

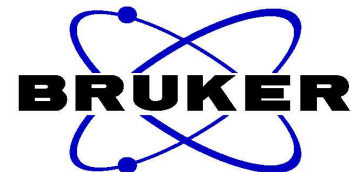
Supporting Information

An Improved Synthesis of BrettPhos and RockPhos-Type Biarylphosphine Ligands

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77 Massachusetts Avenue, Cambridge, MA 02139, USA.*

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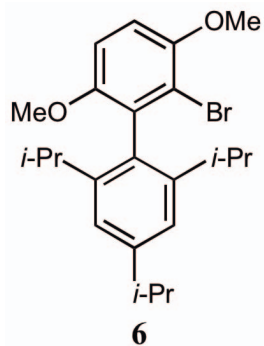


Current Data Parameters
NAME NH5-91-2-1st
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111223
Time 19.42
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 6502
DW 60.400 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

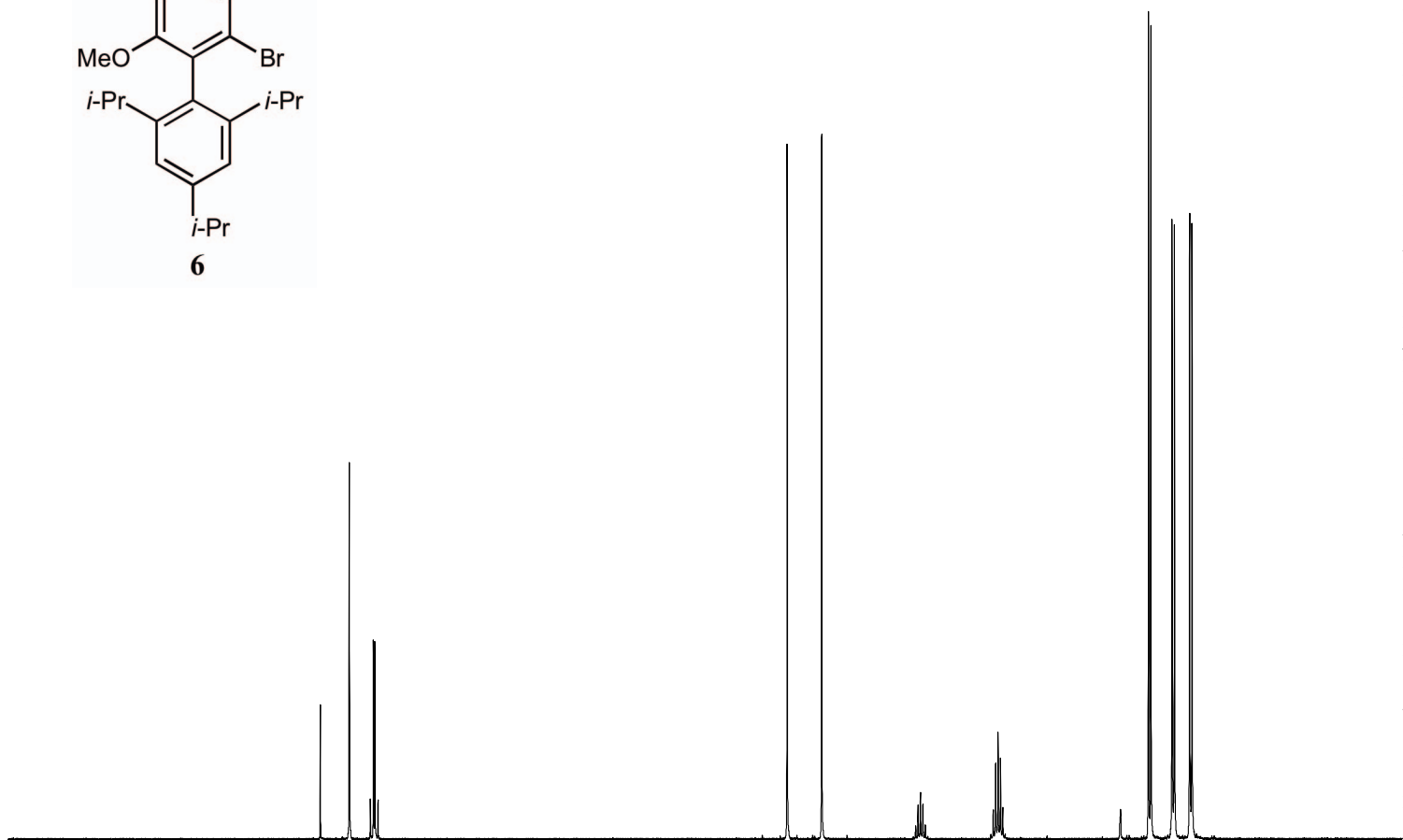
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300096 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



7.053
6.902
6.880
6.869
6.847

3.913
3.665
3.009
2.991
2.974
2.957
2.939
2.922
2.905
2.452
2.435
2.418
2.400
2.383
2.366
2.349
1.321
1.304
1.152
1.135
1.027
1.009



2.05
2.04

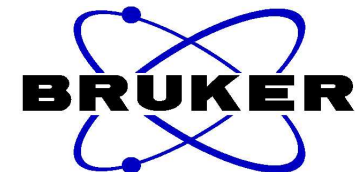
3.08
3.12

1.00

2.05

6.30
6.33
6.32

9 8 7 6 5 4 3 2 1 ppm



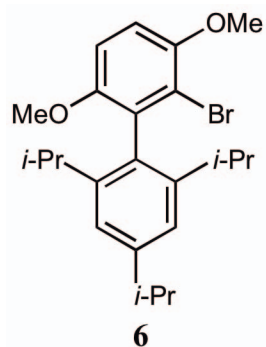
Current Data Parameters
 NAME NH5-68-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111203
 Time 14.31
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 2
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 5792.6
 DW 20.850 usec
 DE 6.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

