

## Studies on the Double Alkylation of 2,2-Disubstituted-1,3-Dithiacycloalkane-S-oxides: Synthesis of Tertiary Thiol Derivatives

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### Supplementary Information

Table 1. Crystallographic data for compounds **9c**, **10**, **12a**, **23**, **24a**, and **24b**.

Compound	<b>9c</b>	<b>10</b>	<b>12a</b>	<b>23</b>
Formula	C <sub>17</sub> H <sub>18</sub> S <sub>2</sub>	C <sub>14</sub> H <sub>28</sub> S <sub>4</sub>	C <sub>7</sub> H <sub>14</sub> OS <sub>2</sub>	C <sub>13</sub> H <sub>24</sub> OS <sub>2</sub>
Formula weight	286.43	324.60	178.30	260.44
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	<i>P2<sub>1</sub>/n</i>	<i>P2<sub>1</sub>/n</i>	<i>P2<sub>1</sub>/n</i>	<i>P2<sub>1</sub></i>
Unit cell dimensions				
<i>a</i> (Å)	13.3194(11)	6.0477(7)	8.2277(8)	8.1567(6)
<i>b</i> (Å)	8.1505(7)	15.1049(18)	10.2736(10)	6.6861(5)
<i>c</i> (Å)	27.370(2)	9.4034(11)	11.2901(11)	12.7905(10)
$\beta$ (°)	103.9079	93.9707(16)	103.5283(15)	97.2784(11)
<i>V</i> (Å <sup>3</sup> )	2884.1(4)	856.94(17)	927.85(16)	691.93(9)
<i>Z</i>	8	2	4	2

$D_{\text{calcd}}$ (g cm <sup>-3</sup> )	1.319	1.258	1.279	1.250
Absorption coefficient (mm <sup>-1</sup> )	0.352	0.538	0.511	0.364
Crystal size (mm)	0.54 × 0.47 × 0.07	0.54 × 0.52 × 0.19	0.55 × 0.15 × 0.14	0.56 × 0.19 × 0.06
$2\theta_{\text{max}}$ (°)	56.82	60.94	61.06	56.62
Reflections measured	28959	9497	10461	6972
Unique reflections, $R_{\text{int}}$	7442, 0.0365	2579, 0.0244	2818, 0.0277	3367, 0.0170
Reflections with $F^2 > 2\sigma(F^2)$	5909	2270	2293	3240
Transmission factors	0.833 to 0.976	0.760 to 0.905	0.766 to 0.932	0.822 to 0.979
Number of parameters	344	84	94	148
$R_1 [F^2 > 2\sigma(F^2)]$	0.0370	0.0243	0.0305	0.0263
$wR_2$ (all data)	0.0926	0.0661	0.0810	0.0665
Largest difference peak and hole (e Å <sup>-3</sup> )	0.56 and - 0.25	0.44 and -0.23	0.38 and - 0.25	0.32 and -0.19

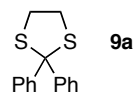
Table 1 Continued.

Compound	<b>24a</b>	<b>24b</b>
Formula	C <sub>14</sub> H <sub>26</sub> OS <sub>2</sub>	C <sub>20</sub> H <sub>30</sub> OS <sub>2</sub>
Formula weight	274.47	350.56
Crystal system	Orthorhombic	Monoclinic
Space group	<i>P</i> 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	<i>P</i> 2 <sub>1</sub>
Unit cell dimensions		
<i>a</i> (Å)	8.1947(5)	8.490(3)
<i>b</i> (Å)	9.7139(6)	20.303(6)
<i>c</i> (Å)	19.6679(11)	11.090(3)
$\beta$ (°)	90	90.152(5)
<i>V</i> (Å <sup>3</sup> )	1565.61(16)	1911.6(10)
<i>Z</i>	4	4
<i>D</i> <sub>calcd</sub> (g cm <sup>-3</sup> )	1.164	1.218
Absorption coefficient (mm <sup>-1</sup> )	0.325	0.281
Crystal size (mm)	1.08 × 0.48 × 0.26	0.68 × 0.56 × 0.33

$2\theta_{\max}$ (°)	63.26	59.46
Reflections measured	18432	19844
Unique reflections, $R_{\text{int}}$	4918, 0.0202	10576, 0.0565
Reflections with $F^2 > 2\sigma(F^2)$	4761	8841
Transmission factors	0.720 to 0.920	0.832 to 0.938
Number of parameters	158	422
$R_1 [F^2 > 2\sigma(F^2)]$	0.0261	0.0793
$wR_2$ (all data)	0.0717	0.2225
Largest difference peak and hole ( $e \text{ \AA}^{-3}$ )	0.33 and -0.15	1.01 and -0.81

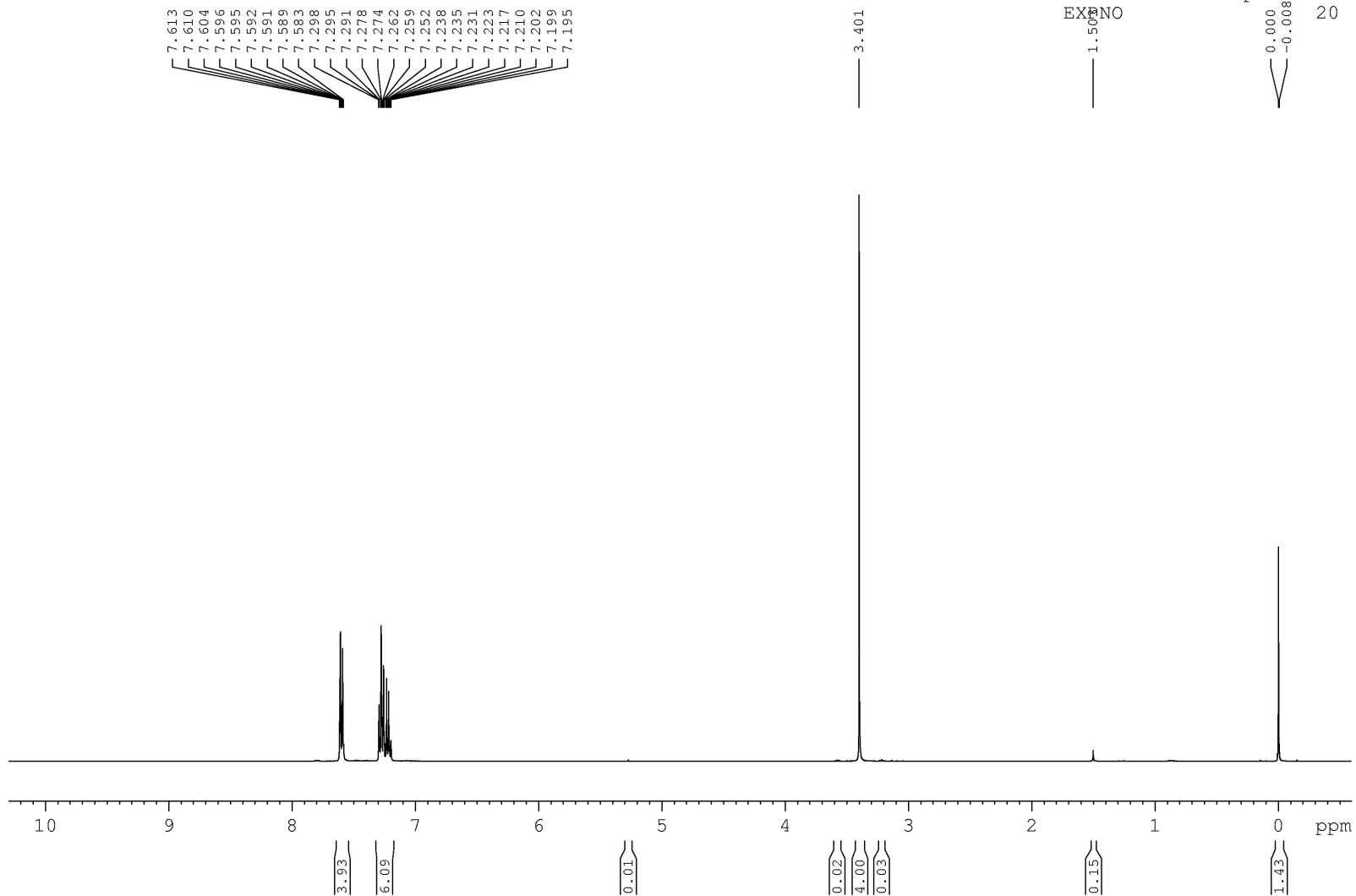
**NMR Spectra of compounds 9a-9c, 10, 12, 12a, 13, 14, 18, 19, 20, 21, 23, 24a, 24b.**

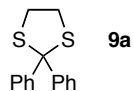




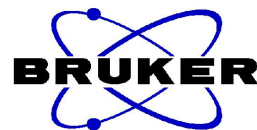
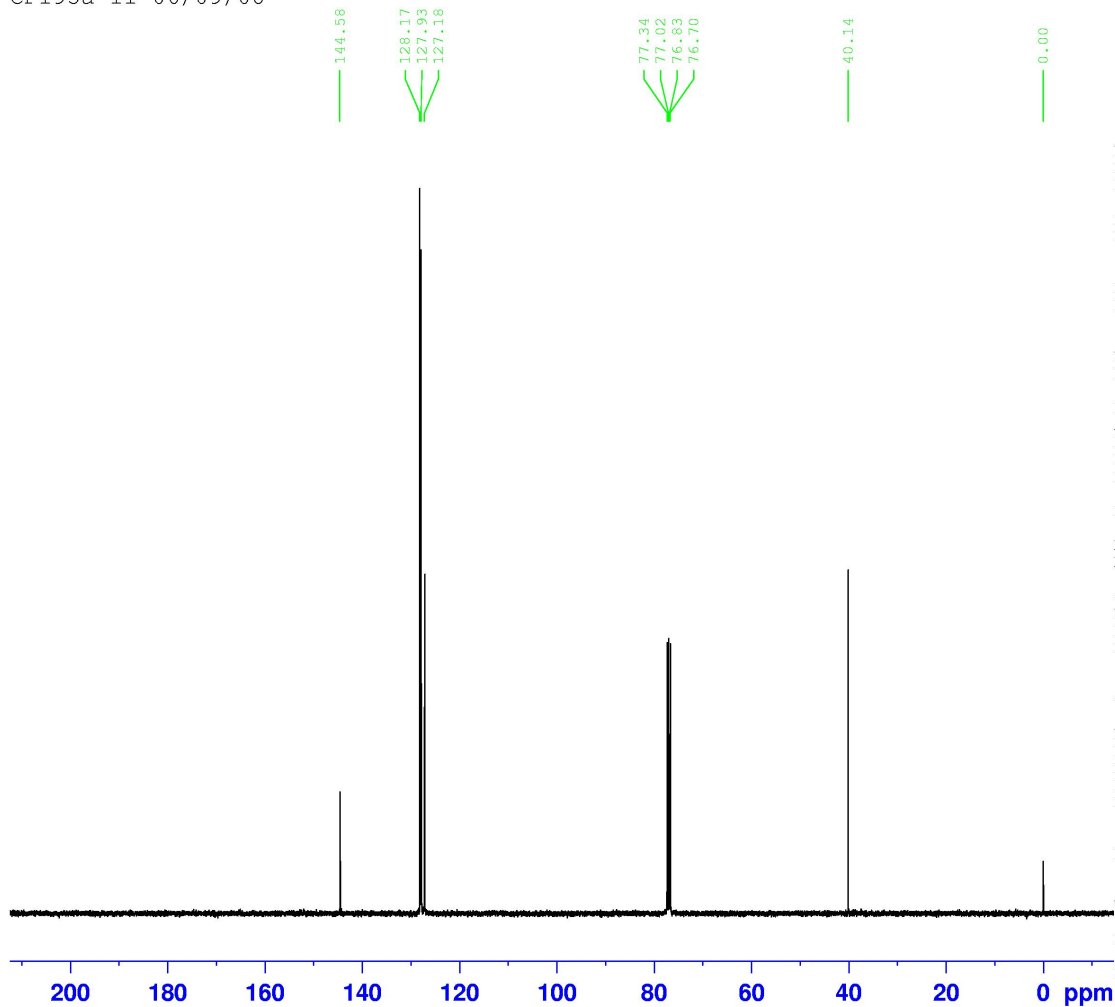
CF195a 20 06/09/08

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NAME  
EXPTNO  
Sep06-2008  
20





CF195a 11 06/09/08



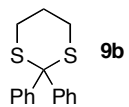
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TD 65536  
SOLVENT CDCl3  
NS 512  
DS 2  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 14596.5  
DW 19.800 usec  
DE 6.00 usec  
TE 295.2 K  
D1 1.00000000 sec  
d11 0.03000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

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NUC1 13C  
P1 8.25 usec  
PL1 -2.00 dB  
SFO1 100.6232777 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 14.00 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz

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LB 1.00 Hz  
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PC 1.40

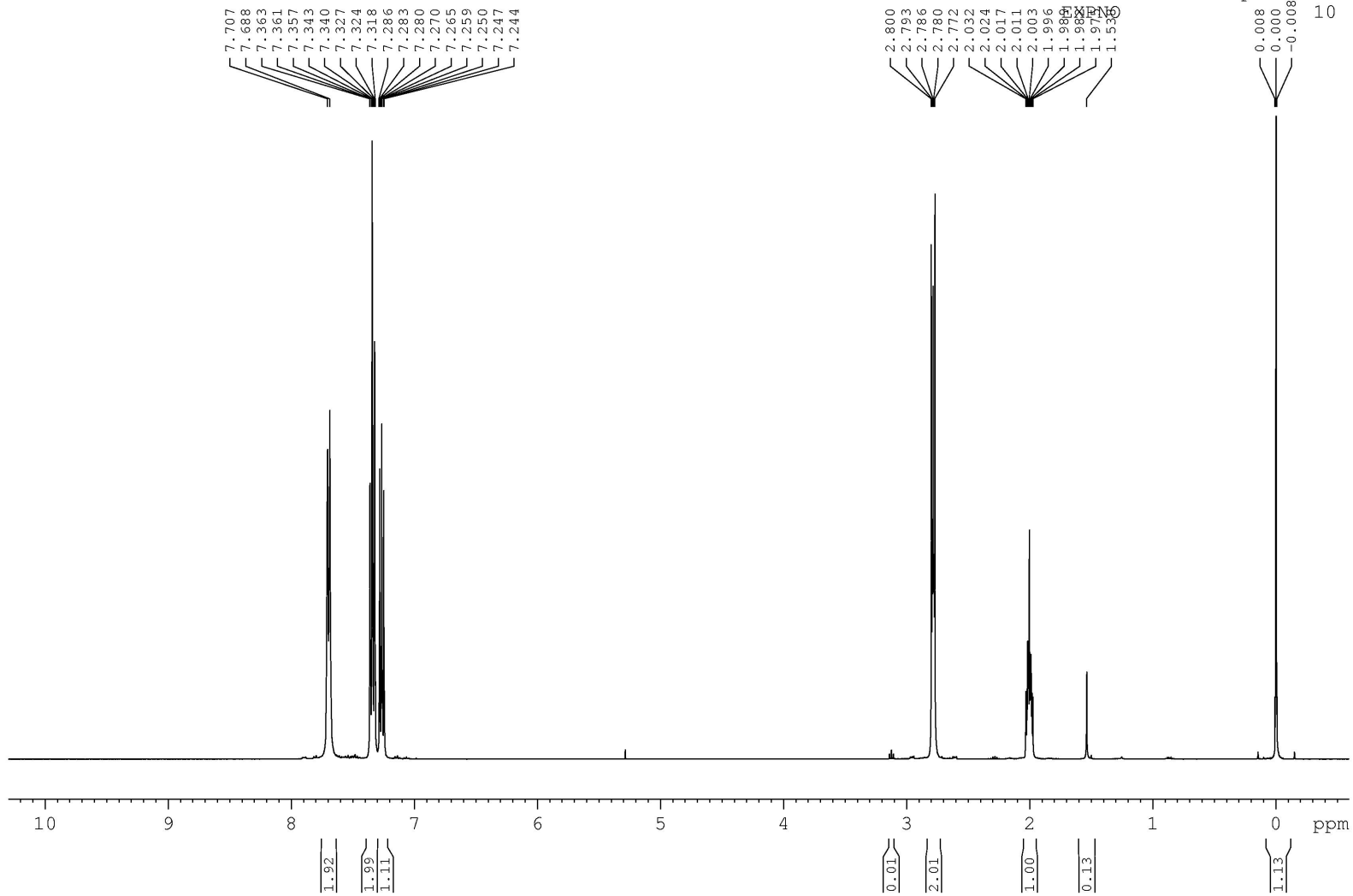


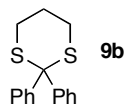
CF196a 10 07/09/08

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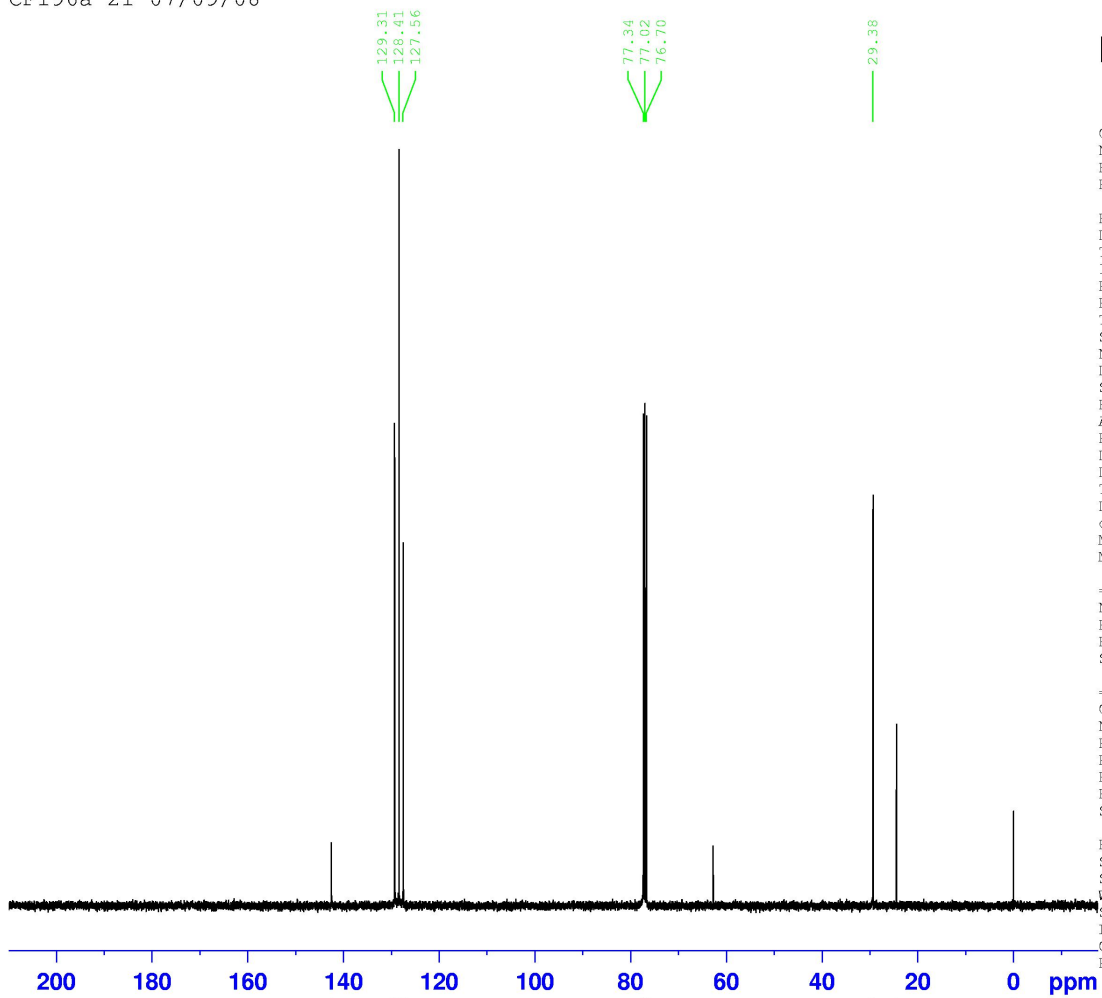
NAME Sep07-2008

10





CF196a 21 07/09/08



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EXPNO 21  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20080907  
Time 11.21  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 512  
DS 2  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 9195.2  
DW 19.800 usec  
DE 6.00 usec  
TE 295.2 K  
D1 1.0000000 sec  
d11 0.0300000 sec  
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MCWRK 0.0150000 sec

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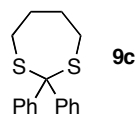
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PL1 -2.00 dB  
SFO1 100.6232777 MHz

===== CHANNEL f2 =====

CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 14.00 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters

SI 131072  
SF 100.6127724 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



CF197 fr 6 210 30/01/09

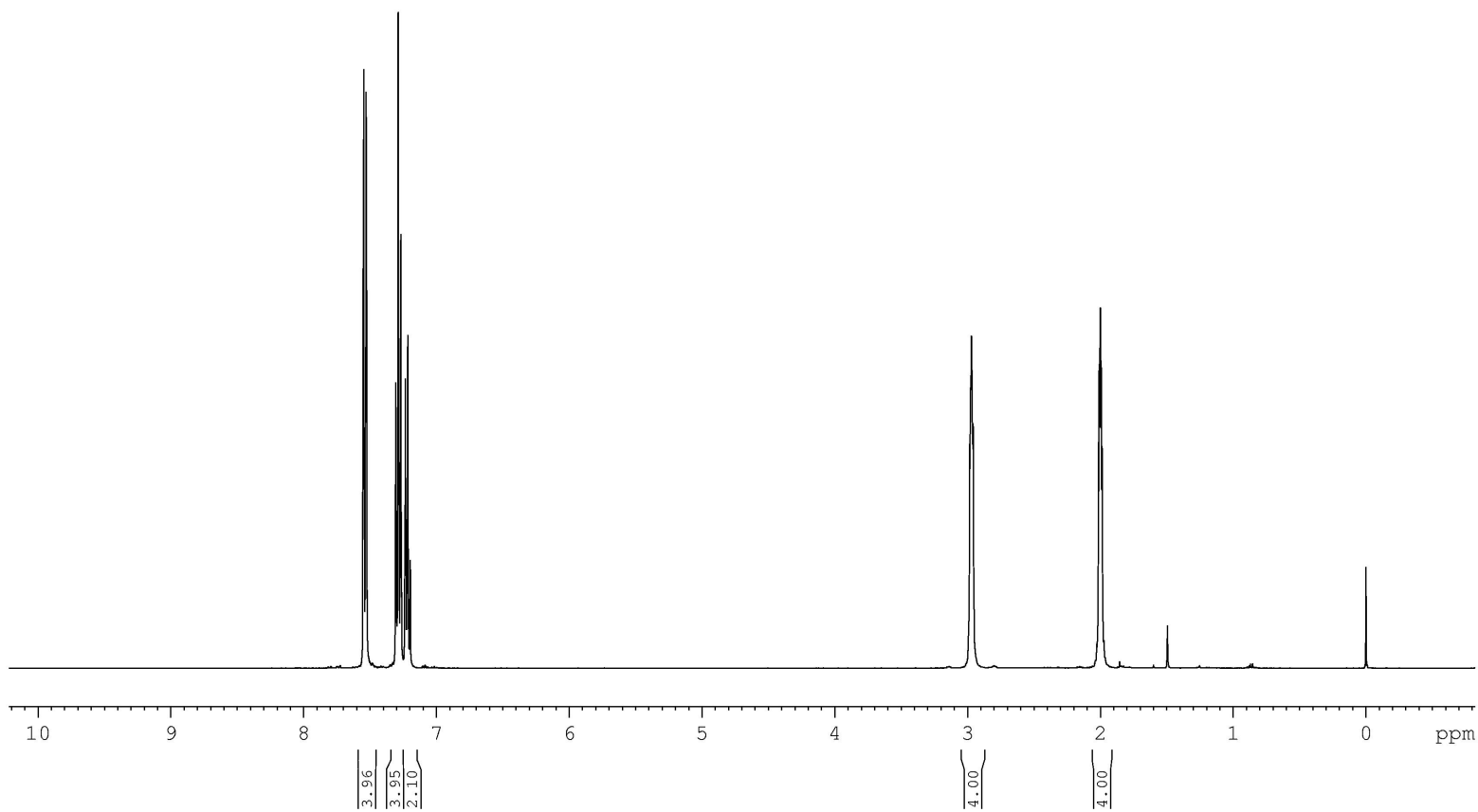
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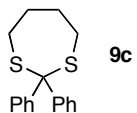
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7.285  
7.273  
7.269  
7.264  
7.238  
7.235  
7.232  
7.229  
7.222  
7.217  
7.211  
7.202  
7.199  
7.196

