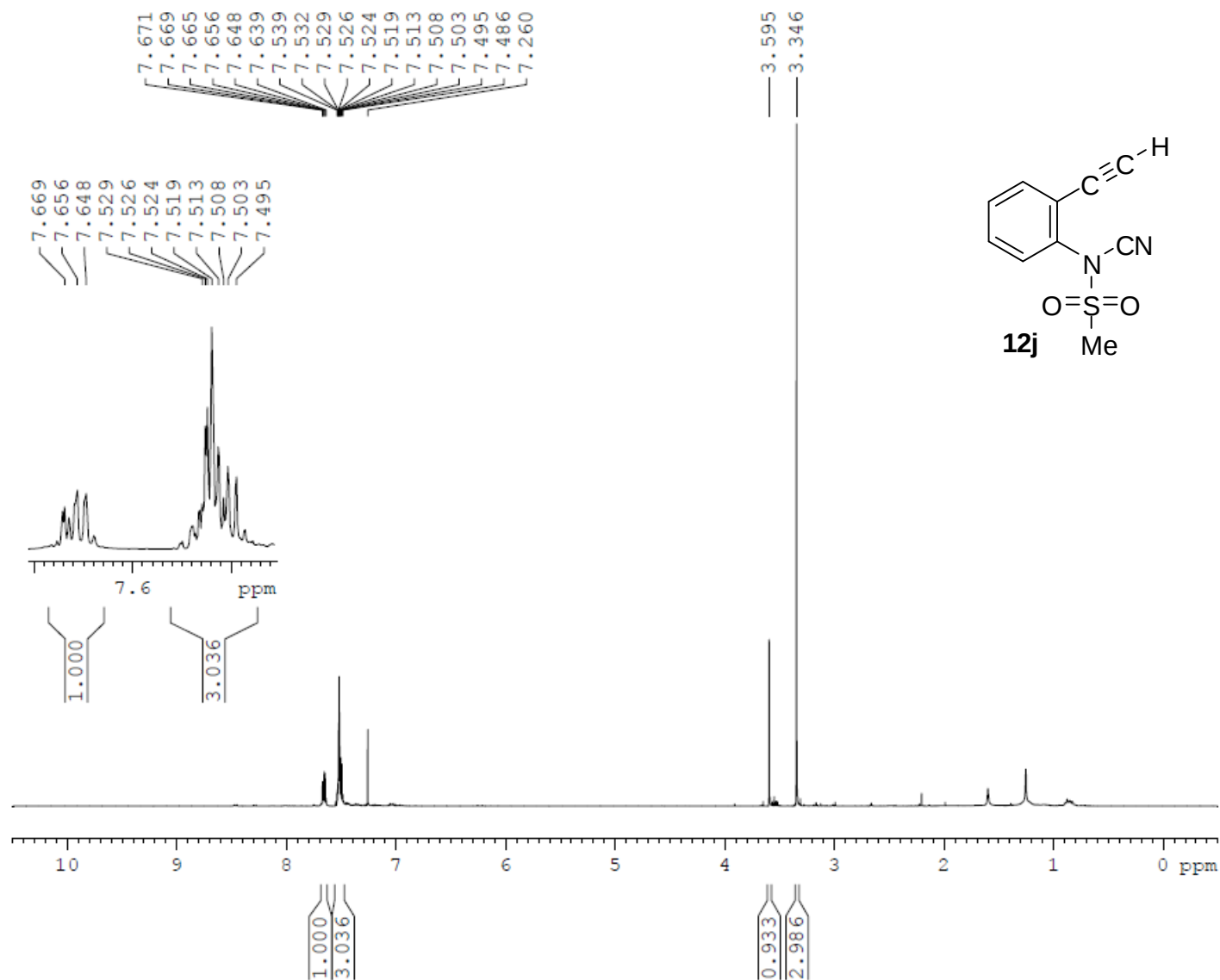
F2 - Acquisition Parameters
Date_ 20150618
Time 9.32
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 769
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 301.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.623319 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



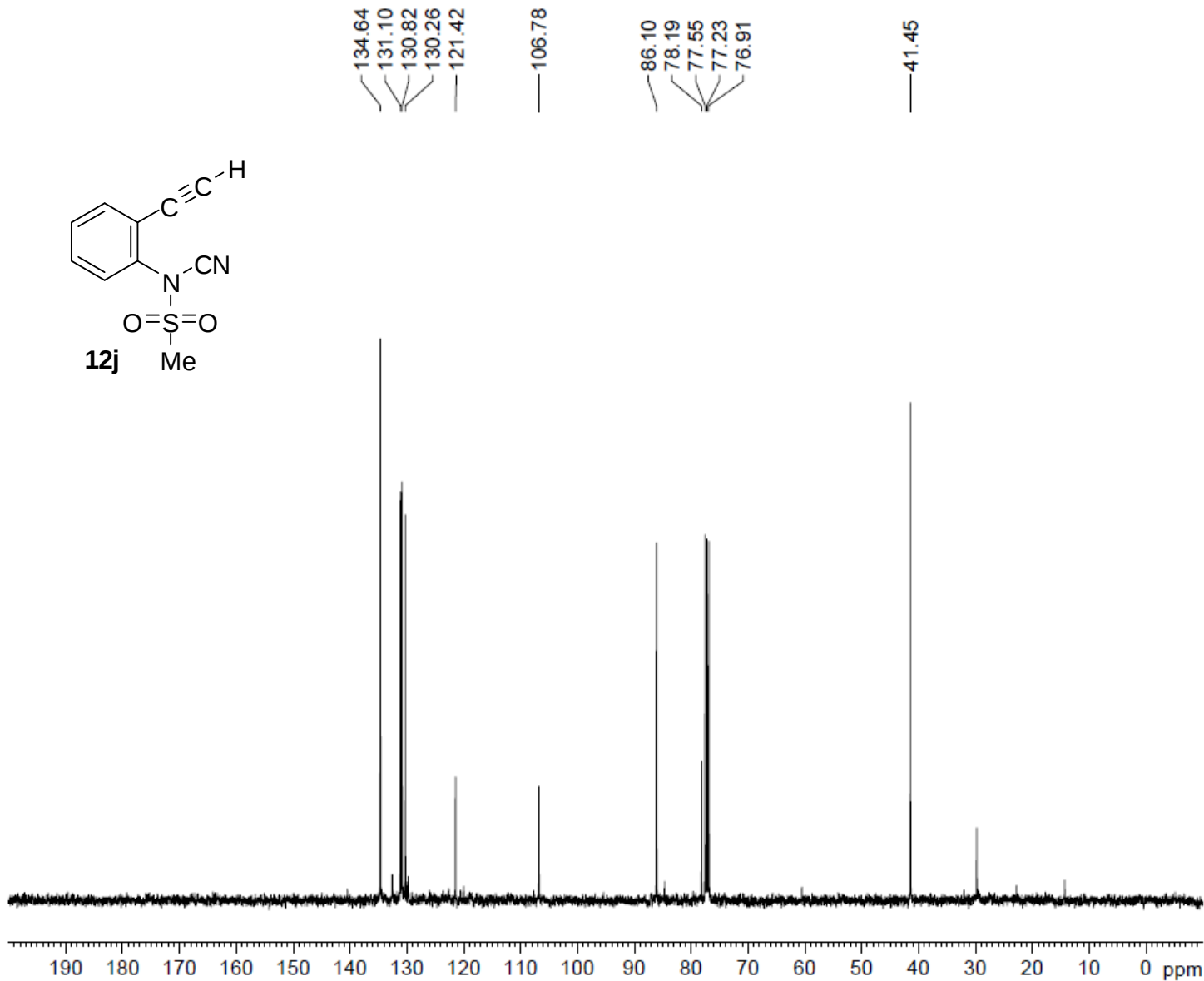
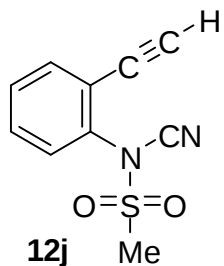


Current Data Parameters
 NAME SO136
 EXPNO 1
 PROCNO 1

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
 TDO 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



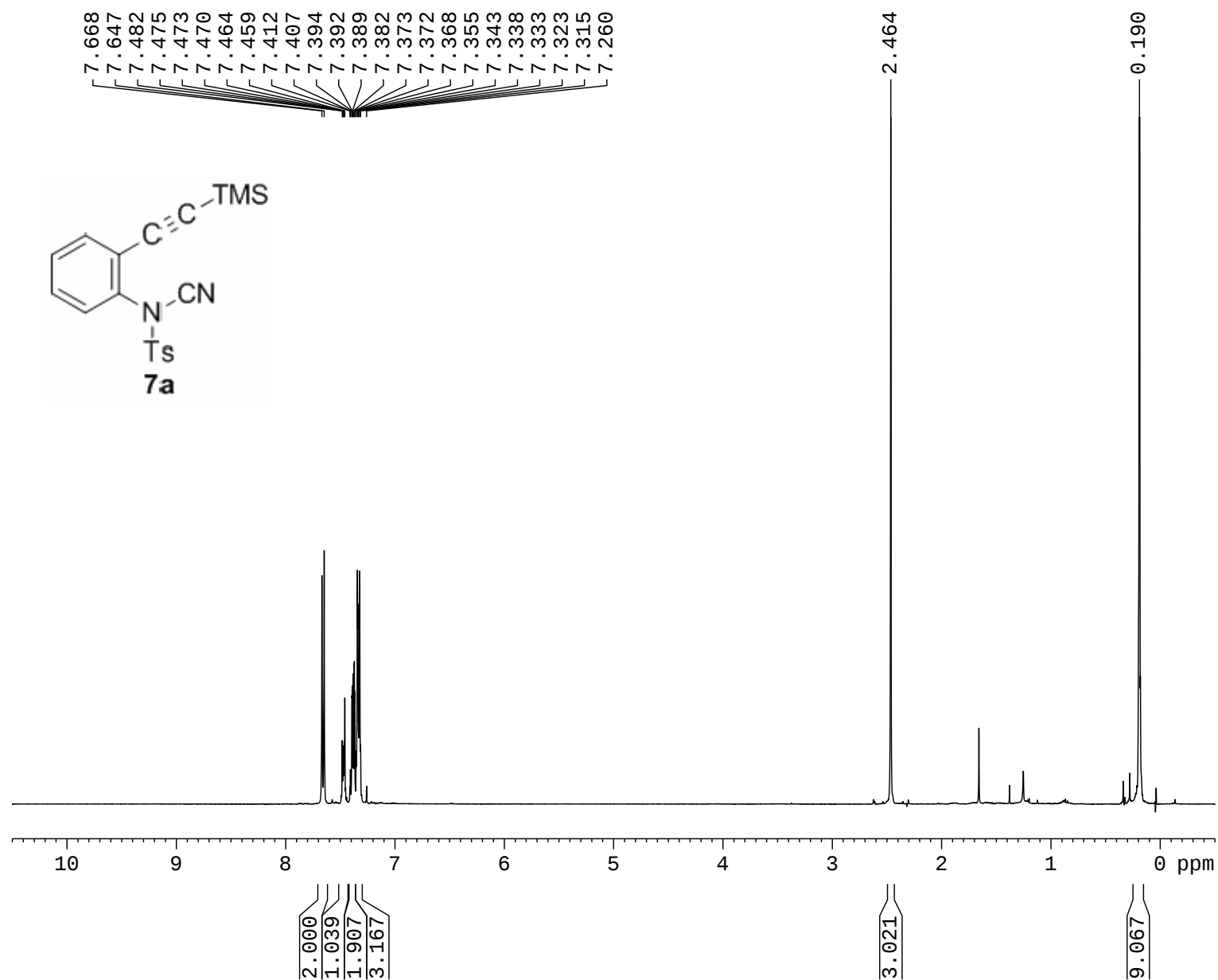
Current Data Parameters
 NAME SO136
 EXPNO 3
 PROCNO 1

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 100.623319 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

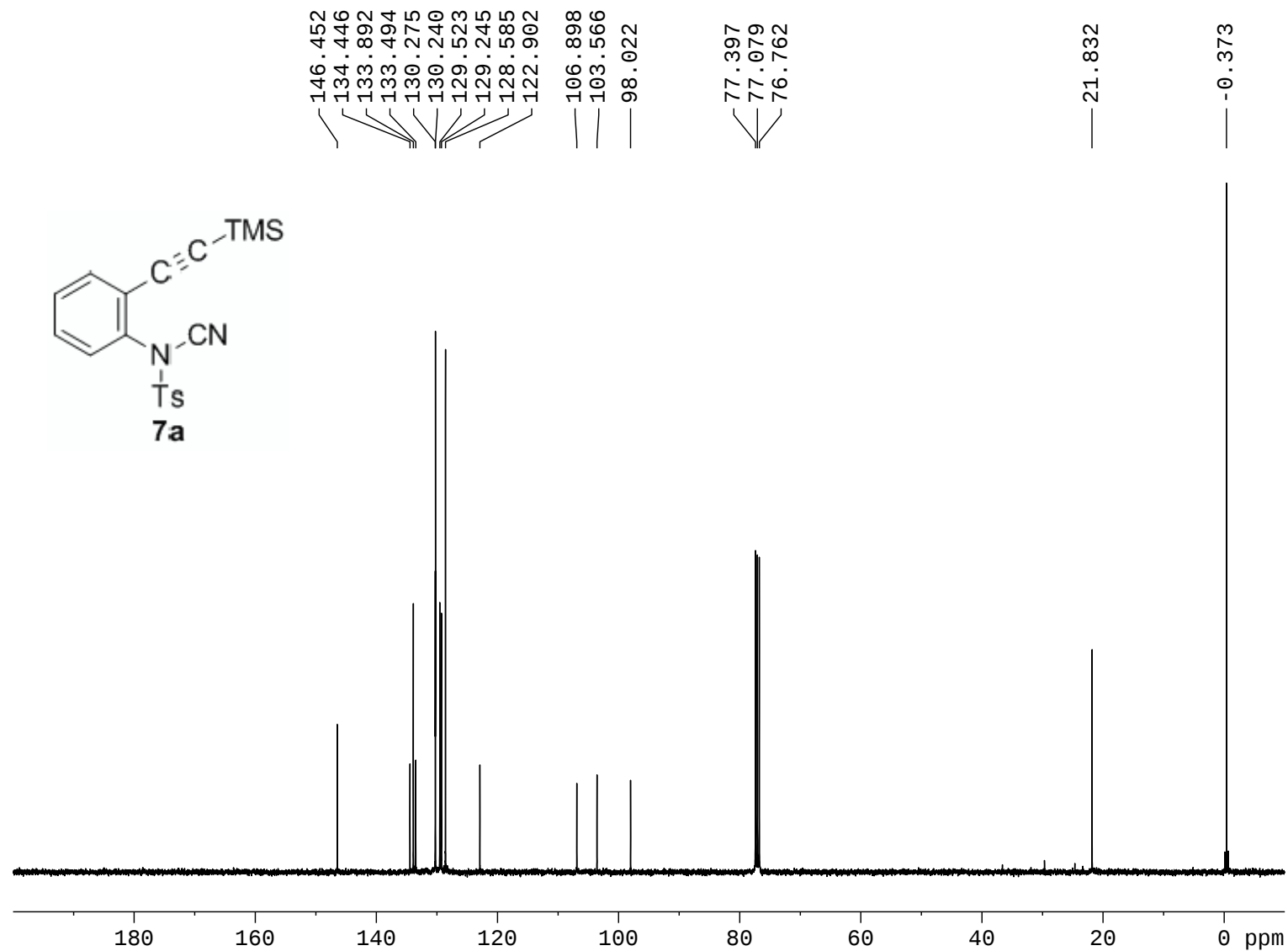


Current Data Parameters
 NAME RV086
 EXPNO 1
 PROCNO 1

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



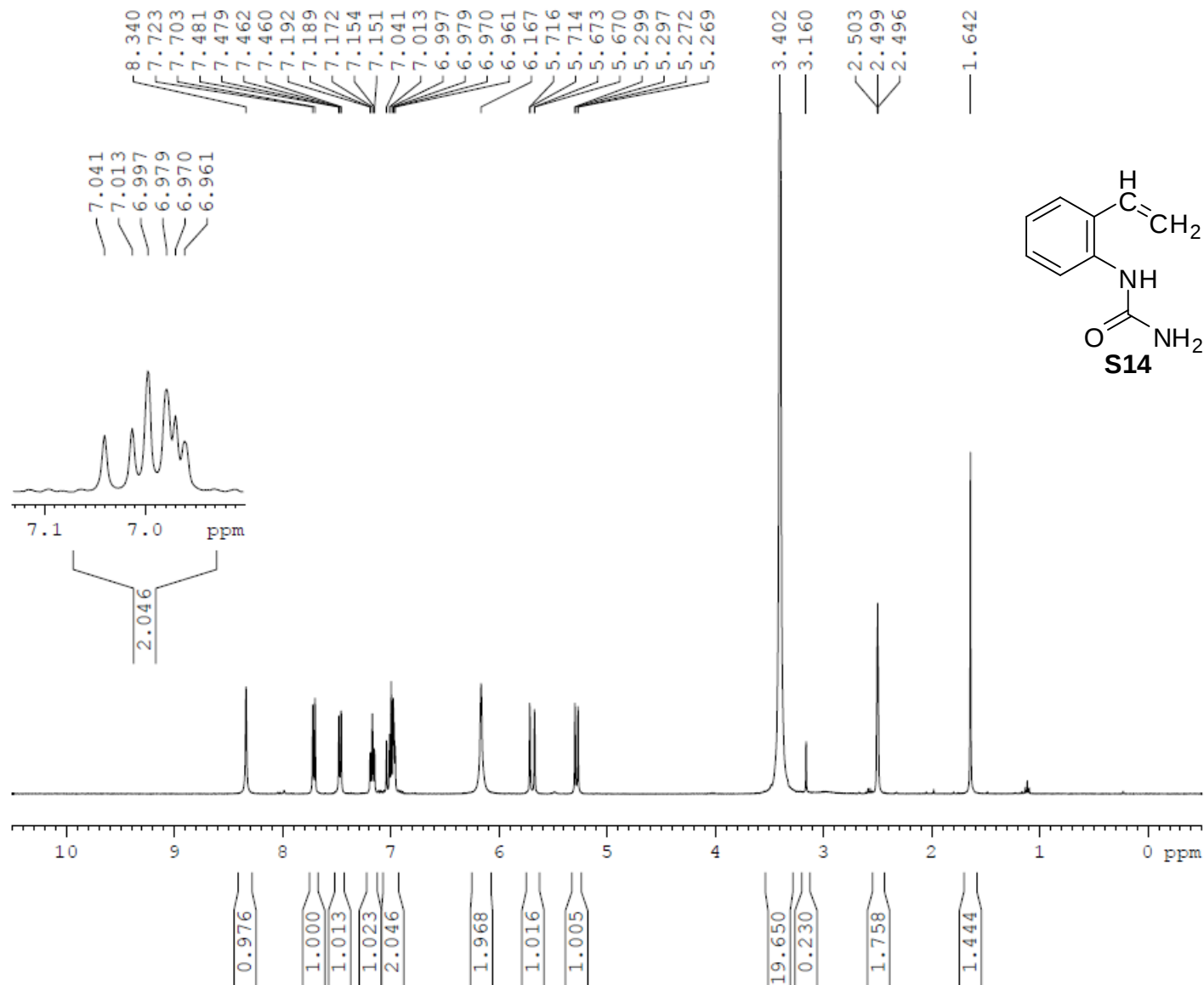
Current Data Parameters
NAME RV086
EXPNO 3
PROCNO 1

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 100.623325 MHz

===== CHANNEL f2 =====
CPDPRG2 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

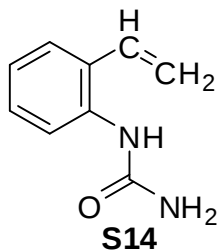


Current Data Parameters
 NAME S0020
 EXPNO 2
 PROCNO 1

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
 TDO 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



— 156.39

137.03
132.57
128.40
127.90
125.45
122.70
122.59
115.40

40.14
39.93
39.72
39.51
39.30
39.09
38.89

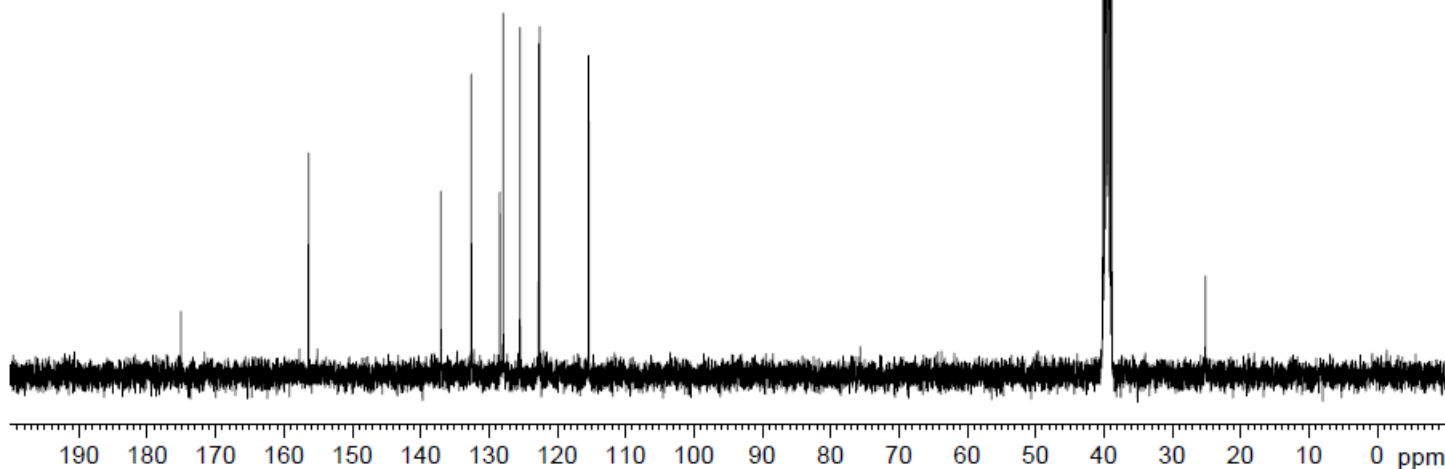
Current Data Parameters
NAME SO020
EXPNO 4
PROCNO 1

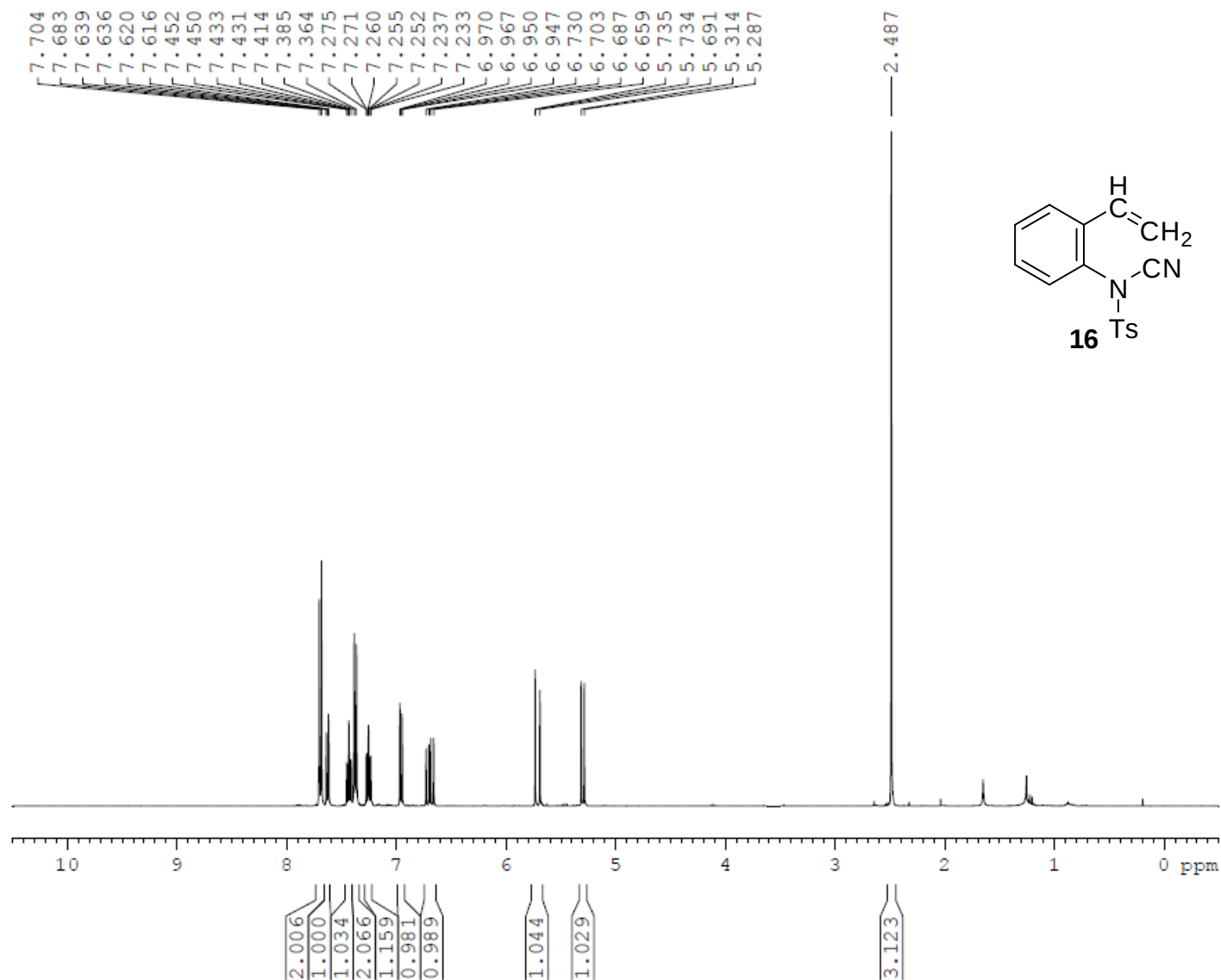
F2 - Acquisition Parameters
Date_ 20141129
Time 9.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 919
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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



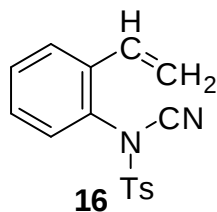


Current Data Parameters
NAME S0021
EXPNO 1
PROCNO 1

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 400.130093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



147.05
137.25
132.98
131.57
131.20
130.51
130.31
129.09
128.88
128.76
127.17
118.53
108.58

77.55
77.23
76.91

21.99

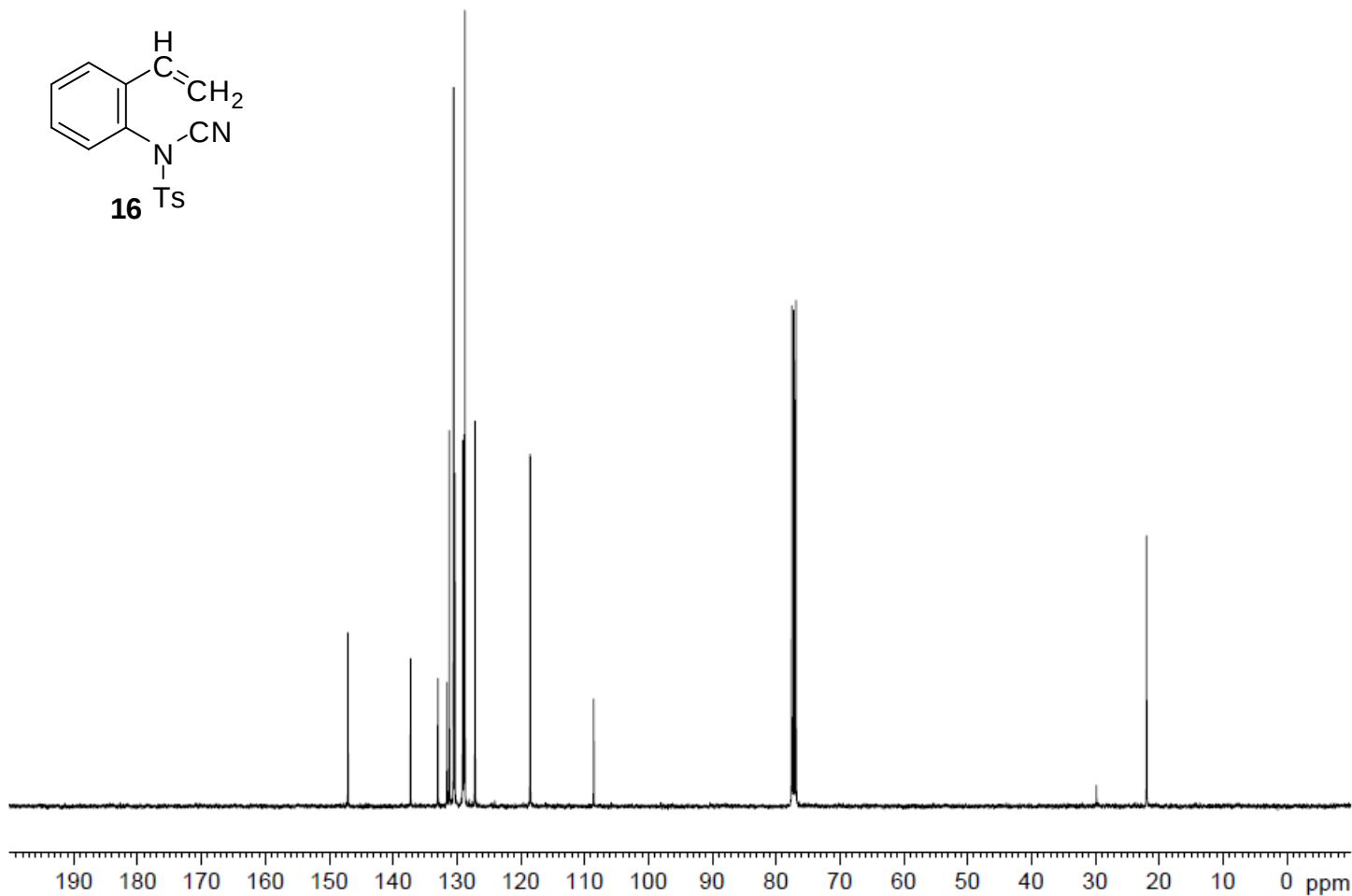
Current Data Parameters
NAME SO021
EXPNO 3
PROCNO 1