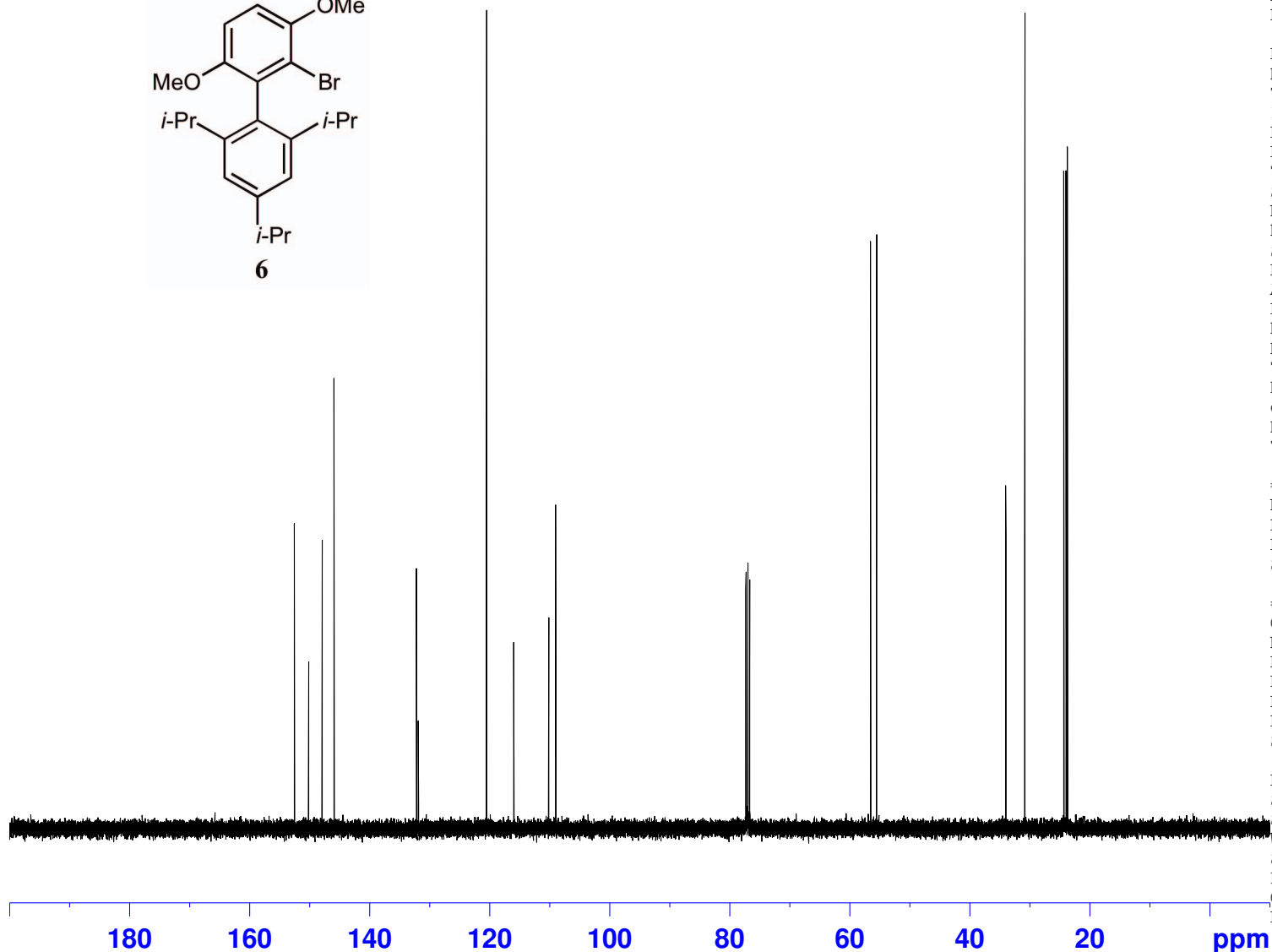
==== CHANNEL f1 =====
 NUC1 13C
 P1 8.75 usec
 PL1 -3.00 dB
 SFO1 100.6228298 MHz

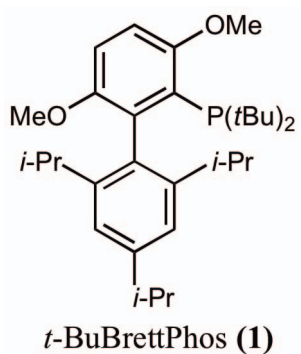
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 -1.00 dB
 PL12 14.52 dB
 PL13 18.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 100.6127769 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40



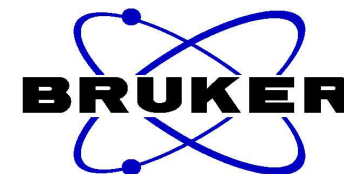
152.57
150.20
147.96
145.97
132.23
131.93
120.55
116.02
110.18
109.02
56.54
55.54
34.00
30.84
24.34
23.97
23.73





6.981
6.896
6.874
6.851
6.829

3.794
3.565
3.016
2.999
2.982
2.965
2.948
2.930
2.913
2.566
2.549
2.532
2.515
2.498
2.482
2.465
1.344
1.327
1.240
1.224
1.160
1.130
0.964
0.948

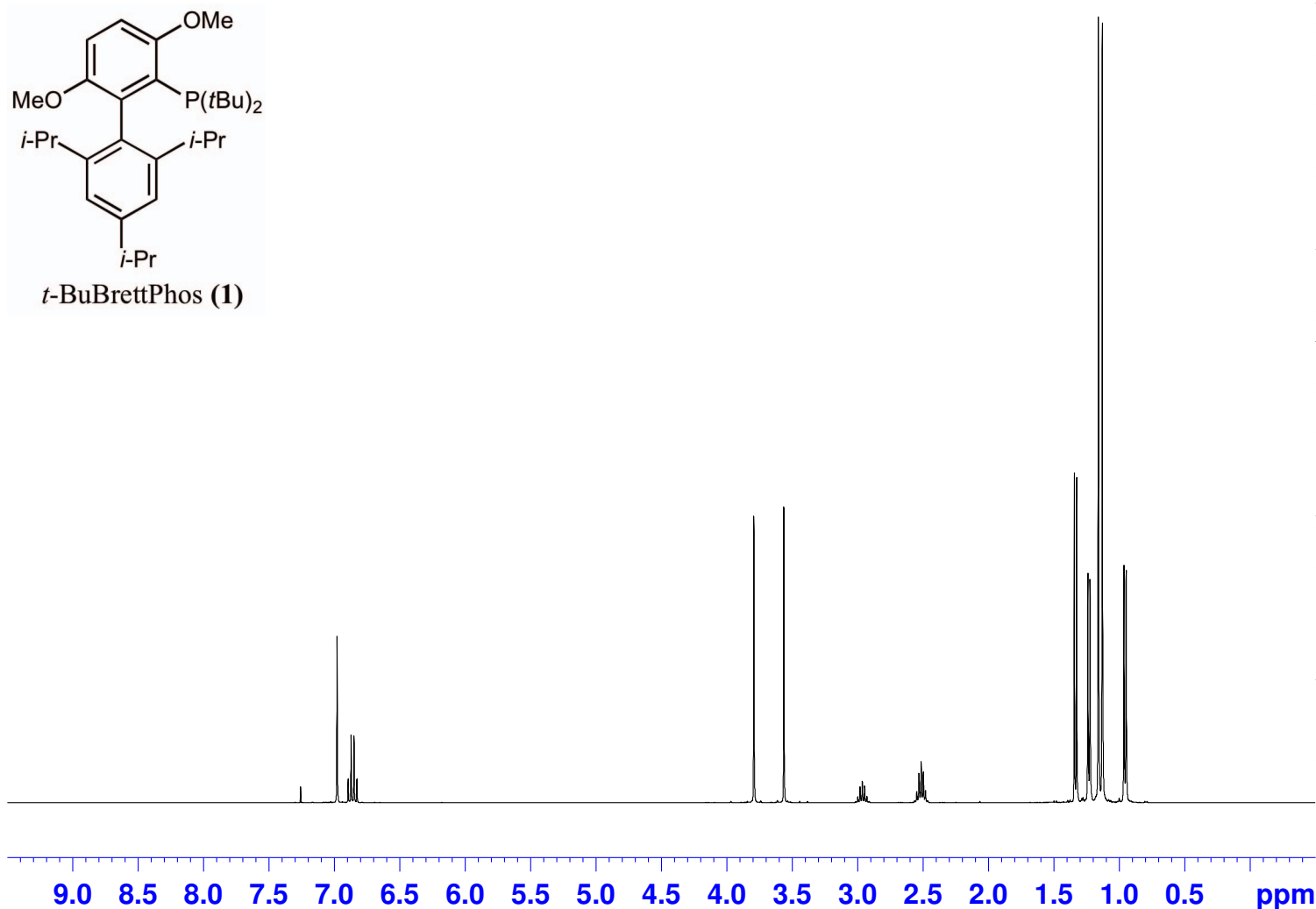


Current Data Parameters
NAME NH5-105-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120106
Time 19.29
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 912.3
DW 60.400 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300098 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



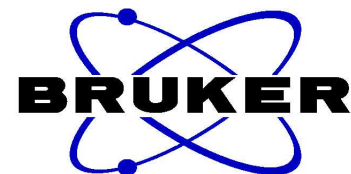
2.00
2.00

3.04
3.02

0.95
1.99

6.30
6.41
18.44
6.19

ppm



Current Data Parameters
 NAME NH5-105-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120106
 Time 19.45
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 1625.5
 DW 20.850 usec
 DE 6.00 usec
 TE 683.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

