

Supporting Information NMR Spectra

A General Gold-Catalyzed Direct Oxidative Coupling of Non-activated Arenes

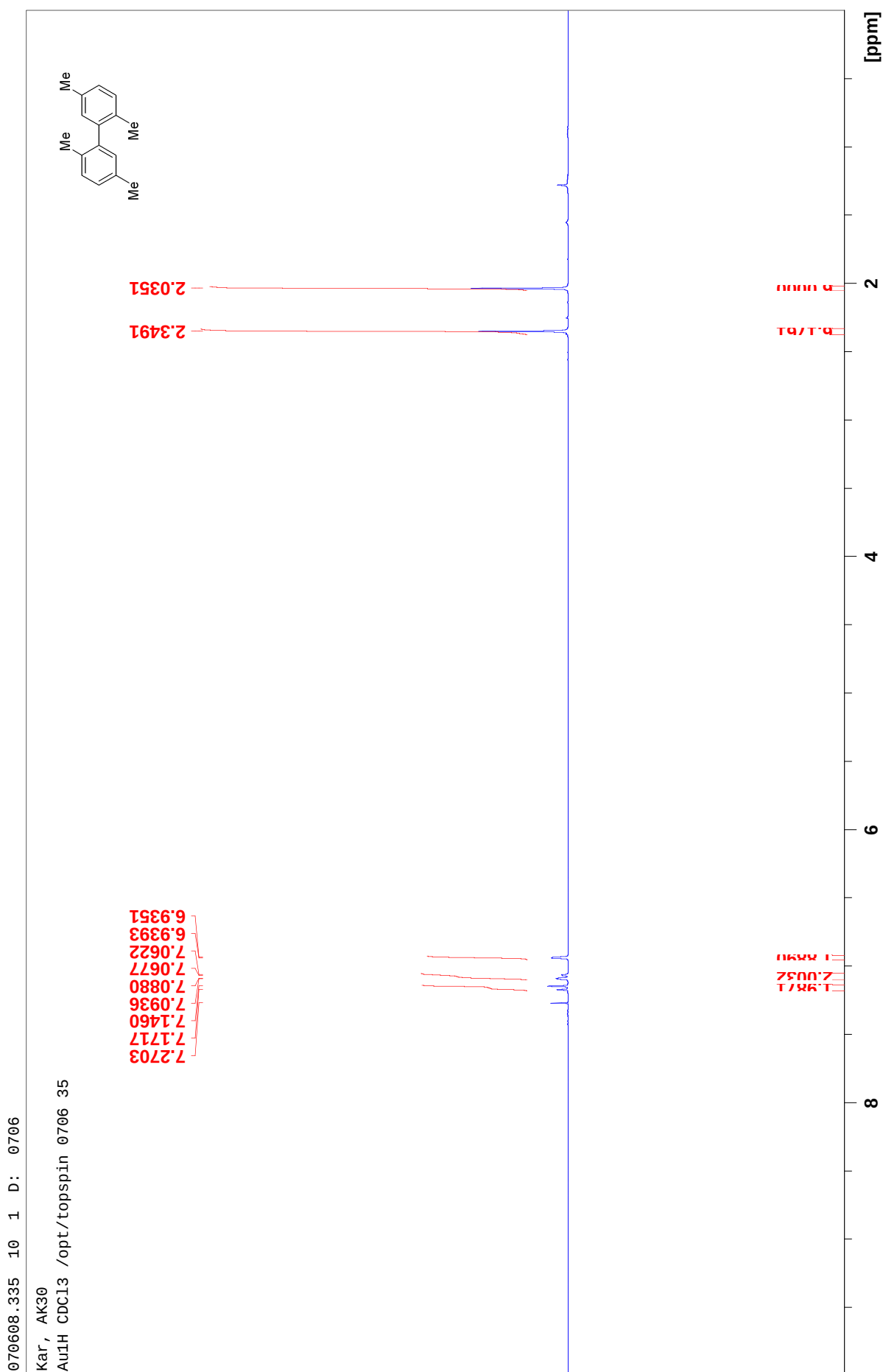
Anirban Kar,^a Naveenkumar Mangu,^a Hanns Martin Kaiser,^{a,b} Matthias Beller^{a,b} and Man Kin Tse^{a,b*}

^aLeibniz-Institut für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Str. 29a, 18059 Rostock, Germany

^bUniversität Rostock, Center for Life Science Automation (CELISCA), Friedrich-Barnewitz-Str. 8, D-18119 Rostock-Warnemünde, Germany

E-mail: man-kin.tse@catalysis.de; fax: +49-381-1281-51193; tel.: +49-381-1281-193

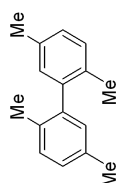
¹ H NMR spectrum of 2,2',5,5'-tetramethylbiphenyl (Table 1, entry 1)	S2
¹³ C NMR spectrum of 2,2',5,5'-tetramethylbiphenyl (Table 1, entry 1)	S3
¹ H NMR spectrum of 2,2',4,4'-tetramethylbiphenyl (Table 1, entry 4)	S4
¹³ C NMR spectrum of 2,2',4,4'-tetramethylbiphenyl (Table 1, entry 4)	S5
¹ H NMR spectrum of 5,5'-di-tert-butyl-2,2'-dimethylbiphenyl (Table 1, entry 5)	S6
¹³ C NMR spectrum of 5,5'-di-tert-butyl-2,2'-dimethylbiphenyl (Table 1, entry 5)	S7
¹ H NMR spectrum of 5,5'-difluoro-2,2'-dimethoxybiphenyl (Table 1, entry 6)	S8
¹³ C NMR spectrum of 5,5'-difluoro-2,2'-dimethoxybiphenyl (Table 1, entry 6)	S9
¹ H NMR spectrum of 3,3'-difluoro-2,4'-dimethoxybiphenyl (minor isomer) (Table 1, entry 7)	S10
¹³ C NMR spectrum of 3,3'-difluoro-2,4'-dimethoxybiphenyl (minor isomer) (Table 1, entry 7)	S11
¹ H NMR spectrum of 3,3'-difluoro-4,4'-dimethoxybiphenyl (major isomer) (Table 1, entry 7)	S12
¹³ C NMR spectrum of 3,3'-difluoro-4,4'-dimethoxybiphenyl (major isomer) (Table 1, entry 7)	S13
¹ H NMR spectrum of 5,5'-dichloro-2,2'-dimethoxybiphenyl (Table 1, entry 8)	S14
¹³ C NMR spectrum of 5,5'-dichloro-2,2'-dimethoxybiphenyl (Table 1, entry 8)	S15
¹ H NMR spectrum of 5,5'-dibromo-2,2'-dimethoxybiphenyl (Table 1, entry 9)	S16
¹³ C NMR spectrum of 5,5'-dibromo-2,2'-dimethoxybiphenyl (Table 1, entry 9)	S17
¹ H NMR spectrum of 3,3'-diiodo-4,4'-dimethoxybiphenyl (major isomer) (Table 1, entry 10)	S18
¹³ C NMR spectrum of 3,3'-diiodo-4,4'-dimethoxybiphenyl (major isomer) (Table 1, entry 10)	S19
¹ H NMR spectrum of 3,3'-diiodo-2,4'-dimethoxybiphenyl (minor isomer) (Table 1, entry 10)	S20
¹³ C NMR spectrum of 3,3'-diiodo-2,4'-dimethoxybiphenyl (minor isomer) (Table 1, entry 10)	S21
¹ H NMR spectrum of 2,2'-dimethoxy-5,5'-dinitrobiphenyl (Table 1, entry 11)	S22
¹³ C NMR spectrum of 2,2'-dimethoxy-5,5'-dinitrobiphenyl (Table 1, entry 11)	S23
¹ H NMR spectrum of dimethyl 4,4'-dimethoxybiphenyl-3,3'-dicarboxylate (major isomer) (Table 1, entry 12)	S24
¹³ C NMR spectrum of dimethyl 4,4'-dimethoxybiphenyl-3,3'-dicarboxylate (major isomer) (Table 1, entry 12)	S25
¹ H NMR spectrum of dimethyl 6,6'-dimethylbiphenyl-3,3'-dicarboxylate (Table 1, entry 13)	S26
¹³ C NMR spectrum of dimethyl 6,6'-dimethylbiphenyl-3,3'-dicarboxylate (Table 1, entry 13)	S27
¹ H NMR spectrum of 5,5'-dimethyl-2,2'-bithiophene (Table 1, entry 14)	S28
¹³ C NMR spectrum of 5,5'-dimethyl-2,2'-bithiophene (Table 1, entry 14)	S29



070608.335 11 1 D: 0706

Kar, AK30

Au13C CDC13 /opt/topspin 0706 35



141.5847
134.8163
132.5876
129.9376
129.5913
127.7020

77.4278
77.0045
76.5817

20.9291
19.3016

[ppm]

