Rh_2(II)-Catalyzed Nitro Migration Reactions: Selective Synthesis of 3-Nitroindoles from β-Nitro Stryryl Azides

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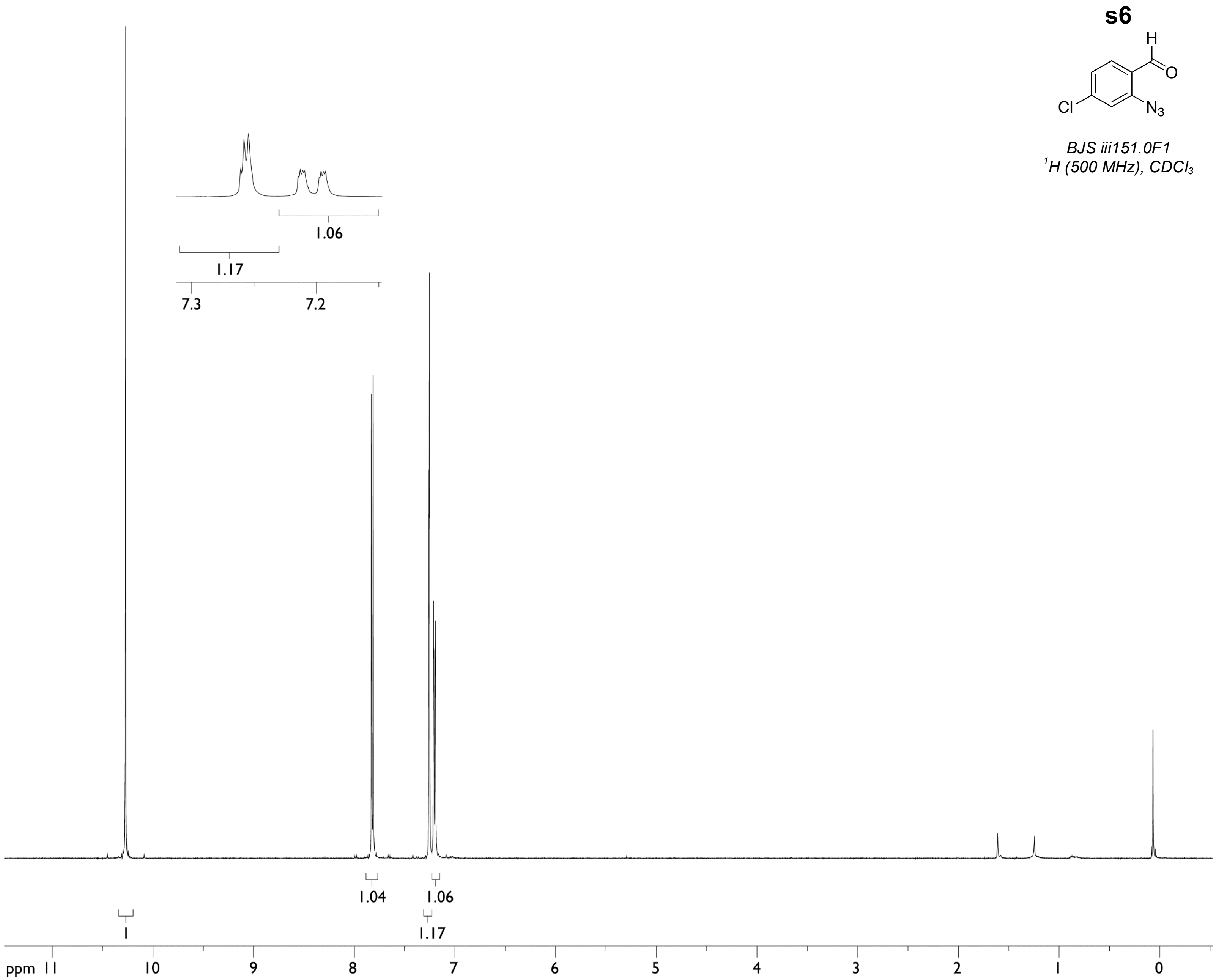
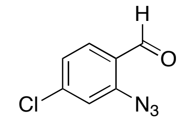
Supporting Information 2

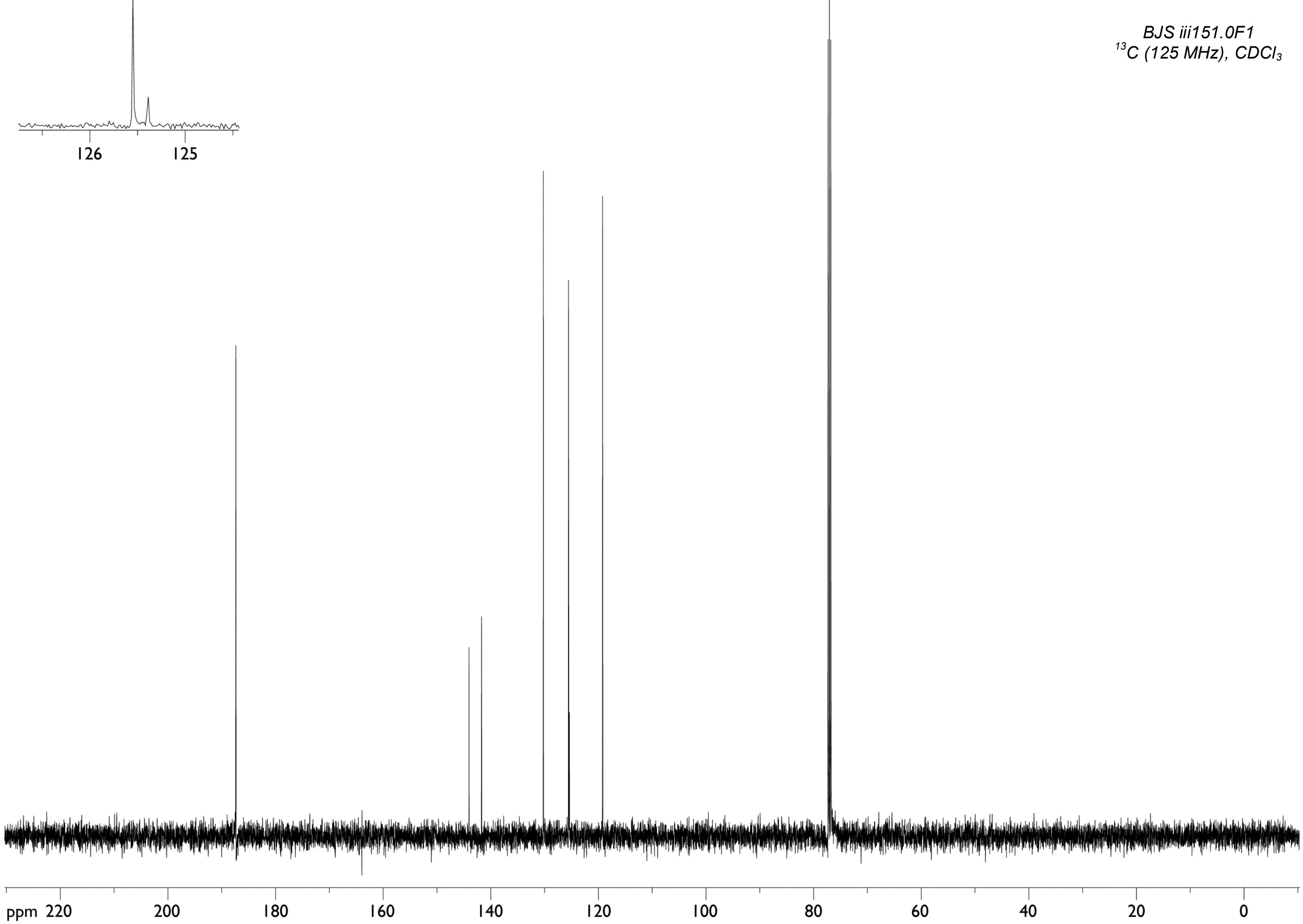
Contents


s6
H
O
Cl
N_3
BJS iii151.0F1
^1H (500 MHz), $CDCl_3$
1.06
1.17
7.3
7.2
1.04
1.06
1
1.17
ppm 11 10 9 8 7 6 5 4 3 2 1 0

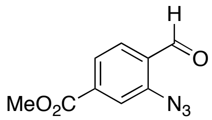
s6



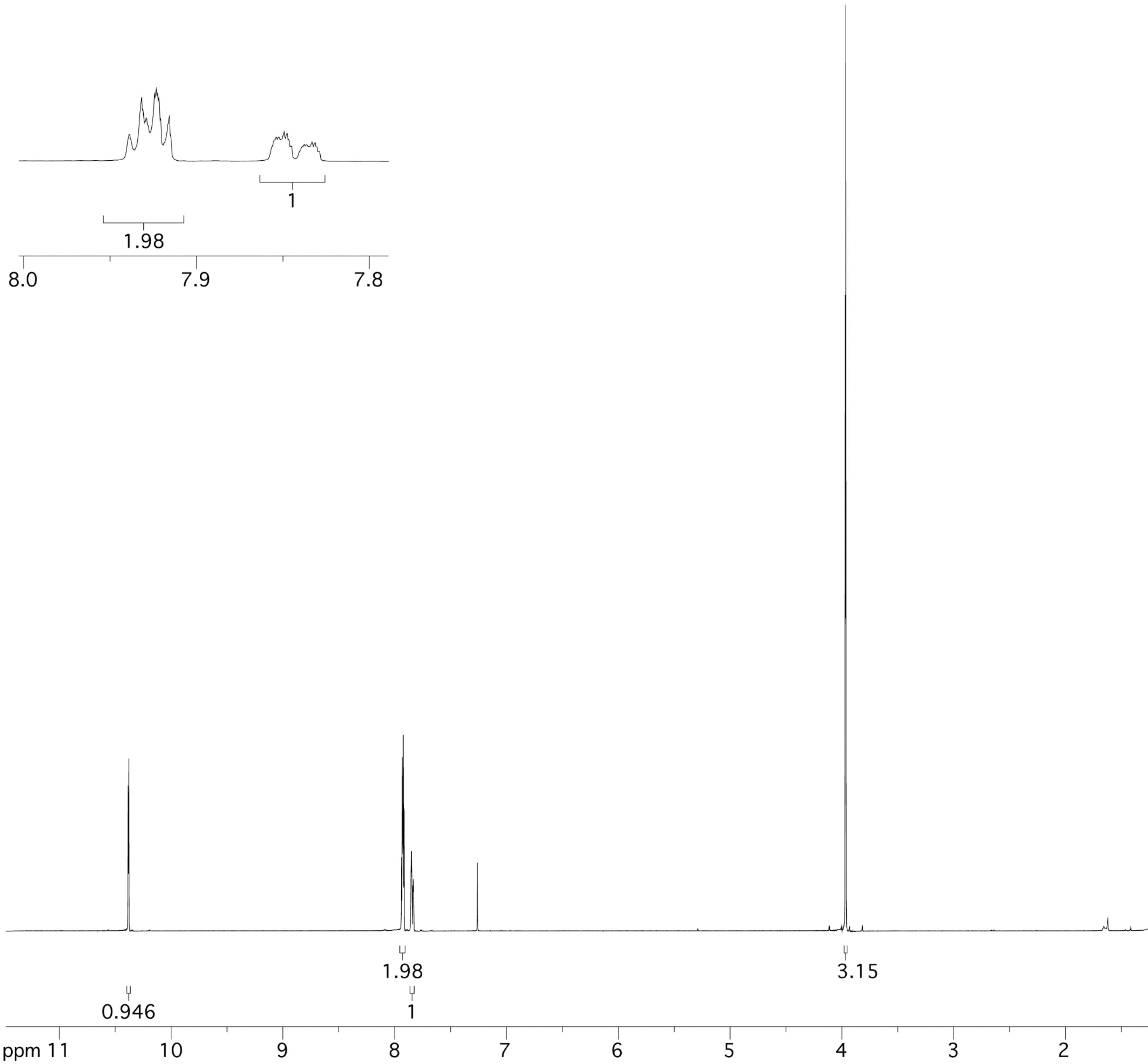
BJS iii151.0F1
^{13}C (125 MHz), $CDCl_3$



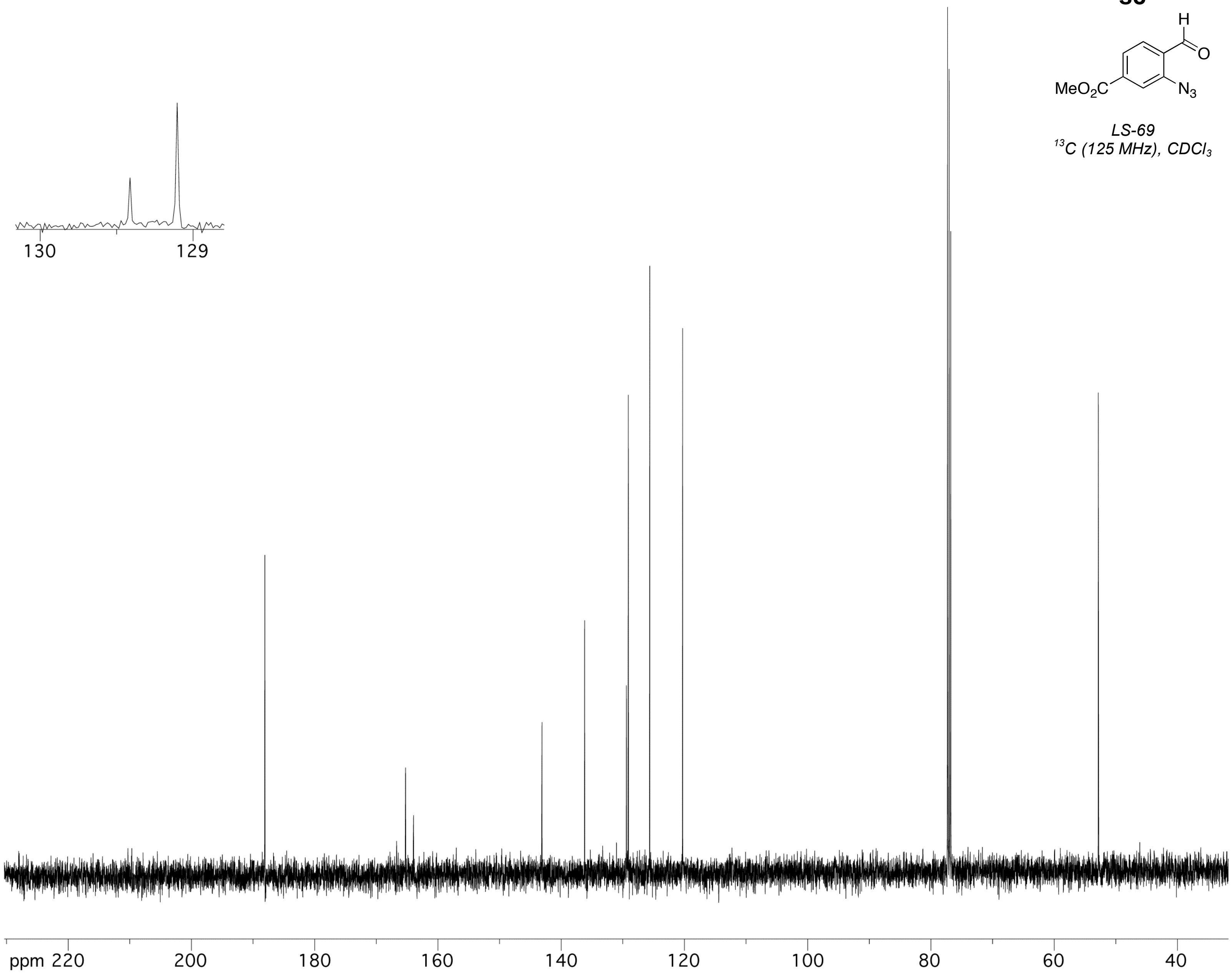
s8



LS-69
[1]H (500 MHz), CDCl3

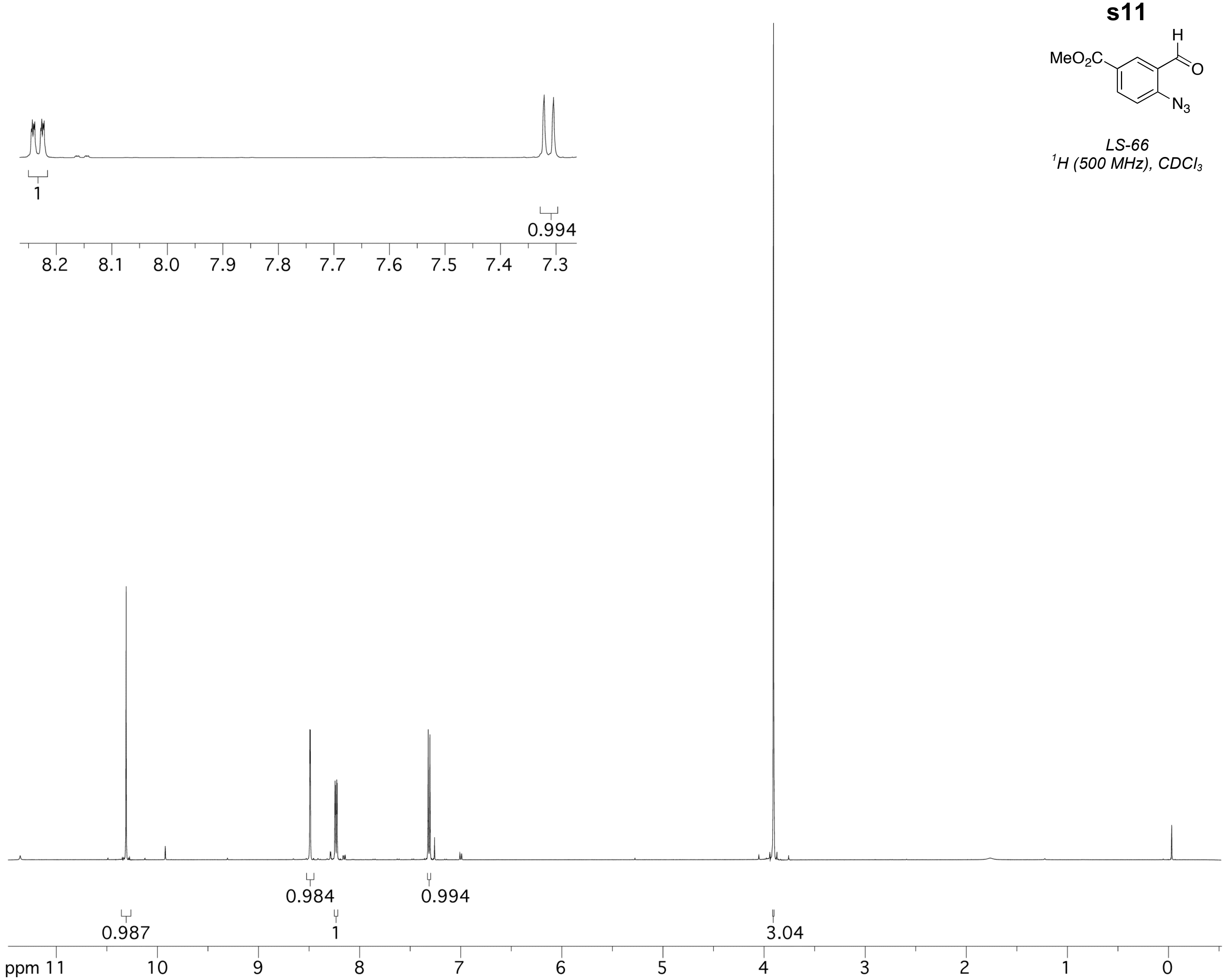


s8

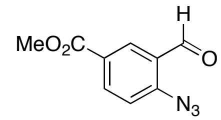


LS-69
^{13}C (125 MHz), CDCl$_3$

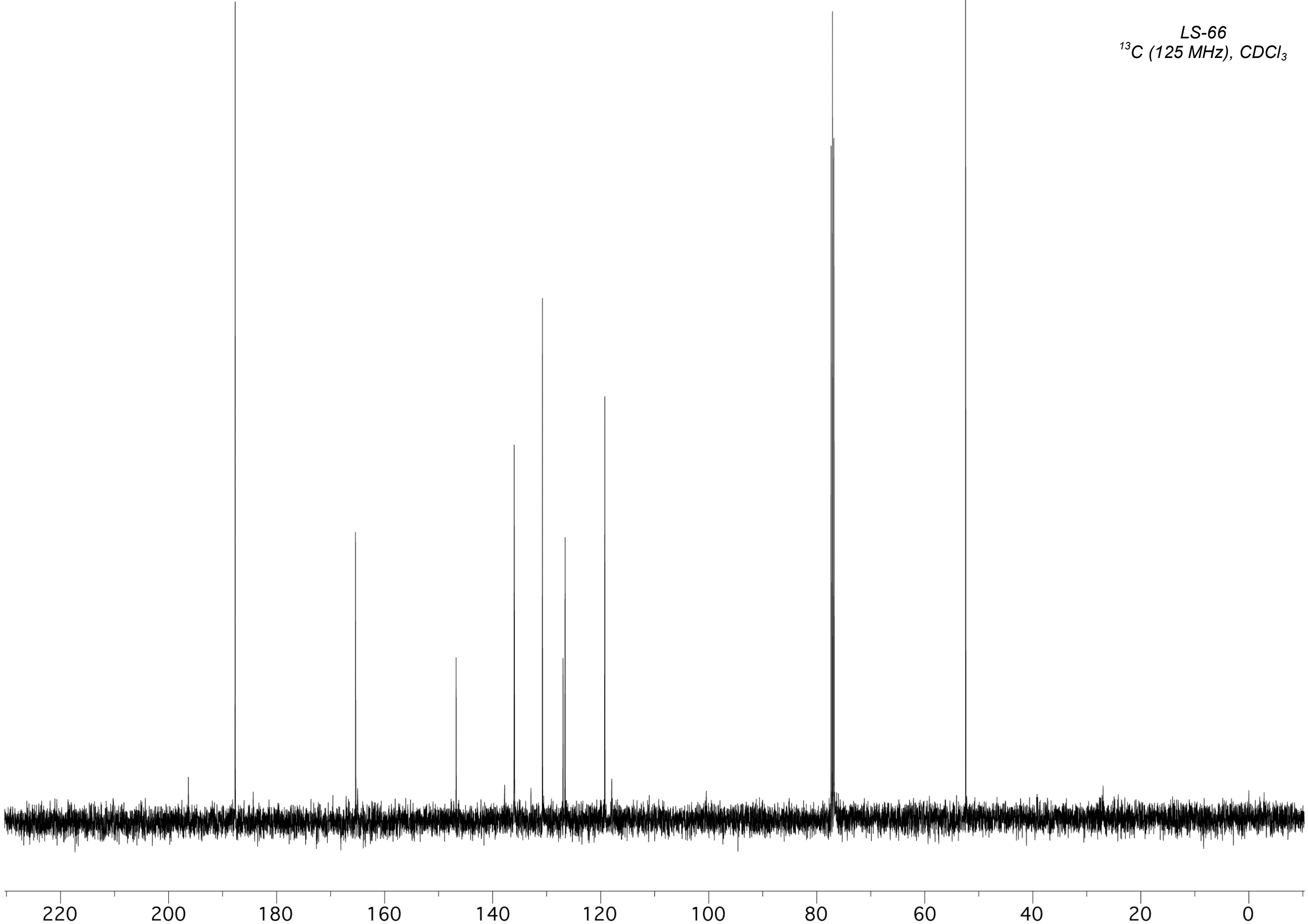
s11


MeO2C
H
O
N3
LS-66
1H (500 MHz), CDCl3
1
0.994
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
0.984
0.994
0.987
1
3.04
ppm 11
10
9
8
7
6
5
4
3
2
1
0

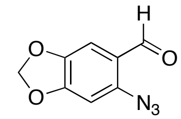
s11



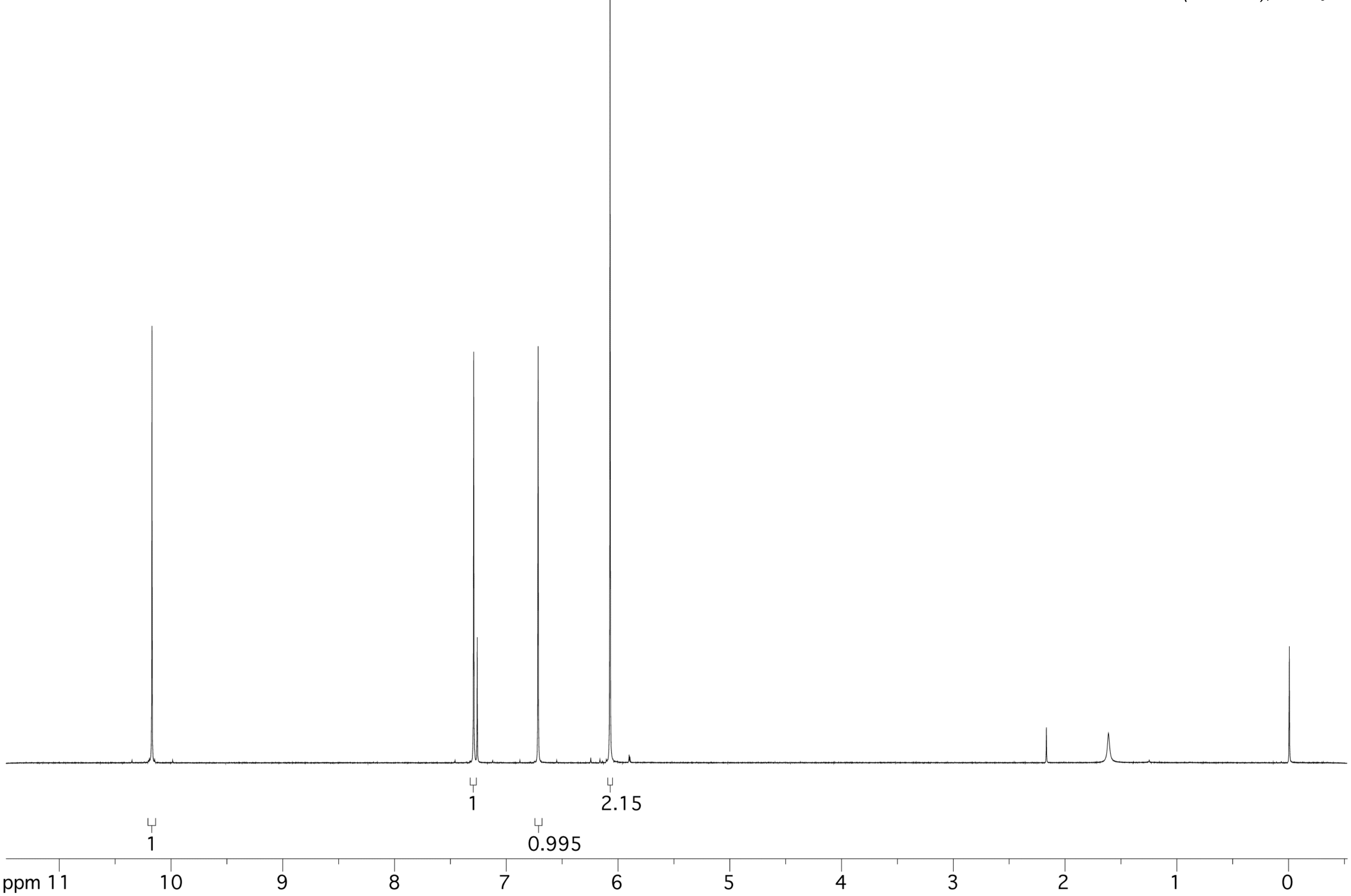
LS-66
^{13}C (125 MHz), CDCl$_3$



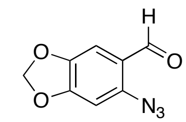
s12



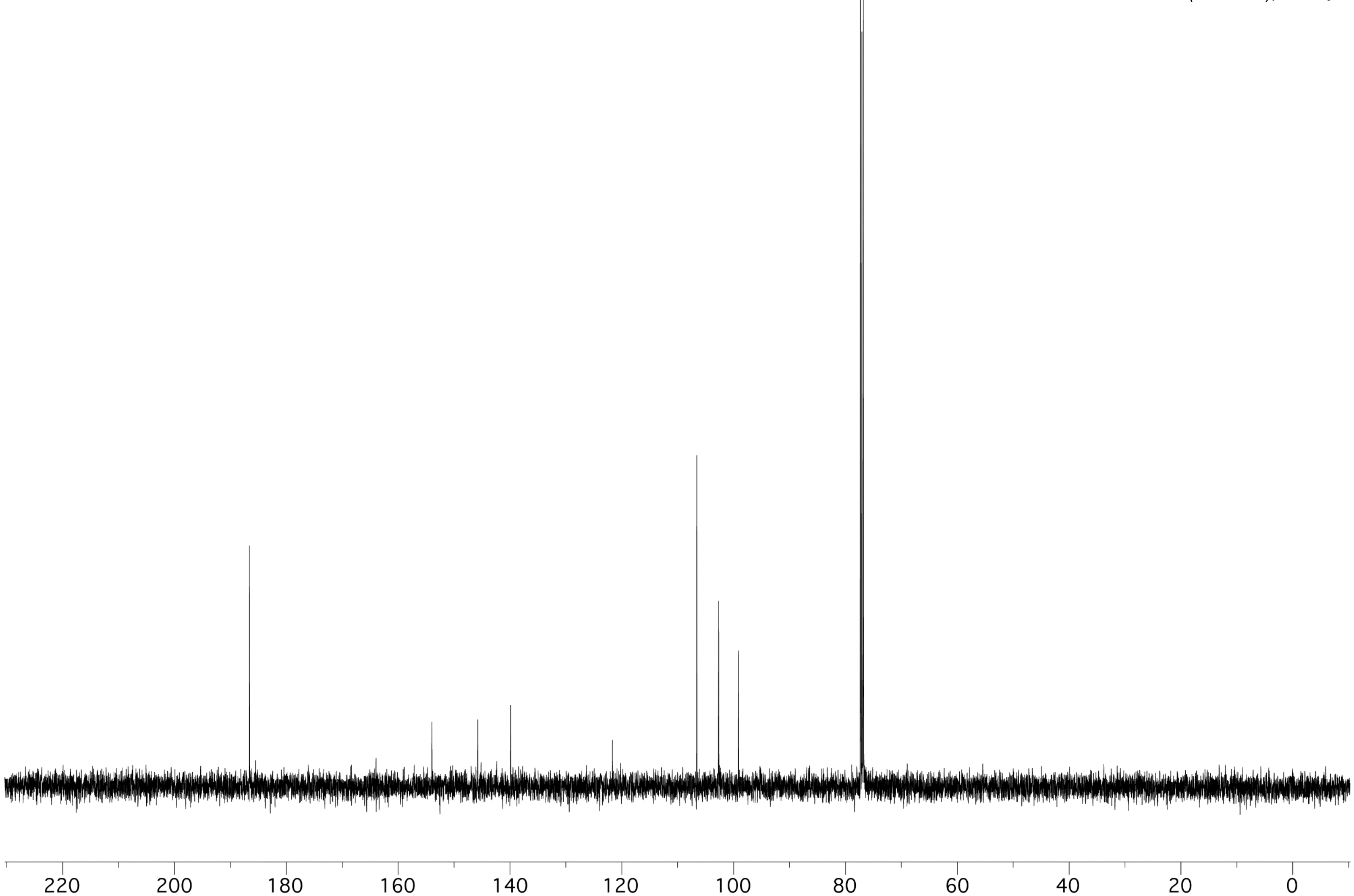
LS-62
^{1}H (500 MHz), $CDCl_3$



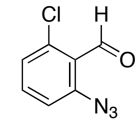
s12



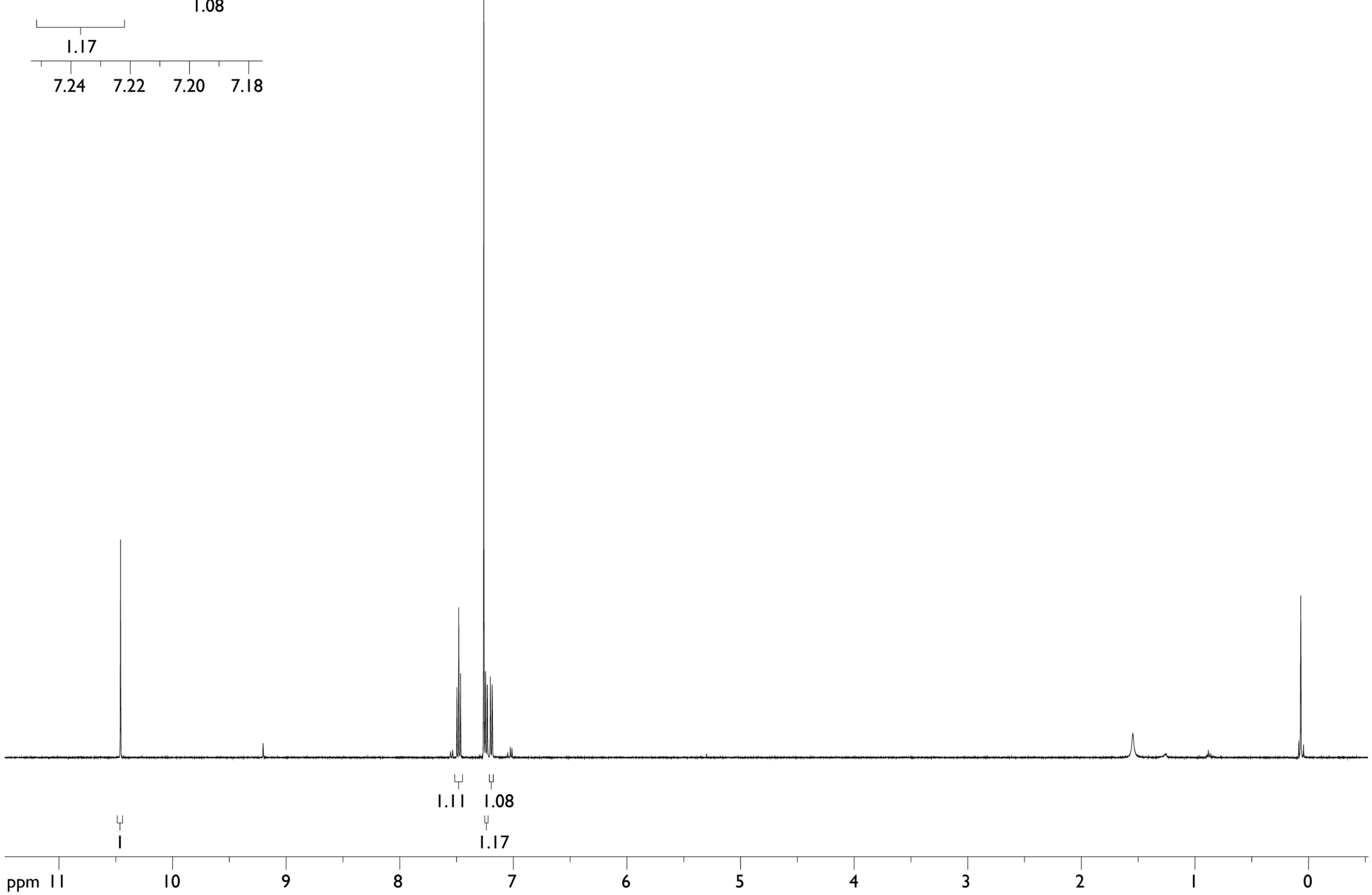
LS-62
^{13}C (125 MHz), CDCl$_3$



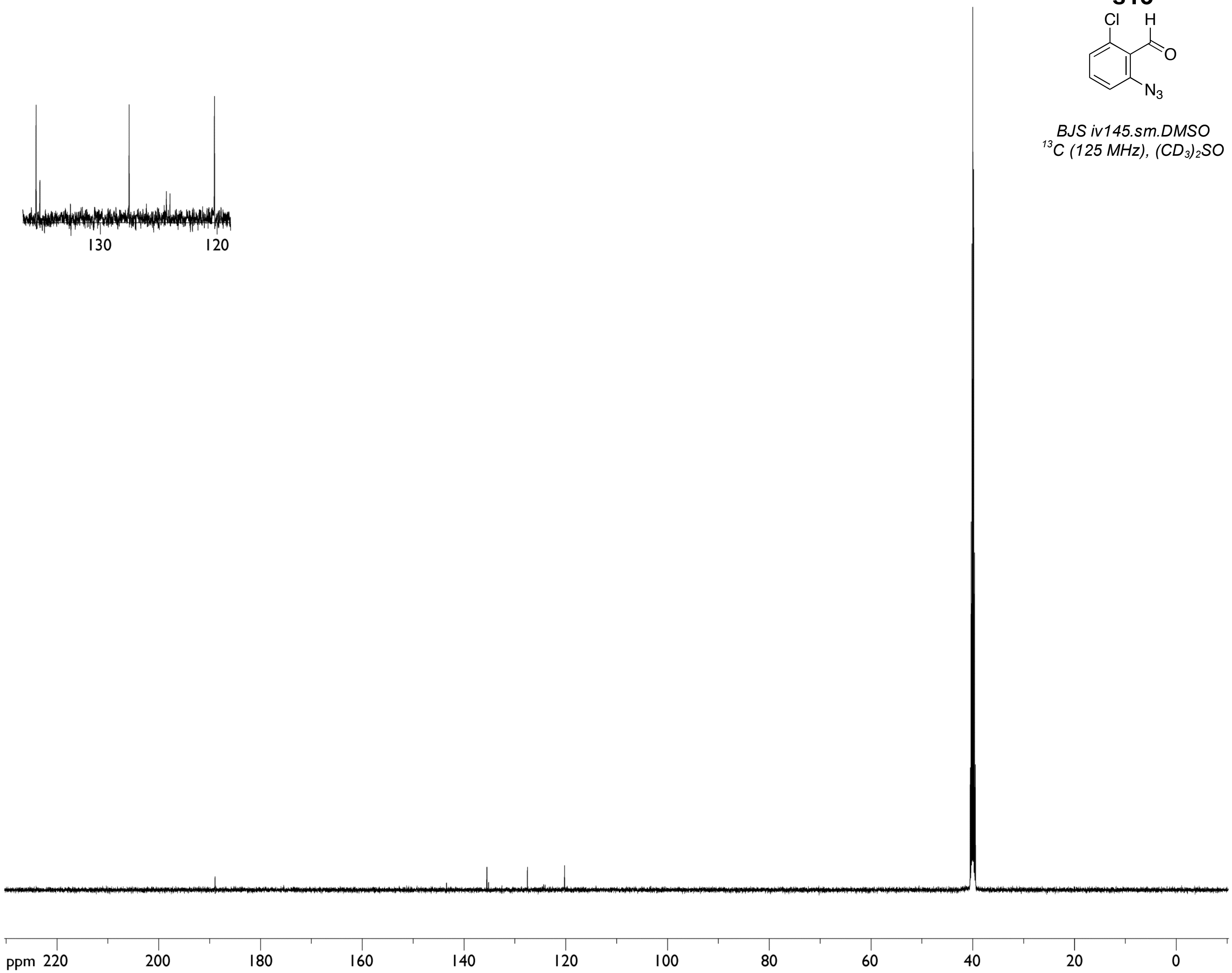
s13



BJS iv145.sm
^{1}H (500 MHz), CDCl$_3$

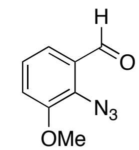


s13

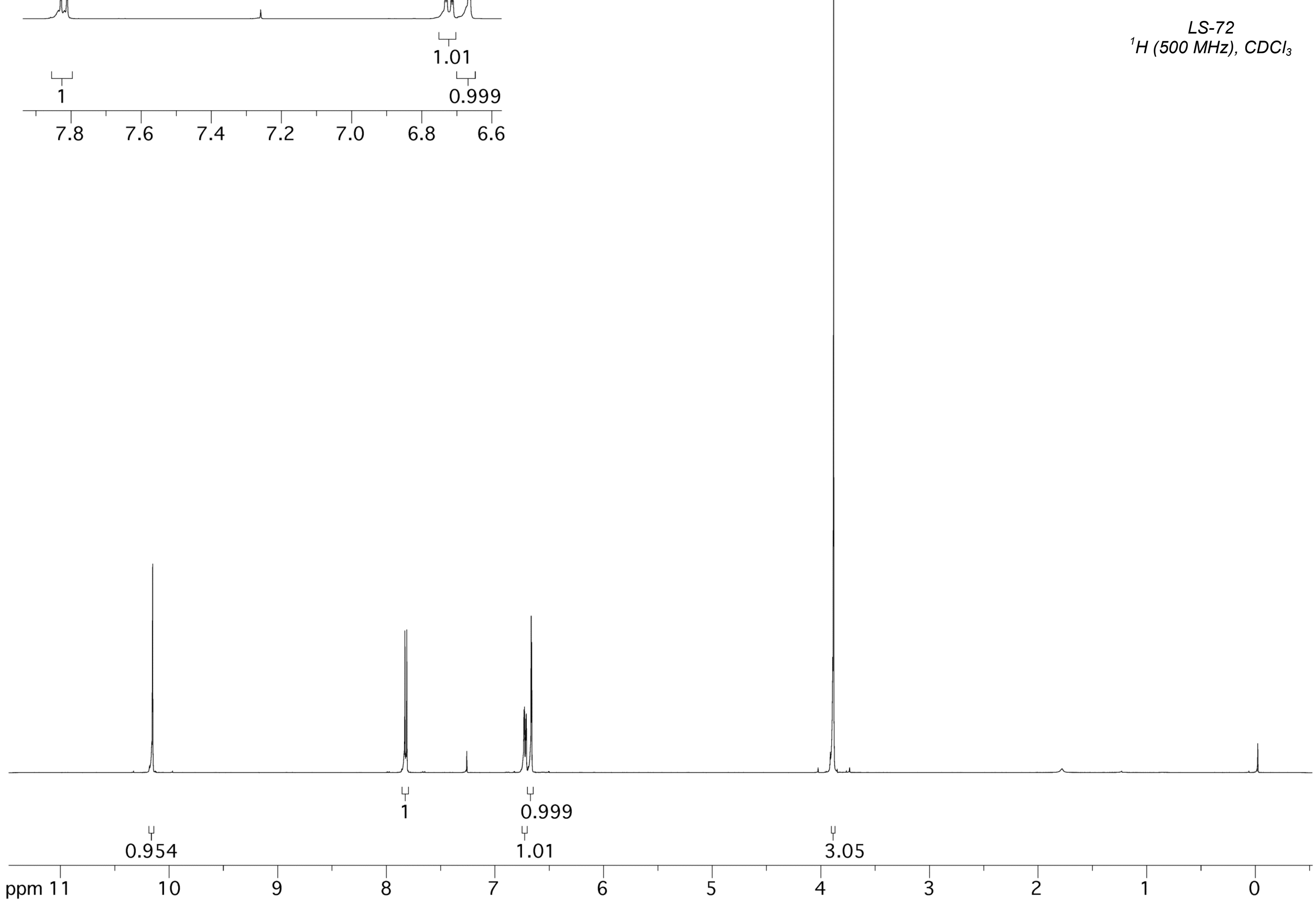


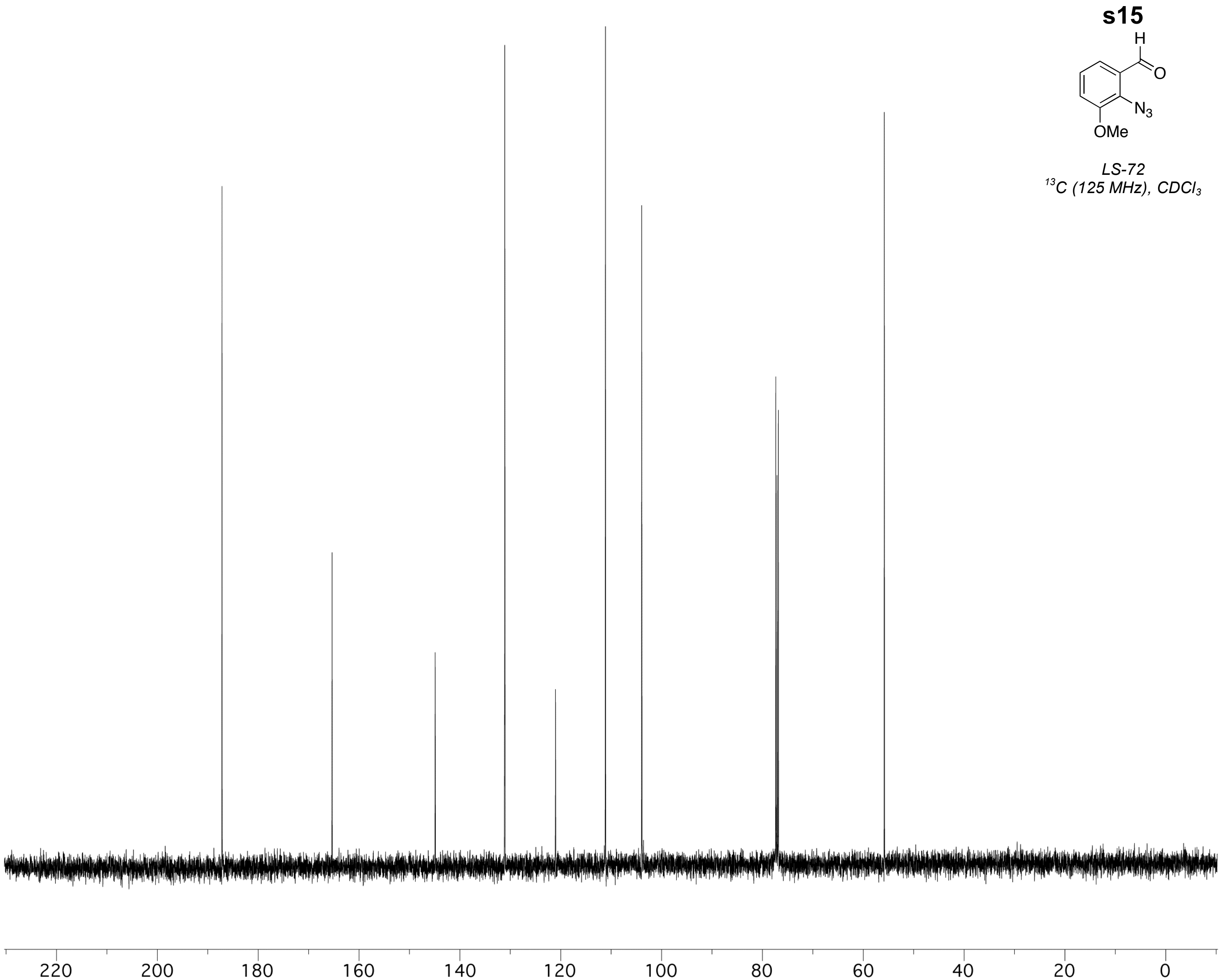
BJS iv145.sm.DMSO
^{13}C (125 MHz), $(CD_3)_2SO$

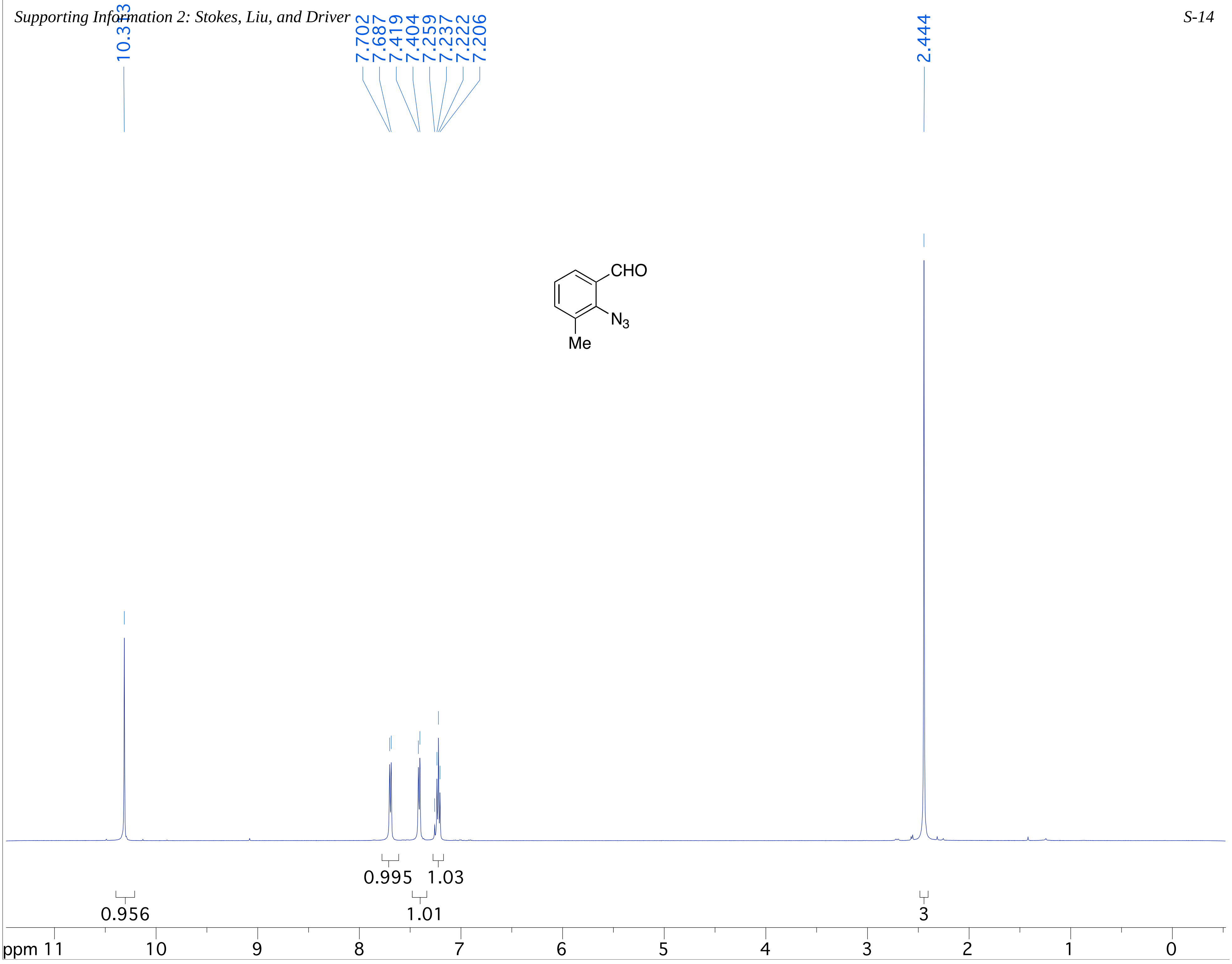
s15

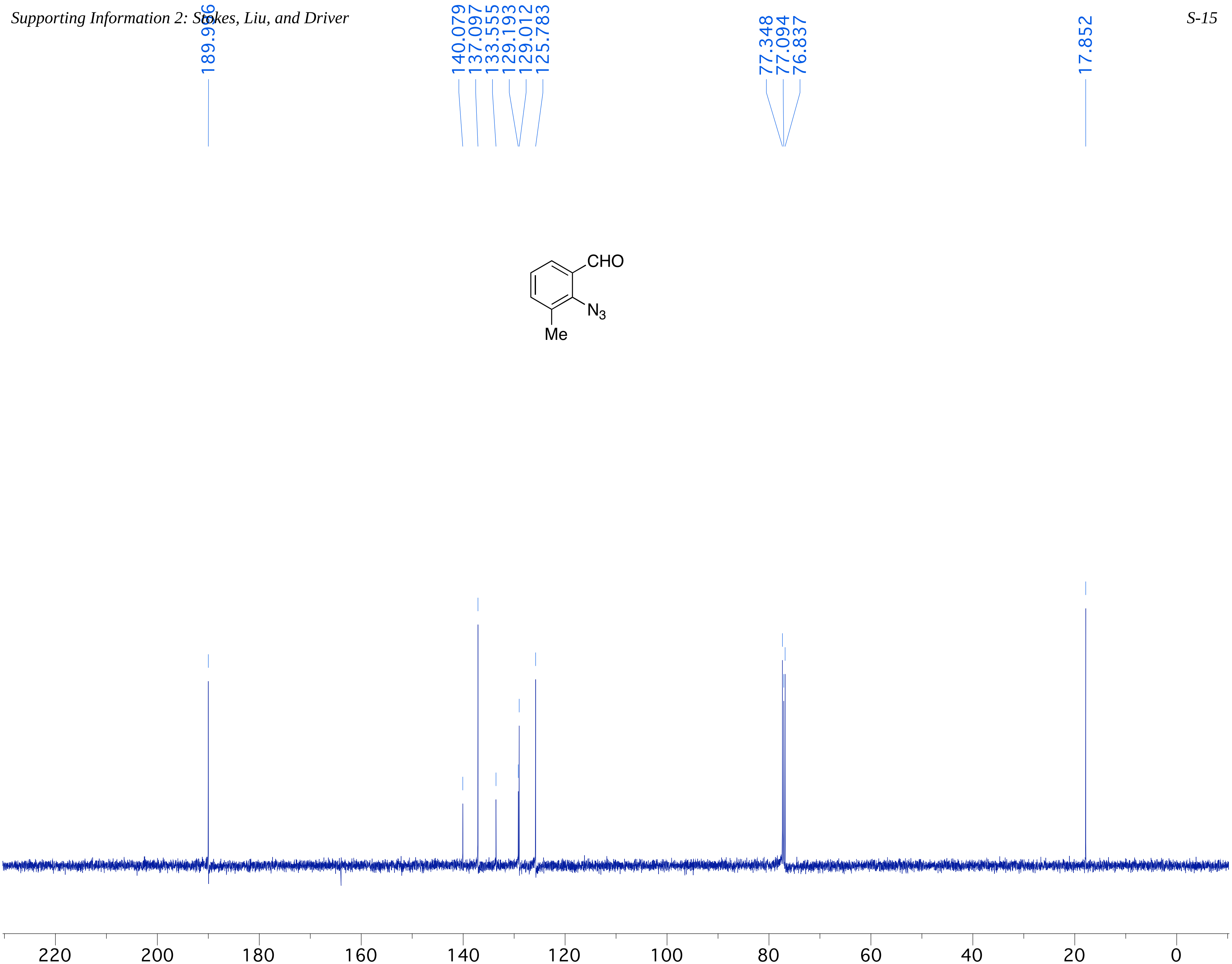


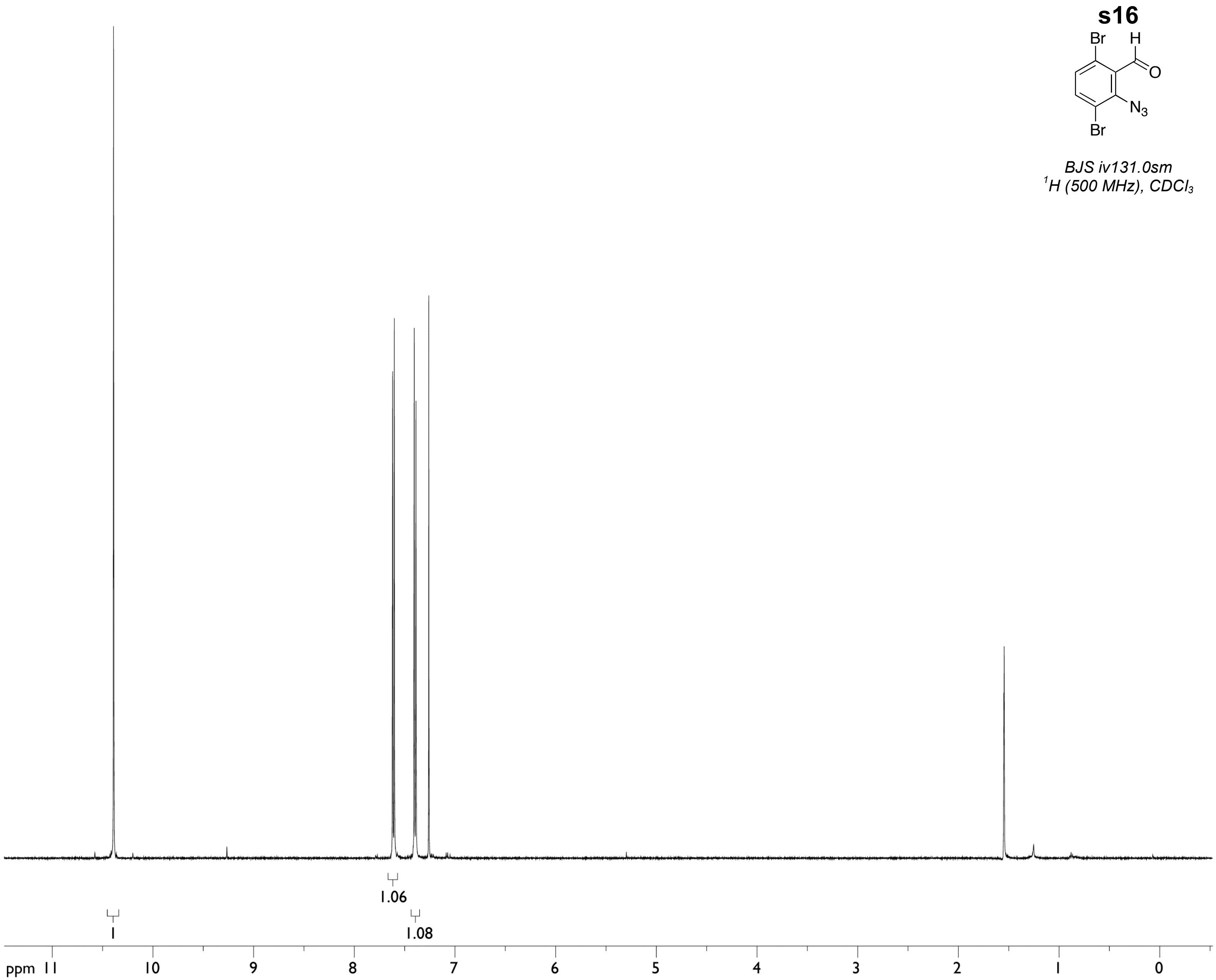
LS-72
^1H (500 MHz), $CDCl_3$




s15
H
O
N_3
OMe
LS-72
^{13}C (125 MHz), $CDCl_3$
220
200
180
160
140
120
100
80
60
40
20
0

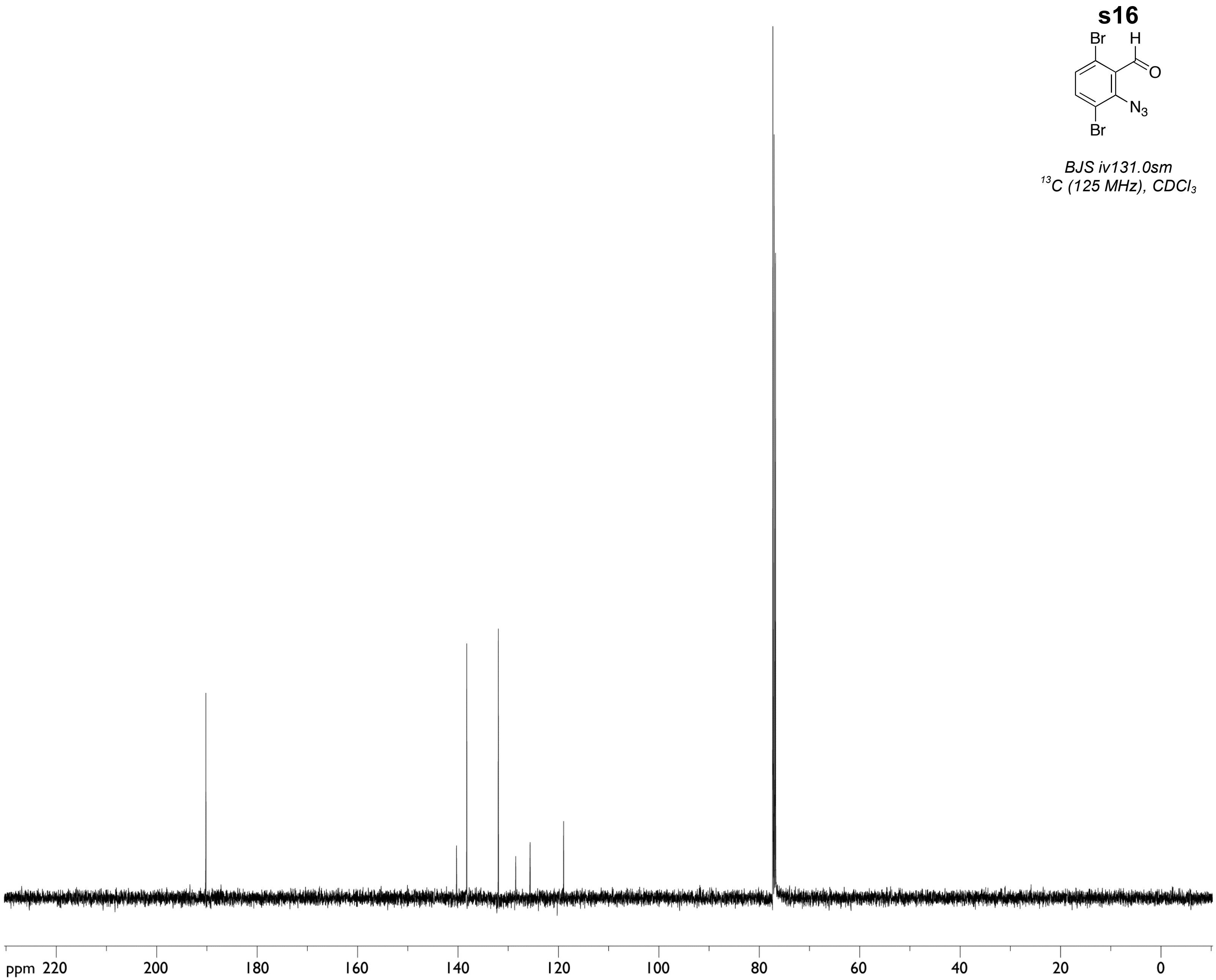

10.313
7.702
7.687
7.419
7.404
7.259
7.237
7.222
7.206
2.444
CHO
N3
Me
0.995
1.03
0.956
1.01
3
ppm 11
10
9
8
7
6
5
4
3
2
1
0

