

Ascertaining the suitability of aryl sulfonyl fluorides for [¹⁸F]radiochemistry applications: a systematic investigation using microfluidics

Electronic Supporting Information

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Table S1. Calculated¹ Hammett constants for sulfonyl fluorides **1b-12b** and **14b**.

Compound	Hammett constant (σ_p)
4b	-0.27
3b	-0.17
10b	-0.17
2b	-0.15
11b	-0.15
1b	0
6b	0.06
9b	0.18
7b	0.23
8b	0.23
14b	0.42
5b	0.78
12b	-

(1) Hansch, C.; Leo, A.; Taft, R. W. *Chem. Rev.* **1991**, *91*, 165.

Table S2. HPLC purity data for sulfonyl fluorides **1b-2b**, **4b-12b** and **14b**.

HPLC purity was determined using an Alltima C18 column (150 × 4.6 mm, 5 μm) with a flow rate of 1 mL/min and CH₃CN/H₂O/1% TFA (solvent system 1) or MeOH/H₂O/1% TFA (solvent system 2) at 254 nm. Gradient elution program was as follows:

(A): CH₃CN or MeOH (B): H₂O (C): 1% TFA

	Time	Flow	%A	%B	%C
1	0	1.00	10	80	10
2	20	1.00	90	0	10
3	21	1.00	10	80	10

Compound	<i>t_R</i> (min)	Purity (%)
1b	18.9 ^a	99.4
2b	14.8 ^b	99.8
4b	22.2 ^b	99.9
5b	20.1 ^b	97.5
6b	19.2 ^a	97.0
7b	17.8 ^b	98.2
8b	23.3 ^b	98.2
9b	21.8 ^a	99.0
10b	23.4 ^a	98.2
11b	15.7 ^a	98.7
12b	20.6 ^b	99.9
14b	17.3 ^a	99.9

^a Solvent system 1: CH₃CN/H₂O/1% TFA gradient

^b Solvent system 2: MeOH/H₂O/1% TFA gradient

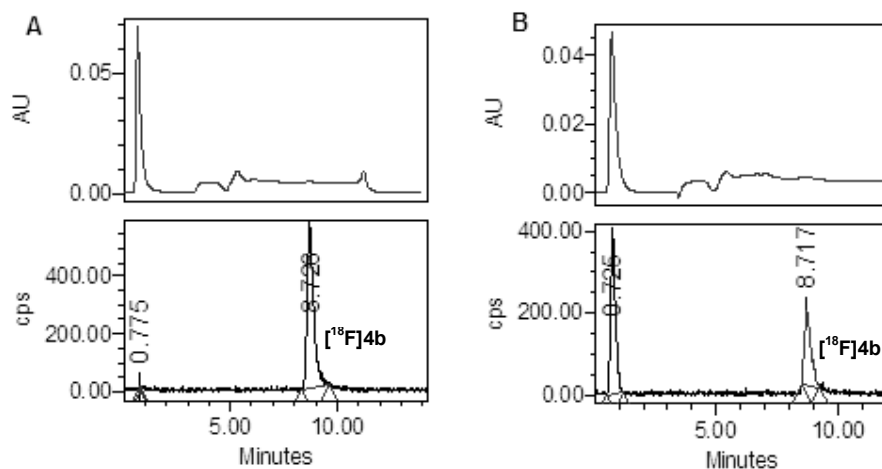
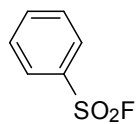


Figure S1. Radio-HPLC chromatograms of [^{18}F]**4b** in normal rat plasma at 37 °C after A) 1 min and B) 120 min. The increase in the presence of an impurity at 0.7 min can be observed at 120 min, as well as fluoride “bleeding”, which leads to an uneven baseline in the chromatogram. Top panel: UV at 254 nm (abs); bottom panel: radioactivity (cps).



1b

8.132
8.119
8.114
8.111
7.994
7.975
7.956
7.845
7.840
7.826
7.824
7.812
7.805

LMF4030

Current Data Parameters
NAME LMF4030
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120412

Time 15.19

INSTRUM spect

PROBHD 5 mm QNP 1H/1

PULPROG zg30

TD 32768

SOLVENT Acetone

NS 8

DS 2

SWH 4789.272 Hz

FIDRES 0.146157 Hz

AQ 3.4210291 sec

RG 1024

DW 104.400 usec

DE 6.00 usec

TE 298.2 K

DI 1.0000000 sec

TDO 1

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

MUCL 1H

PL 12.10 usec

PL1 -3.00 dB

SFO1 400.1322007 MHz

F2 - Processing parameters

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SF 400.130065 MHz

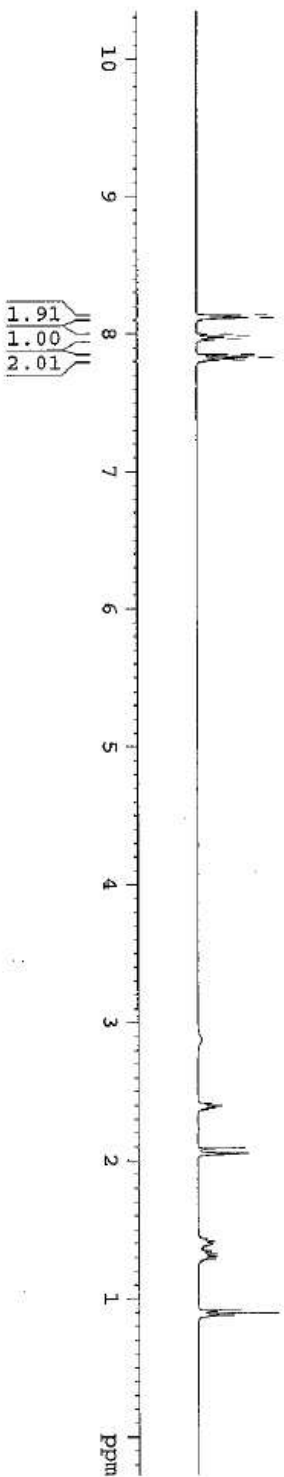
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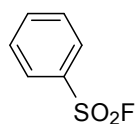
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PC 1.00



LMK4030_13C



1b

137.18
133.70
133.46
131.13
129.24

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Current Data Parameters
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EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
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Time 16.10

INSTRUM spect
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PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2048
DS 4

SPH 23980.814 Hz
FIDRES 0.361913 Hz
AQ 1.3664756 sec
RG 512
DM 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999999 sec
TD0 2

===== CHANNEL F1 =====
NUC1 13C
P1 14.50 usec
PL1 3.00 dB
SFO1 100.628303 MHz

===== CHANNEL F2 =====
CEPRPG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.45 dB
PL13 25.00 dB
SFO2 400.1315006 MHz

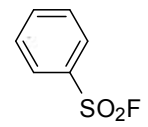
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FIDRES 3.906250 Hz
SW 9.938 ppm
FWDPR Echo-Antiecho

F2 - Processing Parameters
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SF 100.6126775 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing Parameters
SI 1024
MC2 echo-antiecho
SF 100.5046953 MHz
WDW OSINE
SSB 2
LB 0.30 Hz
GB 0.1



IME4030_19F



1b

Current Data Parameters
NAME IME4030
EXPNO 1
PROCNO 1

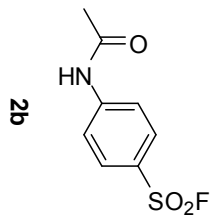
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PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DE 4.400 usec
TE 10.00 usec
TD0 1
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.0002000 sec

CHANNEL F1
NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66949272 W
SFO1 376.4963660 MHz

CHANNEL F2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.50 dB
PL2W 15.33 dB
PL2W 14.77555943 W
PL2W 0.48589671 W
SFO2 400.1316005 MHz

F2 - Processing Parameters
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SF 376.4985467 MHz
WDW no
SSB 0
LB 0
GB 0
PC 1.00

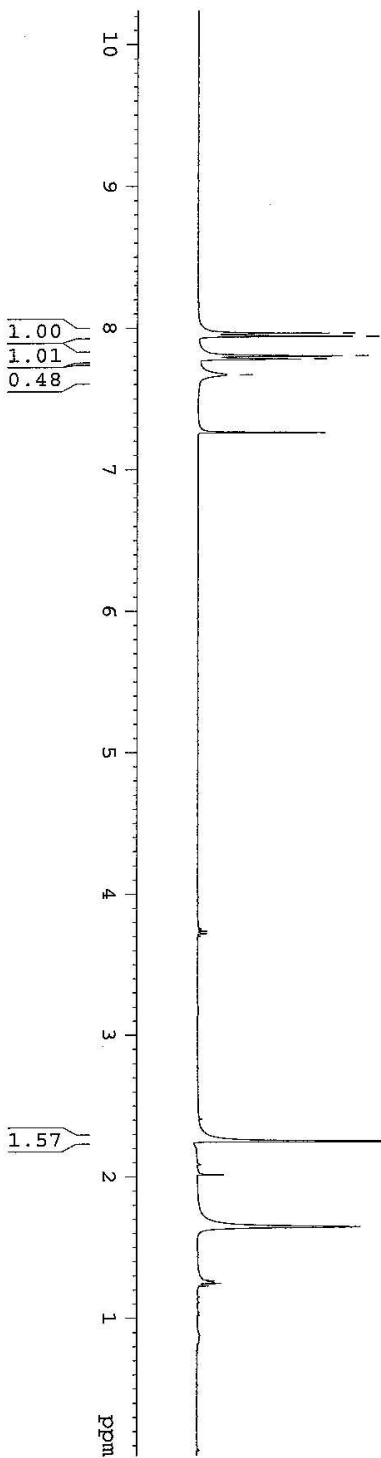




7.962
7.940
7.802
7.780
7.668

bfr0104902 1H

2.248



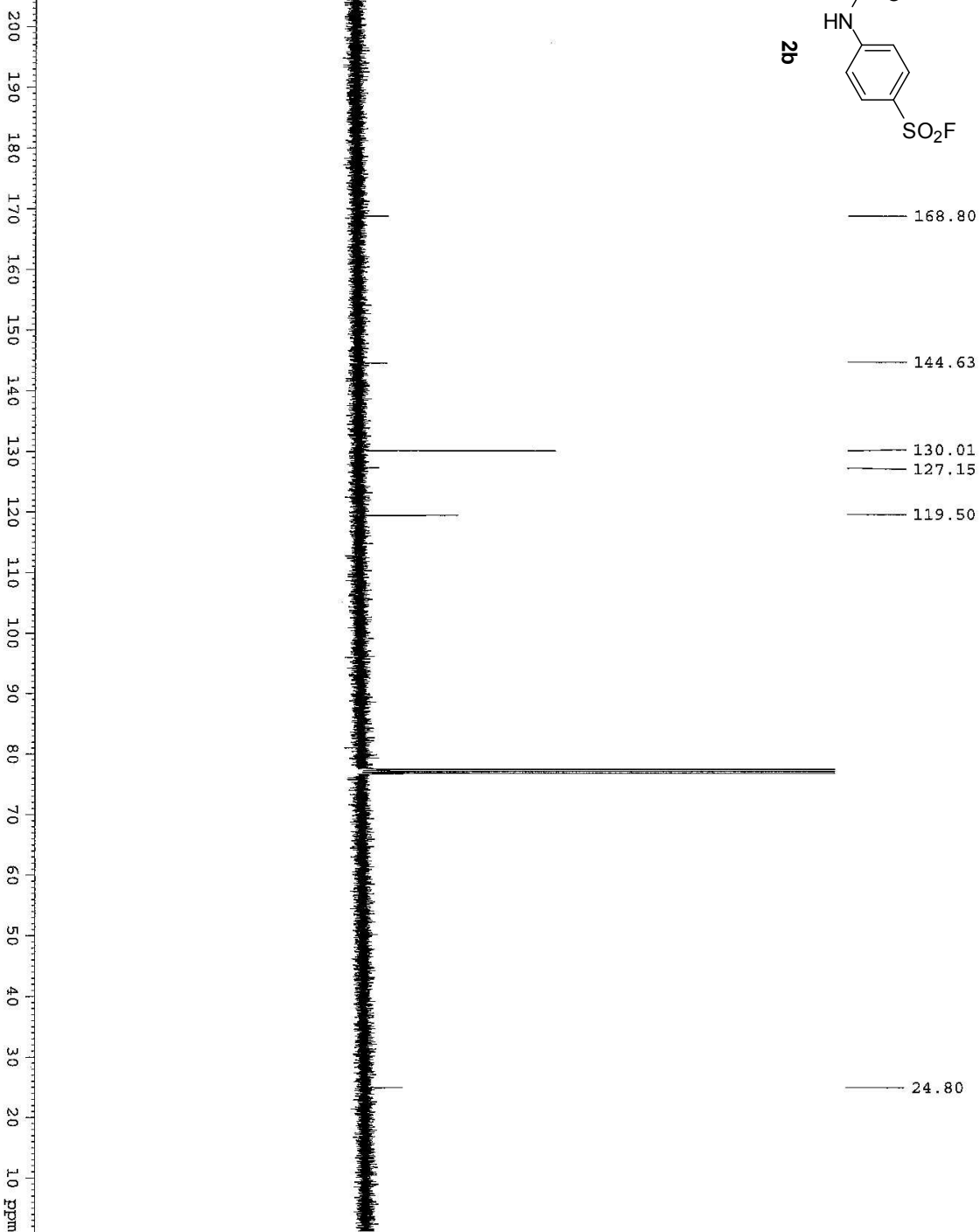
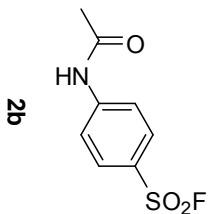
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PULPROG       zg30
TD            32768
SOLVENT       CDCl3
NS            8
DS            2
SWH            4789.272 Hz
FIDRES        0.146157 Hz
AQ            3.4210281 sec
RG            1024
DW            104.400 usec
DE            6.00 usec
TE            298.2 K
D1            1.00000000 sec
TD0           1

