

Synthesis of 2,5-Diaryl-1,5-Dienes from Allylic Bromides Using Visible-Light Photoredox Catalysis

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Optimization of Allylic Bromination of α -Methylstyrene Derivatives.

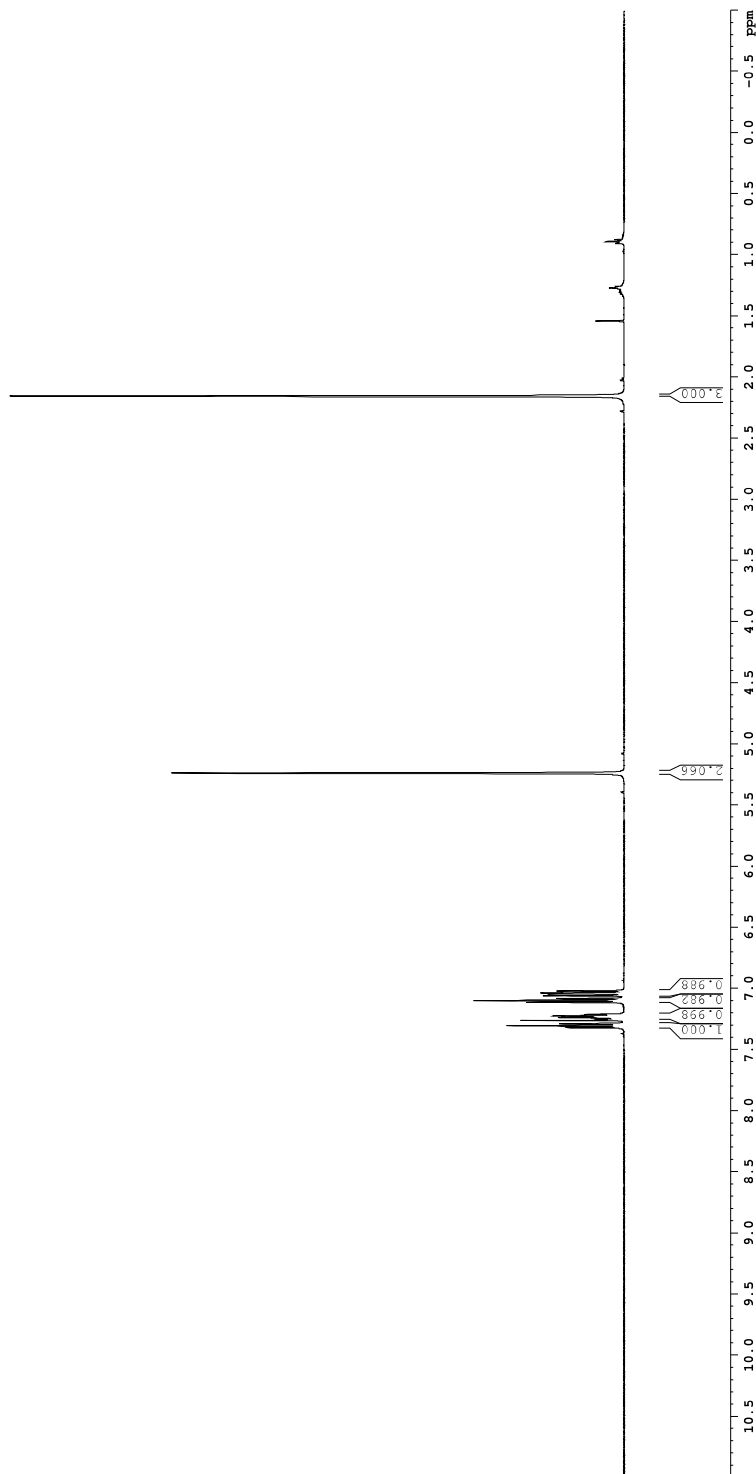
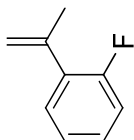
The well-known allylic bromination turned out to be more complex and, in comparison to the Wittig olefination, highly substrate-dependent. Generally, three different approaches starting from α -methylstyrene derivatives can be found in literature: most commonly used are procedures where the starting material and NBS are heated in chlorinated solvents (such as carbon tetrachloride, chloroform or chlorobenzene) in absence¹ or presence of a radical initiator.² Regarding the investigated substrates, yields of the desired product were typically low and the separation from the complex mixture of by-products were often difficult. However, the combination of NBS and dibenzoyl peroxide in refluxing carbon tetrachloride proved to be the only method enabling a successful allylic bromination of electron-rich ortho- and para-methoxy substituted α -methylstyrenes in moderate yields.² Mukherjee *et al.* reported a *p*-toluenesulfonic acid-catalyzed allylic bromination of several α -methylstyrene derivatives with NBS.³ Unfortunately, synthetically useful yields are only obtained for a limited number of substrates. However, we have never been able to reproduce the unusually high reported yields (e.g. 47-65% vs 89% for the preparation of **2a**) and found a significant dependence of the reaction outcome on the nature of the employed sample of *p*-toluenesulfonic acid. The formation of isomeric and double-bromination products additionally complicated the purification which finally excluded this method for our purposes. The broadly applicable and most reliable procedure in our hands was published by Nakagawa and coworkers in 2002.⁴ The allylic bromination with NBS occurs in the presence of catalytic Yb(OTf)₃ and TMS-Cl at room temperature in less than one hour (see Article Scheme 1). Although the reported yields were not fully reproducible (e.g. 43% vs 84% for the preparation of **2a**), this method led to fairly clean product formation of α -(bromomethyl)styrene derivatives **2** in consistent yields up to 60% for a wide array of substituents with only minor modifications necessary.⁵ Even alkyl substitution at the allylic scaffold was tolerated. As mentioned in the original publication, electron-rich ortho- and para-methoxy substituted α -methylstyrenes are incompatible substrates likely due to oligomerization.

^1H NMR Spectra

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2.150

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5.235

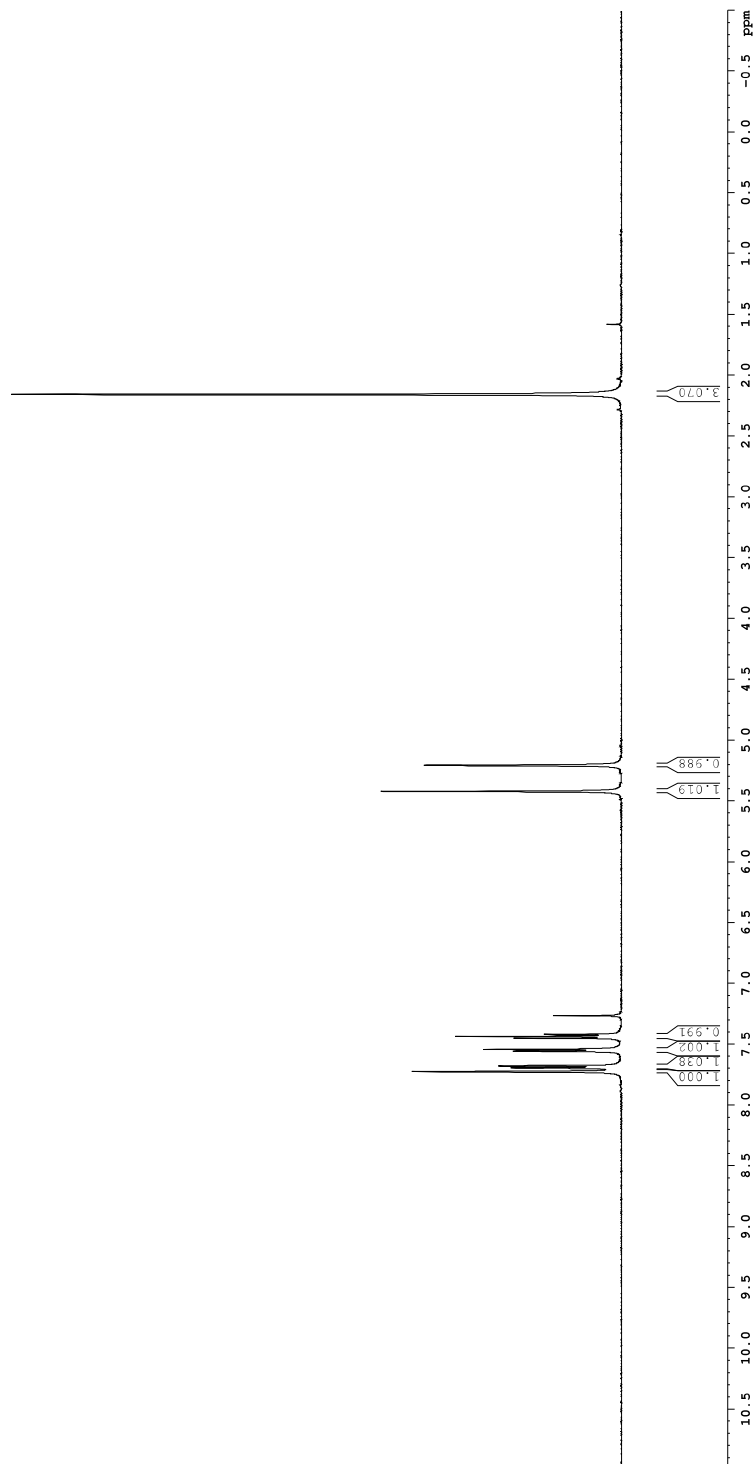
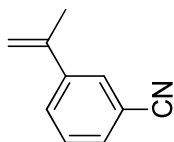


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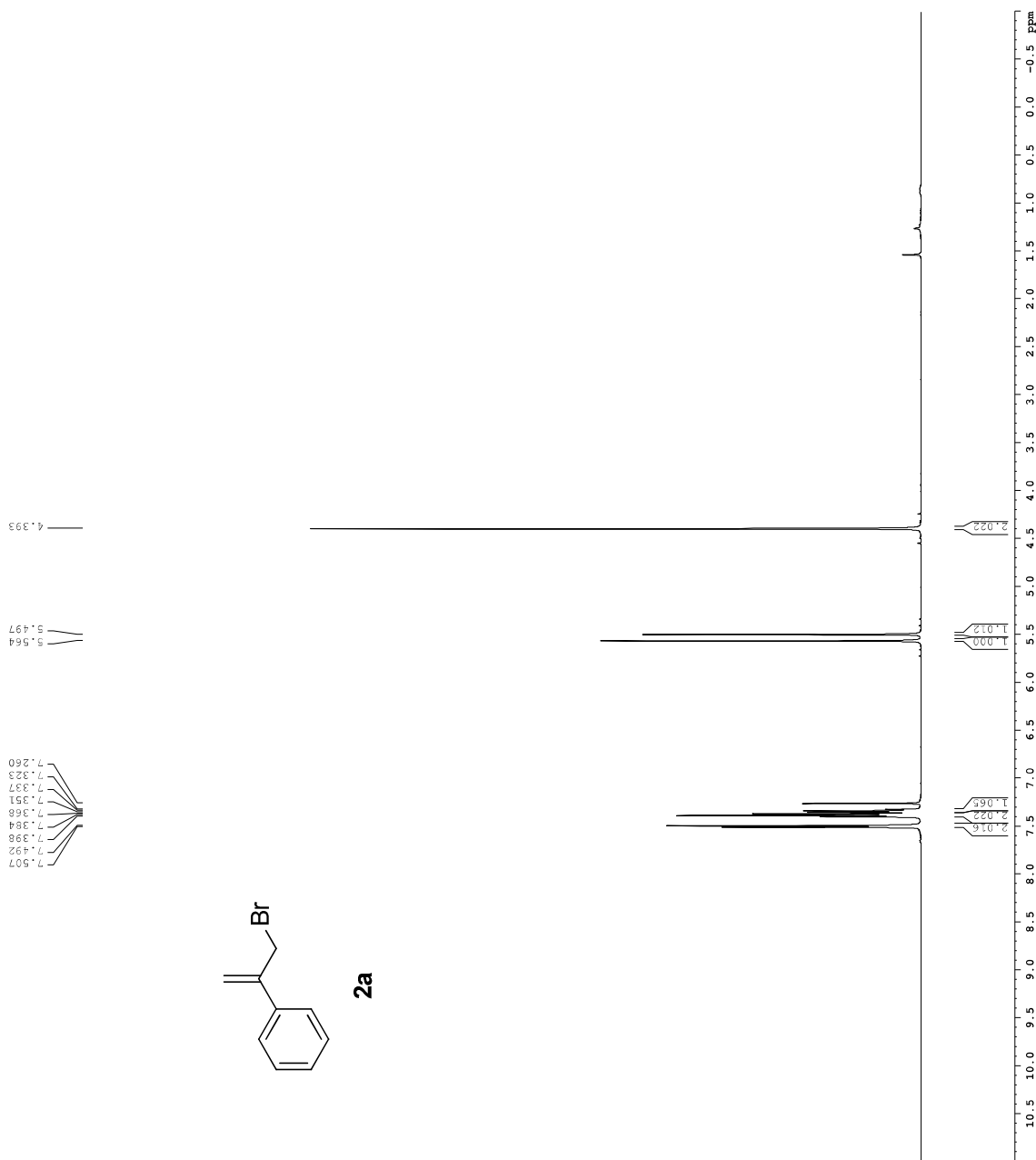
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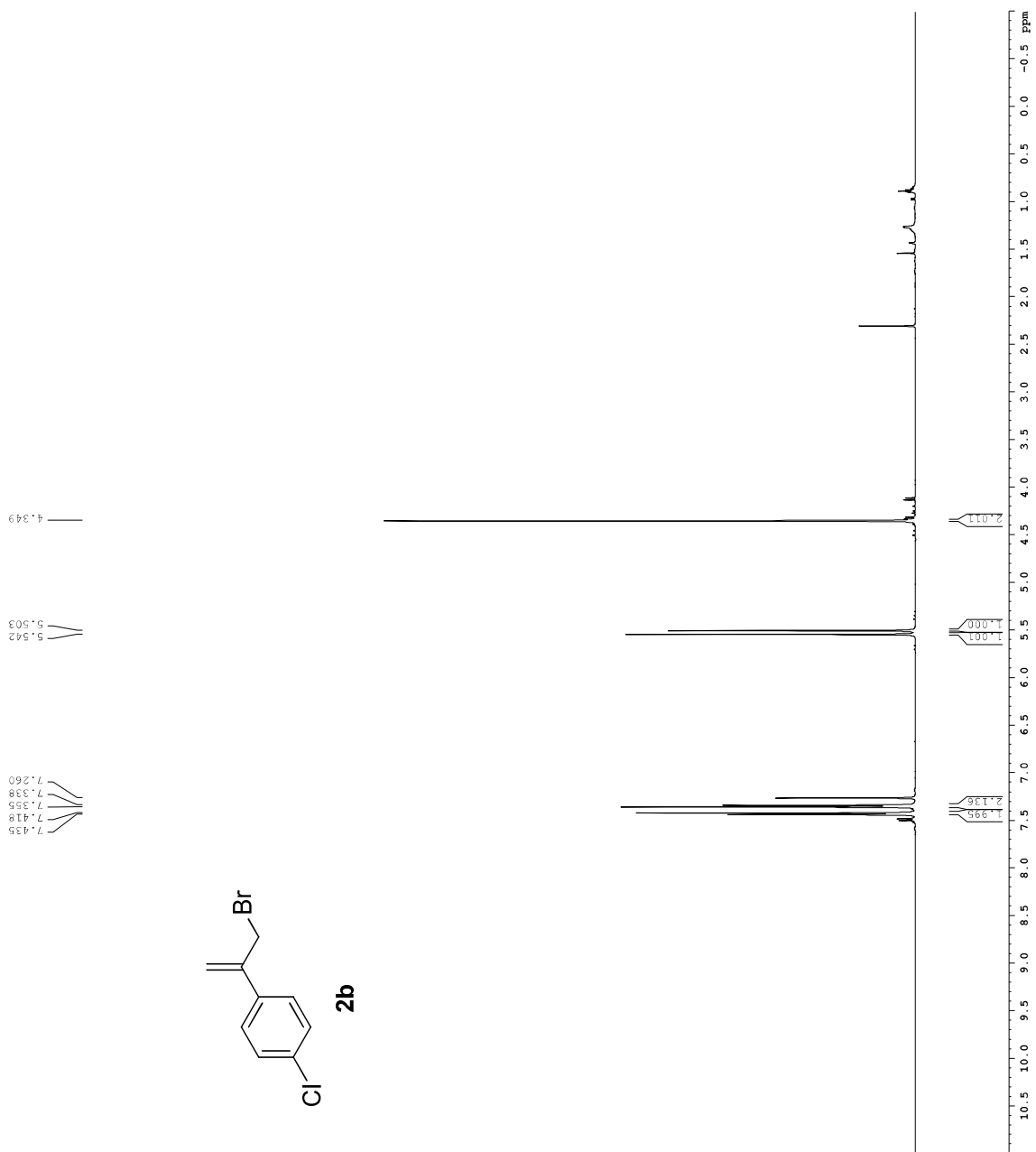
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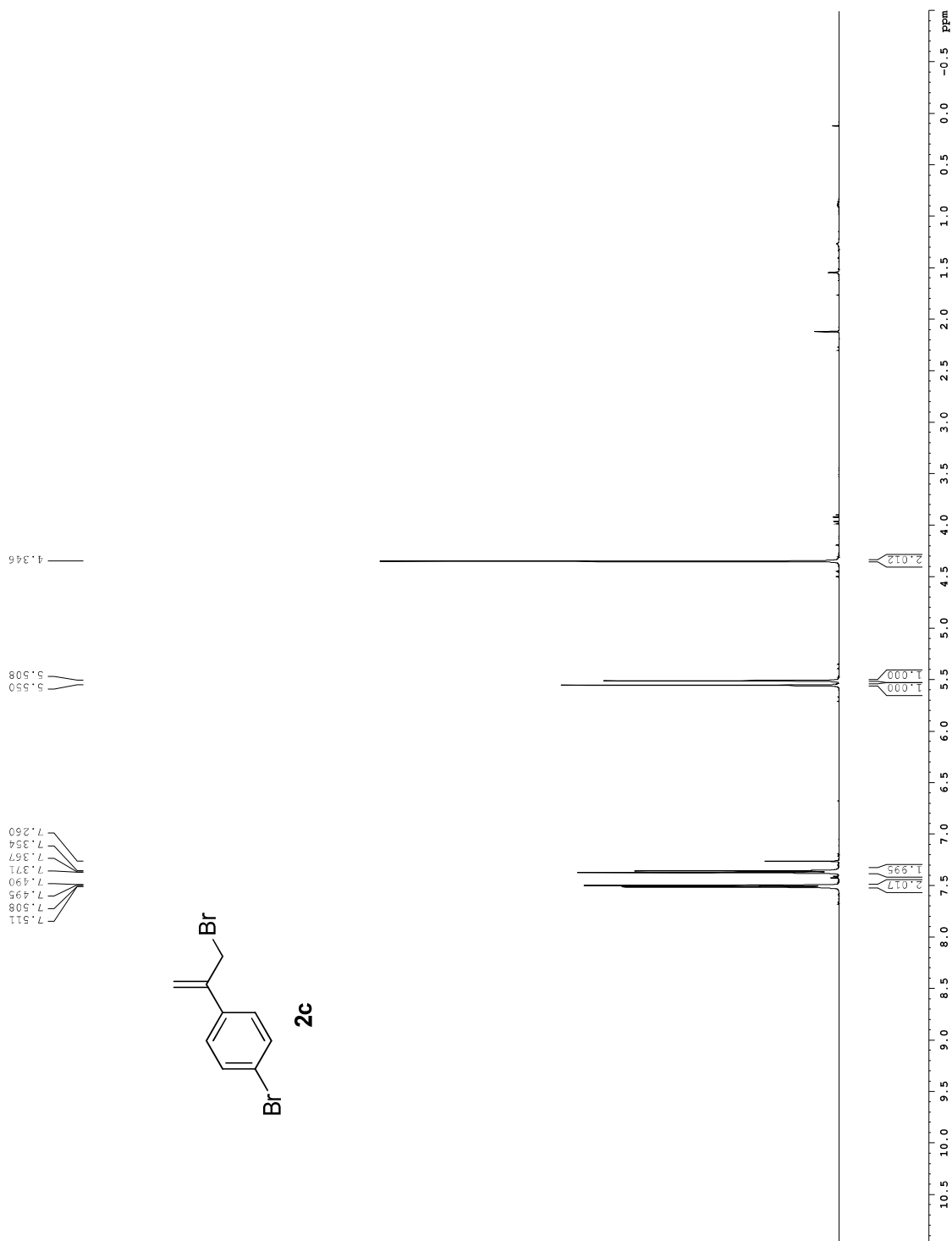
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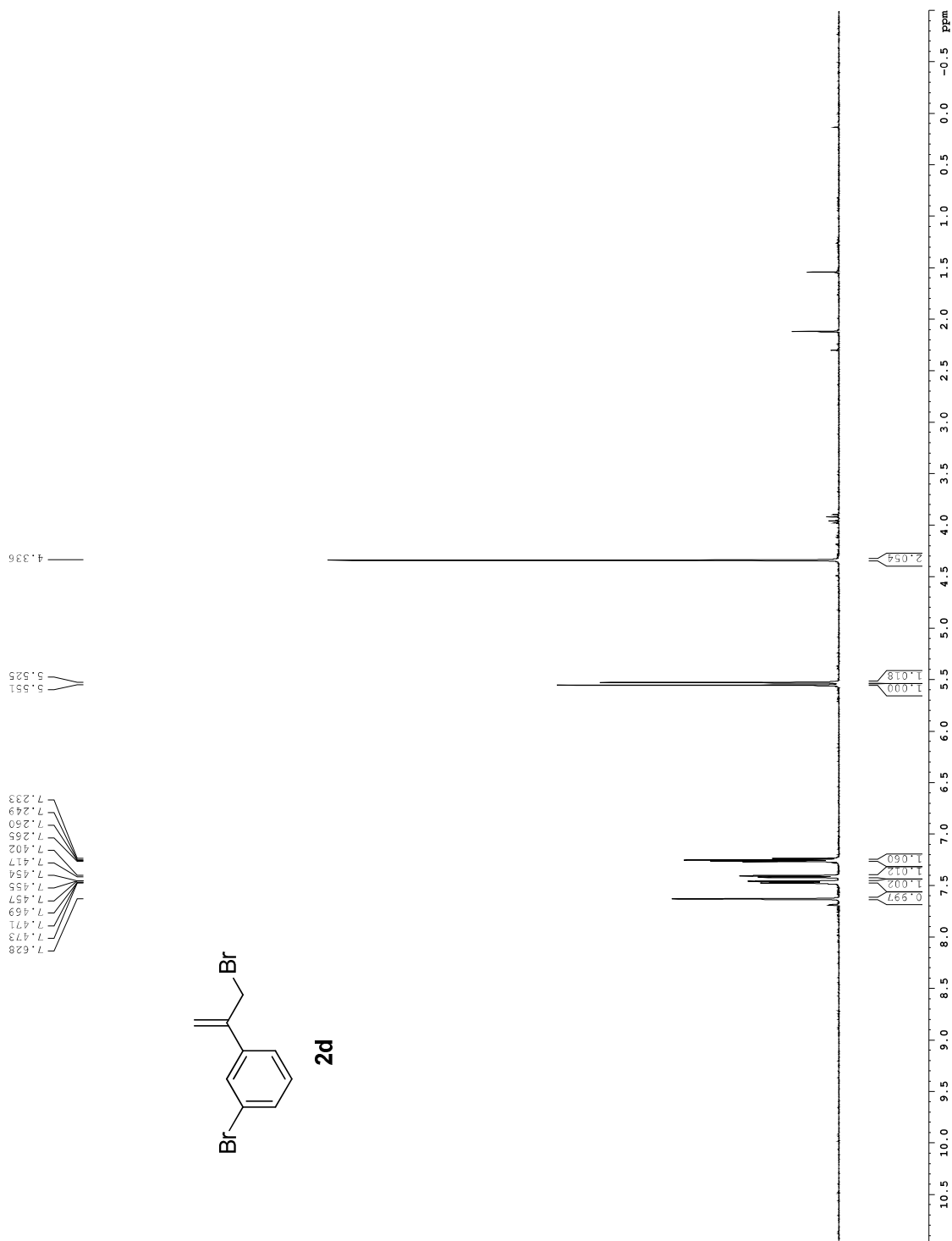
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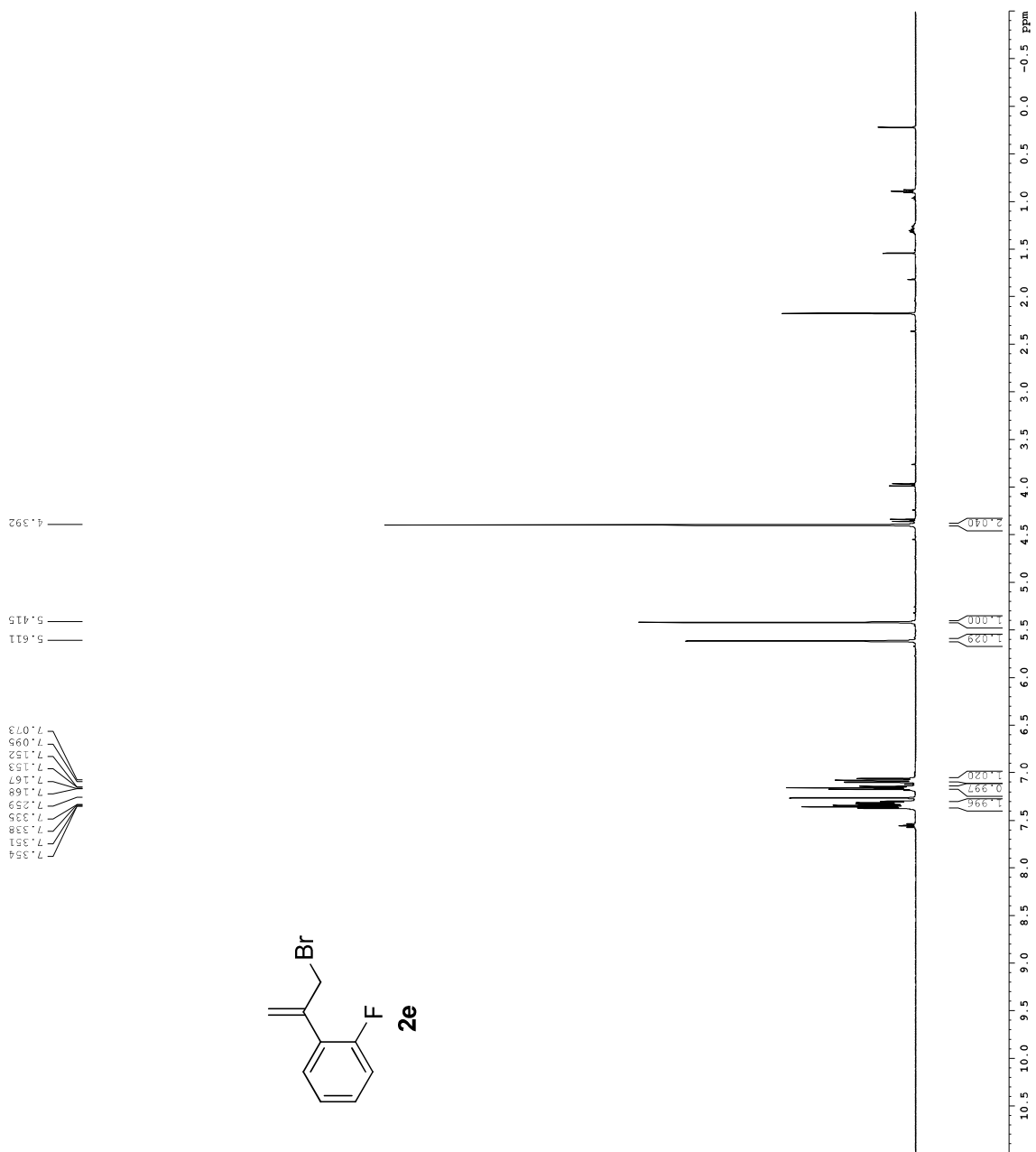
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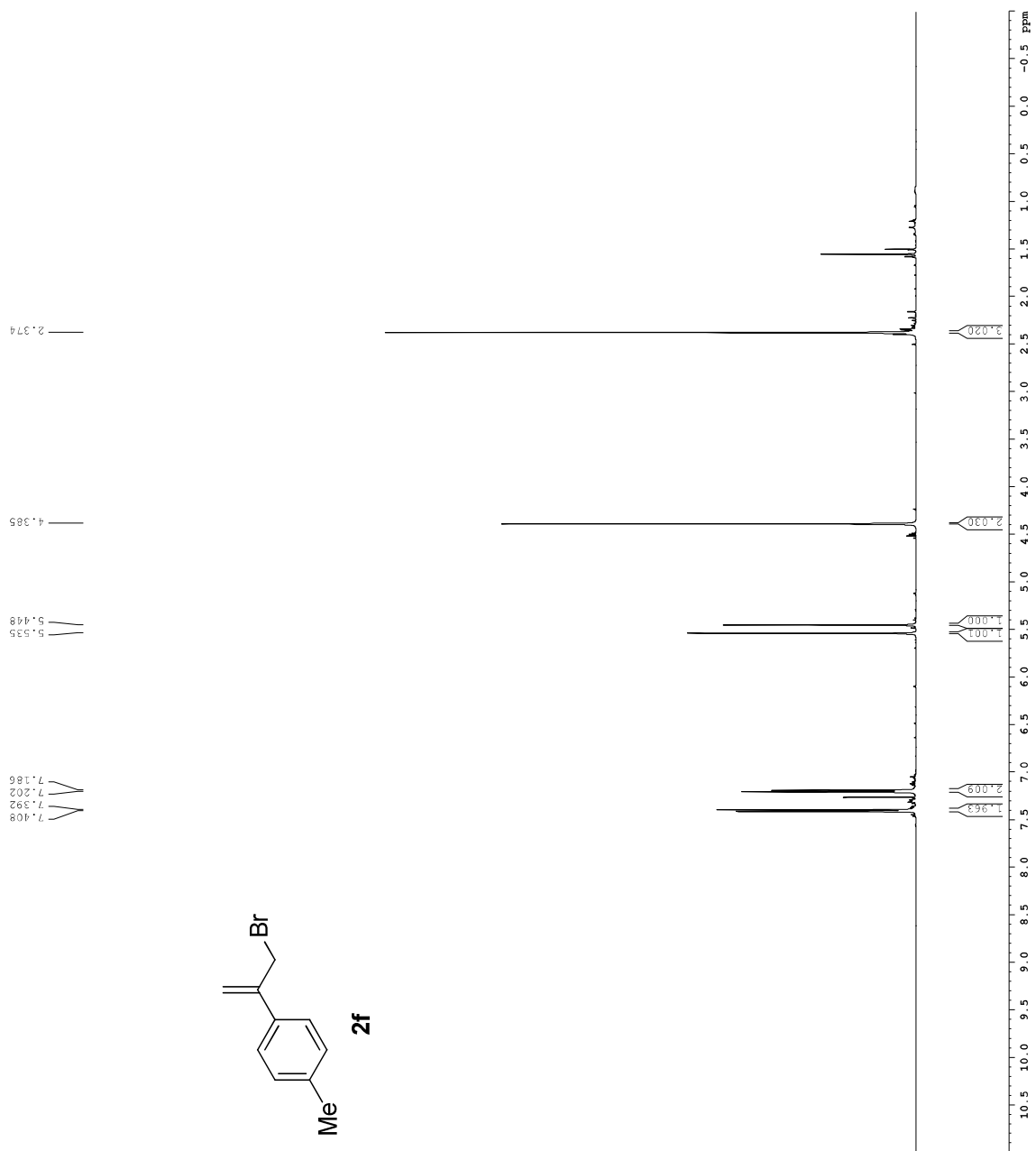
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 FIDRES 0.166677 Hz
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 DW 62.400 usec
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 TE 298.2 K
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 P1 7.50 usec
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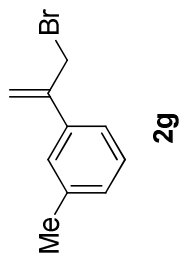
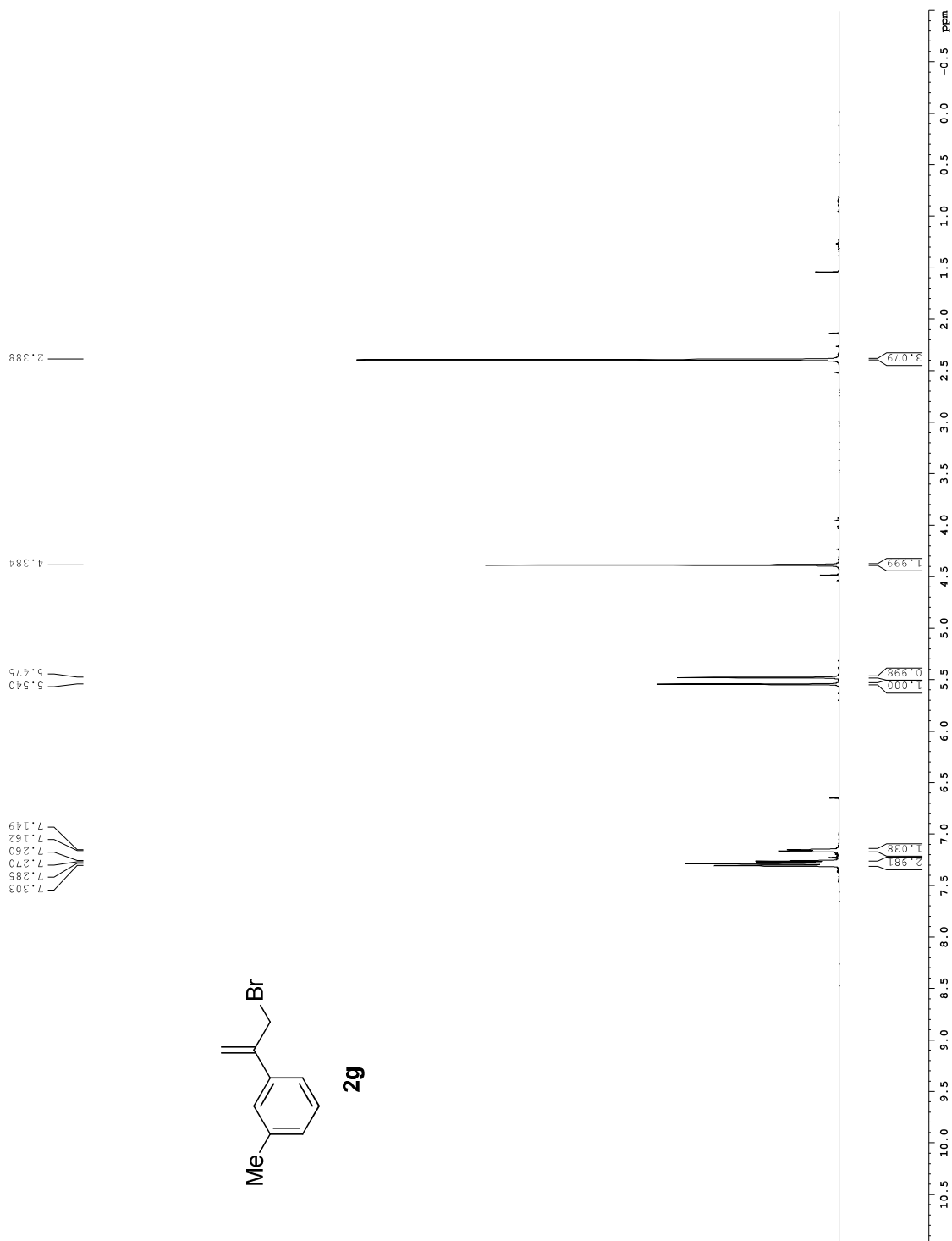
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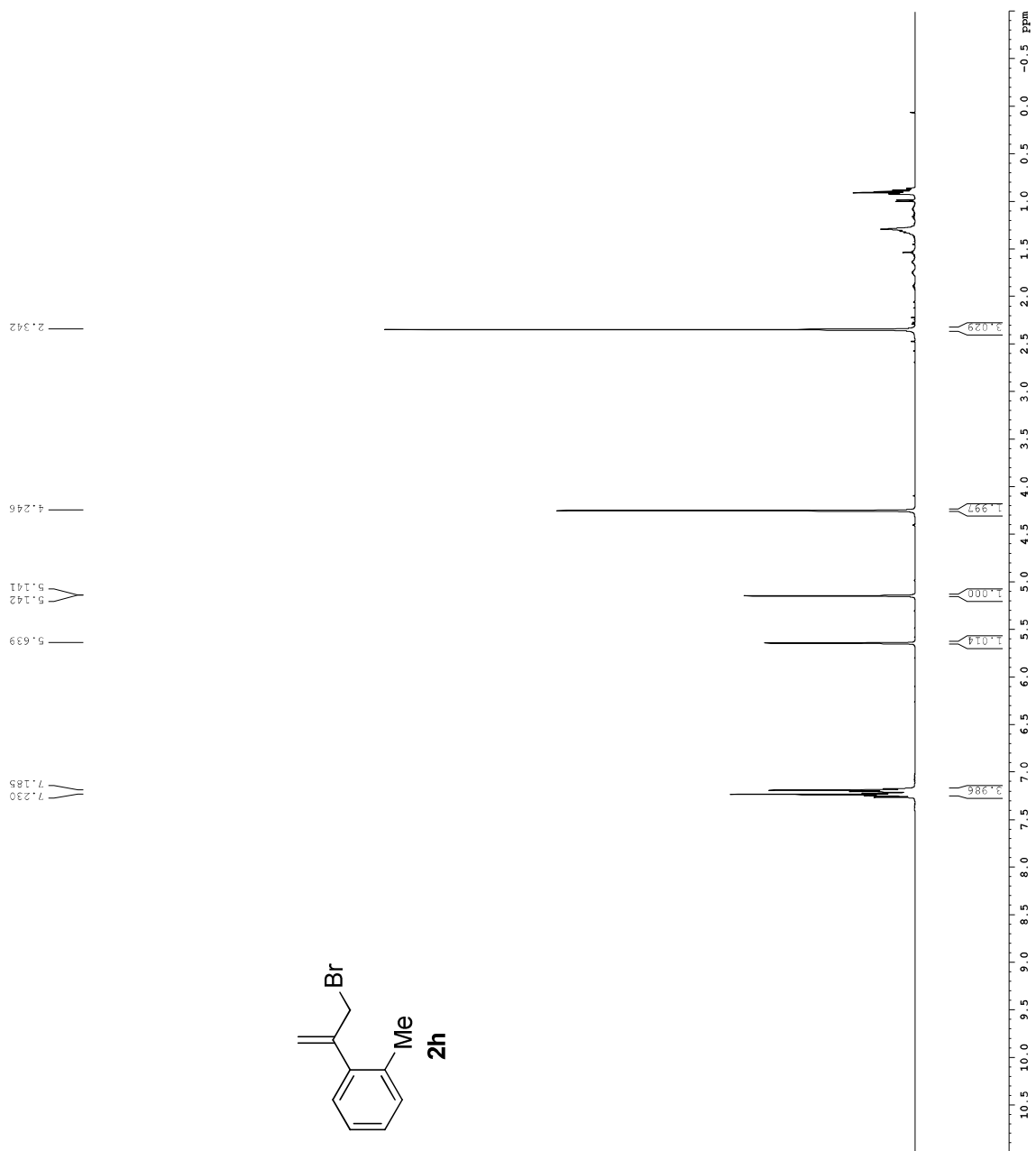
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 SOLVENT CDCl3
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 DS 2
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 FIDRES 0.166677 Hz
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 RG 9
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 DE 1.900 usec
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 NUC1 1H
 F1 7.50 usec
 PC 1.60 dB
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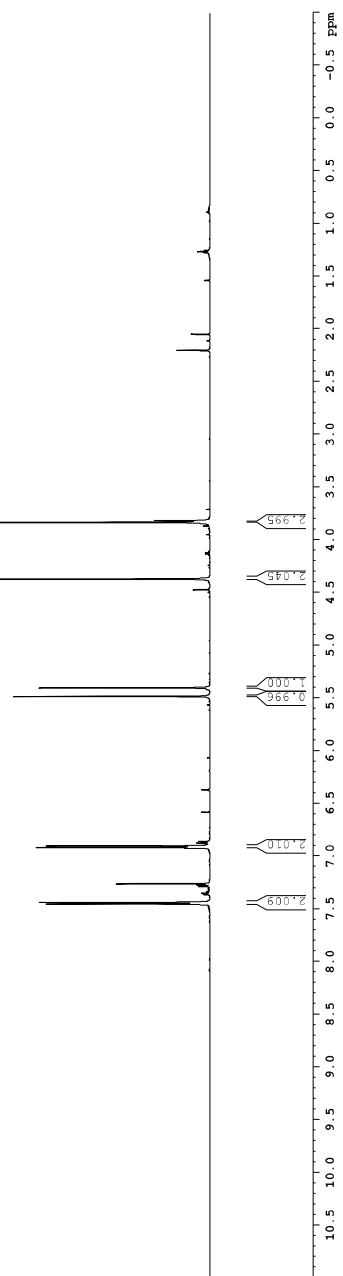
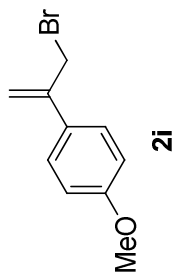


