



Supporting Information

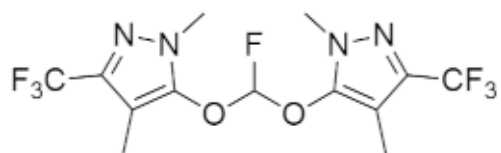
for

Synthesis of bis(aryloxy)fluoromethanes using a heterodihalocarbene strategy

Carl Recsei and Yaniv Barda

Beilstein J. Org. Chem. **2021**, *17*, 813–818. [doi:10.3762/bjoc.17.70](https://doi.org/10.3762/bjoc.17.70)

Copies of NMR spectra



7.272

6.476
6.292

3.752
3.673

2.075
2.039
1.998
1.669

0.000

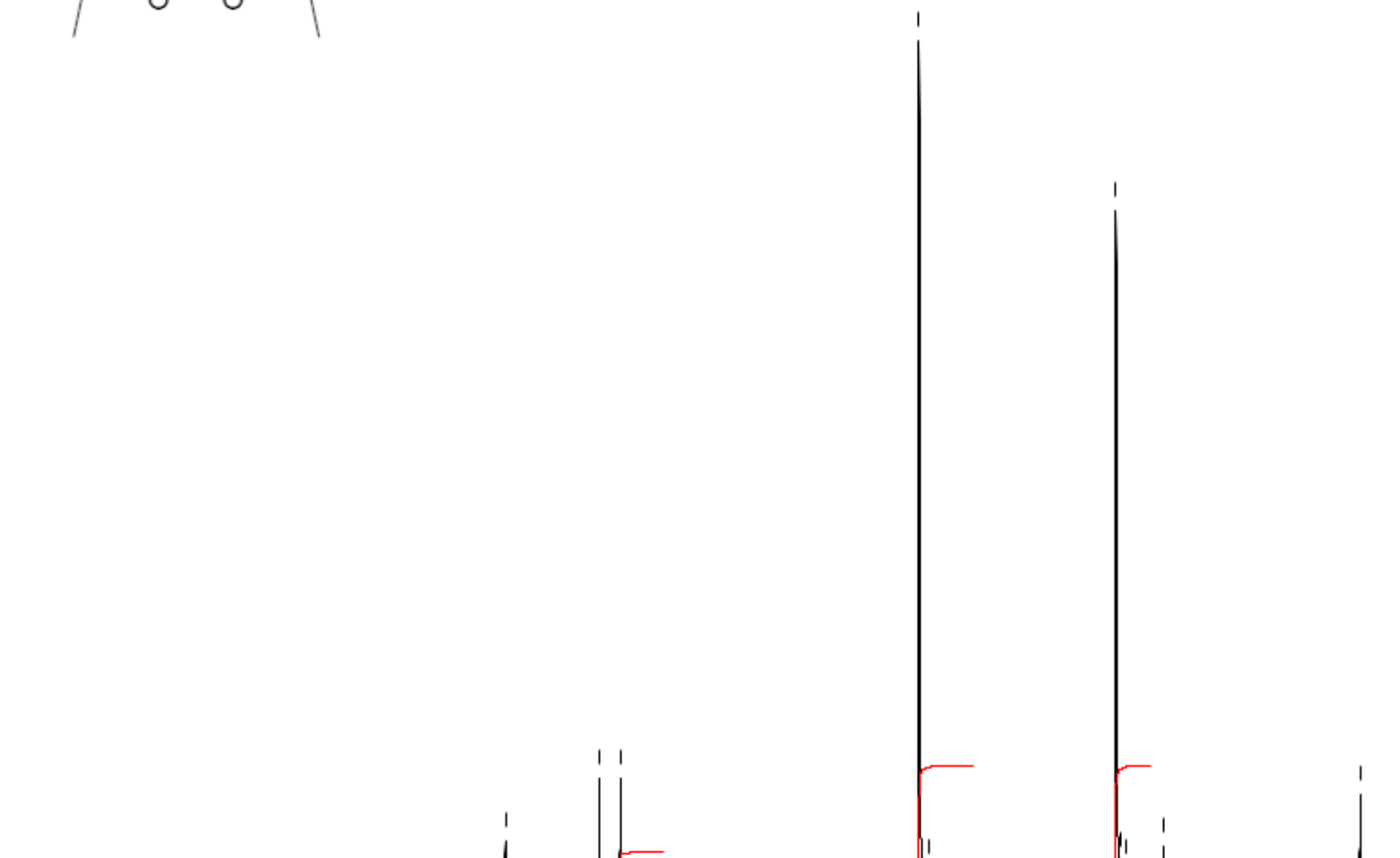


```

NAME          P7K8.12.19
EXPNO         1
PROCNO        1
Date_         20191208
Time          13.13
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            24
DS            0
SWH           7183.908 Hz
FIDRES        0.109618 Hz
AQ            4.5613556 sec
RG            128
DW            69.600 usec
DE            6.50 usec
TE            300.0 K
D1            0.10000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            10.10 usec
PL1           0.00 dB
SFO1          400.1032008 MHz
SI            32768
SF            400.1000058 MHz
WDW           FM
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
  
```

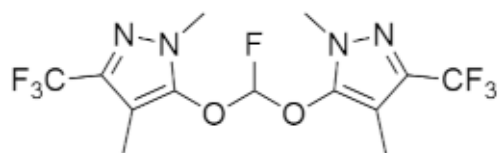


1.000

6.005

6.022

11 10 9 8 7 6 5 4 3 2 1 ppm
Scale: 0.6 ppm/cm, 240.1 Hz/cm



143.769
139.864
139.497
139.129
138.759
125.343
122.667
119.989
117.314
116.754
114.135
103.576

77.401
77.083
76.766

35.554

6.559
-0.001



200 180 160 140 120 100 80 60 40 20 ppm

Scale: 11.25 ppm/cm, 1132 Hz/cm



```

NAME          P7K8.12.19
EXPNO         6
PROCNO        1
Date_         20191209
Time          10.45
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgdc30
TD            32768
SOLVENT       CDC13
NS            6076
DS            0
SWH           24154.590 Hz
FIDRES        0.737140 Hz
AQ            0.6783476 se
RG            71.8
DW            20.700 us
DE            29.57 us
TE            301.1 K
D1            0.10000000 se
D11           0.03000000 se
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          13C
P1            9.20 us
PL1           3.00 dE
SFO1          100.6152865 MHz
  
```

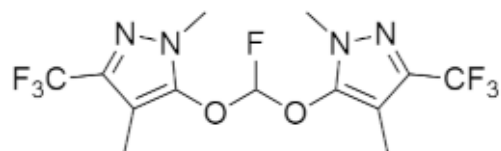
```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 us
PL2            0.00 dE
PL12          18.00 dE
SFO2          400.1009202 MHz
SI            32768
SF            100.6052174 MHz
WDW            EM
SSB            0
LB             2.00 Hz
GB             0
PC             1.00
  
```

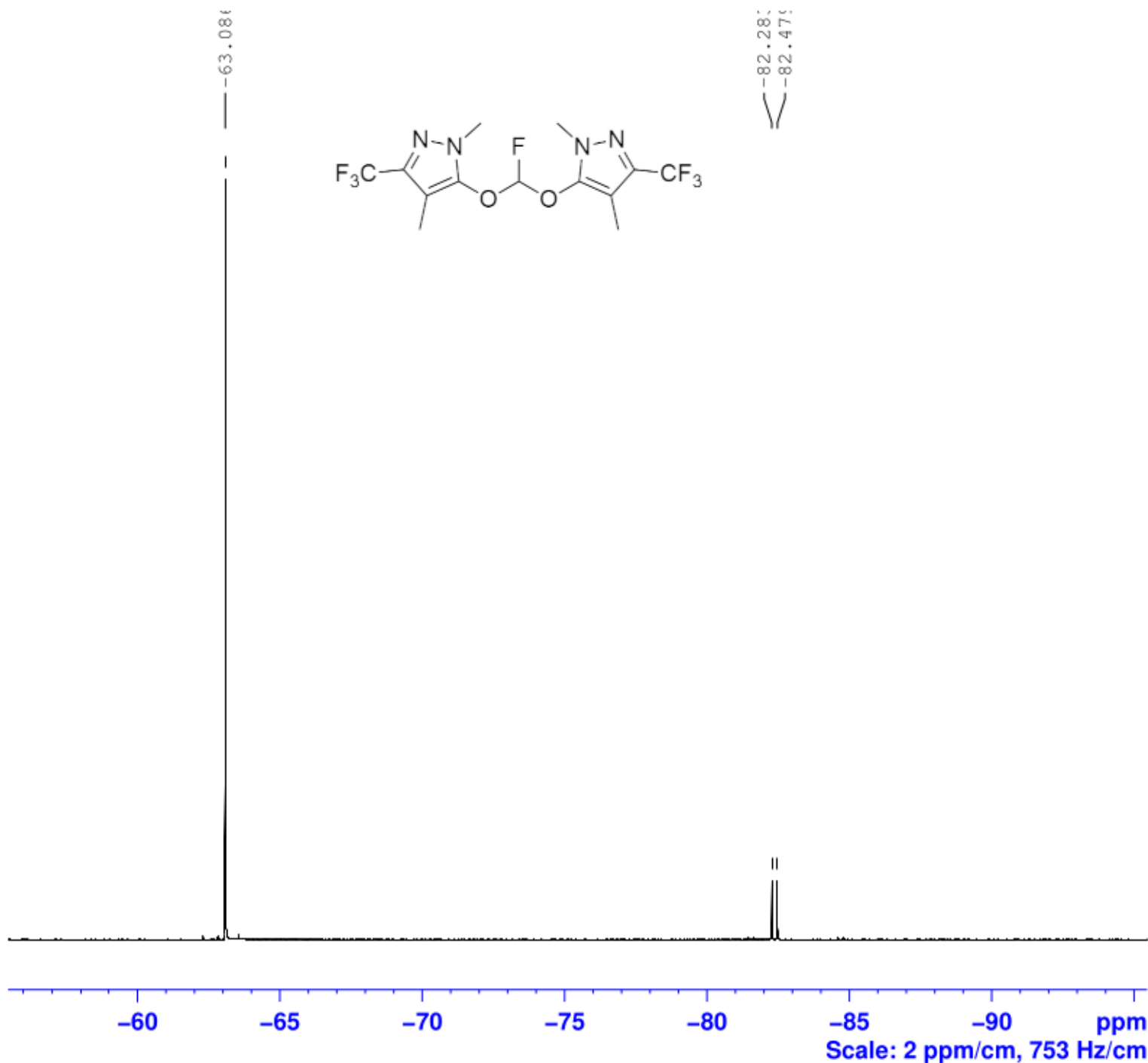


NAME P7K8.12.19
EXPNO 5
PROCNO 1
Date_ 20191208
Time 13.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 15060.241 Hz
FIDRES 0.459602 Hz
AQ 1.0879476 se
RG 1149.4
DW 33.200 us
DE 6.32 us
TE 300.0 K
D1 0.10000000 se
TD0 1

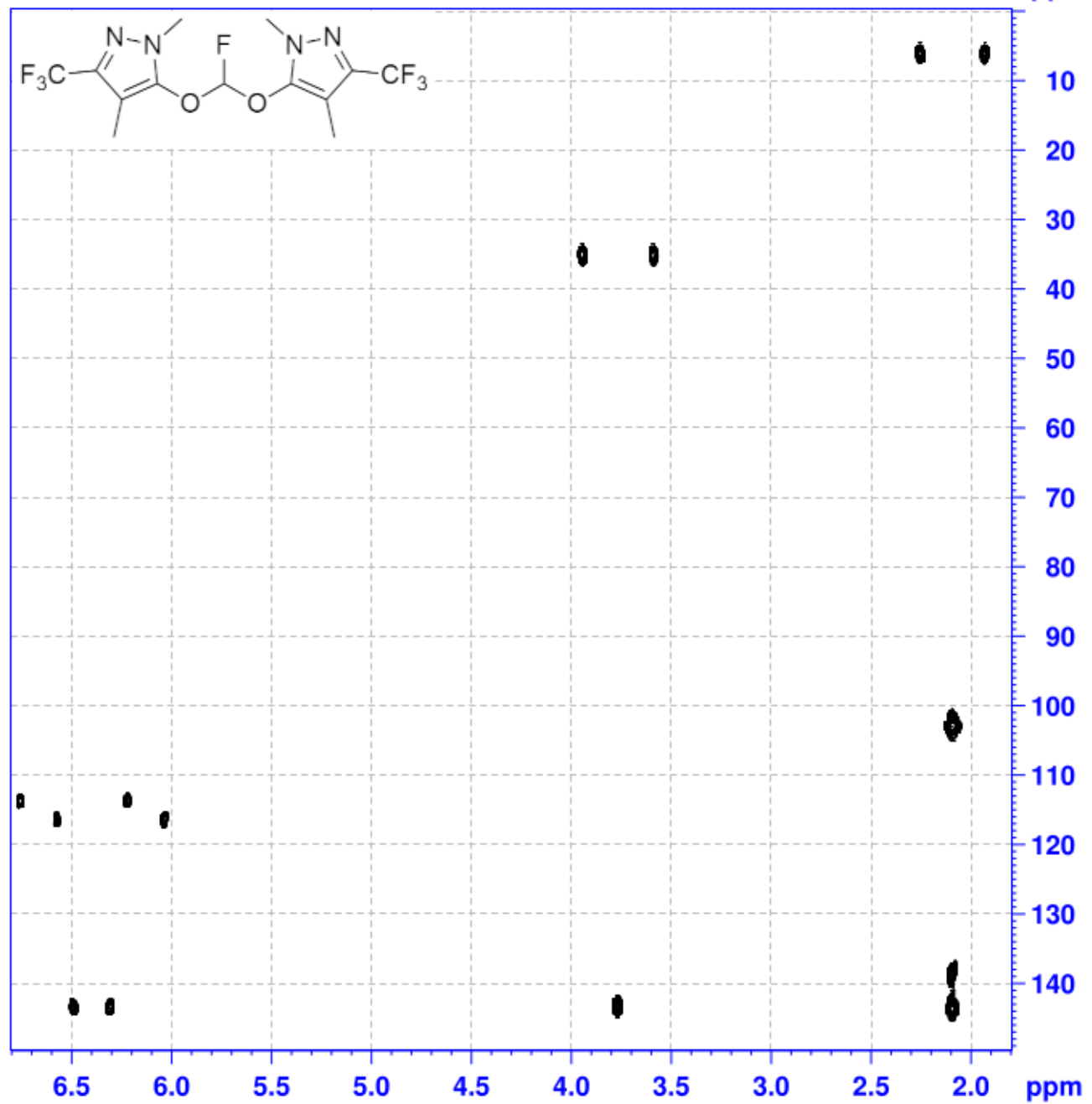
===== CHANNEL f1 =====
NUC1 19F
P1 7.90 us
PL1 0.00 dB
SFO1 376.4419017 MHz
SI 32768
SF 376.4703092 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00



--82.28
--82.47



HMBC



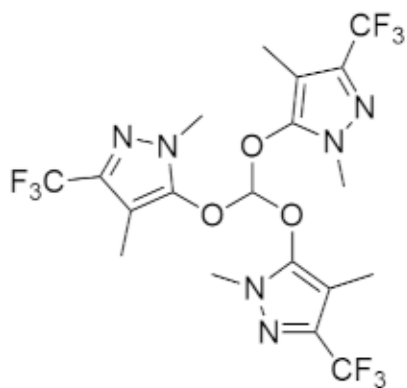
```

NAME          F7K8.12.19
EXPNO         4
PROCNO        1
Date_         20191208
Time          13.49
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       hmbcqp1pndqf
TD            1024
SOLVENT       CDC13
NS            4
DS            2
SWH           2003.205 Hz
FIDRES        1.956255 Hz
AQ            0.2556404 sec
RG            46341
DW            249.600 usec
DE            241.25 usec
TE            300.1 K
CNST2         145.0000000
CNST13        8.0000000
D0            0.00000300 sec
D1            1.00000000 sec
D2            0.00344828 sec
D6            0.06250000 sec
D16           0.00020000 sec
INO           0.00003315 sec

----- CHANNEL f1 -----
NUC1          1H
P1            10.10 usec
P2            20.20 usec
PL1           0.00 dB
SFO1          400.1017204 MHz

----- CHANNEL f2 -----
NUC2          13C
P3            9.20 usec
PL2           0.00 dB
SFO2          100.6127714 MHz

===== GRADIENT CHANNEL =====
GPNAM1       sine.100
GPNAM2       sine.100
GPNAM3       sine.100
GPZ1         50.00 %
GPZ2         30.00 %
GPZ3         40.10 %
PL6          1000.00 usec
ND0          2
TD           67
SFO1         100.6128 MHz
FIDRES       225.252472 Hz
SW           150.000 ppm
FnMODE       QF
SI           1024
SF           400.1000005 MHz
WDW          QSINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.00
SI           512
MC2          QF
SF           100.6052572 MHz
WDW          QSINE
SSB          0
LB           0.00 Hz
GB           0
    
```