50

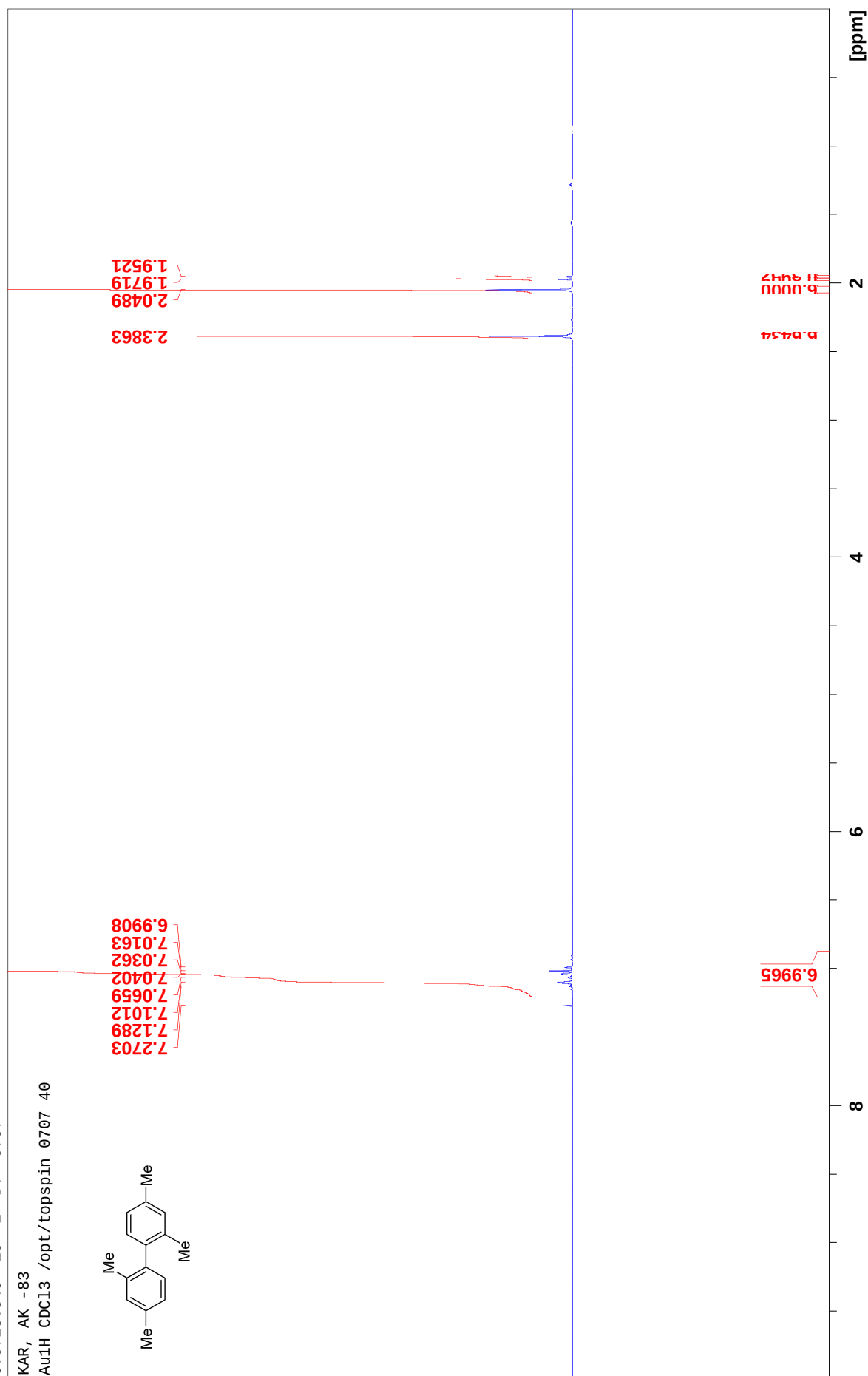
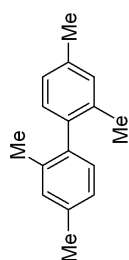
100

150

070718.340 10 1 D: 0707

KAR, AK -83

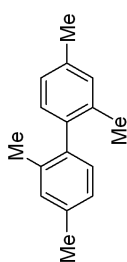
Au1H CDCl3 /opt/topspin 0707 40



070718.340 11 1 D: 0707

KAR, AK -83

Au13C CDC13 /opt/topspin 0707 40



138.6311
136.5143
135.7654
130.5186
129.4265
126.1850

77.4281
77.0048
76.5819

21.1126
19.7899

[ppm]

50

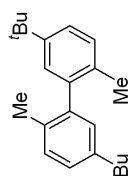
100

150

070808.315 10 1 D: 0708

KAR. AK94

Au1H CDCl3 /opt/topspin 0708 15



7.3281
7.3200
7.3016
7.2936
7.2706
7.2395
7.2120
7.2016
7.1924

2.0529
1.3404

1.9245
1.6785

9.8647

18.0000

[ppm]

2

4

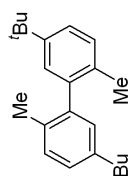
6

8

070808.315 11 1 D: 0708

KAR. AK94

Au13C CDC13 /opt/topspin 0708 15



148.2970
141.5024
132.7754
129.4432
126.6445
123.8294

76.9947

34.4053
31.4450

19.3740

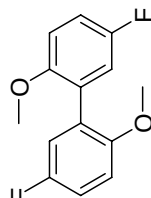
[ppm]

50

100

150

Tse, MKT 1387.B3
Au1H CDCl3 /opt/topspin 0707 26

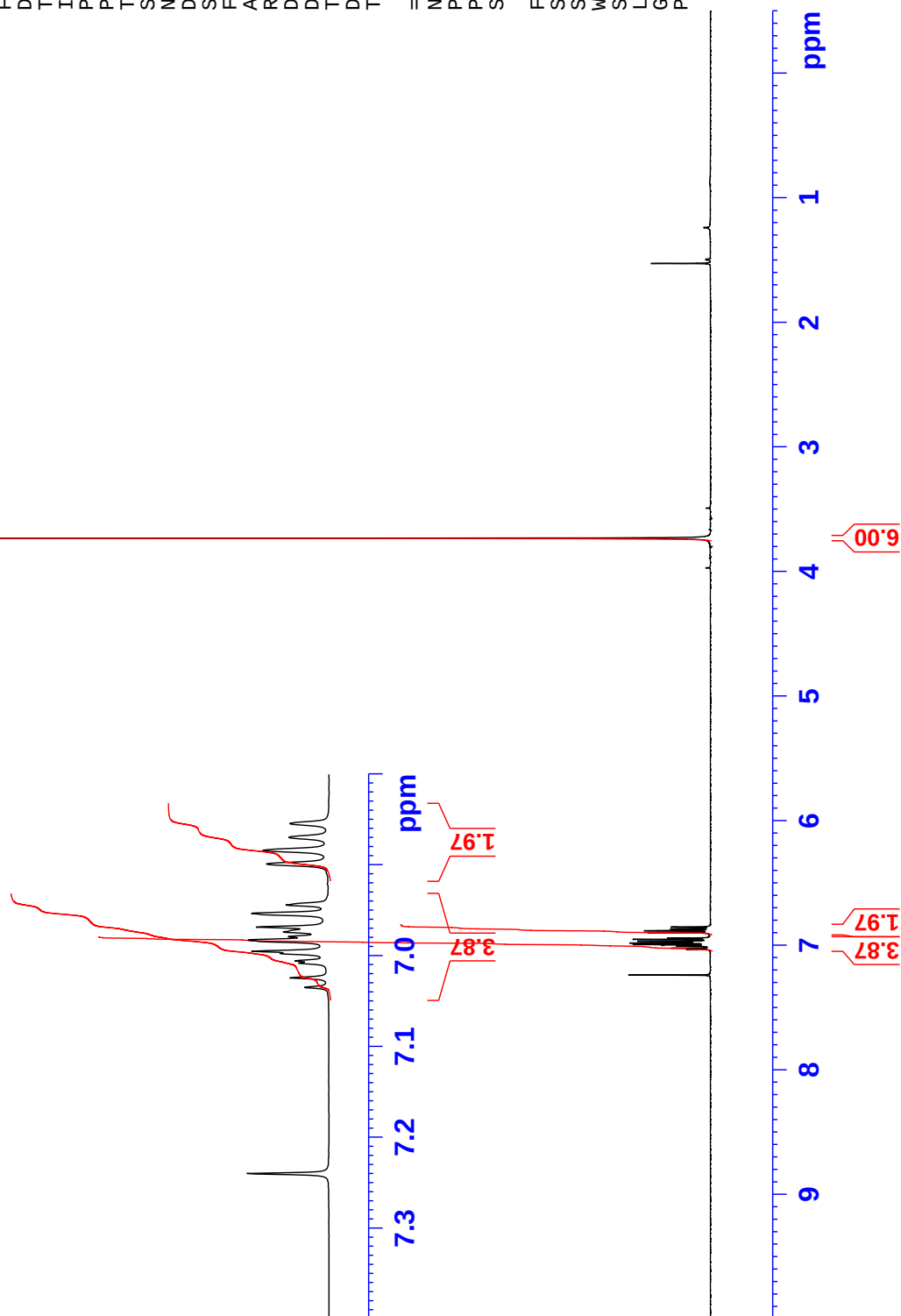


Current Data Parameters
NAME 070720.326
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070721
Time 2.40
INSTRUM spect
PROBHD 5 mm PABBO BB -
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300212 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00





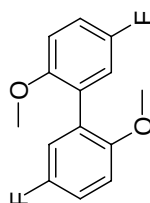
Current Data Parameters
NAME 070720.326
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070721
Time 3.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SF01 75.4771825 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 21.00 dB
SF02 300.1312005 MHz

