

**A General Approach for Preparing Epidithiodioxopiperazines from Trioxopiperazine Precursors.  
Enantioselective Total Syntheses of (+)- and (-)-Glioclazine C, (+)-Leptosin D, (+)-T988C, Bionectin A  
and (+)-Gliocladin A.**

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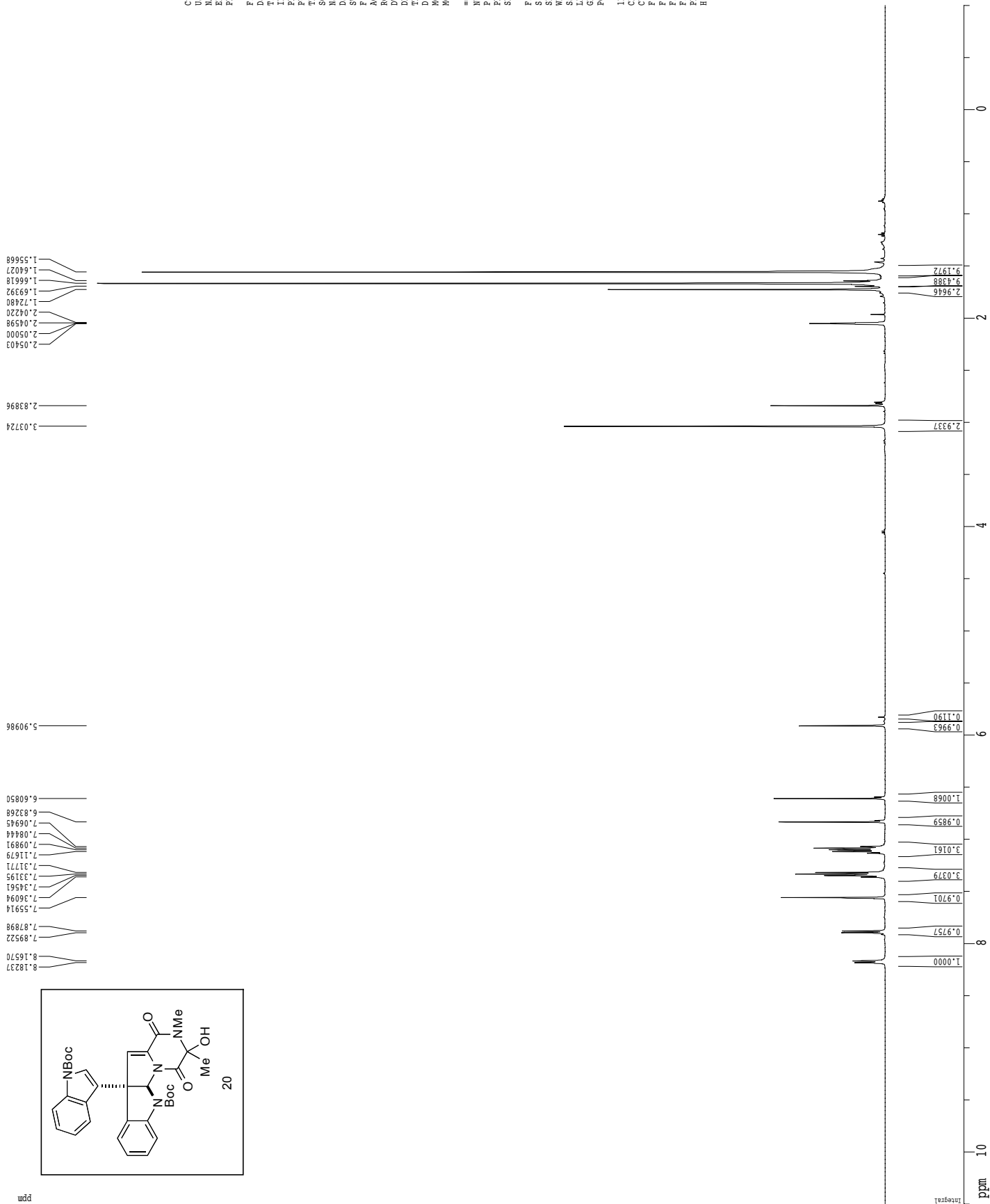
## **Supporting Information Part 2**

### **Table of Contents**

4. NMR Spectra

Page S41–S177

<sup>1</sup>H spectrum



Current Data Parameters  
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 NAME jedl-64  
 EXPNO 3  
 PROCNO 1

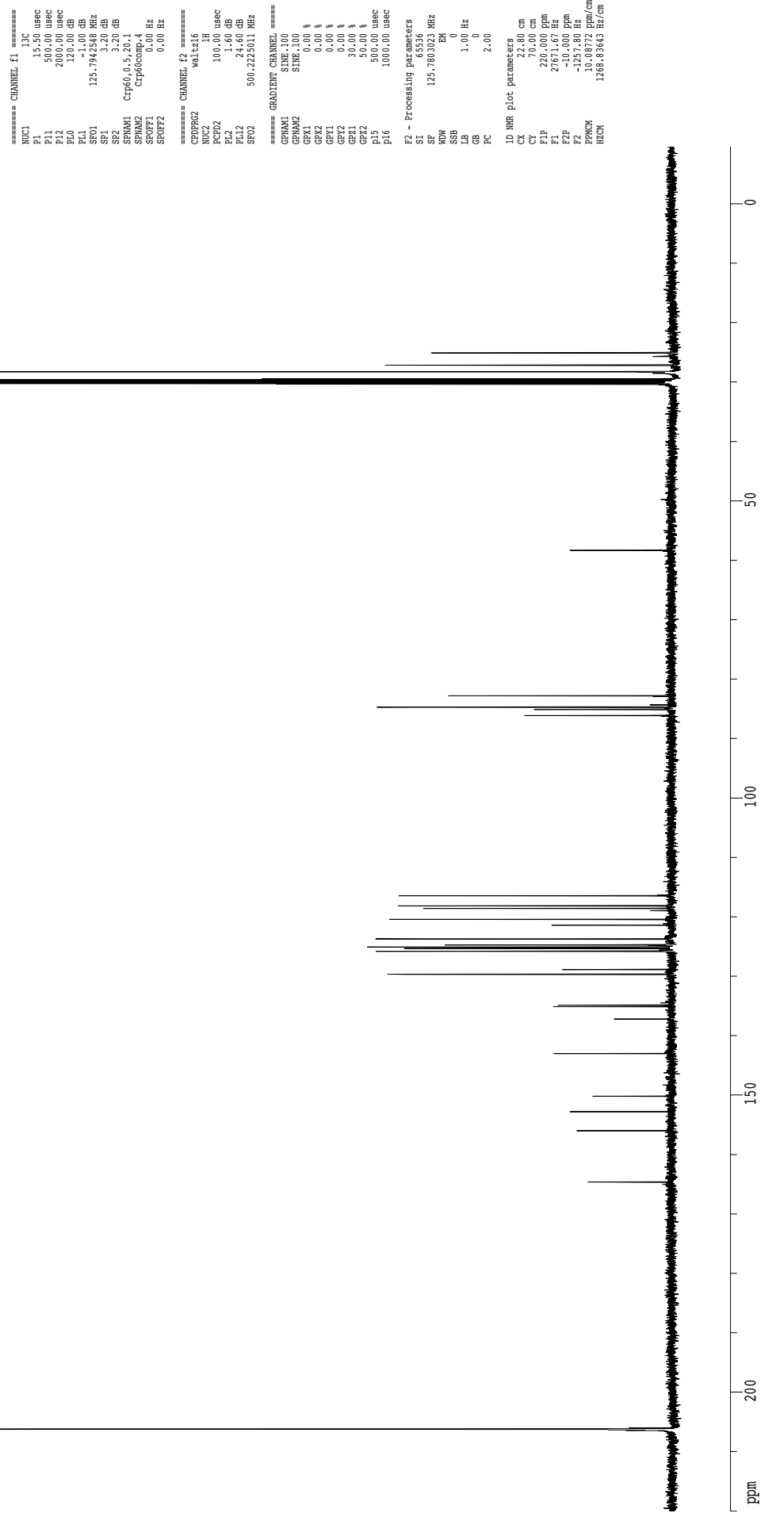
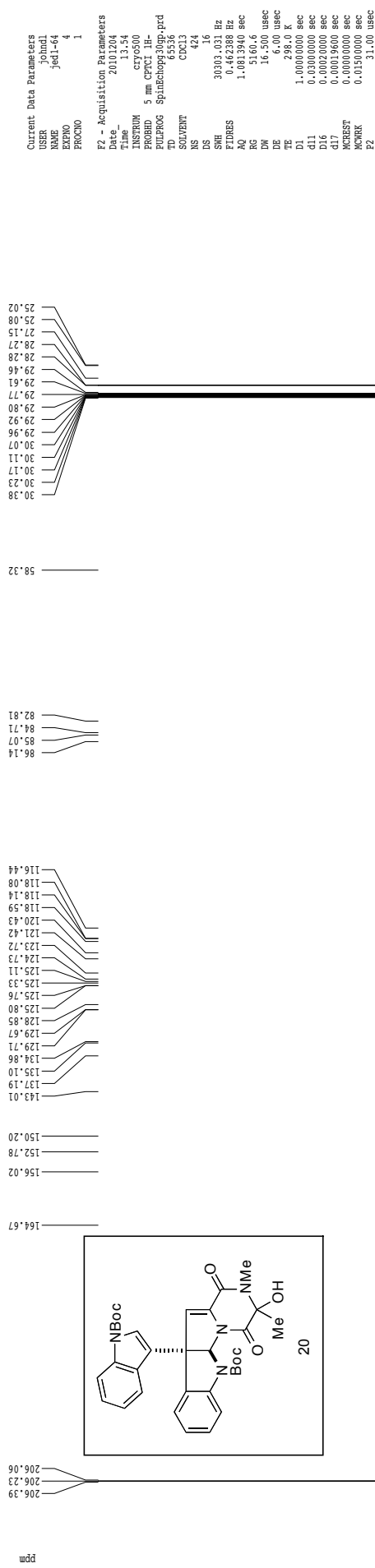
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 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 63  
 DW 6.00 usec  
 DE 15.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
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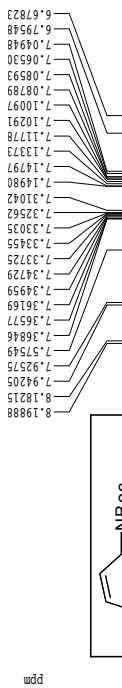
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1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 10.500 ppm  
 F2 9292.31 Hz  
 F3 0.000000 Hz  
 F4 -500.000000 Hz  
 PRMCM 0.50439 ppm/cm  
 HZCM 252.30397 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



<sup>1</sup>H spectrum



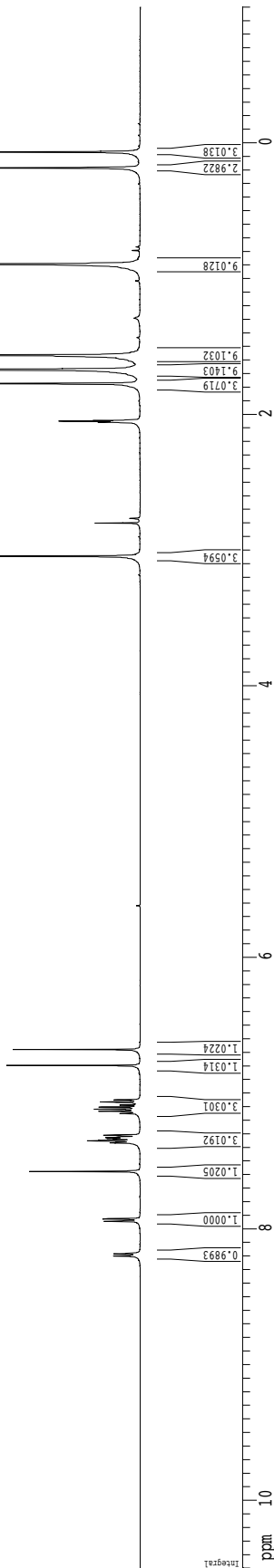
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 INSTRM spect  
 PULPROG zgpg30  
 CHANNEL 5 mm broadband  
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 SOLVENT Acetone  
 NS 48  
 DS 2  
 SWE 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 128  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
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 MCRST 0.00000000 sec  
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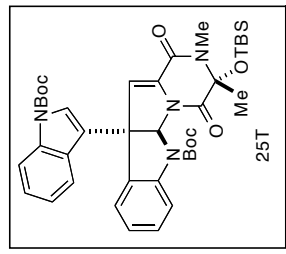
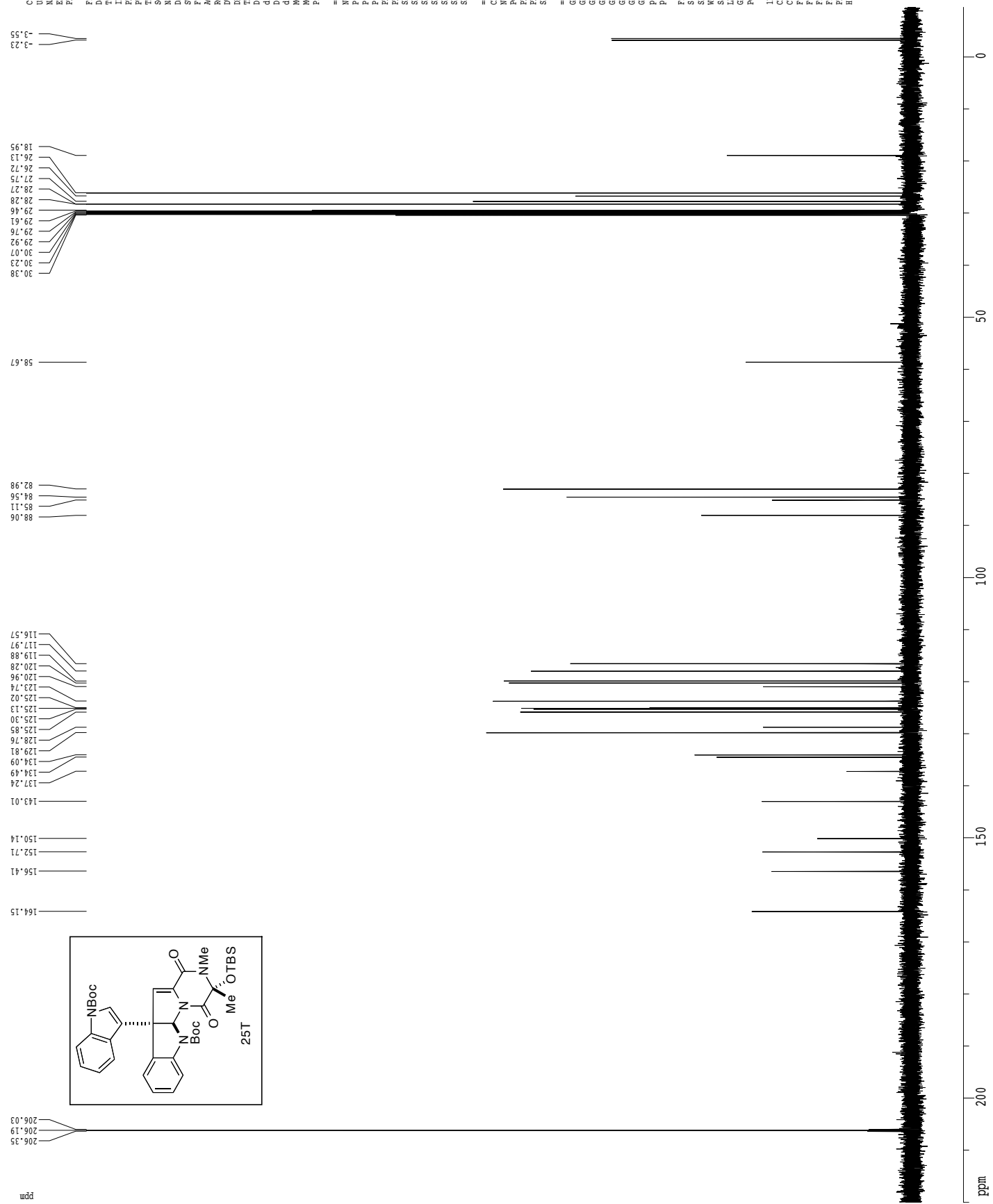
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 GB 0  
 RB 0.30 Hz  
 GC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 10.500 ppm  
 F1 524.85 Hz  
 F2 -1.000 ppm  
 FZ -499.51 Hz  
 PRCH 0.50439 ppm/cm  
 HZCX 251.94385 Hz/cm





Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jound1  
 EXPNO jed1-45-9m3  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20101203  
 Time 13:59  
 INSTRUM cryo500  
 PROBHD 5 mm CPACI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 360  
 DS 16  
 SHF 303.031 Hz  
 FIDRES 0.46238 Hz  
 AQ 1.081940 sec  
 RG 364.1  
 NG 16  
 DR 6.00 usec  
 DE 298.2 K  
 TE 298.2 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.0001960 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 3.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 P12 2000.00 usec  
 PL2 120.00 dB  
 PL0 125.794568 dB  
 SFO1 125.761466 MHz  
 SFO2 500.2225011 MHz  
 SF2 31.20 dB  
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 SFO1M2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

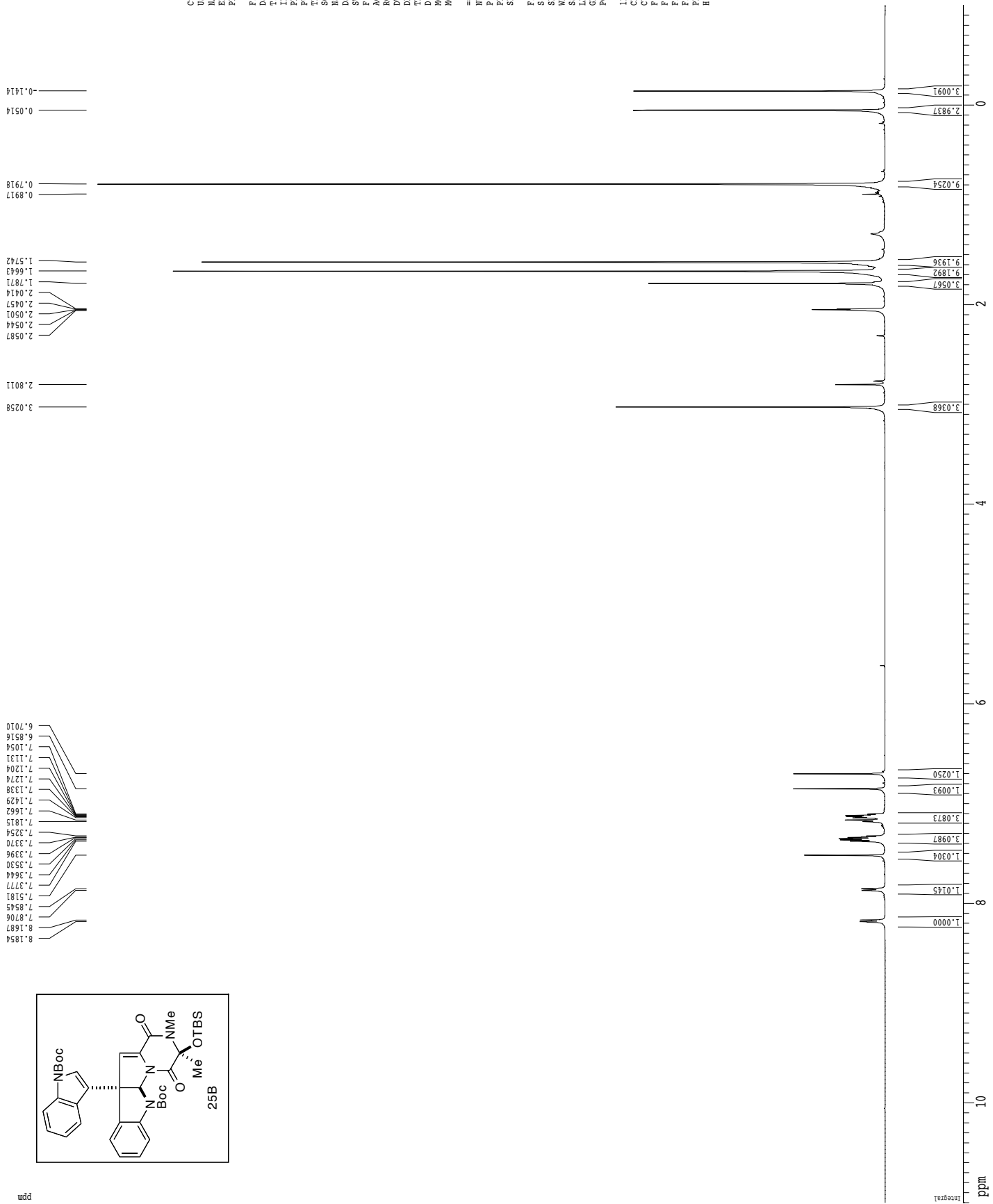
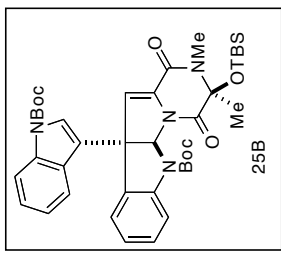
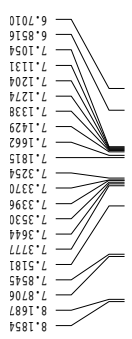
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 GRADPRG3 gpr10  
 GRADPRG4 gpr10  
 GRADPRG5 gpr10  
 GRADPRG6 gpr10  
 GRADPRG7 gpr10  
 GRADPRG8 gpr10  
 GRADPRG9 gpr10  
 GRADPRG10 gpr10  
 GRADPRG11 gpr10  
 GRADPRG12 gpr10  
 GRADPRG13 gpr10  
 GRADPRG14 gpr10  
 GRADPRG15 gpr10  
 GRADPRG16 gpr10  
 GRADPRG17 gpr10  
 GRADPRG18 gpr10  
 GRADPRG19 gpr10  
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 GRADPRG99 gpr10  
 GRADPRG100 gpr10

F2 - Processing parameters  
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 SSB 0  
 LB 0  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 75.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2 -10.000 ppm  
 F2 -125.780 Hz  
 F2 125.7803019 ppm/cm  
 HECK 1268.83649 Hz/cm

**<sup>1</sup>H spectrum**



Current Data Parameters  
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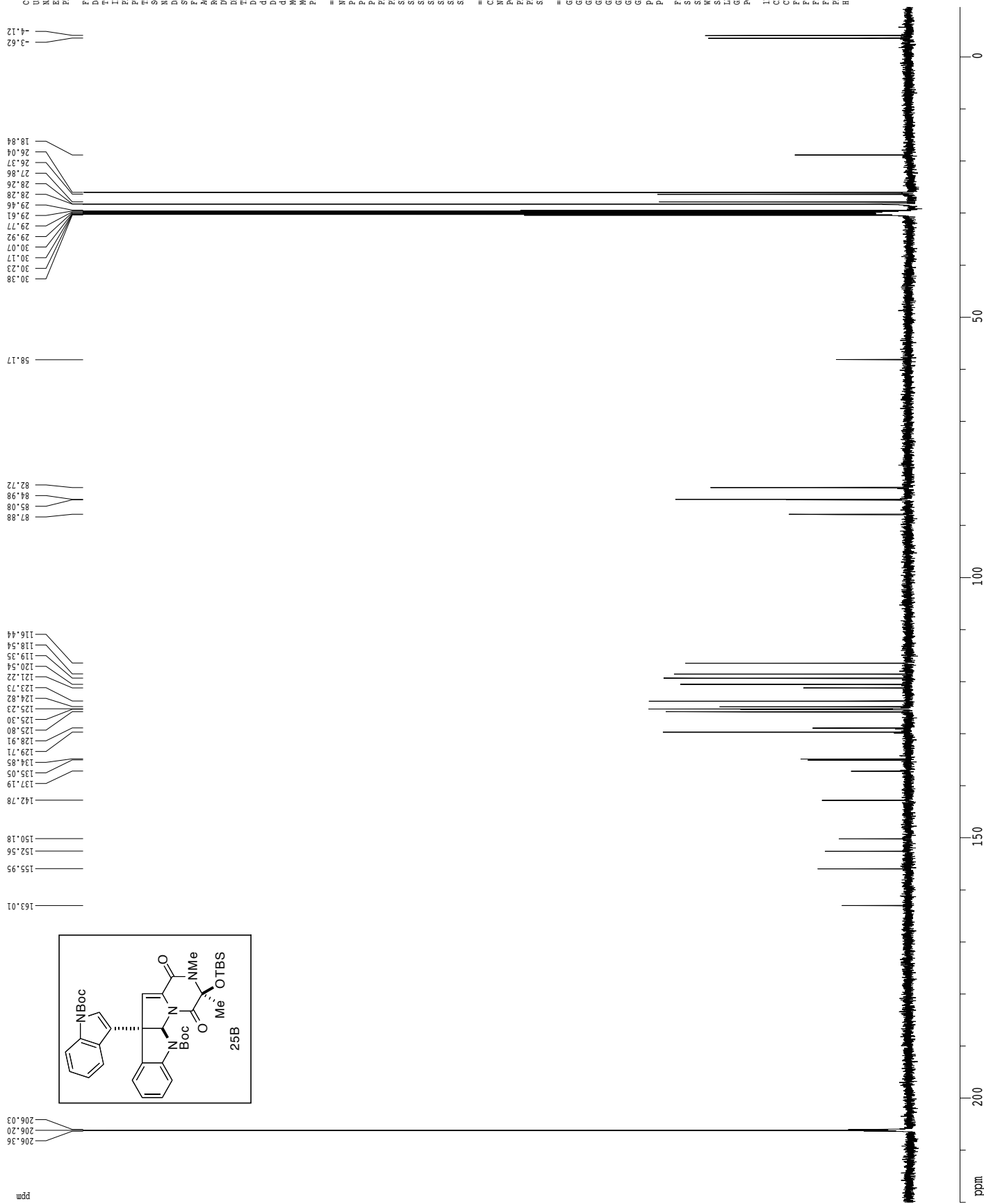
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 SOLVENT Acetone  
 NS 48  
 DS 2  
 SWE 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 128  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
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 MCHRF 0.0000000 sec  
 MCHCK 0.0150000 sec

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 PL1 -4.00 dB  
 SFO1 499.3134966 MHz

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 EN  
 GB 0  
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 PC 1.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 F1 11.000 ppm  
 F2 5494.61 Hz  
 F3 -1.000 ppm  
 F4 -499.51 Hz  
 PRCH 0.52632 ppm/cm  
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Z-restored spin-echo 13C spectrum with 1H decoupling



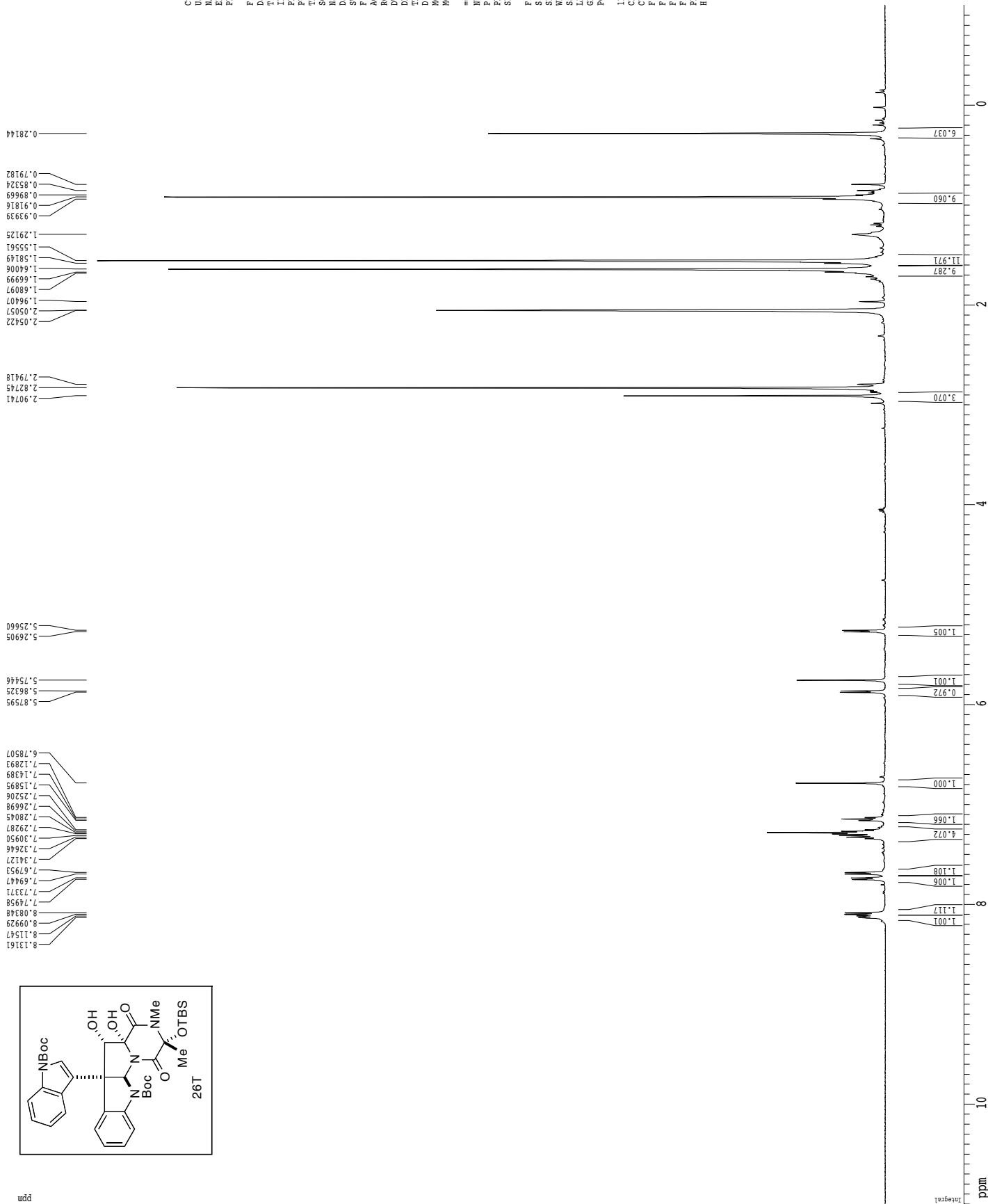
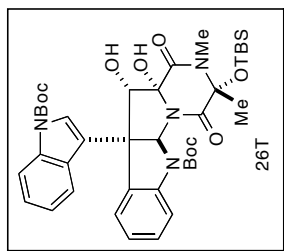
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 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 344  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 632  
 RE 16  
 DR 6.00 usec  
 DE 298.2 K  
 TE 298.2 K  
 D1 1.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.7947548 dB  
 PL2 24.60 dB  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL f2 =====  
 CDPGRZ wd t g1 5  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz  
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 GSPR2 0.00 %  
 GSP3 0.00 %  
 GSP4 0.00 %  
 GSP5 30.00 %  
 GSP6 50.00 %  
 GSP7 100.00 usec  
 GSP8 100.00 usec

F2 - Processing parameters  
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 SF 125.7803014 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 75.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2P -10.000 ppm  
 F2 -125.780 Hz  
 F2PC 10.000 ppm/cm  
 F2PCK 1268.83645 Hz/cm

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jedl-71  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 2011012  
 Time 14.33  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0980774 sec  
 RG 415  
 DE 62.60 usec  
 DR 5.00 usec  
 TE 288.0 K  
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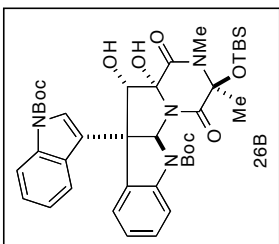
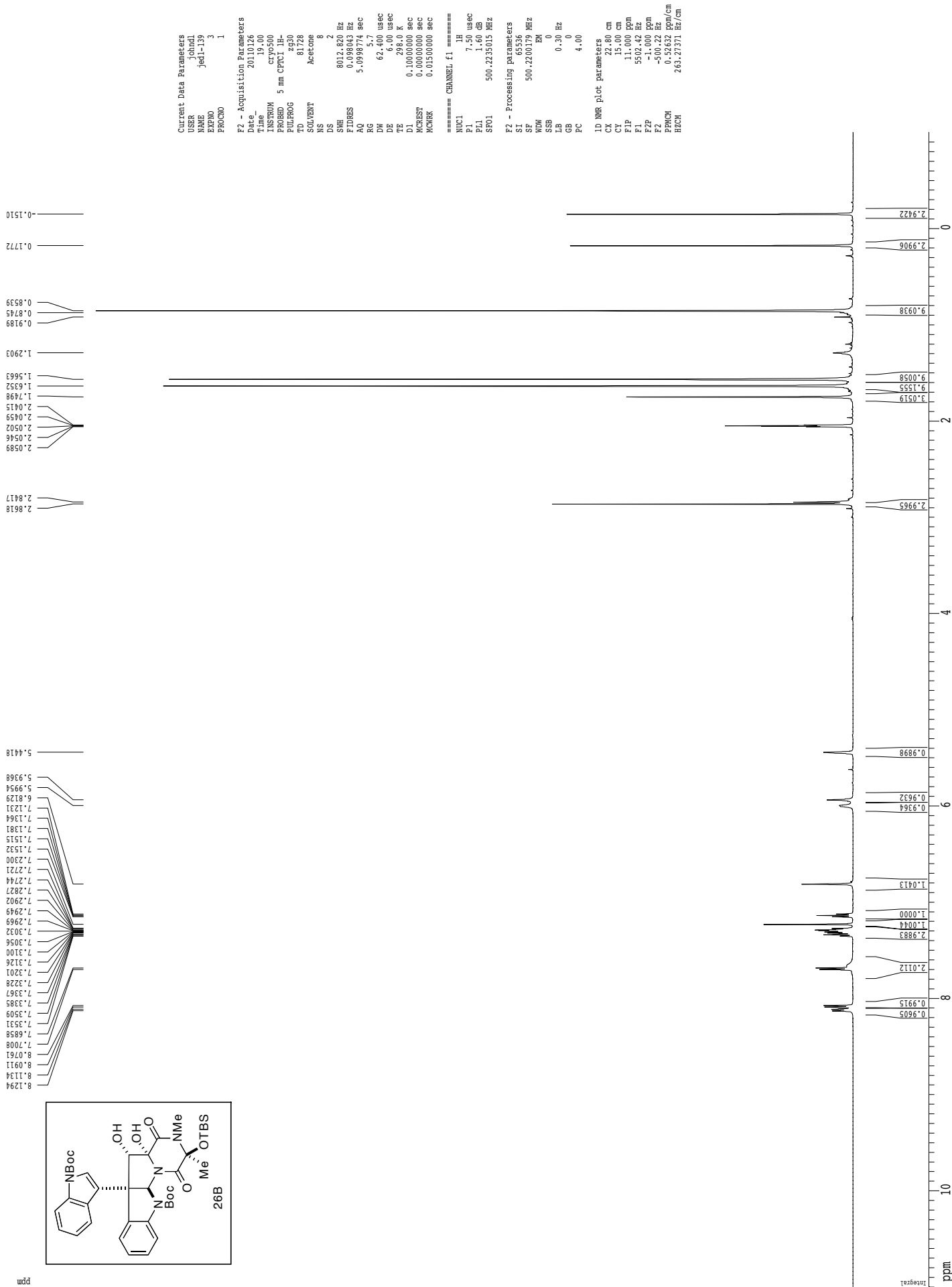
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 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 5902.82 Hz  
 F3 10.000 ppm  
 F4 -50.92 ppm  
 PRMCM 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm





<sup>1</sup>H spectrum



Current Data Parameters  
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 PROCNO 1

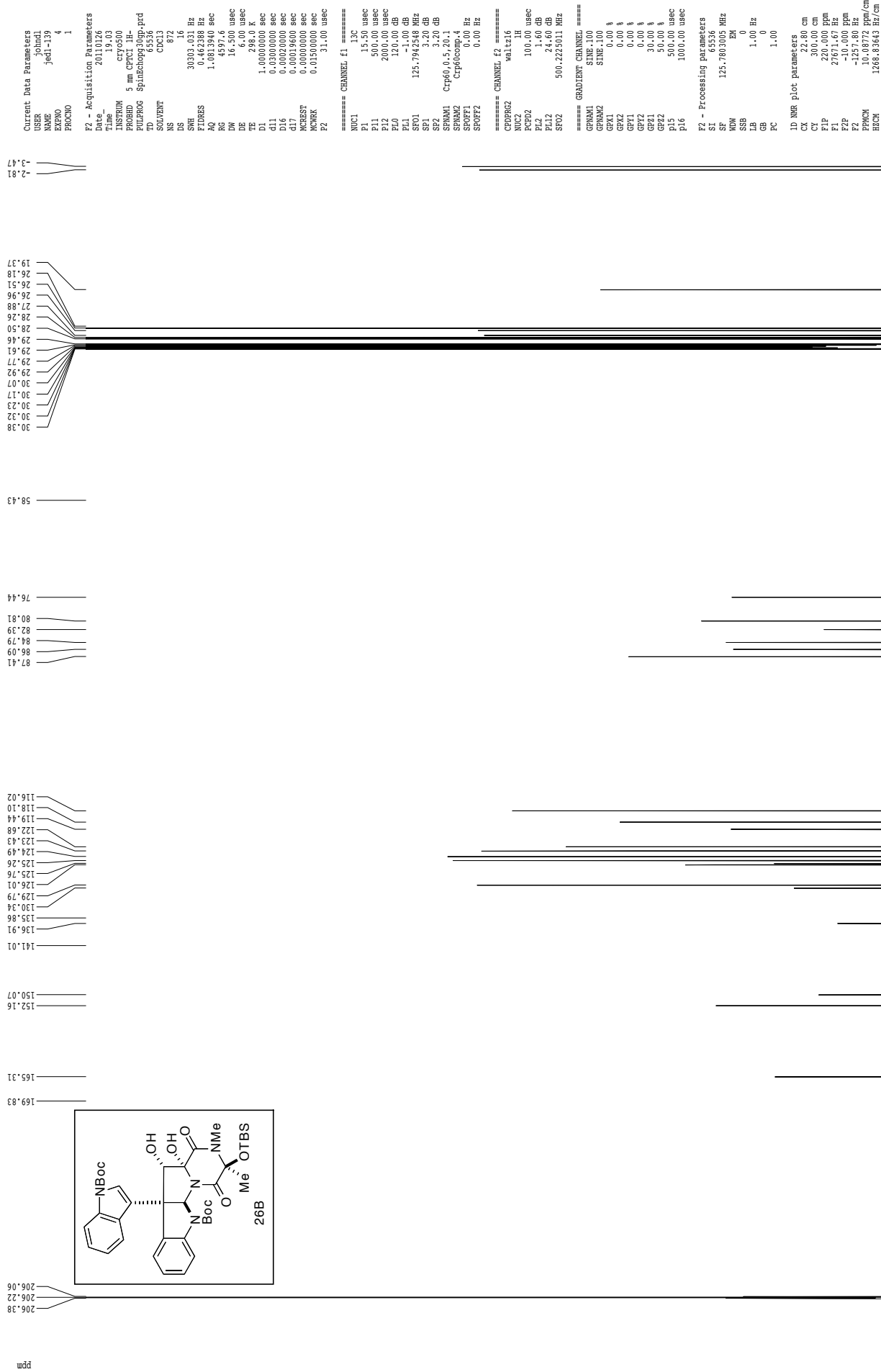
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 PULPROG zg30  
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 SOLVENT Acetone  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 307  
 DE 62.50 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65535  
 SF 500.220179 MHz  
 GB 0  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 590.242 Hz  
 F3 10.000 ppm  
 F4 -50.000 ppm  
 PRGM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
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 EXPNO jedi-112  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20110126  
 Time 19.03  
 INSTRUM cryo500  
 PROBHD 5 mm CPACI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 872  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 457.6  
 DQ 6.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 D11 0.03000000 sec  
 D16 0.00020000 sec  
 D17 0.00015600 sec  
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 ACQRESK 0.01500000 sec  
 F2 31.00 usec

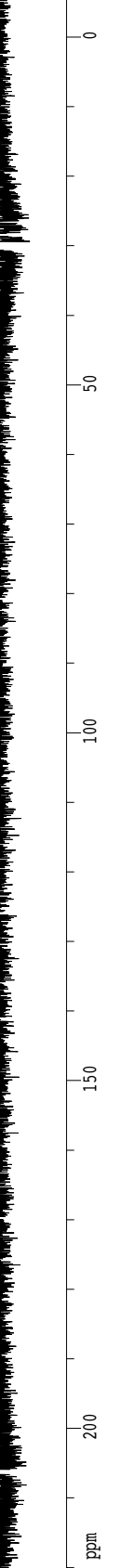
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 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPREG wd t616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
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 GRAB2 10  
 GRAB3 10  
 SINC 1.00  
 GX1 0.00 %  
 GX2 0.00 %  
 GF11 0.00 %  
 GF22 0.00 %  
 GF21 30.00 %  
 GF23 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

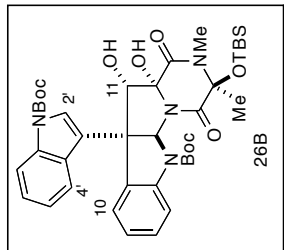
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 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 30.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2P -10.000 ppm  
 F2 -125.780 Hz  
 F2PC 10.000 ppm/cm  
 HPCOM 1268.83645 Hz/cm





gnoe



HO

C10-H

C4'-H

C11-H

Integral

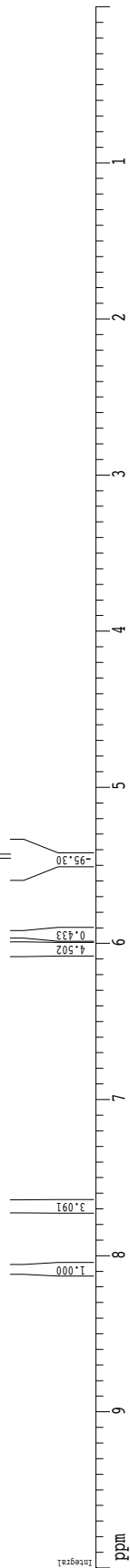
ppm

Current Data Parameters  
 USER JohnHd.  
 NAME jedl-148-bot  
 EXPNO 2  
 PROCNO 1  
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 Time\_ 11.53  
 INSTRUM cryo500  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG gnoe1cc.wu  
 TD 65536  
 SOLVENT Acetone  
 NS 48  
 DS 8  
 SWH 5482.456 Hz  
 FIDRES 0.083656 Hz  
 AQ 5.5769330 sec  
 RG 114  
 DW 91.200 usec  
 DE 6.00 usec  
 TE 298.0 K  
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 D11 0.50000000 sec  
 D16 0.00020000 sec  
 d21 0.33376500 sec  
 d22 0.16399699 sec  
 p2 15.00 usec

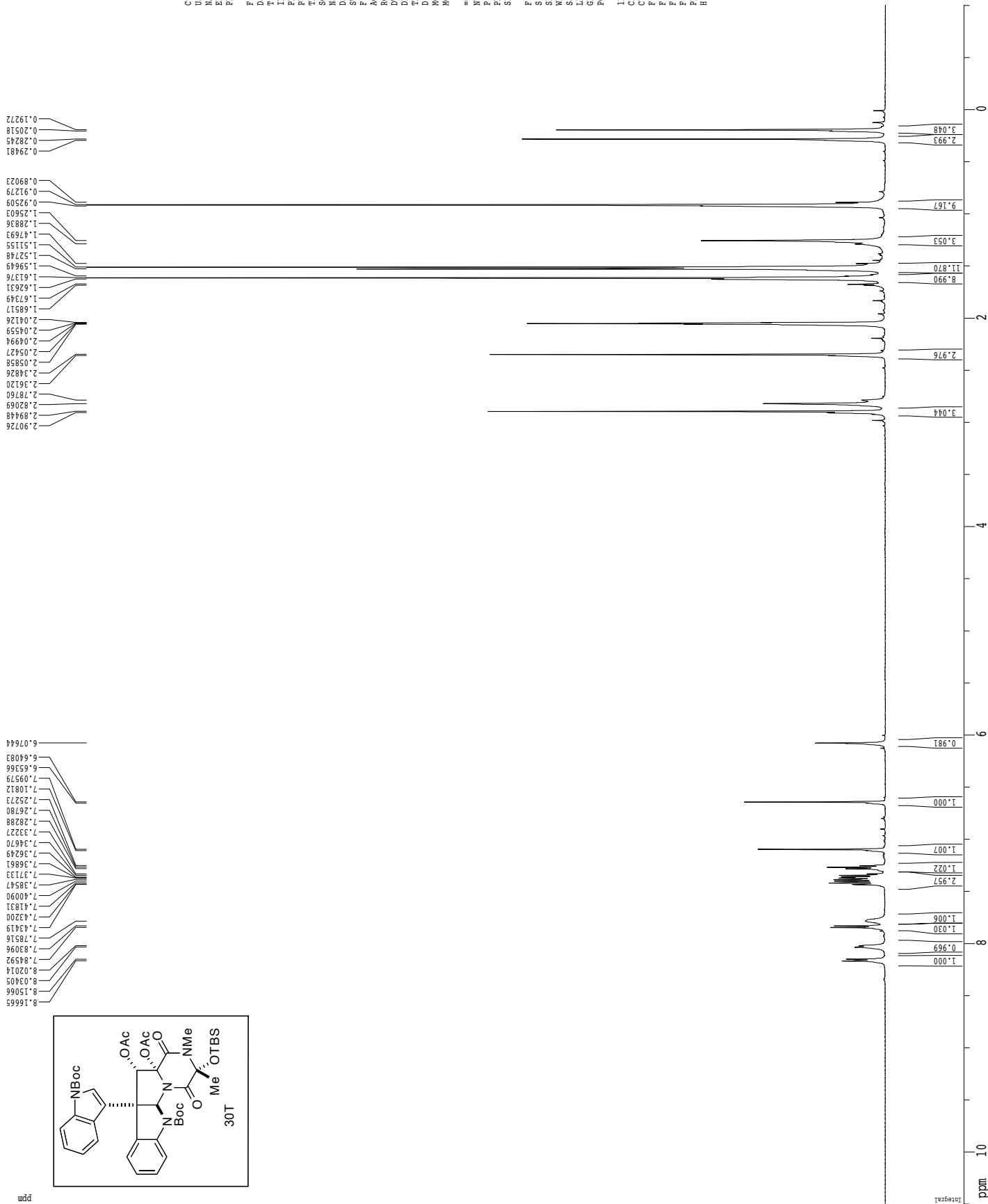
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 P3 22.50 usec  
 P4 30.00 usec  
 P5 20.00 usec  
 P12 40000.00 usec  
 PL1 1.60 dB  
 SFO1 500.2227406 MHz  
 SF1 61.60 dB  
 SPHM1 gauss1.512  
 SPOFF1 0.00 Hz  
 ===== GRADIENT CHANNEL =====  
 GENM1 sine-100  
 GENM2 sine-100  
 GENM3 sine-100  
 GENM4 sine-100  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC5 0.00 %  
 GPC6 0.00 %  
 GPC7 0.00 %  
 GPC8 0.00 %  
 GPC9 0.00 %  
 GPC10 0.00 %  
 GPC11 0.00 %  
 GPC12 0.00 %  
 GPC13 0.00 %  
 GPC14 0.00 %  
 GPC15 0.00 %  
 GPC16 0.00 %  
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F2 - Processing Parameters  
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 SF 500.2200174 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 10.000 ppm  
 F1 5002.20 Hz  
 F2P 0.000 ppm  
 F3 1.00 Hz  
 F3PMH 0.439 ppm/cm  
 HZCM 219.39456 Hz/cm



<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jed1-78-top  
 EXPNO 2  
 PROCNO 1

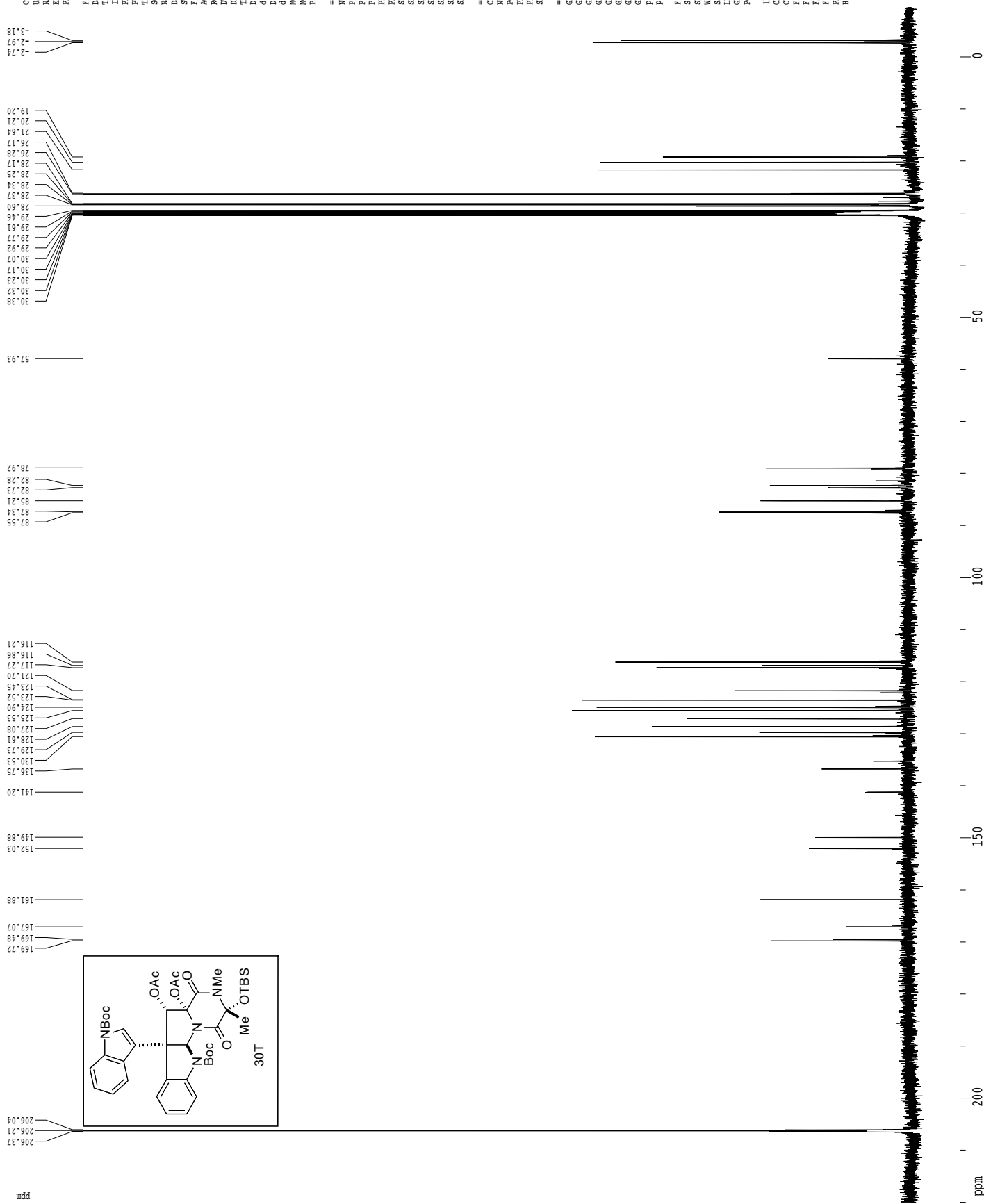
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 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Aceton  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 377  
 DE 62.600 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220181 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 20.00 cm  
 FIP 10.500 ppm  
 F2 5292.31 Hz  
 F3 10.000 ppm  
 F4 -500.22 ppm  
 PRMCM 0.50439 ppm/cm  
 HZCM 252.30397 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jomdl  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20110128  
 Time 17:52  
 INSTRUM cryo500  
 PROBHD 5 mm CPACI JH  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1144  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 4096  
 DR 16  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.100 usec

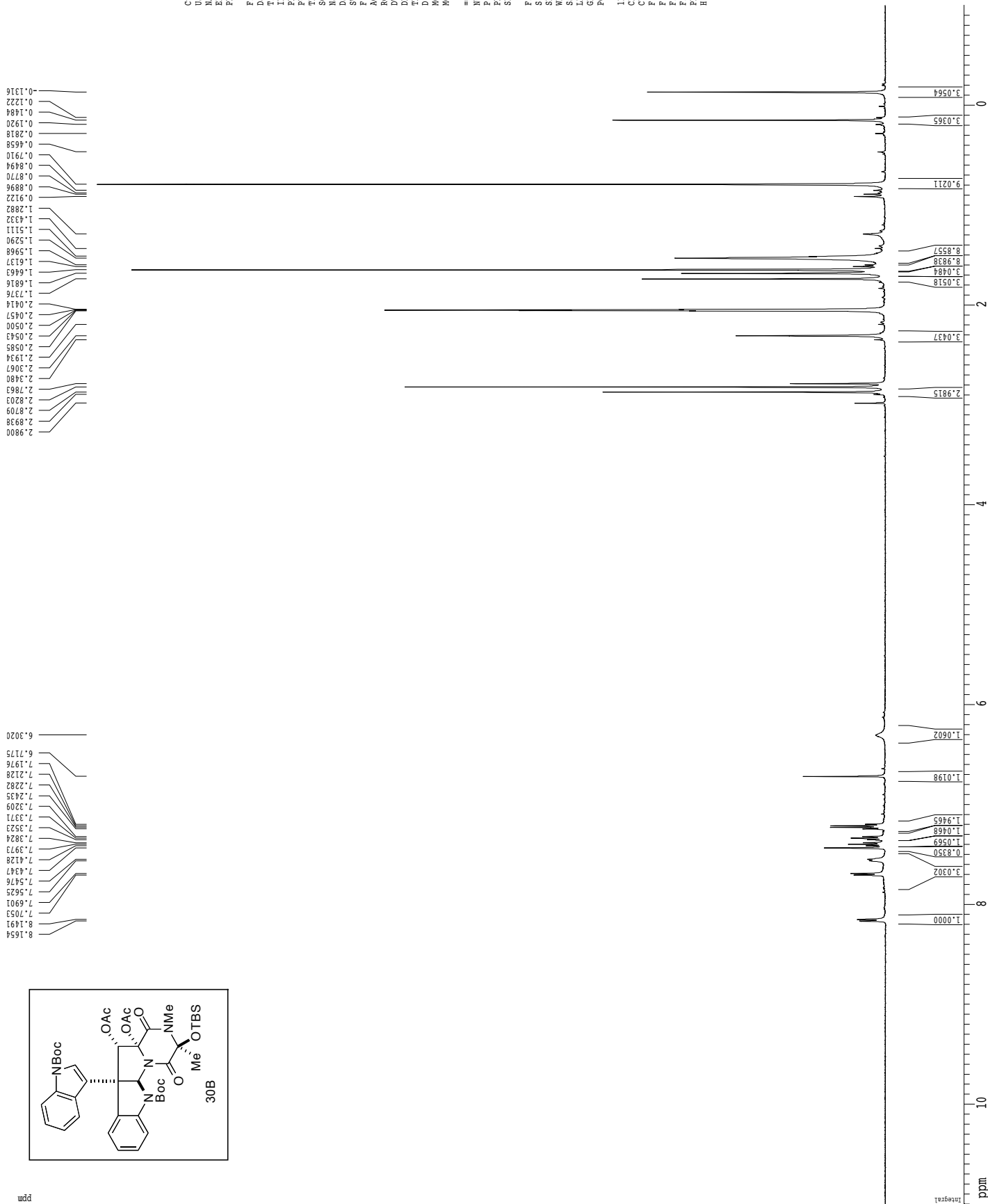
===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 PL2 125.794568 dB  
 SP1 3.20 dB  
 SP2 3.20 dB  
 SFO1 Ccp60.05.20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPGRZ wd t g 1 5  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR1 0.00 %  
 GSPR2 0.00 %  
 GSPR3 0.00 %  
 GSPR4 0.00 %  
 GSPR5 30.00 %  
 GSPR6 50.00 %  
 GSPR7 50.00 usec  
 GSPR8 100.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803005 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 200.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2P -10.000 ppm  
 F2 -125.780 Hz  
 F2PC 10.000 ppm/cm  
 F2PCK 1268.83645 Hz/cm  
 HECK

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johndel  
 NAME jed1-91-bot  
 EXPNO 1  
 PROCNO 1

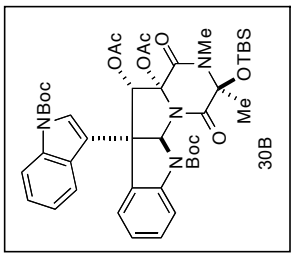
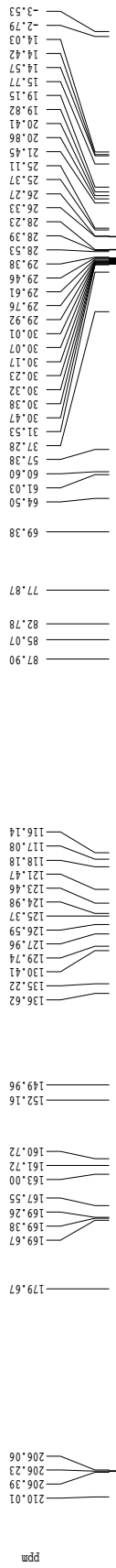
F2 - Acquisition Parameters  
 Date\_ 20101206  
 Time 14.04  
 INSTRUM cryo500  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 48  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099874 sec  
 RG 611  
 DE 62.40 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220187 MHz  
 DS 4  
 WDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 590.242 Hz  
 F3 16.000 ppm  
 F4 -500.92 Hz  
 PRGM 0.52452 ppm/cm  
 HZCN 263.27371 Hz/cm

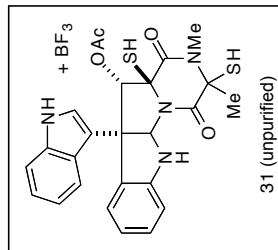
Z-restored spin-echo <sup>13</sup>C spectrum with <sup>1</sup>H decoupling



Current Data Parameters  
 USER zfang  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20100618  
 Time 19.06  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 872  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0812940 sec  
 RG 670  
 AG 16.000 usec  
 DR 6.000 usec  
 TE 298.2 K  
 D1 0.25000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.00 usec  
 ===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 P10 120.00 dB  
 P11 125.794568 dB  
 SFO1 125.761462 MHz  
 SFO2 500.132740 MHz  
 SF2 31.20 dB  
 SFO1 Cpp60.0.5.20.1  
 SFO2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz  
 ===== CHANNEL f2 =====  
 CDPGR2 wd t g1 6  
 NUC2 1H  
 P2 100.00 usec  
 P21 1.60 dB  
 P22 24.60 dB  
 SFO2 500.2225011 MHz  
 ===== GRADIENT CHANNEL =====  
 GRAB1 100.00 usec  
 GRAB2 500.00 usec  
 GRX1 0.00 %  
 GRX2 0.00 %  
 GRX3 0.00 %  
 GRX4 0.00 %  
 GRX5 0.00 %  
 GRX6 0.00 %  
 GRX7 0.00 %  
 GRX8 0.00 %  
 GRX9 0.00 %  
 GRX10 0.00 %  
 GRX11 0.00 %  
 GRX12 0.00 %  
 GRX13 0.00 %  
 GRX14 0.00 %  
 GRX15 0.00 %  
 GRX16 0.00 %  
 F2 - Processing parameters  
 SI 65536  
 SF 125.7803019 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 200.00 cm  
 FIP 220.000 ppm  
 F1 2767.167 Hz  
 F2P -10.000 ppm  
 F2 -125.780 Hz  
 F2P2 10.000 ppm/cm  
 F2P3 1268.83645 Hz/cm  
 HECK



<sup>1</sup>H spectrum



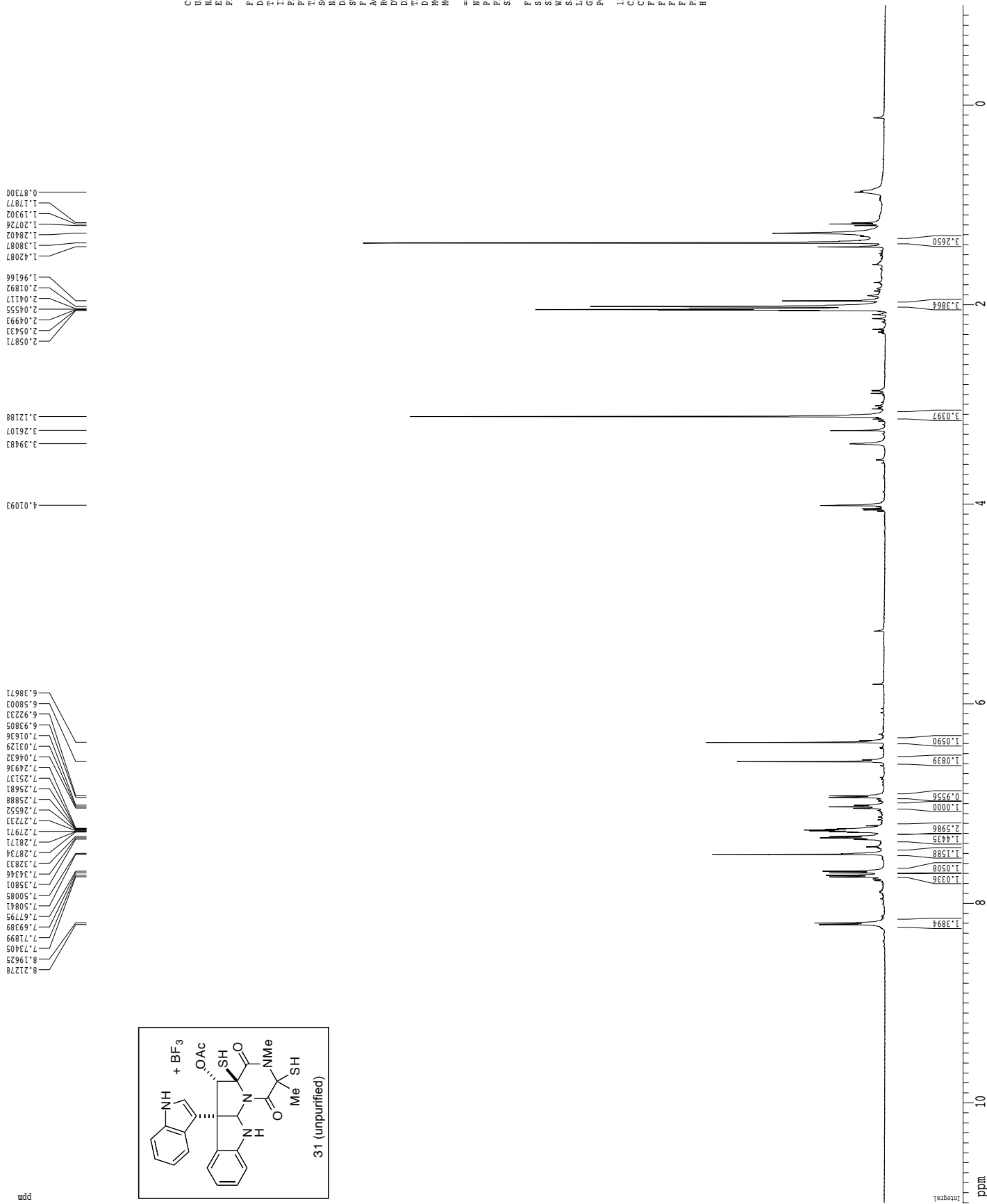
Current Data Parameters  
 USER johnd  
 NAME jes2-120  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120331  
 Time 16.33  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 377  
 DE 62.600 usec  
 DR 5.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWPK 0.01500000 sec

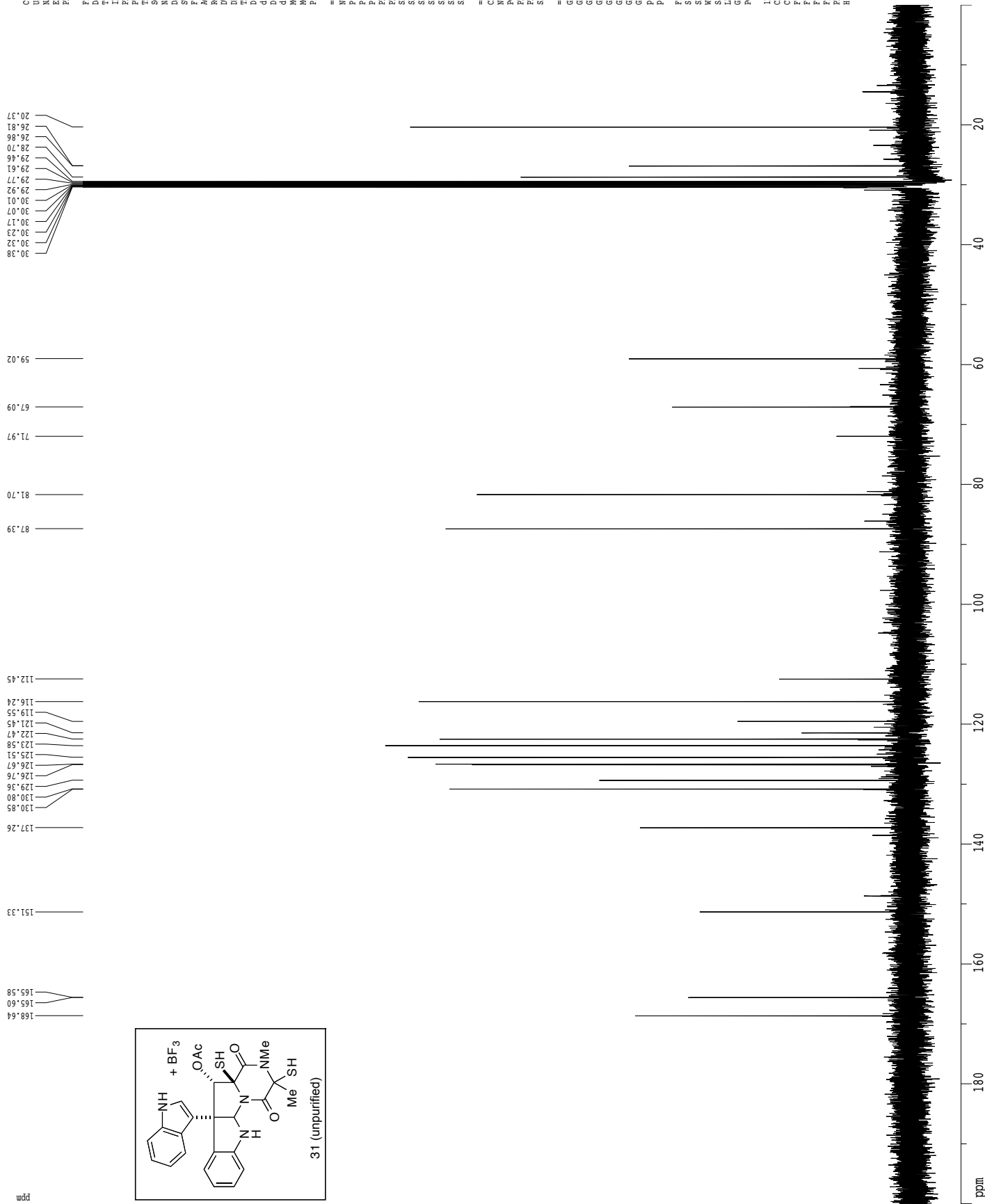
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65535  
 SF 500.220181 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 11.000 ppm  
 F2 5502.82 Hz  
 F3 10.000 ppm  
 F4 -500.32 ppm  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm



Z-restored spin-echo <sup>13</sup>C spectrum with <sup>1</sup>H decoupling



Current Data Parameters  
 USER joundl  
 EXPNO jedz-173  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120331  
 Time 16.17  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT acetone  
 NS 1024  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0812940 sec  
 RG 670  
 NG 16  
 DR 6.00 usec  
 DE 2.00 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 D11 0.03000000 sec  
 D16 0.00020000 sec  
 D17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 31.00 usec

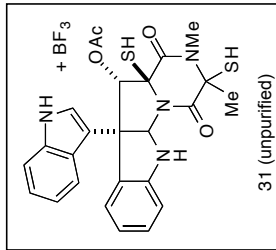
===== CHANNEL F1 =====  
 NUC1 <sup>13</sup>C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 PL2 120.00 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 125.761468 MHz  
 SFO2 500.2225011 MHz  
 SPNAM1 Ccp60.0.5.20.1  
 SPNAM2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPREG wd1615  
 NUC2 <sup>1</sup>H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz  
 ===== GRADIENT CHANGE =====  
 GRAD1 0.00 %  
 GR2 0.00 %  
 GR3 0.00 %  
 GR4 0.00 %  
 GR5 30.00 %  
 GR6 50.00 %  
 p15 500.00 usec  
 p16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803019 MHz  
 WDW EM  
 SSB 0  
 LB 0.10 Hz  
 GB 0  
 PC 2.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 200.000 ppm  
 F1 25156.06 Hz  
 F2 0.000 ppm  
 F3 0.00 Hz  
 F4 0.000 ppm/cm  
 HECK 1103.33606 Hz/cm

11B spectrum with 1H decoupling, using composite pulse for background suppression

ppm



0.983  
0.684

```

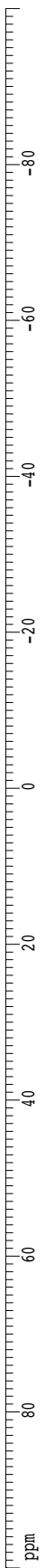
Current Data Parameters
USER          jolnd1
NAME          jes2-120
EXPNO        8
PROCNO       1

F2 - Acquisition Parameters
Date_        20120403
Time         17.25
INSTRUM      av600
PROBHD       5 mm TBI LH/13
PULPROG      zgpg30bs-pdcd
AQ           65536
RG           36
DS           4
SWH          42613.637 Hz
FIDRES       0.650232 Hz
AQ           0.7690057 sec
RG           2050
DW           11.733 usec
DE           6.00 usec
TE           298.0 K
D1           1.00000000 sec
D11          0.03000000 sec

===== CHANNEL f1 =====
NUC1          13C
P1           15.60 usec
F2           31.20 usec

F2 - Processing Parameters
SI           65536
SF           192.545591 MHz
WDW          rso
SSB          0
LB           0.00 Hz
GB           0
PC           1.00

ID NMR plot parameters
CX           22.80 cm
CY           15.65 cm
F1P          100.000 ppm
F1           19254.56 Hz
F2P          -100.000 ppm
F2           -19254.56 Hz
PPMCH        8.7193 ppm/cm
HZCH         1668.99622 Hz/cm
    
```

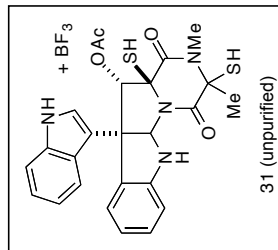






19F spectrum

150.36  
150.30



```

Current Data Parameters
USER          jolnd1
NAME          jes2-120
EXPNO        10
PROCNO       1

F2 - Acquisition Parameters
Date_        20120403
Time         18.06
INSTRUM      dx400
PROBHD       5 mm QNP 1H/1
PULPROG      zgpg30
AQ           0.6536
RG           327.7
NS           77
DS           2
SWH          75187.969 Hz
FIDRES       1.147277 Hz
AQ           0.4358644 sec
RG           2580.3
DW           6.650 usec
DE           9.46 usec
TE           298.0 K
D1           2.0000000 sec

===== CHANNEL f1 =====
NUC1          19F
P1           55.00 usec
PL1          -6.00 dB
SFO1         376.4232343 MHz

F2 - Processing Parameters
SI           65536
SF           376.4984640 MHz
WDW          EM
SSB          0
LB           0.30 Hz
GB           0
PC           1.00

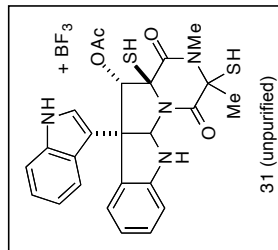
ID NMR plot parameters
CX           22.80 cm
CY           15.00 cm
F1P         -99.962 ppm
F1          -37635.72 Hz
F2P         -299.666 ppm
F2          -112823.70 Hz
PPMCH       8.75891 ppm/cm
HZCH        3297.71802 Hz/cm
    
```