contains ca. 5% Compound 4

7.268

6.452

6.304

5.951

3.744

2.074

1.833

1.831

0.074

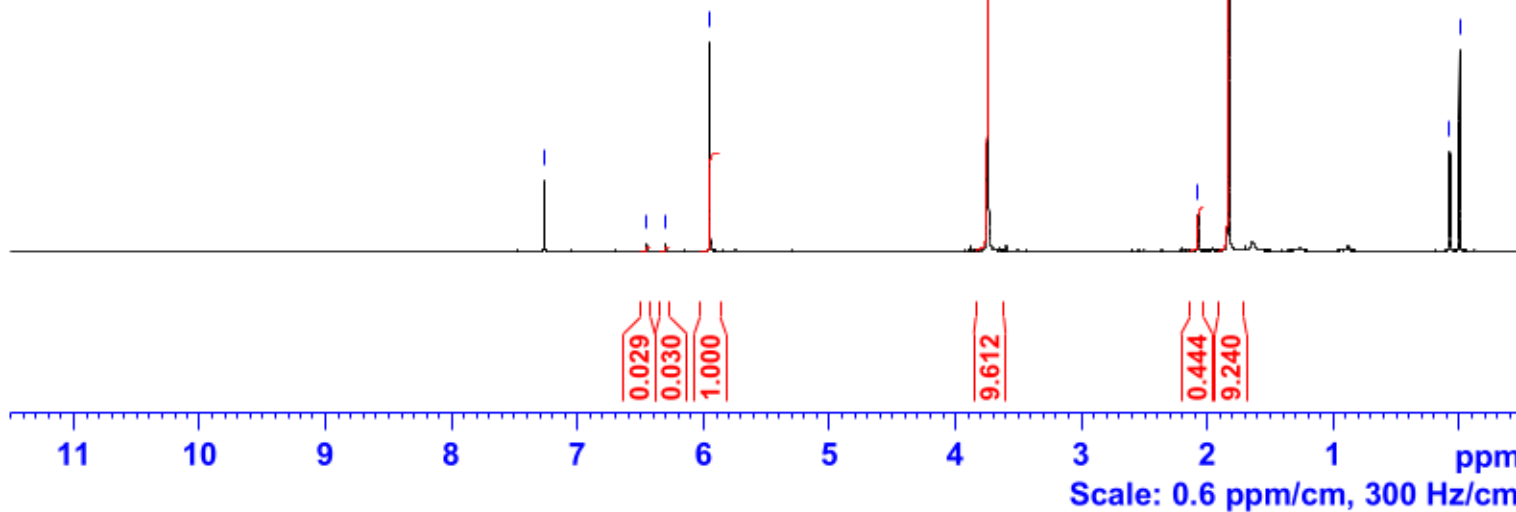
-0.000

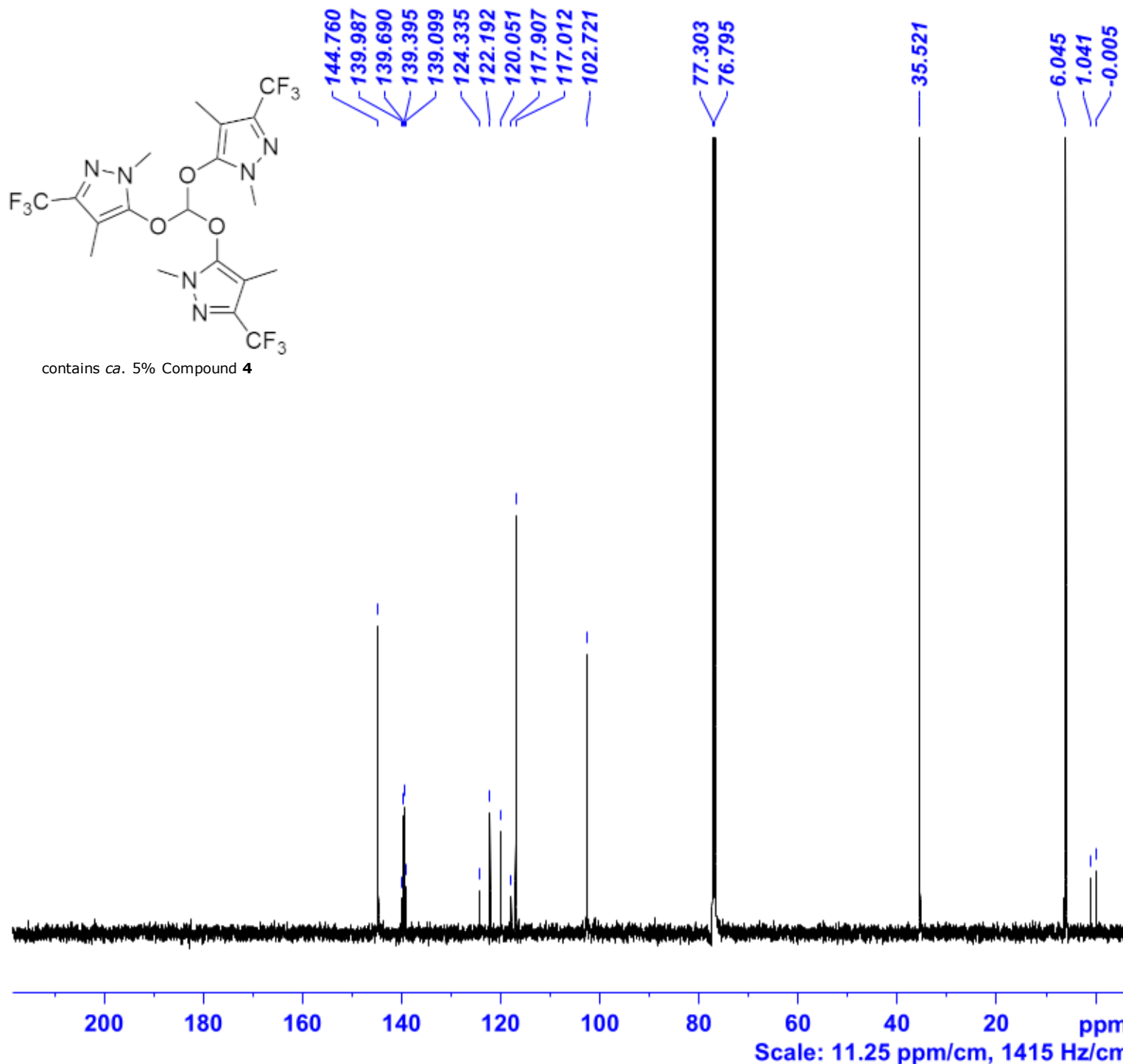


Current Data Parameters
 NAME P7K1.12.20
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201201
 Time_ 10.26 h
 INSTRUM spect
 PROBHD 28420_0082 (PH
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 0
 SWH 7002.801 Hz
 FIDRES 0.213709 Hz
 AQ 4.6792703 sec
 RG 322
 DW 71.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec
 TD0 1
 SFO1 500.0430002 MHz
 NUC1 1H
 P1 10.32 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.0400079 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





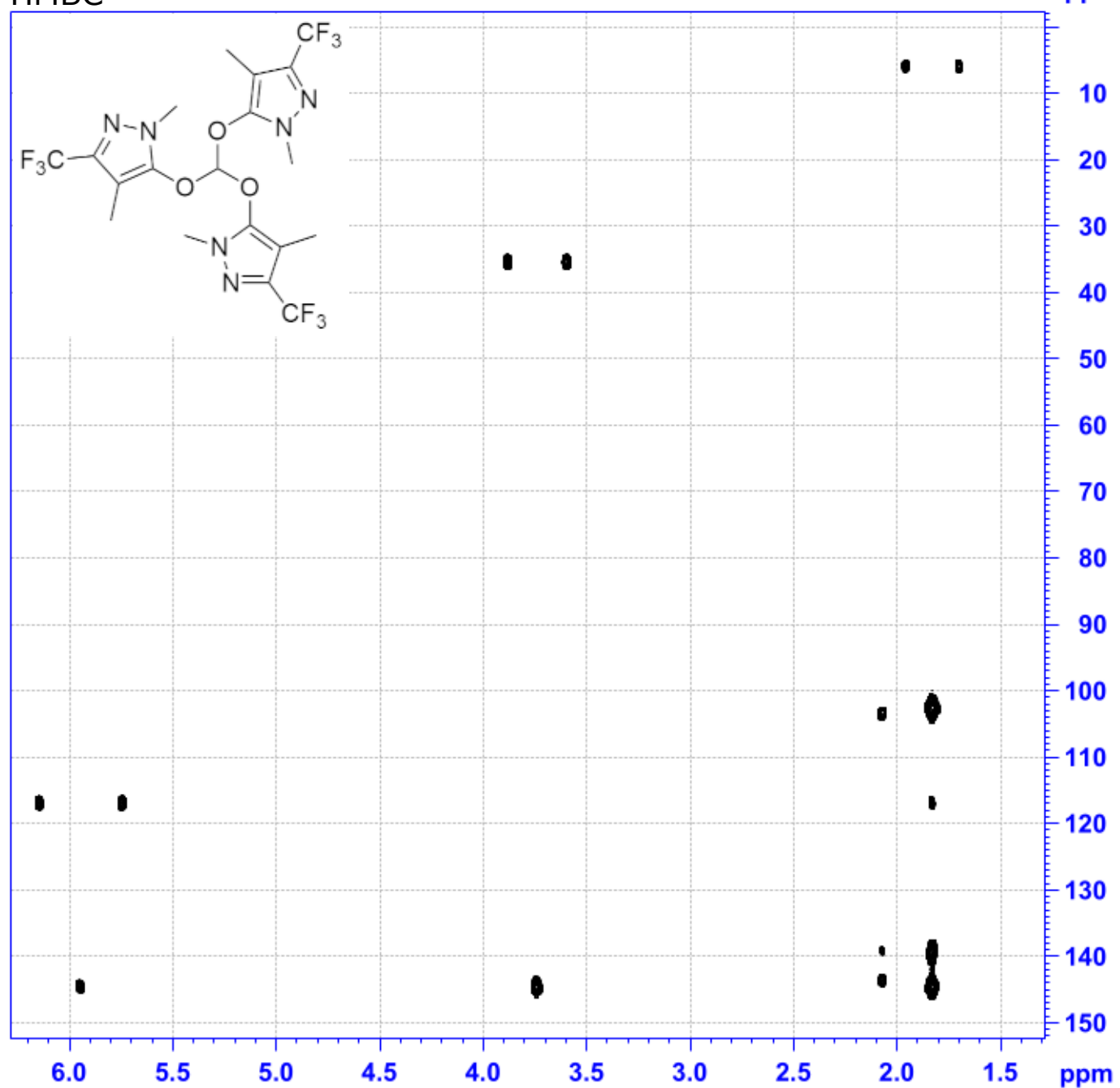
Current Data Parameters
NAME P7K1.12.20
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201201
Time_ 10.49 h
INSTRUM spect
PROBHD Z8420_0082 (PH
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 1046
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7477315 MHz
NUC1 13C
P1 13.00 usec
PLW1 55.00000000 W
SFO2 500.0425002 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.24962001 W

F2 - Processing parameters
SI 32768
SF 125.7351531 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

contains ca. 5% Compound 4

HMBC



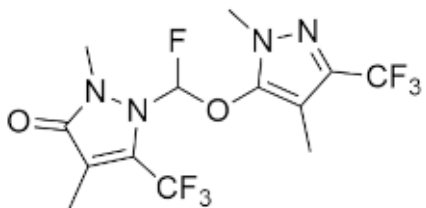
Current Data Parameters
 NAME P7K1.12.20
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201201
 Time 11.21 h
 INSTRUM spect
 PROBHD 28420_0082 (PH
 PULPROG hmbcggplpndqf
 TD 1024
 SOLVENT CDCl3
 NS 8
 DS 2
 SWH 2500.000 Hz
 FIDRES 4.882813 Hz
 AQ 0.2048000 sec
 RG 2050
 DM 200.000 usec
 DE 6.50 usec
 TE 300.0 K
 CNST2 145.0000000
 CNST13 8.0000000
 D0 0.00000300 sec
 D1 1.00000000 sec
 D2 0.00344828 sec
 D6 0.06250000 sec
 D16 0.00020000 sec
 IN0 0.00002570 sec
 TDav 1
 SFO1 500.0419002 MHz
 NUC1 1H
 P1 10.32 usec
 P2 20.64 usec
 PLW1 15.00000000 W
 SFO2 125.7445881 MHz
 NUC2 13C
 P3 13.00 usec
 PLW2 55.00000000 W
 GPNAM[1] SMSQ10.100
 GPZ1 50.00 %
 GPNAM[2] SMSQ10.100
 GPZ2 30.00 %
 GPNAM[3] SMSQ10.100
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 125.7446 MHz
 FIDRES 303.988312 Hz
 SW 154.720 ppm
 FnmODE QF

F2 - Processing parameters
 SI 1024
 SF 500.0400090 MHz
 NDW QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

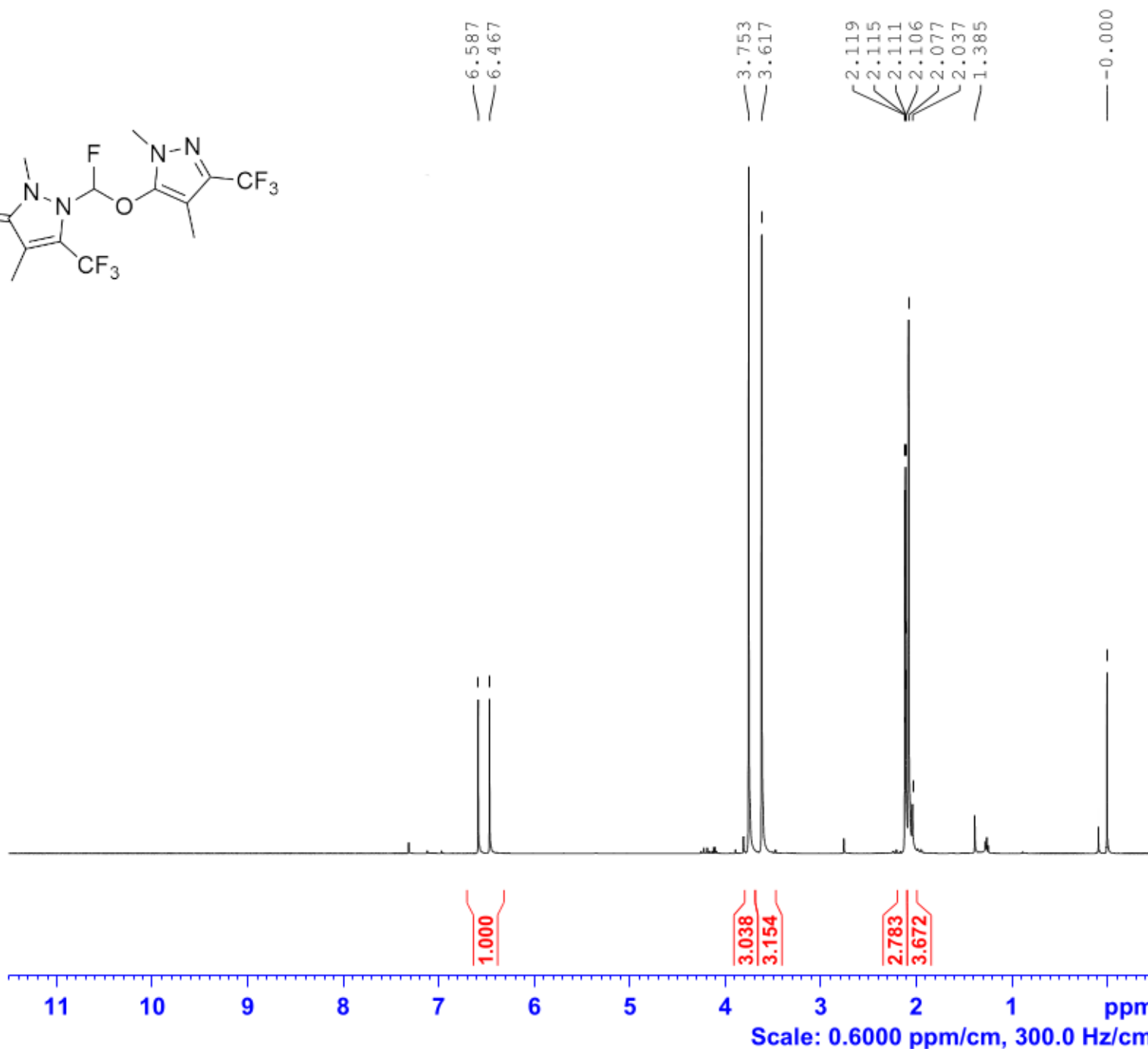
F1 - Processing parameters
 SI 512
 MC2 QF
 SF 125.7351530 MHz
 NDW QSINE
 SSB 0
 LB 0 Hz
 GB 0

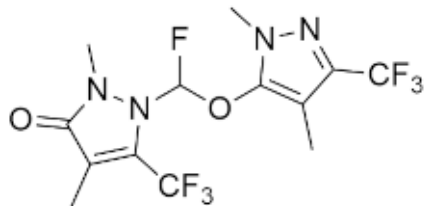


Current Data Parameters
 NAME P7K10.2.21
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210210
 Time_ 14.31 h
 INSTRUM spect
 PROBHD Z8420_0082 (PH
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 24
 DS 0
 SWH 7002.801 Hz
 FIDRES 0.213709 Hz
 AQ 4.6792703 sec
 RG 45.2
 DW 71.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec
 TD0 1
 SFO1 500.0430002 MHz
 NUC1 1H
 P1 10.32 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.0399851 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





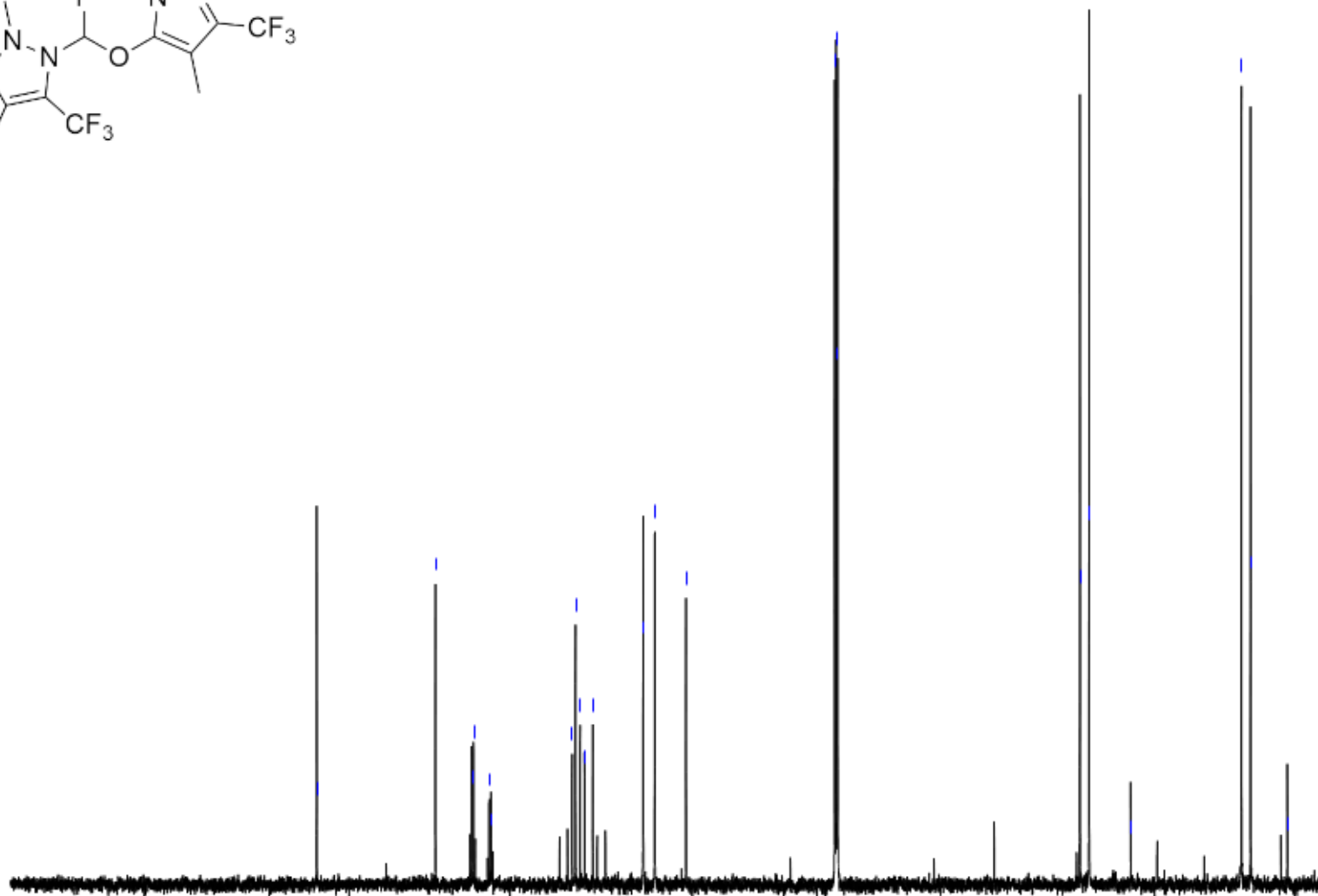
166.089
 145.768
 139.544
 139.250
 136.581
 136.265
 122.387
 121.807
 121.009
 120.246
 118.845
 110.209
 108.233
 102.892
 77.457
 77.202
 76.948
 35.486
 33.923
 33.913
 26.815
 7.843
 6.291
 -0.002



Current Data Parameters
 NAME P7K10.2.21
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210210
 Time 15.51 h
 INSTRUM spect
 PROBHD z8420_0082 (PH
 PULPROG zgdc30
 TD 65536
 SOLVENT CDC13
 NS 900
 DS 0
 SWH 29761.904 Hz
 FIDRES 0.908261 Hz
 AQ 1.1010048 sec
 RG 2050
 DW 16.800 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec
 D11 0.03000000 sec
 TD0 1
 SFO1 125.7477315 MHz
 NUC1 13C
 P1 13.00 usec
 PLW1 55.00000000 W
 SFO2 500.0425002 MHz
 NUC2 1H
 CPDPRG[2] waltz16
 PCPD2 80.00 usec
 PLW2 15.00000000 W
 PLW12 0.24962001 W

F2 - Processing parameters
 SI 32768
 SF 125.7351385 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

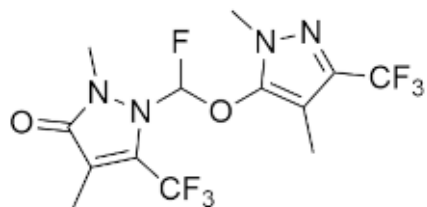


200 180 160 140 120 100 80 60 40 20 ppm
 Scale: 11.25 ppm/cm, 1415 Hz/cm



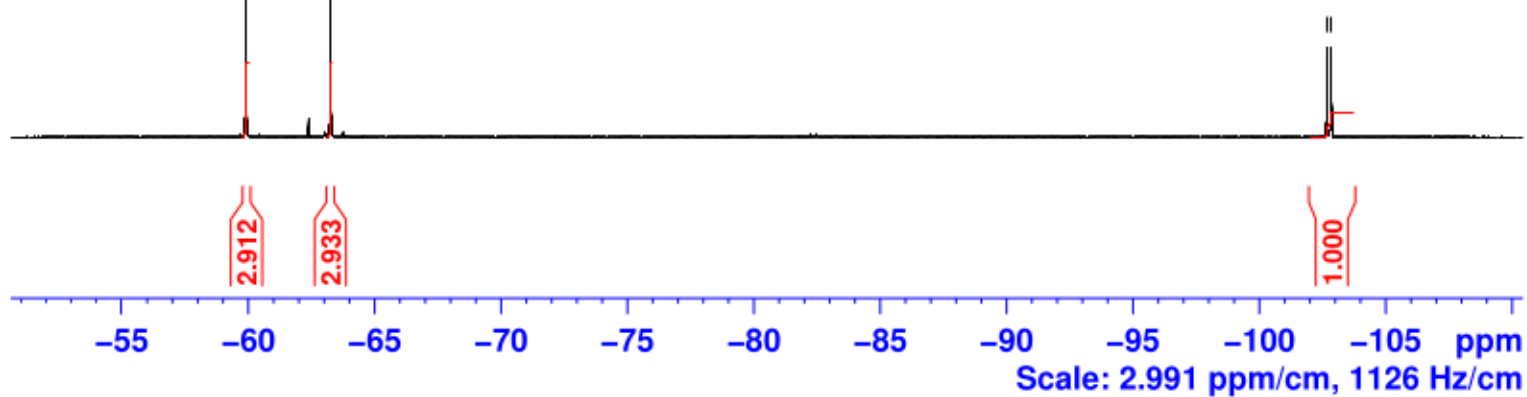
NAME P7K10.2.21
EXPNO 3
PROCNO 1
Date_ 20210214
Time 11.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 48
DS 0
SWH 22522.523 Hz
FIDRES 0.687333 Hz
AQ 0.7274996 se
RG 1625.5
DW 22.200 us
DE 6.32 us
TE 300.1 K
D1 0.10000000 se
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 7.90 us
PL1 0.00 dB
SFO1 376.4400194 MHz
SI 32768
SF 376.4703301 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00



