

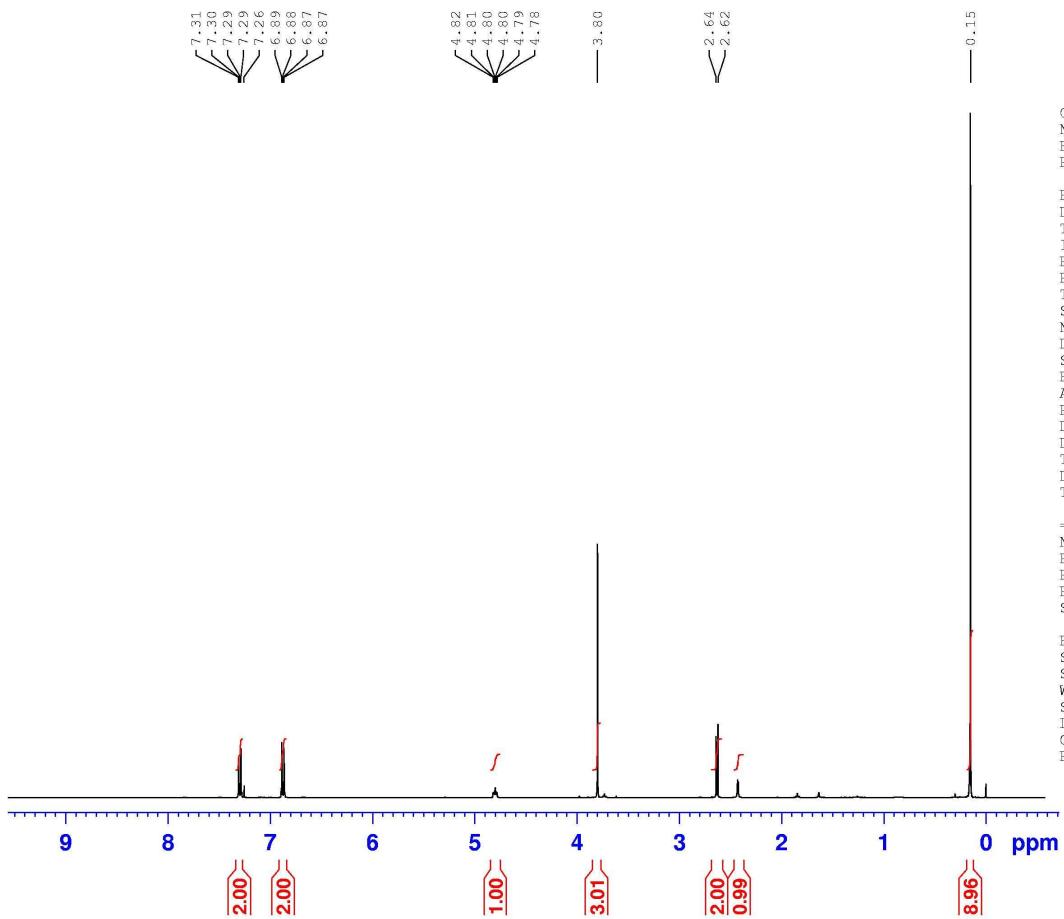
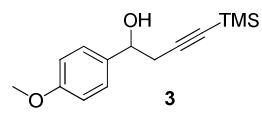
Supporting Information for

Zinc Catalyzed and Mediated Propargylations with Propargyl Boronates

Daniel R. Fandrick,* Keith R. Fandrick,* Jonathan T. Reeves, Zhulin Tan, Courtney S. Johnson, Heewon Lee, Jinhua J. Song, Nathan K. Yee, and Chris H. Senanayake

Department of Chemical Development, Boehringer Ingelheim Pharmaceuticals Inc., 900 Old Ridgebury Road/P.O. Box 368, Ridgefield, Connecticut 06877-0368

II. Spectra

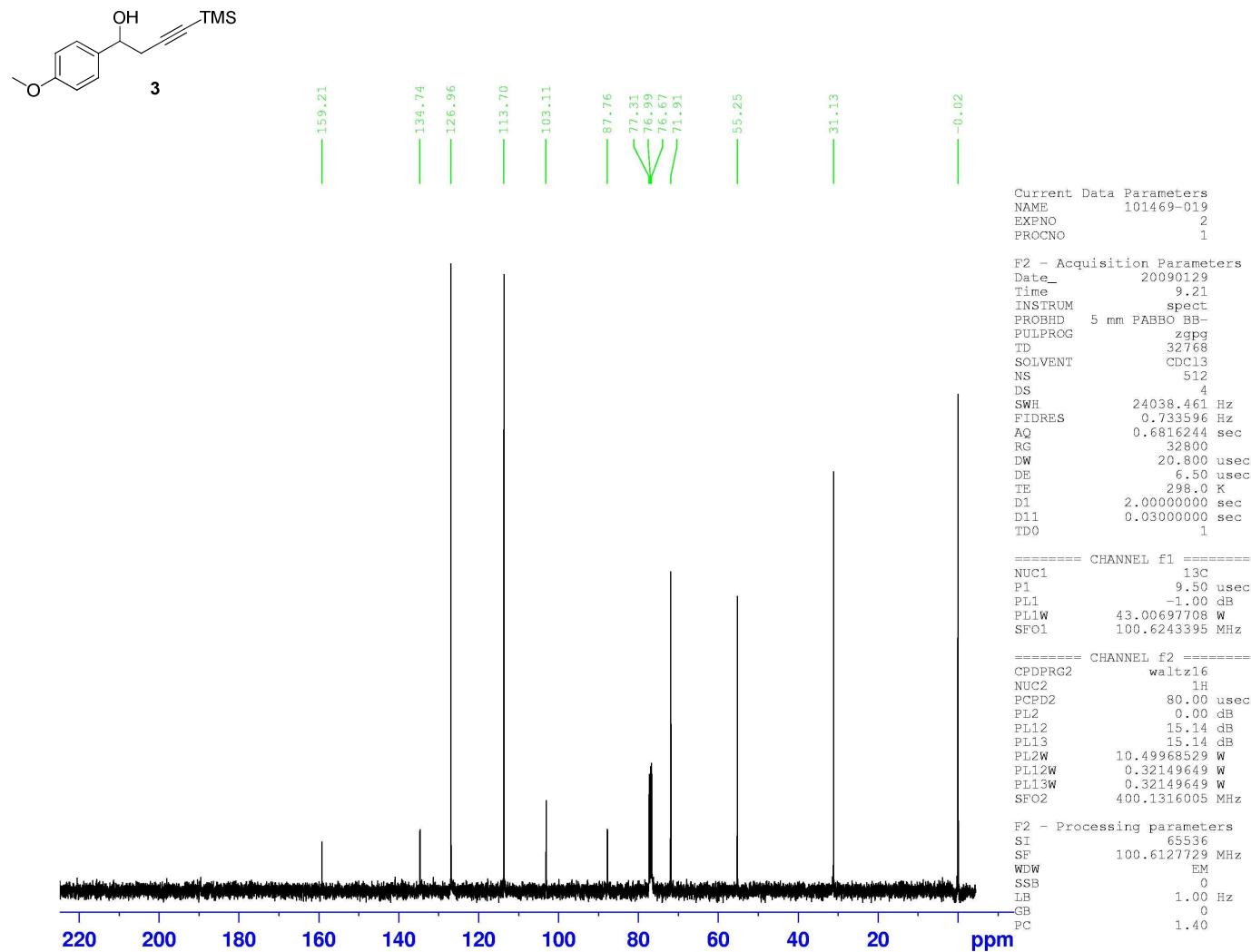


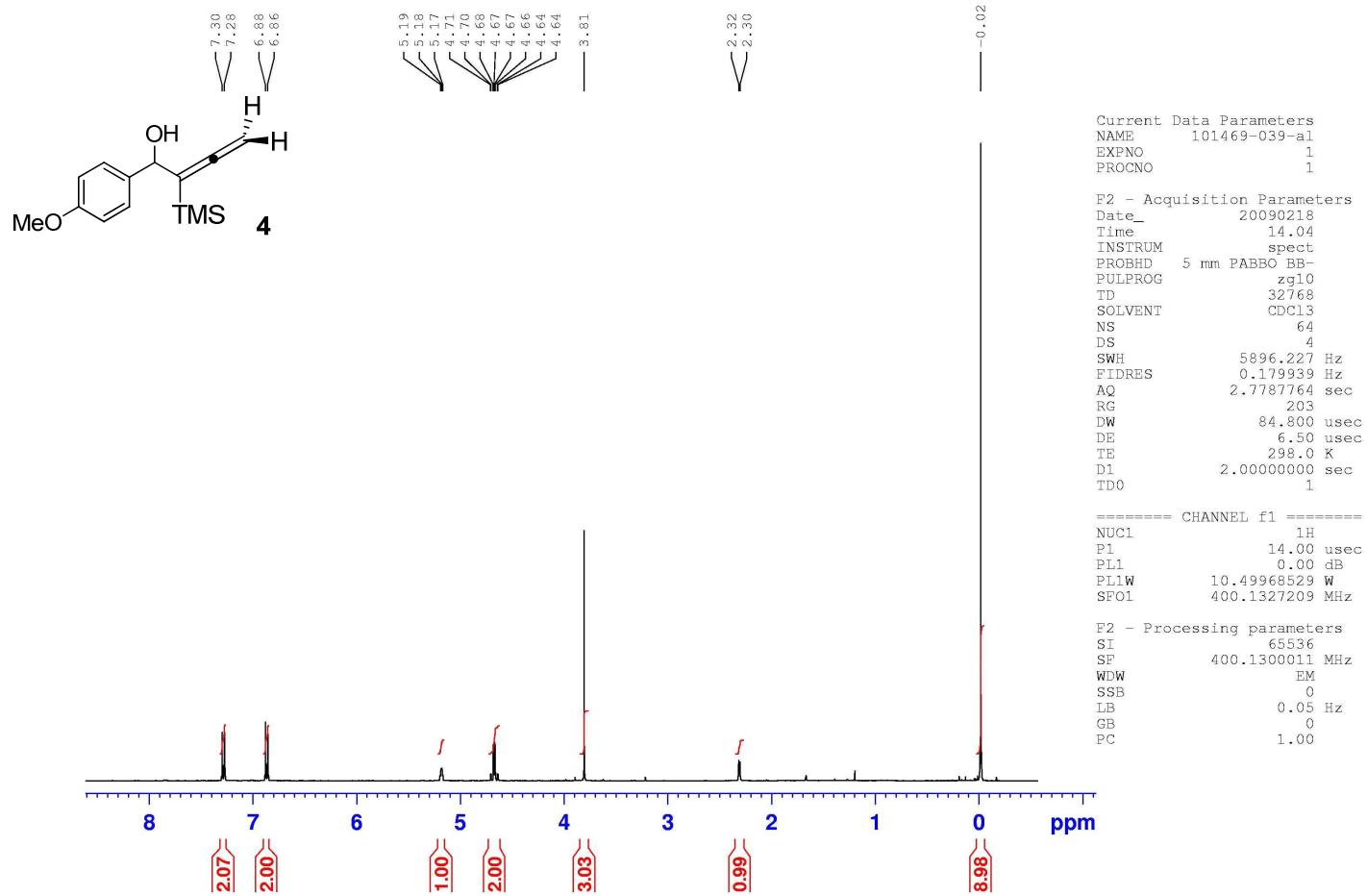
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 EXPNO 4
 PROCNO 1

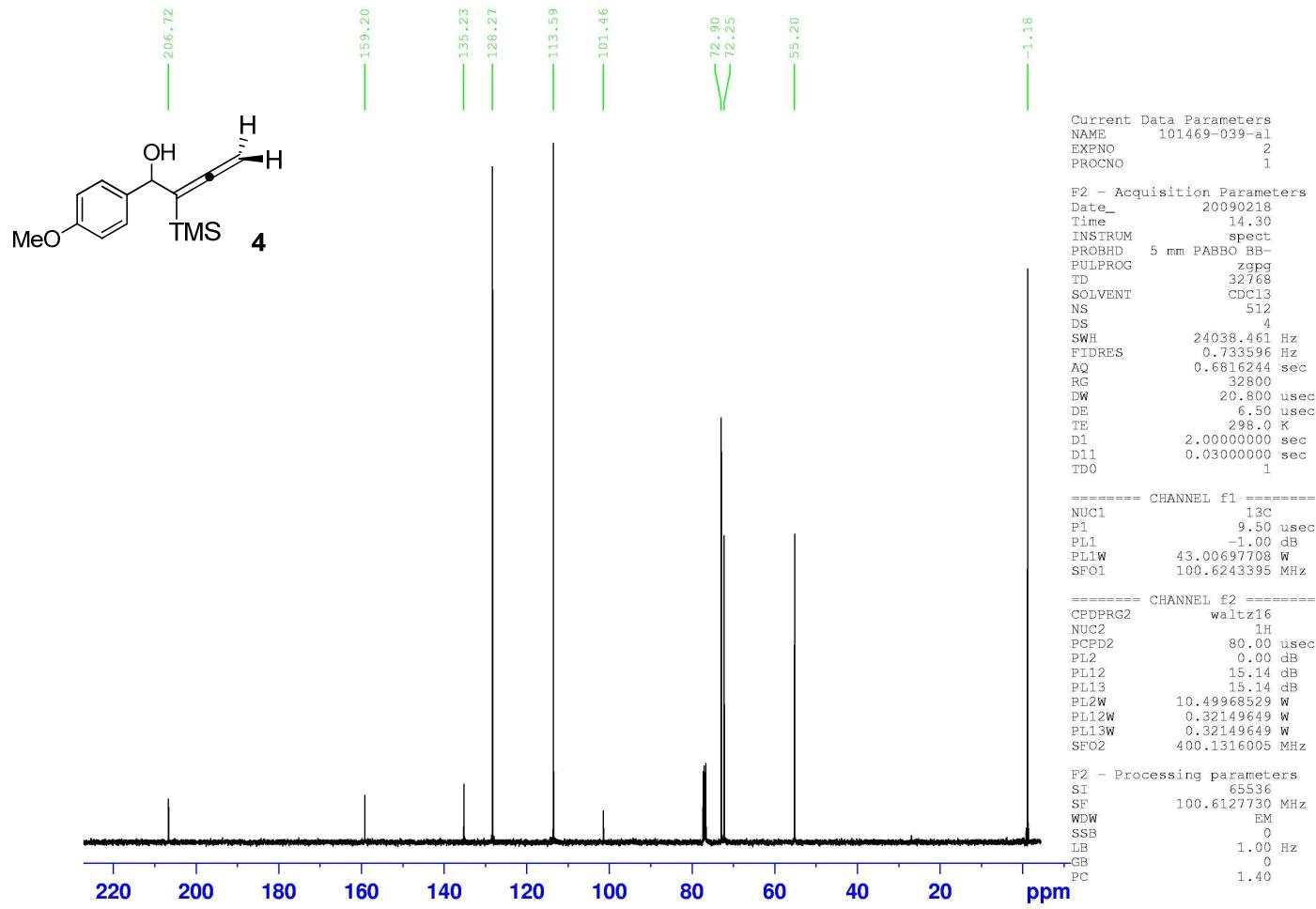
F2 - Acquisition Parameters
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 Time 11.17
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 PULPROG zg10
 TD 32768
 SOLVENT CDCl3
 NS 64
 DS 4
 SWH 5896.227 Hz
 FIDRES 0.179939 Hz
 AQ 2.7787764 sec
 RG 256
 DW 84.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.00000000 sec
 TDO 1

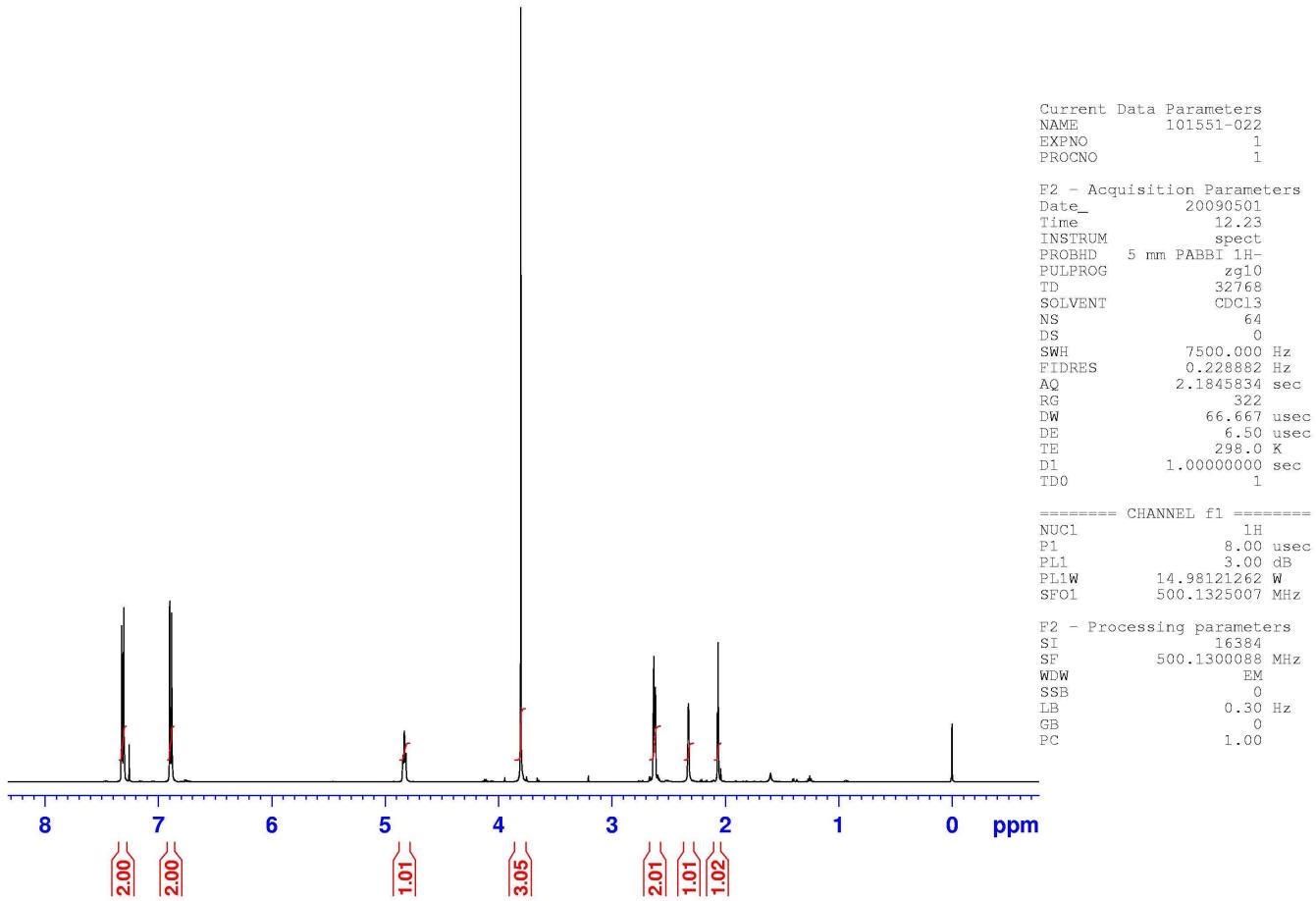
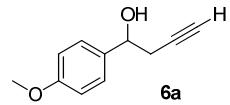
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 P1 14.00 usec
 PL1 0.00 dB
 PL1W 10.49968529 W
 SFO1 400.1327209 MHz

