

Supplementary Material

Synthesis of Imine and Amine-Linked Macrocycles Containing Tris-Indoles

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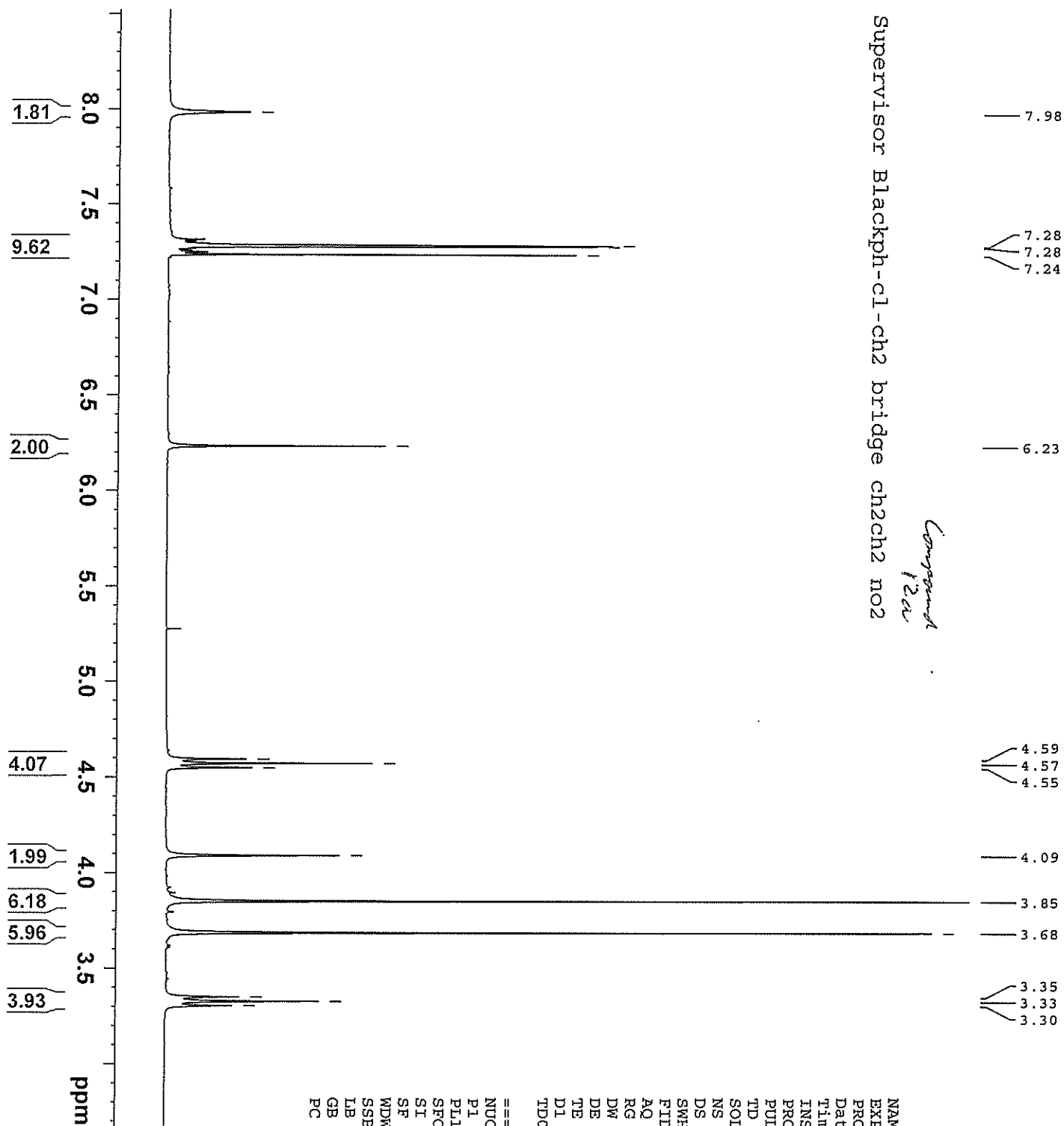
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^DCorresponding author. Email: d.black@unsw.edu.au



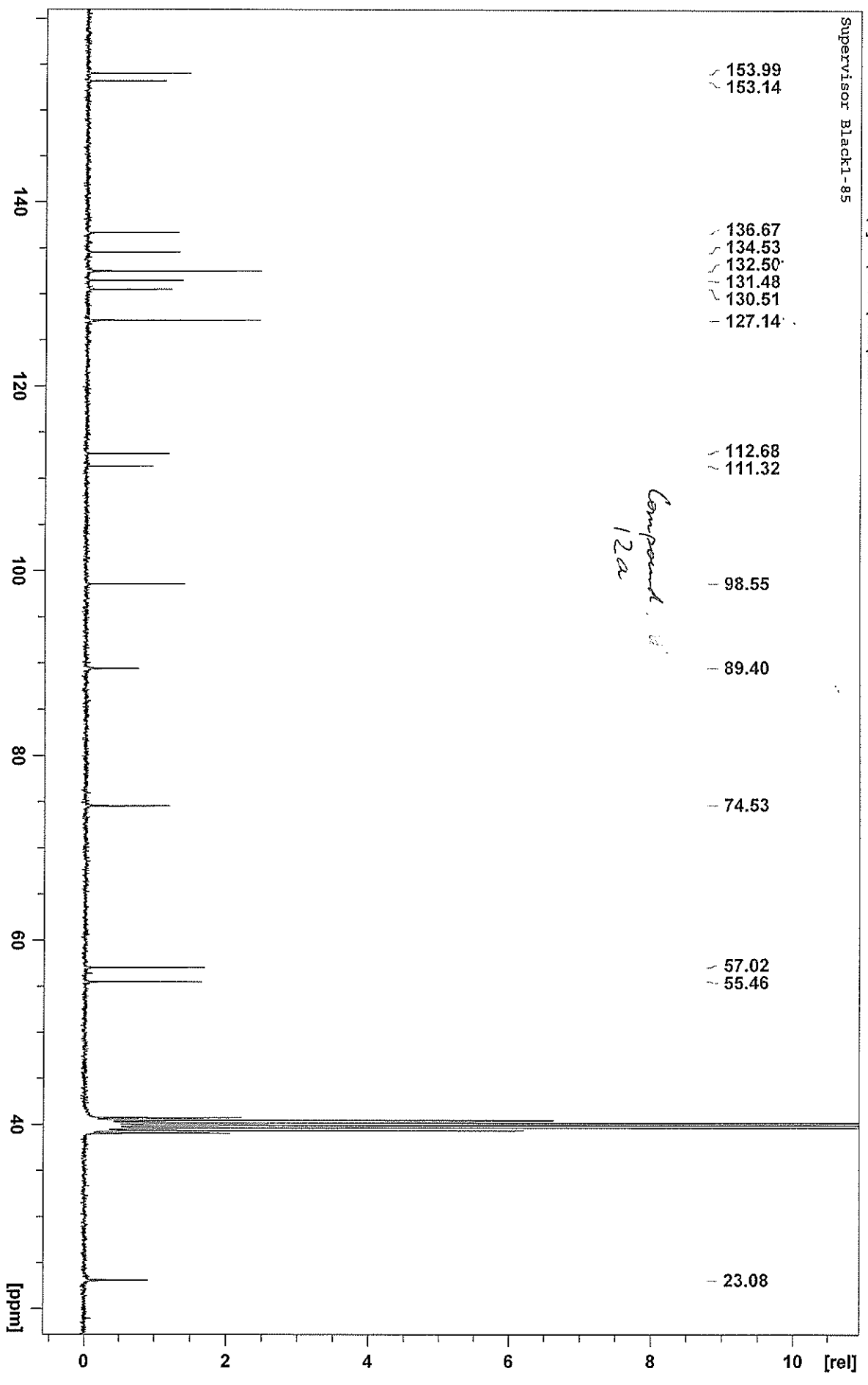
Supervisor Blackph-cl-ch2 bridge ch2ch2 no2