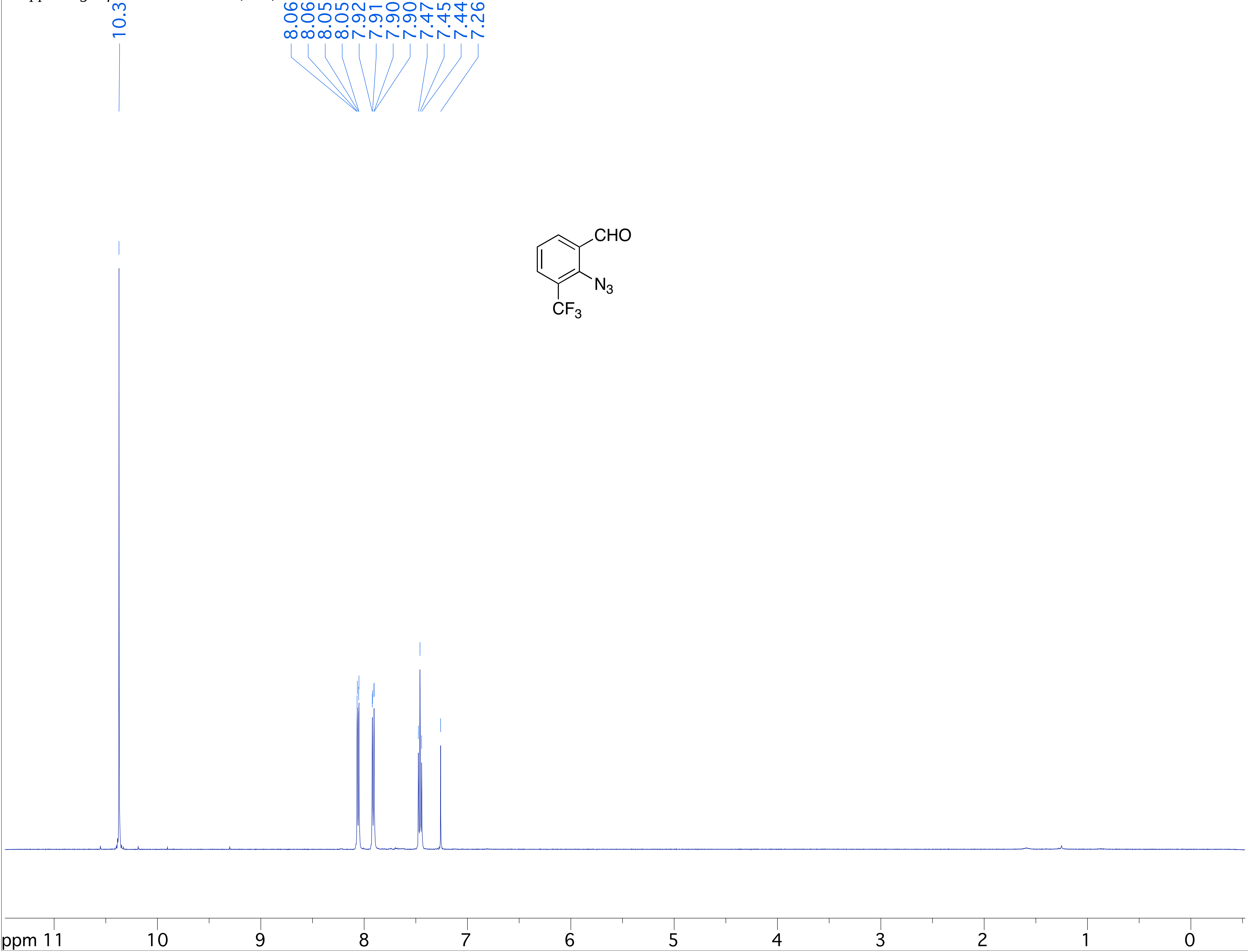

189.966
140.079
137.097
133.555
129.193
129.012
125.783
77.348
77.094
76.837
17.852
CHO
N3
Me
220
200
180
160
140
120
100
80
60
40
20
0

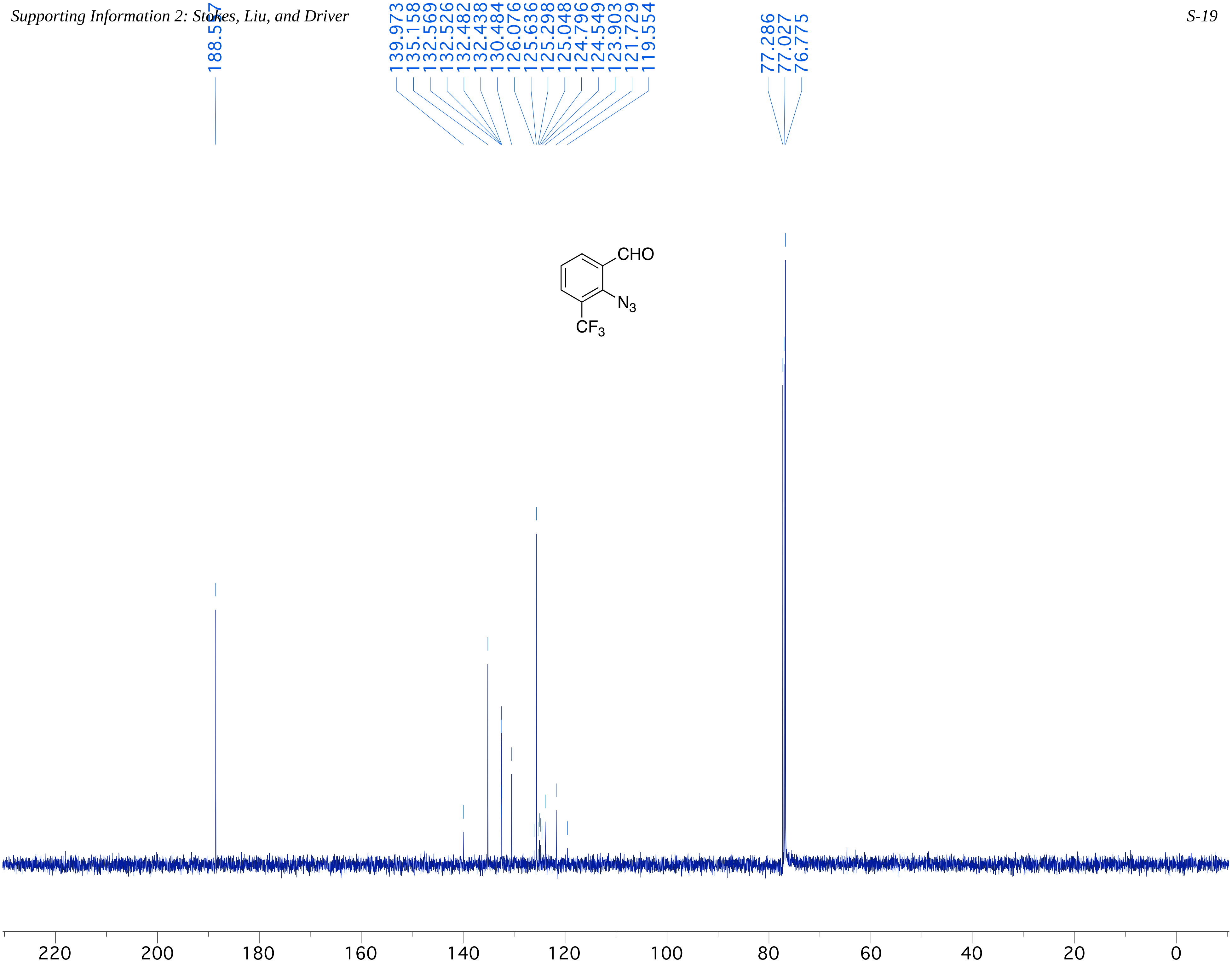

s16
Br
H
O
N3
Br
BJS iv131.0sm
1H (500 MHz), CDCl3
1.06
1
1.08
ppm 11
10
9
8
7
6
5
4
3
2
1
0

s16

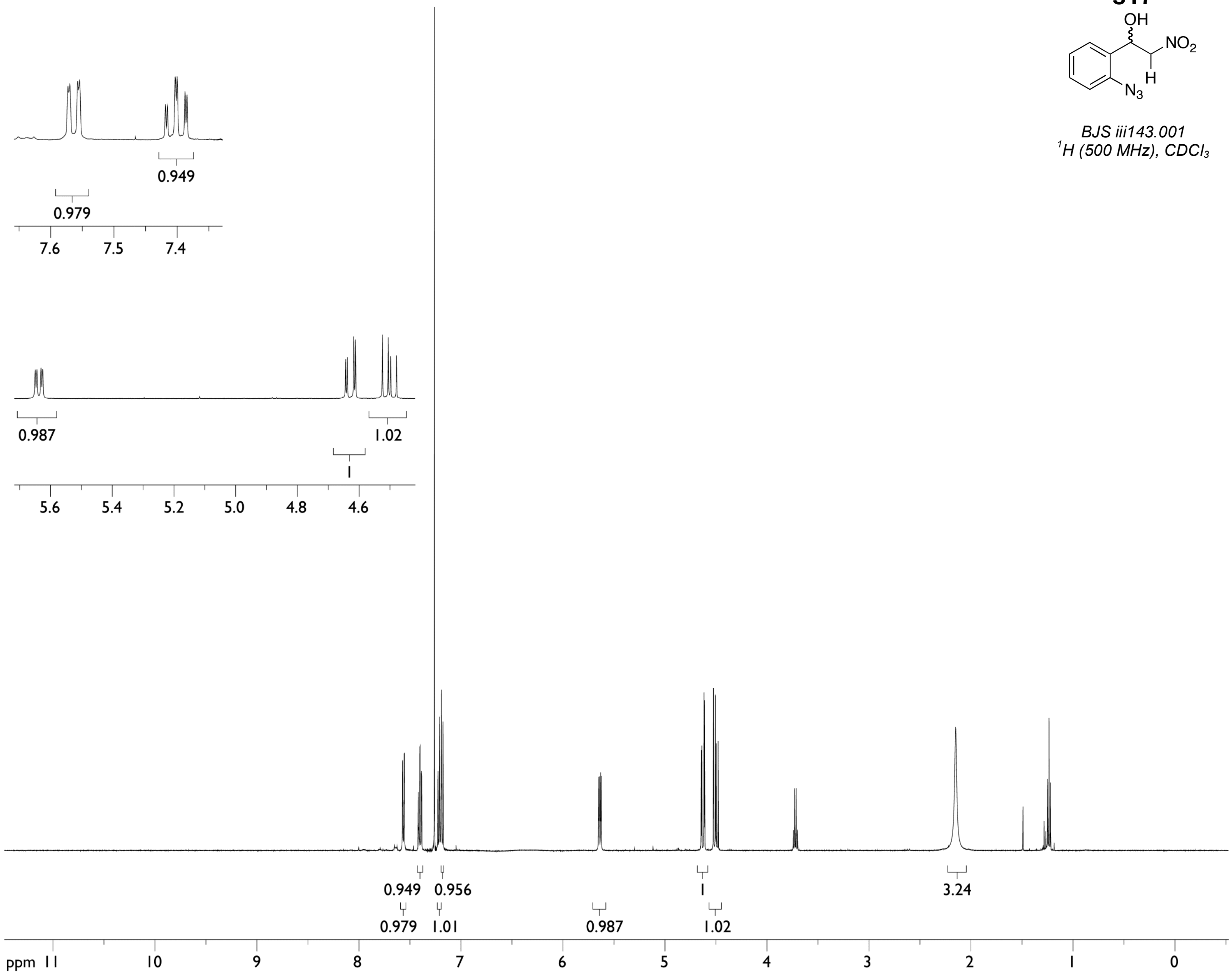
BJS iv131.0sm
^{13}C (125 MHz), $CDCl_3$



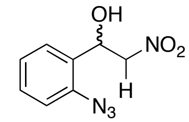

10.372
7.921
7.919
7.905
7.904
7.475
7.459
7.444
7.260
CHO
N_3
CF_3
ppm 11
10
9
8
7
6
5
4
3
2
1
0


188.557
139.973
135.158
132.569
132.526
132.482
132.438
130.484
126.076
125.636
125.298
125.048
124.796
124.549
123.903
121.729
119.554
77.286
77.027
76.775
CHO
N_3
CF_3
220 200 180 160 140 120 100 80 60 40 20 0

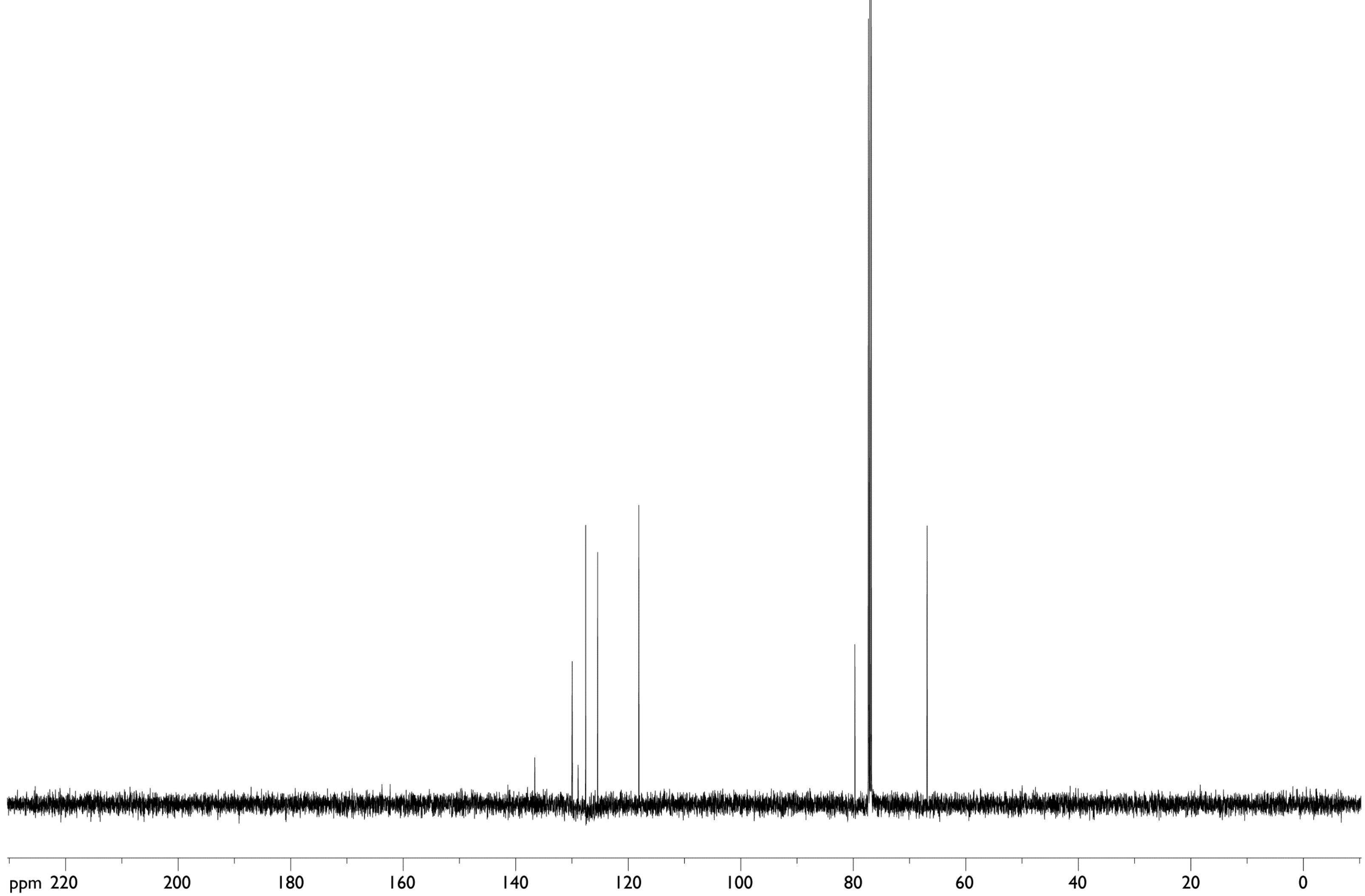
s17

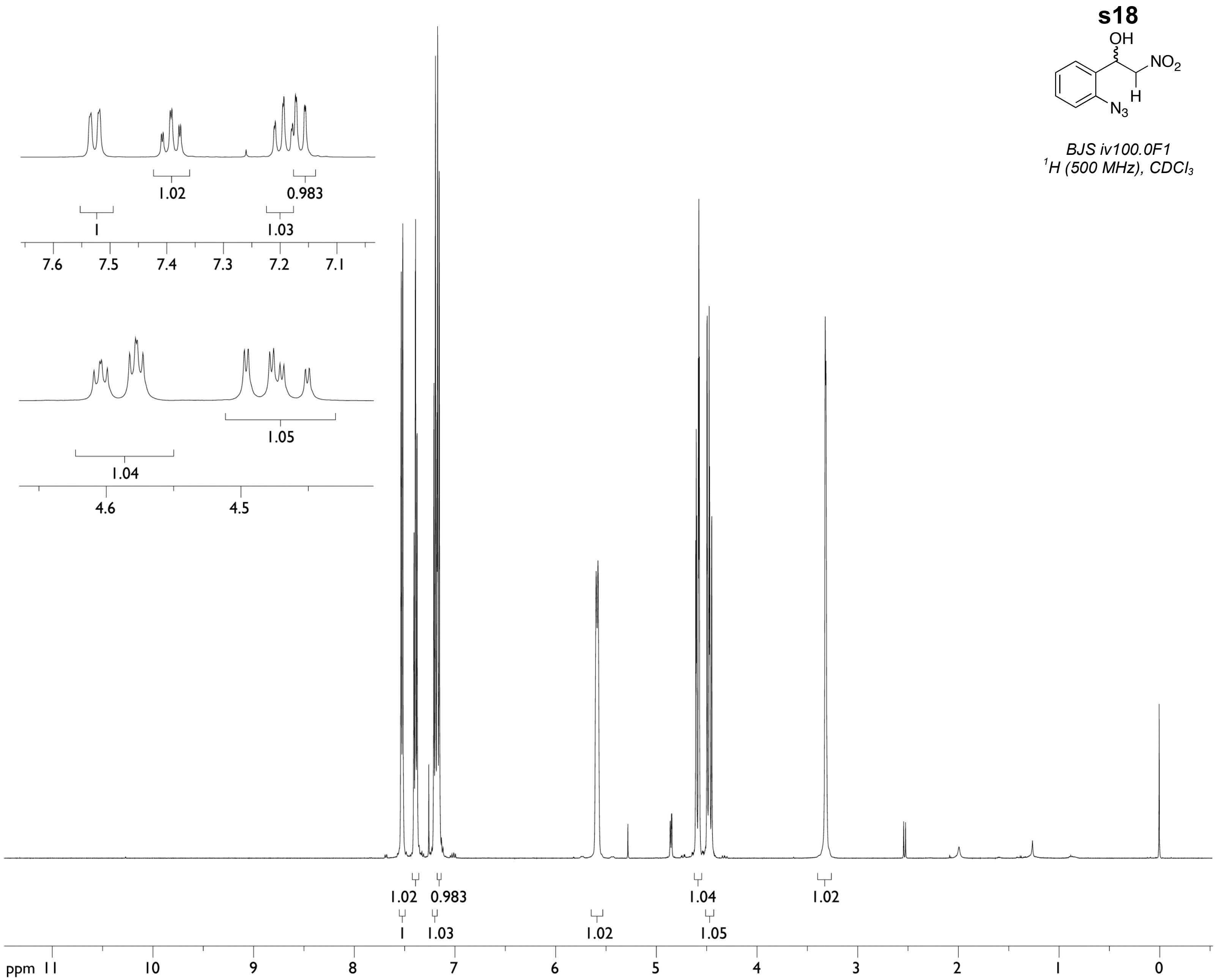

OH
NO_2
H
N_3
BJS iii143.001
^{1}H (500 MHz), $CDCl_3$
0.949
0.979
7.6
7.5
7.4
0.987
1.02
1
5.6
5.4
5.2
5.0
4.8
4.6
0.949
0.956
1
3.24
0.979
1.01
0.987
1.02
ppm 11
10
9
8
7
6
5
4
3
2
1
0

s17

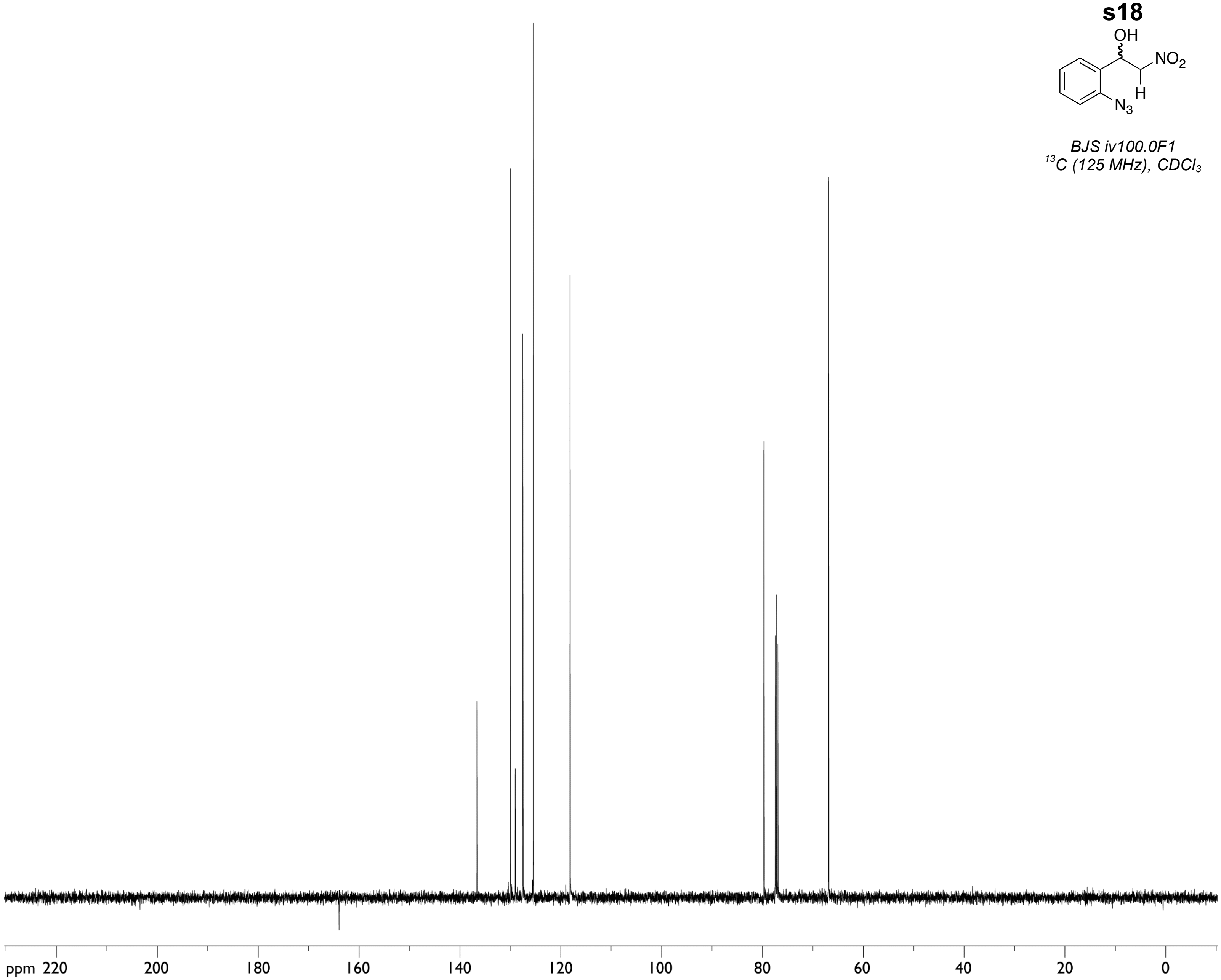


BJS iii143.001
^{13}C (125 MHz), CDCl$_3$

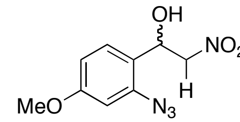



s18
OH
NO_2
H
N_3
BJS iv100.0F1
^{1}H (500 MHz), $CDCl_3$
1.02
0.983
1
1.03
7.6
7.5
7.4
7.3
7.2
7.1
1.05
1.04
4.6
4.5
1.02
0.983
1.04
1.02
1
1.03
1.02
1.05
ppm 11
10
9
8
7
6
5
4
3
2
1
0

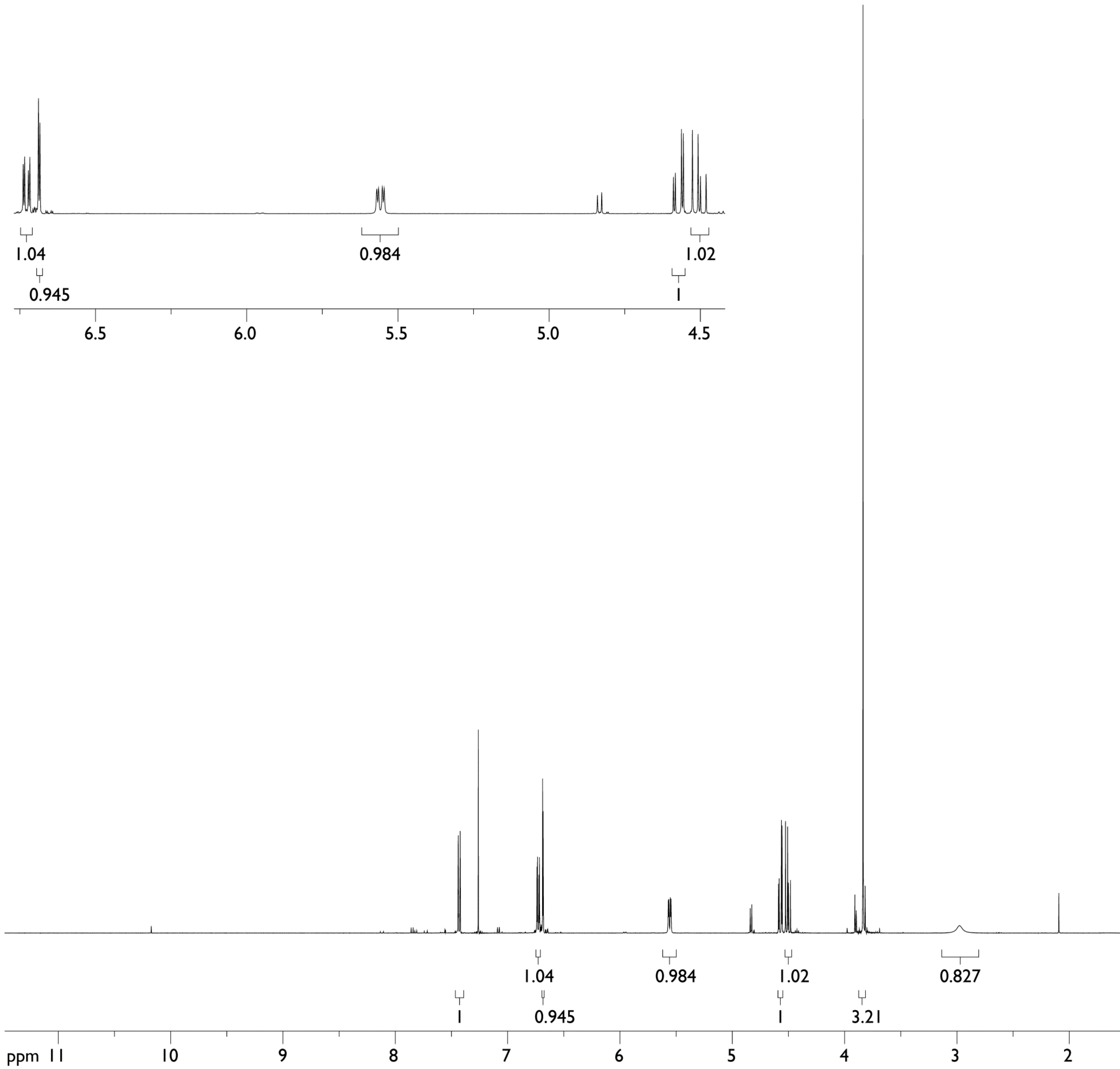
s18

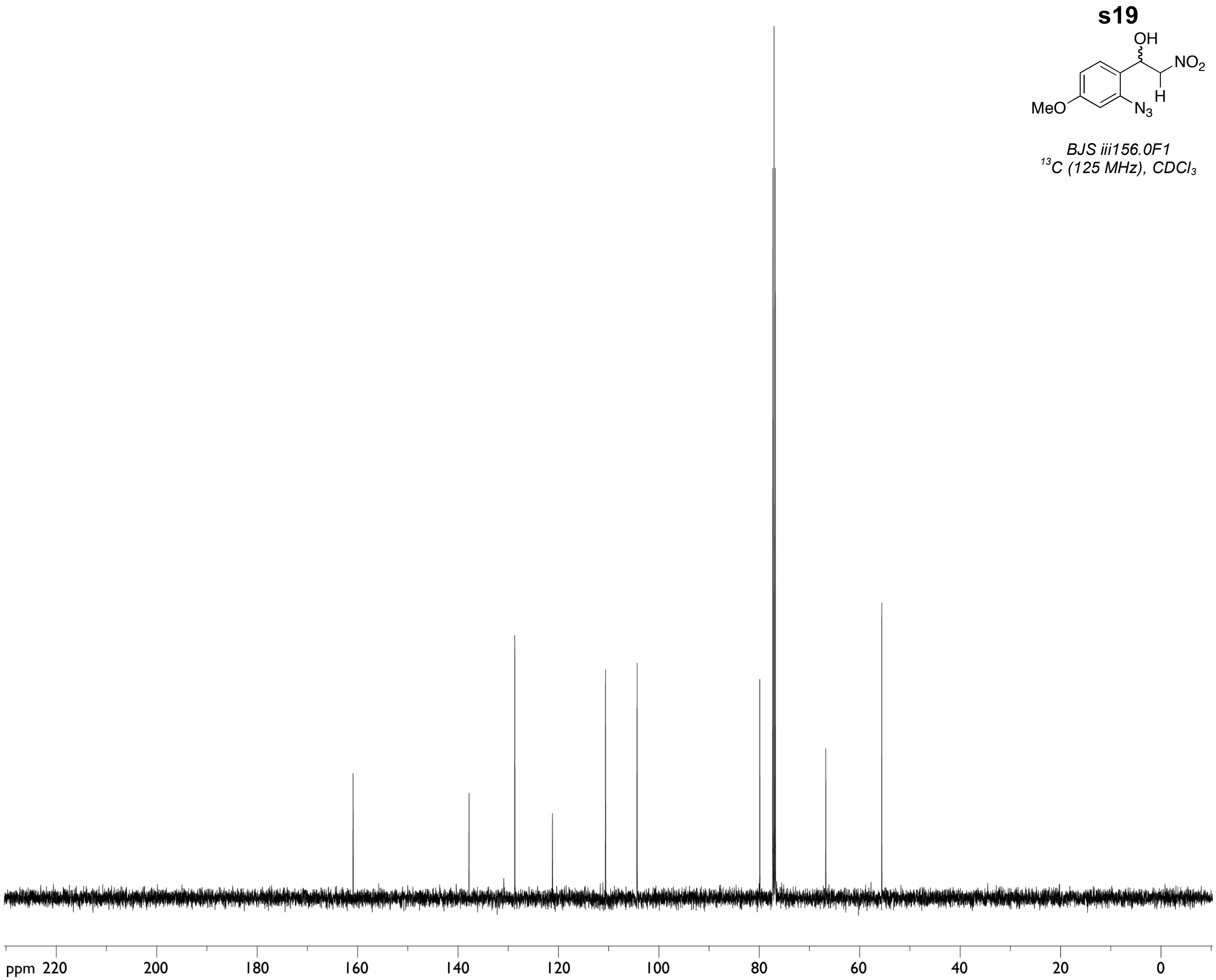

OH
NO2
H
N3
BJS iv100.0F1
13C (125 MHz), CDCl3
ppm 220
200
180
160
140
120
100
80
60
40
20
0

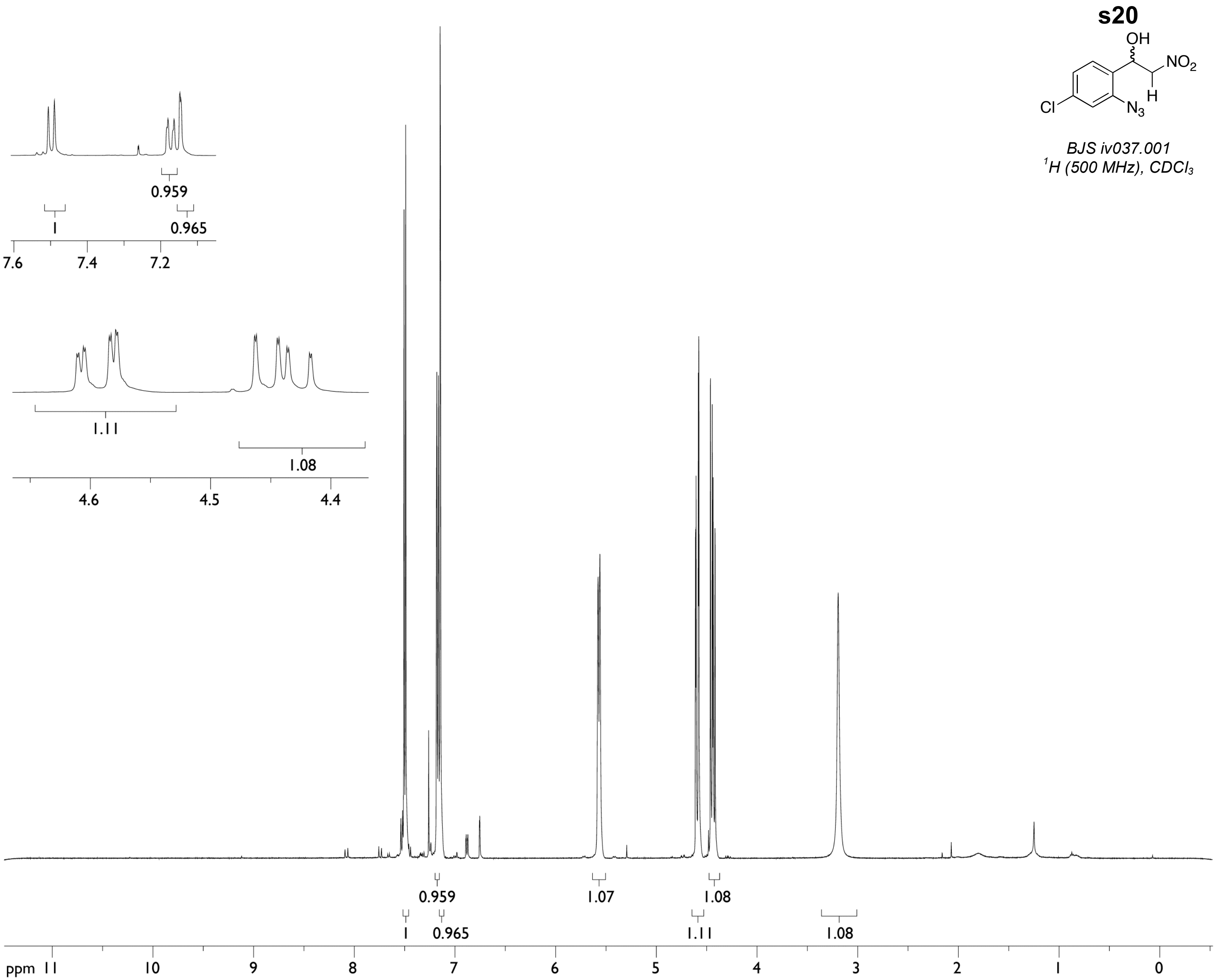
s19



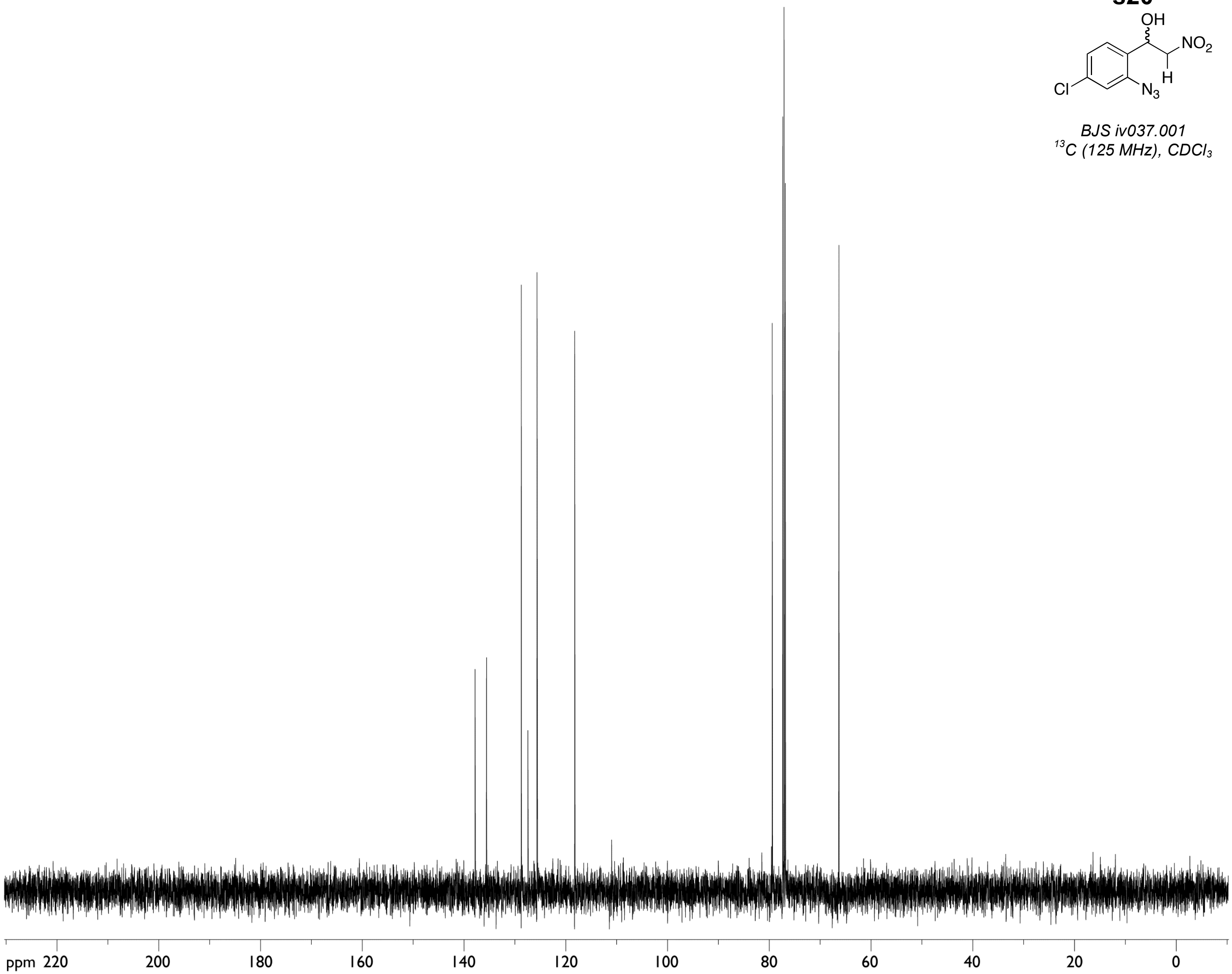
BJS iii156.0F1
^{1}H (500 MHz), CDCl$_3$




s19
OH
NO2
H
MeO
N3
BJS iii156.0F1
13C (125 MHz), CDCl3
ppm 220
200
180
160
140
120
100
80
60
40
20
0

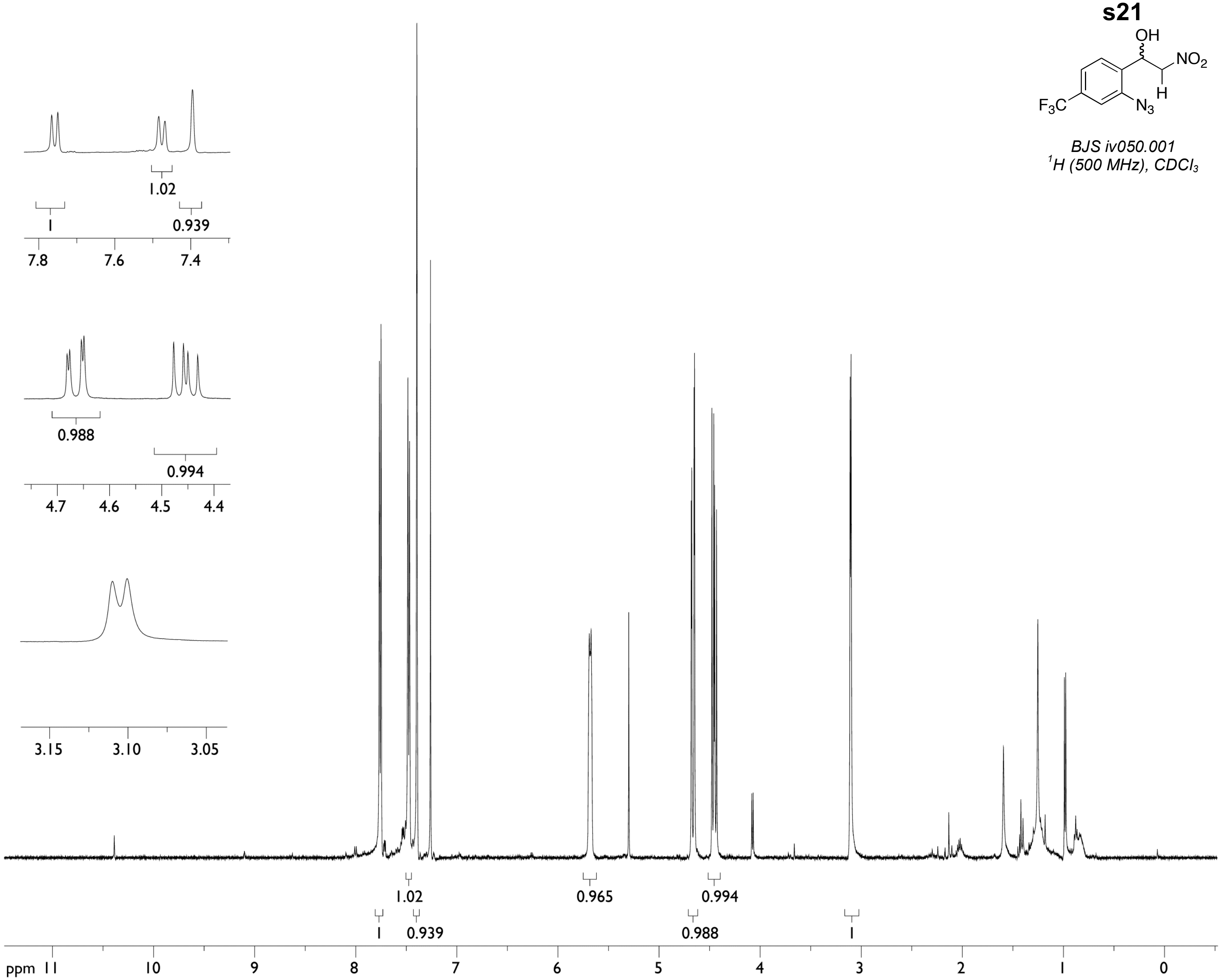

s20
OH
NO2
H
Cl
N3
BJS iv037.001
1H (500 MHz), CDCl3
0.959
1
0.965
7.6
7.4
7.2
1.11
1.08
4.6
4.5
4.4
0.959
1.07
1.08
1
0.965
1.11
1.08
ppm 11
10
9
8
7
6
5
4
3
2
1
0

s20



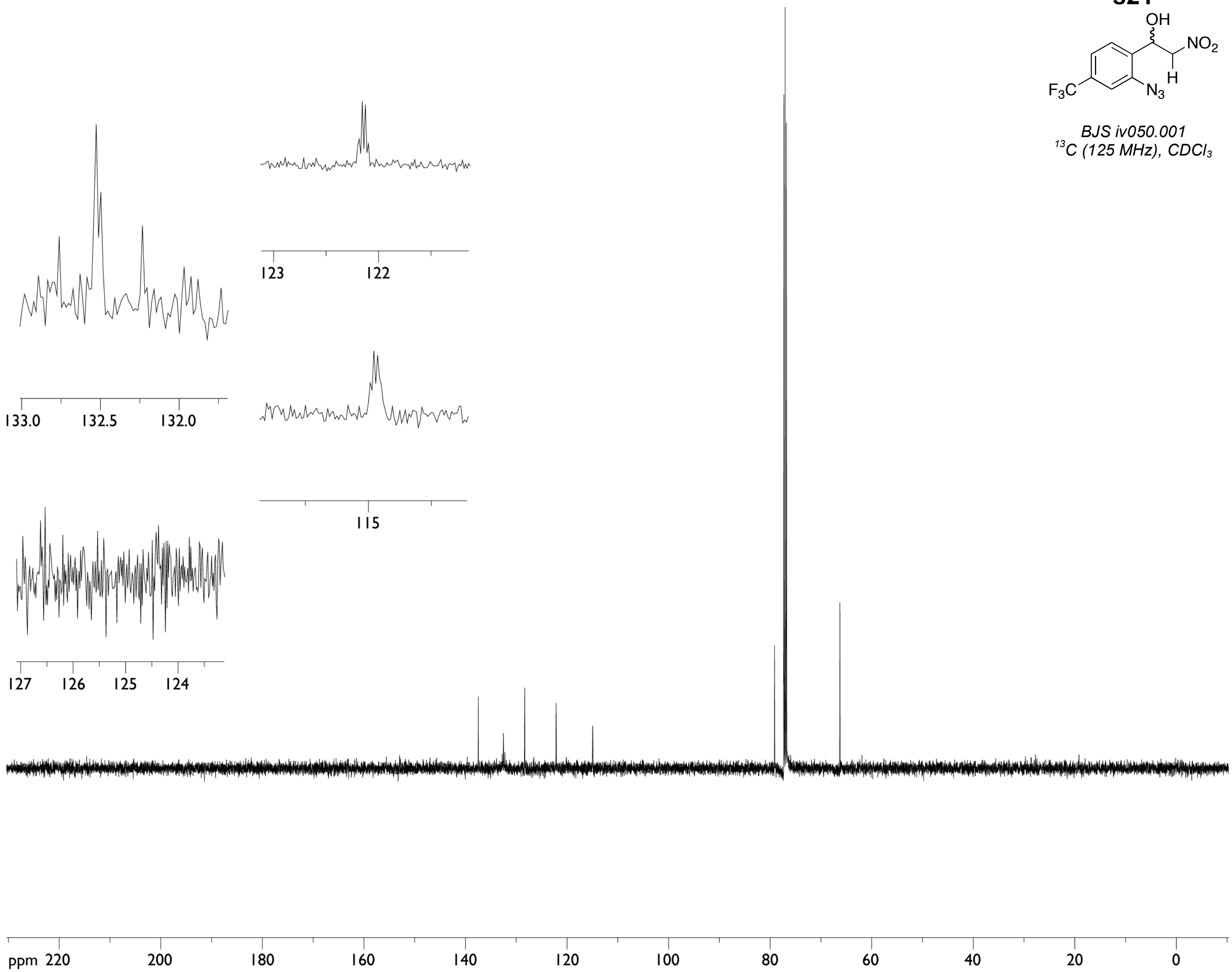
BJS iv037.001
^{13}C (125 MHz), CDCl$_3$

s21



BJS iv050.001
^{1}H (500 MHz), CDCl$_3$

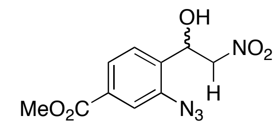
s21



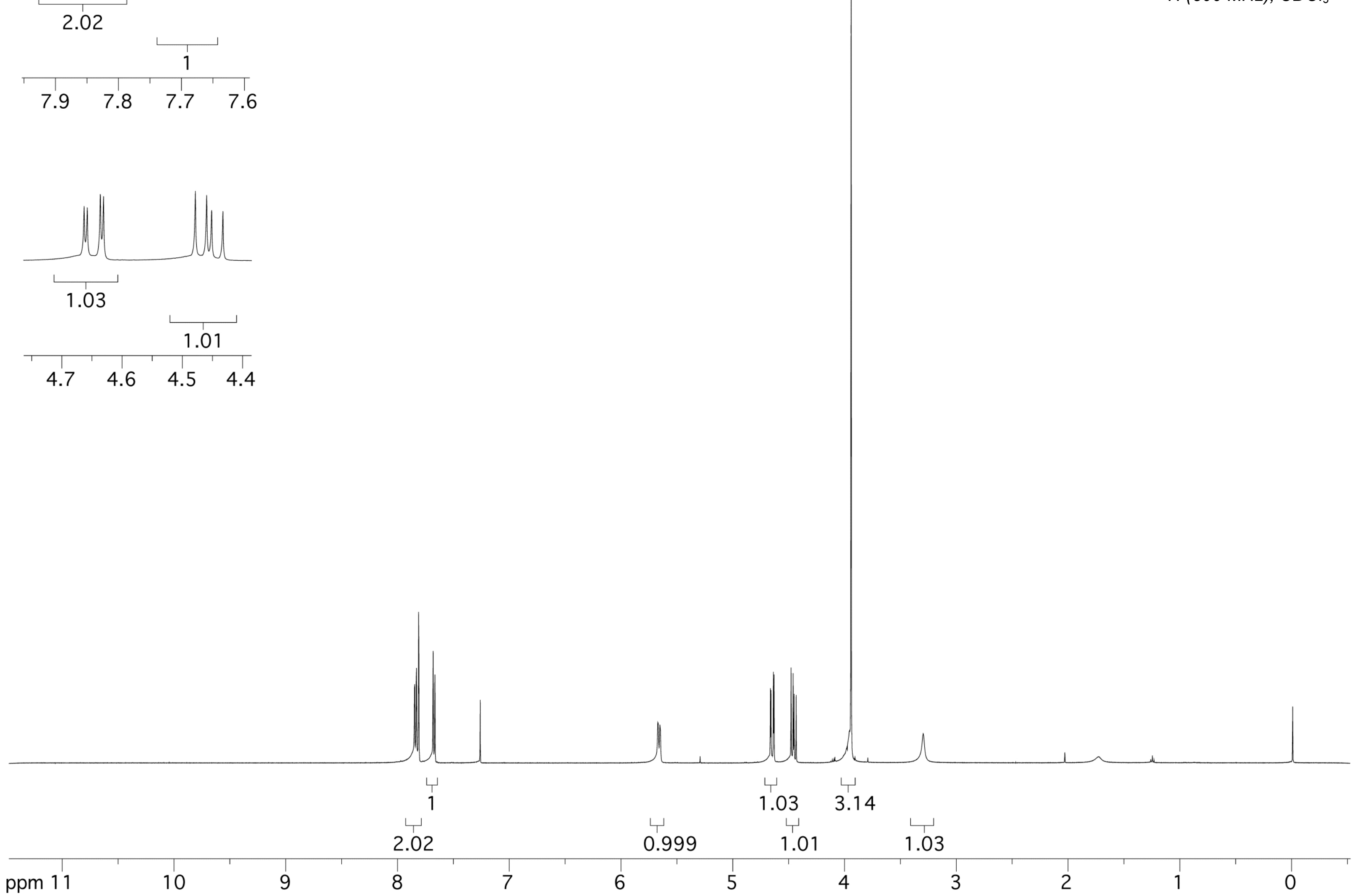
BJS iv050.001

^{13}C (125 MHz), $CDCl_3$

s22

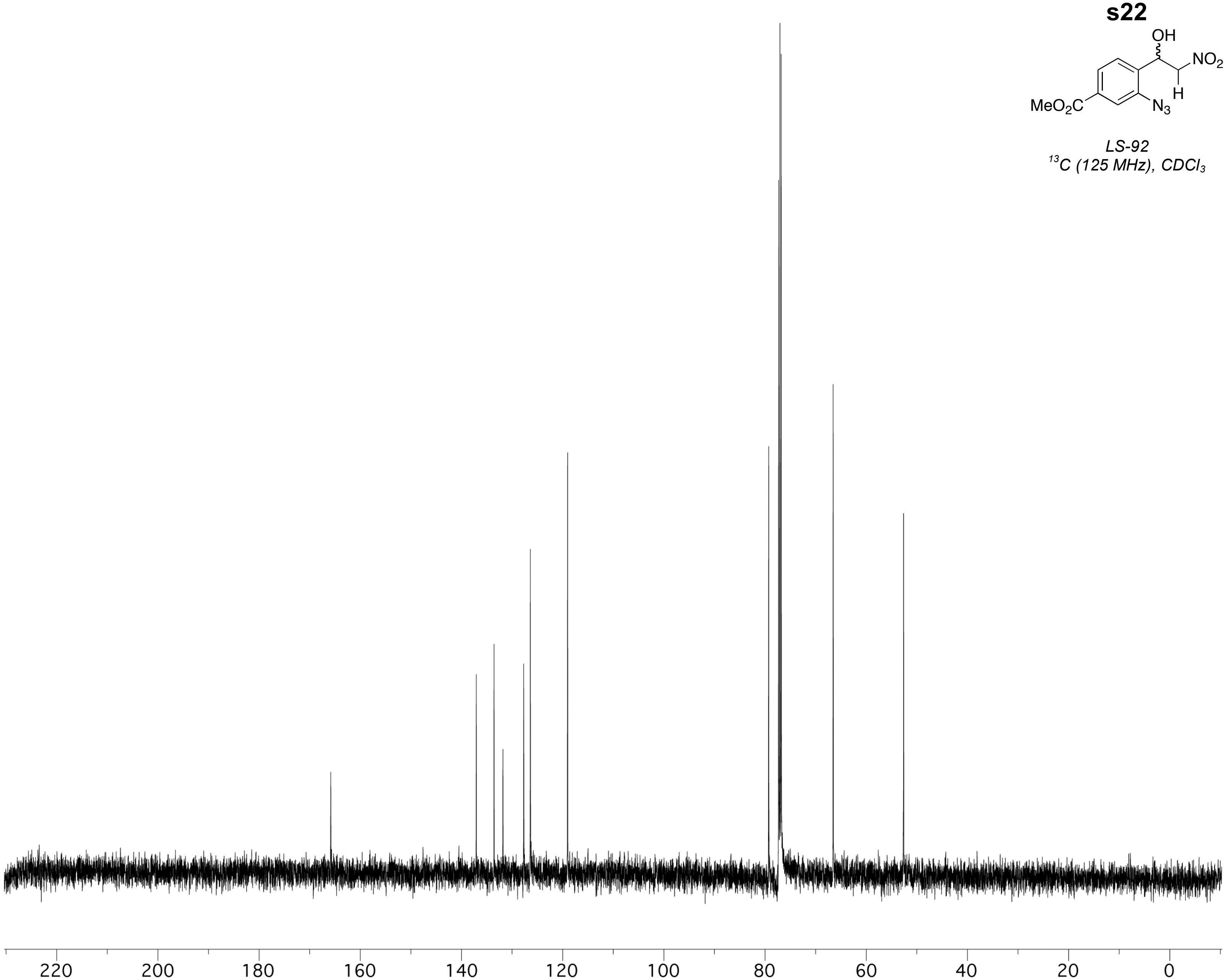


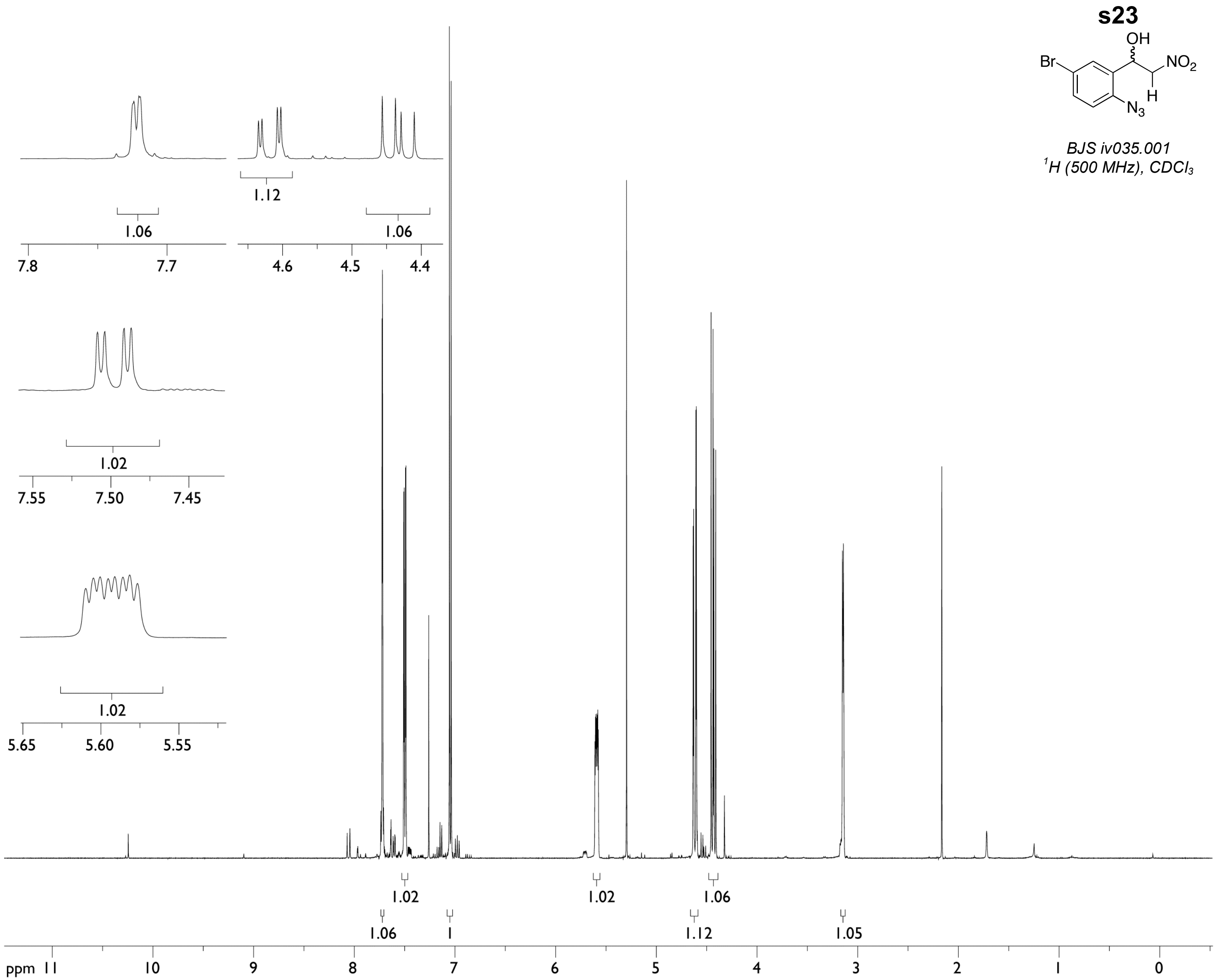
LS-92
^{1}H (500 MHz), $CDCl_3$

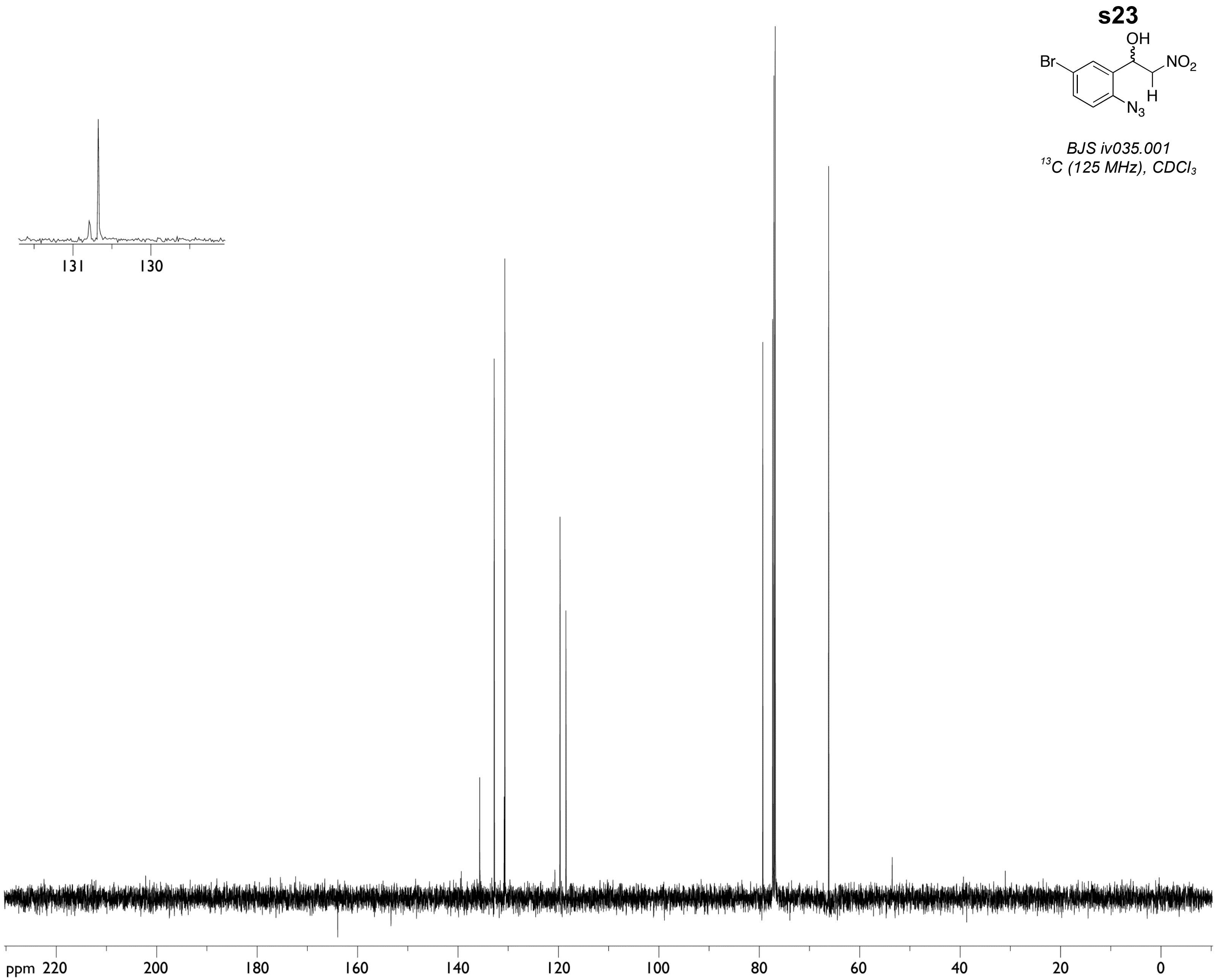


s22

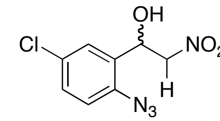
LS-92
^{13}C (125 MHz), $CDCl_3$



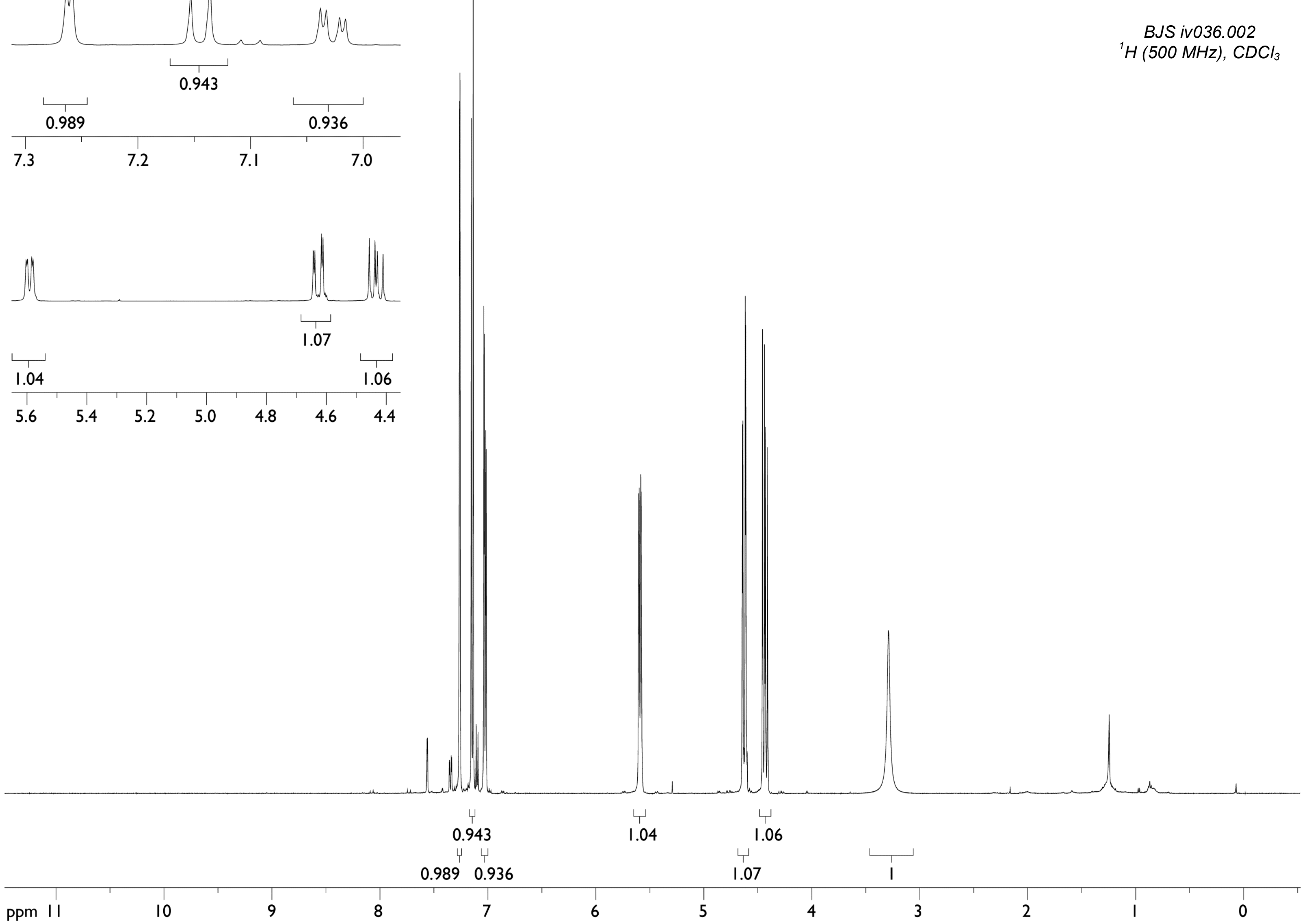

s23
OH
Br
NO2
H
N3
BJS iv035.001
1H (500 MHz), CDCl3
1.06
7.8
7.7
1.12
1.06
4.6
4.5
4.4
1.02
7.55
7.50
7.45
1.02
5.65
5.60
5.55
1.02
1.02
1.06
1.06
1
1.12
1.05
ppm 11
10
9
8
7
6
5
4
3
2
1
0

