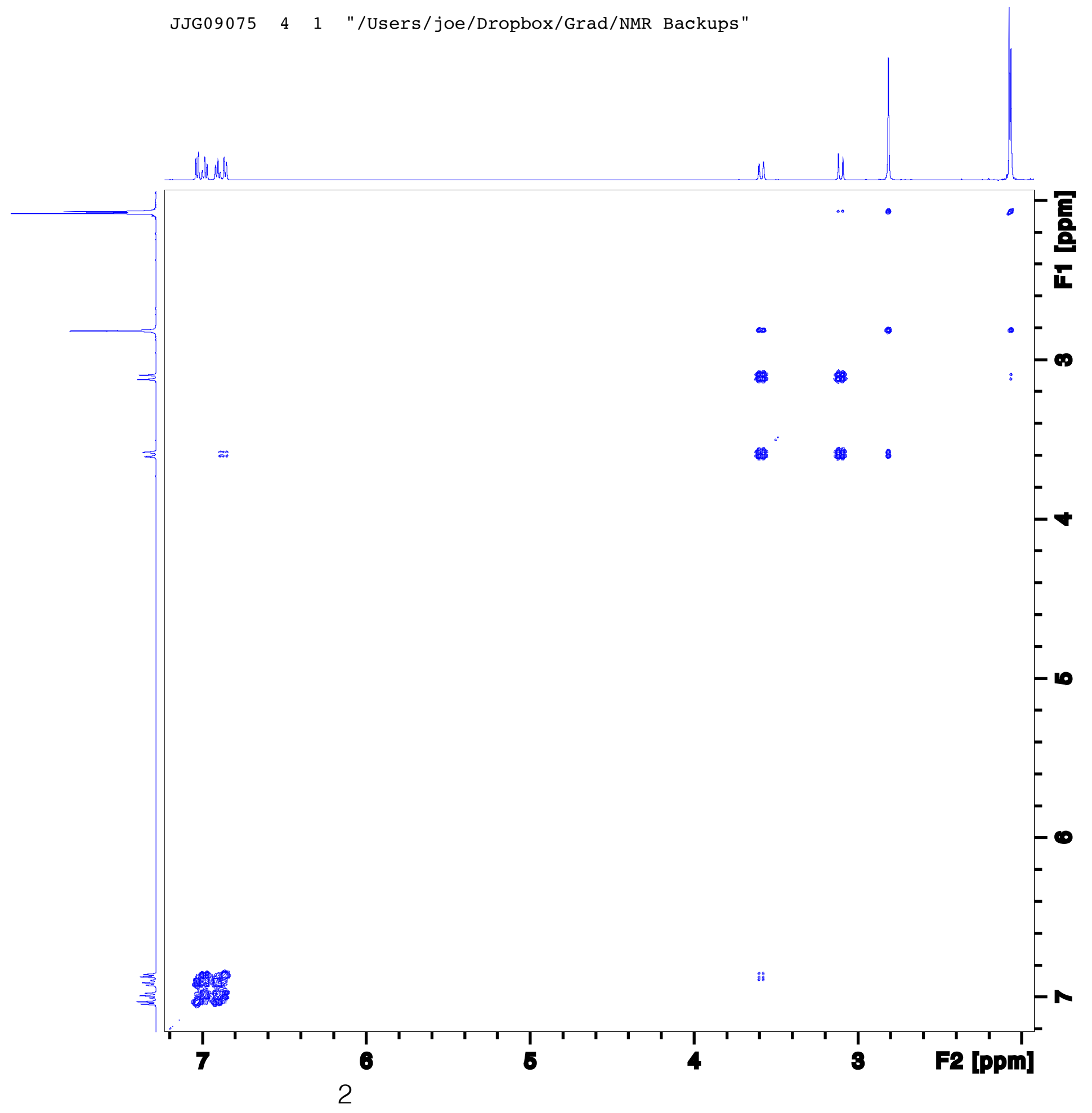
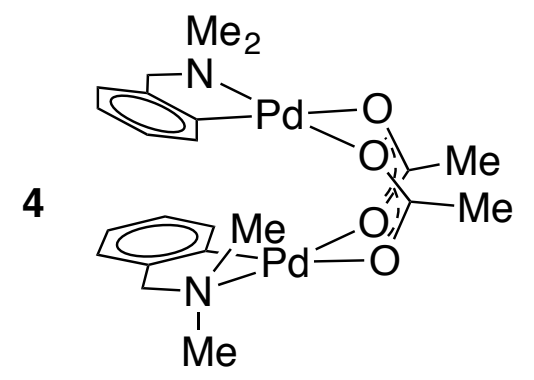


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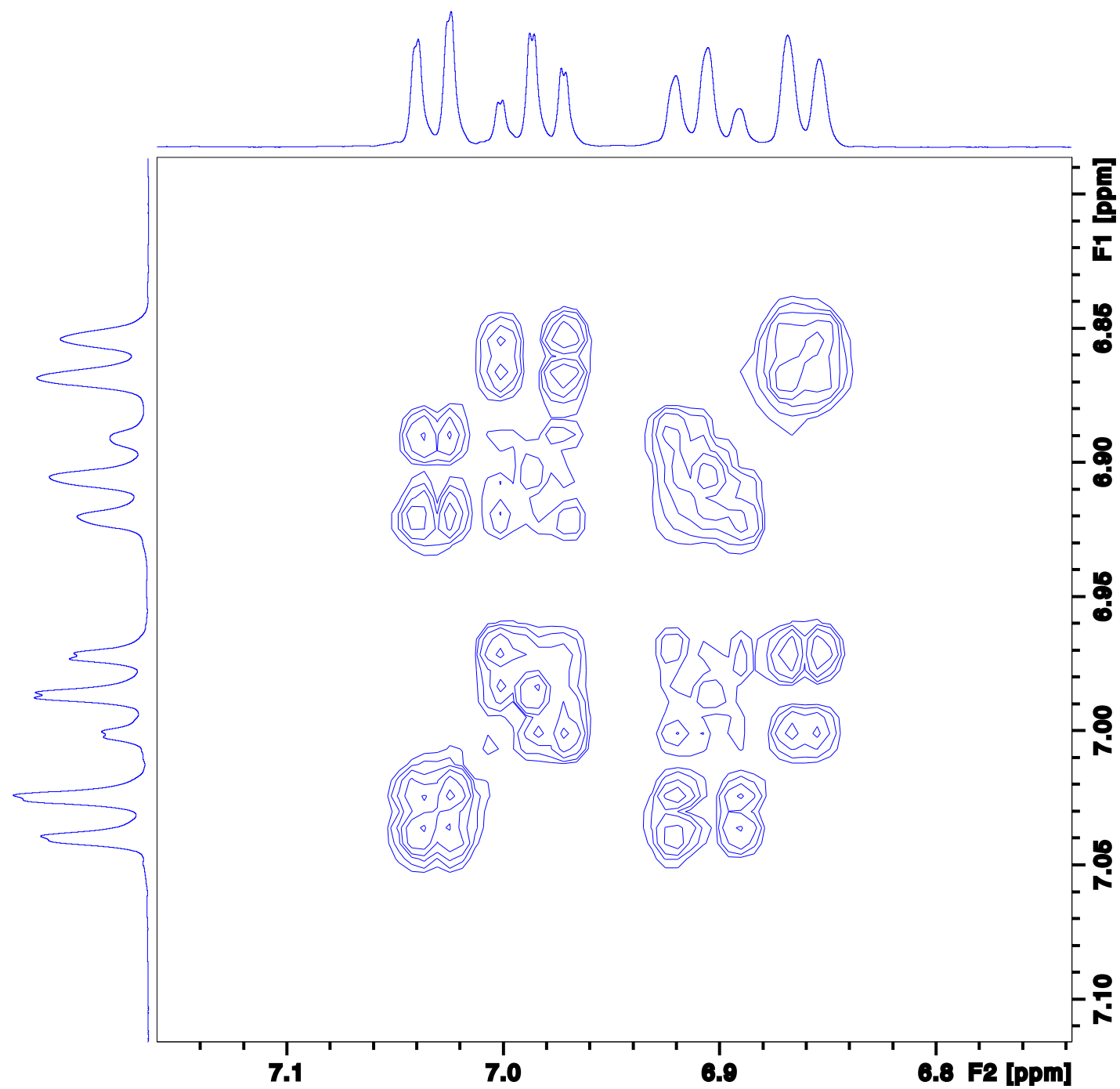
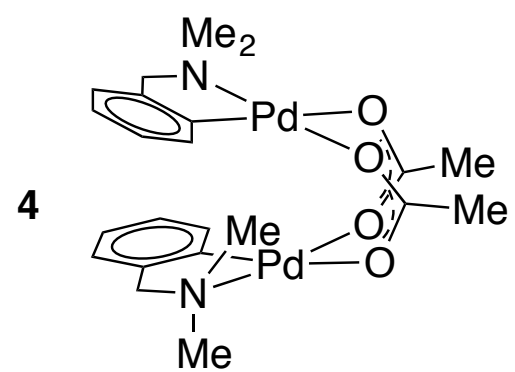
COSY
4 [Pd(dmba)(OAc)]₂



COSY aromatic region

4 [Pd(dmba)(OAc)]₂

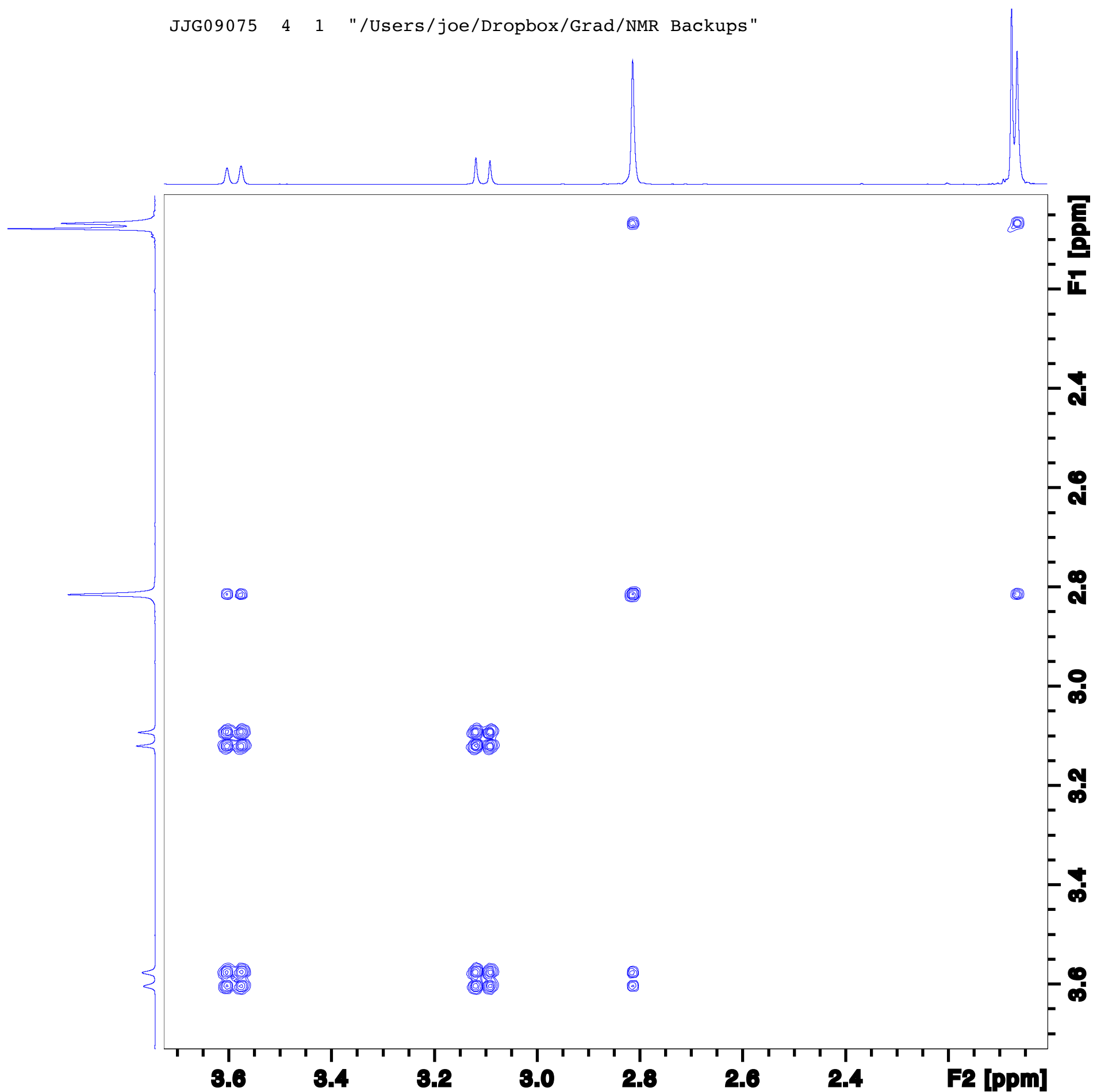
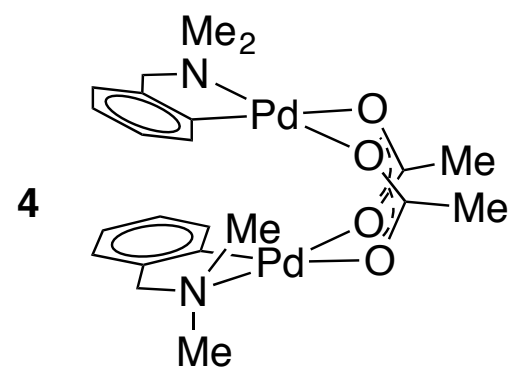
JJG09075 4 1 "/Users/joe/Dropbox/Grad/NMR Backups"



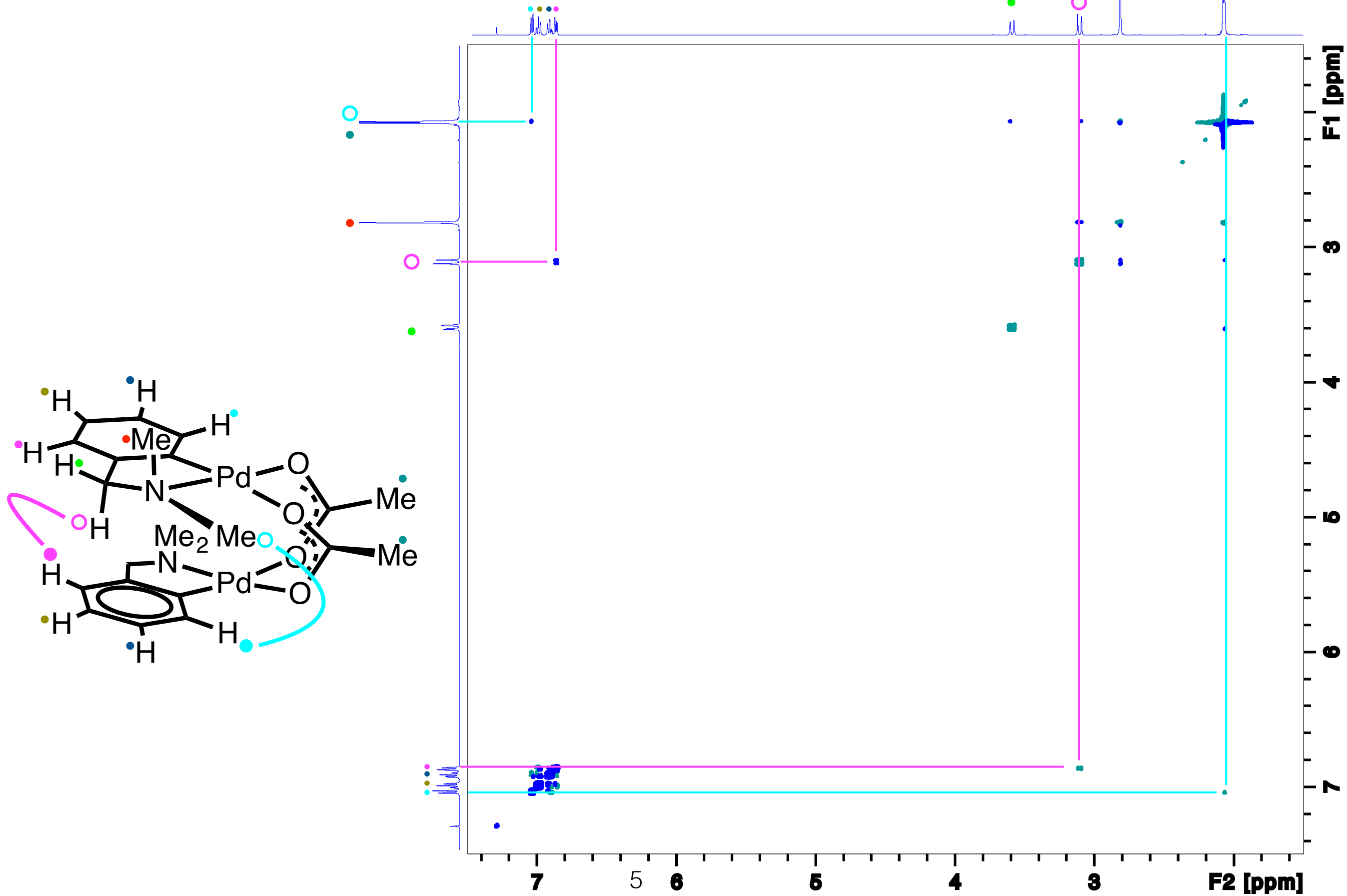
COSY aliphatic region

JJG09075 4 1 "/Users/joe/Dropbox/Grad/NMR Backups"

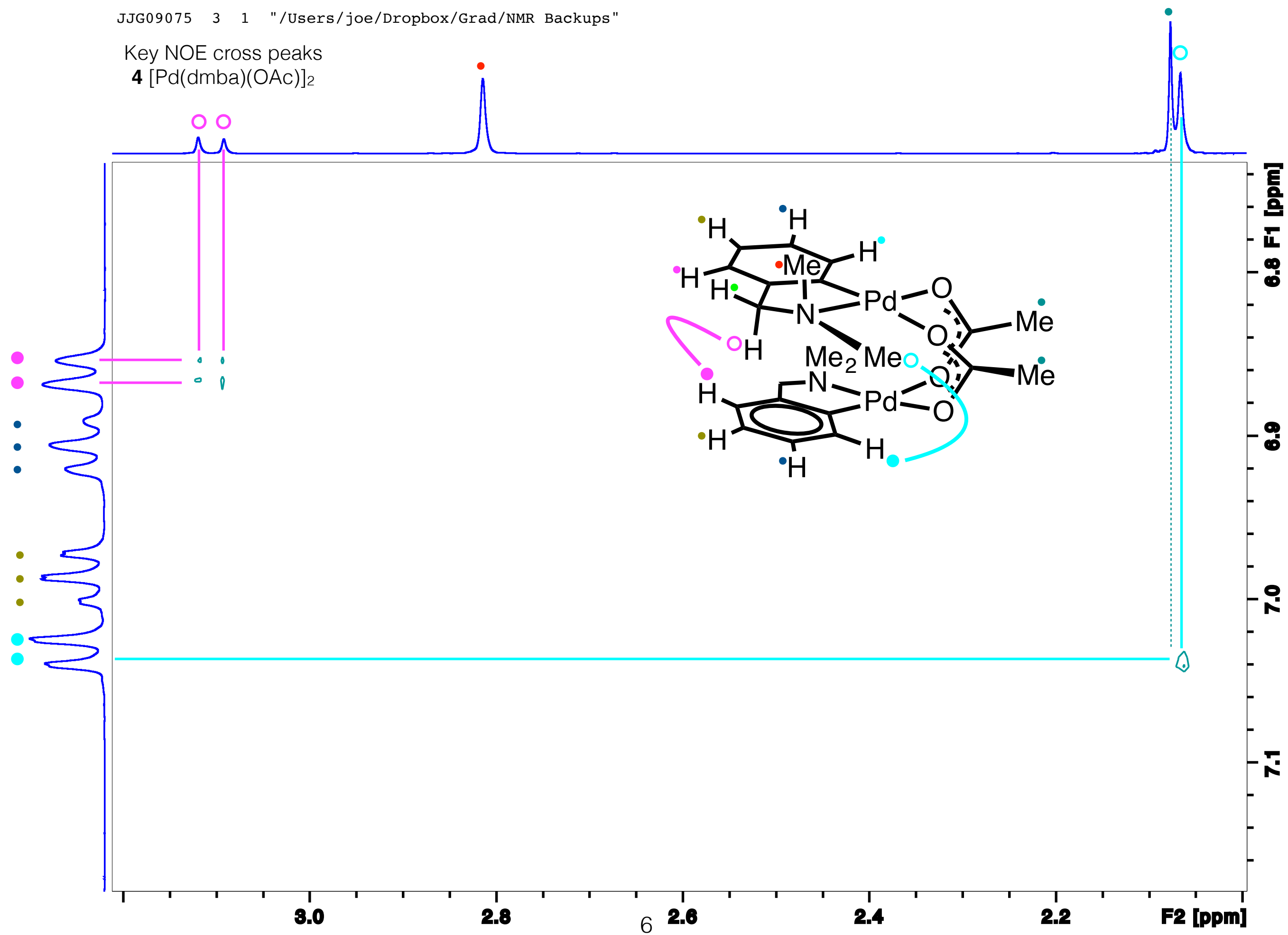
4 [Pd(dmba)(OAc)]₂



NOESY
4 [Pd(dmba)(OAc)]₂

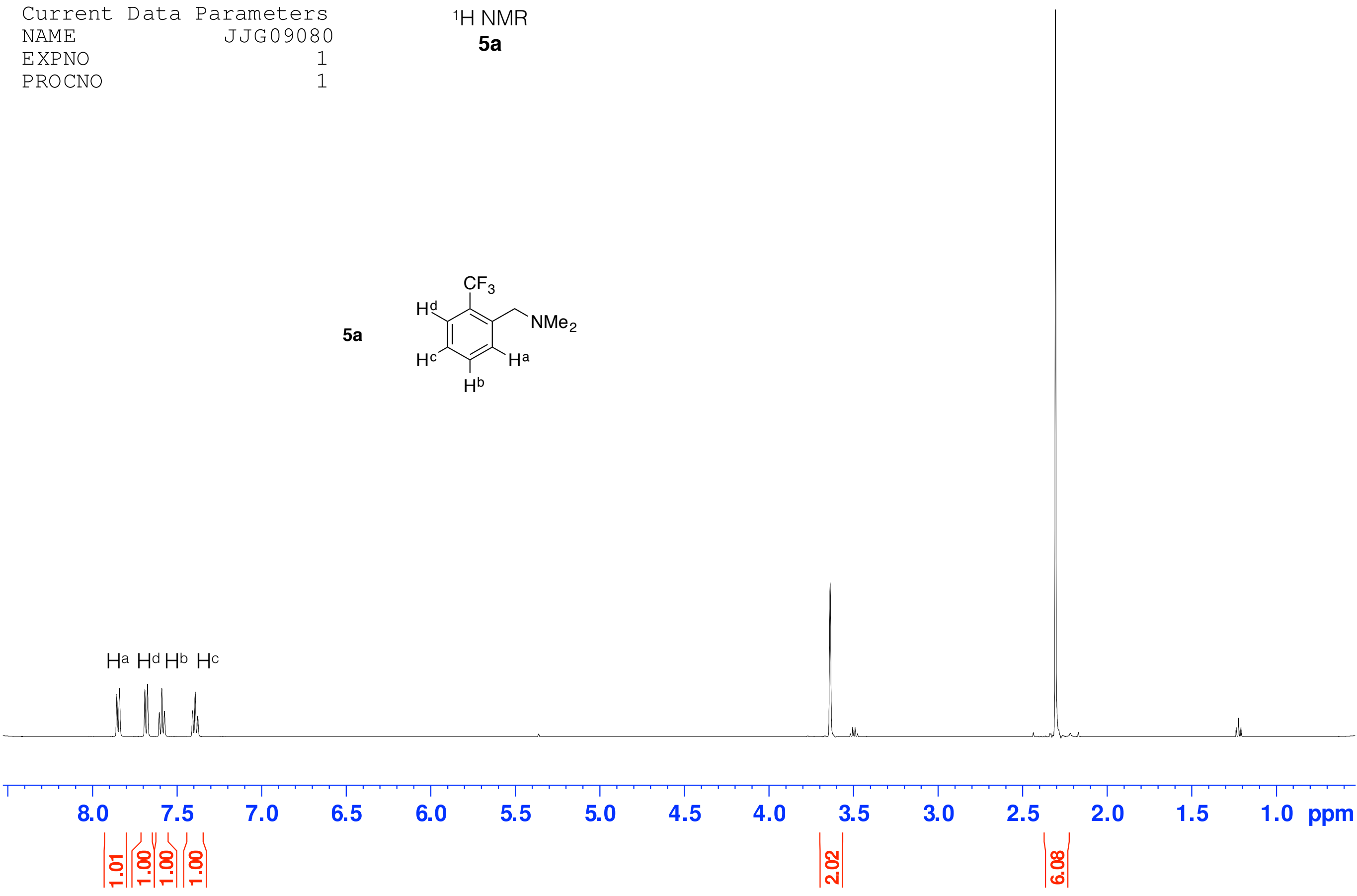
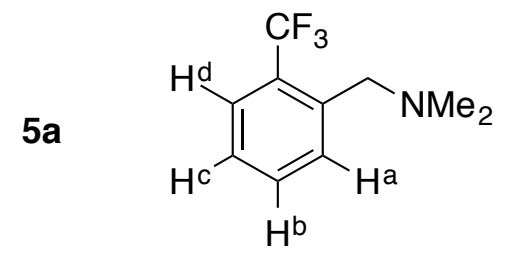


Key NOE cross peaks
4 [Pd(dmba)(OAc)]₂



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EXPNO 1
PROCNO 1

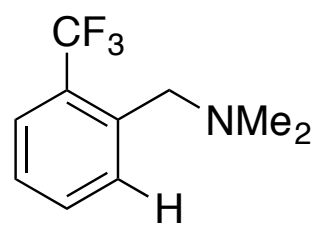
¹H NMR
5a



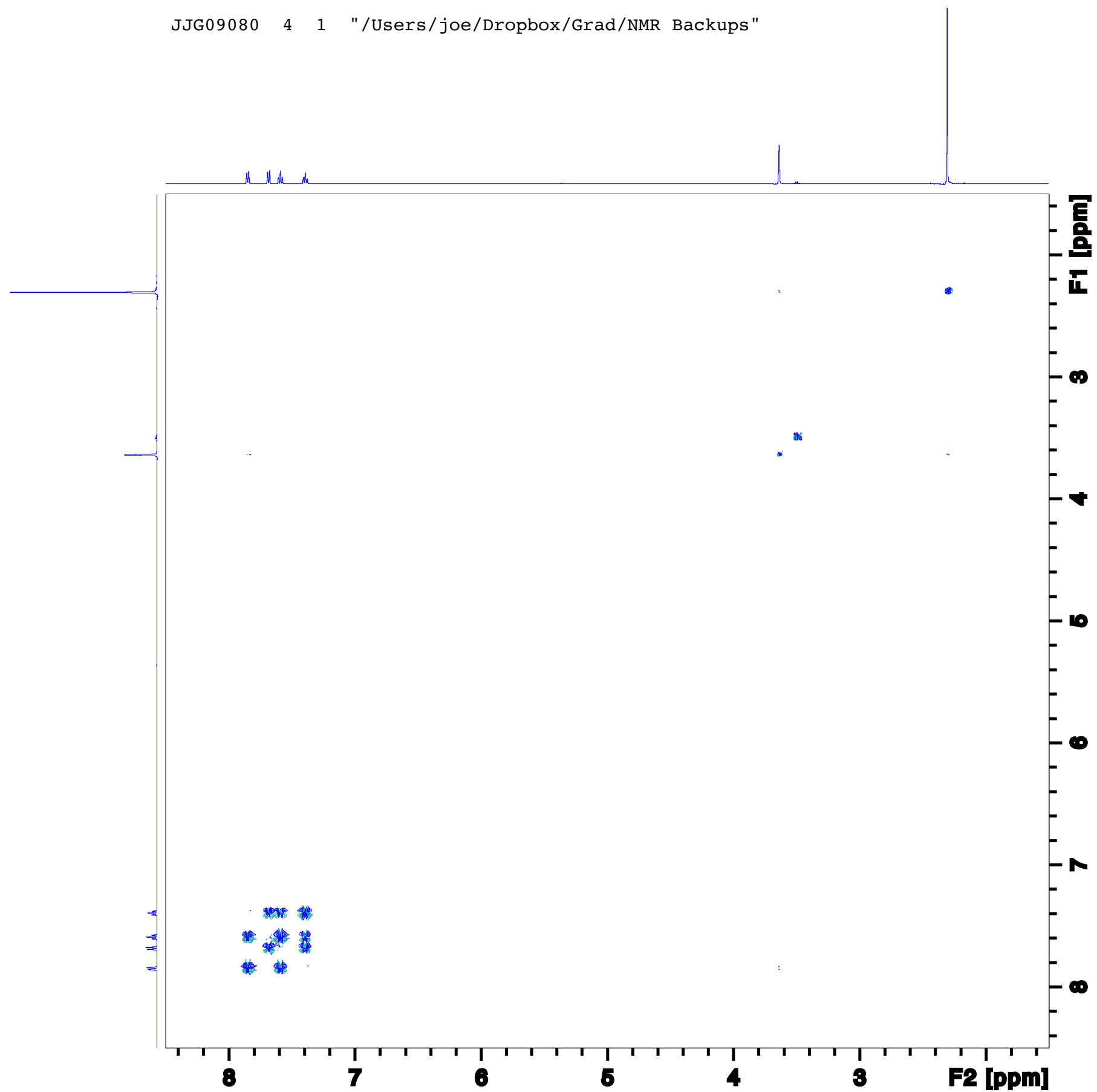
COSY

5a

JJG09080 4 1 "/Users/joe/Dropbox/Grad/NMR Backups"

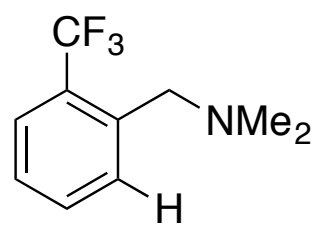


5a



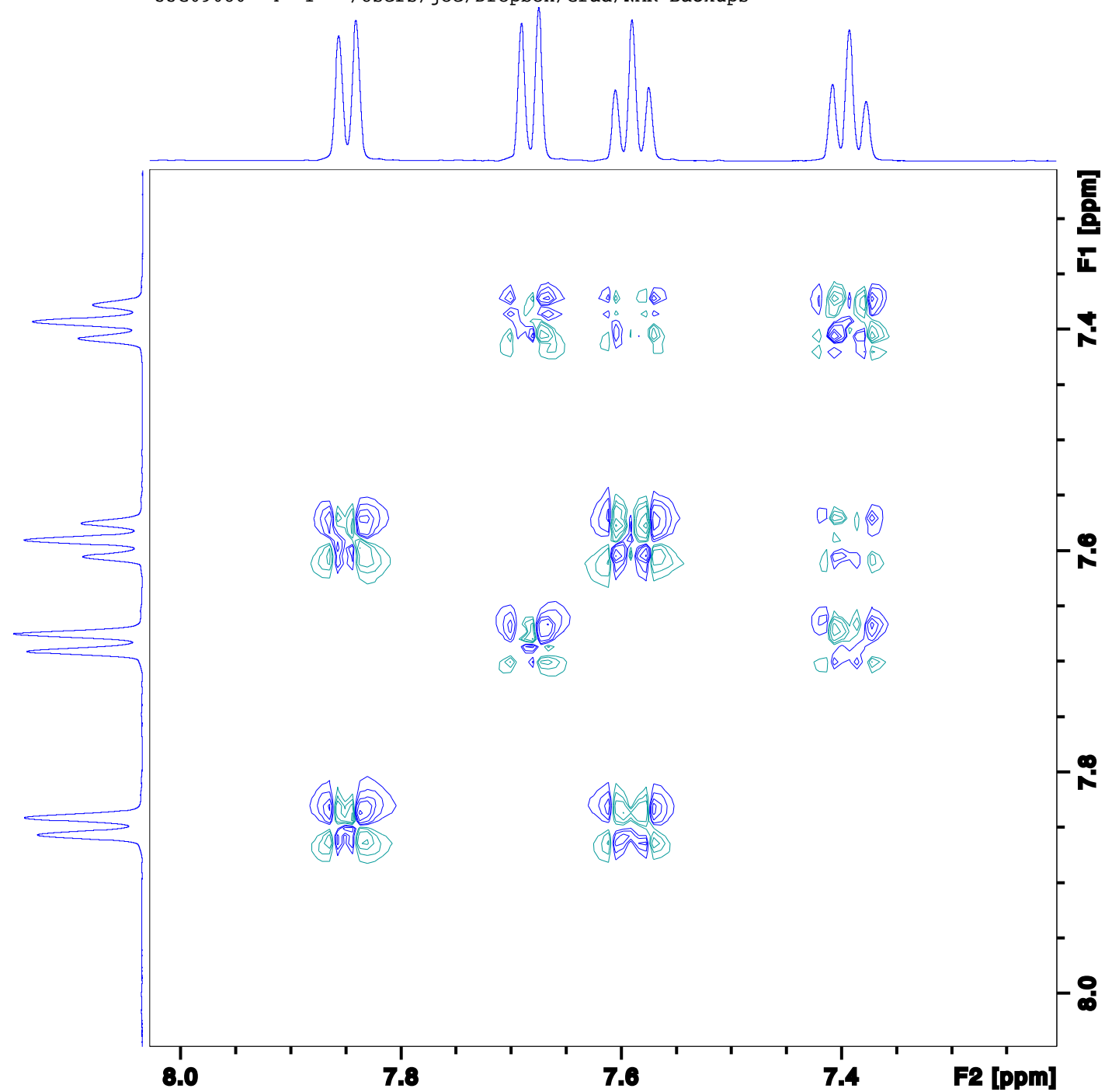
COSY aromatic

5a

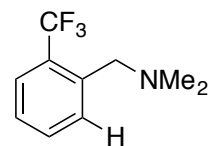


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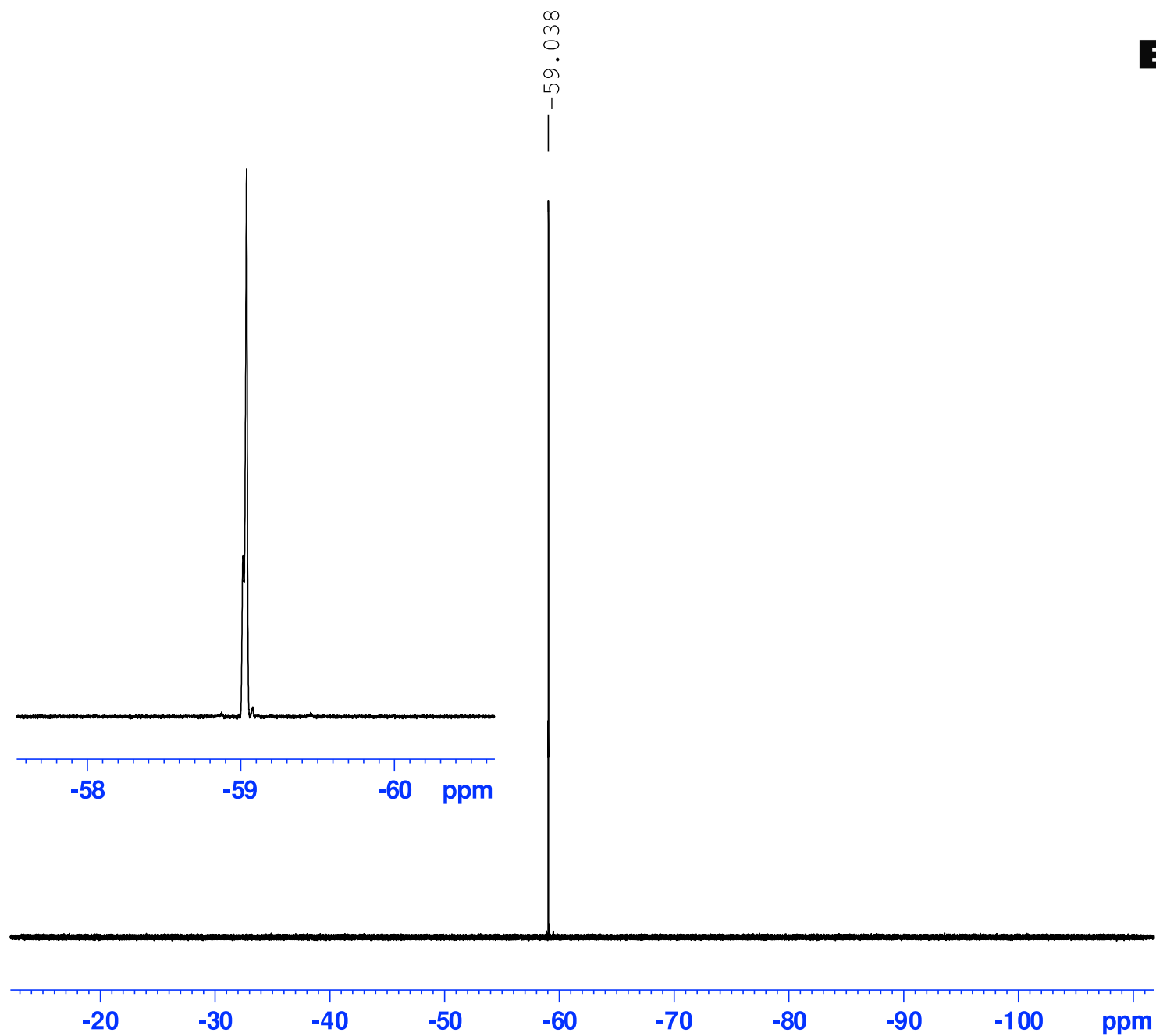
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¹⁹F NMR
5a



5a



Current Data Parameters
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EXPNO 2
PROCNO 1

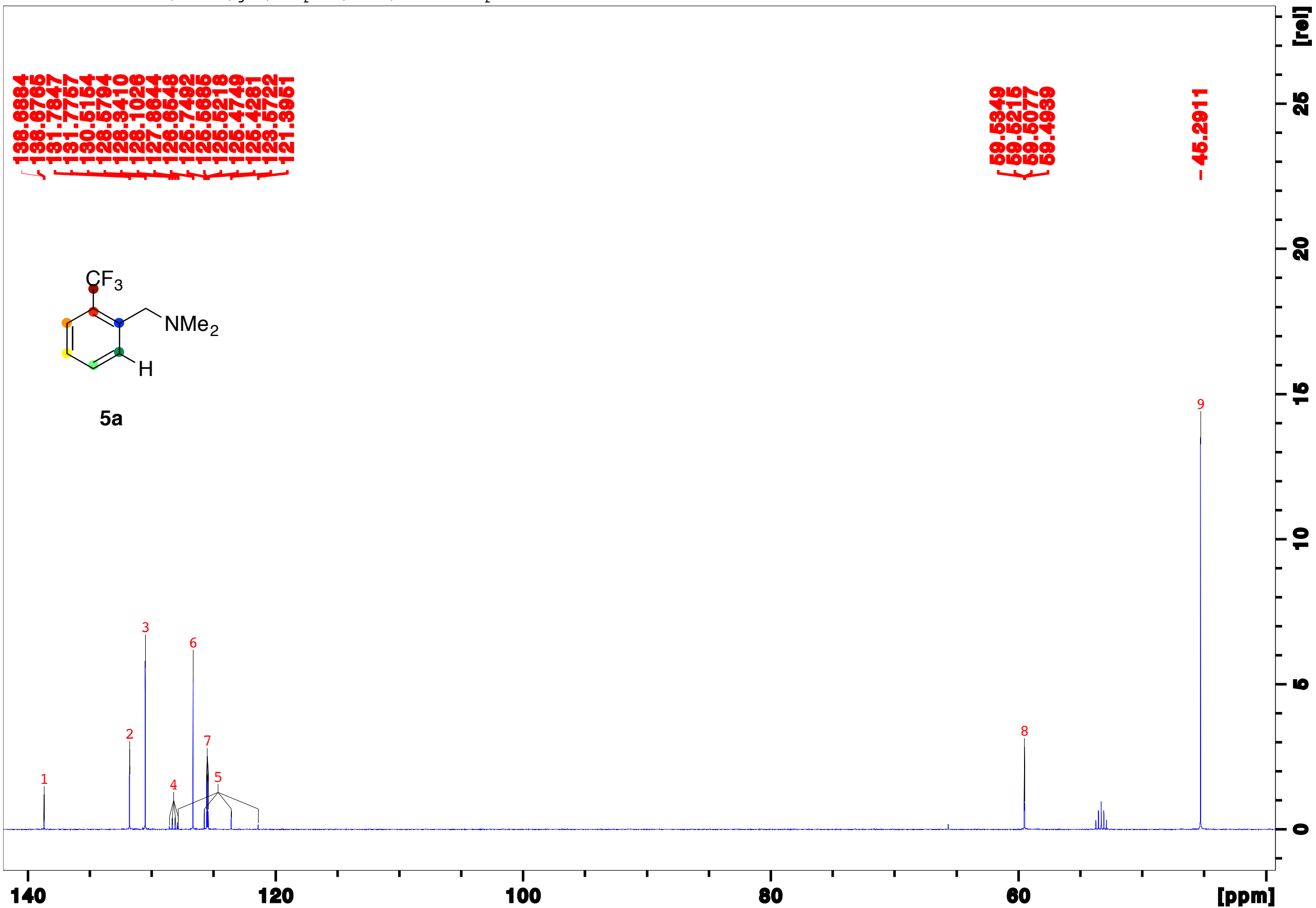
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Date_ 20160916
Time 14.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 281244
SOLVENT CDCl3
NS 1
DS 0
SWH 46875.000 Hz
FIDRES 0.166670 Hz
AQ 2.9999361 sec
RG 435.42
DW 10.667 usec
DE 6.50 usec
TE 296.1 K
D1 3.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 470.3185714 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

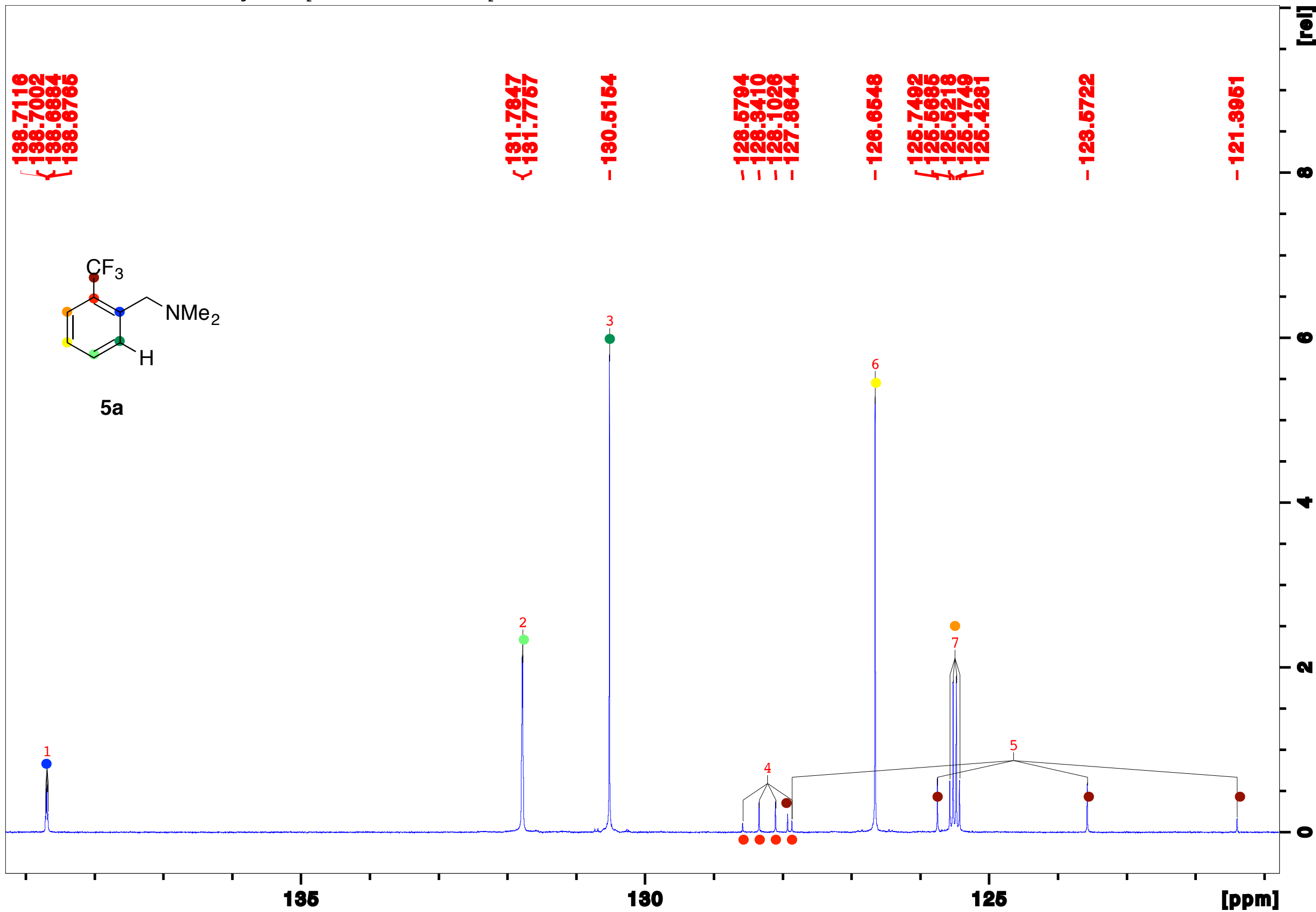
5a

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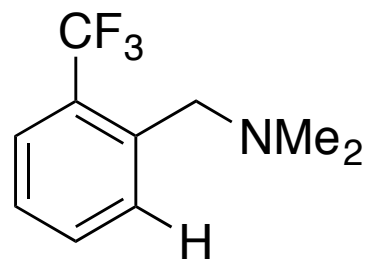
5a

JJG09080 2 1 "/Users/joe/Dropbox/Grad/NMR Backups"

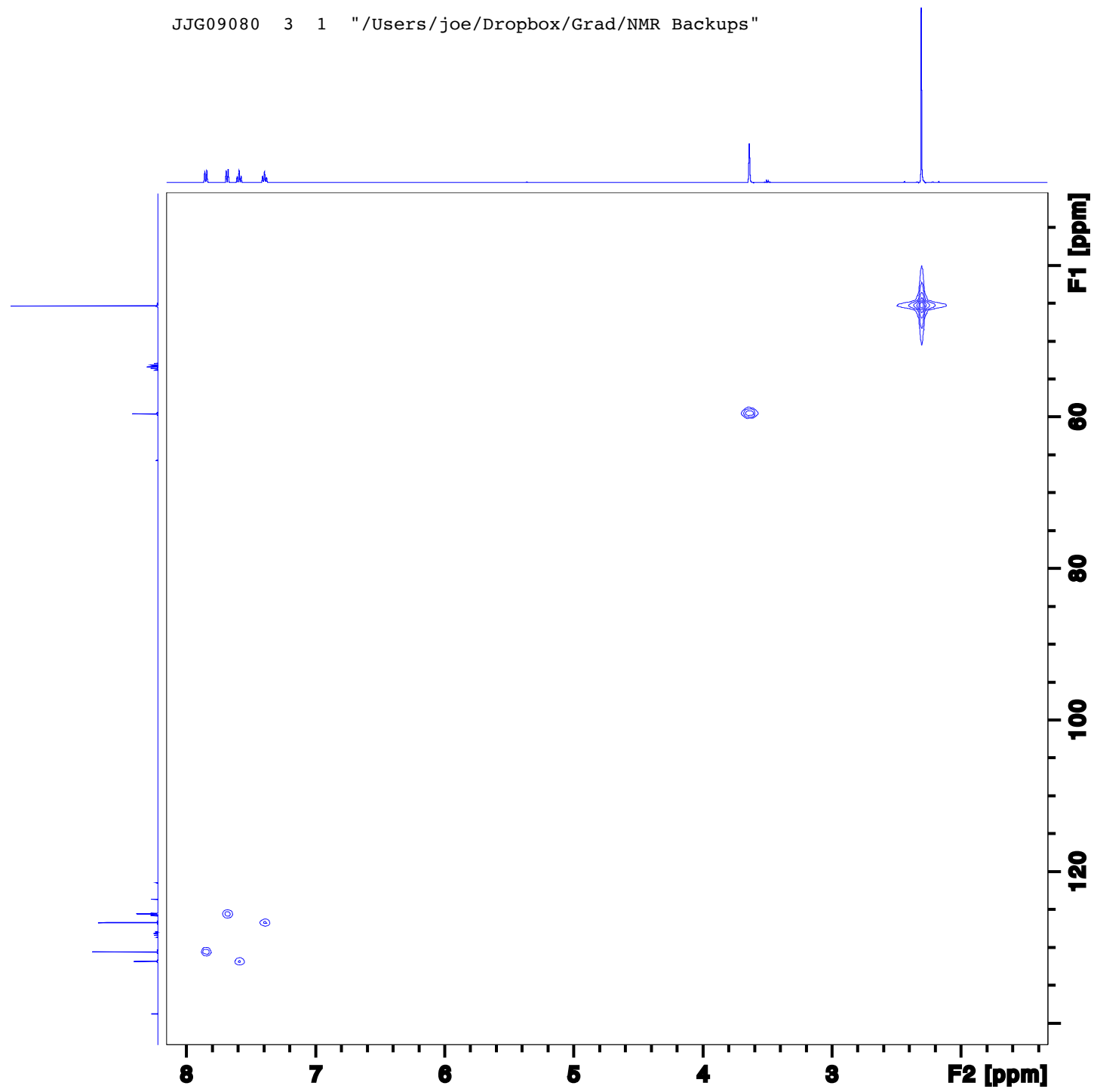


HMQC
5a

JJG09080 3 1 "/Users/joe/Dropbox/Grad/NMR Backups"

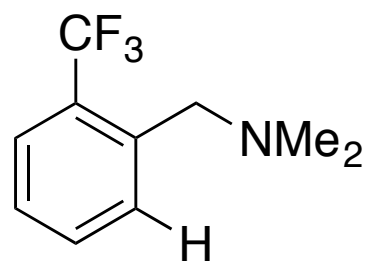


5a

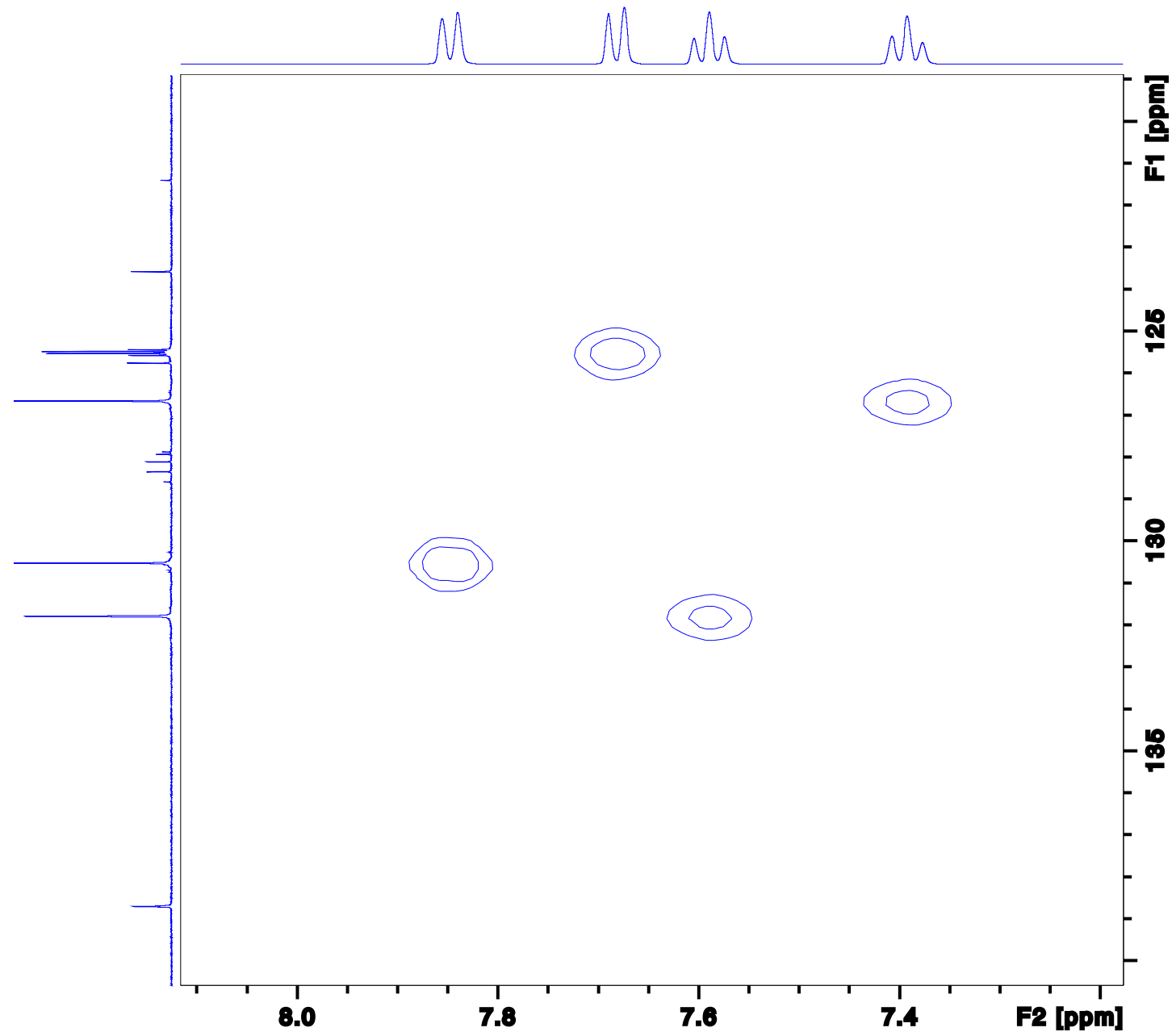


HMQC aromatic
5a

JJG09080 3 1 "/Users/joe/Dropbox/Grad/NMR Backups"



5a



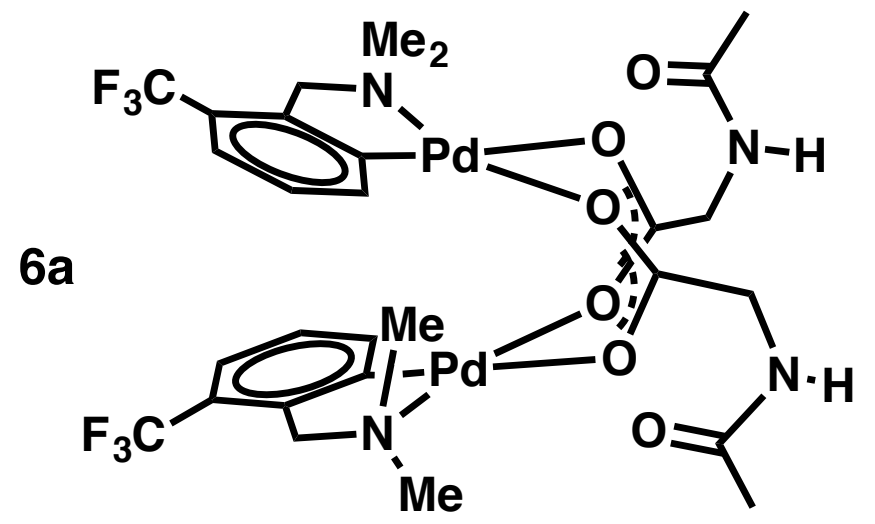
6a [Pd(o-CF₃-dmba)(NAc-Gly)]₂ 5 mM, more dilute sample shows separate NMe and Ac peaks

7.376
7.361
7.232
7.218
7.118
7.103
7.087

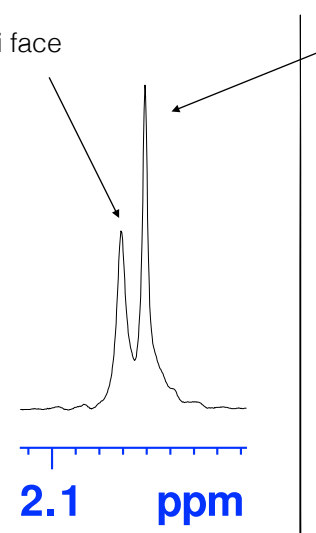
6.375 Current Data Parameters
NAME JJG09068
EXPNO 7
PROCNO 1