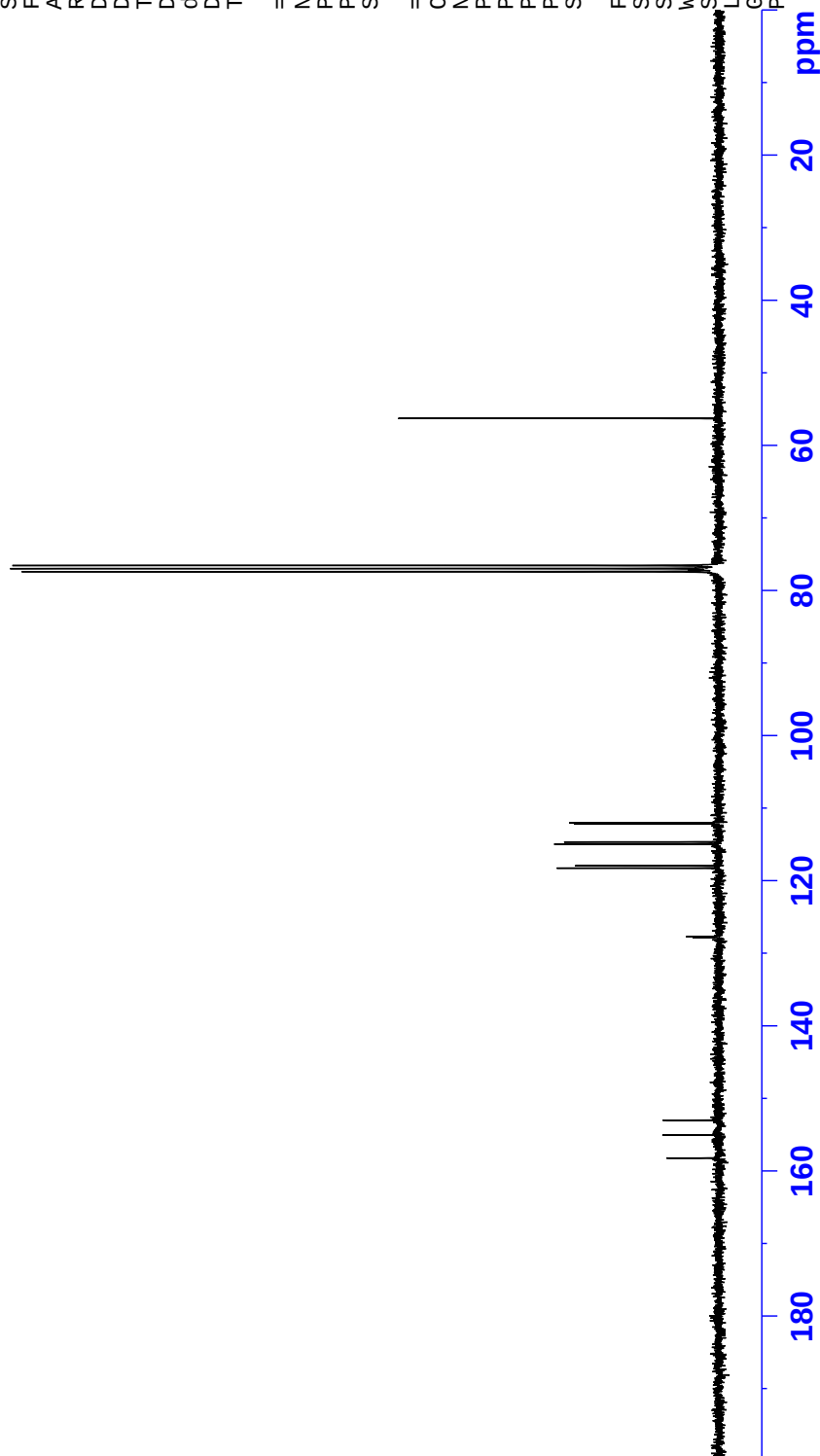
F2 - Processing parameters
SI 32768
SF 75.4677528 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



56.29

77.42
77.00
76.57

158.23
155.07
153.04
153.01
127.84
127.82
127.73
127.71
118.27
117.96
114.96
114.66
112.14
112.03



Tse, MKT 1387.B3
Au13C CDCl3 /opt/topspin 0707 26

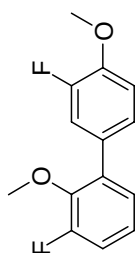


Current Data Parameters
NAME 070718.325
EXPNO 10
PROCNO 1

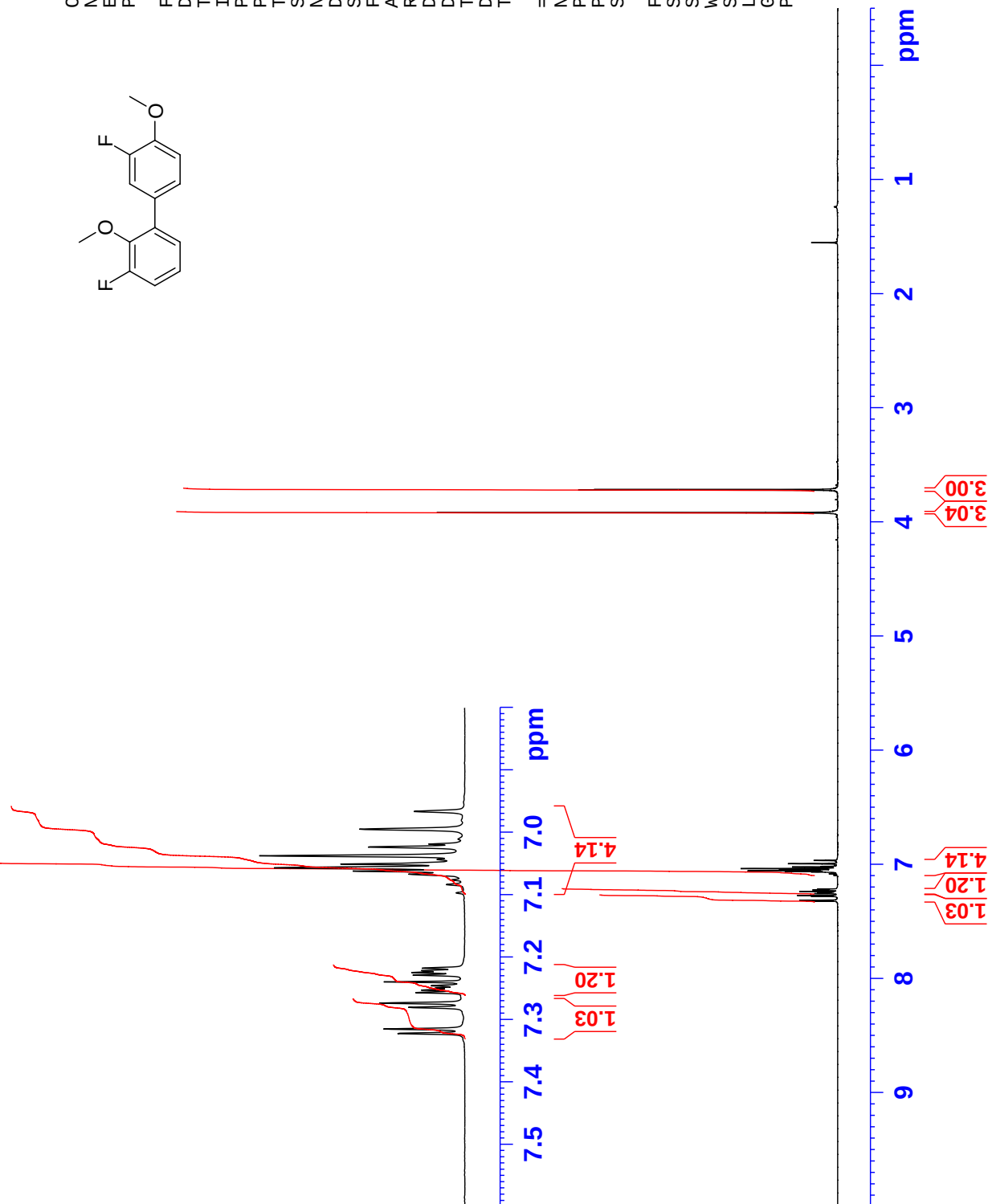
F2 - Acquisition Parameters
Date_ 20070719
Time 2.43
INSTRUM spect
PROBHD 5 mm PABBO BB -
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 4
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 296.3 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300212 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00



Tse, MKT 1382 B1
Au1H CDCl3 /opt/topspin 0707 25





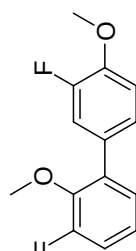
Current Data Parameters
NAME 070718.325
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070719
Time 3.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

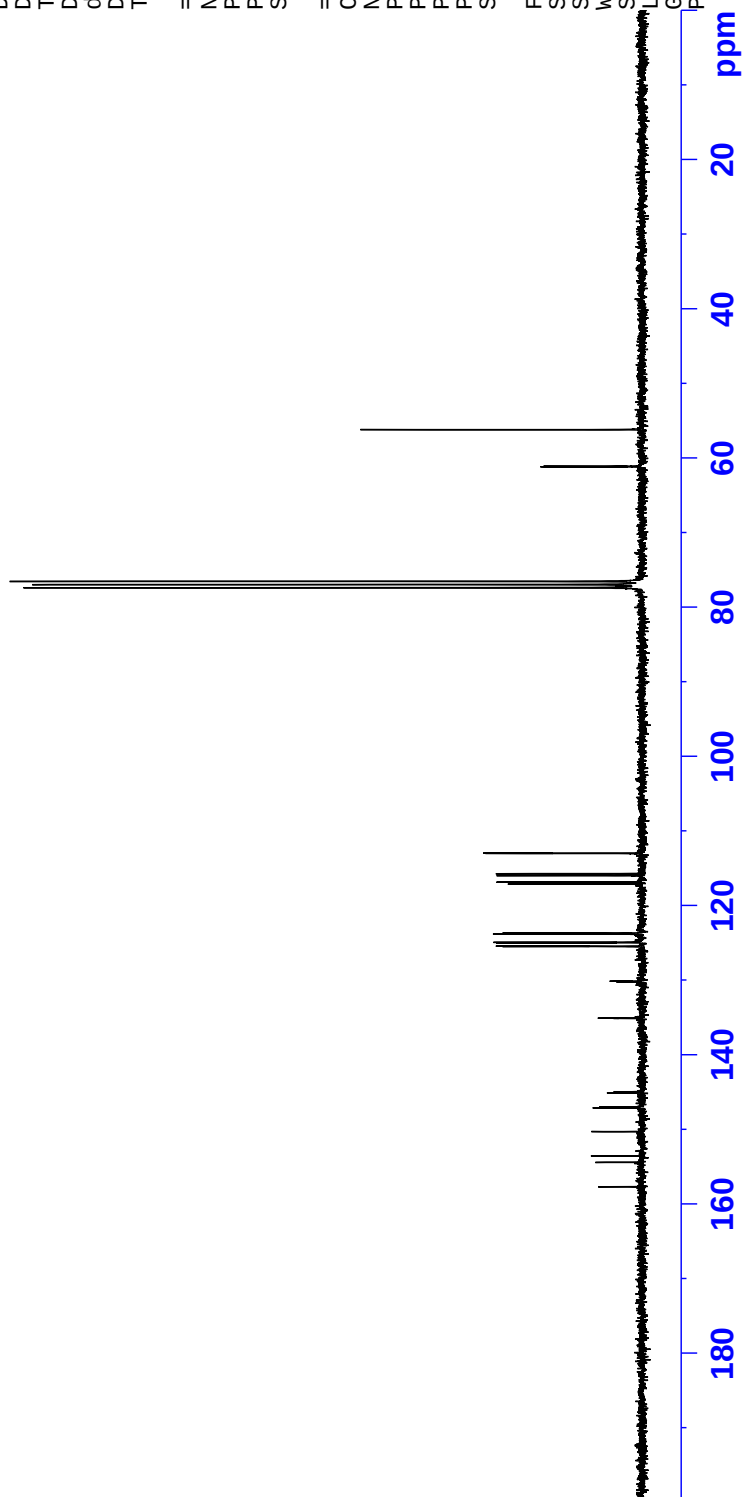
===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SF01 75.4771825 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 21.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