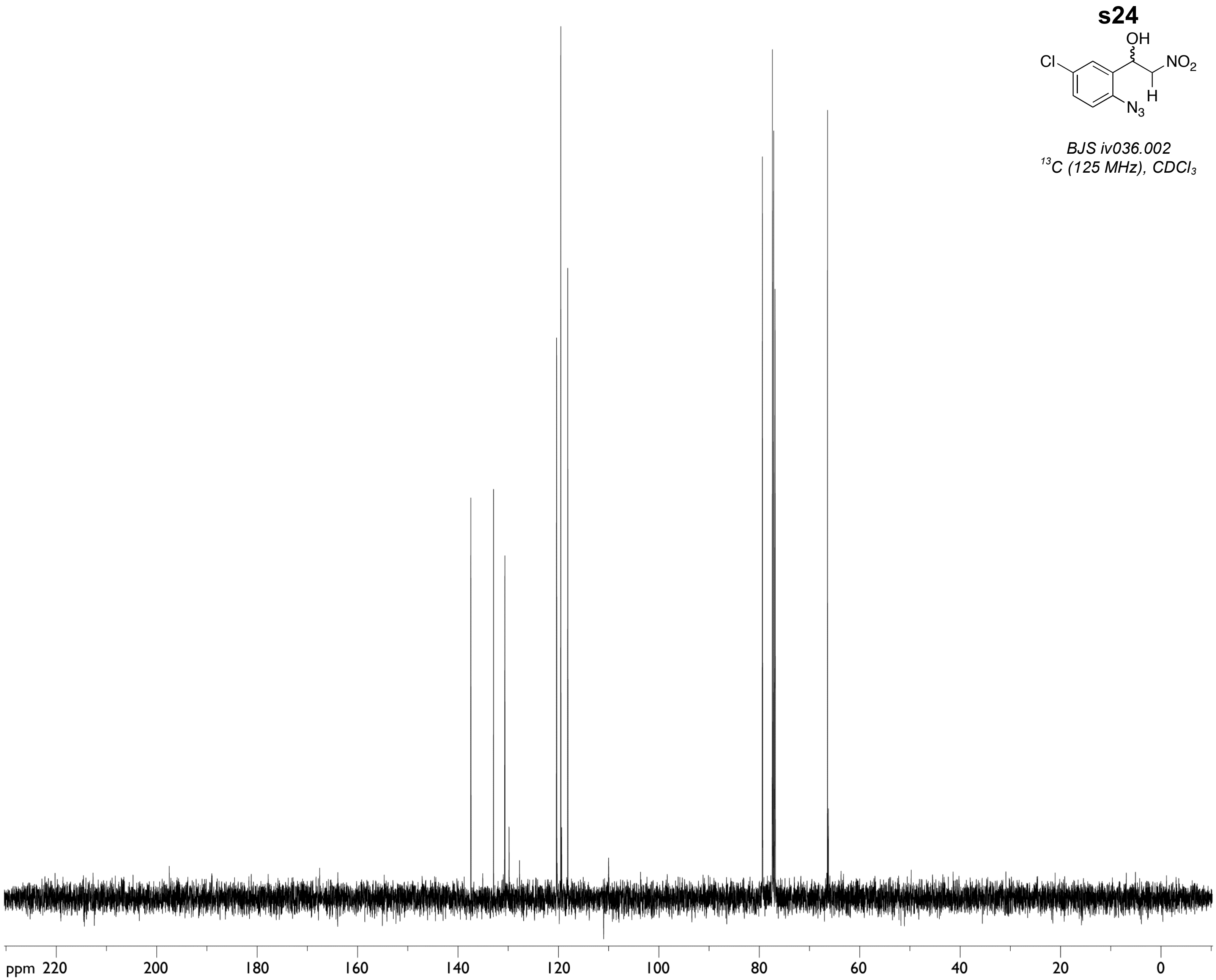

s23
OH
Br
NO_2
H
N_3
BJS iv035.001
^{13}C (125 MHz), $CDCl_3$
131
130
ppm
220
200
180
160
140
120
100
80
60
40
20
0

s24

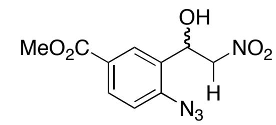


BJS iv036.002
^{1}H (500 MHz), CDCl$_3$

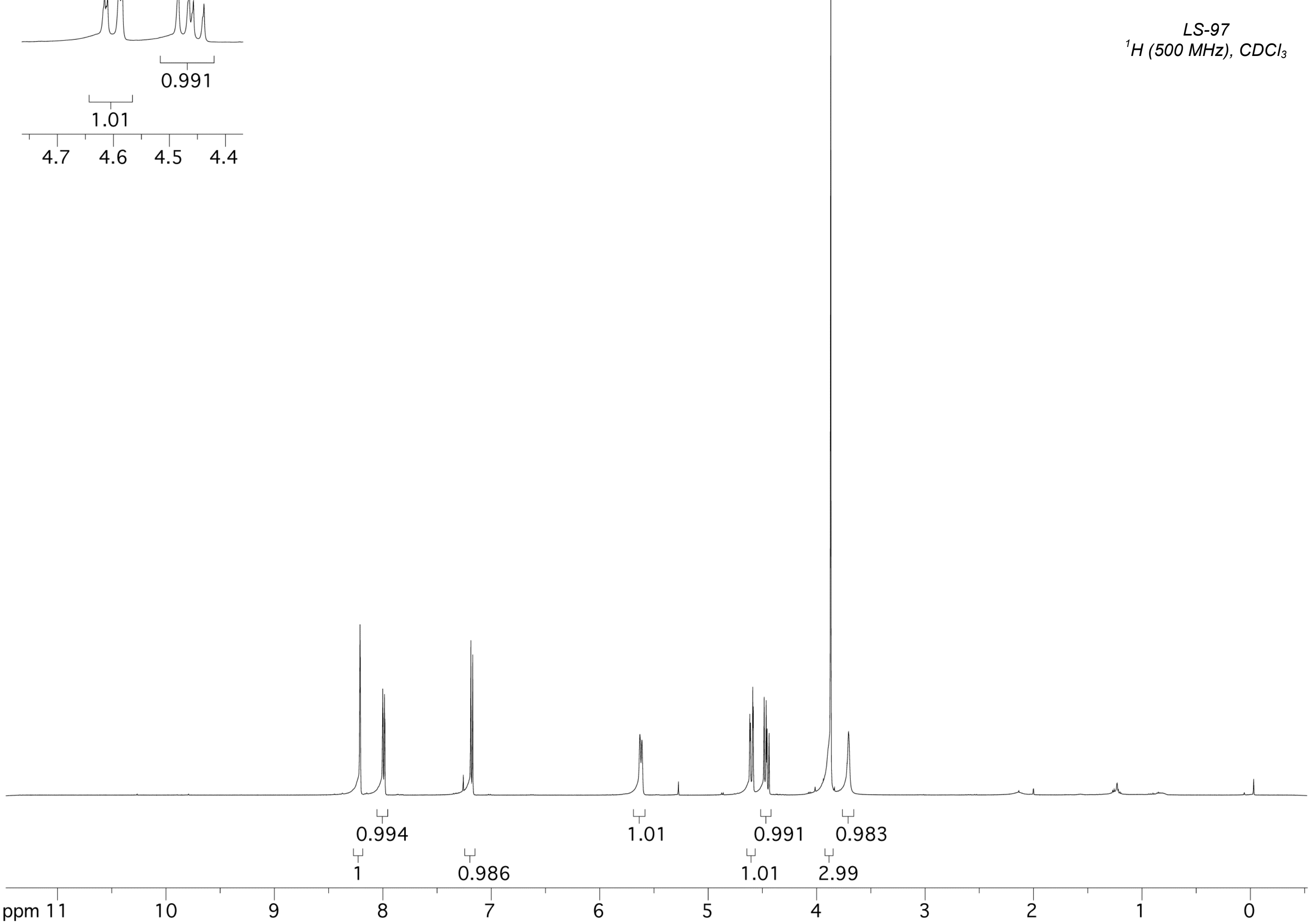



s24
OH
Cl
NO2
H
N3
BJS iv036.002
13C (125 MHz), CDCl3
ppm 220 200 180 160 140 120 100 80 60 40 20 0

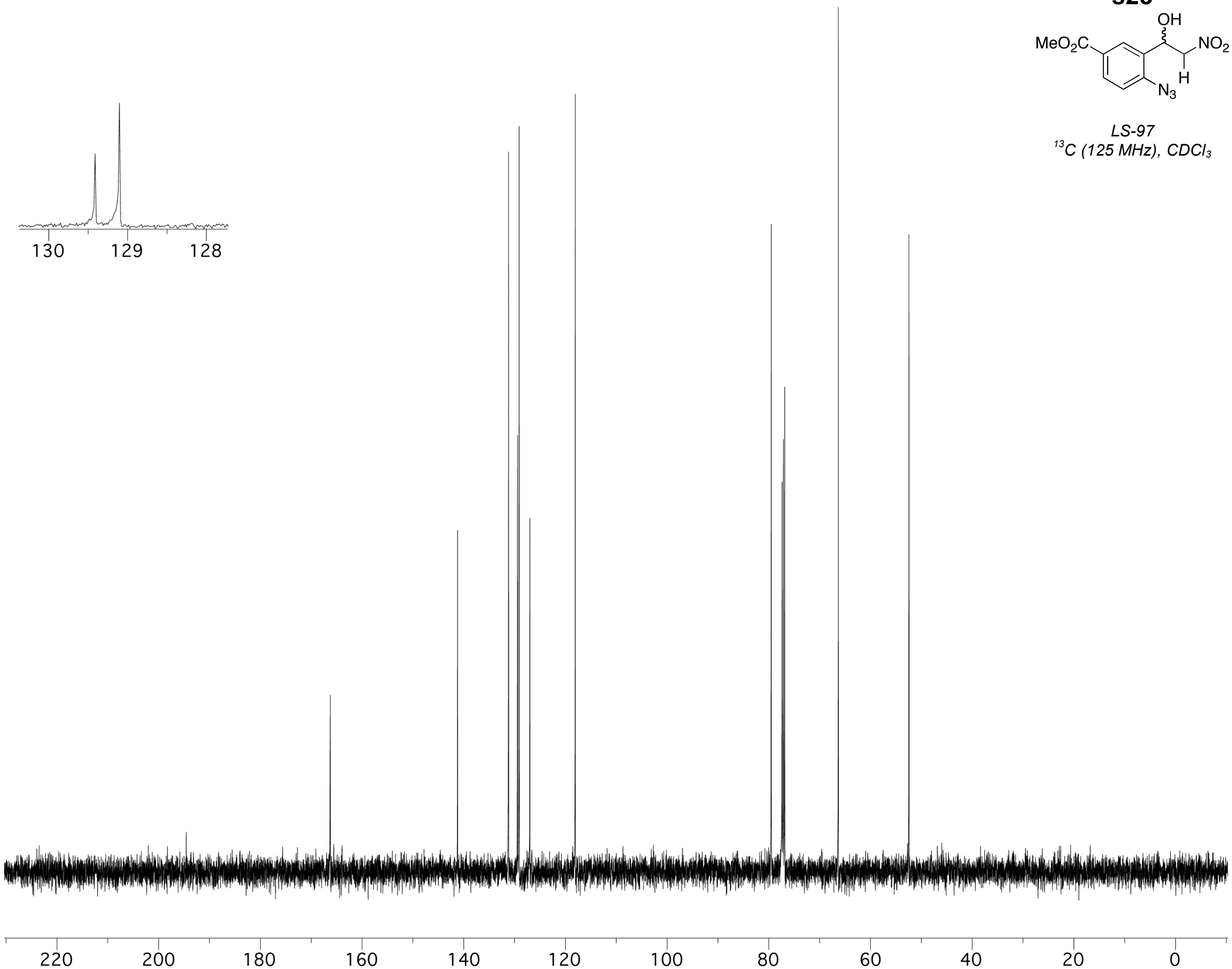
s25



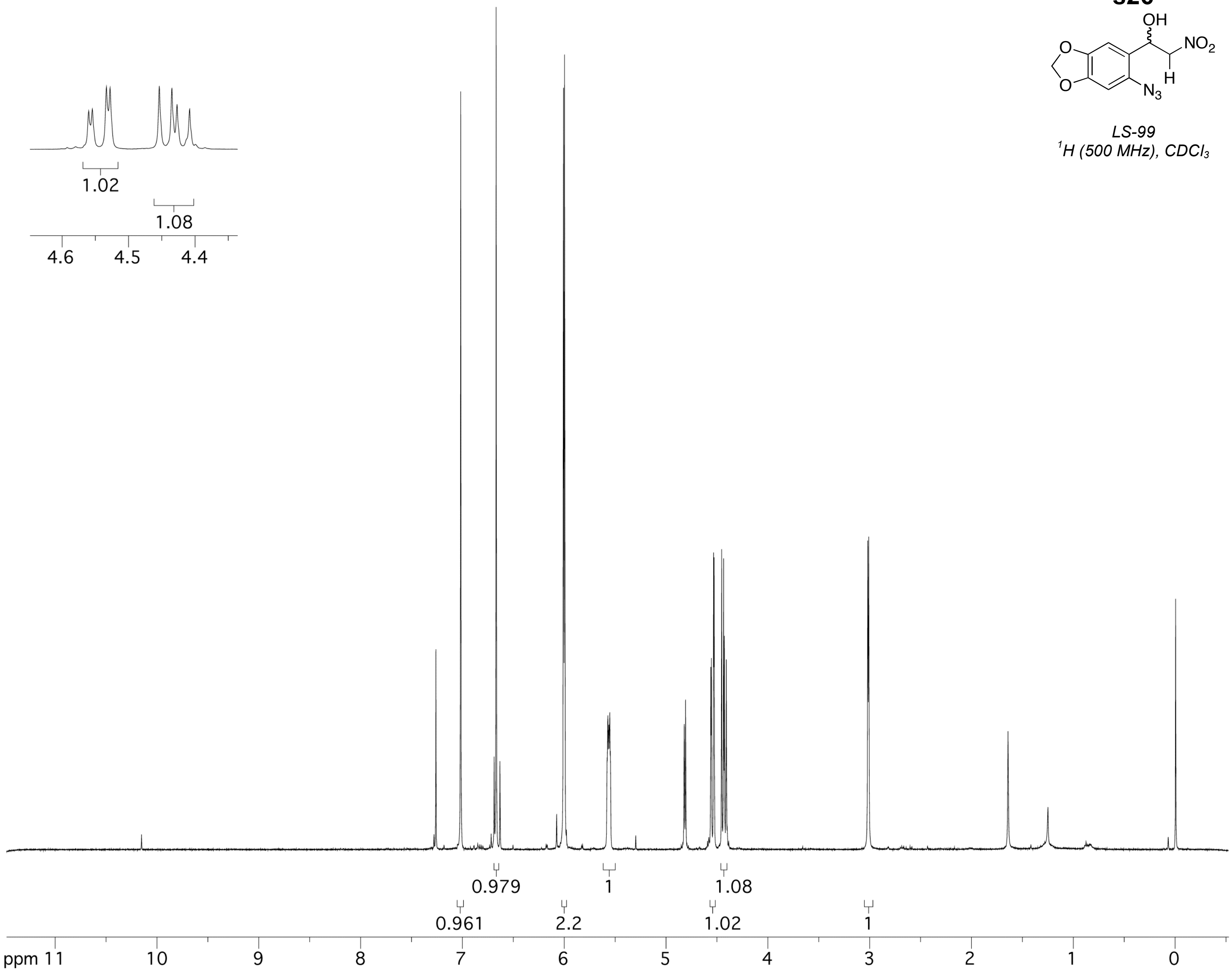
LS-97
¹H (500 MHz), CDCl₃



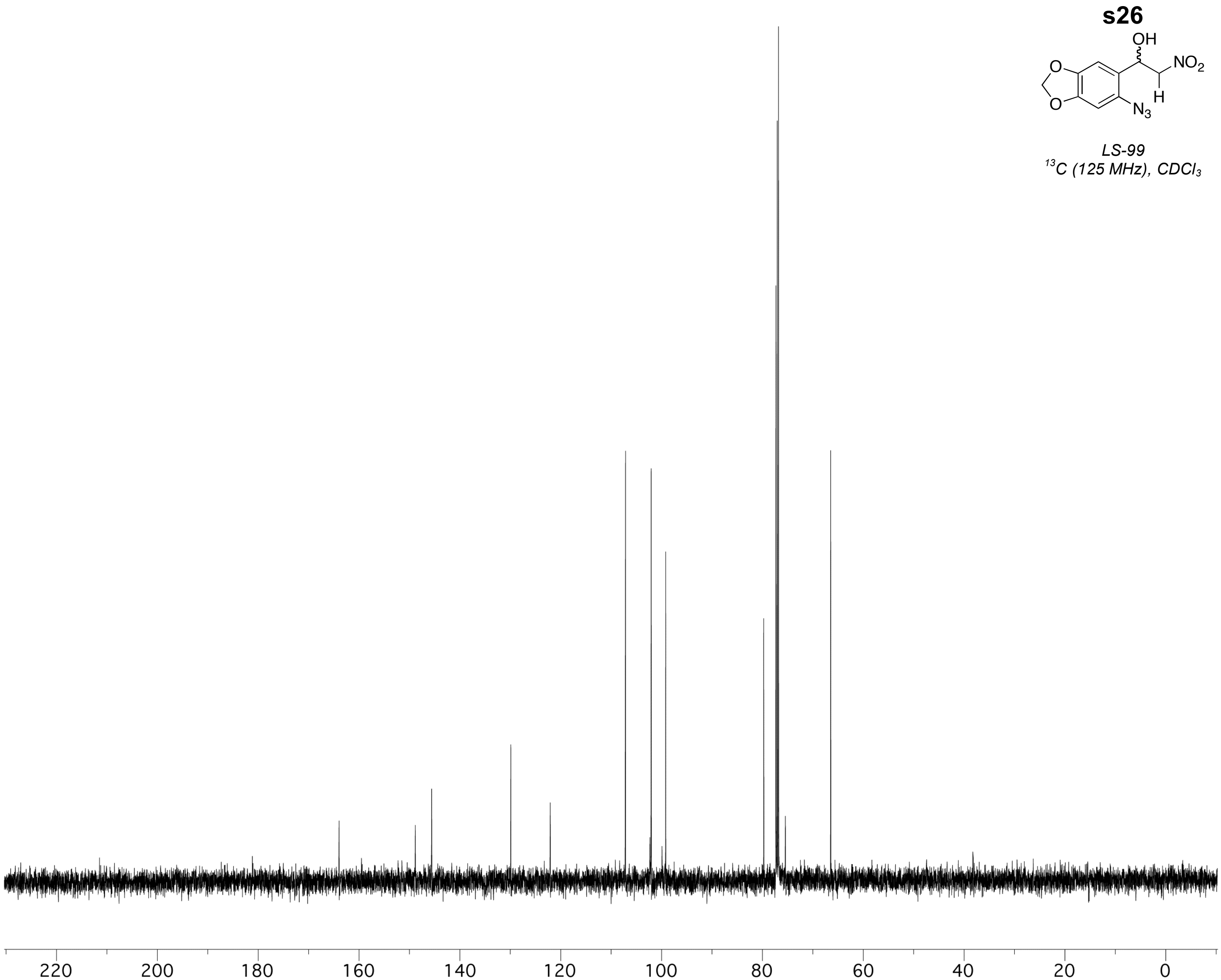
s25


OH
MeO_2C
NO_2
H
N_3
LS-97
^{13}C (125 MHz), $CDCl_3$
130
129
128
220
200
180
160
140
120
100
80
60
40
20
0

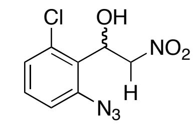
s26



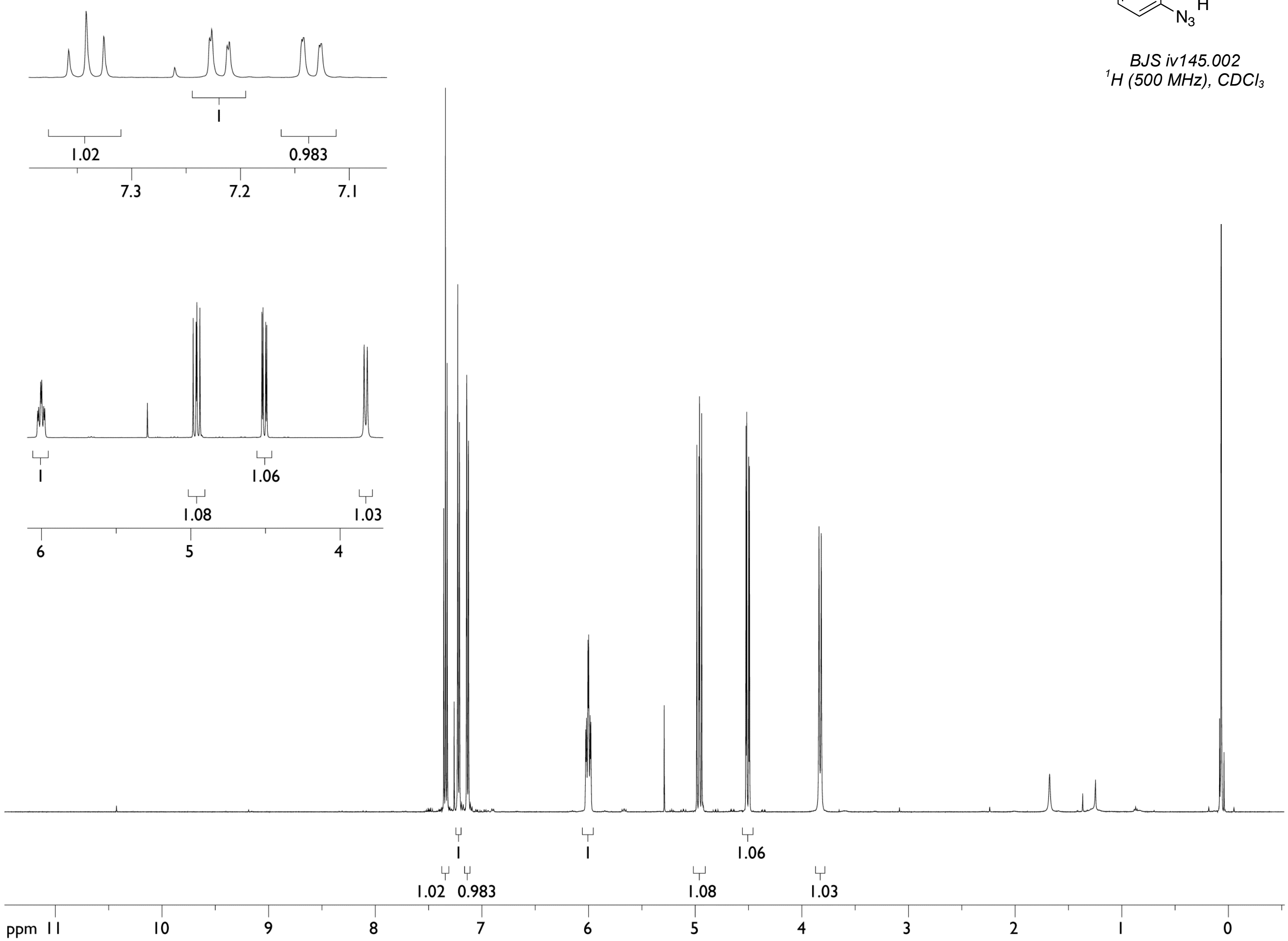
LS-99
¹H (500 MHz), CDCl₃

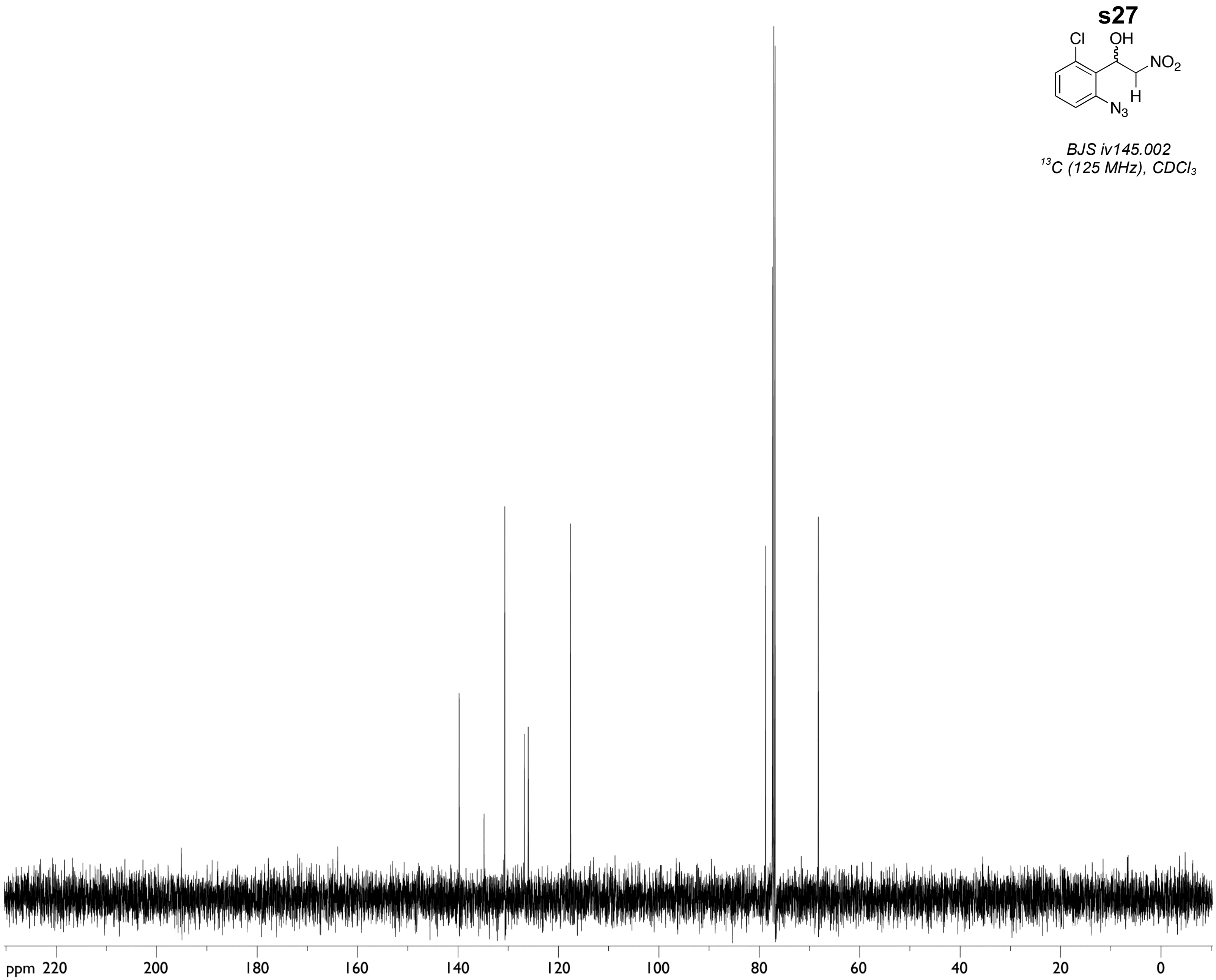

s26
OH
NO2
O
O
H
N3
LS-99
13C (125 MHz), CDCl3
220
200
180
160
140
120
100
80
60
40
20
0

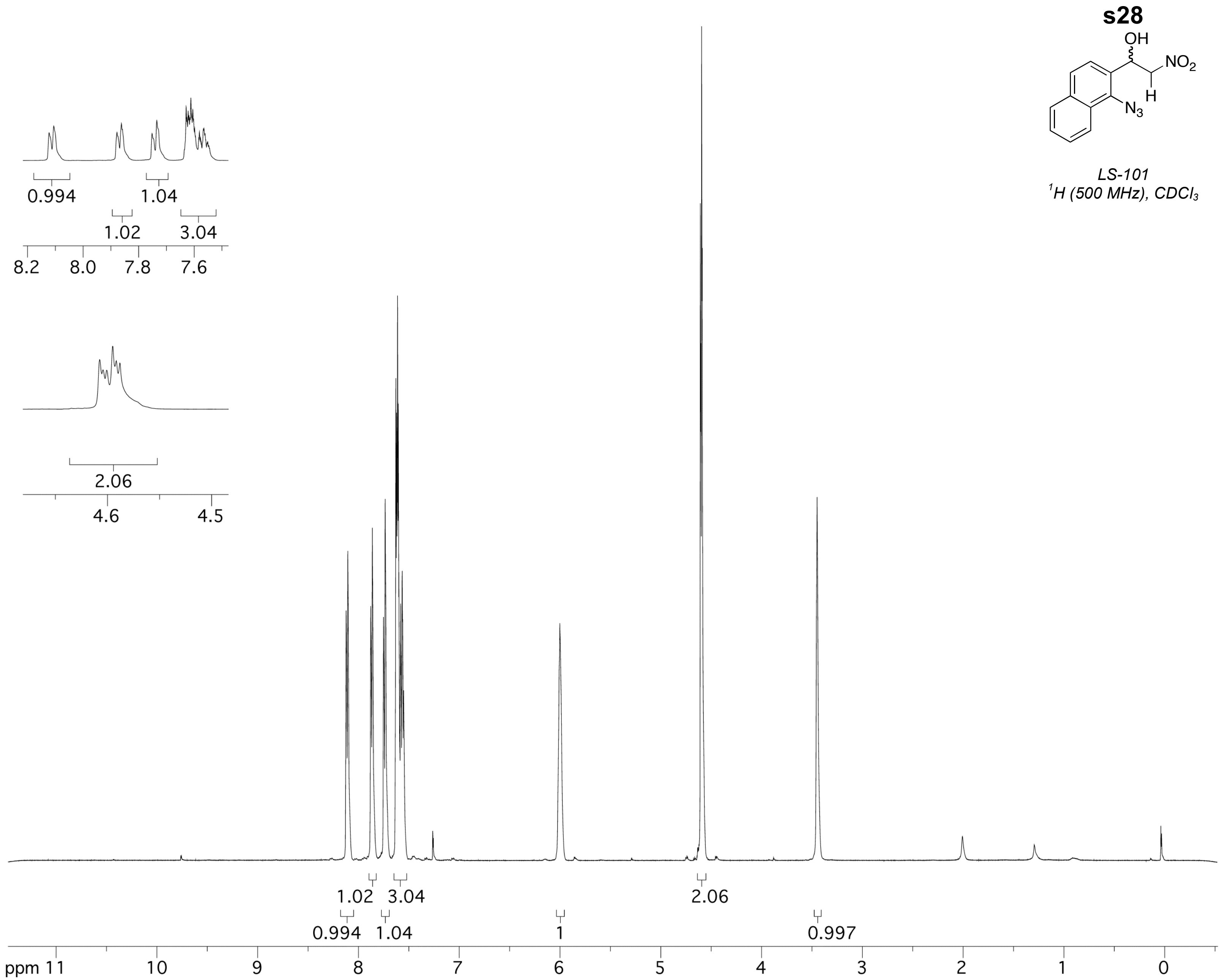
s27



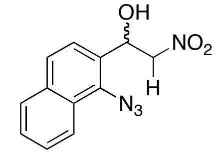
BJS iv145.002
^{1}H (500 MHz), CDCl$_3$



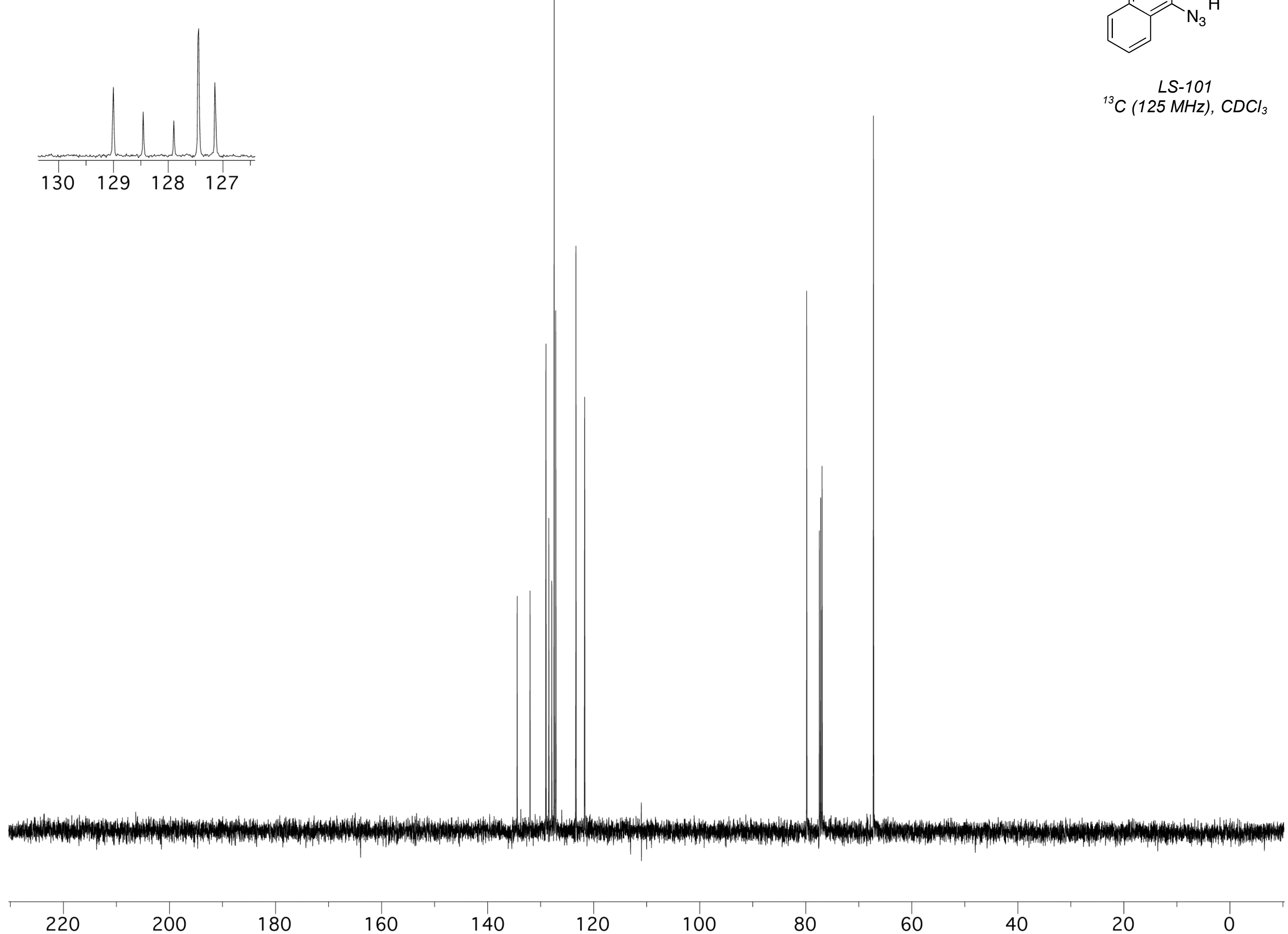

s27
Cl
OH
NO2
H
N3
BJS iv145.002
13C (125 MHz), CDCl3
ppm 220 200 180 160 140 120 100 80 60 40 20 0


s28
OH
NO_2
H
N_3
LS-101
^{1}H (500 MHz), $CDCl_3$
0.994
1.04
1.02
3.04
8.2 8.0 7.8 7.6
2.06
4.6 4.5
1.02 3.04
2.06
0.994 1.04
1
0.997
ppm 11 10 9 8 7 6 5 4 3 2 1 0

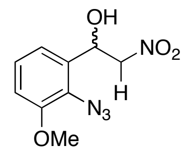
s28



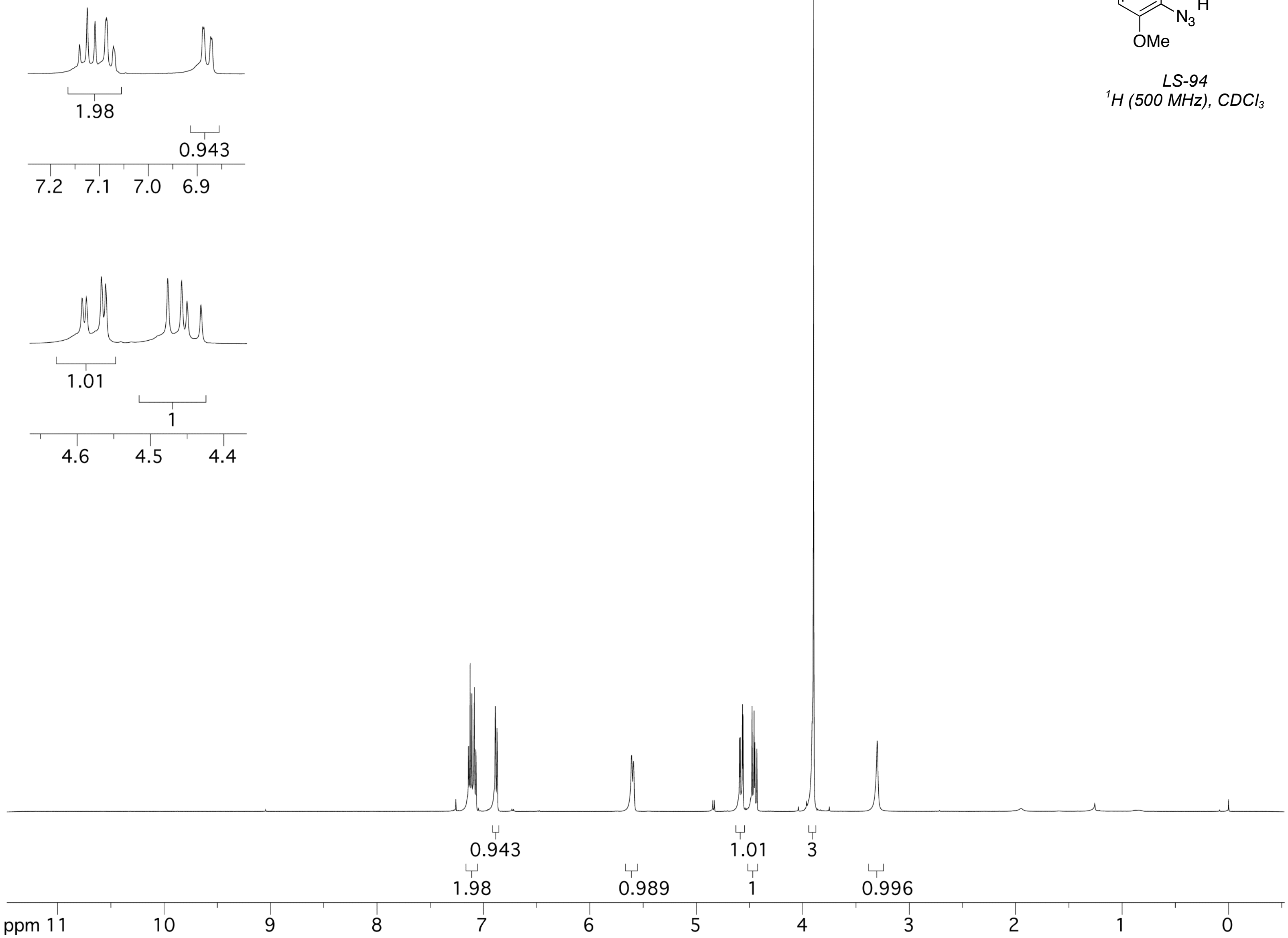
LS-101
^{13}C (125 MHz), $CDCl_3$



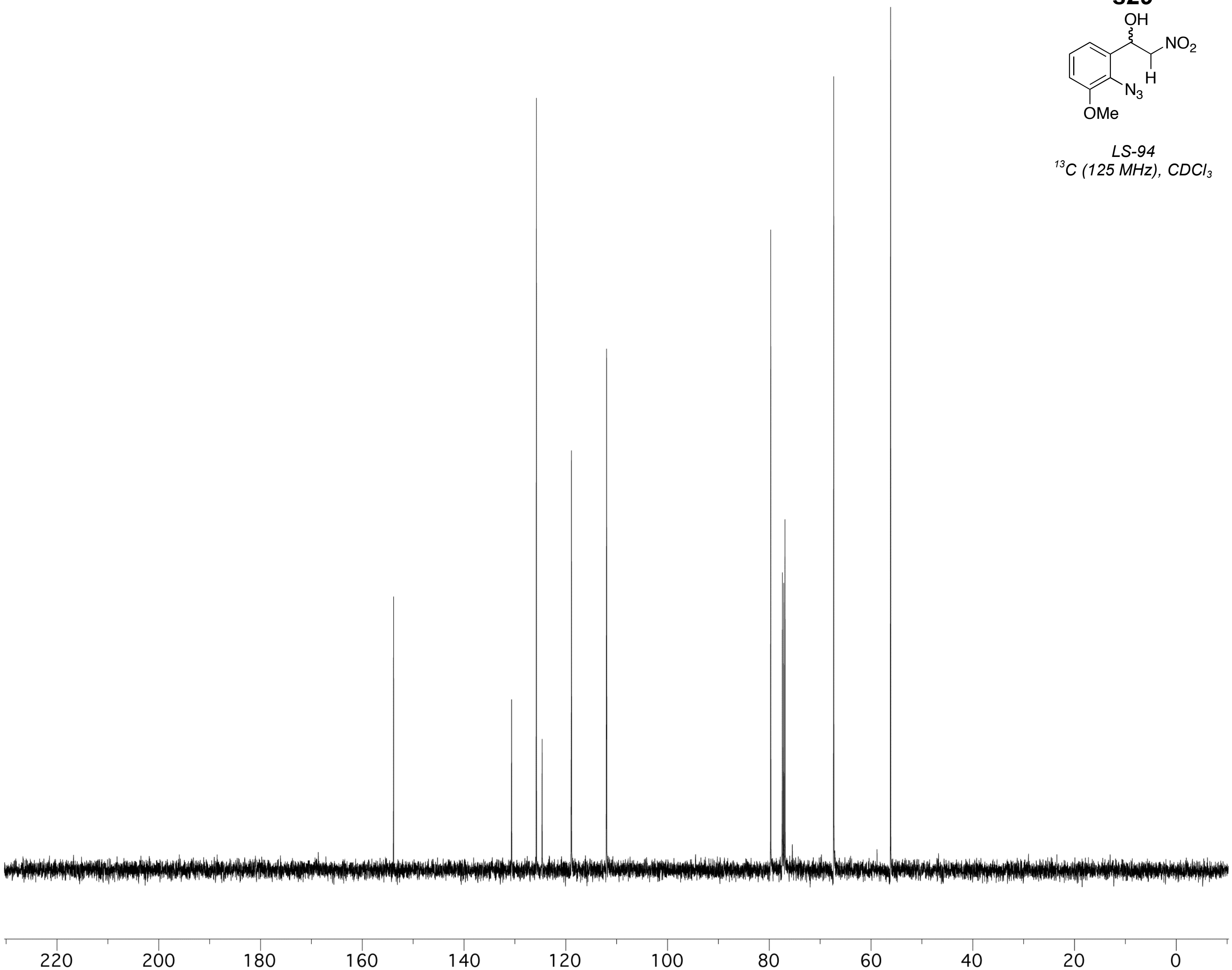
s29



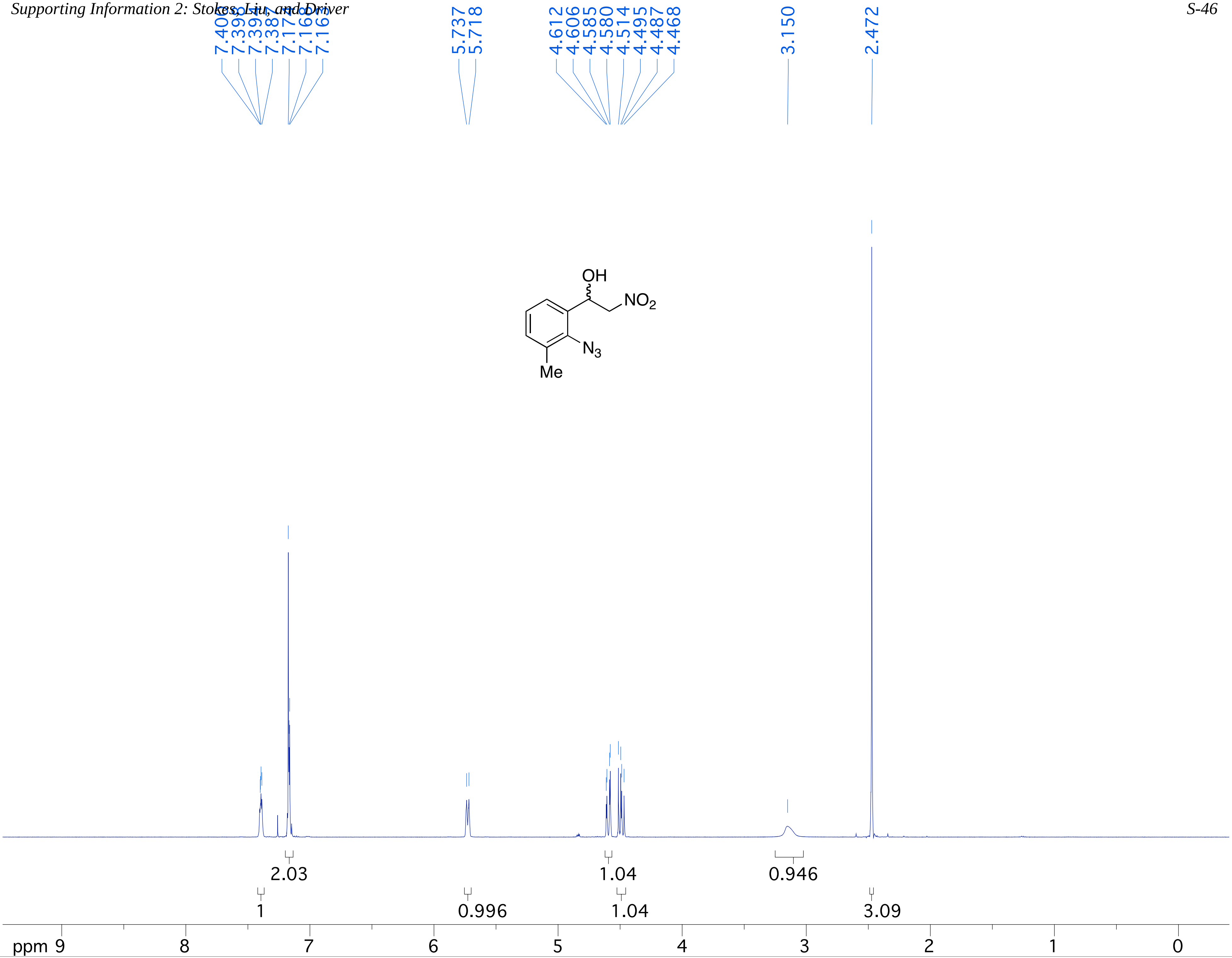
LS-94
^{1}H (500 MHz), $CDCl_3$

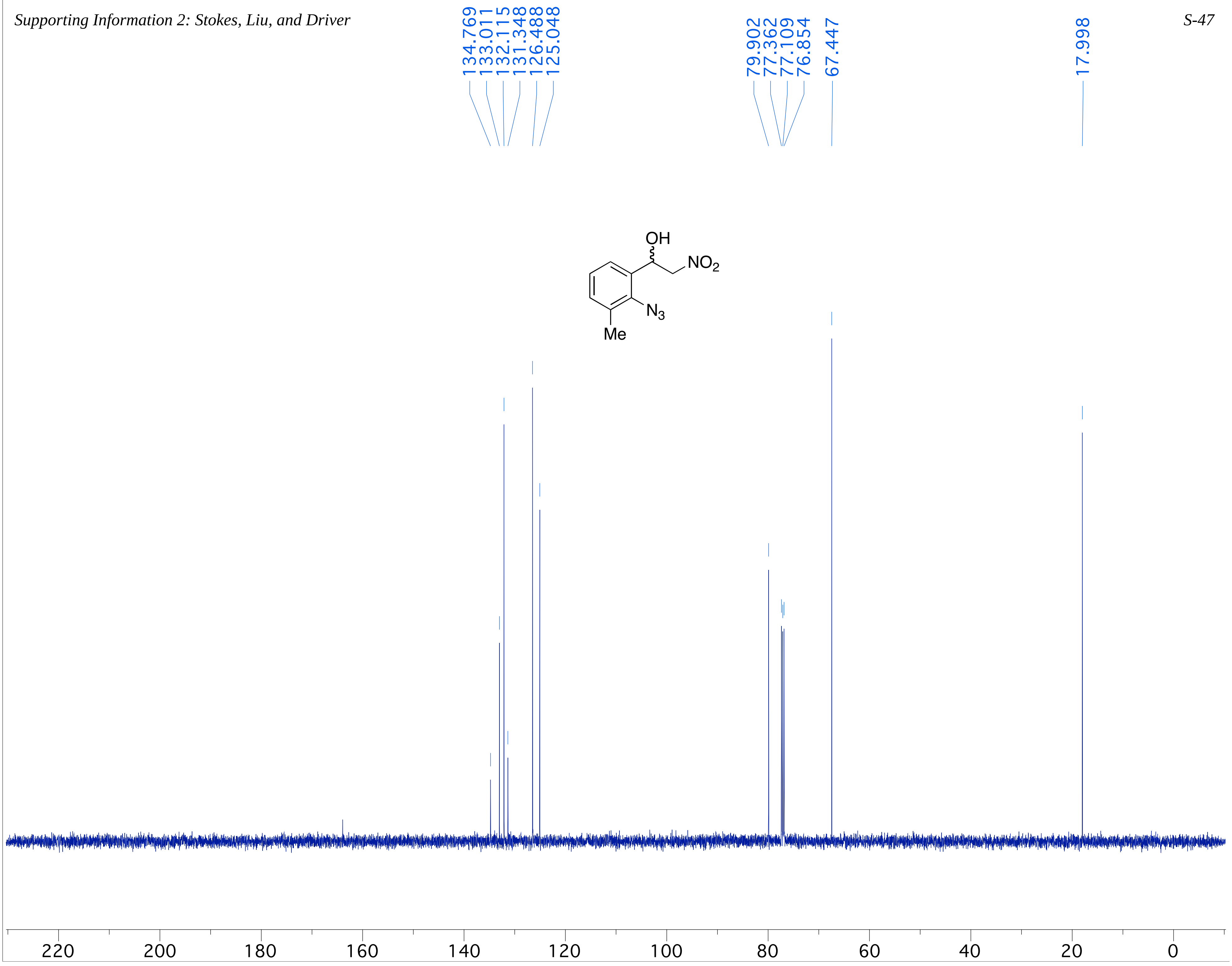


s29

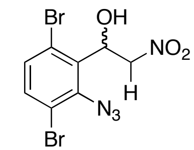


LS-94
^{13}C (125 MHz), CDCl$_3$

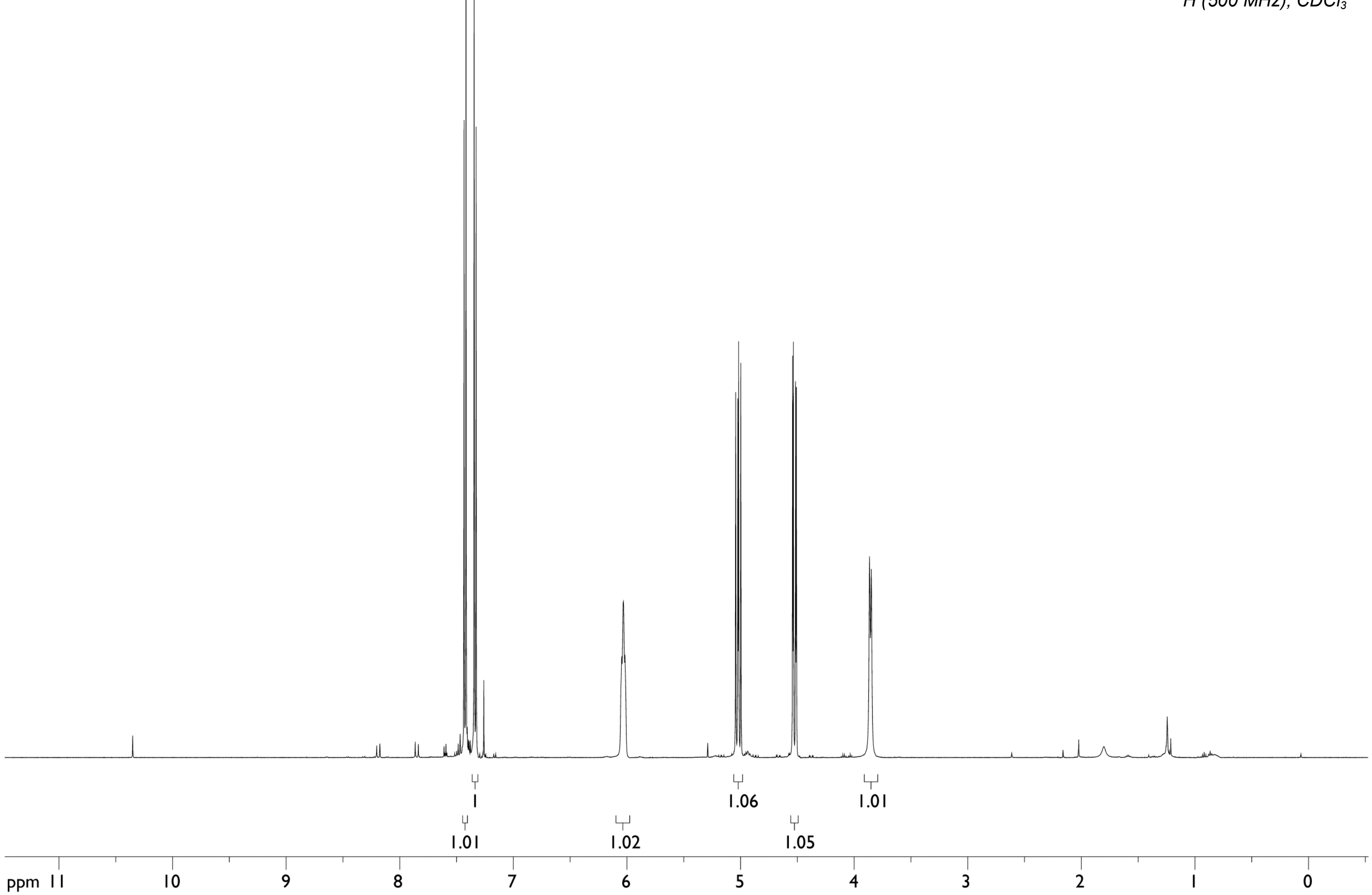

5.737
5.718
4.612
4.606
4.585
4.580
4.514
4.495
4.487
4.468
3.150
2.472
OH
NO_2
N_3
Me
2.03
1.04
0.946
1
0.996
1.04
3.09
ppm 9
8
7
6
5
4
3
2
1
0