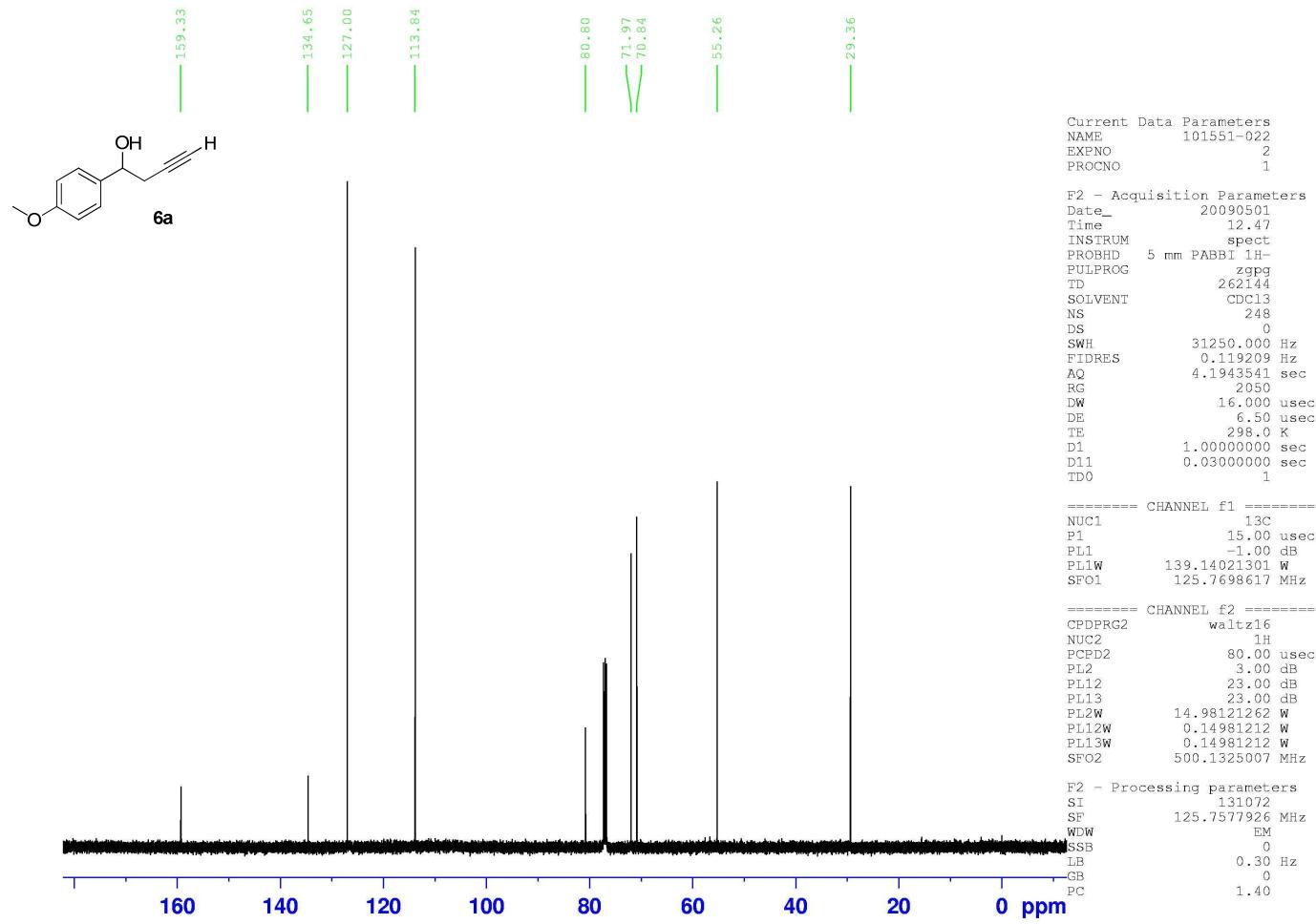
F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 0.05 Hz
 GB 0
 PC 1.00

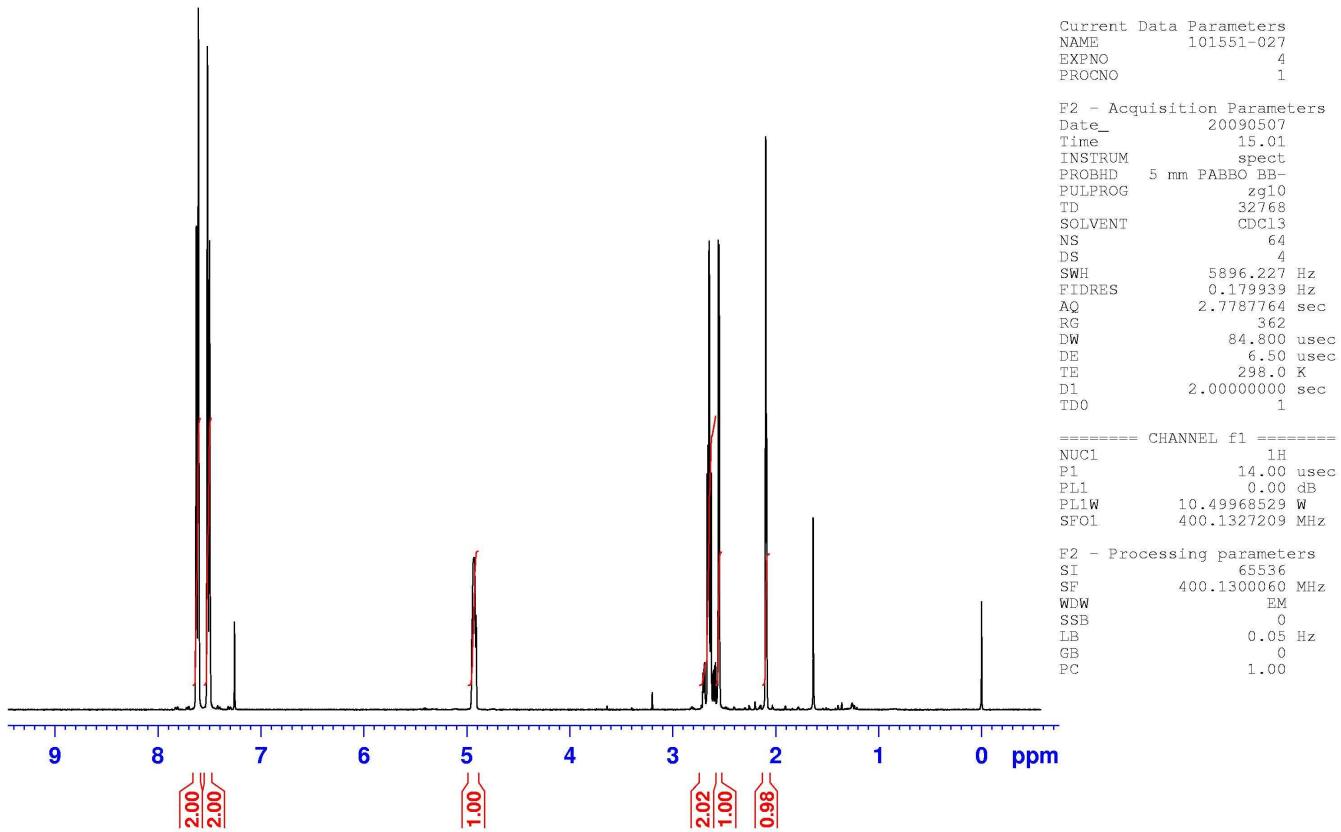
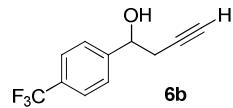


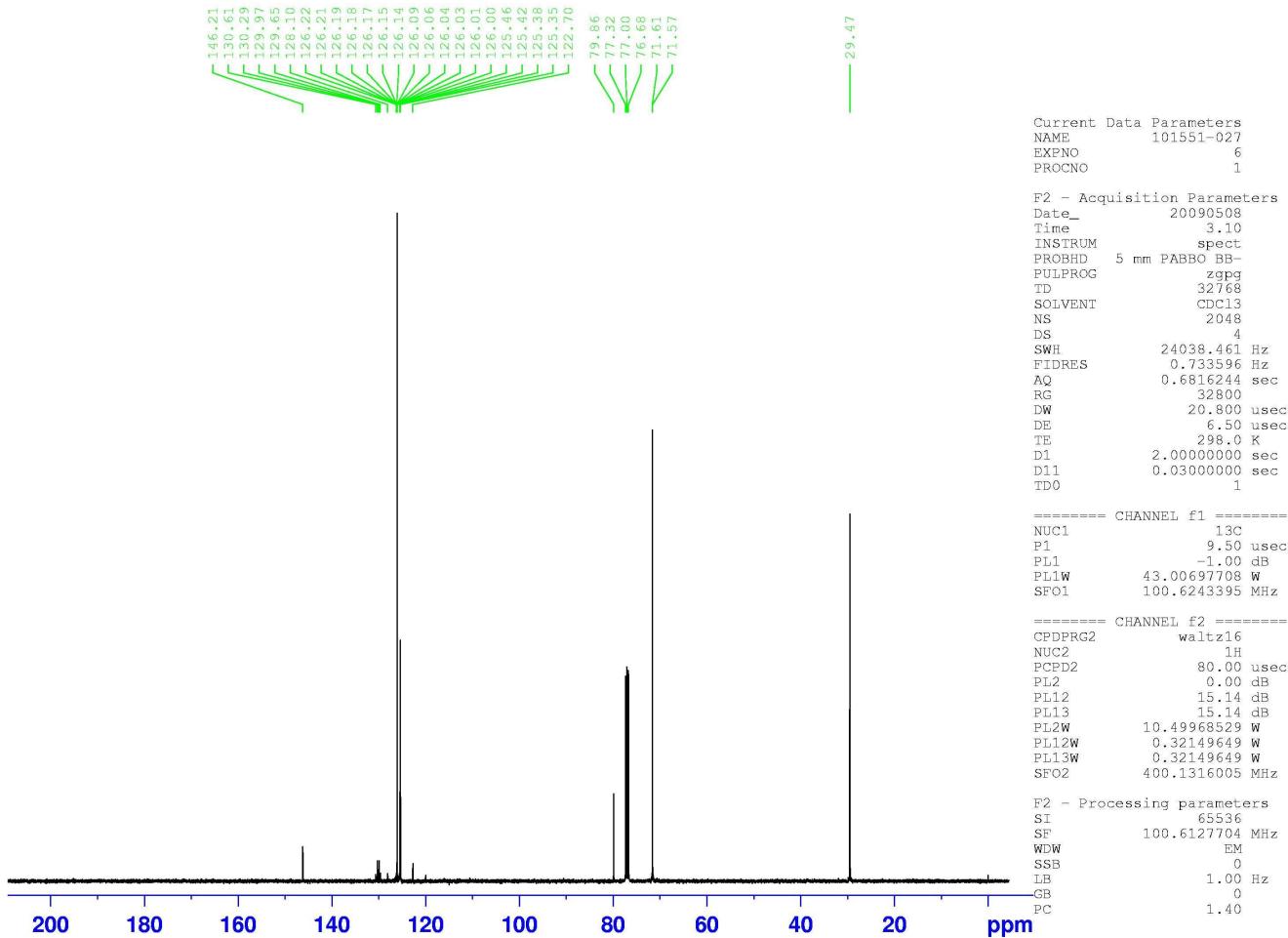
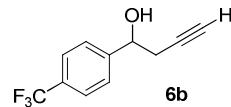


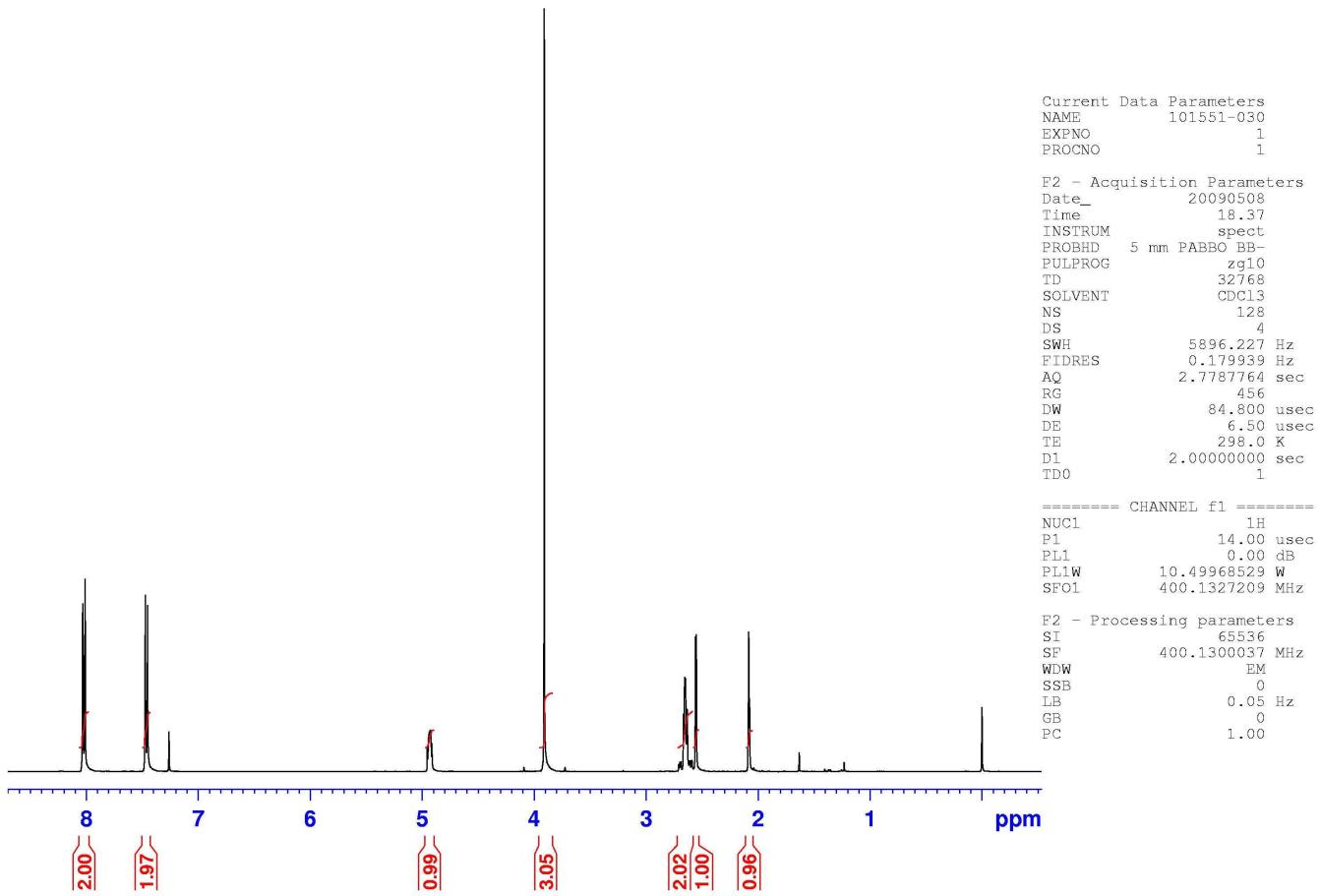
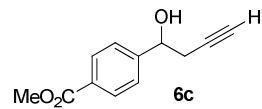


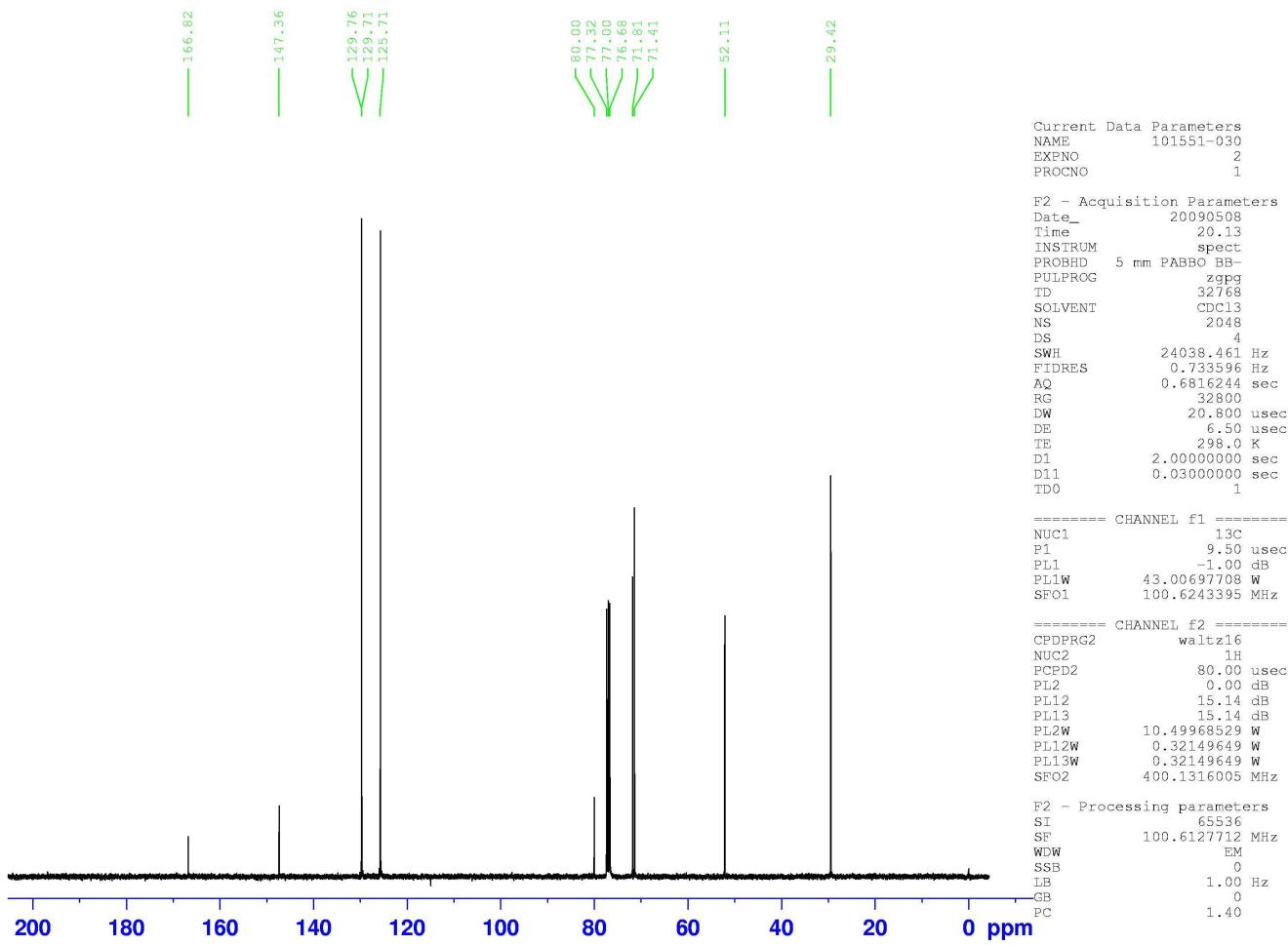
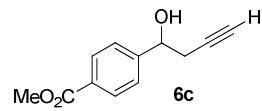