===== CHANNEL f1 =====
NUC1           1H
P1            12.10 usec
PL1           -3.00 dB
SFO1          400.1322007 MHz

F2 - Processing parameters
SI            32768
SF            400.1300084 MHz
WDW           no
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
  
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bfr0104902 13C

Current Data Parameters
NAME IME07044
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20130328
Time 11.07
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1941
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 512
RG 512
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 2

===== CHANNEL f1 =====
NUC1 13C
P1 14.50 usec
PL1 3.00 dB
SFO1 100.6228303 MHz

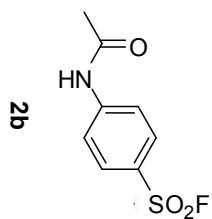
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NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.45 dB
PL13 25.00 dB
SFO2 400.1318006 MHz

F1 - Acquisition Parameters
ND0 1
TD 256
SFO1 100.6228 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FMODE Echo Antiecho

F2 - Processing Parameters
SI 32768
SF 100.6127709 MHz
NDW no
SSB no
TB 0.00 Hz
GB 0
PC 1.40

F1 - Processing Parameters
SI 131072
MC2 echo-antiecho
SF 100.5046553 MHz
WDW QSLINE
SSB 2
TB 0.30 Hz
GB 0.1

BFR01049_19F



65.34

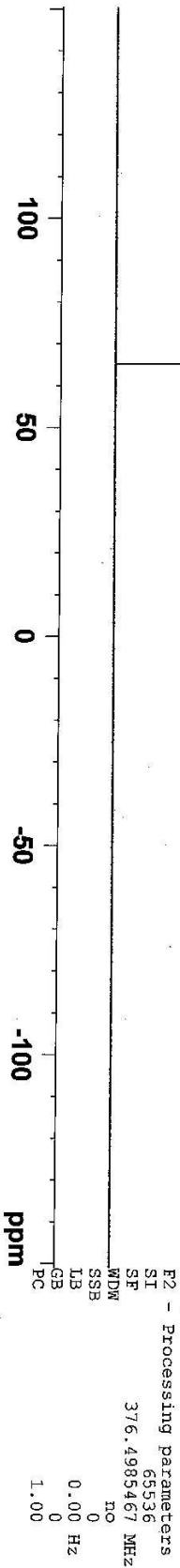


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EXPNO 1
PROCNO 1

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PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DW 4.400 usec
DE 10.00 usec
TE 298.1 K
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D11 0.03000000 sec
D12 0.0002000 sec
TD0 1

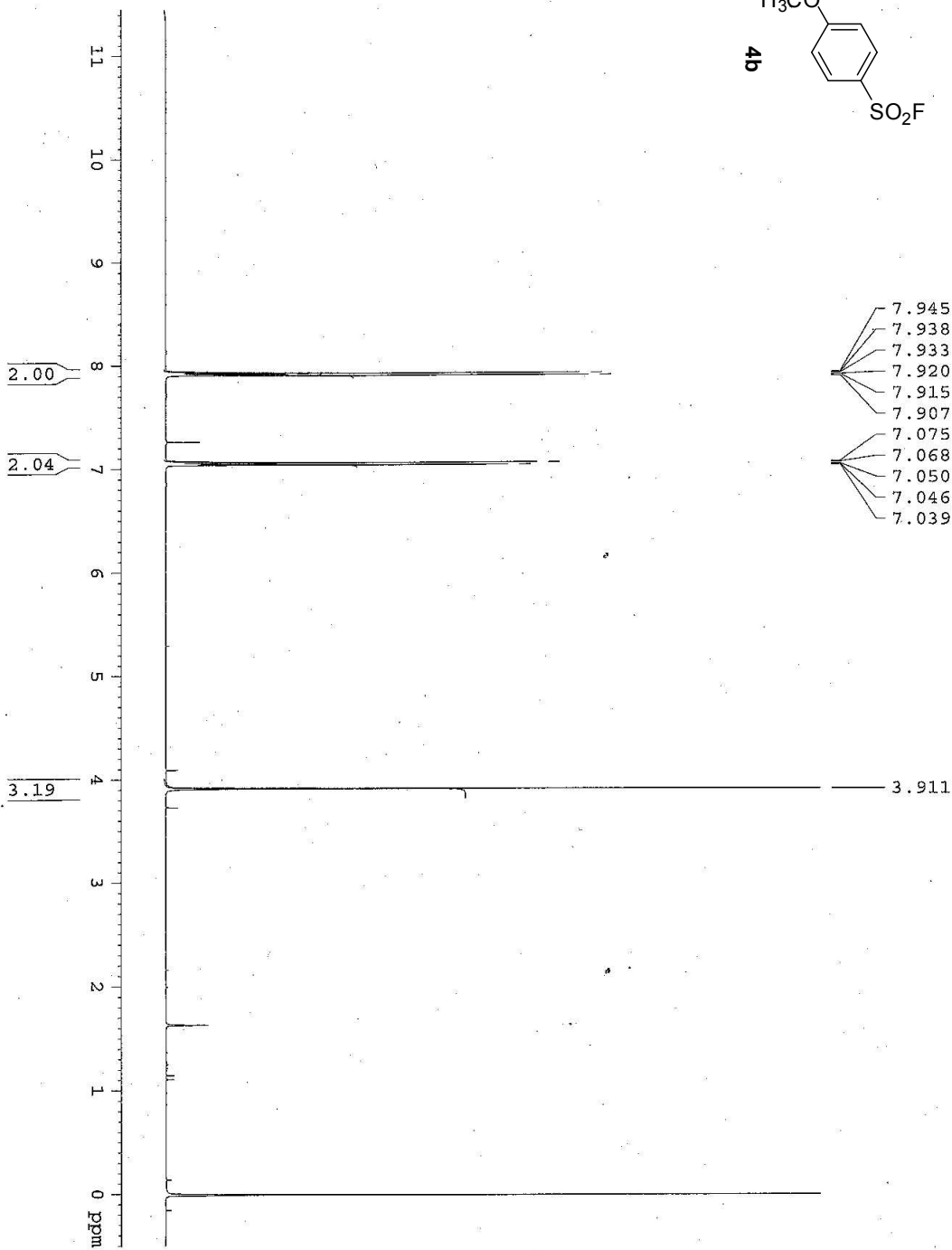
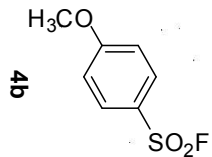
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NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66949272 W
SFO1 376.4983660 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.50 dB
PL12 15.33 dB
PL2W 14.77555943 W
PL12W 0.48589671 W
SFO2 400.1316005 MHz





bfc0104204_1H



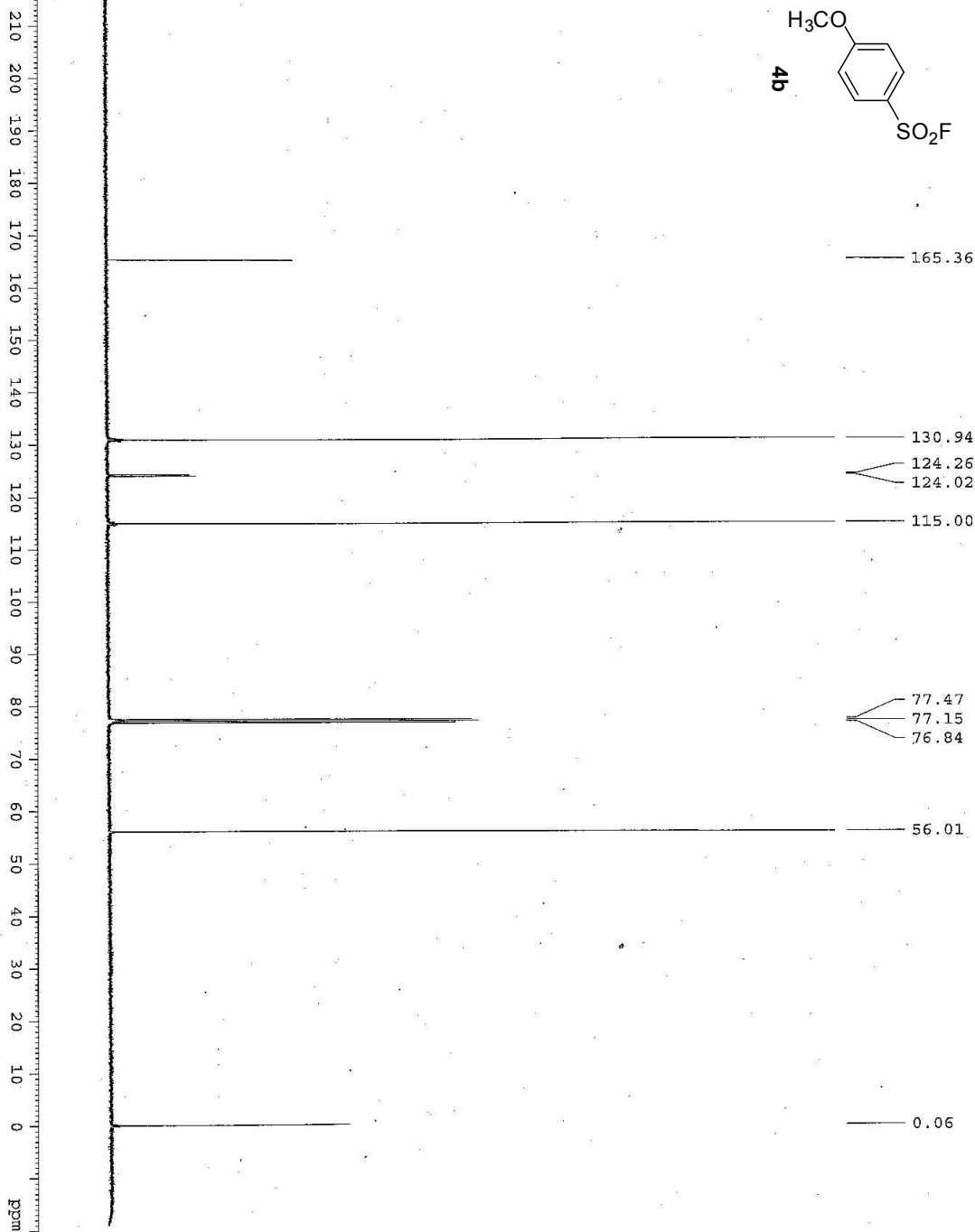
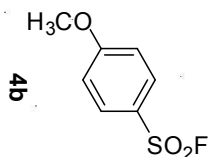
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EXPNO 1
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Time 10.49
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 90.5
DN 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.80 usec
PL 1.80 dB
SFO1 400.1322007 MHz

F2 - Processing parameters
SI 32768
SF 400.130086 MHz
WDW EM
SSB 0
CB 0
GB 0
PC 1.00

bfr0104204_13C



Current Data Parameters
NAME bfr0104204
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120307
Time 11.29
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 4
SWH 23980.814 Hz
FIDRES 0.26512 Hz
AQ 1.366475 sec
RG 386.63
DA 20.850 usec
DE 6.00 usec
TE 284.2 K
D1 1.0000000 sec
d11 0.0300000 sec
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TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 17.50 usec
PL1 3.00 dB
SFO1 100.628303 MHz