2.986  
2.977  
2.972  
2.967  
2.959

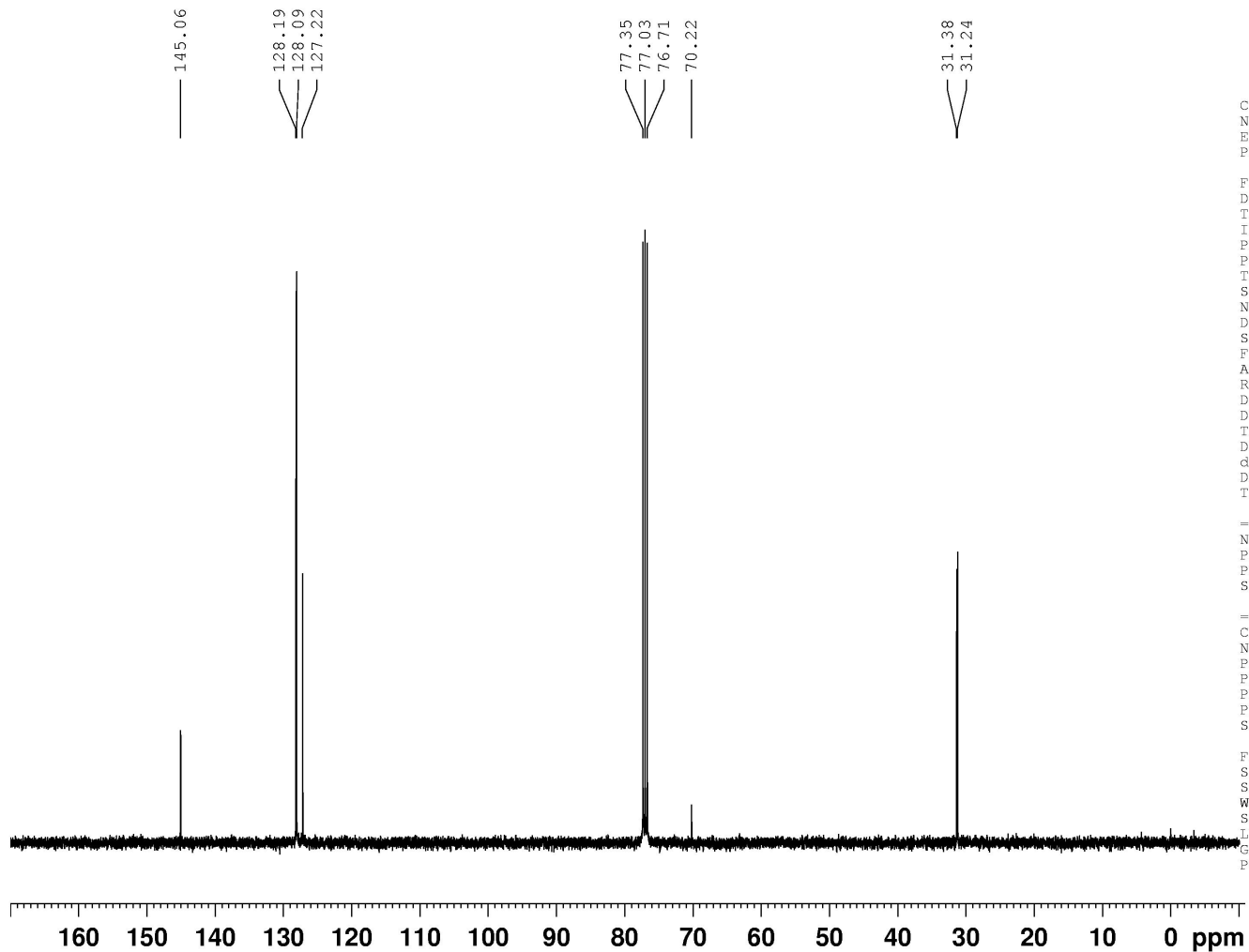
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2.001  
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1.988  
1.974  
1.965

0.000





CF197col 101 27/09/2010



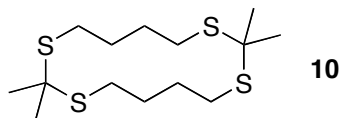
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 512  
DS 2  
SWH 26178.010 E  
FIDRES 0.399445 E  
AQ 1.2517875 s  
RG 16384  
DW 19.100 u  
DE 6.00 u  
TE 298.0 K  
D1 1.00000000 s  
d11 0.03000000 s  
DELTA 0.89999998 s  
TD0 1

===== CHANNEL f1 =====  
NUC1 13C  
P1 9.75 u  
PL1 8.00 c  
SFO1 100.6248425 M

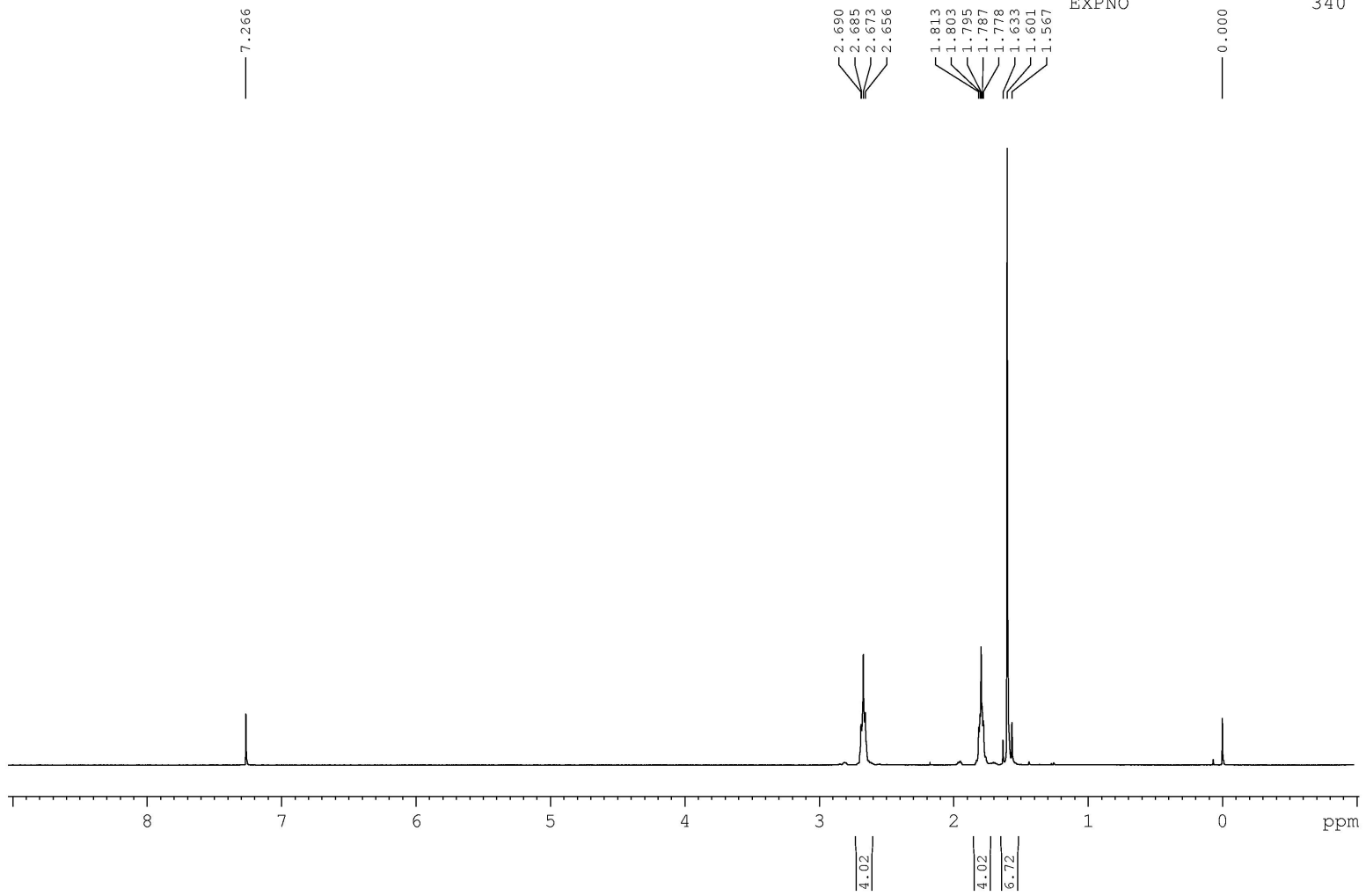
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PCPD2 80.00 u  
PL2 4.00 c  
PL12 18.99 c  
PL13 20.00 c  
SFO2 400.1316005 M

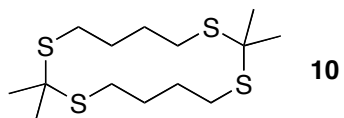
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SF 100.6127690 M  
WDW EM  
SSB 0  
LB 1.00 E  
GB 0  
PC 1.40



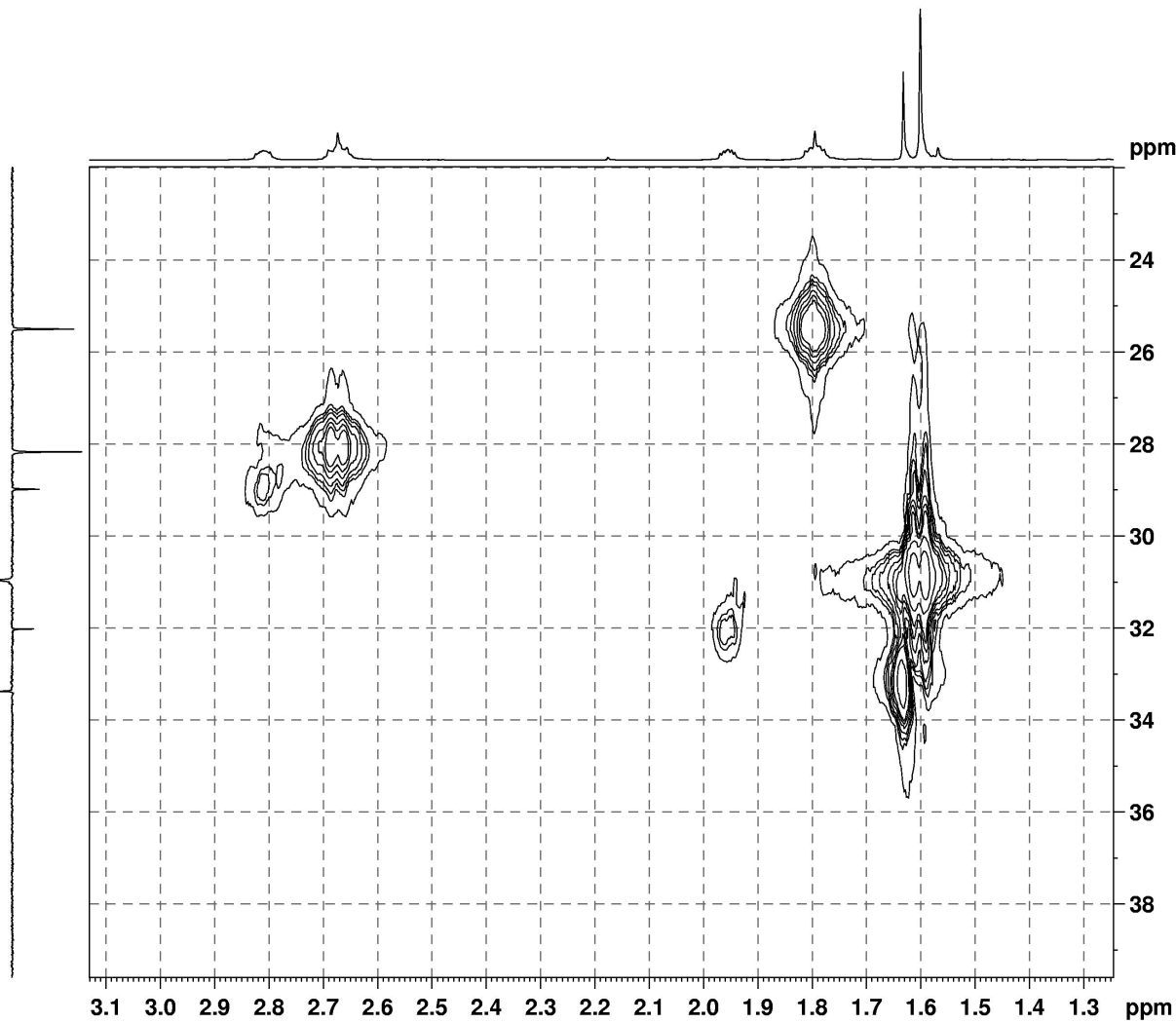
CF114 solid 340 22/09/09

Current Data Parameters  
NAME Sep22-2009  
EXPNO 340





CF114 solid 394 22/09/09



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Current Data Parameters
NAME      Sep22-2009
EXPNO    394
PROCNO    1

F2 - Acquisition Parameters
Date_     20090923
Time      0.57
INSTRUM   spect
PROBHD    5 mm Dual 13C/
PULPROG   hmcqcpqf
TD        2048
SOLVENT   CDCl3
NS         8
DS         16
SWH        3396.739 Hz
FIDRES     1.658564 Hz
AQ         0.3015156 sec
RG         26008
DW         147.200 usec
DE         6.00 usec
TE         293.2 K
CNST2     145.0000000
d0         0.0000300 sec
d1         0.94906878 sec
d2         0.00344828 sec
d12        0.00002000 sec
d13        0.00004000 sec
d16        0.00020000 sec
DELTA1    0.00222428 sec
IN0        0.00002761 sec
MCREST    0.00000000 sec
MCWRK     0.94906878 sec

===== CHANNEL f1 =====
NUC1       1H
P1         11.75 usec
P2         23.50 usec
PL1        -6.00 dB
SFO1       400.1314504 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       13C
P3         8.25 usec
PCPD2     70.00 usec
PL2        -2.00 dB
PL12       15.00 dB
SFO2       100.6213211 MHz

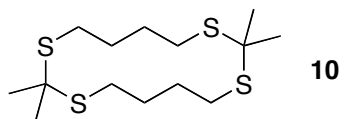
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GPNAM2     SINE.100
GPNAM3     SINE.100
GPX1       0.00 %
GPX2       0.00 %
GPX3       0.00 %
GPY1       0.00 %
GPY2       0.00 %
GPY3       0.00 %
GPZ1       50.00 %
GPZ2       50.00 %
GPZ3       40.10 %
E16        1000.00 usec

F1 - Acquisition parameters
ND0        2
TD         128
SFO1       100.6213 MHz
FIDRES     141.466721 Hz
SW         179.959 ppm
F1MODE     QF

F2 - Processing parameters
SI         4096
SF         400.1300716 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
EC         1.40

F1 - Processing parameters
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MC2        QF
SF         100.6127690 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0
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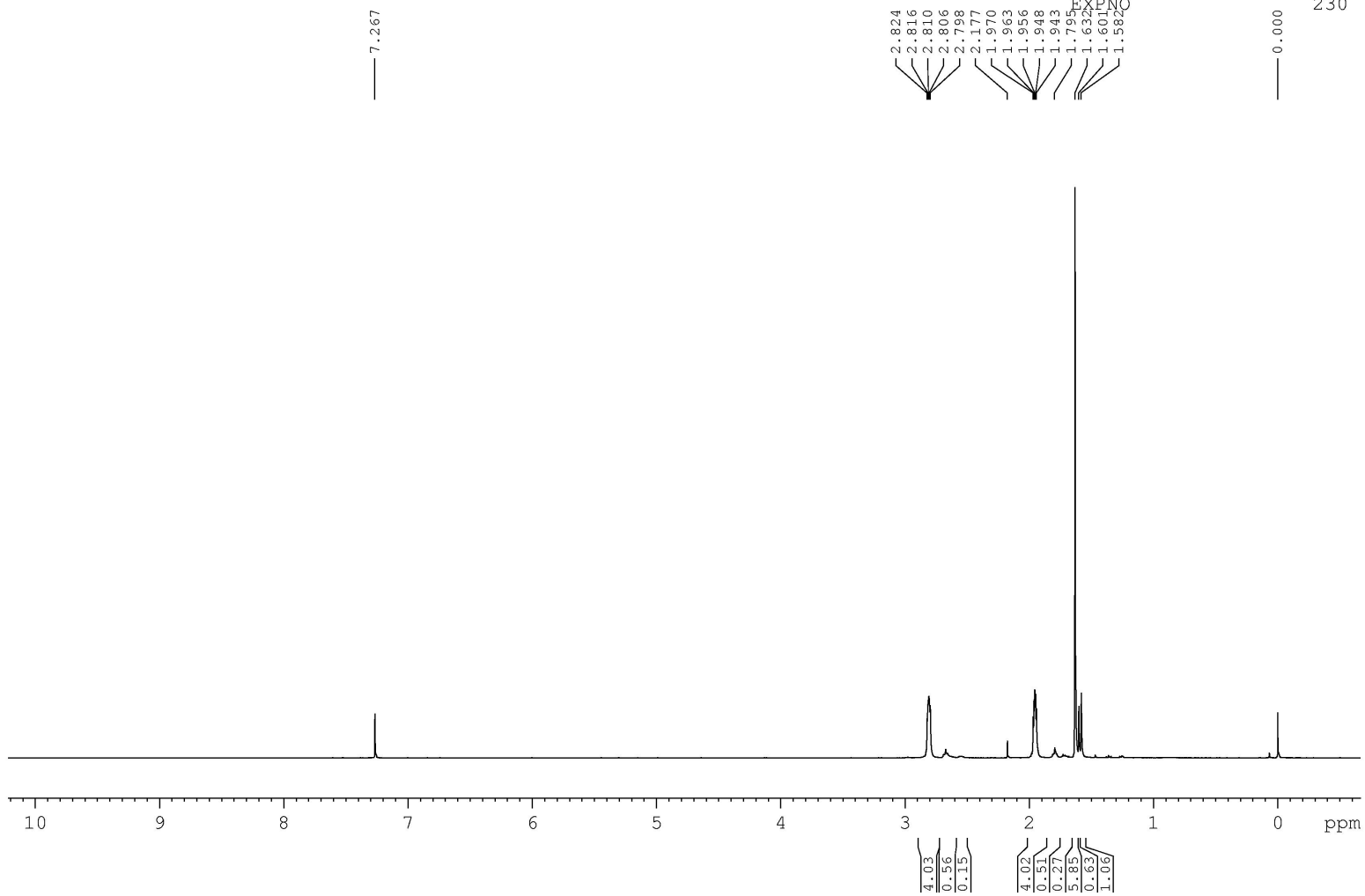


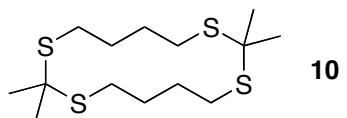


Compound 10 converts after 14 days at room temperature.

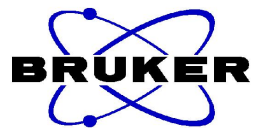
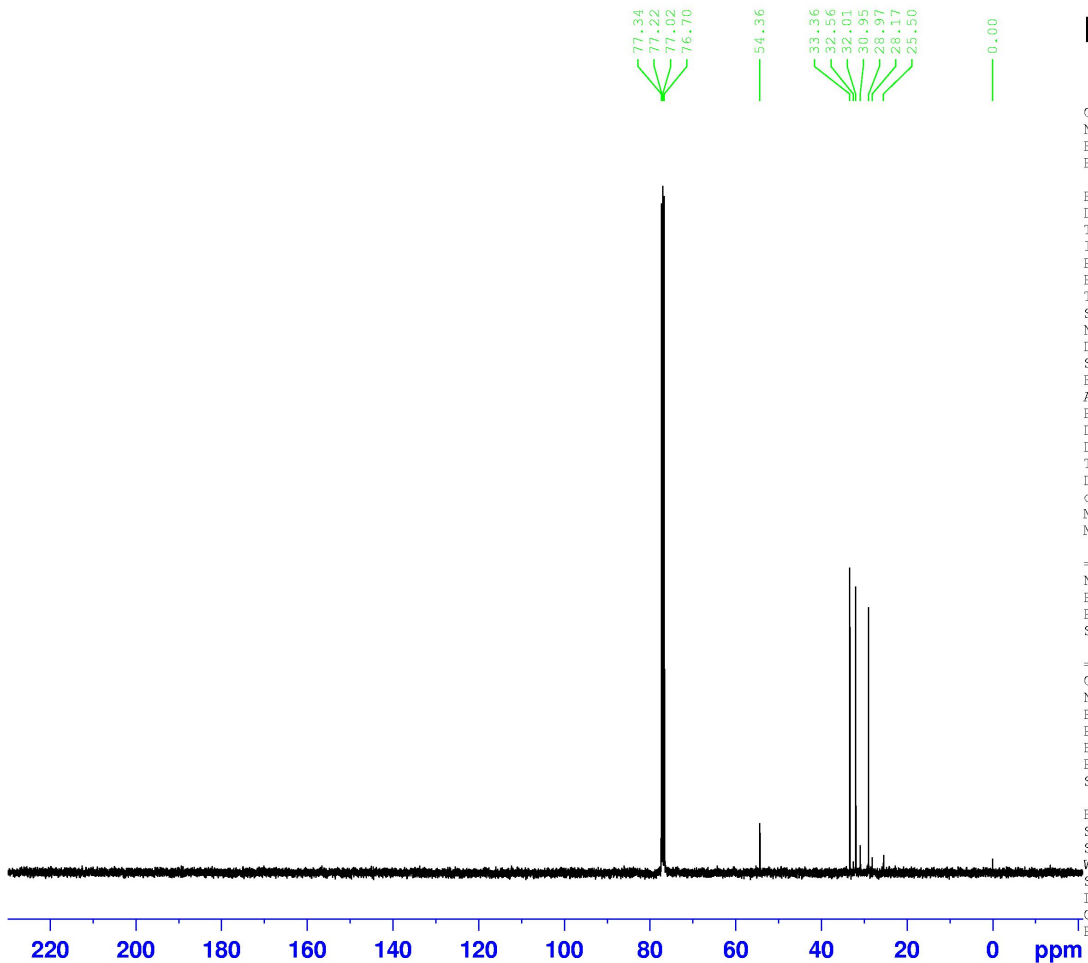
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Current Data Parameters  
NAME Oct06-2009  
EXPNO 230





