

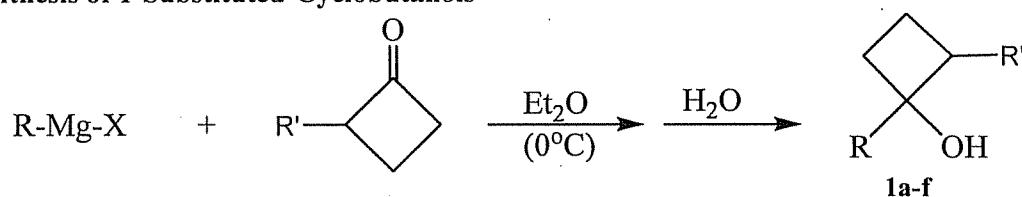
Synthesis of γ -halogenated ketones via the Ce(IV)-mediated oxidative coupling of cyclobutanols and inorganic anions

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Supplemental Information

1. Synthesis of 1-Substituted-Cyclobutanols



Entry	R	R'	X	Product	Yield (%) ^a
1		H	Br	1a	67
2		H	Br	1b	39
3		H	Br	1c	88
4		H	Cl	1d	61
5	$\text{CH}_3(\text{CH}_2)_5$	H	Br	1e	24
6		Et	Br	1f	85

^aIsolated yield

2. Characterization of Compounds

1-Phenyl-1-cyclobutanol (**1a**): ¹H-NMR (CDCl₃, 500MHz) – δ 7.50 (m, 2H), 7.38-7.35 (m, 2H), 7.29-7.27 (m, 2H), 2.58-2.54 (m, 2H), 2.39-2.33 (m, 2H), 2.08-1.97 (m, 1H), 1.96 (s, 1H), 1.72-1.68 (m, 1H).
¹³C-NMR (CDCl₃, 125MHz) – δ 146.22, 128.45, 127.25, 124.93, 36.81, 12.99.

1-*p*-Methoxyphenyl-1-cyclobutanol (**1b**): ¹H-NMR (CDCl₃, 500MHz) – δ 7.42 (m, 2H), 6.90-6.89 (m, 2H), 3.80 (s, 3H), 2.55-2.50 (m, 2H), 2.37-2.32 (m, 2H), 2.01-1.92 (m, 1H), 1.94 (s, 1H), 1.65-1.62 (m,

1H). ¹³C-NMR (CDCl₃, 125MHz) – δ 158.76, 126.34, 113.72, 109.31, 55.29, 36.84, 12.87. Bp 65-68°C (at <25mtorr).

1-*p*-Fluorophenyl-1-cyclobutanol (**1c**): ¹H-NMR (CDCl₃, 500MHz) – δ 7.49-7.46 (m, 2H), 7.07-7.03 (m, 2H), 2.58-2.51 (m, 2H), 2.40-2.33 (m, 2H), 2.05-1.97(m, 1H), 2.01 (s, 1H), 1.72-1.63 (m, 1H). ¹³C-NMR (CDCl₃, 125MHz) – δ 161.96 (d), 142.04 (d), 126.78 (d), 115.13 (d), 37.01, 12.87.

1-Cyclohexyl-1-cyclobutanol (**1d**): ¹H-NMR (CDCl₃, 500MHz) – δ 2.15-2.12 (m, 2H), 1.90-1.65 (m, 8H), 1.59-1.49 (m, 1H), 1.45 (s, 1H), 1.41-1.36 (m, 1H), 1.27-1.09 (m, 3H), 1.06-0.94 (m, 2H). ¹³C-NMR (CDCl₃, 125MHz) – δ 78.02, 45.48, 33.85, 26.47, 26.44, 25.58, 12.36. Bp 34-35°C (at <70mtorr).

1-Hexyl-1-cyclobutanol (**1e**): ¹H-NMR (CDCl₃, 500MHz) – δ 2.05-1.92 (m, 4H), 1.76-1.68 (m, 1H), 1.57 (t, 3H, *J* = 6.75Hz), 1.54-1.44 (m, 1H), 1.35-1.26 (m, 8H), 1.24 (s, 1H), 0.87 (t, 3H, *J* = 6.73Hz). ¹³C-NMR (CDCl₃, 125MHz) – δ 75.40, 39.54, 35.91, 31.88, 29.70, 23.33, 22.62, 14.0008, 12.11. Bp 33-35°C (at <50mtorr).

2-Ethyl-1-*p*-fluorophenyl-1-cyclobutanol (**1f**): ¹H-NMR (CDCl₃, 500MHz) – δ 7.48-7.40 (m, 2H), 7.07-7.01 (m, 2H), 2.55-2.51 (m, 1H), 2.40-2.38 (m, 1H), 2.19-2.14 (m, 1H), 2.00-1.97 (m, 1H), 1.82-1.78 (m, 1H), 1.80 (s, 1H), 1.69-1.51 (m, 2H), 0.90-0.86 (t, 3H, *J* = 7.44 Hz). ¹³C-NMR (CDCl₃, 125MHz) – δ 161.78 (d), 143.12 (d), 126.54 (d), 114.98 (d), 78.29, 47.59, 34.31, 22.33, 21.32, 11.38.

4-Iodo-1-phenyl-1-butanone (**2a**): ¹H-NMR (CDCl₃, 500MHz) – δ 7.97-7.96 (m, 2H), 7.58-7.7.54 (m, 1H), 7.48-7.45 (m, 2H), 3.32 (t, 2H, *J* = 6.70 Hz), 3.12 (t, 2H, *J* = 6.97 Hz), 2.25 (quin, 2H, *J* = 6.83Hz). ¹³C-NMR (CDCl₃, 125MHz) – δ 198.62, 136.72, 133.24, 128.66, 128.02, 38.92, 27.52, 6.78.

4-Iodo-1-*p*-methoxyphenyl-1-butanone (**2b**): ¹H-NMR (CDCl₃, 500MHz) – δ 7.96-7.93 (m, 2H), 6.94-6.92 (m, 2H), 3.87 (s, 3H), 3.31 (t, 2H, *J* = 6.65 Hz), 3.07 (t, 2H, *J* = 7.04), 2.23 (quin, 2H, *J* = 6.84 Hz). ¹³C-NMR (CDCl₃, 125MHz) – δ 197.16, 163.55, 130.28, 129.81, 113.76, 55.47, 38.52, 27.72, 7.02.

1-*p*-Fluorophenyl-4-iodo-1-butanone (**2c**): ¹H-NMR (CDCl₃, 500MHz) – δ 8.03-7.97 (m, 2H), 7.18-7.11 (m, 2H), 3.35-3.29 (t, 2H, *J* = 6.66 Hz), 3.13-3.08 (t, 2H, *J* = 7.01 Hz), 2.29-2.20 (quin, 2H, *J* = 6.84 Hz). ¹³C-NMR (CDCl₃, 125MHz) – δ 196.93, 165.76 (d), 133.11 (d), 130.62 (d), 115.72 (d), 38.78, 27.39, 6.71.

1-Cyclohexyl-4-iodo-1-butanone (**2d**): ¹H-NMR (CDCl₃, 500MHz) – δ 3.20 (t, 2H, *J* = 6.61 Hz), 2.57 (t, 2H, *J* = 7.00 Hz), 2.34-2.30 (m, 1H), 2.04 (quin, 2H, *J* = 6.74 Hz), 1.86-1.62 (m, 5H), 1.36-1.13 (m, 5H). ¹³C-NMR (CDCl₃, 125MHz) – δ 212.63, 50.96, 40.72, 28.48, 26.97, 25.80, 25.63, 6.97. HR-MS (FAB+): *m/z* 281.0397 (M+H)⁺ for C₁₀H₁₈OI: Calcd. 281.04.

1-Iodo-4-decanone (**2e**): ¹H-NMR (CDCl₃, 500MHz) – δ 3.21 (t, 2H, *J* = 6.56 Hz), 2.54 (t, 2H, *J* = 6.91 Hz), 2.39 (t, 2H, *J* = 7.44 Hz), 2.05 (quin, 2H, *J* = 6.73 Hz), 1.58-1.52 (m, 2H), 1.30-1.24 (m, 6H), 0.87 (t, 3H, *J* = 6.91 Hz). ¹³C-NMR (CDCl₃, 125MHz) – δ 209.76, 43.07, 42.79, 31.56, 28.87, 27.02, 23.81, 22.47, 14.02, 6.71.

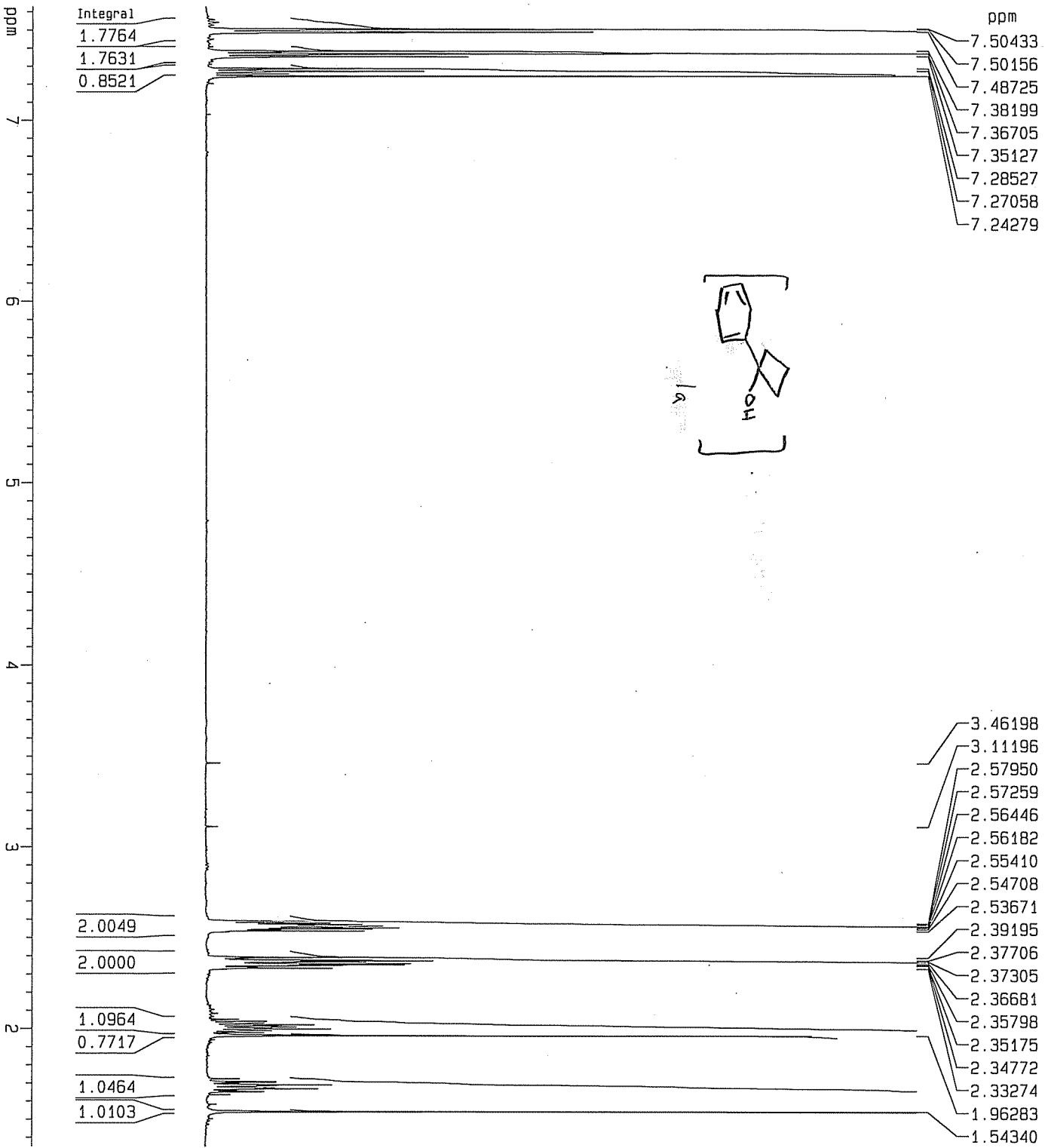
2-Ethyl-1-*p*-fluorophenyl-4-iodo-1-butanone (**2c**): ¹H-NMR (CDCl₃, 500MHz) – δ 8.05-8.00 (m, 2H), 7.18-7.13 (m, 2H), 4.20-4.16 (m, 1H), 3.26-3.14 (m, 2H), 2.22-2.17 (m, 2H), 1.97-1.82 (m, 2H), 1.10-1.06 (t, 3H, *J* = 7.22 Hz). ¹³C-NMR (CDCl₃, 125MHz) – δ 197.38, 165.78 (d), 133.15 (d), 130.66 (d), 115.71 (d), 41.66, 38.72, 34.25, 34.15, 14.12.

4-Bromo-1-phenyl-1-butanone (**3a**): $^1\text{H-NMR}$ (CDCl_3 , 500MHz) – δ 7.98-7.96 (m, 2H), 7.58-7.55 (m, 1H), 7.48-7.45 (m, 2H), 3.54 (t, 2H, $J = 6.27$ Hz), 3.18 (t, 2H, $J = 6.86$ Hz), 2.30 (quin, 2H, $J = 6.64$ Hz). $^{13}\text{C-NMR}$ (CDCl_3 , 125MHz) – δ 198.81, 136.71, 133.24, 128.65, 128.01, 36.54, 33.64, 26.83.

4-Bromo-1-*p*-methoxyphenyl-1-butanone (**3b**): $^1\text{H-NMR}$ (CDCl_3 , 500MHz) – δ 7.96-7.95 (m, 2H), 6.94-6.91 (m, 2H), 3.86 (s, 1H), 3.53 (t, 2H, $J = 6.35$ Hz), 3.12 (t, 2H, $J = 6.96$ Hz), 2.29 (quin, 2H, $J = 6.60$ Hz). $^{13}\text{C-NMR}$ (CDCl_3 , 125MHz) – δ 197.31, 163.52, 130.24, 129.79, 113.72, 55.44, 36.12, 33.76, 27.01.