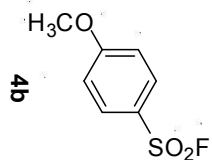
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NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 18.10 dB
PL13 25.00 dB
SFO2 400.131806 MHz

F1 - Acquisition Parameters
ND0 1
TD 256
SFO1 100.6228 MHz
FIDRES 3.906250 Hz
SM 9.938 ppm
FMODE Echo-Antiecho

F2 - Processing Parameters
SI 32768
SF 100.612787 MHz
RG 64
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

F1 - Processing Parameters
SI 1024
MC2 echo-antiecho
SF 100.5046953 MHz
WDW OSINE
SSB 2
LB 0.30 Hz
GB 0.1

BFR01042_19F



65.68



14

Current Data Parameters
 NAME BFR01042
 EXPMO 1
 PROCNO 1

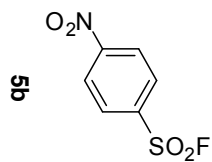
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 Time_ 11.52
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 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 131072
 SOLVENT Acetone
 NS 16
 DS 4
 SMH 113636.367 Hz
 FIDRES 0.866877 Hz
 AQ 0.5767668 sec
 RG 203
 DW 4.400 usec
 DE 10.00 usec
 TE 296.0 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 14.90 usec
 PL1 -1.30 dB
 PL1W 20.66949272 W
 SFO1 376.4983660 MHz

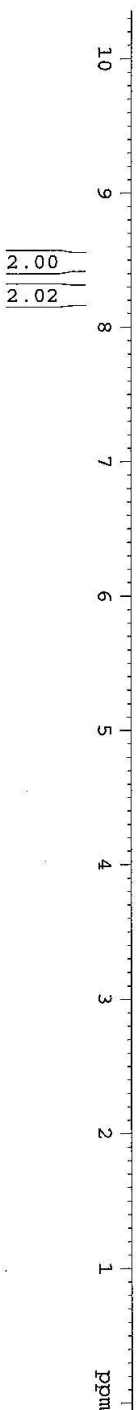
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 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.50 dB
 PL12 15.33 dB
 PL12W 14.77555943 W
 PL12W 0.48589671 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 376.4985467 MHz
 WDW no
 SSB 0
 GB 0
 PC 1.00

100 50 0 -50 -100 ppm



8.495
8.485
8.472
8.251
8.250
8.238
8.228



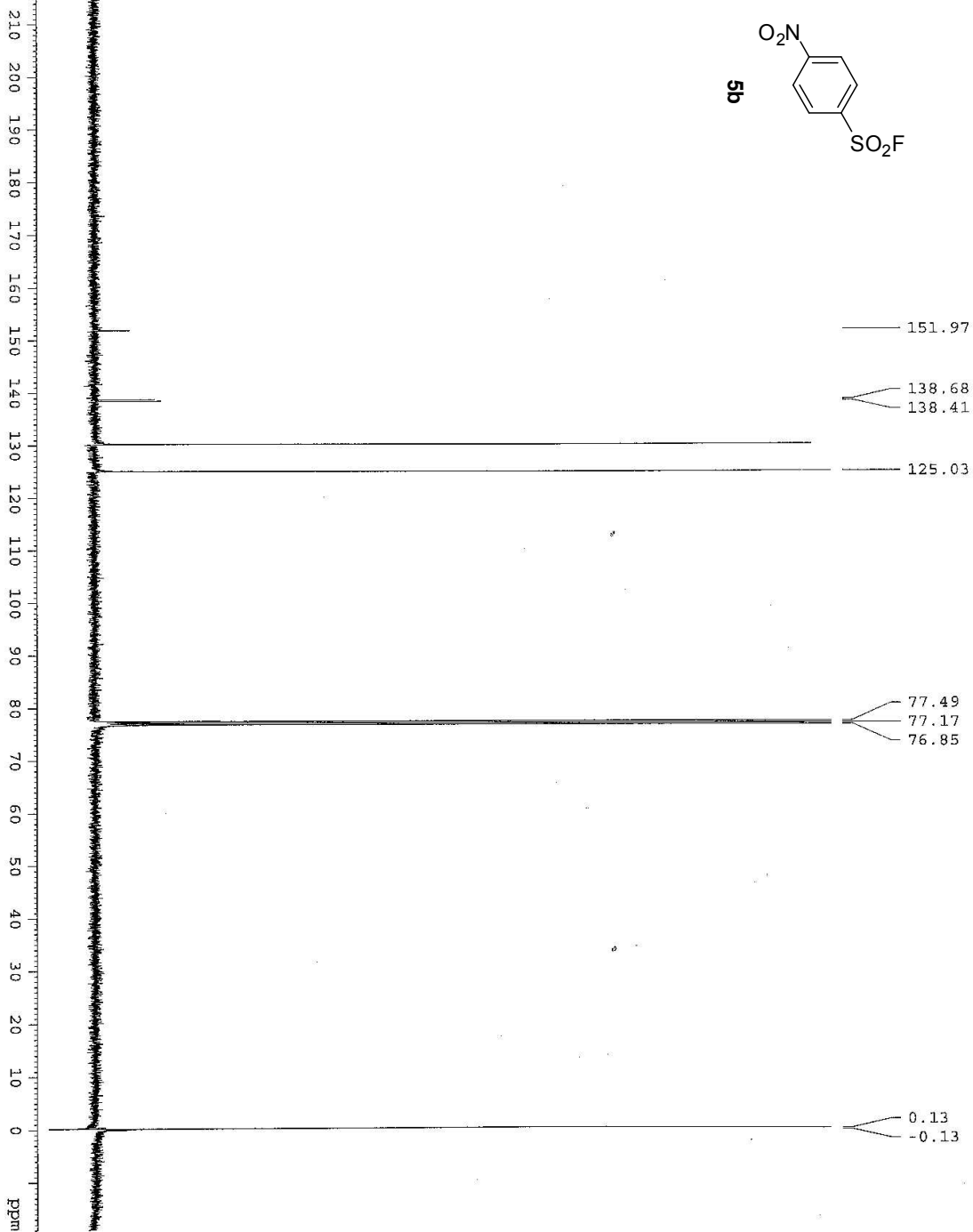
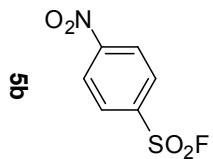
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time_ 17.06
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PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 228.1
DM 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 9.80 usec
PL1 1.80 dB
SFO1 400.1322007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

bfr0103701_13C



Current Data Parameters
NAME bfr0103701
EXPNO 12
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120217
Time 11.16

INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30

TD 65536
SOLVENT CDCl3

NS 710
DS 4

SWH 23980.814 Hz
FIDRES 0.365918 Hz

AQ 1.3664766 sec
RG 1.28963

WDW 20.850 usec
DE 6.00 usec

TE 298.2 K
D1 1.00000000 sec

d11 0.03000000 sec
DELTA 0.89999998 sec

TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 17.50 usec
PL1 3.00 dB

SFO1 100.6228303 MHz

===== CHANNEL f2 =====
CEPPRG2 waltz16

NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB

PL12 18.10 dB
PL13 25.00 dB

SFO2 400.1318006 MHz

F1 - Acquisition Parameters
NDO 1

TD 256
SF01 100.6228 MHz

FIDRES 3.906250 Hz
SW 9.938 ppm

FMODE Echo-Antiecho

F2 - Processing Parameters
SI 32768

SP 100.6127539 MHz
WDW EM

SSB 0
LB 1.00 Hz

GB 0
PC 1.40

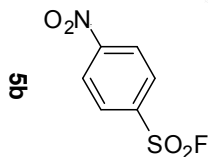
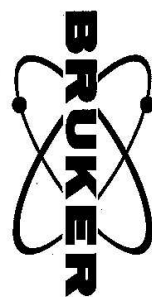
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SI 1024

MC2 echo-antiecho
SF 100.5046953 MHz

WDW QSIKE
SSB 2

LB 0.30 Hz
GB 0.1

BFR01037_19F



63.98

Current Data Parameters
NAME BFR01037
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time_ 11.48

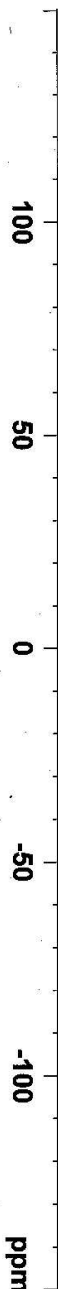
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PROBHD zgpg30
PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4

SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DW 4.400 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66949272 W
SFO1 376.4983660 MHz

===== CHANNEL f2 =====
CEPPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PT2 0.50 dB
PL2 15.33 dB
PL2W 14.77555943 W
PL12W 0.48589671 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 376.4985467 MHz
WDW NO
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



LMF4031

Current Data Parameters
NAME LMF4031
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120413
Time 15.04

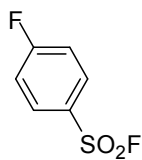
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PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 8
DS 2

SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1024

DW 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

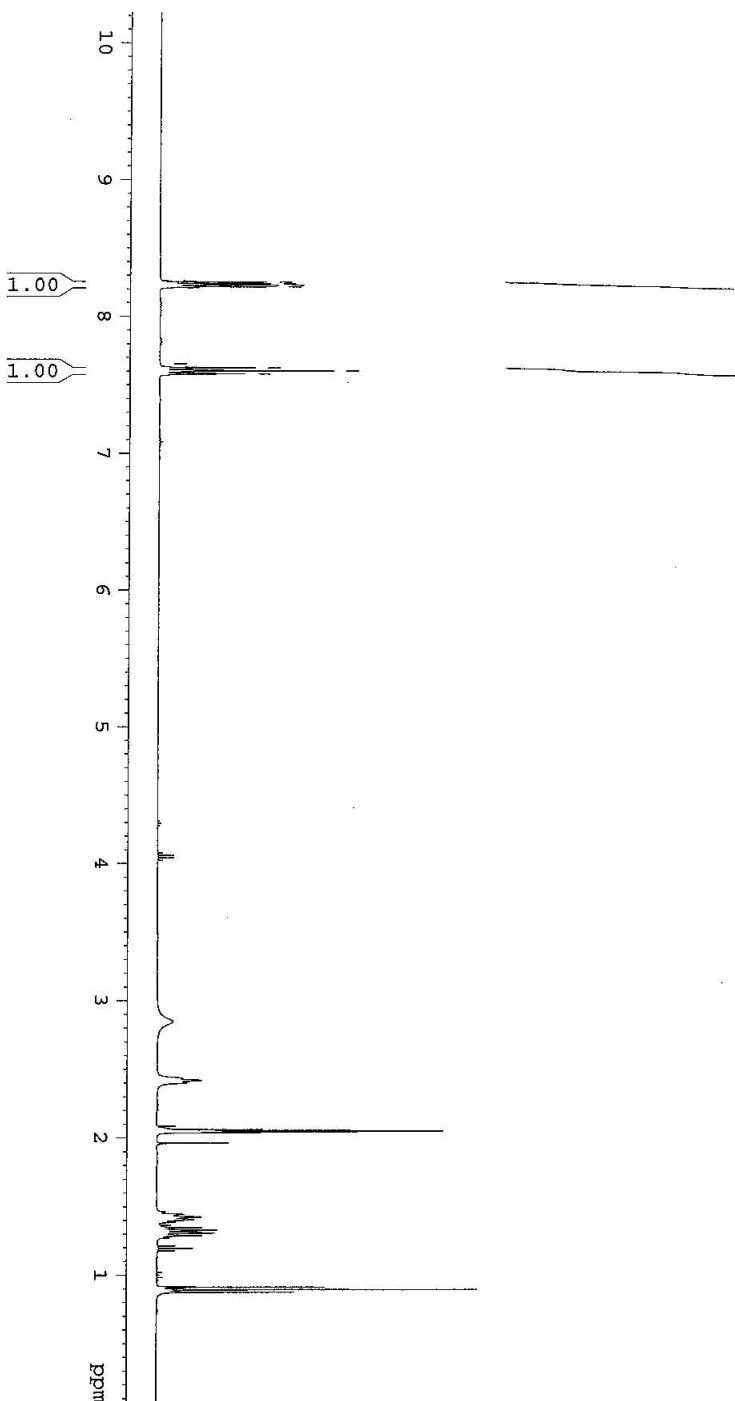
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NUC1 1H
P1 12.10 usec
PL1 -3.00 dB
SFO1 400.1322007 MHz

F2 - Processing parameters
SI 32768
SF 400.130064 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