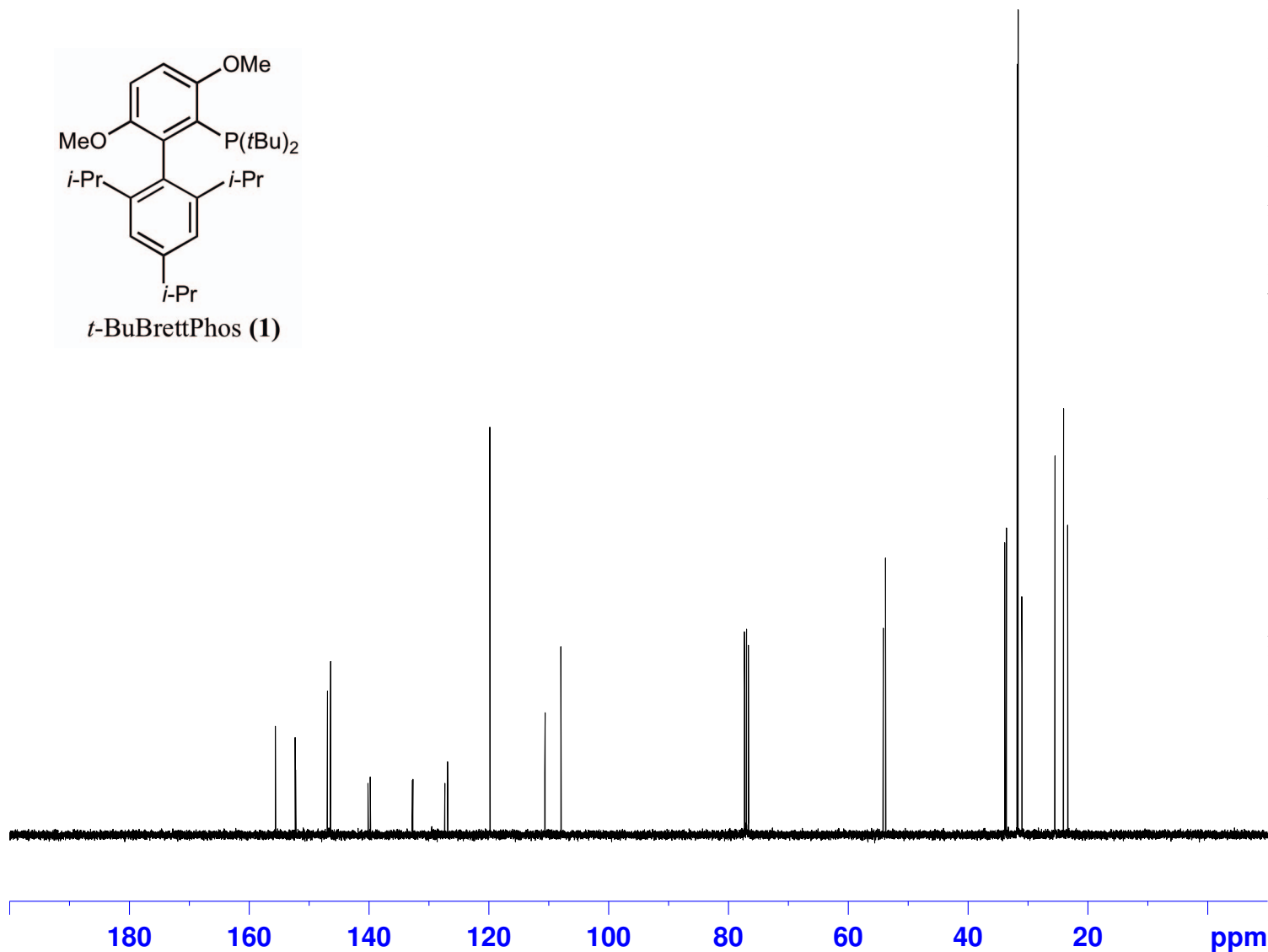
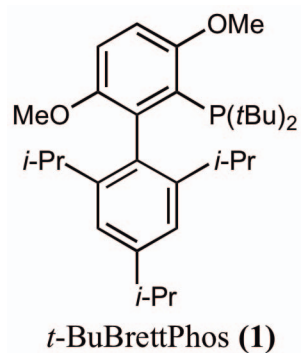
==== CHANNEL f1 =====
 NUC1 13C
 P1 9.38 usec
 PL1 0.00 dB
 SFO1 100.6228298 MHz

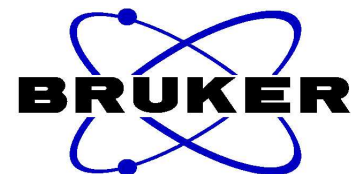
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 16.10 dB
 PL13 19.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127733 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

155.68
 155.66
 152.38
 152.27
 146.96
 146.46
 140.18
 139.80
 132.79
 132.72
 127.37
 126.91
 119.85
 110.66
 110.65
 108.00

54.17
 53.77
 33.91
 33.88
 33.62
 31.81
 31.64
 31.02
 30.99
 25.47
 24.08
 23.36





Current Data Parameters
NAME NH5-105-31P
EXPNO 1
PROCNO 1

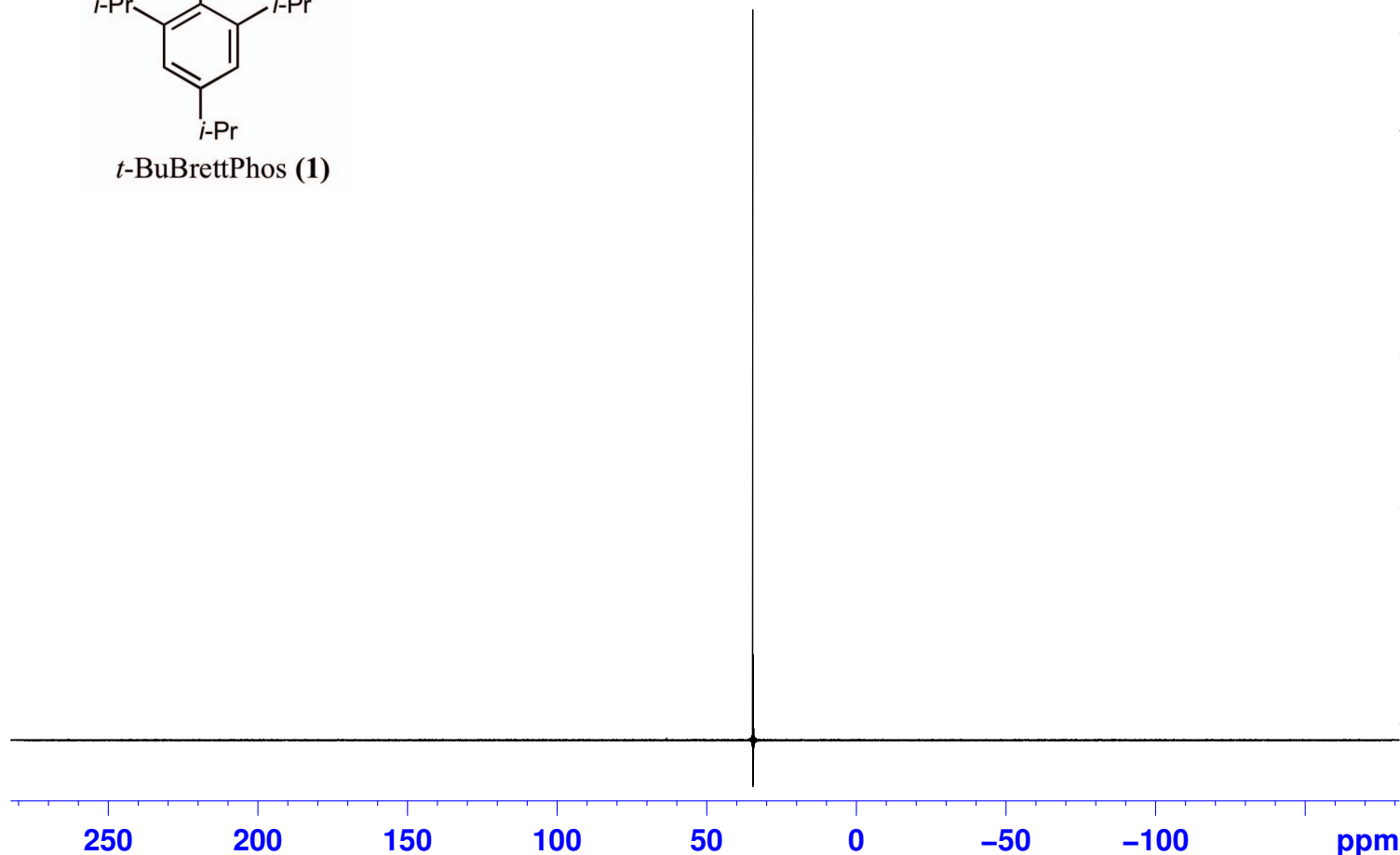
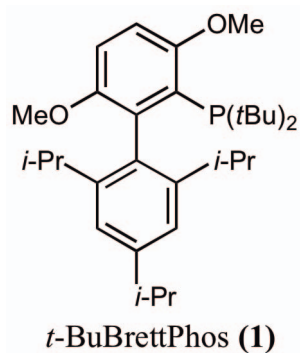
F2 - Acquisition Parameters
Date_ 20120106
Time 19.27
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8
DS 4
SWH 75187.969 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 4597.6
DW 6.650 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

