

Supporting Information

For

4-Halo-1,2,3-triazolyliidenes: Stable Carbenes Featuring Halogen Bonding

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1 X-ray Structural Study Details

All crystallographic data for structures were collected using Bruker D8 venture Kappa Duo diffractometer equipped with a PHOTON 100 detector, a I μ S micro-focus sealed X-ray tube and a Cryostream Cooler (Oxford Cryosystems) using Mo K α radiation ($\lambda = 0.71073$ Å). The crystals were mounted in Cryo-Loops using Paratone oil. The frames were integrated using the SAINT algorithm^[1] to give the hkl files corrected for Lp/decay. Data were corrected for absorption effects using the multi-scan method (SADABS).^[2]

The structures were solved by direct methods using SHELXT^[3] and refined against F² on all data by full-matrix least squares with SHELXL^[4] following established refinement strategies^[5] via the OLEX-2 suite of crystallographic programs.^[6] All non-hydrogen atoms were refined anisotropically ORTEP drawings were prepared using the ORTEP-3 for Windows (version 2014.1).^[7] A very large solvent accessible void in **1-Au**, **2-Au** and **3-Au(I)** were squeezed by using Platon.^[8] In all of the structures, the commands DELU, SIMU and ISOR were applied to mostly restrain the disorders of anions, 2,6-diisopropylphenyl substituents and the solvent molecules. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication nos. CCDC Number: **1-(H⁺)**, 1857789. **2-(H⁺)**, 1857790. **2**, 1857791. **1-Au**, 1857792. **2-Au**, 1857793. **3-Au(I)**, 1857794. **1-Cu**, 1857795. **2-Cu**, 1857796. **3-Cu**, 1857797. **5-(I⁻)**, 1857798. **3-Ir**, 1857800, **3-Au[PF₆]**, 1885414. **7**, 1868802. **4**, 1897693. **5**, 1897694. Copies of these data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

2 Computational Details

Calculations were carried out with the TURBOMOLE program.^[9] In order to reduce the computational cost, the 2,6-diisopropylphenyl groups were replaced by methyl groups. Geometry optimizations were performed with the density functional theory (DFT)/B3LYP, together with def-TZVP basis set. Frequency calculations at the same level of theory were performed.

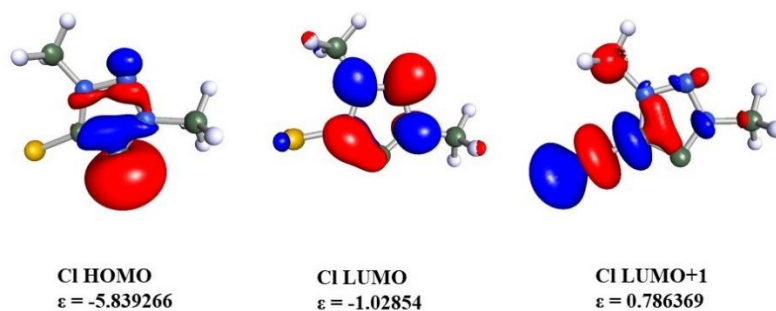


Figure S1 Cl substitution 1,2,3-triazol-5-ylidene orbital energies ϵ at the DFT B3LYP/def-TZVP level of theory.

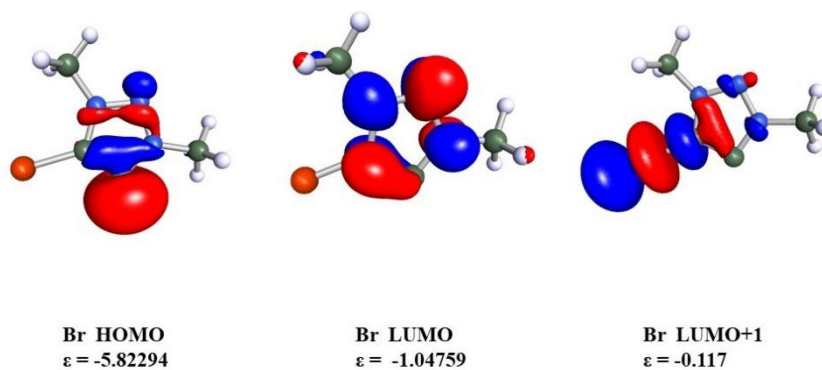


Figure S2 Br substitution 1,2,3-triazol-5-ylidene orbital energies ϵ at the DFT B3LYP/def-TZVP level of theory.

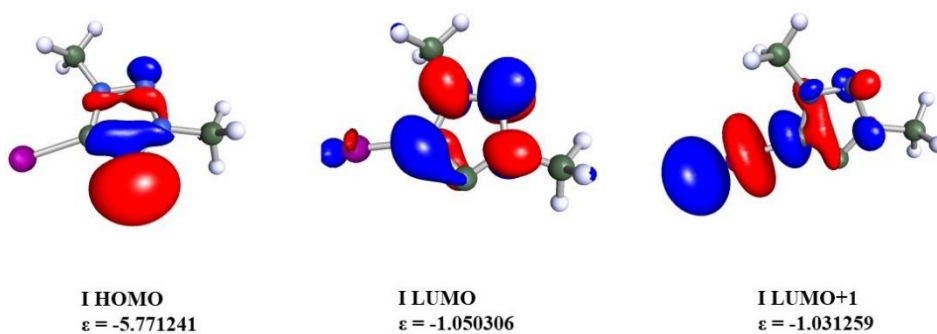


Figure S3 I substitution 1,2,3-triazol-5-ylidene orbital energies ϵ at the DFT/B3LYP-

def-TZVP level of theory.

Table S1 Details of Computation

Substitute	Energy/hatree			Energy/e.V		
Orbital	HOMO	LUMO	LUMO+1	HOMO	LUMO	LUMO+1
H	-0.1999	-0.0307	0.0336	-5.439279	-0.83535	0.914256
Cl	-0.2146	-0.0378	0.0289	-5.839266	-1.02854	0.786369
Br	-0.214	-0.0385	-0.0043	-5.82294	-1.04759	-0.117
I	-0.2121	-0.0386	-0.0379	-5.771241	-1.05031	-1.03126

3 Huynh's Electronic Parameter (HEP) Details

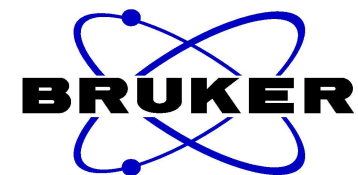
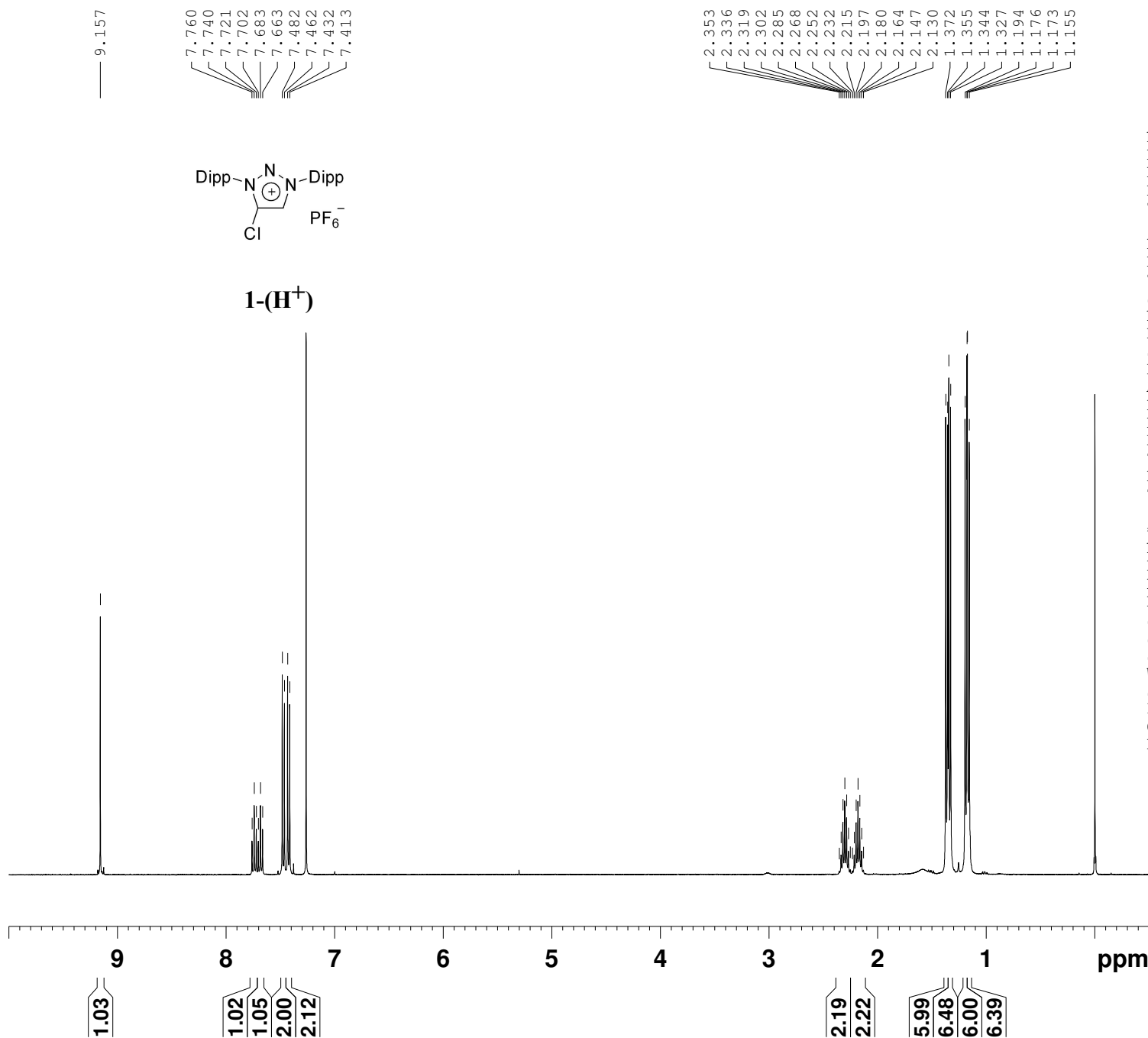
Solution complex **7** (55 mmol/L, CDCl₃) and donors were mixed respectively and then HEP tests were accomplished by Bruker Avance 100MHz (¹³C NMR). The chemical shift data for each HEP test signal are given in units of (ppm) the residual solvent resonances 77.7. The F⁻, Cl⁻, Br⁻ or I⁻ anion is made by using excessive KF, KCl, KBr, KI exchanging the anion BF₄⁻ of **7** in CH₃CN for 24 h.

4 References

- [1] SAINT V7.68A; Bruker AXS, Madison, WI, 2009.
- [2] SADABS V2008/1; Bruker AXS, Madison, WI, 2008.
- [3] G. M. Sheldrick, *Acta Cryst. A*, 2015, **71**, 3.
- [4] G. M. Sheldrick, *Acta Cryst. C*, 2015, **71**, 3.
- [5] P. Müller, *Crystallogr. Rev.*, 2009, **15** (1), 57.
- [6] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard and H. Puschmann, *J. Appl. Cryst.*, 2009, **42**, 339.
- [7] L. J. Farrugia, *J. Appl. Cryst.*, 2012, **45**, 849.
- [8] P. Van der Sluis and A. L. Spek, *Acta Cryst. A* 1990, **46**, 194.

[9] TURBOMOLE V7.0 2015, A development of University of Karlsruhe and Forschungszentrum Karlsruhe GmbH, 1989- 2007, TURBOMOLE GmbH, *since 2007*, Available from <http://www.turbomole.com>.

5 Copies of ^1H NMR and ^{13}C NMR Spectra

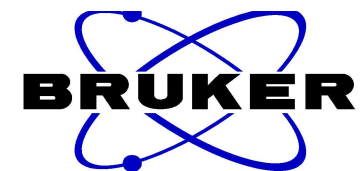
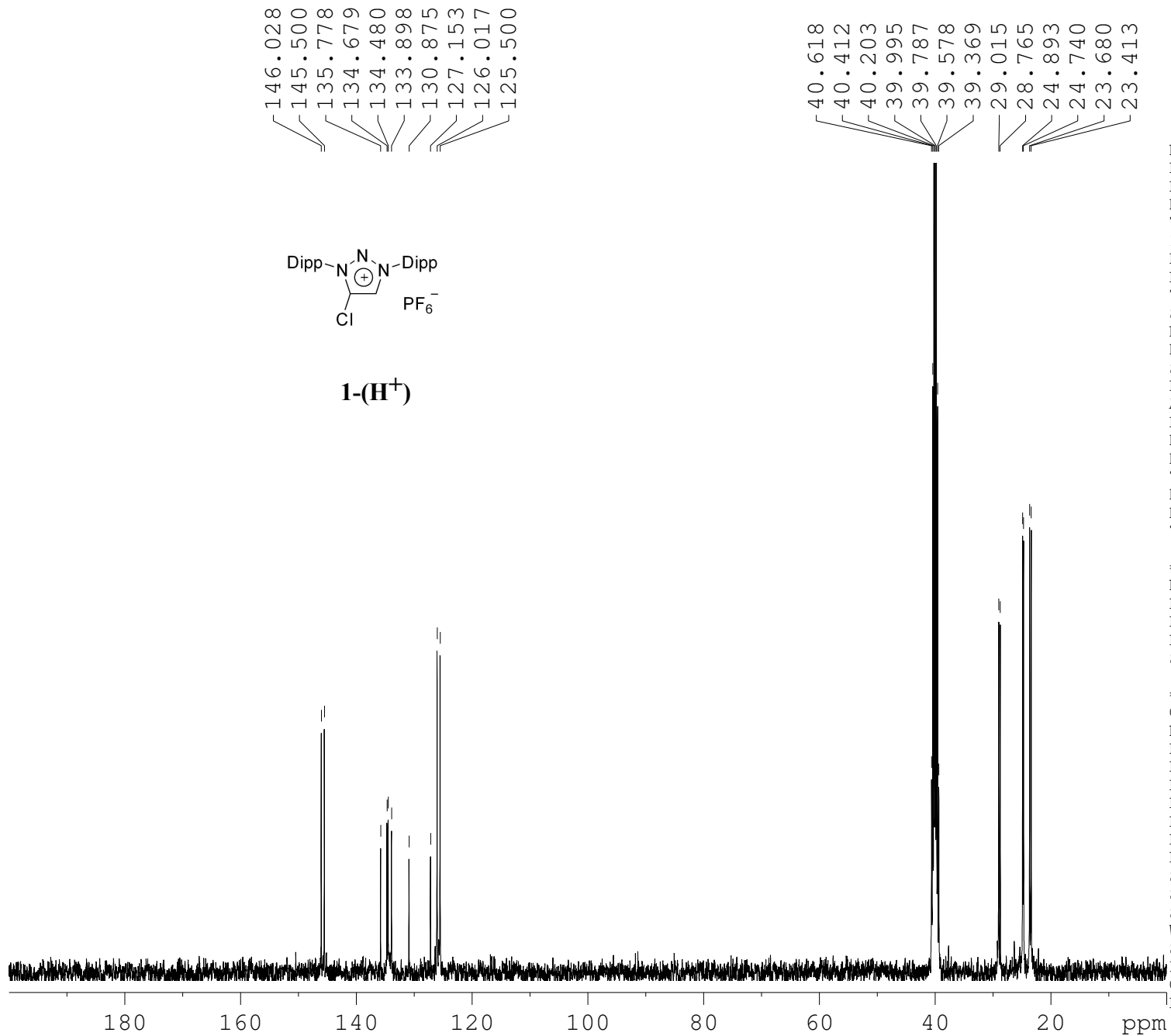


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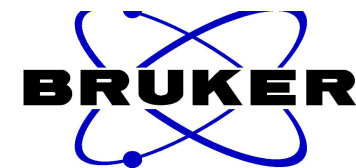
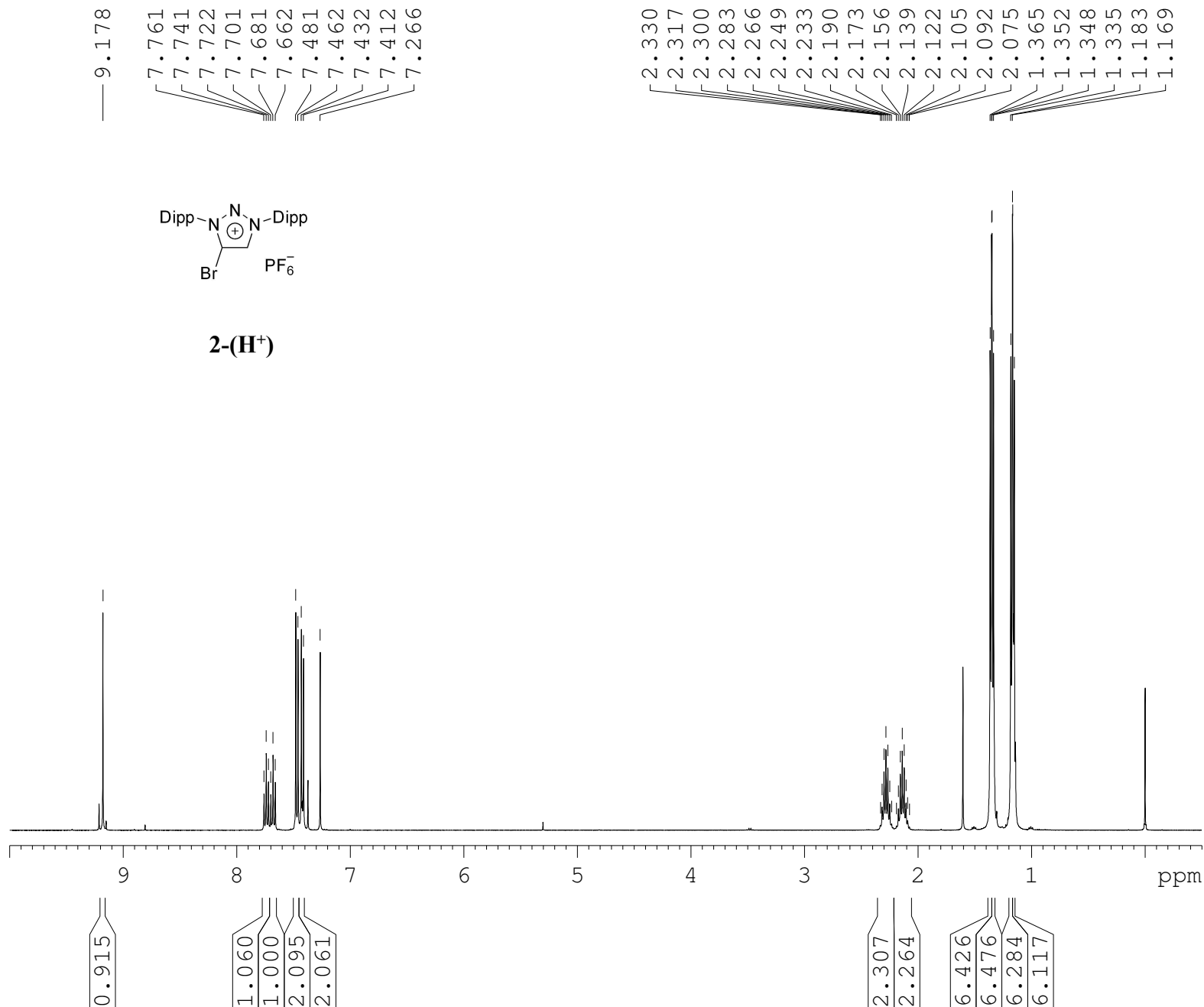
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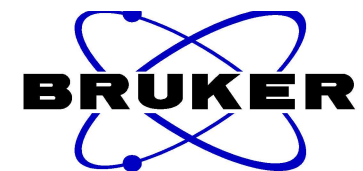
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 PL12 17.19 dB
 PL13 18.46 dB
 PL2W 8.92857742 W
 PL12W 0.25809658 W
 PL13W 0.19265592 W
 SFO2 400.1316005 MHz
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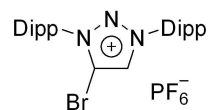
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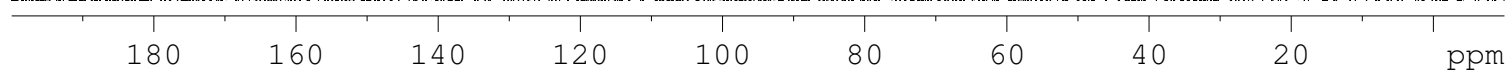


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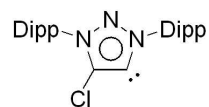
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 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
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 PCPD2 80.00 usec
 PL2 1.80 dB
 PL12 17.19 dB
 PL13 18.46 dB
 PL2W 8.92857742 W
 PL12W 0.25809658 W
 PL13W 0.19265592 W
 SFO2 400.1316005 MHz
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 SF 100.6127690 MHz
 WDW EM
 SSB 0
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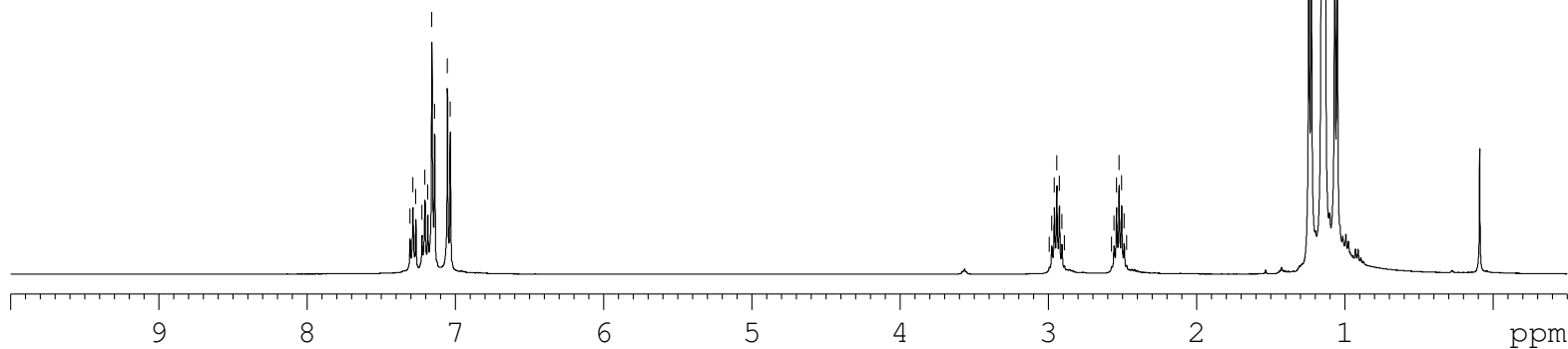
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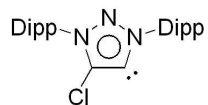