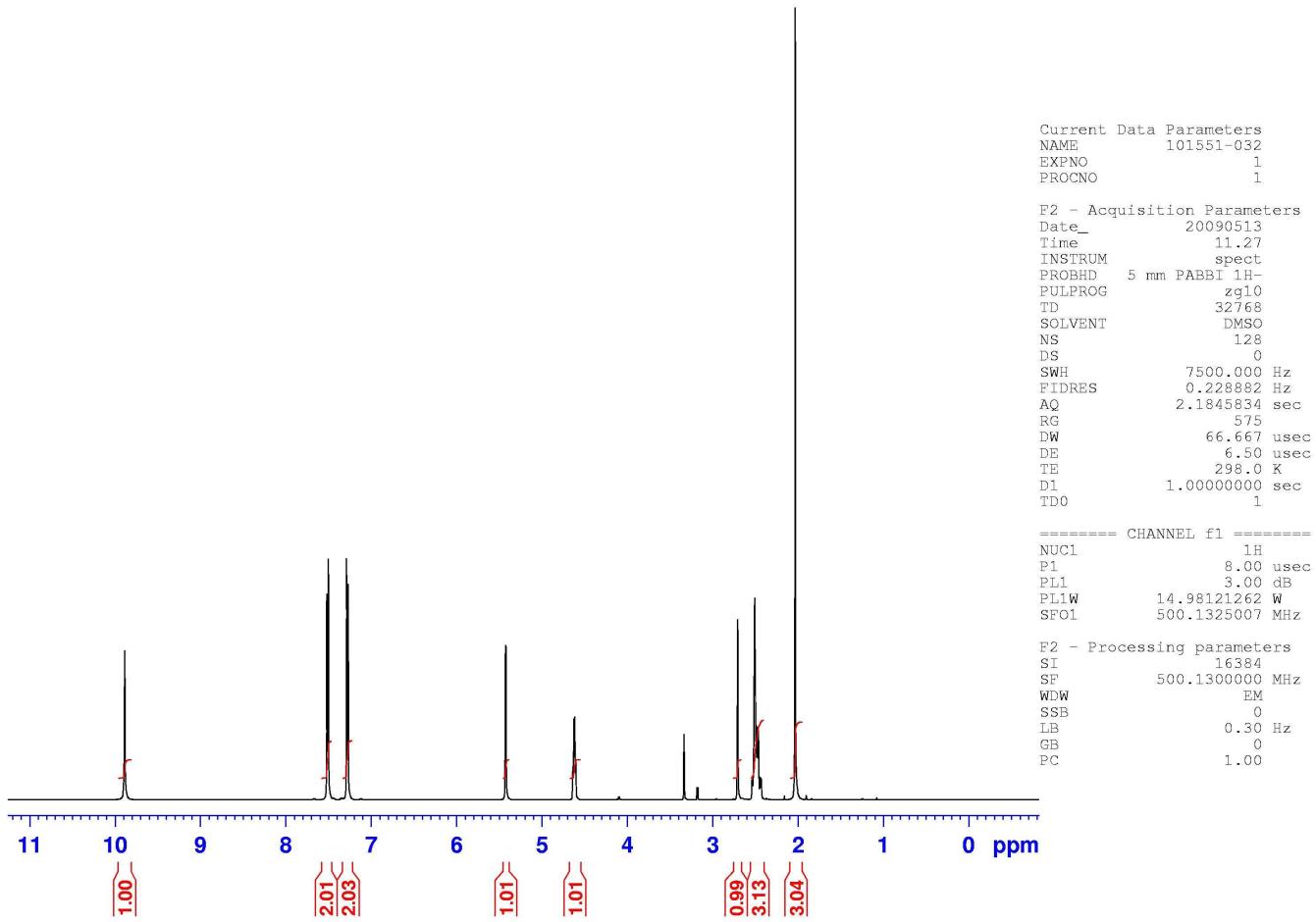
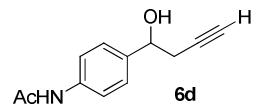


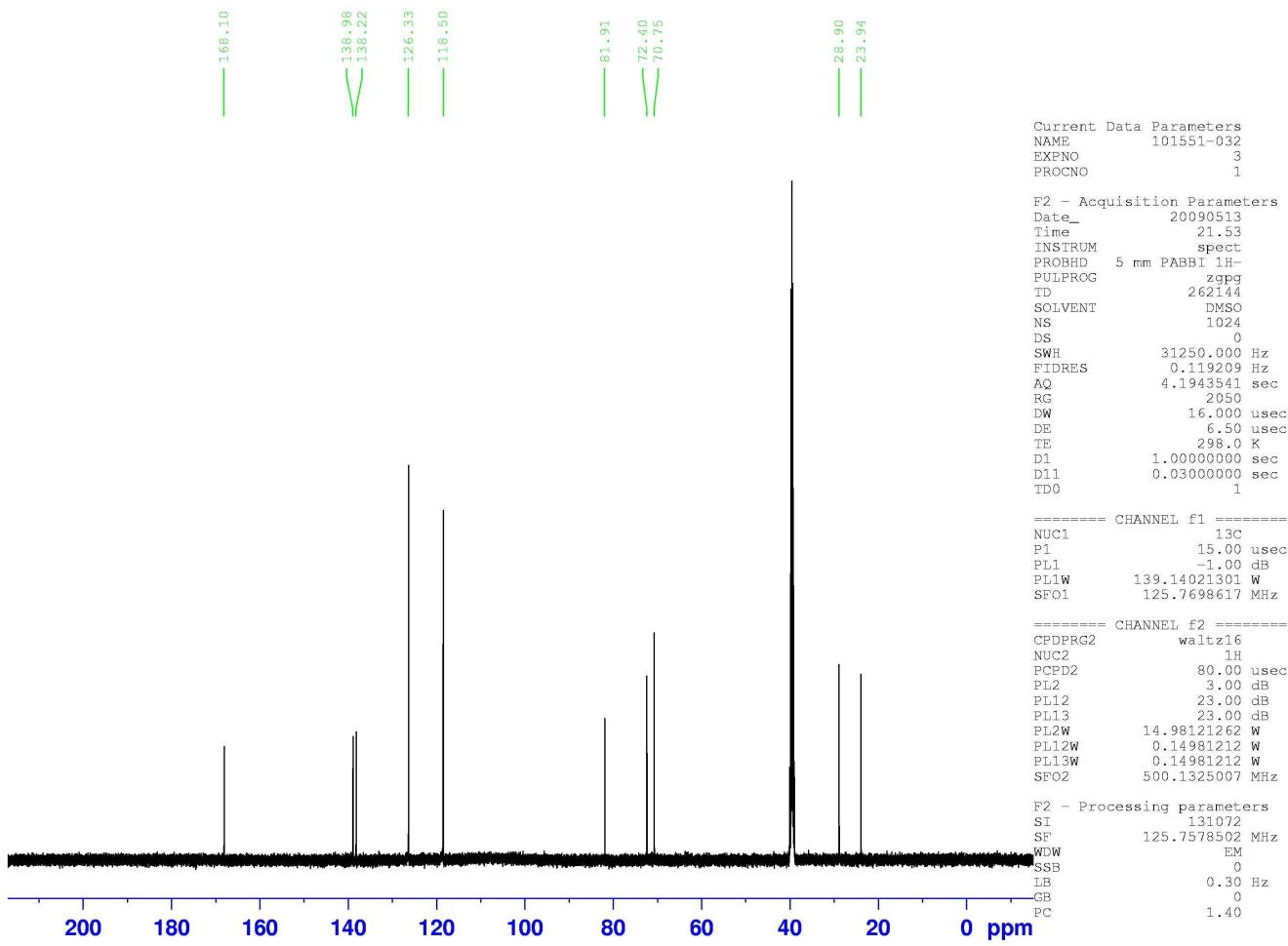
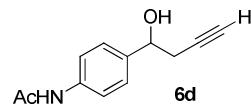




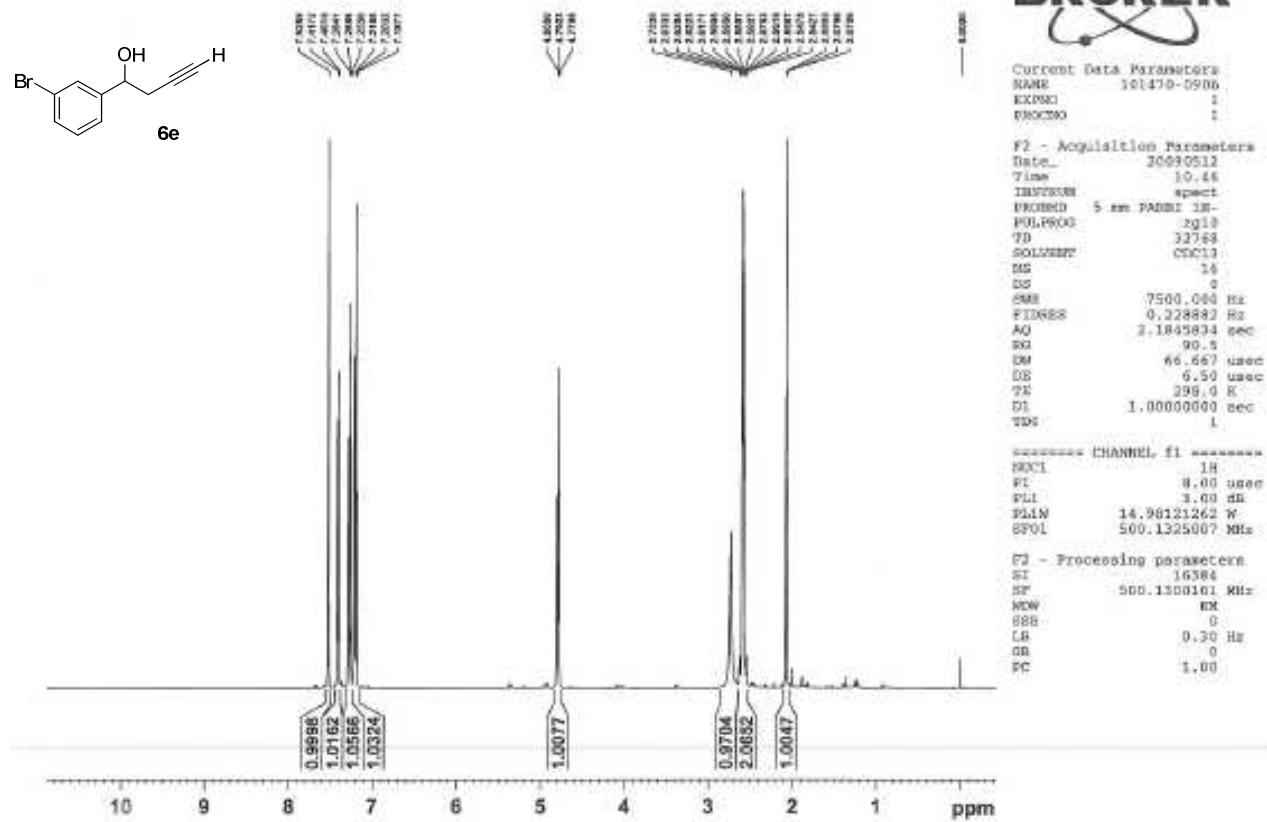


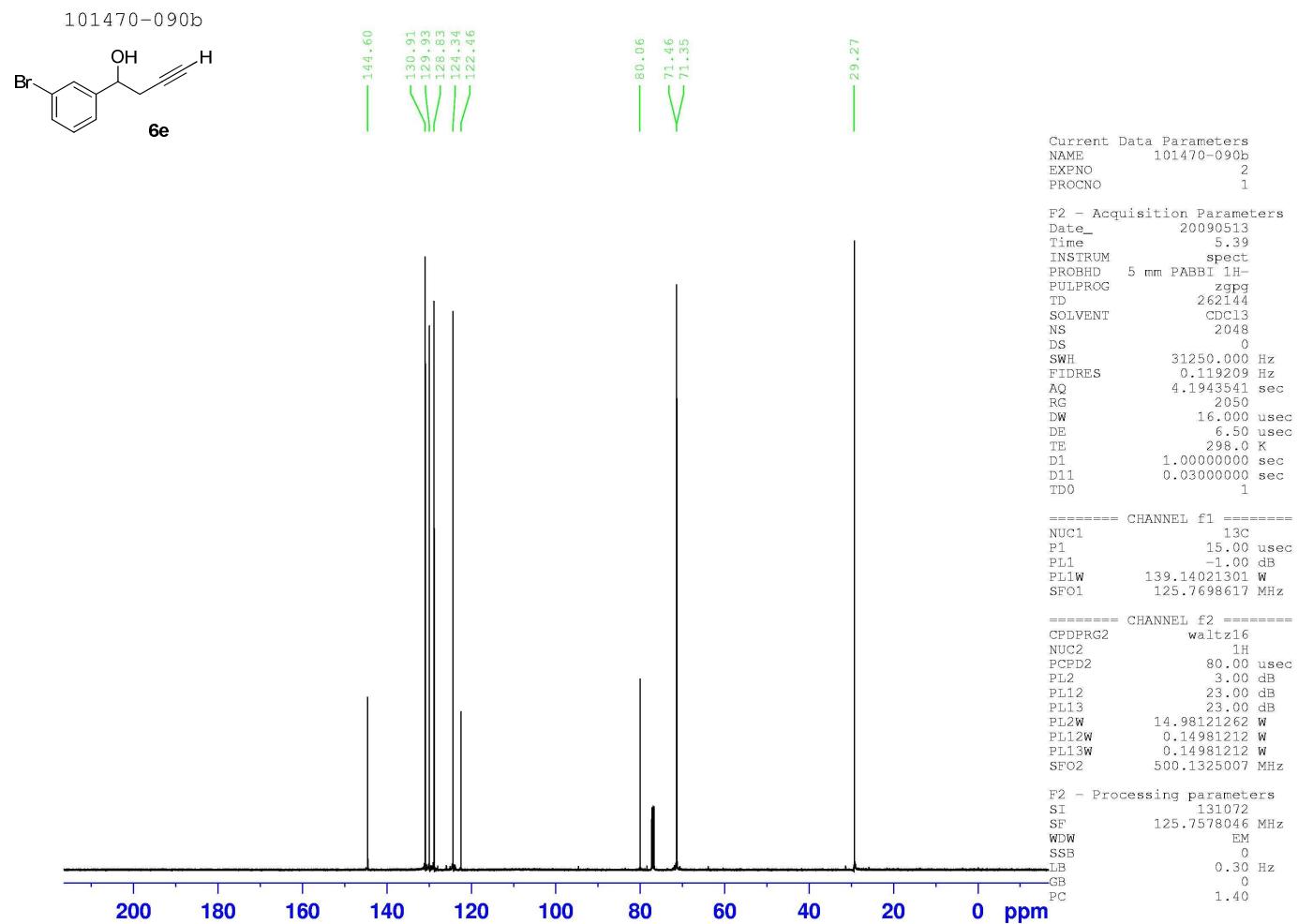


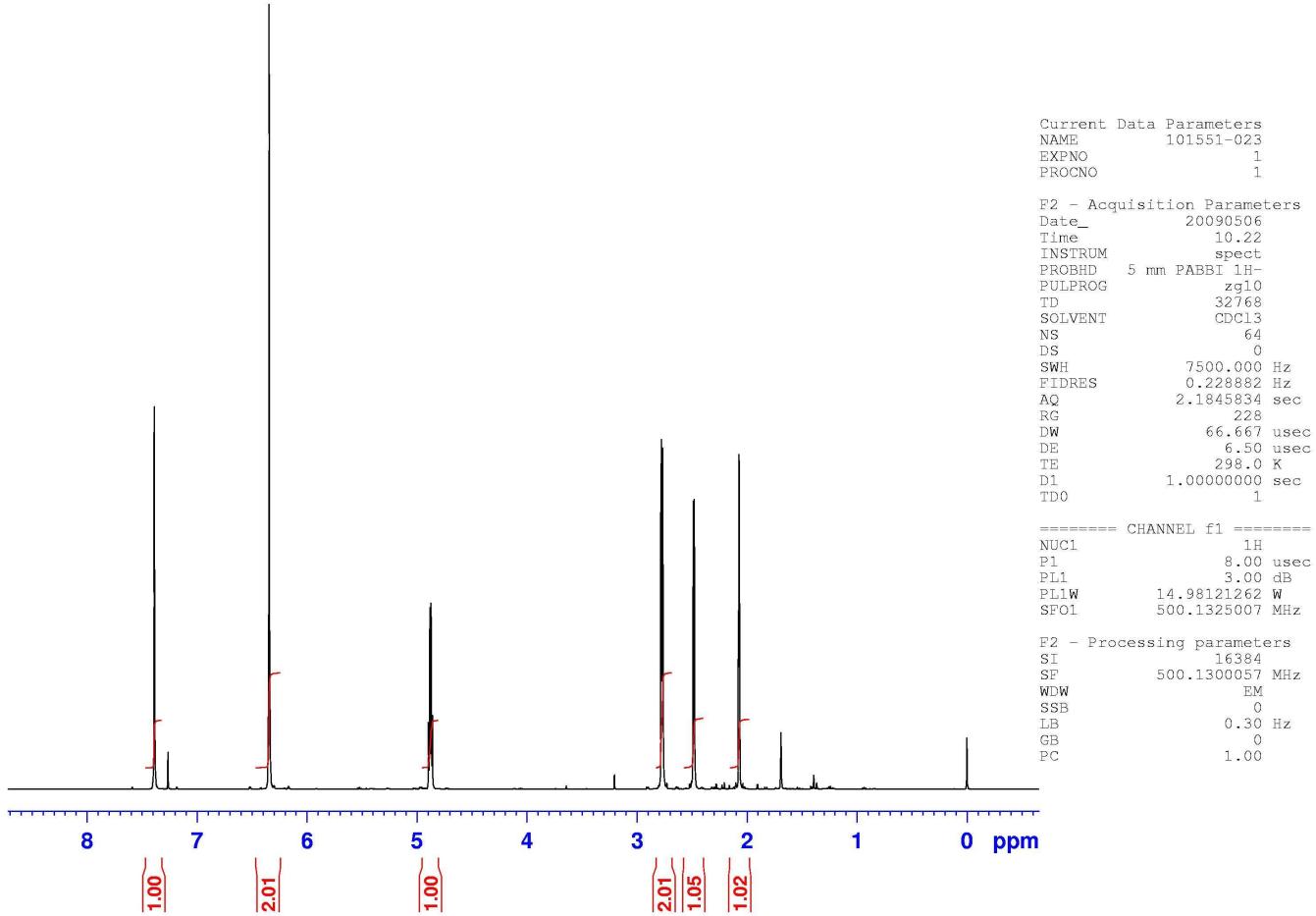
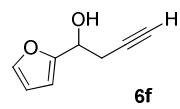