CF114 solid 14d r.t. 361 06/10/09



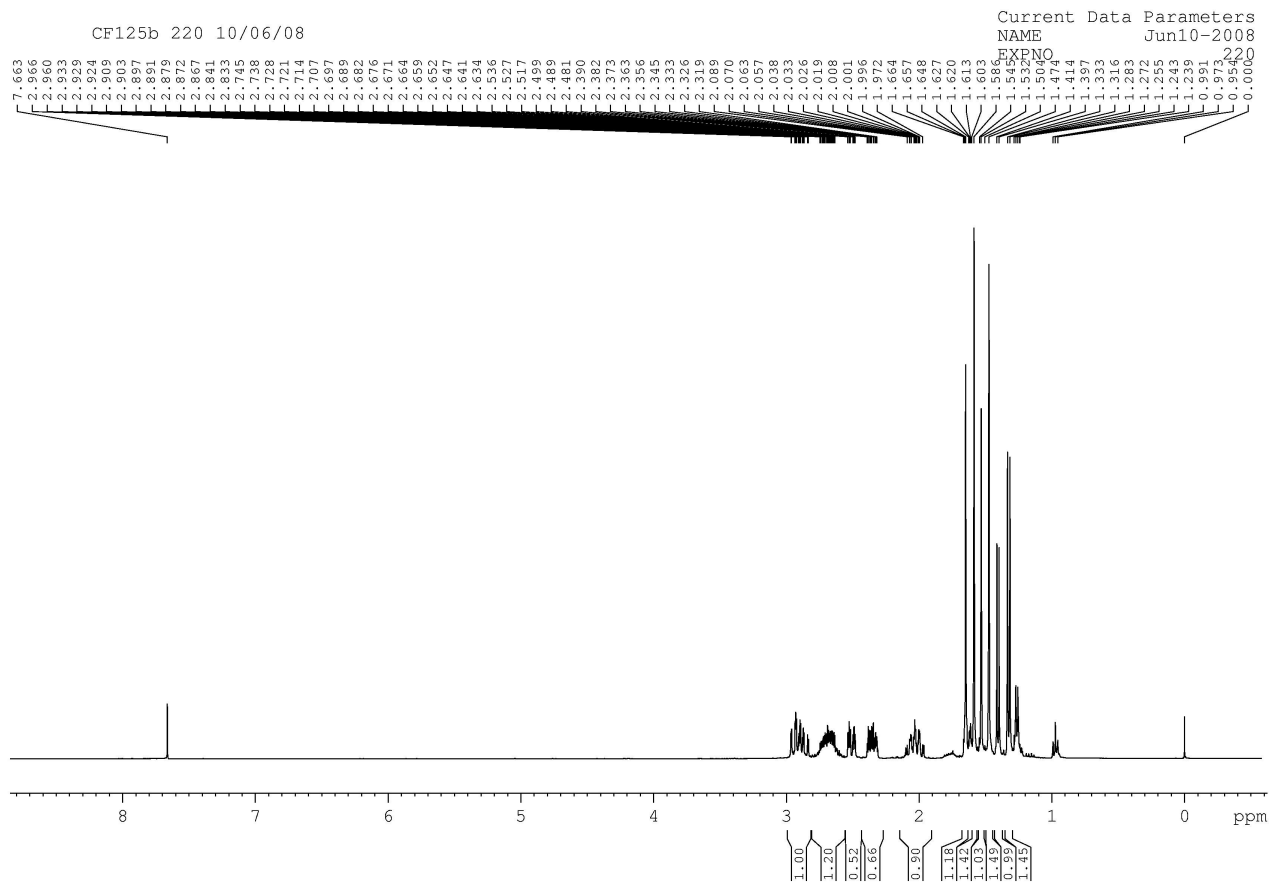
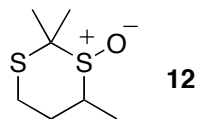
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PROCNO 1

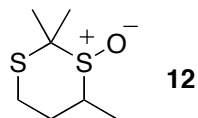
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 13004  
DW 19.800 usec  
DE 6.00 usec  
TE 294.2 K  
D1 1.00000000 sec  
d11 0.03000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.25 usec  
PL1 -2.00 dB  
SFO1 100.6232777 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 14.00 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 131072  
SF 100.6127700 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





CF125b 220 10/06/08



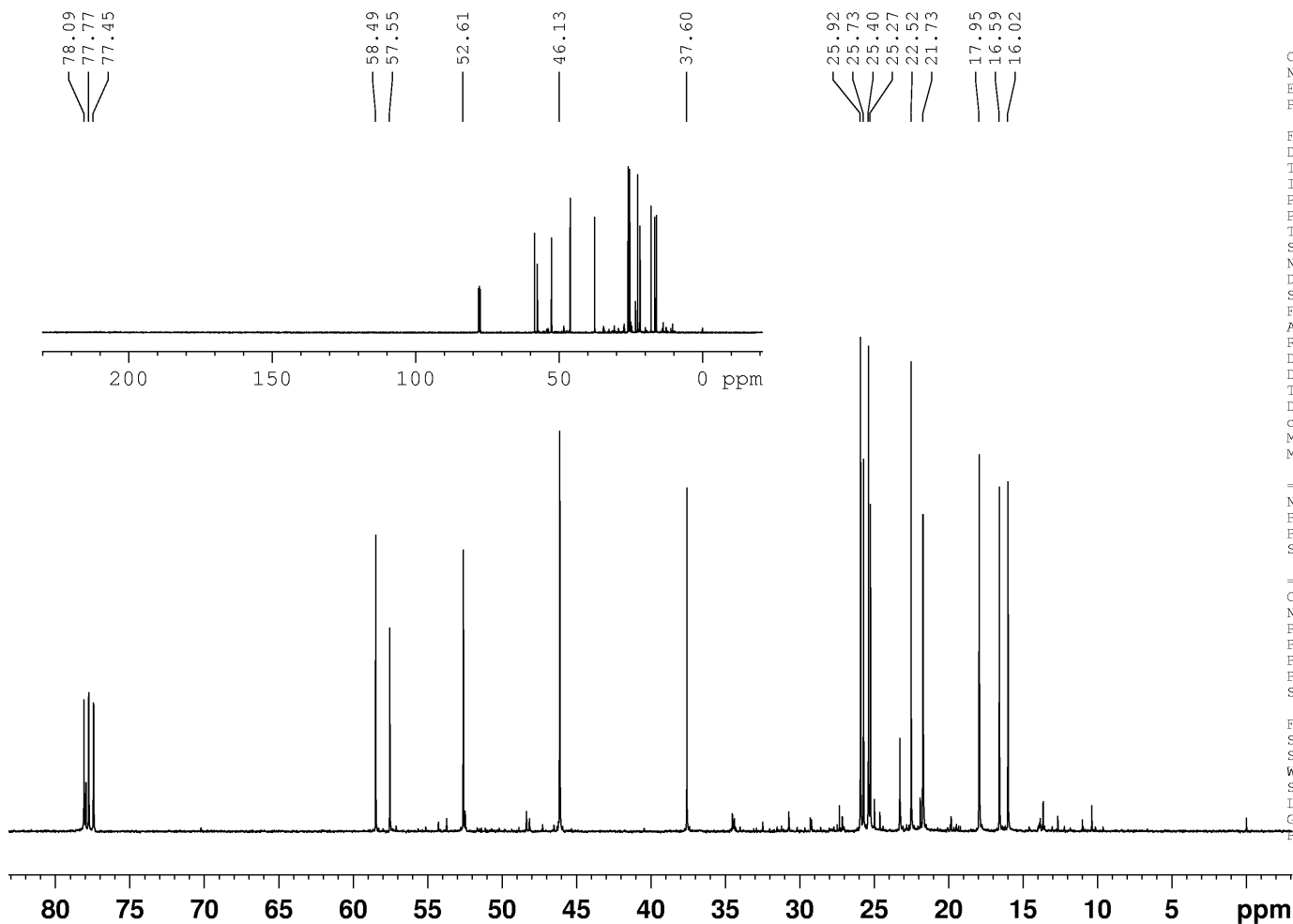
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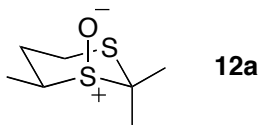
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Date\_ 20080610  
Time 23.31  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 512  
DS 2  
SWH 25252.525 F  
FIDRES 0.385323 F  
AQ 1.2976629 s  
RG 9195.2  
DW 19.800 u  
DE 6.00 u  
TE 294.2 K  
D1 1.00000000 s  
d11 0.03000000 s  
MCREST 0.00000000 s  
MCWRK 0.01500000 s

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.25 u  
PL1 -2.00 c  
SFO1 100.6232777 M

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 u  
PL2 -6.00 c  
PL12 14.00 c  
PL13 15.00 c  
SFO2 400.1316005 M

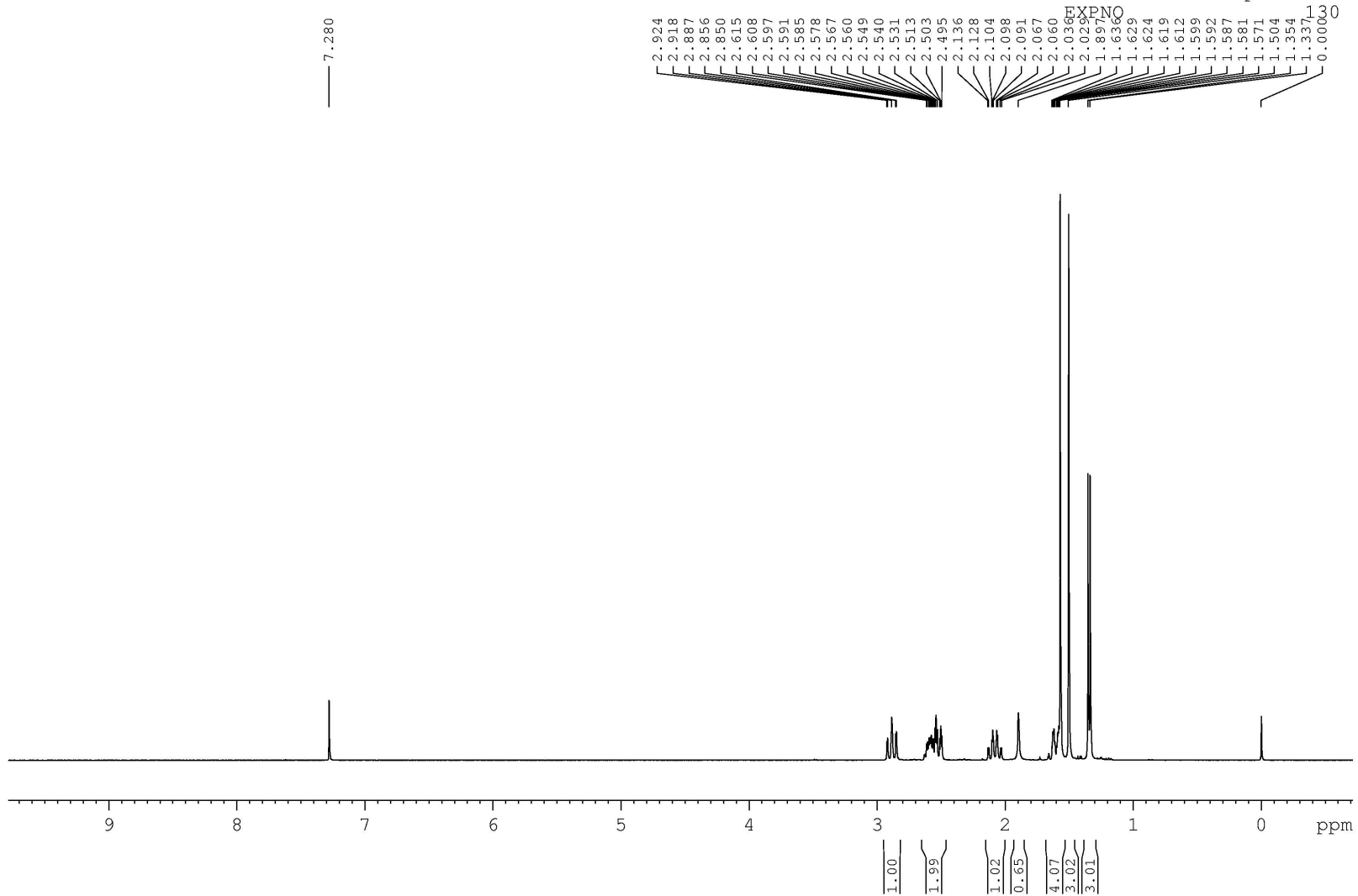
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PC 1.40

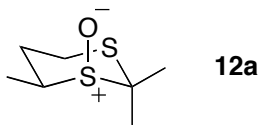




CF399 cryst 130 29/09/09

Current Data Parameters  
NAME Sep29-2009





CF399 cryst 141 29/09/09



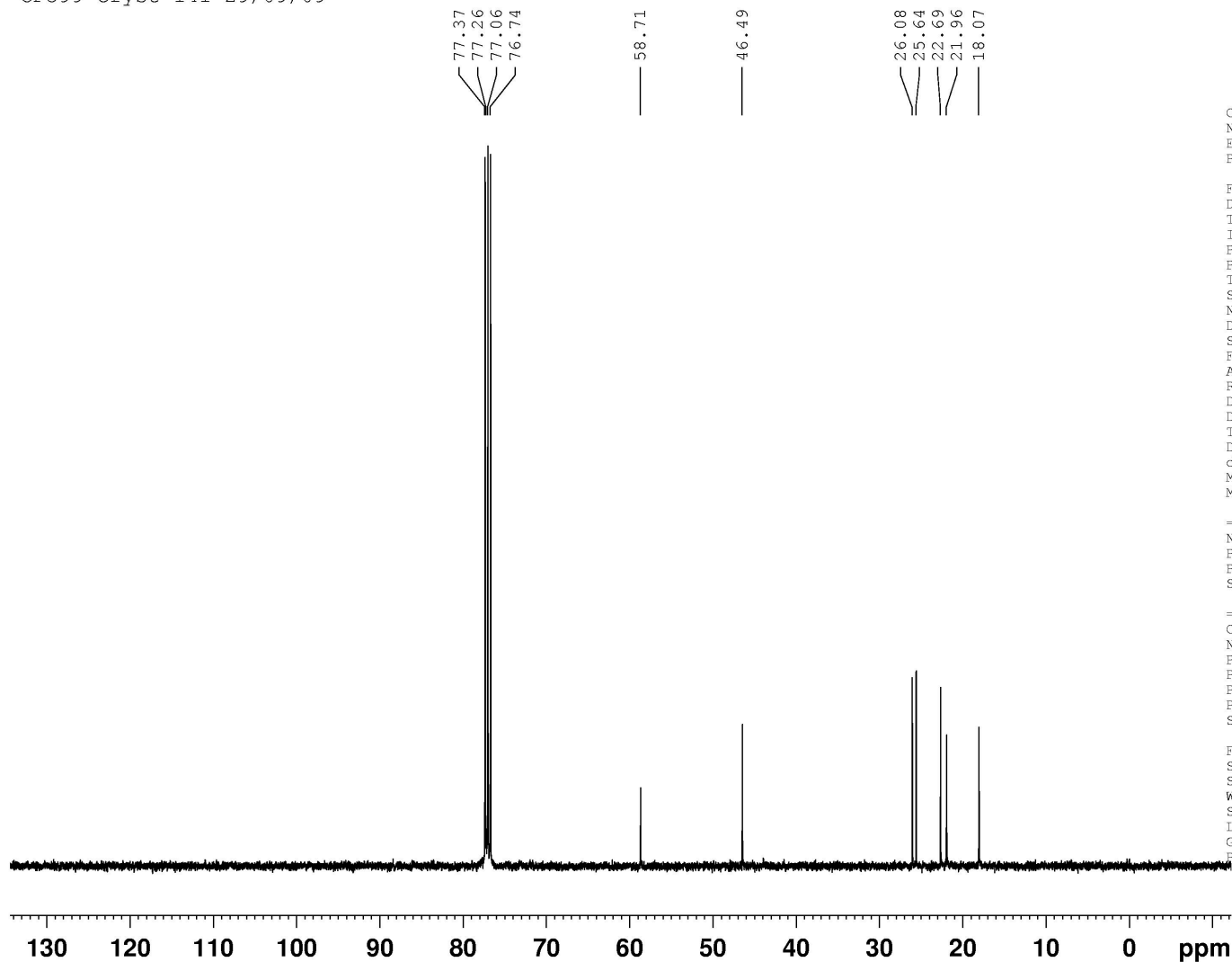
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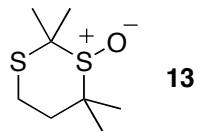
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 25252.525 E  
FIDRES 0.385323 E  
AQ 1.2976629 s  
RG 13004  
DW 19.800 u  
DE 6.00 u  
TE 293.2 K  
D1 1.0000000 s  
d11 0.0300000 s  
MCREST 0.0000000 s  
MCWRK 0.0150000 s

=====  
CHANNEL f1  
NUC1 13C  
P1 8.25 u  
PL1 -2.00 c  
SFO1 100.6232777 M

=====  
CHANNEL f2  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 u  
PL2 -6.00 c  
PL12 14.00 c  
PL13 15.00 c  
SFO2 400.1316005 M

F2 - Processing parameters  
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SF 100.6127690 M  
WDW EM  
SSB 0  
LB 1.00 E  
GB 0  
PC 1.40

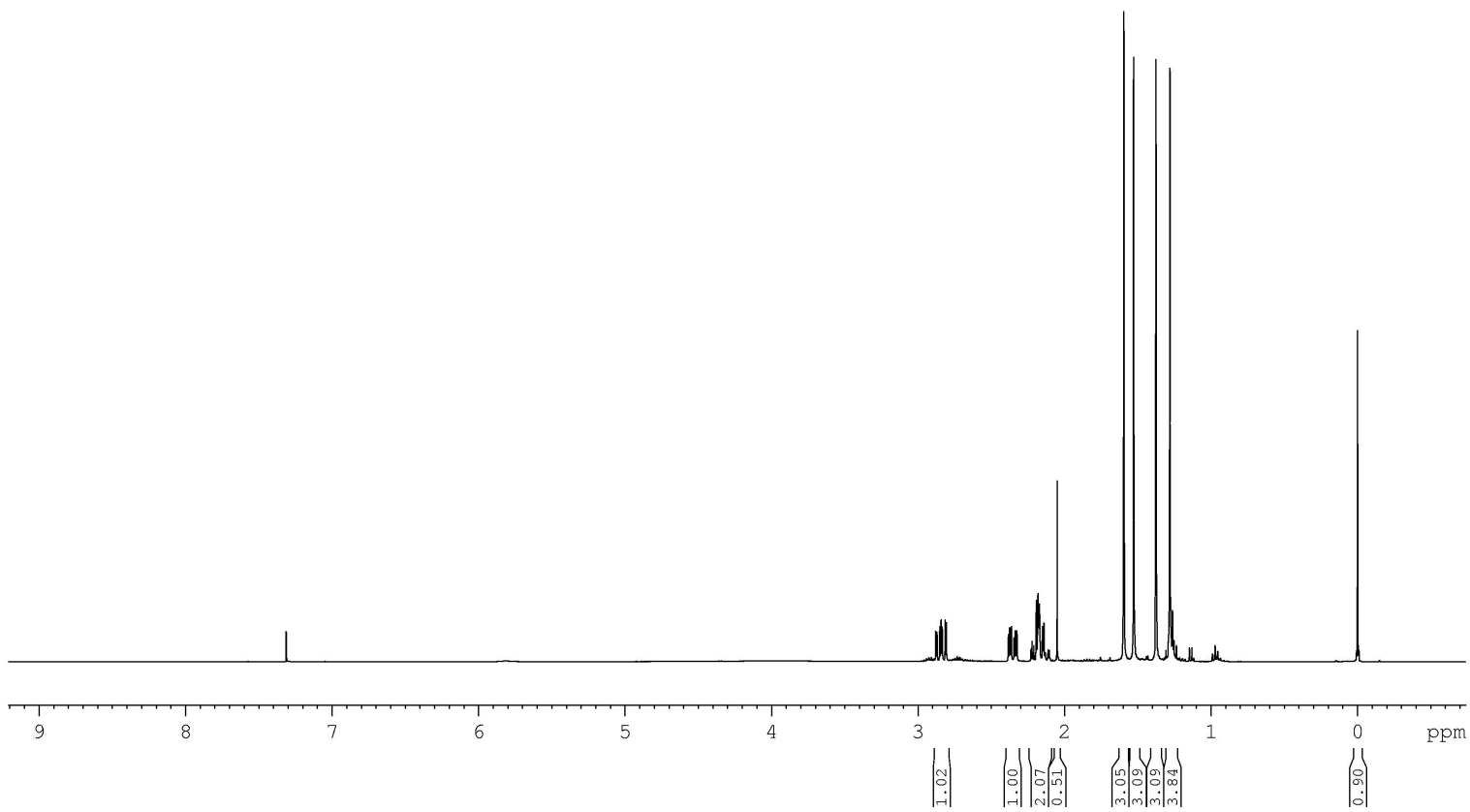


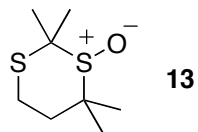


CF134 col 390 10/07/08

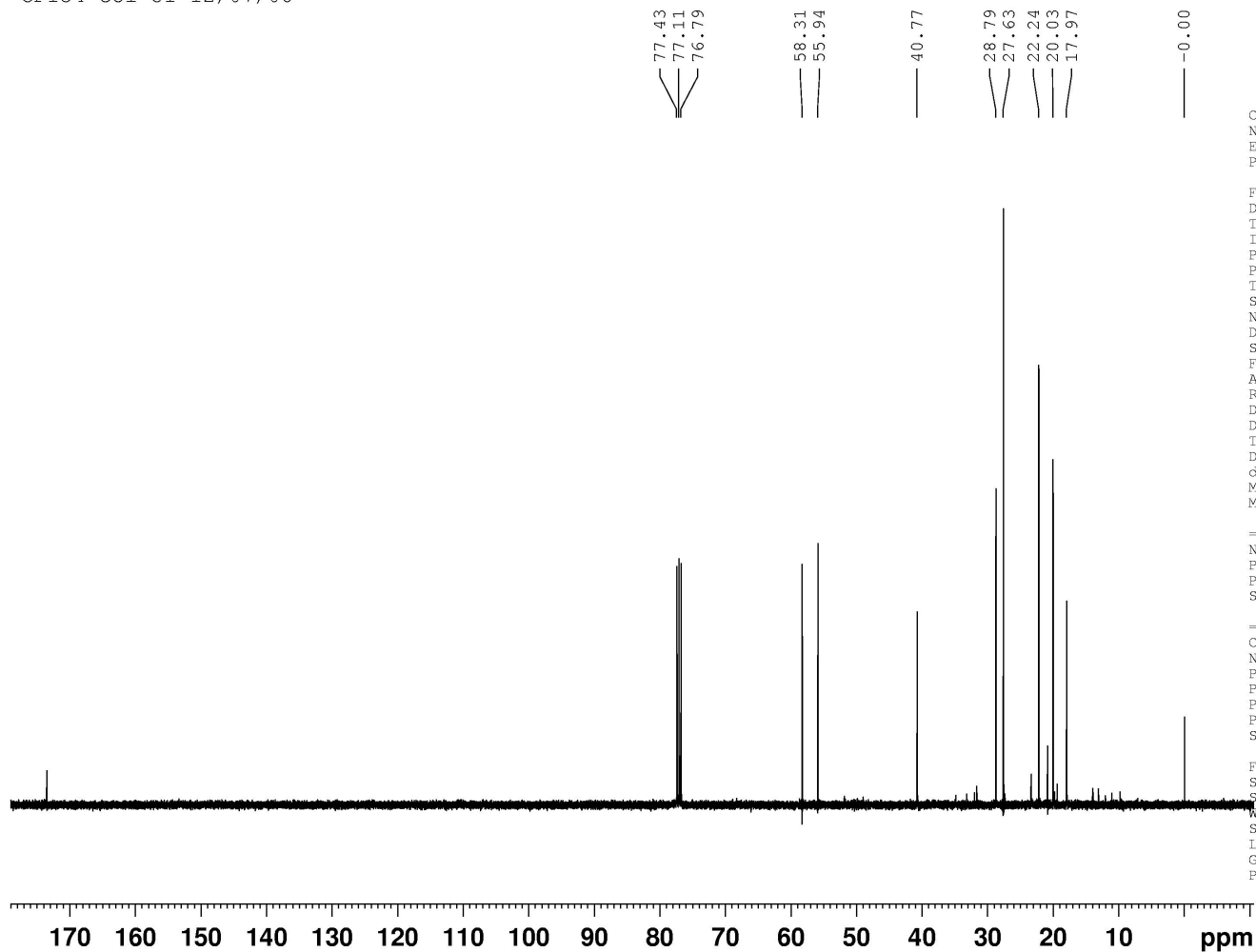
7.313

Current Data Parameters  
NAME: Jul10-2008  
EXPNO: 890  
PROCNO: 1  
F2: 2.880  
F3: 2.872  
F4: 2.853  
F5: 2.845  
F6: 2.843  
F7: 2.835  
F8: 2.815  
F9: 2.807  
F10: 2.384  
F11: 2.376  
F12: 2.371  
F13: 2.363  
F14: 2.346  
F15: 2.337  
F16: 2.334  
F17: 2.326  
F18: 2.251  
F19: 2.210  
F20: 2.193  
F21: 2.186  
F22: 2.182  
F23: 2.178  
F24: 2.173  
F25: 2.159  
F26: 2.150  
F27: 2.144  
F28: 2.104  
F29: 2.052  
F30: 1.596  
F31: 1.529  
F32: 1.377  
F33: 1.309  
F34: 1.282  
F35: 1.265  
F36: 1.255  
F37: 1.238  
F38: 1.149  
F39: 1.132  
F40: 0.974  
F41: 0.000  
F42: -0.000  
F43: -0.000