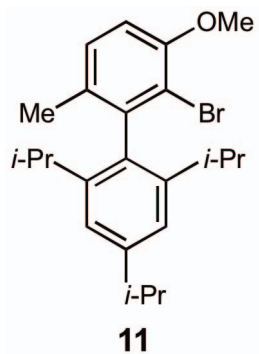
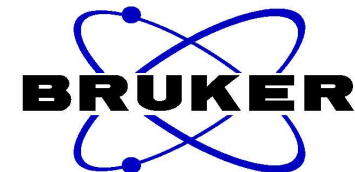
=====
CHANNEL f1
NUC1 31P
P1 9.25 usec
PL1 3.00 dB
SFO1 161.9836918 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
SI 65536
SF 161.9755024 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

34.56





7.196
7.175
7.081
6.847
6.826

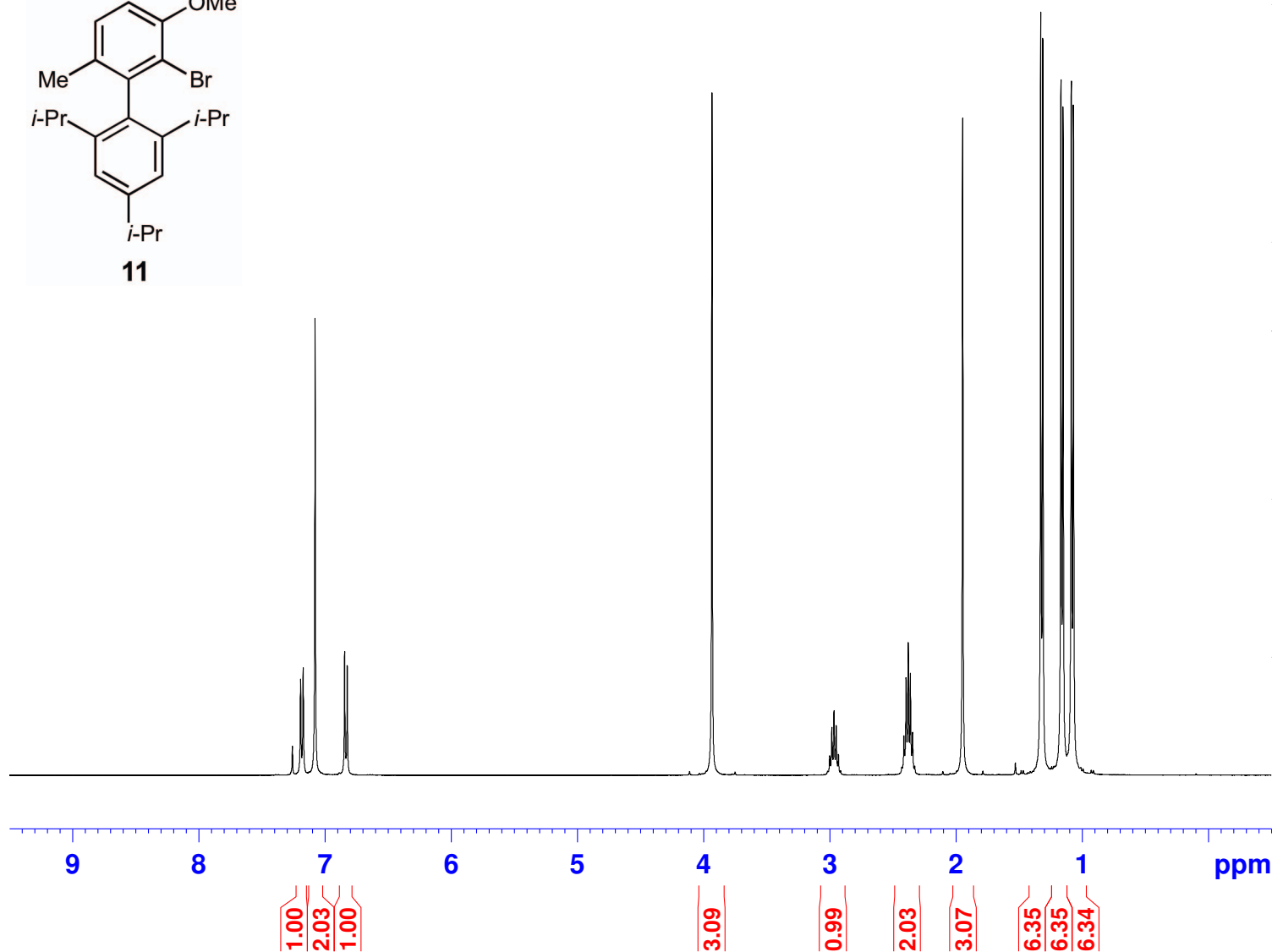
3.935
3.020
3.002
2.985
2.967
2.950
2.933
2.916
2.430
2.413
2.396
2.379
2.362
2.345
2.328
1.948
1.330
1.313
1.169
1.152
1.087
1.070

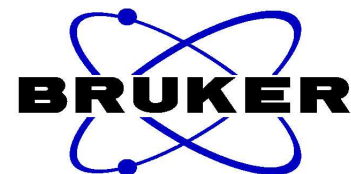
Current Data Parameters
 NAME NH5-79-1st-cry-H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20111203
 Time 14.35
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 8
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 35.9
 DW 60.400 usec
 DE 6.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 15.07 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300092 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00