4.071
4.059
4.035
4.023
3.962
3.951
3.926
3.916
3.550
3.521
3.505
3.475

2.795
2.071
2.061



NMe toward pi face
acetyl Me



glycine methylenes

NMe away from pi face

benzylic methylenes

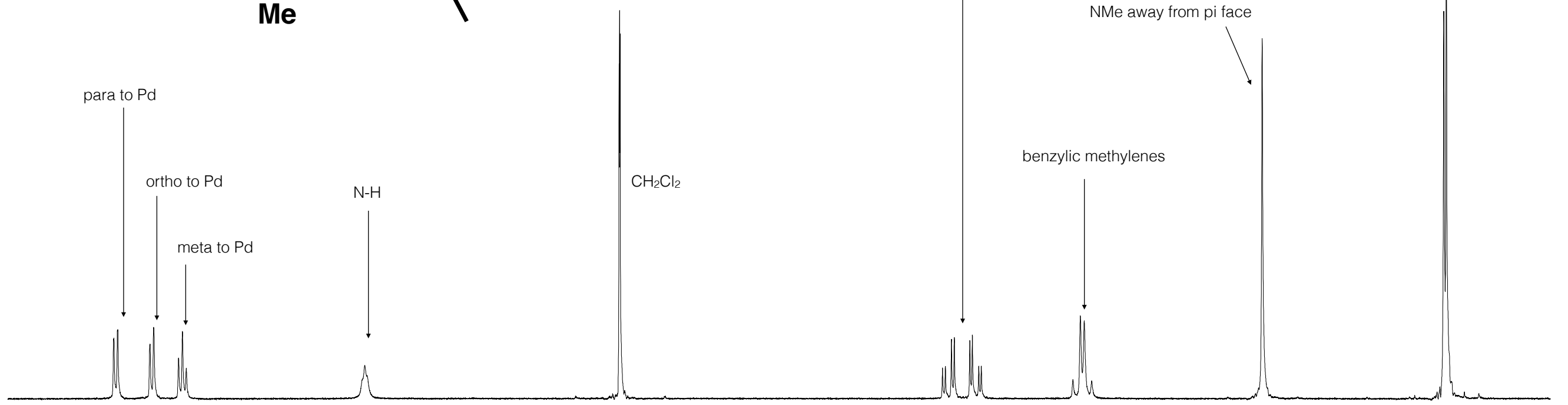
para to Pd

ortho to Pd

meta to Pd

N-H

CH₂Cl₂



7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm

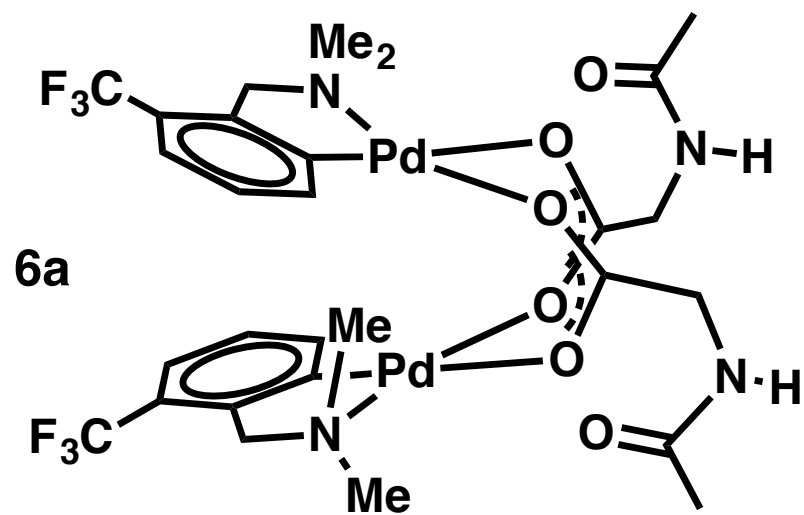
2.01 2.01 2.00 2.00 4.05 4.07 6.00 12.05

^1H [Pd(o-CF₃-dmba)(NAc-Gly)]₂ 30 mM

7.382
7.367
7.252
7.237
7.129
7.113
7.098
— 6.737

4.174
4.161
4.138
4.126
4.043
4.033
4.008
3.998
3.561
3.532
3.510
3.480
— 2.787
— 2.085

Current Data Parameters
NAME JJG06113
EXPNO 1
PROCNO 1



NMe toward pi face
overlapped with acetyl Me

NMe away from pi face

para to Pd

ortho to Pd

meta to Pd

N-H

glycine methylene

benzylic methylenes

7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm

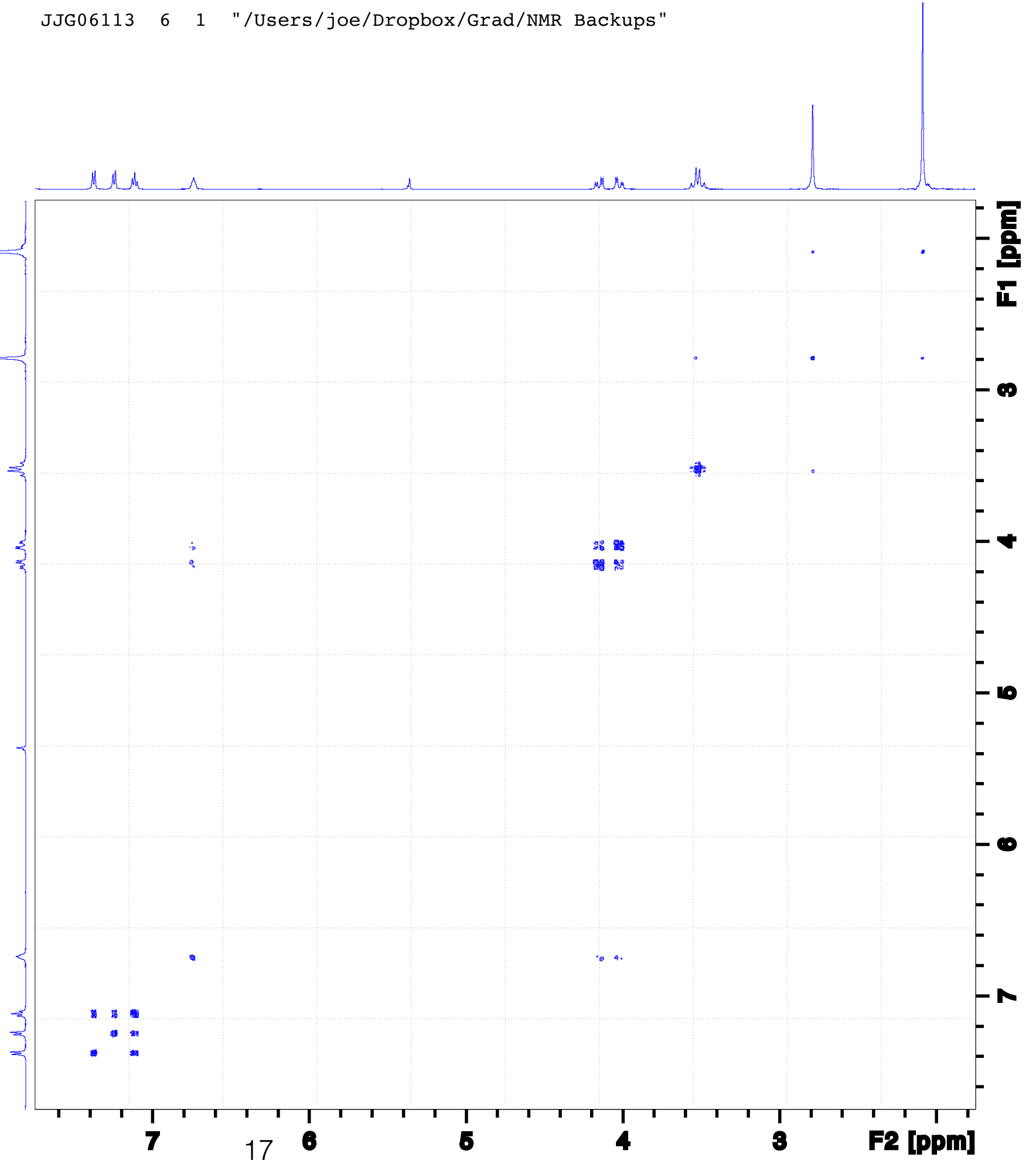
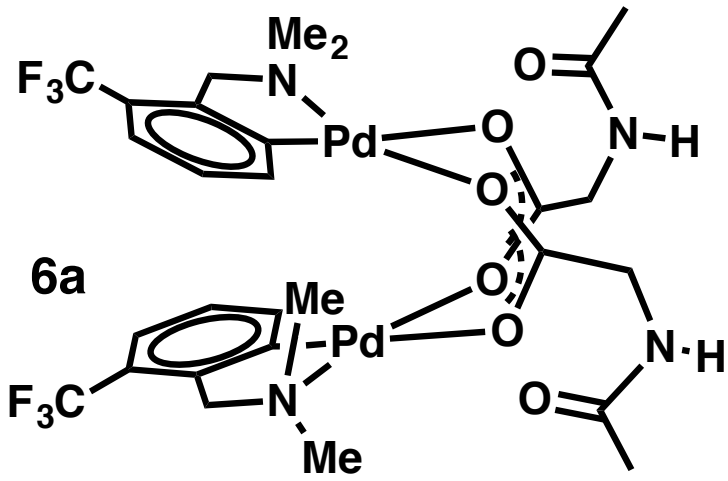
2.02
2.01
2.01
1.83

16

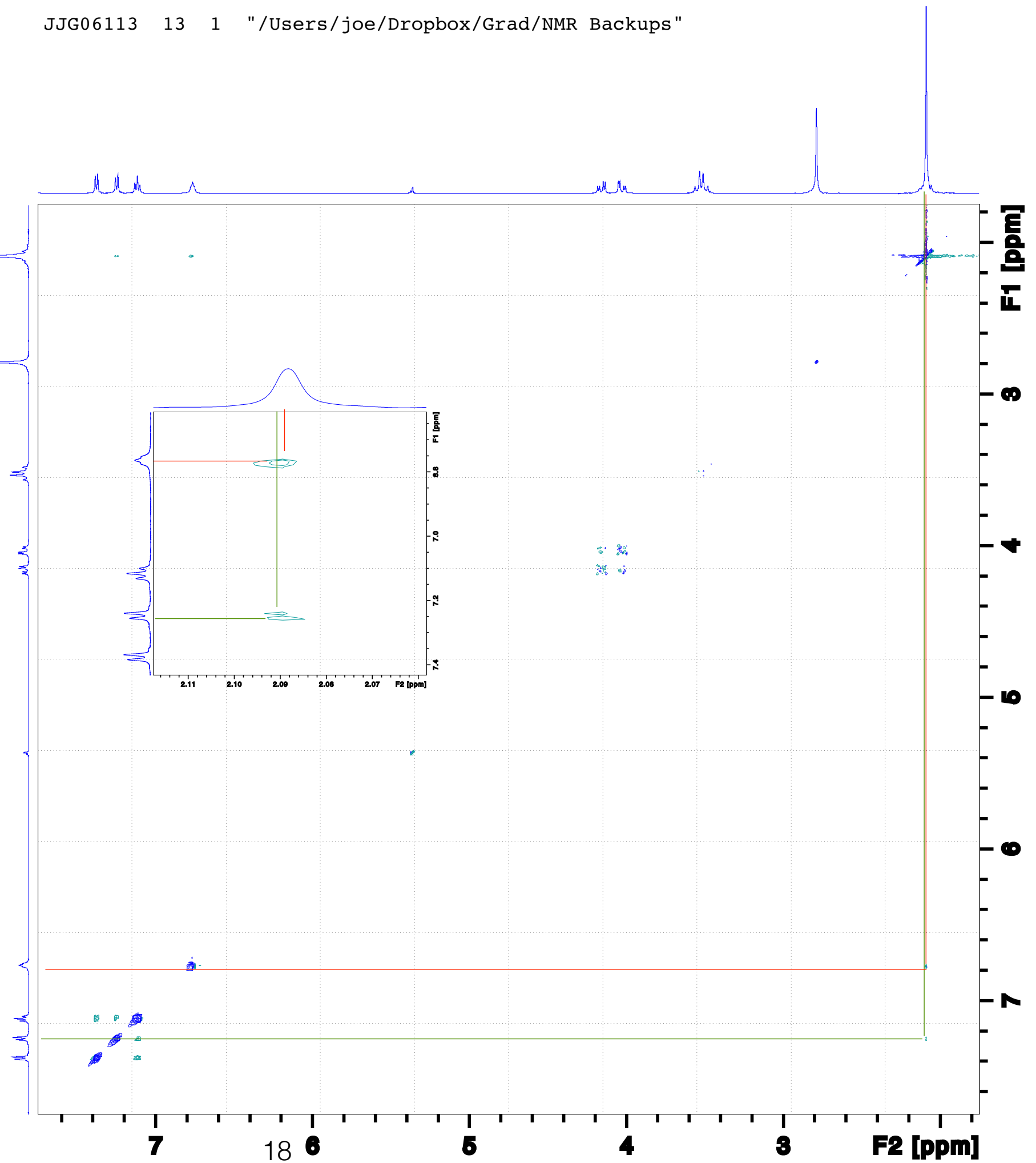
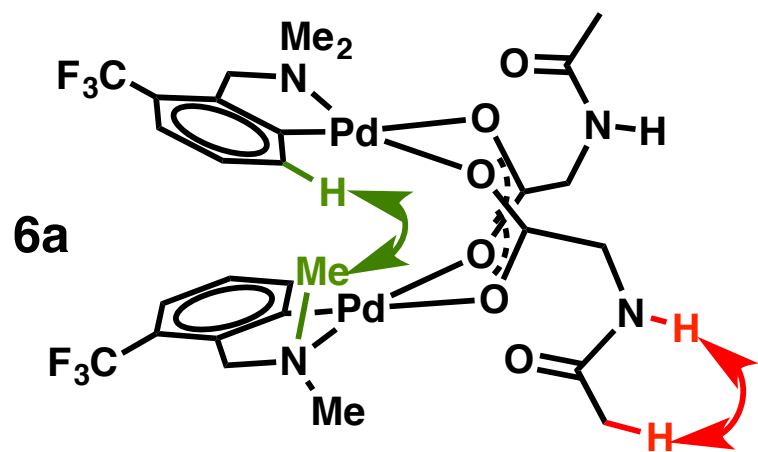
4.00
3.99
6.02
11.88

COSY

[Pd(o-CF₃-dmba)(NAc-Gly)]₂

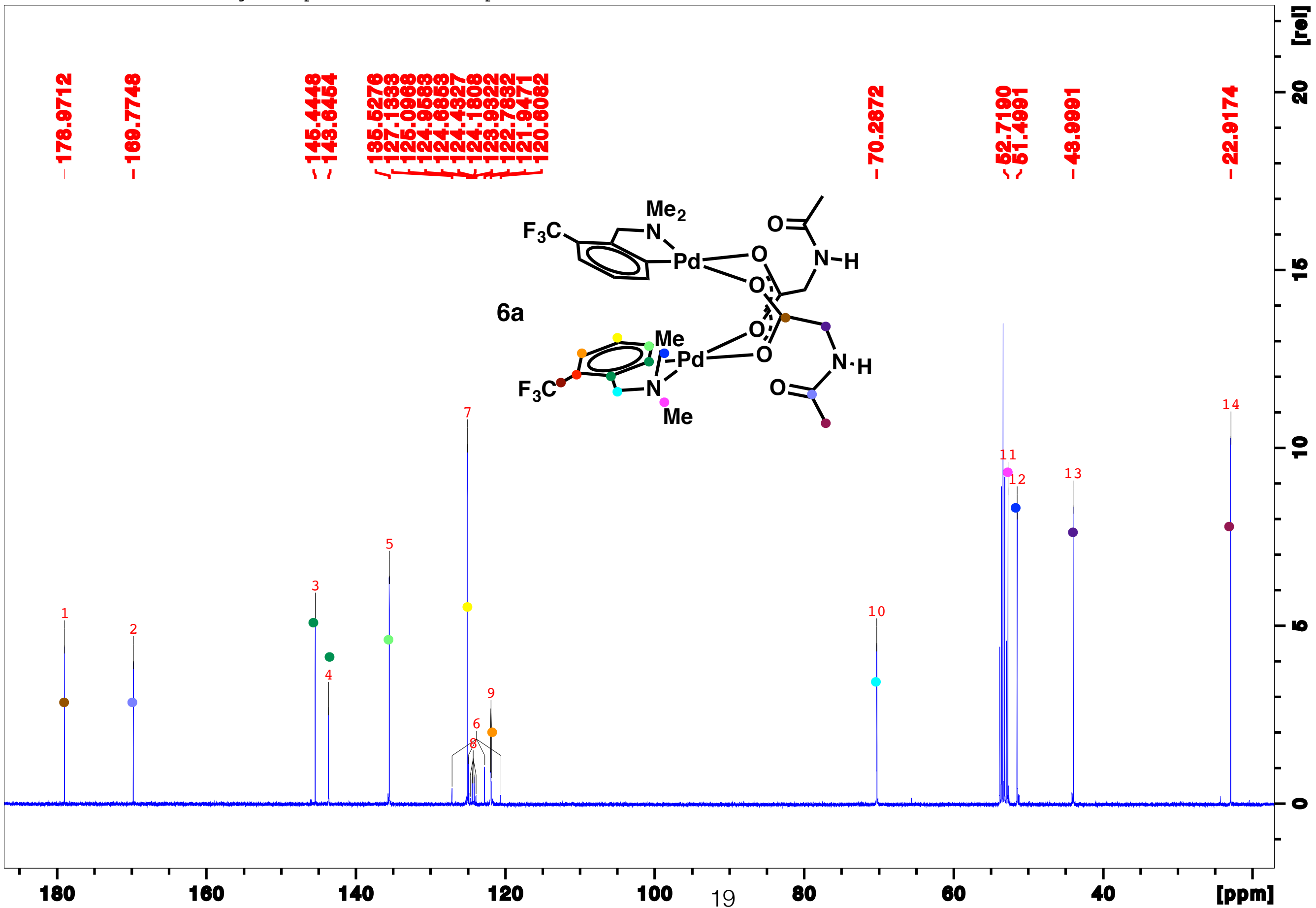


NOESY

 $[\text{Pd}(\text{o-CF}_3\text{-dmba})(\text{NAc-Gly})]_2$ 

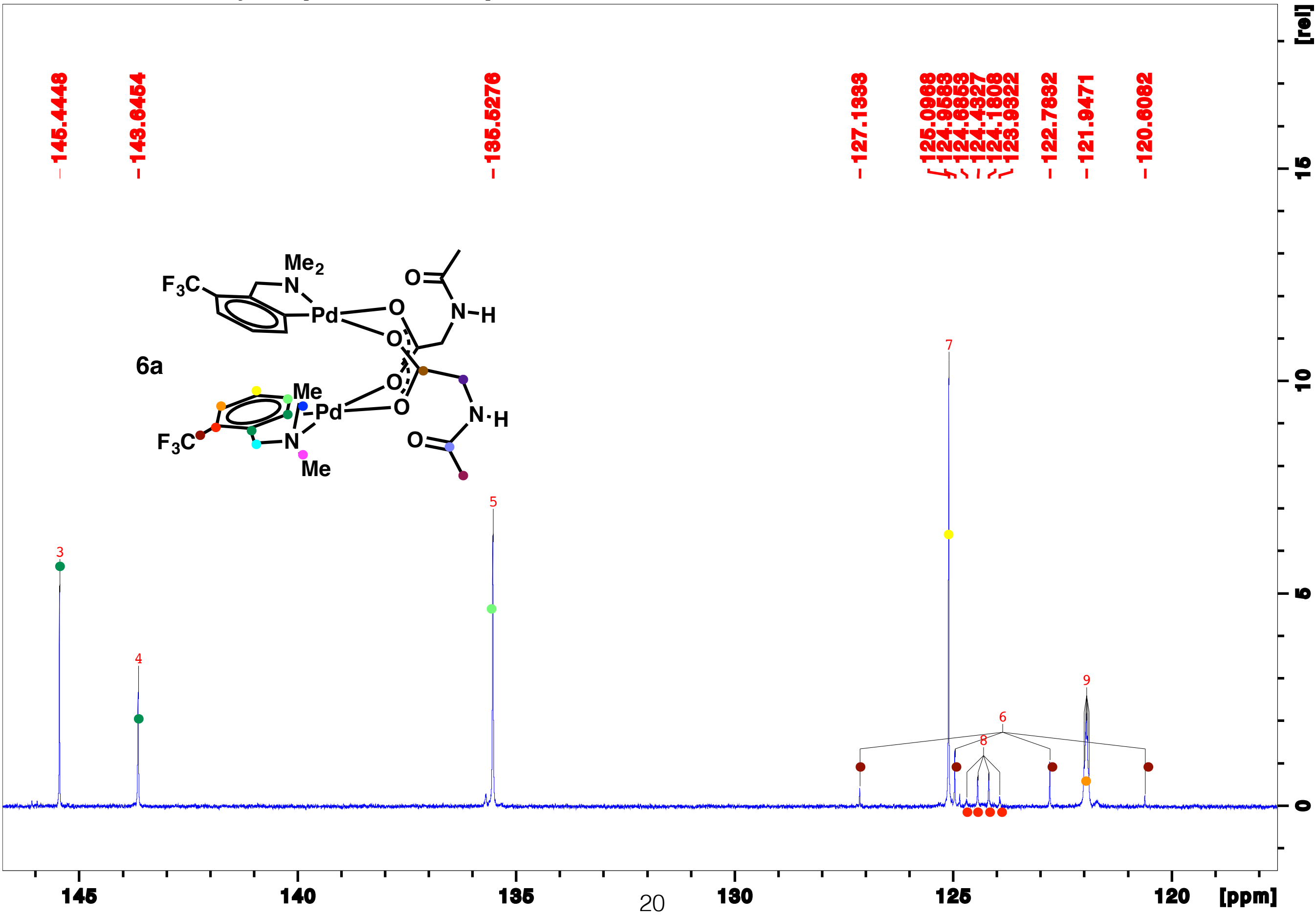
^{13}C [Pd(o-CF₃-dmba)(NAc-Gly)]₂

JJG06113 9 1 "/Users/joe/Dropbox/Grad/NMR Backups"



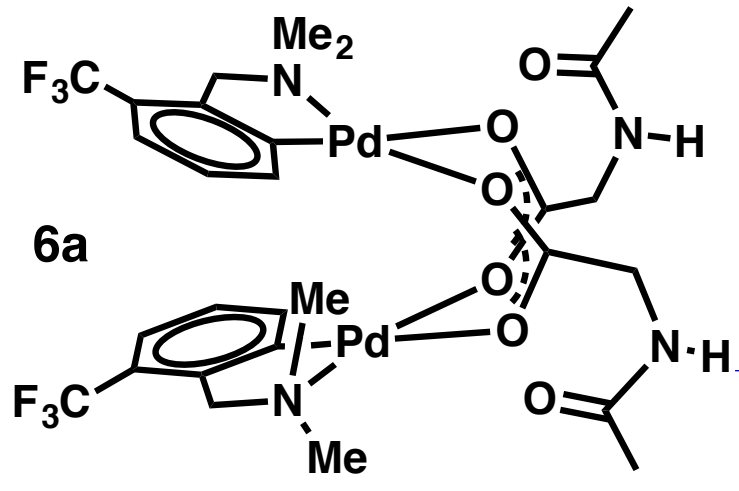
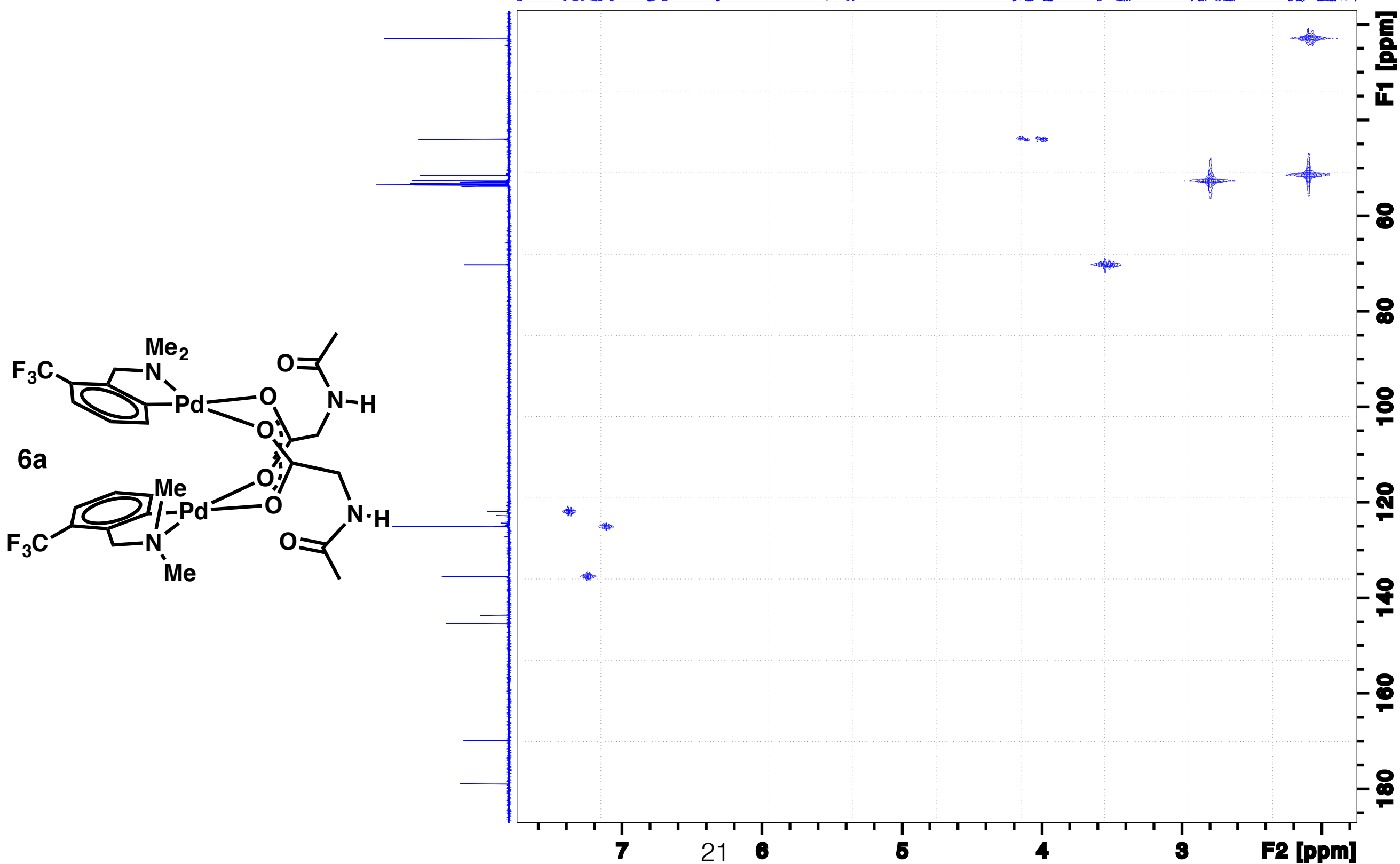
^{13}C aromatic region $[\text{Pd}(\text{o-CF}_3\text{-dmba})(\text{NAc-Gly})]_2$

JJG06113 9 1 "/Users/joe/Dropbox/Grad/NMR Backups"



HMQC

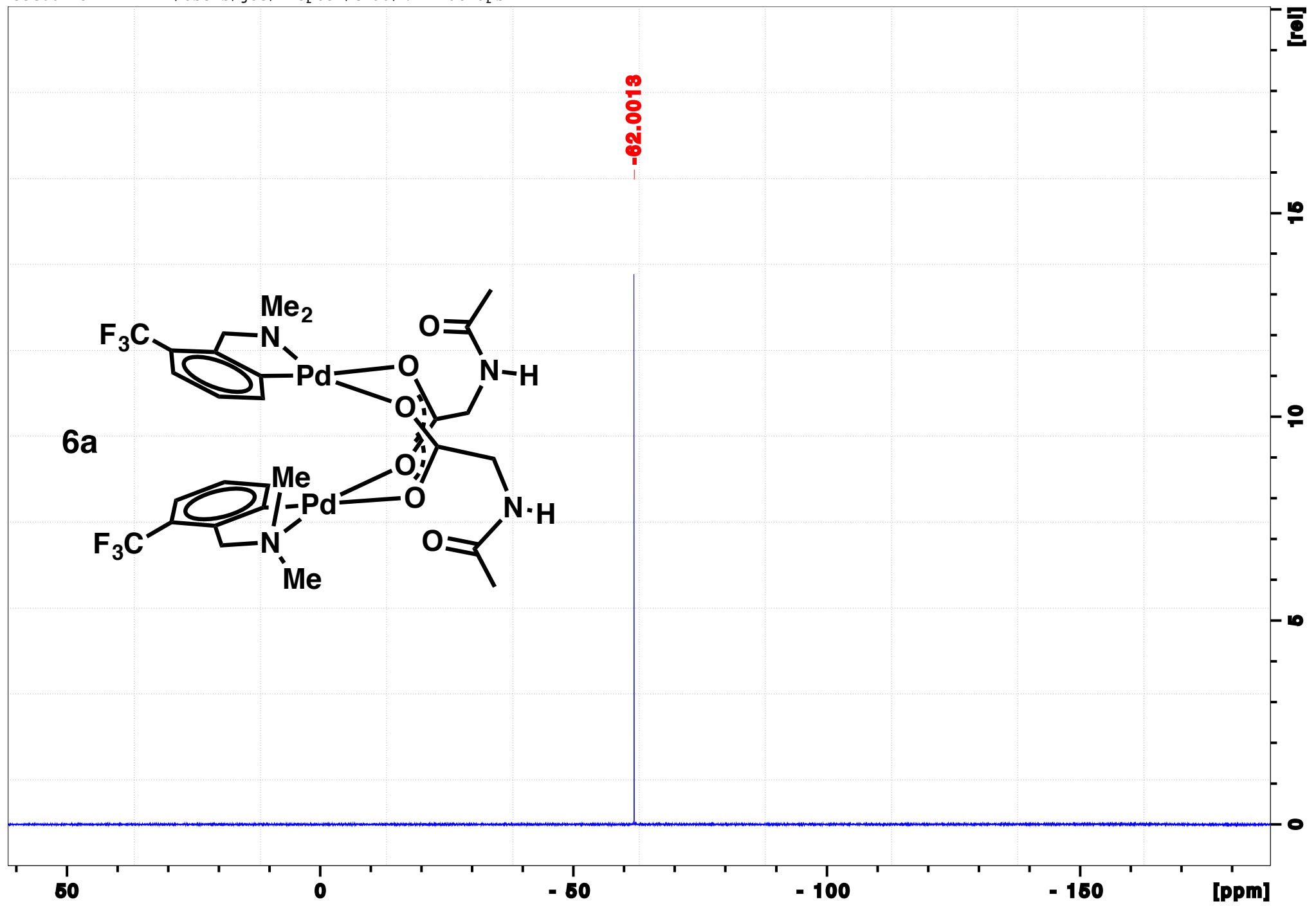
JJG06113 10 1 "/Users/joe/Dropbox/Grad/NMR Backups"



19F



JJG06113 2 1 "/Users/joe/Dropbox/Grad/NMR Backups"



^1H **6b**

7.251
7.236
7.179
7.164
7.118
7.102
7.085
7.069

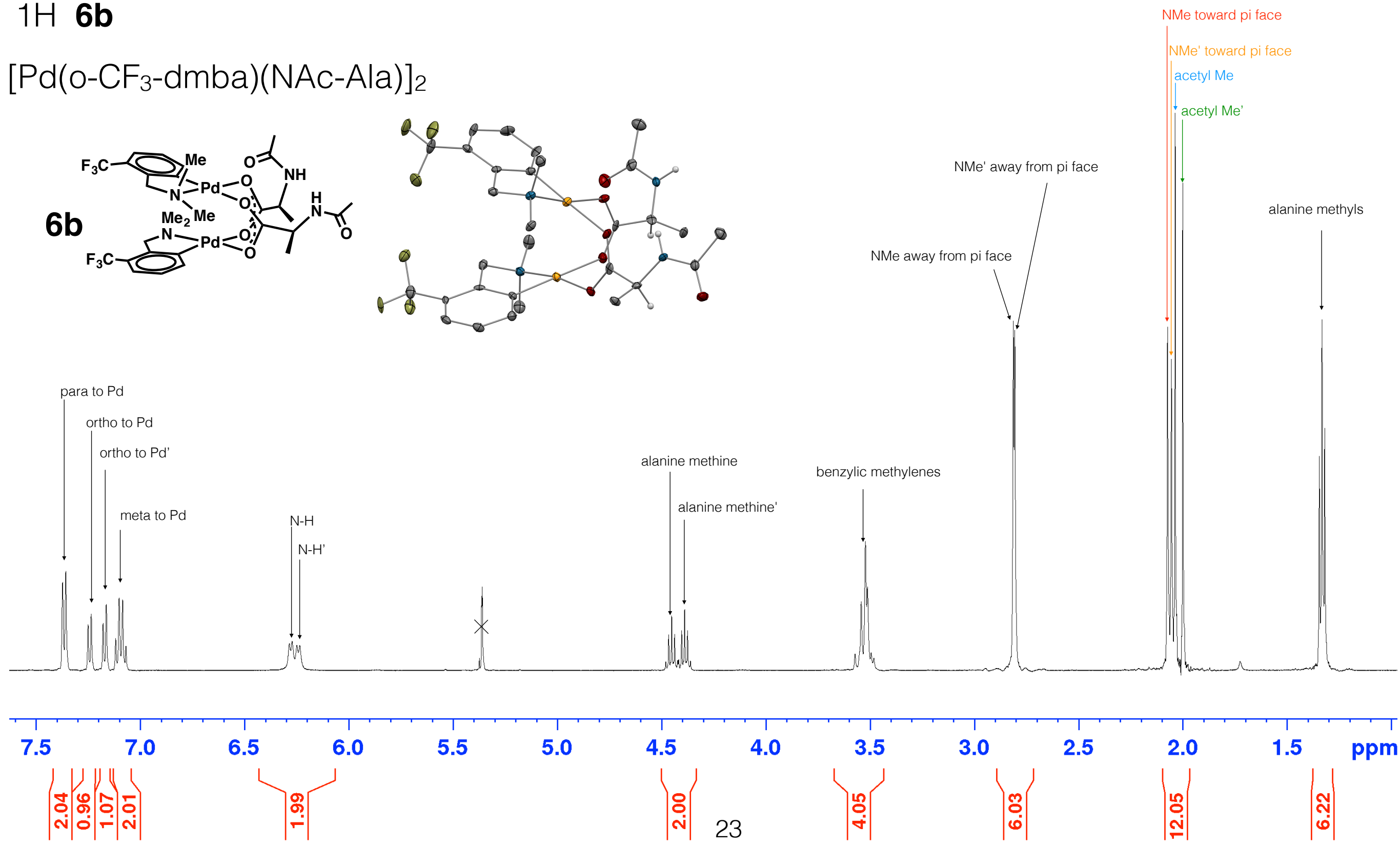
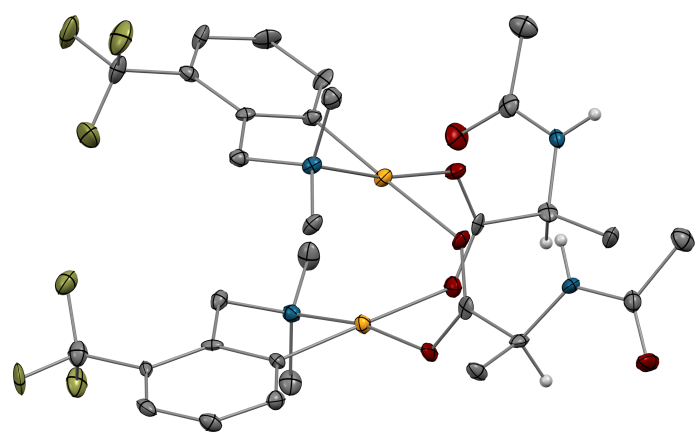
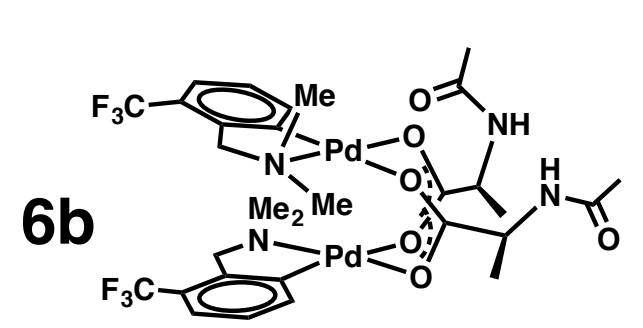
6.285
6.272
6.249
6.235

4.480
4.466
4.452
4.444
4.437
4.423
4.418
4.404
4.390
4.381
4.375
4.361
3.572
3.543
3.523
3.512
3.495
3.482

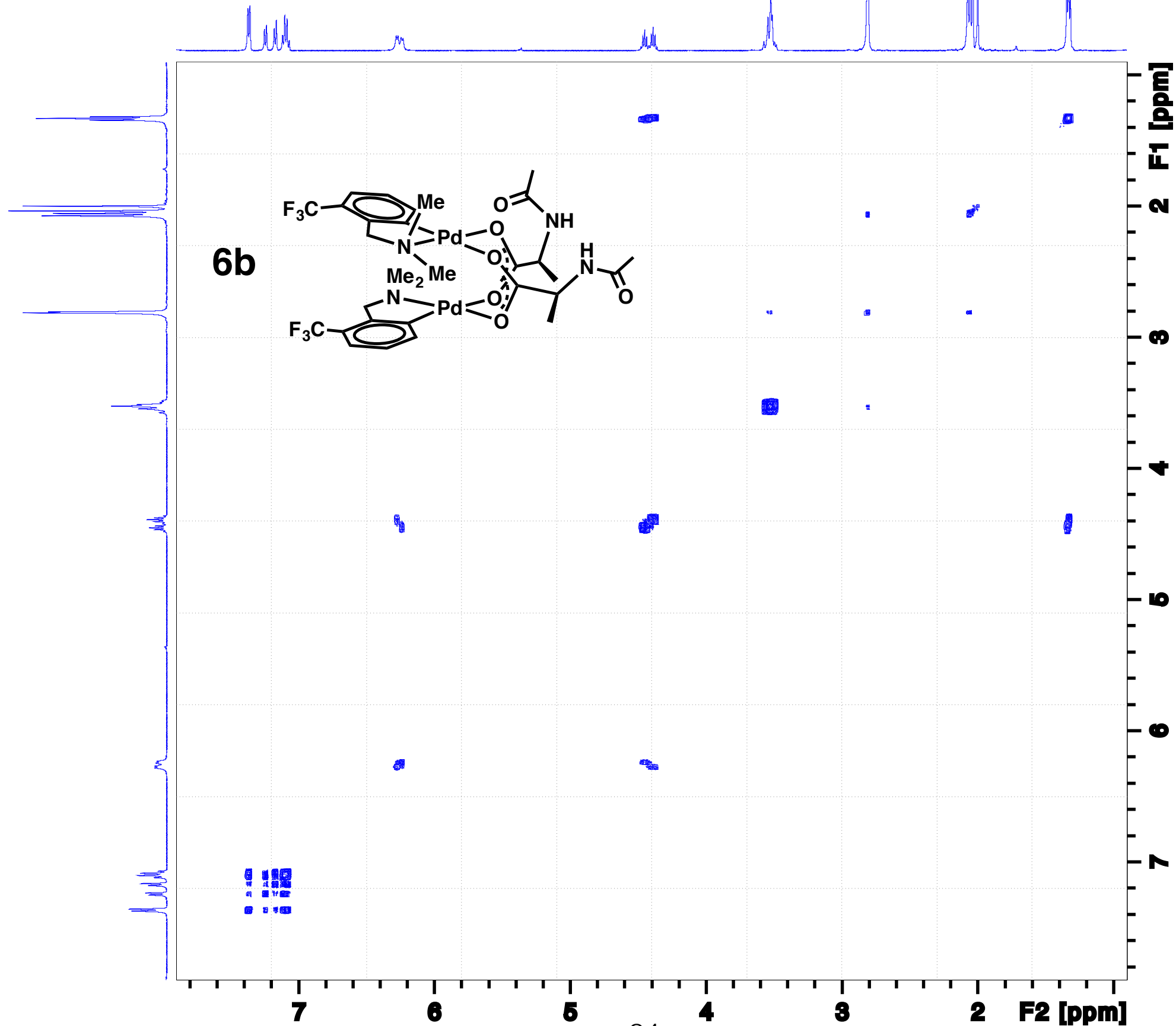
2.813
2.806

2.073
2.055
2.037
2.000

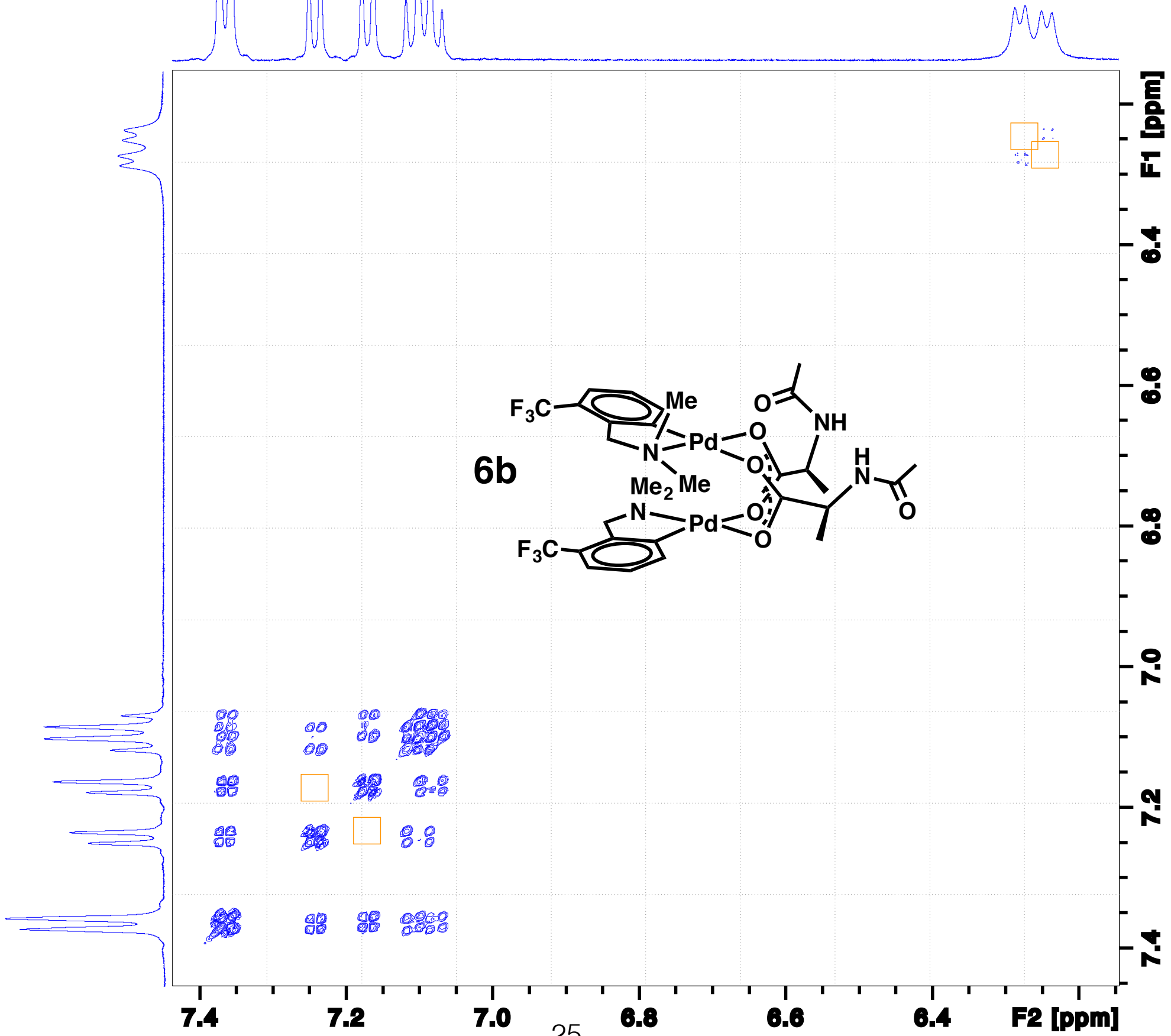
1.345
1.333
1.319



COSY Full



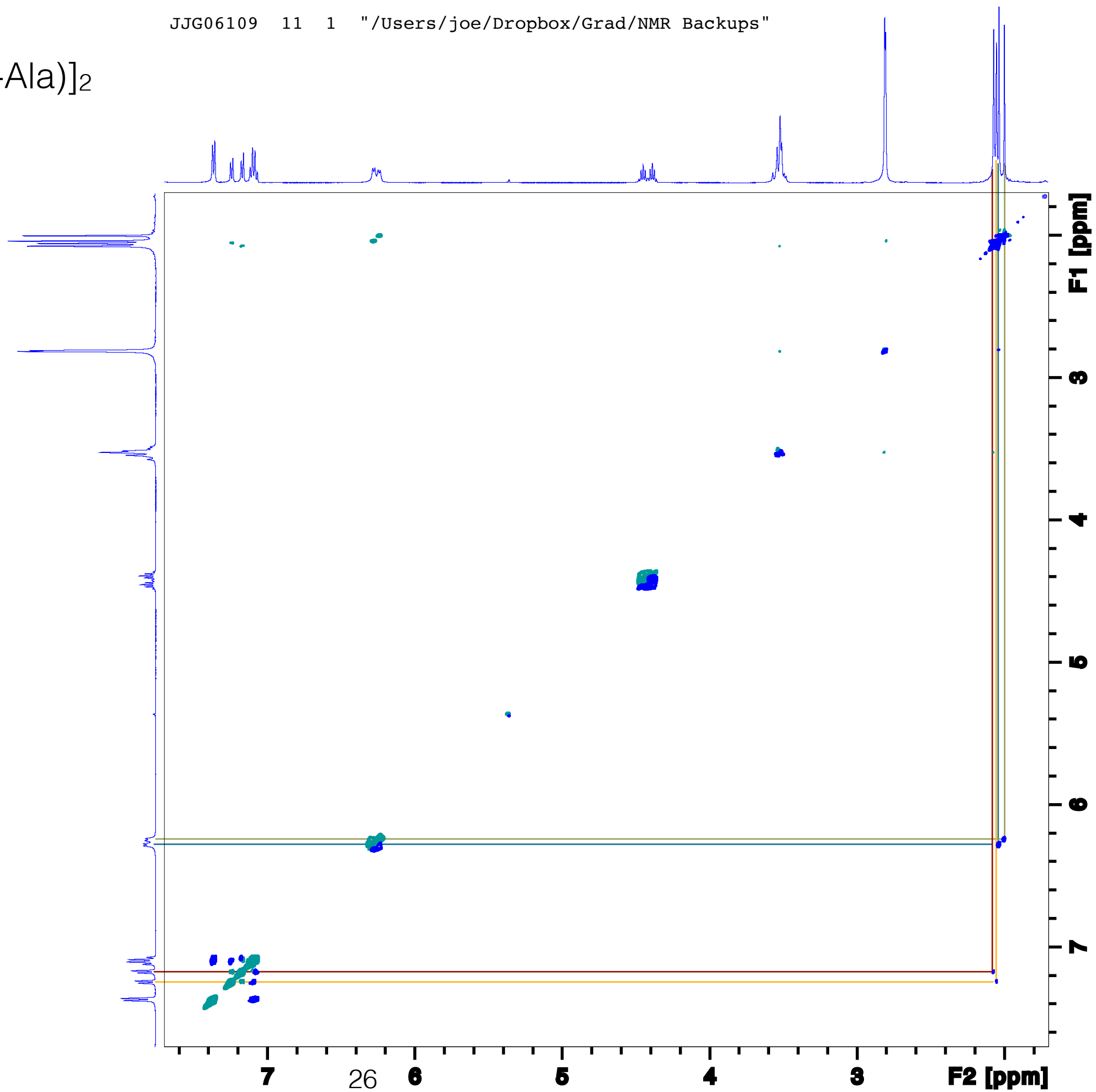
COSY aromatic



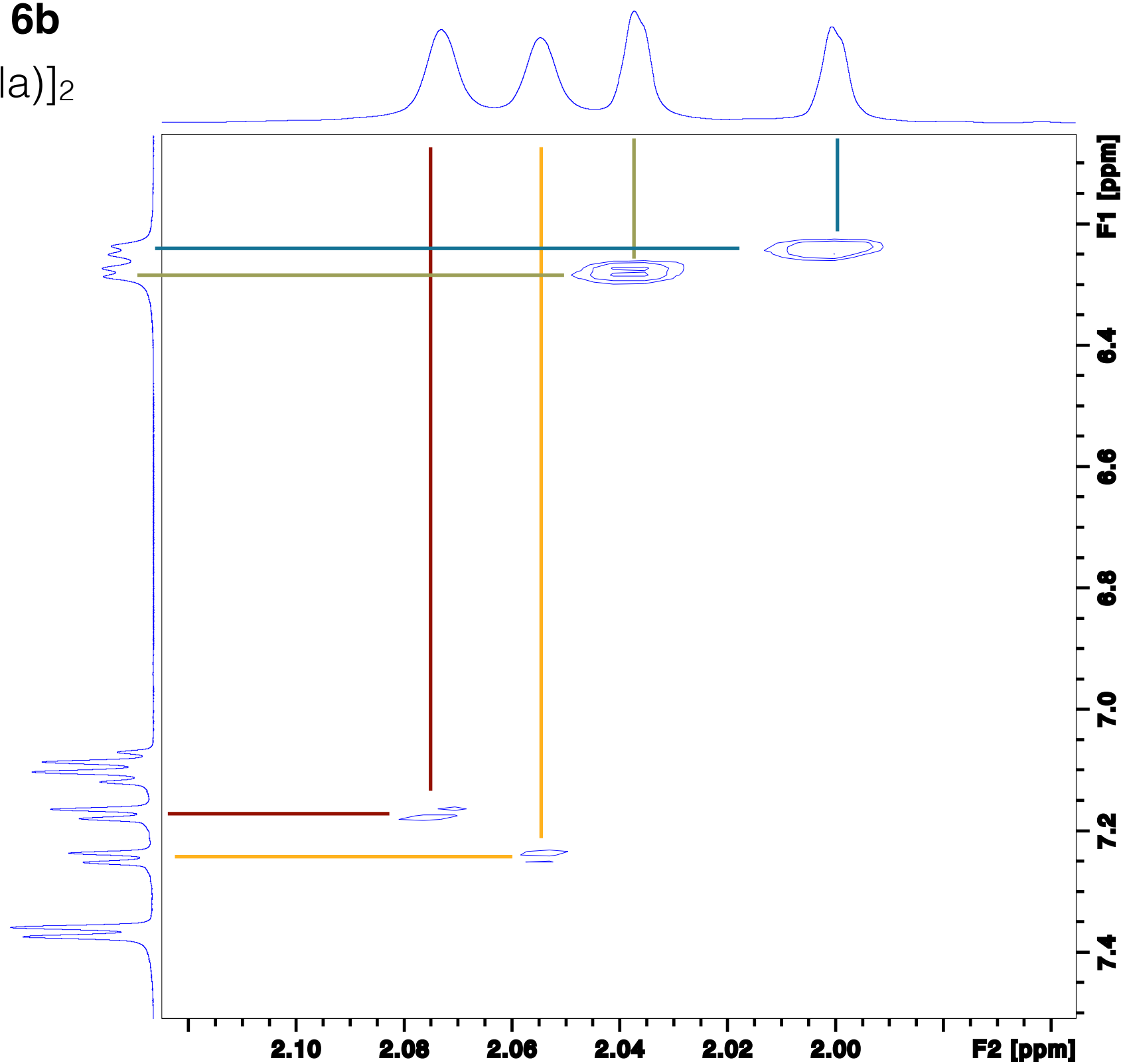
NOESY **6b**

[Pd(o-CF₃-dmba)(NAc-Ala)]₂

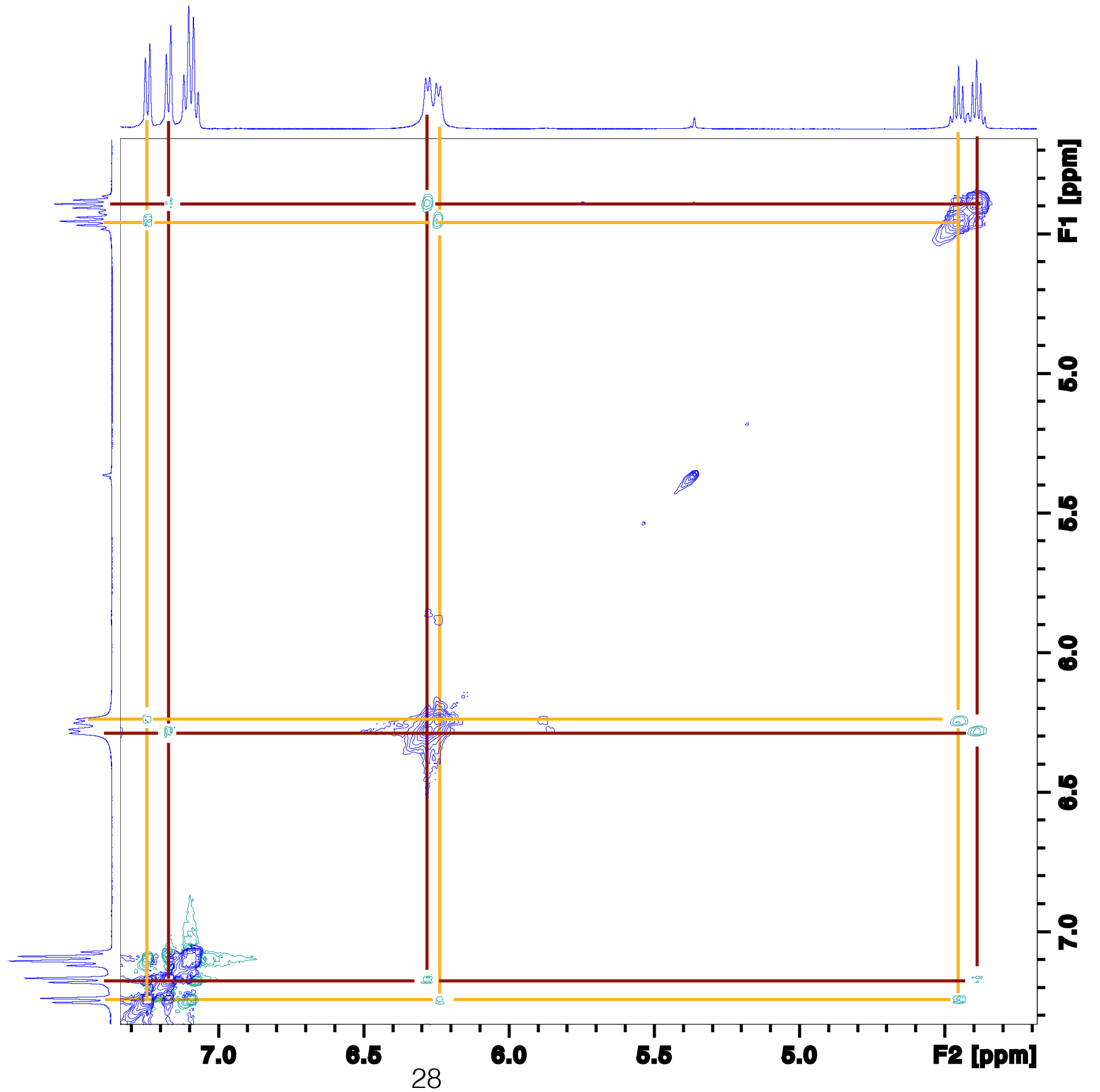
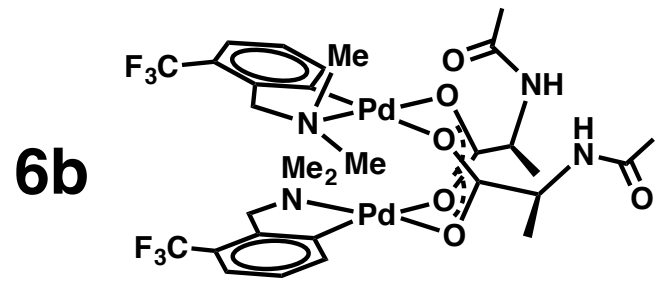
JJG06109 11 1 "/Users/joe/Dropbox/Grad/NMR Backups"



