

Supporting Information

Direct enantioseparation of 1-(2-hydroxyphenyl)ethylamines via diastereomeric salt formation: chiral recognition mechanism based on the crystal structure

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Table of Contents

Thermogravimetric analysis of the diastereomeric salt 1a 6 (Figure S1)	S2
Copies of ¹ H and ¹³ C NMR spectra of the reported compounds	S3 – S9

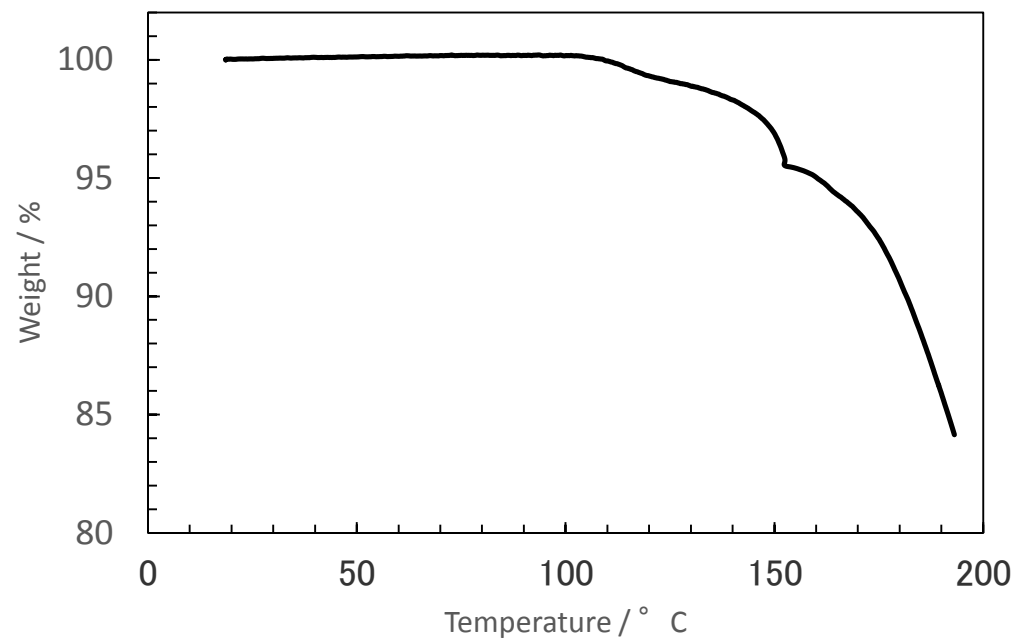


Figure S1. TGA chart of **1a·6** obtained from 50% aqueous EtOH solution.