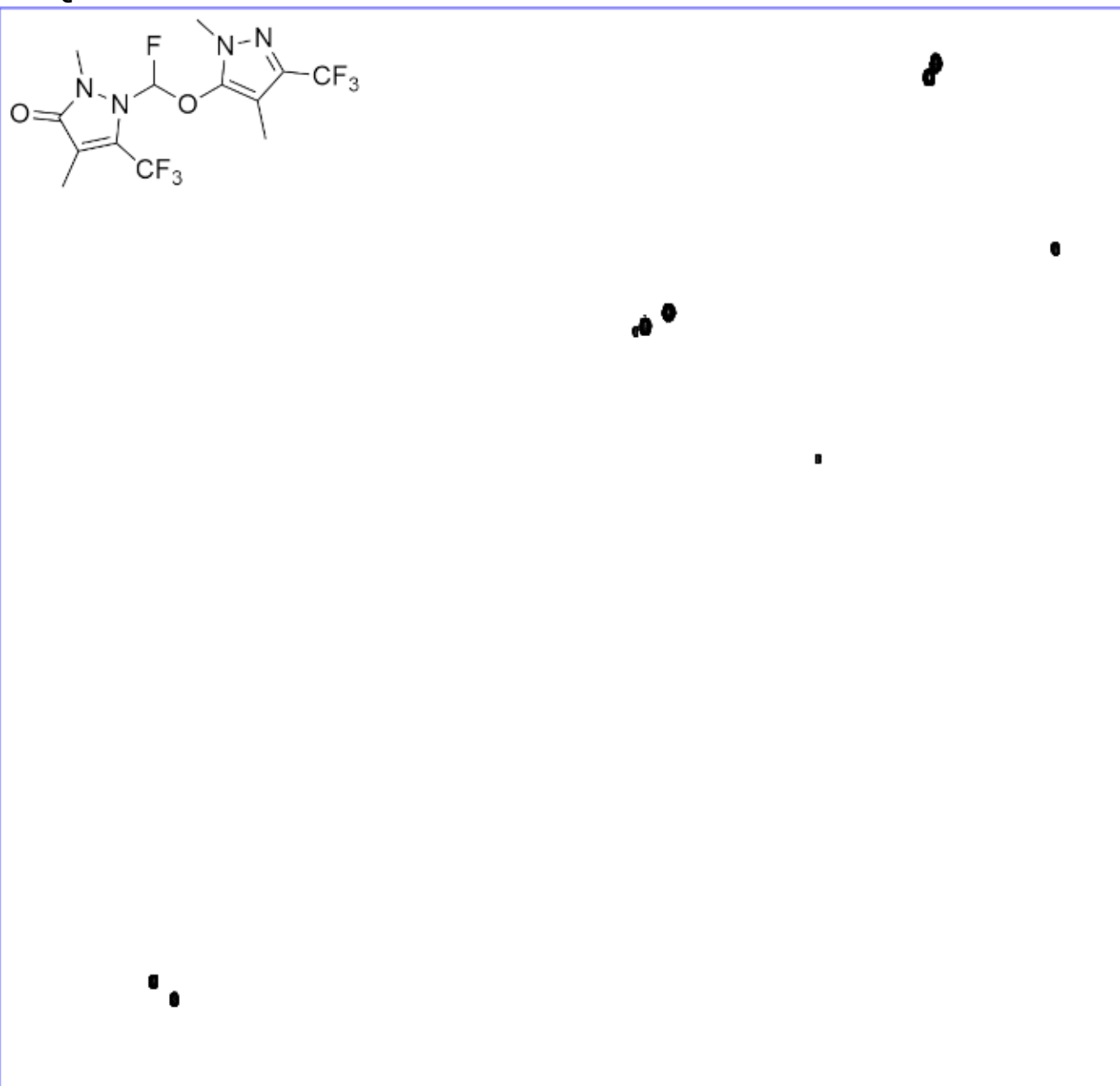
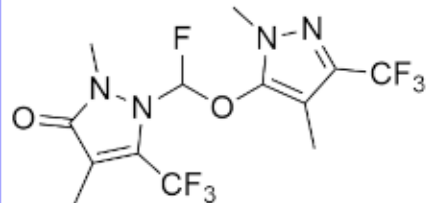
---59.921
---63.271

<---102.61
<---102.81



HMQC

ppm



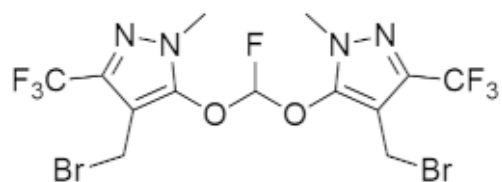
Current Data Parameters
 NAME P7K10.2.21
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20210210
 Time 15.15 h
 INSTRUM spect
 PROBHD z8420_0082 (PH
 PULPROG hmqcpgpgf
 TD 1024
 SOLVENT CDCl3
 NS 4
 DS 2
 SMH 3246.753 Hz
 FIDRES 6.341315 Hz
 AQ 0.1576960 sec
 RG 2050
 DW 154.000 usec
 DE 6.50 usec
 TE 300.1 K
 CNST2 145.0000000
 DO 0.00000300 sec
 D1 1.00000000 sec
 D2 0.00344828 sec
 D12 0.00002000 sec
 D13 0.00000400 sec
 D16 0.00020000 sec
 INO 0.00003310 sec
 TDev 1
 SFO1 500.0421002 MHz
 NUC1 1H
 P1 10.32 usec
 P2 20.64 usec
 PLM1 15.00000000 W
 SFO2 125.7427021 MHz
 NUC2 13C
 CPDPRG2 garp
 P3 13.00 usec
 PCPD2 55.00 usec
 PLM2 55.00000000 W
 PLM12 2.88000011 W
 GPNAM[1] SMSQ10.100
 GPZ1 50.00 %
 GPNAM[2] SMSQ10.100
 GPZ2 30.00 %
 GPNAM[3] SMSQ10.100
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 125.7427 MHz
 FIDRES 236.027191 Hz
 SW 120.132 ppm
 FhMODE QF

F2 - Processing parameters
 SI 1024
 SF 500.0399851 MHz
 WDM QSINR
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 512
 MC2 QF
 SF 125.7351385 MHz
 WDM QSINR
 SSB 0
 LB 0 Hz
 GB 0



7.274
7.015
6.832

4.456
4.411
4.245
3.889
3.867
3.821
3.788
3.782

2.165
2.100
1.466
1.415
1.283
1.261

0.077
0.001

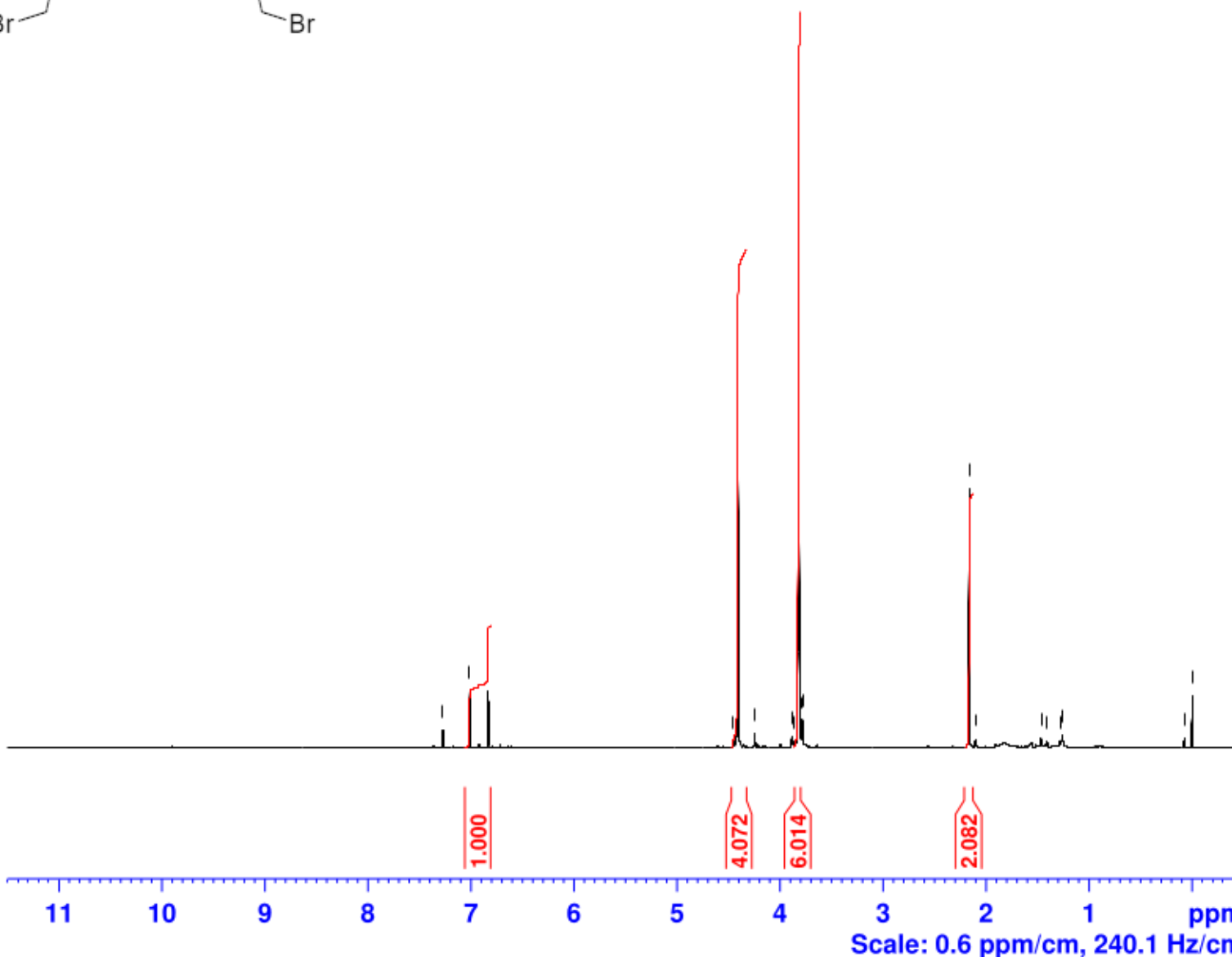


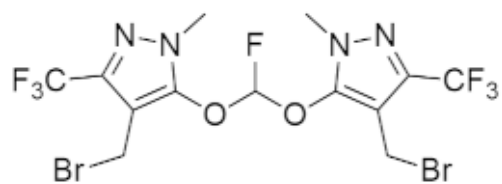
```

NAME          P7K4.5.20
EXPNO         1
PROCNO        1
Date_         20200504
Time          11.18
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            24
DS            0
SWH           7183.908 Hz
FIDRES        0.109618 Hz
AQ            4.5613556 sec
RG            128
DW            69.600 usec
DE            6.50 usec
TE            301.0 K
D1            0.10000000 sec
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          1H
P1            10.10 usec
PL1           0.00 dB
SFO1          400.1032008 MHz
SI            32768
SF            400.1000046 MHz
WDW           EM
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
  
```





144.134
 139.124
 138.744
 138.364
 122.034
 119.354
 115.404
 112.764
 105.944
 102.544
 98.562
 77.399
 77.081
 76.763
 36.032
 30.901
 17.759
 -0.001



```

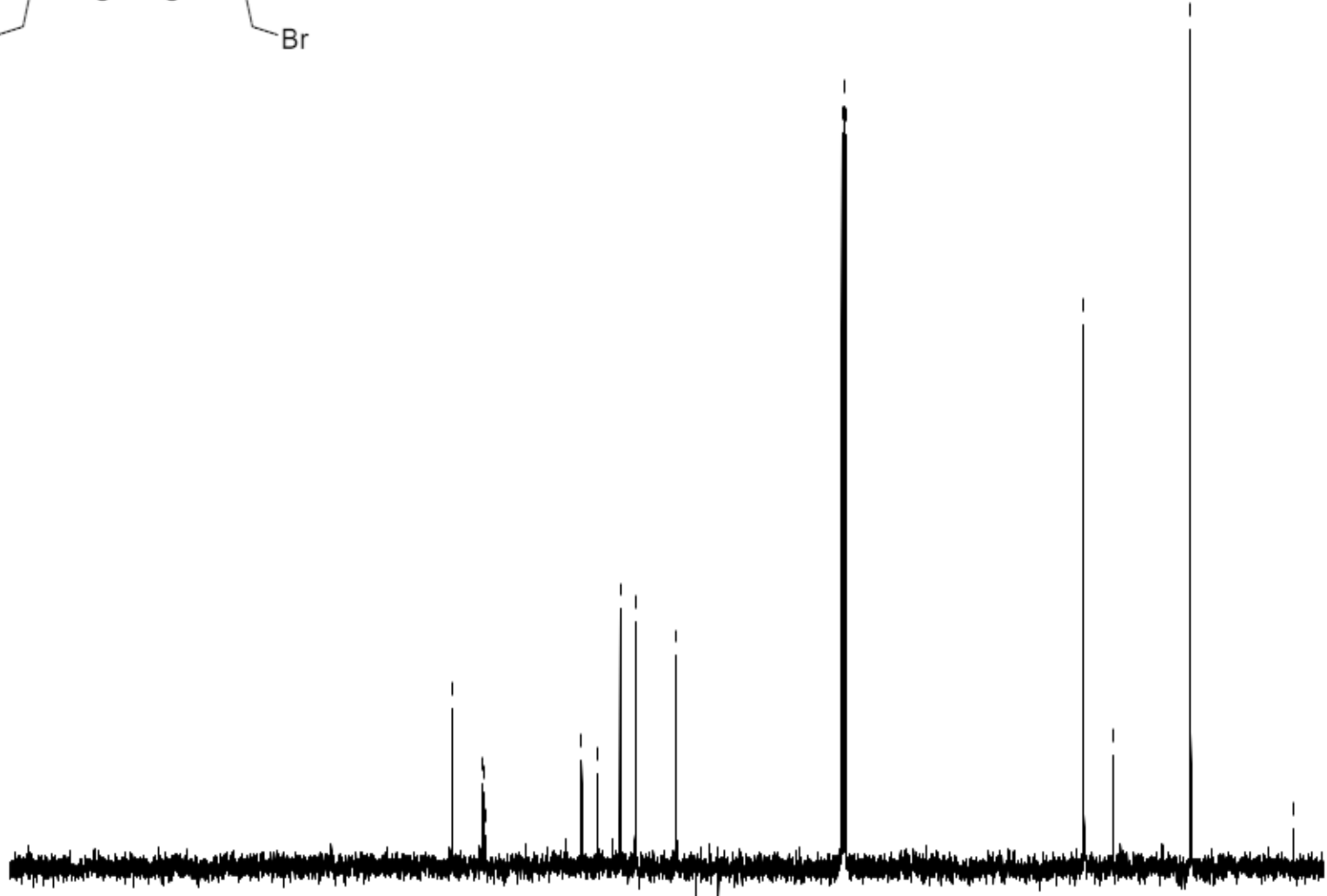
NAME          P7K4.5.20
EXPNO         3
PROCNO        1
Date_         20200504
Time          11.27
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgdc30
TD            32768
SOLVENT       CDC13
NS            2375
DS            0
SWH           24154.590 Hz
FIDRES        0.737140 Hz
AQ            0.6783476 se
RG            71.8
DW            20.700 us
DE            29.57 us
TE            302.3 K
D1            0.10000000 se
D11           0.03000000 se
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1           13C
P1             9.20 us
PL1            3.00 dB
SFO1          100.6152865 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 us
PL2            0.00 dB
PL12          18.00 dB
SFO2          400.1009202 MHz
SI            32768
SF            100.6052190 MHz
WDW            EM
SSB            0
LB             2.00 Hz
GB             0
PC             1.00
  
```

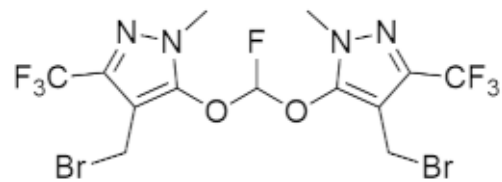


200 180 160 140 120 100 80 60 40 20 ppm
 Scale: 11.25 ppm/cm, 1132 Hz/cm



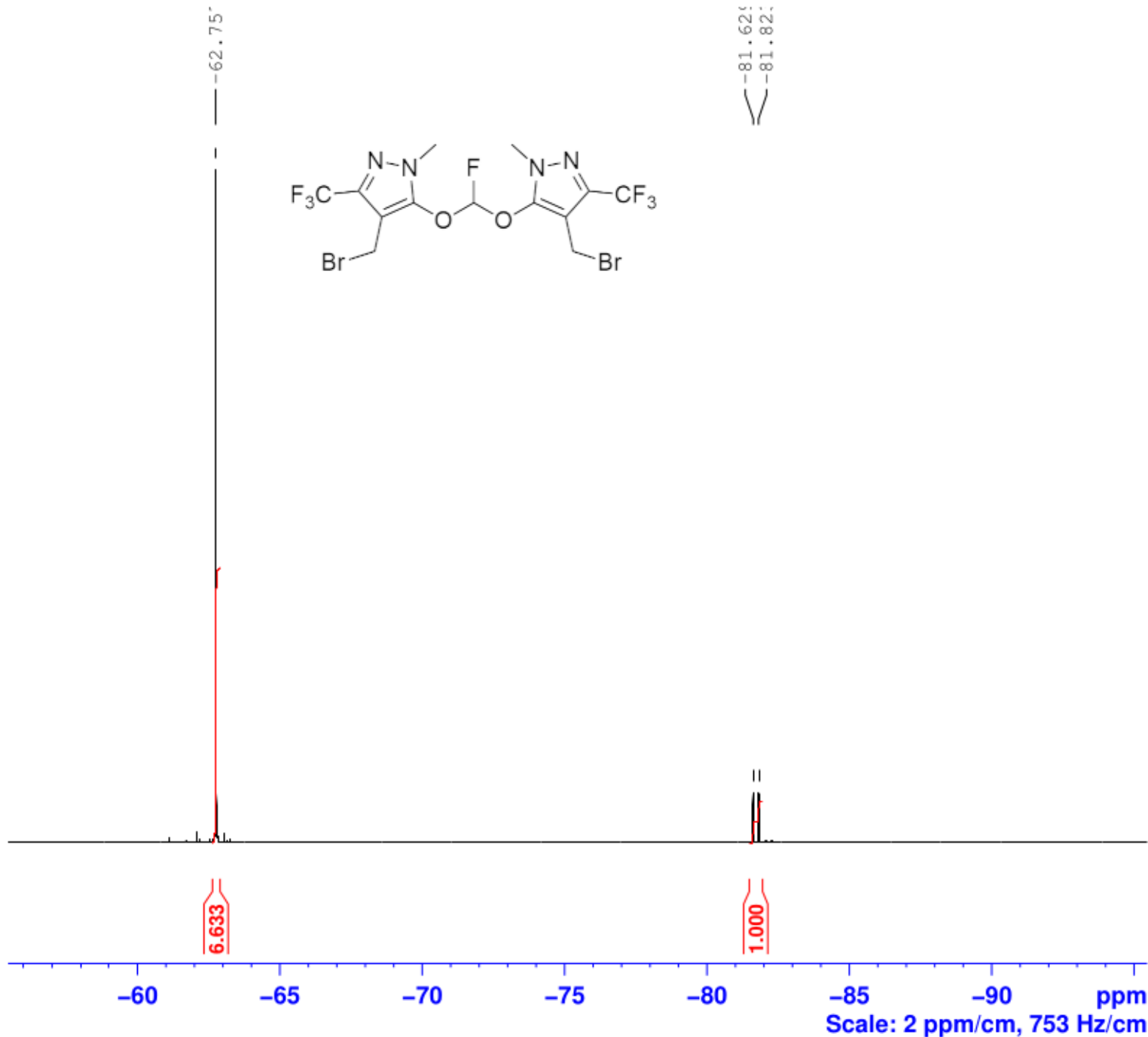
NAME P7K4.5.20
EXPNO 2
PROCNO 1
Date_ 20200504
Time 11.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 0
SWH 15060.241 Hz
FIDRES 0.459602 Hz
AQ 1.0879476 se
RG 71.8
DW 33.200 us
DE 6.32 us
TE 301.0 K
D1 0.10000000 se
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 7.90 us
PL1 0.00 dB
SFO1 376.4419017 MHz
SI 32768
SF 376.4703092 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