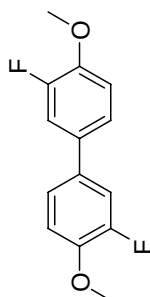


157.70
154.44
153.56
150.31
147.13
147.00
145.11
144.97
135.14
135.11
135.09
130.28
130.24
130.19
130.15
125.49
125.46
124.99
124.94
123.82
123.71
117.12
116.87
115.99
115.73
113.02
112.99
61.20
61.14
56.22
77.42
77.00
76.57



Tse, MKT 1382 B1
Au13C CDCl3 /opt/topspin 0707 25

Tse, MKT 1382 B2
Au1H CDC13 /opt/topspin 0707 27

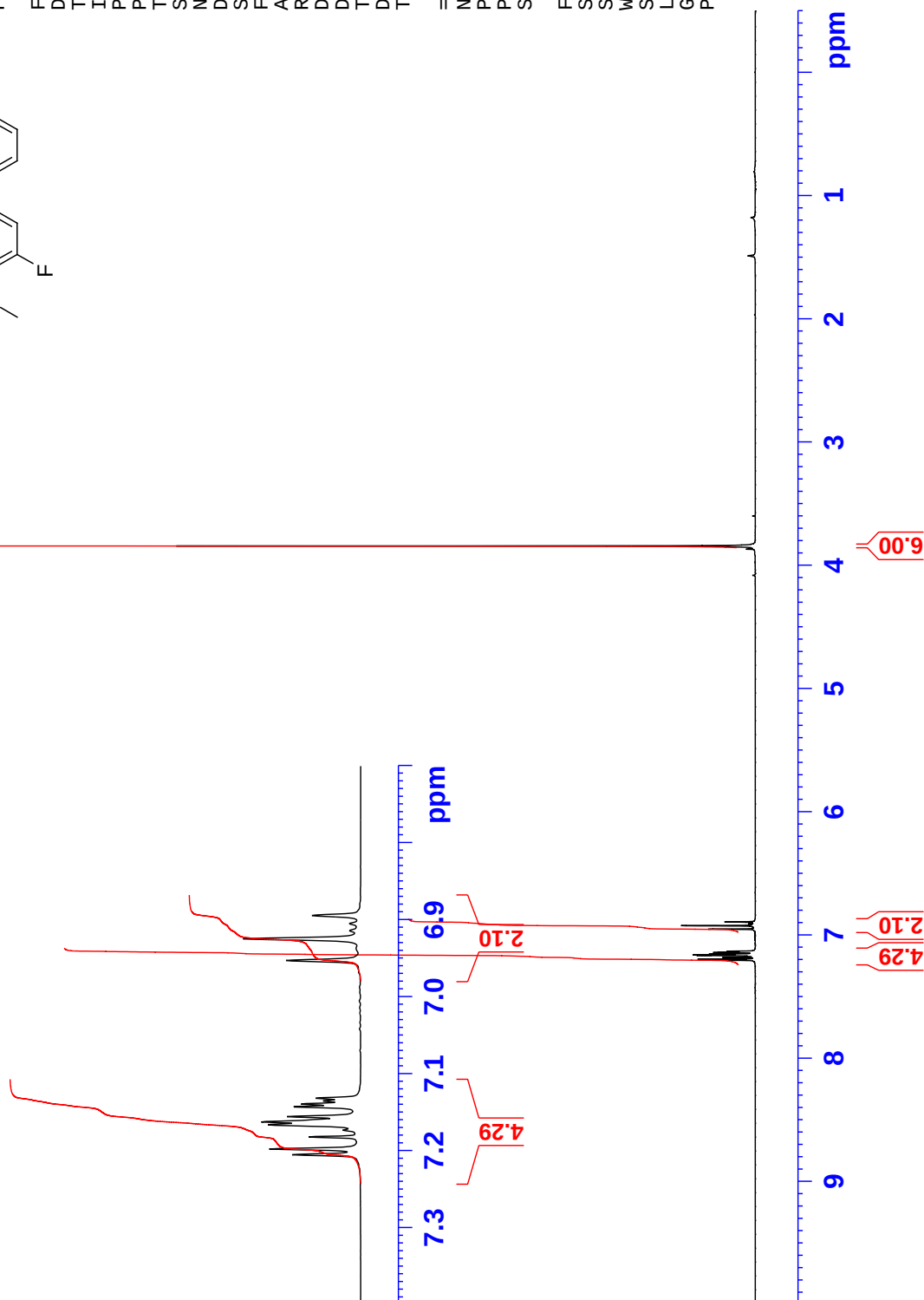


Current Data Parameters
NAME 070718.327
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070719
Time 4.44
INSTRUM spect
PROBHD 5 mm PABBO BB -
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 32
DS 4
SWH 6172.839 Hz
FIDRES 0.188380 Hz
AQ 2.6542580 sec
RG 322.5
DW 81.000 usec
DE 6.00 usec
TE 297.0 K
D1 1.00000000 sec
TD0 1

==== CHANNEL f1 =====
NUC1 1H
P1 11.00 usec
PL1 0.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1300385 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00





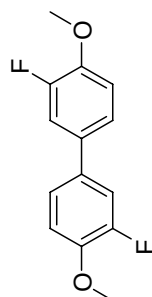
Current Data Parameters
NAME 070718.327
EXPNO 11
PROCNO 1

F2 - Acquisition Parameters
Date_ 20070719
Time 5.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1024
DS 4
SWH 21097.047 Hz
FIDRES 0.643831 Hz
AQ 0.7766516 sec
RG 32768
DW 23.700 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.60 usec
PL1 -1.10 dB
SF01 75.4771825 MHz

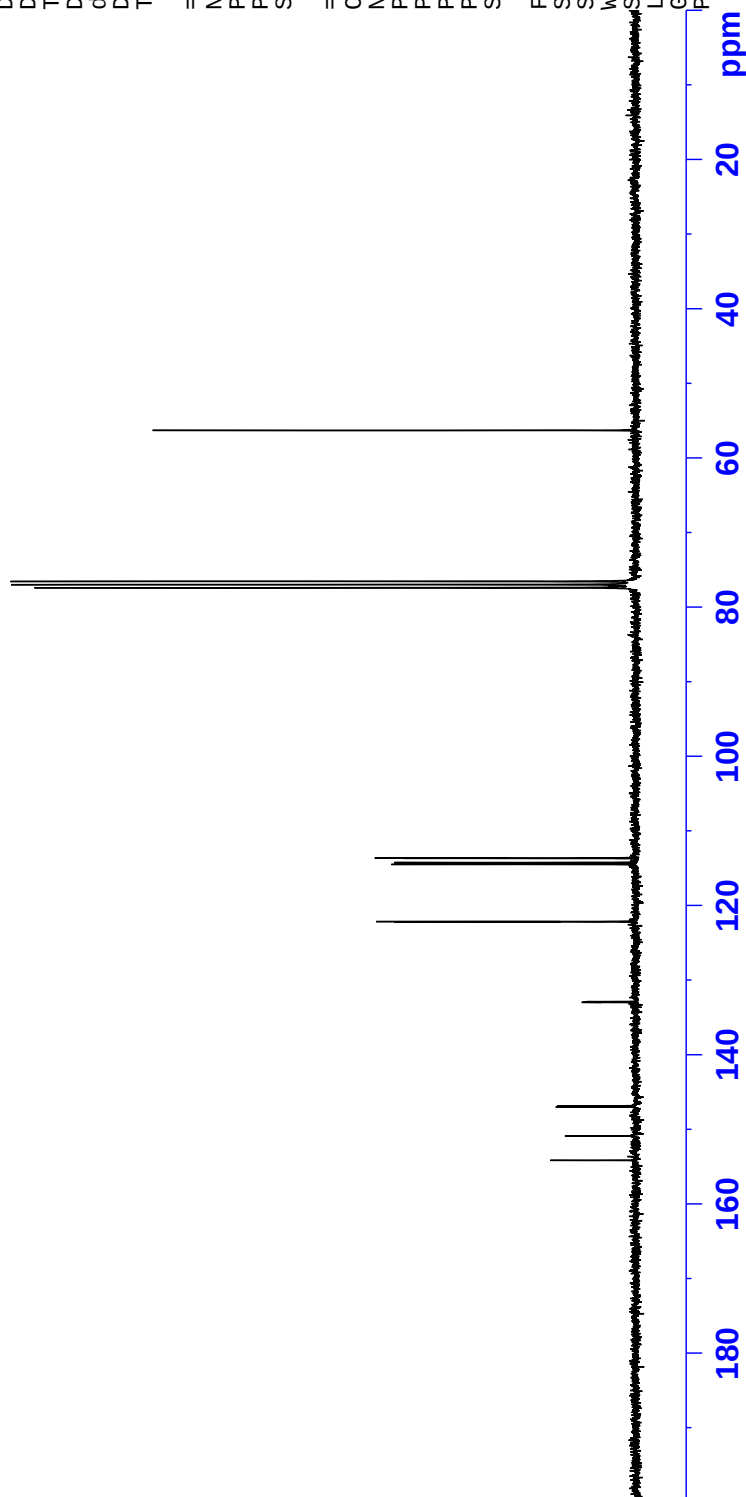
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 0.00 dB
PL12 19.00 dB
PL13 21.00 dB
SF02 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677534 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