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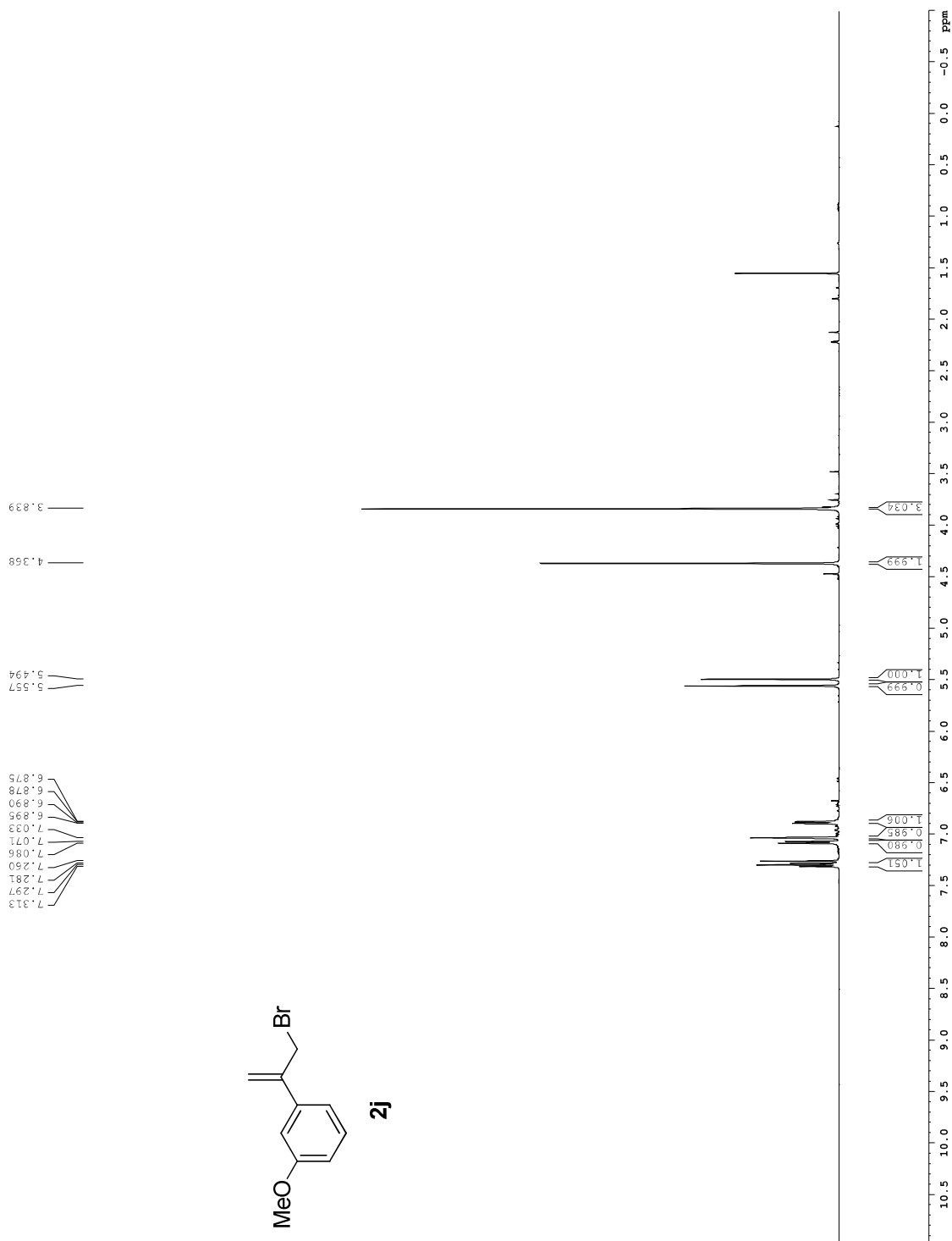


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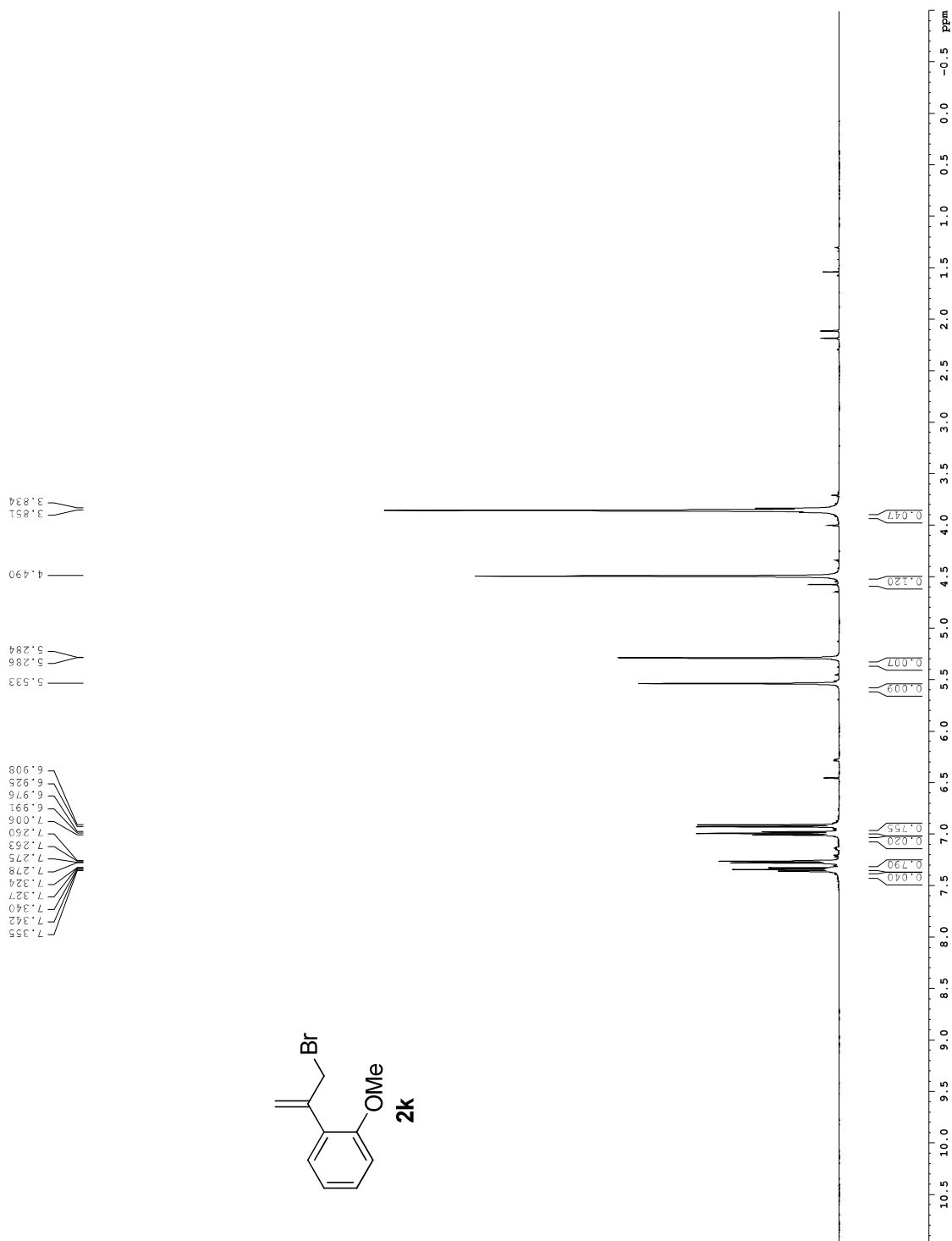
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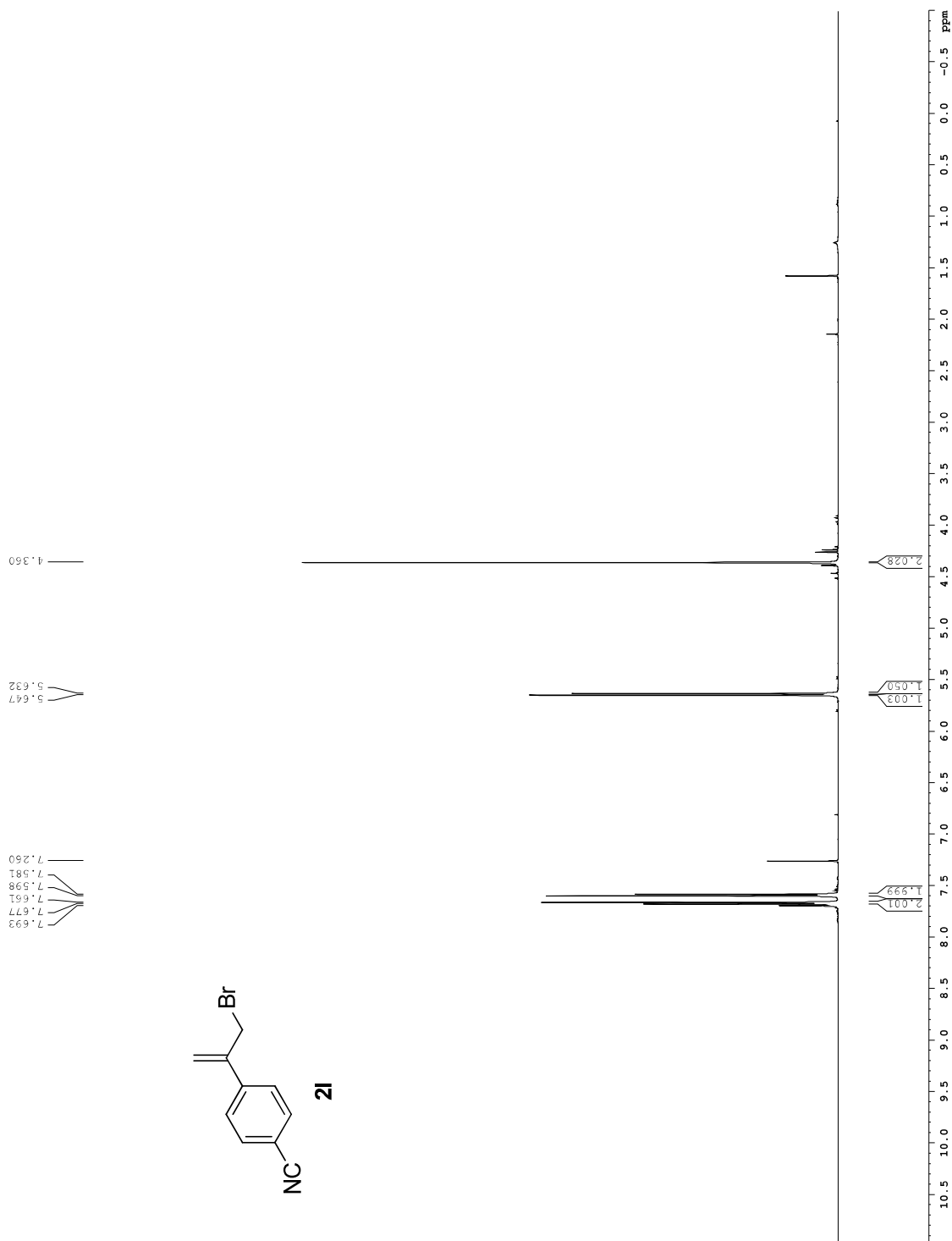
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 PC 1.60 dB
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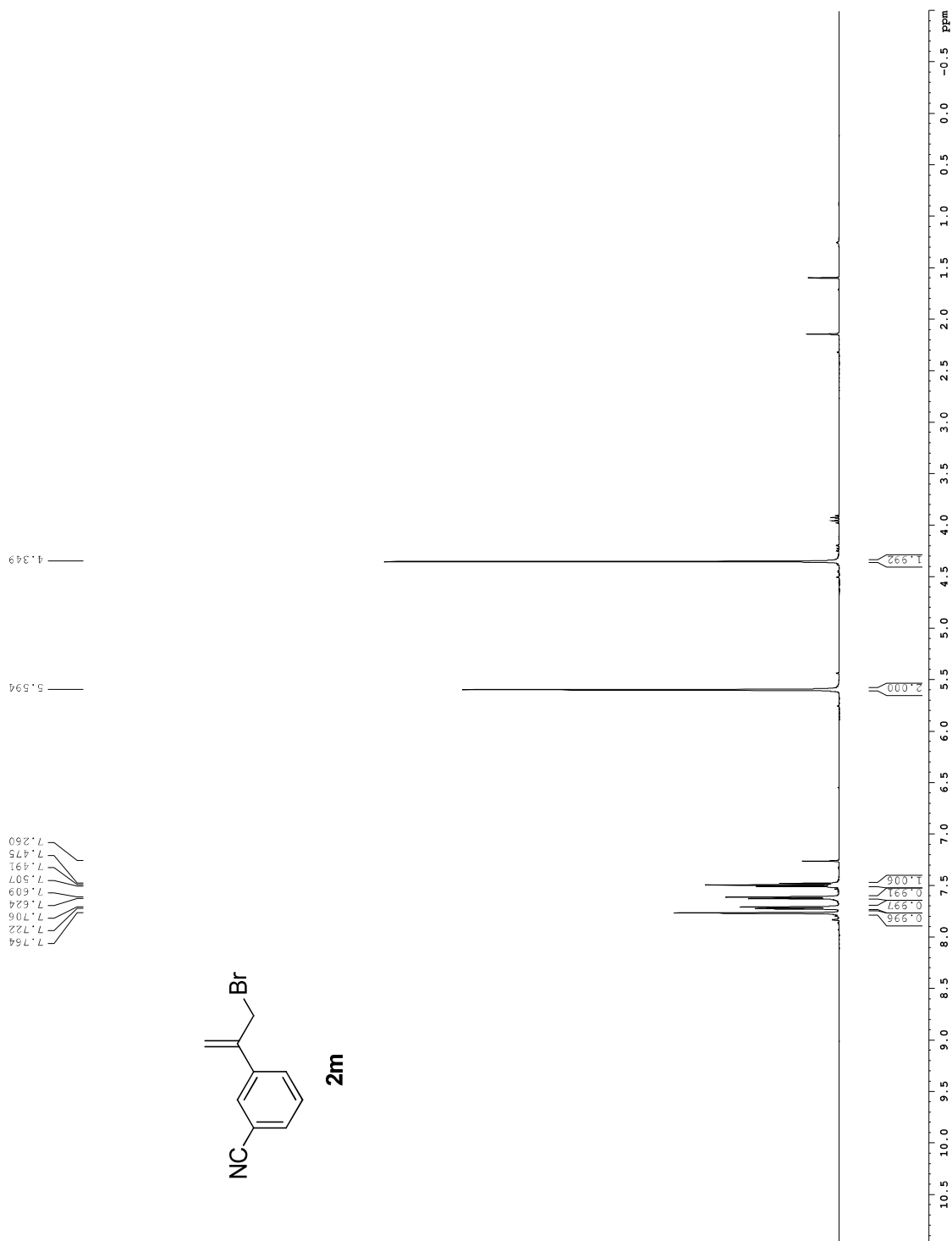
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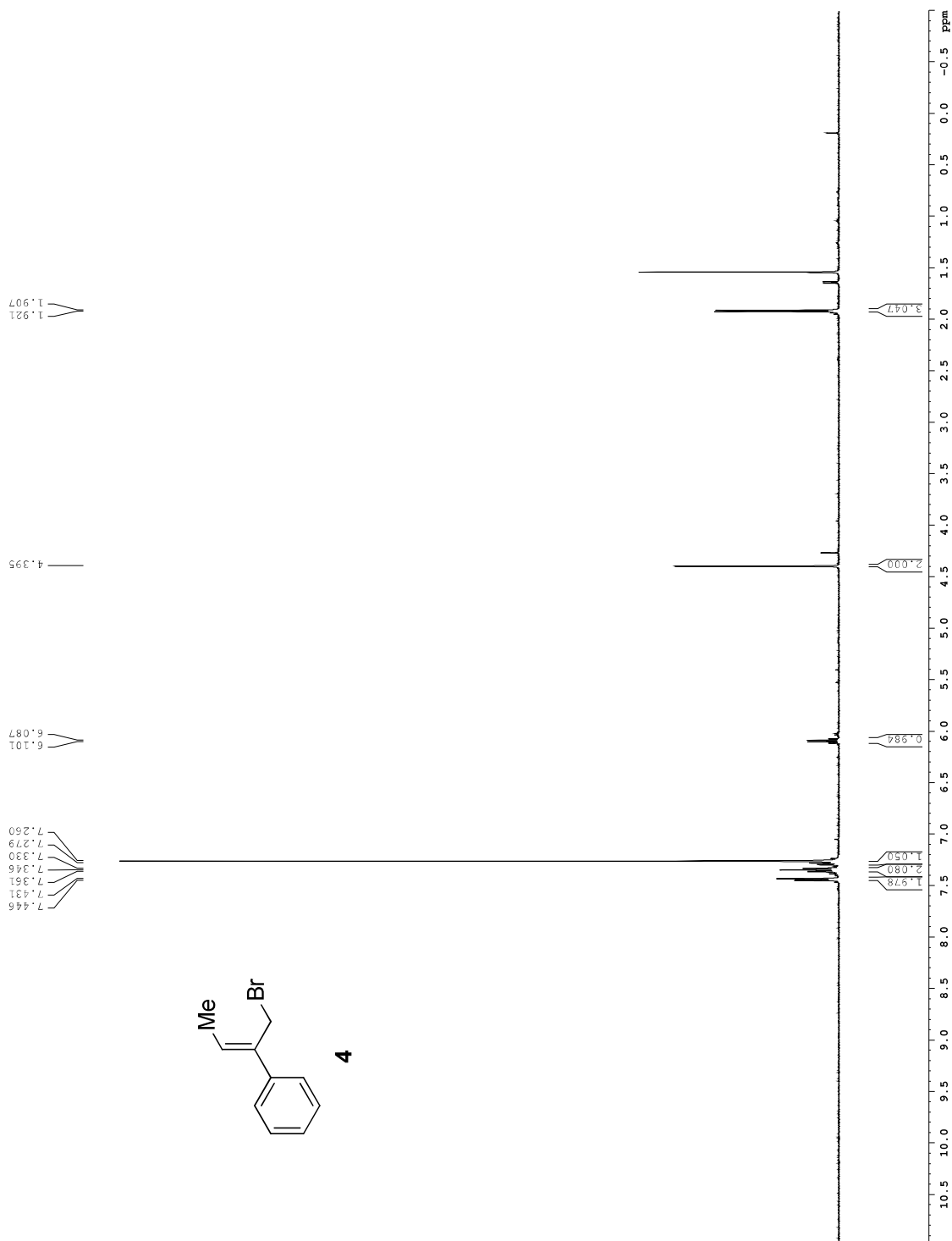
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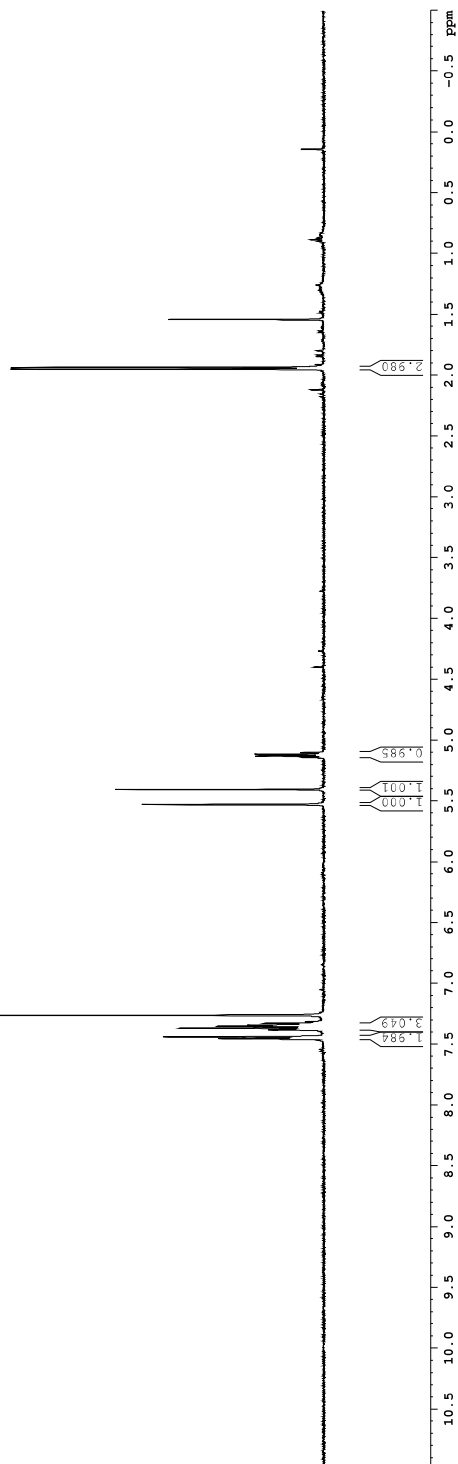
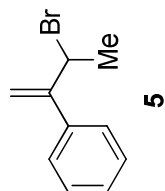