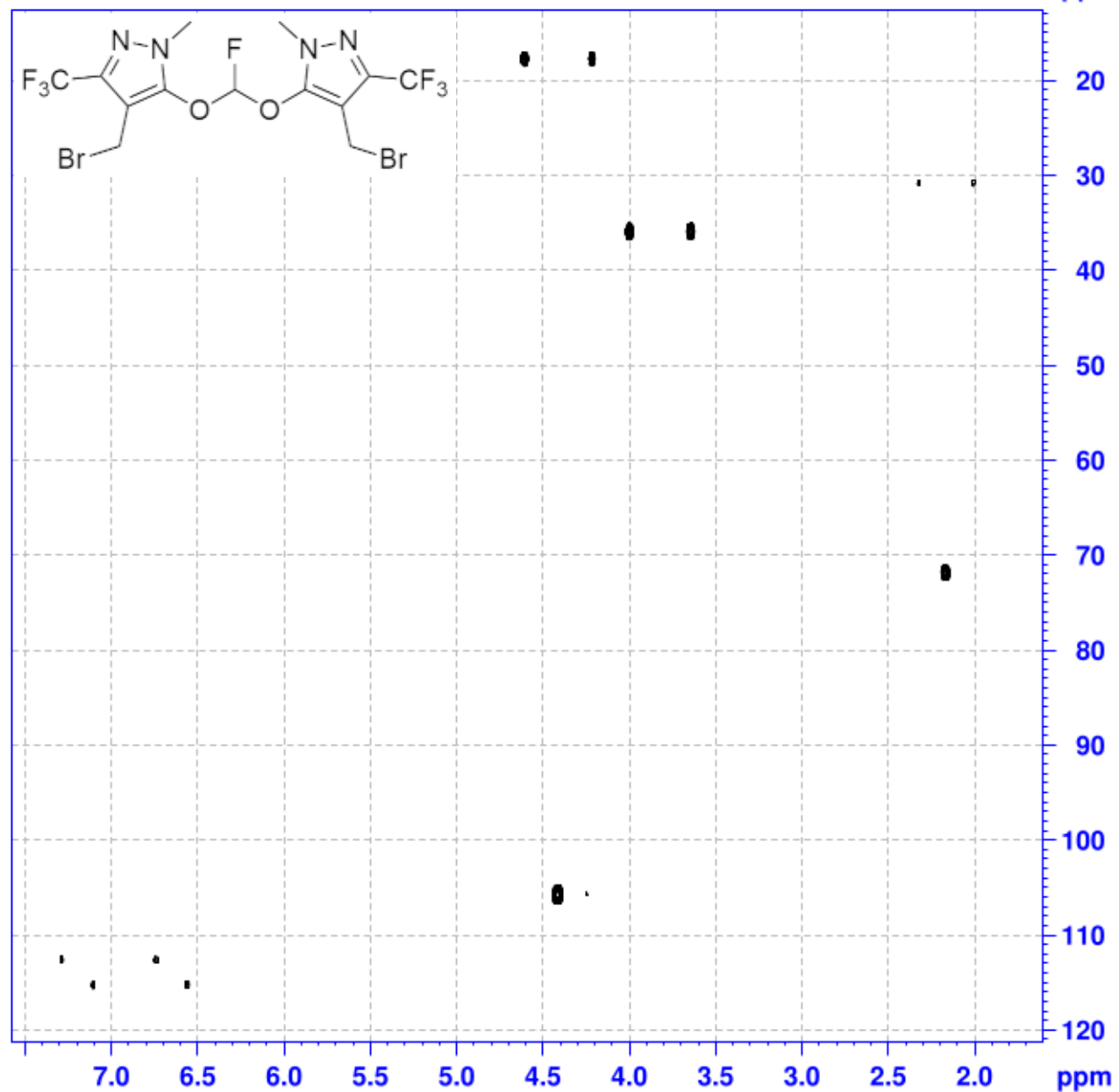


--62.75'

--81.62'
--81.82'



HMBC



```

NAME          P7K4.5.20
EXPNO         6
PROCNO       1
Date_        20200504
Time         12.26
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG     hmbcgp1pndqf
TD           1024
SOLVENT      CDC13
NS           10
DS           2
SWH          2394.636 Hz
FIDRES       2.338512 Hz
AQ           0.2138612 sec
RG           46341
DW           208.800 usec
DE           241.25 usec
TE           302.2 K
CNST2        145.0000000
CNST13        8.0000000
D0           0.00000300 sec
D1           1.00000000 sec
D2           0.00344828 sec
D6           0.06250000 sec
D16          0.00020000 sec
IN0          0.00003680 sec
    
```

```

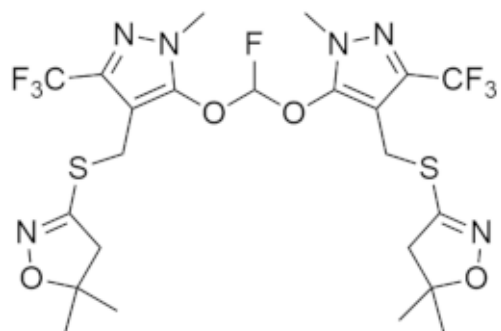
===== CHANNEL f1 =====
NUC1         1H
P1           10.10 usec
P2           20.20 usec
PL1          0.00 dB
SFO1         400.1018405 MHz
    
```

```

===== CHANNEL f2 =====
NUC2         13C
P3           9.20 usec
PL2          0.00 dB
SFO2         100.6132744 MHz
    
```

```

===== GRADIENT CHANNEL =====
GPNAM1      sine.100
GPNAM2      sine.100
GPNAM3      sine.100
GPZ1        50.00 %
GPZ2        30.00 %
GPZ3        40.10 %
P16         1000.00 usec
ND0         2
TD          128
SFO1        100.6133 MHz
FIDRES      106.115562 Hz
SW          135.000 ppm
FnMODE      QF
SI          1024
SF          400.1000046 MHz
WDW         QSINE
SSB         0
LB          0.00 Hz
GB          0
PC          1.00
SI          512
MC2         QF
SF          100.6052190 MHz
WDW         QSINE
SSB         0
LB          0.00 Hz
GB          0
    
```



7.099
6.950

4.244
4.216
4.178
4.150
3.797

2.748

1.381

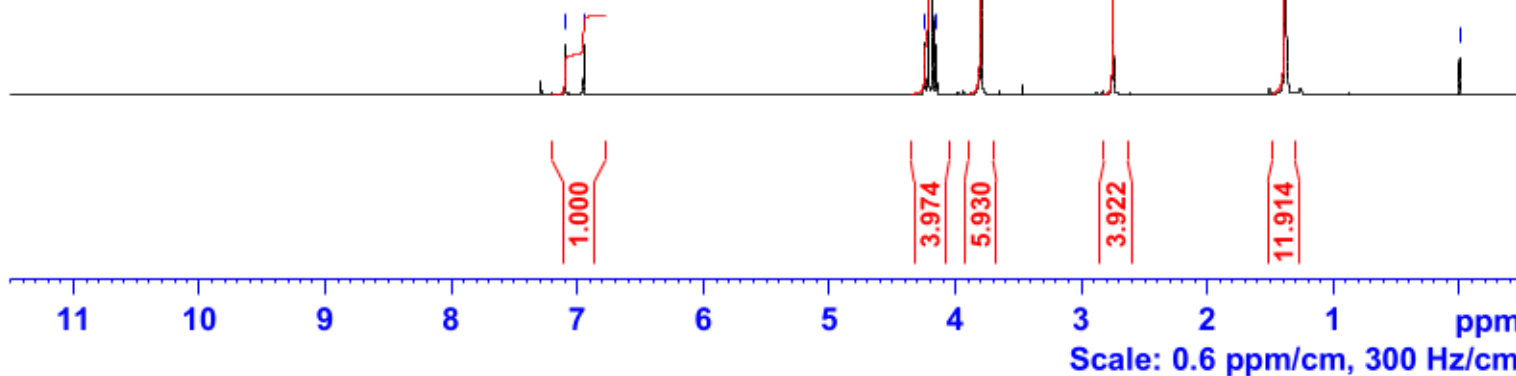
0.000

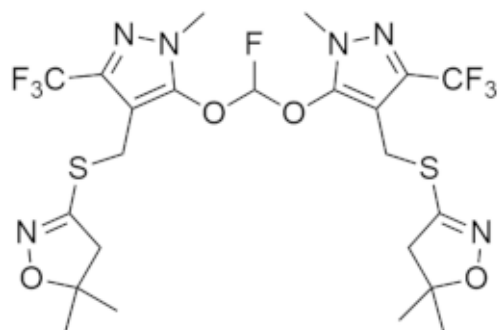


Current Data Parameters
 NAME P7K4.3.21
 EXPNO 1
 PROCNO 1

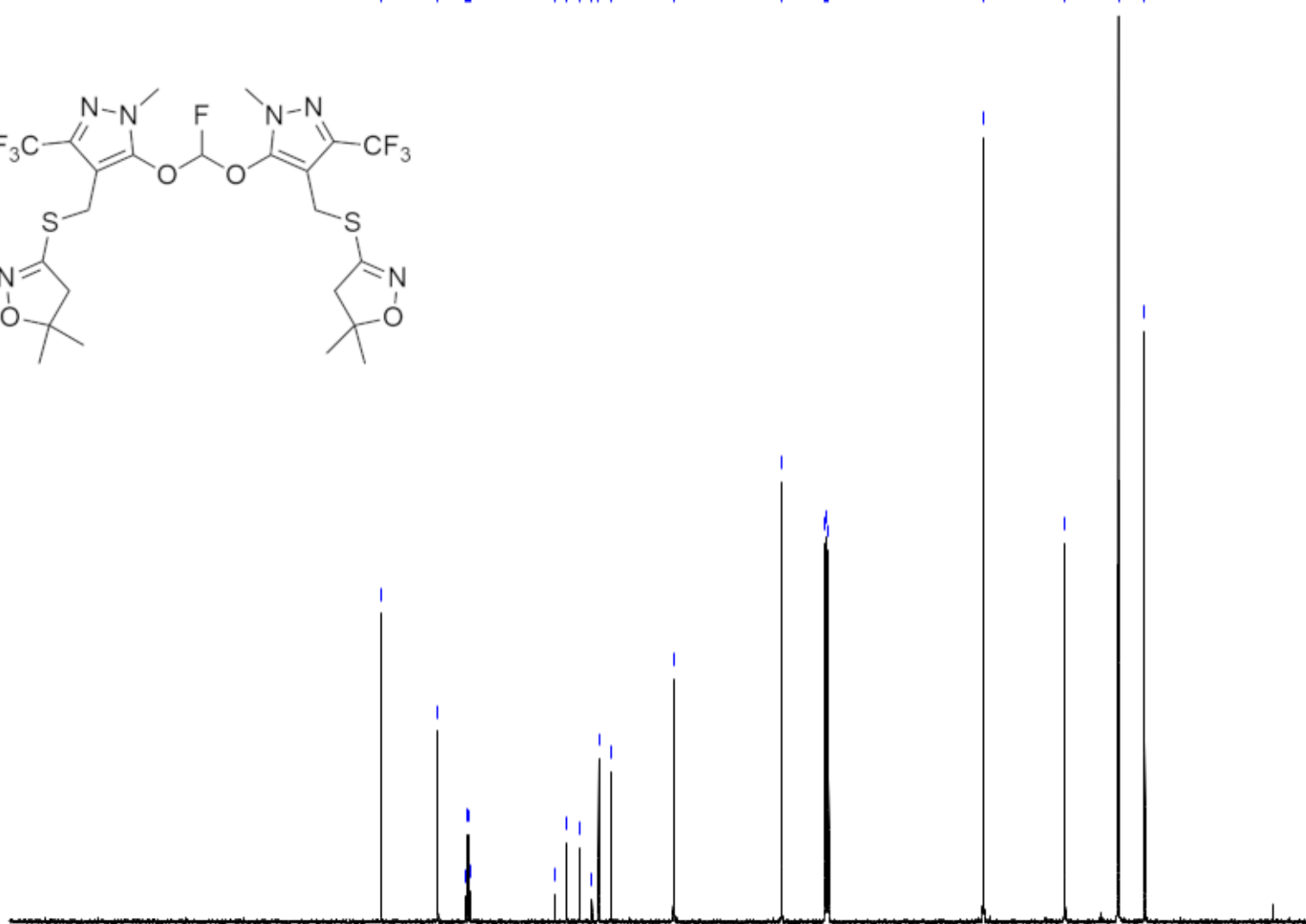
F2 - Acquisition Parameters
 Date_ 20210304
 Time 11.00 h
 INSTRUM spect
 PROBHD 28420_0082 (PH
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 24
 DS 0
 SWH 7002.801 Hz
 FIDRES 0.213709 Hz
 AQ 4.6792703 sec
 RG 128
 DW 71.400 usec
 DE 6.50 usec
 TE 300.0 K
 D1 0.10000000 sec
 TD0 1
 SFO1 500.0430002 MHz
 NUC1 1H
 P1 10.32 usec
 PLW1 15.00000000 W

F2 - Processing parameters
 SI 65536
 SF 500.0399969 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00





154.107
144.358
139.493
139.195
138.894
138.595
124.155
122.009
119.864
117.719
116.555
114.449
103.603
84.947
77.362
77.108
76.854
50.076
35.989
26.773
22.198



Current Data Parameters
NAME P7K4.3.21
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210304
Time 11.31 h
INSTRUM spect
PROBHD 28420_0082 (PH
PULPROG zgdc30
TD 65536
SOLVENT CDC13
NS 1500
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7477315 MHz
NUC1 13C
P1 13.00 usec
PLW1 55.00000000 W
SFO2 500.0425002 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.24962001 W

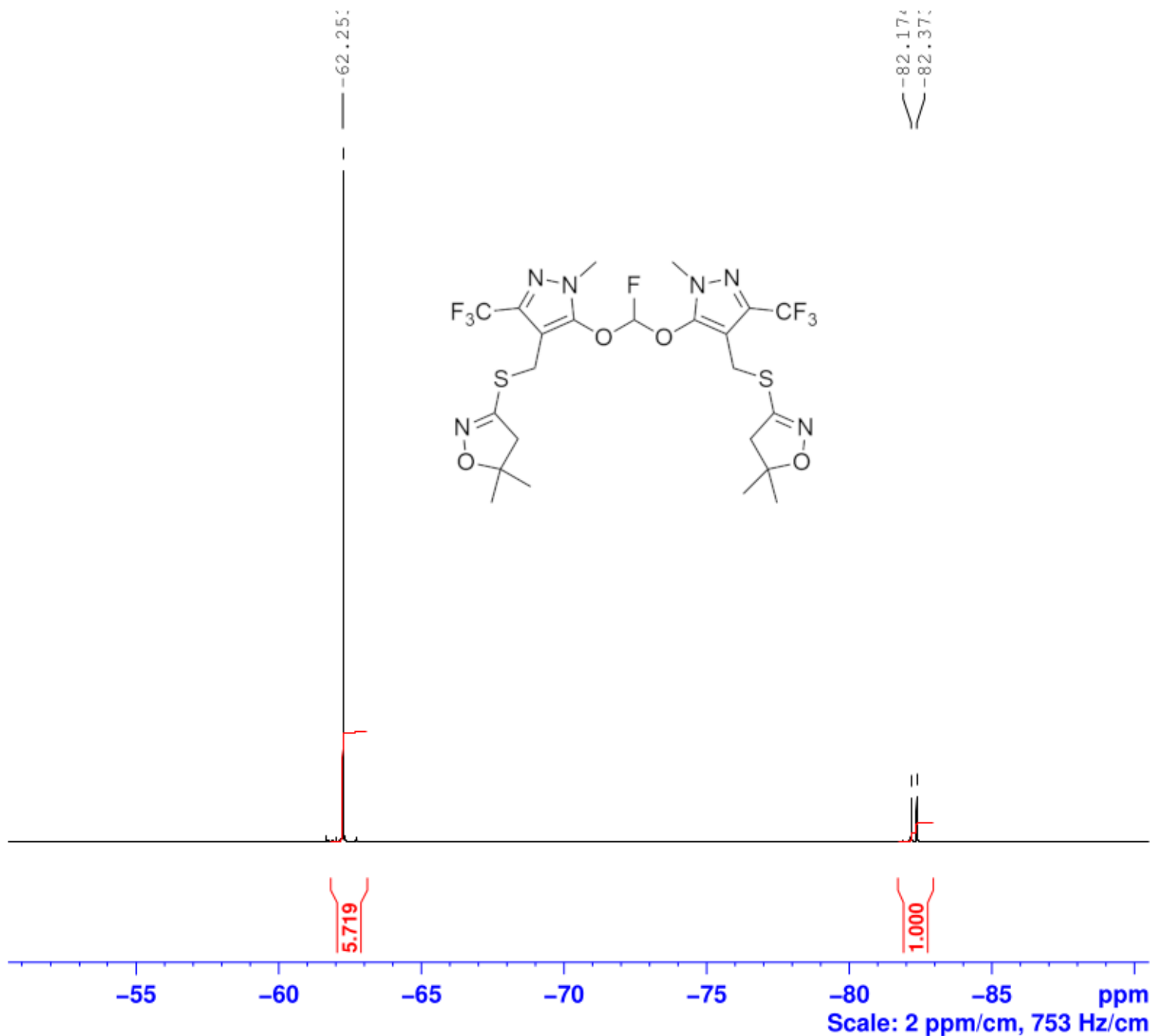
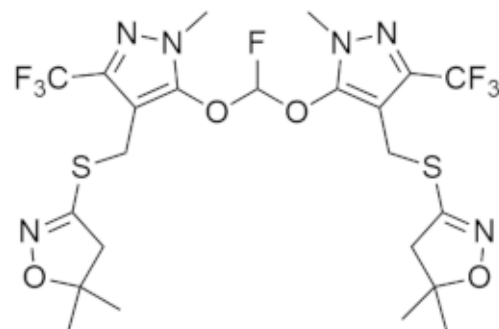
F2 - Processing parameters
SI 32768
SF 125.7351521 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

200 180 160 140 120 100 80 60 40 20 ppm
Scale: 11.25 ppm/cm, 1415 Hz/cm



NAME P7K4.3.21
EXPNO 5
PROCNO 1
Date_ 20210304
Time 12.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 24
DS 0
SWH 15060.241 Hz
FIDRES 0.459602 Hz
AQ 1.0879476 se
RG 1625.5
DW 33.200 us
DE 6.32 us
TE 299.9 K
D1 0.10000000 se
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 7.90 us
PL1 0.00 dB
SFO1 376.4437841 MHz
SI 32768
SF 376.4703301 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

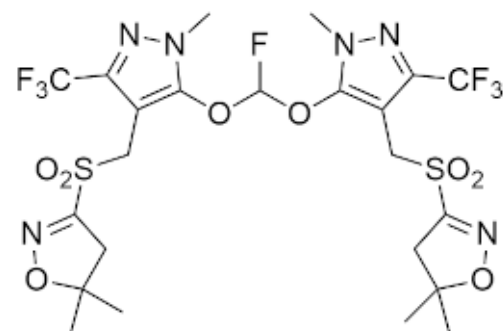




Current Data Parameters
NAME P7K3.11.20
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201103
Time_ 16.47 h
INSTRUM spect
PROBHD Z8420_0082 (PH
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 48
DS 0
SWH 7002.801 Hz
FIDRES 0.213709 Hz
AQ 4.6792703 sec
RG 181
DW 71.400 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec
TD0 1
SFO1 500.0430002 MHz
NUC1 1H
P1 10.32 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 65536
SF 500.0400437 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00