6b

8.257
8.249
8.244
8.237
8.232
8.227
8.220
8.214
8.207
7.651
7.629
7.622
7.601
7.583
7.578
7.572



LMF4031_13C

Current Data Parameters
NAME LMF4031
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120416
Time 13.13

INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2048

DS 4
SWH 23980.814 Hz
FIDRES 0.265216 Hz
AQ 1.366418 sec
RG 512
DM 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 2

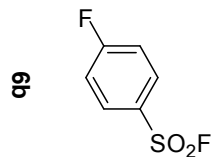
===== CHANNEL f1 =====
NUC1 13C
P1 14.50 usec
PL1 3.00 dB
SFO1 100.6228303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PLA2 11.45 dB
PLA3 25.00 dB
SFO2 400.1318006 MHz

F1 - Acquisition Parameters
ND0 1
TD 256
SFO1 100.6228 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
PwMODE Echo-Antiecho

F2 - Processing parameters
SI 32768
SF 100.6126771 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5046953 MHz
WDW QSINE
SSB 2
LB 0.30 Hz
GB 0.1



169.31
166.73

132.90
132.79

118.63
118.40

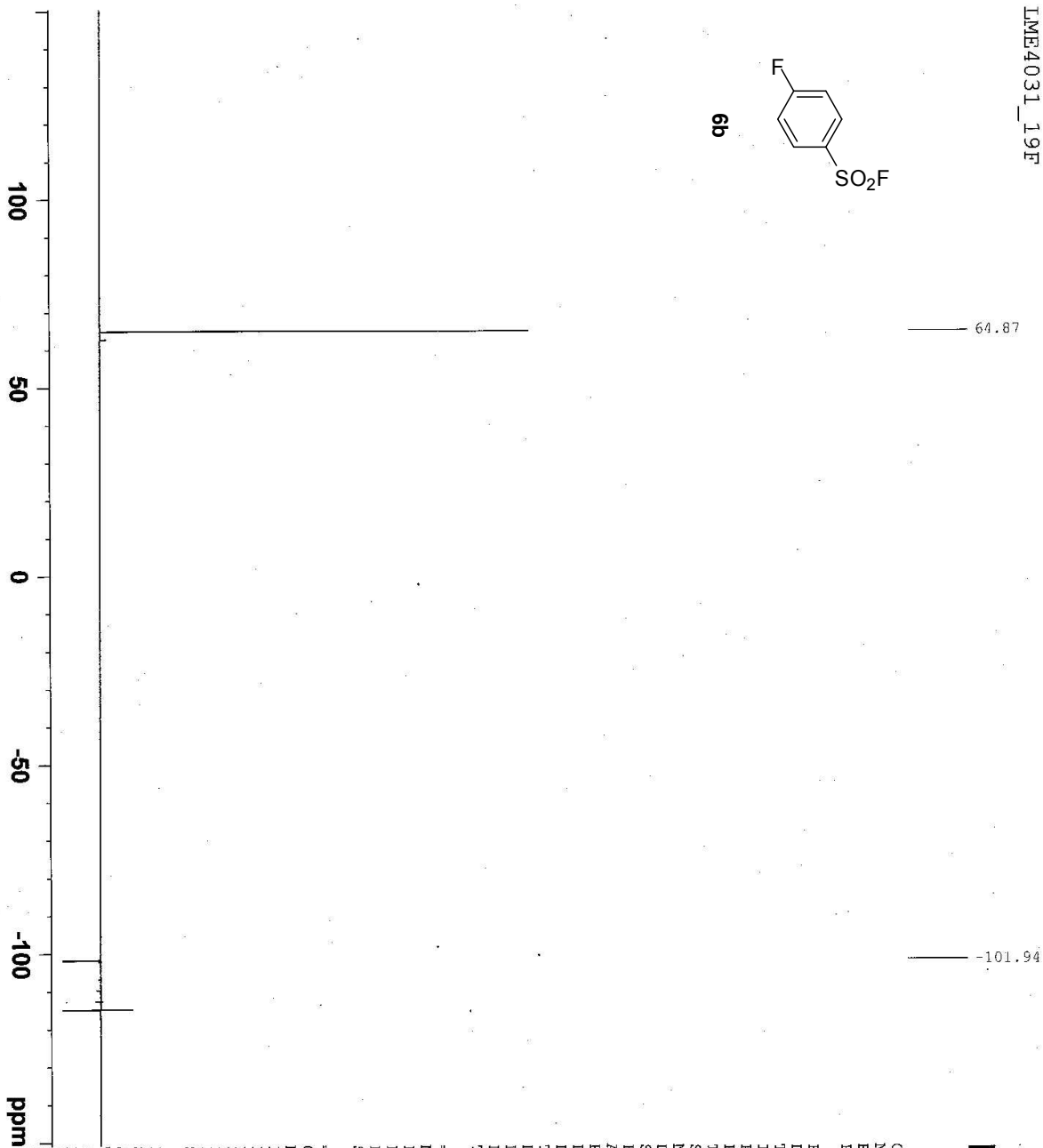
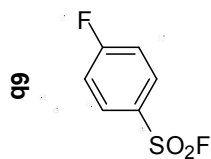
54.51

21.18

14.32

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

LME4031_19F



Current Data Parameters
NAME LME4031
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120801
Time_ 11.38
INSTRUM spect
PROBHD 5 mm PABO BB-
PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DW 4.400 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66949272 W
SFO1 376.4983660 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.50 dB
PL12 15.33 dB
PL2W 14.77555943 W
PL12W 0.48589671 W
SFO2 400.1316005 MHz

F2 - Processing Parameters
SI 376.4985467 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

LMF4035

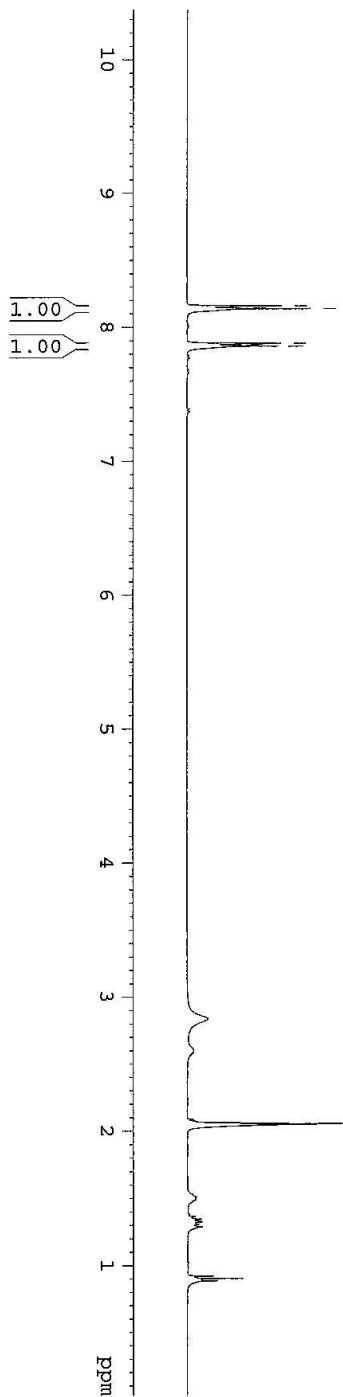
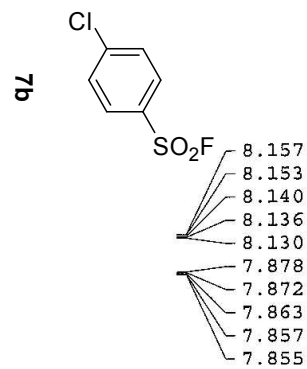
Current Data Parameters
NAME LMF4035
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120419
Time 14.22

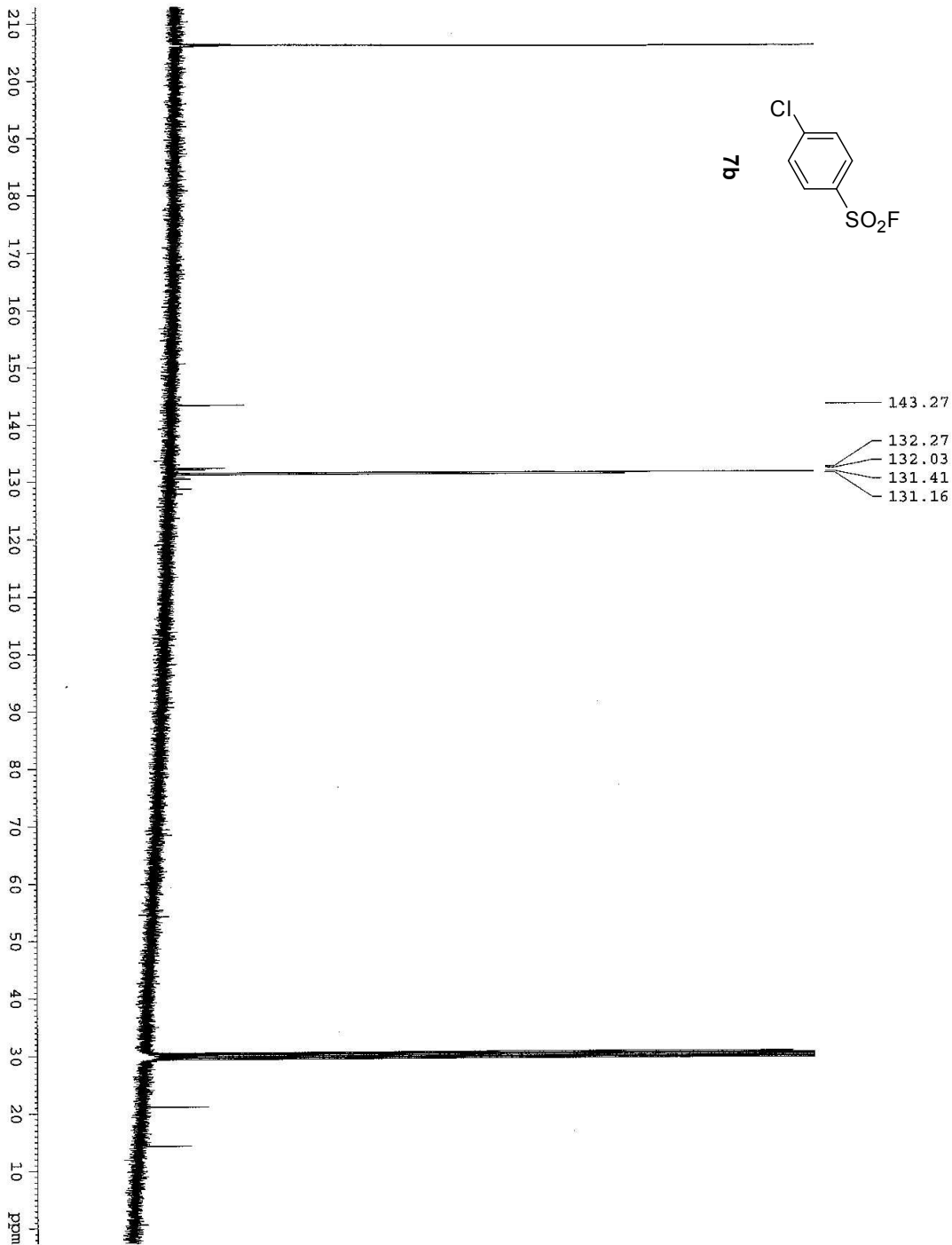
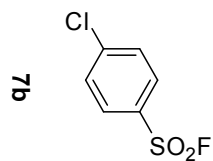
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 8
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1024
DW 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.10 usec
PL1 -3.00 dB
SFO1 400.1322007 MHz

F2 - Processing Parameters
SI 32768
SF 400.130065 MHz
WDW DO
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



IME4035_13C



Current Data Parameters
NAME IME4035
EXNO 3
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120419
Time 15.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2048
DS 4
SWH 23980.814 Hz
FIDRES 0.363218 Hz
AQ 1.3684125 sec
RG 327.5
RG 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 2

===== CHANNEL f1 =====
NUC1 13C
P1 14.50 usec
PL1 3.00 dB
SFO1 100.628303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.45 dB
PL13 25.00 dB
SFO2 400.1318006 MHz

F1 - Acquisition parameters
ND0 251
TD 100.6228 MHz
SFO1 3.906250 Hz
SWH 9.938 PPM
FMODE Echo-Antiecho

F2 - Processing parameters
SI 32768
SF 100.6126771 MHz
WDW TO
SSB 0
LB 0.08 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5046953 MHz
WDW QSINE
SSB 2
LB 0.30 Hz
GB 0.1