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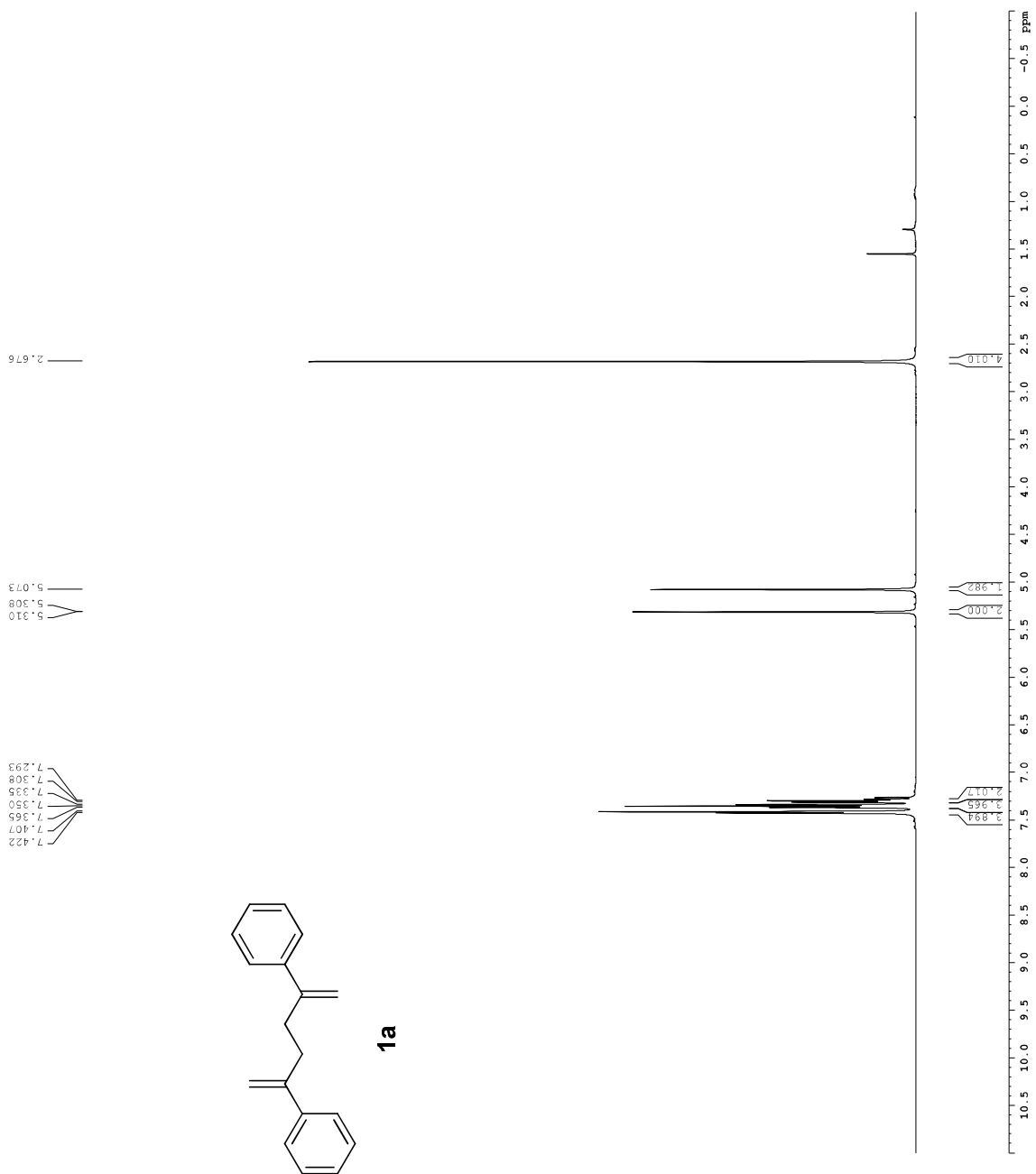
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 PC: 4.00

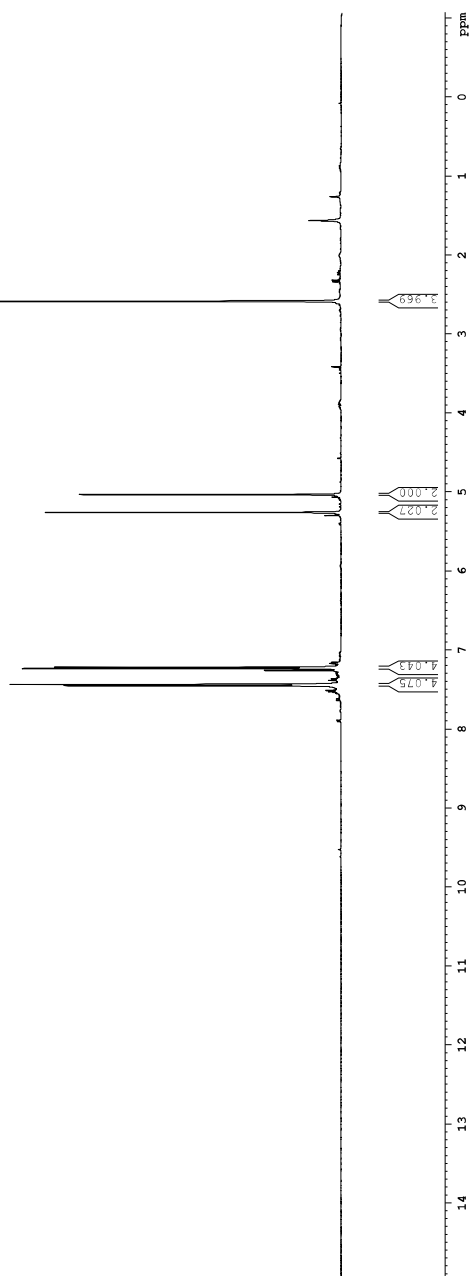
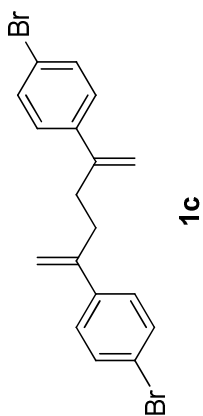


Current Data Parameters
 Name GP-II-19
 EXPNO 30
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20150723
 Time 8:43
 INSTRUM 5 mm CPXI 1H-
 PROBHD 5 mm CPXI 1H-
 PULPROG zg30
 TD 48074
 SOLVENT CDCl3
 NS 2
 DS 2
 SWH 8012.820 Hz
 FIDRES 0.166677 Hz
 AQ 2.9998176 sec
 RG 327.5
 DW 62.400 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.10000000 sec
 MCOREST 0 sec
 LOWRN 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 0.00 dB
 SFO1 500.223013 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200310 MHz
 RG 327.5
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00

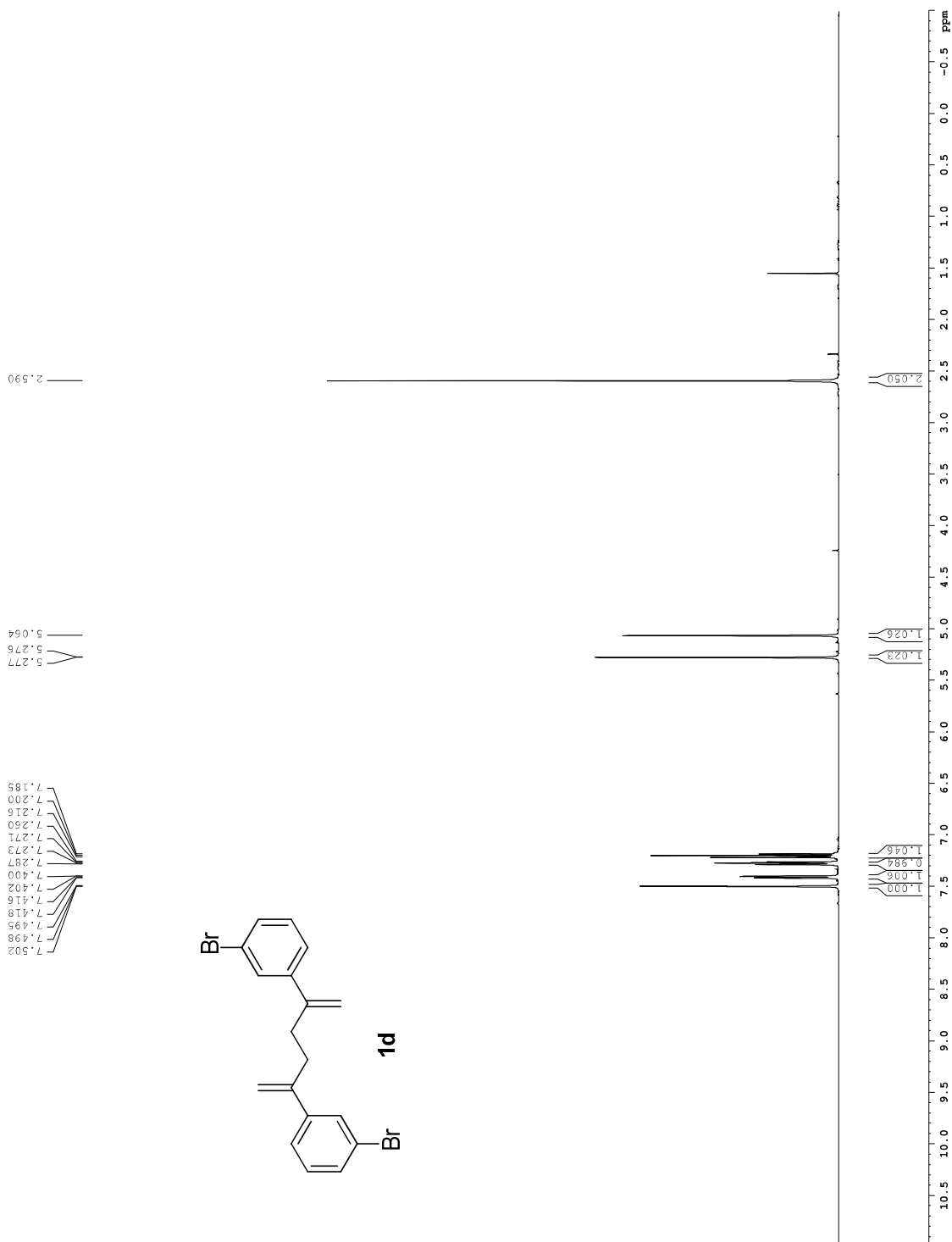
7.453
7.436
7.260
7.234
7.217

5.259
5.033

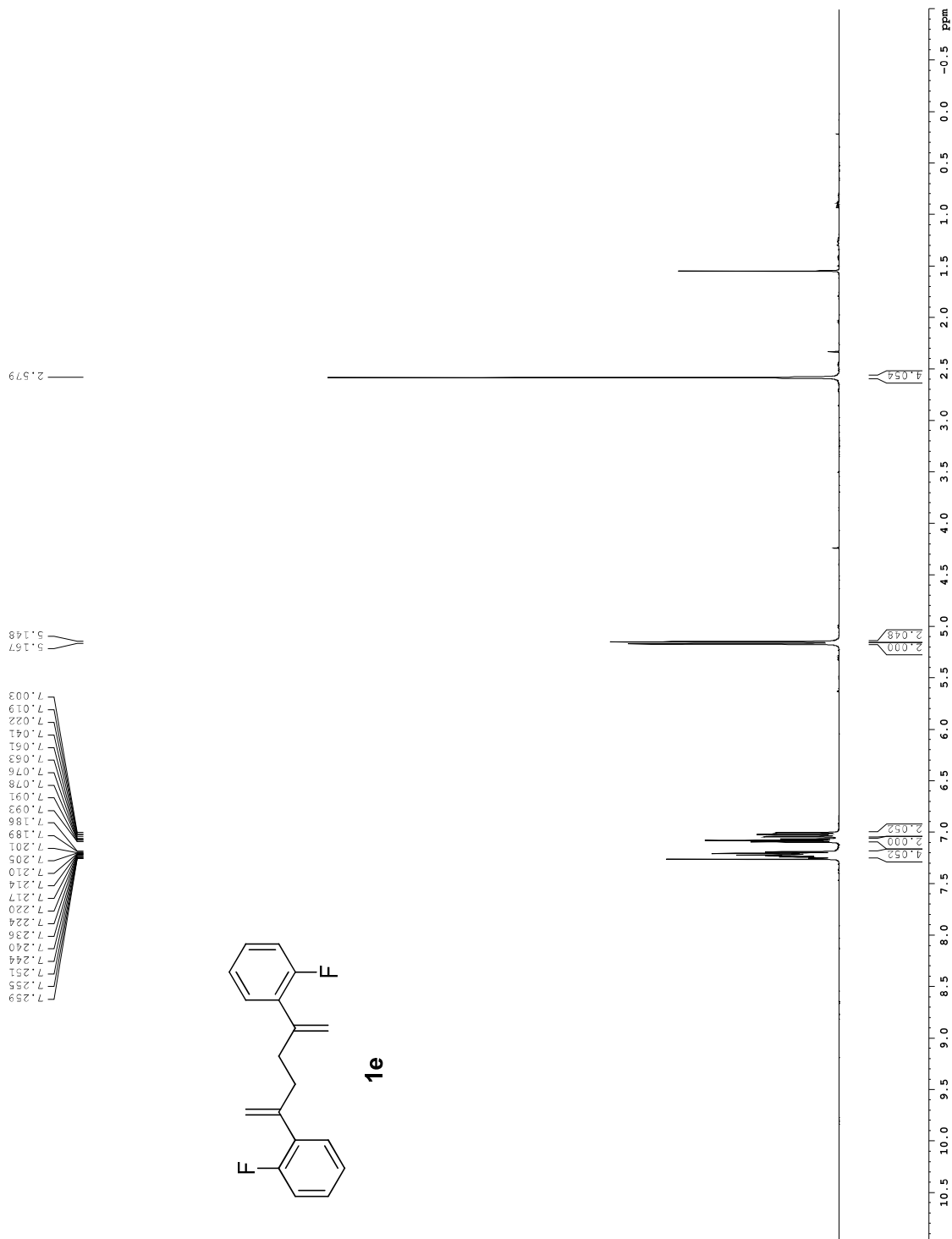
2.584



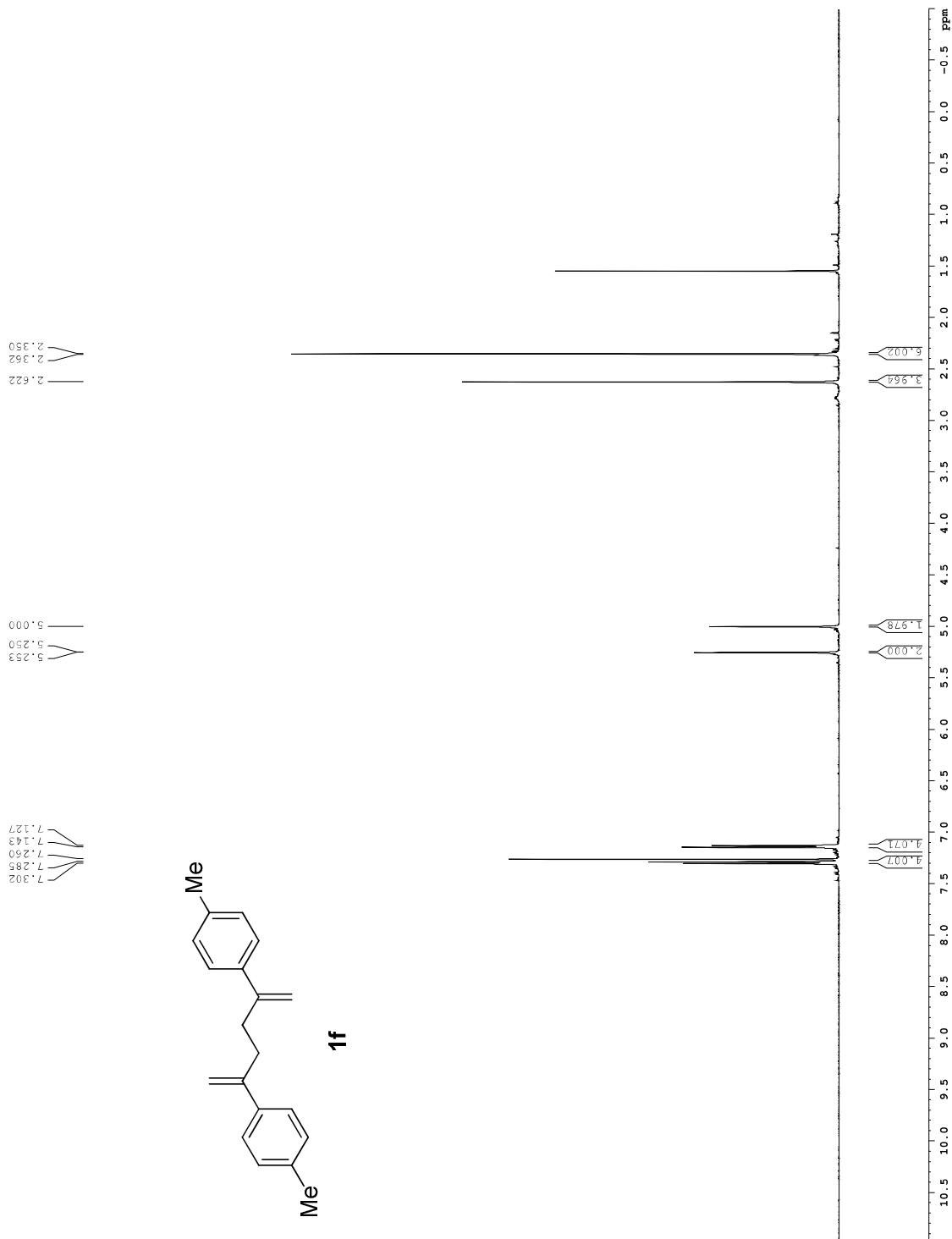
Current Data Parameters
 Name: 1d
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130331
 Time 7:57
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8013.822 Hz
 FWHM 0.16677 Hz
 AQ 2.1998176 sec
 RG 10.1
 DW 62.400 usec
 DE 1.00 usec
 TE 298.2 K
 D1 0.10000000 sec
 NUC1 1H
 F1 7.50 usec
 PC 1.60 dB
 SF 500.2235013 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200713 MHz
 WDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 EC 4.00



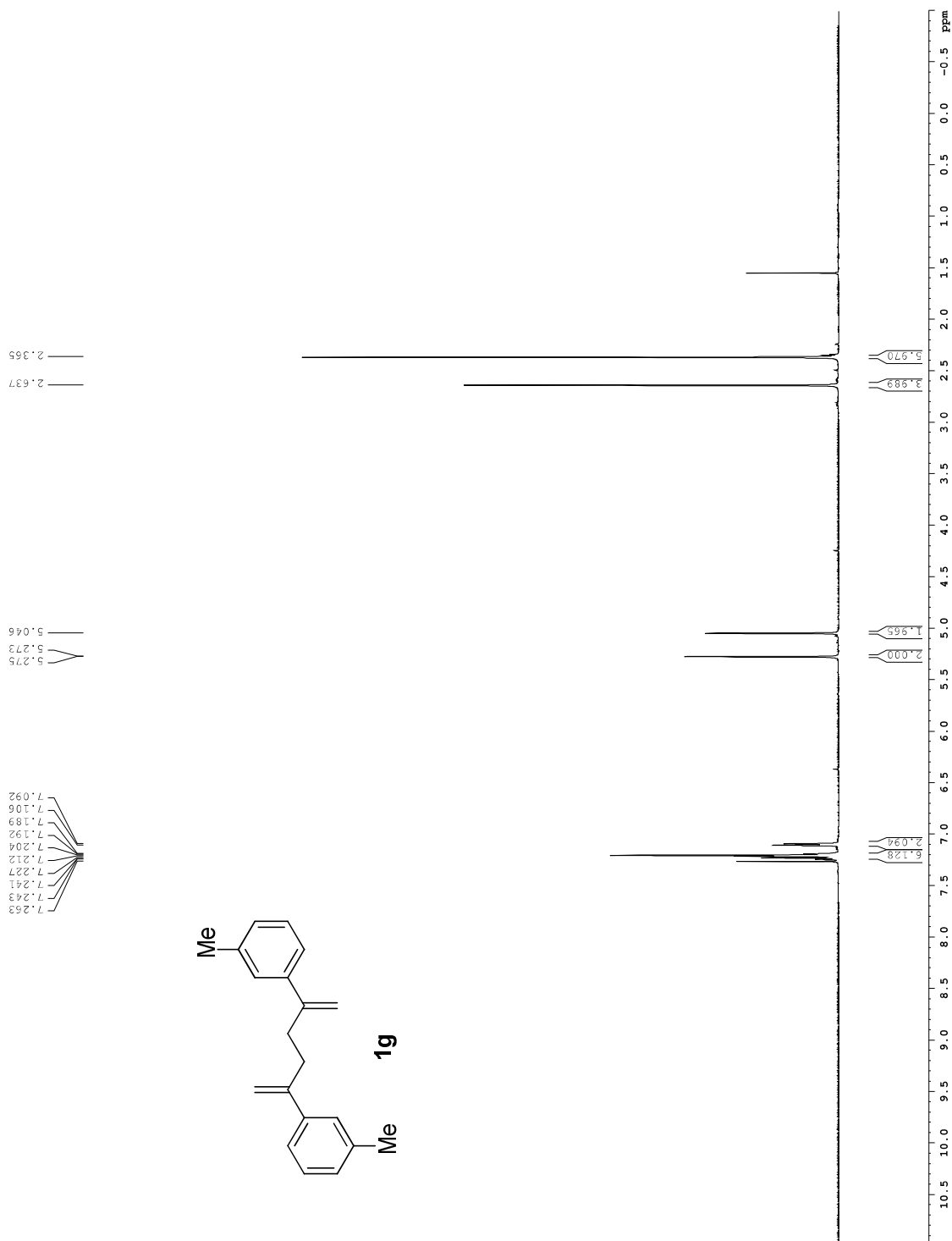
Current Data Parameters
 Name: 1e
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130323
 Time 7.44
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8013.822 Hz
 FIDRES 0.166677 Hz
 AQ 2.9998176 sec
 RG 11.3
 DW 62.400 usec
 DE 1.000 usec
 TE 298.2 K
 D1 0.10000000 sec
 MUREST 0 sec
 KWRRK 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 -6.00 dB
 SFO1 500.225013 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200317 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 EC 4.00