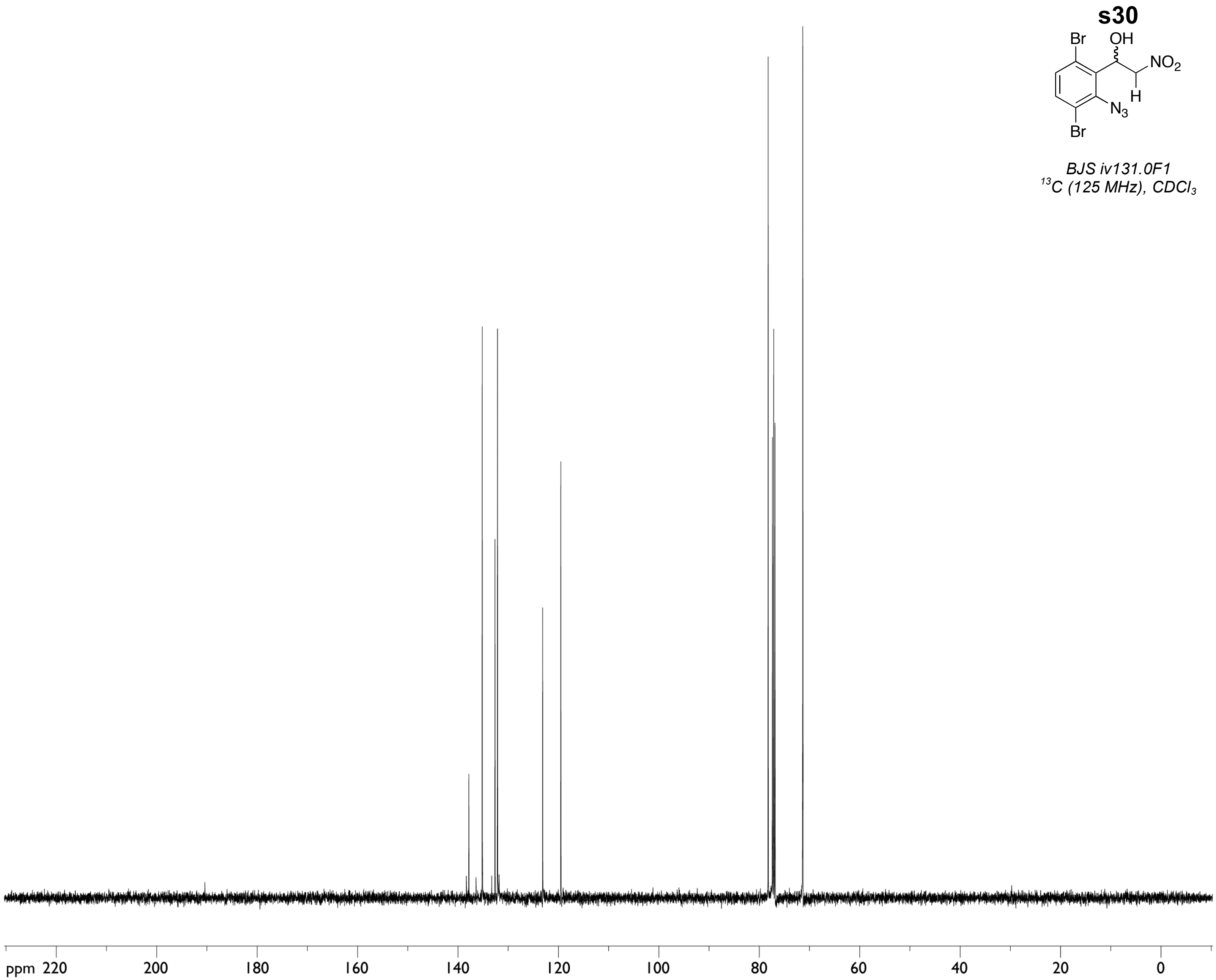

134.769
133.011
132.115
131.348
126.488
125.048
79.902
77.362
77.109
76.854
67.447
17.998
OH
NO2
N3
Me
220
200
180
160
140
120
100
80
60
40
20
0

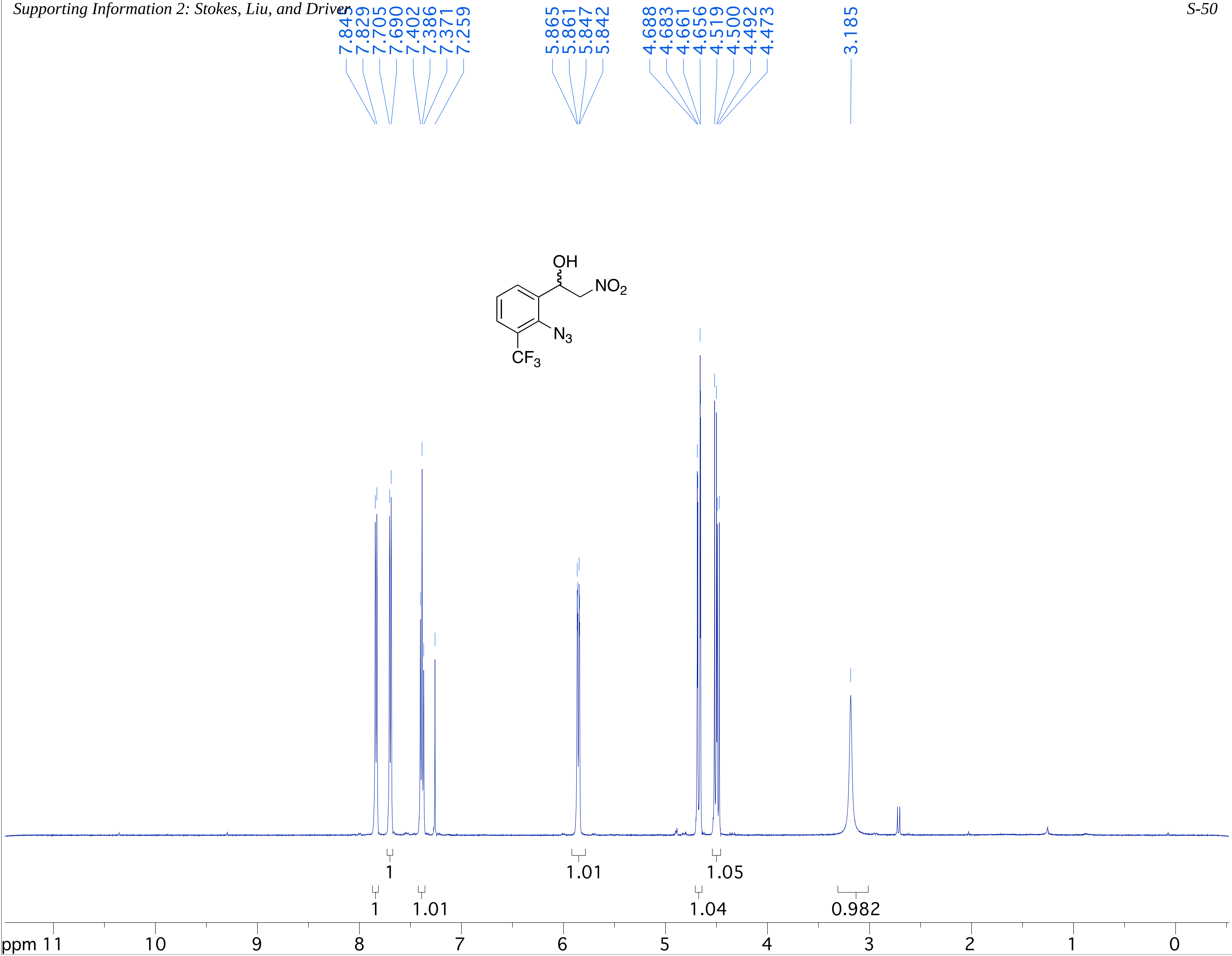
s30

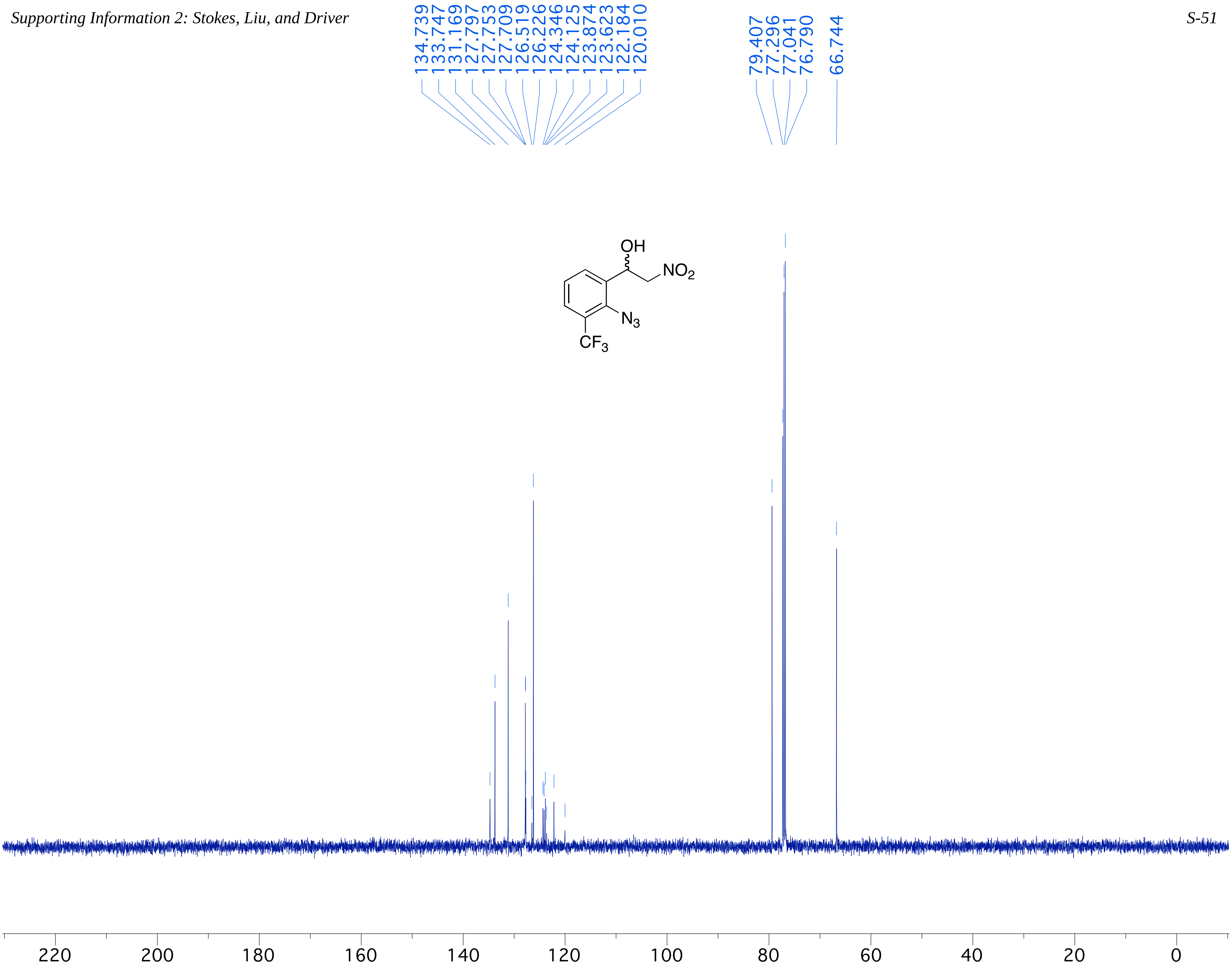


BJS iv131.0F1
^{1}H (500 MHz), $CDCl_3$

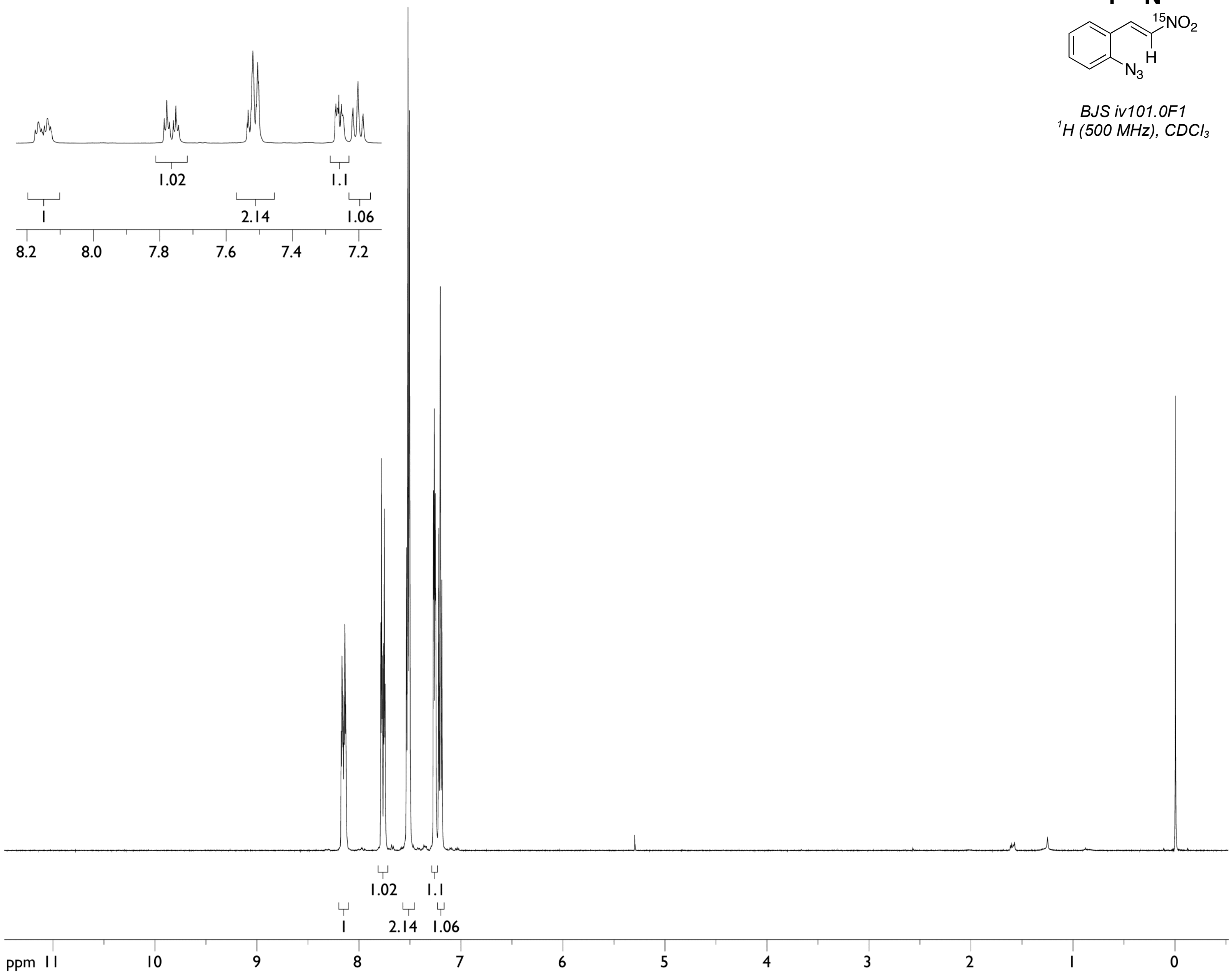



s30
Br
OH
NO_2
H
N_3
Br
BJS iv131.0F1
^{13}C (125 MHz), $CDCl_3$
ppm 220 200 180 160 140 120 100 80 60 40 20 0


7.845
7.829
7.705
7.690
7.402
7.386
7.371
7.259
5.865
5.861
5.847
5.842
4.688
4.683
4.661
4.656
4.519
4.500
4.492
4.473
3.185
OH
NO2
N3
CF3
1
1.01
1.05
1
1.01
1.04
0.982
ppm 11
10
9
8
7
6
5
4
3
2
1
0



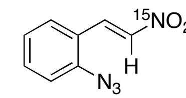
134.739
133.747
131.169
127.797
127.753
127.709
126.519
126.226
124.346
124.125
123.874
123.623
122.184
120.010
79.407
77.296
77.041
76.790
66.744
OH
NO_2
N_3
CF_3
220
200
180
160
140
120
100
80
60
40
20
0



1-^{15}N

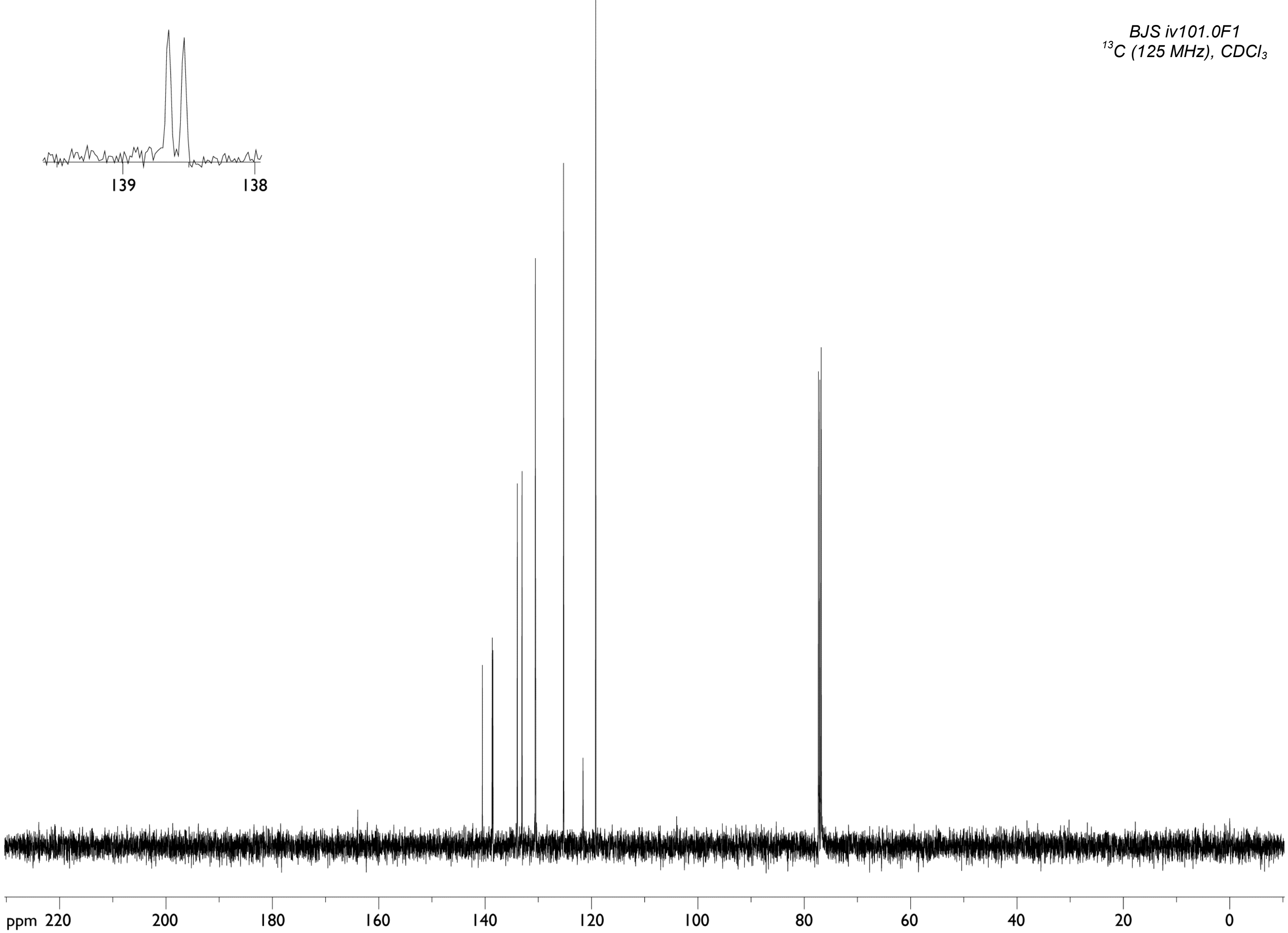
BJS iv101.0F1

^{1}H (500 MHz), $CDCl_3$

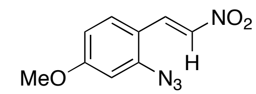


1-^{15}N

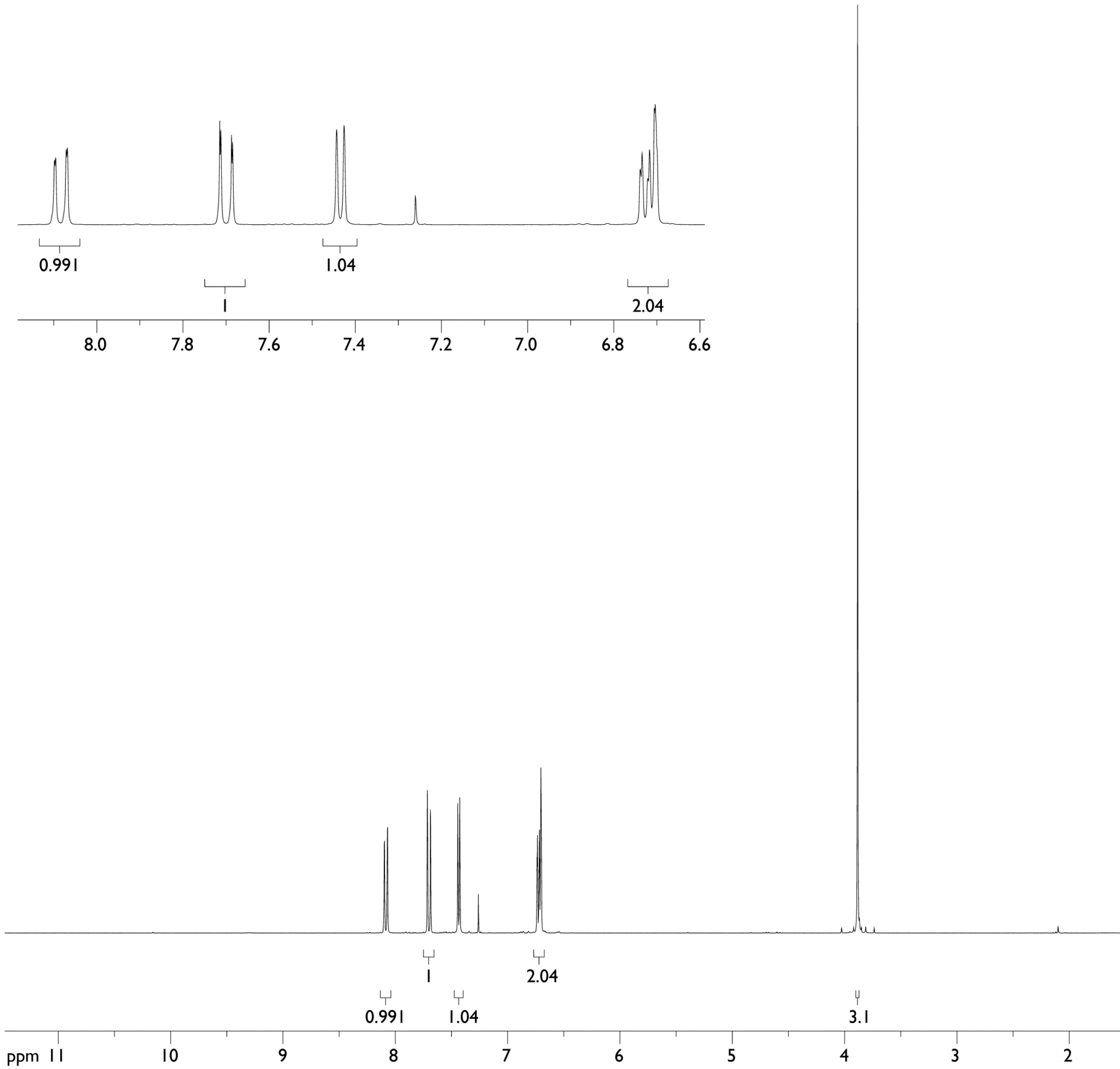
BJS iv101.0F1
^{13}C (125 MHz), CDCl$_3$



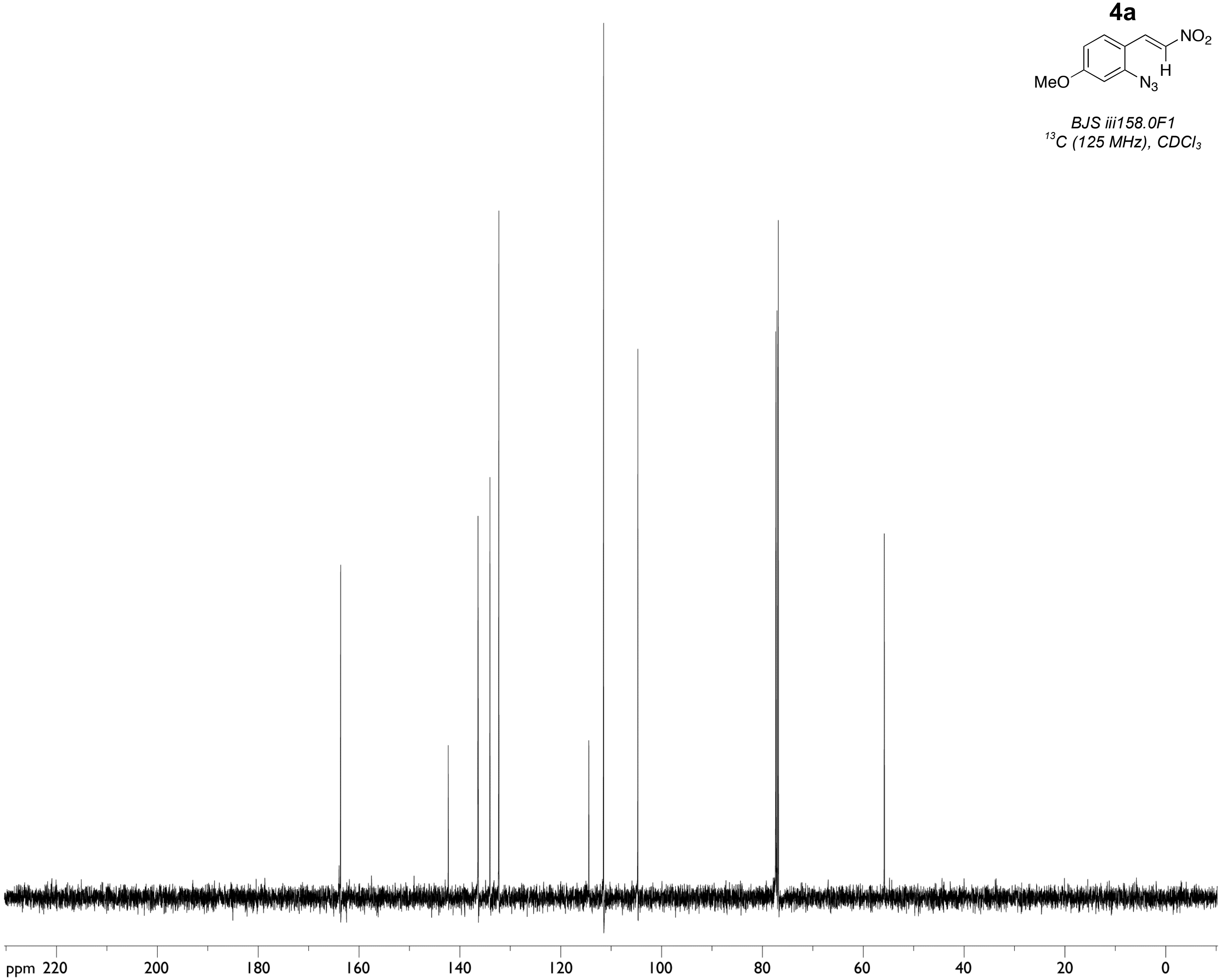
4a



BJS iii158.0F1
^{1}H (500 MHz), $CDCl_3$

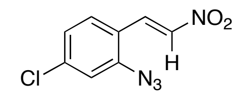


4a

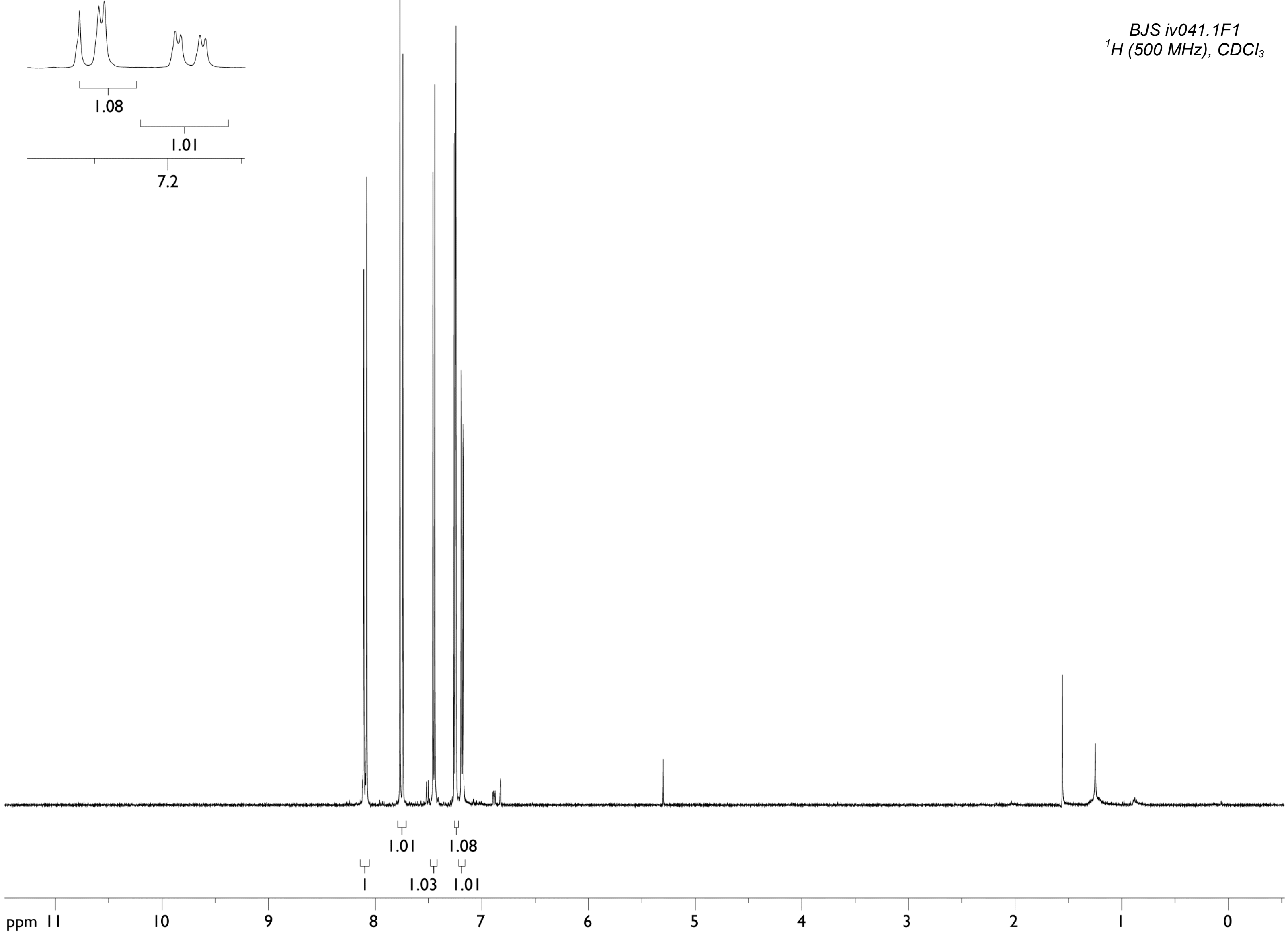


BJS iii158.0F1
^{13}C (125 MHz), $CDCl_3$

4b

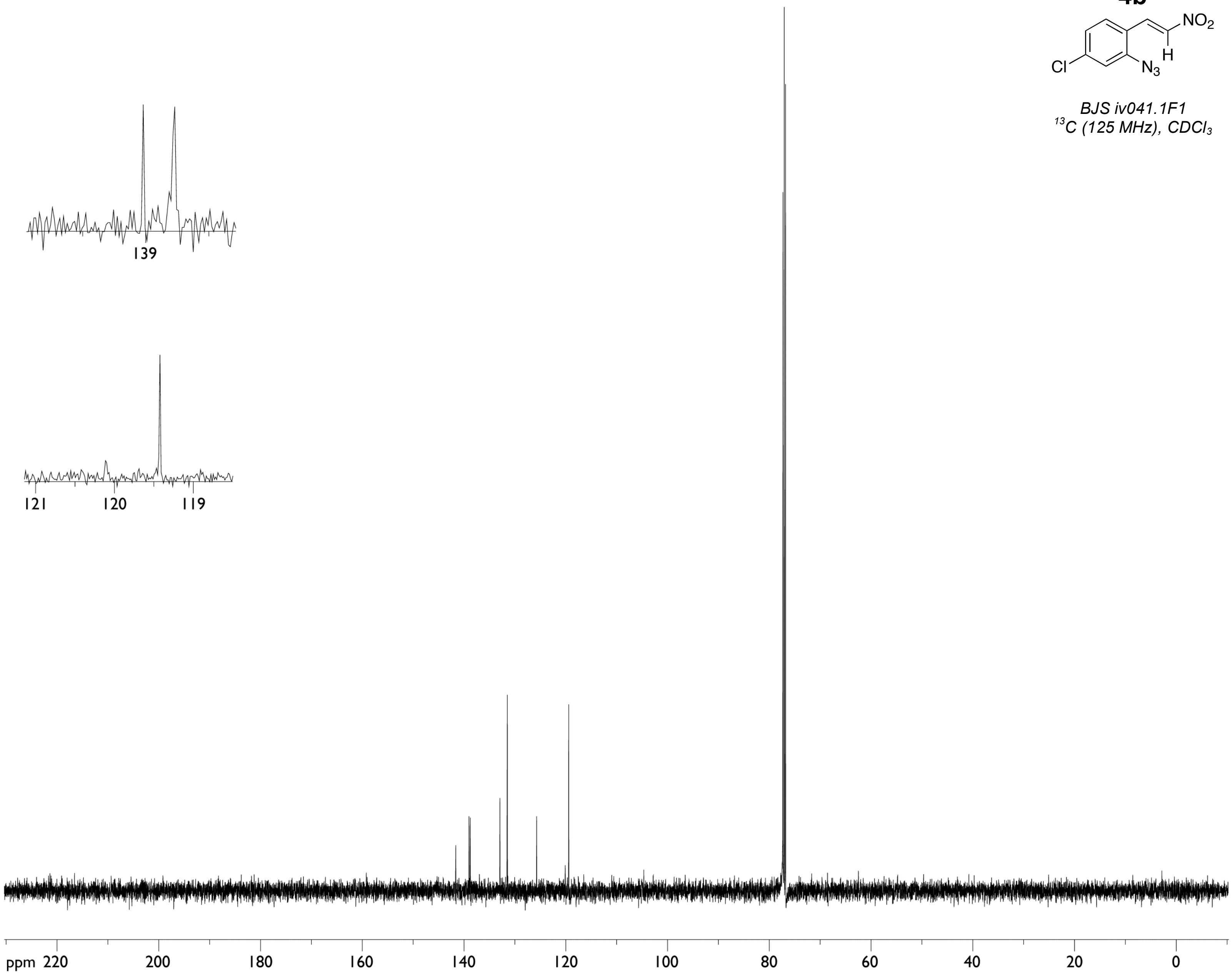


BJS iv041.1F1
^{1}H (500 MHz), $CDCl_3$

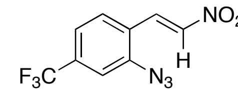


4b

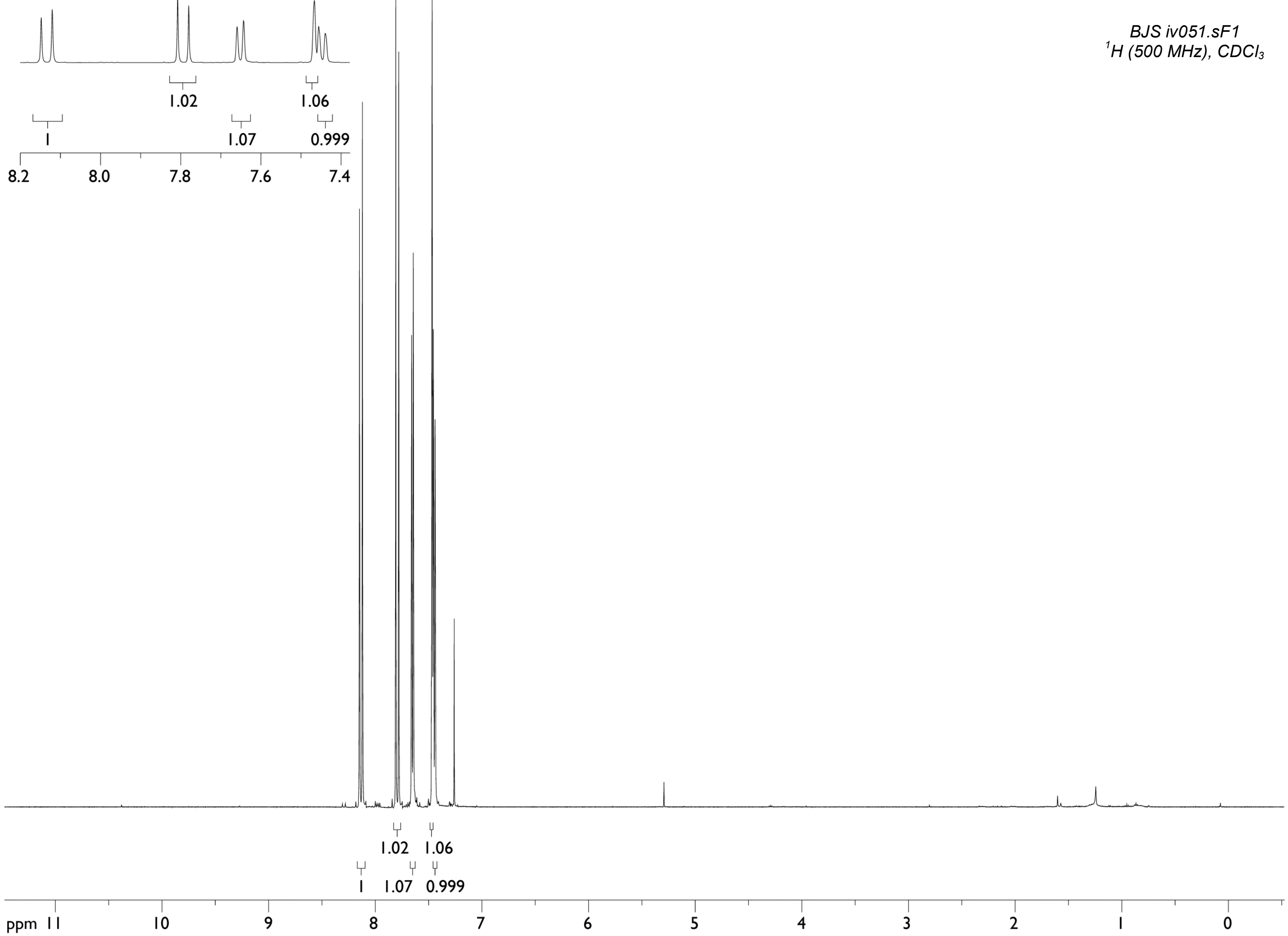
BJS iv041.1F1
^{13}C (125 MHz), $CDCl_3$



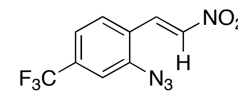
4c



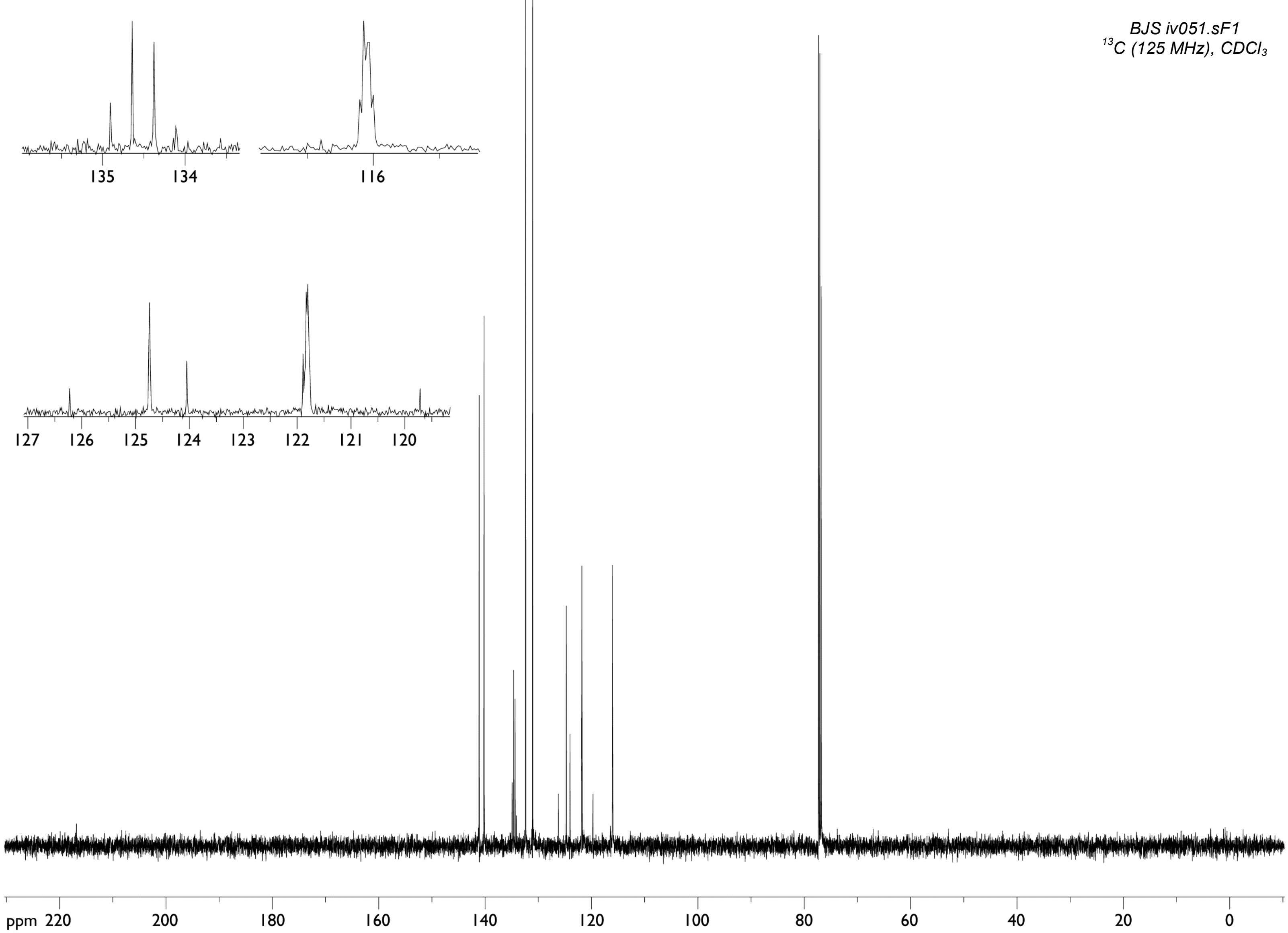
BJS iv051.sF1
^{1}H (500 MHz), $CDCl_3$



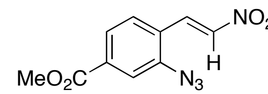
4c



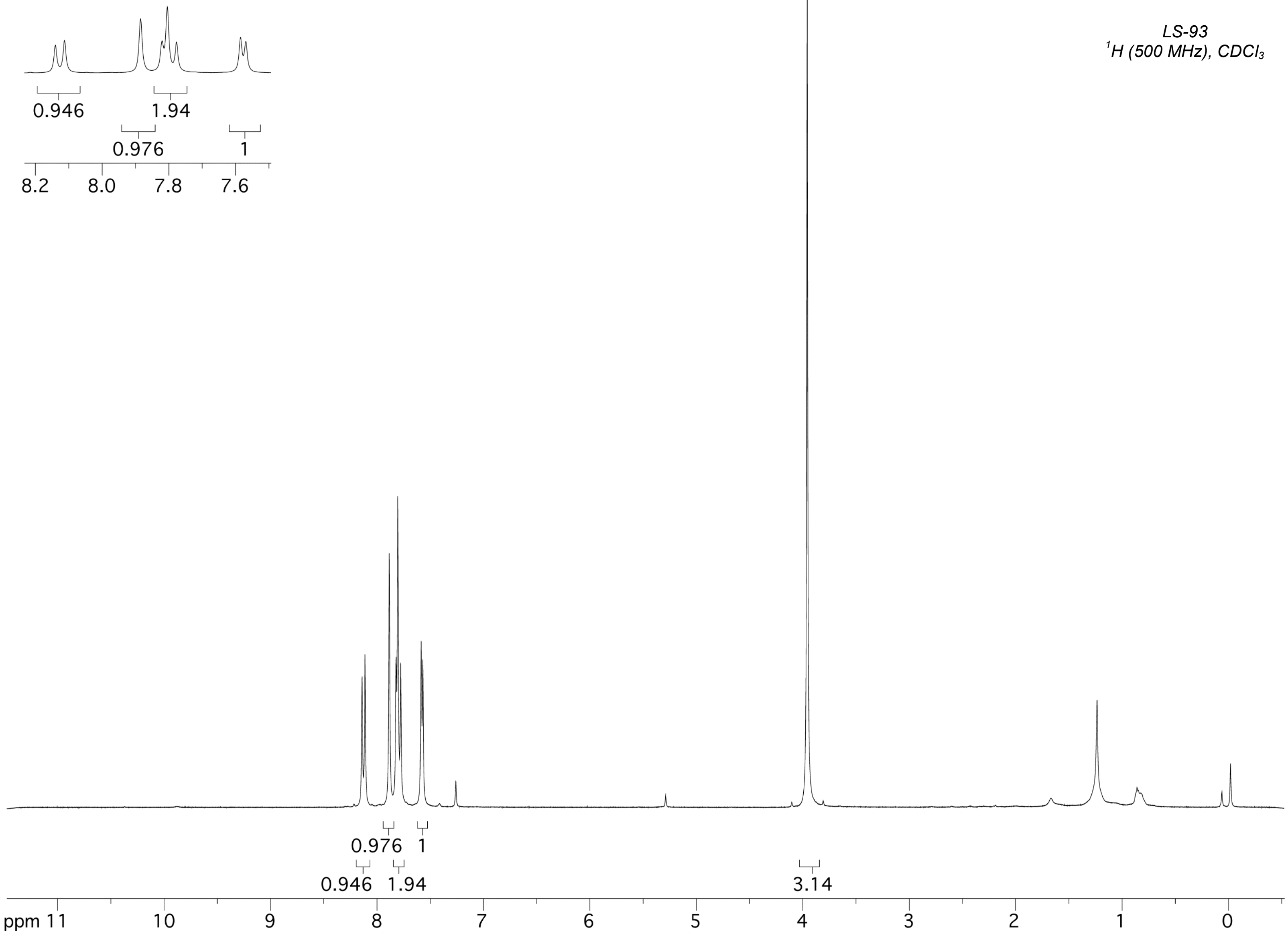
BJS iv051.sF1
^{13}C (125 MHz), $CDCl_3$



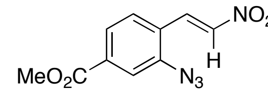
4d



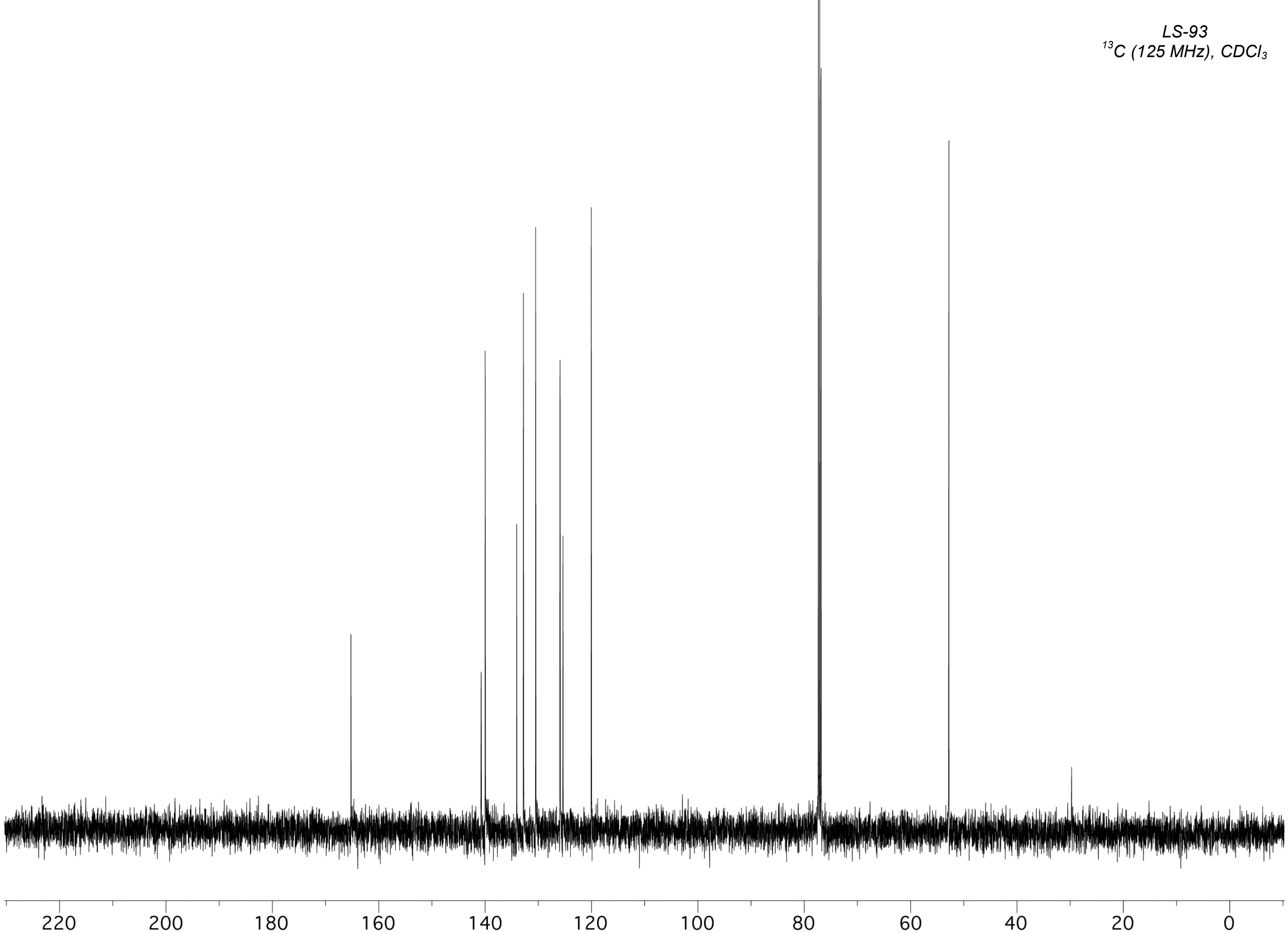
LS-93
^{1}H (500 MHz), CDCl$_3$

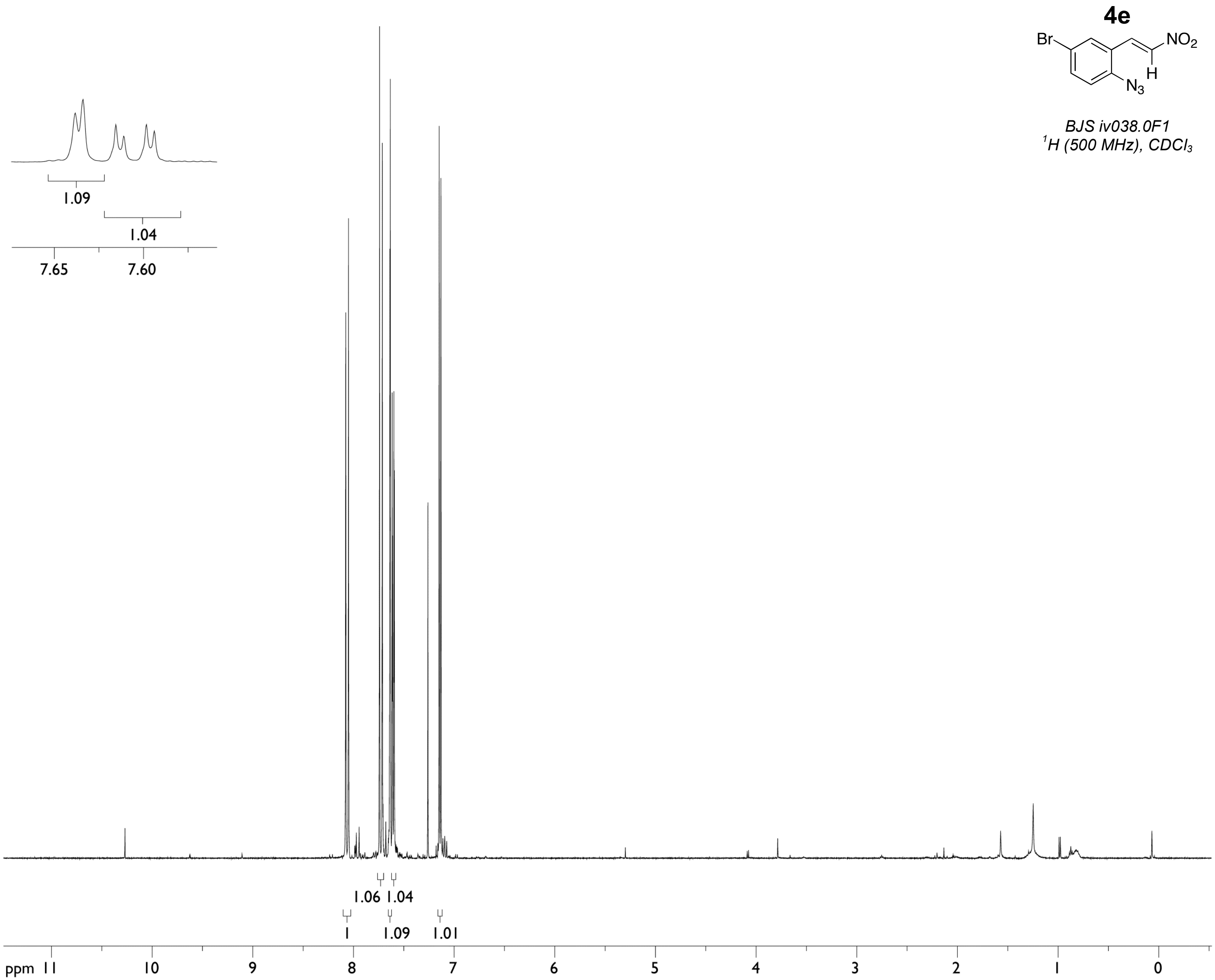


4d

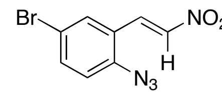


LS-93
^{13}C (125 MHz), CDCl$_3$

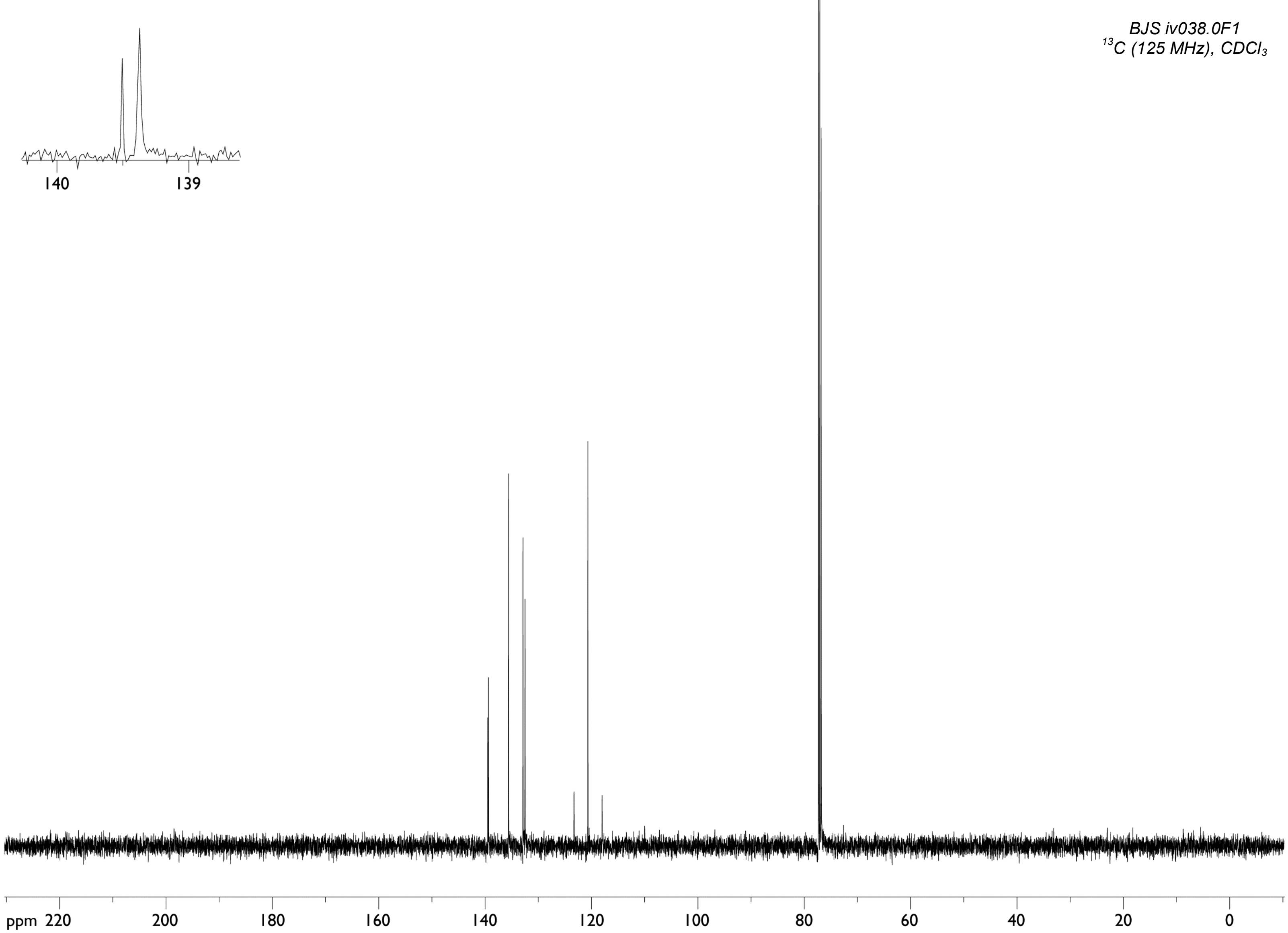



4e
Br
NO_2
H
N_3
BJS iv038.0F1
^{1}H (500 MHz), CDCl$_3$
1.09
1.04
7.65
7.60
1.06
1.04
1
1.09
1.01
ppm
11
10
9
8
7
6
5
4
3
2
1
0