Key NOE cross peaks **6b**

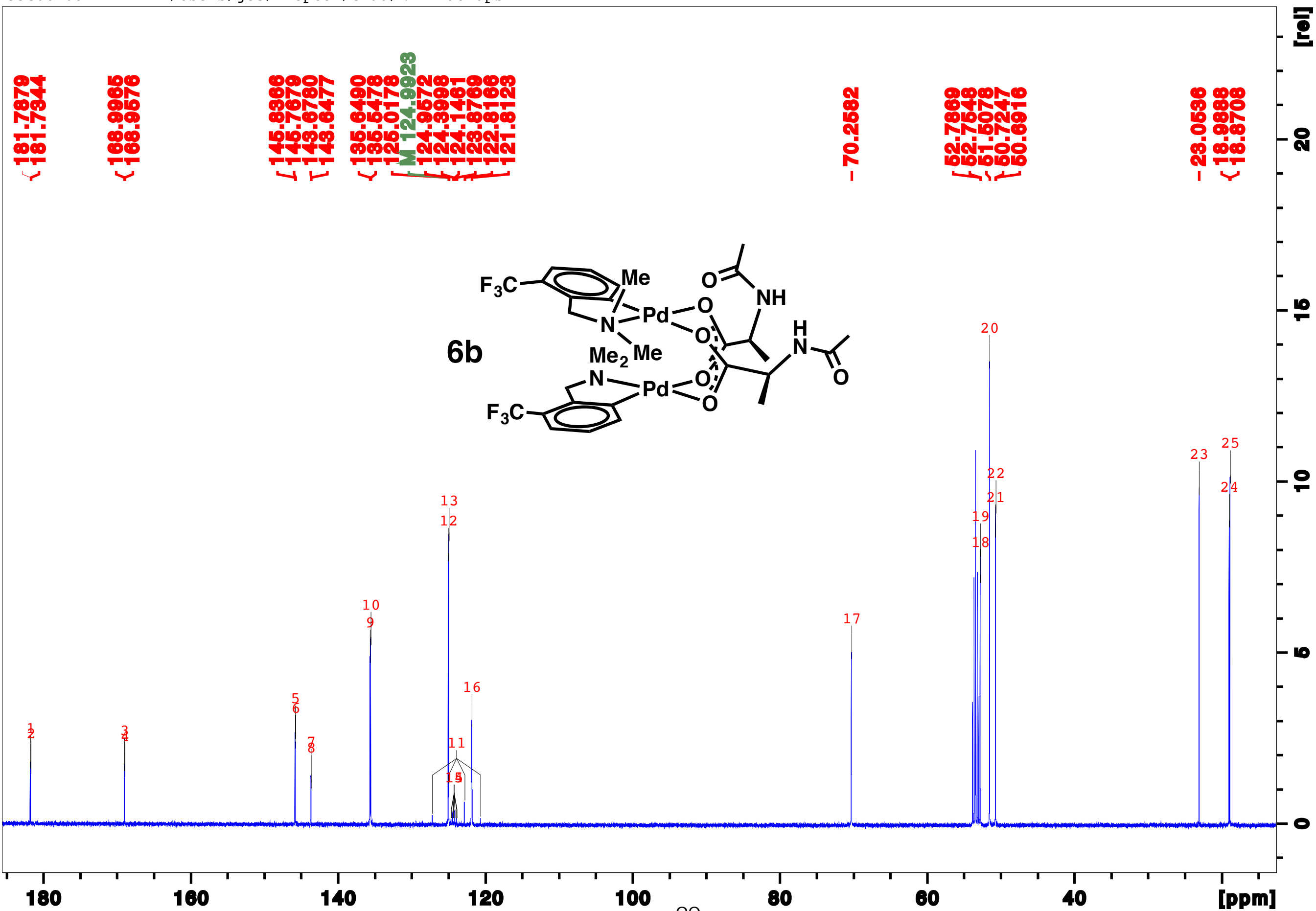


weak NOE cross peaks **6b**
 from MPAA to substrate
 [Pd(CF₃-dmba)(NAC-Ala)]₂



¹³C [Pd(o-CF₃-dmba)(NAc-Ala)]₂

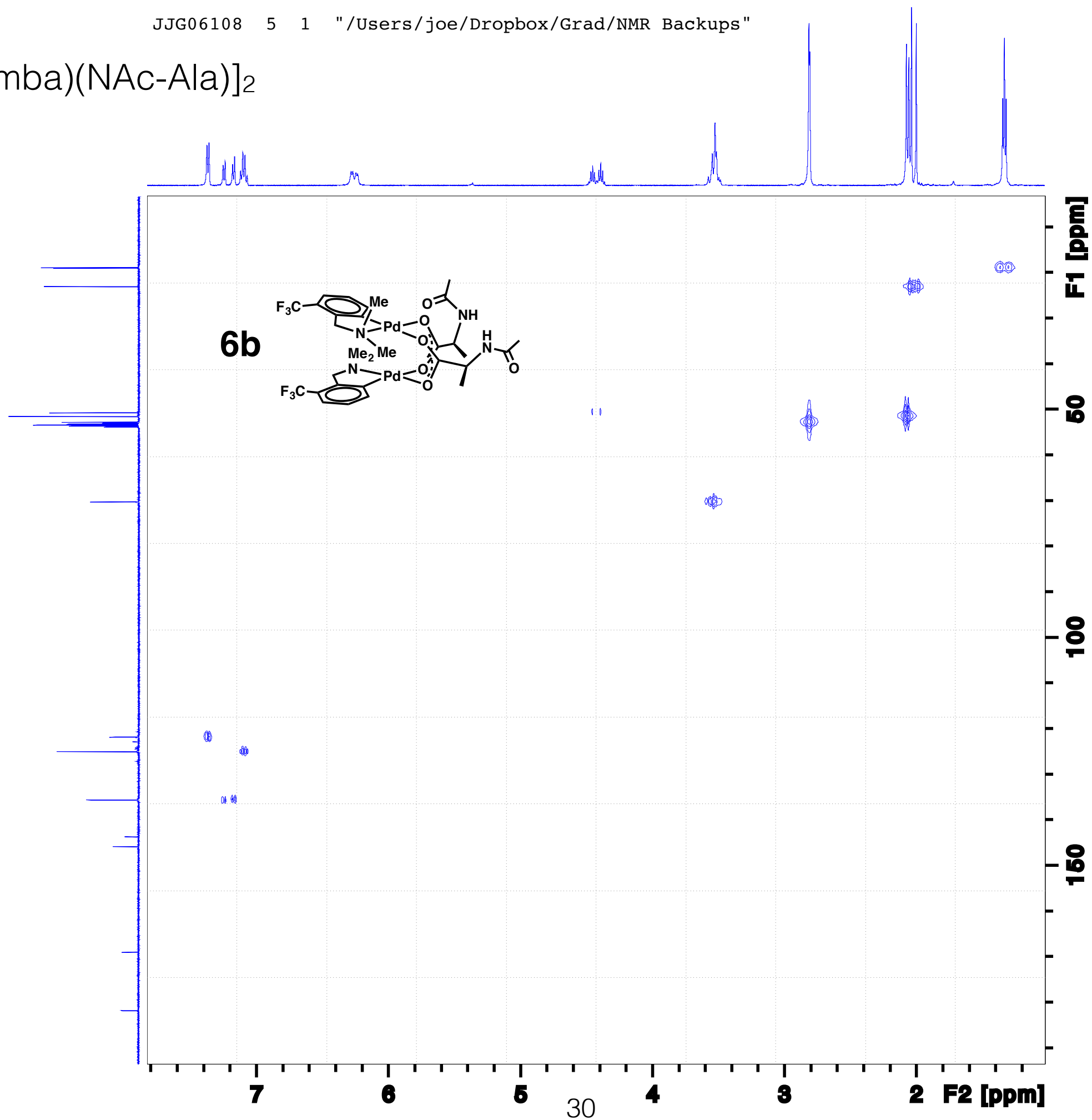
JJG06108 4 1 "/Users/joe/Dropbox/Grad/NMR Backups"



HMCQ

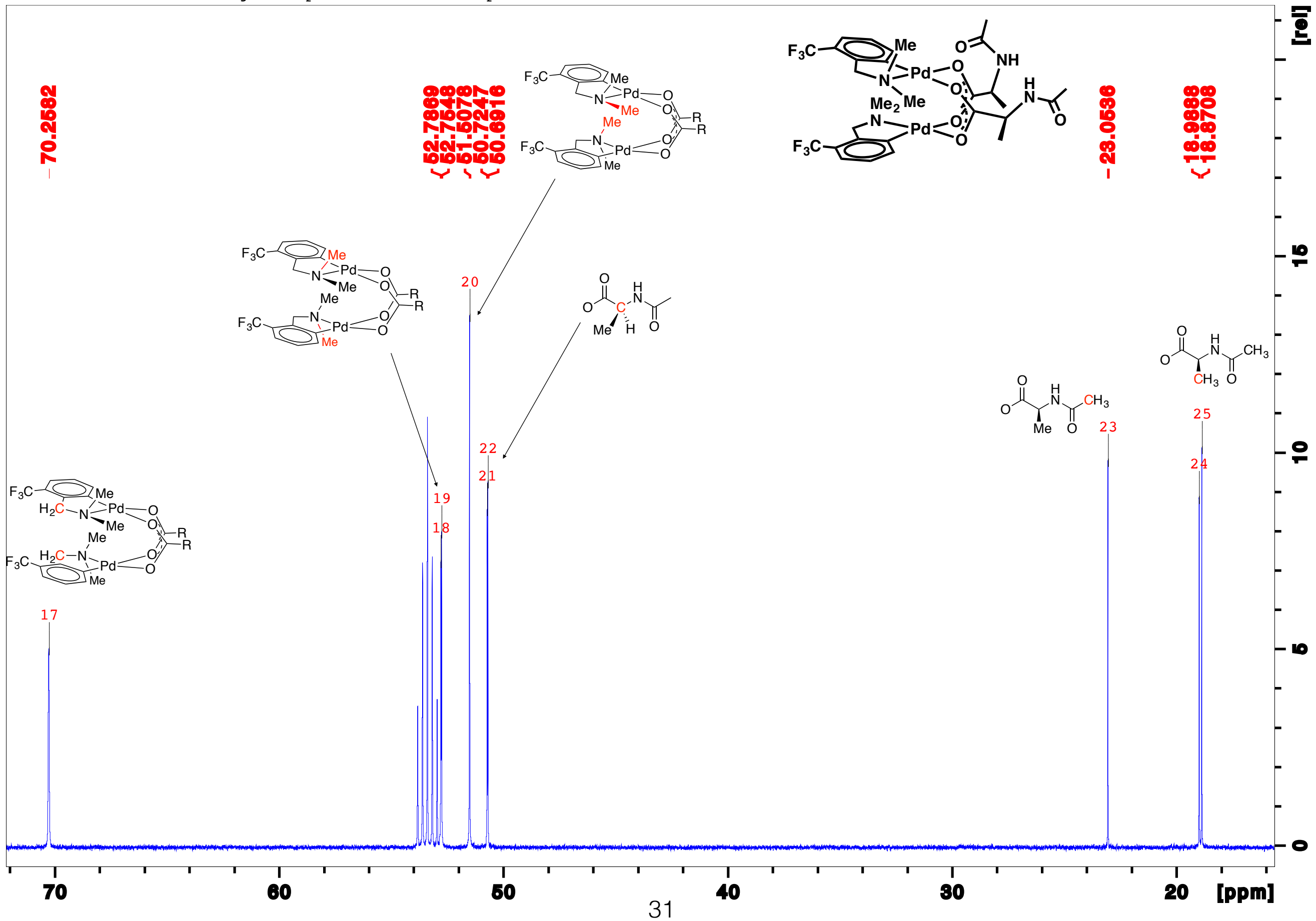
JJG06108 5 1 "/Users/joe/Dropbox/Grad/NMR Backups"

[Pd(o-CF₃-dmba)(NAc-Ala)]₂



13C aliphatic [Pd(o-CF₃-dmba)(NAc-Ala)]₂

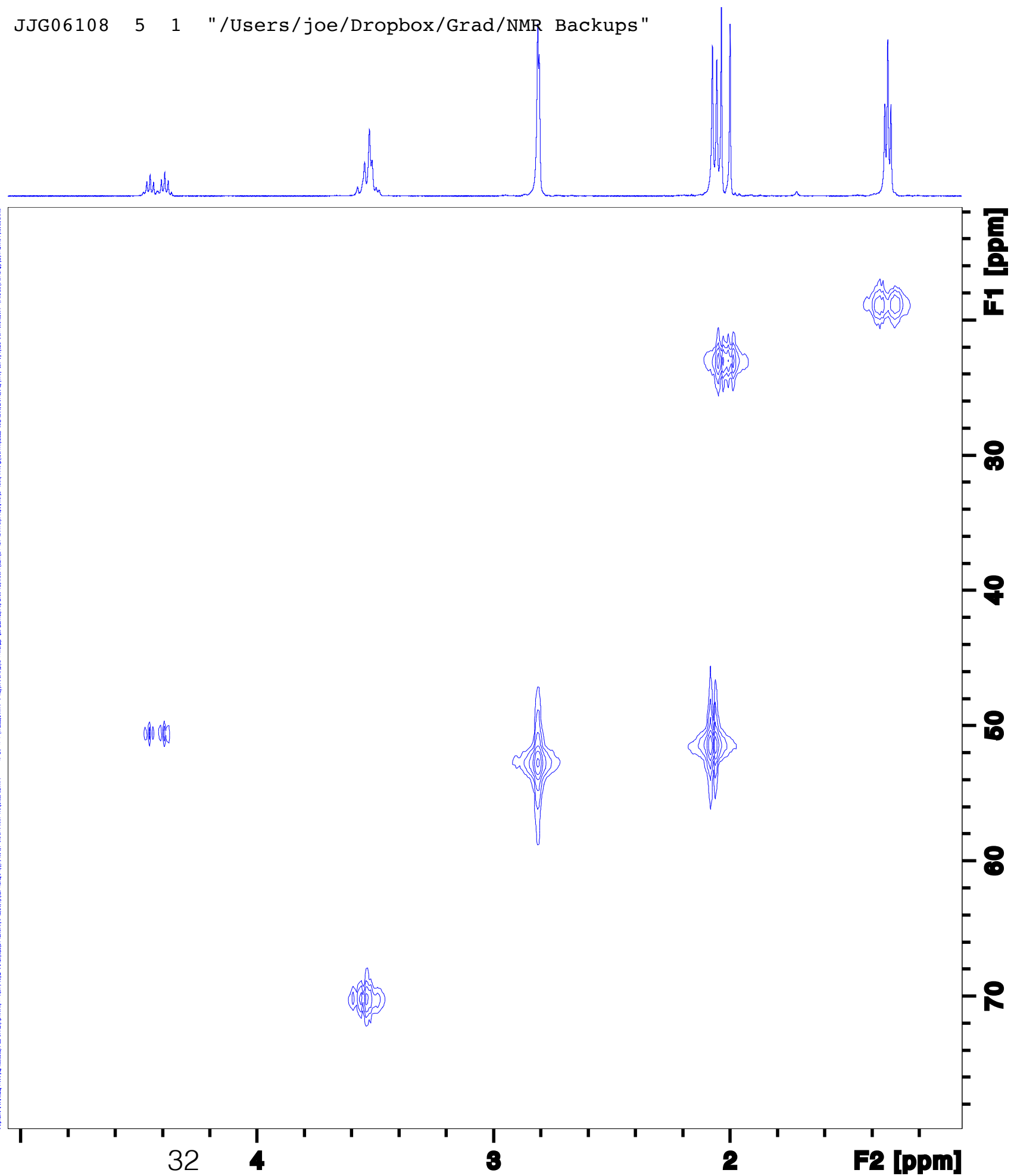
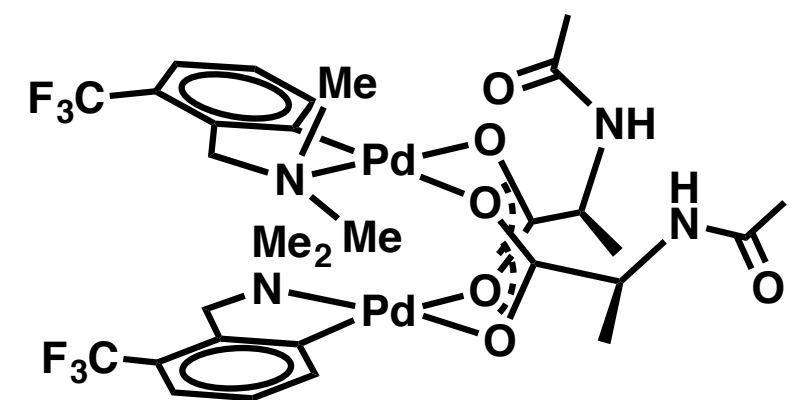
JJG06108 4 1 "/Users/joe/Dropbox/Grad/NMR Backups"



HMCQ aliphatic

[Pd(o-CF₃-dmba)(NAC-Ala)]₂

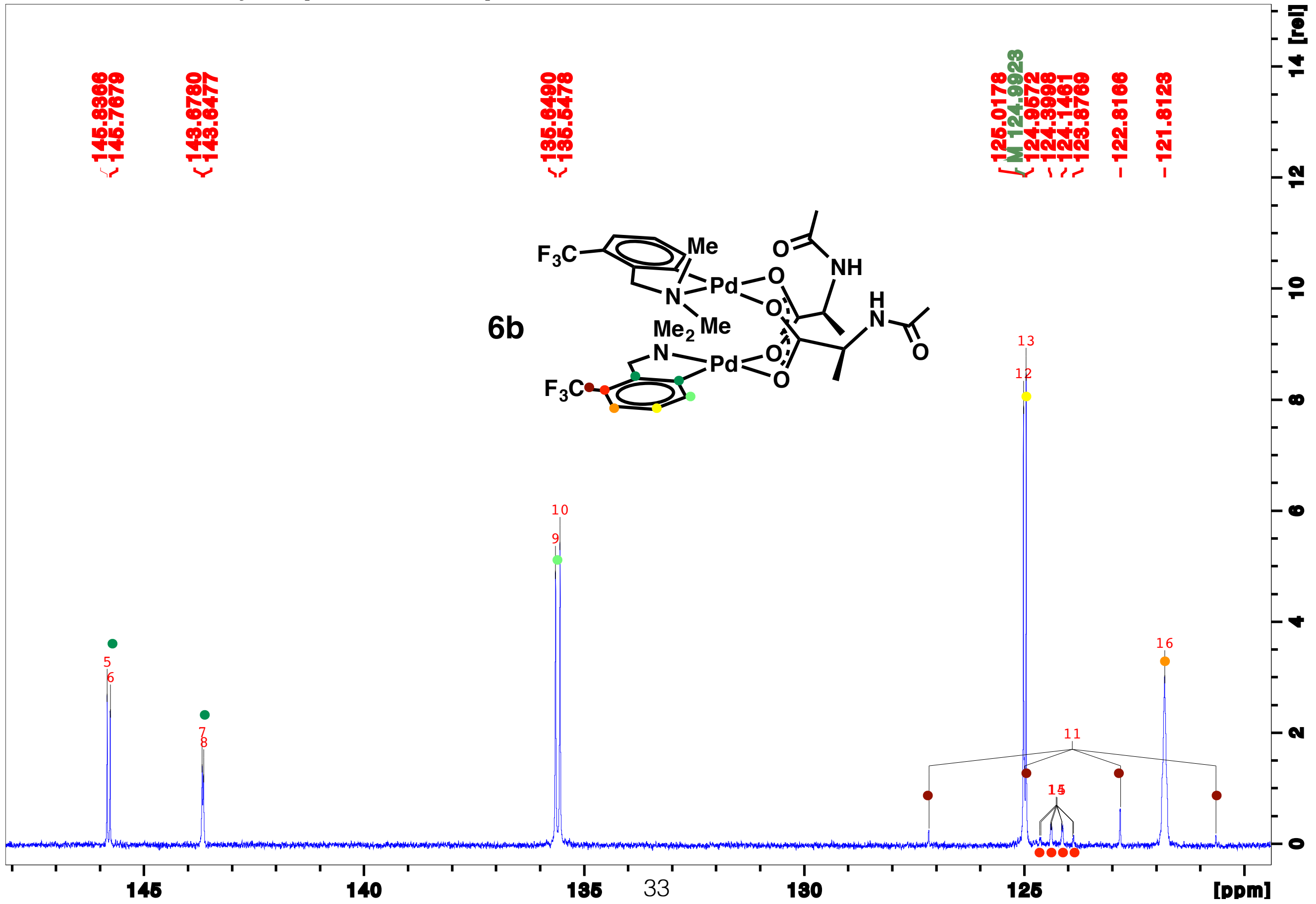
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¹³C aromatic



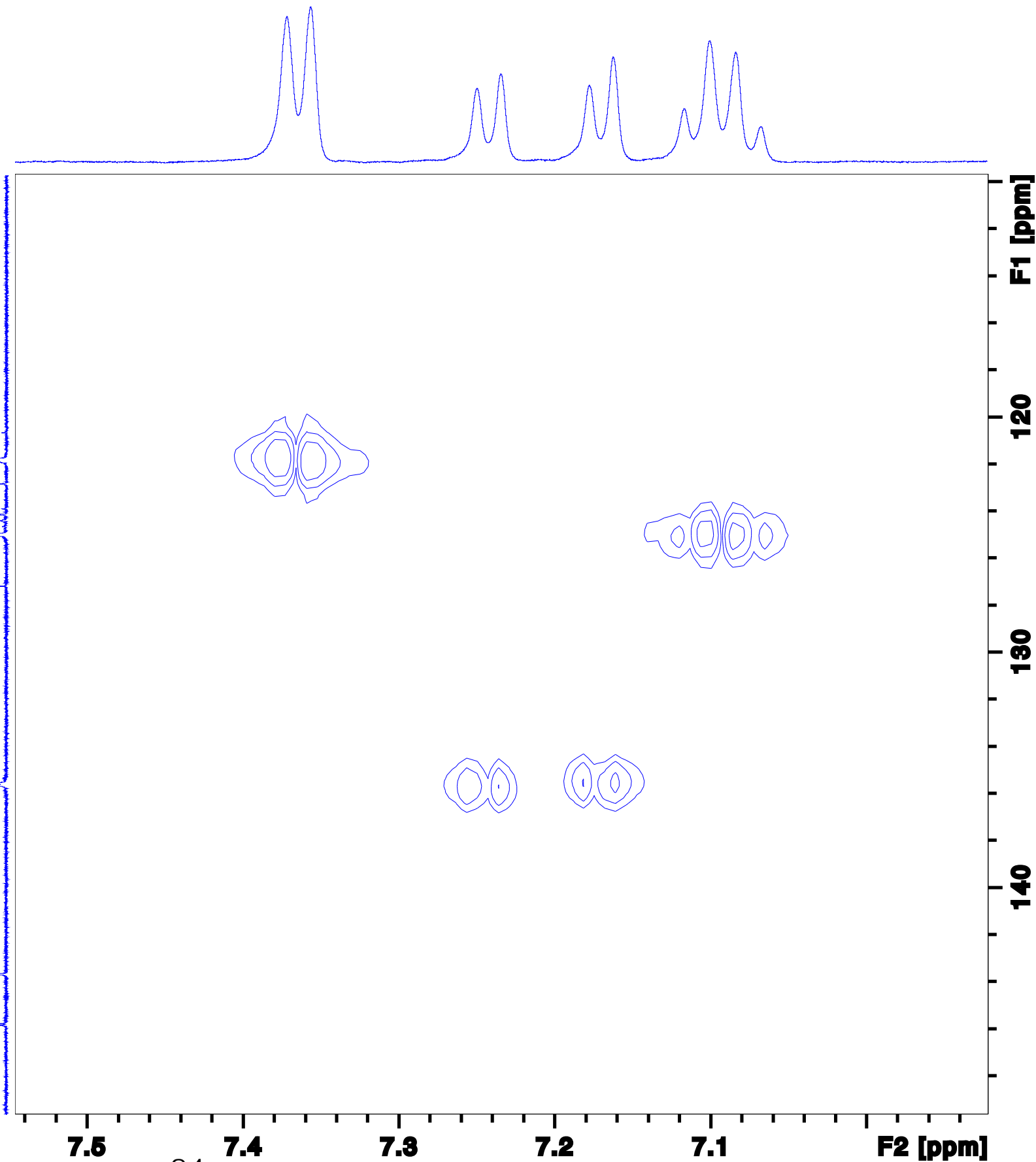
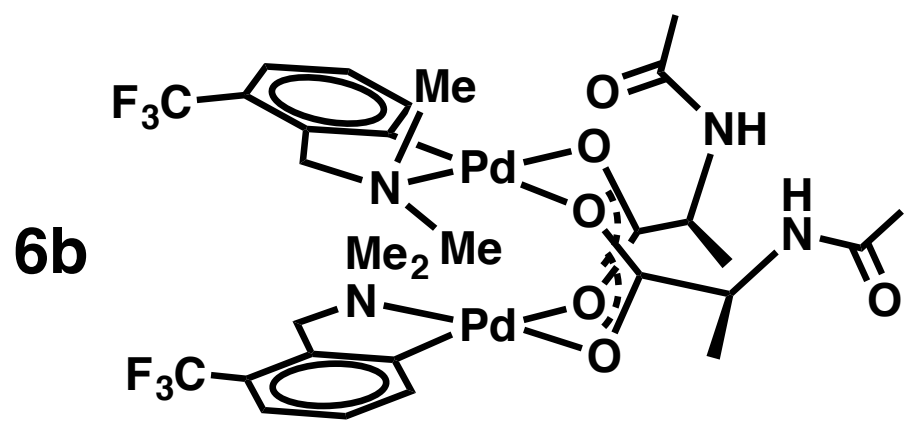
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HMCQ aromatic

[Pd(o-CF₃-dmba)(NAc-Ala)]₂

JJG06108 5 1 "/Users/joe/Dropbox/Grad/NMR Backups"

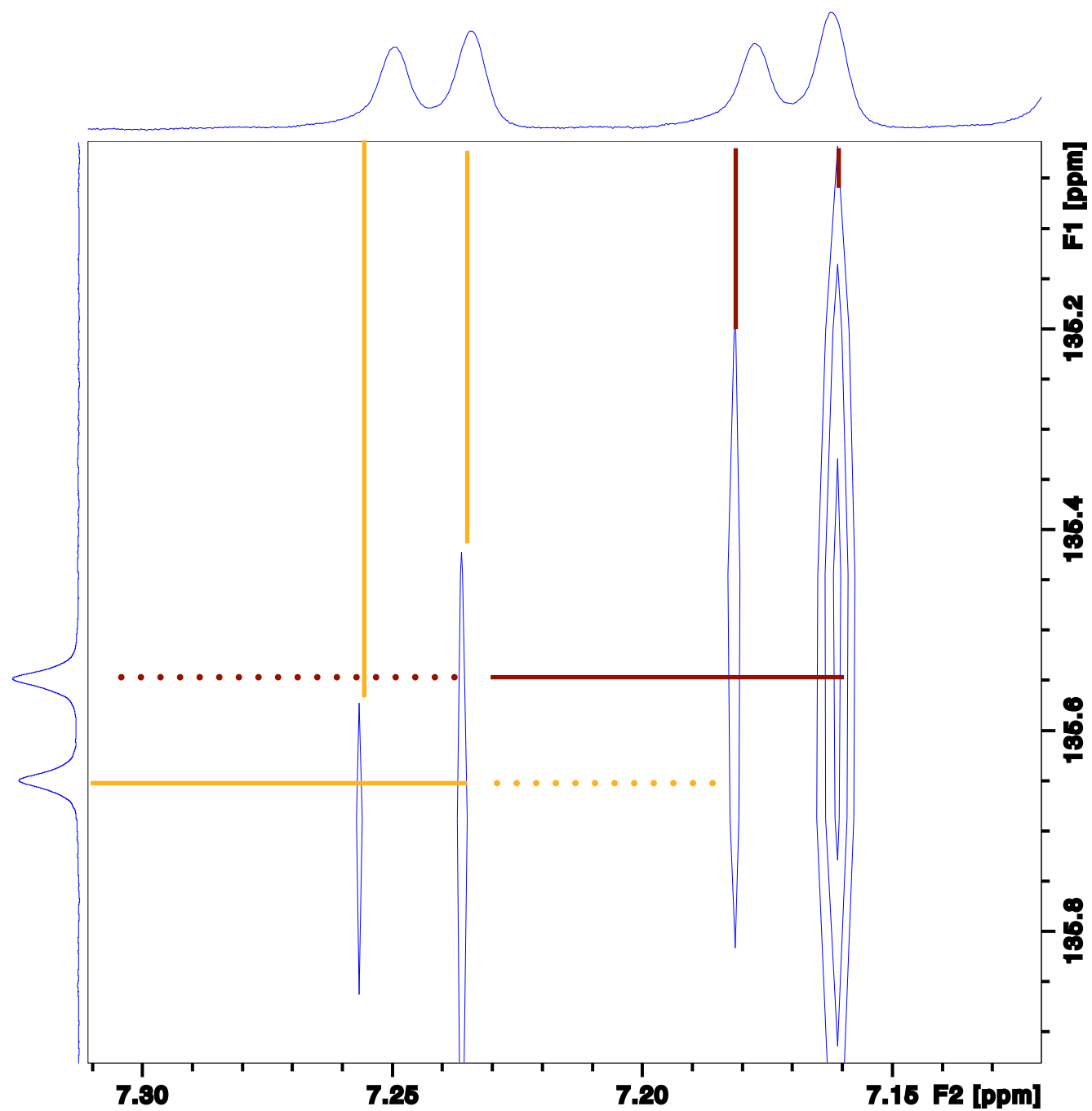
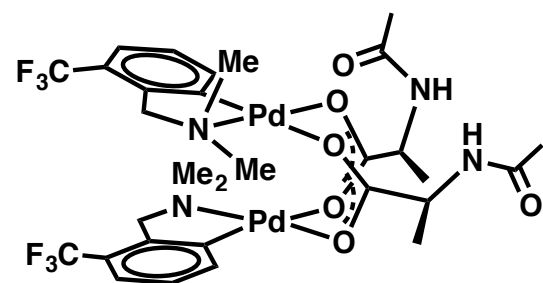


HMCQ of inequivalent C-H's ortho to Pd



JJG06108 5 1 "/Users/joe/Dropbox/Grad/NMR Backups"

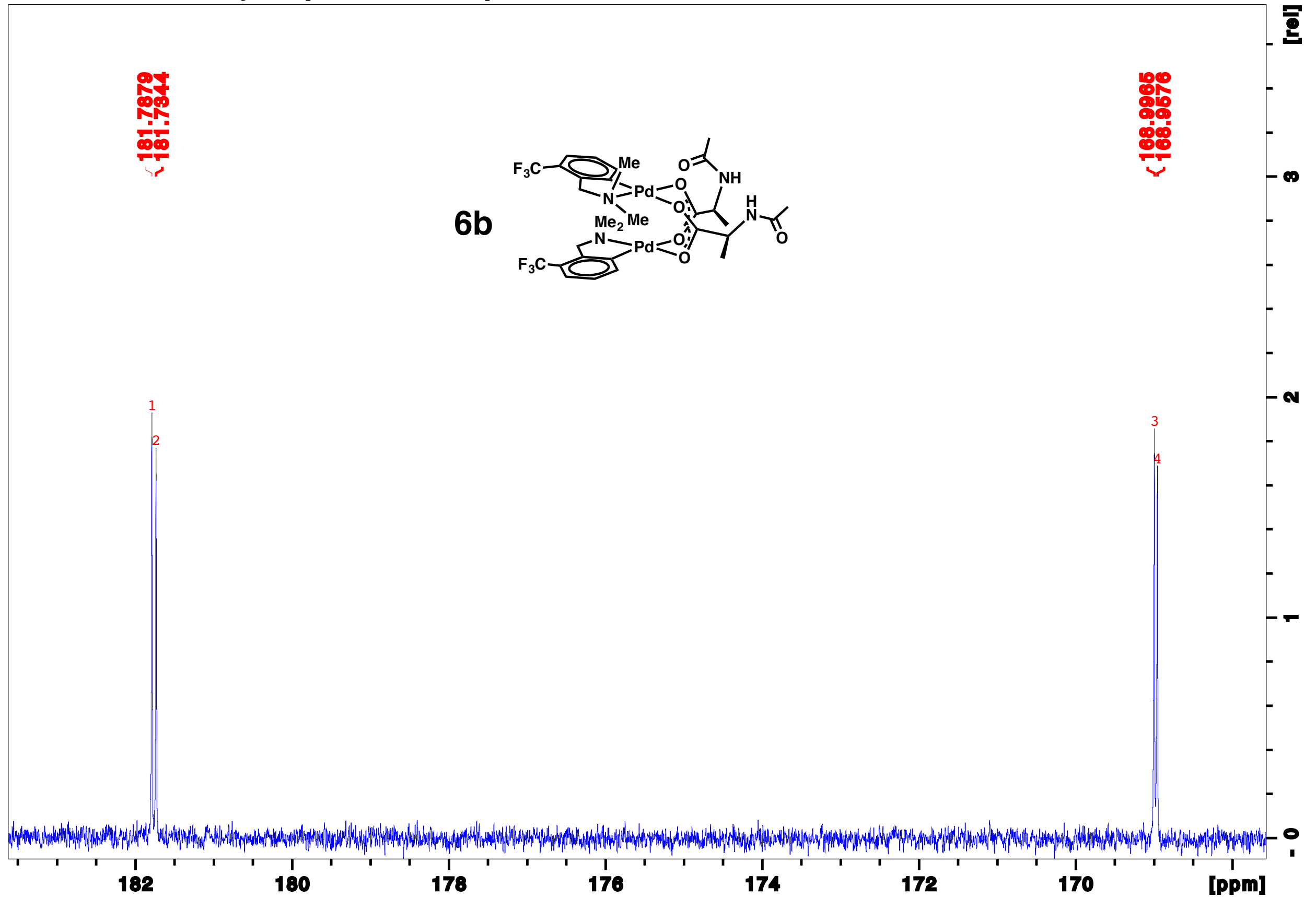
6b



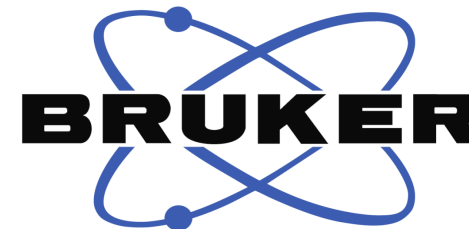
¹³C carbonyls



JJG06108 4 1 "/Users/joe/Dropbox/Grad/NMR Backups"



^{19}F [Pd(o-CF₃-dmba)(NAc-Ala)]₂

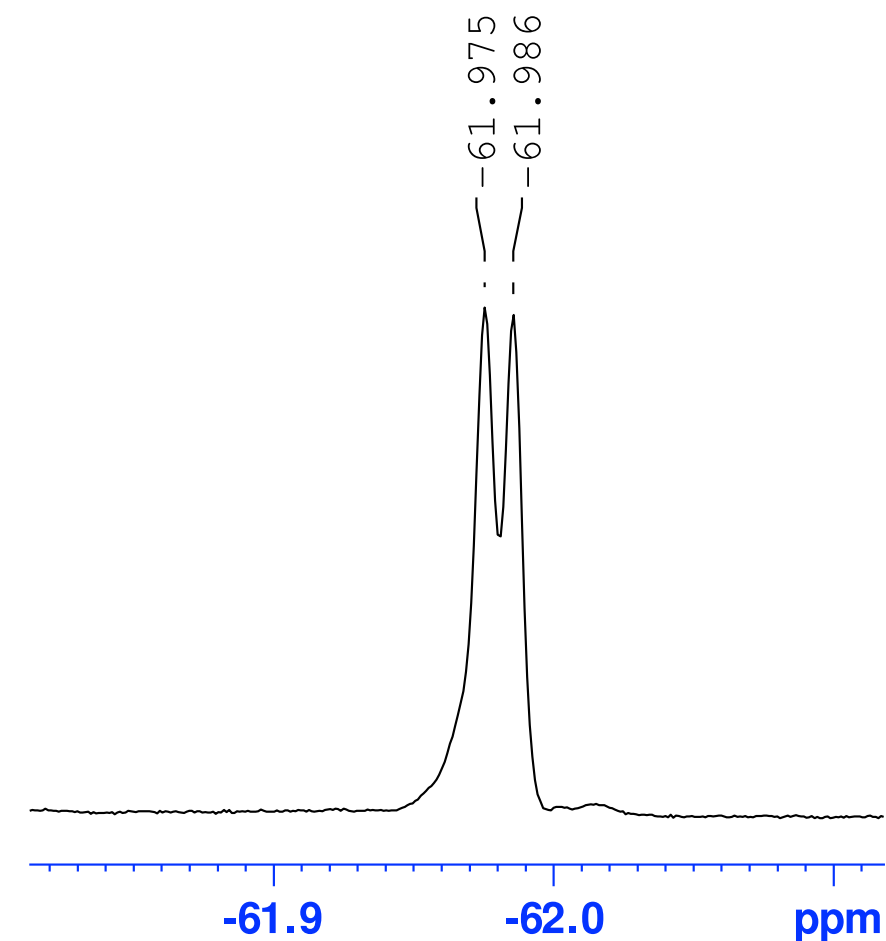
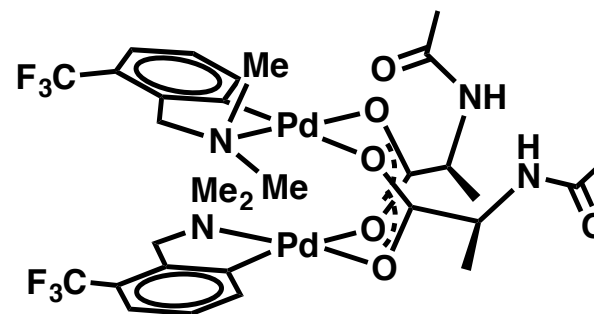


Current Data Parameters
NAME JYG06109
EXPNO 13
PROCNO 1

F2 - Acquisition Parameter
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Time 11.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 703112
SOLVENT CD2Cl2
NS 1
DS 0
SWH 117187.500 Hz
FIDRES 0.166670 Hz
AQ 2.9999444 sec
RG 499.75
DW 4.267 usec
DE 6.50 usec
TE 295.5 K
D1 3.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 470.3185714 MHz
NUC1 19F
P1 14.80 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



-61.975
-61.986

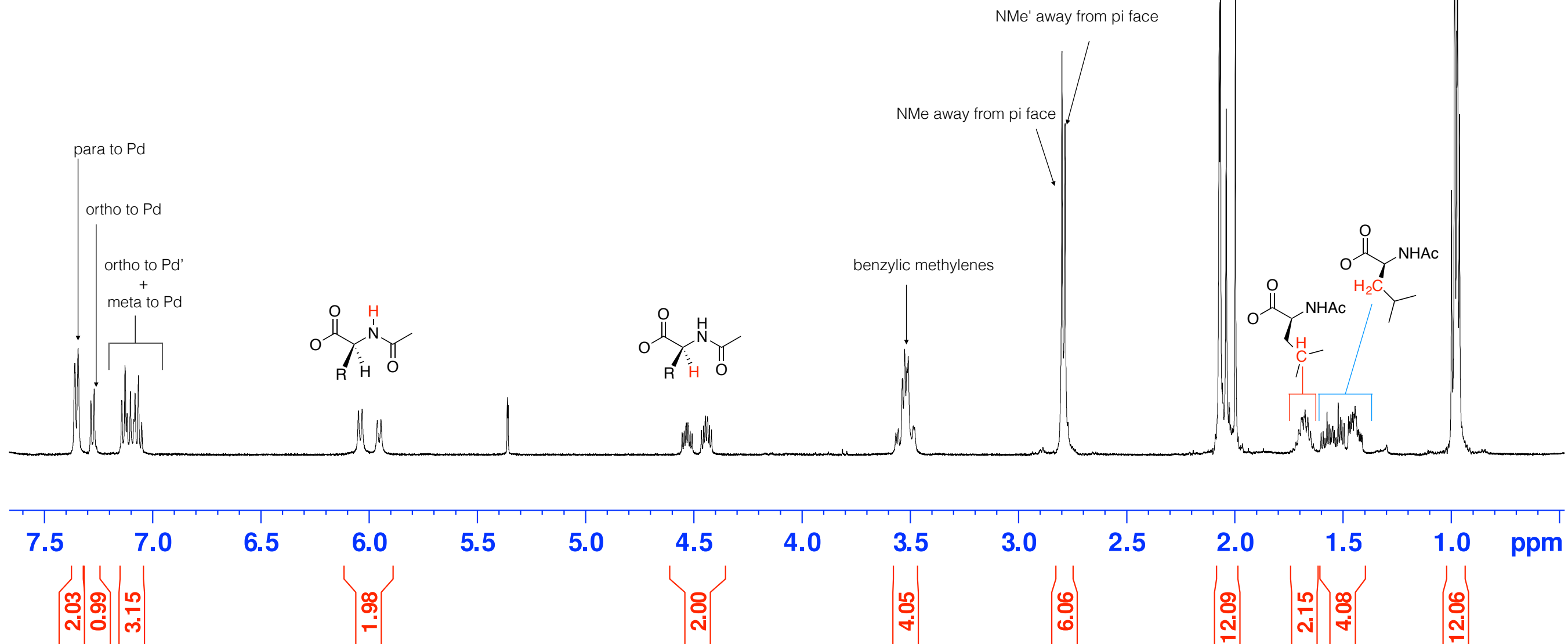
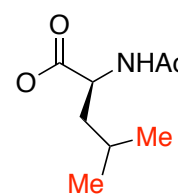
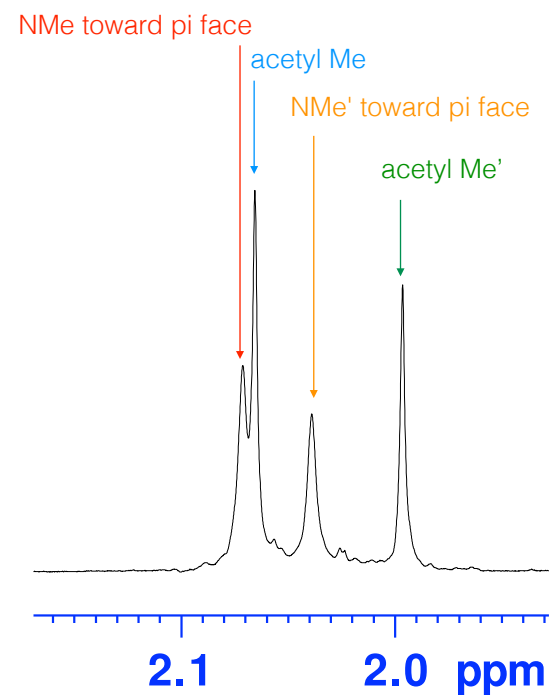
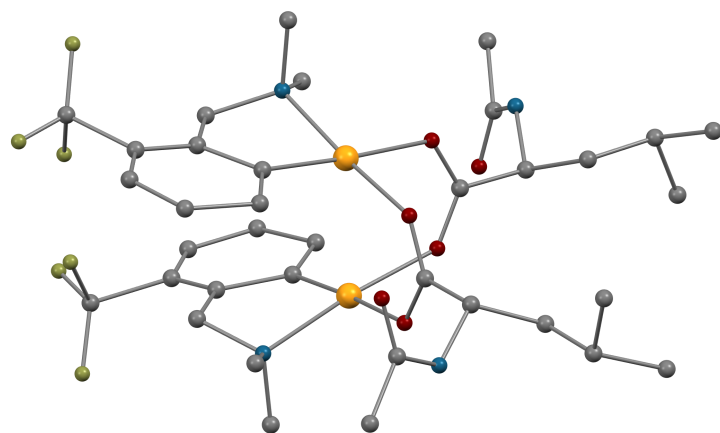
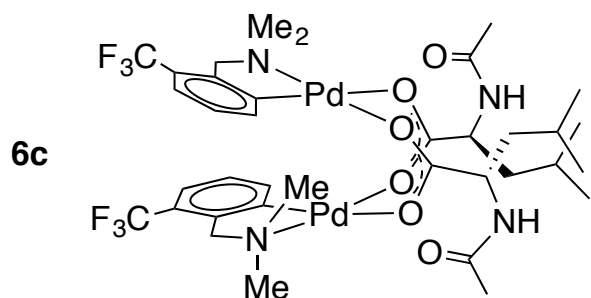


Current Data Parameters

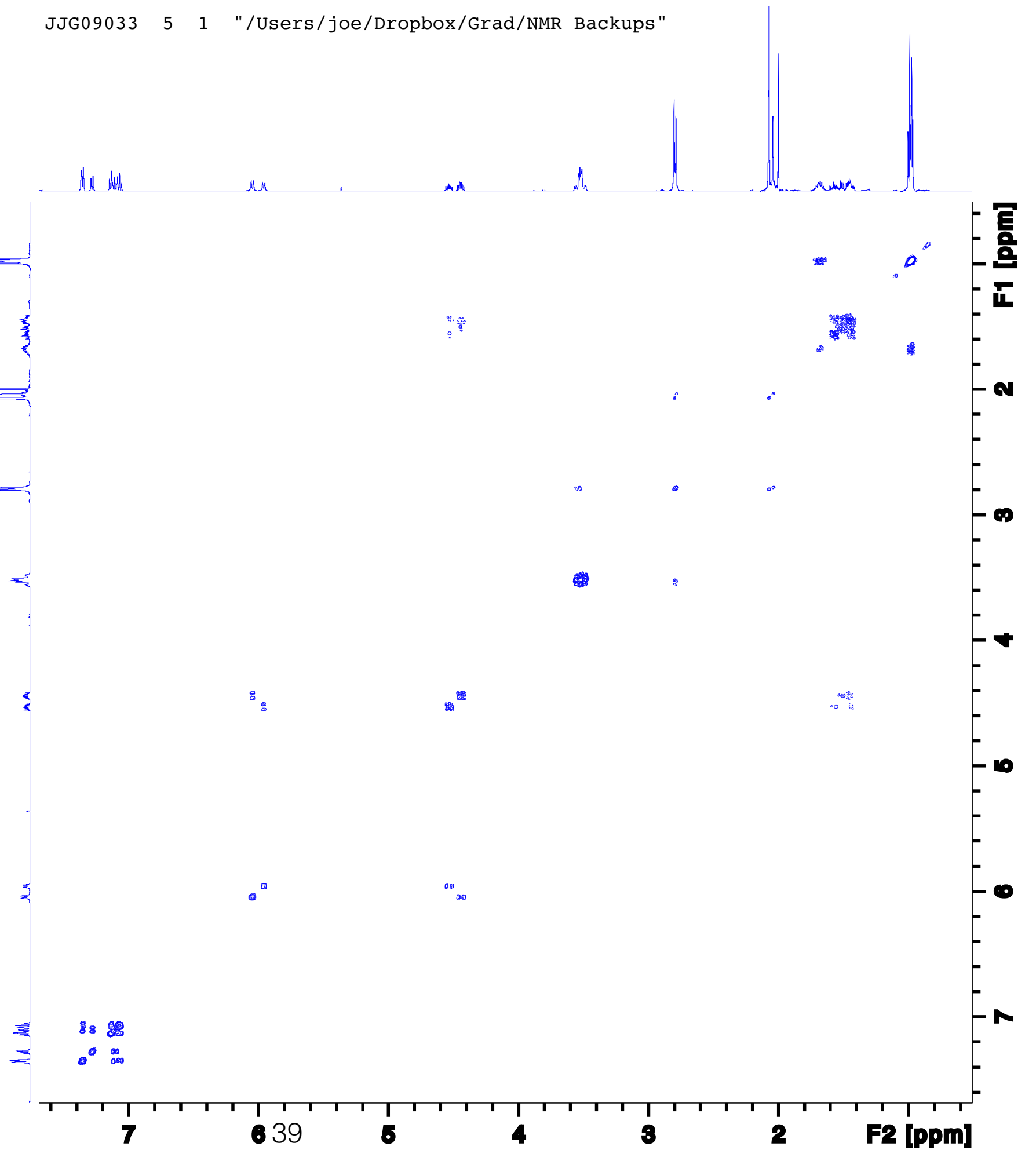
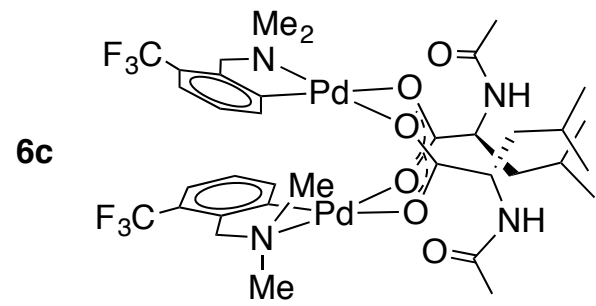
NAME JJG09032

EXPNO 7

PROCNO 1

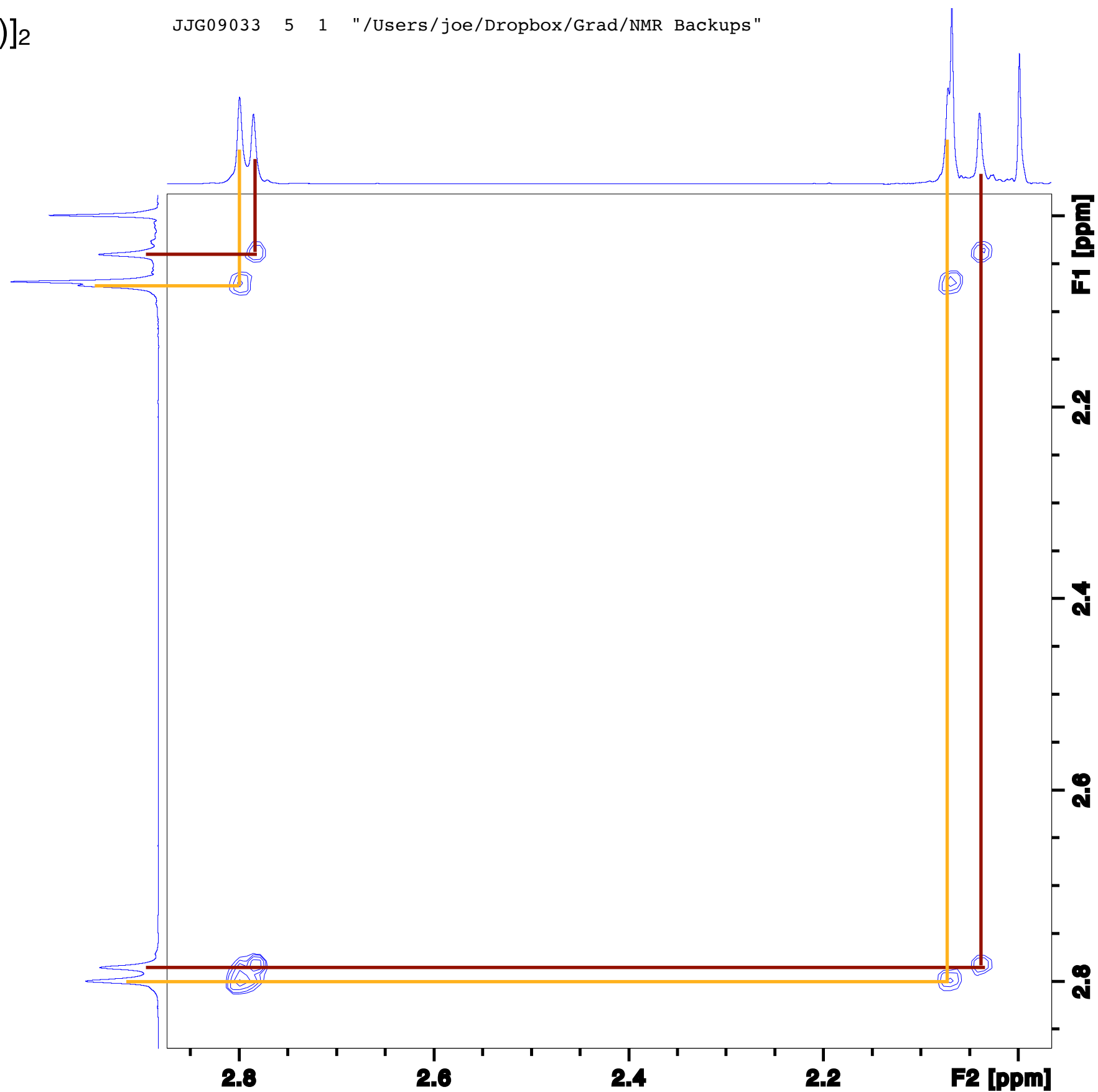
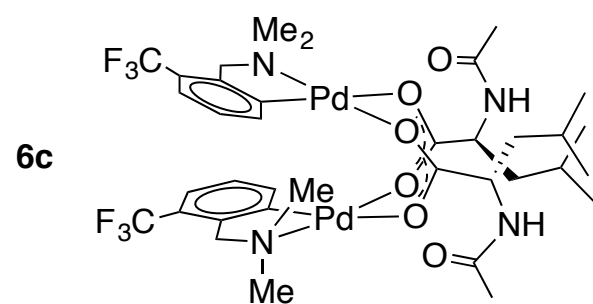


COSY [Pd(CF₃-dmba)(NAc-Leu)]₂

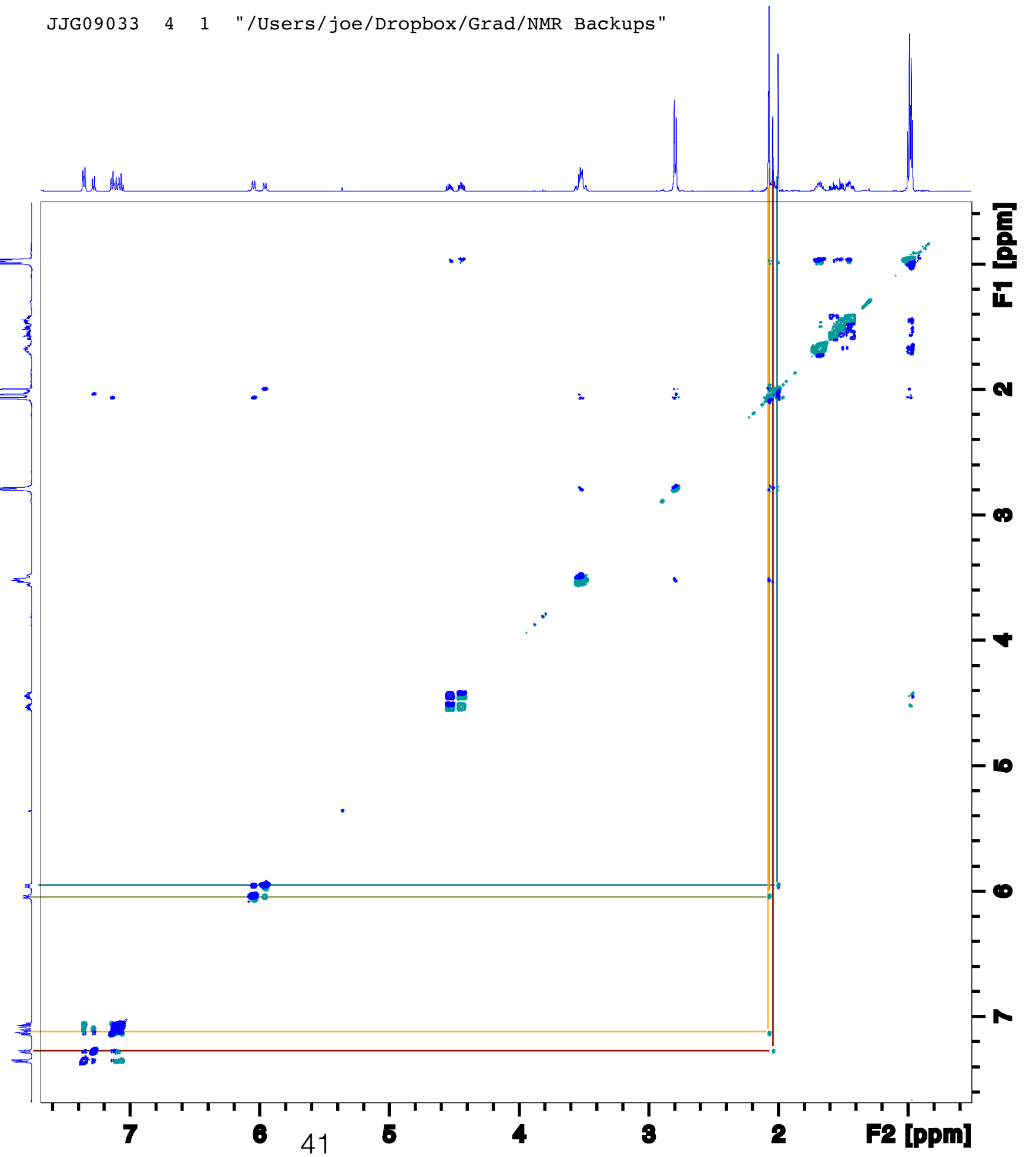
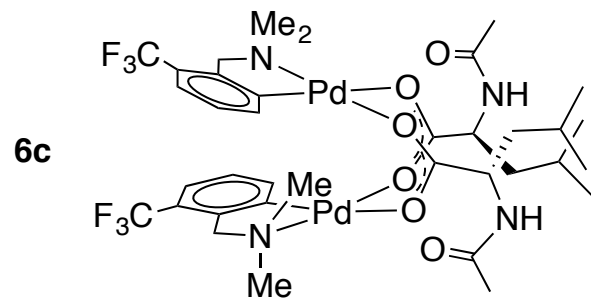