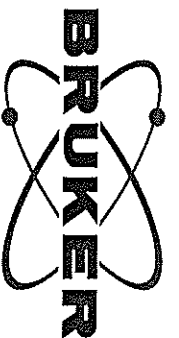
Compound 12a



NAME 100814-hkn
EXPNO 30
PROCNO 1
Date_ 20100815
Time 16.47
INSTRUM dpx1
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SMH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 574.7
DW 83.400 usec
DE 12.00 usec
TE 293.9 K
D1 1.50000000 sec
TD0 1

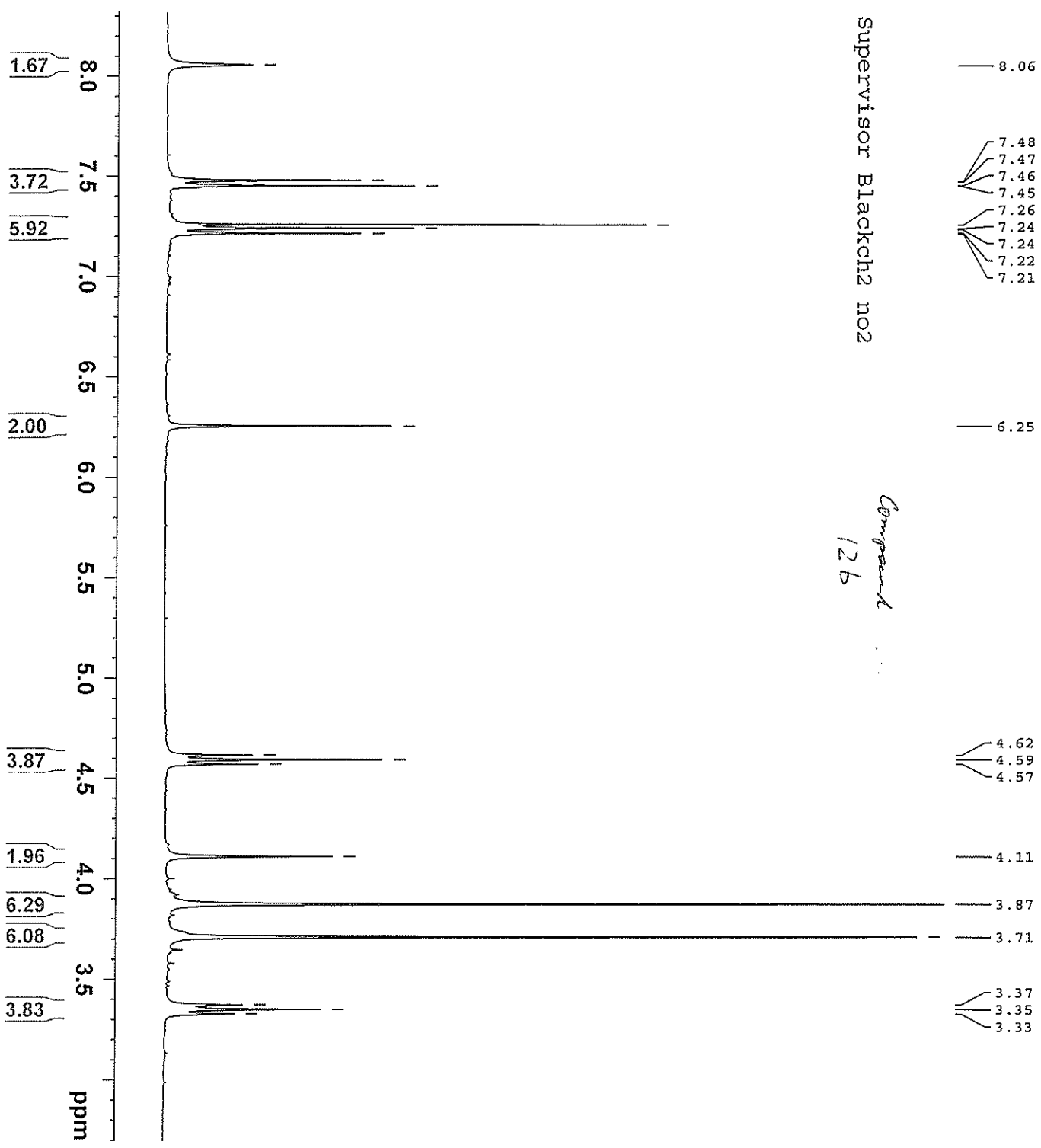
==== CHANNEL f1 =====
NUC1 1H
PI 10.10 usec
PL1 -3.00 dB
SFO1 300.1719511 MHz
SI 65536
SF 300.1700120 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00