IME4035_19F



Current Data Parameters
NAME IME4035
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date_ 20120801
Time_ 11.29
INSTRUM 5 mm PABBO BB-
PROBHD zgpg30
PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DM 4.400 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.0002000 sec
TD0 1

==== CHANNEL f1 =====

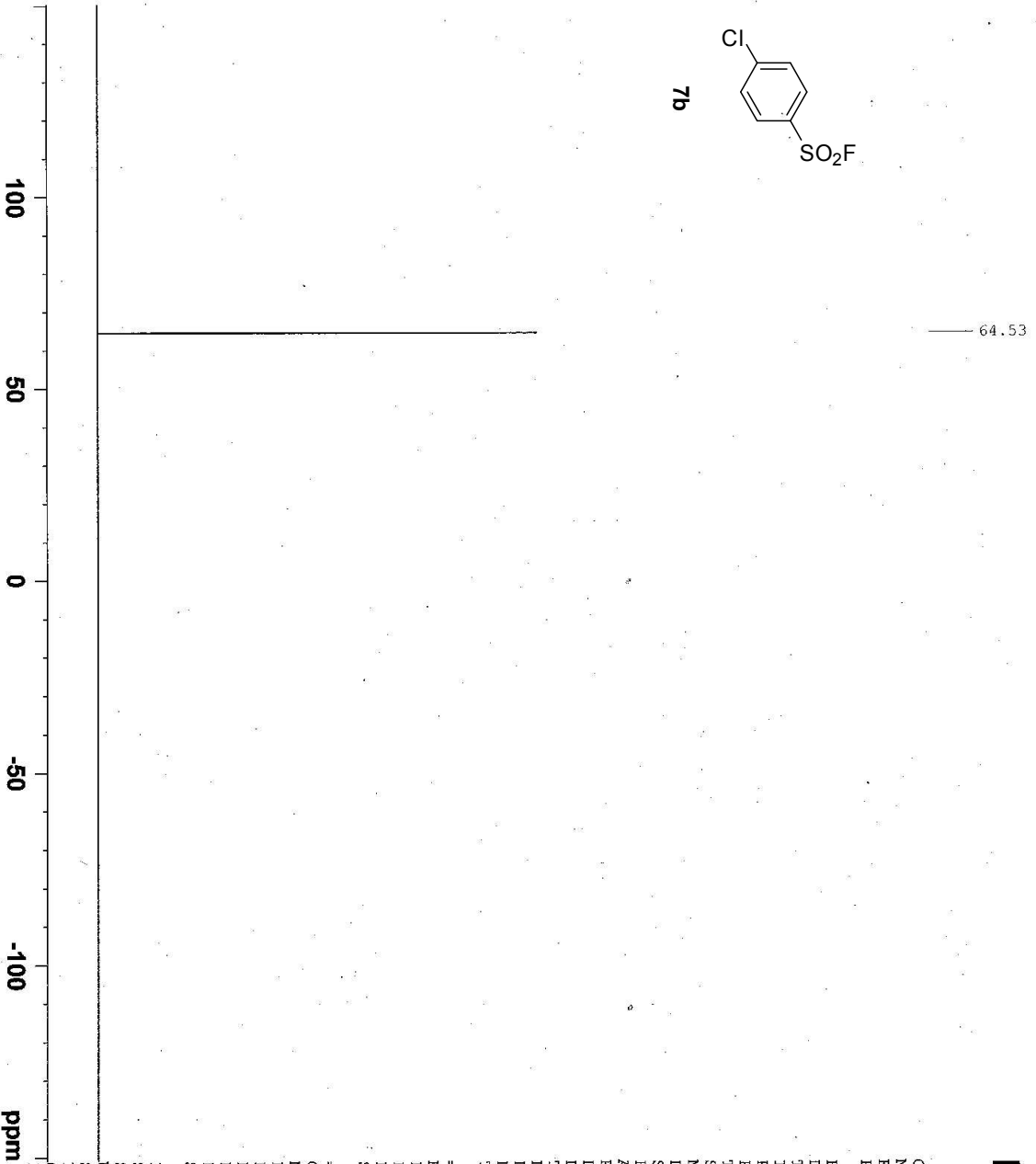
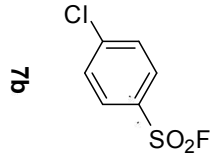
NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66949272 W
SFO1 376.4983660 MHz

==== CHANNEL f2 =====

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.50 dB
PL12 15.33 dB
PL2W 14.77555943 W
PL12W 0.48589671 W
SFO2 400.1316005 MHz

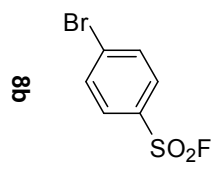
F2 - Processing parameters

SI 65536
SF 376.4985467 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



IME4033

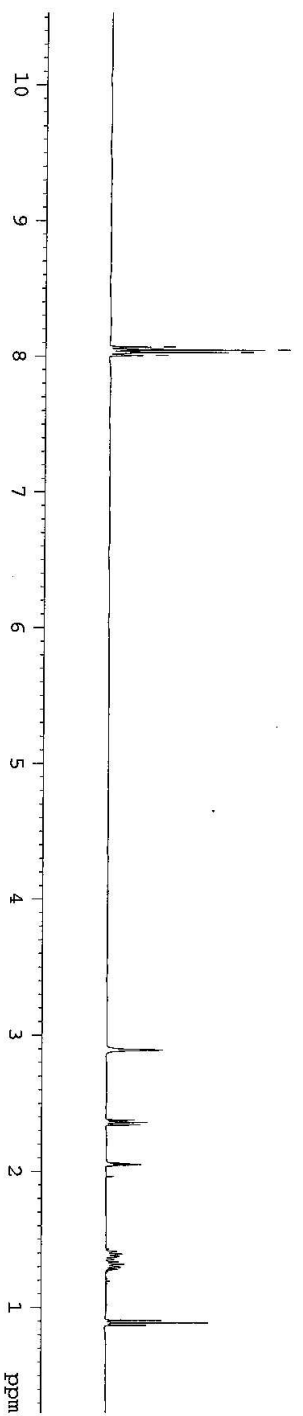
- 8.068
- 8.063
- 8.052
- 8.046
- 8.042
- 8.028
- 8.023
- 8.006



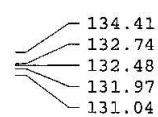
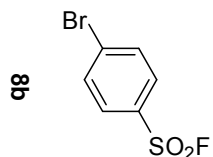
Current Data Parameters
NAME IME4033
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120417
Time 14.23
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 8
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1024
DW 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.10 usec
PL1 -3.00 dB
SFO1 400.1322007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300064 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



LME4033_13C



Current Data Parameters
NAME LME4033
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120417
Time 15.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 512
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec
d11 0.0300000 sec
DELTA 0.8999998 sec
TD0 2

===== CHANNEL f1 =====
NUC1 13C
P1 14.50 usec
PL1 3.00 dB
SFO1 100.628303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.45 dB
PL13 25.00 dB
SFO2 400.1318006 MHz

F1 - Acquisition Parameters
ND0 1
TD 256
SFO1 100.6228 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FMODE Echo-Antiecho

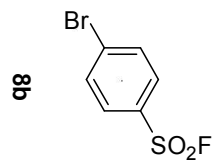
F2 - Processing Parameters
SI 32768
SF 100.6126800 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing Parameters
SI 1024
MC2 echo-antiecho
SP 100.5046953 MHz
WDW QSINE
SSB 2
LB 0.30 Hz
GB 0.1

IME4033_19F



Current Data Parameters
NAME IME4033
EXPNO 1
PROCNO 1



F2 - Acquisition Parameters

Date_ 20120801
Time_ 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DW 4.400 usec
DE 10.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.0002000 sec
TD0 1

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

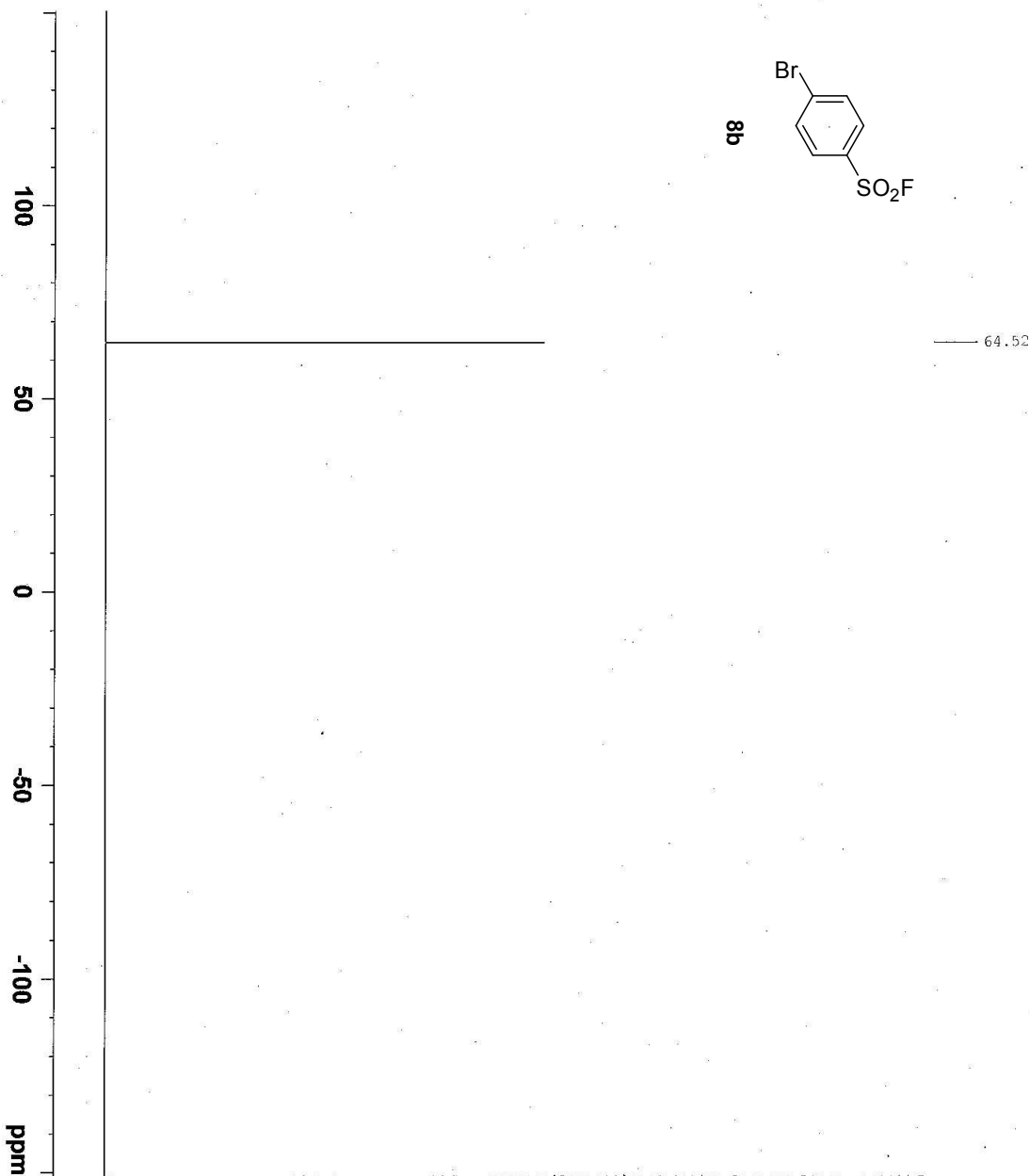
NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66949272 W
SFO1 376.4983660 MHz

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

CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.50 dB
PL12 15.33 dB
PL12W 14.77555943 W
PL12W 0.48589671 W
SFO2 400.1316005 MHz

F2 - Processing Parameters

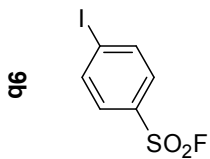
SI 65536
SF 376.498467 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