4-Bromo-1-*p*-fluorophenyl-1-butanone (**3c**): $^1\text{H-NMR}$ (CDCl_3 , 500MHz) – δ 8.03-7.98 (m, 2H), 7.17-7.11 (m, 2H), 3.57-3.53 (t, 2H, $J = 6.33$ Hz), 3.18-3.13 (t, 2H, $J = 6.97$ Hz), 2.33-2.26 (quin, 2H, $J = 6.58$ Hz). $^{13}\text{C-NMR}$ (CDCl_3 , 125MHz) – δ 197.13, 165.77 (d), 133.12 (d), 130.62 (d), 115.72 (d), 36.41, 33.53, 26.74.

3. Spectral Data for 1a-f, 2a-f and 3a-c



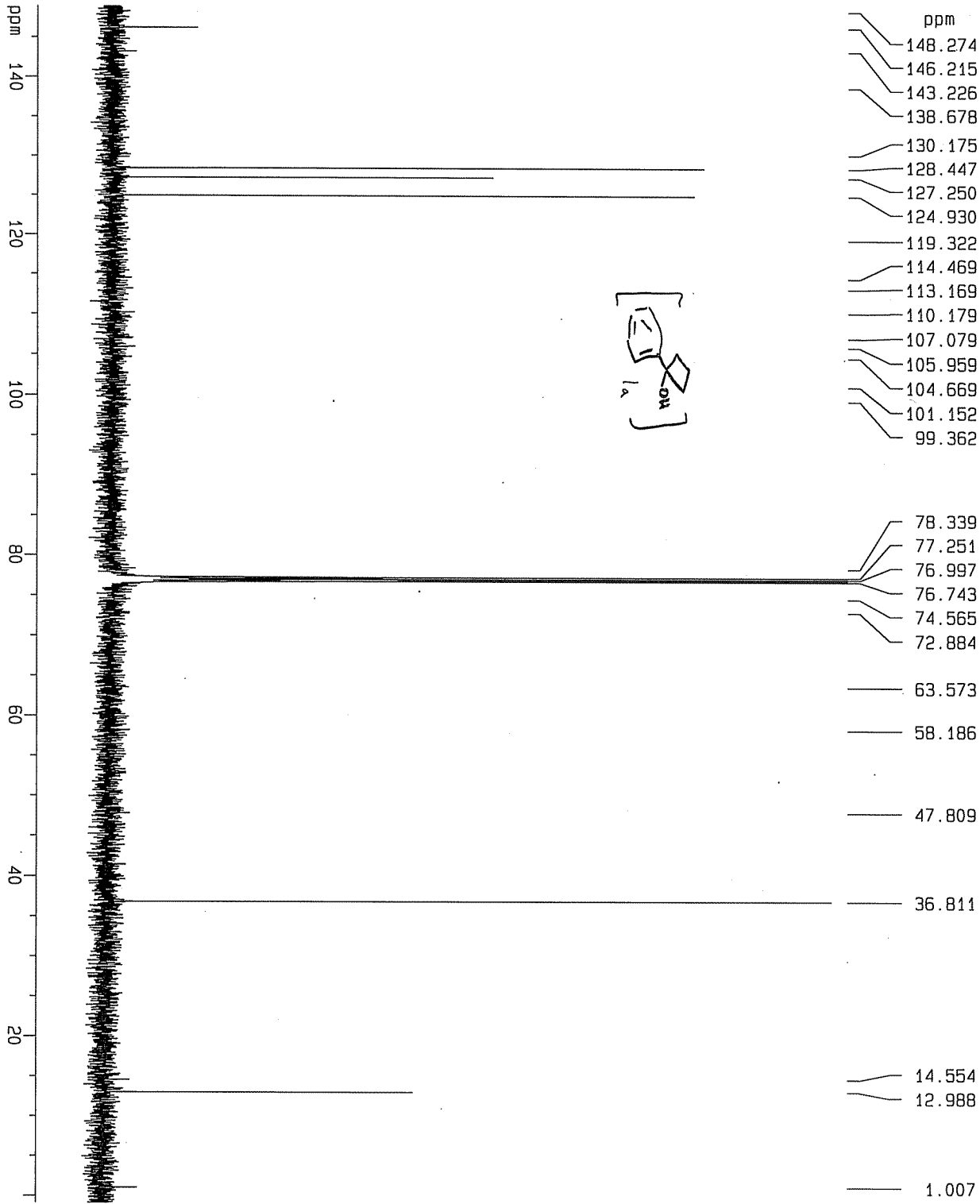
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Current Data Parameters
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 DE 7.00 usec

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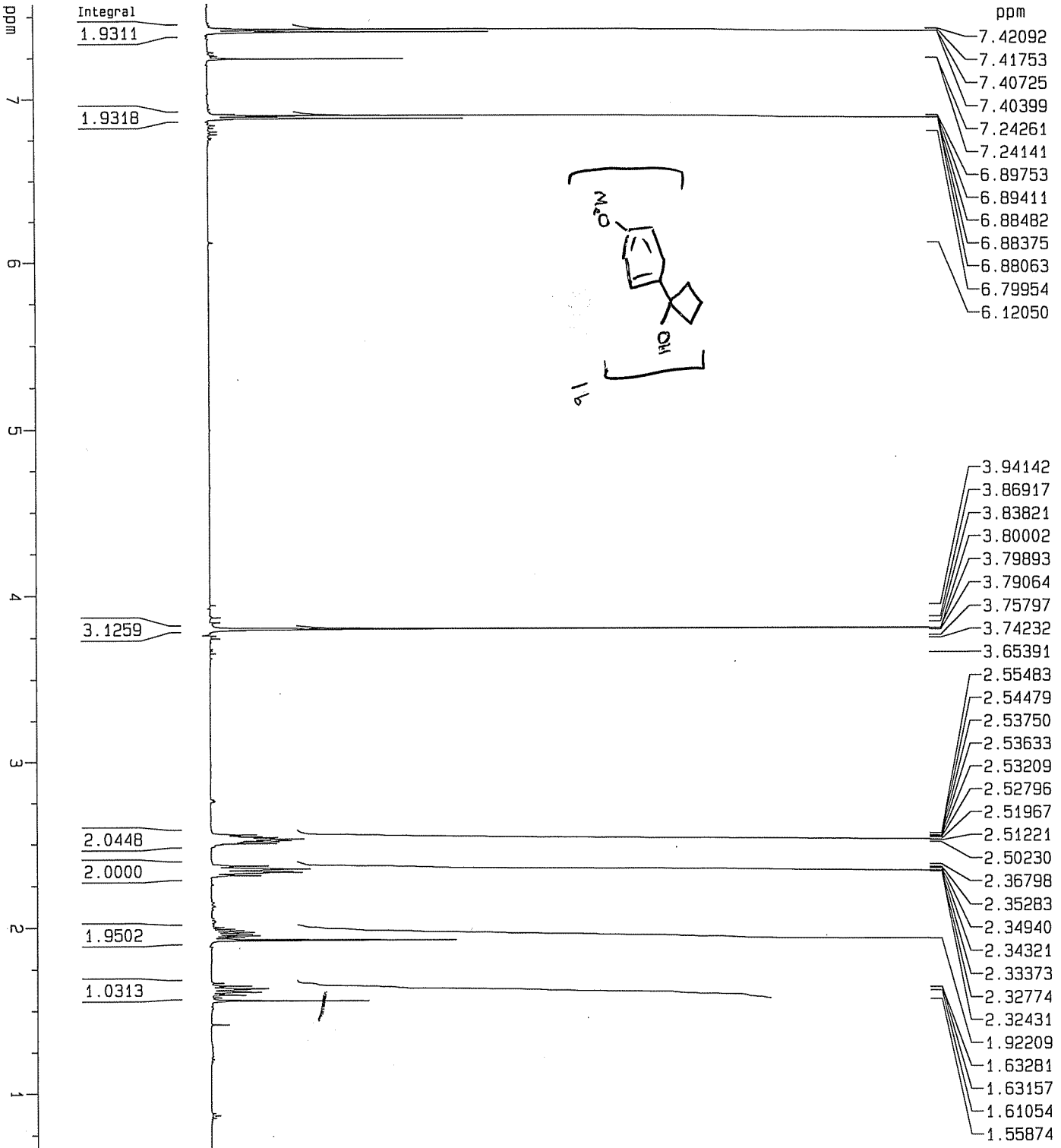
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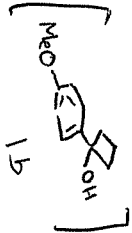
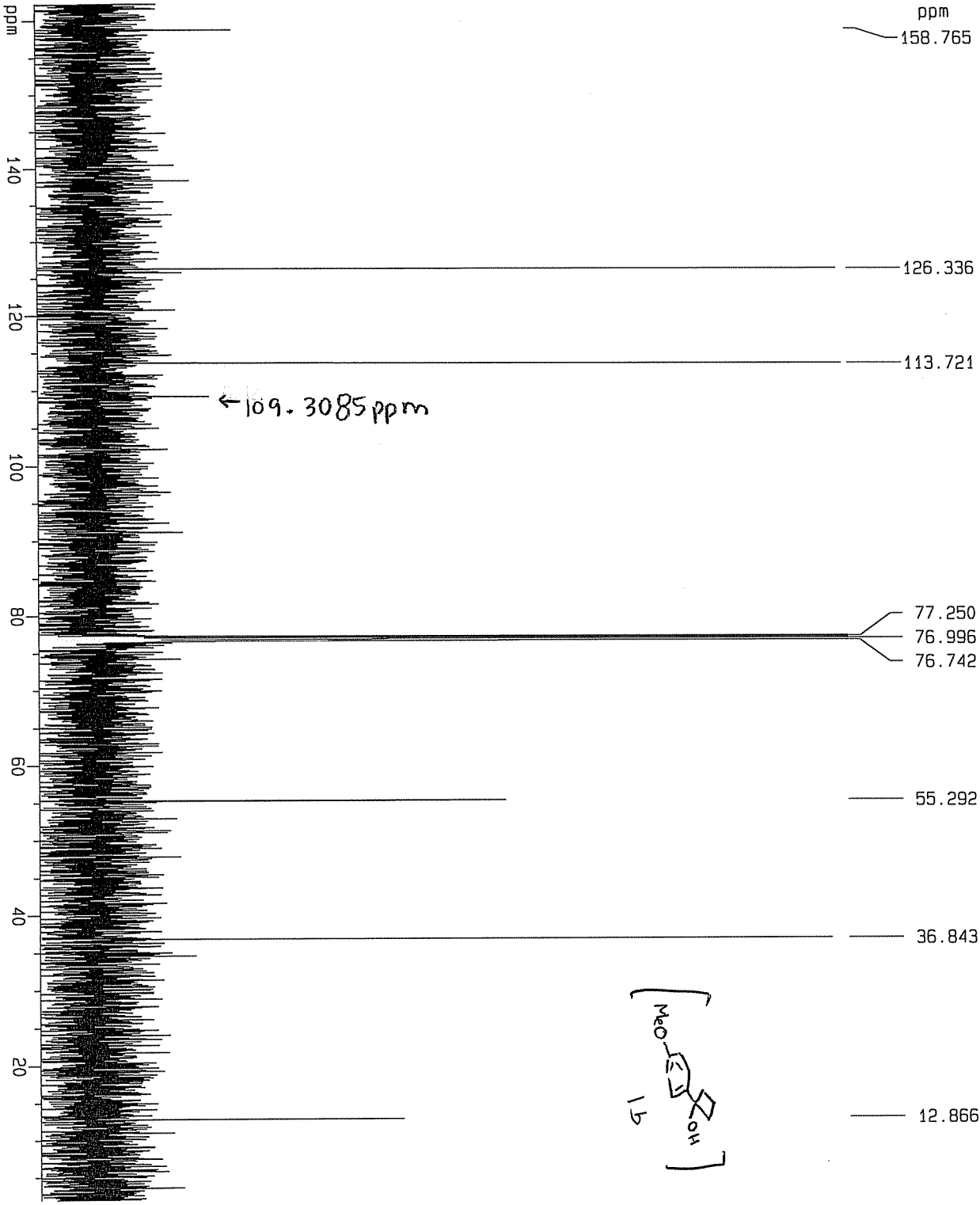
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1D NMR plot parameters

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Crude

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7.04

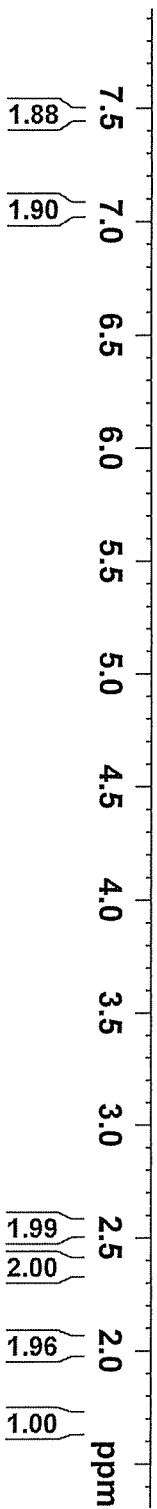
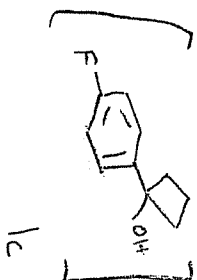
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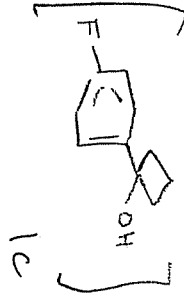
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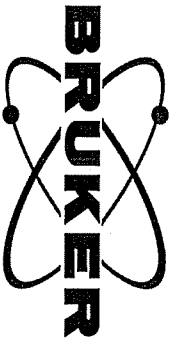