Current Data Parameters
NAME NH5-79-1st-cry-13C
EXPNO 1
PROCNO 1

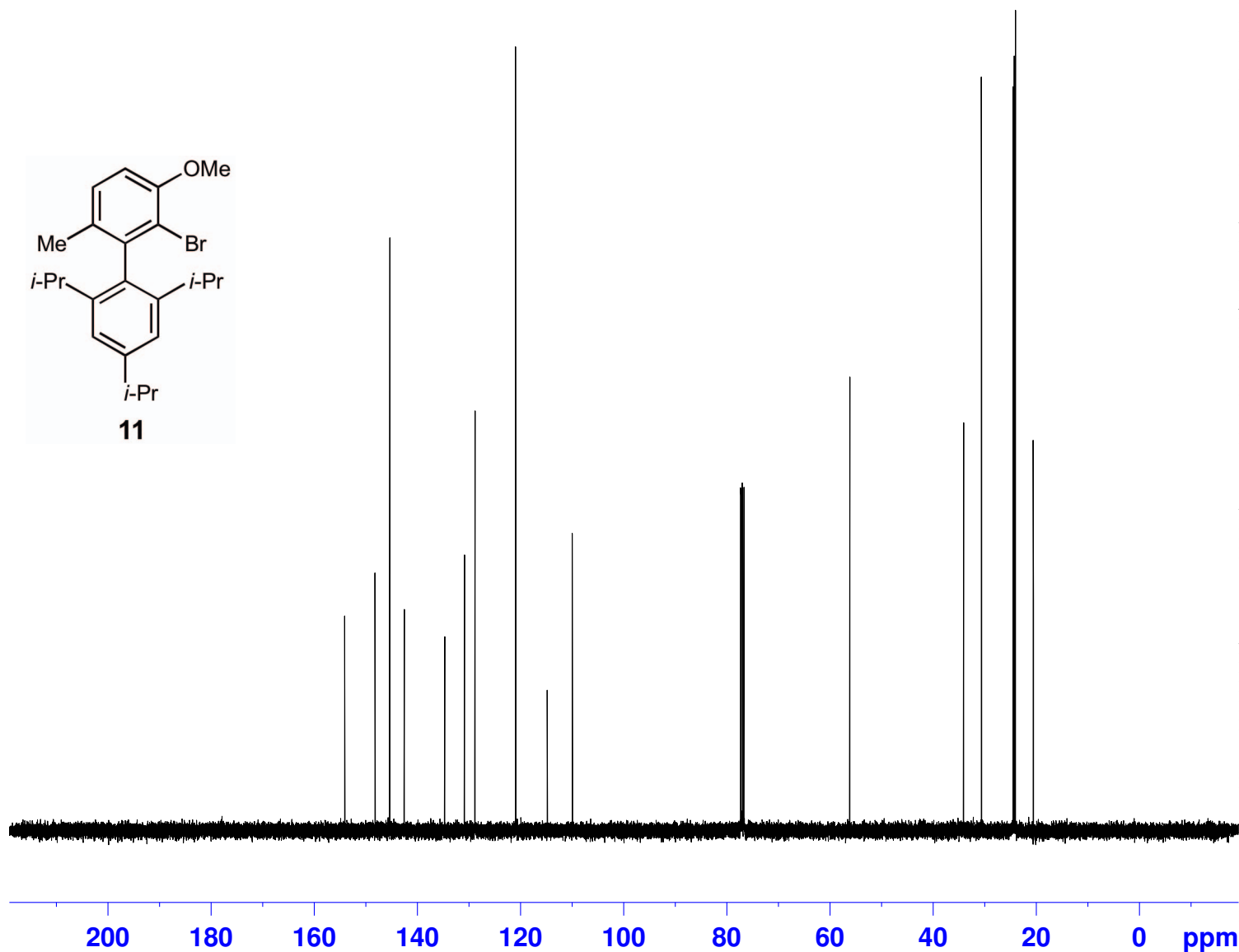
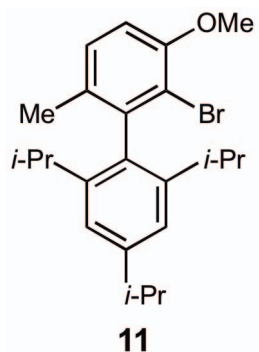
F2 - Acquisition Parameters
Date_ 20111203
Time 14.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 18390.4
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

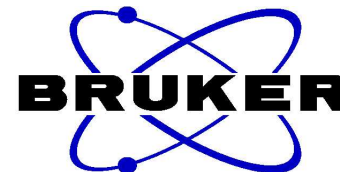
==== CHANNEL f1 =====
NUC1 13C
P1 8.75 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.00 dB
PL12 14.52 dB
PL13 18.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 100.6127742 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

154.11
148.24
145.39
142.59
134.70
130.88
128.87
120.96
114.86
109.97
56.17
34.08
30.62
24.51
24.27
24.05
20.56





Current Data Parameters
NAME NH5-90-1H
EXPNO 1
PROCNO 1

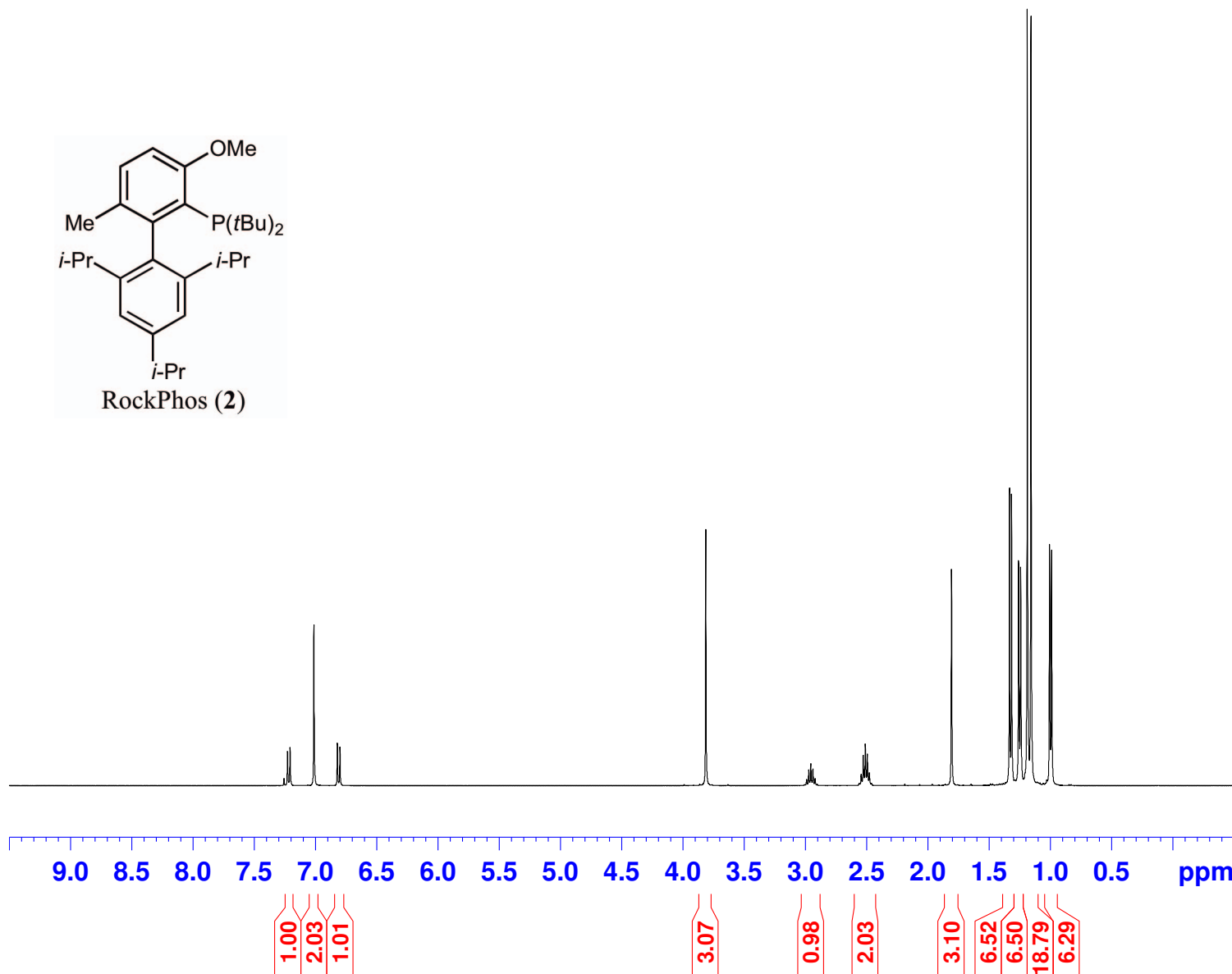
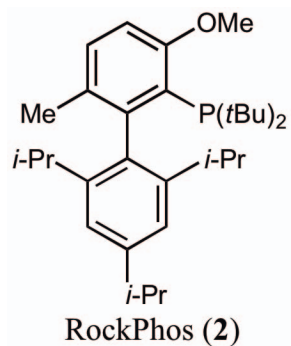
F2 - Acquisition Parameters
Date_ 20120106
Time 20.13
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 724.1
DW 60.400 usec
DE 6.00 usec
TE 683.2 K
D1 1.00000000 sec
TD0 1

