

Supporting Information

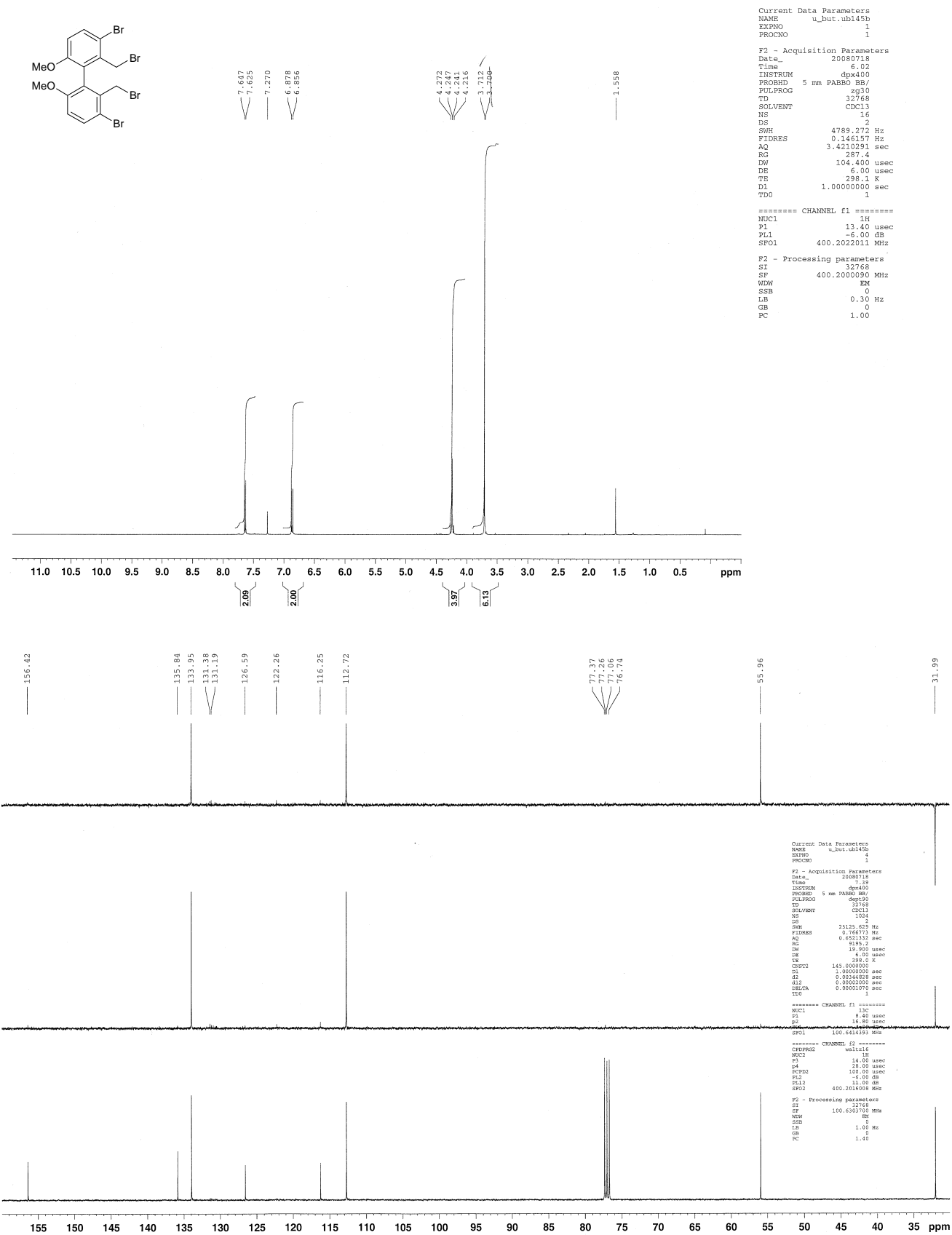
Synthesis and evaluation of *atropos* dihydro-5*H*-dibenzazepinium halide PTCs derived from α -methylbenzylamine

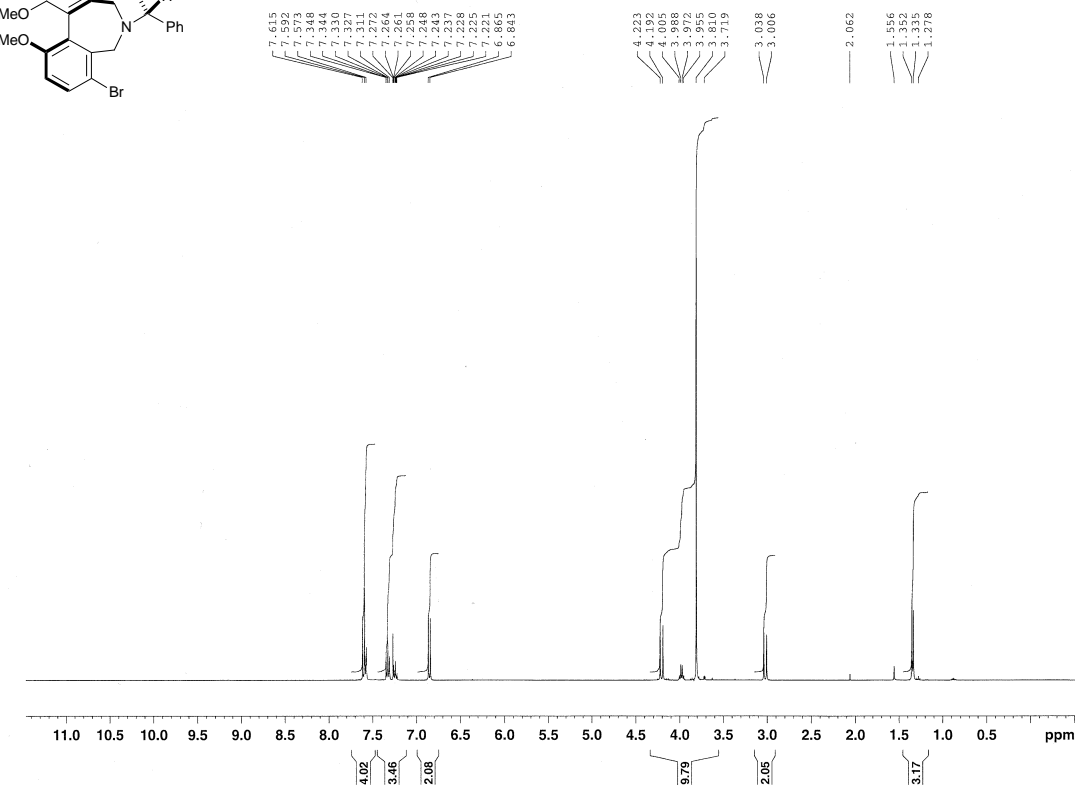
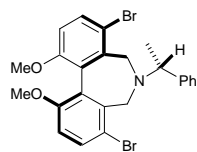
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Table of Contents