150  
140  
120  
160  
180  
200  
220  
240  
260  
280

19F spectrum

ppm



150.36  
150.30

```

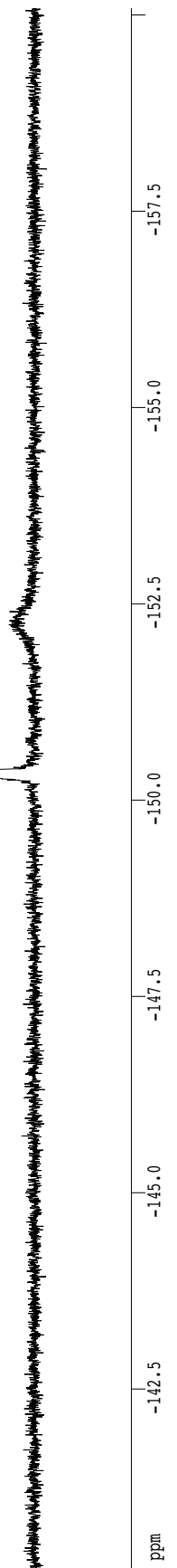
Current Data Parameters
USER          jolmd1
NAME          jes2-120
EXPNO         10
PROCNO        1

F2 - Acquisition Parameters
Date_         20120403
Time          18.06
INSTRUM       dx400
PROBHD        5 mm QNP 1H/13
PULPROG       zgpg30
AQ            6536
RG            327
DS            2
SWH           75187.969 Hz
FIDRES        1.147277 Hz
AQ            0.4358644 sec
RG            2580.3
DW            6.650 usec
DE            9.46 usec
TE            298.0 K
D1            2.0000000 sec

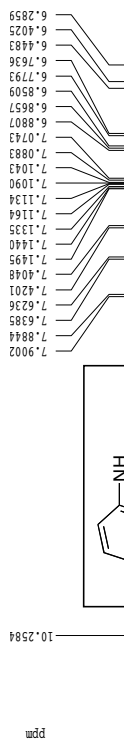
===== CHANNEL f1 =====
NUC1          19F
P1            55.00 usec
PL1           -6.00 dB
SFO1          376.4232343 MHz

F2 - Processing Parameters
SI            65536
SF            376.4984640 MHz
WDW           EM
SSB           0
LB            0.30 Hz
GB            0
PC            1.00

ID NMR plot parameters
CX            22.80 cm
CY            15.00 cm
F1P          -140.223 ppm
F1           -52793.71 Hz
F2P          -160.061 ppm
F2           -60270.27 Hz
PPMACH        0.87097 ppm/cm
HZCH          327.91953 Hz/cm
    
```



<sup>1</sup>H spectrum



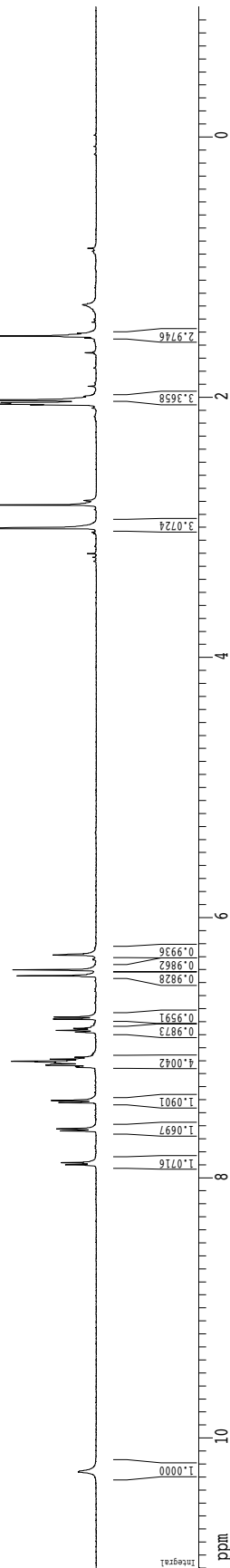
Current Data Parameters  
 USER johnd  
 NAME jedl-84  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 2011025  
 Time 11.34  
 INSTRUM crys500  
 PROBRD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 32  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 377  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

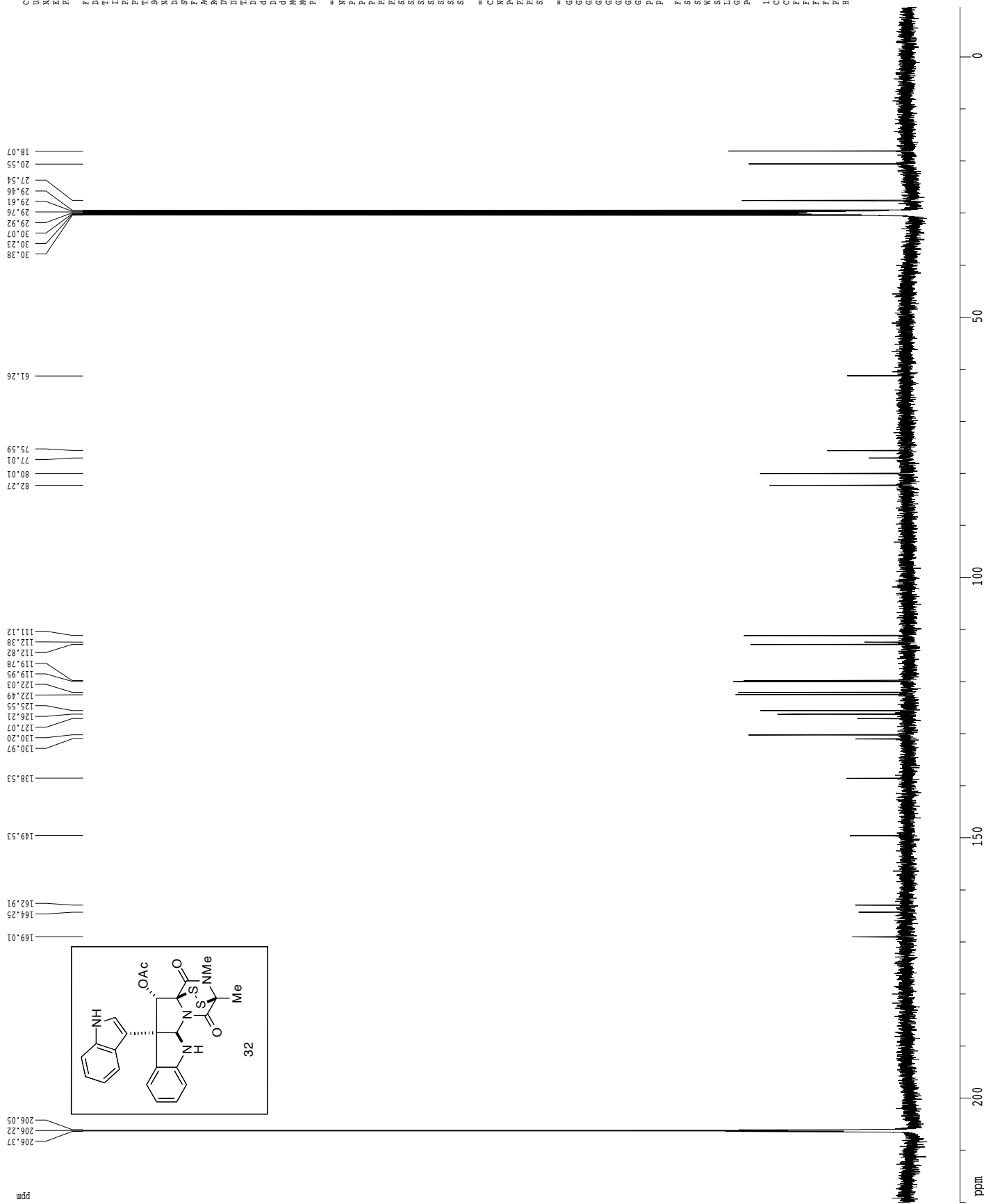
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65535  
 SF 500.220179 MHz  
 WDW rto  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 5.00 cm  
 FIP 11.000 ppm  
 F2 590.242 Hz  
 F3 10.000 ppm  
 FZ -50.92  
 PRMCM 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER joudal  
 EXPNO jed1-56  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110125  
 Time 13:30  
 INSTRUM cryo500  
 PROBRID 5 mm CPAC1 JH  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 1312  
 DS 16  
 SMR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 1298.2  
 DR 16.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 D17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.100 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 P12 2000.00 usec  
 PL2 120.00 dB  
 PLO 120.00 dB  
 SFO1 125.7645680 MHz  
 SF2 51.20 dB  
 SFO2 31.20 dB  
 SFO3 125.7645680 MHz  
 SFO4 31.20 dB  
 SFO5 125.7645680 MHz  
 SFO6 31.20 dB  
 SFO7 125.7645680 MHz  
 SFO8 31.20 dB  
 SFO9 125.7645680 MHz  
 SFO10 31.20 dB  
 SFO11 125.7645680 MHz  
 SFO12 31.20 dB  
 SFO13 125.7645680 MHz  
 SFO14 31.20 dB  
 SFO15 125.7645680 MHz  
 SFO16 31.20 dB  
 SFO17 125.7645680 MHz  
 SFO18 31.20 dB  
 SFO19 125.7645680 MHz  
 SFO20 31.20 dB  
 SFO21 125.7645680 MHz  
 SFO22 31.20 dB  
 SFO23 125.7645680 MHz  
 SFO24 31.20 dB  
 SFO25 125.7645680 MHz  
 SFO26 31.20 dB  
 SFO27 125.7645680 MHz  
 SFO28 31.20 dB  
 SFO29 125.7645680 MHz  
 SFO30 31.20 dB  
 SFO31 125.7645680 MHz  
 SFO32 31.20 dB  
 SFO33 125.7645680 MHz  
 SFO34 31.20 dB  
 SFO35 125.7645680 MHz  
 SFO36 31.20 dB  
 SFO37 125.7645680 MHz  
 SFO38 31.20 dB  
 SFO39 125.7645680 MHz  
 SFO40 31.20 dB  
 SFO41 125.7645680 MHz  
 SFO42 31.20 dB  
 SFO43 125.7645680 MHz  
 SFO44 31.20 dB  
 SFO45 125.7645680 MHz  
 SFO46 31.20 dB  
 SFO47 125.7645680 MHz  
 SFO48 31.20 dB  
 SFO49 125.7645680 MHz  
 SFO50 31.20 dB  
 SFO51 125.7645680 MHz  
 SFO52 31.20 dB  
 SFO53 125.7645680 MHz  
 SFO54 31.20 dB  
 SFO55 125.7645680 MHz  
 SFO56 31.20 dB  
 SFO57 125.7645680 MHz  
 SFO58 31.20 dB  
 SFO59 125.7645680 MHz  
 SFO60 31.20 dB  
 SFO61 125.7645680 MHz  
 SFO62 31.20 dB  
 SFO63 125.7645680 MHz  
 SFO64 31.20 dB  
 SFO65 125.7645680 MHz  
 SFO66 31.20 dB  
 SFO67 125.7645680 MHz  
 SFO68 31.20 dB  
 SFO69 125.7645680 MHz  
 SFO70 31.20 dB  
 SFO71 125.7645680 MHz  
 SFO72 31.20 dB  
 SFO73 125.7645680 MHz  
 SFO74 31.20 dB  
 SFO75 125.7645680 MHz  
 SFO76 31.20 dB  
 SFO77 125.7645680 MHz  
 SFO78 31.20 dB  
 SFO79 125.7645680 MHz  
 SFO80 31.20 dB  
 SFO81 125.7645680 MHz  
 SFO82 31.20 dB  
 SFO83 125.7645680 MHz  
 SFO84 31.20 dB  
 SFO85 125.7645680 MHz  
 SFO86 31.20 dB  
 SFO87 125.7645680 MHz  
 SFO88 31.20 dB  
 SFO89 125.7645680 MHz  
 SFO90 31.20 dB  
 SFO91 125.7645680 MHz  
 SFO92 31.20 dB  
 SFO93 125.7645680 MHz  
 SFO94 31.20 dB  
 SFO95 125.7645680 MHz  
 SFO96 31.20 dB  
 SFO97 125.7645680 MHz  
 SFO98 31.20 dB  
 SFO99 125.7645680 MHz  
 SFO100 31.20 dB

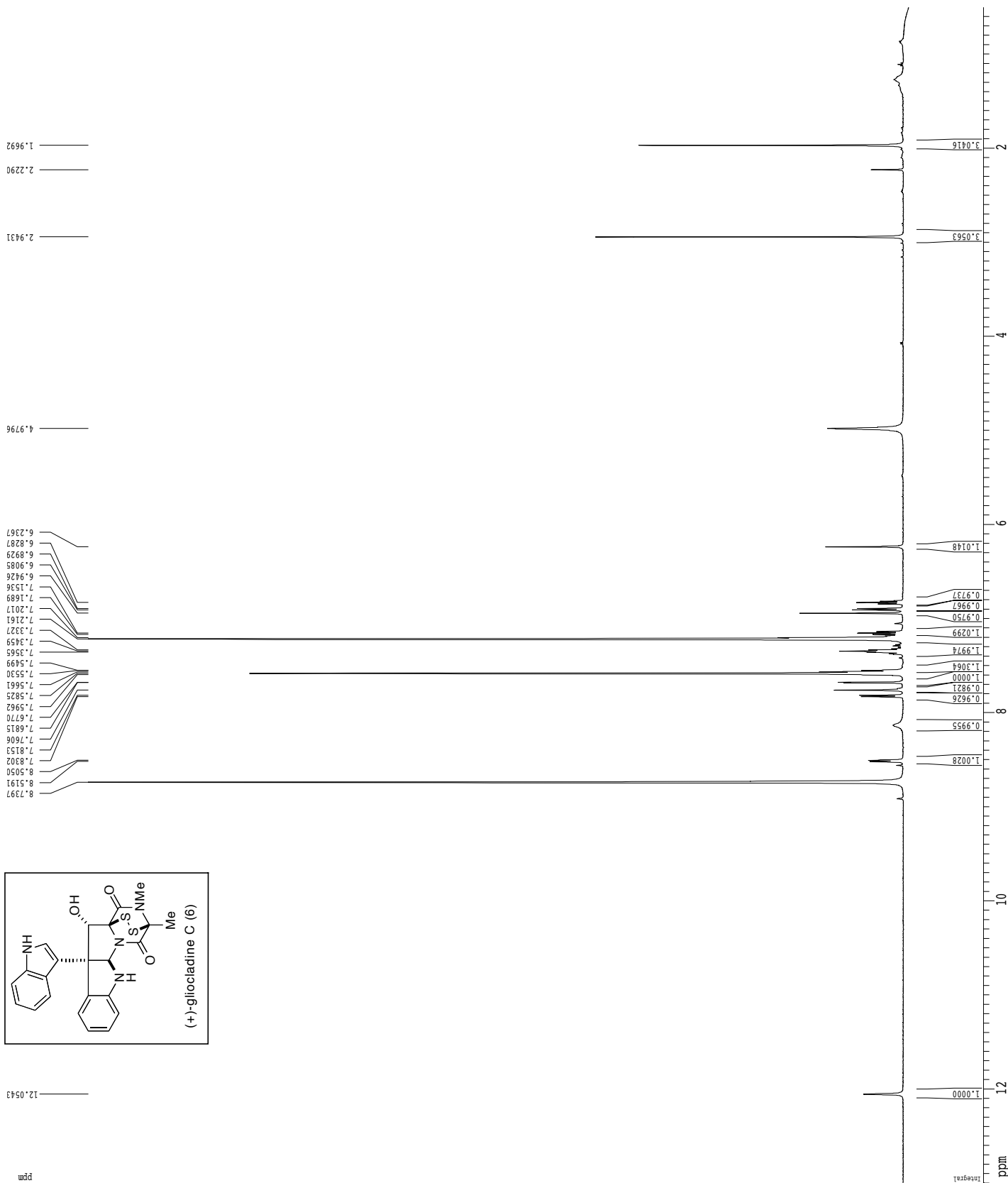
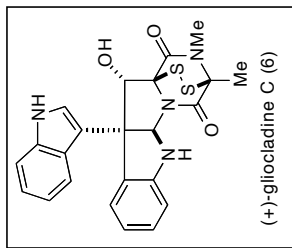
===== CHANNEL F2 =====  
 CDPGRZ wd1616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GRAD1 100.00 usec  
 GRAD2 100.00 usec  
 GRAD3 100.00 usec  
 GRAD4 100.00 usec  
 GRAD5 100.00 usec  
 GRAD6 100.00 usec  
 GRAD7 100.00 usec  
 GRAD8 100.00 usec  
 GRAD9 100.00 usec  
 GRAD10 100.00 usec  
 GRAD11 100.00 usec  
 GRAD12 100.00 usec  
 GRAD13 100.00 usec  
 GRAD14 100.00 usec  
 GRAD15 100.00 usec  
 GRAD16 100.00 usec  
 GRAD17 100.00 usec  
 GRAD18 100.00 usec  
 GRAD19 100.00 usec  
 GRAD20 100.00 usec  
 GRAD21 100.00 usec  
 GRAD22 100.00 usec  
 GRAD23 100.00 usec  
 GRAD24 100.00 usec  
 GRAD25 100.00 usec  
 GRAD26 100.00 usec  
 GRAD27 100.00 usec  
 GRAD28 100.00 usec  
 GRAD29 100.00 usec  
 GRAD30 100.00 usec  
 GRAD31 100.00 usec  
 GRAD32 100.00 usec  
 GRAD33 100.00 usec  
 GRAD34 100.00 usec  
 GRAD35 100.00 usec  
 GRAD36 100.00 usec  
 GRAD37 100.00 usec  
 GRAD38 100.00 usec  
 GRAD39 100.00 usec  
 GRAD40 100.00 usec  
 GRAD41 100.00 usec  
 GRAD42 100.00 usec  
 GRAD43 100.00 usec  
 GRAD44 100.00 usec  
 GRAD45 100.00 usec  
 GRAD46 100.00 usec  
 GRAD47 100.00 usec  
 GRAD48 100.00 usec  
 GRAD49 100.00 usec  
 GRAD50 100.00 usec  
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 GRAD67 100.00 usec  
 GRAD68 100.00 usec  
 GRAD69 100.00 usec  
 GRAD70 100.00 usec  
 GRAD71 100.00 usec  
 GRAD72 100.00 usec  
 GRAD73 100.00 usec  
 GRAD74 100.00 usec  
 GRAD75 100.00 usec  
 GRAD76 100.00 usec  
 GRAD77 100.00 usec  
 GRAD78 100.00 usec  
 GRAD79 100.00 usec  
 GRAD80 100.00 usec  
 GRAD81 100.00 usec  
 GRAD82 100.00 usec  
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 GRAD86 100.00 usec  
 GRAD87 100.00 usec  
 GRAD88 100.00 usec  
 GRAD89 100.00 usec  
 GRAD90 100.00 usec  
 GRAD91 100.00 usec  
 GRAD92 100.00 usec  
 GRAD93 100.00 usec  
 GRAD94 100.00 usec  
 GRAD95 100.00 usec  
 GRAD96 100.00 usec  
 GRAD97 100.00 usec  
 GRAD98 100.00 usec  
 GRAD99 100.00 usec  
 GRAD100 100.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803005 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

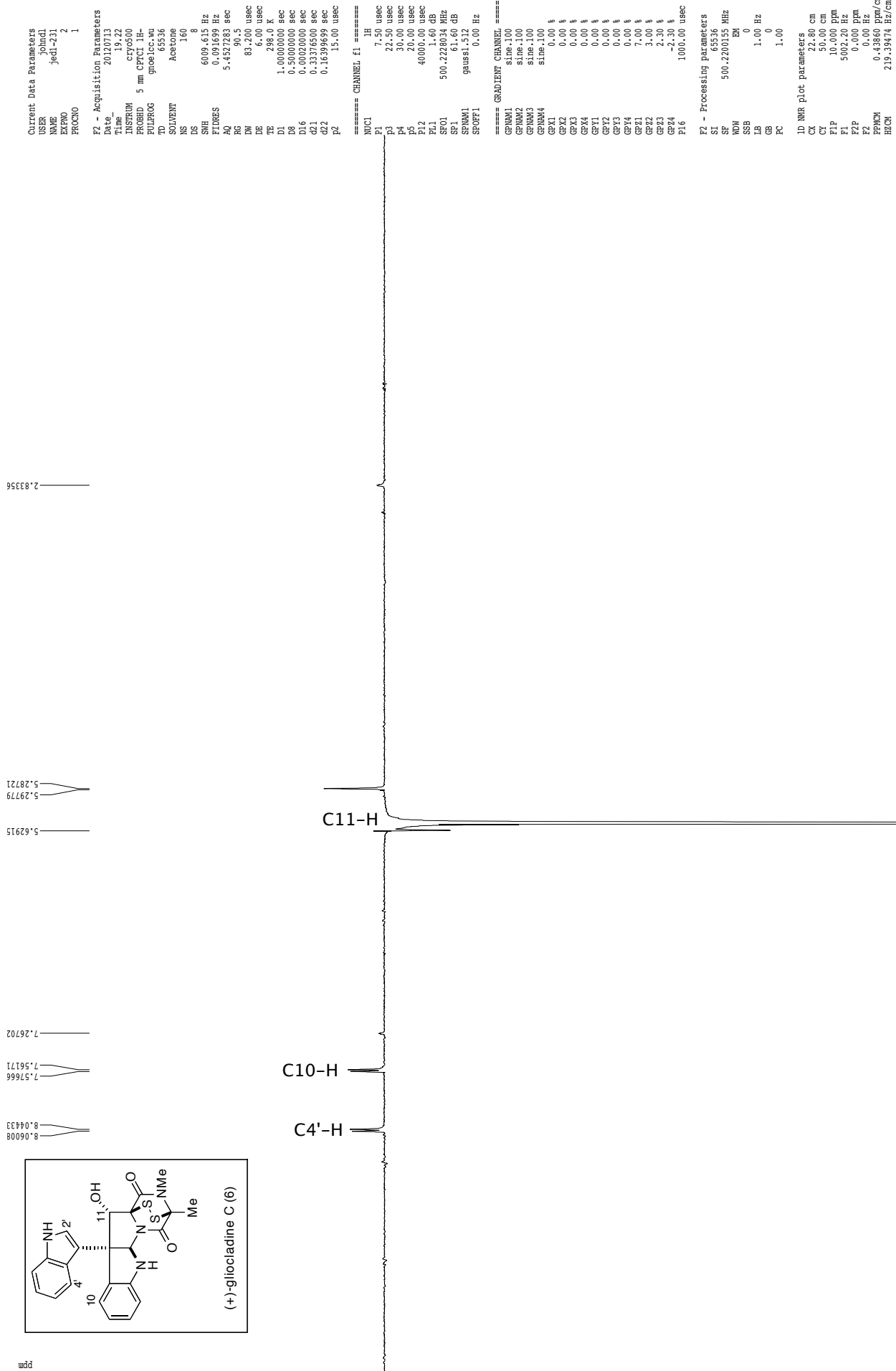
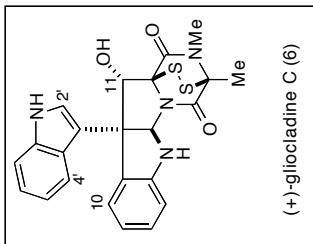
ID NMR plot parameters  
 CX 22.80 cm  
 CY 250.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -10.000 ppm  
 F2 125.780 Hz  
 F2 125.780 Hz  
 F2 125.780 Hz  
 HECK 1248.8363 Hz/cm

<sup>1</sup>H spectrum





gnoe

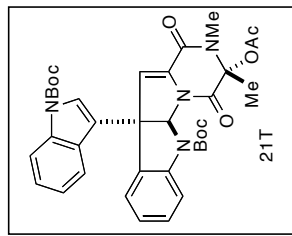


ppm

Integral



<sup>1</sup>H spectrum

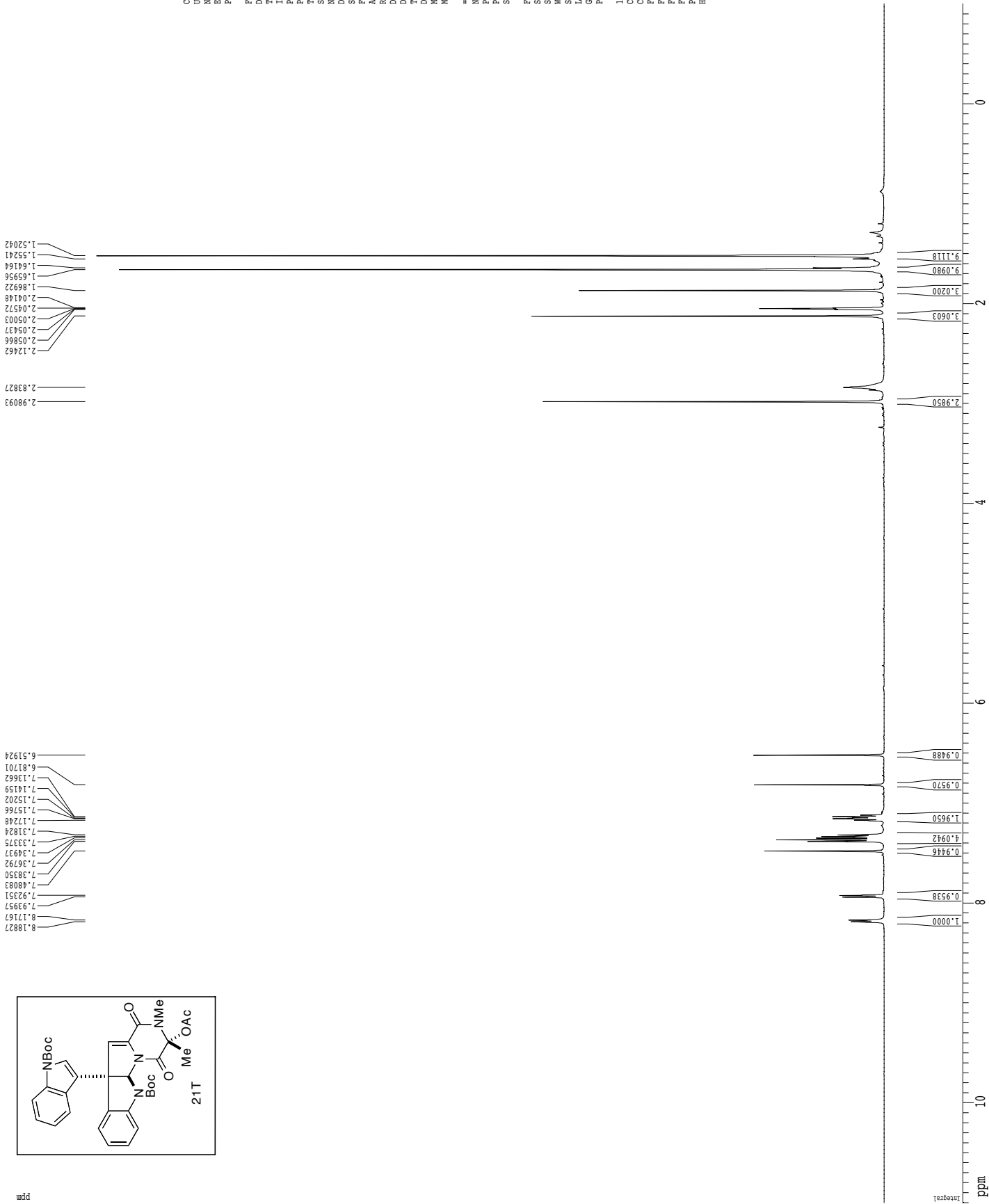


8.18827  
8.17167  
7.93957  
7.92351  
7.48083  
7.38350  
7.36792  
7.34937  
7.33375  
7.31824  
7.17248  
7.15766  
7.15282  
7.14159  
7.13662  
7.13662  
6.81701  
6.51924

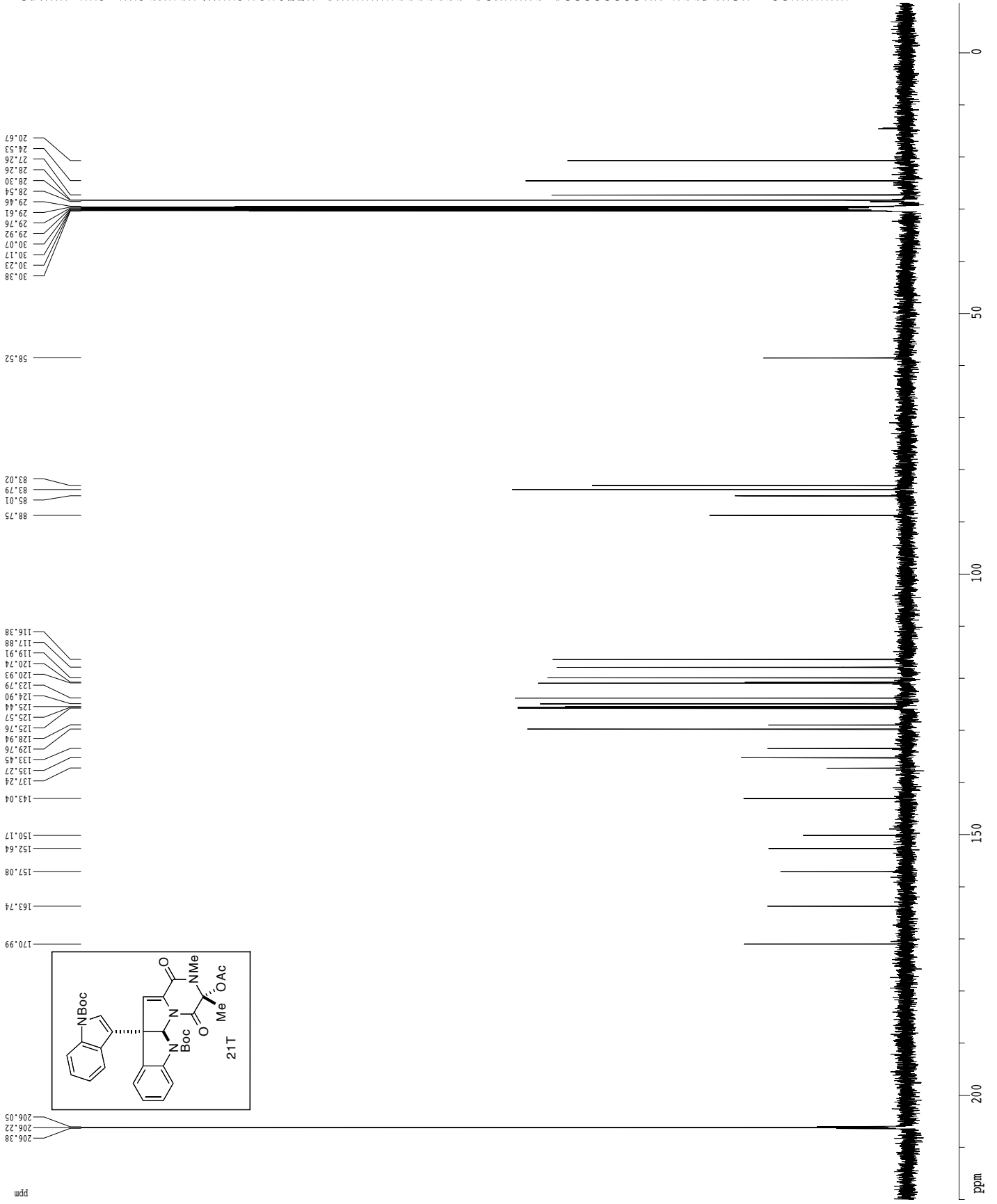
2.98093  
2.83827

2.12462  
2.05866  
2.05437  
2.05003  
2.04572  
2.04148  
1.86922  
1.65956  
1.64164  
1.55241  
1.52042

Current Data Parameters  
 USER johnd  
 NAME jed7-122-top  
 EXPNO 8  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120601  
 Time 10.23  
 INSTRUM cryo500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099774 sec  
 RG 45  
 DE 62.600 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 500.220182 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 FZ 5902.82 Hz  
 HZ 10.000 ppm  
 F2 -500.22 MHz  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jomdl  
 EXPNO jedi-12-409  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120529  
 Time 9:59  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 304  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 1288.7  
 DR 6.00 usec  
 DE 19.00 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACRESK 0.01500000 sec  
 F2 3.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

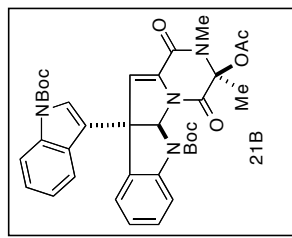
===== CHANNEL f2 =====  
 CDPREG wd1615  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GRAB1 0  
 GRAB2 10  
 GRAB3 10  
 SINC 10  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC5 30.00 %  
 GPC6 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803019 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 25.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2 -10.000 ppm  
 F2 -125.780 Hz  
 F2 10.000 ppm/cm  
 HECK 1268.8365 Hz/cm

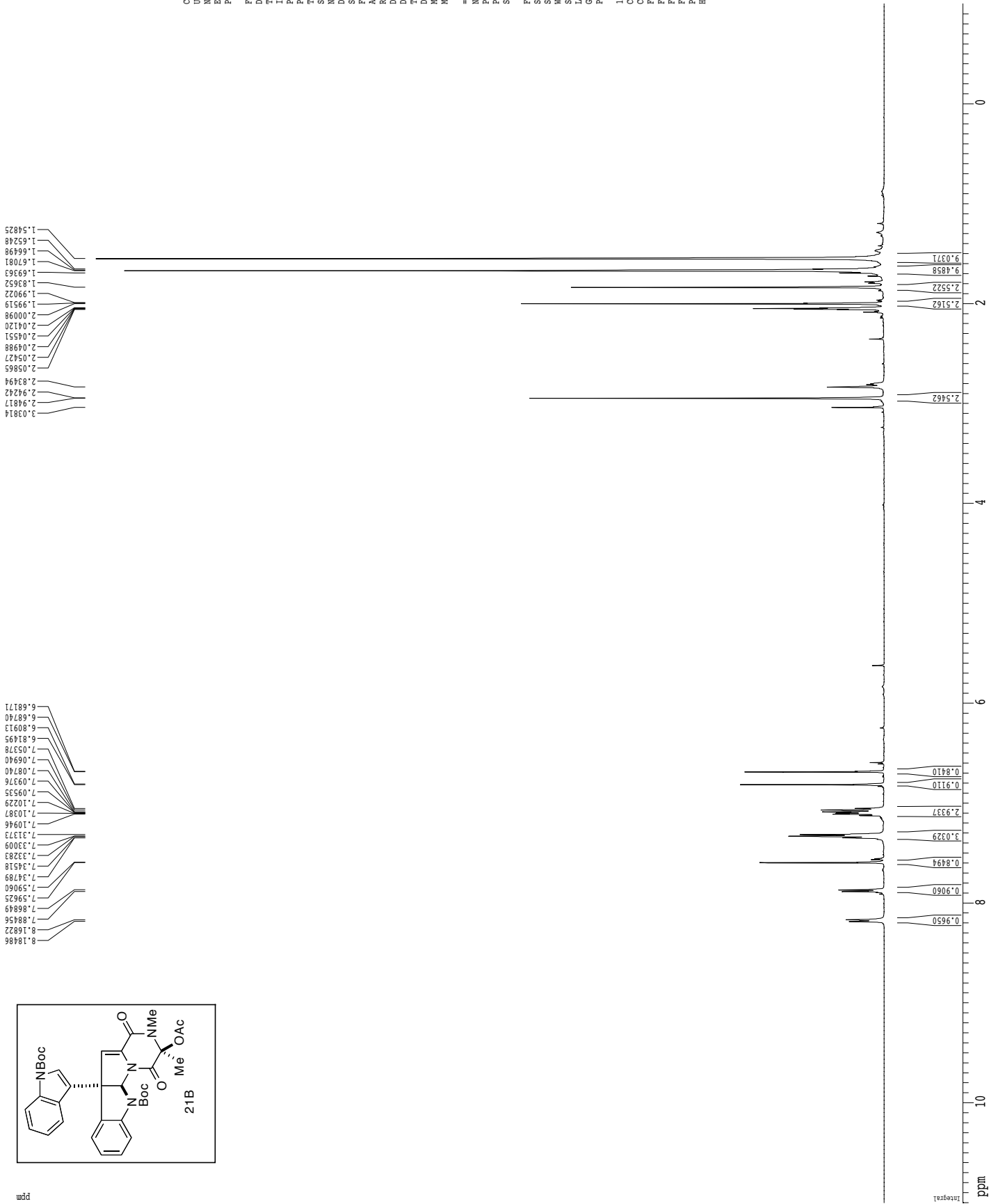
**<sup>1</sup>H spectrum**



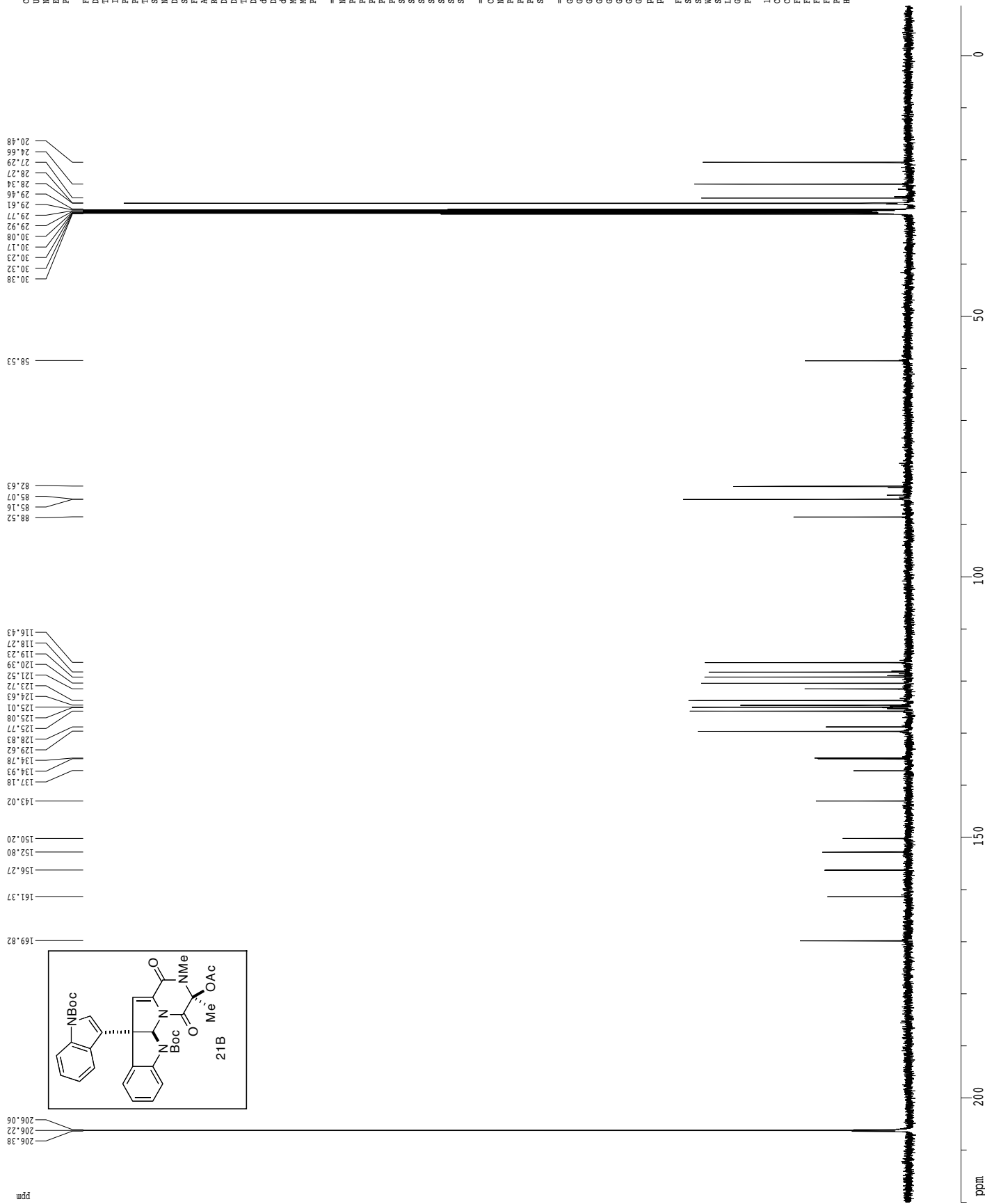
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2.94817  
2.94242  
2.83494  
2.05865  
2.05427  
2.04988  
2.04120  
2.00098  
1.99519  
1.99022  
1.98652  
1.69363  
1.67081  
1.66498  
1.65248  
1.54825

8.18486  
8.16822  
7.88456  
7.86849  
7.59625  
7.59060  
7.54189  
7.54518  
7.33283  
7.33009  
7.31373  
7.10946  
7.10387  
7.10229  
7.09535  
7.09376  
7.08740  
7.06940  
7.05378  
6.81495  
6.80913  
6.80740  
6.68171

Current Data Parameters  
 USER johnd  
 NAME jed2-122-bot  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120528  
 Time 15.43  
 INSTRUM cryo500  
 PROBRD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099874 sec  
 RG 62.400 usec  
 DR 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz  
 F2 - Processing parameters  
 SI 65535  
 SF 500.220183 MHz  
 GM 0.00000000 sec  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 590.242 Hz  
 F3 0.00000000 Hz  
 F4 -500.92000000 Hz  
 PRGM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jced1  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120528  
 Time 15.46  
 INSTRUM cryo500  
 PROBHD 5 mm CPACI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 352  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.081940 sec  
 RG 364.71  
 AG 19.60 usec  
 DR 6.00 usec  
 DE 298.0 K  
 TE 298.0 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.00015600 sec  
 WREST 0.0000000 sec  
 WTRK 0.0150000 sec  
 F2 31.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 PL2 120.00 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

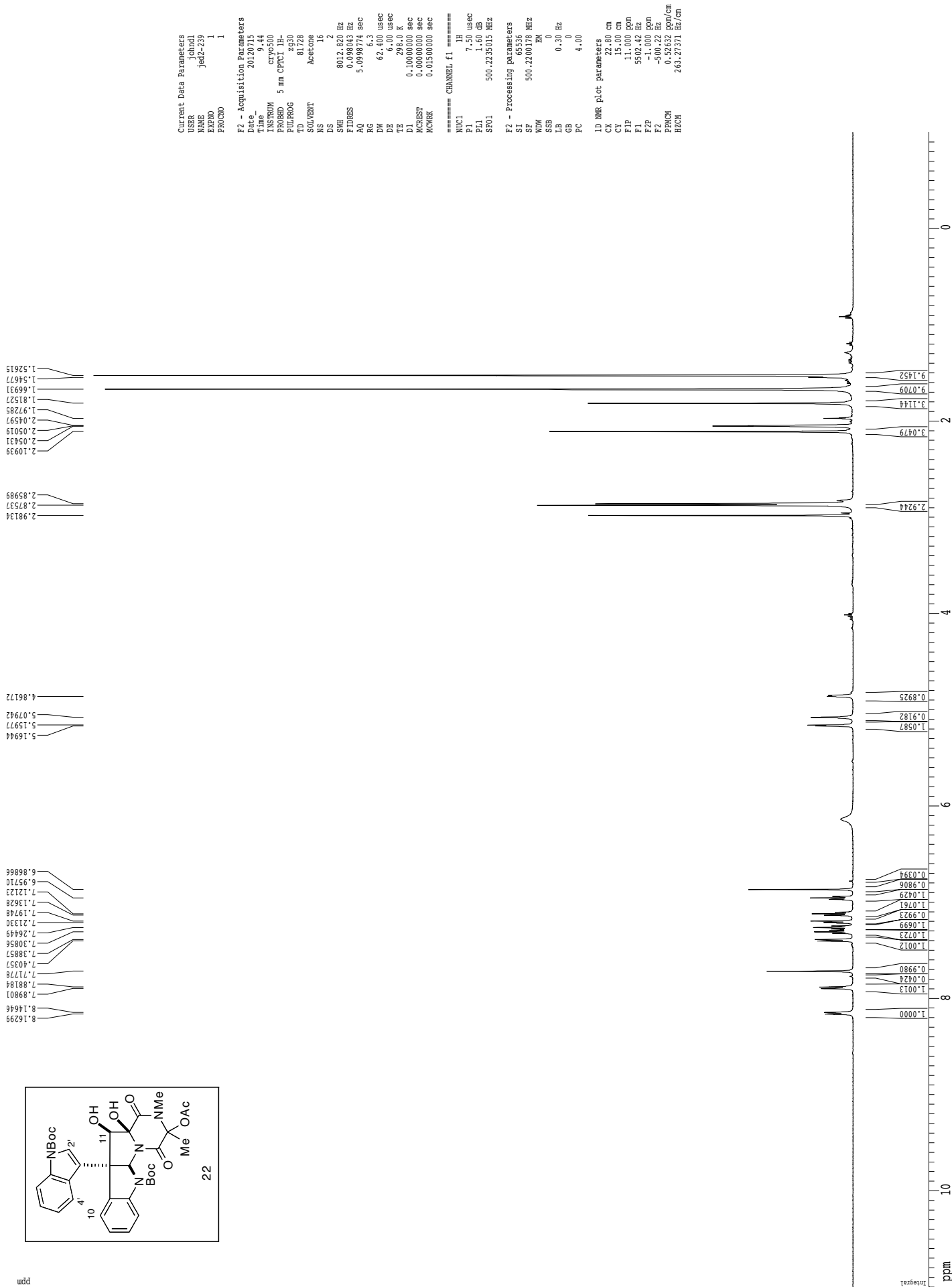
===== CHANNEL f2 =====  
 CDPGRZ wd1615  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR1 0.00 %  
 GSPR2 0.00 %  
 GSPR3 0.00 %  
 GSPR4 0.00 %  
 GSPR5 30.00 %  
 GSPR6 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

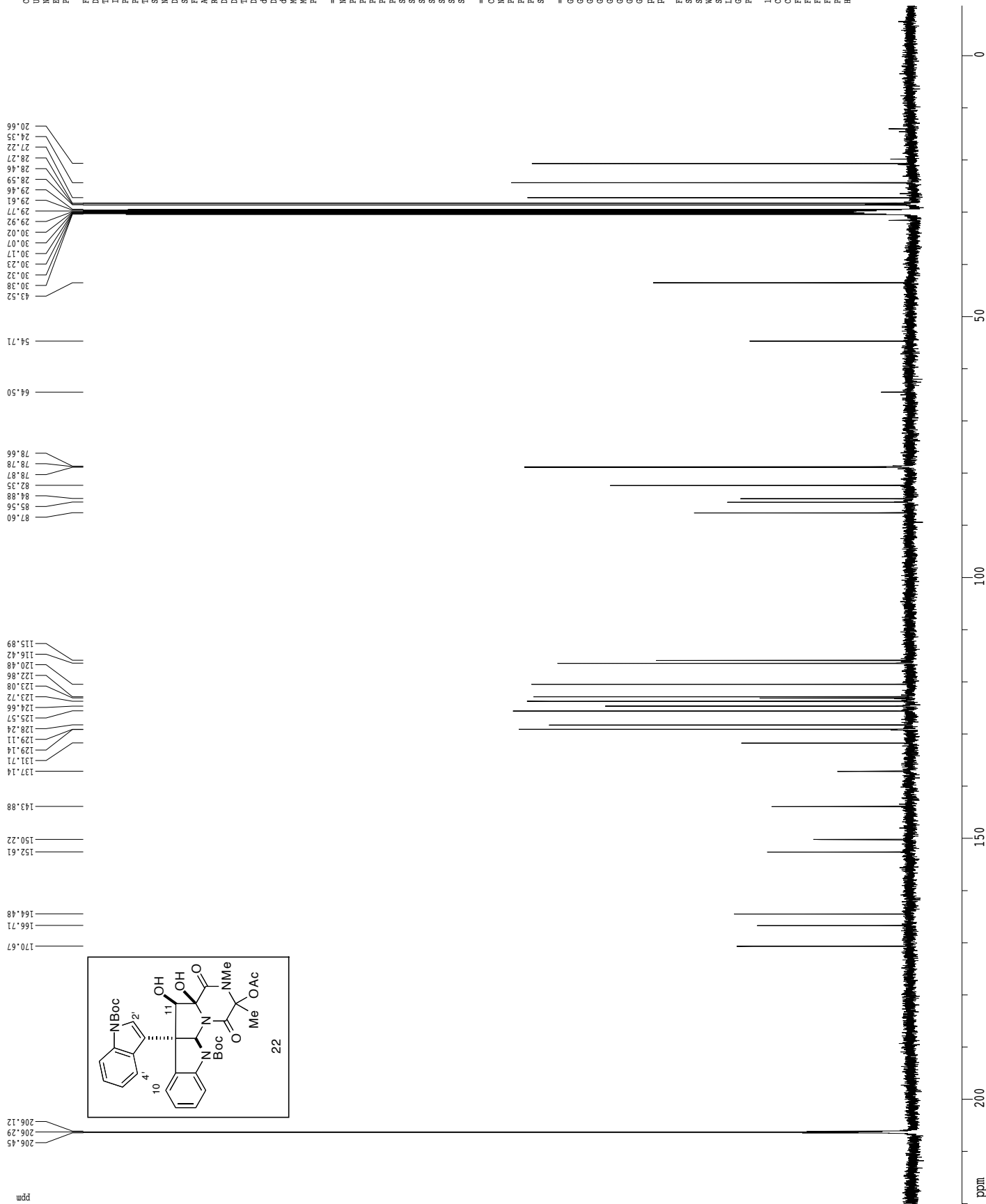
F2 - Processing parameters  
 SI 65536  
 SF 125.7803019 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -10.000 ppm  
 F2 -125.780 Hz  
 F2 1000.000 ppm/cm  
 HPCW 1268.83649 Hz/cm

<sup>1</sup>H spectrum



Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER joundl  
 EXPNO jedz-4.9  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120715  
 Time 10.31  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 1000  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 4597.6  
 DW 6.00 usec  
 DE 298.0 K  
 TE 298.0 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.00015600 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 31.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.7945648 dB  
 PL2 125.7945648 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Ccp60.0.5.20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL f2 =====  
 CDPGRZ wd1cp15  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GRAMZ 0  
 GRAM1 0  
 GRAM2 0  
 GRX1 0.00 %  
 GRX2 0.00 %  
 GRP1 0.00 %  
 GRP2 0.00 %  
 GRZ1 30.00 %  
 GRZ2 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803019 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 2.00

ID WDR plot parameters  
 CX 22.80 cm  
 CY 150.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -10.000 ppm  
 FZ -125.780 Hz  
 FWHM 1.000 ppm/cm  
 HECM 1268.83649 Hz/cm

ppm

200

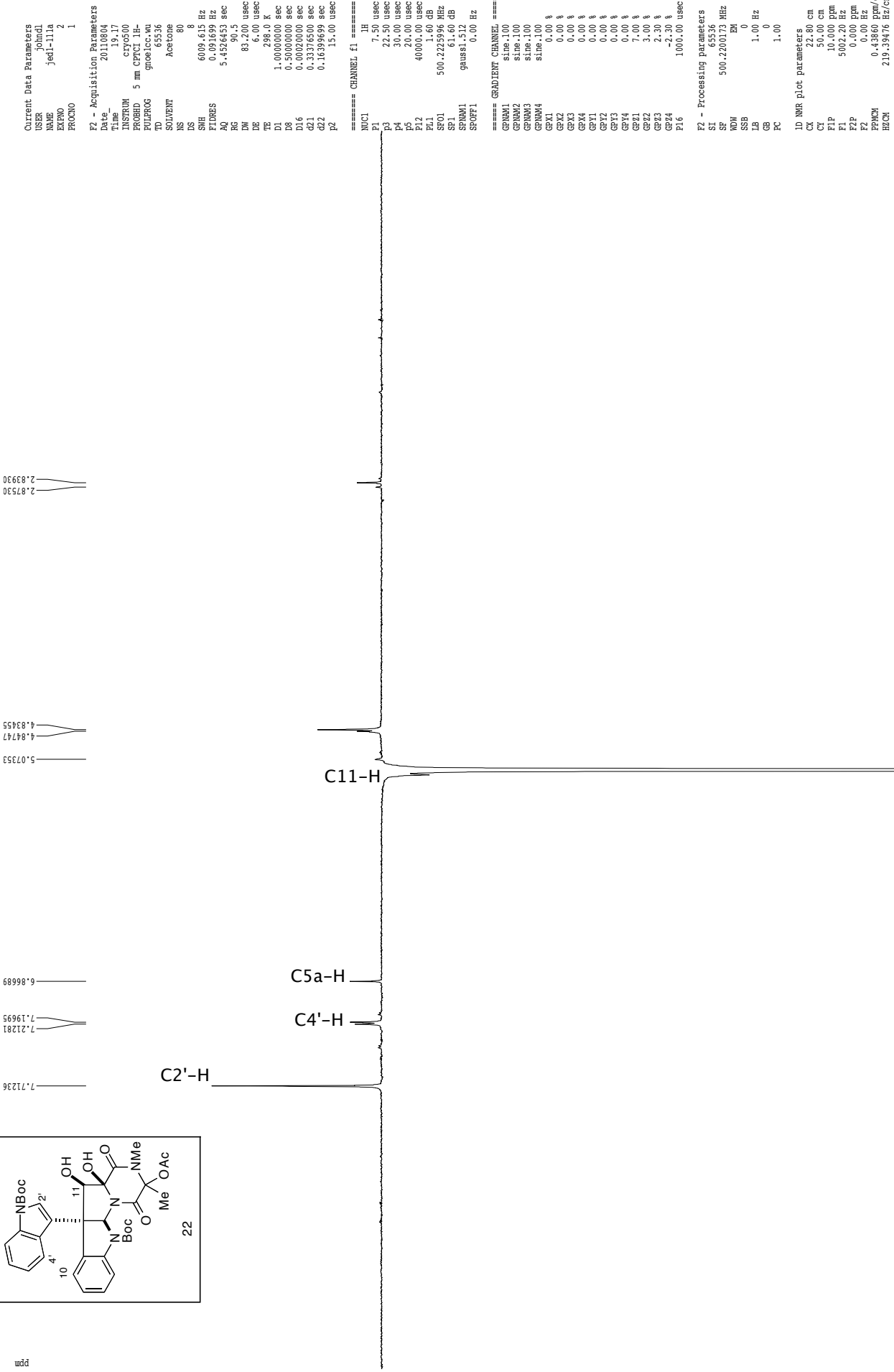
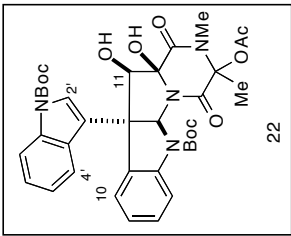
150

100

50

0

gnoe



```

Current Data Parameters
USER      johndl
NAME      jcdl-111a
EXPNO     2
PROCNO    1

F2 - Acquisition Parameters
Date_     20110804
Time      19.17
INSTRUM   cryo500
PROBHD    5 mm CPYCI 1H-
PULPROG   gnoe1cc.wu
TD         65536
SOLVENT   Acetone
NS         80
DS         8
SWH        6009.615 Hz
FIDRES     0.091699 Hz
AQ         5.4526453 sec
RG         99.5
DW         83.200 usec
DE         6.00 usec
TE         298.0 K
D1         1.0000000 sec
D11        0.5000000 sec
D16        0.0002000 sec
d21        0.33376500 sec
d22        0.16396999 sec
p2         15.00 usec

===== CHANNEL f1 =====
NUC1       1H
P1         7.50 usec
P3         22.50 usec
P4         30.00 usec
P5         20.00 usec
P12        40000.00 usec
PL1        1.60 dB
SFO1       500.2225996 MHz
SF1        61.60 GB
SFOFF1     0.00 Hz

===== GRADIENT CHANNEL =====
GEM11     sine.100
GEM12     sine.100
GEM13     sine.100
GEM14     sine.100
GFX1      0.00 %
GFX2      0.00 %
GFX3      0.00 %
GFX4      0.00 %
GFY1      0.00 %
GFY2      0.00 %
GFY3      0.00 %
GFY4      0.00 %
GZ1       7.00 %
GZ2       3.00 %
GZ3       2.30 %
GZ4       -2.30 %
F16       1000.00 usec

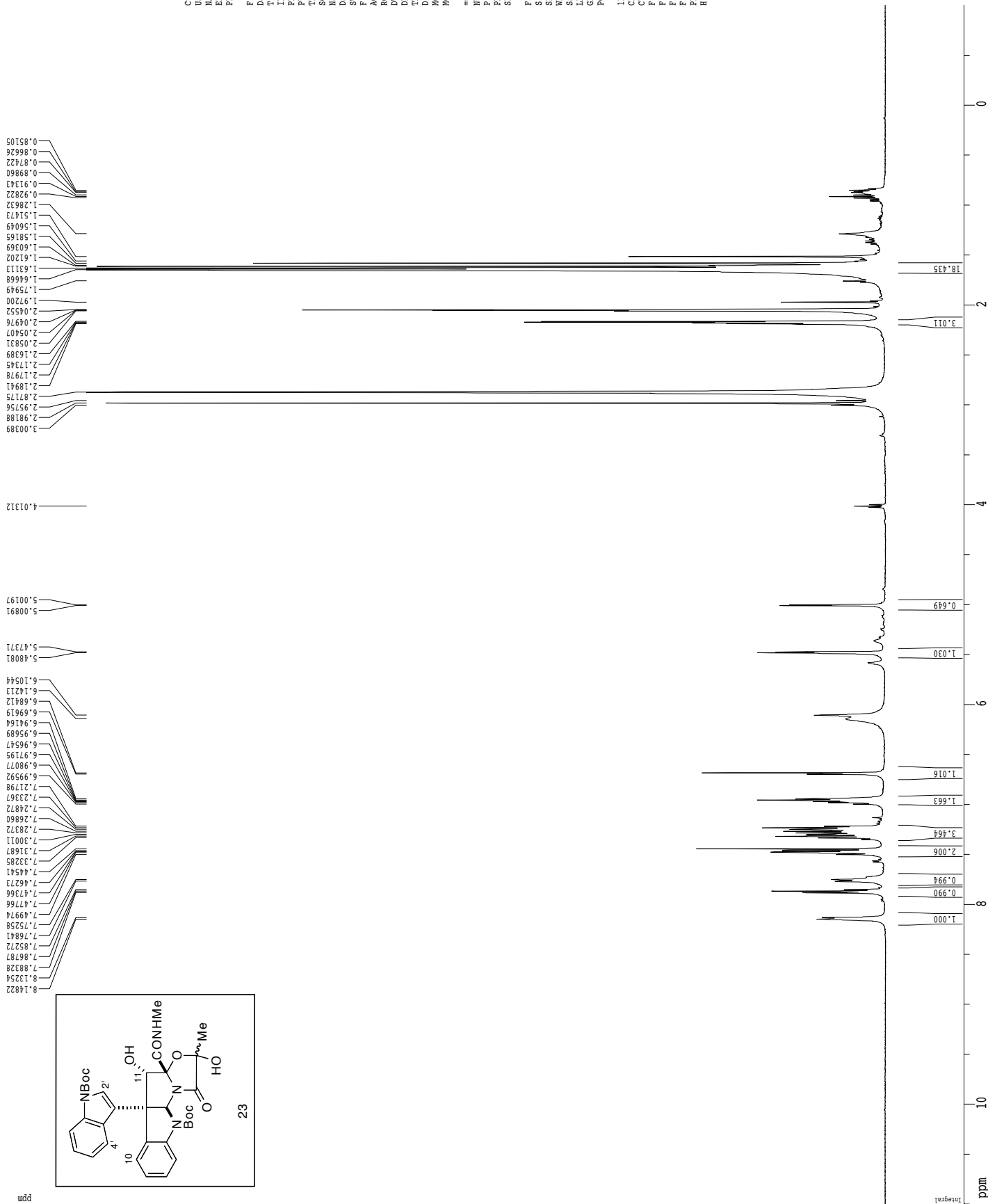
F2 - Processing Parameters
SI         65536
SF         500.2200173 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.00

ID NMR plot parameters
CX         22.80 cm
CY         50.00 cm
F1P        10.000 ppm
F1         5002.20 Hz
F2P        0.000 ppm
F2         0.00 Hz
FREQMCH    0.4396 ppm/cm
HZCM       219.39496 Hz/cm
    
```

Integral

ppm

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jes2-219  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120715  
 Time 14.04  
 INSTRUM cryo500  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 63  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

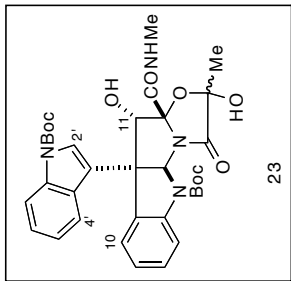
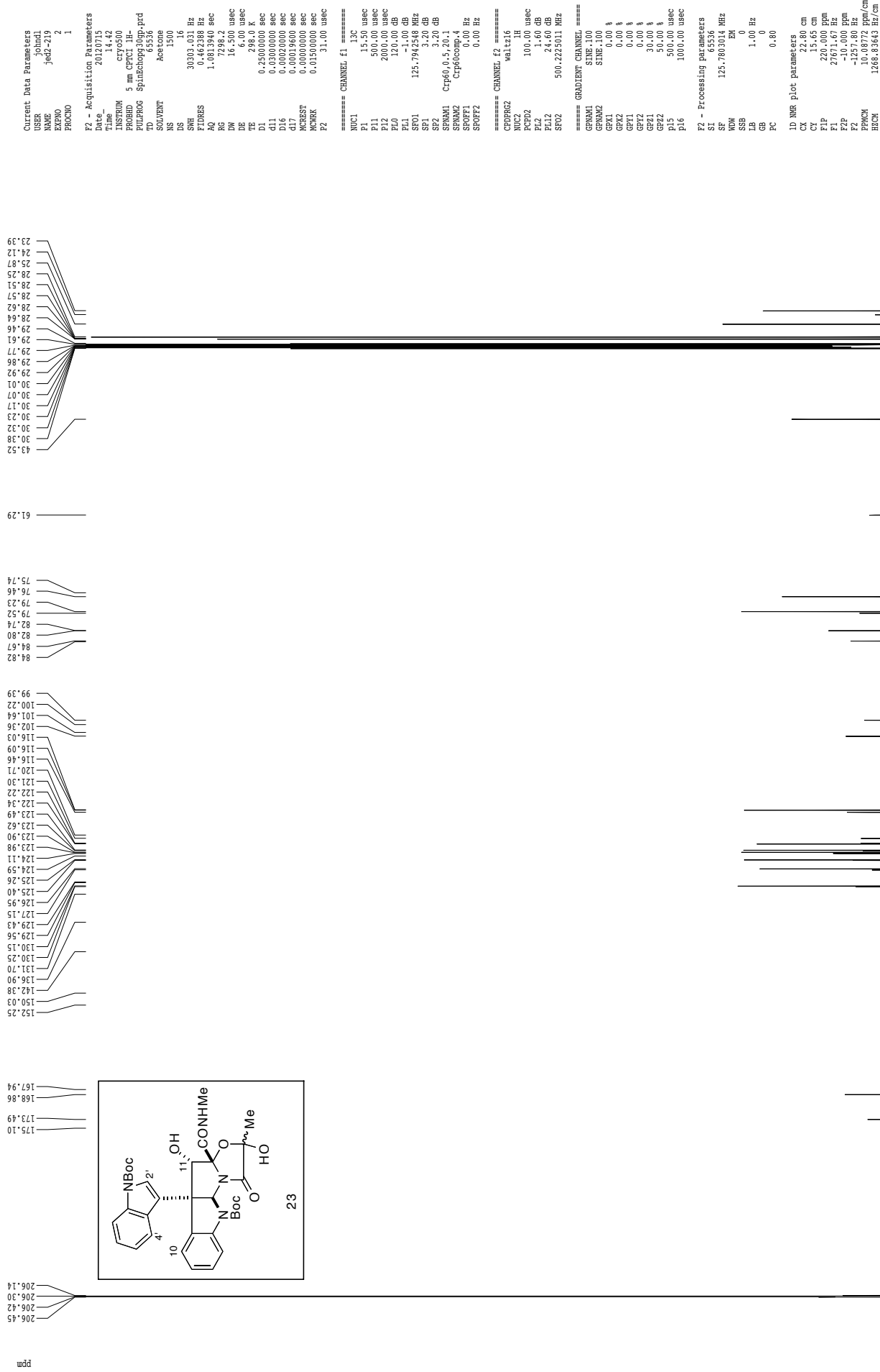
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220181 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 11.000 ppm  
 F1 590.242 Hz  
 F2 10.000 ppm  
 F3 -500.92 ppm  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

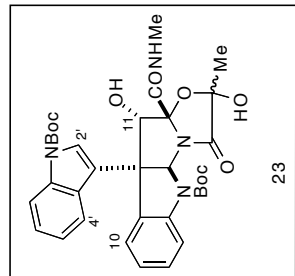


Z-restored spin-echo 13C spectrum with 1H decoupling



206.45  
206.42  
206.30  
206.14  
175.10  
173.49  
168.86  
167.94  
152.25  
150.03  
142.38  
136.90  
131.70  
130.25  
130.15  
129.56  
129.43  
127.15  
126.95  
125.40  
125.26  
124.11  
123.98  
123.90  
123.82  
123.49  
122.24  
122.22  
121.32  
121.30  
120.71  
116.46  
116.09  
102.36  
101.64  
100.22  
99.39  
84.82  
84.67  
82.80  
82.74  
79.23  
79.22  
76.46  
75.74  
61.29  
43.52  
30.38  
30.32  
30.23  
30.17  
30.07  
30.01  
29.92  
29.77  
29.66  
29.61  
28.64  
28.57  
28.42  
28.21  
28.12  
27.97  
24.12

gnoe



Current Data Parameters  
 USER JohnHJ  
 NAME jedz-2.1j  
 EXPNO 6  
 PROCNO 1

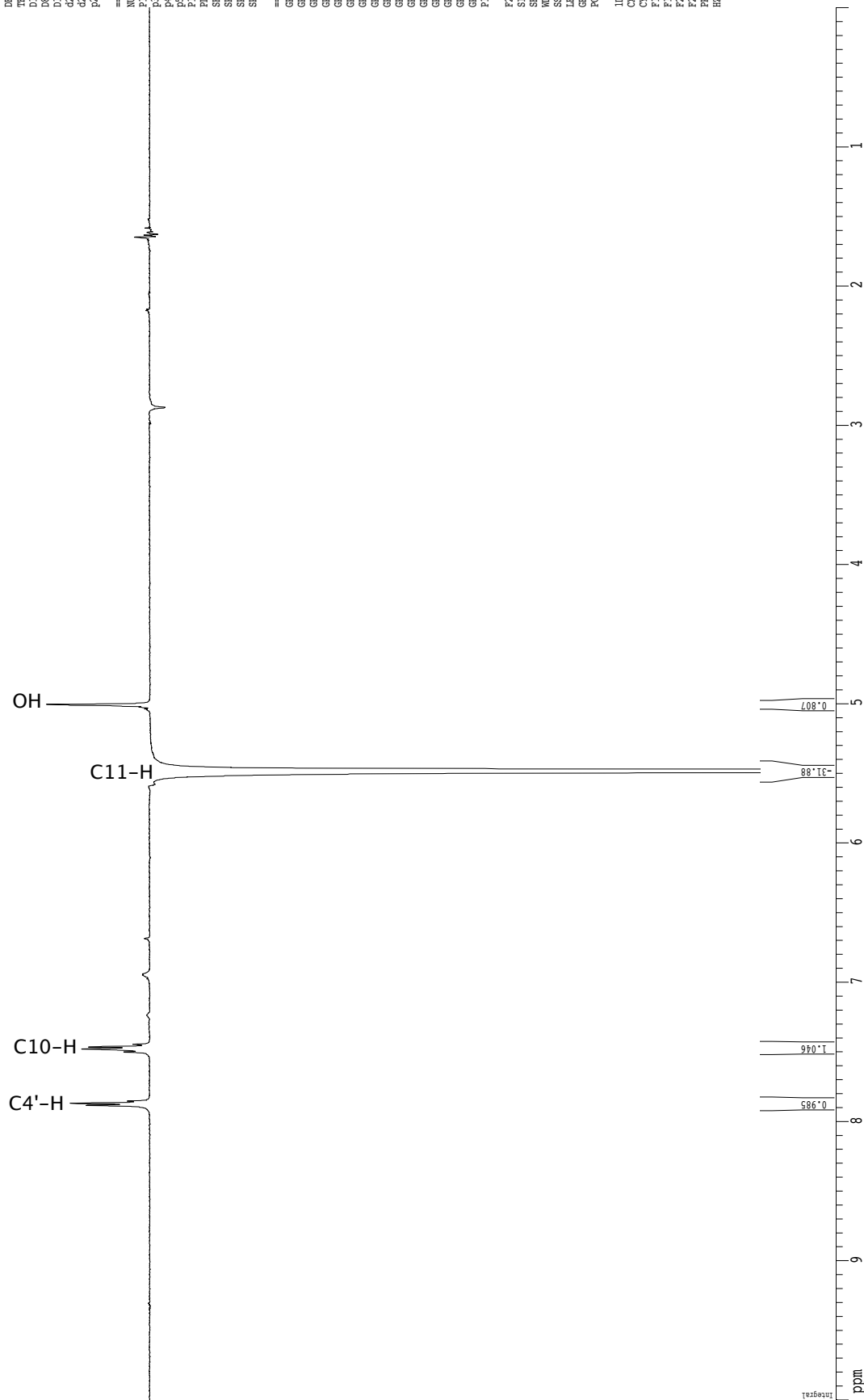
F2 - Acquisition Parameters  
 Date\_ 20120715  
 Time\_ 15.17  
 INSTRUM cryo500  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG gnoe1cc.wu  
 TD 65536  
 SOLVENT CDCl3  
 NS 56  
 DS 8  
 SWH 5482.456 Hz  
 FIDRES 0.083656 Hz  
 AQ 5.5769330 sec  
 RG 101.6  
 DW 91.200 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.000000 sec  
 D11 0.500000 sec  
 D16 0.002000 sec  
 d21 0.3337690 sec  
 d22 0.1639699 sec  
 p2 15.00 usec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 P2 22.50 usec  
 P3 30.00 usec  
 P4 20.00 usec  
 P5 40000.00 usec  
 P12 1.60 dB  
 P11 500.2227591 MHz  
 SF1 61.60 GB  
 SP1 gauss1.512  
 SFOFF1 0.00 Hz