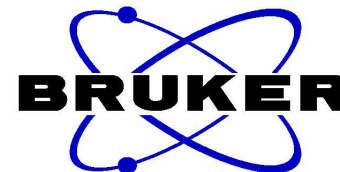
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 65536
SF 400.1300104 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

7.231
7.210
7.015
6.823
6.802

3.814
3.008
2.991
2.974
2.956
2.939
2.922
2.904
2.562
2.545
2.529
2.512
2.495
2.478
2.462
1.808
1.334
1.317
1.259
1.243
1.189
1.159
1.007
0.990





Current Data Parameters
 NAME NH5-90-13C
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120106
 Time 20.29
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 23980.814 Hz
 FIDRES 0.365918 Hz
 AQ 1.3664756 sec
 RG 3649.1
 DW 20.850 usec
 DE 6.00 usec
 TE 683.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

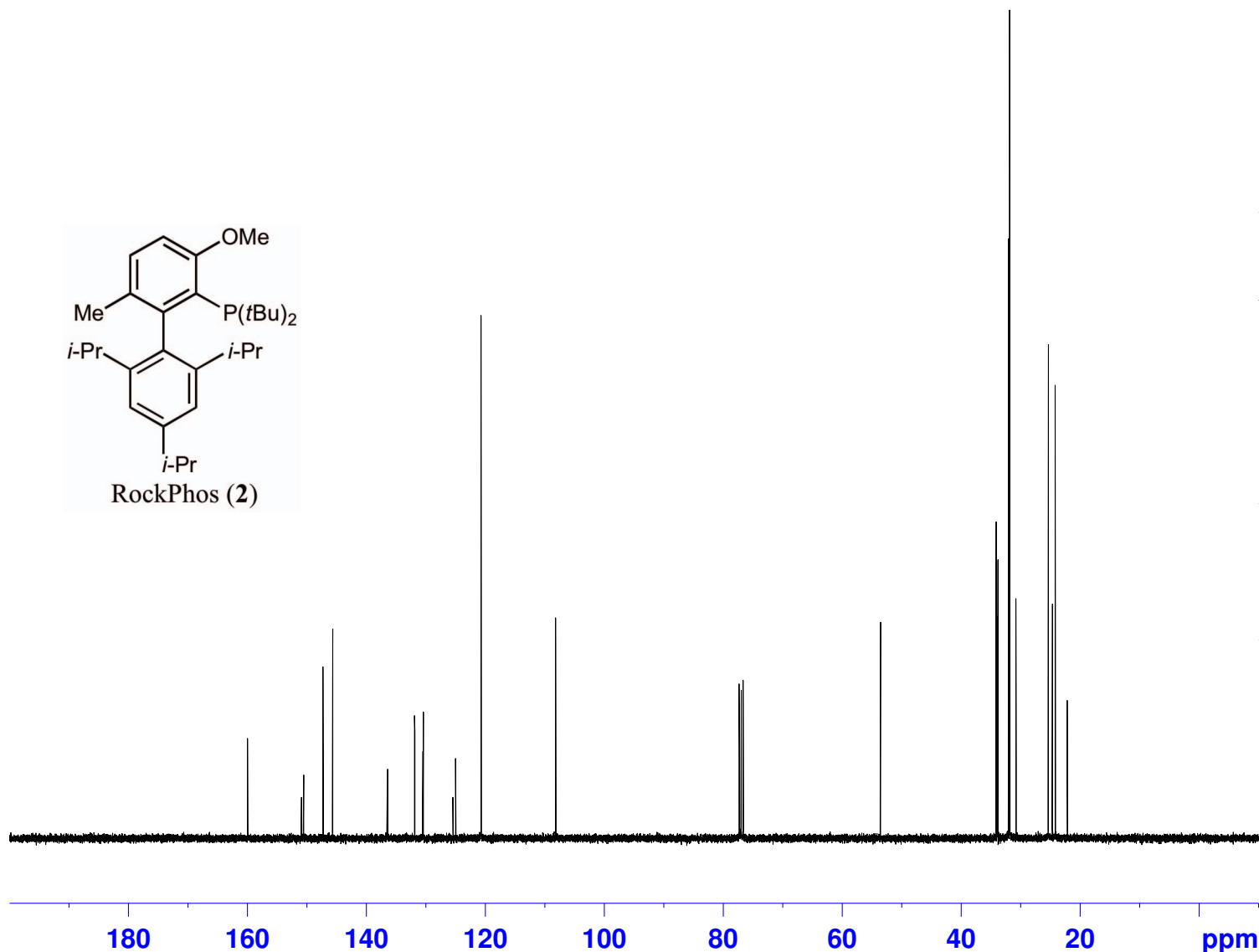
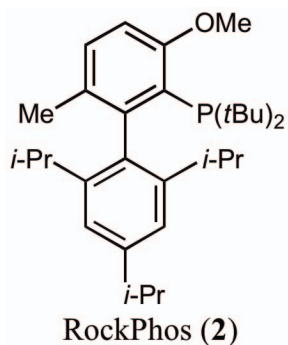
==== CHANNEL f1 =====
 NUC1 13C
 P1 9.38 usec
 PL1 0.00 dB
 SFO1 100.6228298 MHz

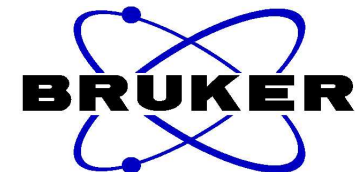
==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 0.00 dB
 PL12 16.10 dB
 PL13 19.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127724 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.40

160.05
 160.03
 150.97
 150.59
 147.33
 145.72
 145.71
 136.55
 136.48
 131.91
 131.90
 130.54
 130.46
 125.46
 125.01
 120.74
 108.19

53.58
 34.13
 33.99
 33.84
 32.01
 31.85
 30.79
 30.77
 25.35
 24.66
 24.64
 24.17
 22.17
 22.15





Current Data Parameters
NAME NH5-90-31P
EXPNO 1
PROCNO 1

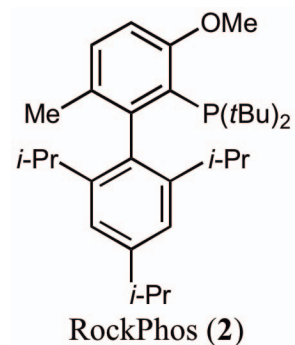
F2 - Acquisition Parameters
Date_ 20120106
Time 20.11
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 4
SWH 75187.969 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 3251
DW 6.650 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

=====
CHANNEL f1
NUC1 31P
P1 9.25 usec
PL1 3.00 dB
SFO1 161.9836918 MHz

=====
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316000 MHz

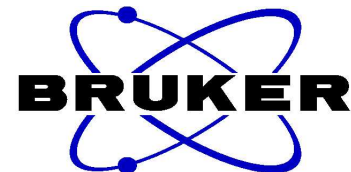
F2 - Processing parameters
SI 65536
SF 161.9755024 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

