

Highly Regioselective Nitrile Oxide Dipolar Cycloadditions with *ortho*-Nitrophenyl Alkynes

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and Rich G. Carter*

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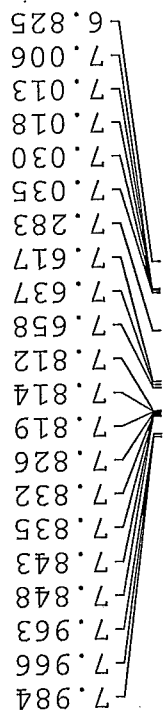
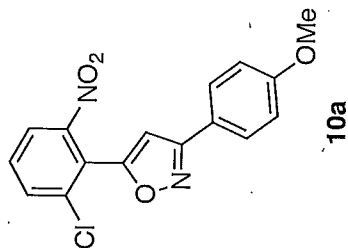
Electronic Supplementary Information: NMR Spectra

Highly Regioselective Nitrile Oxide Dipolar Cycloadditions with *ortho*-Nitrophenyl Alkynes

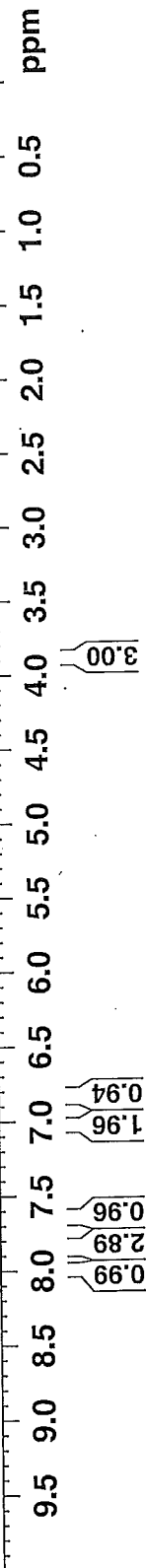
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Compound #	Page Number
10a	S3
11	S5
13a	S7
13b	S9
13c	S11
13d	S13
13e	S15
13f	S17
13g	S19
13h	S21
13i	S23
13j	S25
15b	S27
17a	S29
17b	S31
17c	S33
18	S35
19	S37
22	S39
23	S41
24	S43
25	S45

NAME Isoxazole1C1R2HAR40K
EXPNO 3
PROCNO 1
Date_ 20120502
Time 17.38
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 18
DS 2
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 sec
RG 181
DE 69.600 usec
TE 6.50 usec
D1 298.2 K
D0 2.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL1 0.00 dB
SF01 400.1428010 MHz
SI 32768
SF 400.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



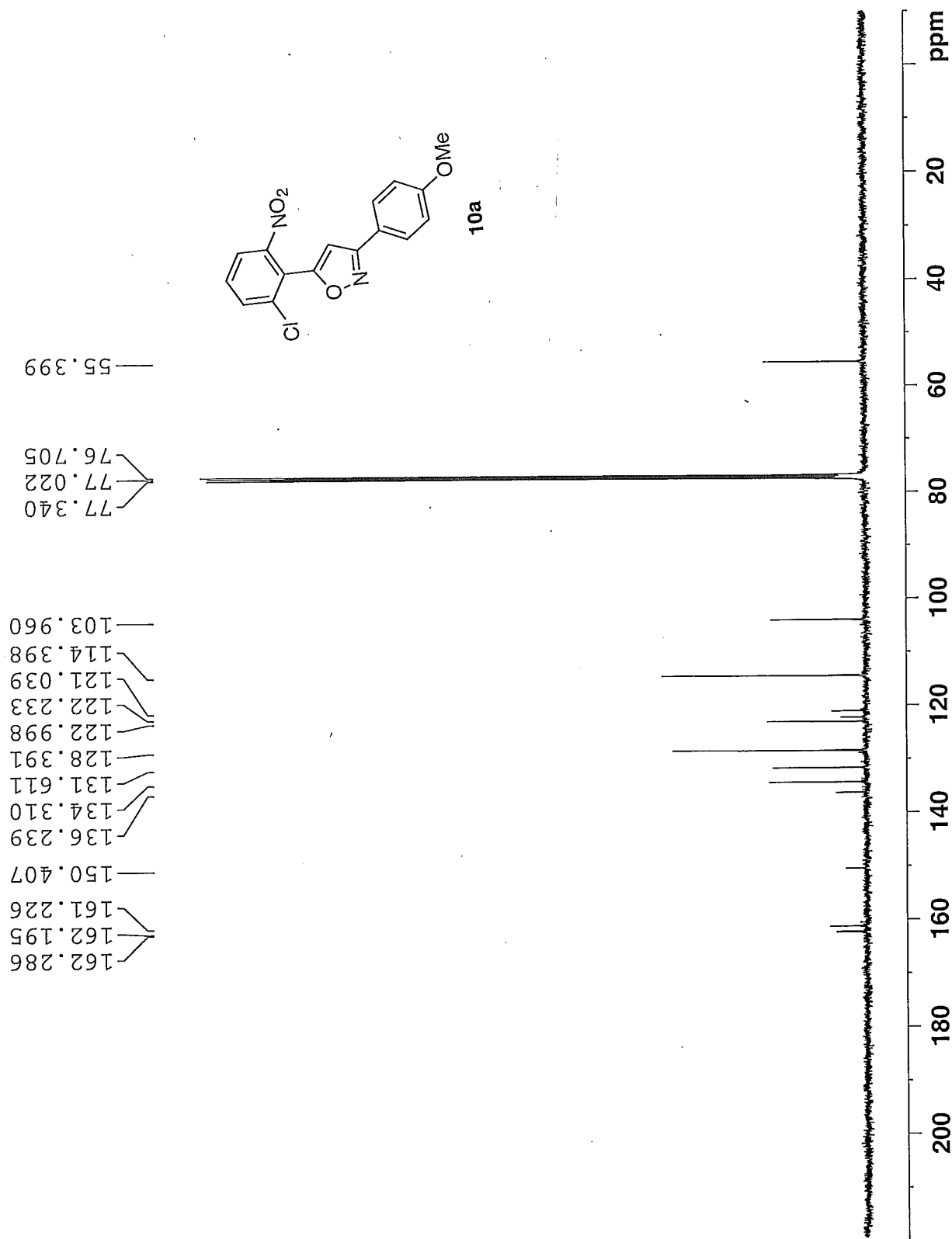
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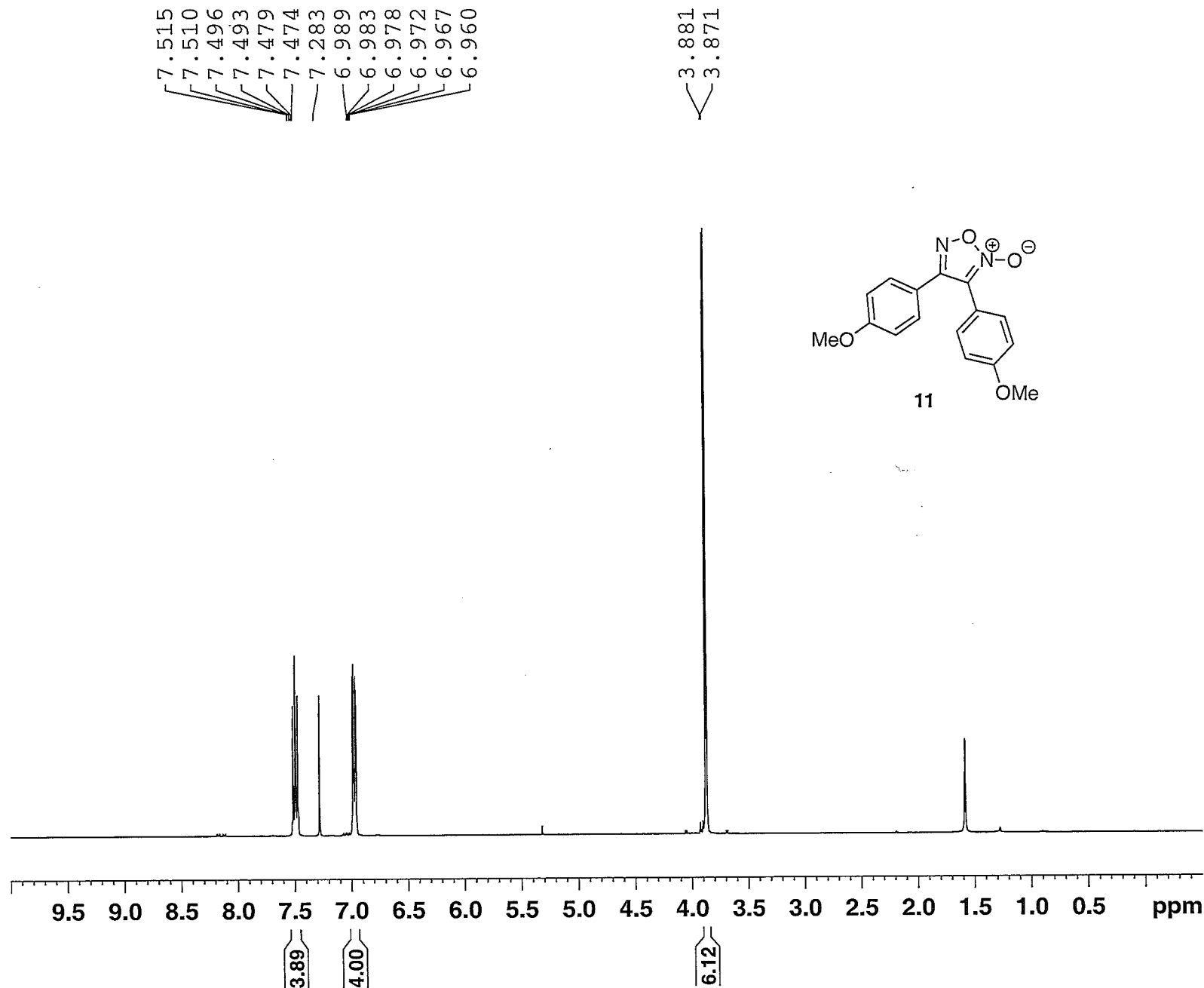


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PROCNO 1
Date_ 20120502
Time 17.42
INSTRUM robinson
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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 724
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
SFO1 100.6253446 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.16 dB
PL13 17.00 dB
SFO2 400.1416006 MHz
SI 32768
SF 100.6152830 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40





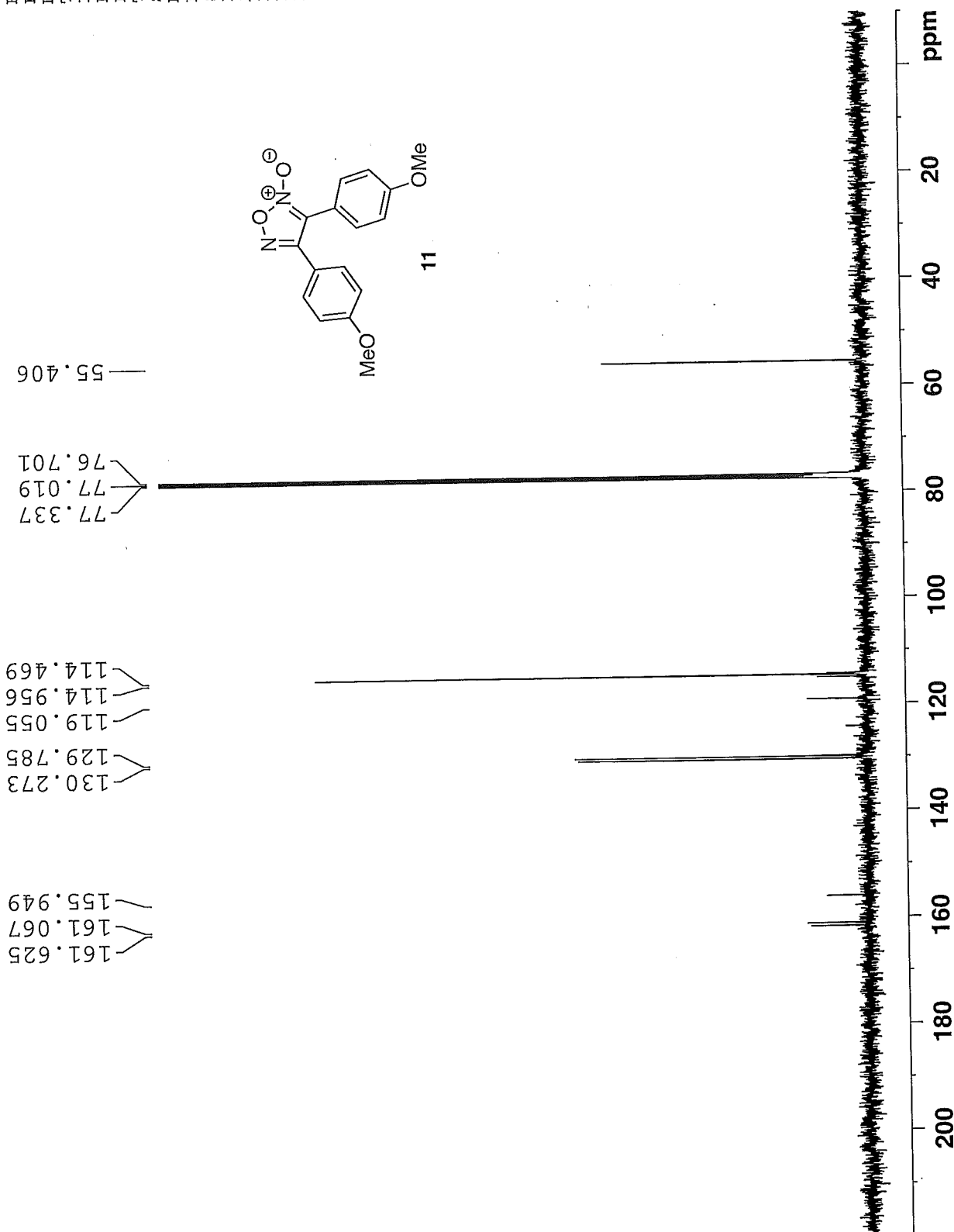
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EXPNO         5
PROCNO        1
Date_         20120906
Time          18.44
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PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            6
DS            0
SWH           7183.908 H.
FIDRES        0.219235 H.
AQ            2.2807028 s.
RG            161.3
DW            69.600 u.
DE            6.50 u.
TE            298.2 K
D1            2.00000000 s.
TD0           1
  
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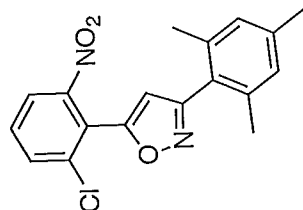
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===== CHANNEL f1 =====
NUC1          1H
P1            14.00 u.
PL1           0.00 d.
SFO1          400.1428010 M
SI            32768
SF            400.1400000 M
WDW           EM
SSB           0
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GB            0
PC            1.00
  
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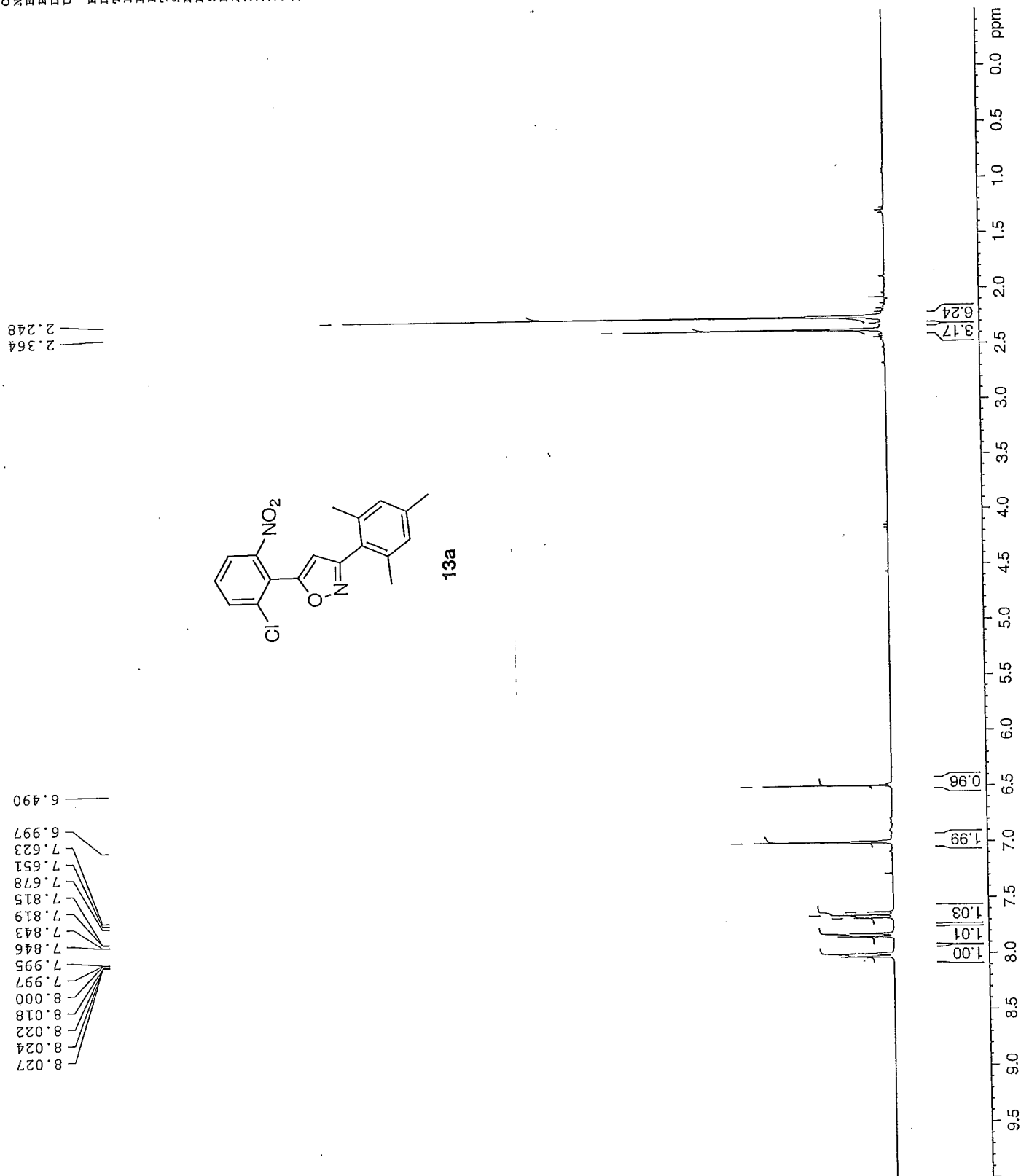
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TD 65536
SOLVENT CDCl3
NS 562
DS 0
SWH 23980.814 H
FIDRES 0.365918 H
AQ 1.3664756 s
RG 32768
DW 20.850 u
DE 6.50 u
TE 298.9 K
D1 1.00000000 s
D11 0.03000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 u
PL1 -2.00 d
SFO1 100.6253446 M
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PL2 0.00 d
PL12 16.16 d
PL13 17.00 d
SFO2 400.1416006 M
SI 32768
SF 100.6152830 M
WDW EM
SSB 0
LB 3.00 H
GB 0
PC 1.40