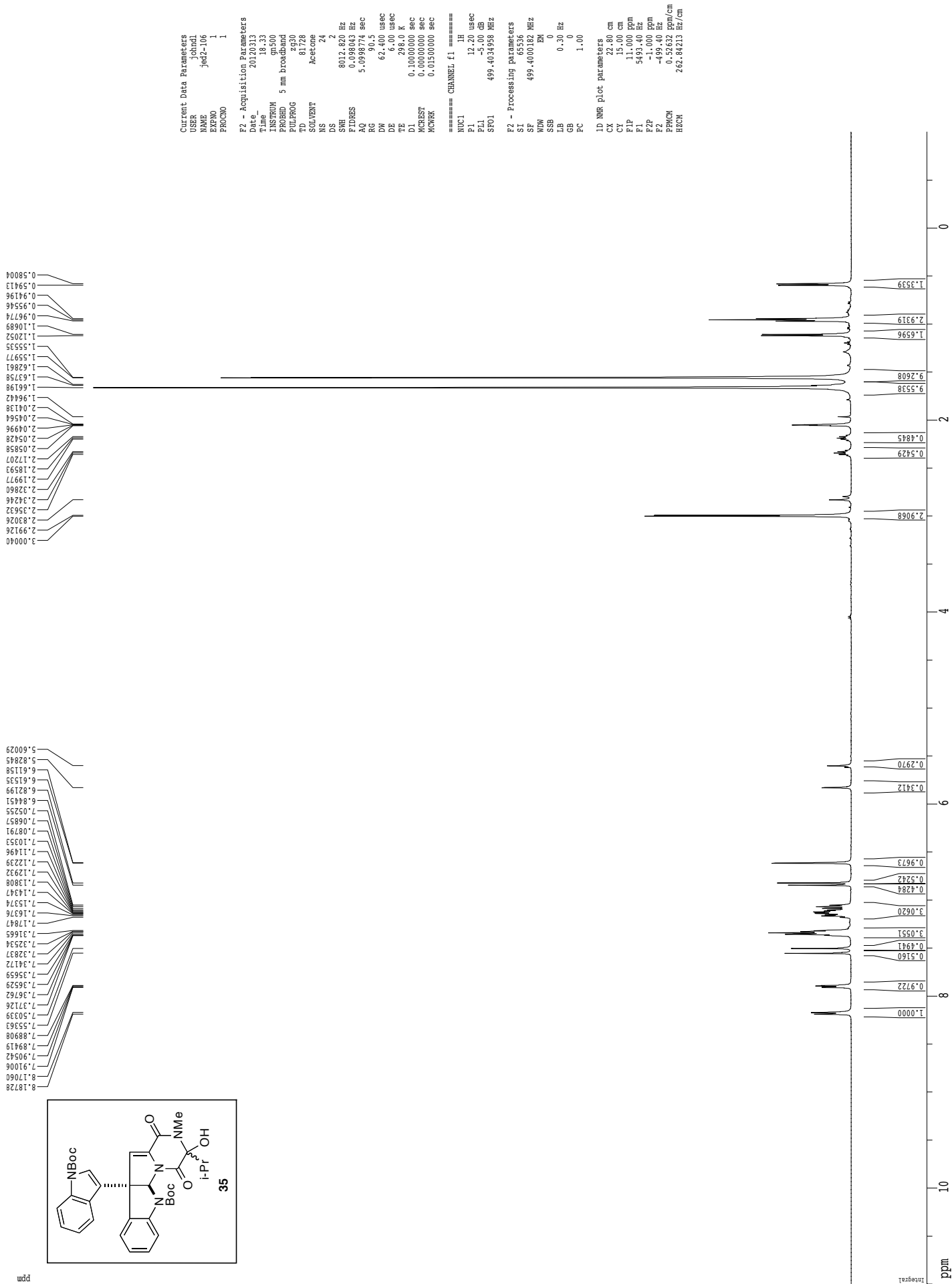
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 GENAM1 sine.100  
 GENAM2 sine.100  
 GENAM3 sine.100  
 GENAM4 sine.100  
 GFX1 0.00 %  
 GFX2 0.00 %  
 GFX3 0.00 %  
 GFX4 0.00 %  
 GFY1 0.00 %  
 GFY2 0.00 %  
 GFY3 0.00 %  
 GFY4 0.00 %  
 GZ1 7.00 %  
 GZ2 3.00 %  
 GZ3 2.30 %  
 GZ4 -2.30 %  
 F16 1000.00 usec

F2 - Processing Parameters  
 SI 65536  
 SF 500.2200180 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

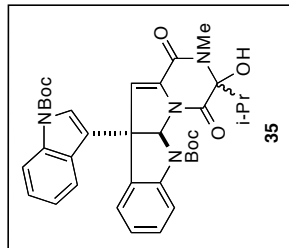
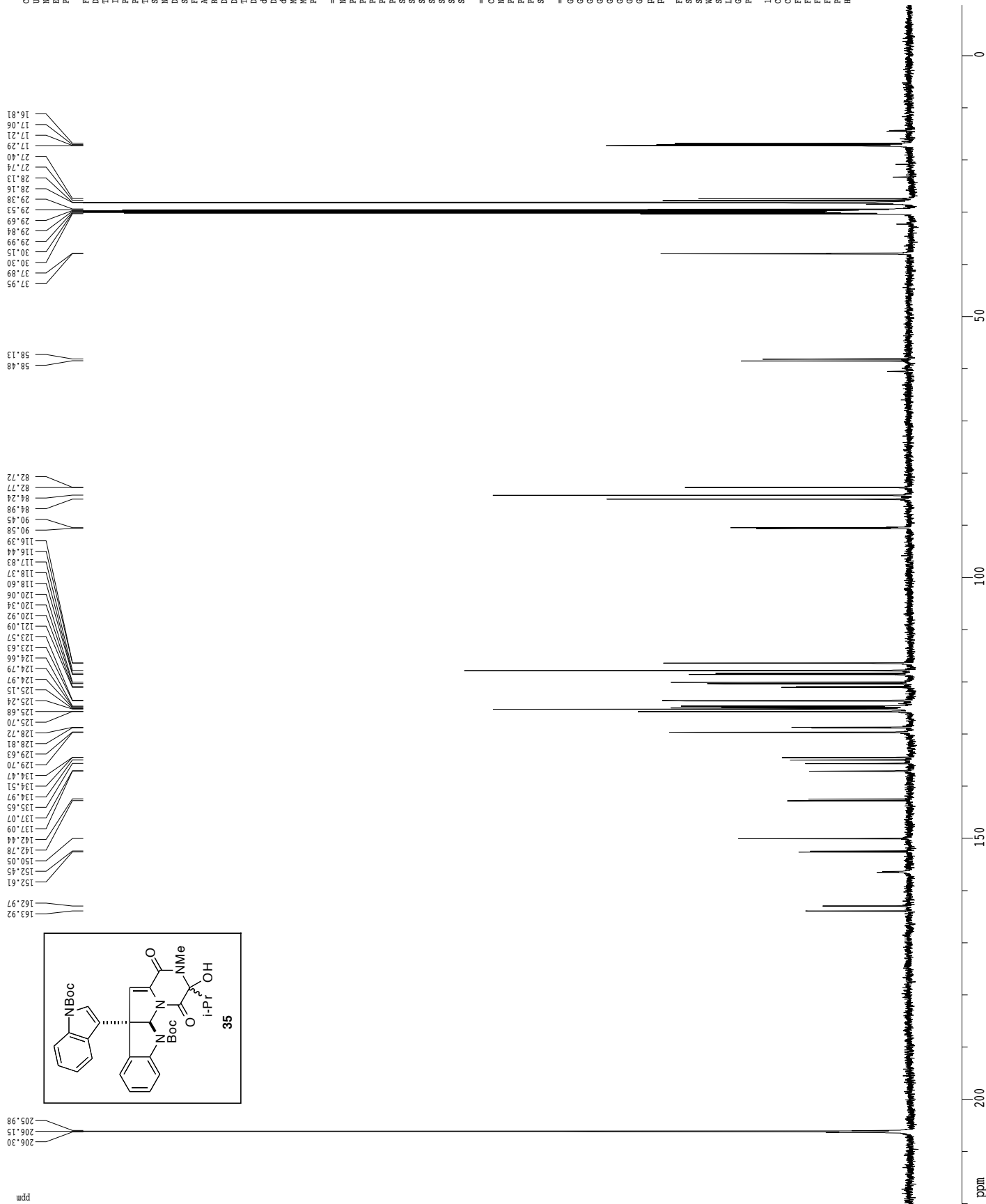
ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 10.000 ppm  
 F1 5002.20 Hz  
 F2 0.000 ppm  
 F3 0.00 Hz  
 F4 0.439 ppm/cm  
 HZCM 219.39476 Hz/cm



## 1H spectrum



Z-restored spin-echo <sup>13</sup>C spectrum with <sup>1</sup>H decoupling



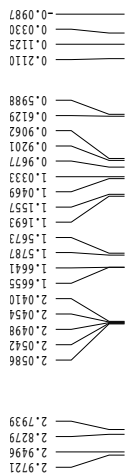
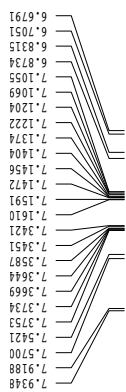
Current Data Parameters  
 USER jomdl  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120313  
 Time 15.46  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 320  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813941 sec  
 RG 432  
 DR 6.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.50000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACQRESF 0.00000000 sec  
 ACQBRK 0.01500000 sec  
 F2 31.00 usec

===== CHANNEL f1 =====  
 NUC1 <sup>13</sup>C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.7947548 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60.05, 20.1  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL f2 =====  
 NUC2 <sup>1</sup>H  
 P2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz  
 ===== GRADIENT CHANNEL =====  
 GSPR1 100.00 usec  
 GSPR2 510.00 usec  
 GFL1 0.00 %  
 GFL2 0.00 %  
 GFL3 0.00 %  
 GFL4 0.00 %  
 GFL5 30.00 %  
 GFL6 50.00 %  
 GFL7 100.00 usec  
 GFL8 100.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803184 MHz  
 WDW EM  
 SSB 0  
 LB 2.00 Hz  
 GB 0  
 PC 0.20  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 75.00 cm  
 FIP 220.000 ppm  
 F1 2767.167 Hz  
 F2 -10.000 ppm  
 F2 -125.780 Hz  
 F2 100.625 Hz/cm  
 HZCM 1268.83655 Hz/cm

<sup>1</sup>H spectrum



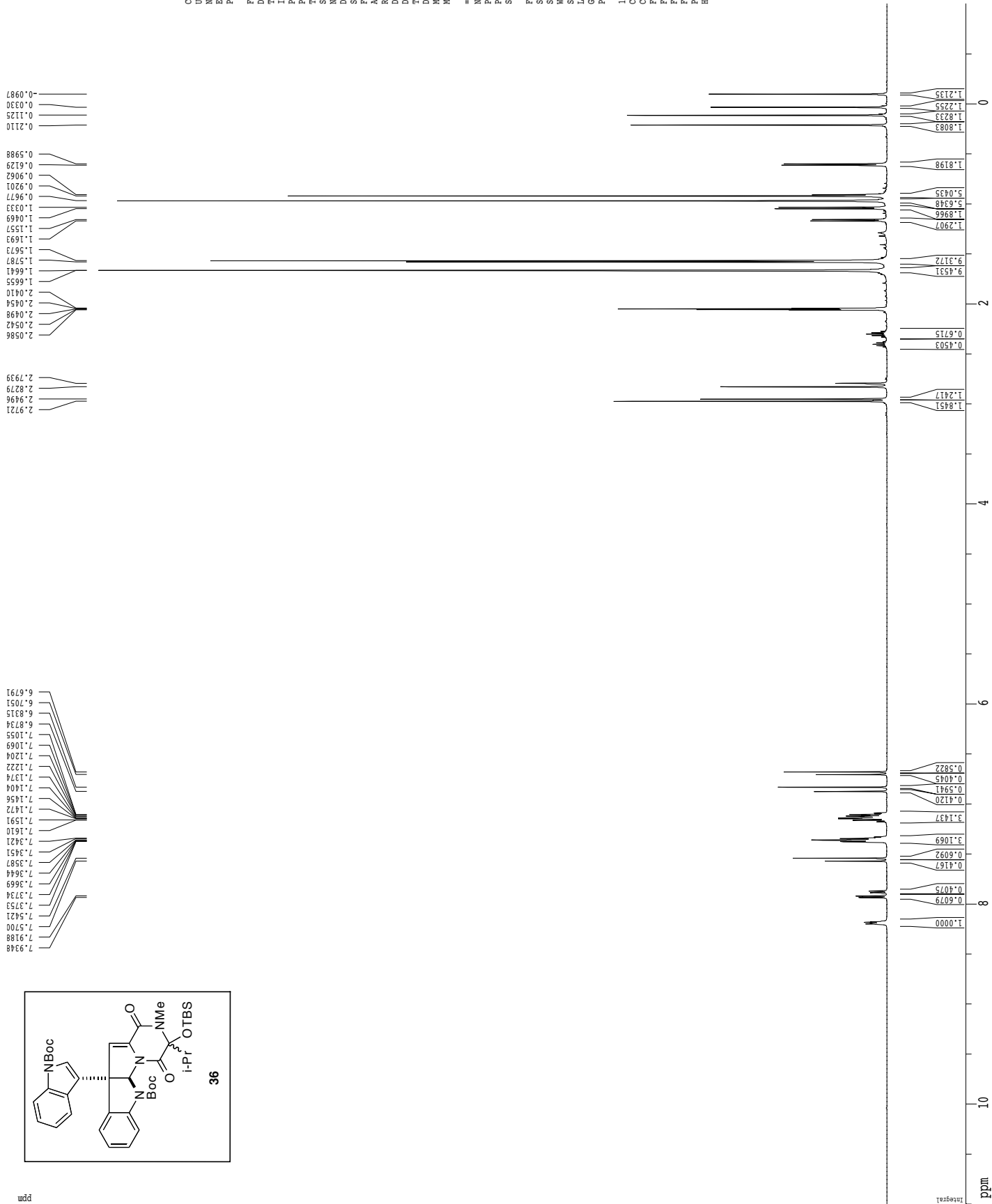
Current Data Parameters  
 USER JohnDl  
 NAME Jesk2-109  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120316  
 Time 13.44  
 INSTRUM cryo500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0996774 sec  
 RG 62.01  
 DW 6.00 usec  
 DE 288.0 K  
 TE 0.10000000 sec  
 D1 0.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

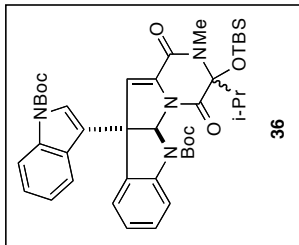
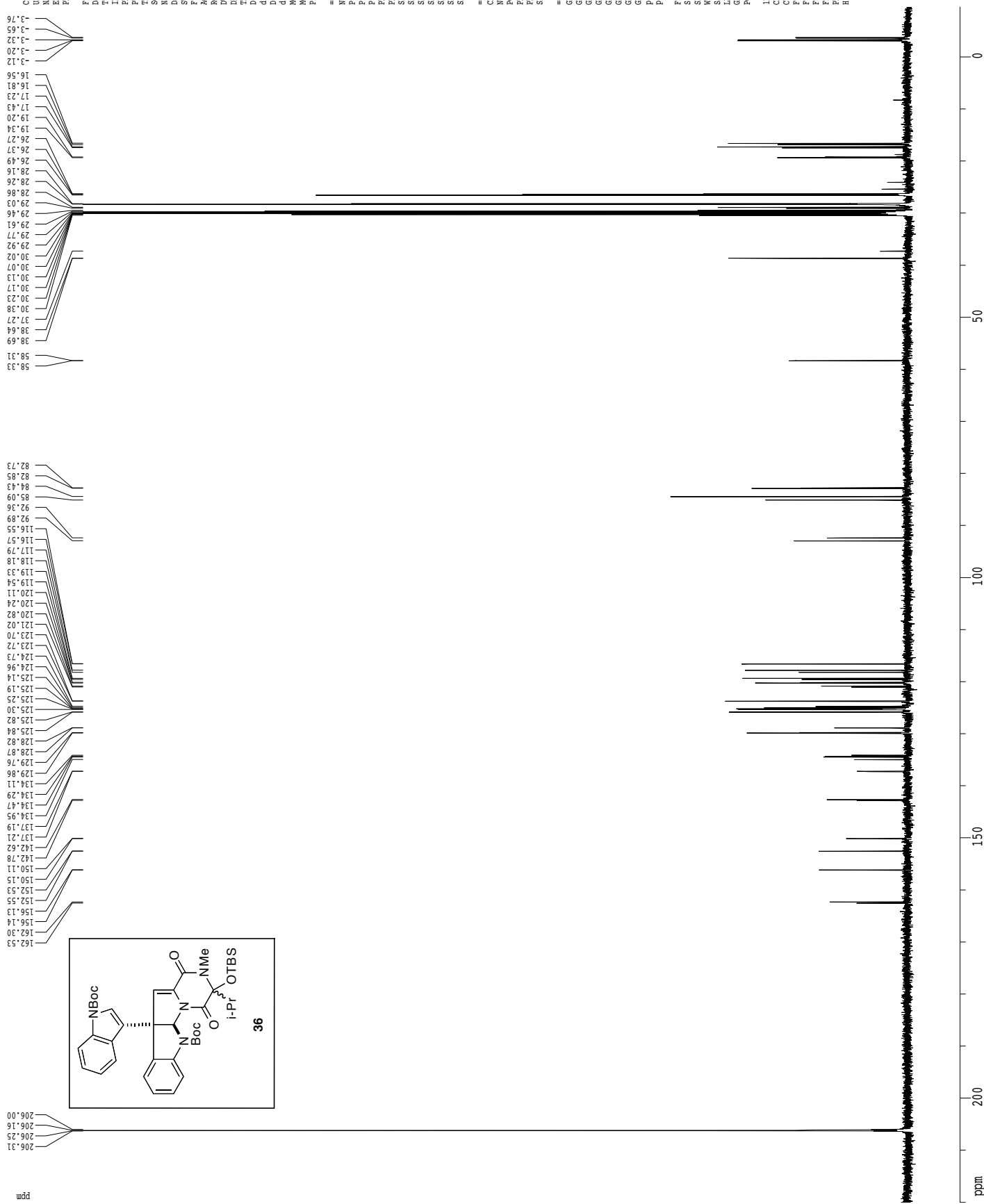
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.220183 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 590.242 Hz  
 F3 10.000 ppm  
 FZ -50.92  
 PPM0 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



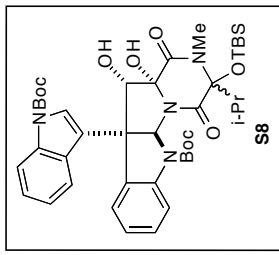
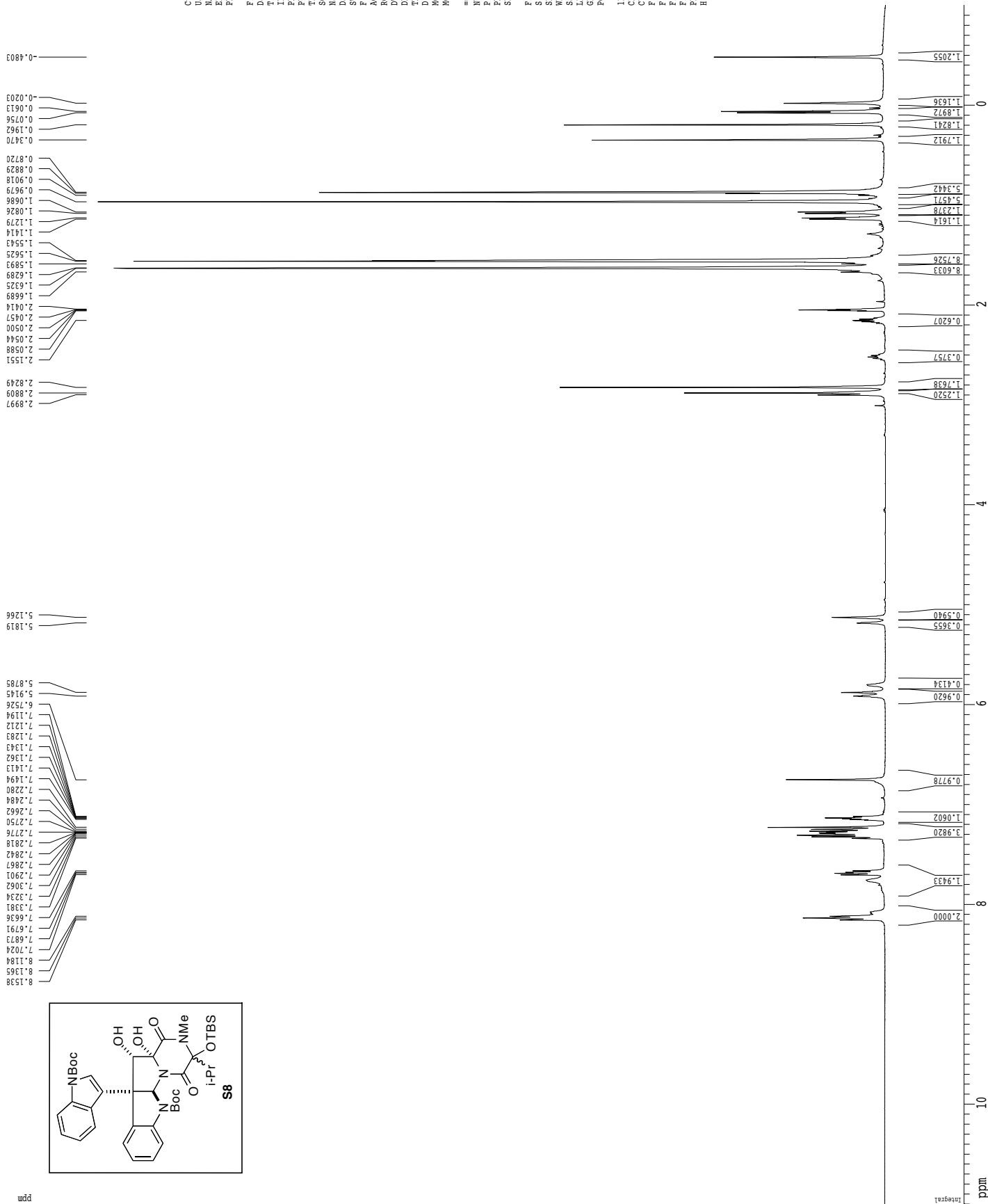
Current Data Parameters  
 USER jomdl  
 JUNIT jed-102  
 EXNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120316  
 Time 15:58  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 216  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 572.6  
 NG 16  
 DR 6.00 usec  
 DE 298.2 K  
 TE 298.2 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.00015600 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 3.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 P12 2000.00 usec  
 PL2 120.00 dB  
 P13 125.7947548 Hz  
 SFO1 500.1362997 MHz  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO2 500.2225011 MHz  
 SFO3 500.2225011 MHz  
 SFO4 500.2225011 MHz  
 SFO5 500.2225011 MHz  
 SFO6 500.2225011 MHz  
 SFO7 500.2225011 MHz  
 SFO8 500.2225011 MHz  
 SFO9 500.2225011 MHz  
 SFO10 500.2225011 MHz  
 SFO11 500.2225011 MHz  
 SFO12 500.2225011 MHz  
 SFO13 500.2225011 MHz  
 SFO14 500.2225011 MHz  
 SFO15 500.2225011 MHz  
 SFO16 500.2225011 MHz  
 SFO17 500.2225011 MHz  
 SFO18 500.2225011 MHz  
 SFO19 500.2225011 MHz  
 SFO20 500.2225011 MHz  
 SFO21 500.2225011 MHz  
 SFO22 500.2225011 MHz  
 SFO23 500.2225011 MHz  
 SFO24 500.2225011 MHz  
 SFO25 500.2225011 MHz  
 SFO26 500.2225011 MHz  
 SFO27 500.2225011 MHz  
 SFO28 500.2225011 MHz  
 SFO29 500.2225011 MHz  
 SFO30 500.2225011 MHz  
 SFO31 500.2225011 MHz  
 SFO32 500.2225011 MHz  
 SFO33 500.2225011 MHz  
 SFO34 500.2225011 MHz  
 SFO35 500.2225011 MHz  
 SFO36 500.2225011 MHz  
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 SFO38 500.2225011 MHz  
 SFO39 500.2225011 MHz  
 SFO40 500.2225011 MHz  
 SFO41 500.2225011 MHz  
 SFO42 500.2225011 MHz  
 SFO43 500.2225011 MHz  
 SFO44 500.2225011 MHz  
 SFO45 500.2225011 MHz  
 SFO46 500.2225011 MHz  
 SFO47 500.2225011 MHz  
 SFO48 500.2225011 MHz  
 SFO49 500.2225011 MHz  
 SFO50 500.2225011 MHz  
 SFO51 500.2225011 MHz  
 SFO52 500.2225011 MHz  
 SFO53 500.2225011 MHz  
 SFO54 500.2225011 MHz  
 SFO55 500.2225011 MHz  
 SFO56 500.2225011 MHz  
 SFO57 500.2225011 MHz  
 SFO58 500.2225011 MHz  
 SFO59 500.2225011 MHz  
 SFO60 500.2225011 MHz  
 SFO61 500.2225011 MHz  
 SFO62 500.2225011 MHz  
 SFO63 500.2225011 MHz  
 SFO64 500.2225011 MHz  
 SFO65 500.2225011 MHz  
 SFO66 500.2225011 MHz  
 SFO67 500.2225011 MHz  
 SFO68 500.2225011 MHz  
 SFO69 500.2225011 MHz  
 SFO70 500.2225011 MHz  
 SFO71 500.2225011 MHz  
 SFO72 500.2225011 MHz  
 SFO73 500.2225011 MHz  
 SFO74 500.2225011 MHz  
 SFO75 500.2225011 MHz  
 SFO76 500.2225011 MHz  
 SFO77 500.2225011 MHz  
 SFO78 500.2225011 MHz  
 SFO79 500.2225011 MHz  
 SFO80 500.2225011 MHz  
 SFO81 500.2225011 MHz  
 SFO82 500.2225011 MHz  
 SFO83 500.2225011 MHz  
 SFO84 500.2225011 MHz  
 SFO85 500.2225011 MHz  
 SFO86 500.2225011 MHz  
 SFO87 500.2225011 MHz  
 SFO88 500.2225011 MHz  
 SFO89 500.2225011 MHz  
 SFO90 500.2225011 MHz  
 SFO91 500.2225011 MHz  
 SFO92 500.2225011 MHz  
 SFO93 500.2225011 MHz  
 SFO94 500.2225011 MHz  
 SFO95 500.2225011 MHz  
 SFO96 500.2225011 MHz  
 SFO97 500.2225011 MHz  
 SFO98 500.2225011 MHz  
 SFO99 500.2225011 MHz  
 SFO100 500.2225011 MHz

ppm

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jes2-111  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120319  
 Time 11.22  
 INSTRUM cryo500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099874 sec  
 RG 307  
 DR 62.600 usec  
 DE 6.600 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220183 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

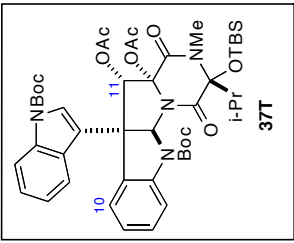
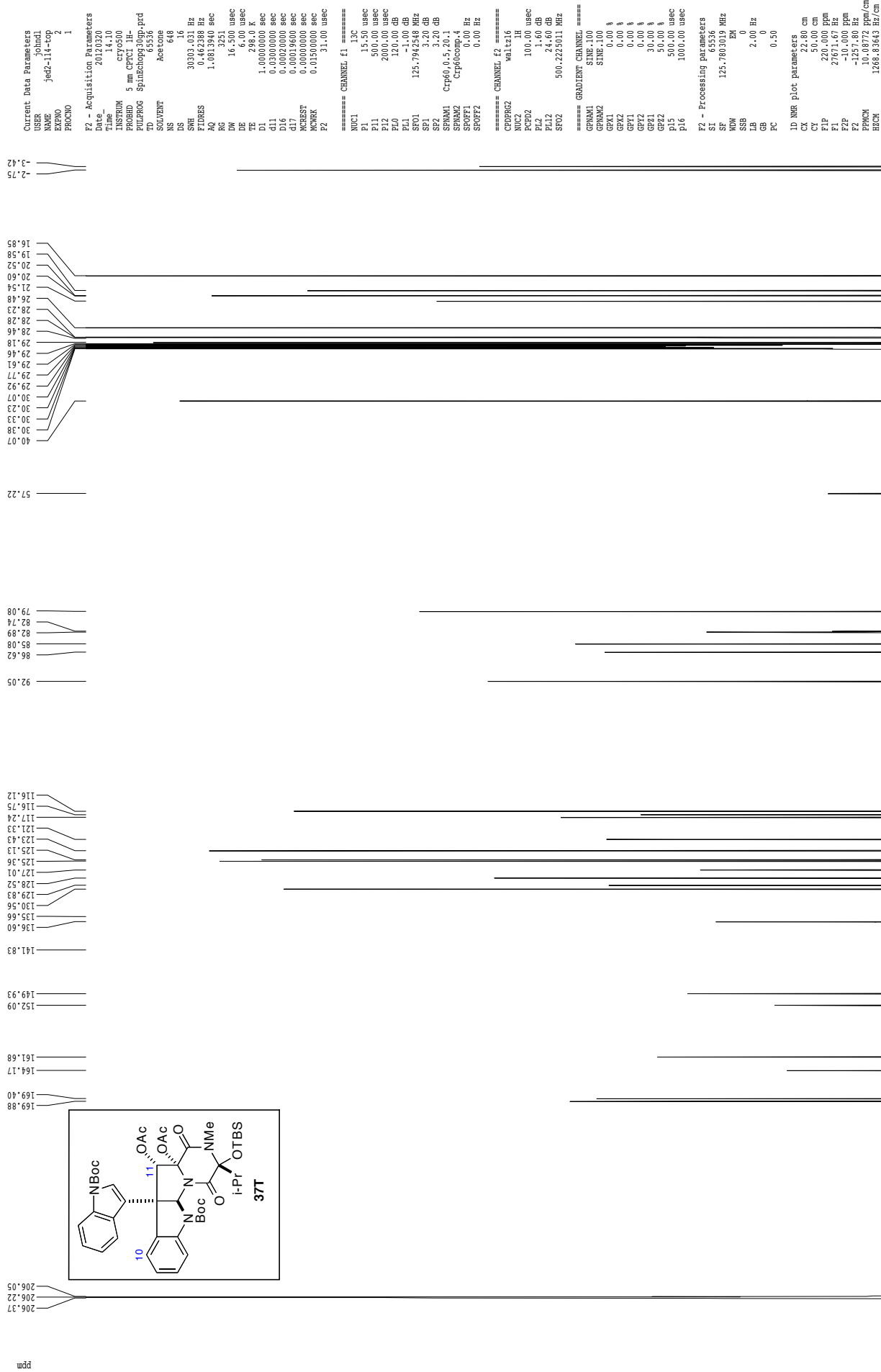
1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 5902.82 Hz  
 F2 500.220183 MHz  
 F2 -500.92 MHz  
 PRMCM 0.52632 ppm/cm  
 HZCM 263.27371 Hz/cm



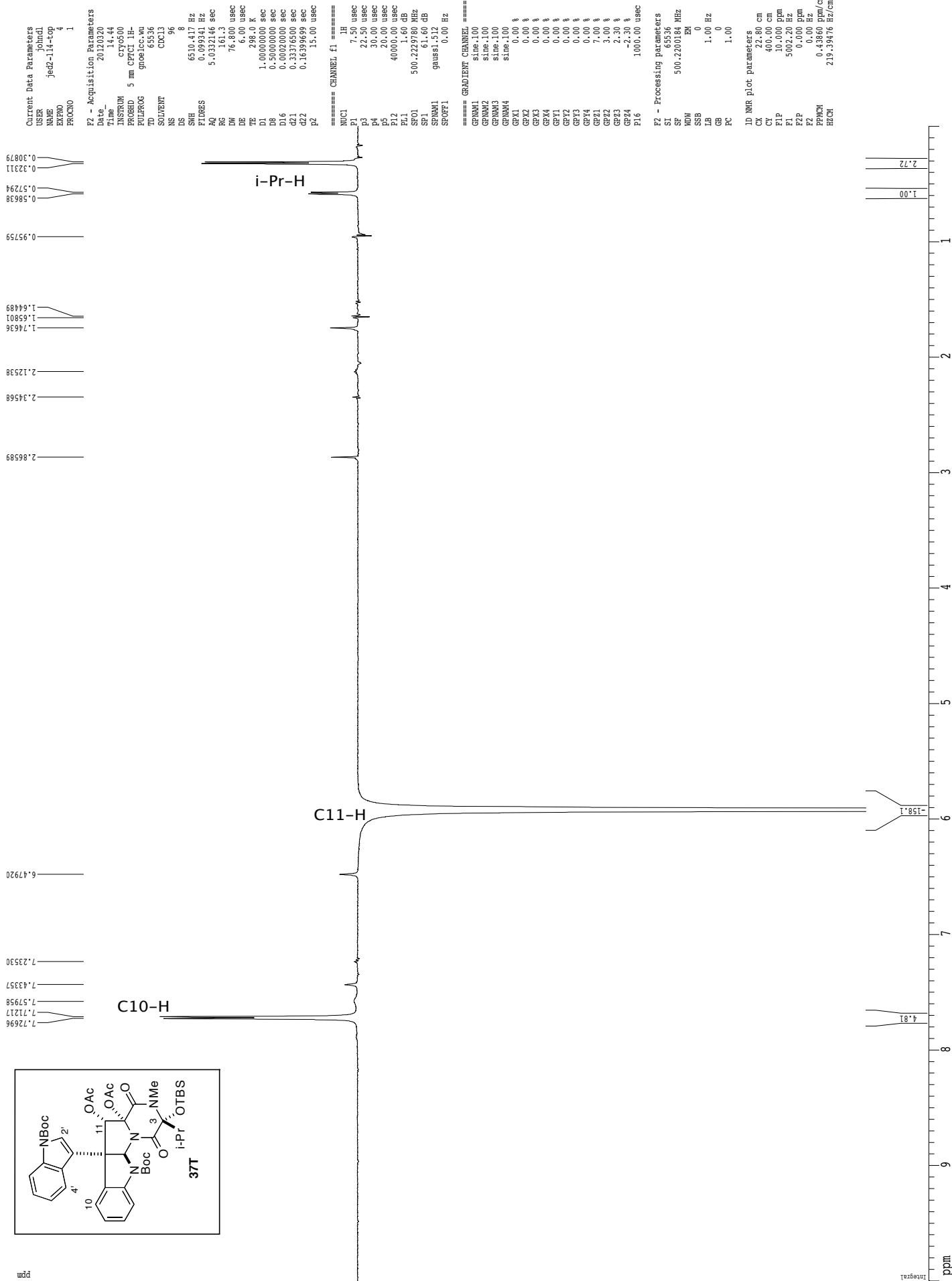
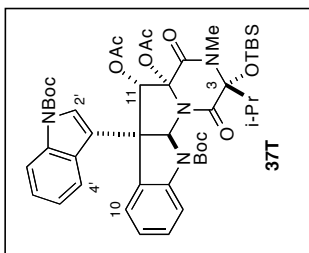




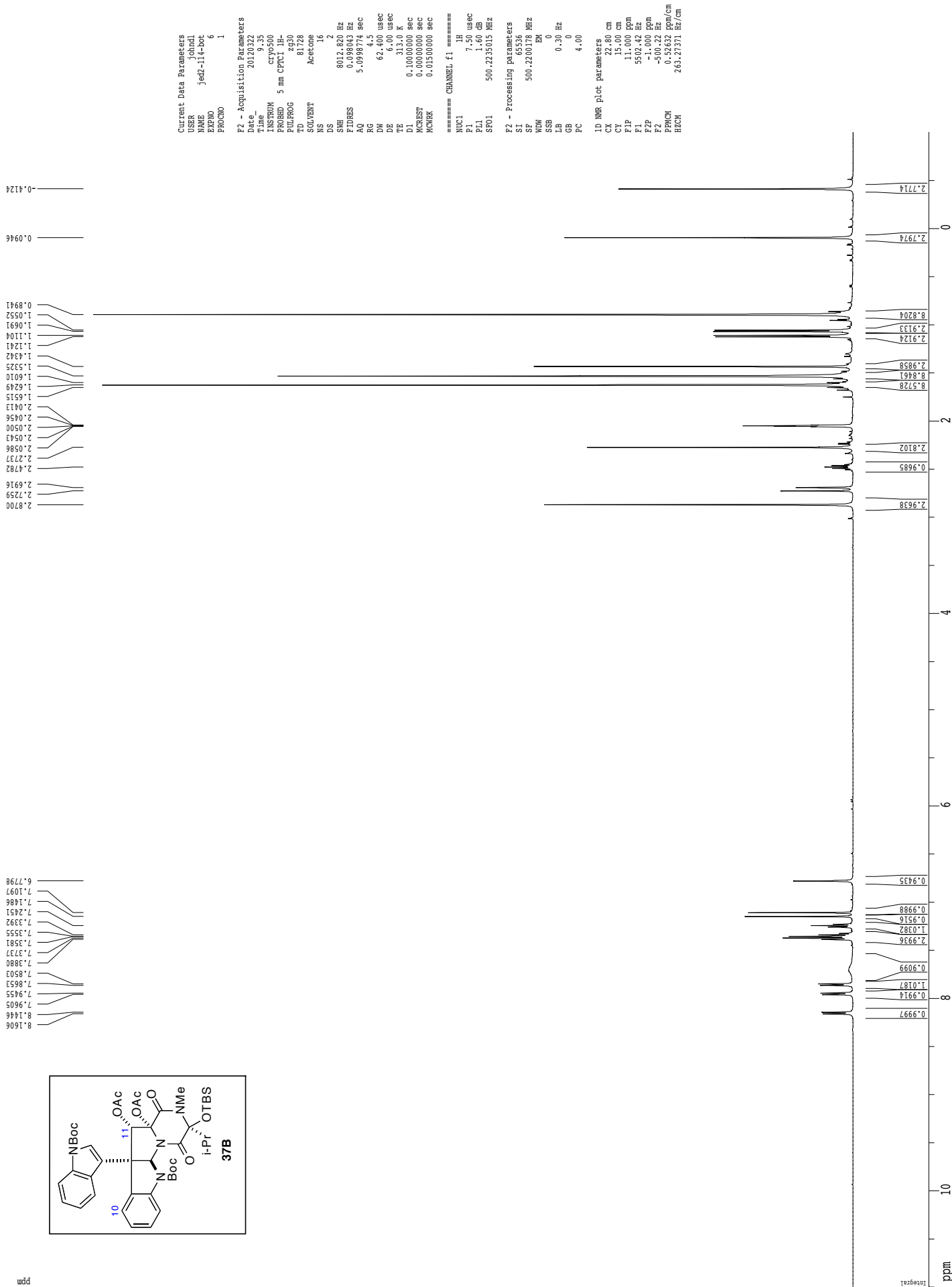
Z-restored spin-echo 13C spectrum with 1H decoupling



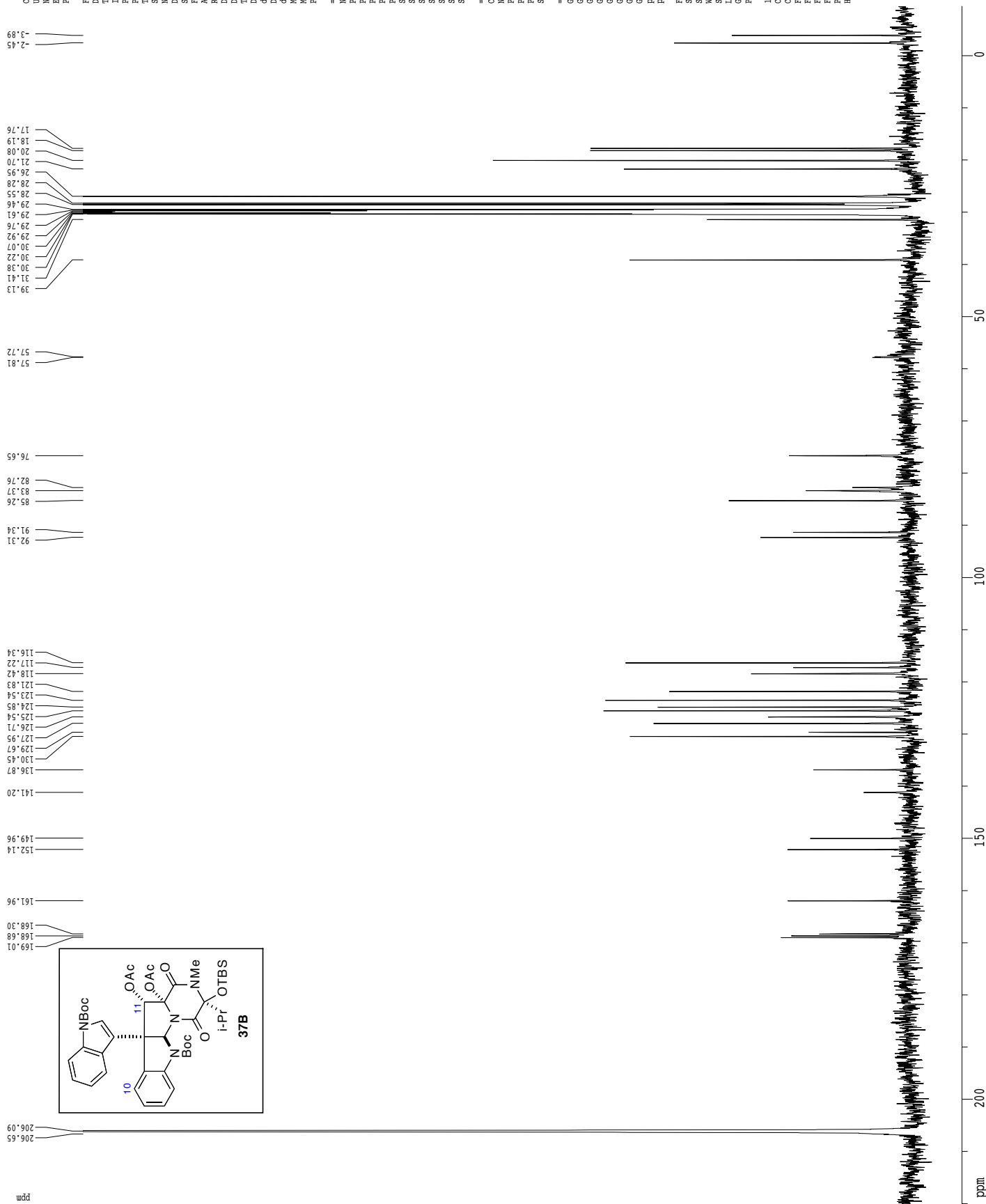
gnoe



<sup>1</sup>H spectrum



Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jound1  
 EXPNO jed3-114-467  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120322  
 Time 9:38  
 INSTRUM cryo500  
 PROBHD 5 mm CPACI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 608  
 DS 16  
 SHF 303.03 Hz  
 FIDRES 0.46238 Hz  
 AQ 1.081394 sec  
 RG 432  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 313.0 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.0001500 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 3.00 usec

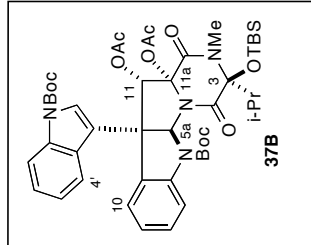
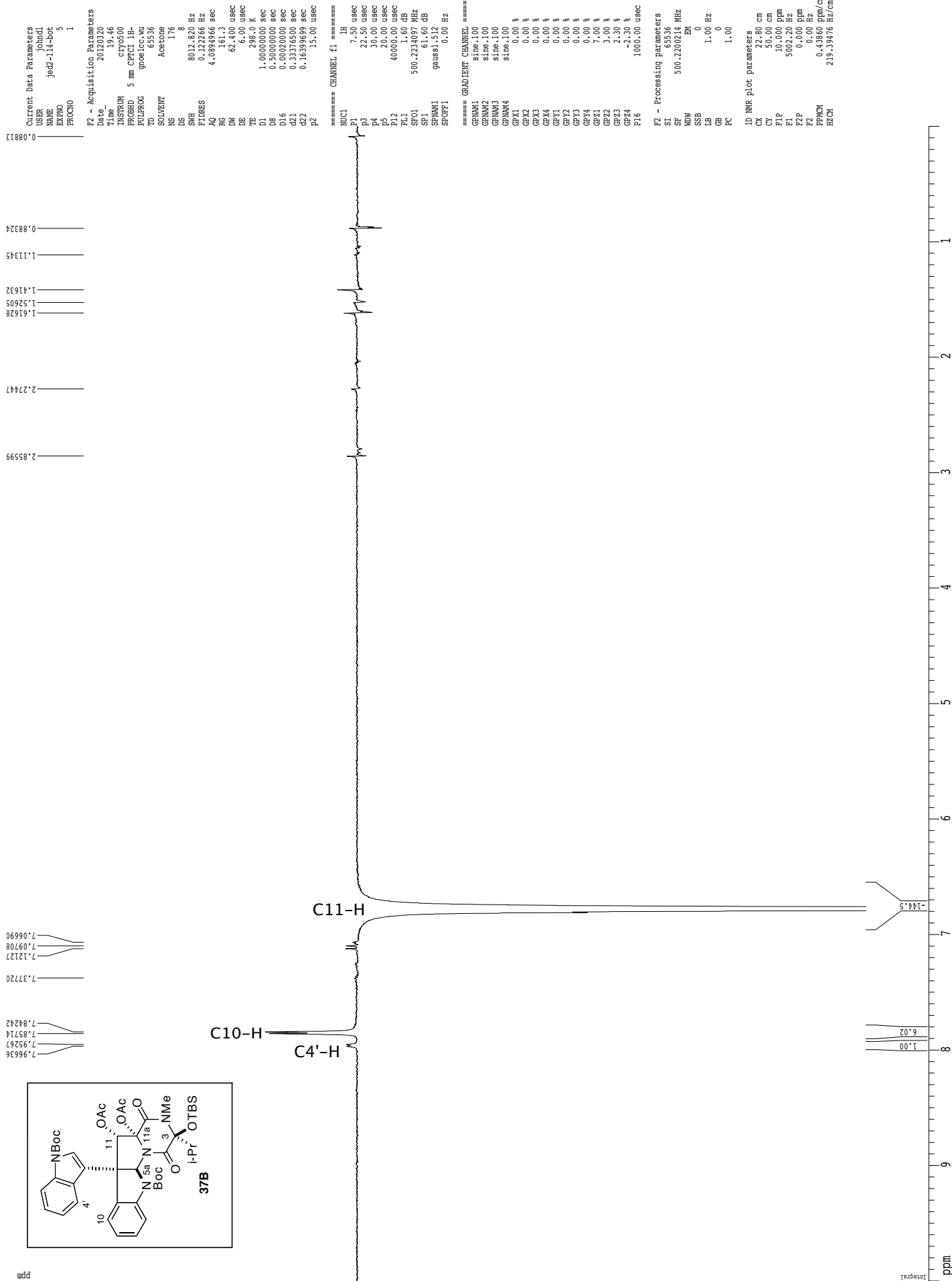
===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 P10 120.00 dB  
 P11 125.794548 dB  
 SFO1 125.760462 MHz  
 SFO2 500.222501 MHz  
 SP1 3.20 dB  
 SP2 3.20 dB  
 SPNAM1 Cpp60.0.5.20.1  
 SPNAM2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPGRZ wd1616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.222501 MHz  
 ===== GRADIENT CHANNEL =====  
 GRNAM1 G10  
 GRNAM2 G10  
 GRAM1 0.00 %  
 GRAM2 0.00 %  
 GRP1 0.00 %  
 GRP2 0.00 %  
 GRP3 30.00 %  
 GRP4 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.780292 MHz  
 WDW EM  
 SSB 0  
 LB 5.00 Hz  
 GB 0  
 PC 0.10

ID NMR plot parameters  
 CX 22.80 cm  
 CY 30.00 cm  
 FIP 220.000 ppm  
 F1 2767.66 Hz  
 F2P -10.000 ppm  
 F2 -125.780 Hz  
 F2PCH 10.000 ppm/cm  
 HZCX 1268.8353 Hz/cm

gnoe

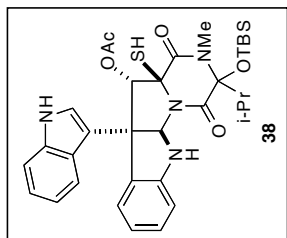


ppm

Integral

<sup>1</sup>H spectrum

7.74320  
7.72704  
7.61883  
7.60186  
7.40229  
7.38802  
7.15223  
7.15062  
7.11925  
7.10567  
7.10156  
6.86519  
6.86349  
6.73351  
6.71787  
6.70010  
6.69651  
6.69336  
6.29621



1.34728  
1.08723  
1.07374  
1.03827  
1.00504  
0.99134  
0.44430  
0.29862

2.05855  
2.05419  
2.04981  
2.04541  
2.04103

3.04602  
2.82815  
2.79406

2.9977  
1.0051

3.0625  
3.0513  
3.0034

2.9725

0.8471

0.9996  
1.0000  
0.9779

1.0916  
2.1370  
1.0706  
0.9478  
0.9270  
0.9455

0.7254  
1.0122

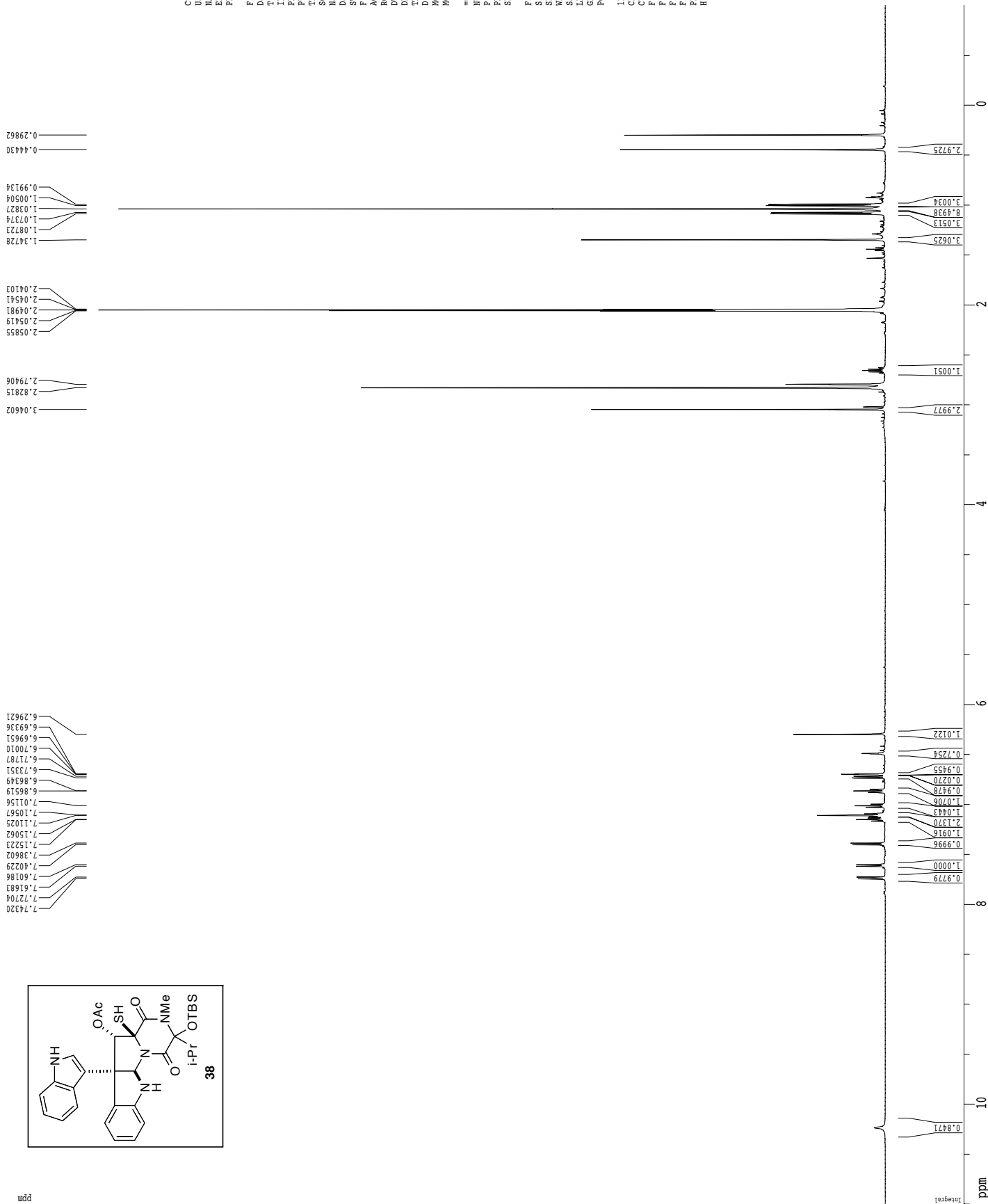
Current Data Parameters  
USER johnd  
NAME jes2-161  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20120519  
Time 15.58  
INSTRUM cryo500  
PROBHD 5 mm CPXI 1H-  
PULPROG zg30  
TD 81728  
SOLVENT Acetone  
NS 32  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.098043 Hz  
AQ 5.0998774 sec  
RG 8  
DE 62.40 usec  
TE 288.0 K  
D1 0.10000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

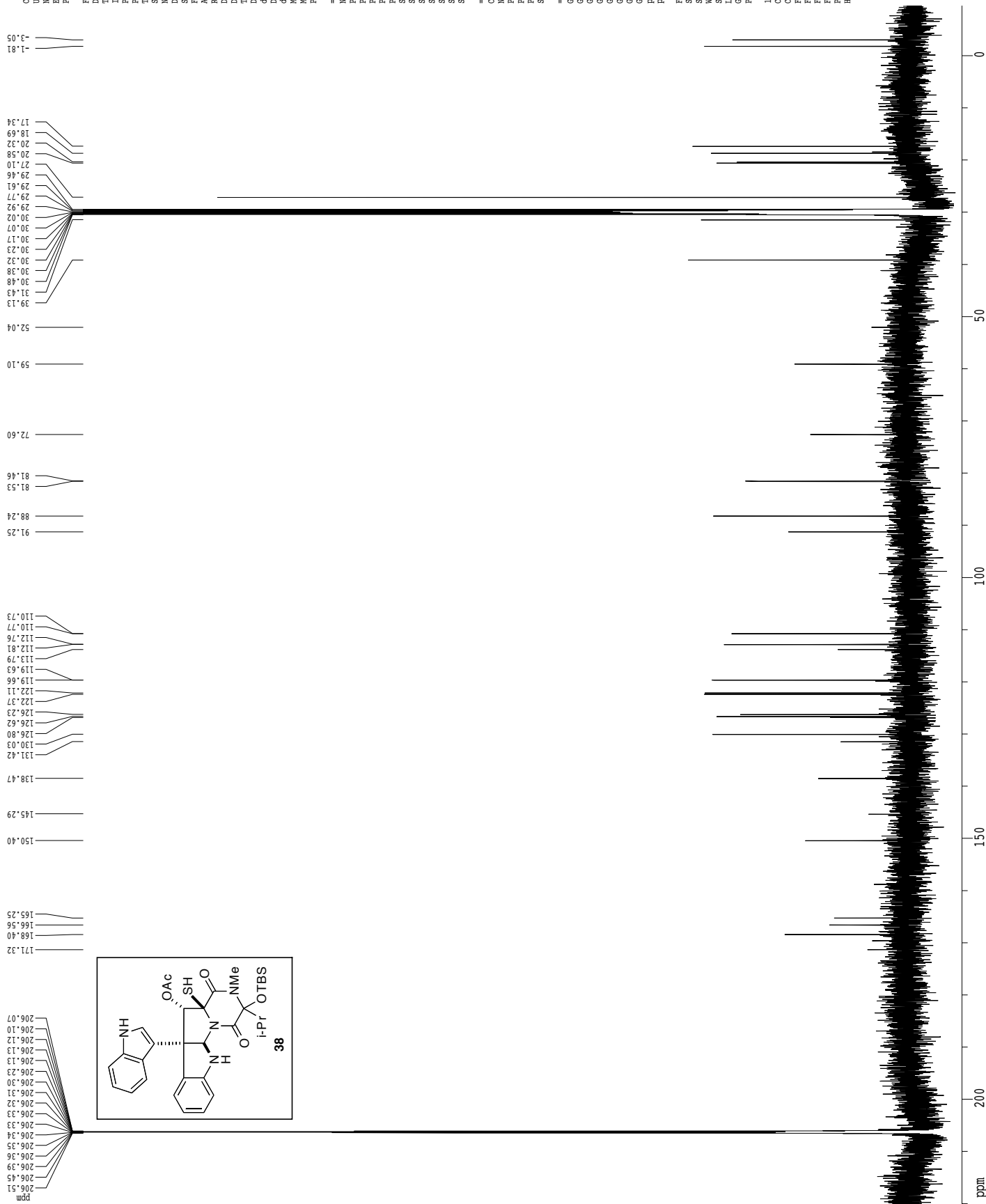
==== CHANNEL f1 =====  
NUC1 1H  
P1 7.50 usec  
PL1 1.00 dB  
SFO1 500.2235015 MHz

F2 - Processing parameters  
SI 65536  
SF 500.220183 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 22.80 cm  
CY 15.00 cm  
FIP 11.000 ppm  
F1 550.242 Hz  
F2 11.000 ppm  
F3 -500.922 ppm  
PRCM 0.52452 ppm/cm  
HZCM 263.27371 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



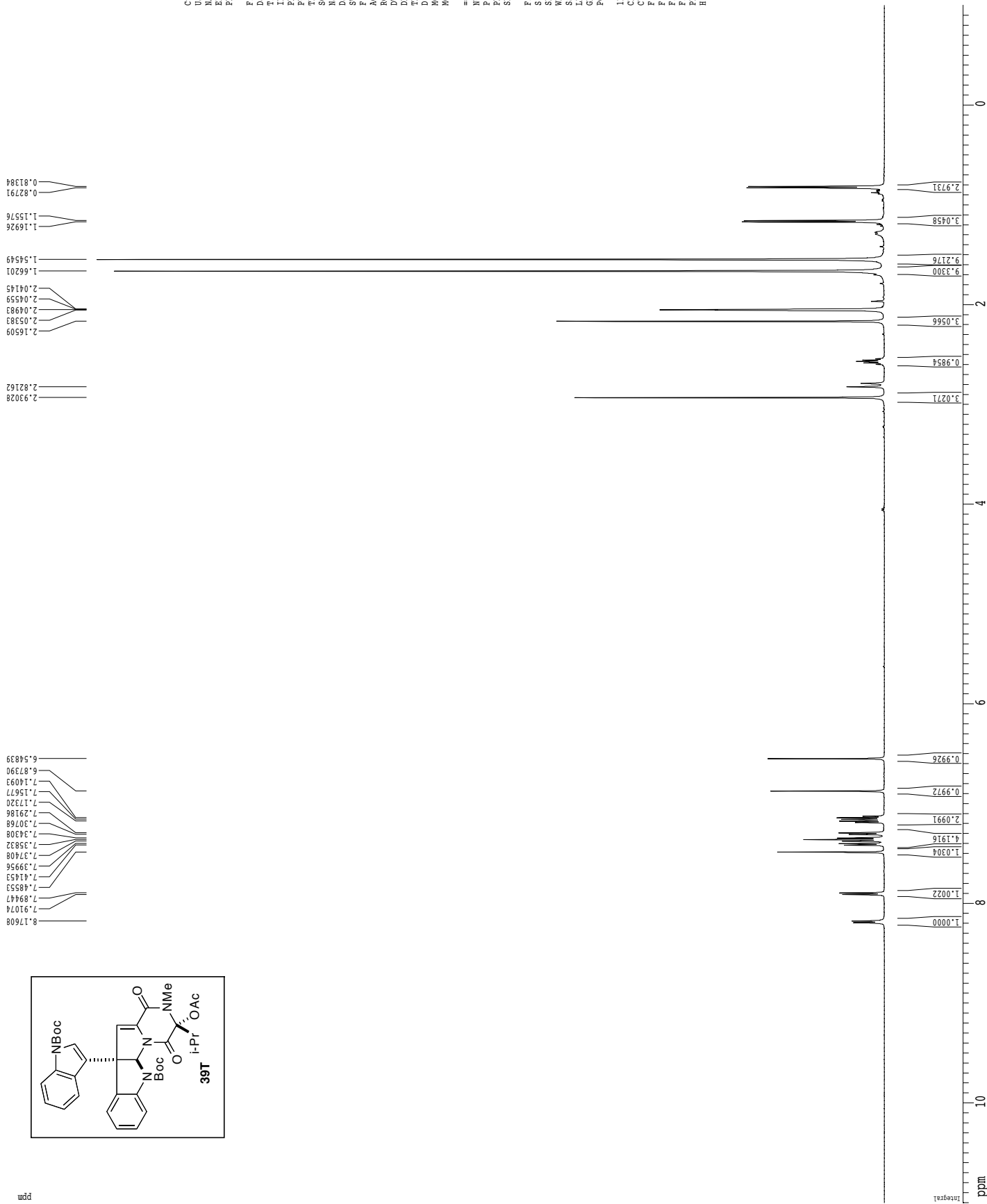
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Current Data Parameters
USER          jomdl
EXPNO         jedz-10
PROCNO       1
F2 - Acquisition Parameters
Date_         20120519
Time         16.05
INSTRUM      cryo500
PROBHD       5 mm CPAC1 1H
PULPROG      zgpg30
SOLVENT      Acetone
NS           1024
DS           16
SFR          303.034031 Hz
FIDRES       0.462388 Hz
AQ           1.0815940 sec
RG           1824.6
AQ           16.000000 sec
DR           6.000000 sec
TE           298.2 K
D1           1.50000000 sec
d11          0.03000000 sec
D16         0.00020000 sec
D17         0.00015600 sec
ACRESF       0.00000000 sec
ACWRK        0.01500000 sec
F2           31.00 usec
===== CHANNEL f1 =====
NUC1         13C
P1           15.50 usec
PL1          500.00 usec
P12          2000.00 usec
PL2          120.00 dB
SFO1         125.7645680 MHz
SFO2         500.2225011 MHz
SFO3         31.20 dB
SFO4         31.20 dB
SFO5         Ccp60.0.5.20.1
SFO6         Ccp60comp.4
SFO7         0.00 Hz
SFO8         0.00 Hz
SFO9         0.00 Hz
===== CHANNEL f2 =====
CPDPRG2     wd1cp15
NUC2         1H
PCPD2       100.00 usec
PL2         1.60 dB
PL12        24.60 dB
SFO2        500.2225011 MHz
===== GRADIENT CHANNEL =====
GSPR1       0.00 %
GSPR2       0.00 %
GSPR3       0.00 %
GSPR4       0.00 %
GSPR5       30.00 %
GSPR6       50.00 %
GSPR7       500.00 usec
GSPR8       1000.00 usec
F2 - Processing parameters
SI          65536
SF          125.7803000 MHz
WDW         EM
SSB         0
LB          1.00 Hz
GB          0
PC          1.10
ID NMR plot parameters
CX          22.80 cm
CY          800.00 cm
FIP         220.000 ppm
F1          2767.167 Hz
F2          -10.000 ppm
F3          -125.780 Hz
F4          125.780 ppm/cm
HEXC       1268.83649 Hz/cm
    