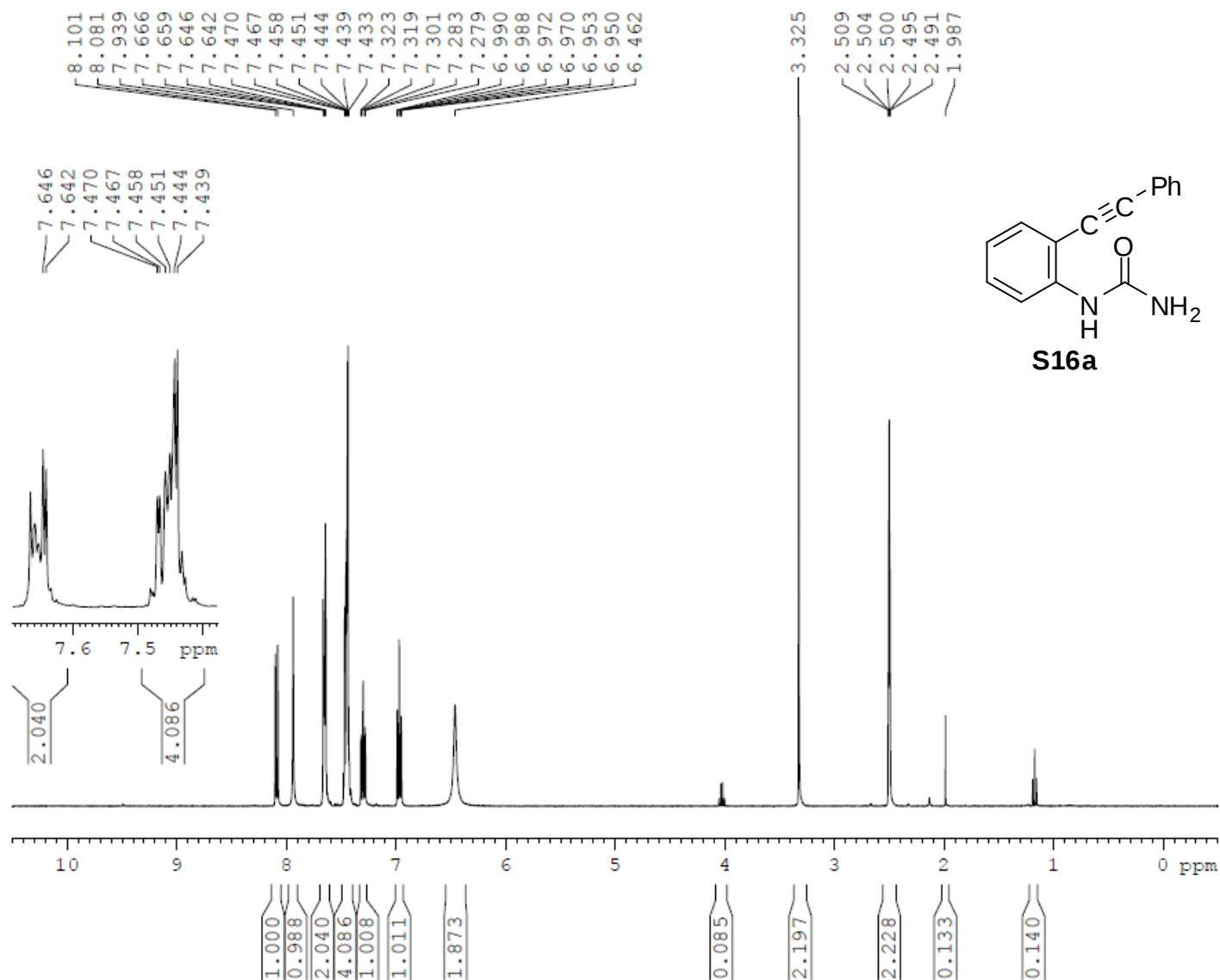
F2 - Acquisition Parameters
Date_ 20141129
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.623319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 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



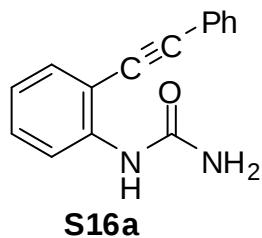


Current Data Parameters
 NAME S0038
 EXPNO 1
 PROCNO 1

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
 TDO 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



155.55
140.92
132.02
131.57
129.28
128.79
128.57
122.35
121.42
119.39
110.85
94.96
85.37

40.14
39.93
39.72
39.51
39.30
39.09
38.88

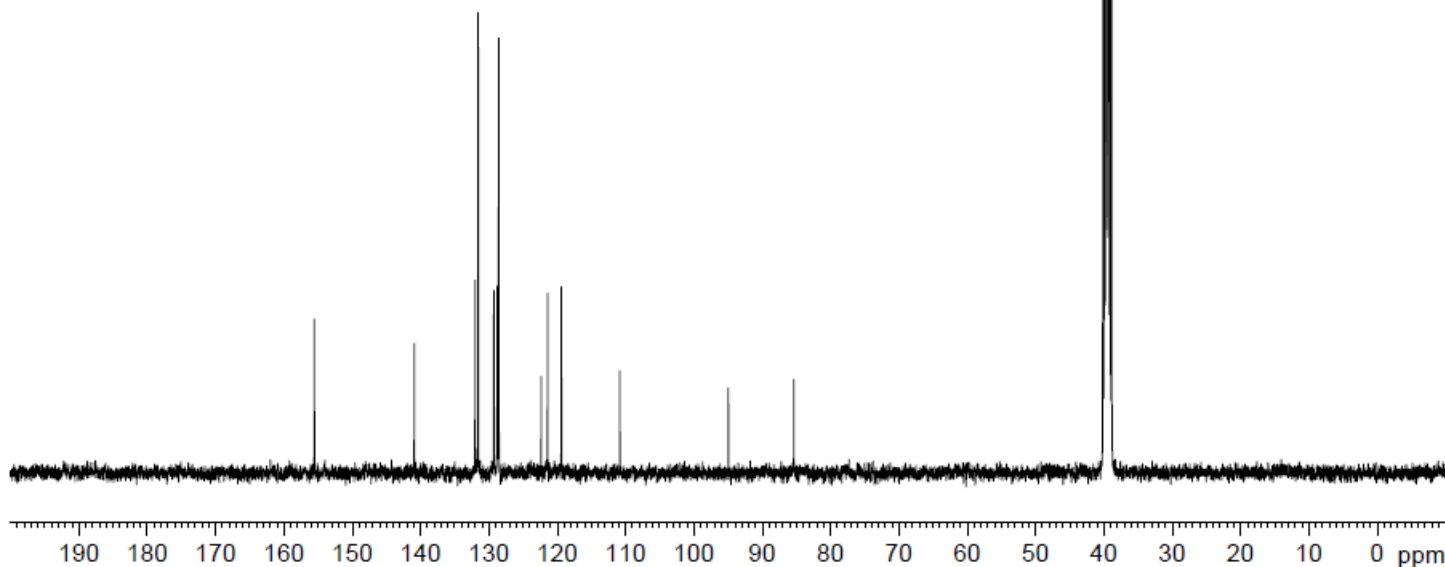
Current Data Parameters
NAME SO038
EXPNO 3
PROCNO 1

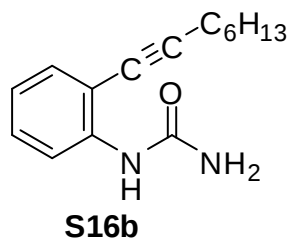
F2 - Acquisition Parameters
Date_ 20141220
Time 10.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT DMSO
NS 1408
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.623319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 90.00 usec
PLW2 15.00000000 W
PLW12 0.34252000 W
PLW13 0.27744001 W

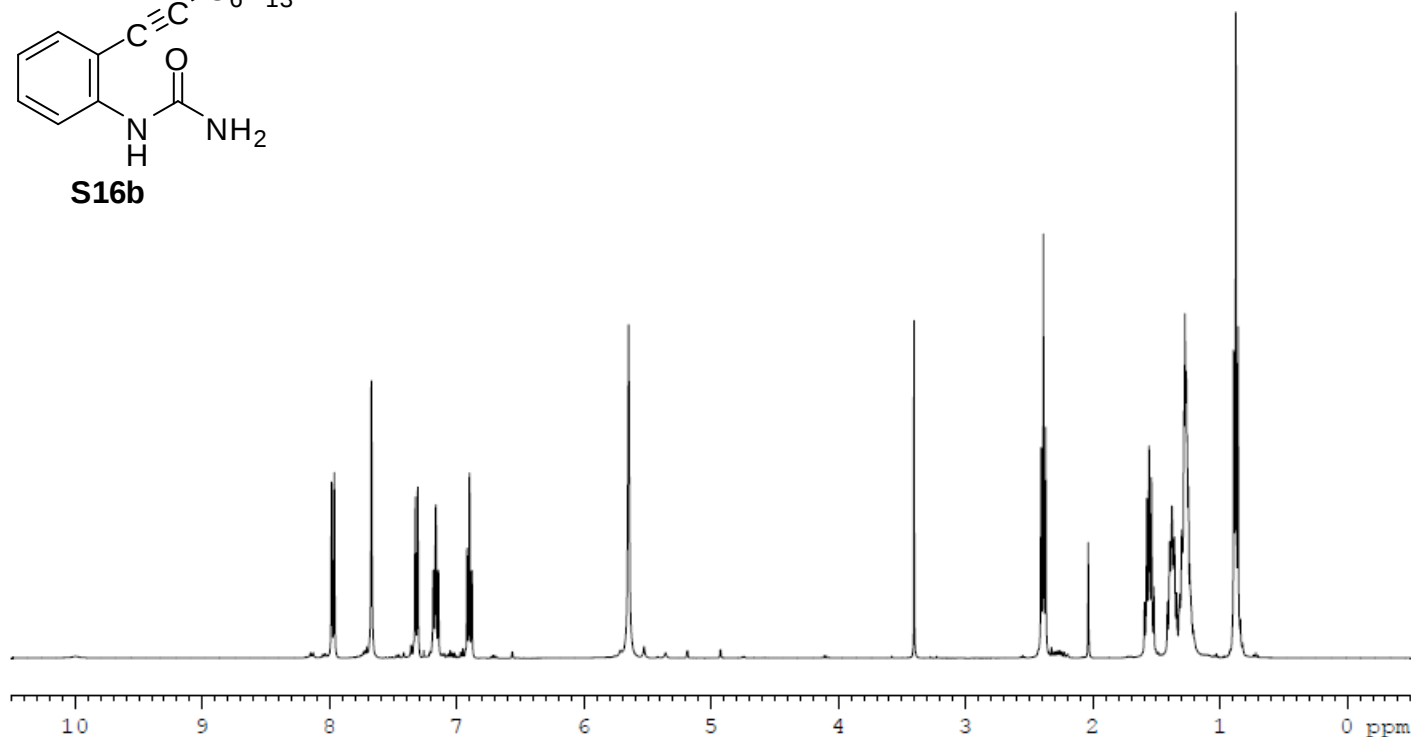
F2 - Processing parameters
SI 32768
SF 100.6128202 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00





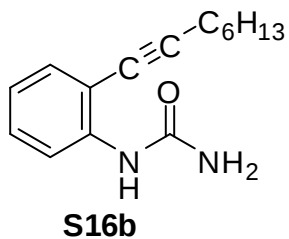
7.985
 7.964
 7.962
 7.329
 7.325
 7.309
 7.306
 7.187
 7.184
 7.166
 7.148
 7.144
 6.921
 6.920
 6.901
 6.883
 6.881
 5.650

3.406
 2.407
 2.389
 2.371
 2.036
 1.594
 1.576
 1.558
 1.539
 1.520
 1.415
 1.397
 1.393
 1.378
 1.366
 1.359
 1.341
 1.323
 1.315
 1.300
 1.283
 1.275
 1.267
 1.258



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



—157.08
 —139.71
 —132.11
 —128.51
 —122.47
 —119.68
 —113.70
 —97.50
 77.55
 77.23
 76.91
 76.26
 —50.22
 31.38
 28.73
 22.59
 19.63
 14.07

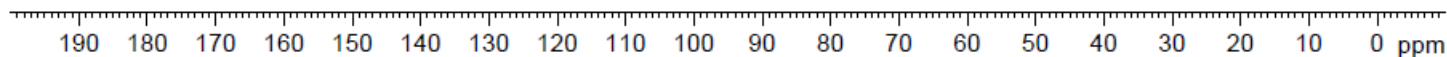
Current Data Parameters
 NAME SC127
 EXPNO 3
 PROCNO 1

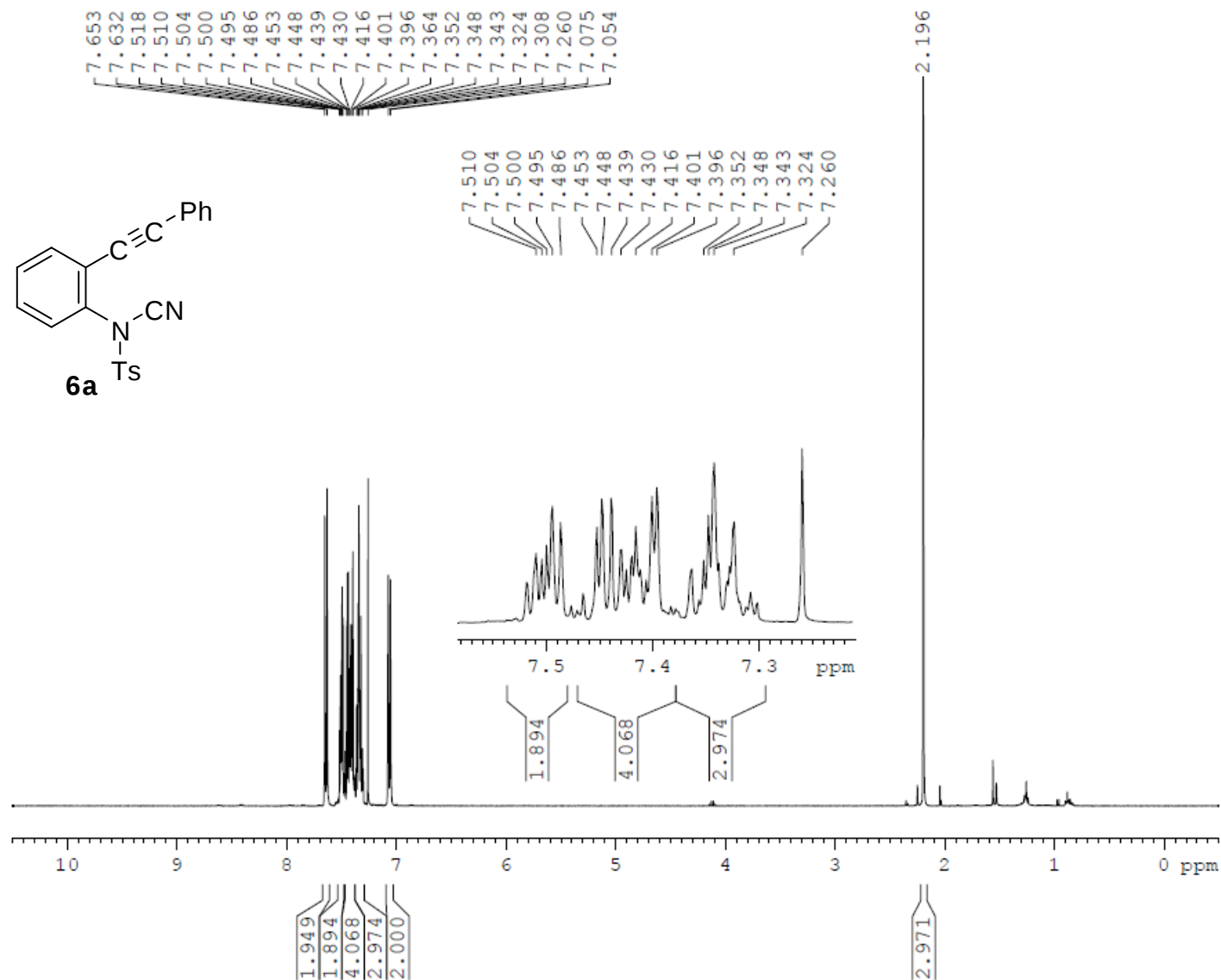
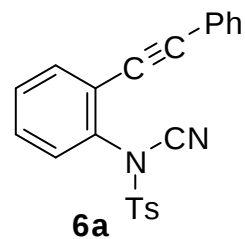
F2 - Acquisition Parameters
 Date_ 20140514
 Time 8.46
 INSTRUM spect
 PROBHD 5 mm SEI 1H-13
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 100
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 32768
 DW 20.800 usec
 DE 6.50 usec
 TE 296.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

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

===== CHANNEL f2 =====
 CPDPRG2 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



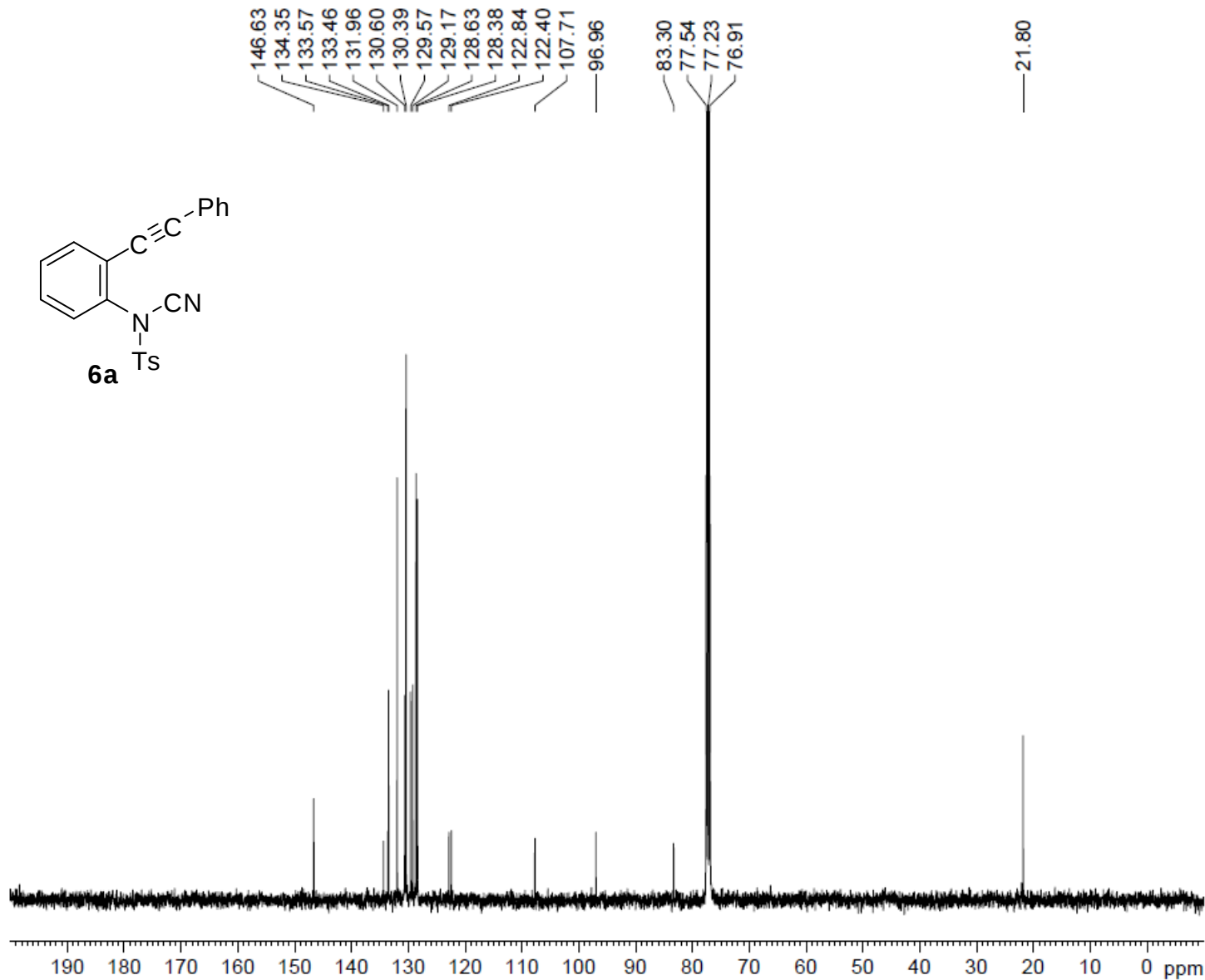
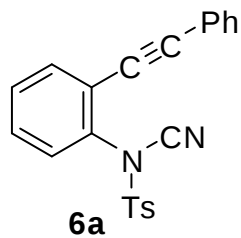


Current Data Parameters
 NAME S0041
 EXPNO 1
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130093 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



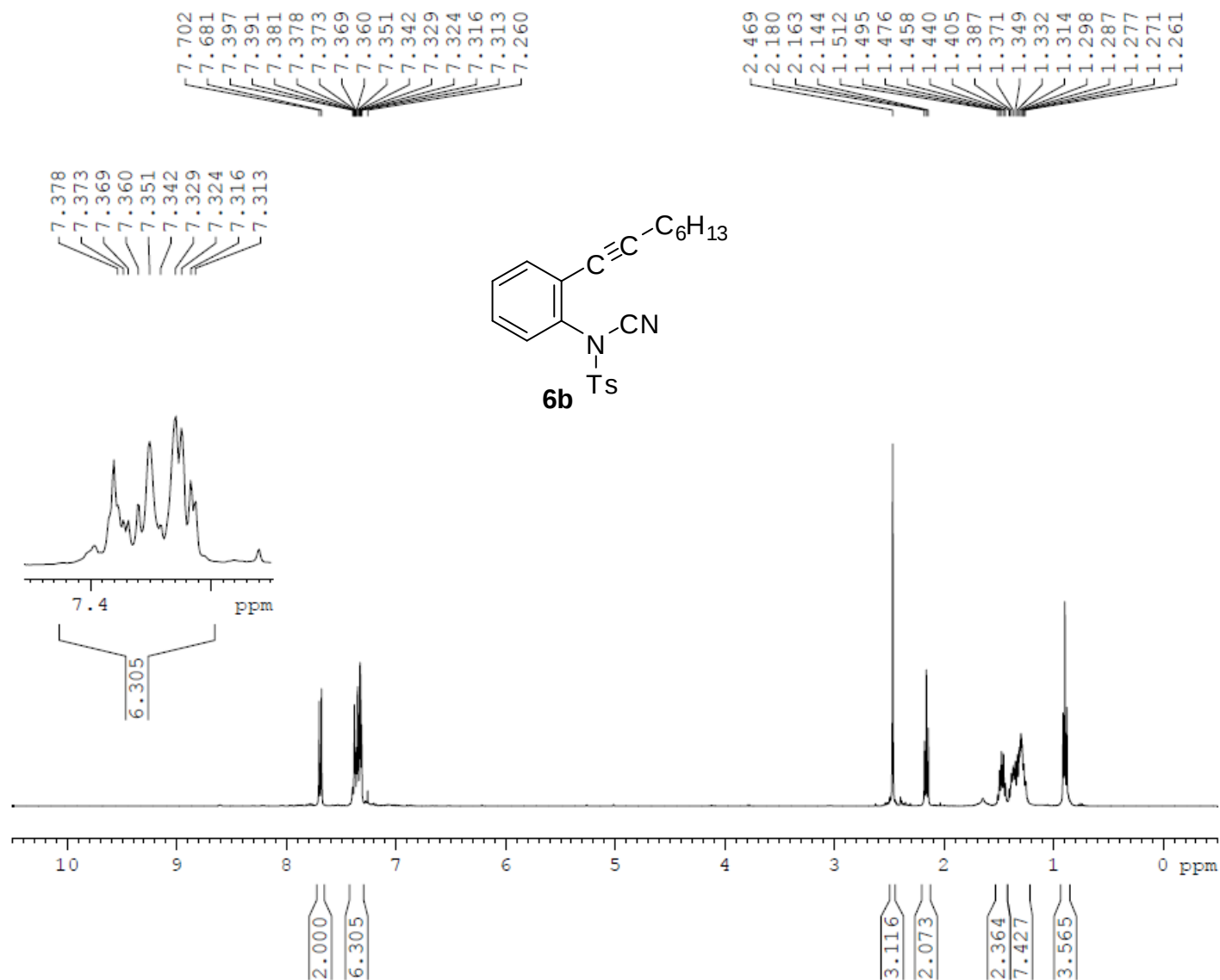
Current Data Parameters
 NAME SO041
 EXPNO 3
 PROCNO 1

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 100.623319 MHz
 NUC1 ¹³C
 P1 10.00 usec
 PLW1 46.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 ¹H
 CPDPRG2 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

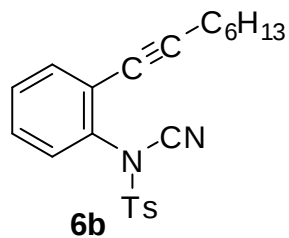


Current Data Parameters
 NAME SC131
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140518
 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
 TDO 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
 WDWH EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



146.43
 134.37
 133.96
 133.71
 130.45
 130.24
 129.62
 128.79
 128.72
 123.95
 107.47
 99.19

77.55
 77.23
 76.91
 74.72

31.51
 28.86
 28.46
 22.70
 21.95
 19.73
 14.23

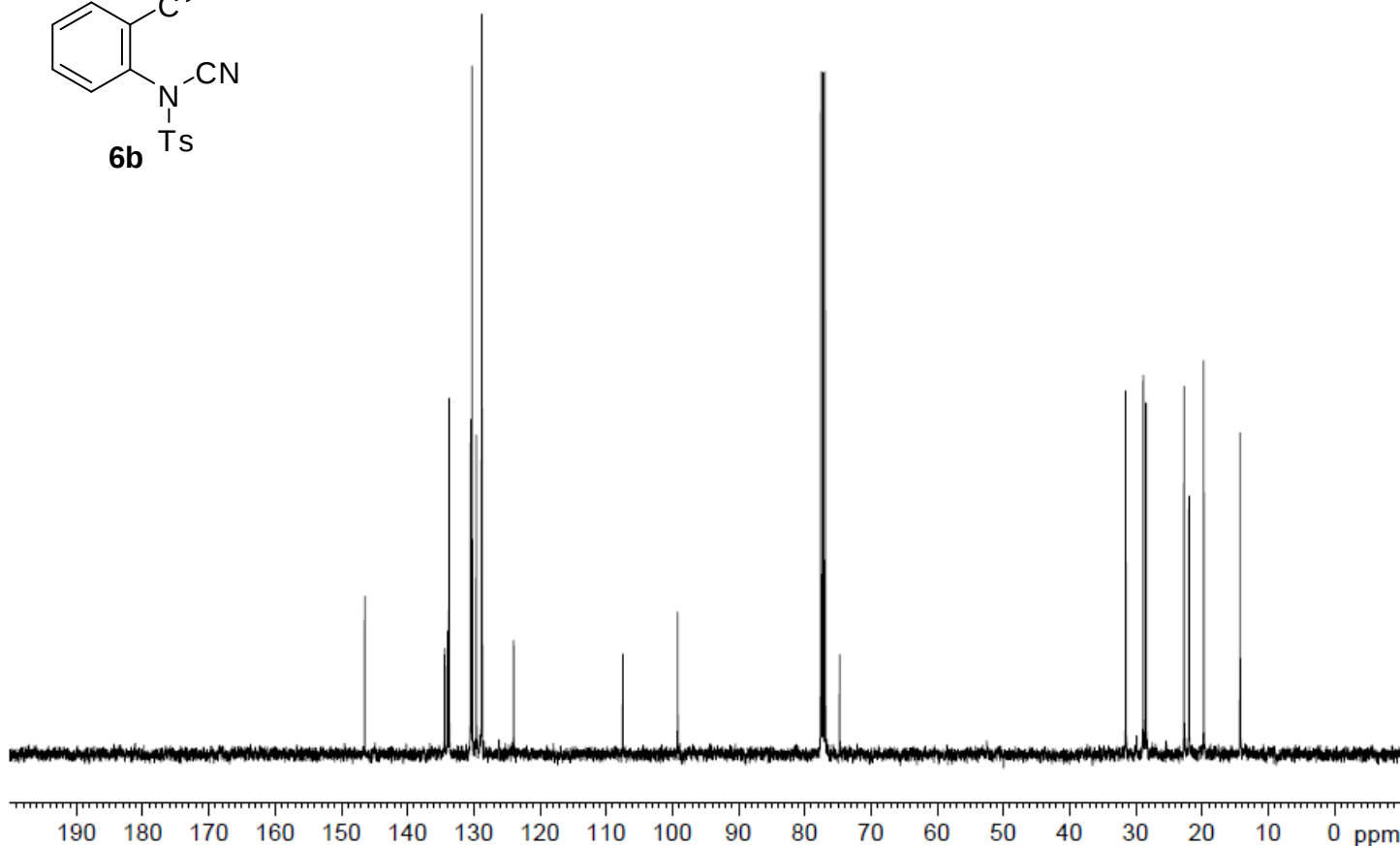
Current Data Parameters
 NAME SC131
 EXPNO 3
 PROCNO 1