Crude

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 115.04



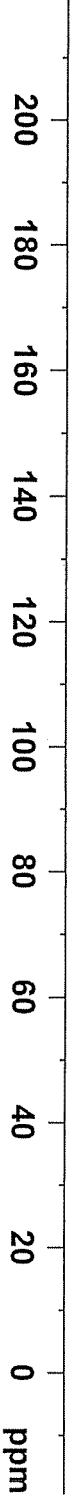
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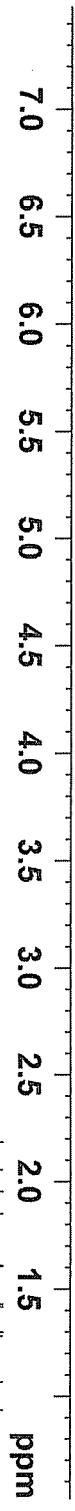
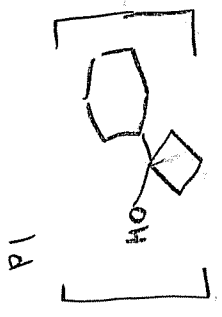
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CYHexCyButol-0522208

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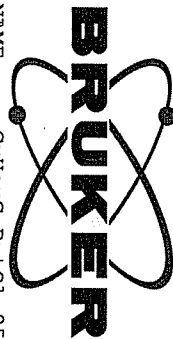


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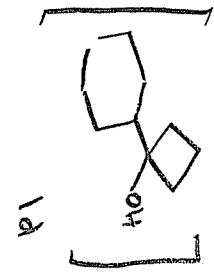
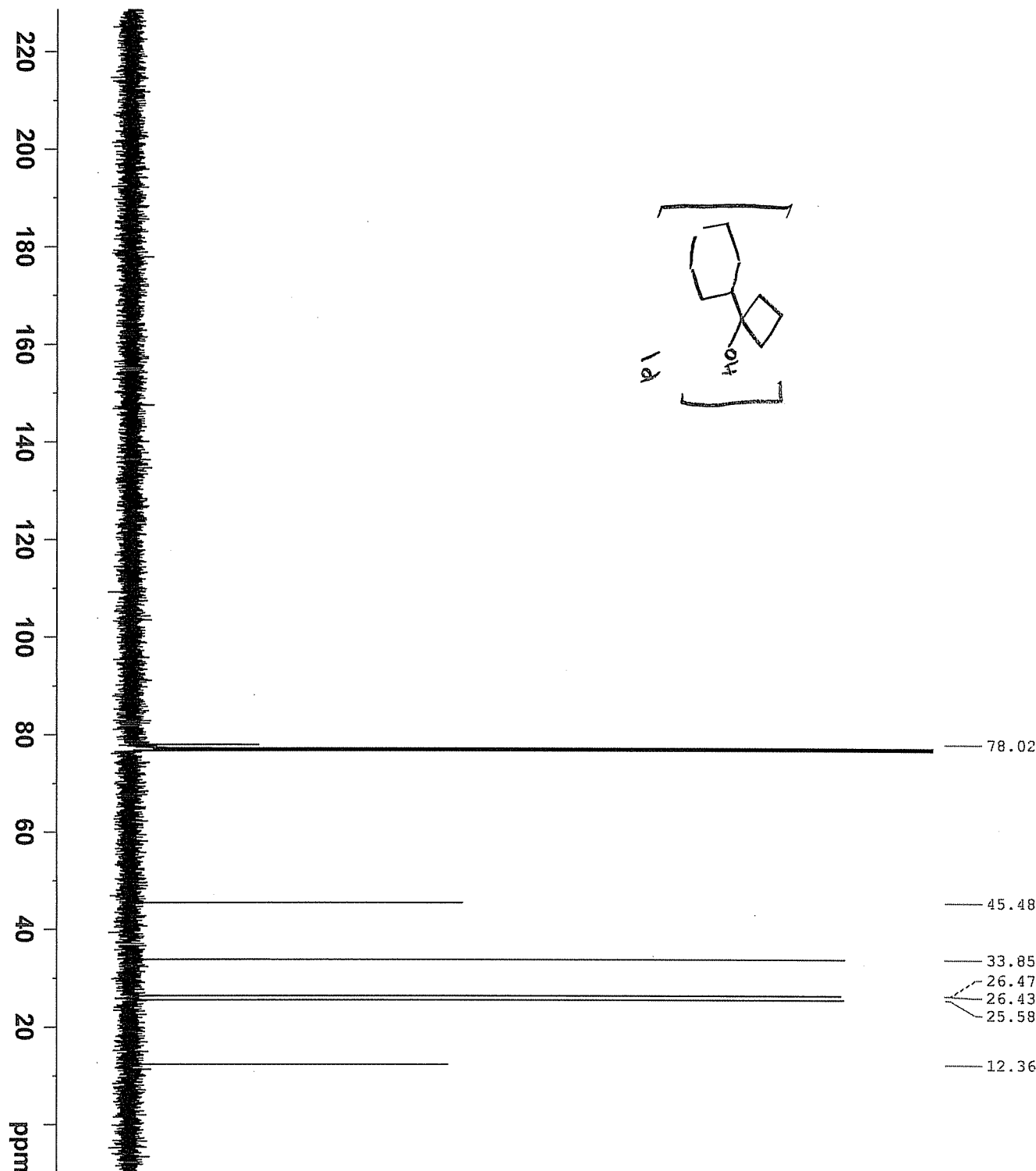
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CYHexCyBut01-052208

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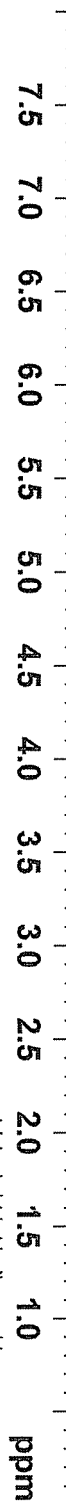
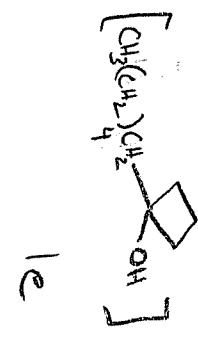


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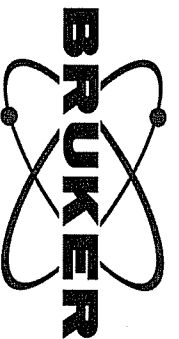
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 SI 32768
 SF 500.1300225 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 4.00

2.04
2.04
2.03
2.03
2.02
2.02
2.01
2.01
2.01
2.00
1.99
1.97
1.97
1.96
1.95
1.73
1.73
1.71
1.58
1.57
1.55
1.52
1.50
1.49
1.48
1.48
1.46
1.46
1.35
1.34
1.33
1.31
1.30

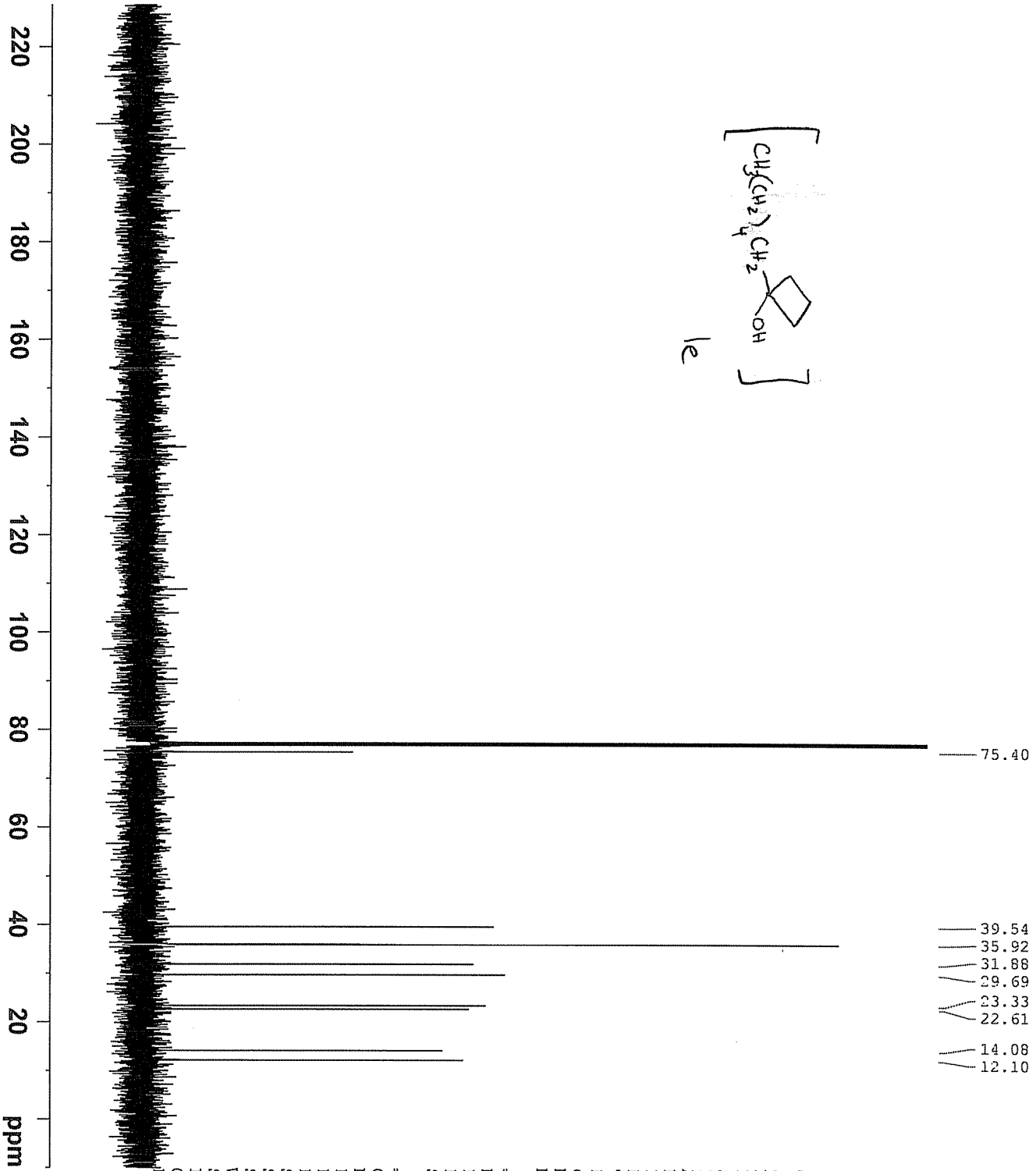
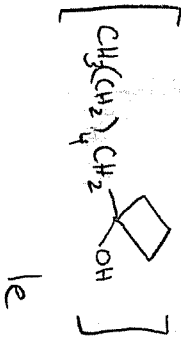


1.93
2.03
1.00
3.07
1.07
8.04
0.41
3.10

ppm



39.54
 35.92
 31.88
 29.69
 23.33
 22.61
 14.08
 12.10



```

NAME HexBut01-052608
EXPNO 2
PROCNO 1
Date_ 20080527
Time 8.08
INSTRUM spect
PROBHD 5 mm PHBBO BB-
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 112
DS 0
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0912410 sec
RG 9195.2
DW 16.650 usec
DE 7.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
  
```

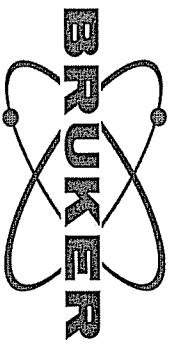
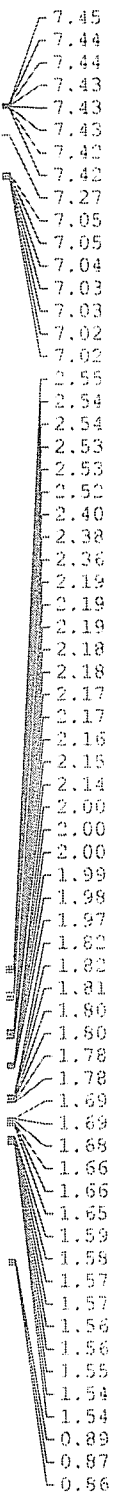
```

===== CHANNEL F1 =====
NUC1 13C
P1 5.00 usec
PL1 -1.00 dB
SFO1 125.7715390 MHz
  
```

```

===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 110.00 usec
PL2 17.50 dB
PL12 17.00 dB
SFO2 500.1325000 MHz
SI 65536
SF 125.7577931 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
  
```

High Vac

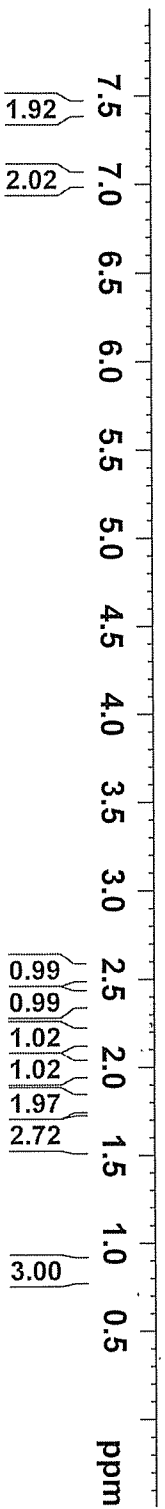


Current Data Parameters
 NAME p-F-Pn-CyButol-2EtHy1-120508
 EXPMO 8
 PROCNO 1

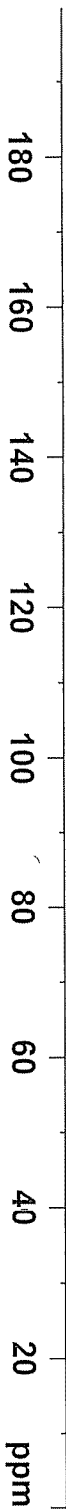
F2 - Acquisition Parameters
 Date_ 20081206
 Time_ 11.21
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 6
 DS 0
 SWH 6009.615 Hz
 FIDKRS 0.183399 Hz
 AQ 2.7264509 sec
 RG 256
 DW 83.200 usec
 DE 6.00 usec
 TE 297.5 K
 D1 1.00000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 1H
 P1 14.00 usec
 PL1 1.00 dB
 SFO1 500.1327510 MHz