```

Chemical shift values (ppm): 206.10, 206.12, 206.13, 206.13, 206.23, 206.30, 206.31, 206.32, 206.33, 206.34, 206.35, 206.36, 206.39, 206.45, 206.51, 206.51, 171.32, 168.40, 166.56, 165.25, 150.40, 145.29, 138.47, 131.42, 130.03, 126.80, 126.62, 126.23, 122.37, 122.11, 119.66, 119.63, 113.79, 112.81, 112.76, 110.77, 110.73, 91.25, 88.24, 81.53, 81.46, 72.60, 59.10, 52.04, 39.13, 31.43, 30.48, 30.38, 30.32, 30.17, 30.07, 30.02, 29.92, 29.77, 29.61, 29.46, 29.10, 27.10, 20.52, 18.69, 17.34, -1.01, -3.05



<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jedi-104-top  
 EXPNO 1  
 PROCNO 1

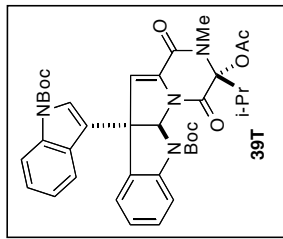
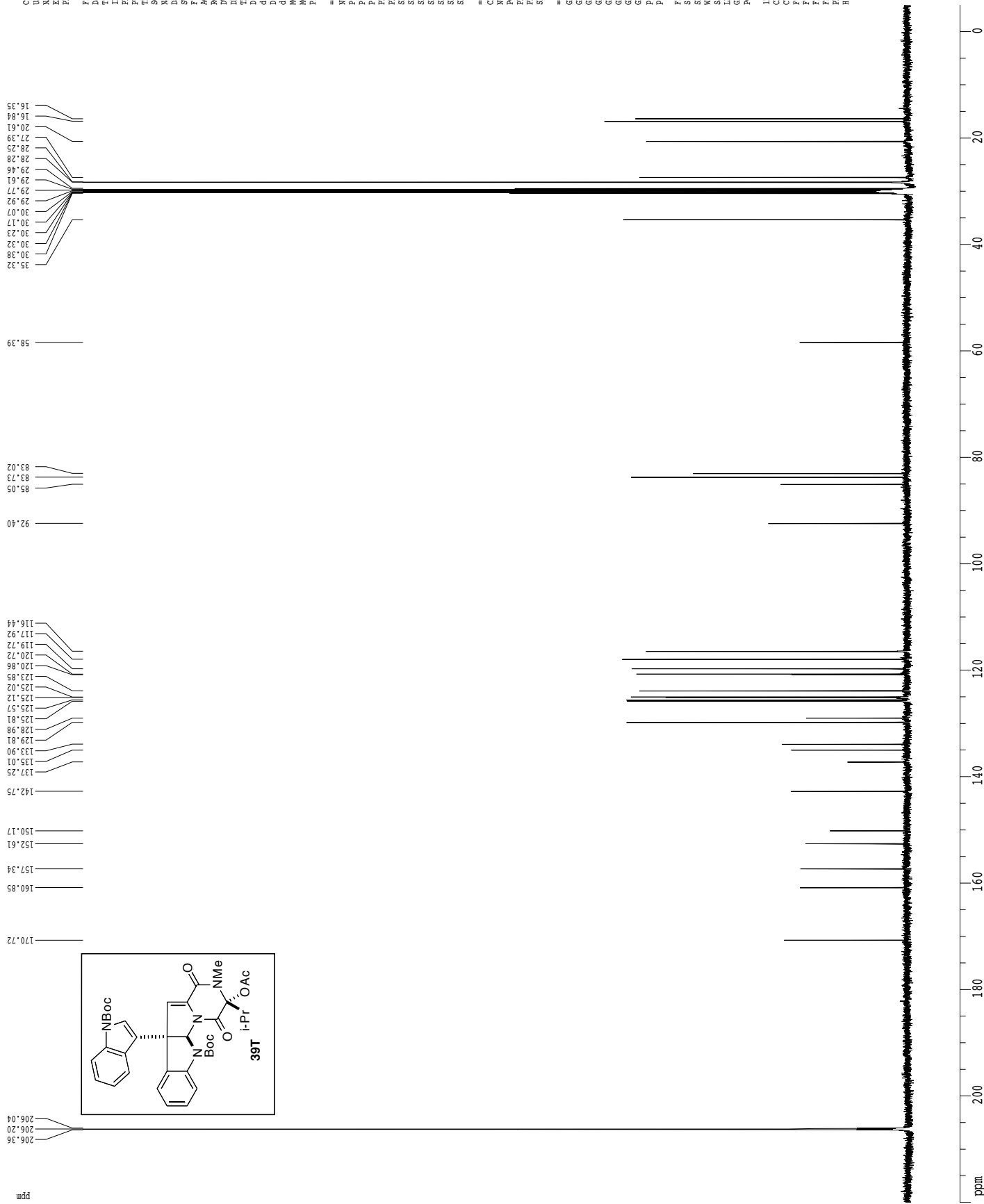
F2 - Acquisition Parameters  
 Date\_ 20101201  
 Time 14.04  
 INSTRUM cryo500  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 63  
 DR 6.00 usec  
 DE 15.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220187 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 590.242 Hz  
 F3 10.000 ppm  
 F4 -500.922 ppm  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jomdl  
 EXNO jedi-104-409  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20101201  
 Time 19.06  
 INSTRUM cryo500  
 PROBHD 5 mm CPACI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 576  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 2048  
 DW 6.00 usec  
 DE 298.0 K  
 TE 298.0 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 D17 0.00015600 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 31.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPGRZ wd t616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

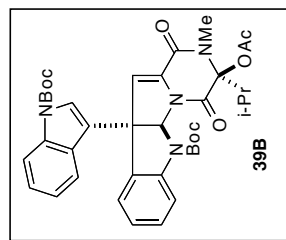
===== GRADIENT CHANNEL =====  
 GSPR1 0.00 %  
 GSPR2 0.00 %  
 GSPR3 0.00 %  
 GSPR4 0.00 %  
 GSPR5 30.00 %  
 GSPR6 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803019 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

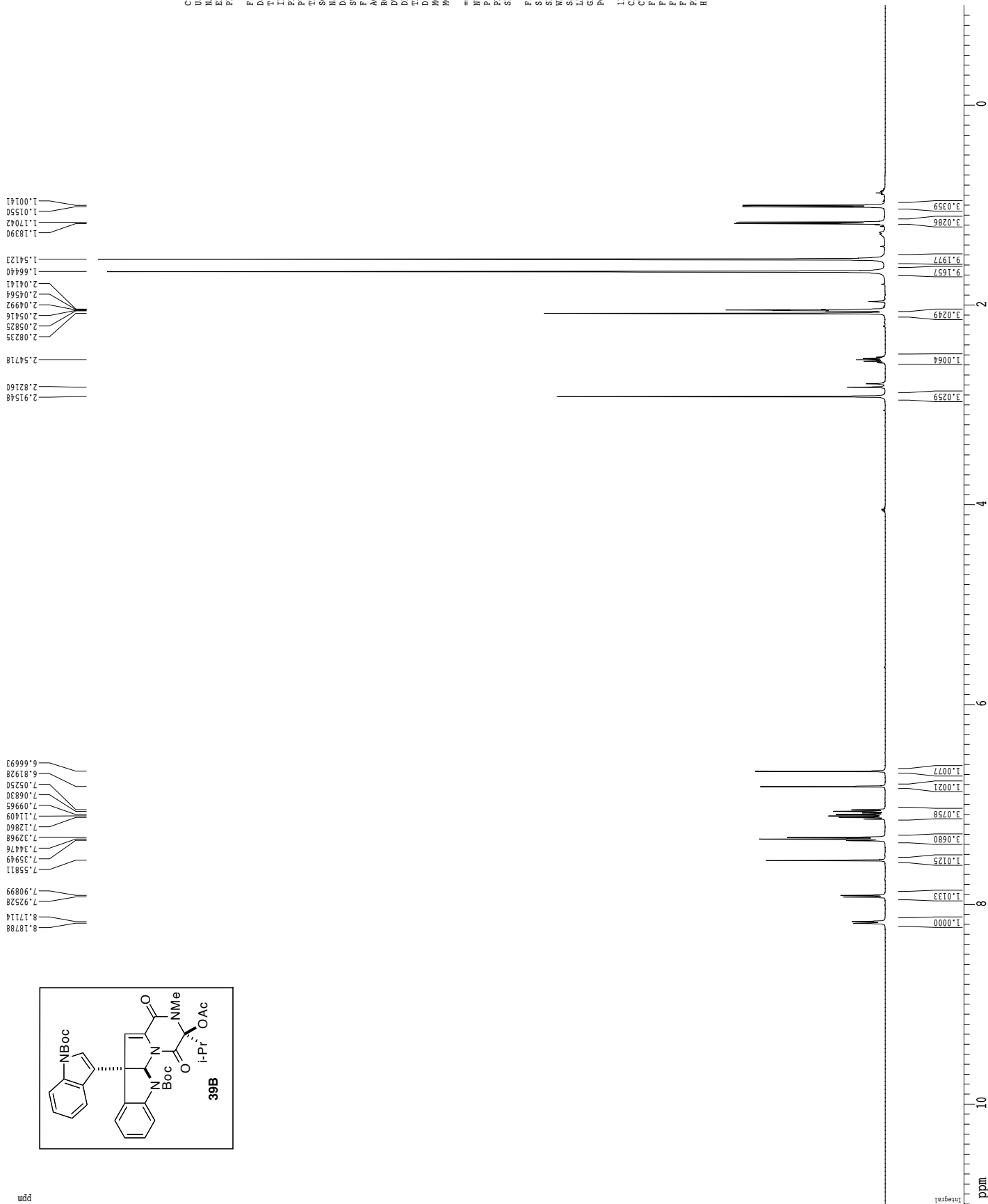
ID NMR plot parameters  
 CX 22.80 cm  
 CY 75.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -5.000 ppm  
 F3 -628.90 Hz  
 FWHM 0.000 ppm/cm  
 HECK 1241.2530 Hz/cm

<sup>1</sup>H spectrum

8.18788  
8.17114  
7.92528  
7.90899  
7.55811  
7.35949  
7.34476  
7.32986  
7.12860  
7.11409  
7.09965  
7.06830  
7.05250  
6.81928  
6.66693

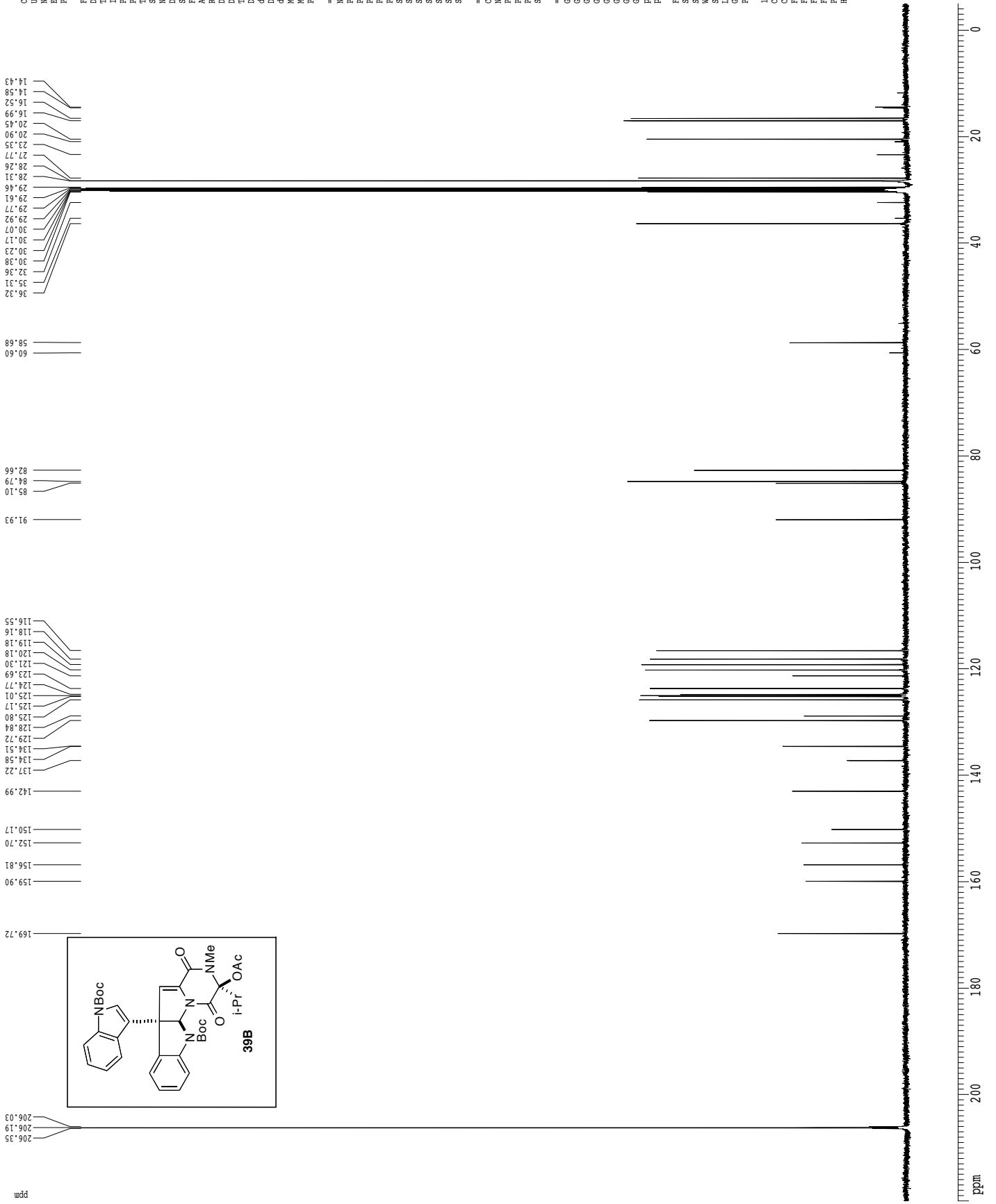


2.91948  
2.82160  
2.54718  
2.08235  
2.05825  
2.05416  
2.04992  
2.04564  
2.04141  
1.66440  
1.54123  
1.18390  
1.17042  
1.01550  
1.00141



Current Data Parameters  
 USER johnd  
 NAME jed1-104-bot  
 EXPNO 1  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20101201  
 Time 14.08  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099874 sec  
 RG 63  
 DE 6.00 usec  
 DR 15.00 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec  
 ===== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz  
 F2 - Processing parameters  
 SI 32768  
 SF 500.220185 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 2.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F1 590.242 Hz  
 F2 16.000 ppm  
 F3 -500.922 ppm  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jound1  
 EXPNO jedi-104-462  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20101201  
 Time 16.08  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 512  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 5100.6  
 DR 6.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 D17 0.00015600 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 31.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 PL2 120.00 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Ccp60.05, 20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

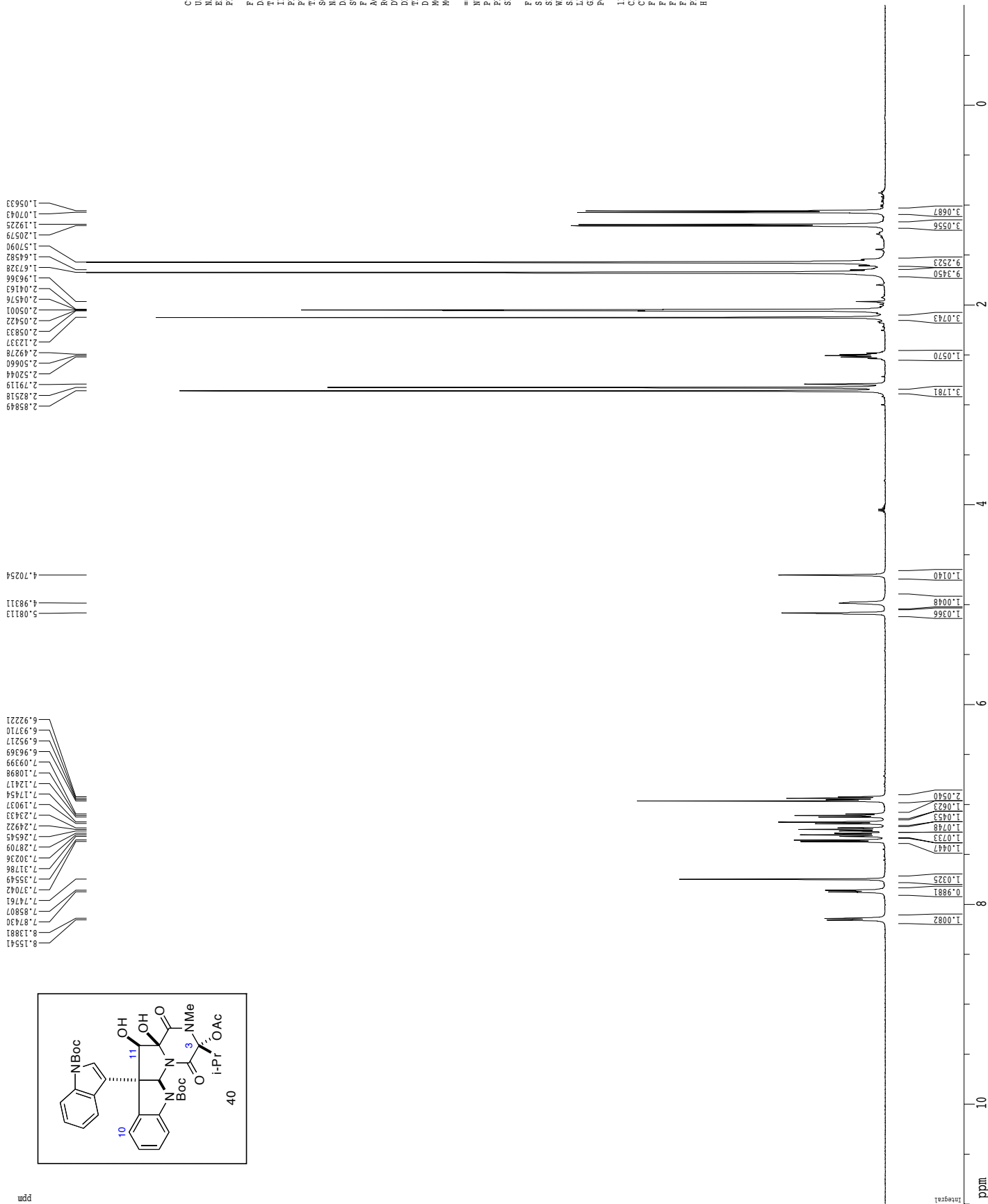
===== CHANNEL f2 =====  
 CDPGRZ wd1615  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GRAMZ 0  
 GRAPZ 0  
 GRMZ 0.00 %  
 GRXZ 0.00 %  
 GRYZ 0.00 %  
 GRZ1 30.00 %  
 GRZ2 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803028 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2P -5.000 ppm  
 F2 8283.90 Hz  
 FWHM 0.95000 ppm/cm  
 HECM 1241.25300 Hz/cm

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jed1-105  
 EXPNO 1  
 PROCNO 1

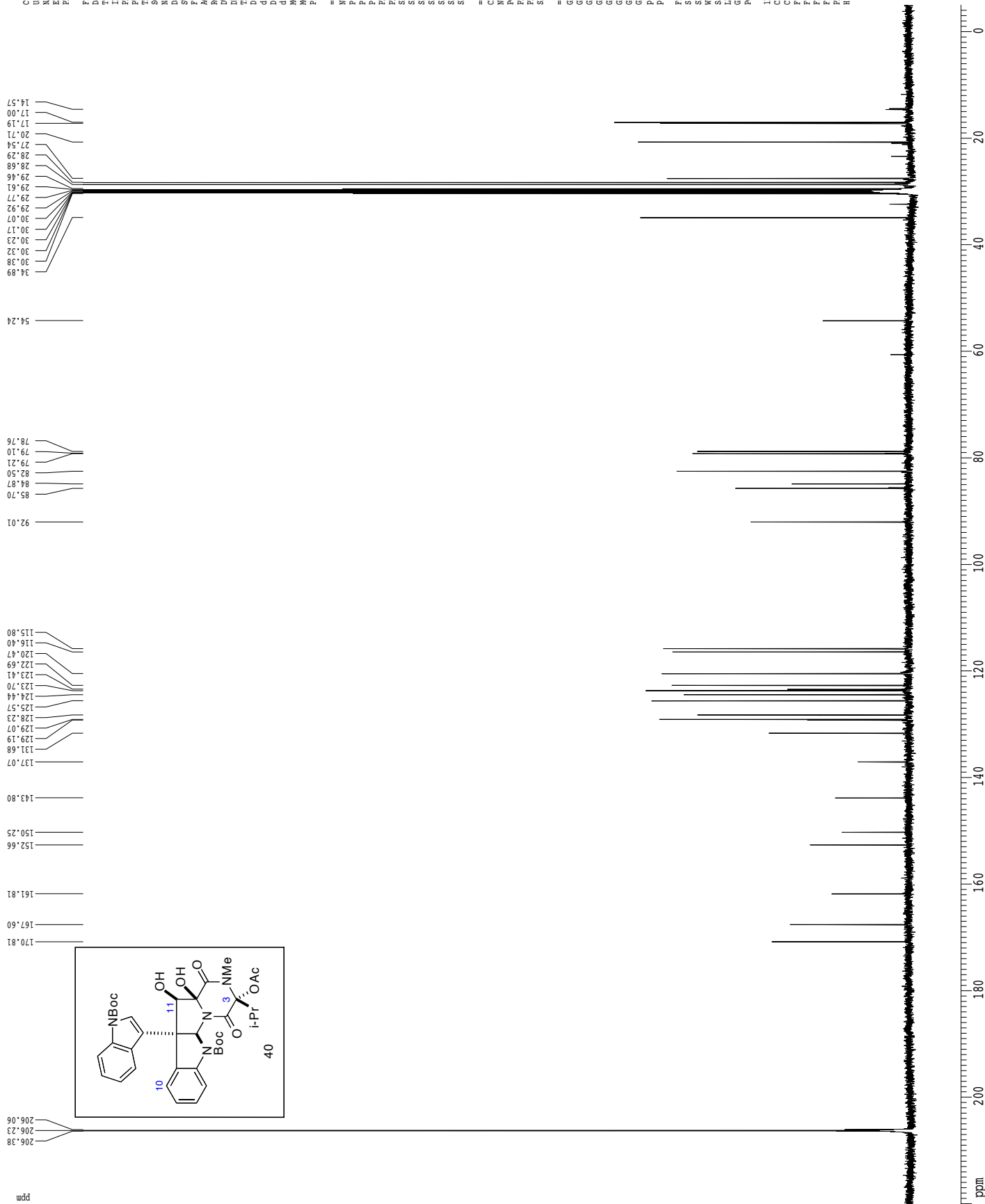
F2 - Acquisition Parameters  
 Date\_ 20101204  
 Time 13.42  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 48  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 63  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220185 MHz  
 GM 1.00000000  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 35.00 cm  
 FIP 11.000 ppm  
 F2 5902.82 Hz  
 F3 10.000 ppm  
 FZ -500.92 Hz  
 PRMCM 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER joud1  
 EXPNO jedi-102  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20101204  
 Time 17:19  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 640  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815941 sec  
 RG 432  
 DW 6.00 usec  
 DE 16.00 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 D17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 31.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PLO 120.00 dB  
 P1L1 125.794548 MHz  
 SFO1 500.136299 MHz  
 SFO2 125.794548 MHz  
 SP1 3.20 dB  
 SP2 3.20 dB  
 SPNAM1 Cpp60.0.5.20.1  
 SPNAM2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

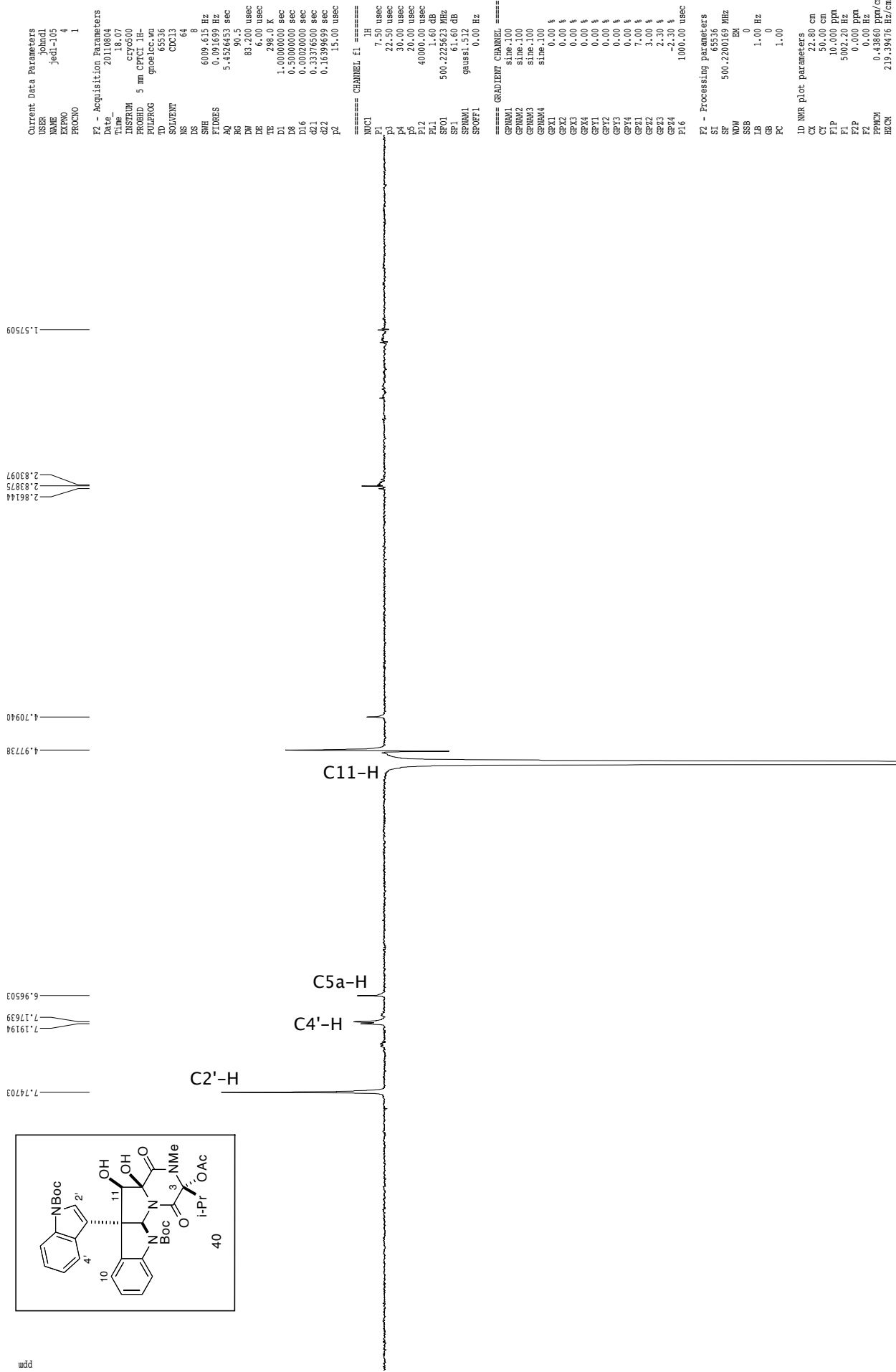
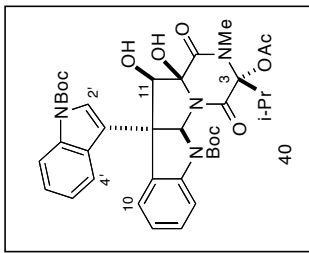
===== CHANNEL F2 =====  
 CDPREG wd1615  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPAM1 0.00 usec  
 GSPAM2 0.00 usec  
 GFL1 0.00 %  
 GFL2 0.00 %  
 GFL3 0.00 %  
 GFL4 0.00 %  
 GFL5 0.00 %  
 GFL6 0.00 %  
 GFL7 0.00 %  
 GFL8 0.00 %  
 GFL9 0.00 %  
 GFL10 0.00 %  
 GFL11 0.00 %  
 GFL12 0.00 %  
 GFL13 0.00 %  
 GFL14 0.00 %  
 GFL15 0.00 %  
 GFL16 0.00 %  
 GFL17 0.00 %  
 GFL18 0.00 %  
 GFL19 0.00 %  
 GFL20 0.00 %

F2 - Processing parameters  
 SI 65536  
 SF 125.7803019 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 100.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -5.000 ppm  
 F2 0.62830 Hz  
 F2 0.62830 ppm/cm  
 HECK 1241.2530 Hz/cm

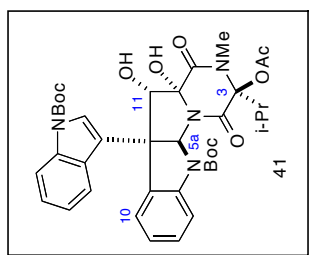
gnoe



ppm

Integral

<sup>1</sup>H spectrum



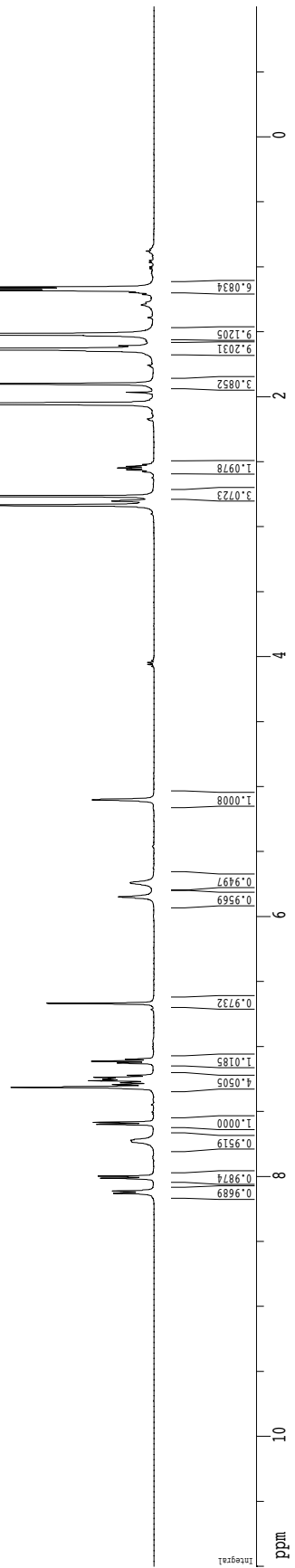
Current Data Parameters  
 USER johnd  
 NAME jed1-106  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20101204  
 Time 17.06  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 36  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.098674 sec  
 RG 0  
 DR 62.40 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

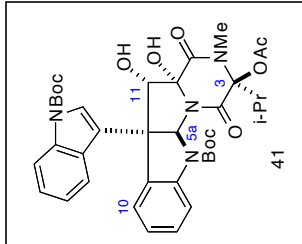
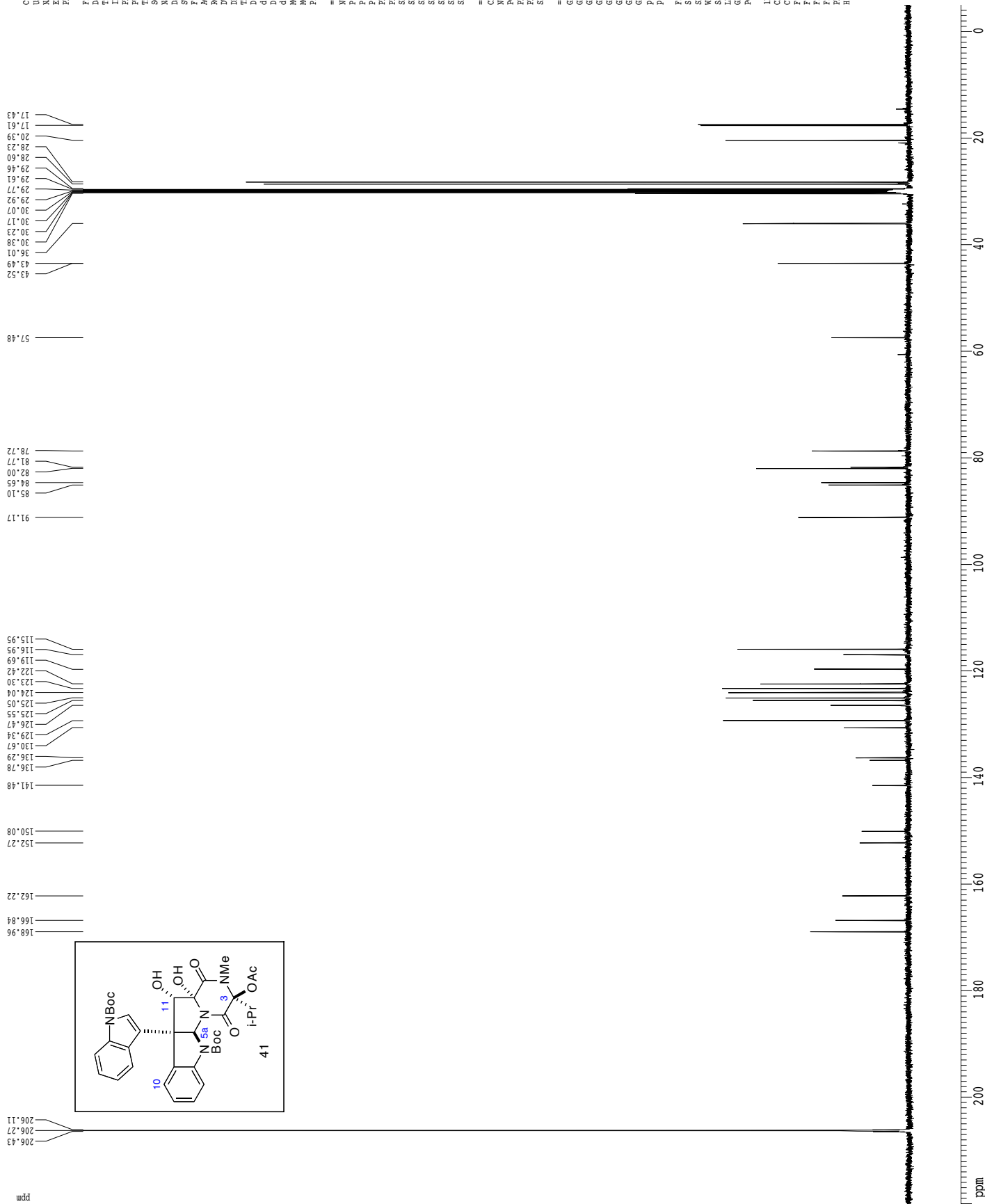
F2 - Processing parameters  
 SI 32768  
 SF 500.220183 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 550.242 Hz  
 F3 10.000 ppm  
 F4 -50.922 ppm  
 PPM0 0.52432 ppm/cm  
 HZ00 263.27371 Hz/cm





Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jomdl  
 EXPNO jedi-102  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20101204  
 Time 17:47  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 336  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 4597.6  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.00015600 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 31.00 usec

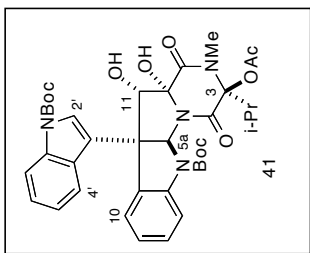
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 PL2 125.794568 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Ccp60.0.5.20.1  
 SFO2 Ccp60.0.5.20.1  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL f2 =====  
 CDPGRG2 wd1616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR1 0.00 %  
 GSPR2 0.00 %  
 GSPR3 0.00 %  
 GSPR4 0.00 %  
 GSPR5 0.00 %  
 GSPR6 0.00 %  
 GSPR7 0.00 %  
 GSPR8 0.00 %  
 GSPR9 0.00 %  
 GSPR10 0.00 %  
 GSPR11 0.00 %  
 GSPR12 0.00 %  
 GSPR13 0.00 %  
 GSPR14 0.00 %  
 GSPR15 0.00 %  
 GSPR16 0.00 %  
 GSPR17 0.00 %  
 GSPR18 0.00 %  
 GSPR19 0.00 %  
 GSPR20 0.00 %  
 GSPR21 0.00 %  
 GSPR22 0.00 %  
 GSPR23 0.00 %  
 GSPR24 0.00 %  
 GSPR25 0.00 %  
 GSPR26 0.00 %  
 GSPR27 0.00 %  
 GSPR28 0.00 %  
 GSPR29 0.00 %  
 GSPR30 0.00 %  
 GSPR31 0.00 %  
 GSPR32 0.00 %  
 GSPR33 0.00 %  
 GSPR34 0.00 %  
 GSPR35 0.00 %  
 GSPR36 0.00 %  
 GSPR37 0.00 %  
 GSPR38 0.00 %  
 GSPR39 0.00 %  
 GSPR40 0.00 %  
 GSPR41 0.00 %  
 GSPR42 0.00 %  
 GSPR43 0.00 %  
 GSPR44 0.00 %  
 GSPR45 0.00 %  
 GSPR46 0.00 %  
 GSPR47 0.00 %  
 GSPR48 0.00 %  
 GSPR49 0.00 %  
 GSPR50 0.00 %  
 GSPR51 0.00 %  
 GSPR52 0.00 %  
 GSPR53 0.00 %  
 GSPR54 0.00 %  
 GSPR55 0.00 %  
 GSPR56 0.00 %  
 GSPR57 0.00 %  
 GSPR58 0.00 %  
 GSPR59 0.00 %  
 GSPR60 0.00 %  
 GSPR61 0.00 %  
 GSPR62 0.00 %  
 GSPR63 0.00 %  
 GSPR64 0.00 %  
 GSPR65 0.00 %  
 GSPR66 0.00 %  
 GSPR67 0.00 %  
 GSPR68 0.00 %  
 GSPR69 0.00 %  
 GSPR70 0.00 %  
 GSPR71 0.00 %  
 GSPR72 0.00 %  
 GSPR73 0.00 %  
 GSPR74 0.00 %  
 GSPR75 0.00 %  
 GSPR76 0.00 %  
 GSPR77 0.00 %  
 GSPR78 0.00 %  
 GSPR79 0.00 %  
 GSPR80 0.00 %  
 GSPR81 0.00 %  
 GSPR82 0.00 %  
 GSPR83 0.00 %  
 GSPR84 0.00 %  
 GSPR85 0.00 %  
 GSPR86 0.00 %  
 GSPR87 0.00 %  
 GSPR88 0.00 %  
 GSPR89 0.00 %  
 GSPR90 0.00 %  
 GSPR91 0.00 %  
 GSPR92 0.00 %  
 GSPR93 0.00 %  
 GSPR94 0.00 %  
 GSPR95 0.00 %  
 GSPR96 0.00 %  
 GSPR97 0.00 %  
 GSPR98 0.00 %  
 GSPR99 0.00 %  
 GSPR100 0.00 %

F2 - Processing parameters  
 SI 65536  
 SF 125.7803037 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -5.000 ppm  
 F3 6283.90 Hz  
 F4 11.111 ppm/cm  
 F5 1241.2530 Hz/cm  
 HECK 1241.2530 Hz/cm

gnoe



Current Data Parameters  
 USER johnd  
 NAME jedl-106  
 EXPMO 4  
 PROCNO 1

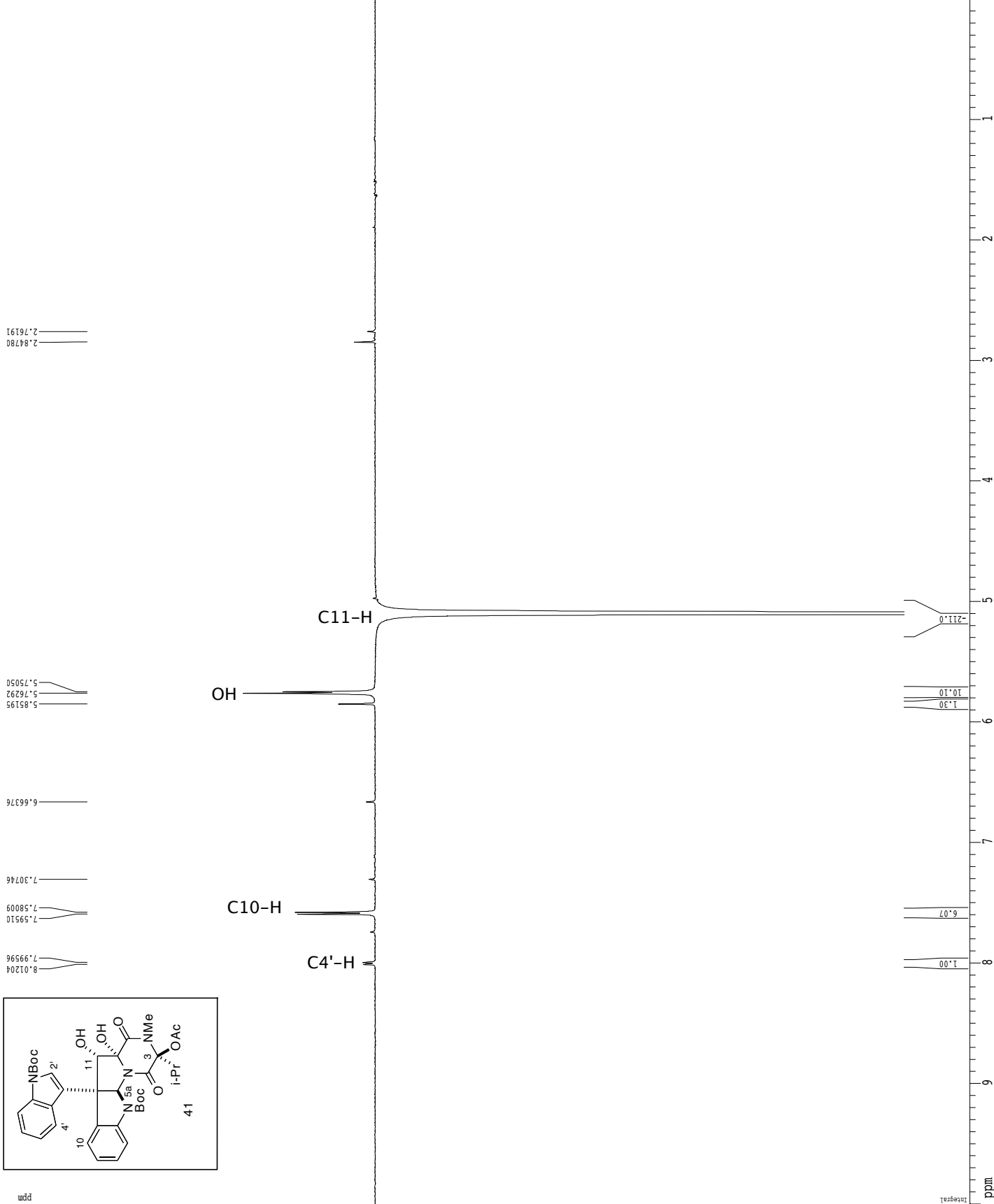
F2 - Acquisition Parameters  
 Date\_ 20110804  
 Time\_ 17.20  
 INSTRUM cty6500  
 PROBRD 5 mm CPXI 1H-  
 PULPROG gnoelcc.wu  
 TD 65536  
 SOLVENT Acetone  
 NS 120  
 DS 8  
 SWH 6009.615 Hz  
 FIDRES 0.091699 Hz  
 AQ 5.4526453 sec  
 RG 101.6  
 DW 83.200 usec  
 DE 6.0 usec  
 TE 298.0 K  
 D1 1.000000 sec  
 D11 0.500000 sec  
 D16 0.002000 sec  
 d21 0.33376500 sec  
 d22 0.16396999 sec  
 p2 15.00 usec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 P3 22.50 usec  
 P4 30.00 usec  
 P5 20.00 usec  
 P12 40000.00 usec  
 PL1 1.60 dB  
 SF01 500.222594 MHz  
 SE1 61.60 dB  
 SP0M1 gauss1.512  
 SP0F1 0.00 Hz

==== GRADIENT CHANNEL =====  
 GENM1 sine.100  
 GENM2 sine.100  
 GENM3 sine.100  
 GENM4 sine.100  
 GFX1 0.00 %  
 GFX2 0.00 %  
 GFX3 0.00 %  
 GFX4 0.00 %  
 GFY1 0.00 %  
 GFY2 0.00 %  
 GFY3 0.00 %  
 GFY4 0.00 %  
 GZ1 7.00 %  
 GZ2 3.00 %  
 GZ3 2.30 %  
 GZ4 -  
 F16 1000.00 usec

F2 - Processing Parameters  
 SI 65536  
 SF 500.2200179 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

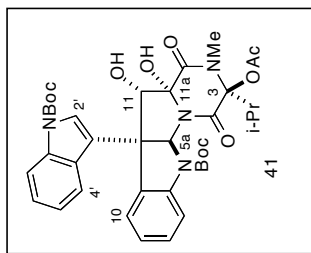
ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 10.000 ppm  
 F1 5002.20 Hz  
 F2P 0.000 ppm  
 F2 1.00 Hz  
 FREQM 0.439 ppm/cm  
 HZCM 219.39456 Hz/cm



Integral

ppm

gnoe



Current Data Parameters  
 USER JohnHd.  
 NAME jeo2-115-boc  
 EXPMO 3  
 PROCNO 1

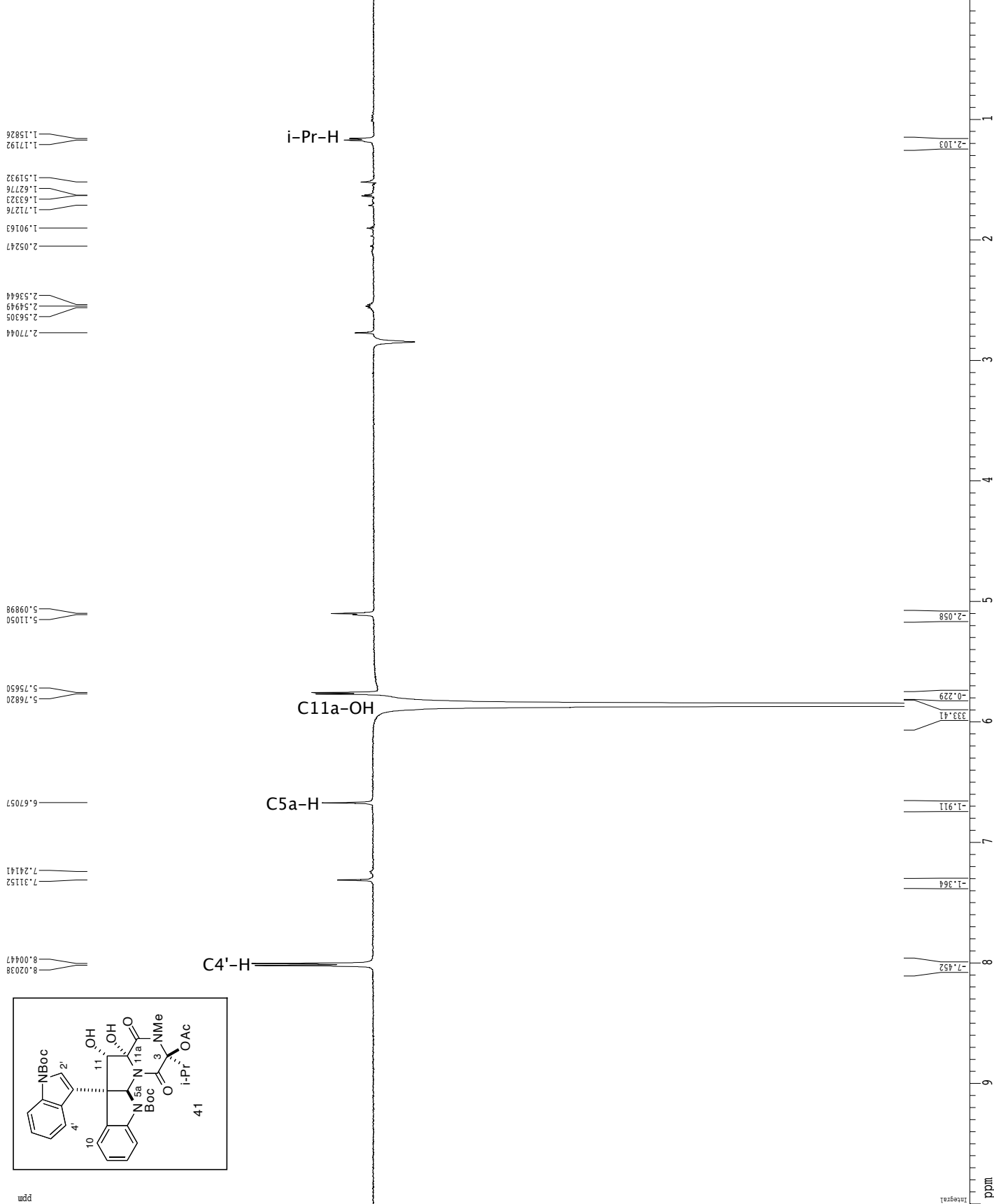
F2 - Acquisition Parameters  
 Date\_ 20120327  
 Time\_ 16.04  
 INSTRUM cryo590  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG gnoe1cc.wu  
 TD 65536  
 SOLVENT CDC13  
 NS 160  
 DS 8  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894966 sec  
 RG 161.3  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 D11 0.50000000 sec  
 D16 0.00020000 sec  
 d21 0.33376500 sec  
 d22 0.16399699 sec  
 p2 15.00 usec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 P3 22.50 usec  
 P4 30.00 usec  
 P5 20.00 usec  
 P12 40000.00 usec  
 P11 1.60 dB  
 SF01 500.2229463 MHz  
 SF1 61.60 dB  
 SPHM1 gauss1.512  
 SFOF1 0.00 Hz

==== GRADIENT CHANNEL =====  
 GENM1 sine.100  
 GENM2 sine.100  
 GENM3 sine.100  
 GENM4 sine.100  
 GFX1 0.00 %  
 GFX2 0.00 %  
 GFX3 0.00 %  
 GFX4 0.00 %  
 GFY1 0.00 %  
 GFY2 0.00 %  
 GFY3 0.00 %  
 GFY4 0.00 %  
 GZ1 7.00 %  
 GZ2 3.00 %  
 GZ3 2.30 %  
 GZ4 -2.30 %  
 F16 1000.00 usec

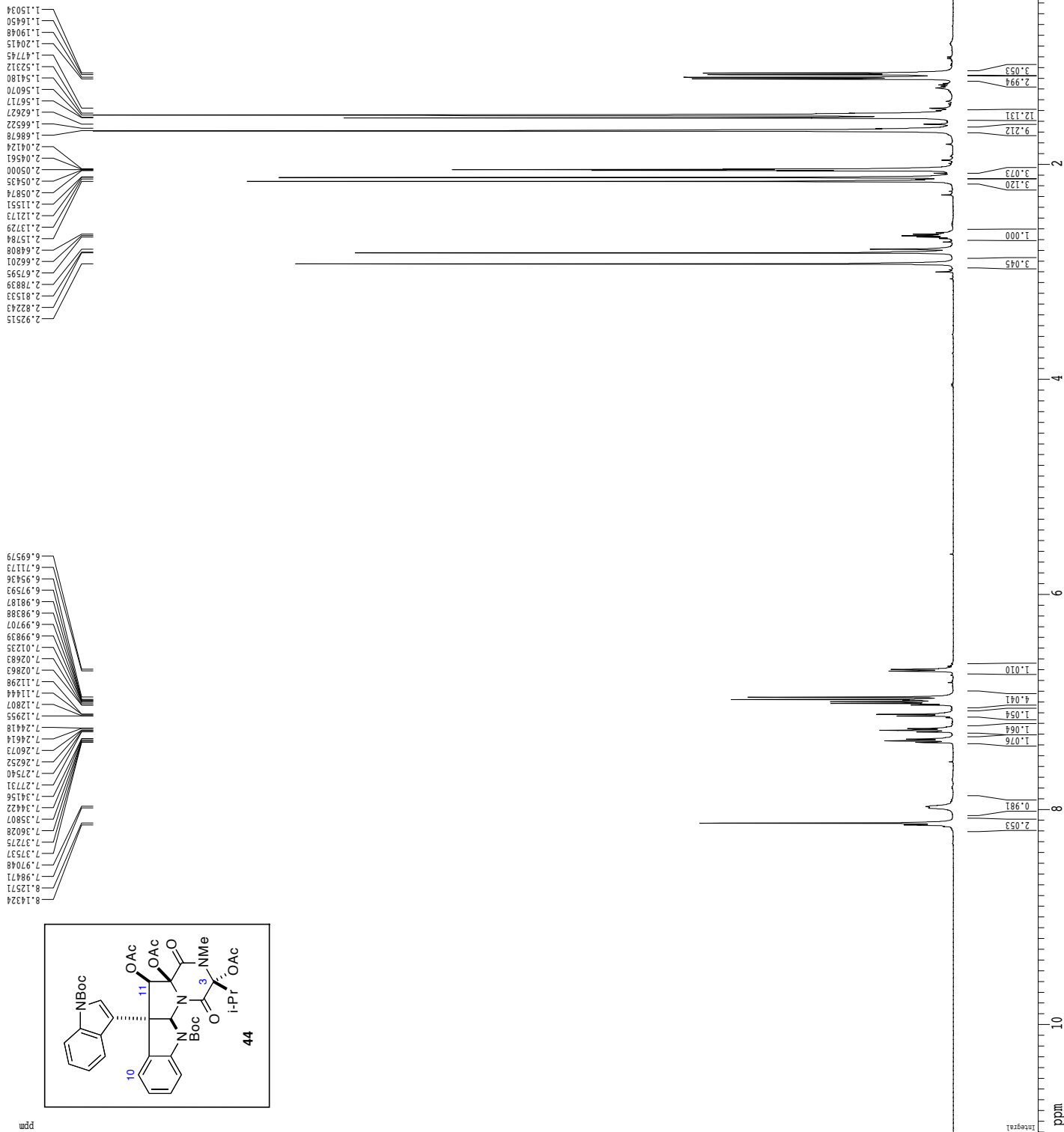
F2 - Processing Parameters  
 SI 65536  
 SF 500.2200165 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 250.00 cm  
 FIP 10.000 ppm  
 F1 5002.20 Hz  
 F2P 0.000 ppm  
 F3P 0.000 Hz  
 FREQM 0.439 ppm/cm  
 HZCM 219.39476 Hz/cm



ppm

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jed1-107  
 EXPNO 1  
 PROCNO 1

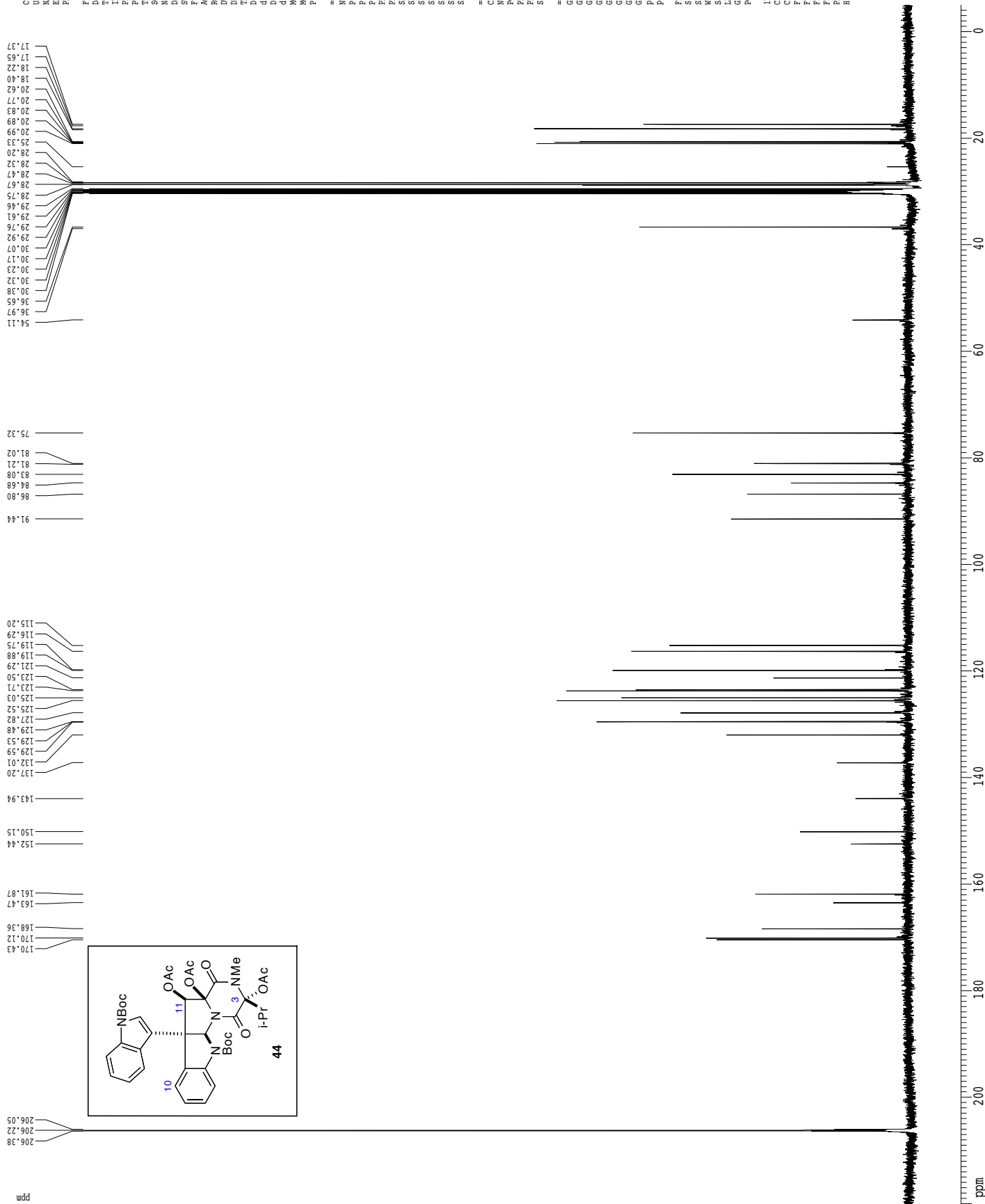
F2 - Acquisition Parameters  
 Date\_ 20101209  
 Time 14.04  
 INSTRUM crys500  
 PROBRD 5 mm CPXI H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 36  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 63  
 DE 6.00 usec  
 DR 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65535  
 SF 500.220184 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.50

1D NMR plot parameters  
 CX 22.80 cm  
 CY 30.00 cm  
 FIP 11.000 ppm  
 F1 5907.82 Hz  
 F2 10.000 ppm  
 F3 -500.92 ppm  
 PPMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



```

Current Data Parameters
USER          joudi1
JOB           jedi-10
EXNO         1
PROCNO       1

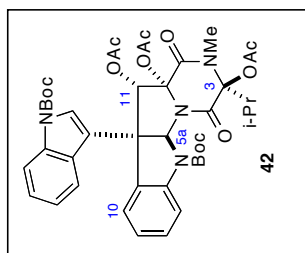
F2 - Acquisition Parameters
Date_        20101210
Time         19.24
INSTRUM      cryo500
PROBHD       5 mm CPXI 1H
PULPROG      zgpg30
TD           65536
SOLVENT      Acetone
NS           824
DS           16
SHR          30303.031 Hz
FIDRES       0.462388 Hz
AQ           1.0815940 sec
RG           3260.75
DR           6.00 usec
TE           298.2 K
D1           1.00000000 sec
d11          0.03000000 sec
D16         0.00020000 sec
d17         0.00015600 sec
ACQRESF     0.00000000 sec
AQSWH       0.01500000 sec
F2          500.130000 MHz
===== CHANNEL F1 =====
NUC1         13C
P1          15.50 usec
P11         500.00 usec
P12         2000.00 usec
PL0         120.00 dB
PL1         125.794568 dB
PL2         125.794568 dB
PL3         125.794568 dB
PL4         125.794568 dB
PL5         125.794568 dB
PL6         125.794568 dB
SFO1        500.130000 MHz
SFO2        500.130000 MHz
SFO3        500.130000 MHz
SFO4        500.130000 MHz
SFO5        500.130000 MHz
SFO6        500.130000 MHz
SFO7        500.130000 MHz
SFO8        500.130000 MHz
SFO9        500.130000 MHz
SFO10       500.130000 MHz
===== CHANNEL F2 =====
CPDPRG2     wd1cp15
NUC2         1H
PCPD2       100.00 usec
PL2         1.60 dB
PL12        24.60 dB
SFO2        500.2225011 MHz
===== GRADIENT CHANNEL =====
GSPRNG1     0.00 %
GSPRNG2     0.00 %
GSPRNG3     0.00 %
GSPRNG4     0.00 %
GSPRNG5     0.00 %
GSPRNG6     0.00 %
GSPRNG7     0.00 %
GSPRNG8     0.00 %
GSPRNG9     0.00 %
GSPRNG10    0.00 %
GSPRNG11    0.00 %
GSPRNG12    0.00 %
===== Processing parameters =====
SI          65536
SF          125.7803019 MHz
WDW         EM
SSB         0
LB          0
GB          0
PC          2.00

1D NMR plot parameters
CX          22.80 cm
CY          140.00 cm
FIP         220.000 ppm
F1          2767.167 Hz
F2          -5.000 ppm
F3          -628.90 Hz
F4          0.000 Hz
NUC1        13C
HEXC       1241.25305 Hz/cm
    