Supervisor Blackch2 no2

Compound 12b



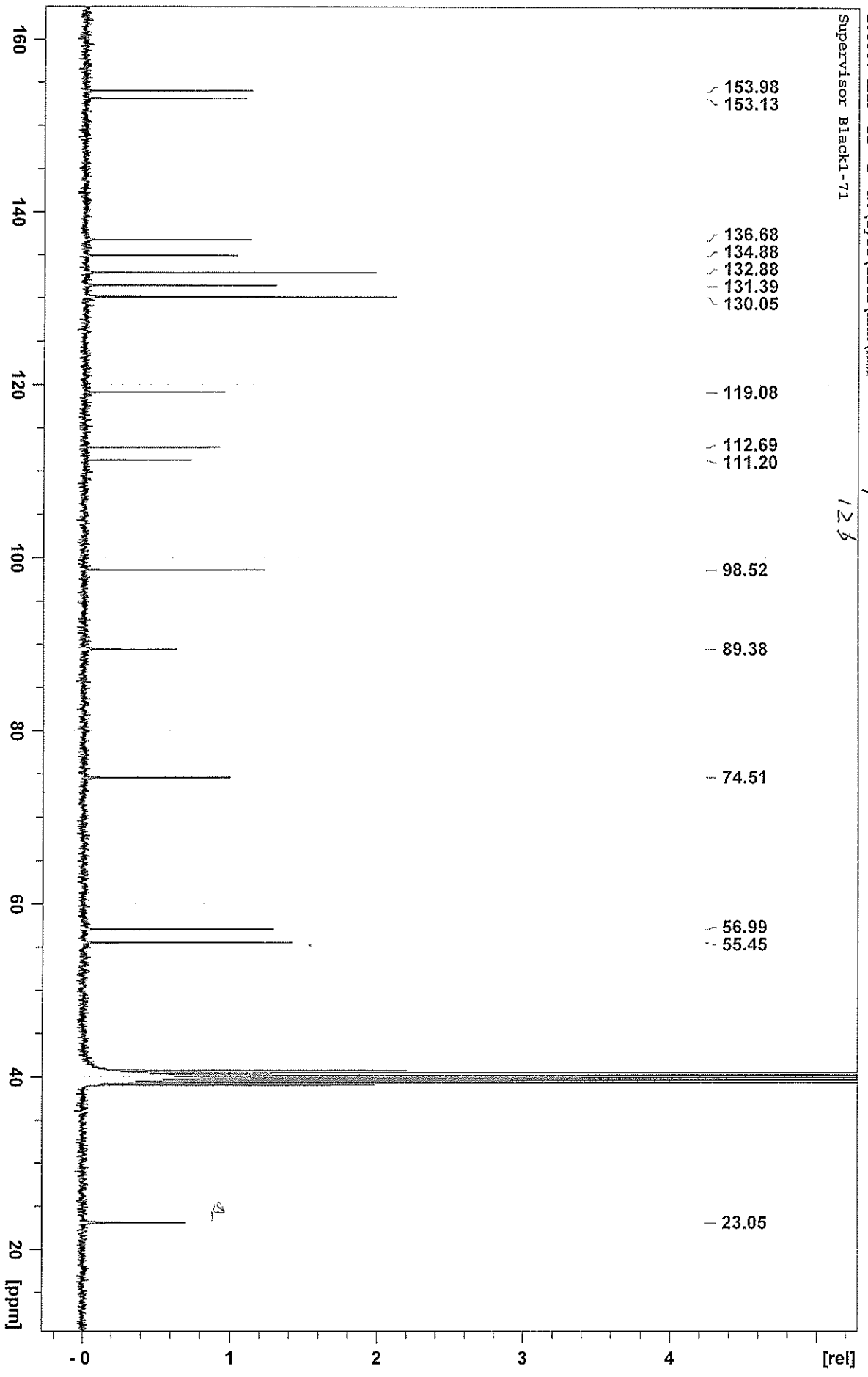
- 8.06
- 7.48
- 7.47
- 7.46
- 7.45
- 7.26
- 7.24
- 7.24
- 7.22
- 7.21
- 6.25
- 4.62
- 4.59
- 4.57
- 4.11
- 3.87
- 3.71
- 3.37
- 3.35
- 3.33

NAME 100419-hken
 EXPNO 10
 PROCNO 1
 Date_ 20100419
 Time_ 10.48
 INSTRUM dpx1
 PROBHD 5 mm QNP 1H/13
 PULPROG zg
 TD 32768
 SOLVENT CDCl3
 NS 64
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.188380 Hz
 AQ 2.6542580 sec
 RG 645.1
 DW 81.000 usec
 DE 12.00 usec
 TE 297.2 K
 DL 1.50000000 sec
 TD0 1

==== CHANNEL F1 =====
 NUCL1 1H
 P1 10.10 usec
 PL1 -3.00 dB
 SFO1 300.1718537 MHz
 SI 65536
 SF 300.1700120 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

100807-hkn 21 1 N:\Gyro\data\hkn\mr
Supervisor Black1-71

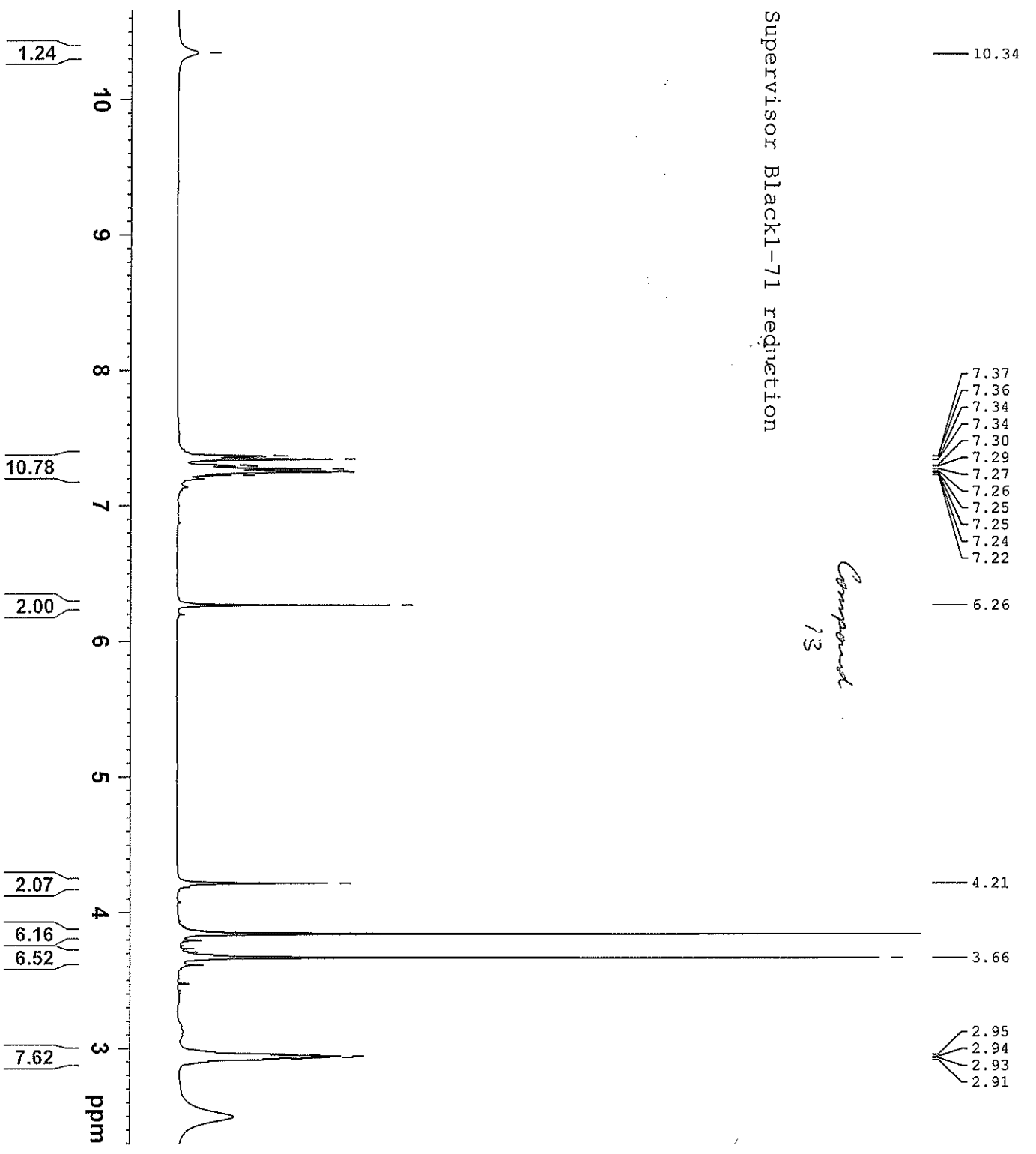
Compound
125





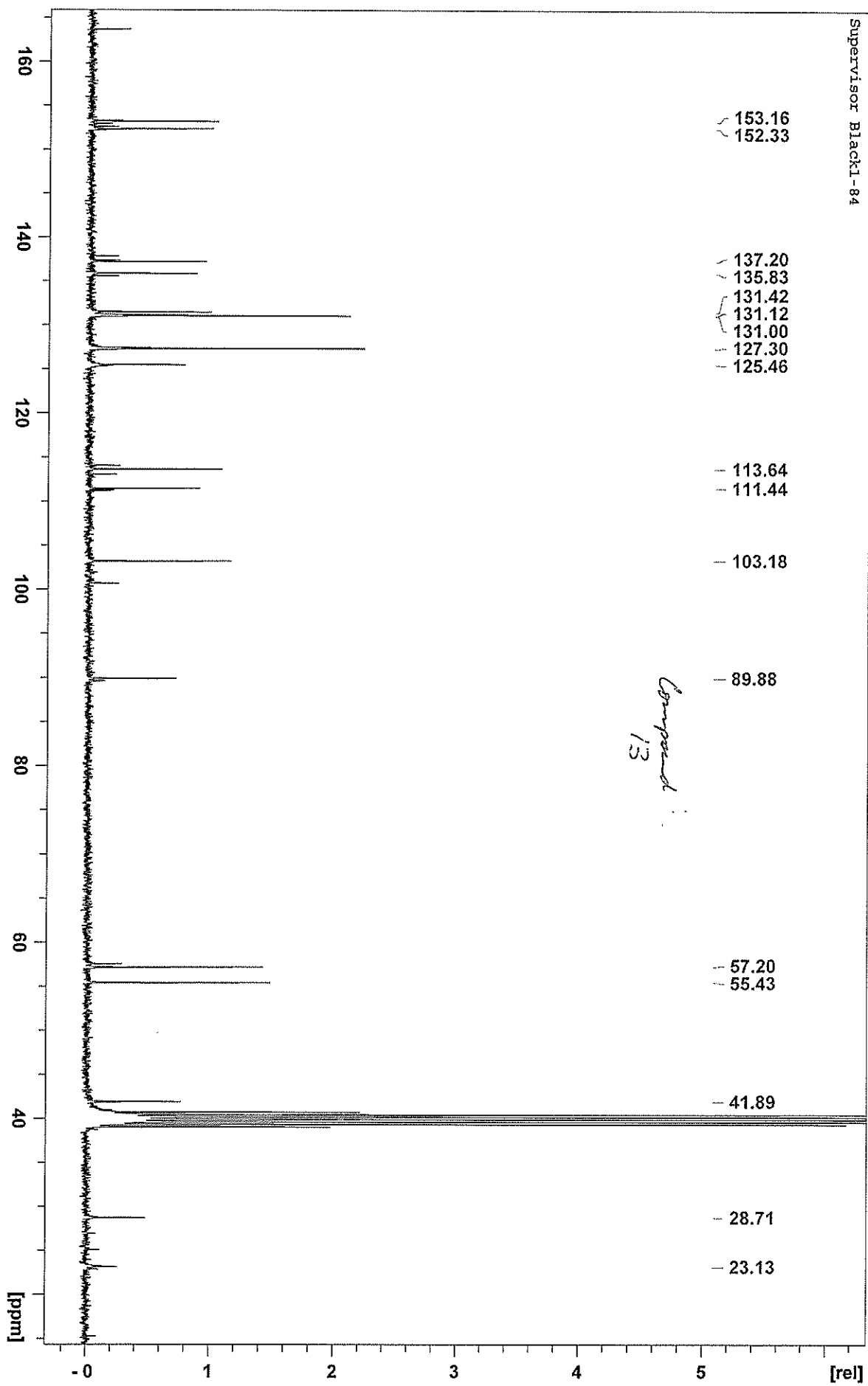
Supervisor Black1-71 rednetion

Compound 13



NAME 100529-hkn
EXPNO 20
PROCNO 1
Date_ 20100531
Time_ 9.10
INSTRUM dpx1
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 64
DS 2
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 161.3
DW 81.000 usec
DE 12.00 usec
TE 298.2 K
D1 1.50000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL1 -3.00 dB
SFO1 300.1718537 MHz
SI 65536
SF 300.1700120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



12.03

9.55

8.79
8.40
7.34
7.24
7.09
7.08
7.08
7.07
7.06
7.05
7.05
7.04
7.03
7.02
7.01
7.01
7.00
7.00
6.99
6.98
6.98
6.97
6.91
6.90
6.89
6.88
6.69
6.67
6.33
6.33
6.10

4.03
3.93
3.87
3.83
3.76
3.71
3.63
3.16
3.15
2.87

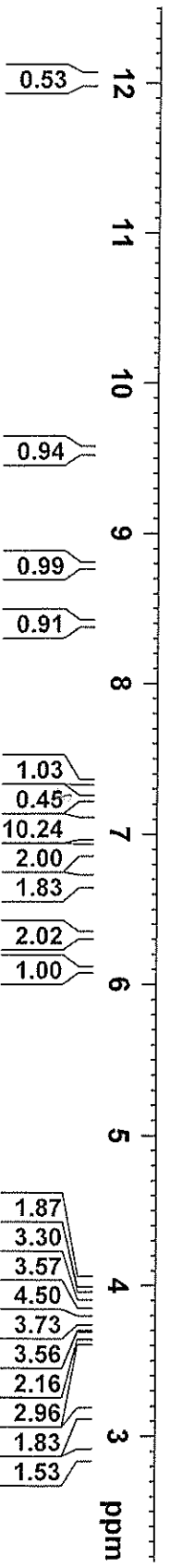
Supervisor BlackC-4

Compound 15a



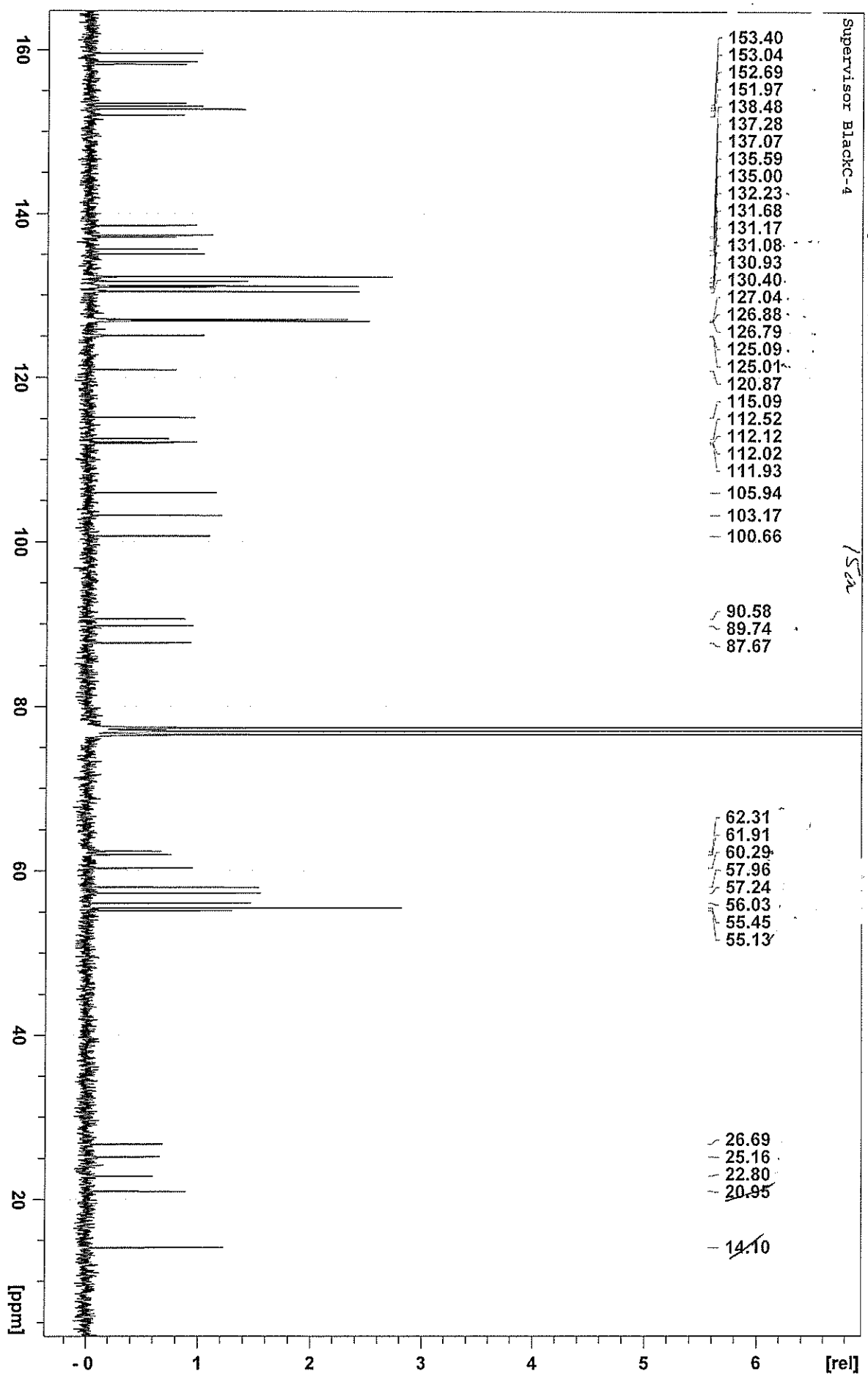
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EXPNO 10
PROCNO 1
Date_ 20100821
Time 15.03
INSTRUM dpx1
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5935.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 143.7
DE 83.400 usec
TE 294.6 K
D1 1.50000000 sec
TD0 1

===== CHANNEL F1 =====
NUC1 1H
P1 10.10 usec
PL1 -3.00 dB
SFO1 300.1719511 MHz
SI 65536
SF 300.1700120 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00



100821-hkn 11 1 N:\gyro\data\hkn\mr
Supervisor BlackC-4

Comparison
15a



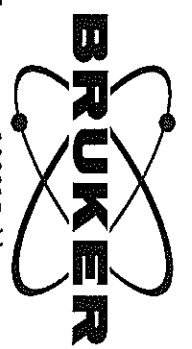
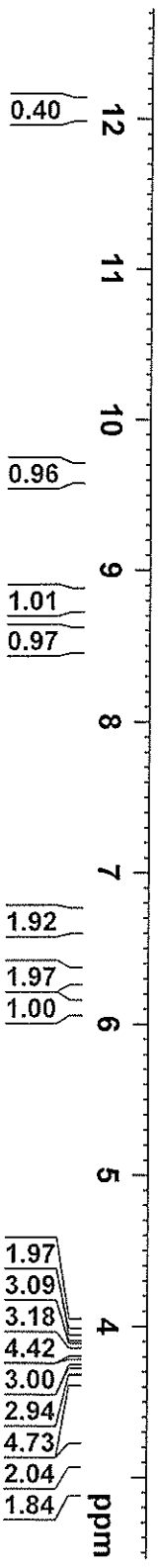
12.07
12.05
12.04
12.03

9.64
8.80
8.55
7.39
7.24
7.21
7.18
7.09
7.08
7.06
7.05
7.02
7.01
6.99
6.99
6.93
6.92
6.91
6.90
6.69
6.66
6.33
6.32
6.11

Compound 15b

3.92
3.87
3.84
3.77
3.70
3.63
3.16
3.14
2.97

Supervisor BlackC-2

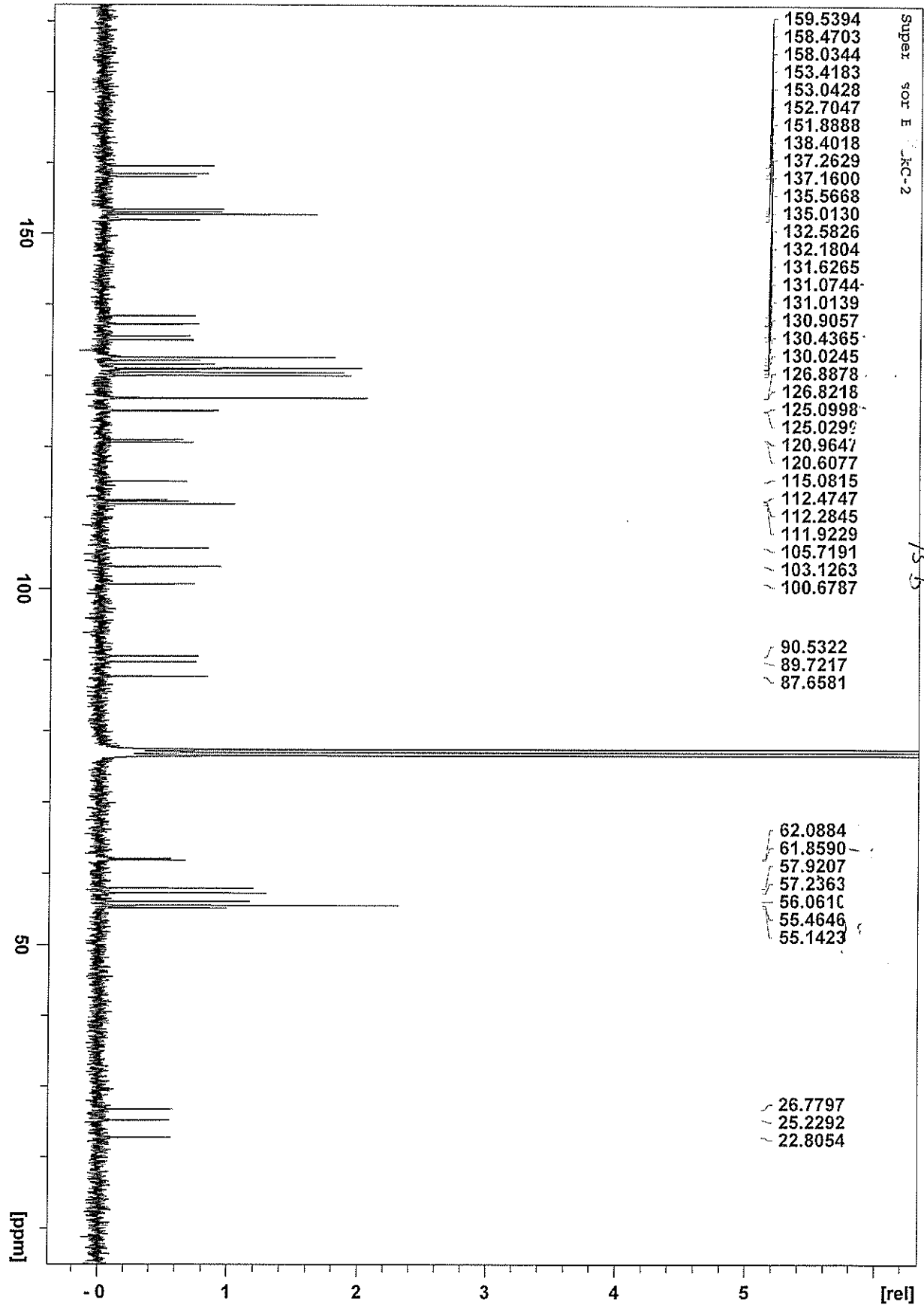


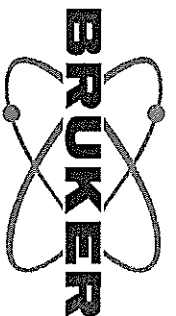
100815-hkm
NAME
EXPNO 20
PROCNO 1
Date_ 20100815
Time 17.33
INSTRUM dpx1
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 143.7
DM 83.400 usec
DE 12.00 usec
TE 293.7 K
D1 1.50000000 sec
TDO 1

==== CHANNEL F1 =====
NUC1 1H
P1 10.10 usec
PL1 -3.00 dB
SF01 300.1719511 MHz
SI 65536
SP 300.1700120 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

100815-hkm 21 1 N:\Gyro\data\hkm\mr
Super sor E JC-2

Compound 15-B

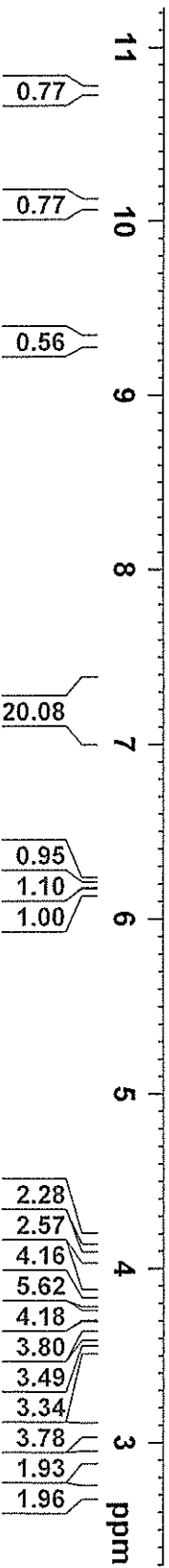




- 10.752
- 10.097
- 9.312
- 7.340
- 7.312
- 7.224
- 7.208
- 7.166
- 7.147
- 7.120
- 7.056
- 7.032
- 6.222
- 6.199
- 6.156
- 4.171
- 4.062
- 3.848
- 3.812
- 3.728
- 3.670
- 3.566
- 3.551
- 3.072
- 2.917
- 2.713

Supervisor Black
C-7
1H CDCl3 F:\ \ hkn 10

Compound 15C



Current Data Parameters
NAME 110503-hkn
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110503
Time 17.33
INSTRUM dpx2
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 4816.956 Hz
FIDRES 0.147002 Hz
AQ 3.4013684 sec
RG 128
DW 103.800 usec
DE 12.00 usec
TE 299.2 K
D1 2.00000000 sec
TD0 1

==== CHANNEL F1 =====
NUC1 1H
P1 14.90 usec
PL1 2.50 dB
SFO1 300.3019519 MHz
F2 - Processing parameters
SI 65536
SF 300.3000341 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00



Current Data Parameters
 NAME 110503-hkn
 EXPNO 3
 PROCNO 1

Compound
 15c

Supervisor Black
 C-7
 13C(1H) CDC13 hkn 10

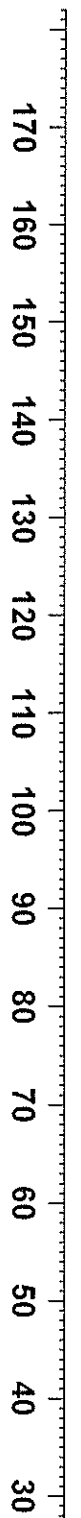
F2 - Acquisition Parameters

Date_ 20110503
 Time 19.17
 INSTRUM dpx2
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 32768
 SOLVENT CDC13
 NS 2048
 DS 0
 SWH 18832.393 Hz
 FIDRES 0.574719 Hz
 AQ 0.8700404 sec
 RG 16384
 DM 26.550 usec
 DE 25.00 usec
 TE 299.2 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 L31 1
 TDO 1

==== CHANNEL F1 =====
 NUCL 13C
 P1 9.80 usec
 PL1 -1.20 dB
 SFO1 75.5191787 MHz

==== CHANNEL F2 =====
 CPDPRG2 bi_waltz65_256
 NUCL 1H
 PCPD2 80.00 usec
 PL2 2.50 dB
 PL12 17.10 dB
 PL13 20.10 dB
 SFO2 300.3015017 MHz

Processing parameters
 SI 32768
 WDW 75.5104950 MHz
 SSB EM
 LB 0
 GB 0
 PC 1.40
 ppm



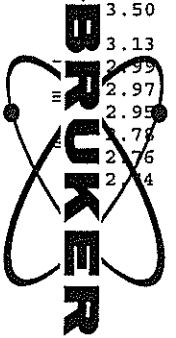
Supervisor BlackC-5

10.72
10.11
9.39

7.35
7.26
7.25
7.25
7.25
7.24
7.24
7.23
7.22
7.20
7.20
7.18
7.17
7.16
7.16
7.14
7.12
7.12
7.09
6.30
6.27
6.24

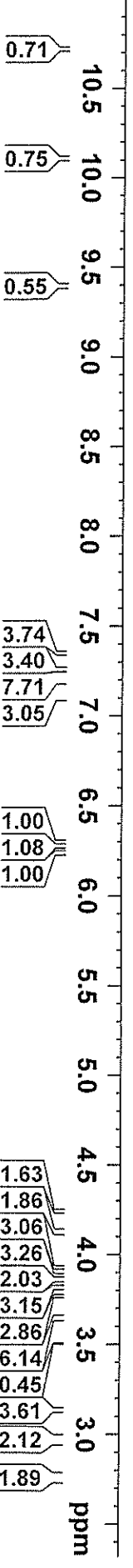
Compound Ka

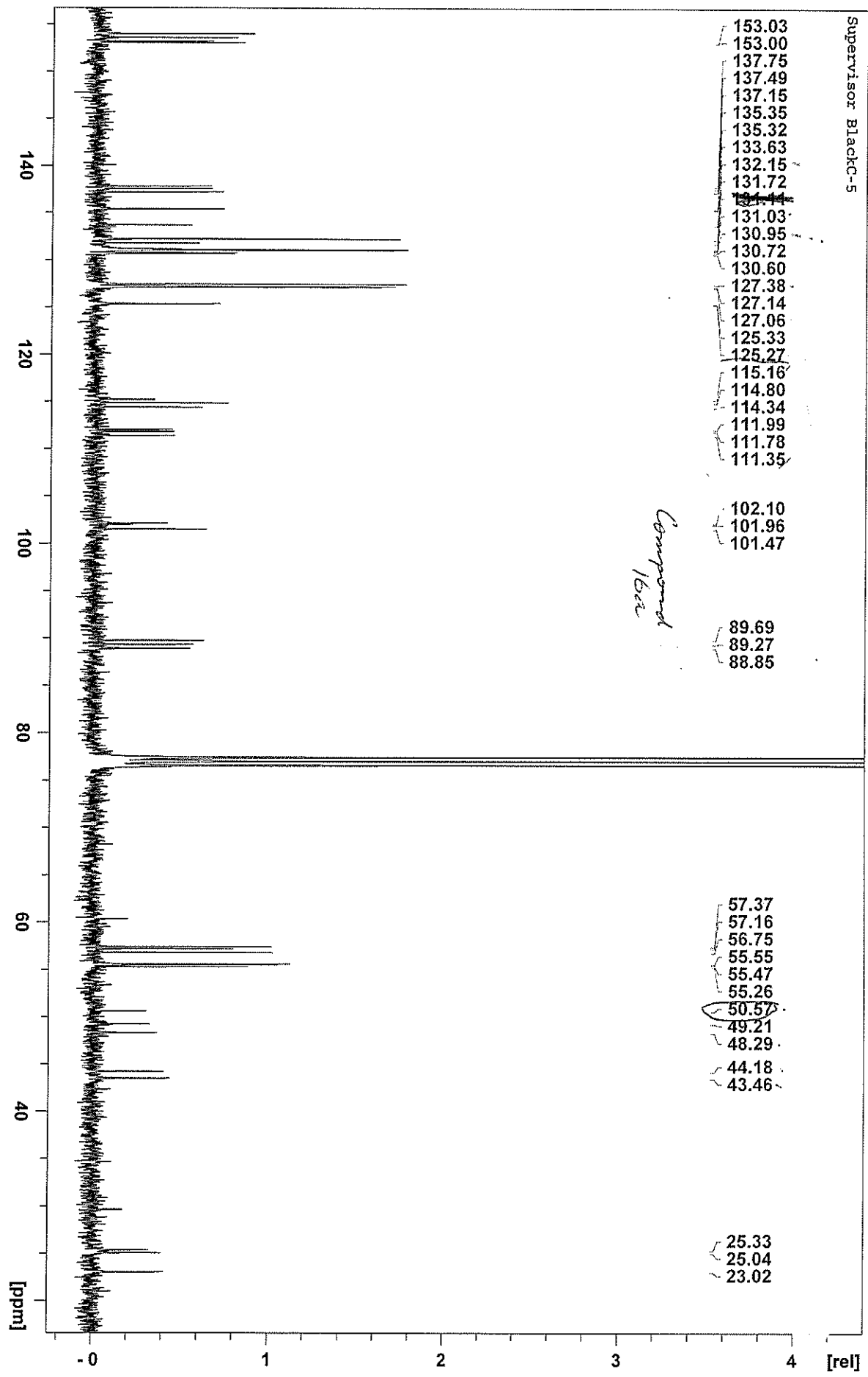
4.24
4.13
3.93
3.88
3.86
3.82
3.77
3.65
3.64
3.50
3.13
2.99
2.97
2.95
2.78
2.76
2.74

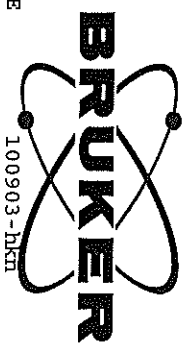


NAME 100825-nkn
EXPNO 10
PROCNO 1
Date_ 20100825
Time 15.51
INSTRUM dpx1
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 574.7
DW 83.400 usec
DE 12.00 usec
TE 294.1 K
D1 1.50000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL -3.00 dB
SFO1 300.1719511 MHz
SI 65536
SF 300.1700120 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00



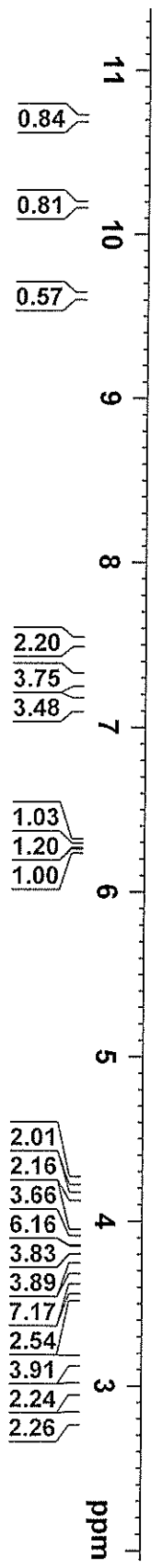




Supervisor BlackC-3

Compound 168

- 10.71
- 10.18
- 9.62
- 7.53
- 7.50
- 7.31
- 7.28
- 7.26
- 7.23
- 7.21
- 7.17
- 7.15
- 7.13
- 7.10
- 6.30
- 6.28
- 6.25
- 5.30
- 4.24
- 4.15
- 3.93
- 3.89
- 3.82
- 3.77
- 3.65
- 3.65
- 3.54
- 3.14
- 2.98
- 2.97
- 2.82
- 2.80



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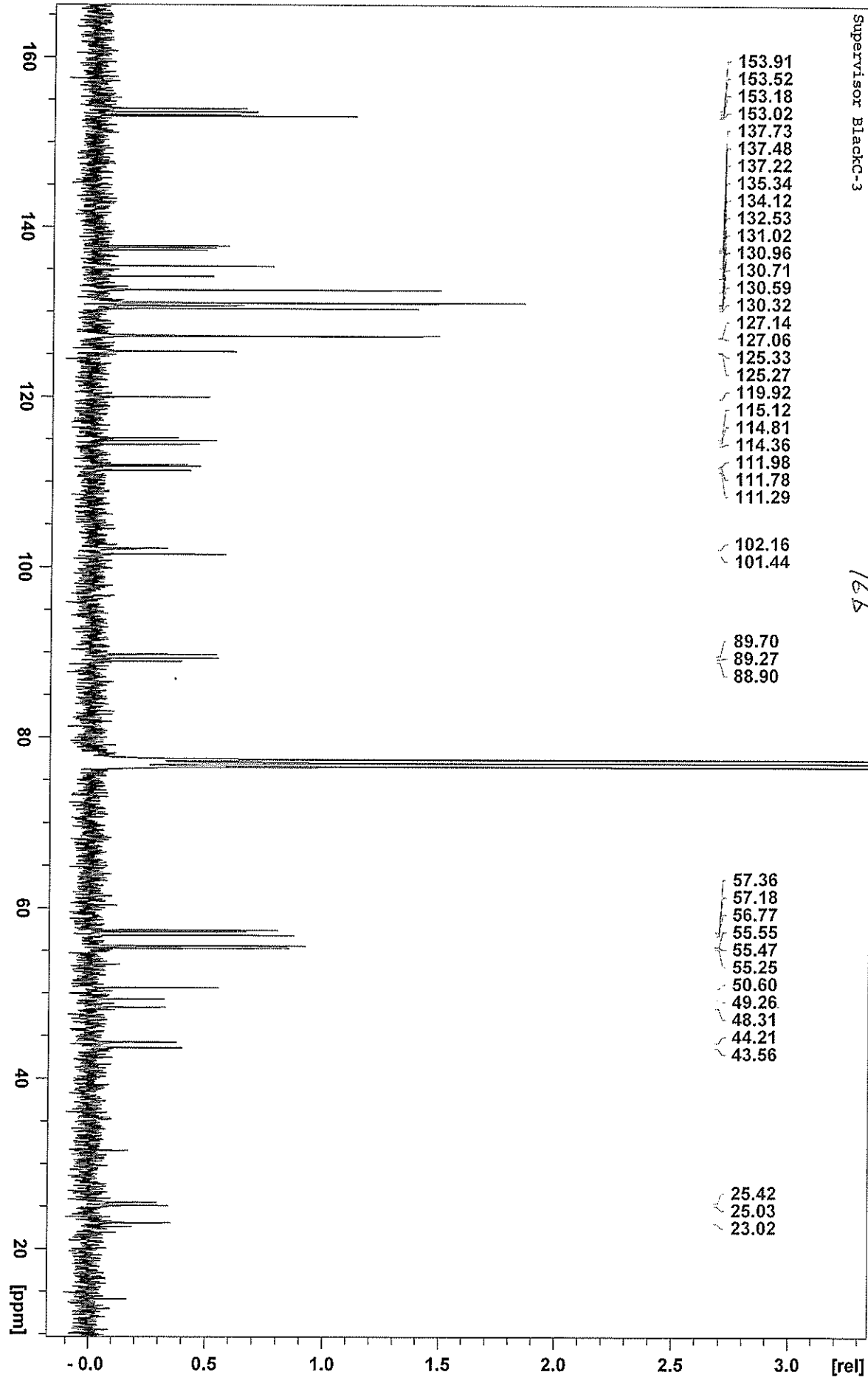
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EXPNO 60
PROCNO 1
Date_ 20100903
Time 20.59
INSTRUM dpx1
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 161.3
DW 83.400 usec
DE 12.00 usec
TE 294.2 K
D1 1.50000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.10 usec
PL -3.00 dB
SFO1 300.1719511 MHz
SI 65536
SF 300.1700120 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

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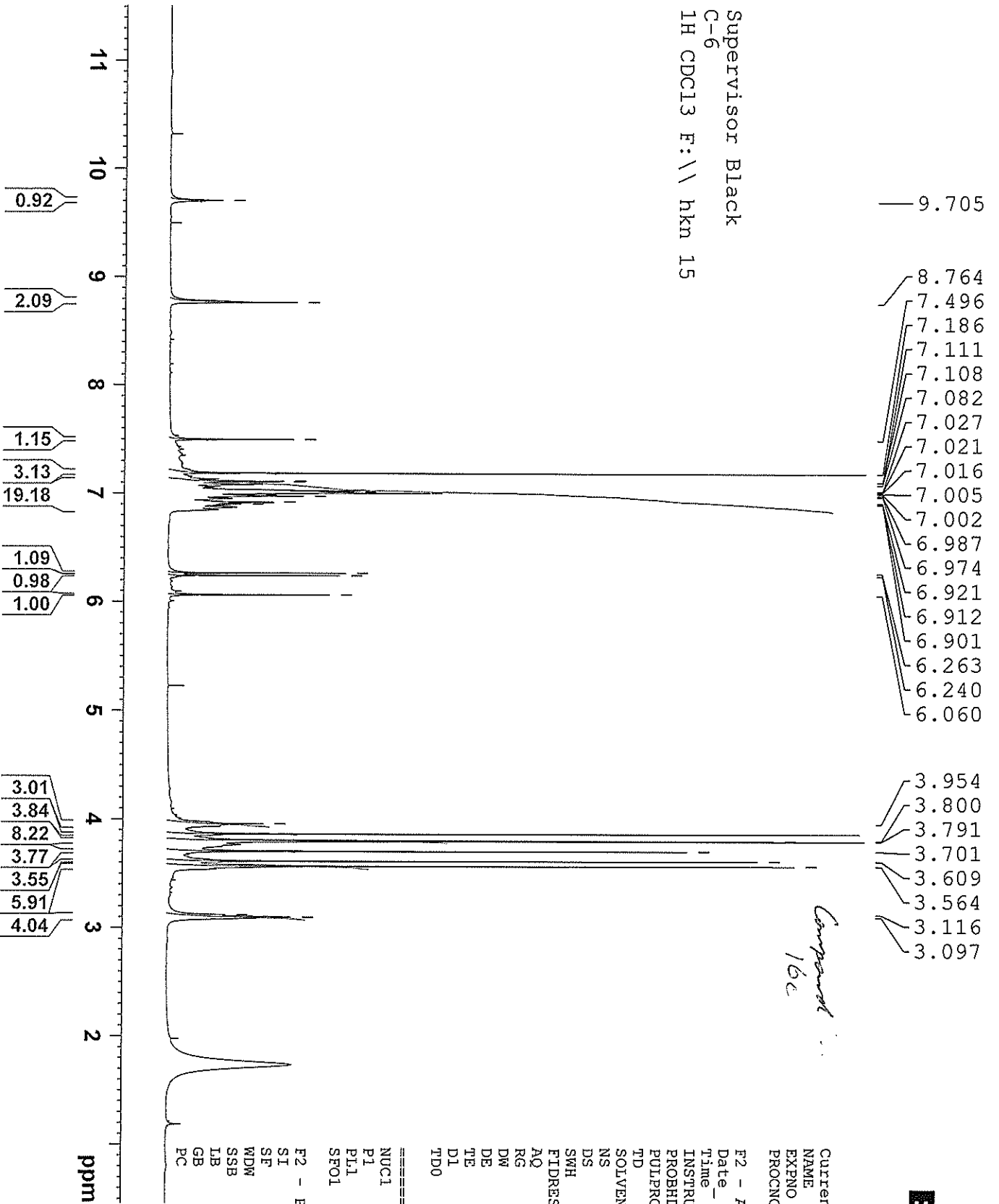

100903-hkm 61 1 N:\Gyro\data\hkm\mr
Supervisor BlackC-3

Campana
165





Supervisor Black
C-6
1H CDCl3 F:\ hkn 15



- 9.705
- 8.764
- 7.496
- 7.186
- 7.111
- 7.108
- 7.082
- 7.027
- 7.021
- 7.016
- 7.005
- 7.002
- 6.987
- 6.974
- 6.921
- 6.912
- 6.901
- 6.263
- 6.240
- 6.060
- 3.954
- 3.800
- 3.791
- 3.701
- 3.609
- 3.564
- 3.116
- 3.097

- 0.92
- 2.09
- 1.15
- 3.13
- 19.18
- 1.09
- 0.98
- 1.00
- 3.01
- 3.84
- 8.22
- 3.77
- 3.55
- 5.91
- 4.04

Compound 16c

Current Data Parameters
NAME 110209-hkn
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20110209
Time 14.57
INSTRUM dpx2
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 4816.956 Hz
FIDRES 0.147002 Hz
AQ 3.4013684 sec
RG 322.5
DW 103.800 usec
DE 12.00 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 14.90 usec
PL1 2.50 dB
SFO1 300.3019519 MHz
F2 - Processing parameters
SI 65536
SF 300.3000280 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00

110303-hkn 3 1 "C:\Users\Hakan\Documents\NMR Data\F11p"

Supervisor Black

C-6

13C{1H} CDCl3 F:\hkn 10

Component 1: 13c