1H

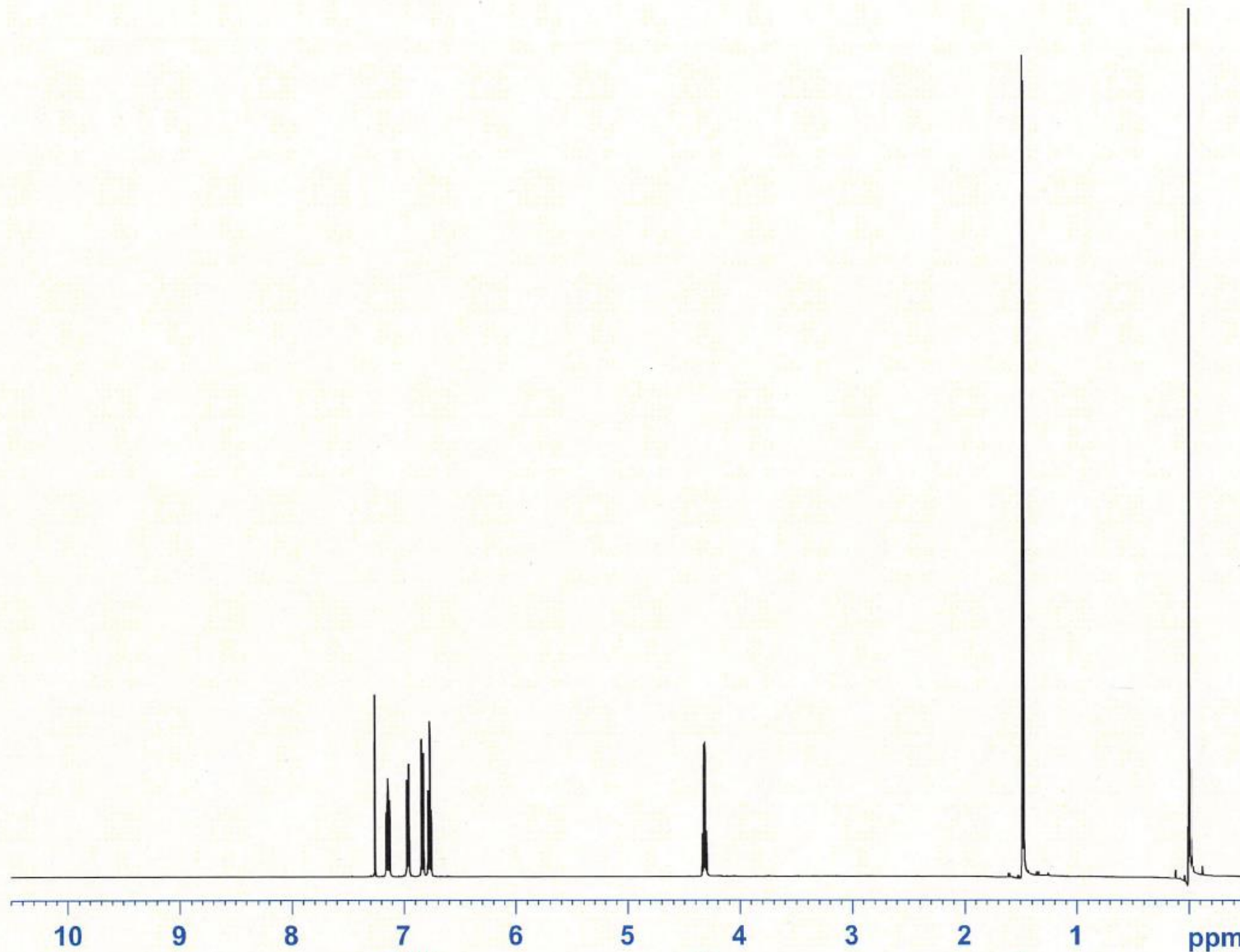
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7.157
7.154
7.141
7.139
7.127
7.123
6.971
6.968
6.956
6.953
6.844
6.842
6.828
6.826
6.787
6.785
6.772
6.770
6.757
6.755
4.342
4.329
4.316
4.302

1.482
1.469



NAME kodama
EXPNO 7
PROCNO 1
Date_ 20121213
Time_ 20.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
DW 48.400 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
TD0 1

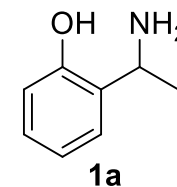
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NUC1 1H
P1 11.80 usec
PL1 2.40 dB
PL1W 15.17711735 W
SFO1 500.0330885 MHz
SI 32768
SF 500.0300133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