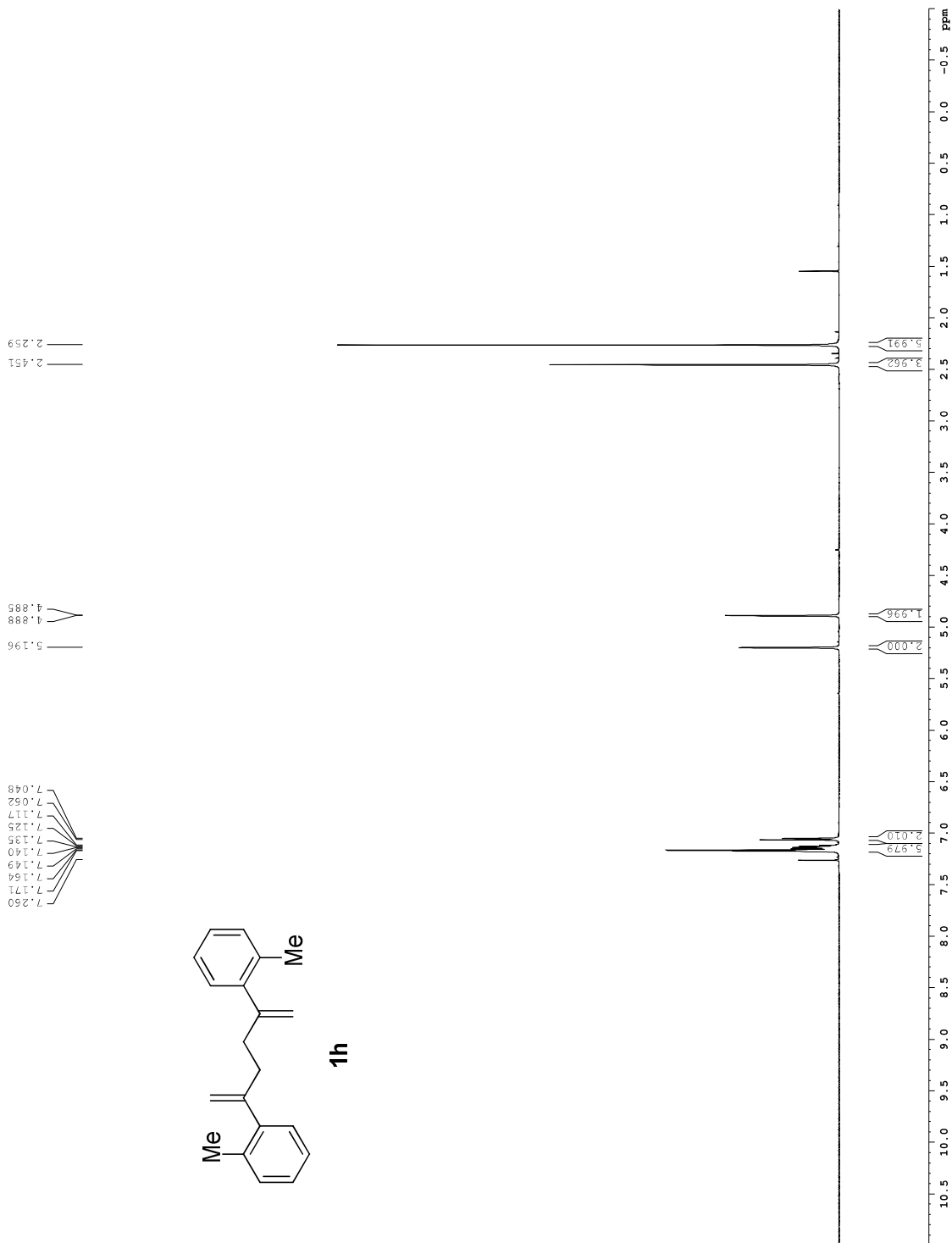
Current Data Parameters
 Name: 2f
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130331
 Time 7.36
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TOFPROG 48274
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8013.822 Hz
 FWHM 0.16677 Hz
 AQ 2.9998176 sec
 RG 11.3
 DW 62.400 usec
 DE 19.00 usec
 TE 298.2 K
 D1 0.10000000 sec
 D11 0.01500000 sec
 NUC1 1H
 F1 7.50 usec
 PC 1.60 dB
 SF 500.2235015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200314 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 EC 4.00



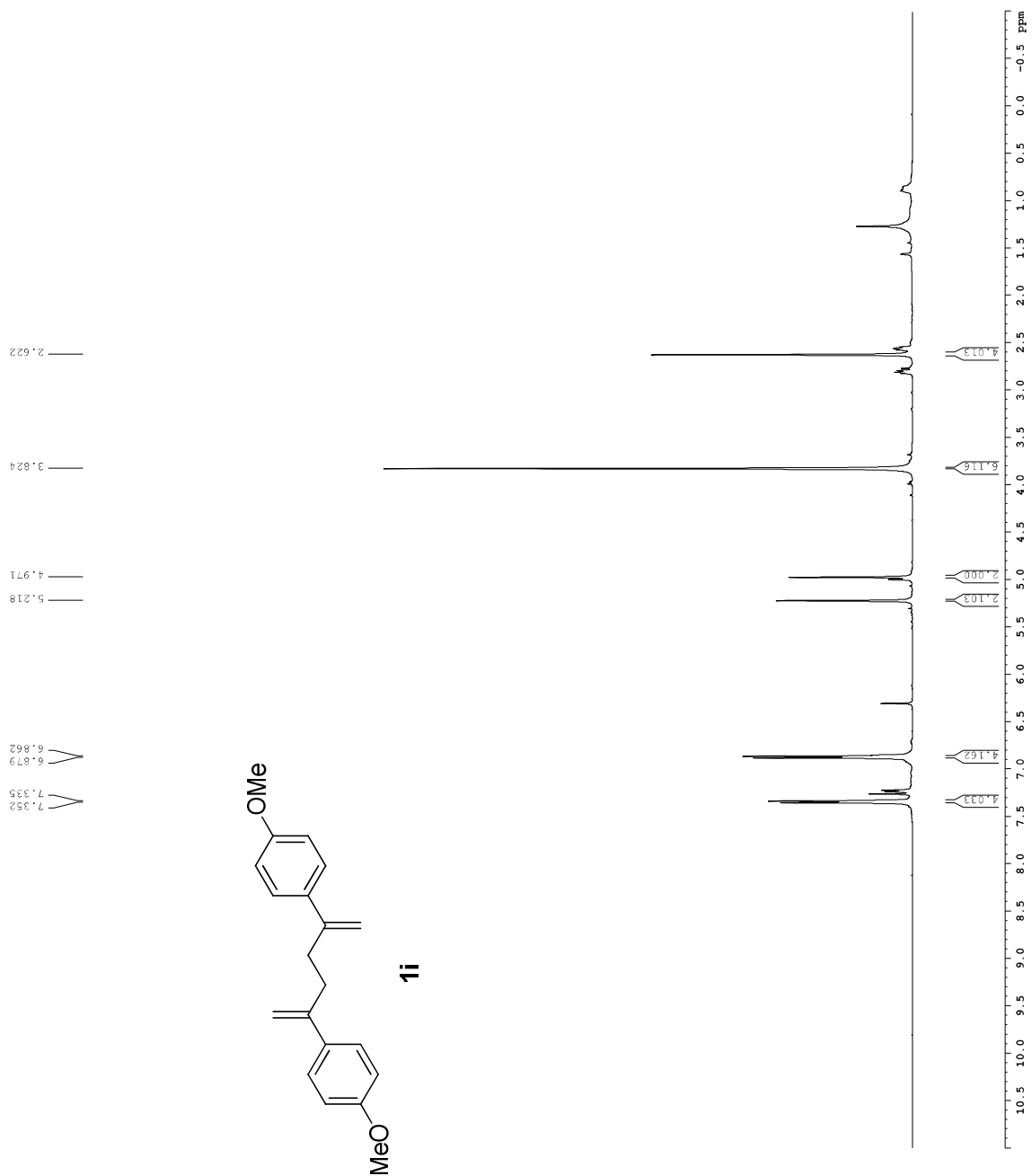
Current Data Parameters
 Name: 1g
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130313
 Time 7.51
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8013.822 Hz
 FIDRES 0.166677 Hz
 AQ 2.1998176 sec
 RG 10.1
 DW 62.400 usec
 DE 1.000 usec
 TE 298.2 K
 D1 0.10000000 sec
 D11 0.10000000 sec
 NUC1 1H
 F1 7.50 usec
 PC 1.60 dB
 SFO1 500.225015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200298 MHz
 WDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 EC 4.00



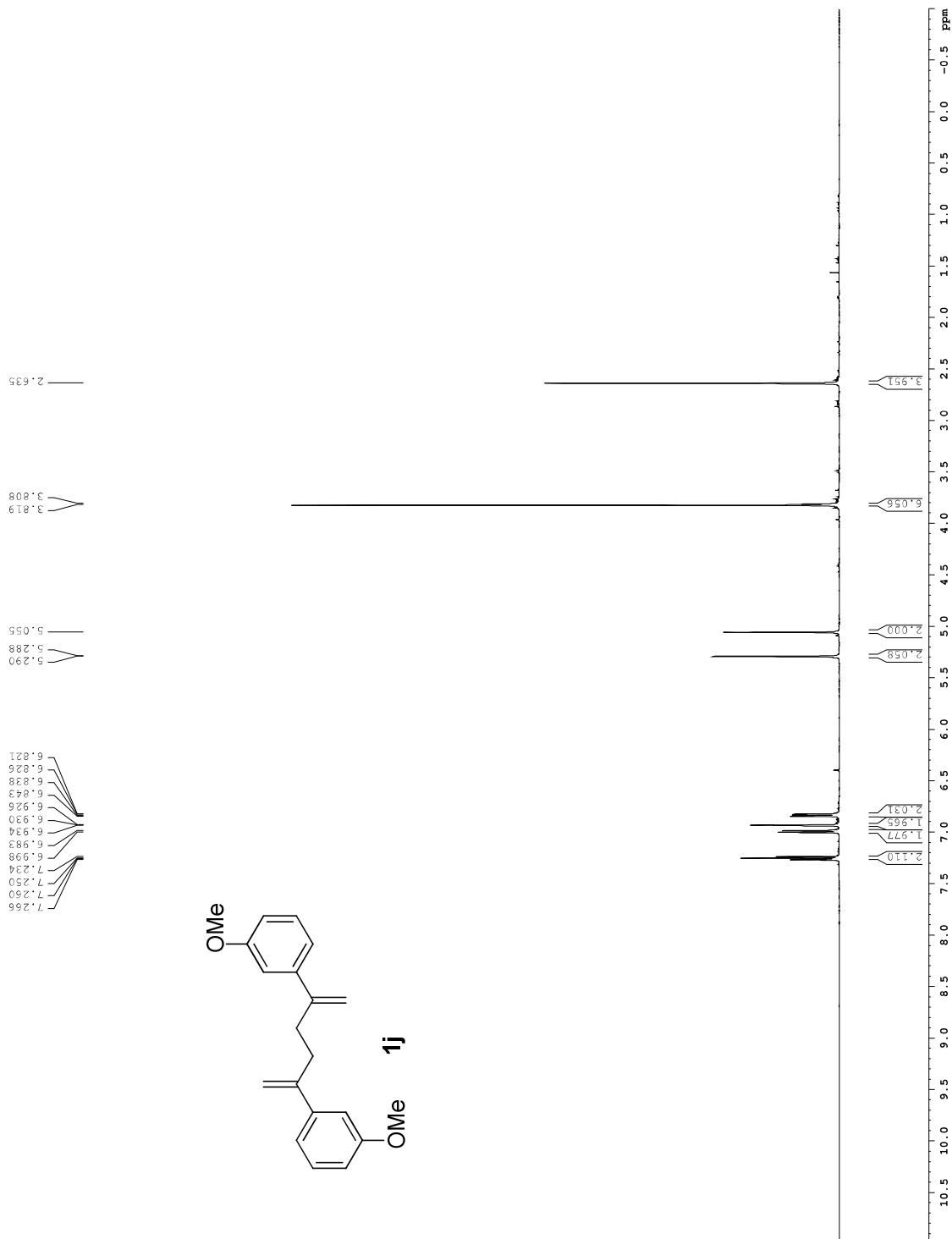
Current Data Parameters
 Name: 2
 EXPNO 90
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130331
 Time 7.29
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8013.822 Hz
 FIDRES 0.166677 Hz
 AQ 2.1998176 sec
 RG 8
 DW 62.400 usec
 DE 1.000 usec
 TE 298.2 K
 D1 0.10000000 sec
 D11 0.01500000 sec
 NUC1 1H
 F1 7.50 usec
 P1 1.60 dB
 SFO1 500.2235013 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200313 MHz
 WDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 FC 4.00

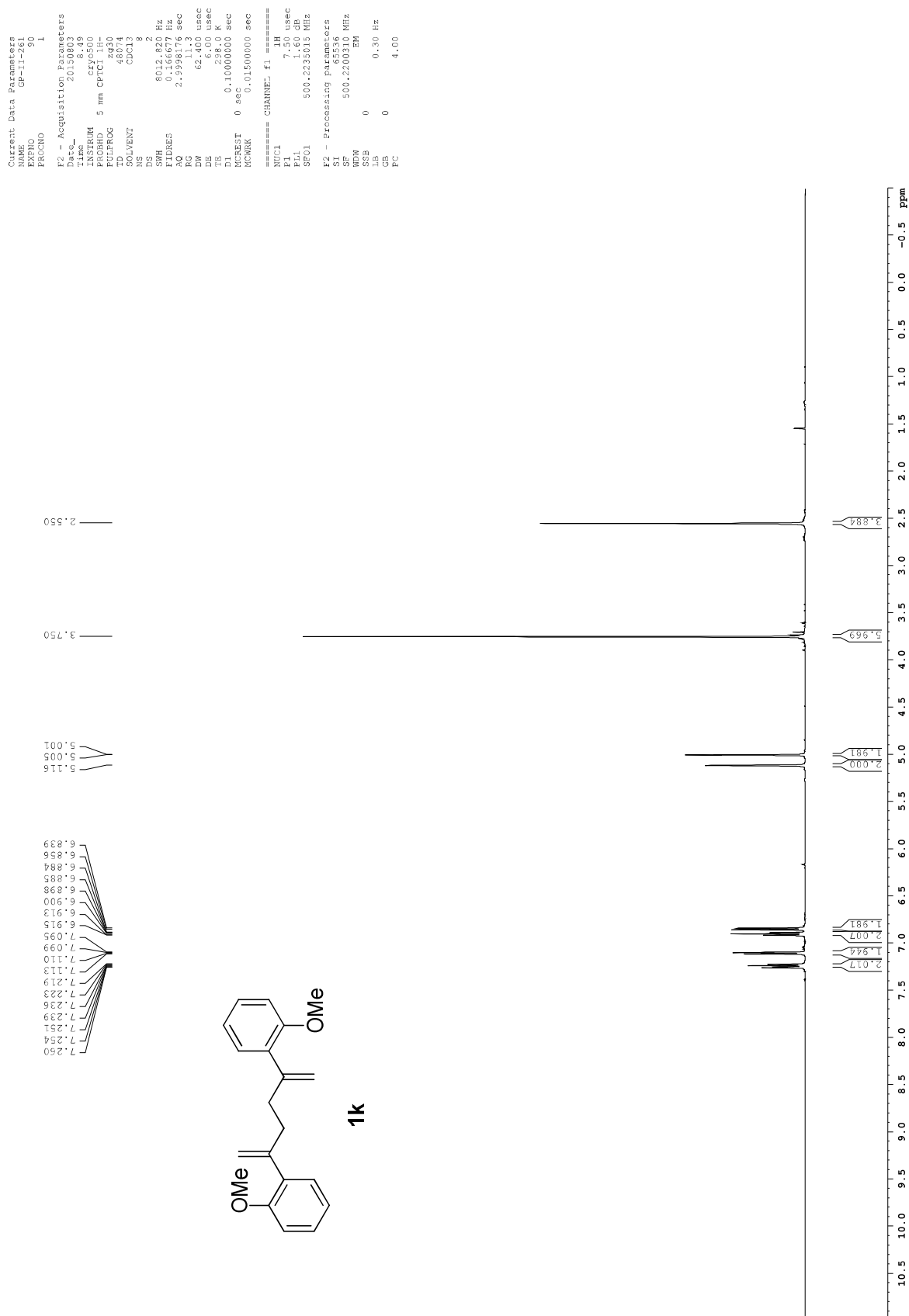


Current Data Parameters
 Name: 1i
 EXPNO: 3
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20150723
 Time: 18.00
 INSTRUM: spect
 PROBHD: 5 mm CPXI 1H-
 PULPROG: zg30
 TD: 48074
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.166677 Hz
 AQ: 2.9998176 sec
 RG: 327.500
 DW: 62.400 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 0.10000000 sec
 MCREST: 0 sec
 LOWRN: 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.223015 MHz
 F2 - Processing parameters
 SI: 65536
 SF: 500.2200315 MHz
 RG: 327.500
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 4.00



Current Data Parameters
 Name: 1j
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20100808
 Time 9.06
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8013.822 Hz
 FWHM 0.16677 Hz
 AQ 2.9998176 sec
 RG 10.1
 DW 62.400 usec
 DE 1.900 usec
 TE 298.2 K
 D1 0.10000000 sec
 NUC1 1H
 F1 7.50 usec
 PL1 0.00 dB
 SFO1 500.225013 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200713 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00

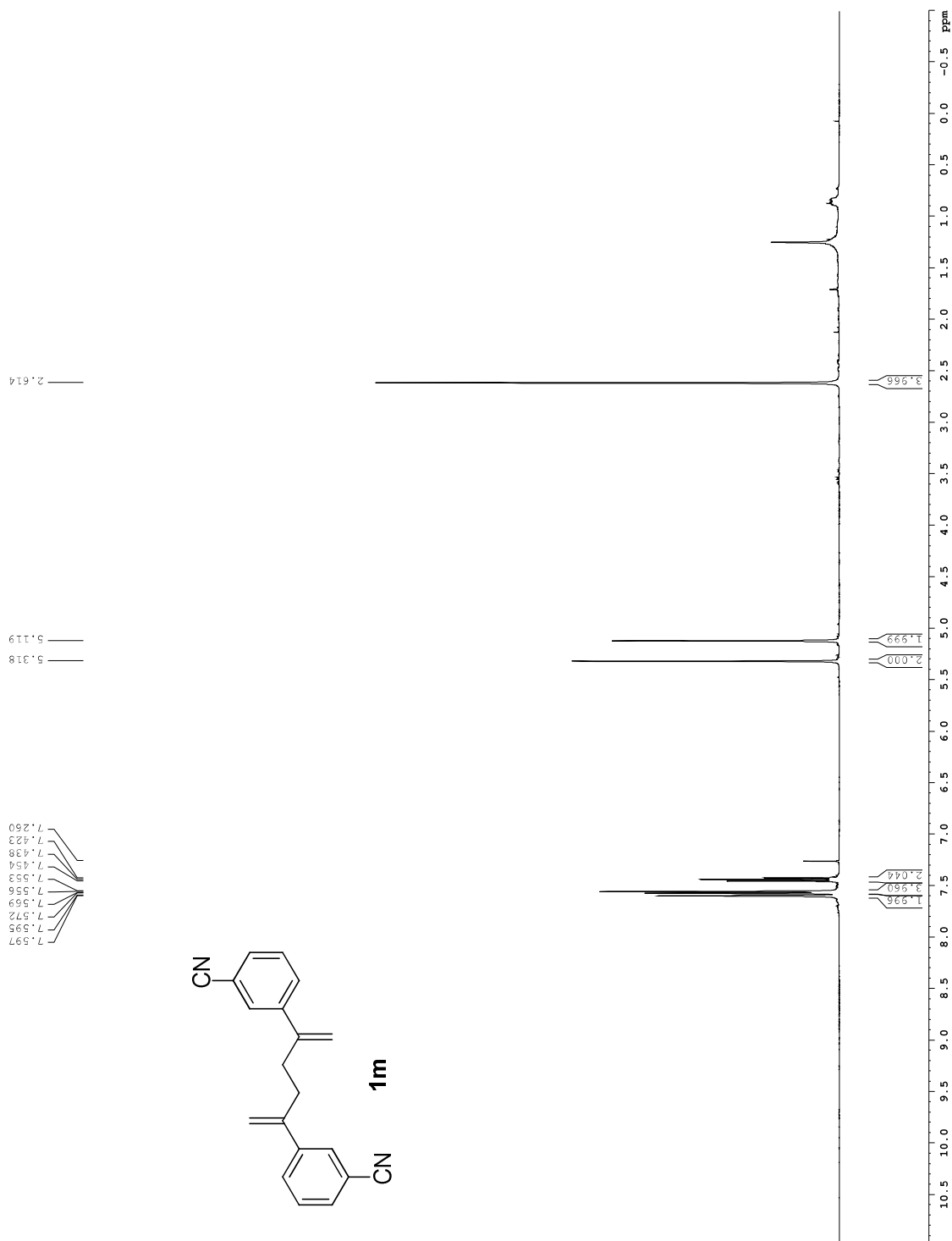




Current Data Parameters
 Name: 11-85
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130808
 Time 8.15
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TOFPROG 48274
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8013.822 Hz
 FWHM 0.16677 Hz
 AQ 2.9998176 sec
 RG 9
 DW 62.400 usec
 DE 1.0000000 usec
 TE 298.2 K
 D1 0.10000000 sec
 D11 0.10000000 sec
 NUC1 1H
 F1 7.50 usec
 PC 1.60 dB
 SF 500.2235015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200315 MHz
 WDW 0
 SSB 0
 LB 0.30 Hz
 GB 0
 EC 4.00



Current Data Parameters
 Name: 20130003
 EXPNO 2
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20130003
 Time 9.23
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TOFPROG 48274
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8013.822 Hz
 FWHM 0.16677 Hz
 AQ 2.1998176 sec
 RG 9
 DW 62.400 usec
 DE 19.000 usec
 TE 298.2 K
 D1 0.10000000 sec
 D11 0.10000000 sec
 NUREST 0 sec
 NUC1 1H
 F1 7.50 usec
 PC 1.60 dB
 SF01 500.2235015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200312 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 EC 4.00



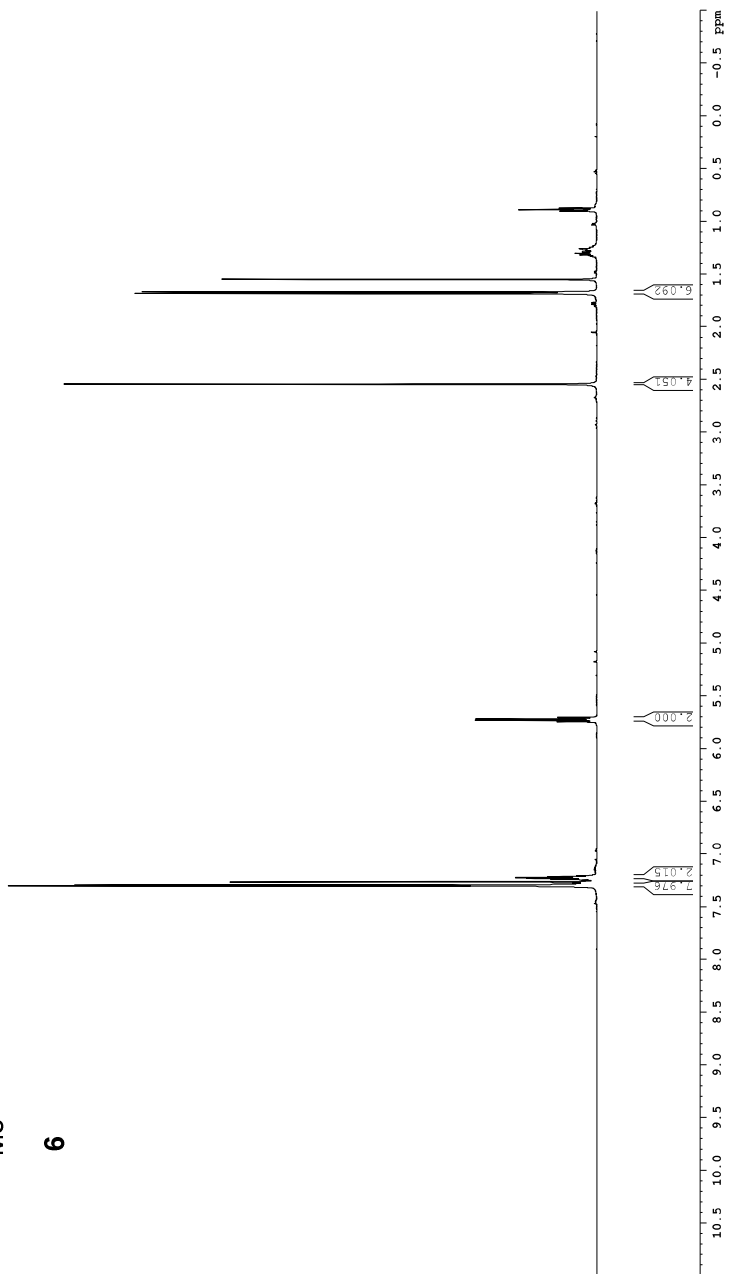
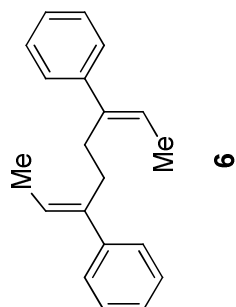
Current Data Parameters
 Name: 6
 EXPNO: 31
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20150804
 Time: 15:24
 INSTRUM: spect
 PROBHD: 5 mm CPXI 1H-
 PULPROG: zg30
 TD: 48074
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.166677 Hz
 AQ: 2.9998176 sec
 RG: 327.67
 DW: 62.400 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 0.10000000 sec
 MCOREST: 0 sec
 FLOWN: 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.223013 MHz
 F2 - Processing parameters
 SI: 65536
 SF: 500.2200311 MHz
 RG: 327.67
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 4.00

1.678
1.664

2.539

5.727
5.714

7.298
7.290
7.260
7.219



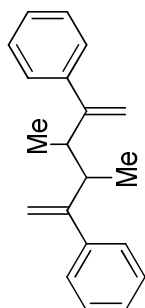
Current Data Parameters
 Name: 8
 EXPNO: 100
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20150806
 Time: 22:25
 INSTRUM: spect
 PROBHD: 5 mm CPXI 1H-
 PULPROG: zg30
 TD: 48074
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.166677 Hz
 AQ: 2.9998176 sec
 RG: 327.5
 DW: 62.400 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 0.10000000 sec
 MCHRG: 0
 LOWRN: 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.223013 MHz
 F2 - Processing parameters
 SI: 65536
 SF: 500.2200314 MHz
 RG: 327.5
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 4.00