7.196
7.116
6.965

4.565
4.558

3.807

3.045
3.010
2.998
2.963

1.967

1.430
1.421

-0.000

1.000

4.060

6.258

4.108

12.754

11 10 9 8 7 6 5 4 3 2 1 ppm

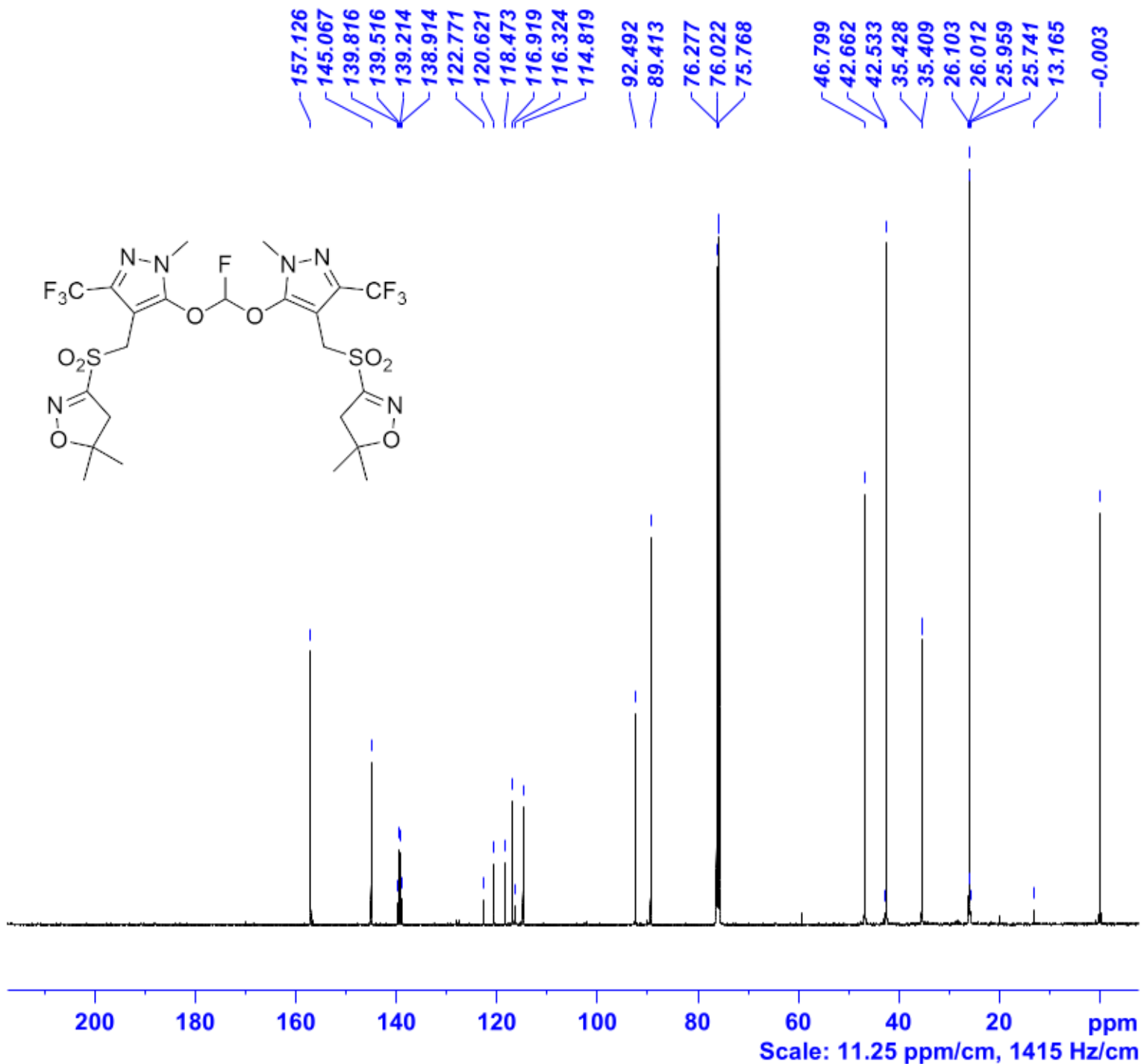
Scale: 0.6 ppm/cm, 300 Hz/cm



Current Data Parameters
NAME P7K3.11.20
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201104
Time_ 7.59 h
INSTRUM spect
PROBHD 28420_0082 (PH
PULPROG zgdc30
TD 65536
SOLVENT CDCl3
NS 33323
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7477315 MHz
NUC1 13C
P1 13.00 usec
PLW1 55.00000000 W
SFO2 500.0425002 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.24962001 W

F2 - Processing parameters
SI 32768
SF 125.7352853 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00





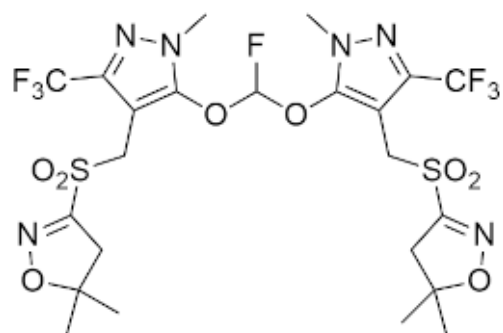
Current Data Parameters
NAME P7K3.11.20
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201103
Time_ 14.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 11261.262 Hz
FIDRES 0.343666 Hz
AQ 1.4548992 sec
RG 3251
DW 44.400 usec
DE 6.32 usec
TE 301.0 K
D1 0.1000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 19F
P1 7.90 usec
PL1 0 dB
SF01 376.4437841 MHz

F2 - Processing parameters
SI 32768
SF 376.4703301 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

-81.995
-82.196



-61.705

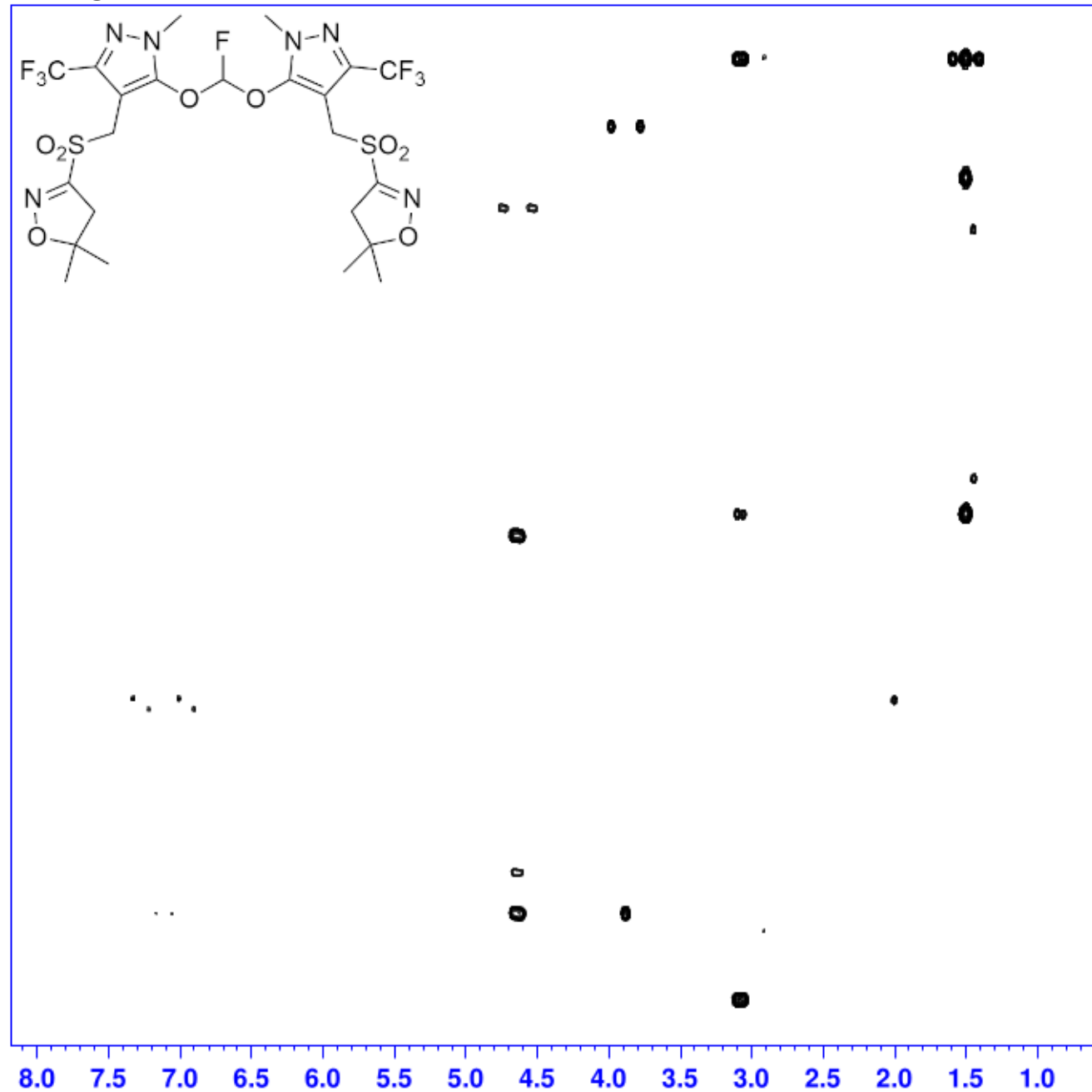
5.879

1.000

-58 -60 -62 -64 -66 -68 -70 -72 -74 -76 -78 -80 -82 ppm

Scale: 1.496 ppm/cm, 563.1 Hz/cm

HMBC



ppm



Current Data Parameters
 NAME P7K3.9.19
 EXPNO 6
 PROCNO 1

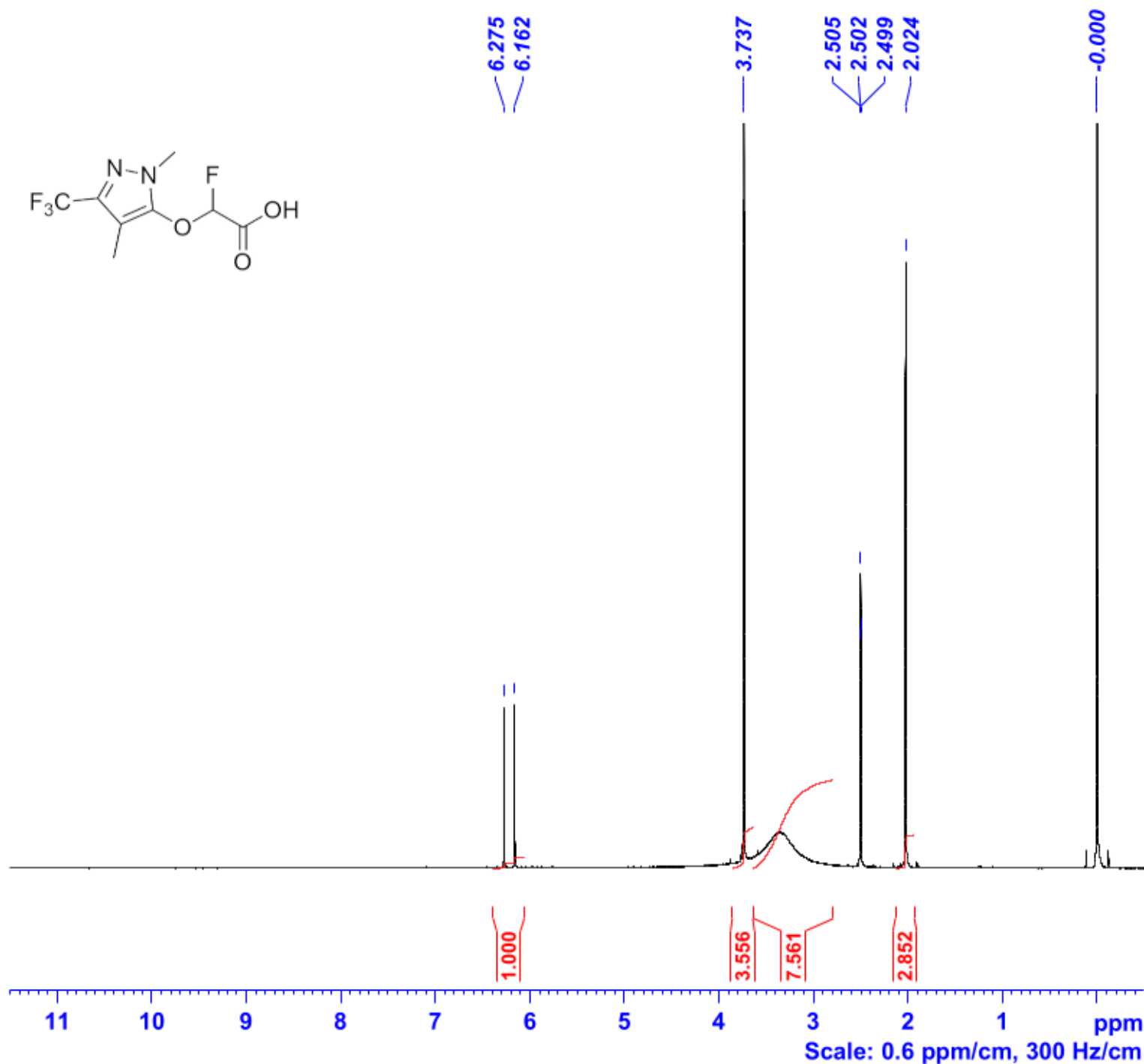
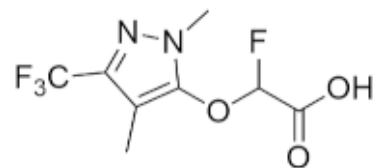
F2 - Acquisition Parameters
 Date_ 20190903
 Time 9.20 h
 INSTRUM spect
 PROBHD Z44908_0030 (C
 PULPROG hmbcgp1pndqf
 TD 1024
 SOLVENT CDCl3
 NS 4
 DS 2
 SWH 5326.705 Hz
 FIDRES 10.403720 Hz
 AQ 0.0961195 sec
 RG 2050
 DW 93.867 usec
 DE 10.00 usec
 TE 300.0 K
 CNST2 145.0000000
 CNST13 8.0000000
 D0 0.00000300 sec
 D1 1.00000000 sec
 D2 0.00344828 sec
 D6 0.06250000 sec
 D16 0.00020000 sec
 IN0 0.00001960 sec
 TDav 1
 SFO1 700.4530820 MHz
 NUC1 1H
 P1 9.32 usec
 P2 18.64 usec
 PLW1 9.00000000 W
 SFO2 176.1444968 MHz
 NUC2 13C
 P3 14.00 usec
 PLW2 18.94499969 W
 GPNAM[1] SINE.100
 GPZ1 50.00 %
 GPNAM[2] SINE.100
 GPZ2 30.00 %
 GPNAM[3] SINE.100
 GPZ3 40.10 %
 P16 1000.00 usec

F1 - Acquisition parameters
 TD 128
 SFO1 176.1445 MHz
 FIDRES 398.596924 Hz
 SW 144.825 ppm
 FMODE QF

F2 - Processing parameters
 SI 1024
 SF 700.4500162 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

F1 - Processing parameters
 SI 512
 MC2 QF
 SF 176.1282756 MHz
 WDW QSINE
 SSB 0
 LB 0 Hz
 GB 0

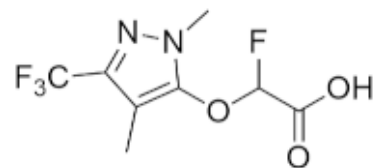
ppm



Current Data Parameters
NAME P7K18.2.21
EXPNO 11
PROCNO 1

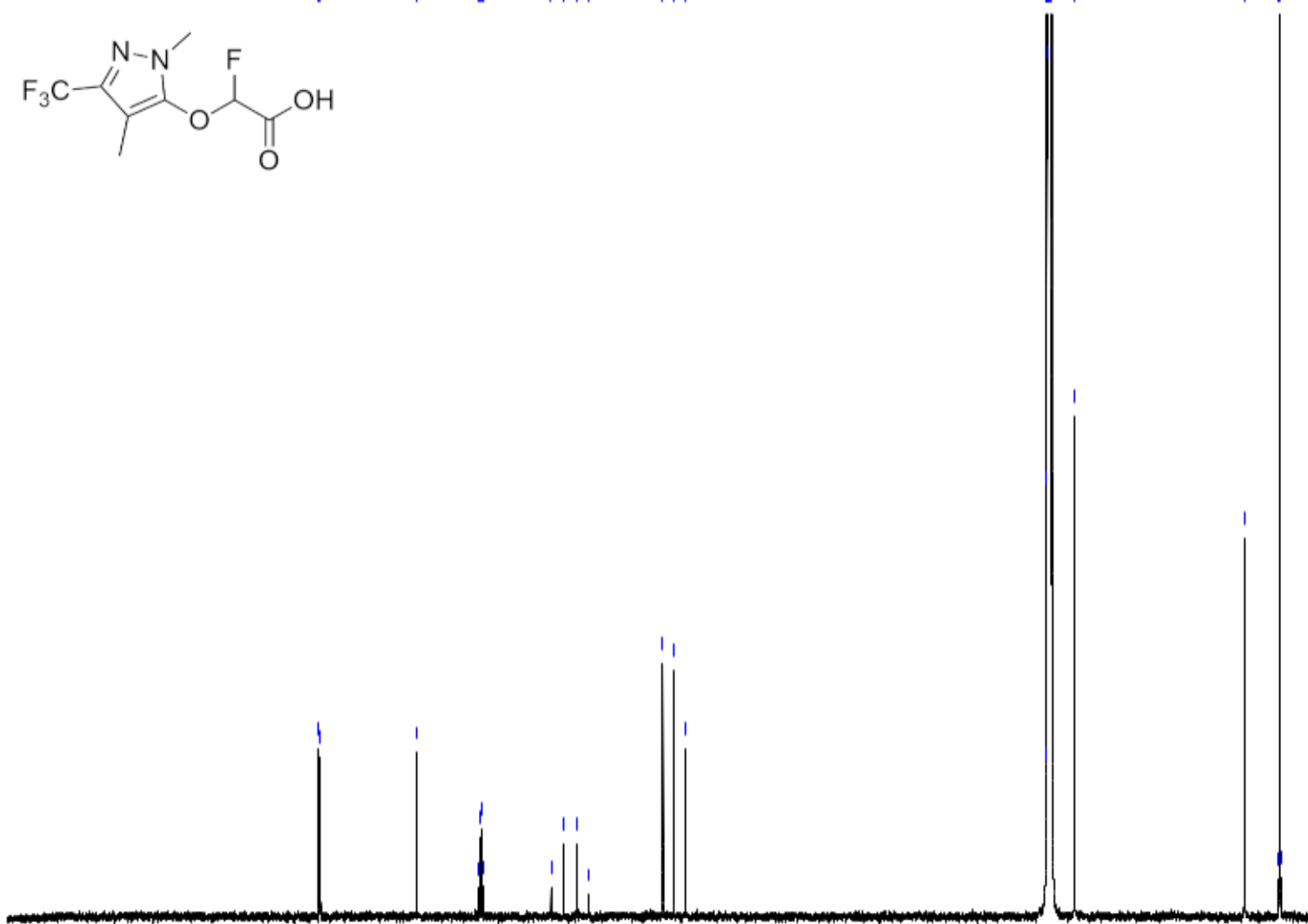
F2 - Acquisition Parameters
Date_ 20210220
Time 3.36 h
INSTRUM spect
PROBHD 28420_0082 (PH
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 24
DS 0
SWH 7002.801 Hz
FIDRES 0.213709 Hz
AQ 4.6792703 sec
RG 512
DW 71.400 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec
TDO 1
SFO1 500.0430002 MHz
NUC1 1H
P1 10.32 usec
PLW1 15.00000000 W

F2 - Processing parameters
SI 65536
SF 500.0400026 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00



164.501
164.264
147.848
137.248
136.963
136.676
136.390
124.707
122.568
120.430
118.292
105.591
103.710
101.739

40.027
39.939
39.863
39.772
39.699
39.605
39.438
39.271
39.104
38.937
35.113
5.956
0.195
-0.003



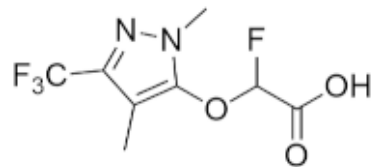
Current Data Parameters
NAME P7K18.2.21
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210220
Time 3.34 h
INSTRUM spect
PROBHD 28420_0082 (PH
PULPROG zgdc30
TD 65536
SOLVENT DMSO
NS 100000
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 2050
DW 16.800 usec
DE 6.50 usec
TE 300.0 K
D1 0.10000000 sec
D11 0.03000000 sec
TDO 1
SFO1 125.7477315 MHz
NUC1 13C
P1 13.00 usec
PLW1 55.00000000 W
SFO2 500.0425002 MHz
NUC2 1H
CPDPRG[2] waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.24962001 W

F2 - Processing parameters
SI 32768
SF 125.7352290 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