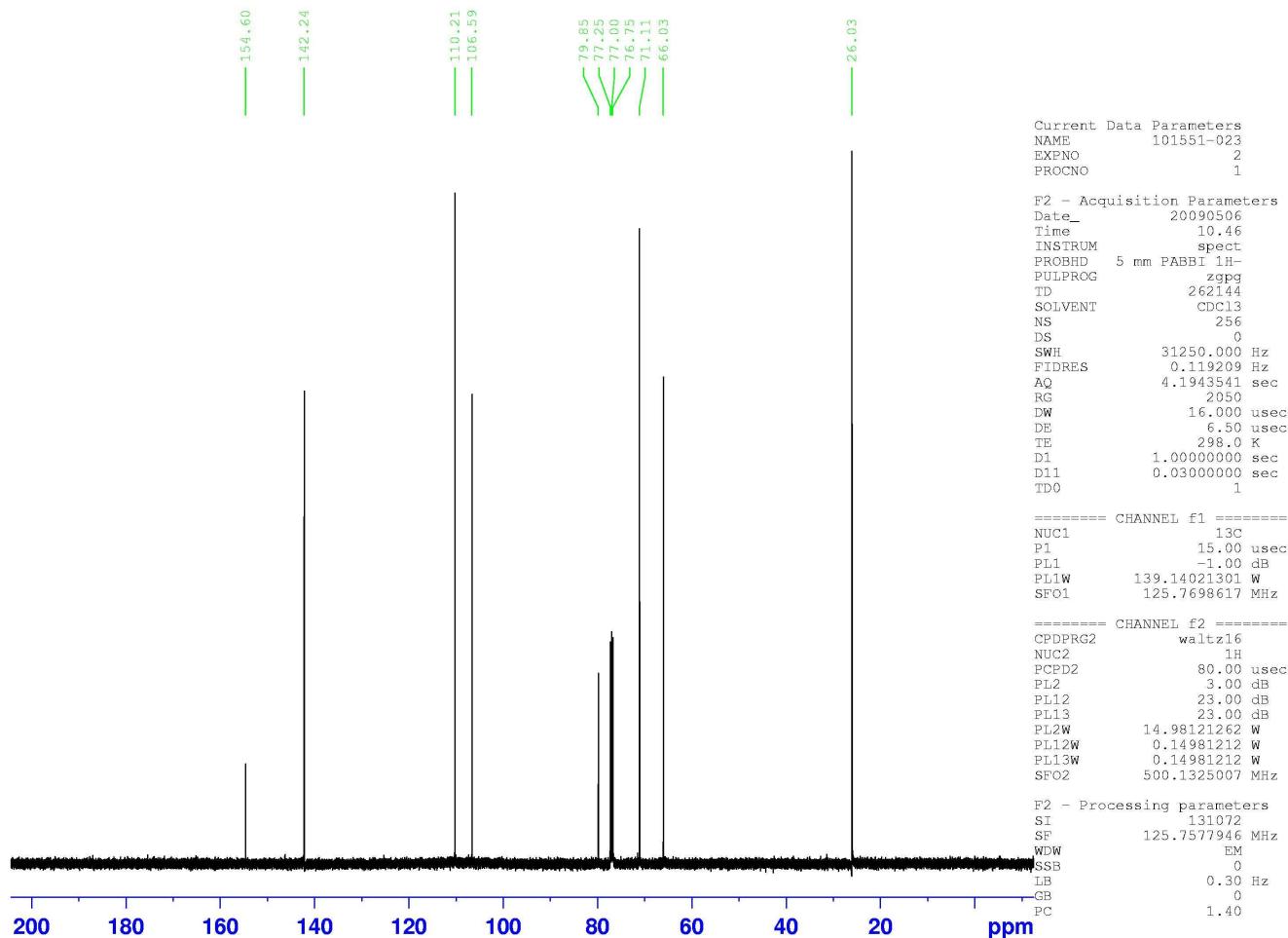
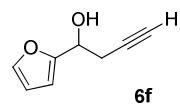


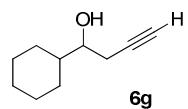
101470-090b



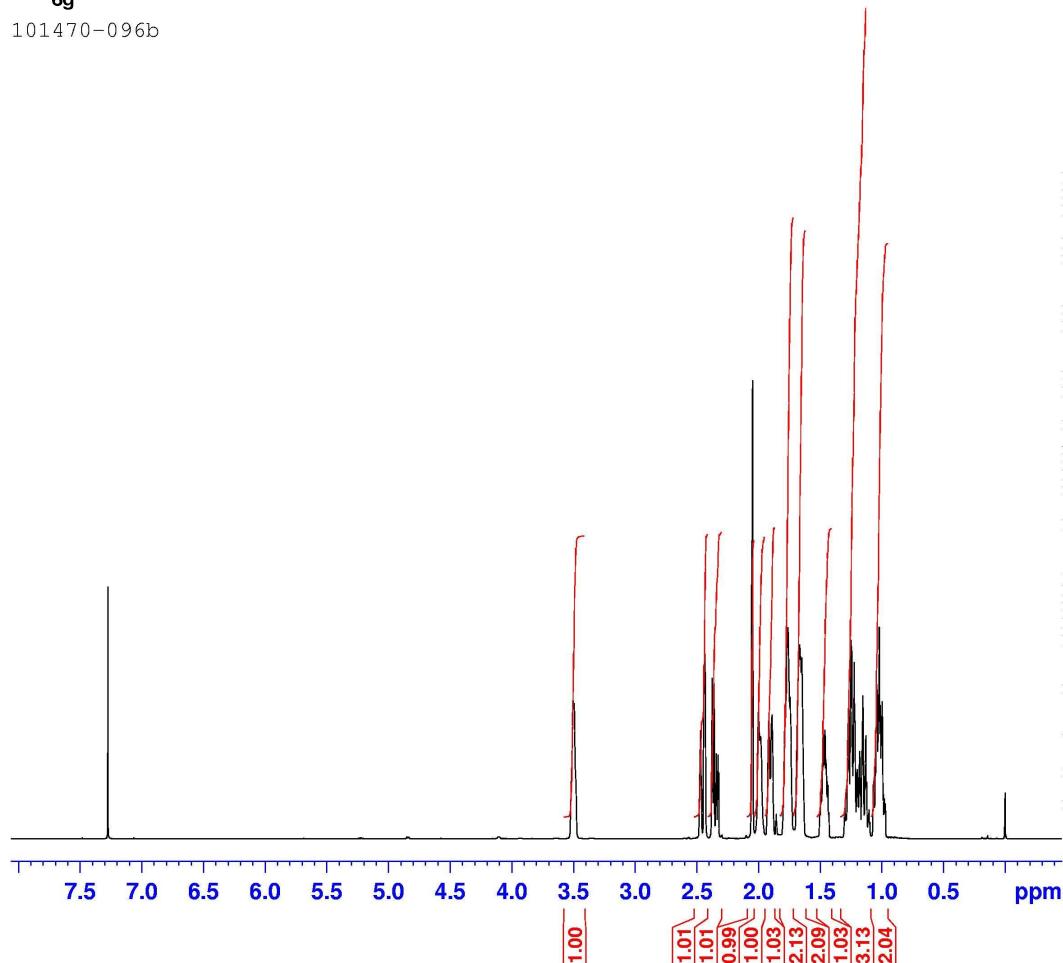








101470-096b

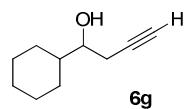


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PROCNO 1

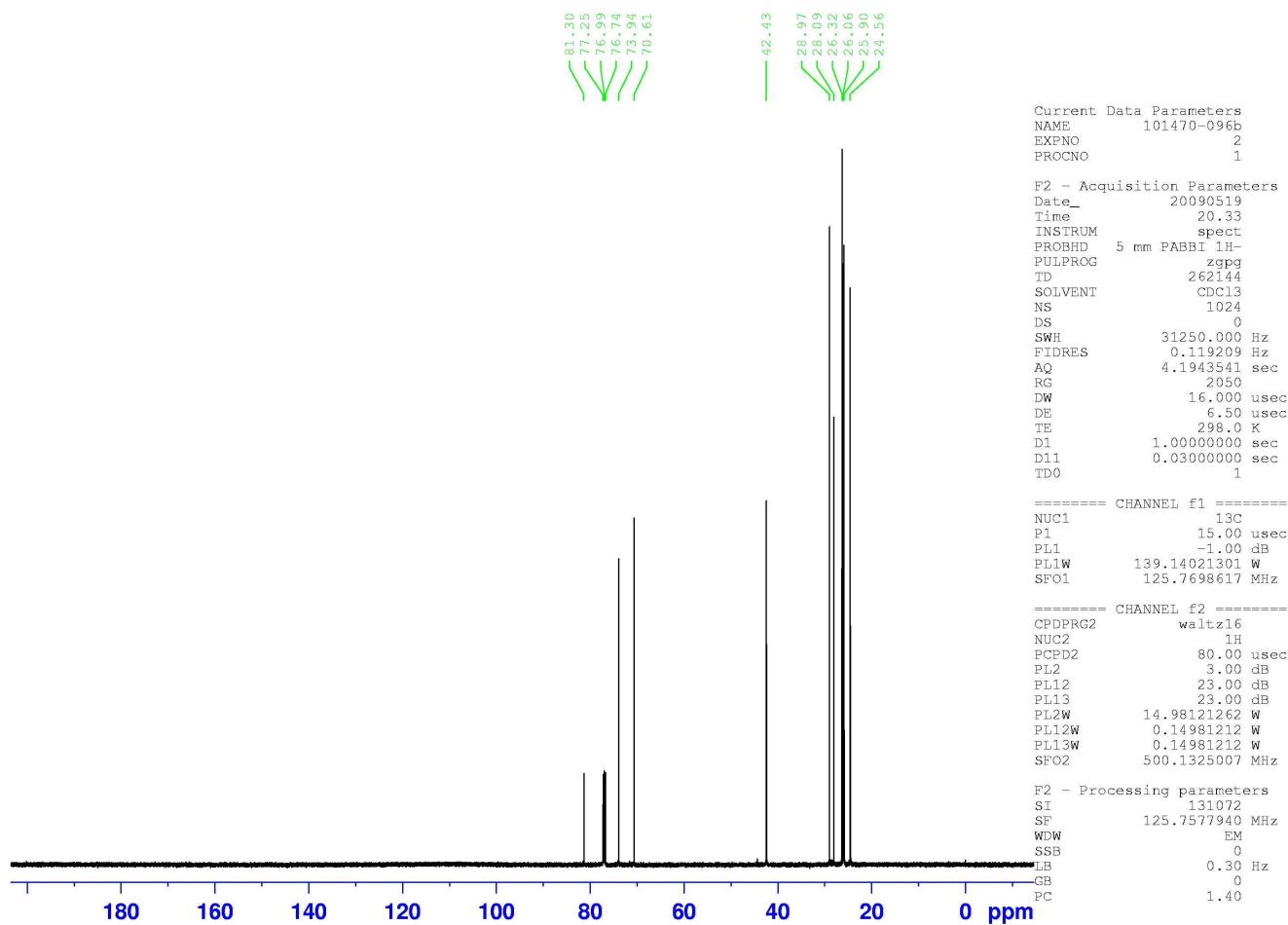
F2 - Acquisition Parameters
Date_ 20090519
Time 11.58
INSTRUM spect
PROBHD 5 mm PABBI 1H-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 144
DW 66.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TDO 1

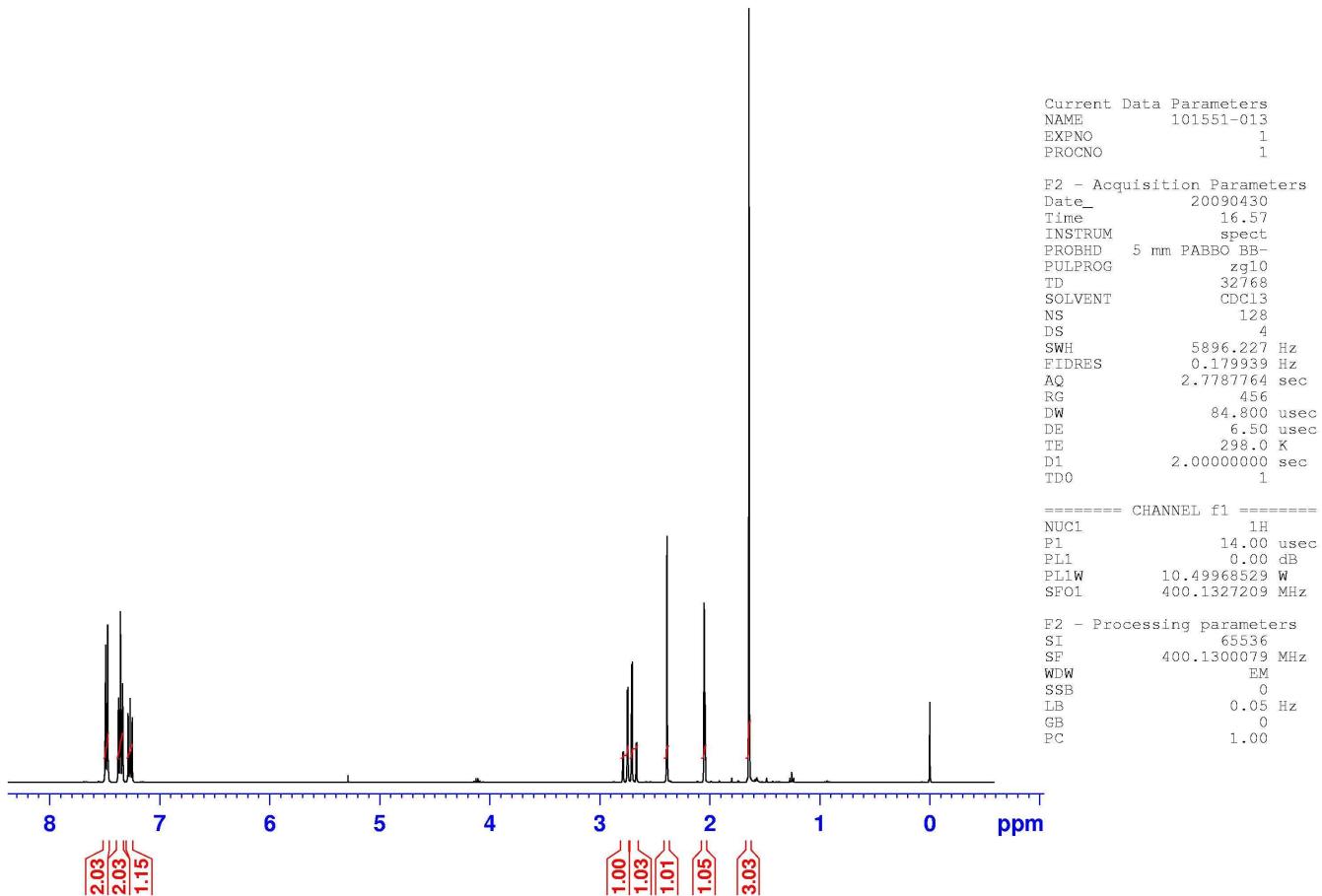
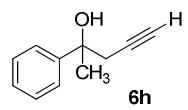
===== CHANNEL f1 ======
NUC1 1H
P1 8.00 usec
PL1 3.00 dB
PL1W 14.98121262 W
SFO1 500.1325007 MHz