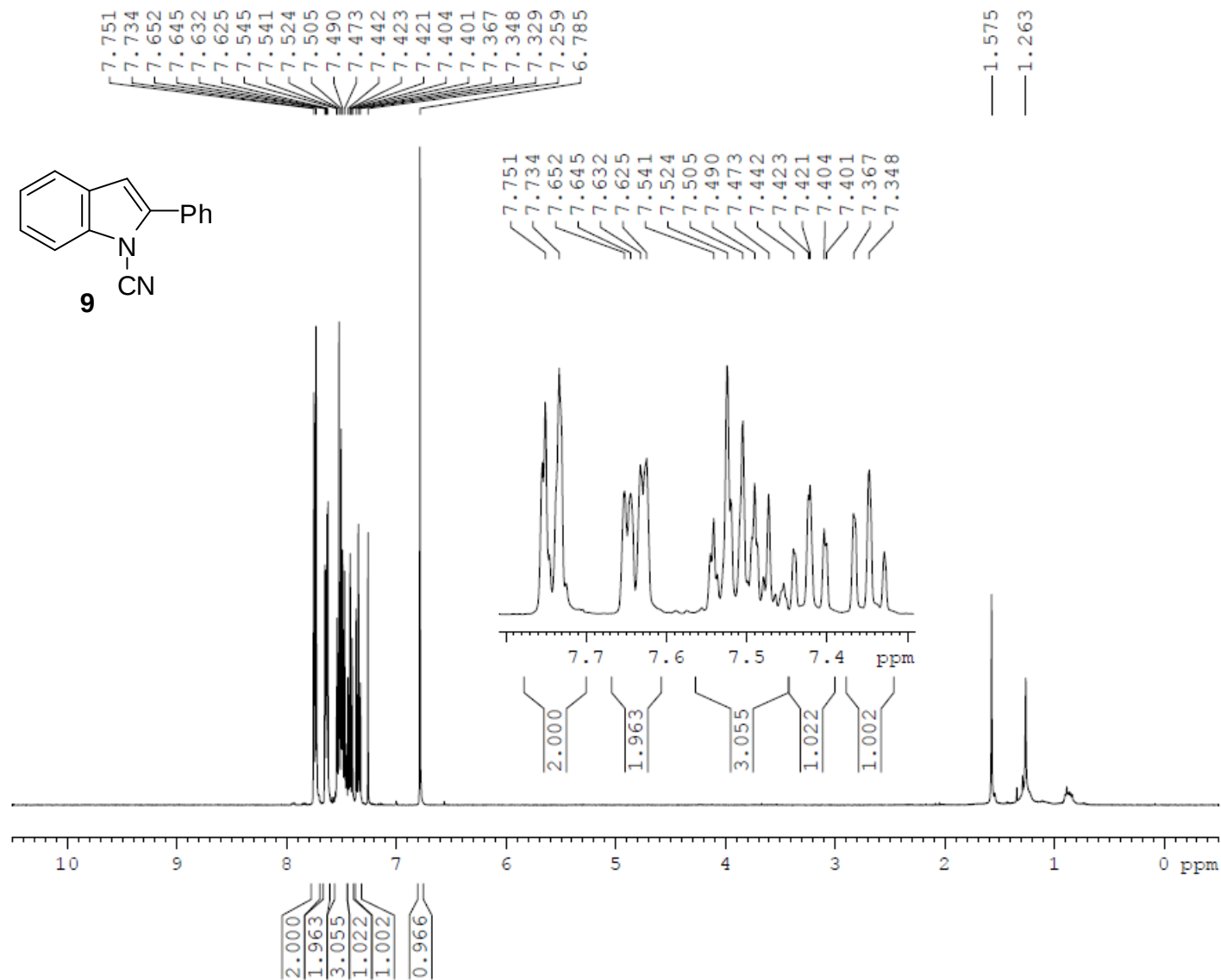
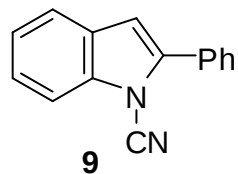
F2 - Acquisition Parameters
 Date_ 20140516
 Time 10.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 173
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 299.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

===== CHANNEL f1 =====
 SFO1 100.623319 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



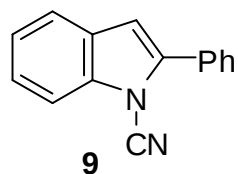


Current Data Parameters
 NAME S0091
 EXPNO 1
 PROCNO 1

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
 TDO 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



139.80
 138.37
 129.78
 129.32
 129.30
 128.84
 127.81
 125.36
 124.68
 121.81
 111.77
 107.60
 107.32

77.55
 77.23
 76.91

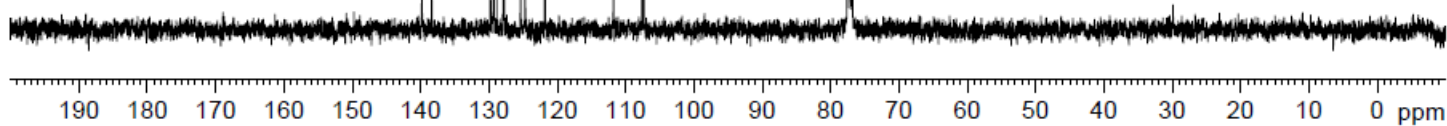
Current Data Parameters
 NAME SO091
 EXPNO 2
 PROCNO 1

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

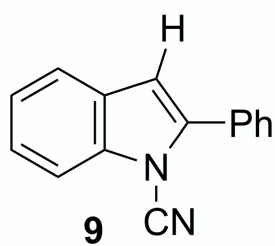
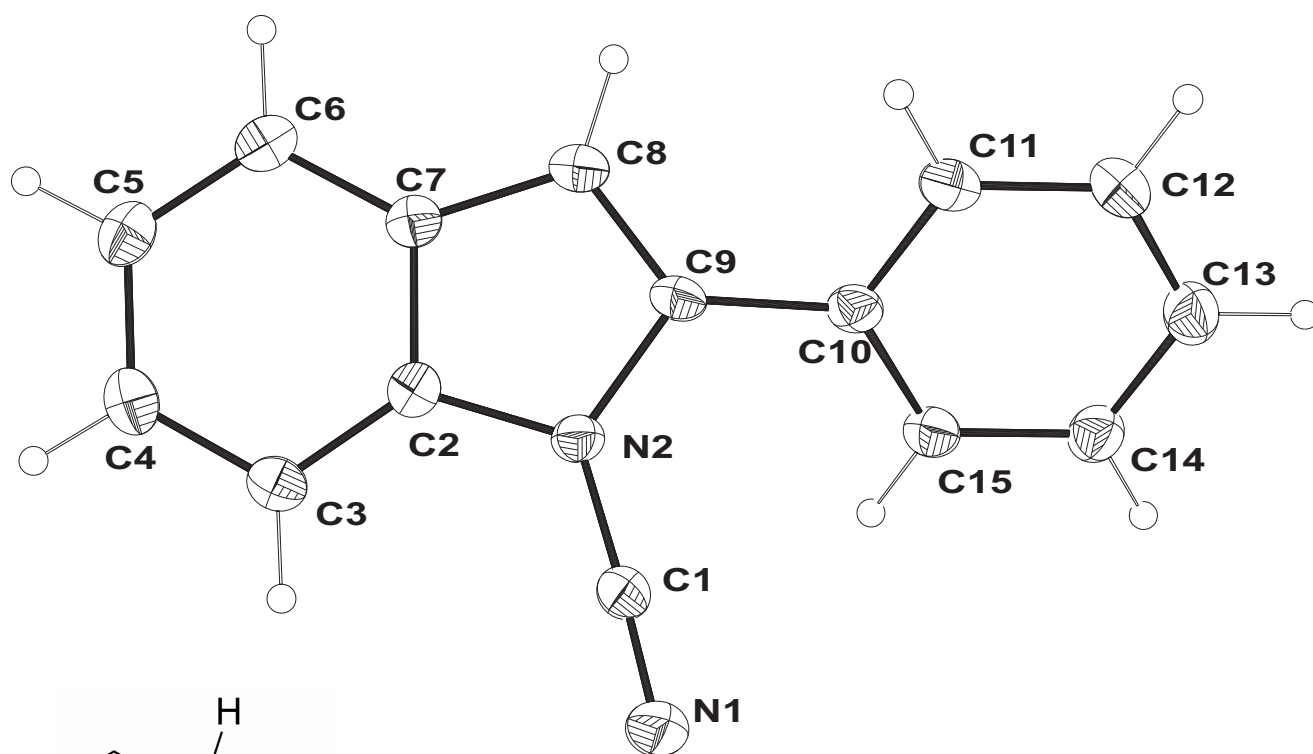
===== CHANNEL f1 =====
 SFO1 100.6233319 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 46.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 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



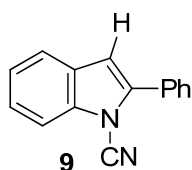


Table 1. Crystal data and structure refinement for a15780.

Identification code	a15780	
Empirical formula	C ₁₅ H ₁₀ N ₂	
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 > 2σ(I)]	R ₁ = 0.0582, wR ₂ = 0.1137	
R indices (all data)	R ₁ = 0.1301, wR ₂ = 0.1461	
Largest diff. peak and hole	0.213 and -0.222 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for a15780. $U(\text{eq})$ 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)

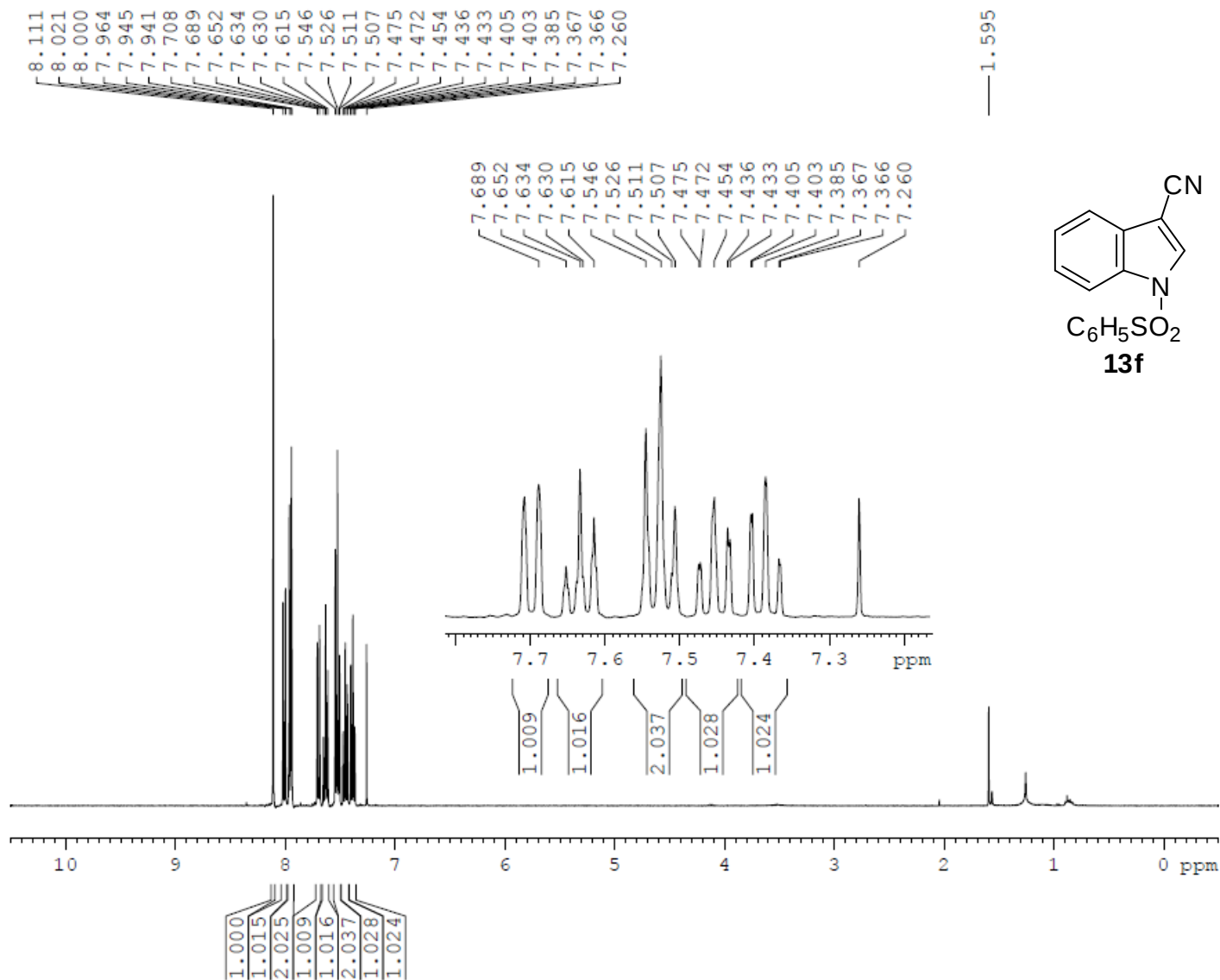
Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
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 ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) 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

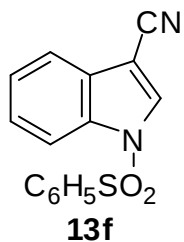


Current Data Parameters
NAME SO125
EXPNO 1
PROCNO 1

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 7248.377 Hz
FIDRES 0.221142 Hz
AQ 2.200921 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 400.130095 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



137.35
135.11
133.89
133.29
129.99
128.52
127.35
126.84
125.09
120.54
113.97
113.57
— 94.16
77.55
77.23
76.91

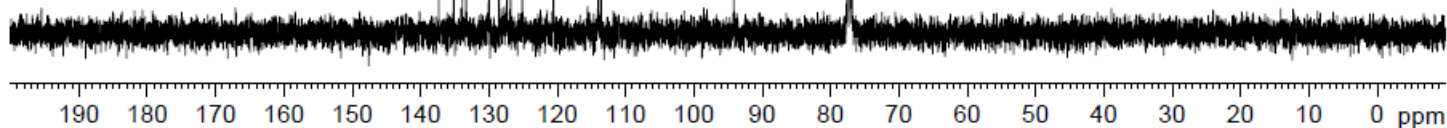
Current Data Parameters
NAME SO125
EXPNO 3
PROCNO 1

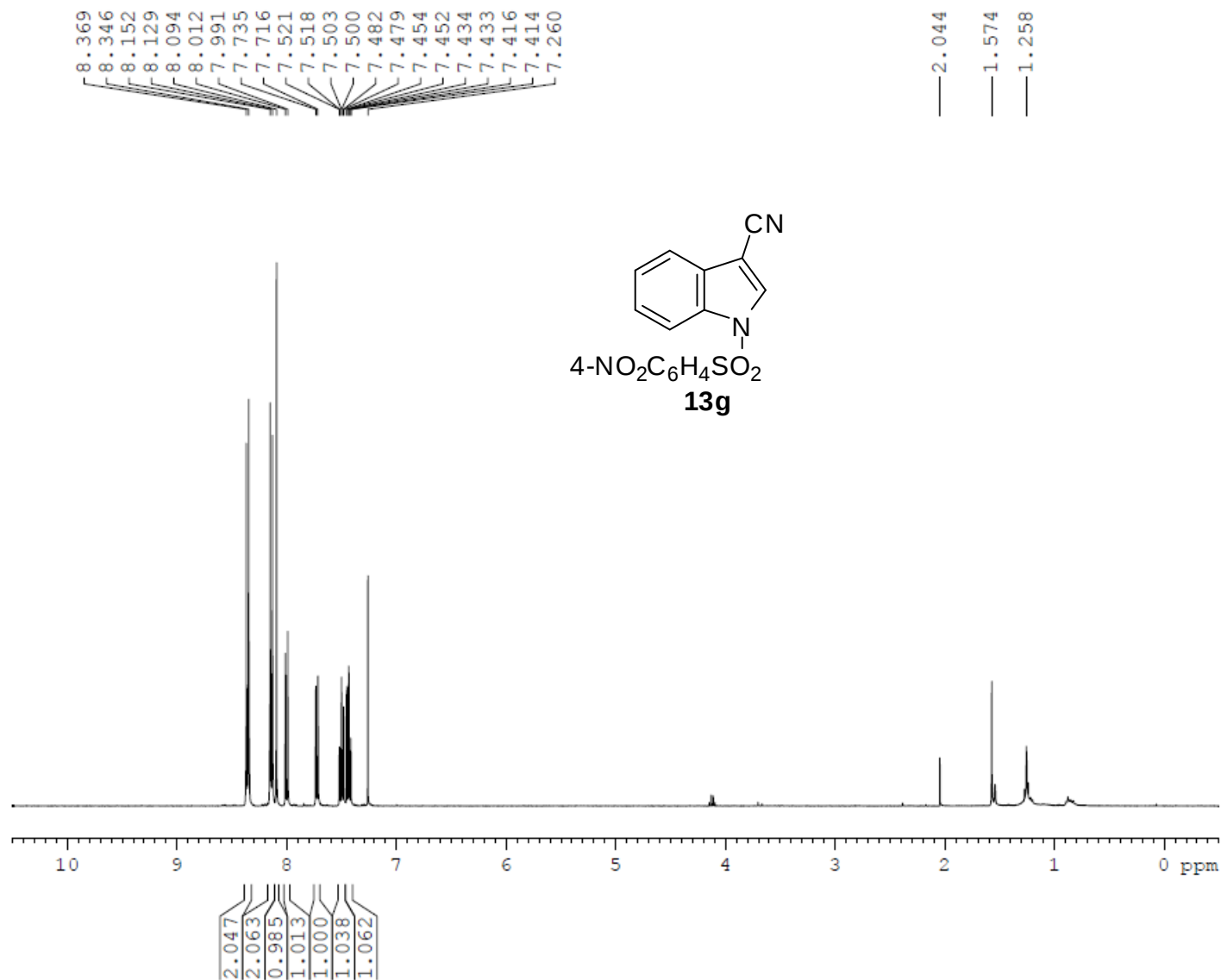
F2 - Acquisition Parameters
Date_ 20150609
Time 9.27
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 131
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 9195.2
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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



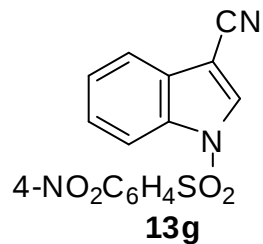


Current Data Parameters
 NAME S0030
 EXPNO 1
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130093 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



151.45
 142.57
 133.82
 132.87
 128.73
 128.60
 127.46
 125.76
 125.22
 120.96
 113.77
 113.01
 95.73
 77.55
 77.23
 76.91

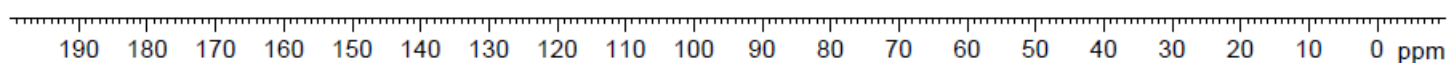
Current Data Parameters
 NAME SO030
 EXPNO 3
 PROCNO 1

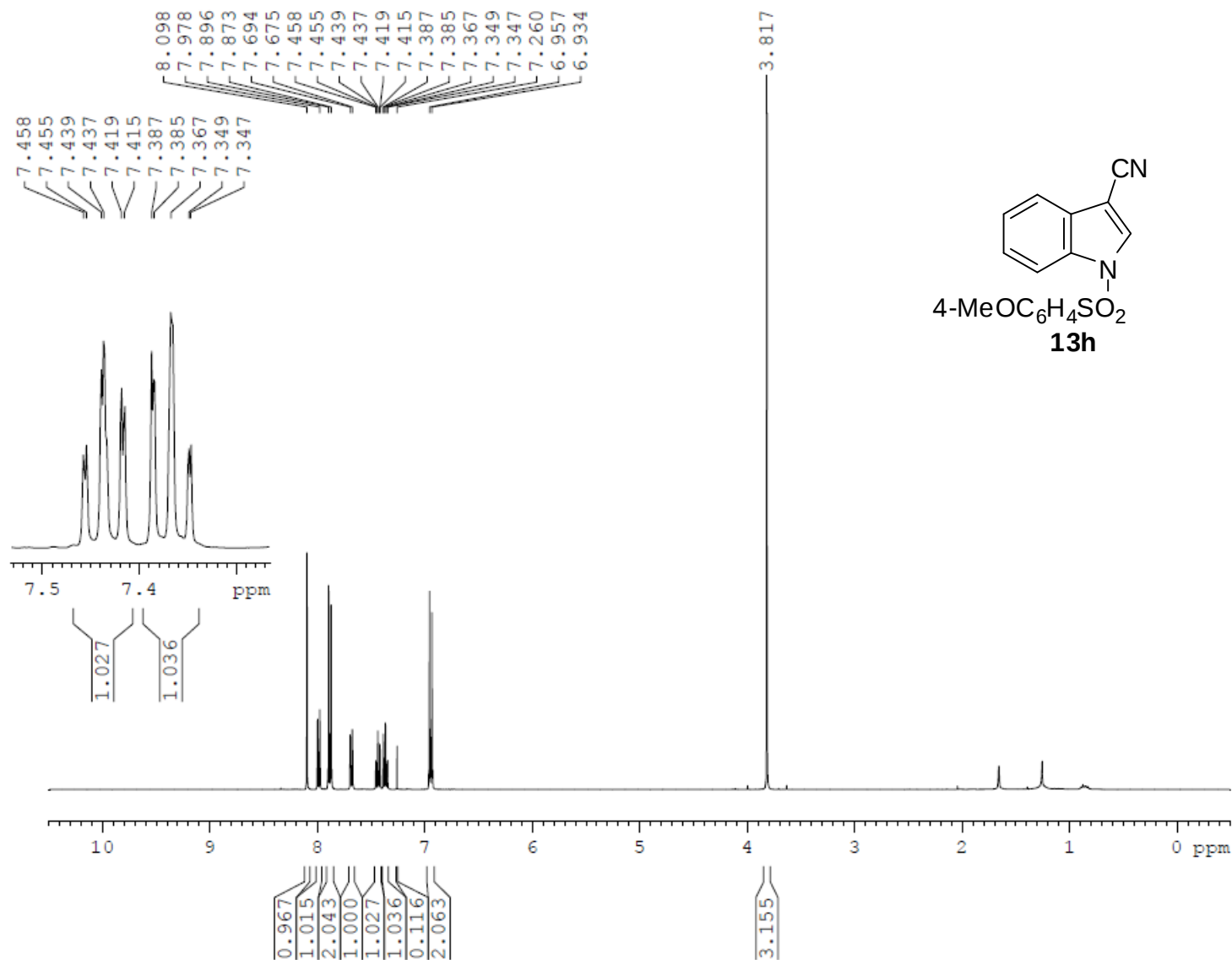
F2 - Acquisition Parameters
 Date_ 20141210
 Time 9.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1229
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 299.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

===== CHANNEL f1 =====
 SFO1 100.623319 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



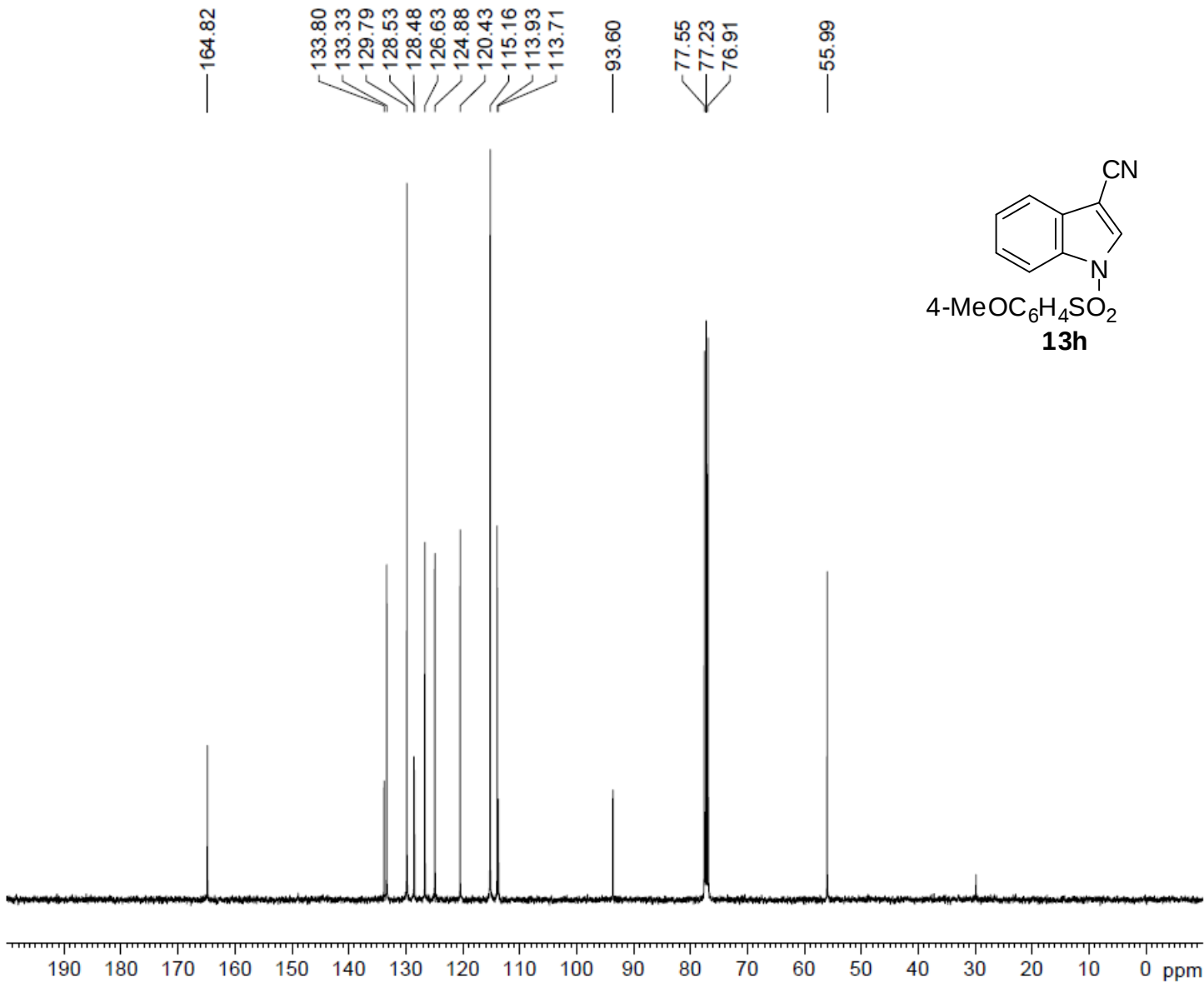


Current Data Parameters
NAME SO128
EXPNO 1
PROCNO 1

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 18384
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



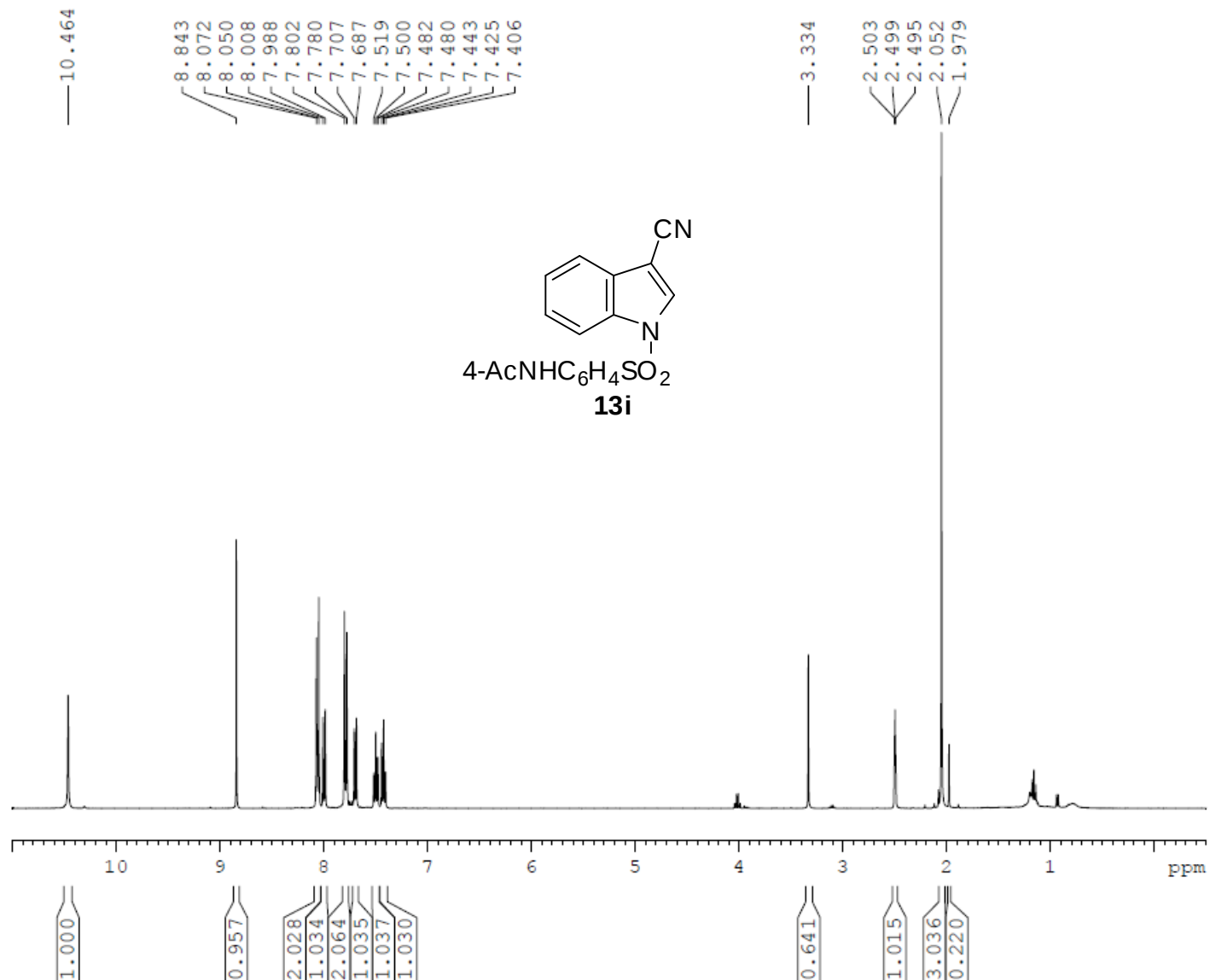
Current Data Parameters
NAME SO128
EXPNO 2
PROCNO 1