Year	Number of employees (thousands)
1997	6,500
1998	7,000
1999	6,900
2000	7,100
2001	7,200
2002	7,300
2003	7,400
2004	7,500
2005	7,600
2006	7,700
2007	8,000



13a



prep

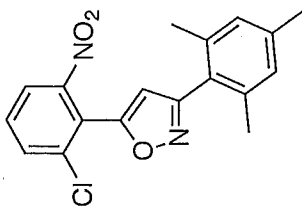
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EXPNO 13
PROCNO 1
DU /n
USER michaeln

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Time_ 10.47
INSTRUM DPX300
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 5
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 9195.2
DW 26.550 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.80 usec
PL1 -3.00 dB
SFO1 75.4760505 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.55 dB
PL13 17.55 dB
SFO2 300.1312005 MHz

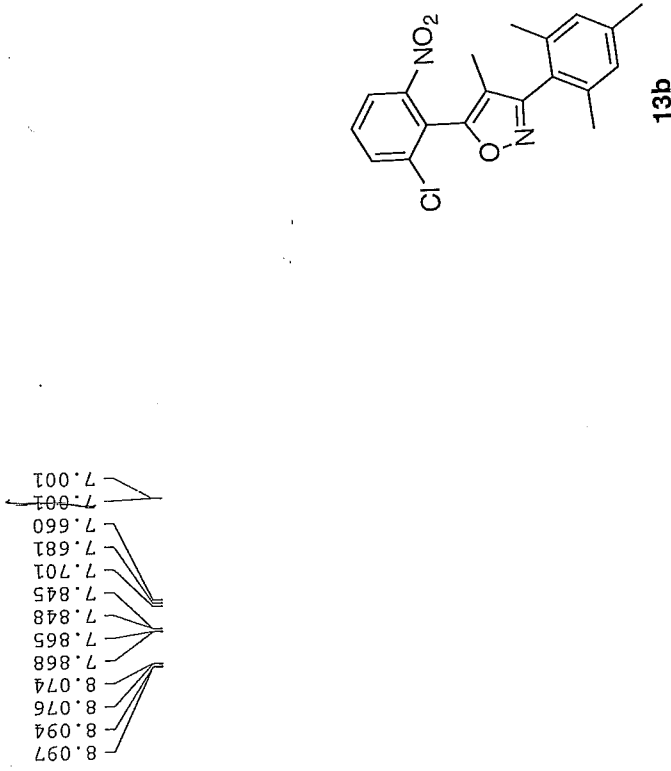
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LB 3.00 Hz
GB 0
PC 1.40



13a

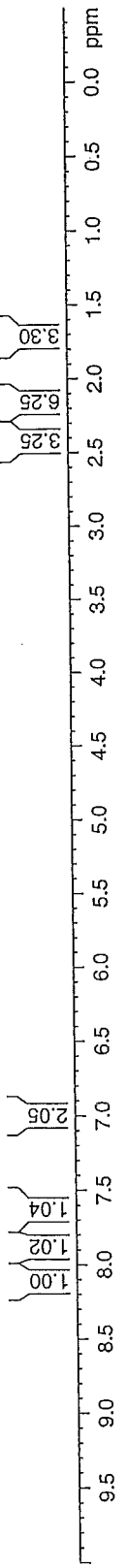


oxazole



8.097
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8.076
8.074
7.868
7.865
7.848
7.845
7.701
7.681
7.660
7.001
7.001

2.368
2.179
1.750



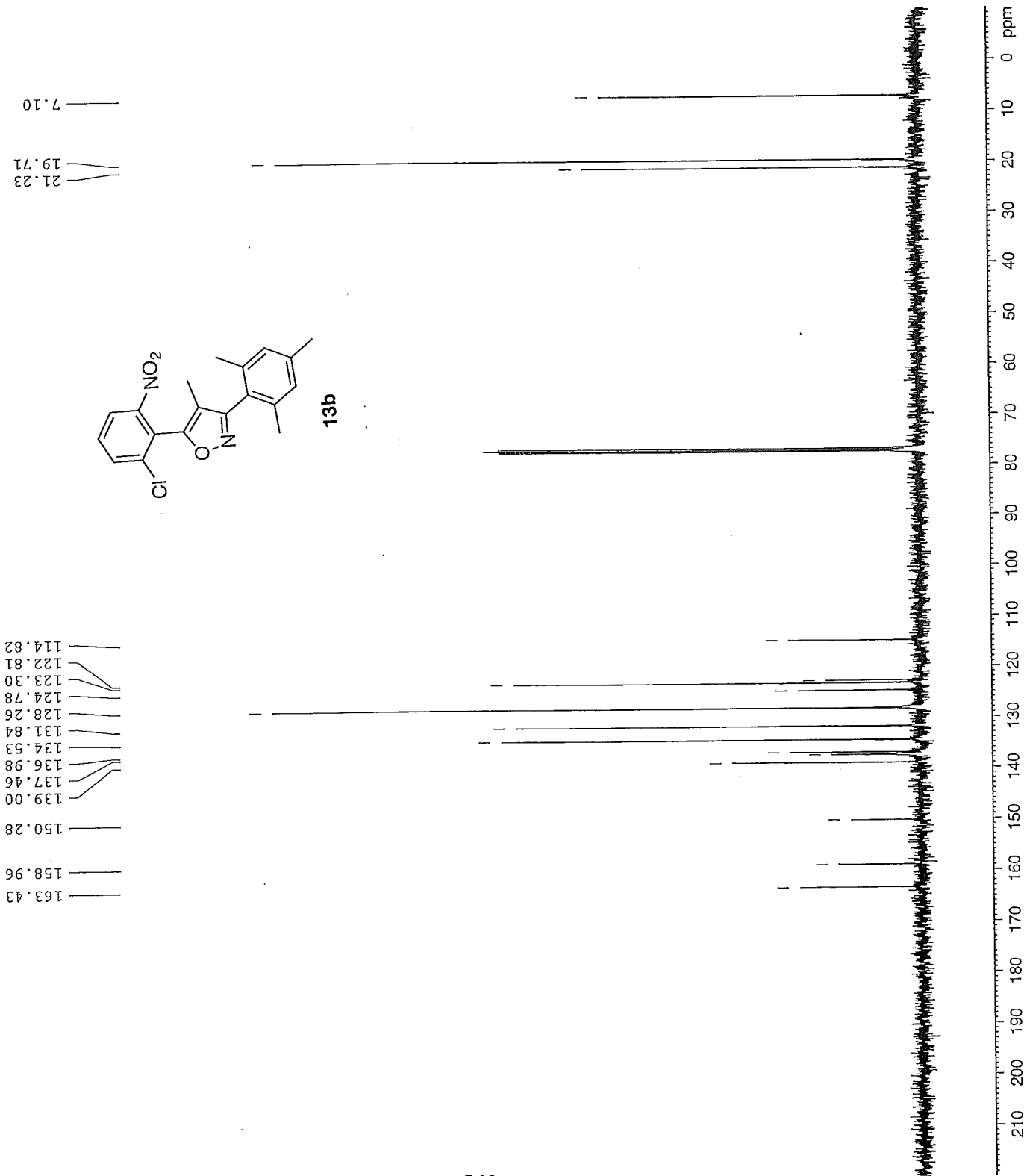
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PROCNO 1
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PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT
NS 6
DS 2
SWH 6410.256 Hz
FIDRES 0.195425 Hz
AQ 2.555940 sec
RG 128
DW 78.000 usec
DE 6.00 usec
TE 299.2 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
SF01 399.9528000 MHz

F2 - Processing parameters
SI 32768
SF 399.9500000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

oxazole



Current Data Parameters

NAME u
EXPNO 22
PROCNO 1
DU /m
USER michaeln

F2 - Acquisition Parameters

Date_ 20090720
Time 13.52
INSTRUM DFX400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT
NS 296
DS 4
SWH 25125.629 Hz
FIDRES 0.138387 Hz
AQ 1.3042164 sec
RG 5160.6
DW 19.900 usec
DE 6.00 usec
TE 299.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TDO 1

===== CHANNEL f1 =====

NUC1 13C
P1 7.80 usec
PL1 -3.00 dB
SFO1 100.5785700 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 135.00 usec
PL2 17.40 dB
PL12 17.40 dB
PL13 17.40 dB
SFO2 399.9516000 MHz

F2 - Processing parameters

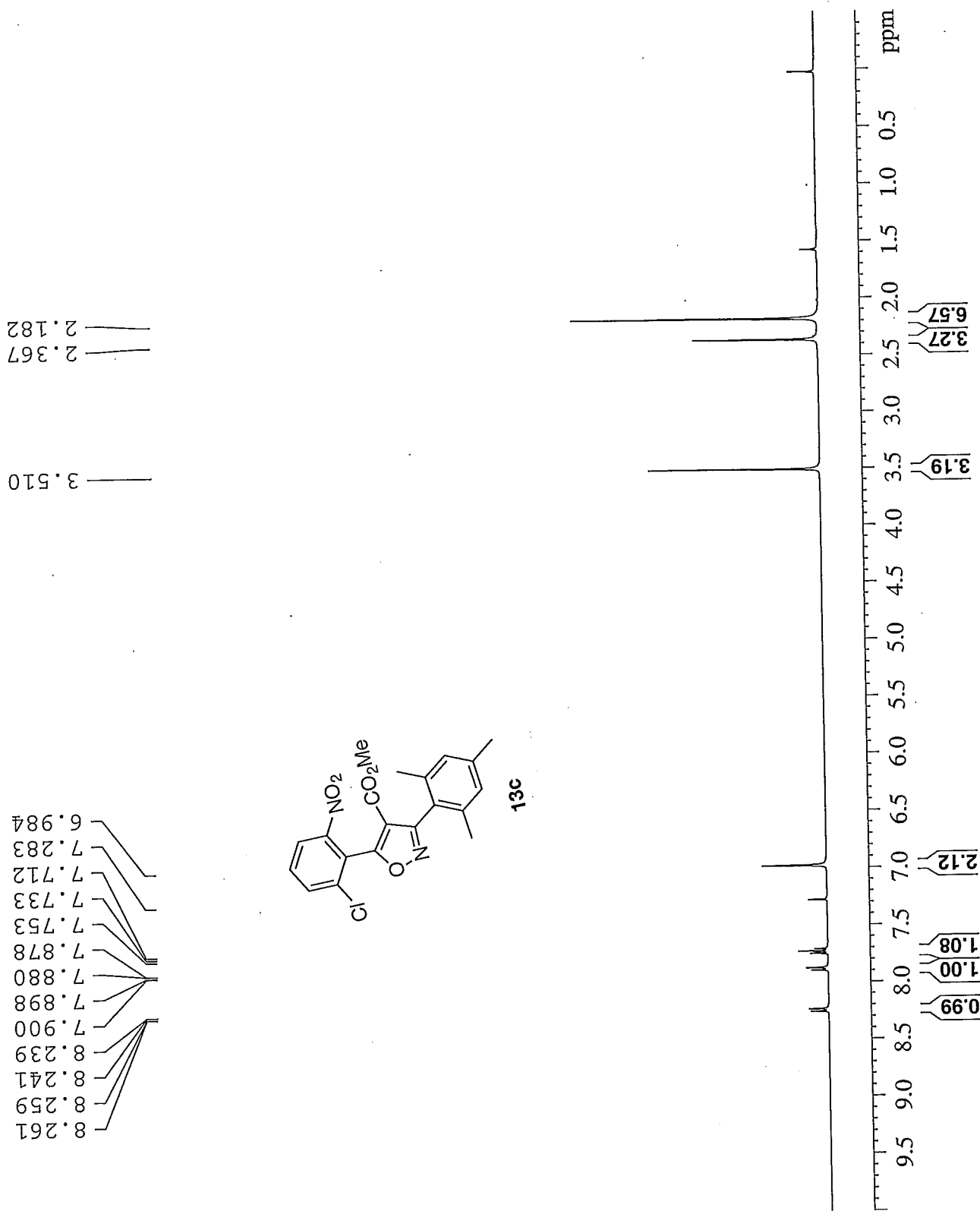
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LB 3.00 Hz
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Current Data Parameters
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EXPNO 4
PROCNO 1

F2 - Acquisition Parameters:
Date_ 20100712
Time 10.13
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6793.478 Hz
FIDRES 0.207320 Hz
AQ 2.4117749 sec
RG 128
DM 73.600 us
DE 6.50 us
TE 298.7 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.00 us
PL1 0.00 dB
SFO1 400.1424008 MHz

F2 - Processing parameters
SI 65536
SF 400.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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Current Data Parameters
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EXPNO     5
PROCNO    1

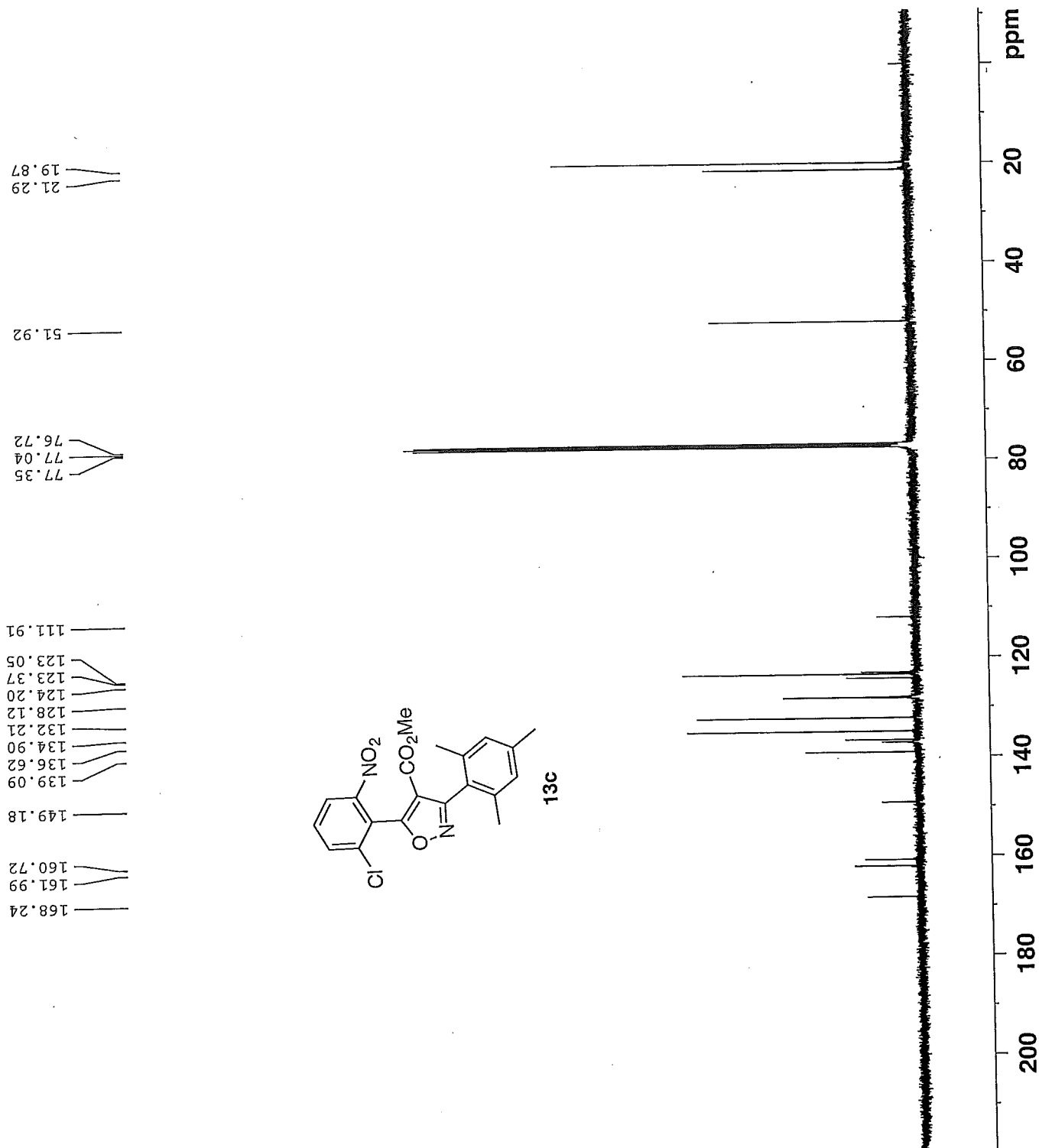
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Time      13.19
INSTRUM   DPX400
PROBHD    5 mm BBO BB-1H
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         3000
DS         4
SWH        23980.814 Hz
FIDRES     0.365918 Hz
AQ         1.3664756 sec
RG         18390.4
DE         20.850 usec
TE         299.2 K
D1         0.20000000 sec
d11        0.03000000 sec
DELTA      0.10000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         8.30 usec
PL1        -3.00 dB
SFO1       100.6517495 MHz

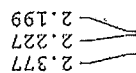
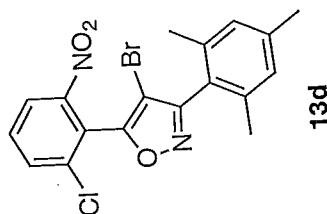
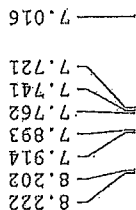
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      90.00 usec
PL2        -3.00 dB
PL12       15.00 dB
PL13       15.00 dB
SFO2       400.2466010 MHz