IME4034

Current Data Parameters
NAME IME4034
EXPNO 2
PROCNO 1

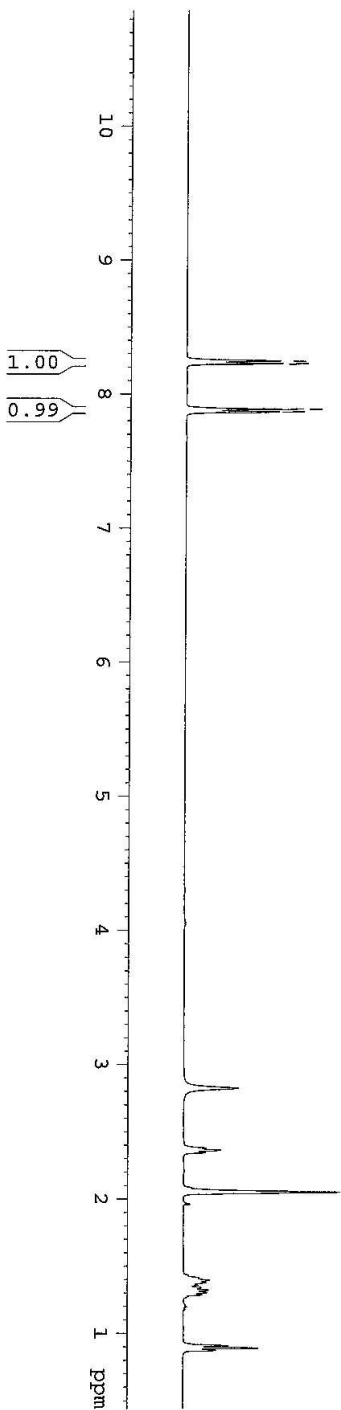
8.246
8.228
8.224
7.891
7.886
7.869
7.864



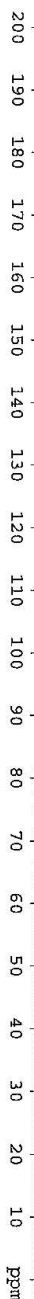
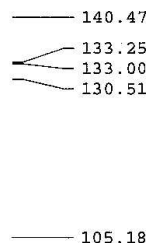
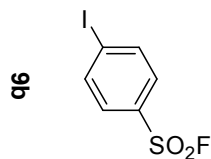
F2 - Acquisition Parameters
Date_ 20120417
Time_ 14.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 8
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1024
DM 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.10 usec
PL1 -3.00 dB
SFO1 400.1322007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300055 MHz
WDW DO
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



LME4034_13C



Current Data Parameters
NAME LME4034
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120418
Time 10.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
ID 65536
SOLVENT Acetone
NS 2048
DS 4
SWH 23980.814 Hz
FIDRES 0.36328 Hz
AQ 1.368452 sec
RG 1.368452
DM 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec
d11 0.0300000 sec
DELTA 0.8999998 sec
TD0 2

===== CHANNEL F1 =====
NUC1 13C
P1 14.50 usec
PL1 1.50 dB
SFO1 100.622803 MHz

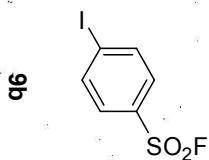
===== CHANNEL F2 =====
CDDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 11.45 dB
PL13 25.00 dB
SFO2 400.1318006 MHz

F1 - Acquisition parameters
MD0 1
NU0 255
SFO1 100.6228 MHz
FIDRES 3.906250 Hz
SW 9.998 ppm
FMODE Echo-Antlecho

F2 - Processing parameters
SI 32768
SF 100.6126787 MHz
WDW DO
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 65536
SF 400.1318006 MHz
WDW QSIINE
SSB 2
LB 0.30 Hz
GB 0.1

IME4034_19F



64.31



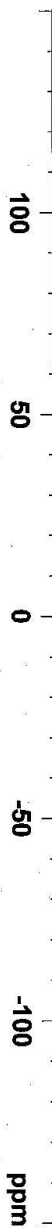
Current Data Parameters
NAME IME4034
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120801
Time 11.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866877 Hz
AQ 0.576766 sec
RG 203
DW 4.400 usec
DE 10.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66849272 W
SFO1 376.4983660 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PT2 0.50 dB
PL12 15.33 dB
PL1W 14.77555943 W
PL12W 0.48589671 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 376.4983467 MHz
WDW no
SSB 0
GB 0
PC 1.00



bfr0105802_1h



30

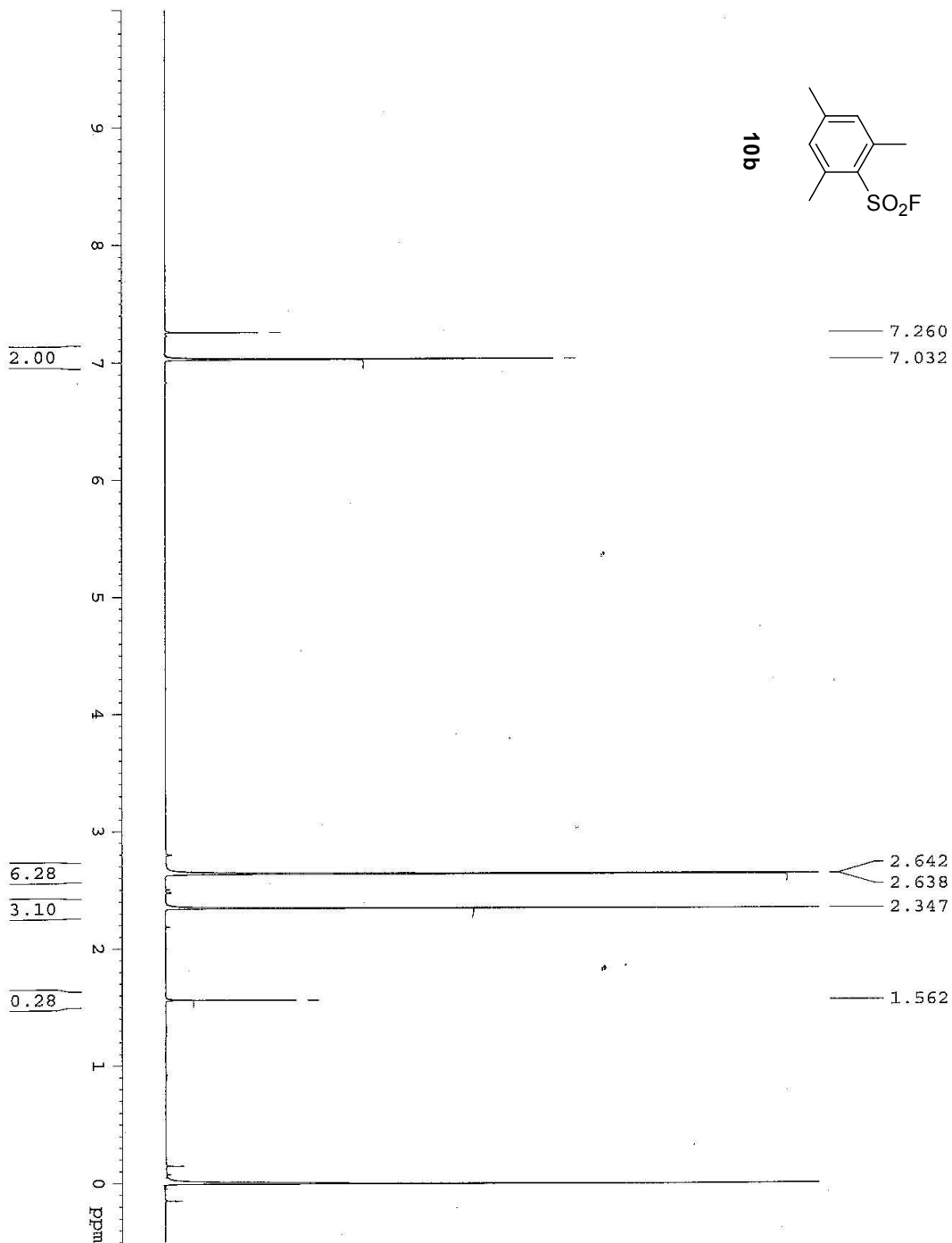
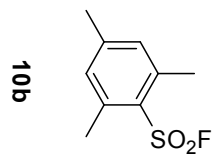
Current Data Parameters
 NAME bfr0105802
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120217
 Time 11.45

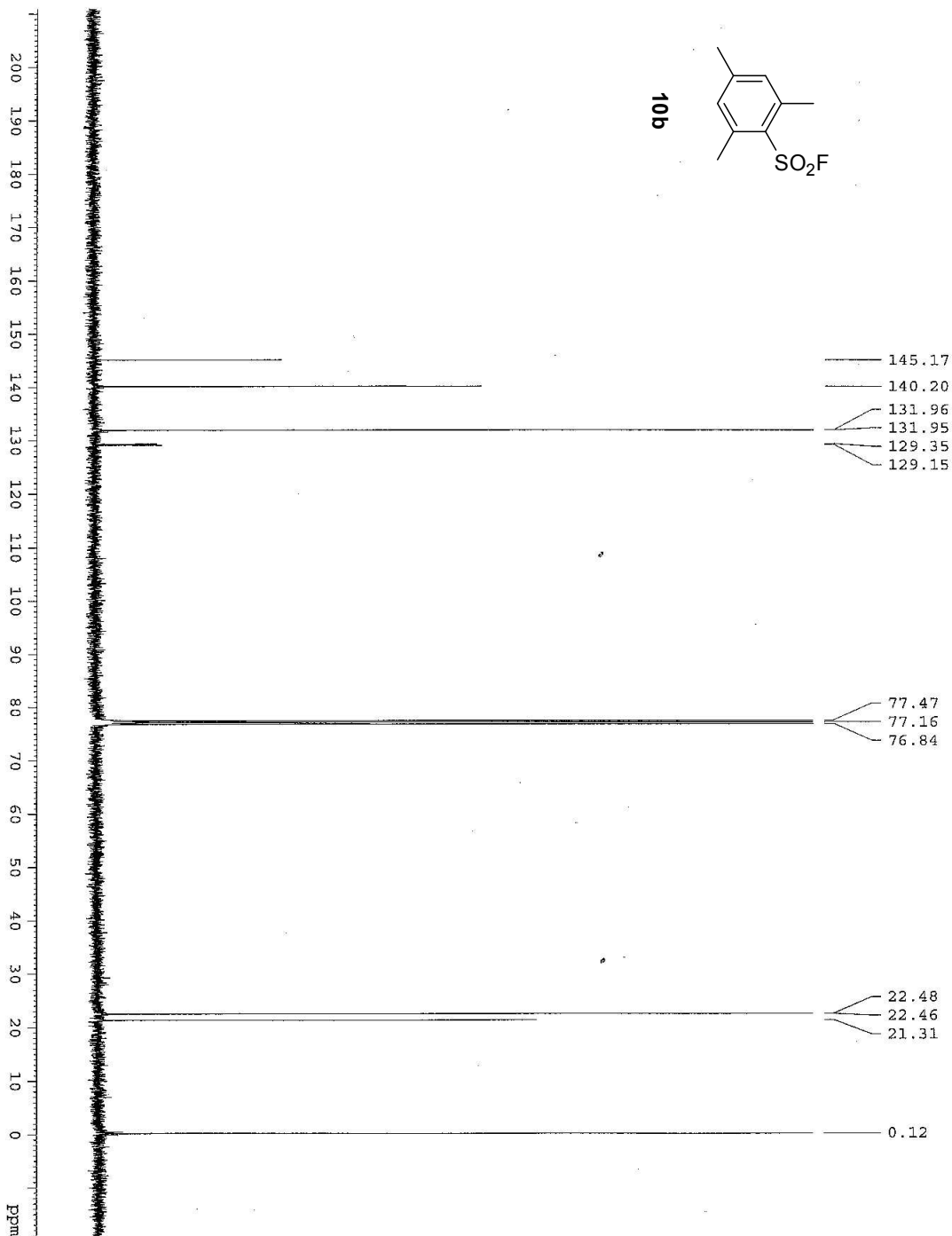
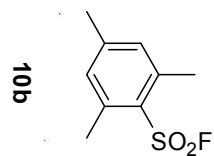
INSTRUM spect
 PROBHD 5 mm QNP 1H/1
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 2

SWH 4789.272 Hz
 FIDRES 0.146157 Hz
 AQ 3.4210291 sec
 RG 90.5
 DW 104.400 usec
 DE 6.00 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 9.80 usec
 PL1 1.80 dB
 SFO1 400.132007 MHz
 F2 - Processing parameters
 SI 32768
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



bfr0105802_13C



Current Data Parameters
NAME bfr0105802
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120217
Time 12.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 8192
DW 20.850 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec
d11 0.0300000 sec
DELTA 0.8999999 sec
TD0 1

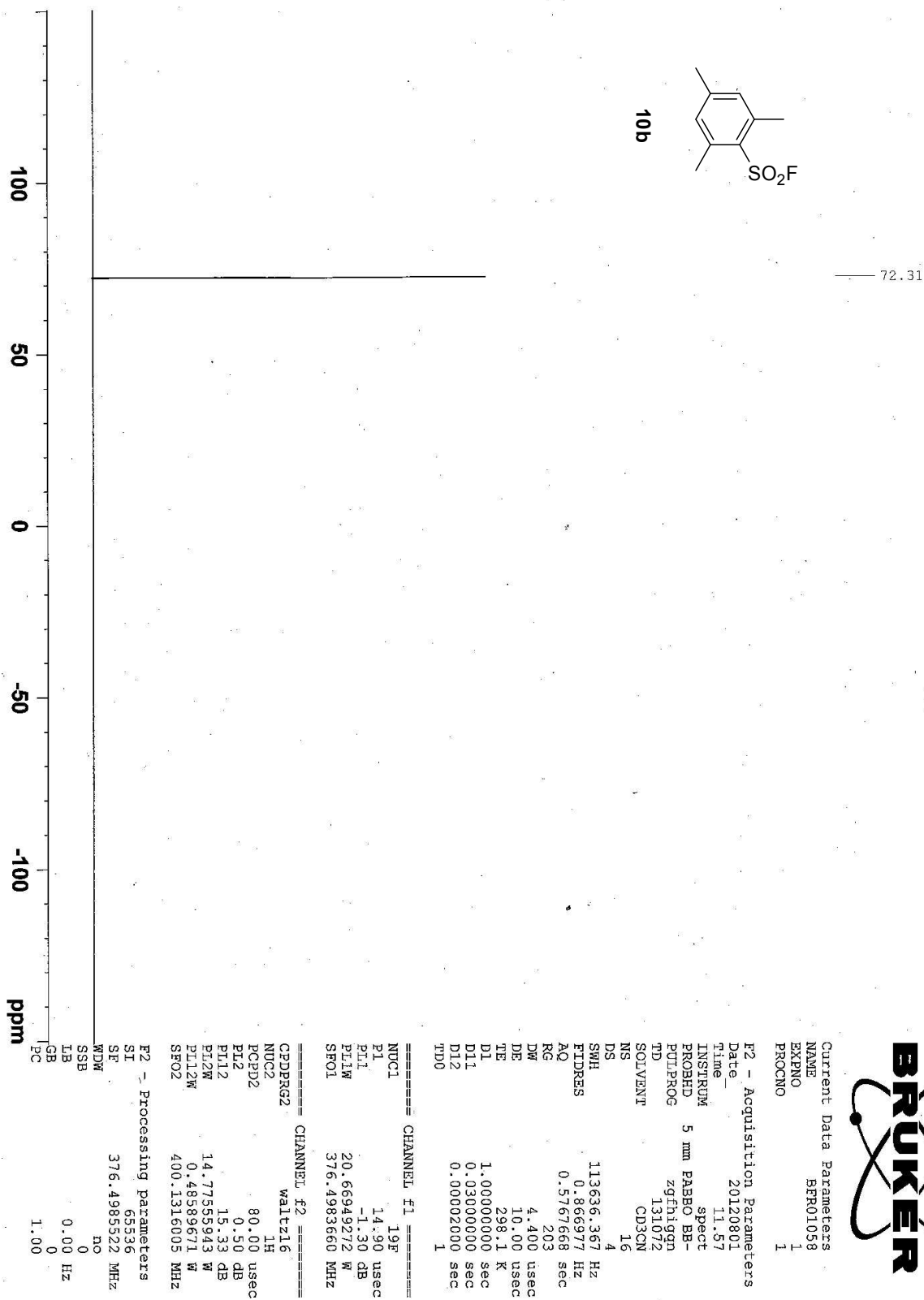
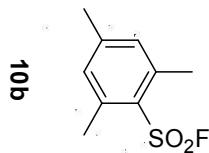
===== CHANNEL f1 =====
NUC1 13C
P1 17.50 usec
PL1 3.00 dB
SFO1 100.6228303 MHz

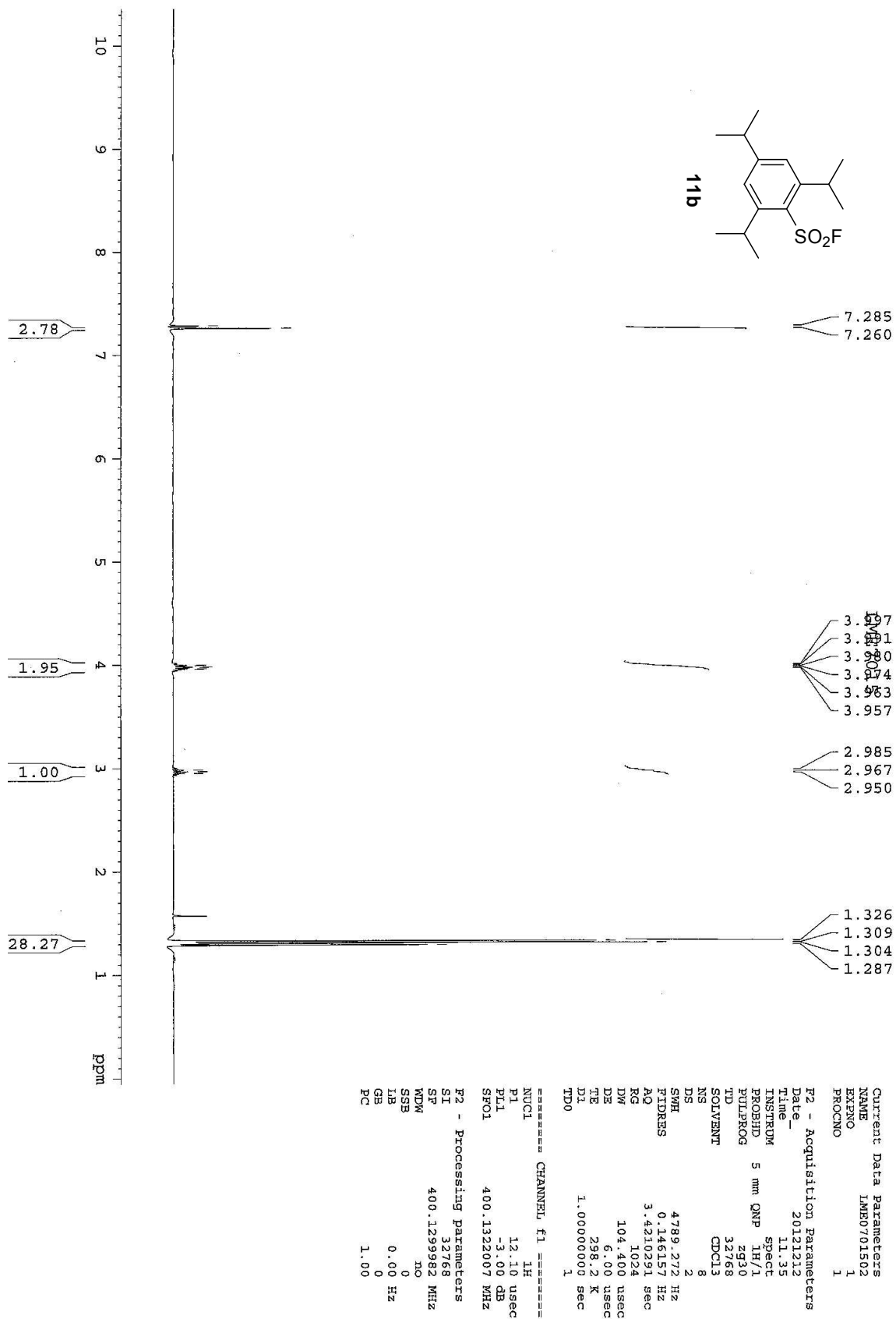
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.90 dB
PL12 18.10 dB
PL13 25.00 dB
SFO2 400.1318006 MHz

F1 - Acquisition parameters
ND0 1
TD 256
SF01 100.6228 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FMODE Echo-Antiecho

F2 - Processing parameters
SI 32768
SF 100.6127551 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5046953 MHz
WDW QSINE
SS2 2
LB 0.30 Hz
GB 0.1





bfr0104901_13C

Current Data Parameters
NAME bfr0104901
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120217
Time 13.01

INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30

TD 29932
SOLVENT CDCl3
NS 800

DS 4
SWH 23960.814 Hz
FIDRES 0.365918 Hz

AQ 1.3664756 sec
RG 2580.3
DW 20.850 usec

DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec

d11 0.03000000 sec
DELTA 0.89999998 sec
TD0 1

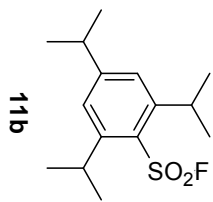
===== CHANNEL f1 =====
NUC1 13C
P1 17.50 usec
PL1 3.00 dB
SFO1 100.628303 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 18.10 dB
PL13 25.00 dB
SFO2 400.1318006 MHz

F1 - Acquisition Parameters
ND0 255
TD0 1
SFO1 100.6228 MHz
FIDRES 3.906250 Hz
SW 39.938 ppm
PRMODE Echo-Antiecho

F2 - Processing Parameters
SI 32768
SF 100.6127557 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

F1 - Processing Parameters
SI 1024
MC2 echo-antiecho
SF 100.5046953 MHz
WDW QSINE
SSB 2
LB 0.30 Hz
GB 0.1



11b

155.46
150.91

128.25
128.06
124.11

77.46
77.14
76.83

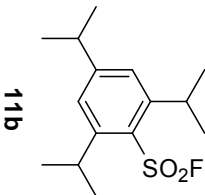
34.54
30.27
30.25
24.63
23.61

0.12

190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



67.08



Current Data Parameters
 NAME BFR0104901
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20120801
 Time 12.02

INSTNUM 5 mm PABBO BB-
 PROBD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 131072
 SOLVENT CD3CN
 NS 16
 DS 4

SWH 113636.367 Hz
 FIDRES 0.866977 Hz
 AQ 0.5767668 sec
 RG 203

DW 4.400 usec
 DE 10.00 usec
 TE 298.1 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 D12 0.00002000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 19F
 P1 14.90 usec
 PL1 -1.30 dB
 PL1W 20.66949272 W
 SFO1 376.4983660 MHz

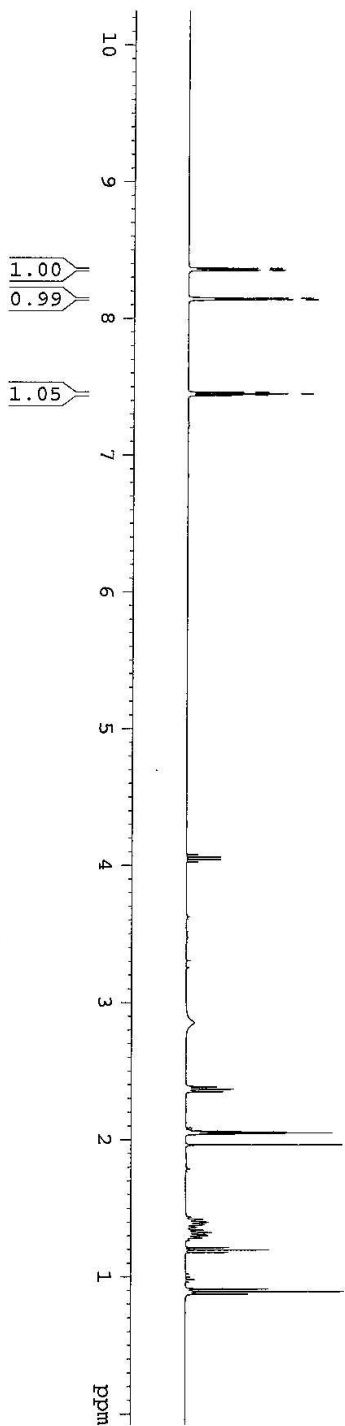
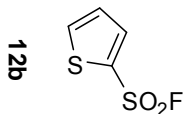
===== CHANNEL f2 =====
 CPDPRG2 waitz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.50 dB
 PL12 15.33 dB
 PL2W 14.77555943 W
 PL12W 0.48589671 W
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 65536
 SF 376.4985522 MHz
 WDW no
 SSB 0
 LB 0.00 Hz
 GB 0
 PC 1.00



IME4032_UVfraction

8.364
8.362
8.361
8.353
8.352
8.349
8.348
8.149
8.146
8.142
8.139
8.136
8.132
7.459
7.457
7.449
7.446
7.444
7.436
7.434

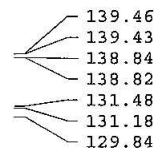
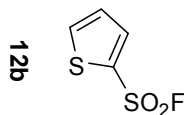


Current Data Parameters
NAME IME4032
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120413
Time 15.19
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 8
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1024
DM 104.400 usec
DE 6.00 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.10 usec
PL1 -3.00 dB
SFO1 400.1322007 MHz
F2 - Processing parameters
SI 32768
SF 400.1300064 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00