200 180 160 140 120 100 80 60 40 20 ppm

Scale: 11.25 ppm/cm, 1415 Hz/cm

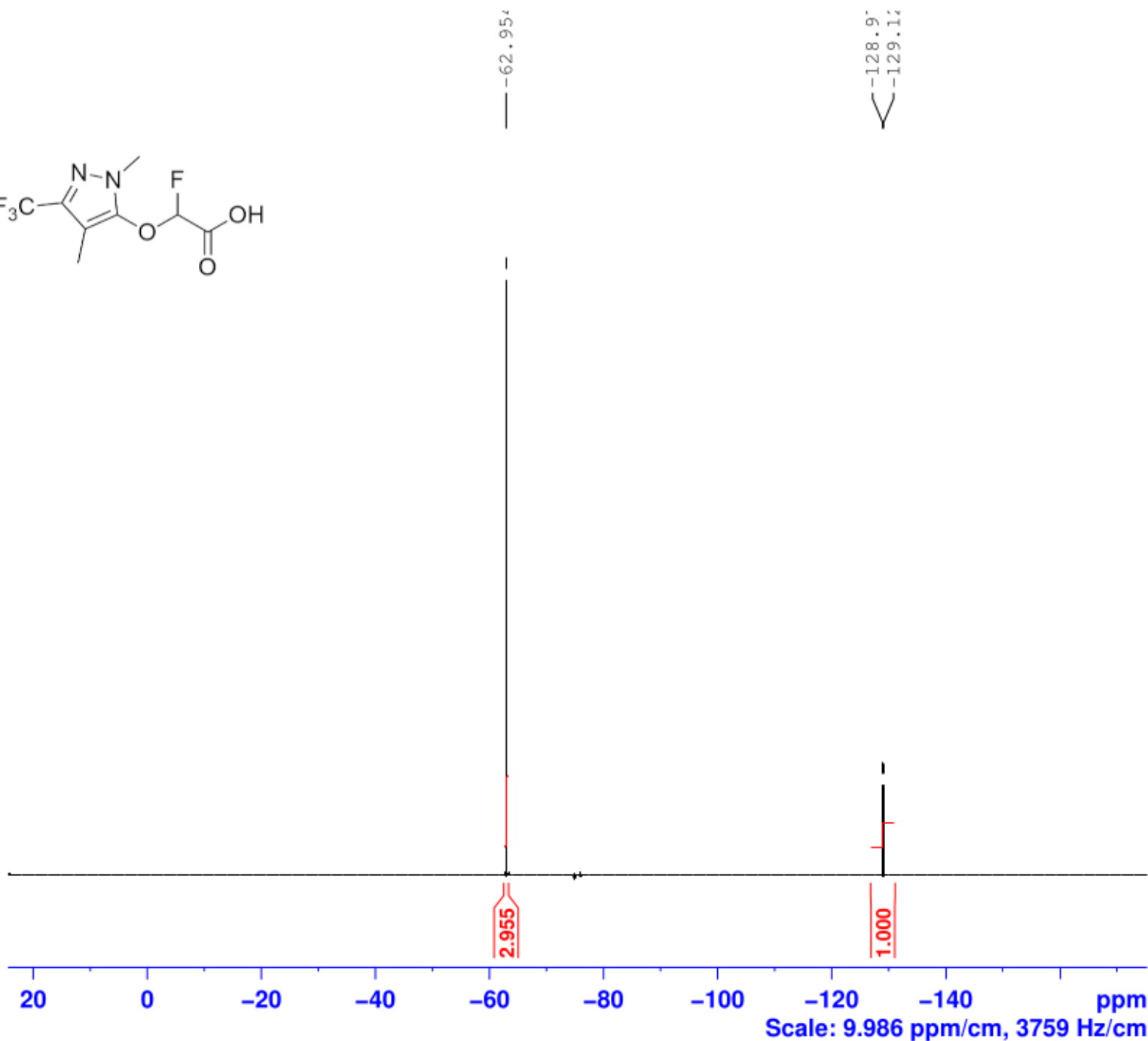


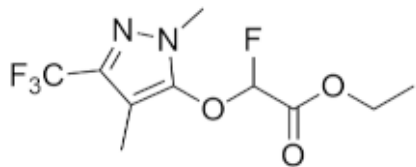
```

NAME          P7K2.9.19
EXPNO         1
PROCNO        1
Date_         20190902
Time          11.04
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            32768
SOLVENT       CDC13
NS            8
DS            0
SWH           75187.969 Hz
FIDRES        2.294555 Hz
AQ            0.2179572 se
RG            71.8
DW            6.650 us
DE            6.32 us
TE            300.2 K
D1            0.10000000 se
TD0           1
  
```

```

===== CHANNEL f1 =====
NUC1          19F
P1            7.90 us
PL1           0.00 dB
SFO1          376.4419017 MHz
SI            32768
SF            376.4703092 MHz
WDW           EM
SSB           0
LB            0.50 Hz
GB            0
PC            1.00
  
```





5.852
5.710
4.410
4.392
4.374
4.356
3.788
2.097
1.399
1.381
1.363
0.000

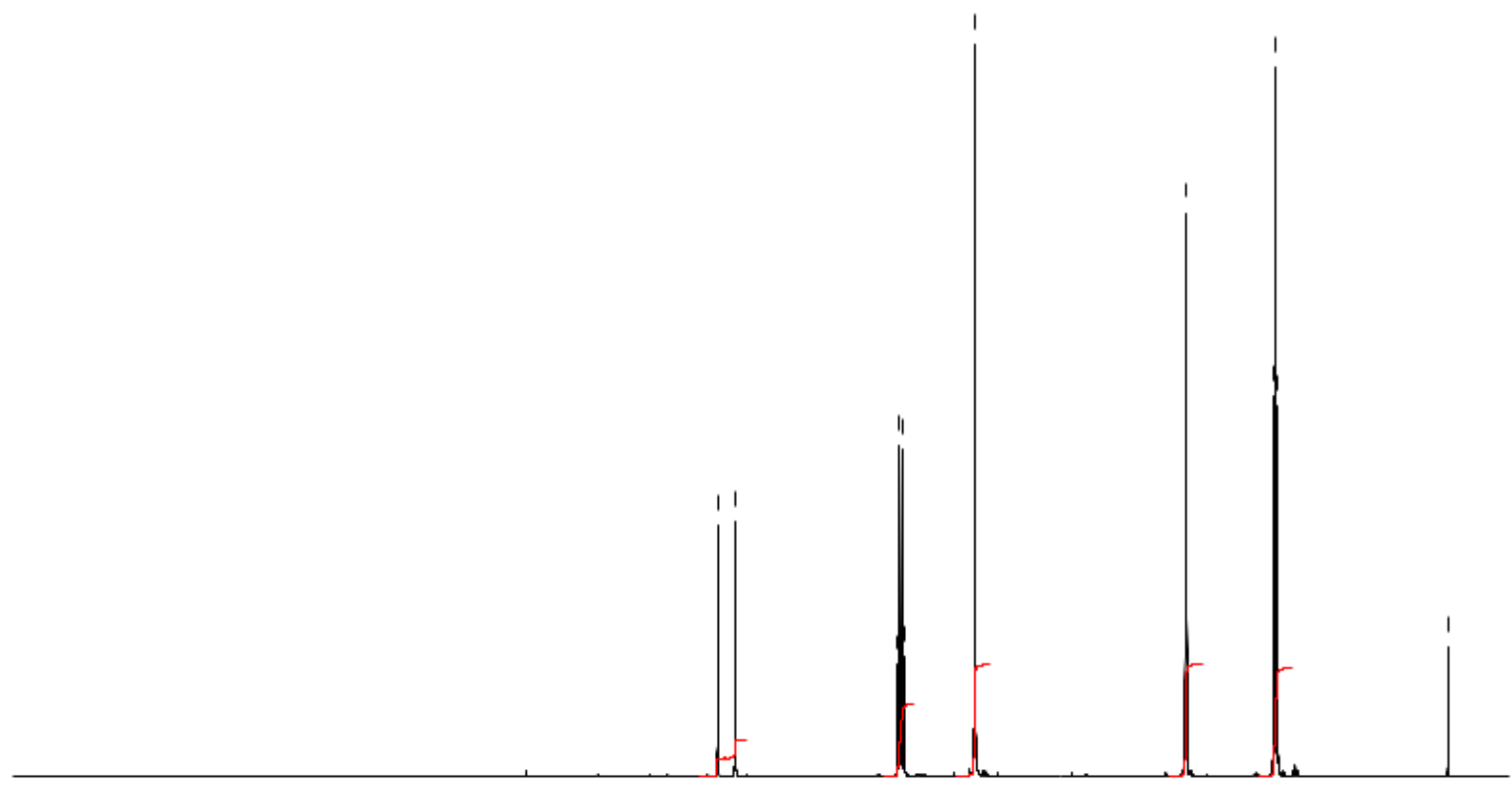


```

NAME          P7K15.2.21
EXPNO         15
PROCNO        1
Date_         20210216
Time          7.55
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            8
DS            0
SWH           7183.908 Hz
FIDRES        0.109618 Hz
AQ            4.5613556 sec
RG            20.2
DW            69.600 usec
DE            6.50 usec
TE            299.7 K
D1            0.10000000 sec
TD0           1
  
```

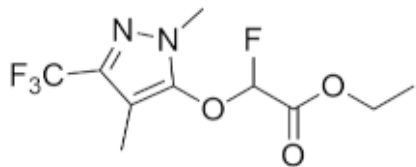
```

===== CHANNEL f1 =====
NUC1          1H
P1            10.10 usec
PL1           0.00 dB
SFO1          400.1032008 MHz
SI            32768
SF            400.0999574 MHz
WDW           FM
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
  
```

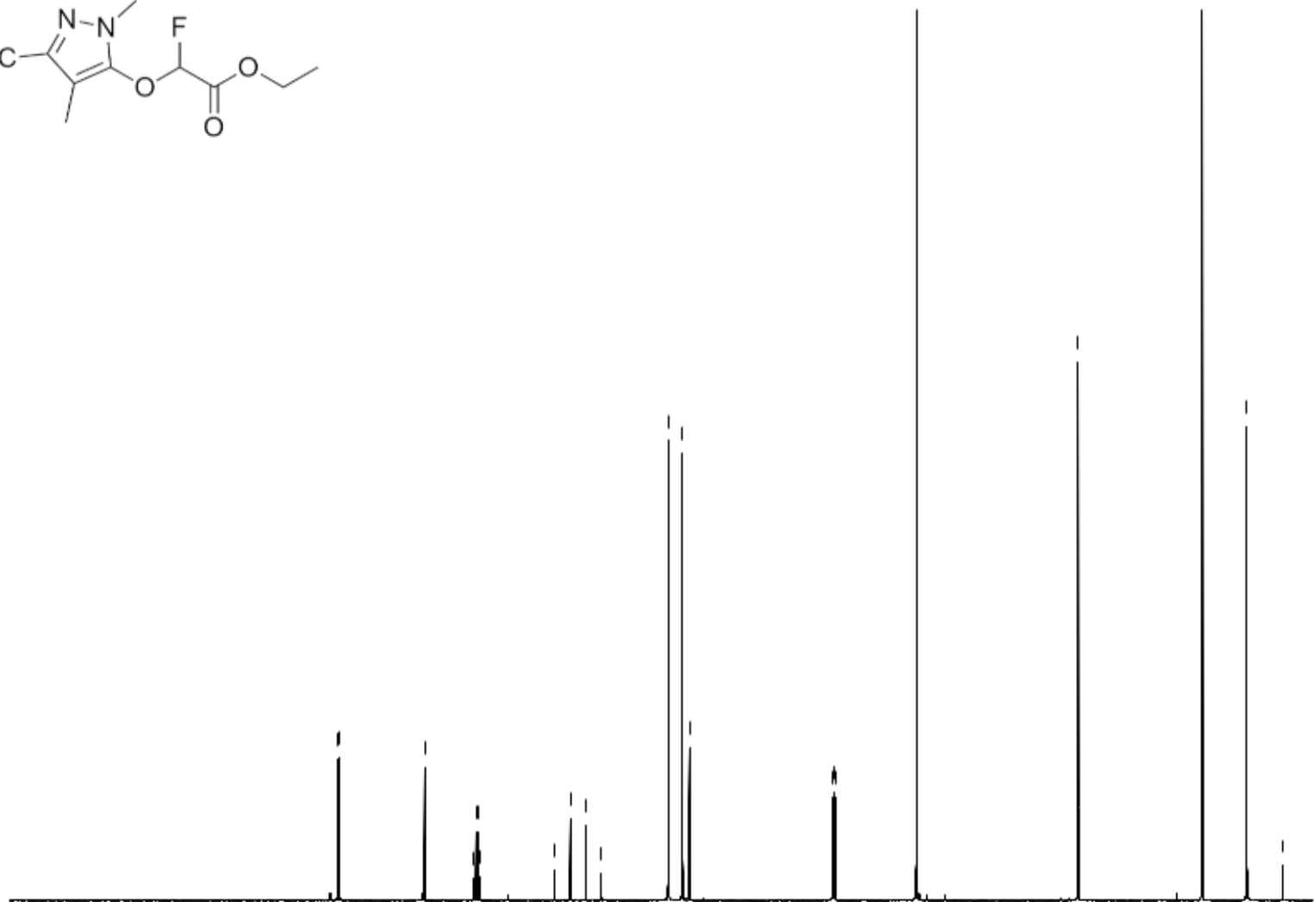


1.000
1.983
3.105
3.082
3.007

11 10 9 8 7 6 5 4 3 2 1 ppm
Scale: 0.6 ppm/cm, 240.1 Hz/cm



163.235
162.929
148.289
139.764
139.399
139.033
138.668
125.805
123.130
120.456
117.781
106.118
103.730
102.560
77.847
77.528
77.208
63.370
35.442
13.991
6.336
-0.000



200 180 160 140 120 100 80 60 40 20 ppm
Scale: 11.25 ppm/cm, 1132 Hz/cm



```

NAME          P7K15.2.21
EXPNO         14
PROCNO        1
Date_         20210216
Time          3.06
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgdc30
TD            32768
SOLVENT       CDC13
NS            40000
DS            0
SWH           24154.590 Hz
FIDRES        0.737140 Hz
AQ            0.6783476 se
RG            71.8
DW            20.700 us
DE            29.57 us
TE            299.9 K
D1            0.10000000 se
D11           0.03000000 se
TD0           1

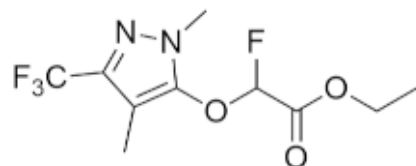
===== CHANNEL f1 =====
NUC1           13C
P1             9.20 us
PL1            3.00 dB
SFO1          100.6152865 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2         80.00 us
PL2            0.00 dB
PL12          18.00 dB
SFO2          400.1009202 MHz
SI            32768
SF            100.6051785 MHz
WDW           EM
SSB           0
LB            2.00 Hz
GB            0
PC            1.00
  
```



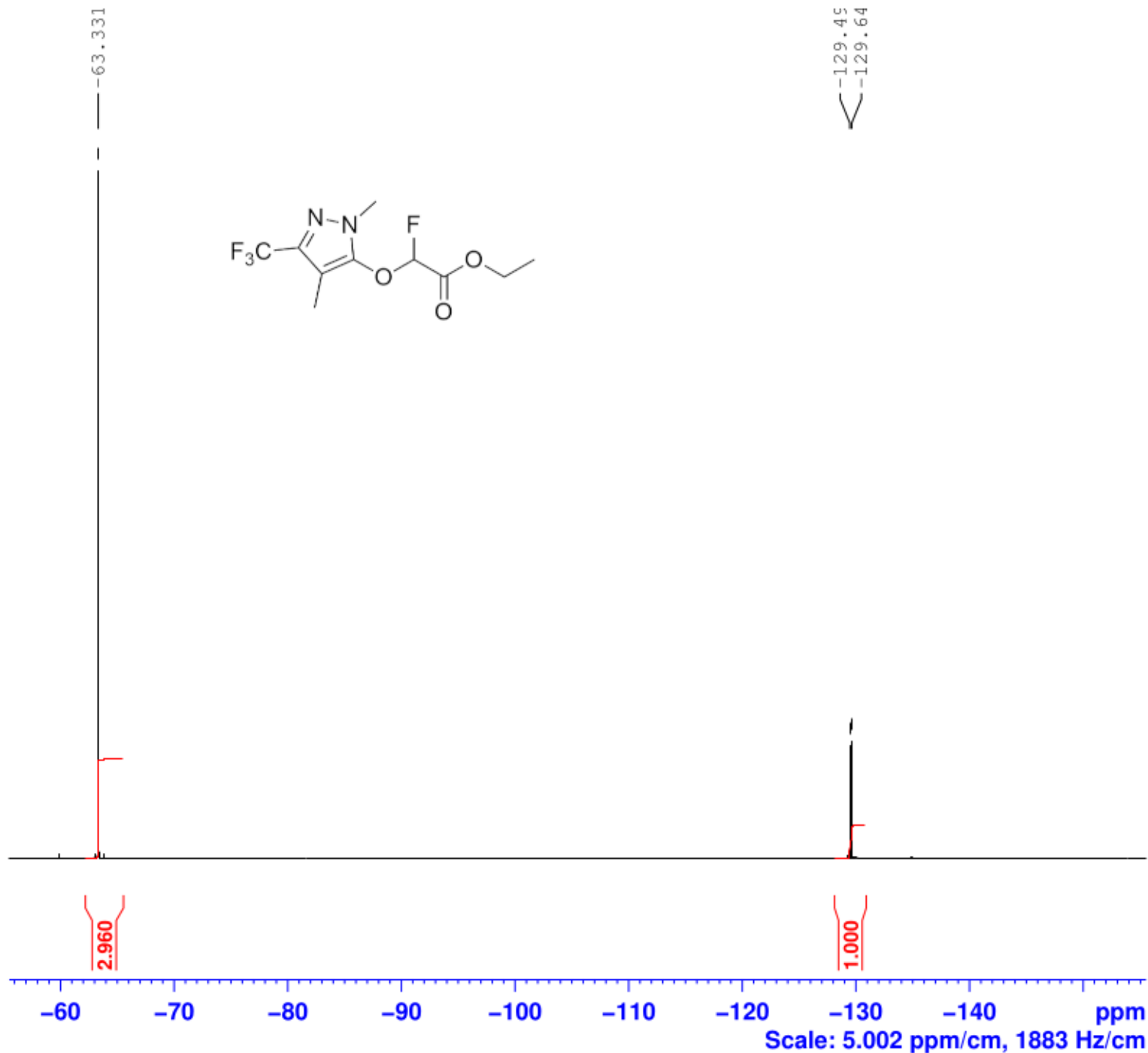
NAME P7K15.2.21
EXPNO 6
PROCNO 1
Date_ 20210215
Time 9.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 48
DS 0
SWH 37664.785 Hz
FIDRES 1.149438 Hz
AQ 0.4350452 se
RG 1290.2
DW 13.275 us
DE 6.32 us
TE 300.0 K
D1 0.10000000 se
TD0 1

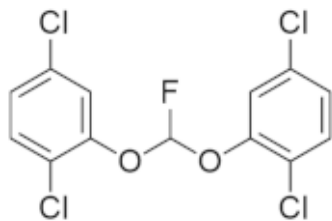
===== CHANNEL f1 =====
NUC1 19F
P1 7.90 us
PL1 0.00 dB
SFO1 376.4306076 MHz
SI 32768
SF 376.4703301 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00



63.331

-129.45
-129.64





7.651
7.640
7.638
7.634
7.631
7.629
7.607
7.582
7.464
7.346
7.340
7.324
7.318

3.340

2.521
2.517

0.000



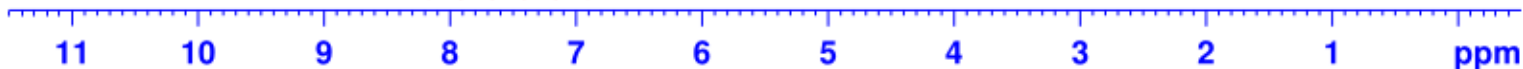
```

NAME          P7K26.1.21
EXPNO          4
PROCNO         1
Date_         20210126
Time          10.05
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            24
DS            0
SWH           7183.908 Hz
FIDRES        0.109618 Hz
AQ            4.5613556 sec
RG            362
DW            69.600 usec
DE            6.50 usec
TE            299.9 K
D1            0.10000000 sec
TD0           1
  
```

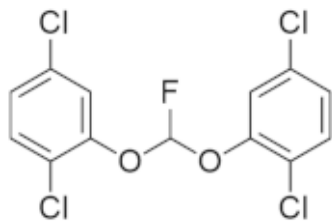
```

===== CHANNEL f1 =====
NUC1           1H
P1             10.10 usec
PL1            0.00 dB
SFO1           400.1032008 MHz
SI             32768
SF             400.0999959 MHz
WDW            FM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
  