F2 - Processing parameters
SI         65536
SF         100.6416850 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```



chloro bromo mesityl oxazole

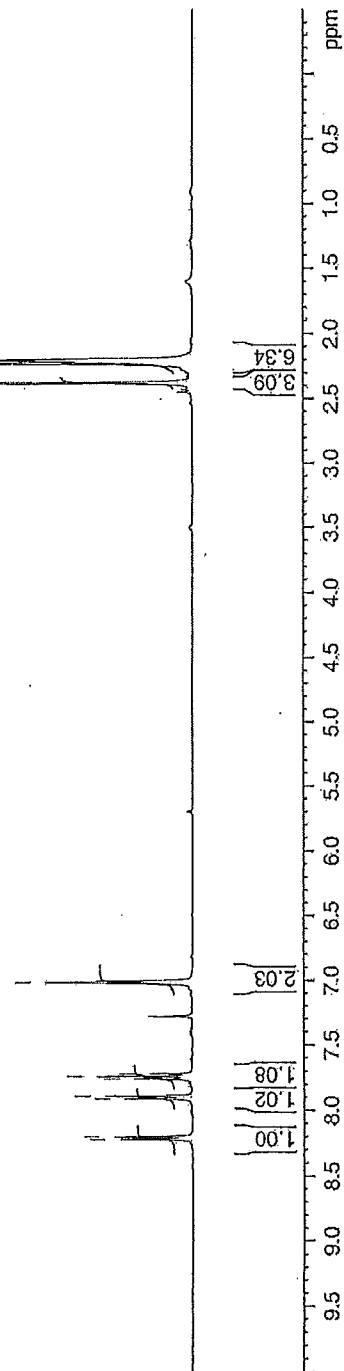


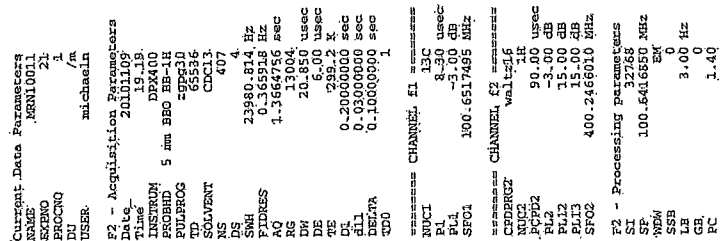
Current Data Parameters
NAME MEN10011
EXPNO 20
PROCNO 1
DT /m
USER michaeln

F2 - Acquisition Parameters
Date_ 20101109
Time_ 19.16
INSTRUM DEK400
PROBHD 5 mm BBO BB-4H
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 10
DS 2
SWH 6410.256 Hz
FIDRES 0.185623 Hz
AQ 2.5559540 sec
RG 322.5
DM 78.000 usec
DE 6.00 usec
TE 298.2 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.50 usec
PL -3.00 dB
SFO1 400.2478017 MHz

F2 - Processing parameters
SI 32768
SF 400.2450000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



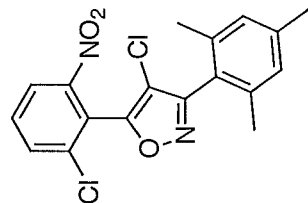


NAME MRN10010
EXPNO 1
PROCNO 1
Date_ 20101107
Time 23.09
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDC13
NS 15
DS 2
SWE 6793.478 Hz
FIDRES 0.207320 Hz
AQ 2.4117749 sec
RG 90.5
DW 73.600 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
TD0 1

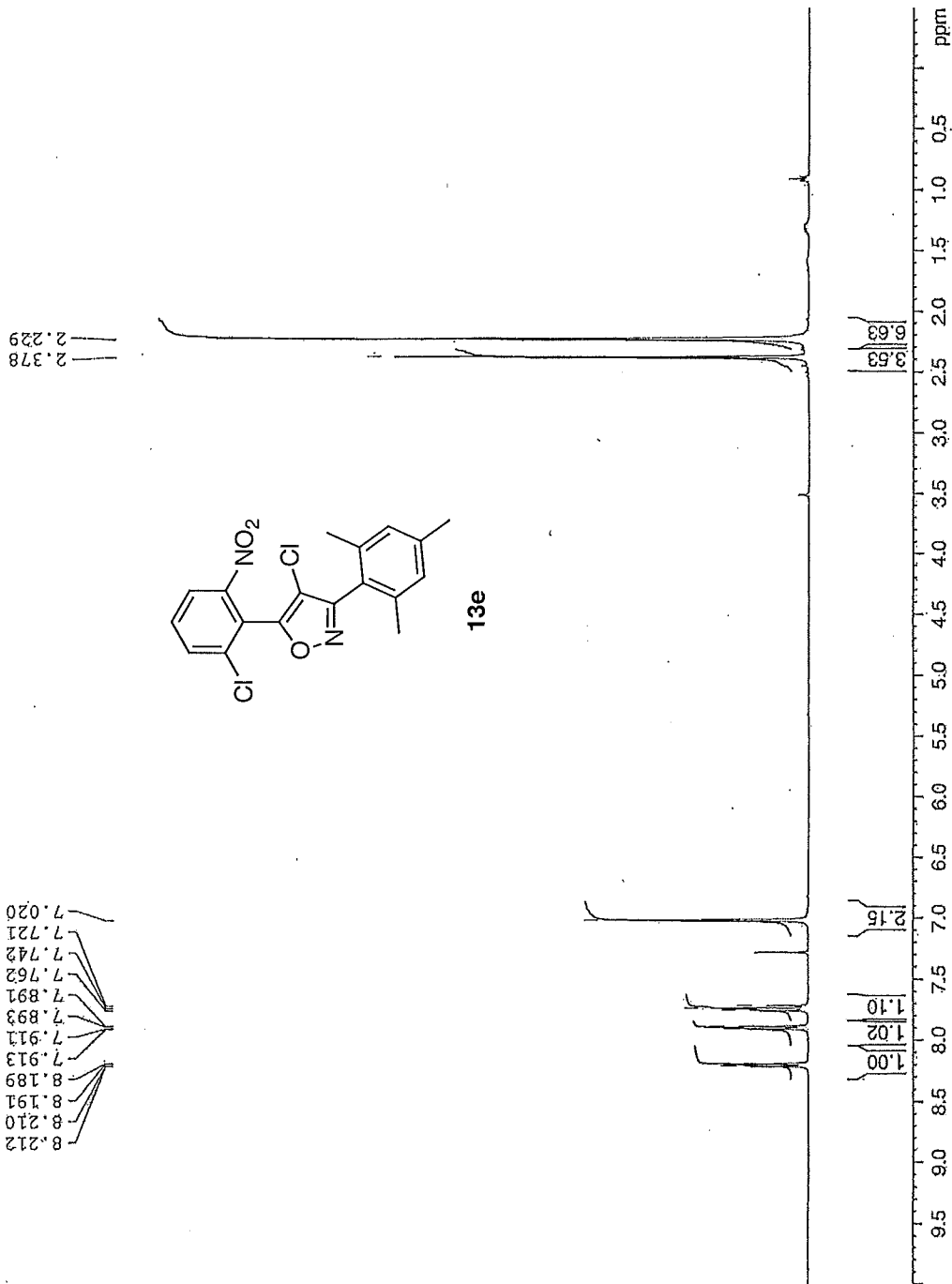
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 usec
PL 0.00 dB
SF01 400.1424008 MHz
SI 32768
SF 400.1400000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

bis chloro oxazole

7.020
7.721
7.742
7.762
7.891
7.893
7.911
7.913
8.189
8.191
8.210
8.212



13e

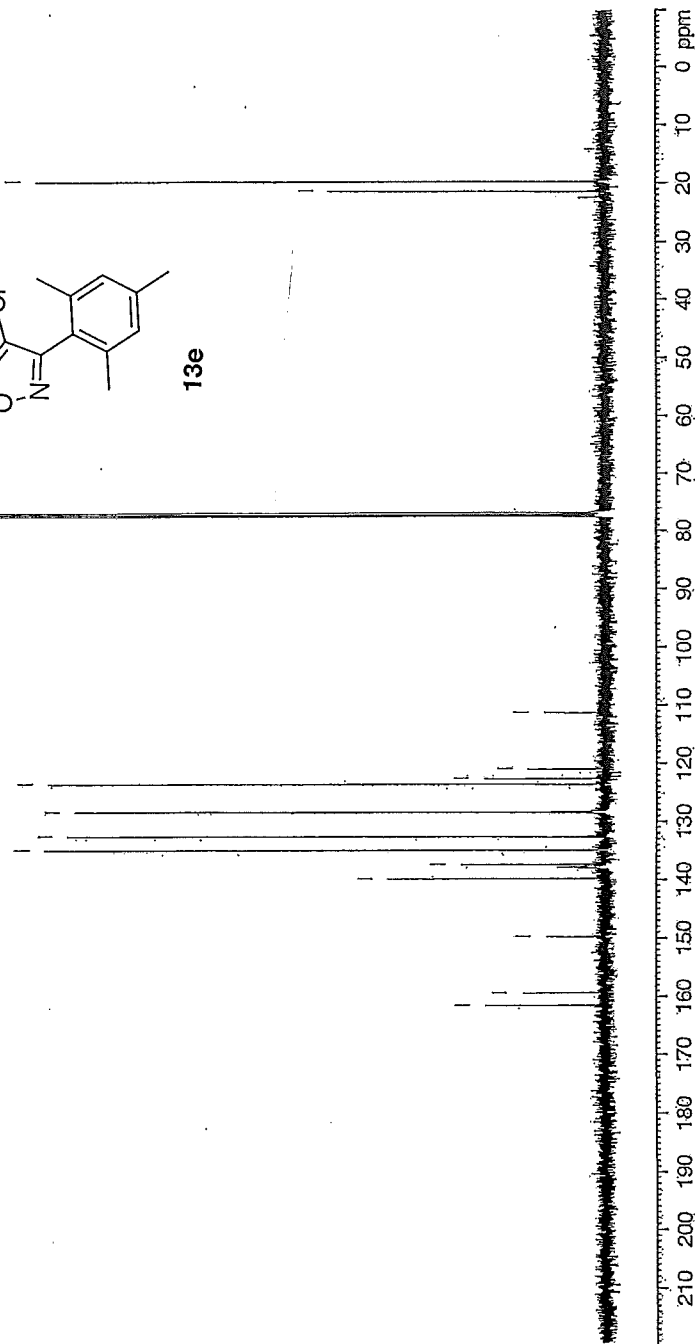
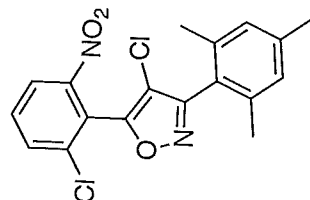


bis chloro oxazole

NAME MRN10010
EXPNO 2
PROCNO 1
Date_ 20101107
Time 23.13
INSTRUM robinson
PROBHD 5 mm PABBO-
PULPROG zgpg30
TD 65536
SOLVENT CCl₄
NS 1584
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.366756 sec
RG 14396.5
DW 20.850 usec
DE 6.50 usec
TE 301.3 K
D1 0.20000000 sec
D11 0.03000000 sec
TD0 1
===== CHANNEL F1 =====
NUC1 ¹³C
P1 9.00 usec
PL1 -2.00 dB
SFO1 100.6259446 MHz
===== CHANNEL F2 =====
CPDPRG2 waltz16
NUC2 ¹H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.16 dB
PL13 17.00 dB
SFO2 400.1416006 MHz
SI 32768
SF 100.6152830 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

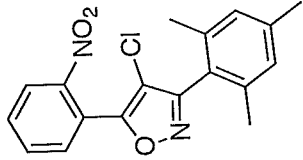
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149.7
139.8
137.9
137.4
134.9
132.6
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123.6
122.6
120.9
111.2



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2.215

8.207
8.187
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7.821
7.760
7.281
7.012



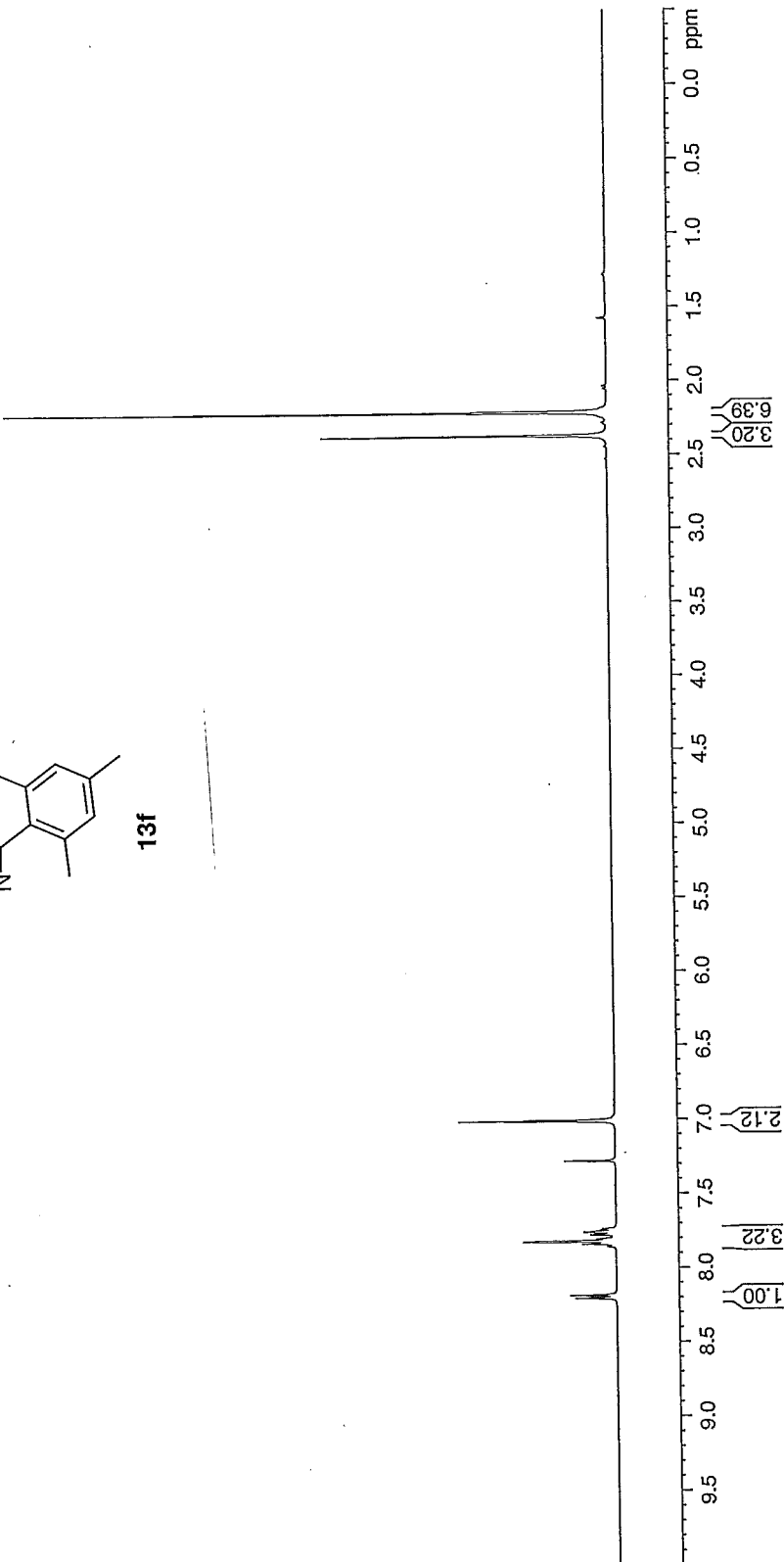
13f

Current Data Parameters
NAME MLM-I-020
EXPNO 6
PROCNO 1
DU /m
USER melissa

F2 - Acquisition Parameters
Date_ 20100828
Time 12.06
INSTRUM DEX400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5539540 sec
RG 406.4
RW 78.000 usec
DE 6.00 usec
TE 298.2 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.50 usec
PL 3.00 dB
SFO1 400.2478017 MHz

F2 - Processing parameters
SI 65536
SF 400.2450000 MHz
WDW no
SSB 0
LB 0
GB 0
PC 1.00

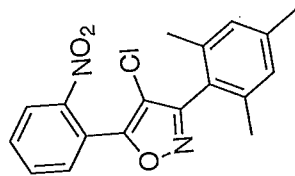


Current Data Parameters
NAME MMN-I-020
EXPNO 7
PROCNO 1
DT /m
DI melissa
F2 - Acquisition Parameters
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Time 12.14
INSTRUM DPX400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3820
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3684756 sec
RG 14596.5
RG 20.850 usec
DE 6.00 usec
TE 299.2 K
D1 0.20000000 sec
d11 0.03000000 sec
DELTA 0.10000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 8.30 usec
PL1 -3.00 dB
SFO1 100.6517495 MHz
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.2466010 MHz
F2 - Processing parameters
SI 65536
SF 100.6416850 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