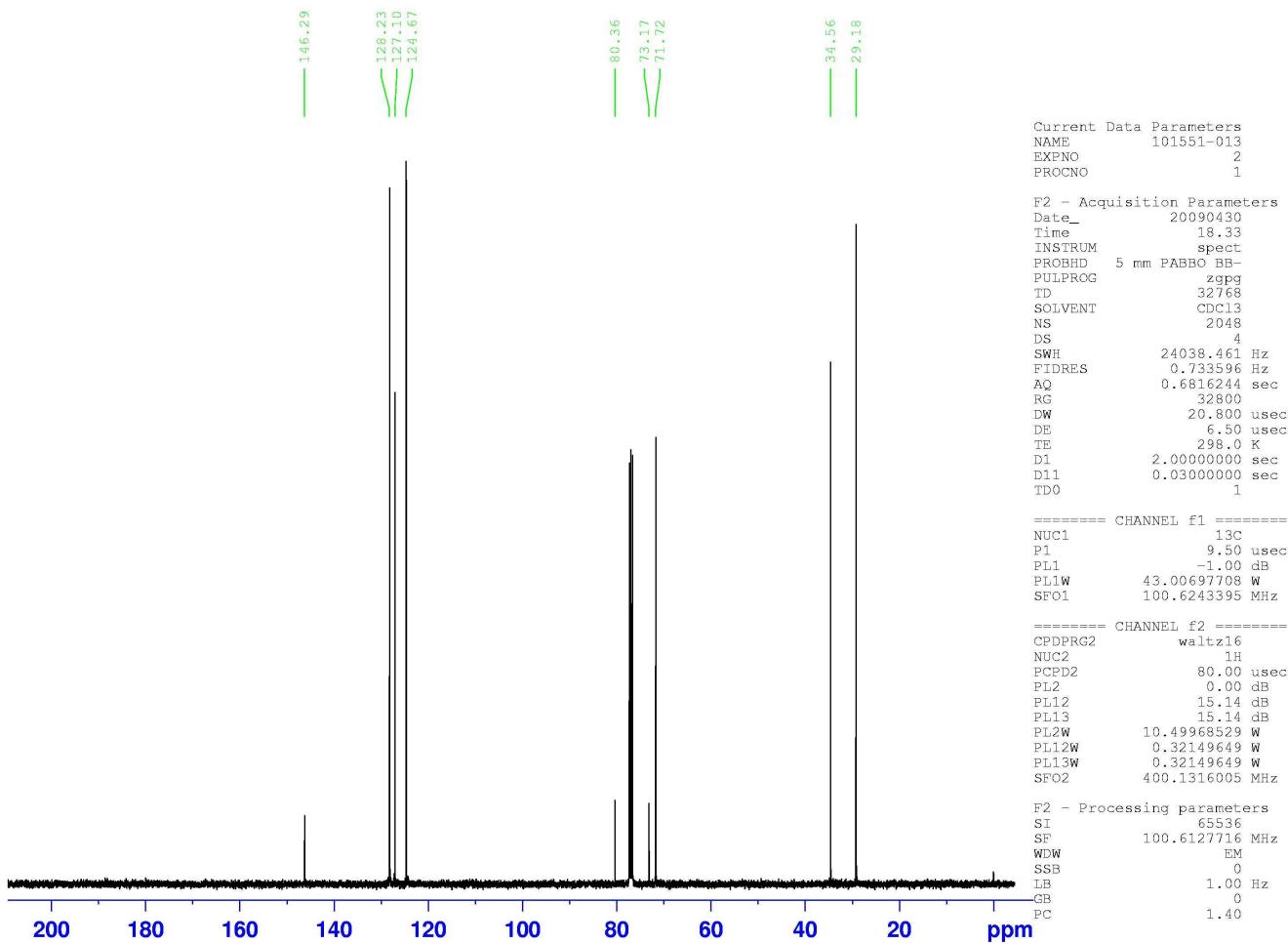
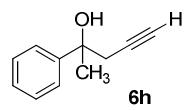
F2 - Processing parameters
SI 16384
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

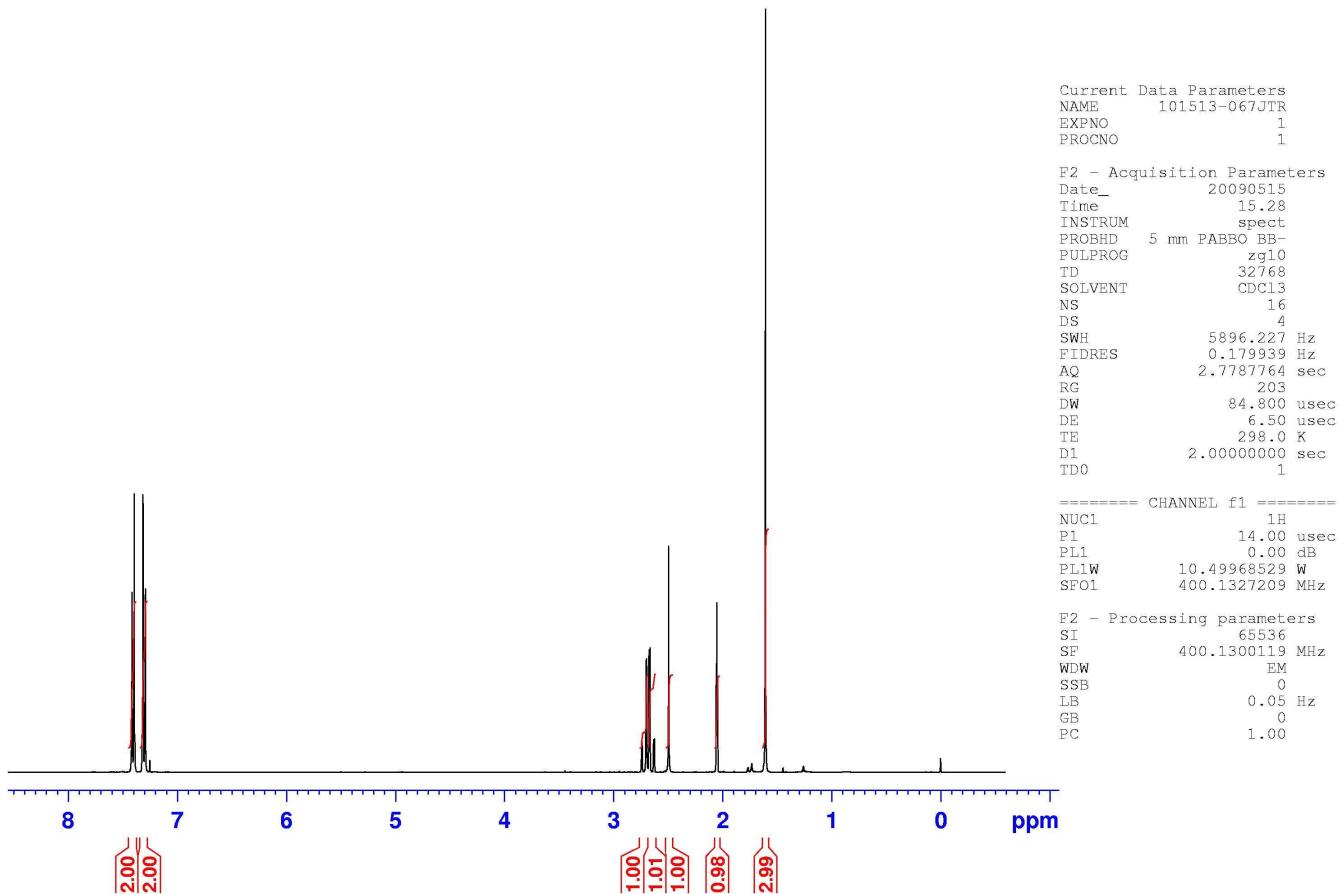
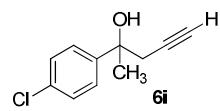


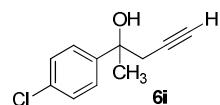
101470-096b



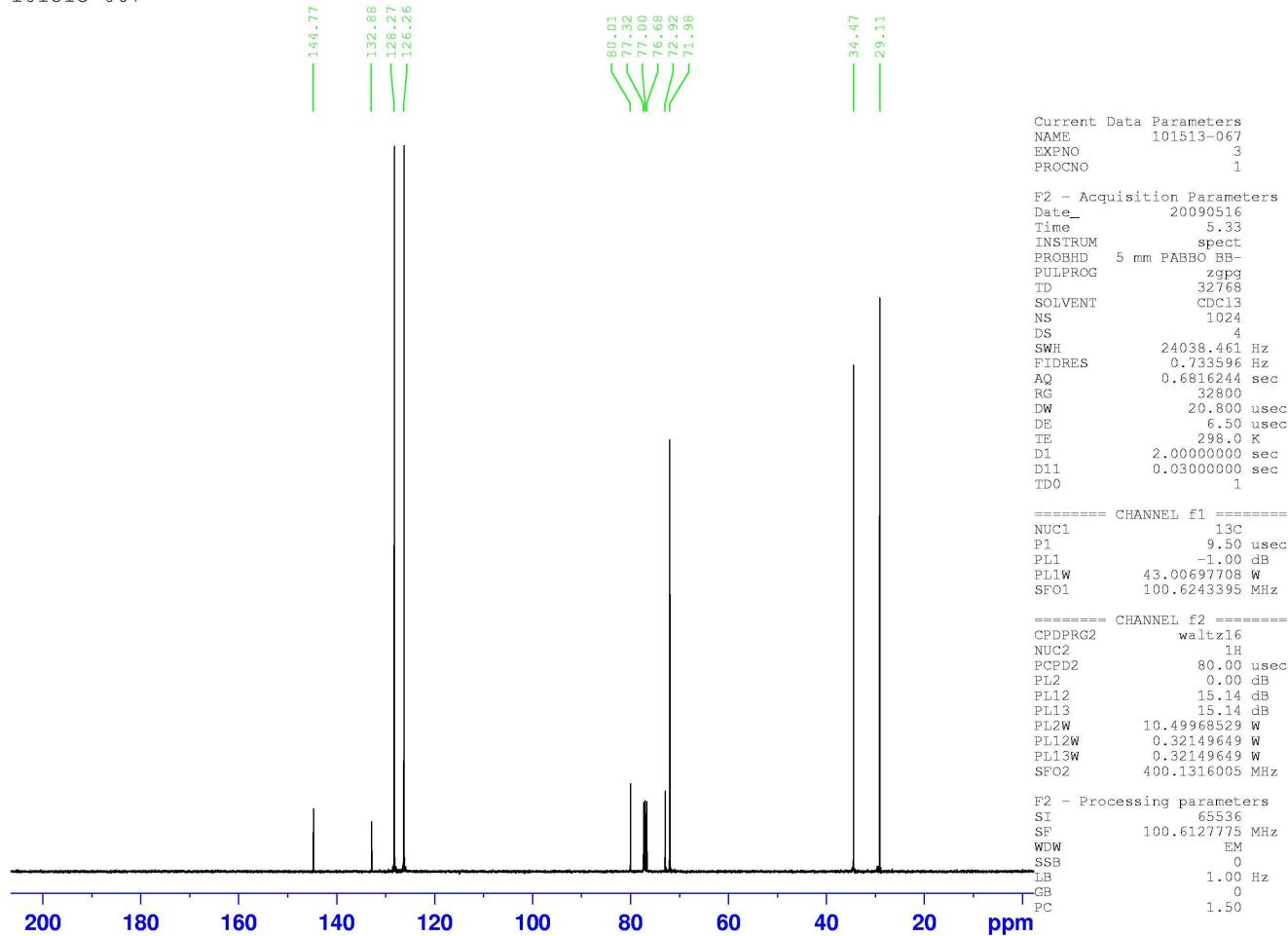


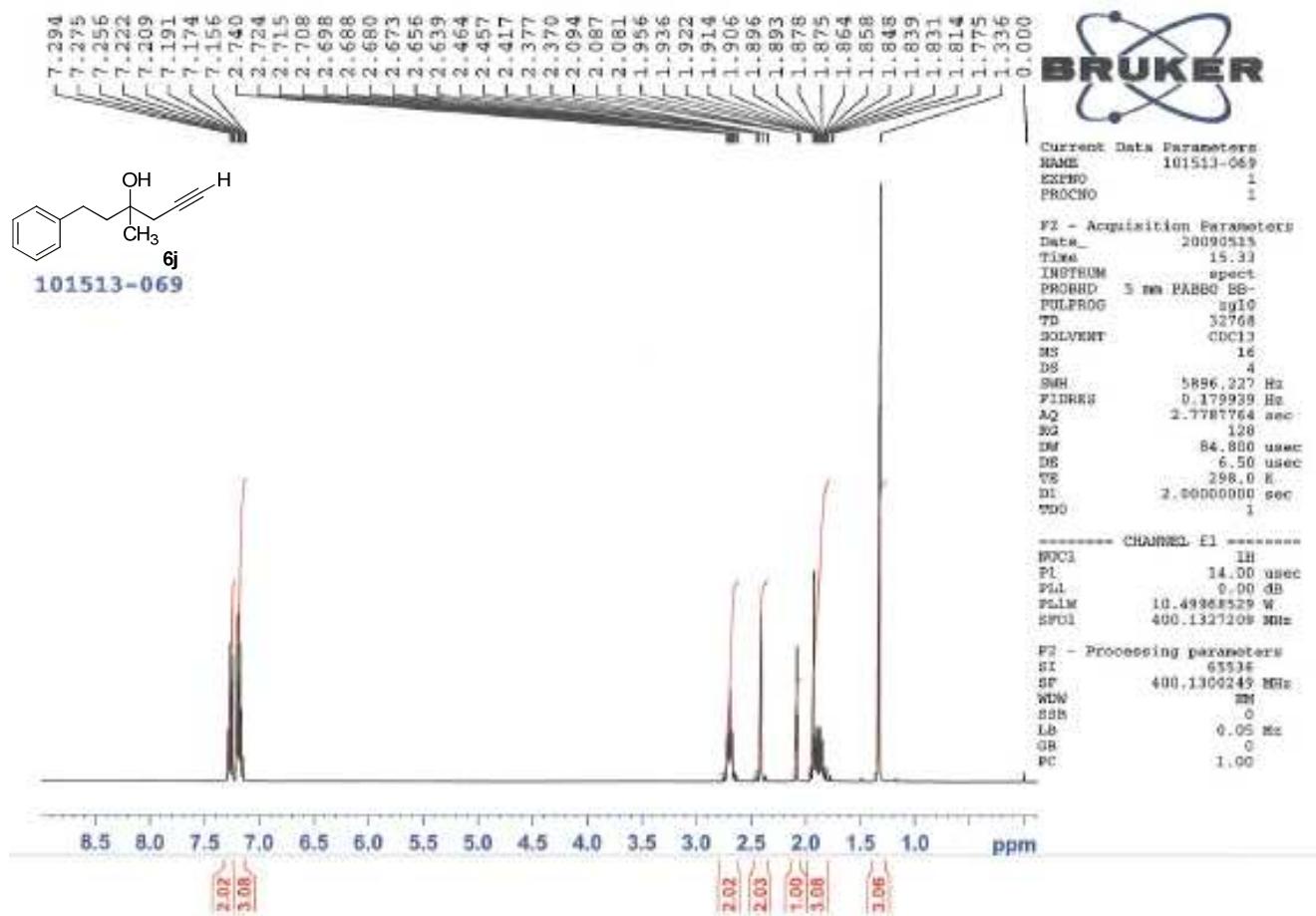


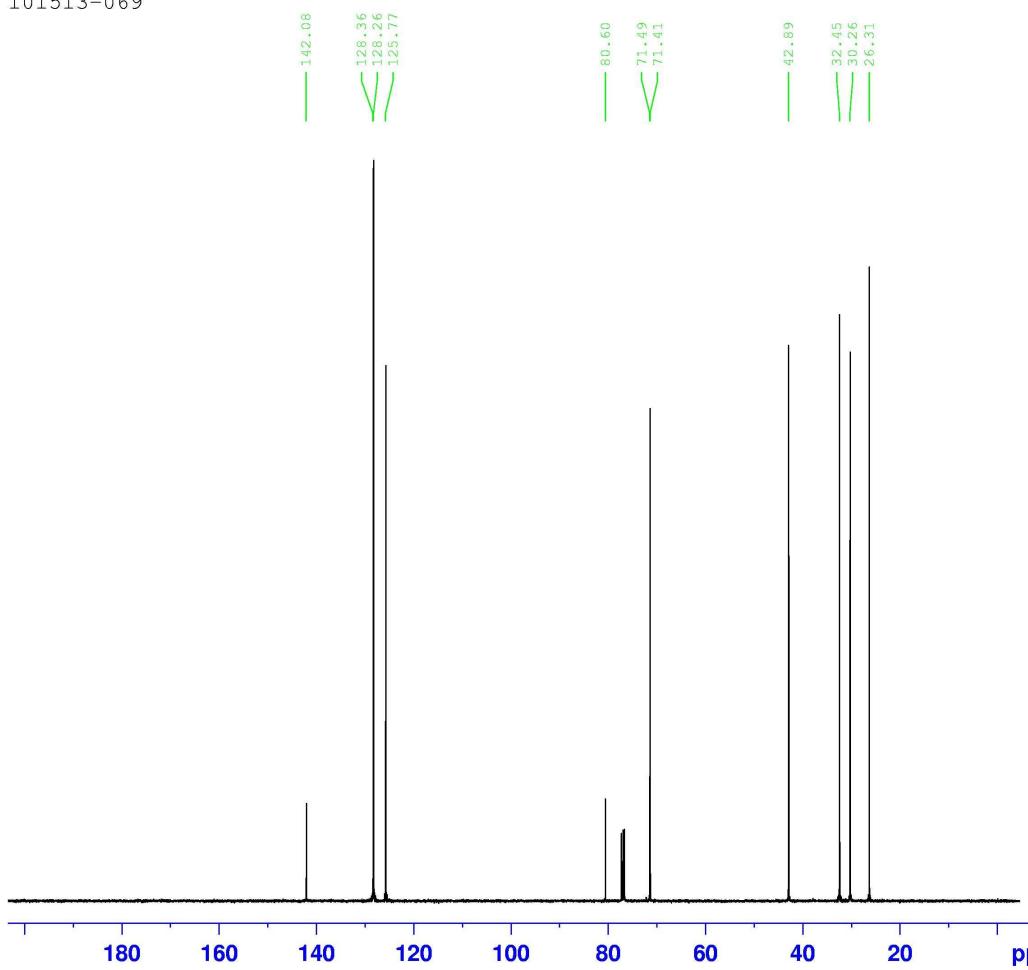
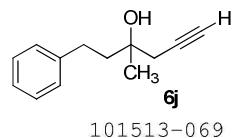




101513-067







Current Data Parameters
 NAME 101513-069
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20090516
 Time 6.24
 INSTRUM spect
 PROBID 5 mm PABBO BB-
 PULPROG zgpg
 TD 32768
 SOLVENT CDCl3
 NS 1024
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.733596 Hz
 AQ 0.6816244 sec
 RG 32800
 DW 20.800 usec
 DE 6.50 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