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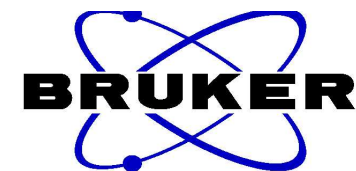
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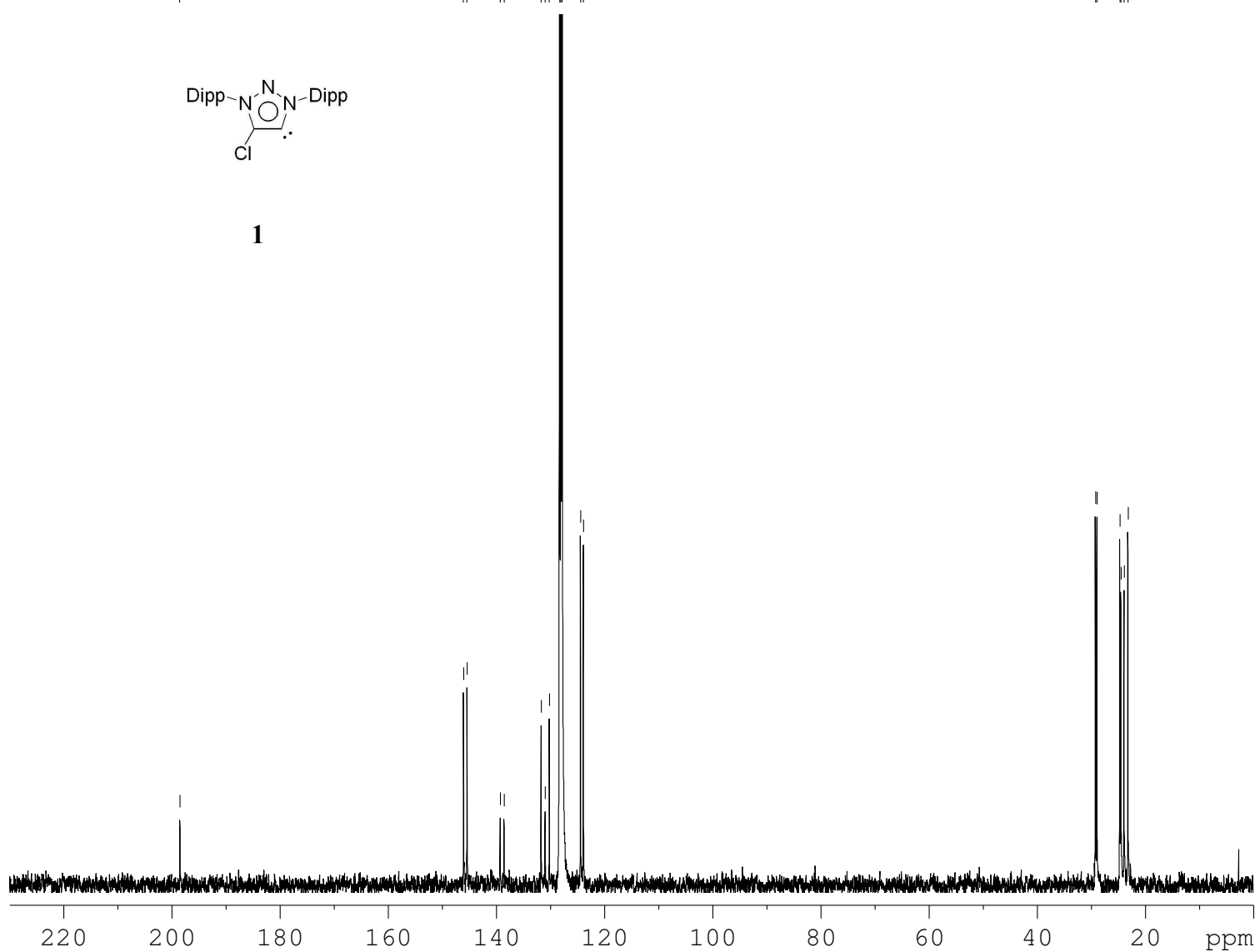
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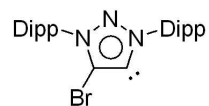
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===== CHANNEL f2 =====
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PCPD2 80.00 usec
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PL12 17.19 dB
PL13 18.46 dB
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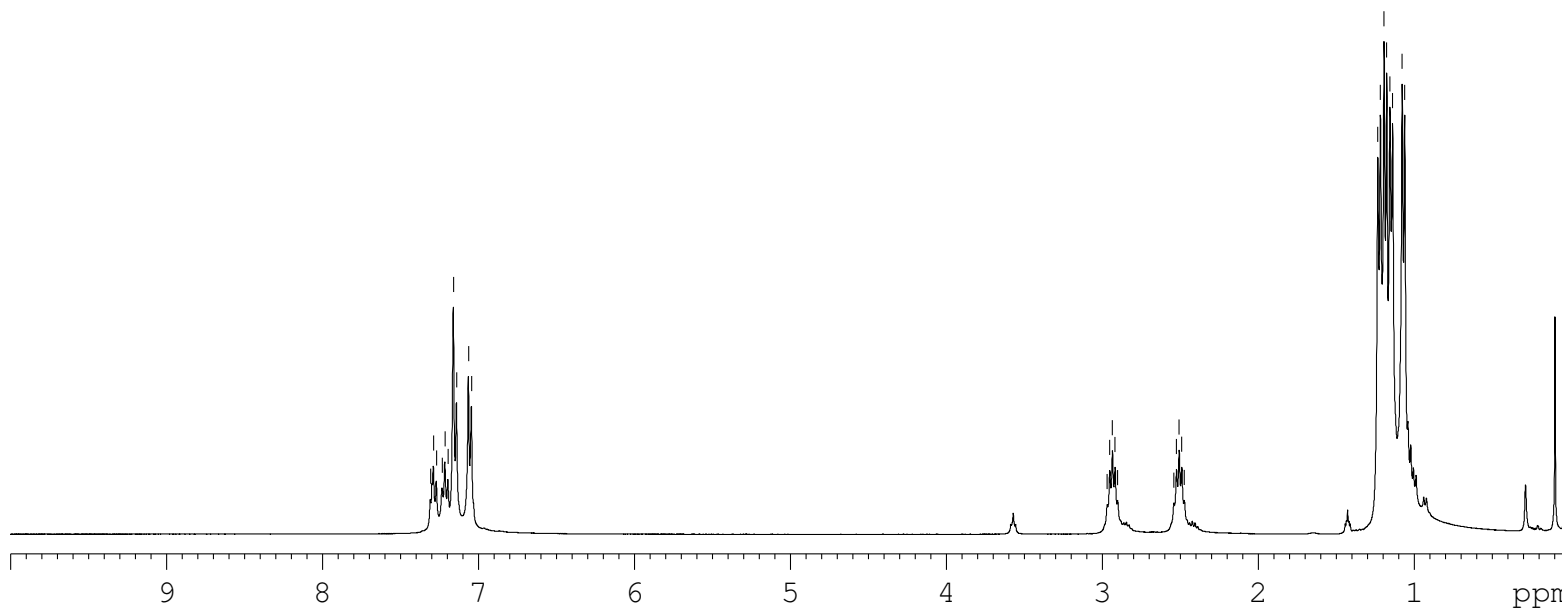
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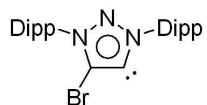


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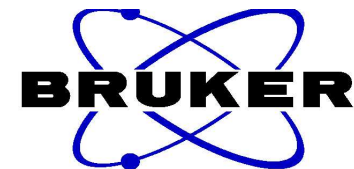
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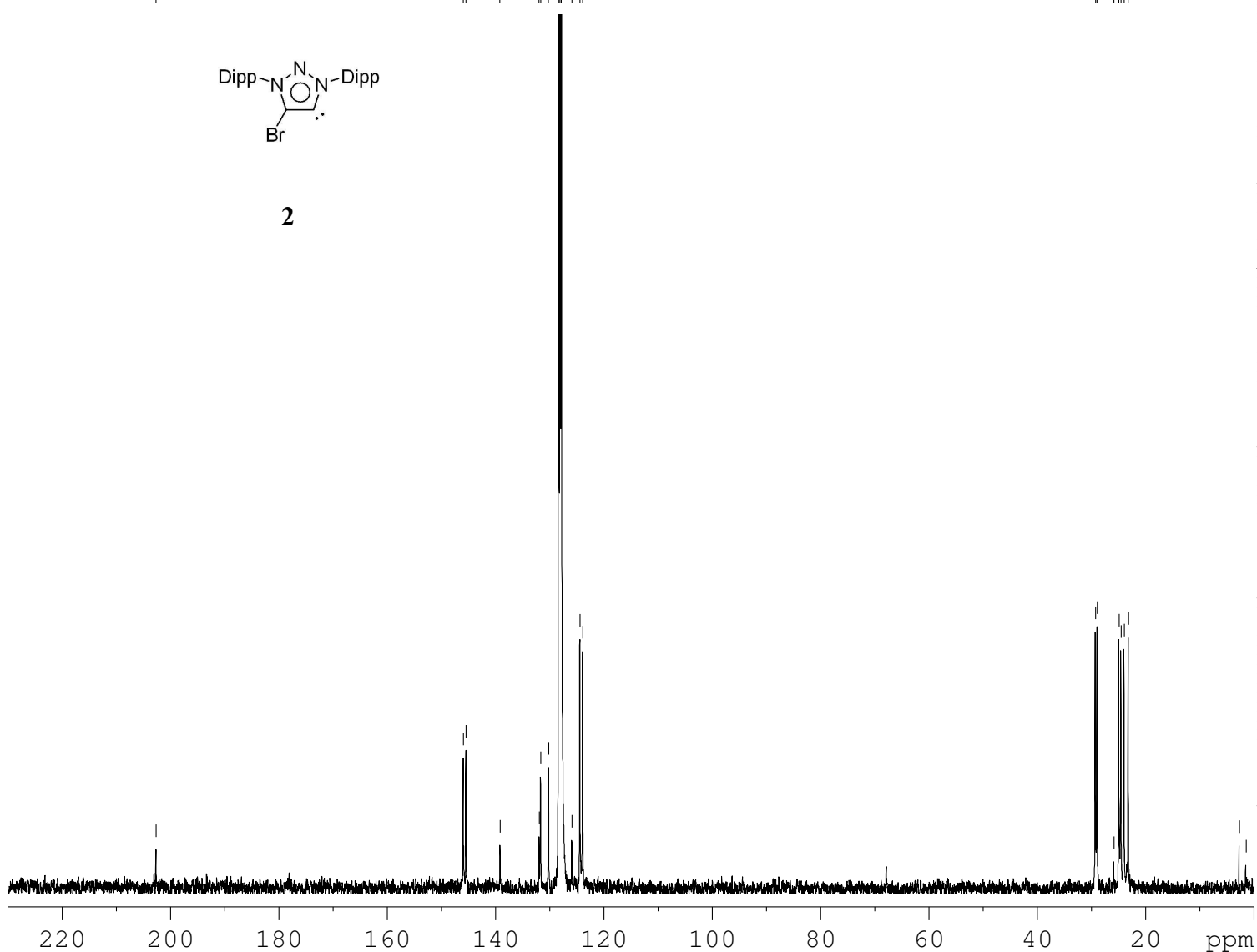
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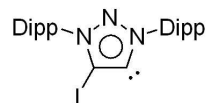


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PL1 3.00 dB
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NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 17.19 dB
PL13 18.46 dB
PL2W 8.92857742 W
PL12W 0.25809658 W
PL13W 0.19265592 W
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3

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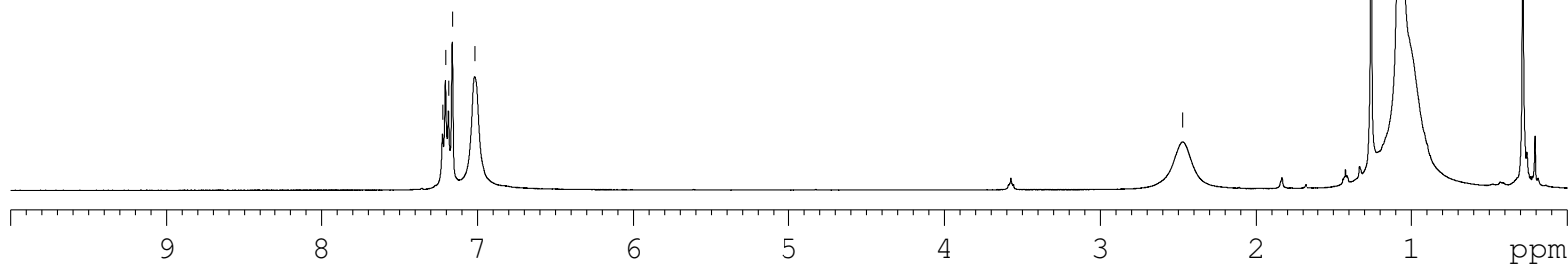
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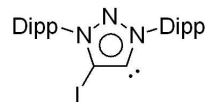
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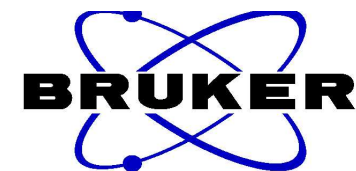
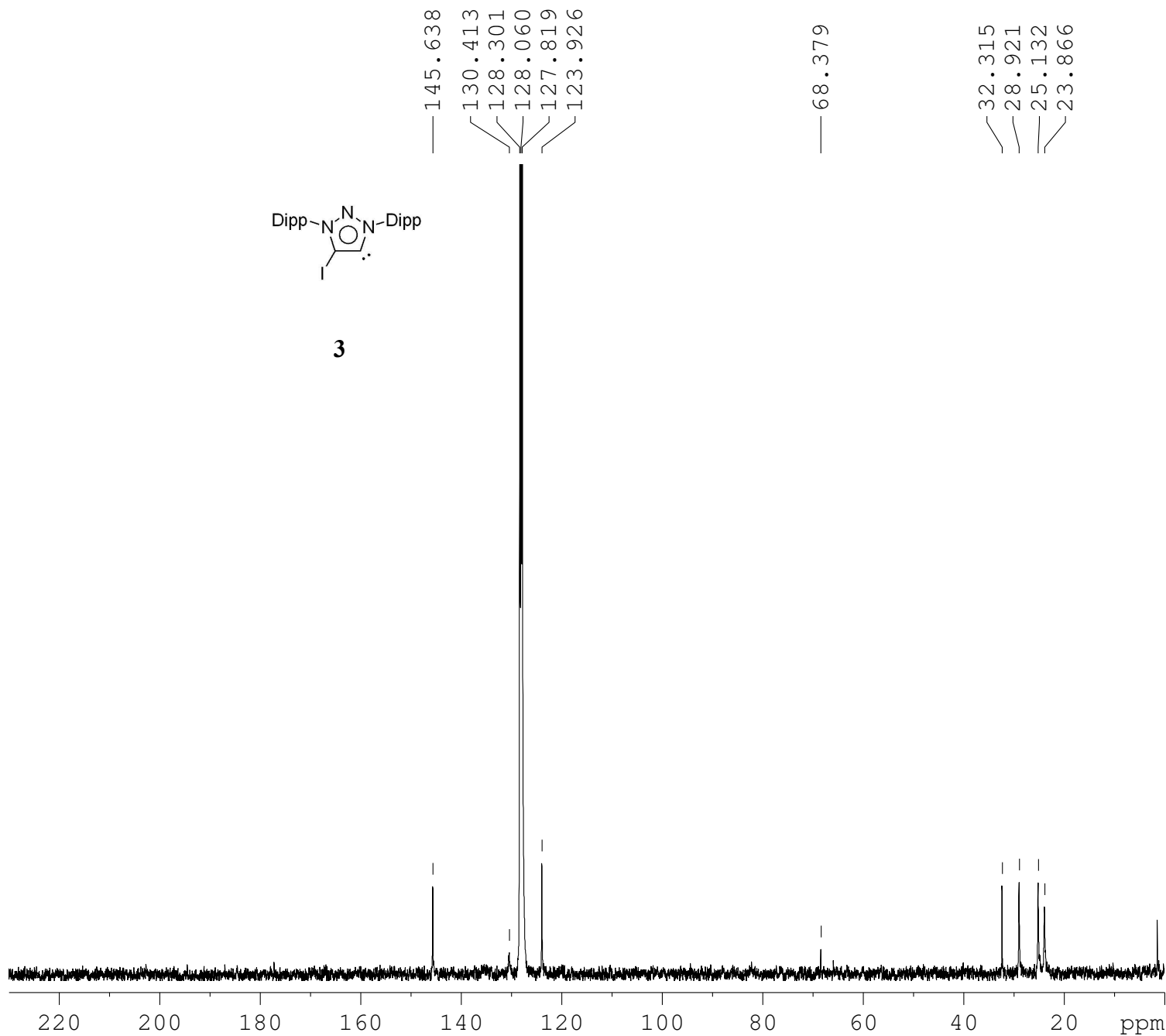
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RG          2050
DW          19.800 usec
DE          8.00 usec
TE          297.6 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1
  
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PL1         3.00 dB
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SFO1        100.6238364 MHz
  
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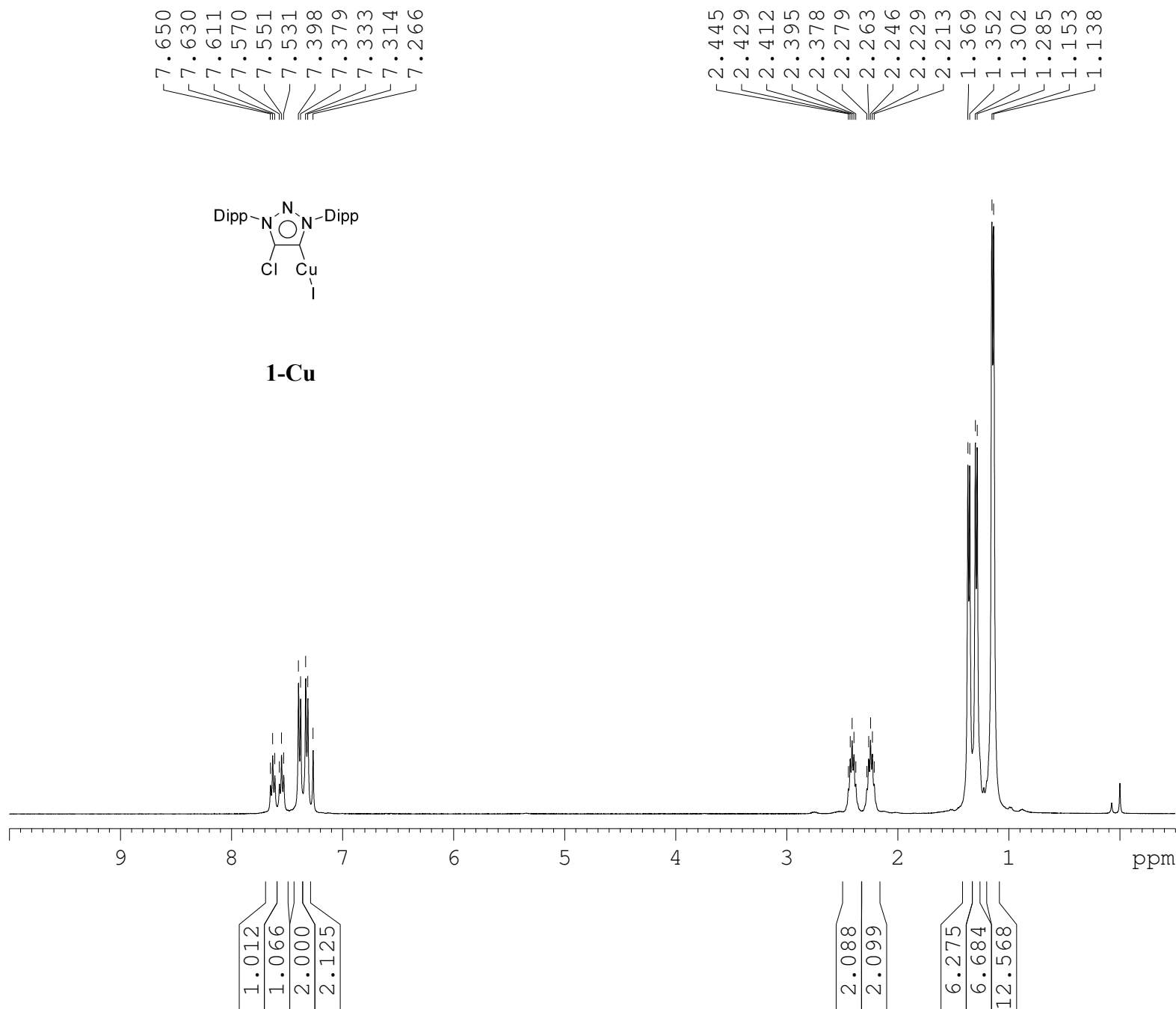
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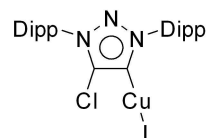
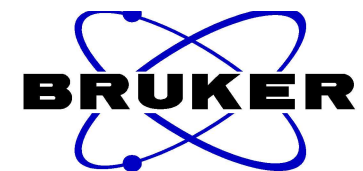
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PL2         1.80 dB
PL12        17.19 dB
PL13        18.46 dB
PL2W        8.92857742 W
PL12W       0.25809658 W
PL13W       0.19265592 W
SFO2        400.1316005 MHz
SI          32768
SF          100.6127425 MHz
WDW         EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
  
```



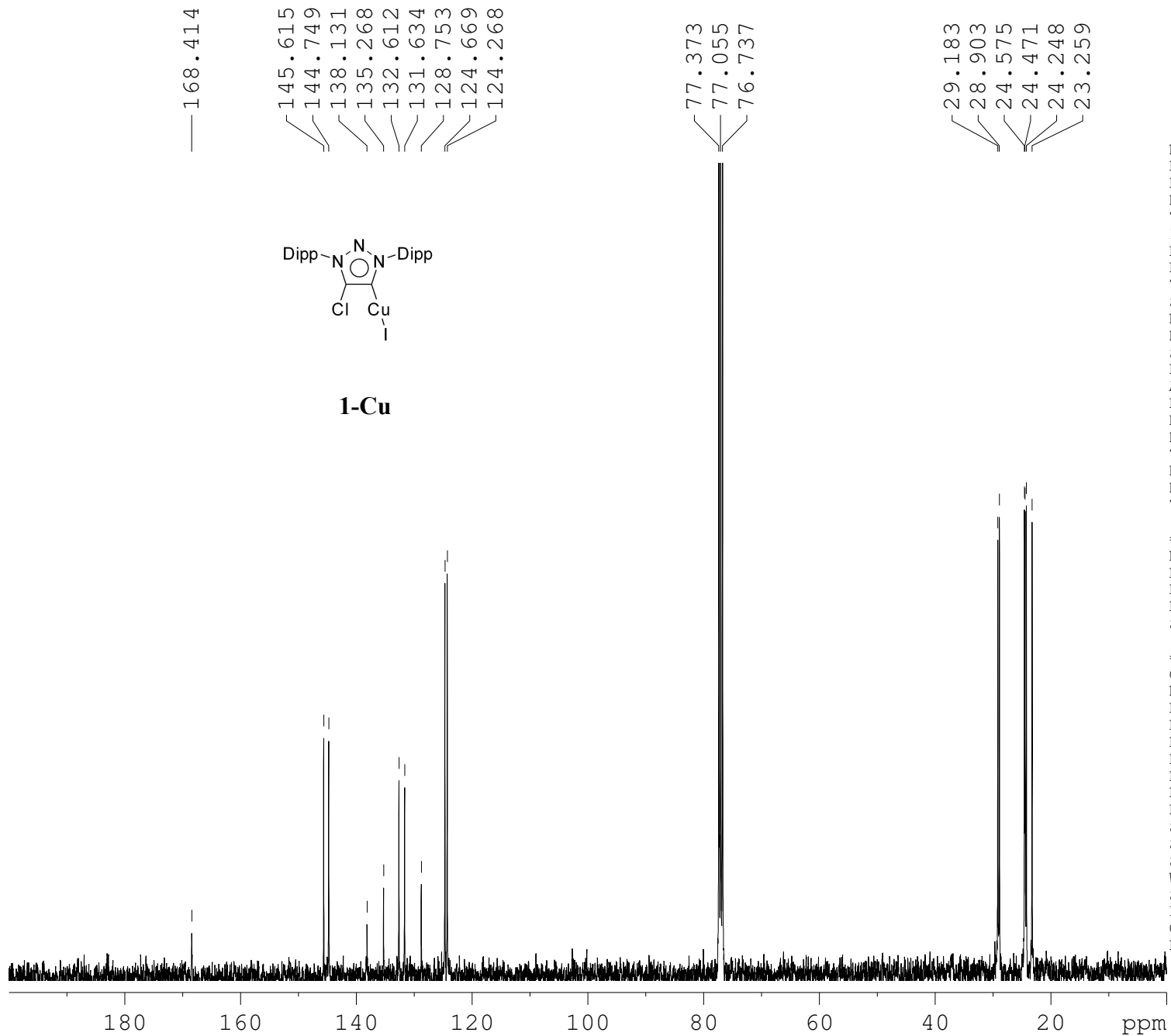
NAME xxy-11-20-cu-20171121
 EXPNO 1
 PROCNO 1
 Date_ 20171121
 Time 14.09
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zg30
 TD 32768
 SOLVENT CDC13
 NS 8
 DS 0
 SWH 6393.862 Hz
 FIDRES 0.195125 Hz
 AQ 2.5625076 sec
 RG 128
 DW 78.200 usec
 DE 6.50 usec
 TE 297.9 K
 D1 2.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.10 usec
 PL1 1.80 dB
 PL1W 8.92857742 W
 SFO1 400.1326008 MHz
 SI 32768
 SF 400.1300076 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





1-Cu