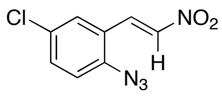
4e



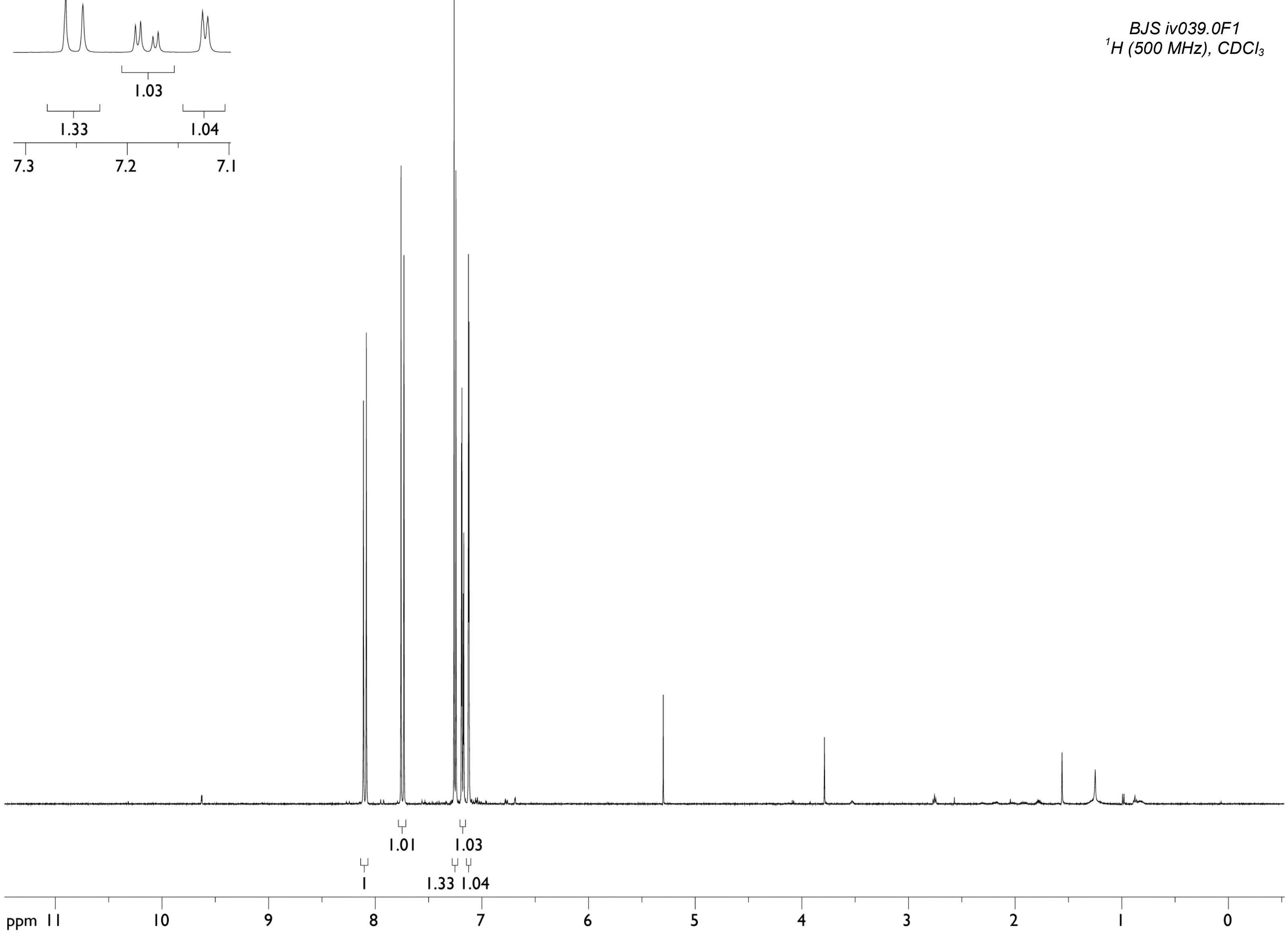
BJS iv038.0F1
^{13}C (125 MHz), $CDCl_3$



4f

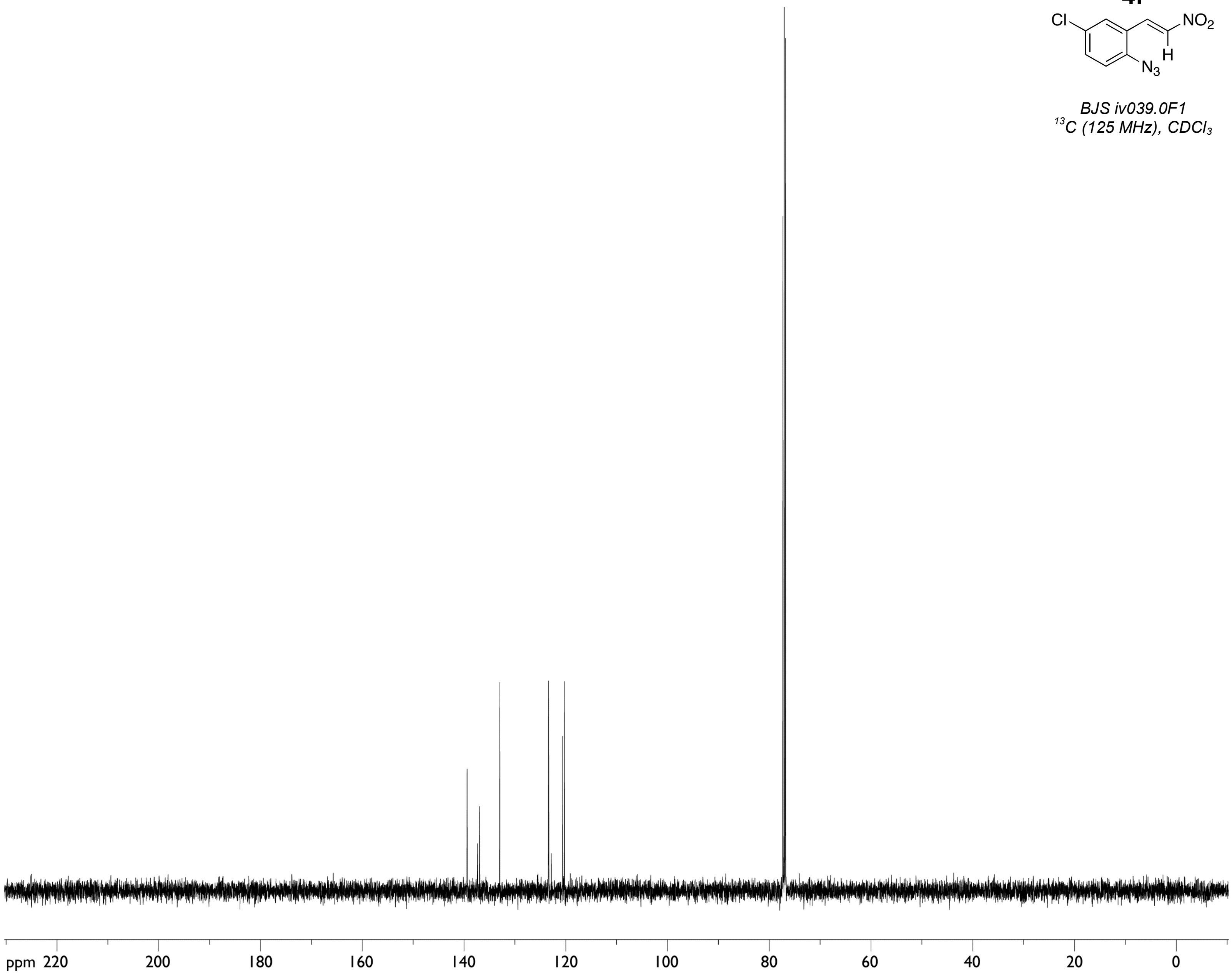


BJS iv039.0F1
^{1}H (500 MHz), CDCl$_3$

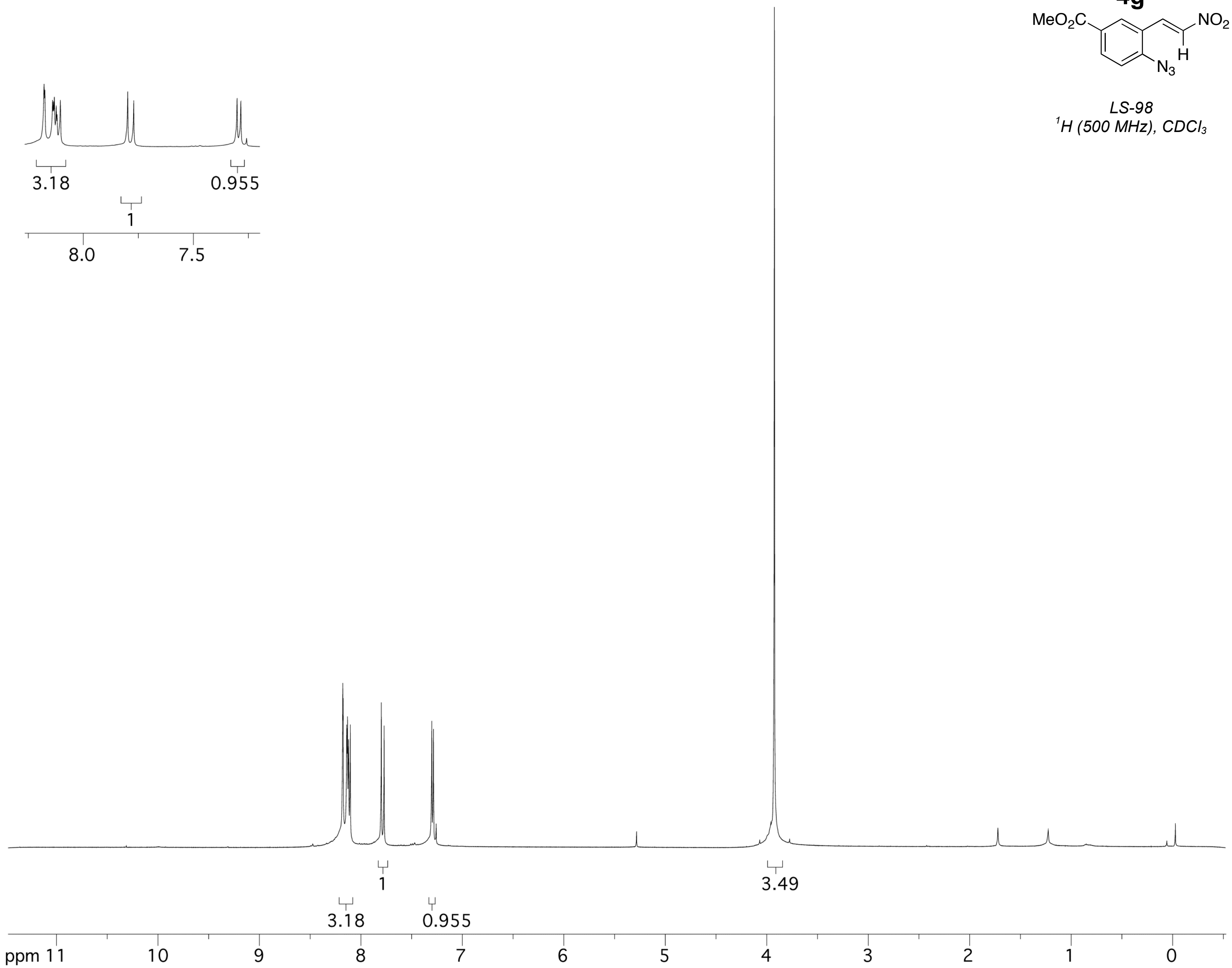


4f

BJS iv039.0F1
^{13}C (125 MHz), $CDCl_3$

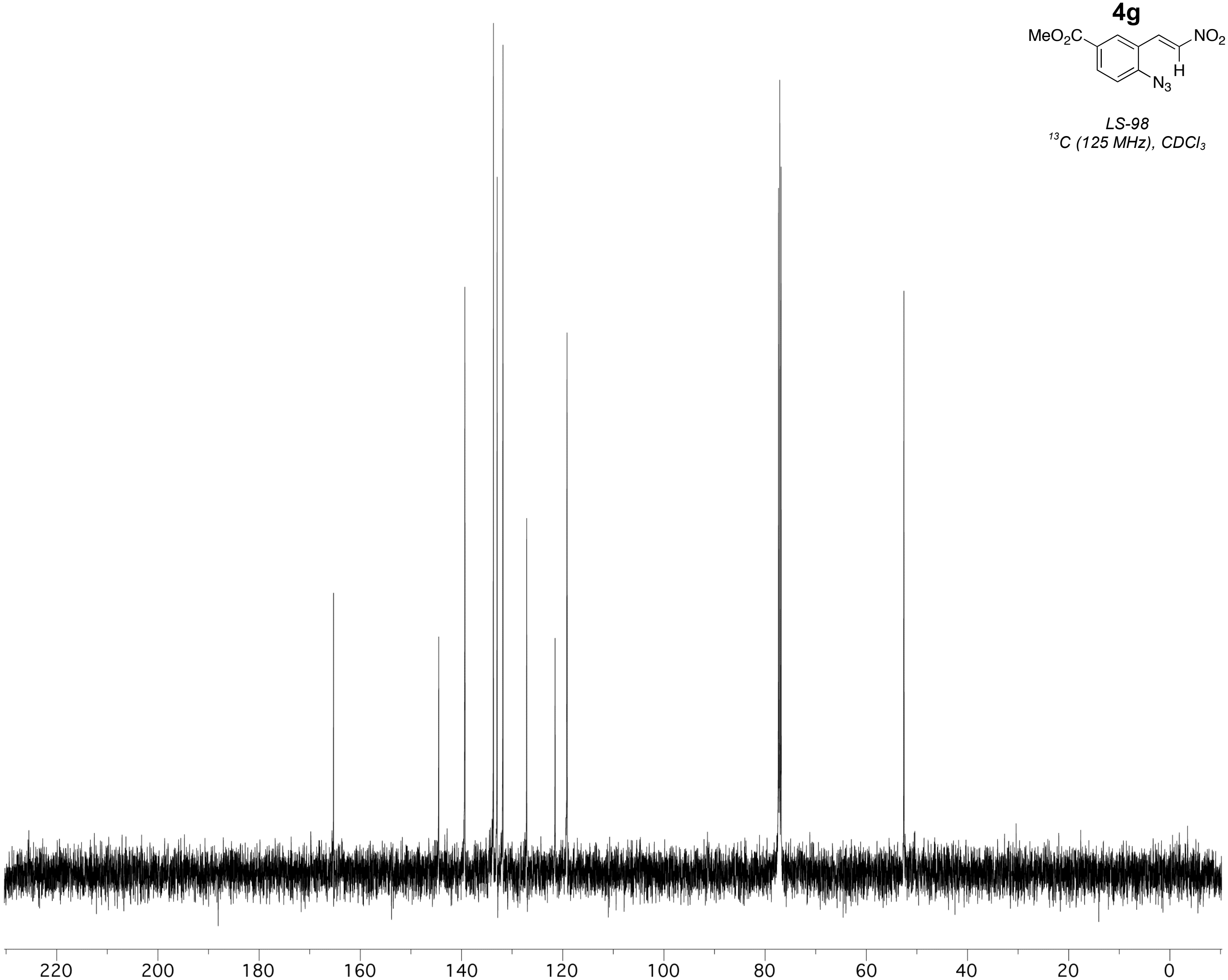


4g



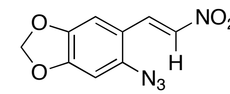
LS-98
^{1}H (500 MHz), $CDCl_3$

4g

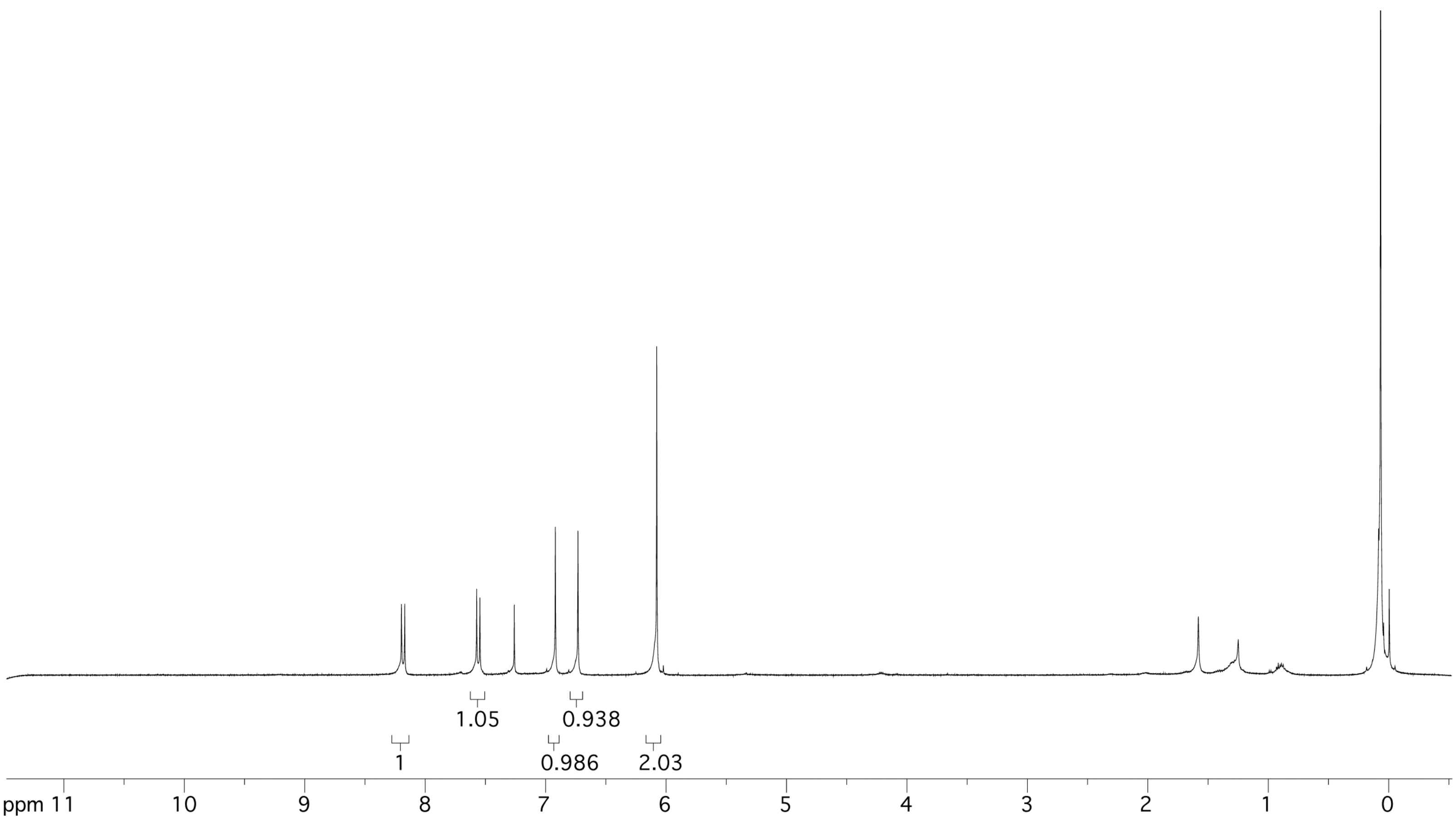


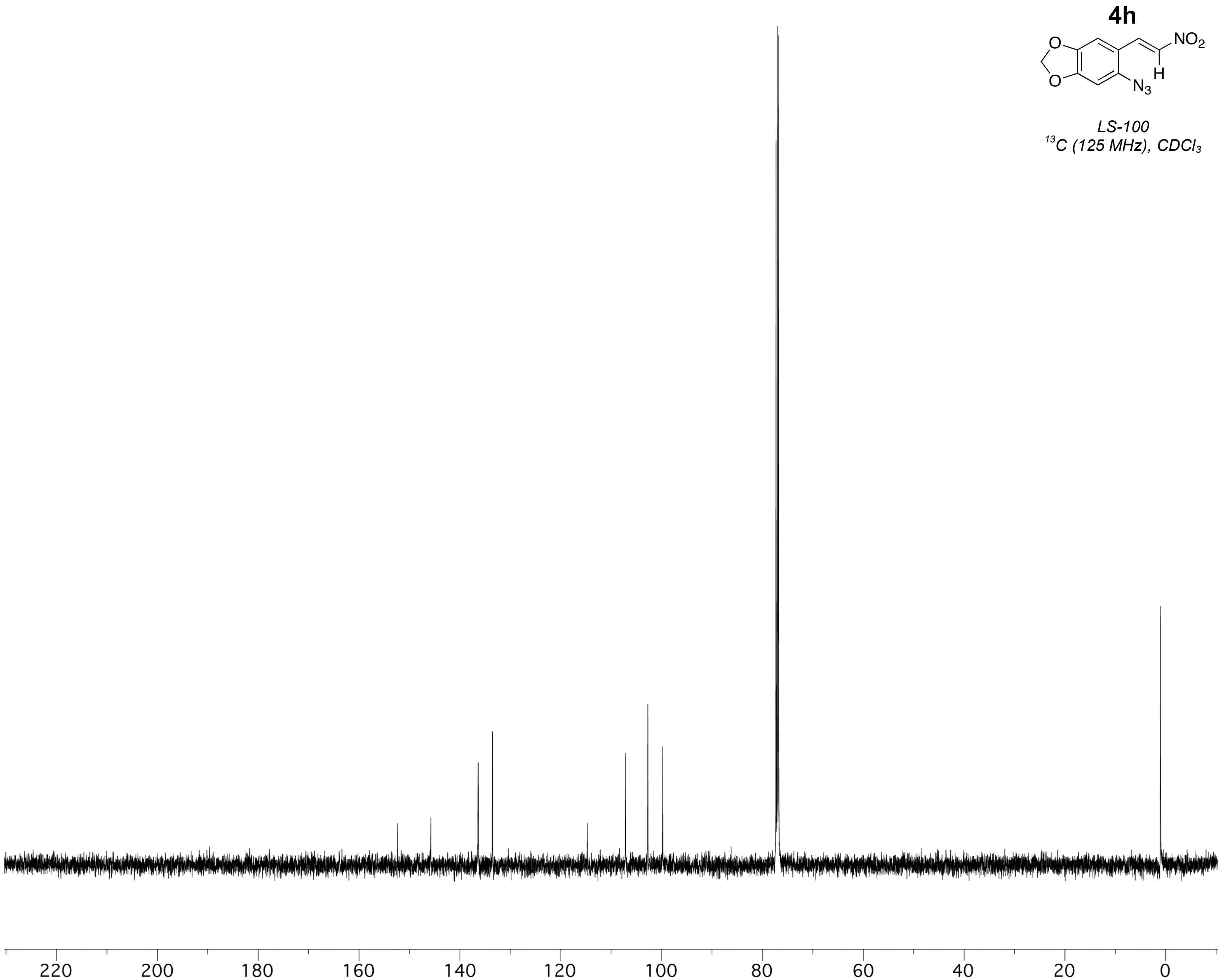
LS-98
^{13}*C (125 MHz), CDCl$_3$*

4h

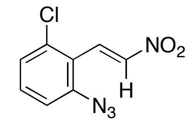


LS-100
^{1}H (500 MHz), $CDCl_3$



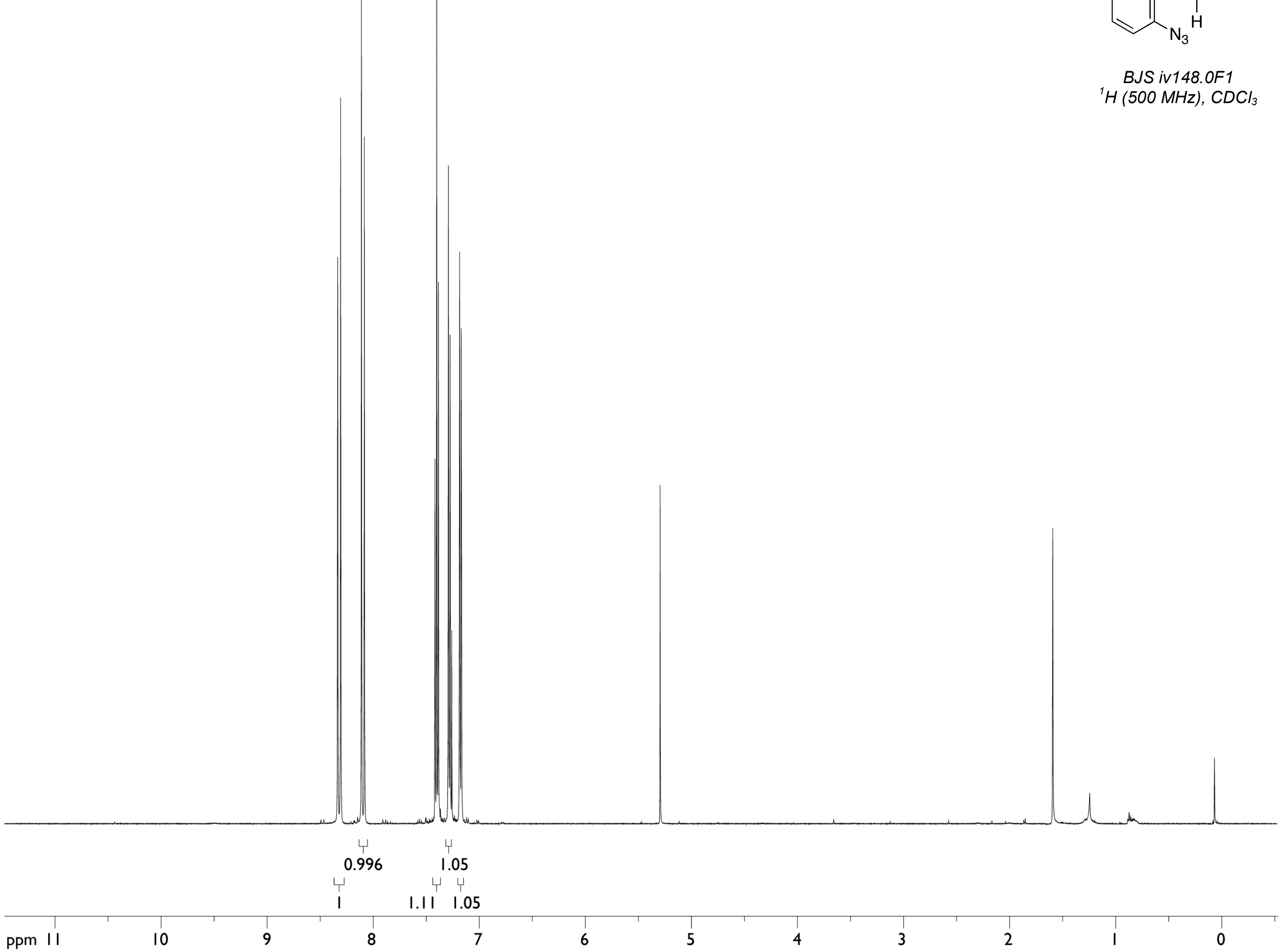

4h
NO2
O
O
H
N3
LS-100
13C (125 MHz), CDCl3
220
200
180
160
140
120
100
80
60
40
20
0

4i

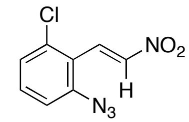


BJS iv148.0F1

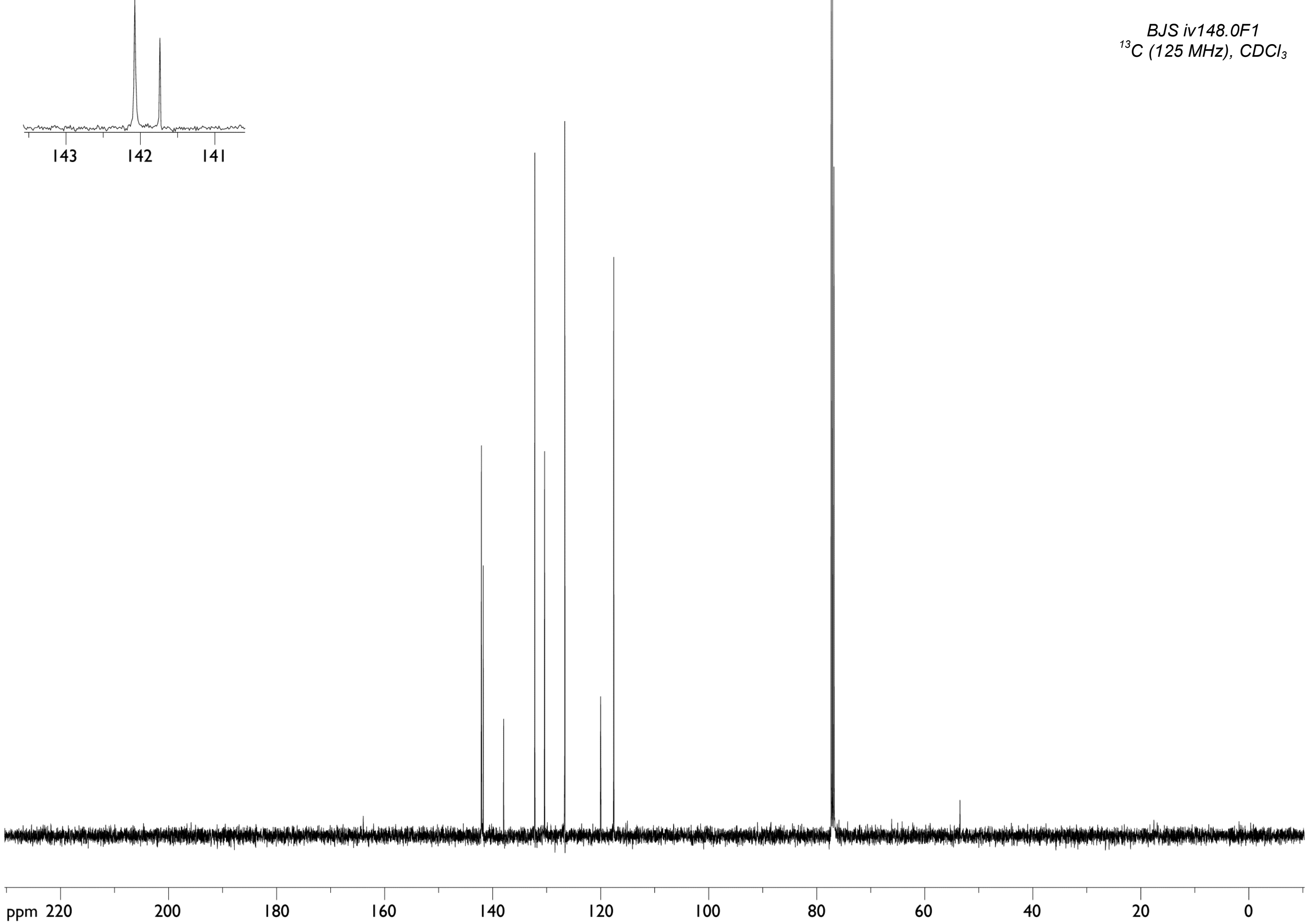
^{1}H (500 MHz), CDCl$_3$



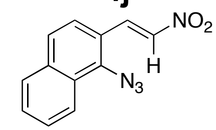
4i



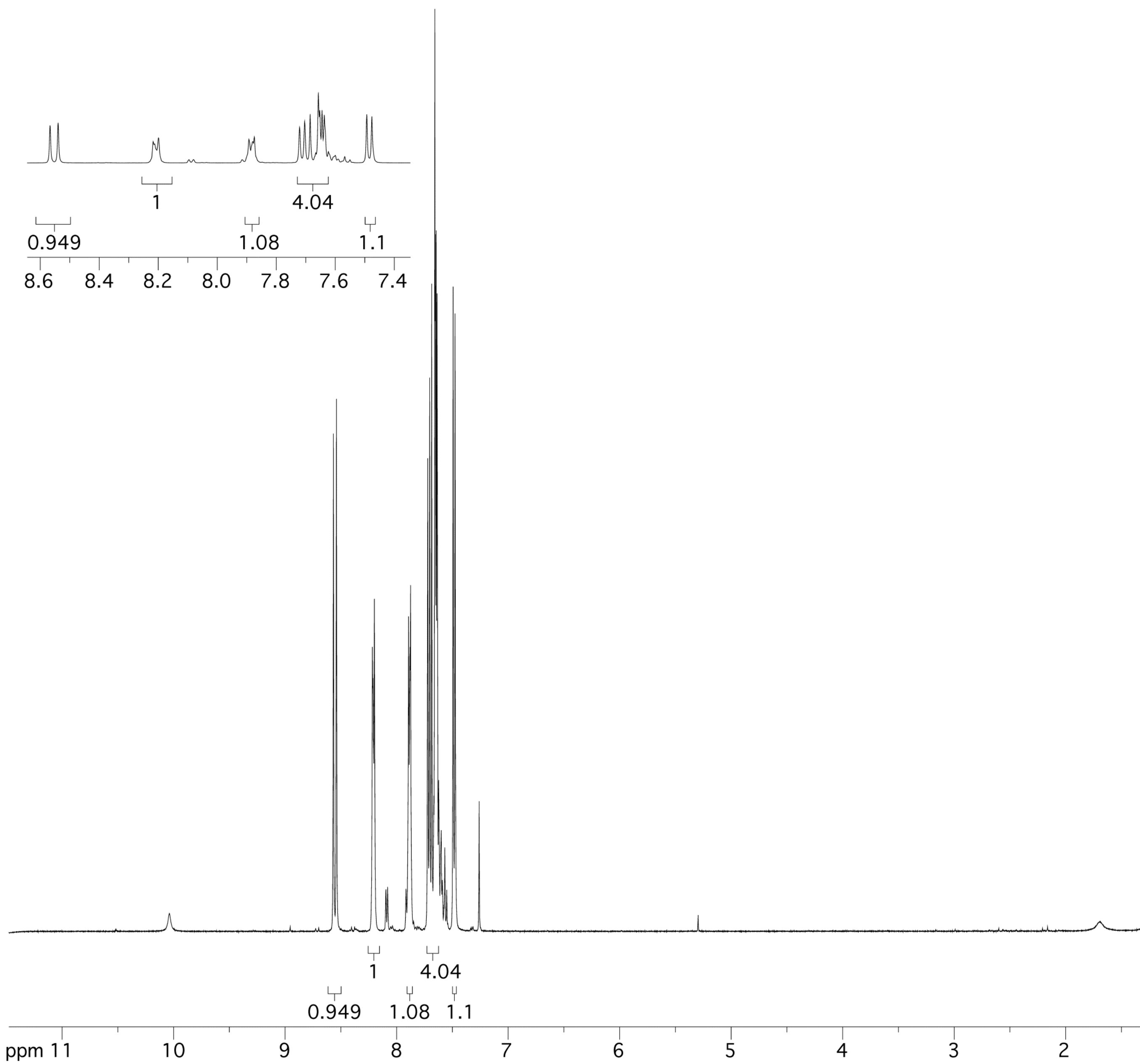
BJS iv148.0F1
^{13}C (125 MHz), $CDCl_3$



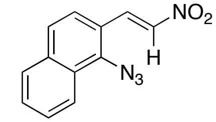
4j



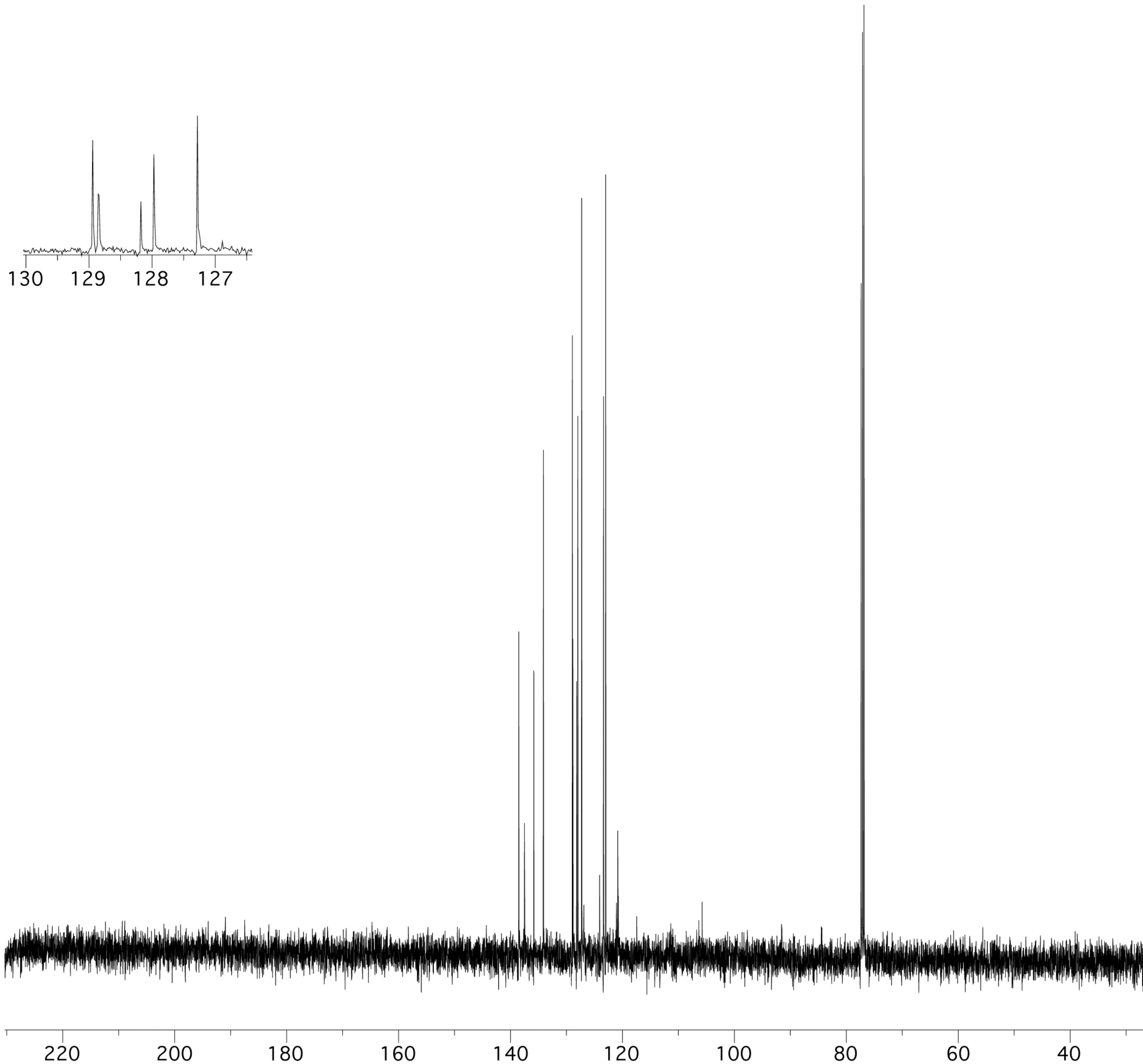
LS-102
^{1}H (500 MHz), $CDCl_3$



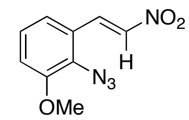
4j



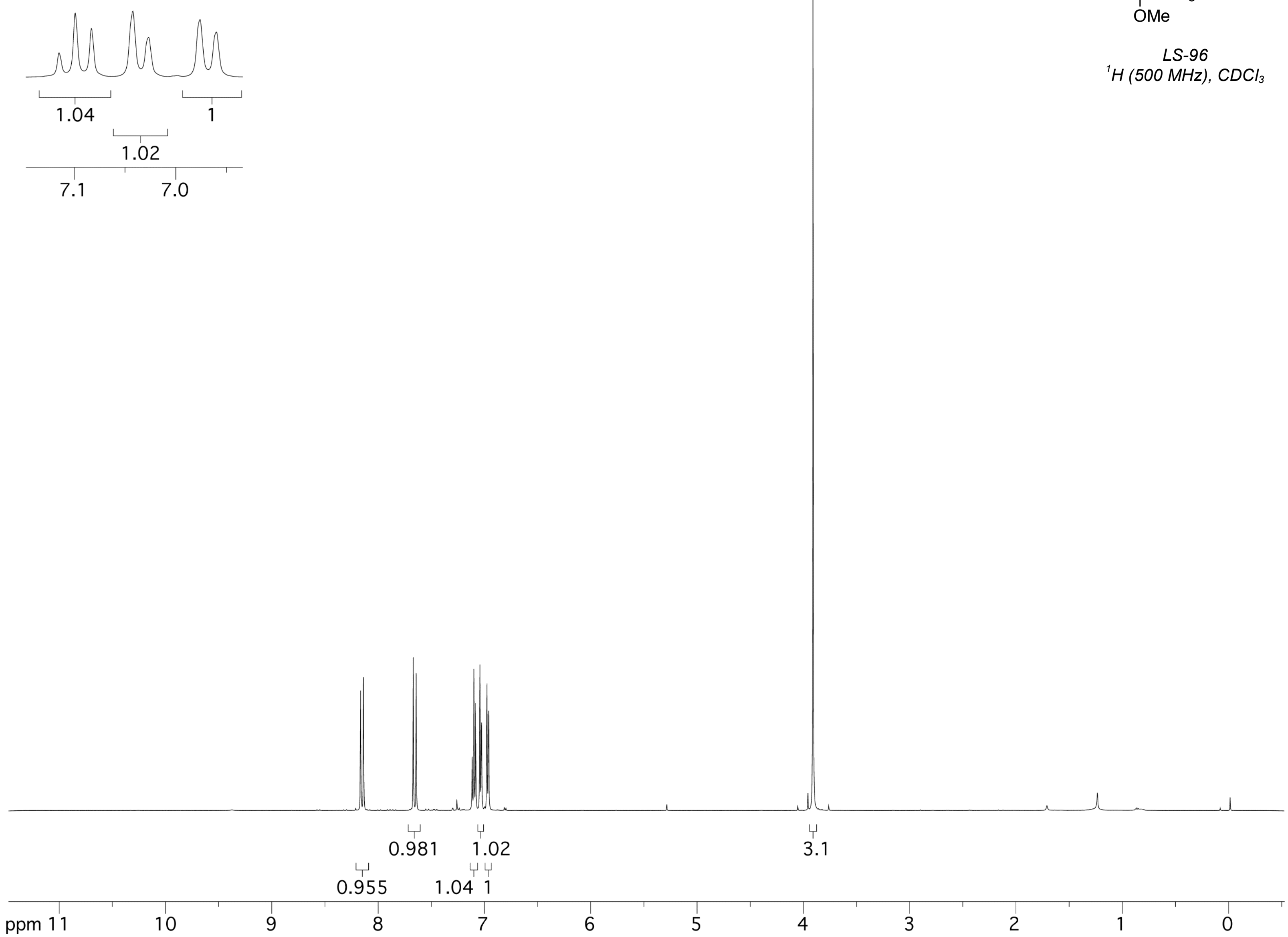
LS-102
^{13}C (125 MHz), $CDCl_3$



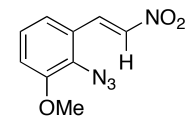
4k



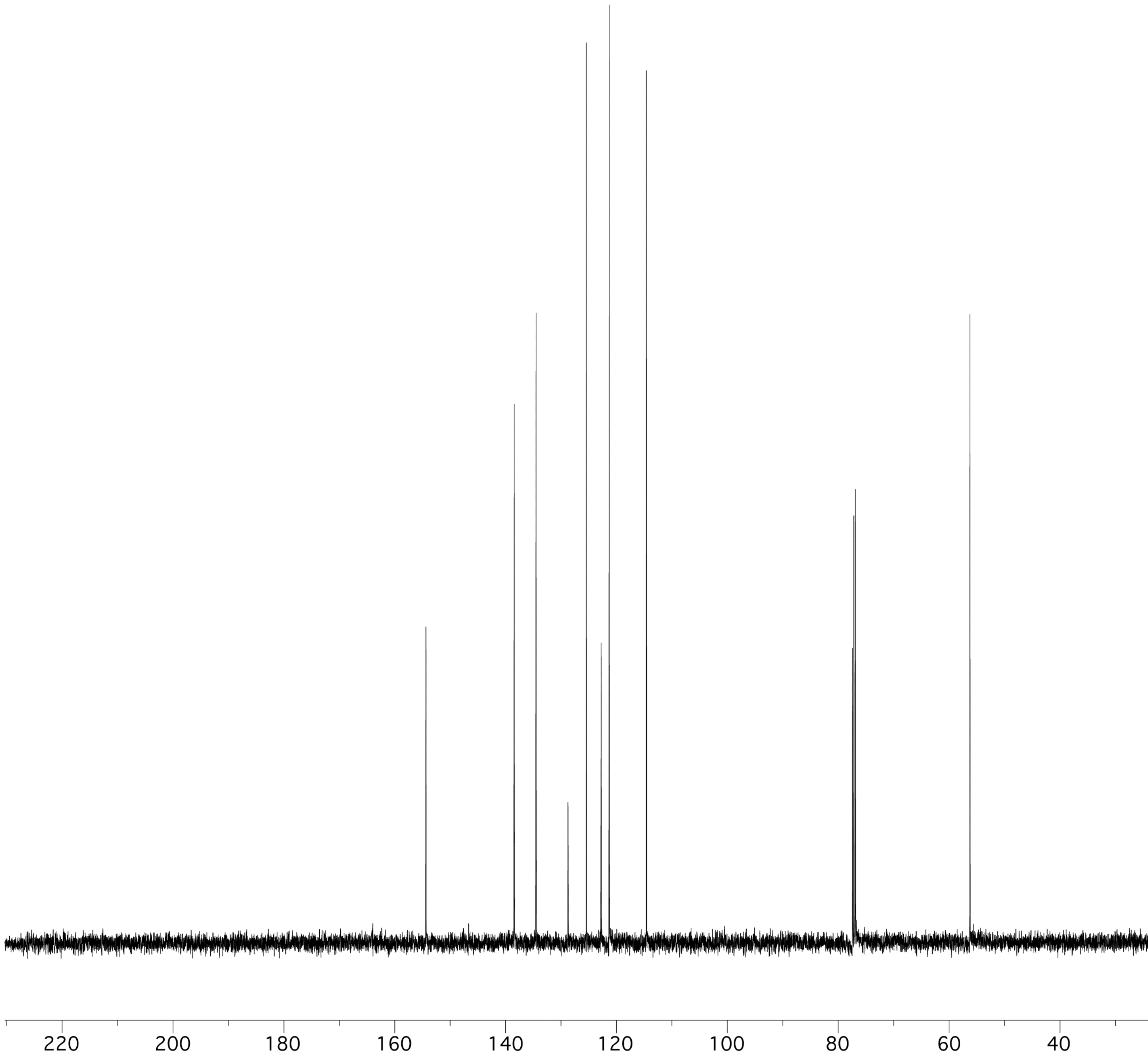
LS-96
^{1}H (500 MHz), CDCl$_3$

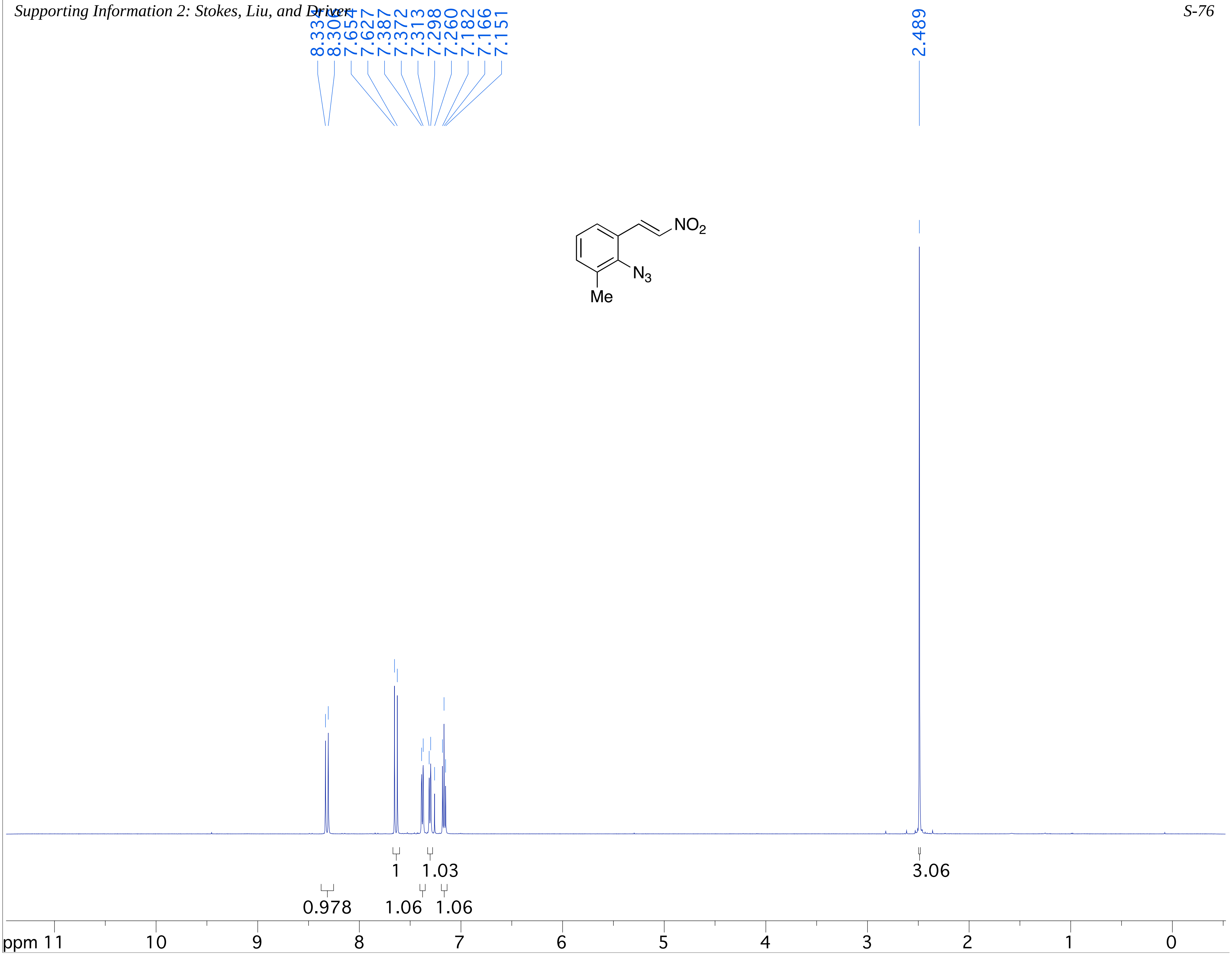


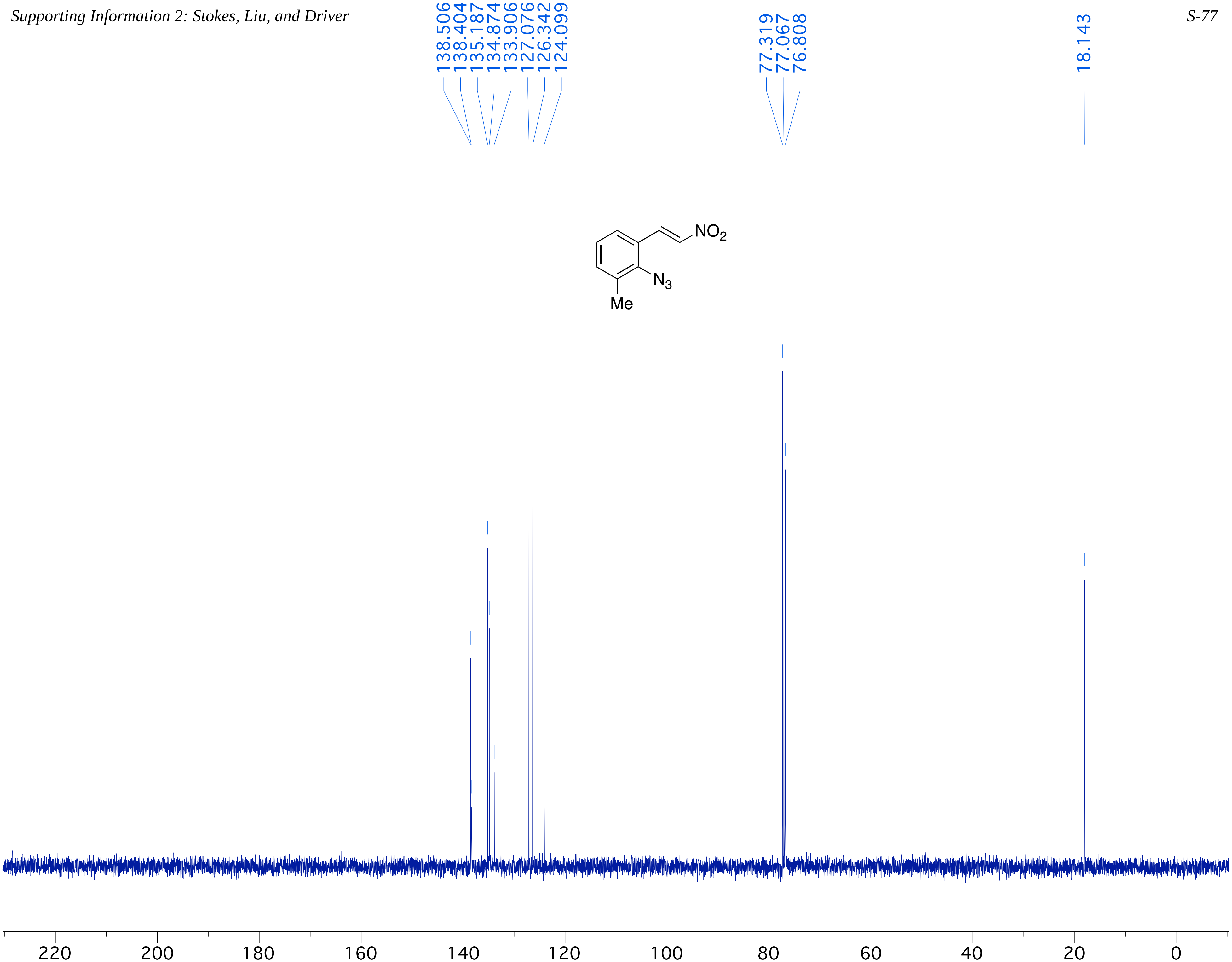
4k



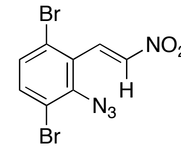
LS-96
^{13}C (125 MHz), CDCl$_3$



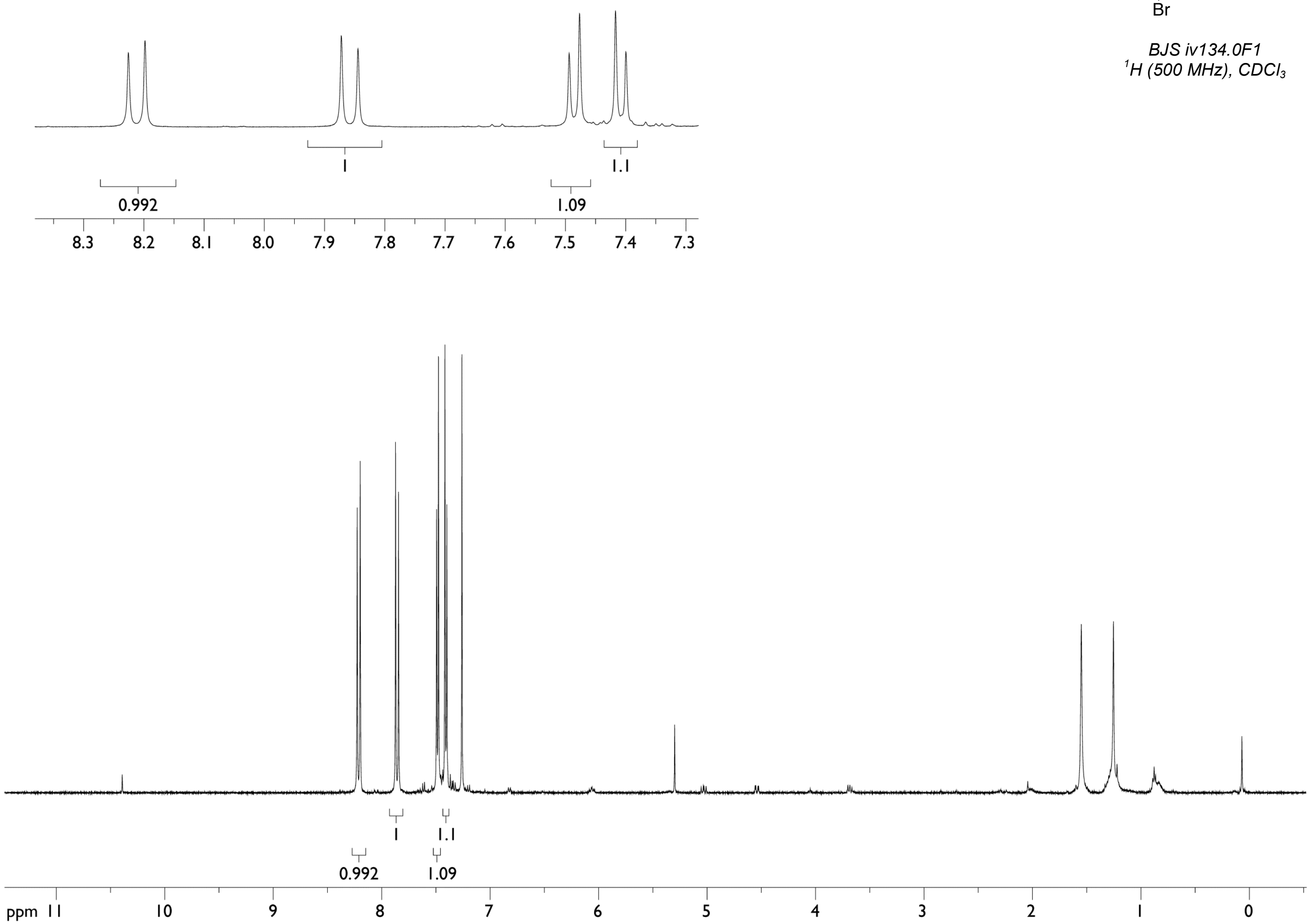

8.334
8.306
7.654
7.627
7.387
7.372
7.313
7.298
7.260
7.182
7.166
7.151
2.489
NO2
N3
Me
1
1.03
3.06
0.978
1.06
1.06
ppm 11
10
9
8
7
6
5
4
3
2
1
0


138.506
138.404
135.187
134.874
133.906
127.076
126.342
124.099
77.319
77.067
76.808
18.143
NO2
N3
Me
220
200
180
160
140
120
100
80
60
40
20
0