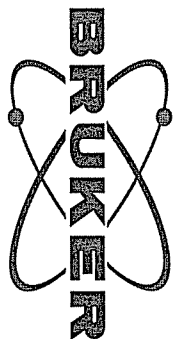
F2 - Processing parameters
 SI 32768
 SF 500.1300102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



13C-NMR-Clean



Current Data Parameters
 NAME p-F-ph-Cybutol-2Ethy-1-120508
 EXPNO 9
 PROCNO 1



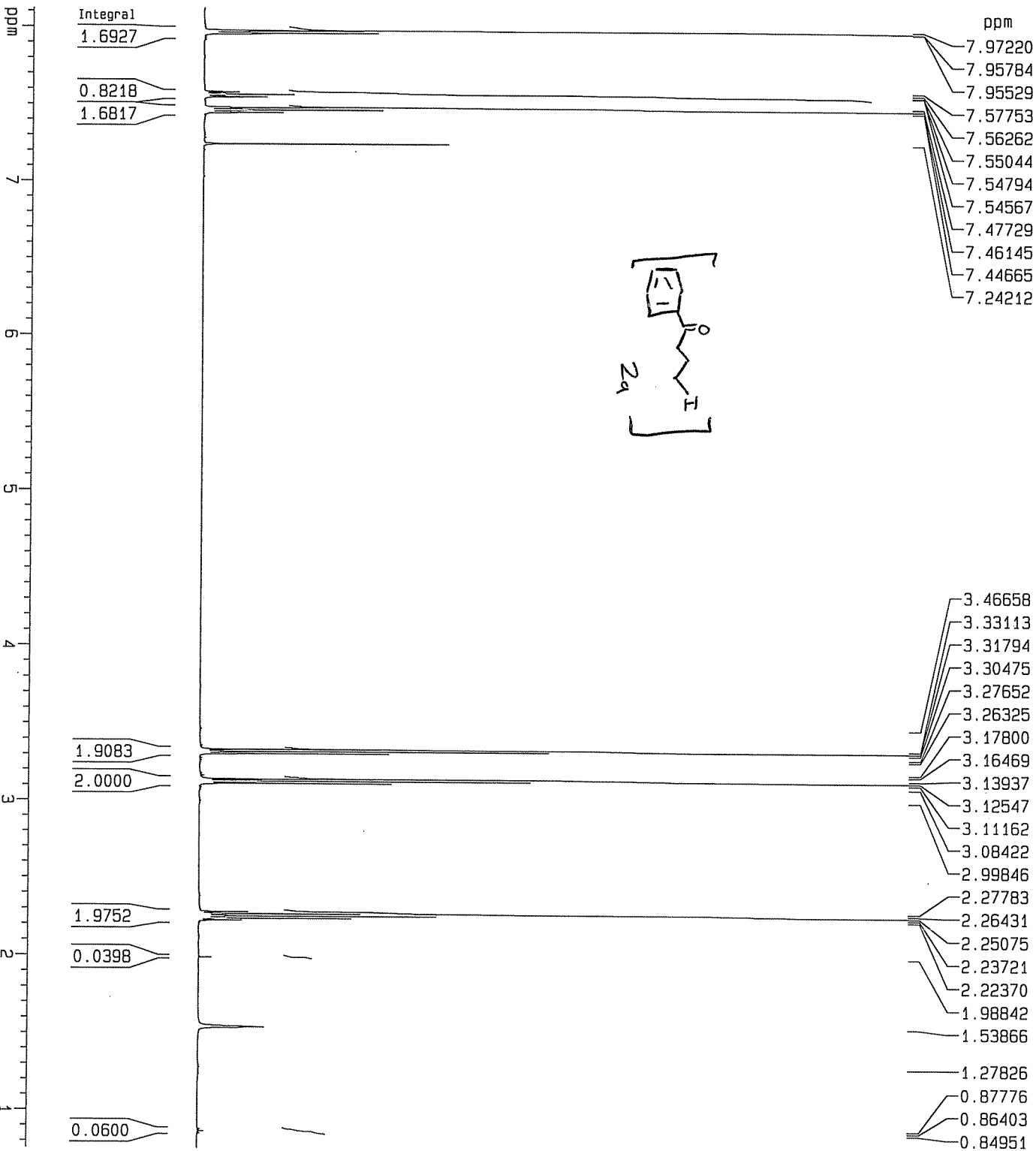
F2 - Acquisition Parameters
 Date_ 20081206
 Time_ 11.24
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 401
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 3251
 DM 16.650 usec
 DE 7.00 usec
 TE 297.9 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.35 usec
 PL1 1.00 dB
 SFO1 125.7703640 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPDD2 100.00 usec
 PL2 17.50 dB
 PL12 17.50 dB
 SFO2 500.1322150 MHz

F2 - Processing parameters
 SI 32768
 SF 125.757923 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

ppm



Current Data Parameters
 NAME 4-I-ButPhenone-051408
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080515
 Time 13.51

INSTRUM spect
 PROBHD 5 mm PHEB0 BB-
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 10
 DS 0

SMH 7507.507 Hz
 FIDRES 0.229111 Hz
 AG 2.1824653 sec
 RG 287.4

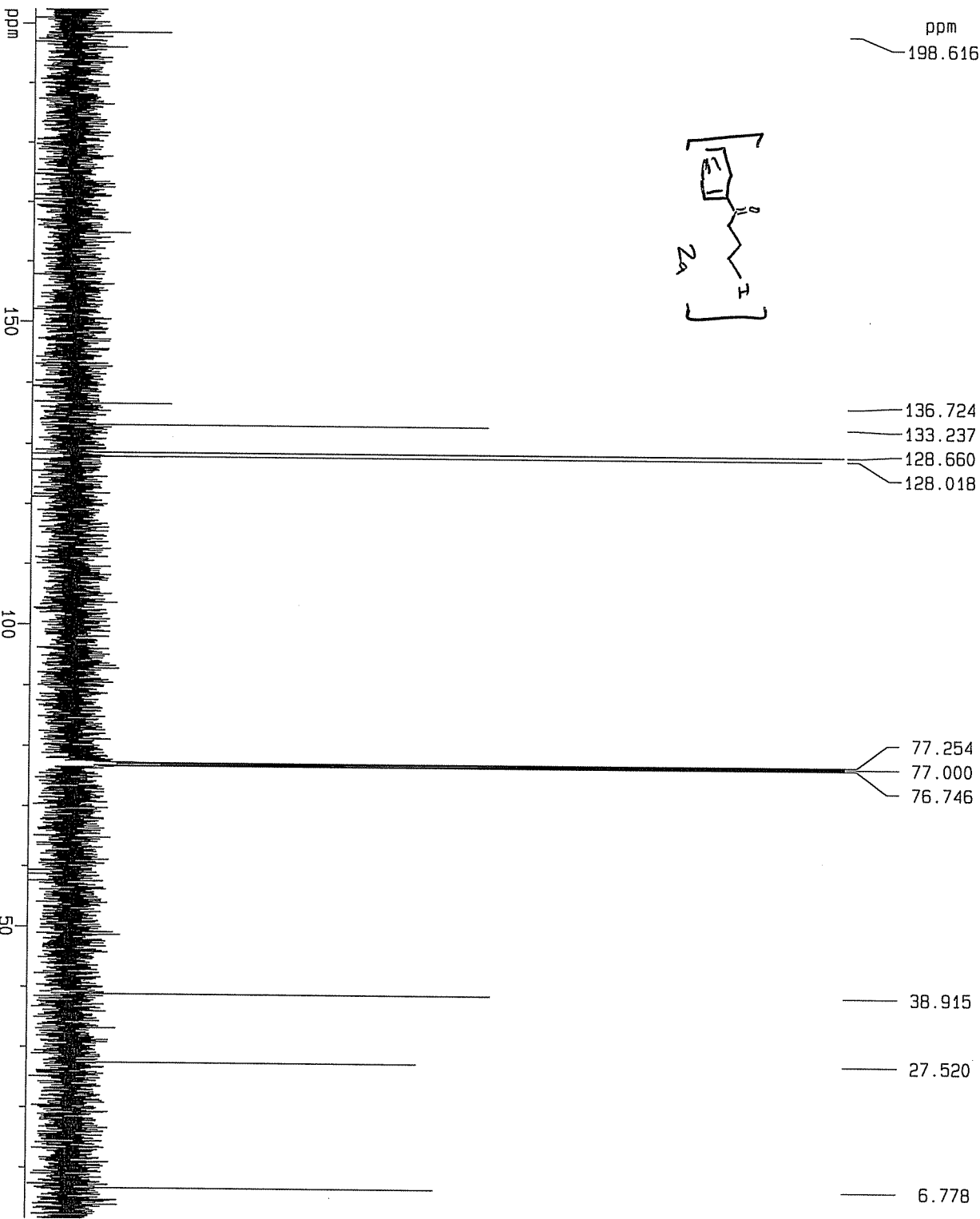
DW 66.600 usec
 DE 7.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 6.00 usec
 PL1 -4.00 dB
 SFO1 500.1323989 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 off
 PCPD2 100.00 usec
 PL2 120.00 dB
 PL12 120.00 dB
 SFO2 500.1300000 MHz

F2 - Processing parameters
 S1 32768
 SF 500.1300225 MHz
 WDM EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 8.119 ppm
 F1 4060.34 Hz
 F2P 0.753 ppm
 F2 376.75 Hz
 PPMCM 0.36826 ppm/cm
 HZCM 184.17952 Hz/cm



Current Data Parameters
 NAME 4-1-ButPhenone-051408
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080515
 Time 13.56
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg
 TD 65536
 SOLVENT CDCl3
 NS 252
 DS 0
 SMH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 1250.2
 DW 16.650 usec
 DE 7.00 usec
 TE 298.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 -1.00 dB
 SF01 125.7715390 MHz

===== CHANNEL f2 =====
 CPDPRG2 wa1tz16
 NUC2 1H
 PCPD2 110.00 usec
 PL2 17.50 dB
 PL12 17.00 dB
 SF02 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577921 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 202.486 ppm
 F1 25464.18 Hz
 F2P 1.632 ppm
 F2 205.28 Hz
 PPMCM 10.04268 ppm/cm
 HZCM 1262.94531 Hz/cm

Current Data Parameters
 NAME 4-I-pMeOPhBut-062308
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080624
 Time 17.05

INSTAUM Spect
 PROBHD 5 mm PHBBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0

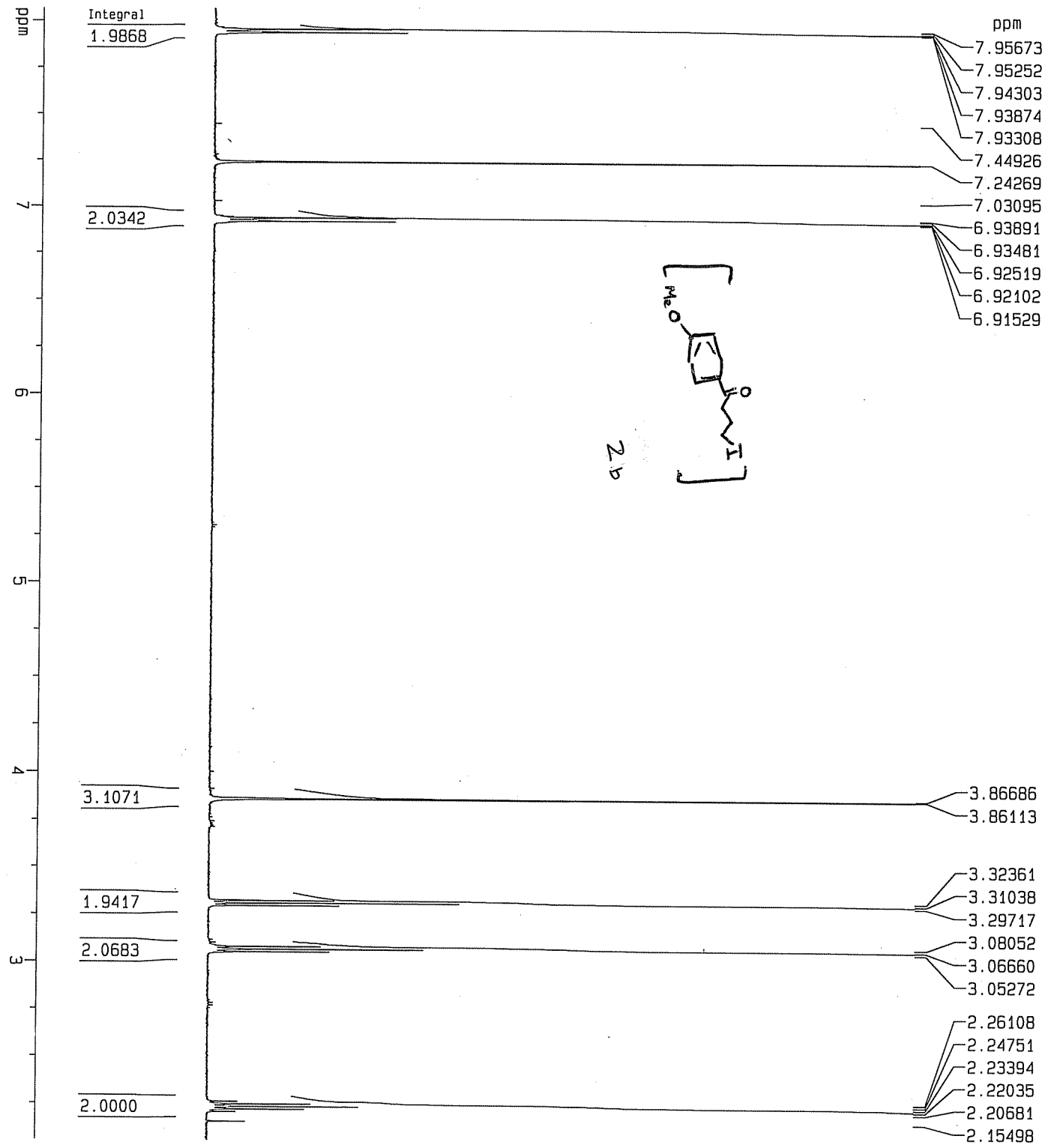
SMH 7507.507 Hz
 FIDRES 0.229114 Hz
 AQ 2.1824653 sec
 RG 362
 DW 66.600 usec
 DE 7.00 usec
 TE 296.8 K