```

NAME      xxy-11-20-cu-20171121
EXPNO      2
PROCNO     1
Date_      20171121
Time       14.13
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         128
DS         4
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         114
DW         19.800 usec
DE         8.00 usec
TE         298.4 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

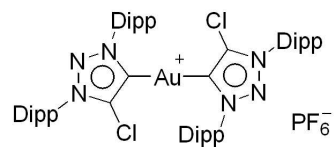
```

===== CHANNEL f1 =====
NUC1       13C
P1         13.50 usec
PL1        3.00 dB
PL1W       43.93649673 W
SFO1       100.6238364 MHz
  
```

```

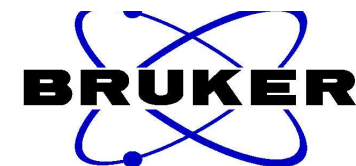
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.80 dB
PL12       17.19 dB
PL13       18.46 dB
PL2W       8.92857742 W
PL12W      0.25809658 W
PL13W      0.19265592 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```

7.714
7.694
7.674
7.646
7.627
7.607
7.445
7.425
7.329
7.310
7.285



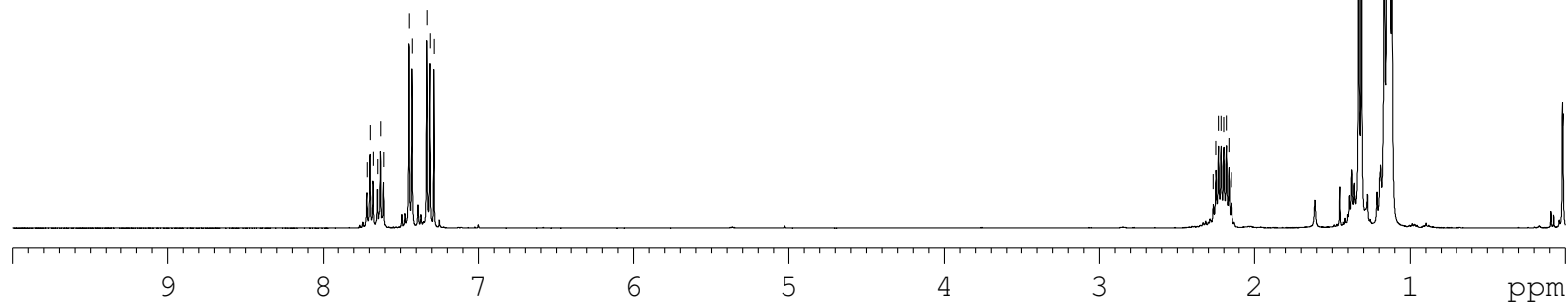
1-Au

2.270
2.253
2.236
2.219
2.201
2.184
2.167
2.150
1.332
1.315
1.167
1.149
1.135
1.131
1.119



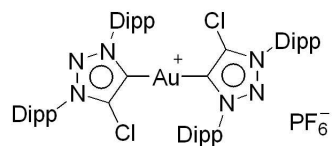
NAME xxy-11-20-au-20171121
EXPNO 1
PROCNO 1
Date_ 20171121
Time 14.24
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 181
DW 78.200 usec
DE 6.50 usec
TE 298.1 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

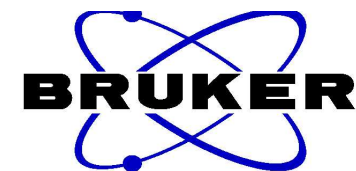
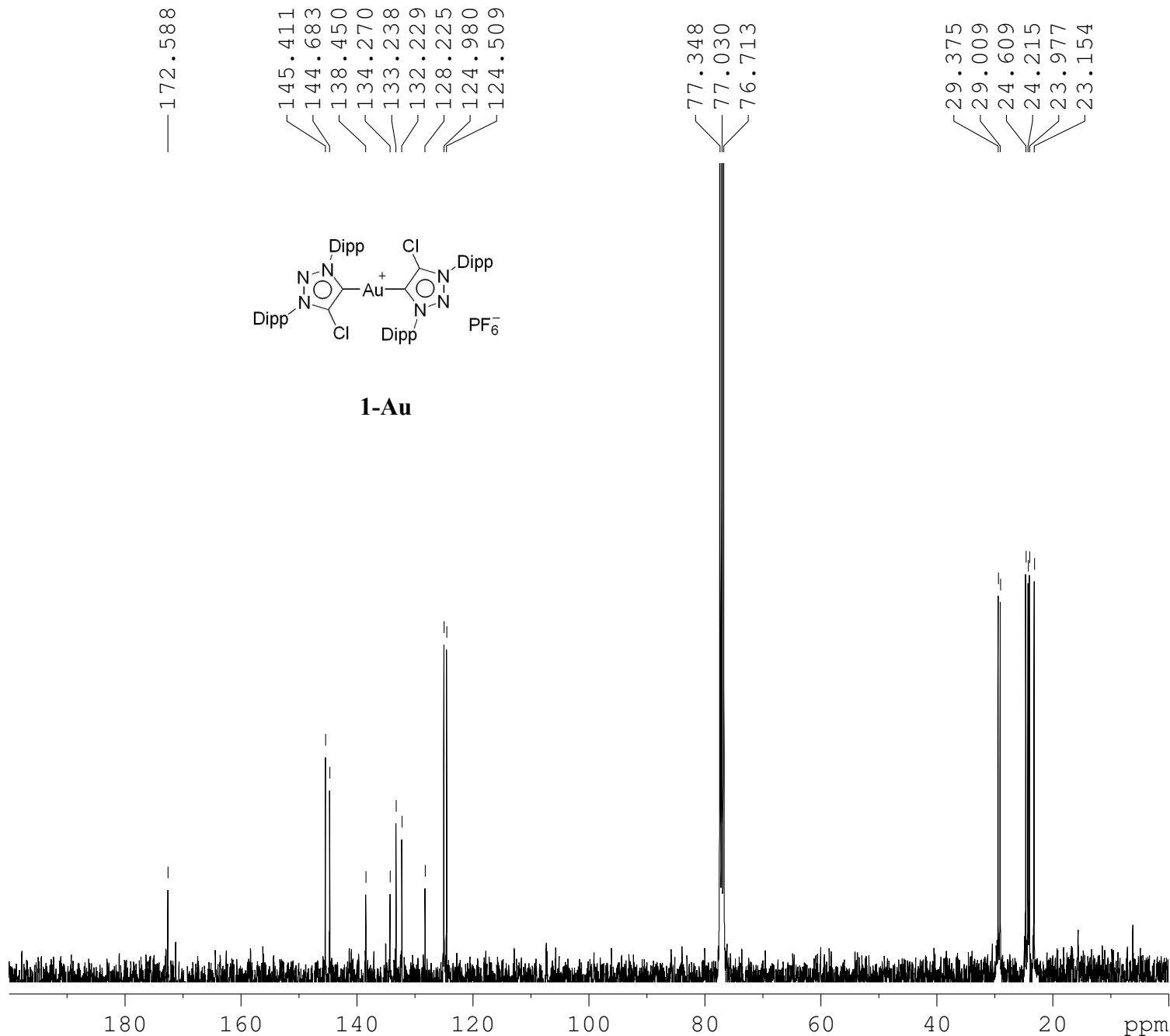


2.000
2.079
3.844
3.815

8.402
12.369
34.714



1-Au

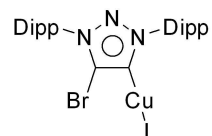


NAME xxy-11-20-au-20171121
 EXPNO 2
 PROCNO 1
 Date_ 20171121
 Time 14.27
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 248
 DS 4
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 114
 DW 19.800 usec
 DE 8.00 usec
 TE 298.7 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 13.50 usec
 PL1 3.00 dB
 PL1W 43.93649673 W
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.80 dB
 PL12 17.19 dB
 PL13 18.46 dB
 PL2W 8.92857742 W
 PL12W 0.25809658 W
 PL13W 0.19265592 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

7.670
7.650
7.631
7.596
7.576
7.557
7.416
7.396
7.356
7.337
7.285



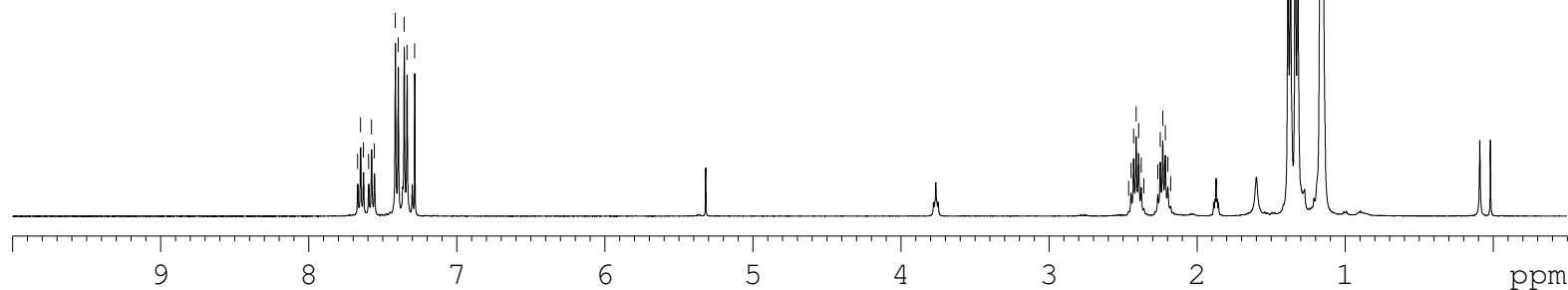
2-Cu

2.463
2.446
2.429
2.412
2.395
2.378
2.360
2.266
2.249
2.232
2.215
2.198
2.179
1.386
1.369
1.337
1.320
1.168
1.151



NAME xxy 9-22-dipp-Br-CuI-rongjica
EXPNO 1
PROCNO 1
Date_ 20170925
Time 13.31
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 181
DW 78.200 usec
DE 6.50 usec
TE 295.2 K
D1 2.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.000
0.972
2.004
1.965

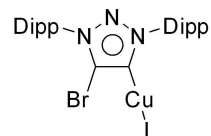
2.129
2.173
6.298
6.477
12.501

— 171.840

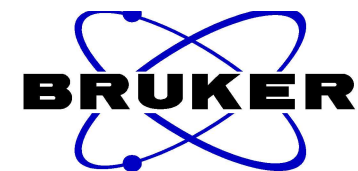
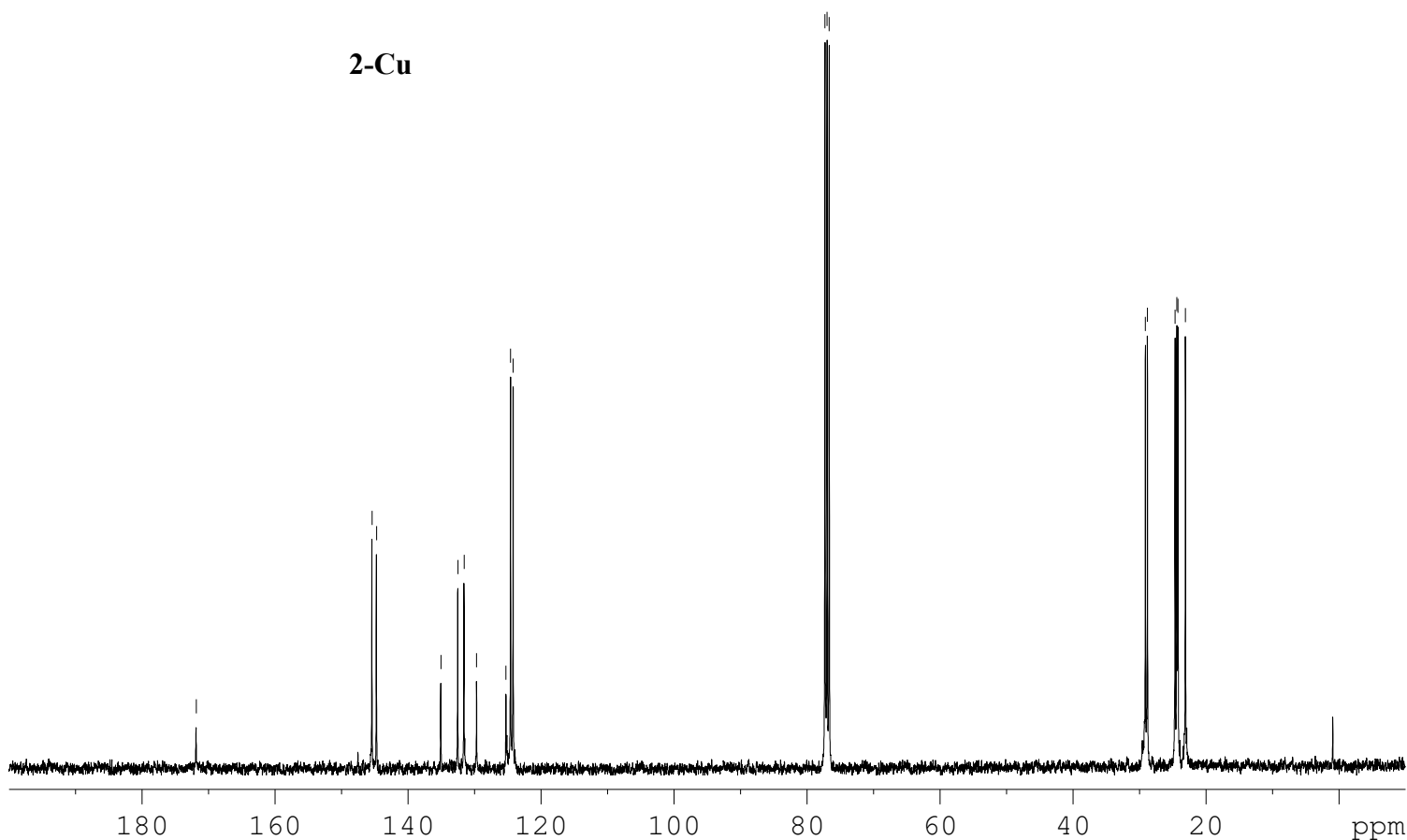
145.404
144.726
135.047
132.491
131.556
129.705
125.286
124.589
124.204

77.315
76.997
76.680

29.133
28.817
24.659
24.396
24.230
23.105



2-Cu

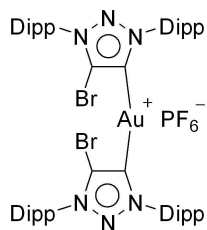


NAME xxy-9-22-dbrcu-20170925
EXPNO 2
PROCNO 1
Date_ 20170925
Time 17.03
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 613
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 8.00 usec
TE 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.50 usec
PL1 3.00 dB
PL1W 43.93649673 W
SFO1 100.6238364 MHz

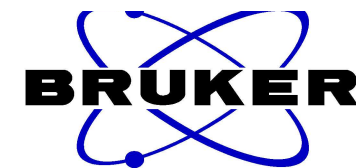
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 17.19 dB
PL13 18.46 dB
PL2W 8.92857742 W
PL12W 0.25809658 W
PL13W 0.19265592 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127764 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

7.700
7.680
7.660
7.635
7.615
7.596
7.429
7.409
7.316
7.297
7.285



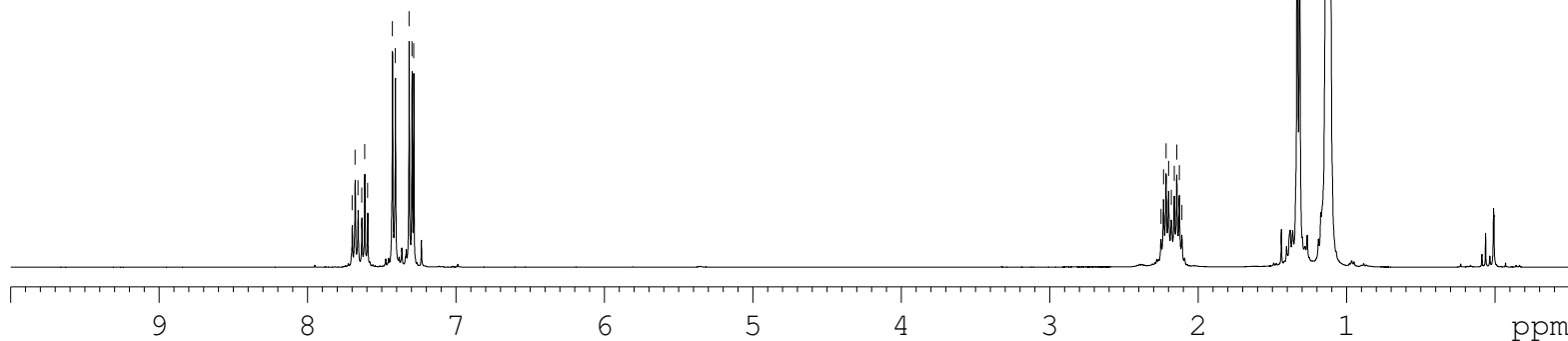
2-Au

2.250
2.233
2.216
2.199
2.181
2.161
2.144
2.127
2.110
1.333
1.316
1.141
1.127
1.110



NAME xxy-dipp-Br-Au
EXPNO 1
PROCNO 1
Date_ 20171110
Time 19.02
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 80.6
DW 78.200 usec
DE 6.50 usec
TE 293.9 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.029
1.935
3.949
4.743

4.000
4.219

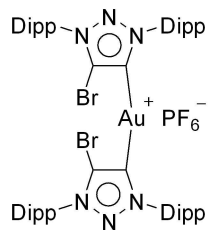
12.268
36.369

— 176.242

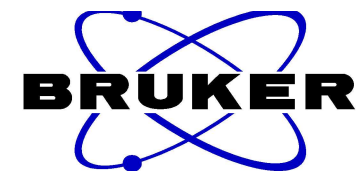
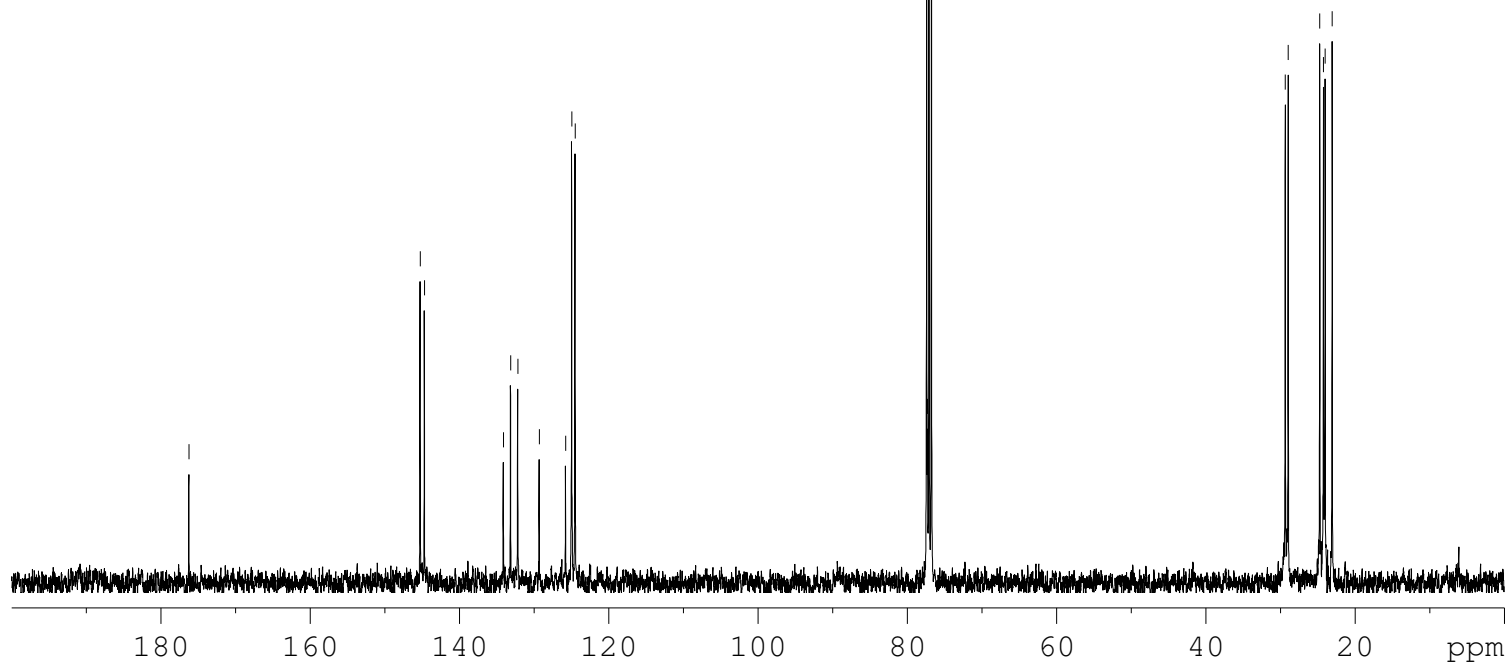
145.254
144.686
134.106
133.141
132.174
129.299
125.775
124.950
124.495

77.421
77.306
77.103
76.785

29.371
28.976
24.754
24.253
24.026
23.085



2-Au

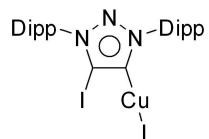


NAME xxy-dipp-Br-Au
EXPNO 2
PROCNO 1
Date_ 20171110
Time 19.05
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 104
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 114
DW 19.800 usec
DE 8.00 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 13.50 usec
PL1 3.00 dB
PL1W 43.93649673 W
SFO1 100.6238364 MHz

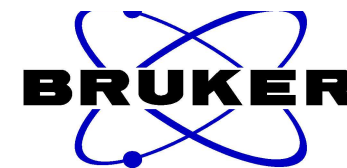
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 17.19 dB
PL13 18.46 dB
PL2W 8.92857742 W
PL12W 0.25809658 W
PL13W 0.19265592 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

7.647
7.627
7.607