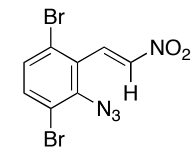
4l



BJS iv134.0F1
^1H (500 MHz), $CDCl_3$

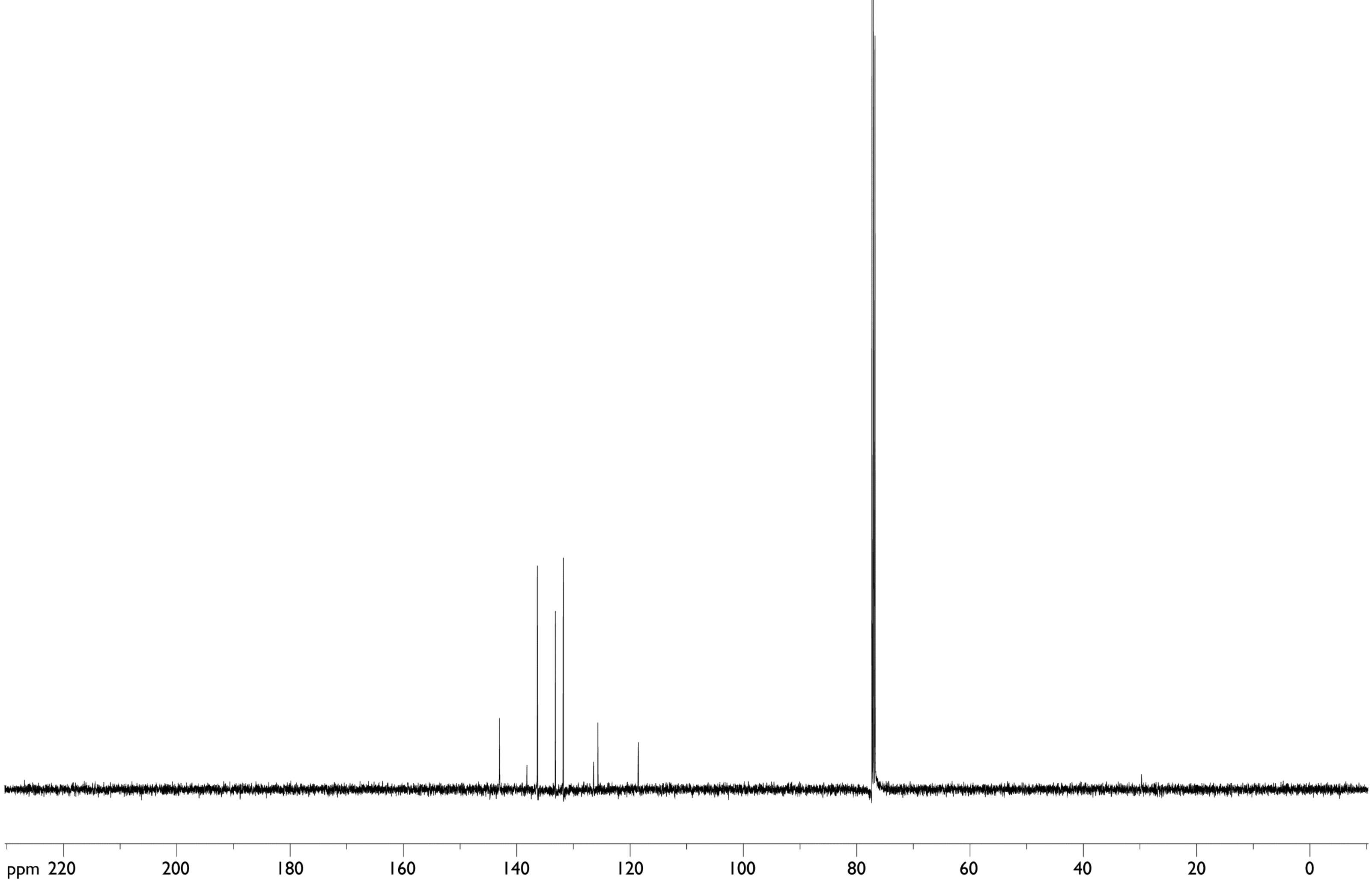


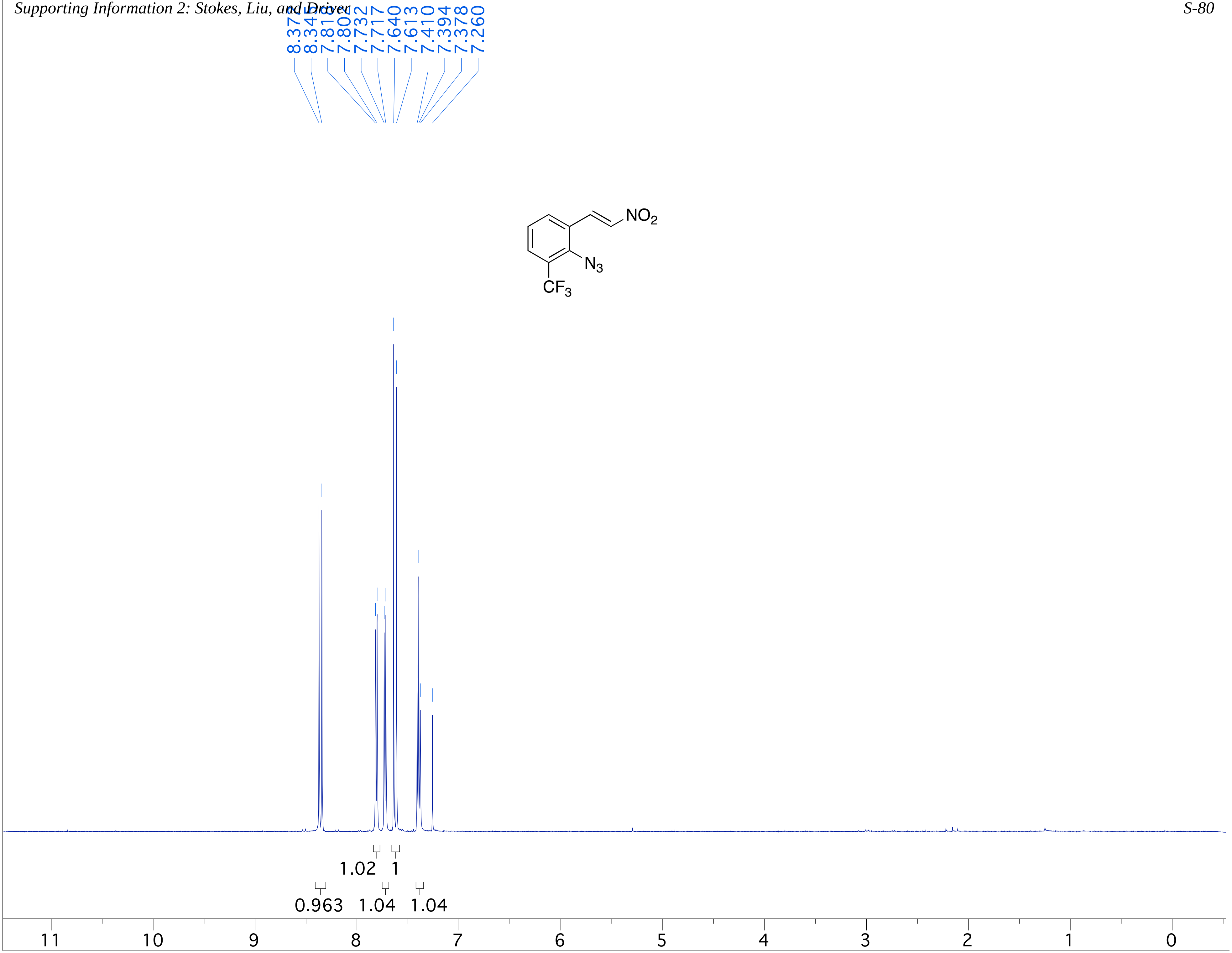
4l

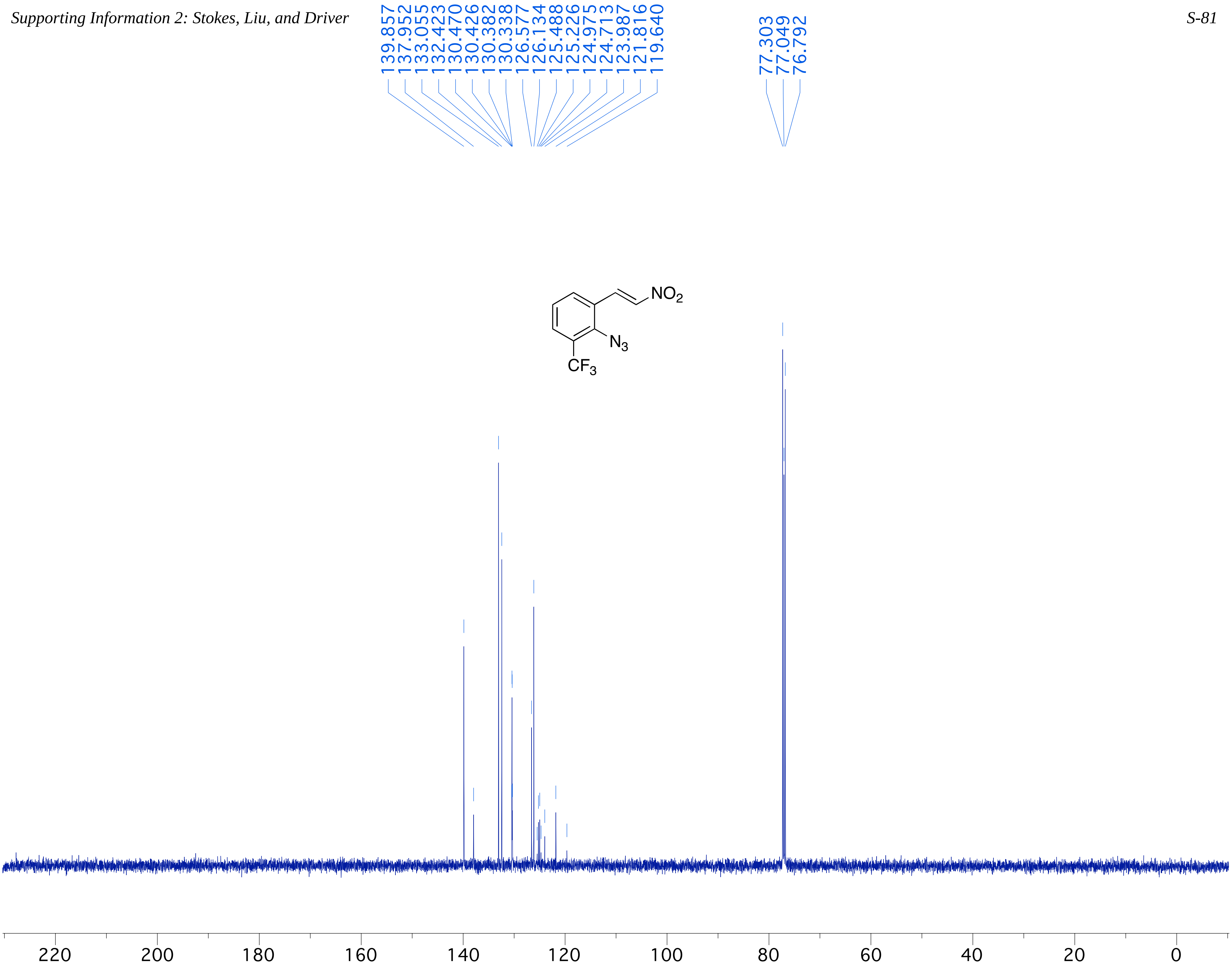


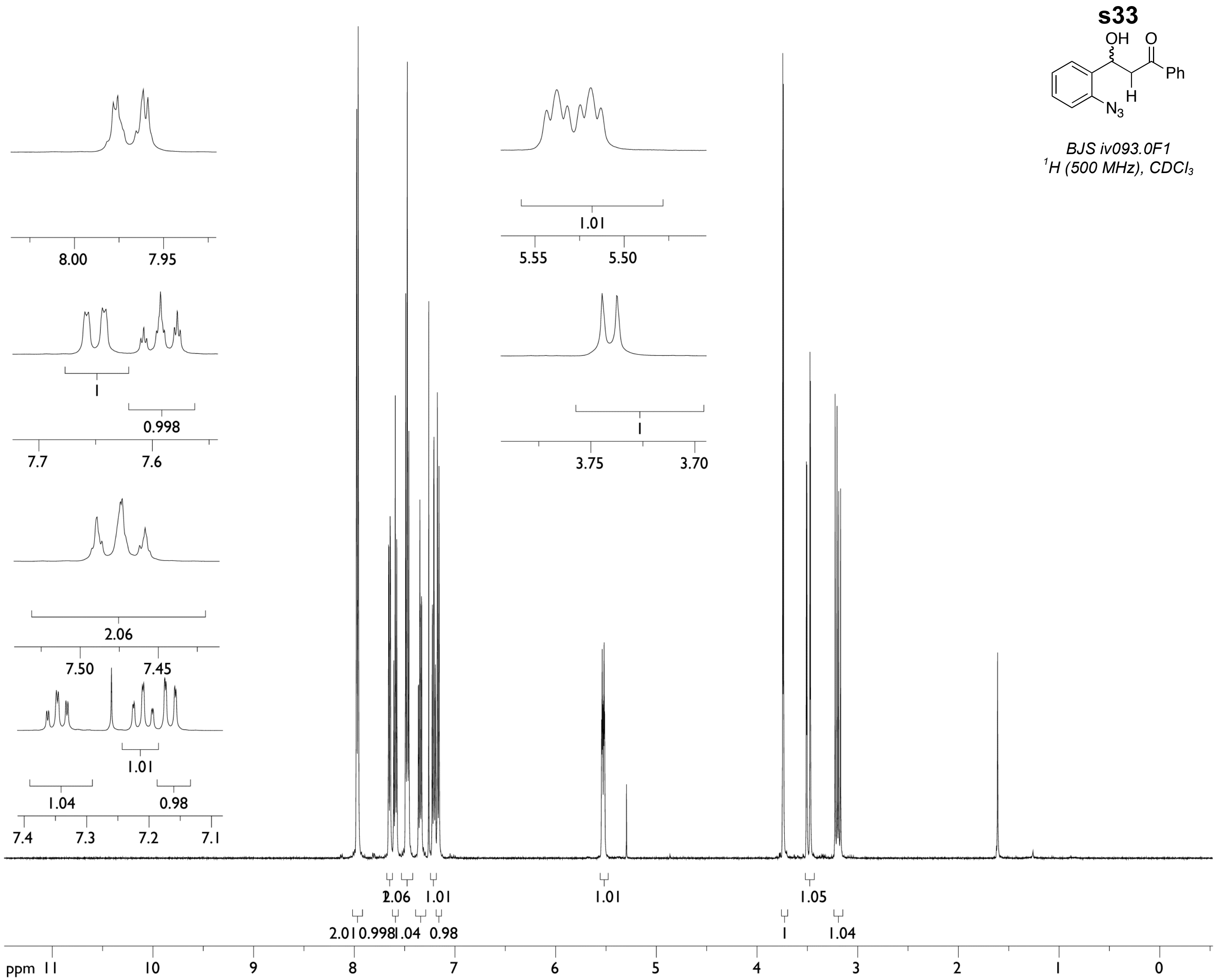
BJS iv134.0F1

^{13}C (125 MHz), CDCl$_3$

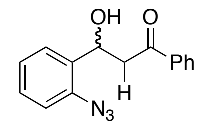



8.372
8.340
7.818
7.803
7.732
7.717
7.640
7.613
7.410
7.394
7.378
7.260
NO_2
N_3
CF_3
1.02
1
0.963
1.04
1.04
11
10
9
8
7
6
5
4
3
2
1
0

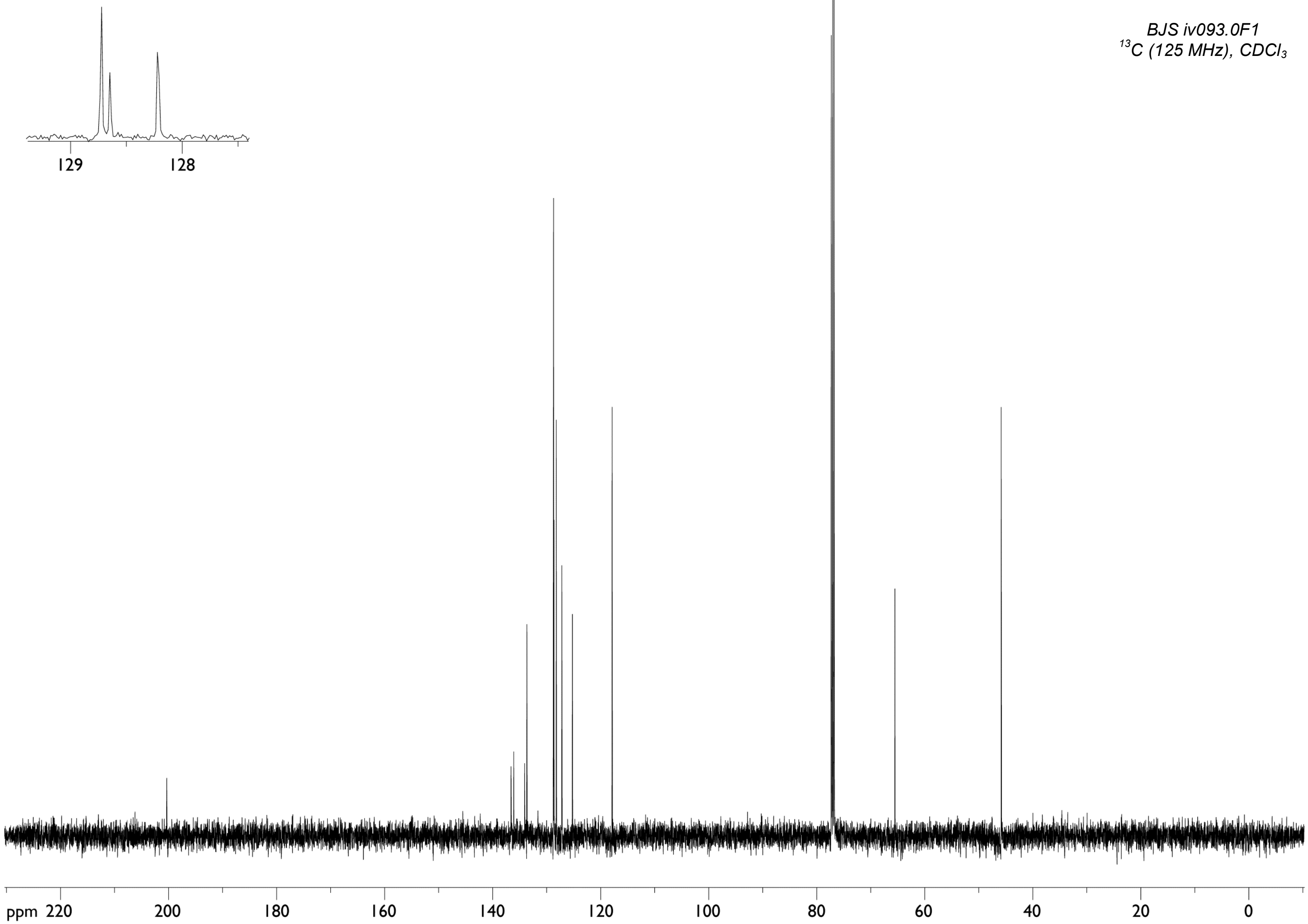

139.857
137.952
133.055
132.423
130.470
130.426
130.382
130.338
126.577
126.134
125.488
125.226
124.975
124.713
123.987
121.816
119.640
77.303
77.049
76.792
NO_2
N_3
CF_3
220
200
180
160
140
120
100
80
60
40
20
0


s33
OH
O
Ph
H
N3
BJS iv093.0F1
1H (500 MHz), CDCl3
8.00
7.95
1.01
5.55
5.50
1
0.998
7.7
7.6
1
3.75
3.70
2.06
7.50
7.45
1.01
1.04
0.98
7.4
7.3
7.2
7.1
2.06
1.01
1.01
1.05
2.01
0.998
1.04
0.98
1
1.04
ppm
11
10
9
8
7
6
5
4
3
2
1
0

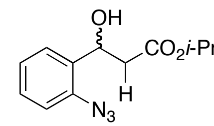
s33



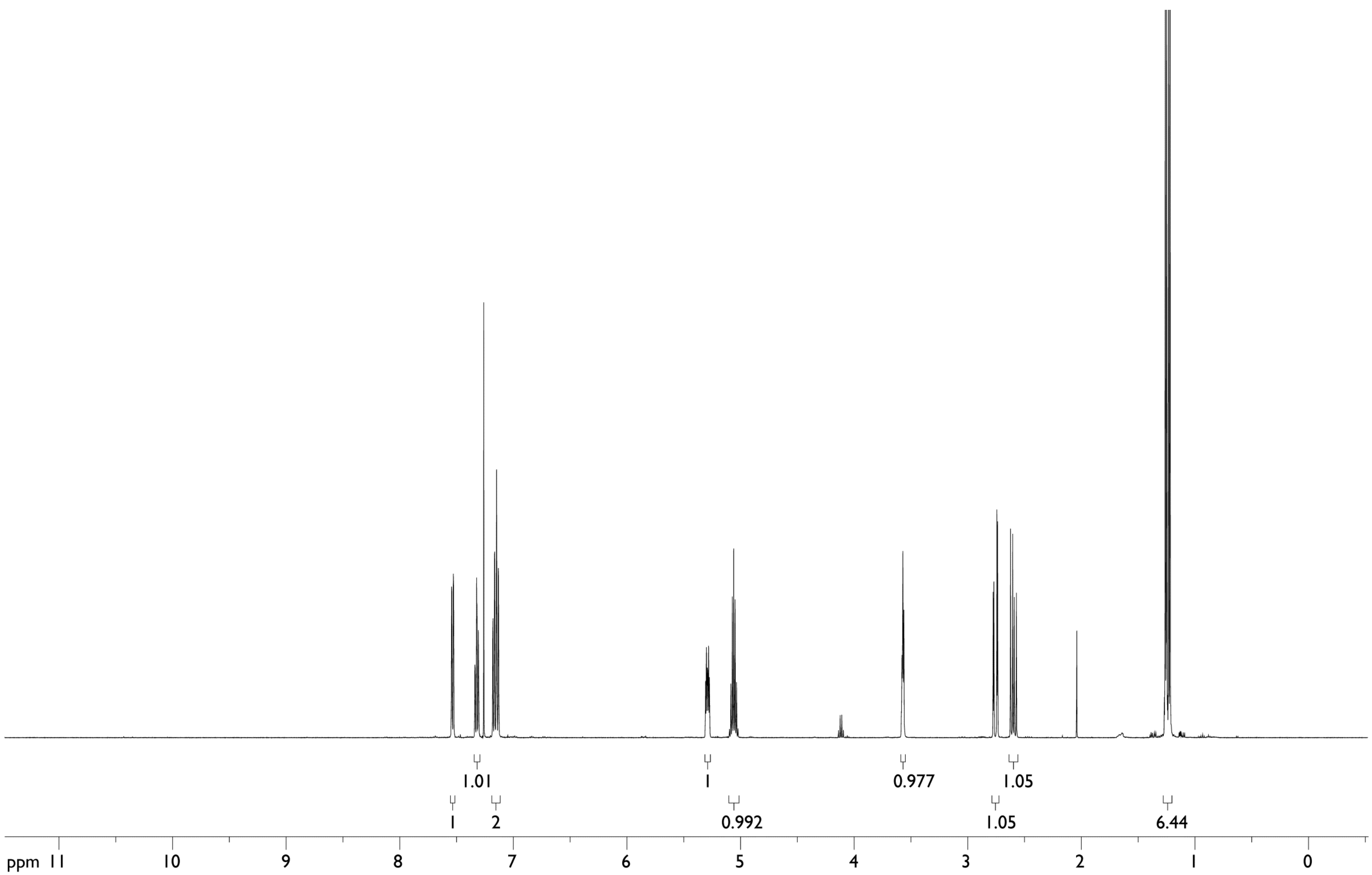
BJS iv093.0F1
^{13}C (125 MHz), $CDCl_3$

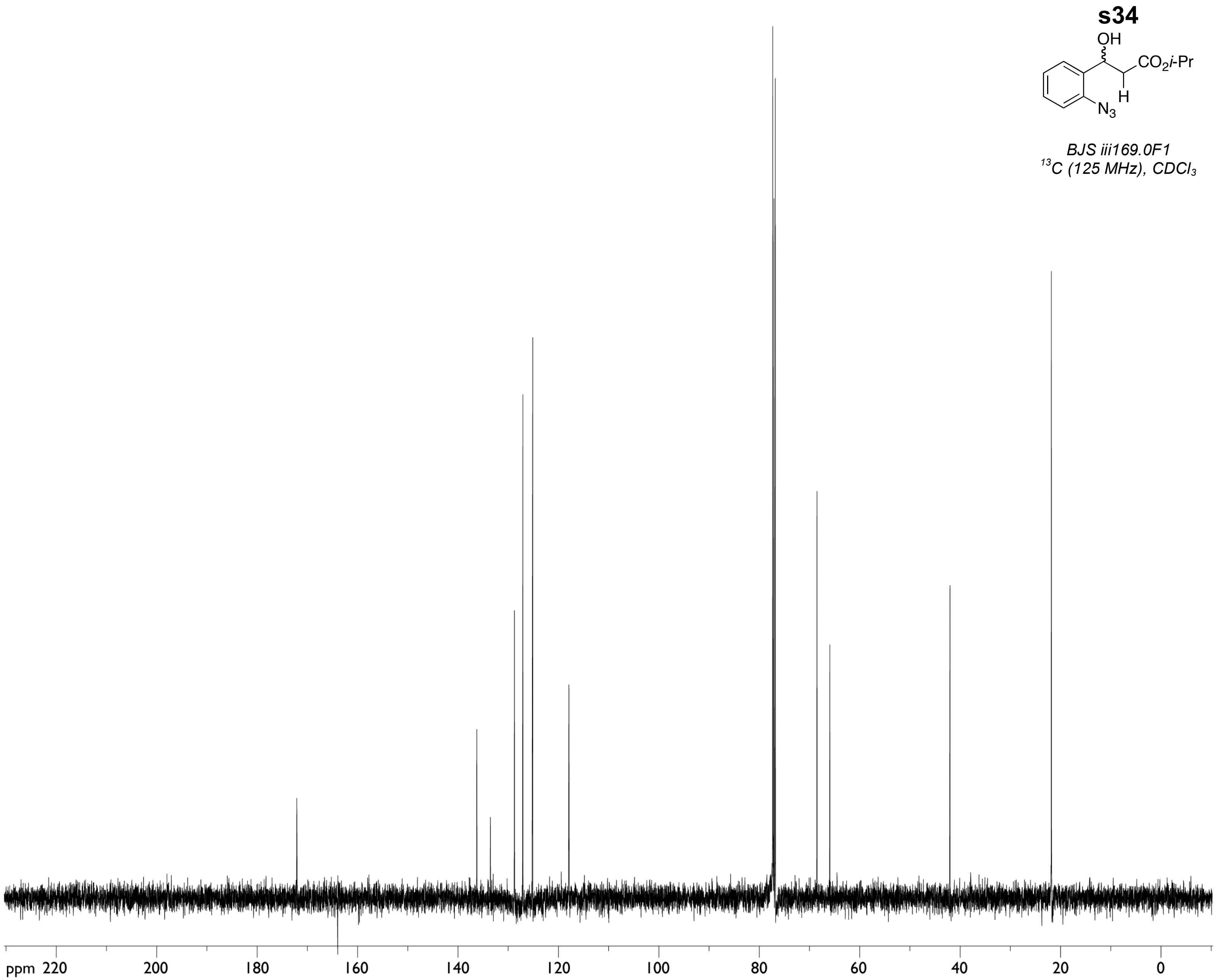


s34

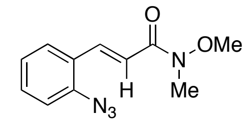


BJS iii169.0F1
^{1}H (500 MHz), $CDCl_3$

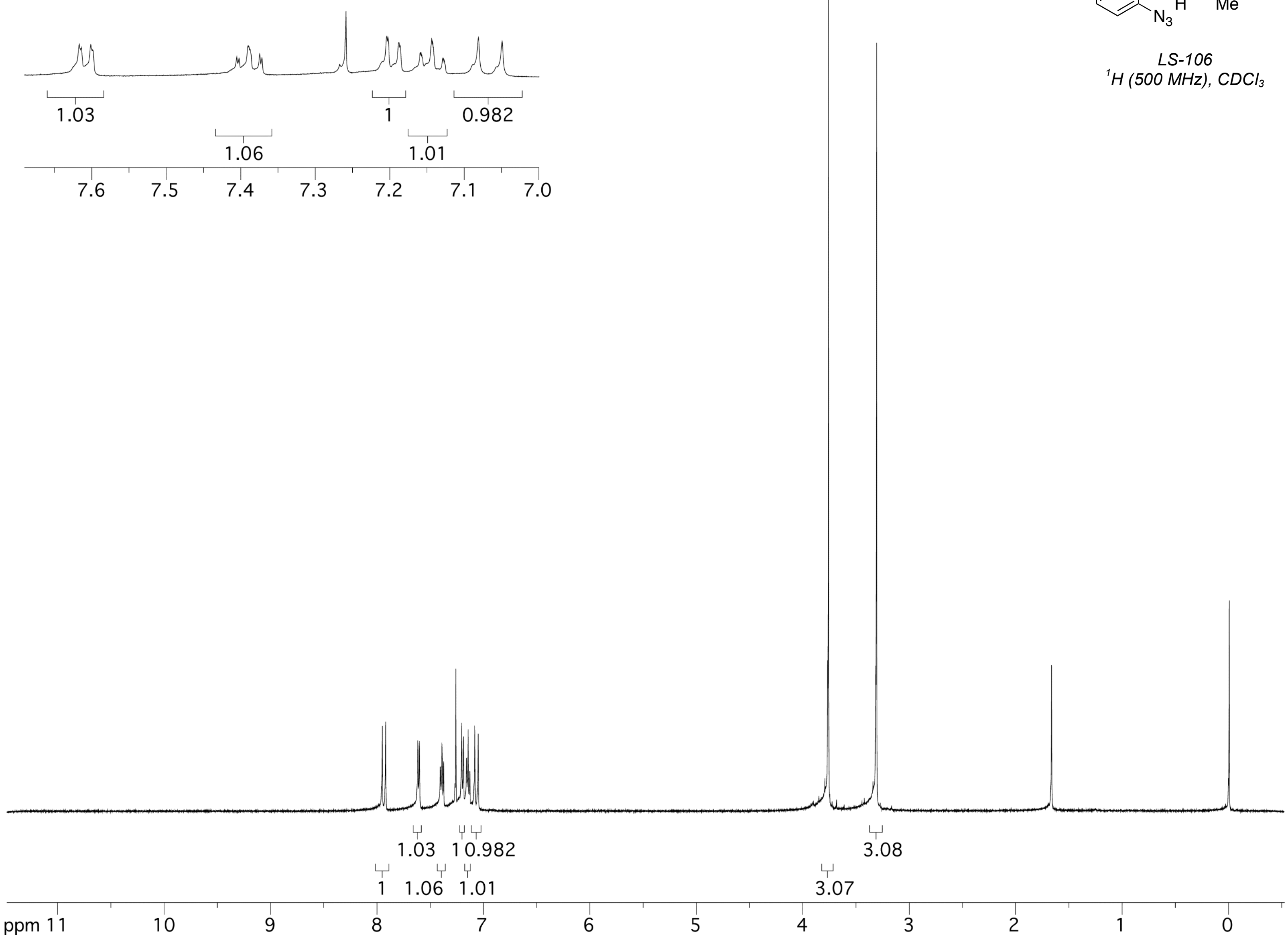



s34
OH
CO_2i-Pr
H
N_3
BJS iii169.0F1
^{13}C (125 MHz), $CDCl_3$
ppm 220 200 180 160 140 120 100 80 60 40 20 0

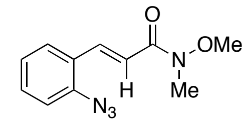
7d



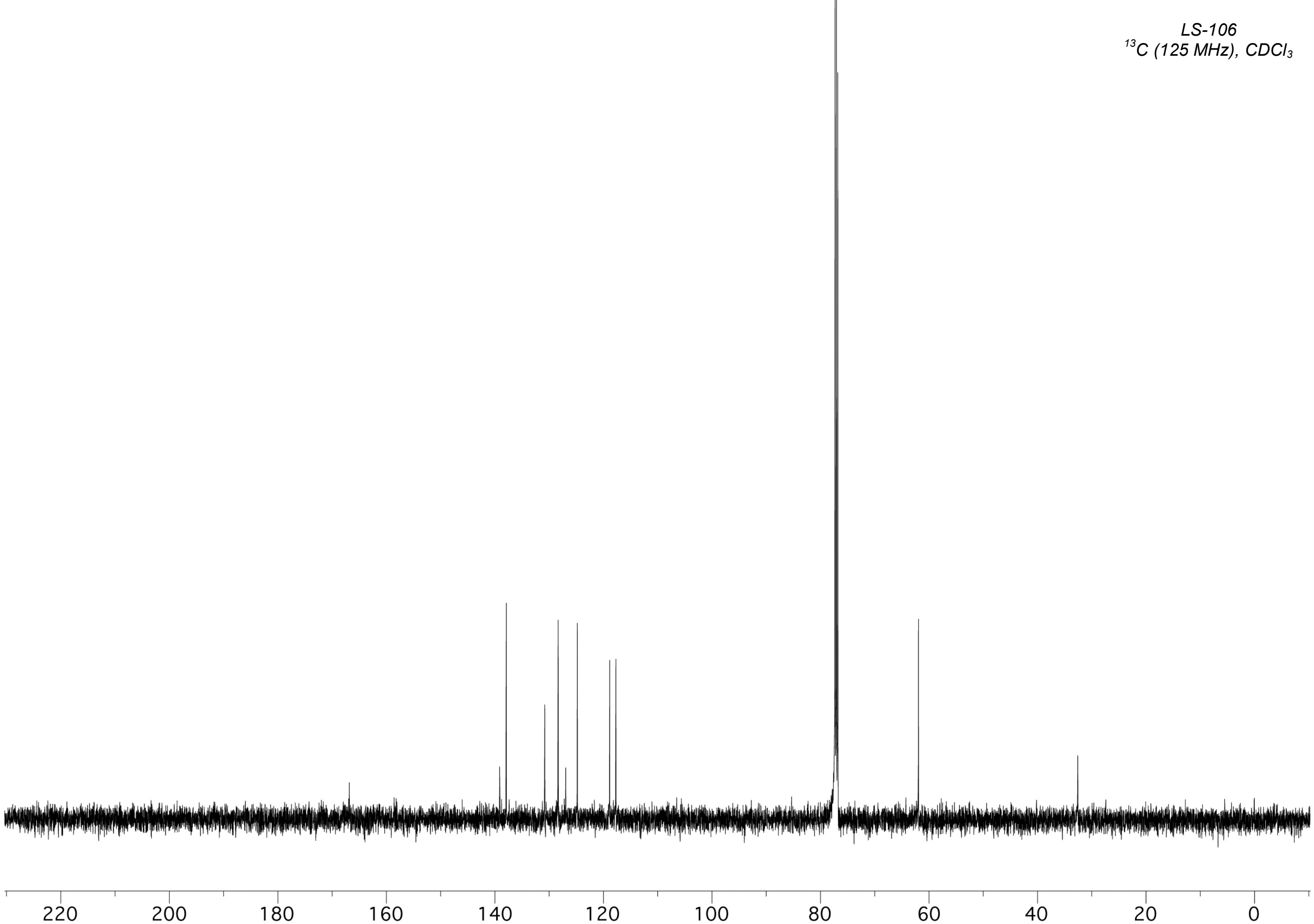
LS-106
¹H (500 MHz), CDCl₃



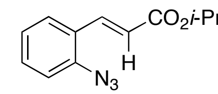
7d



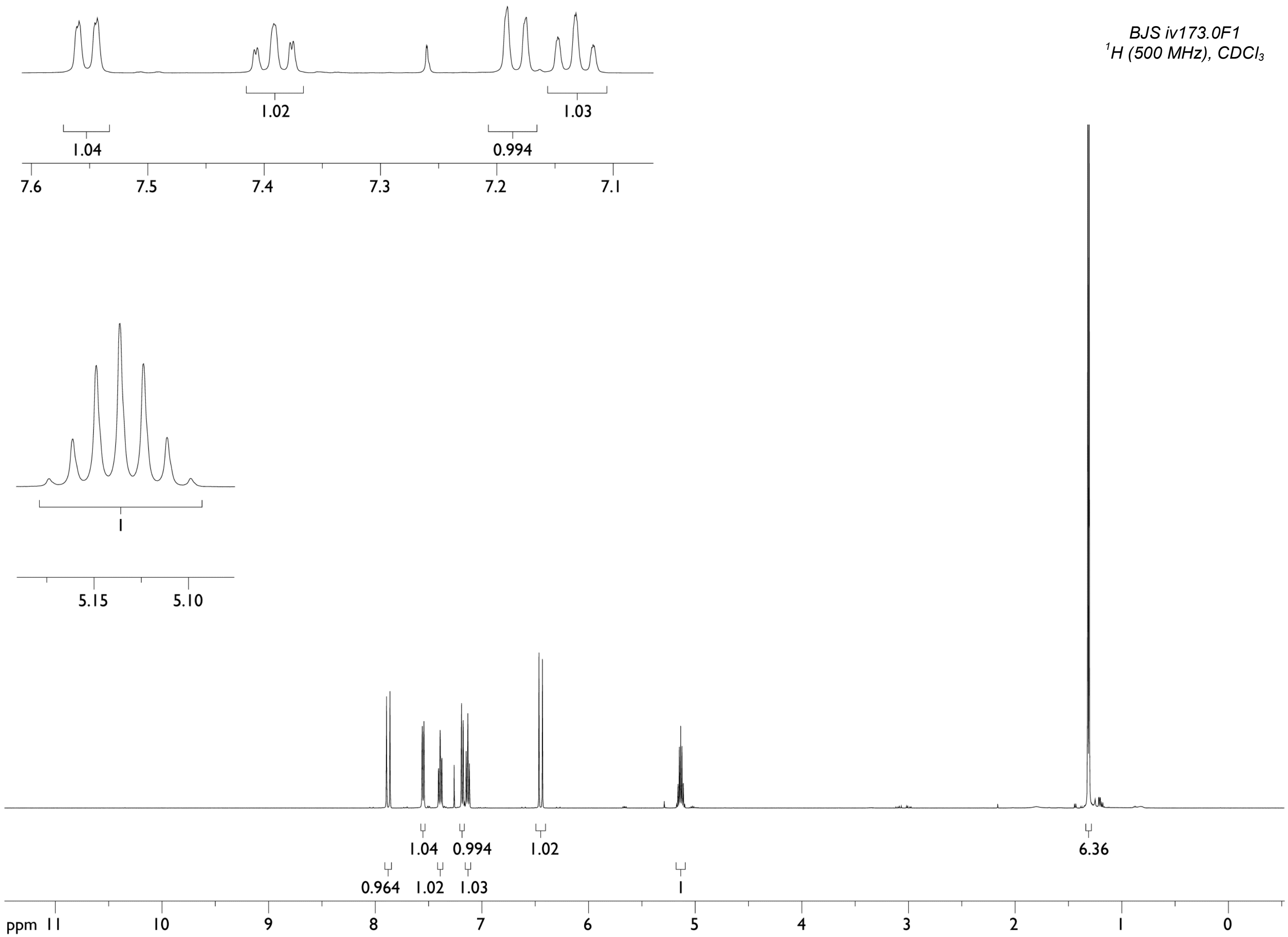
LS-106
^{13}C (125 MHz), $CDCl_3$



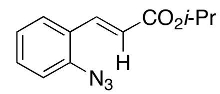
7e



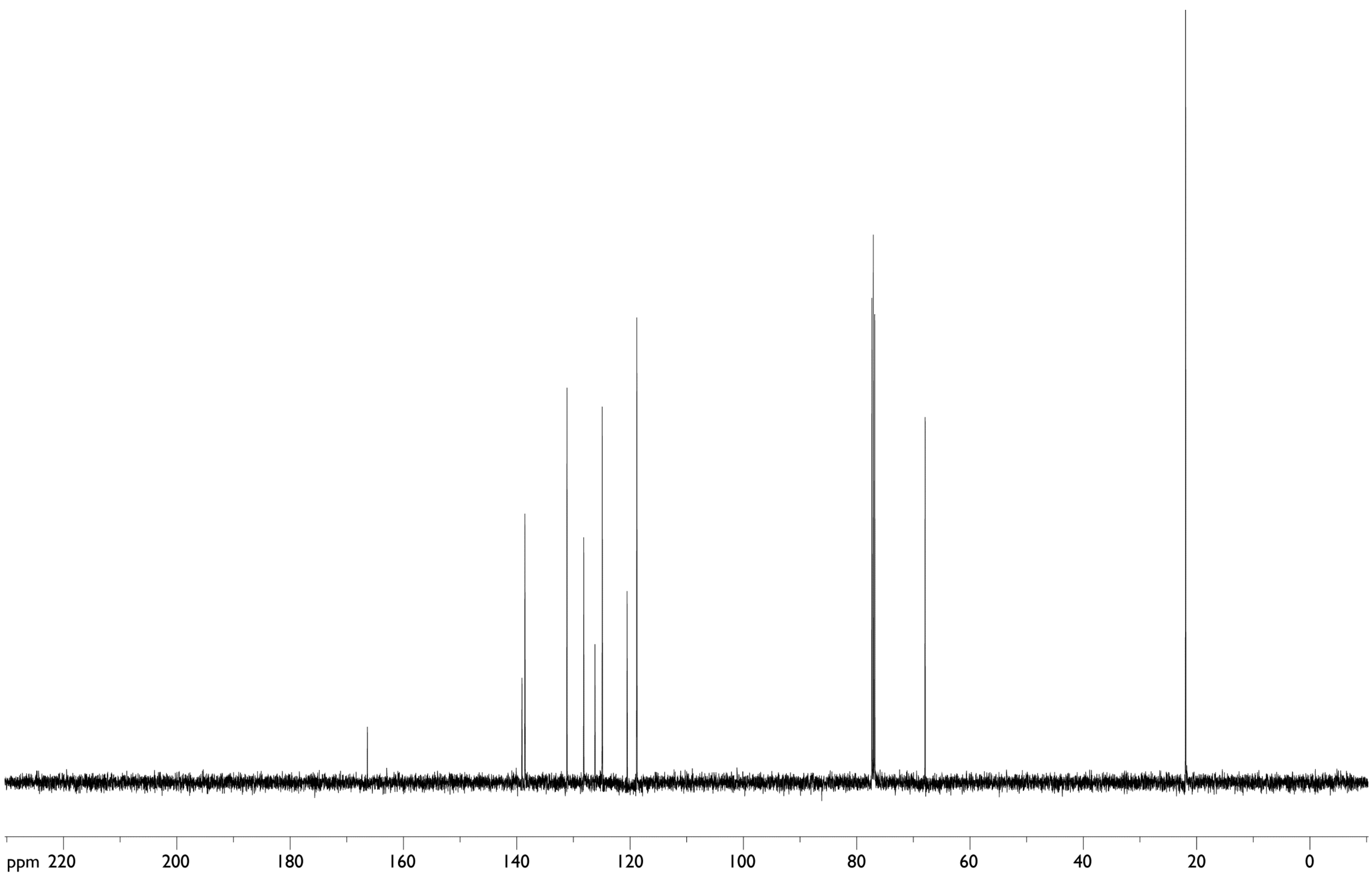
BJS iv173.0F1
^{1}H (500 MHz), CDCl$_3$



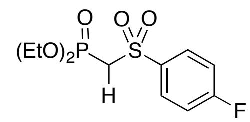
7e



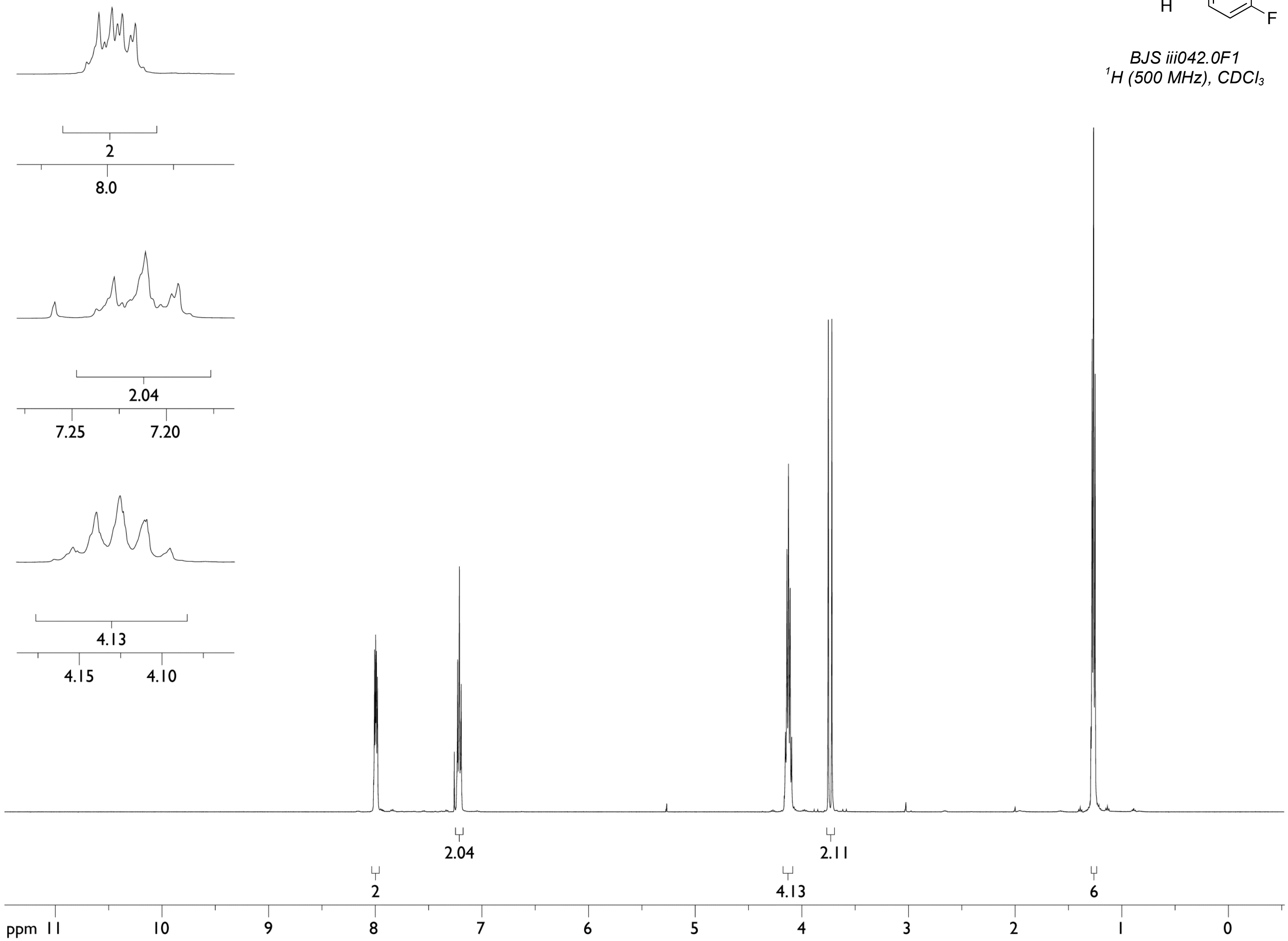
BJS iv173.0F1
^{13}C (125 MHz), $CDCl_3$



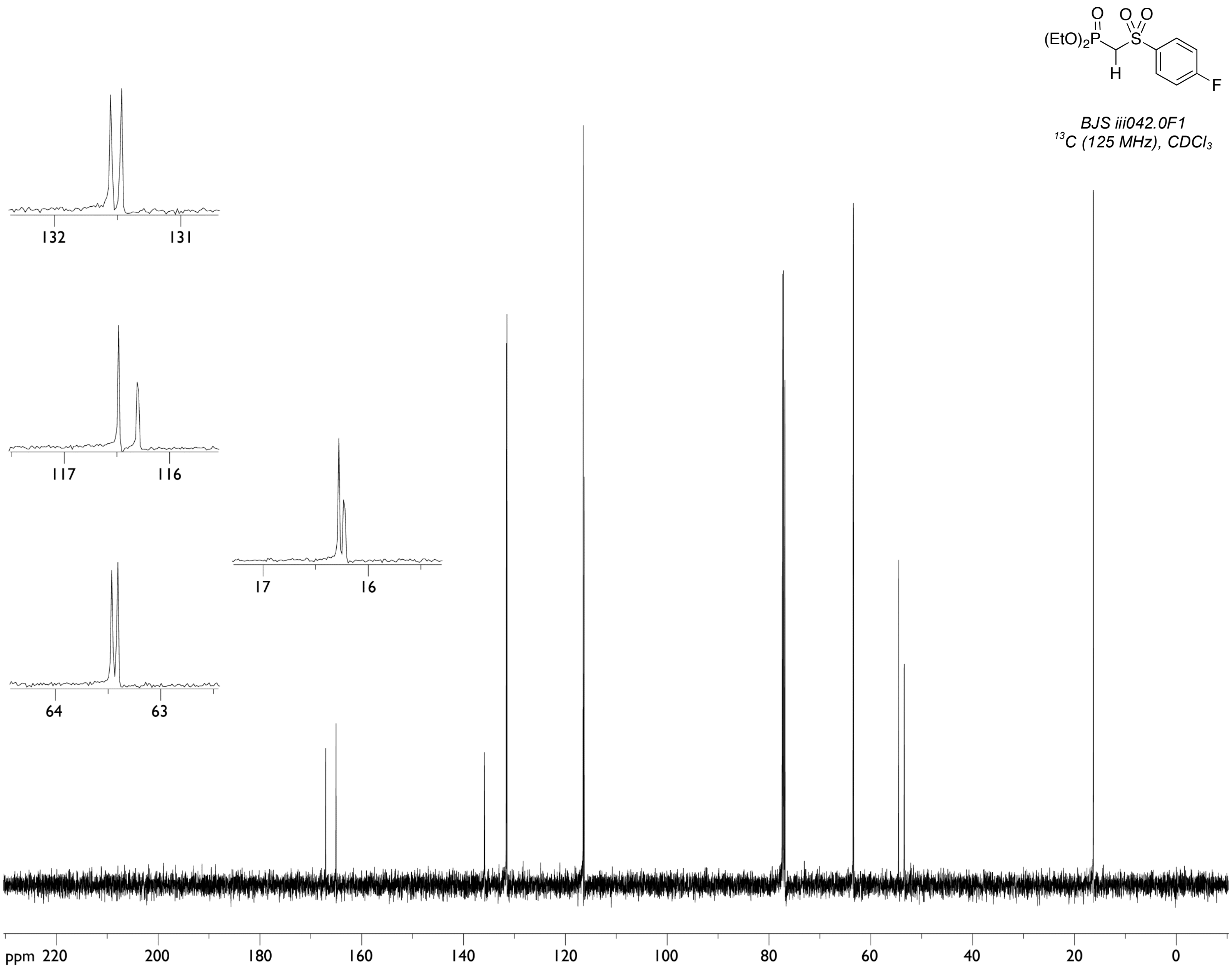
s41



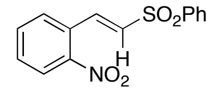
BJS iii042.0F1
¹H (500 MHz), CDCl₃



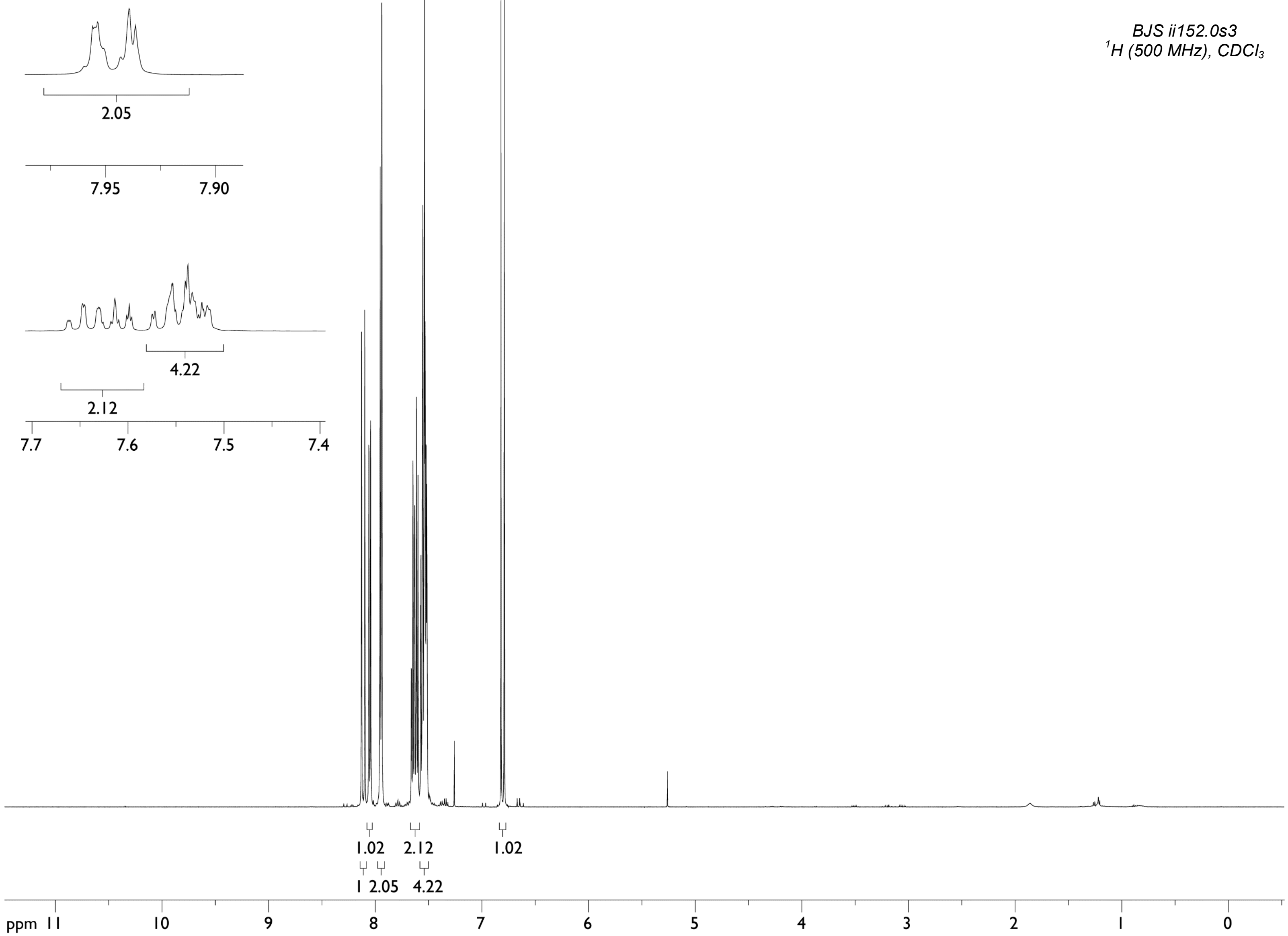
s41


(EtO)2P
O
O O
S
H
F
BJS iii042.0F1
13C (125 MHz), CDCl3
132
131
117
116
17
16
64
63
ppm 220
200
180
160
140
120
100
80
60
40
20
0

s42

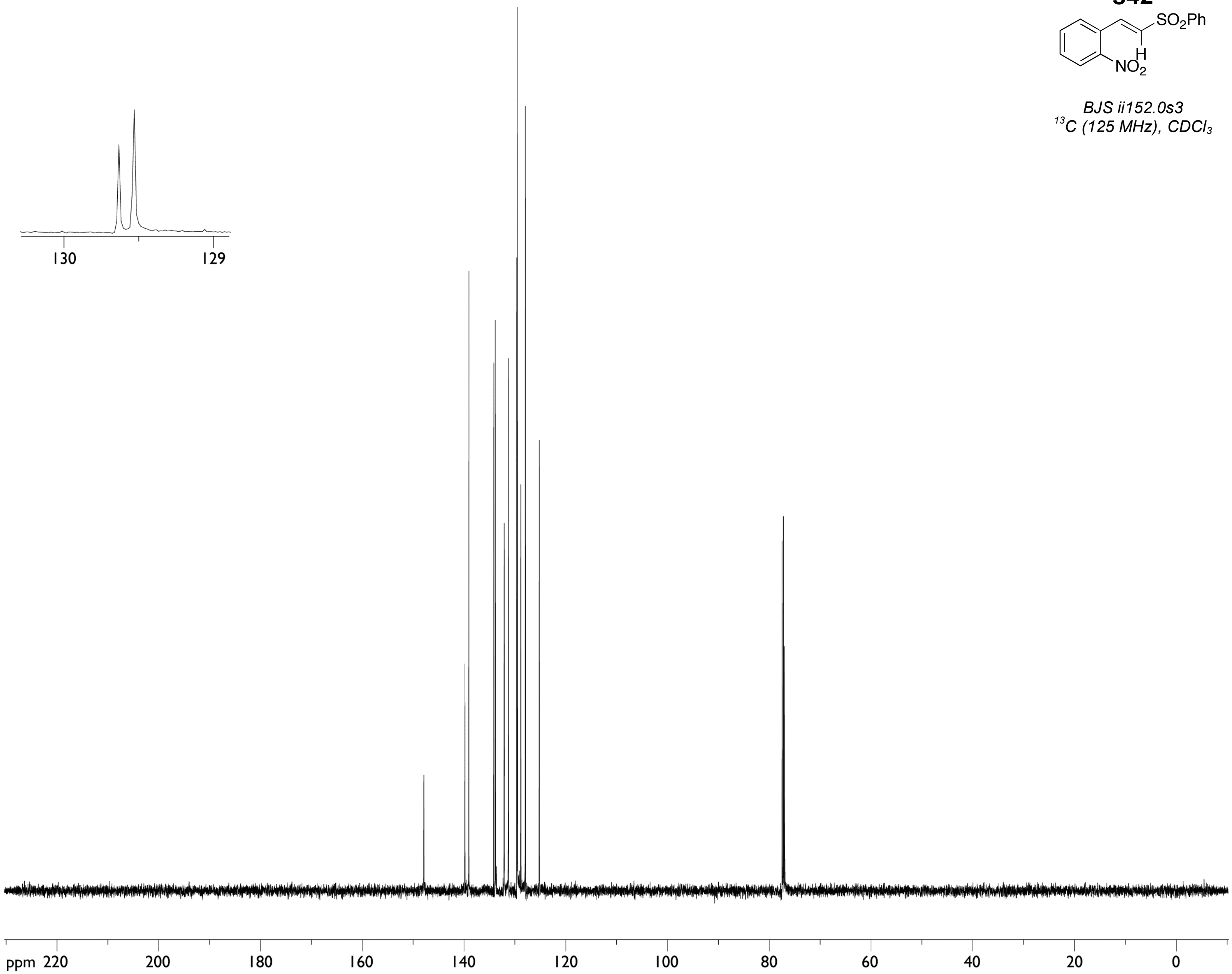


BJS ii152.0s3
^{1}H (500 MHz), $CDCl_3$

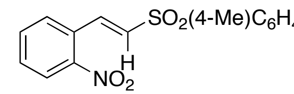


s42

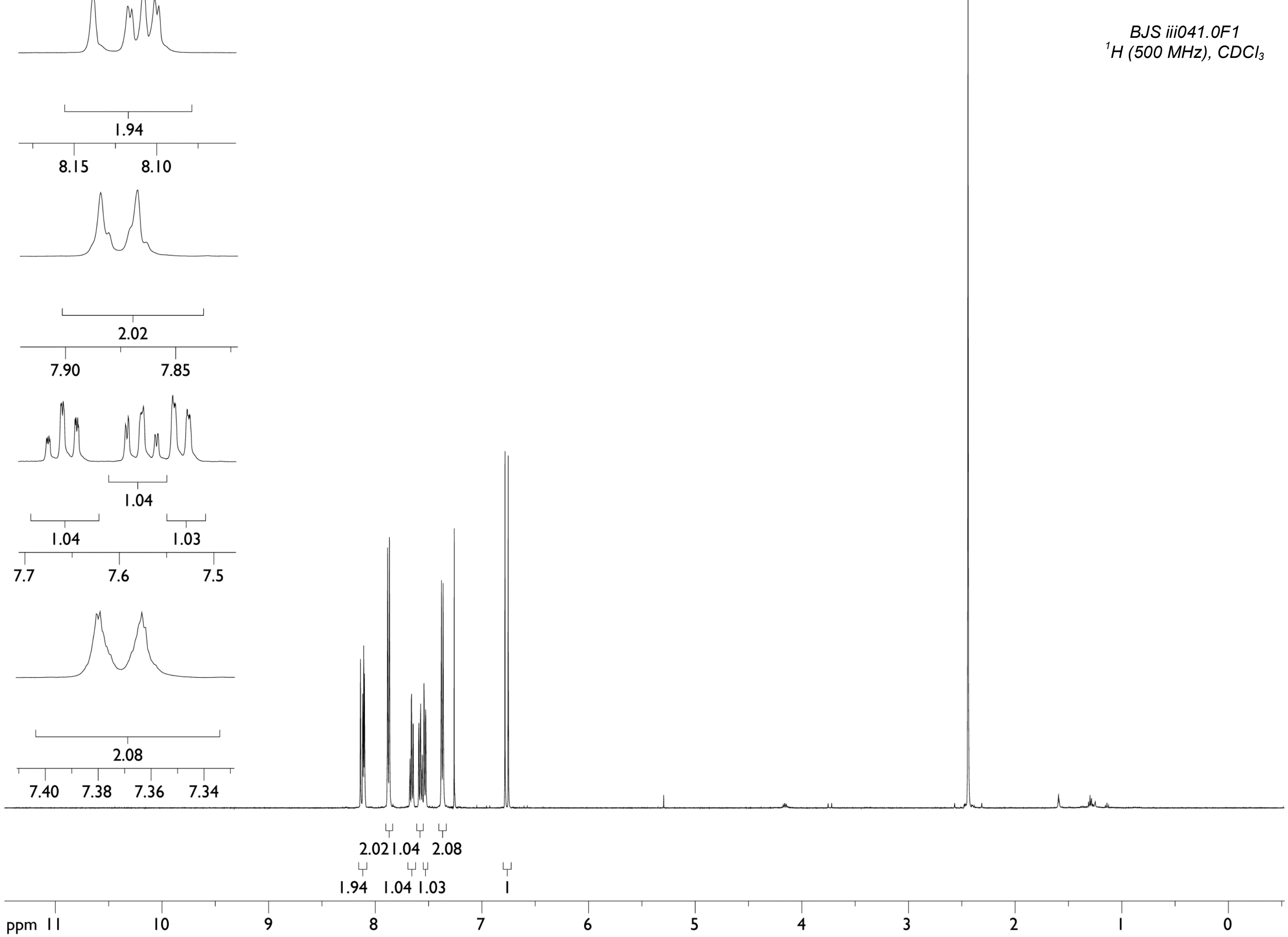
BJS ii152.0s3
^{13}C (125 MHz), CDCl$_3$