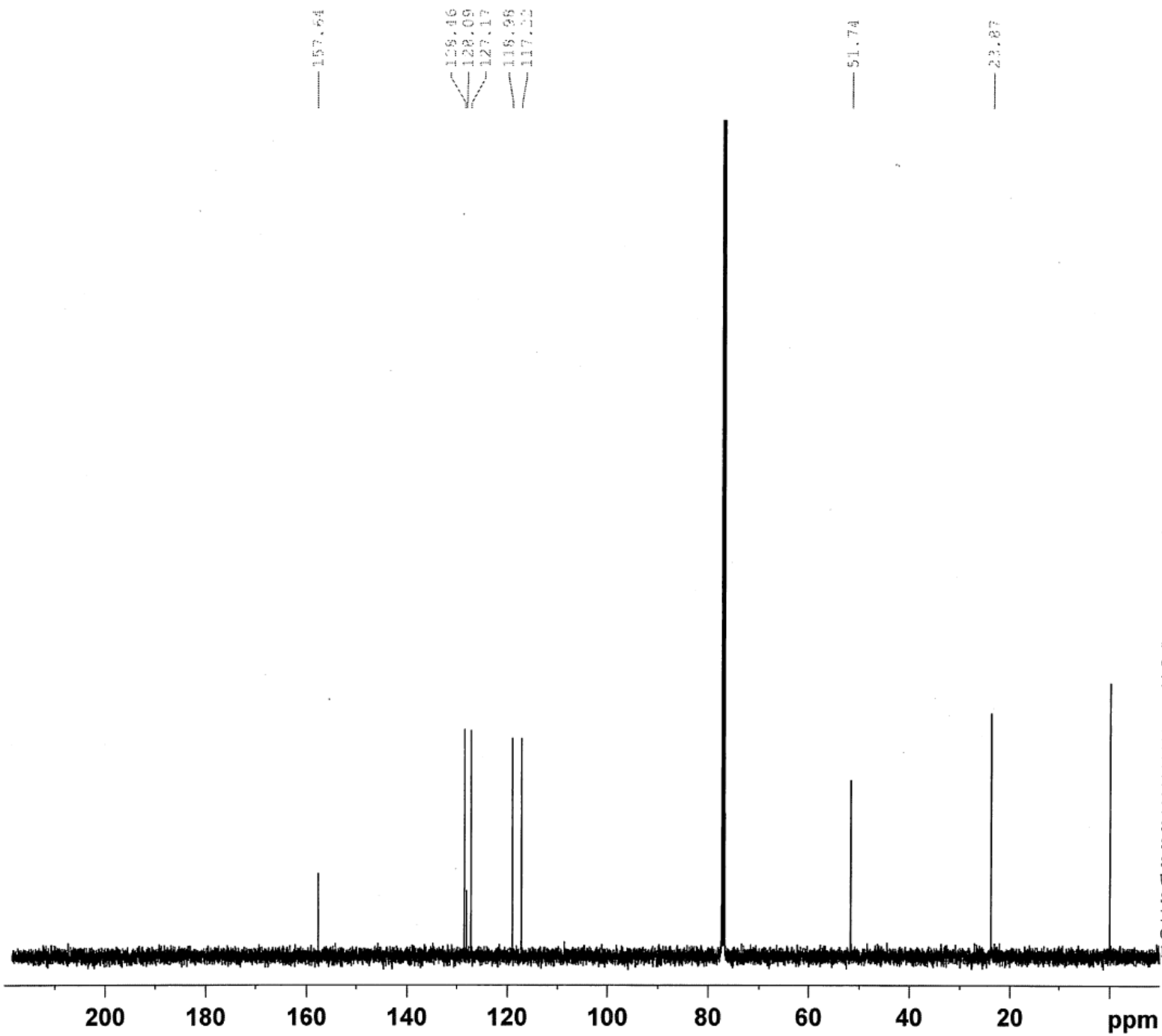
0.974
0.986
0.954
0.980

1.000

3.060



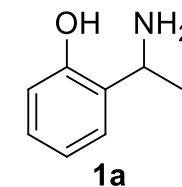
13C with 1H decoupling



NAME kodama
EXPNO 2
PROCNO 1
Date_ 20121213
Time_ 21.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 202
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -0.30 dB
PL1W 93.66541290 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.75 dB
PL12 19.50 dB
PL13 19.50 dB
PL2W 18.63472366 W
PL12W 0.31284049 W
PL13W 0.31284049 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577896 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