7.572
7.552
7.533
7.392
7.372
7.325
7.306
7.261



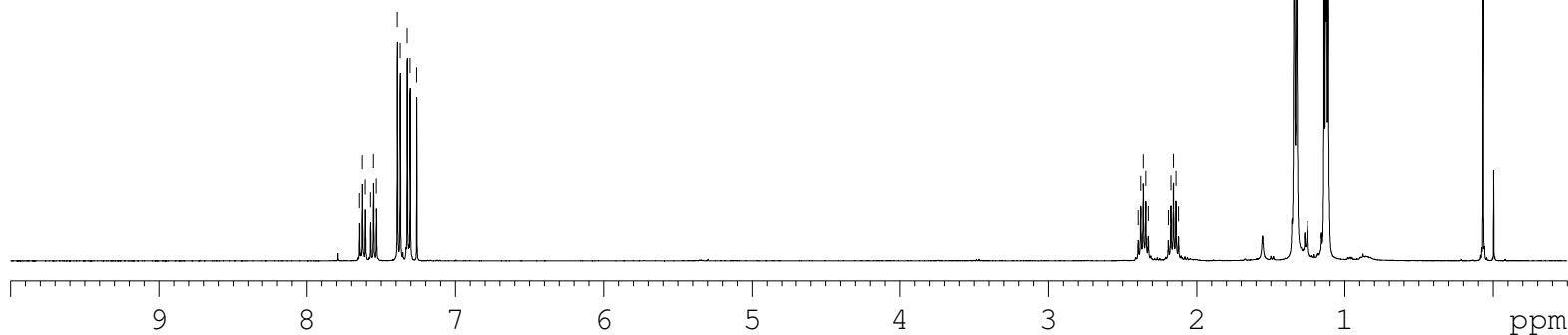
3-Cu

2.395
2.378
2.361
2.344
2.327
2.192
2.175
2.158
2.141
2.124
1.342
1.325
1.139
1.129
1.122
1.112



NAME xxy-9-25-dipp-2iicu-20171011
EXPNO 1
PROCNO 1
Date_ 20171011
Time 16.25
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 203
DW 78.200 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

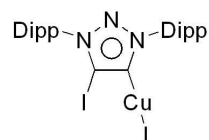
===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.000
1.082
2.141
2.000

1.993
1.969
12.224
5.806
6.227

145.267
144.756
134.698
132.419
131.542
131.306
124.582
124.226

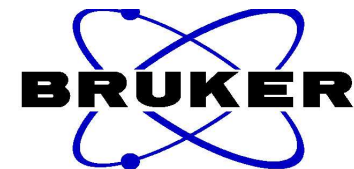


3-Cu

77.286
76.969
76.651

29.189
28.799
24.905
24.354
22.994

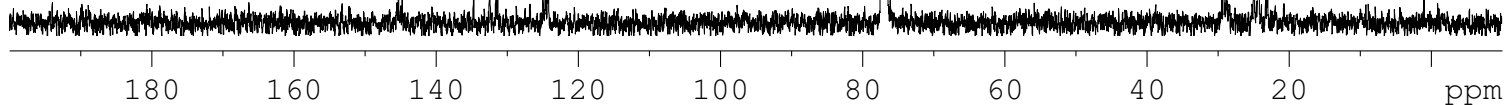
— 0.959



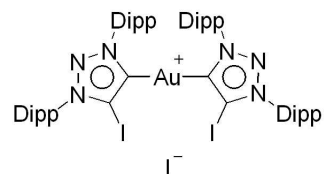
NAME xxy-9-25-dipp-2iicu-20171011
EXPNO 2
PROCNO 1
Date_ 20171011
Time 16.28
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 536
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 8.00 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.50 usec
PL1 3.00 dB
PL1W 43.93649673 W
SFO1 100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 17.19 dB
PL13 18.46 dB
PL2W 8.92857742 W
PL12W 0.25809658 W
PL13W 0.19265592 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127764 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40



7.606
7.586
7.567
7.515
7.496
7.476
7.354
7.334
7.265
7.169
7.150



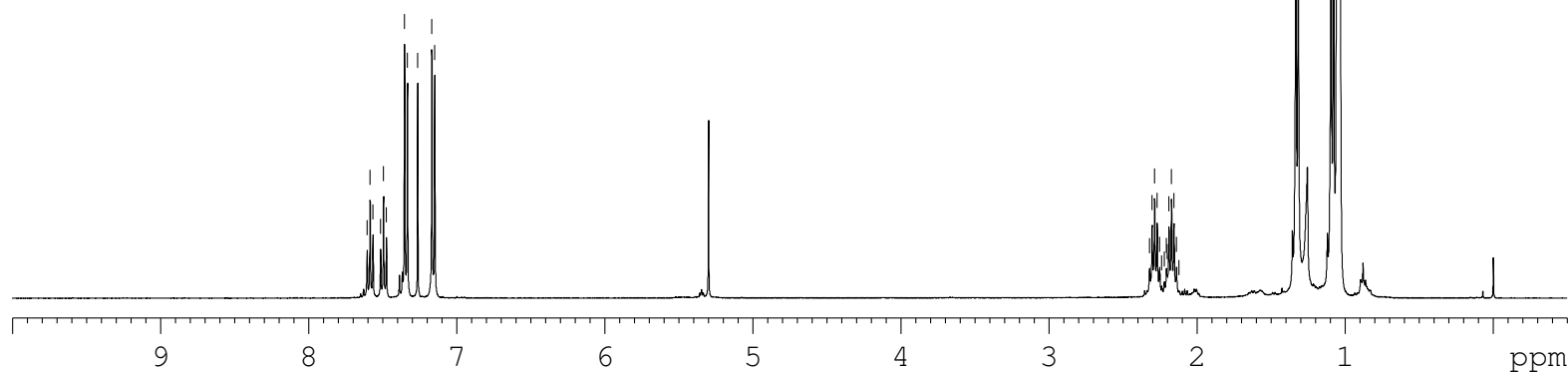
3-Au(I)

2.322
2.305
2.288
2.271
2.254
2.240
2.222
2.208
2.202
2.191
2.174
2.157
2.140
2.123
1.334
1.317
1.096
1.079
1.058
1.051



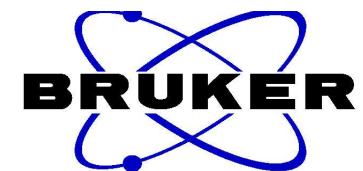
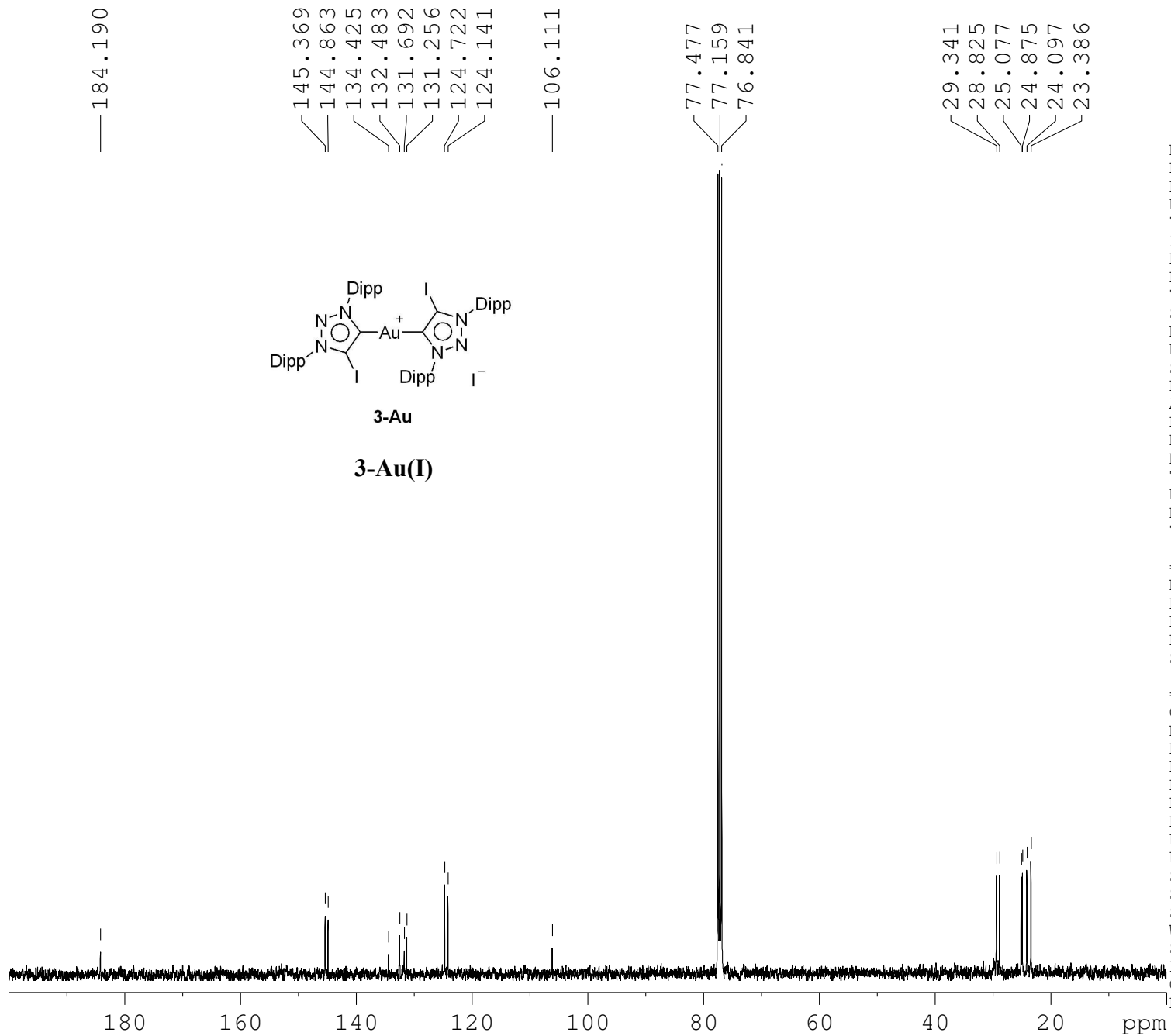
NAME xxy-Au-2
EXPNO 1
PROCNO 1
Date_ 20180228
Time 15.37
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 287
DW 78.200 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300081 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



2.000
1.915
3.828
3.960

4.201
4.248
12.485
12.389
11.142
11.383

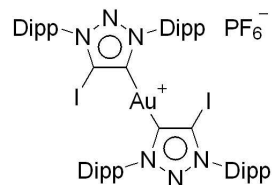


NAME xxy-au-i-i-20180228
 EXPNO 2
 PROCNO 1
 Date_ 20180228
 Time 17.42
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 200
 DS 4
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 2050
 DW 19.800 usec
 DE 8.00 usec
 TE 298.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 10

===== CHANNEL f1 =====
 NUC1 13C
 P1 13.50 usec
 PL1 3.00 dB
 PL1W 43.93649673 W
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.80 dB
 PL12 17.19 dB
 PL13 18.46 dB
 PL2W 8.92857742 W
 PL12W 0.25809658 W
 PL13W 0.19265592 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127557 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

7.657
7.637
7.618
7.596
7.577
7.557
7.391
7.371
7.280
7.261
7.254



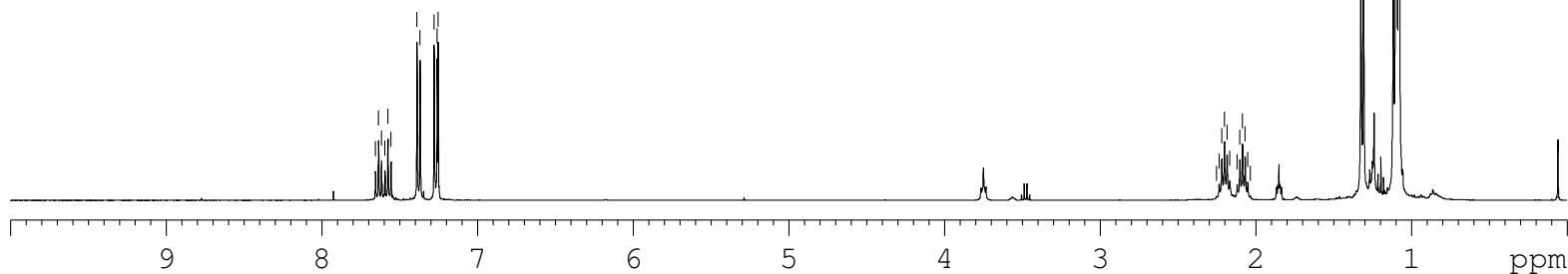
3-Au[PF₆]

2.253
2.237
2.220
2.203
2.186
2.169
2.121
2.104
2.087
2.070
2.053
2.036
1.327
1.310
1.118
1.102
1.098



NAME xxy1211pf-3-20181211
EXPNO 1
PROCNO 1
Date_ 20181211
Time 17.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl₃
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 114
DW 78.200 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

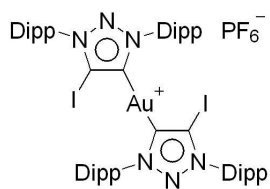
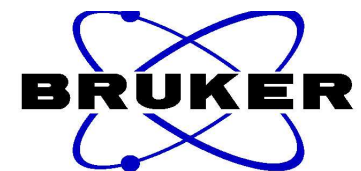
===== CHANNEL f1 =====
NUC1 1H
P1 10.40 usec
PL1 -1.00 dB
PL1W 17.01305389 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300128 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



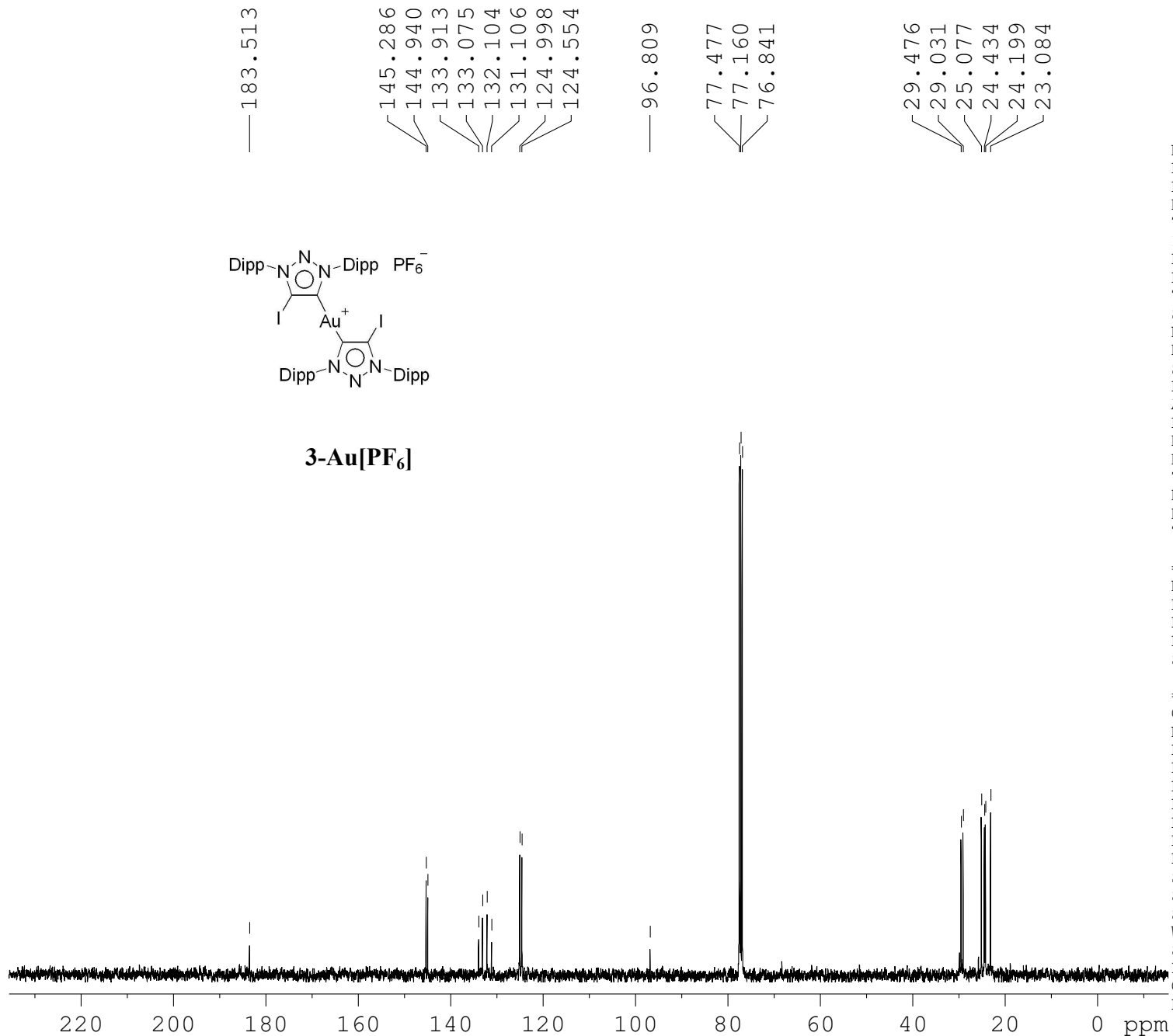
2.034
2.003
3.898
3.567

4.448
4.000

12.079
35.447



3-Au[PF₆]

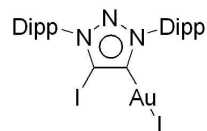


NAME xxy1211pf-20181211
 EXPNO 2
 PROCNO 1
 Date_ 20181211
 Time 17.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 120
 DS 4
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 181
 DW 19.800 usec
 DE 6.50 usec
 TE 296.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 3

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 2.00 dB
 PL1W 55.31277084 W
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 16.72 dB
 PL13 15.50 dB
 PL2W 17.01305389 W
 PL12W 0.28759566 W
 PL13W 0.38087484 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127589 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

7.663
7.643
7.623
7.591
7.572
7.552
7.404
7.385
7.330
7.311
7.262



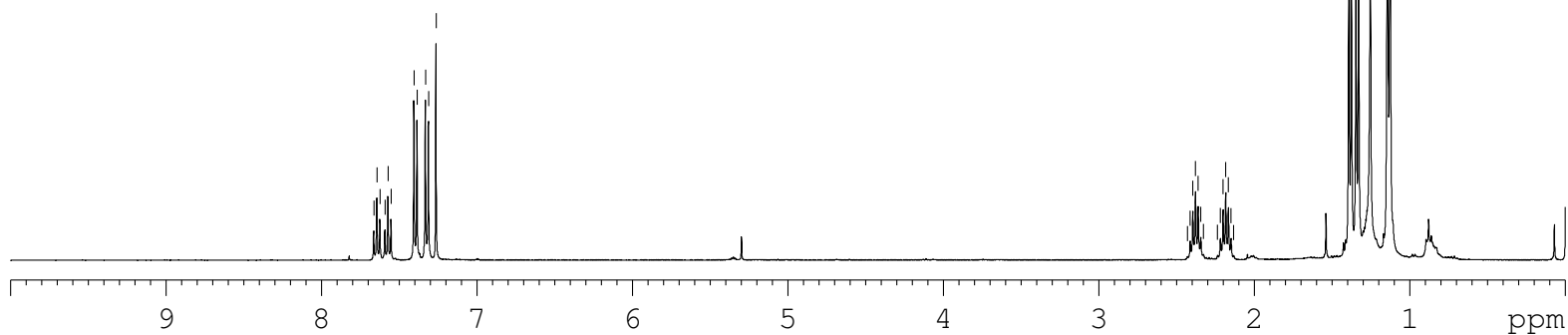
4

2.430
2.413
2.396
2.379
2.362
2.345
2.328
2.238
2.219
2.202
2.185
2.168
2.151
2.134
1.394
1.377
1.347
1.330



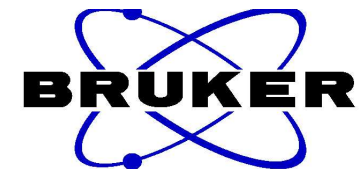
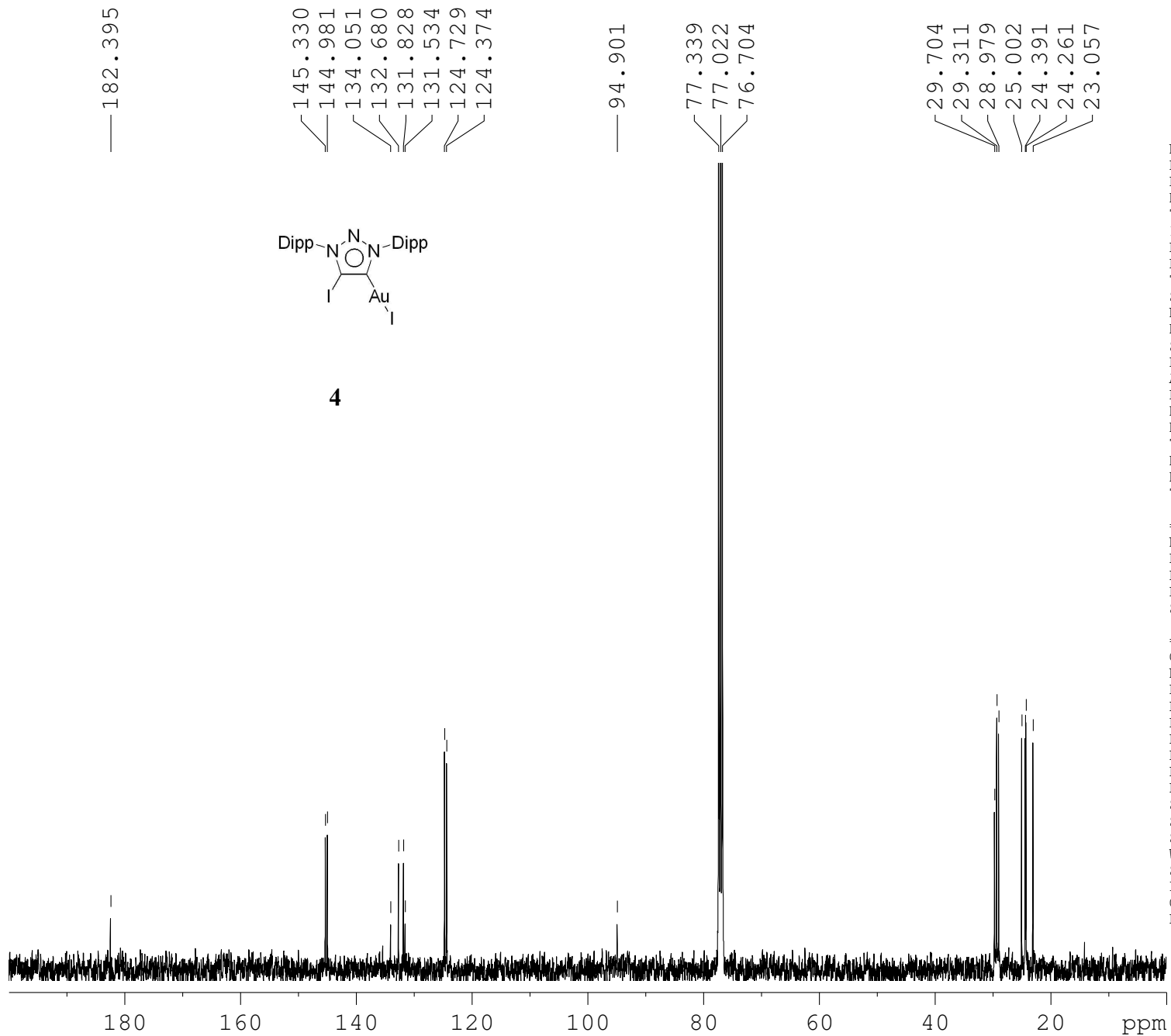
NAME xxy-314-c-a-1-20180316
EXPNO 1
PROCNO 1
Date_ 20180317
Time 14.31
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 203
DW 78.200 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SF01 400.1326008 MHz
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



1.000
1.043
2.001
2.033

2.132
2.111
6.274
6.444
12.872