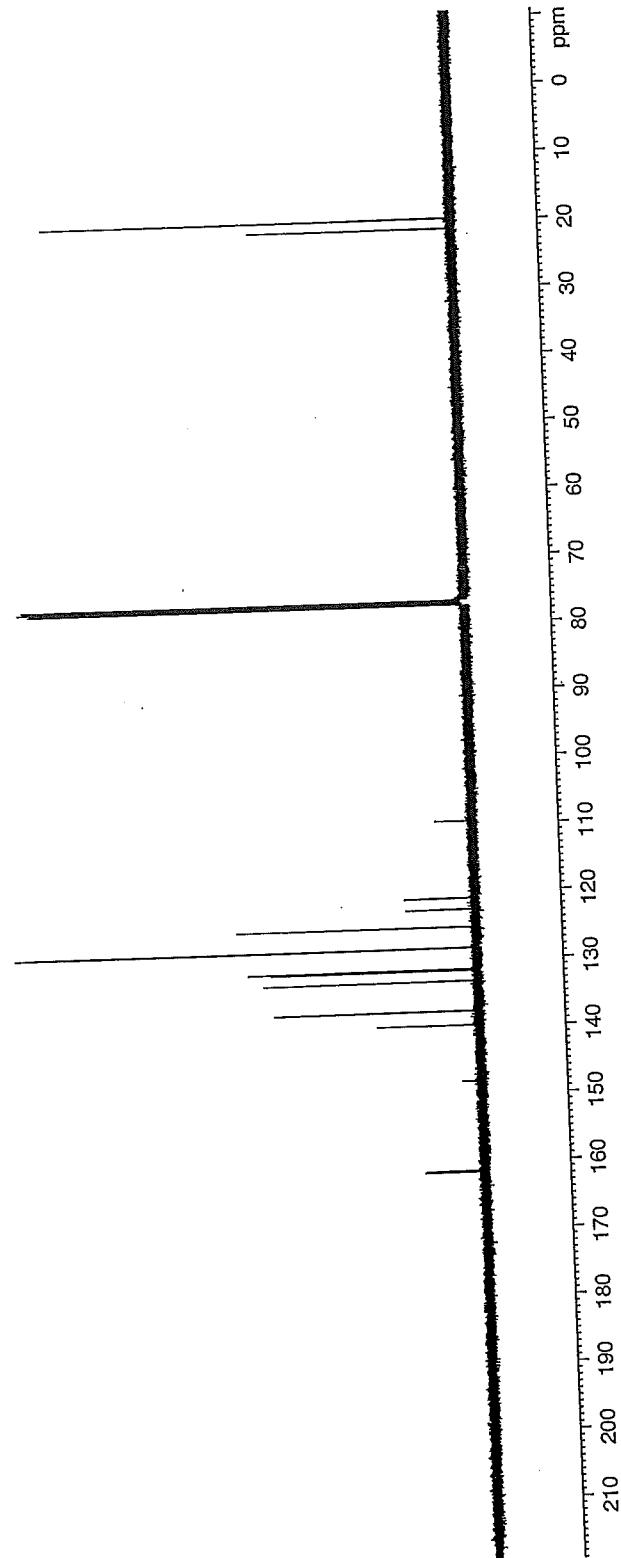
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77.23
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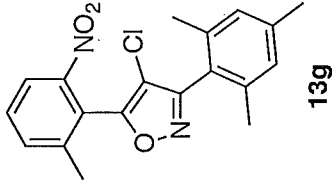
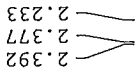
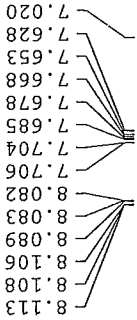
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131.76
131.59
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125.30
122.71
121.05
109.63



13f



insoluble wht solid



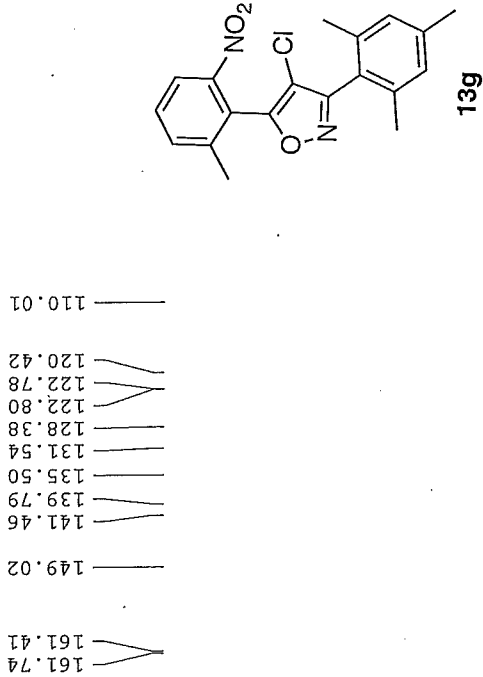
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NAME MRN9035
EXPNO 22
PROCNO 1
DU /n
USER michaeln

F2 - Acquisition Parameters
Date_ 20090311
Time 13.24
INSTRUM DFX300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 203.2
DW 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL -3.00 dB
PL1 300.1321009 MHz
SF01 300.1321009 MHz

F2 - Processing parameters
SI 32768
SF 300.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

insoluable wht solid



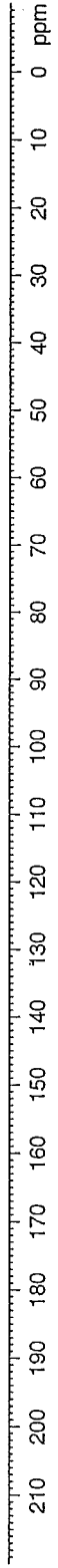
Current Data Parameters
NAME MN9095
EXPNO 23
PROCNO 1
DO /n
USER michaeln

F2 - Acquisition Parameters
Date_ 20090311
Time 13.29
INSTRUM DFX300
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 475
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 812.7
DM 26.550 usec
DE 6.00 usec
TE 298.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 8.80 usec
PL1 -3.00 dB
SFO1 75.4760505 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.55 dB
PL13 17.55 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



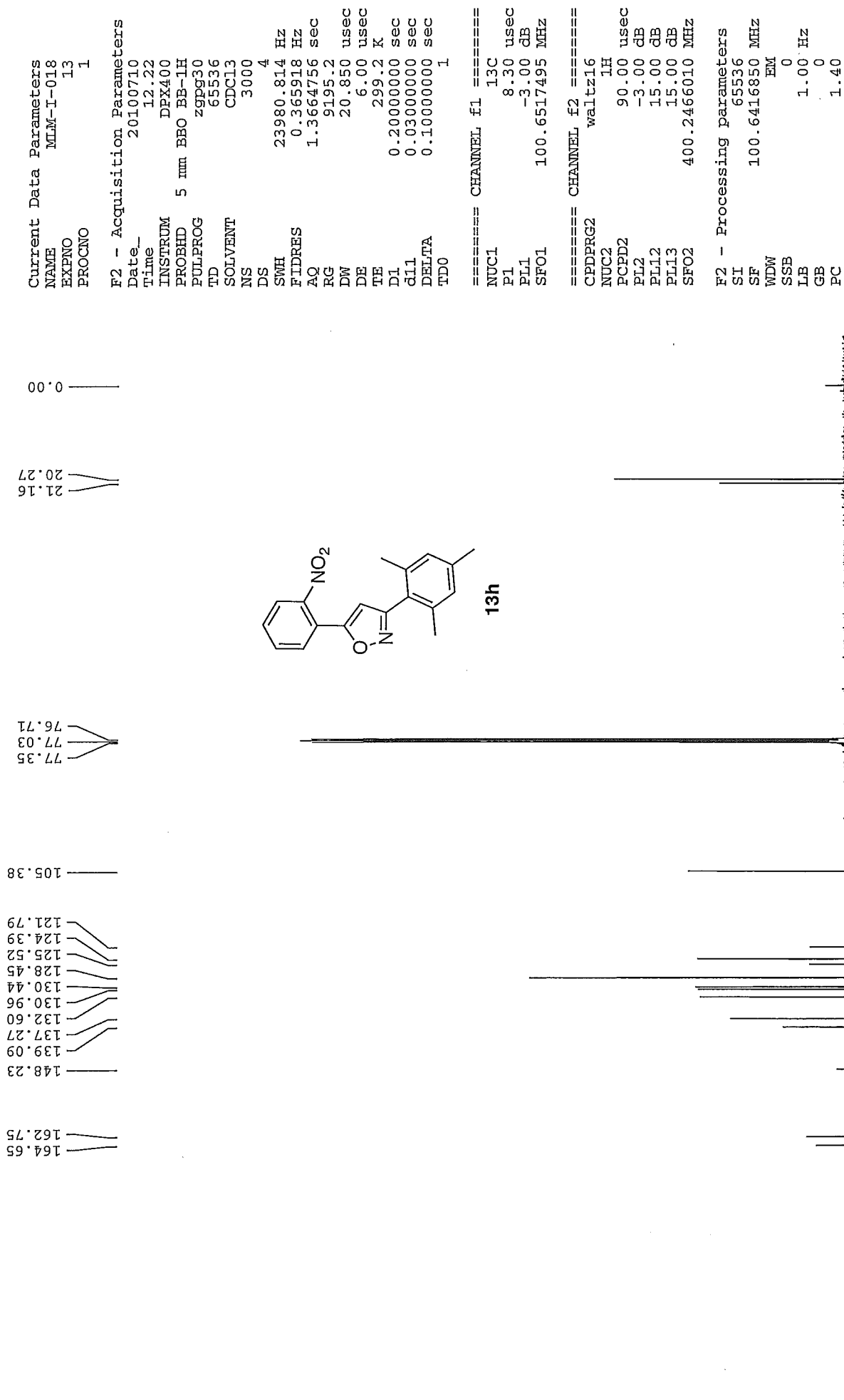
Current Data Parameters
NAME MLM-I-018
EXPNO 8
PROCNO 1

F2 - Acquisition Parameter:
Date_ 20100708
Time 12.36
INSTRUM DPX400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 27
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 812.7
DW 78.000 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

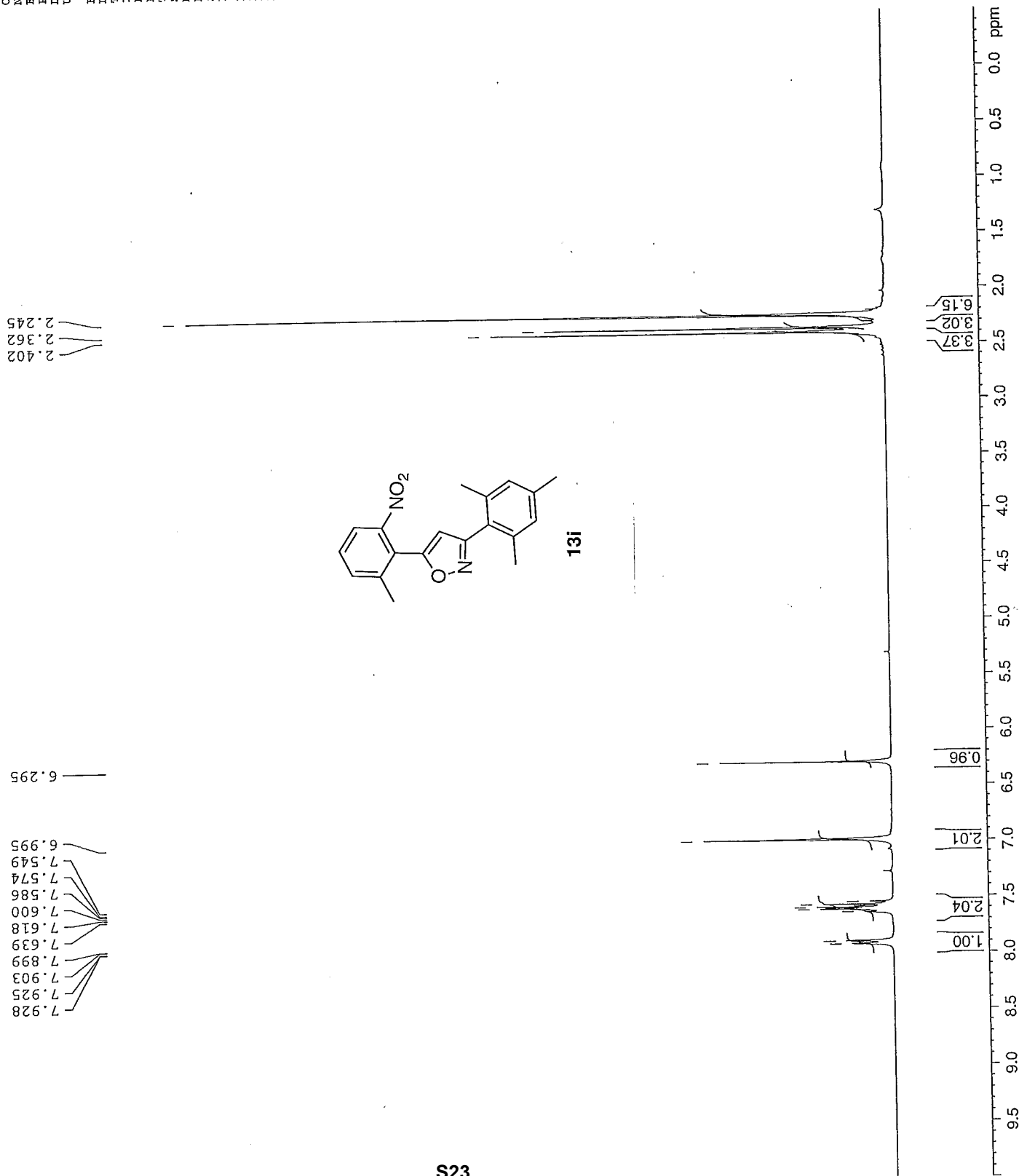
===== CHANNEL f1 =====
NUC1 1H
P1 13.50 usec
PL1 -3.00 dB
SFO1 400.2478017 MHz

F2 - Processing parameters
SI 65536
SF 400.2450000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





Current Data Parameters
NAME MEN10014
EXNO 10
PROCNO 1
DU /h
USER michaeln
F2 - Acquisition Parameters
Date_ 20090429
Time 10.11
INSTRUM DPX300
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 64
DW 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 2.0000000 sec
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 9.00 usec
PL1 -3.00 dB
SFO1 300.1321009 MHz
F2 - Processing Parameters
SI 32768
SF 300.1300000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters
NAME KEN10014
EXPNO 12
PROCNO 1
DU /h
USER michaeln

F2 - Acquisition Parameters
Date_ 20090429
Time 10.26
INSTRUM DEX300
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 186
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 645.1
DM 26.550 usec
DE 6.00 usec
TE 298.2 K
TD0 1
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

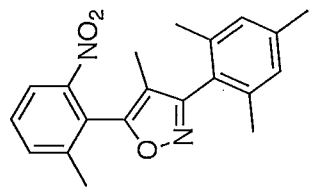
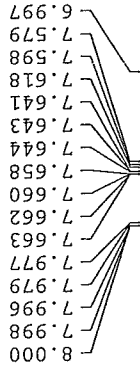
===== CHANNEL f1 =====
NUC1 13C
P1 8.80 usec
PL1 -3.00 dB
SFO1 75.4760505 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 17.55 dB
PL13 17.55 dB
SFO2 300.1312005 MHz

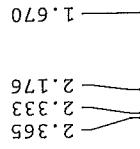
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
TM 0
WDW 0
SSB 3.00 Hz
LB 0
GB 0
PC 1.40



bismethyloxazole



13j



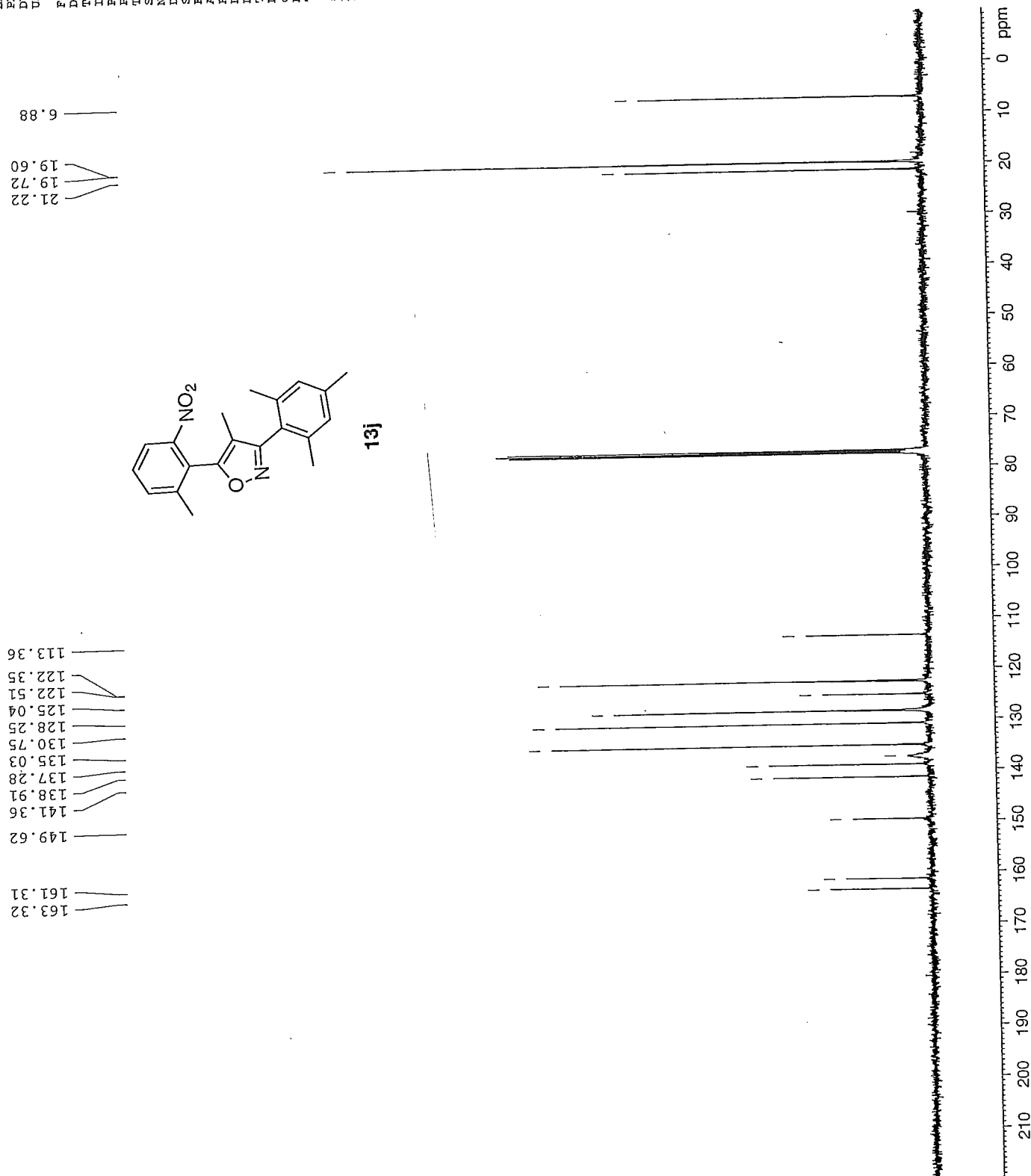
Current Data Parameters
NAME MXN10049
EXPNO 30
PROCNO 1
DU /m
USER michaeln