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Current Data Parameters  
NAME Jul12-2008  
EXPNO 51  
PROCNO 1

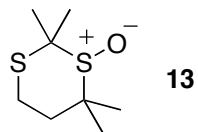
F2 - Acquisition Parameters  
Date\_ 20080712  
Time 12.26  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 512  
DS 2  
SWH 25252.525 E  
FIDRES 0.385323 E  
AQ 1.2976629 s  
RG 9195.2  
DW 19.800 u  
DE 6.00 u  
TE 294.2 K  
D1 1.0000000 s  
a11 0.0300000 s  
MCREST 0.0000000 s  
MCWRK 0.0150000 s

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.25 u  
PL1 -2.00 c  
SFO1 100.6232777 M

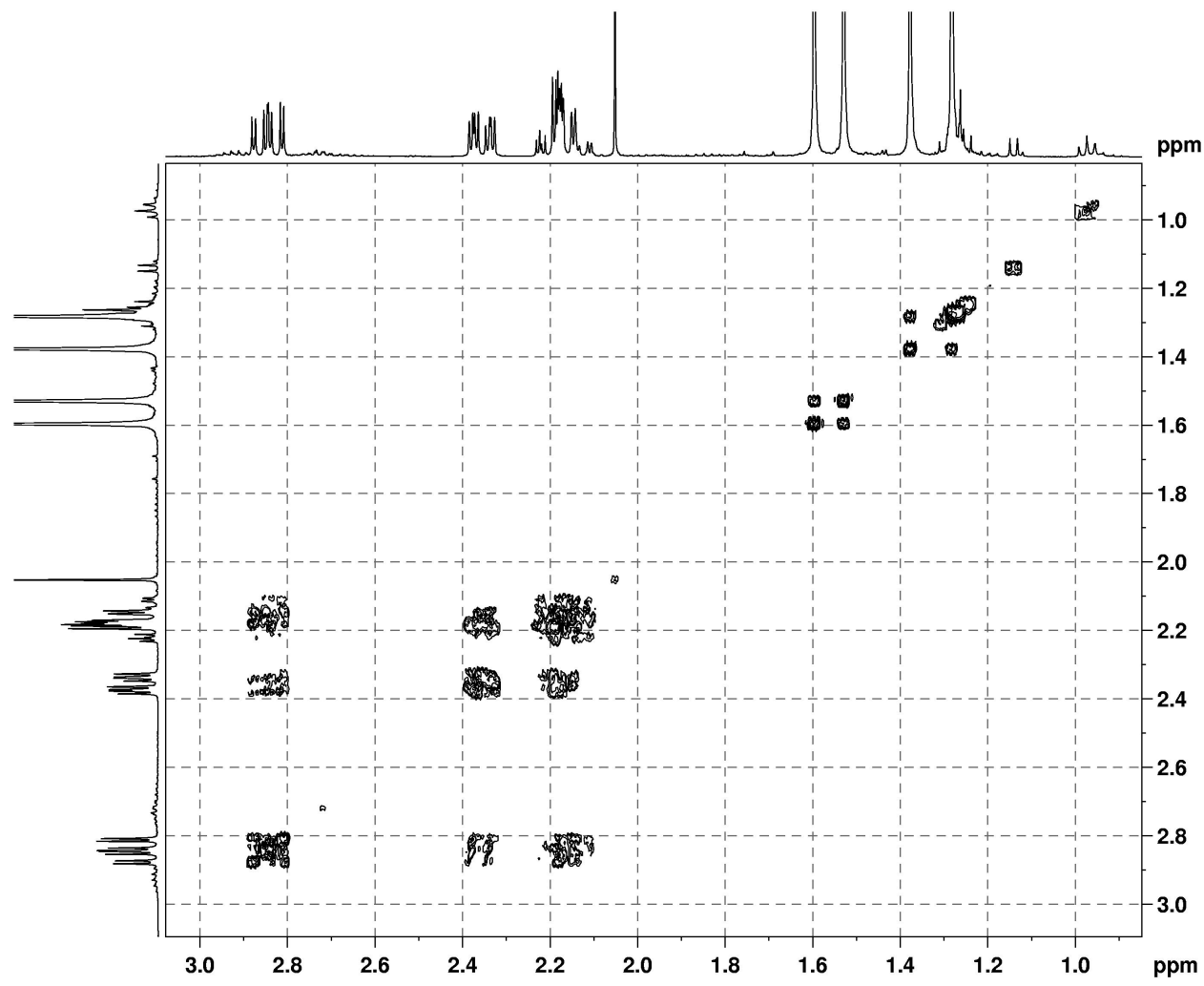
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 u  
PL2 -6.00 c  
PL12 14.00 c  
PL13 15.00 c  
SFO2 400.1316005 M

F2 - Processing parameters  
SI 131072  
SF 100.6127685 M  
WDW no  
SSB 0  
LB 0.00 E  
GB 0  
PC 1.40





CF134 col 53 12/07/08



Current Data Parameters  
NAME Jul12-2008  
EXPNO 53  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080712  
Time 12.57  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG cosygmrfqf  
TD 2048  
SOLVENT CDCl3  
NS 1  
DS 16  
SWH 3834.356 Hz  
FIDRES 1.872244 Hz  
AQ 0.2671092 sec  
RG 4597.6  
DW 130.400 usec  
DE 6.00 usec  
TE 294.2 K  
D0 0.0000300 sec  
D1 0.99016541 sec  
d13 0.0000400 sec  
D16 0.00020000 sec  
INO 0.00026080 sec  
MCREST 0.00000000 sec  
MCWRK 0.99016541 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 11.75 usec  
PL1 -6.00 dB  
SFO1 400.1313532 MHz

===== GRADIENT CHANNEL =====  
GPNAM1 SINE.100  
GPNAM2 SINE.100  
GPNAM3 SINE.100  
GPX1 0.00 %  
GPX2 0.00 %  
GPX3 0.00 %  
GPY1 0.00 %  
GPY2 0.00 %  
GPY3 0.00 %  
GPZ1 16.00 %  
GPZ2 12.00 %  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
ND0 1  
TD 256  
SFO1 400.1314 MHz  
FIDRES 14.977952 Hz  
SW 9.583 ppm  
FMODE QF

F2 - Processing parameters  
SI 4096  
SF 400.1299871 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40

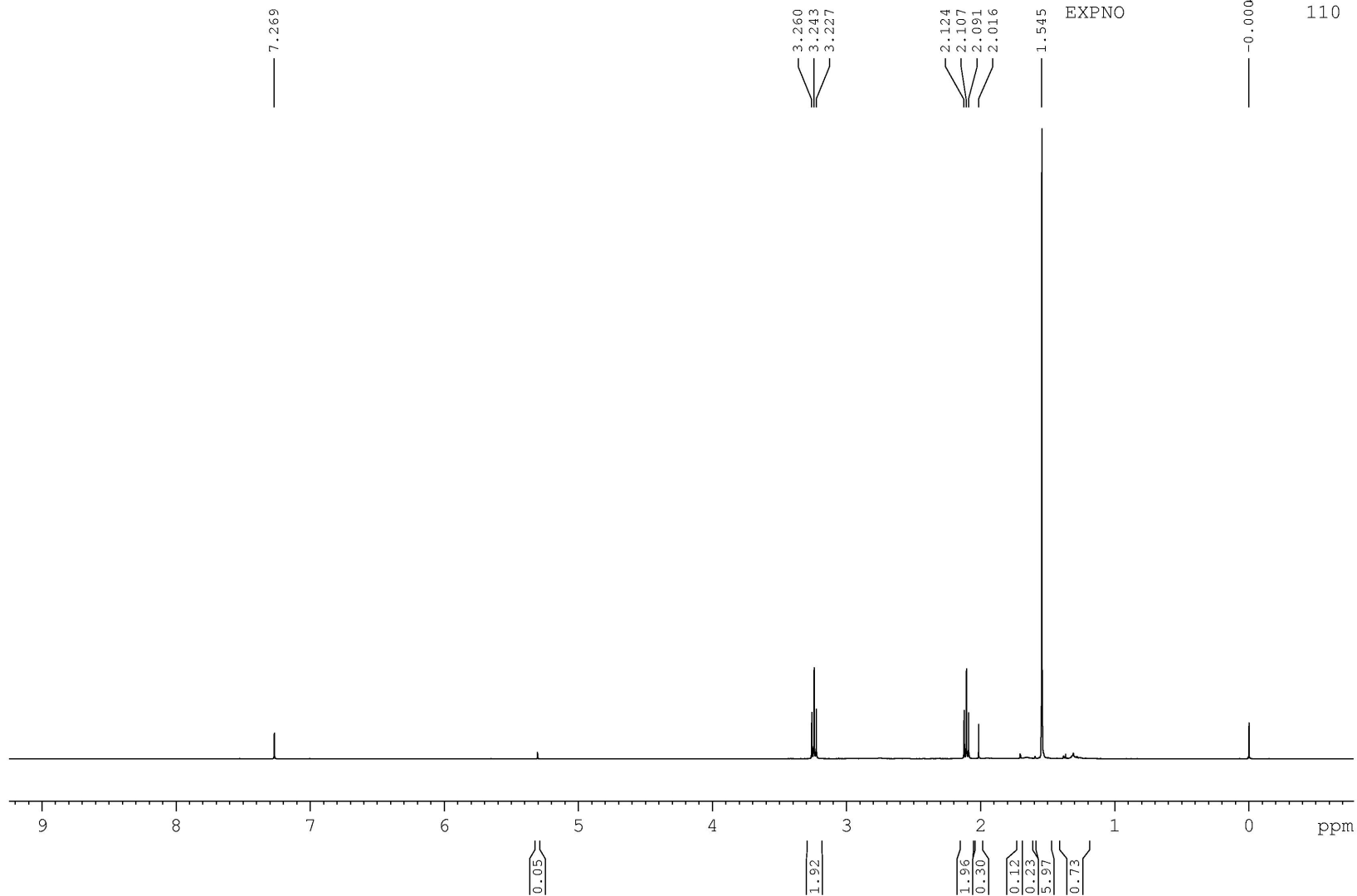
F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 400.1299871 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0



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CF402 crude 110 05/05/09

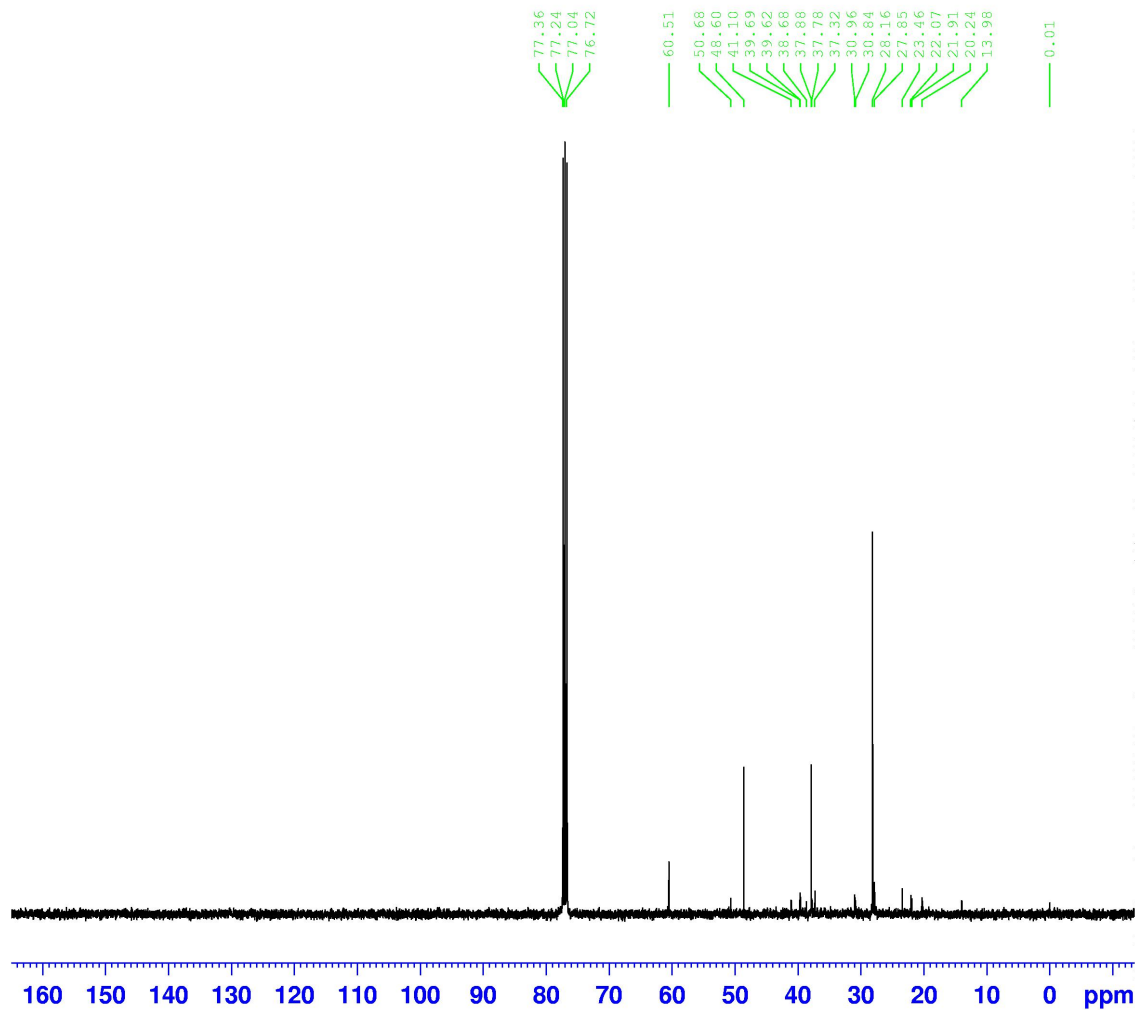
Current Data Parameters  
NAME May05-2009  
EXPNO 110





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CF326a 81 05/02/09



Current Data Parameters  
NAME Feb05-2009  
EXPNO 81  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20090205  
Time 22.13  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 9195.2  
DW 19.800 usec  
DE 6.00 usec  
TE 294.2 K  
D1 1.00000000 sec  
d11 0.03000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.25 usec  
PL1 -2.00 dB  
SFO1 100.6232777 MHz

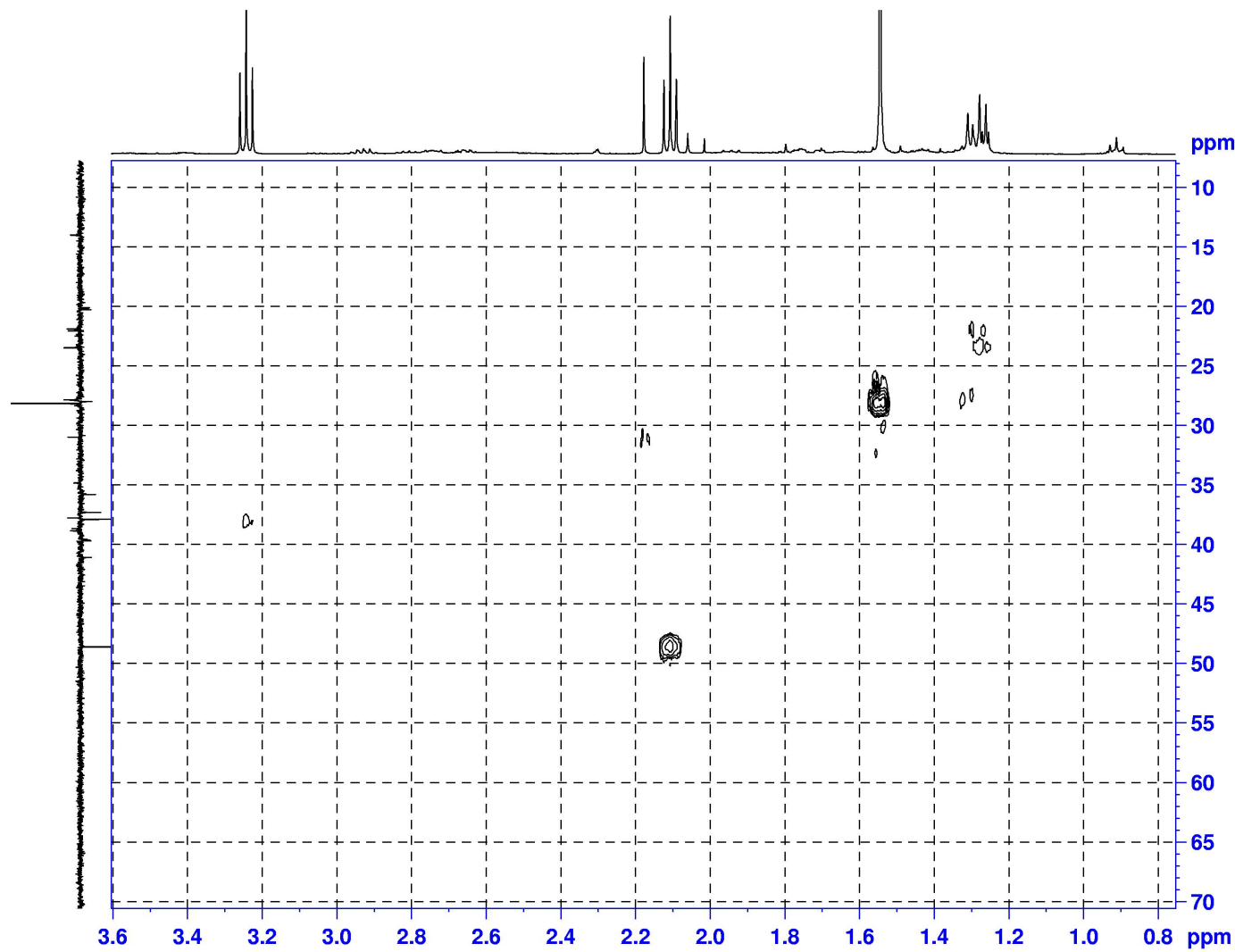
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 14.00 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 131072  
SF 100.6127690 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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CF326a 84 05/02/09



```
Current Data Parameters
NAME      Feb05-2009
EXPNO     84
PROCNO    1

F2 - Acquisition Parameters
Date_     20090205
Time      23.01
INSTRUM   gp400
PROBHD    5 mm Dual 13C/
PULPROG   hmqcgpqf
TD         2048
SOLVENT   cdcl3
NS         8
DS         16
SWH        2934.272 Hz
FIDRES     1.432750 Hz
AQ         0.3490292 sec
RG         26008
DW         170.400 usec
DE         6.00 usec
TE         293.2 K
CNST2     145.0000000
d0         0.00000300 sec
D1         0.90196478 sec
d2         0.0034828 sec
d12        0.00002000 sec
d13        0.00000400 sec
D16        0.00020000 sec
DELTA1     0.00222428 sec
IN0        0.00002761 sec
MCREST     0.00000000 sec
MCWRK     0.90196478 sec

===== CHANNEL f1 =====
NUC1       1H
P1         11.75 usec
p2         23.50 usec
PL1        -6.00 dB
SFO1       400.1316258 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2       13C
P3         8.25 usec
PCPD2     70.00 usec
PL2        -2.00 dB
PL12       15.00 dB
SFO2       100.6213211 MHz

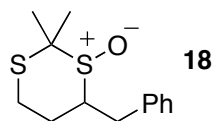
===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPNAM3    SINE.100
GPX1      0.00 %
GPX2      0.00 %
GPX3      0.00 %
GPY1      0.00 %
GPY2      0.00 %
GPY3      0.00 %
GPZ1      50.00 %
GPZ2      30.00 %
GPZ3      40.10 %
P16       1000.00 usec

F1 - Acquisition parameters
NDO        2
TD         128
SFO1       100.6213 MHz
FIDRES     141.466721 Hz
SW         179.959 ppm
FrMODE     QF

F2 - Processing parameters
SI         4096
SF         400.130064 MHz
WDW        QSINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

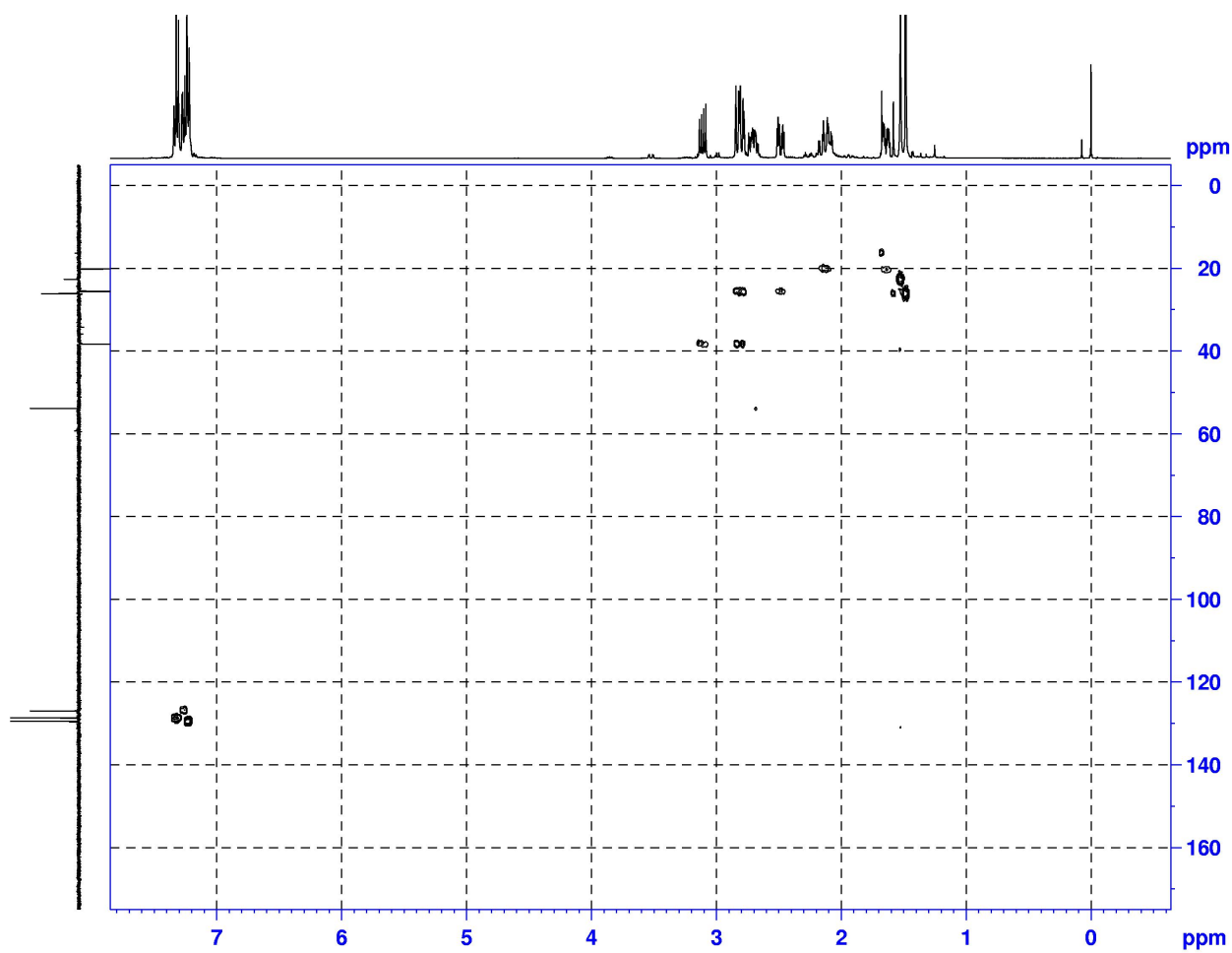
F1 - Processing parameters
SI         1024
MC2        QF
SF         100.6127690 MHz
WDW        QSINE
SSB        0
LB         0.00 Hz
GB         0
```





The diastereoisomer which resisted alkylation.

CF371 11-13 674 20/10/2010



```
Current Data Parameters
NAME      Oct20-2010
EXPNO    674
PROCNO    1

F2 - Acquisition Parameters
Date_    20101020
Time     18.39
INSTRUM  av400
PROBHD   5 mm PABBO BB-
PULPROG  hmzgpgpgf
TD       2048
SOLVENT  CDCl3
NS       8
DS       16
SWH      3491.620 Hz
FIDRES   1.704893 Hz
AQ       0.2933236 sec
RG       20642.5
DW       143.200 usec
DE       6.00 usec
TE       298.0 K
CNST2    145.0000000
d0       0.00000300 sec
d1       0.92094648 sec
d2       0.00344828 sec
d12      0.00002000 sec
d13      0.00000400 sec
d16      0.00020000 sec
DELTA1   0.00222428 sec
INO      0.00002615 sec

===== CHANNEL f1 =====
NUC1     1H
P1       14.25 usec
p2       28.50 usec
PL1      4.00 dB
SFO1     400.1314804 MHz

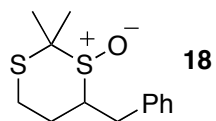
===== CHANNEL f2 =====
CPDPRG2  garp
NUC2     13C
P3       9.75 usec
PCPD2    70.00 usec
PL2      8.00 dB
PL12     25.12 dB
SFO2     100.6218241 MHz

===== GRADIENT CHANNEL =====
GPNAM1   SINE.100
GPNAM2   SINE.100
GPNAM3   SINE.100
GPZ1     50.00 %
GPZ2     30.00 %
GPZ3     40.10 %
PL6      1000.00 usec

F1 - Acquisition parameters:
NDO      2
TD       128
SFO1     100.6218 MHz
FIDRES   149.378586 Hz
SW       190.023 MHz
FnMODE   QF

F2 - Processing parameters:
SI       4096
SF       400.1300017 MHz
WDW      QSINE
SSB      0
LB       0.00 Hz
GB       0
PC       1.40

F1 - Processing parameters:
SI       1024
MC2      QF
SF       100.6127690 MHz
WDW      QSINE
SSB      0
LB       0.00 Hz
GB       0
```



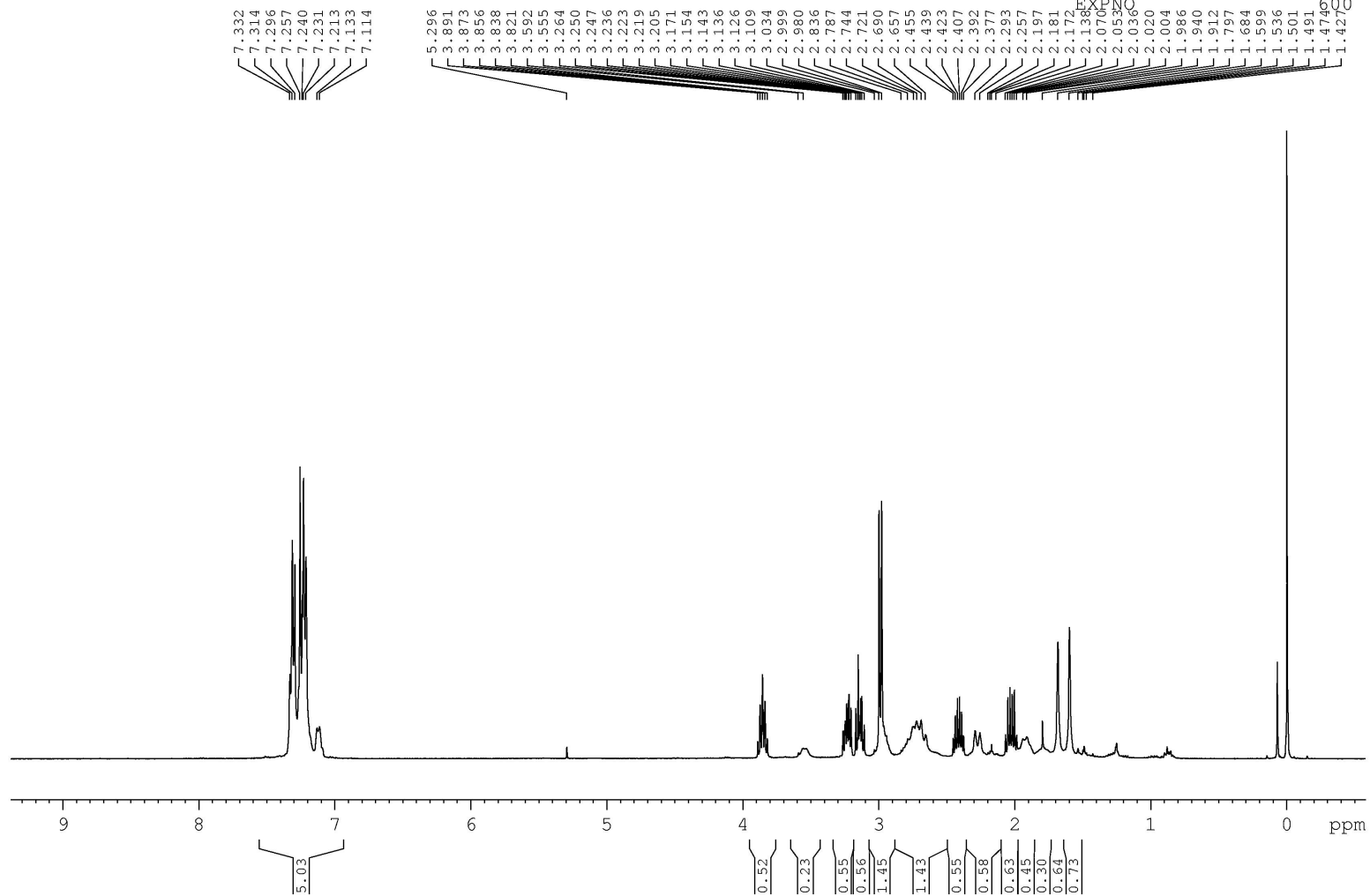
The diastereoisomer which was cleaved more slowly by acid.

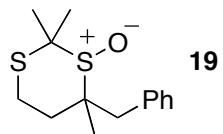
CF368a 600 24/03/09

Current Data Parameters

NAME Mar24-2009

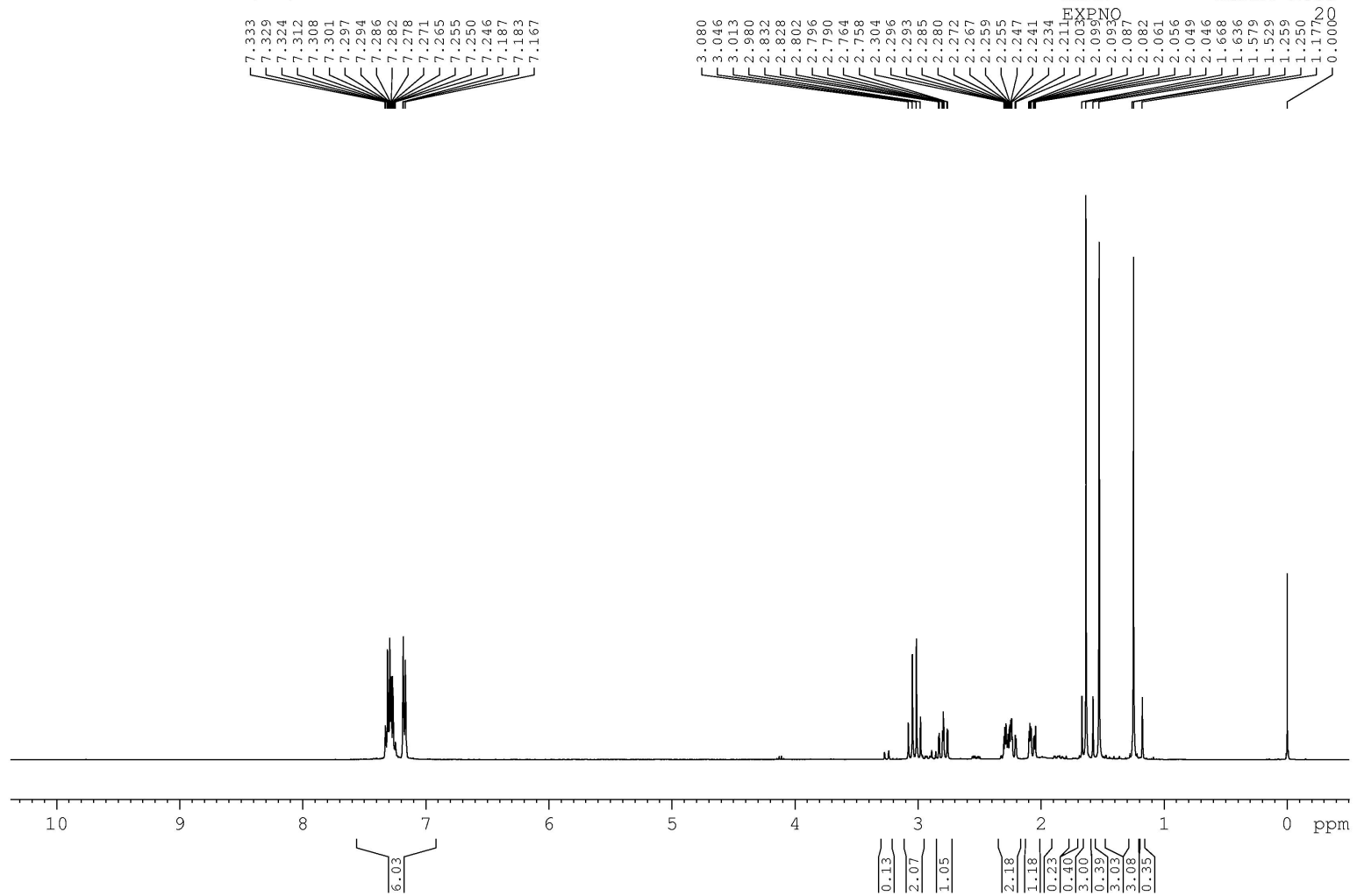
EXPNO 600



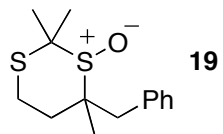


CF371-6 20 24/03/09

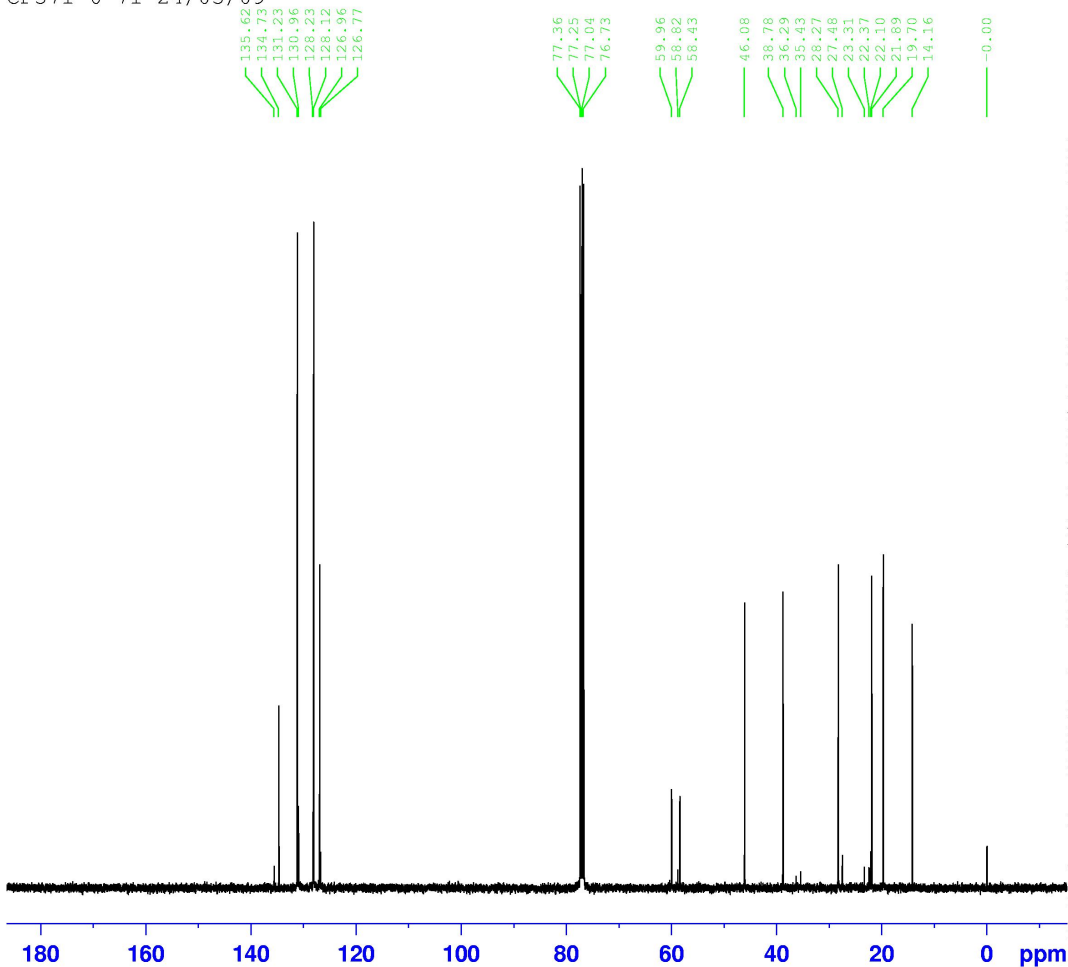
Current Data Parameters  
NAME Mar24-2009







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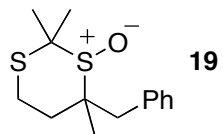
Current Data Parameters  
NAME Mar24-2009  
EXPNO 71  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20090325  
Time 1.05  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 9195.2  
DW 19.800 usec  
DE 6.00 usec  
TE 294.2 K  
D1 1.00000000 sec  
d11 0.03000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

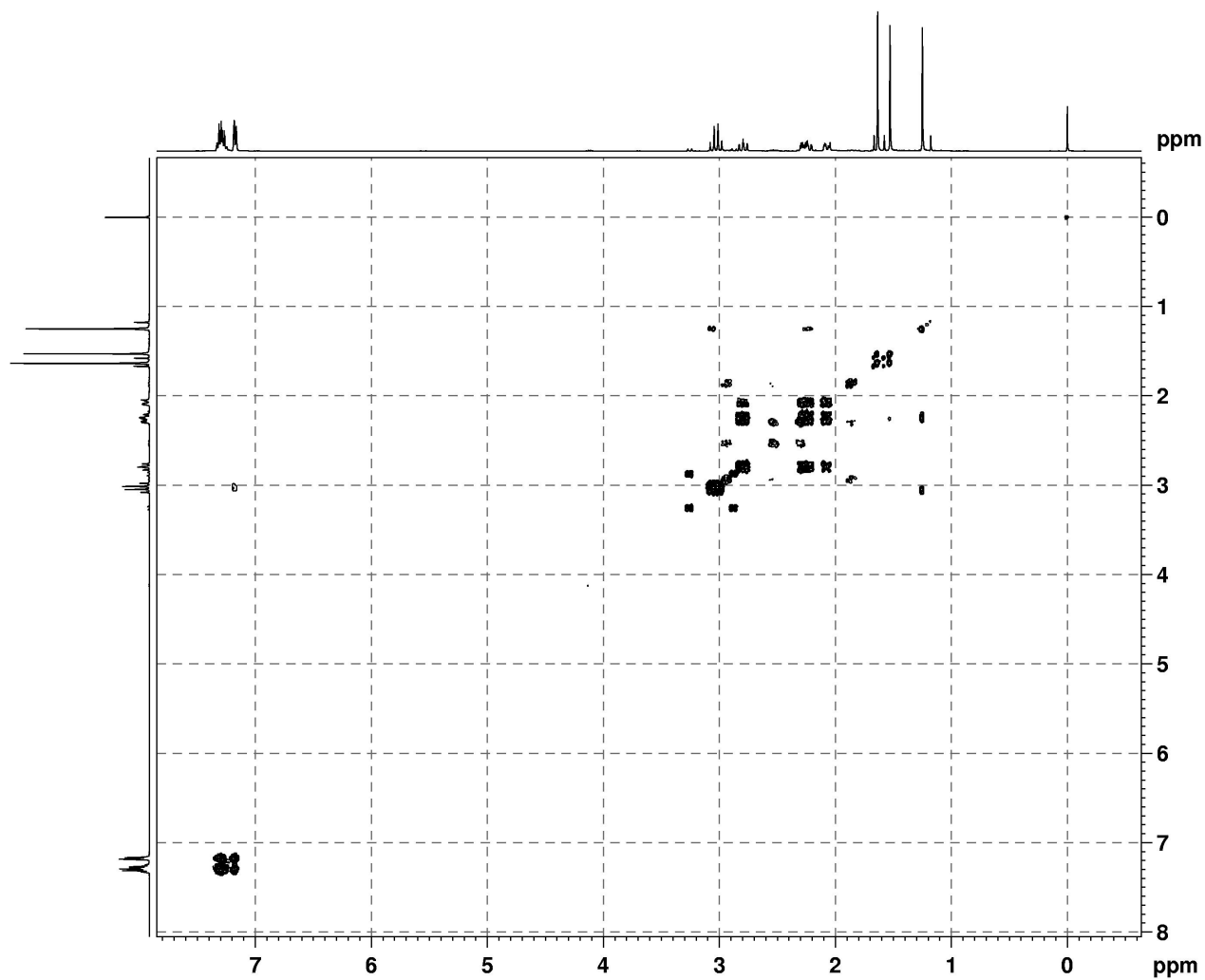
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.25 usec  
PL1 -2.00 dB  
SFO1 100.6232777 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 14.00 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 131072  
SF 100.6127713 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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Current Data Parameters  
NAME Mar24-2009  
EXPNO 73  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20090325  
Time 1.47  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG cosygmfzf  
TD 2048  
SOLVENT CDCl3  
NS 1  
DS 16  
SWH 3491.620 Hz  
FIDRES 1.704893 Hz  
AQ 0.2933236 sec  
RG 2896.3  
DW 143.200 usec  
DE 6.00 usec  
TE 293.2 K  
D0 0.0000300 sec  
D1 0.96354133 sec  
d13 0.0000400 sec  
D16 0.0002000 sec  
-fno 0.00028640 sec  
MCREST 0.0000000 sec  
MCWRK 0.96354133 sec

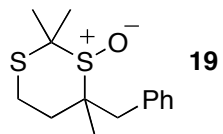
----- CHANNEL f1 -----  
NUC1 1H  
P1 11.75 usec  
PL1 -6.00 dB  
SFO1 400.1314821 MHz

===== GRADIENT CHANNEL =====  
GPNAM1 SINE.100  
GPNAM2 SINE.100  
GPNAM3 SINE.100  
GPX1 0.00 %  
GPX2 0.00 %  
GPX3 0.00 %  
GPY1 0.00 %  
GPY2 0.00 %  
GPY3 0.00 %  
GPZ1 16.00 %  
GPZ2 12.00 %  
GPZ3 40.00 %  
P16 1000.00 usec

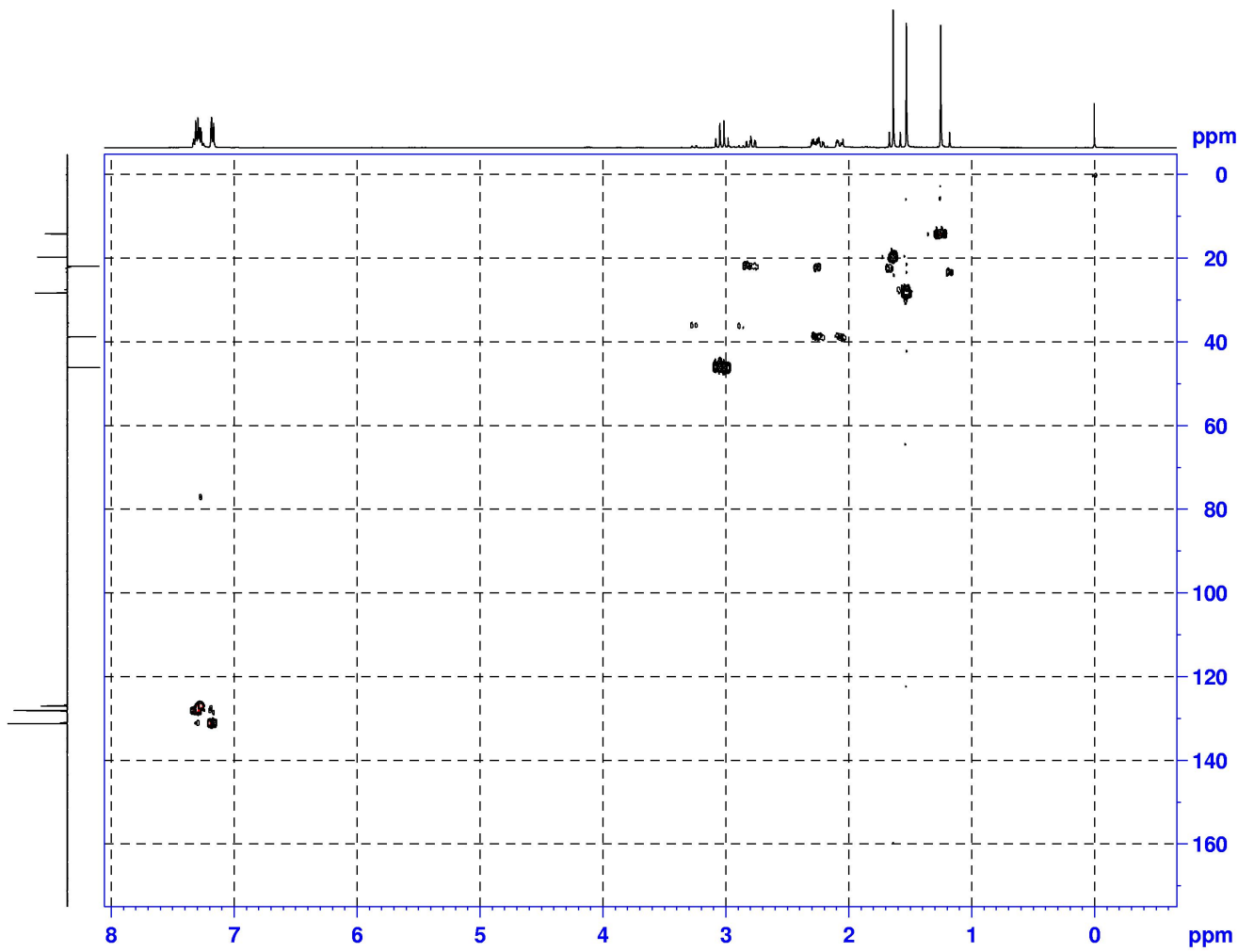
F1 - Acquisition parameters  
ND0 1  
TD 256  
SFO1 400.1315 MHz  
FIDRES 13.639141 Hz  
SW 8.726 ppm  
FrMODE QF

F2 - Processing parameters  
SI 4096  
SF 400.130052 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 400.130052 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0



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```
Current Data Parameters
NAME      Mar24-2009
EXPNO    74
PROCNO   1

F2 - Acquisition Parameters
Date_    20090325
Time     1.53
INSTRUM  dpx400
PROBHD   5 mm Dual 13C/
PULPROG  hmqcpgpf
TD       2048
SOLVENT  cdcl3
NS       8
DS       16
SWH      3491.620 Hz
FIDRES   1.704893 Hz
AQ       0.2933256 sec
RG       26008
DW       143.200 usec
DE       6.00 usec
TE       293.2 K
CNST2    145.0000000
d0       0.0000300 sec
d1       0.95726079 sec
d2       0.00344828 sec
d12      0.00002000 sec
d13      0.00000400 sec
d16      0.00020000 sec
DELTA1   0.00222428 sec
lNO      0.00002761 sec
MCREST   0.00000000 sec
MCWEX    0.95726079 sec

===== CHANNEL f1 =====
NUC1     1H
P1       11.75 usec
P2       23.50 usec
PL1      -6.00 dB
SFO1     400.1314821 MHz

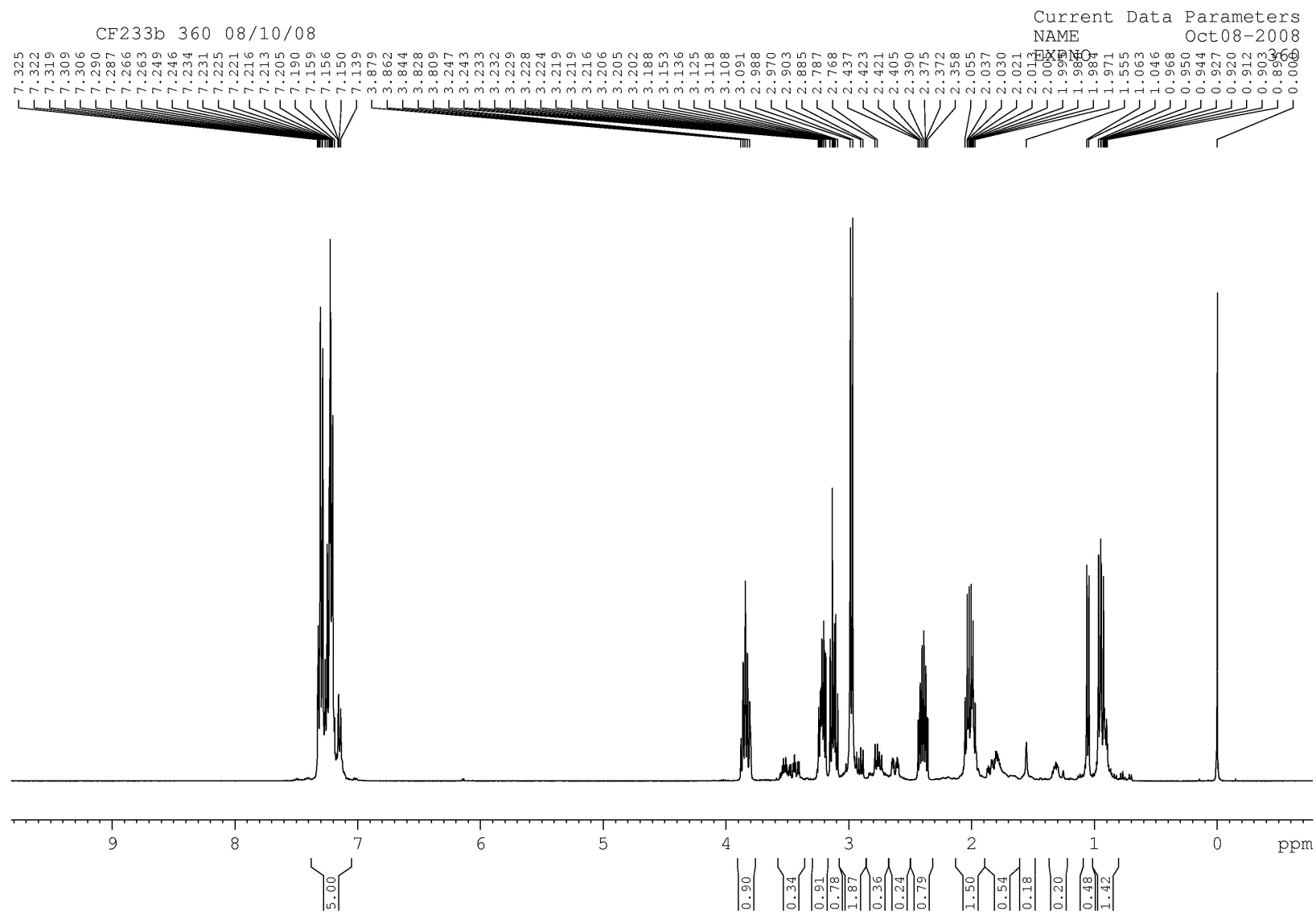
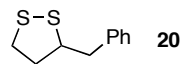
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     13C
P3       8.25 usec
PCPD2    70.00 usec
PL2      -2.00 dB
PL12     15.00 dB
SFO2     100.6213211 MHz

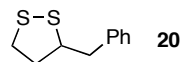
===== GRADIENT CHANNEL =====
GPNAM1   SINE.100
GPNAM2   SINE.100
GPNAM3   SINE.100
GPX1     0.00 %
GPX2     0.00 %
GPX3     0.00 %
GPY1     0.00 %
GPY2     0.00 %
GPY3     0.00 %
GPZ1     50.00 %
GPZ2     30.00 %
GPZ3     40.10 %
P16      1000.00 usec

F1 - Acquisition parameters
ND0      2
TD       128
SFO1     100.6213 MHz
FIDRES   141.466721 Hz
SW       179.959 ppm
FHM0MODE QF

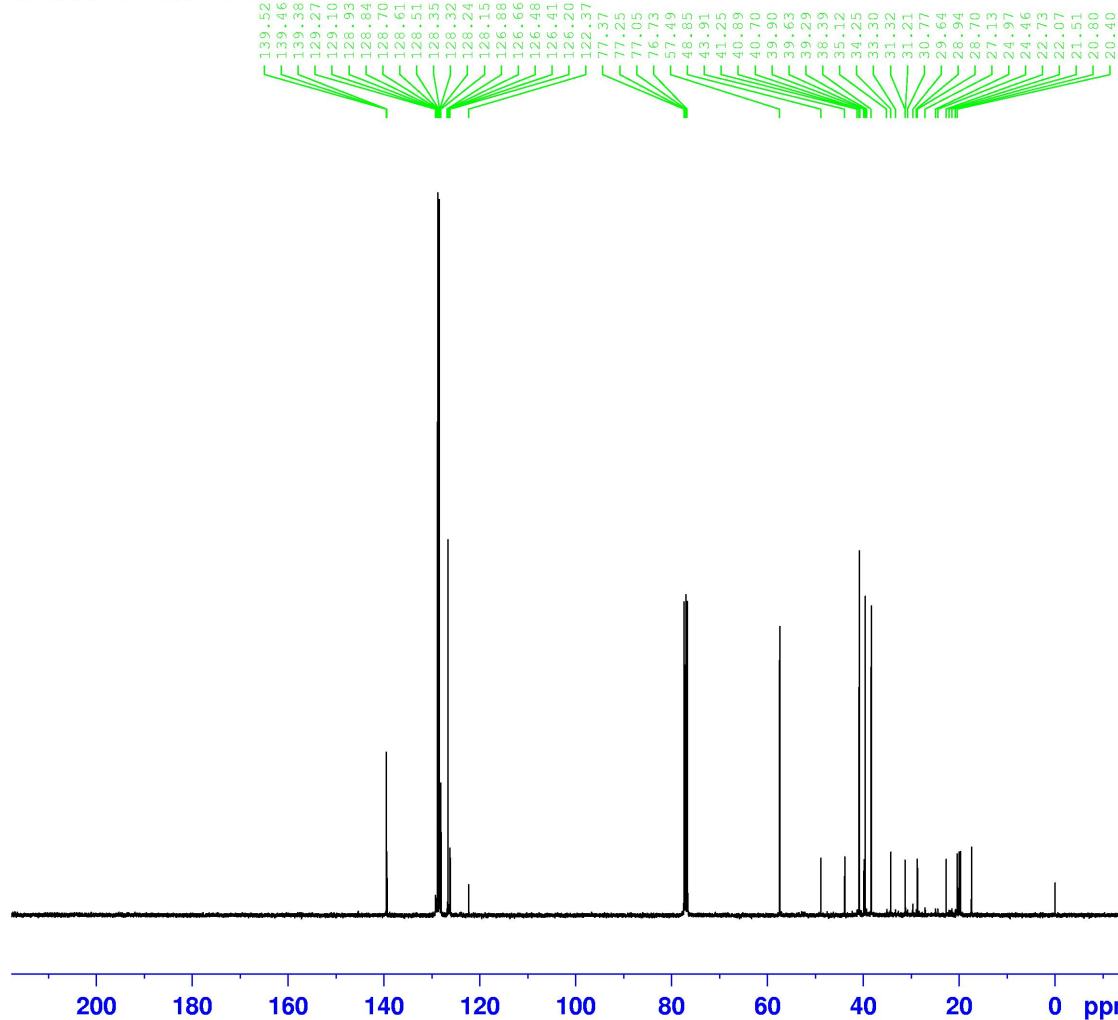
F2 - Processing parameters
SI       4096
SF       400.130052 MHz
WDW      QSINE
SSB      0
LB       0.00 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      QF
SF       100.6127690 MHz
WDW      QSINE
SSB      0
LB       0.00 Hz
GB       0
```





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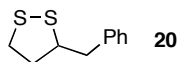
Current Data Parameters  
NAME Oct09-2008  
EXPNO 41  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20081009  
Time 18.48  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 9195.2  
DW 19.800 usec  
DE 6.00 usec  
TE 295.2 K  
D1 1.0000000 sec  
d11 0.0300000 sec  
MCREST 0.0000000 sec  
MCWRK 0.01500000 sec

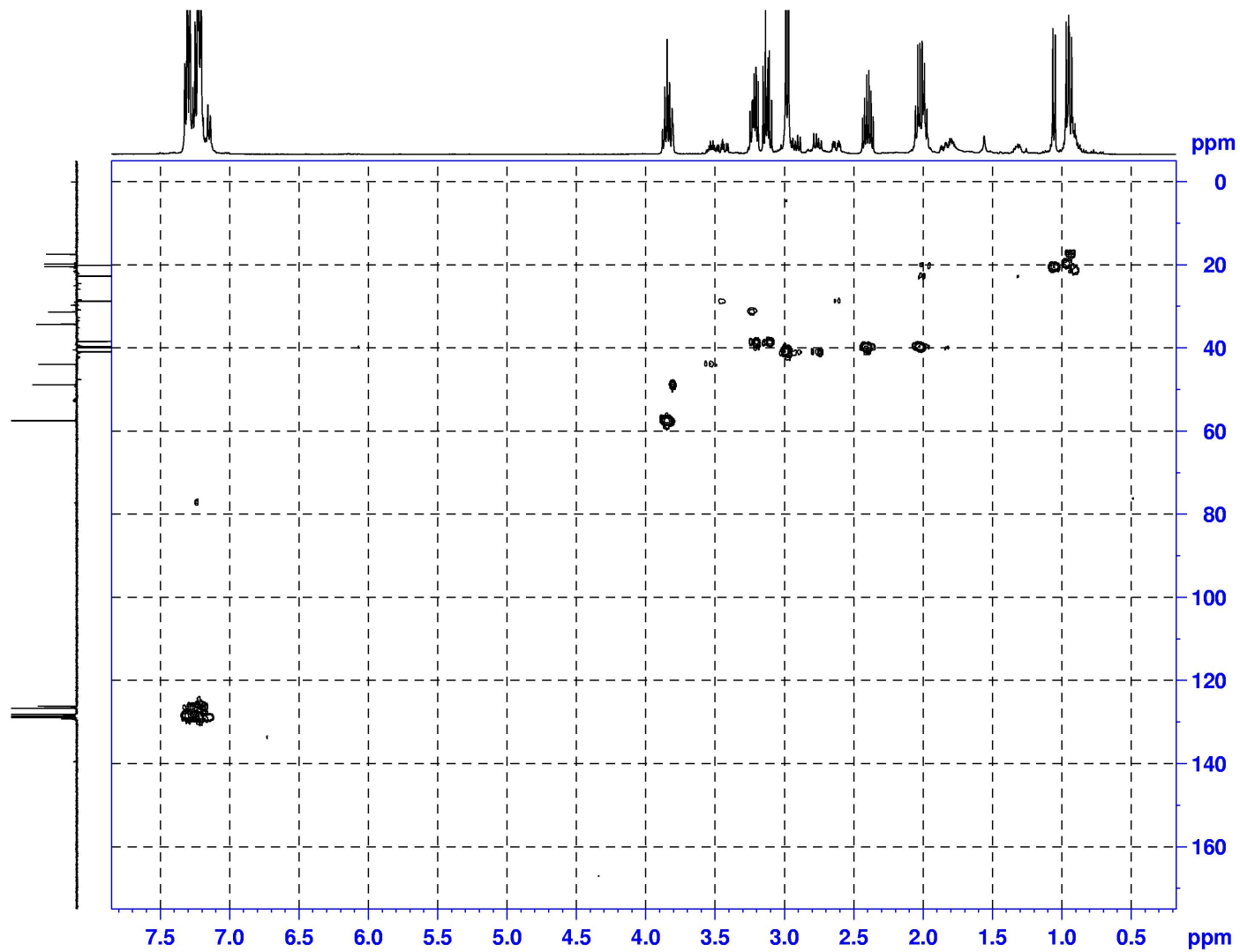
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.25 usec  
PL1 -2.00 dB  
SFO1 100.6232777 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 14.00 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 131072  
SF 100.6127773 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



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```
Current Data Parameters
NAME      Oct09-2008
EXPNO    44
PROCNO    1

F2 - Acquisition Parameters
Date_     20081009
Time      19.36
INSTRUM   dpx400
PROBHD    5 mm Dual 13C/
PULPROG   hmqcpgqf
TD         2048
SOLVENT   cdcl3
NS         8
DS         16
SWH        3205.128 Hz
FIDRES     1.565004 Hz
AQ         0.3195380 sec
RG         18390.4
DW         156.000 usec
DE         6.00 usec
TE         294.2 K
CNST2     145.0000000
d0         0.0000300 sec
d1         0.93063688 sec
d2         0.00344828 sec
d12        0.00002000 sec
d13        0.00000400 sec
d16        0.00020000 sec
DELTAT1   0.00222428 sec
INO        0.00002761 sec
MCWREST   0.00000000 sec
MCWRK     0.93063688 sec

===== CHANNEL f1 =====
NUC1       1H
F1         11.75 usec
p2         23.50 usec
PL1        -6.00 dB
SFO1       400.1316924 MHz

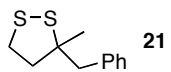
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       13C
P3         8.25 usec
PCPD2      70.00 usec
PL2        -2.00 dB
PL12       15.00 dB
SFO2       100.6213211 MHz

===== GRADIENT CHANNEL =====
GPNAM1     SINE.100
GPNAM2     SINE.100
GPNAM3     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       40.10 %
P16        1000.00 usec

F1 - Acquisition parameters
ND0        2
TD         128
SFO1       100.6213 MHz
FIDRES     141.466721 Hz
SW         179.959 ppm
FqMODE     QF

F2 - Processing parameters
SI         4096
SF         400.1300202 MHz
WDW        QSINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         100.6127690 MHz
WDW        QSINE
SSB        0
LB         0.00 Hz
GB         0
```

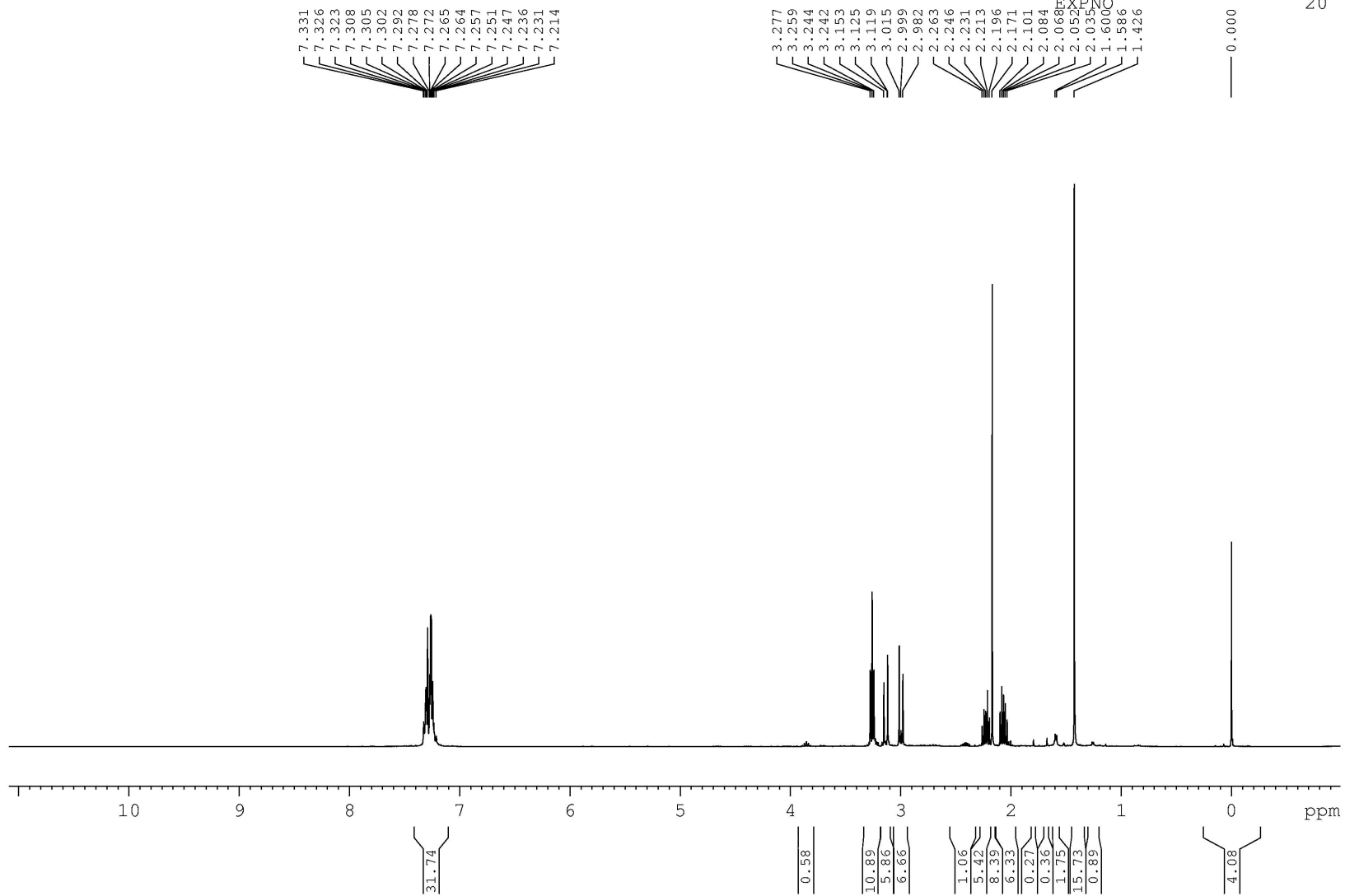


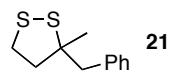
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Current Data Parameters

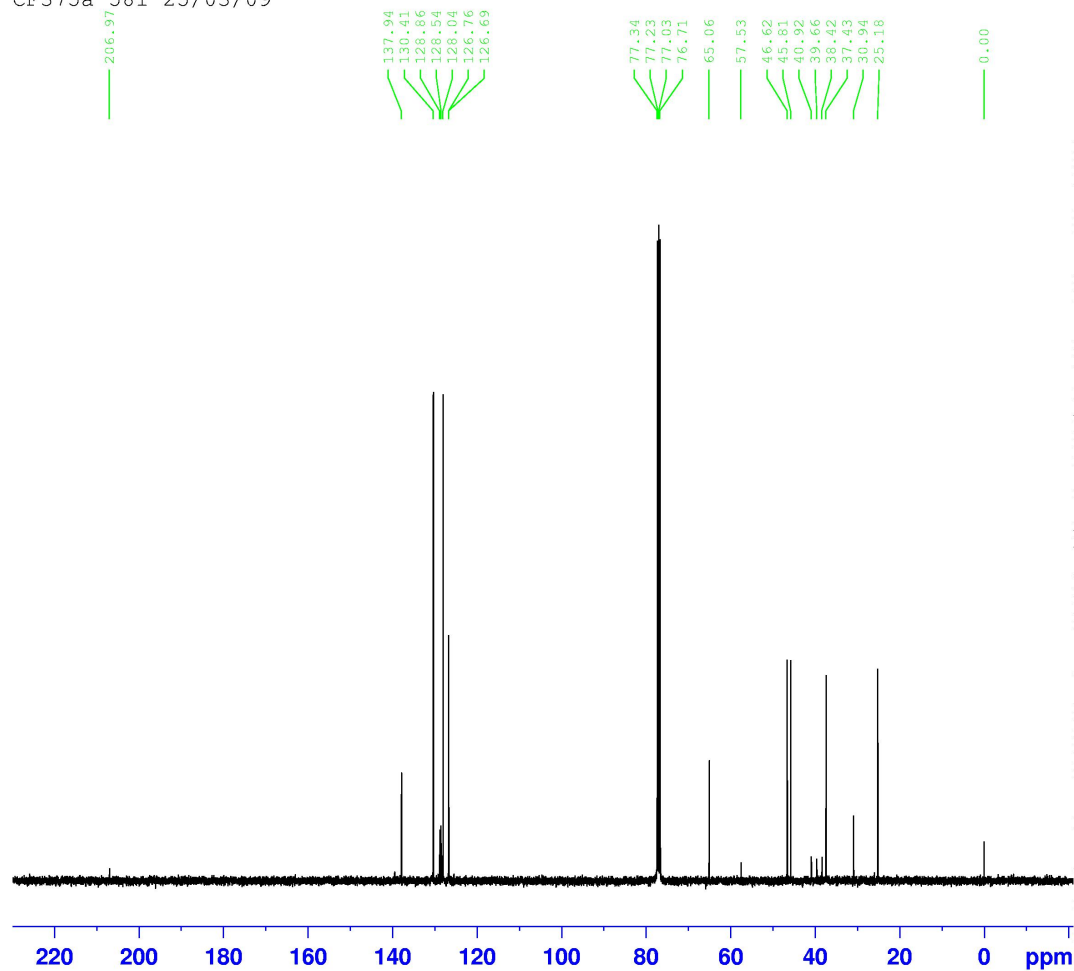
NAME Mar29-2009

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Current Data Parameters  
NAME Mar25-2009  
EXPNO 581  
PROCNO 1

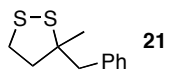
F2 - Acquisition Parameters  
Date\_ 20090326  
Time 20.49  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 13004  
DW 19.800 usec  
DE 6.00 usec  
TE 294.2 K  
D1 1.0000000 sec  
d11 0.0300000 sec  
MCREST 0.0000000 sec  
MCWRK 0.0150000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 8.25 usec  
PL1 -2.00 dB  
SFO1 100.6232777 MHz

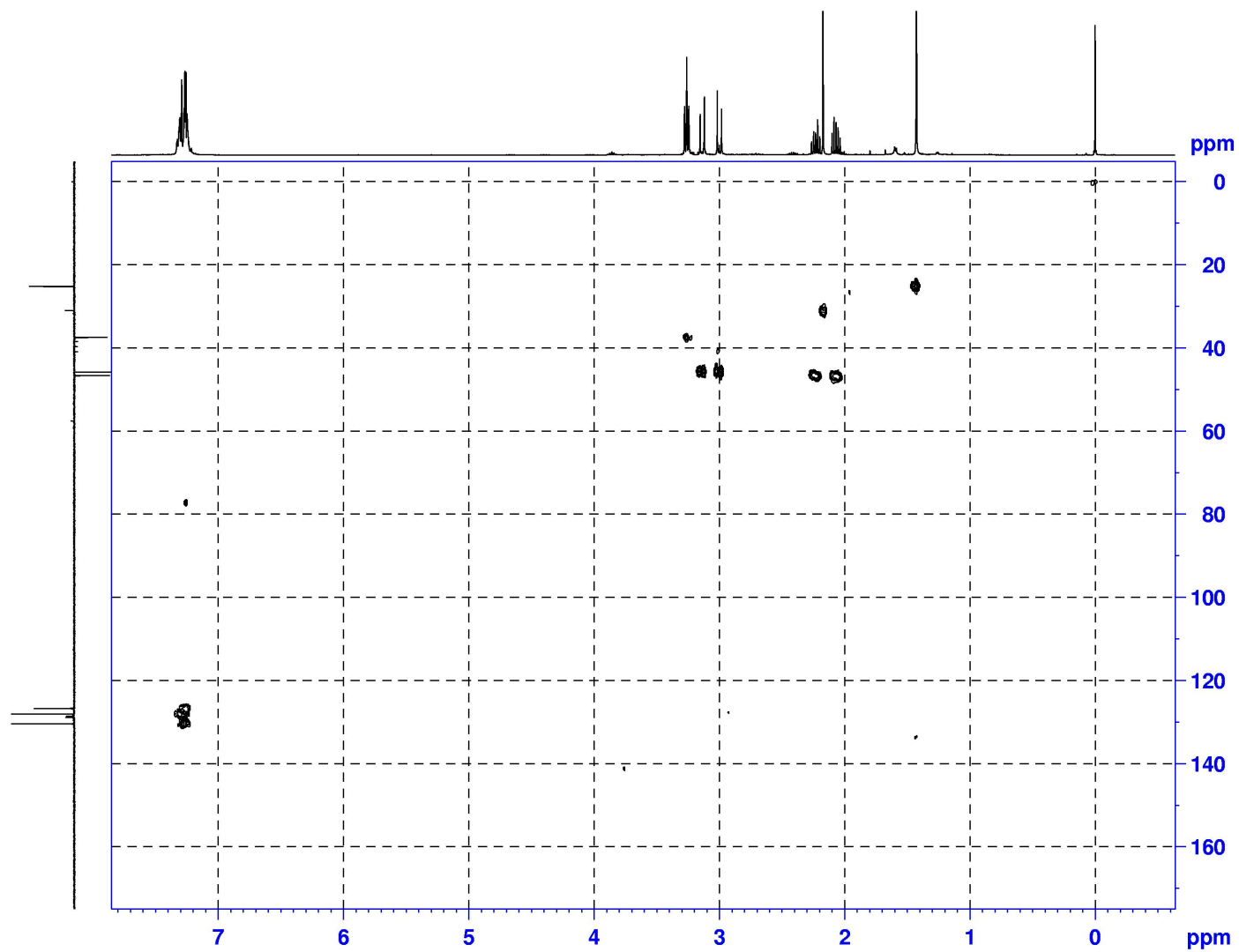
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 14.00 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 131072  
SF 100.6127716 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





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```
Current Data Parameters
NAME      Mar29-2009
EXPNO    24
PROCNO   1

F2 - Acquisition Parameters
Date_    20090329
Time     13.41
INSTRUM  dpx400
PROBHD   5 mm Dual 13C/
PULPROG  hmqcpgqf
TD       2048
SOLVENT  CDCl3
NS       8
DS       16
SWH      3551.136 Hz
FIDRES   1.733953 Hz
AQ       0.2884084 sec
RG       26008
DW       140.800 usec
DE       6.00 usec
TE       293.2 K
CNST2    145.0000000
d0       0.0000000 sec
d1       0.96135688 sec
d2       0.00344828 sec
d12      0.00002000 sec
d13      0.00000400 sec
d16      0.00020000 sec
DELTA1   0.0022428 sec
INO      0.00002761 sec
MCREST   0.00000000 sec
MCWRK    0.96135688 sec

===== CHANNEL f1 =====
NUC1     1H
P1       11.75 usec
P2       23.50 usec
PL1      -6.00 dB
SFO1     400.1315131 MHz

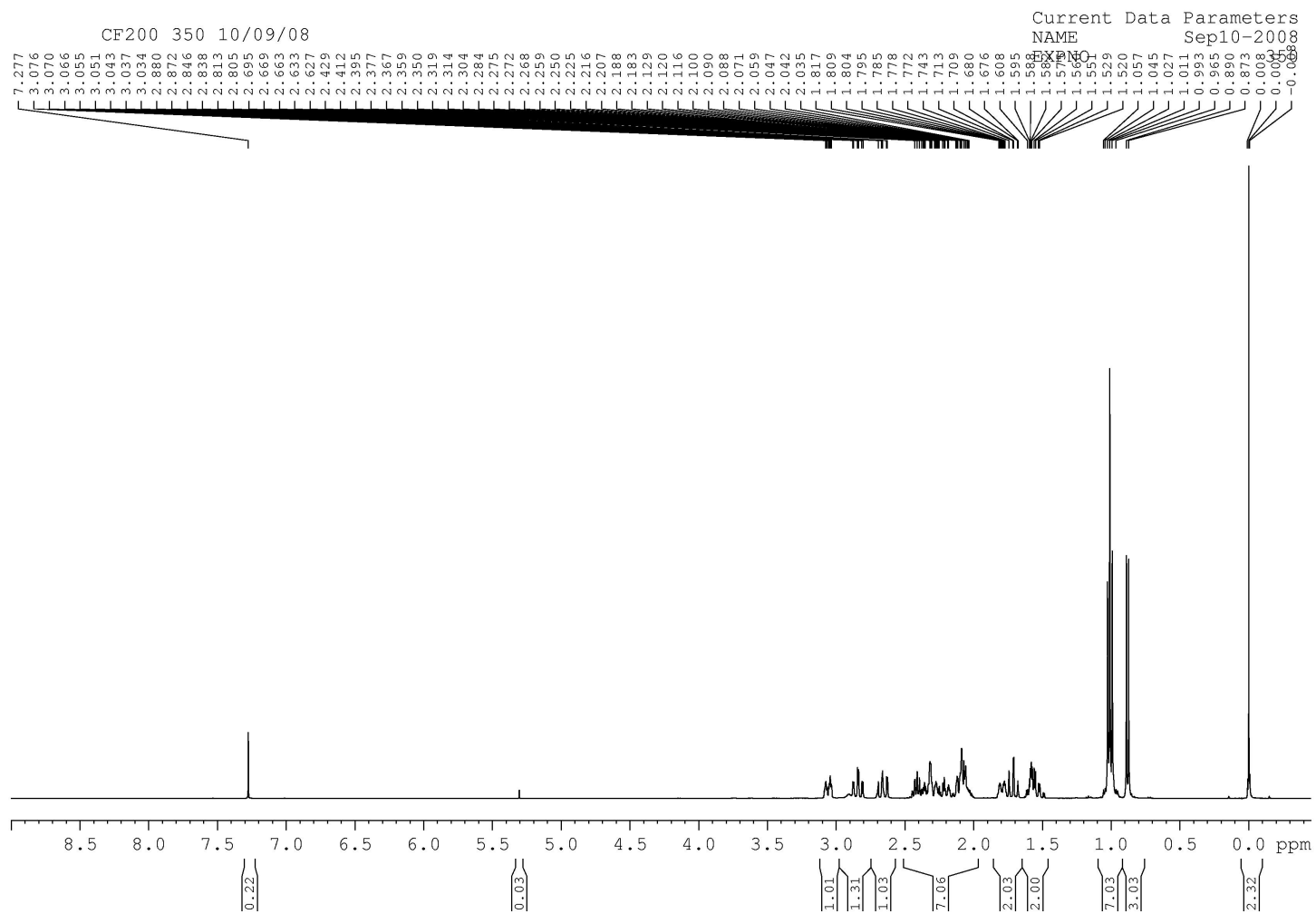
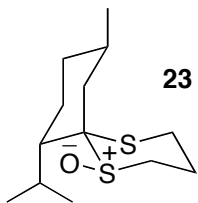
===== CHANNEL f2 =====
CPDPRG2  waltz16
NUC2     13C
P3       8.25 usec
PCPD2    70.00 usec
PL2      -2.00 dB
PL12     15.00 dB
SFO2     100.6213211 MHz

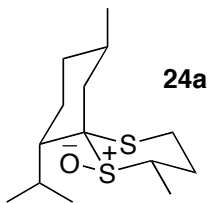
===== GRADIENT CHANNEL =====
GPNAM1   SINE.100
GPNAM2   SINE.100
GPNAM3   SINE.100
GFX1     0.00 %
GFX2     0.00 %
GFX3     0.00 %
GFY1     0.00 %
GFY2     0.00 %
GFY3     0.00 %
GPZ1     50.00 %
GPZ2     30.00 %
GPZ3     40.10 %
P16      1000.00 usec

F1 - Acquisition parameters
ND0      2
TD       128
SFO1     100.6213 MHz
FIDRES   141.466721 Hz
SW       179.959 ppm
FIRMODE  QF

F2 - Processing parameters
SI       4096
SF       400.1300109 MHz
WDW      QSI
SSB      0
LB       0.00 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
MC2      QF
SF       100.6127690 MHz
WDW      QSI
SSB      0
LB       0.00 Hz
GB       0
```

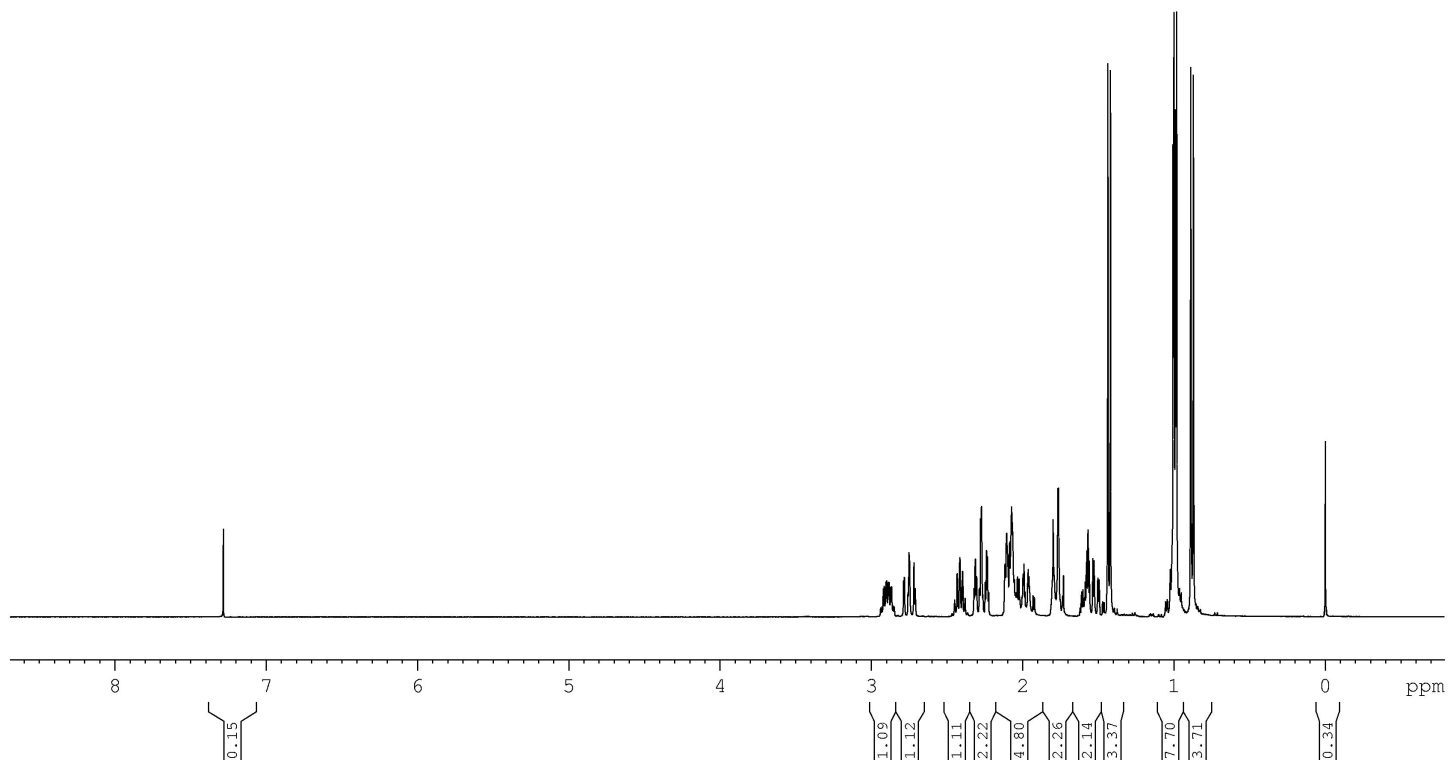


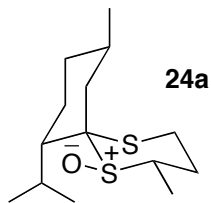


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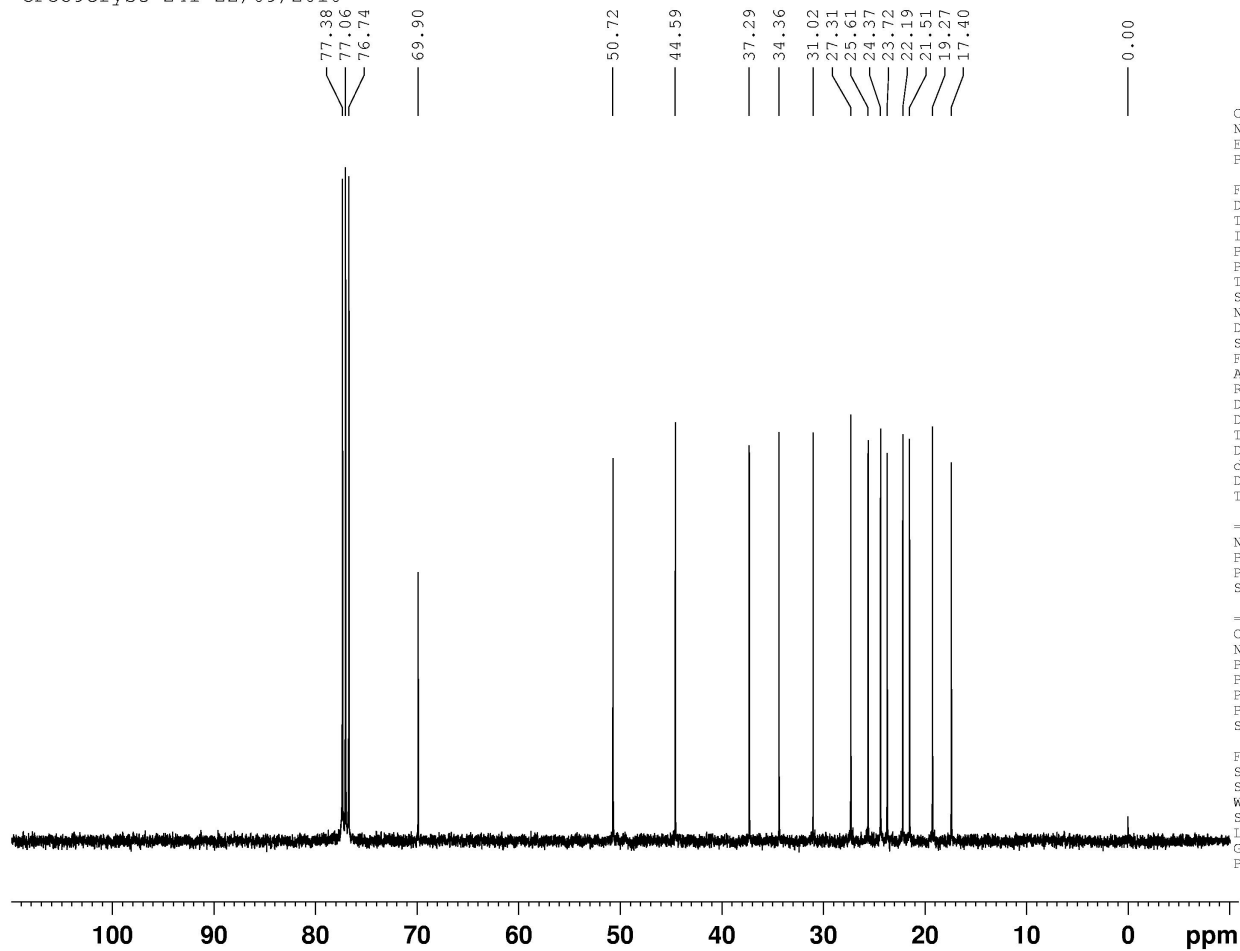
Current Data Parameters  
NAME Sep22-2010

Chemical Shift (ppm)	Integration
7.285	
2.922	
2.915	
2.906	
2.898	
2.890	
2.884	
2.874	
2.867	
2.789	
2.783	
2.758	
2.752	
2.746	
2.720	
2.711	
2.711	
2.433	
2.416	
2.399	
2.382	
2.321	
2.313	
2.307	
2.304	
2.285	
2.279	
2.273	
2.263	
2.248	
2.241	
2.234	
2.226	
2.118	
2.106	
2.097	
2.087	
2.074	
2.069	
2.057	
2.048	
2.044	
2.035	
2.024	
2.000	
1.997	
1.992	
1.986	
1.969	
1.964	
1.960	
1.955	
1.932	
1.923	
1.769	
1.763	
1.783	
1.768	
1.764	
1.736	
1.732	
1.611	
1.603	
1.593	
1.588	
1.577	
1.569	
1.559	
1.537	
1.528	
1.504	
1.496	
1.438	
1.421	
1.045	
1.025	
1.006	
1.001	
0.990	
0.984	
0.967	
0.963	
0.952	
0.890	
0.873	
0.000	





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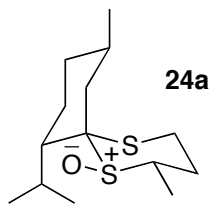
Current Data Parameters  
NAME Sep22-2010  
EXPNO 241  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20100922  
Time 18.34  
INSTRUM av400  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 512  
DS 2  
SWH 26178.010 Hz  
FIDRES 0.399445 Hz  
AQ 1.2517875 s  
RG 16384  
DW 19.100 u  
DE 6.00 u  
TE 298.0 K  
D1 1.0000000 s  
d11 0.0300000 s  
DELTA 0.89999998 s  
TDG 1

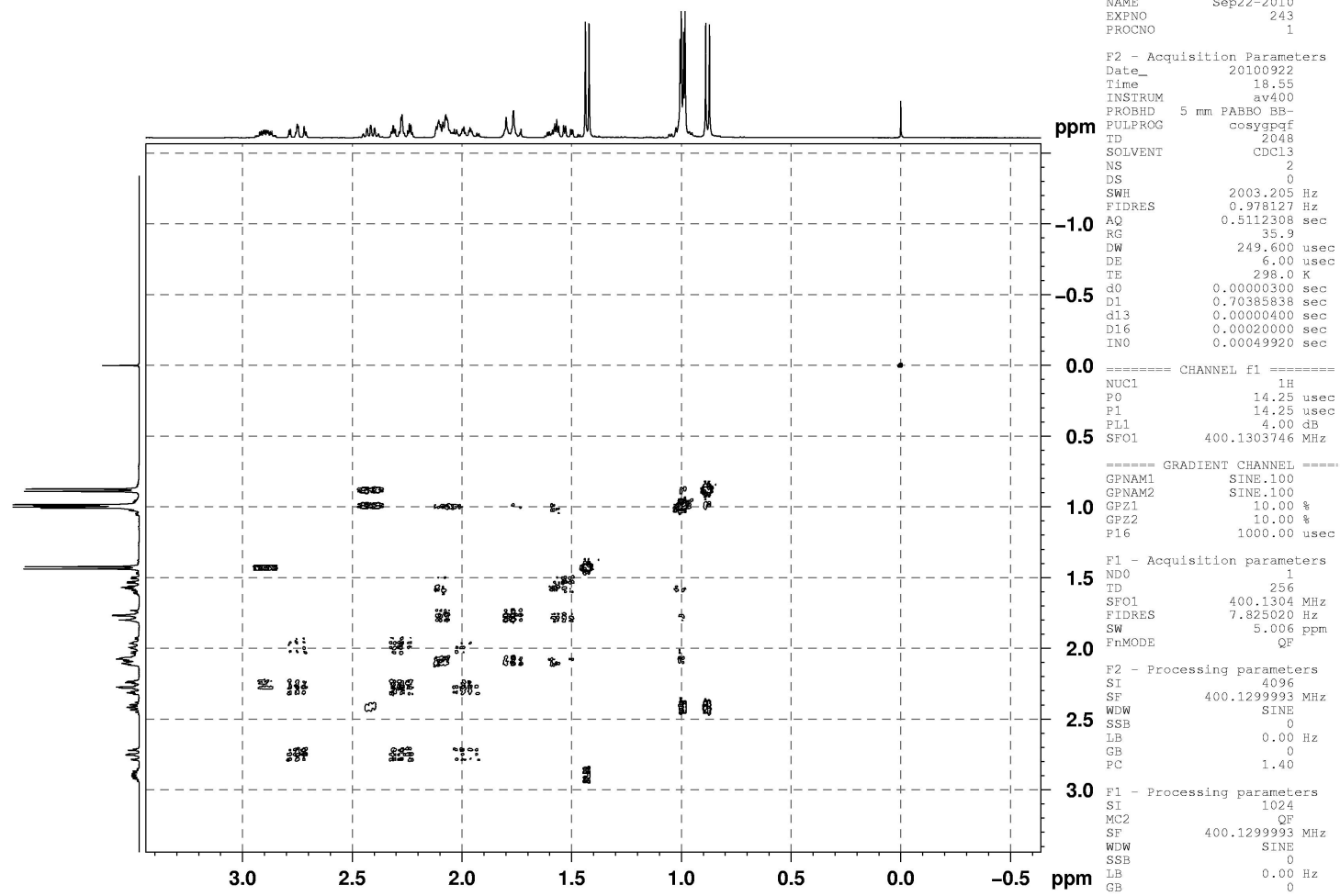
===== CHANNEL f1 =====  
NUC1 13C  
P1 9.75 u  
PL1 8.00 c  
SFO1 100.6248425 MHz

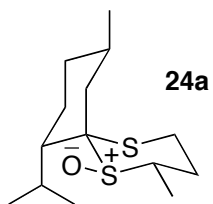
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 u  
PL2 4.00 c  
PL12 18.99 c  
PL13 20.00 c  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 131072  
SF 100.6127679 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

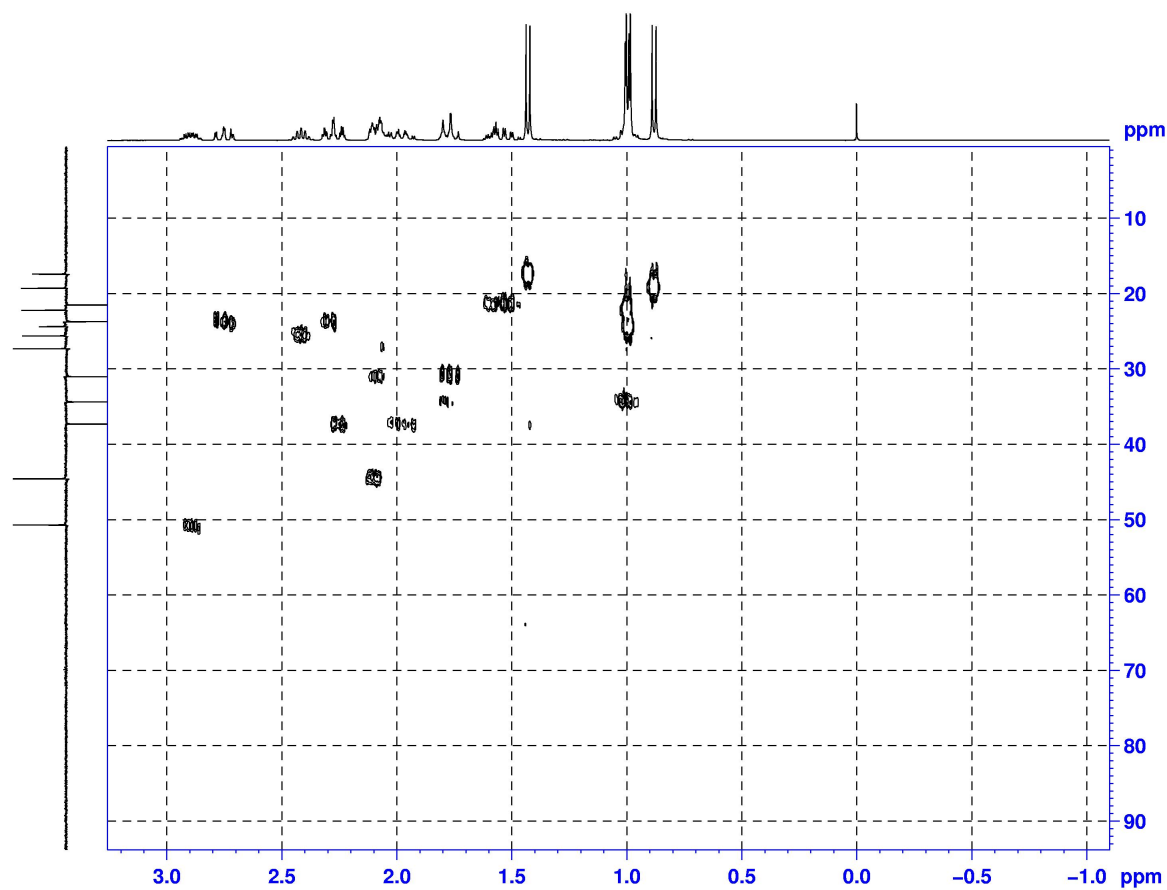


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```
Current Data Parameters
NAME          Sep22-2010
EXPNO        244
PROCNO       1

F2 - Acquisition Parameters
Date_        20100922
Time         19:07
INSTRUM      av400
PROBHD       5 mm PABBO BB-
PULPROG      hmcqcpqf
TD           2048
SOLVENT      CDCl3
NS           8
DS           16
SWH          2003.205 Hz
FIDRES       0.978127 Hz
AQ           0.5112308 sec
RG           20642.5
DW           249.600 us
DE           6.00 us
TE           298.2 K
CONST2       145.0000000
d0           0.00000300 sec
d1           0.70385861 sec
d2           0.00344828 sec
d12          0.00002000 sec
d13          0.00000400 sec
d16          0.00020030 sec
DELTA1       0.00222428 sec
IN0          0.0002615 sec

----- CHANNEL f1 -----
NUC1         1H
P1           14.25 us
p2           28.50 us
PL1          4.00 dB
SFO1         400.1303746 MHz

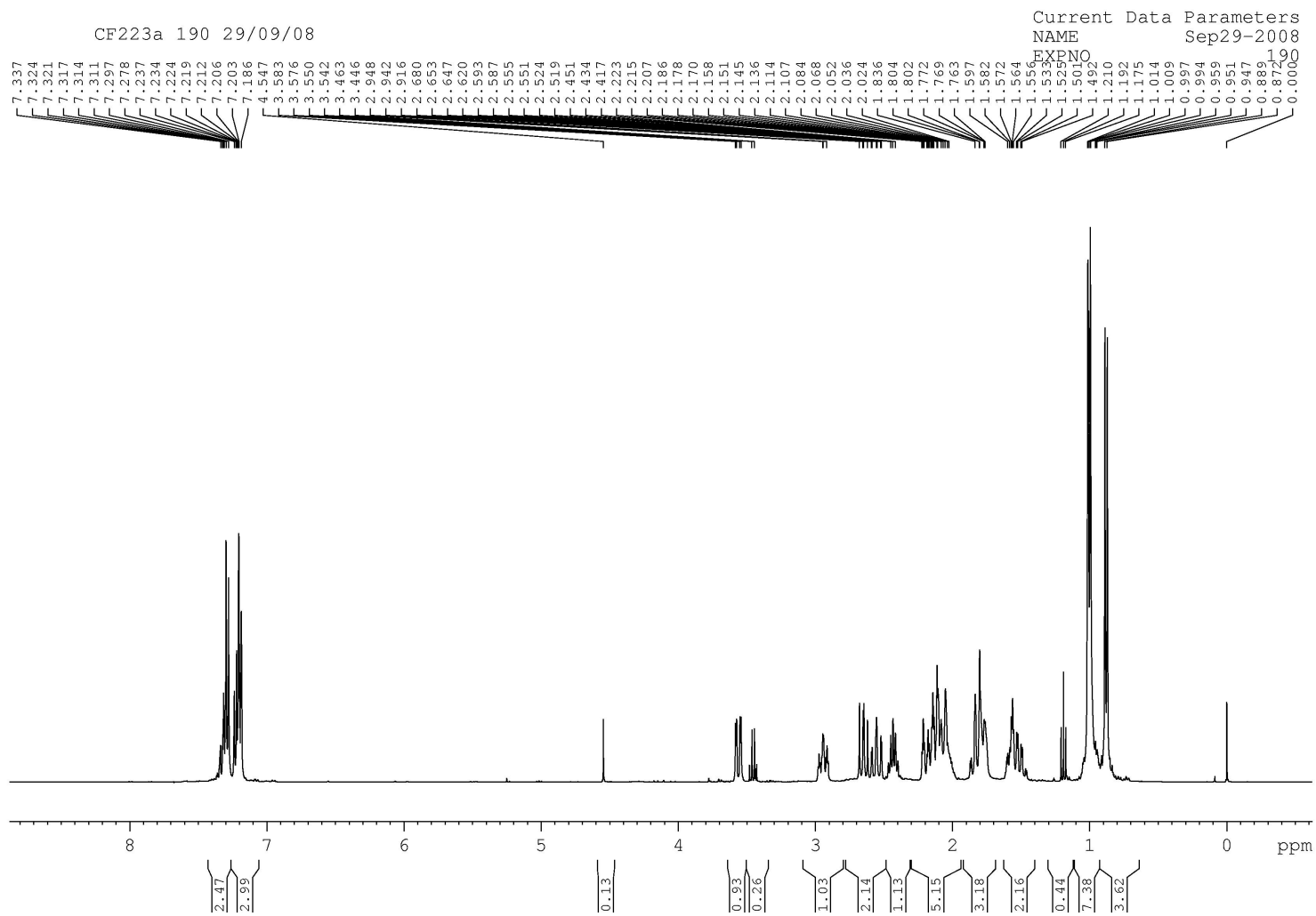
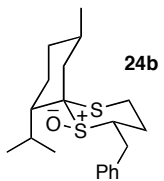
----- CHANNEL f2 -----
CPDPRG2      gntp
NUC2         13C
P3           9.75 us
PCPD2       70.00 us
PL2          8.00 dB
PL12        25.12 dB
SFO2         100.6218241 MHz

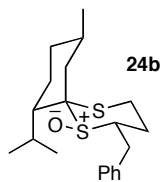
----- GRADIENT CHANNEL -----
GPNAM1       SINE.100
GPNAM2       SINE.100
GPNAM3       SINE.100
GPZ1         50.00 %
GPZ2         30.00 %
GPF3         40.10 %
P16          1000.00 us

F1 - Acquisition parameters:
ND0          2
TD           128
SFO1         100.6218 MHz
FIDRES       149.378586 Hz
SW           190.023 Hz
FmMODE       QF

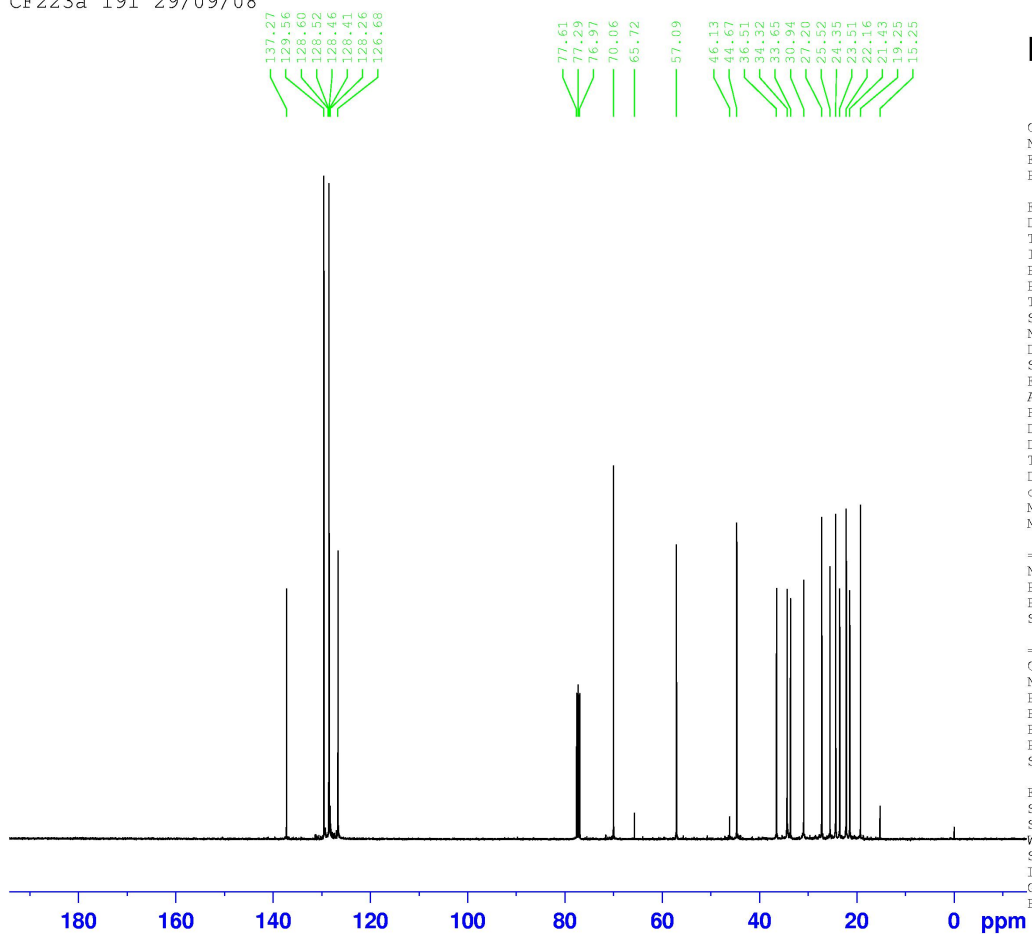
F2 - Processing parameters:
SI           4096
SF           400.1299993 MHz
WDW          QSINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.40

F1 - Processing parameters:
SI           1024
MC2          QF
SF           100.6127690 MHz
WDW          QSINE
SSB          0
LB           0.00 Hz
GB           0
```