```

NAME      xxy-314-c-a-1-20180316
EXPNO      2
PROCNO     1
Date_      20180317
Time       14.35
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         296
DS         4
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DW         19.800 usec
DE         8.00 usec
TE         296.9 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        10
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         13.50 usec
PL1        3.00 dB
PL1W       43.93649673 W
SFO1       100.6238364 MHz
  
```

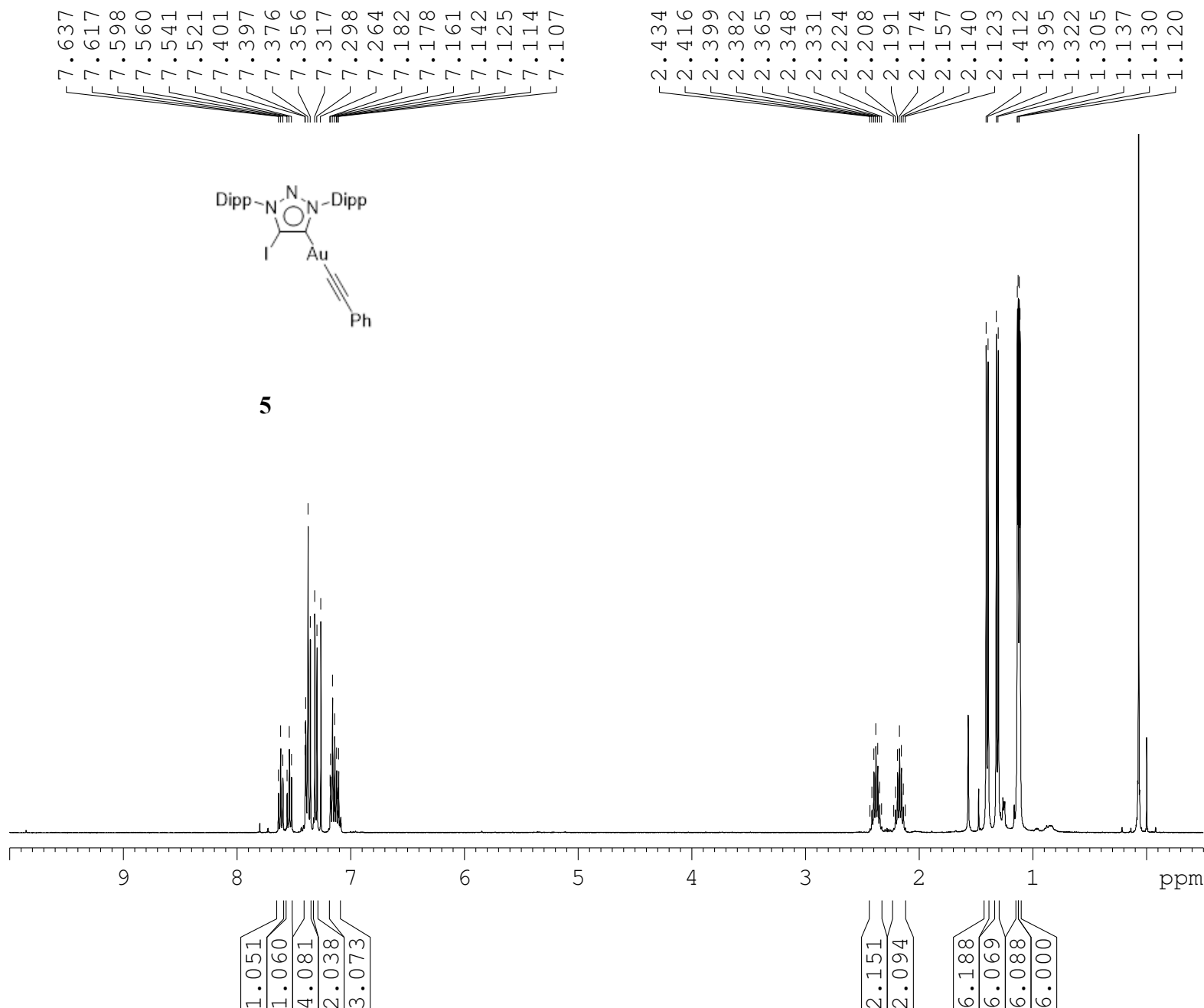
```

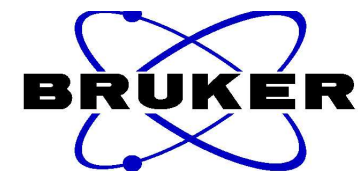
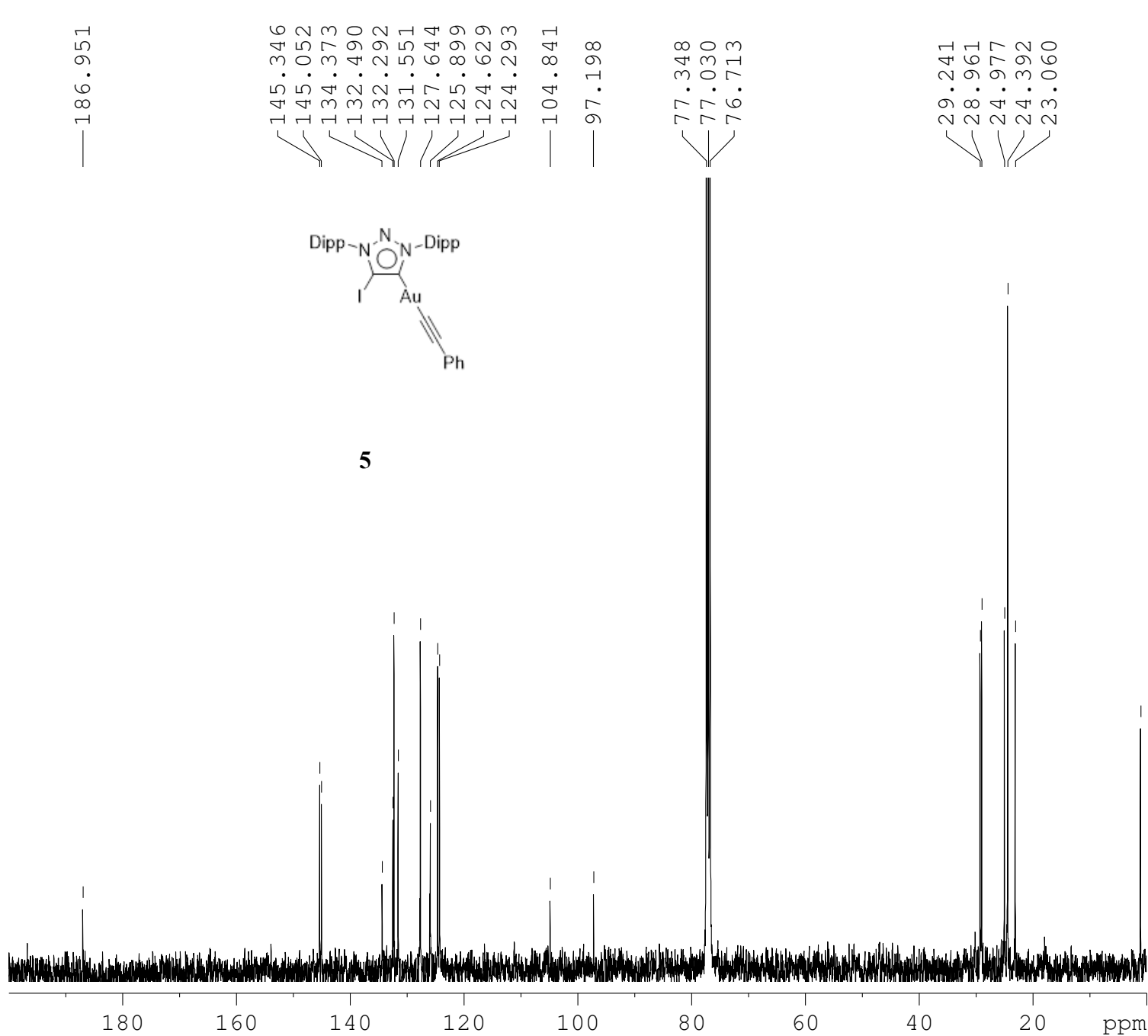
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.80 dB
PL12       17.19 dB
PL13       18.46 dB
PL2W       8.92857742 W
PL12W      0.25809658 W
PL13W      0.19265592 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127690 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```



NAME xxy-7-7-2-20180710
 EXPNO 1
 PROCNO 1
 Date_ 20180710
 Time 13.27
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 6393.862 Hz
 FIDRES 0.195125 Hz
 AQ 2.5625076 sec
 RG 228
 DW 78.200 usec
 DE 6.50 usec
 TE 293.7 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 10.40 usec
 PL1 -1.00 dB
 PL1W 17.01305389 W
 SFO1 400.1326008 MHz
 SI 32768
 SF 400.1300091 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



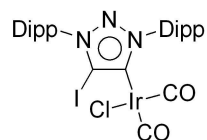


NAME xxy-7-2-2-20180711
 EXPNO 2
 PROCNO 1
 Date_ 20180710
 Time 13.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 368
 DS 4
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 181
 DW 19.800 usec
 DE 6.50 usec
 TE 294.8 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 3

===== CHANNEL f1 =====
 NUC1 13C
 P1 15.00 usec
 PL1 2.00 dB
 PL1W 55.31277084 W
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 16.72 dB
 PL13 15.50 dB
 PL2W 17.01305389 W
 PL12W 0.28759566 W
 PL13W 0.38087484 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127690 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

7.651
7.631
7.612
7.603
7.583
7.564
7.400
7.381
7.357
7.338
7.261



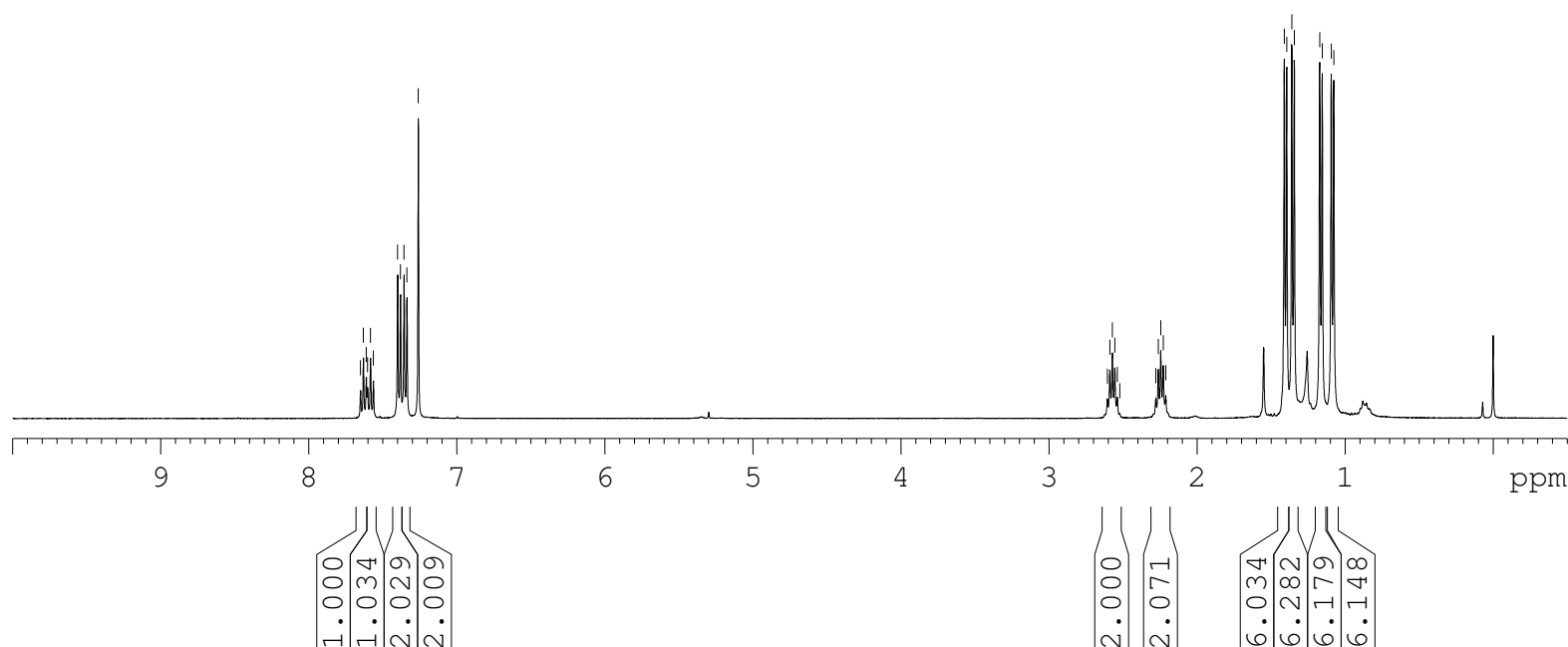
3-Ir

2.606
2.589
2.572
2.556
2.539
2.522
2.279
2.262
2.245
2.228
2.212
1.411
1.395
1.360
1.343
1.172
1.155
1.094
1.077



NAME xxy-Ir-2-20171229
EXPNO 1
PROCNO 1
Date_ 20171229
Time 17.53
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 0
SWH 6393.862 Hz
FIDRES 0.195125 Hz
AQ 2.5625076 sec
RG 203
DW 78.200 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.10 usec
PL1 1.80 dB
PL1W 8.92857742 W
SFO1 400.1326008 MHz
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



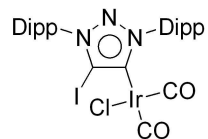
— 180.44
— 174.54
— 168.58

— 145.68

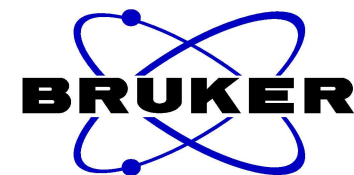
— 134.42
— 132.50
— 131.71
— 131.50
— 124.75
— 124.10

— 98.68

— 29.28
— 29.06
— 26.54
— 25.01
— 23.58
— 22.65



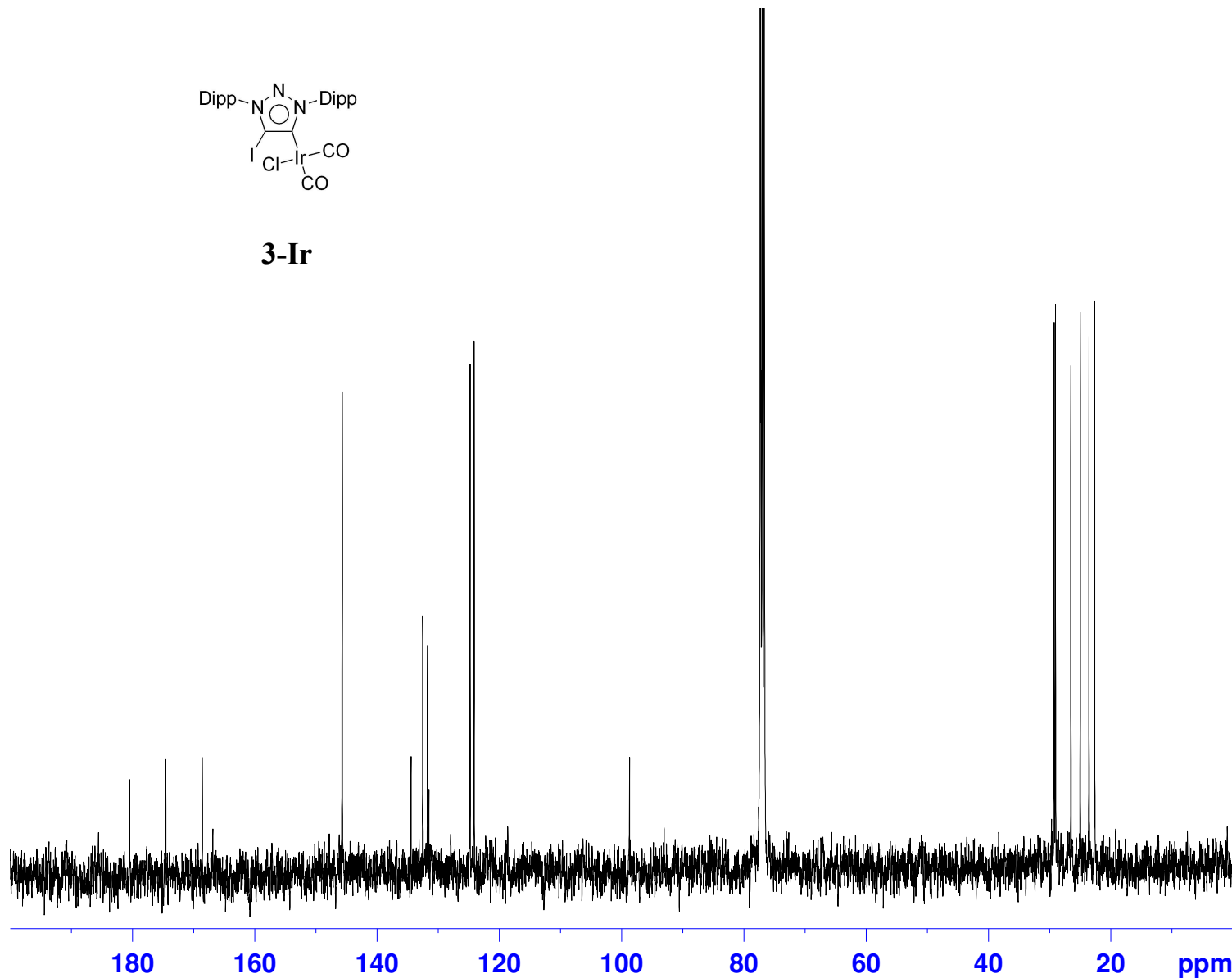
3-Ir



```
NAME      xxy-Ir-2-20171229
EXPNO      2
PROCNO      1
Date_      20171229
Time       17.55
INSTRUM     spect
PROBHD      5 mm PADUL 13C
PULPROG     zgpg30
TD          65536
SOLVENT     CDC13
NS          528
DS          4
SWH         25252.525 Hz
FIDRES      0.385323 Hz
AQ          1.2976629 sec
RG          114
DW          19.800 usec
DE          8.00 usec
TE          297.5 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0         1
```

```
===== CHANNEL f1 =====
NUC1        13C
P1          13.50 usec
PL1         3.00 dB
PL1W        43.93649673 W
SFO1        100.6238364 MHz
```

```
===== CHANNEL f2 =====
CPDPRG2     waltz16
NUC2        1H
PCPD2       80.00 usec
PL2         1.80 dB
PL12        17.19 dB
PL13        18.46 dB
PL2W        8.92857742 W
PL12W       0.25809658 W
PL13W       0.19265592 W
SFO2        400.1316005 MHz
SI          32768
SF          100.6127690 MHz
WDW         EM
SSB         0
LB          3.00 Hz
GB          0
PC          1.40
```

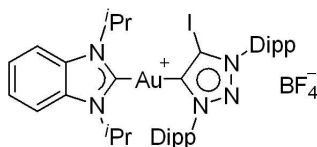




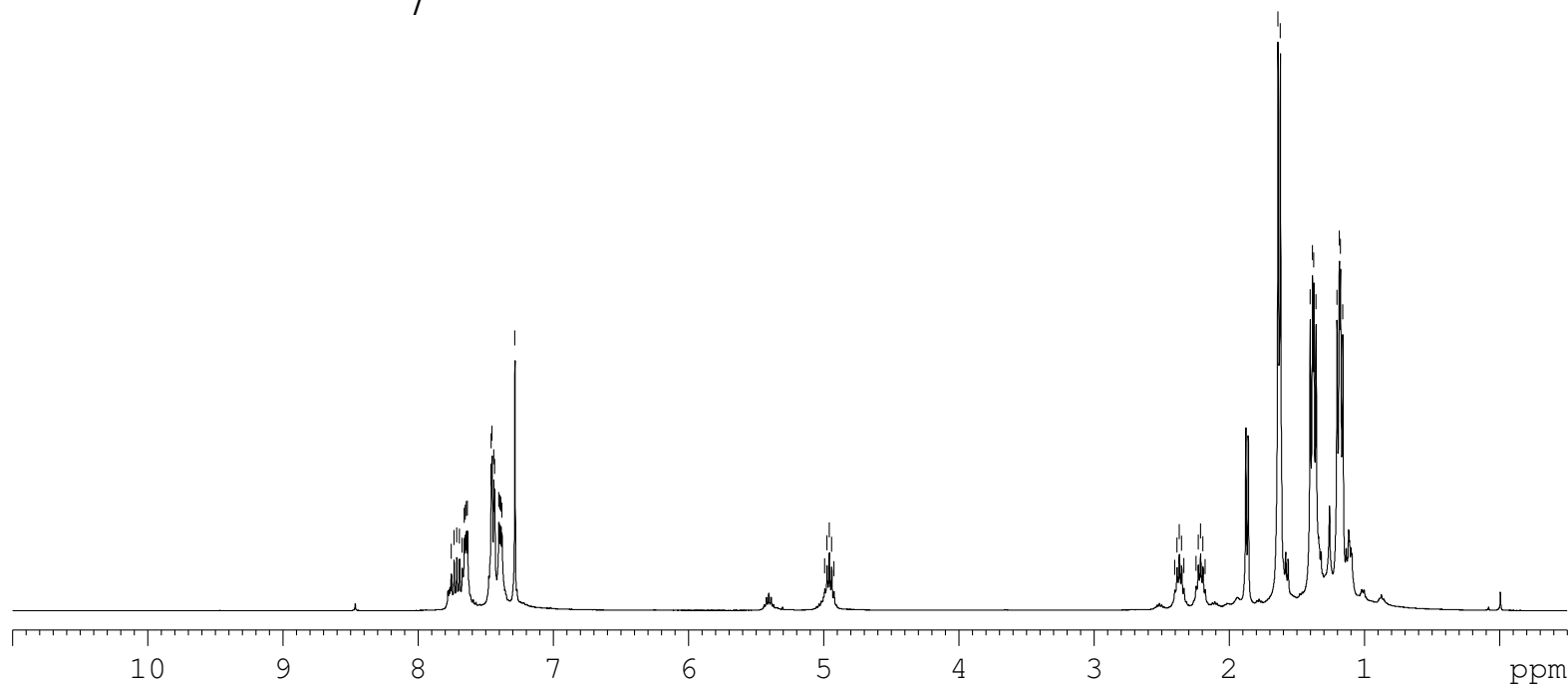
NAME xxy-5h-bf-20180511
 EXPNO 1
 PROCNO 1
 Date_ 20180511
 Time 14.20
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zg30
 TD 32768
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 6393.862 Hz
 FIDRES 0.195125 Hz
 AQ 2.5625076 sec
 RG 80.6
 DW 78.200 usec
 DE 6.50 usec
 TE 299.4 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.10 usec
 PL1 1.80 dB
 PL1W 8.92857742 W
 SFO1 400.1326008 MHz
 SI 32768
 SF 400.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