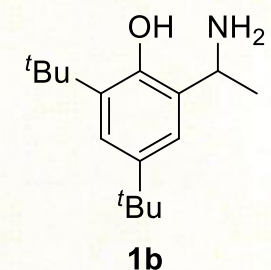
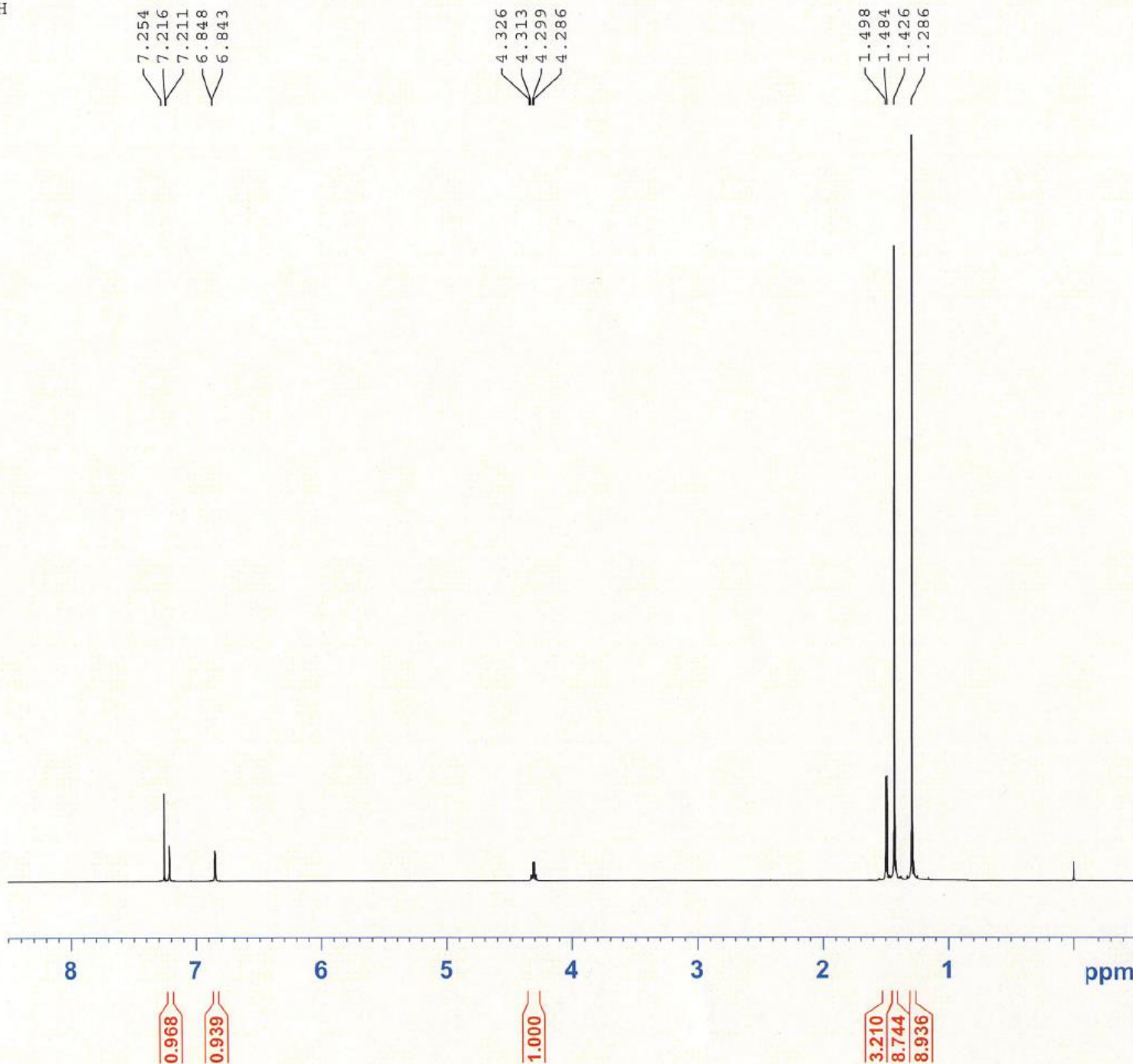