```

0.490
2.858
1.225
0.516
2.000



Scale: 0.6 ppm/cm, 240.1 Hz/cm



7.651
7.640
7.638
7.634
7.631
7.629
7.607
7.582
— 7.464
7.346
7.340
7.324
7.318

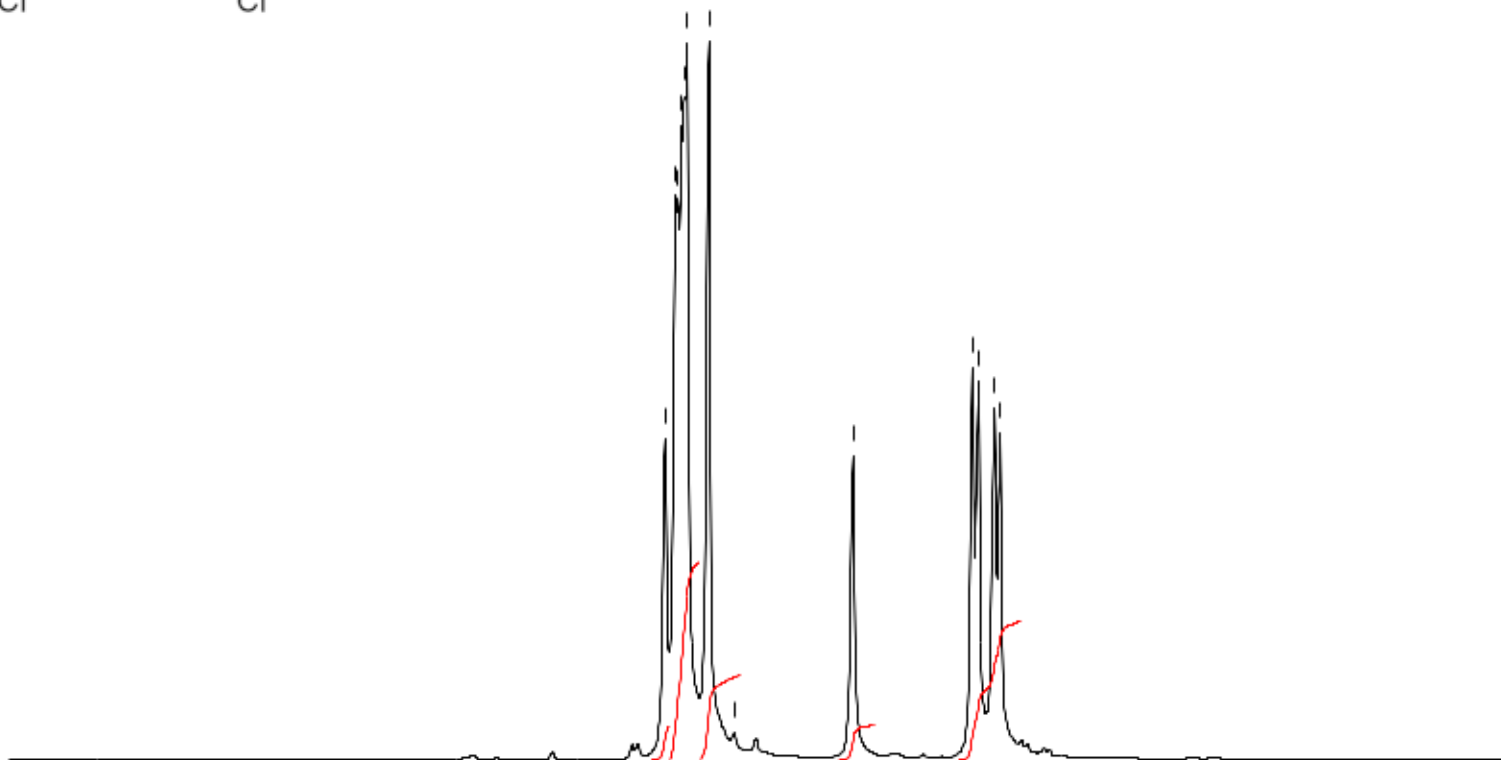


```

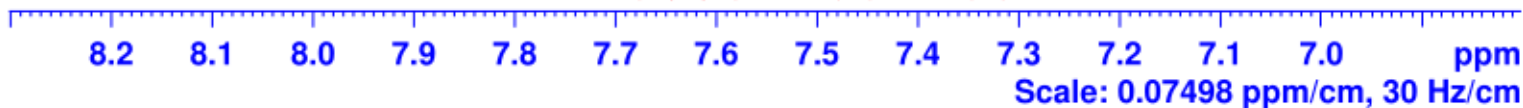
NAME          P7K26.1.21
EXPNO         4
PROCNO        1
Date_         20210126
Time          10.05
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       DMSO
NS            24
DS            0
SWH           7183.908 Hz
FIDRES        0.109618 Hz
AQ            4.5613556 sec
RG            362
DW            69.600 usec
DE            6.50 usec
TE            299.9 K
D1            0.10000000 sec
TD0           1
  
```

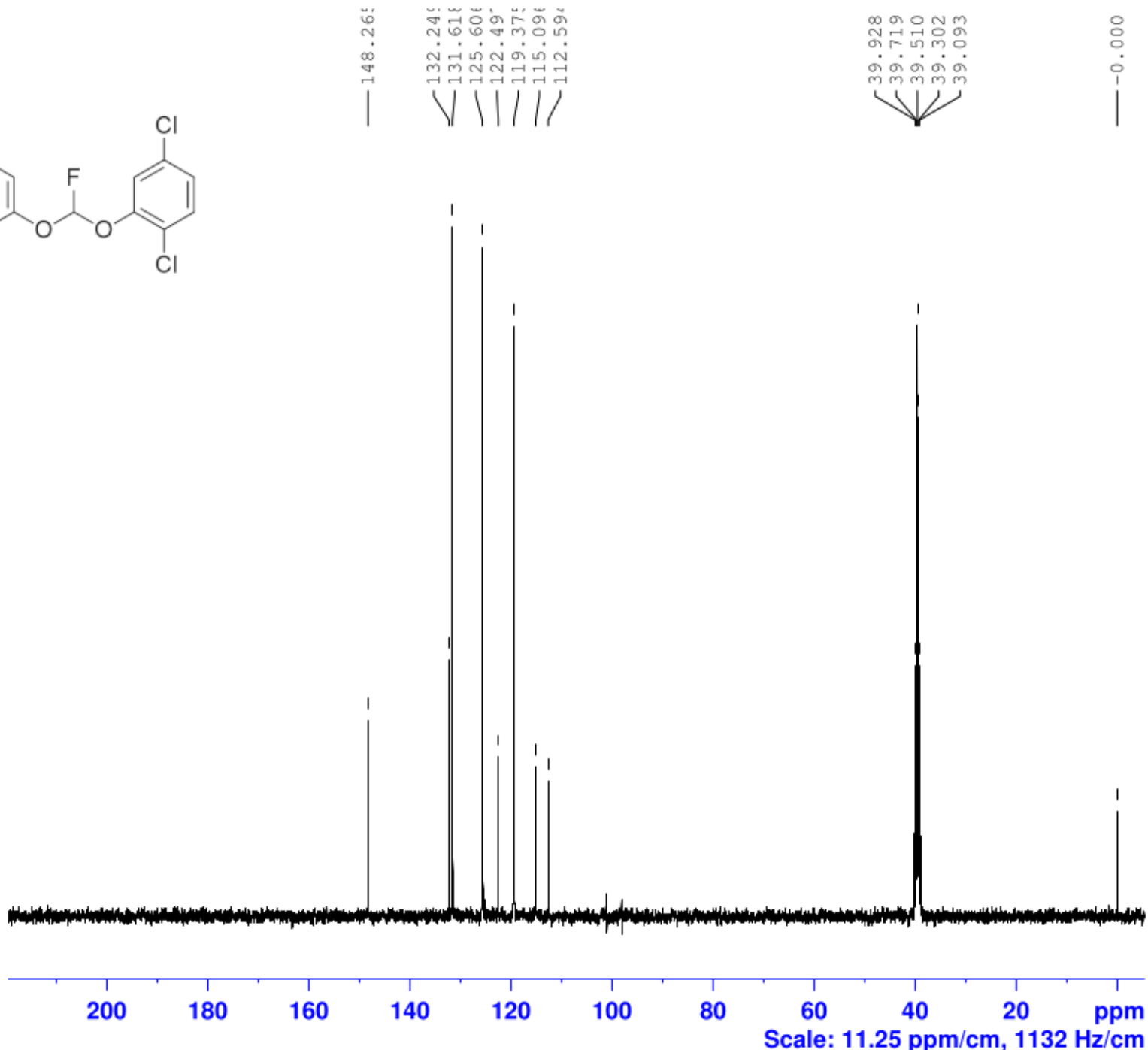
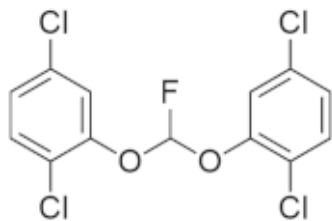
```

===== CHANNEL f1 =====
NUC1           1H
P1             10.10 usec
PL1            0.00 dB
SFO1           400.1032008 MHz
SI             32768
SF             400.0999959 MHz
WDW            FM
SSB            0
LB             0.30 Hz
GB             0
PC             1.00
  
```



0.490
2.858
1.225
0.516
2.000





— 148.26
 132.24
 131.61
 125.60
 122.49
 119.37
 115.09
 112.59
 39.928
 39.719
 39.510
 39.302
 39.093
 — 0.000

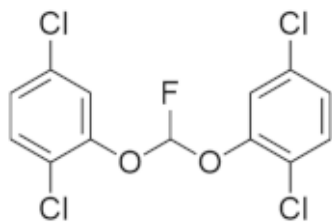


```

NAME          P7K26.1.21
EXPNO         7
PROCNO        1
Date_         20210126
Time          10.10
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zgdc30
TD            32768
SOLVENT       DMSO
NS            1200
DS            0
SWH           24154.590 Hz
FIDRES        0.737140 Hz
AQ            0.6783476 se
RG            71.8
DW            20.700 us
DE            29.57 us
TE            300.5 K
D1            0.10000000 se
D11           0.03000000 se
TD0           1

===== CHANNEL f1 =====
NUC1           13C
P1             9.20 us
PL1            3.00 dB
SFO1           100.6152865 MHz

===== CHANNEL f2 =====
CPDPRG2       waltz16
NUC2           1H
PCPD2          80.00 us
PL2            0.00 dB
PL12           18.00 dB
SFO2           400.1009202 MHz
SI            32768
SF            100.6052769 MHz
WDW            EM
SSB            0
LB             2.00 Hz
GB             0
PC             1.00
  
```



--87.01!
--87.21!



NAME P7K26.1.21
EXPNO 6
PROCNO 1
Date_ 20210126
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 24
DS 0
SWH 11261.262 Hz
FIDRES 0.343666 Hz
AQ 1.4549491 se
RG 1625.5
DW 44.400 us
DE 6.32 us
TE 299.9 K
D1 0.10000000 se
TD0 1

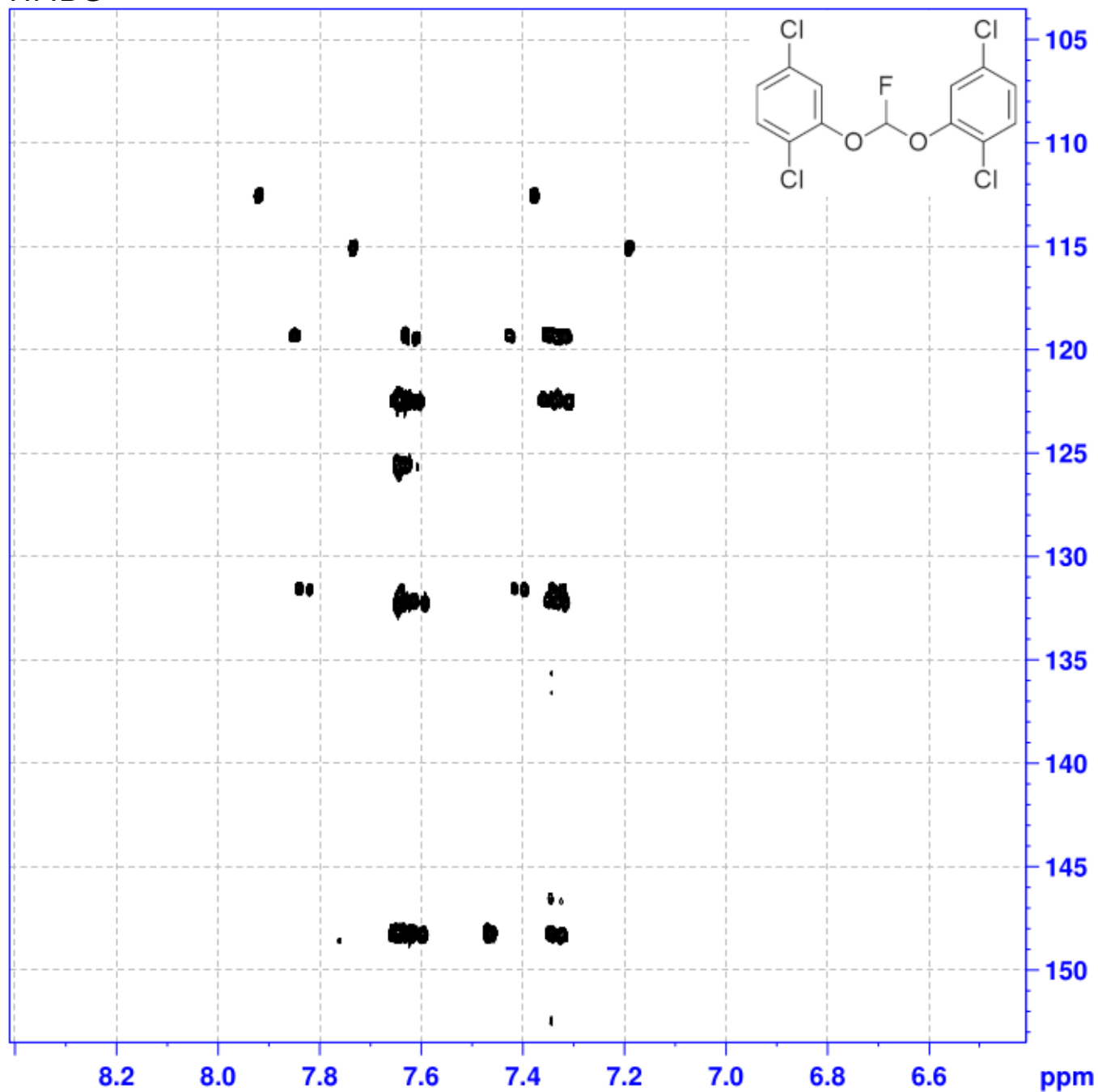
==== CHANNEL f1 =====
NUC1 19F
P1 7.90 us
PL1 0.00 dB
SFO1 376.4381370 MHz
SI 32768
SF 376.4703301 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00



-75 -80 -85 -90 -95 ppm

Scale: 1.496 ppm/cm, 563.1 Hz/cm

HMBC



```

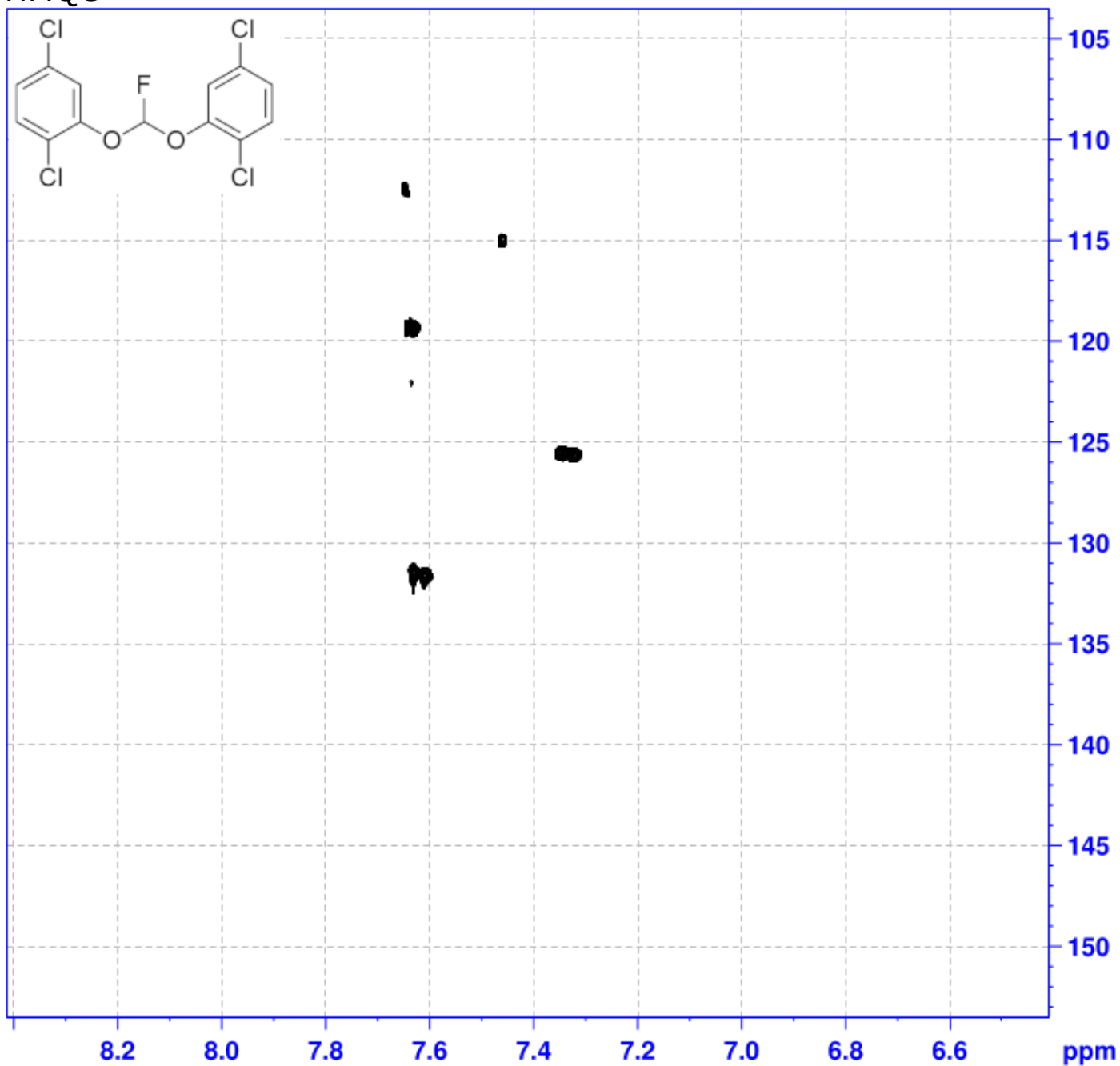
NAME          P7K26.1.21
EXPNO         11
PROCNO        1
Date_         20210126
Time          10.56
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       hmbcqp1pndqf
TD            1024
SOLVENT       DMSO
NS            8
DS            2
SWH           801.282 Hz
FIDRES        0.782502 Hz
AQ            0.6390260 sec
RG            46341
DW            624.000 usec
DE            241.25 usec
TE            299.2 K
CNST2         145.0000000
CNST13        8.0000000
D0            0.00000300 sec
D1            1.00000000 sec
D2            0.00344828 sec
D6            0.06250000 sec
D16           0.00020000 sec
INO           0.00009940 sec

----- CHANNEL f1 -----
NUC1          1H
P1            10.10 usec
P2            20.20 usec
PL1           0.00 dB
SFO1          400.1029607 MHz

----- CHANNEL f2 -----
NUC2          13C
P3            9.20 usec
PL2           0.00 dB
SFO2          100.6182041 MHz

===== GRADIENT CHANNEL =====
GPNAM1       sine.100
GPNAM2       sine.100
GPNAM3       sine.100
GPZ1         50.00 %
GPZ2         30.00 %
GPZ3         40.10 %
PL6          1000.00 usec
ND0          2
TD           128
SFO1         100.6182 MHz
FIDRES       39.303986 Hz
SW           50.000 ppm
FmMODE       QF
SI           1024
SF           400.0999959 MHz
WDW          QSINE
SSB          0
LB           0.00 Hz
GB           0
PC           1.00
SI           512
MC2          QF
SF           100.6052769 MHz
WDW          QSINE
SSB          0
LB           0.00 Hz
GB           0
    
```

HMQC



```

NAME          P7K26.1.21
EXPNO         10
PROCNO        1
Date_         20210126
Time_         10.41
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       hmqcpgqf
TD            1024
SOLVENT       DMSO
NS            4
DS            2
SWH           801.282 Hz
FIDRES        0.782502 Hz
AQ            0.6390260 sec
RG            46341
DW            624.000 usec
DE            241.25 usec
TE            300.1 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00009940 sec
    
```

```

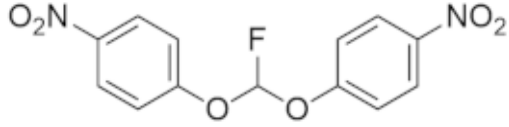
===== CHANNEL f1 =====
NUC1          1H
P1            10.50 usec
P2            21.00 usec
PL1           0.00 dB
SFO1          400.1029607 MHz
    
```

```

===== CHANNEL f2 =====
CPDPRG2       gaXP
NUC2          13C
P3            9.10 usec
PCPD2         55.00 usec
PL2           3.00 dB
PL12          18.40 dB
SFO2          100.6182041 MHz
    
```

```

----- GRADIENT CHANNEL -----
GPNAM1        sine.100
GPNAM2        sine.100
GPNAM3        sine.100
GPZ1          50.00 %
GPZ2          30.00 %
GPZ3          40.10 %
P16           1000.00 usec
ND0           2
TD            128
SFO1          100.6182 MHz
FIDRES        39.303986 Hz
SW            50.000 ppm
FnMODE        QF
SI            1024
SF            400.0999959 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
SI            512
MC2           QF
SF            100.6052769 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
    
```



8.280
8.258
7.424
7.401
7.295
7.273
6.938
6.758

3.484

2.042
1.691
1.275
1.258

0.092
-0.000

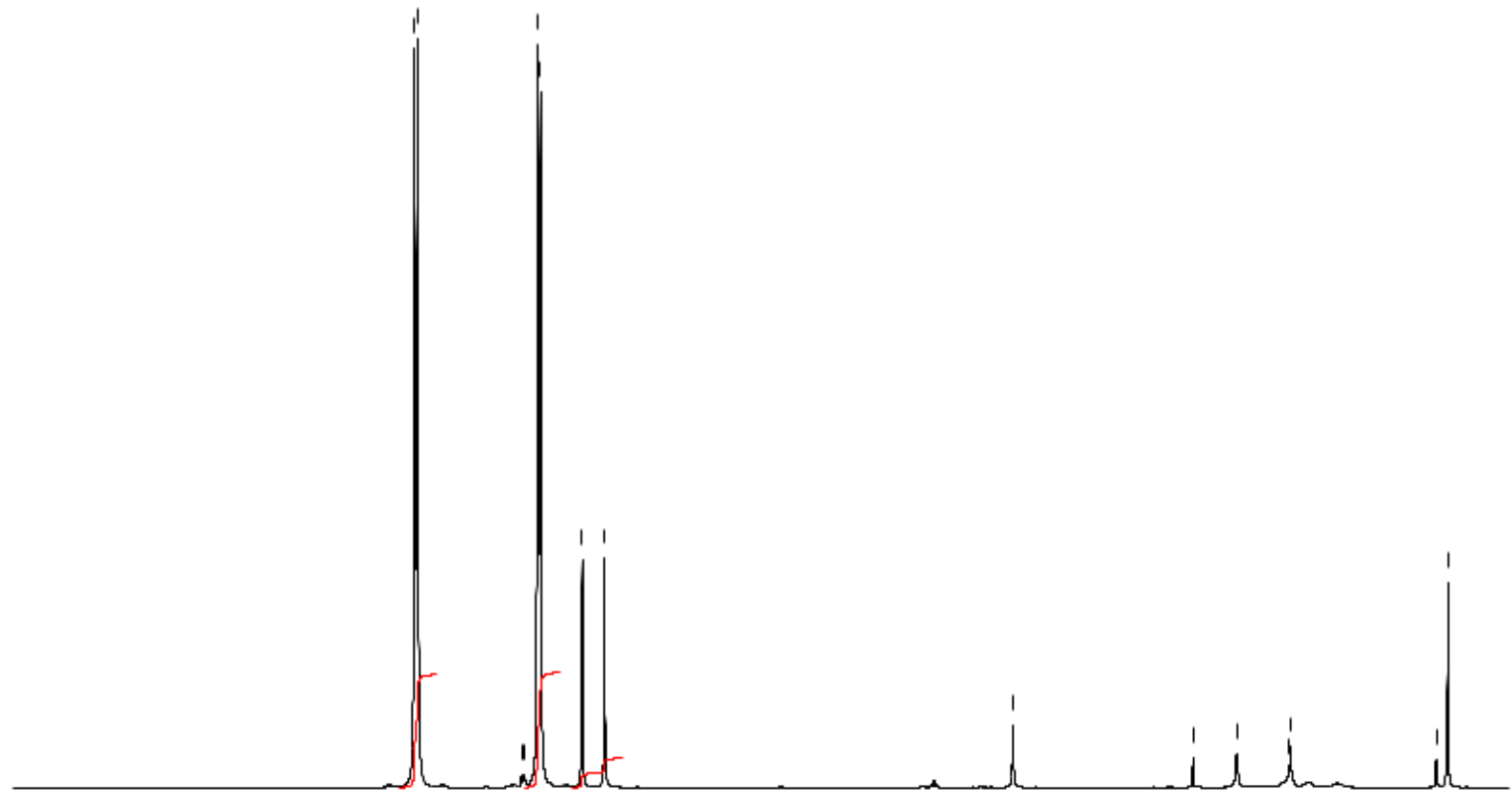


```

NAME          P7K1.2.21
EXPNO         1
PROCNO        1
Date_         20210201
Time          8.35
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       zg30
TD            65536
SOLVENT       CDCl3
NS            24
DS            0
SWH           7183.908 Hz
FIDRES        0.109618 Hz
AQ            4.5613556 sec
RG            114
DW            69.600 usec
DE            6.50 usec
TE            299.9 K
D1            0.10000000 sec
TD0           1
  
```

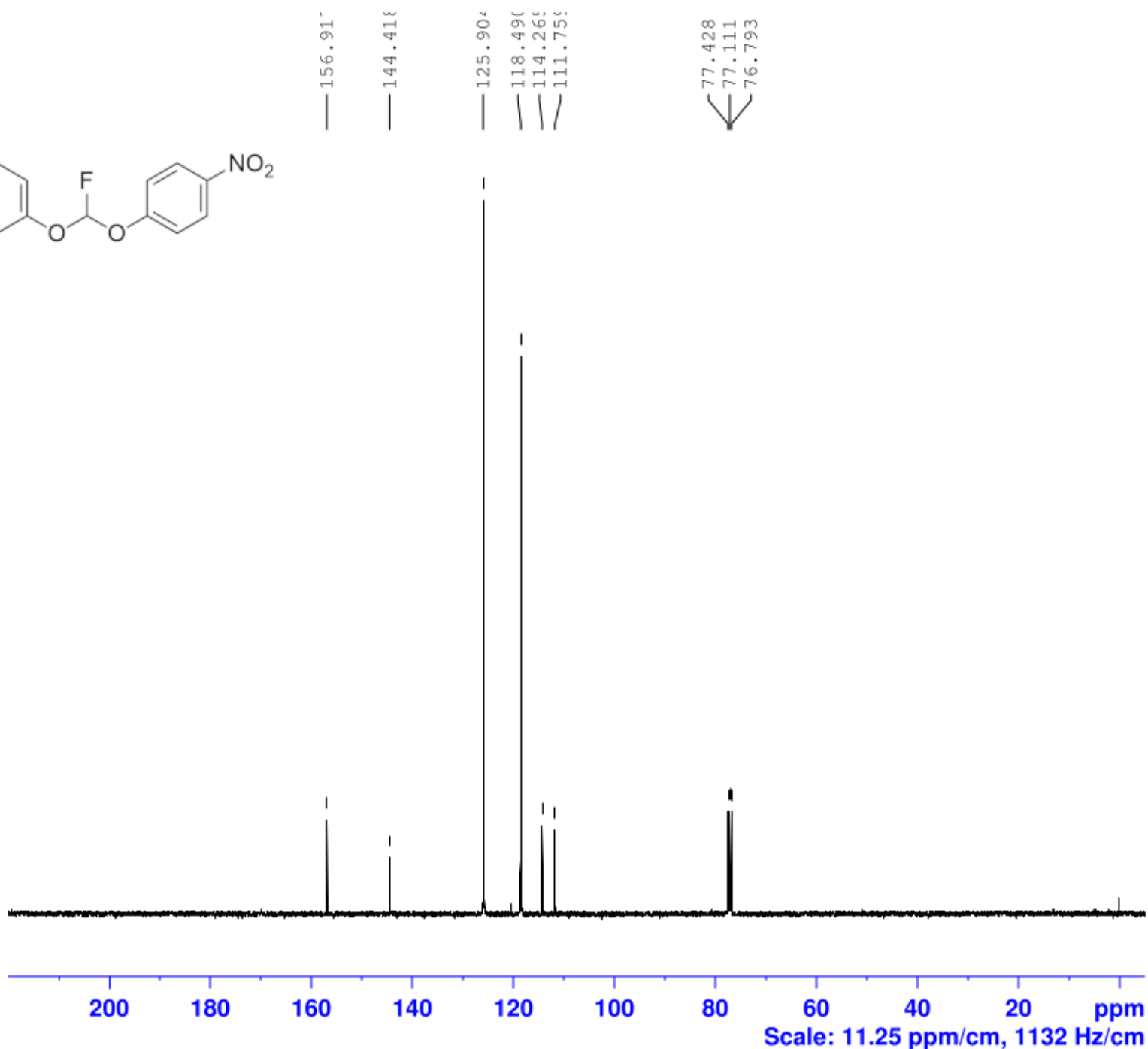
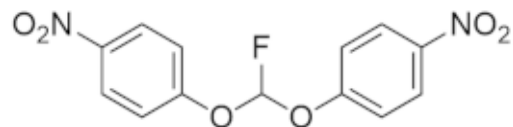
```

===== CHANNEL f1 =====
NUC1           1H
P1             10.10 usec
PL1            0.00 dB
SFO1          400.1032008 MHz
SI            32768
SF            400.1000013 MHz
WDW            FM
SSB            0
LB            0.30 Hz
GB            0
PC            1.00
  
```



4.000
4.063
1.035

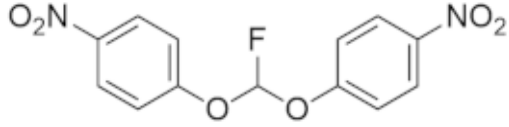
11 10 9 8 7 6 5 4 3 2 1 ppm
Scale: 0.6 nm/cm. 240.1 Hz/cm



NAME P7K1.2.21
EXPNO 3
PROCNO 1
Date_ 20210201
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgdc30
TD 32768
SOLVENT CDCl3
NS 1000
DS 0
SWH 24154.590 Hz
FIDRES 0.737140 Hz
AQ 0.6783476 se
RG 71.8
DW 20.700 us
DE 29.57 us
TE 300.5 K
D1 0.10000000 se
D11 0.03000000 se
TD0 1

=====
CHANNEL f1
=====
NUC1 13C
P1 9.20 us
PL1 3.00 dB
SFO1 100.6152865 MHz

=====
CHANNEL f2
=====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 us
PL2 0.00 dB
PL12 18.00 dB
SFO2 400.1009202 MHz
SI 32768
SF 100.6052219 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00



85.672
85.862

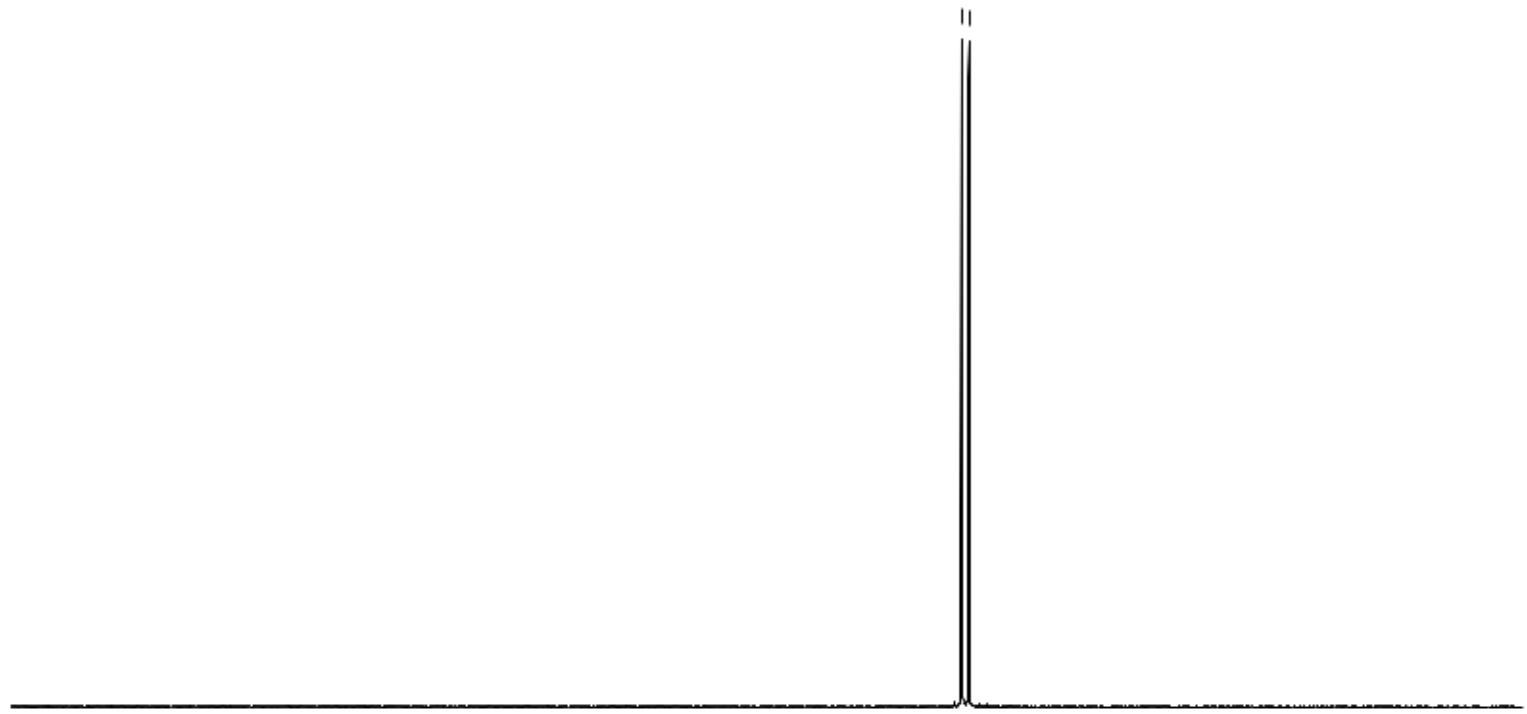


```

NAME          P7K1.2.21
EXPNO         2
PROCNO       1
Date_        20210201
Time         8.36
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           32768
SOLVENT      CDC13
NS           8
DS           0
SWH          15060.241 Hz
FIDRES       0.459602 Hz
AQ           1.0879476 se
RG           2580.3
DW           33.200 us
DE           6.32 us
TE           299.9 K
D1           0.10000000 se
TDO          1
  
```

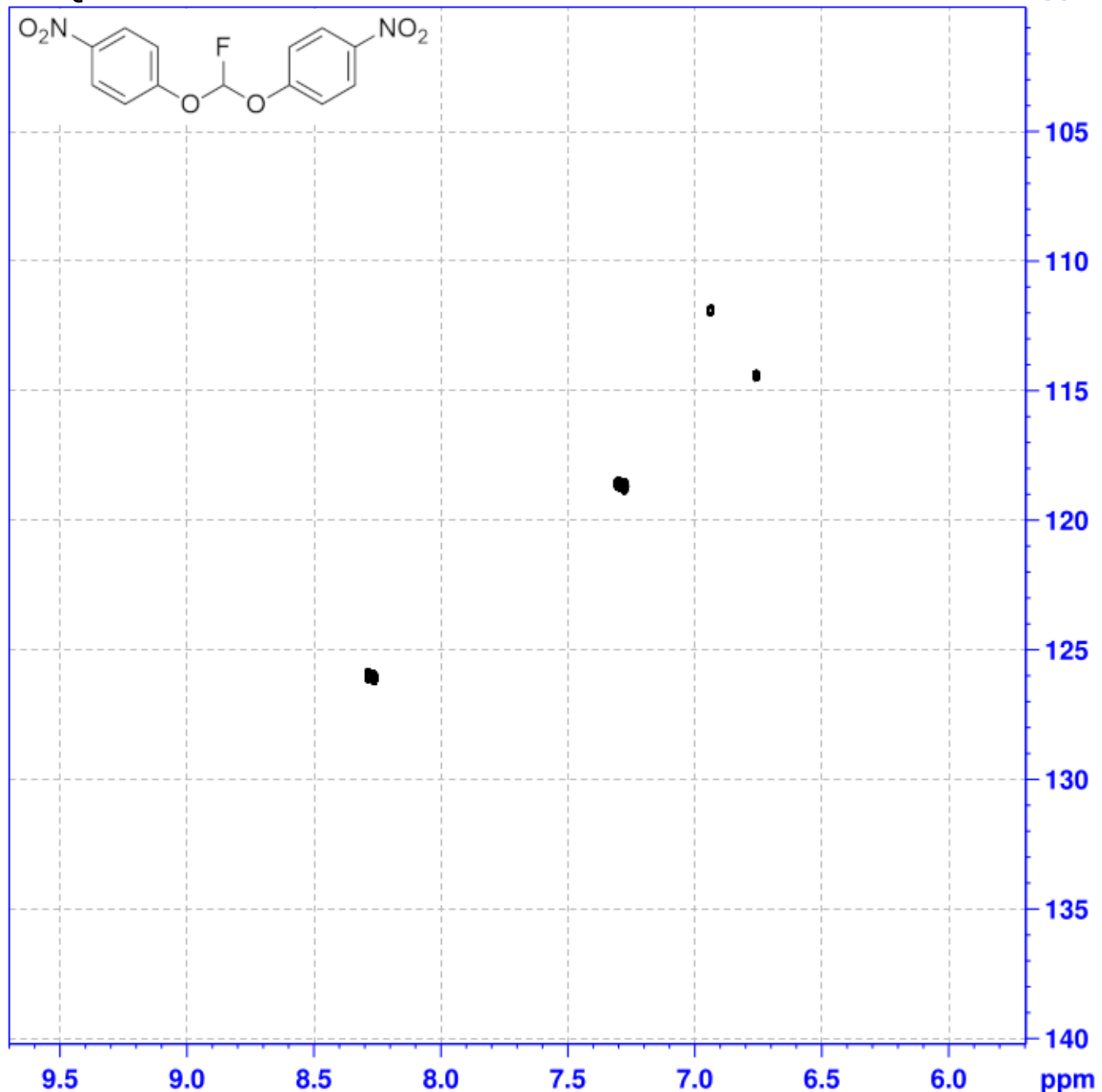
```

===== CHANNEL f1 =====
NUC1          19F
P1            7.90 us
PL1           0.00 dB
SFO1         376.4400194 MHz
SI            32768
SF           376.4703301 MHz
WDW           EM
SSB           0
LB            0.50 Hz
GB            0
PC            1.00
  
```



-65 -70 -75 -80 -85 -90 -95 ppm
Scale: 2 ppm/cm, 753 Hz/cm

HMQC



```

NAME          P7K1.2.21
EXPNO         5
PROCNO        1
Date_         20210201
Time          9.11
INSTRUM       spect
PROBHD        5 mm PABBO BB-
PULPROG       hmqcpgqf
TD            1024
SOLVENT       CDCl3
NS            4
DS            2
SWH           1602.564 Hz
FIDRES        1.565004 Hz
AQ            0.3195380 sec
RG            20642.5
DW            312.000 usec
DE            241.25 usec
TE            300.2 K
CNST2         145.0000000
D0            0.00000300 sec
D1            1.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00012425 sec

===== CHANNEL f1 =====
NUC1           1H
P1             10.50 usec
P2             21.00 usec
PL1            0.00 dB
SFO1          400.1030808 MHz

===== CHANNEL f2 =====
CPDPRG2       gaXp
NUC2           13C
P3             9.10 usec
PCPD2         55.00 usec
PL2            3.00 dB
PL12          18.40 dB
SFO2          100.6172986 MHz

----- GRADIENT CHANNEL -----
GPNAM1        sine.100
GPNAM2        sine.100
GPNAM3        sine.100
GPZ1          50.00 %
GPZ2          30.00 %
GPZ3          40.10 %
P16           1000.00 usec
ND0           2
TD            128
SFO1          100.6173 MHz
FIDRES        31.442905 Hz
SW            40.000 ppm
FnMODE        QF
SI            1024
SF            400.1000009 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
PC            1.00
SI            512
MC2           QF
SF            100.6052043 MHz
WDW           QSINE
SSB           0
LB            0.00 Hz
GB            0
    
```