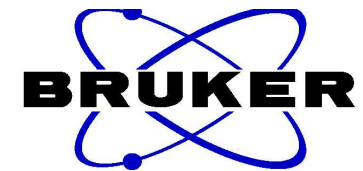
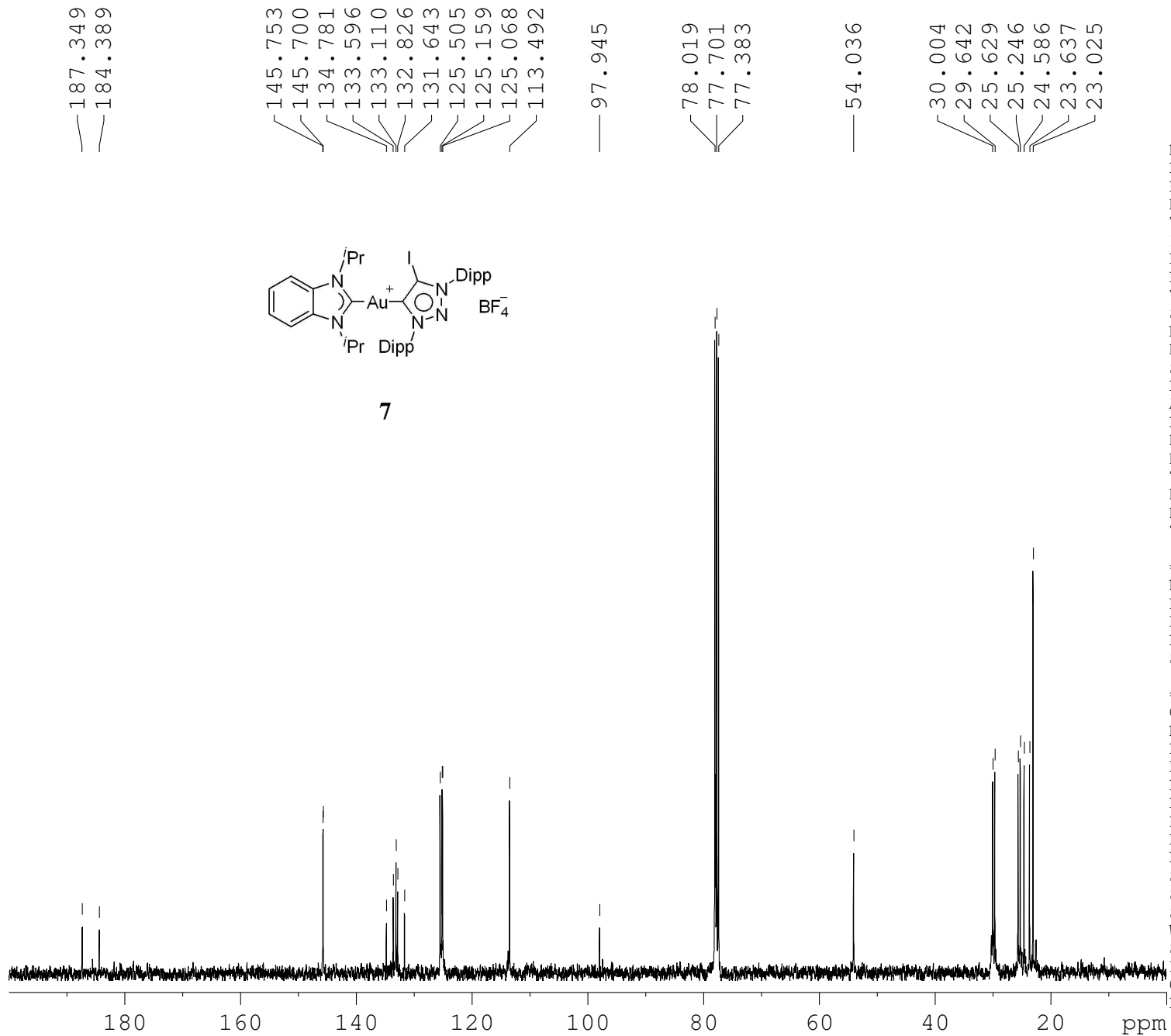
7.756
 7.735
 7.715
 7.695
 7.675
 7.660
 7.652
 7.644
 7.636
 7.460
 7.454
 7.441
 7.435
 7.404
 7.396
 7.389
 7.381
 7.286
 4.994
 4.977
 4.959
 4.942
 4.925
 2.404
 2.387
 2.370
 2.353
 2.337
 2.246
 2.230
 2.213
 2.196
 2.179
 1.641
 1.623
 1.402
 1.385
 1.376
 1.359
 1.204
 1.187



7



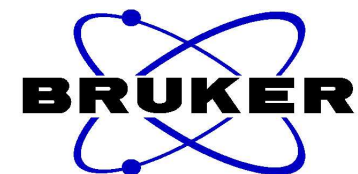
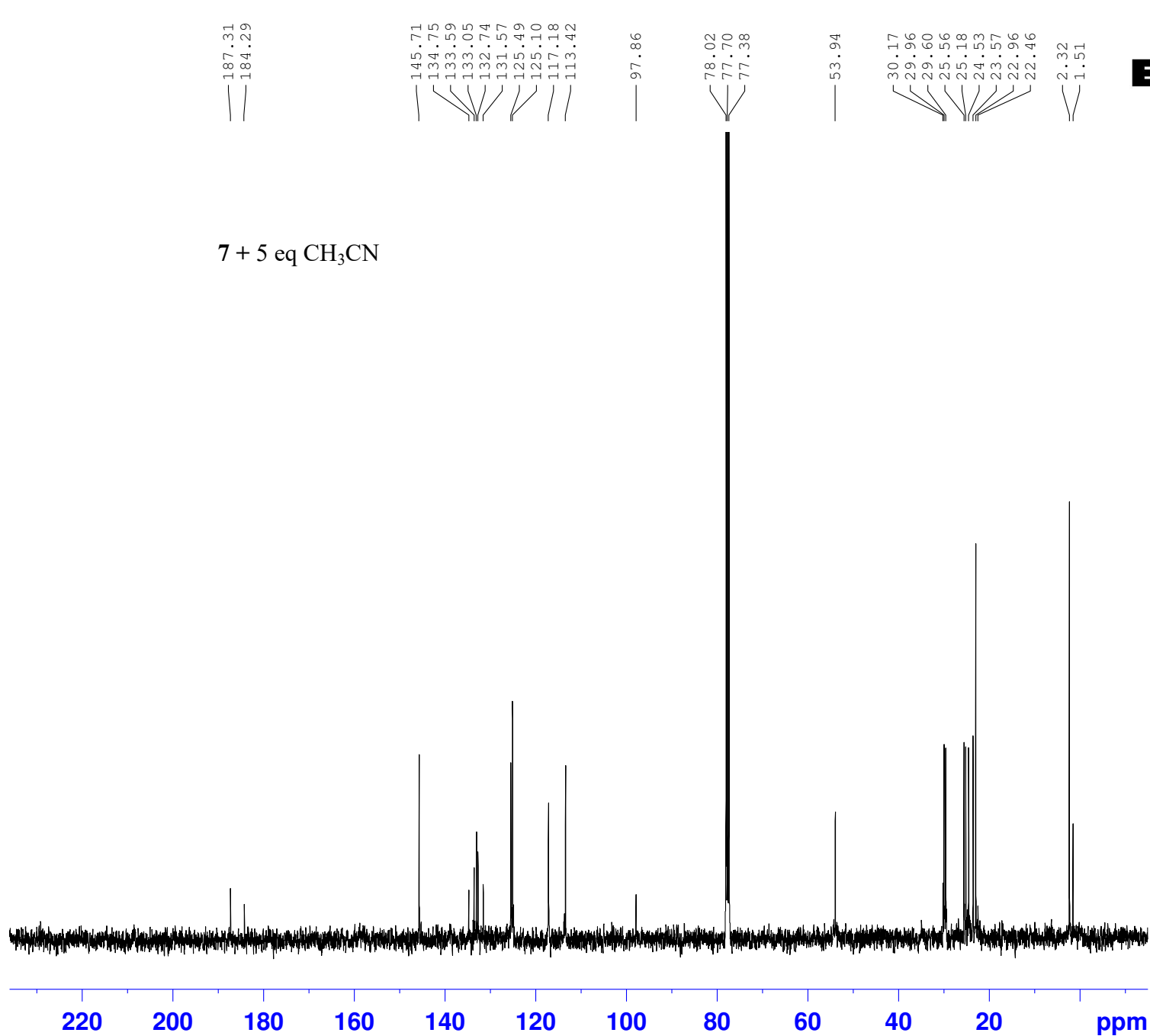
2.475
 2.427
 4.725
 2.477
 2.156
 2.344
 2.424
 12.077
 6.259
 5.843
 6.000
 5.998



NAME xxy-423bf-20180425
 EXPNO 2
 PROCNO 1
 Date_ 20180425
 Time 19.28
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 96
 DS 4
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 2050
 DW 19.800 usec
 DE 8.00 usec
 TE 297.6 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 10

===== CHANNEL f1 =====
 NUC1 13C
 P1 13.50 usec
 PL1 3.00 dB
 PL1W 43.93649673 W
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.80 dB
 PL12 17.19 dB
 PL13 18.46 dB
 PL2W 8.92857742 W
 PL12W 0.25809658 W
 PL13W 0.19265592 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127131 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



```

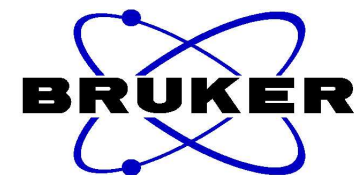
NAME      xxy-bf-cn-20180426
EXPNO      2
PROCNO     1
Date_      20180426
Time       20.20
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         128
DS         4
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DW         19.800 usec
DE         8.00 usec
TE         297.6 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        10
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         13.50 usec
PL1        3.00 dB
PL1W       43.93649673 W
SFO1       100.6238364 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.80 dB
PL12       17.19 dB
PL13       18.46 dB
PL2W       8.92857742 W
PL12W      0.25809658 W
PL13W      0.19265592 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127162 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```



```

NAME      xxy-bf-dmap-20180427
EXPNO     2
PROCNO    1
Date_     20180427
Time      14.18
INSTRUM   spect
PROBHD    5 mm PADUL 13C
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        152
DS        4
SWH       25252.525 Hz
FIDRES    0.385323 Hz
AQ        1.2976629 sec
RG        2050
DW        19.800 usec
DE        8.00 usec
TE        298.2 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       10

```

```

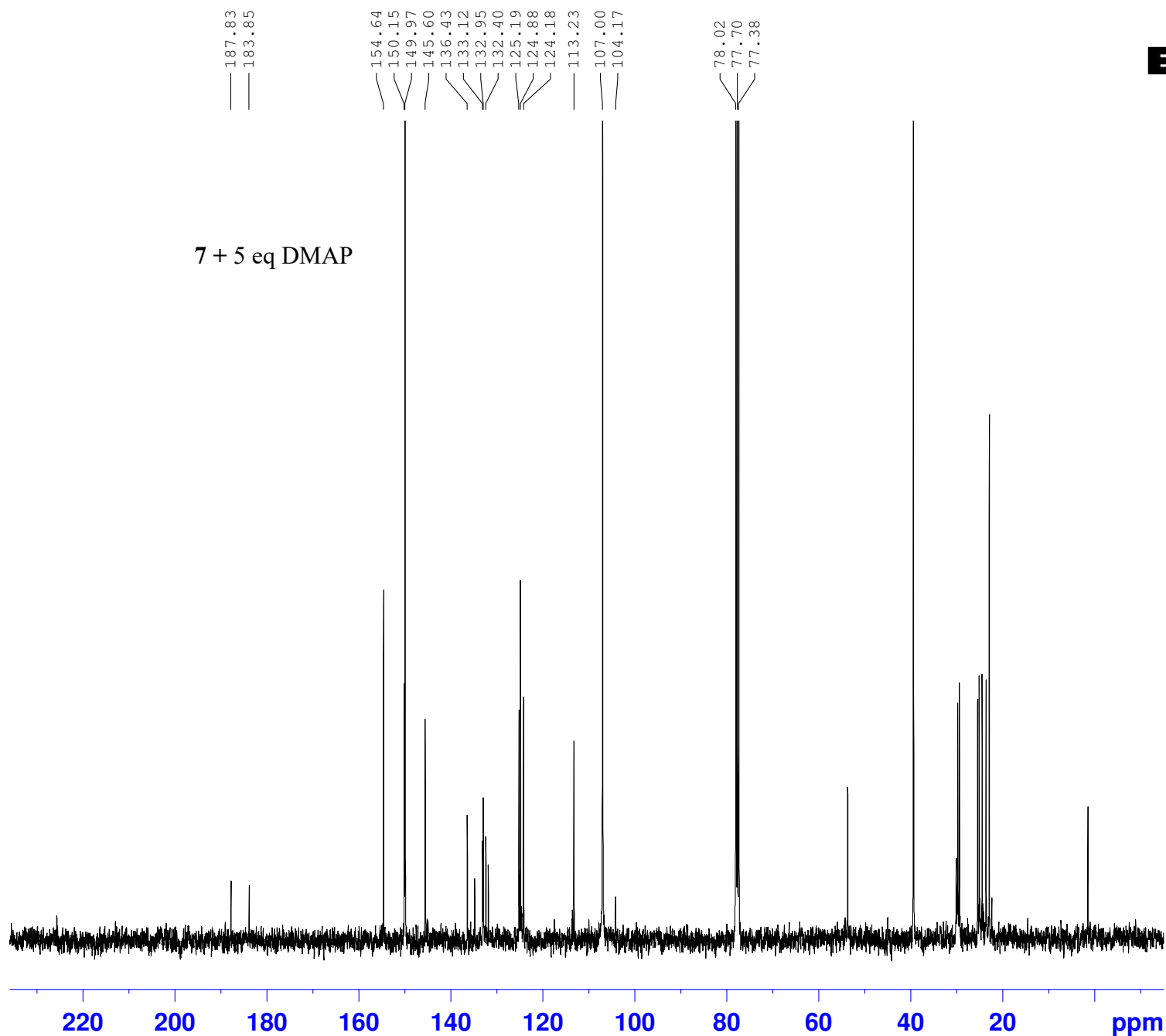
===== CHANNEL f1 =====
NUC1      13C
P1        13.50 usec
PL1       3.00 dB
PL1W      43.93649673 W
SFO1      100.6238364 MHz

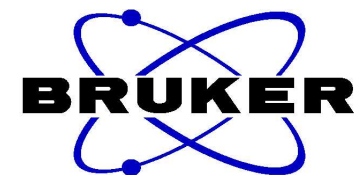
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.80 dB
PL12      17.19 dB
PL13      18.46 dB
PL2W      8.92857742 W
PL12W     0.25809658 W
PL13W     0.19265592 W
SFO2      400.1316005 MHz
SI        32768
SF        100.6127238 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40

```





```

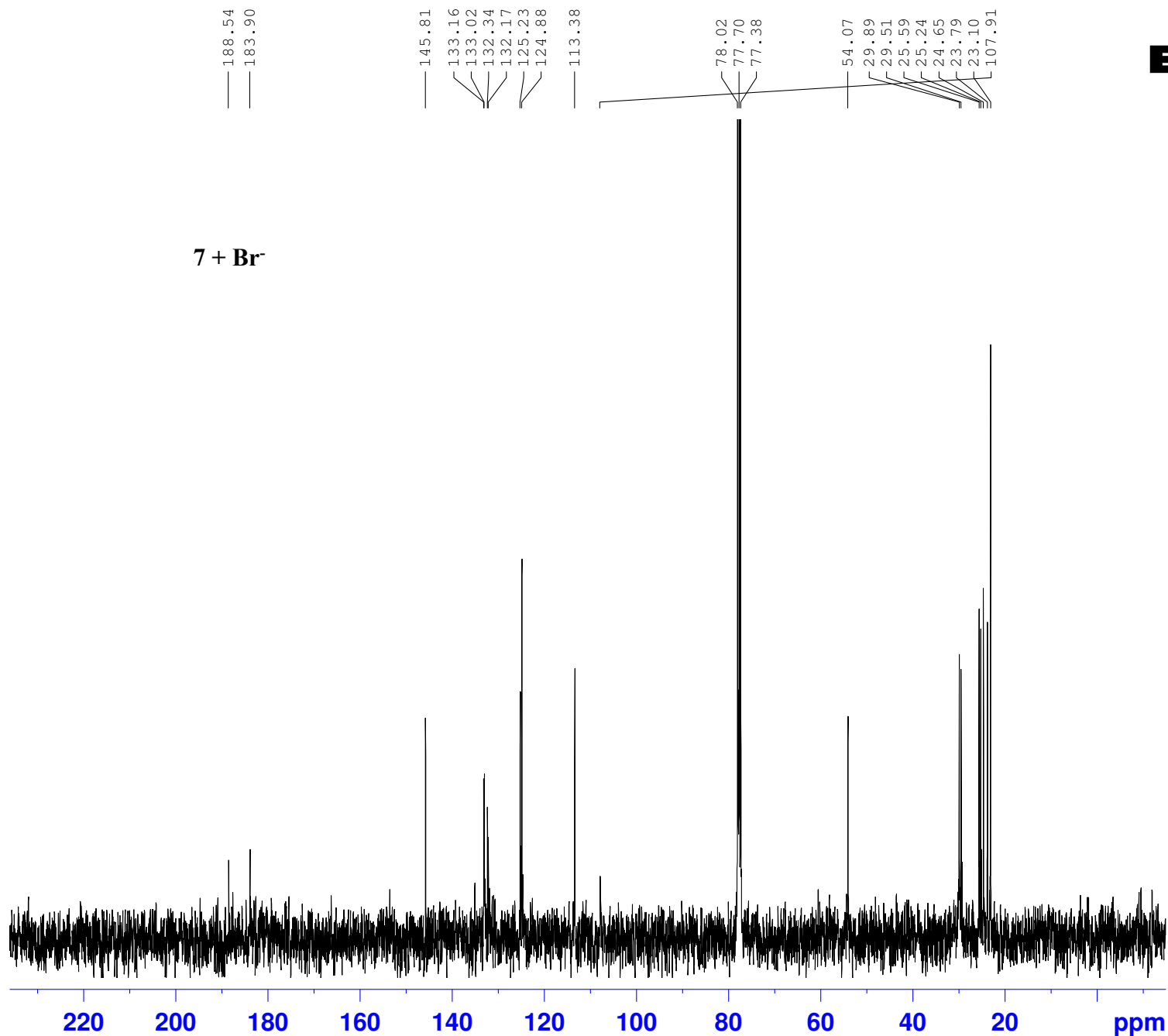
NAME      xxy-518kbr-20180518
EXPNO     2
PROCNO    1
Date_     20180518
Time      14.21
INSTRUM   spect
PROBHD    5 mm PADUL 13C
PULPROG   zgpg30
TD        65536
SOLVENT   CDCl3
NS        56
DS        4
SWH       25252.525 Hz
FIDRES    0.385323 Hz
AQ        1.2976629 sec
RG        2050
DW        19.800 usec
DE        8.00 usec
TE        296.4 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
  
```

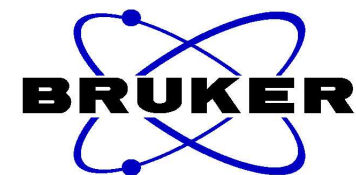
```