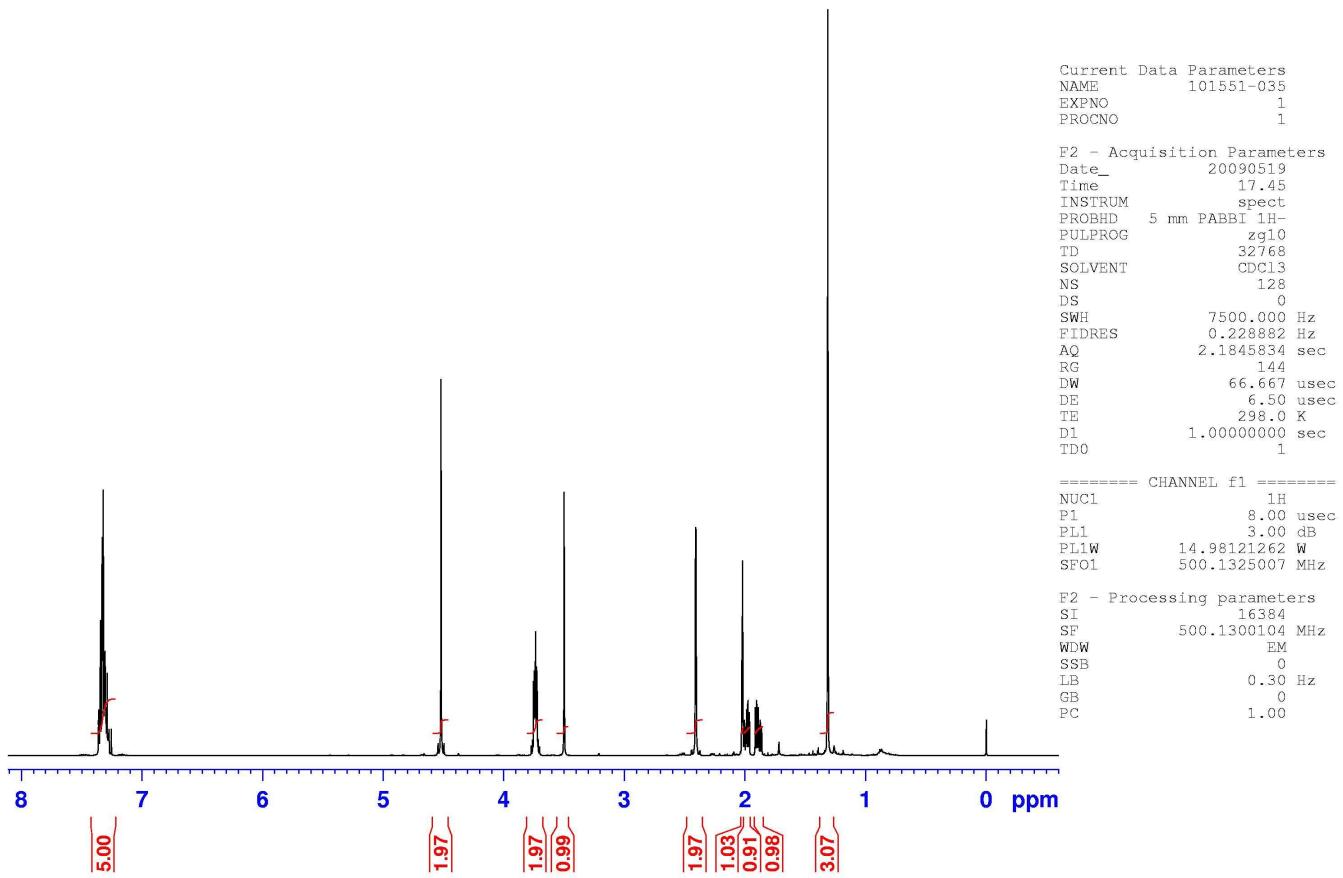
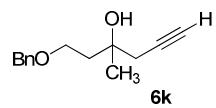
===== CHANNEL f1 ======

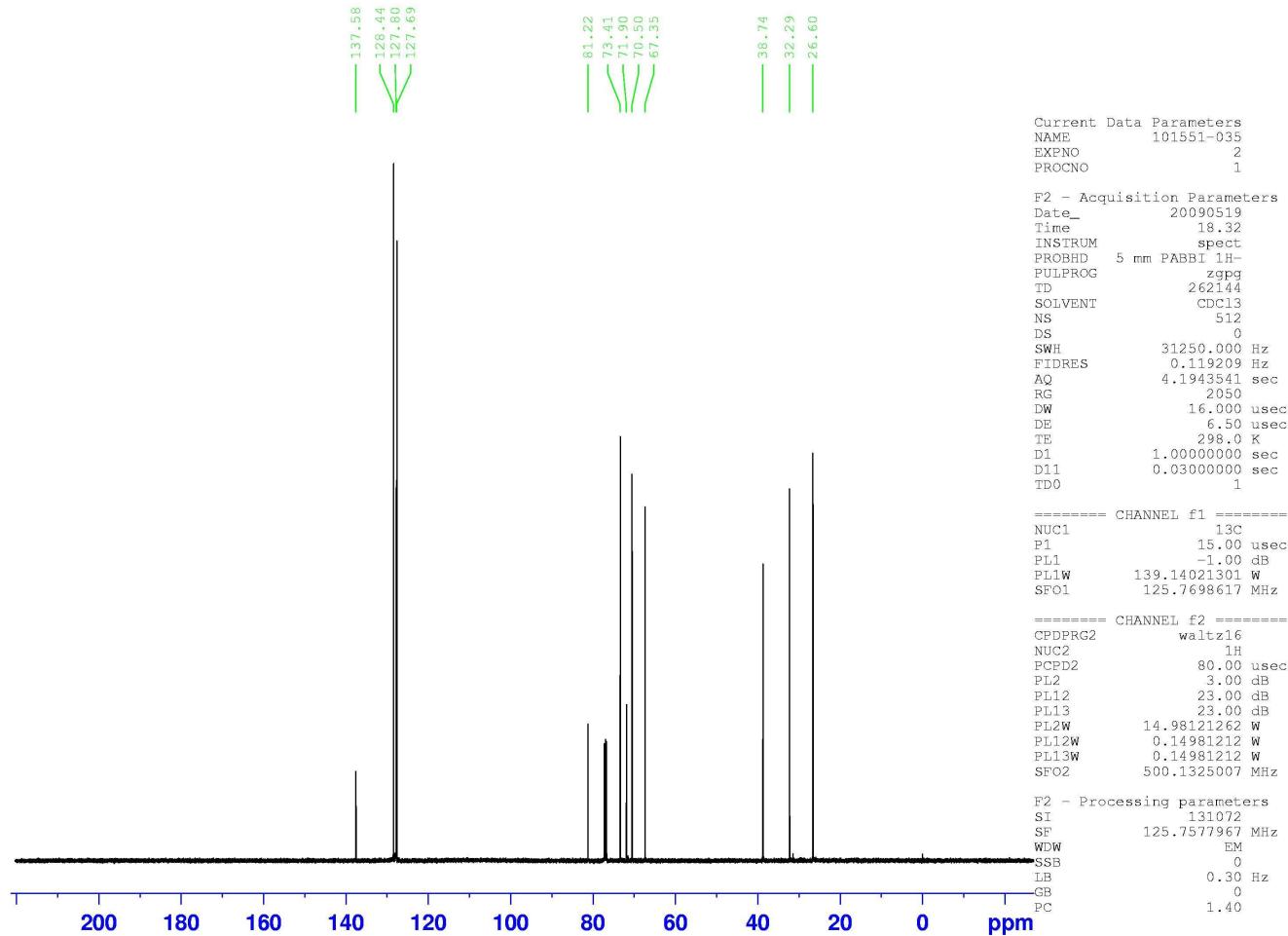
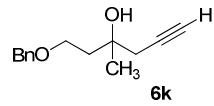
NUC1	13C
P1	9.50 usec
PL1	-1.00 dB
PL1W	43.00697708 W
SFO1	100.6243395 MHz

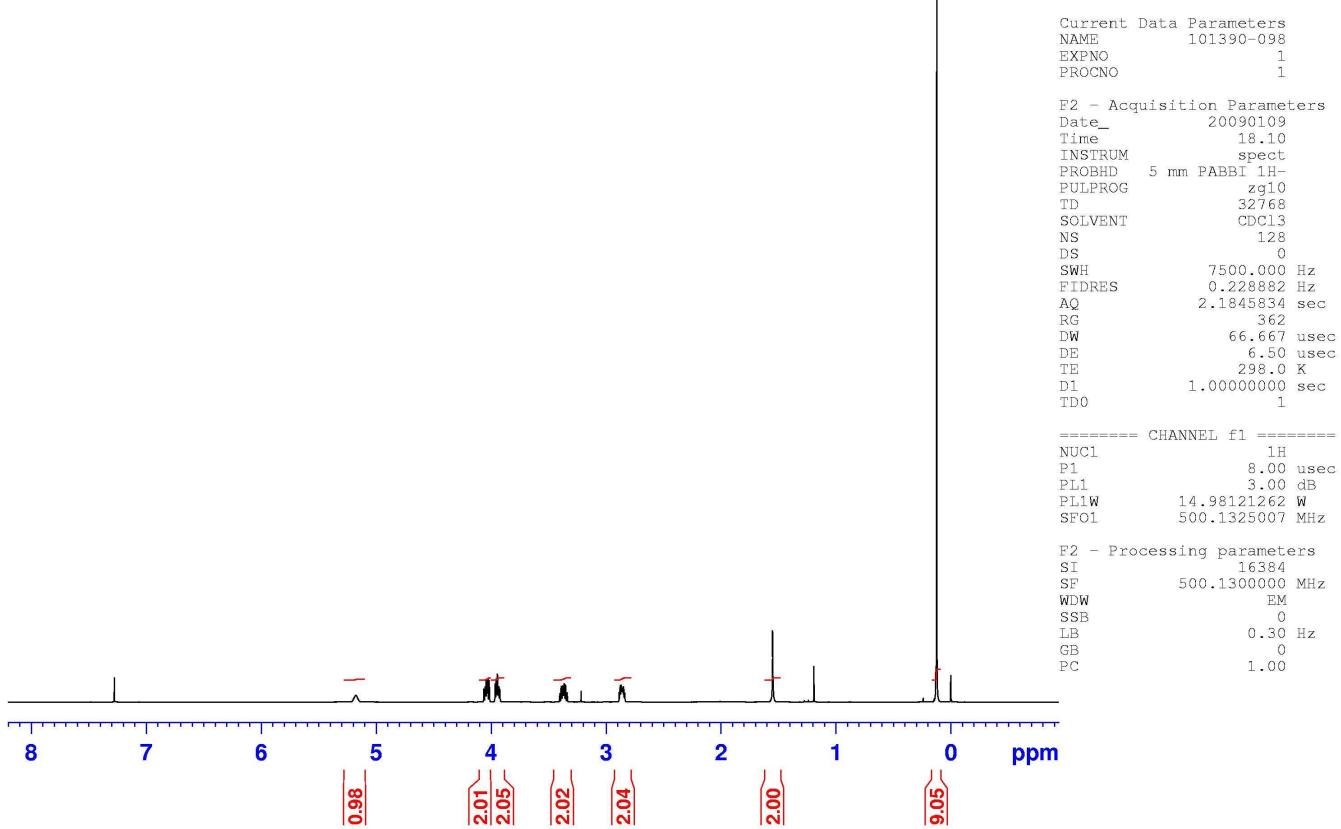
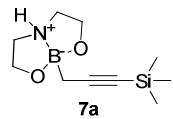
===== CHANNEL f2 ======

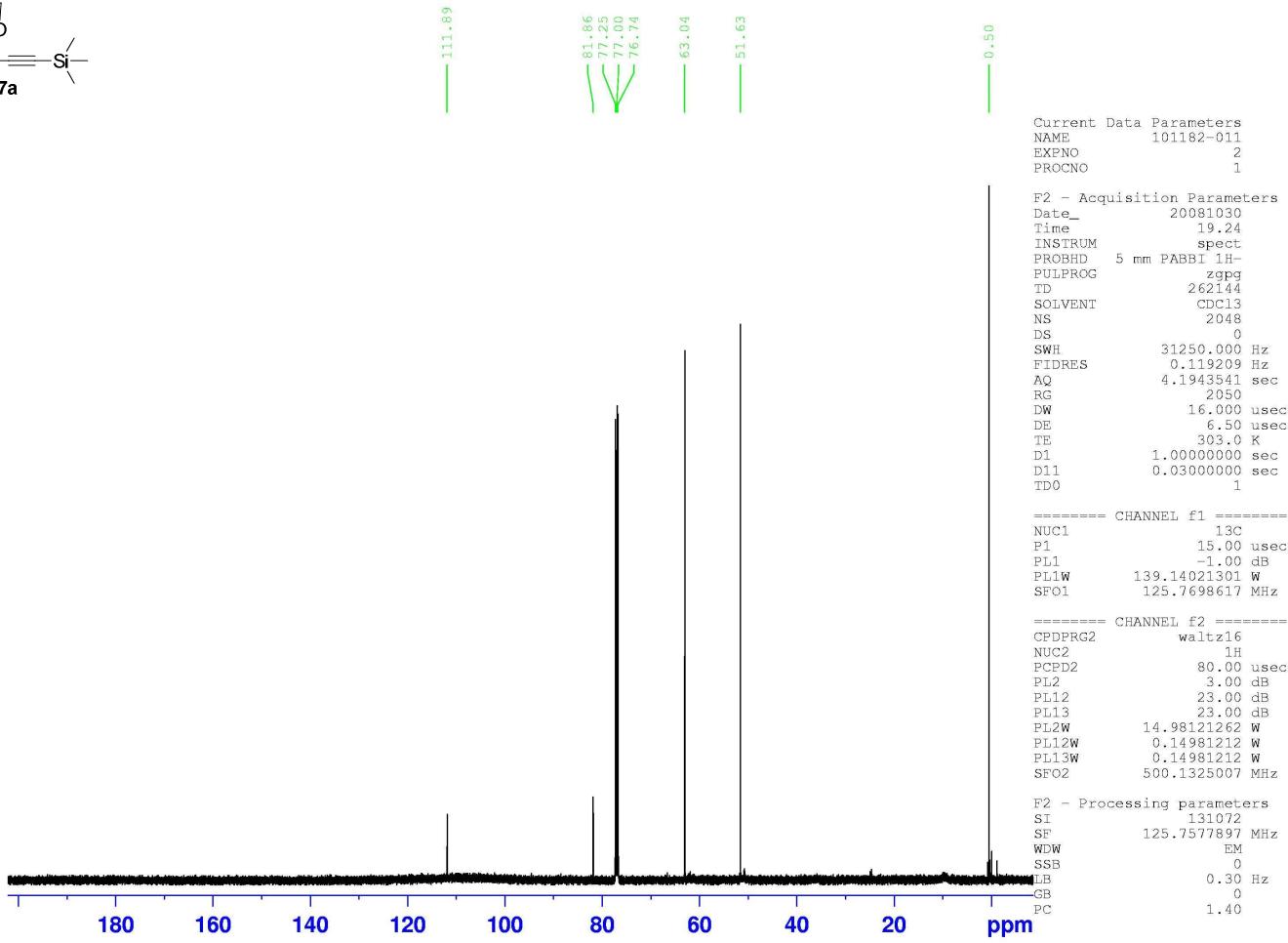
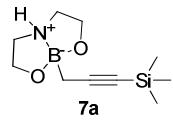
CEDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	15.14 dB
PL13	15.14 dB
PL2W	10.49968529 W
PL12W	0.32149649 W
PL13W	0.32149649 W
SFO2	400.1316005 MHz

F2 - Processing parameters
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 SF 100.6127817 MHz
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 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

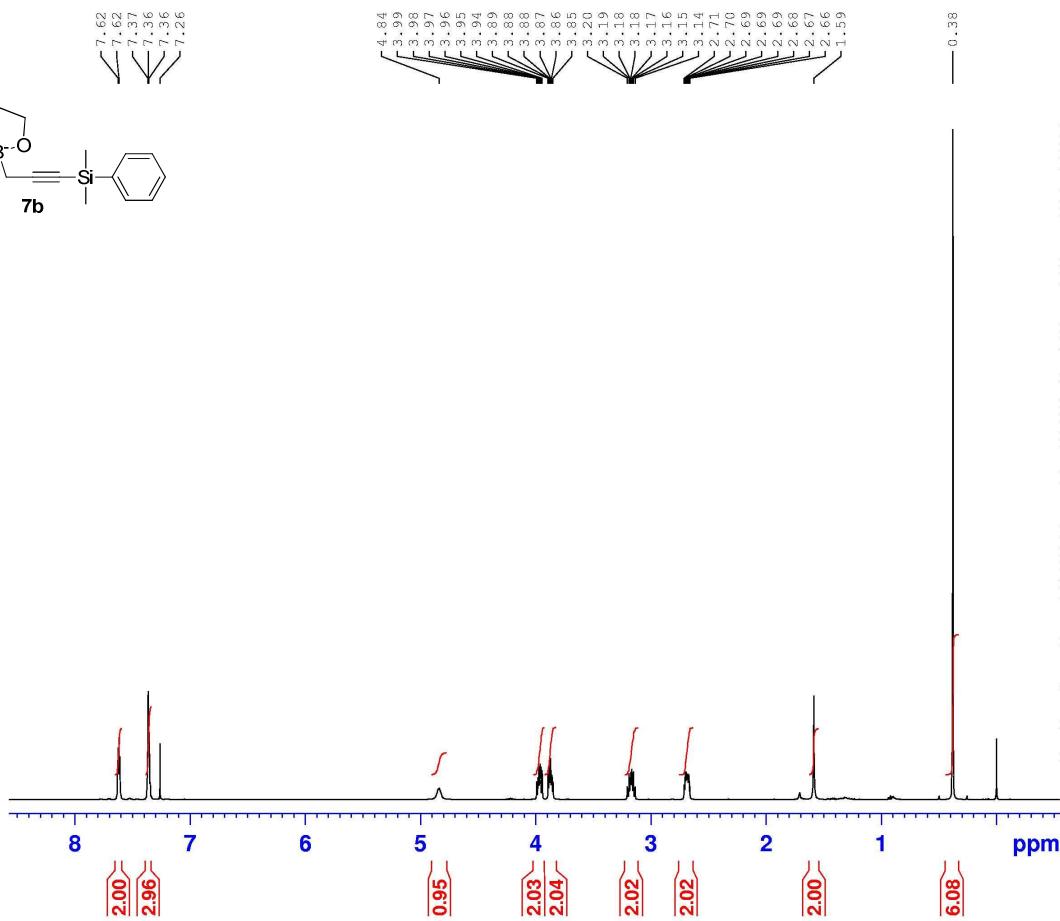
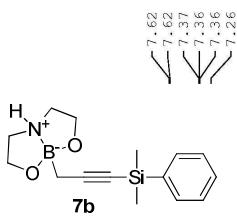