35.71



250 200 150 100 50 0 -50 -100 ppm

6.983
6.873
6.851
6.810
6.788
3.832
3.569
2.990
2.973
2.956
2.939
2.921
2.498
2.482
2.465
2.448
2.431
2.414
2.398
2.254
2.246
2.238
2.231
2.224
2.216
2.208
2.201
2.193
2.186
2.178
1.847
1.818
1.728
1.696
1.657
1.638
1.431
1.398
1.339
1.321
1.303
1.299
1.291
1.260
1.229
1.212
1.181
1.171
1.163
1.149
1.141
1.133
1.118
1.111
0.989
0.980
0.958
0.941

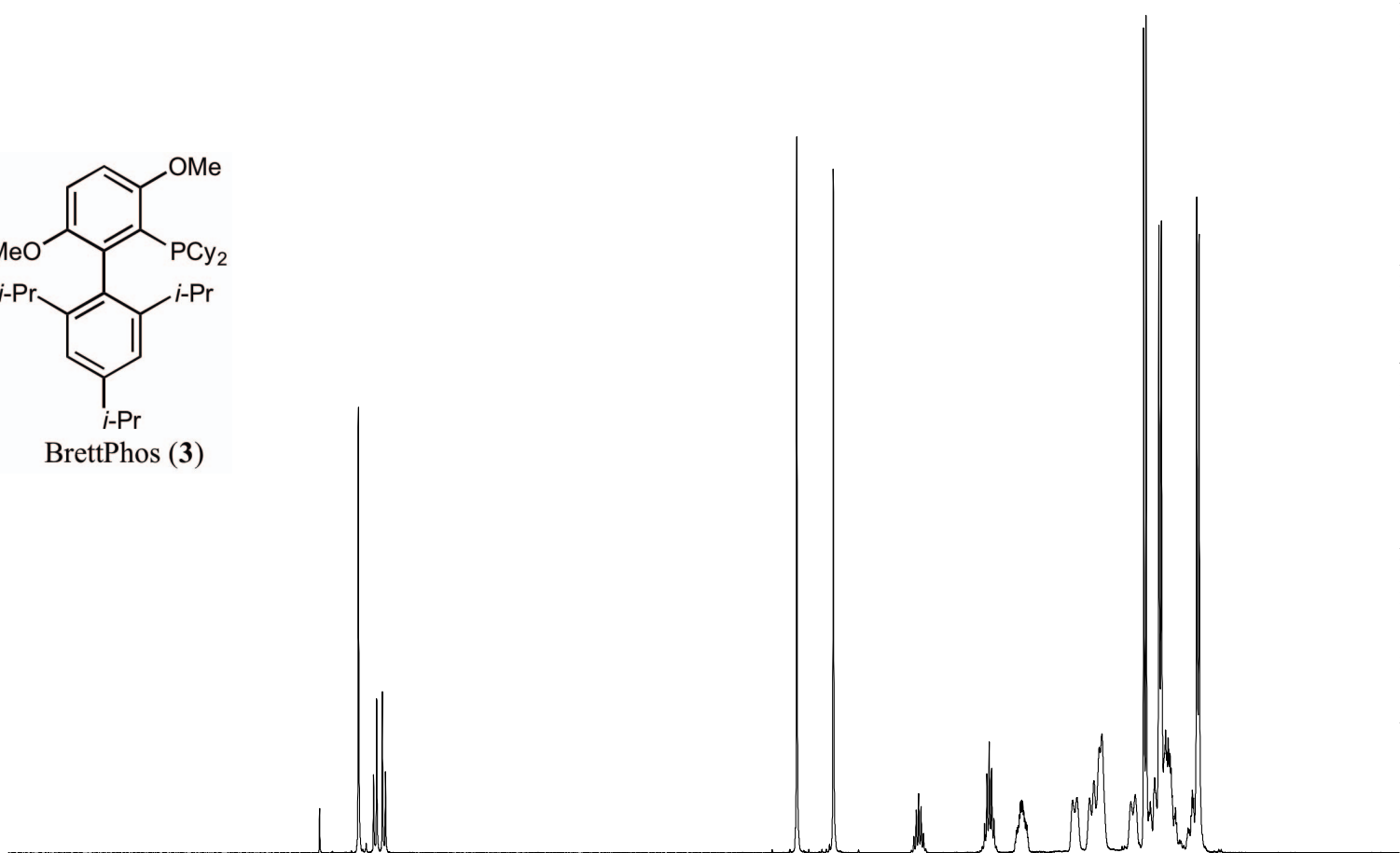
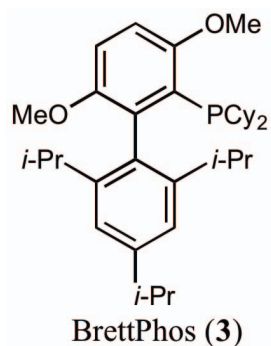


Current Data Parameters
 NAME NH5-104-1H
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120106
 Time 19.51
 INSTRUM spect
 PROBHD 5 mm QNP 1H/13
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8278.146 Hz
 FIDRES 0.126314 Hz
 AQ 3.9584243 sec
 RG 1149.4
 DW 60.400 usec
 DE 6.00 usec
 TE 683.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 0.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 65536
 SF 400.1300097 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



9 8 7 6 5 4 3 2 1 ppm

2.00
2.03

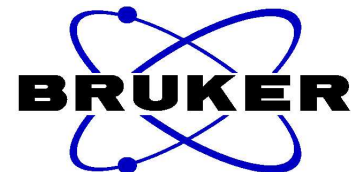
3.09
3.11

0.97

2.04
2.04

2.12
6.31

2.23
21.22
8.42



Current Data Parameters
NAME NH5-104-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120106
Time 20.07
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1625.5
DW 20.850 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