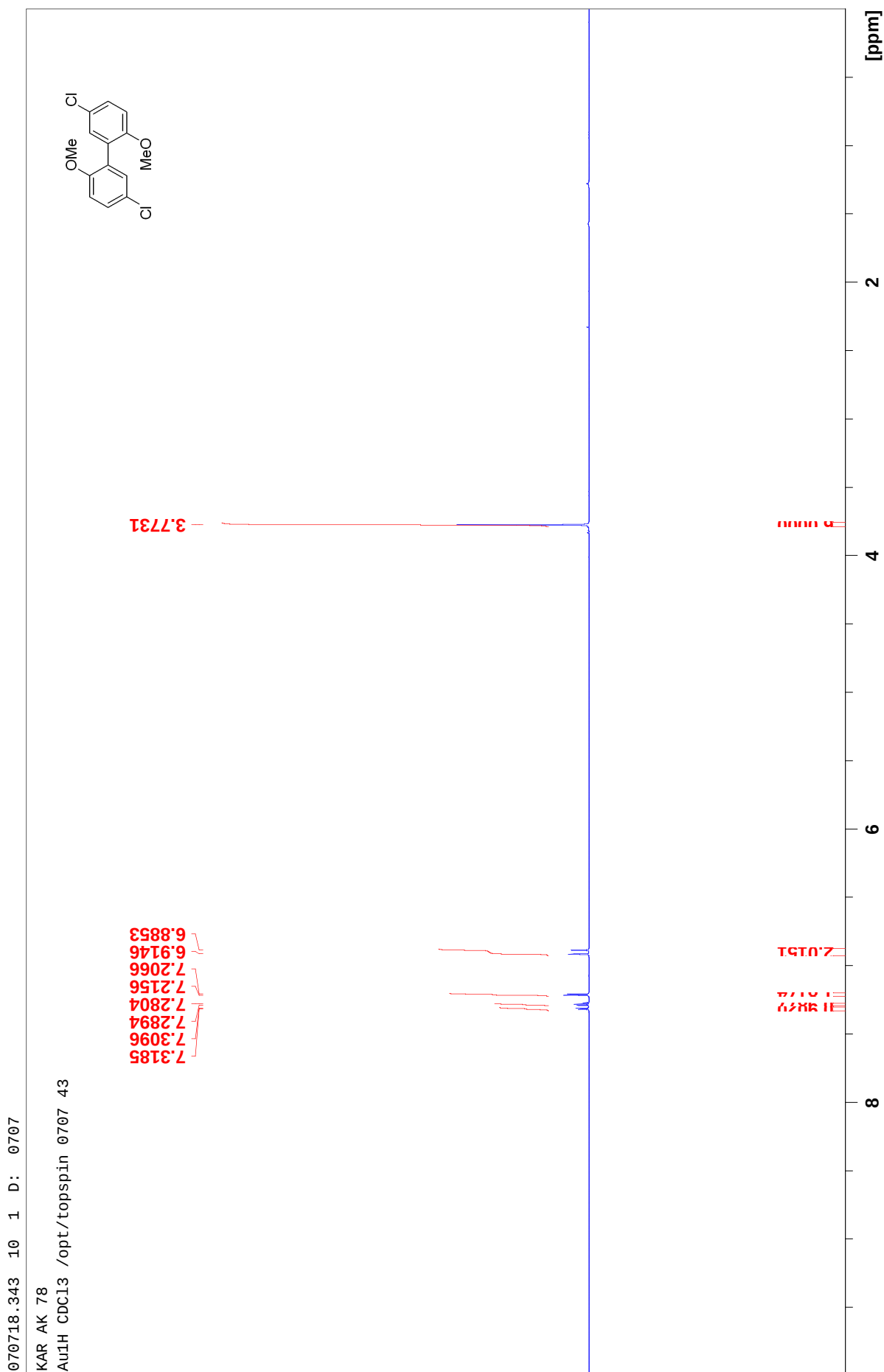


56.33

113.68
113.68
154.18
150.91
147.01
146.87
133.00
132.97
132.91
132.89
122.19
122.15
114.49
114.24
113.65



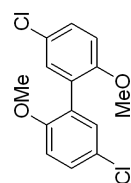
Tse, MKT 1382 B2
Au13C CDCl3 /opt/topspin 0707 27



070718.343 11 1 D: 0707

KAR AK 78

Au13C CDC13 /opt/topspin 0707 43



155.5603

131.0085
128.6179
127.9404
125.1779

112.2277

77.4270
77.0034
76.5794

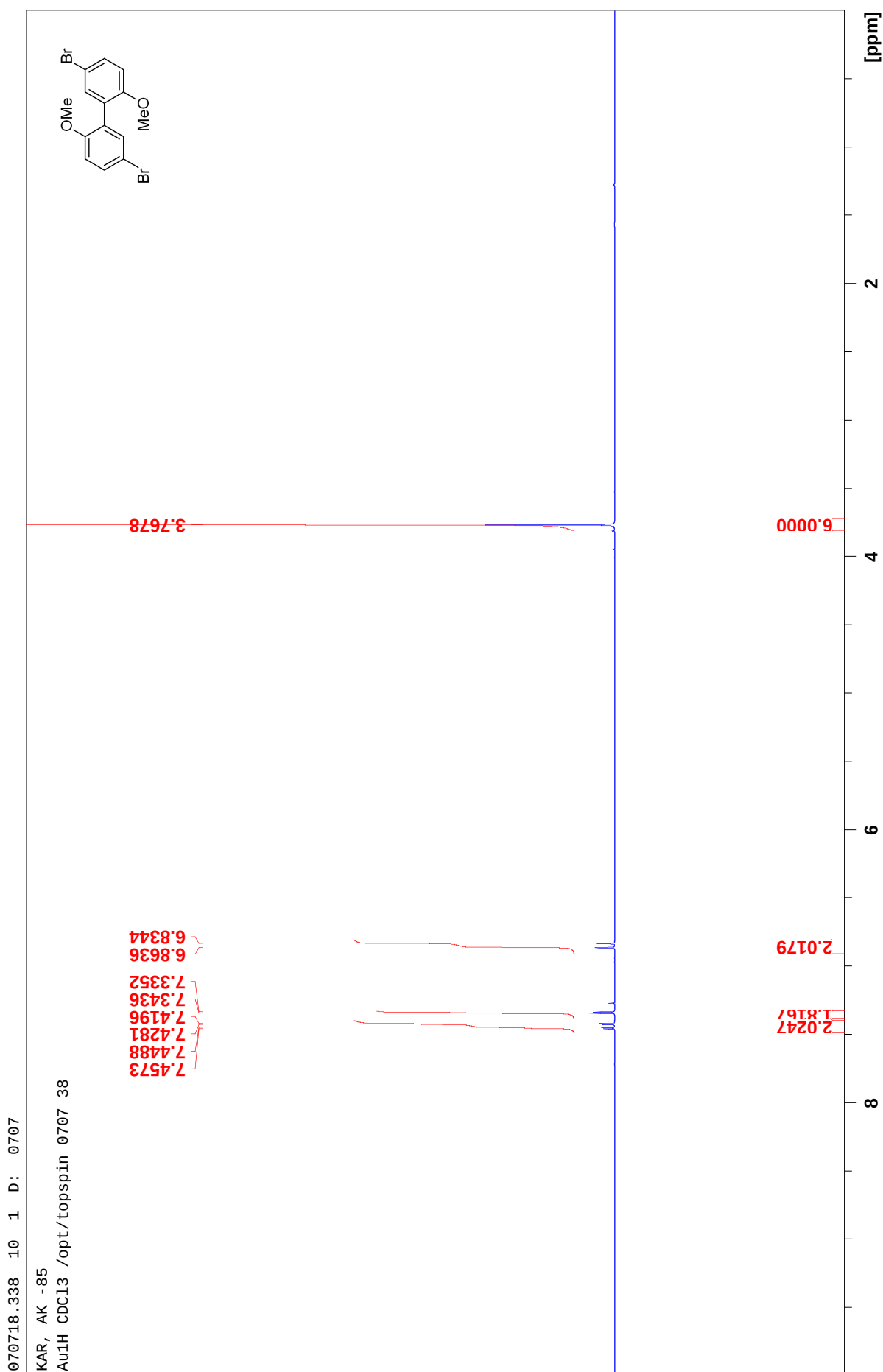
55.9720

[ppm]