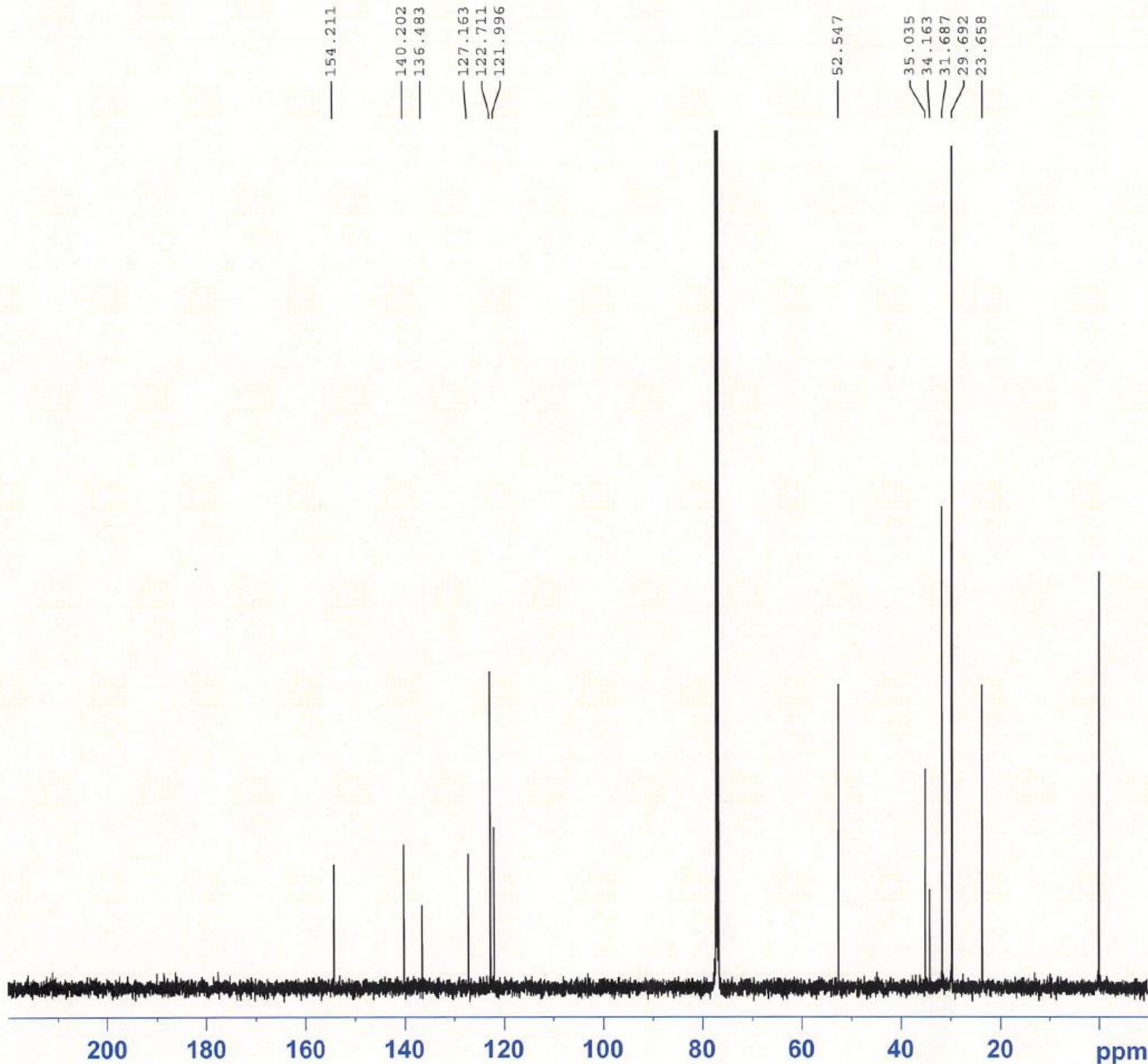
1H



NAME kodama
EXPNO 6
PROCNO 1
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Time 10.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
DW 48.400 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.80 usec
PL1 2.40 dB
PL1W 15.17711735 W
SFO1 500.0330885 MHz
SI 32768
SF 500.0300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