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

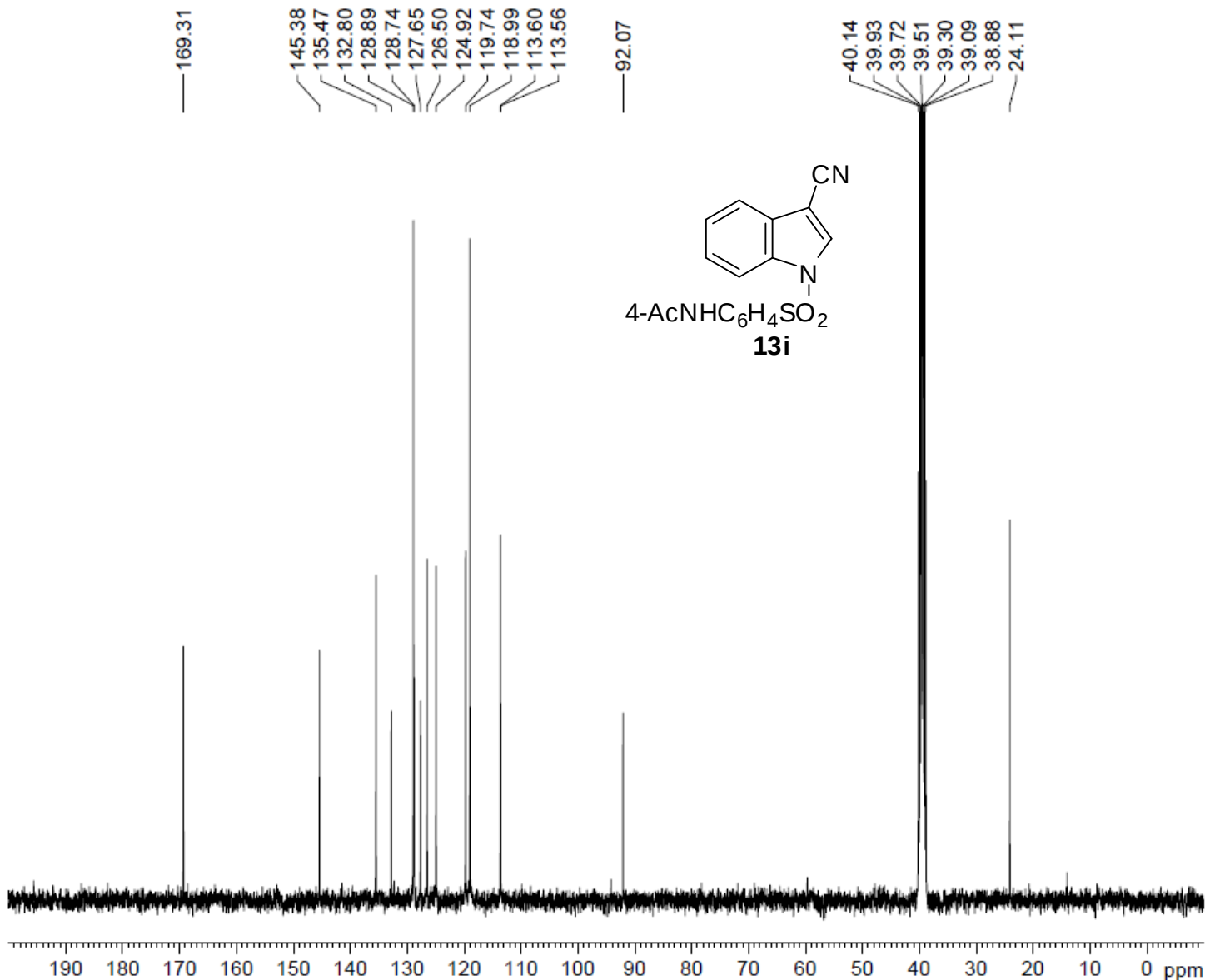


Current Data Parameters
 NAME SO133
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20150822
 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



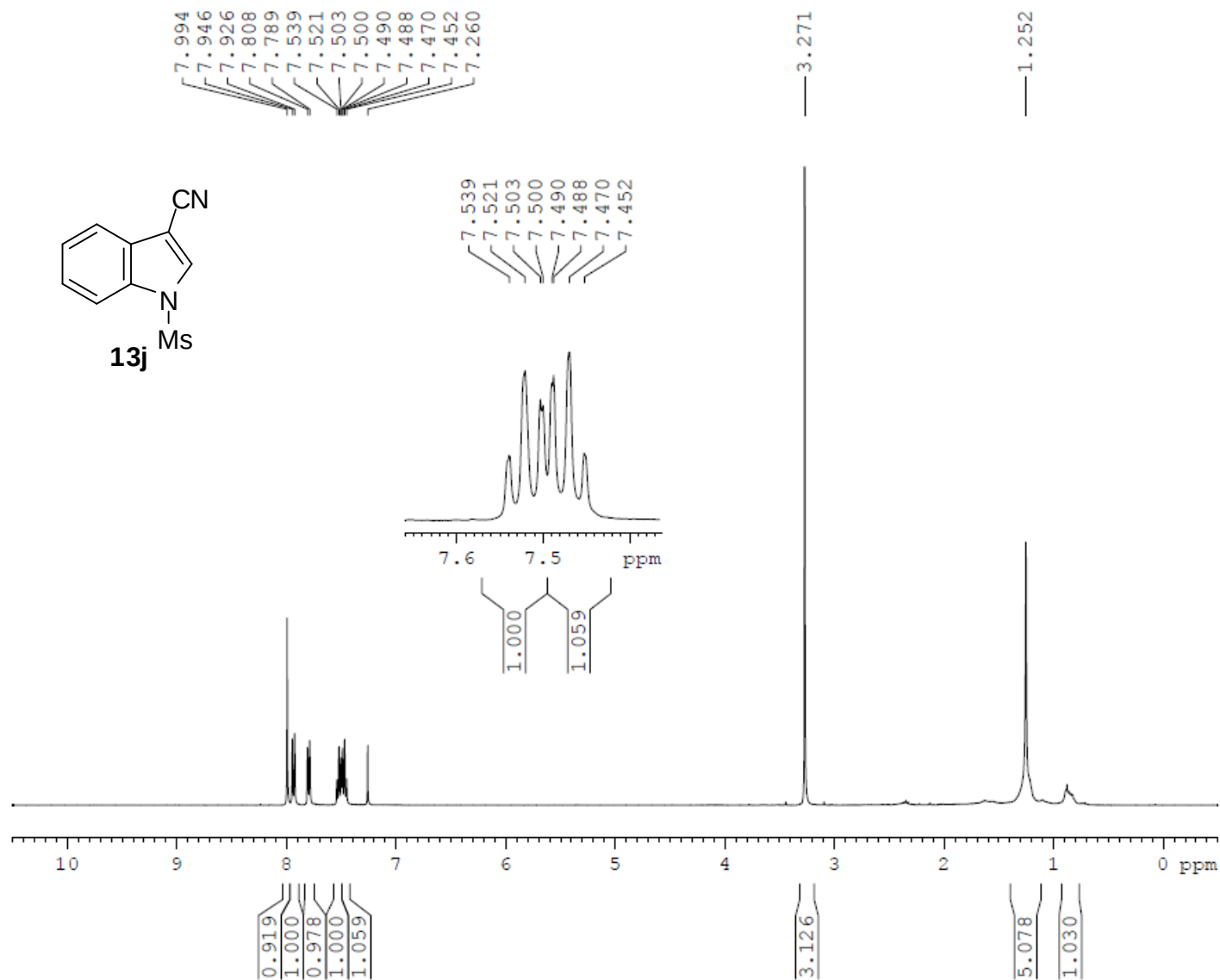
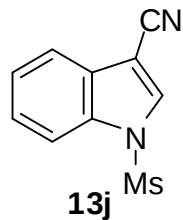
Current Data Parameters
 NAME SO133
 EXPNO 3
 PROCNO 1

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
 CPDPRG2 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



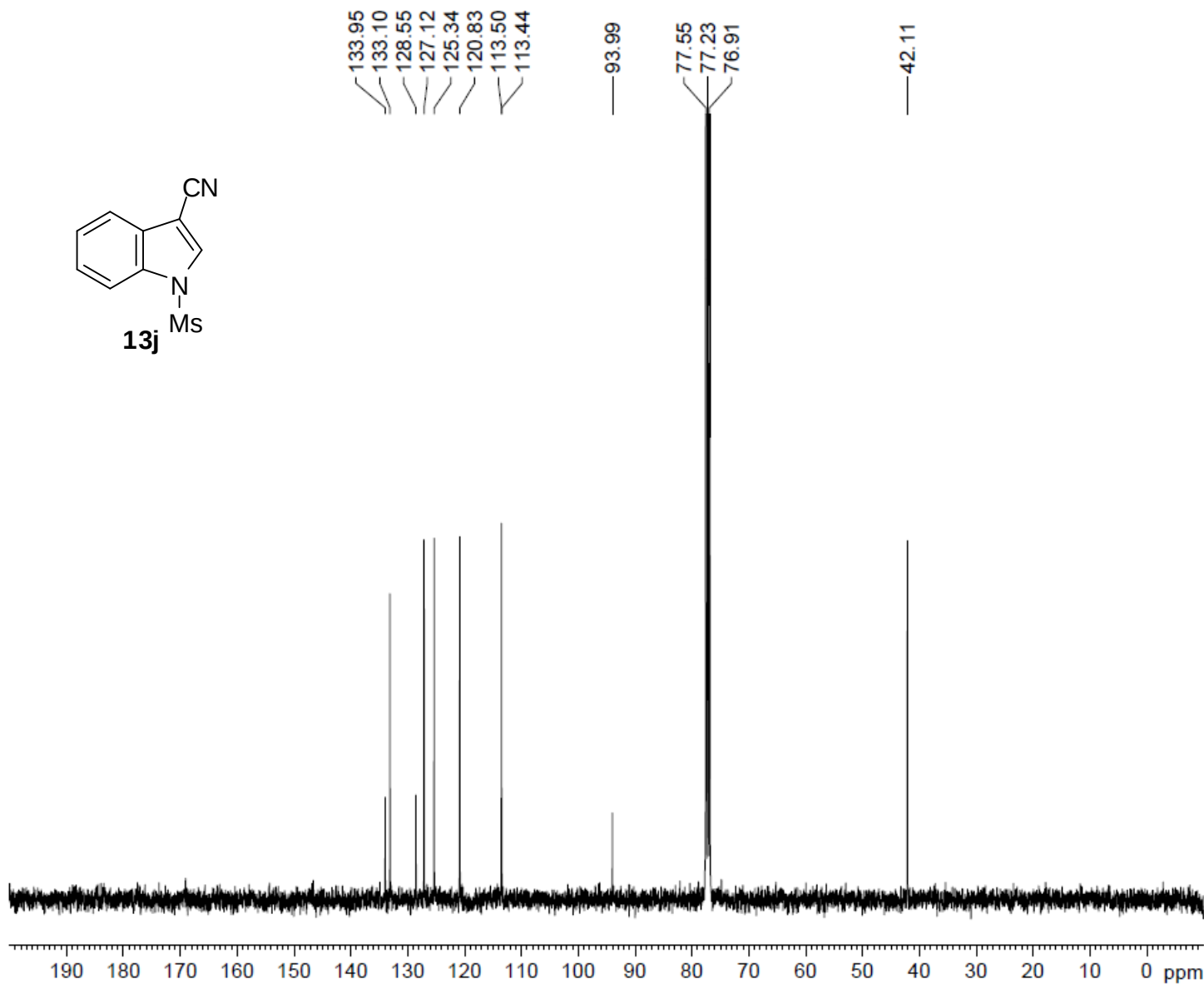
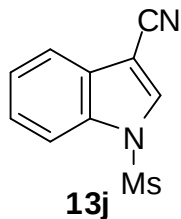
Current Data Parameters
 NAME SO137
 EXPNO 1
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130093 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

recrystallized



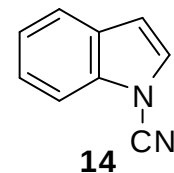
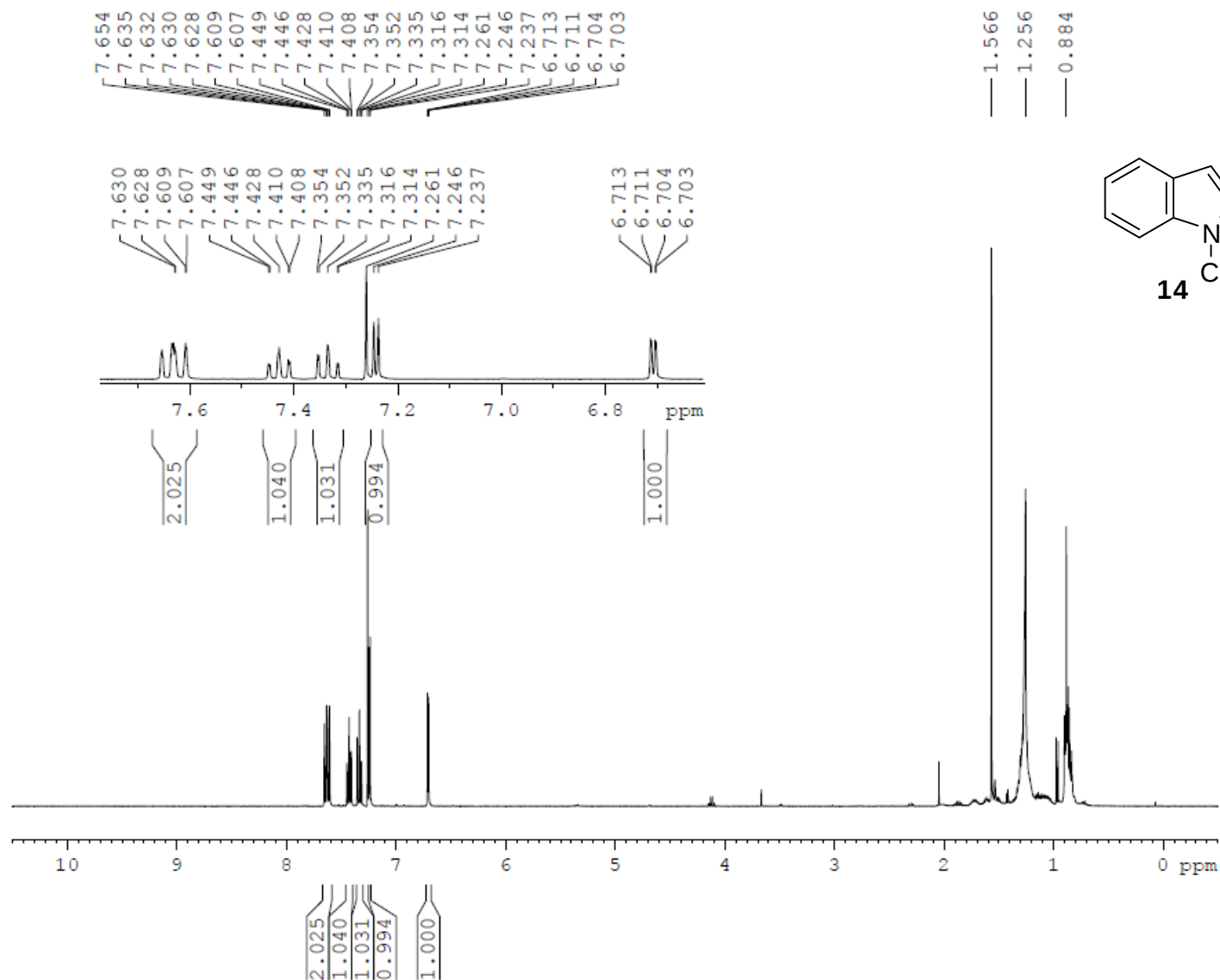
Current Data Parameters
NAME SO137
EXPNO 4
PROCNO 1

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
CPDPRG2 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

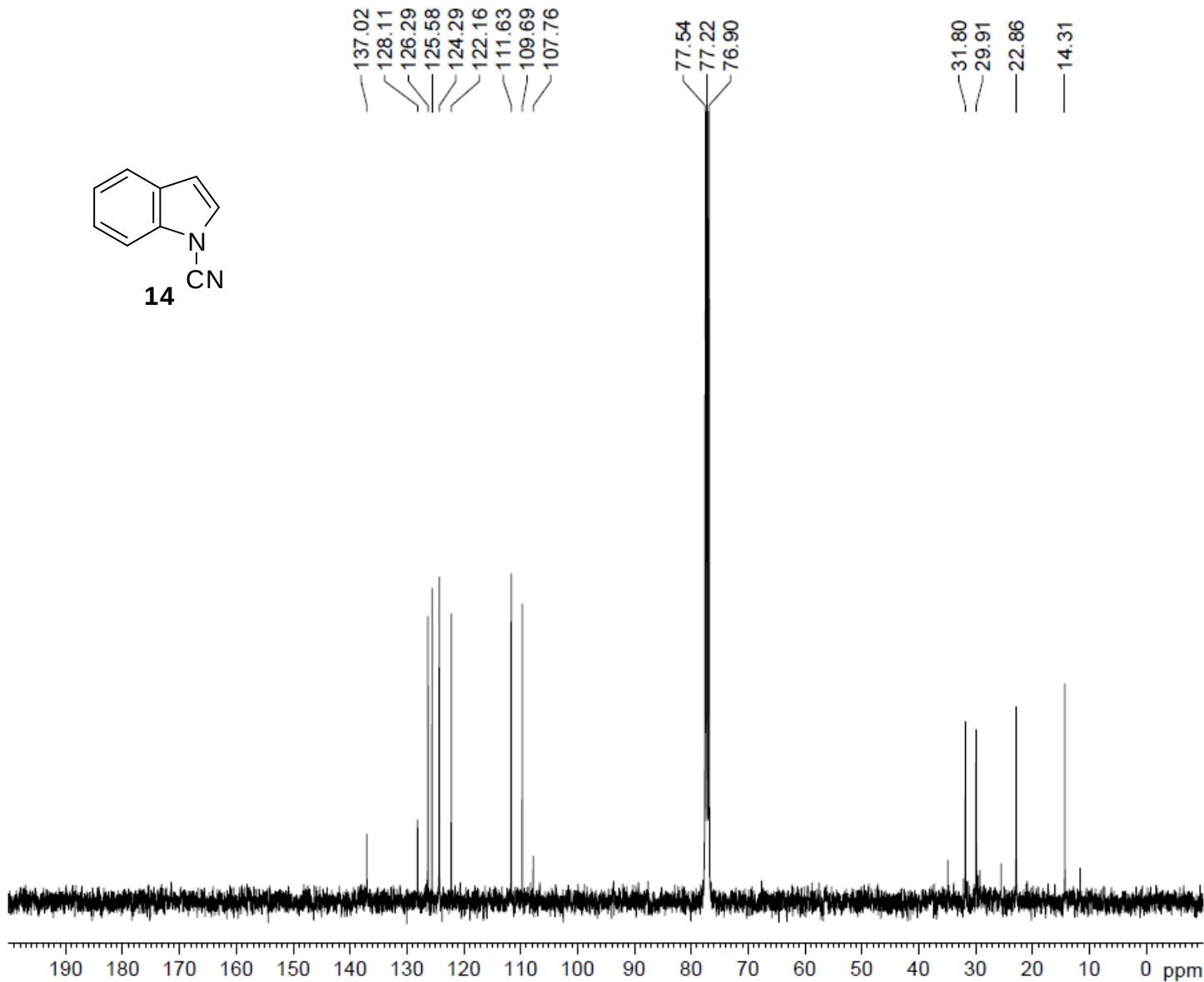
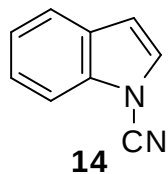


Current Data Parameters
 NAME S0034
 EXPNO 1
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130093 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



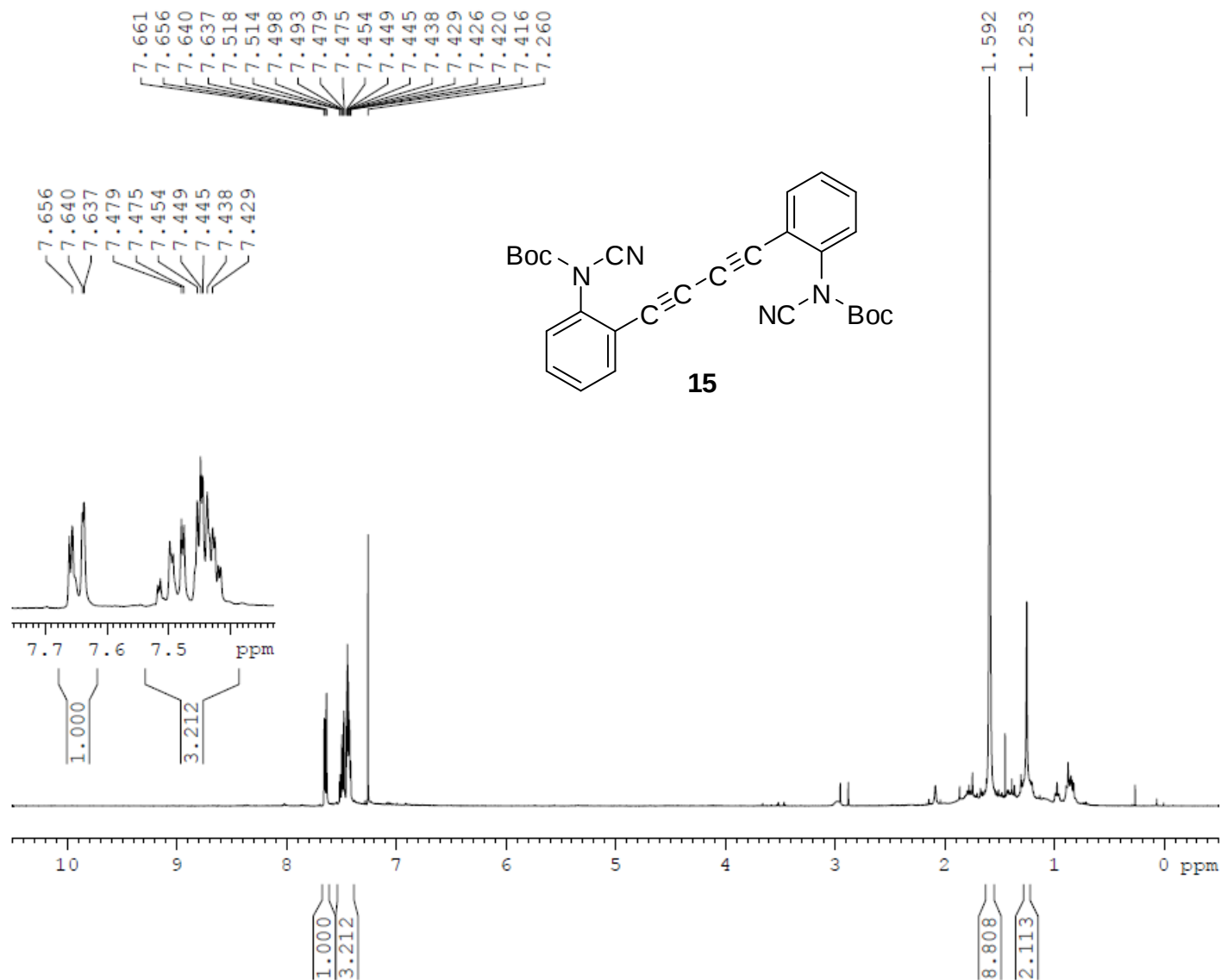
Current Data Parameters
NAME SO034
EXPNO 3
PROCNO 1

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

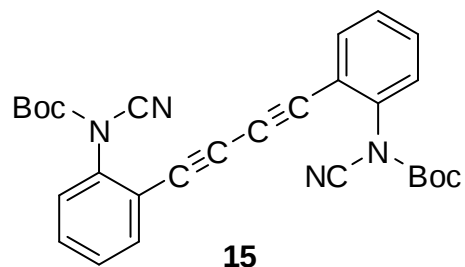


Current Data Parameters
 NAME SO155
 EXPNO 1
 PROCNO 1

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
 TDO 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



149.70
137.18
134.67
130.97
129.87
127.70
121.11
108.50
87.25
79.43
78.01
77.55
77.23
76.91
27.96

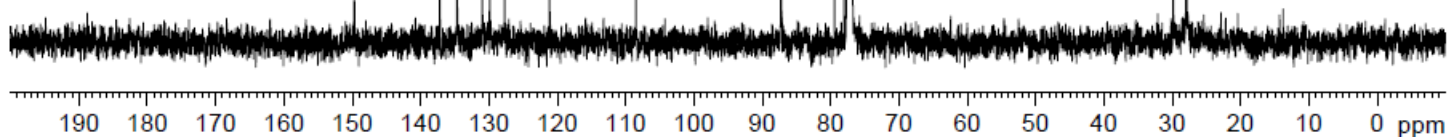
Current Data Parameters
NAME SO155
EXPNO 3
PROCNO 1

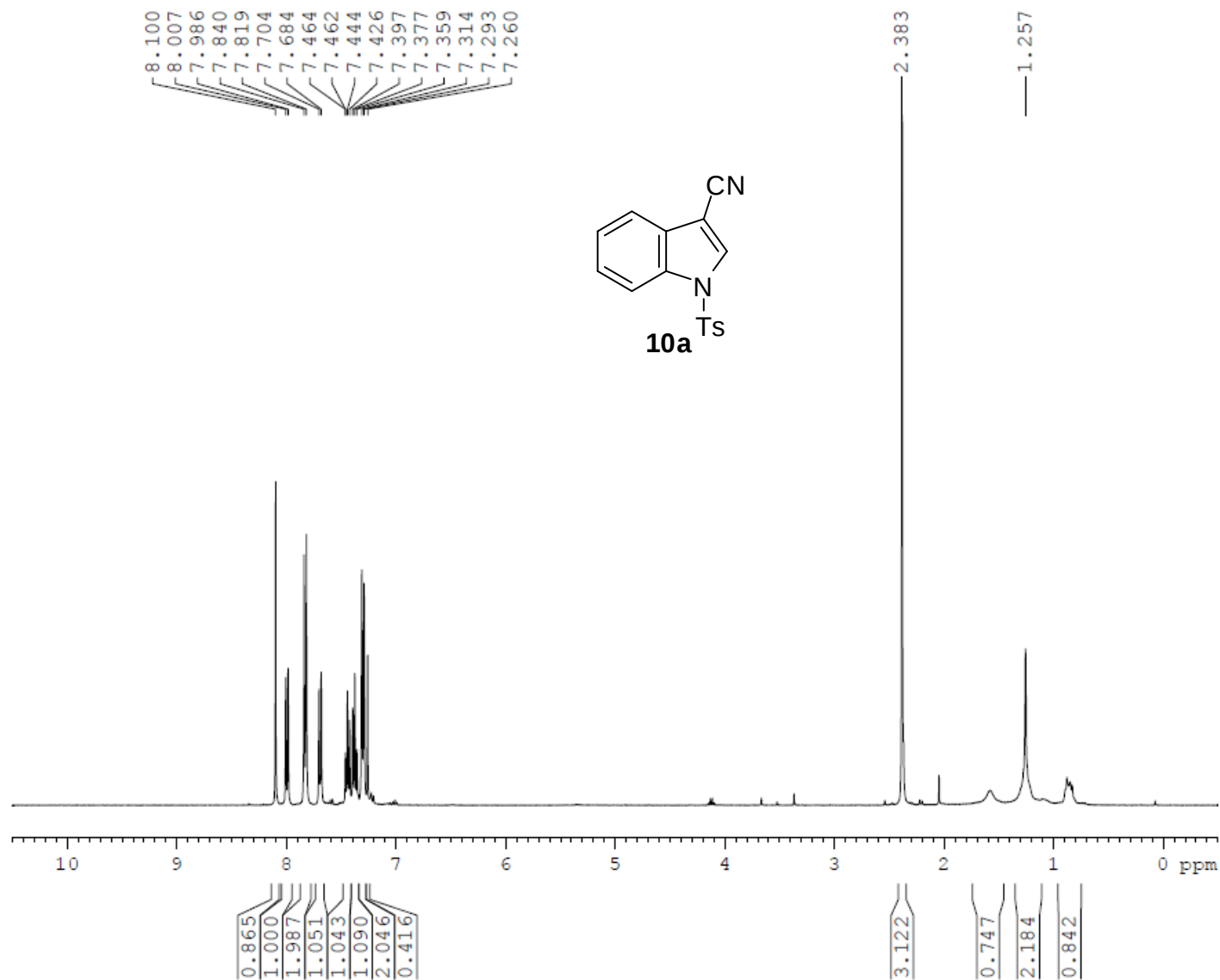
F2 - Acquisition Parameters
Date_ 20150917
Time 14.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 271
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 198.09
DW 20.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.623319 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