F2 - Acquisition Parameters
Date_ 20090721
Time 12.31
INSTRUM DFX400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT
NS 12
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 114
DW 78.000 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.70 usec
PL 0.00 dB
SFO1 399.9528000 MHz

F2 - Processing parameters
SI 32768
SF 399.9500000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

bismethyloxazole



Current Data Parameters
NAME MEN10049
EXPNO 31
PROCNO 1
DU /m
USER michaeln

F2 - Acquisition Parameters
Date_ 20090721
Time 12.35
INSTRUM DFX400
PROBHD 5 mm BBO BB-IH
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1112
DS 4
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 16384
DM 19.900 usec
DE 6.00 usec
TE 299.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 7.80 usec
PL1 -3.00 dB
SFO1 100.5785700 MHz

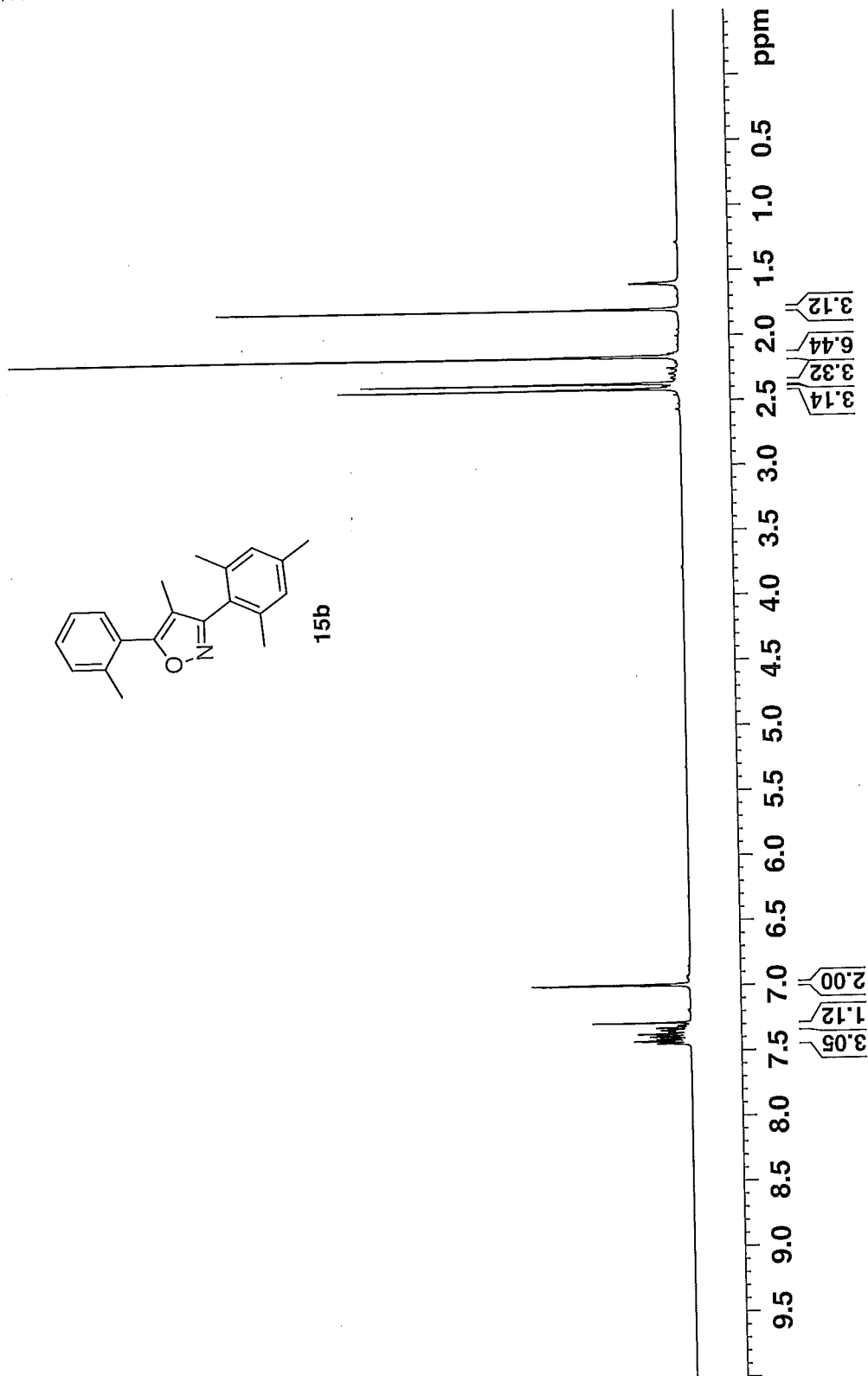
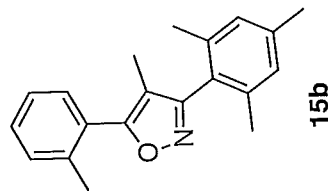
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 135.00 usec
PL2 17.40 dB
PL12 17.40 dB
PL13 17.40 dB
SFO2 399.9516000 MHz

F2 - Processing parameters
SI 32768
SF 100.5675080 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

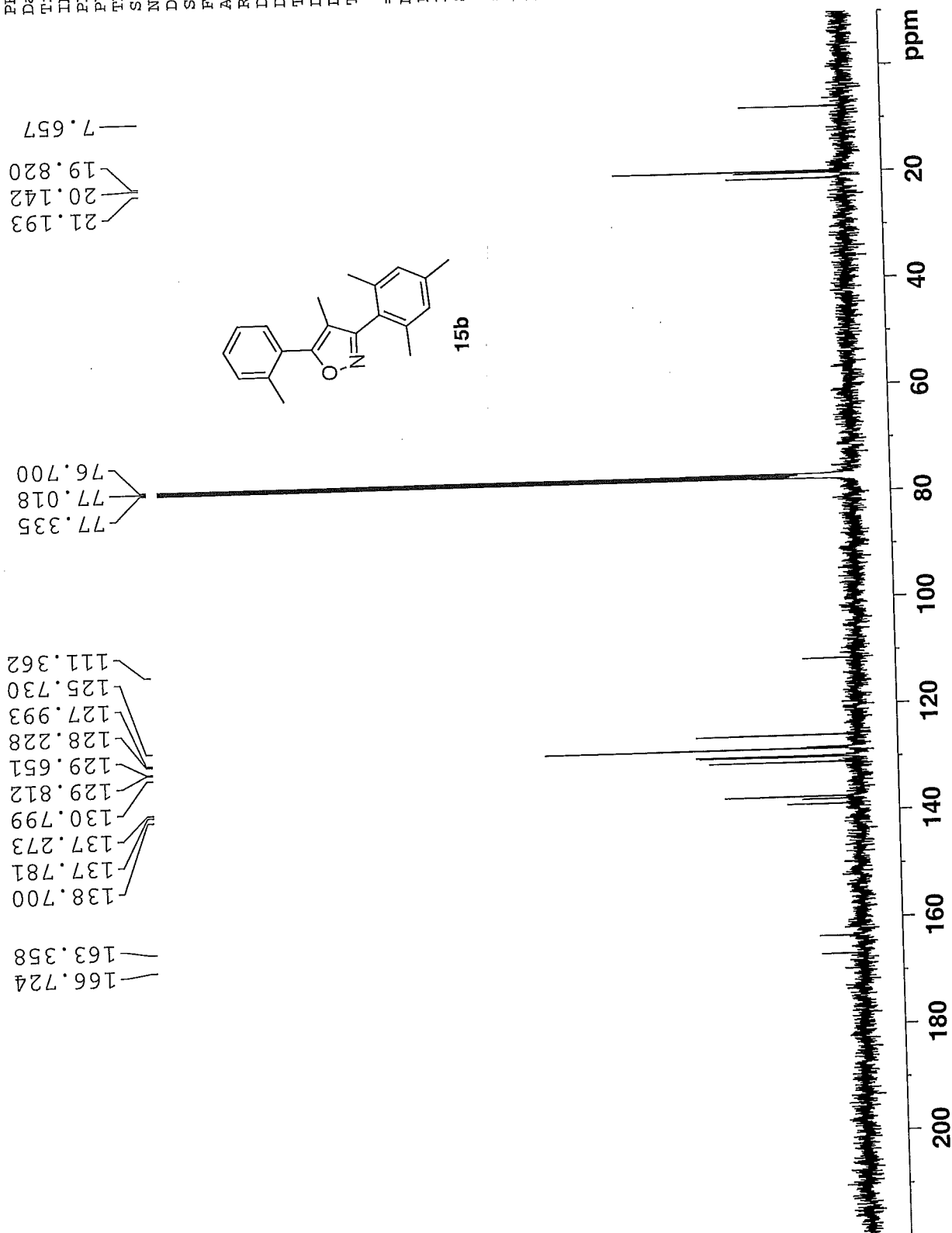
NAME MLM-V-012
EXPNO 7
PROCNO 1
Date_ 20120906
Time 15.30
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 2
SWH 7183.908 H
FIDRES 0.219235 H
AQ 2.2807028 s
RG 128
DW 69.600 u
DE 6.50 u
TE 298.2 K
D1 2.00000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 u
PL1 0.00 d
SFO1 400.1428010 M
SI 32768
SF 400.1400000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

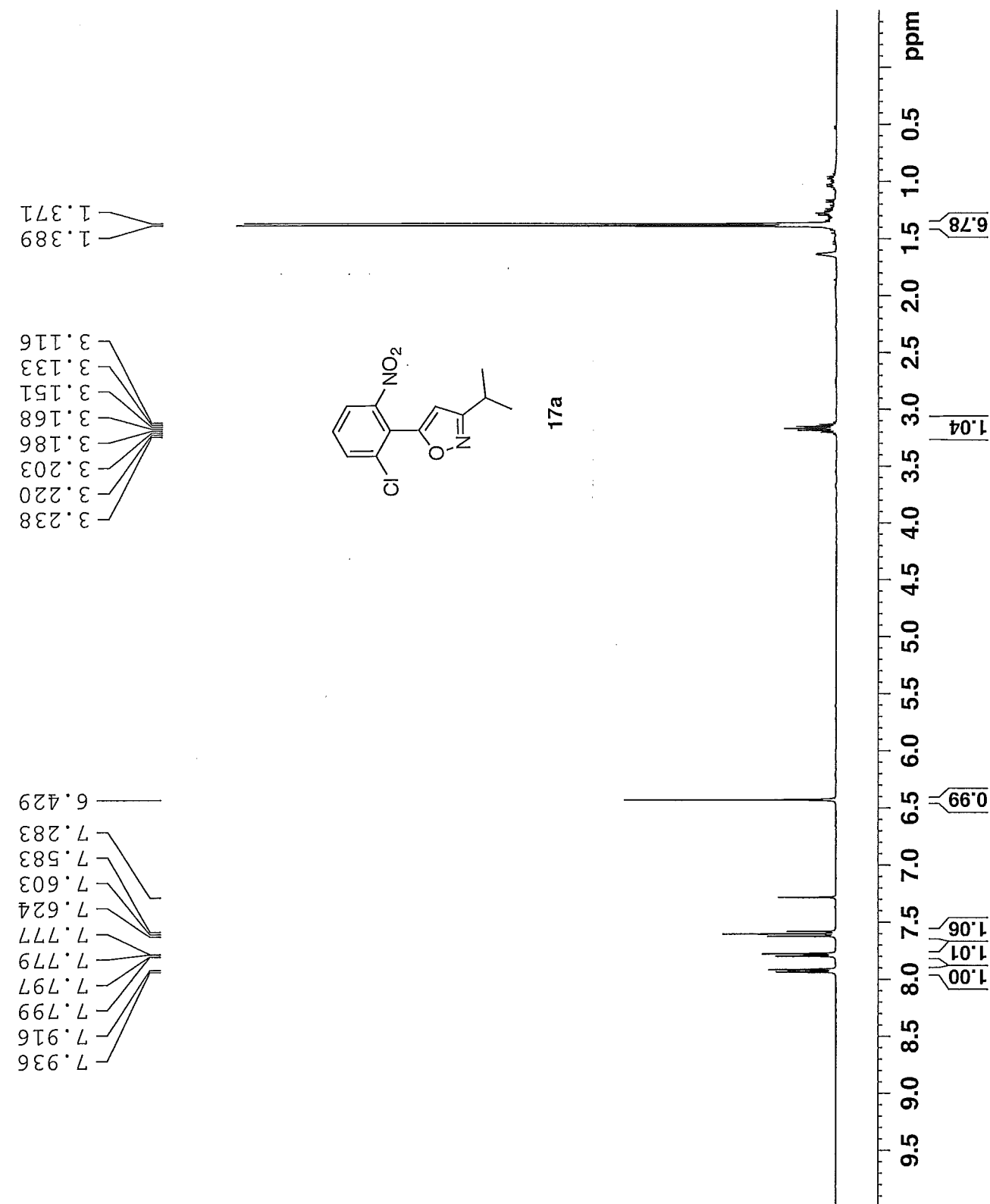
2.410
2.368
2.162
1.796
1.599

7.444
7.425
7.410
7.407
7.392
7.389
7.371
7.354
7.344
7.325
7.307
7.283
6.993



NAME MLM-V-012
EXPNO 9
PROCNO 1
Date_ 20120906
Time 19.13
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 412
DS 4
SWH 23980.814 H
FIDRES 0.365918 H
AQ 1.3664756 s
RG 16384
DW 20.850 u
DE 6.50 u
TE 298.9 K
D1 1.00000000 s
D11 0.03000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 u
PL1 -2.00 d
SFO1 100.6253446 M
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PL2 0.00 d
PL12 16.16 d
PL13 17.00 d
SFO2 400.1416006 M
SI 32768
SF 100.6152830 M
WDW EM
SSB 0
LB 3.00 H
GB 0
PC 1.40





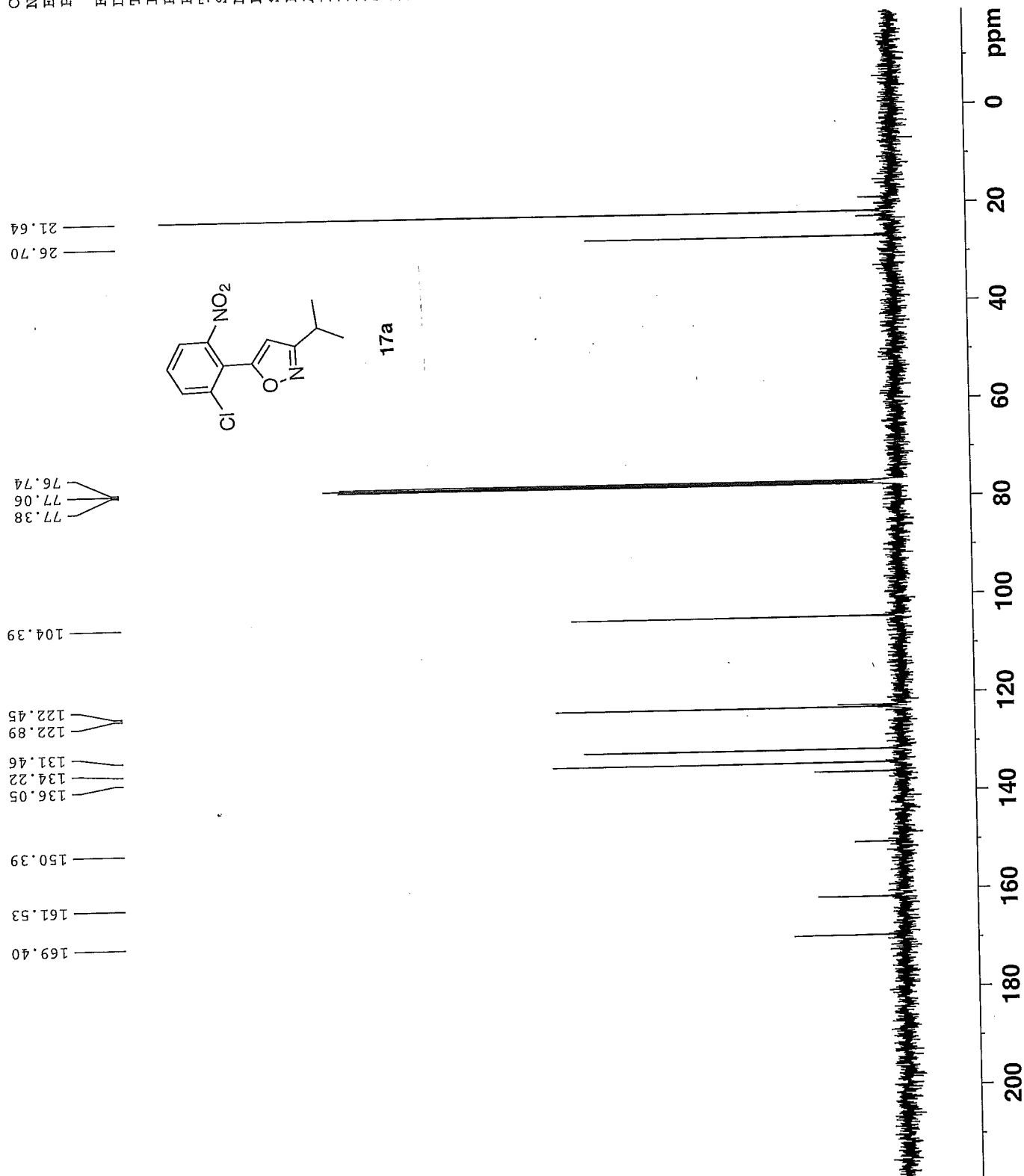
Current Data Parameters
NAME MLM-V-022
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters:
Date_ 20120905
Time 10.44
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 98
DS 0
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -2.00 dB
SFO1 100.6253446 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 0.00 dB
PL12 16.16 dB
PL13 17.00 dB
SFO2 400.1416006 MHz

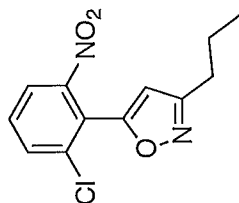
F2 - Processing parameters
SI 32768
SF 100.6152830 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