COSY [Pd(CF₃-dmba)(NAC-Leu)]₂
inequivalent pairs of NMe's

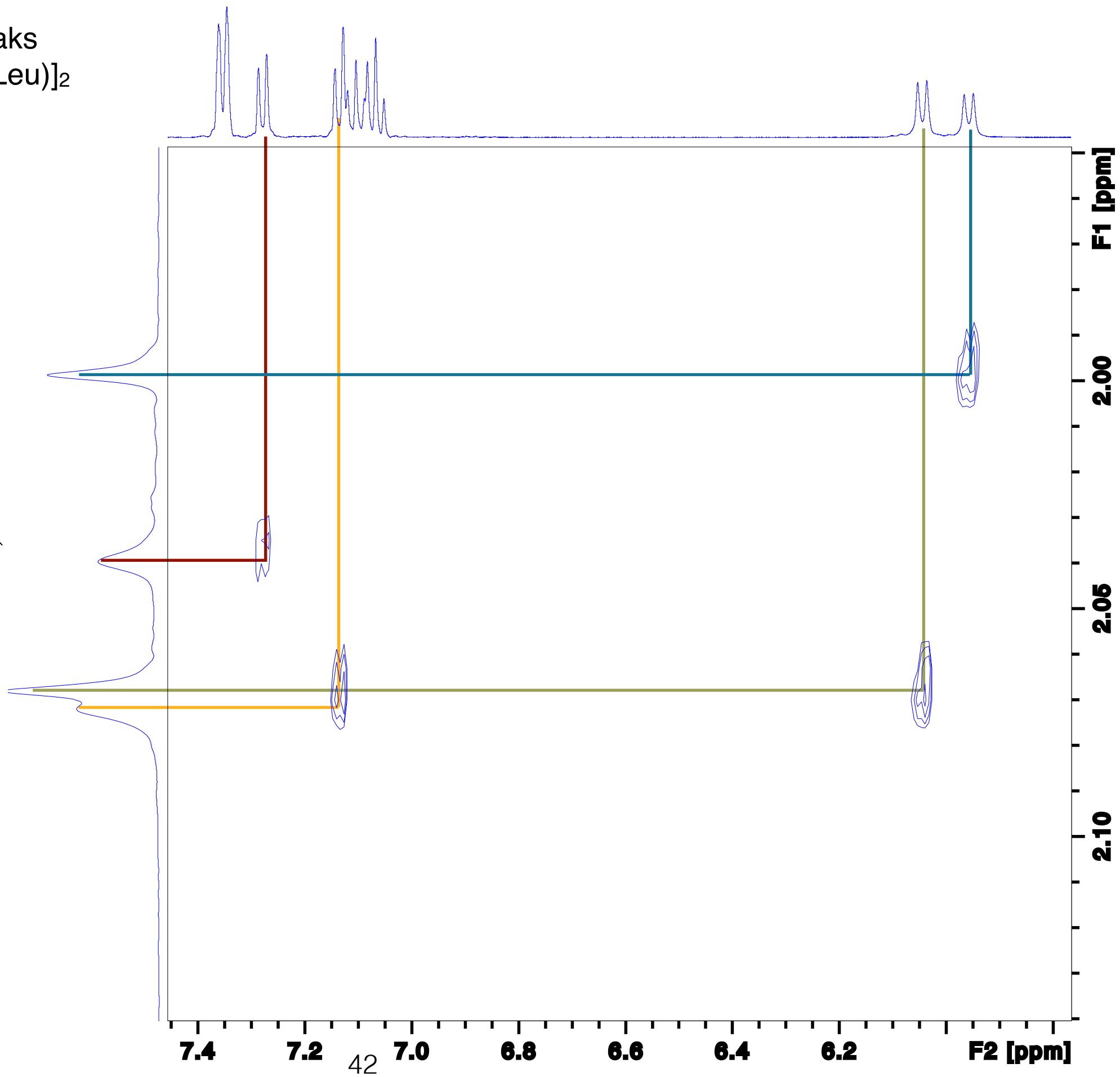
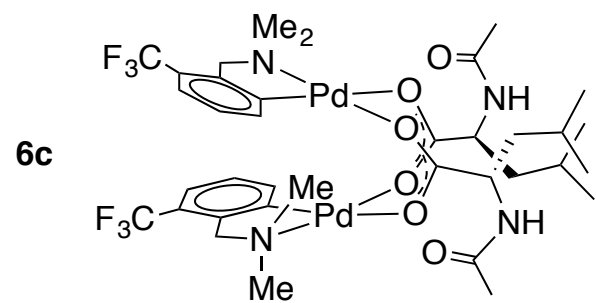
JJG09033 5 1 "/Users/joe/Dropbox/Grad/NMR Backups"



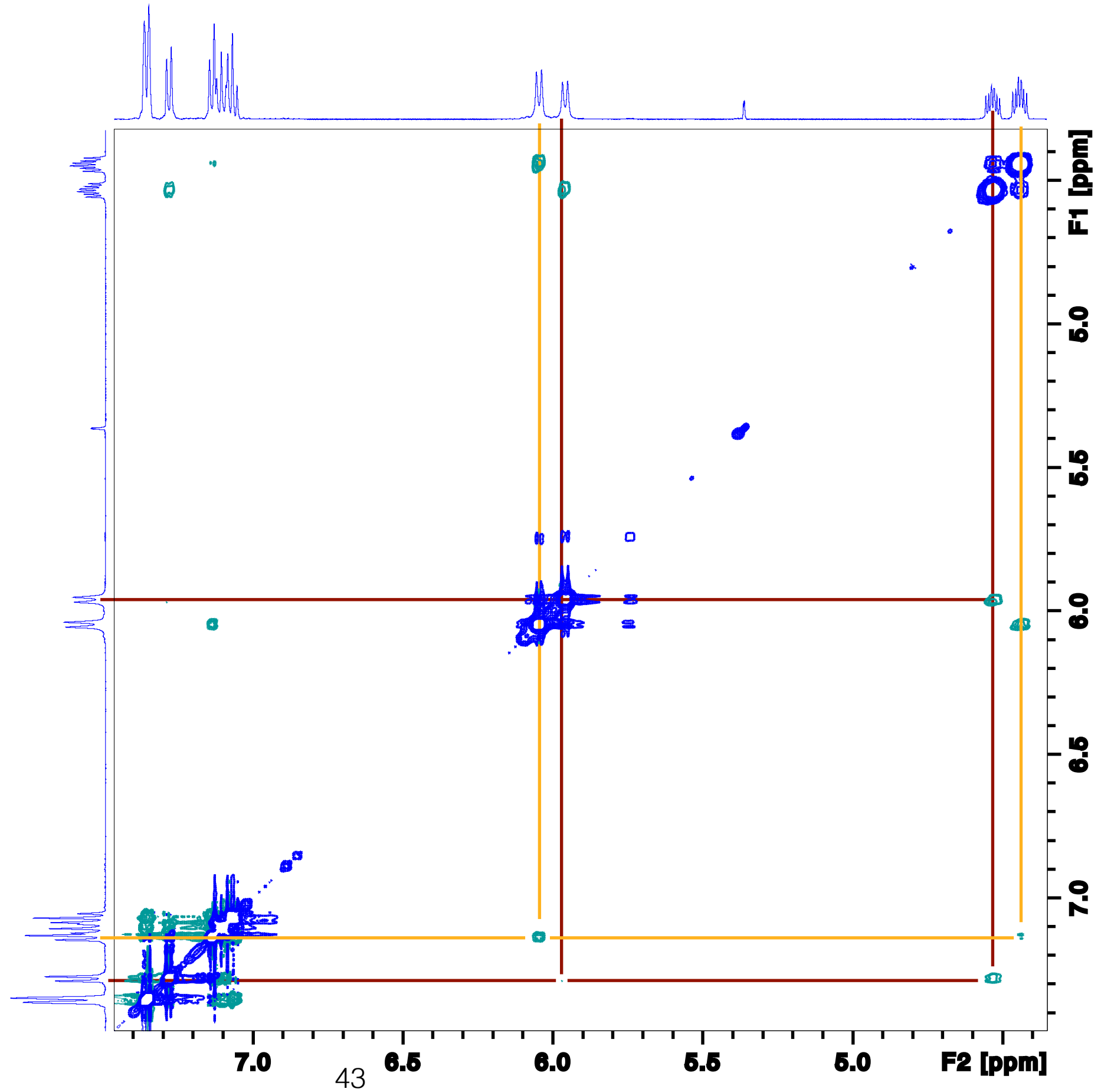
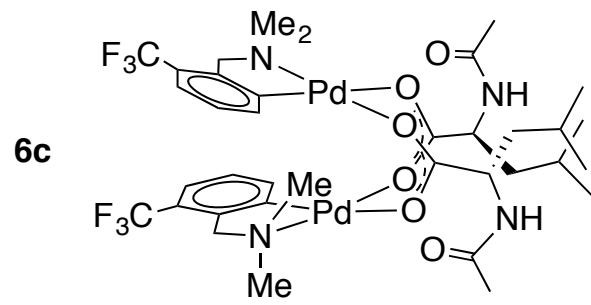
NOESY [Pd(CF₃-dmba)(NAc-Leu)]₂

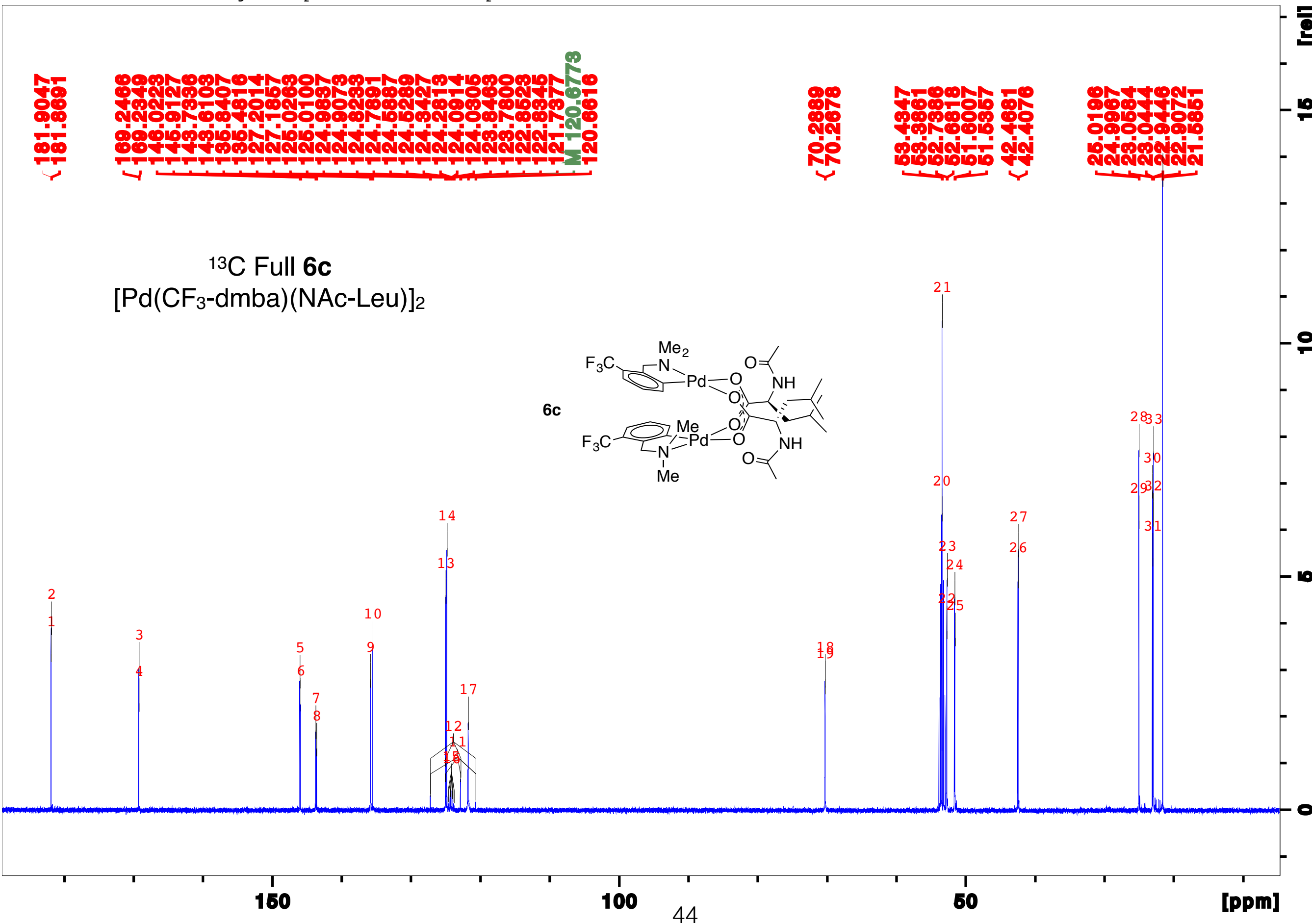


Key NOE cross peaks
 [Pd(CF₃-dmba)(NAC-Leu)]₂

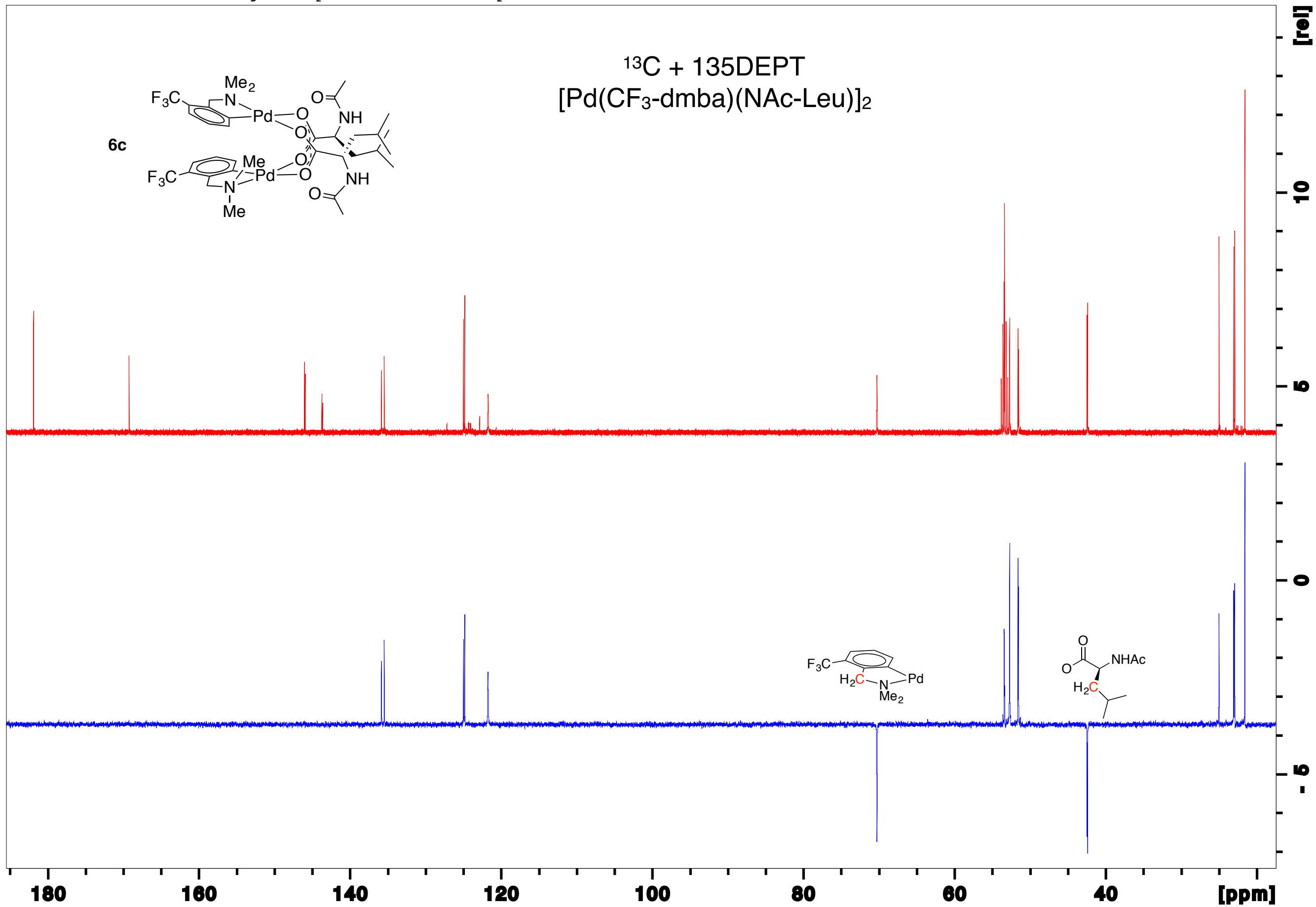
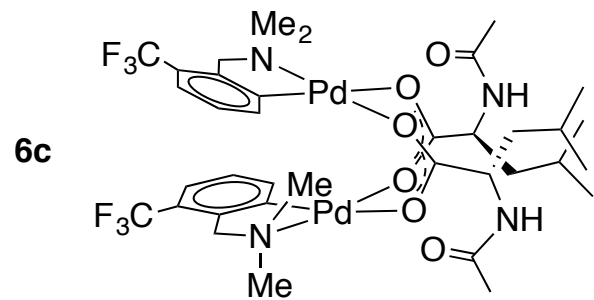


weak NOE cross peaks
from MPAA to substrate
[Pd(CF₃-dmba)(NAc-Leu)]₂



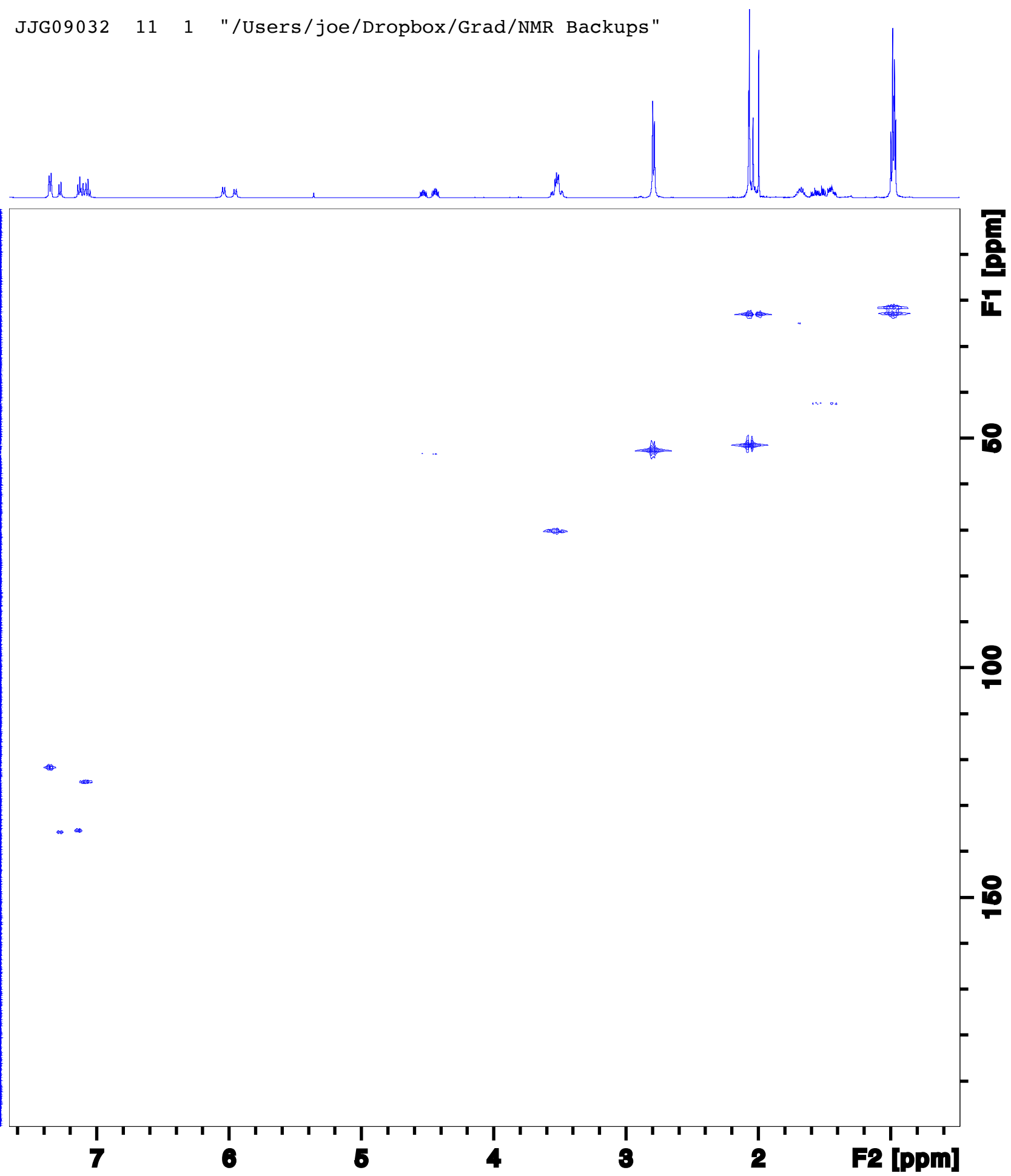
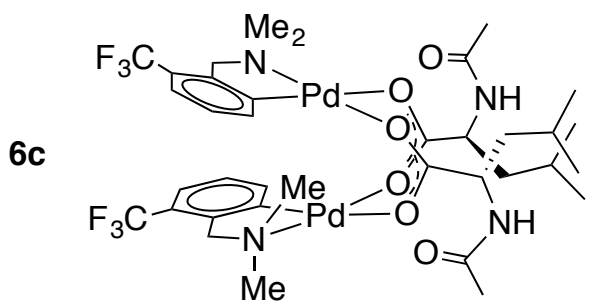


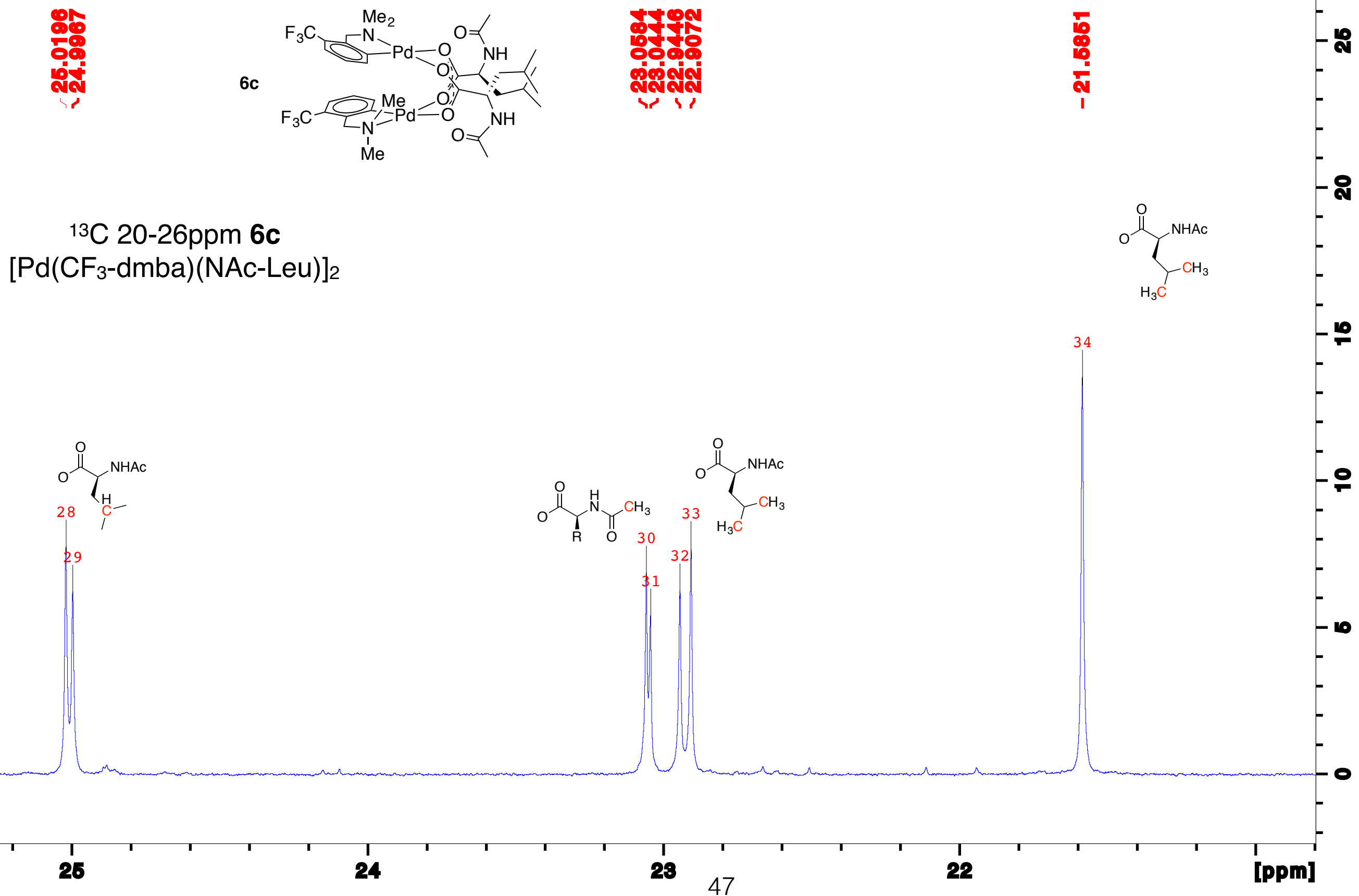
¹³C + 135DEPT
[Pd(CF₃-dmba)(NAc-Leu)]₂



HMQC

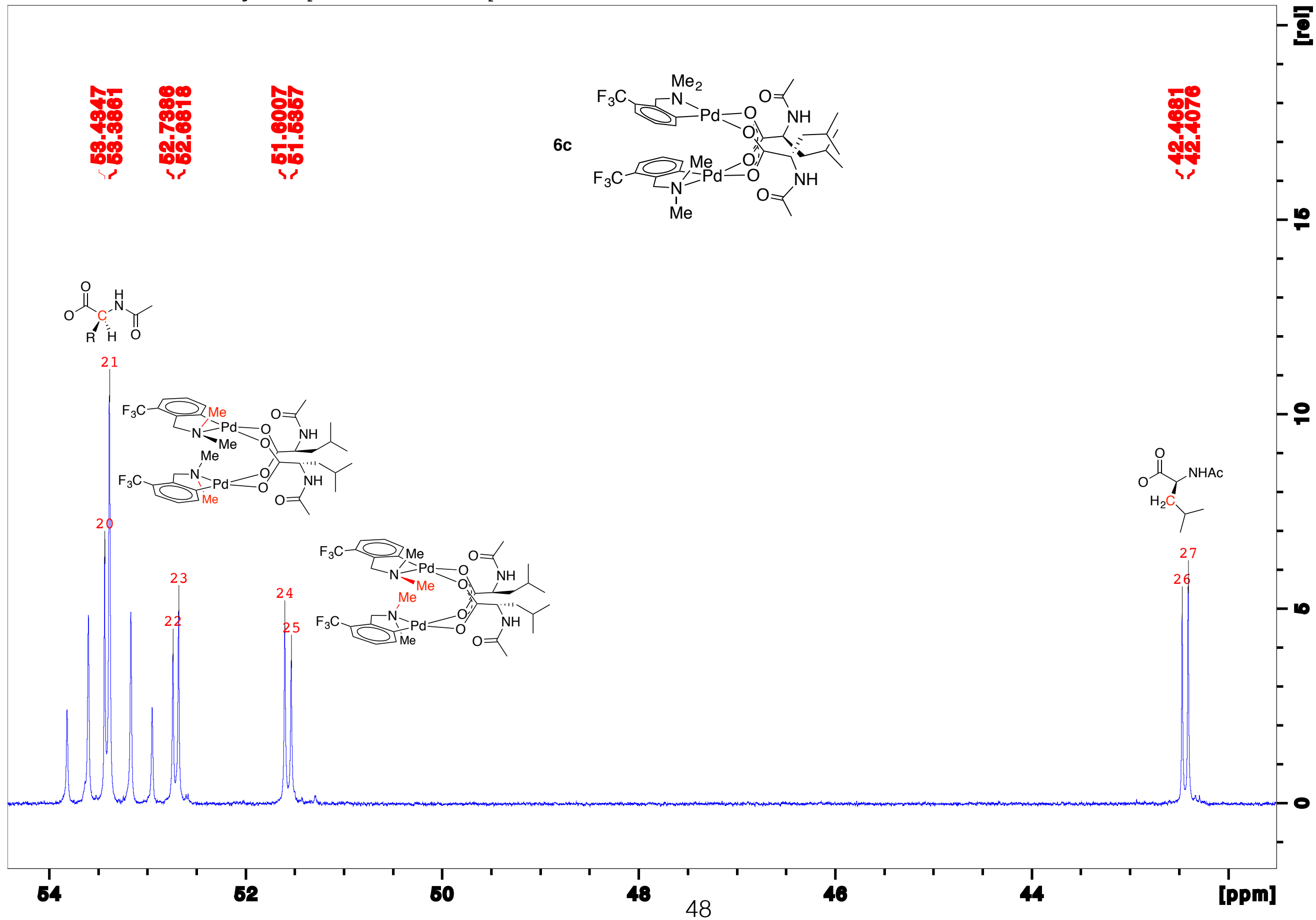
[Pd(CF₃-dmba)(NAc-Leu)]₂



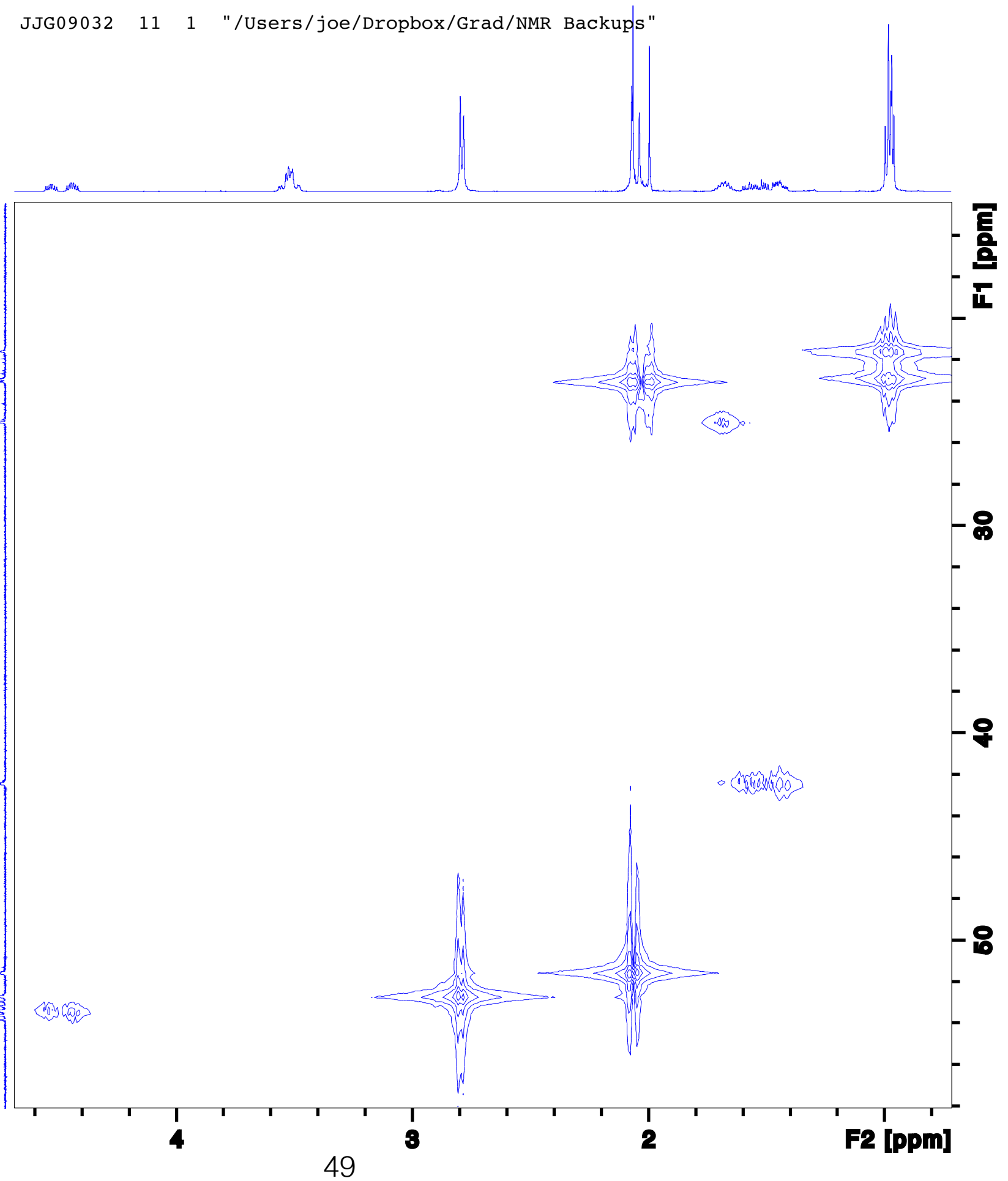
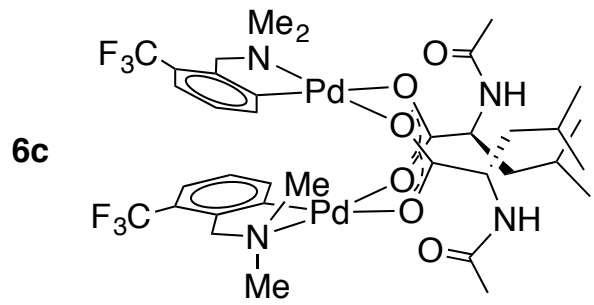


^{13}C 43-56ppm **6c**
[Pd(CF₃-dmba)(NAC-Leu)]₂

JJG09032 8 1 "/Users/joe/Dropbox/Grad/NMR Backups"

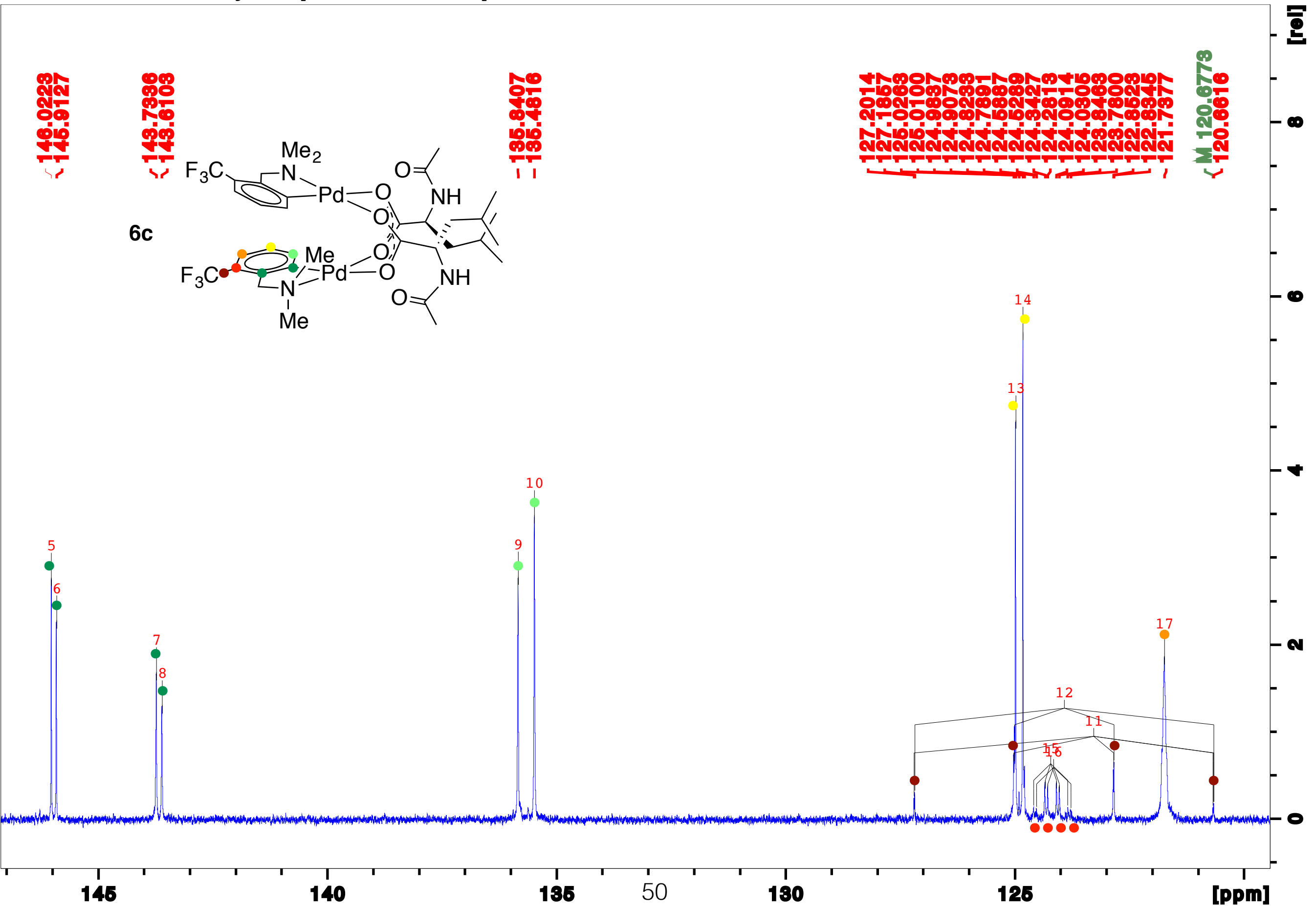


HMQC aliphatic region [Pd(CF₃-dmba)(NAC-Leu)]₂

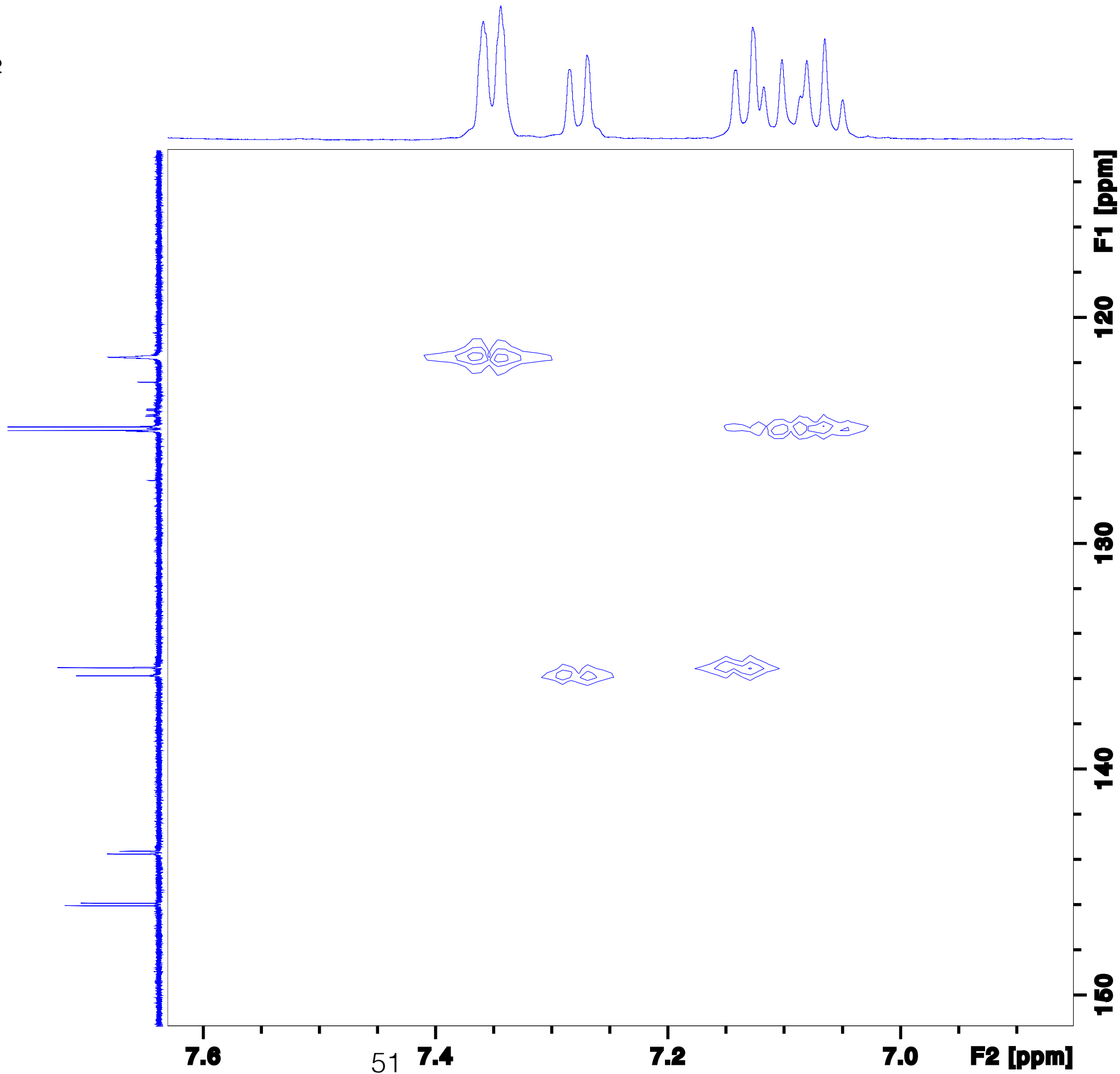
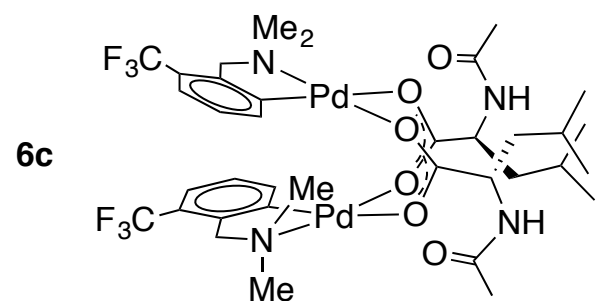


¹³C aromatic region **6c**
[Pd(CF₃-dmba)(NAc-Leu)]₂

JJG09032 8 1 "/Users/joe/Dropbox/Grad/NMR Backups"



HMQC aromatic region [Pd(CF₃-dmba)(NAC-Leu)]₂

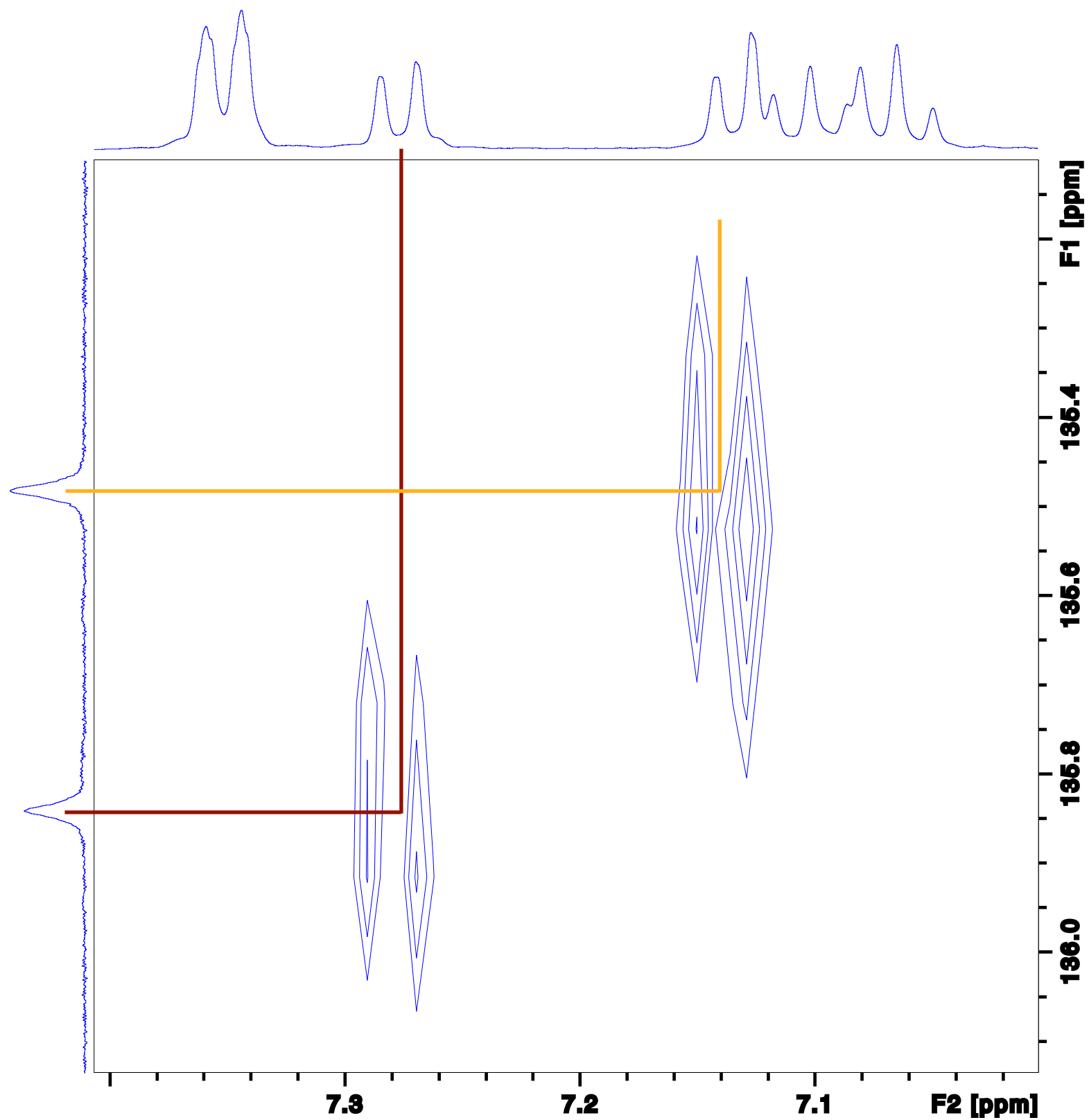
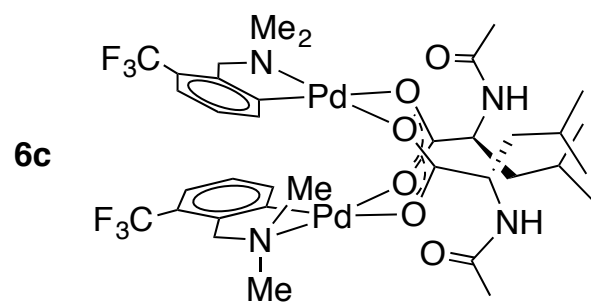


HMQC

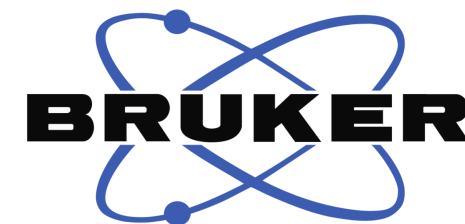
C-H's ortho to Pd

[Pd(CF₃-dmba)(NAc-Leu)]₂

JJG09032 11 1 "/Users/joe/Dropbox/Grad/NMR Backups"



¹⁹F Full **6c**
[Pd(CF₃-dmba)(NAc-Leu)]₂

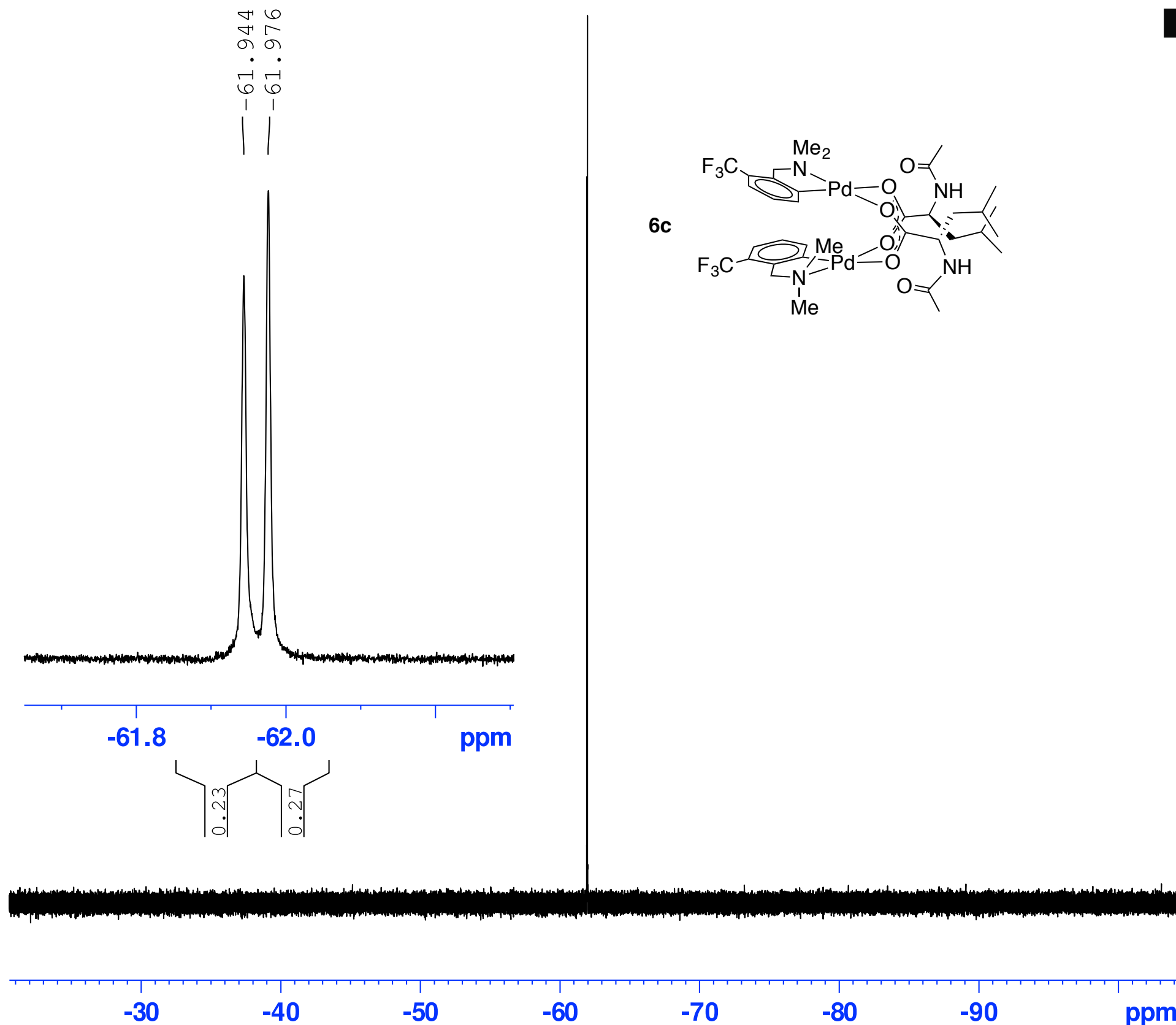
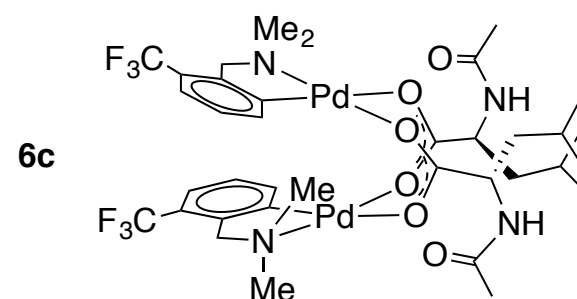


Current Data Parameters
NAME JJG09031
EXPNO 10
PROCNO 1

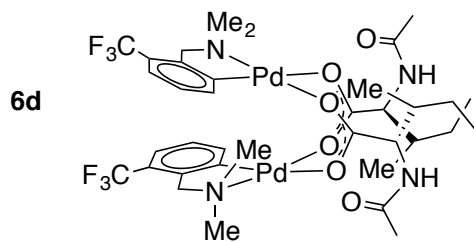
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Date_ 20161205
Time 12.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 281244
SOLVENT CD2Cl2
NS 1
DS 0
SWH 46875.000 Hz
FIDRES 0.166670 Hz
AQ 2.9999361 sec
RG 554.84
DW 10.667 usec
DE 6.50 usec
TE 296.9 K
D1 13.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 470.3176307 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



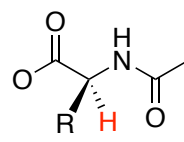
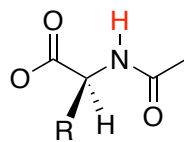
Current Data Parameters
 NAME JJG07019
 EXPNO 5
 PROCNO 1



para to Pd
+
para to Pd'

ortho to Pd

ortho to Pd'
+
meta to Pd
+
meta to Pd'



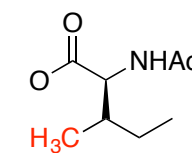
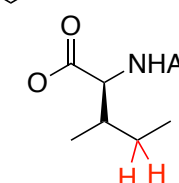
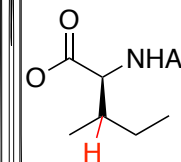
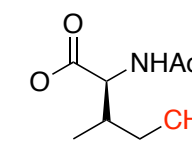
benzylic CH₂

NMe toward pi face

NMe away from pi face

NMe' away from pi face

NMe' toward pi face



7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

2.02
0.97
3.03

2.01

2.00

4.06

6.04

12.00
2.07

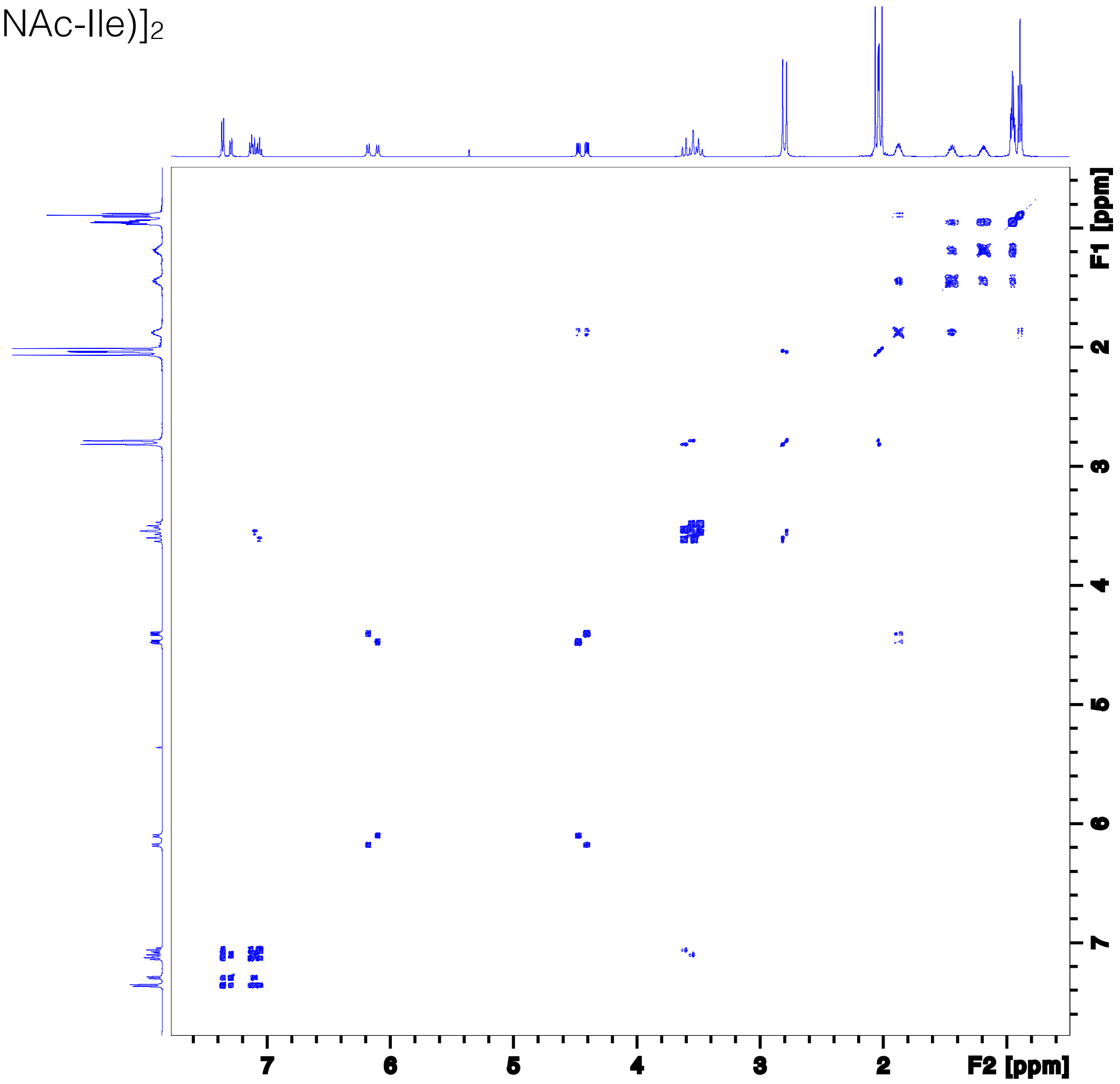
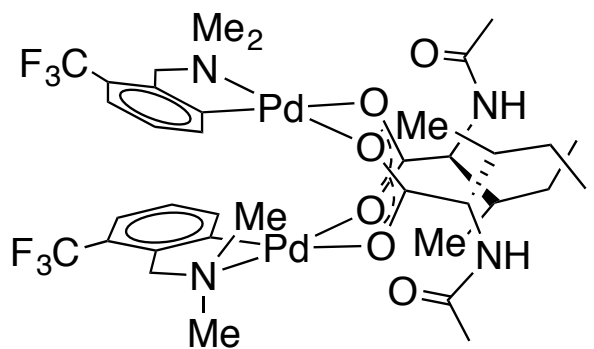
1.99