¹ H NMR and ¹³ C NMR Spectra	S2-S17
HPLC data	S18



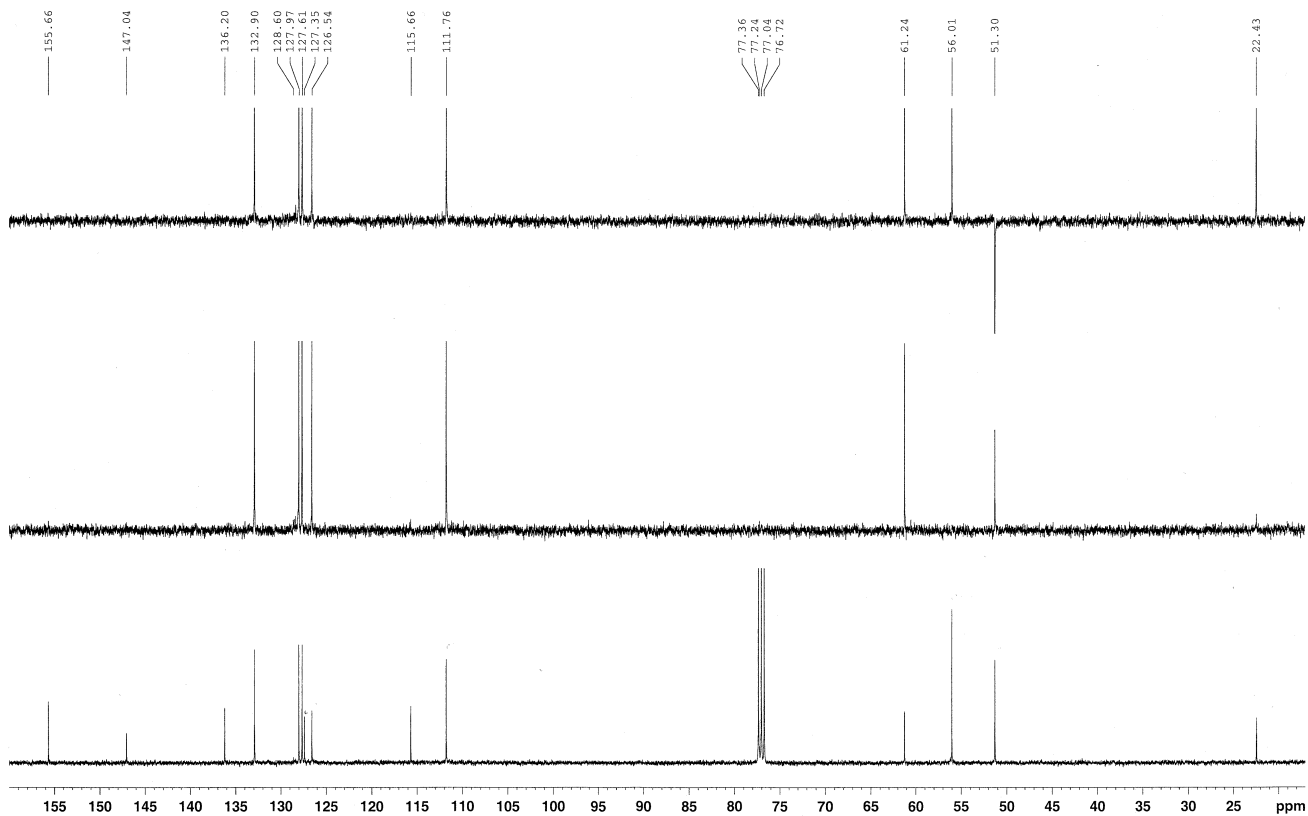


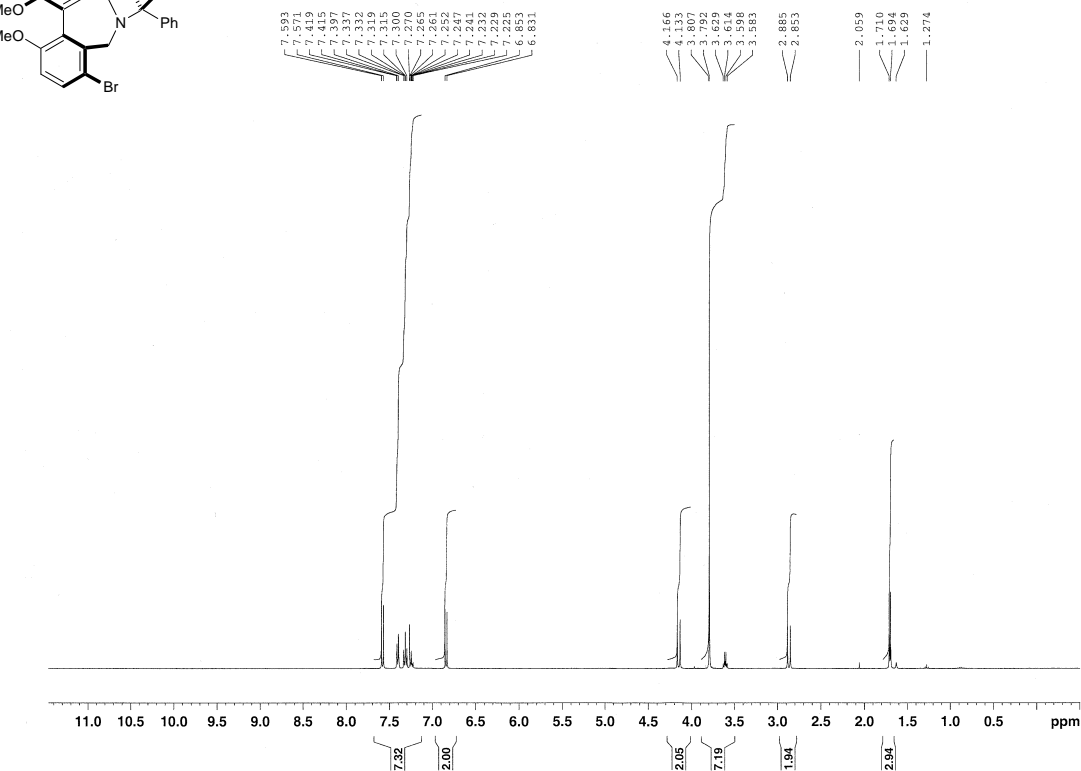
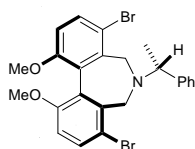
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NAME u_but.ub186c11
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090109
Time 10.09
INSTRUM dpx400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 15
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 456.1
DW 104.400 usec
DE 6.00 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1

***** CHANNEL f1 *****
NUC1 1H
P1 13.40 usec
PL1 -6.00 dB
SFO1 400.2022011 MHz

F2 - Processing parameters
SI 32768
SF 400.2000085 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





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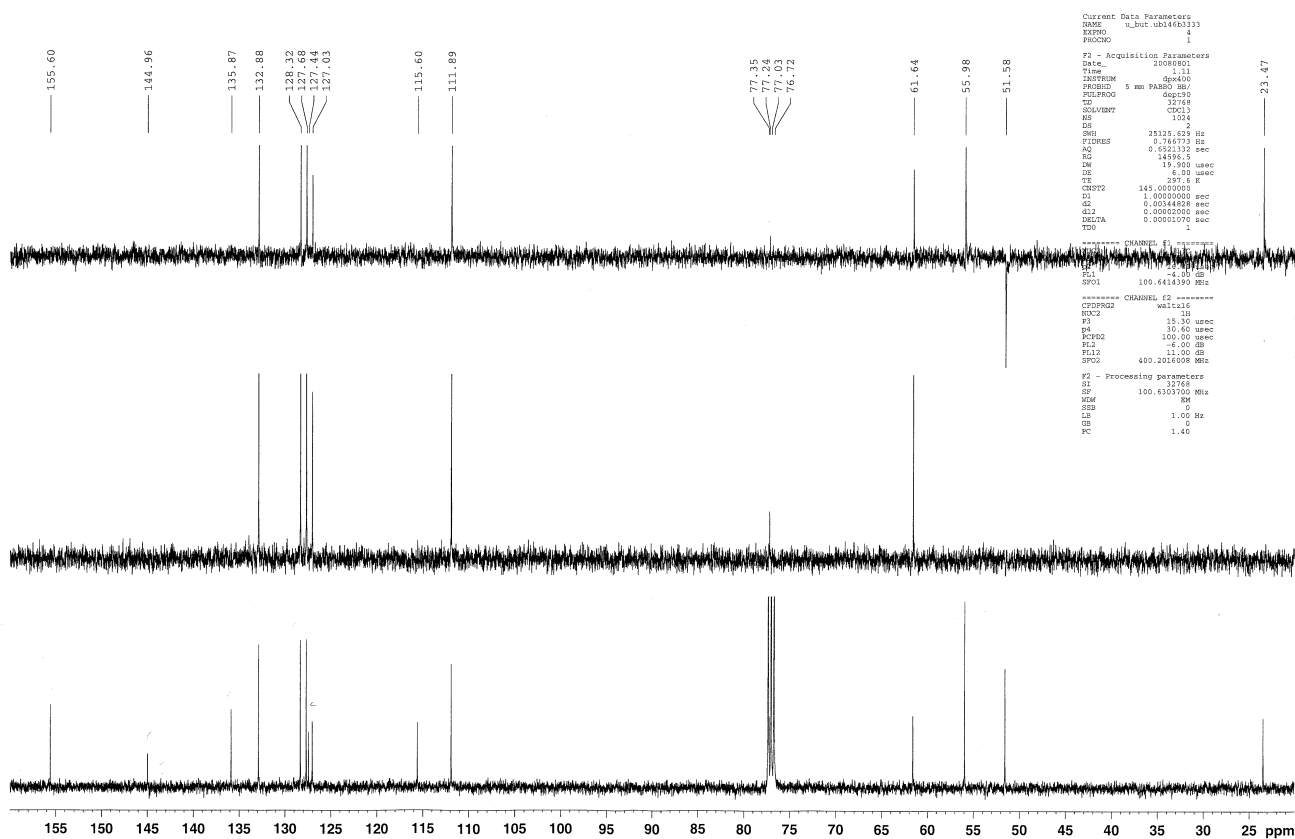
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EXPNO     1
PROCNO    1

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Date_      20090110
Time       10 15
INSTRUM    dp4x40
PROBHD      5 mm PABBO BB/
PULPROG     zgpg
TD          32768
SOLVENT     DMSO
DS          15
DE          2
SNR         4789.272 Hz
FIDRES      0.146157 Hz
AQ          0.000000 sec
RG          456.1
TE          104.400 usec
DE          6.00 usec
TD          299.1 K
D1          1.0000000 sec
TDO         1

===== CHANNEL f1 =====
NUC1        13
P1           1.34 usec
PL1          -6.00 dB
SFO1        400.2022011 MHz

F2 - Processing parameters
SI          32768
SF          400.200091 MHz
NUM         EM
SSB         0
LB          0.30 Hz
GB          0
PC          1.00

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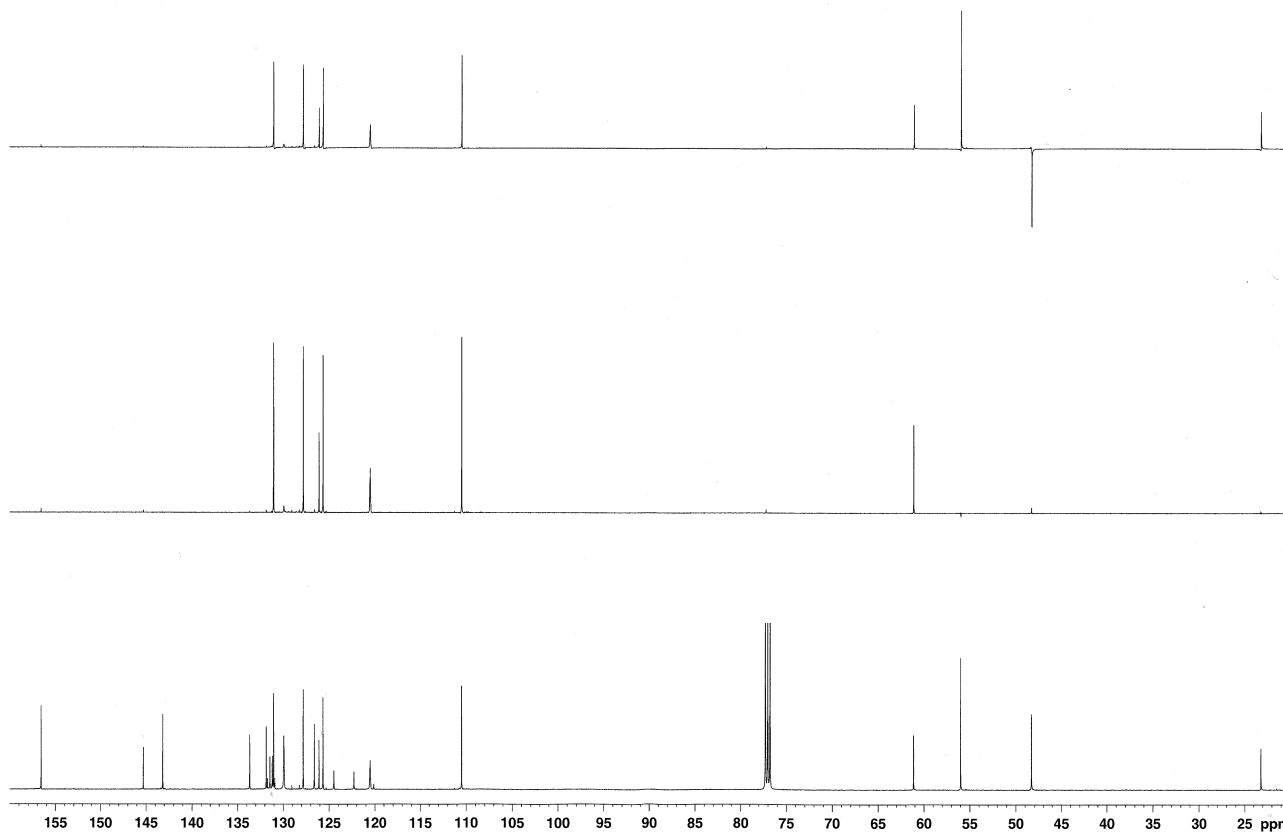
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Current Data Parameters
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PROGNO       1