1.171
1.159
0.949
0.935

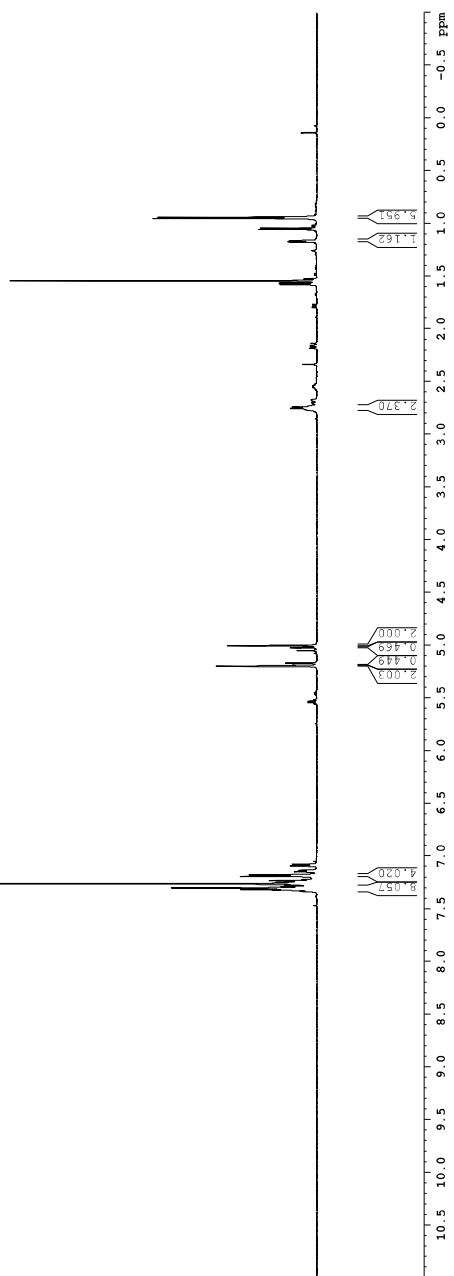
2.751
2.737

5.194
5.020
5.001

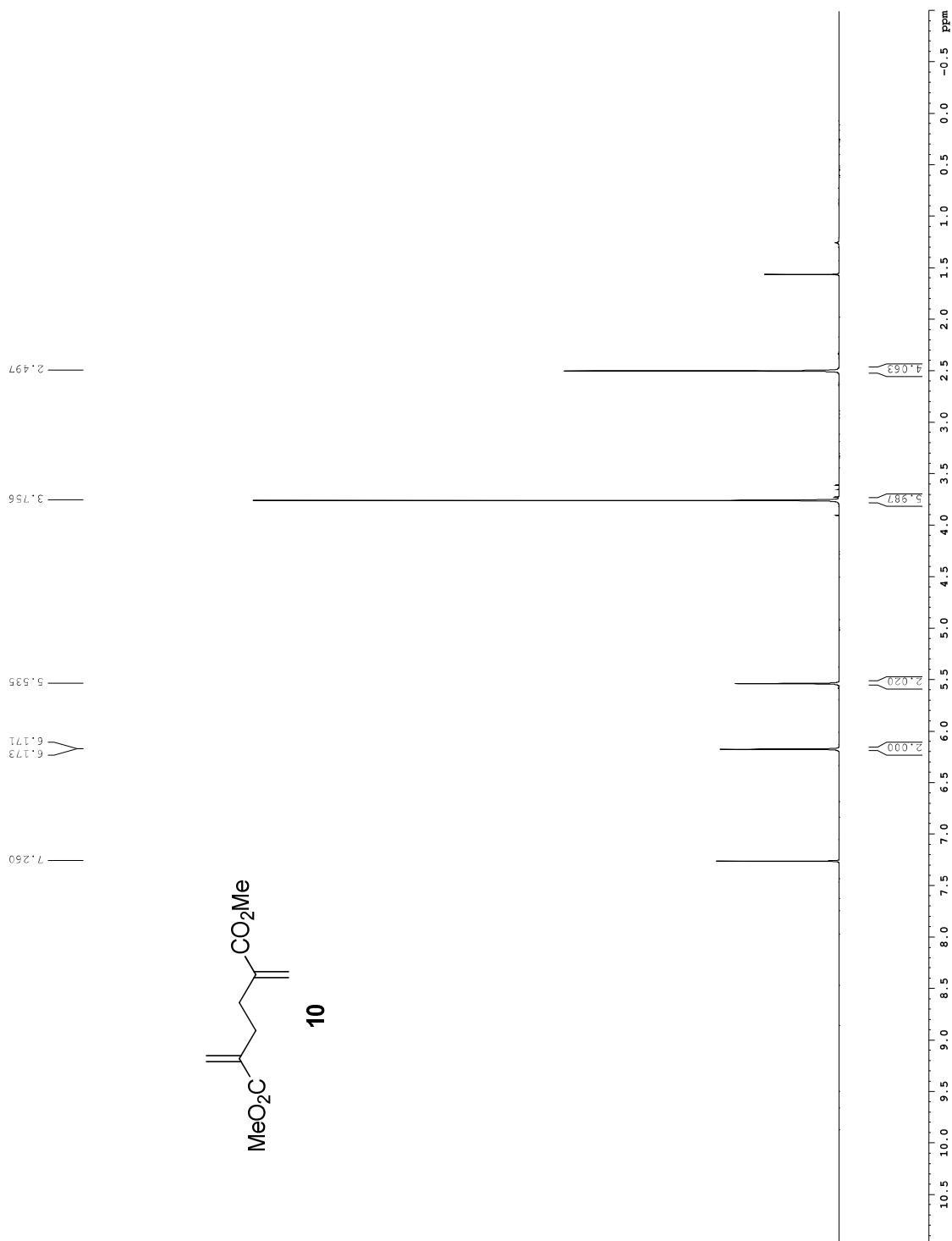
7.320
7.314
7.287
7.190
7.186
7.174



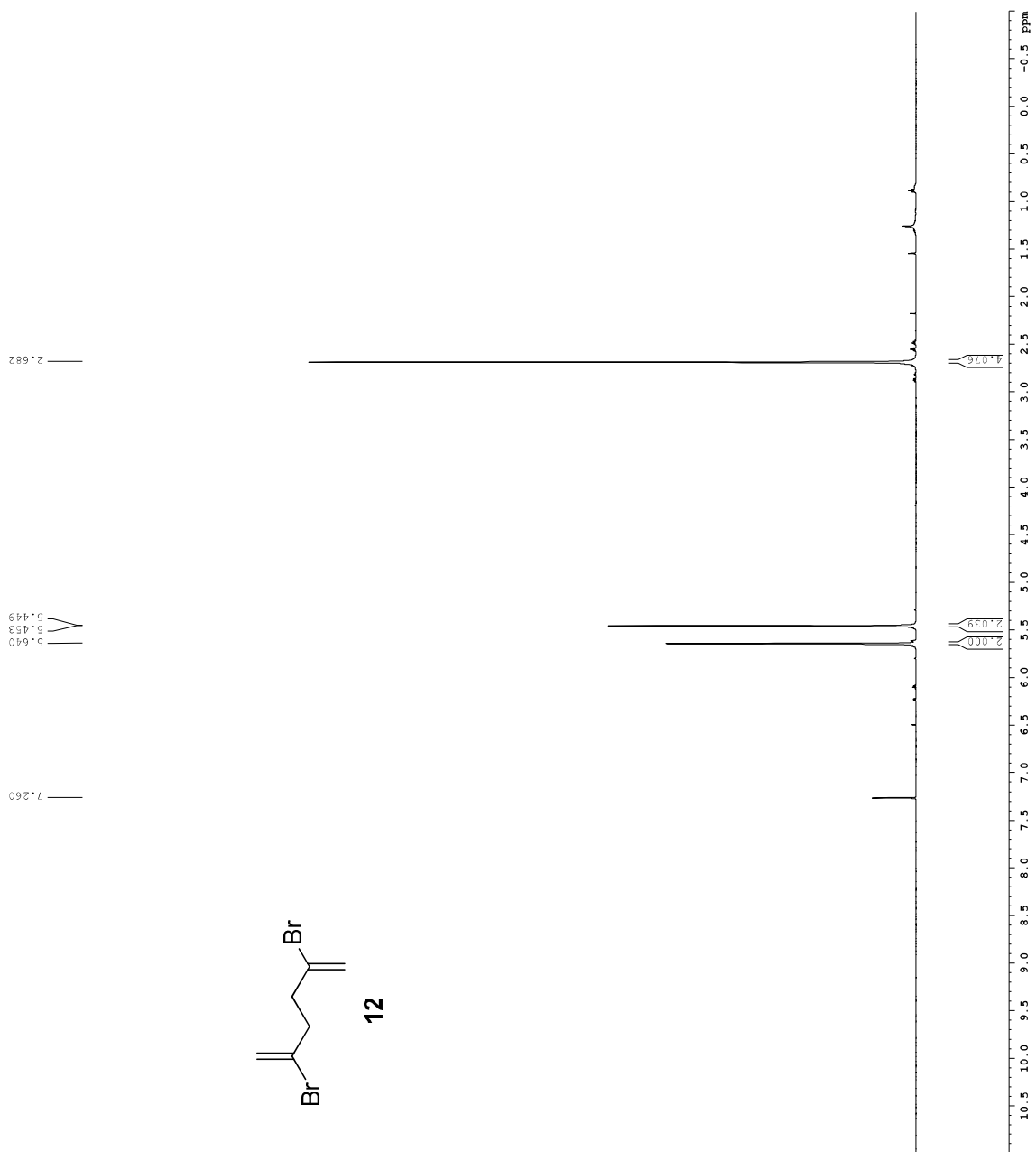
8 (dr 5:1)



Current Data Parameters
 Name: 10
 EXPNO 100
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20190808
 Time 8.39
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TOFPROG 48274
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 6013.822 Hz
 FWHM 0.16677 Hz
 AQ 2.1998176 sec
 RG 8
 DW 62.400 usec
 DE 1.000 usec
 TE 298.2 K
 D1 0.10000000 sec
 MUREST 0 sec
 KWARK 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1 1H
 P1 7.50 usec
 PL1 0.00 dB
 SFO1 500.225015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200312 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 EC 4.00



Current Data Parameters
 Name: 20151007
 EXPNO: 2
 PROCNO: 1
 F2 - Acquisition Parameters
 Date_: 20151007
 Time: 15:02
 INSTRUM: spect
 PROBHD: 5 mm CPIC1 1H-
 PULPROG: zg30
 TD: 48074
 SOLVENT: CDCl3
 NS: 2
 DS: 2
 SWH: 8012.820 Hz
 FIDRES: 0.166677 Hz
 AQ: 2.9998176 sec
 RG: 327.500
 DW: 62.400 usec
 DE: 6.00 usec
 TE: 298.0 K
 D1: 0.10000000 sec
 MCOREST: 0 sec
 LOWRN: 0.01500000 sec
 ===== CHANNEL f1 =====
 NUC1: 1H
 P1: 7.50 usec
 PL1: 0.00 dB
 SFO1: 500.223013 MHz
 F2 - Processing parameters
 SI: 65536
 SF: 500.2200314 MHz
 RG: 327.500
 SSB: 0
 LB: 0.30 Hz
 GB: 0
 PC: 4.00

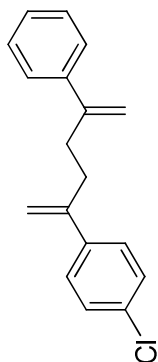


Current Data Parameters
 Name: 15-1-2015
 EXPNO 1
 PROCNO 1
 F2 - Acquisition Parameters
 Date_ 20150801
 Time 8.21
 INSTRUM cryo500
 PROBHD 5 mm OPTCI 1H-
 PULPROG zgpg30
 TO 48274
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 8012.822 Hz
 FWHM 0.16677 Hz
 AQ 2.9998176 sec
 RG 12.7
 DW 62.400 usec
 DE 19.80 usec
 TE 298.2 K
 D1 0.10000000 sec
 MUREST 0 sec
 NUC1 1H
 F1 7.50 usec
 PD1 1.60 dB
 SFOL 500.2235015 MHz
 F2 - Processing parameters
 SI 65536
 SF 500.2200316 MHz
 WDW EN
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 4.00

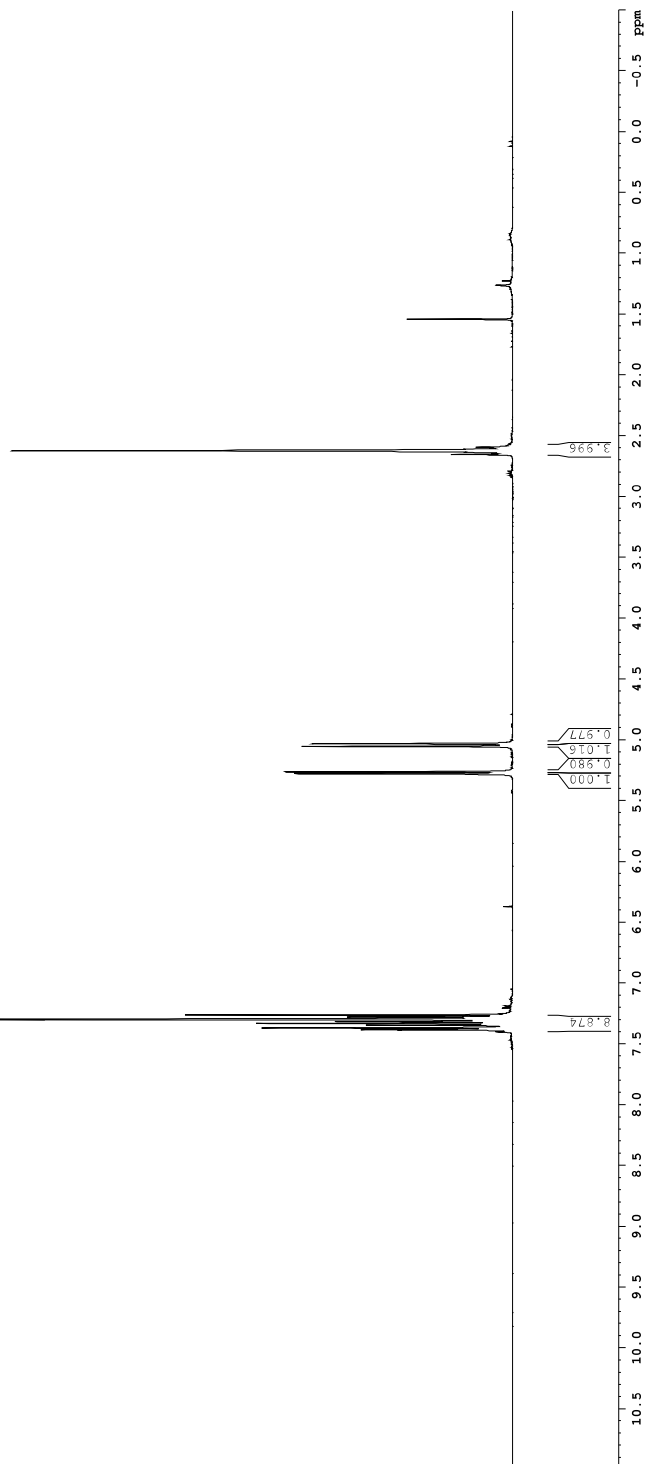
7.384
7.381
7.367
7.344
7.340
7.330
7.315
7.298
7.294
7.281
7.276
7.260

5.276
5.274
5.261
5.260
5.050
5.029

2.552
2.526
2.522
2.470
2.460
2.390



15



^{13}C NMR Spectra

Current Data Parameters
 NAME GP-11-216
 EXPNO 52
 PROCNO 1

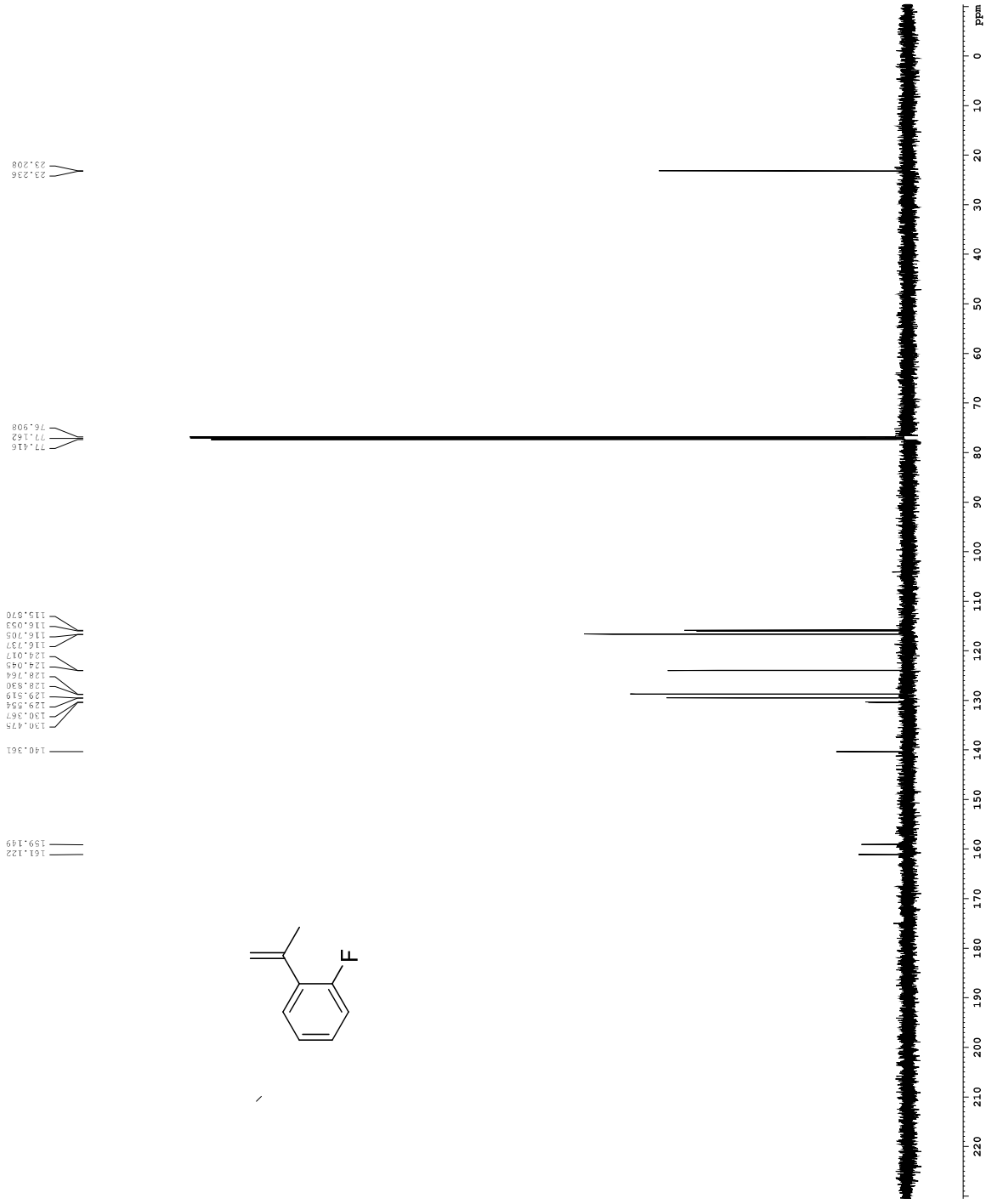
F2 - Acquisition Parameters
 Date_ 20150918
 Time 15.35
 INSTRUM cryo500
 PROBD 5 mm CPTCI 1H-
 PULPROG Spinecho90ap-prd
 TD 65536
 SOLVENT CDCl3
 NS 128
 DS 16
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0413440 sec
 RG 128.000
 DW 16.500 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 d12 0.06000000 sec
 d17 0.00015000 sec
 MCRST 0 sec
 MCWRK 0.01500000 sec
 P2 33.10 usec

===== CHANNEL f1 =====
 NUC1 13C
 P1 16.55 usec
 P11 500.00 usec
 P12 2000.00 usec
 FLO 120.00 dB
 PL1 125.794558 MHz
 SE1 2.70 dB
 SE2 2.70 dB
 SFNAM[1] Ctp60,0.5,20.1
 SFNAM[2] Ctp60comp.4
 SFOF1 0 Hz
 SFOF2 0 Hz

===== CHANNEL f2 =====
 CPDPRG12 waltz16
 NUC2 1H
 P2D2 100.00 usec
 P2F2 24.50 dB
 PL2 500.2225011 MHz
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
 GPNAM[1] SINE.100
 GPNAM[2] SINE.100
 GEX1 0 %
 GEX2 0 %
 GFY1 0 %
 GFY2 0 %
 GRZ1 30.00 %
 GRZ2 0.00 %
 GRZ3 50.00 %
 P16 1000.00 usec

F2 - Processing parameters
 SI 65536
 SF 125.7804074 MHz
 RG 128
 SSF 0
 LB 1.00 Hz
 GB 0
 FC 2.00



220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

Current Data Parameters
 NAME GF-II-258
 EXPNO 5
 PROCNO 1

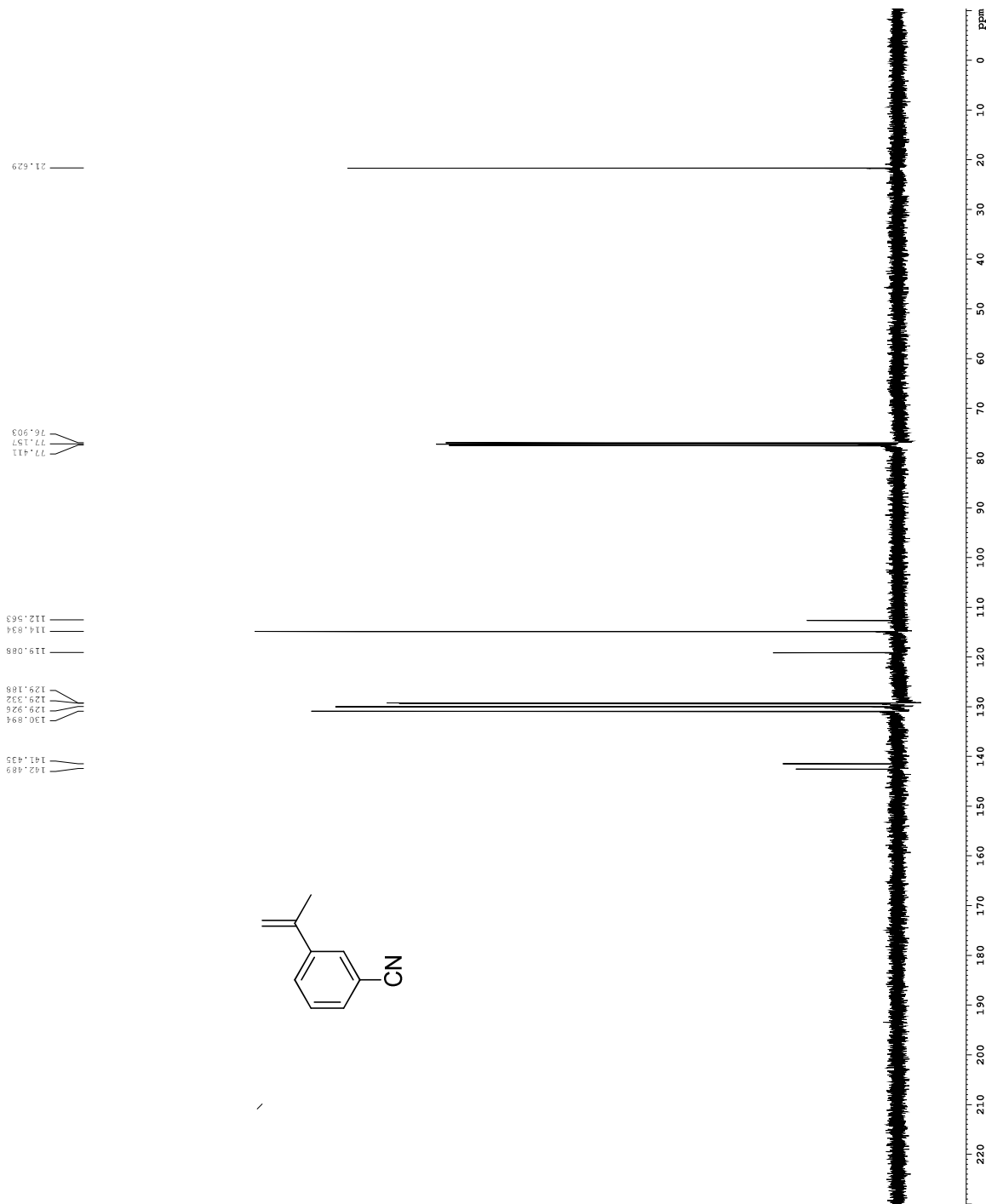
F2 - Acquisition Parameters
 Date_ 2019.9.43
 Time_ 9.43
 INSTRUM cryo500
 PROBHD 5 mm CFTCI 1H-
 PULPROG SpinEcho90pp-prd
 TD 65536
 SFO 500.130000 MHz
 SOLVENT CDCl₃
 NS 128
 DS 16
 SWH 30303.031 Hz
 FIDRES 0.462388 Hz
 AQ 1.0413640 sec
 RG 327.62
 DW 16.500 usec
 DE 6.00 usec
 TE 298.0 K
 D1 0.25000000 sec
 d11 0.03000000 sec
 d12 0.00200000 sec
 d17 0.00015600 sec
 MCGRST 0 sec
 MCWREK 0.01500000 sec
 P2 33.10 usec

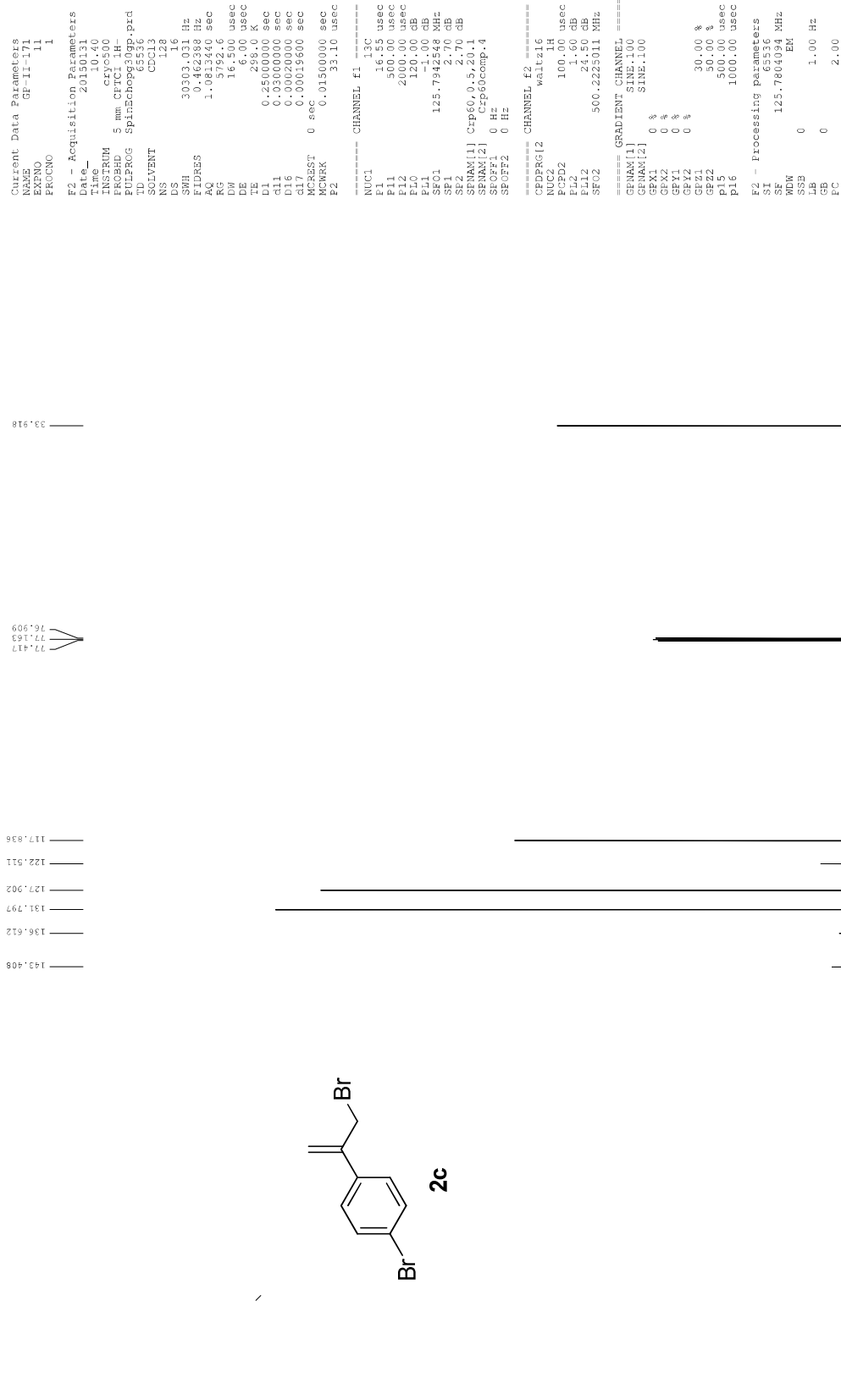
===== CHANNEL f1 13C =====
 NUC1 13C
 P1 16.55 usec
 P11 500.00 usec
 P12 2000.00 usec
 PLO 120.00 dB
 PL1 120.00 dB
 PL2 120.00 dB
 SFO1 125.764500 MHz
 SE1 2.70 dB
 SE2 2.70 dB
 SENAM[1] Crp60, 0.5, 20.1
 SENAM[2] Crp60comp, 4
 SFOFF1 0 Hz
 SFOFF2 0 Hz