50

100

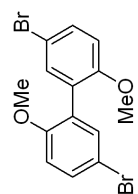
150



070718.338 11 1 D: 0707

KAR, AK -85

Au13C CDC13 /opt/topspin 0707 38



156.0900

133.7712
131.6156
128.3528

112.7084
112.4776

77.4295
77.0059
76.5831

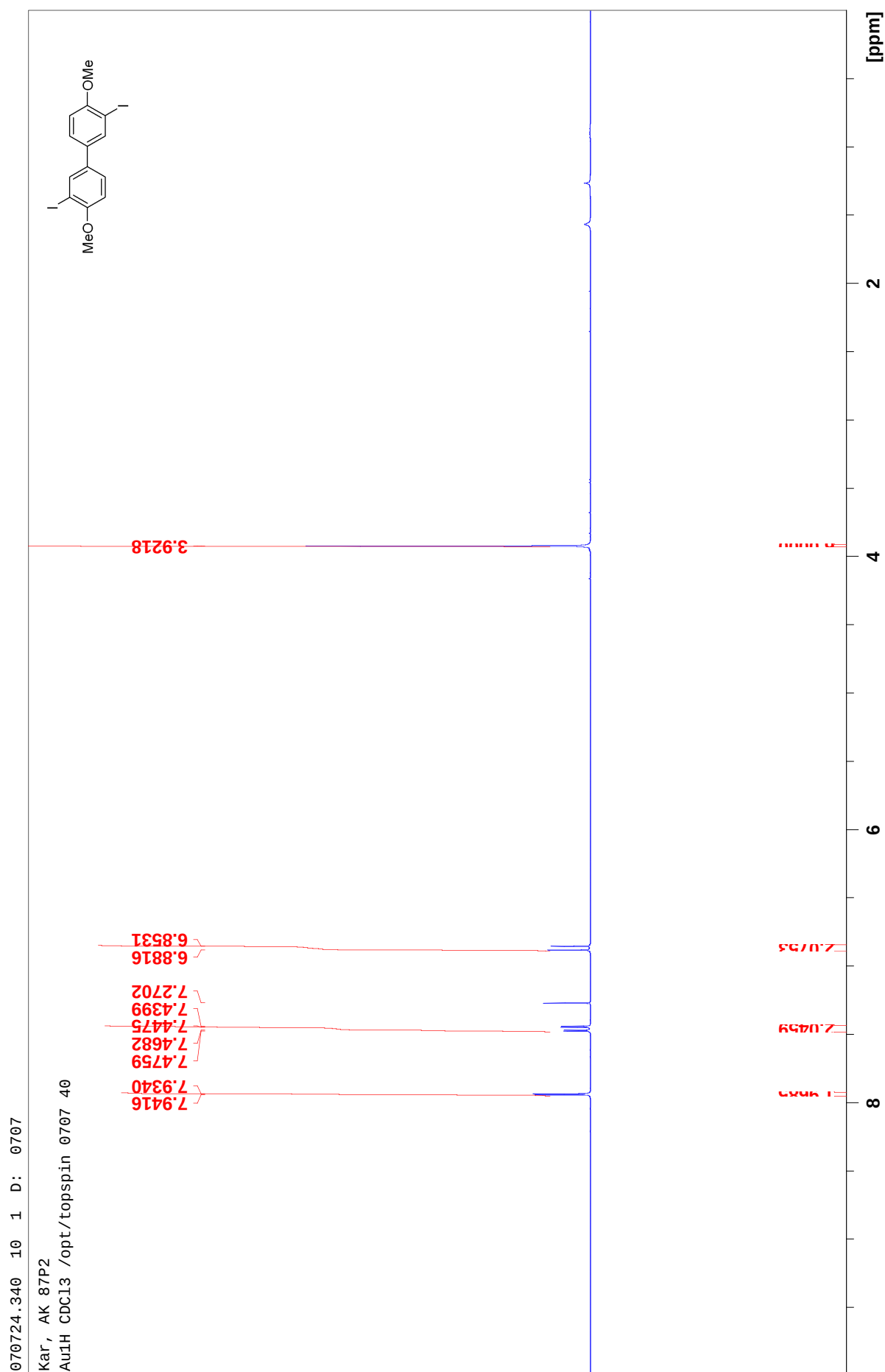
55.9103

[ppm]

50

100

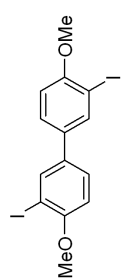
150



070724.340 11 1 D: 0707

Kar, AK 87P2

Au13C CDC13 /opt/topspin 0707 40



— 157.4535

— 137.5721

— 133.8996

— 127.7312

— 110.9619

— 86.4138

77.4249

77.0019

76.5783

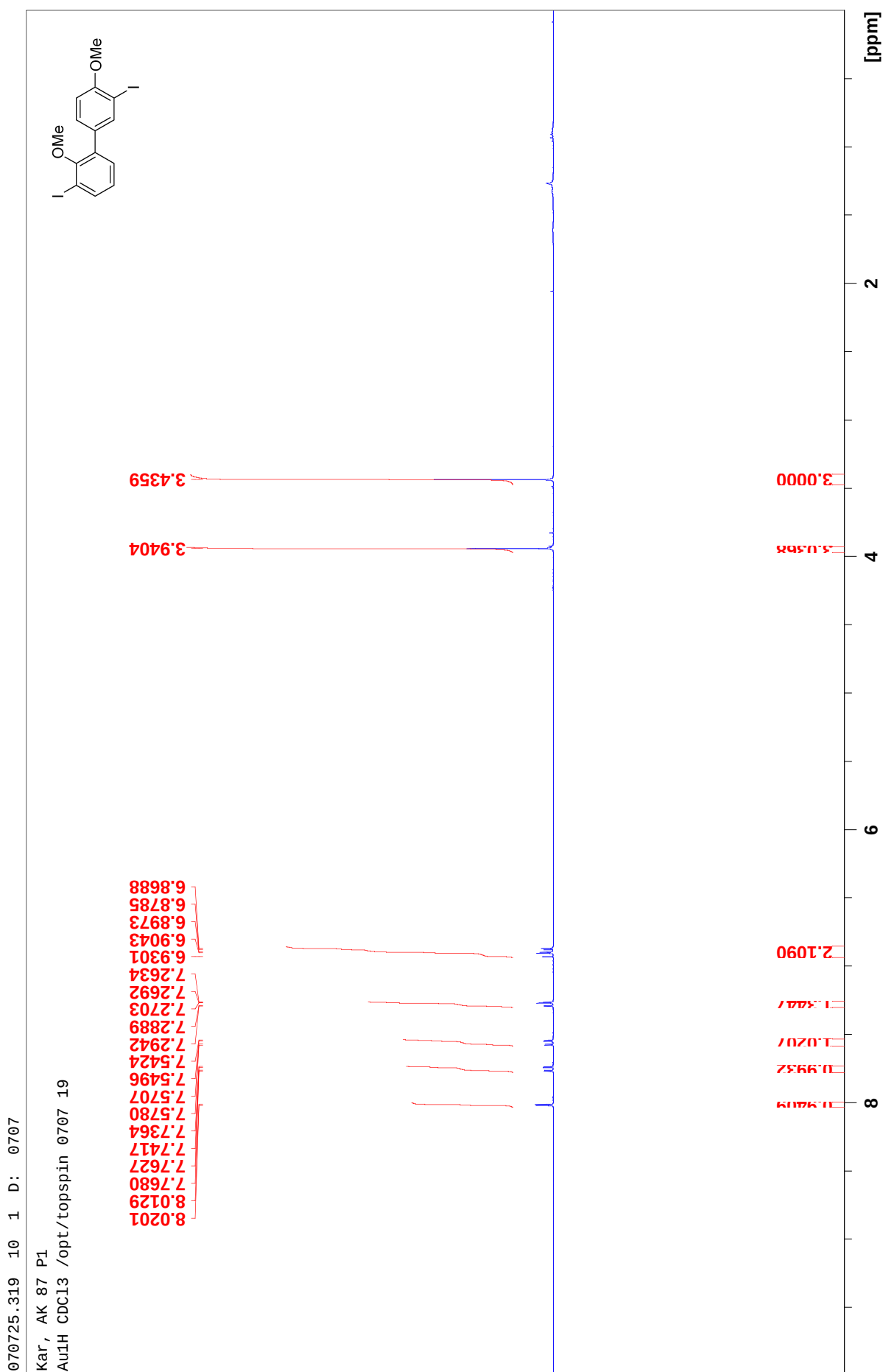
— 56.4709

[ppm]