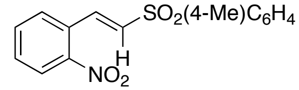
s43



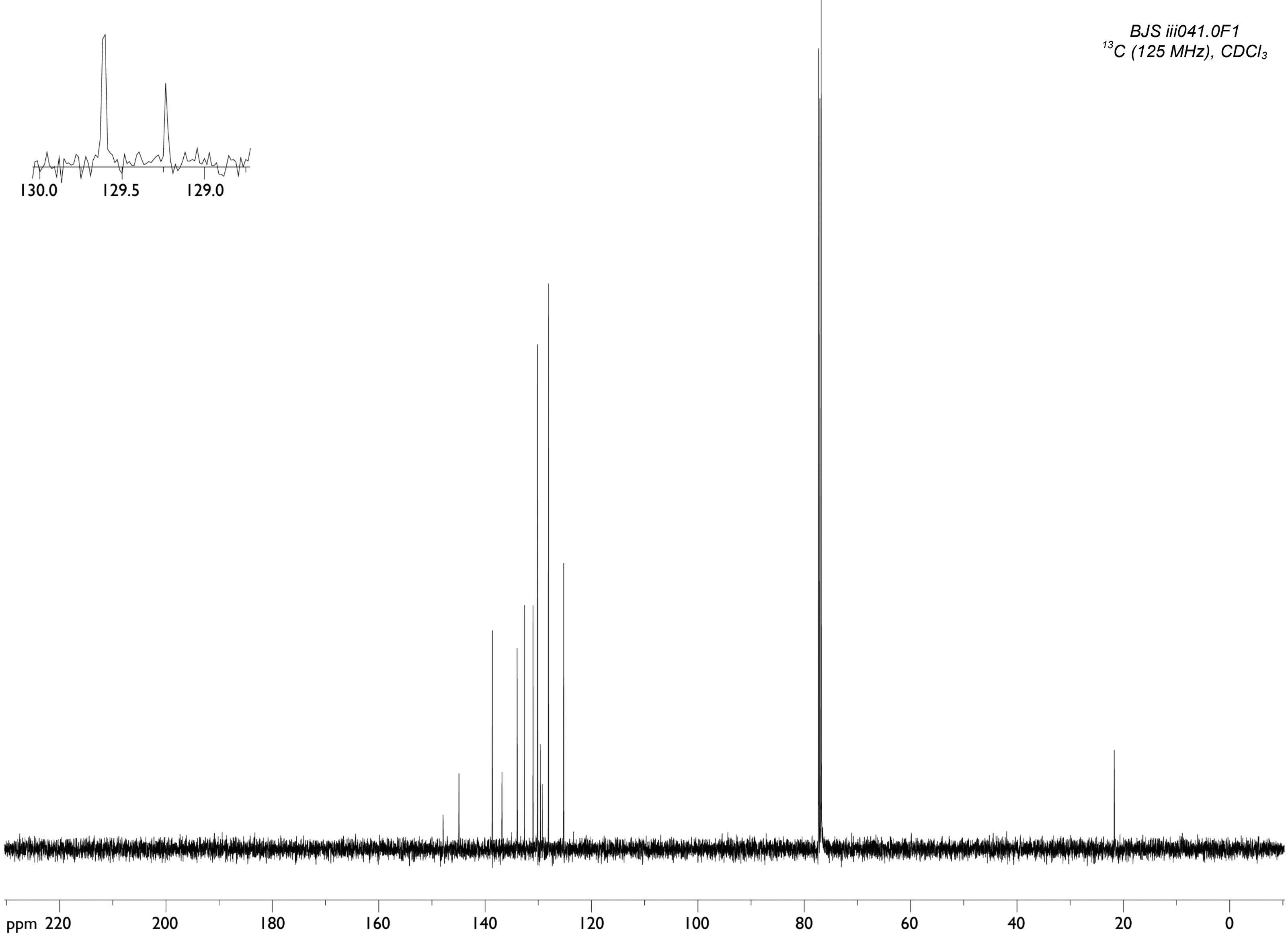
BJS iii041.0F1
^{1}H (500 MHz), CDCl$_3$



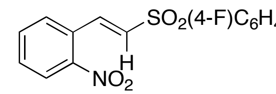
s43



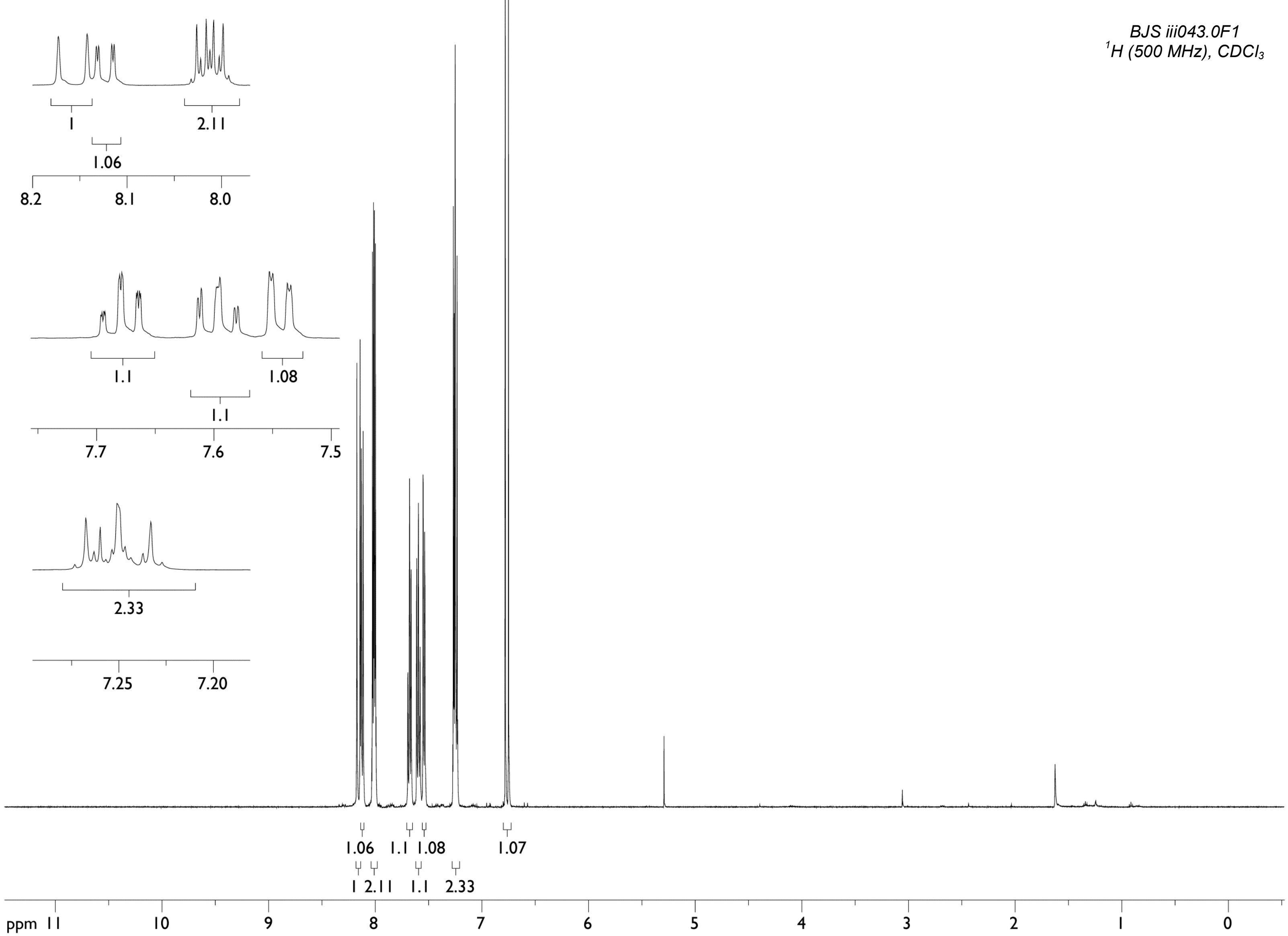
BJS iii041.0F1
^{13}C (125 MHz), $CDCl_3$



s44

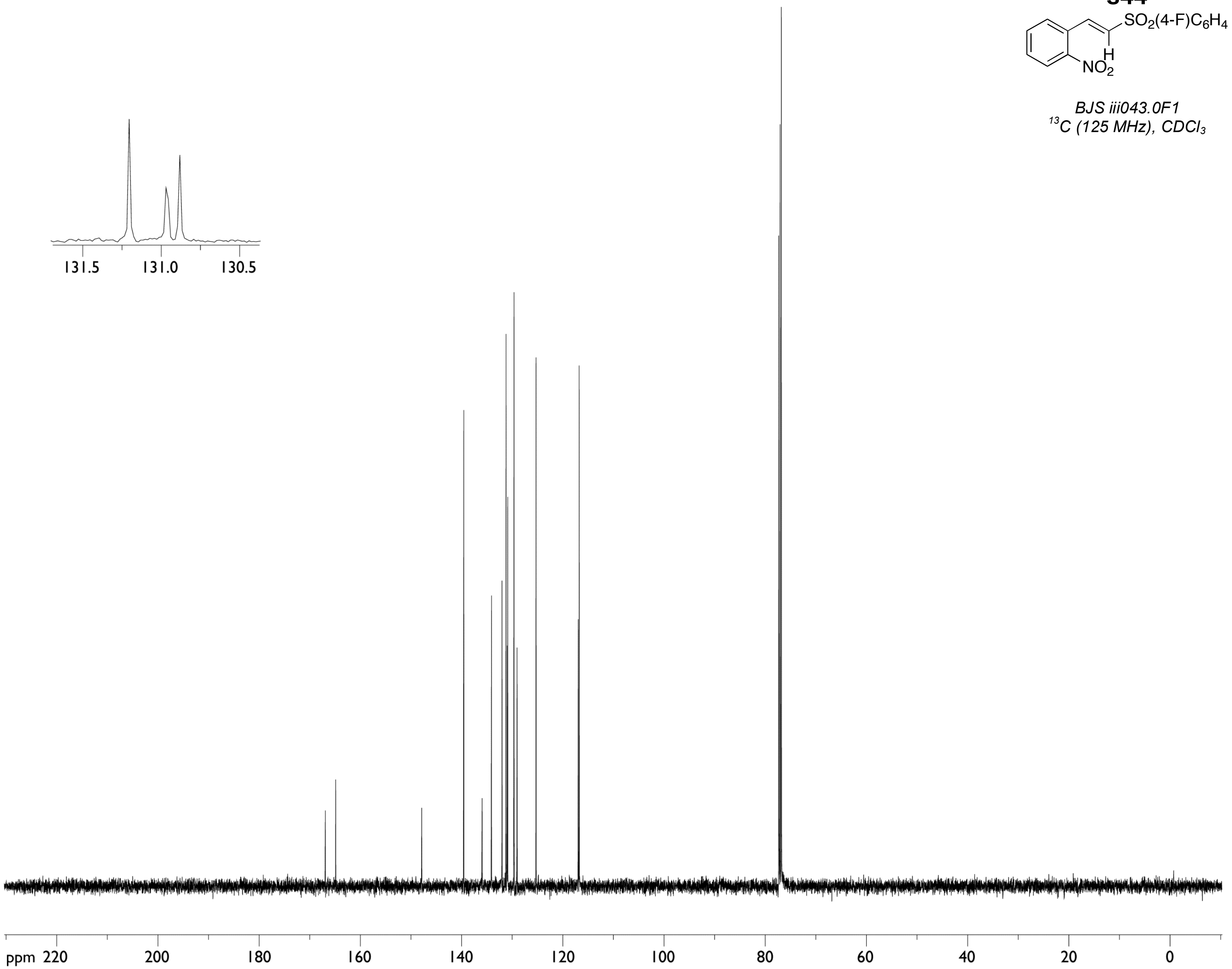


BJS iii043.0F1
^{1}H (500 MHz), $CDCl_3$



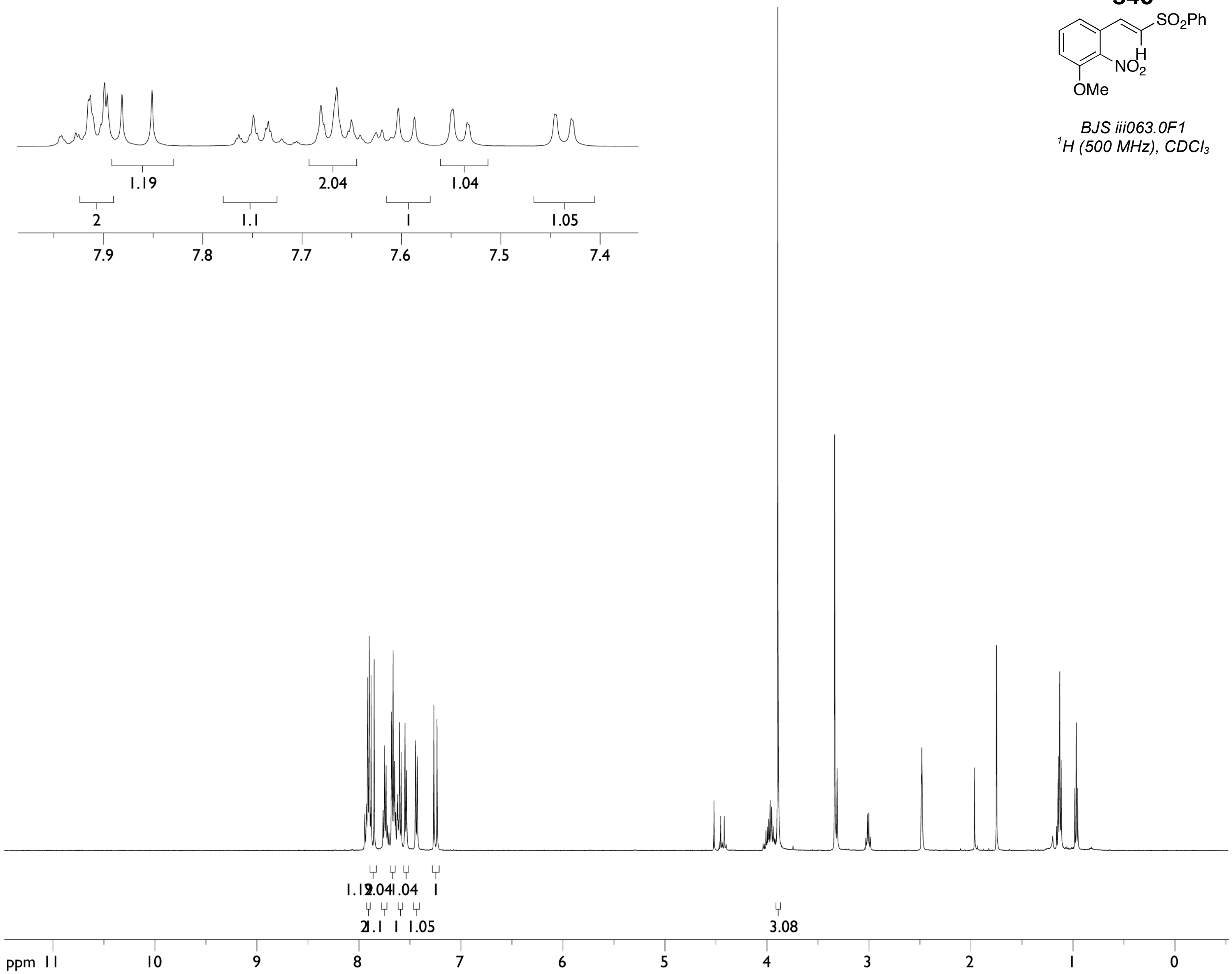
s44

BJS iii043.0F1
^{13}C (125 MHz), $CDCl_3$

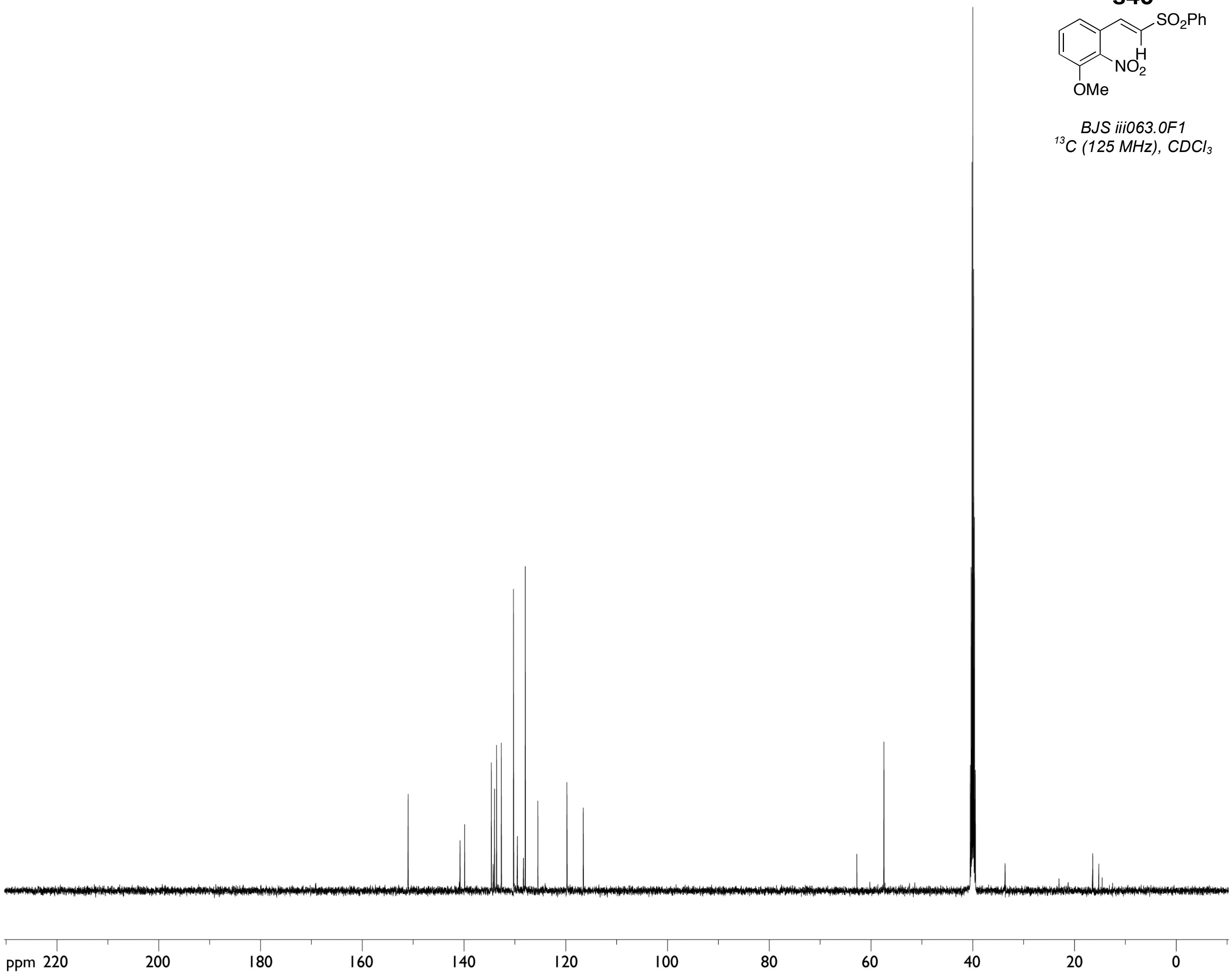


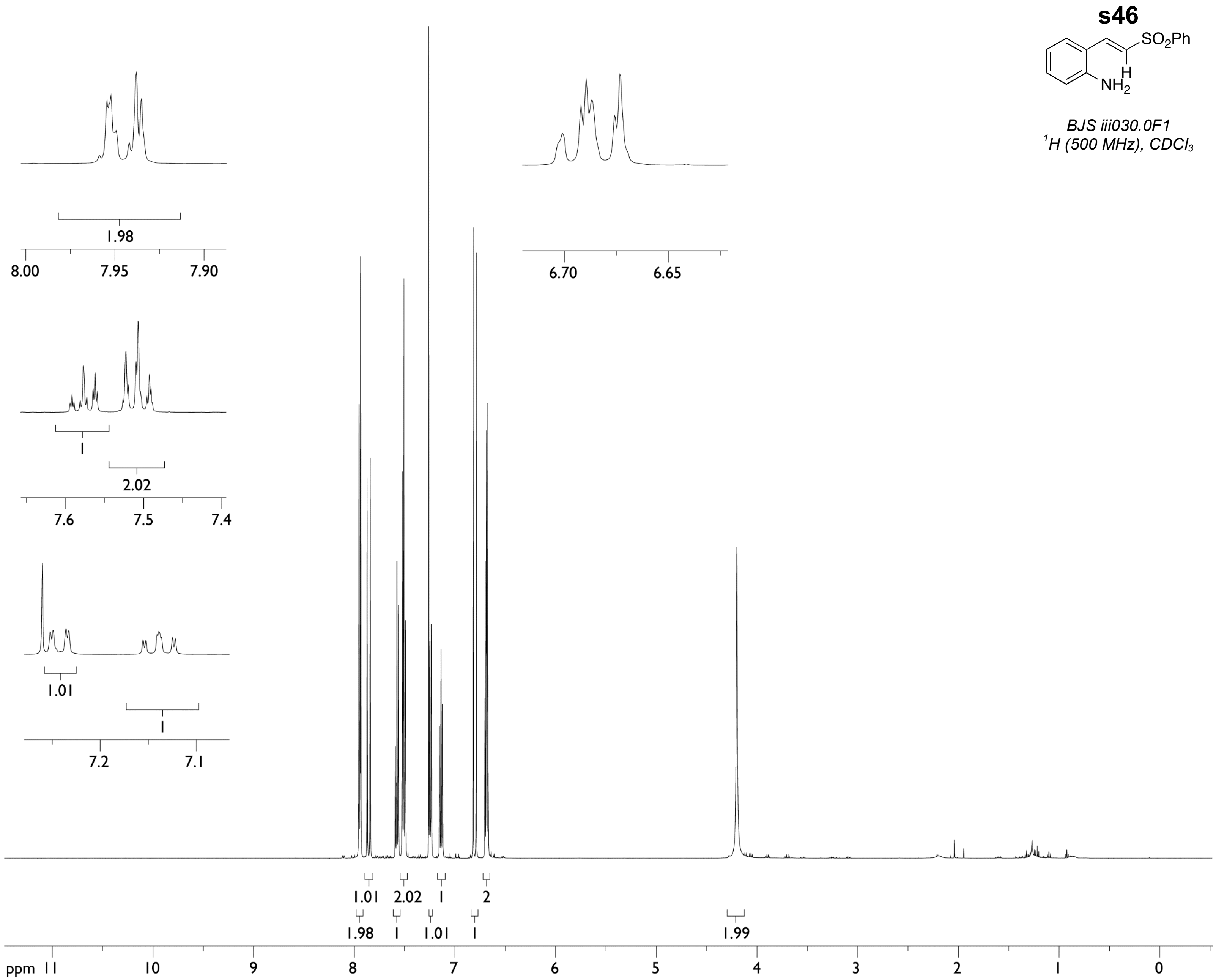
s45

BJS iii063.0F1
^{1}H (500 MHz), $CDCl_3$

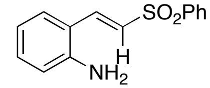


s45

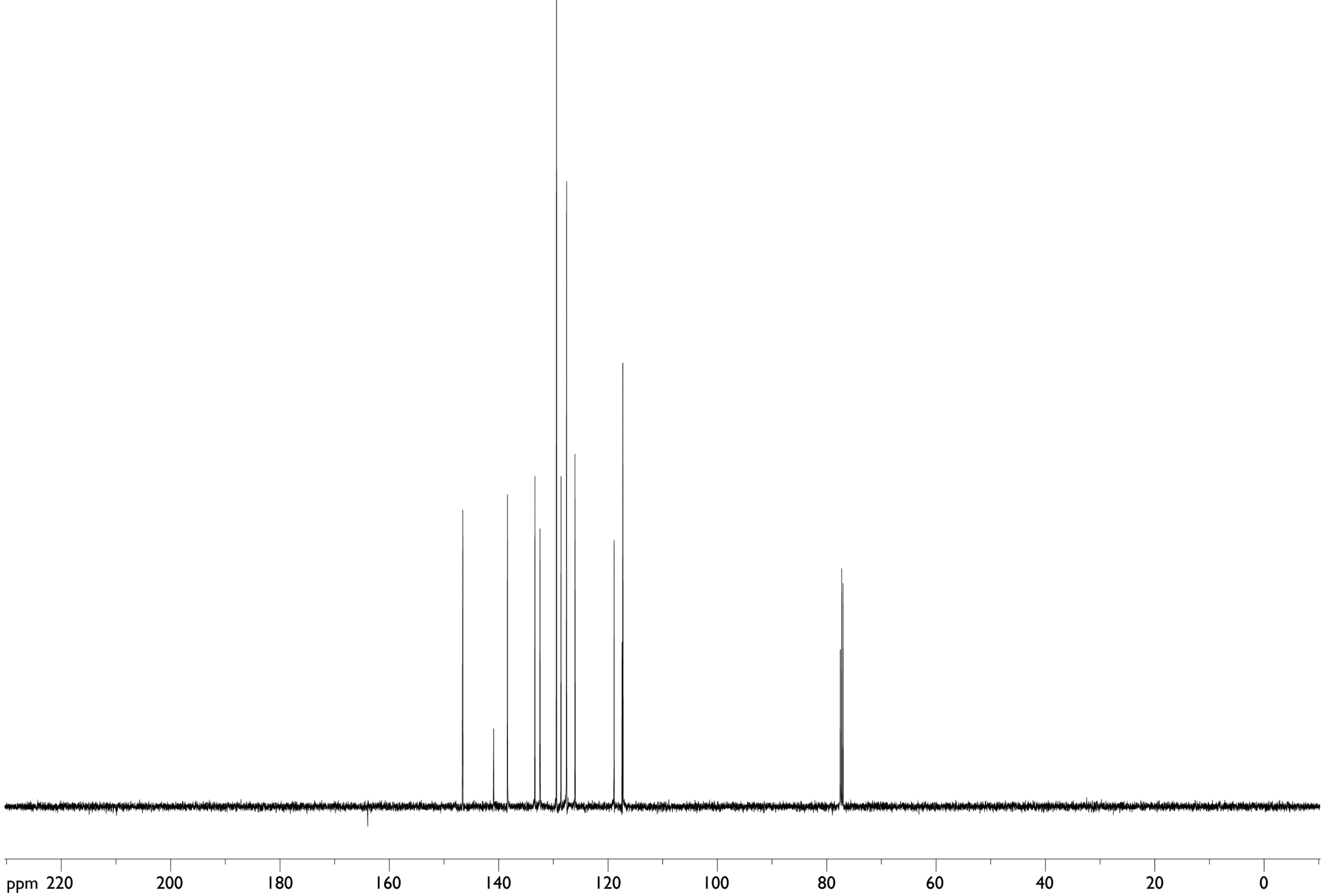

SO2Ph
H
NO2
OMe
BJS iii063.0F1
13C (125 MHz), CDCl3
ppm 220
200
180
160
140
120
100
80
60
40
20
0


s46
SO2Ph
H
NH2
BJS iii030.0F1
1H (500 MHz), CDCl3
1.98
8.00 7.95 7.90
6.70 6.65
1
2.02
7.6 7.5 7.4
1.01
1
7.2 7.1
1.01 2.02 1 2
1.98 1 1.01 1
1.99
ppm 11 10 9 8 7 6 5 4 3 2 1 0

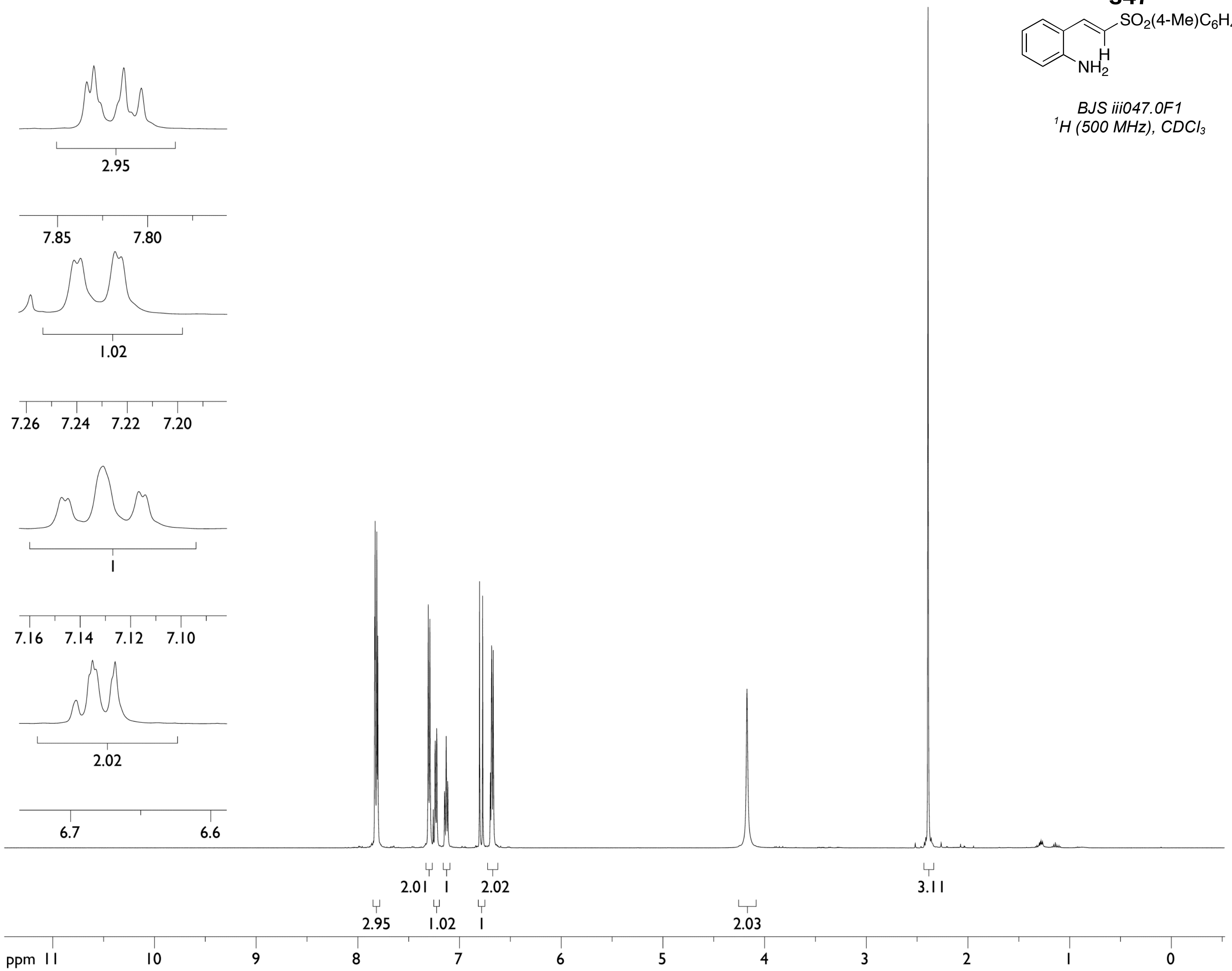
s46



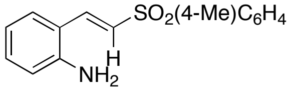
BJS iii030.0F1
^{13}C (125 MHz), $CDCl_3$



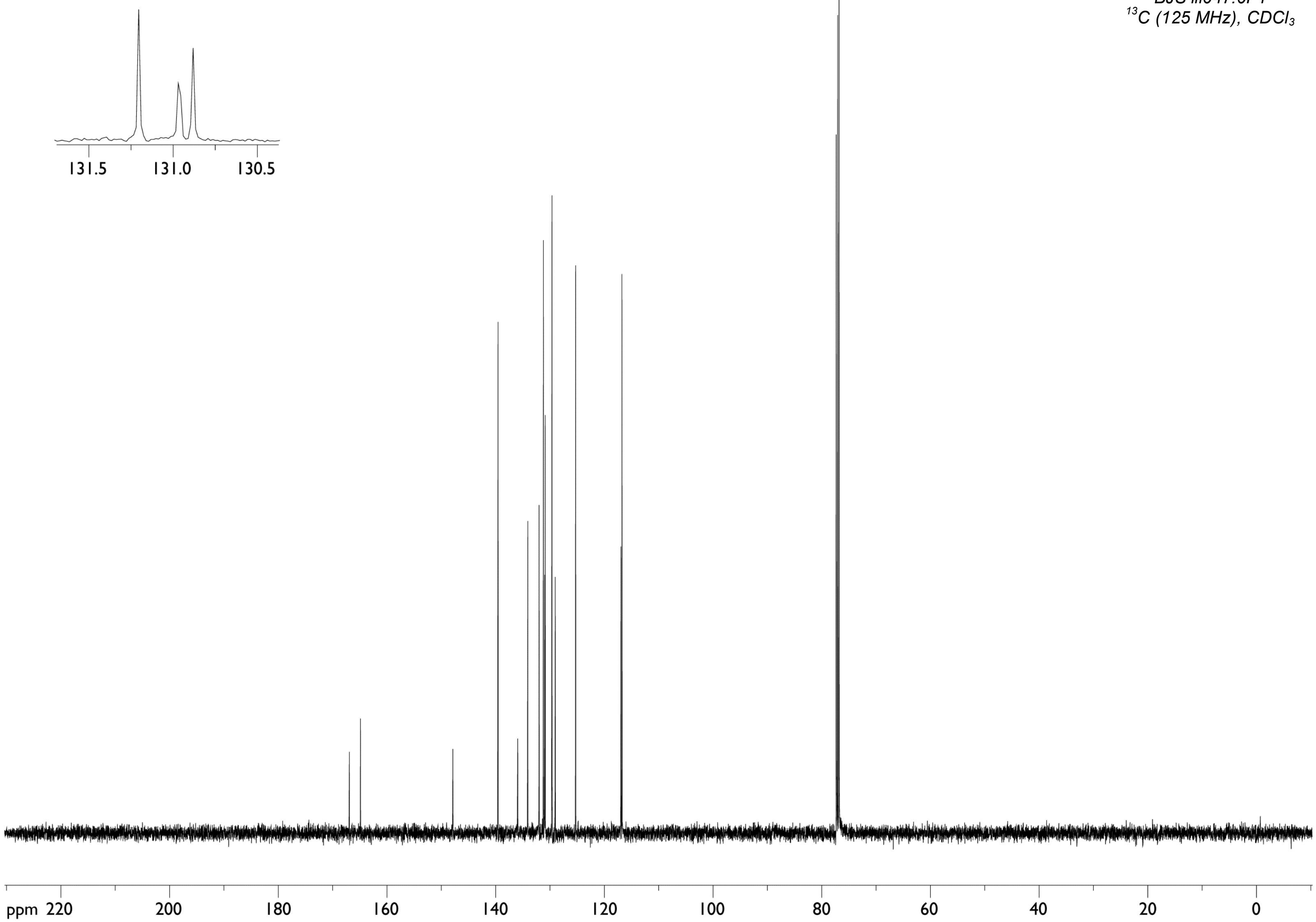
s47


SO2(4-Me)C6H4
H
NH2
BJS iii047.0F1
1H (500 MHz), CDCl3
2.95
7.85
7.80
1.02
7.26
7.24
7.22
7.20
1
7.16
7.14
7.12
7.10
2.02
6.7
6.6
2.01
1
2.02
3.11
2.95
1.02
1
2.03
ppm
11
10
9
8
7
6
5
4
3
2
1
0

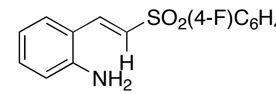
s47



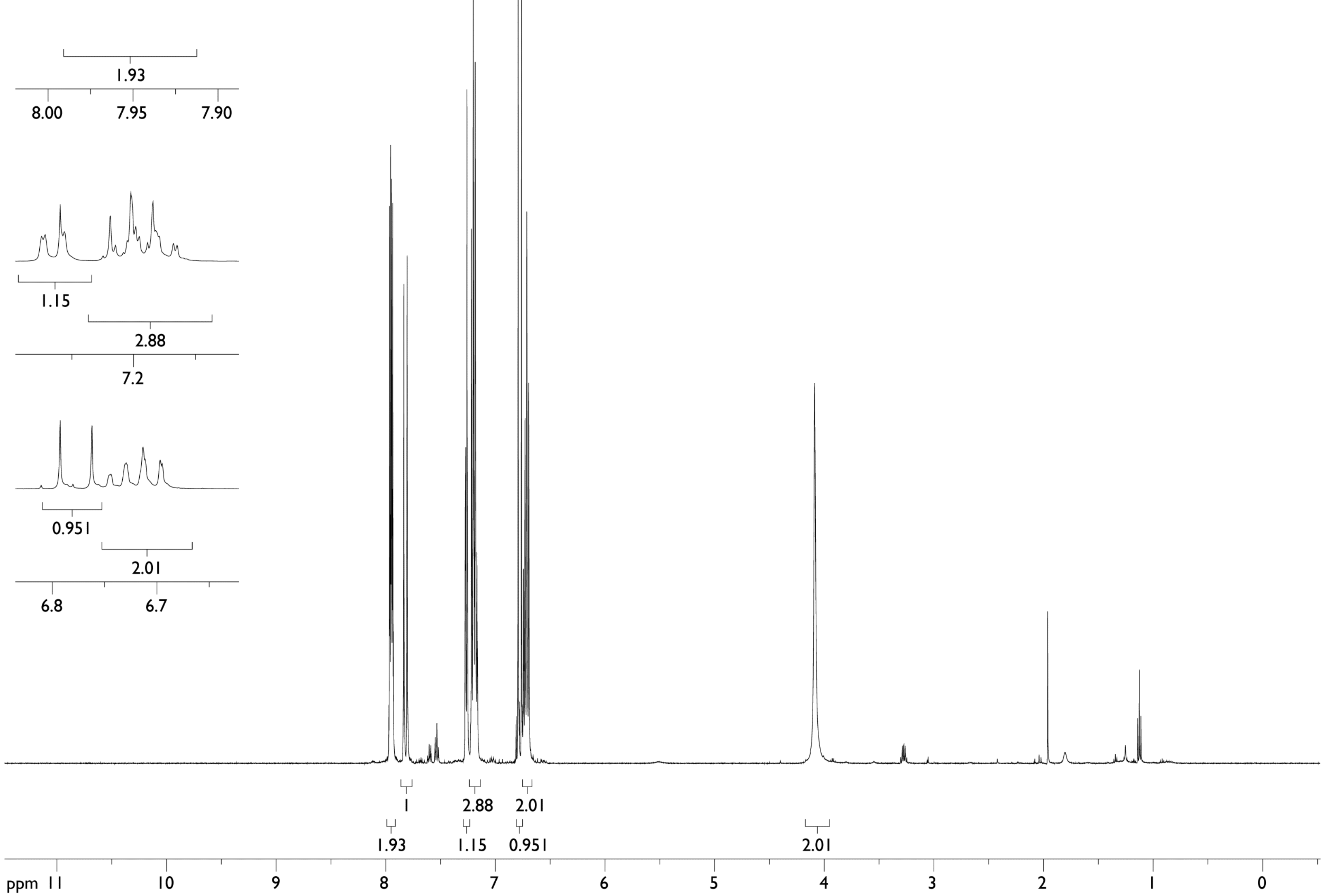
BJS iii047.0F1
^{13}C (125 MHz), $CDCl_3$



s48

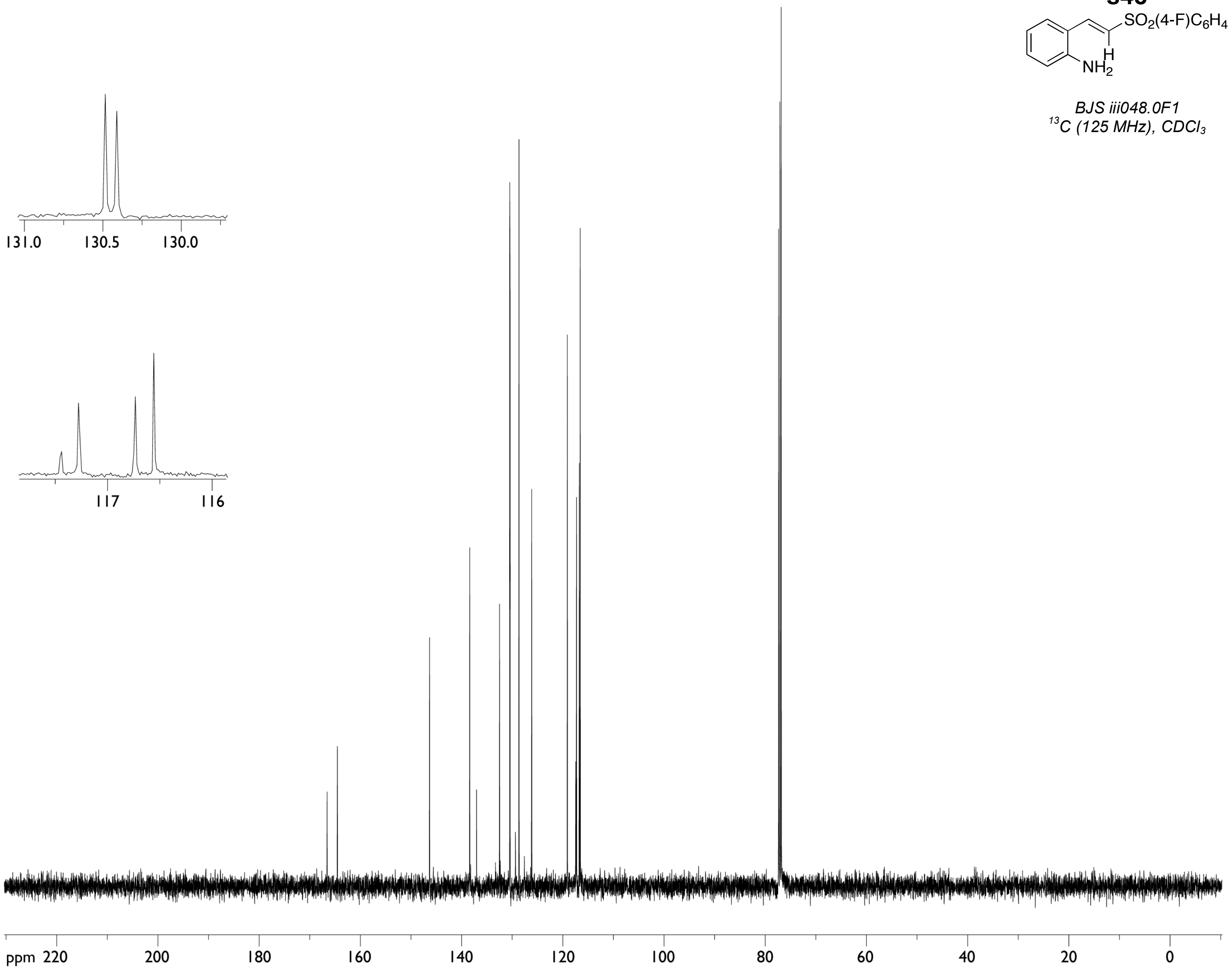


BJS iii048.0F1
^{1}H (500 MHz), $CDCl_3$

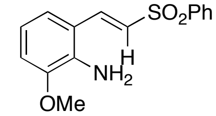


s48

BJS iii048.0F1
^{13}C (125 MHz), $CDCl_3$

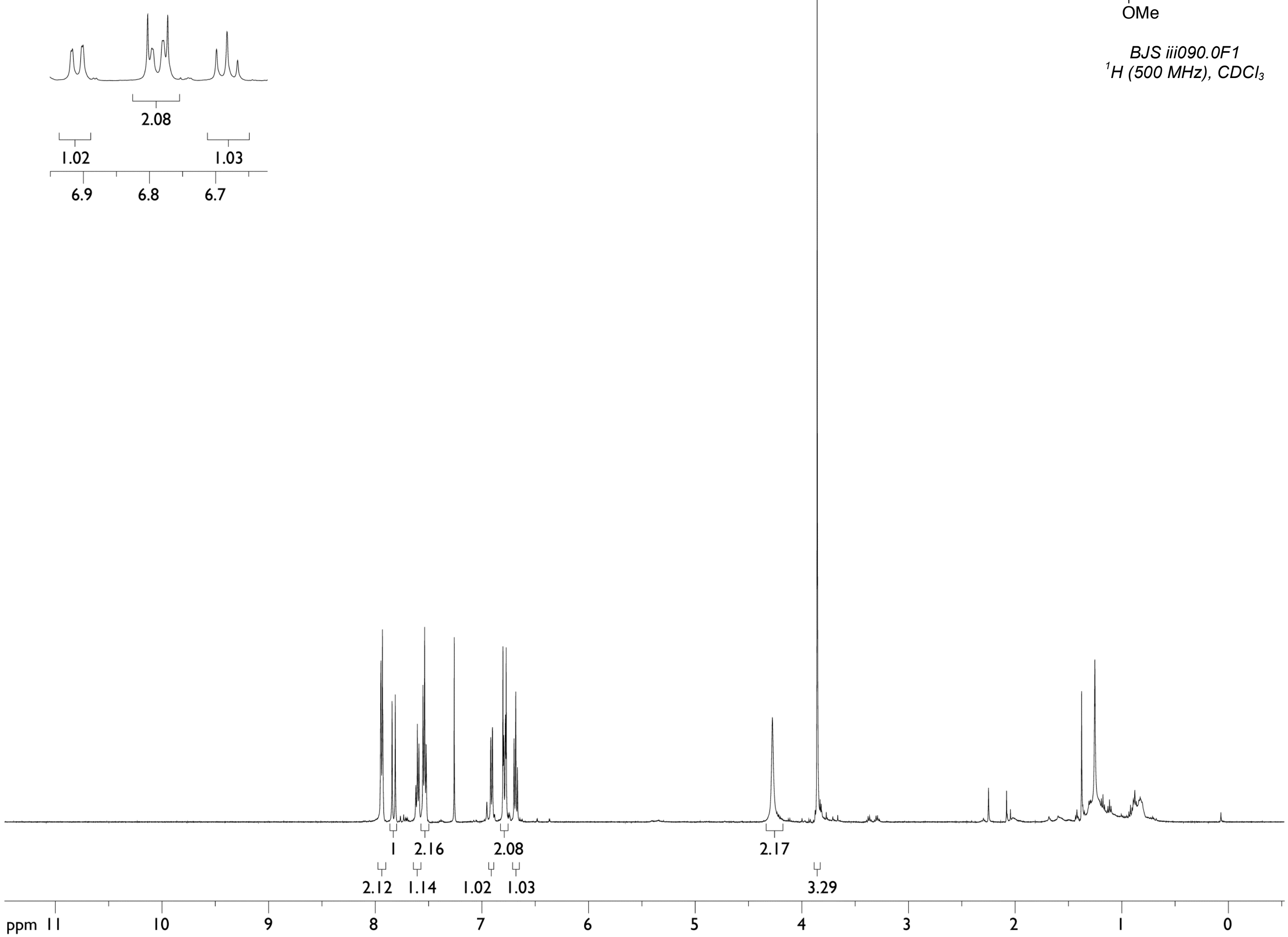


s49

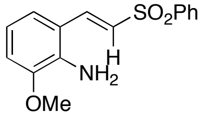


BJS iii090.0F1

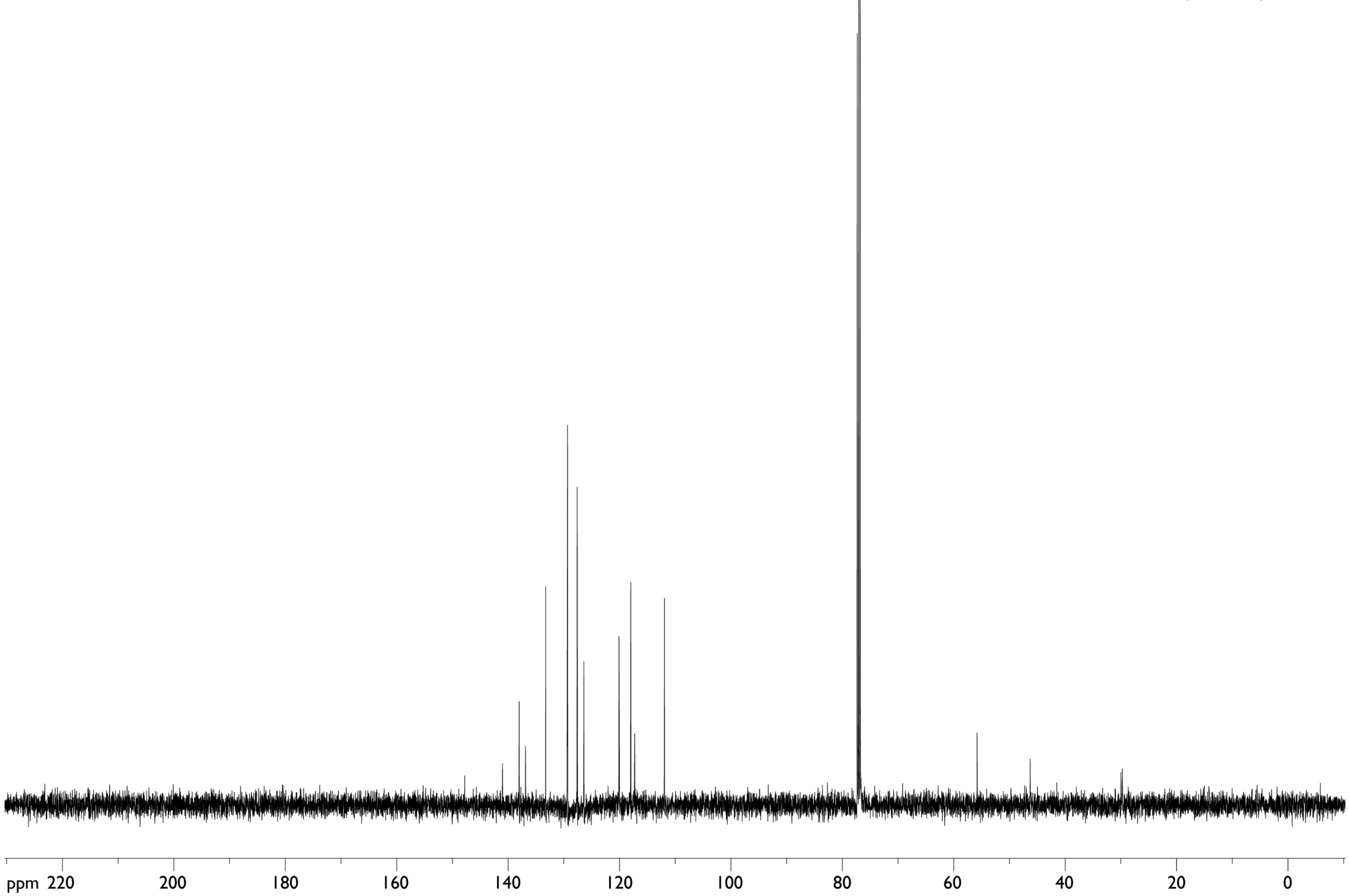
^{1}H (500 MHz), CDCl$_3$

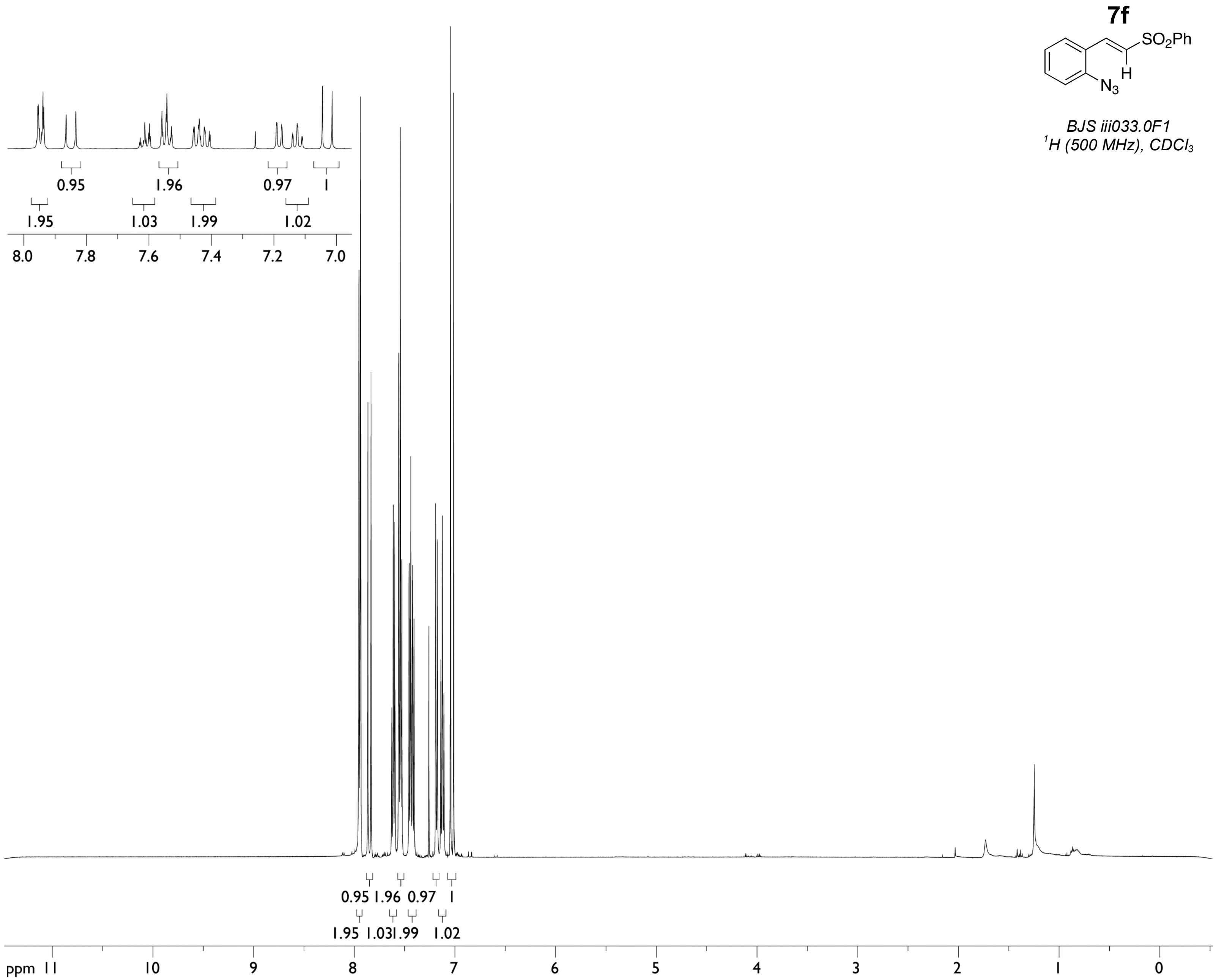


s49

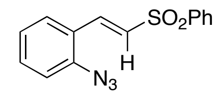


BJS iii090.0F1
^{13}C (125 MHz), CDCl$_3$

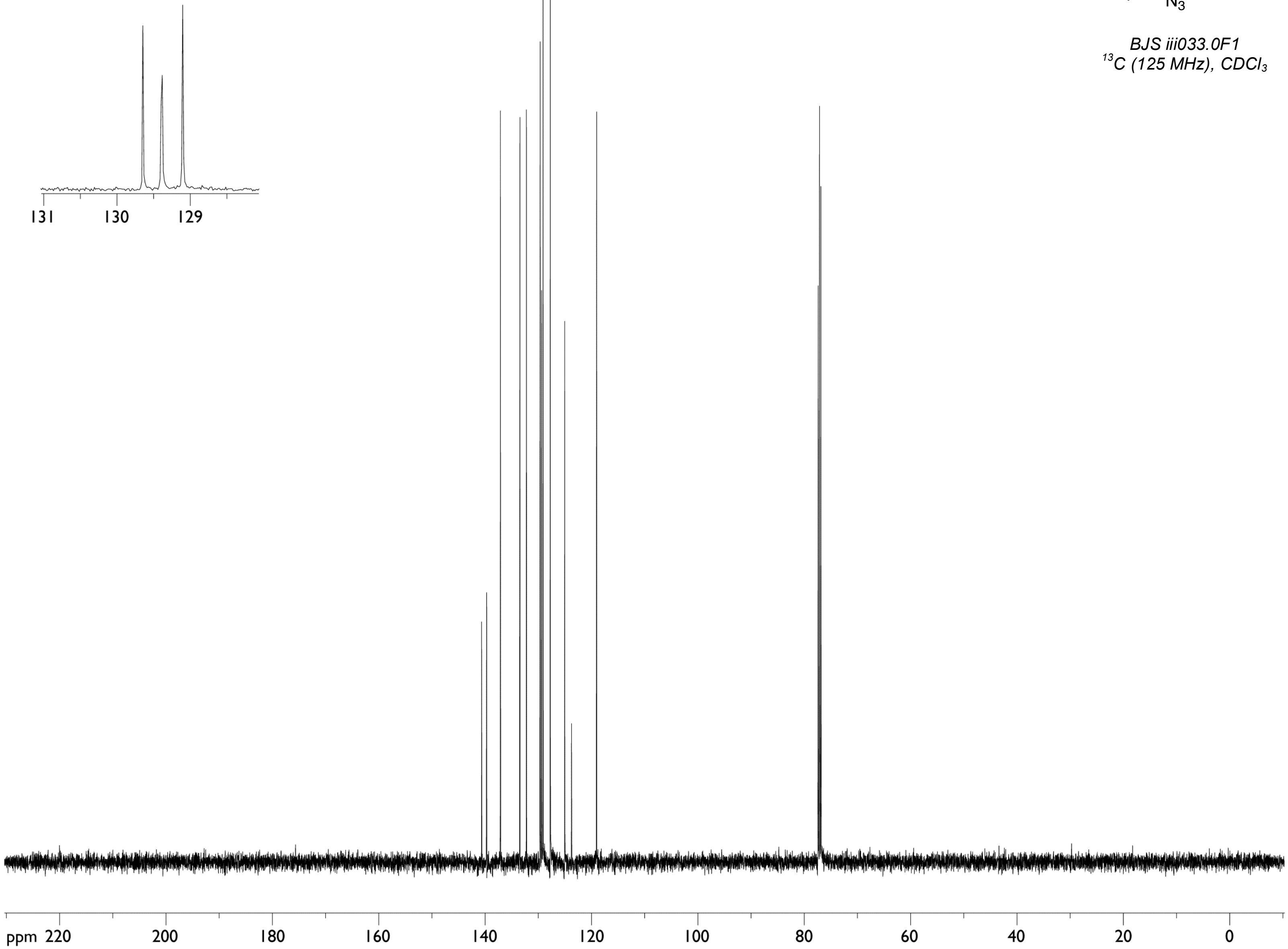



7f
SO2Ph
H
N3
BJS iii033.0F1
1H (500 MHz), CDCl3
0.95
1.96
0.97
1
1.95
1.03
1.99
1.02
8.0
7.8
7.6
7.4
7.2
7.0
ppm
11
10
9
8
7
6
5
4
3
2
1
0