recrystallized

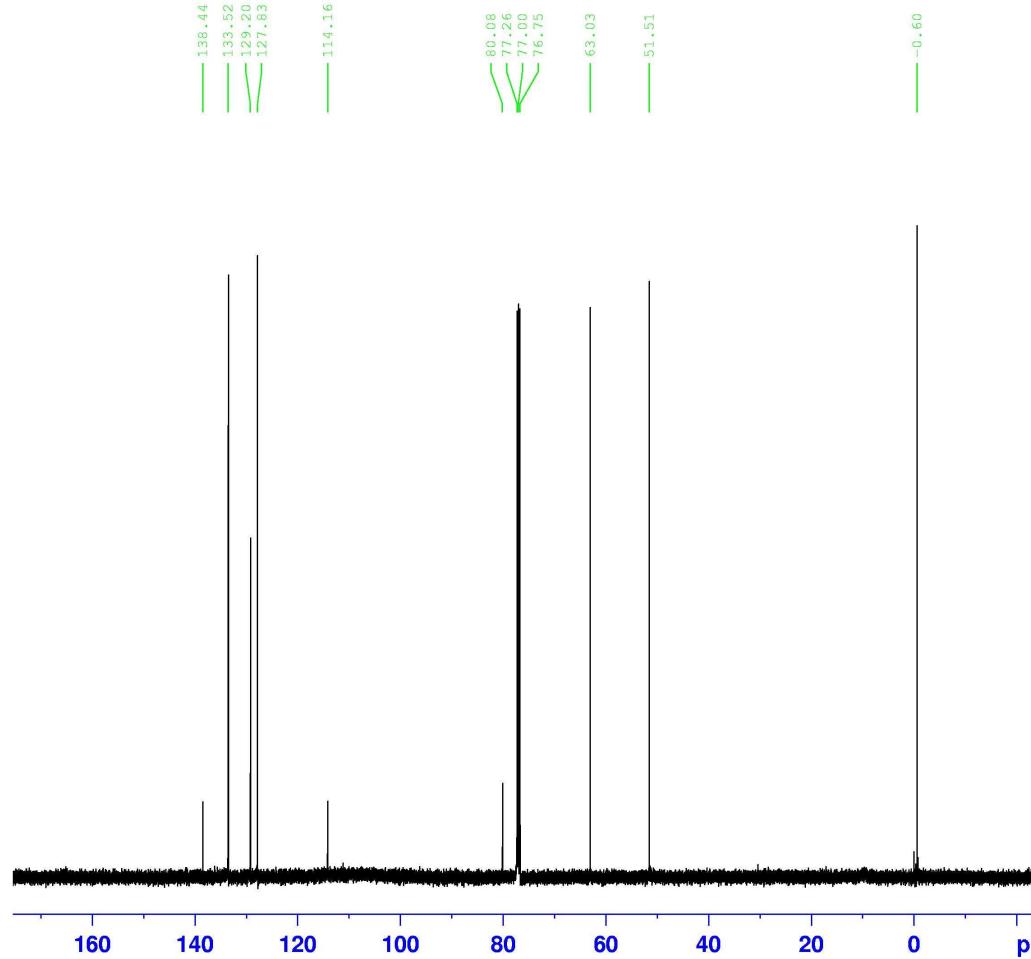
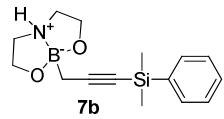


Current Data Parameters
NAME 101390-058
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date 20081111
Time 8.55
INSTRUM spect
PROBHD 5 mm PABBI 1H-
PULPROG zg10
TD 32768
SOLVENT CDCl₃
NS 128
DS 0
SWH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 456
DW 66.667 usec
DE 6.50 usec
TE 303.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.00 usec
PL1 3.00 dB
PL1W 14.98121262 W
SF01 500.1325007 MHz

F2 - Processing parameters
SI 16384
SF 500.1300070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



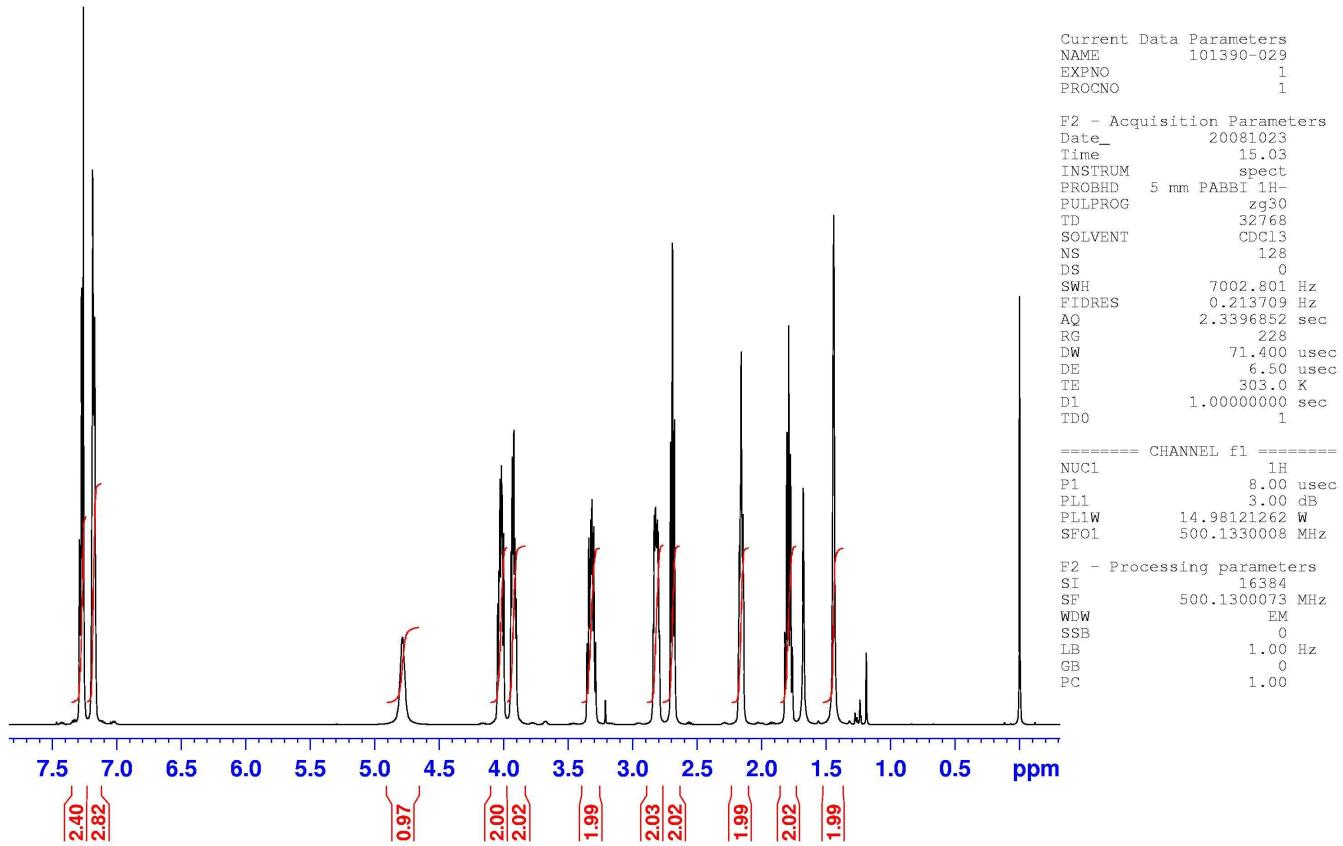
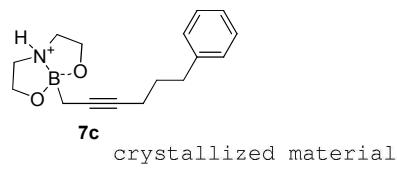
Current Data Parameters
NAME 101390-058
EXPNO 7
PROCNO 1

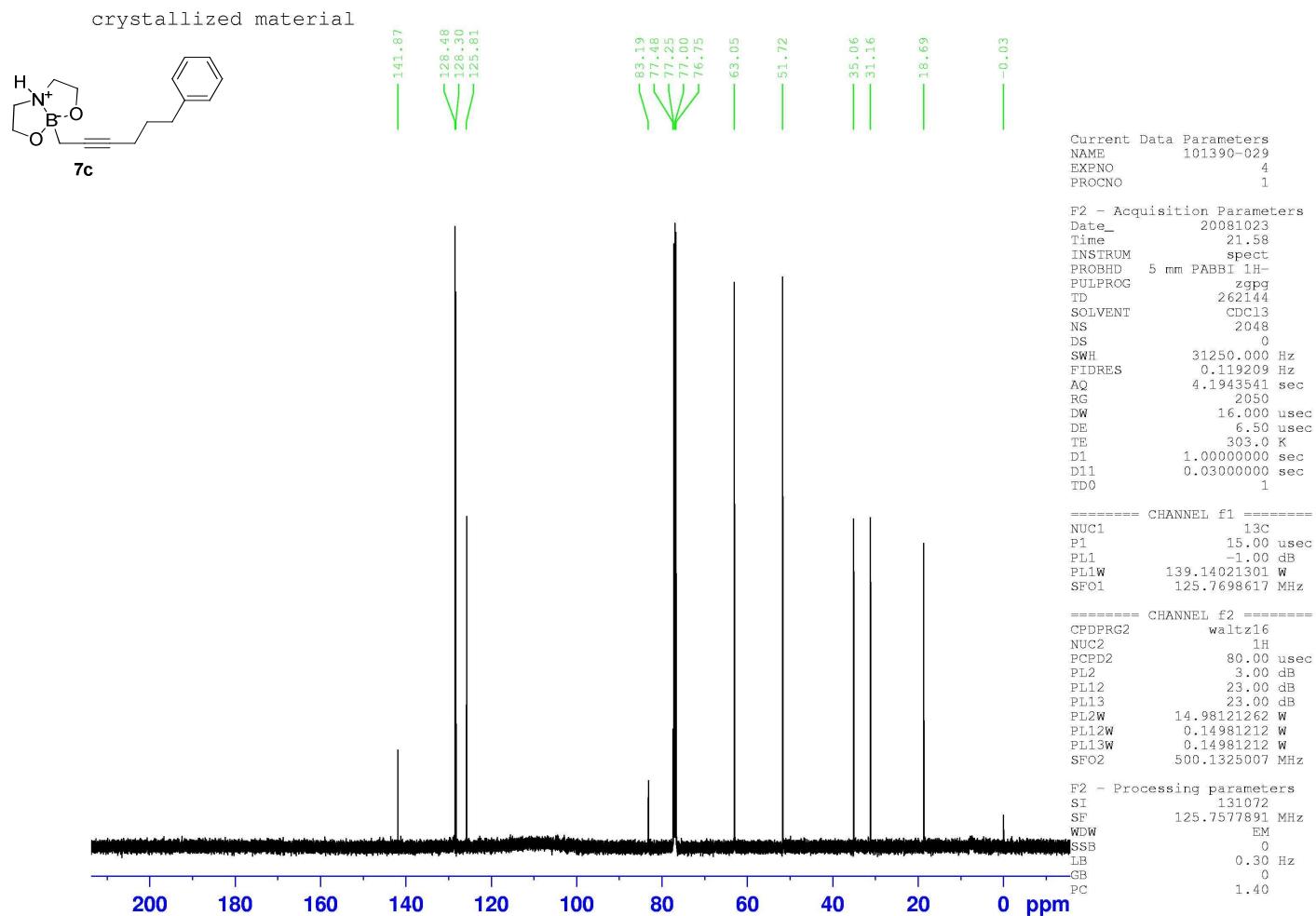
F2 - Acquisition Parameters
Date_ 20081111
Time 22.53
INSTRUM spect
PROBHD 5 mm PABBI 1H-
PULPROG zgpg
TD 262144
SOLVENT CDCl3
NS 1024
DS 0
SWH 31250.000 Hz
FIDRES 0.119209 Hz
AQ 4.1943541 sec
RG 2050
DW 16.000 usec
DE 6.50 usec
TE 303.0 K
D1 1.0000000 sec
D11 0.03000000 sec
TD0 1

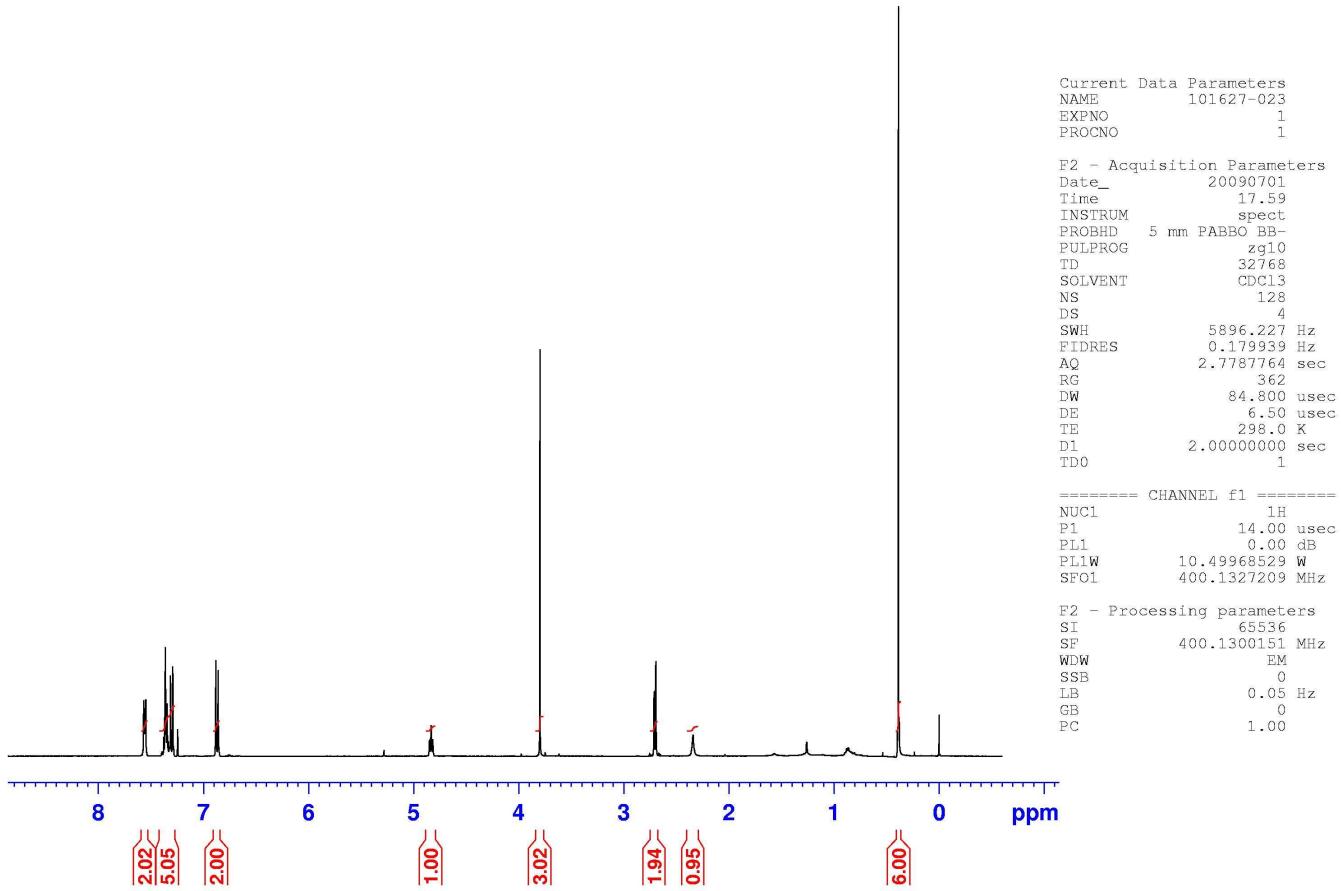
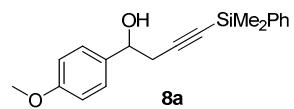
===== CHANNEL f1 =====
NUC1 13C
P1 15.00 usec
PL1 -1.00 dB
PL1W 139.14021301 W
SFO1 125.7698617 MHz

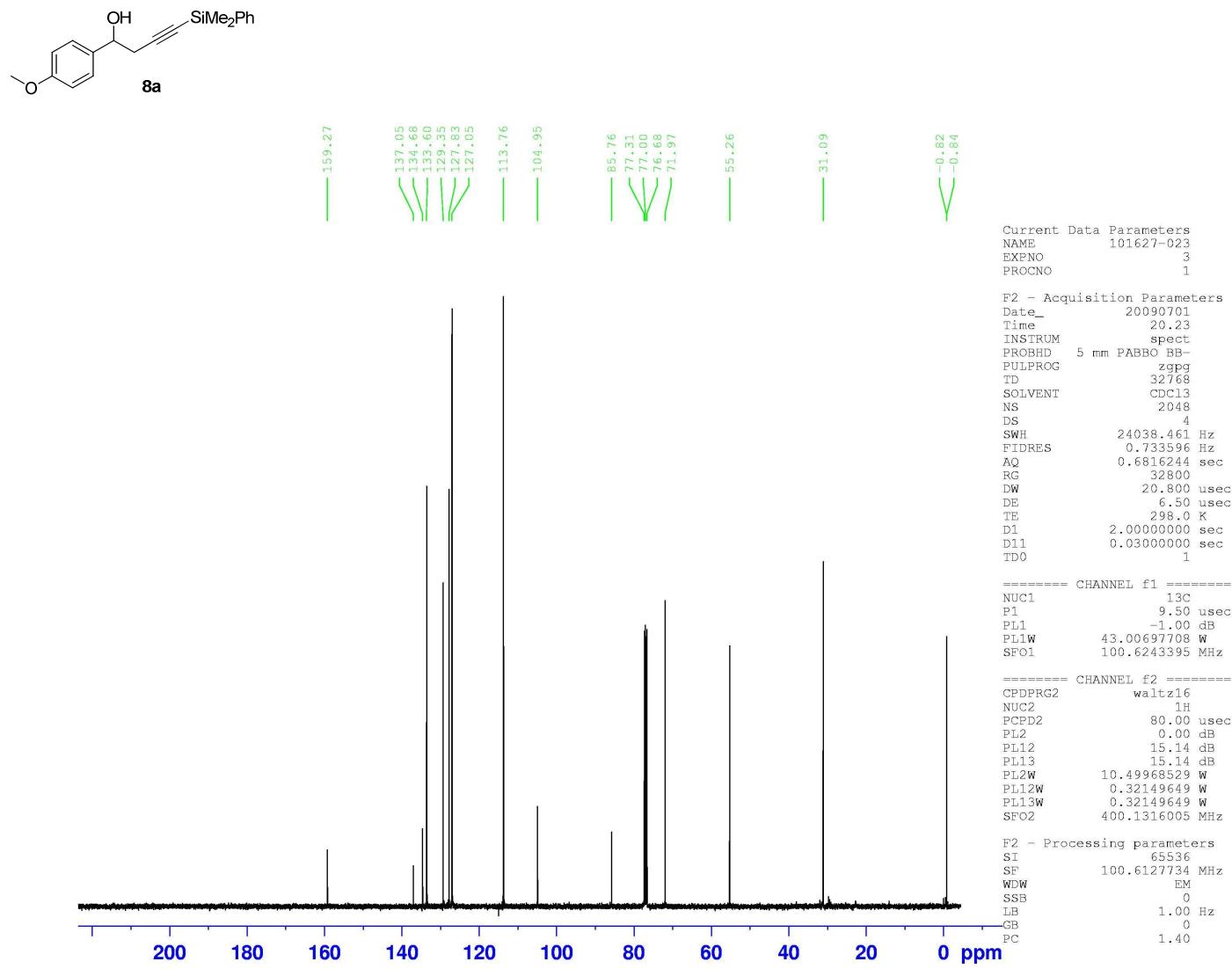
===== CHANNEL f2 =====
CPDPGR2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 3.00 dB
PL12 23.00 dB
PL13 23.00 dB
PL2W 14.98121262 W
PL12W 0.14981212 W
PL13W 0.14981212 W
SFO2 500.1325007 MHz