```

<sup>1</sup>H spectrum

1.14216  
1.15597  
1.28901  
1.47764  
1.49557  
1.59454  
1.60371  
1.62950  
1.96222  
2.04156  
2.04230  
2.04581  
2.05012  
2.05447  
2.05881  
2.28273  
2.53436  
2.54811  
2.56190  
2.57574  
2.58953  
2.72276  
2.78729  
2.82146

6.75040  
6.92492  
7.18534  
7.20030  
7.21535  
7.23118  
7.28327  
7.29796  
7.31321  
7.33330  
7.34404  
7.34959  
7.35595  
7.36419  
7.37078  
7.68494  
7.80791  
7.80297  
8.14206  
8.15855



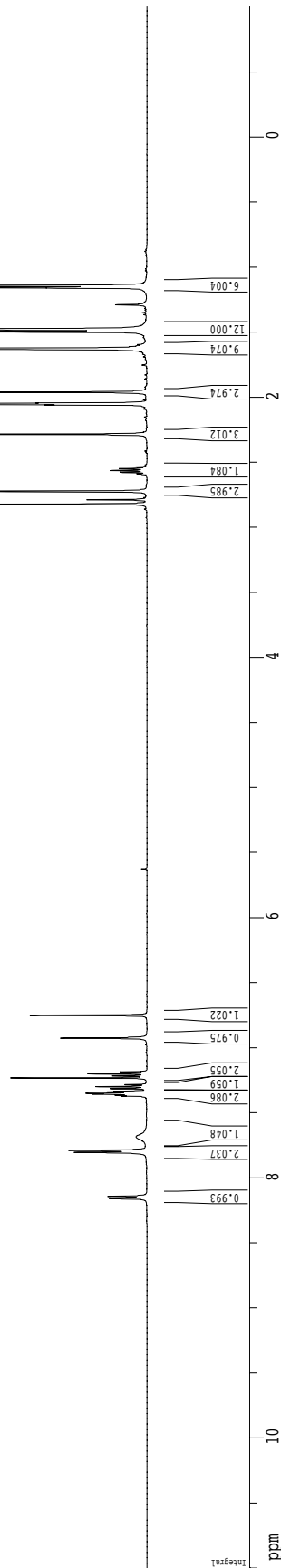
Current Data Parameters  
USER johnd  
NAME jed1-108  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20101208  
Time 14.30  
INSTRUM crys500  
PROBHD 5 mm CPXI 1H-  
PULPROG zg30  
TD 81728  
SOLVENT Acetone  
NS 48  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.098043 Hz  
AQ 5.0996774 sec  
RG 64.00  
DE 6.00 usec  
TE 288.0 K  
D1 0.10000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 7.50 usec  
PL1 1.00 dB  
SFO1 500.2235015 MHz

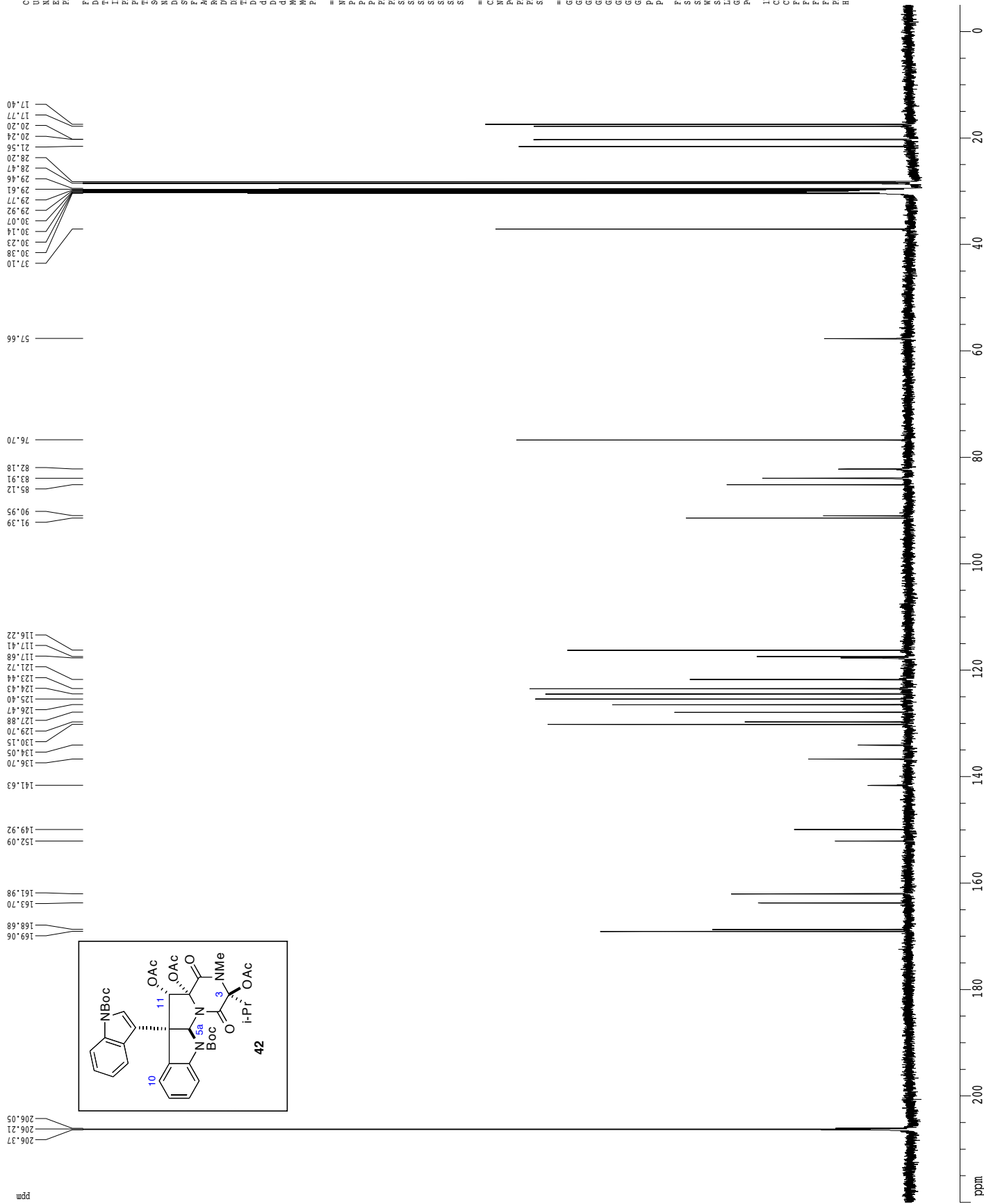
F2 - Processing parameters  
SI 32768  
SF 500.220184 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 0.50

1D NMR plot parameters  
CX 22.80 cm  
CY 15.00 cm  
FIP 11.000 ppm  
F2 590.242 Hz  
F3 10.000 ppm  
F4 -500.92 Hz  
PRCM 0.52432 ppm/cm  
HZCM 263.27371 Hz/cm



Integral

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER joudi  
 EXPNO jedi-102  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20101209  
 Time 14:10  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 472  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 5100.6  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 D17 0.00015600 sec  
 ACQRESF 0.00000000 sec  
 ACQBRK 0.01500000 sec  
 F2 31.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 78.00 dB  
 PL2 125.7947548 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Ccp60.05, 20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

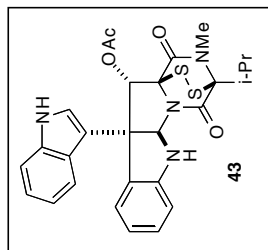
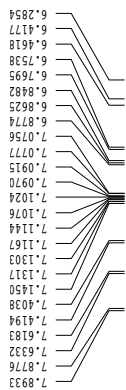
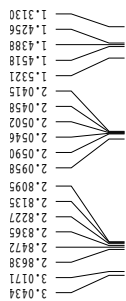
===== CHANNEL f2 =====  
 CPMRGZ wd1616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GMRG1 0.00 %  
 GMRG2 0.00 %  
 GMRG3 0.00 %  
 GMRG4 0.00 %  
 GMRG5 30.00 %  
 GMRG6 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803023 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 120.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -5.000 ppm  
 F3 -6283.90 Hz  
 GPCOM 0.00000000 ppm/cm  
 HPCOM 1241.25305 Hz/cm

<sup>1</sup>H spectrum



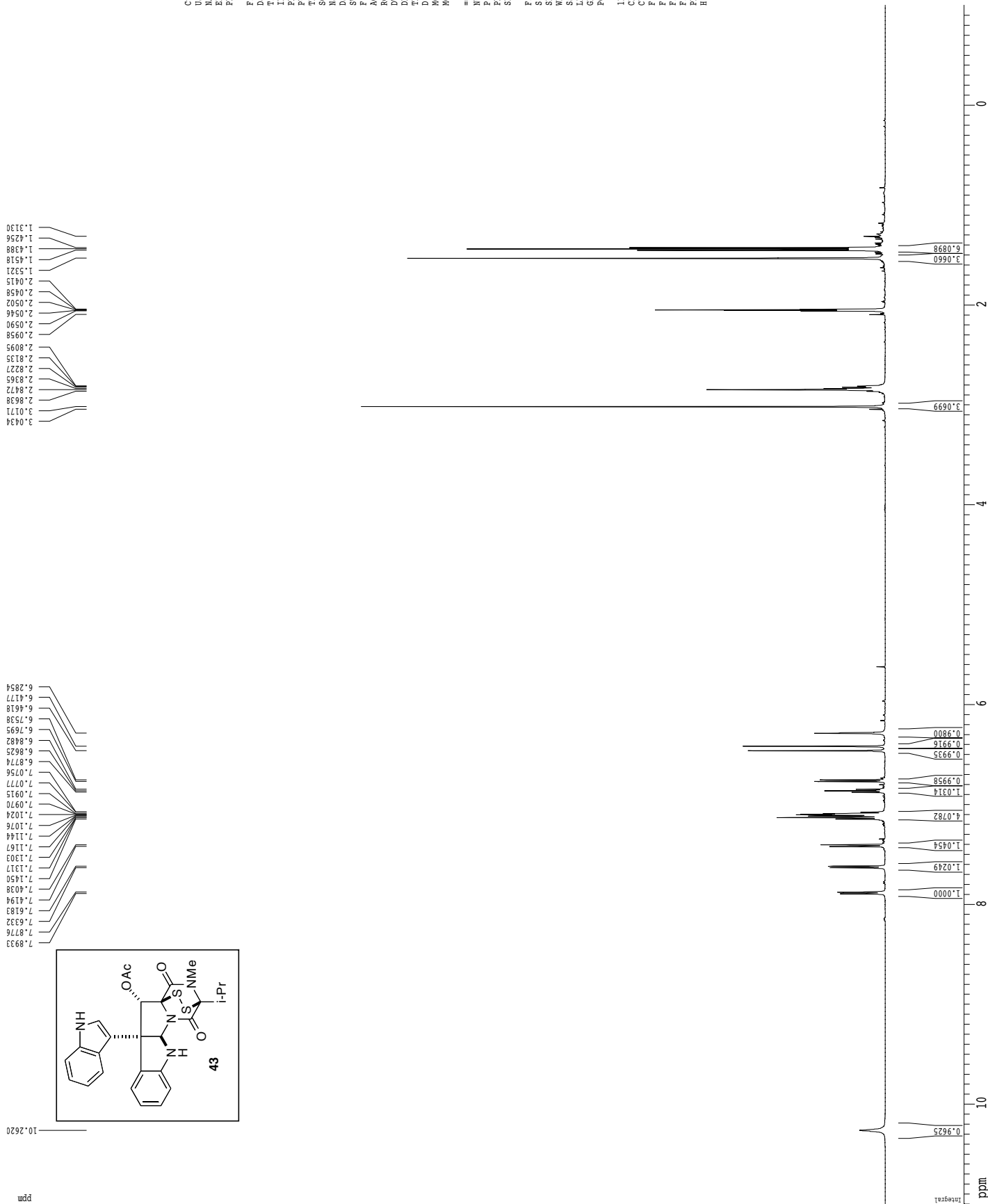
Current Data Parameters  
 USER johndel  
 NAME jes2-167  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120531  
 Time 9.21  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0990774 sec  
 RG 415  
 DE 62.600 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

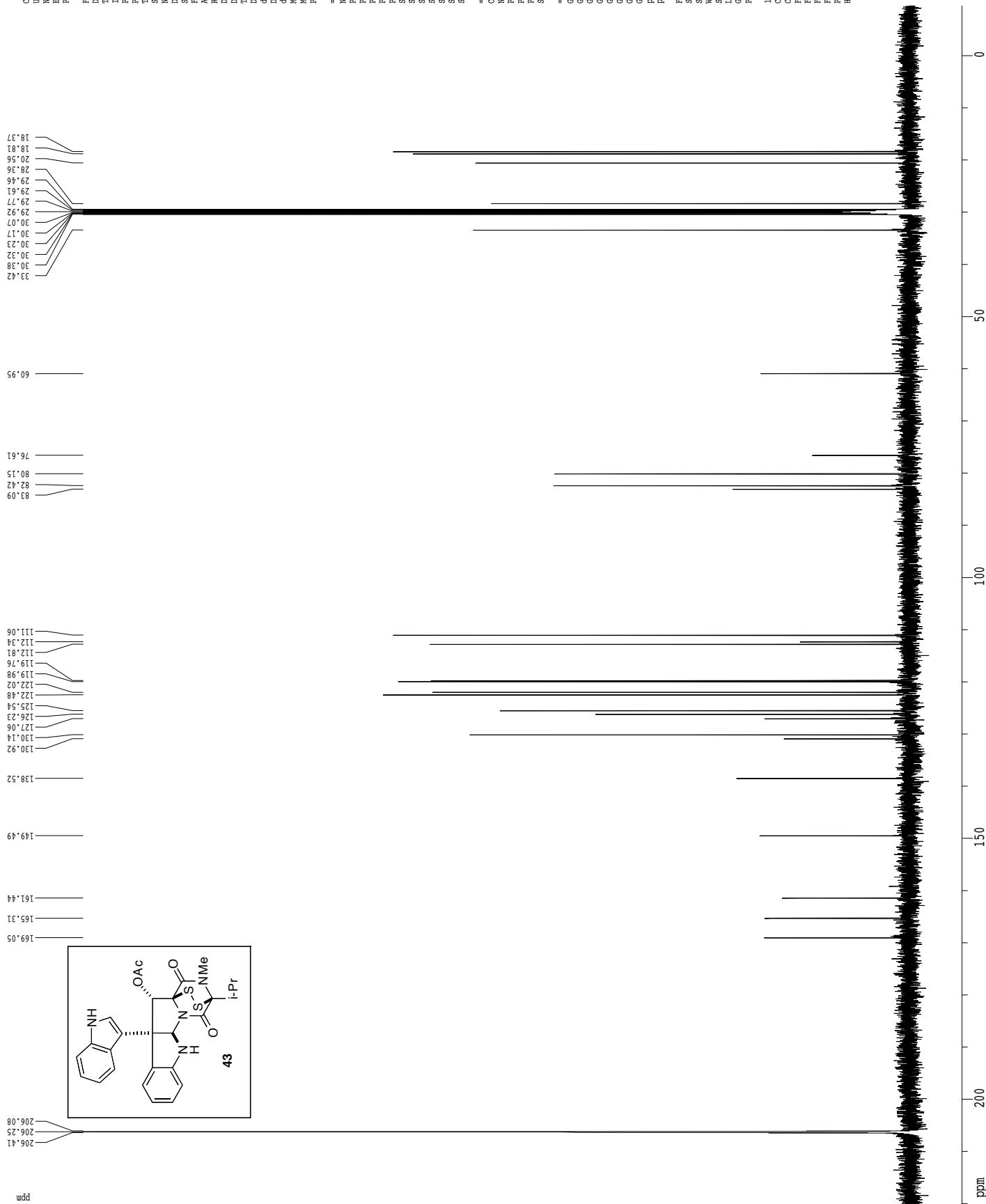
F2 - Processing parameters  
 SI 65535  
 SF 500.220181 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 11.000 ppm  
 F2 550.22 Hz  
 F3 10.000 ppm  
 F4 -50.92 ppm  
 PPM0 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

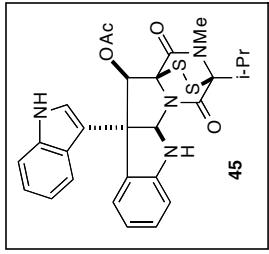
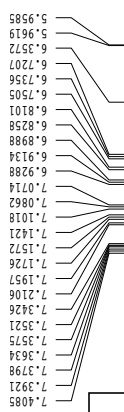
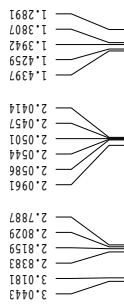




Z-restored spin-echo 13C spectrum with 1H decoupling



<sup>1</sup>H spectrum



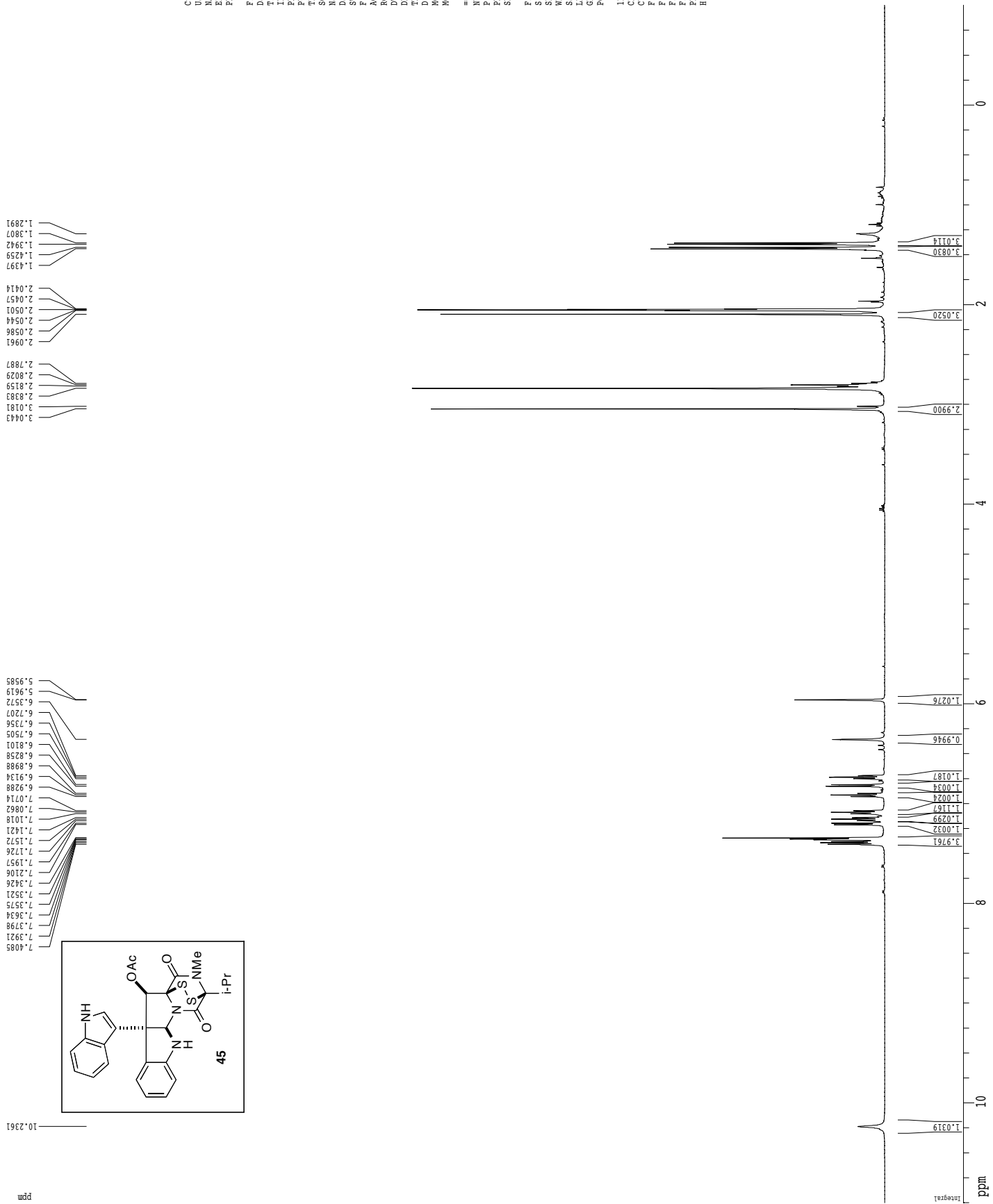
Current Data Parameters  
 USER JohnDl  
 NAME Jes2-169  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120602  
 Time 18.32  
 INSTRUM cryo500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 62.400 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

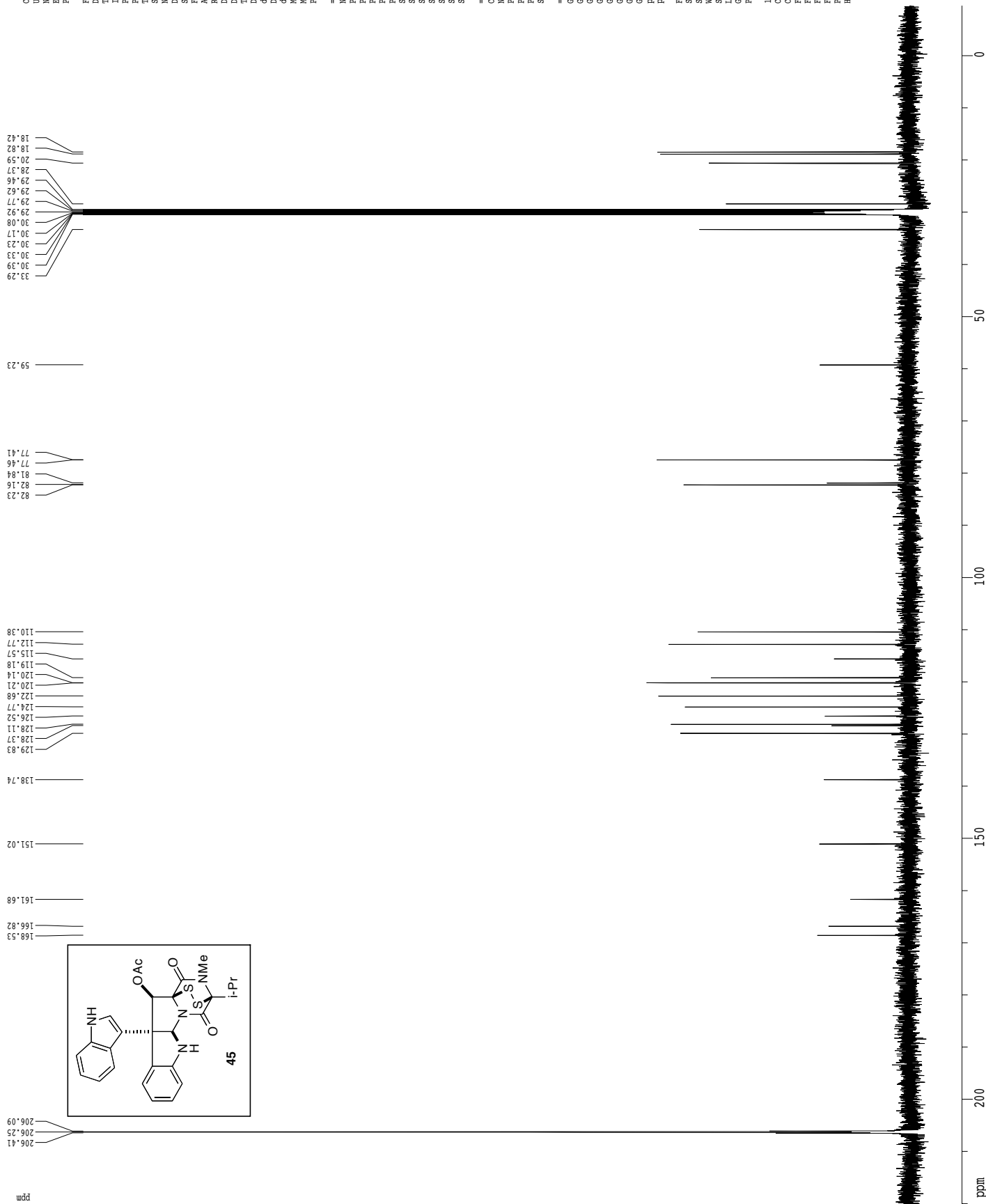
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220183 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 9.00 cm  
 FIP 11.000 ppm  
 F2 550.22 Hz  
 F3 -50.92 ppm  
 FPMCM 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jomdl  
 EXPNO jed-419  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120602  
 Time 18.40  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 JH  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 816  
 DS 16  
 SHR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 3260.5  
 DW 6.00 usec  
 DE 19.00 usec  
 TE 298.2 K  
 D1 0.25000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.00 usec

===== CHANNEL f1 =====  
 NU1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 MHz  
 PL2 125.761868 MHz  
 SP1 3.20 dB  
 SP2 3.20 dB  
 SFO1 Ccp60.0.5.20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

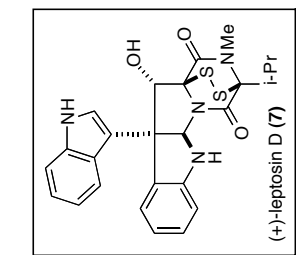
===== CHANNEL f2 =====  
 CPDPRG2 wd1616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR1 0.00 %  
 GSPR2 0.00 %  
 GSPR3 0.00 %  
 GSPR4 0.00 %  
 GSPR5 30.00 %  
 GSPR6 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803005 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 5.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2P -10.000 ppm  
 F2 -125.780 Hz  
 F2PCH 10.000 ppm/cm  
 HECN 1268.83645 Hz/cm

<sup>1</sup>H spectrum



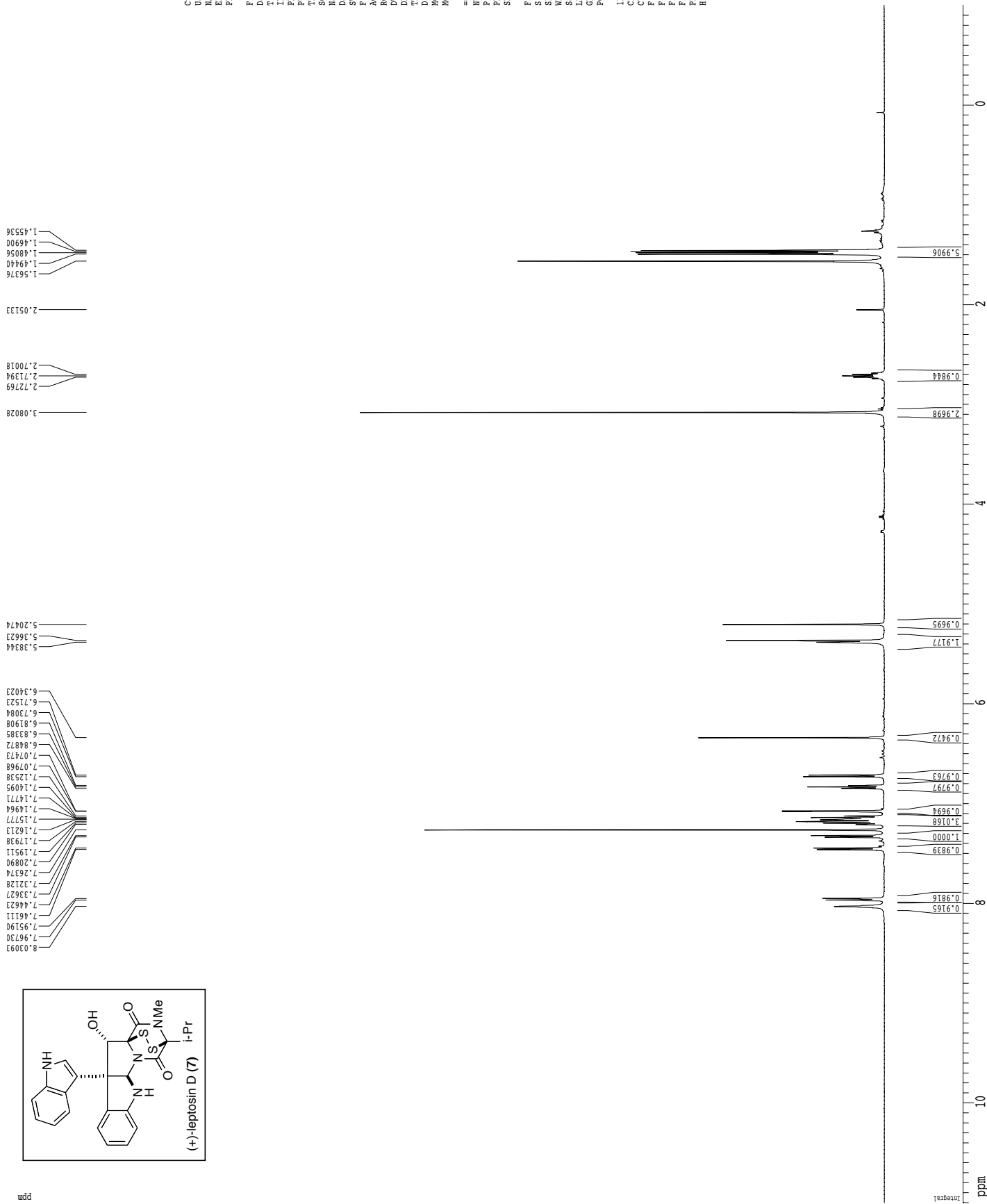
Current Data Parameters  
 USER johnd  
 NAME jes2-185  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120615  
 Time 19.27  
 INSTRUM crys500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CCl3  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 127.0  
 DR 6.00 usec  
 DE 5.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

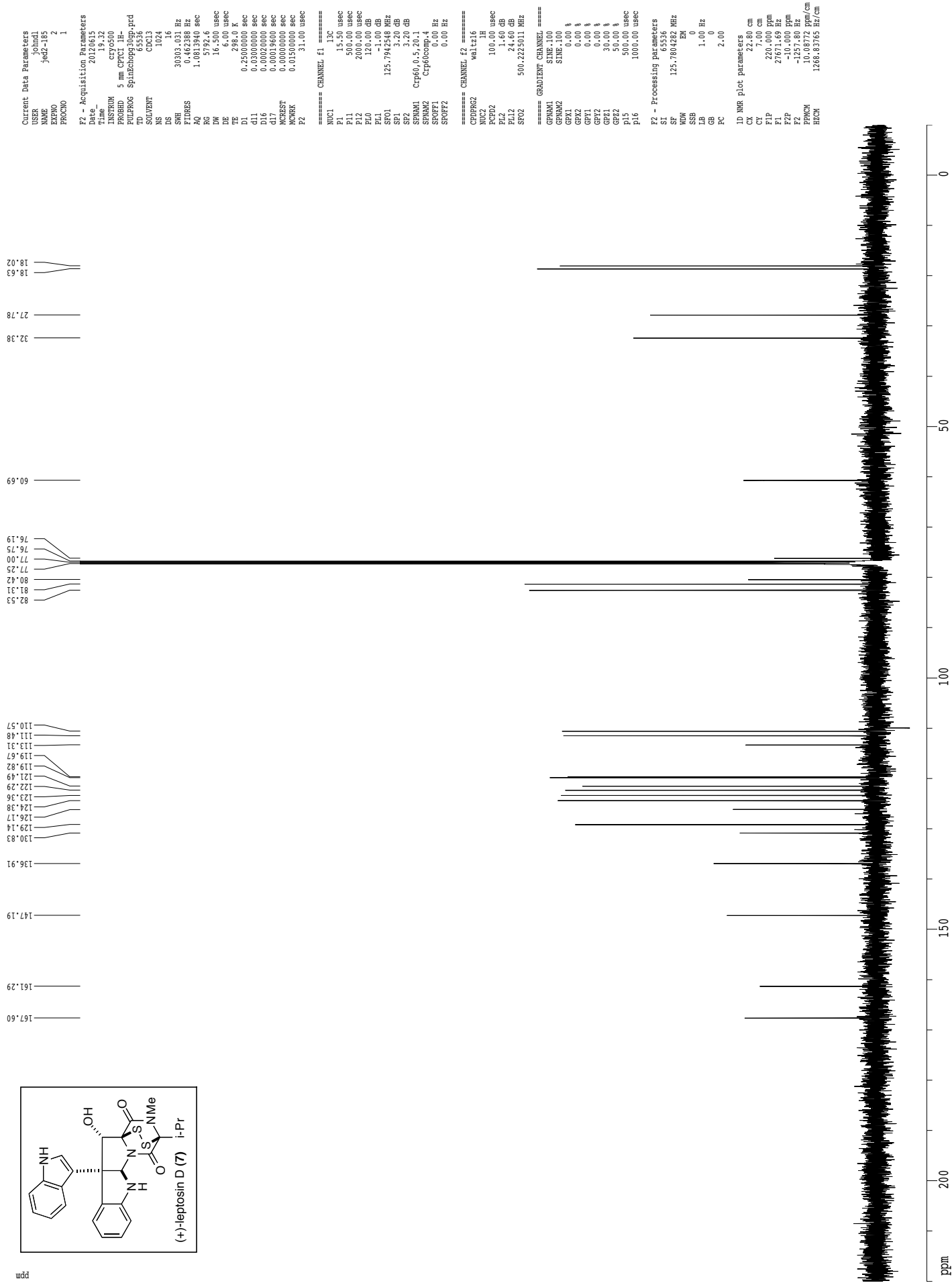
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65535  
 SF 500.220291 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 11.000 ppm  
 F2 42.82 Hz  
 F3 16.00 ppm  
 F4 -50.92 ppm  
 PPM0 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm



## Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER johnd1  
 NAME jes2-185  
 EXNO 4  
 PROCNO 1

F2 - Acquisition Parameters

Date 20120615  
 Time 20.12  
 INSTRUM cryo500  
 PROBDH 5 mm CPXI IH-  
 PULPROG invfqp.wu  
 TD 2048  
 SOLVENT CDCl3  
 NS 12  
 DS 2  
 SWH 3763.754 Hz  
 FIDRES 1.832888 Hz  
 AQ 0.2728436 sec  
 RG 11585.2  
 DW 133.200 usec  
 DE 6.50 usec  
 TE 298.0 K  
 CHSTZ 145.000000  
 U1 0.000000 sec  
 U2 2.000000 sec  
 d1 0.00344828 sec  
 d2 0.0002000 sec  
 d12 0.0000300 sec  
 d13 0.0000300 sec  
 D16 0.0020000 sec  
 d20 0.0024258 sec  
 INO 0.0002400 sec

\*\*\*\*\* CHANNEL F1 \*\*\*\*\*

NUC1 1H  
 P1 7.50 usec  
 P2 15.00 usec  
 PL1 1.60 dB  
 SFO1 500.2224021 MHz

\*\*\*\*\* CHANNEL F2 \*\*\*\*\*

CPDPRG2 gact  
 NUC2 15N  
 P1 15.50 usec  
 P2 65.00 usec  
 PL2 -1.00 dB  
 PL12 11.30 dB  
 SFO2 125.7920628 MHz

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*

GPMAX1 size-100  
 GMXZ2 size-100  
 GMXZ3 size-100  
 GXY1 0.00 %  
 GPX2 0.00 %  
 GPX3 0.00 %  
 GPY1 0.00 %  
 GPY2 0.00 %  
 GPY3 0.00 %  
 GPZ1 30.00 %  
 GPZ2 0.00 %  
 GPZ3 2.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters

ND0 2  
 TD 128  
 SFO1 125.7921 MHz  
 FIDRES 162.760422 Hz  
 SW 465.617 Ppm  
 FWHM undefined

F2 - Processing parameters

SI 1024  
 SF 500.2200291 MHz  
 WDM EM  
 SSB 0  
 LB 5.00 Hz  
 GB 0  
 PC 2.00

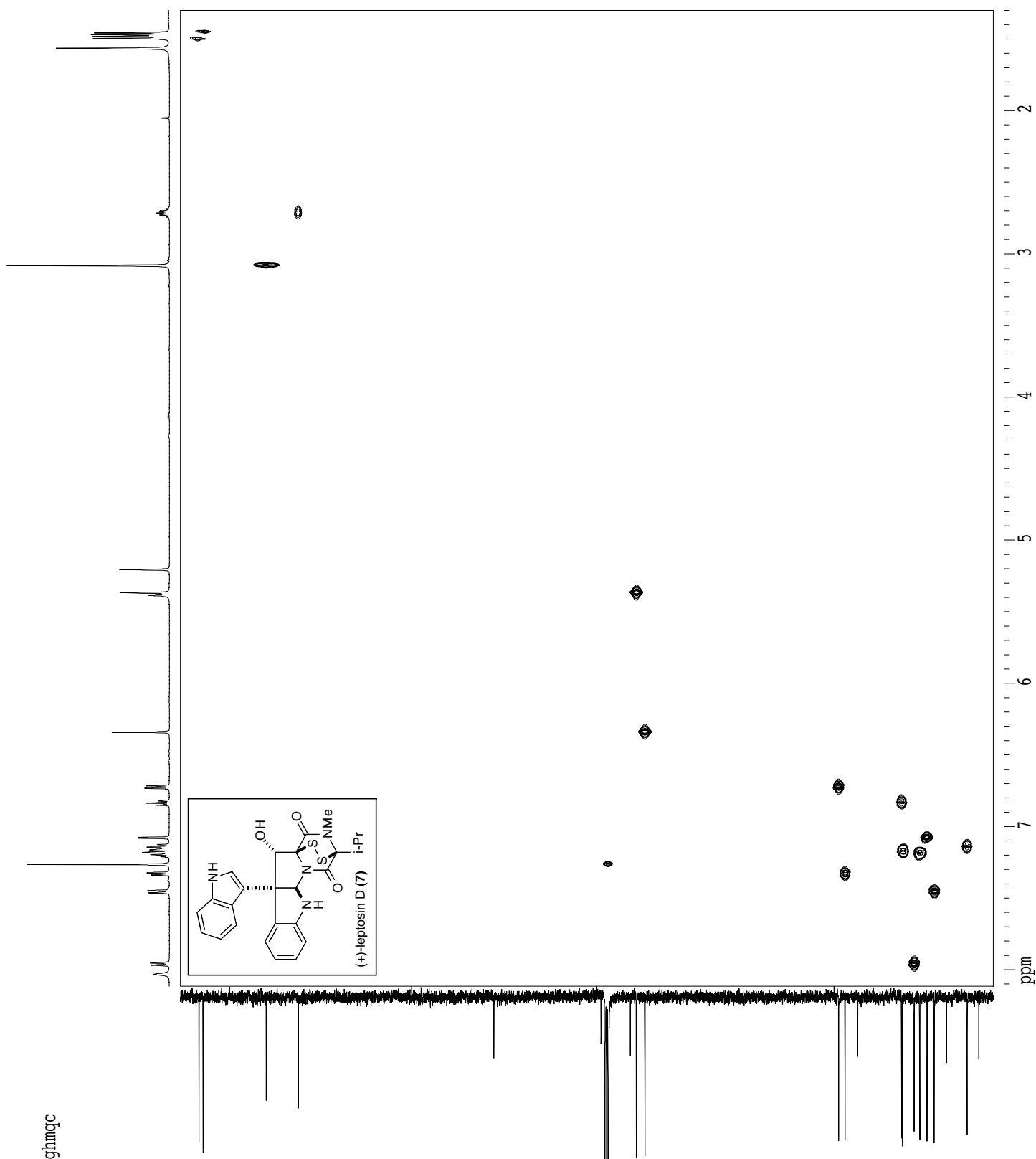
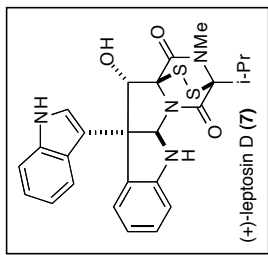
F1 - Processing parameters

SI 1024  
 MCX QF  
 SF 125.7804282 MHz  
 WDM Q8INE  
 SSB 3  
 LB 0.00 Hz  
 GB 0

2D NMR plot parameters

CX2 18.00 cm  
 CX1 15.00 cm  
 F2PLO 8.115 ppm  
 F2LO 4059.26 Hz  
 F2PHI 1.300 ppm  
 F2HI 650.09 Hz  
 F1PLO 1622.98 ppm  
 F1PHI 15.345 ppm  
 F1HI 1030.10 Hz  
 F2PMCH 0.37863 ppm/cm  
 F2HCM 189.38939 Hz/cm  
 F1PMCH 7.83951 ppm/cm  
 F1HCM 966.05676 Hz/cm

ghmqc



ppm

2

3

4

5

6

7

Current Data Parameters  
 USER johnd1  
 NAME j642-185  
 EXPTNO 3  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20120615  
 Time 19:55  
 INSTRUM spect  
 PROBEID 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 4096  
 SOLVENT gdmco  
 NS 2  
 DS 16  
 SWH 3753.754 Hz  
 FIDRES 0.516444 Hz  
 AQ 0.5456372 sec  
 RG 14596.5  
 DW 133.200 usec  
 DE 9.00 usec  
 TE 300.2 K  
 C13F2 145.000000 sec  
 d0 0.00000300 sec  
 D1 1.25900000 sec  
 d2 0.00344828 sec  
 D6 0.05900000 sec  
 d13 0.00000300 sec  
 D16 0.00020000 sec  
 INO 0.00002400 sec

==== CHANNEL f1 =====

NVC1 1H  
 P1 7.50 usec  
 PL 15.00 usec  
 PL2 -1.00 dB  
 SF01 500.2224021 MHz

==== CHANNEL f2 =====

NVC2 13C  
 P3 15.50 usec  
 PL2 -1.00 dB  
 SF02 125.7920628 MHz

==== GRADIENT CHANNEL =====

GPW01 sine,100  
 GPW02 sine,100  
 GPW03 sine,100  
 GPX1 0.00 %  
 GPX2 0.00 %  
 GPX3 0.00 %  
 GPY1 0.00 %  
 GPY2 0.00 %  
 GPY3 0.00 %  
 GPZ1 50.00 %  
 GPZ2 30.00 %  
 GPZ3 40.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters

NU0 95.2  
 SF01 125.7923 MHz  
 FIDRES 81.380211 Hz  
 SW 165.617 ppm  
 FWHM undefined

F2 - Processing parameters

SF 2648  
 SF 500.2200291 MHz  
 WDW SINE  
 SSB 0  
 GB 0  
 PC 2.00

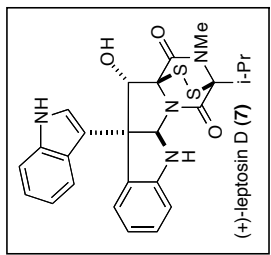
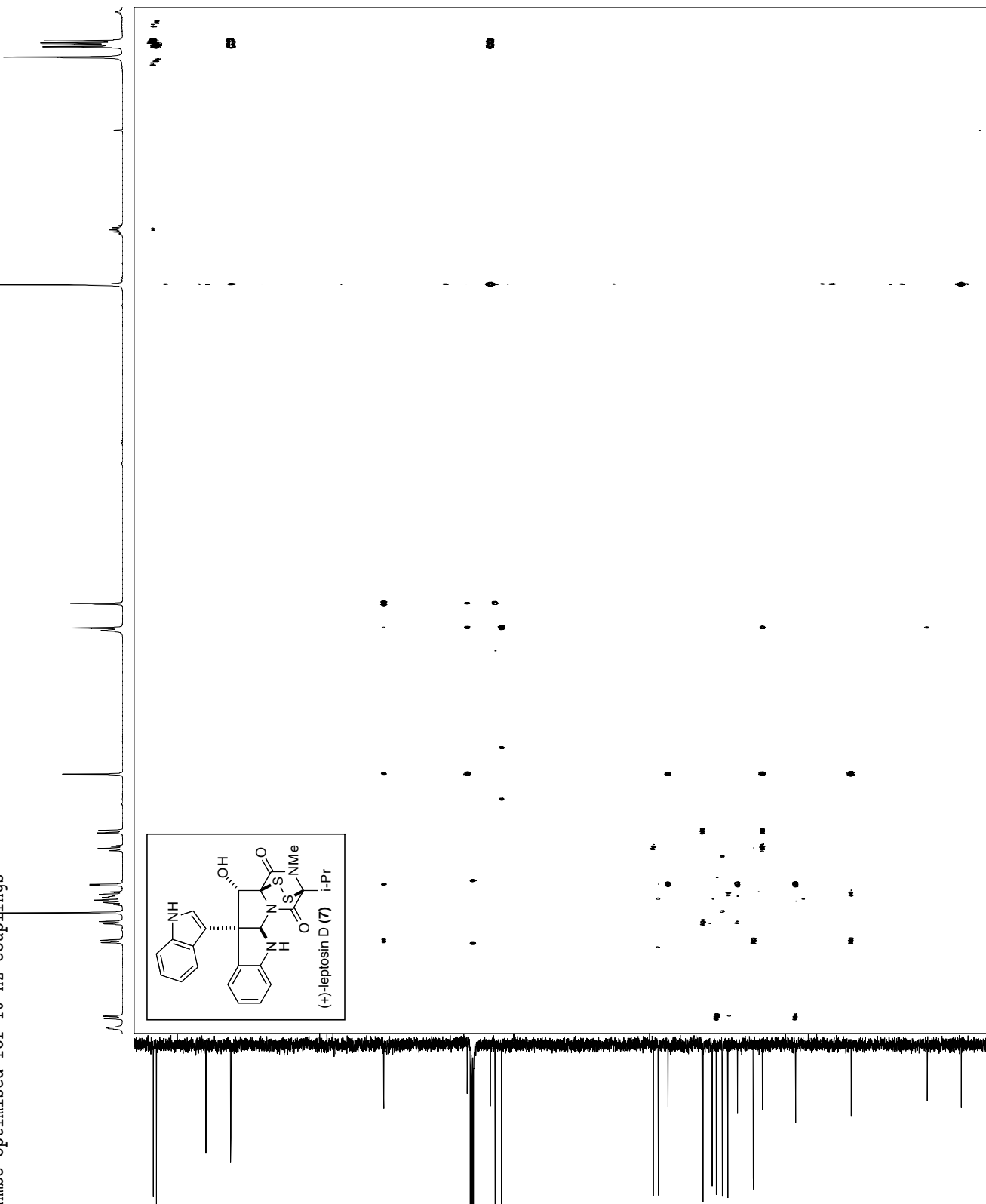
F1 - Processing parameters

SI 1024  
 MC2 CF  
 SF 125.7804282 MHz  
 WDW SINE  
 SSB 0  
 GB 0

2D NMR plot parameters

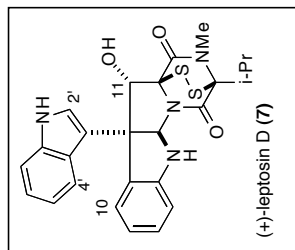
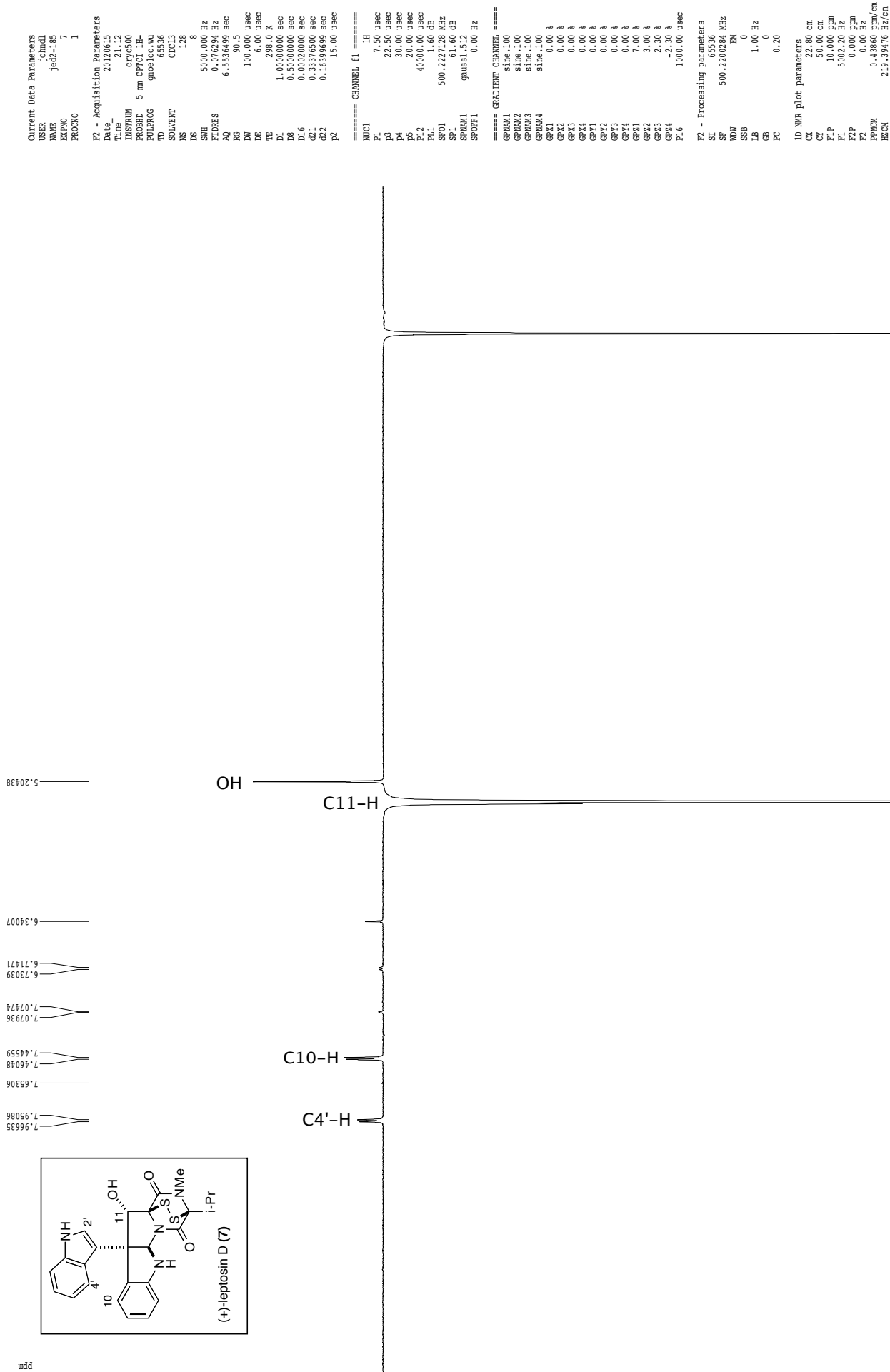
CX2 18.00 cm  
 CX1 15.00 cm  
 FZEO 8.00 ppm  
 FZFO 403.20 Hz  
 FZHI 11.20 ppm  
 FZHI 615.26 Hz  
 F1FO 172.890 ppm  
 F1LO 21146.18 Hz  
 F1HI 14.536 ppm  
 F1HI 1828.38 Hz  
 F2P0ACH 0.37985 ppm/cm  
 F2H0CH 190.00935 Hz/cm  
 F1P0ACH 10.55692 ppm/cm  
 F1H0CH 1327.85364 Hz/cm

ghmhc optimised for 10 Hz couplings

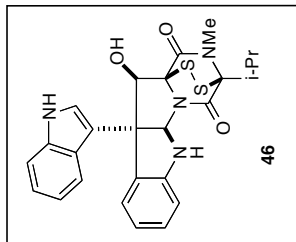


ppm

gnoe





<sup>1</sup>H spectrum

1.58952  
1.50022  
1.48639  
1.45531  
1.44166

3.09271

5.32512

5.95814  
6.06979

6.75965  
6.77532  
6.85771  
7.10260  
7.10789  
7.19969  
7.21478  
7.23030  
7.27008  
7.27008  
7.38165  
7.39793  
7.56826  
7.58436  
7.60138  
7.61625

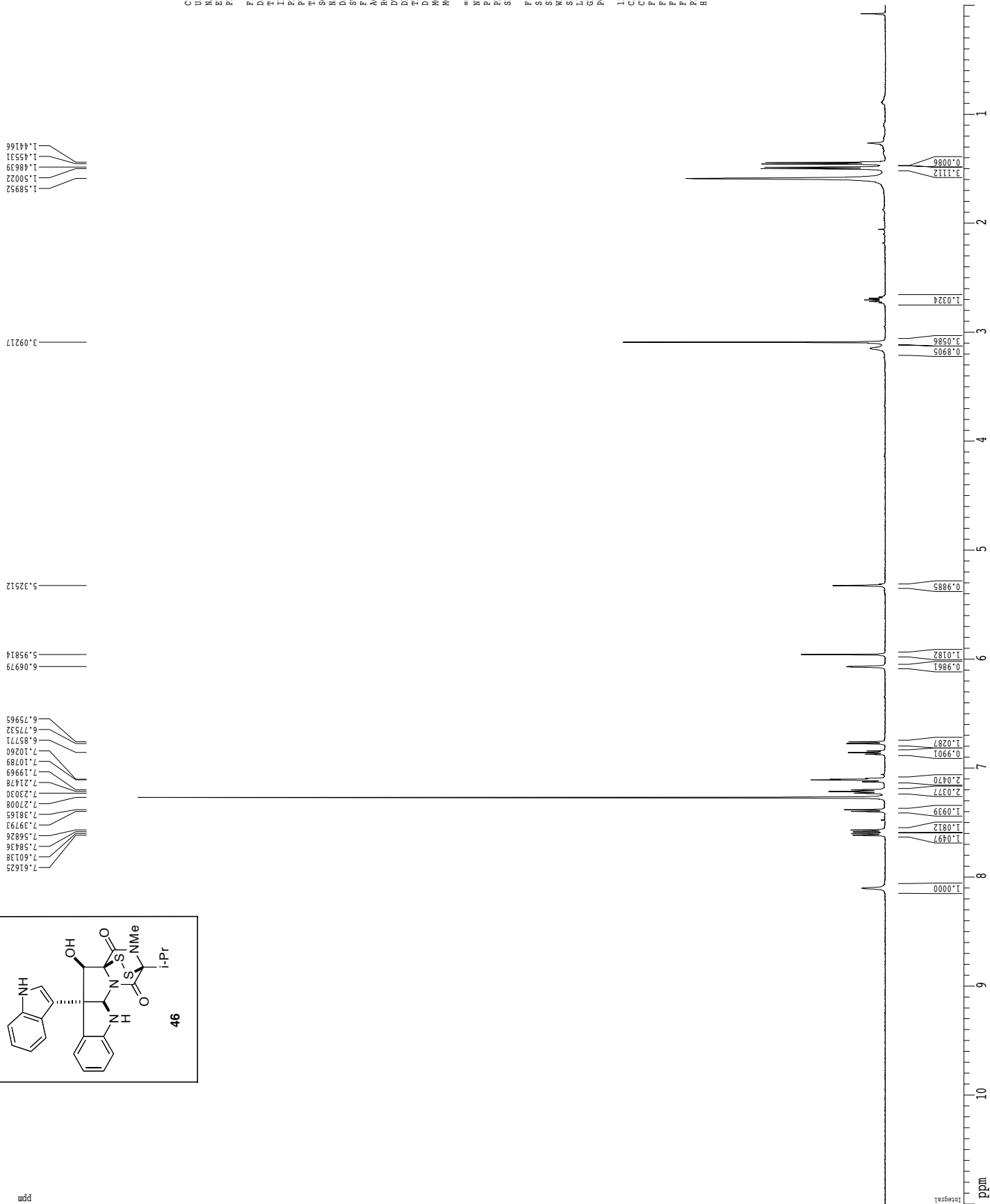
Current Data Parameters  
 USER johndf  
 NAME jes2-186  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120615  
 Time 19.18  
 INSTRUM crys500  
 PROBRD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 8  
 DE 62.40 usec  
 DR 5.00 usec  
 TE 298.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

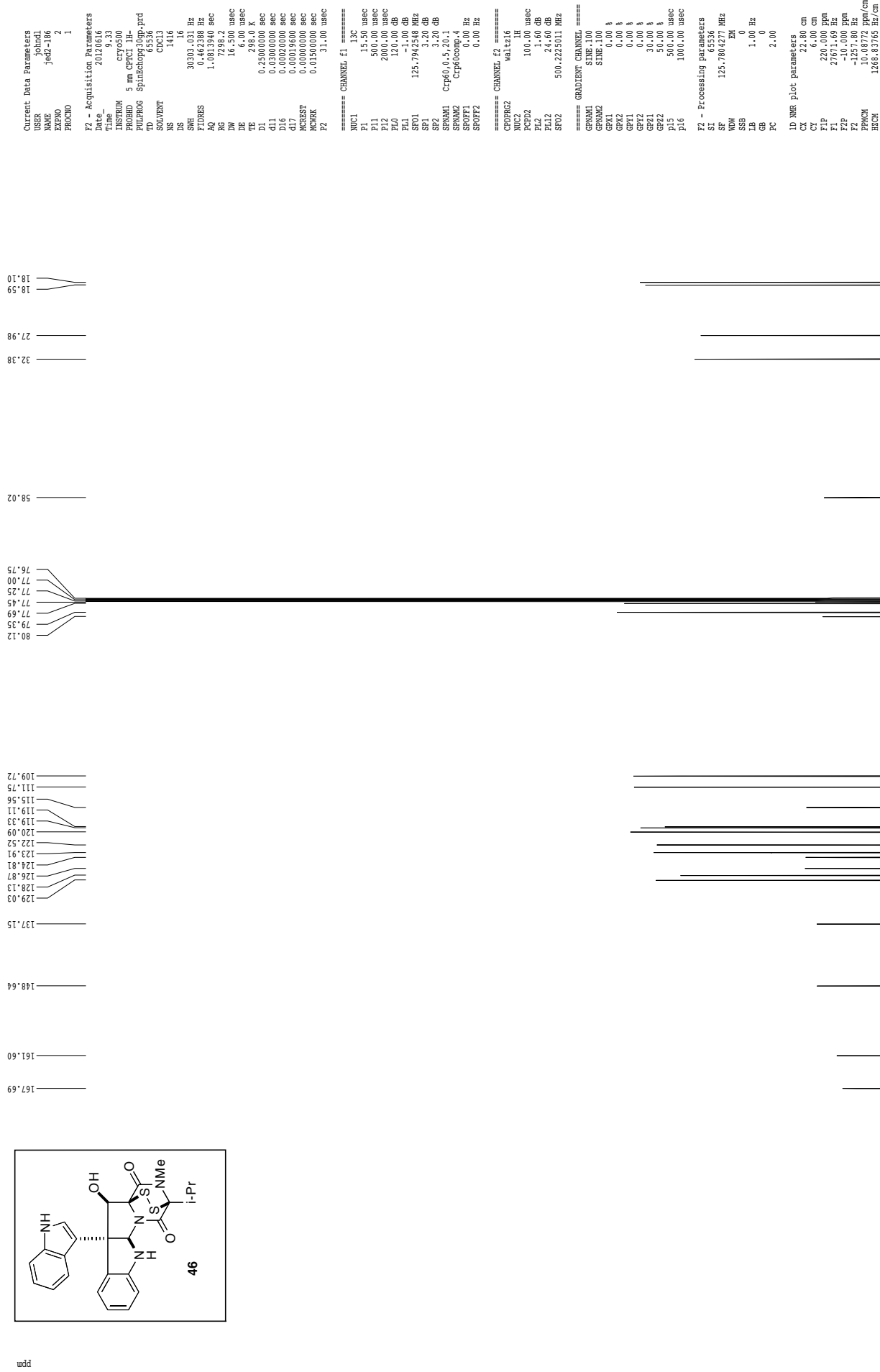
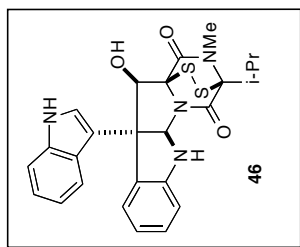
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2020260 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.50

1D NMR plot parameters  
 CX 22.80 cm  
 CY 5.00 cm  
 FIP 11.000 ppm  
 SFO2 550.242 Hz  
 F2 0.00 ppm  
 F2 0.00 ppm  
 PPMCM 0.48246 ppm/cm  
 HZCM 241.33423 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER johnd1  
 NAME jes42-186  
 EXNO 4  
 PROCNO 1

F2 - Acquisition Parameters

Date 20121016  
 Time 10.23  
 INSTRUM cryo500  
 PROBDH 5 mm CPXI IH-  
 PULPROG invf4gpr.wu  
 TD 2048  
 SOLVENT CDCl3  
 NS 12  
 DS 1  
 SWH 3591.954 Hz  
 FIDRES 1.753884 Hz  
 AQ 0.2851316 sec  
 RG 18390.4  
 DW 139.200 usec  
 DE 6.50 usec  
 TE 298.0 K  
 CHSYZ 145.000000  
 U 1.000000 sec  
 D1 2.000000 sec  
 d2 0.00344828 sec  
 d12 0.00002000 sec  
 d13 0.00003000 sec  
 D16 0.00020000 sec  
 d20 0.00242528 sec  
 INO 0.00002340 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

NUC1 <sup>1</sup>H  
 P1 7.50 usec  
 P2 15.00 usec  
 PL1 1.60 dB  
 SFO1 500.2223770 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*

CPDPRG2 garr  
 NU2 <sup>13</sup>C  
 P1 15.50 usec  
 P2 65.00 usec  
 PL2 -1.00 dB  
 PL12 11.30 dB  
 SFO2 125.7923768 MHz

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*

GPM11 size:100  
 GMX2 size:100  
 GMX3 size:100  
 GXY1 0.00 %  
 GPX2 0.00 %  
 GPX3 0.00 %  
 GPY1 0.00 %  
 GPY2 0.00 %  
 GPY3 0.00 %  
 GPZ1 30.00 %  
 GPZ2 0.00 %  
 GPZ3 2.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters

ND0 2  
 TD 64  
 SFO1 125.7924 MHz  
 FIDRES 333.867523 Hz  
 SW 169.863 ppm  
 FWHM undefined

F2 - Processing parameters

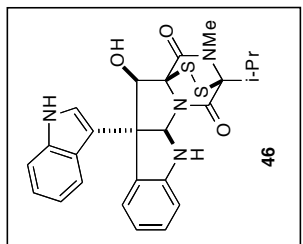
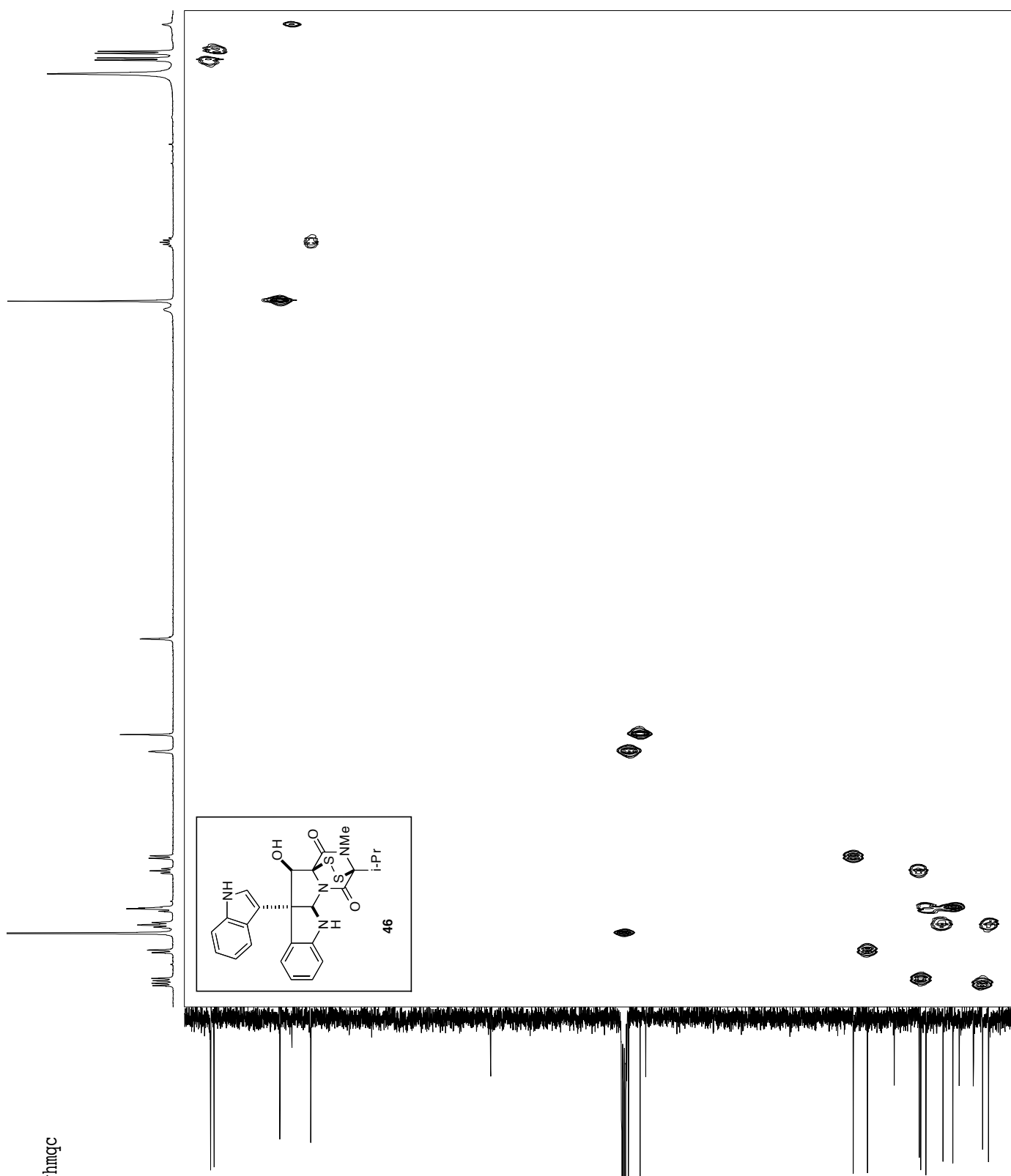
SI 1024  
 SF 500.2200260 MHz  
 WDM EM  
 SSB 0  
 LB 5.00 Hz  
 GB 0  
 PC 4.00

F1 - Processing parameters

SI 1024  
 MC2 OF  
 SF 125.7804277 MHz  
 WDM QSIDE  
 SSB 3  
 LB 0.00 Hz  
 GB 0

ZD NMR plot parameters

CX2 18.00 cm  
 CX1 15.00 cm  
 F2PLO 7.757 ppm  
 FZLO 3880.42 Hz  
 FZHI 1.173 ppm  
 FZHI 586.62 Hz  
 F1PLO 132.825 ppm  
 F1PLO 162.825 ppm  
 F1PHI 14.374 ppm  
 F1HI 1807.92 Hz  
 F2FPMCH 0.36582 ppm/cm  
 F2HCM 182.98854 Hz/cm  
 F1FPMCH 7.89674 ppm/cm  
 F1HCM 991.25586 Hz/cm



ghmqc

Current Data Parameters  
 USER johnd1  
 NAME j642-186  
 EXPTNO 3  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20120616  
 Time 10:07  
 INSTRUM spect  
 PROBRD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 4096  
 SOLVENT CDCl3  
 NS 2  
 DS 16  
 SWH 3591.954 Hz  
 FIDRES 0.876942 Hz  
 AQ 0.5702132 sec  
 RG 14596.5  
 DW 139.200 usec  
 DE 9.00 usec  
 TE 300.2 K  
 CREST2 145.0000000  
 d0 0.00000300 sec  
 D1 1.25000000 sec  
 d1 0.00344828 sec  
 D6 0.05000000 sec  
 d13 0.00000300 sec  
 D16 0.00020000 sec  
 INO 0.00002340 sec

==== CHANNEL f1 =====

NVC1 IH  
 F1 7.50 usec  
 PL 15.00 usec  
 PL2 -1.00 dB  
 SF01 500.2223770 MHz

==== CHANNEL f2 =====

NVC2 13C  
 F2 15.50 usec  
 PL2 -1.00 dB  
 SF02 125.7923768 MHz

==== GRADIENT CHANNEL =====

GPW01 sine,100  
 GPW02 sine,100  
 GPW03 sine,100  
 GPW04 0.00 %  
 GPW05 0.00 %  
 GPW06 0.00 %  
 GPW07 0.00 %  
 GPW08 0.00 %  
 GPW09 0.00 %  
 GPW10 0.00 %  
 GPW11 0.00 %  
 GPW12 0.00 %  
 GPW13 50.00 %  
 GPW14 30.00 %  
 GPW15 40.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters

NU0 95.2  
 SF01 125.7923 MHz  
 FIDRES 83.666881 Hz  
 SW 169.843 ppm  
 FWHM undefined

F2 - Processing parameters

SF 2648  
 SF 500.2200260 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 4.00

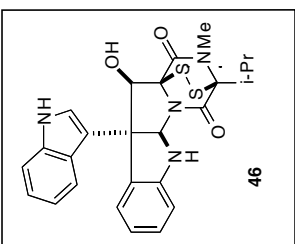
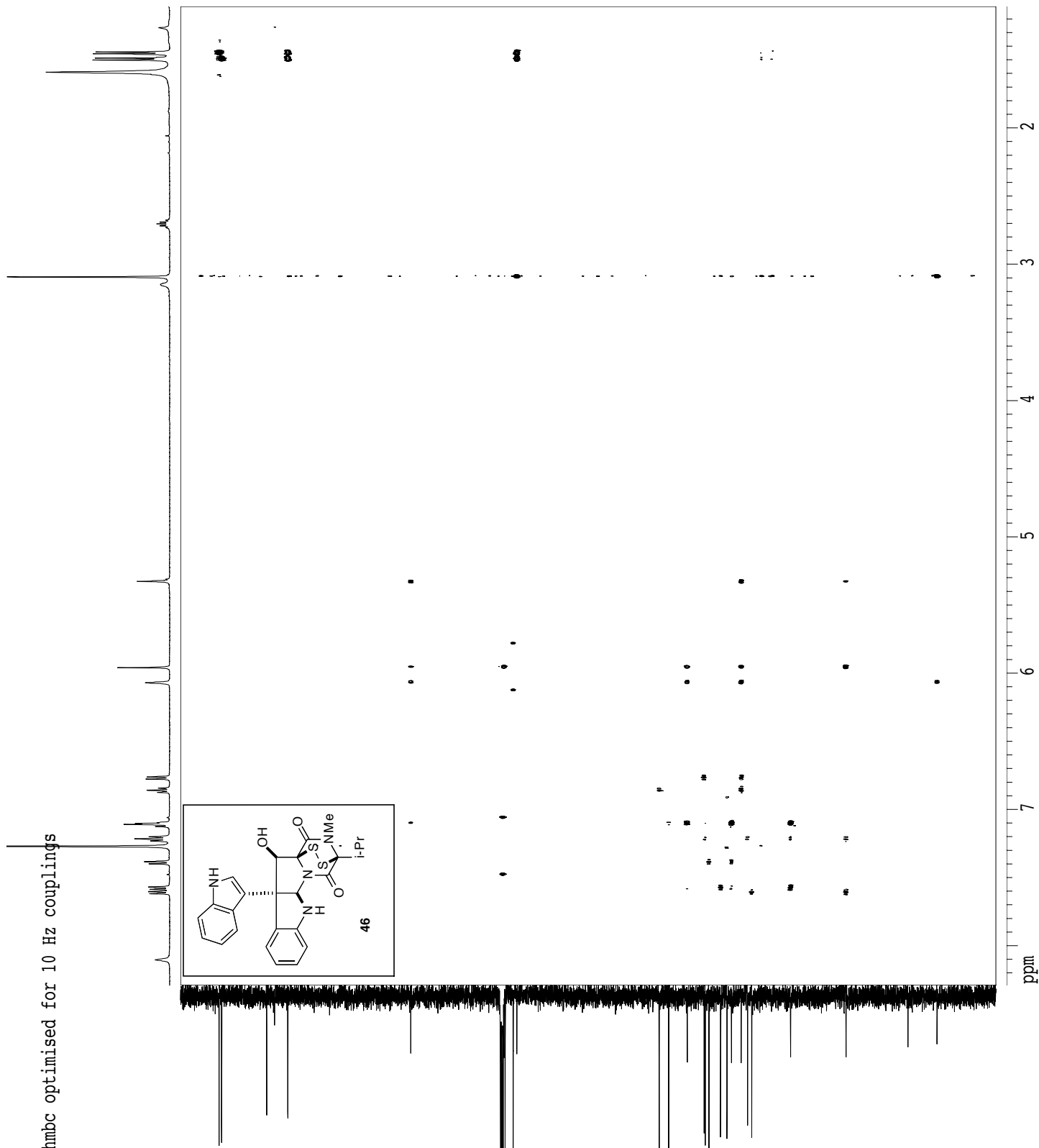
F1 - Processing parameters

NU2 102.0  
 SF 125.7804277 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

2D NMR plot parameters

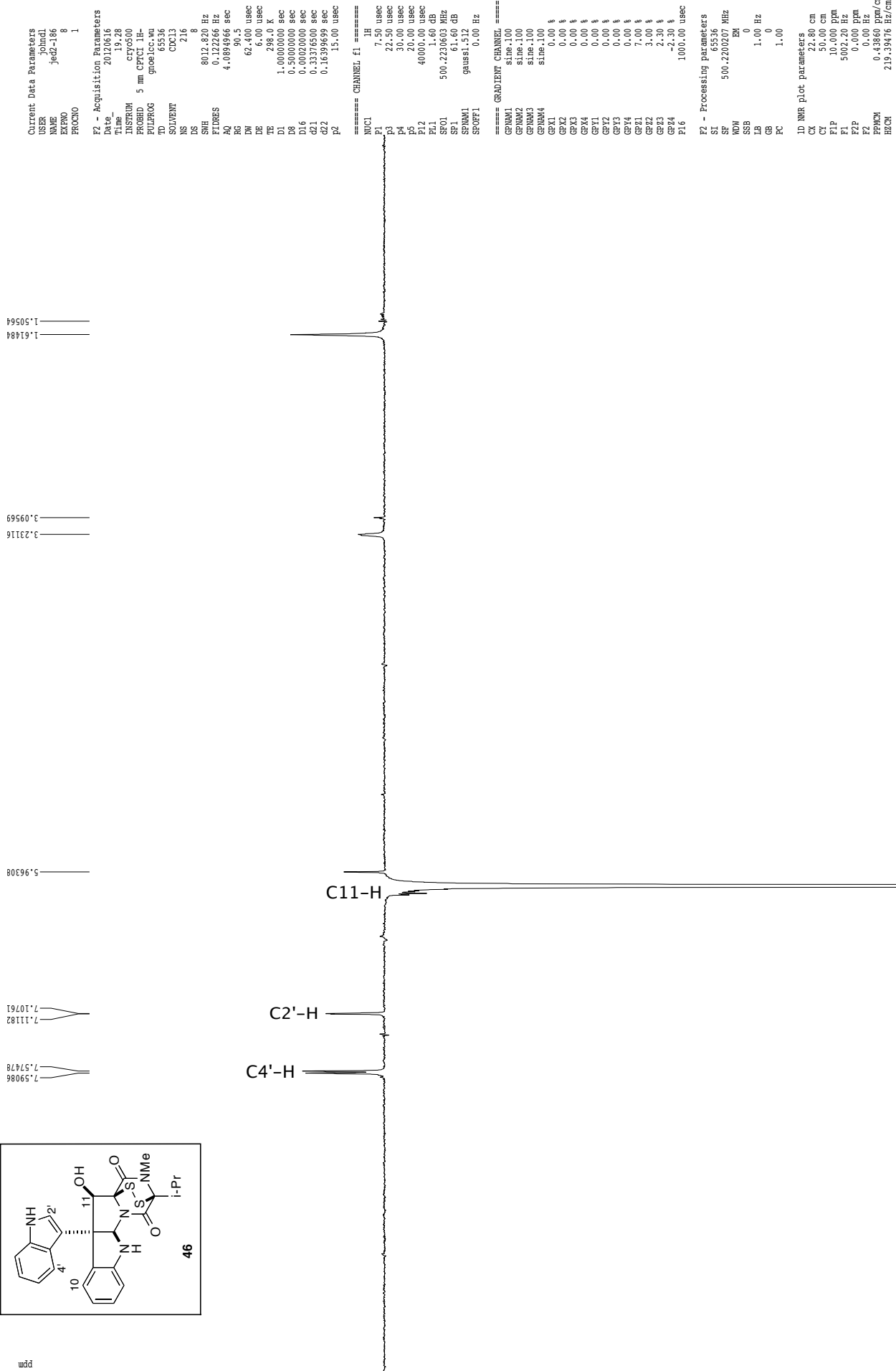
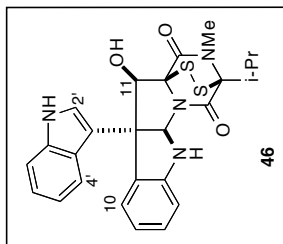
CX2 18.00 cm  
 CX1 15.00 cm  
 FZPZ0 8.230 ppm  
 FZPZ1 11.110 Hz  
 FZPHI 555.05 Hz  
 F1F0 179.940 ppm  
 F1F1 22632.90 Hz  
 F1PHI 10.060 ppm  
 F1H 1265.38 Hz  
 F2PZPACH 0.39893 ppm/cm  
 F2HZCN 199.55299 Hz/cm  
 F1PZPACH 11.32530 ppm/cm  
 F1HZCN 1424.50146 Hz/cm

ghmhc optimised for 10 Hz couplings



ppm

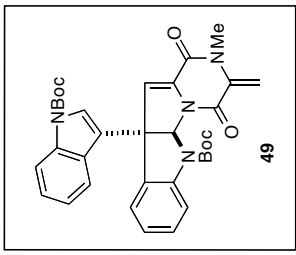
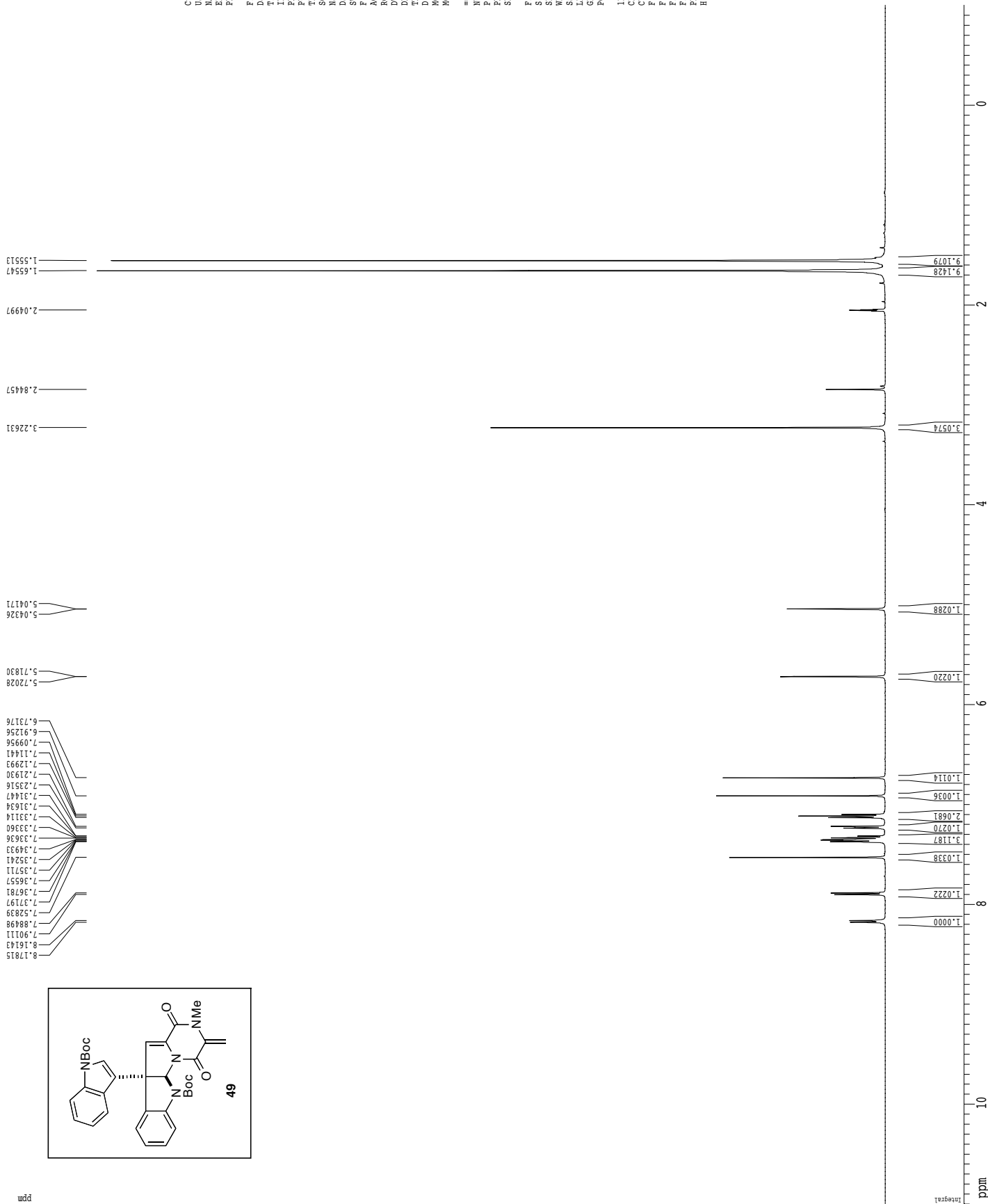
gnoe



ppm

Integral

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jed1-216  
 EXPNO 1  
 PROCNO 1

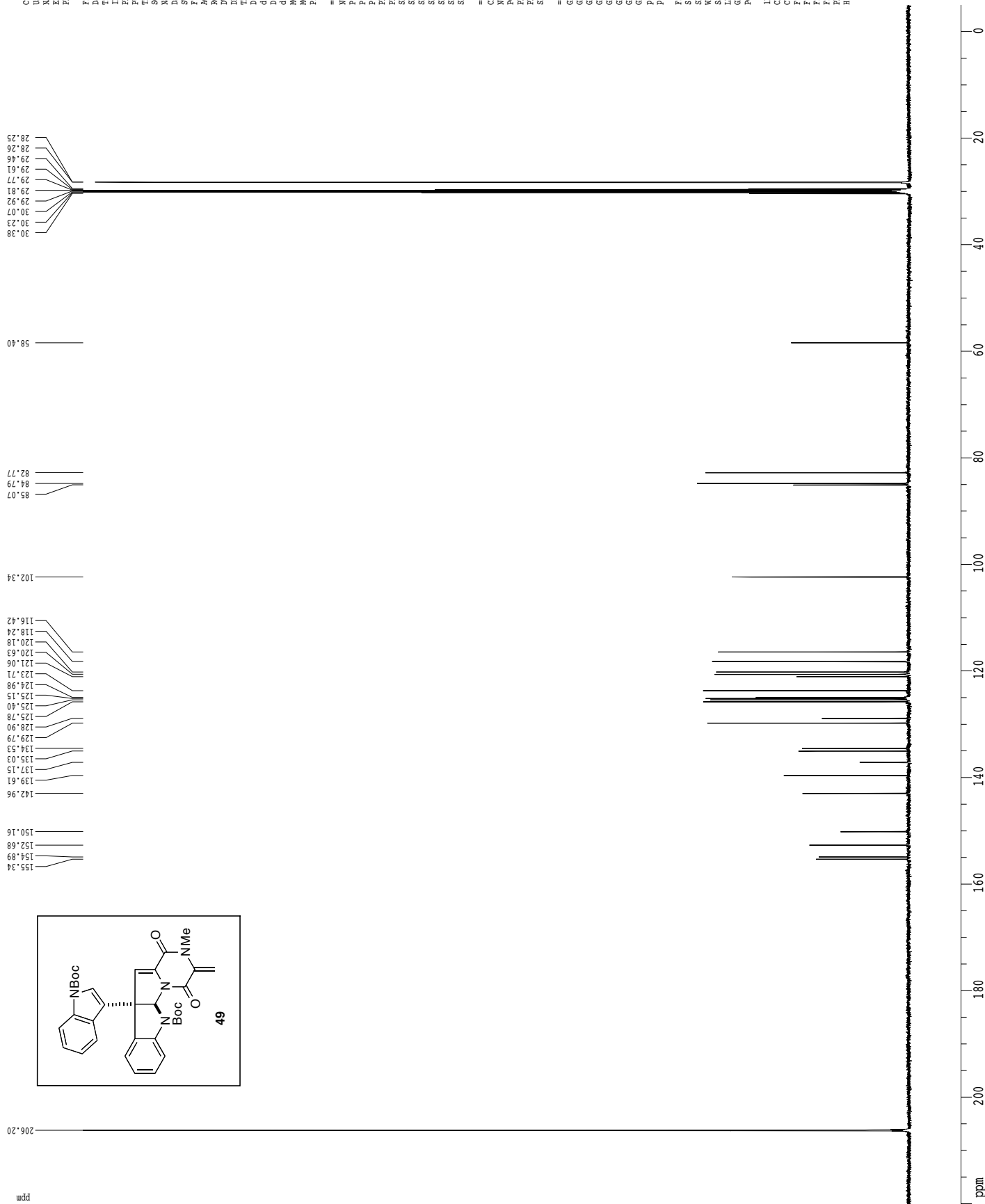
F2 - Acquisition Parameters  
 Date\_ 20110527  
 Time 16.21  
 INSTRUM cryo500  
 PROBRID 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0990774 sec  
 RG 415  
 DE 62.60 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220184 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 3.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F1 5902.82 Hz  
 F2 10.000 ppm  
 F3 -500.92 ppm  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER joudl  
 EXPNO jedi-212  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 2011027  
 Time 16.24  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 160  
 DS 16  
 SHR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813941 sec  
 RG 4096  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.50000000 sec  
 D11 0.03000000 sec  
 D16 0.00020000 sec  
 D17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.00 usec

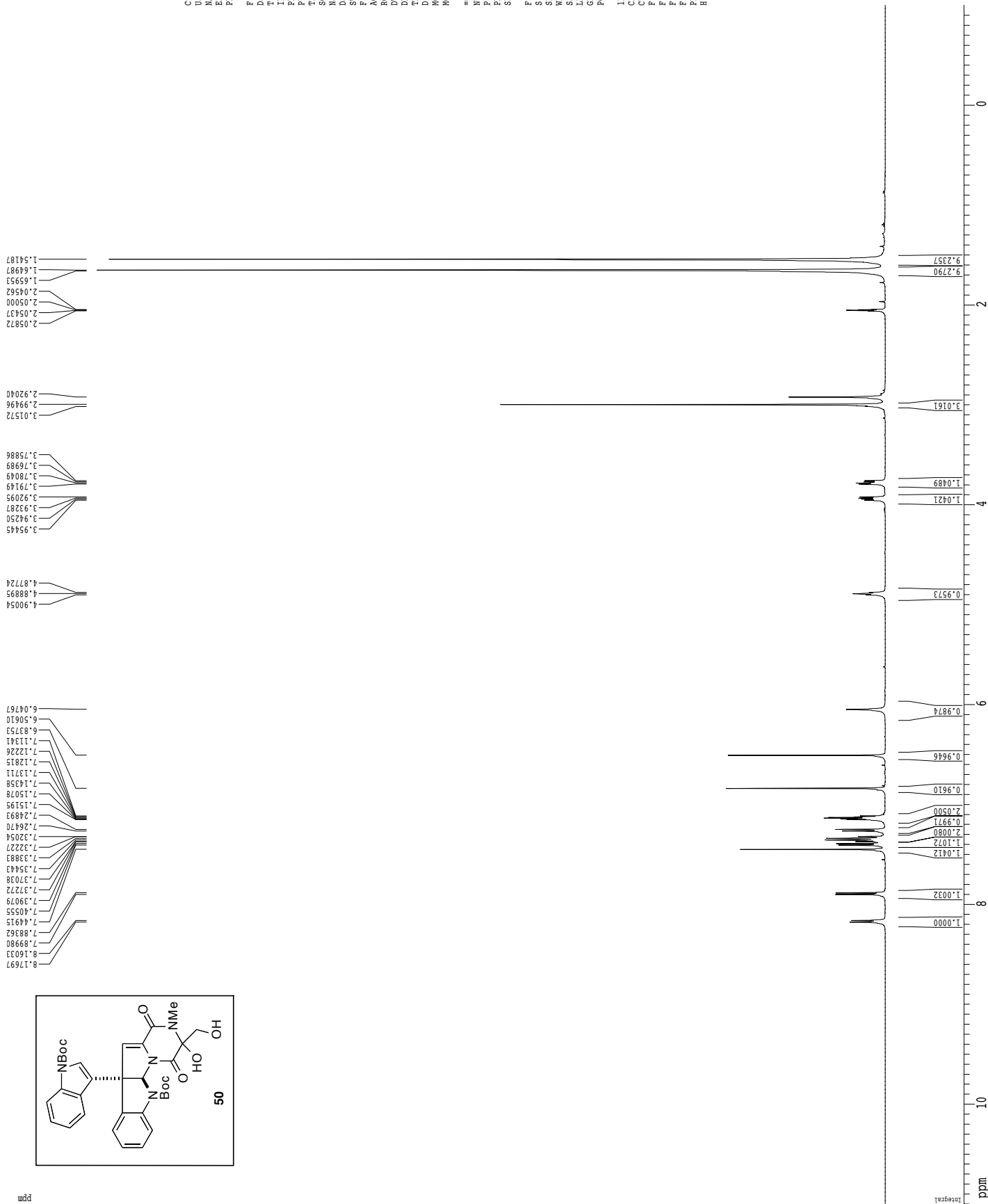
===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794548 dB  
 PL2 125.794548 dB  
 SP1 3.20 dB  
 SP2 3.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CPDPRG2 wd1cp15  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPRMR SFO 0  
 GSPRMR SFO 10  
 GSPRMR SFO 10  
 GX1 0.00 %  
 GX2 0.00 %  
 GX3 0.00 %  
 GX4 0.00 %  
 GX5 0.00 %  
 GX6 0.00 %  
 GX7 0.00 %  
 GX8 0.00 %  
 GX9 0.00 %  
 GX10 0.00 %  
 GX11 0.00 %  
 GX12 0.00 %  
 GX13 0.00 %  
 GX14 0.00 %  
 GX15 0.00 %  
 GX16 0.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803056 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 15.65 cm  
 FIP 220.000 ppm  
 F1 2767.167 Hz  
 F2 -5.000 ppm  
 F3 -628.90 Hz  
 FWHM 0.000000 ppm/cm  
 HZCM 1241.2530 Hz/cm

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jed1-217  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110530  
 Time 15.32  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0990774 sec  
 RG 415  
 DE 62.60 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRK 0.01500000 sec

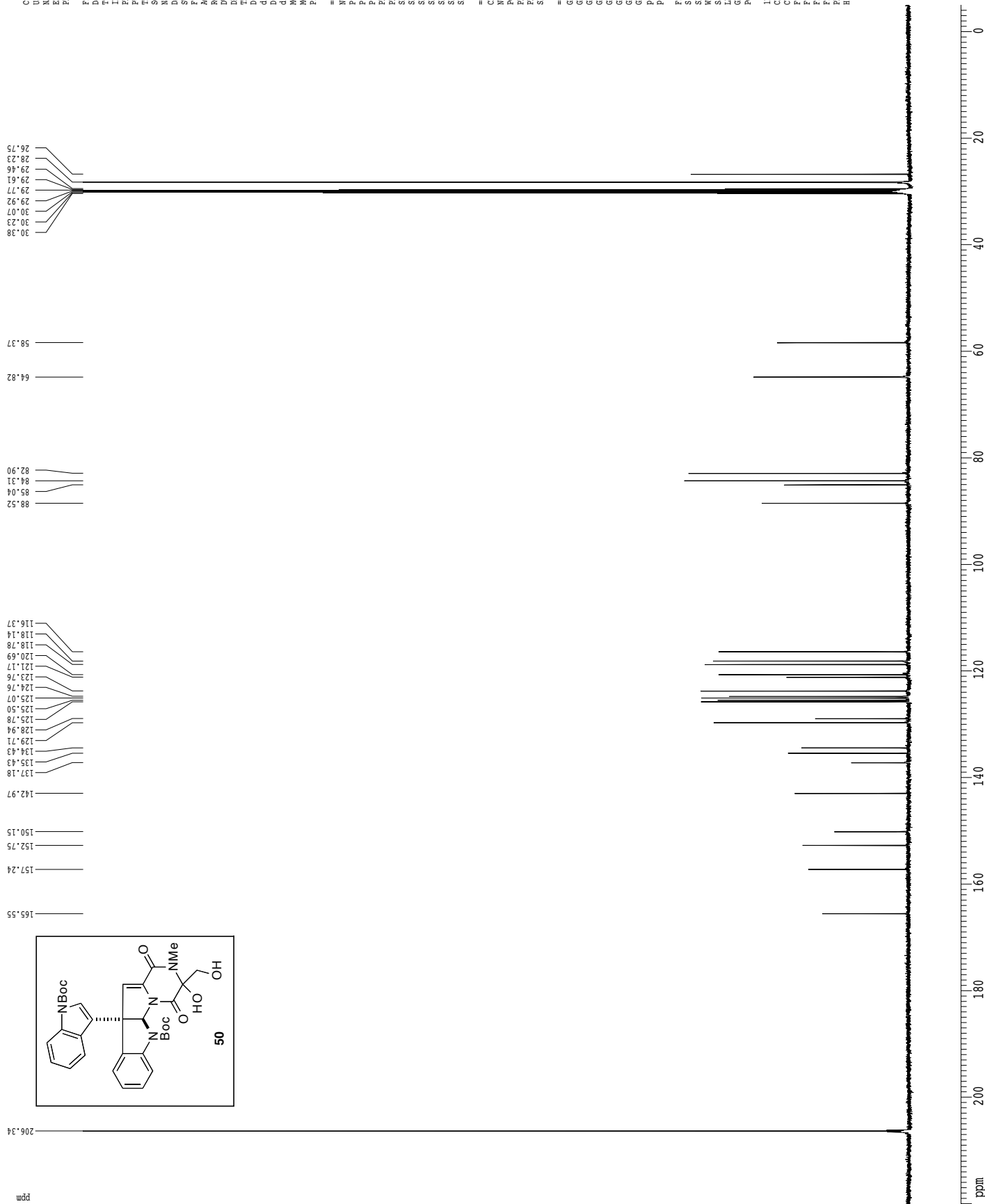
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220184 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.50

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F1 590.242 Hz  
 F2 10.000 ppm  
 F3 -500.92 ppm  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm



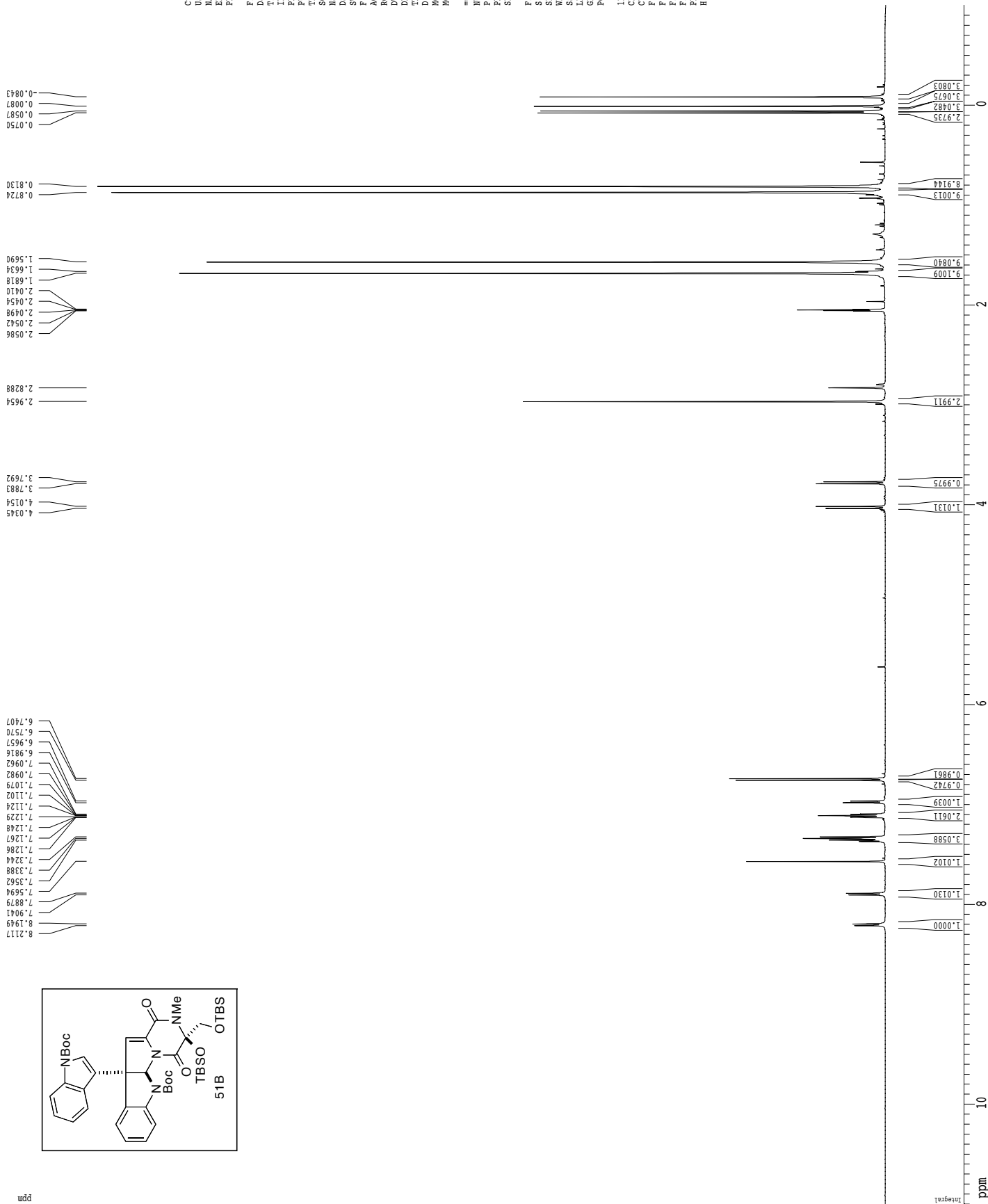
Z-restored spin-echo 13C spectrum with 1H decoupling







<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jedi-218-bot  
 EXPNO 1  
 PROCNO 1

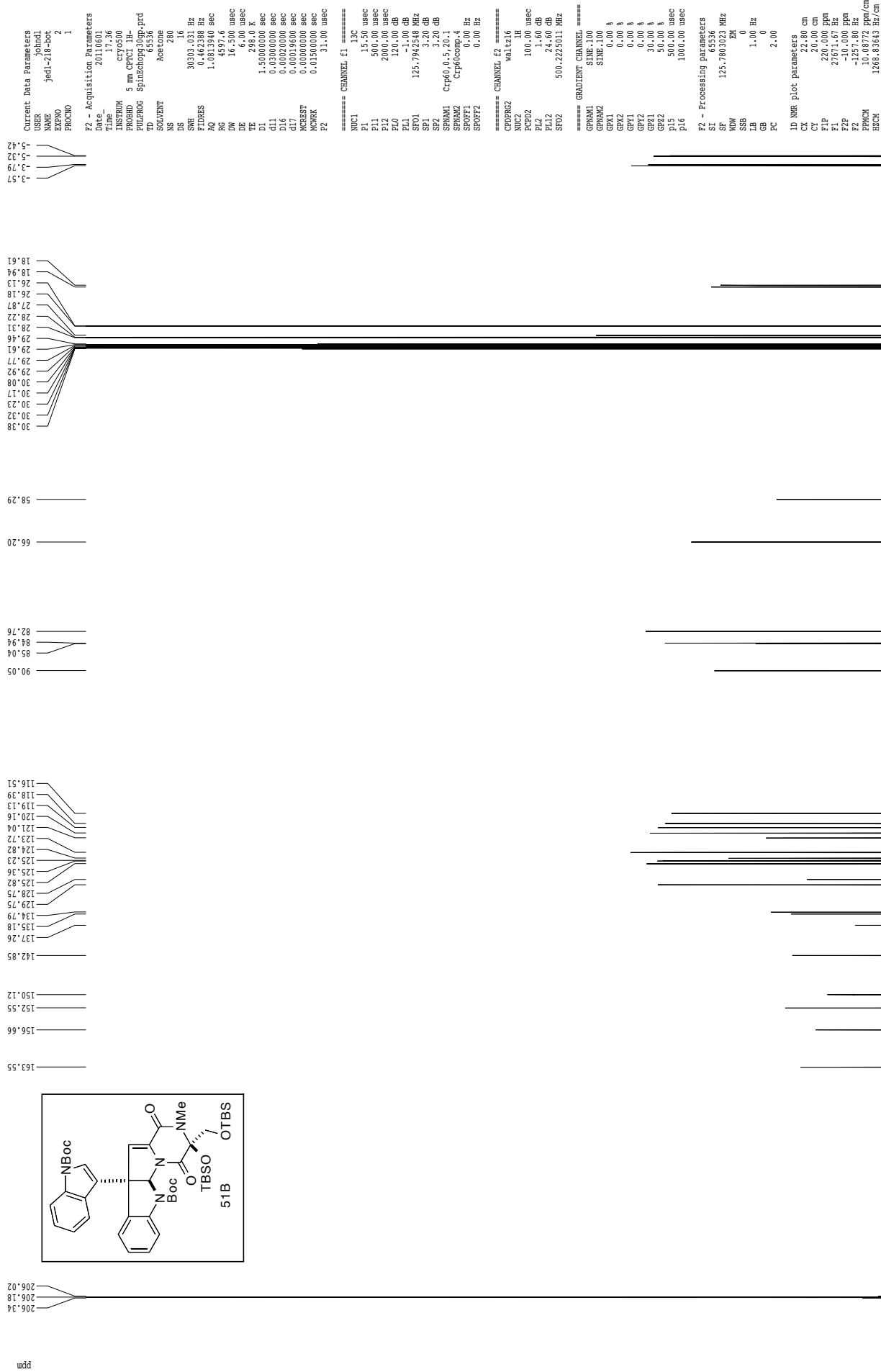
F2 - Acquisition Parameters  
 Date\_ 20110601  
 Time 17.31  
 INSTRUM cryo500  
 PROBRD 5 mm CPXI H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 62.400 usec  
 DR 6.00 usec  
 DE 288.0 K  
 TE 0.10000000 sec  
 D1 0.00000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

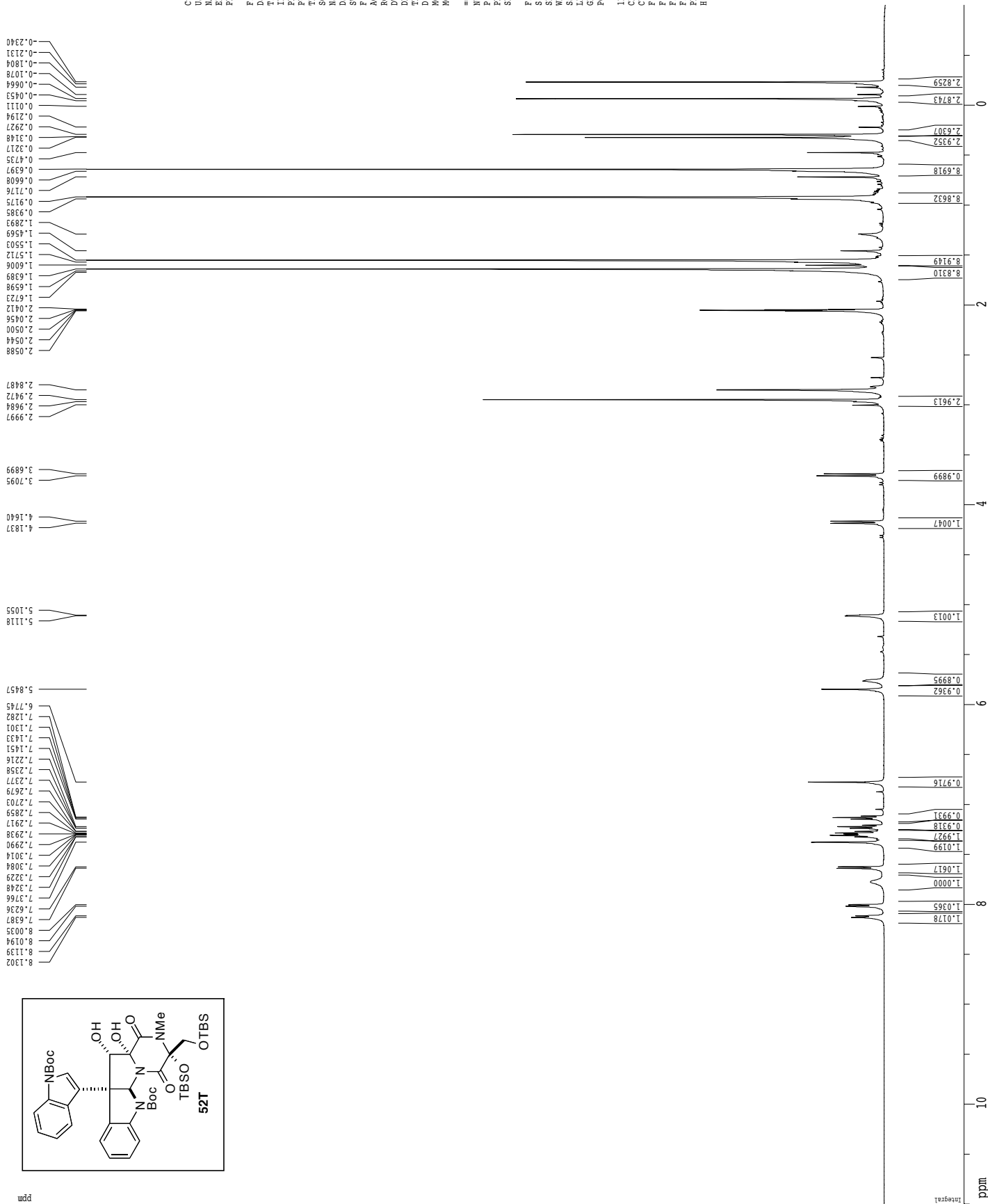
F2 - Processing parameters  
 SI 32768  
 SF 500.220184 MHz  
 DS 4  
 MVM EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 5907.82 Hz  
 F3 10.000 ppm  
 F4 -500.92 Hz  
 PRGM 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jedl-220  
 EXPNO 1  
 PROCNO 1

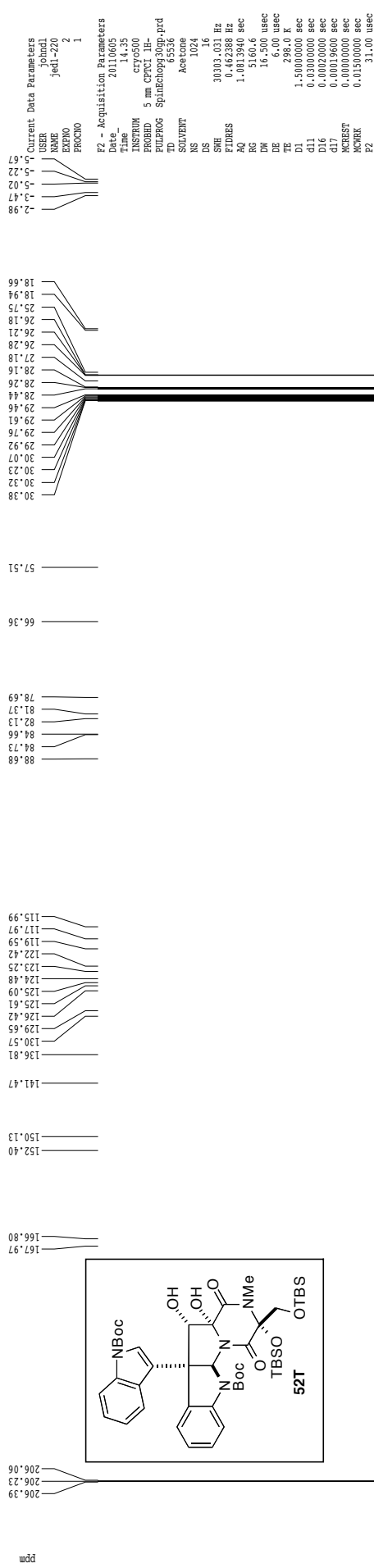
F2 - Acquisition Parameters  
 Date\_ 20110605  
 Time 14.32  
 INSTRUM cryo500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.096043 Hz  
 AQ 5.0998774 sec  
 RG 63  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220183 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.10

1D NMR plot parameters  
 CX 22.80 cm  
 CY 20.00 cm  
 FIP 11.000 ppm  
 F2 5902.82 Hz  
 F3 10.000 ppm  
 F4 -500.92 ppm  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