D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWRRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 7.90 usec
 PL1 -4.00 dB
 SFO1 500.1323989 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300225 MHz
 MDM EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 8.067 ppm
 F1 4034.43 Hz
 F2P 2.055 ppm
 F2 1027.89 Hz
 PPMCM 0.30058 ppm/c
 HZCM 150.32701 Hz/cm



ppm
197.161

163.552

130.282
129.812

113.755

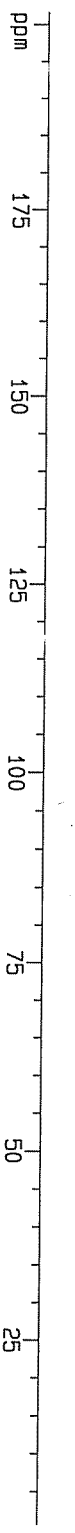
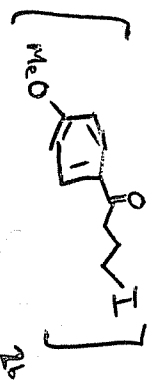
77.252
76.998
76.744

55.473

38.515

27.718

7.021



Current Data Parameters
 NAME 4-I-pMeOPhBut-062308
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20080624
 Time 17.17
 INSTRUM spect
 PROBRD 5 mm PHEB0 B9-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 53
 DS 0
 SMH 30030.029 HZ
 FIDRES 0.458222 HZ
 AQ 1.0912410 sec
 RG 2580.3
 DW 16.650 usec
 DE 7.00 usec
 TE 297.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCNMRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 1.00 DB
 SFO1 125.7715390 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 17.50 DB
 PL12 17.50 DB
 SFO2 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577949 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 5.00 cm
 F1P 201.695 ppm
 F1 25363.50 Hz
 F2P 0.582 ppm
 F2 73.19 Hz
 PPMCM 10.0517 ppm/cm
 HZCM 1264.51536 Hz/cm

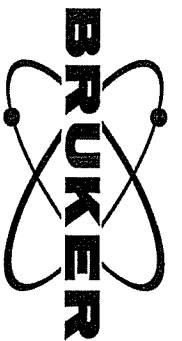
Frac3-4

8.00
8.01
8.00
7.99

7.16
7.14
7.12

3.34
3.32
3.31
3.12
3.11
3.10

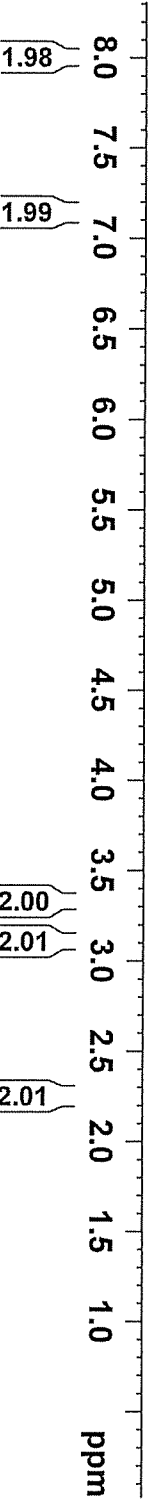
2.28
2.26
2.25
2.24
2.23

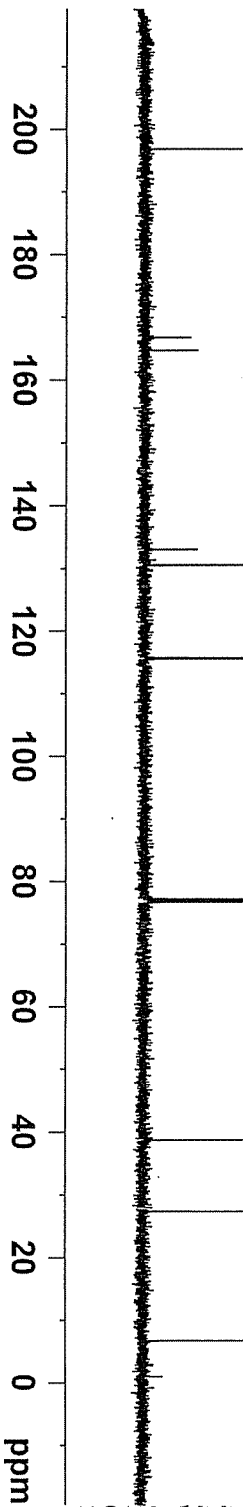
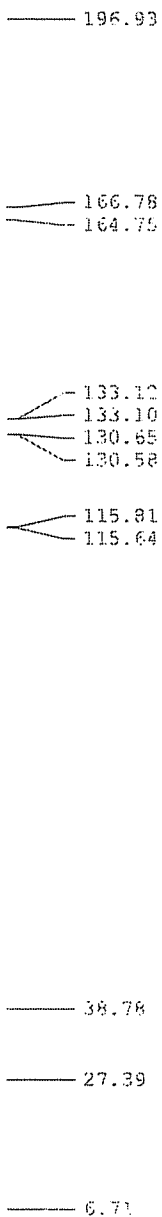


Current Data Parameters
 NAME 4-I-pf-PnBut-090808
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080908
 Time 13.56
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 6
 DS 0
 SWH 6009.615 Hz
 FIDRES 0.183399 Hz
 AQ 2.7264309 sec
 RG 90.5
 DW 83.200 usec
 DE 6.00 usec
 TE 296.4 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL F1 =====
 NUCL1 1H
 P1 7.35 usec
 PL1 1.00 dB
 SFO1 500.1327510 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.1300102 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters
 NAME 4-I-pf-PhBut-090808
 EXPNO 3
 PROCNO 1

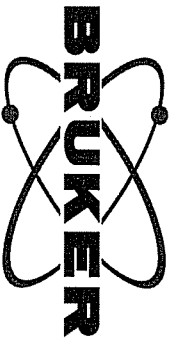


F2 - Acquisition Parameters
 Date_ 20080908
 Time 13.59
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 85
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 1448.2
 DW 16.650 usec
 DE 7.00 usec
 TE 297.5 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

==== CHANNEL F1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 1.00 dB
 SFO1 125.7703640 MHz

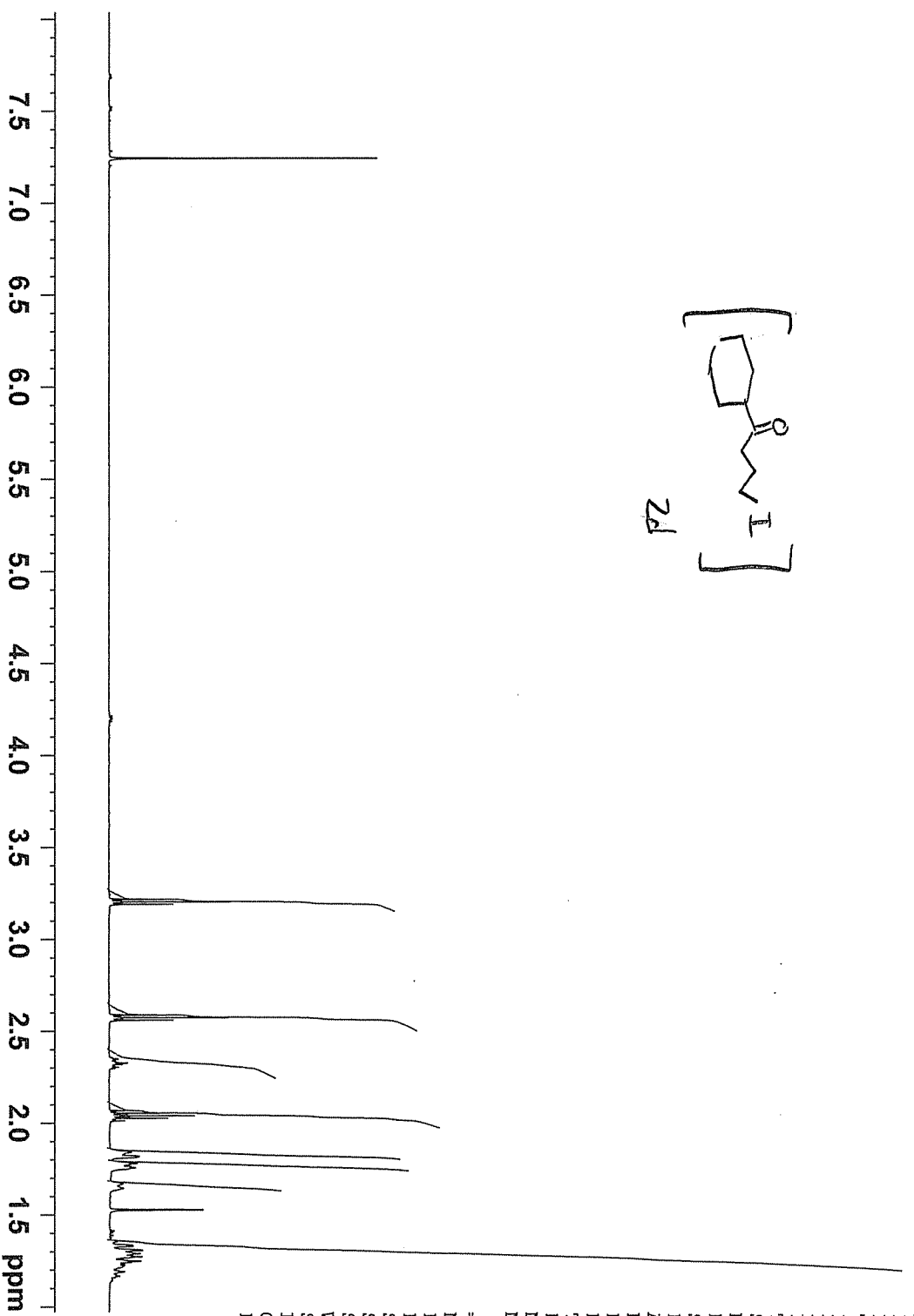
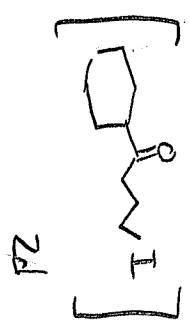
==== CHANNEL F2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 24.00 dB
 PL12 24.00 dB
 SFO2 500.1322150 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577969 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



4-I-CyHexPro-052308

- 3.22
- 3.20
- 3.19
- 2.59
- 2.57
- 2.56
- 2.33
- 2.32
- 2.07
- 2.05
- 2.04
- 2.03
- 2.01
- 1.84
- 1.82
- 1.78
- 1.76
- 1.67
- 1.64
- 1.53
- 1.33
- 1.31