F2 - Acquisition Parameters
Date         20080801
Time         1:11
FREQ         15.000000 MHz
PULSE        5 mm PABBO dB0
PRF          27268
TID          27268
TID_ADJUSTED 27268
TID_OFFSET   0
DS           2     1024
SW           25328.629 Hz
BW           57.7975 Hz
AQ           0.0523132 sec
DM           6.00 uSec
DMT          10.1900 uSec
DMT_OFFSET   0.00 uSec
TDE          2.971 K
D1           145.000000 sec
D2           1.00000000 sec
D3           0.50000000 sec
D4           0.00000000 sec
D5           0.00000000 sec
D6           0.00000000 sec
D7           0.00000000 sec
D8           0.00000000 sec
D9           0.00000000 sec
D10          0.00000000 sec
D11          0.00000000 sec
D12          0.00000000 sec
D13          0.00000000 sec
D14          0.00000000 sec
D15          0.00000000 sec
D16          0.00000000 sec
D17          0.00000000 sec
D18          0.00000000 sec
D19          0.00000000 sec
D20          0.00000000 sec
D21          0.00000000 sec
D22          0.00000000 sec
D23          0.00000000 sec
D24          0.00000000 sec
D25          0.00000000 sec
D26          0.00000000 sec
D27          0.00000000 sec
D28          0.00000000 sec
D29          0.00000000 sec
D30          0.00000000 sec
D31          0.00000000 sec
D32          0.00000000 sec
D33          0.00000000 sec
D34          0.00000000 sec
D35          0.00000000 sec
D36          0.00000000 sec
D37          0.00000000 sec
D38          0.00000000 sec
D39          0.00000000 sec
D40          0.00000000 sec
D41          0.00000000 sec
D42          0.00000000 sec
D43          0.00000000 sec
D44          0.00000000 sec
D45          0.00000000 sec
D46          0.00000000 sec
D47          0.00000000 sec
D48          0.00000000 sec
D49          0.00000000 sec
D50          0.00000000 sec
D51          0.00000000 sec
D52          0.00000000 sec
D53          0.00000000 sec
D54          0.00000000 sec
D55          0.00000000 sec
D56          0.00000000 sec
D57          0.00000000 sec
D58          0.00000000 sec
D59          0.00000000 sec
D60          0.00000000 sec
D61          0.00000000 sec
D62          0.00000000 sec
D63          0.00000000 sec
D64          0.00000000 sec
D65          0.00000000 sec
D66          0.00000000 sec
D67          0.00000000 sec
D68          0.00000000 sec
D69          0.00000000 sec
D70          0.00000000 sec
D71          0.00000000 sec
D72          0.00000000 sec
D73          0.00000000 sec
D74          0.00000000 sec
D75          0.00000000 sec
D76          0.00000000 sec
D77          0.00000000 sec
D78          0.00000000 sec
D79          0.00000000 sec
D80          0.00000000 sec
D81          0.00000000 sec
D82          0.00000000 sec
D83          0.00000000 sec
D84          0.00000000 sec
D85          0.00000000 sec
D86          0.00000000 sec
D87          0.00000000 sec
D88          0.00000000 sec
D89          0.00000000 sec
D90          0.00000000 sec
D91          0.00000000 sec
D92          0.00000000 sec
D93          0.00000000 sec
D94          0.00000000 sec
D95          0.00000000 sec
D96          0.00000000 sec
D97          0.00000000 sec
D98          0.00000000 sec
D99          0.00000000 sec
D100         0.00000000 sec

***** CHANNEL 1 *****
F1          15.000000 MHz
F2          15.000000 MHz
F3          15.000000 MHz
F4          15.000000 MHz
F5          15.000000 MHz
F6          15.000000 MHz
F7          15.000000 MHz
F8          15.000000 MHz
F9          15.000000 MHz
F10         15.000000 MHz
F11         15.000000 MHz
F12         15.000000 MHz
F13         15.000000 MHz
F14         15.000000 MHz
F15         15.000000 MHz
F16         15.000000 MHz
F17         15.000000 MHz
F18         15.000000 MHz
F19         15.000000 MHz
F20         15.000000 MHz
F21         15.000000 MHz
F22         15.000000 MHz
F23         15.000000 MHz
F24         15.000000 MHz
F25         15.000000 MHz
F26         15.000000 MHz
F27         15.000000 MHz
F28         15.000000 MHz
F29         15.000000 MHz
F30         15.000000 MHz
F31         15.000000 MHz
F32         15.000000 MHz
F33         15.000000 MHz
F34         15.000000 MHz
F35         15.000000 MHz
F36         15.000000 MHz
F37         15.000000 MHz
F38         15.000000 MHz
F39         15.000000 MHz
F40         15.000000 MHz
F41         15.000000 MHz
F42         15.000000 MHz
F43         15.000000 MHz
F44         15.000000 MHz
F45         15.000000 MHz
F46         15.000000 MHz
F47         15.000000 MHz
F48         15.000000 MHz
F49         15.000000 MHz
F50         15.000000 MHz
F51         15.000000 MHz
F52         15.000000 MHz
F53         15.000000 MHz
F54         15.000000 MHz
F55         15.000000 MHz
F56         15.000000 MHz
F57         15.000000 MHz
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F61         15.000000 MHz
F62         15.000000 MHz
F63         15.000000 MHz
F64         15.000000 MHz
F65         15.000000 MHz
F66         15.000000 MHz
F67         15.000000 MHz
F68         15.000000 MHz
F69         15.000000 MHz
F70         15.000000 MHz
F71         15.000000 MHz
F72         15.000000 MHz
F73         15.000000 MHz
F74         15.000000 MHz
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F76         15.000000 MHz
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F95         15.000000 MHz
F96         15.000000 MHz
F97         15.000000 MHz
F98         15.000000 MHz
F99         15.000000 MHz
F100        15.000000 MHz

F2 - Processing parameters
F1          15.000000 MHz
F2          15.000000 MHz
F3          15.000000 MHz
F4          15.000000 MHz
F5          15.000000 MHz
F6          15.000000 MHz
F7          15.000000 MHz
F8          15.000000 MHz
F9          15.000000 MHz
F10         15.000000 MHz
F11         15.000000 MHz
F12         15.000000 MHz
F13         15.000000 MHz
F14         15.000000 MHz
F15         15.000000 MHz
F16         15.000000 MHz
F17         15.000000 MHz
F18         15.000000 MHz
F19         15.000000 MHz
F20         15.000000 MHz
F21         15.000000 MHz
F22         15.000000 MHz
F23         15.000000 MHz
F24         15.000000 MHz
F25         15.000000 MHz
F26         15.000000 MHz
F27         15.000000 MHz
F28         15.000000 MHz
F29         15.000000 MHz
F30         15.000000 MHz
F31         15.000000 MHz
F32         15.000000 MHz
F33         15.000000 MHz
F34         15.000000 MHz
F35         15.000000 MHz
F36         15.000000 MHz
F37         15.000000 MHz
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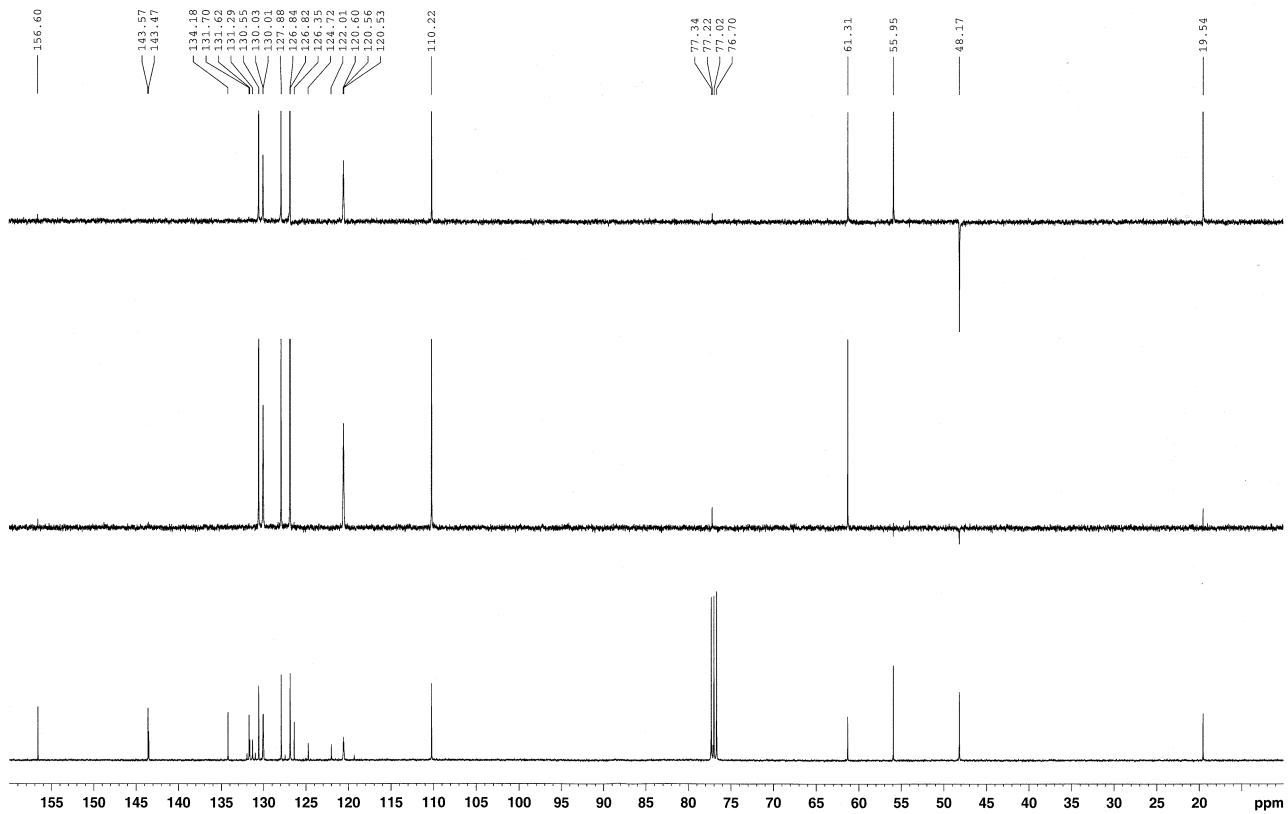
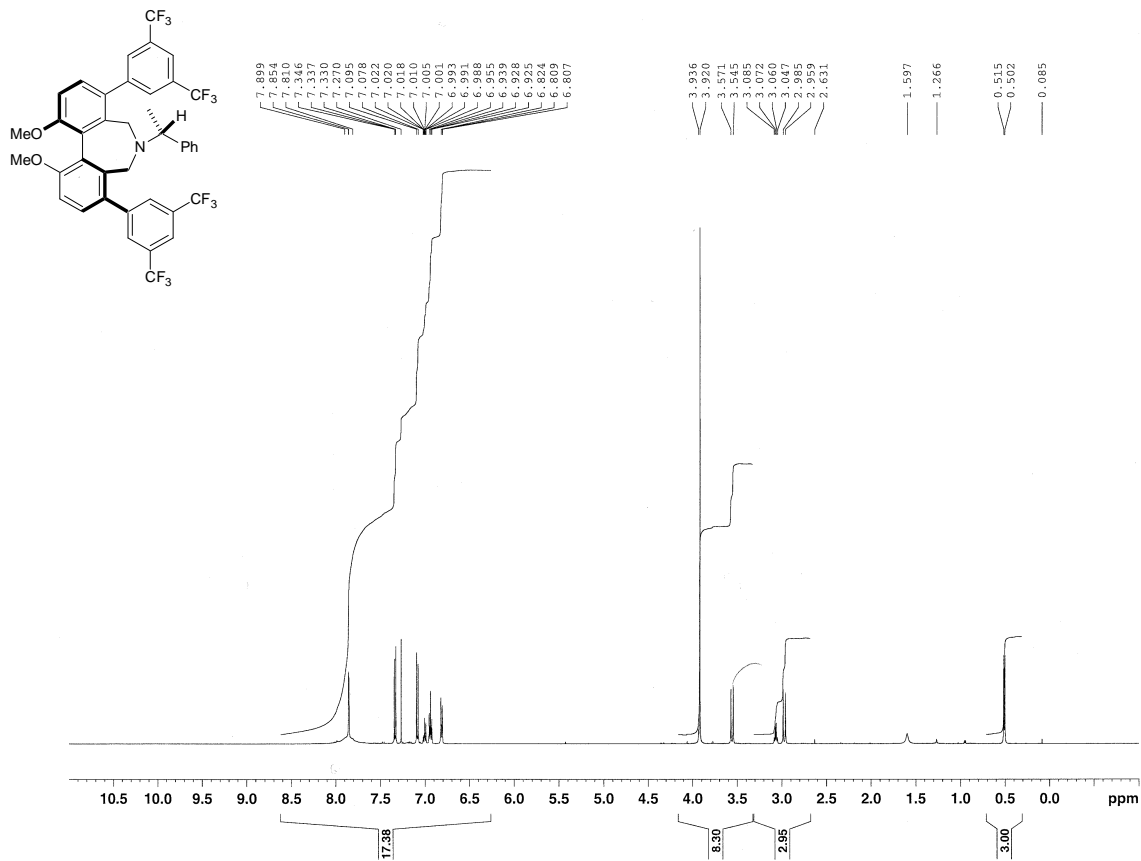