50

100

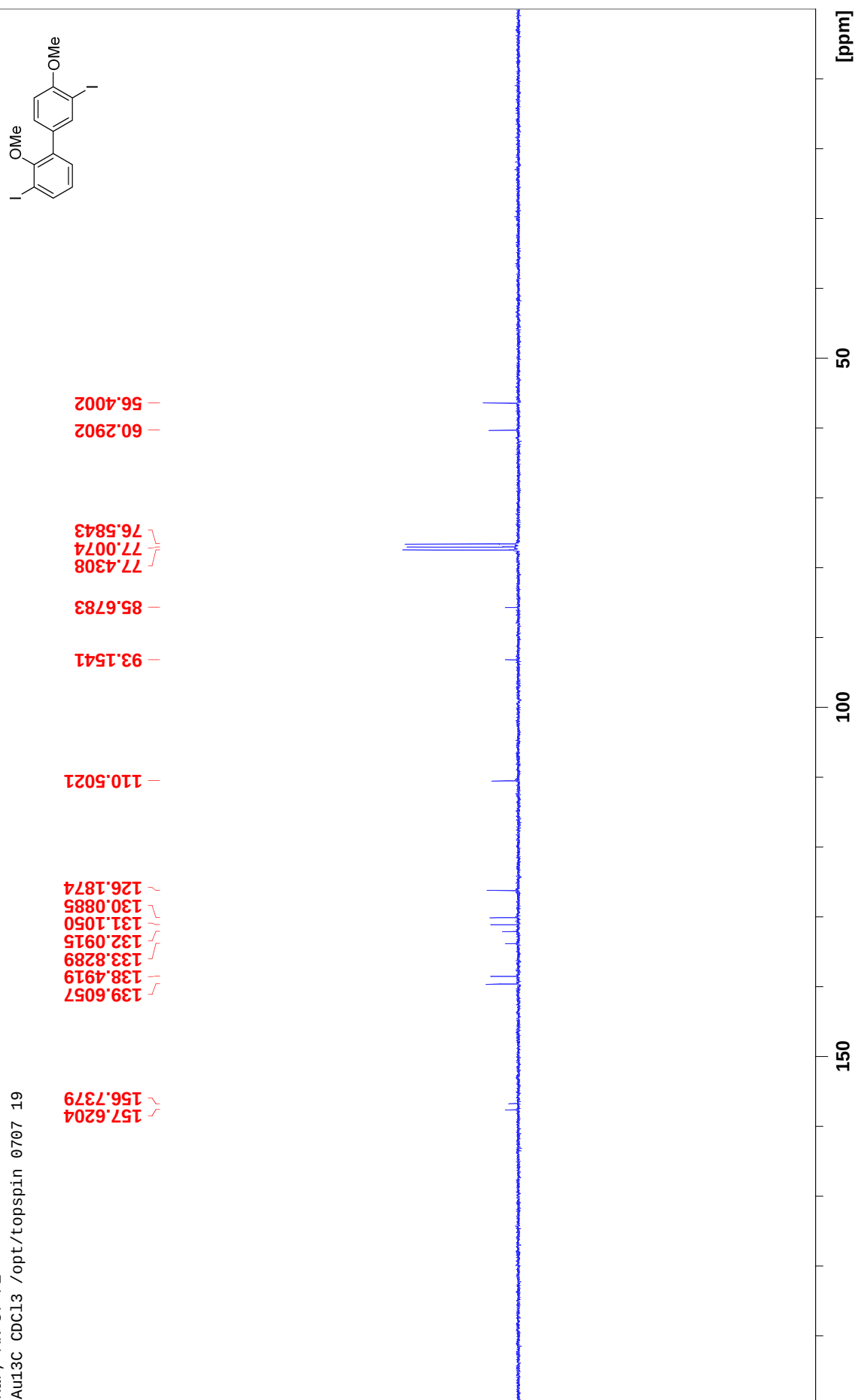
150

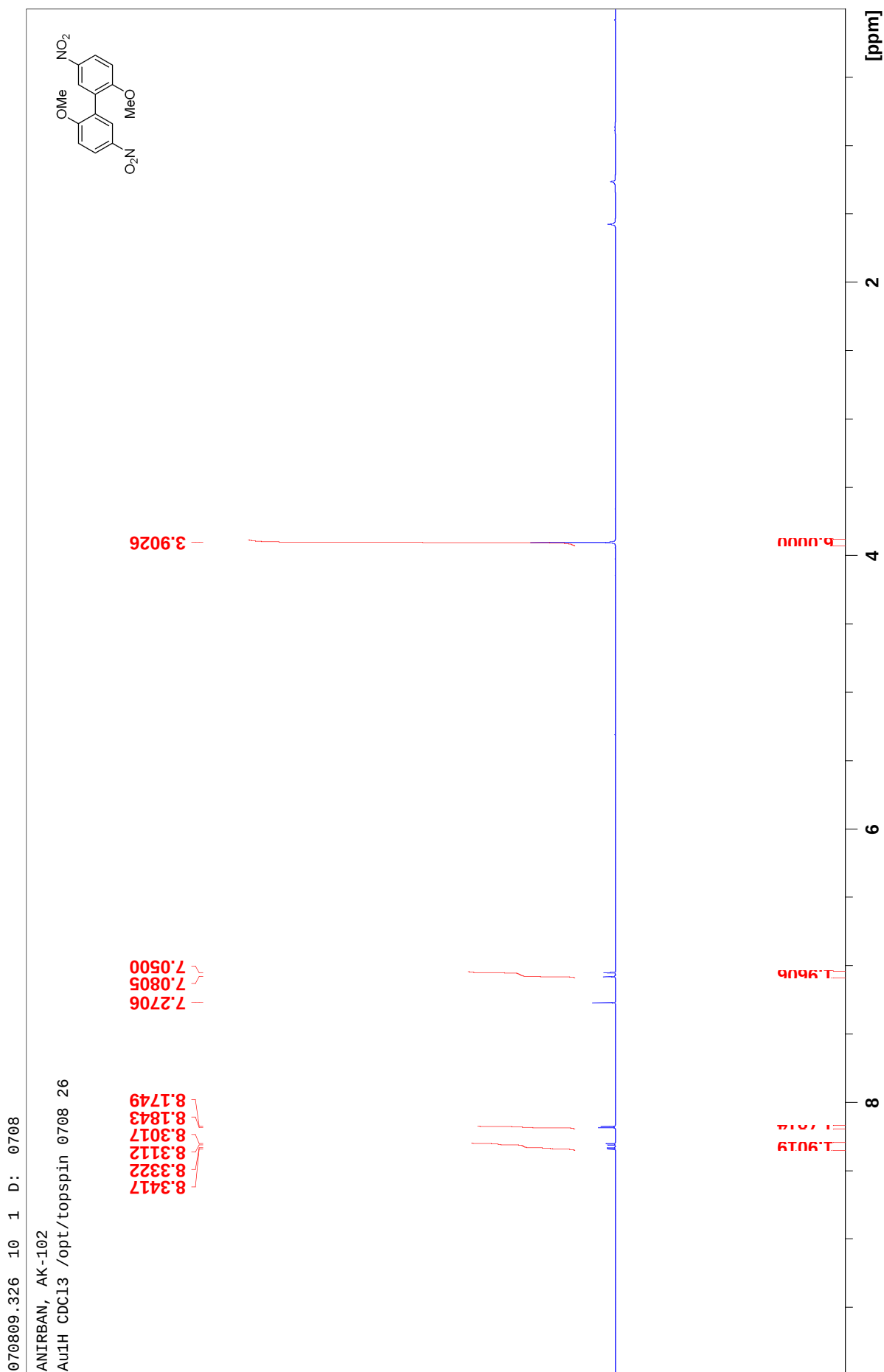


070725.319 11 1 D: 0707

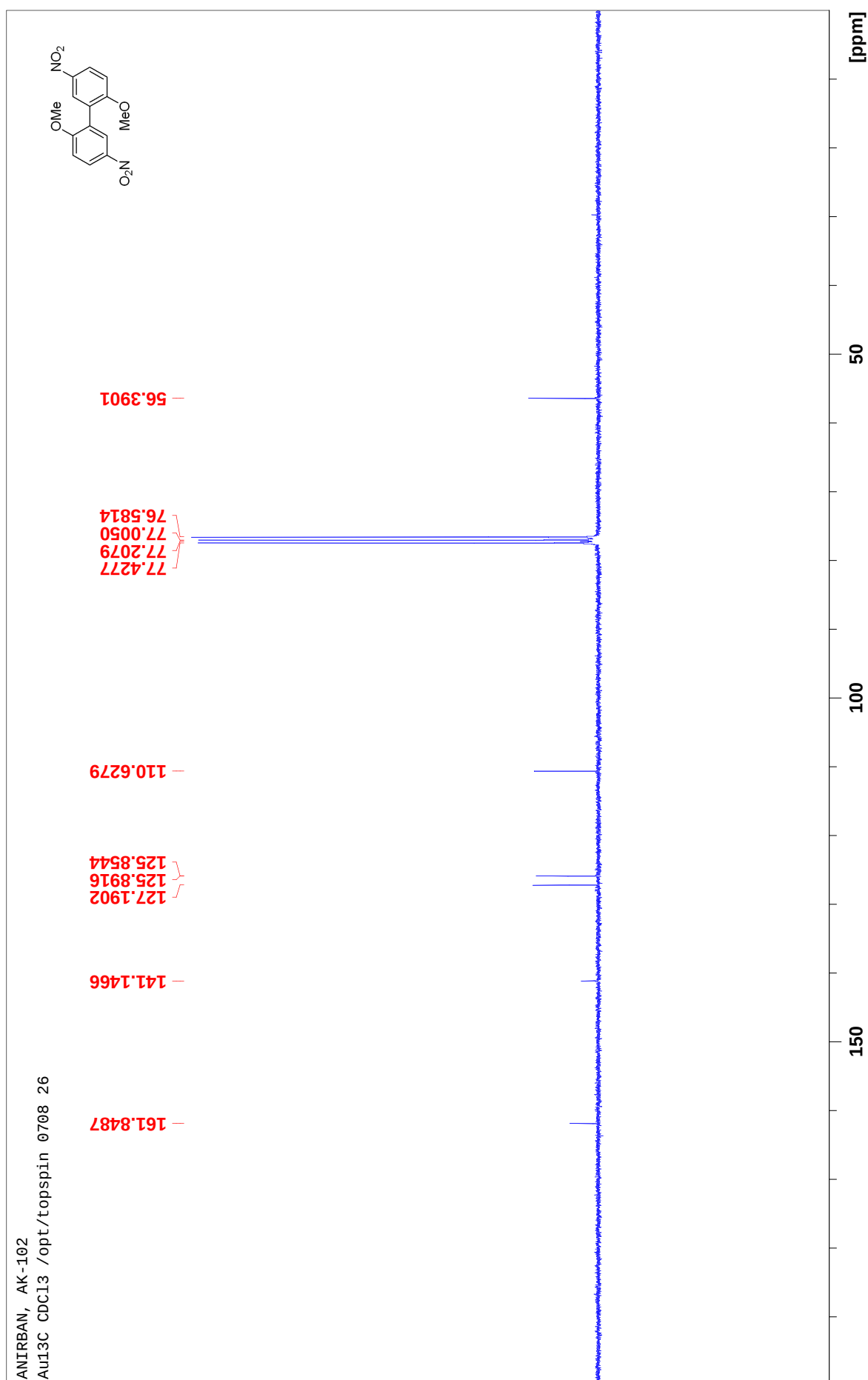
Kar, AK 87 P1

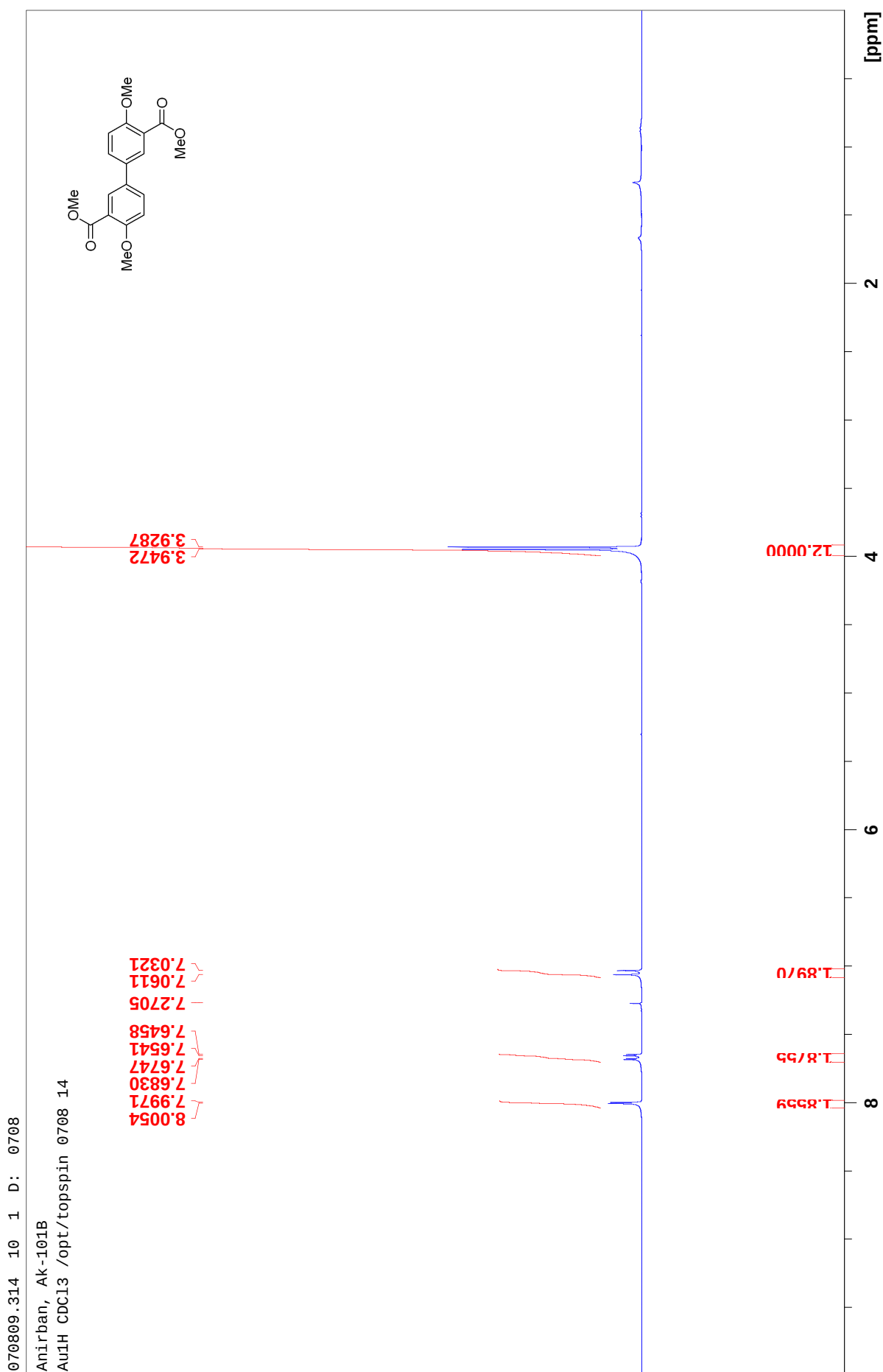
Au13C CDC13 /opt/topspin 0707 19





070809.326 11 1 D: 0708
ANIRBAN, AK-102
Au13C CDC13 /opt/topspin 0708 26

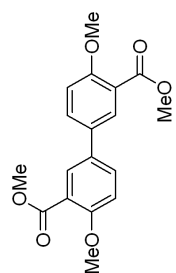




070809.314 11 1 D: 0708

Anirban, Ak-101B

Au13C CDC13 /opt/topspin 0708 14



— 166.6033
— 158.3725

— 131.8606
— 131.4831
— 129.7915

— 120.2916
— 112.4905

— 77.4296
— 77.0057
— 76.5820