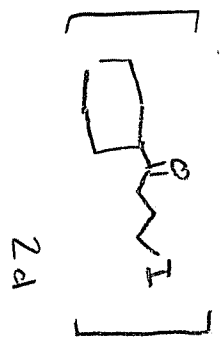
- 1.88
- 2.02
- 1.10
- 2.17
- 1.92
- 1.97
- 1.15
- 5.18

```

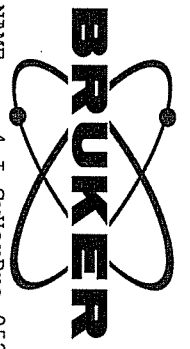
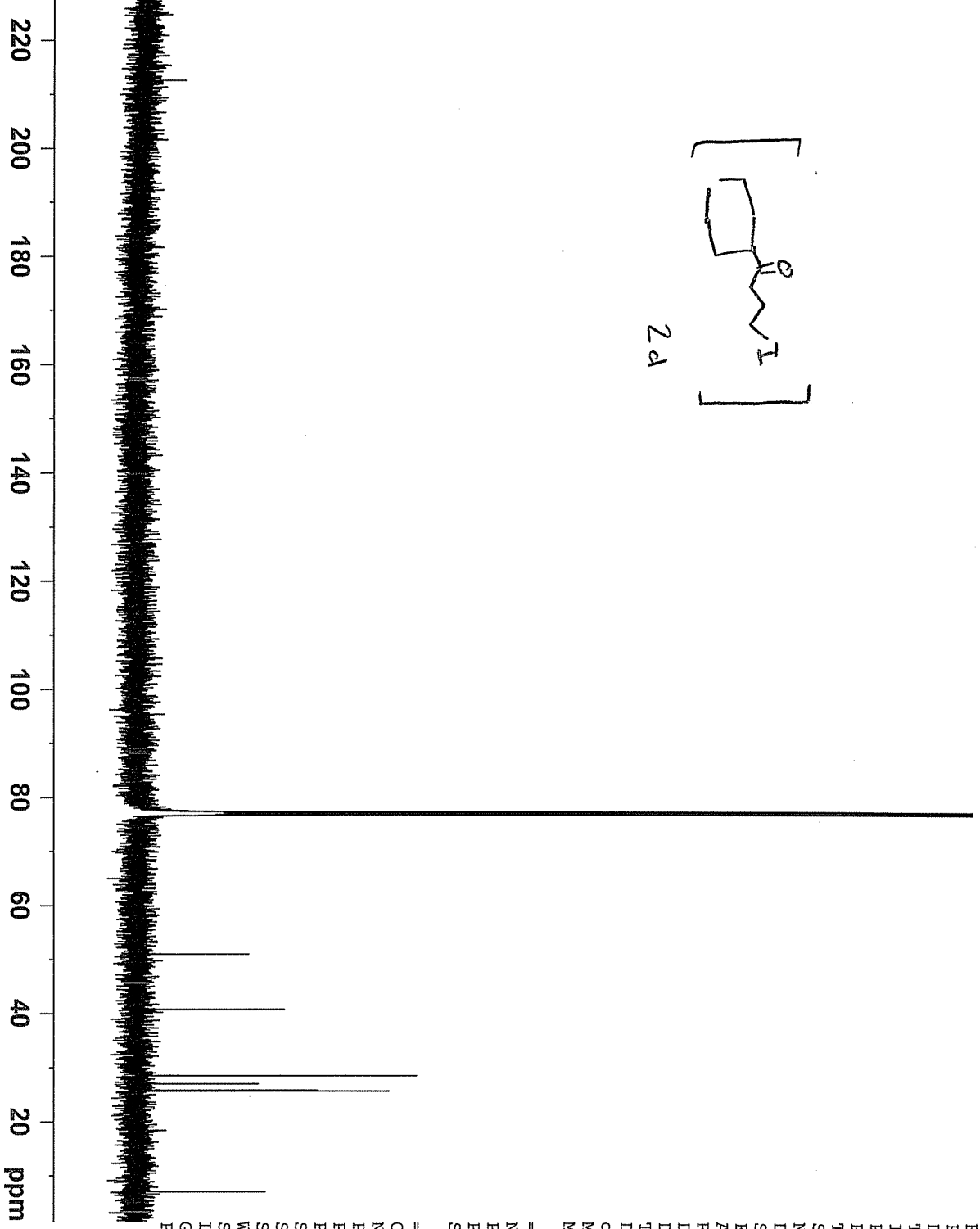
NAME 4-I-CyHexPro-052308
EXPNO 4
PROCNO 1
Date_ 20080523
Time 17.04
INSTRUM spect
PROBHD 5 mm PNBBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 7507.507 Hz
FIDRES 0.2229111 Hz
AQ 2.1824653 sec
RG 256
DW 66.600 usec
DE 7.00 usec
TE 295.5 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCTWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 6.00 usec
PL1 -4.00 dB
SFO1 500.1323989 MHz
SI 32768
SF 500.1300225 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 4.00
  
```

212.63



50.96
 40.72
 28.48
 26.97
 25.80
 25.63
 6.96

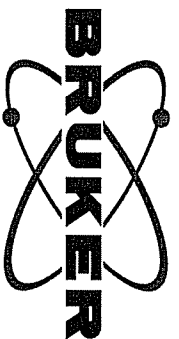


NAME 4-I-CyHexPro-052308

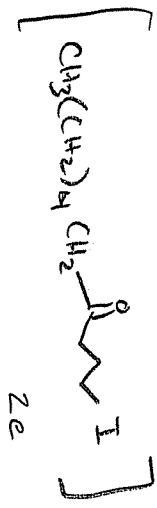
EXPNO 3
 PROCNO 1
 Date_ 20080523
 Time 13.11
 INSTRUM spect
 PROBHD 5 mm PNBBO BB-
 PULPROG zgpg
 TD 65536
 SOLVENT CDCl3
 NS 2789
 DS 0
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 5160.6
 DW 16.650 usec
 DE 7.00 usec
 TE 296.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCWRK 0.01500000 sec

==== CHANNEL F1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 -1.00 dB
 SFO1 125.7715390 MHz

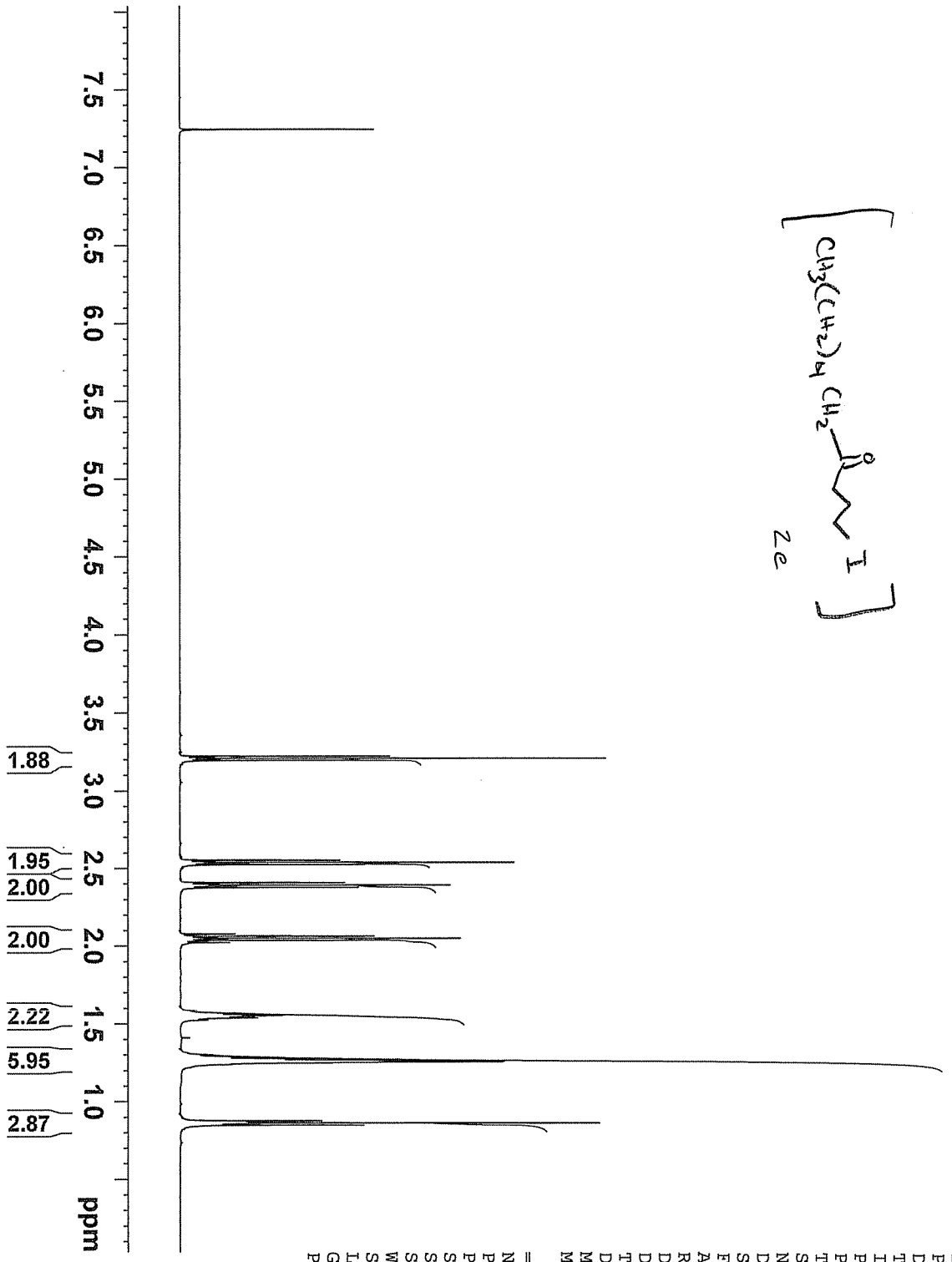
==== CHANNEL F2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 110.00 usec
 PL2 17.50 dB
 PL12 17.00 dB
 SFO2 500.1325000 MHz
 SI 65536
 SF 125.7577926 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



4-I-HexBut2-060408



- 3.22
- 3.21
- 3.19
- 2.55
- 2.54
- 2.52
- 2.41
- 2.39
- 2.38
- 2.06
- 2.05
- 2.04
- 1.55
- 1.54
- 1.29
- 1.27
- 1.26
- 1.26
- 1.25
- 0.88
- 0.87
- 0.86
- 0.85



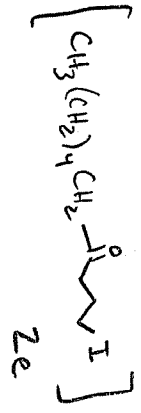
```

NAME 4-I-HexBut2-060408
EXPNO 1
PROCNO 1
Date_ 20080604
Time 16.31
INSTRUM spect
PROBHD 5 mm PHEBO BB-
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 7507.507 Hz
FIDRES 0.229111 Hz
AQ 2.1824653 sec
RG 161.3
DW 66.600 usec
DE 7.00 usec
TE 295.4 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
  
```

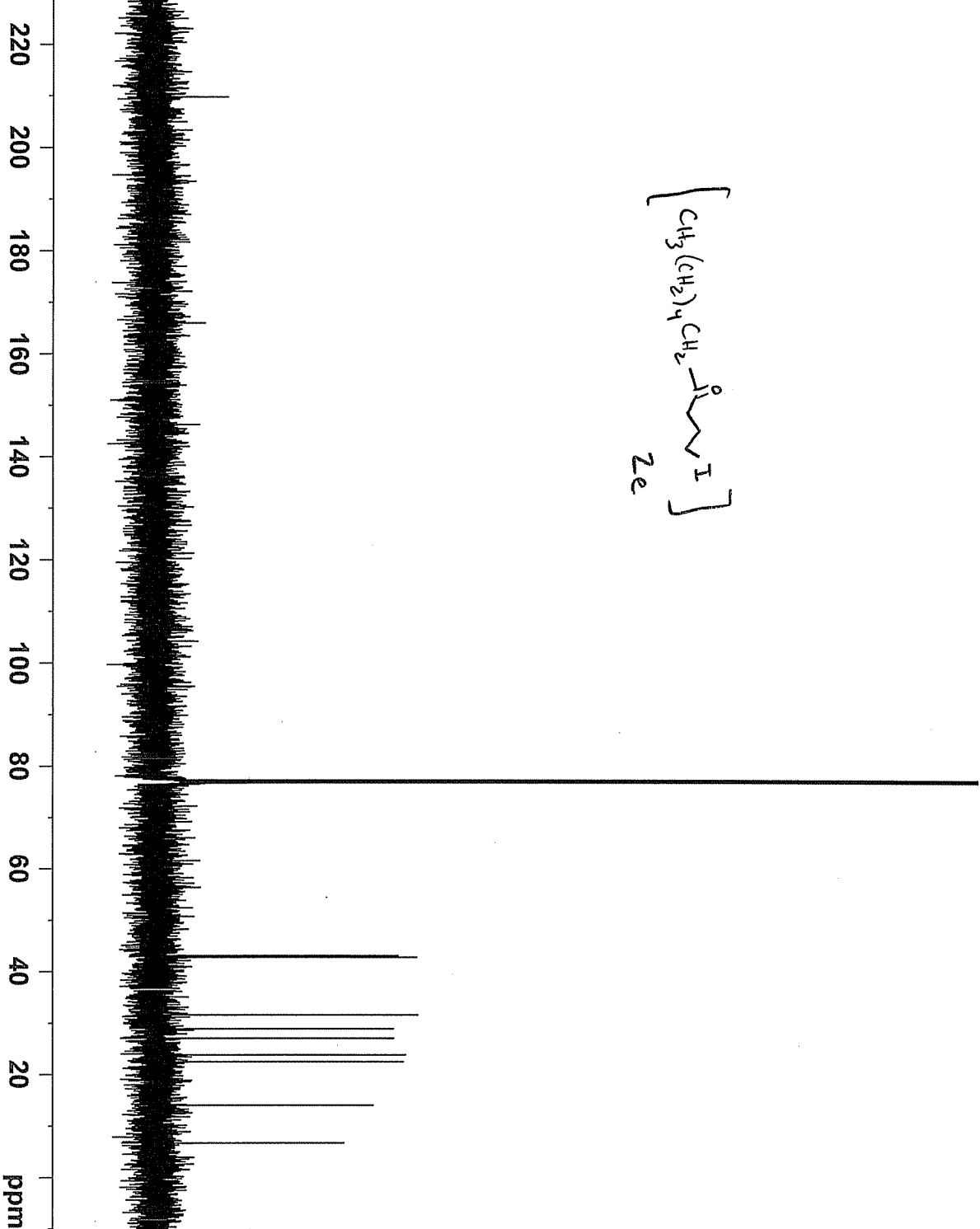
```

===== CHANNEL f1 =====
NUC1 1H
P1 6.00 usec
PL1 -4.00 dB
SFO1 500.1323989 MHz
SI 32768
SF 500.1300225 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 4.00
  
```

209.76



- 43.07
- 42.79
- 31.56
- 28.87
- 27.02
- 23.81
- 22.47
- 14.02
- 6.71



4-I-HexBut-060408

```

NAME
EXPNO          3
PROCNO         1
Date_          20080604
Time           16.25
INSTRUM        spect
PROBHD         5 mm PHBBO BB-
PULPROG        zgdc30
TD             65536
SOLVENT        CDCl3
NS             92
DS             0
SWH            30030.029 Hz
FIDRES        0.458222 Hz
AQ            1.0912410 sec
RG            1625.5
DW            16.650 usec
DE            7.00 usec
TE            295.6 K
D1            2.00000000 sec
d11           0.03000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec
  
```

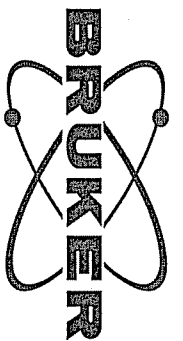
```

===== CHANNEL F1 =====
NUC1          13C
P1            9.30 usec
PL1           1.00 dB
SFO1         125.7715390 MHz
  