IMB4032_UVfraction_13C



```

Current Data Parameters
NAME          IMB4032
EXPNO         4
PROCNO        1

F2 - Acquisition Parameters
Date_         20120403
Time         14.07
INSTRUM       spect
PROBHD        5 mm QNP 1H/1
PULPROG       zgpg30
TD            65536
SOLVENT       Acetone
NS            2048
DS            4
SWH           23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG            512
RG            20.850 usec
DE            6.00 usec
TE            298.2 K
D1            1.00000000 sec
d11           0.03000000 sec
DELTA         0.89999998 sec
TD0           2

===== CHANNEL f1 =====
NUC1          13C
P1            14.50 usec
PL1           3.00 dB
SFO1          100.626303 MHz

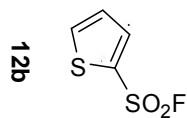
===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 usec
PL2           -3.00 dB
PL12          11.45 dB
PL13          25.00 dB
SFO2          400.1318006 MHz

F1 - Acquisition Parameters
ND0           1
TD            256
SFO1          100.6228 MHz
FIDRES        3.906250 Hz
SW            9.938 PPM
PULPROG       Echo-Antiecho

F2 - Processing Parameters
SI            32768
SF            100.6126787 MHz
WDW           DO
SSB           0
GB            0
PC            1.40

F1 - Processing Parameters
SI            1024
MC2           echo-antiecho
SF            100.5046953 MHz
WDW           QSTINE
SSB           2
GB            0.30 Hz
GB            0.1
  
```

IME4032_19F



70.19



Current Data Parameters
NAME IME4032
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120801
Time 11.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203
DM 4.400 usec
DE 10.00 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66949272 W
SFO1 376.4983660 MHz

===== CHANNEL f2 =====
CPDPRG2 wait216
NUC2 1H
PCPD2 80.00 usec
PL2 0.50 dB
PL12 15.33 dB
PL2W 14.77555943 W
PL12W 0.48589671 W
SFO2 400.1316005 MHz

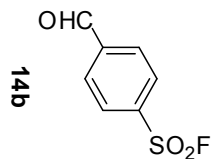
F2 - Processing parameters
SI 65536
SF 376.4985467 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



LME4099_F1

Current Data Parameters
NAME LME4099
EXPNO 3
PROCNO 1

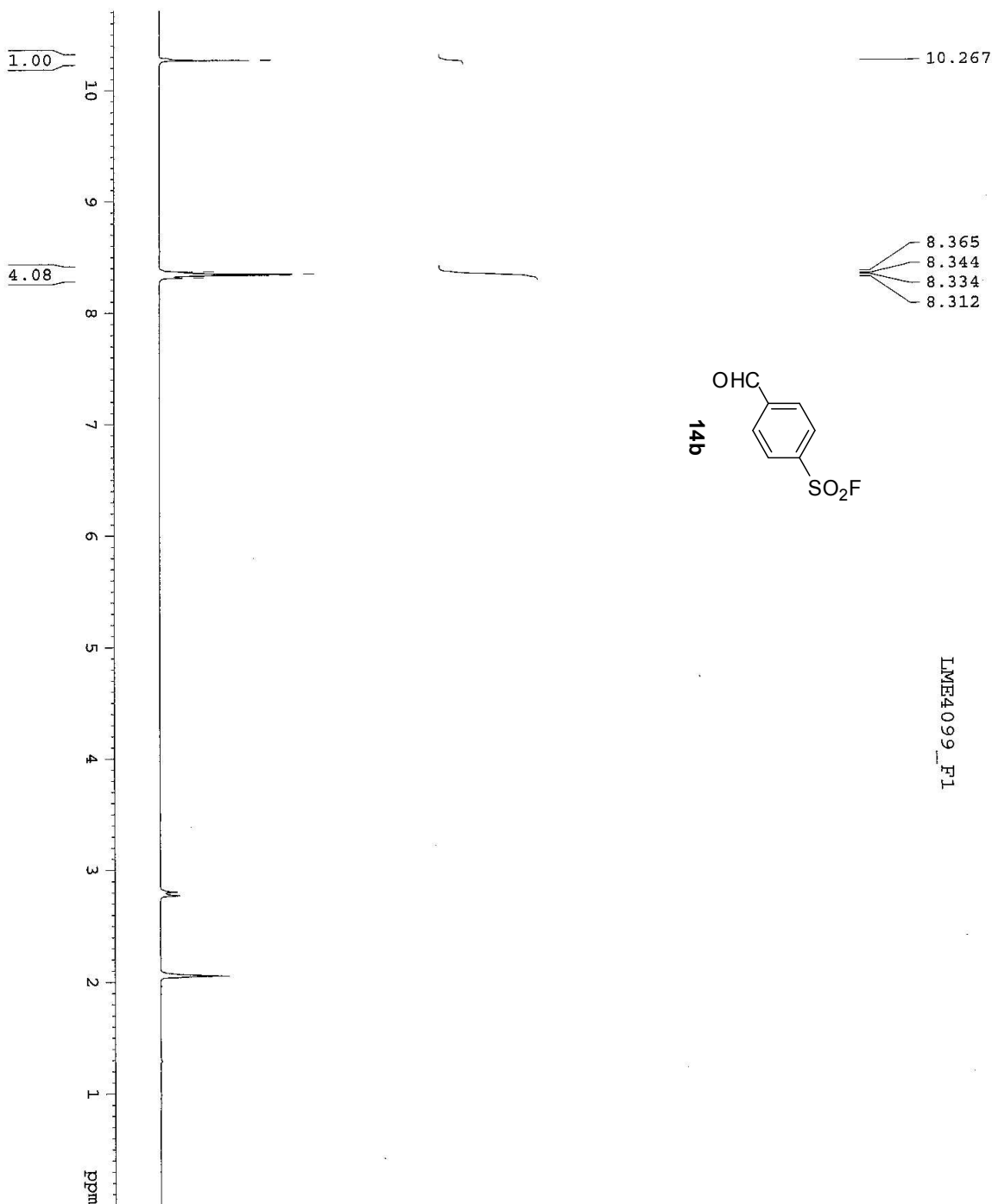
8.365
8.344
8.334
8.312



F2 - Acquisition Parameters
Date_ 20120718
Time 16.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg30
TD 32768
SOLVENT Acetone
NS 8
DS 2
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 1024
DW 104.400 usec
DE 6.00 usec
TE 301.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 12.10 usec
PL1 -3.00 dB
SFO1 400.1322007 MHz

F2 - Processing parameters
SI 32768
SF 400.1300060 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00



Current Data Parameters
NAME LME4099
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20120718
Time 16:36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 8192
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 512
DM 20.850 usec
DE 6.00 usec
TE 301.2 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89939998 sec
TD0 8

===== CHANNEL f1 =====
NUC1 13C
P1 14.50 usec
PL1 3.00 dB
SFO1 100.6228303 MHz

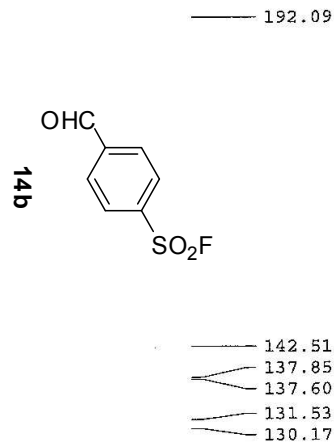
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.40 dB
PL12 11.40 dB
PL13 21.00 dB
SFO2 400.1318006 MHz

f1 - Acquisition parameters
ND0 1
TD 256
SFO1 100.6228 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FMODE Echo-Antiecho

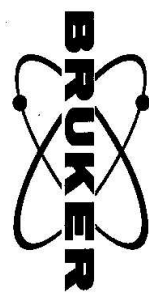
F2 - Processing parameters
SI 32768
SF 100.6126767 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

f1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.5046953 MHz
WDW QSINE
SSB 2
LB 0.30 Hz
GB 0.1

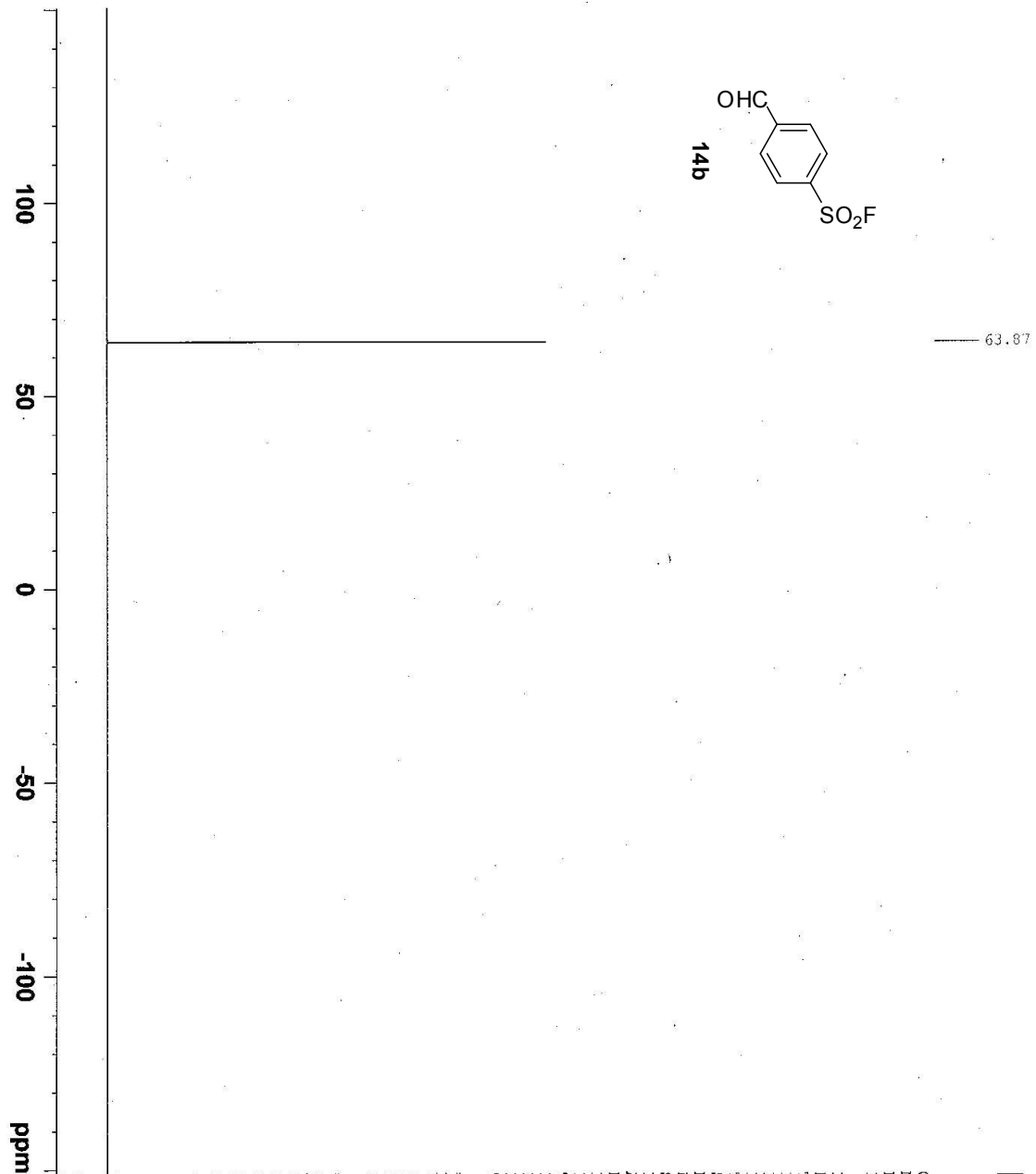
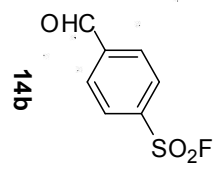
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



LME4099



Current Data Parameters
NAME LME4099
EXPNO 1
PROCNO 1



F2 - Acquisition Parameters
Date_ 20120801
Time_ 11.05

INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 131072
SOLVENT Acetone
NS 16
DS 4

SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 203

DW 4.400 usec
DE 10.00 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 14.90 usec
PL1 -1.30 dB
PL1W 20.66949272 W
SFO1 376.4983660 MHz

===== CHANNEL f2 =====
CDEPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.50 dB
PL12 15.33 dB
PL2W 14.77555943 W
PL12W 0.48589671 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 65536
SF 376.4985467 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00