2.01

6.08
5.86

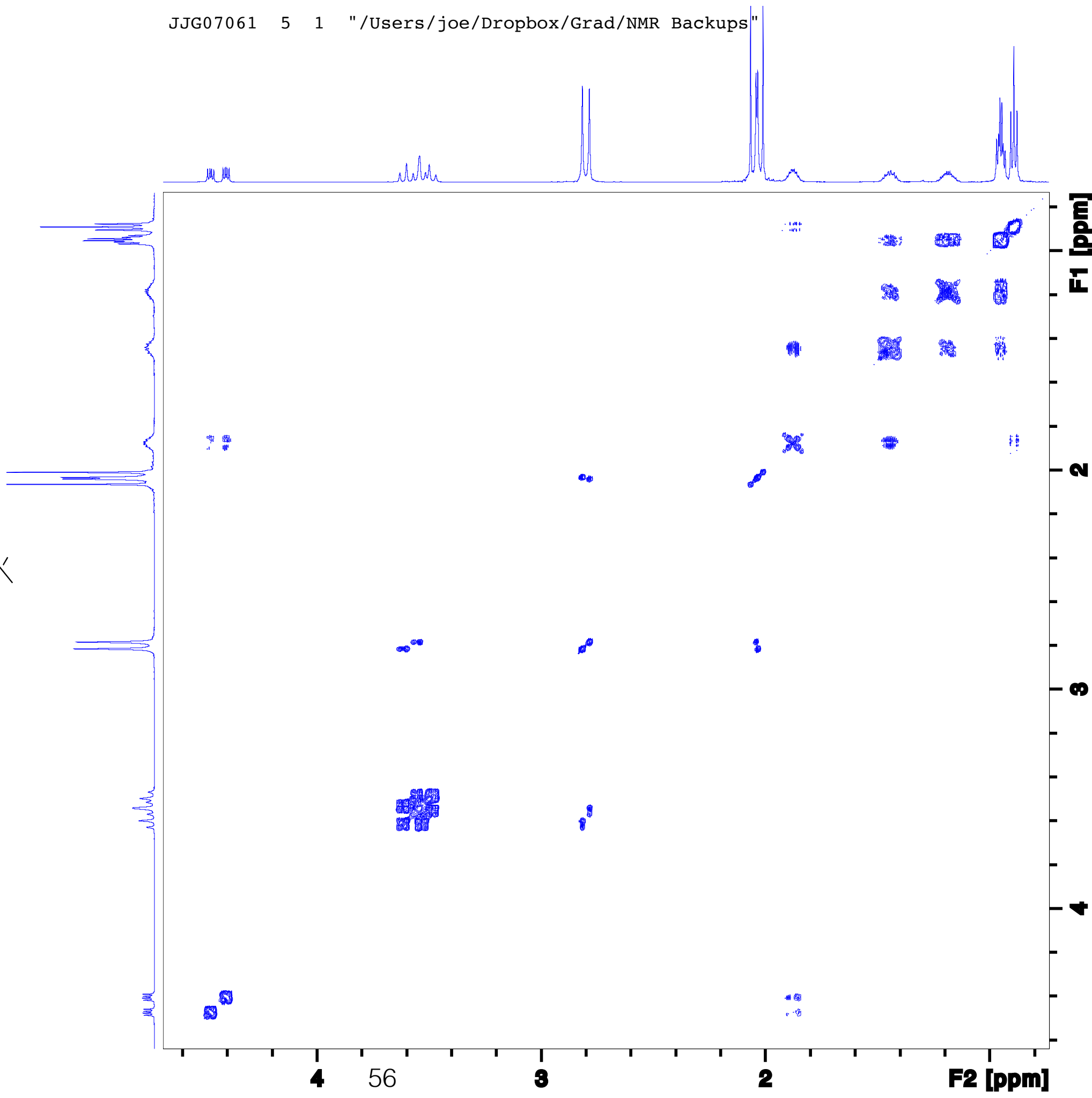
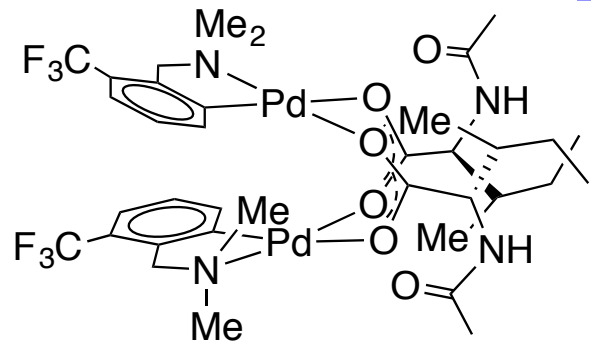
COSY [Pd(o-CF₃-dmba)(NAc-Ile)]₂

6d



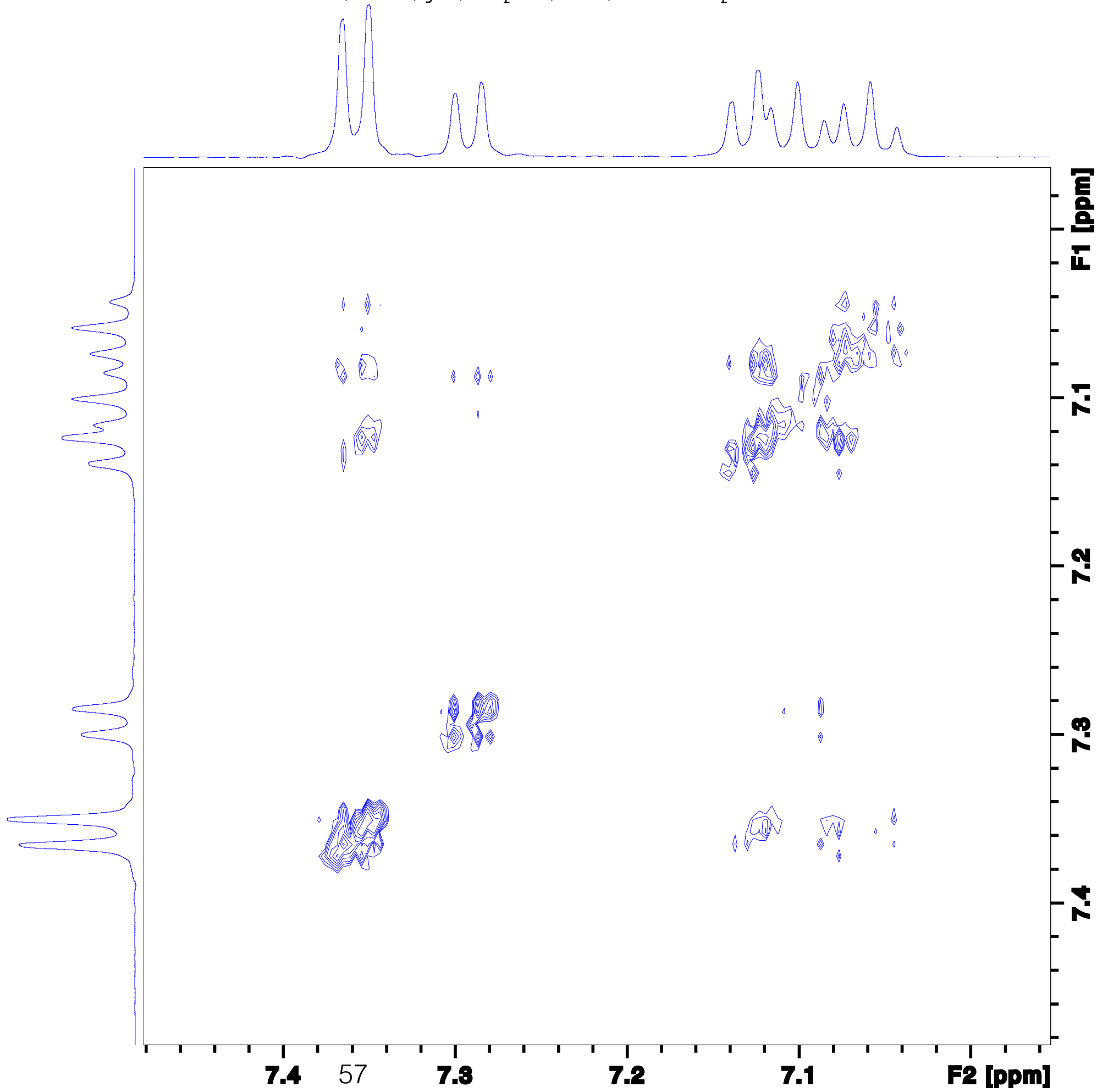
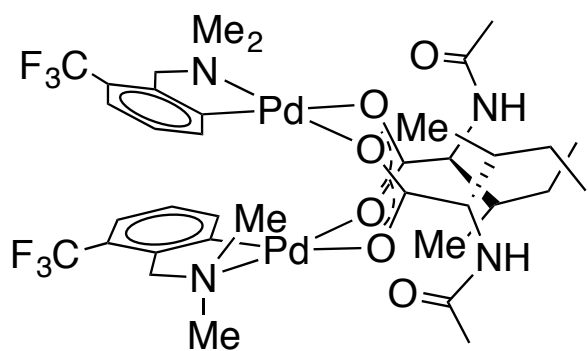
COSY aliphatic
 [Pd(o-CF₃-dmba)(NAc-Ile)]₂

6d



COSY aromatic
 [Pd(o-CF₃-dmba)(NAC-Ile)]₂

6d

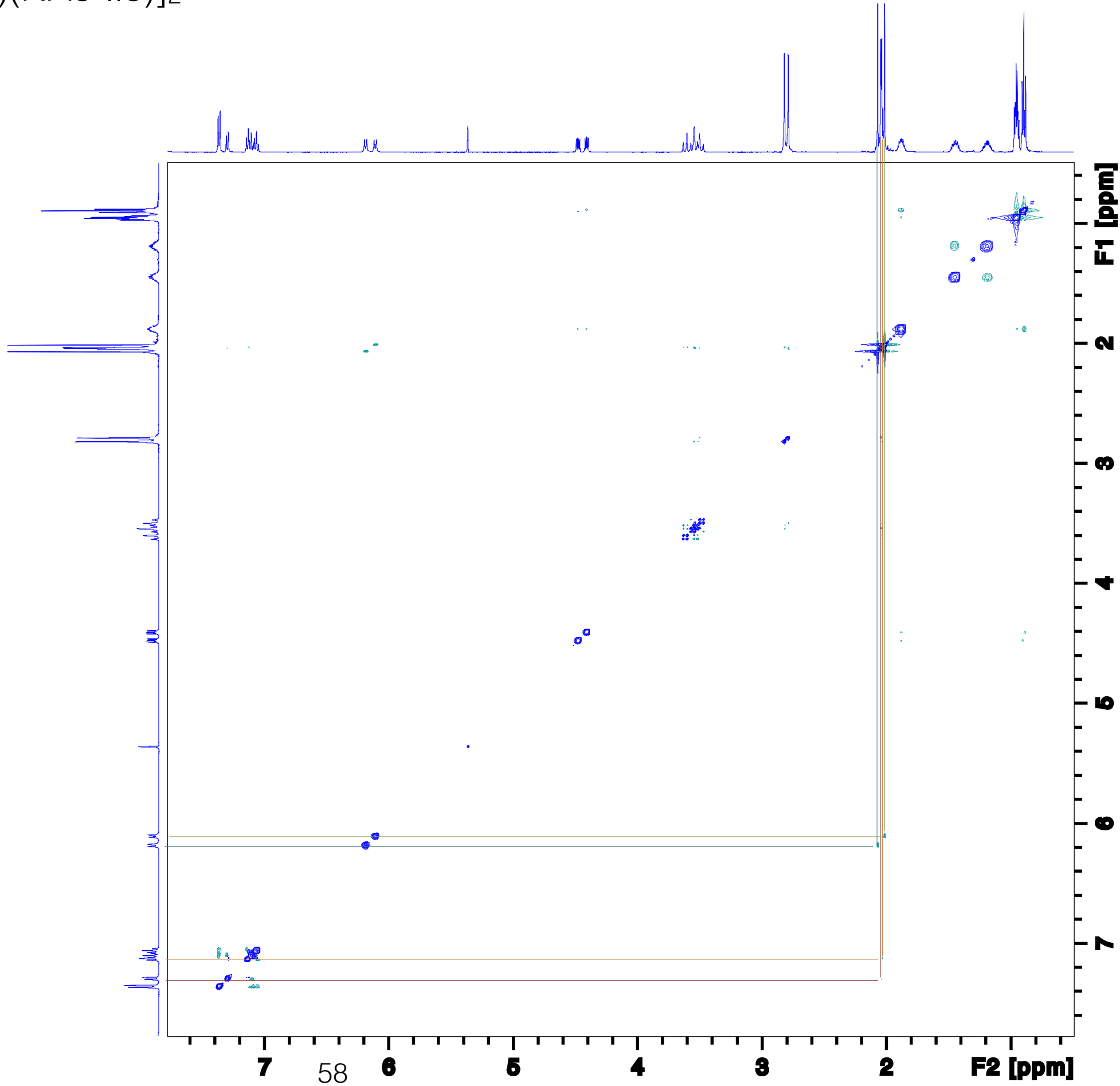
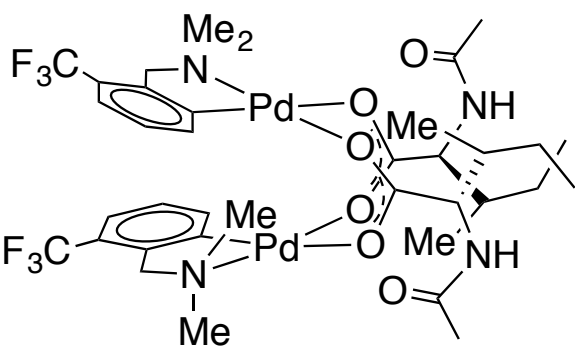


7.4 57 7.3 7.2 7.1 F2 [ppm]

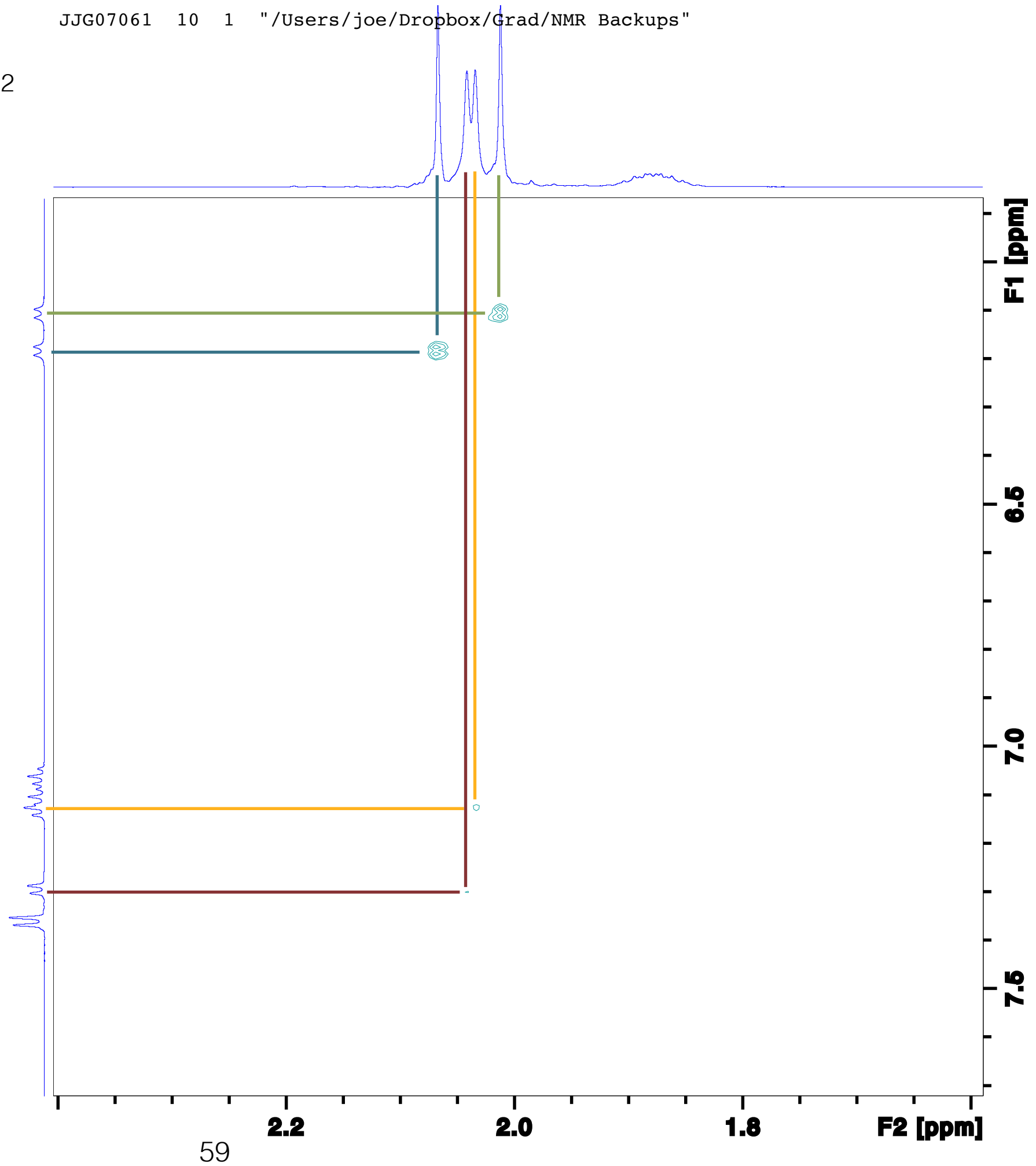
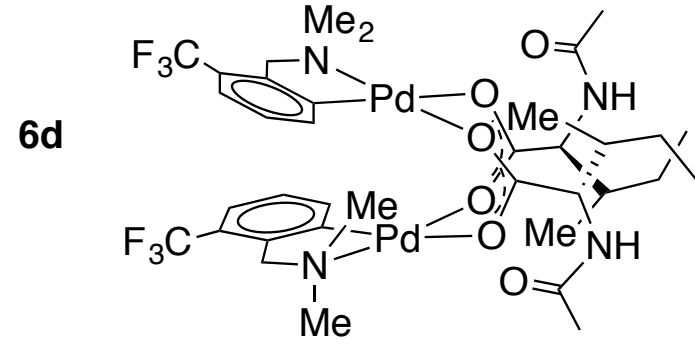
F1 [ppm]
 7.1
 7.2
 7.3
 7.4

NOESY [Pd(o-CF₃-dmba)(NAc-Ile)]₂

6d

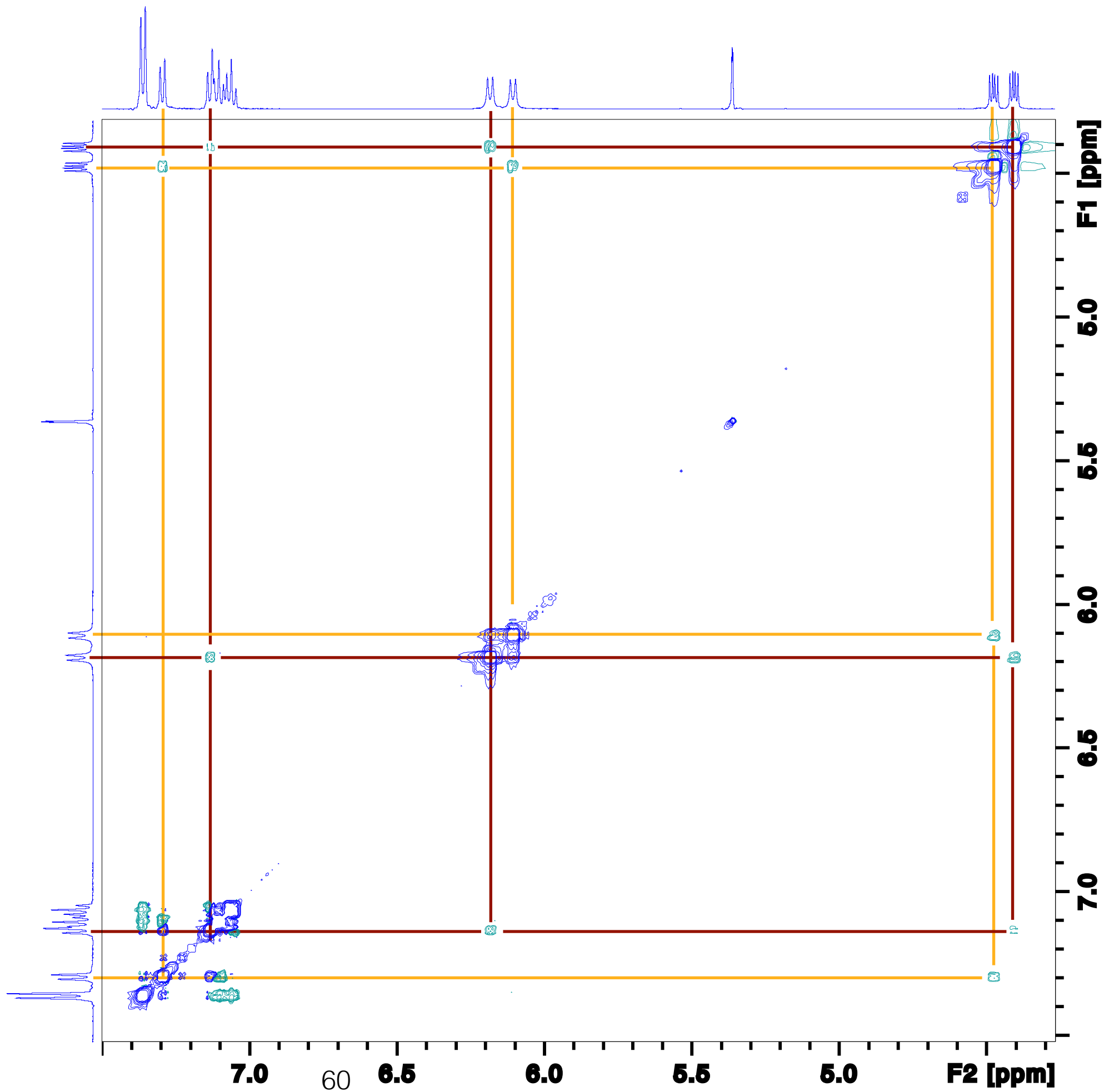
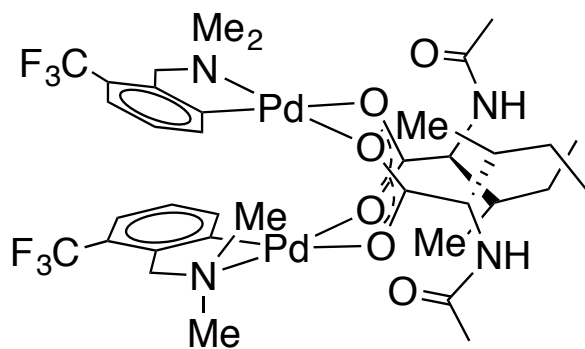


Key NOE cross peaks [Pd(o-CF₃-dmba)(NAc-Ile)]₂

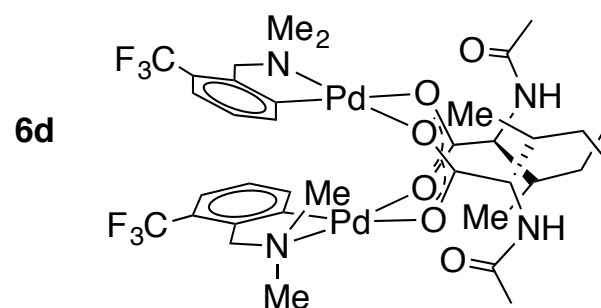


weak NOE cross peaks
between MPAA and substrate
[Pd(o-CF₃-dmba)(NAc-Ile)]₂

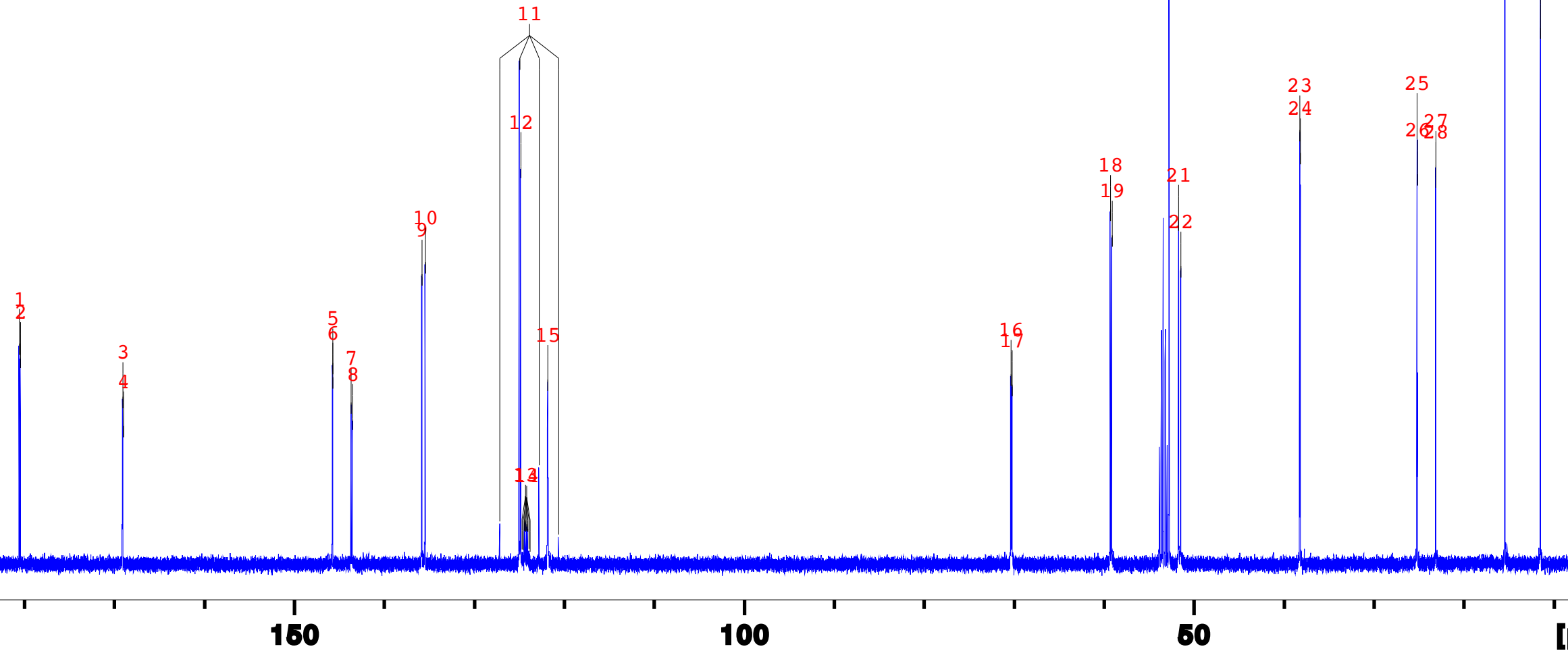
6d



^{13}C [Pd(o-CF₃-dmba)(NAc-Ile)]₂



180.5876
180.4444
169.0684
169.0401
145.7696
145.7288
143.6801
143.5425
135.8208
135.4616
127.1678
124.9898
124.8468
124.4924
124.3415
124.1809
124.0884
122.8166
121.8209
120.6384
70.9591
70.2240
59.9066
59.1947
52.7722
51.7192
51.4738
38.2461
38.1964
25.2197
25.1712
23.1939
23.1242
15.4845
15.4000
11.4886
11.4789

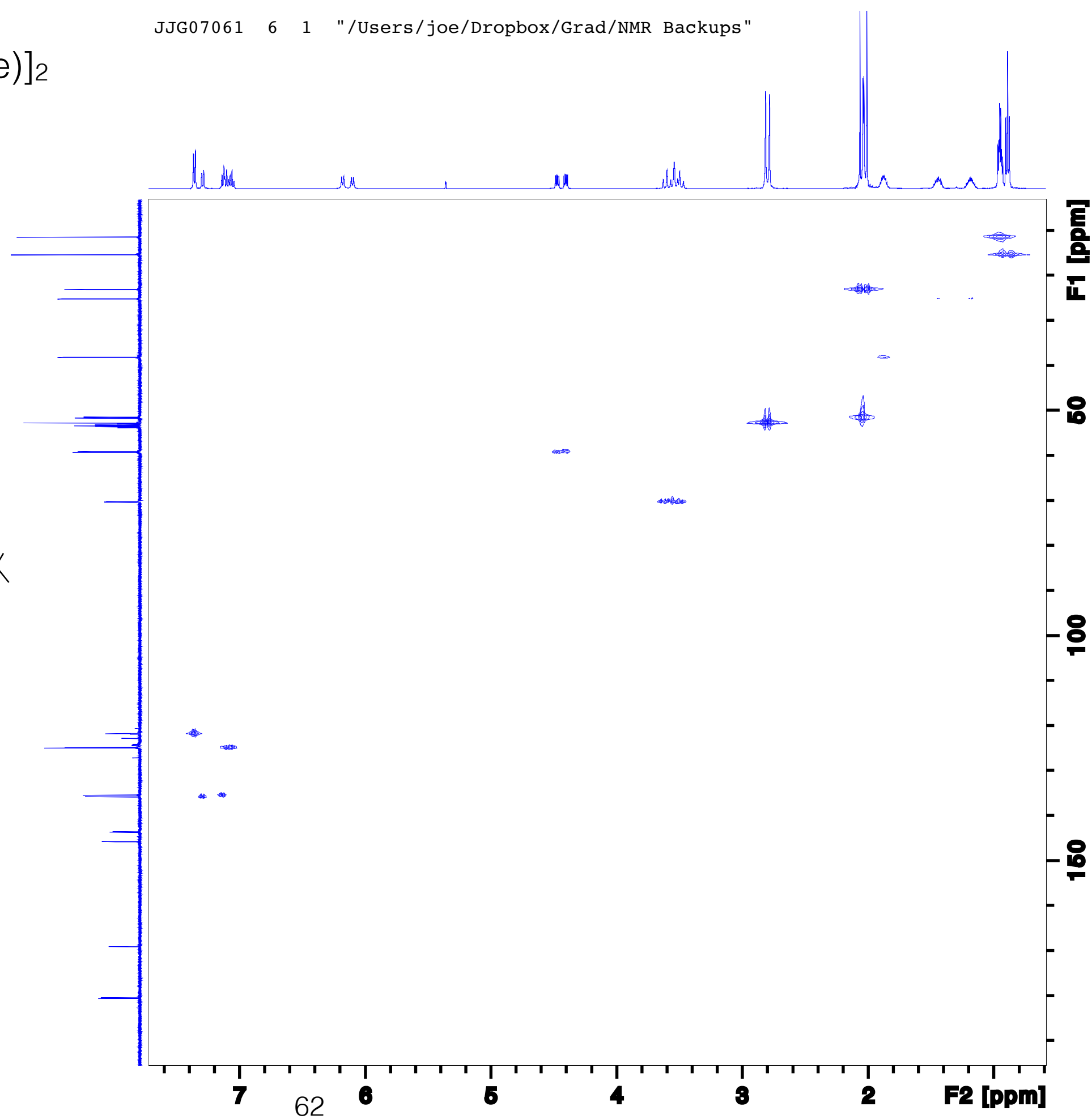
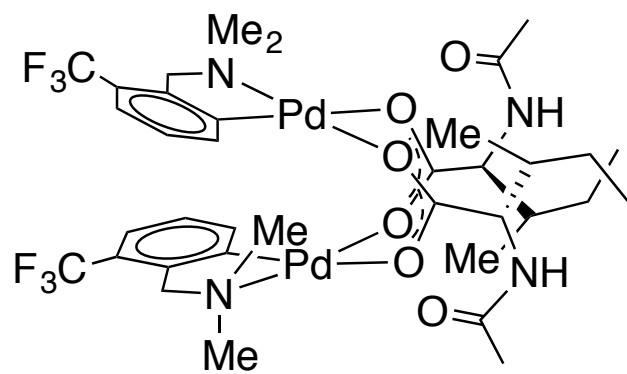


HMQC

JJG07061 6 1 "/Users/joe/Dropbox/Grad/NMR Backups"

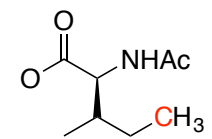
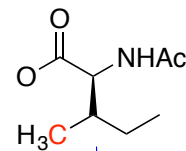
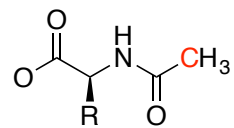
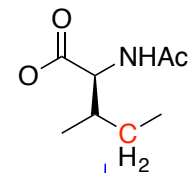
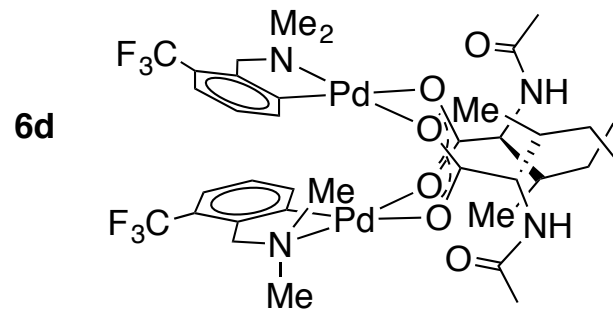


6d



¹³C 7-27 ppm
[Pd(o-CF₃-dmba)(NAc-Ile)]₂

JJG07019 7 1 "/Users/joe/Dropbox/Grad/NMR Backups"



25.2187
25.1712

28.1889
28.1242

15.4846
15.4000

11.4886
11.4789

25

20

63

15

[ppm]

[rel]

25

20

15

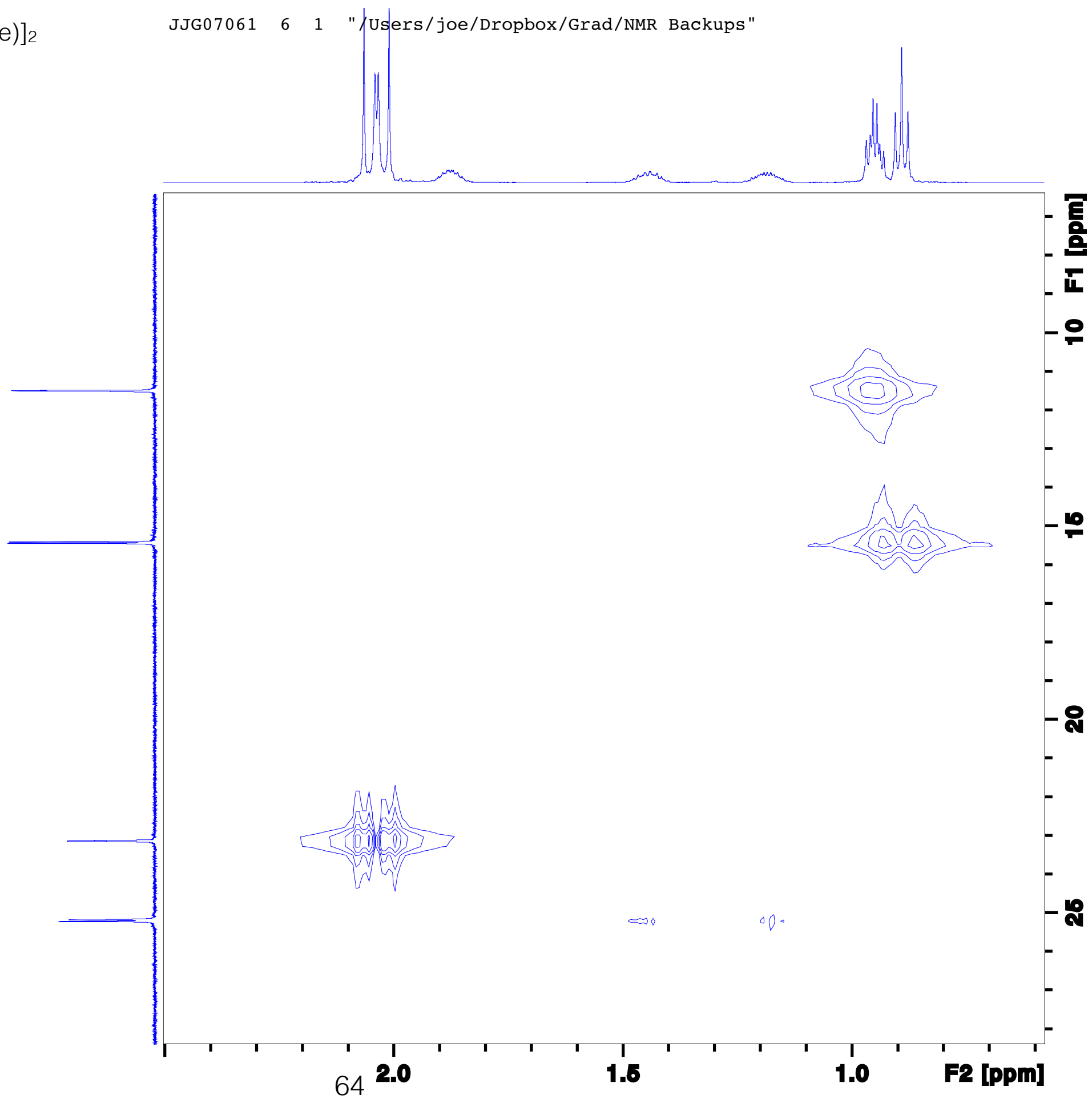
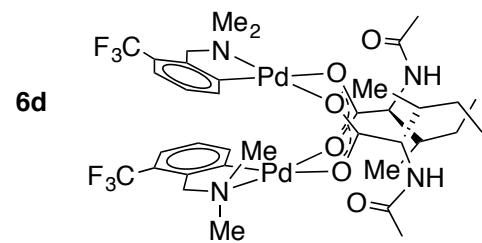
10

5

0

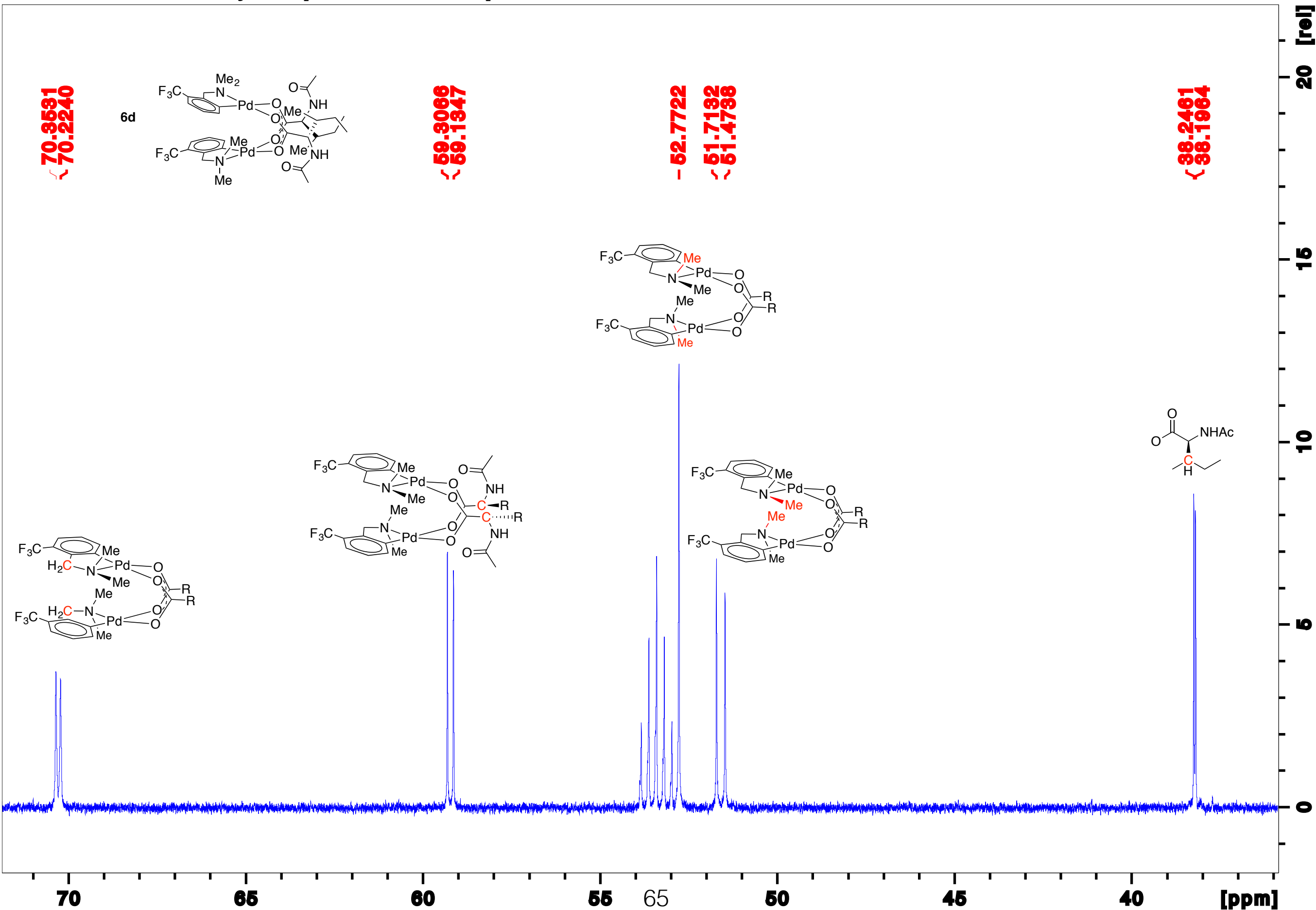
^{13}C HMQC 7-27 ppm
[Pd(o-CF₃-dmba)(NAc-Ile)]₂

JJG07061 6 1 "/Users/joe/Dropbox/Grad/NMR Backups"



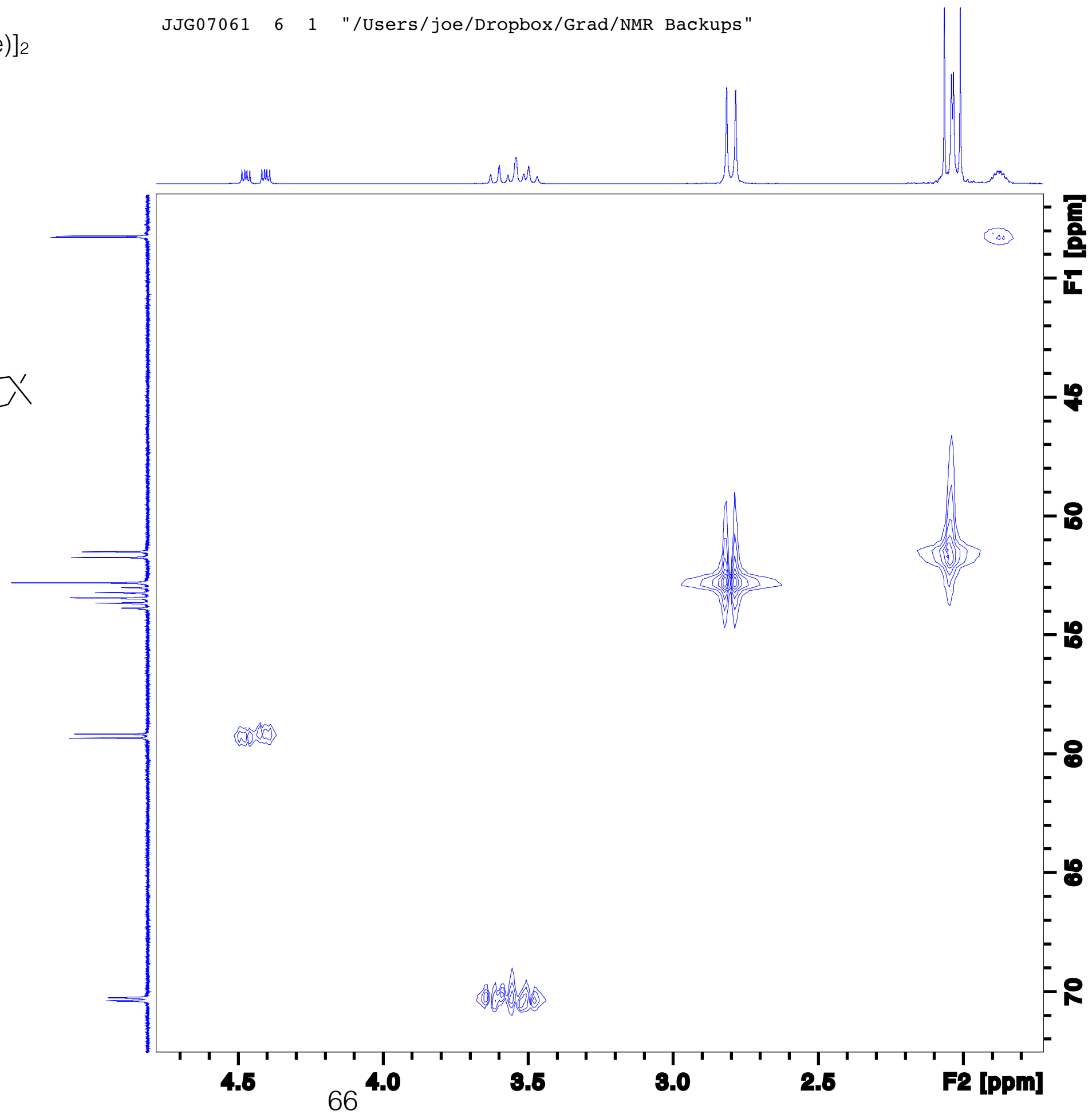
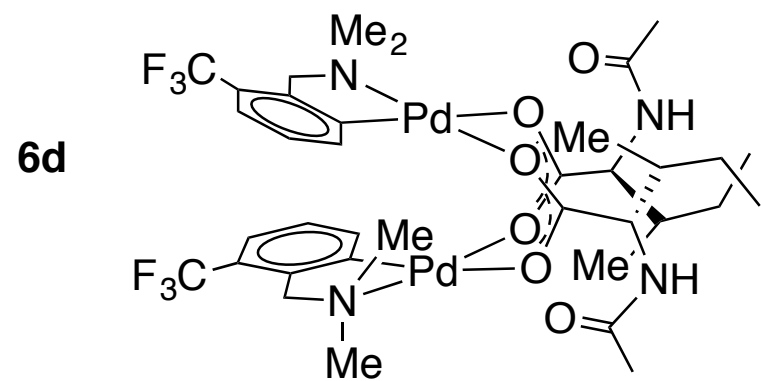
^{13}C 38-73 ppm
[Pd(o-CF₃-dmba)(NAC-Ile)]₂

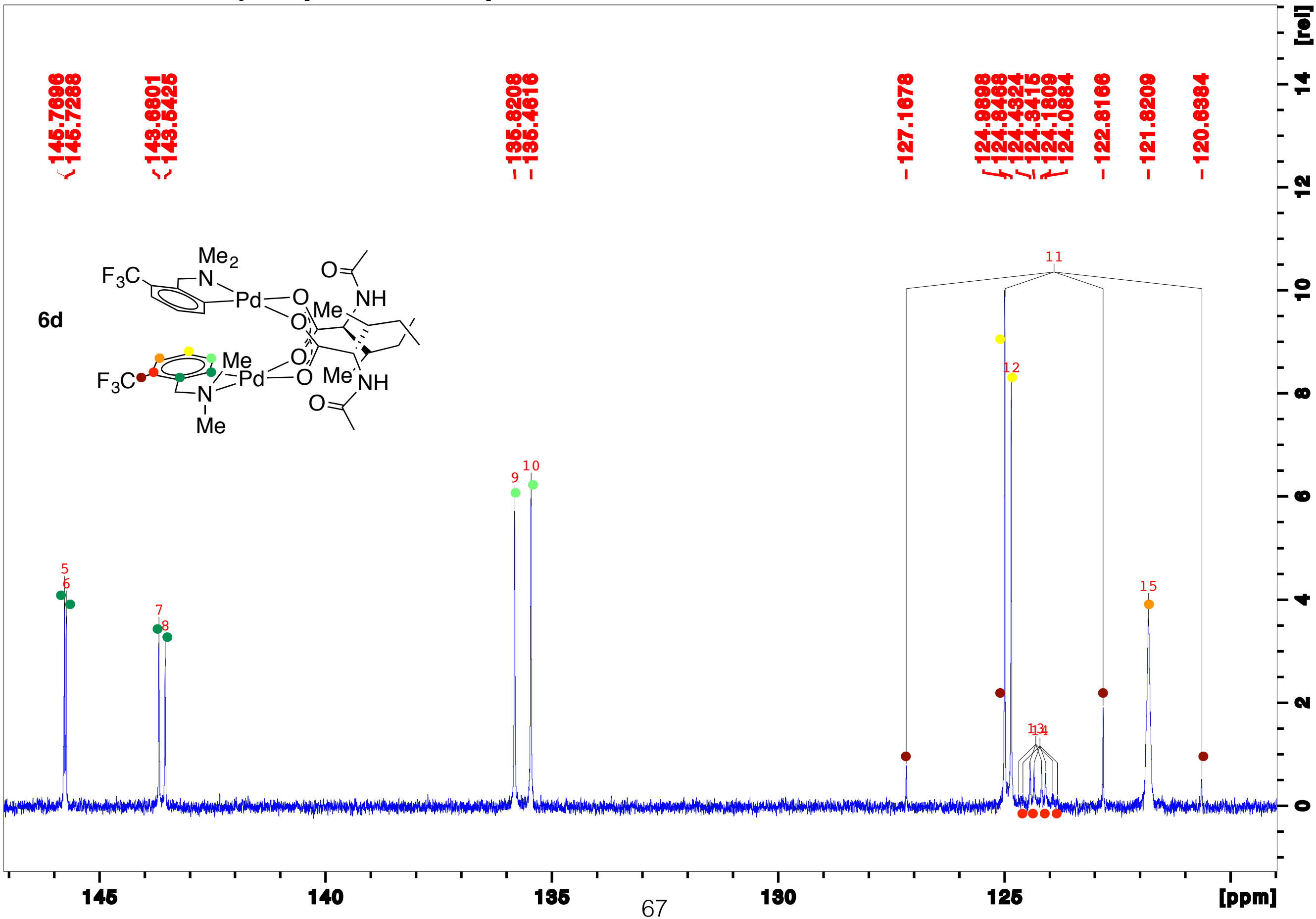
JJG07019 7 1 "/Users/joe/Dropbox/Grad/NMR Backups"



^{13}C HMQC 38-73 ppm
[Pd(o-CF₃-dmba)(NAc-Ile)]₂

JJG07061 6 1 "/Users/joe/Dropbox/Grad/NMR Backups"

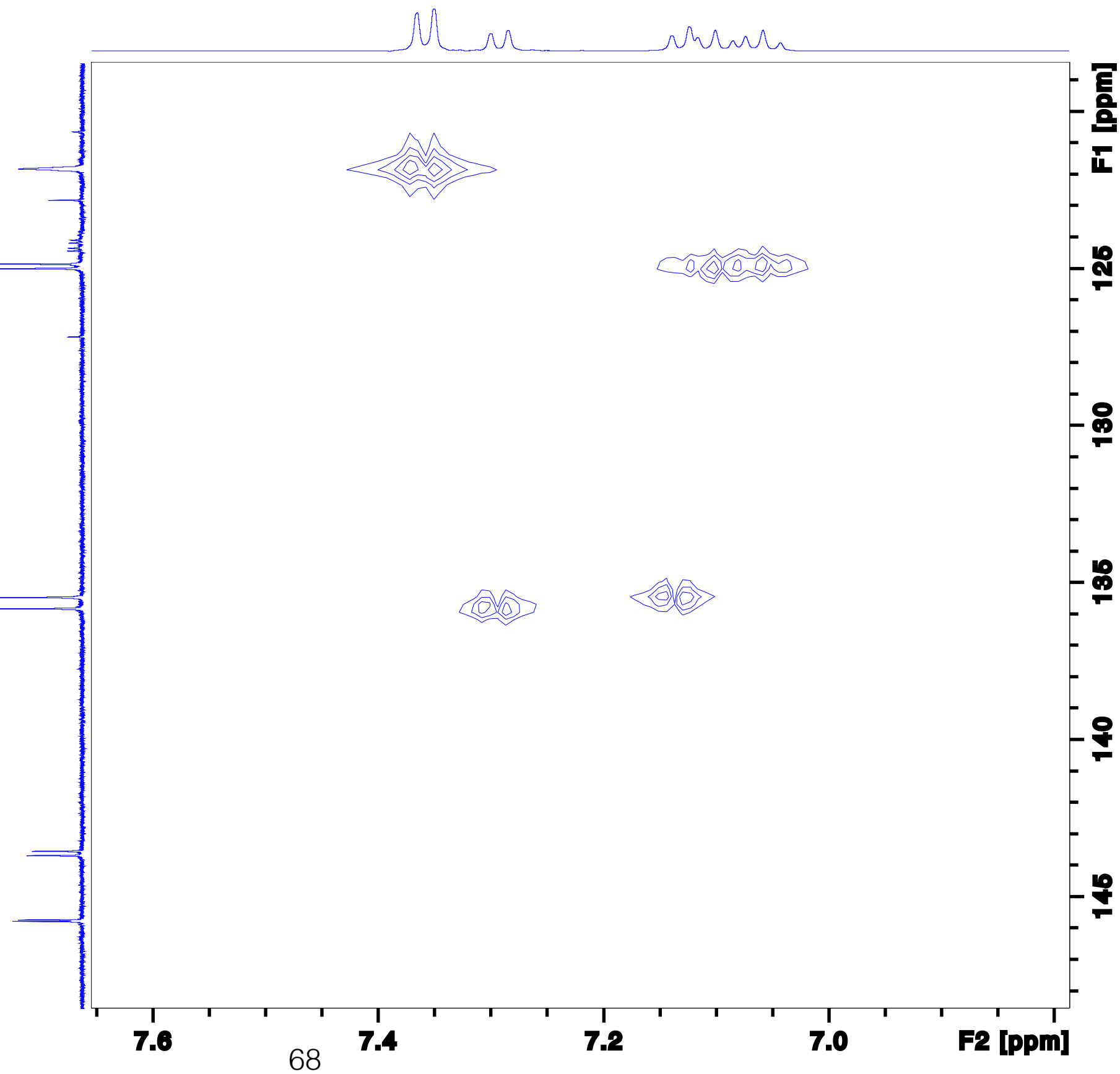
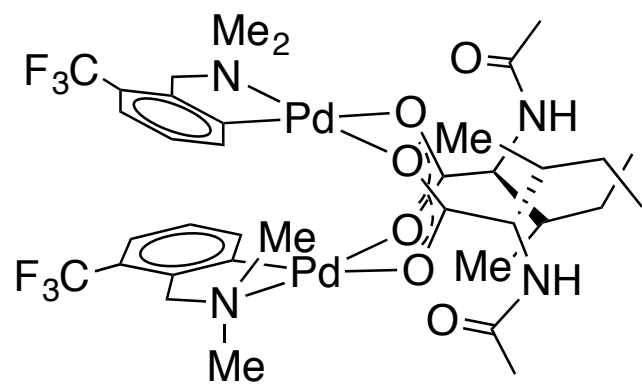




^{13}C HMQC aromatic region
[Pd(o-CF₃-dmba)(NAc-Ile)]₂

JJG07061 6 1 "/Users/joe/Dropbox/Grad/NMR Backups"