===== CHANNEL f1 =====
NUC1      13C
P1        13.50 usec
PL1       3.00 dB
PL1W      43.93649673 W
SFO1      100.6238364 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.80 dB
PL12      17.19 dB
PL13      18.46 dB
PL2W      8.92857742 W
PL12W     0.25809658 W
PL13W     0.19265592 W
SFO2      400.1316005 MHz
SI        32768
SF        100.6127120 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40
  
```

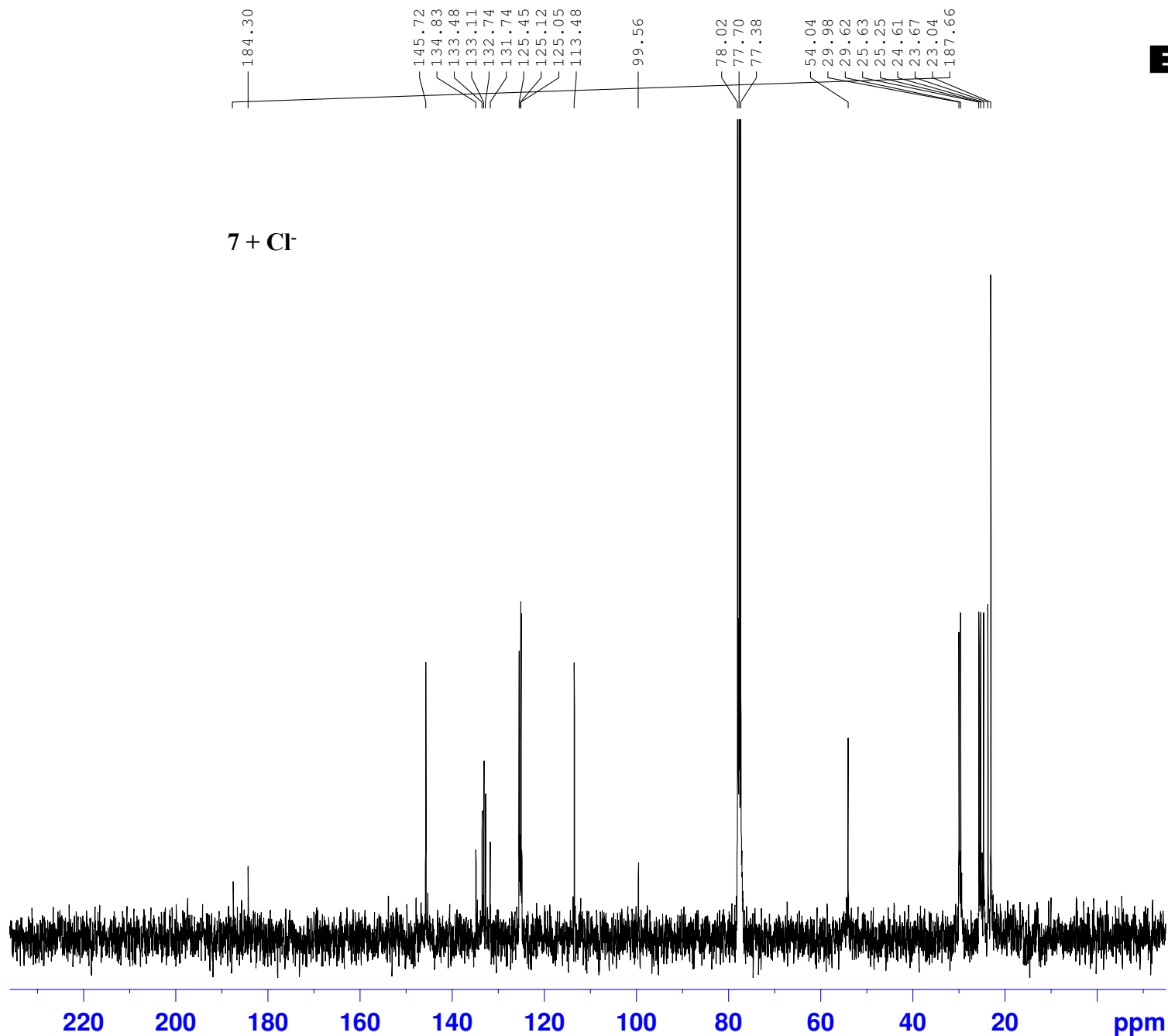


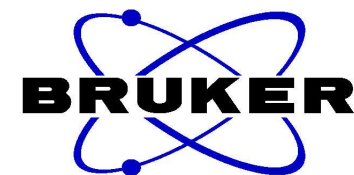


NAME xxy-518kc1-20180518
 EXPNO 2
 PROCNO 1
 Date_ 20180518
 Time 14.38
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 72
 DS 4
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 2050
 DW 19.800 usec
 DE 8.00 usec
 TE 296.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

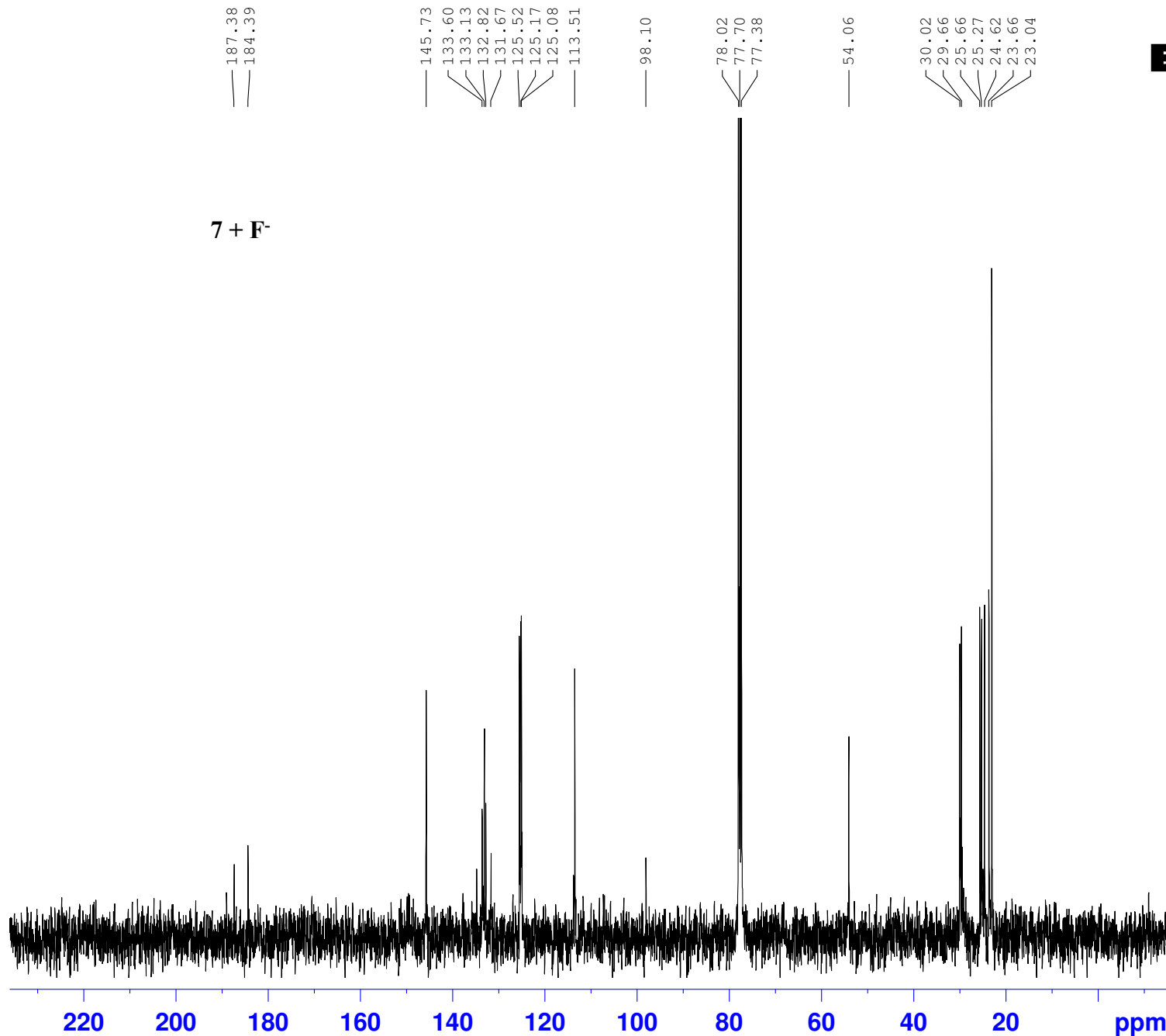
===== CHANNEL f1 =====
 NUC1 13C
 P1 13.50 usec
 PL1 3.00 dB
 PL1W 43.93649673 W
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.80 dB
 PL12 17.19 dB
 PL13 18.46 dB
 PL2W 8.92857742 W
 PL12W 0.25809658 W
 PL13W 0.19265592 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127131 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40





7 + F⁻



```

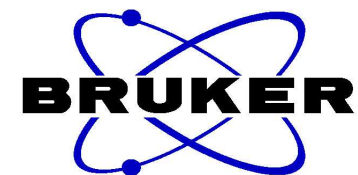
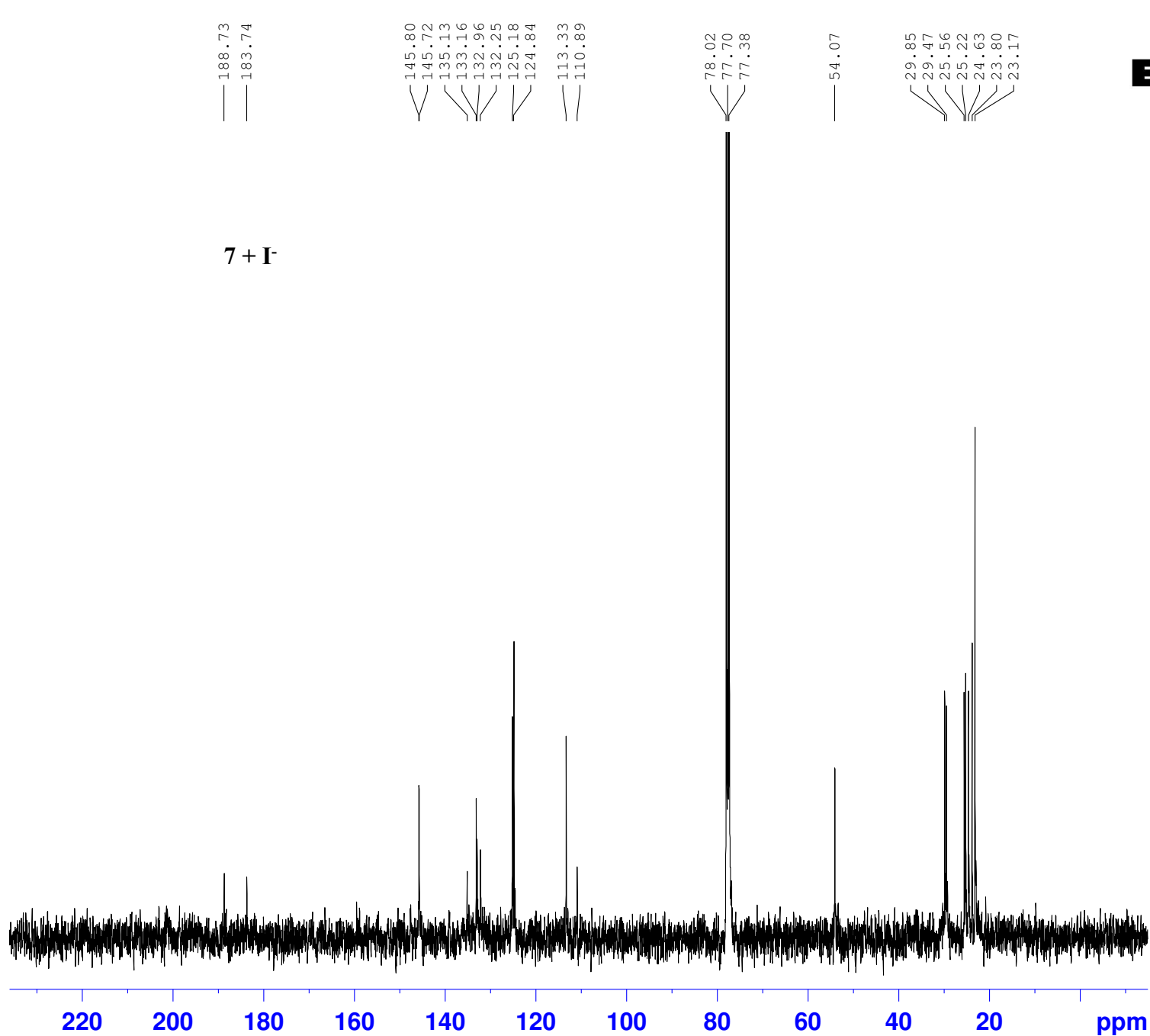
NAME      xxy-518kf-20180518
EXPNO      2
PROCNO     1
Date_      20180518
Time       14.30
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         48
DS         4
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DW         19.800 usec
DE         8.00 usec
TE         295.9 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        13.50 usec
PL1       3.00 dB
PL1W      43.93649673 W
SFO1      100.6238364 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.80 dB
PL12      17.19 dB
PL13      18.46 dB
PL2W      8.92857742 W
PL12W     0.25809658 W
PL13W     0.19265592 W
SFO2      400.1316005 MHz
SI        32768
SF        100.6127113 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40
  
```



```

NAME      xxy-518ik-20180518
EXPNO      2
PROCNO     1
Date_      20180518
Time       14.08
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         112
DS         4
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DW         19.800 usec
DE         8.00 usec
TE         295.8 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

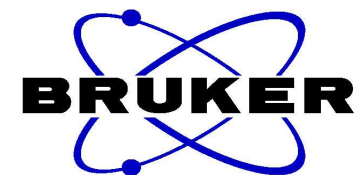
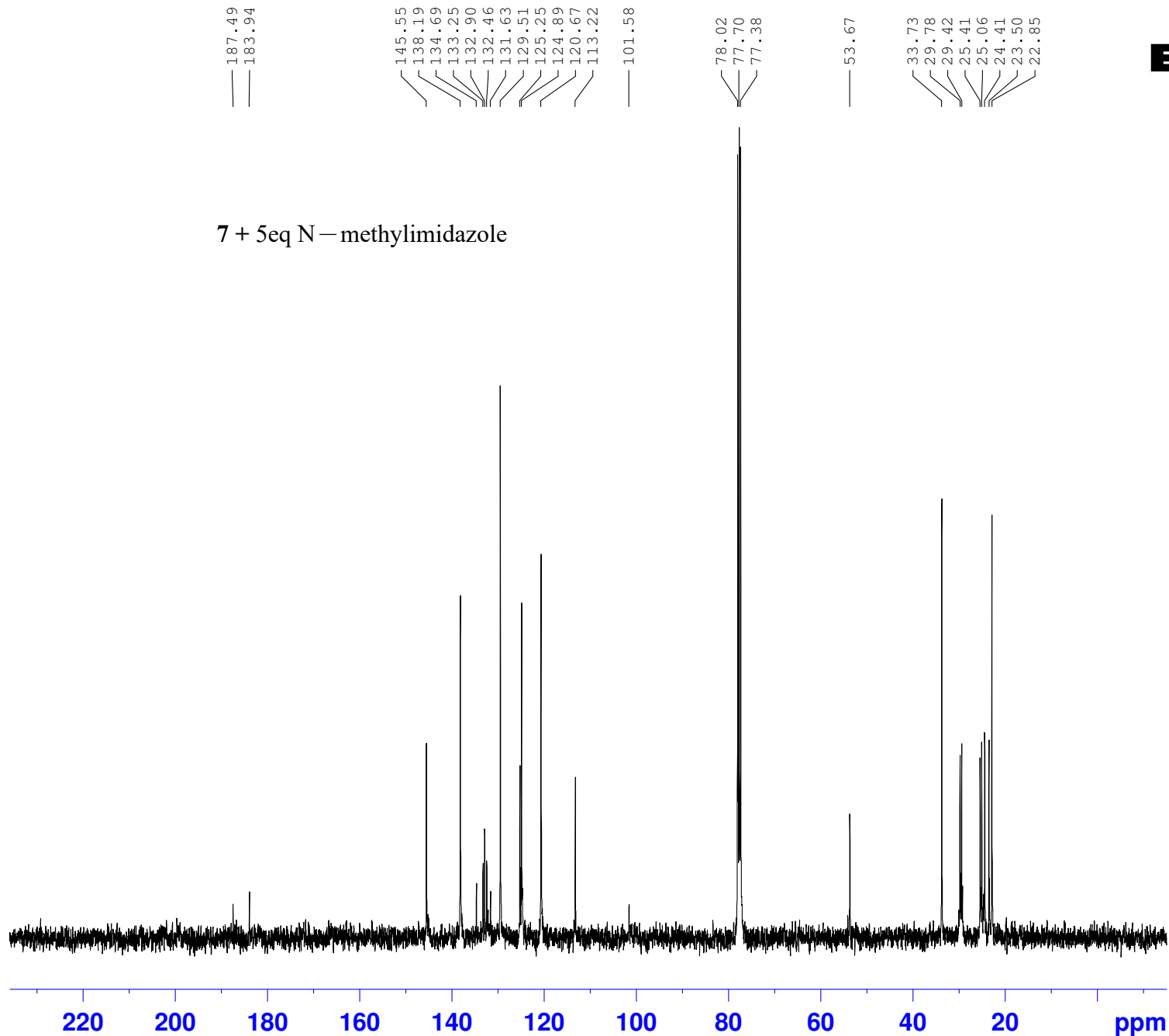
```

===== CHANNEL f1 =====
NUC1       13C
P1         13.50 usec
PL1        3.00 dB
PL1W       43.93649673 W
SFO1       100.6238364 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.80 dB
PL12       17.19 dB
PL13       18.46 dB
PL2W       8.92857742 W
PL12W      0.25809658 W
PL13W      0.19265592 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127139 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```

7 + 5eq N—methylimidazole



```

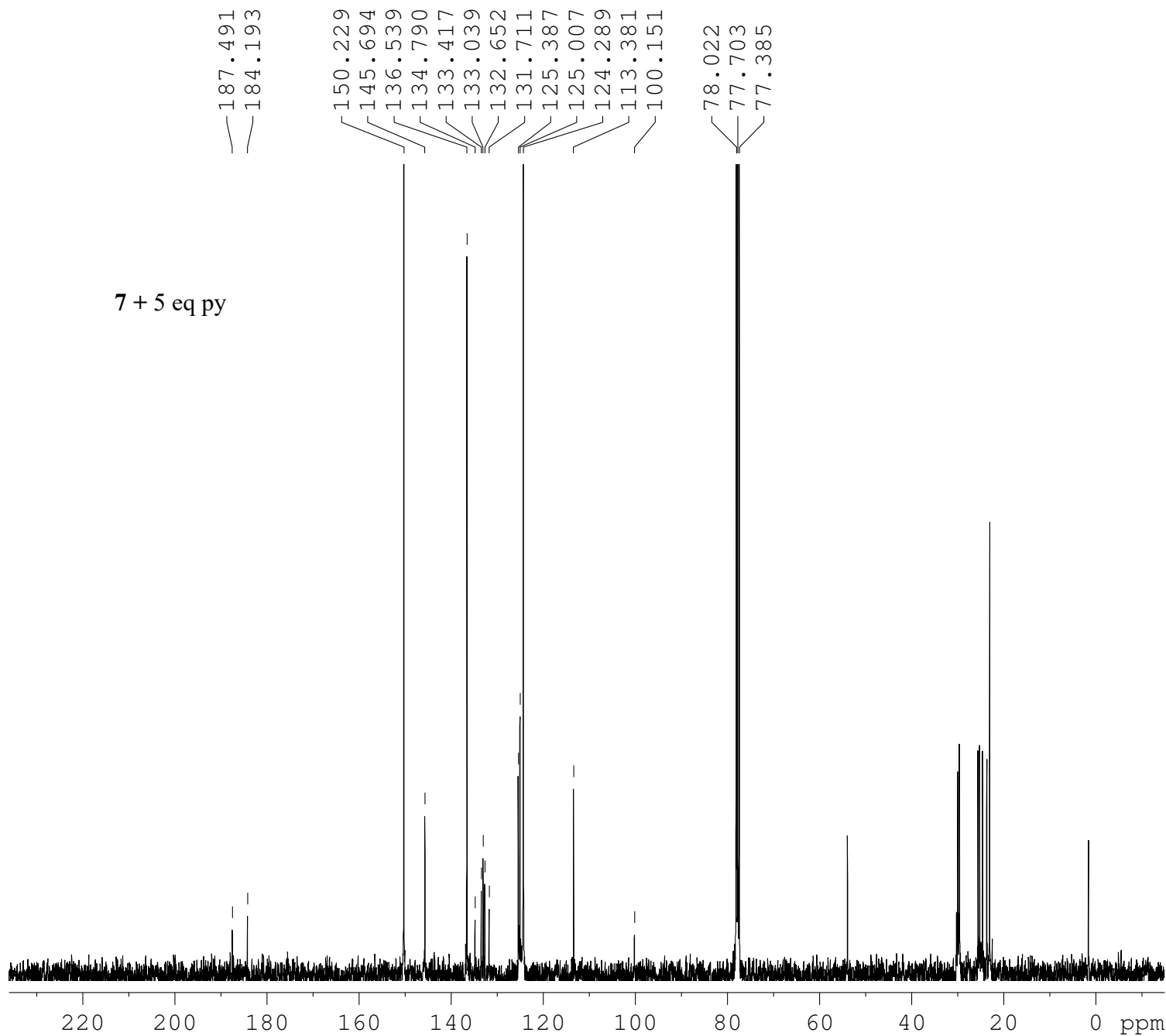
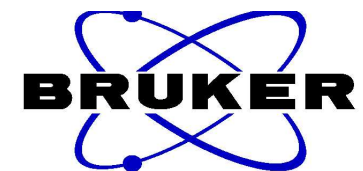
NAME      xxy-518NME mz-20180518
EXPNO      2
PROCNO     1
Date_      20180518
Time       21.50
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         136
DS         4
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DW         19.800 usec
DE         8.00 usec
TE         295.0 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1
  
```

```

===== CHANNEL f1 =====
NUC1      13C
P1        13.50 usec
PL1       3.00 dB
PL1W      43.93649673 W
SFO1      100.6238364 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2   waltz16
NUC2      1H
PCPD2     80.00 usec
PL2       1.80 dB
PL12      17.19 dB
PL13      18.46 dB
PL2W      8.92857742 W
PL12W     0.25809658 W
PL13W     0.19265592 W
SFO2      400.1316005 MHz
SI        32768
SF        100.6127262 MHz
WDW       EM
SSB       0
LB        3.00 Hz
GB        0
PC        1.40
  
```



```

NAME      xxy-bf-py2-20180427
EXPNO      2
PROCNO     1
Date_      20180427
Time       13.50
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDC13
NS         96
DS         4
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DW         19.800 usec
DE         8.00 usec
TE         297.8 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        10
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         13.50 usec
PL1        3.00 dB
PL1W       43.93649673 W
SFO1       100.6238364 MHz
  
```

```

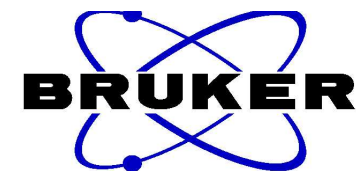
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.80 dB
PL12       17.19 dB
PL13       18.46 dB
PL2W       8.92857742 W
PL12W      0.25809658 W
PL13W      0.19265592 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127161 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```