```

===== CHANNEL F1 =====
NUC1 13C
P1 15.50 usec
P11 500.00 usec
P12 2000.00 usec
P10 120.00 dB
P11 125.7947548 dB
SP1 5.20 dB
SP2 3.20 dB
SPNAM1 Cpp60.0.5.20.1
SPNAM2 Cpp60comp.4
SPOFF1 0.00 Hz
SPOFF2 0.00 Hz

===== CHANNEL F2 =====
CPDPRG2 wd1cp15
NUC2 1H
PCPD2 100.00 usec
PL2 1.60 dB
PL12 24.60 dB
SFO2 500.2225011 MHz

===== GRADIENT CHANGE =====
GRAB1 20.00 usec
GRAB2 510.00 usec
GRX1 0.00 %
GRX2 0.00 %
GRY1 0.00 %
GRY2 0.00 %
GRZ1 30.00 %
GRZ2 50.00 %
P15 500.00 usec
P16 1000.00 usec

F2 - Processing parameters
SI 65536
SF 125.7803019 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 2.00

ID NMR plot parameters
CX 22.80 cm
CY 400.00 cm
FIP 220.000 ppm
F1 2767.67 Hz
F2 -10.000 ppm
F3 -125.780 Hz
F4 10.000 Hz
HECN 1268.83649 Hz/cm
    
```

```

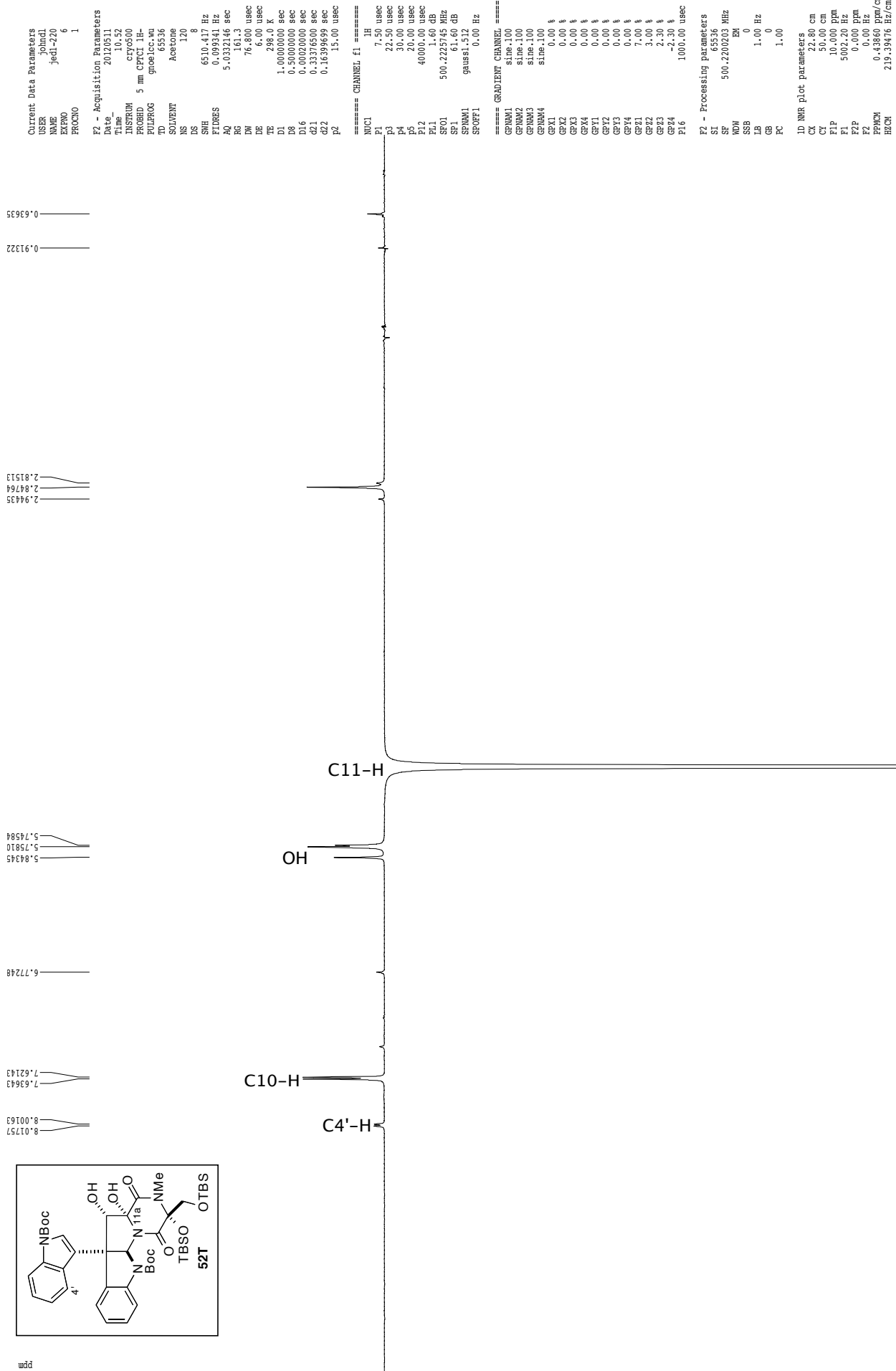
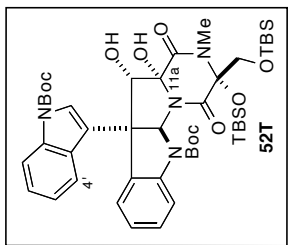
===== CHANNEL F1 =====
Date_ 20110605
Time_ 14.35
INSTRUM cryo500
PROBHD 5 mm CPXI 1H
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1024
DS 16
SHR 30303.031 Hz
FIDRES 0.462388 Hz
AQ 1.0815940 sec
RG 5100.6
DR 6.00 usec
DE 298.0 K
TE 298.0 K
D1 1.50000000 sec
d11 0.03000000 sec
D16 0.00020000 sec
d17 0.00015600 sec
ACRESF 0.00000000 sec
ACWRK 0.01500000 sec
F2 31.00 usec
    
```

```

===== CHANNEL F1 =====
===== CHANNEL F2 =====
===== GRADIENT CHANGE =====
===== ID NMR plot parameters =====
===== Processing parameters =====
===== Acquisition Parameters =====
===== Current Data Parameters =====
===== USER =====
===== PROCNO =====
===== EXNO =====
===== FID =====
===== F2 =====
===== F1 =====
===== F3 =====
===== F4 =====
===== HECS =====
===== HECN =====
===== HZ =====
===== LB =====
===== PC =====
===== SSB =====
===== WDW =====
===== SI =====
===== SF =====
===== WDW =====
===== EM =====
===== SSB =====
===== LB =====
===== GB =====
===== PC =====
===== CX =====
===== CY =====
===== FIP =====
===== F1 =====
===== F2 =====
===== F3 =====
===== F4 =====
===== HECS =====
===== HECN =====
===== HZ =====
    