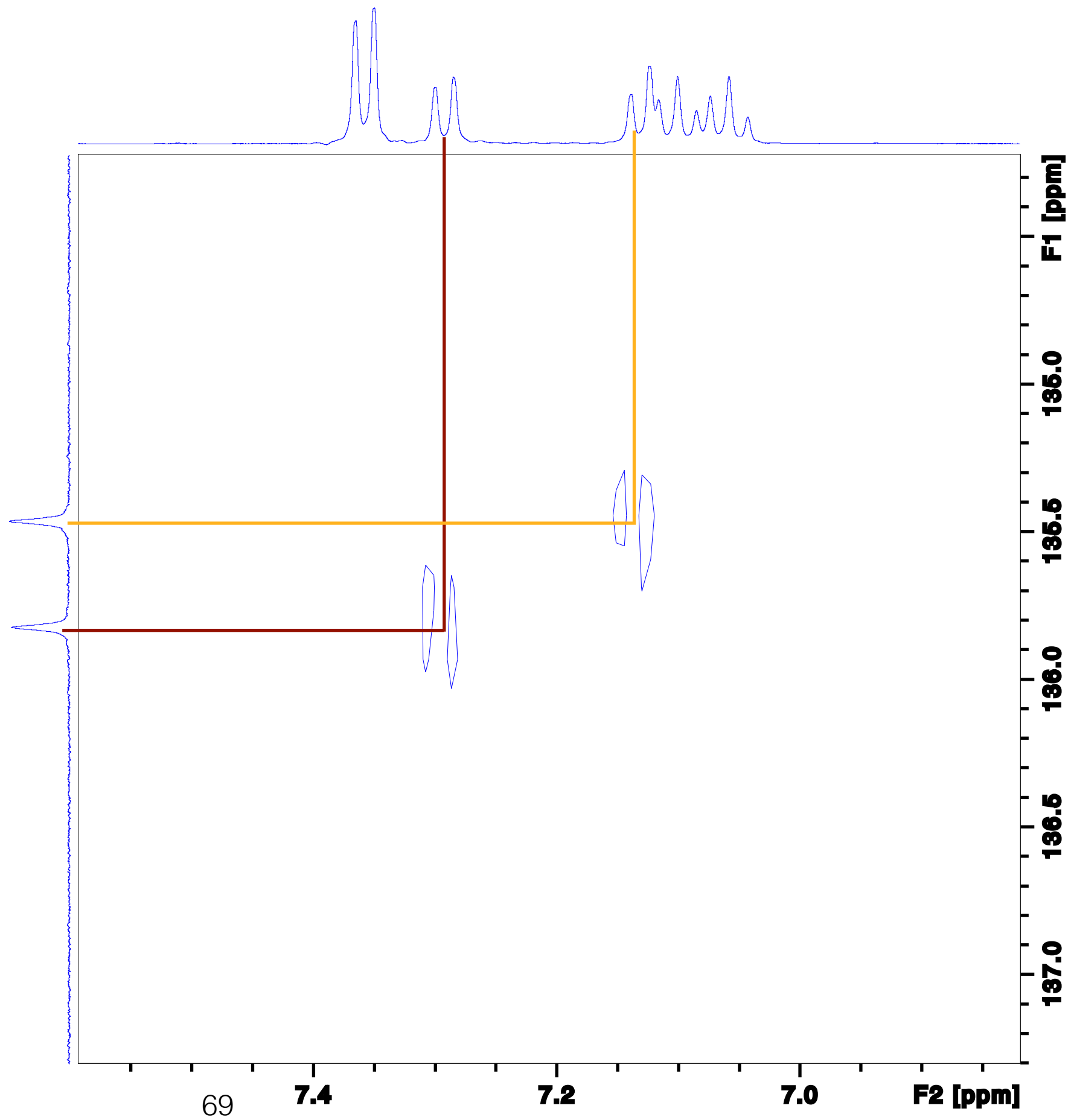
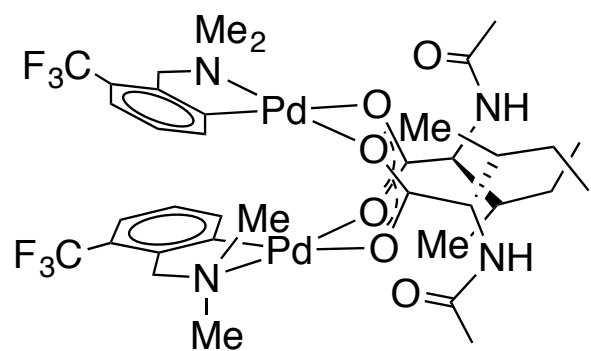
6d



HMQC C-H's ortho to Pd
[Pd(o-CF₃-dmba)(NAC-Ile)]₂

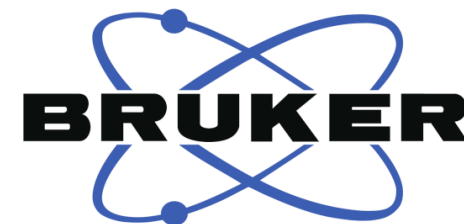
JJG07061 6 1 "/Users/joe/Dropbox/Grad/NMR Backups"

6d



^{19}F [Pd(o-CF₃-dmba)(NAc-Ile)]₂

∨
-61.923
-61.976

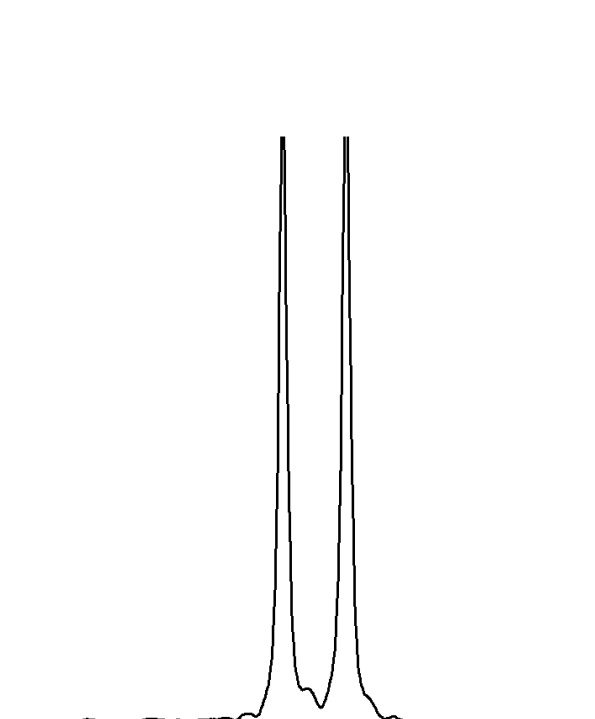
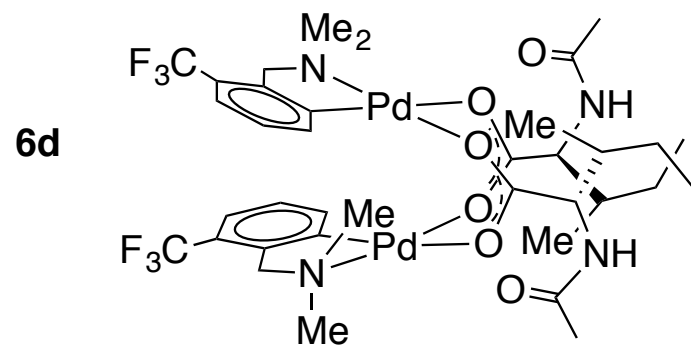


Current Data Parameters
NAME JYG07019
EXPNO 6
PROCNO 1

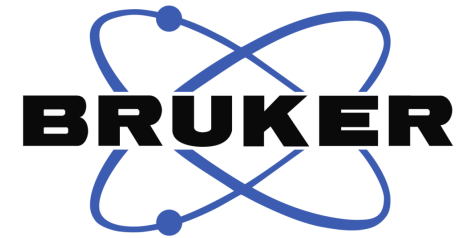
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Date_ 20160622
Time 10.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 703112
SOLVENT CD₂Cl₂
NS 1
DS 0
SWH 117187.500 Hz
FIDRES 0.166670 Hz
AQ 2.9999444 sec
RG 189.89
DW 4.267 usec
DE 6.50 usec
TE 296.0 K
D1 12.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 470.3195121 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



¹H [Pd(o-CF₃-dmba)(OAc)]₂

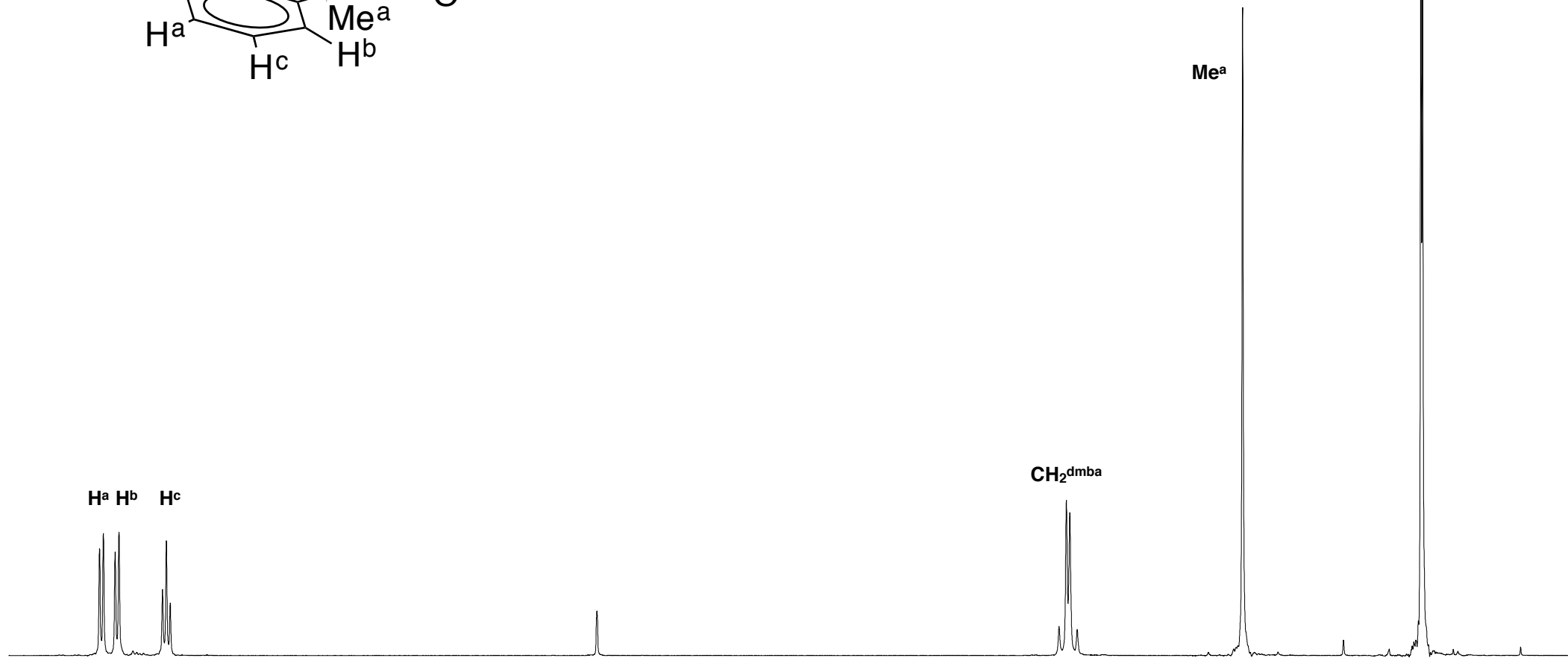
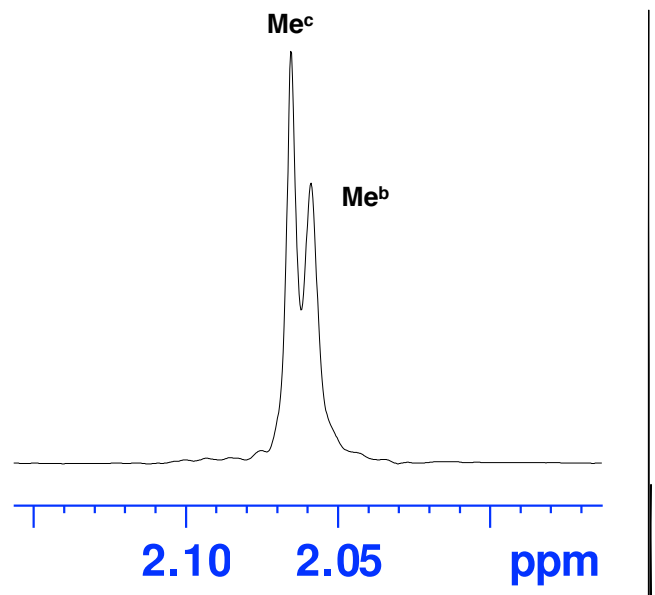
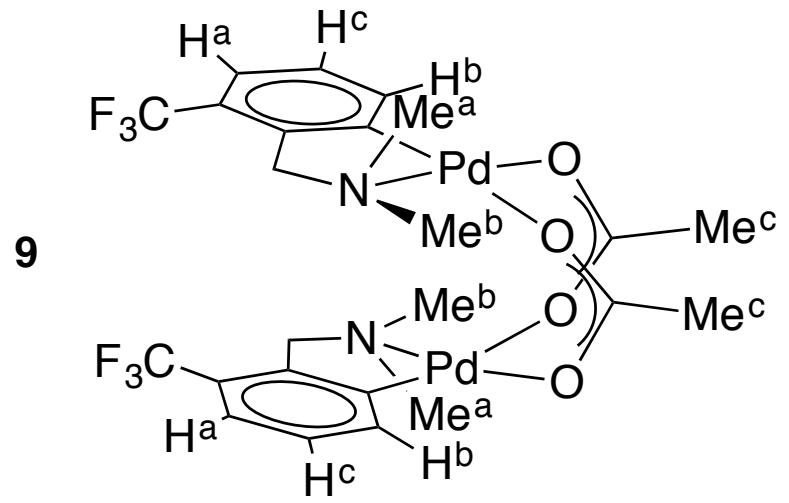


Current Data Parameters
NAME JYG09042
EXPNO 1
PROCNO 1

F2 - Acquisition Parameter
Date_ 20161208
Time 5.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 59998
SOLVENT CD2Cl2
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 0.166672 Hz
AQ 2.9999001 sec
RG 29.95
DW 50.000 usec
DE 6.50 usec
TE 297.0 K
D1 30.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 499.8730869 MHz
NUC1 1H
P1 10.75 usec
PLW1 18.25000000 W

F2 - Processing parameters
SI 65536
SF 499.8700000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

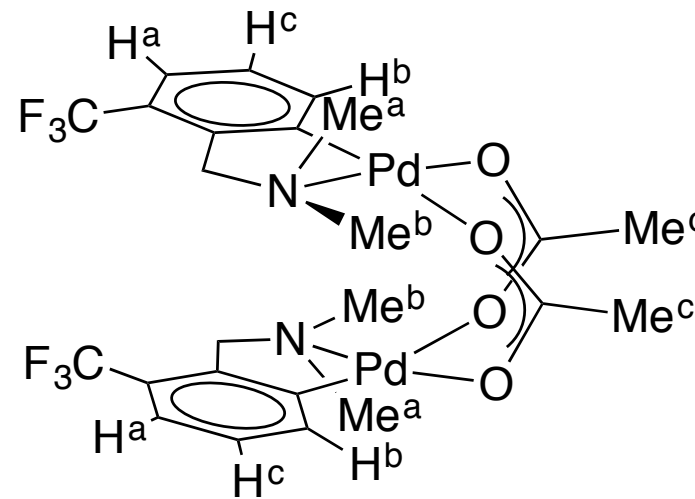


7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 ppm

2.02 2.06 2.03 4.02 6.00 12.02

71

^{19}F [Pd(o-CF₃-dmba)(OAc)]₂

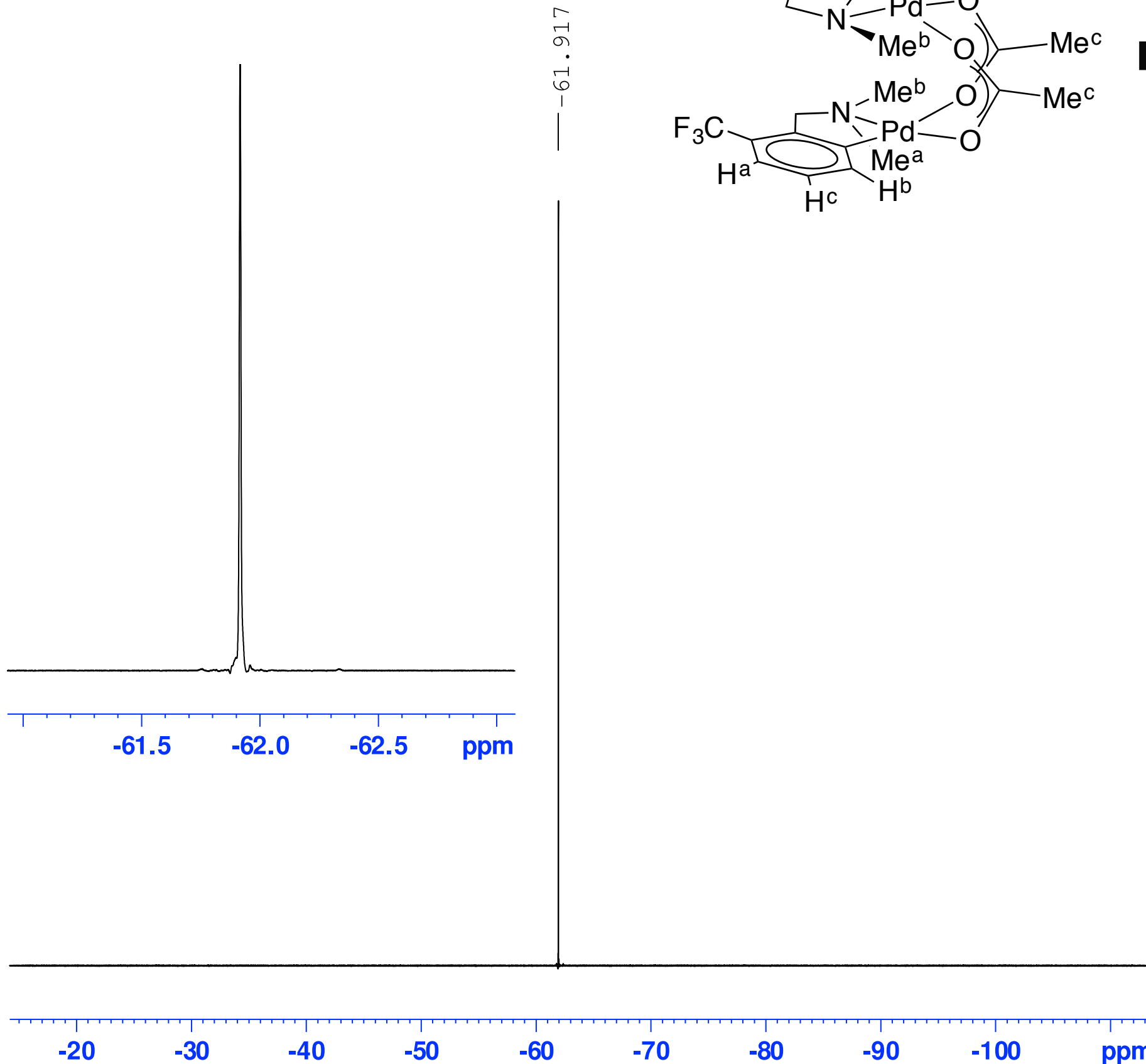


Current Data Parameters
NAME JYG09042
EXPNO 6
PROCNO 1

F2 - Acquisition Parameter
Date_ 20161208
Time 6.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqg
TD 281244
SOLVENT CD2Cl2
NS 1
DS 0
SWH 46875.000 Hz
FIDRES 0.166670 Hz
AQ 2.9999361 sec
RG 310.79
DW 10.667 usec
DE 6.50 usec
TE 297.7 K
D1 3.00000000 sec
TD0 1

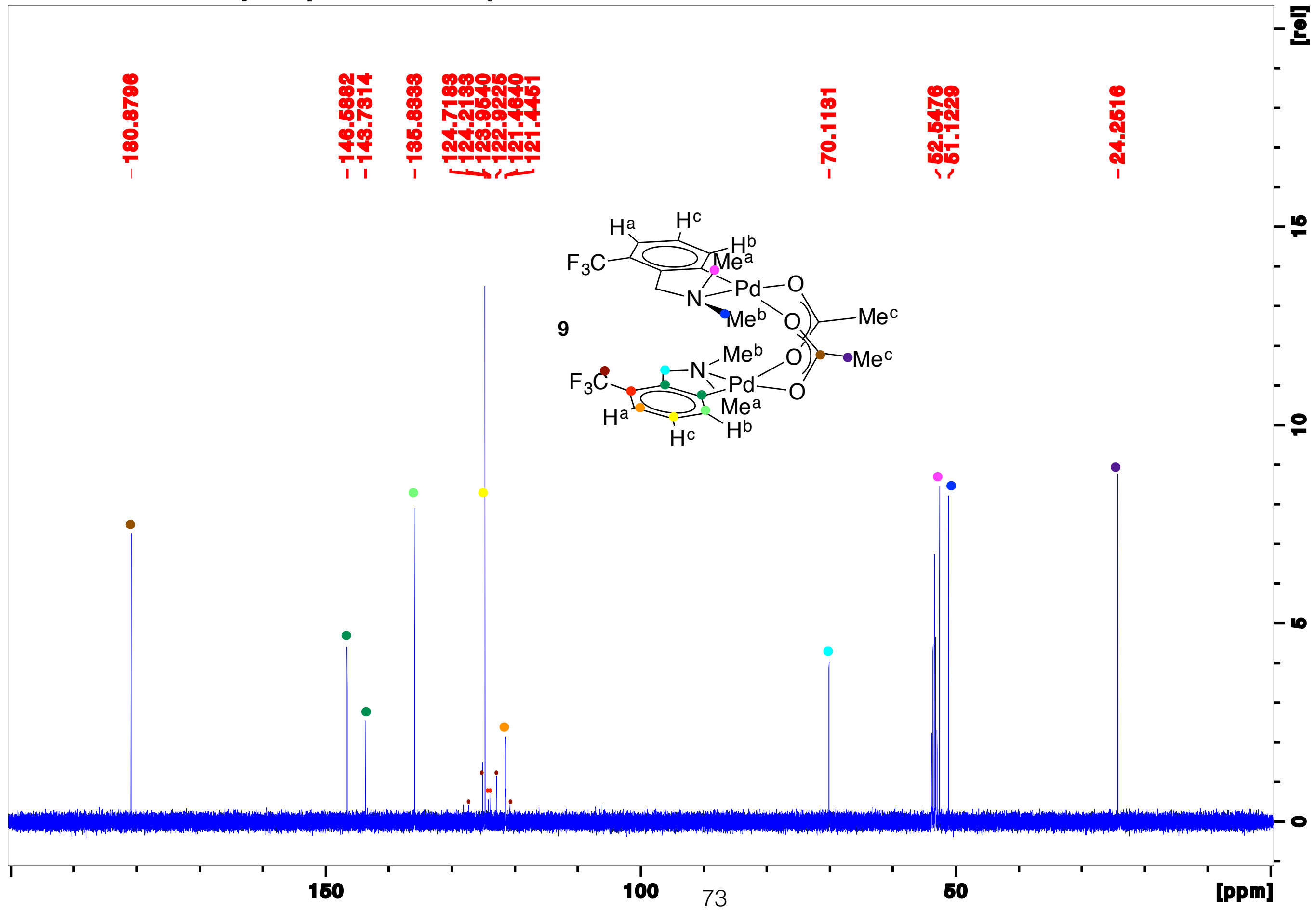
==== CHANNEL f1 =====
SF01 470.3176307 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



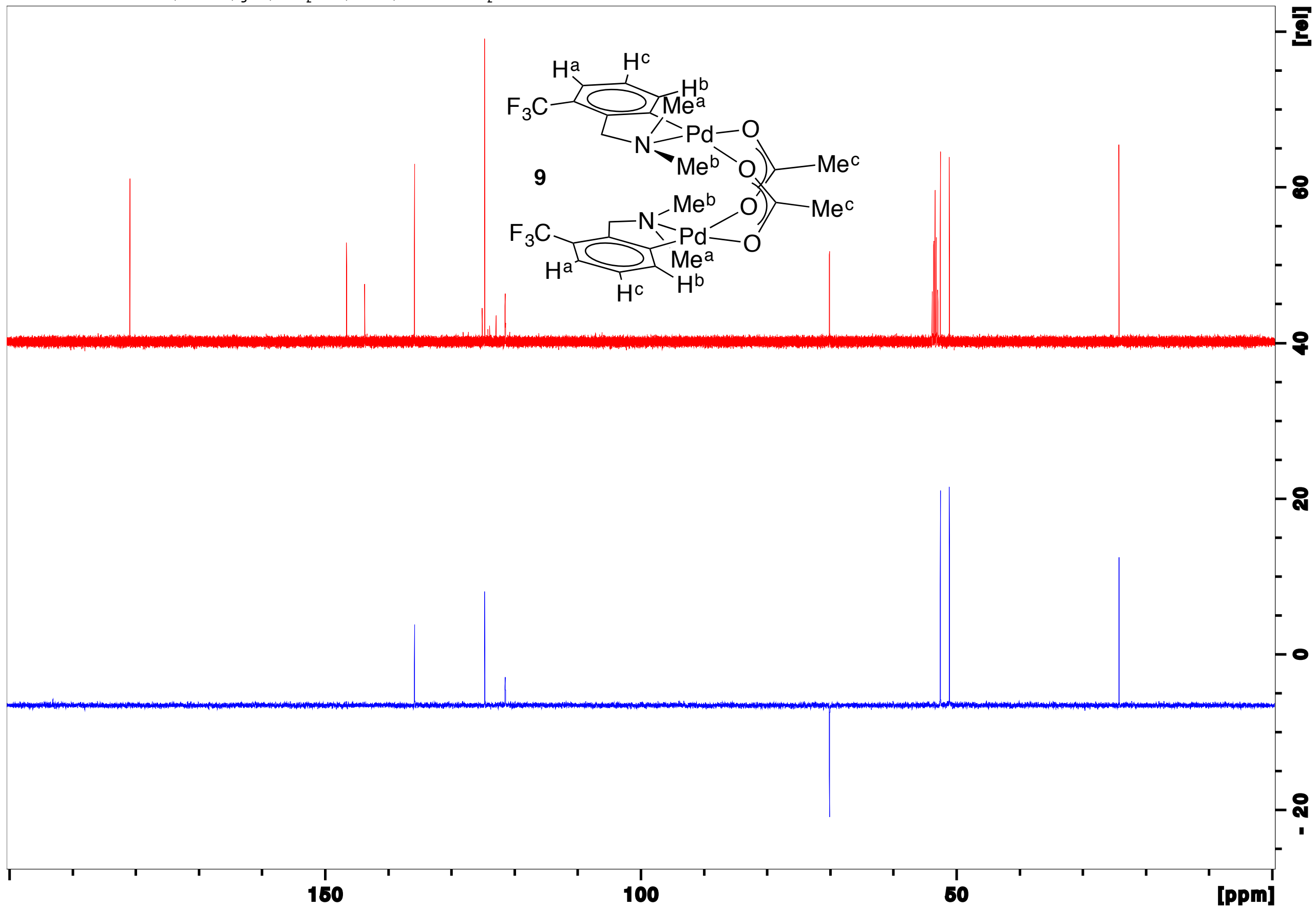
$^{13}\text{C}\{^1\text{H}\}$ [Pd(*o*-CF₃-dmba)(OAc)]₂

JJG09042 2 1 "/Users/joe/Dropbox/Grad/NMR Backups"



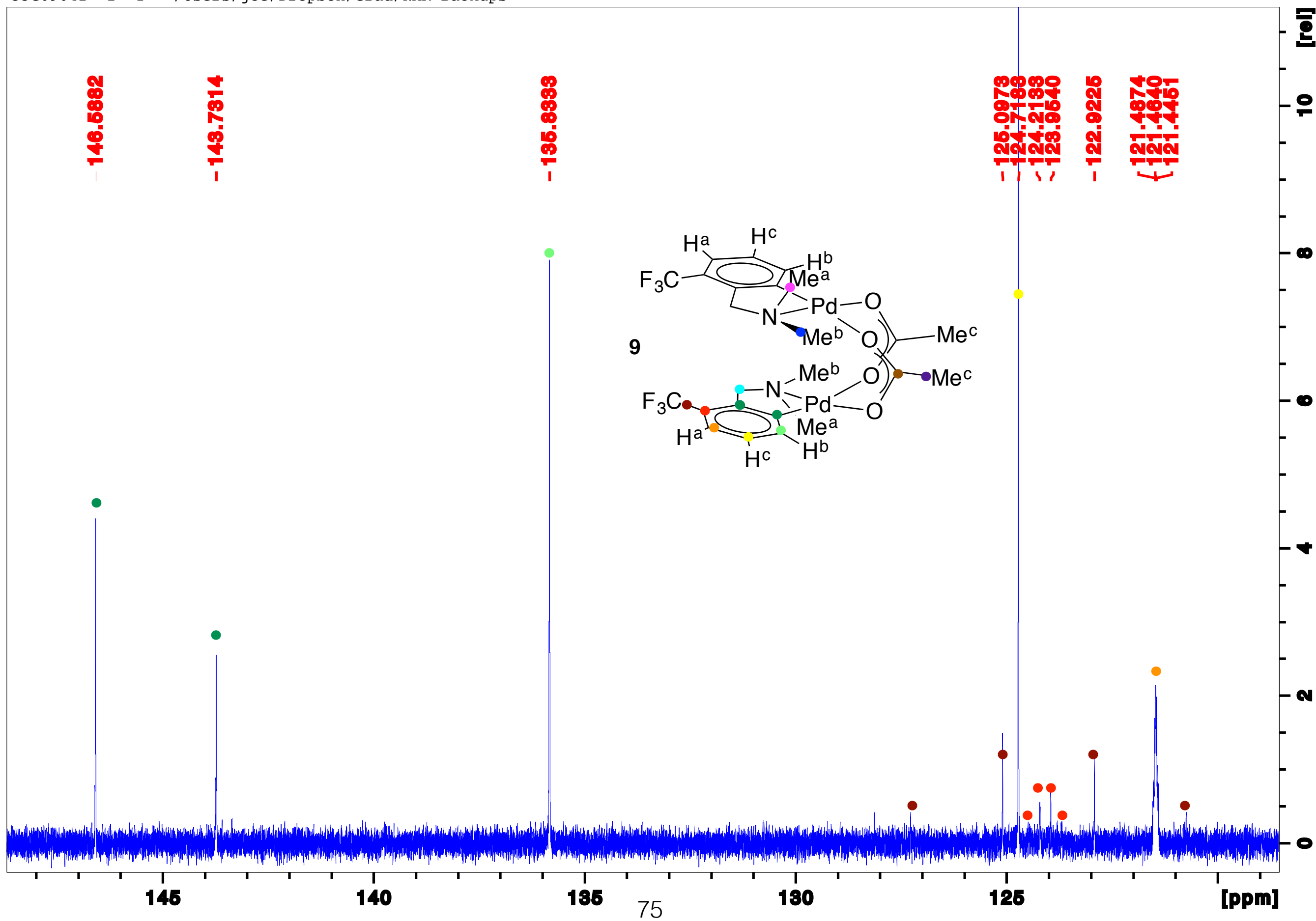
$^{13}\text{C}\{^1\text{H}\}$ [Pd(*o*-CF₃-dmba)(OAc)]₂ : overlaid with DEPT 135

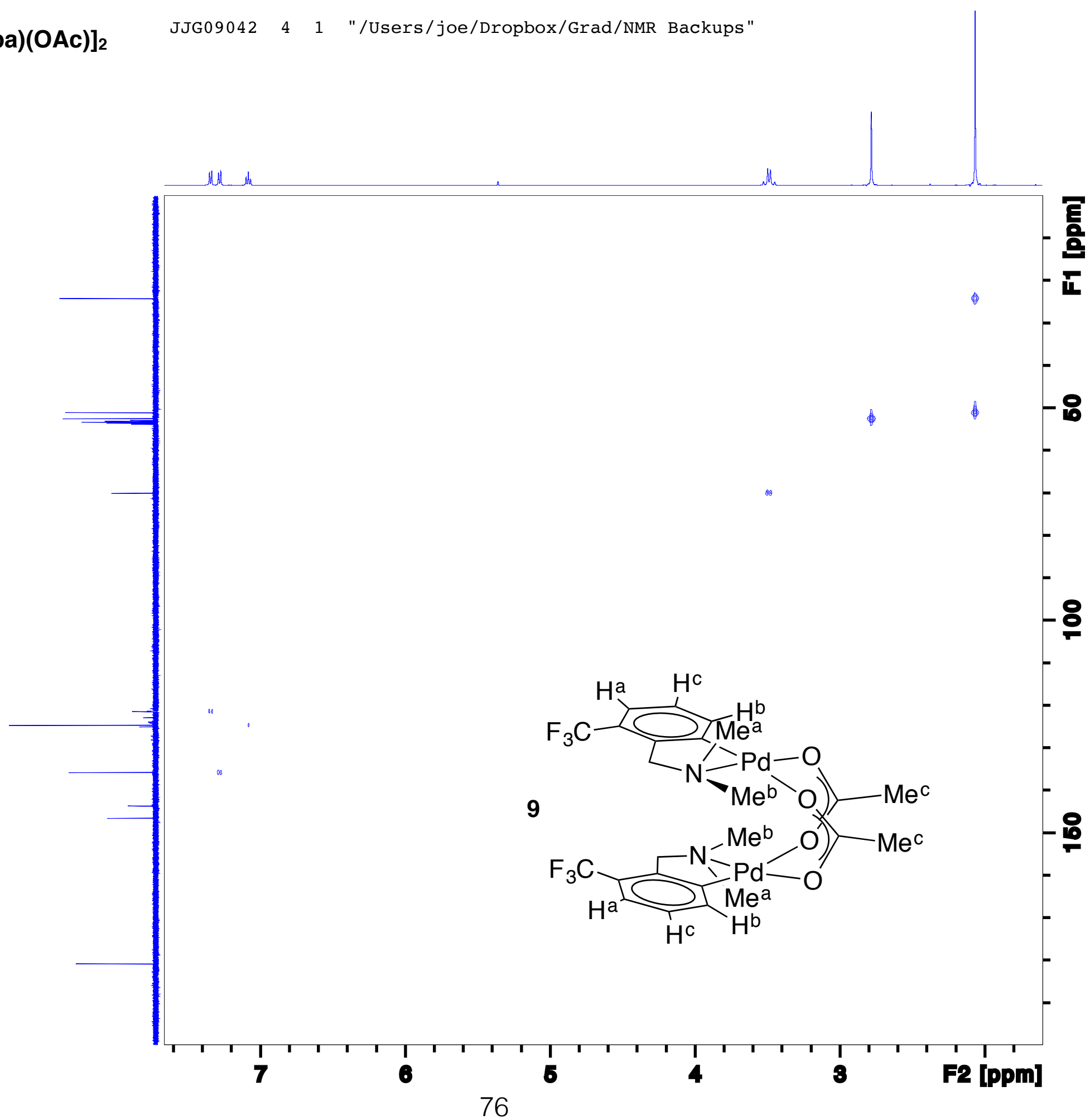
JJG09042 3 1 "/Users/joe/Dropbox/Grad/NMR Backups"



$^{13}\text{C}\{^1\text{H}\}$ [Pd(*o*-CF₃-dmba)(OAc)₂] ^{13}C aromatic region

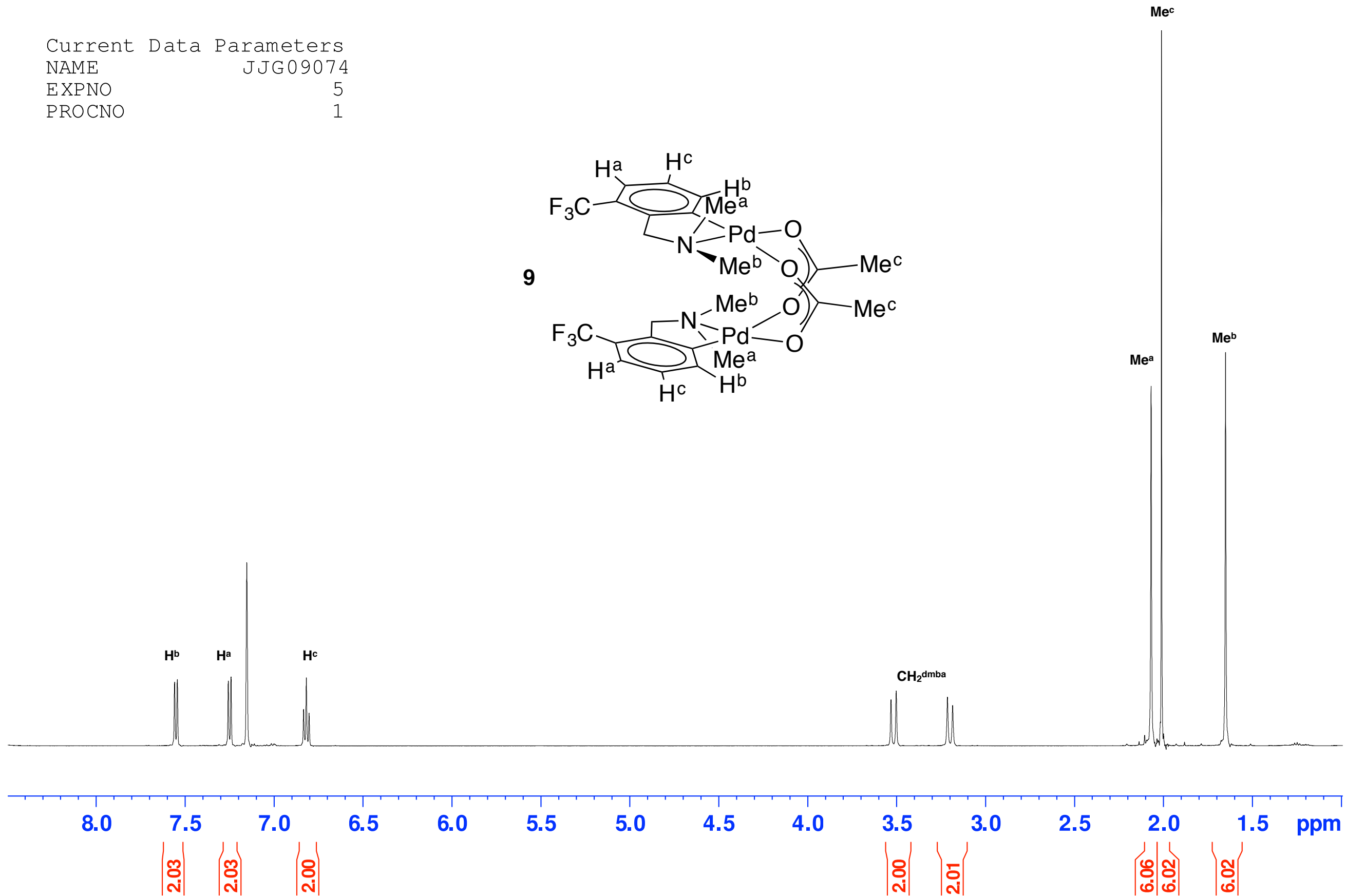
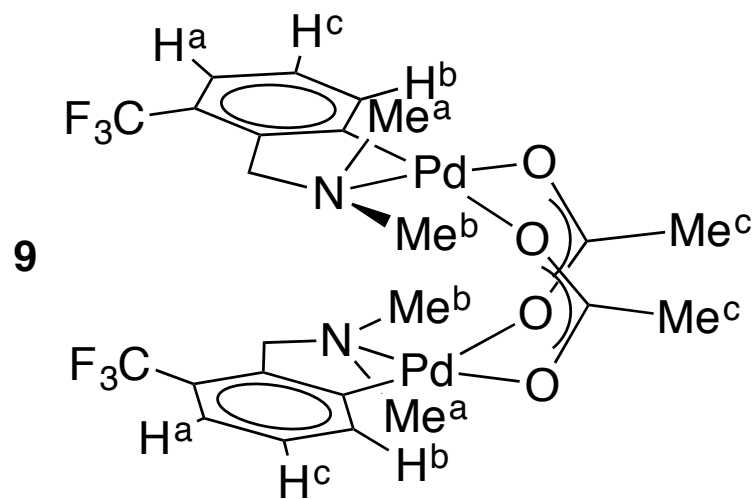
JJG09042 2 1 "/Users/joe/Dropbox/Grad/NMR Backups"



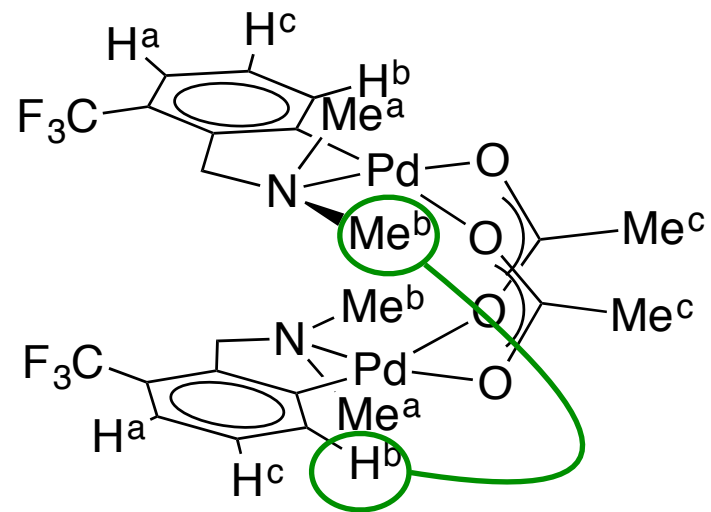
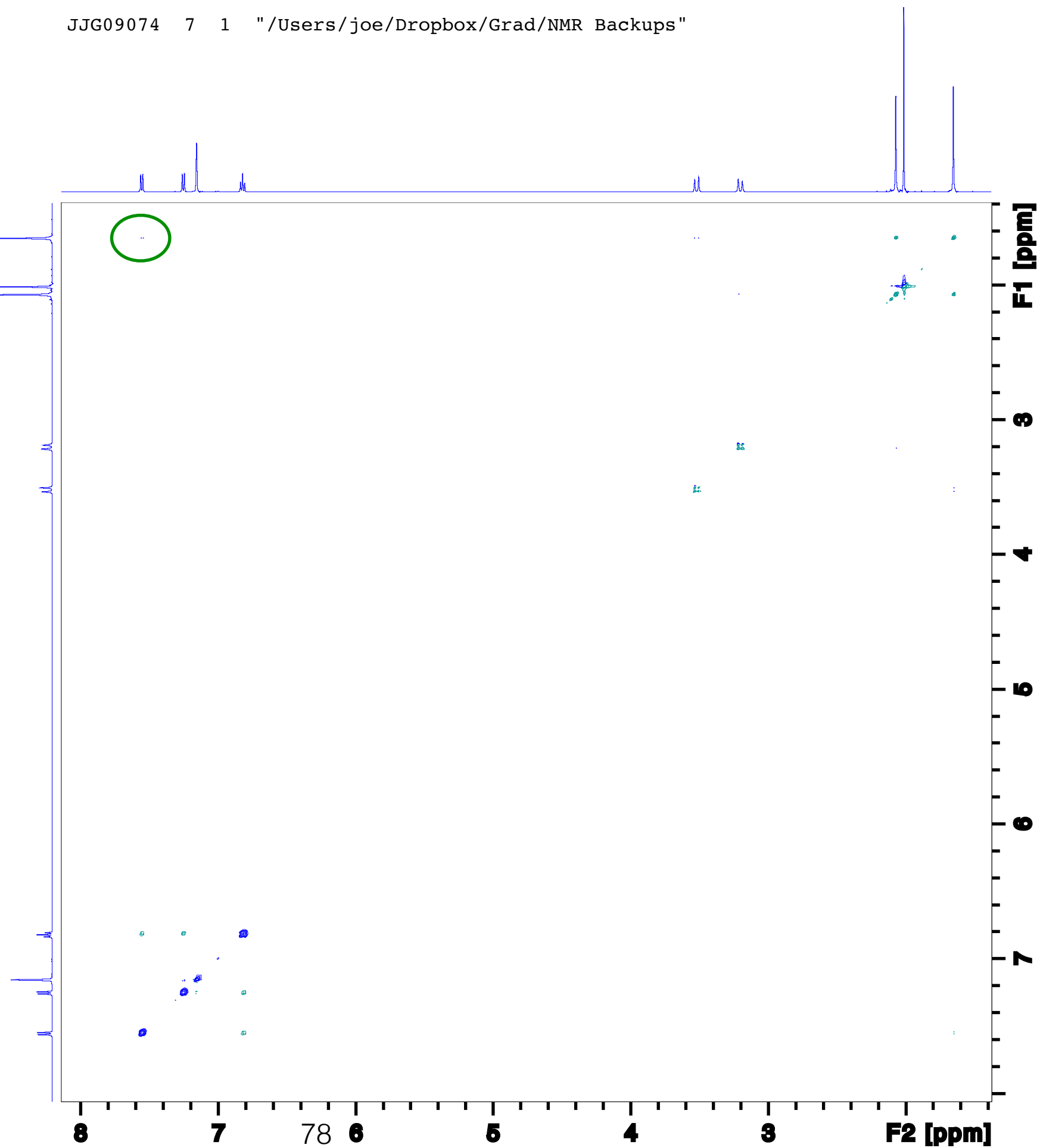


^1H in C_6D_6 $[\text{Pd}(\text{o-CF}_3\text{-dmba})(\text{OAc})_2]$

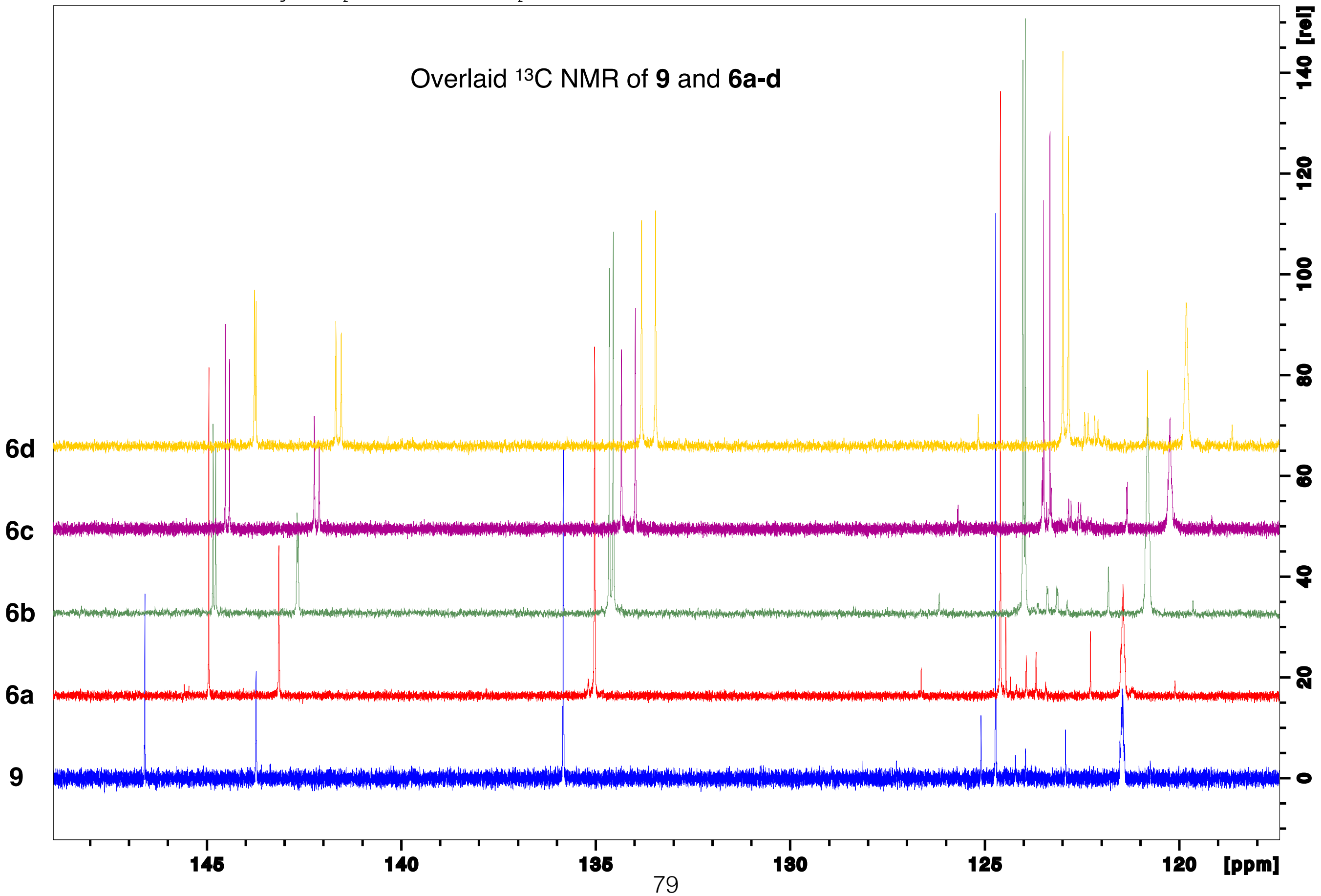
Current Data Parameters
NAME JYG09074
EXPNO 5
PROCNO 1



Key NOE cross peak
9 [Pd(CF₃-dmba)(OAc)]₂



Overlaid ^{13}C NMR of **9** and **6a-d**

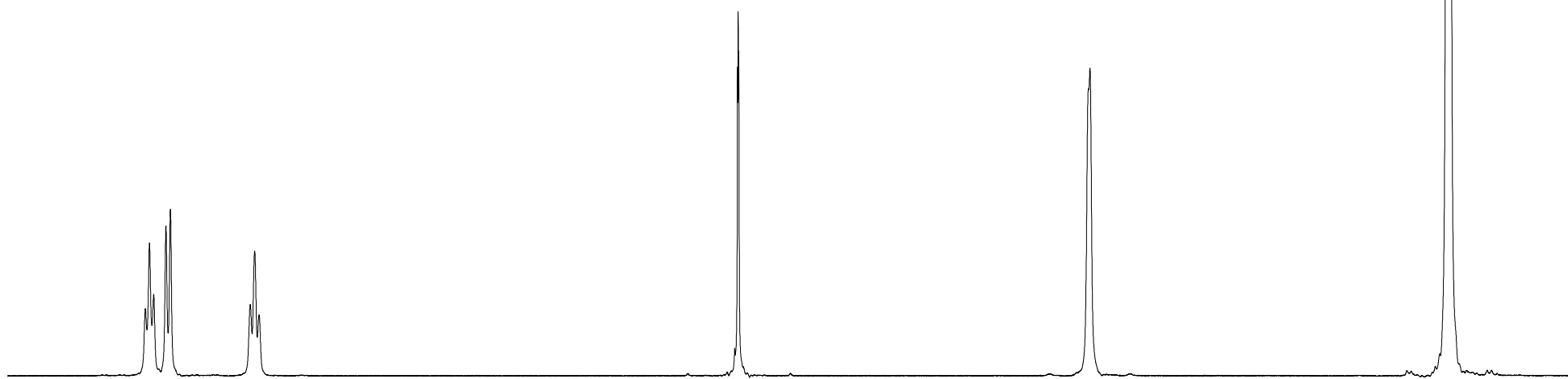
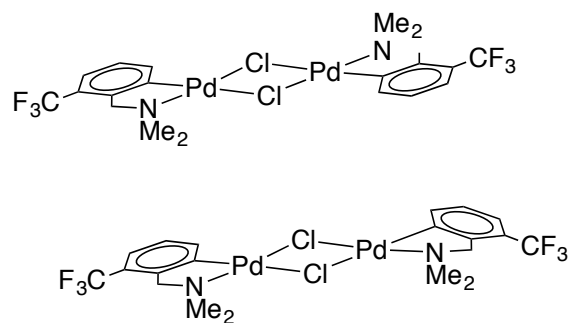


7.415
7.401
7.386
7.344
7.328
7.051
7.036
7.020

¹H 8
[Pd(CF₃-dmba)(Cl)]₂

4.144
4.139

2.903
2.888



Current Data Parameters
NAME JYG06187
EXPNO 1
PROCNO 1

F2 - Acquisition Parameter
Date_ 20160521
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 59998
SOLVENT CD2Cl2
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 0.166672 Hz
AQ 2.9999001 sec
RG 51.11
DW 50.000 usec
DE 6.50 usec
TE 296.9 K
D1 20.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 499.8730869 MHz
NUC1 1H
P1 10.75 usec
PLW1 18.25000000 W

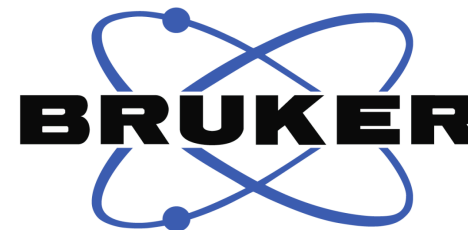
F2 - Processing parameters
SI 65536
SF 499.8700000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 ppm

1.00
0.99
1.00

2.00

6.01



Current Data Parameters
NAME JYG06187
EXPNO 2
PROCNO 1

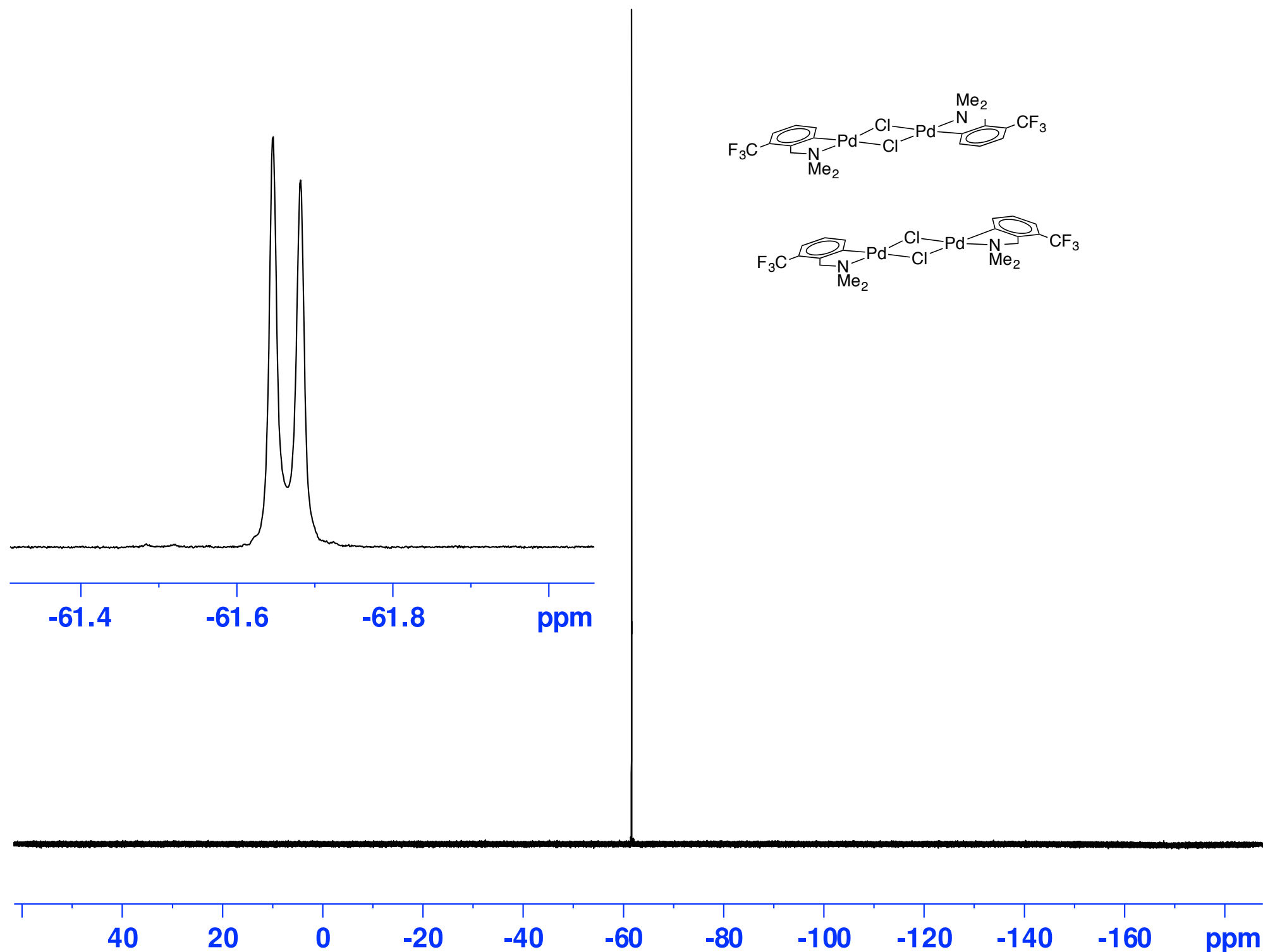
F2 - Acquisition Parameter
Date_ 20160521
Time 14.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqr
TD 524288
SOLVENT CD2Cl2
NS 1
DS 0
SWH 117187.500 Hz
FIDRES 0.223517 Hz
AQ 2.2369621 sec
RG 435.42
DW 4.267 usec
DE 6.50 usec
TE 296.9 K
D1 3.00000000 sec
TD0 1