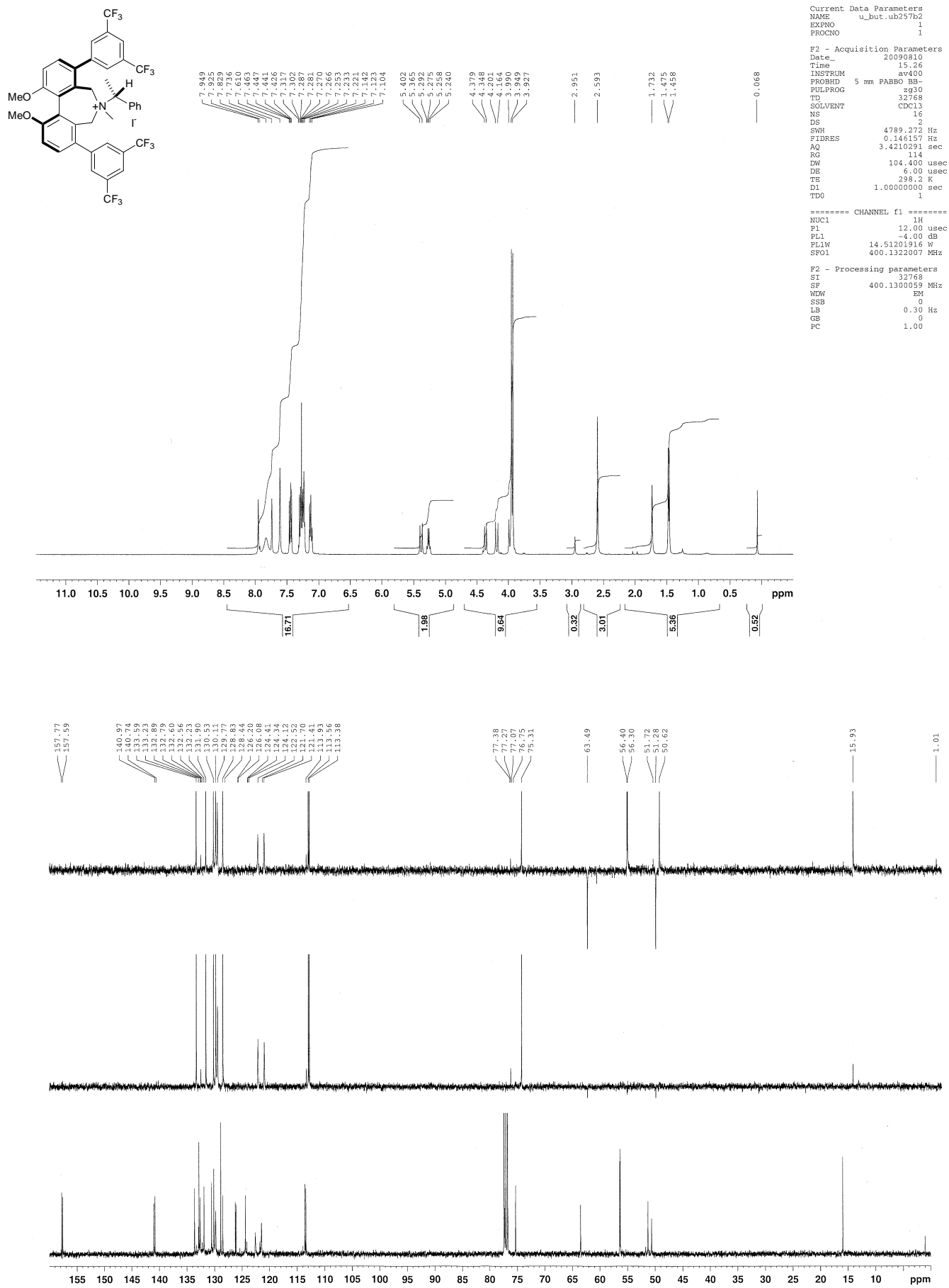
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EXPNO 1
PROCNO 1

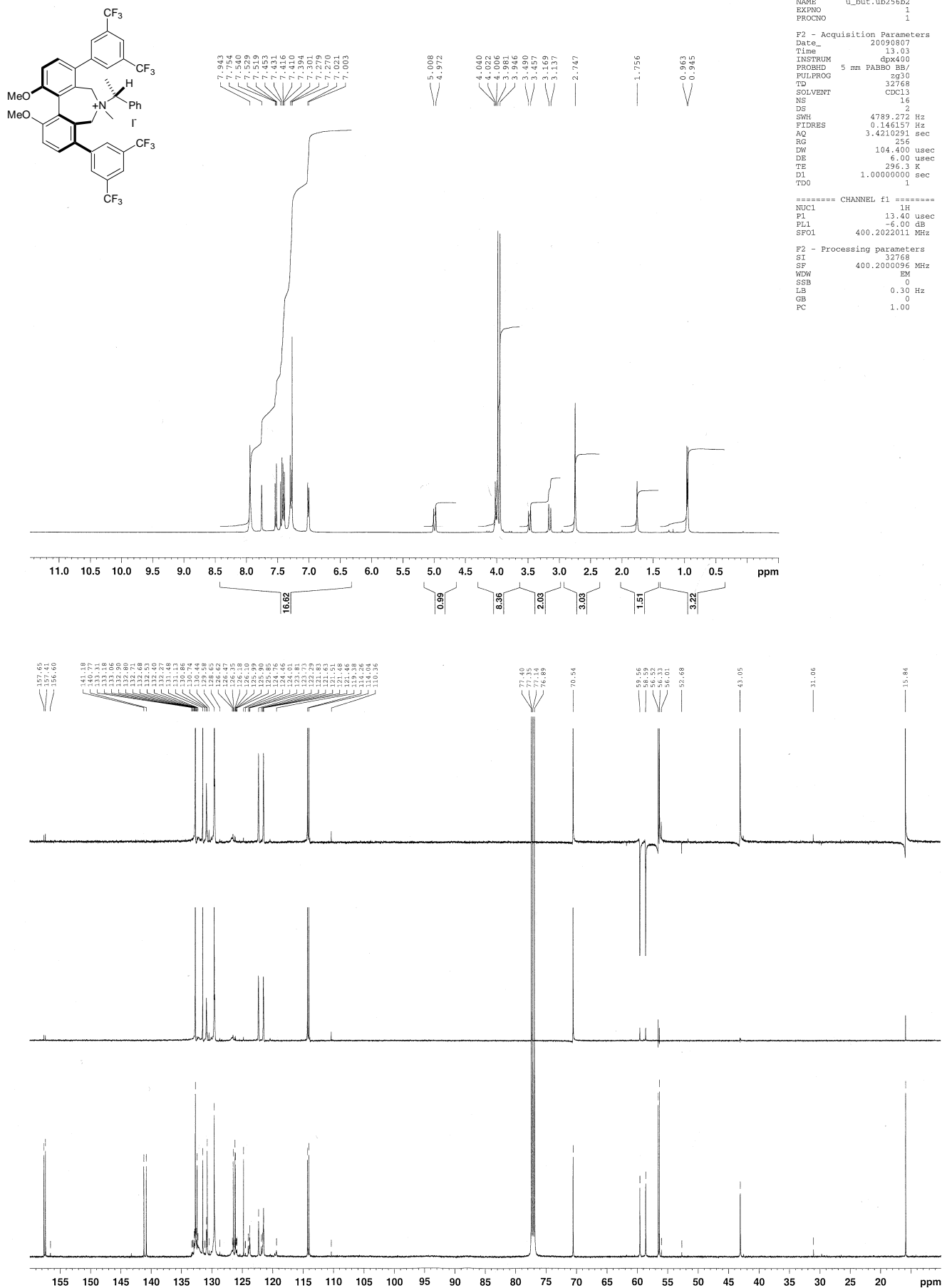
F2 - Acquisition Parameters
Date_ 20090725
Time 1.10
INSTRUM av3500
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 8
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 203
RW 48.400 usec
DE 82.19 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

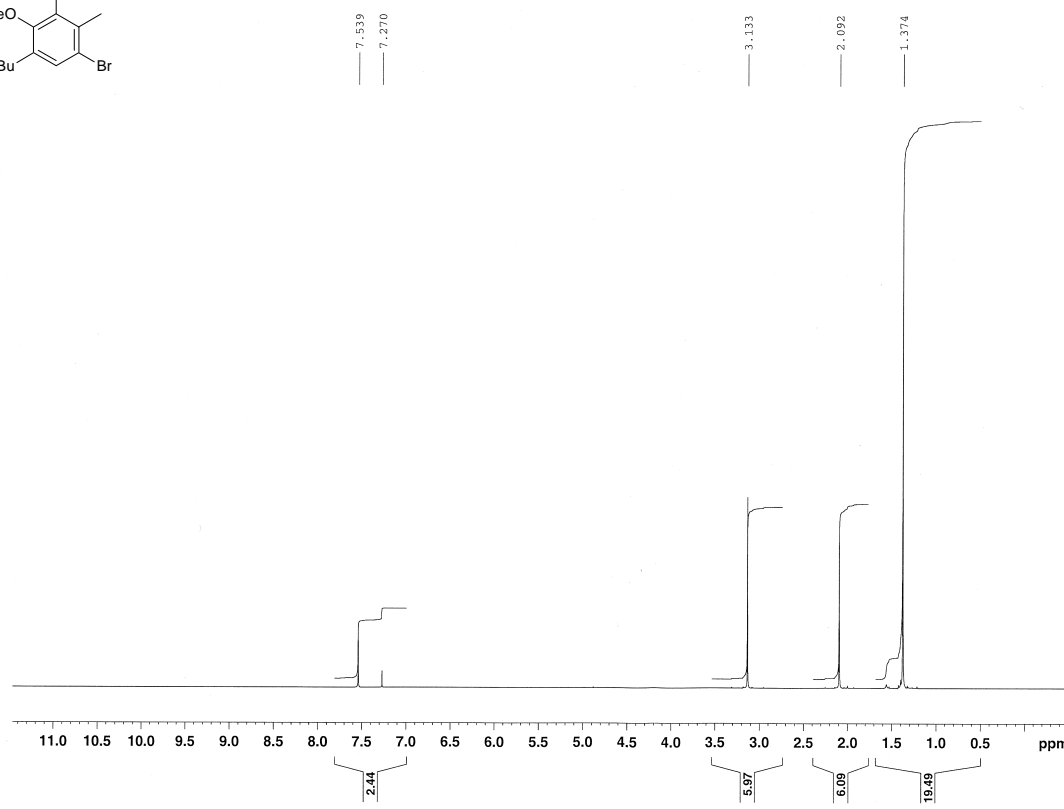
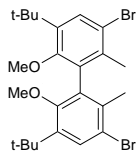
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NUC1 13H
P1 7.90 usec
PL1 1.60 dB
PL1W 20.50605011 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 65536
SF 500.1300029 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00