```

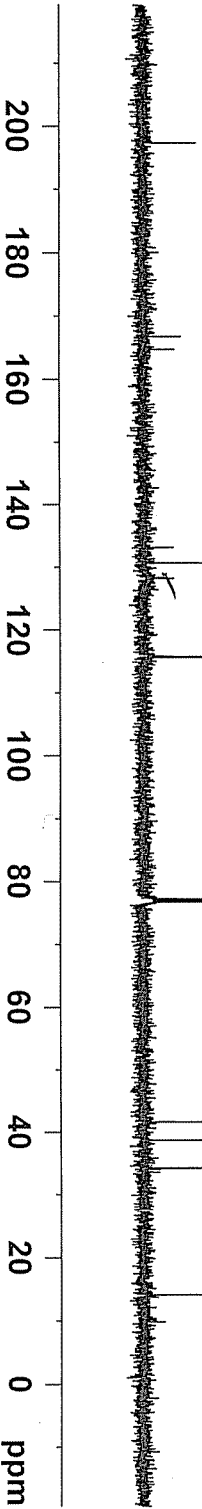
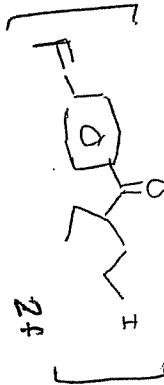
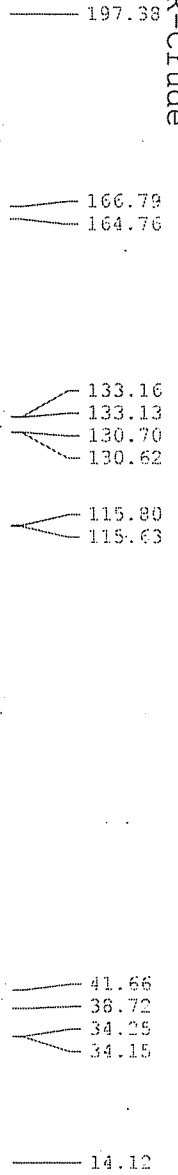
```

===== CHANNEL F2 =====
CPDPRG2      waltz16
NUC2          1H
PCPD2        110.00 usec
PL2          -4.00 dB
PL12         18.88 dB
SFO2         500.1325000 MHz
SI           65536
SF           125.7577935 MHz
WDW          EM
SSB          0
LB           1.00 Hz
GB           0
PC           1.40
  
```

13C-NMR-Crude



Current Data Parameters
 NAME 4-I-p-F-Ph-But-2Etyl-120908
 EXPNO 3
 PROCNO 1



F2 - Acquisition Parameters
 Date_ 20081209
 Time 18.17
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 121
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0512410 sec
 RG 3251
 DW 16.650 usec
 DE 7.00 usec
 TE 298.1 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

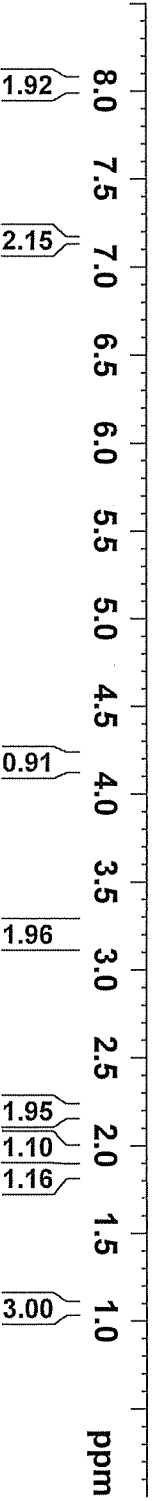
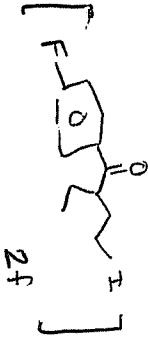
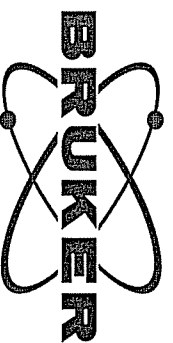
==== CHANNEL F1 =====
 NUC1 13C
 P1 9.35 usec
 PL1 1.00 dB
 SFO1 125.7703640 MHz

==== CHANNEL F2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 100.00 usec
 PL2 17.50 dB
 PL12 17.50 dB
 SFO2 500.1322150 MHz

F2 - Processing parameters
 SI 32768
 SF 125.7577976 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Minicol

8.04
8.04
8.03
8.03
8.02
8.02
8.01
8.01
7.27
7.17
7.17
7.16
7.16
7.15
7.15
7.15
7.14
7.14
7.13
7.13
4.19
4.19
4.18
4.17
4.16
4.16
3.49
3.25
3.24
3.23
3.22
3.20
3.19
3.17
3.16
3.16
3.14
2.21
2.20
2.20
2.19
2.19
2.18
2.18
2.17
2.17
1.96
1.94
1.93
1.91
1.88
1.87
1.86
1.85
1.85
1.84
1.83
1.83
1.44
1.31
1.26
1.09
1.08
1.07
1.06
1.06
0.98
0.89
0.88
0.86



Current Data Parameters
 NAME 4-I-p-F-PI-BUT-2Ethy1-120908
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20081210
 Time 10.01
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 6
 DS 0
 SWH 6009.615 Hz
 FIDRES 0.183399 Hz
 AQ 2.7264309 sec
 RG 90.5
 DW 83.200 usec
 DE 6.00 usec
 TE 297.4 K
 D1 1.00000000 sec
 TDO 1

==== CHANNEL F1 =====
 NUC1 1H
 P1 14.00 usec
 PL 1.00 dB
 SFO1 500.1327510 MHz
 F2 - Processing parameters
 SI 32768
 SF 500.1300102 MHz
 WDW EM
 SSB 0
 GB 0
 PC 1.00

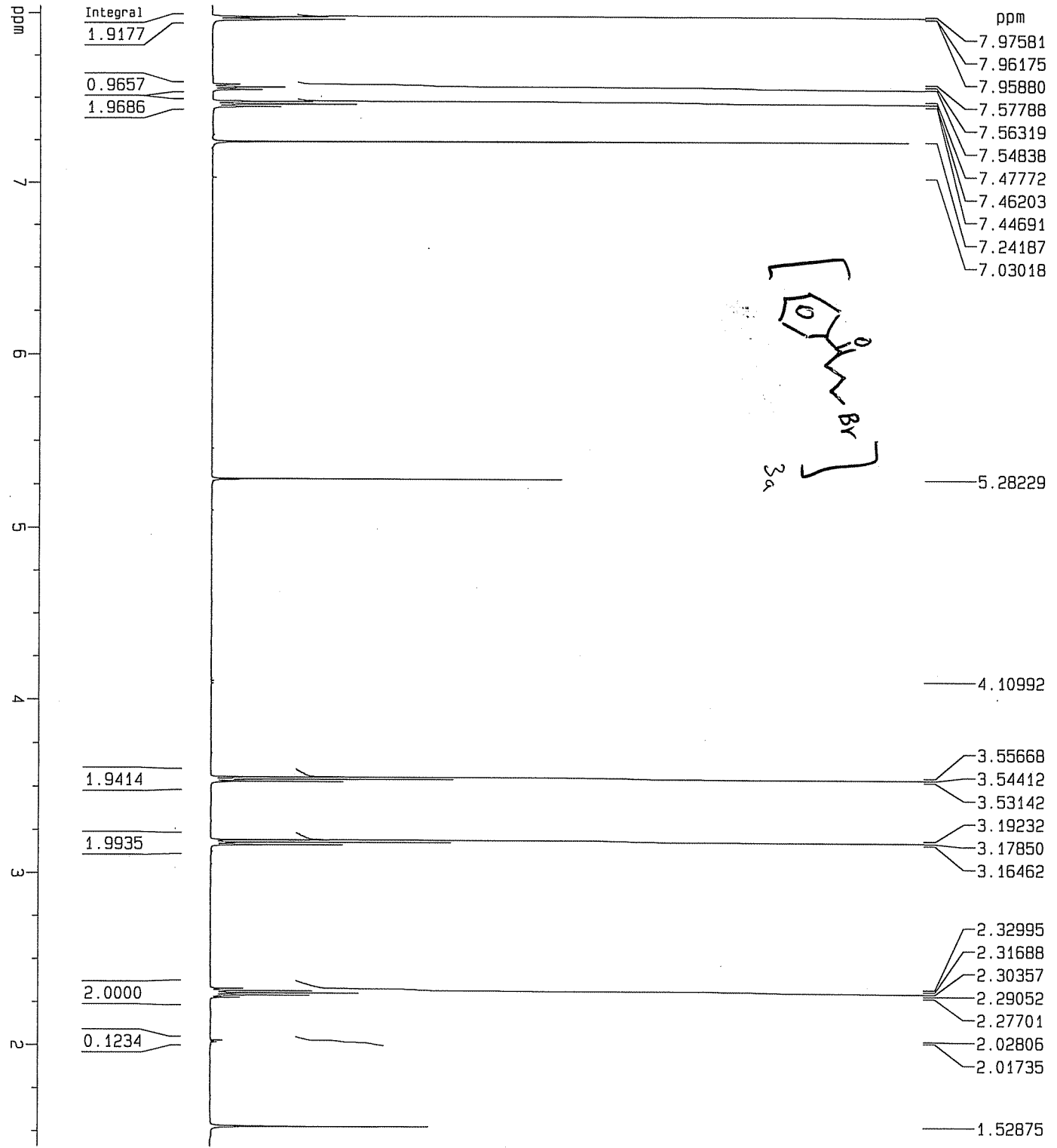
Current Data Parameters
 NAME 4-Br-PhBut-053008
 EXPNO 3
 PROCNO 1

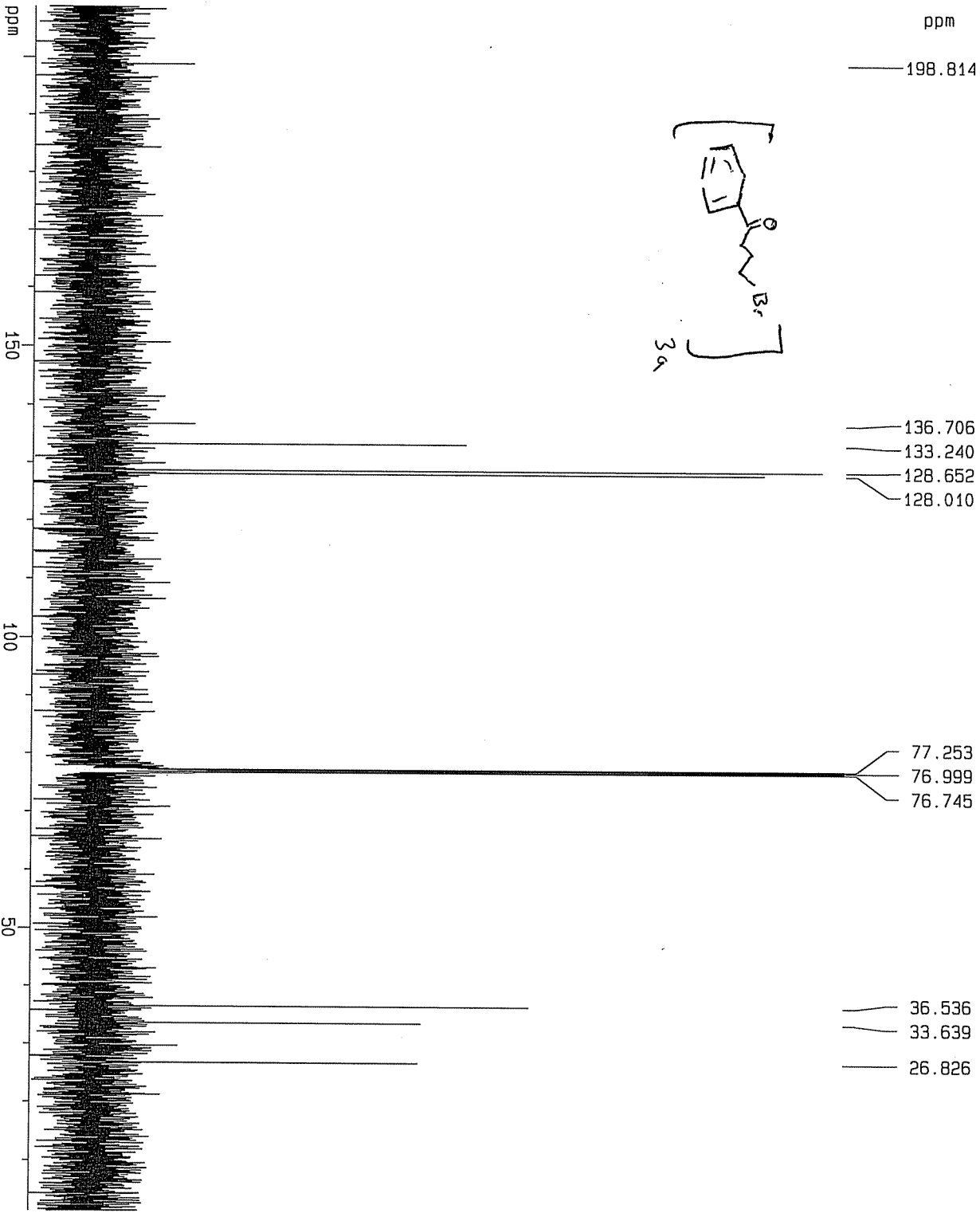
F2 - Acquisition Parameters
 Date_ 20080530
 Time 11.47
 INSTRUM spect
 PROBHD 5 mm TXI 1H/2H
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 7507.507 Hz
 FIDRES 0.229111 Hz
 AQ 2.1824653 sec
 RG 724.1
 DW 66.600 use
 DE 7.00 use
 TE 294.7 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCWPK 0.01500000 sec