```



gnoe



Current Data Parameters  
 USER johnd.  
 NAME jedl-220  
 EXPNO 6  
 PROCNO 1

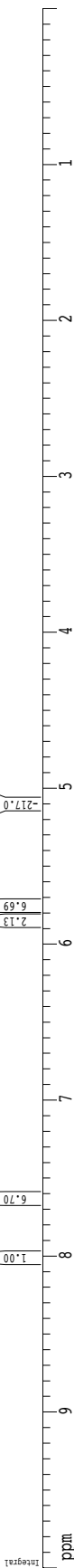
F2 - Acquisition Parameters  
 Date\_ 20120511  
 Time\_ 10.52  
 INSTRUM cryo6500  
 PROBRD 5 mm CPYCI 1H-  
 PULPROG gnoe1cc.wu  
 TD 65536  
 SOLVENT Acetone  
 NS 120  
 DS 8  
 SWH 6510.417 Hz  
 FIDRES 0.099341 Hz  
 AQ 5.0332146 sec  
 RG 161.3  
 DW 76.800 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 D11 0.50000000 sec  
 D16 0.00020000 sec  
 d21 0.33376500 sec  
 d22 0.16396999 sec  
 p2 15.00 usec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 P3 22.50 usec  
 P4 30.00 usec  
 P5 20.00 usec  
 P12 40000.00 usec  
 PL1 1.60 dB  
 SF01 500.2225745 MHz  
 SF1 61.60 dB  
 SP0M1 gauss1.512  
 SFOF1 0.00 Hz

==== GRADIENT CHANNEL =====  
 GENM1 sine.100  
 GENM2 sine.100  
 GENM3 sine.100  
 GENM4 sine.100  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC5 0.00 %  
 GPC6 0.00 %  
 GPC7 0.00 %  
 GPC8 0.00 %  
 GPC9 0.00 %  
 GPC10 0.00 %  
 GPC11 0.00 %  
 GPC12 0.00 %  
 GPC13 0.00 %  
 GPC14 0.00 %  
 GPC15 0.00 %  
 GPC16 1000.00 usec

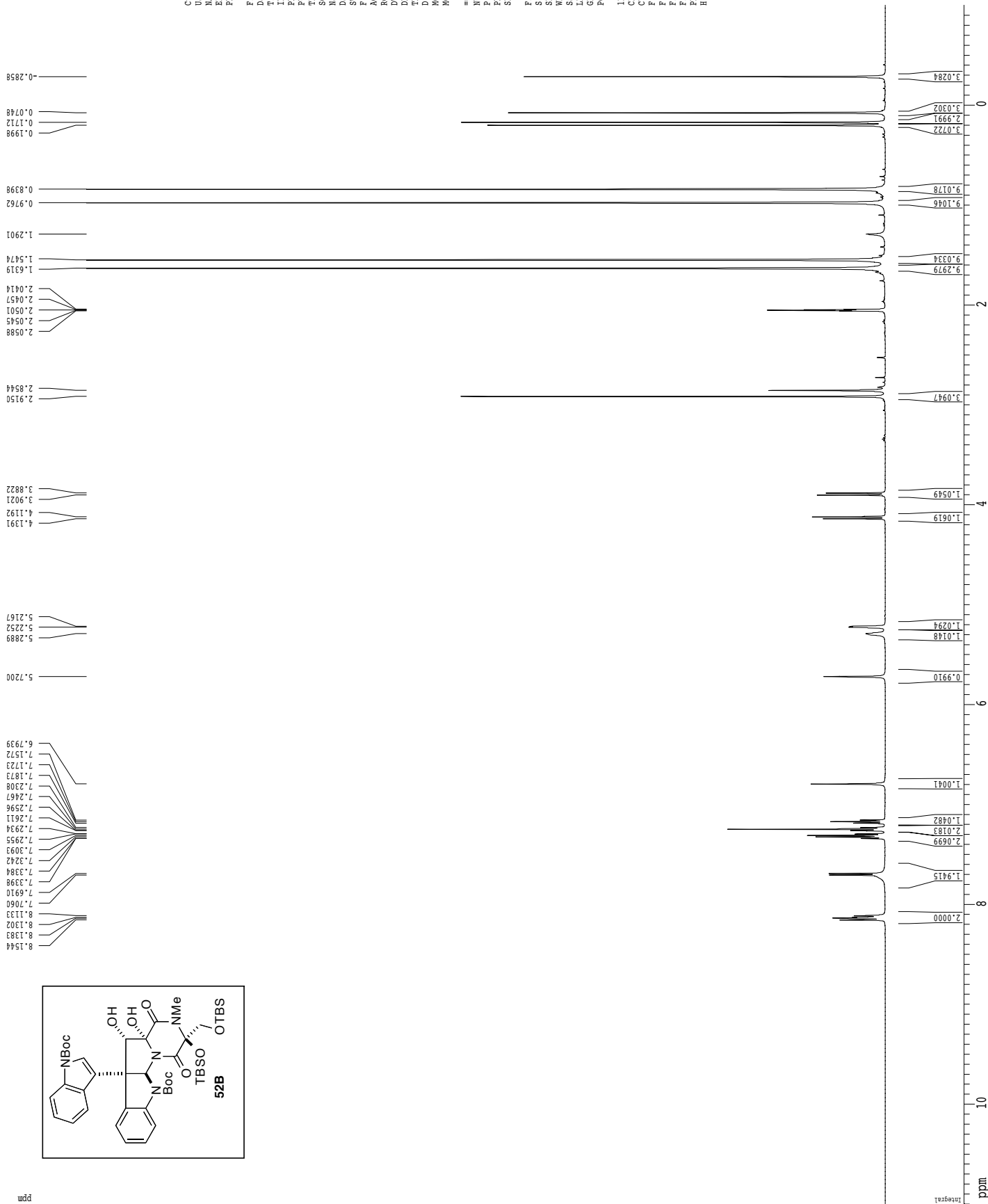
F2 - Processing Parameters  
 SI 65536  
 SF 500.220203 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 10.000 ppm  
 F1 5002.20 Hz  
 F2 0.000 ppm  
 F3 0.00 Hz  
 F4 0.439 ppm/cm  
 HZCM 219.39476 Hz/cm





<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jed1-219  
 EXPNO 1  
 PROCNO 1

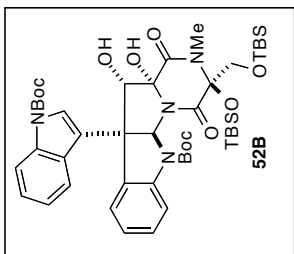
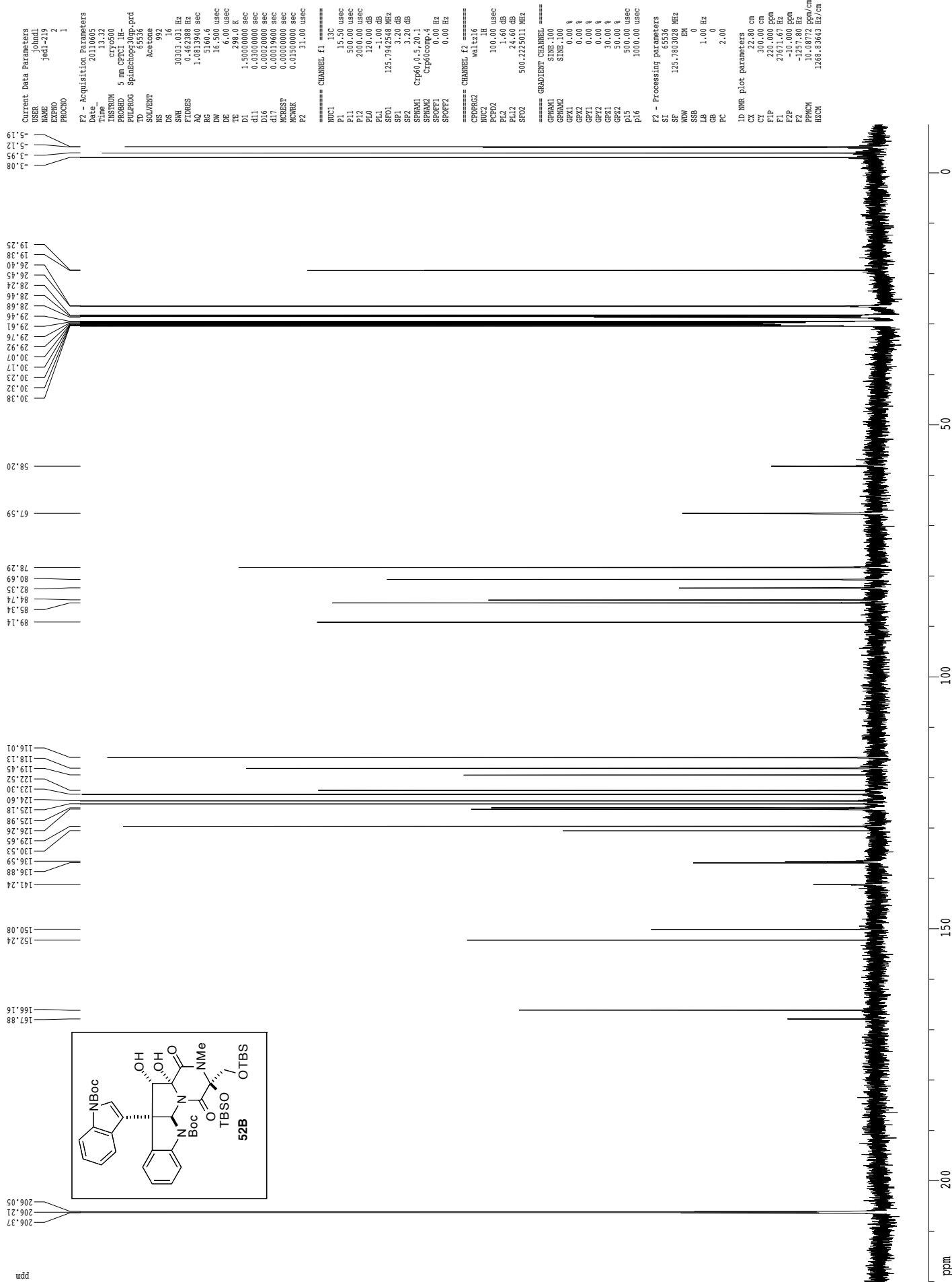
F2 - Acquisition Parameters  
 Date\_ 20110605  
 Time 13.25  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.098674 sec  
 RG 62.40  
 DR 5.00 usec  
 DE 288.0 K  
 TE 0.1000000 sec  
 D1 0.0000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

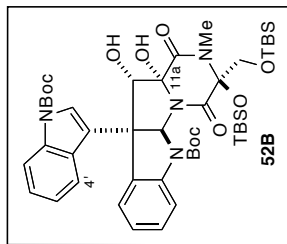
F2 - Processing parameters  
 SI 32768  
 SF 500.220183 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.50

1D NMR plot parameters  
 CX 22.80 cm  
 CY 20.00 cm  
 FIP 11.000 ppm  
 F1 5907.82 Hz  
 F2 -500.92 ppm  
 FREQM 0.52632 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



gnoe



Current Data Parameters  
 USER JohnHd  
 NAME jedl-219  
 EXPNO 6  
 PROCNO 1

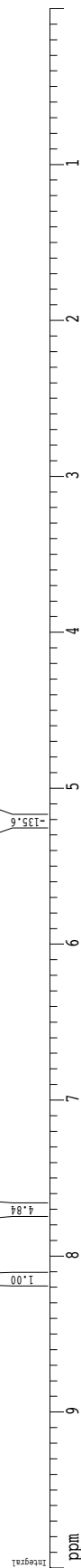
F2 - Acquisition Parameters  
 Date\_ 20120511  
 Time\_ 11.18  
 INSTRUM cryo500  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG gnoe1cc.wu  
 TD 65536  
 SOLVENT Acetone  
 NS 88  
 DS 8  
 SWH 6510.417 Hz  
 FIDRES 0.099341 Hz  
 AQ 5.0332146 sec  
 RG 114  
 DW 76.800 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.000000 sec  
 D11 0.500000 sec  
 D16 0.0002000 sec  
 d21 0.33376500 sec  
 d22 0.16399699 sec  
 p2 15.00 usec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 P3 22.50 usec  
 P4 30.00 usec  
 P5 20.00 usec  
 P12 40000.00 usec  
 P11 1.60 dB  
 SFO1 500.2226299 MHz  
 SF1 61.60 dB  
 SPHM1 gauss1.512  
 SFOFF 0.00 Hz

==== GRADIENT CHANNEL =====  
 GENM1 sine-100  
 GENM2 sine-100  
 GENM3 sine-100  
 GENM4 sine-100  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC1 7.00 %  
 GPC2 3.00 %  
 GPC3 2.30 %  
 GPC4 2.30 %  
 P16 1000.00 usec

F2 - Processing Parameters  
 SI 65536  
 SF 500.220200 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 10.000 ppm  
 F1 5002.20 Hz  
 F2P 0.000 ppm  
 F3 1.00 Hz  
 FREQM 0.439 ppm/cm  
 HZCM 219.39456 Hz/cm

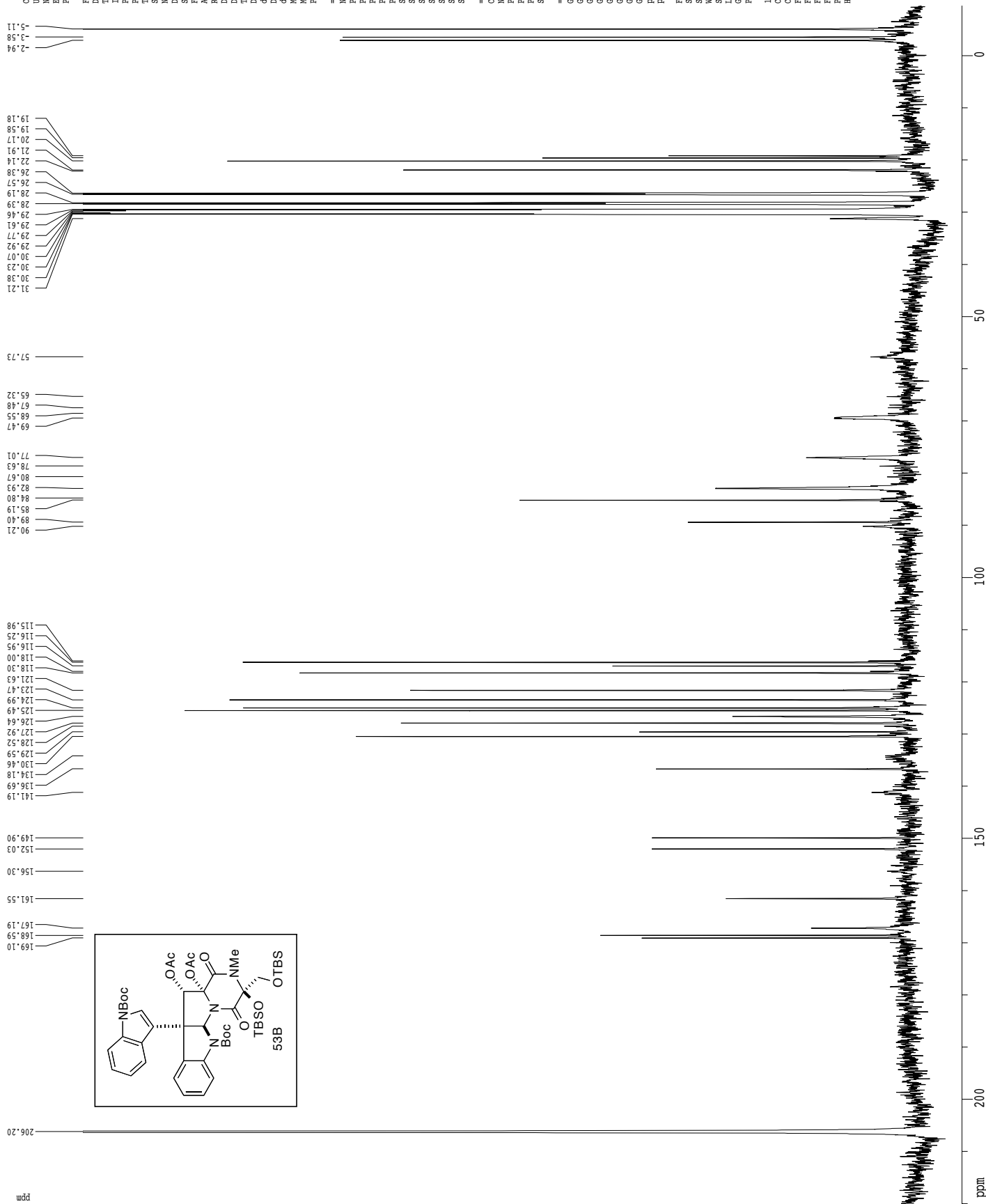








Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER joudi  
 EXPNO jedi-7472  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20110607  
 Time 16.35  
 INSTRUM cryso500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 1024  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 7298.7  
 AG 16.00 usec  
 DR 6.00 usec  
 DE 298.0 K  
 TE 298.0 K  
 D1 1.5000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.00015600 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 31.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.7947548 dB  
 PL2 120.00 dB  
 SP1 5.20 dB  
 SP2 31.20 dB  
 SFO1 Cyp60.0.5.20.1  
 SFO2 Cyp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

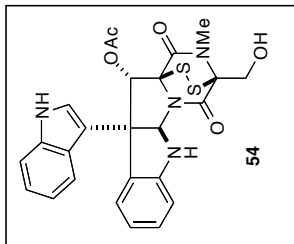
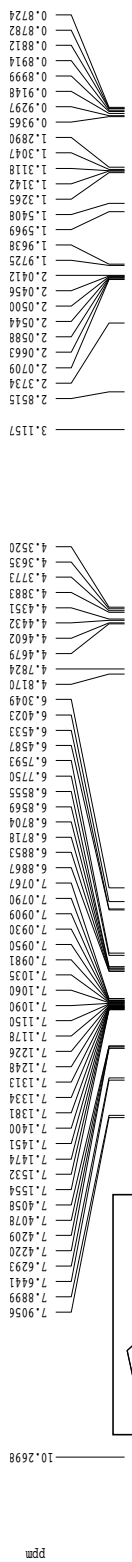
===== CHANNEL F2 =====  
 CPDPRG2 wd1cp15  
 NUC2 1H  
 P2 100.00 usec  
 PCPD2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR10 0.00 %  
 GSPR11 0.00 %  
 GSPR12 0.00 %  
 GSPR13 0.00 %  
 GSPR14 30.00 %  
 GSPR15 50.00 %  
 GSPR16 100.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803023 MHz  
 WDW EM  
 SSB 0  
 LB 0  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 400.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -10.000 ppm  
 F2 -125.780 Hz  
 F2 125.7803023 ppm/cm  
 HZCM 1268.83645 Hz/cm

<sup>1</sup>H spectrum



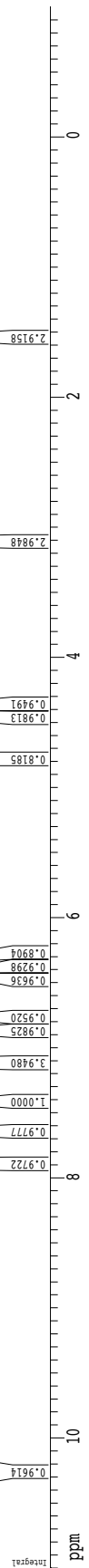
Current Data Parameters  
 USER Johnel  
 NAME Jes2-159  
 EXPNO 6  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120519  
 Time 15.50  
 INSTRUM cryo500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0996774 sec  
 RG 611  
 DE 62.40 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCPRK 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

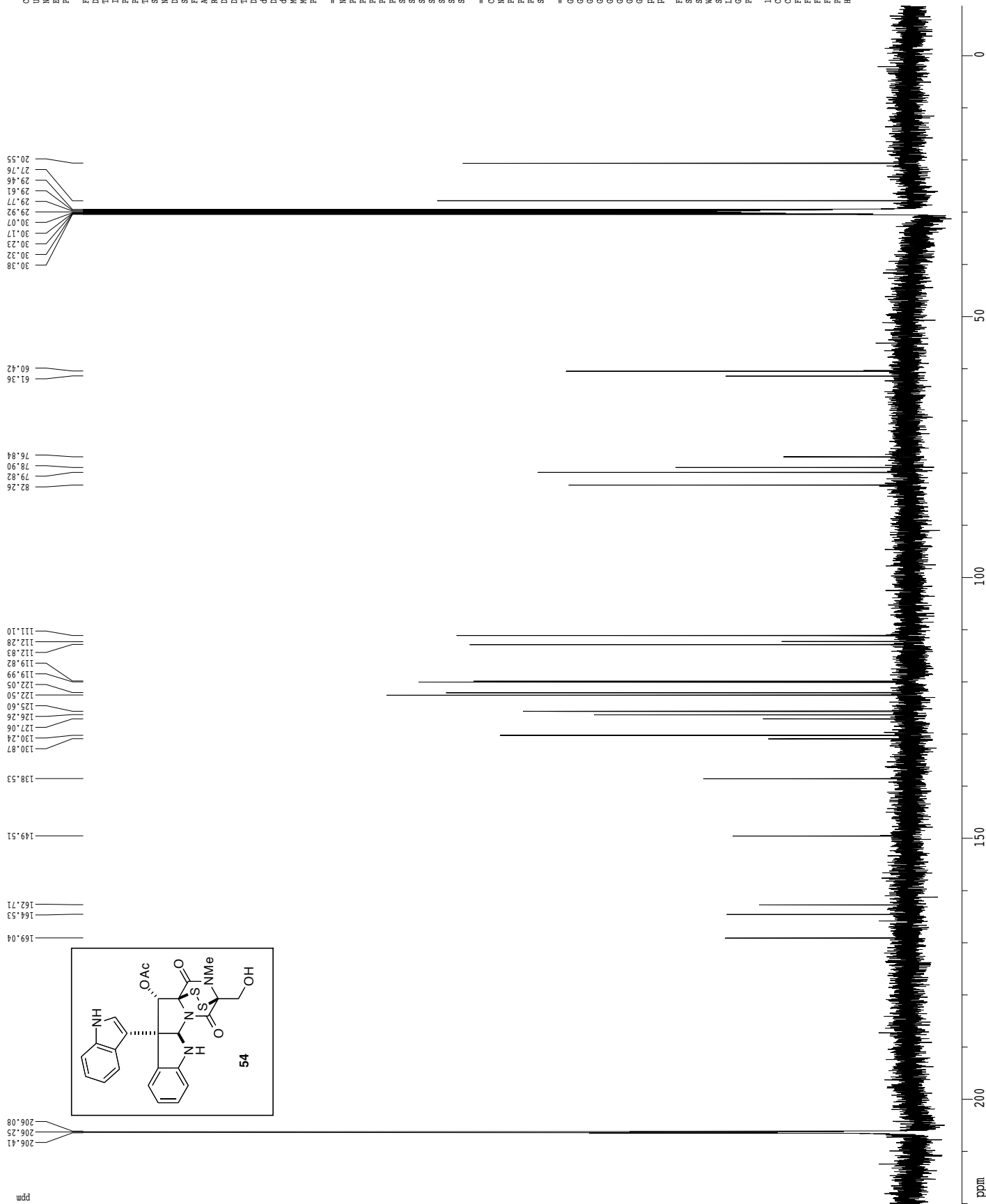
F2 - Processing parameters  
 SI 65536  
 SF 500.220182 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.01

1D NMR plot parameters  
 CX 22.80 cm  
 CY 12.00 cm  
 FIP 11.000 ppm  
 F2 5902.82 Hz  
 F3 10.000 ppm  
 F4 -500.92 ppm  
 PRCM 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm





Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER joudl  
 NAME jed-112  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120518  
 Time 9.22  
 INSTRUM cryo500  
 PROBRD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 536  
 DS 16  
 SFR 30303.031 Hz  
 SHR 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 1824.6  
 DR 6.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.50000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 D17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

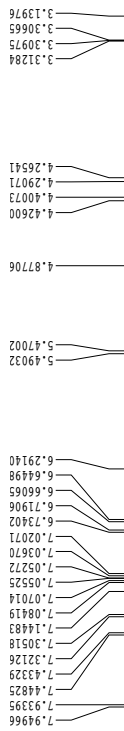
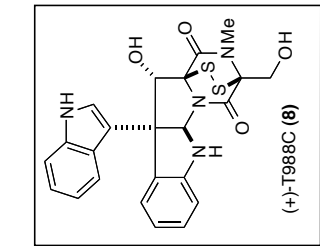
===== CHANNEL F2 =====  
 CDPGRZ wd1615  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPRZ 0.00 %  
 GSPRZ 0.00 %  
 GSPRZ 0.00 %  
 GSPRZ 0.00 %  
 GSPRZ 30.00 %  
 GSPRZ 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7803009 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2P -10.000 ppm  
 F2 -125.780 Hz  
 F2PCK 1268.3865 Hz/cm  
 HZCK 1268.3865 Hz/cm

<sup>1</sup>H spectrum



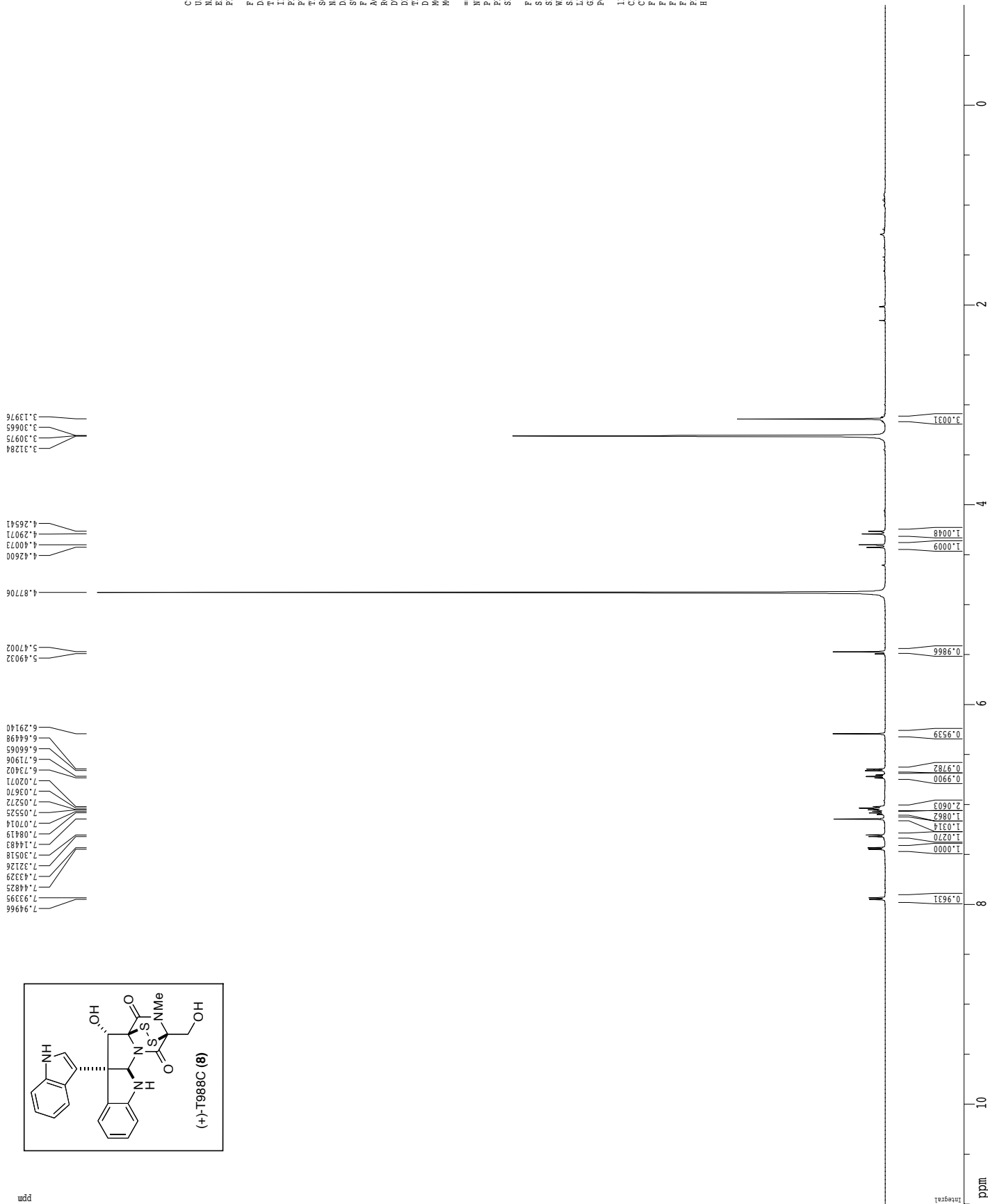
Current Data Parameters  
 USER johnd  
 NAME jes2-164  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120528  
 Time 10.37  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CD300  
 NS 32  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099674 sec  
 RG 671  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.220193 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

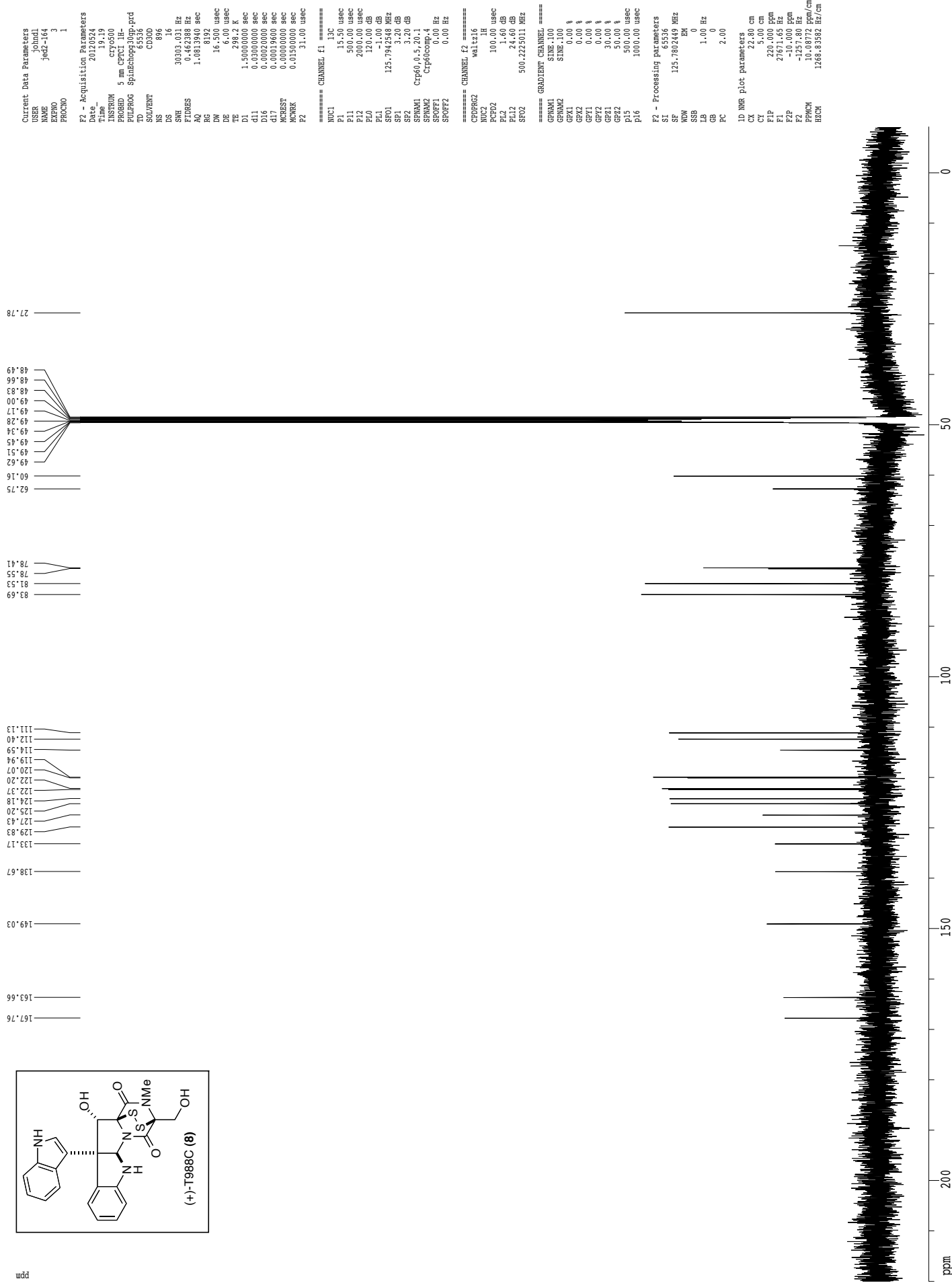
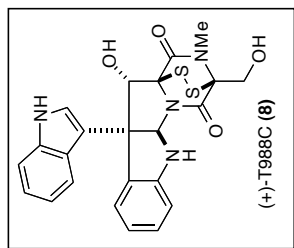
1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 550.242 Hz  
 F3 10.000 ppm  
 F4 -50.000 ppm  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm



Integrat

ppm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jomdl  
 EXPNO jed-193  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20120524  
 Time 19.19  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CD300  
 NS 896  
 DS 16  
 SHR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0813940 sec  
 RG 432  
 DR 16  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.50000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.7947648 dB  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60.05, 20.1  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPREG wd1616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR1 0  
 GSPR2 0  
 GSTR1 0.00 %  
 GSTR2 0.00 %  
 GPF1 0.00 %  
 GPF2 0.00 %  
 GZ1 30.00 %  
 GZ2 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7802449 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00  
 ID NMR plot parameters  
 CX 22.80 cm  
 CY 5.00 cm  
 FIP 220.000 ppm  
 F1 27671.65 Hz  
 F2P -10.000 ppm  
 F2 -125.780 Hz  
 F2PCH 125.7802449 ppm/cm  
 HECN 1248.8382 Hz/cm

Current Data Parameters  
 USER johnd  
 NAME jeh2-164  
 EXNO 5  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20120225  
 Time 13.48  
 INSTRUM cryo500  
 PROBDH 5 mm CPXI IH-  
 PULPROG invgfp.wu  
 TD 2048  
 SOLVENT CD3OD  
 NS 2  
 DS 12  
 SWH 4606.403 Hz  
 FIDRES 2.195509 Hz  
 AQ 0.2277876 sec  
 RG 11585.2  
 DW 111.200 usec  
 DE 6.50 usec  
 TE 298.0 K  
 CH2Z 145.000000  
 CH2Y 0.000000  
 CH2X 2.000000  
 d1 2.000000 sec  
 d2 0.00344828 sec  
 d12 0.00002000 sec  
 d13 0.00003000 sec  
 D16 0.00020000 sec  
 d20 0.00242528 sec  
 d21 0.00002000 sec  
 INO 0.00002000 sec

20

==== CHANNEL f1 =====  
 NU1C1 H  
 P1 7.50 usec  
 P2 15.00 usec  
 PL1 1.60 dB  
 SF01 500.2222510 MHz

40

==== CHANNEL f2 =====  
 CPDPRG2 gald  
 NU2 C  
 P1 15.50 usec  
 PCPD2 65.00 usec  
 PL2 -1.00 dB  
 PL12 11.30 dB  
 SF02 125.7915647 MHz

60

==== GRADIENT CHANNEL =====  
 GPM11 size-100  
 GMX2 size-100  
 GMB3 size-100  
 GXY1 0.00 %  
 GPX2 0.00 %  
 GPX3 0.00 %  
 GPY1 0.00 %  
 GPY2 0.00 %  
 GPY3 0.00 %  
 GPZ1 30.00 %  
 GPZ2 0.00 %  
 GPZ3 2.00 %  
 GPC5 0.00 %  
 P16 1000.00 usec

80

F1 - Acquisition parameters  
 ND0 2  
 TD 86  
 SF01 125.7916 MHz  
 FIDRES 264.270599 Hz  
 SW 480.674 ppm  
 FREQDE undefined

F2 - Processing parameters  
 SI 1024  
 SF 500.220193 MHz  
 WDM EM  
 SSB 0  
 LB 5.00 Hz  
 GB 0  
 FC 2.00

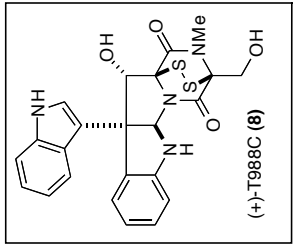
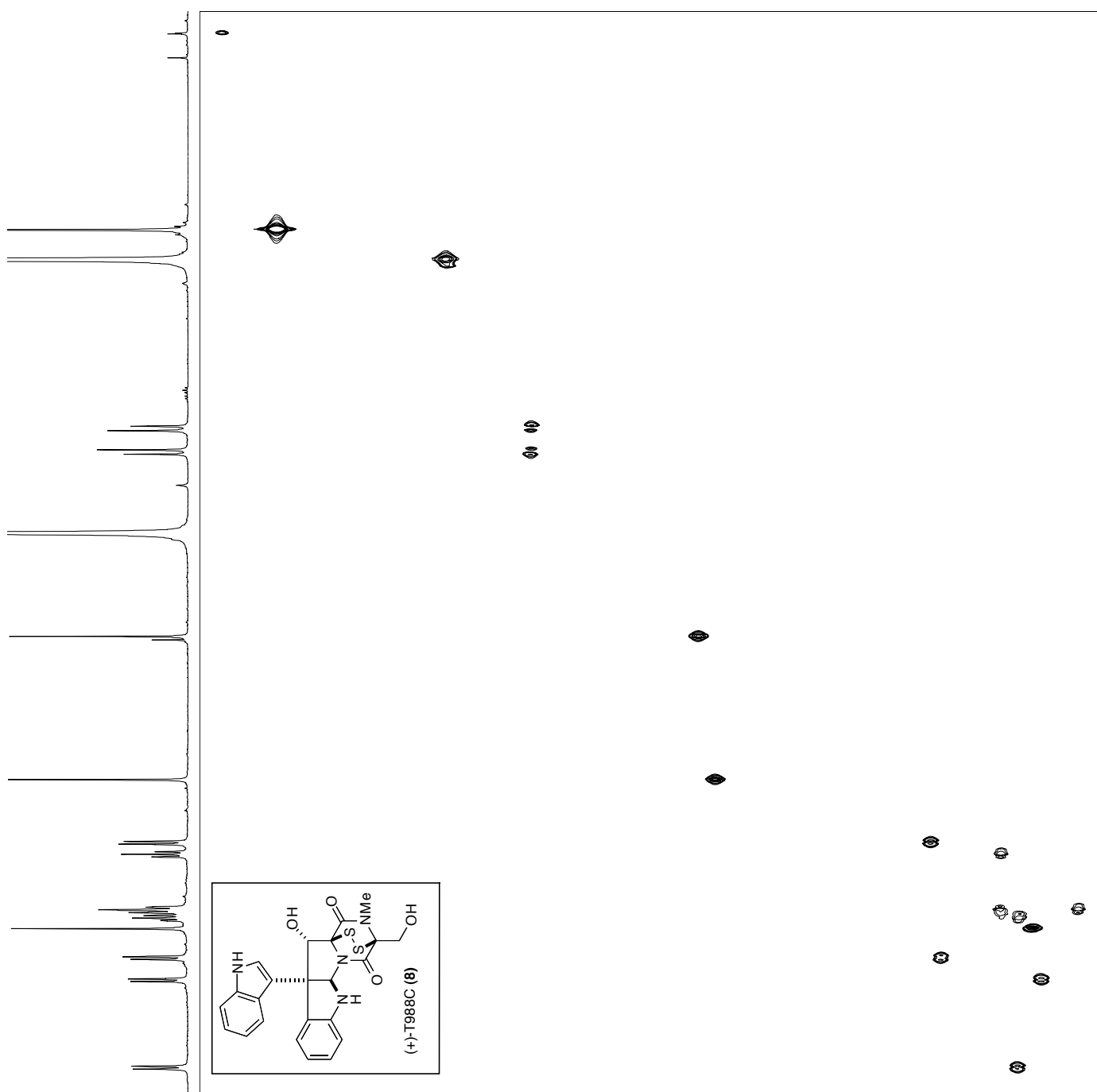
100

F1 - Processing parameters  
 SI 1024  
 MC2 OF  
 SF 125.780244 MHz  
 WDM QSTINE  
 SSB 3  
 LB 0.00 Hz  
 GB 0

120

ZD NMR plot parameters  
 CX2 18.00 cm  
 CX1 15.00 cm  
 F2PLO 8.087 ppm  
 FZLO 4045.20 Hz  
 FZHI 1.889 ppm  
 FZHI 945.14 Hz  
 F1PLO 137.879 ppm  
 F1PLO 162.000 ppm  
 F1PHI 18.006 ppm  
 F1HI 2264.82 Hz  
 F2PFCM 0.34430 ppm/cm  
 F2HCM 172.2251 Hz/cm  
 F1PFCM 7.68816 ppm/cm  
 F1HCM 961.24573 Hz/cm

ppm



ghmqc

Current Data Parameters  
 USER johnd1  
 NAME j6e2-164  
 EXNO 4  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20120525  
 Time 13:53  
 INSTRUM spect  
 PROBEID 5 mm CPXI 1H  
 PULPROG ghmhbcx9  
 TD 4096  
 SOLVENT CD300  
 NS 2  
 DS 16  
 SWH 4496.403 Hz  
 FIDRES 1.097755 Hz  
 AQ 0.4555252 sec  
 RG 14596.5  
 DW 111.200 usec  
 DE 6.00 usec  
 TE 300.2 K  
 CNUF2 145.0000030 sec  
 d0 0.00000300 sec  
 d1 1.25000000 sec  
 d2 0.00344828 sec  
 d6 0.05000000 sec  
 d13 0.00000300 sec  
 D16 0.00020000 sec  
 INO 0.00002200 sec

==== CHANNEL F1 =====

NVC1 IH  
 F1 7.50 usec  
 P1 15.00 usec  
 P2 15.00 usec  
 SF01 500.2222510 MHz

==== CHANNEL F2 =====

NVC2 13C  
 F2 15.50 usec  
 P3 15.50 usec  
 P4 -1.00 dB  
 SF02 125.7915647 MHz

==== GRADIENT CHANNEL =====

GPWA1 sine,100  
 GPWA2 sine,100  
 GPWA3 sine,100  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC5 0.00 %  
 GPC6 0.00 %  
 GPC7 0.00 %  
 GPC8 0.00 %  
 GPC9 0.00 %  
 GPC10 0.00 %  
 GPC11 0.00 %  
 GPC12 0.00 %  
 GPC13 0.00 %  
 GPC14 0.00 %  
 GPC15 0.00 %  
 GPC16 0.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters

NU0 246  
 SF01 125.7915647 MHz  
 FIDRES 91.642237 Hz  
 SW 180.674 ppm  
 FWHM undefined

F2 - Processing parameters

SI 2048  
 SF 500.2200193 MHz  
 SINE SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 2.00

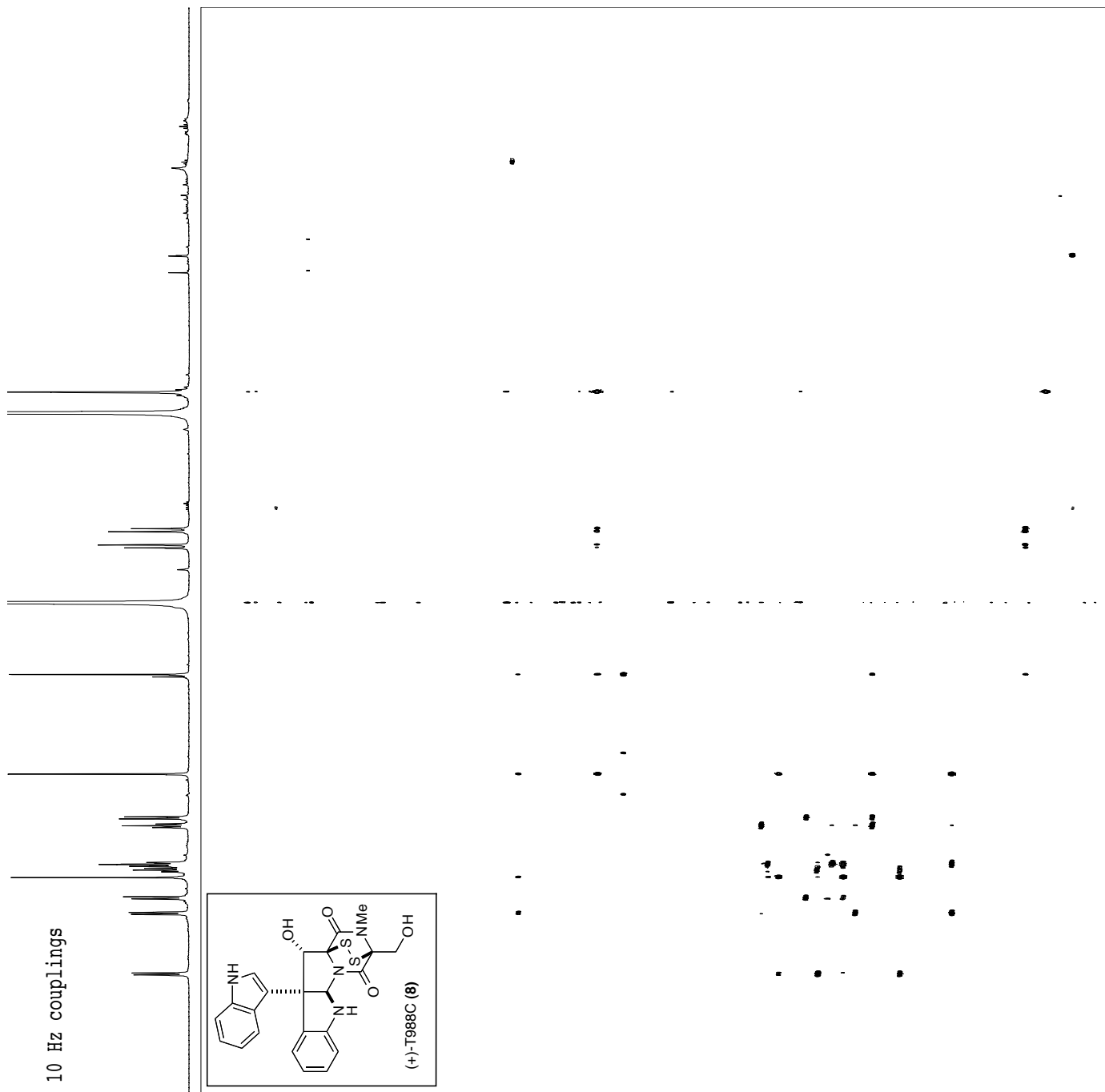
F1 - Processing parameters

SI 1024  
 MC2 CF  
 SF 125.7802444 MHz  
 SINE SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

2D NMR plot parameters

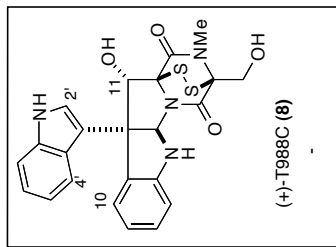
CX2 18.00 cm  
 CX1 15.00 cm  
 FZEO 8.956 ppm  
 FZFO 44.9033 Hz  
 FZHI -0.345 ppm  
 FZHI -16.49 Hz  
 F1FO 180.345 ppm  
 F1LO 22683.85 Hz  
 F1HI -0.345 ppm  
 F1HI -43.42 Hz  
 F2PACH 0.49938 ppm/cm  
 F2HCN 249.80017 Hz/cm  
 F1PPACH 12.04602 ppm/cm  
 F1HCN 1515.15149 Hz/cm

ghmhc optimised for 10 Hz couplings



ppm

gnoe



Current Data Parameters  
 USER johndi  
 NAME jedz-164  
 EXPNO 6  
 PROCNO 1

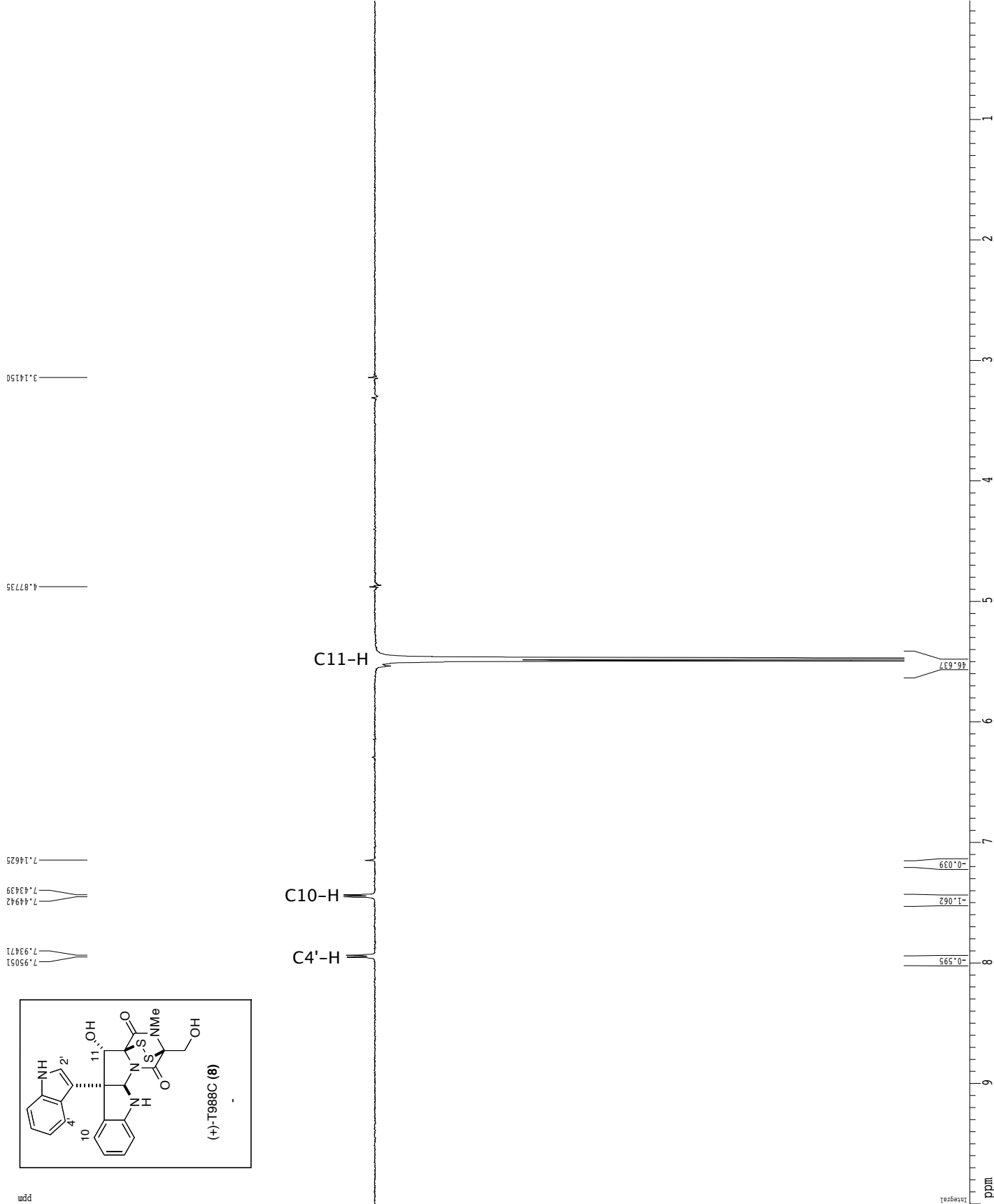
F2 - Acquisition Parameters  
 Date\_ 20120524  
 Time\_ 20.00  
 INSTRUM cty6500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG gnoe1cc.wu  
 TD 65536  
 SOLVENT CD3OD  
 NS 72  
 DS 8  
 SWH 5482.456 Hz  
 FIDRES 0.083656 Hz  
 AQ 5.5769330 sec  
 RG 228.1  
 DW 91.200 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 D11 0.50000000 sec  
 D16 0.00020000 sec  
 d21 0.33376500 sec  
 d22 0.16399699 sec  
 p2 15.00 usec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 P3 22.50 usec  
 P4 30.00 usec  
 P5 20.00 usec  
 P12 40000.00 usec  
 PL1 1.60 dB  
 SF01 500.2227686 MHz  
 SE1 61.60 dB  
 SP0M1 gauss1.512  
 SPOFF1 0.00 Hz

==== GRADIENT CHANNEL =====  
 GENM1 sine.100  
 GENM2 sine.100  
 GENM3 sine.100  
 GENM4 sine.100  
 GFX1 0.00 %  
 GFX2 0.00 %  
 GFX3 0.00 %  
 GFX4 0.00 %  
 GFY1 0.00 %  
 GFY2 0.00 %  
 GFY3 0.00 %  
 GFY4 0.00 %  
 GZ1 7.00 %  
 GZ2 3.00 %  
 GZ3 2.30 %  
 GZ4 -2.30 %  
 F16 1000.00 usec

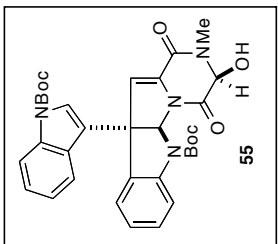
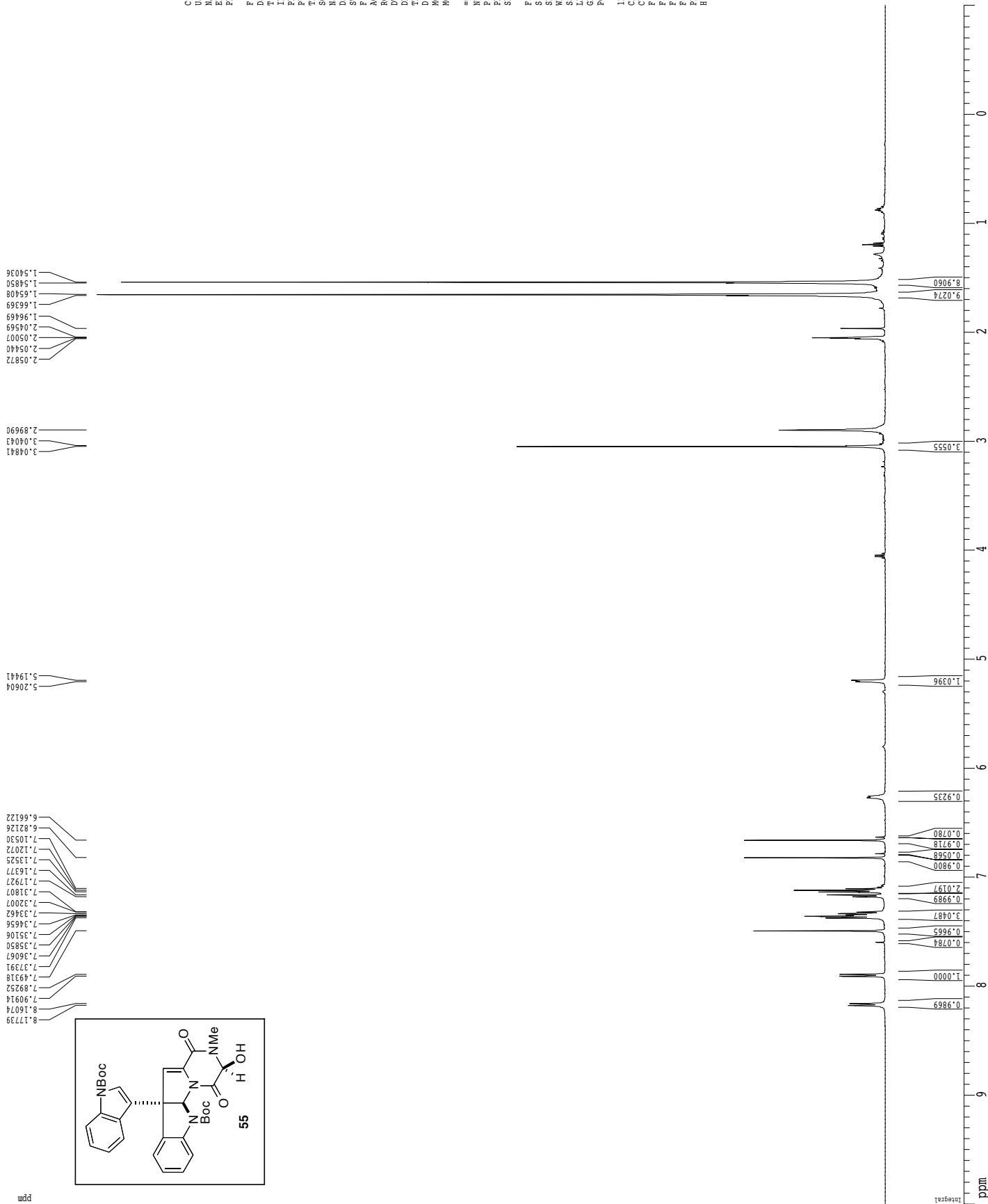
F2 - Processing Parameters  
 SI 65536  
 SF 500.2200193 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 10.000 ppm  
 F1 5002.20 Hz  
 F2P 0.000 ppm  
 F3 1.00 Hz  
 F3MCH 0.439 ppm/cm  
 HZCM 219.39456 Hz/cm



Integral

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jedq-28  
 EXPNO 1  
 PROCNO 1

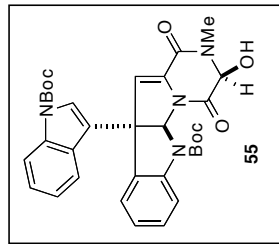
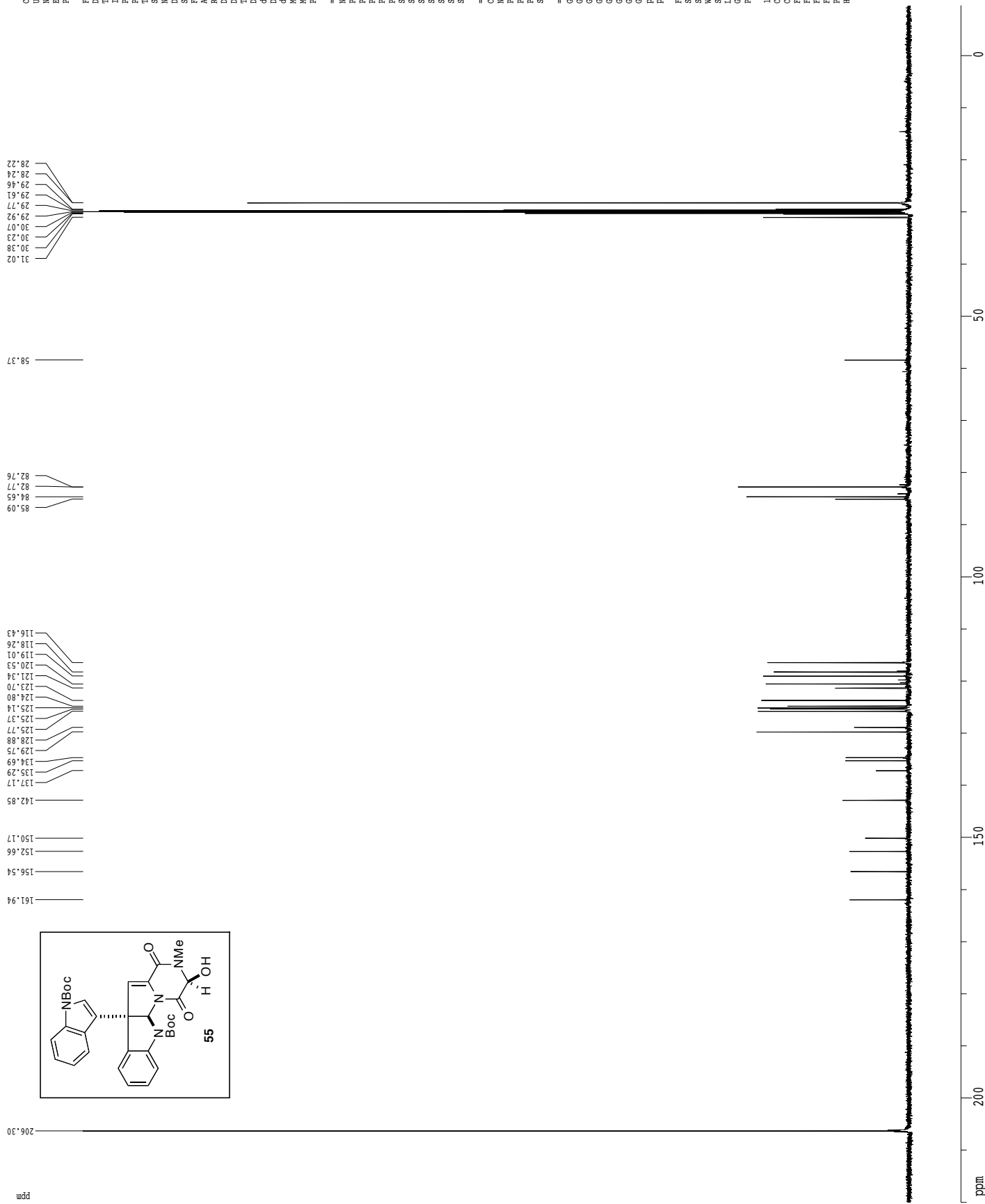
F2 - Acquisition Parameters  
 Date\_ 20120715  
 Time 13.01  
 INSTRUM cryo500  
 PROBRD 5 mm CPXI H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099674 sec  
 RG 62.40  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.225015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.220178 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 10.000 ppm  
 F2 500.220 Hz  
 F3 10.000 ppm  
 F4 -500.32 ppm  
 PRMCM 0.48246 ppm/cm  
 HZCM 241.33423 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jomid1  
 EXPNO jedz-2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120715  
 Time 13.06  
 INSTRUM cryo500  
 PROBHD 5 mm CPAC1 JH  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 176  
 DS 16  
 SHR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 3649.1  
 AG 6.00 usec  
 DR 2.00 usec  
 DE 298.2 K  
 TE 298.2 K  
 D1 0.25000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794568 dB  
 PL2 125.794568 dB  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO1 Cpp60.05, 20.1  
 SFO2 Cpp60.05, 20.1  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

===== CHANNEL F2 =====  
 CDPREG wd t615  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR1 0  
 GSPR2 0  
 GSPR3 0  
 GSPR4 0  
 GSPR5 0  
 GSPR6 0  
 GSPR7 0  
 GSPR8 0  
 GSPR9 0  
 GSPR10 0  
 GSPR11 0  
 GSPR12 0  
 GSPR13 0  
 GSPR14 0  
 GSPR15 0  
 GSPR16 0  
 GSPR17 0  
 GSPR18 0  
 GSPR19 0  
 GSPR20 0  
 GSPR21 0  
 GSPR22 0  
 GSPR23 0  
 GSPR24 0  
 GSPR25 0  
 GSPR26 0  
 GSPR27 0  
 GSPR28 0  
 GSPR29 0  
 GSPR30 0  
 GSPR31 0  
 GSPR32 0  
 GSPR33 0  
 GSPR34 0  
 GSPR35 0  
 GSPR36 0  
 GSPR37 0  
 GSPR38 0  
 GSPR39 0  
 GSPR40 0  
 GSPR41 0  
 GSPR42 0  
 GSPR43 0  
 GSPR44 0  
 GSPR45 0  
 GSPR46 0  
 GSPR47 0  
 GSPR48 0  
 GSPR49 0  
 GSPR50 0  
 GSPR51 0  
 GSPR52 0  
 GSPR53 0  
 GSPR54 0  
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 GSPR60 0  
 GSPR61 0  
 GSPR62 0  
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 GSPR64 0  
 GSPR65 0  
 GSPR66 0  
 GSPR67 0  
 GSPR68 0  
 GSPR69 0  
 GSPR70 0  
 GSPR71 0  
 GSPR72 0  
 GSPR73 0  
 GSPR74 0  
 GSPR75 0  
 GSPR76 0  
 GSPR77 0  
 GSPR78 0  
 GSPR79 0  
 GSPR80 0  
 GSPR81 0  
 GSPR82 0  
 GSPR83 0  
 GSPR84 0  
 GSPR85 0  
 GSPR86 0  
 GSPR87 0  
 GSPR88 0  
 GSPR89 0  
 GSPR90 0  
 GSPR91 0  
 GSPR92 0  
 GSPR93 0  
 GSPR94 0  
 GSPR95 0  
 GSPR96 0  
 GSPR97 0  
 GSPR98 0  
 GSPR99 0  
 GSPR100 0

F2 - Processing parameters  
 SI 65536  
 SF 125.7803042 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 25.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2 -30.000 ppm  
 FZ 1.25780 Hz  
 FWHM 1.00000 ppm/cm  
 HECM 1268.83645 Hz/cm

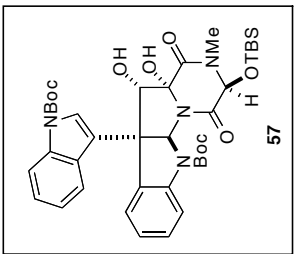
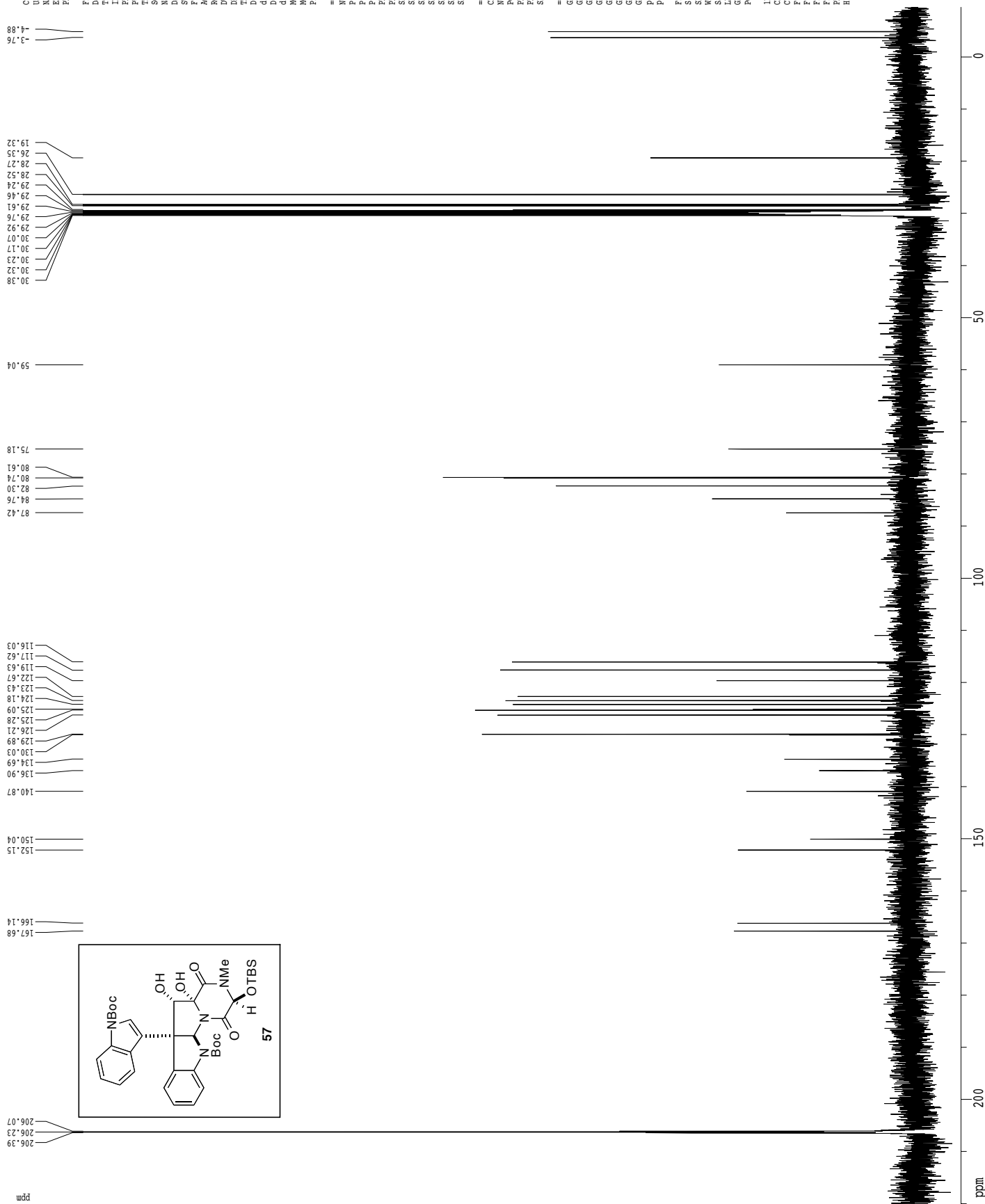








Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jound1  
 NAME jedi-112  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20110107  
 Time 14.08  
 INSTRUM cryso00  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 512  
 DS 16  
 SHR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 7298.7  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 298.2 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 d16 0.0002000 sec  
 d17 0.00015600 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 31.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 P11 500.00 usec  
 P12 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794548 dB  
 PL2 120.00 dB  
 SP1 51.20 dB  
 SP2 31.20 dB  
 SFO1 Ccp60.0.5.20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

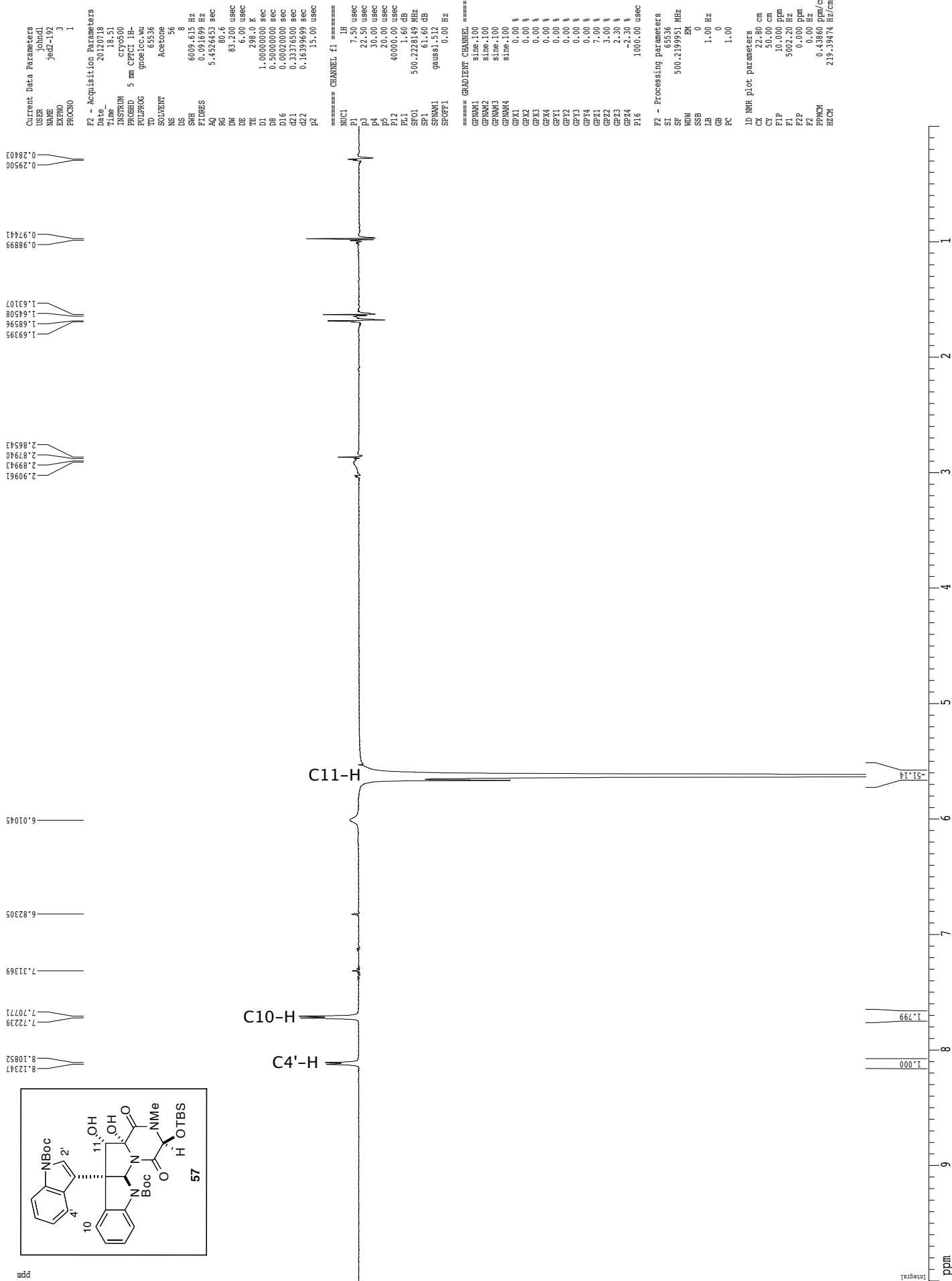
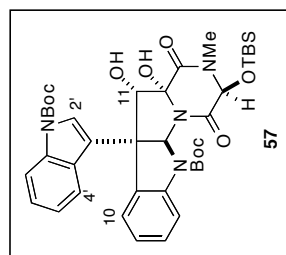
===== CHANNEL f2 =====  
 CDPGRG2 wd1cp15  
 NUC2 1H  
 P2 100.00 usec  
 P21 1.60 dB  
 P22 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR10 0.00 %  
 GSPR11 0.00 %  
 GSPR12 0.00 %  
 GSPR13 0.00 %  
 GSPR14 0.00 %  
 GSPR15 30.00 %  
 GSPR16 50.00 %  
 GSPR17 50.00 usec  
 GSPR18 100.00 usec

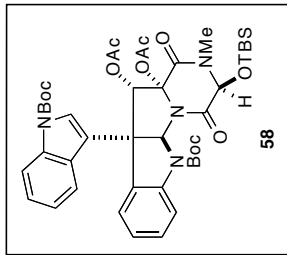
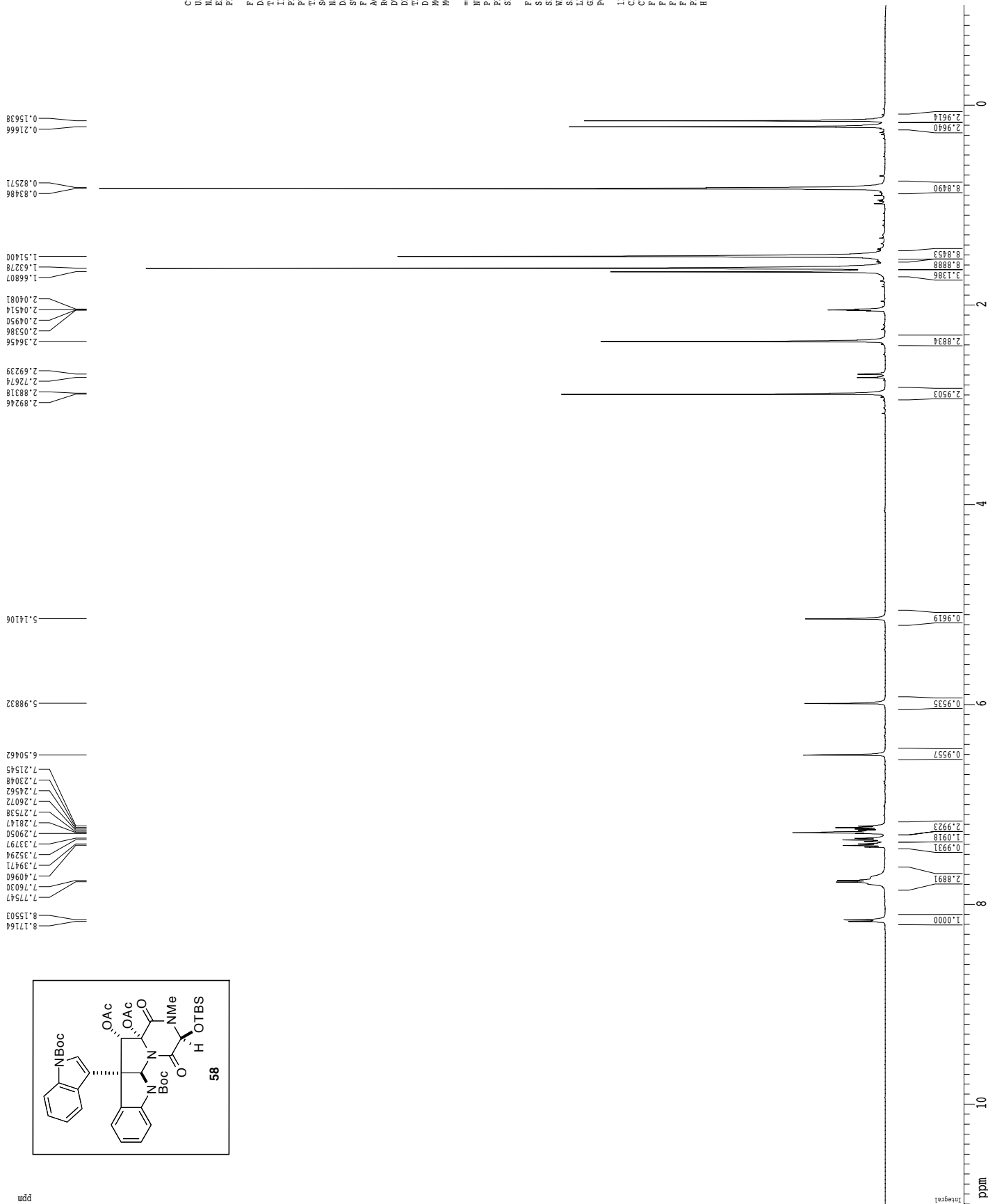
F2 - Processing parameters  
 SI 65536  
 SF 125.7803005 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 400.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2 -10.000 ppm  
 F2 -125.780 Hz  
 F2 125.7803005 ppm/cm  
 HECK 1248.83645 Hz/cm

gnoe



<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jed2-116-bot  
 EXPNO 2  
 PROCNO 1

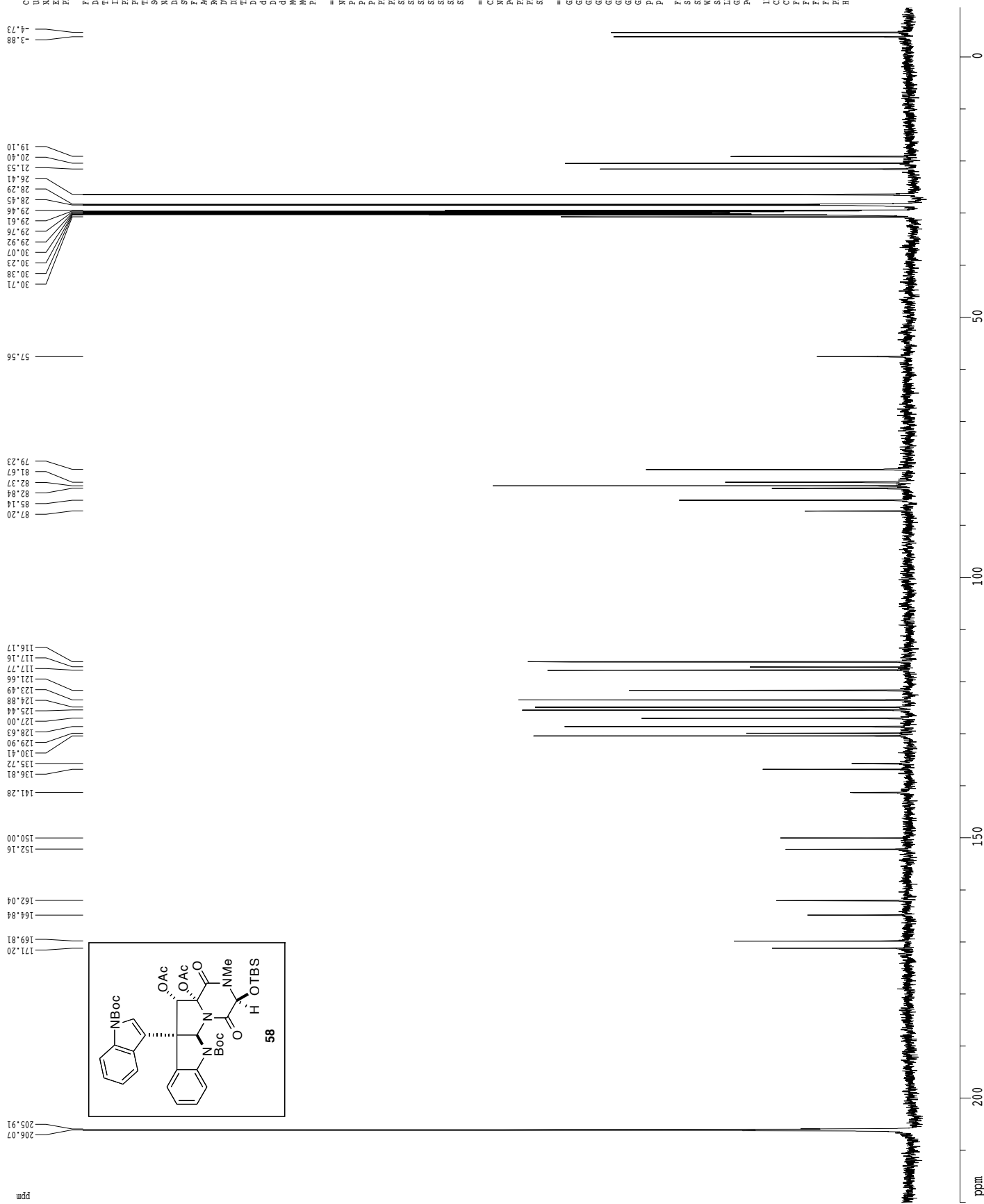
F2 - Acquisition Parameters  
 Date\_ 20120328  
 Time 14.07  
 INSTRUM cryo500  
 PROBRD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 8  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 65  
 DE 62.40 usec  
 DF 6.00 usec  
 TE 313.3 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220179 MHz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 15.00 cm  
 FIP 11.000 ppm  
 F2 5907.82 Hz  
 F3 10.000 ppm  
 F4 -500.92 ppm  
 PRMCM 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER jound1  
 EXPNO jed1-116-4605  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120328  
 Time 14:09  
 INSTRUM cryo500  
 PROBHD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 312  
 DS 16  
 SFR 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 7298.7  
 DW 6.00 usec  
 DE 6.00 usec  
 TE 313.0 K  
 D1 1.0000000 sec  
 d11 0.0300000 sec  
 D16 0.0002000 sec  
 d17 0.0001560 sec  
 ACRESF 0.0000000 sec  
 ACWRK 0.0150000 sec  
 F2 3.00 usec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.7945648 dB  
 PL2 125.7945648 dB  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO1 Ccp60.0.5.20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

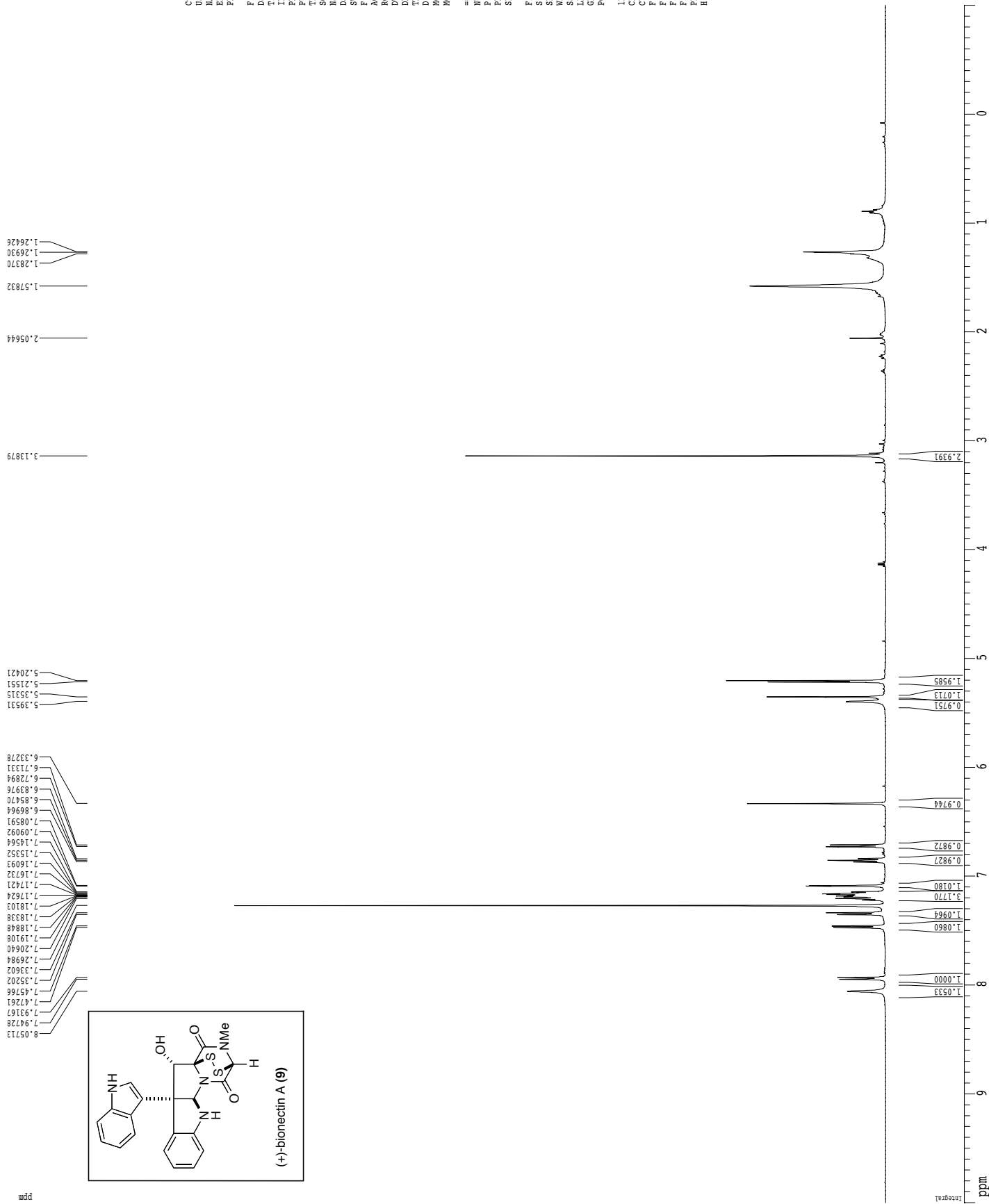
===== CHANNEL f2 =====  
 CDPGR2 wd1616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GRAM1 0.00 %  
 GRAM2 0.00 %  
 GRAM3 0.00 %  
 GRAM4 0.00 %  
 GRAM5 0.00 %  
 GRAM6 0.00 %  
 GRAM7 30.00 %  
 GRAM8 50.00 %  
 P15 500.00 usec  
 P16 1000.00 usec

F2 - Processing parameters  
 SI 65536  
 SF 125.7802935 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 2.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 25.00 cm  
 FIP 220.000 ppm  
 F1 2767.67 Hz  
 F2 -10.000 ppm  
 F2 -125.780 Hz  
 F2 125.780 ppm/cm  
 HZCM 1268.83645 Hz/cm

CDCl3  
1H spectrum



Current Data Parameters  
 USER JohnM  
 NAME jek2-224  
 EXPNO 7  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120714  
 Time 0.31  
 INSTRUM cryo500  
 PROBRD 5 mm CPXI IH-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 48  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.096943 Hz  
 AQ 5.0939718 sec  
 RG 384.5  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

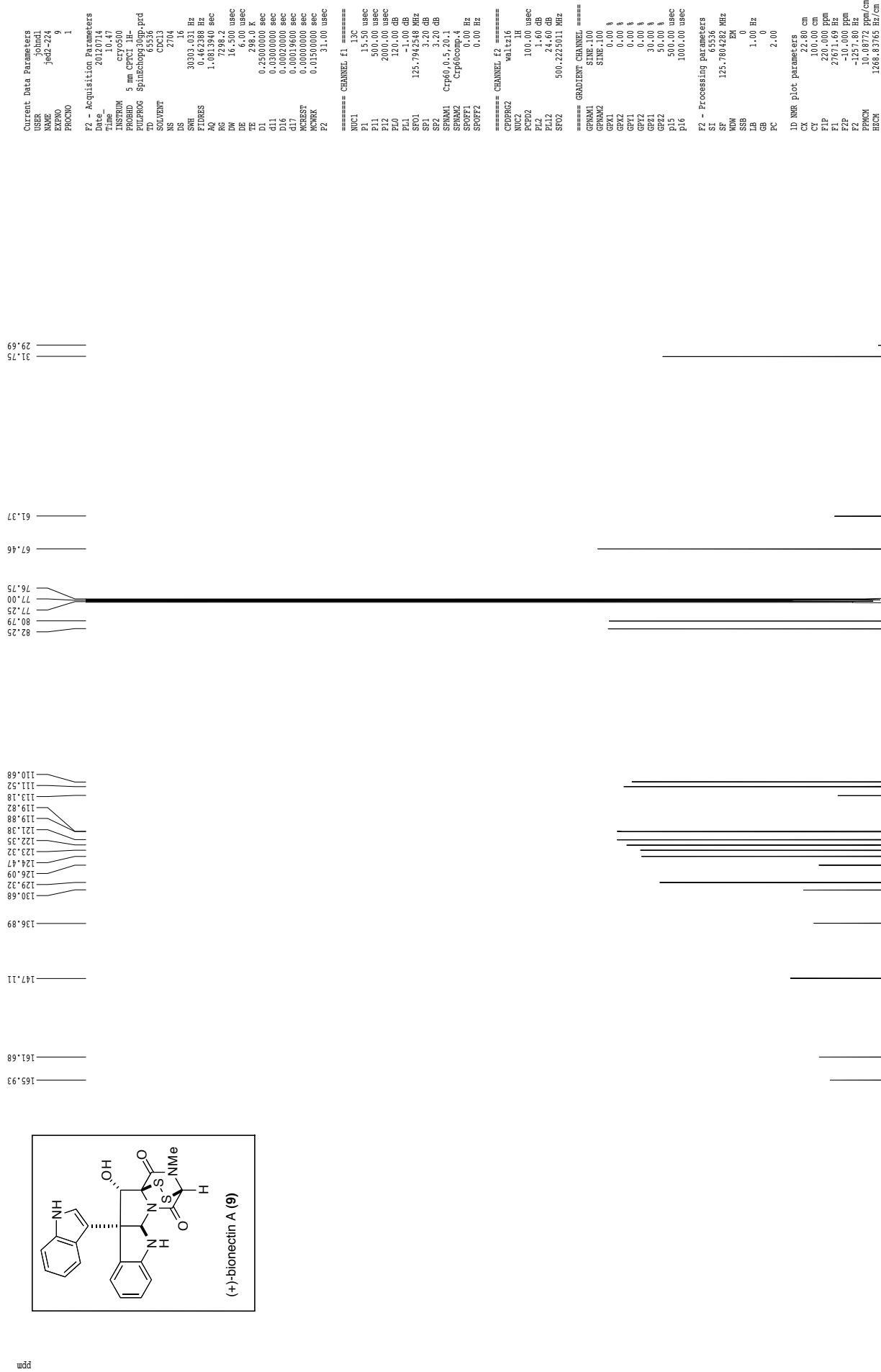
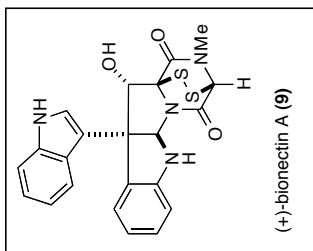
==== CHANNEL F1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.223015 MHz

F2 - Processing Parameters  
 SI 65536  
 SF 500.2200262 MHz  
 WDW EM  
 SSF 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

ID NMR plot parameters  
 CX 22.80 cm  
 CI 8.00 cm  
 F1 10.00 ppm  
 F2 5002.200 ppm  
 F3 1.000 ppm  
 F4 -500.22 Hz  
 PRMCM 0.48246 ppm/cm  
 HZCM 241.33423 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER johndel  
 NAME jes42-224  
 EXNO 4  
 PROCNO 1

F2 - Acquisition Parameters

Date 20120713  
 Time 23.33  
 INSTRUM cryo500  
 PROBDH 5 mm CPXI IH-  
 PULPROG invv4gpr.wu  
 TD 2048  
 SOLVENT CDCl3  
 NS 1  
 DS 1  
 SWH 5252.101 Hz  
 FIDRES 2.564502 Hz  
 AQ 0.1950196 sec  
 RG 20642.5  
 DW 95.200 usec  
 DE 6.50 usec  
 TE 298.0 K  
 CHSTZ 145.000000  
 U 0.000000 sec  
 D1 1.000000 sec  
 d2 0.00344828 sec  
 d12 0.00002000 sec  
 d13 0.00003000 sec  
 D16 0.00020000 sec  
 d20 0.00242528 sec  
 INO 0.00002100 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*

NUC1 1H  
 P1 7.50 usec  
 P2 15.00 usec  
 PL1 1.60 dB  
 SFO1 500.222653 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*

CPDPRG2 garrd  
 NUC2 15N  
 P2 15.50 usec  
 PCPD2 65.00 usec  
 PL2 -1.00 dB  
 PL12 11.30 dB  
 SFO2 125.792373 MHz

\*\*\*\*\* GRADIENT CHANNEL \*\*\*\*\*

GPM1G1 size-100  
 GMX2 size-100  
 GMRMS size-100  
 GXY1 0.00 %  
 GPX2 0.00 %  
 GPX3 0.00 %  
 GPY1 0.00 %  
 GPY2 0.00 %  
 GPY3 0.00 %  
 GPZ1 30.00 %  
 GPZ2 0.00 %  
 GPZ3 2.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters

ND0 2  
 TD 512  
 SFO1 125.7924 MHz  
 FIDRES 46.502975 Hz  
 SW 49.276 ppm  
 FWHM undefined

F2 - Processing parameters

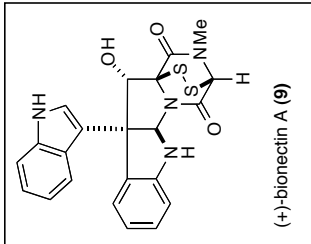
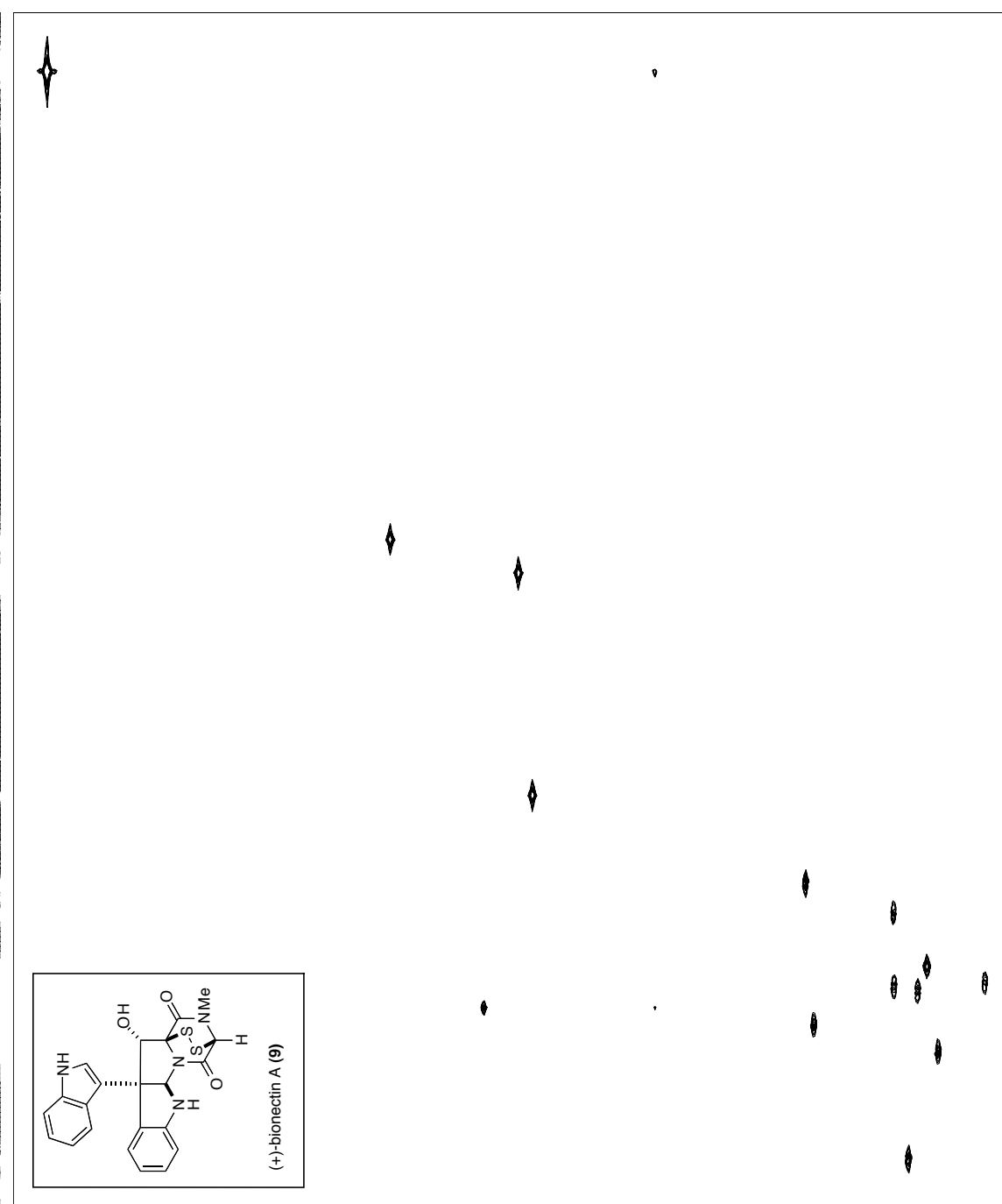
SI 1024  
 SF 500.220262 MHz  
 WDM EM  
 SSB 0  
 LB 5.00 Hz  
 GB 0  
 PC 1.40

F1 - Processing parameters

SI 1024  
 MC2 OF  
 SF 125.7804282 MHz  
 WDM QSTINE  
 SSB 3  
 LB 0.00 Hz  
 GB 0

ZD NMR plot parameters

CX2 18.00 cm  
 CX1 15.00 cm  
 F2PLO 8.137 ppm  
 FZLO 4070.32 Hz  
 F2PHI 2.877 ppm  
 FZHI 1439.14 Hz  
 F1PLO 155.602 ppm  
 F1PHI 28.766 ppm  
 F1HI 3556.36 Hz  
 F2PFCM 0.29222 ppm/cm  
 F2HCM 146.17664 Hz/cm  
 F1PFCM 6.88903 ppm/cm  
 F1HCM 866.50543 Hz/cm



ghmbc optimised for 10 Hz couplings

Current Data Parameters  
USER johnd1  
NAME j642-224  
EXNO 5  
PROCNO 1

F2 - Acquisition Parameters

Date 20120713  
Time 23:44  
INSTRUM spect  
PROBHD 5 mm CPXI 1H  
PULPROG ghmbo20  
TD 4096  
SOLVENT CDCl3  
NS 2  
DS 16  
SWH 5252.101 Hz  
FIDRES 1.282251 Hz  
AQ 0.3899892 sec  
RG 14596.5  
DM 95.200 usec  
DE 9.00 usec  
TE 300.2 K  
CNSF2 145.000000 sec  
d0 0.00000300 sec  
D1 1.25000000 sec  
d2 0.00344828 sec  
D6 0.05000000 sec  
d13 0.00000300 sec  
D16 0.00020000 sec  
IN0 0.00002100 sec

40

==== CHANNEL F1 =====

NVC1 1H  
P1 7.50 usec  
PL 15.00 dB  
SFO1 500.226559 MHz

60

==== CHANNEL F2 =====

NVC2 13C  
P3 15.50 usec  
PL2 -1.00 dB  
SFO2 125.792373 MHz

==== GRADIENT CHANNEL =====

GPW01 sine,100  
GPW02 sine,100  
GPW03 sine,100  
GPR0 0.00 %  
GPR1 0.00 %  
GPR2 0.00 %  
GPR3 0.00 %  
GPR4 0.00 %  
GPR5 0.00 %  
GPR6 0.00 %  
GPR7 0.00 %  
GPR8 0.00 %  
GPR9 0.00 %  
GPR10 0.00 %  
GPR11 0.00 %  
GPR12 0.00 %  
GPR13 0.00 %  
GPR14 0.00 %  
GPR15 0.00 %  
GPR16 0.00 %  
GPR17 0.00 %  
GPR18 0.00 %  
GPR19 0.00 %  
GPR20 0.00 %  
GPR21 0.00 %  
GPR22 0.00 %  
GPR23 0.00 %  
GPR24 0.00 %  
GPR25 0.00 %  
GPR26 0.00 %  
GPR27 0.00 %  
GPR28 0.00 %  
GPR29 0.00 %  
GPR30 0.00 %  
GPR31 0.00 %  
GPR32 0.00 %  
GPR33 0.00 %  
GPR34 0.00 %  
GPR35 0.00 %  
GPR36 0.00 %  
GPR37 0.00 %  
GPR38 0.00 %  
GPR39 0.00 %  
GPR40 0.00 %  
GPR41 0.00 %  
GPR42 0.00 %  
GPR43 0.00 %  
GPR44 0.00 %  
GPR45 0.00 %  
GPR46 0.00 %  
GPR47 0.00 %  
GPR48 0.00 %  
GPR49 0.00 %  
GPR50 0.00 %  
GPR51 0.00 %  
GPR52 0.00 %  
GPR53 0.00 %  
GPR54 0.00 %  
GPR55 0.00 %  
GPR56 0.00 %  
GPR57 0.00 %  
GPR58 0.00 %  
GPR59 0.00 %  
GPR60 0.00 %  
GPR61 0.00 %  
GPR62 0.00 %  
GPR63 0.00 %  
GPR64 0.00 %  
GPR65 0.00 %  
GPR66 0.00 %  
GPR67 0.00 %  
GPR68 0.00 %  
GPR69 0.00 %  
GPR70 0.00 %  
GPR71 0.00 %  
GPR72 0.00 %  
GPR73 0.00 %  
GPR74 0.00 %  
GPR75 0.00 %  
GPR76 0.00 %  
GPR77 0.00 %  
GPR78 0.00 %  
GPR79 0.00 %  
GPR80 0.00 %  
GPR81 0.00 %  
GPR82 0.00 %  
GPR83 0.00 %  
GPR84 0.00 %  
GPR85 0.00 %  
GPR86 0.00 %  
GPR87 0.00 %  
GPR88 0.00 %  
GPR89 0.00 %  
GPR90 0.00 %  
GPR91 0.00 %  
GPR92 0.00 %  
GPR93 0.00 %  
GPR94 0.00 %  
GPR95 0.00 %  
GPR96 0.00 %  
GPR97 0.00 %  
GPR98 0.00 %  
GPR99 0.00 %  
GPR100 0.00 %

80

100

==== GRADIENT CHANNEL =====

GPW01 sine,100  
GPW02 sine,100  
GPW03 sine,100  
GPR0 0.00 %  
GPR1 0.00 %  
GPR2 0.00 %  
GPR3 0.00 %  
GPR4 0.00 %  
GPR5 0.00 %  
GPR6 0.00 %  
GPR7 0.00 %  
GPR8 0.00 %  
GPR9 0.00 %  
GPR10 0.00 %  
GPR11 0.00 %  
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GPR13 0.00 %  
GPR14 0.00 %  
GPR15 0.00 %  
GPR16 0.00 %  
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GPR18 0.00 %  
GPR19 0.00 %  
GPR20 0.00 %  
GPR21 0.00 %  
GPR22 0.00 %  
GPR23 0.00 %  
GPR24 0.00 %  
GPR25 0.00 %  
GPR26 0.00 %  
GPR27 0.00 %  
GPR28 0.00 %  
GPR29 0.00 %  
GPR30 0.00 %  
GPR31 0.00 %  
GPR32 0.00 %  
GPR33 0.00 %  
GPR34 0.00 %  
GPR35 0.00 %  
GPR36 0.00 %  
GPR37 0.00 %  
GPR38 0.00 %  
GPR39 0.00 %  
GPR40 0.00 %  
GPR41 0.00 %  
GPR42 0.00 %  
GPR43 0.00 %  
GPR44 0.00 %  
GPR45 0.00 %  
GPR46 0.00 %  
GPR47 0.00 %  
GPR48 0.00 %  
GPR49 0.00 %  
GPR50 0.00 %  
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GPR55 0.00 %  
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GPR58 0.00 %  
GPR59 0.00 %  
GPR60 0.00 %  
GPR61 0.00 %  
GPR62 0.00 %  
GPR63 0.00 %  
GPR64 0.00 %  
GPR65 0.00 %  
GPR66 0.00 %  
GPR67 0.00 %  
GPR68 0.00 %  
GPR69 0.00 %  
GPR70 0.00 %  
GPR71 0.00 %  
GPR72 0.00 %  
GPR73 0.00 %  
GPR74 0.00 %  
GPR75 0.00 %  
GPR76 0.00 %  
GPR77 0.00 %  
GPR78 0.00 %  
GPR79 0.00 %  
GPR80 0.00 %  
GPR81 0.00 %  
GPR82 0.00 %  
GPR83 0.00 %  
GPR84 0.00 %  
GPR85 0.00 %  
GPR86 0.00 %  
GPR87 0.00 %  
GPR88 0.00 %  
GPR89 0.00 %  
GPR90 0.00 %  
GPR91 0.00 %  
GPR92 0.00 %  
GPR93 0.00 %  
GPR94 0.00 %  
GPR95 0.00 %  
GPR96 0.00 %  
GPR97 0.00 %  
GPR98 0.00 %  
GPR99 0.00 %  
GPR100 0.00 %

100

120

==== GRADIENT CHANNEL =====

GPW01 sine,100  
GPW02 sine,100  
GPW03 sine,100  
GPR0 0.00 %  
GPR1 0.00 %  
GPR2 0.00 %  
GPR3 0.00 %  
GPR4 0.00 %  
GPR5 0.00 %  
GPR6 0.00 %  
GPR7 0.00 %  
GPR8 0.00 %  
GPR9 0.00 %  
GPR10 0.00 %  
GPR11 0.00 %  
GPR12 0.00 %  
GPR13 0.00 %  
GPR14 0.00 %  
GPR15 0.00 %  
GPR16 0.00 %  
GPR17 0.00 %  
GPR18 0.00 %  
GPR19 0.00 %  
GPR20 0.00 %  
GPR21 0.00 %  
GPR22 0.00 %  
GPR23 0.00 %  
GPR24 0.00 %  
GPR25 0.00 %  
GPR26 0.00 %  
GPR27 0.00 %  
GPR28 0.00 %  
GPR29 0.00 %  
GPR30 0.00 %  
GPR31 0.00 %  
GPR32 0.00 %  
GPR33 0.00 %  
GPR34 0.00 %  
GPR35 0.00 %  
GPR36 0.00 %  
GPR37 0.00 %  
GPR38 0.00 %  
GPR39 0.00 %  
GPR40 0.00 %  
GPR41 0.00 %  
GPR42 0.00 %  
GPR43 0.00 %  
GPR44 0.00 %  
GPR45 0.00 %  
GPR46 0.00 %  
GPR47 0.00 %  
GPR48 0.00 %  
GPR49 0.00 %  
GPR50 0.00 %  
GPR51 0.00 %  
GPR52 0.00 %  
GPR53 0.00 %  
GPR54 0.00 %  
GPR55 0.00 %  
GPR56 0.00 %  
GPR57 0.00 %  
GPR58 0.00 %  
GPR59 0.00 %  
GPR60 0.00 %  
GPR61 0.00 %  
GPR62 0.00 %  
GPR63 0.00 %  
GPR64 0.00 %  
GPR65 0.00 %  
GPR66 0.00 %  
GPR67 0.00 %  
GPR68 0.00 %  
GPR69 0.00 %  
GPR70 0.00 %  
GPR71 0.00 %  
GPR72 0.00 %  
GPR73 0.00 %  
GPR74 0.00 %  
GPR75 0.00 %  
GPR76 0.00 %  
GPR77 0.00 %  
GPR78 0.00 %  
GPR79 0.00 %  
GPR80 0.00 %  
GPR81 0.00 %  
GPR82 0.00 %  
GPR83 0.00 %  
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GPR85 0.00 %  
GPR86 0.00 %  
GPR87 0.00 %  
GPR88 0.00 %  
GPR89 0.00 %  
GPR90 0.00 %  
GPR91 0.00 %  
GPR92 0.00 %  
GPR93 0.00 %  
GPR94 0.00 %  
GPR95 0.00 %  
GPR96 0.00 %  
GPR97 0.00 %  
GPR98 0.00 %  
GPR99 0.00 %  
GPR100 0.00 %

120

140

==== GRADIENT CHANNEL =====

GPW01 sine,100  
GPW02 sine,100  
GPW03 sine,100  
GPR0 0.00 %  
GPR1 0.00 %  
GPR2 0.00 %  
GPR3 0.00 %  
GPR4 0.00 %  
GPR5 0.00 %  
GPR6 0.00 %  
GPR7 0.00 %  
GPR8 0.00 %  
GPR9 0.00 %  
GPR10 0.00 %  
GPR11 0.00 %  
GPR12 0.00 %  
GPR13 0.00 %  
GPR14 0.00 %  
GPR15 0.00 %  
GPR16 0.00 %  
GPR17 0.00 %  
GPR18 0.00 %  
GPR19 0.00 %  
GPR20 0.00 %  
GPR21 0.00 %  
GPR22 0.00 %  
GPR23 0.00 %  
GPR24 0.00 %  
GPR25 0.00 %  
GPR26 0.00 %  
GPR27 0.00 %  
GPR28 0.00 %  
GPR29 0.00 %  
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GPR35 0.00 %  
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GPR41 0.00 %  
GPR42 0.00 %  
GPR43 0.00 %  
GPR44 0.00 %  
GPR45 0.00 %  
GPR46 0.00 %  
GPR47 0.00 %  
GPR48 0.00 %  
GPR49 0.00 %  
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GPR53 0.00 %  
GPR54 0.00 %  
GPR55 0.00 %  
GPR56 0.00 %  
GPR57 0.00 %  
GPR58 0.00 %  
GPR59 0.00 %  
GPR60 0.00 %  
GPR61 0.00 %  
GPR62 0.00 %  
GPR63 0.00 %  
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GPR68 0.00 %  
GPR69 0.00 %  
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GPR73 0.00 %  
GPR74 0.00 %  
GPR75 0.00 %  
GPR76 0.00 %  
GPR77 0.00 %  
GPR78 0.00 %  
GPR79 0.00 %  
GPR80 0.00 %  
GPR81 0.00 %  
GPR82 0.00 %  
GPR83 0.00 %  
GPR84 0.00 %  
GPR85 0.00 %  
GPR86 0.00 %  
GPR87 0.00 %  
GPR88 0.00 %  
GPR89 0.00 %  
GPR90 0.00 %  
GPR91 0.00 %  
GPR92 0.00 %  
GPR93 0.00 %  
GPR94 0.00 %  
GPR95 0.00 %  
GPR96 0.00 %  
GPR97 0.00 %  
GPR98 0.00 %  
GPR99 0.00 %  
GPR100 0.00 %

140

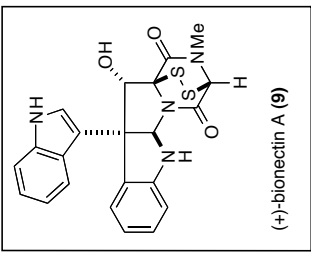
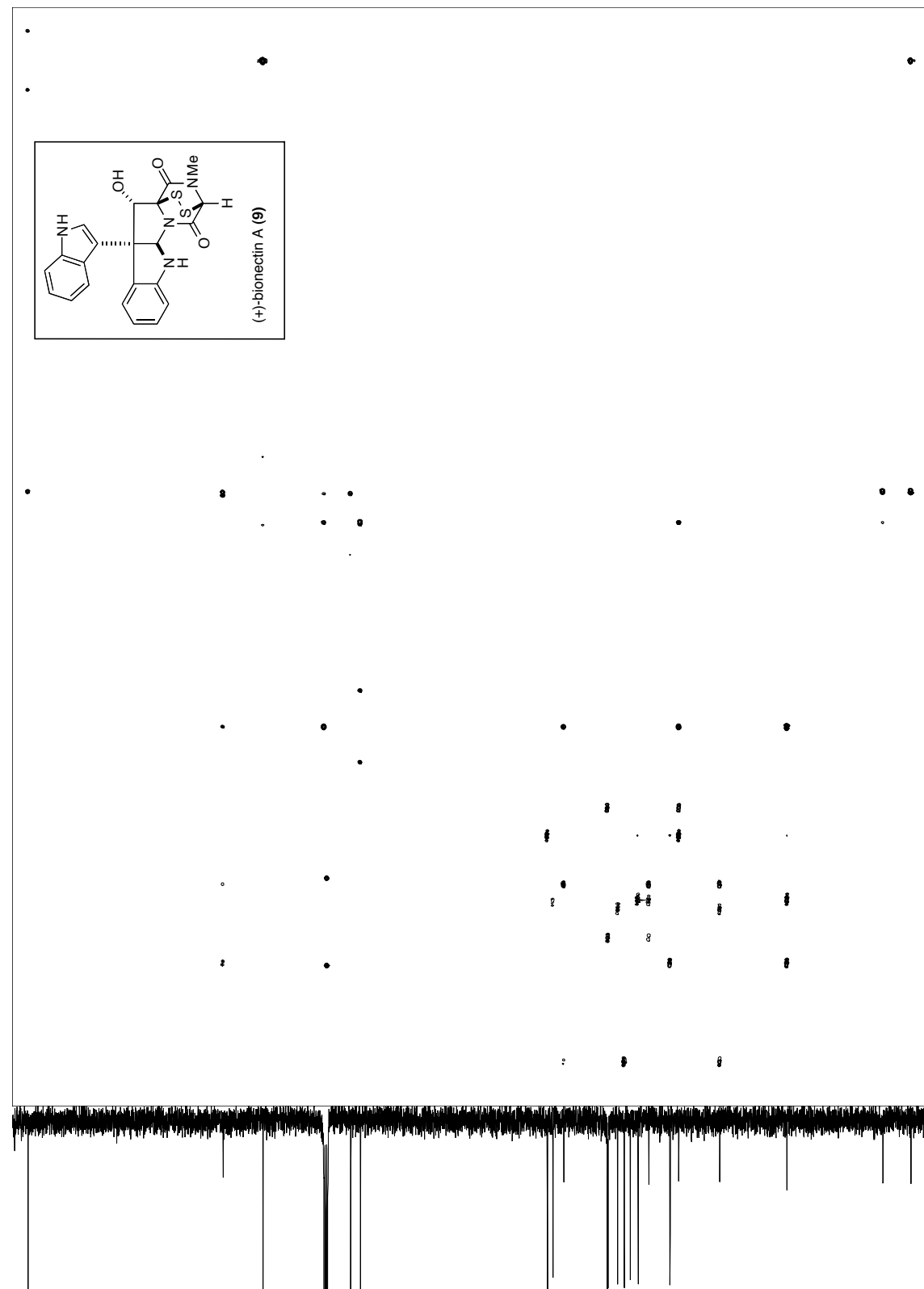
160

==== GRADIENT CHANNEL =====

GPW01 sine,100  
GPW02 sine,100  
GPW03 sine,100  
GPR0 0.00 %  
GPR1 0.00 %  
GPR2 0.00 %  
GPR3 0.00 %  
GPR4 0.00 %  
GPR5 0.00 %  
GPR6 0.00 %  
GPR7 0.00 %  
GPR8 0.00 %  
GPR9 0.00 %  
GPR10 0.00 %  
GPR11 0.00 %  
GPR12 0.00 %  
GPR13 0.00 %  
GPR14 0.00 %  
GPR15 0.00 %  
GPR16 0.00 %  
GPR17 0.00 %  
GPR18 0.00 %  
GPR19 0.00 %  
GPR20 0.00 %  
GPR21 0.00 %  
GPR22 0.00 %  
GPR23 0.00 %  
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GPR25 0.00 %  
GPR26 0.00 %  
GPR27 0.00 %  
GPR28 0.00 %  
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GPR30 0.00 %  
GPR31 0.00 %  
GPR32 0.00 %  
GPR33 0.00 %  
GPR34 0.00 %  
GPR35 0.00 %  
GPR36 0.00 %  
GPR37 0.00 %  
GPR38 0.00 %  
GPR39 0.00 %  
GPR40 0.00 %  
GPR41 0.00 %  
GPR42 0.00 %  
GPR43 0.00 %  
GPR44 0.00 %  
GPR45 0.00 %  
GPR46 0.00 %  
GPR47 0.00 %  
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GPR51 0.00 %  
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GPR59 0.00 %  
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GPR63 0.00 %  
GPR64 0.00 %  
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GPR67 0.00 %  
GPR68 0.00 %  
GPR69 0.00 %  
GPR70 0.00 %  
GPR71 0.00 %  
GPR72 0.00 %  
GPR73 0.00 %  
GPR74 0.00 %  
GPR75 0.00 %  
GPR76 0.00 %  
GPR77 0.00 %  
GPR78 0.00 %  
GPR79 0.00 %  
GPR80 0.00 %  
GPR81 0.00 %  
GPR82 0.00 %  
GPR83 0.00 %  
GPR84 0.00 %  
GPR85 0.00 %  
GPR86 0.00 %  
GPR87 0.00 %  
GPR88 0.00 %  
GPR89 0.00 %  
GPR90 0.00 %  
GPR91 0.00 %  
GPR92 0.00 %  
GPR93 0.00 %  
GPR94 0.00 %  
GPR95 0.00 %  
GPR96 0.00 %  
GPR97 0.00 %  
GPR98 0.00 %  
GPR99 0.00 %  
GPR100 0.00 %

160

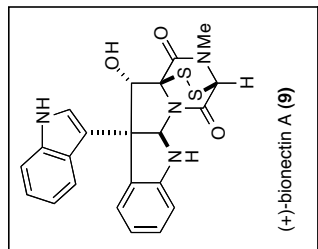
ppm



2D NMR plot parameters  
CX2 18.00 cm  
CX1 15.00 cm  
F2Z0 8.152 ppm  
F2Z1 40.882 Hz  
F2Z2 2.882 Hz  
F2Z3 1441.71 Hz  
F2Z4 168.573 ppm  
F2Z5 21203.24 Hz  
F1Z1 29.376 ppm  
F1Z2 3694.87 Hz  
F2P0 0.29279 ppm/cm  
F2P1 146.46158 Hz/cm  
F1P0 9.27986 ppm/cm  
F1P1 1167.22473 Hz/cm

gnoe

5.21630  
7.94854  
7.93291  
7.47377  
7.45898



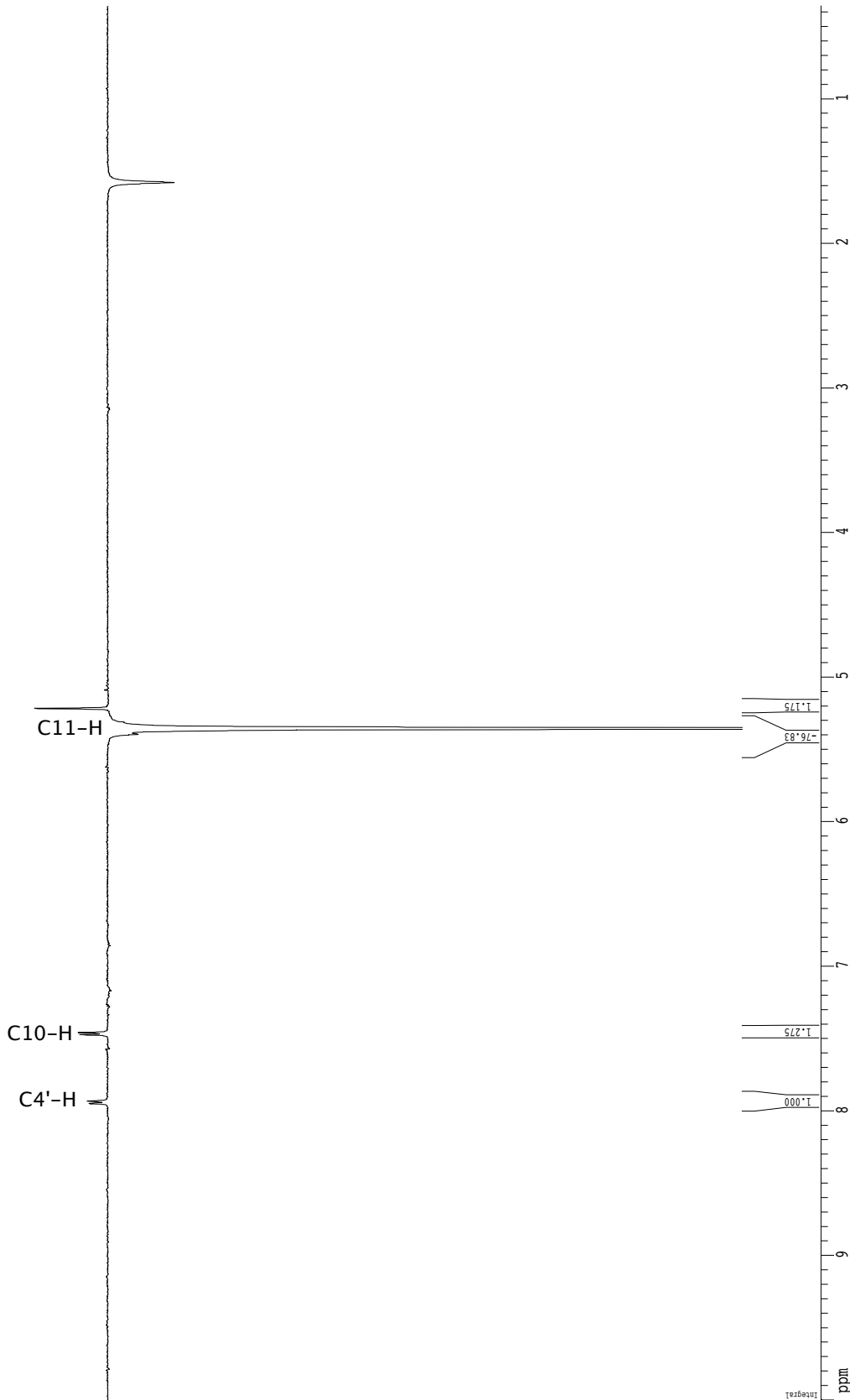
Current Data Parameters  
 USER JohnHd.  
 NAME jed2-224  
 EXPNO 11  
 PROCNO 1  
 P2 - Acquisition Parameters  
 Date\_ 20120714  
 Time\_ 16.35  
 INSTRUM cryo500  
 PROBHD 5 mm CPYCI 1H-  
 PULPROG gnoe1cc.wu  
 TD 65536  
 SOLVENT CDC13  
 NS 40  
 DS 8  
 SWH 5000.000 Hz  
 FIDRES 0.076294 Hz  
 AQ 6.5536499 sec  
 RG 64  
 DW 100.000 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.000000 sec  
 D11 0.500000 sec  
 D16 0.1002000 sec  
 d21 0.33376500 sec  
 d22 0.16399699 sec  
 p2 15.00 usec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 P3 22.50 usec  
 P4 30.00 usec  
 P5 20.00 usec  
 P12 40000.00 usec  
 PL1 1.60 dB  
 SF01 500.2227040 MHz  
 SF1 61.60 dB  
 SP0M1 gauss1.512  
 SPOFF1 0.00 Hz

==== GRADIENT CHANNEL =====  
 GENM1 slope:100  
 GENM2 slope:100  
 GENM3 slope:100  
 GENM4 slope:100  
 GFX1 0.00 %  
 GFX2 0.00 %  
 GFX3 0.00 %  
 GFX4 0.00 %  
 GFY1 0.00 %  
 GFY2 0.00 %  
 GFY3 0.00 %  
 GFY4 0.00 %  
 GZ1 7.00 %  
 GZ2 3.00 %  
 GZ3 2.30 %  
 GZ4 -2.30 %  
 P16 1000.00 usec

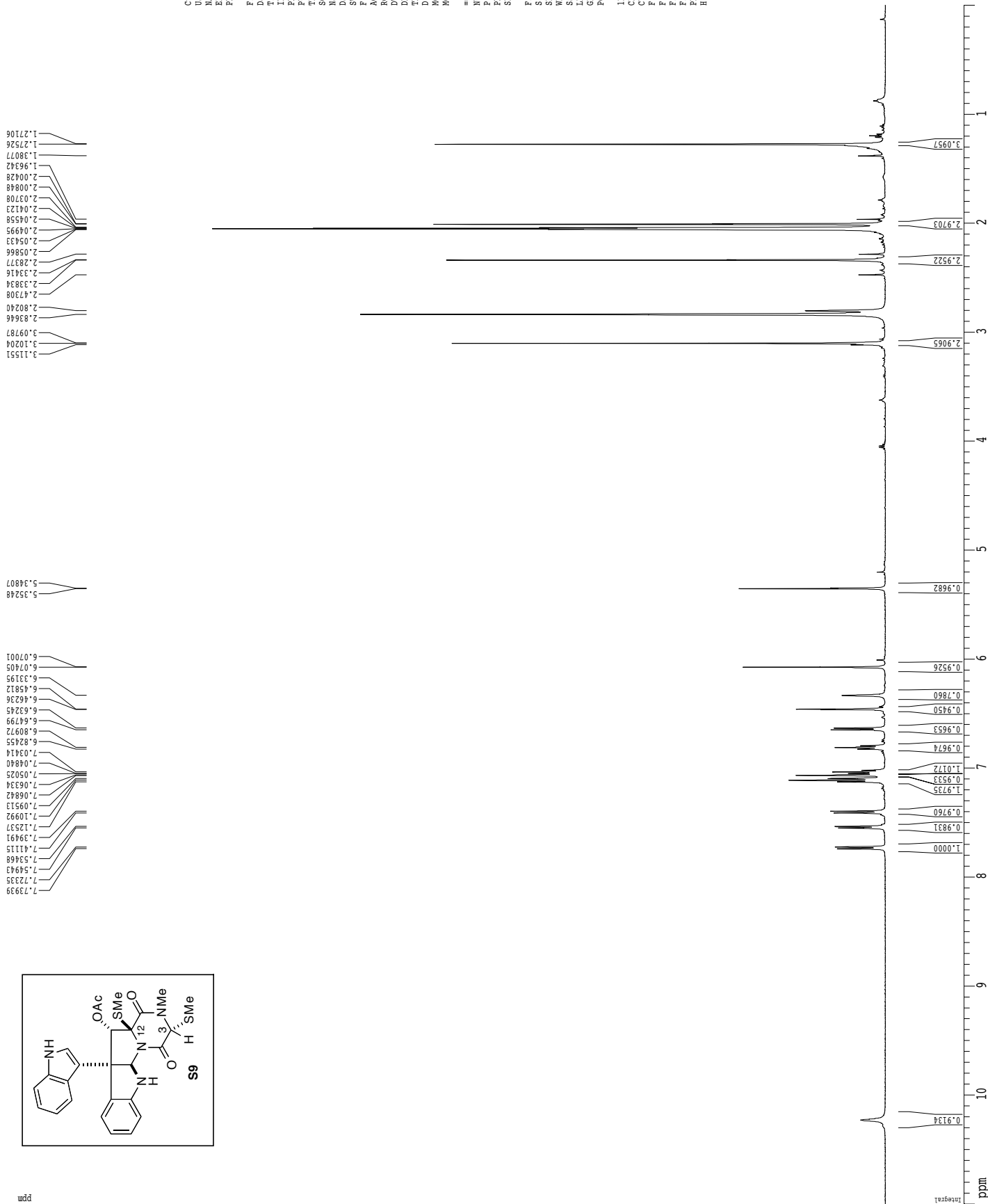
P2 - Processing Parameters  
 SI 65536  
 SF 500.220250 MHz  
 MDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 F1P 10.000 ppm  
 F1 5002.20 Hz  
 F2P 0.000 ppm  
 F2 1.000 Hz  
 FREQM 0.4396 ppm/cm  
 HZCM 219.39456 Hz/cm



Integral

<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jed7-172-bot  
 EXPNO 1  
 PROCNO 1

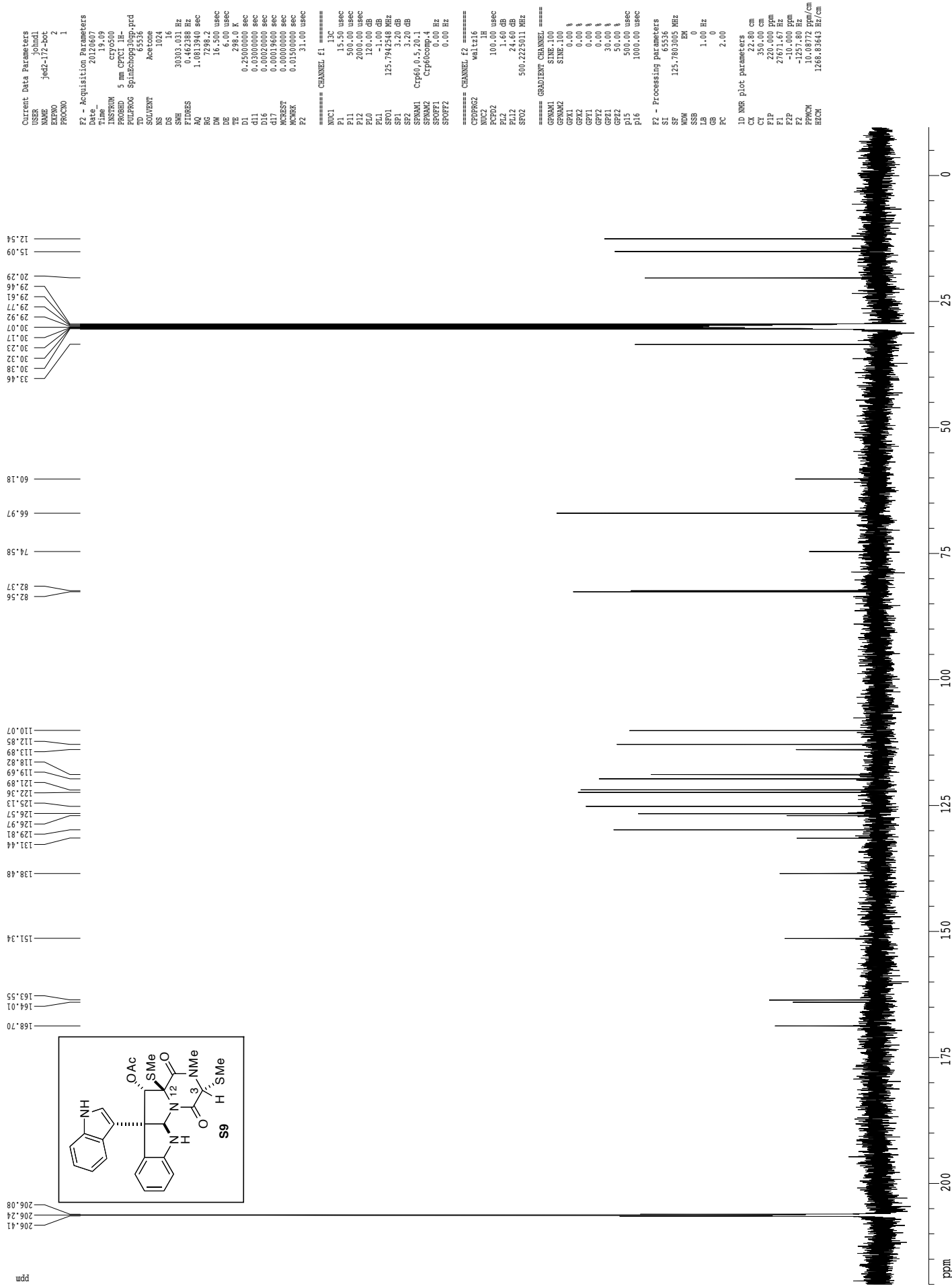
F2 - Acquisition Parameters  
 Date\_ 20120607  
 Time 19.06  
 INSTRUM crys500  
 PROBHD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 377  
 DE 62.600 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.225015 MHz

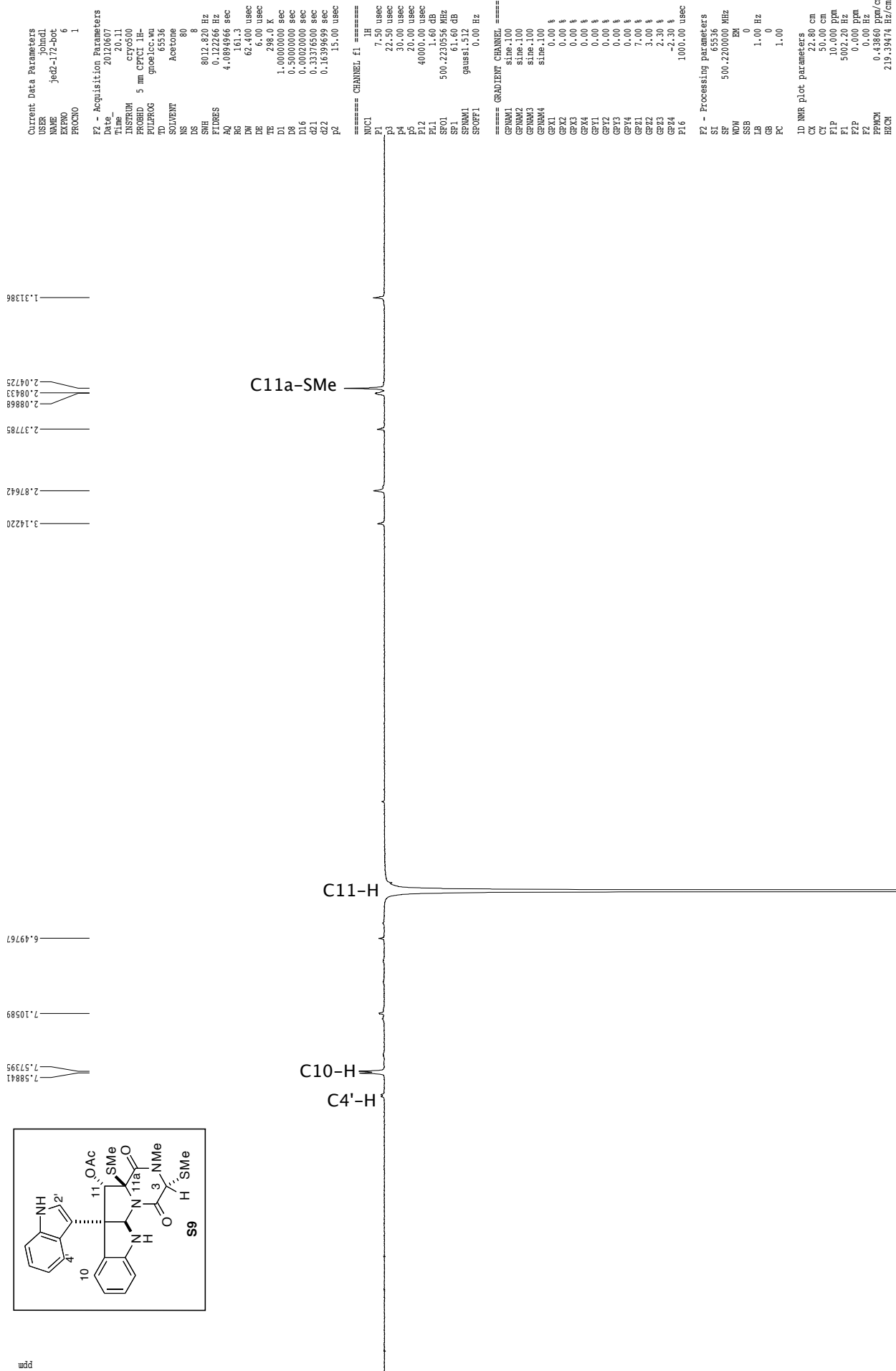
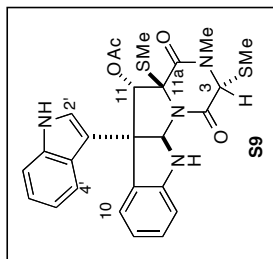
F2 - Processing parameters  
 SI 65536  
 SF 500.220183 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 11.000 ppm  
 SFO 5502.82 Hz  
 F2 0.00 ppm  
 F3 0.00 ppm  
 PRGM 0.48246 ppm/cm  
 HZCN 241.33423 Hz/cm

Z-restored spin-echo <sup>13</sup>C spectrum with <sup>1</sup>H decoupling



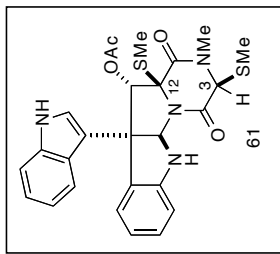
gnoe



Integral

ppm

<sup>1</sup>H spectrum



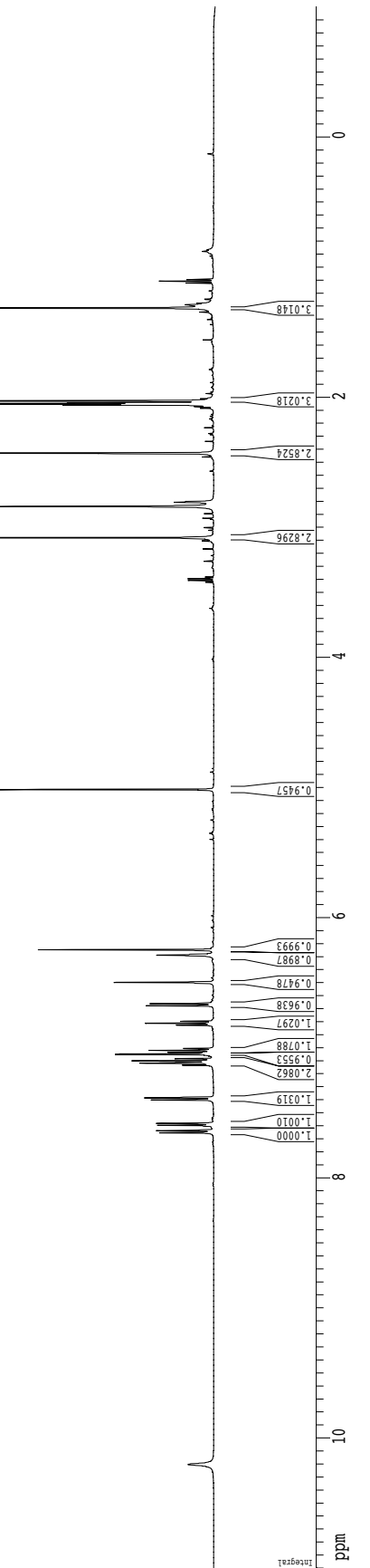
Current Data Parameters  
 USER johnd  
 NAME jed2-172-top  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120607  
 Time 9.35  
 INSTRUM cryo500  
 PROBRD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 62.40  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220181 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 9.00 cm  
 FIP 11.000 ppm  
 F1 550.22 Hz  
 F2 11.000 ppm  
 F3 -50.00 Hz  
 PRMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

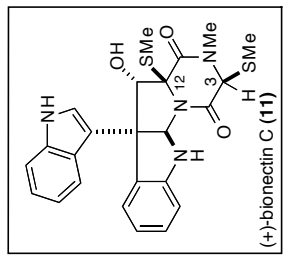
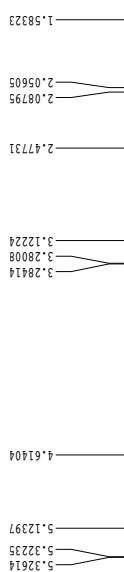
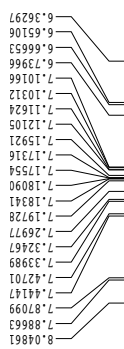








<sup>1</sup>H spectrum



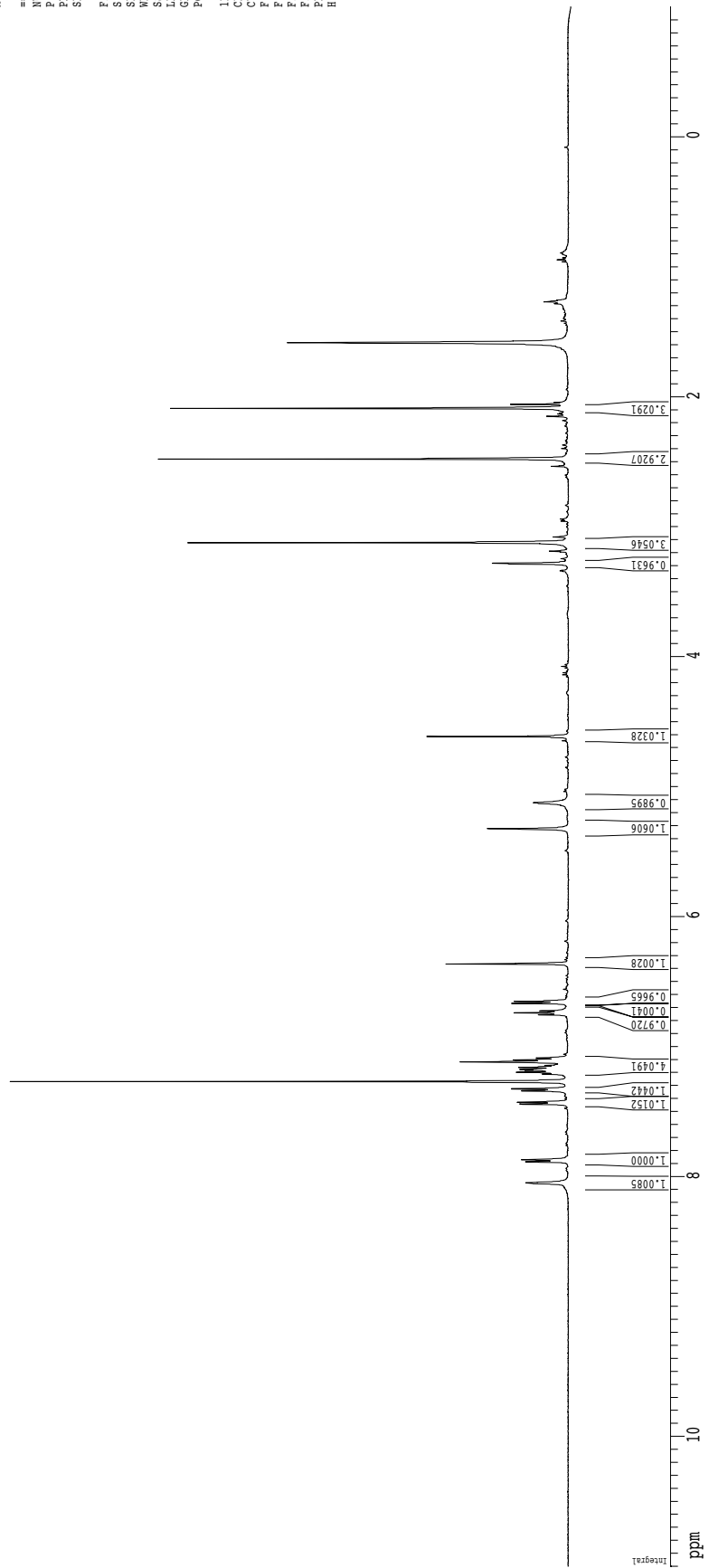
Current Data Parameters  
 USER johnd  
 NAME jes2-193  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120618  
 Time 16.34  
 INSTRUM cryo500  
 PROBRID 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CCl3  
 NS 24  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0996774 sec  
 RG 671  
 SW 62.401 usec  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.220262 MHz  
 DS 4  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 0.50

1D NMR plot parameters  
 CX 22.80 cm  
 CY 6.00 cm  
 FIP 11.000 ppm  
 F2 5502.82 Hz  
 F3 10.000 ppm  
 FZ -50.92 ppm  
 PRMCM 0.52432 ppm/cm  
 HZCM 263.27371 Hz/cm



ppm



Current Data Parameters  
 USER johnd  
 NAME jes2-193  
 EXNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20120619  
 Time 8.56  
 INSTRUM cryo500  
 PROBDH 5 mm CPXI IH-  
 PULPROG invv4gpp.wu  
 TD 2048  
 SOLVENT CDCl3  
 NS 12  
 DS 2  
 SWH 3387.534 Hz  
 FIDRES 1.654069 Hz  
 AQ 0.3023348 sec  
 RG 11585.2  
 DW 147.600 usec  
 DE 6.50 usec  
 TE 298.0 K  
 CHS22 145.000000  
 CHS23 145.000000  
 CHS24 2.00000000  
 d1 0.00344828 sec  
 d2 0.00344828 sec  
 d12 0.00002000 sec  
 d13 0.00003000 sec  
 D16 0.00020000 sec  
 d20 0.00242528 sec  
 d20 0.00024800 sec  
 INO 0.00024800 sec

20

40

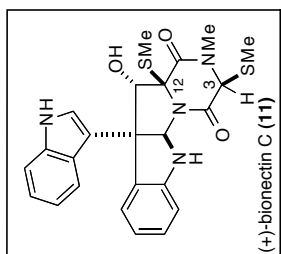
60

80

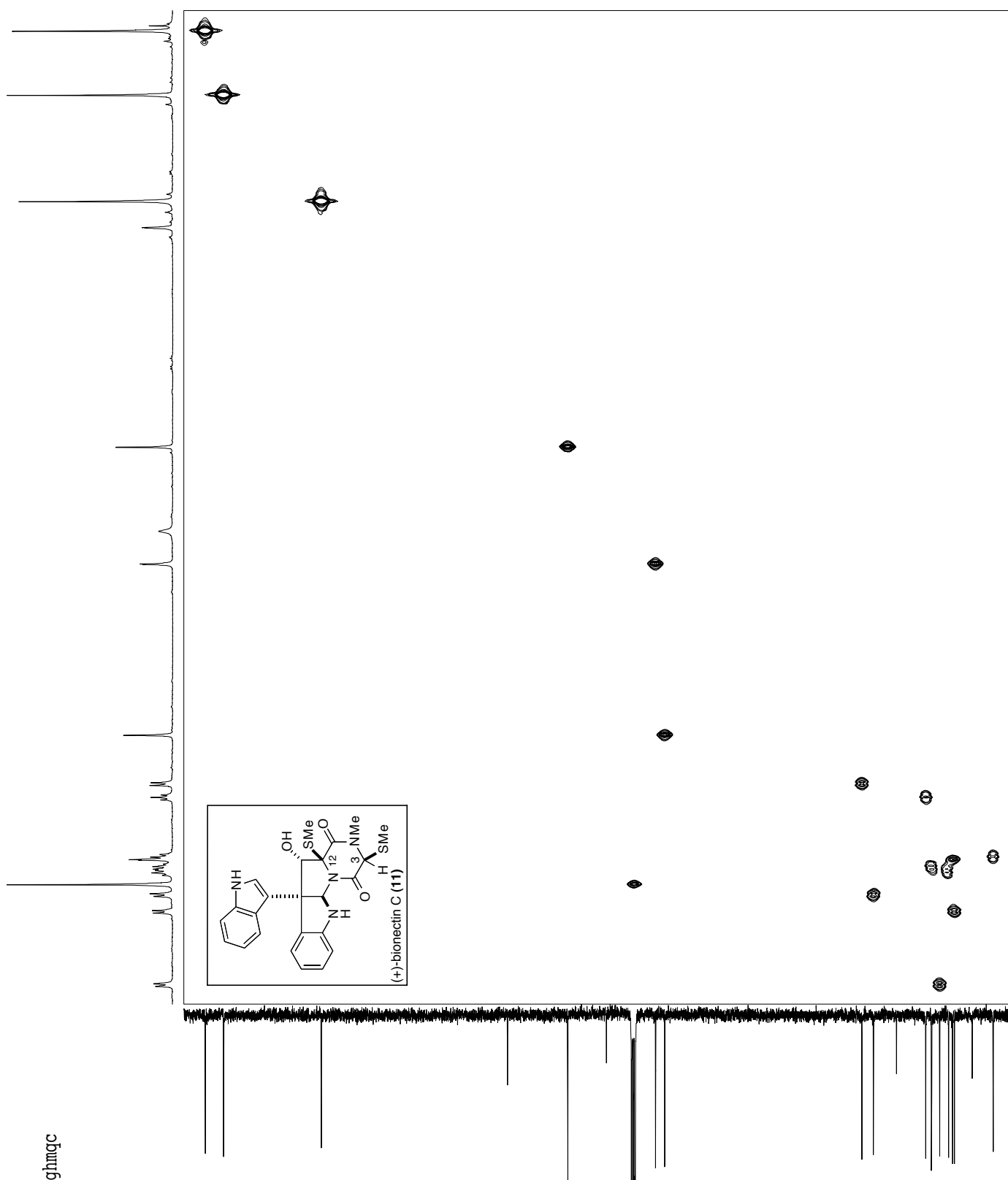
100

120

ppm



(+)-bionelectin C (11)



ghmqc

ppm

7

6

5

4

3

2D NMR plot parameters

CX2 18.00 cm  
 CX1 15.00 cm  
 F2PLO 7.995 ppm  
 FZLO 399.36 Hz  
 F2PHI 1.964 ppm  
 F2HI 982.34 Hz  
 F1PLO 1632.461 ppm  
 F1PHI 1632.461 ppm  
 F1HI 1554.61 Hz  
 F2PQMC 0.33508 ppm/cm  
 F2HCOC 167.61235 Hz/cm  
 F1PQMC 7.94143 ppm/cm  
 F1HCOC 998.87646 Hz/cm

F1 - Processing parameters

SI 1024  
 MC 0F  
 SF 125.7804282 MHz  
 QSTINE 3  
 LB 0.00 Hz  
 GB 0

F2 - Processing parameters

SI 1024  
 SF 500.2200262 MHz  
 EM 0  
 WDM 5.00 Hz  
 SSB 0  
 LB 0  
 GB 0  
 PC 2.00

F1 - Acquisition parameters

ND0 2  
 TD 88  
 SF01 125.7917 MHz  
 SF02 229.10576 Hz  
 SW 460.275 ppm  
 FREQ0E undefined

==== GRADIENT CHANNEL =====

GPM01 size:100  
 GPM02 size:100  
 GPM03 size:100  
 GPM04 size:100  
 GPX1 0.00 %  
 GPX2 0.00 %  
 GPX3 0.00 %  
 GPY1 0.00 %  
 GPY2 0.00 %  
 GPY3 0.00 %  
 GPZ1 30.00 %  
 GPZ2 0.00 %  
 GPZ3 0.00 %  
 GPC1 2.00 usec  
 GPC2 2.00 usec  
 GPC3 2.00 usec  
 GPC4 2.00 usec  
 GPC5 2.00 usec  
 GPC6 2.00 usec  
 GPC7 2.00 usec  
 GPC8 2.00 usec  
 GPC9 2.00 usec  
 GPC10 2.00 usec  
 GPC11 2.00 usec  
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 GPC95 2.00 usec  
 GPC96 2.00 usec  
 GPC97 2.00 usec  
 GPC98 2.00 usec  
 GPC99 2.00 usec  
 GPC100 2.00 usec

==== CHANNEL F1 =====

CPDPRG2 gact  
 NU1 H  
 P1 7.50 usec  
 P2 15.00 usec  
 PL1 1.60 dB  
 SF01 500.222598 MHz

==== CHANNEL F2 =====

CPDPRG2 gact  
 NU2 H  
 P1 7.50 usec  
 P2 15.00 usec  
 PL1 1.60 dB  
 SF01 500.222598 MHz  
 PCPD2 65.00 usec  
 PL2 -1.00 dB  
 PL12 11.30 dB  
 SF02 125.7917484 MHz

Current Data Parameters  
 USER johnd1  
 NAME j642-193  
 EXPTNO 3  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20120619  
 Time 8:11  
 INSTRUM spect  
 PROBRD 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 4096  
 SOLVENT CDCl3  
 NS 3  
 DS 16  
 SWH 3387.534 Hz  
 FIDRES 0.827035 Hz  
 AQ 0.6046196 sec  
 RG 14596.5  
 DW 147.600 usec  
 DE 9.00 usec  
 TE 300.2 K  
 CNSF2 145.0000000  
 d0 0.00000300 sec  
 D1 1.25000000 sec  
 d2 0.00344828 sec  
 D6 0.05000000 sec  
 d13 0.00000300 sec  
 D16 0.00020000 sec  
 INO 0.00002480 sec

==== CHANNEL f1 =====

NVC1 IH  
 P1 7.50 usec  
 PL1 15.00 dB  
 P2 7.50 usec  
 PL2 -1.00 dB  
 SF01 500.2225898 MHz

==== CHANNEL f2 =====

NVC2 13C  
 P3 15.50 usec  
 PL2 -1.00 dB  
 SF02 125.7917484 MHz

==== GRADIENT CHANNEL =====

GPWA1 sine,100  
 GPWA2 sine,100  
 GPWA3 sine,100  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC5 0.00 %  
 GPC6 0.00 %  
 GPC7 0.00 %  
 GPC8 0.00 %  
 GPC9 0.00 %  
 GPC10 0.00 %  
 GPC11 0.00 %  
 GPC12 0.00 %  
 GPC13 0.00 %  
 GPC14 0.00 %  
 GPC15 0.00 %  
 GPC16 0.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters

NU0 2  
 SF01 125.7917 MHz  
 FIDRES 78.7555043 Hz  
 SW 160.275 ppm  
 FWHM undefined

F2 - Processing parameters

SI 2648  
 SF 500.2200262 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 2.00

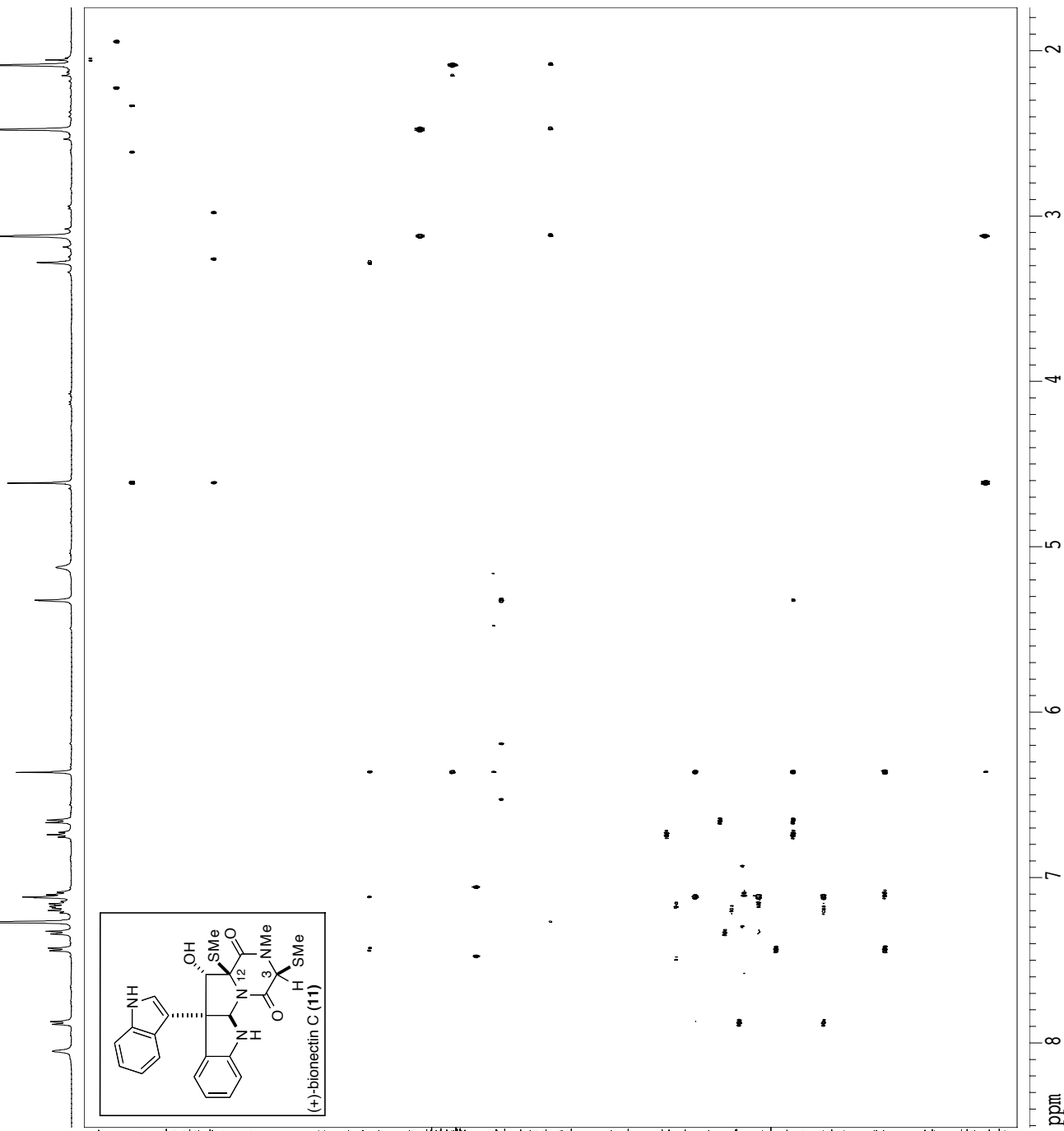
F1 - Processing parameters

SI 1024  
 SF 125.7804282 MHz  
 WDW SINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

2D NMR plot parameters

CX2 18.00 cm  
 CX1 15.00 cm  
 FZEO 8.31 ppm  
 FZOH 43.79 Hz  
 FZHI 869.86 Hz  
 F1F0 170.145 ppm  
 F1LO 21400.89 Hz  
 F1F1 9.855 ppm  
 F1H1 1239.60 Hz  
 F2PACH 0.3762 ppm/cm  
 F2HCN 188.19632 Hz/cm  
 F1PACH 10.68597 ppm/cm  
 F1HCN 1344.08594 Hz/cm

ghmhc optimised for 10 Hz couplings



25

50

75

100

125

150

ppm

2

3

4

5

6

7

8

ppm

gnoe

Current Data Parameters  
 USER Johnhd  
 NAME jedz-193  
 EXPNO 6  
 PROCNO 1

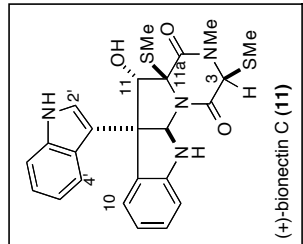
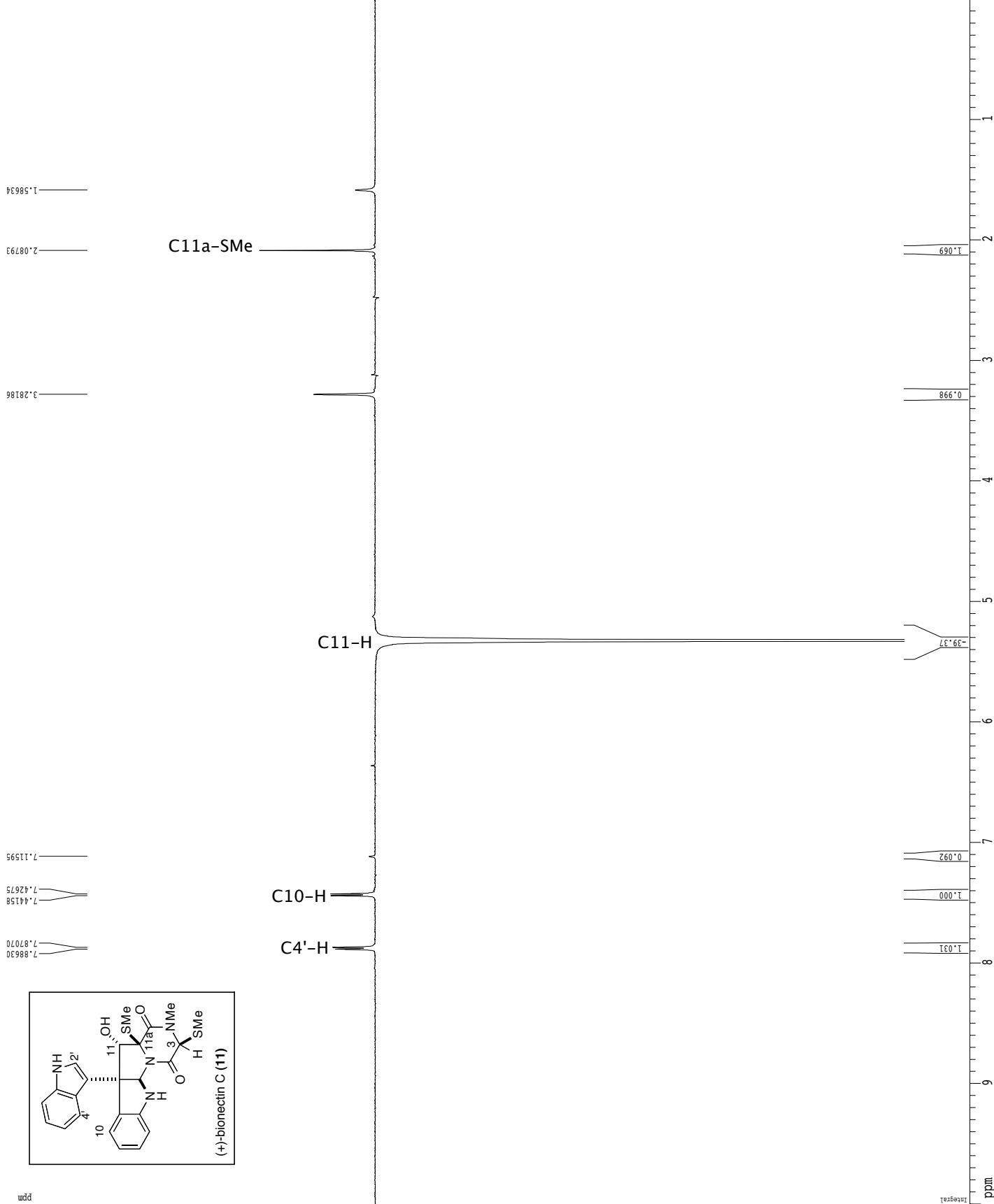
F2 - Acquisition Parameters  
 Date\_ 20120618  
 Time\_ 19.56  
 INSTRUM cty6590  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG gnoe1cc.wu  
 TD 65536  
 SOLVENT Acetone  
 NS 72  
 DS 8  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQAQ 4.0894966 sec  
 RG 406.4  
 DW 62.400 usec  
 DE 6.00 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 D11 0.50000000 sec  
 D16 0.10020000 sec  
 d21 0.33376500 sec  
 d22 0.16396999 sec  
 p2 15.00 usec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 P3 22.50 usec  
 P4 30.00 usec  
 P5 20.00 usec  
 P12 40000.00 usec  
 PL1 1.60 dB  
 SF01 500.222897 MHz  
 SF1 61.60 dB  
 SP0M1 gauss1.512  
 SP0F1 0.00 Hz

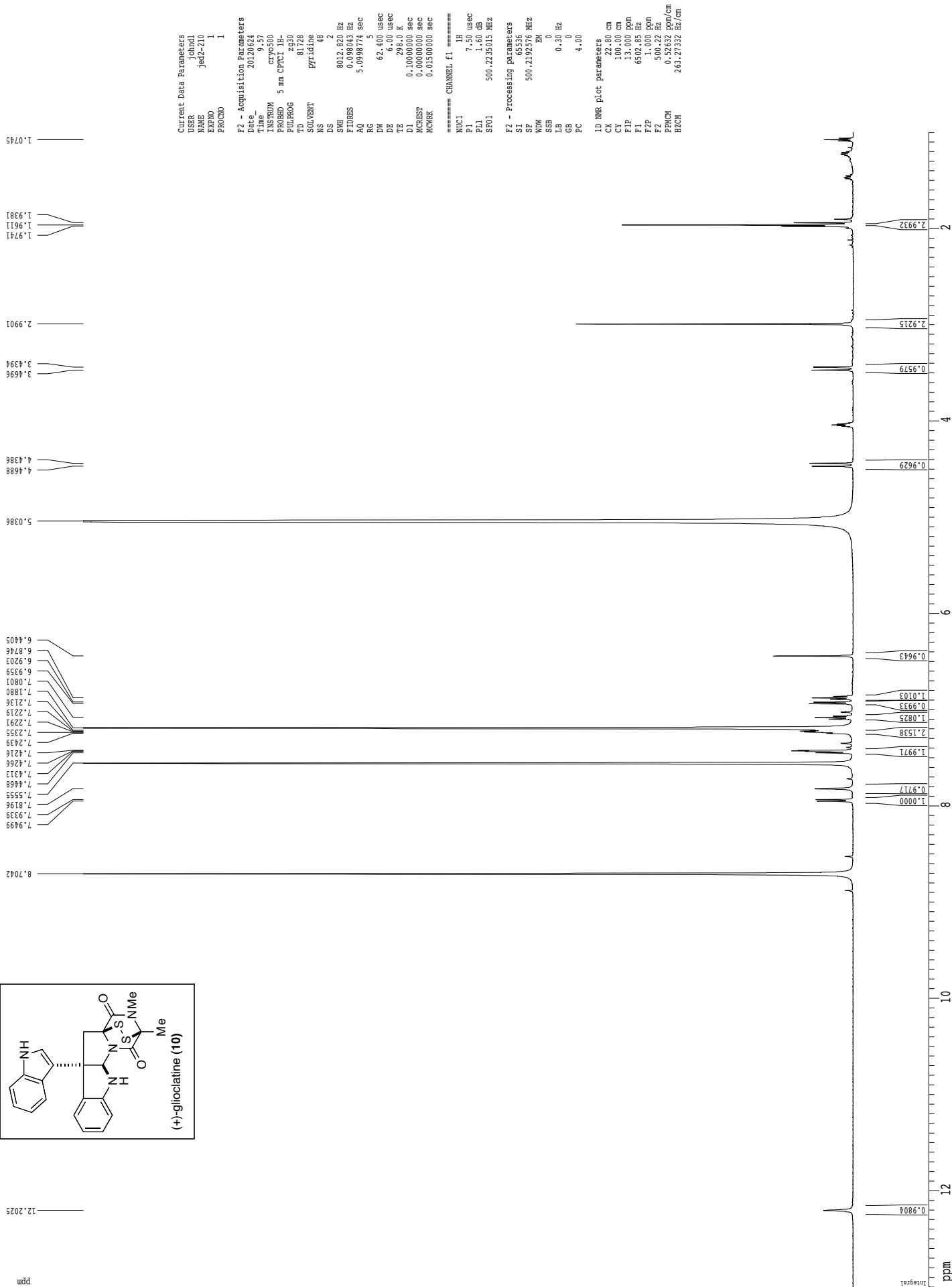
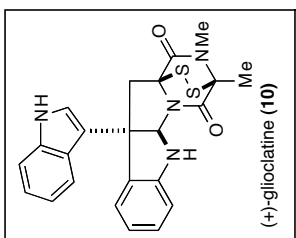
==== GRADIENT CHANNEL =====  
 GENM1 1000.00 usec  
 GENM2 1000.00 usec  
 GENM3 1000.00 usec  
 GENM4 1000.00 usec  
 GPC1 0.00 %  
 GPC2 0.00 %  
 GPC3 0.00 %  
 GPC4 0.00 %  
 GPC5 0.00 %  
 GPC6 0.00 %  
 GPC7 0.00 %  
 GPC8 0.00 %  
 GPC9 0.00 %  
 GPC10 0.00 %  
 GPC11 0.00 %  
 GPC12 0.00 %  
 GPC13 0.00 %  
 GPC14 0.00 %  
 GPC15 0.00 %  
 GPC16 0.00 %  
 GPC17 0.00 %  
 GPC18 0.00 %  
 GPC19 0.00 %  
 GPC20 0.00 %  
 GPC21 0.00 %  
 GPC22 0.00 %  
 GPC23 0.00 %  
 GPC24 0.00 %  
 P16 1000.00 usec

F2 - Processing Parameters  
 SI 65536  
 SF 500.220253 MHz  
 MDW 0  
 EM 0  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 50.00 cm  
 FIP 10.000 ppm  
 F1 5002.20 Hz  
 F2P 0.000 ppm  
 F2 100.620 Hz  
 FREQM 0.4396 ppm/cm  
 HZCM 219.39456 Hz/cm



<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jes2-210  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 2012054  
 Time 9 57  
 INSTRUM crys500  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT pyridine  
 NS 48  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 63  
 DE 6.00 usec  
 TE 288.0 K  
 D1 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

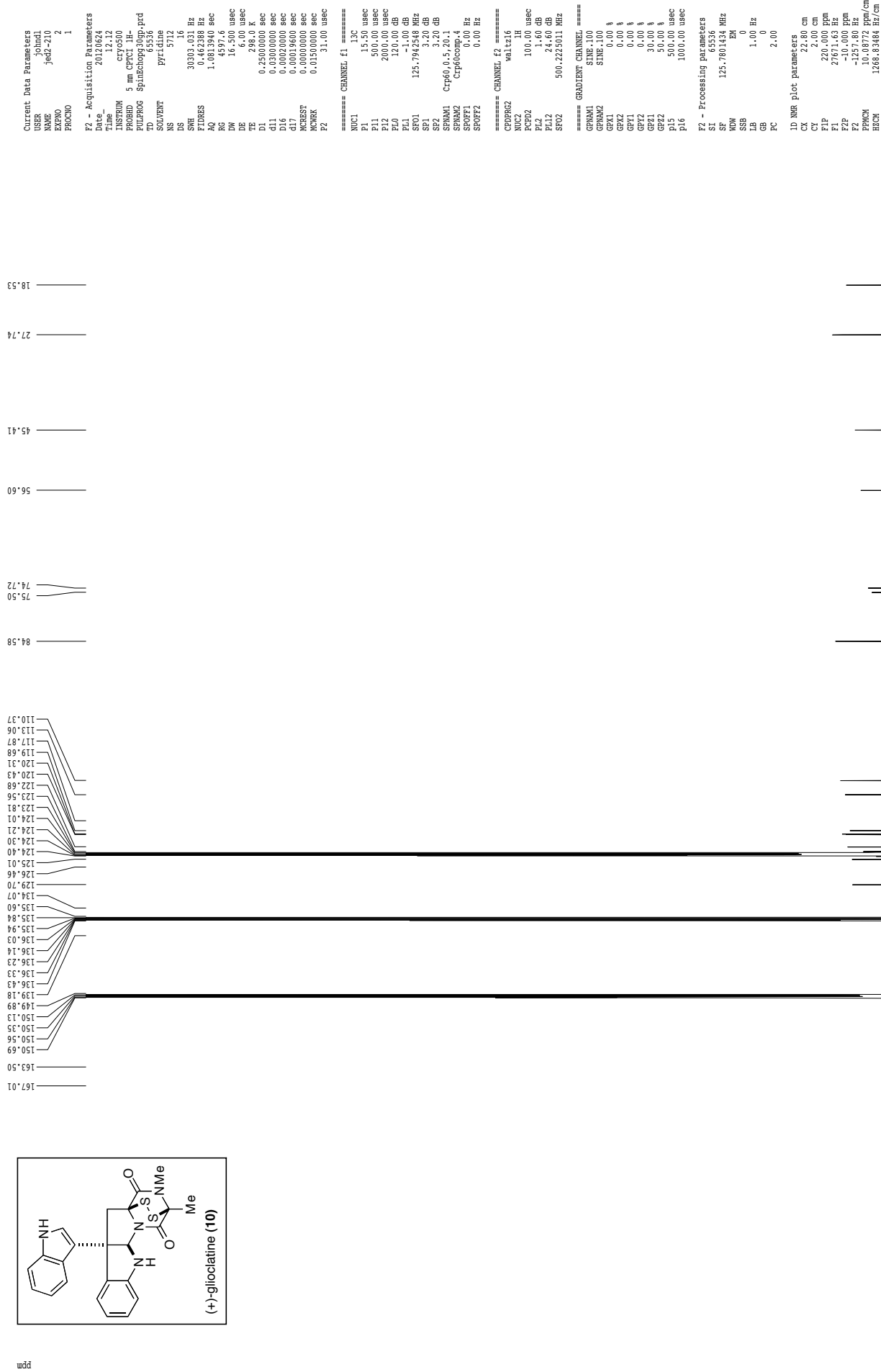
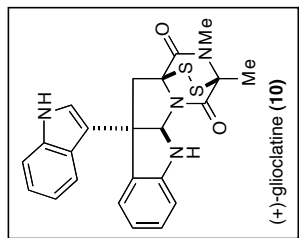
==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2192576 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

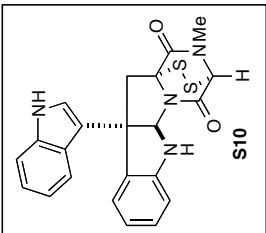
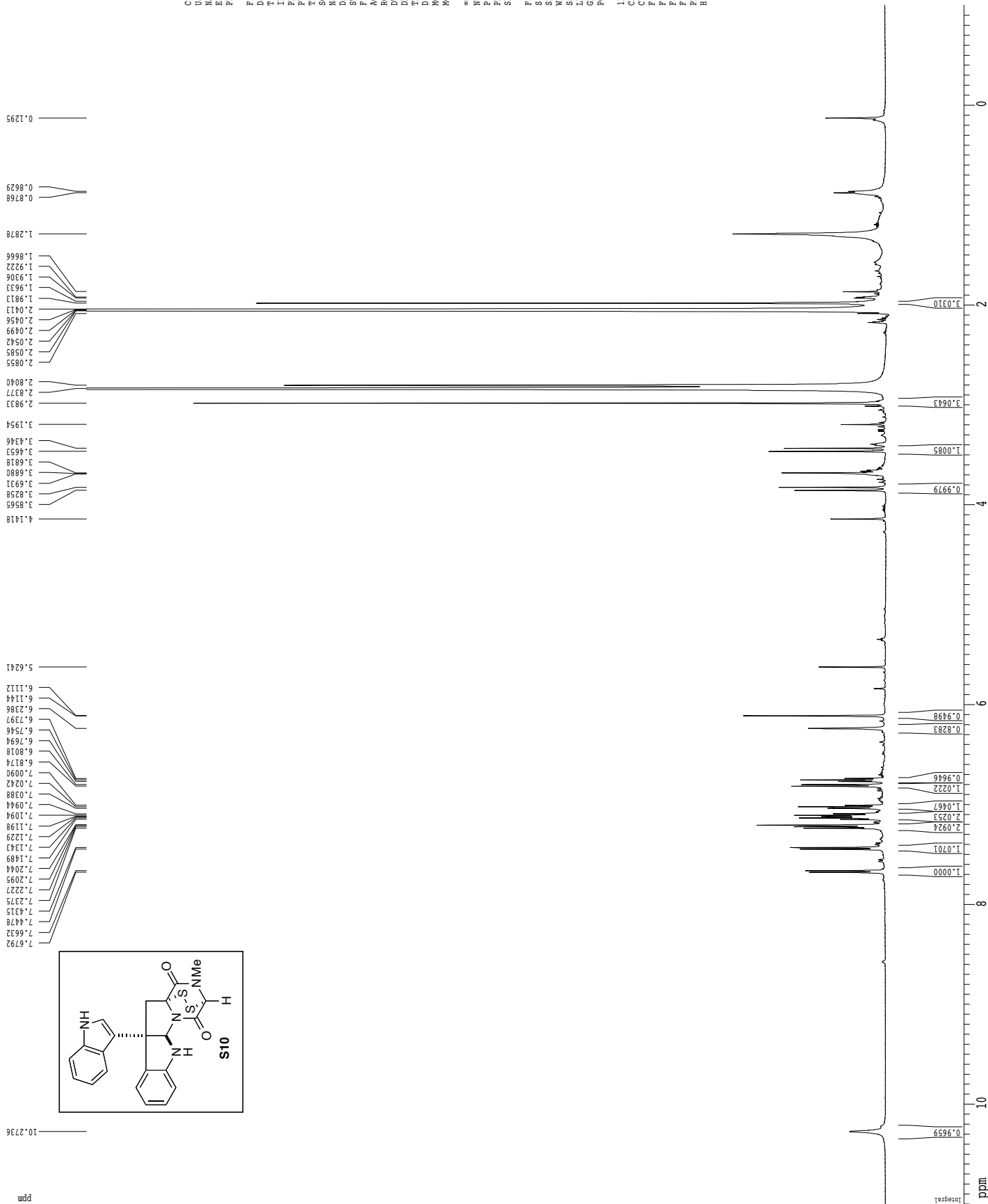
1D NMR plot parameters  
 CX 22.80 cm  
 CY 100.00 cm  
 FIP 13.000 ppm  
 F2 6502.85 Hz  
 F3 10.000 ppm  
 F4 500.22 MHz  
 PRMCM 0.52432 ppm/cm  
 HZCM 263.27332 Hz/cm



Z-restored spin-echo 13C spectrum with 1H decoupling



<sup>1</sup>H spectrum



Current Data Parameters  
 USER johnd  
 NAME jes2-216  
 EXPNO 1  
 PROCNO 1

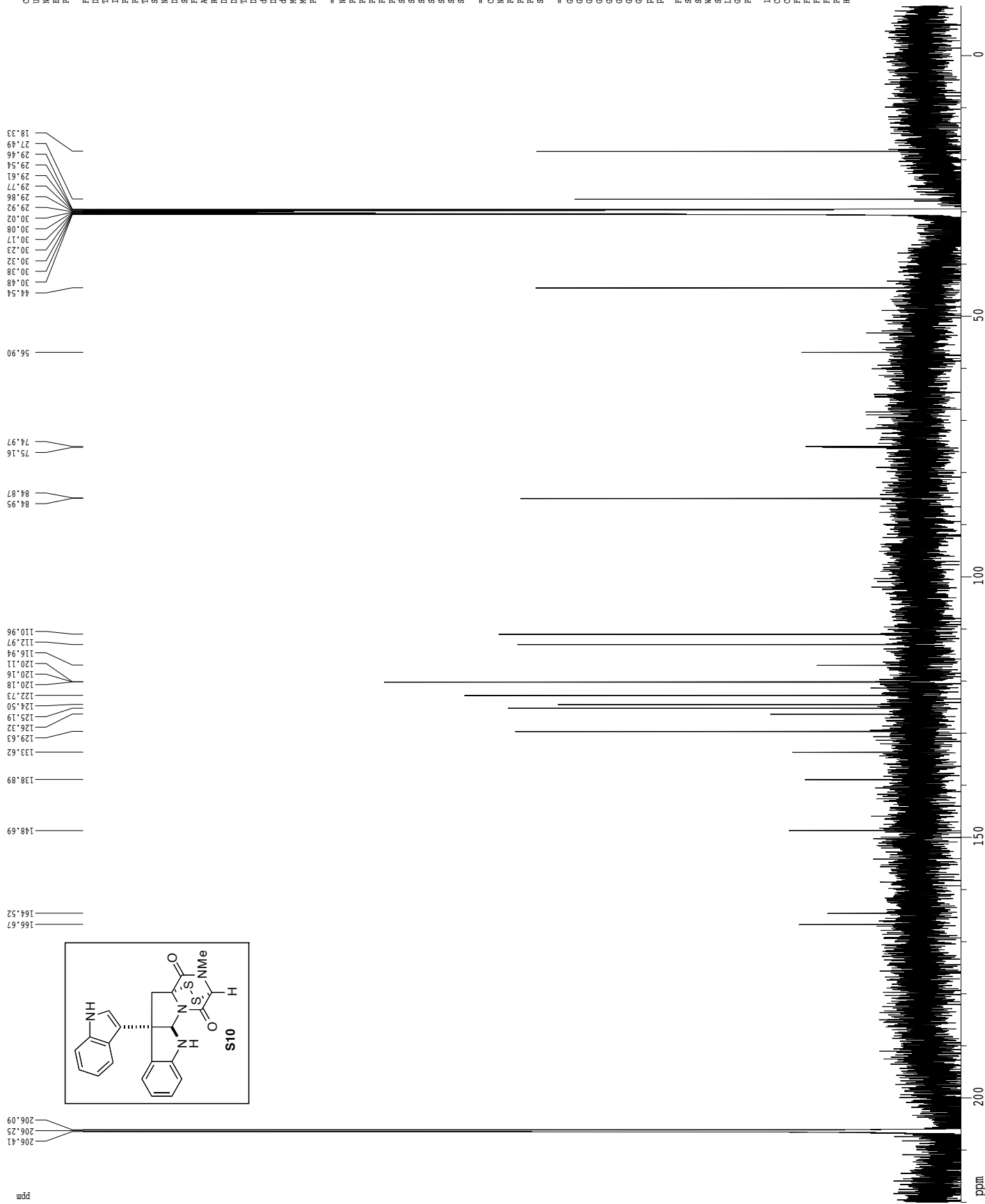
F2 - Acquisition Parameters  
 Date\_ 20120714  
 Time 1.36  
 INSTRUM crys500  
 PROBRD 5 mm CPXI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 64  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.099874 sec  
 RG 403  
 DE 62.60 usec  
 TE 288.0 K  
 D1 0.10000000 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.00 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.220179 MHz  
 MDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.80 cm  
 CY 100.00 cm  
 FIP 11.000 ppm  
 F2 5502.82 Hz  
 F3 -500.92 ppm  
 FPMCM 0.52452 ppm/cm  
 HZCM 263.27371 Hz/cm

Z-restored spin-echo 13C spectrum with 1H decoupling



Current Data Parameters  
 USER joundl  
 EXPNO jed-212  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20120714  
 Time 4:39  
 INSTRUM cryo500  
 PROBRID 5 mm CPXI 1H  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT Acetone  
 NS 8000  
 DS 16  
 SWH 30303.031 Hz  
 FIDRES 0.462388 Hz  
 AQ 1.0815940 sec  
 RG 1.258  
 RW 6.00 usec  
 DR 6.00 usec  
 DE 298.2 K  
 TE 298.2 K  
 D1 0.25000000 sec  
 d11 0.03000000 sec  
 D16 0.00020000 sec  
 d17 0.00015600 sec  
 ACRESF 0.00000000 sec  
 ACWRK 0.01500000 sec  
 F2 3.00 usec

===== CHANNEL F1 =====  
 NUC1 13C  
 P1 15.50 usec  
 PL1 500.00 usec  
 PL2 2000.00 usec  
 PL0 120.00 dB  
 PL1 125.794548 dB  
 PL2 125.794548 dB  
 SP1 5.20 dB  
 SP2 3.20 dB  
 SFO1 Ccp60.0.5.20.1  
 SFO2 Ccp60comp.4  
 SFOFF1 0.00 Hz  
 SFOFF2 0.00 Hz

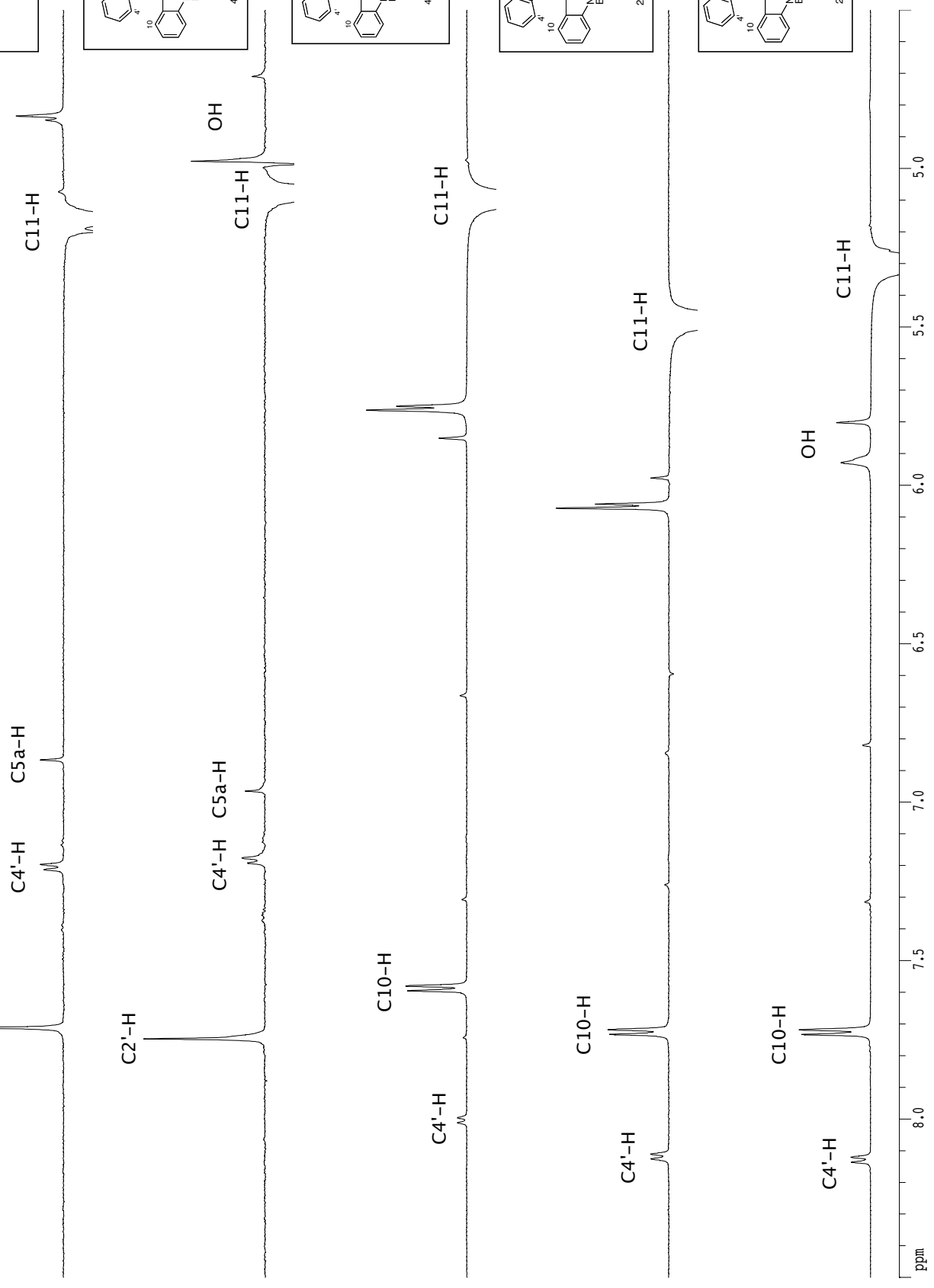
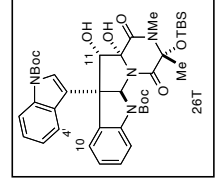
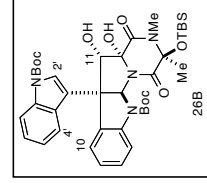
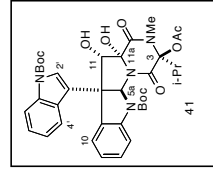
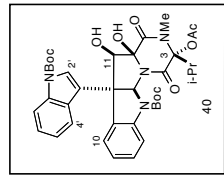
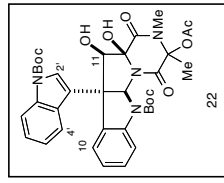
===== CHANNEL F2 =====  
 CDPGRZ wd1616  
 NUC2 1H  
 PCPD2 100.00 usec  
 PL2 1.60 dB  
 PL12 24.60 dB  
 SFO2 500.2225011 MHz

===== GRADIENT CHANNEL =====  
 GSPR1 0.00 %  
 GSPR2 0.00 %  
 GSPR3 0.00 %  
 GSPR4 0.00 %  
 GSPR5 0.00 %  
 GSPR6 0.00 %  
 GSPR7 0.00 %  
 GSPR8 0.00 %  
 GSPR9 0.00 %  
 GSPR10 0.00 %  
 GSPR11 0.00 %  
 GSPR12 0.00 %  
 GSPR13 0.00 %  
 GSPR14 0.00 %  
 GSPR15 0.00 %  
 GSPR16 0.00 %

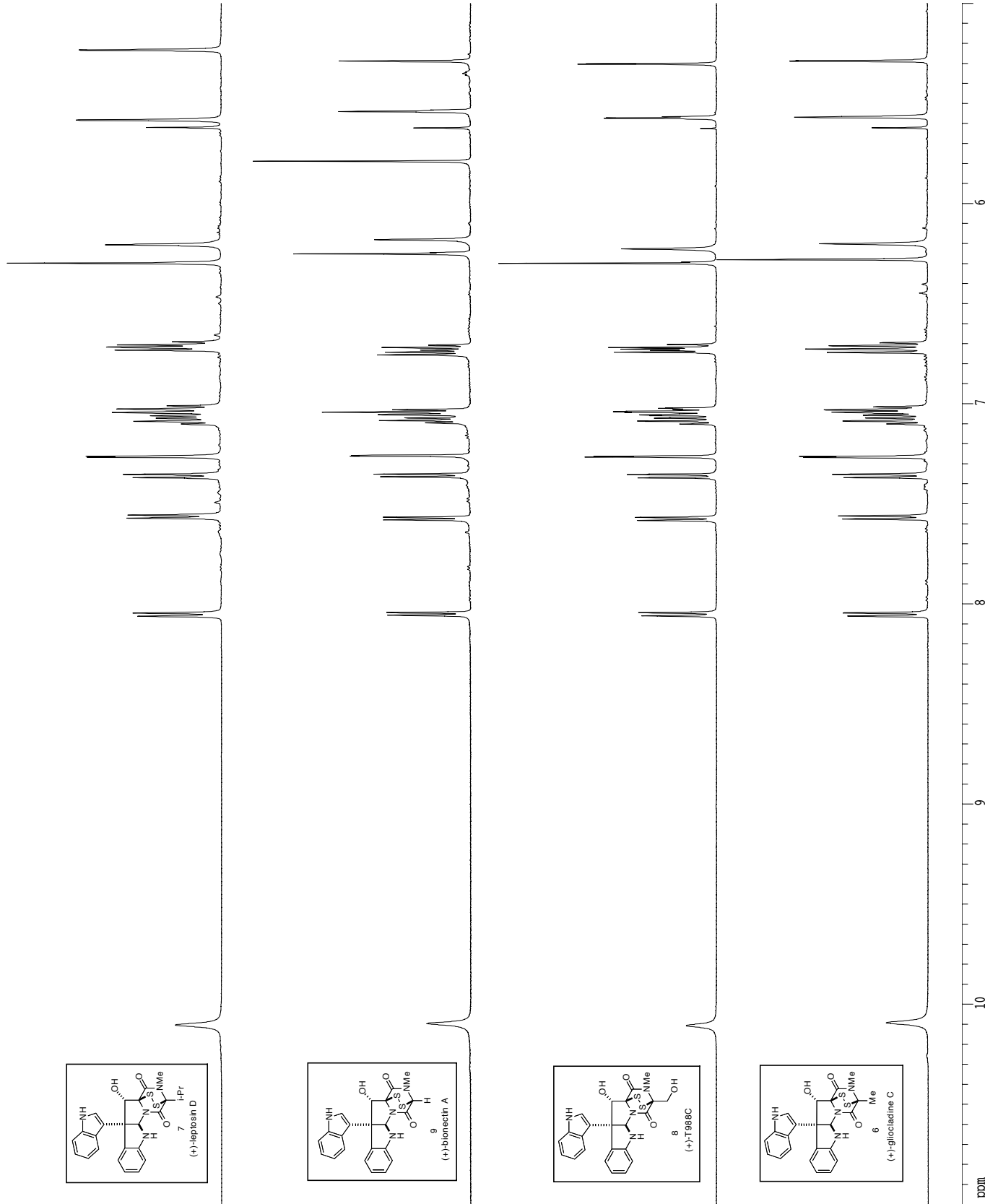
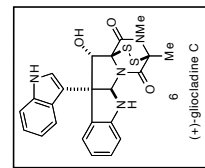
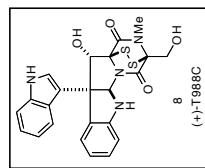
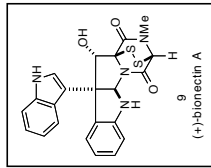
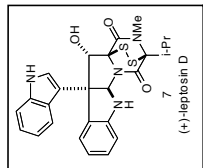
F2 - Processing parameters  
 SI 65536  
 SF 125.7802996 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.00

ID NMR plot parameters  
 CX 22.80 cm  
 CY 10.00 cm  
 FIP 220.000 ppm  
 F1 27671.67 Hz  
 F2P -10.000 ppm  
 F2 125.780 Hz  
 F2P2CM 10.000 ppm/cm  
 HPCOM 1268.83645 Hz/cm

NOE\_Dihydroxylation Stack  
gnoe



ETP Natural Products  
1H spectrum



Current Data Parameters  
 USER johnd1  
 NAME ETP  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 201013  
 Time 01:05  
 INSTRUM cty650  
 PROBRID 5 mm CPYCI 1H-  
 PULPROG zg30  
 TD 81728  
 SOLVENT Acetone  
 NS 8  
 DS 2  
 SFO 801.2820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.098774 sec  
 RG 6.3  
 DW 62.400 usec  
 DE 0.000000 sec  
 TE 298.0 K usec  
 DI 0.1000000 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 65536  
 SF 500.2235015 MHz  
 EQ 0  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.00 cm  
 CY 0.00 cm  
 FIP 11.000 ppm  
 FI 590.242 Hz  
 FZP 5.000 ppm  
 FZ 2.000 Hz  
 FRACM 0.2173 Hz  
 RECN 136.48365 Hz/cm

Bionectin A TFA titration (0.2 eq increments)  
 1H spectrum

2.0 equiv TFA

1.2 equiv TFA

1.0 equiv TFA

0.8 equiv TFA

0.6 equiv TFA

0.4 equiv TFA

0.2 equiv TFA

in K<sub>2</sub>CO<sub>3</sub>  
treated CDCl<sub>3</sub>in CDCl<sub>3</sub>

ppm

8.0

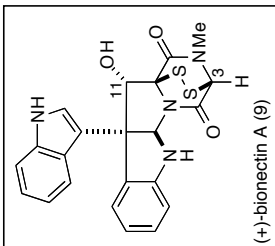
7.5

7.0

6.5

6.0

5.5



(+)-bionectin A (9)

Current Data Parameters  
 USER johnd1  
 NAME bionectinTFA  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 2012.04  
 Time 0.14  
 INSTRUM crys600  
 PROBHD 5 mm CPCTC IH-  
 PULPROG zg30  
 TD 81728  
 SOLVENT CDCl3  
 NS 48  
 DS 2  
 SHF 801.2820 Hz  
 FIDRES 0.098043 Hz  
 AQ 5.0998774 sec  
 RG 28.5  
 DW 62.400 usec  
 DE 0.000000 usec  
 TE 298.0 K  
 DT 0.10000000 sec  
 MCOREF 0.00000000 sec  
 MCHRG 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 7.50 usec  
 PL1 1.60 dB  
 SFO1 500.2235015 MHz

F2 - Processing parameters  
 SI 6556  
 SF 500.2200000 MHz  
 EQ  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 4.00

1D NMR plot parameters  
 CX 22.00 cm  
 CY 0.00 cm  
 FIP 8.500 bpm  
 FI 425.187 Hz  
 FZP 5.000 bpm  
 ZF 23.000 Hz  
 BRACH 0.5500 Hz/cm  
 RECN 79.58046 Hz/cm