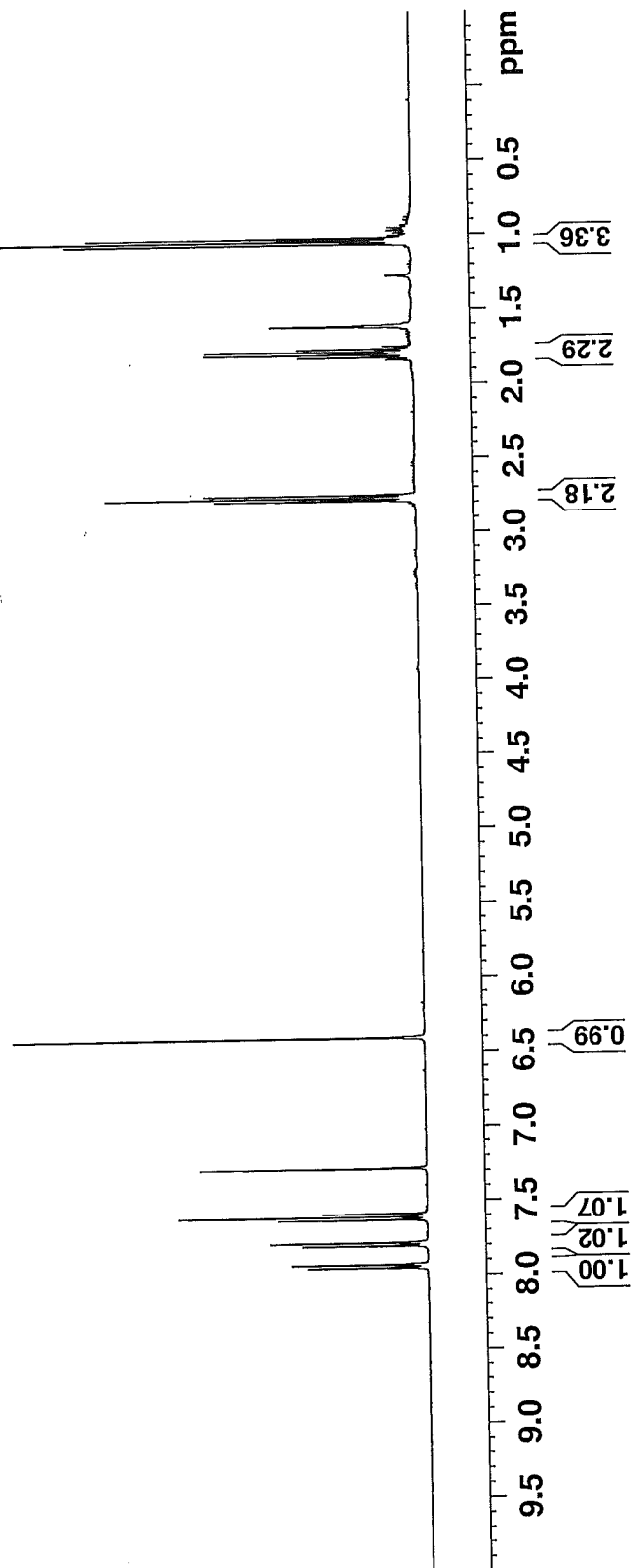
NAME MLM-V-023
EXPNO 2
PROCNO 1
Date_ 20120830
Time 12.32
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 6
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2807028 s
RG 161.3
DW 69.600 us
DE 6.50 us
TE 298.2 K
D1 2.00000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 us
PL1 0.00 dB
SFO1 400.1428010 MHz
SI 32768
SF 400.1400000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

2.787
2.768
2.749
1.840
1.821
1.803
1.784
1.766
1.747
1.059
1.041
1.022

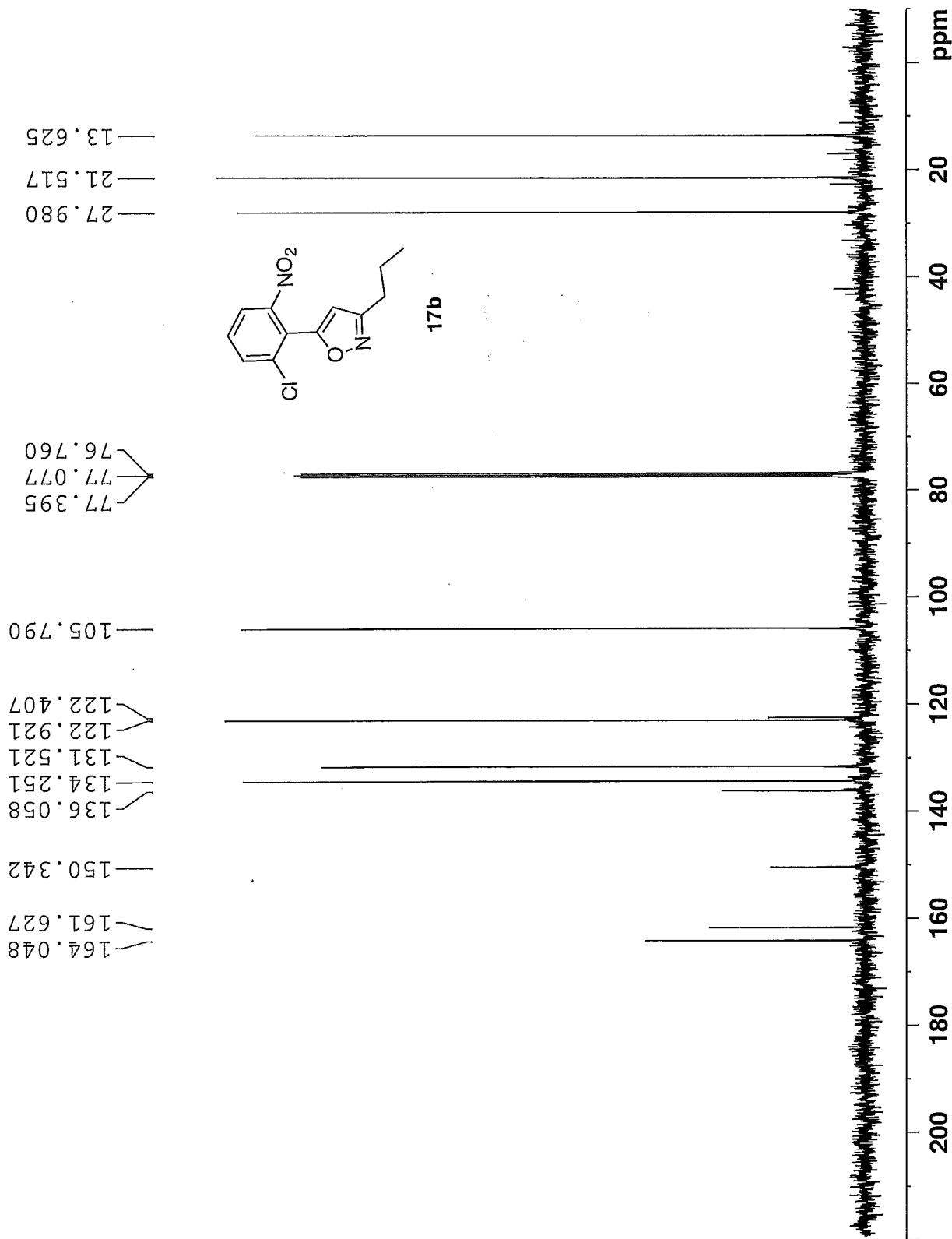
7.952
7.949
7.931
7.928
7.804
7.801
7.784
7.781
7.628
7.608
7.587
7.282
6.406



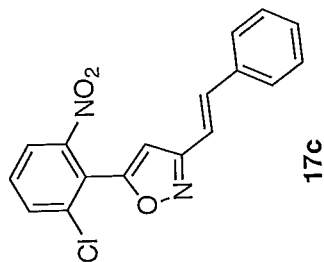
17b



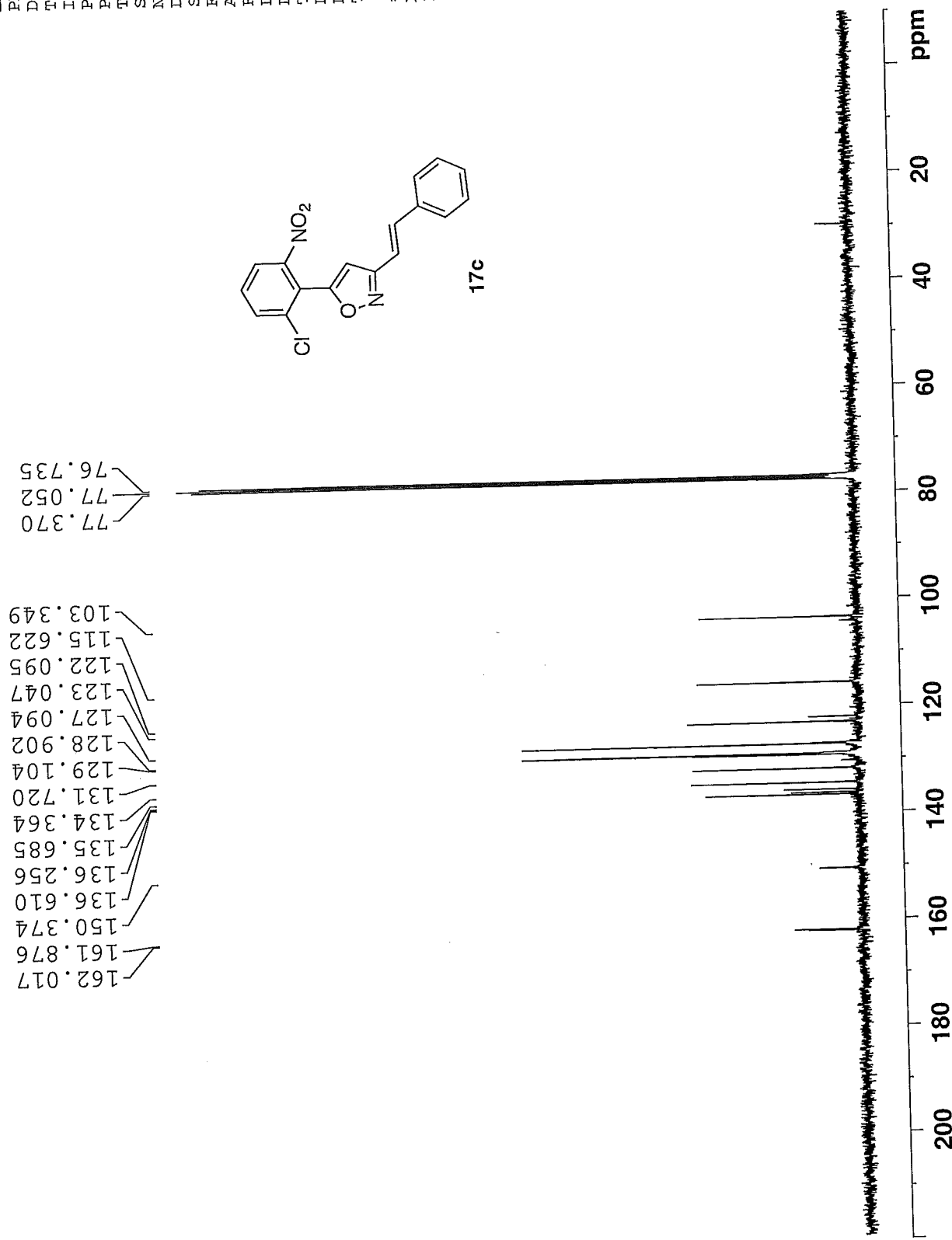
NAME MLM-V-023
EXPNO 6
PROCNO 1
Date_ 20120906
Time 11.54
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 146
DS 0
SWH 23980.814 H
FIDRES 0.365918 H
AQ 1.3664756 s
RG 32768
DW 20.850 u
DE 6.50 u
TE 298.3 K
D1 1.00000000 s
D11 0.03000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 u
PL1 -2.00 d
SFO1 100.6253446 M
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PL2 0.00 d
PL12 16.16 d
PL13 17.00 d
SFO2 400.1416006 M
SI 32768
SF 100.6152830 M
WDW EM
SSB 0
LB 3.00 H
GB 0
PC 1.40



NAME MLM-V-025
EXPNO 11
PROCNO 1
Date_ 20120910
Time 15.17
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 7183.908 H
FIDRES 0.219235 H
AQ 2.2807028 s
RG 90.5
DM 69.600 u
DE 6.50 u
TE 298.2 K
D1 2.0000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 u
PL1 0.00 d
SFO1 400.1428010 M
SI 32768
SF 400.1400000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

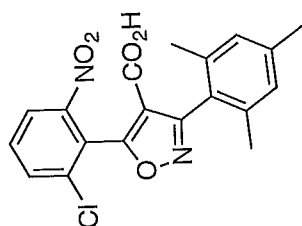


NAME MLM-V-025
EXPNO 12
PROCNO 1
Date_ 20120910
Time 15.22
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 327
DS 4
SWH 23980.814 H
FIDRES 0.365918 H
AQ 1.3664756 s
RG 32768
DW 20.850 u
DE 6.50 u
TE 299.3 K
D1 1.00000000 s
D11 0.03000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 u
PL1 -2.00 d
SFO1 100.6253446 M
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 u
PL2 0.00 d
PL12 16.16 d
PL13 17.00 d
SFO2 400.1416006 M
SI 32768
SF 100.6152830 M
WDW EM
SSB 0
LB 3.00 H
GB 0
PC 1.40



NAME MLM-IV-020
EXPNO 6
PROCNO 1
Date_ 20120329
Time 18.00
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 2
SWH 7183.908 H
FIDRES 0.219235 H
AQ 2.2807028 s
RG 228.1
DW 69.600 u
DE 6.50 u
TE 298.2 K
D1 2.00000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 u
PL1 0.00 dB
SFO1 400.1428010 M
SI 32768
SF 400.1400000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