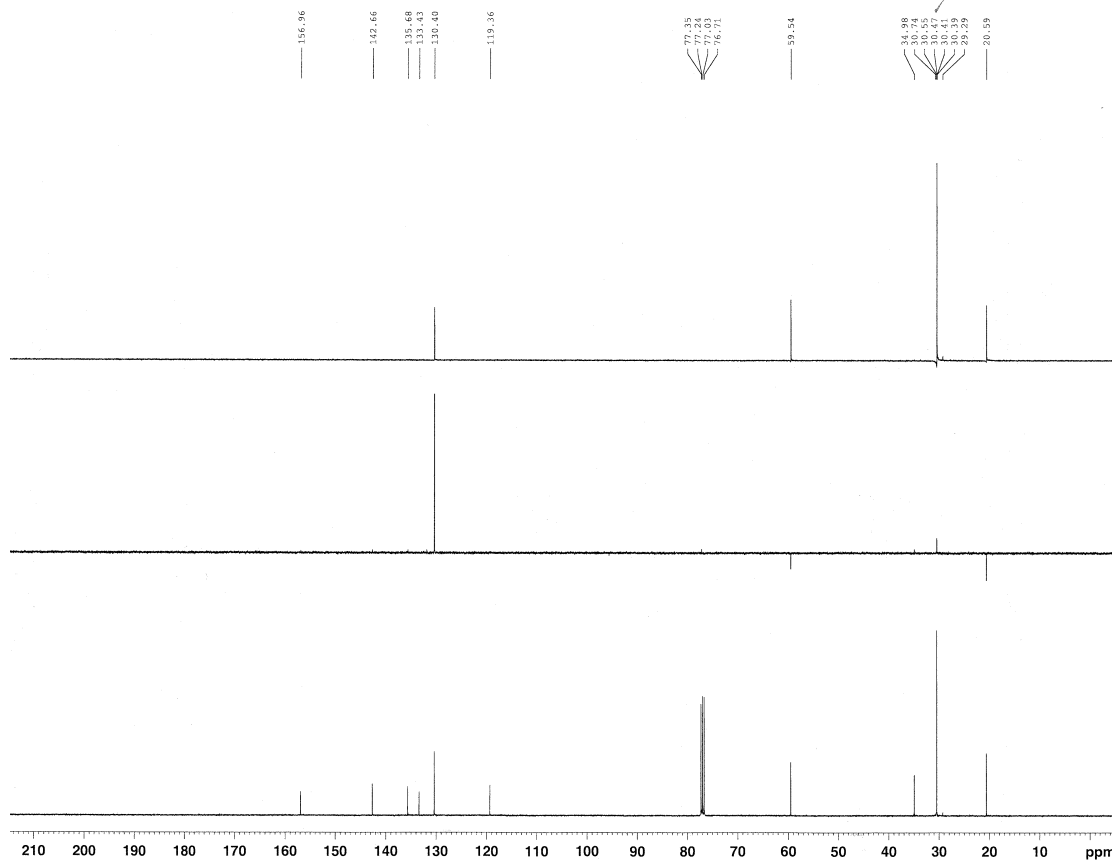


Current Data Parameters
NAME u_but.ub217b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090409
Time 14.51
INSTRUM dpx400
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 322.5
DW 104.400 usec
DE 6.00 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.40 usec
PL1 -6.00 dB
SFO1 400.2022011 MHz

F2 - Processing parameters
SI 32768
SF 400.2000090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



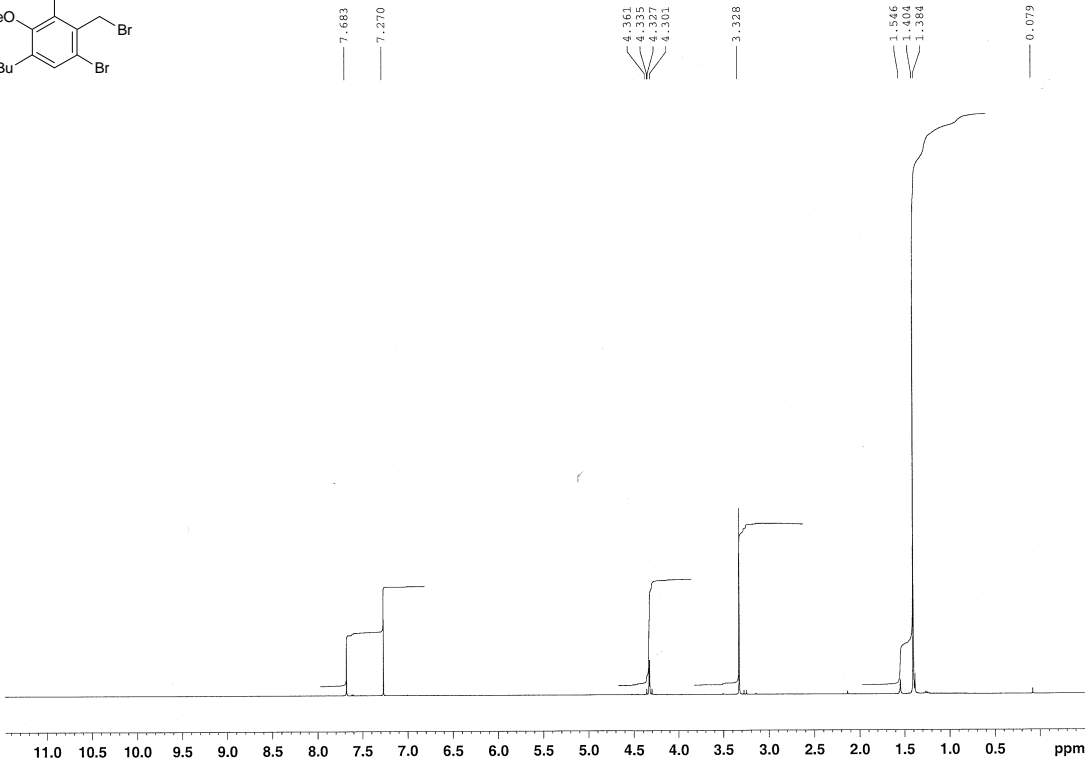
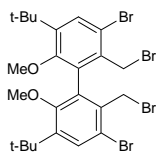
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NAME u_but.ub217b
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090409
Time 23.20
INSTRUM dpx400
PROBHD 5 mm PABBO BB/
PULPROG dept135
TD 32768
SOLVENT CDCl3
NS 1024
DS 2
SWH 25125.629 Hz
FIDRES 0.766773 Hz
AQ 0.6521332 sec
RG 6502
DW 19.900 usec
DE 6.00 usec
TE 298.1 K
CHST2 145.00000000
D1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001070 sec
TD0 1

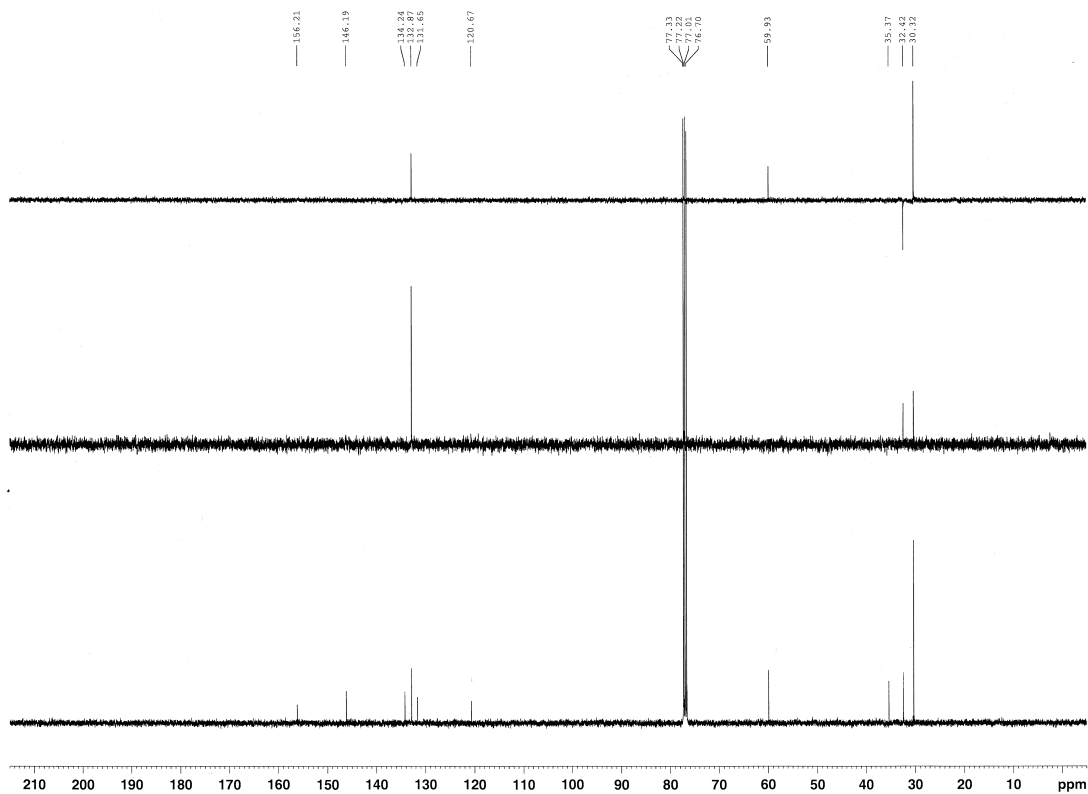
===== CHANNEL f1 =====
NUC1 13C
P1 8.40 usec
p2 16.80 usec
PL1 -4.00 dB
SFO1 100.6414390 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 15.30 usec
p4 30.60 usec
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 11.00 dB
SFO2 400.2016008 MHz