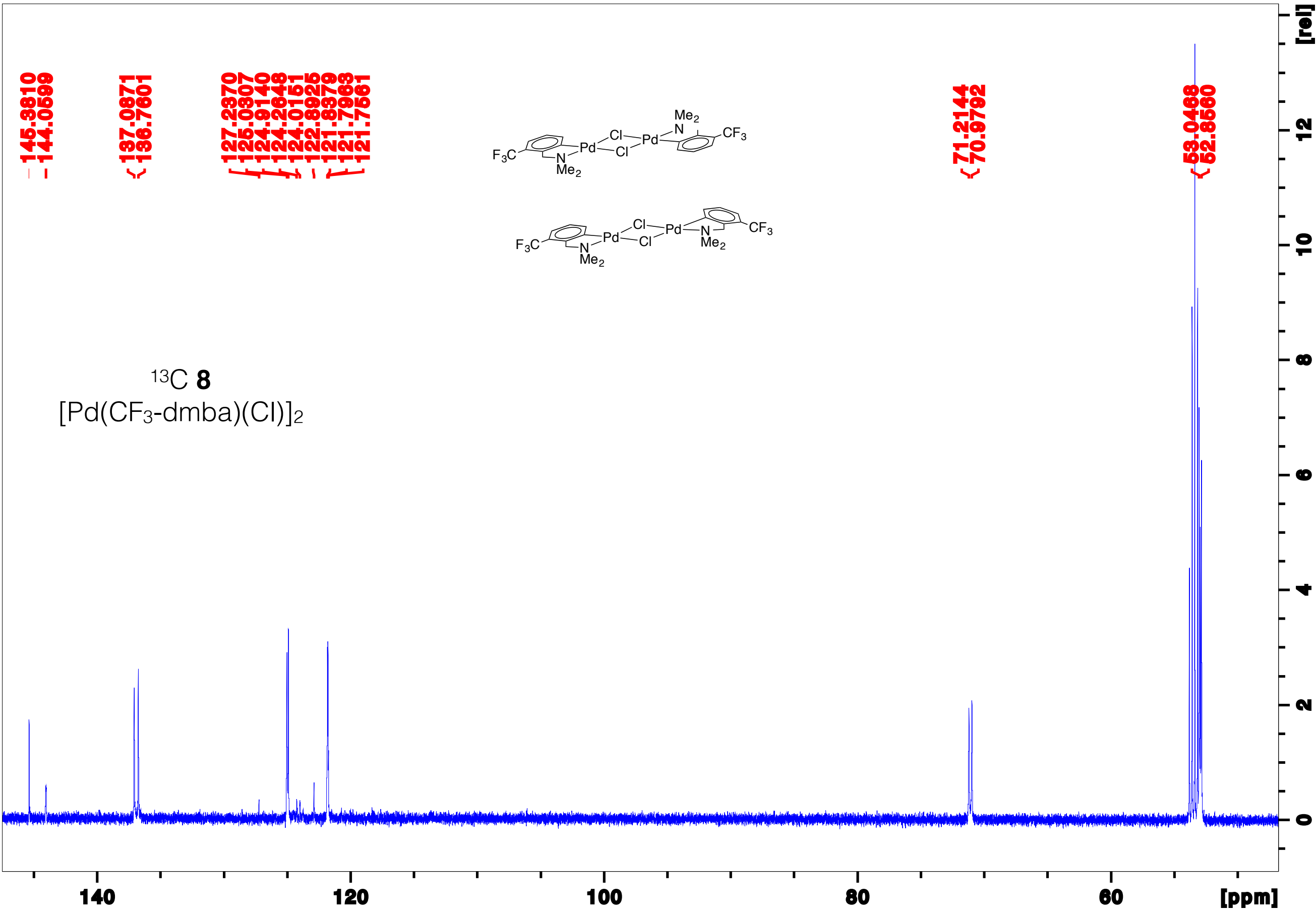
==== CHANNEL f1 =====
SFO1 470.3181011 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

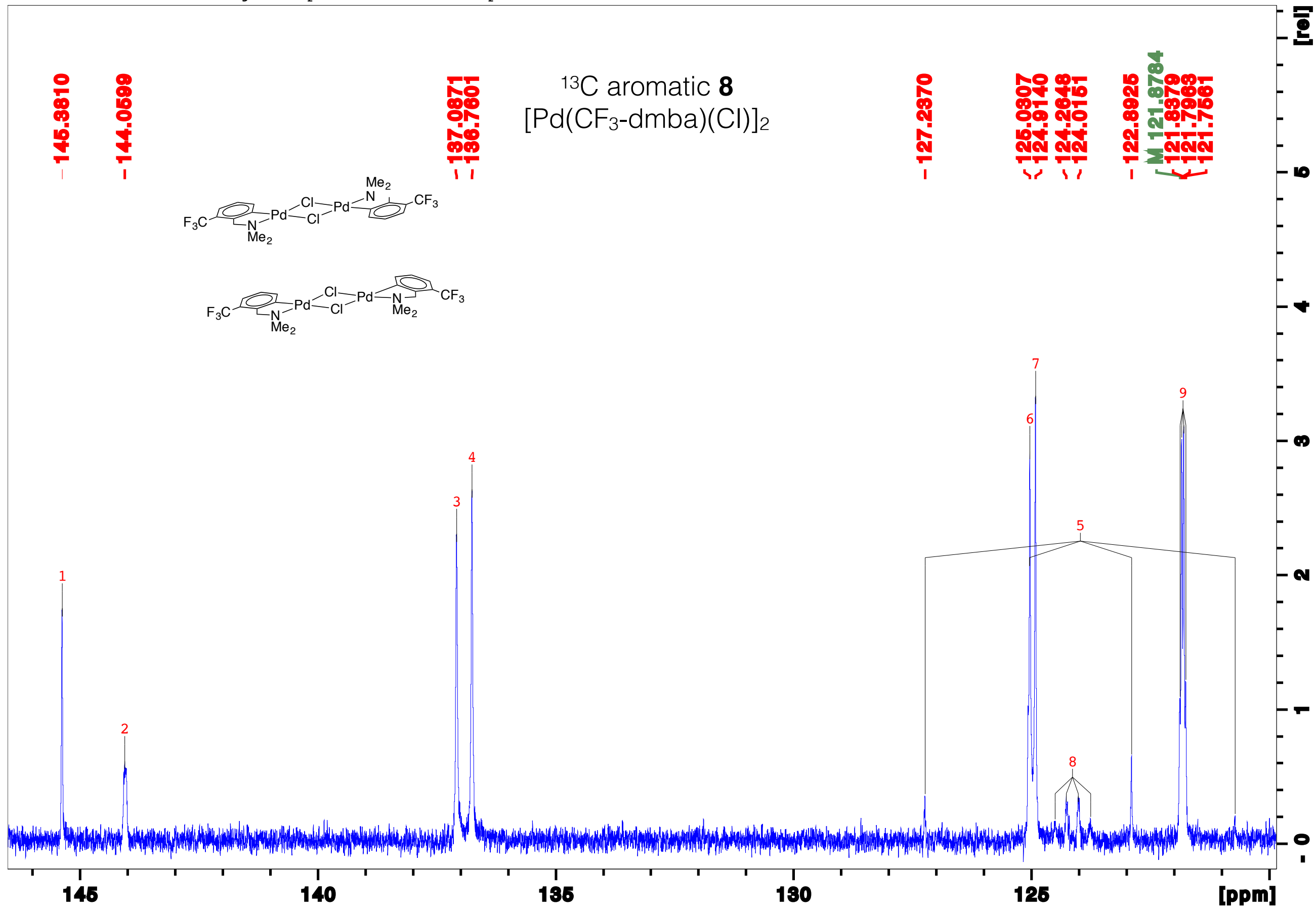
F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

^{19}F 8
[Pd(CF₃-dmba)(Cl)]₂

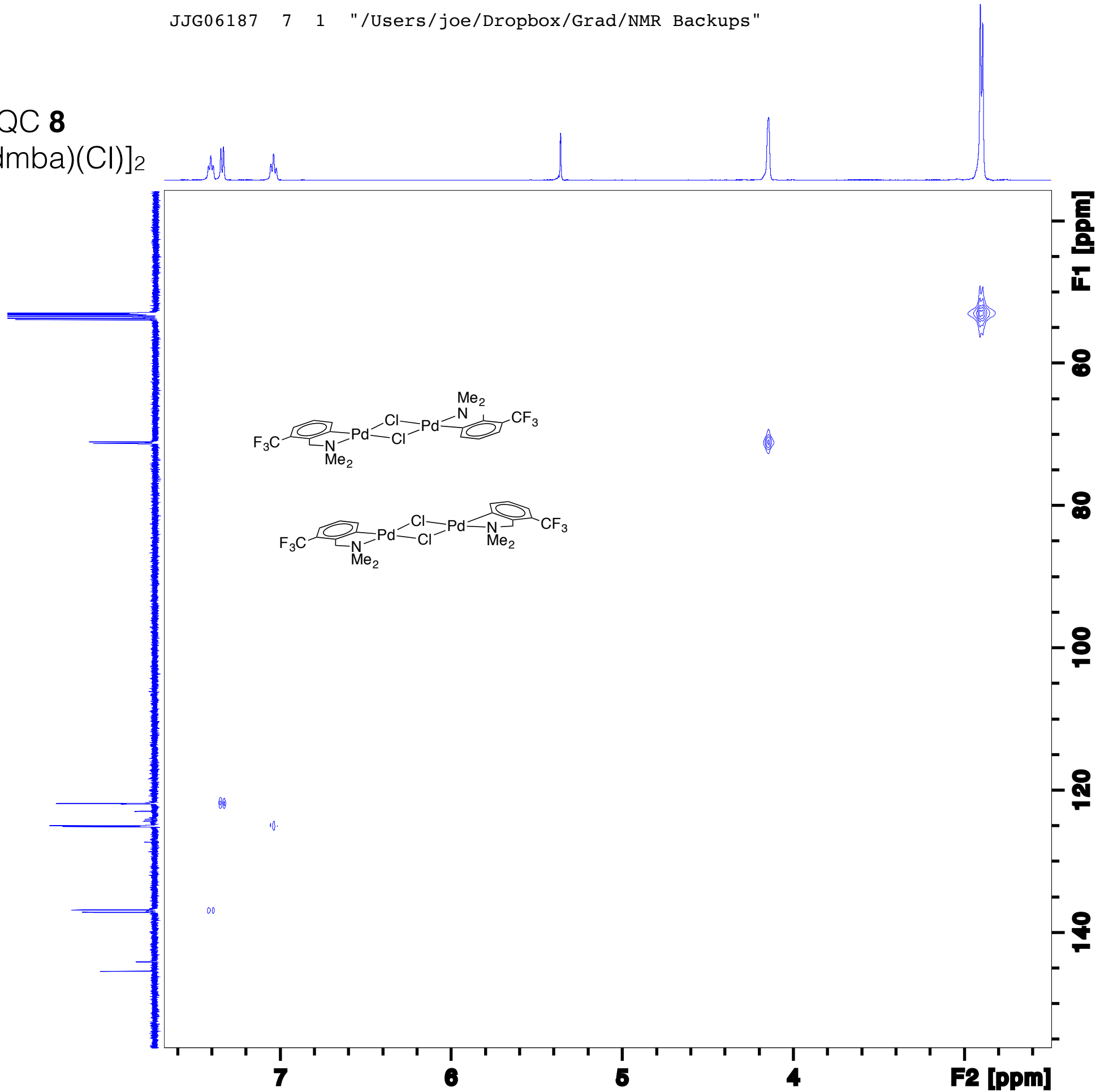
-61.646
-61.682





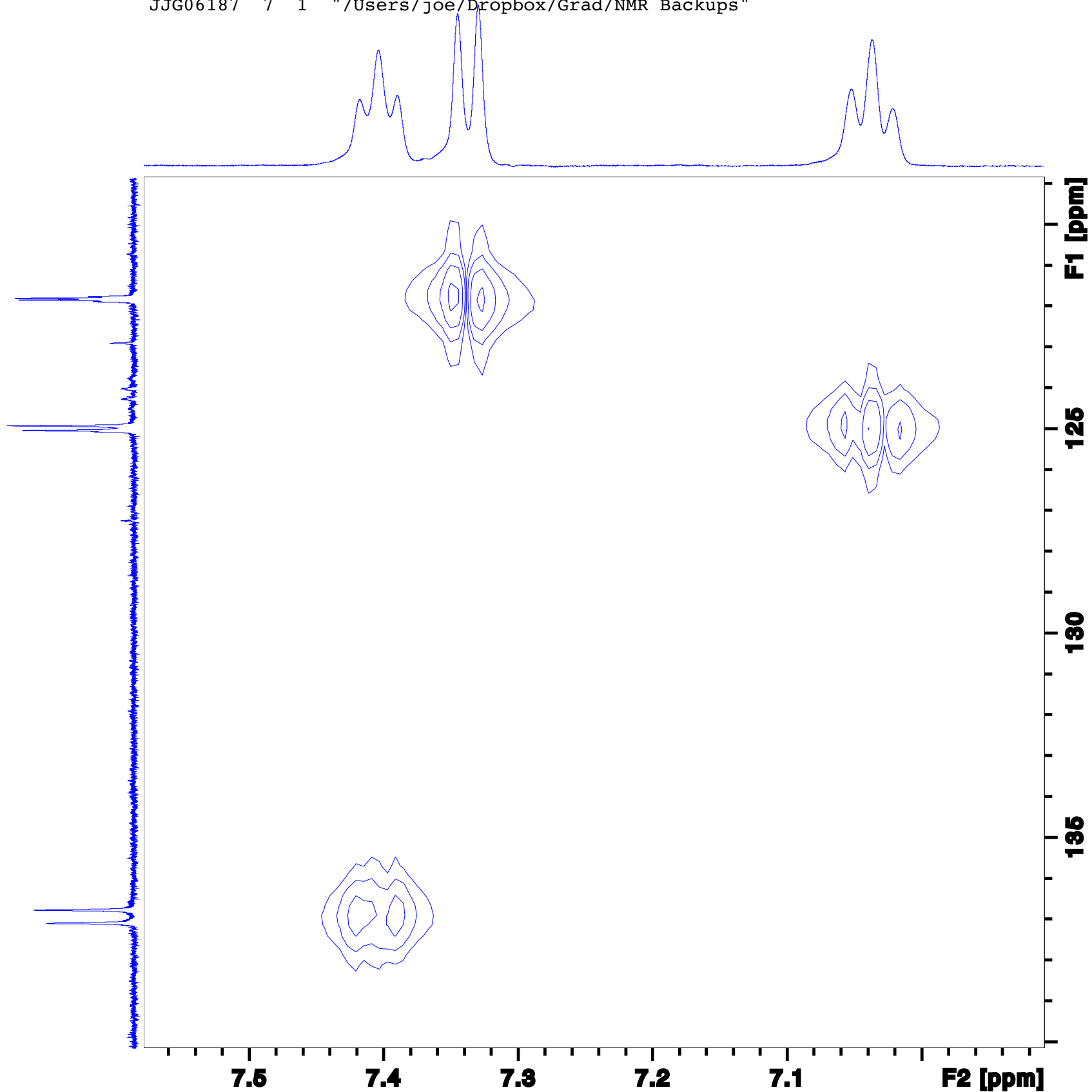
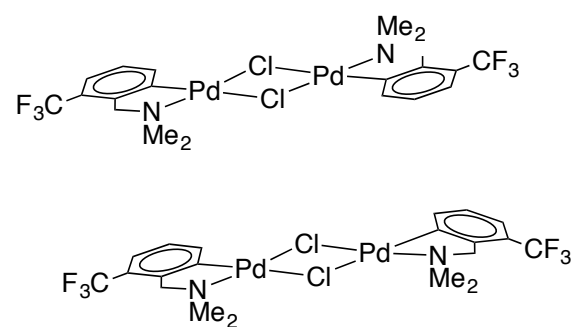


HMQC **8**
 [Pd(CF₃-dmba)(Cl)]₂



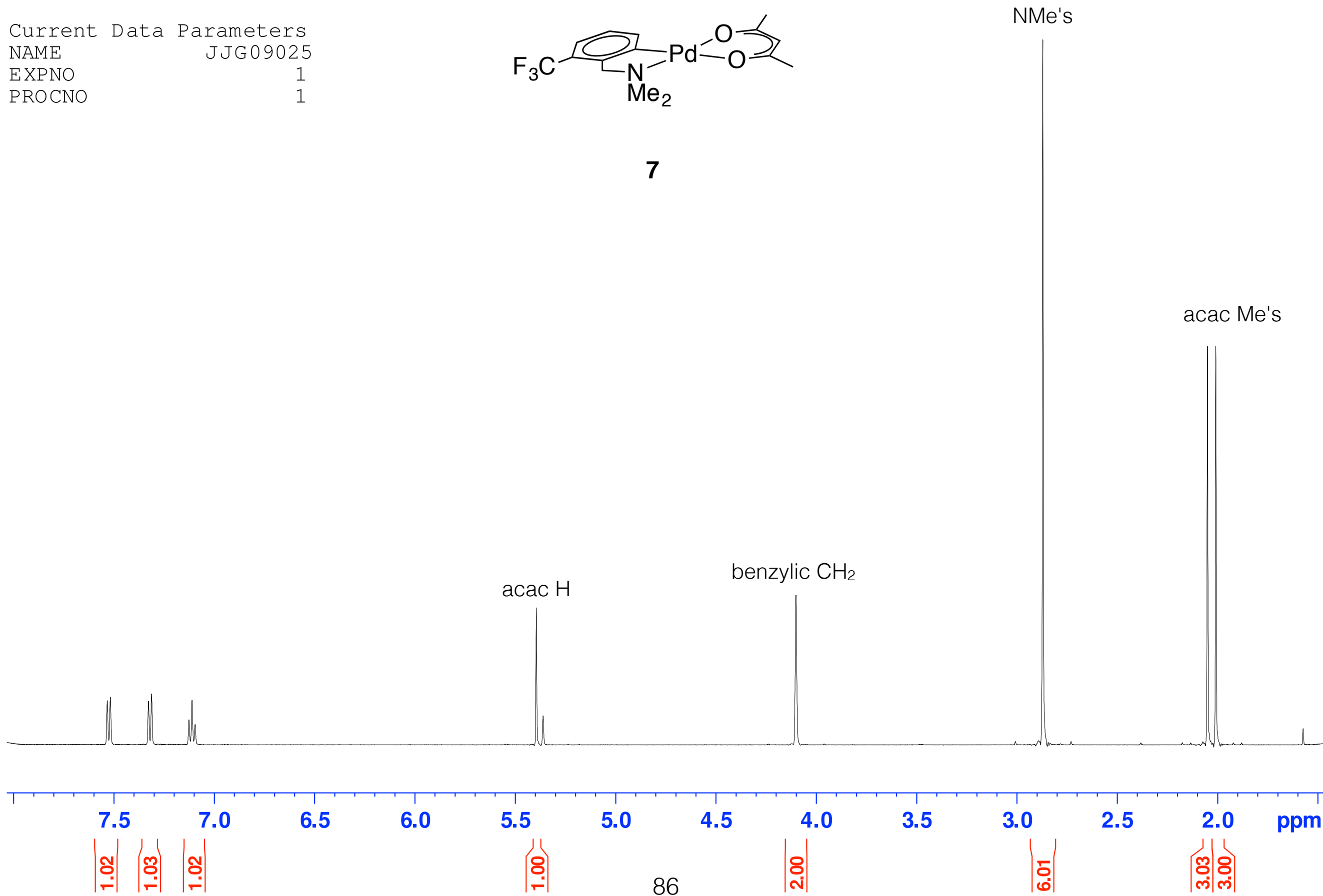
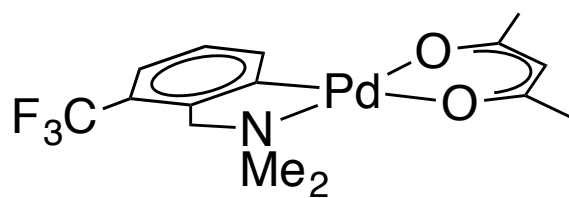
HMQC aromatic **8**
[Pd(CF₃-dmba)(Cl)]₂

JJG06187 7 1 "/Users/joe/Dropbox/Grad/NMR Backups"



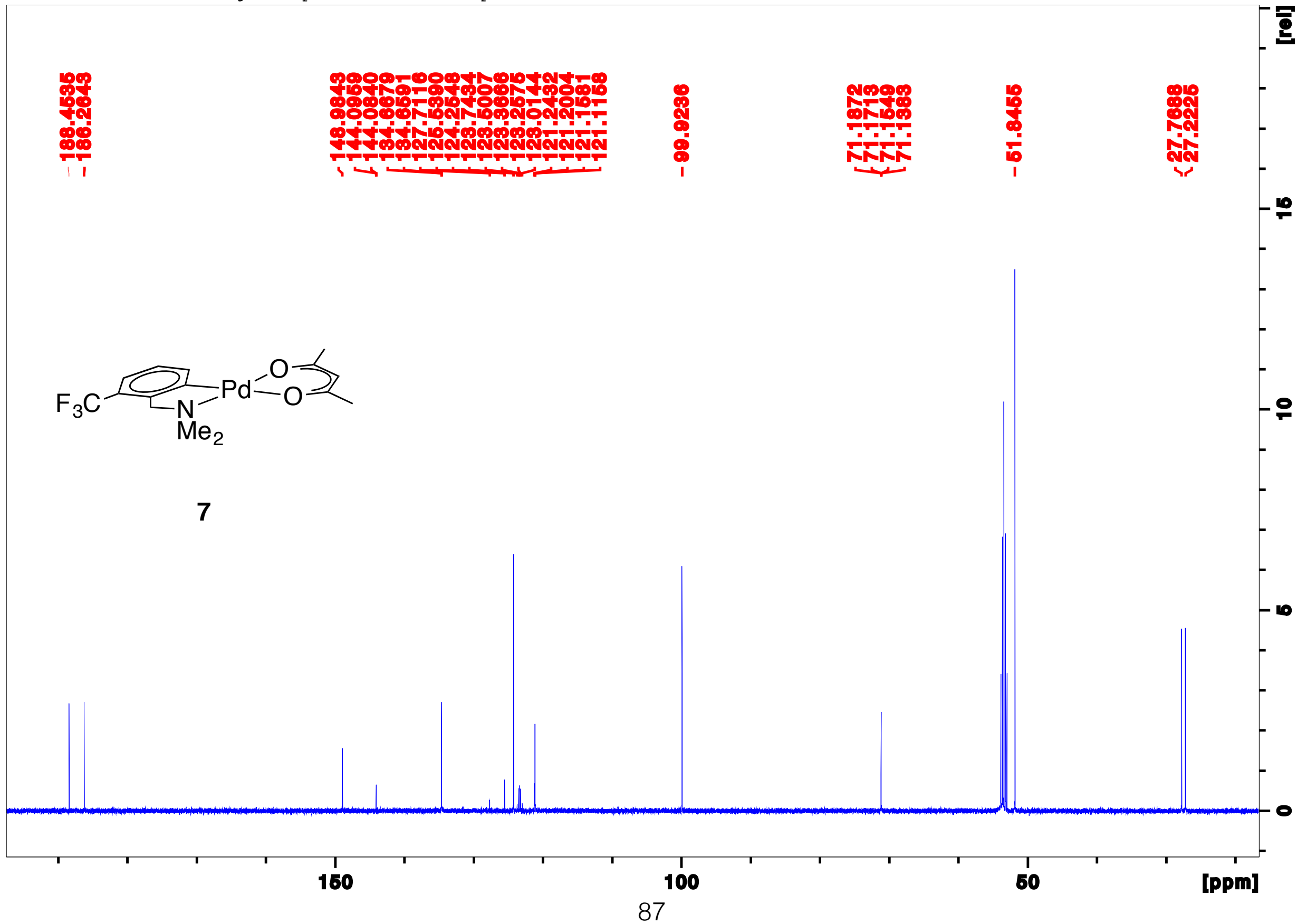
¹H NMR
Pd(CF₃-dmba)(acac)

Current Data Parameters
NAME JYG09025
EXPNO 1
PROCNO 1



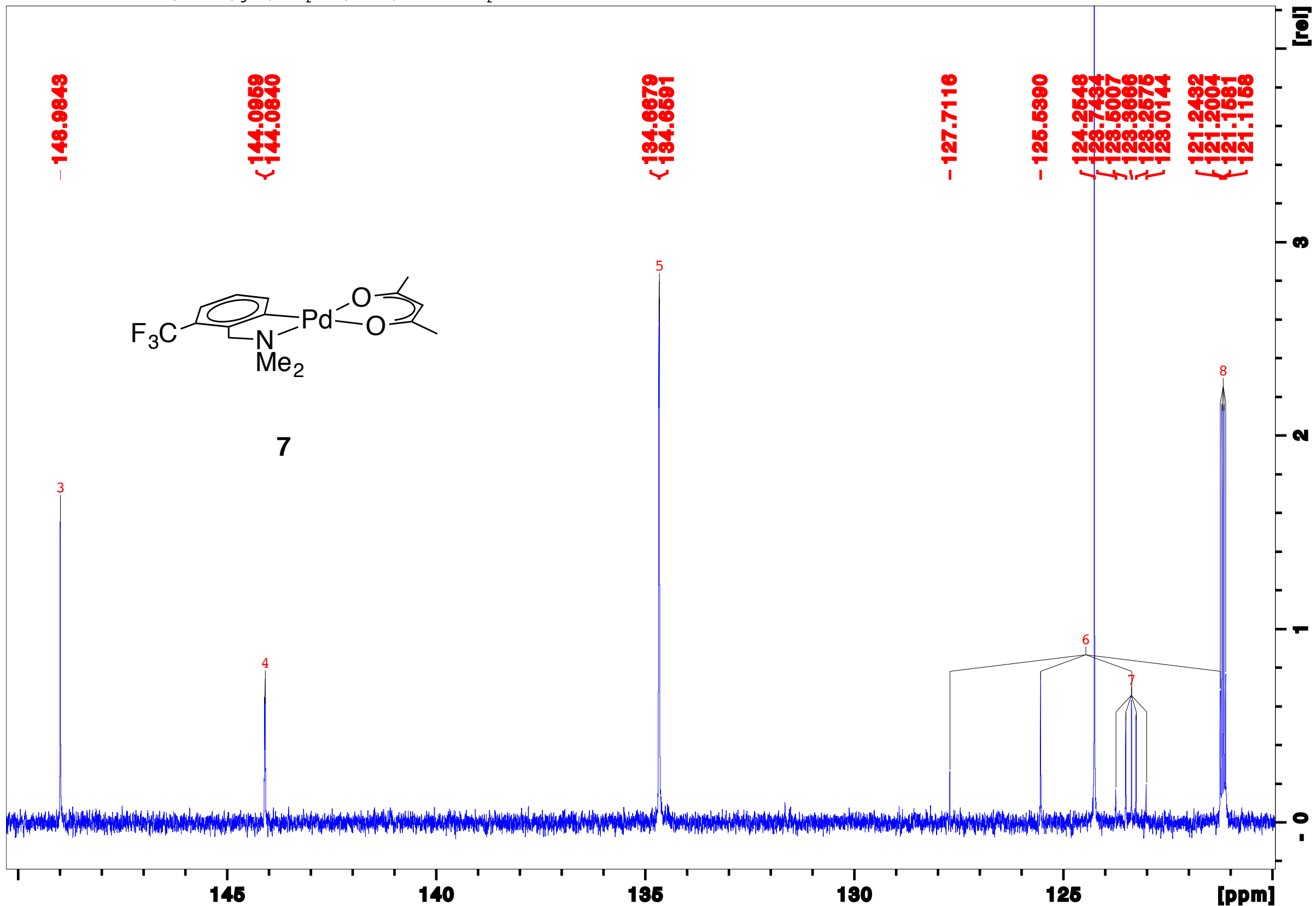
¹³C NMR
Pd(CF₃-dmba)(acac)

JJG09025 2 1 "/Users/joe/Dropbox/Grad/NMR Backups"



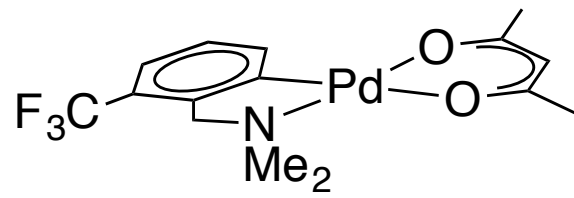
¹³C NMR aromatic region
Pd(CF₃-dmba)(acac)

JJG09025 2 1 "/Users/joe/Dropbox/Grad/NMR Backups"

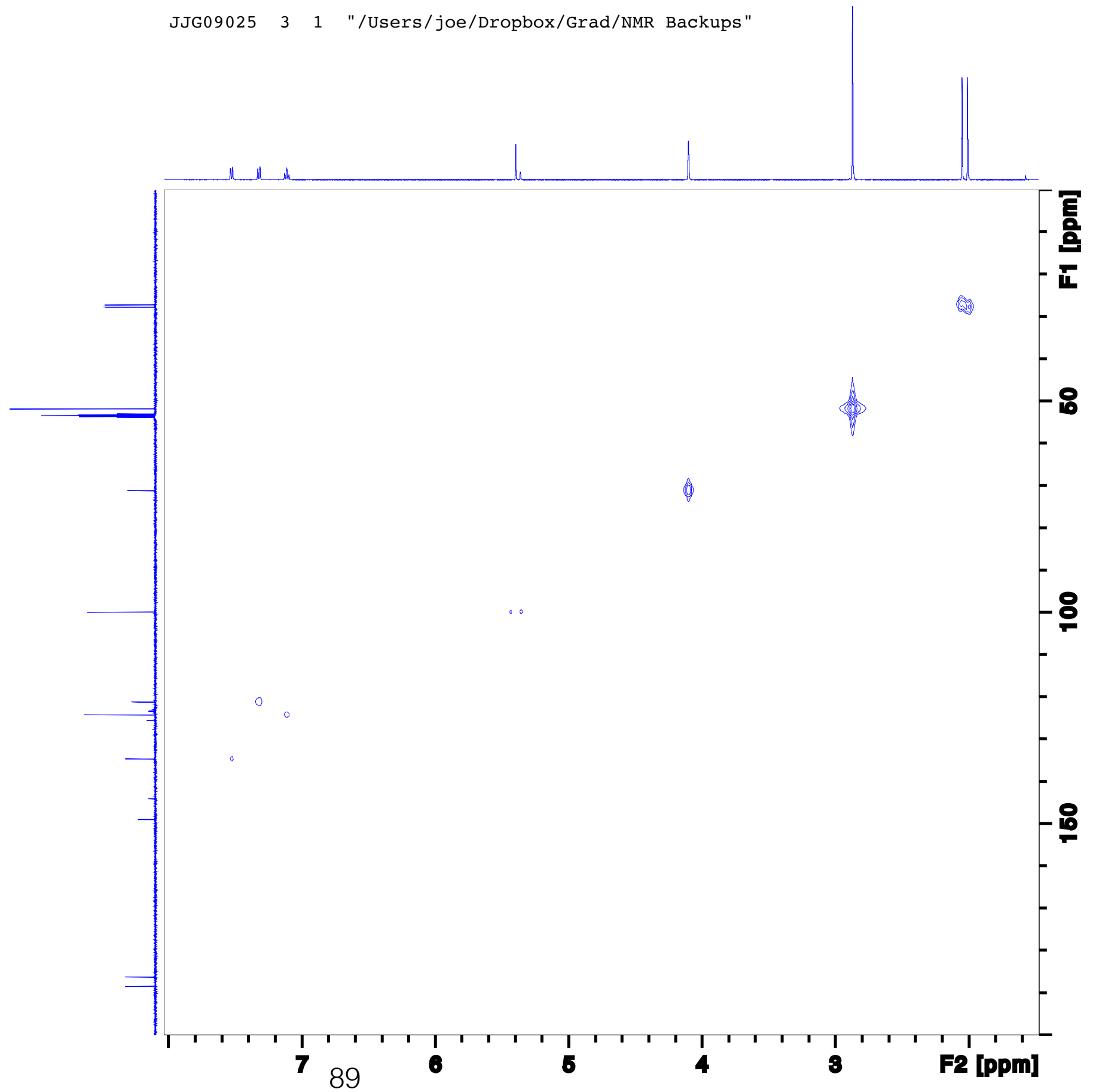


¹³C HMQC
Pd(CF₃-dmba)(acac)

JJG09025 3 1 "/Users/joe/Dropbox/Grad/NMR Backups"

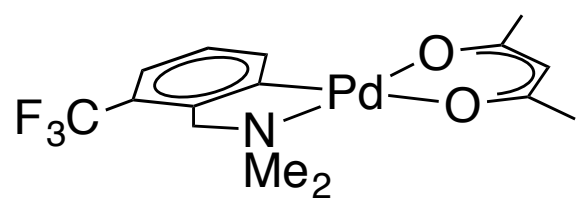


7

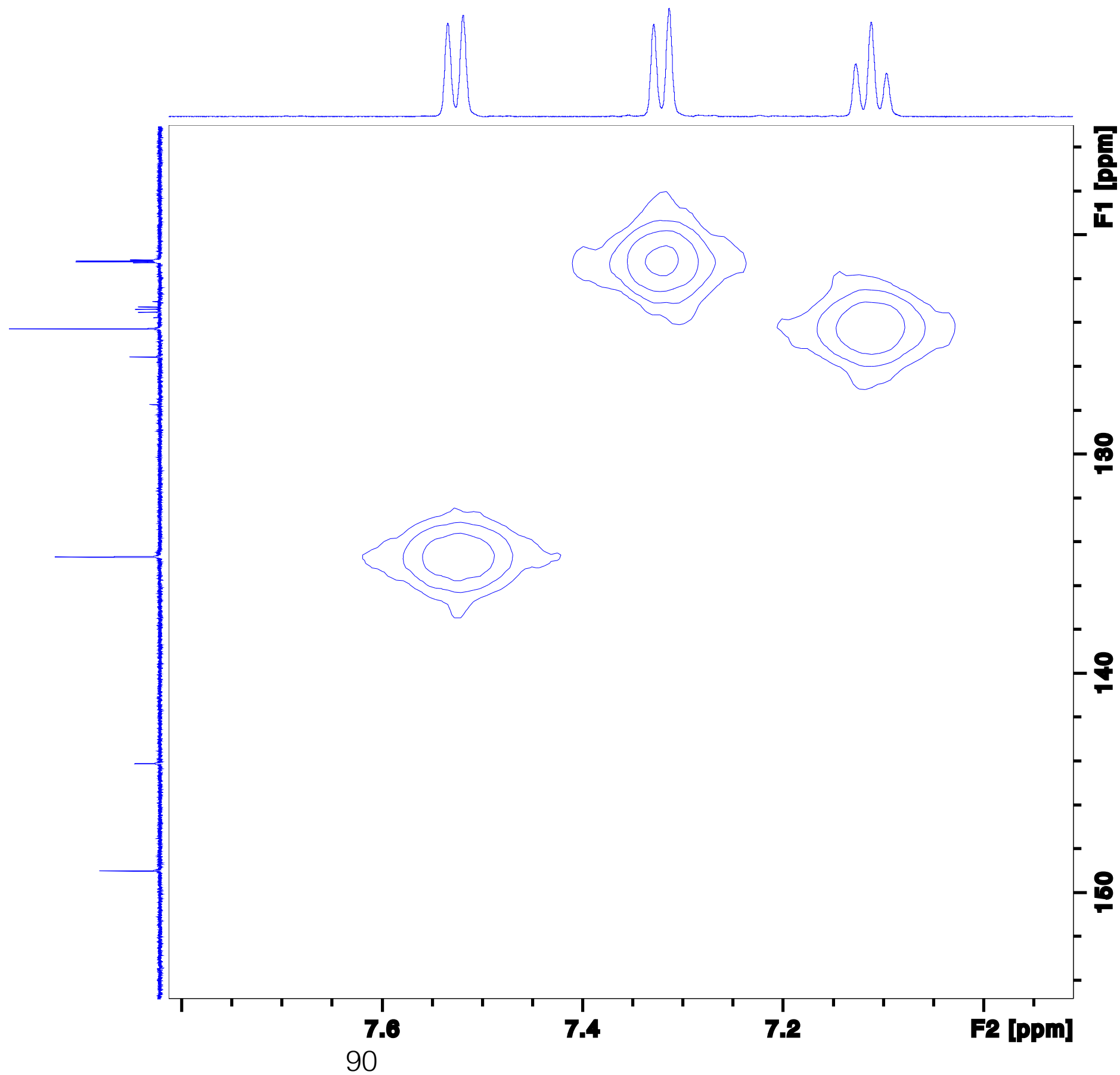


¹³C HMQC aromatic region
Pd(CF₃-dmba)(acac)

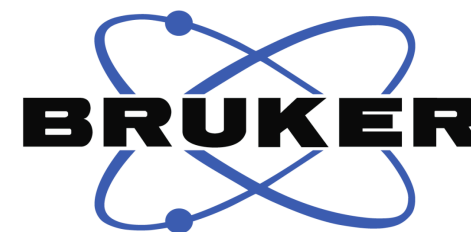
JJG09025 3 1 "/Users/joe/Dropbox/Grad/NMR Backups"



7



¹⁹F NMR
Pd(CF₃-dmba)(acac)



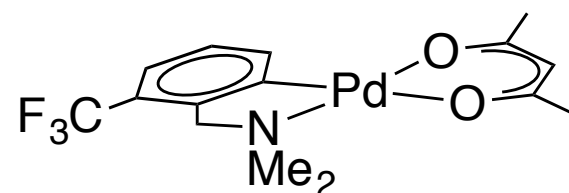
Current Data Parameters
NAME JYG07009
EXPNO 4
PROCNO 1

F2 - Acquisition Parameter
Date_ 20160610
Time 14.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 524288
SOLVENT CD2Cl2
NS 8
DS 0
SWH 117187.500 Hz
FIDRES 0.223517 Hz
AQ 2.2369621 sec
RG 554.84
DW 4.267 usec
DE 6.50 usec
TE 295.6 K
D1 3.00000000 sec
TD0 1

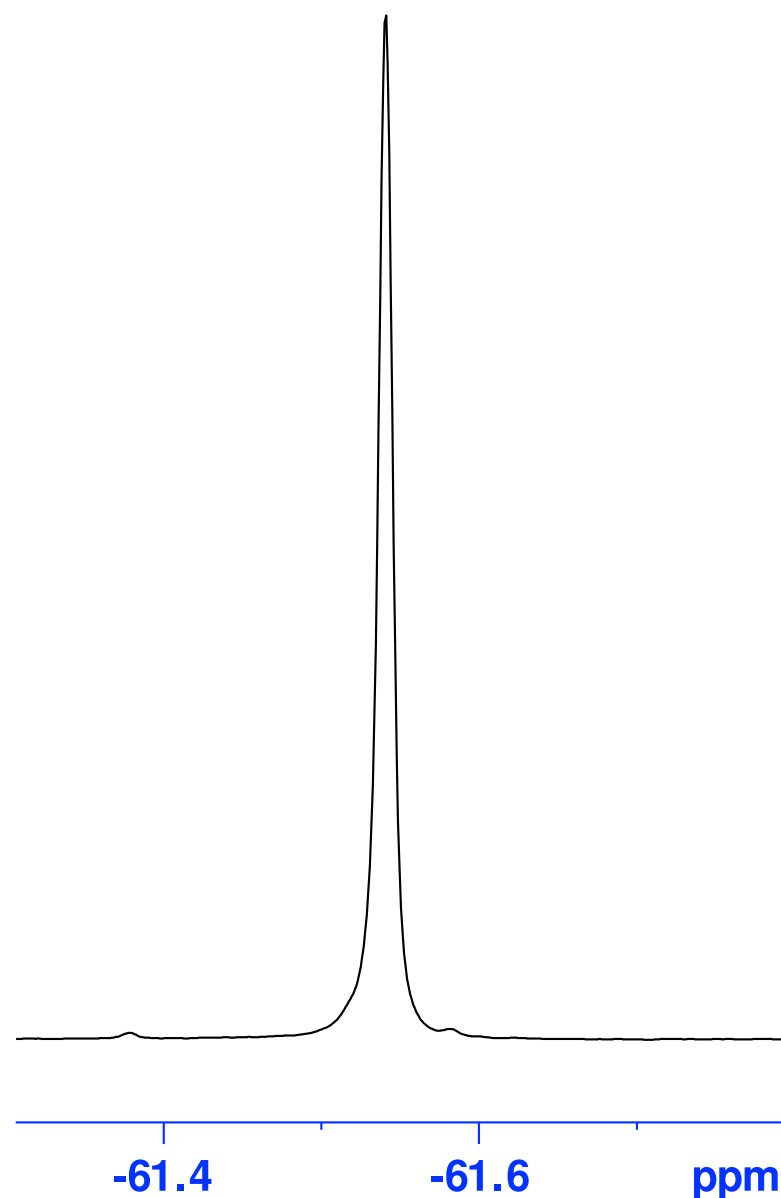
==== CHANNEL f1 =====
SFO1 470.3181011 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

-61.541



7



¹H NMR
5b

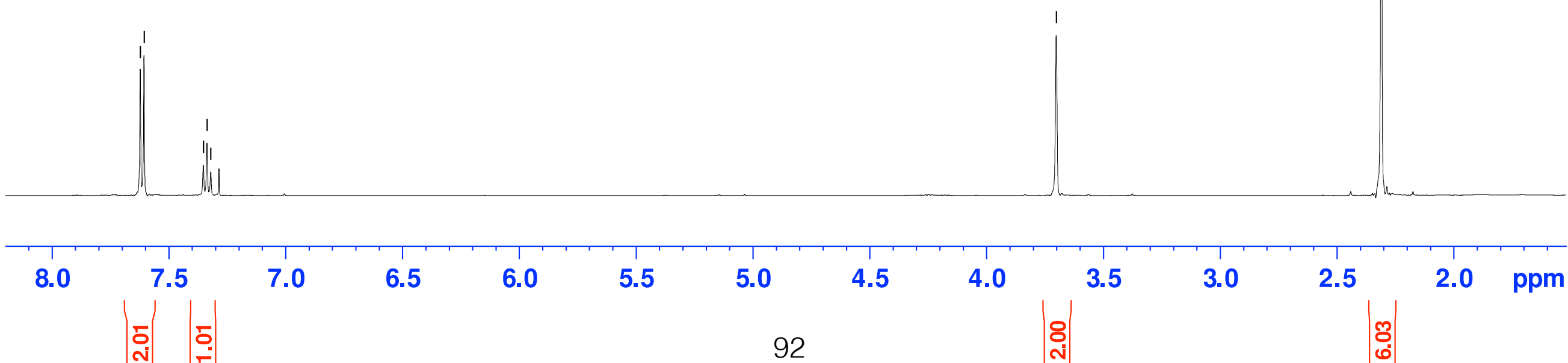
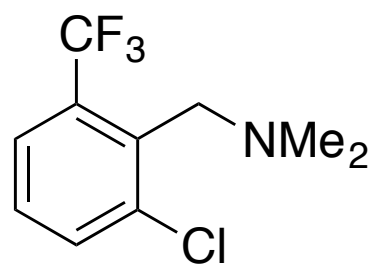
7.622
7.606
7.353
7.336
7.321

Current Data Parameters
NAME JYG07178
EXPNO 1
PROCNO 1

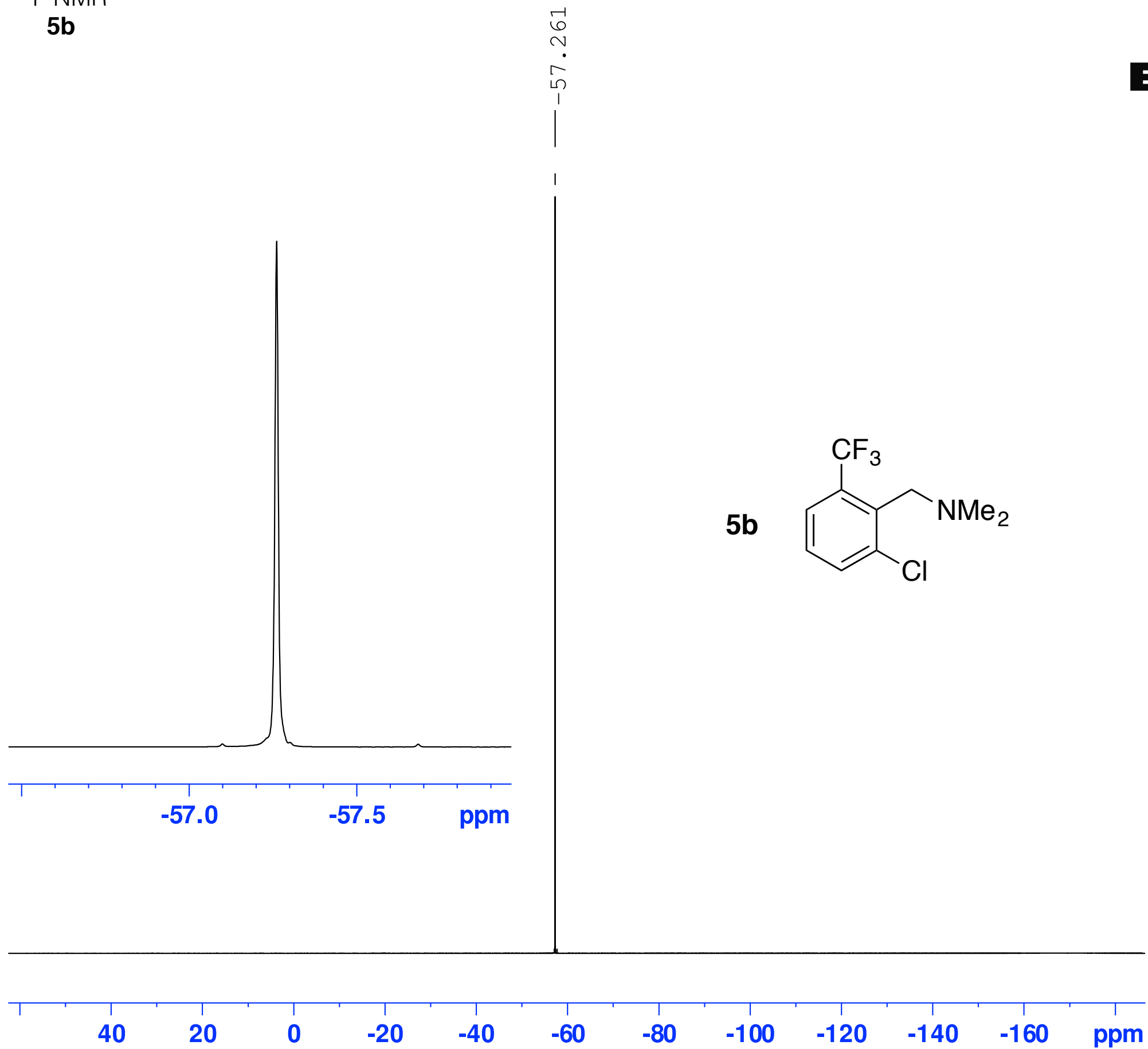
3.701

2.309

5b



¹⁹F NMR
5b



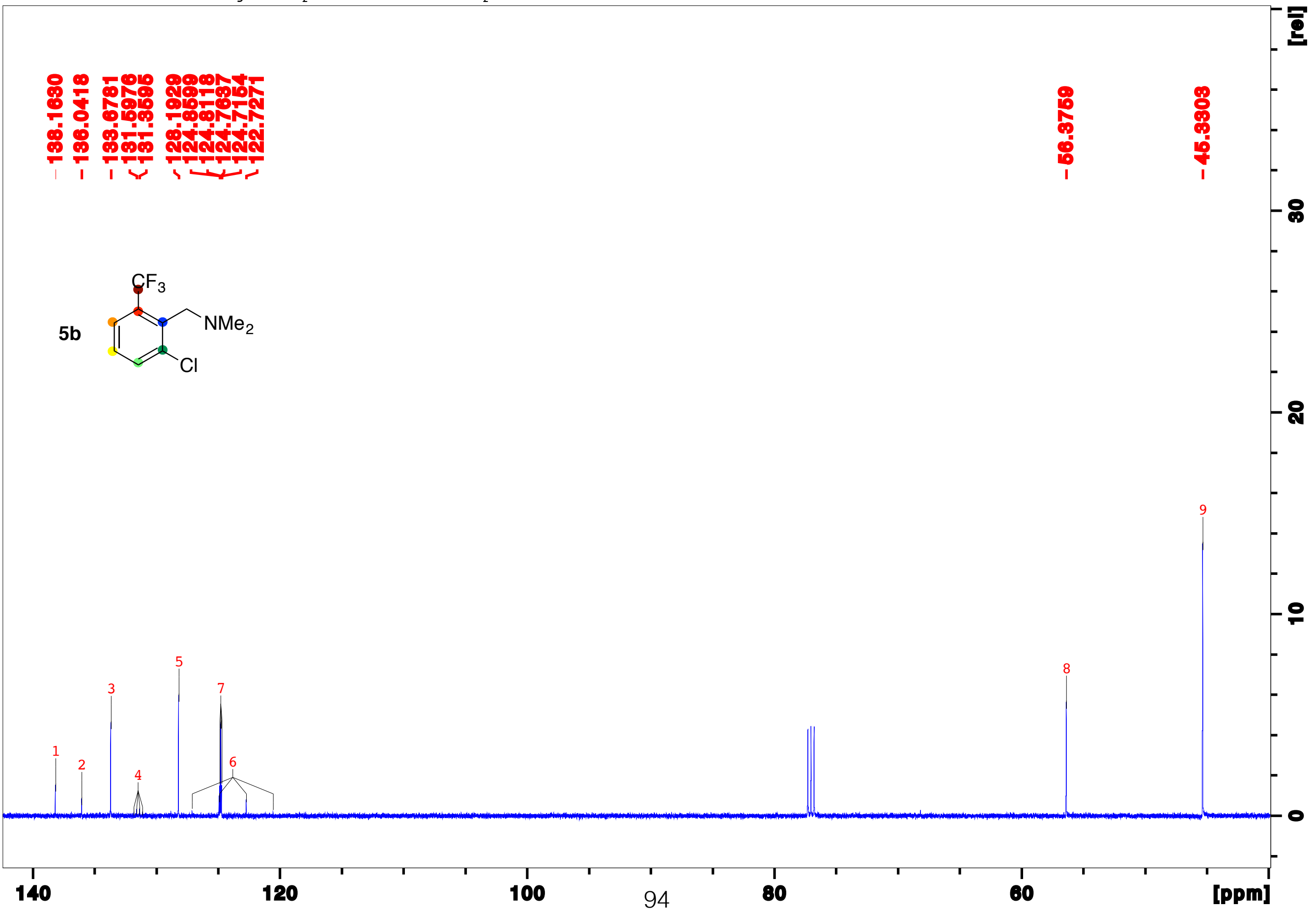
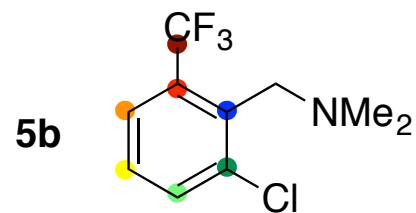
Current Data Parameters
NAME JJG07178
EXPNO 2
PROCNO 1

F2 - Acquisition Parameter
Date_ 20160830
Time 9.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 524288
SOLVENT CDCl3
NS 1
DS 0
SWH 117187.500 Hz
FIDRES 0.223517 Hz
AQ 2.2369621 sec
RG 249.19
DW 4.267 usec
DE 6.50 usec
TE 295.8 K
D1 3.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 470.3185714 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00

138.1630
136.0418
133.6781
131.5976
131.3595
128.1929
124.8599
124.8118
124.7697
124.7154
122.7271

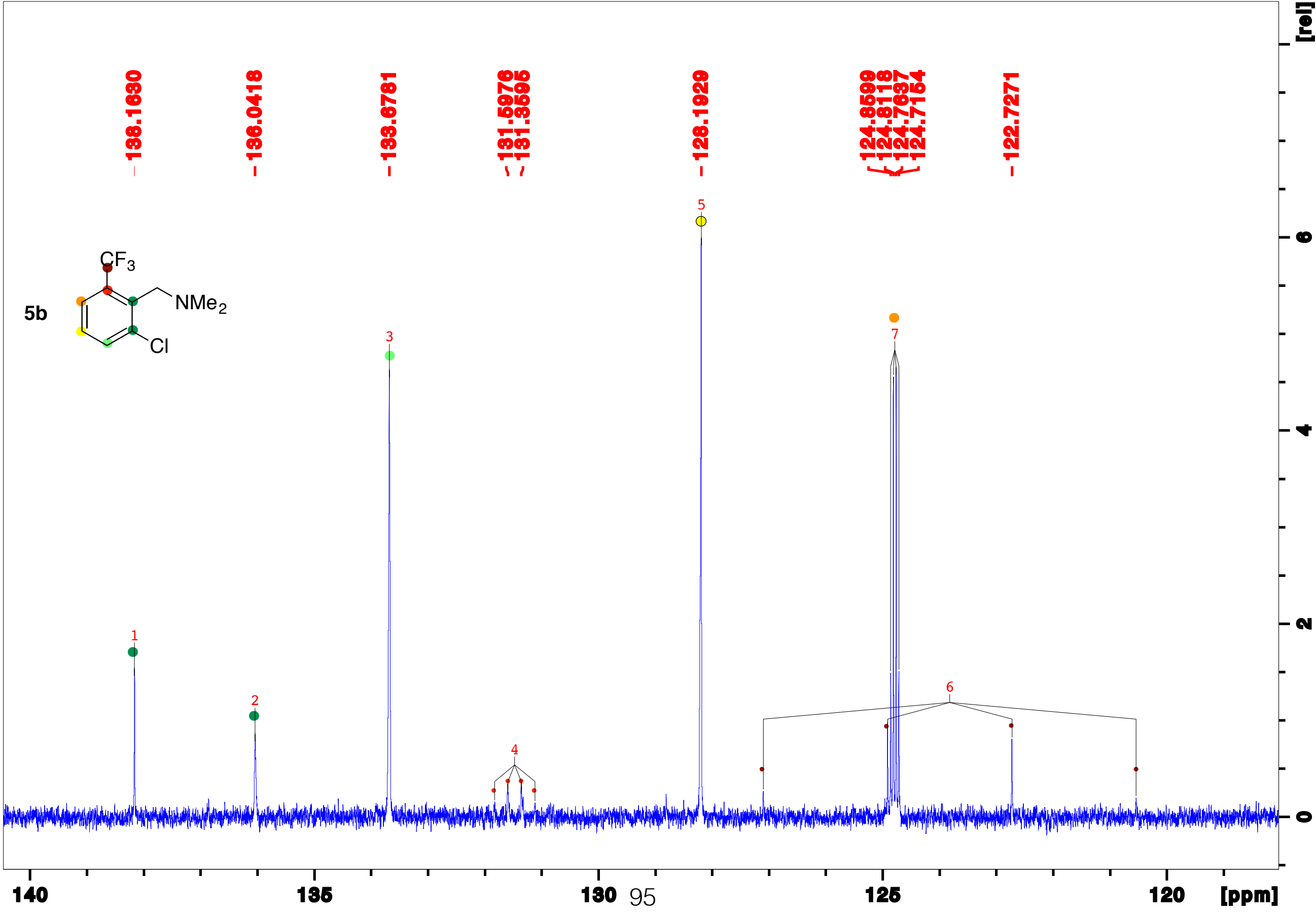


140 120 100 94 80 60 [ppm]

[rel]

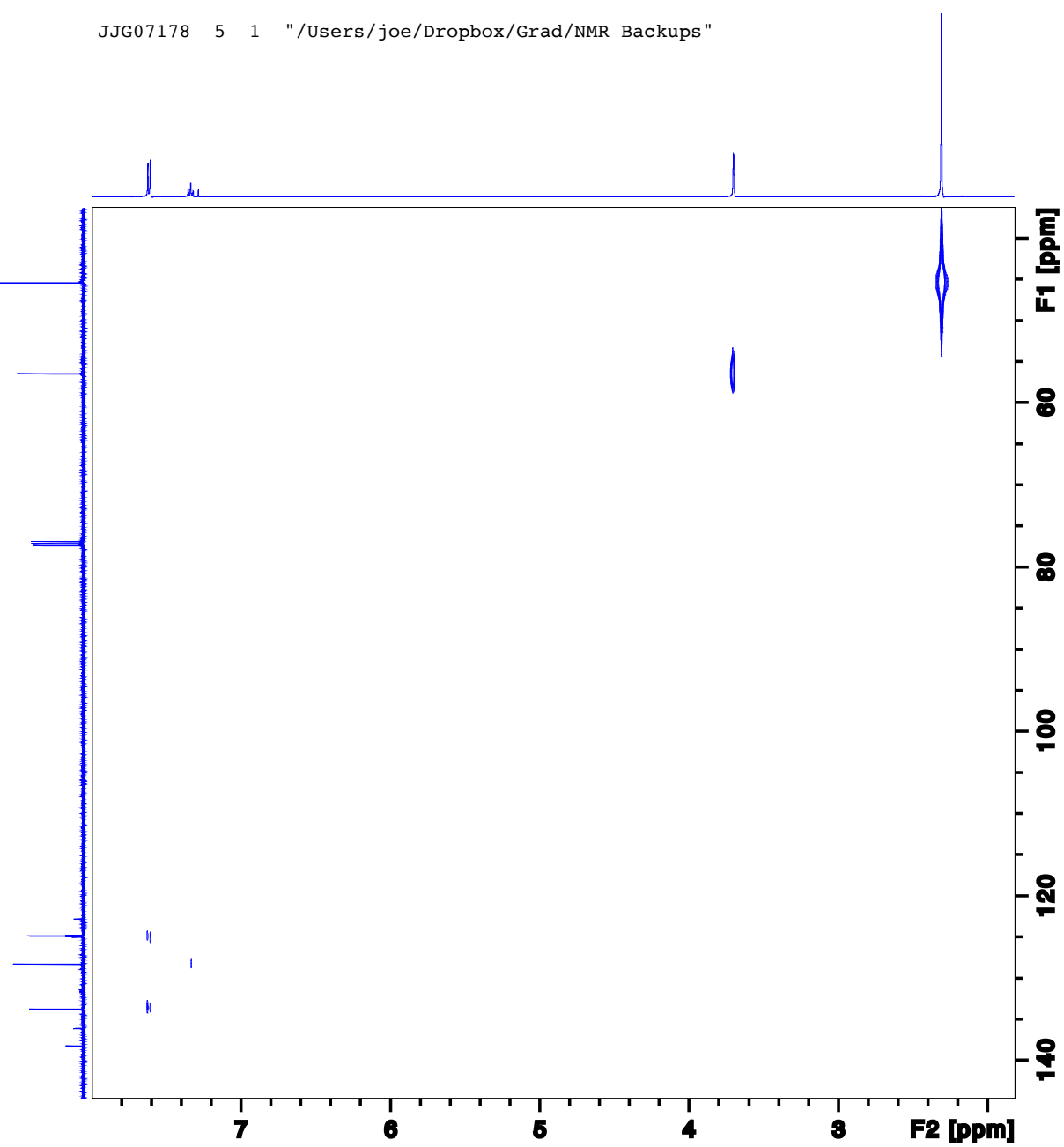
¹³C NMR aromatic
5b

JJG07178 4 1 "/Users/joe/Dropbox/Grad/NMR Backups"

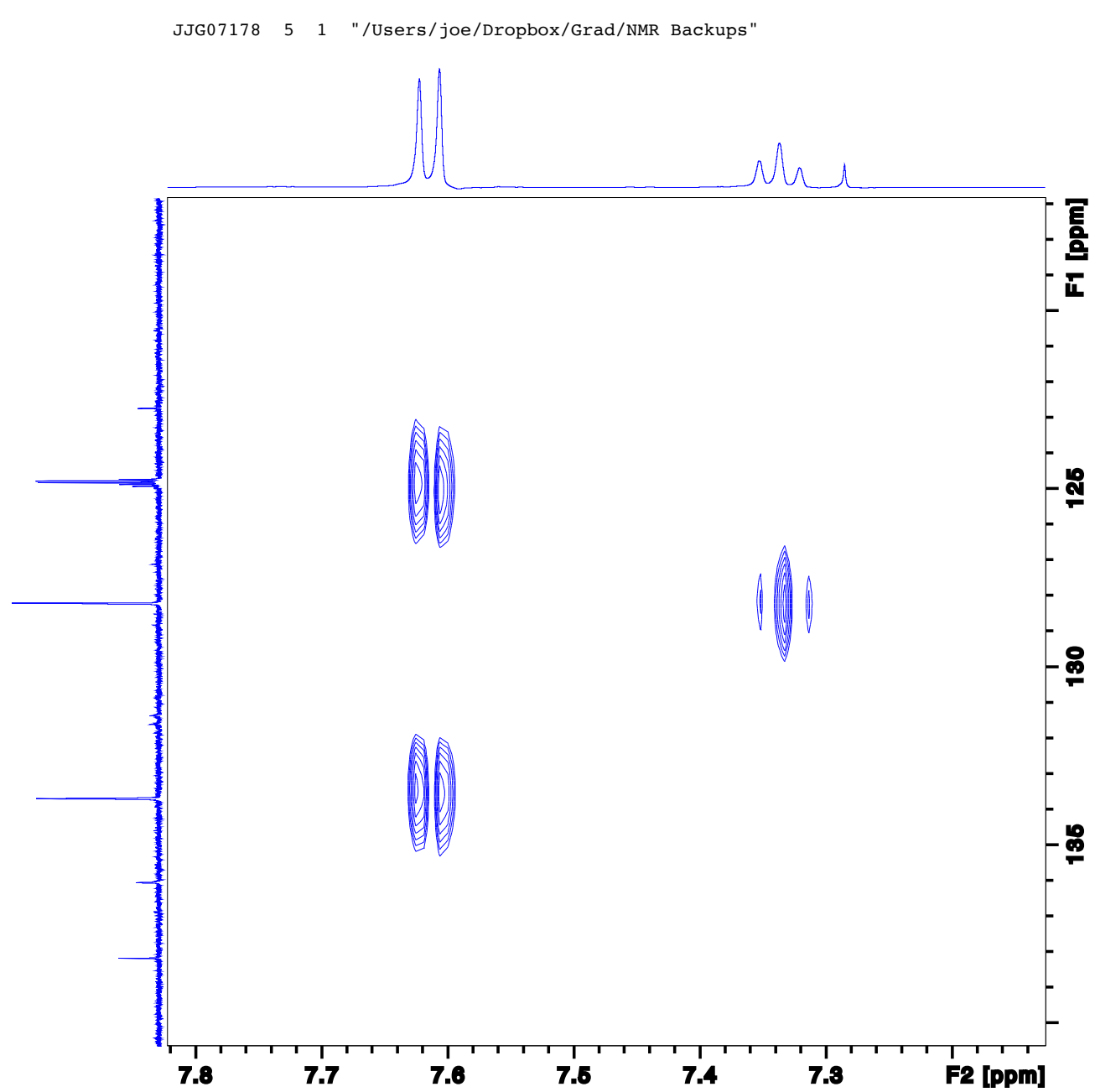


HMQC
5b

JJG07178 5 1 "/Users/joe/Dropbox/Grad/NMR Backups"



JJG07178 5 1 "/Users/joe/Dropbox/Grad/NMR Backups"



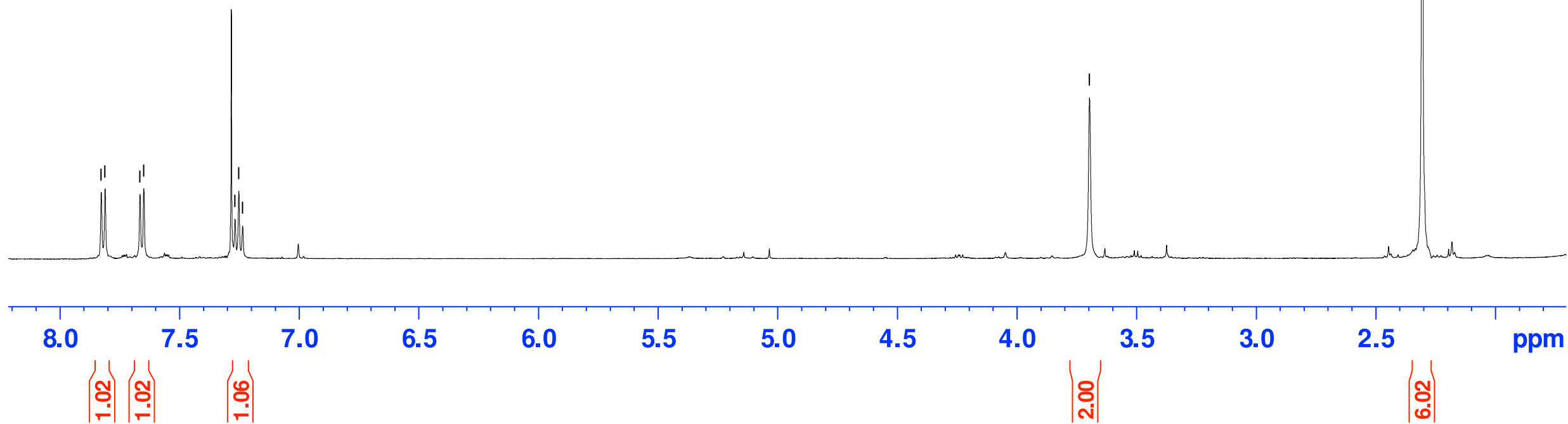
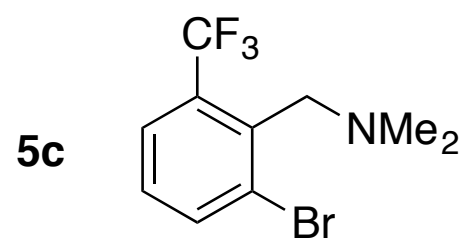
¹H NMR
5c

7.829
7.813
7.667
7.651
7.269
7.254
7.238

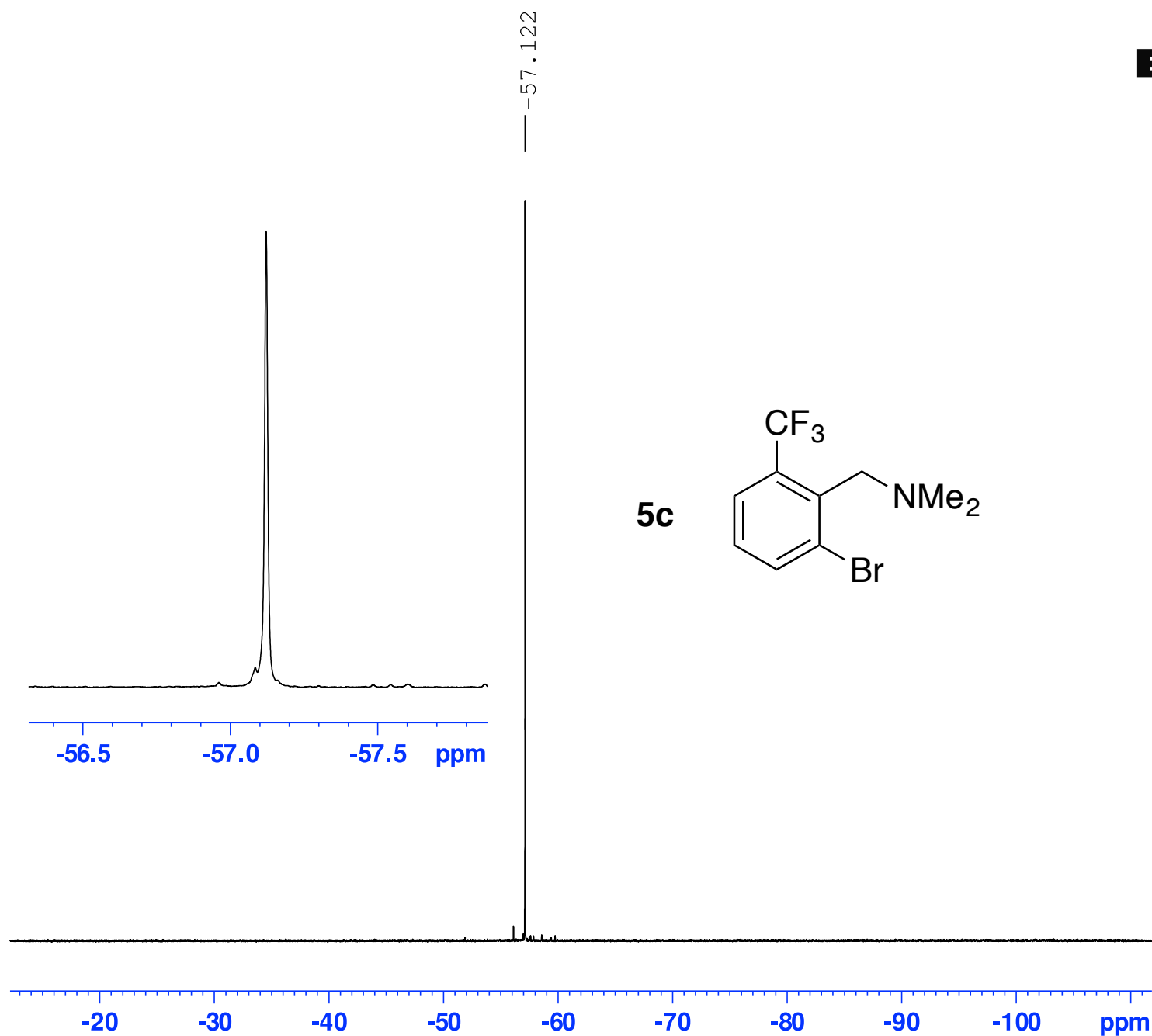
Current Data Parameters
NAME JYG07179b
EXPNO 3
PROCNO 1

3.698

2.307



¹⁹F NMR
5c

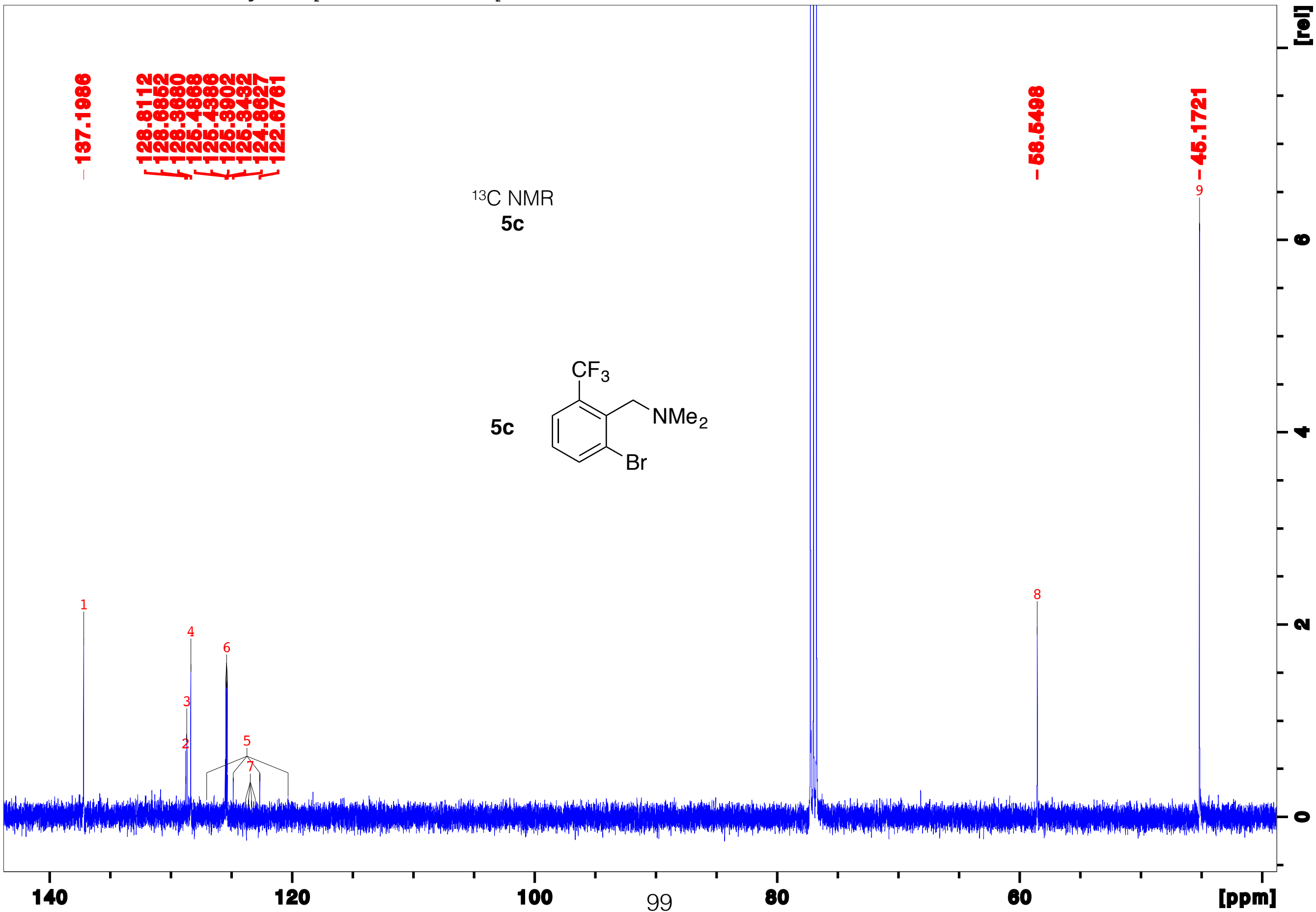


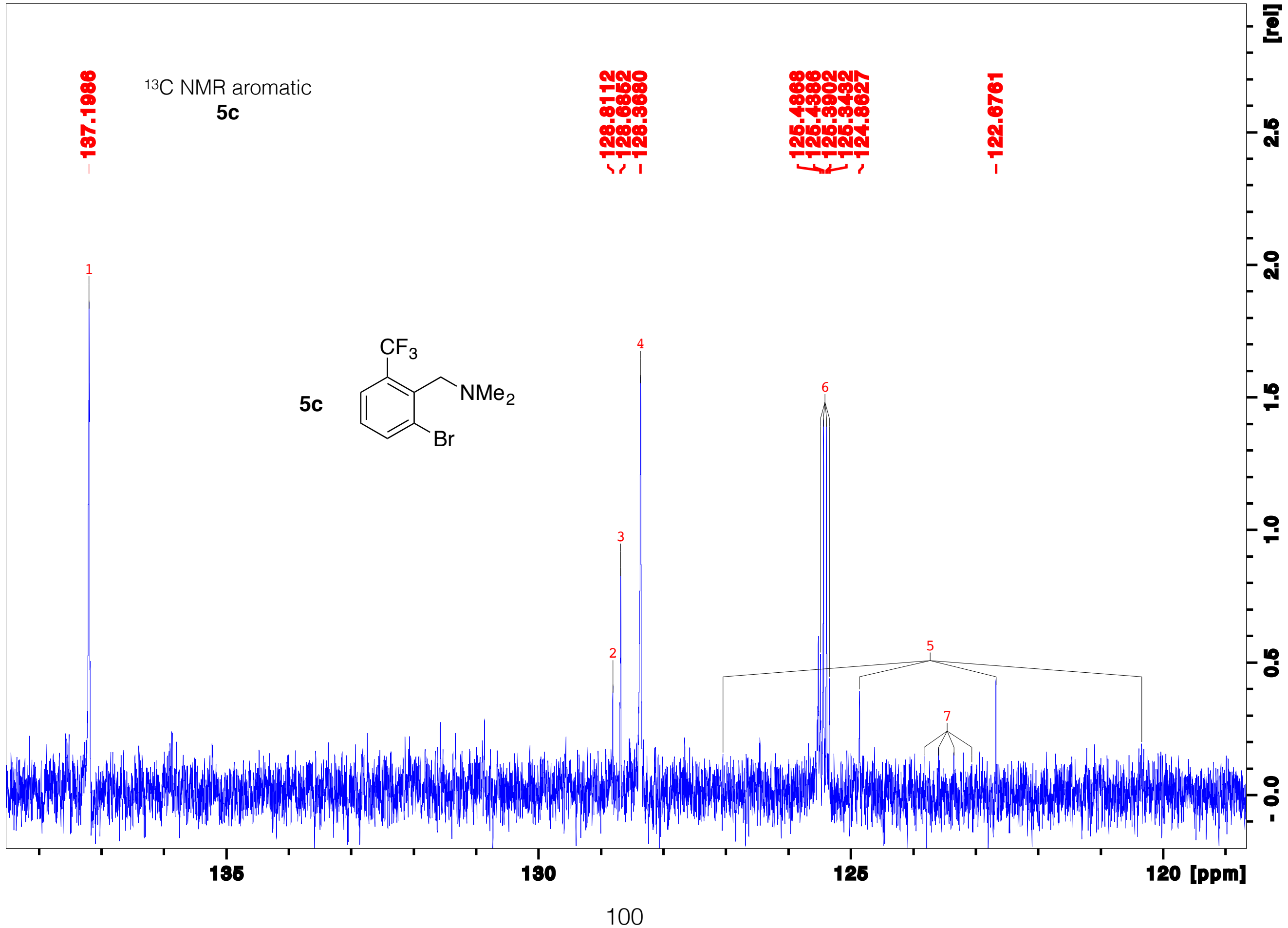
Current Data Parameters
NAME JYG07179
EXPNO 4
PROCNO 1

F2 - Acquisition Parameter
Date_ 20160831
Time 9.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 281244
SOLVENT CDCl3
NS 1
DS 0
SWH 46875.000 Hz
FIDRES 0.166670 Hz
AQ 2.9999361 sec
RG 695.65
DW 10.667 usec
DE 6.50 usec
TE 295.8 K
D1 3.00000000 sec
TD0 1

===== CHANNEL f1 =====
SF01 470.3185714 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.00





¹H NMR
5d

8.126
8.110

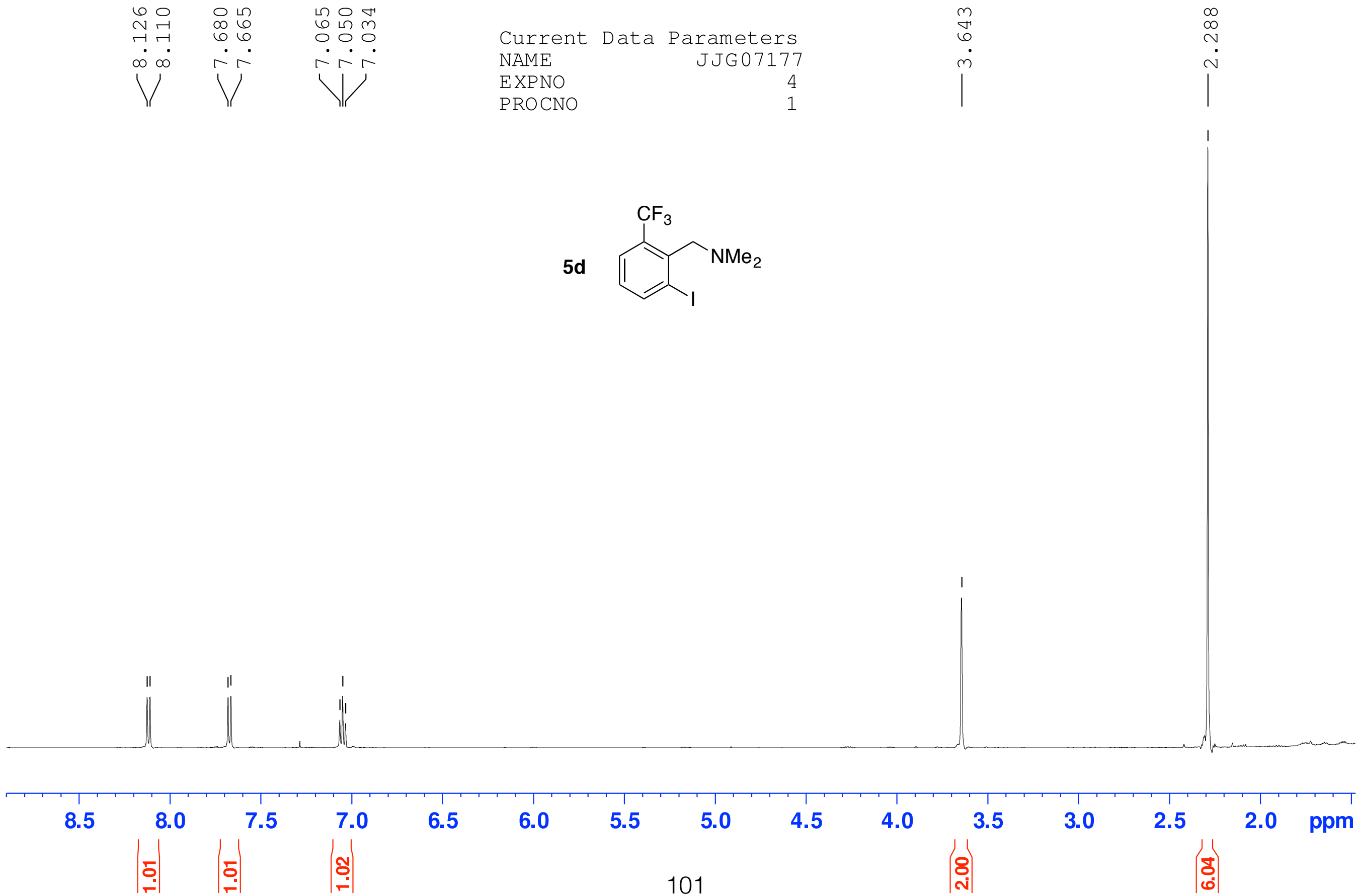
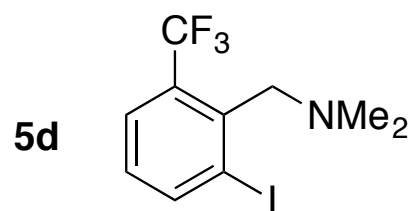
7.680
7.665

7.065
7.050
7.034

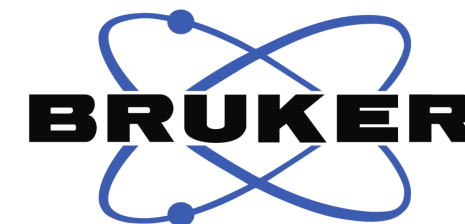
Current Data Parameters
NAME JYG07177
EXPNO 4
PROCNO 1

3.643

2.288



¹⁹F NMR
5d



Current Data Parameters
NAME JYG07177
EXPNO 6
PROCNO 1

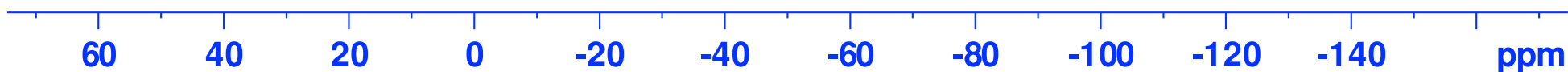
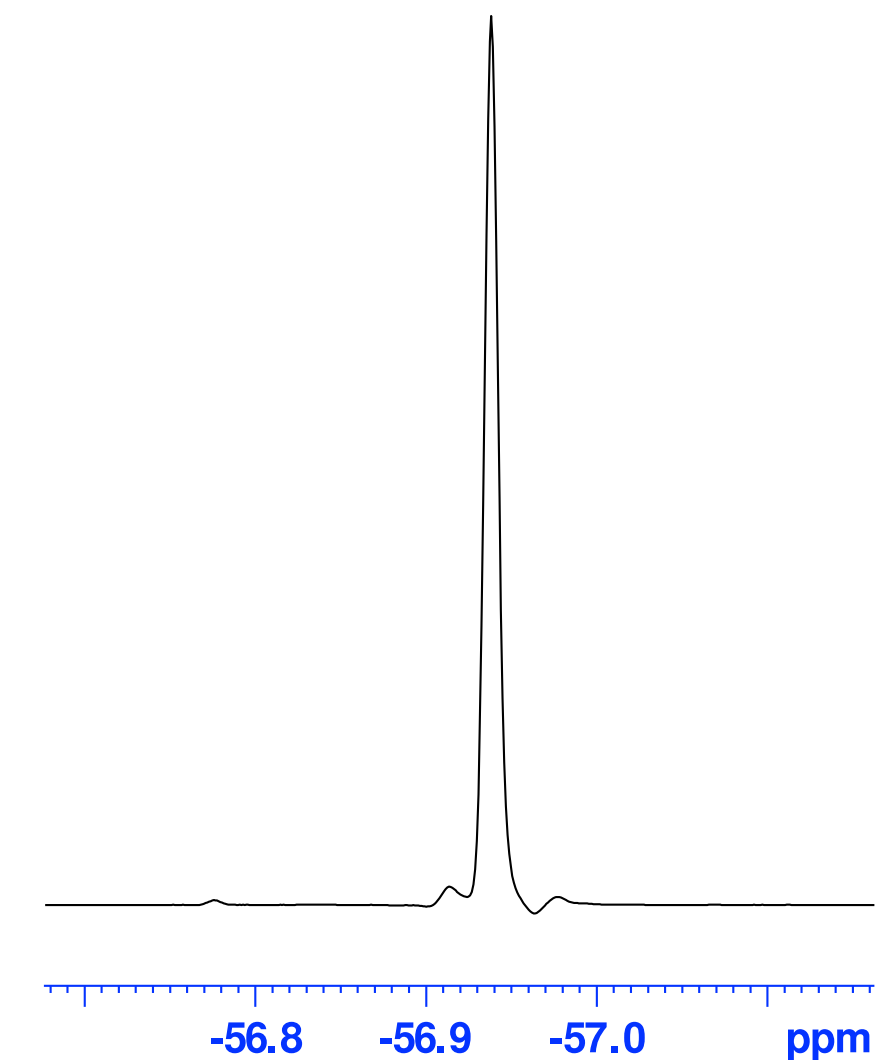
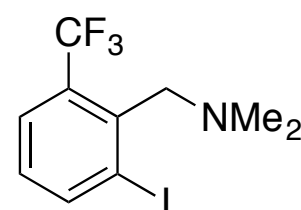
F2 - Acquisition Parameter
Date_ 20160820
Time 11.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgflqn
TD 703112
SOLVENT CDCl3
NS 1
DS 0
SWH 117187.500 Hz
FIDRES 0.166670 Hz
AQ 2.9999444 sec
RG 118.99
DW 4.267 usec
DE 6.50 usec
TE 295.8 K
D1 5.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 470.3242156 MHz
NUC1 19F
P1 15.00 usec
PLW1 37.79999924 W

F2 - Processing parameters
SI 262144
SF 470.3477328 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

-56.938

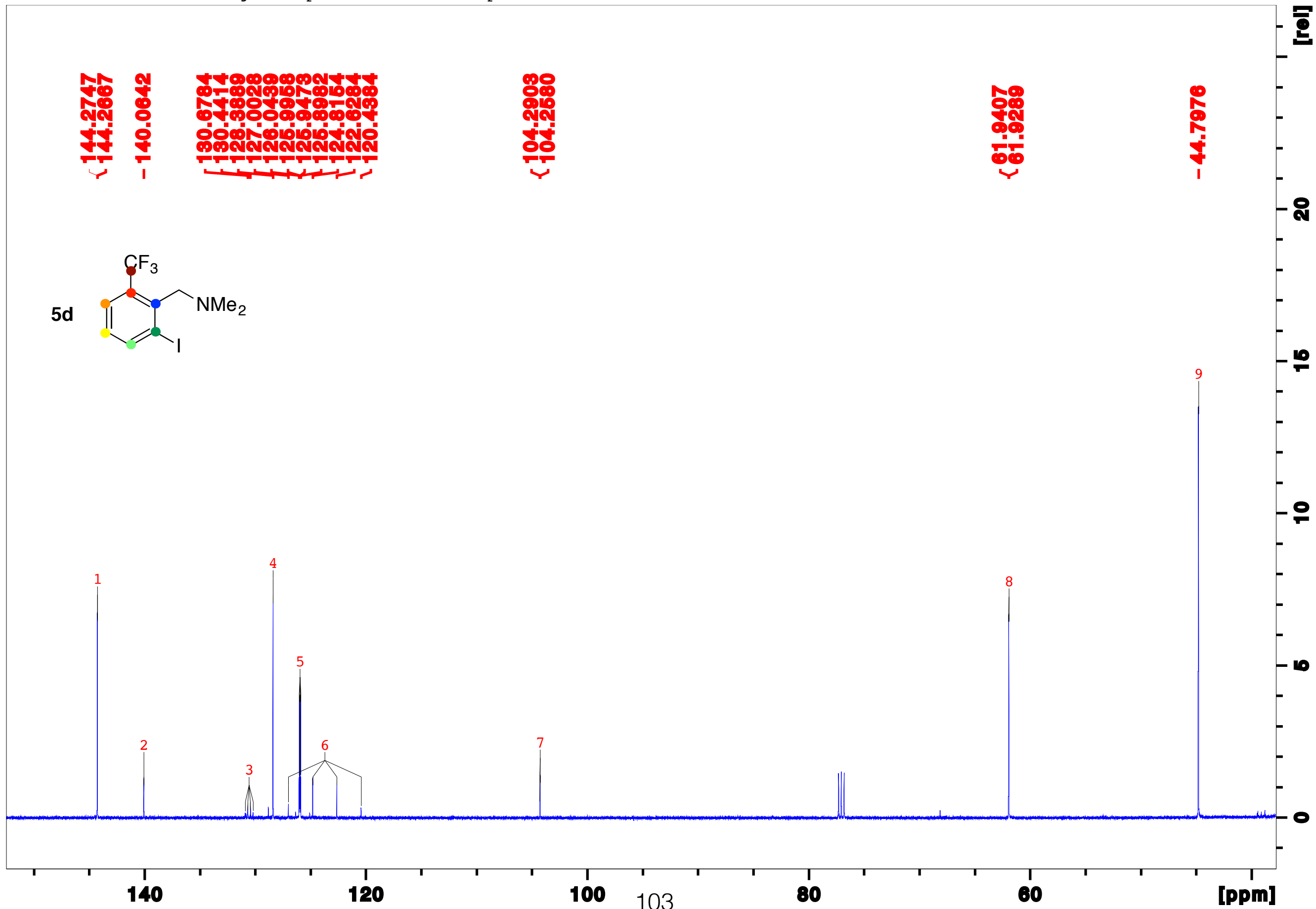
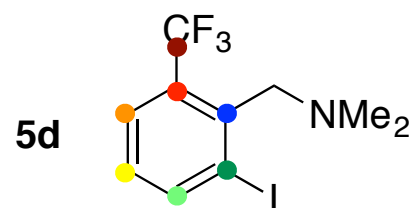
5d



¹³C NMR

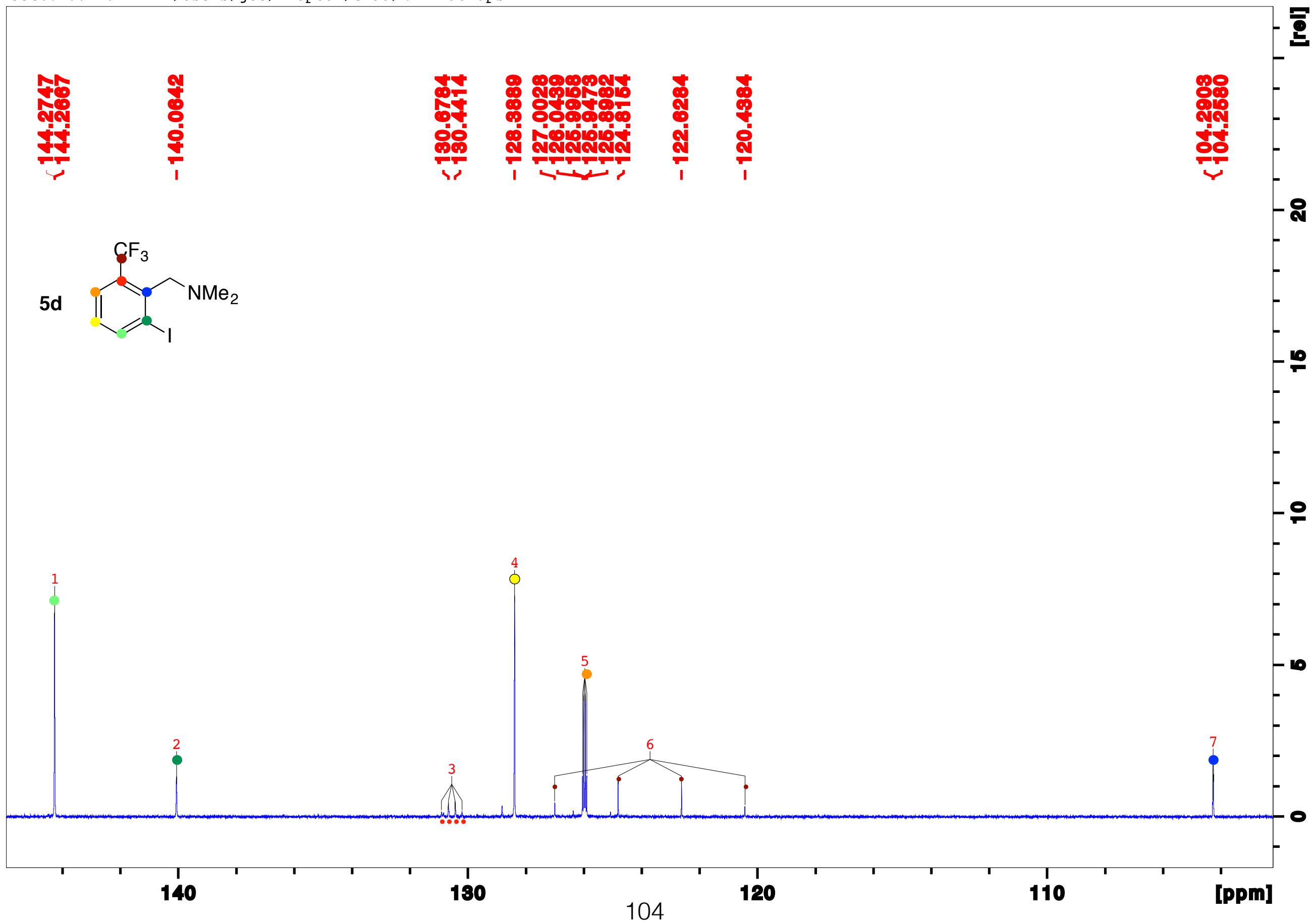
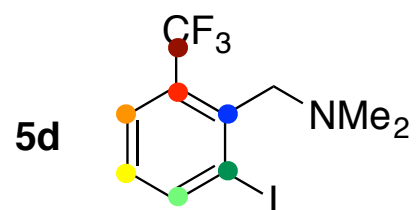
5d

JJG07177 7 1 "/Users/joe/Dropbox/Grad/NMR Backups"



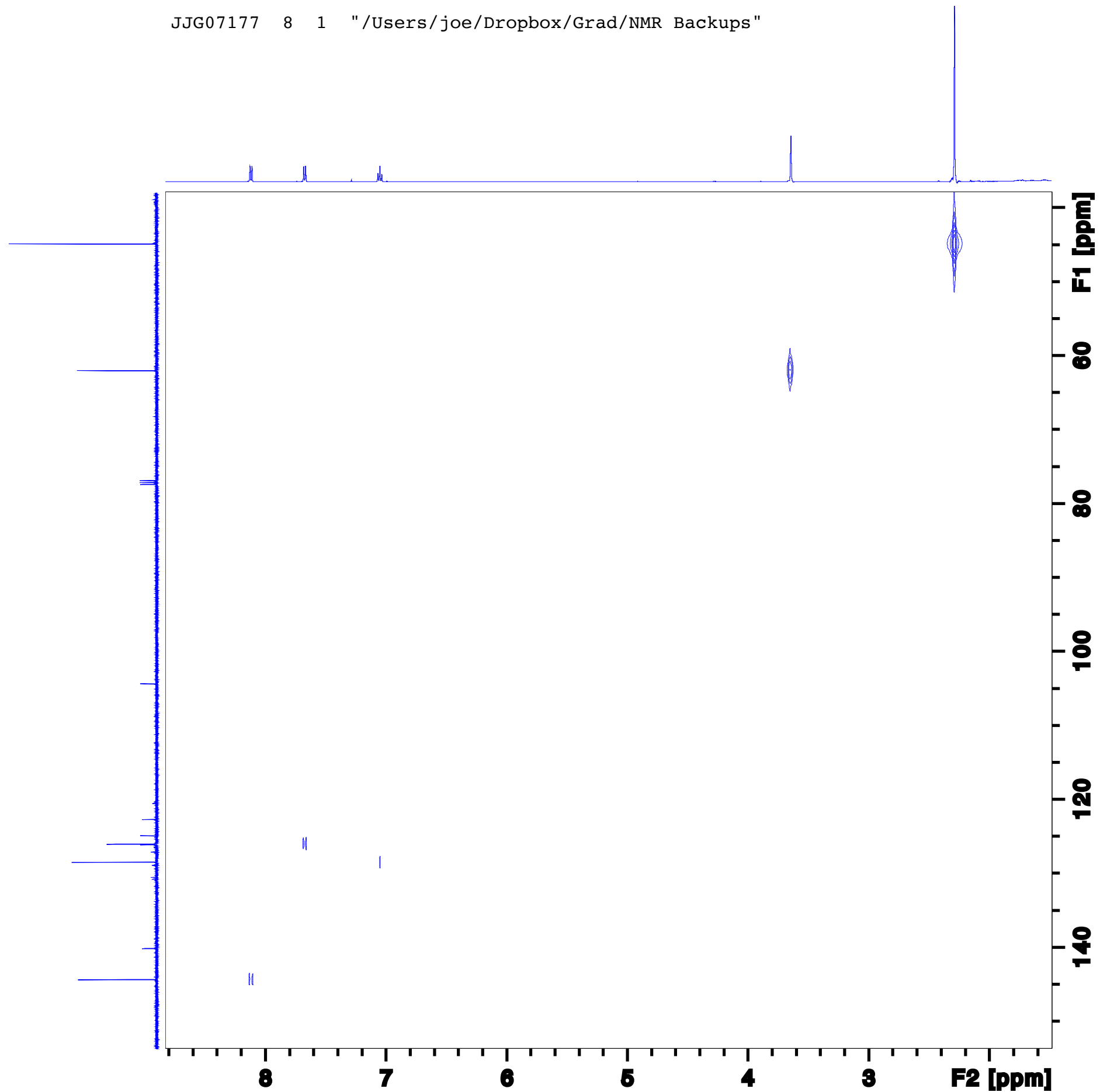
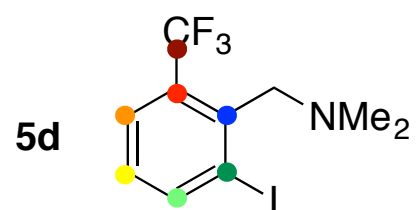
5d

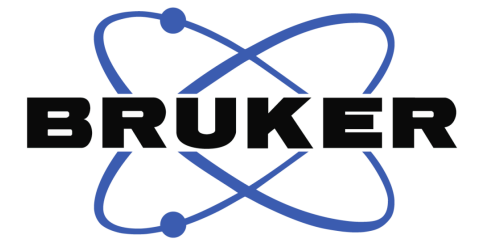
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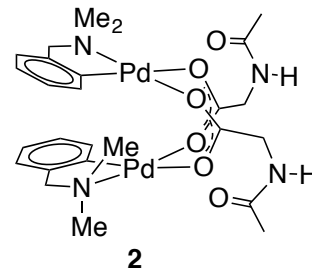
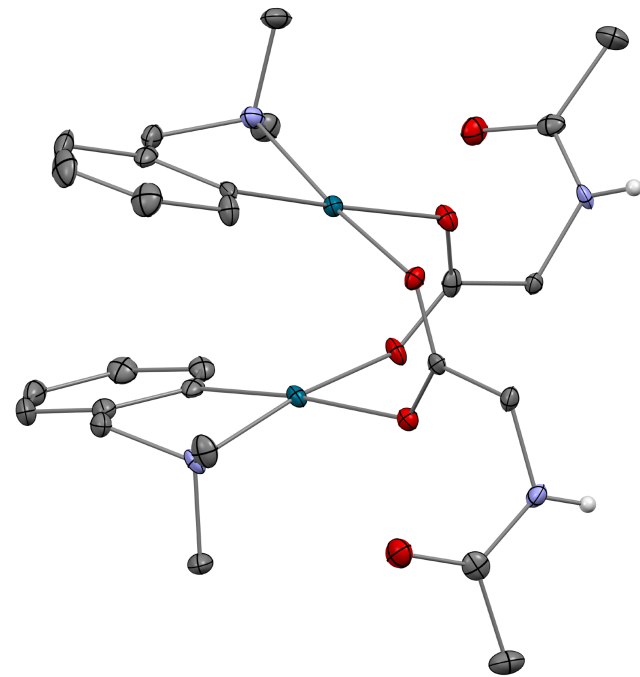
HMQC
5d

JJG07177 8 1 "/Users/joe/Dropbox/Grad/NMR Backups"





¹H NMR in CDCl₃
2 [Pd(dmba)(NAc-Gly)]₂

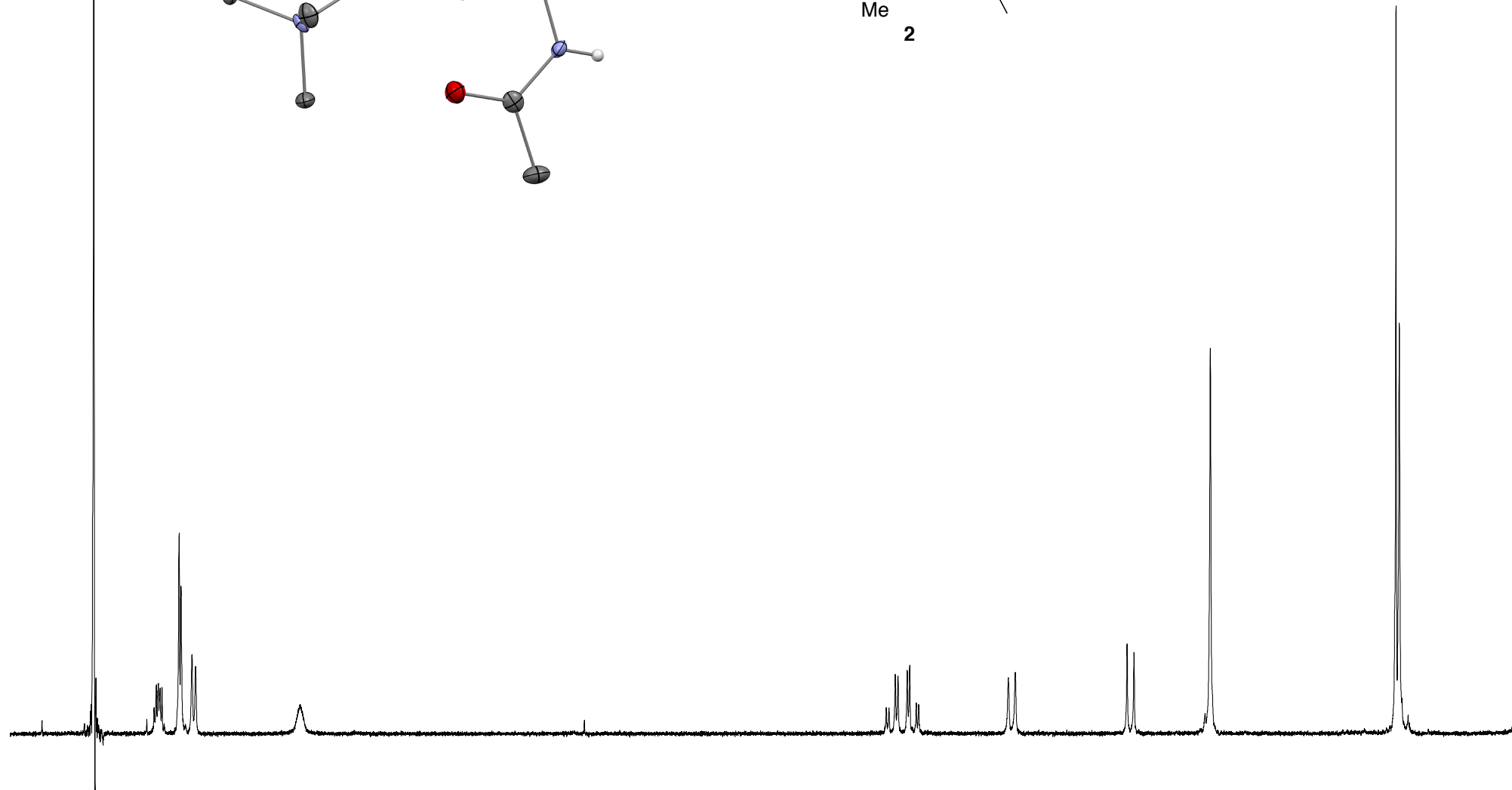


Current Data Parameters
NAME JYG08091
EXPNO 4
PROCNO 1

F2 - Acquisition Parameter
Date_ 20160916
Time 12.15
INSTRUM spect
PROBHD 5 mm PATXI 1H/
PULPROG zg
TD 59998
SOLVENT CDCl₃
NS 1
DS 0
SWH 10000.000 Hz
FIDRES 0.166672 Hz
AQ 2.9999001 sec
RG 196.79
DW 50.000 usec
DE 10.00 usec
TE 293.5 K
D1 10.00000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 500.1330885 MHz
NUC1 1H
P1 8.00 usec
PLW1 12.19999981 W

F2 - Processing parameters
SI 65536
SF 500.1300000 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00



7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 ppm

6.00

2.07

1.81

4.00

2.02

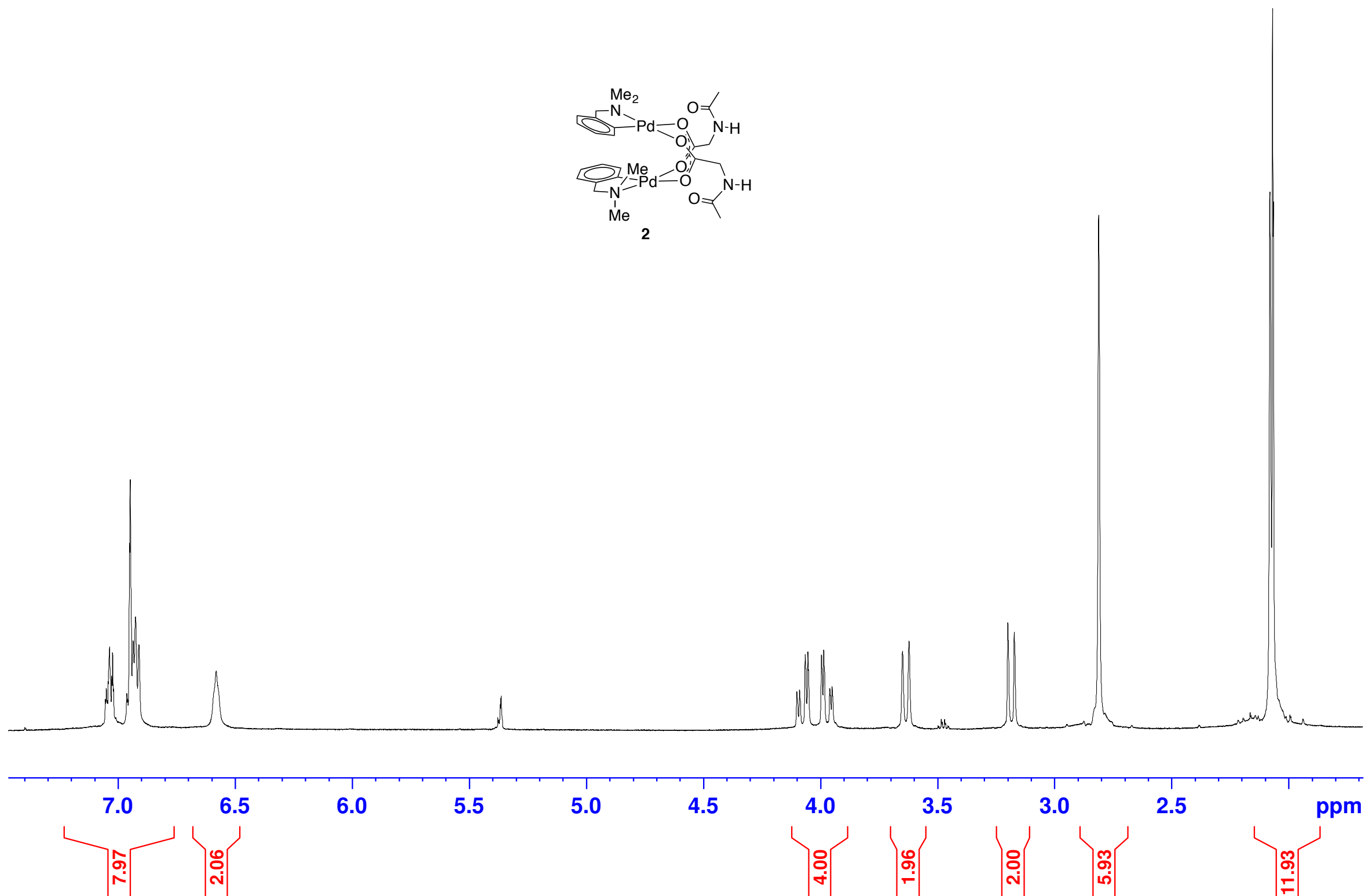
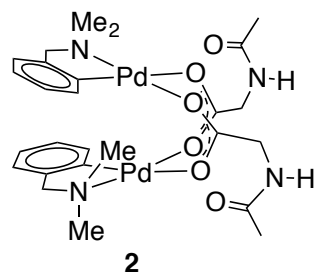
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6.04

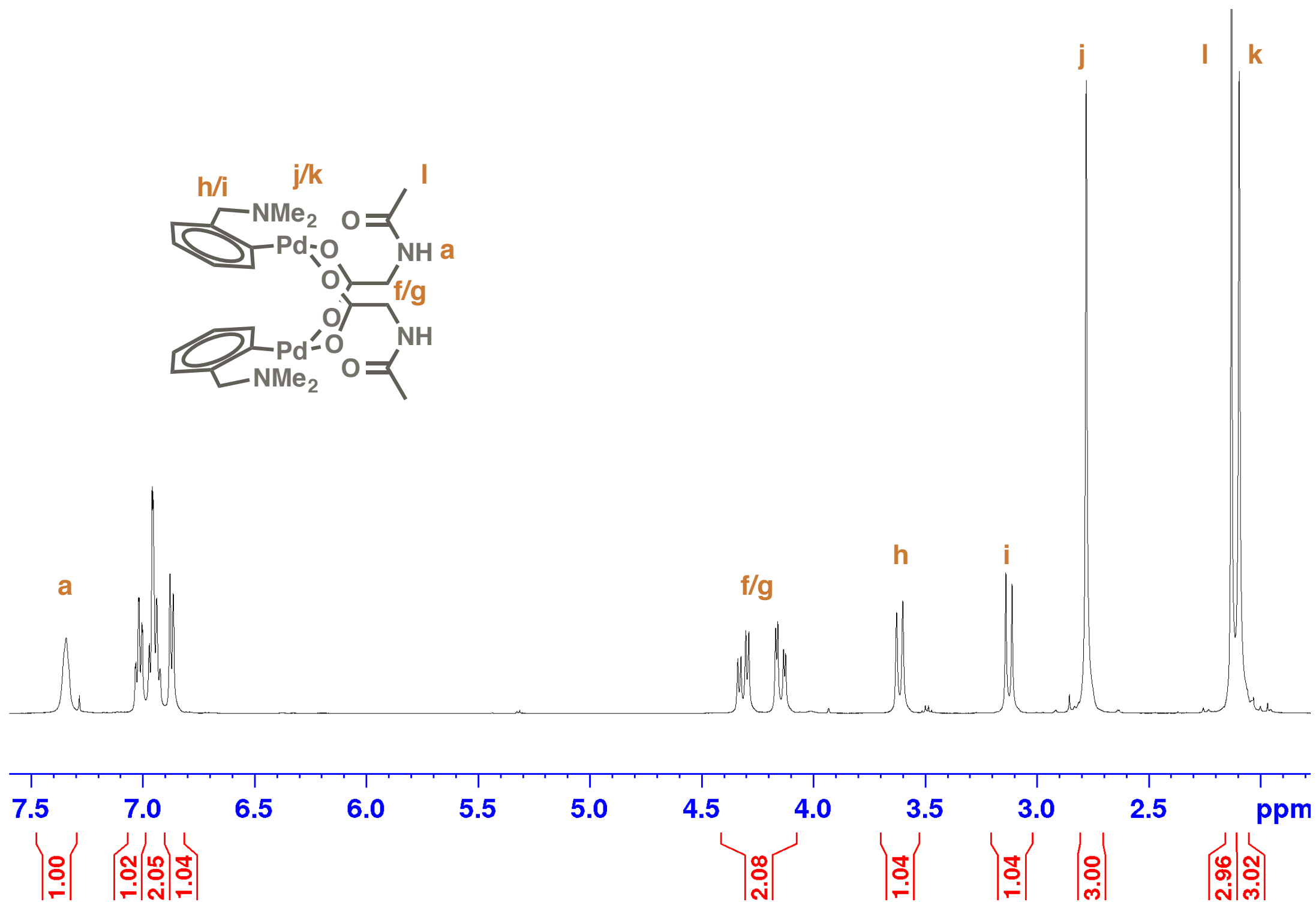
12.01

106

^1H NMR in CD_2Cl_2
2 $[\text{Pd}(\text{dmba})(\text{NAc-Gly})]_2$



^1H NMR in THF- d_8
2 $[\text{Pd}(\text{dmba})(\text{NAc-Gly})]_2$



NOESY in THF-d₈
2 [Pd(dmba)(NAc-Gly)]₂

JJG03016 4 1 /opt/topspin/data/jgair/nmr