2.361
2.180



18

8.271
8.251
7.893
7.873
7.750
7.729
7.709
7.283
6.976

2.91
5.93

1.84

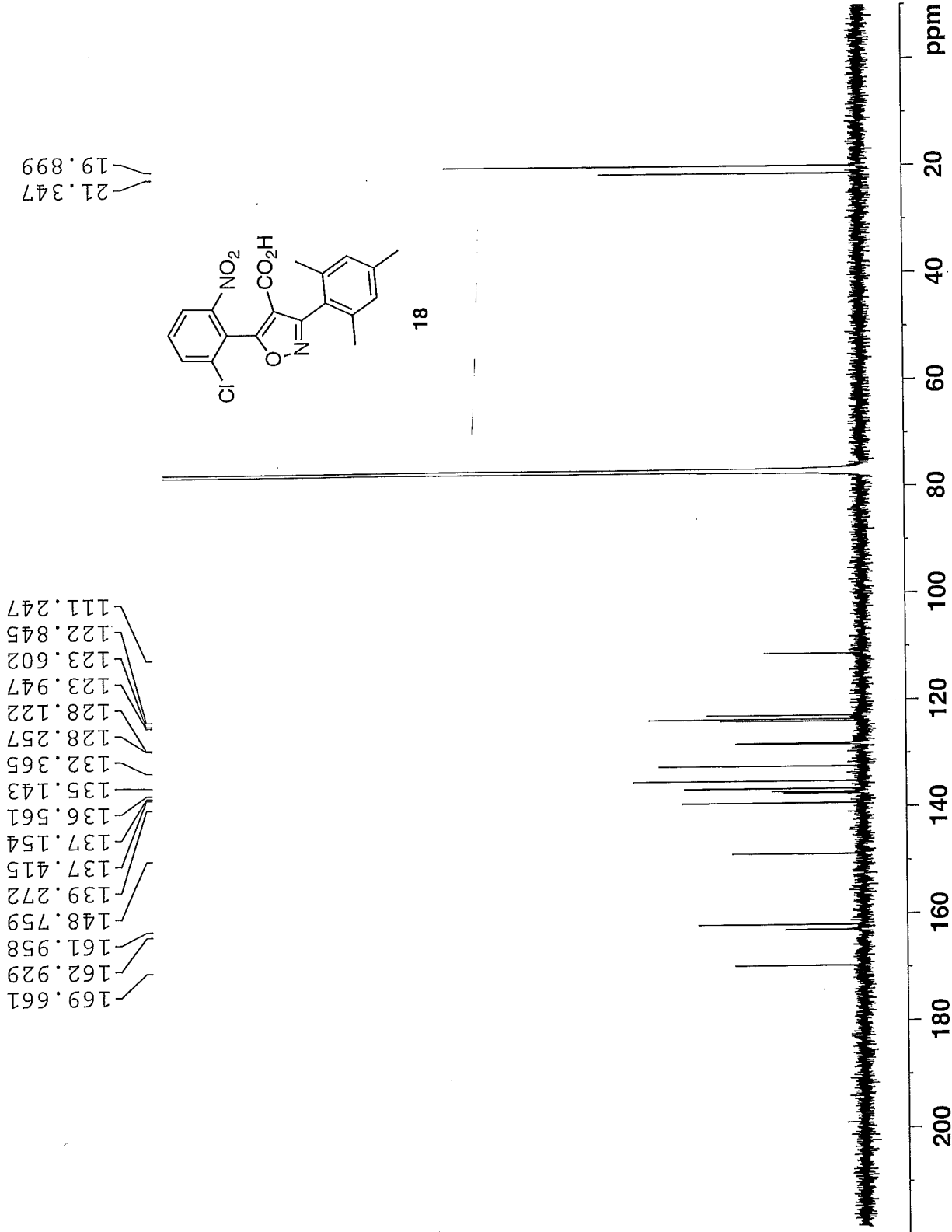
0.98

0.94

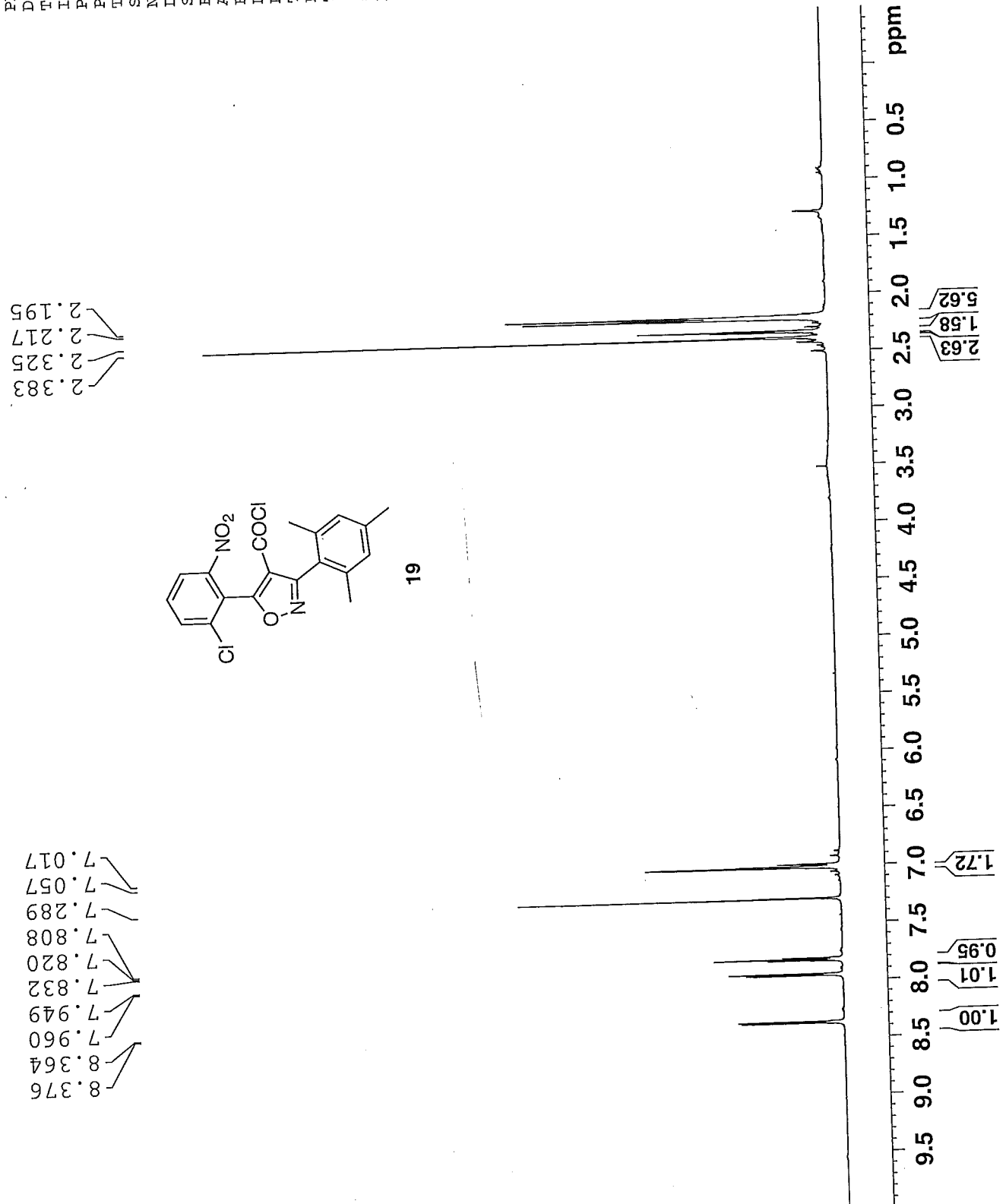
1.00

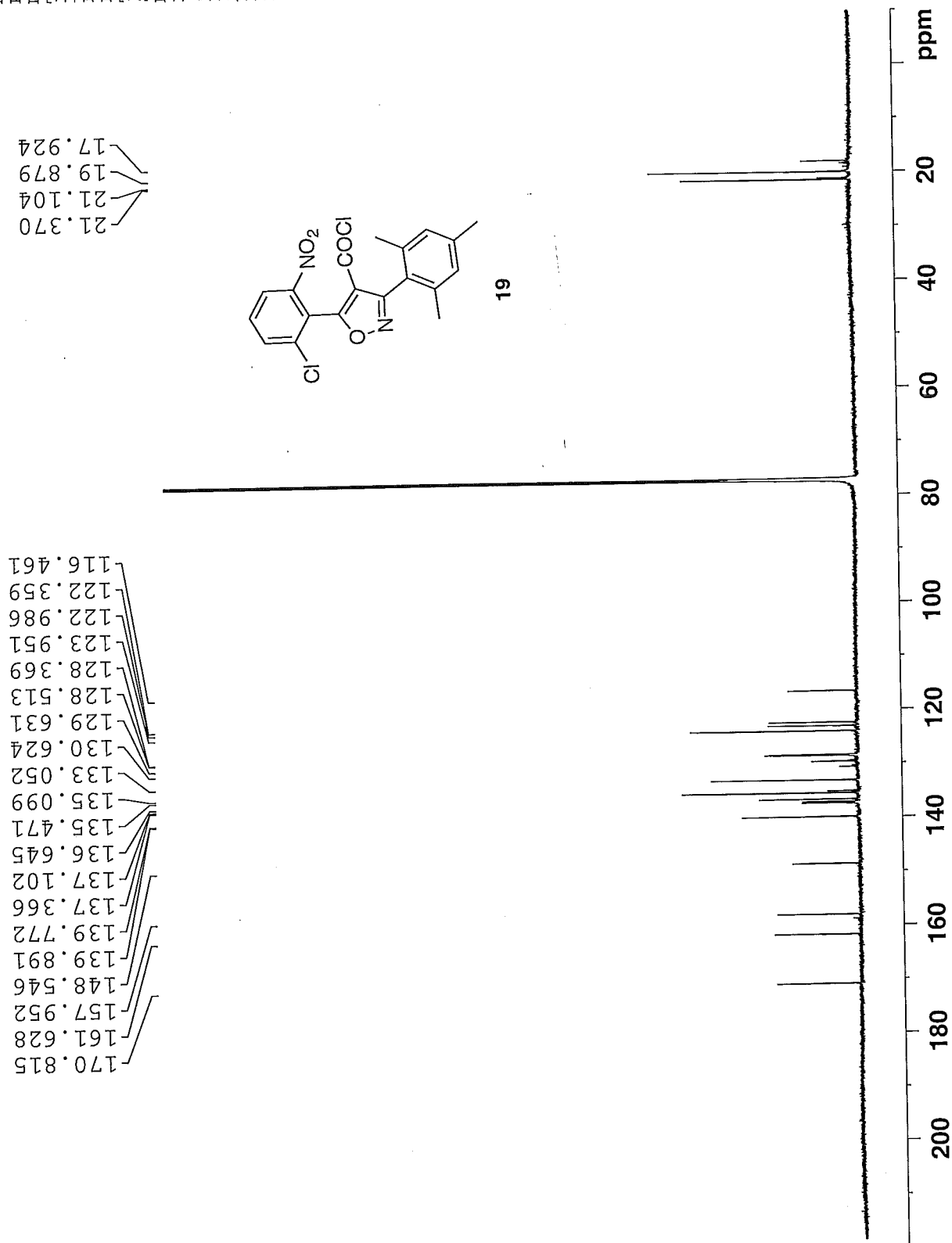
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm

NAME MLM-IV-020
EXPNO 6
PROCNO 1
Date_ 20120330
Time 11.12
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 845
DS 4
SMH 41666.668 H
FIDRES 0.635783 H
AQ 0.7864820 S
RG 203
DW 12.000 u
DE 16.50 u
TE 298.2 K
D1 2.00000000 S
D11 0.03000000 S
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 u
PL1 4.50 d
PL1W 38.14553833 W
SFO1 176.0697436 M
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 65.00 u
PL2 -3.20 d
PL12 13.60 d
PL13 120.00 d
PL2W 33.59817505 W
PL12W 0.70196527 W
PL13W 0.00000000 W
SFO2 700.1499406 M
SI 32768
SF 176.0521380 M
WDW EM
SSB 0
LB 3.00 H
GB 0
PC 1.40



NAME MLM-IV-023
EXPNO 1
PROCNO 1
Date_ 20120327
Time 15.04
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 95236
SOLVENT CDCl3
NS 5
DS 2
SWH 11904.762 H
FIDRES 0.125003 H
AQ 3.9999621 s
RG 203
DW 42.000 u
DE 6.50 u
TE 298.2 K
D1 2.0000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 9.40 u
PL1 -3.20 d
PL1W 33.59817505 W
SFO1 700.1516910 M
SI 131072
SF 700.1471400 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00



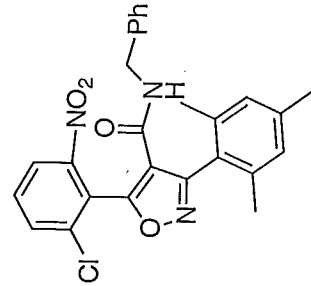


fractions 13-16

8.268
8.256
7.878
7.866
7.717
7.705
7.694
7.288
7.249
7.239
7.234
7.231
7.226
6.929
6.865
6.864
6.855
5.519

4.258
4.252
4.186
4.181

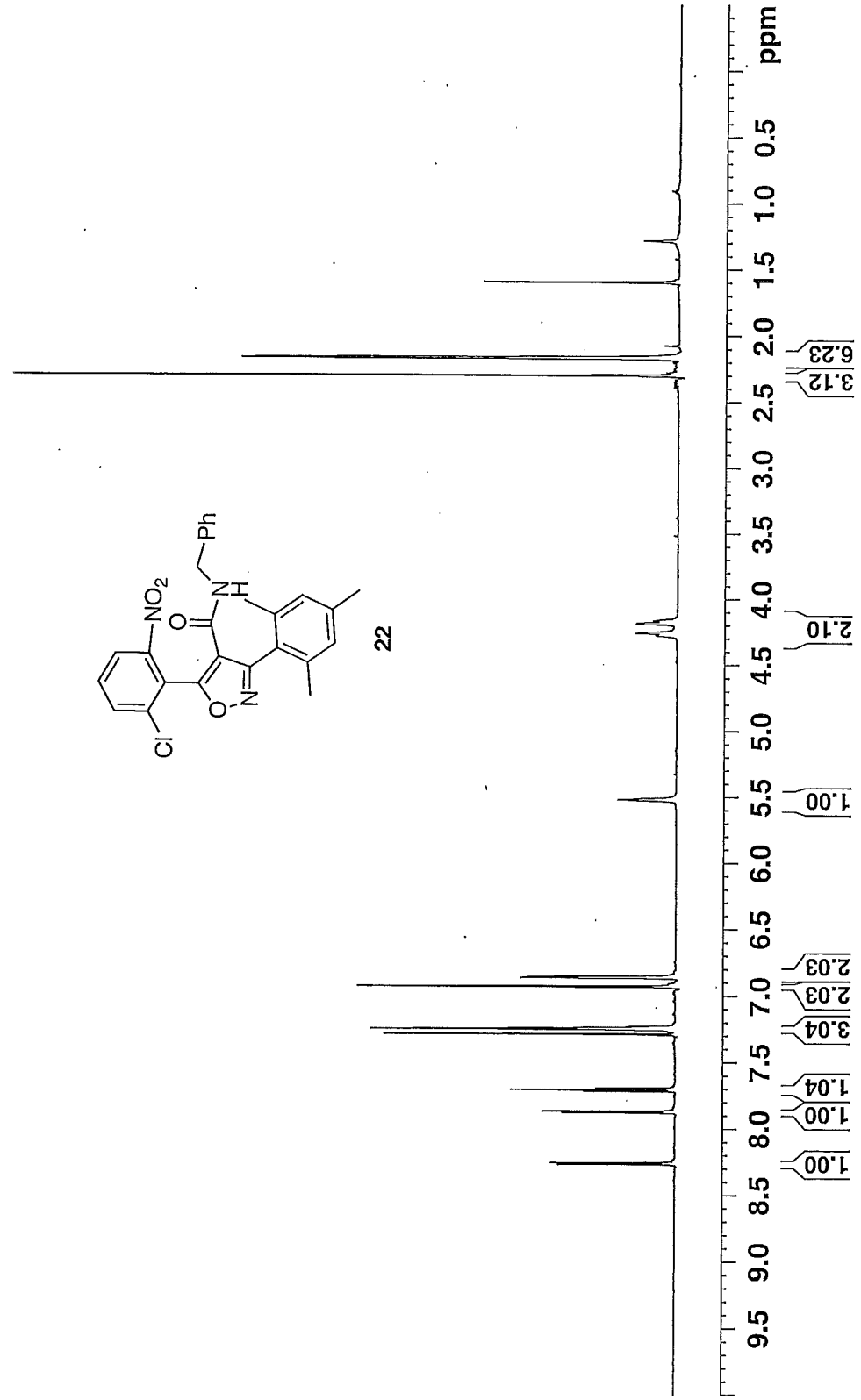
2.298
2.167
1.596
1.283



22

NAME MLM-IV-033
EXPNO 3
PROCNO 1
Date_ 20120416
Time 11.59
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zg30
TD 95236
SOLVENT CDC13
NS 3
DS 2
SWH 11904.762 Hz
FIDRES 0.125003 Hz
AQ 3.9999621 s
RG 36
DW 42.000 us
DE 6.50 us
TE 303.2 K
D1 303.2 K
TD0 2.0000000 s
1

===== CHANNEL f1 =====
NUC1 1H
P1 9.40 us
PL1 -3.20 dB
PL1W 33.59817505 W
SFO1 700.1516910 MHz
SI 131072
SF 700.1471400 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



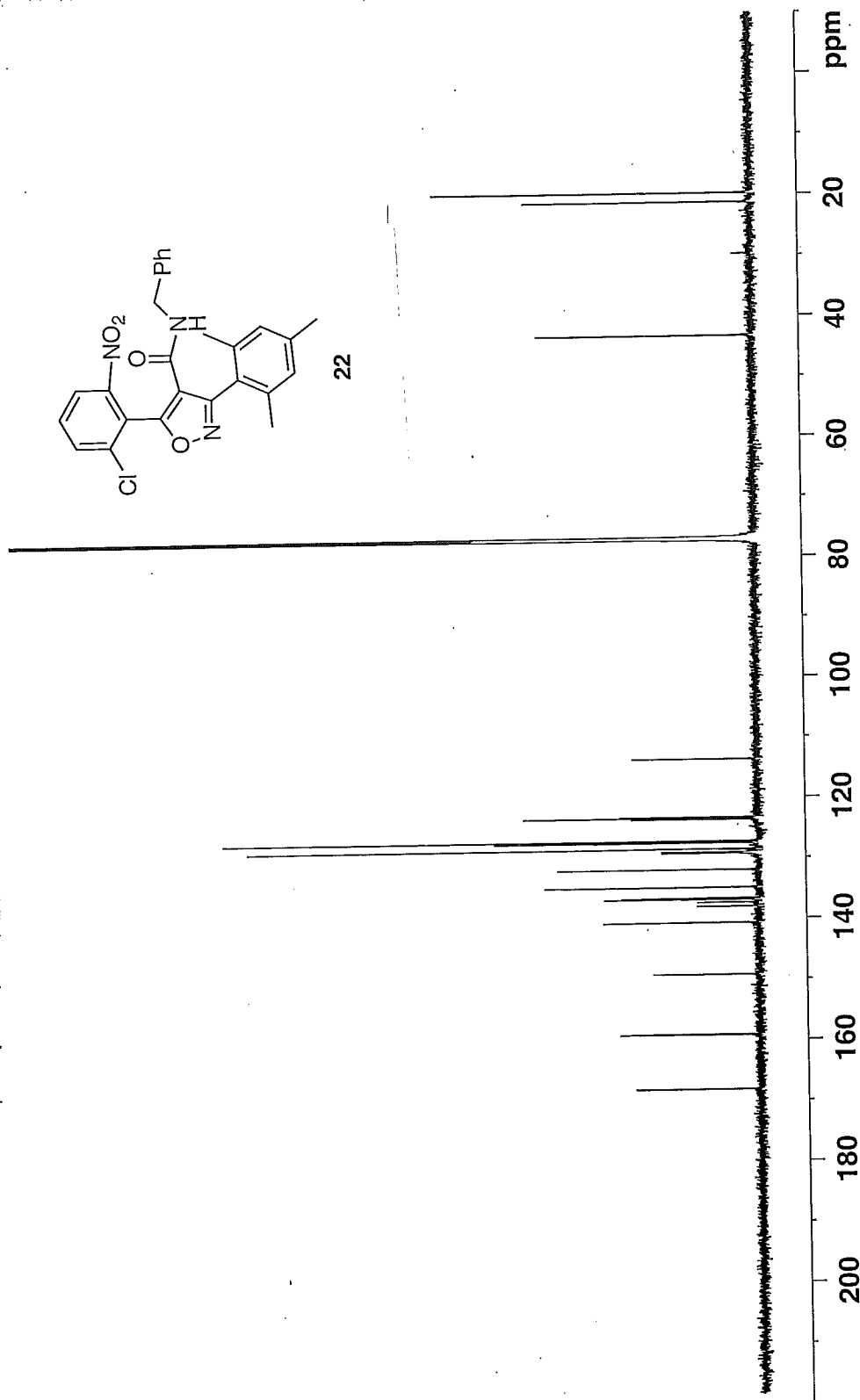
NAME MLM-IV-033
EXPNO 4
PROCNO 1
Date_ 20120416
Time 12.02
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 103
DS 4
SWH 41666.668 H
FIDRES 0.635783 H
AQ 0.7864820 s
RG 203
DW 12.000 u
DE 16.50 u
TE 303.2 K
D1 2.00000000 s
D11 0.03000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 u
PL1 4.50 d
PL1W 38.14553833 W
SFO1 176.0697436 M
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 65.00 u
PL2 -3.20 d
PL12 13.60 d
PL13 120.00 d
PL2W 33.59817505 W
PL12W 0.70196527 W
PL13W 0.00000000 W
SFO2 700.1499406 M
SI 32768
SF 176.0521380 M
WDW EM
SSB 0
LB 3.00 H
GB 0
PC 1.40

fractions 13-16

168.169
159.192
159.104
149.227
140.664
138.002
137.336
136.843
136.649
134.845
131.895
129.235
129.025
128.548
127.468
127.184
123.615
123.392
123.257
113.634