===== CHANNEL f2 1H =====
 CPDPRG2 waltz16
 NUC2 1H
 P2 100.00 usec
 P21 100.00 dB
 P22 2.50 dB
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
 GENAM[1] SINE, 100
 GENAM[2] SINE, 100
 GENP1 0 %
 GENP2 0 %
 GENP3 0 %
 GENP4 0 %
 GENP5 0 %
 GENP6 0 %
 GENP7 0 %
 GENP8 0 %
 GENP9 0 %
 GENP10 0 %
 GENP11 0 %
 GENP12 0 %
 GENP13 0 %
 GENP14 0 %
 GENP15 0 %
 GENP16 0 %
 GENP17 0 %
 GENP18 0 %
 GENP19 0 %
 GENP20 0 %
 GENP21 0 %
 GENP22 0 %
 GENP23 0 %
 GENP24 0 %
 GENP25 0 %
 GENP26 0 %
 GENP27 0 %
 GENP28 0 %
 GENP29 0 %
 GENP30 0 %
 GENP31 0 %
 GENP32 0 %
 GENP33 0 %
 GENP34 0 %
 GENP35 0 %
 GENP36 0 %
 GENP37 0 %
 GENP38 0 %
 GENP39 0 %
 GENP40 0 %
 GENP41 0 %
 GENP42 0 %
 GENP43 0 %
 GENP44 0 %
 GENP45 0 %
 GENP46 0 %
 GENP47 0 %
 GENP48 0 %
 GENP49 0 %
 GENP50 0 %
 GENP51 0 %
 GENP52 0 %
 GENP53 0 %
 GENP54 0 %
 GENP55 0 %
 GENP56 0 %
 GENP57 0 %
 GENP58 0 %
 GENP59 0 %
 GENP60 0 %
 GENP61 0 %
 GENP62 0 %
 GENP63 0 %
 GENP64 0 %
 GENP65 0 %
 GENP66 0 %
 GENP67 0 %
 GENP68 0 %
 GENP69 0 %
 GENP70 0 %
 GENP71 0 %
 GENP72 0 %
 GENP73 0 %
 GENP74 0 %
 GENP75 0 %
 GENP76 0 %
 GENP77 0 %
 GENP78 0 %
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 GENP80 0 %
 GENP81 0 %
 GENP82 0 %
 GENP83 0 %
 GENP84 0 %
 GENP85 0 %
 GENP86 0 %
 GENP87 0 %
 GENP88 0 %
 GENP89 0 %
 GENP90 0 %
 GENP91 0 %
 GENP92 0 %
 GENP93 0 %
 GENP94 0 %
 GENP95 0 %
 GENP96 0 %
 GENP97 0 %
 GENP98 0 %
 GENP99 0 %
 GENP100 0 %

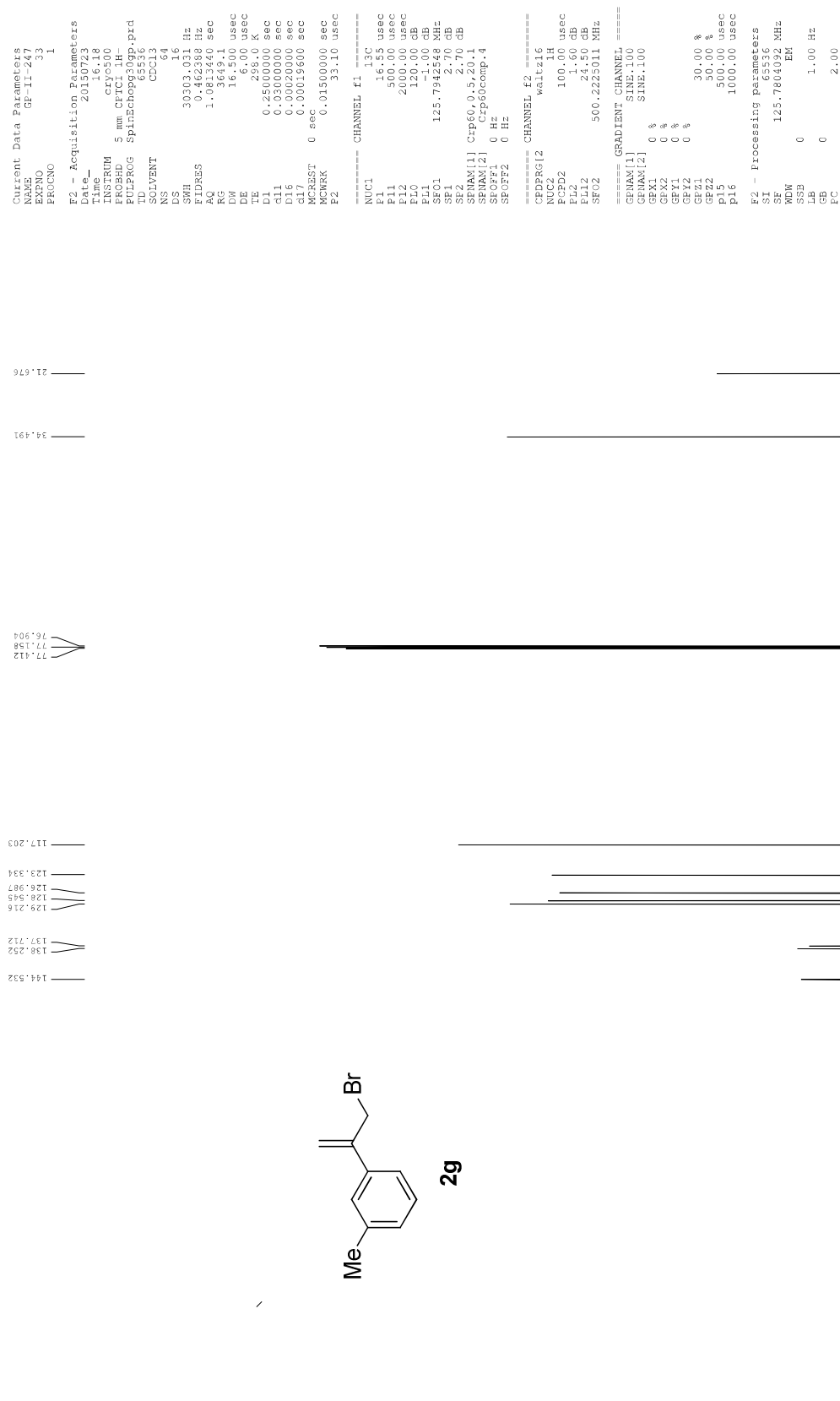
F2 - Processing parameters
 SI 65536
 SF 125.7604105 MHz
 SFO 500.130000 MHz
 SFW 50.00 %
 SFL 50.00 %
 SFR 50.00 %
 SFS 50.00 %
 SFT 50.00 %
 SFT2 50.00 %
 SFT3 50.00 %
 SFT4 50.00 %
 SFT5 50.00 %
 SFT6 50.00 %
 SFT7 50.00 %
 SFT8 50.00 %
 SFT9 50.00 %
 SFT10 50.00 %
 SFT11 50.00 %
 SFT12 50.00 %
 SFT13 50.00 %
 SFT14 50.00 %
 SFT15 50.00 %
 SFT16 50.00 %
 SFT17 50.00 %
 SFT18 50.00 %
 SFT19 50.00 %
 SFT20 50.00 %
 SFT21 50.00 %
 SFT22 50.00 %
 SFT23 50.00 %
 SFT24 50.00 %
 SFT25 50.00 %
 SFT26 50.00 %
 SFT27 50.00 %
 SFT28 50.00 %
 SFT29 50.00 %
 SFT30 50.00 %
 SFT31 50.00 %
 SFT32 50.00 %
 SFT33 50.00 %
 SFT34 50.00 %
 SFT35 50.00 %
 SFT36 50.00 %
 SFT37 50.00 %
 SFT38 50.00 %
 SFT39 50.00 %
 SFT40 50.00 %
 SFT41 50.00 %
 SFT42 50.00 %
 SFT43 50.00 %
 SFT44 50.00 %
 SFT45 50.00 %
 SFT46 50.00 %
 SFT47 50.00 %
 SFT48 50.00 %
 SFT49 50.00 %
 SFT50 50.00 %
 SFT51 50.00 %
 SFT52 50.00 %
 SFT53 50.00 %
 SFT54 50.00 %
 SFT55 50.00 %
 SFT56 50.00 %
 SFT57 50.00 %
 SFT58 50.00 %
 SFT59 50.00 %
 SFT60 50.00 %
 SFT61 50.00 %
 SFT62 50.00 %
 SFT63 50.00 %
 SFT64 50.00 %
 SFT65 50.00 %
 SFT66 50.00 %
 SFT67 50.00 %
 SFT68 50.00 %
 SFT69 50.00 %
 SFT70 50.00 %
 SFT71 50.00 %
 SFT72 50.00 %
 SFT73 50.00 %
 SFT74 50.00 %
 SFT75 50.00 %
 SFT76 50.00 %
 SFT77 50.00 %
 SFT78 50.00 %
 SFT79 50.00 %
 SFT80 50.00 %
 SFT81 50.00 %
 SFT82 50.00 %
 SFT83 50.00 %
 SFT84 50.00 %
 SFT85 50.00 %
 SFT86 50.00 %
 SFT87 50.00 %
 SFT88 50.00 %
 SFT89 50.00 %
 SFT90 50.00 %
 SFT91 50.00 %
 SFT92 50.00 %
 SFT93 50.00 %
 SFT94 50.00 %
 SFT95 50.00 %
 SFT96 50.00 %
 SFT97 50.00 %
 SFT98 50.00 %
 SFT99 50.00 %
 SFT100 50.00 %







2d



Current Data Parameters
NAME GF-II-218
EXPNO 41
PROCNO 1

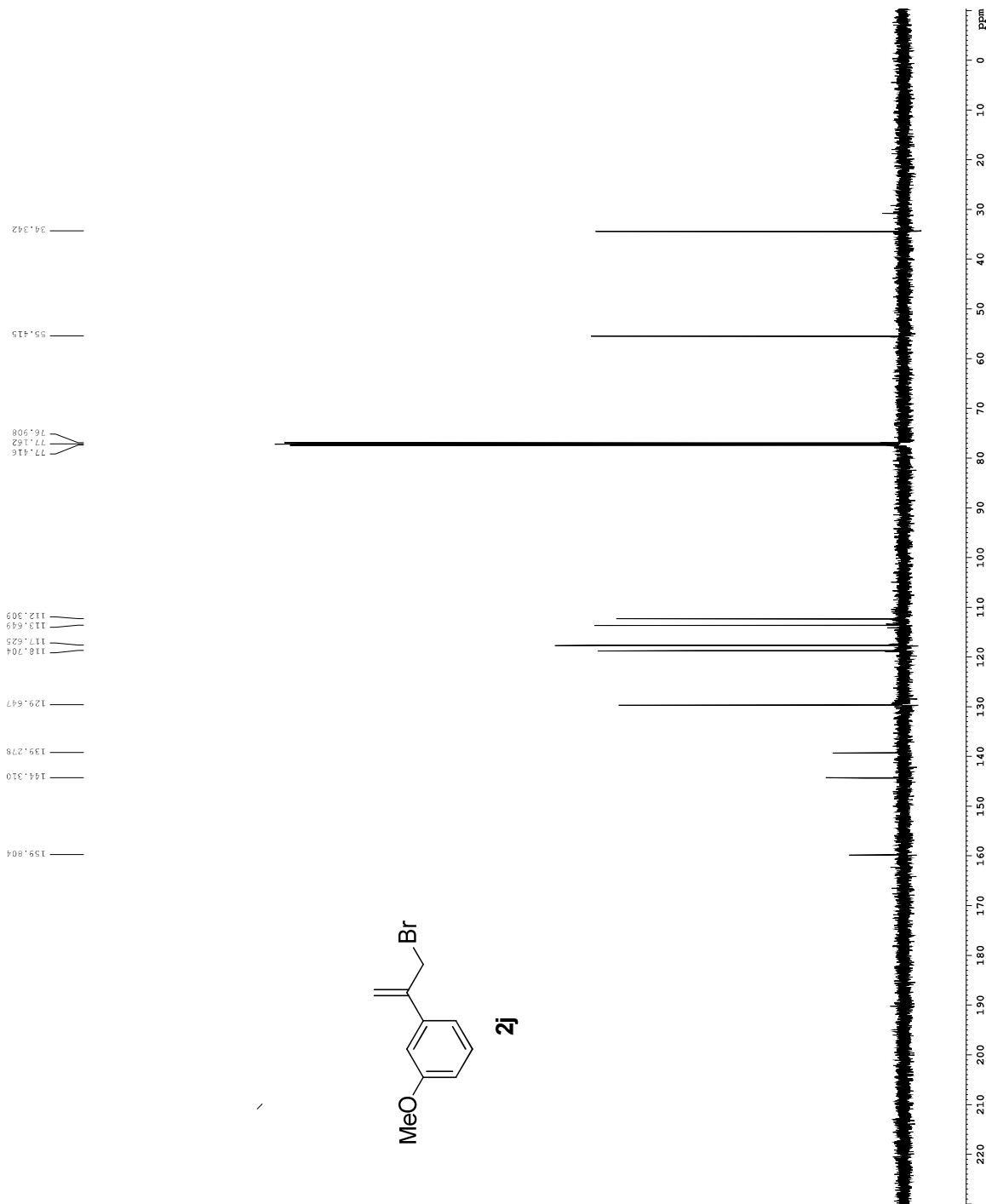
F2 - Acquisition Parameters
Date_ 20150723
Time 16.24
INSTRUM cryo500
PROBHD 5 mm CFTCI 1H-
PULPROG Spinecho90gp-prd
TD 65536
SOLVENT CDCl3
NS 160
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.081340 sec
RG 1024
DW 16.500 usec
DE 6.00 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00015600 sec
MCREST 0 sec
MCWCK 0.01500000 sec
P2 33.10 usec

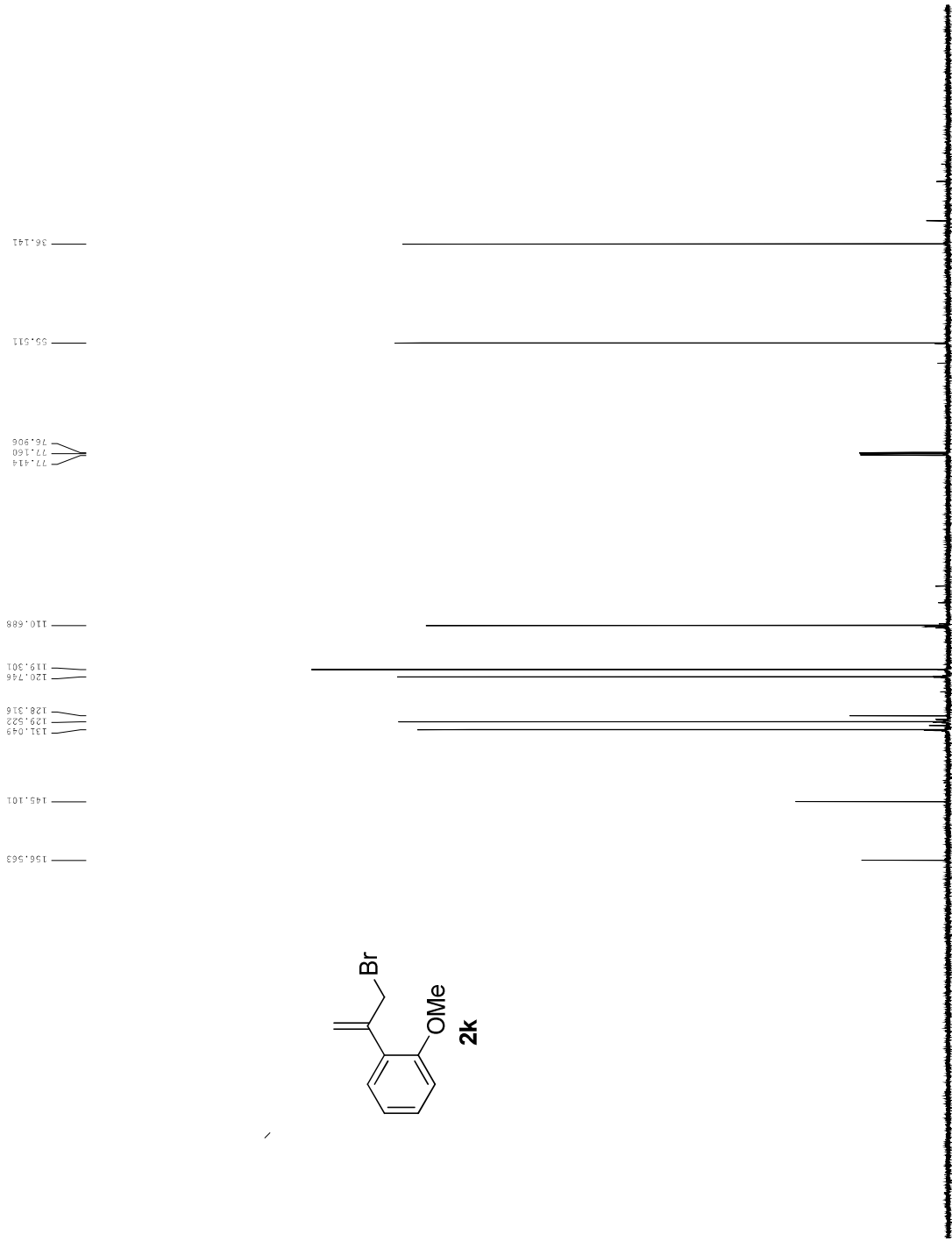
===== CHANNEL f1 13C =====
NUC1 13C
P1 16.55 usec
P11 500.00 usec
P12 2000.00 usec
PL0 120.00 dB
PL1 125.794570 dB
PL2 120.00 dB
SE1 2.70 dB
SE2 2.70 dB
SFOFF1 Cfp60, 0.5, 20.1
SFOFF2 0 Hz
SFOFF3 0 Hz

===== CHANNEL f2 1H =====
CFDPRG12 waltz16
NUC2 1H
P2P02 100.00 usec
P2P03 1.00 dB
P2P04 2.50 dB
P2P05 2.50 dB
SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GEN[1] 0 %
GEN[2] 0 %
GFY1 0 %
GFY2 0 %
GFZ1 30.00 %
GFZ2 50.00 %
P15 500.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7604084 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 2.00



COc1ccccc1C(=C)CBr **2k**

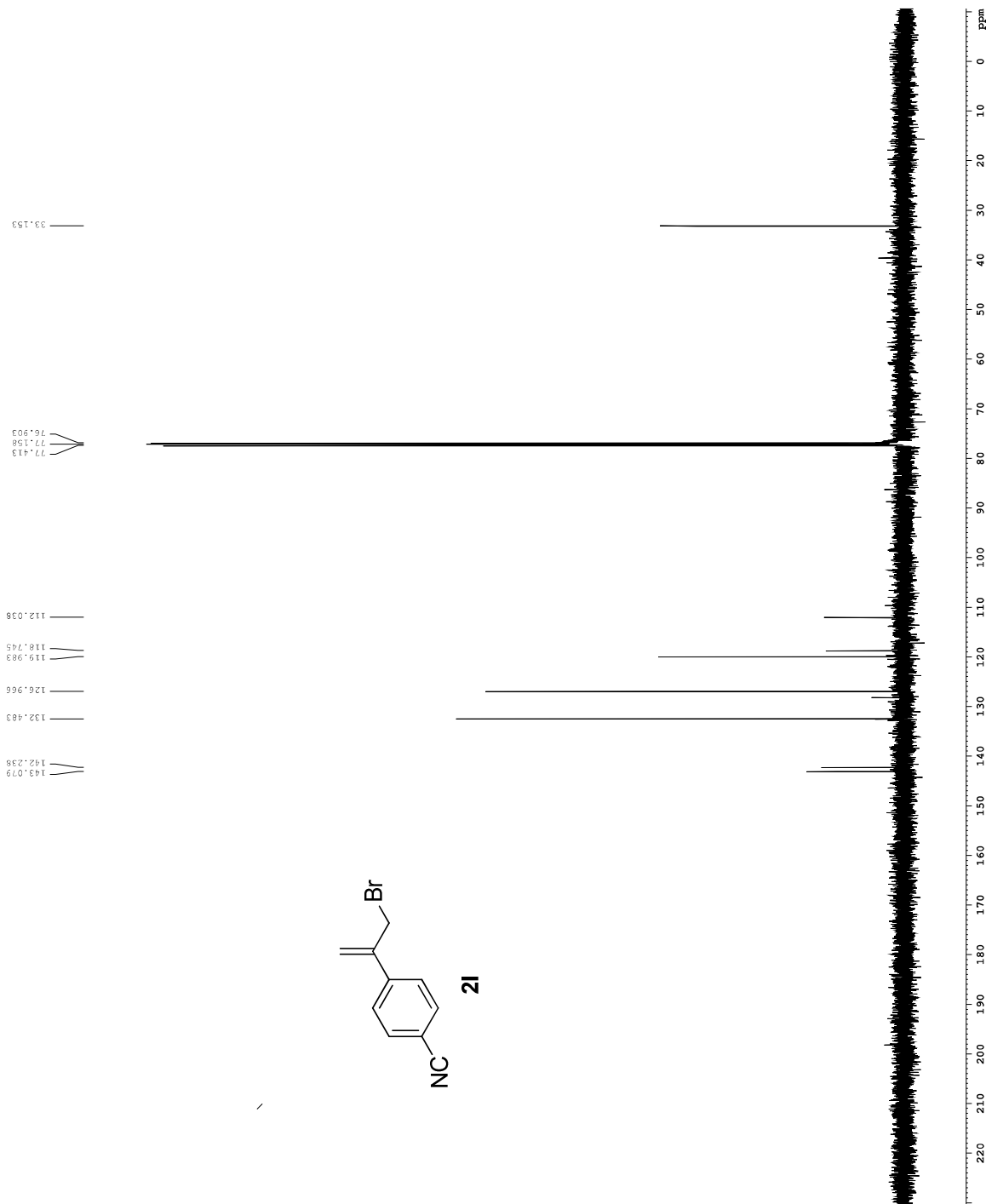
Current Data Parameters
NAME GF-II-190
EXPNO 93
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150707
Time 10.43
INSTRUM gn500
PROBHD 5 mm broadband
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 116
DS 4
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0013640 sec
RG 327.6
DE 16.500 usec
TE 298.0 K
d11 0.25000000 sec
d1 0.03000000 sec
ACQRES 0 sec
MORCK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 0.80 dB
SFO1 125.532191 MHz

===== CHANNEL f2 =====
CFPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 12.00 dB
PL12 12.80 dB
SFO2 499.1824959 MHz

F2 - Processing parameters
SI 65536
SF 125.5185905 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 2.00



Current Data Parameters
NAME GF-11-259
EXPNO 91
PROCNO 1

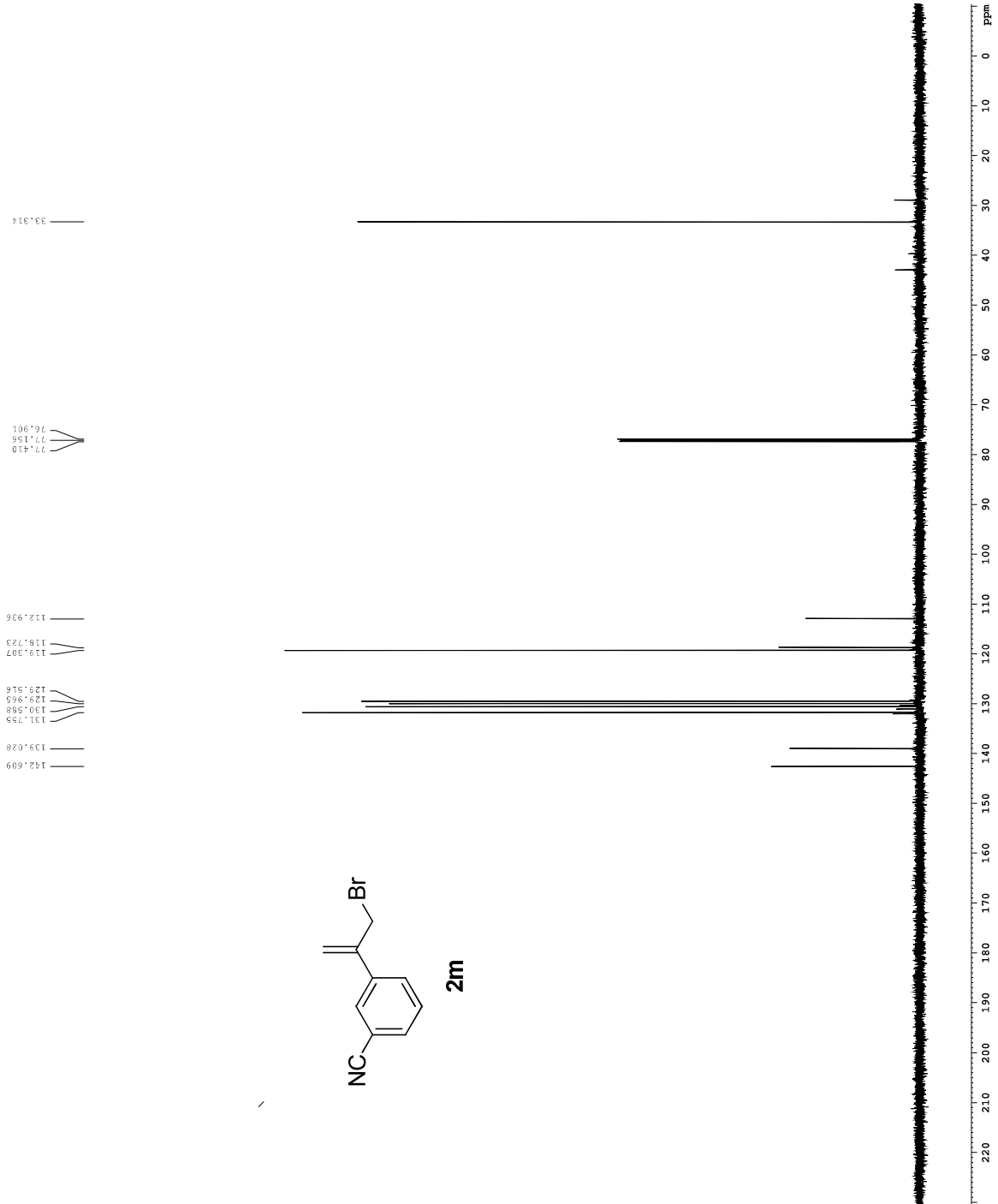
F2 - Acquisition Parameters
Date_ 2019.8.43
Time 20:58:43
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG SpinEcho90gp-p1d
TD 65536
SOLVENT CDCl3
NS 16
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0413440 sec
RG 128.000
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00019000 sec
MCREST 0 sec
MCWRE 0.01500000 sec
F2 33.10 usec

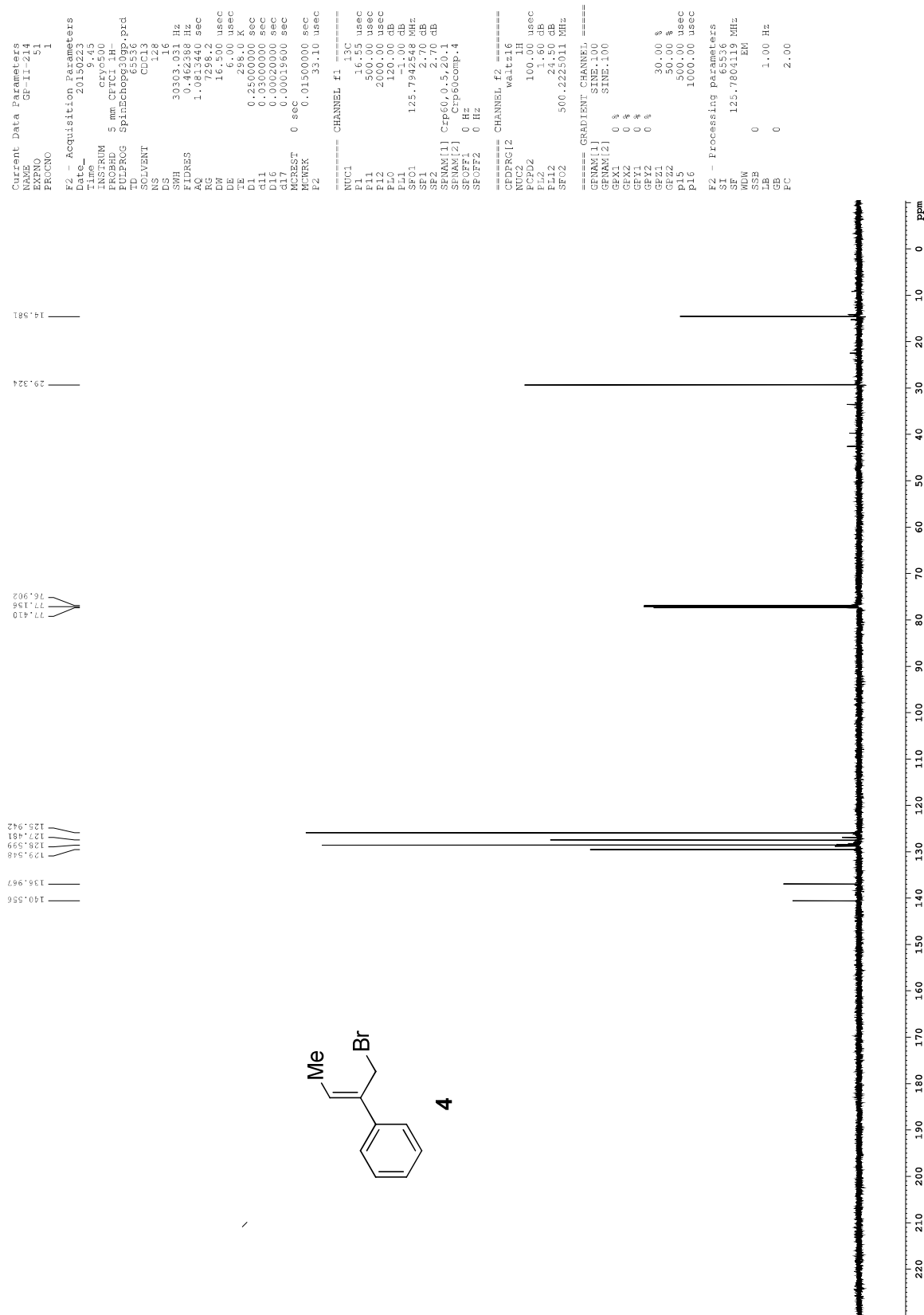
===== CHANNEL f1 =====
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
P11 120.00 dB
P12 120.00 dB
SF1 125.794586 MHz
SF2 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