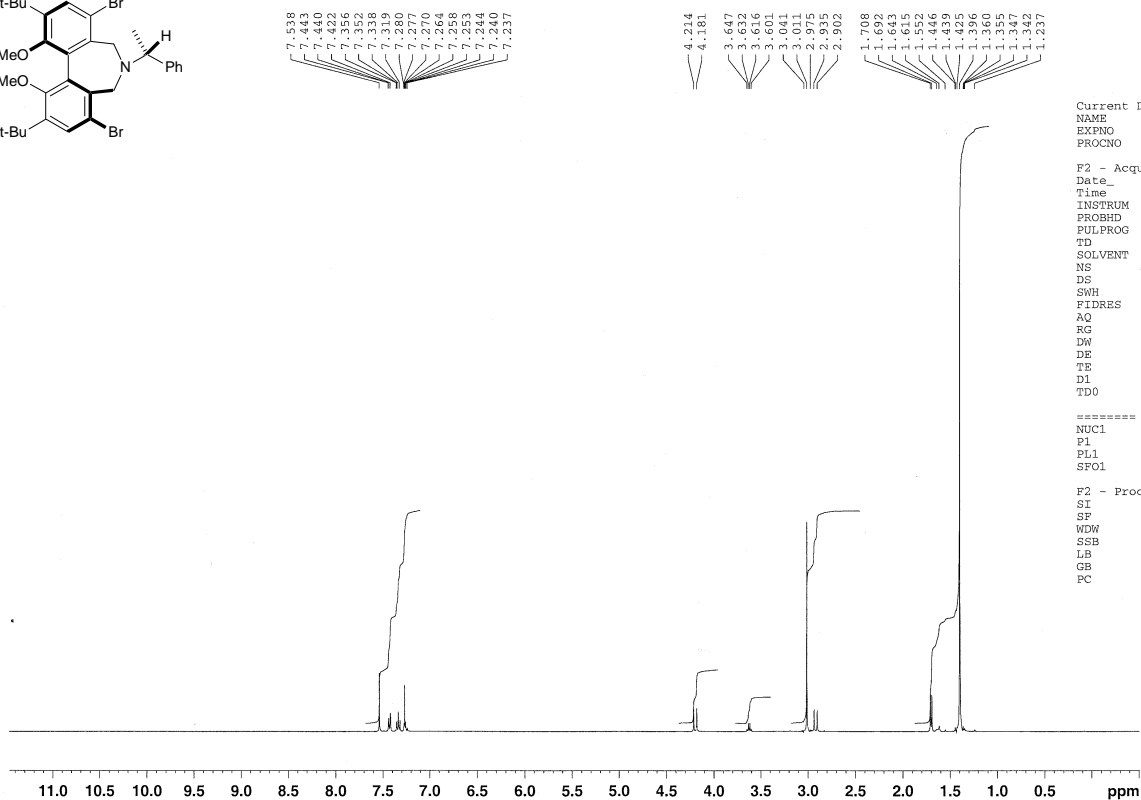
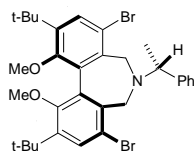
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SI 32768
SF 100.6303700 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME u_but.ub218c
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090417
Time 16.25
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 256
DW 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 12.00 usec
PL1 -4.00 dB
PL1W 14.51201916 W
SFO1 400.1322007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



NAME u_but.ub218c
EXPNO 4
PROCNO 1
Date_ 20090417
Time 23.49
INSTRUM av400
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 23980.814 Hz
FIDRES 0.731836 Hz
AQ 0.6832628 sec
RG 13004
DW 20.850 usec
DE 10.00 usec
TE 298.2 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 7.90 usec
P2 15.80 usec
PL1 -3.00 dB
PL1W 70.66739655 W
SFO1 100.6238345 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
P3 10.90 usec
P4 21.80 usec
PCPD2 100.00 usec
PL2 -4.00 dB
PL12 15.25 dB
PL2W 14.51201916 W
PL12W 0.17247567 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



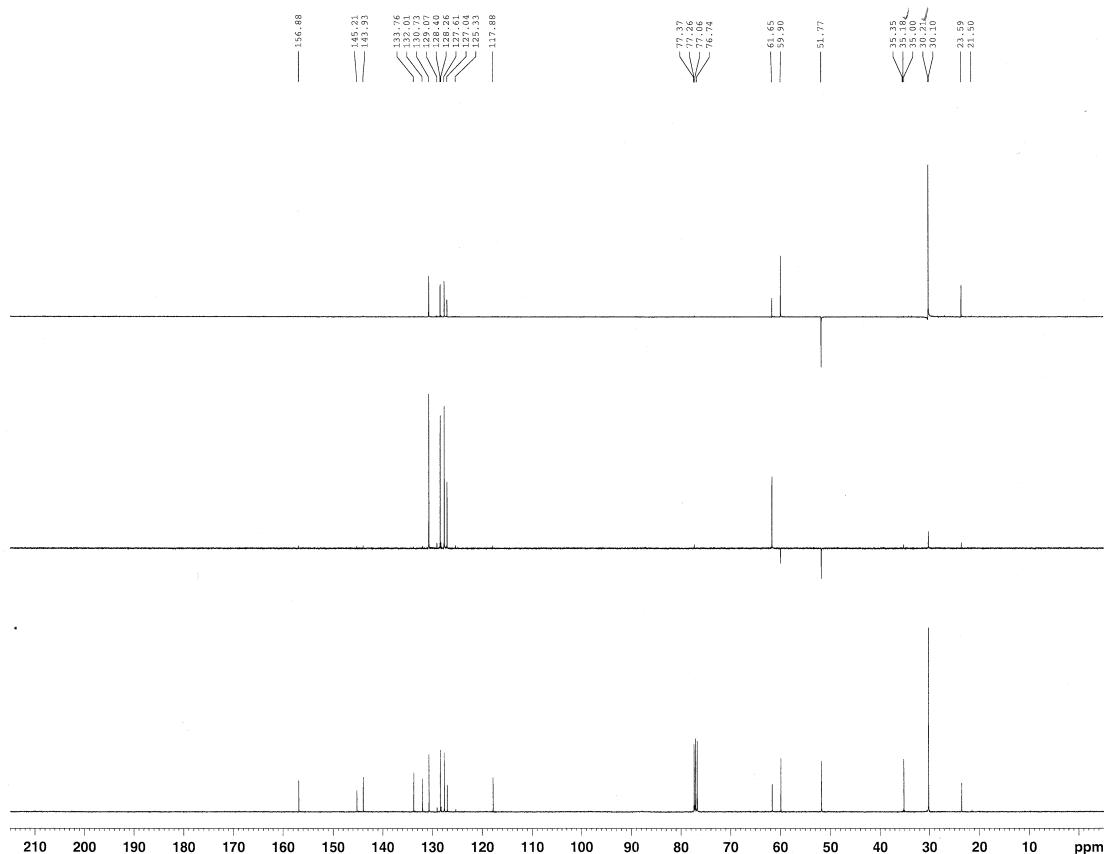
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Current Data Parameters
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EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20091009
Time      3.47
INSTRUM    dpx400
PROBHD     5 mm PABBO BB/
PULPROG    zg30
TD         32768
SOLVENT    CDCl3
NS         16
DS         2
SWH         4789.272 Hz
FIDRES     0.146157 Hz
AQ         3.4210291 sec
RG          322.5
WDW         104.400 usec
DE         6.00 usec
TE         295.4 K
D1         1.00000000 sec
TD0
===== CHANNEL f1 =====
NUC1       1H
P1         13.40 usec
PL1        -6.00 db
SFO1       400.2022011 MHz

F2 - Processing parameters
SI         32768
AQ         400.200093 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00

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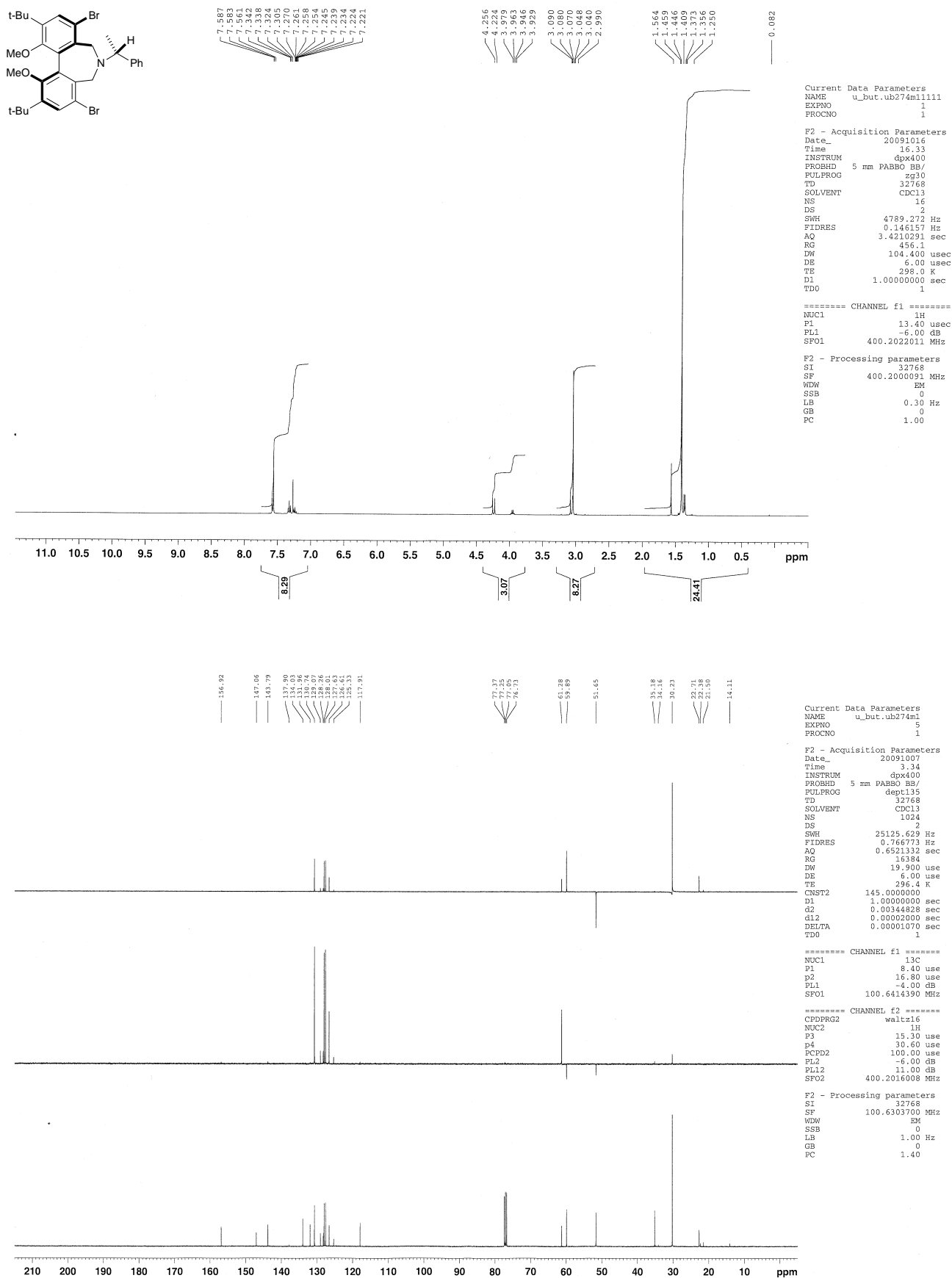
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EXPNO     5
PROCNO    1