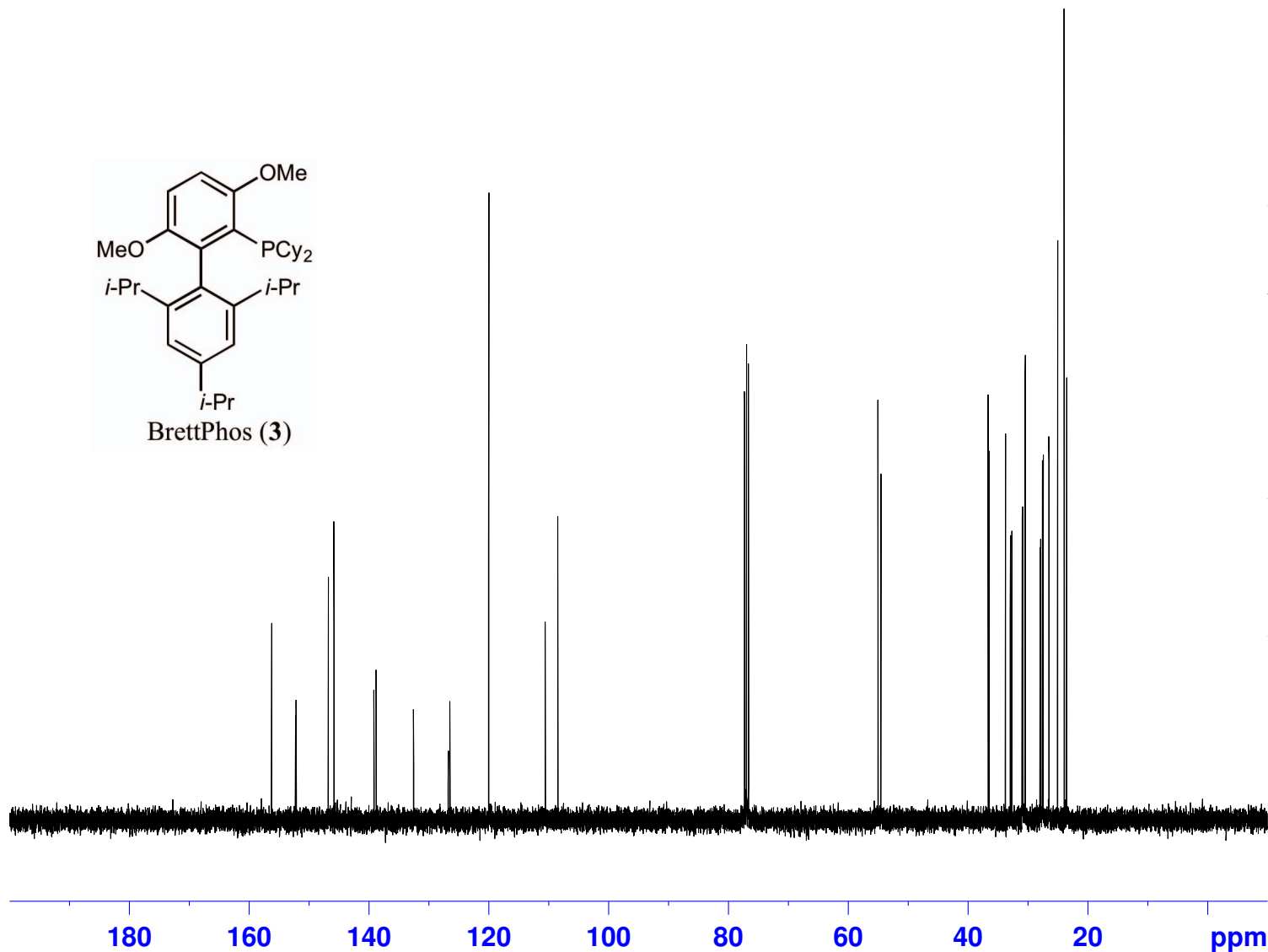
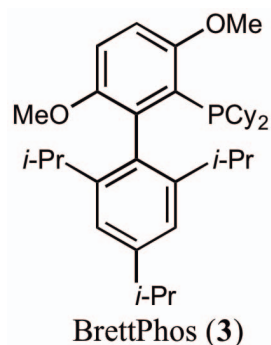
==== CHANNEL f1 =====
NUC1 13C
P1 9.38 usec
PL1 0.00 dB
SFO1 100.6228298 MHz

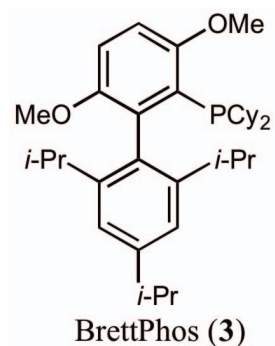
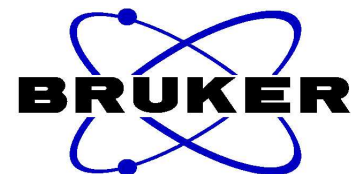
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

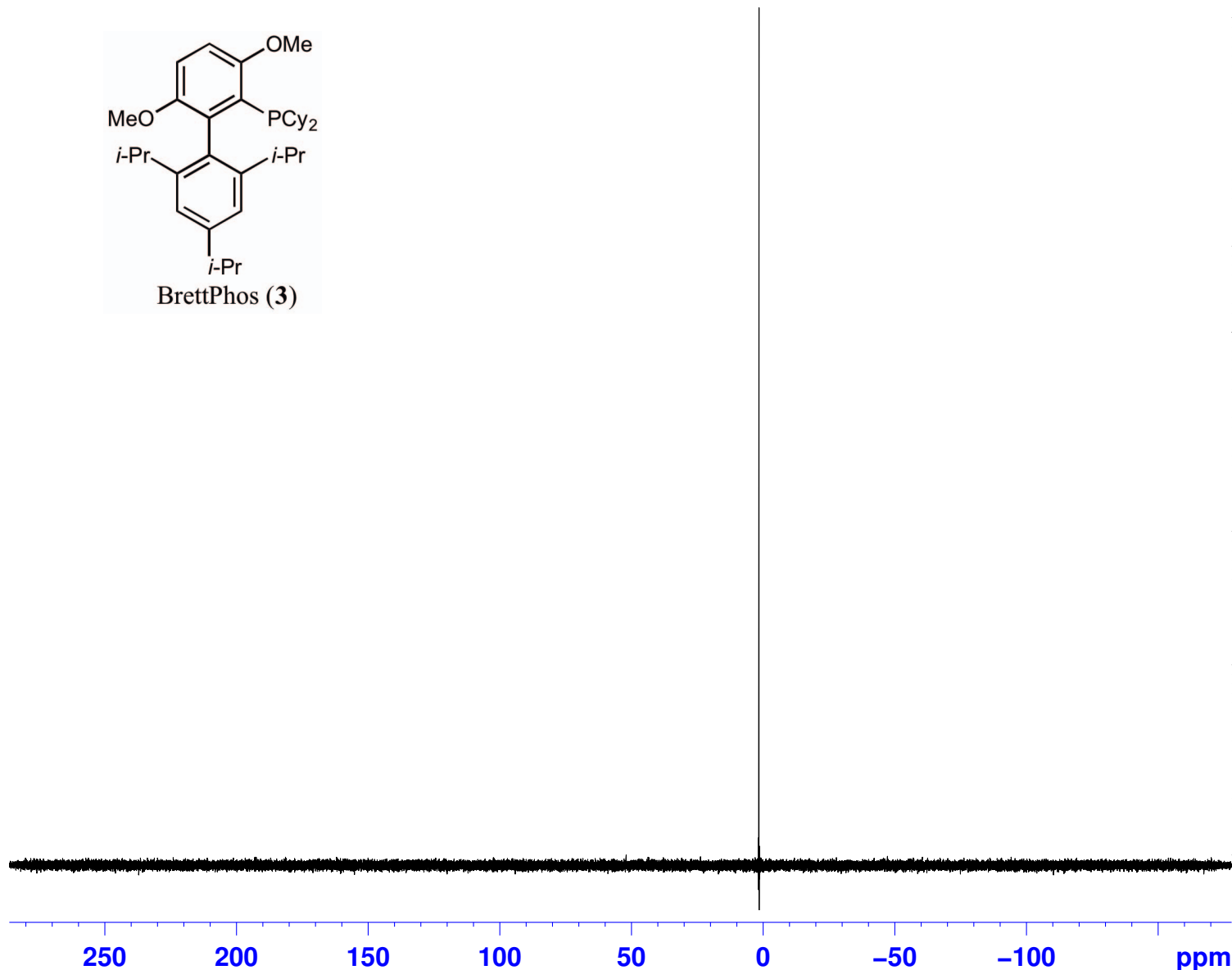
156.29
156.27
152.29
152.18
146.82
145.88
145.86
139.19
138.83
132.64
132.56
126.79
126.51
120.04
110.60
108.51

55.05
54.53
36.63
36.49
33.76
32.94
32.71
30.96
30.85
30.47
27.97
27.88
27.59
27.45
26.49
26.48
25.05
23.95
23.52





1.61



Current Data Parameters
NAME NH5-104-1st-cry-31P
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120102
Time 14.55
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8
DS 4
SWH 75187.969 Hz
FIDRES 1.147277 Hz
AQ 0.4358644 sec
RG 11585.2
DW 6.650 usec
DE 6.00 usec
TE 683.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

==== CHANNEL f1 =====
NUC1 31P
P1 9.25 usec
PL1 3.00 dB
SFO1 161.9836918 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.10 dB
PL13 19.00 dB
SFO2 400.1316000 MHz

F2 - Processing parameters
SI 65536
SF 161.9749159 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40