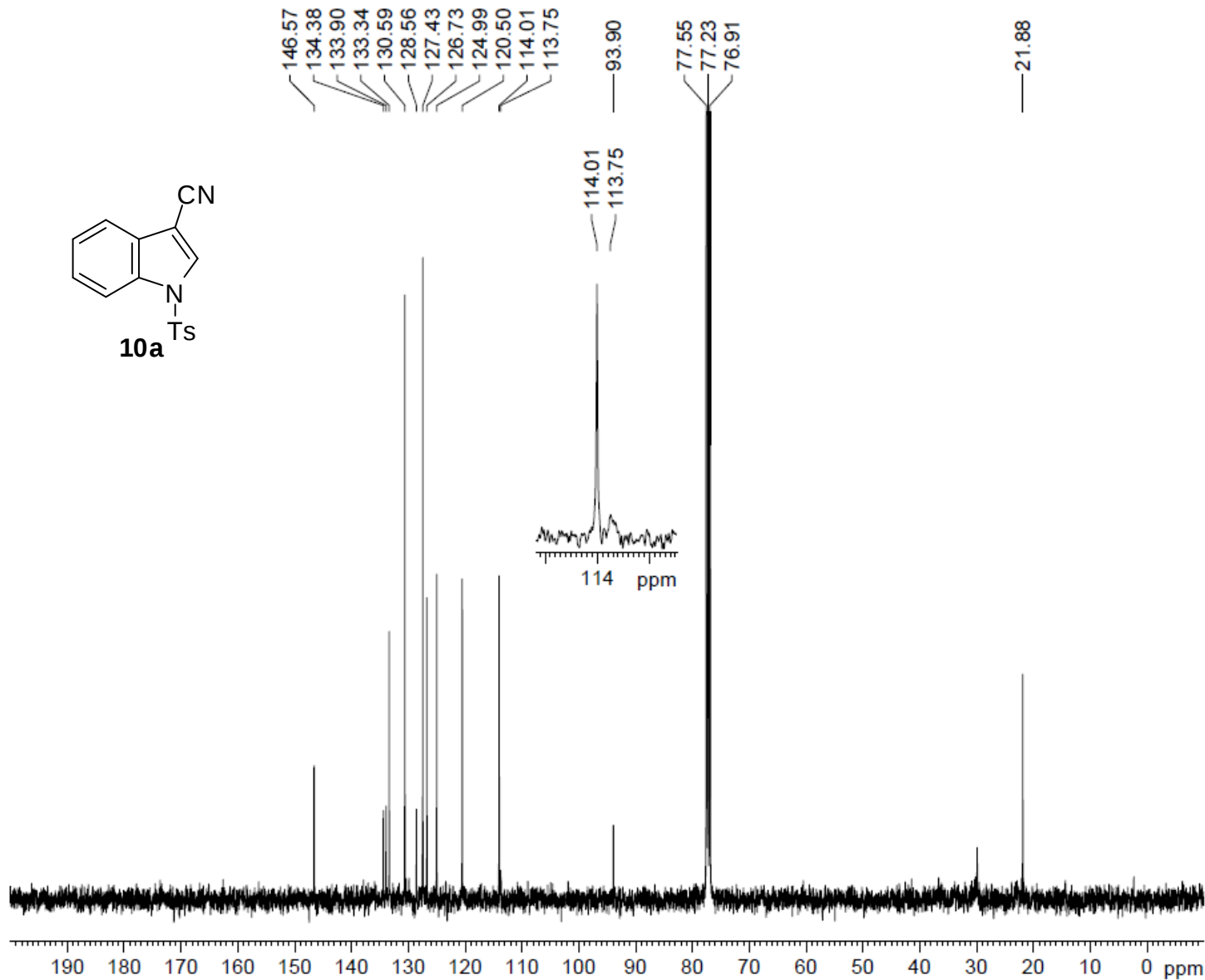
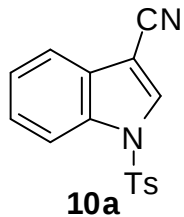


Current Data Parameters
 NAME S0050indole
 EXPNO 1
 PROCNO 1

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
 TDO 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

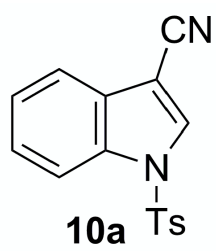
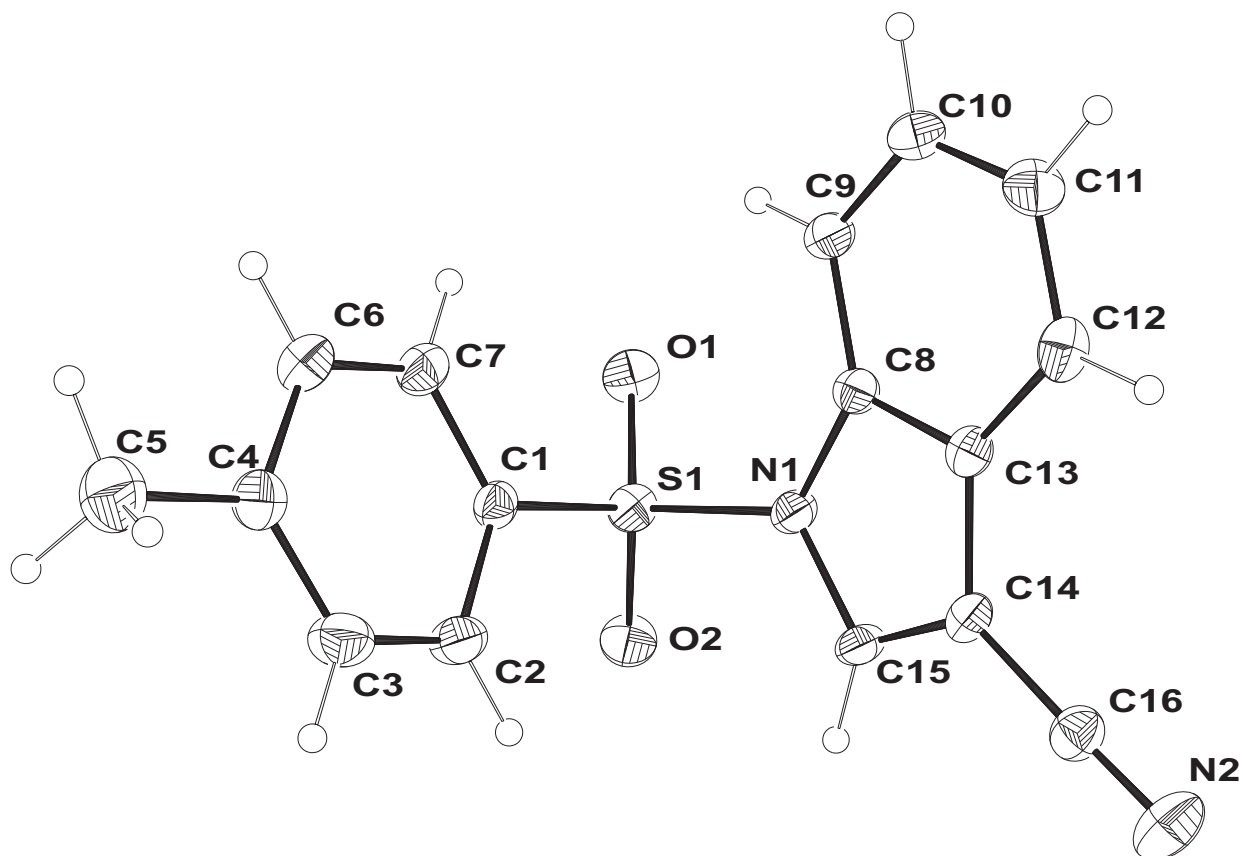
F2 - Acquisition Parameters
 Date_ 20150209
 Time 9.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 262
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 298.4 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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

===== CHANNEL f1 =====
 SFO1 100.623319 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 46.00000000 W

===== CHANNEL f2 =====
 SFO2 400.1316005 MHz
 NUC2 1H
 CPDPRG2 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



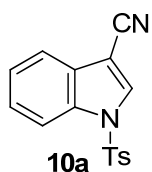


Table 1. Crystal data and structure refinement for a15781.

Identification code	a15781	
Empirical formula	C ₁₆ H ₁₂ N ₂ O ₂ S	
Formula weight	296.34	
Temperature	200(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /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 > 2σ(I)]	R ₁ = 0.0529, wR ₂ = 0.1059	
R indices (all data)	R ₁ = 0.1015, wR ₂ = 0.1274	
Largest diff. peak and hole	0.314 and -0.317 e.Å ⁻³	

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

	x	y	z	$U(\text{eq})$
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)

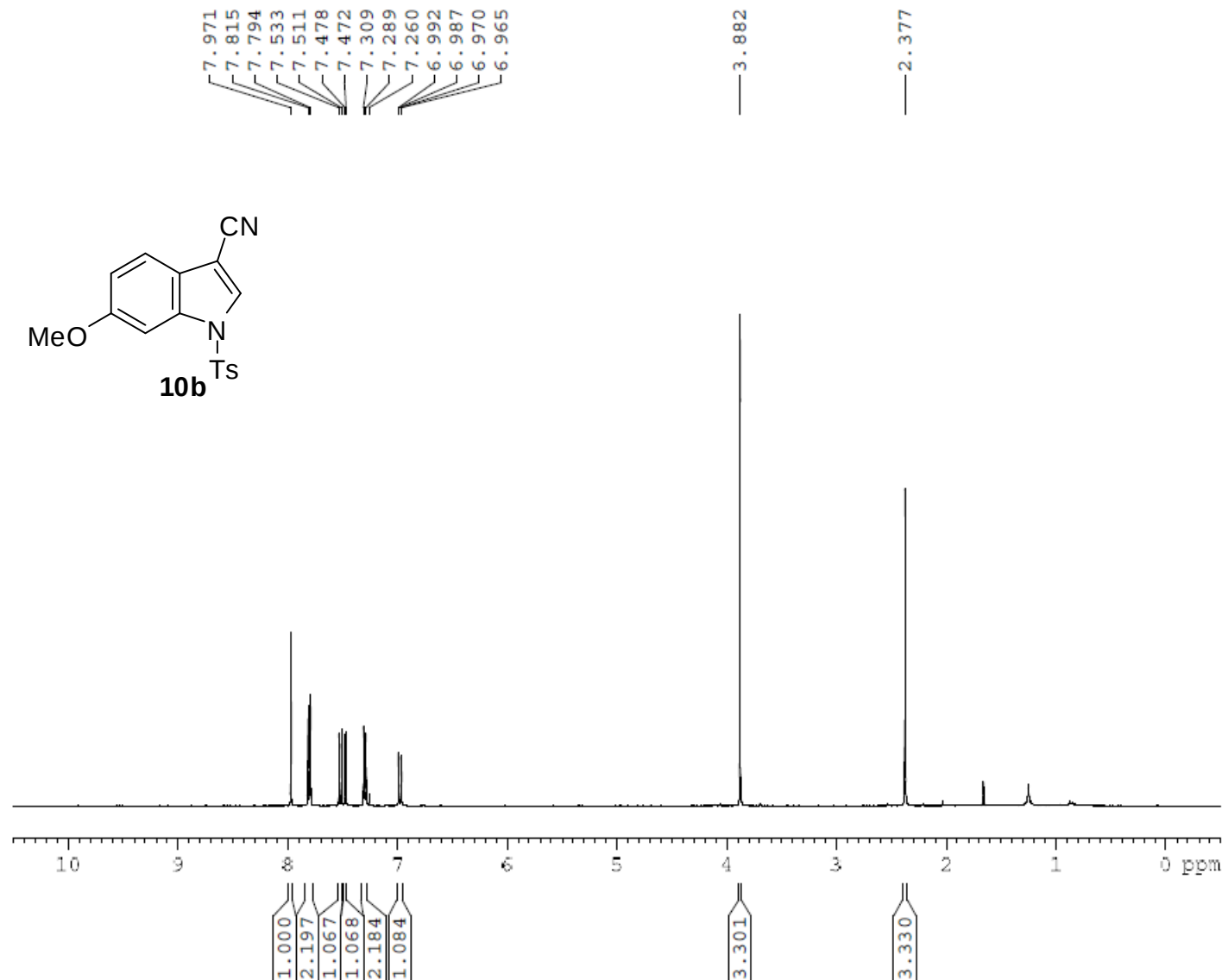
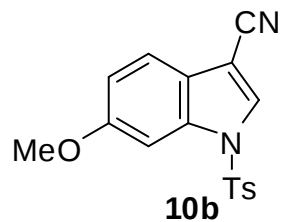
Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
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 ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) 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

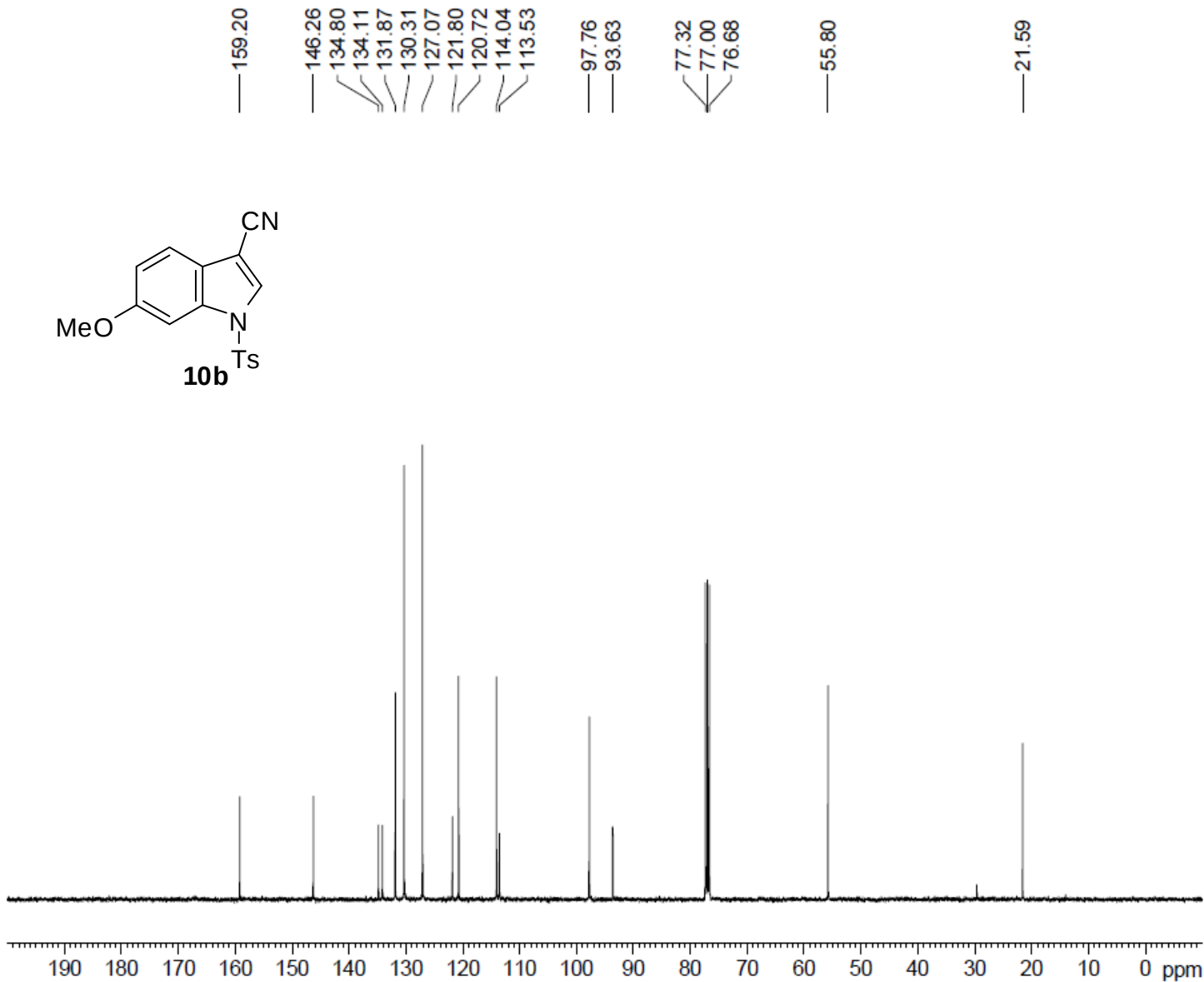
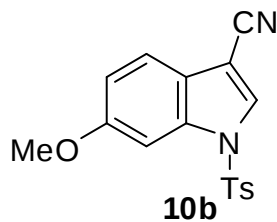


Current Data Parameters
 NAME SD-103(new)
 EXPNO 1
 PROCNO 1

F2: Acquisition Parameters
 Date 20140707
 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 2.0000000 sec
 D0 1

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

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



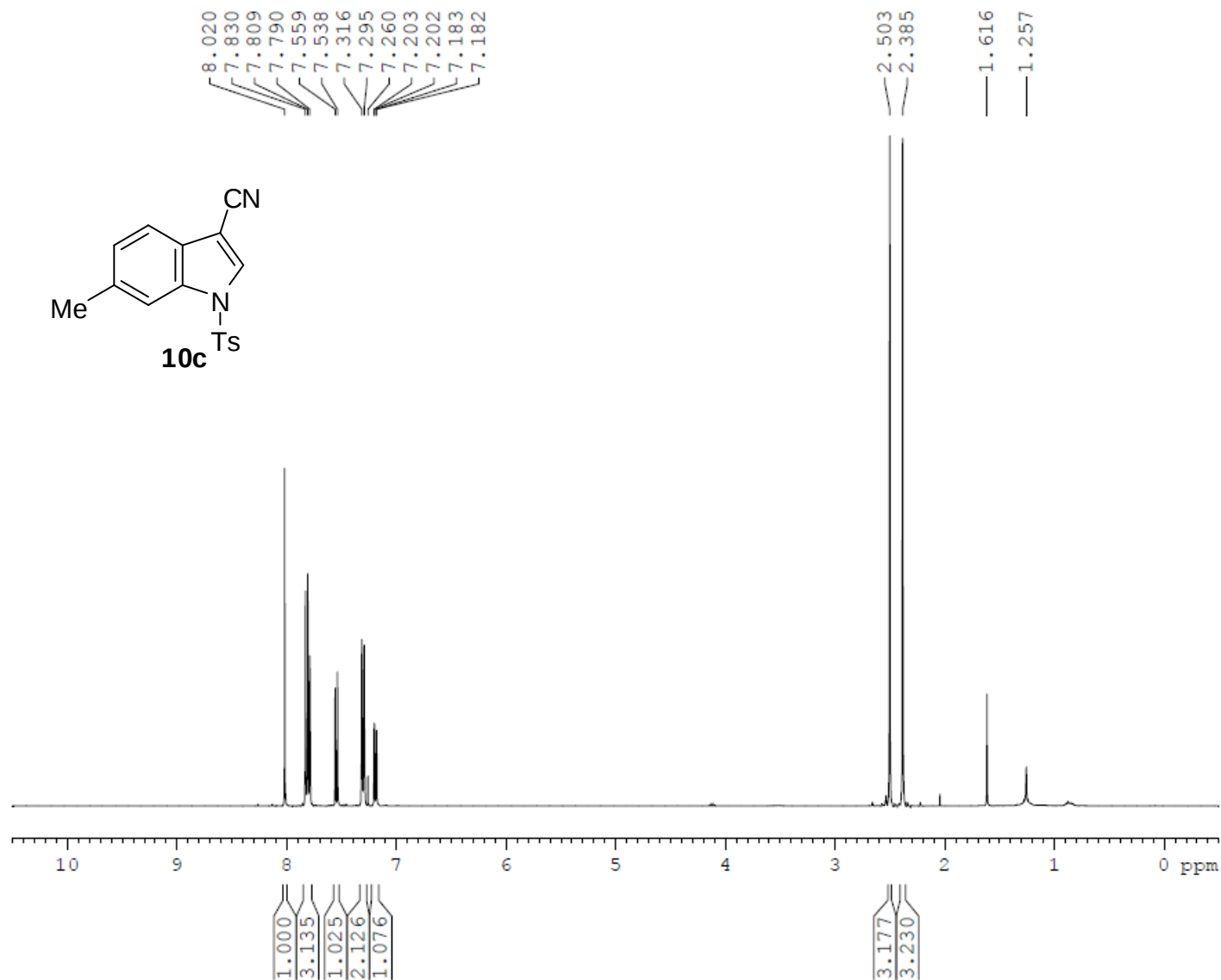
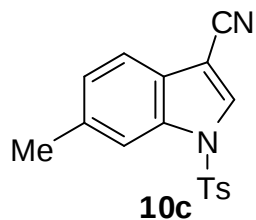
Current Data Parameters
 NAME SD-103(new)
 EXPNO 4
 PROCNO 1

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

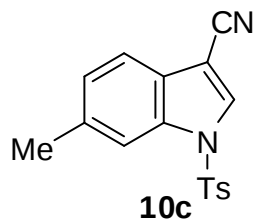


Current Data Parameters
 NAME SC183-1
 EXPNO 1
 PROCNO 1

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
 TDO 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



146.43
 137.26
 134.50
 134.31
 132.75
 130.55
 127.35
 126.59
 126.25
 119.99
 113.91
 113.81

93.79

77.55
 77.23
 76.91

22.20
 21.85

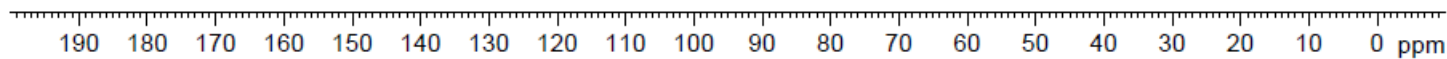
Current Data Parameters
 NAME SC163-1
 EXPNO 2
 PROCNO 1

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

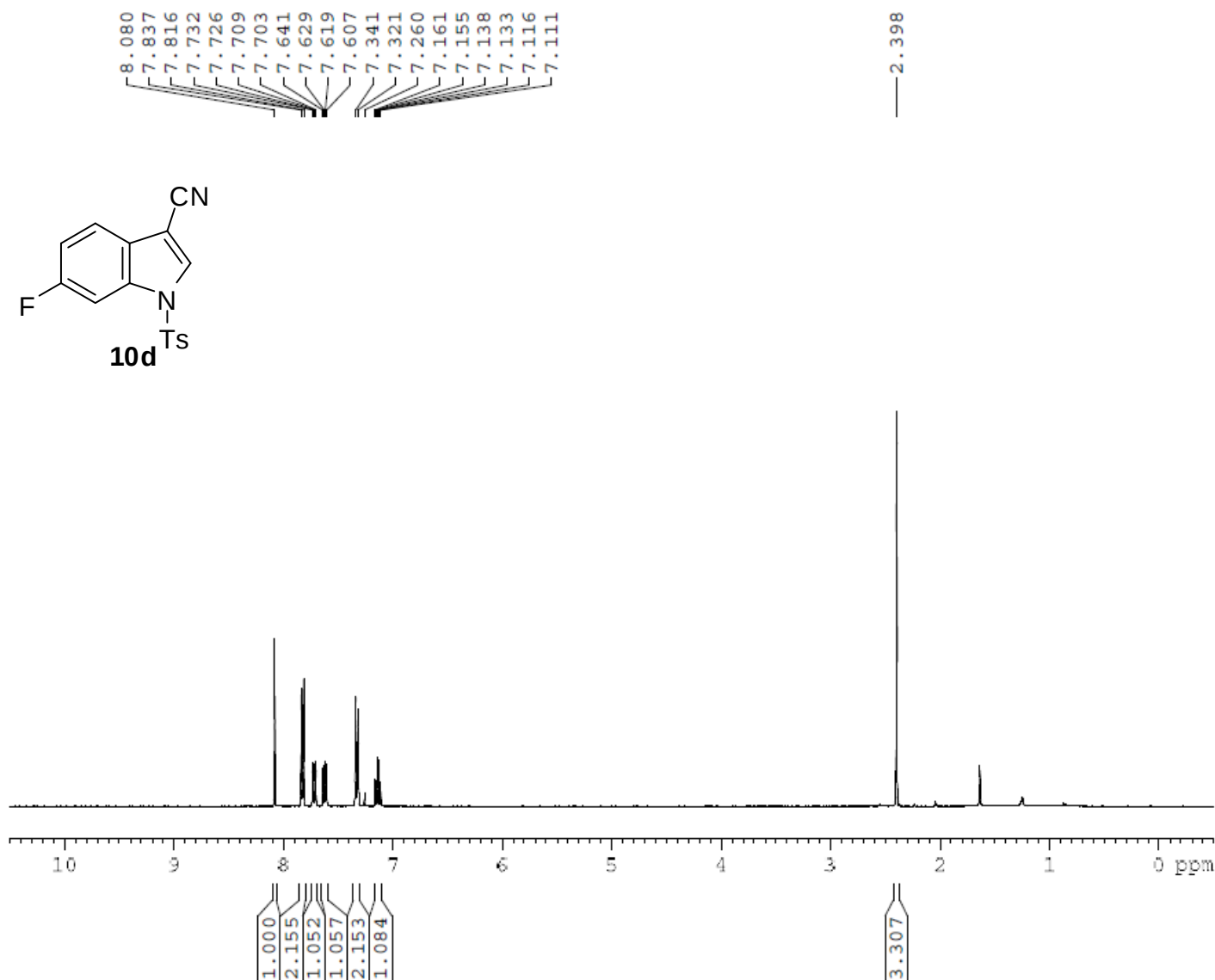
===== CHANNEL f1 =====
 SFO1 100.623319 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 46.00000000 W

===== 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



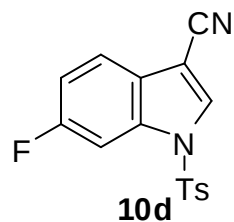
Current Data Parameters
 NAME SD-084(old)
 EXPNO 1
 PROCNO 1

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 2.0000000 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



162.90
160.46
146.65
133.95
133.82
133.42
133.39
130.49
127.21
124.49
121.40
121.30
113.73
113.49
113.08
101.38
101.09
93.60
77.32
77.00
76.68

21.66

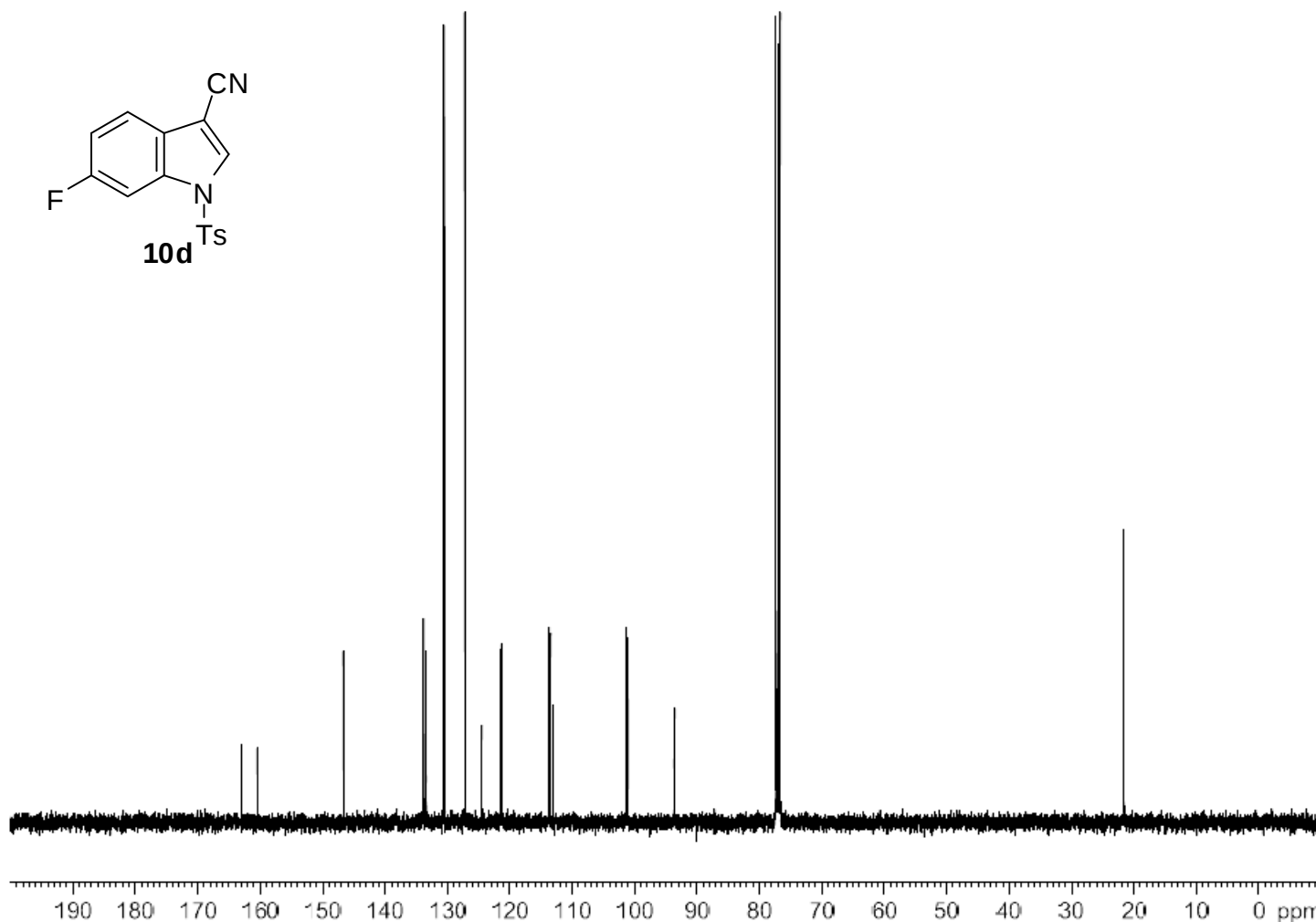
Current Data Parameters
NAME SD-084(pld)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140607
Time 16.54
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 381
CS 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