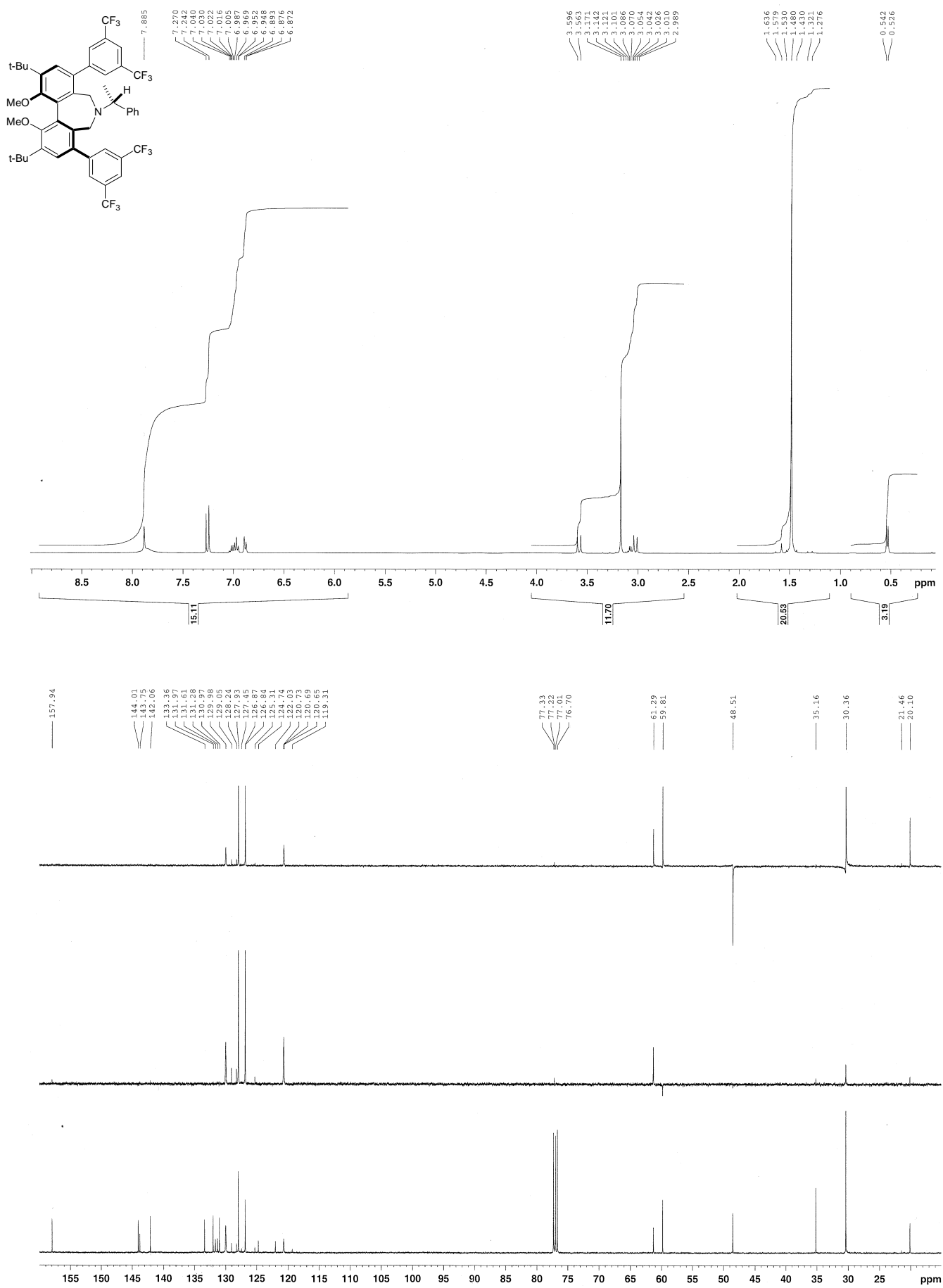
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Date_     20091007
Time      5.38
INSTRUM    dp4x000
PROBHD     5 mm PABBO BB/
PULPROG    dept135
TD          32768
FIDRES     CD13
SOLVENT     NS
DS          1024
NS          2
SWH         25125.629 Hz
FIDRES      0.766773 Hz
AQ          0.6521332 sec
RG          13004
DE          19.900 use
TE          6.00 use
TD          296.3 K
===== CHANNEL f1 =====
NUC1        13C
P1          8.40 use
PL1         16.80 use
PL12        -4.00 dB
SF01        100.61434390 MHz

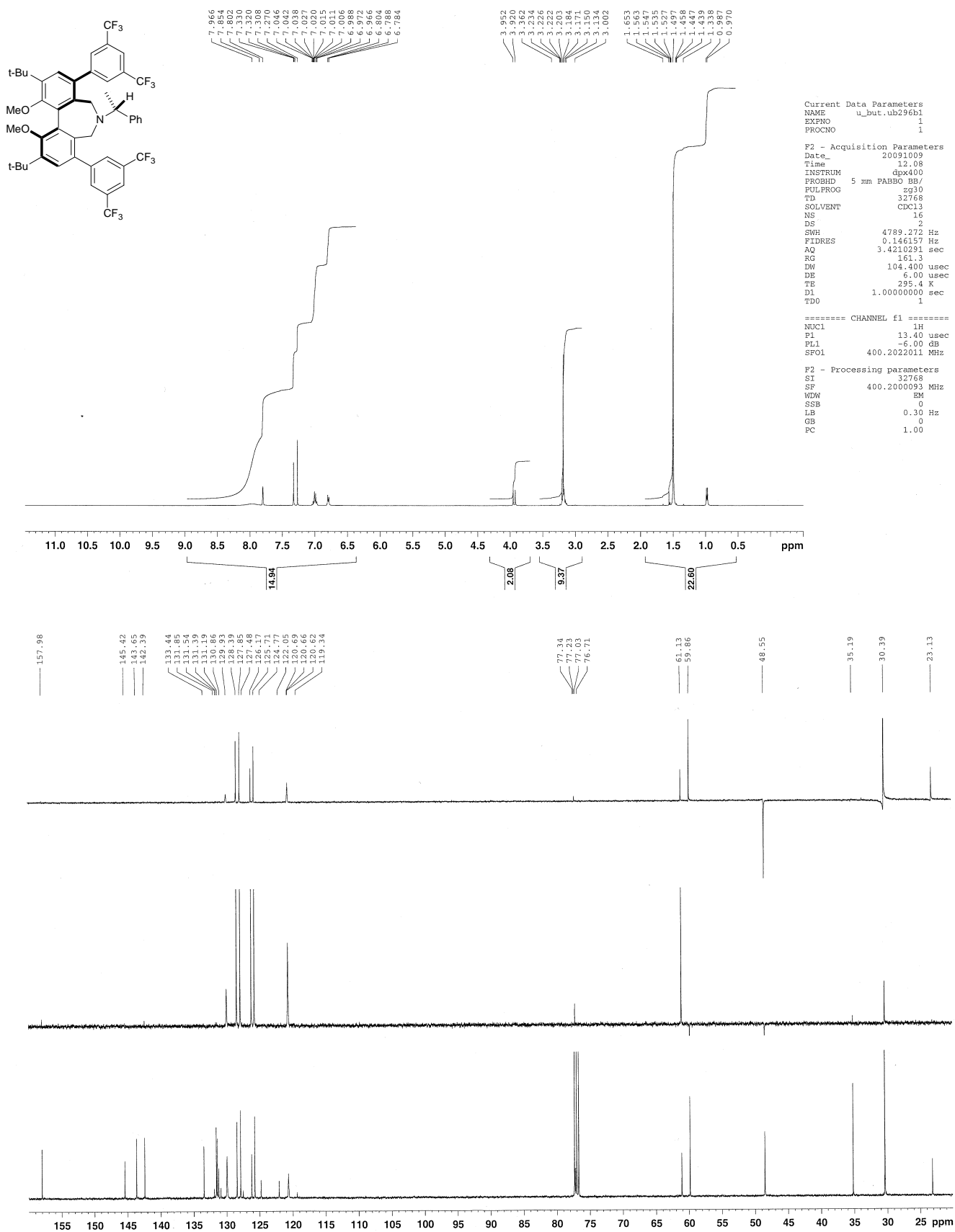
===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2        1H
P3          15.30 use
PL3         30.60 use
PCPD2       19.00 use
PL2         -6.00 dB
PL12        11.00 dB
SF02        400.2016080 MHz

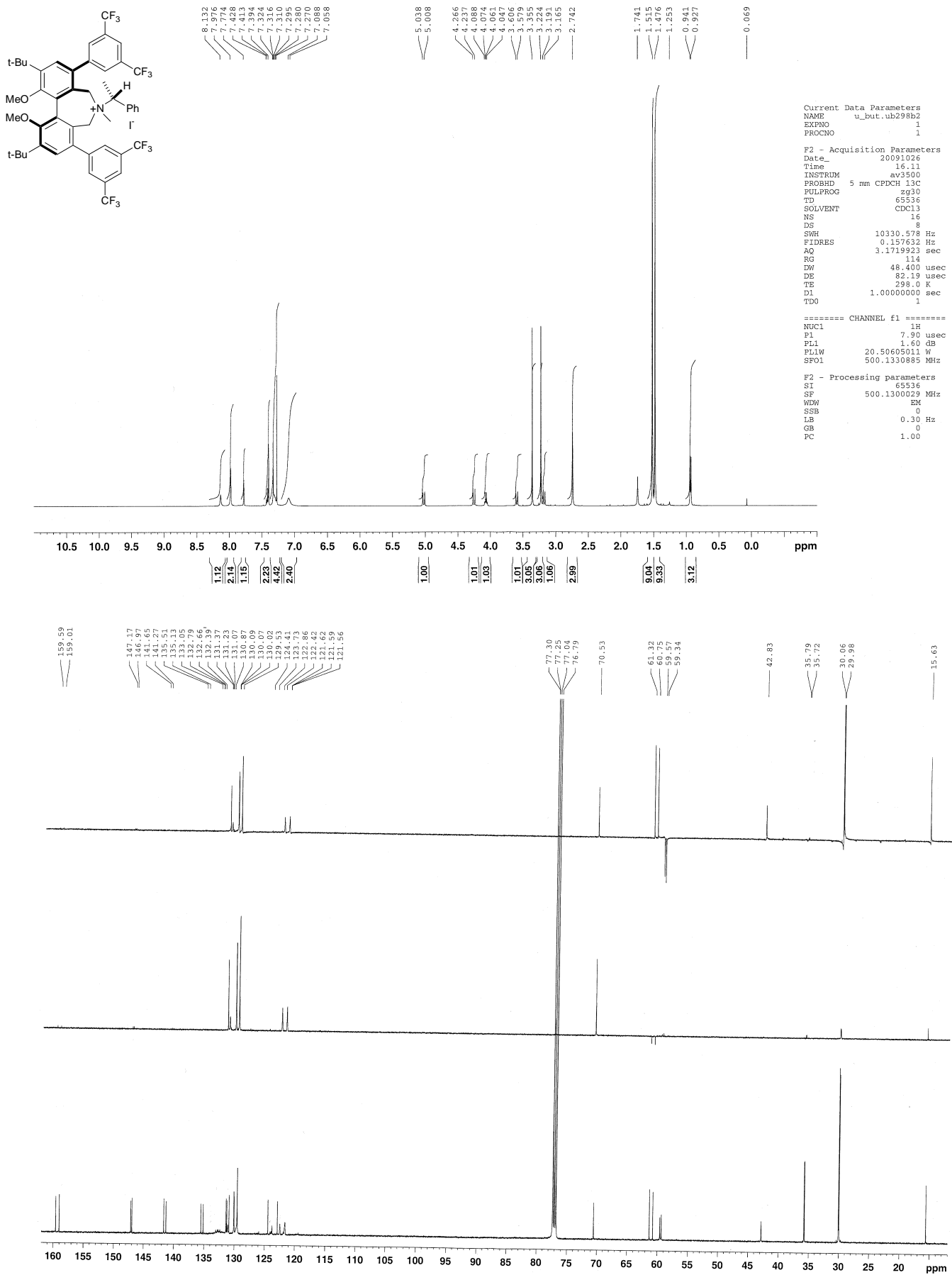
F2 - Processing parameters
SI          32768
SF          100.6303700 MHz
SD          EM
WSB         0
GB          0.100 Hz
LB          0
GB          0
PC          1.40