187.480
184.309

7 + 1eq NEt₃

145.765
134.866
133.579
133.146
132.803
131.744
125.510
125.167
125.111
113.524

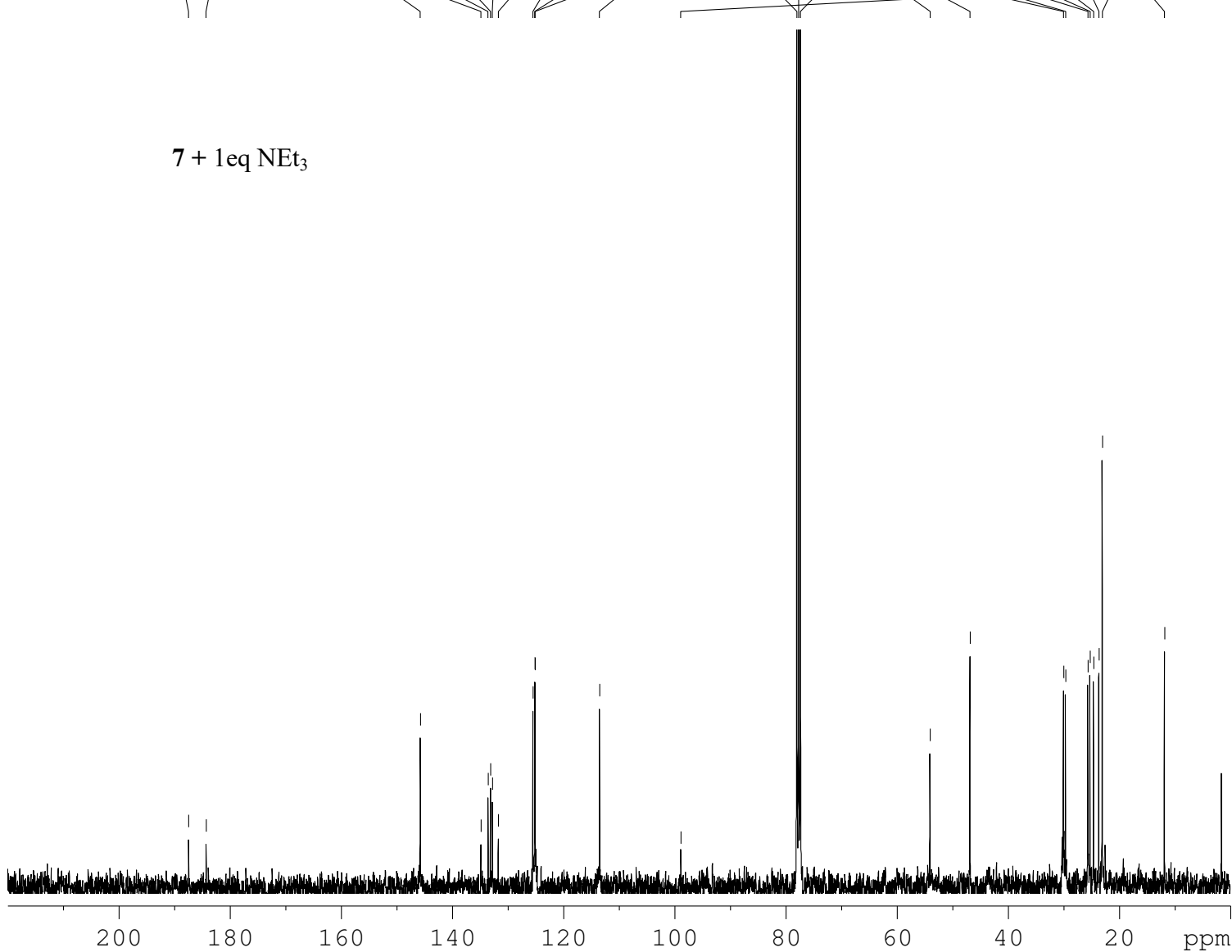
78.017
77.699
77.381
54.066
46.864
30.032
29.671
25.662
25.279
24.629
23.674
23.057
11.863
98.904

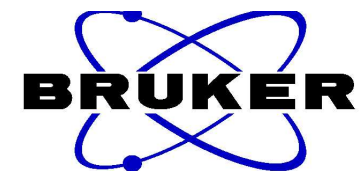
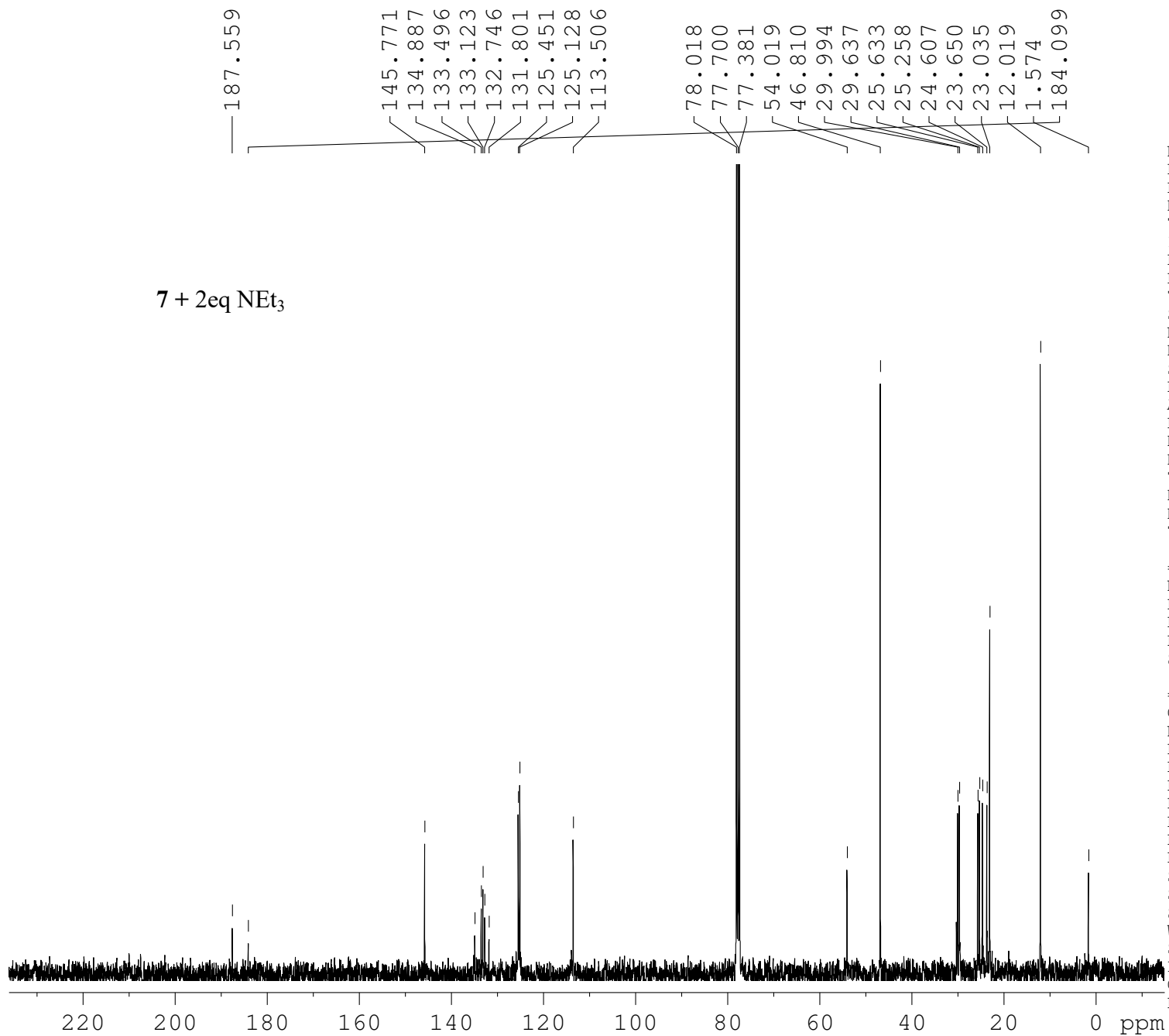


NAME xxy-bf-1b
EXPNO 2
PROCNO 1
Date_ 20180426
Time 18.19
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl₃
NS 80
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 2050
DW 19.800 usec
DE 8.00 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 10

===== CHANNEL f1 =====
NUC1 13C
P1 13.50 usec
PL1 3.00 dB
PL1W 43.93649673 W
SFO1 100.6238364 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.80 dB
PL12 17.19 dB
PL13 18.46 dB
PL2W 8.92857742 W
PL12W 0.25809658 W
PL13W 0.19265592 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127091 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40





```

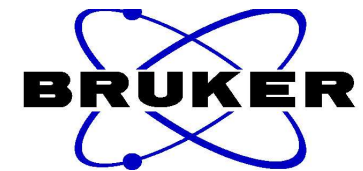
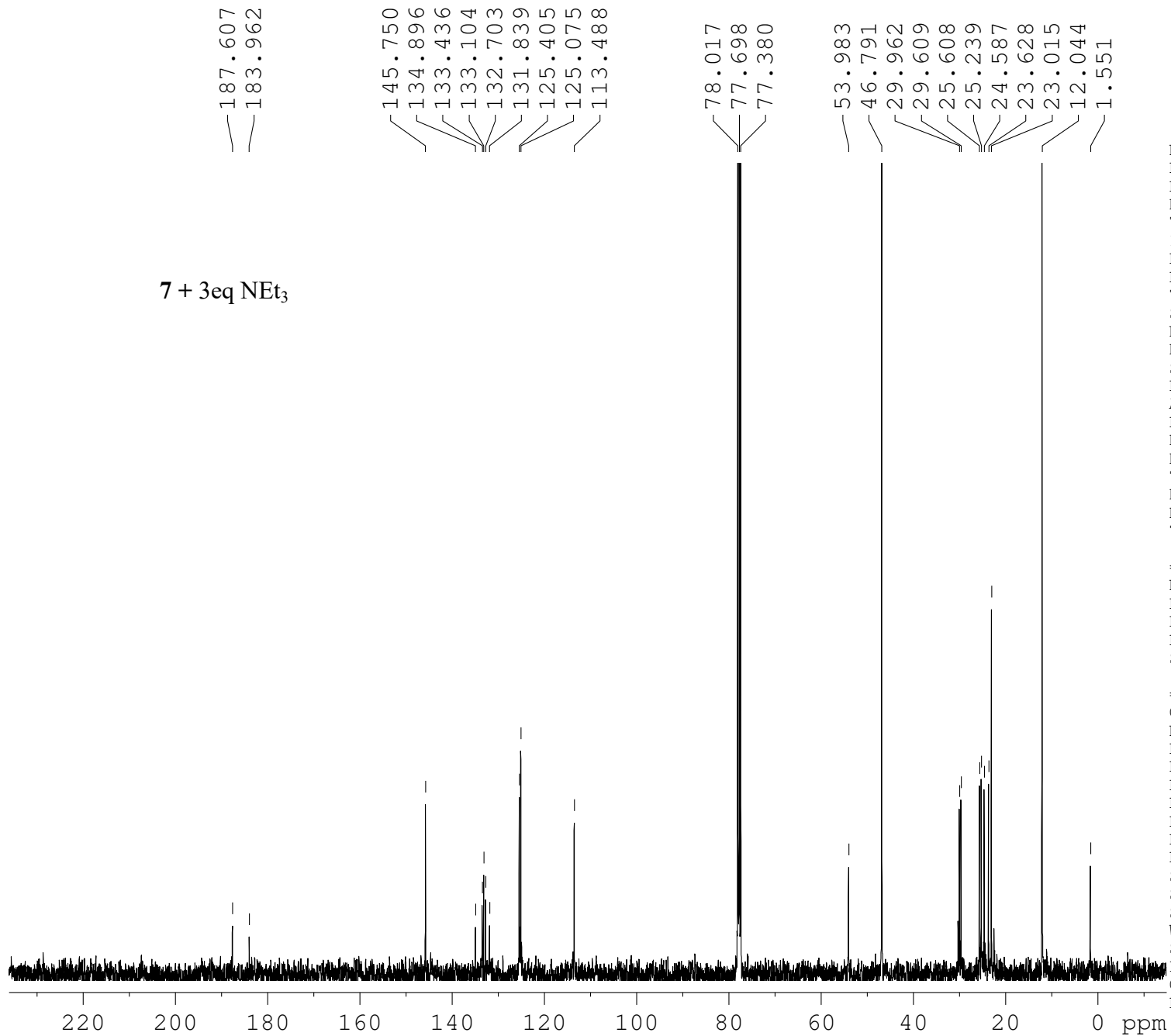
NAME          xxy-bf-2b
EXPNO          2
PROCNO         1
Date_          20180426
Time           18.30
INSTRUM        spect
PROBHD         5 mm PADUL 13C
PULPROG        zgpg30
TD             65536
SOLVENT        CDC13
NS             72
DS             4
SWH            25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976629 sec
RG            2050
DW            19.800 usec
DE            8.00 usec
TE            298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           10
  
```

```

===== CHANNEL f1 =====
NUC1           13C
P1            13.50 usec
PL1           3.00 dB
PL1W          43.93649673 W
SFO1          100.6238364 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2           1H
PCPD2          80.00 usec
PL2           1.80 dB
PL12          17.19 dB
PL13          18.46 dB
PL2W          8.92857742 W
PL12W         0.25809658 W
PL13W         0.19265592 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127100 MHz
WDW            EM
SSB            0
LB            3.00 Hz
GB            0
PC            1.40
  
```



```

NAME          xxy-bf-3b
EXPNO          2
PROCNO         1
Date_          20180426
Time           18.40
INSTRUM        spect
PROBHD         5 mm PADUL 13C
PULPROG        zgpg30
TD             65536
SOLVENT        CDCl3
NS             80
DS             4
SWH            25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976629 sec
RG            2050
DW            19.800 usec
DE            8.00 usec
TE            298.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0           10
  
```

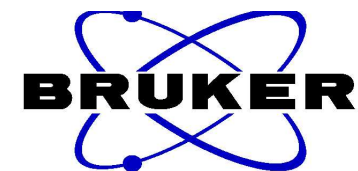
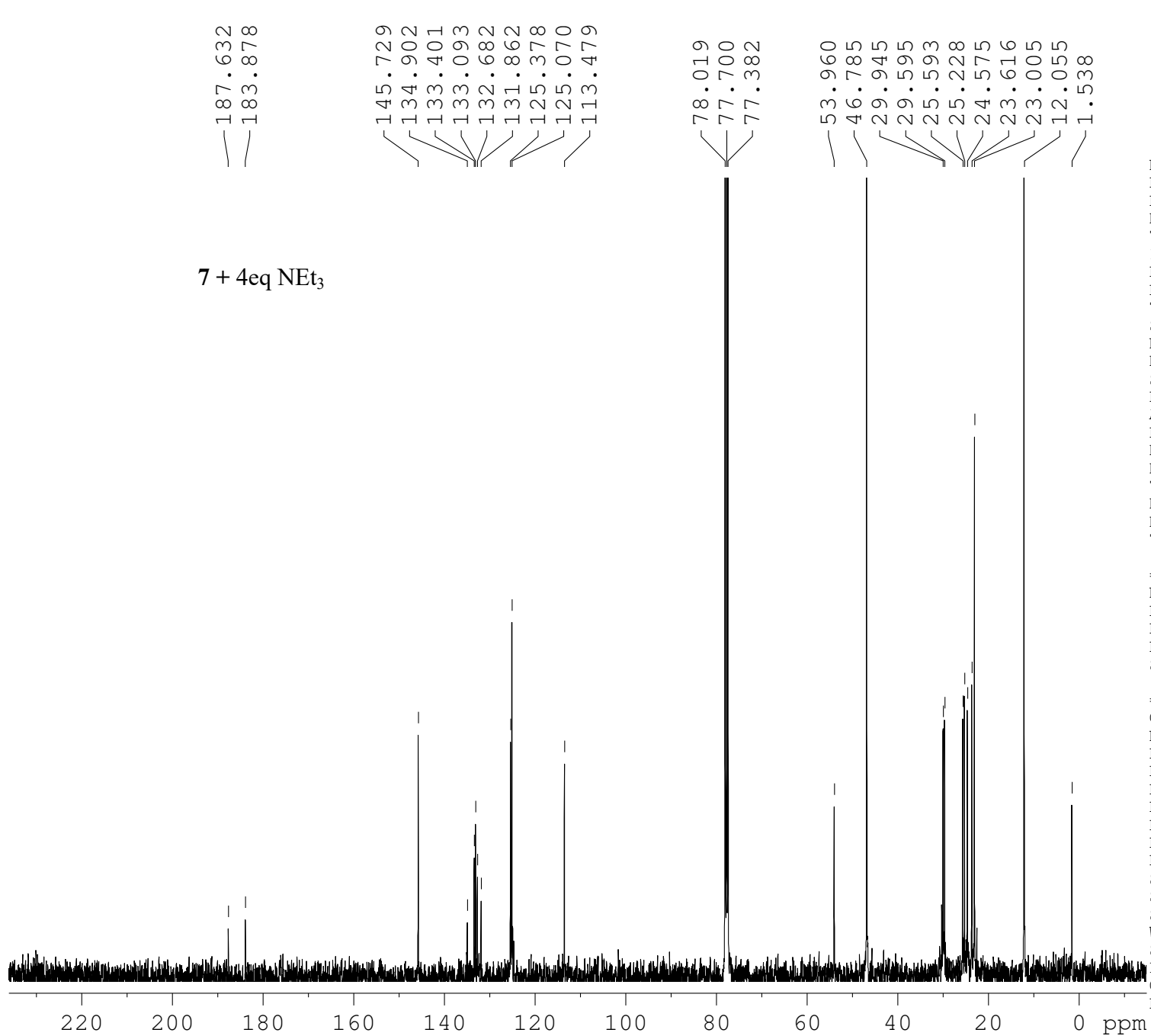
```

===== CHANNEL f1 =====
NUC1           13C
P1            13.50 usec
PL1           3.00 dB
PL1W          43.93649673 W
SFO1          100.6238364 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2        waltz16
NUC2           1H
PCPD2          80.00 usec
PL2           1.80 dB
PL12          17.19 dB
PL13          18.46 dB
PL2W          8.92857742 W
PL12W         0.25809658 W
PL13W         0.19265592 W
SFO2          400.1316005 MHz
SI            32768
SF            100.6127107 MHz
WDW            EM
SSB            0
LB            3.00 Hz
GB            0
PC            1.40
  
```

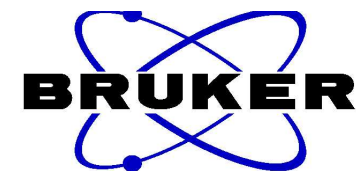
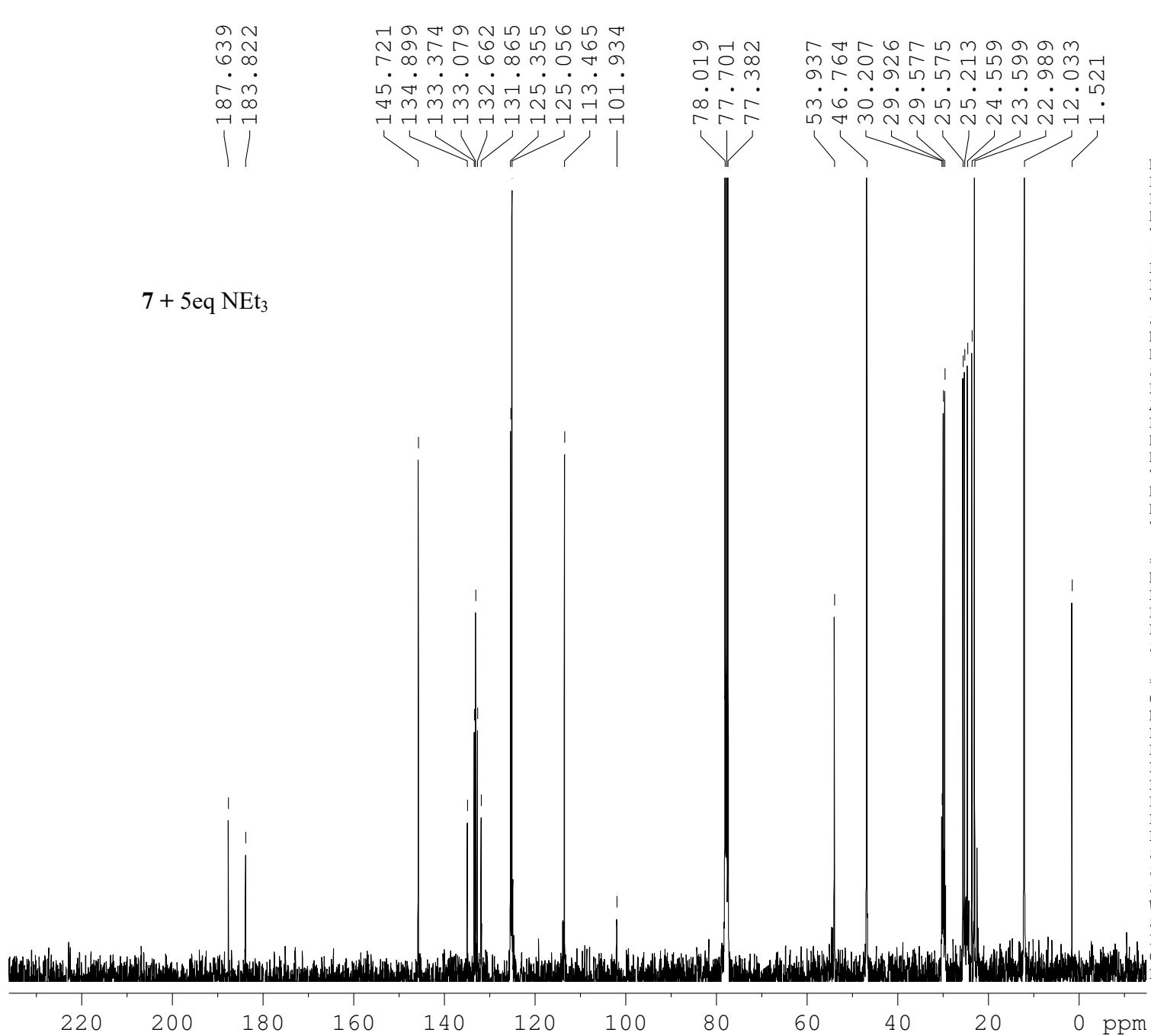
7 + 4eq NEt₃



NAME xxy-bf-4b
 EXPNO 2
 PROCNO 1
 Date_ 20180426
 Time 18.51
 INSTRUM spect
 PROBHD 5 mm PADUL 13C
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 120
 DS 4
 SWH 25252.525 Hz
 FIDRES 0.385323 Hz
 AQ 1.2976629 sec
 RG 2050
 DW 19.800 usec
 DE 8.00 usec
 TE 298.3 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 10

===== CHANNEL f1 =====
 NUC1 13C
 P1 13.50 usec
 PL1 3.00 dB
 PL1W 43.93649673 W
 SFO1 100.6238364 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 1.80 dB
 PL12 17.19 dB
 PL13 18.46 dB
 PL2W 8.92857742 W
 PL12W 0.25809658 W
 PL13W 0.19265592 W
 SFO2 400.1316005 MHz
 SI 32768
 SF 100.6127109 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40



```

NAME      xxy-bf-net3-20180426
EXPNO      2
PROCNO     1
Date_      20180426
Time       20.31
INSTRUM    spect
PROBHD     5 mm PADUL 13C
PULPROG    zgpg30
TD         65536
SOLVENT    CDCl3
NS         240
DS         4
SWH        25252.525 Hz
FIDRES     0.385323 Hz
AQ         1.2976629 sec
RG         2050
DW         19.800 usec
DE         8.00 usec
TE         297.7 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        10
  
```

```

===== CHANNEL f1 =====
NUC1       13C
P1         13.50 usec
PL1        3.00 dB
PL1W       43.93649673 W
SFO1       100.6238364 MHz
  
```

```

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        1.80 dB
PL12       17.19 dB
PL13       18.46 dB
PL2W       8.92857742 W
PL12W      0.25809658 W
PL13W      0.19265592 W
SFO2       400.1316005 MHz
SI         32768
SF         100.6127116 MHz
WDW        EM
SSB        0
LB         3.00 Hz
GB         0
PC         1.40
  
```