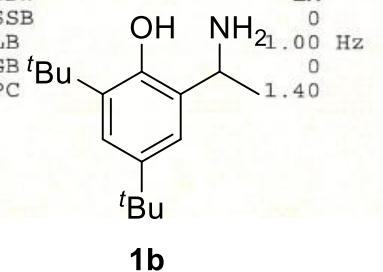




NAME kodama
EXPNO 17
PROCNO 1
Date_ 20121116
Time 21.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 2
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039582 sec
RG 203
DW 12.267 usec
DE 6.50 usec
TE 300.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

==== CHANNEL f1 =====
NUC1 13C
P1 9.80 usec
PL1 0.00 dB
PL1W 100.47545624 W
SFO1 125.7477319 MHz

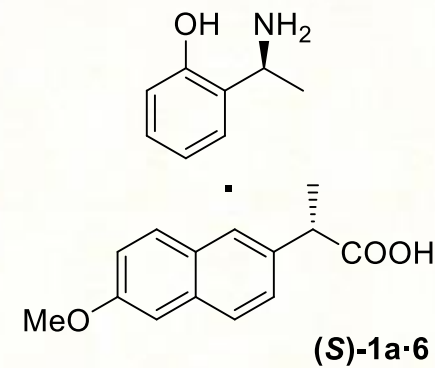
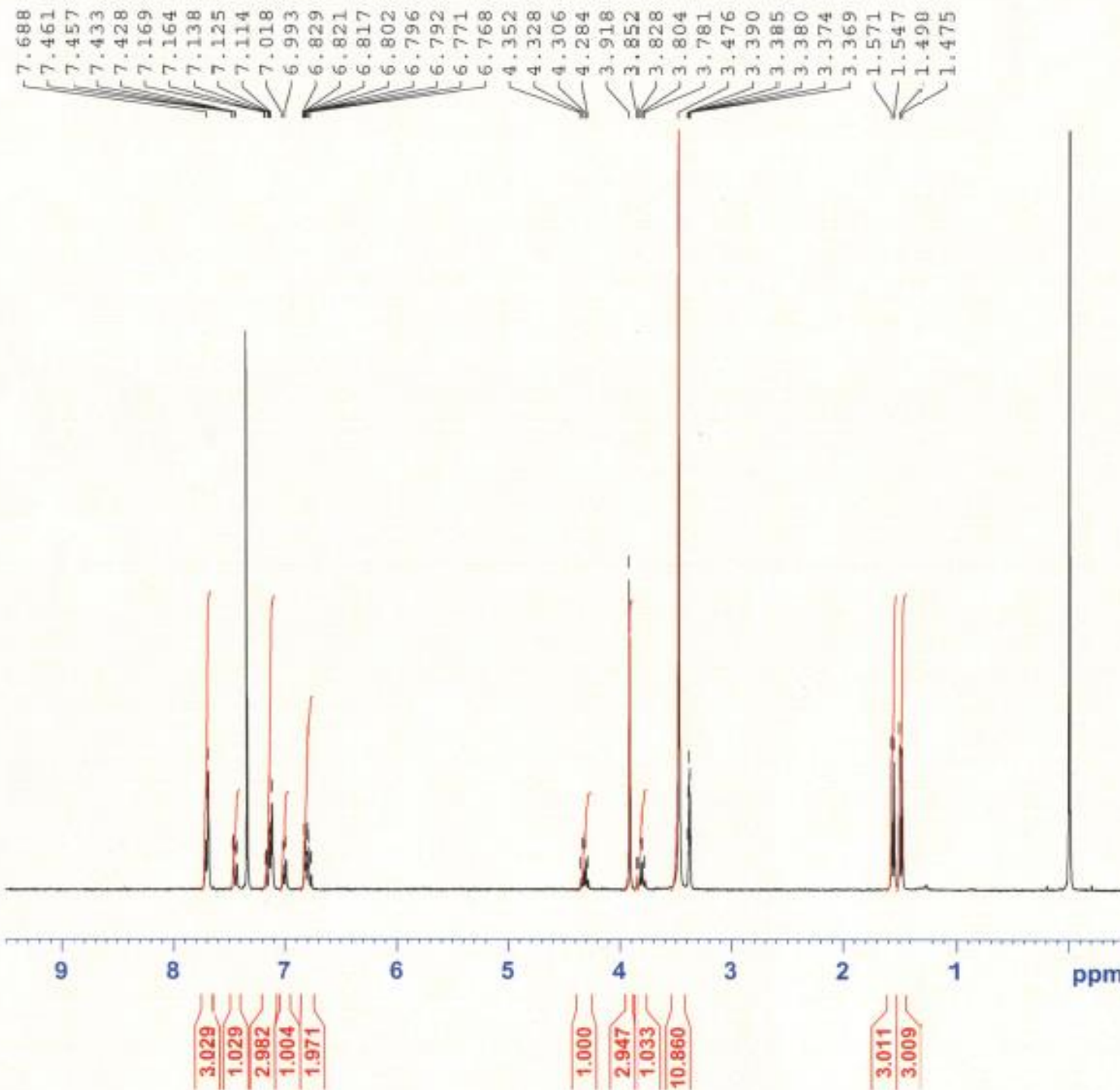
==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.40 dB
PL12 19.02 dB
PL13 22.02 dB
PL2W 15.17711735 W
PL12W 0.33051354 W
PL13W 0.16564916 W
SFO2 500.0316016 MHz
SI 16384
SF 125.7326453 MHz
WDW EM
SSB 0
LB 21.00 Hz
GB 0
PC 1.40