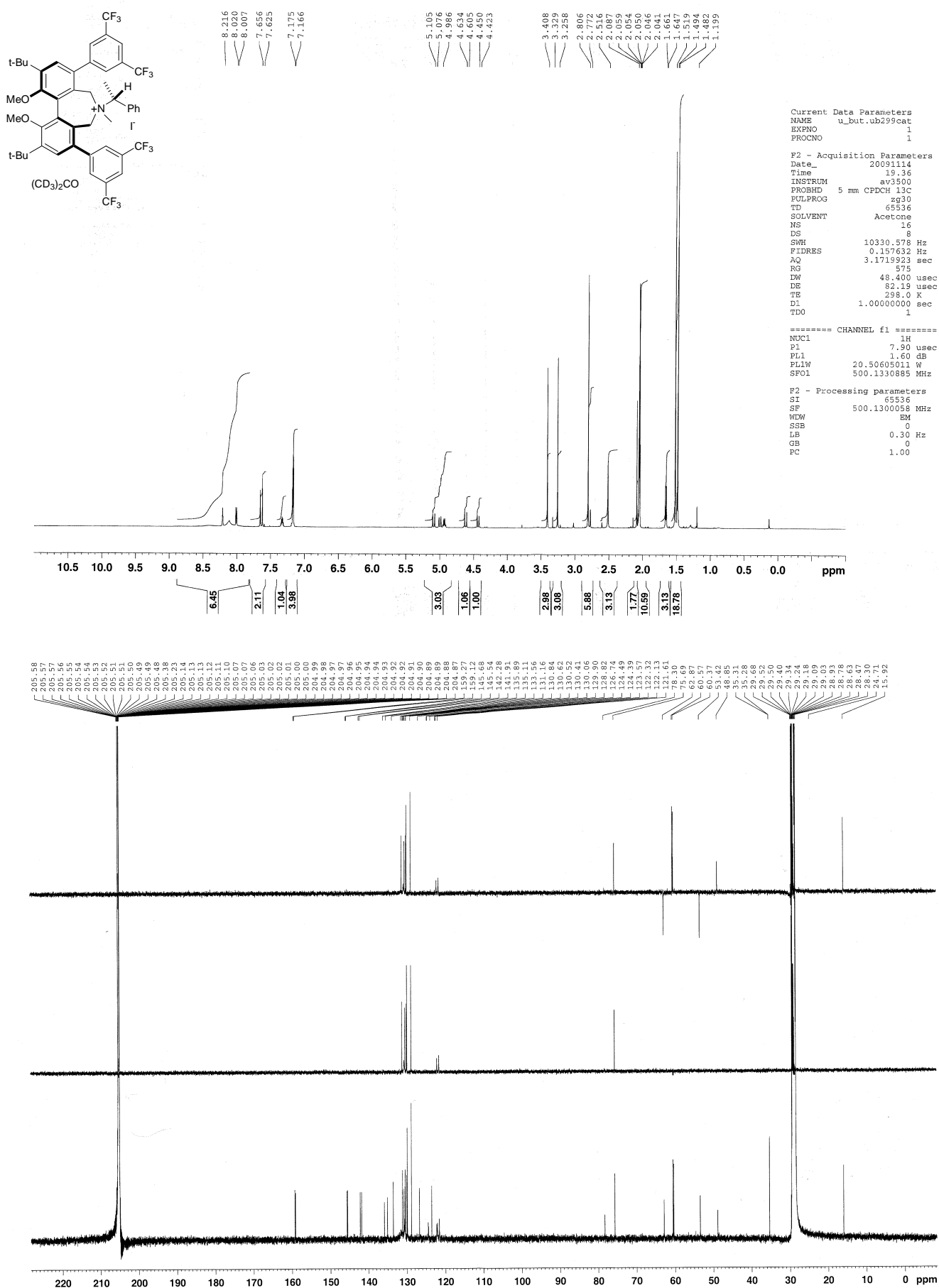
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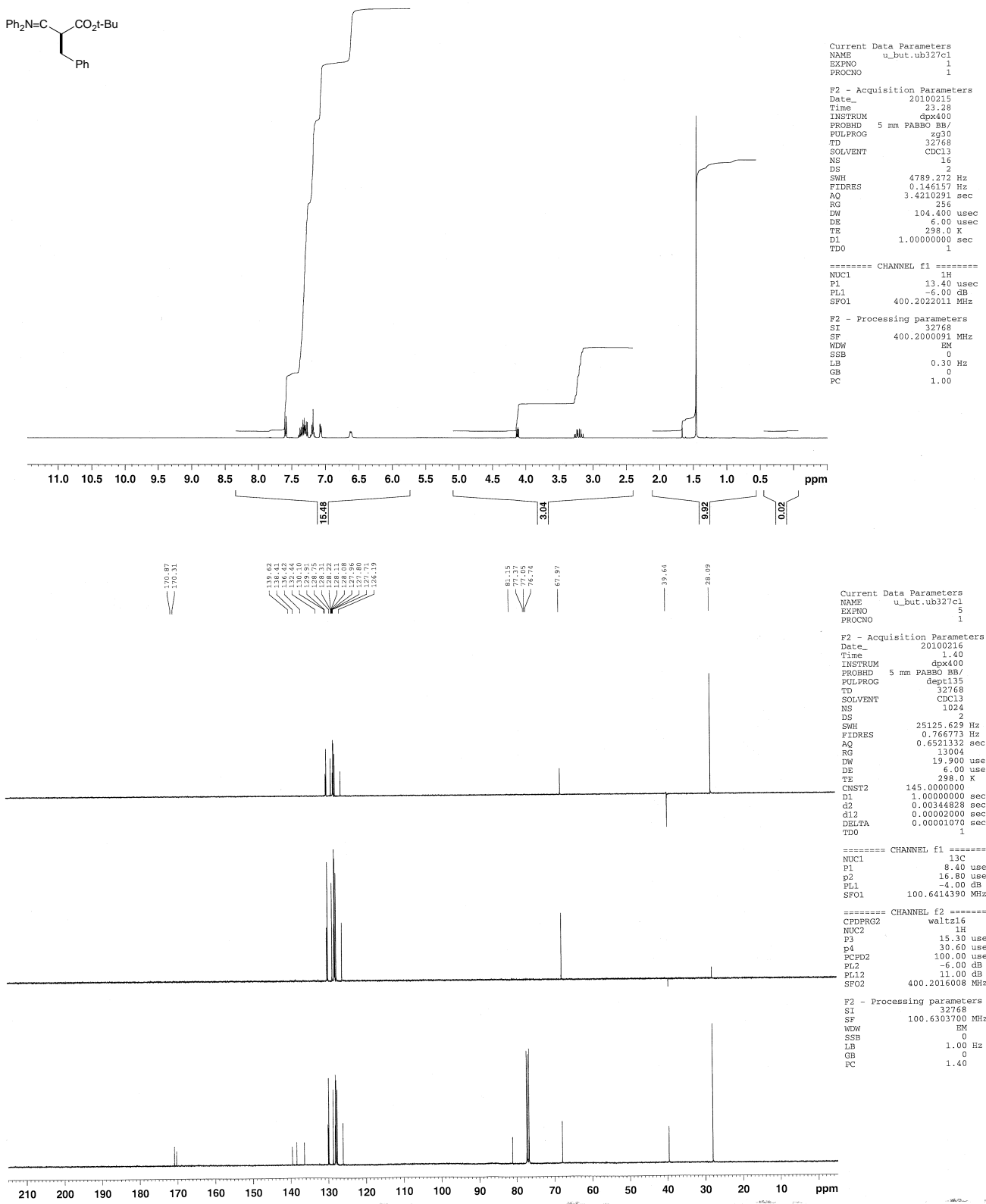




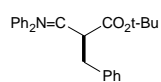




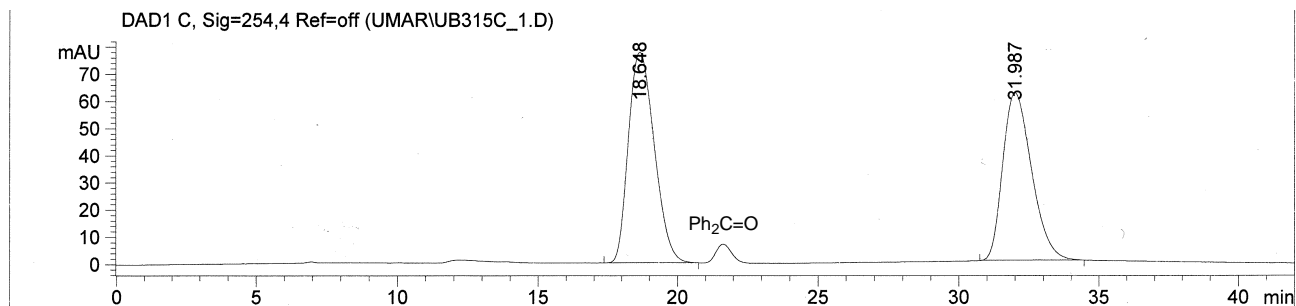




HPLC:



Racemate:



92% e.e.:

