

Supporting Information for:

Nickel-Catalyzed Decarboxylative Arylation of Azoles with Perfluoro- and Nitrobenzoates

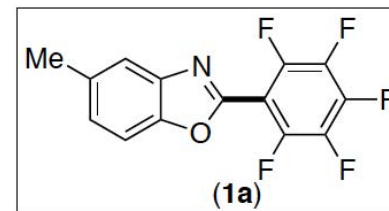
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and Dipannita Kalyani*

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Email: kalyani@stolaf.edu

¹H NMR and ¹³C NMR spectra

DK-XXIV-JC-156 PURE

user: sa...
team: research-kalyani holder: 15
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

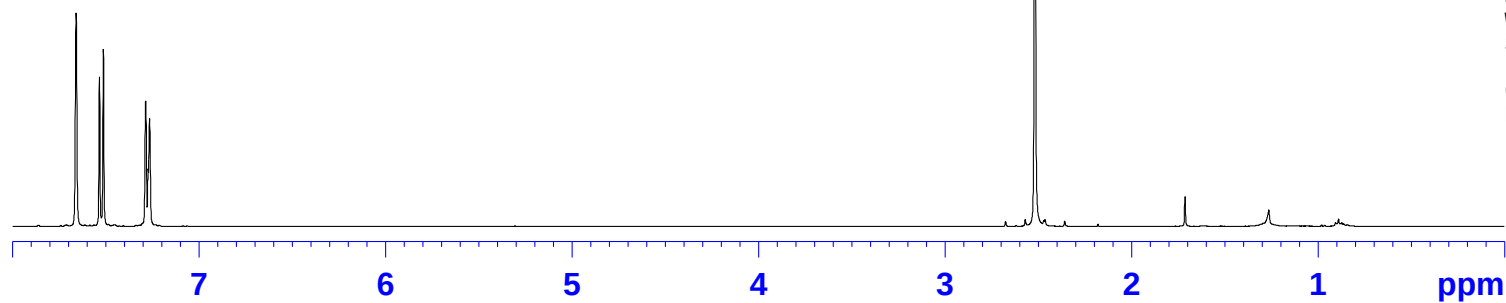


Current Data Parameters
NAME Nov23-2014
EXPNO 1014810
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141124
Time 3.23
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 256
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

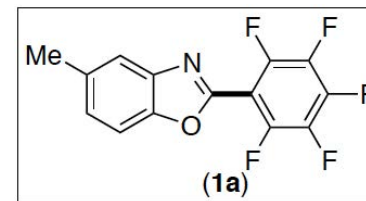


1.00
1.01
1.13

3.27

DK-XXIV-JC-156 PURE

user: sa...
team: research-kalyani holder: 15
solvent: CDCl₃ expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



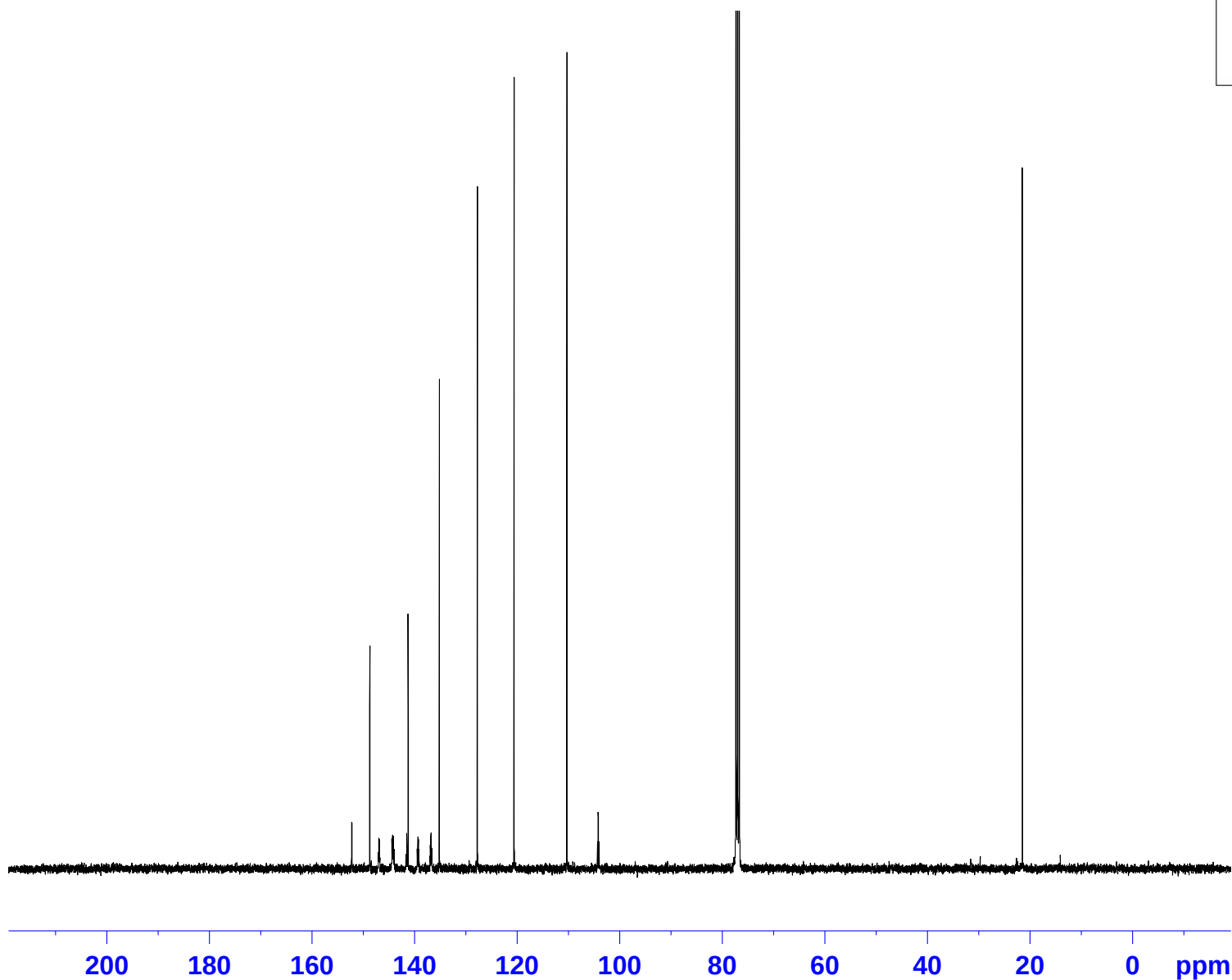
Current Data Parameters
NAME Nov23-2014
EXPNO 1014910
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141124
Time 11.04
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4096
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

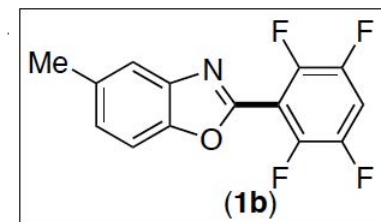
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XXIV-JC-121 dry, pure

user: cr...
team: research-kalyani-crawforj holder: 12
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

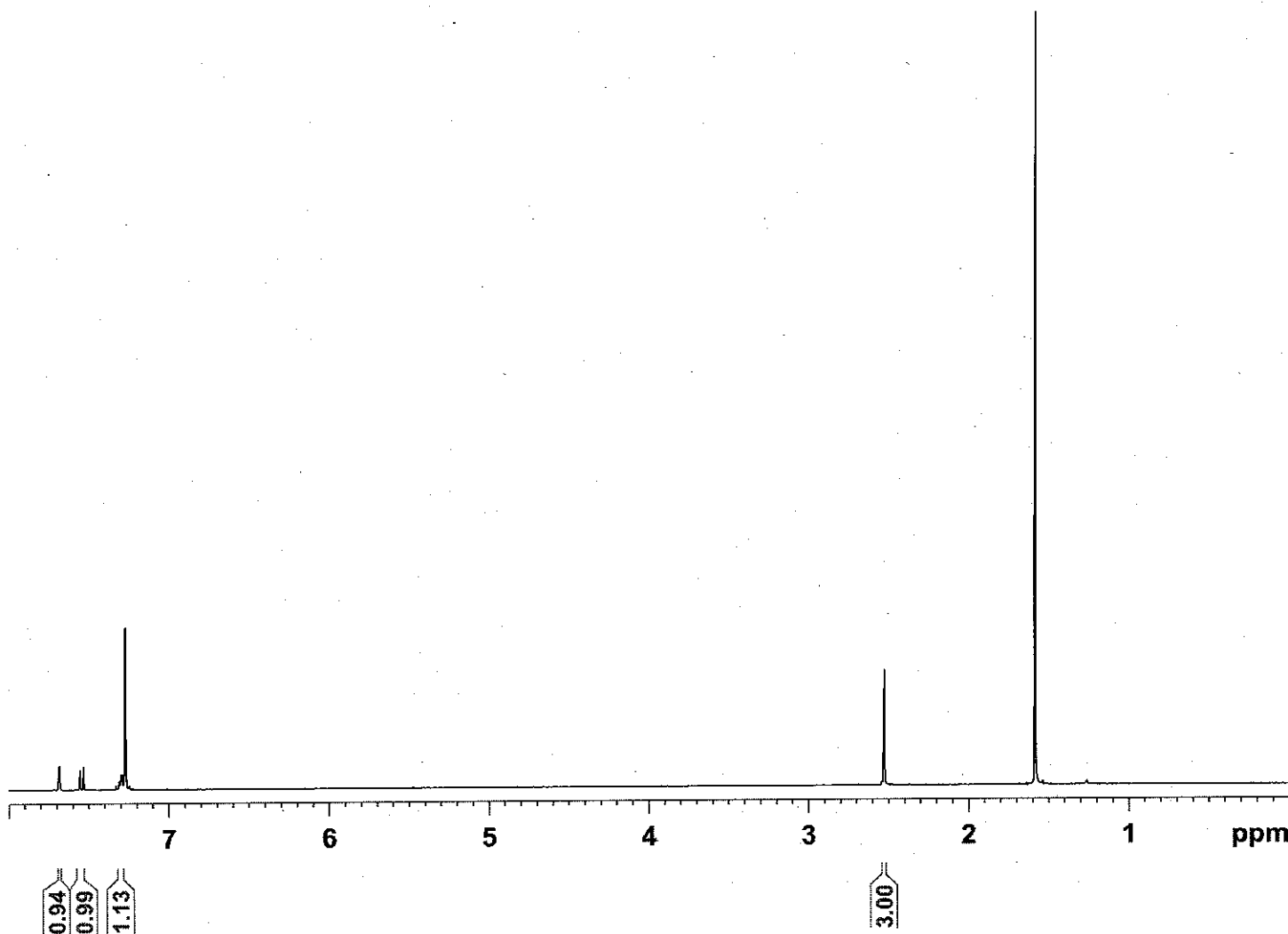


Current Data Parameters
NAME Jul31-2014
EXPNO 1913310
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140731
Time 14.50
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 724.1
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

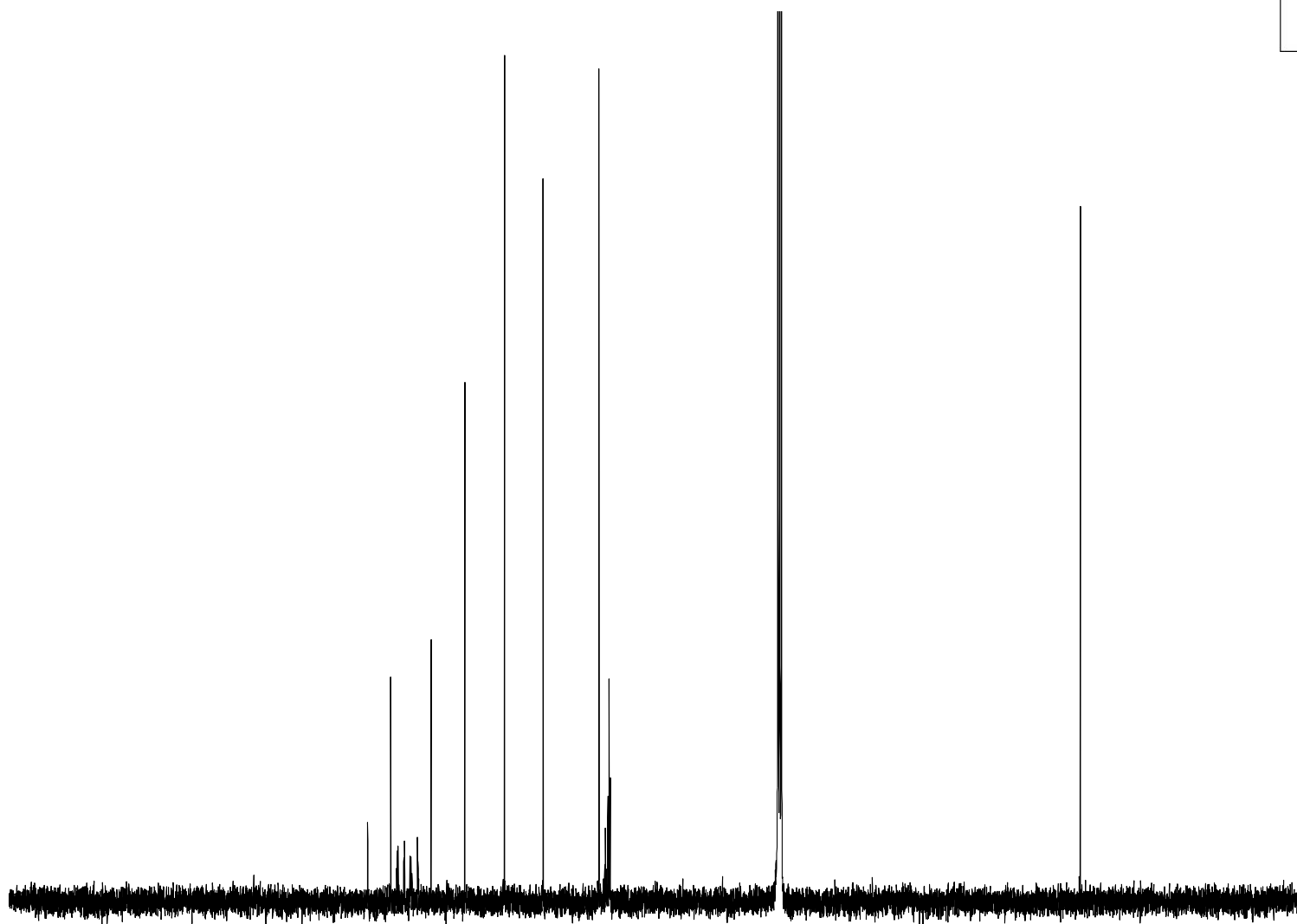
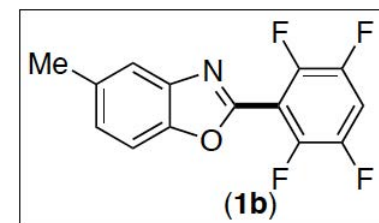
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-121 (C13)

user: sh...
team: research-kalyani-shelton holder: 9
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



Current Data Parameters
NAME Nov13-2014
EXPNO 1006210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141114
Time 11.30
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 14596.5
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

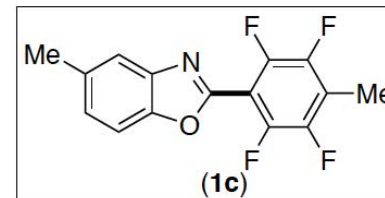
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM

200 180 160 140 120 100 80 60 40 20 0 ppm

DK-XXIV-JC-60 isolated x2

user: cr...
team: research-kalyani holder: 12
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment (1 Min 17 Sec)

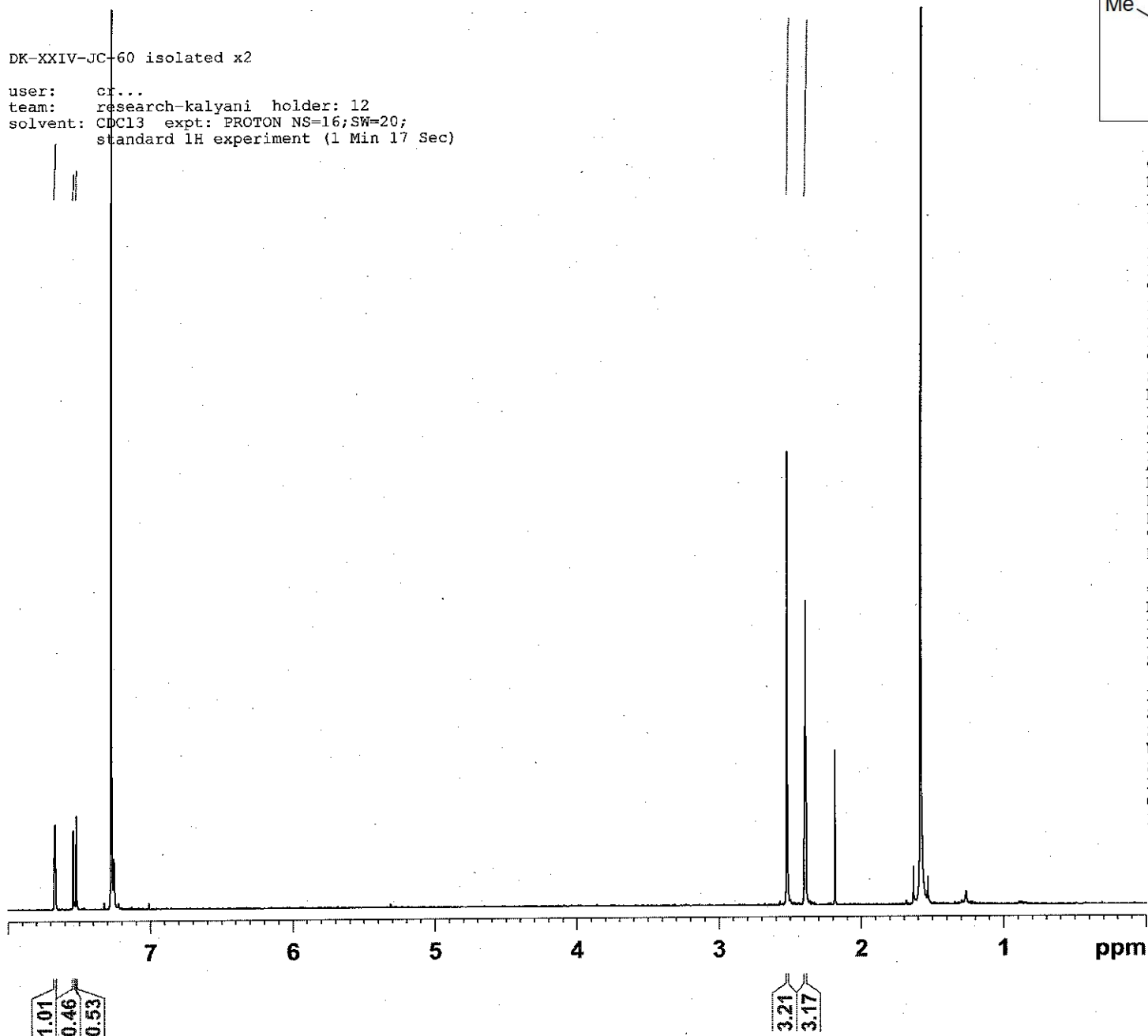


Current Data Parameters
NAME Jun19-2014
EXPNO 1866010
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140619
Time_ 15.30
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

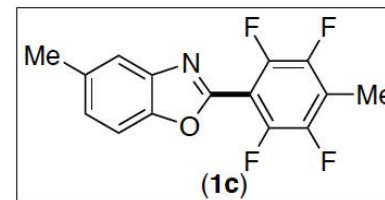
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-60 PURE

user: sa...
team: research-kalyani holder: 14
solvent: CDCl₃ expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



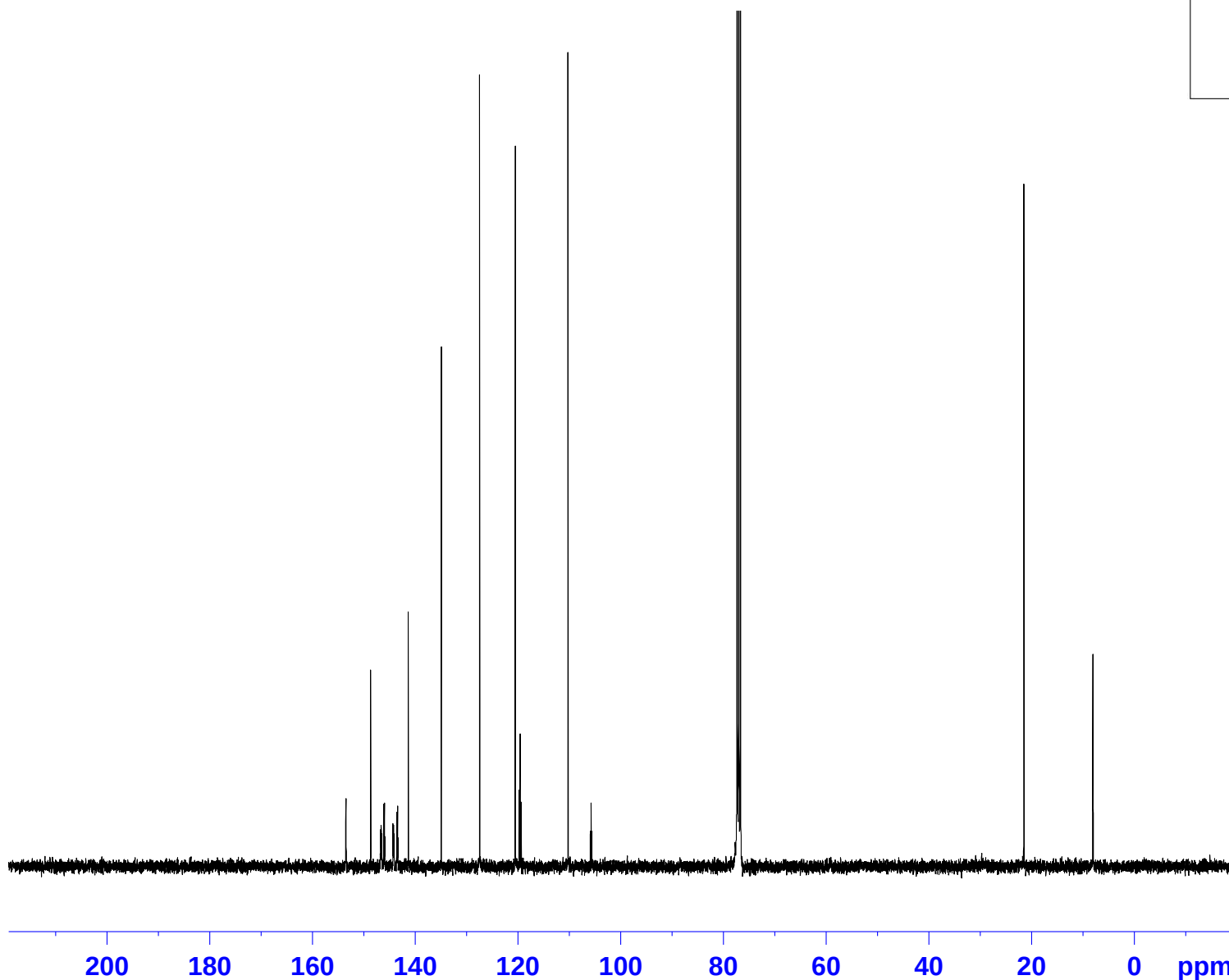
Current Data Parameters
NAME Nov23-2014
EXPNO 1014710
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141124
Time 3.17
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 14596.5
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

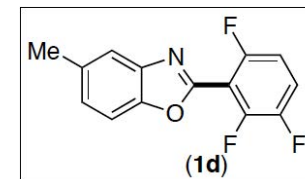
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XXIV-JC-114-2 PURE, DRY

user: cr...
team: research-kalyani-crawforj holder: 9
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

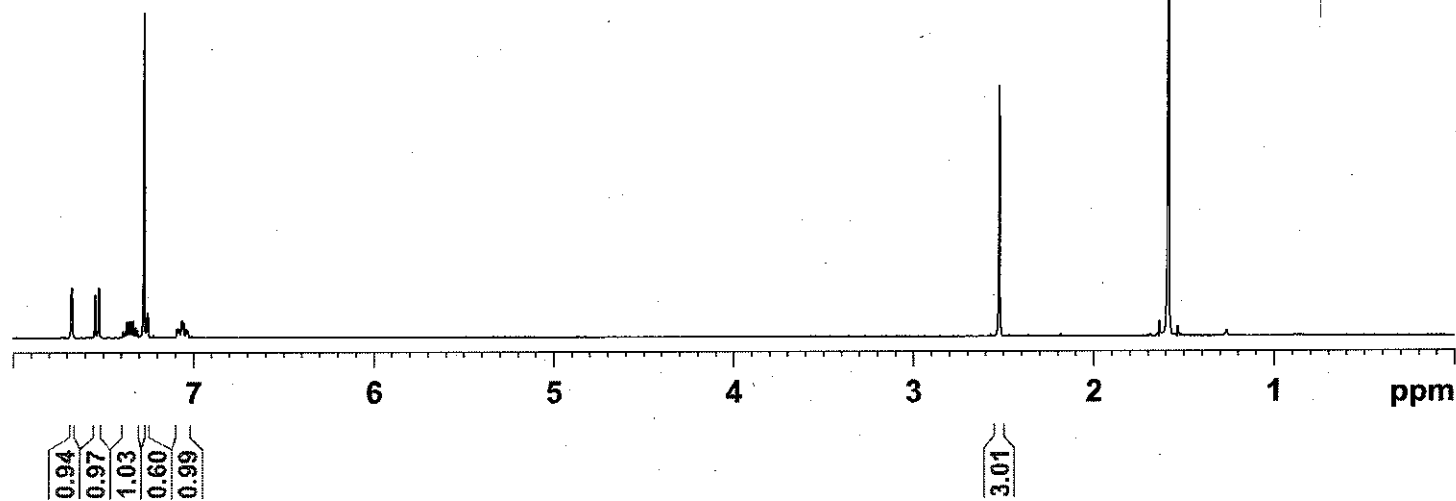


Current Data Parameters
NAME Jul23-2014
EXPNO 1900010
PROCNO 1

F2 - Acquisition Parameters
Date 20140723
Time 10.39
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

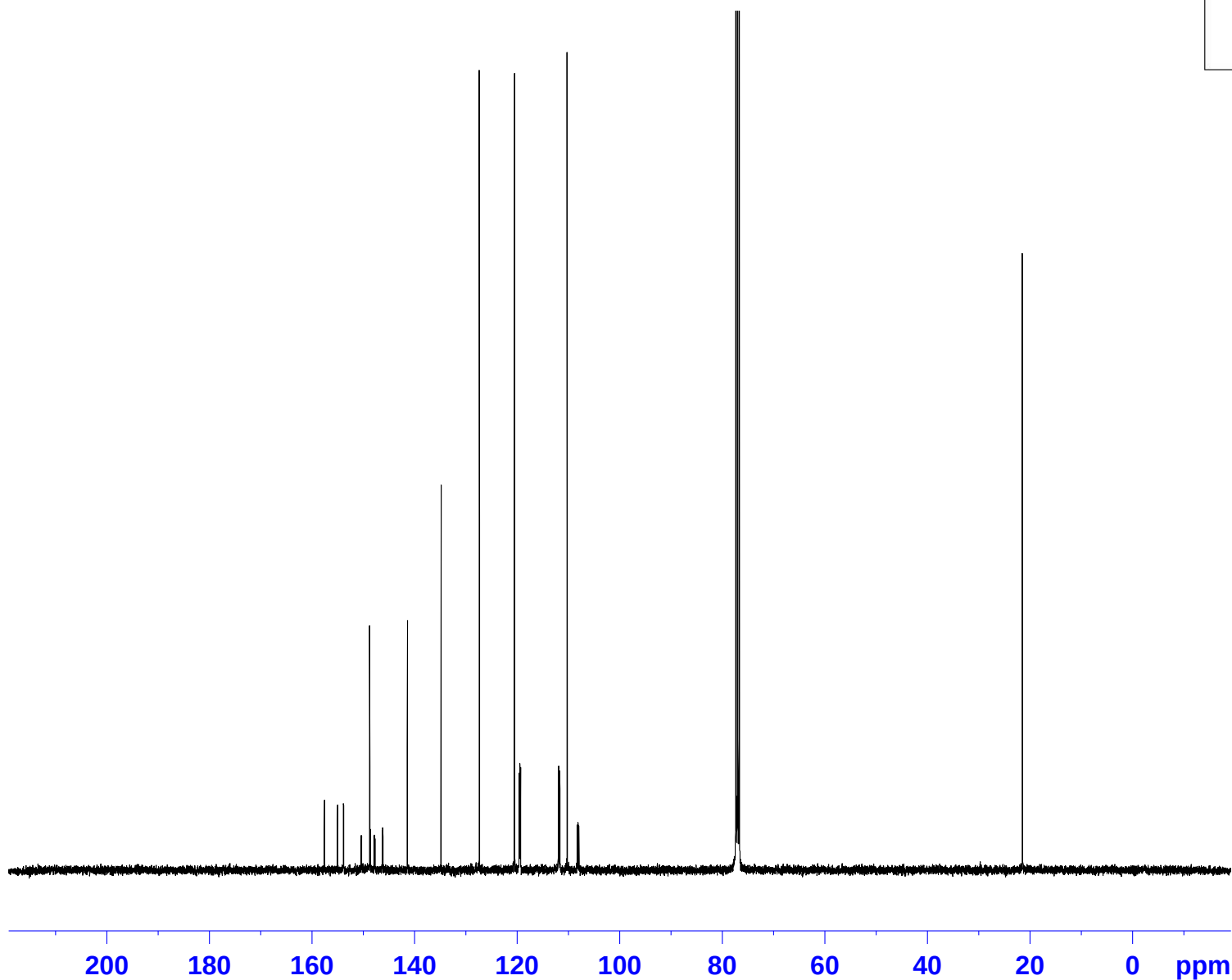
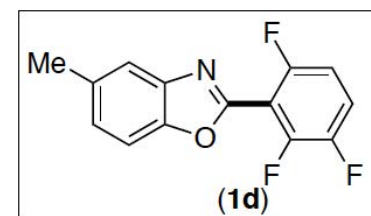
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-114-2 C13

user: cr...
team: research-kalyani-crawforj holder: 3
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



Current Data Parameters
NAME Nov04-2014
EXPNO 1978910
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141105
Time 3.09
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 3251
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

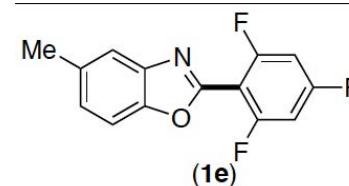
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM

DK-XVII-KS-108 fr. 51-70 pure dry

user: cr...
team: research-kalyani-shelton holder: 1
solvent: CDCl3 expt: PROTON NS=128;SW=20;
standard 1H experiment ()

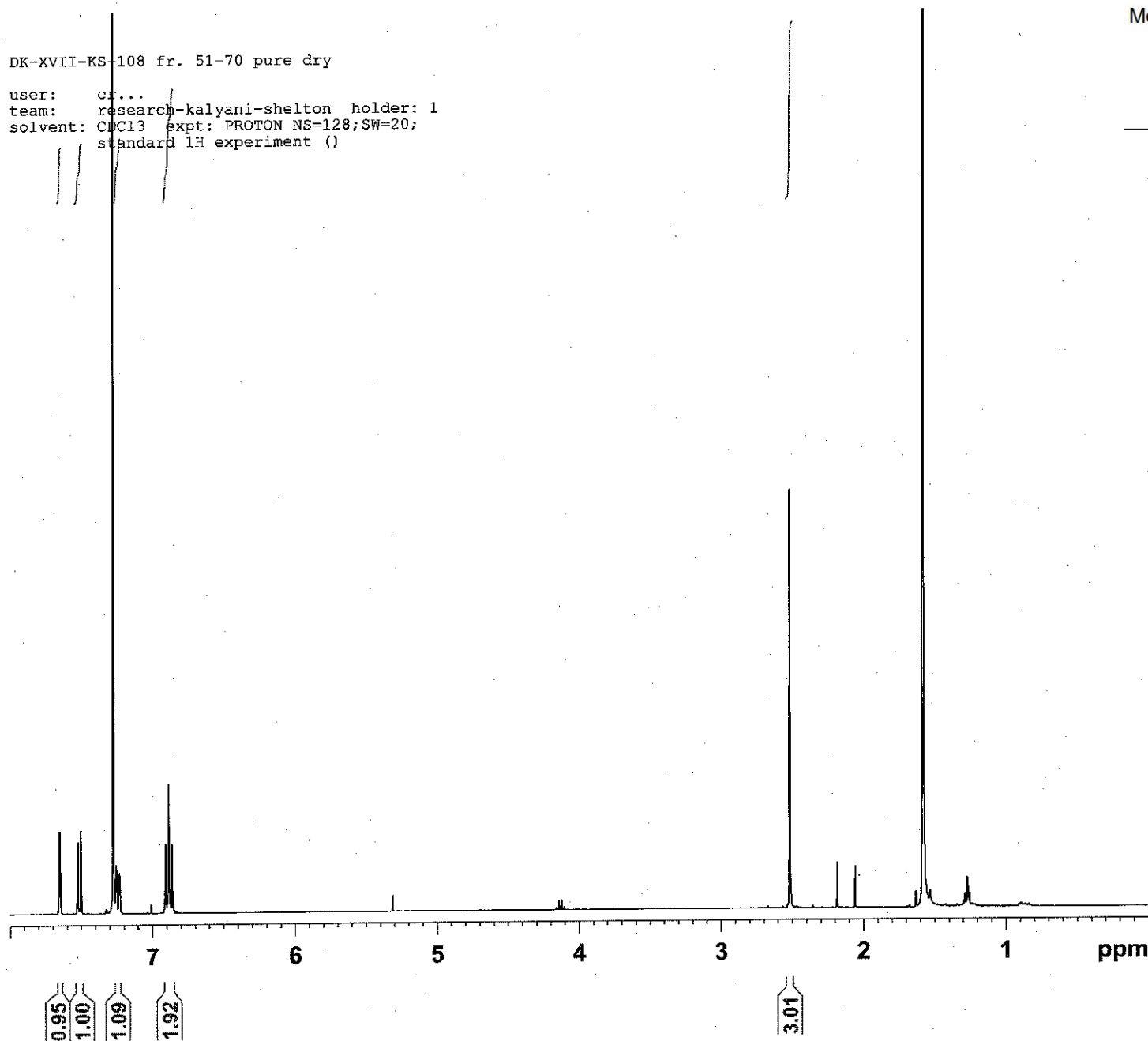


Current Data Parameters
NAME Jul04-2014
EXPNO 1880910
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140704
Time_ 15.20
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

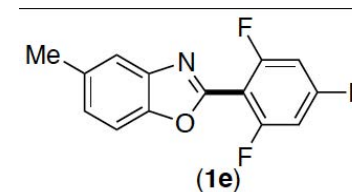
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XVII-KS-104? (2,4,6-TRIFLUORO) (C13)

user: sh...
team: research-kalyani-shelton holder: 6
solvent: CDCl3 expt: C13CPD32 NS=8000;D1=2;
standard C13 experiment (1 Min 36 Sec)



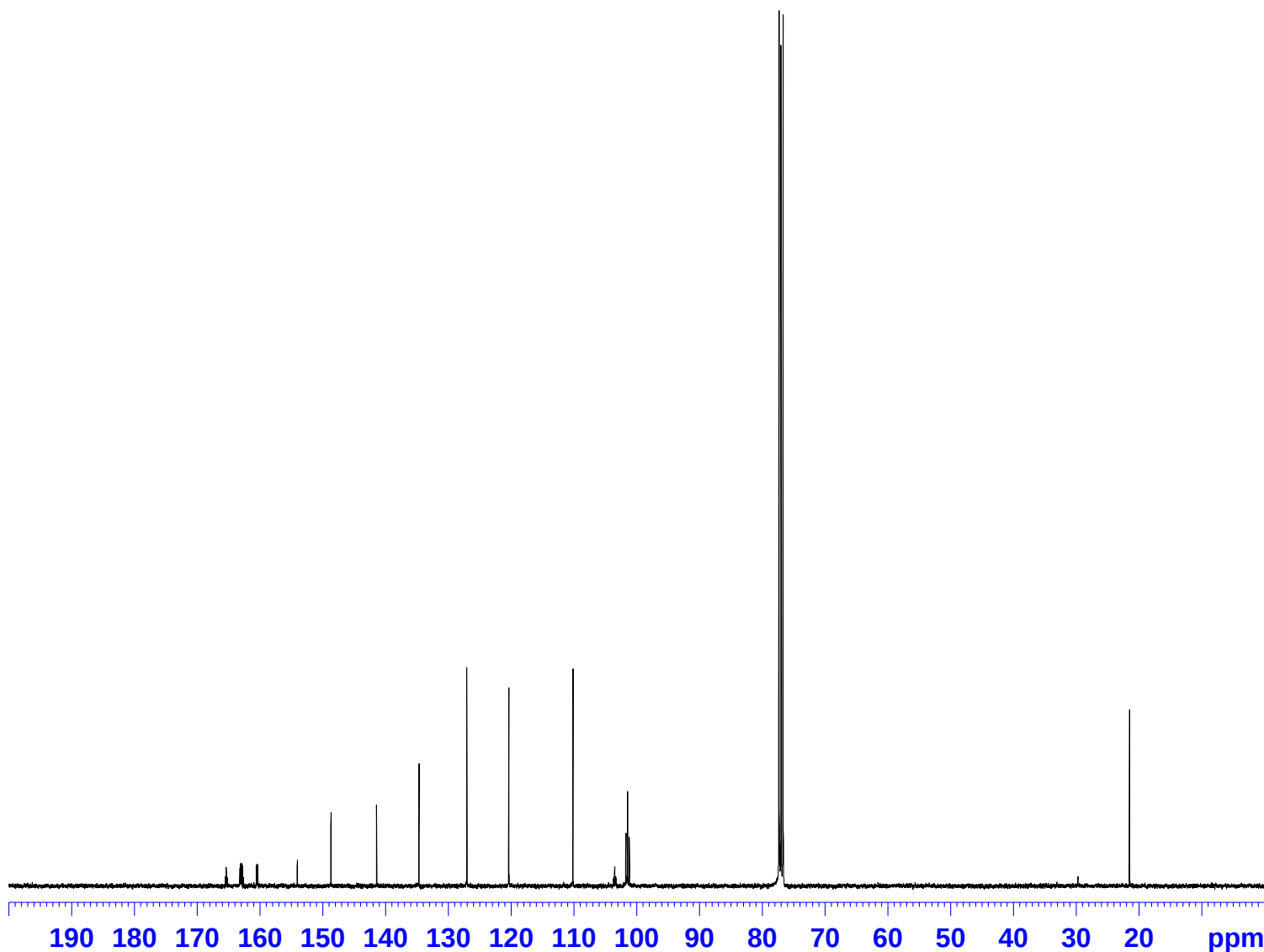
Current Data Parameters
NAME Oct30-2014
EXPNO 1968710
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141031
Time 5.22
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2048
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

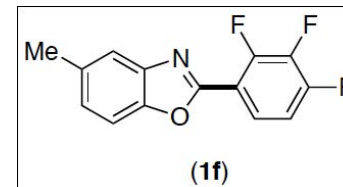
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XXIV-JC-152 (PURE FRACTIONS)

user: sa...
team: research-kalyani-sadarana holder: 7
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

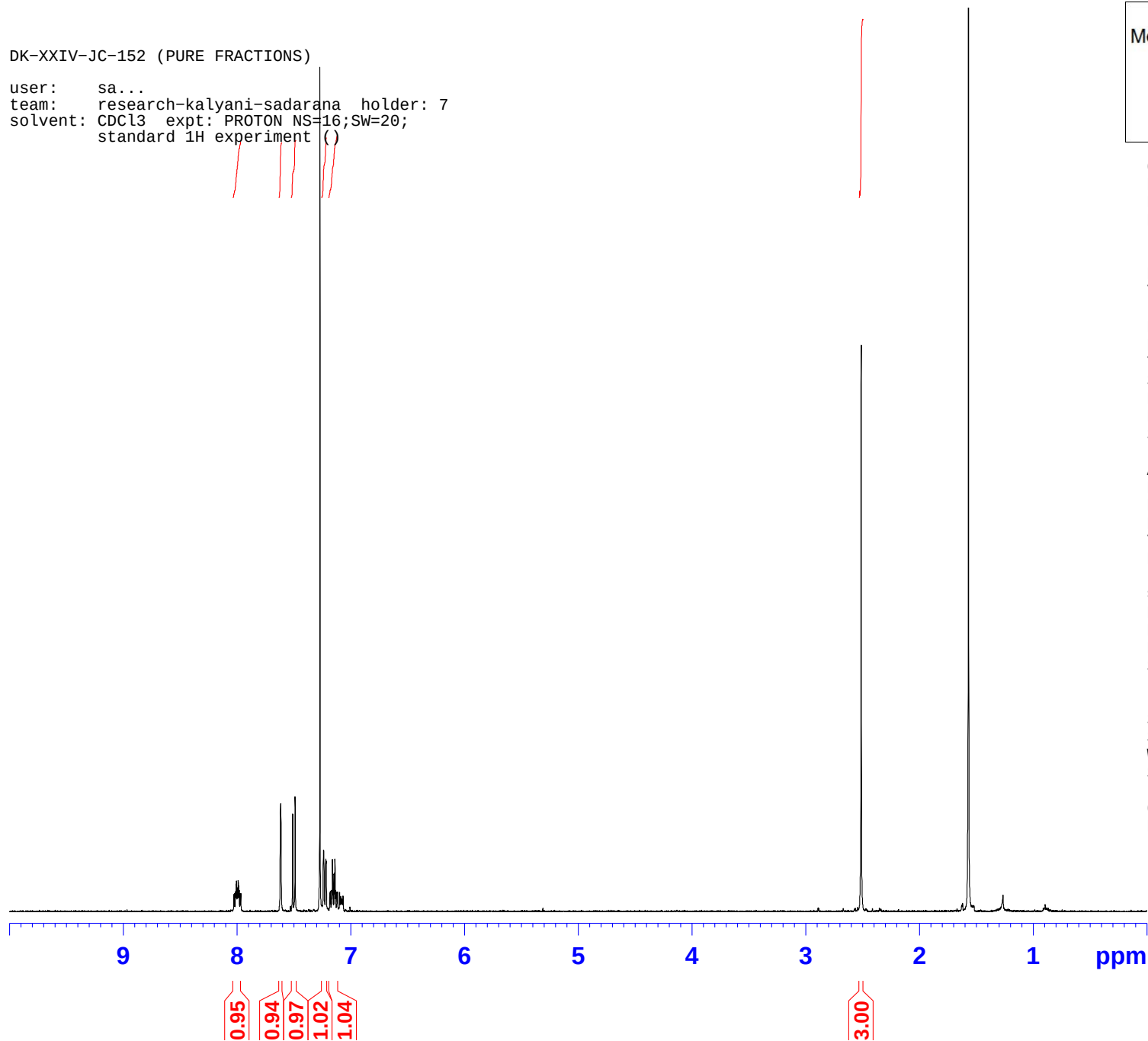


Current Data Parameters
NAME Nov02-2014
EXPNO 1969810
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141102
Time 15.15
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

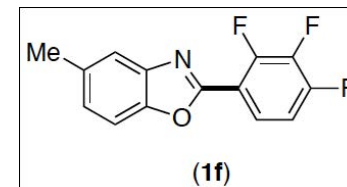
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-152 (C13)

user: sh...
team: research-kalyani-shelton holder: 8
solvent: CDCl3 expt: C13CPD32 NS=8000;D1=2;
standard C13 experiment ()



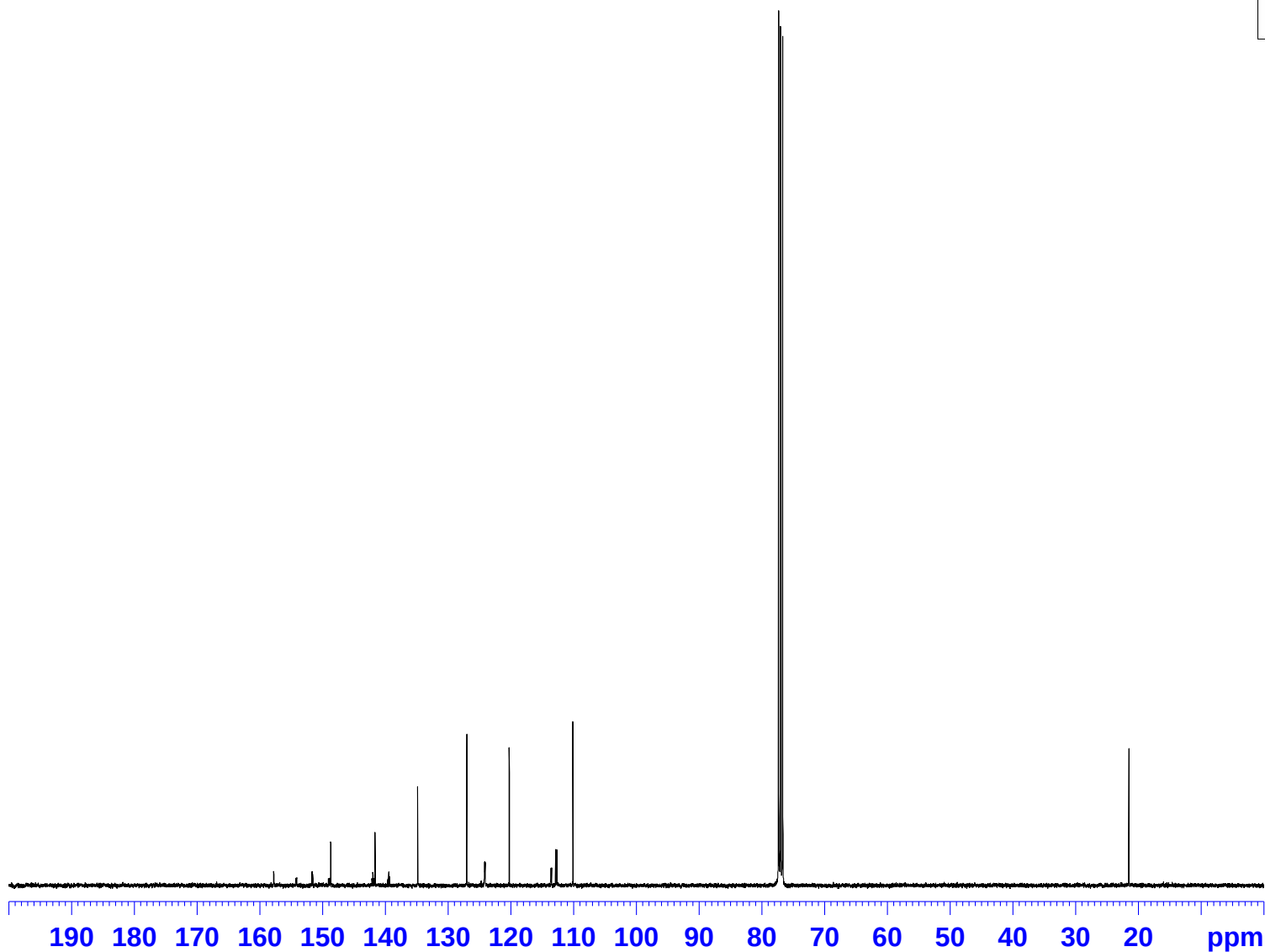
Current Data Parameters
NAME Nov08-2014
EXPNO 1987810
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141109
Time 10.18
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8000
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4096
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

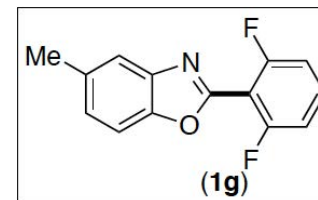
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XXIV-JC-82 pure, dry

user: cr...
team: research-kalyani-crawforj holder: 3
solvent: CDC13 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

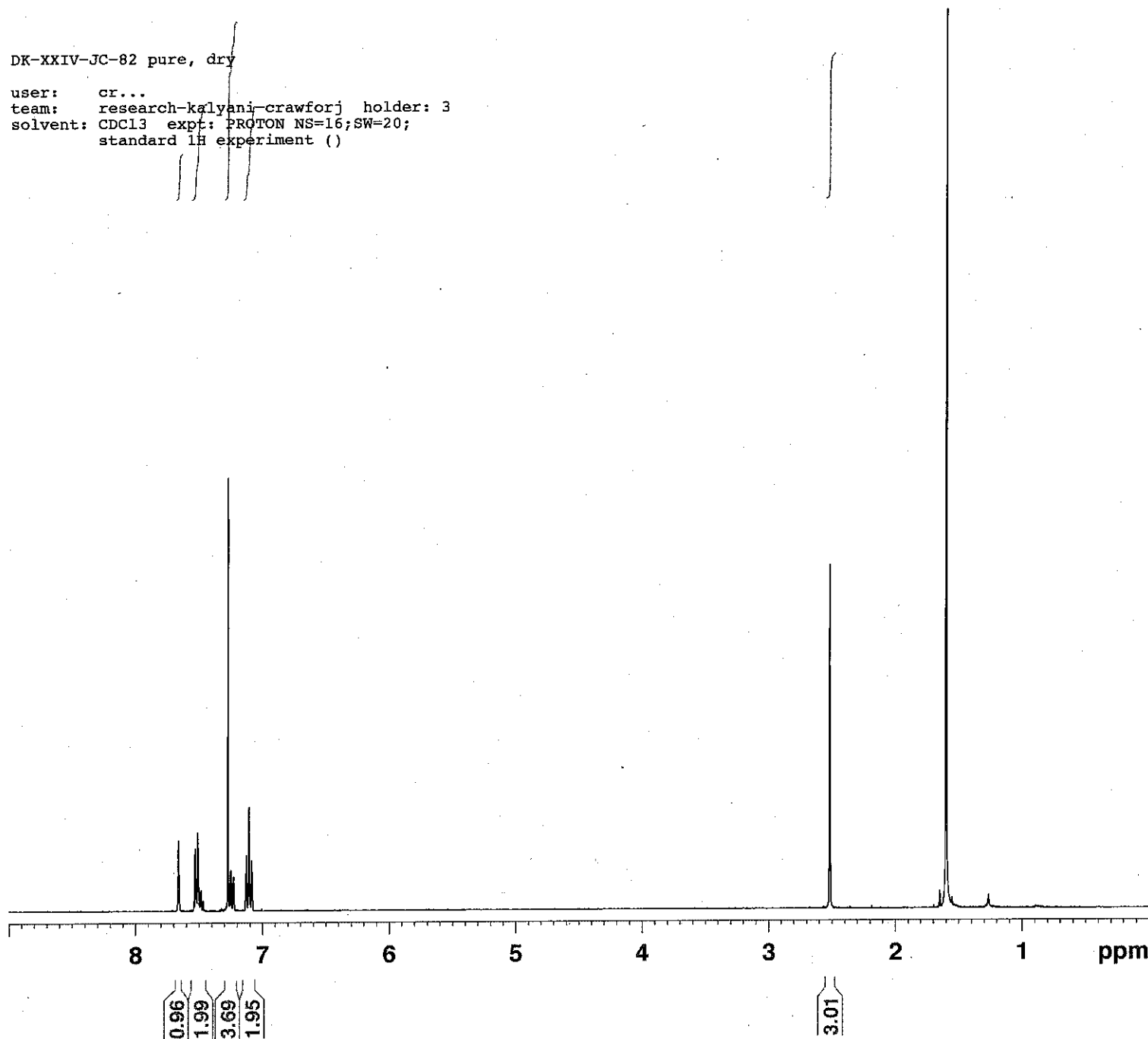


Current Data Parameters
NAME Jul01-2014
EXPNO 1877710
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140701
Time 15.25
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 724.1
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

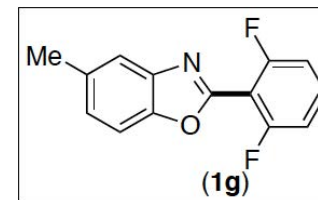
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-82 PURE

user: sa...
team: research-kalyani holder: 1
solvent: CDCl₃ expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



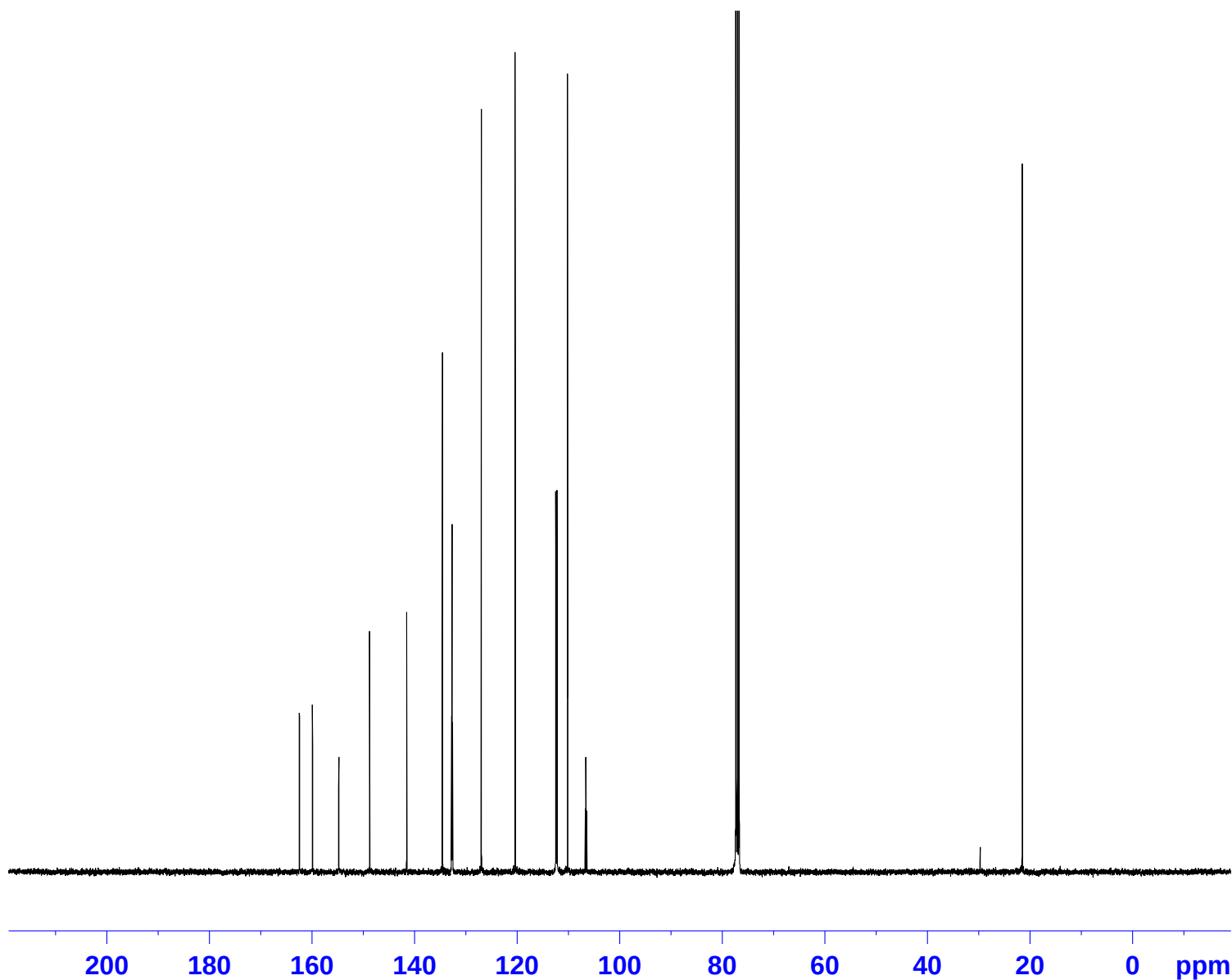
Current Data Parameters
NAME Dec08-2014
EXPNO 1021610
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141209
Time 16.49
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2298.8
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

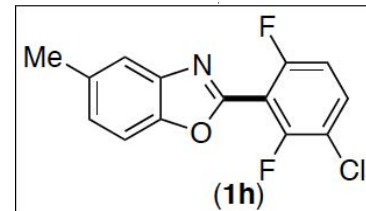
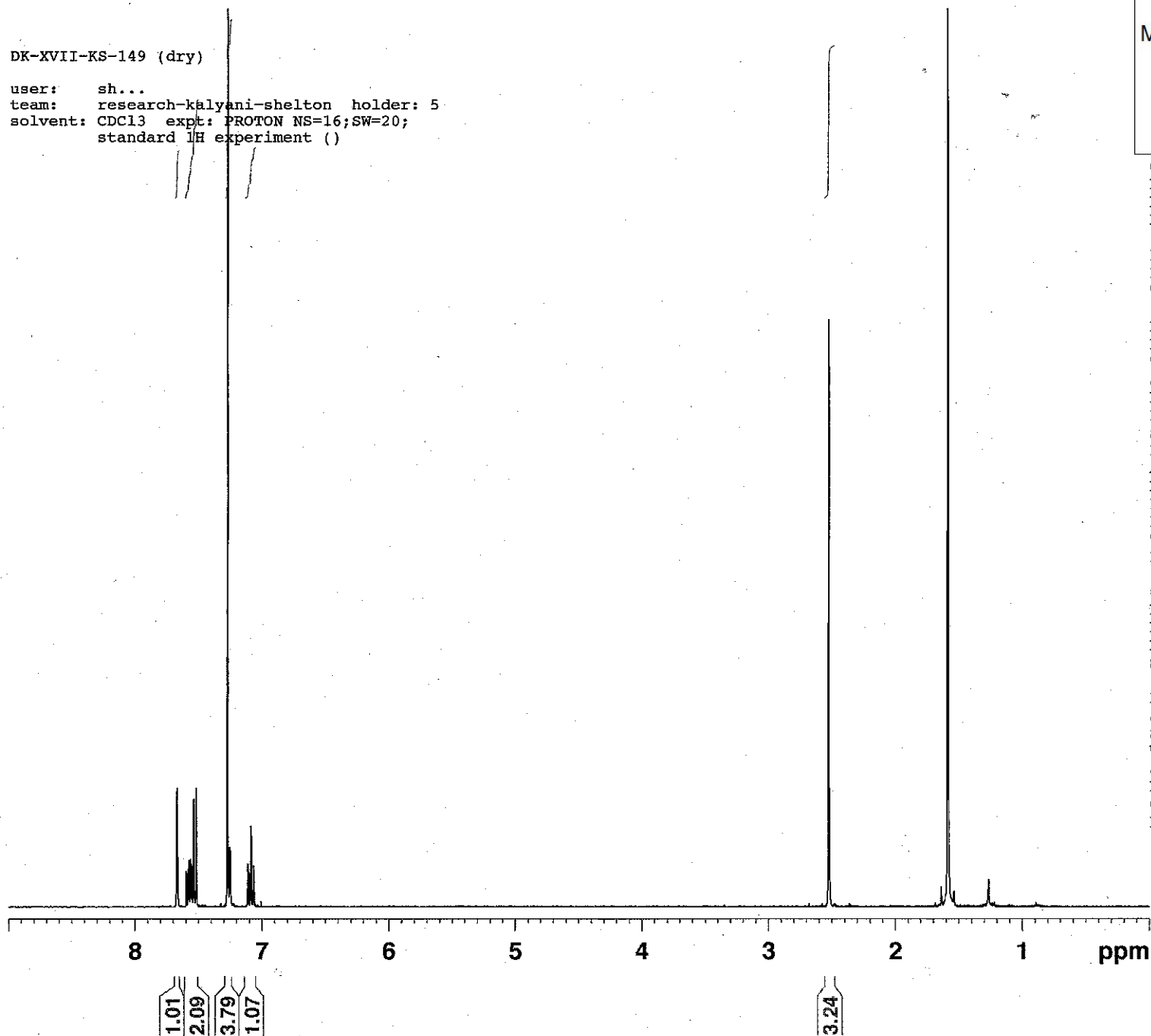
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XVII-KS-149 (dry)

user: sh...
team: research-kalyani-shelton holder: 5
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()



Current Data Parameters
NAME Jul31-2014
EXPNO 1913710
PROCNO 1

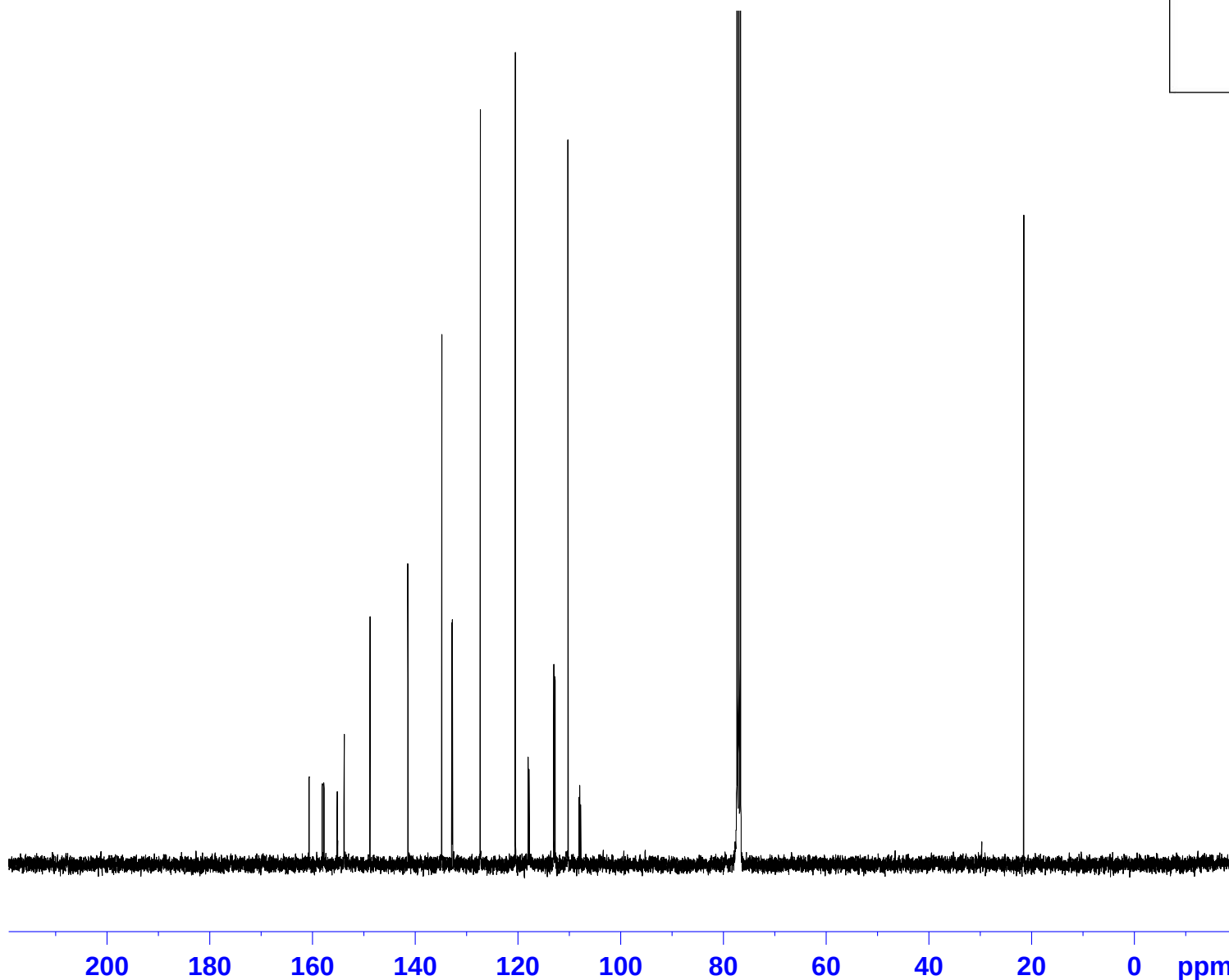
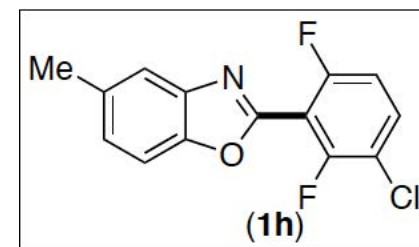
F2 - Acquisition Parameters
Date_ 20140731
Time_ 20.51
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

DK-XVII-KS-149 (C13)

user: sh...
team: research-kalyani-shelton holder: 1
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



Current Data Parameters
NAME Nov12-2014
EXPNO 1000910
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141113
Time 6.04
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 16384
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

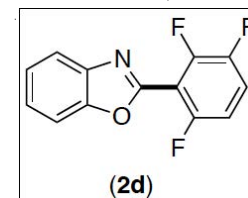
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM

DK-XXIV-JC-128 pure, dry

user: cr...
team: research-kalyani-crawforj holder: 4
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

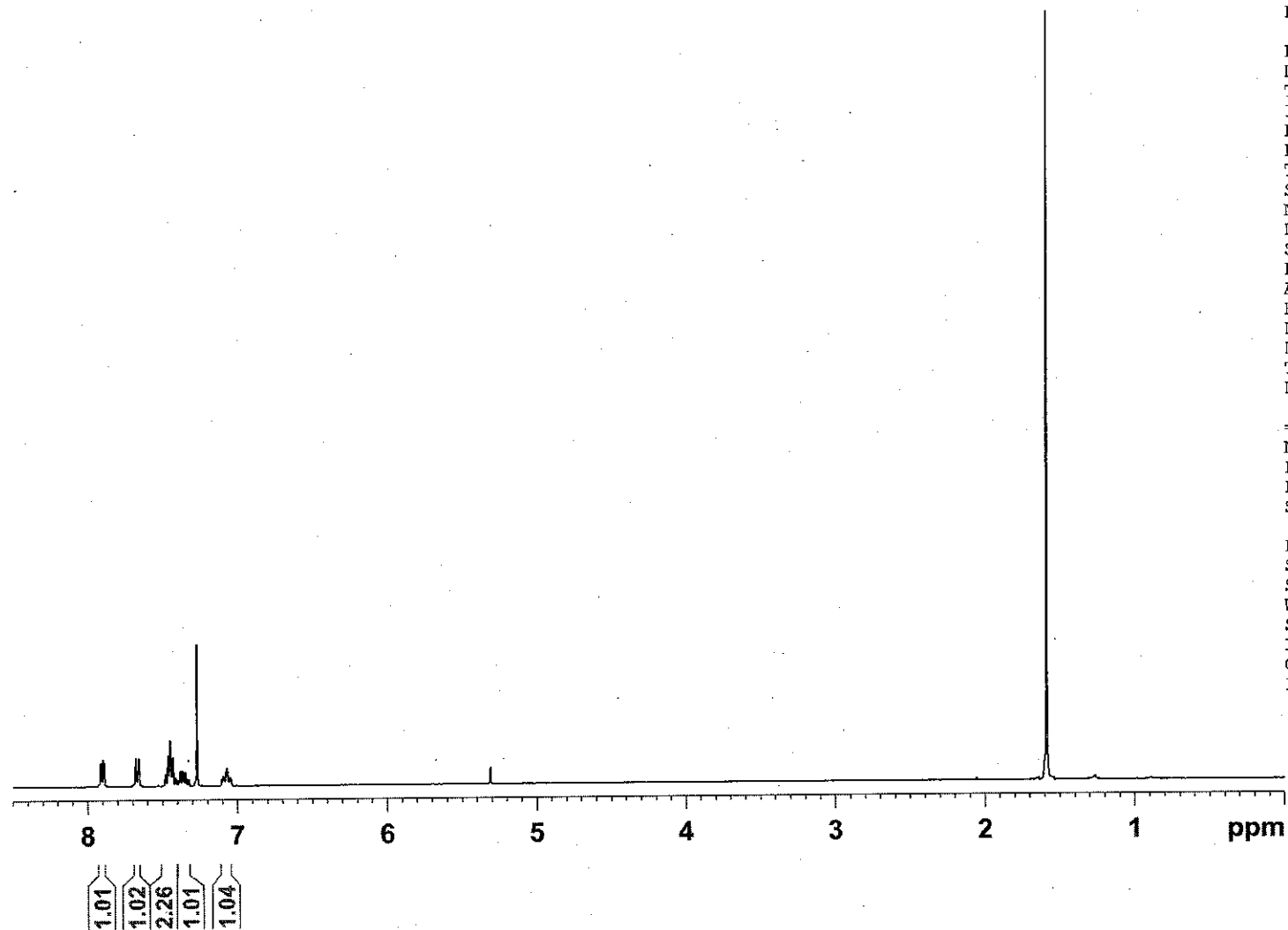


Current Data Parameters
NAME Jul28-2014
EXPNO 1905910
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140728
Time 19.02
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 724.1
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

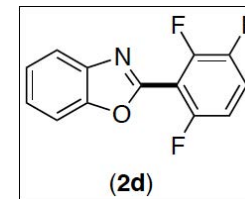
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-128 C13

user: cr...
team: research-kalyani-crawforj holder: 14
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



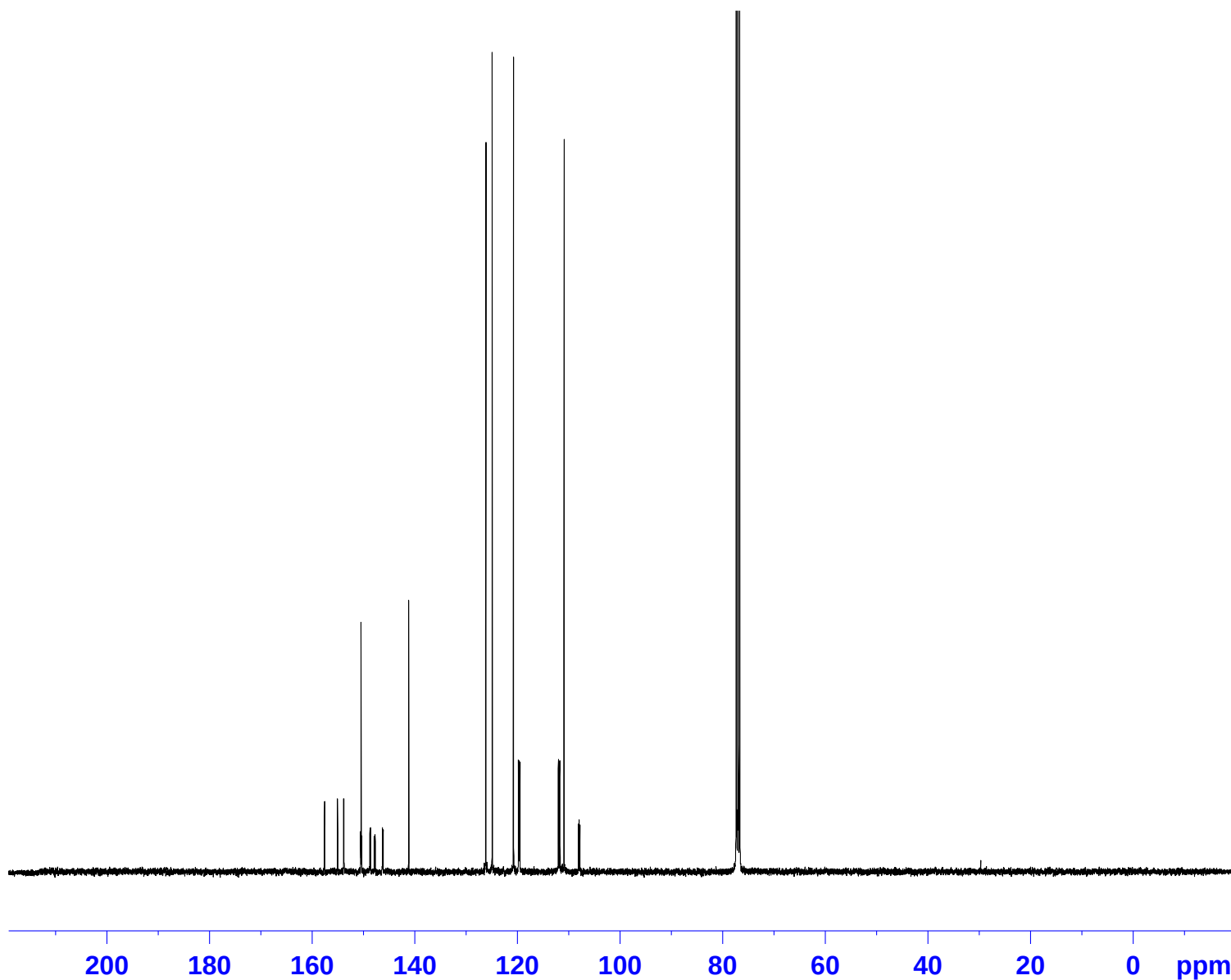
Current Data Parameters
NAME Nov22-2014
EXPNO 1014210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141123
Time 4.32
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2896.3
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

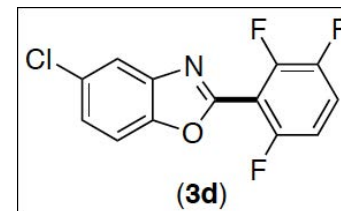
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XXIV-JC-120 pure, dry

user: cr...
team: research-kalyani-crawforj holder: 2
solvent: CDC13 expt: PROTON NS=128;SW=20;
standard 1H experiment ()

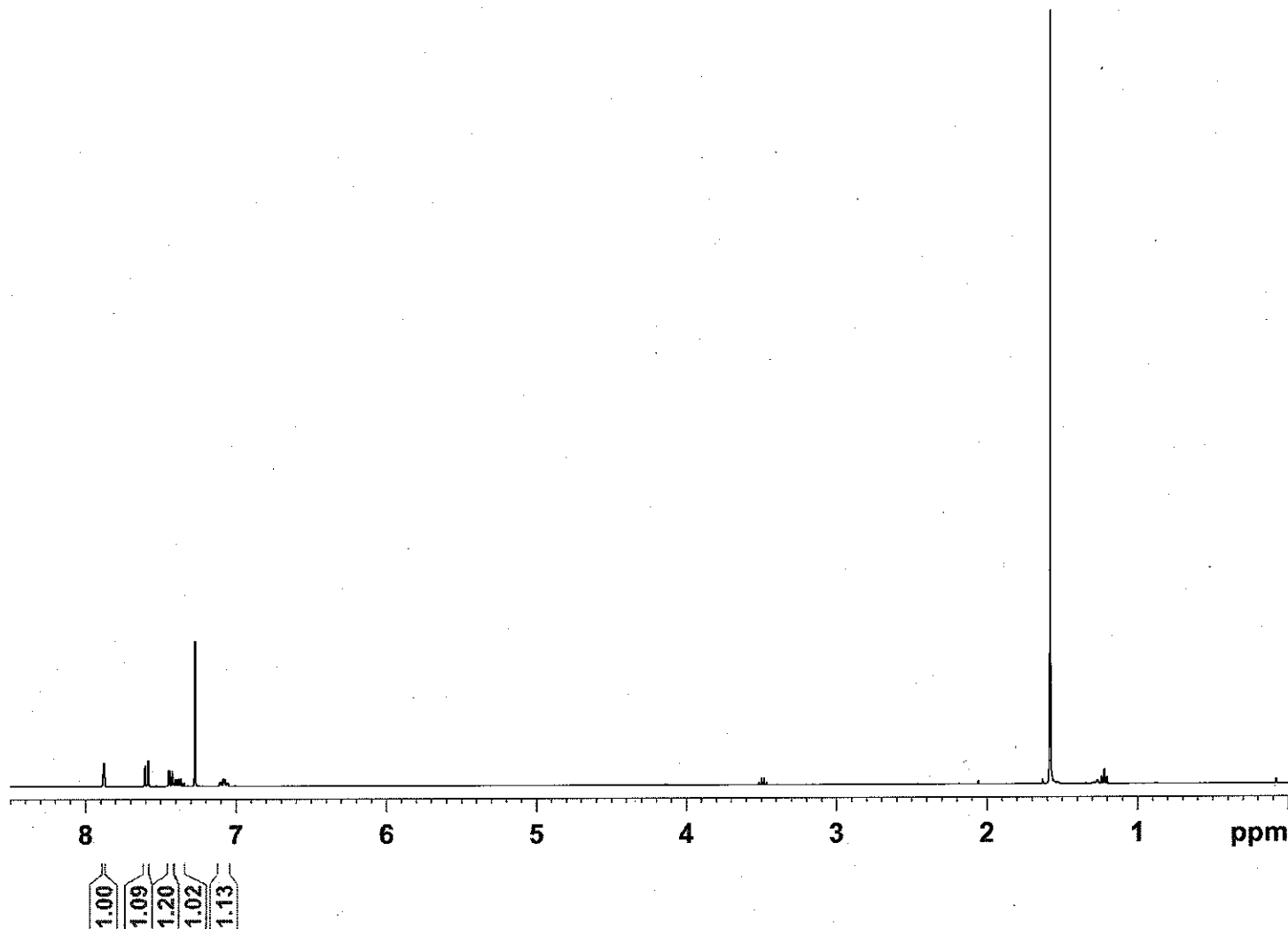


Current Data Parameters
NAME Jul24-2014
EXPNO 1902510
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140724
Time 16.50
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 128
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

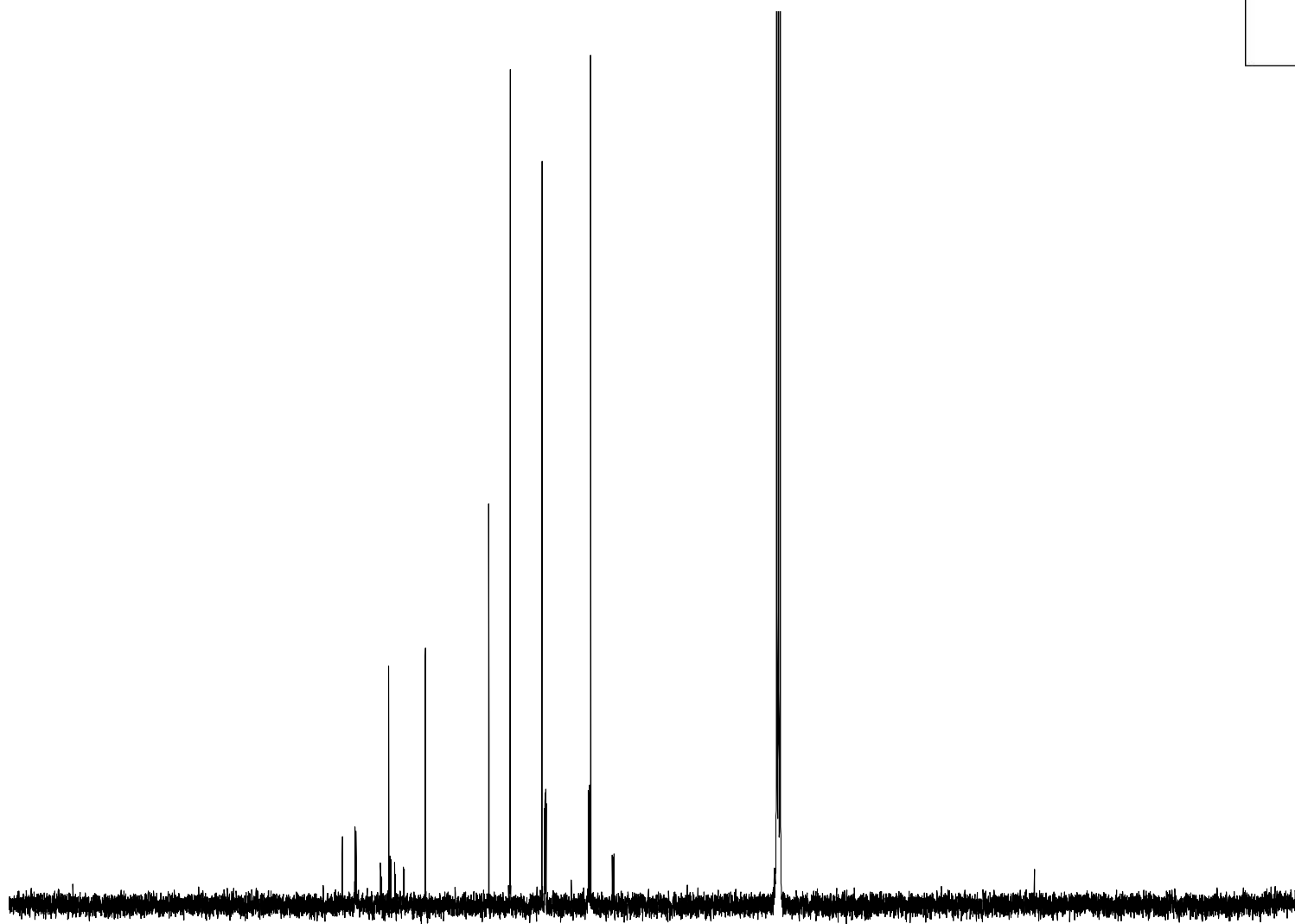
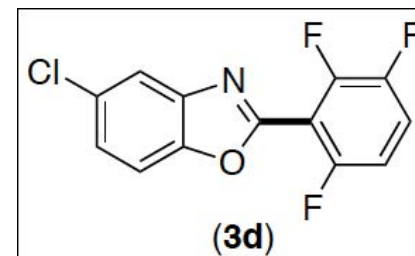
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-120 (C13)

user: sh...
team: research-kalyani-shelton holder: 10
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



Current Data Parameters
NAME Dec01-2014
EXPNO 1019310
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141202
Time 3.26
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 1824.6
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

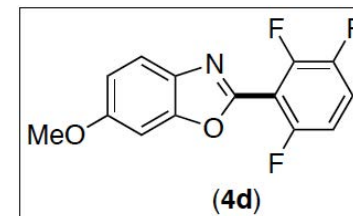
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM

DK-XXVI-JC-106 PURE DRY

user: cr...
team: research-kalyani holder: 2
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

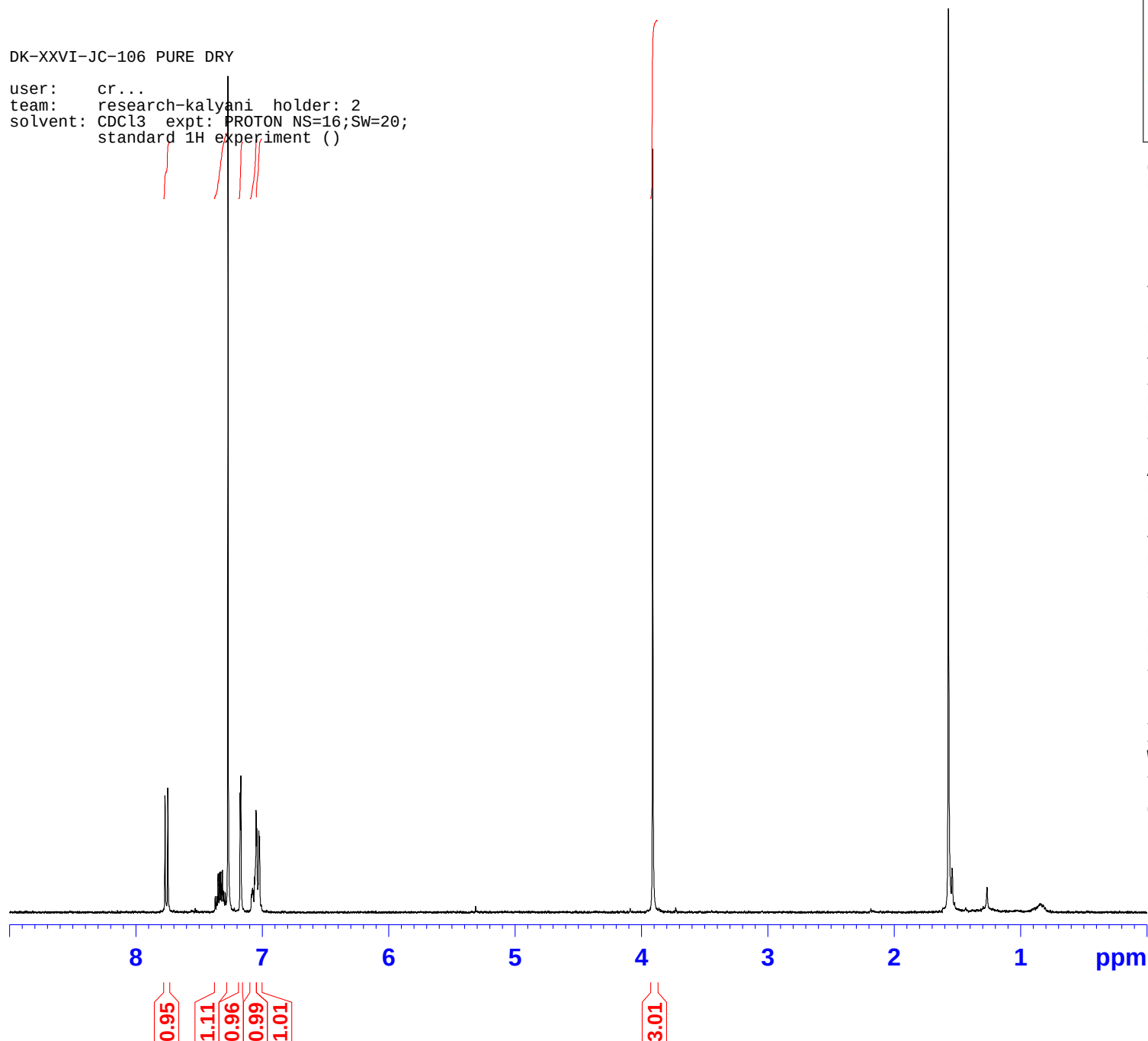


Current Data Parameters
NAME Apr09-2015
EXPNO 1076410
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150409
Time 14.14
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

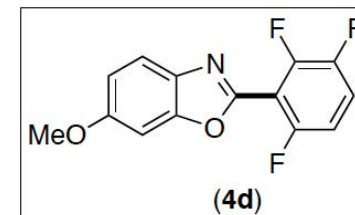
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-123 (C13)

user: sh...
team: research-kalyani-shelton holder: 14
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



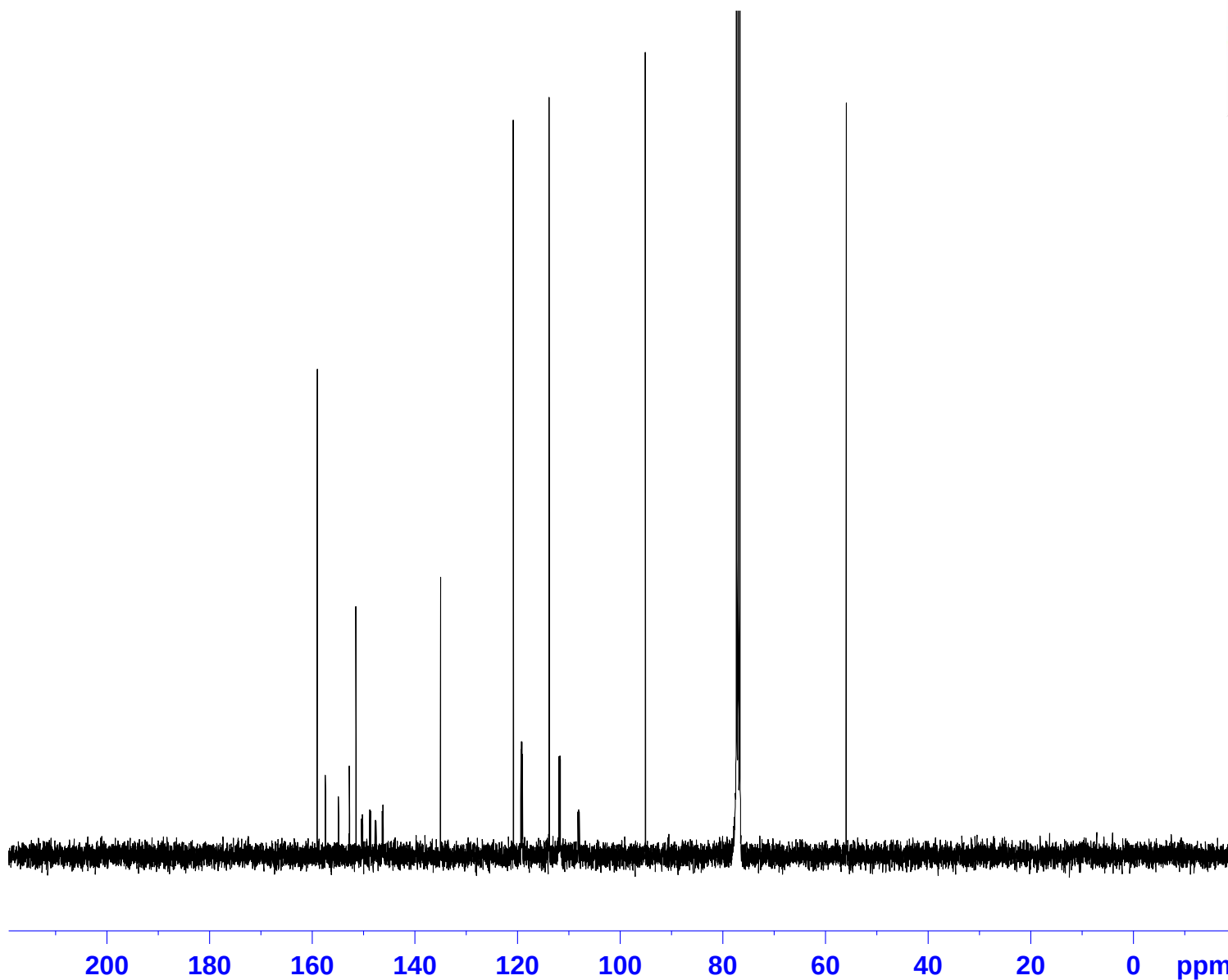
Current Data Parameters
NAME Nov15-2014
EXPNO 1009210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141116
Time 3.51
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 5792.6
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

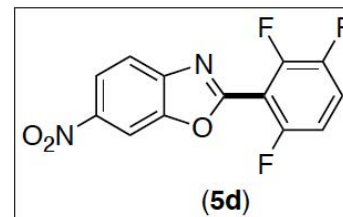
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XXIV-JC-124 pure, dry (16 scans)

user: cr...
team: research-kalyani-crawforj holder: 9
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()



Current Data Parameters

NAME Jul25-2014
EXPNO 1903910
PROCNO 1

F2 - Acquisition Parameters

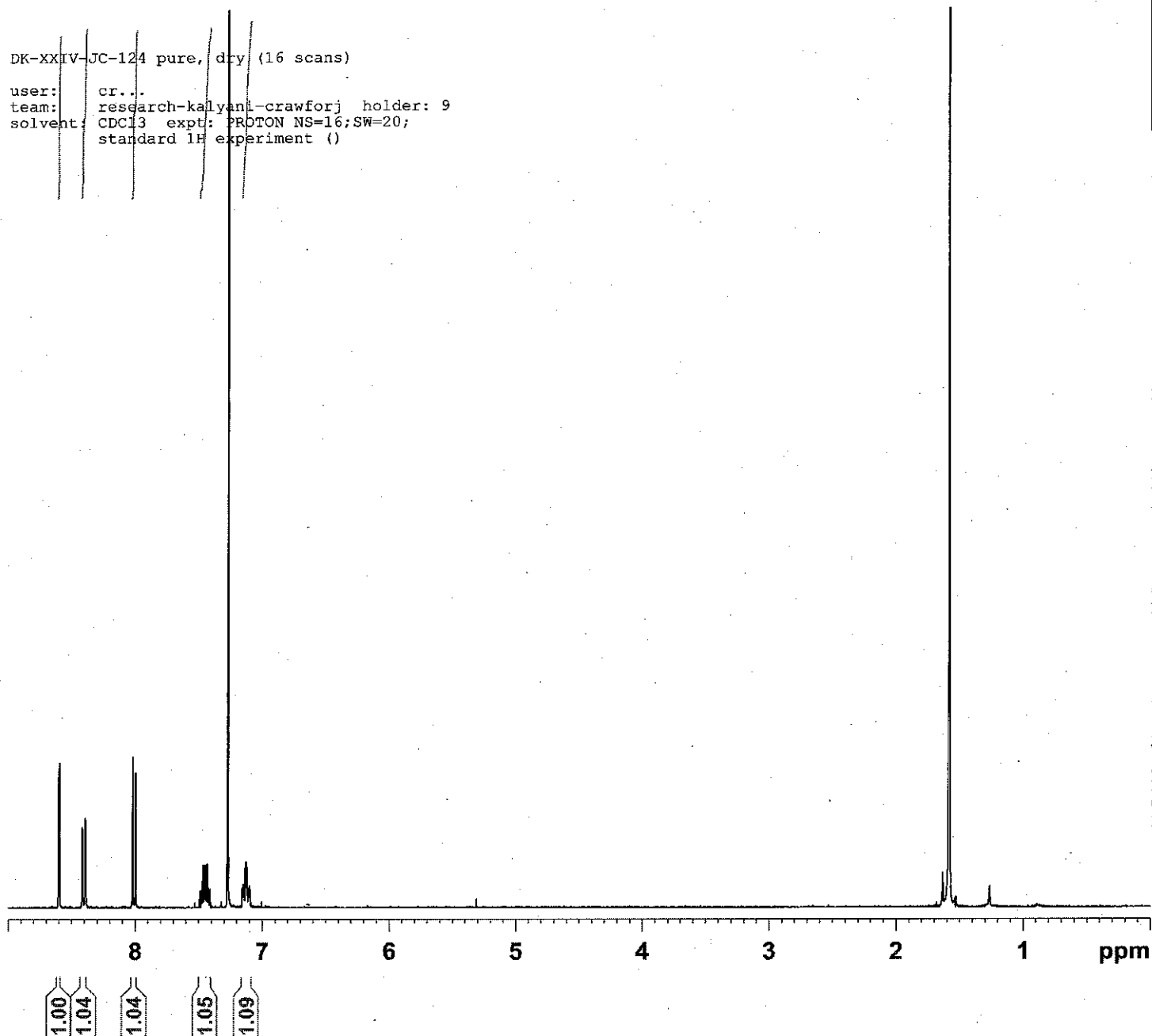
Date_ 20140725
Time 19.57
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

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

NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

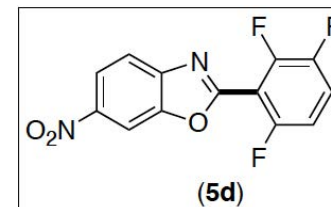
F2 - Processing parameters

SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-124

user: cr...
team: research-kalyani-crawforj holder: 2
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



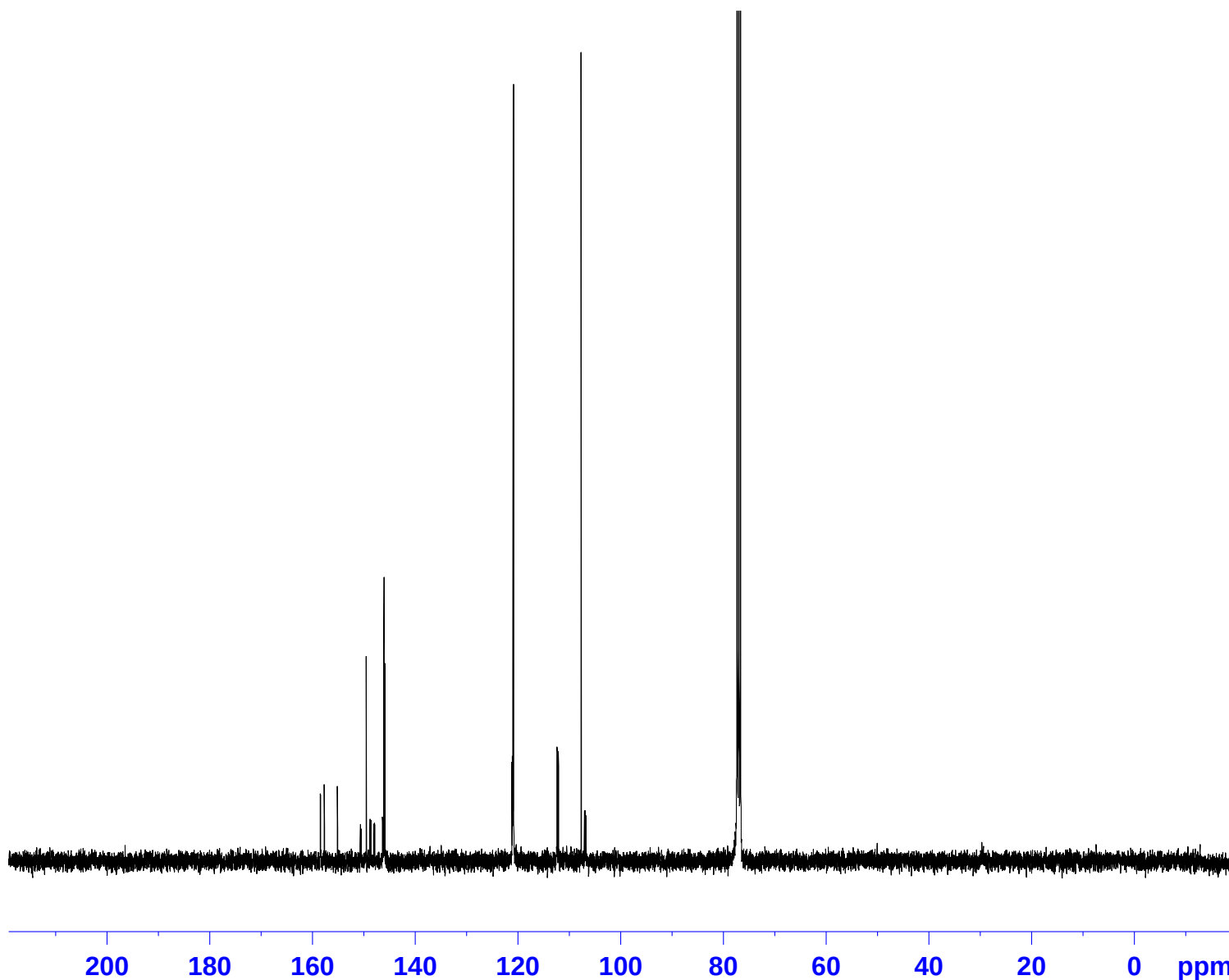
Current Data Parameters
NAME Oct24-2014
EXPNO 1960910
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141025
Time 11.25
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 4597.6
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

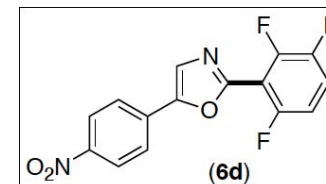
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XVII-KS-146 (dry)

user: sh...
team: research-kalyani-shelton holder: 5
solvent: CDC13 (expt: PROTON NS=16;SW=20;
standard 1H experiment (14 Min 43 Sec)

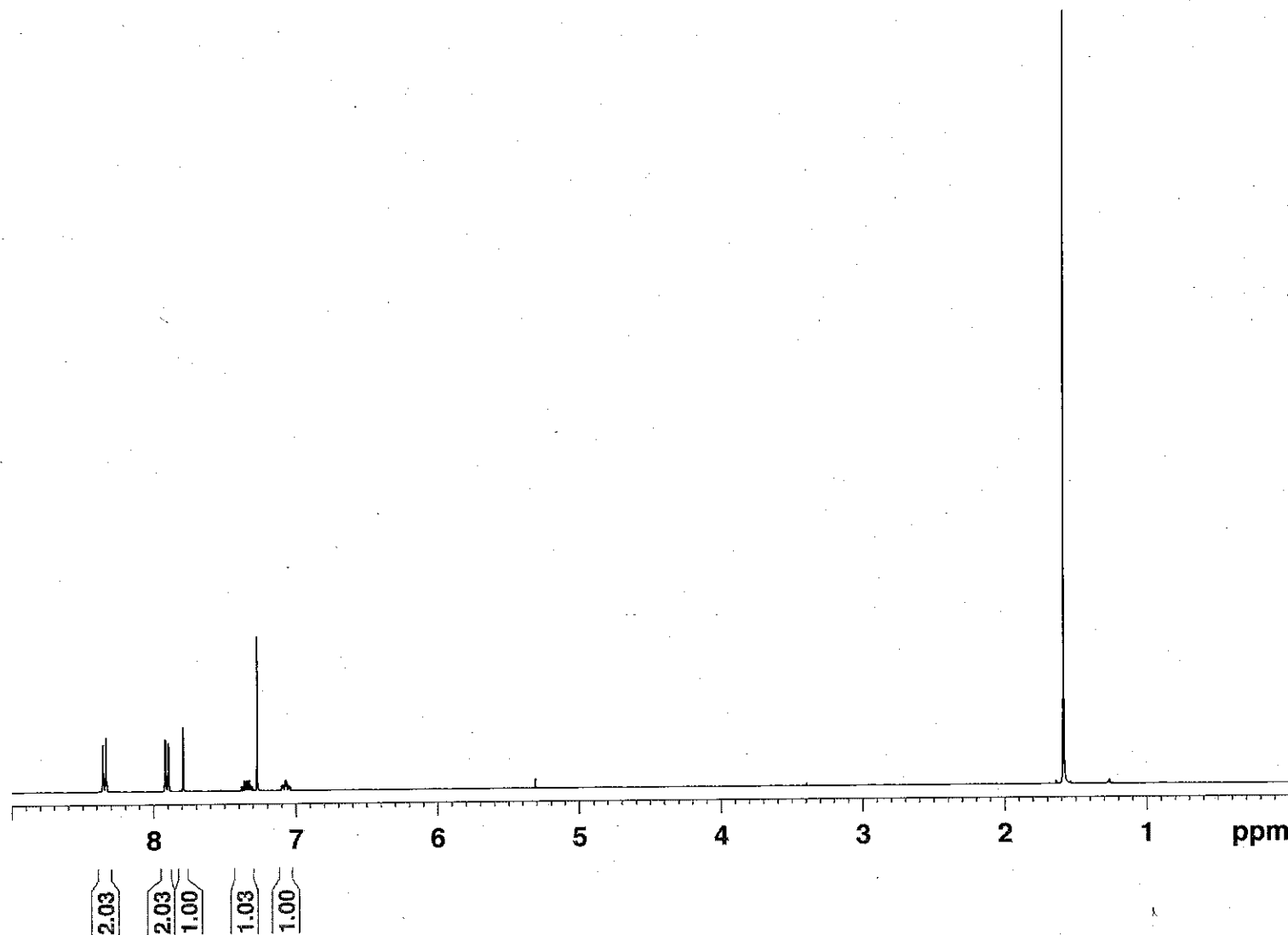


Current Data Parameters
NAME Jul29-2014
EXPNO 1908710
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140729
Time 13.17
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 724.1
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

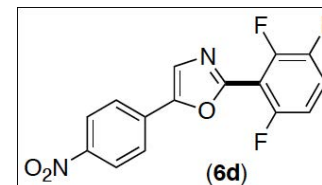
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XVII-KS-146

user: sa...
team: research-kalyani holder: 15
solvent: CDCl₃ expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



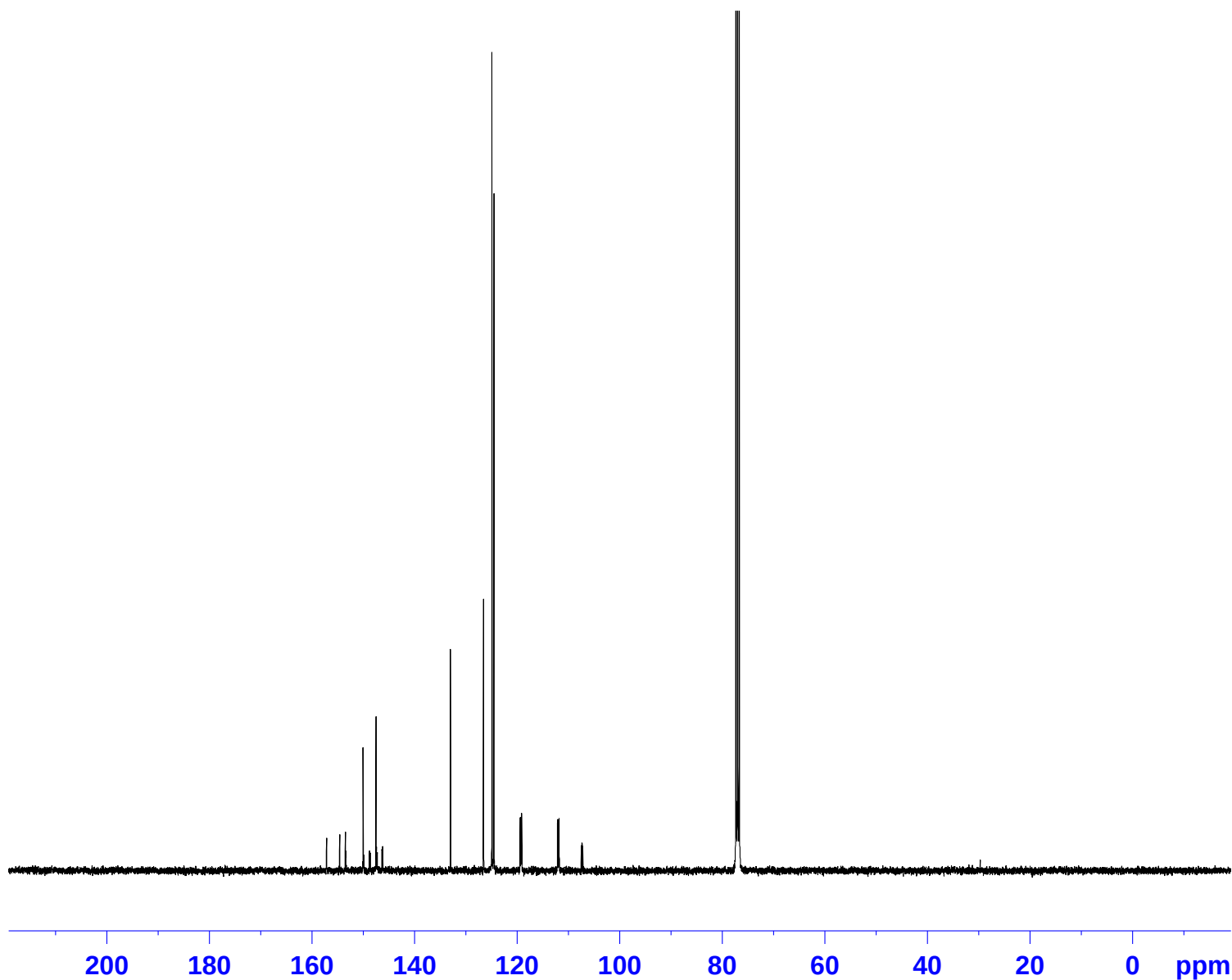
Current Data Parameters
NAME Dec14-2014
EXPNO 1024610
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141214
Time 8.36
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 2048
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

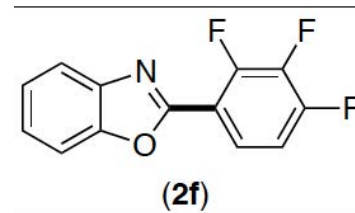
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XXVI-JC-55 pure fractions

user: we...
team: research-kalyani holder: 4
solvent: CDCl3 expt: PROTON NS=16; Sw=20;
standard 1H experiment ()

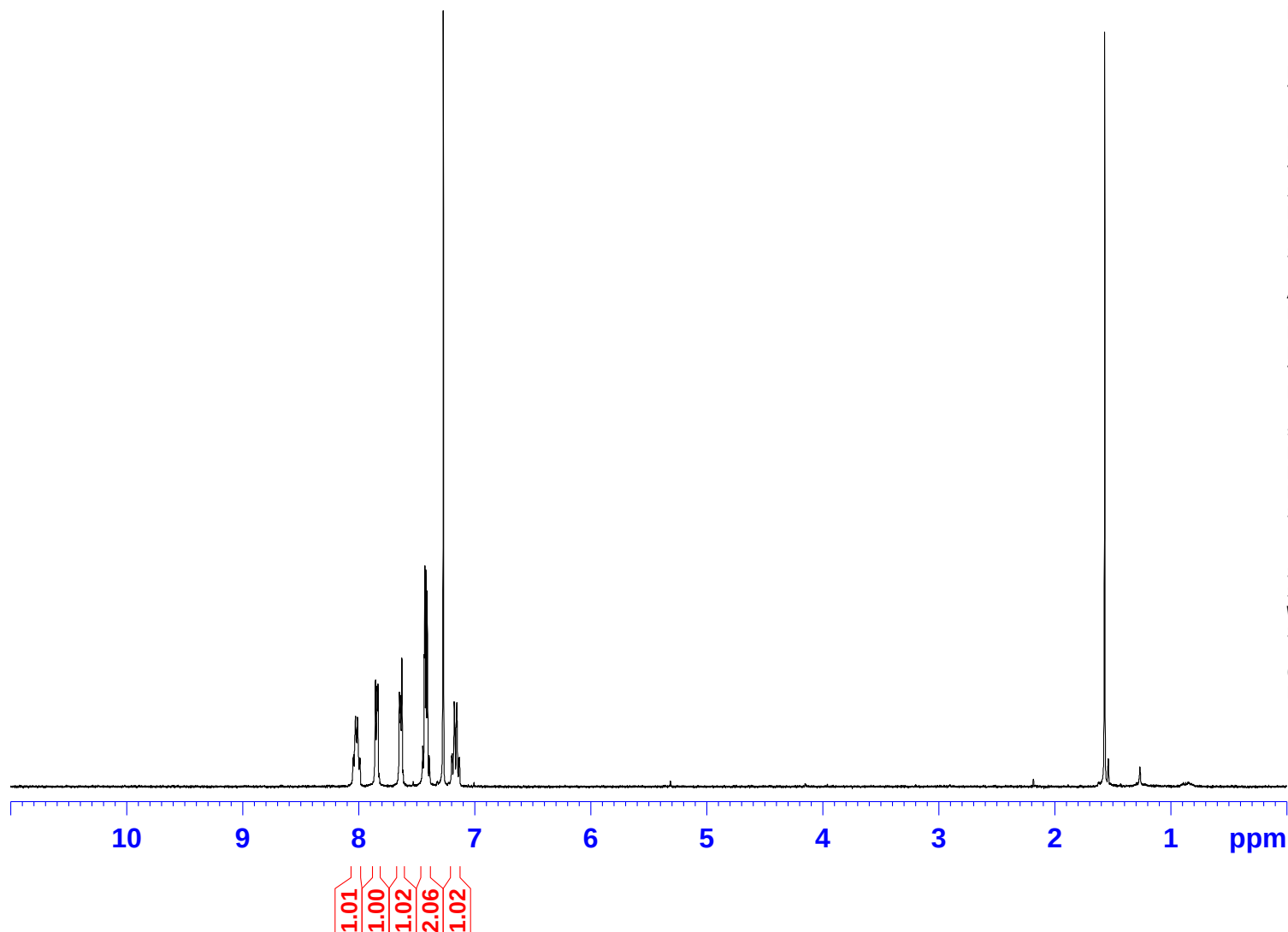


Current Data Parameters
NAME Jan22-2015
EXPNO 1038310
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150122
Time 22.24
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

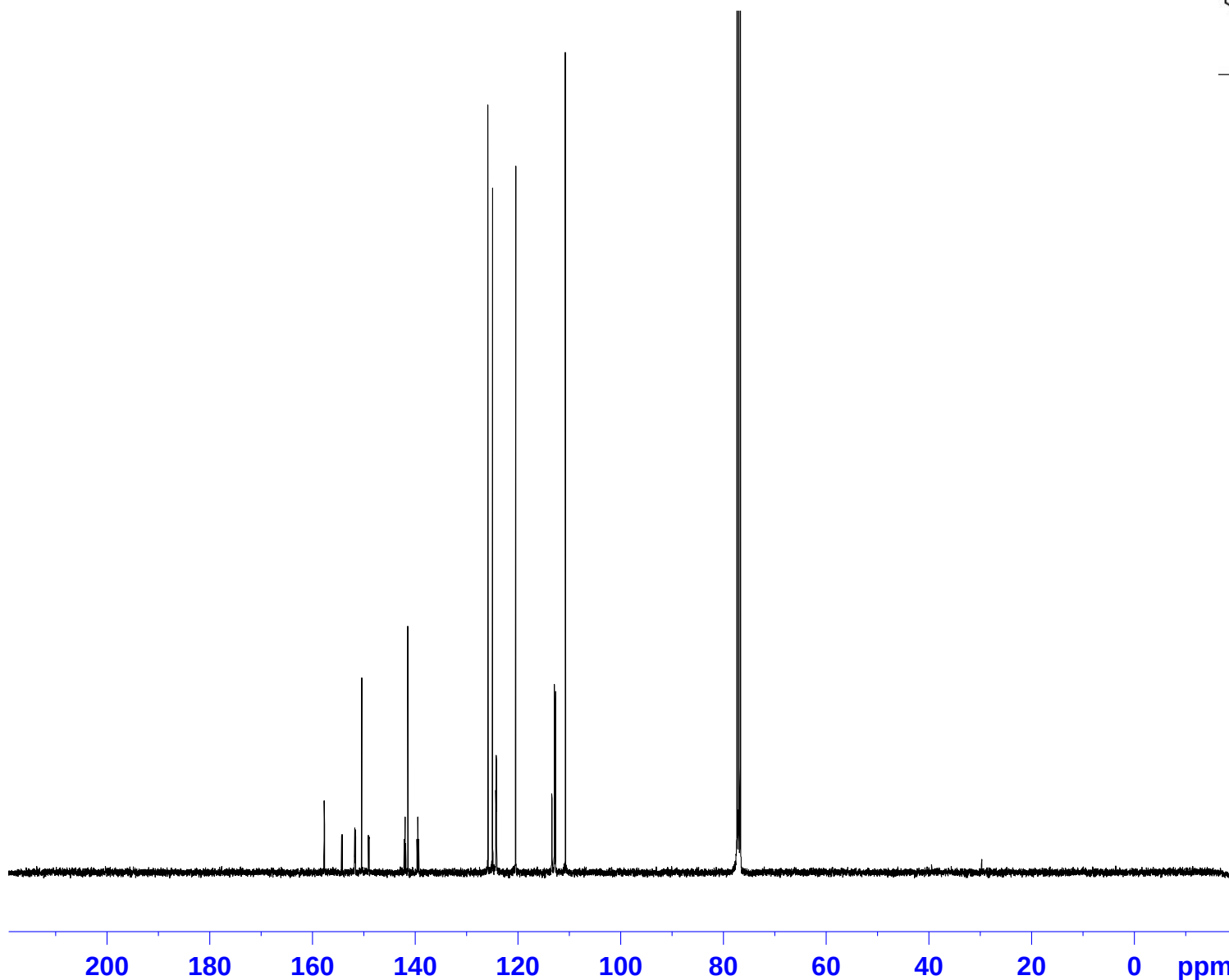
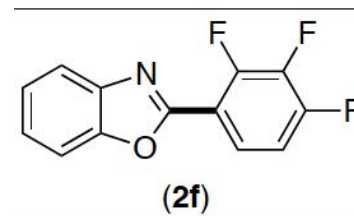
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXVI-JC-55 carbon

user: cr...
team: research-kalyani holder: 8
solvent: CDCl₃ expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



Current Data Parameters
NAME Jan29-2015
EXPNO 1041610
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150130
Time 1.17
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 13004
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

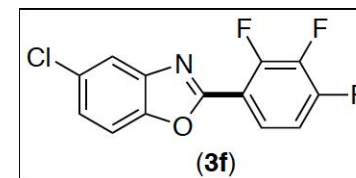
===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM

DK-XXVI-JC-61 mixed fractions

user: re...
team: research-kalyani-reeves holder: 5
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

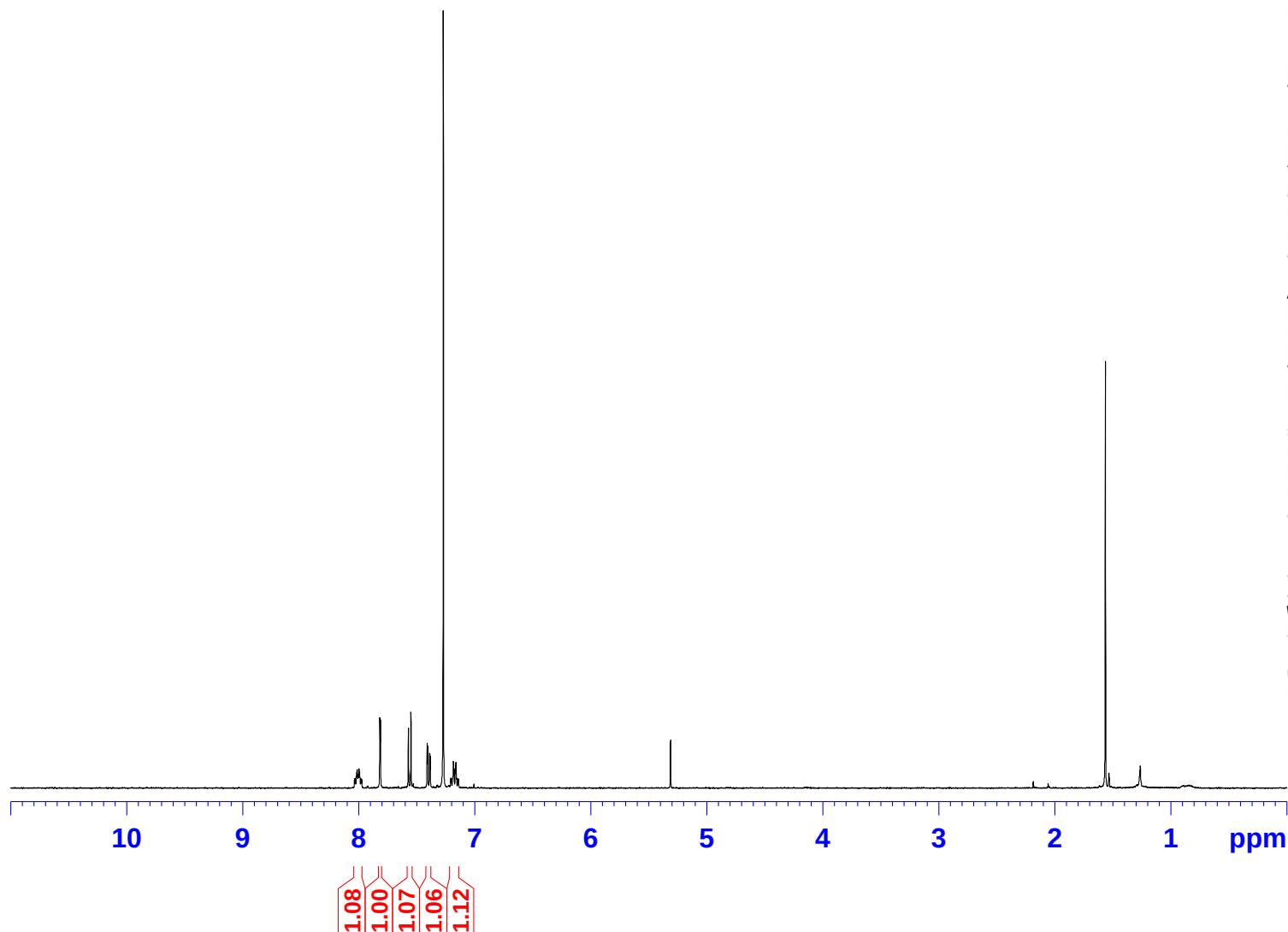


Current Data Parameters
NAME Jan24-2015
EXPNO 1039210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150124
Time 11.17
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

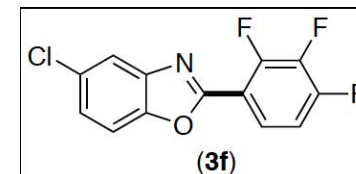
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXVI-JC-13 MAYBE MIXED

user: sa...
team: research-kalyani holder: 15
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



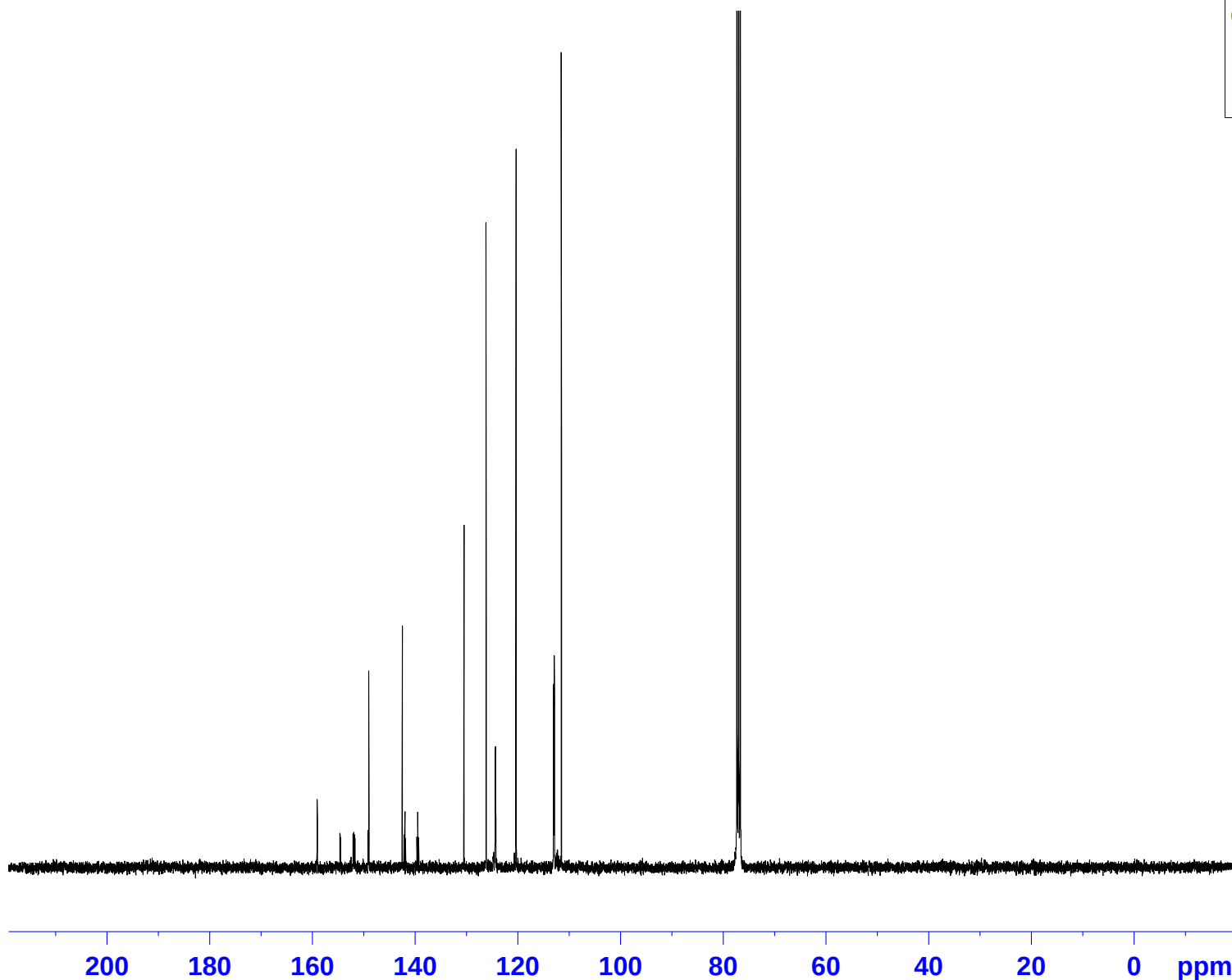
Current Data Parameters
NAME Nov21-2014
EXPNO 1013110
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141122
Time 3.15
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

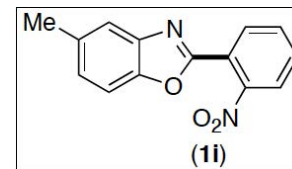
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM



DK-XXIV-JC-136 (pure)

user: sh...
team: research-kalyani-shelton holder: 10
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

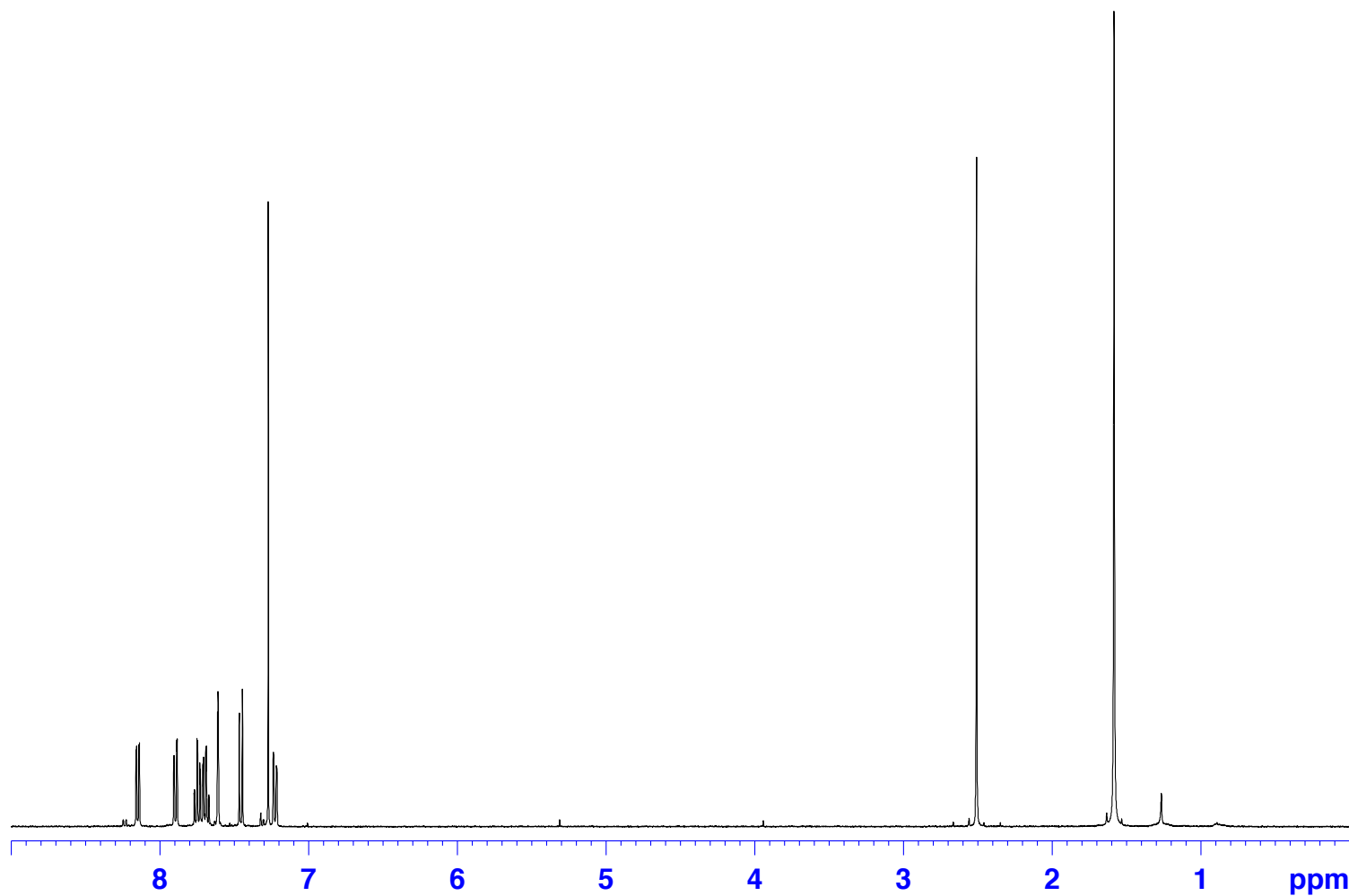


Current Data Parameters
NAME Oct24-2014
EXPNO 1960410
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141024
Time 10.26
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 645.1
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

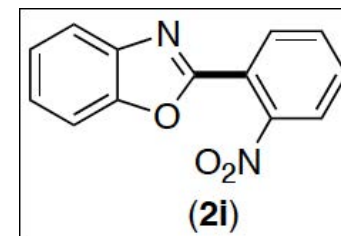
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXVI-JC-80 redried

user: re...
team: research-kalyani-reeves holder: 4
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

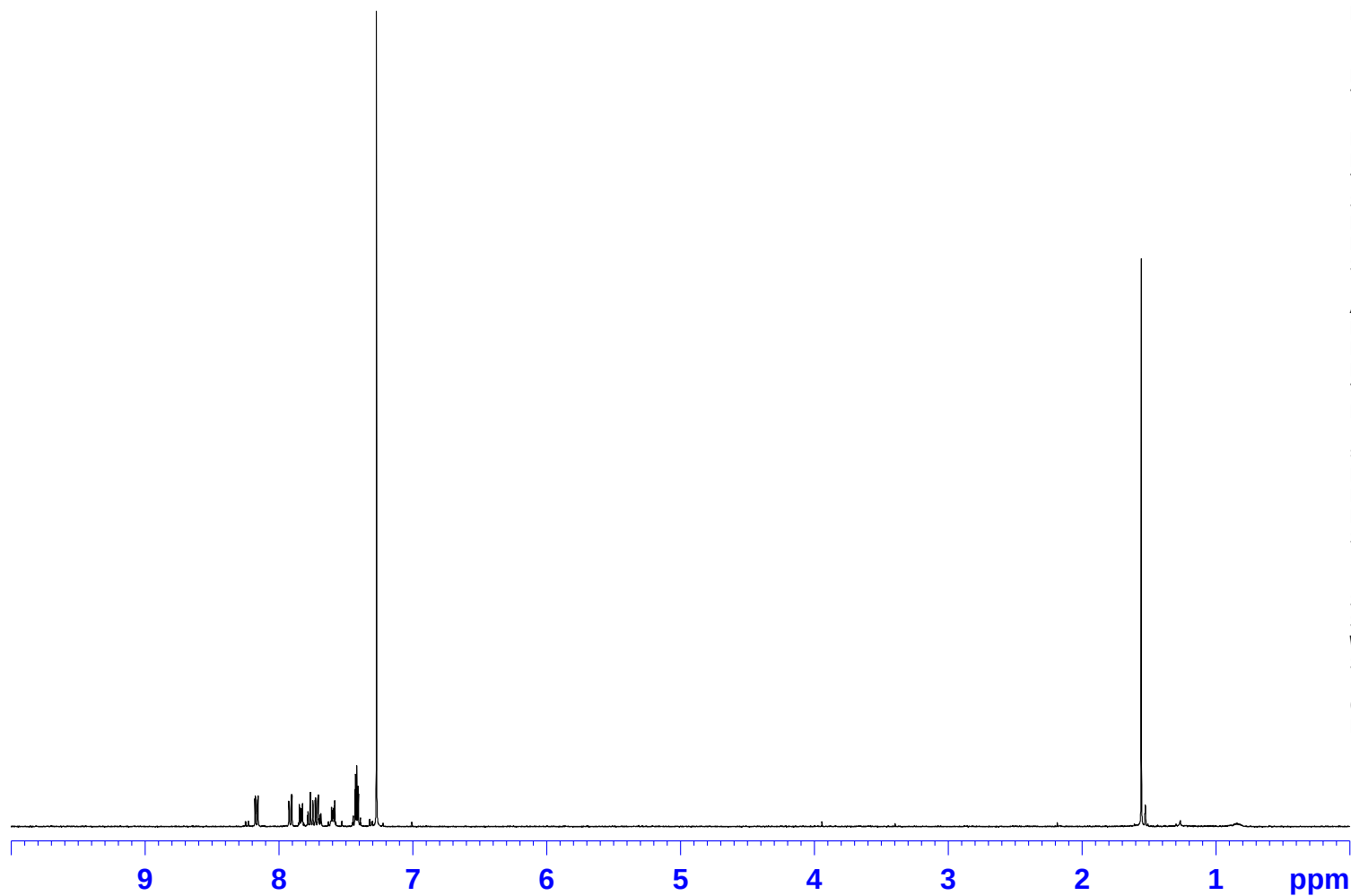


Current Data Parameters
NAME Jan30-2015
EXPNO 1042210
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150130
Time 15.13
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 912.3
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SF01 400.1324710 MHz

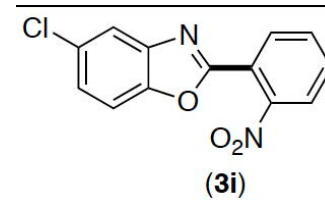
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.03
1.00
0.97
2.41
1.04
1.91

DK-XXIV-JC-154 (mixed)

user: sh...
team: research-kalyani-shelton holder: 8
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

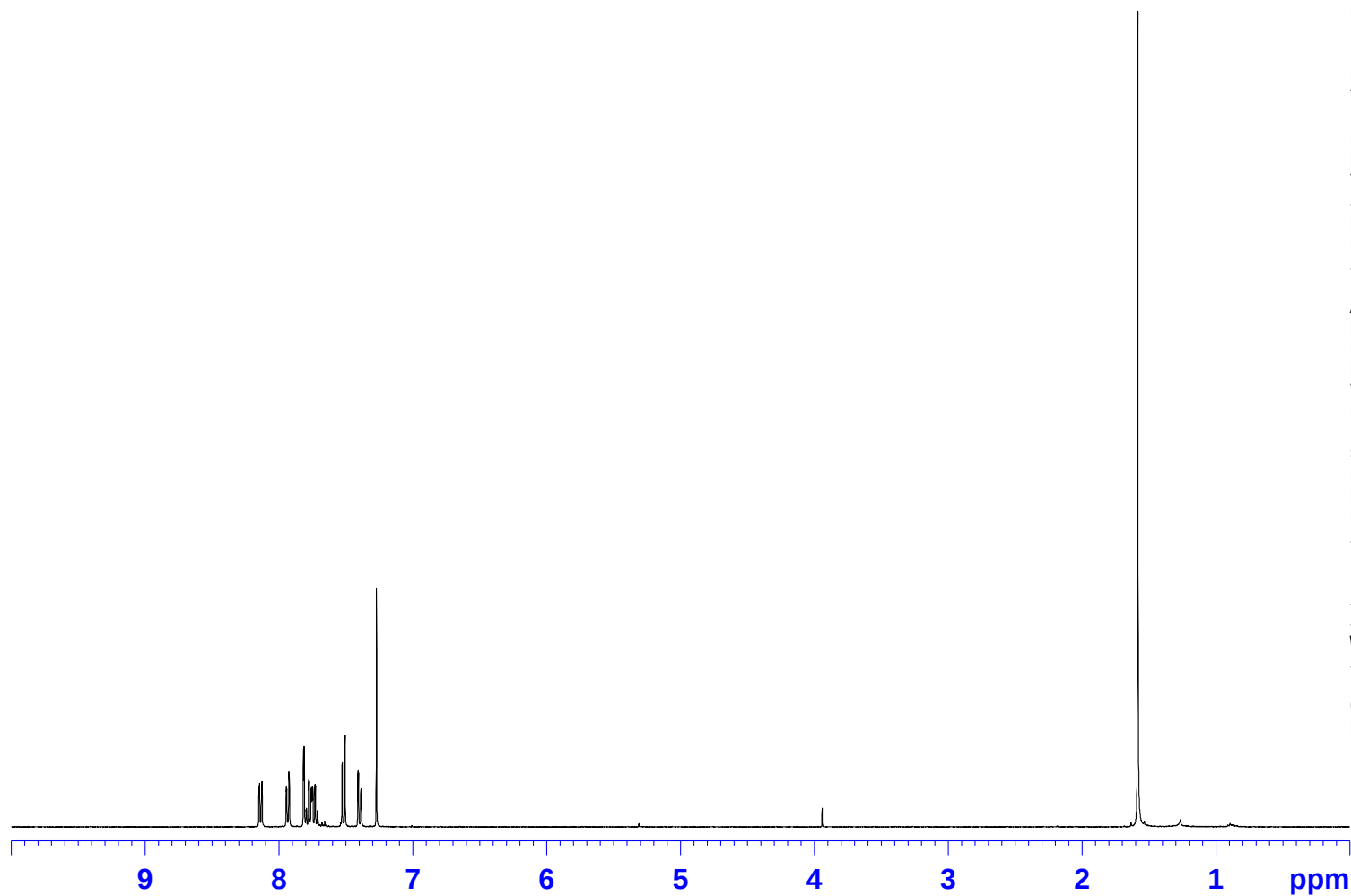


Current Data Parameters
NAME Nov07-2014
EXPNO 1987010
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141107
Time 17.48
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 724.1
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

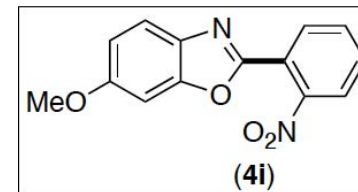
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-151 no grease dry

user: cr...
team: research-kalyani-crawforj holder: 2
solvent: CDCl3 expt: PROTON NS=16;SW=20;
standard 1H experiment ()

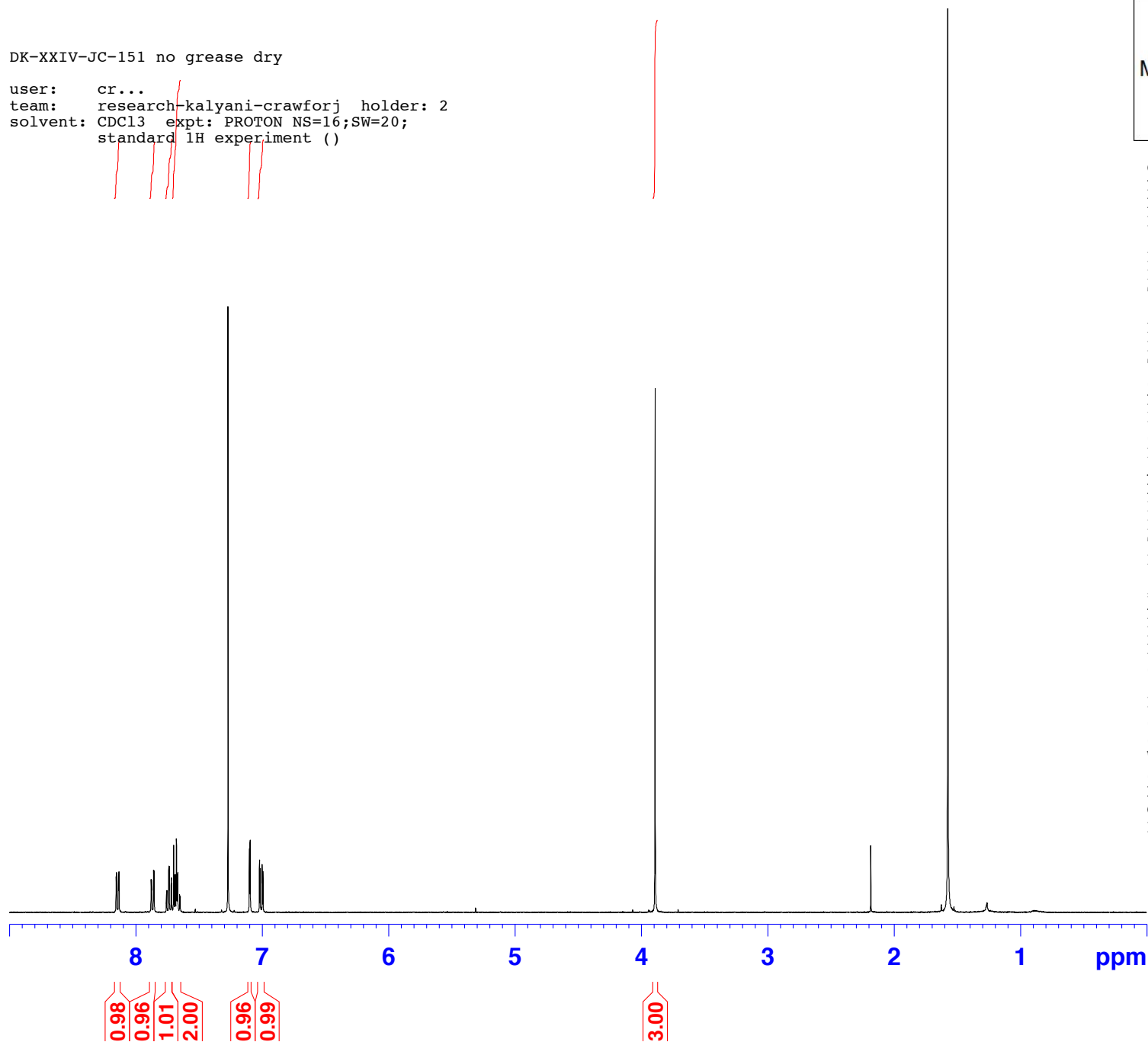


Current Data Parameters
NAME Nov07-2014
EXPNO 1986310
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141107
Time 9.56
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894966 sec
RG 812.7
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

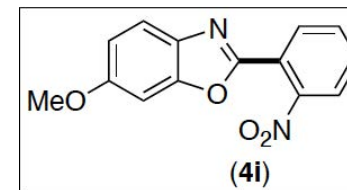
===== CHANNEL f1 =====
NUC1 1H
P1 11.75 usec
PL1 -4.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



DK-XXIV-JC-151 C13

user: cr...
team: research-kalyani-crawforj holder: 13
solvent: CDCl3 expt: C13CPD32 NS=8192;D1=2;
standard C13 experiment ()



Current Data Parameters
NAME Nov21-2014
EXPNO 1013310
PROCNO 1

F2 - Acquisition Parameters
Date_ 20141122
Time 11.02
INSTRUM spect
PROBHD 5 mm BBO 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 8192
DS 2
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 10321.3
DW 20.850 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 9.00 usec
PL1 -4.50 dB
SF01 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -4.00 dB
PL12 13.68 dB
PL13 17.24 dB
SF02 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127690 MHz
WDW EM