===== CHANNEL f2 =====
CFDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
P22 1.00 dB
P23 2.50 dB
P24 2.50 dB
SF02 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GEC1 0 %
GEX2 0 %
GEY1 0 %
GEY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P13 100.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.77804137 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00





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Current Data Parameters
NAME      GF-11-215
EXPNO     81
PROCNO    1

F2 - Acquisition Parameters
Date_     20090707
Time      14.50
INSTRUM   cryo500
PROBHD    5 mm CFTCI 1H-
PULPROG   SpinEchozgpgpzd
TD         65536
SOLVENT   CDCl3
NS         32
DS         16
SWH        30303.031 Hz
FIDRES     0.462388 Hz
AQ          1.0813440 sec
RG          3272.6
DE         16.500 usec
TE          298.0 K
D1          0.25000000 sec
d11         0.03000000 sec
d12         0.00200000 sec
d17         0.00019000 sec
MCREST     0 sec
MCWK       0.01500000 sec
F2         33.10 usec

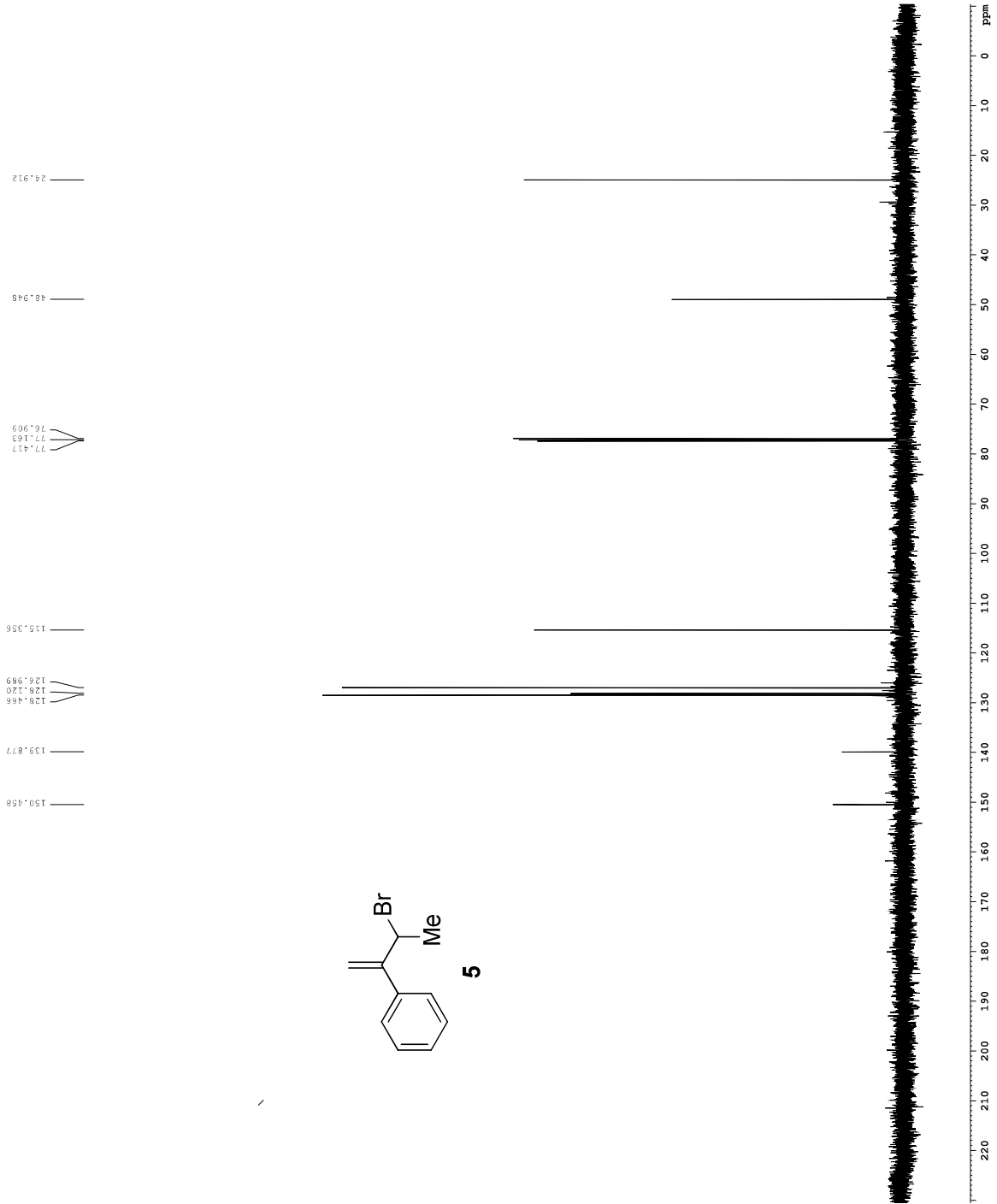
===== CHANNEL f1 =====
NUC1       13C
P1         16.55 usec
PL1        500.00 usec
F11        2000.00 usec
PL2        120.00 dB
PL0         120.00 dB
PL11       125.794358 dB
PL12       120.00 dB
SF1         2.70 dB
SF2         2.70 dB
SFNAM[1]   Crp60,0.5,20.1
SFNAM[2]   Crp60comp.4
SFOFF1     0 Hz
SFOFF2     0 Hz

===== CHANNEL f2 =====
CFDPRG[2]  waltz16
NUC2       1H
PCPDZ      100.00 usec
PL22       1.00 dB
PL12       2.50 dB
SF12       500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1]   SINE.100
GENAM[2]   SINE.100
GEC1       0 %
GEC2       0 %
GFY1       0 %
GFY2       0 %
GRZ1       30.00 %
GRZ2       50.00 %
PL13       100.00 usec
PL14       100.00 usec
PL16       1000.00 usec