43.252

21.256
19.751

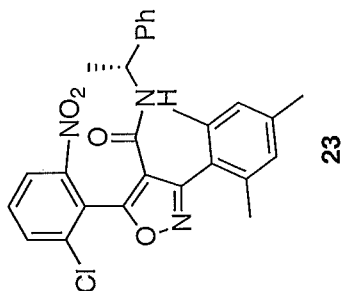


NAME MLM-IV-038
EXPNO 3
PROCNO 1
Date_ 20120503
Time 21.05
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 14
DS 2
SWH 7183.908 H
FIDRES 0.219235 H
AQ 2.2807028 s
RG 161.3
DW 69.600 u
DE 6.50 u
TE 298.3 K
D1 2.0000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 u
PL1 0.00 d
SF01 400.1428010 M
SI 32768
SF 400.1400000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00

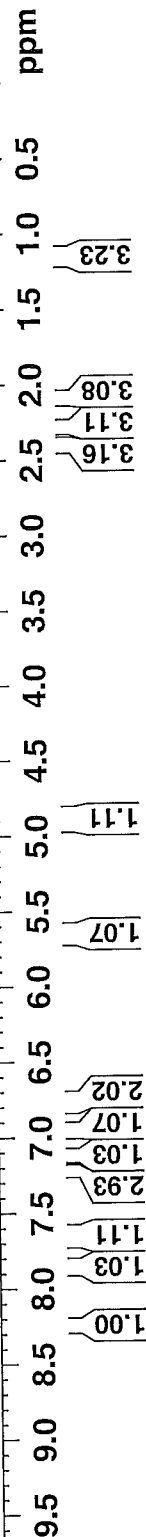
Fractions 18-22

8.245
8.225
7.845
7.698
7.677
7.657
7.282
7.228
7.220
7.212
7.202
7.128
7.101
6.963
6.941
6.808
6.801
6.793
6.785
5.655
5.636
4.899
4.882
4.864

2.393
2.283
2.263
2.091
1.572
1.278
1.150

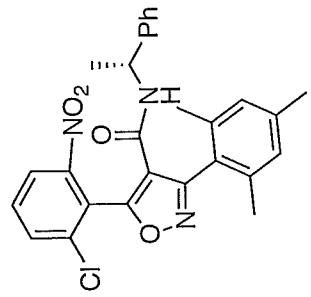


23

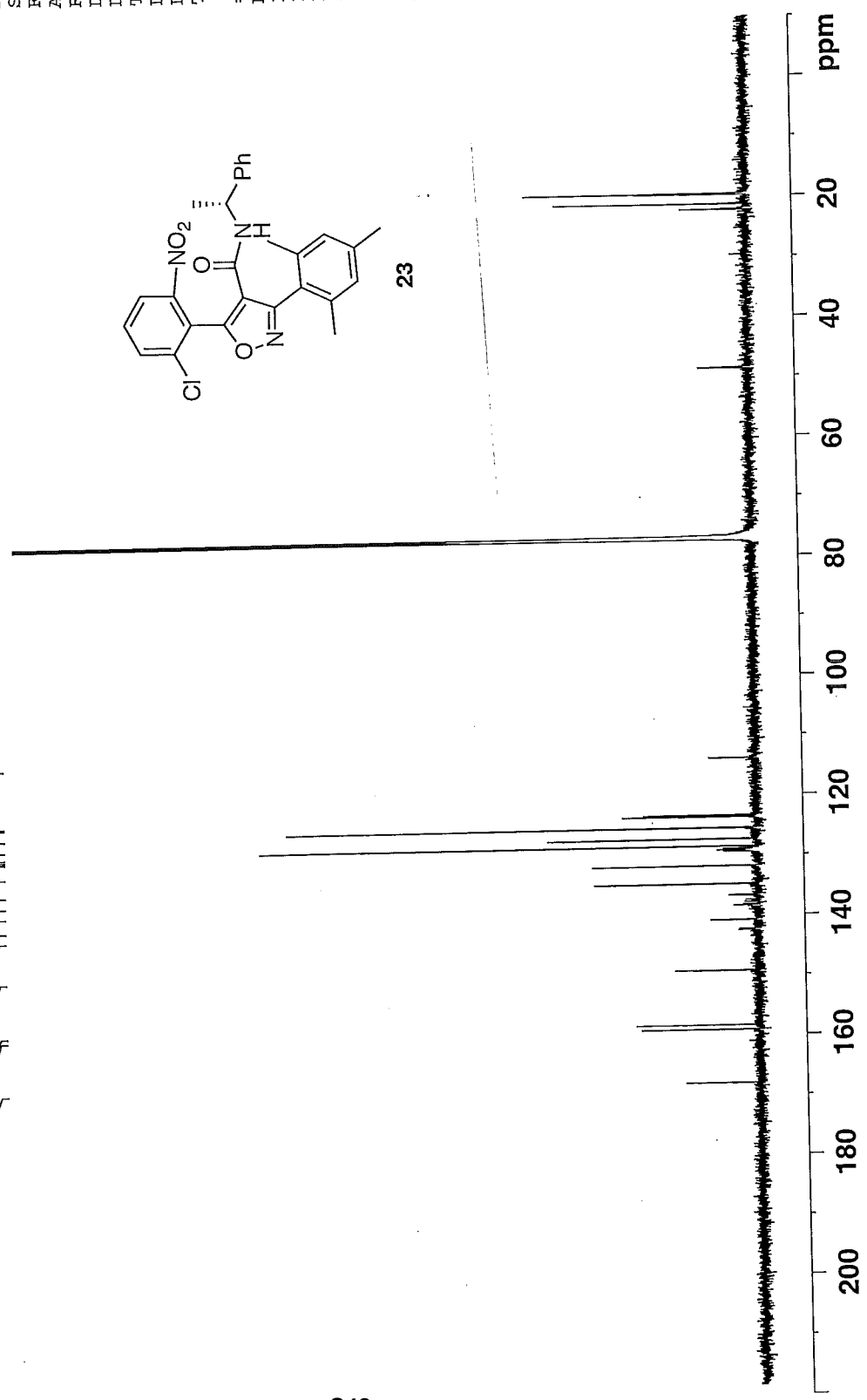


NAME MLM-IV-038
EXPNO 6
PROCNO 1
Date_ 20120503
Time 21.36
INSTRUM spect
PROBHD 5 mm CPDCH 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 239
DS 4
SWH 41666.668 H
FIDRES 0.635783 H
AQ 0.7864820 s
RG 203
DE 12.000 u
TE 16.50 u
D1 298.2 K
D11 2.00000000 s
D11 0.03000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 u
PL1 4.50 d
PL1W 38.14553833 W
SFO1 176.0697436 M
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 65.00 u
PL2 -3.20 d
PL12 13.60 d
PL13 120.00 d
PL2W 33.59817505 W
PL12W 0.70196527 W
PL13W 0.00000000 W
SFO2 700.1499406 M
SI 32768
SF 176.0521380 M
EM 0
SSB 3.00 H
LB 0
GB 0
PC 1.40

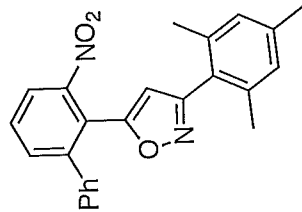
19.639
19.725
21.282
22.196
48.545



167.981
159.095
158.309
149.225
142.436
140.784
138.358
136.642
134.778
131.768
129.357
129.175
128.881
128.514
127.290
125.453
123.633
123.343
113.826

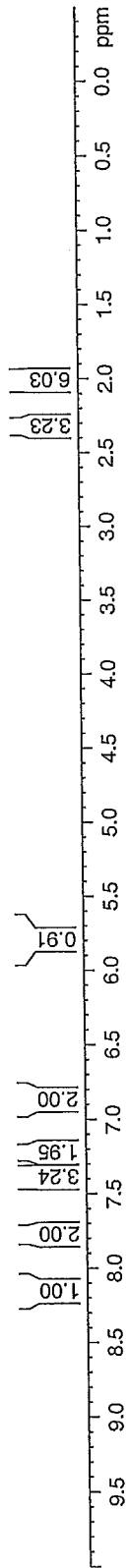


ph coupled oxazole



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2.322
2.025



Current Data Parameters
NAME MRN10079
EXPNO 10
PROCNO 1
DU /n
USER michaeln

F2 - Acquisition Parameters
Date_ 20090703
Time 10.57
INSTRUM DFX400
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT
NS 20
DS 2
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 80.6
DW 78.000 usec
DE 6.00 usec
TE 299.2 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.70 usec
PL1 0.00 dB
SFO1 399.9528000 MHz

F2 - Processing parameters
SI 32768
SF 399.9500000 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

ph coupled oxazole

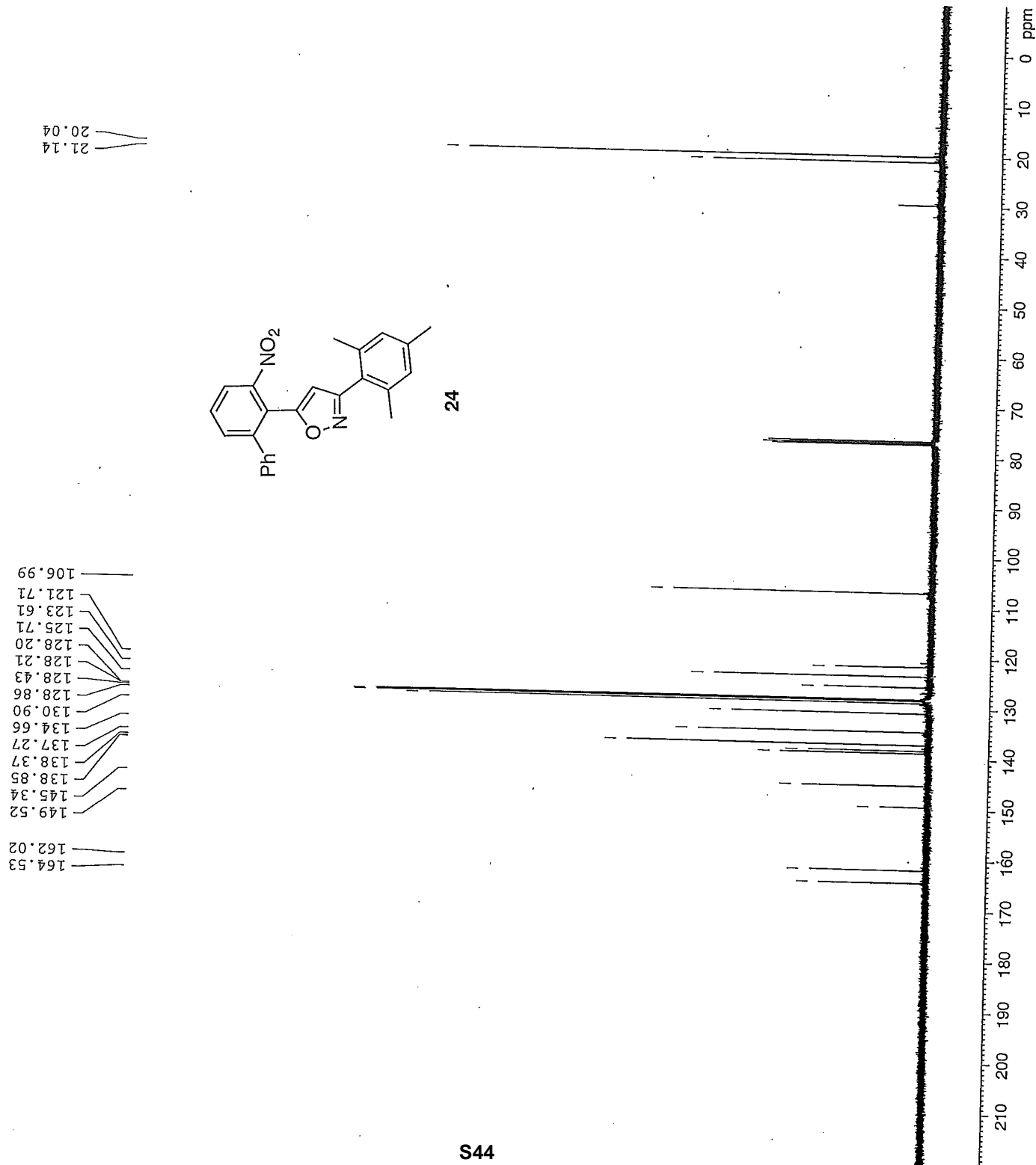
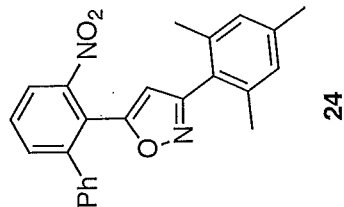
Current Data Parameters
NAME MRN10079
EXPNO 11
PROCNO 2
DU /n
USER michaeln

F2 - Acquisition Parameters
Date_ 20090703
Time 11.13
INSTRUM DPK400
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT
NS 507
DS 4
SWH 25125.629 Hz
FIDRES 0.383387 Hz
AQ 1.3042164 sec
RG 16384
DW 19.900 usec
DE 6.00 usec
TE 299.2 K
D1 0.15000001 sec
d11 0.03000000 sec
DELTA 0.05000000 sec
TD0 1

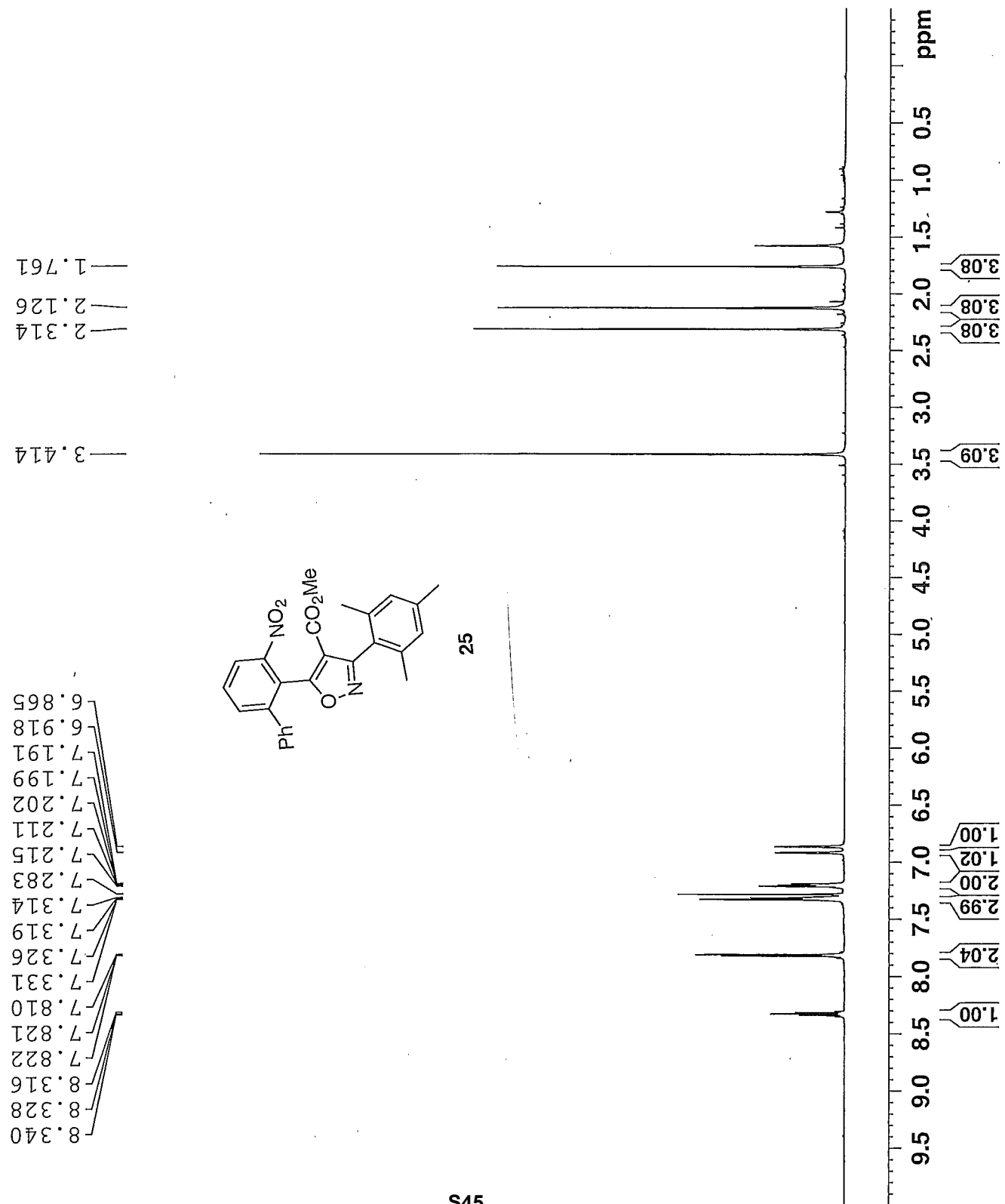
==== CHANNEL f1 =====
NUC1 13C
P1 13C
PL1 7.80 usec
SF01 100.5785700 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 135.00 usec
PL2 17.40 dB
PL12 17.40 dB
PL13 17.40 dB
SF02 399.9516000 MHz

F2 - Processing parameters
SI 65536
SF 100.5675080 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40



NAME MLM-TV-039
EXPNO 2
PROCNO 1
Date_ 20120503
Time_ 19.50
INSTRUM robinson
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 7
DS 2
SWH 7183.908 H
FIDRES 0.219235 H
AQ 2.2807028 s
RG 161.3
DW 69.600 u
DE 6.50 u
TE 298.2 K
D1 2.00000000 s
TD0 1
===== CHANNEL f1 =====
NUC1 1H
P1 14.00 u
PL1 0.00 d
SFO1 400.1428010 M
SI 32768
SF 400.1400000 M
WDW EM
SSB 0
LB 0.30 H
GB 0
PC 1.00



Current Data Parameters
NAME MLM-I-047
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120501
Time 11.20
INSTRUM DFX400
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3884
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 32768
DW 20.850 usec
DE 6.00 usec
TE 299.2 K
D1 0.20000000 sec
d11 0.03000000 sec
DELTA 0.10000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 13C
P1 8.30 usec
PL1 -3.00 dB
SFO1 100.6555216 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -3.00 dB
PL12 15.00 dB
PL13 15.00 dB
SFO2 400.2620013 MHz

F2 - Processing parameters
SI 32768
SF 100.6454570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