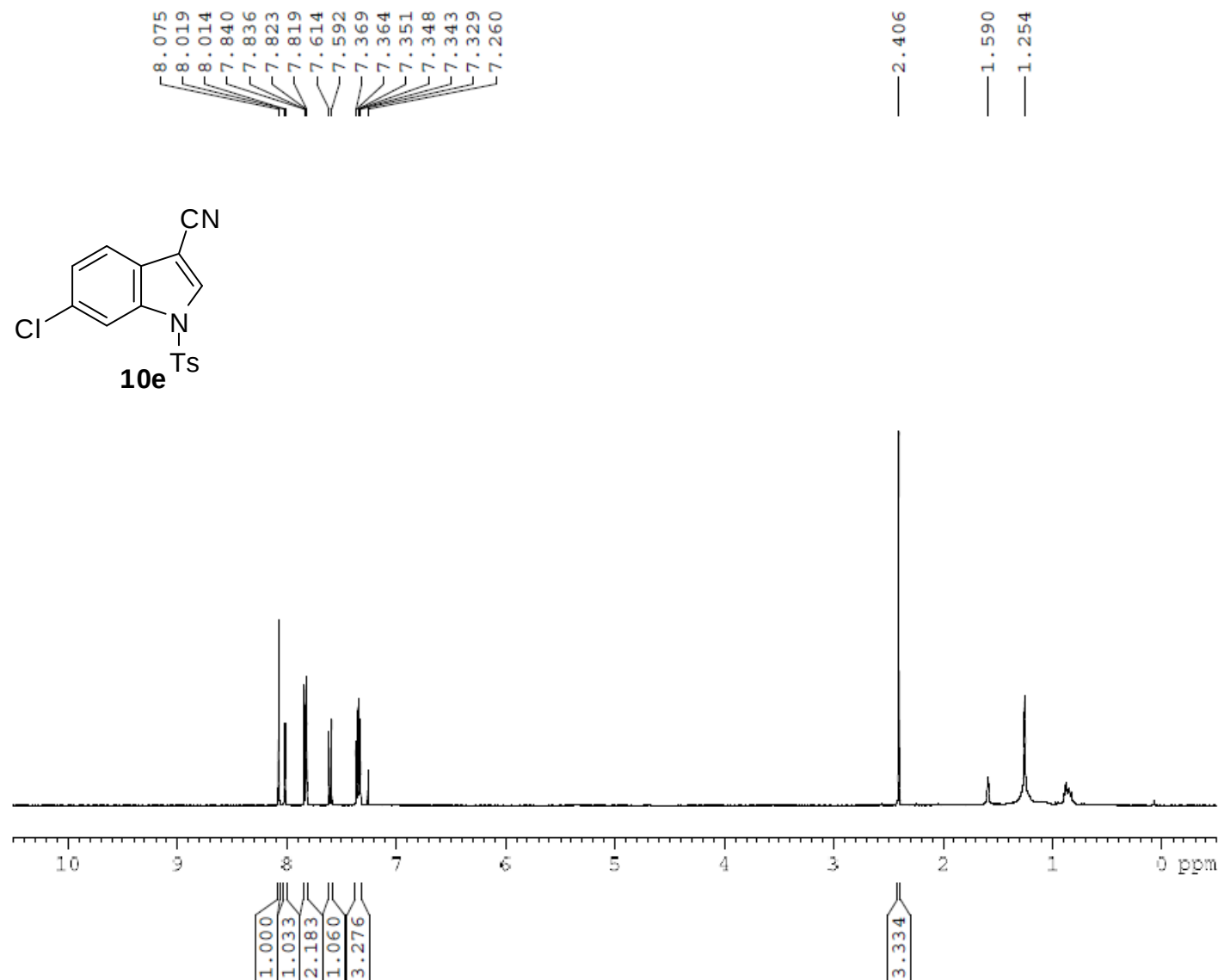
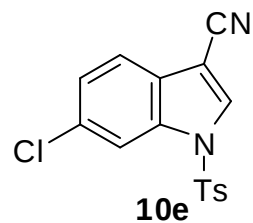
===== CHANNEL f1 =====
NUC1 13C
P1 15.50 usec
PL1 7.30 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG2 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



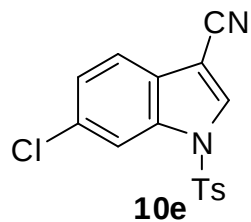
Current Data Parameters
NAME SD-079(old)
EXPNO 1
PROCNO 1

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 2.0000000 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 400.1300992 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

pure



146.72
133.98
133.84
133.52
132.81
130.55
127.22
126.76
125.63
121.09
114.01
112.95

93.61

77.31
76.99
76.68

21.70

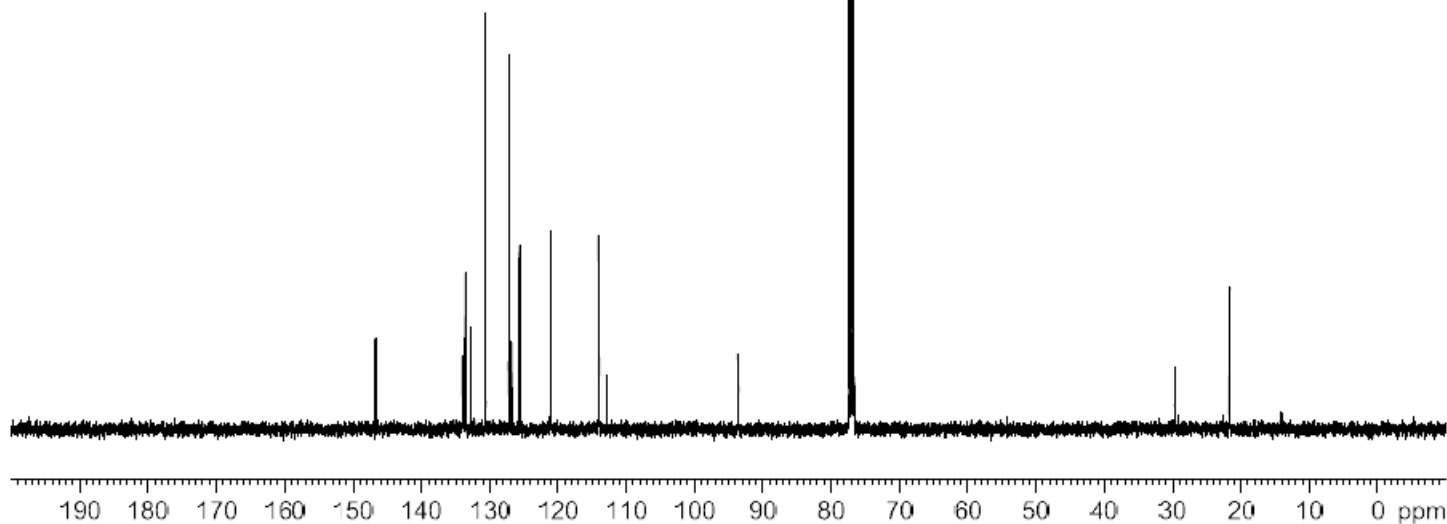
Current Data Parameters
NAME SD-079(old)
EXPNO 5
PROCNO 1

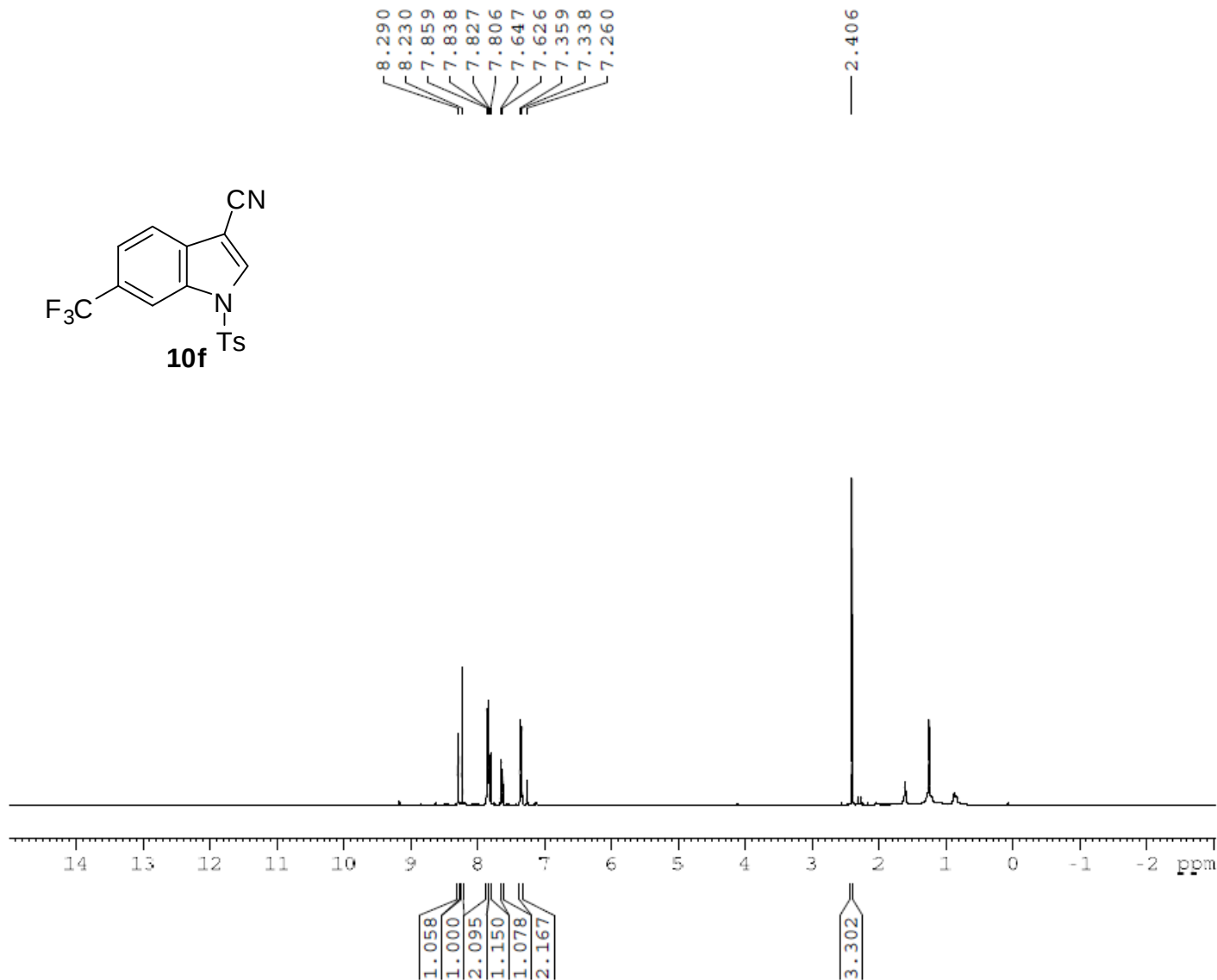
F2 - Acquisition Parameters
Date 20140528
Time 12.05
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1331
CS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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





```

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

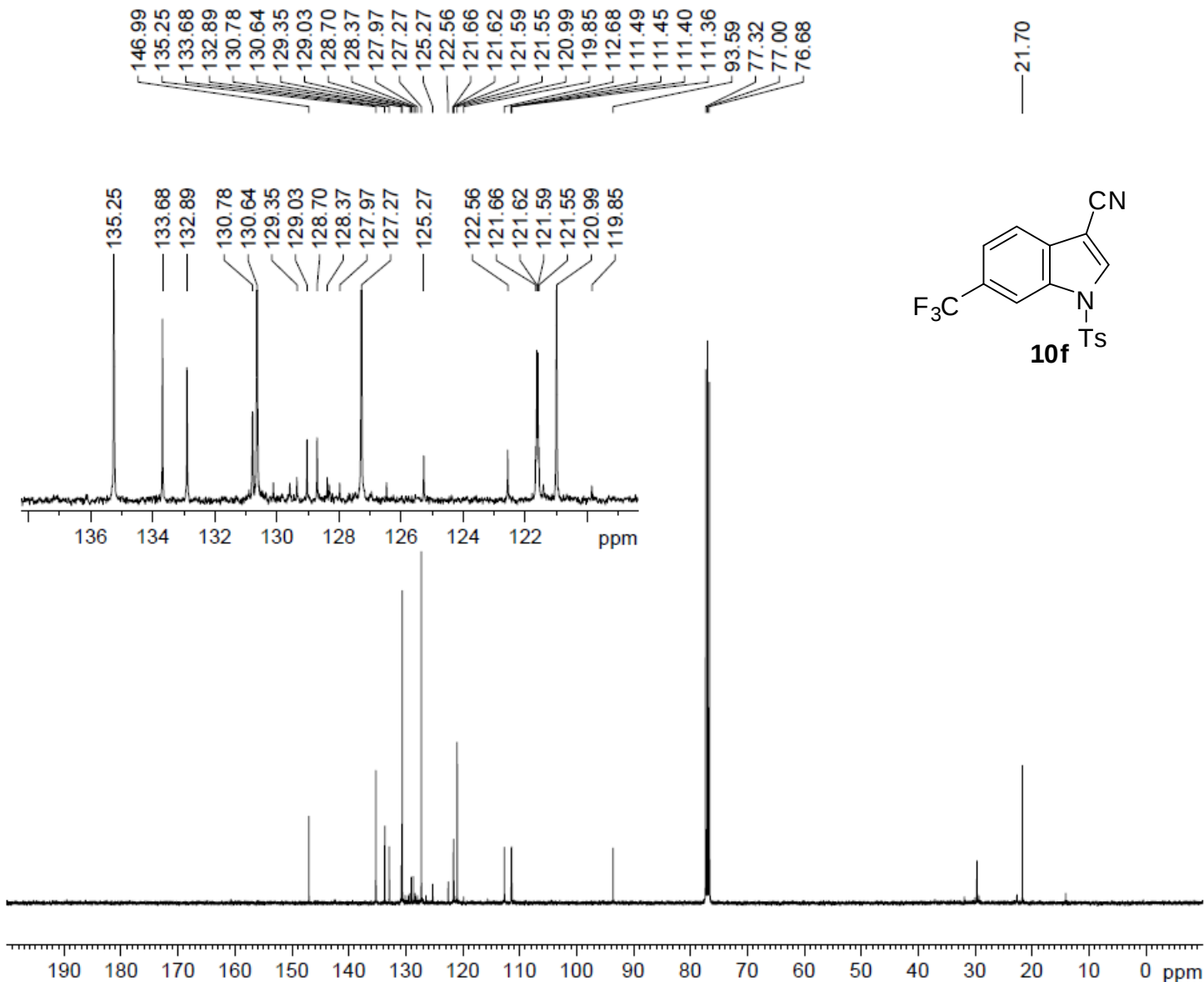
```

```

===== 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



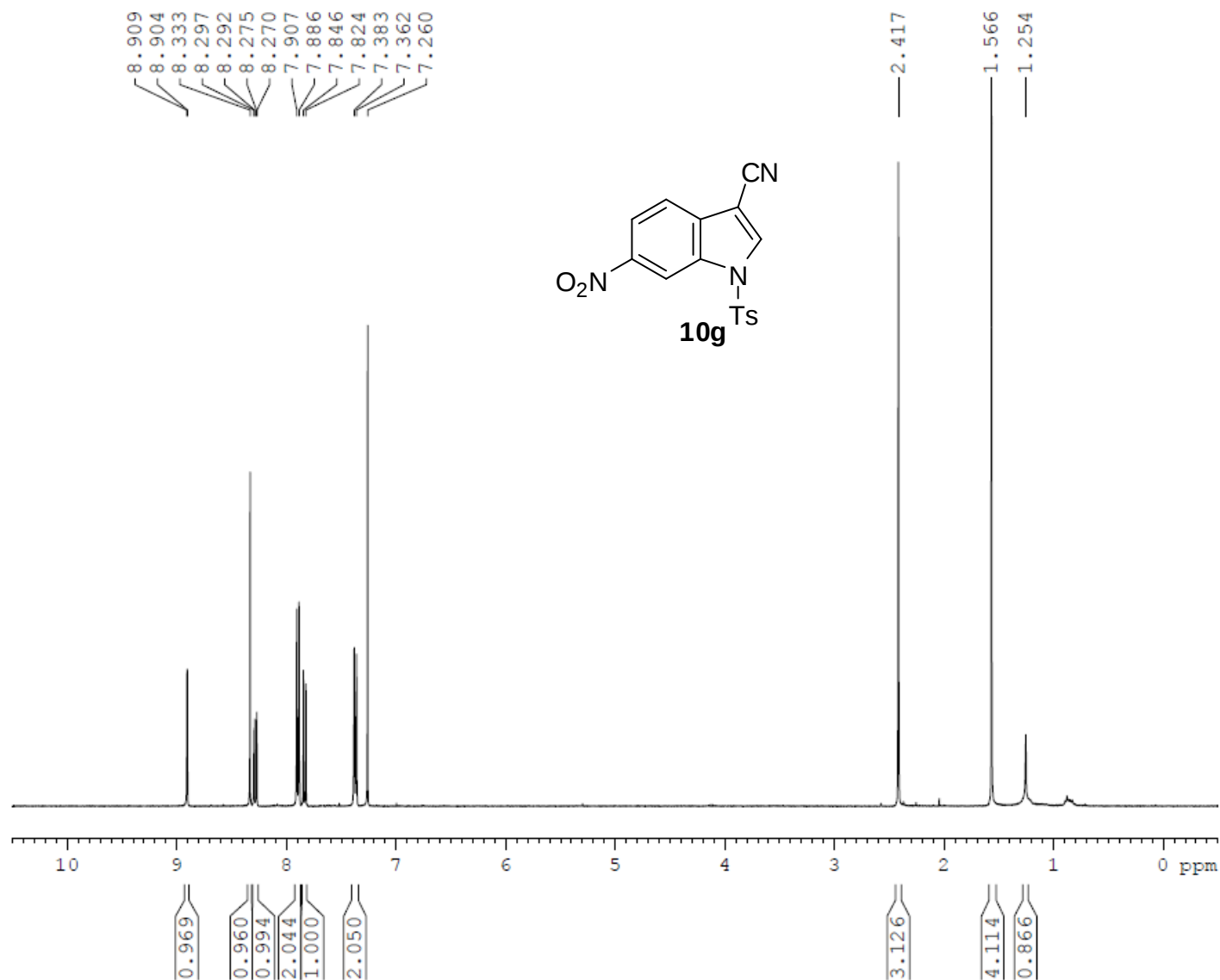
Current Data Parameters
 NAME SD-080-2(old)
 EXPNO 3
 PROCNO 1

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 100.623325 MHz

===== CHANNEL f2 =====
 CPDPRG2 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

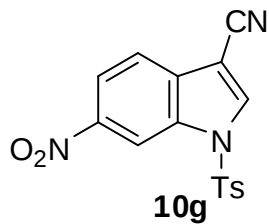


Current Data Parameters
 NAME SC184
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20140918
 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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130093 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



147.60
 146.68
 137.37
 133.68
 133.05
 132.86
 131.05
 127.71
 121.11
 120.16
 112.46
 110.55
 — 93.90
 77.55
 77.23
 76.92
 — 21.99

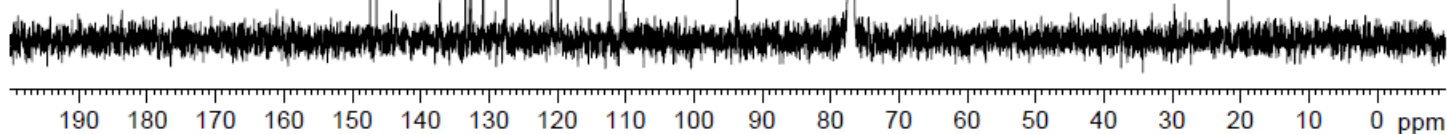
Current Data Parameters
 NAME SC184
 EXPNO 2
 PROCNO 1

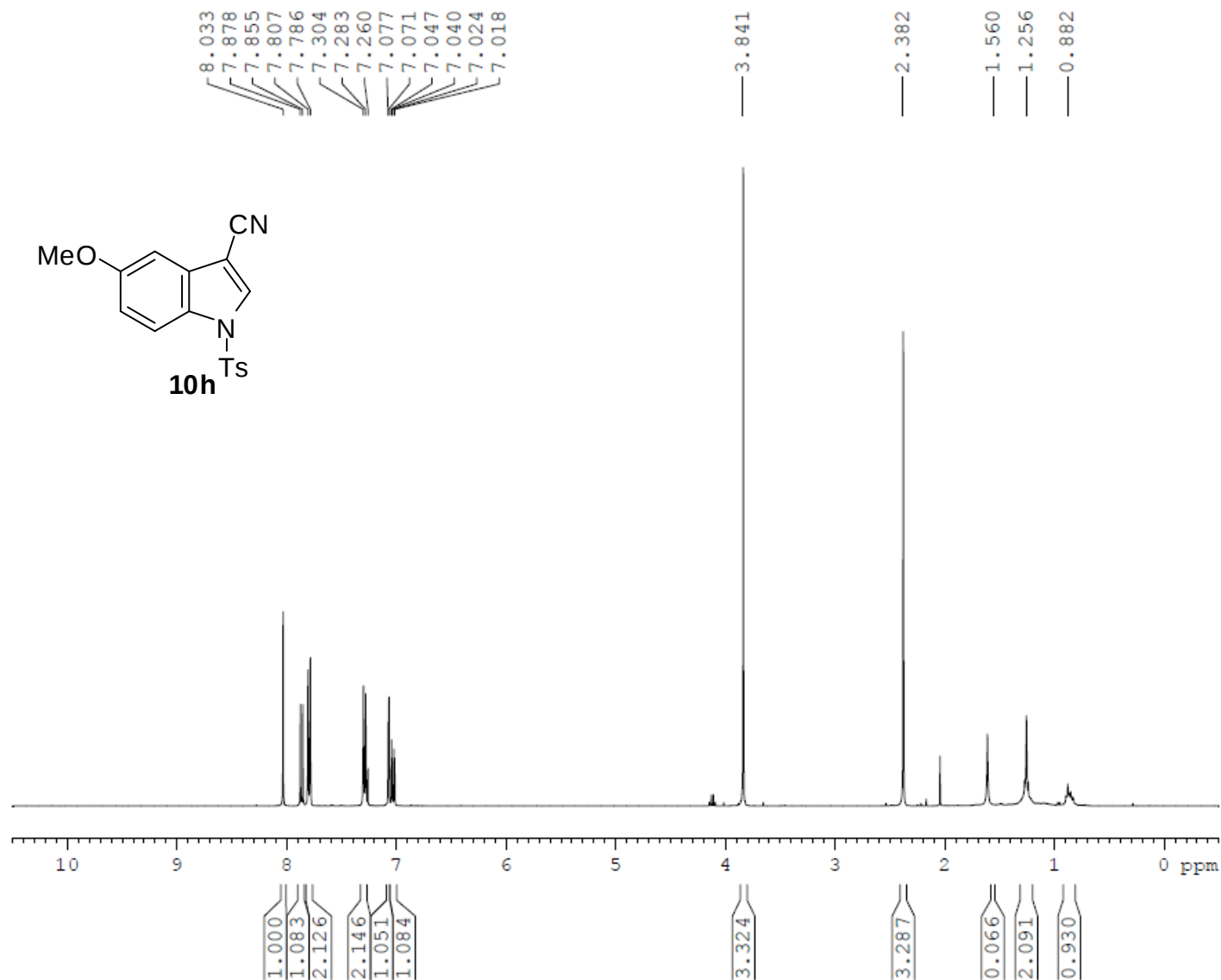
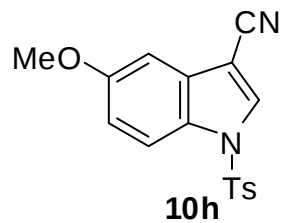
F2 - Acquisition Parameters
 Date_ 20140916
 Time 9.29
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDCl3
 NS 1645
 DS 0
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6815744 sec
 RG 198.09
 DW 20.800 usec
 DE 6.50 usec
 TE 300.5 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0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



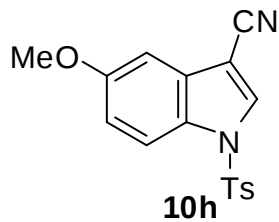


Current Data Parameters
 NAME SC115a
 EXPNO 1
 PROCNO 1

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
 TDO 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



—157.76
 —146.46
 —134.42
 —133.54
 —130.55
 —129.73
 —128.44
 —127.34
 —116.75
 —114.98
 —113.84
 —101.87
 —93.72
 —77.55
 —77.23
 —76.91
 —55.98
 —21.86

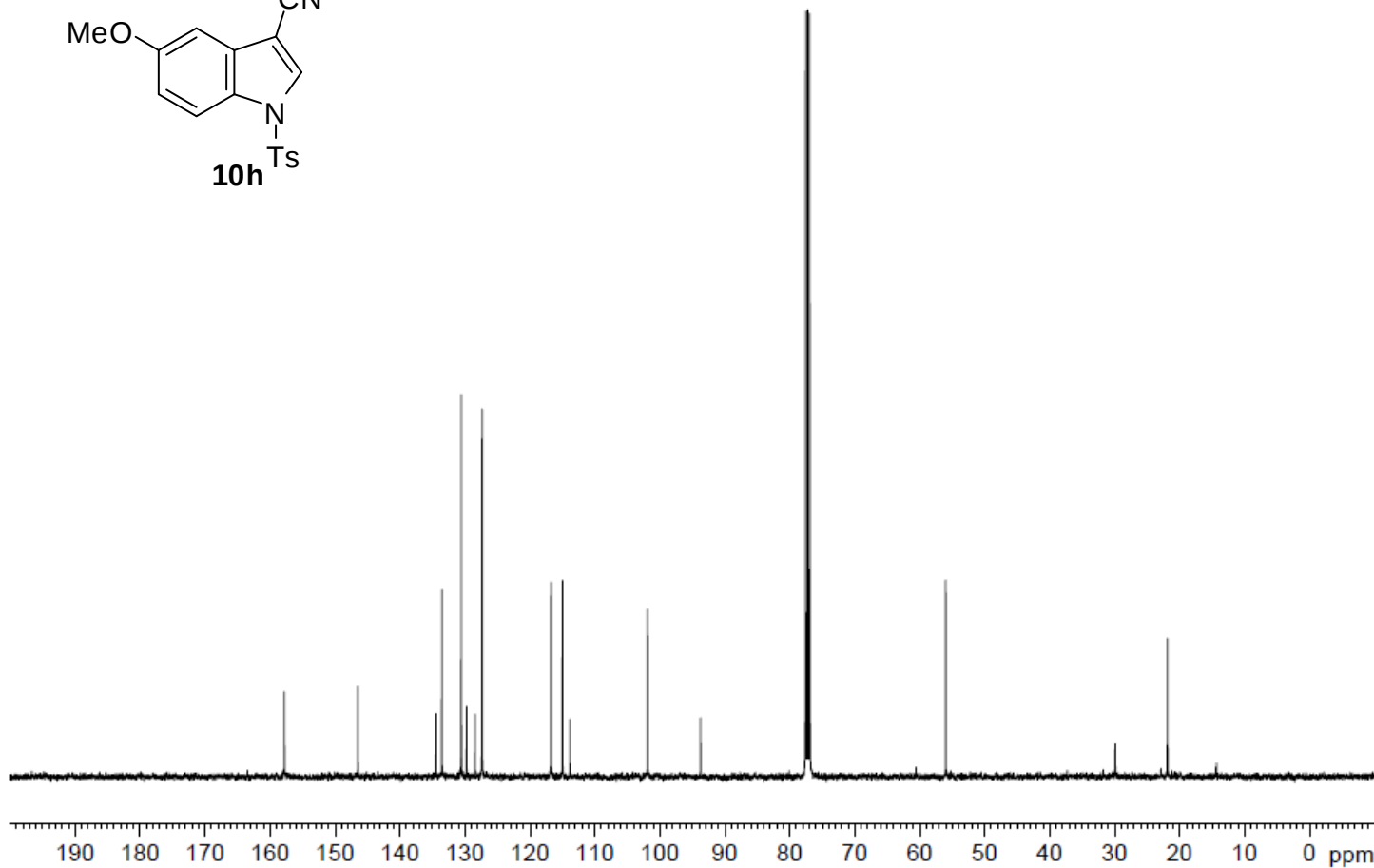
Current Data Parameters
 NAME SC115a
 EXPNO 3
 PROCNO 1

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

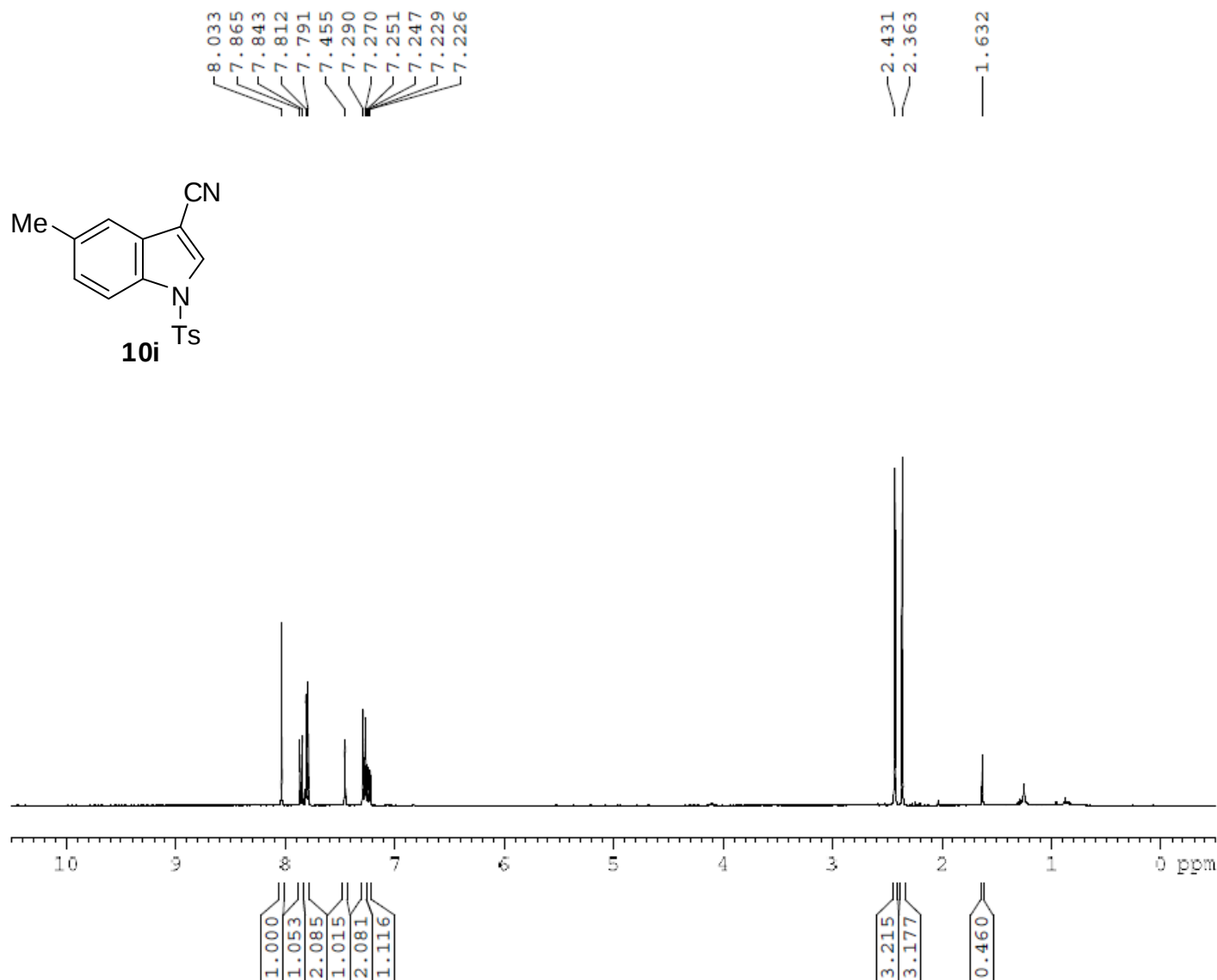
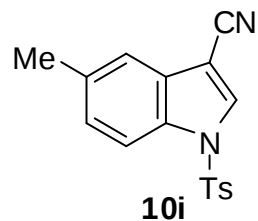
===== CHANNEL f1 =====
 SFO1 100.623319 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 46.00000000 W

===== 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



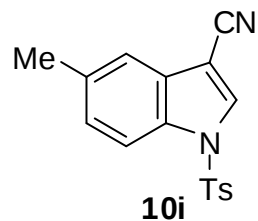
Current Data Parameters
NAME SD-063(old)
EXPNO 5
PROCNO 1

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 2.0000000 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

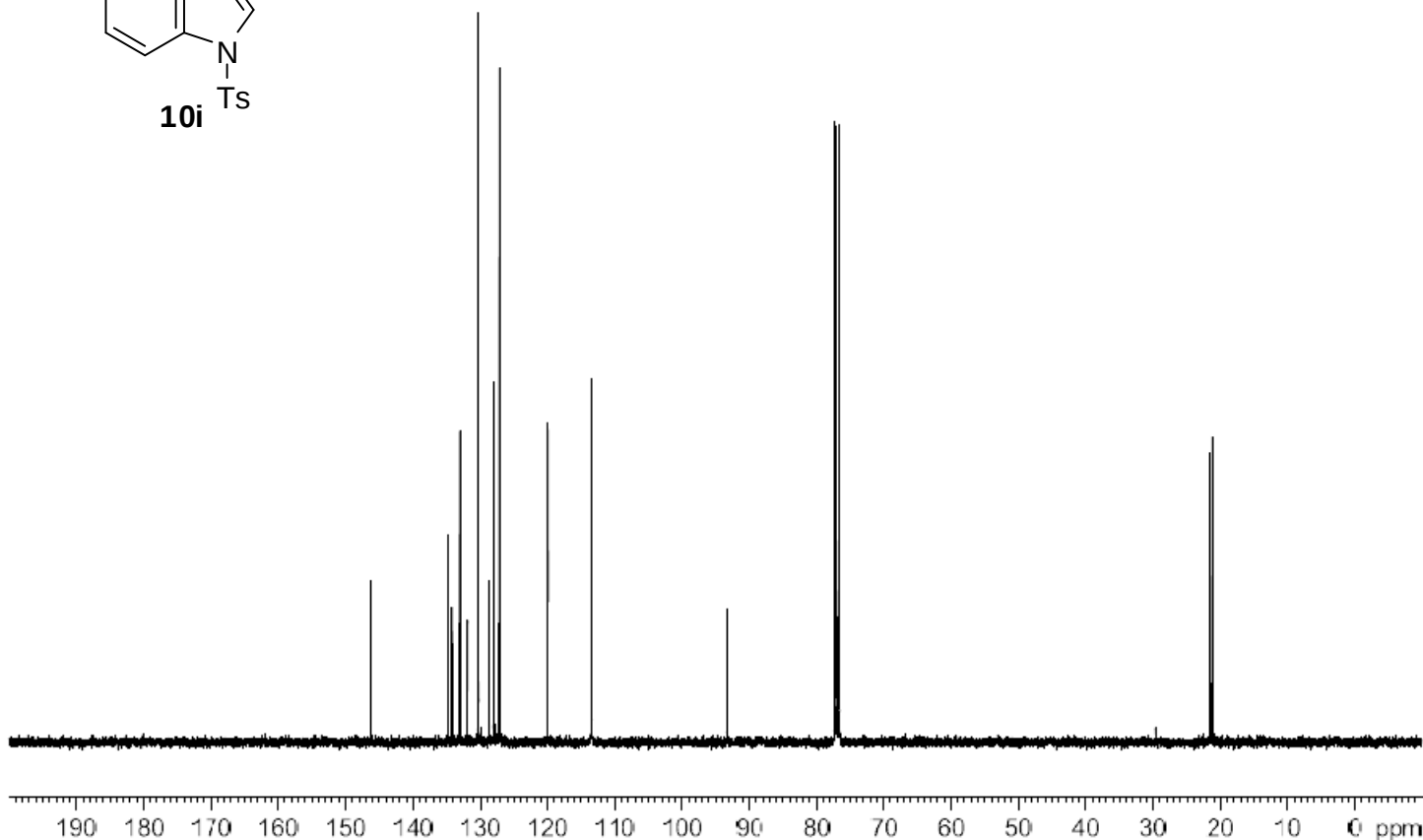


146.17
134.78
134.12
133.01
131.85
130.26
128.53
127.94
127.10
119.91
113.54
113.36

93.28

77.32
77.00
76.68

21.58
21.19



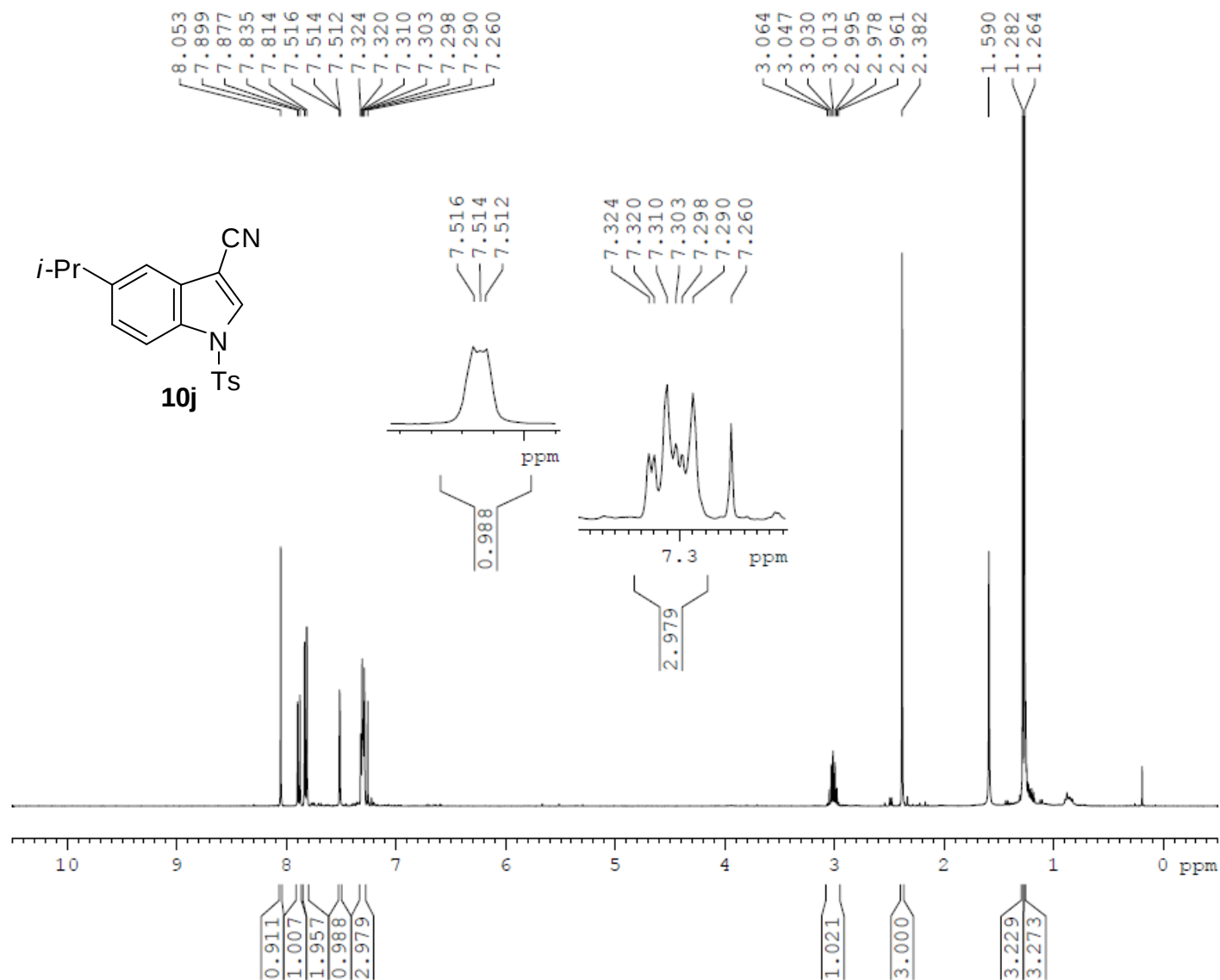
Current Data Parameters
NAME SD-063(old)
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date 20140425
Time 19.35
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 968
CS 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 =====
CPDPRG2 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



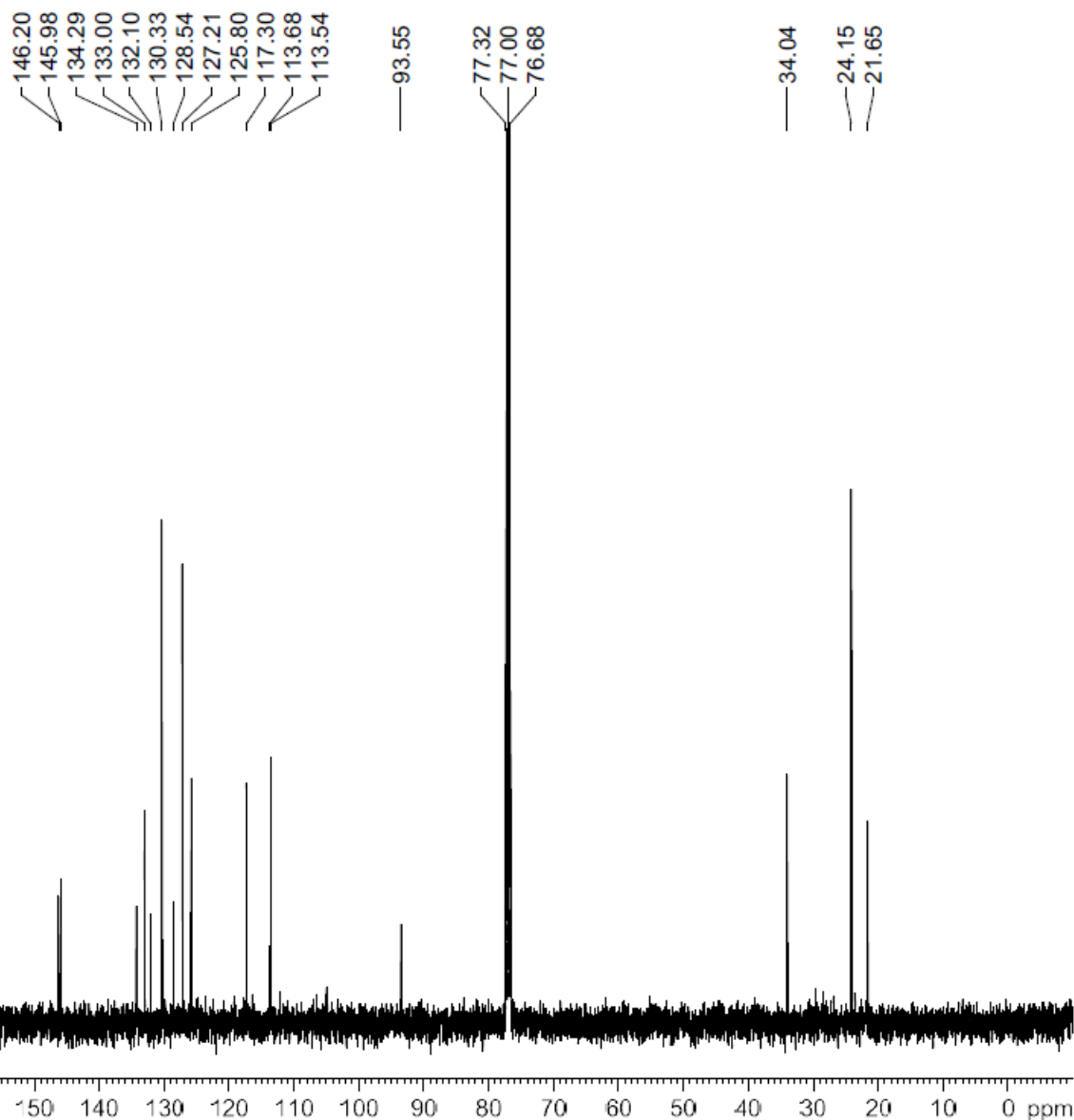
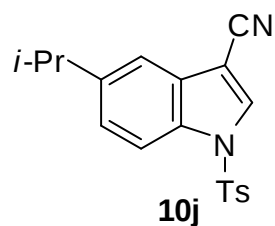
Current Data Parameters
 NAME SD-093
 EXPNO 1
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.1300991 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

pure



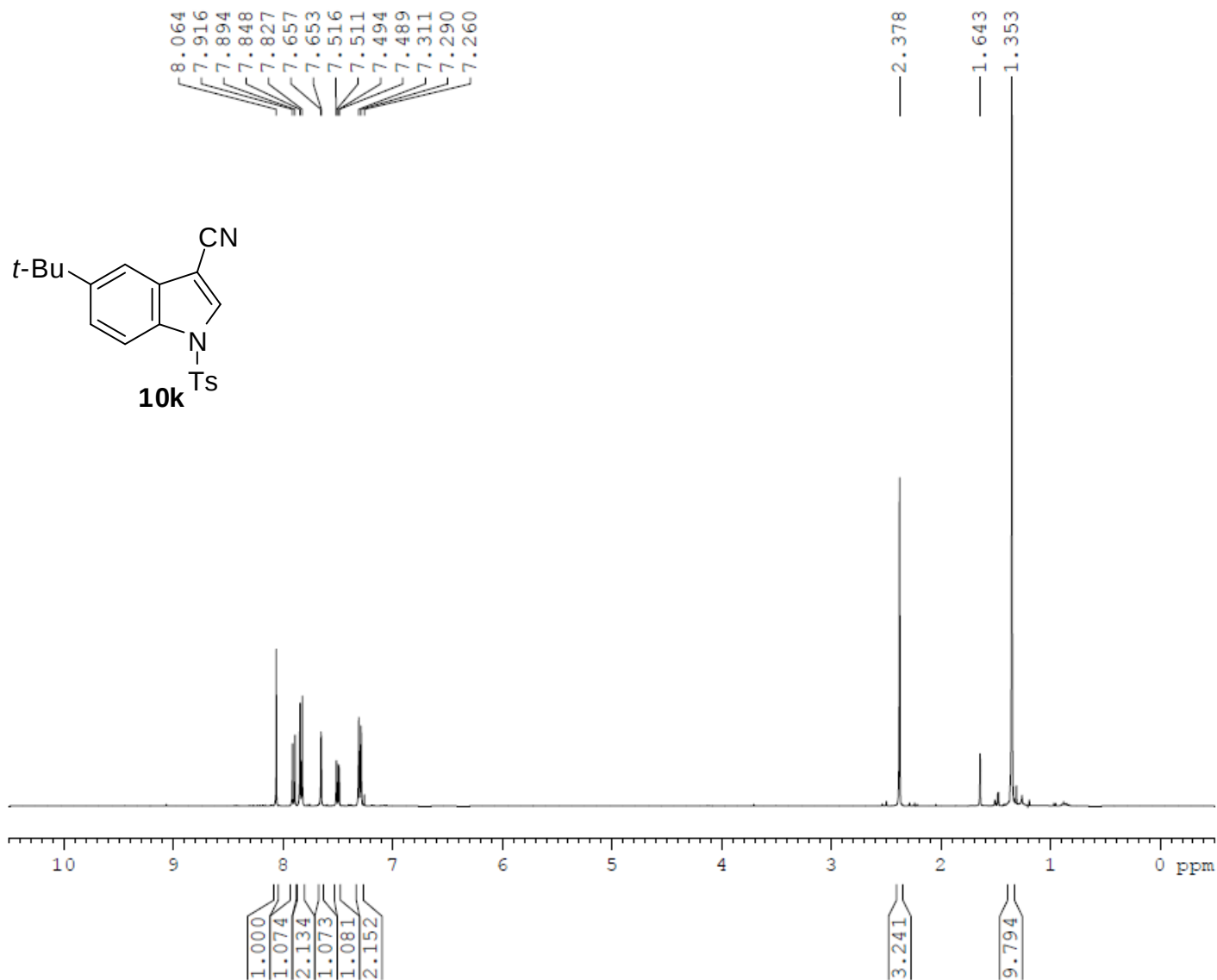
Current Data Parameters
NAME SD-093(OLD)
EXPNO 4
PROCNO 1

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 =====
CPDPRG2 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

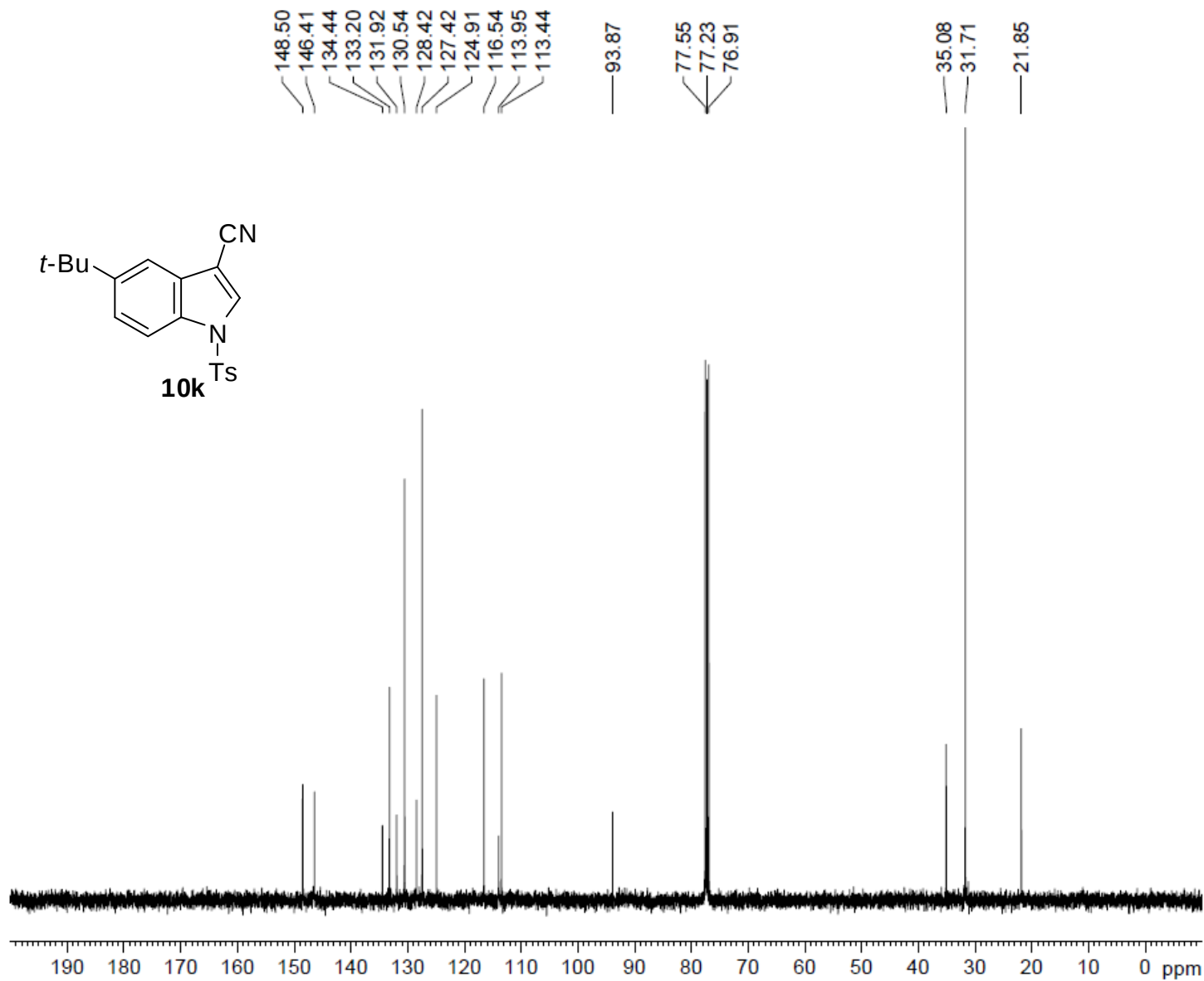


Current Data Parameters
 NAME SC159-1
 EXPNO 1
 PROCNO 1

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
 TDO 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