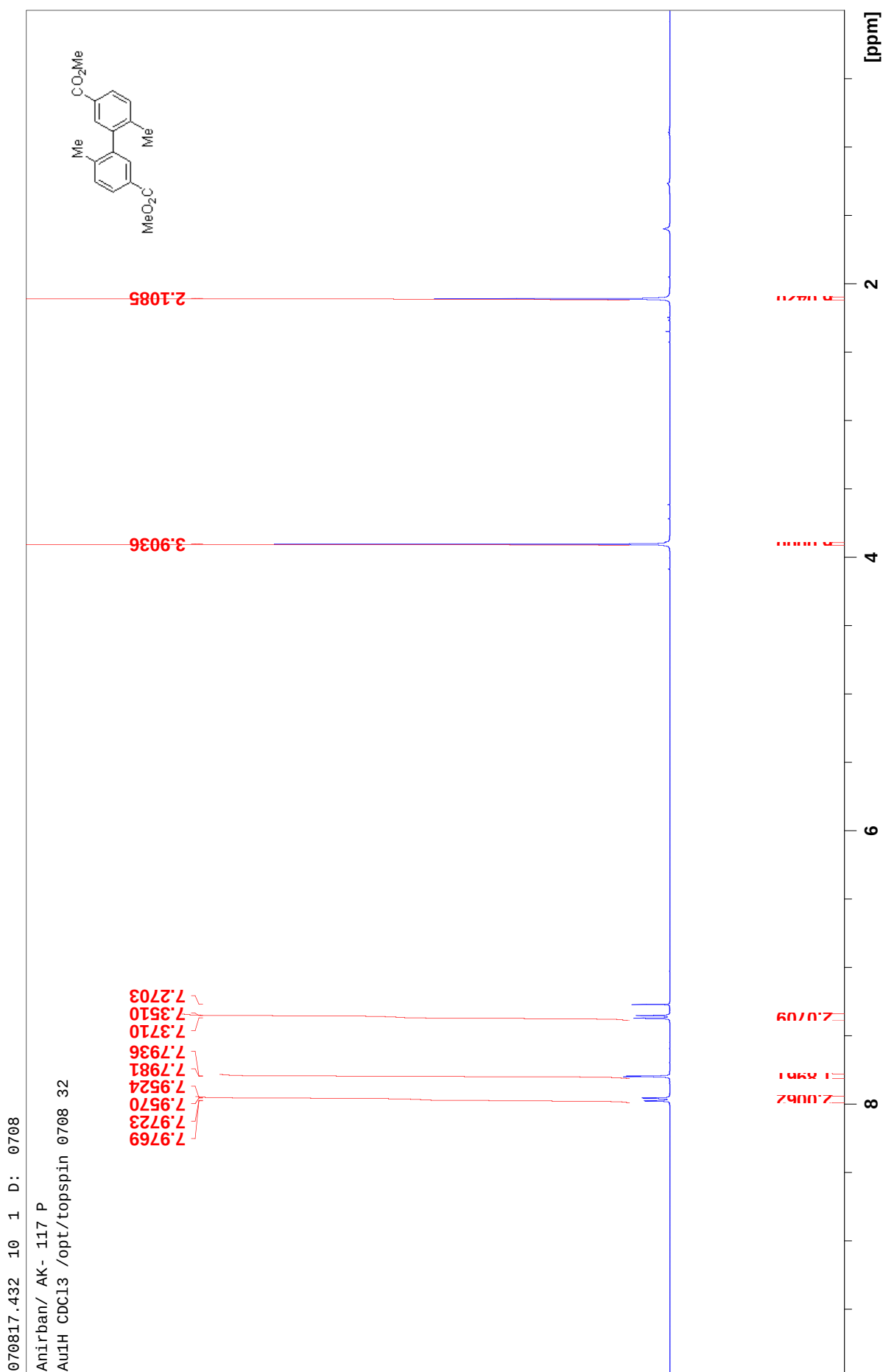
— 56.1709
— 52.1283

[ppm]

50

100

150



070817.432 11 1 D: 0708

Anirban/ AK- 117 P

Au13C CDC13 /opt/topspin 0708 32

167.0163

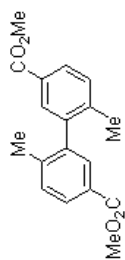
141.4870
140.6512

130.4226
130.1425
128.7809
127.8371

77.3221
77.0046
76.6872

52.0149

20.0374

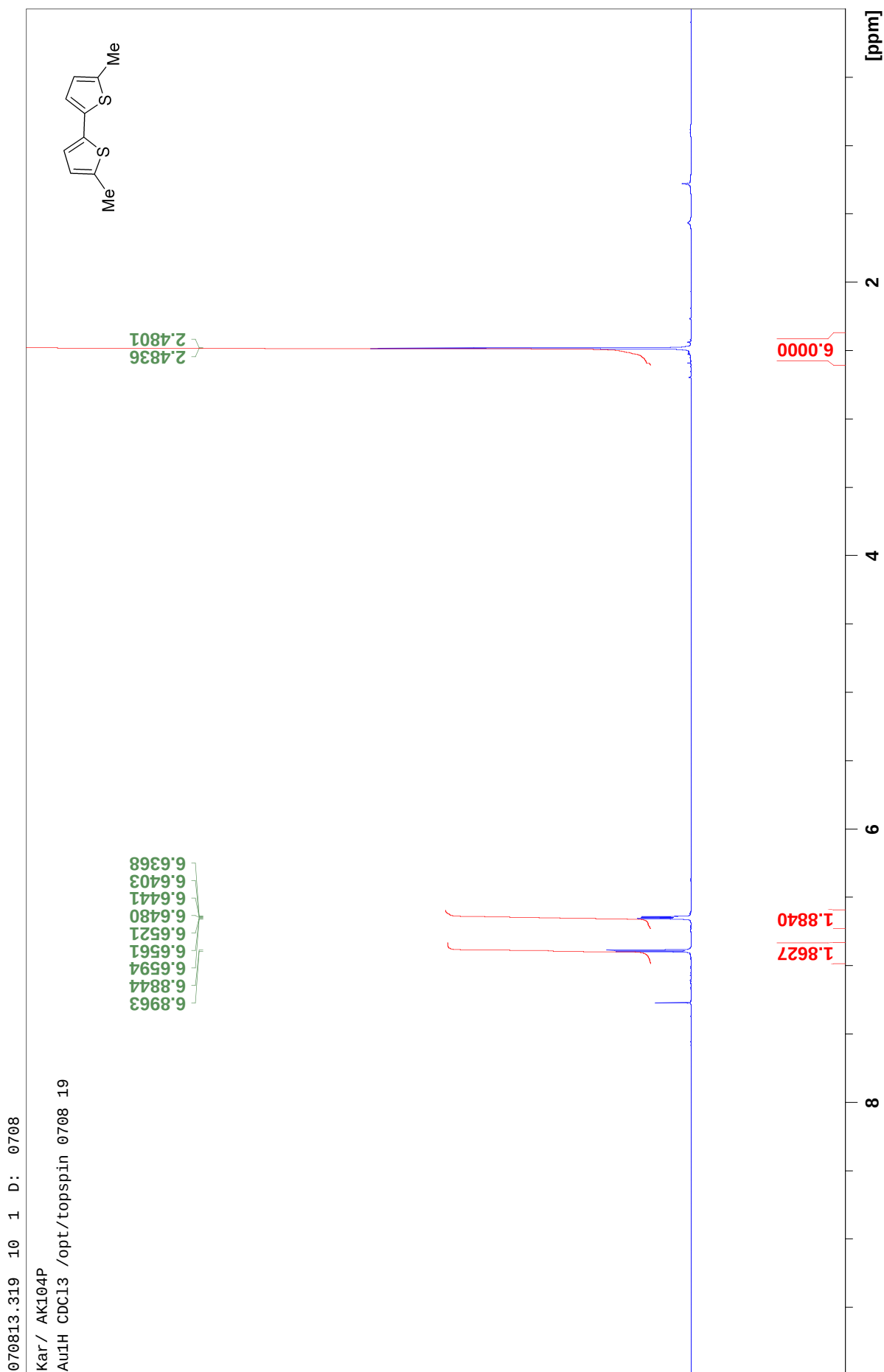


[ppm]

50

100

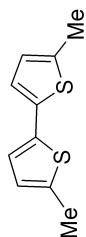
150



070813.319 11 1 D: 0708

Kar / AK104P

Au13C CDC13 /opt/topspin 0708 19



138.4514
135.4895
125.7242
122.8385
77.4240
76.9989
76.5737
15.2967

[ppm]

150
100
50