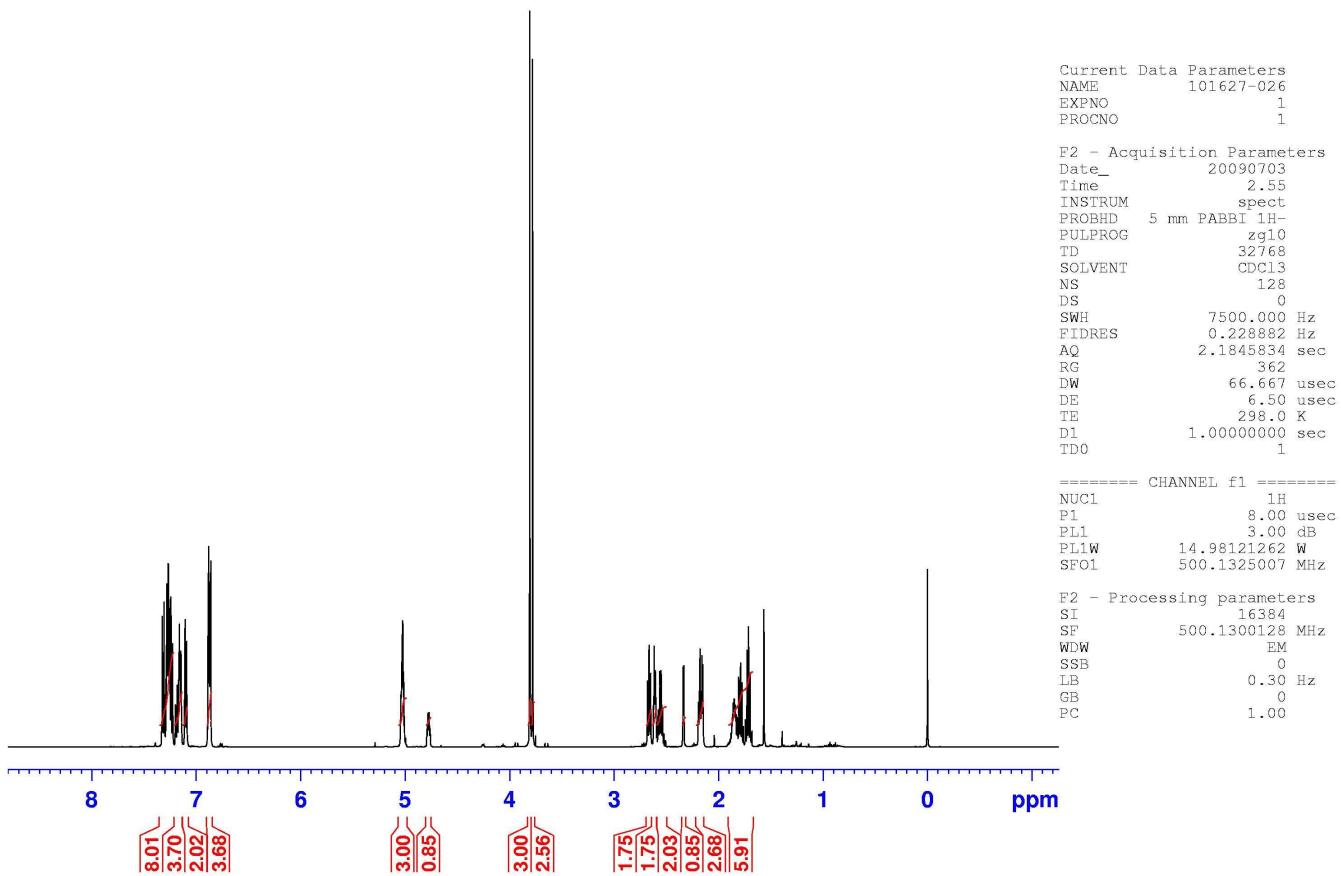
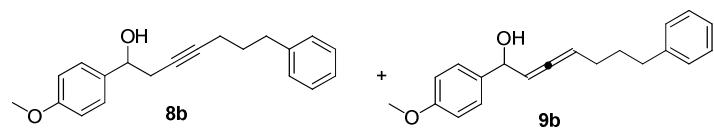
F2 - Processing parameters
SI 131072
SF 125.7577895 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

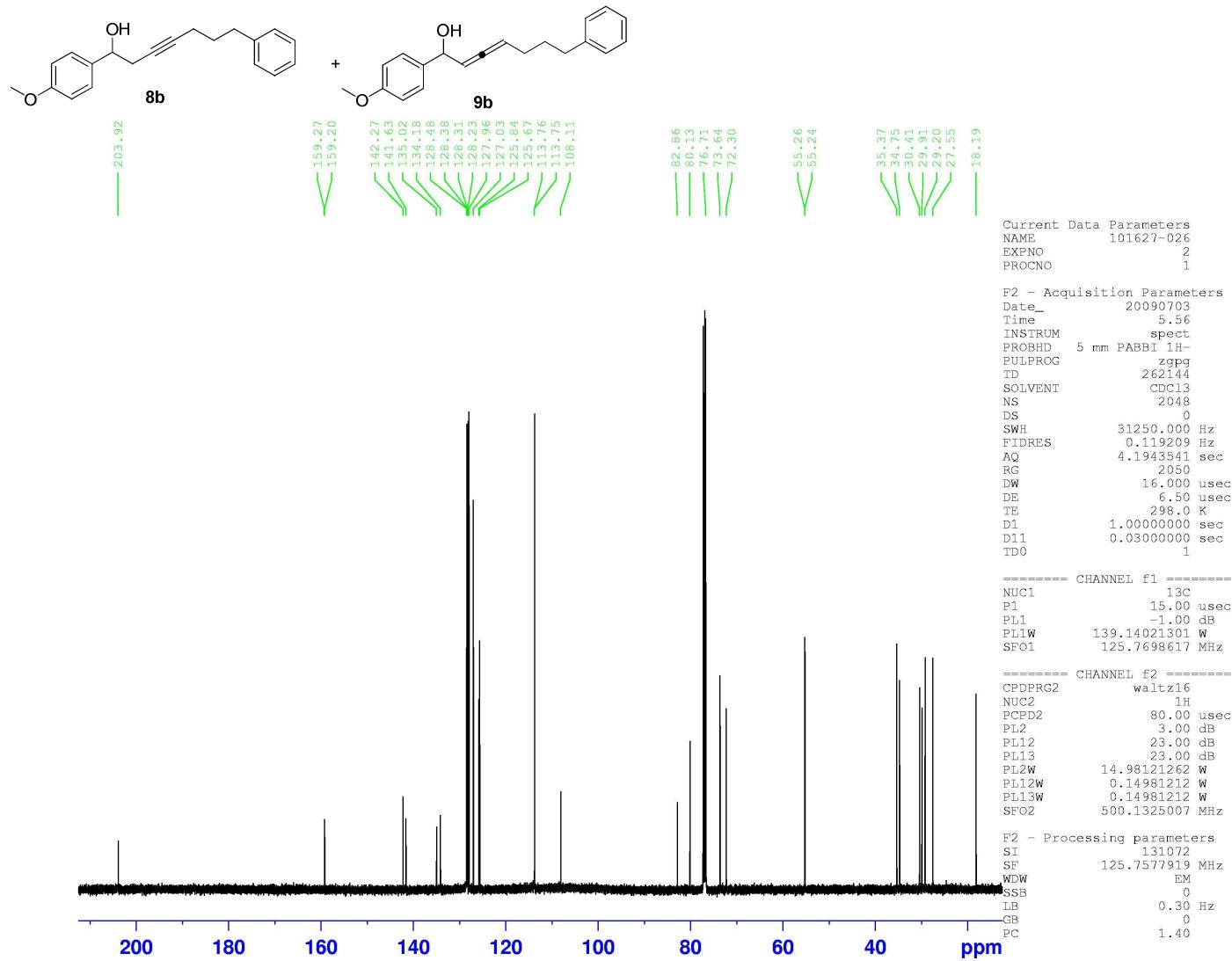


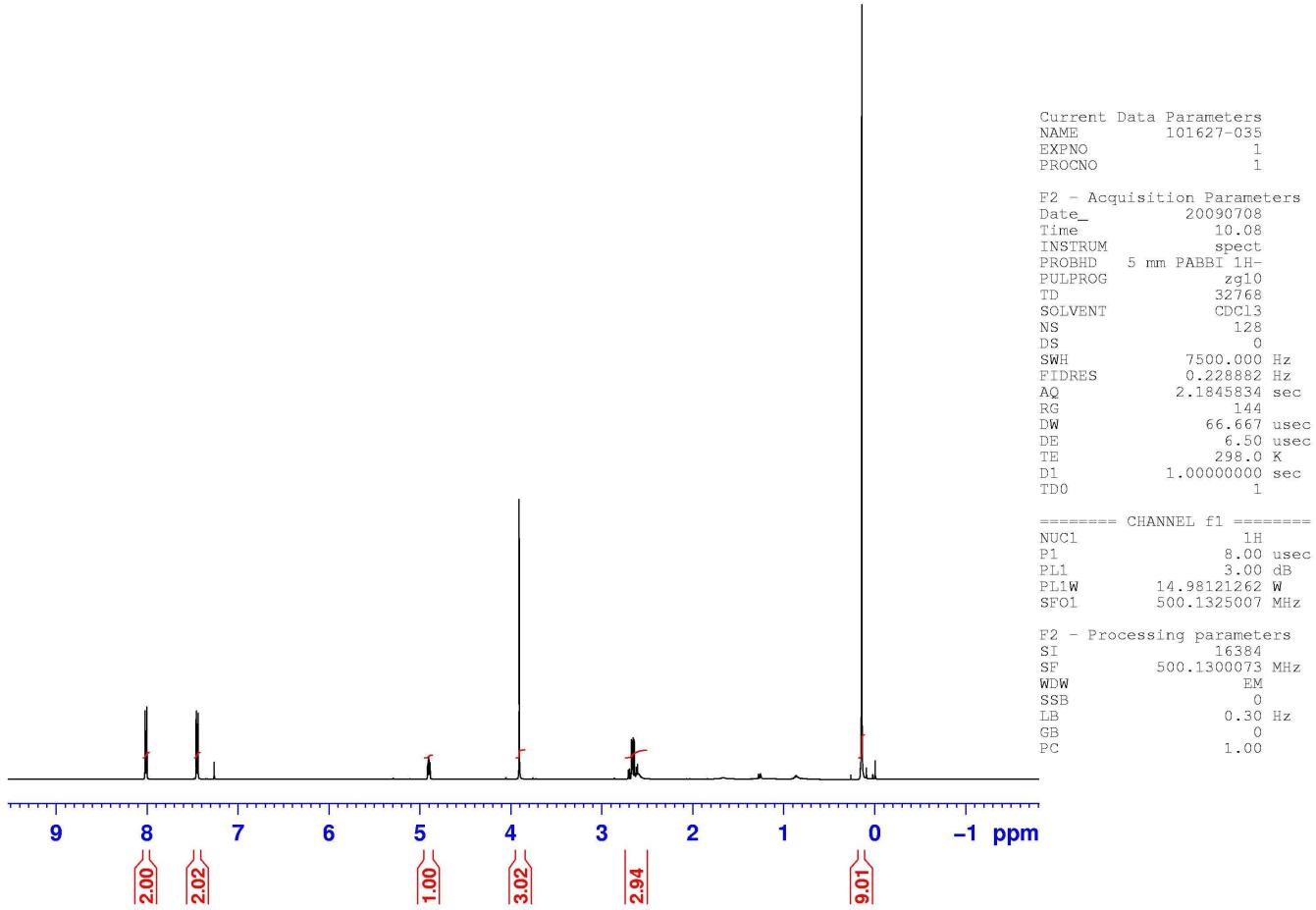
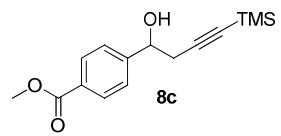


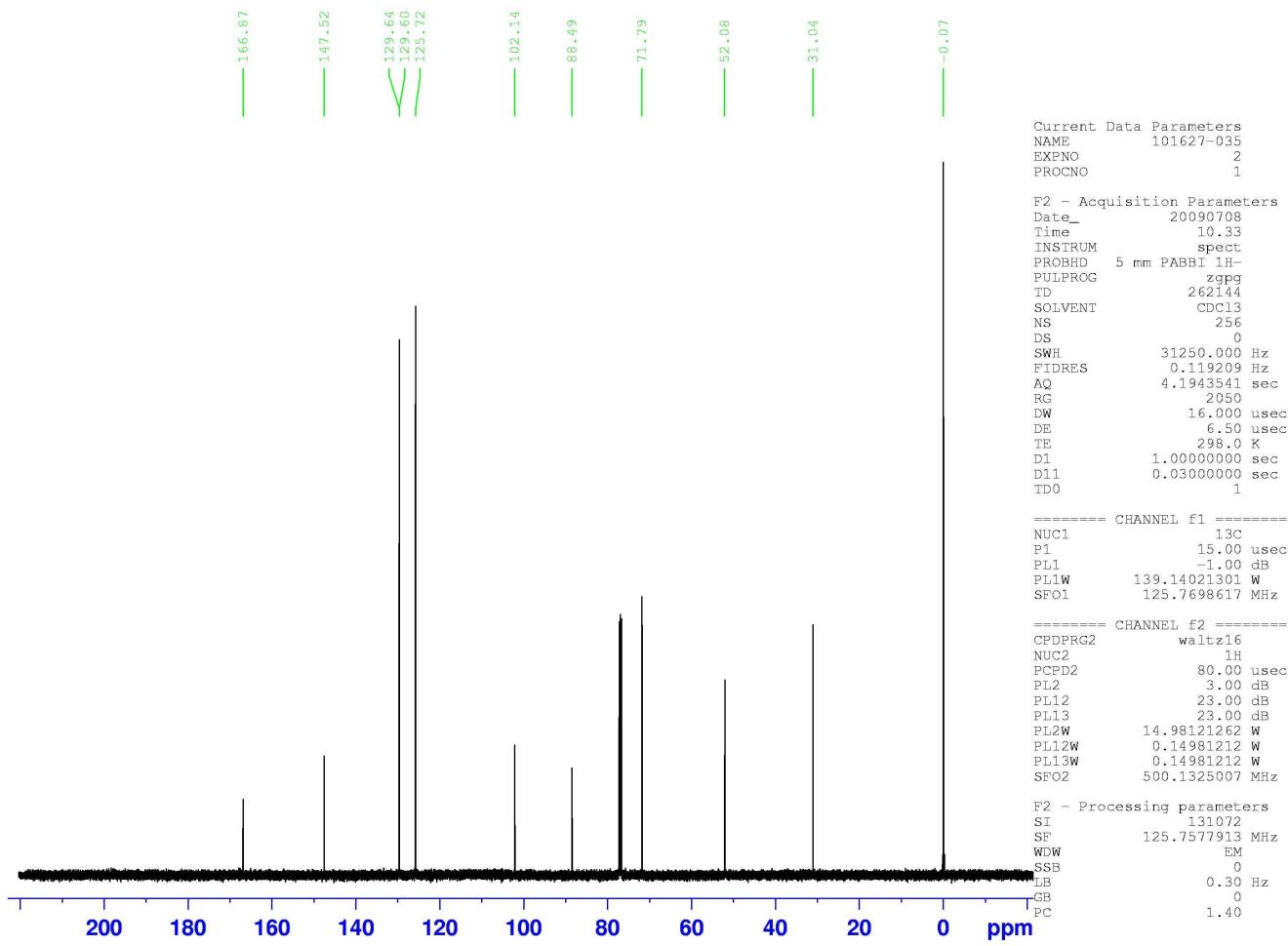
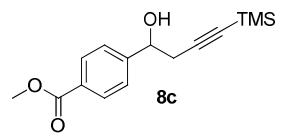














7.48
7.48
7.46
7.46
7.46
7.46
7.36
7.34
7.33
7.27
7.27
7.26
7.24

2.16
2.73
2.71
2.68
2.45

1.64

0.12

Current Data Parameters
NAME 101627-028
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090704
Time 15.57
INSTRUM spect
PROBHD 5 mm PABBI 1H-
PULPROG zg10
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 7500.000 Hz
FIDRES 0.228882 Hz
AQ 2.1845834 sec
RG 287
DW 66.667 usec
DE 6.50 usec
TE 298.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 ======
NUC1 1H
P1 8.00 usec
PL1 3.00 dB
PL1W 14.98121262 W
SFO1 500.1325007 MHz

F2 - Processing parameters
SI 16384
SF 500.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