F2 - Processing parameters
SI          65536
SF          125.7604089 MHz
RG          3272.6
SSB         0
LB          1.00 Hz
GB          0
PC          2.00

```



Current Data Parameters
NAME GF-11-253
EXPNO 91
PROCNO 1

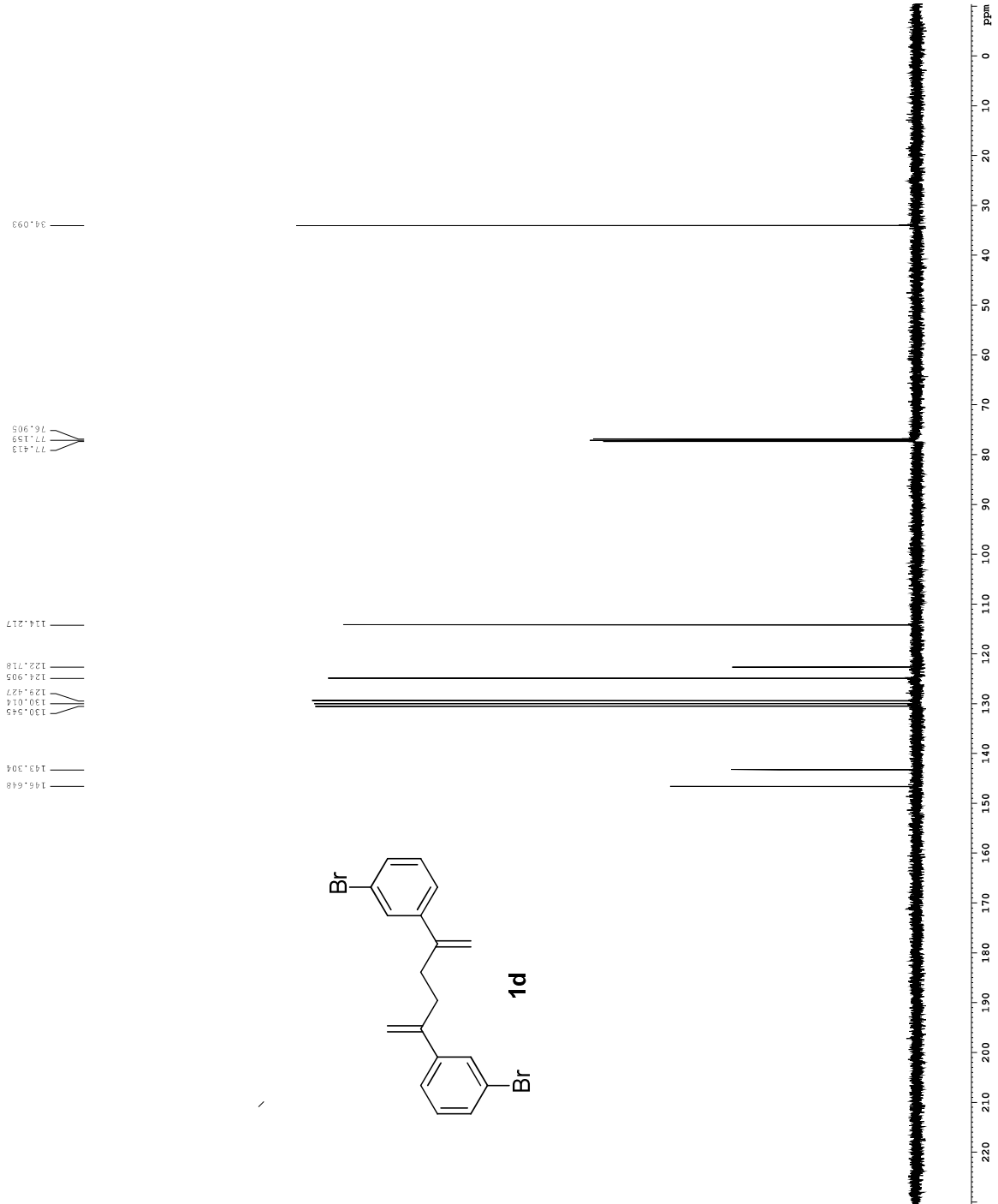
F2 - Acquisition Parameters
Date_ 2017.7.59
Time 7.59
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG Spinchose20gp.prd
TD 65536
SOLVENT CCl4
NS 40
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 327.500
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00200000 sec
MCREST 0 sec
MCWREK 0.01500000 sec
F2 33.10 usec

===== CHANNEL f1 =====
NUC1 ¹³C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
P11 120.00 dB
P12 120.00 dB
SF1 125.7945384 MHz
SF2 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

===== CHANNEL f2 =====
CFDPRG[2] waltz16
NUC2 ¹H
PCPDZ 100.00 usec
P22 1.00 dB
P12 2.50 dB
SF2 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GEX1 0 %
GEX2 0 %
GEY1 0 %
GEY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P15 100.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.77804094 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00



Current Data Parameters
NAME GF-11-250
EXPNO 91
PROCNO 1

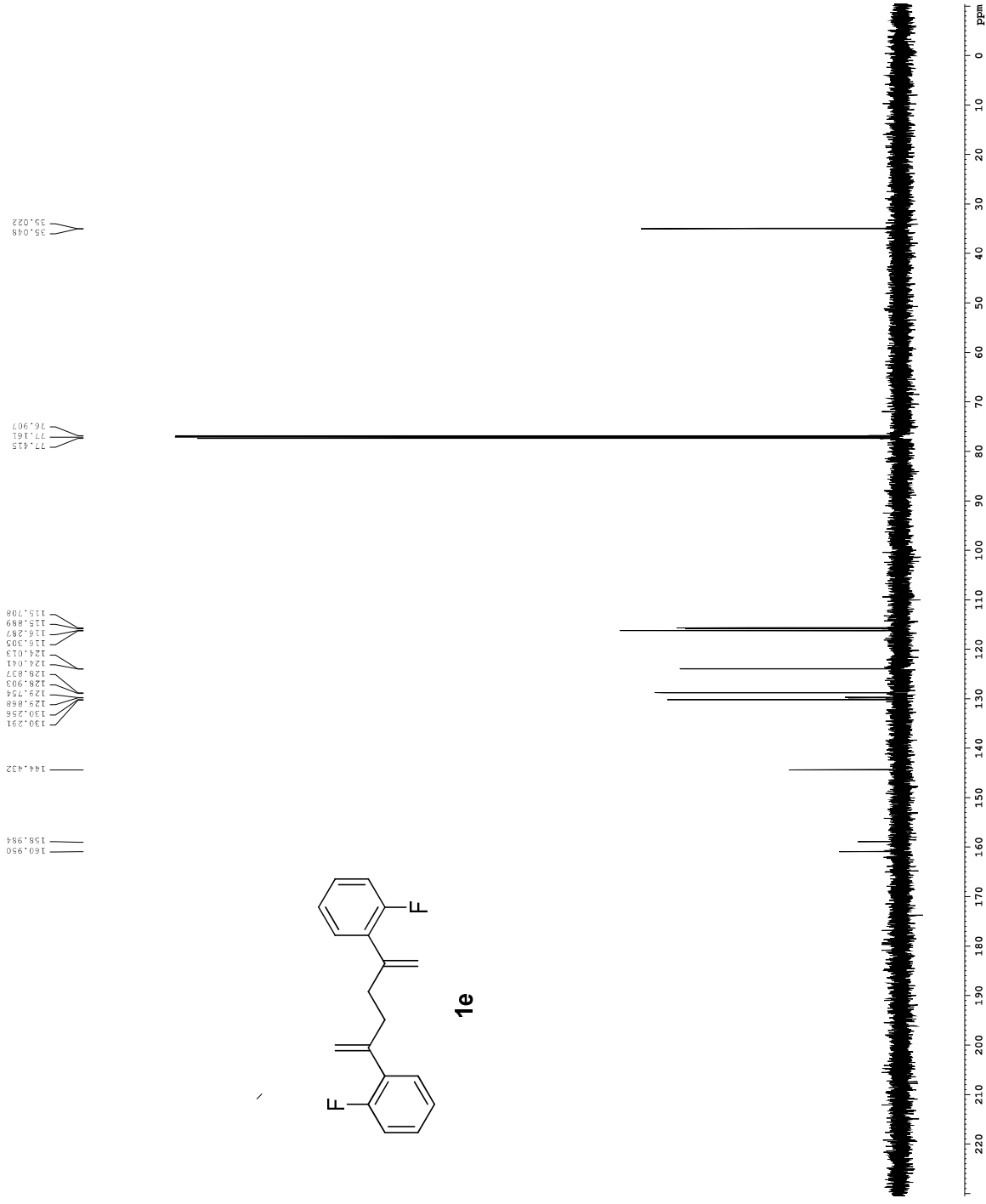
F2 - Acquisition Parameters
Date_ 2017.7.46
Time 7.46
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
FULPROG SpinEcho90gp-p1d
D 65536
SOLVENT CDCl3
NS 104
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0413440 sec
RG 655.1
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00019000 sec
MCREST 0 sec
MCWREK 0.01500000 sec
F2 33.10 usec

CHANNEL f1
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
FLO 120.00 dB
SFO1 125.794526 MHz
SF1 125.00 dB
SF2 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

CHANNEL f2
CFDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
F22 1.00 dB
F12 2.50 dB
SF02 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GFL1 0 %
GFL2 0 %
GFY1 0 %
GFY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P15 500.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7904075 MHz
WREK 0
LB 0
GB 0
PC 2.00



Current Data Parameters
NAME GF-11-227
EXPNO 91
PROCNO 1

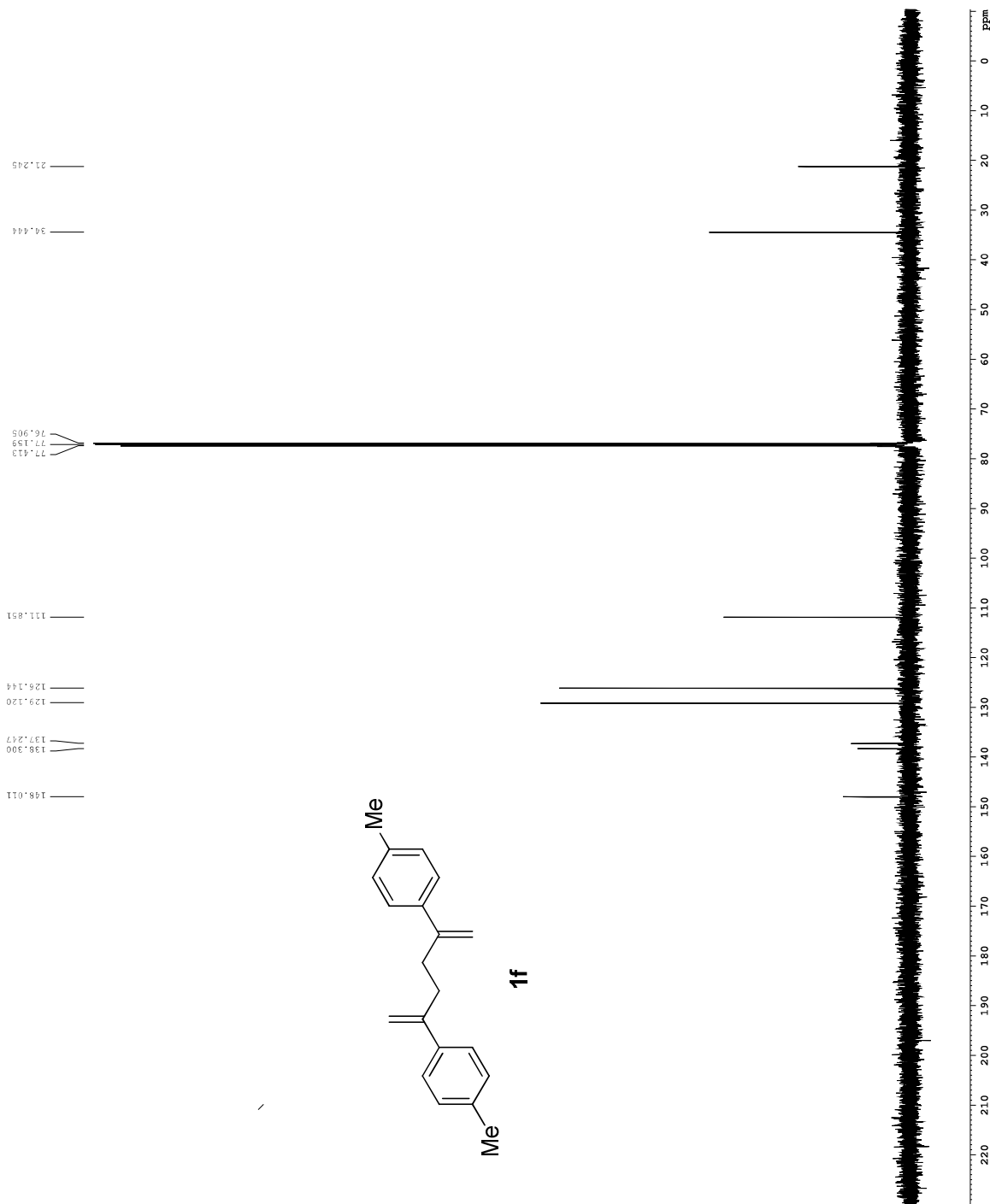
F2 - Acquisition Parameters
Date_ 2017.7.39
Time 7.39
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG Spinchose20gp.prd
TD 65536
SOLVENT CDCl3
NS 160
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0413440 sec
RG 1280
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00019000 sec
MCREST 0 sec
MCWRE 0.01500000 sec
F2 33.10 usec

CHANNEL f1
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
P11 120.00 dB
P12 120.00 dB
SF1 125.794526 MHz
SF2 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

CHANNEL f2
CFDPRG[2] waltz16
NUC2 1H
PCPDZ 100.00 usec
P2 1.00 dB
P22 2.50 dB
P21 2.50 dB
SF02 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GFX1 0 %
GFY1 0 %
GFZ1 0 %
GFX2 0 %
GFY2 0 %
GFZ2 0 %
P15 30.00 %
P16 50.00 %
P17 100.00 usec
P18 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7904076 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00





Current Data Parameters
NAME GF-11-225
EXPNO 91
PROCNO 1

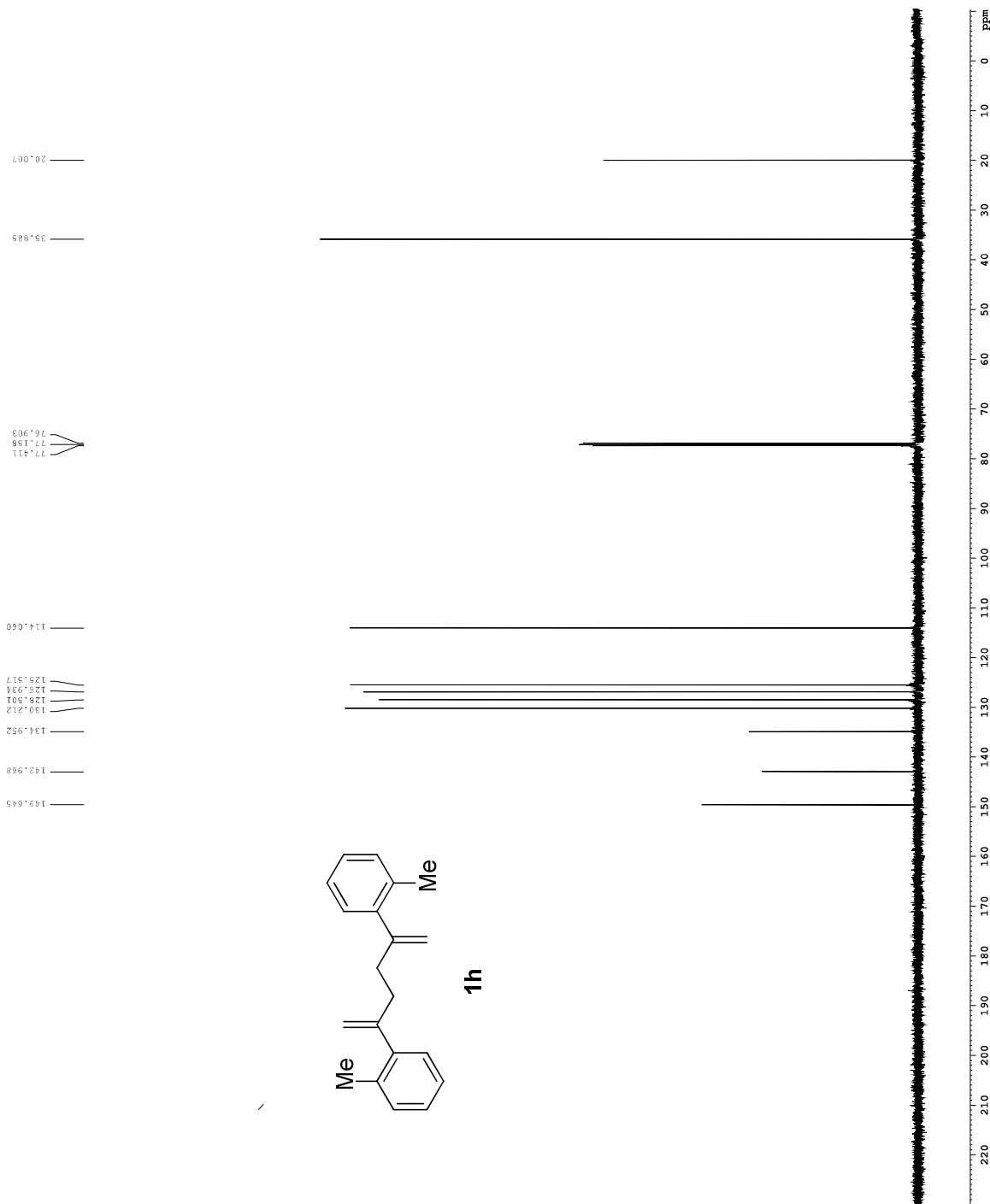
F2 - Acquisition Parameters
Date_ 2017.7.33
Time 7.33
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG SpinEcho90gp.prd
TD 65536
SOLVENT CDCl3
NS 120
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0413440 sec
RG 657.6
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00000000 sec
MCREST 0 sec
MCWRE 0.01500000 sec
F2 33.10 usec

===== CHANNEL f1 =====
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
P11 120.00 dB
P12 120.00 dB
SF1 125.794388 MHz
SF2 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

===== CHANNEL f2 =====
CFDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
P22 1.00 dB
P12 2.50 dB
SF2 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GEX1 0 %
GEX2 0 %
GEY1 0 %
GEY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P13 500.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.77804099 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00



Current Data Parameters
NAME GF-11-246
EXPNO 91
PROCNO 1

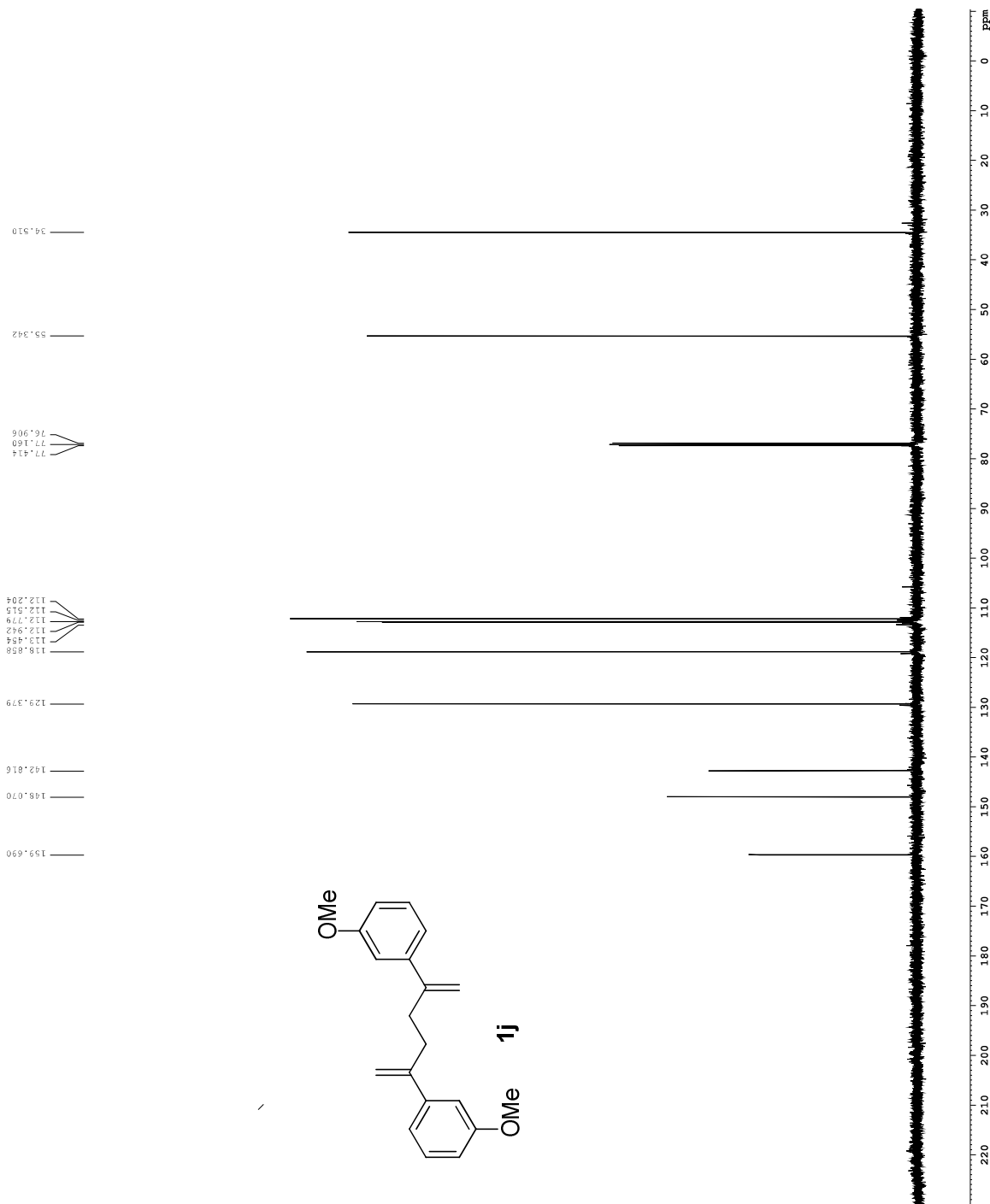
F2 - Acquisition Parameters
Date_ 2019.09
Time 20:59:09
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG SpinEcho90gp-p1d
TD 65536
SOLVENT CDCl3
NS 16
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0413440 sec
RG 128.000
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00200000 sec
MCREST 0 sec
MCWRE 0.01500000 sec
F2 33.10 usec

===== CHANNEL f1 =====
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
FLO 120.00 dB
SFO1 125.7704093 MHz
SF1 120.00 dB
SF2 2.70 dB
SFNAM[1] Crp60,0.5,20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

===== CHANNEL f2 =====
CFDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
F22 1.00000000 dB
F12 2.50 dB
SF02 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GFX1 0 %
GFX2 0 %
GFY1 0 %
GFY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P15 500.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7704093 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00



Current Data Parameters
NAME GF-11-261
EXPNO 91
PROCNO 1

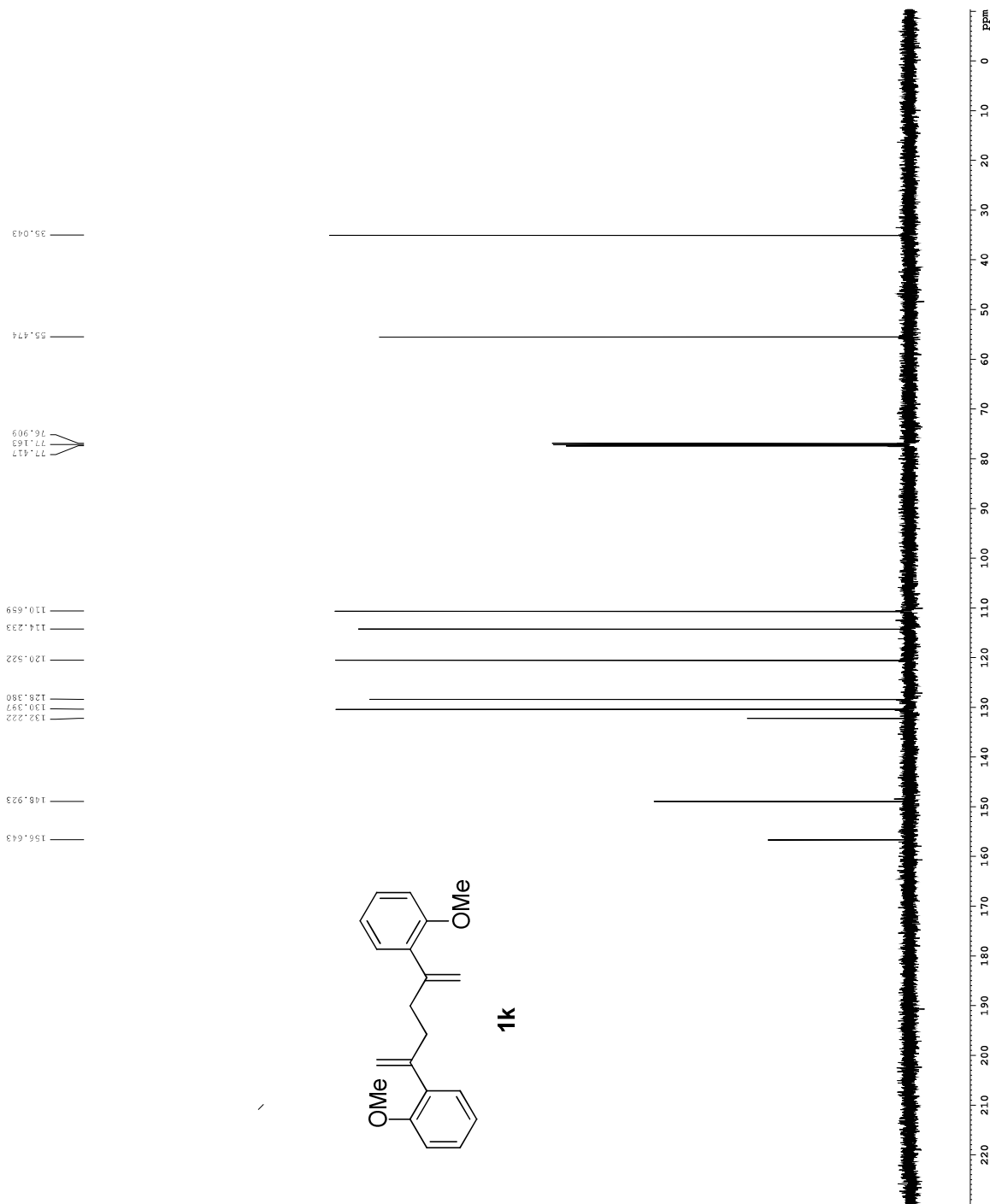
F2 - Acquisition Parameters
Date_ 20150815
Time 20:58:52
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG SpinEcho90gp-p1d
TD 65536
SOLVENT CDCl3
NS 112
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.041340 sec
RG 183.004
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00200000 sec
MCREST 0 sec
MCWREK 0.01500000 sec
F2 33.10 usec

===== CHANNEL f1 =====
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
P11 120.00 dB
P12 120.00 dB
SFO1 125.764505 MHz
SF2 2.70 dB
SF1 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

===== CHANNEL f2 =====
CFDPRG12 waltz16
NUC2 1H
PCPD2 100.00 usec
P22 1.00 dB
P23 2.50 dB
P12 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GENP1 0 %
GENP2 0 %
GFY1 0 %
GFY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P13 500.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7604085 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00



Current Data Parameters
NAME GF-11-235
EXPNO 86
PROCNO 1

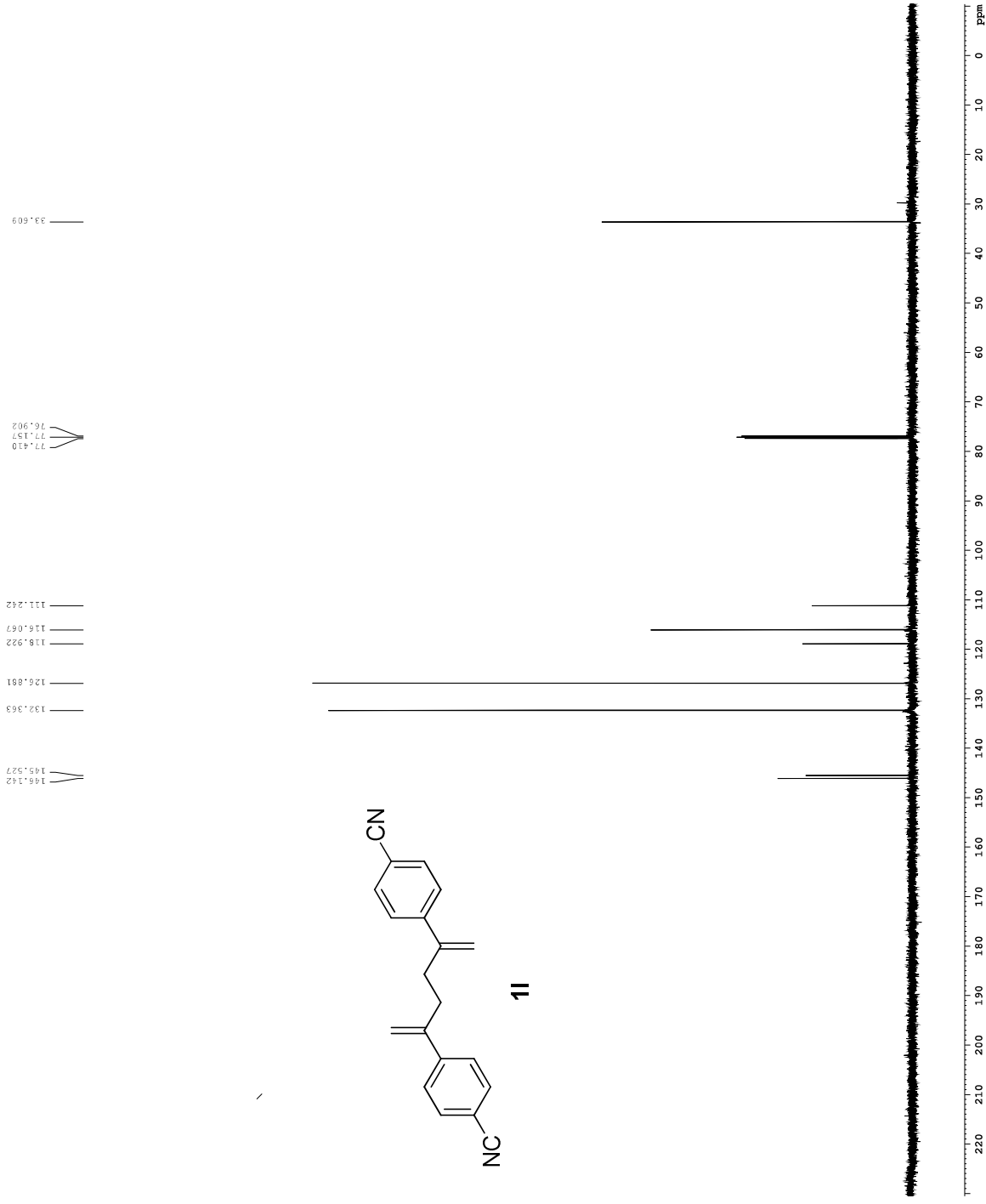
F2 - Acquisition Parameters
Date_ 2013.8.17
Time 20:58:17
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG Spinchoir20p-prd
TD 65536
SOLVENT CDCl3
NS 16
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0813440 sec
RG 327.8100000
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00200000 sec
MCREST 0 sec
MCWRE 0.01500000 sec
F2 33.10 usec

CHANNEL f1
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
SFO1 125.7704123 MHz
SFO2 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

CHANNEL f2
CFDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
P22 1.00 dB
F12 2.50 dB
SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GFL1 0 %
GFL2 0 %
GFY1 0 %
GFY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P15 100.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7704123 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00



Current Data Parameters
NAME GF-11-262
EXPNO 91
PROCNO 1

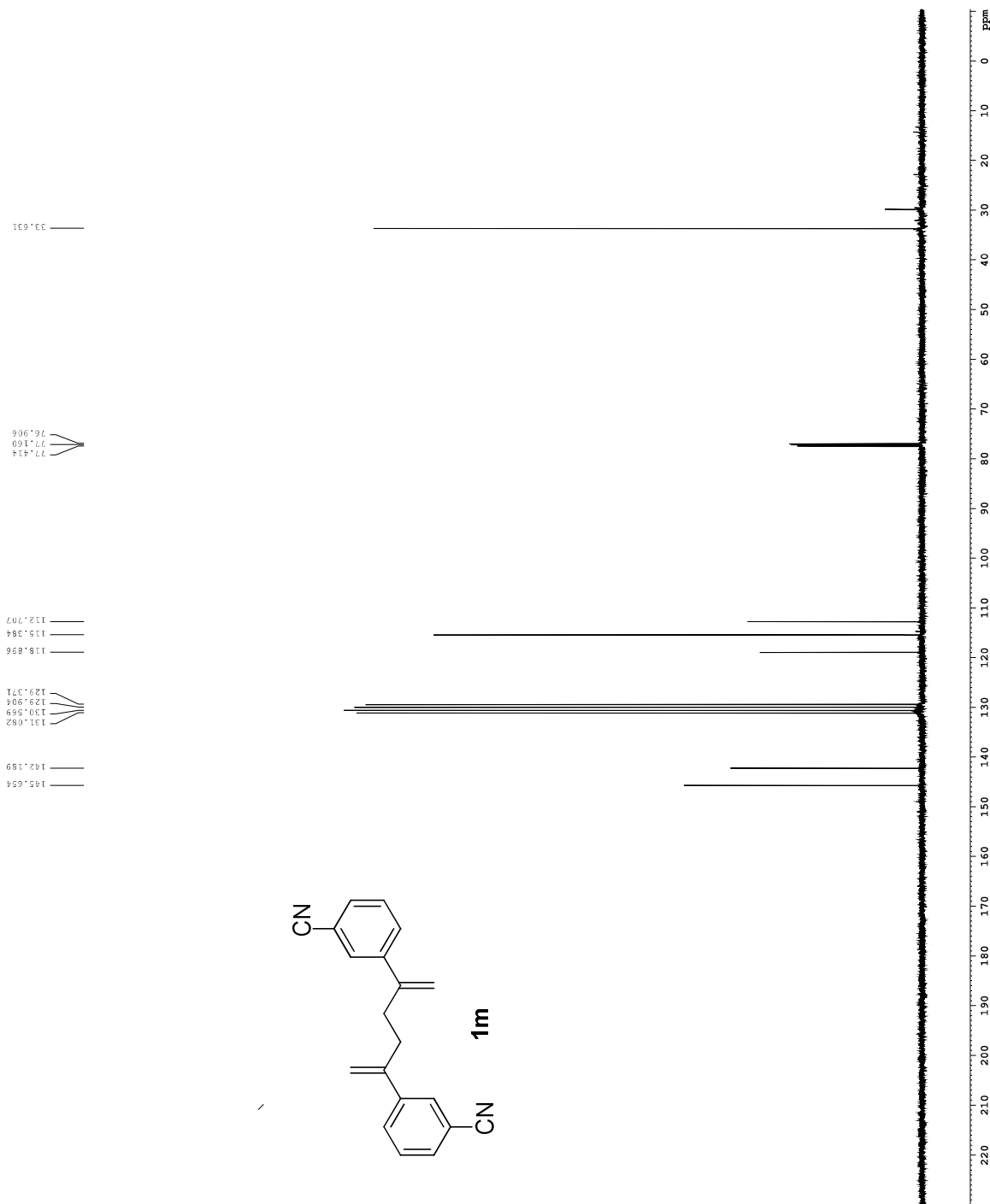
F2 - Acquisition Parameters
Date_ 2019.9.23
Time 20:59:23
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG SpinEcho90gp.prd
TD 65536
SOLVENT CDCl3
NS 40
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0413440 sec
RG 1280
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00200000 sec
MCREST 0 sec
MCWREK 0.01500000 sec
F2 33.10 usec

===== CHANNEL f1 =====
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
P11 120.00 dB
P12 120.00 dB
SFO1 125.7645611 MHz
SF2 2.70 dB
SF1 2.70 dB
SF2 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

===== CHANNEL f2 =====
CFDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
P22 1.00 dB
P21 2.50 dB
P22 2.50 dB
SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GENP1 0 %
GENP2 0 %
GENP3 0 %
GENP4 0 %
GENP5 0 %
GENP6 0 %
GENP7 0 %
GENP8 0 %
GENP9 0 %
GENP10 0 %
GENP11 0 %
GENP12 0 %
GENP13 0 %
GENP14 0 %
GENP15 0 %
GENP16 0 %
GENP17 0 %
GENP18 0 %
GENP19 0 %
GENP20 0 %
GENP21 0 %
GENP22 0 %
GENP23 0 %
GENP24 0 %
GENP25 0 %
GENP26 0 %
GENP27 0 %
GENP28 0 %
GENP29 0 %
GENP30 0 %
GENP31 0 %
GENP32 0 %
GENP33 0 %
GENP34 0 %
GENP35 0 %
GENP36 0 %
GENP37 0 %
GENP38 0 %
GENP39 0 %
GENP40 0 %
GENP41 0 %
GENP42 0 %
GENP43 0 %
GENP44 0 %
GENP45 0 %
GENP46 0 %
GENP47 0 %
GENP48 0 %
GENP49 0 %
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GENP57 0 %
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GENP66 0 %
GENP67 0 %
GENP68 0 %
GENP69 0 %
GENP70 0 %
GENP71 0 %
GENP72 0 %
GENP73 0 %
GENP74 0 %
GENP75 0 %
GENP76 0 %
GENP77 0 %
GENP78 0 %
GENP79 0 %
GENP80 0 %
GENP81 0 %
GENP82 0 %
GENP83 0 %
GENP84 0 %
GENP85 0 %
GENP86 0 %
GENP87 0 %
GENP88 0 %
GENP89 0 %
GENP90 0 %
GENP91 0 %
GENP92 0 %
GENP93 0 %
GENP94 0 %
GENP95 0 %
GENP96 0 %
GENP97 0 %
GENP98 0 %
GENP99 0 %
GENP100 0 %

F2 - Processing parameters
SI 65536
SF 125.7604135 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00



Current Data Parameters
NAME GF-11-277
EXPNO 101
PROCNO 1

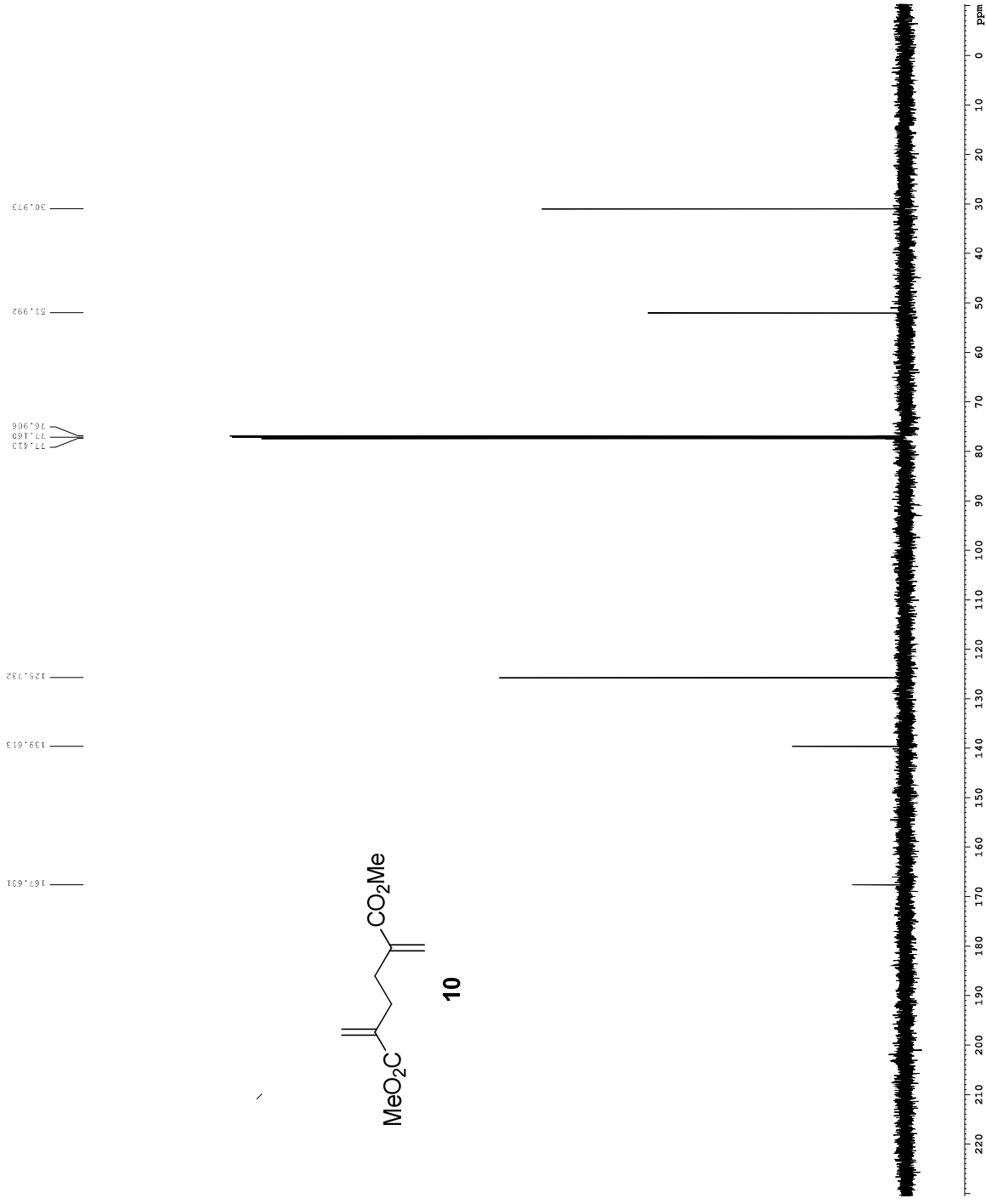
F2 - Acquisition Parameters
Date_ 20150802
Time 20:58:42
INSTRUM cryo500
PROBHD 5 mm CFTCI 1H-
PULPROG SpinEchozgpgp-
D 65536
SOLVENT CDCl3
NS 192
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0413440 sec
RG 650.0
DW 16.500 usec
DE 6.000 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00200000 sec
MCREST 0 sec
MCWREK 0.01500000 sec
F2 33.10 usec

==== CHANNEL f1 =====
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
P11 120.00 dB
SFO1 125.794538 MHz
SF1 125.794538 MHz
SF2 2.70 dB
SFNAM[1] Cfp60, 0.5, 20.1
SFNAM[2] Cfp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

==== CHANNEL f2 =====
CFDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
P2 1.00 dB
P21 2.50 dB
P22 2.50 dB
SF02 500.2225011 MHz

==== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
PCPD1 0 %
PCPD2 0 %
GFY1 0 %
GFY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P15 100.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.794067 MHz
RG 650
SFOFF 0
LB 1.00 Hz
GB 0
PC 2.00



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Current Data Parameters
NAME GF-11-287
EXPNO 96
PROCNO 1

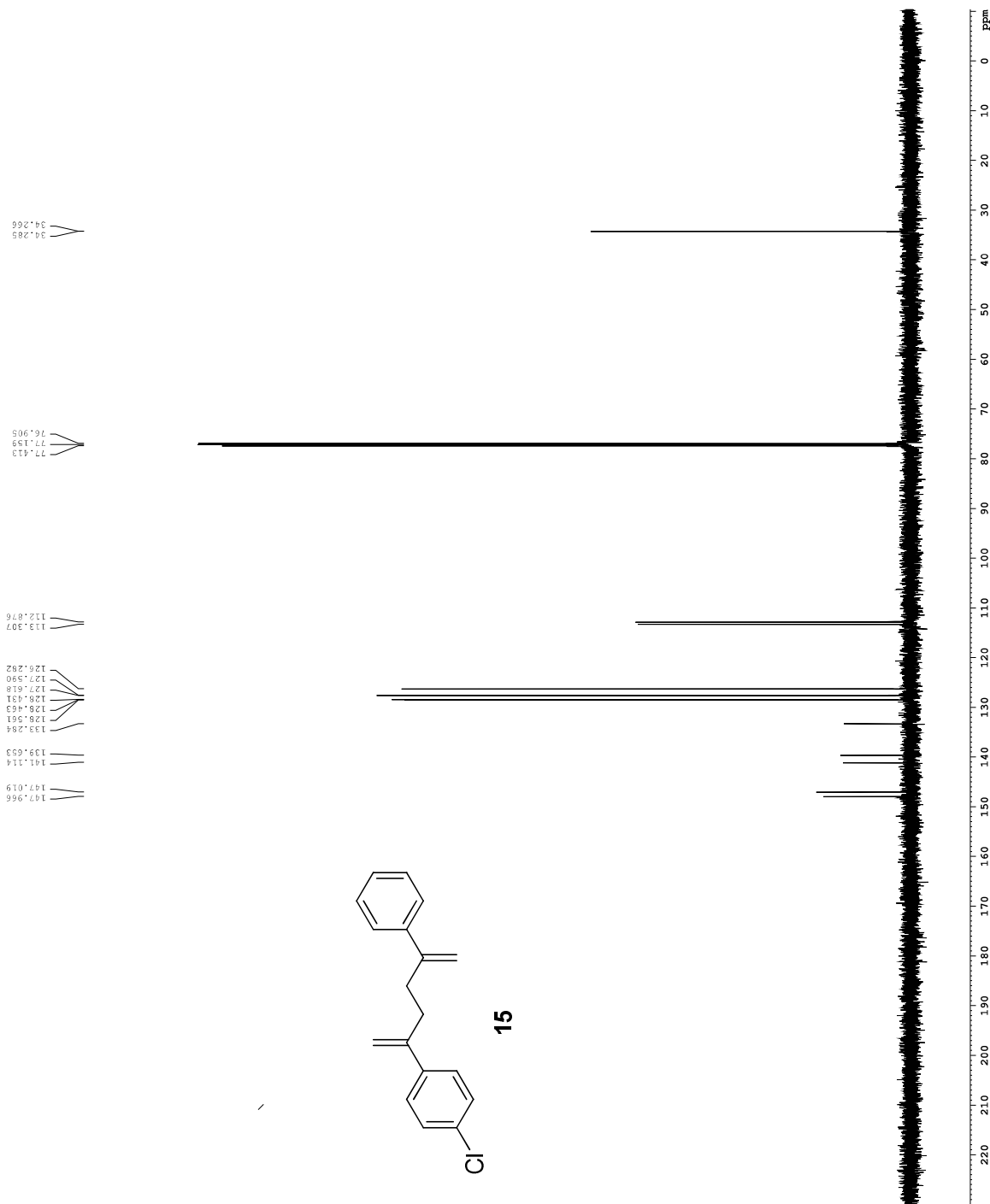
F2 - Acquisition Parameters
Date_ 20150824
Time 20:58:24
INSTRUM cryo500
PROBHD 5 mm CFC1 1H-
PULPROG SpinEcho90gp-prd
TD 65536
SOLVENT CDCl3
NS 160
DS 16
SWH 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.081340 sec
RG 320.00
DE 16.500 usec
TE 298.0 K
D1 0.25000000 sec
d11 0.03000000 sec
d12 0.00200000 sec
d17 0.00200000 sec
MCREST 0 sec
MCREK 0.01500000 sec
F2 33.10 usec

===== CHANNEL f1 =====
NUC1 13C
P1 16.55 usec
F11 500.00 usec
F12 2000.00 usec
P10 120.00 dB
P11 120.00 dB
P12 120.00 dB
SFO1 125.764500 MHz
SF1 2.70 dB
SF2 2.70 dB
SFNAM[1] Crp60, 0.5, 20.1
SFNAM[2] Crp60comp.4
SFOFF1 0 Hz
SFOFF2 0 Hz

===== CHANNEL f2 =====
CFDPRG[2] waltz16
NUC2 1H
PCPD2 100.00 usec
P21 1.00 dB
P22 2.50 dB
P23 2.50 dB
SF02 500.2225011 MHz

===== GRADIENT CHANNEL =====
GENAM[1] SINE.100
GENAM[2] SINE.100
GEC1 0 %
GEV1 0 %
GEV2 0 %
GFY1 0 %
GFY2 0 %
GRZ1 30.00 %
GRZ2 50.00 %
P13 500.00 usec
P14 1000.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7604080 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00



References.

¹ For an example of heating the substrate with NBS in chlorobenzene without a radical initiator, see:

Vaccher, B.; Flouquet, D. *Synth Commun.* **1993**, *23*, 671–679.

² For an example of heating the substrate with NBS in carbon tetrachloride in the presence of dibenzoyl peroxide, see: Baird, L. J.; Timmer, M. S. M.; Teesdale-Spittle, P. H.; Harvey, J. E. *J. Org. Chem.*

2009, *74*, 2271–2277.

³ Tripathi, C. B.; Mukherjee, S. *Angew. Chem., Int. Ed.* **2013**, *52*, 8450–8453. For the original publication of the herein described procedure for allylic bromination of α -methylstyrene derivatives, see: Harrison, C. R. *US Patent No.* 5474998 (**1995**).

⁴ Yamanaka, M.; Arisawa, M.; Nishida, A.; Nakagawa, M. *Tetrahedron Lett.* **2002**, *43*, 2403–2406.

⁵ The yield of product formation is dependent on the combination of substituents on the aromatic core and the amount of Yb(OTf)₃ (0.1-10 mol%) added to the reaction mixture. The optimized conditions for all substrates depicted in Scheme 1 (Article) are summarized in the Experimental Section.