```

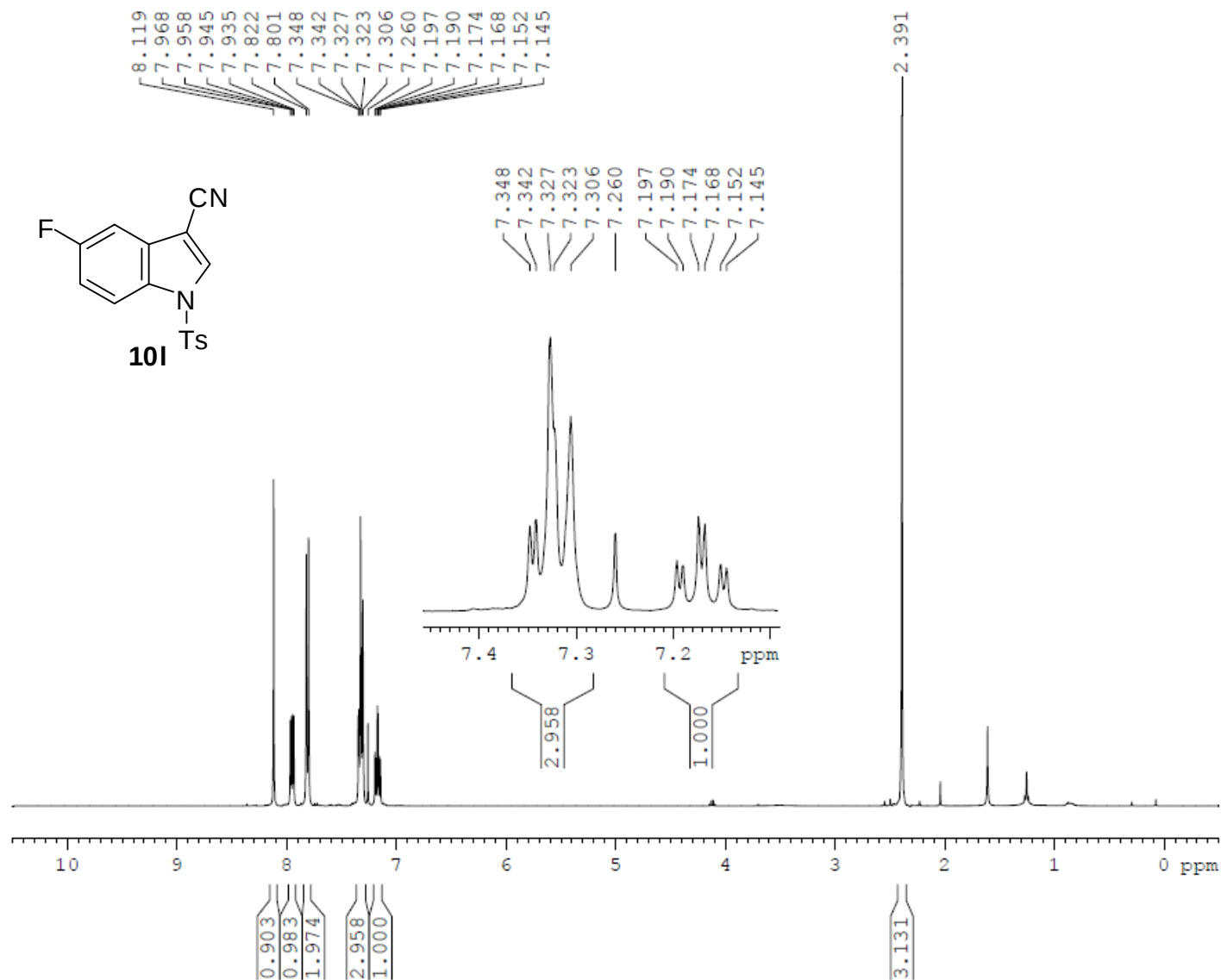
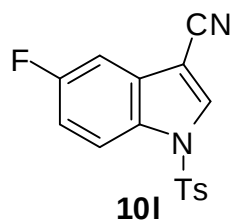
F2 - Acquisition Parameters
Date_      20140711
Time       9.43
INSTRUM    spect
PROBHD     5 mm BBO BB-H
PULPROG    zgpg30
TD          32768
SOLVENT     CDCl3
NS          68
DS          0
SWH         24038.461 Hz
FIDRES      0.733596 Hz
AQ          0.6815744 sec
RG          2048
DW          20.800 usec
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

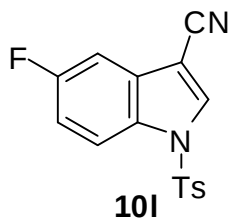


Current Data Parameters
 NAME SC172
 EXPNO 2
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.1300998 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



161.70
159.27
146.82
134.69
134.18
130.68
130.28
129.73
129.63
127.41
115.43
115.34
115.08
113.14
106.41
106.16
93.84
93.80
77.55
77.23
76.91

21.87

Current Data Parameters
NAME SC172
EXPNO 4
PROCNO 1

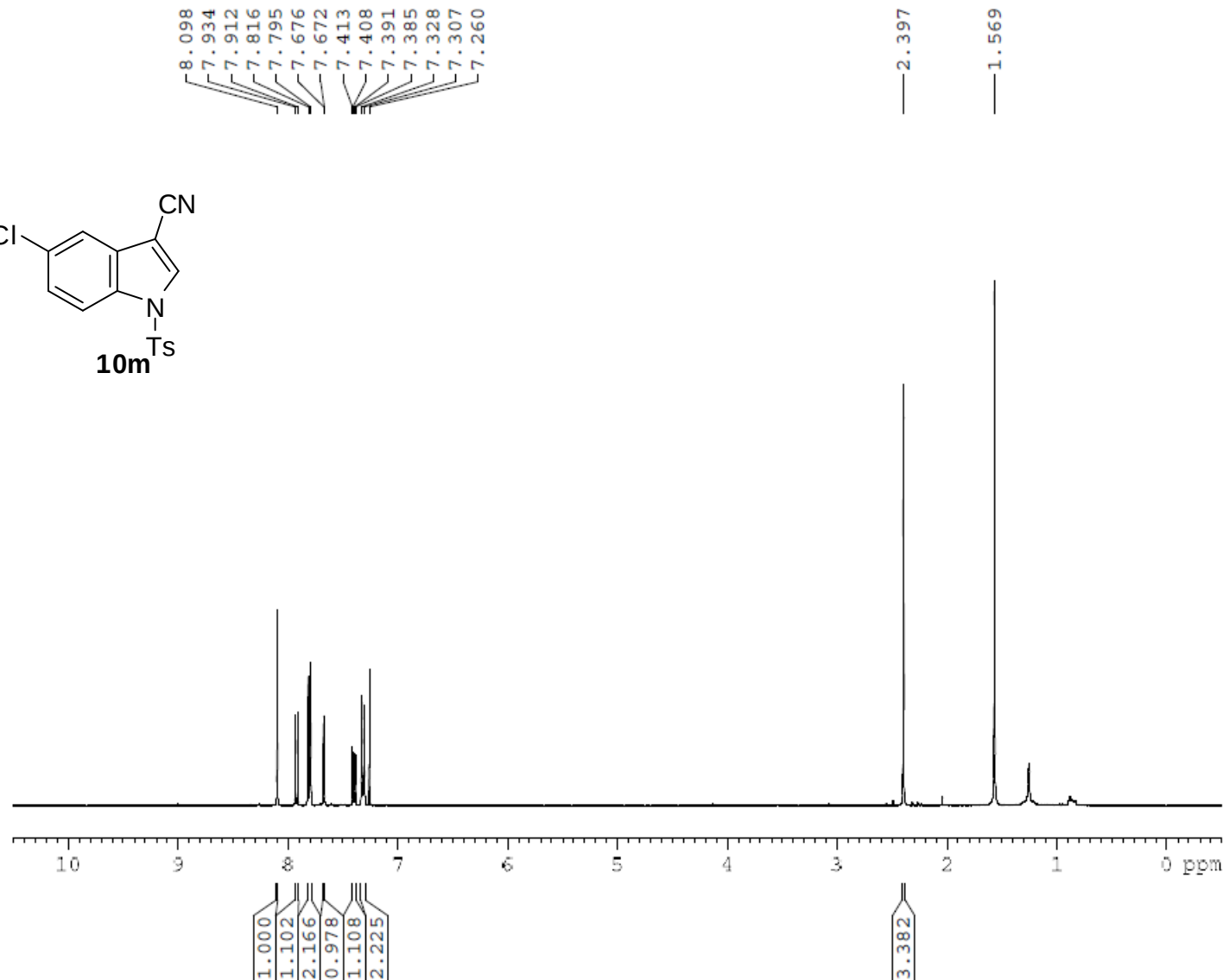
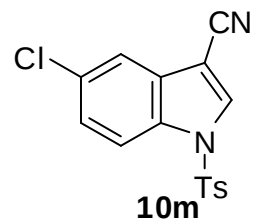
F2 - Acquisition Parameters
Date_ 20140818
Time 10.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 382
DS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 2896.3
DW 20.800 usec
DE 6.50 usec
TE 302.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

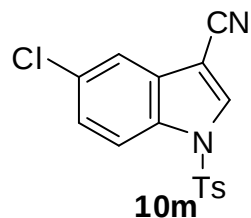


Current Data Parameters
 NAME SD-089(old)
 EXPNO 1
 PROCNO 1

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 2.0000000 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



146.70
134.16
133.89
132.05
131.09
130.50
129.50
127.21
127.03
119.98
114.91
112.81