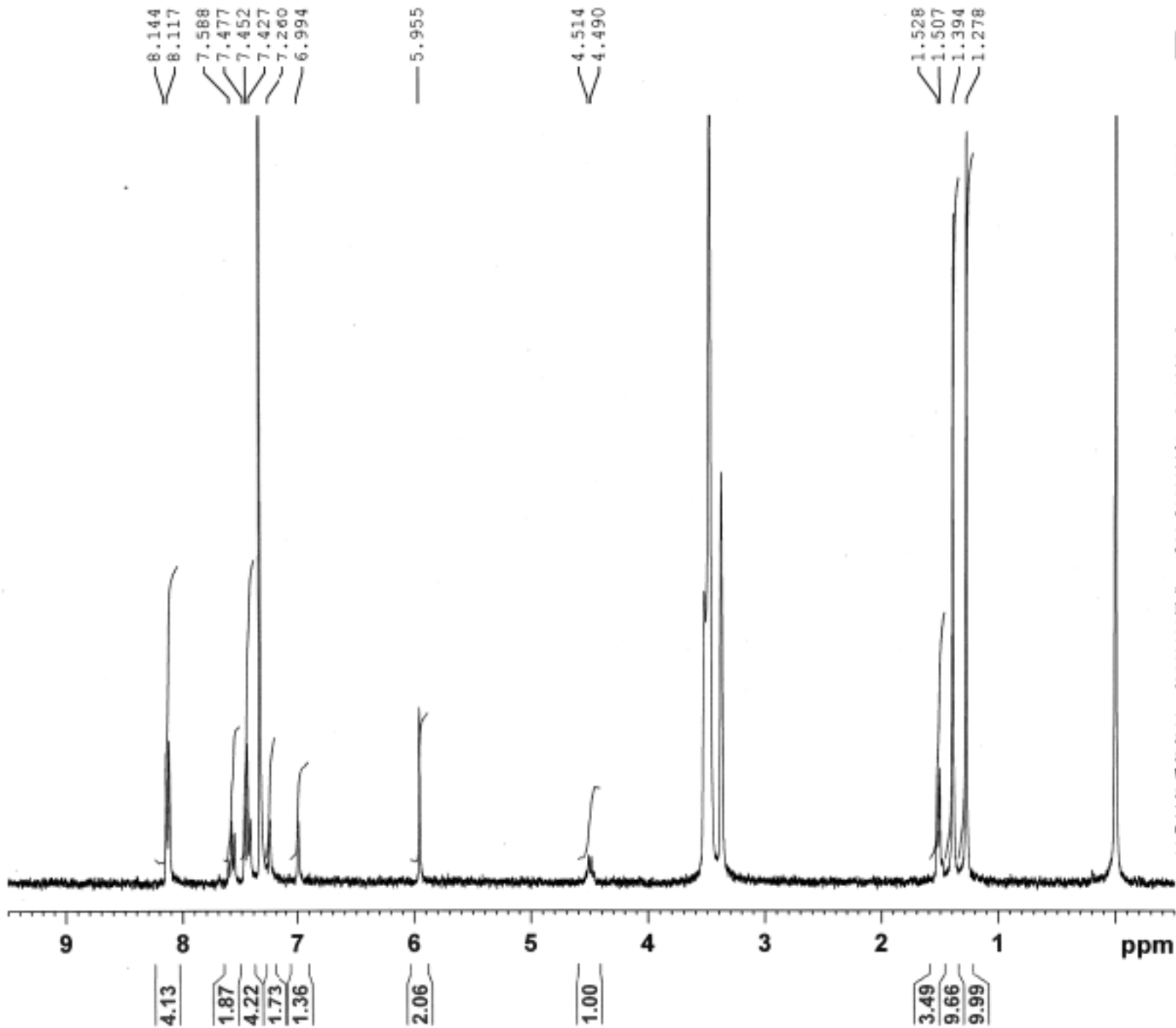




NAME A13my019nh
EXPNO 14022807
PROCNO 1
Date_ 20140228
Time_ 18.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 15.00 usec
PL1 1.20 dB
PL1W 8.19348145 W
SFO1 300.1318534 MHz
SI 32768
SF 300.1299823 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



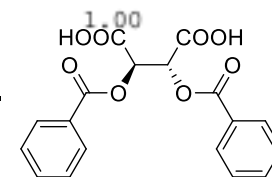
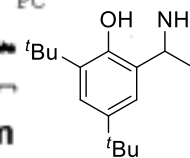


Current Data Parameters
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 EXPNO 29
 PROCNO 1

F2 - Acquisition Parameters
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 Time_ 9.25
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6188.119 Hz
 FIDRES 0.094423 Hz
 AQ 5.2953587 sec
 RG 203
 DW 80.800 usec
 DE 6.50 usec
 TE 296.5 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 15.00 usec
 PL1 1.20 dB
 PL1W 8.19348145 W
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1299808 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



1b-5

7.435
7.287
7.279
7.055
7.047

4.589
4.566
4.544
4.522
4.280
4.177
4.158
4.147
4.129
2.535
2.514
2.506
2.495
2.484
2.477
2.467
2.462
2.455
2.450
2.444
2.432
2.426
2.415
2.387
2.377
2.370
2.358
2.353
2.337
2.323
2.297
2.267
2.224
2.204
2.191
2.184
2.171
2.164
2.160
2.153
2.141
2.136
2.132
1.585
1.562
1.426
1.300



Current Data Parameters
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EXPNO 30
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111007
Time_ 15.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 6188.119 Hz
FIDRES 0.094423 Hz
AQ 5.2953587 sec
RG 203
DW 80.800 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 15.00 usec
PL1 1.20 dB
PL1W 8.19348145 W
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1311721 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