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.30 use
 PL1 1.00 dB
 SFO1 500.1323989 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300225 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F4P 8.041 ppm
 F1 4021.73 Hz
 F2P 1.412 ppm
 F2 706.17 Hz
 PPMCM 0.33147 ppm
 HZCM 165.77797 Hz/





Current Data Parameters
 NAME 4-Br-PhBut-050408
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080604
 Time 11.37

INSTRUM spect
 PROBHD 5 mm PHB80 B8-
 PULPROG zgpg

TD 65536
 SOLVENT CDCl3
 NS 256

DS 0
 SWH 30030.029 HZ
 FIDRES 0.458222 HZ

RG 1.0912410 sec
 RG 1625.5
 DW 16.650 usec

DE 7.00 usec
 TE 295.5 K

D1 2.00000000 sec
 d11 0.03000000 sec
 MCOREST 0.00000000 sec
 MCMRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 -1.00 dB
 SF01 125.7715390 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 140.00 usec
 PL2 17.50 dB
 PL12 17.00 dB
 SF02 500.1325000 MHz

F2 - Processing Parameters
 SI 65536
 SF 125.7577930 MHz
 WDM EM
 SSB 0
 LB 1.00 HZ
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 12.50 cm
 F1P 208.895 ppm
 F1 26270.16 HZ
 F2P 1.346 ppm
 F2 169.30 HZ

PPMCM 10.37743 ppm/cm
 HZCM 1305.04321 HZ/cm

Current Data Parameters
 NAME 4-Br-pMeOPhBut-061606
 EXPNO 2
 PROCNO 1

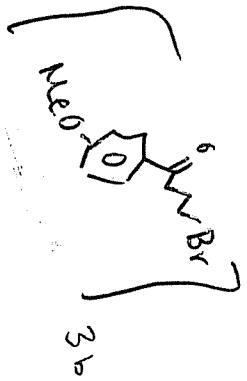
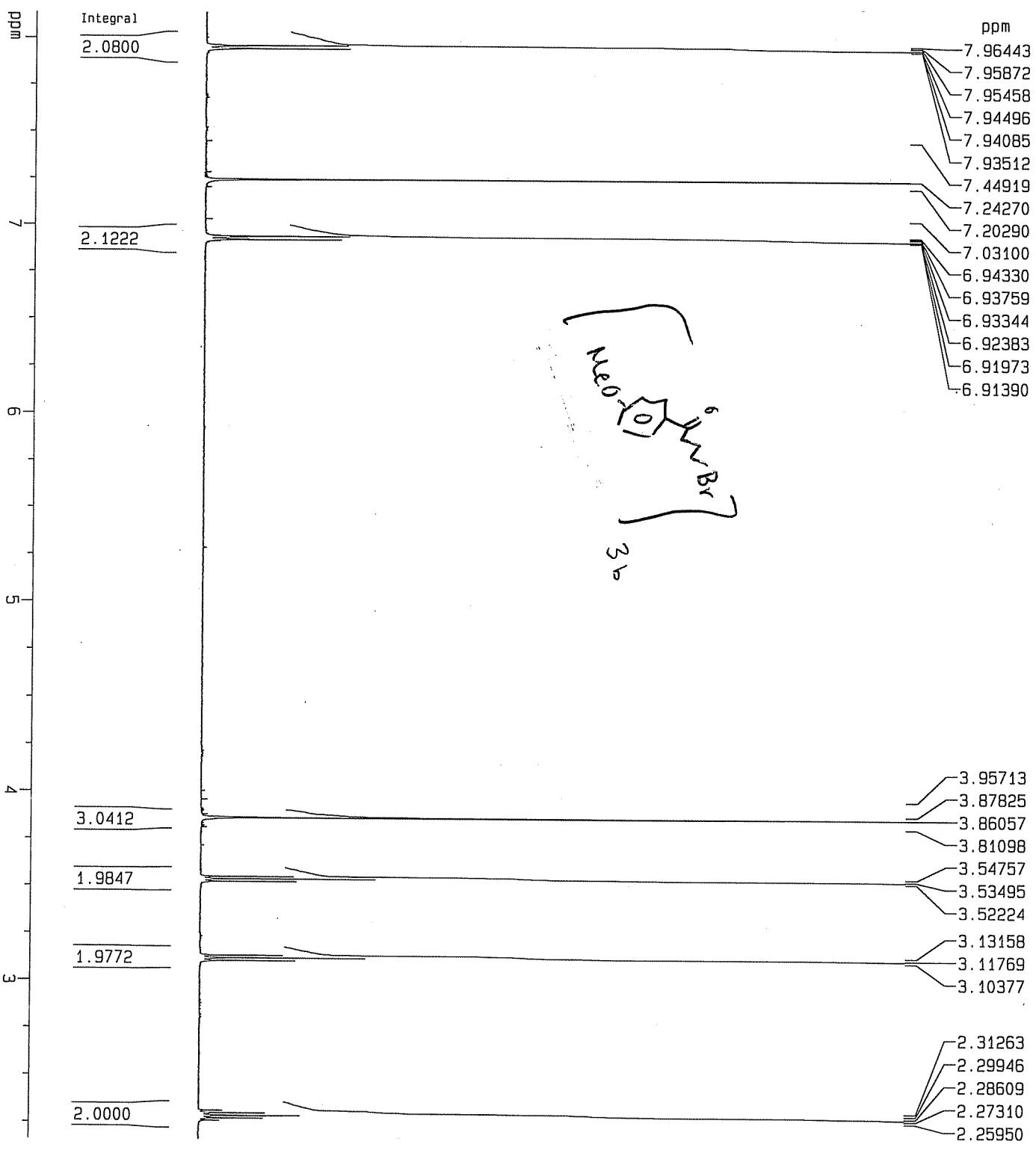
F2 - Acquisition Parameters

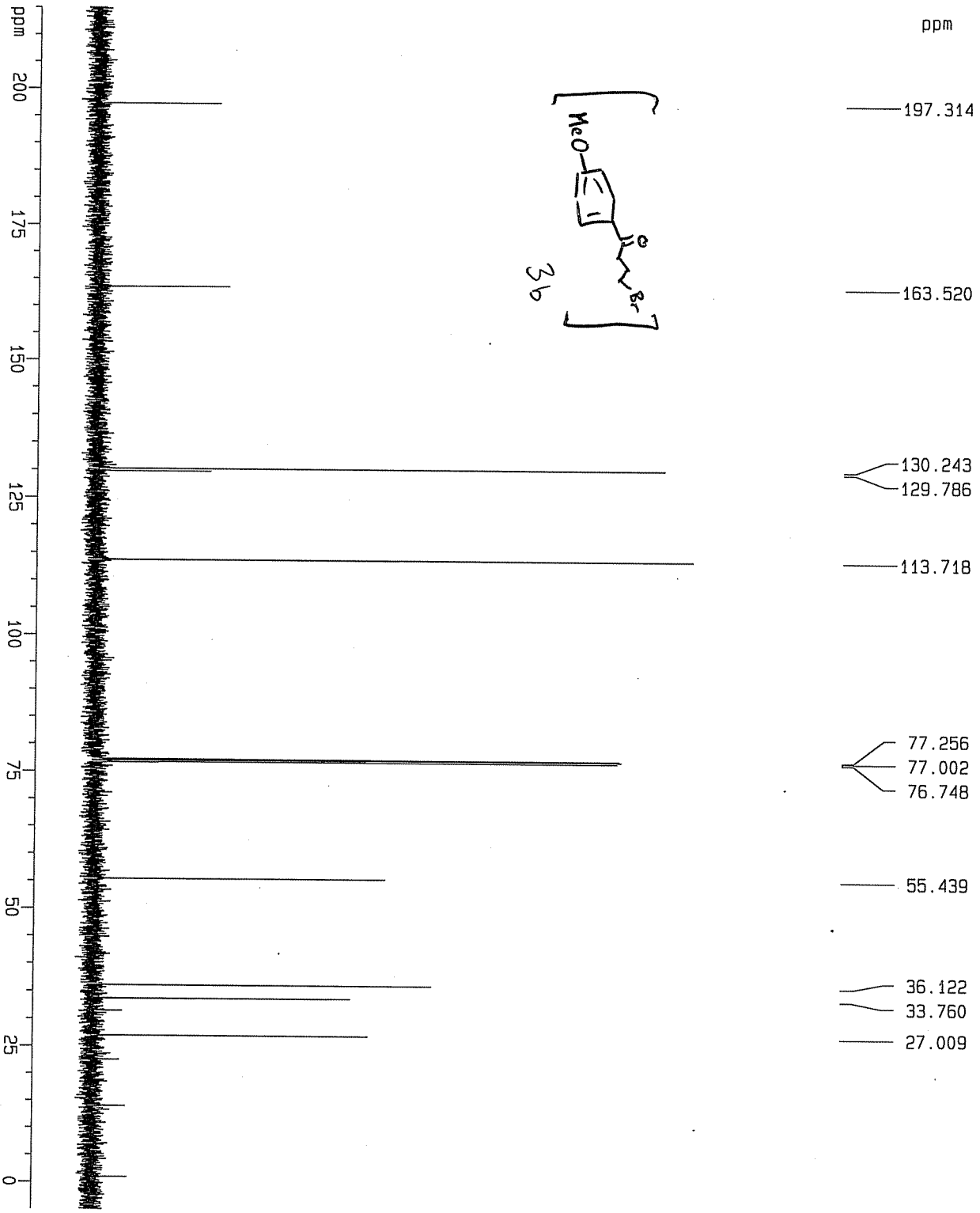
Date_ 20080616
 Time 14.46
 INSTRUM spect
 PROBRD 5 mm PHB80 BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 7507.507 Hz
 FIDRES 0.229111 Hz
 AQ 2.1824653 sec
 RG 912.3
 DW 66.600 usec
 DE 7.00 usec
 TE 296.1 K
 D1 1.00000000 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 1H
 P1 8.30 usec
 PL1 1.00 dB
 SFO1 500.1323989 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1300225 MHz
 WDW EM
 SSB 0
 LB 0.20 Hz
 GB 0
 PC 4.00

1D NMR plot parameters
 CX 20.00 cm
 CY 0.00 cm
 F1P 8.137 ppm
 F1 4069.80 Hz
 F2P 2.161 ppm
 F2 1080.94 Hz
 PPMCM 0.29881 ppm/cm
 HZCM 149.44272 Hz/cm





ppm

197.314
 163.520
 130.243
 129.786
 113.718
 77.256
 77.002
 76.748
 55.439
 36.122
 33.760
 27.009

Current Data Parameters
 NAME 4-Br-methoxybut-061808
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080616
 Time 17.58
 INSTRUM spect
 PROBD 5 mm PHEB0 9B-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 37
 DS 0
 SMH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 2048
 DW 16.650 usec
 DE 7.00 usec
 TE 296.9 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 MCREST 0.00000000 sec
 MCMRK 0.01500000 sec

==== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 1.00 dB
 SF01 125.7715390 MHz

==== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 100.00 usec
 PL2 17.50 dB
 PL12 17.50 dB
 SF02 500.1325000 MHz

F2 - Processing parameters
 SI 65536
 SF 125.7577976 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

1D NMR plot parameters
 CX 20.00 cm
 CY 10.00 cm
 F1P 215.000 ppm
 F1 27037.93 Hz
 F2P -5.000 ppm
 F2 -628.79 Hz
 PPMCKM 11.00000 ppm/cm
 HZCM 1383.33582 Hz/cm

Column

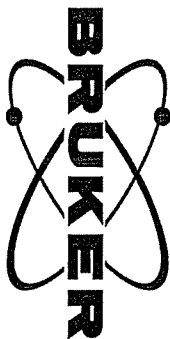
8.02
8.01
8.01
8.00

7.16
7.14
7.12

3.56
3.55
3.54

3.17
3.16
3.15

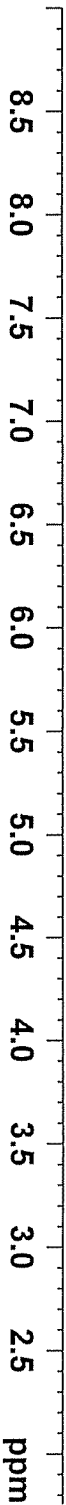
2.38
2.32
2.31
2.28
2.28



Current Data Parameters
NAME 4-Br-Pf-PhBut-090808
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080909
Time_ 11.47
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 6009.615 Hz
FIDRES 0.183399 Hz
AQ 2.7264309 sec
RG 128
DW 83.200 usec
DE 6.00 usec
TE 296.3 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 7.35 usec
PL1 1.00 dB
SFO1 500.1327510 MHz
F2 - Processing parameters
SI 32768
SF 500.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.96

1.95

1.99

2.00

2.01

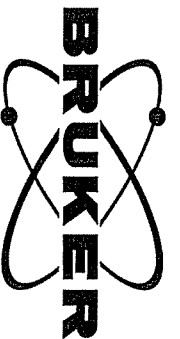
ppm

Column

197.13
 166.76
 164.76
 133.13
 133.11
 130.65
 130.58
 115.80
 115.63



36.41
 33.53
 26.74



Current Data Parameters
 NAME 4-Br-pF-PHbUt-090808
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20080909
 Time_ 11.51
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpgc30
 TD 65536
 SOLVENT CDCl3
 NS 42
 DS 4
 SWH 30030.029 Hz
 FIDRES 0.458222 Hz
 AQ 1.0912410 sec
 RG 3251
 DW 16.650 usec
 DE 7.00 usec
 TE 297.0 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 TD0 1

==== CHANNEL f1 =====
 NUC1 13C
 P1 5.00 usec
 PL1 1.00 dB
 SFO1 125.7703640 MHz
 ===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 24.00 dB
 PL12 24.00 dB
 SFO2 500.1322150 MHz
 F2 - Processing parameters
 SI 32768
 SF 125.7577962 MHz
 WDW EM
 SSB 0
 IB 1.00 Hz
 GB 0
 PC 1.40