93.19

77.32
77.00
76.68

21.69

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

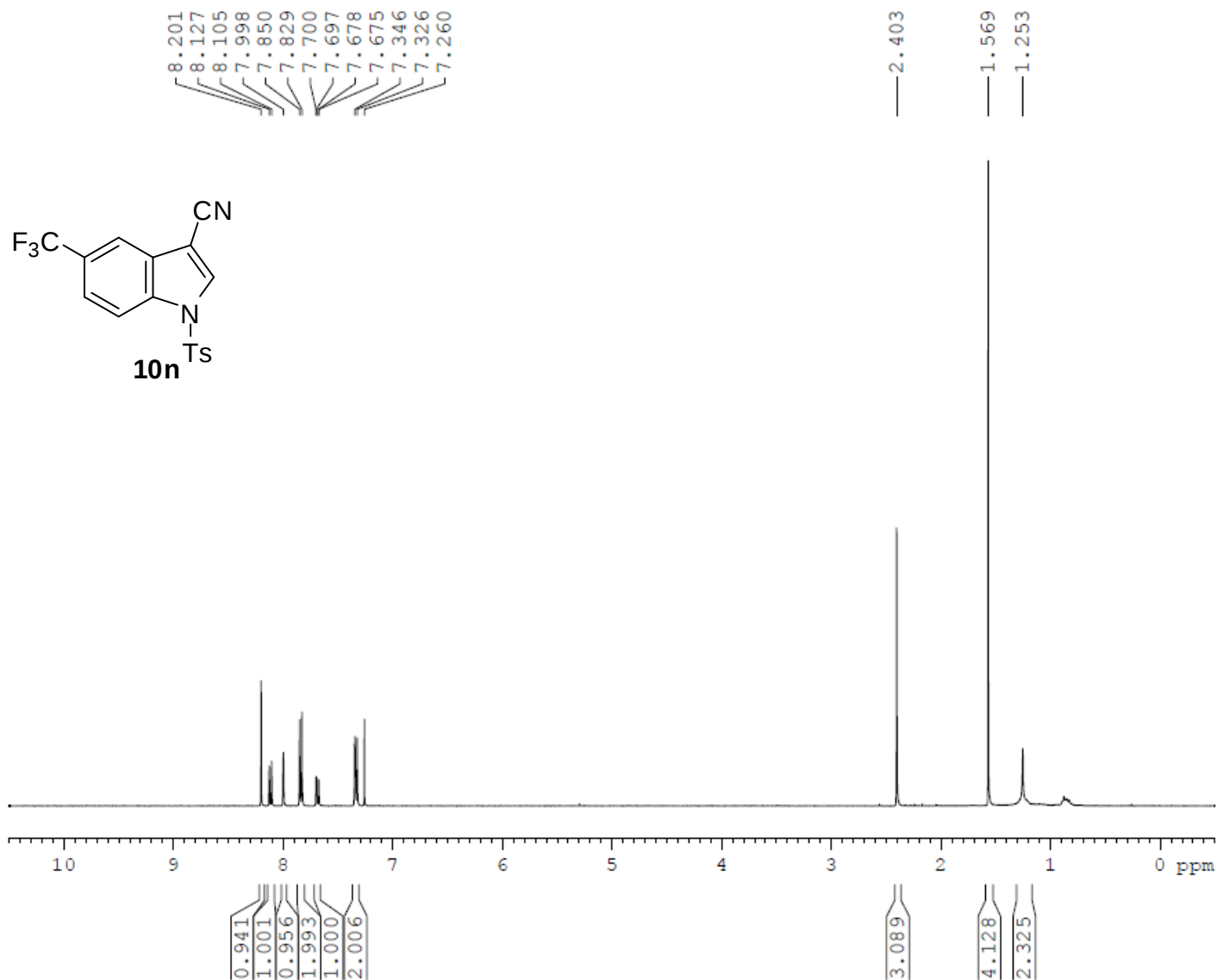
F2 - Acquisition Parameters
Date_ 20140701
Time_ 1.44
INSTRUM spect
PROBHD 5 mm SEI 1H-13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4210
CS 0
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 0.6815744 sec
RG 8192
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

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

===== CHANNEL f2 =====
CPDPRG2 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

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

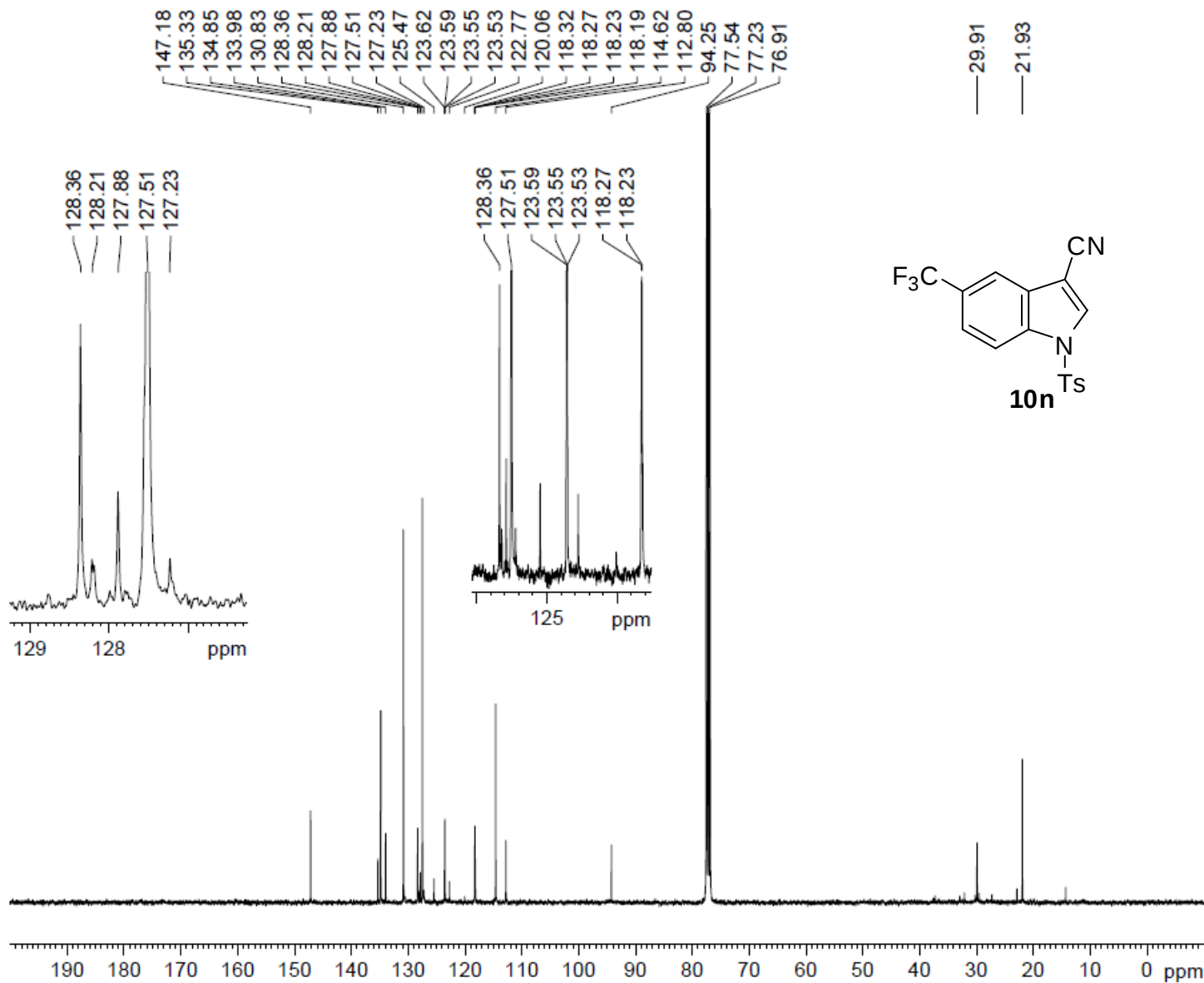


Current Data Parameters
 NAME SC180
 EXPNO 2
 PROCNO 1

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
 TDO 1

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

F2 - Processing parameters
 SI 16384
 SF 400.130097 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00



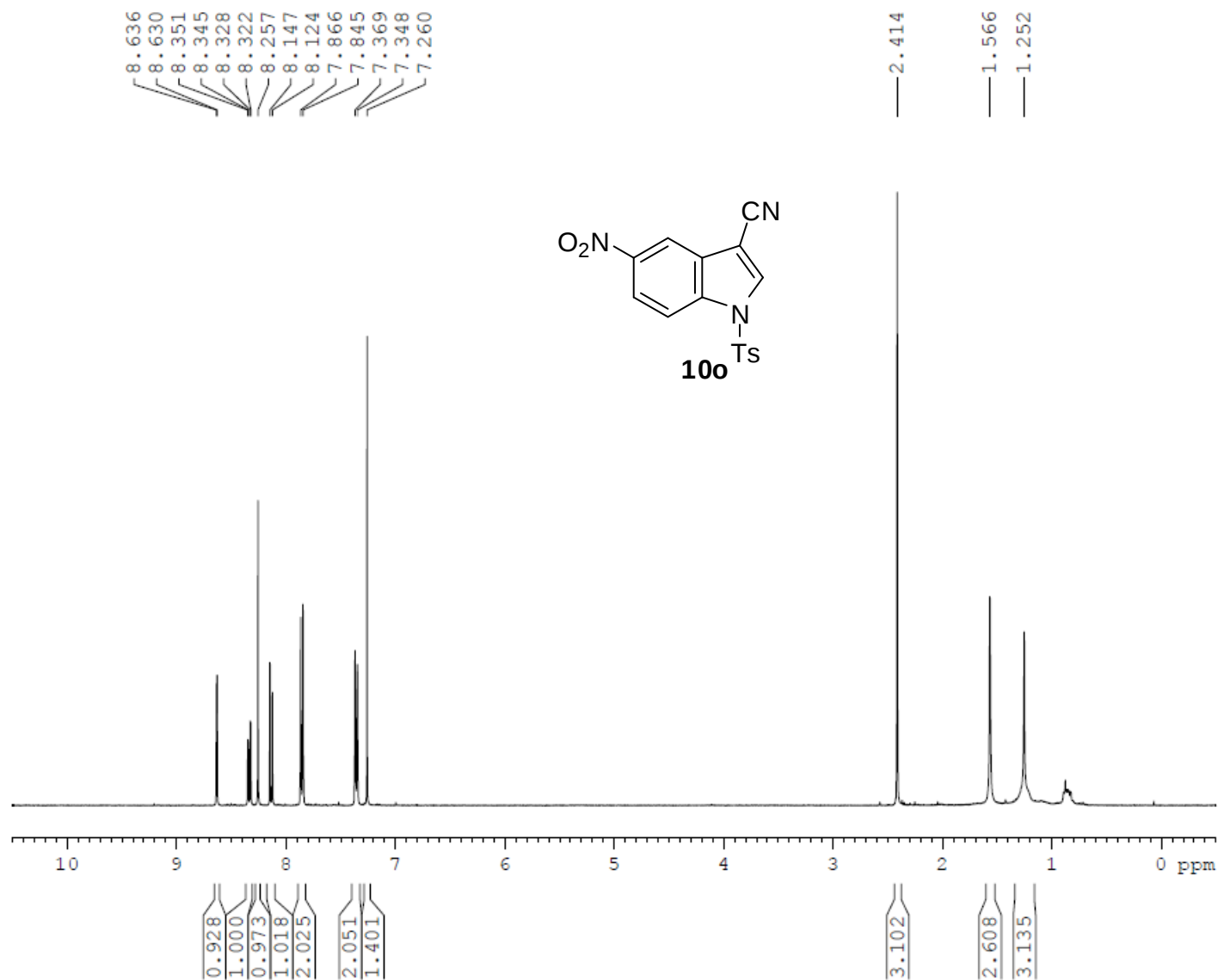
Current Data Parameters
 NAME SC180
 EXPNO 4
 PROCNO 1

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
 CPDPRG2 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

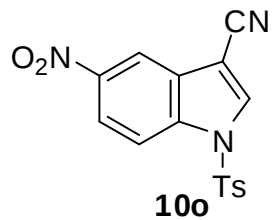


Current Data Parameters
 NAME SC198
 EXPNO 1
 PROCNO 1

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
 TDO 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



147.58
145.42
136.56
135.99
133.72
130.98
128.60
127.59
121.88
117.00
114.63
112.29

— 94.91

77.55
77.23
76.91

— 21.98

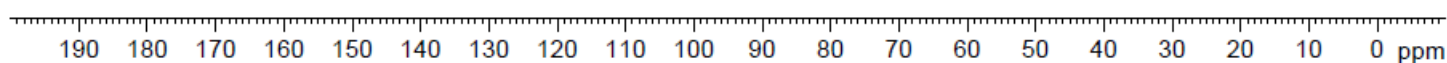
Current Data Parameters
NAME SC196
EXPNO 2
PROCNO 1

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

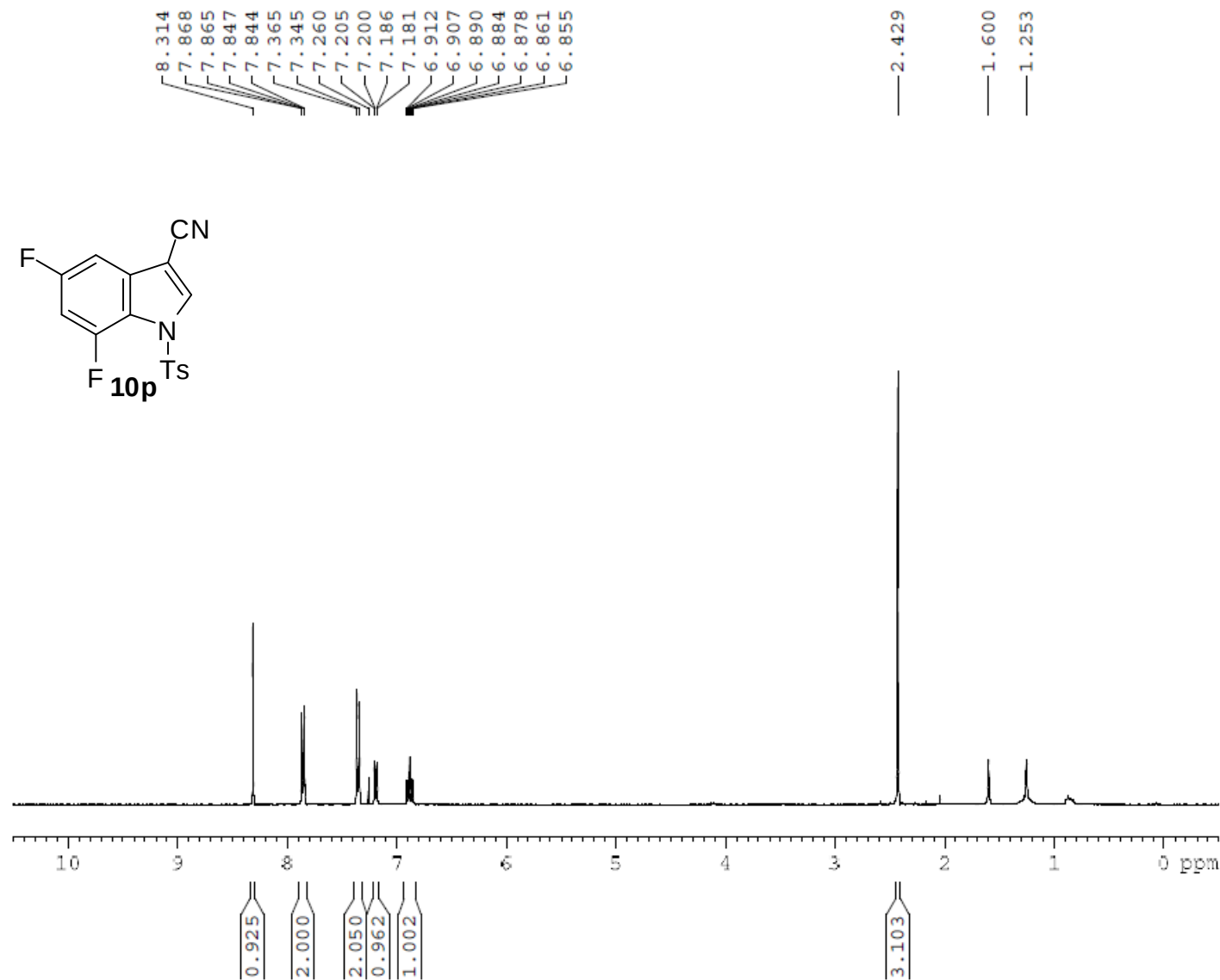
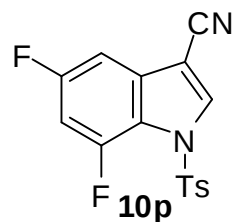
===== CHANNEL f1 =====
SFO1 100.6233319 MHz
NUC1 13C
P1 10.00 usec
PLW1 46.00000000 W

===== CHANNEL f2 =====
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 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



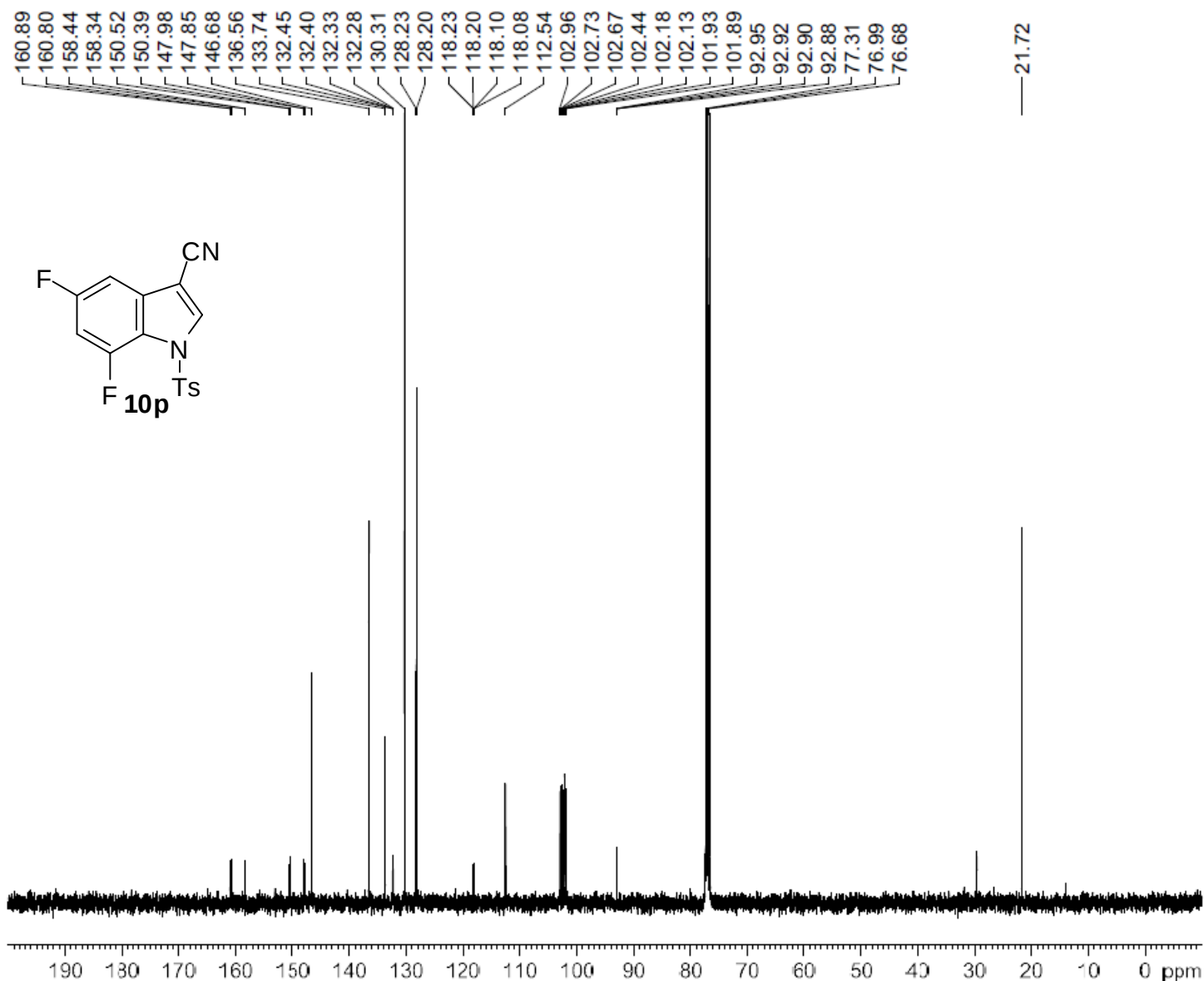
Current Data Parameters
NAME SD-075(old)
EXPNO 1
PROCNO 1

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 2.0000000 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



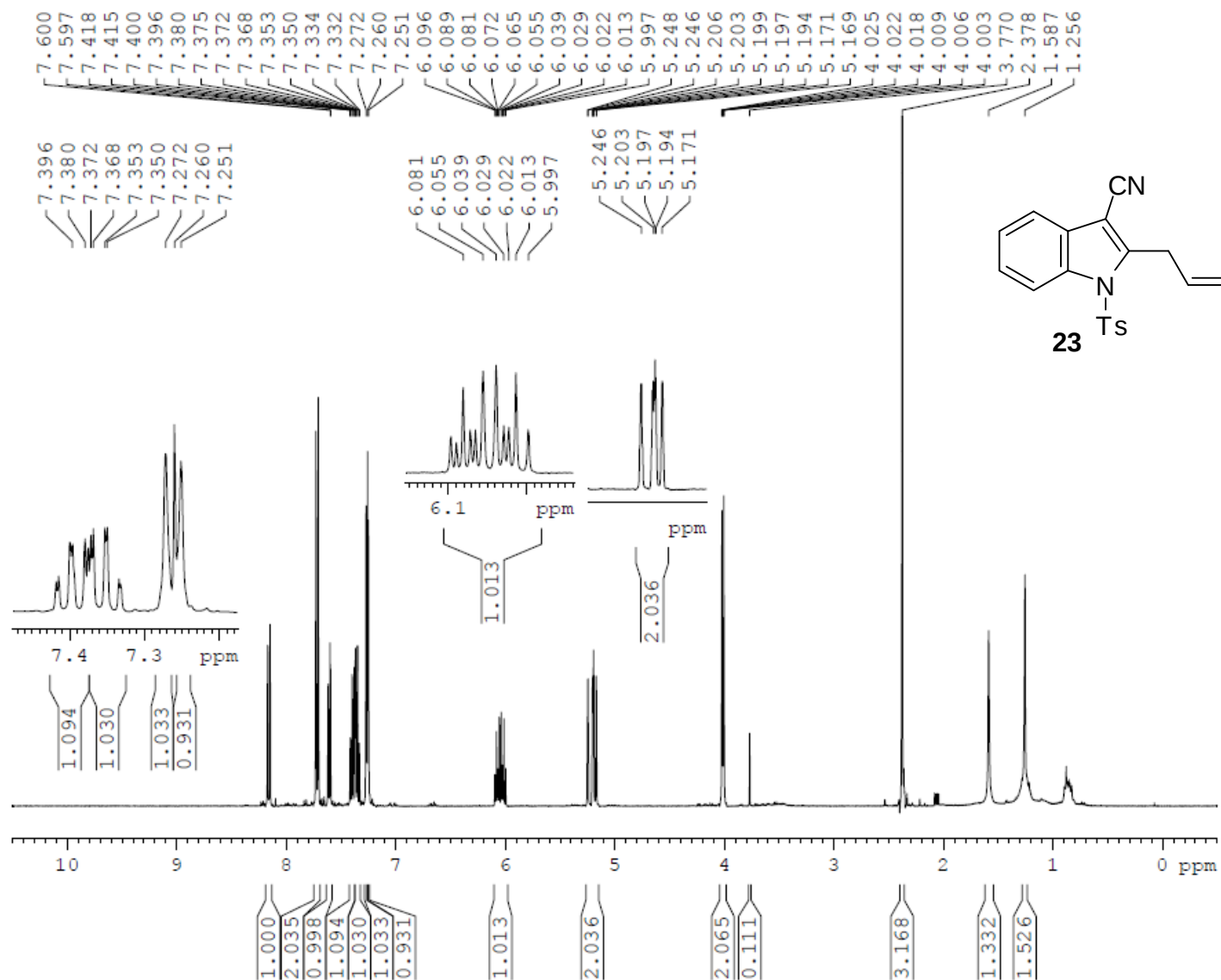
Current Data Parameters
NAME SD-075(old)
EXPNO 2
PROCNO 1

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 =====
CPDPRG2 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

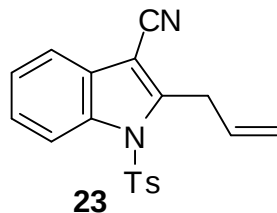


Current Data Parameters
NAME SO119a-1
EXPNO 1
PROCNO 1

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
TDO 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



148.28
146.28
135.73
135.43
133.05
130.42
127.40
126.96
126.23
125.07
119.56
118.79
115.25
114.06
95.23

77.55
77.23
76.91

32.39

21.85

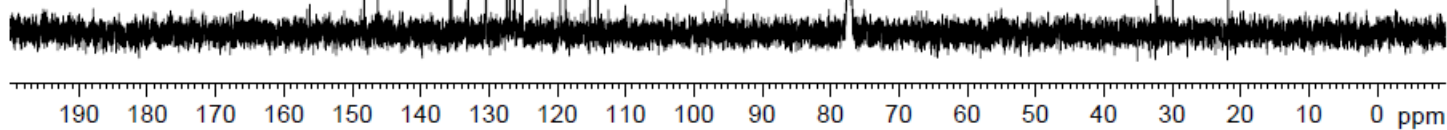
Current Data Parameters
NAME SO119a-1
EXPNO 3
PROCNO 1

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

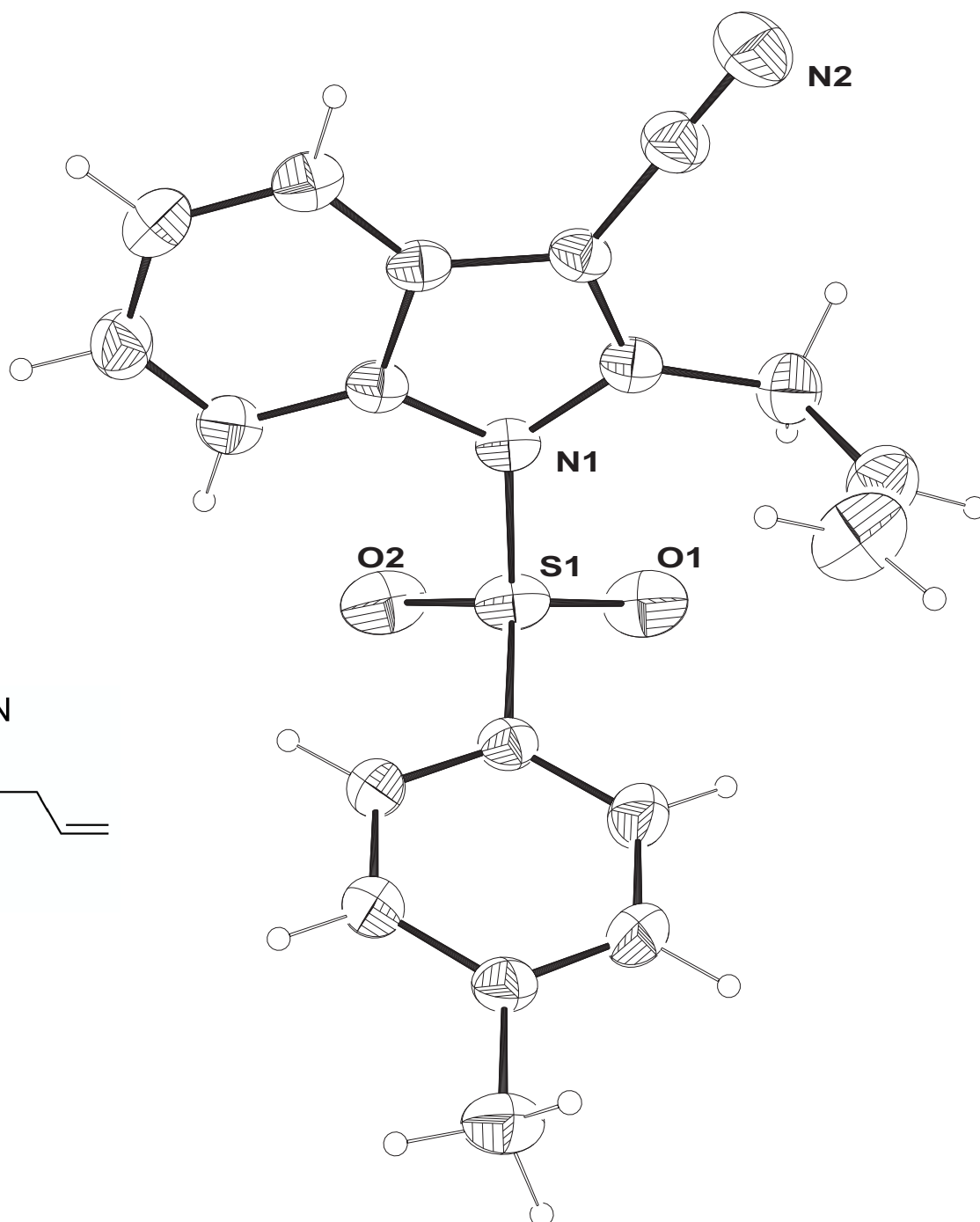
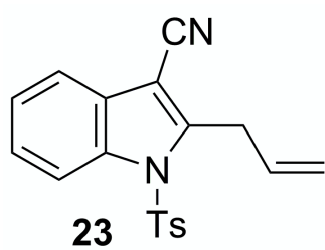
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 6.70 dB
SFO1 100.6233325 MHz

===== CHANNEL f2 =====
CPDPRG2 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



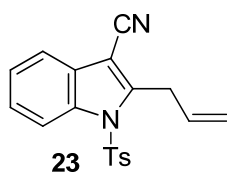


Table 1. Crystal data and structure refinement for a17991.

Identification code	a17991	
Empirical formula	C ₁₉ H ₁₆ N ₂ O ₂ S	
Formula weight	336.40	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /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 > 2σ(I)]	R ₁ = 0.0536, wR ₂ = 0.1392	
R indices (all data)	R ₁ = 0.0786, wR ₂ = 0.1575	
Largest diff. peak and hole	0.296 and -0.228 e.Å ⁻³	

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

	x	y	z	$U(\text{eq})$
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 ($\text{\AA}^2 \times 10^3$) for a17991. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
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 ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) 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