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Current Data Parameters  
NAME Sep29-2008  
EXPNO 191  
PROCNO 1

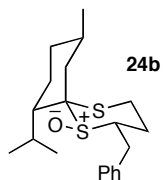
F2 - Acquisition Parameters  
Date\_ 20080929  
Time 22.38  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 2  
SWH 25252.525 Hz  
FIDRES 0.385323 Hz  
AQ 1.2976629 sec  
RG 9195.2  
DW 19.800 usec  
DE 6.00 usec  
TE 295.2 K  
D1 1.0000000 sec  
d11 0.0300000 sec  
MCREST 0.0000000 sec  
MCWRK 0.0150000 sec

==== CHANNEL f1 =====  
NUC1 13C  
P1 8.25 usec  
PL1 -2.00 dB  
SFO1 100.6232777 MHz

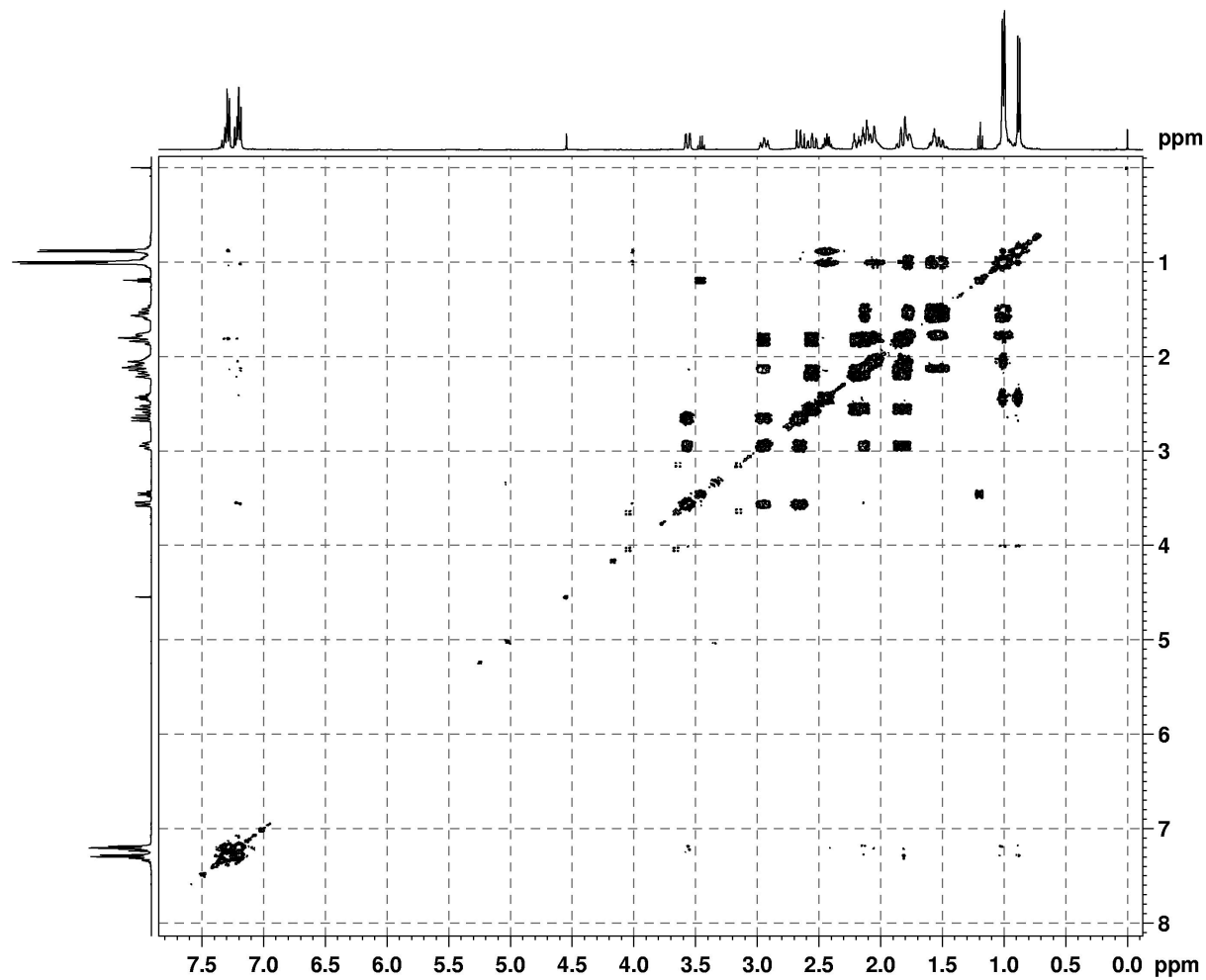
==== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -6.00 dB  
PL12 14.00 dB  
PL13 15.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
SI 131072  
SF 100.6127743 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





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Current Data Parameters  
NAME Sep29-2008  
EXPNO 193  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080929  
Time 23.20  
INSTRUM dpx400  
PROBHD 5 mm Dual 13C/  
PULPROG cosygmzgfg  
TD 2048  
SOLVENT CDCl3  
NS 1  
DS 16  
SWH 3306.878 Hz  
FIDRES 1.614687 Hz  
AQ 0.3097076 sec  
RG 406.4  
DW 151.200 usec  
DE 6.00 usec  
TE 294.2 K  
D0 0.0000300 sec  
D1 0.94715732 sec  
d13 0.0000400 sec  
D16 0.0002000 sec  
IN0 0.00030240 sec  
MCREST 0.0000000 sec  
MCWRK 0.94715732 sec

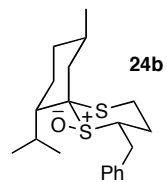
----- CHANNEL f1 -----  
NUC1 1H  
P1 11.75 usec  
PL1 -6.00 dB  
SFO1 400.1315823 MHz

----- GRADIENT CHANNEL -----  
GPNAM1 SINE.100  
GPNAM2 SINE.100  
GPNAM3 SINE.100  
GPX1 0.00 %  
GPX2 0.00 %  
GPX3 0.00 %  
GPY1 0.00 %  
GPY2 0.00 %  
GPY3 0.00 %  
GPZ1 16.00 %  
GPZ2 12.00 %  
GPZ3 40.00 %  
P16 1000.00 usec

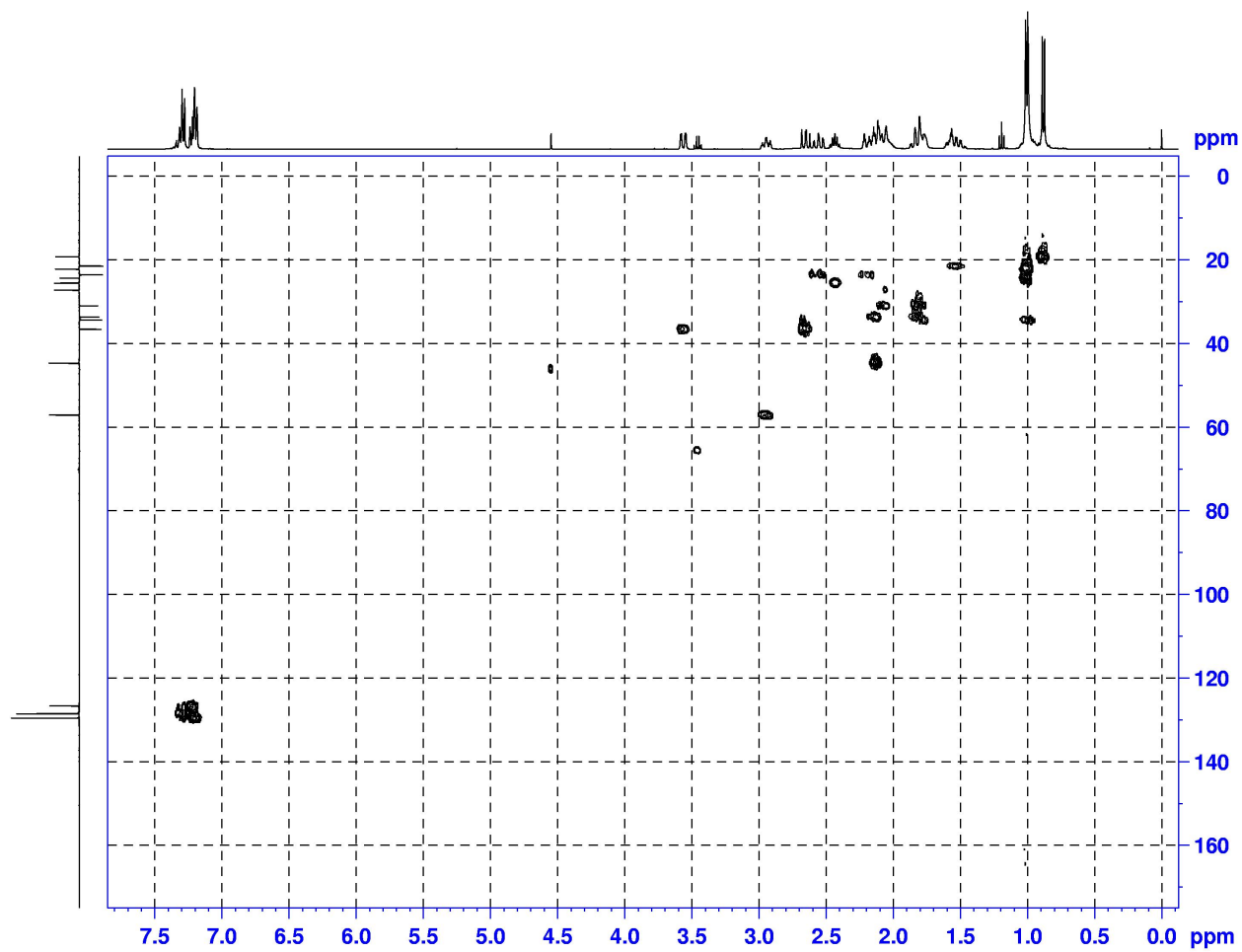
F1 - Acquisition parameters  
ND0 1  
TD 256  
SFO1 400.1316 MHz  
FIDRES 12.917494 Hz  
SW 8.264 ppm  
FrMODE QF

F2 - Processing parameters  
SI 4096  
SF 400.1299791 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 400.1299791 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0



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```
Current Data Parameters
NAME      Sep29-2008
EXPNO    194
PROCNO    1

F2 - Acquisition Parameters
Date_     20080929
Time      23.26
INSTRUM   qnx400
PROBHD    5 mm Dual 13c/
PULPROG   hmqcpgpgf
TD         2048
SOLVENT   cdcl3
NS         8
DS         16
SWH        3306.878 Hz
FIDRES     1.614687 Hz
AQ         0.3097076 sec
RG         7298.2
DW         151.200 usec
DE         6.00 usec
TE         294.2 K
CNS12     145.0000000
d0         0.0000000 sec
D1         0.94087678 sec
d2         0.00344828 sec
d12        0.0002000 sec
d13        0.0000400 sec
D16        0.00020000 sec
DELTA1    0.0022428 sec
TNO       0.00002761 sec
MCREST    0.0000000 sec
MCWRK     0.94087678 sec

===== CHANNEL f1 =====
NUC1      1H
P1        11.75 usec
P2        23.50 usec
PL1       -6.00 dB
SFO1      400.1315823 MHz

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      13C
P3        8.25 usec
PCPD2     70.00 usec
PL2       -2.00 dB
PL12      15.00 dB
SFO2      100.6213211 MHz

===== GRADIENT CHANNEL =====
GPNAM1    SINE.100
GPNAM2    SINE.100
GPNAM3    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      40.10 %
P16       1000.00 usec

F1 - Acquisition parameters
ND0        2
TD         128
SFO1       100.6213 MHz
FIDRES     141.466721 Hz
SW         179.959 ppm
FhMODE     QF

F2 - Processing parameters
SI         4096
SF         400.1299791 MHz
WDW        QSINE
SSB        0
LB         0.00 Hz
GB         0
PC         1.40

F1 - Processing parameters
SI         1024
MC2        QF
SF         100.6127690 MHz
WDW        QSINE
SSB        0
LB         0.00 Hz
GB         0
```