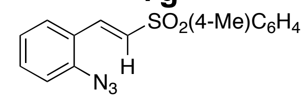
7f



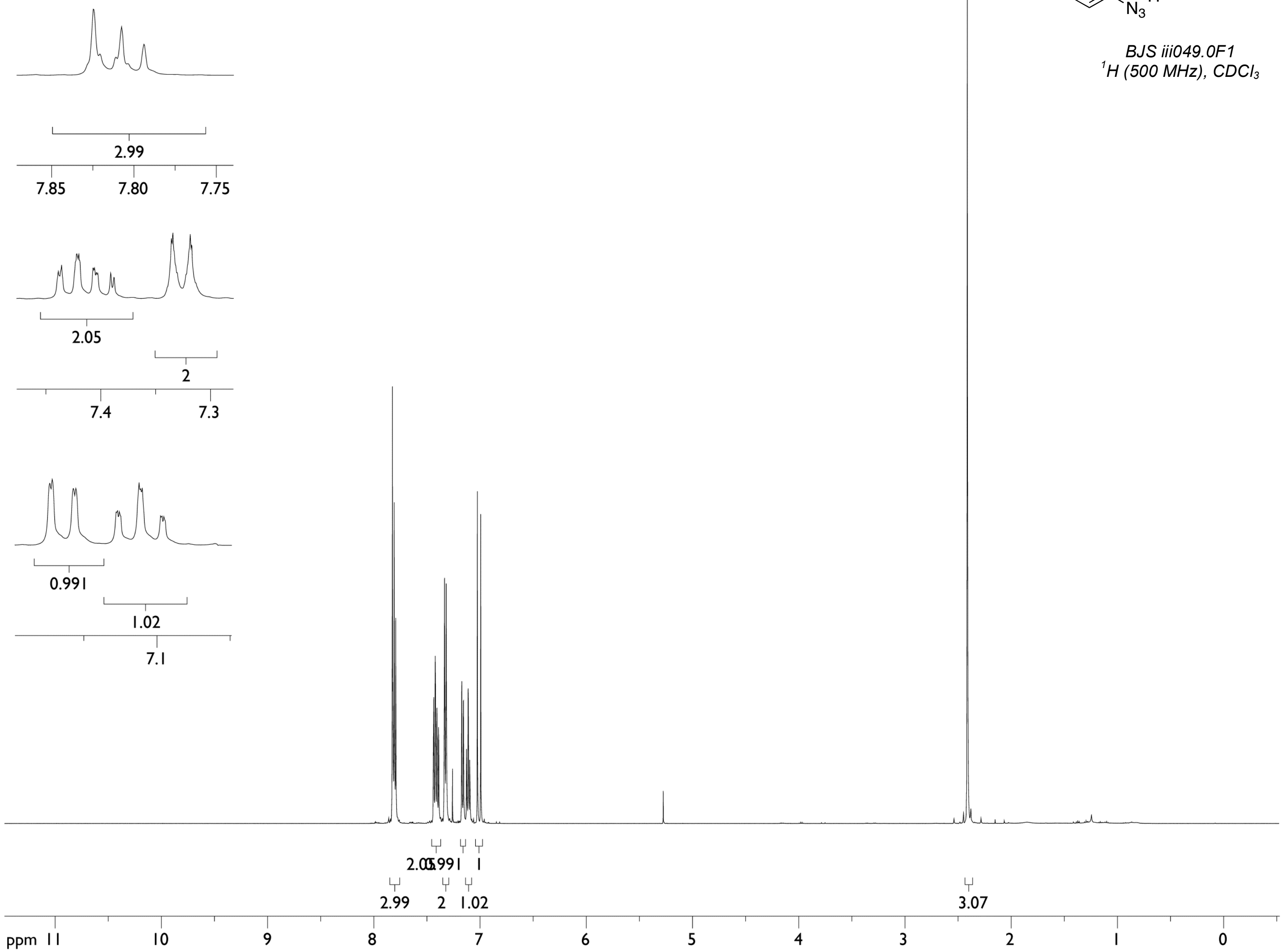
BJS iii033.0F1
^{13}C (125 MHz), $CDCl_3$



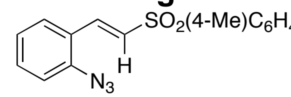
7g



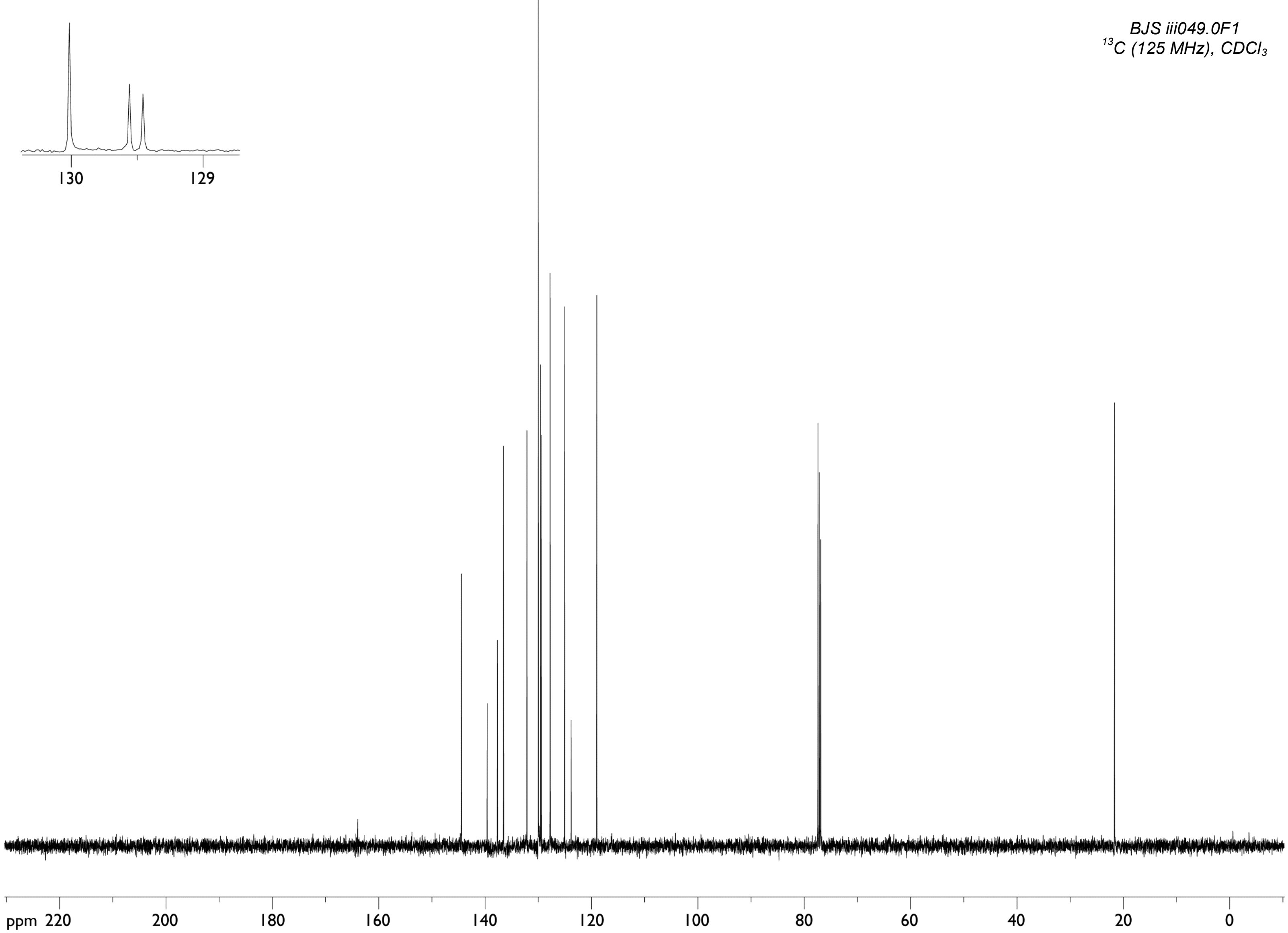
BJS iii049.0F1
[1]H (500 MHz), CDCl3

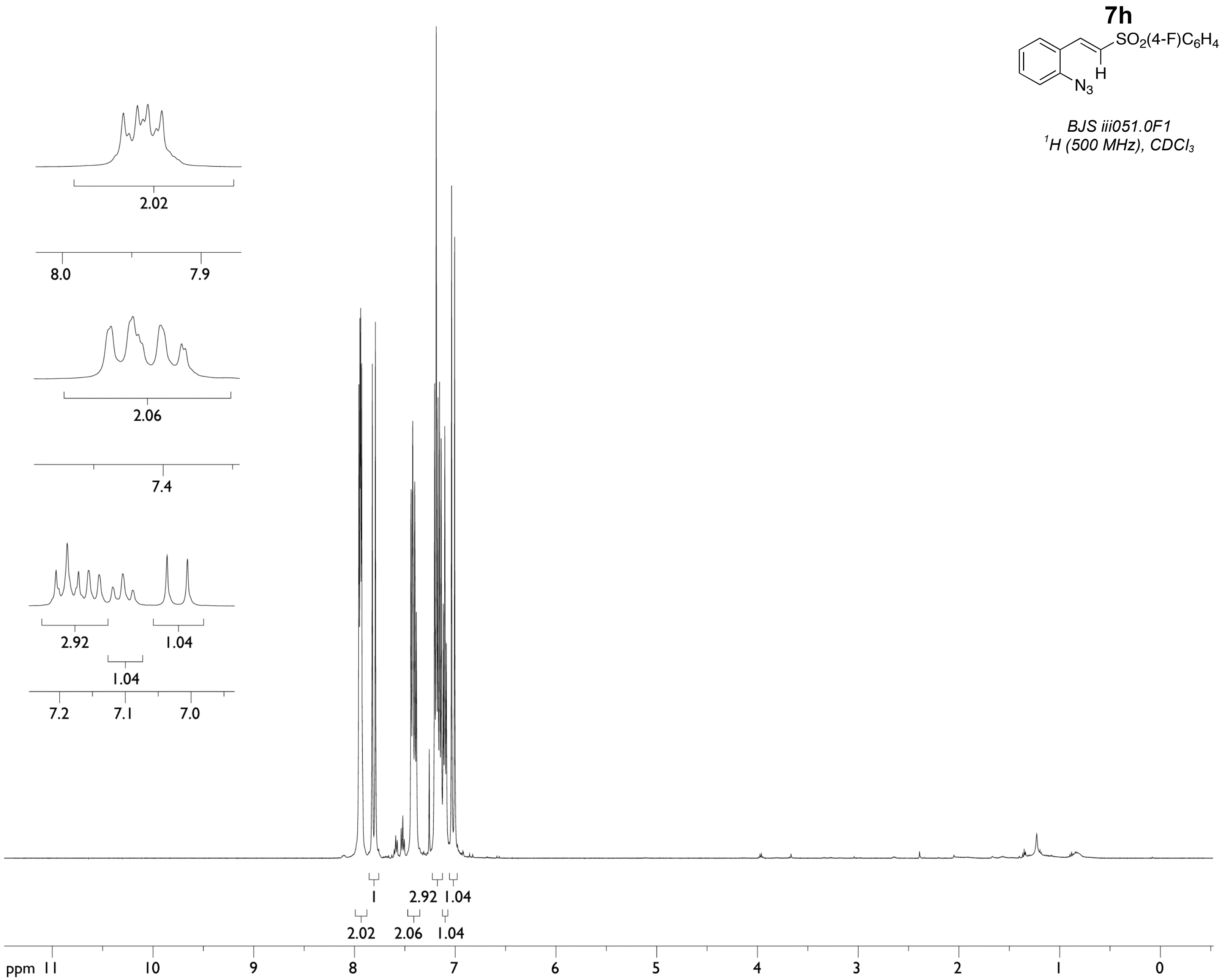


7g

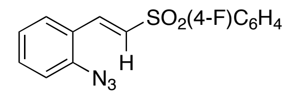


BJS iii049.0F1
^{13}C (125 MHz), $CDCl_3$

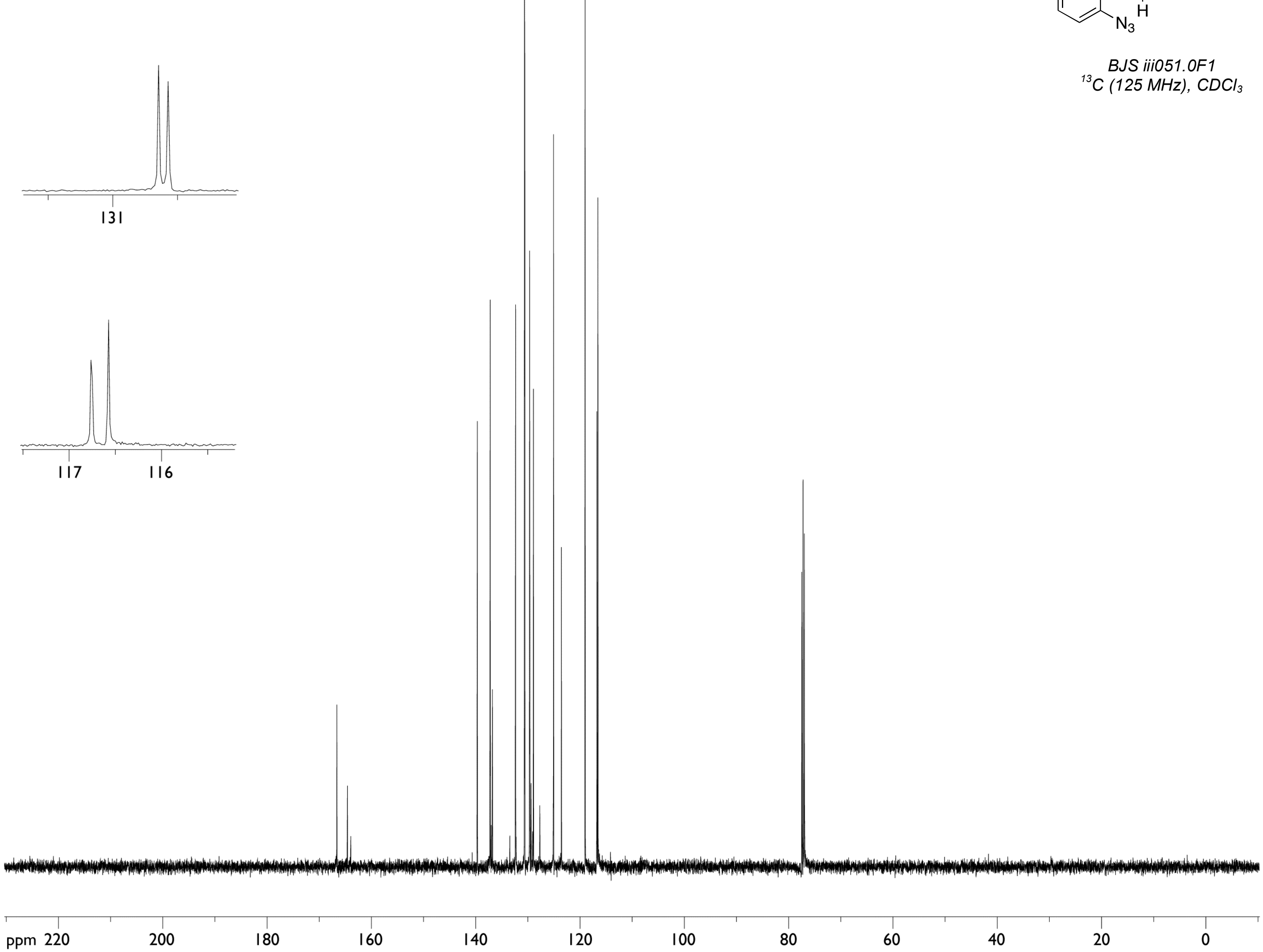



7h
$SO_2(4\text{-}F)C_6H_4$
H
N_3
BJS iii051.0F1
^1H (500 MHz), $CDCl_3$
2.02
8.0
7.9
2.06
7.4
2.92
1.04
1.04
7.2
7.1
7.0
1
2.92
1.04
2.02
2.06
1.04
ppm 11
10
9
8
7
6
5
4
3
2
1
0

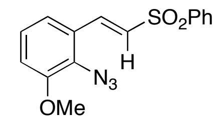
7h



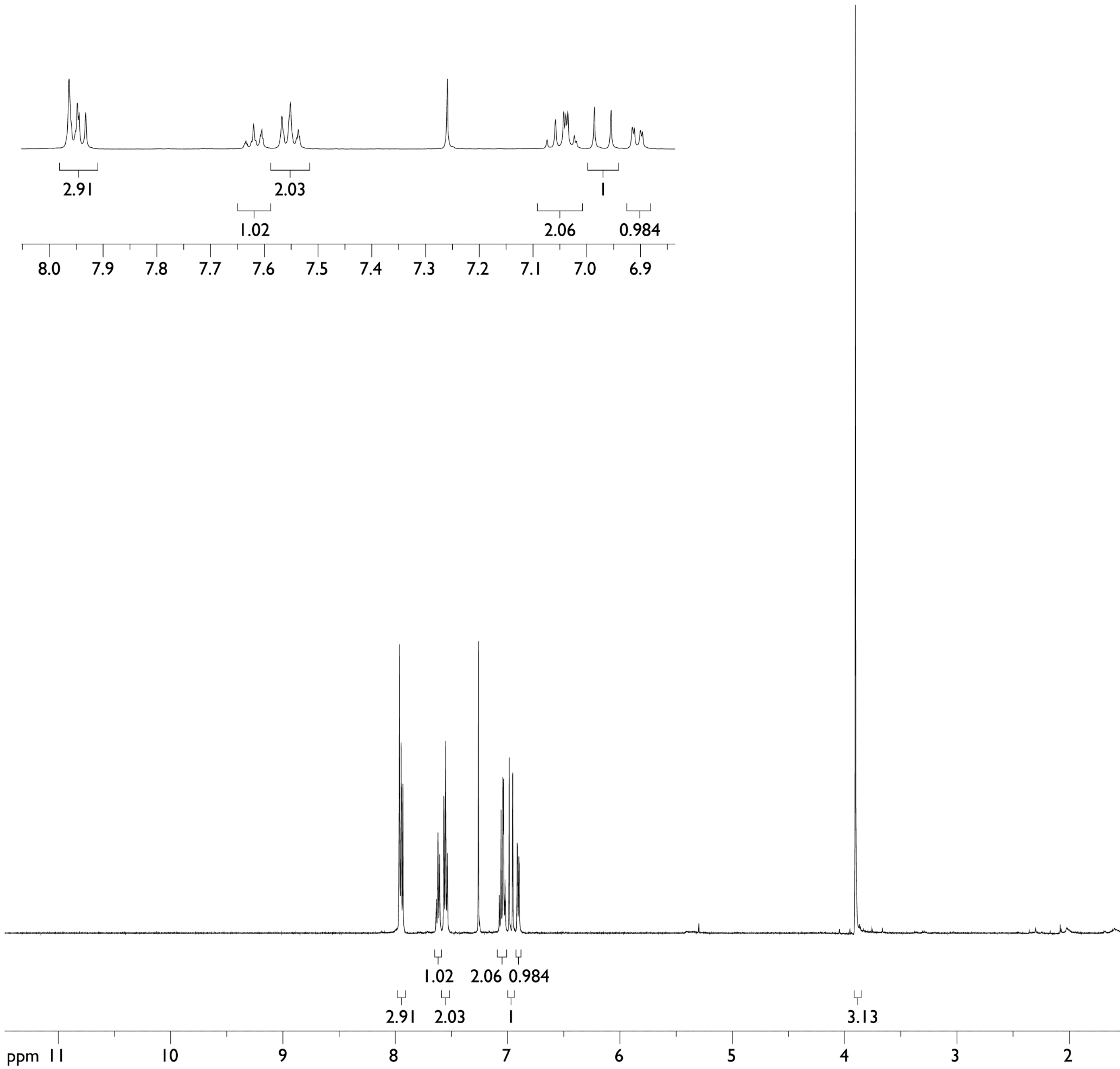
BJS iii051.0F1
^{13}C (125 MHz), $CDCl_3$



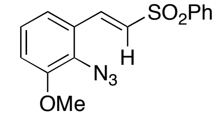
7i



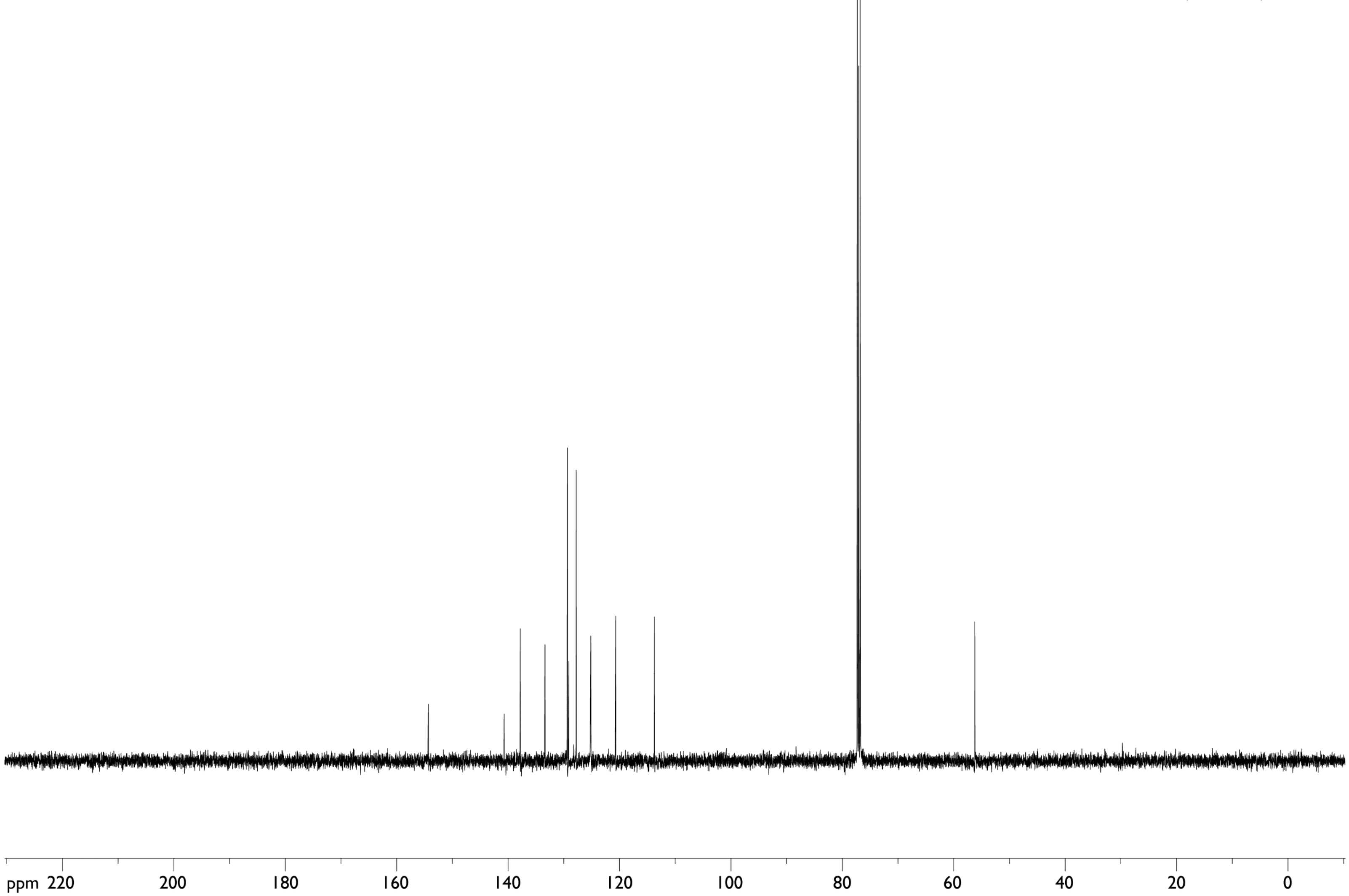
BJS iii096.0F2
^{1}H (500 MHz), $CDCl_3$

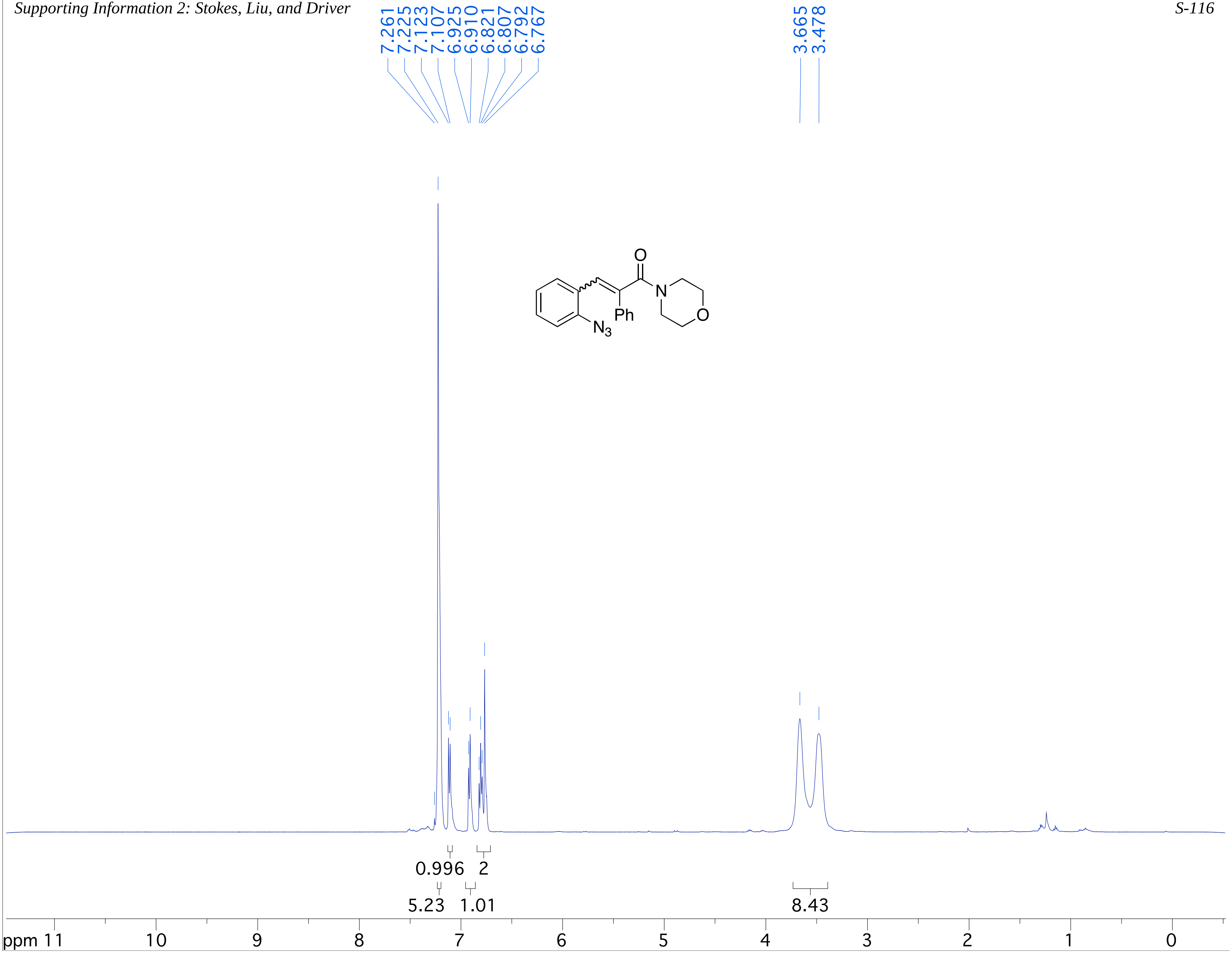


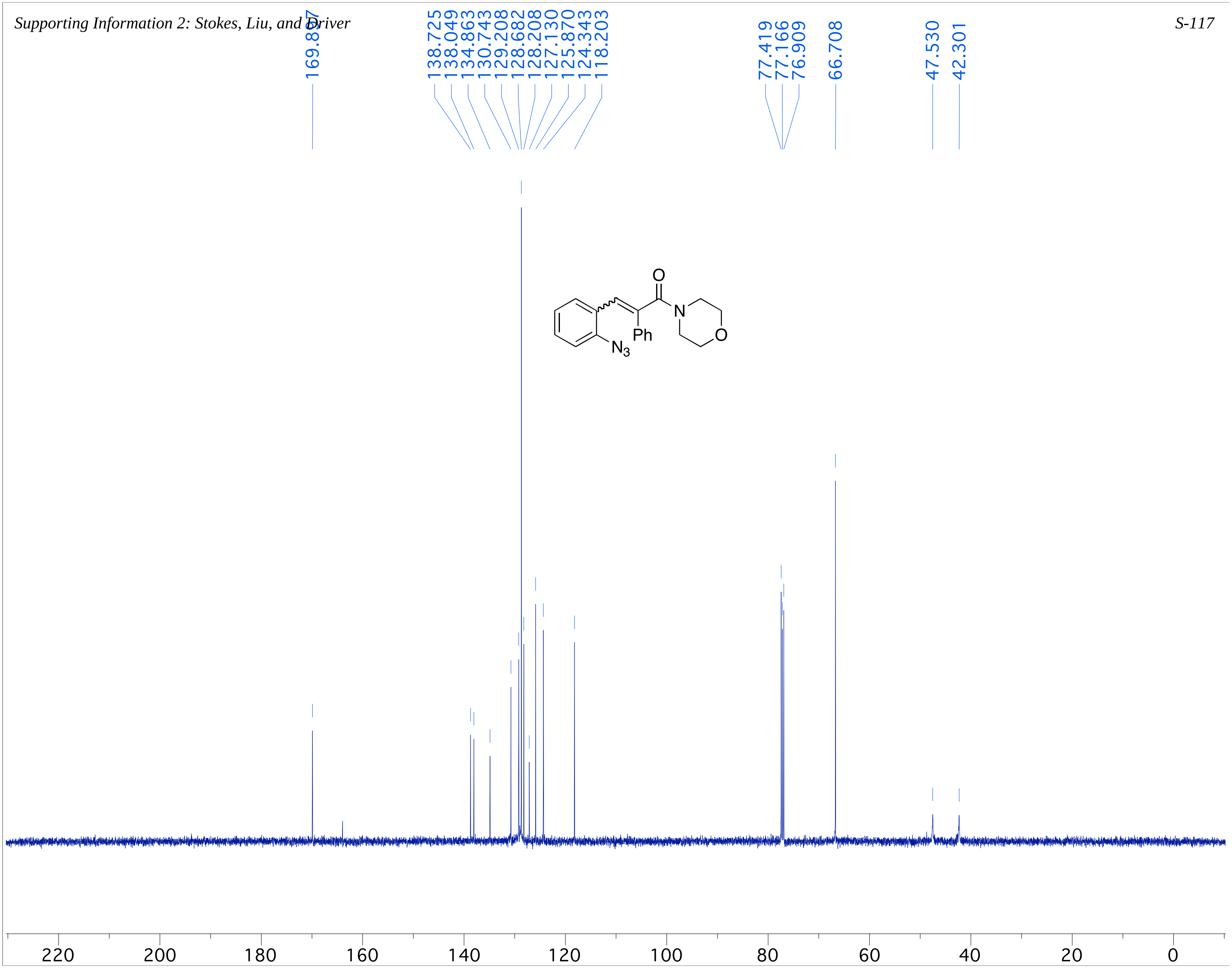
7i



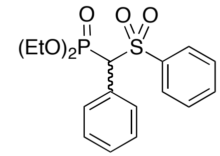
BJS iii096.0F2
^{13}C (125 MHz), $CDCl_3$



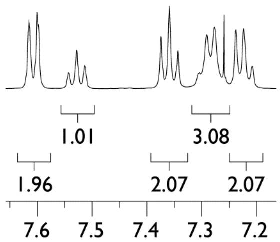

7.261
7.225
7.123
7.107
6.925
6.910
6.821
6.807
6.792
6.767
3.665
3.478
O
N
O
Ph
N3
0.996
2
5.23
1.01
8.43
ppm 11
10
9
8
7
6
5
4
3
2
1
0

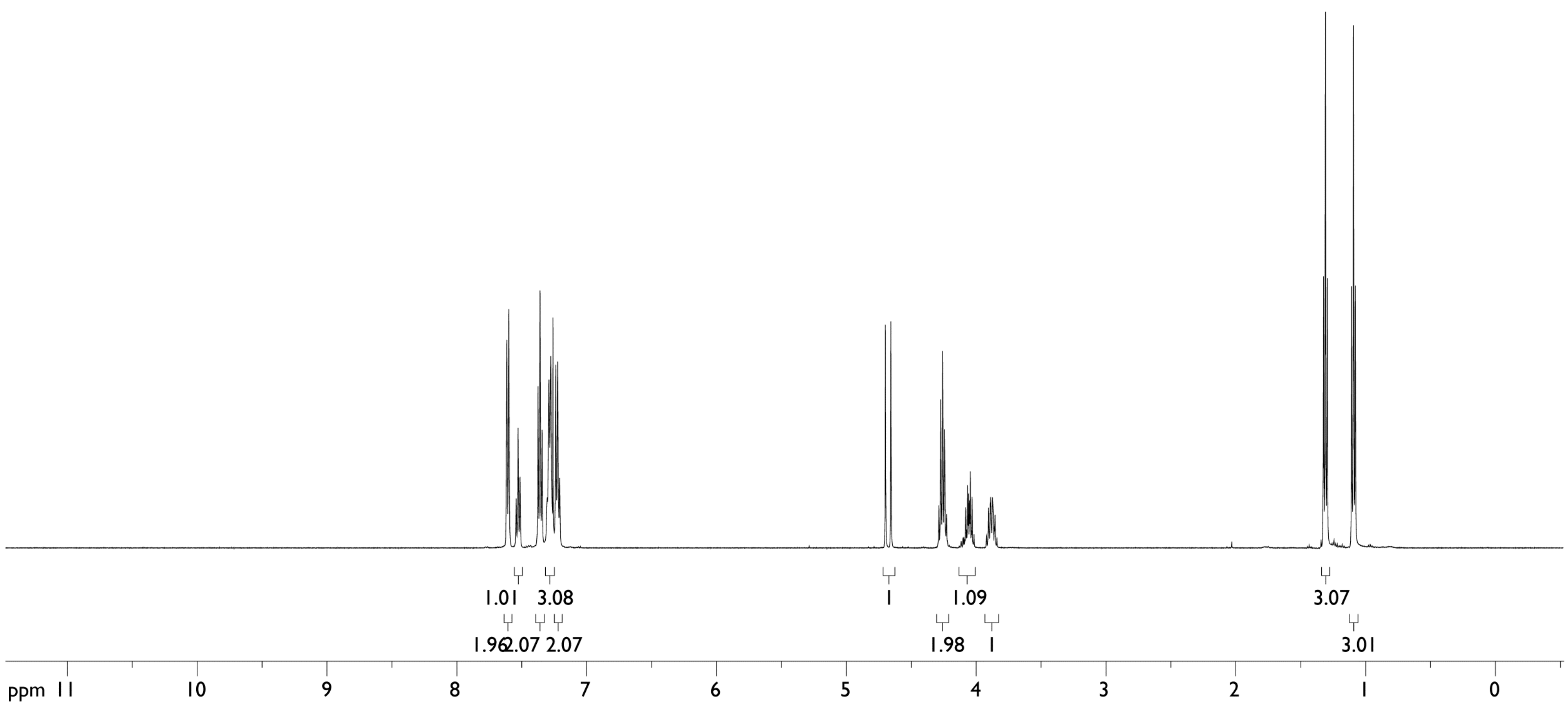

169.857
138.725
138.049
134.863
130.743
129.208
128.682
128.208
127.130
125.870
124.343
118.203
77.419
77.166
76.909
66.708
47.530
42.301
O
N
O
Ph
N_3
220
200
180
160
140
120
100
80
60
40
20
0

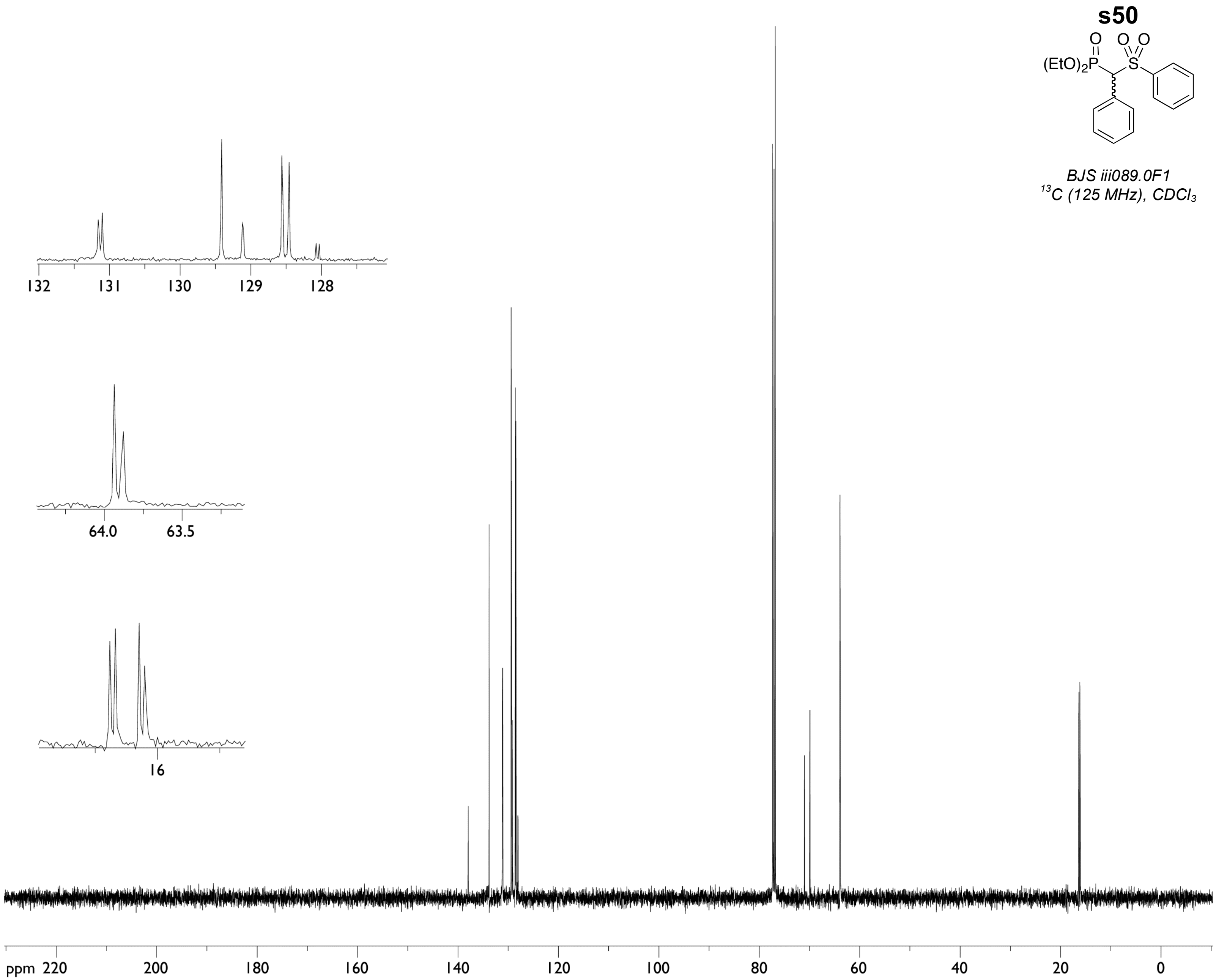
s50



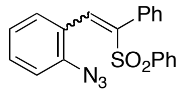
BJS iii089.0F1
^{1}H (500 MHz), CDCl$_3$



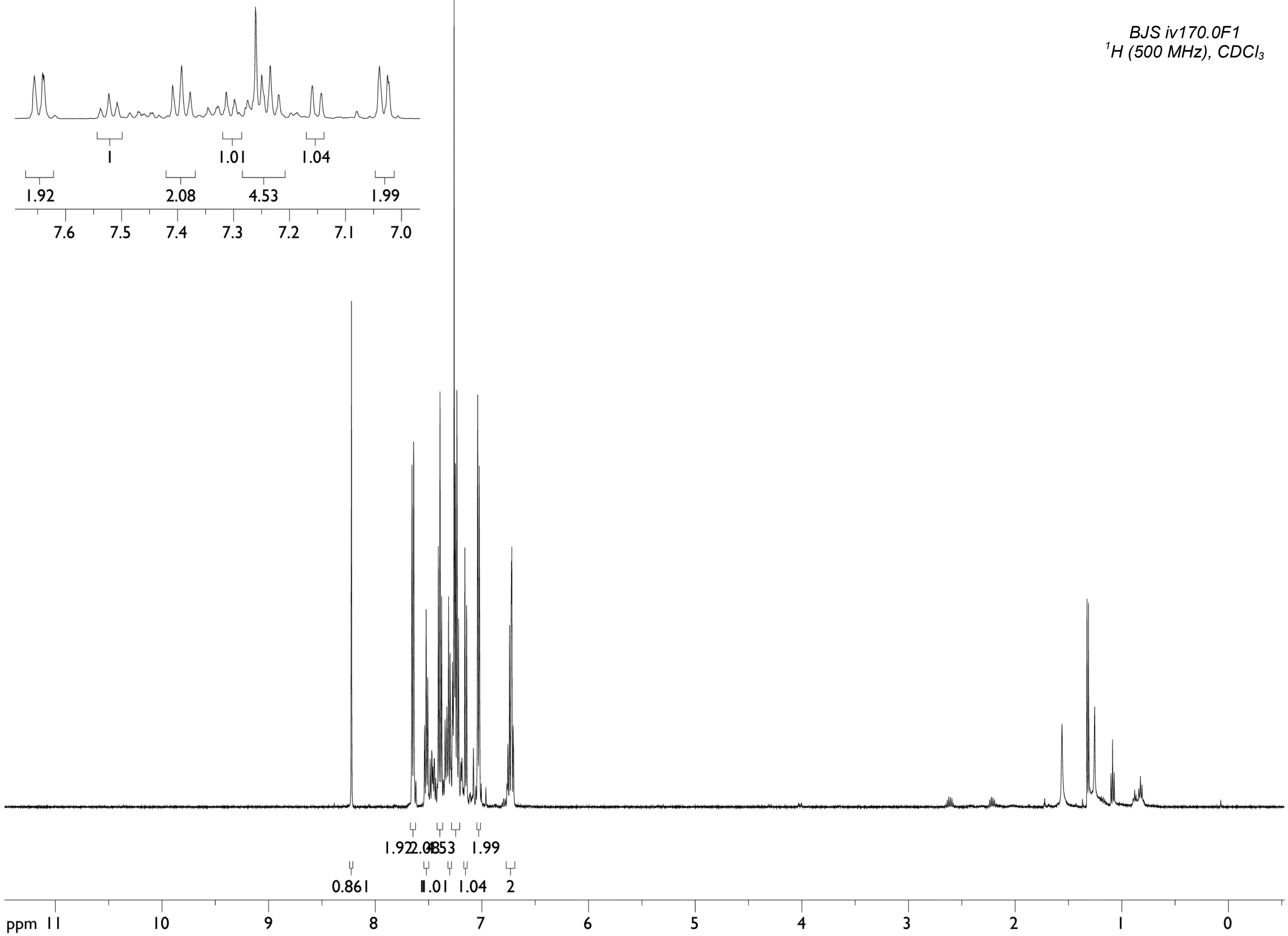



s50
(EtO)2P
S
BJS iii089.0F1
13C (125 MHz), CDCl3
132
131
130
129
128
64.0
63.5
16
ppm 220
200
180
160
140
120
100
80
60
40
20
0

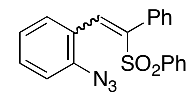
10d



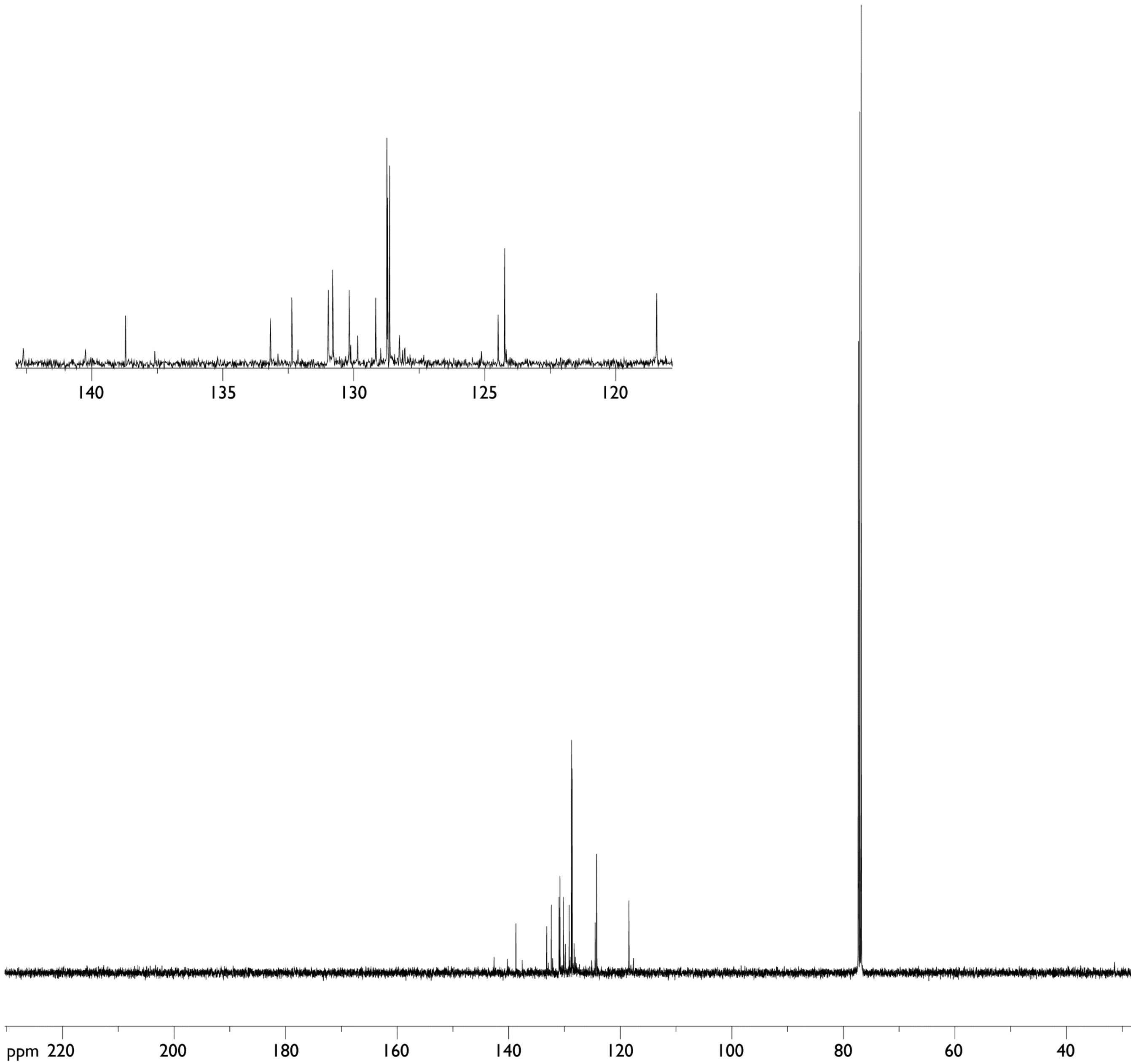
BJS iv170.0F1
^1H (500 MHz), $CDCl_3$



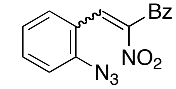
10d



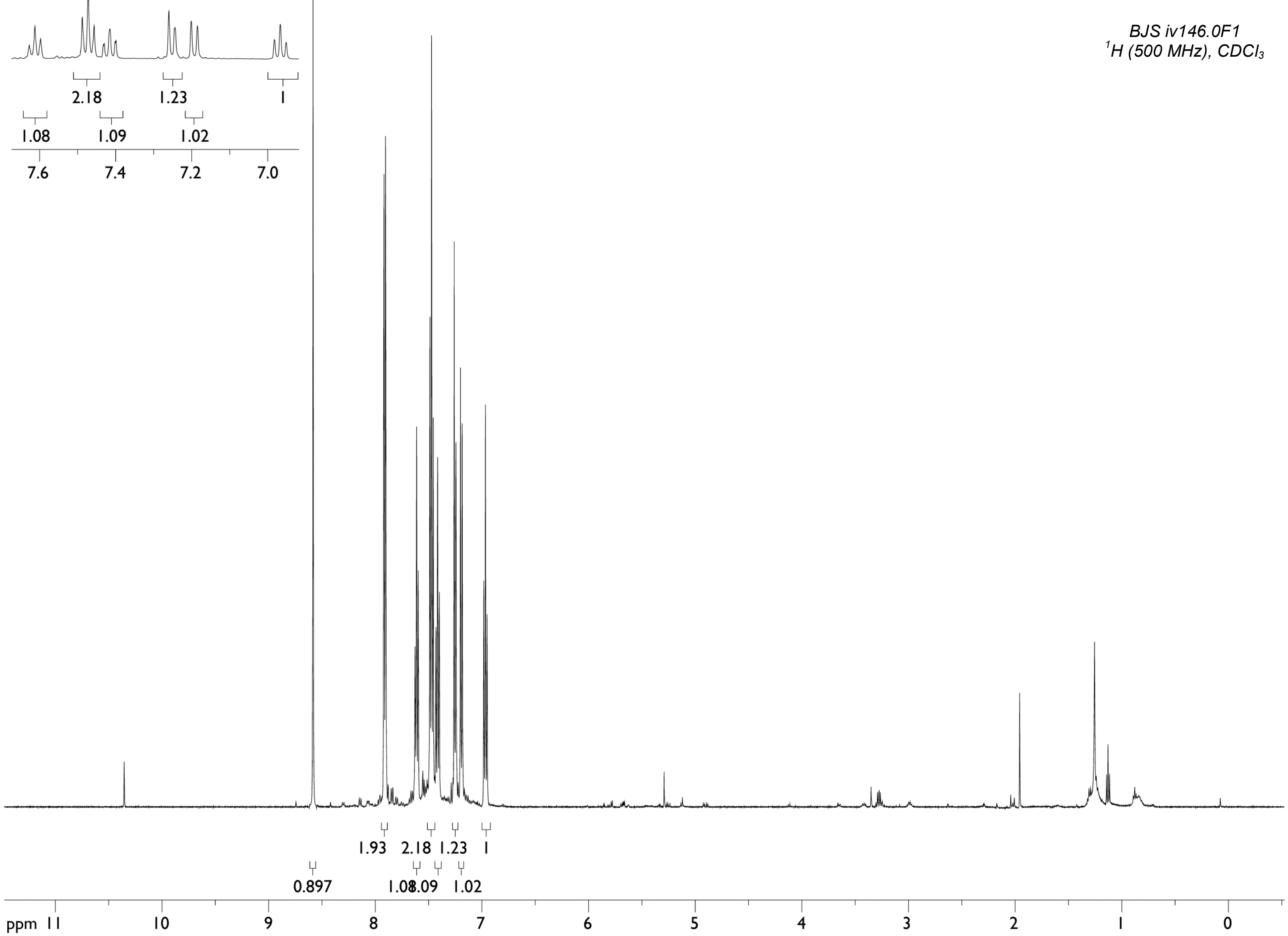
BJS iv170.0F1
^{13}C (125 MHz), $CDCl_3$



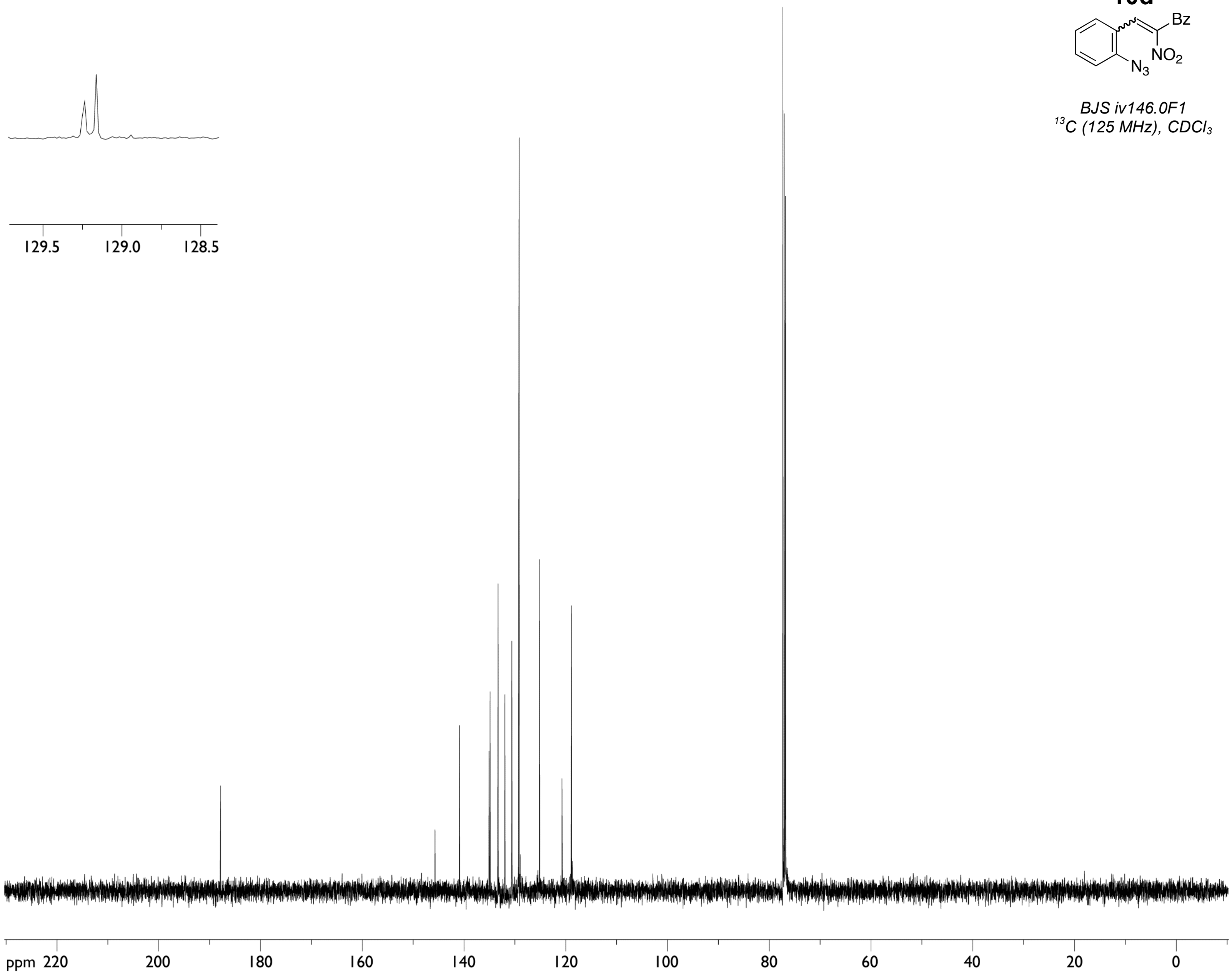
10d



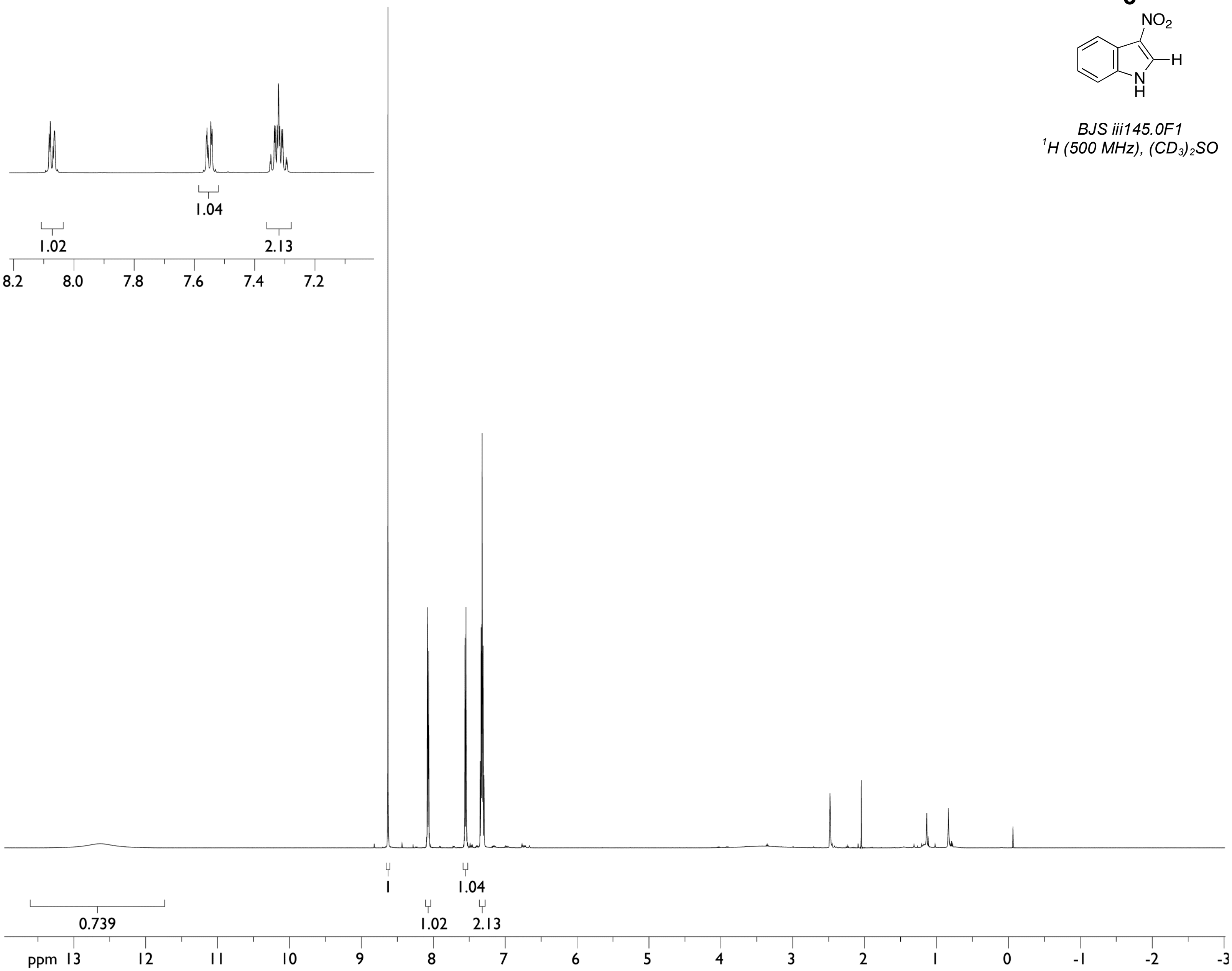
BJS iv146.0F1
^{1}H (500 MHz), $CDCl_3$



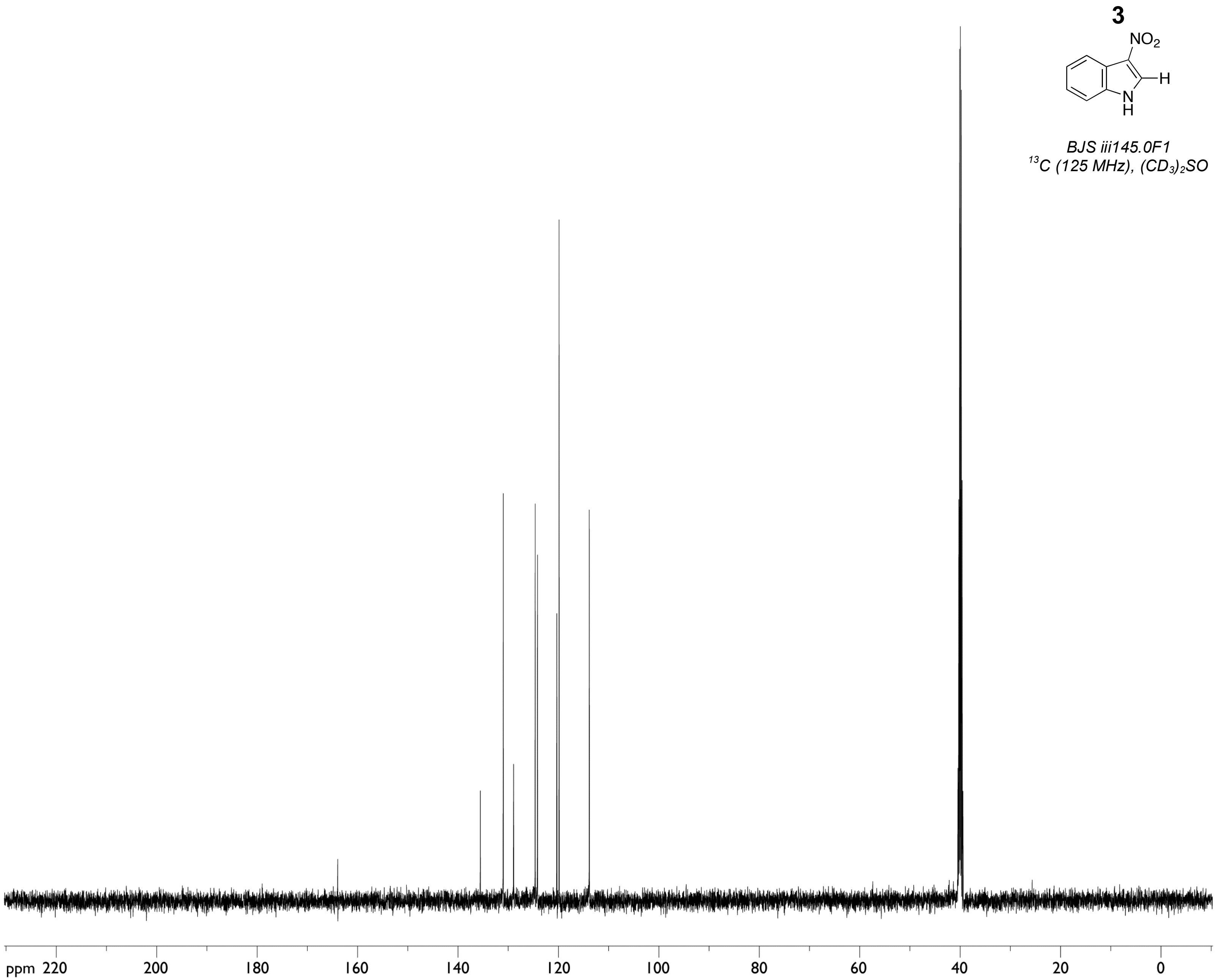
10d

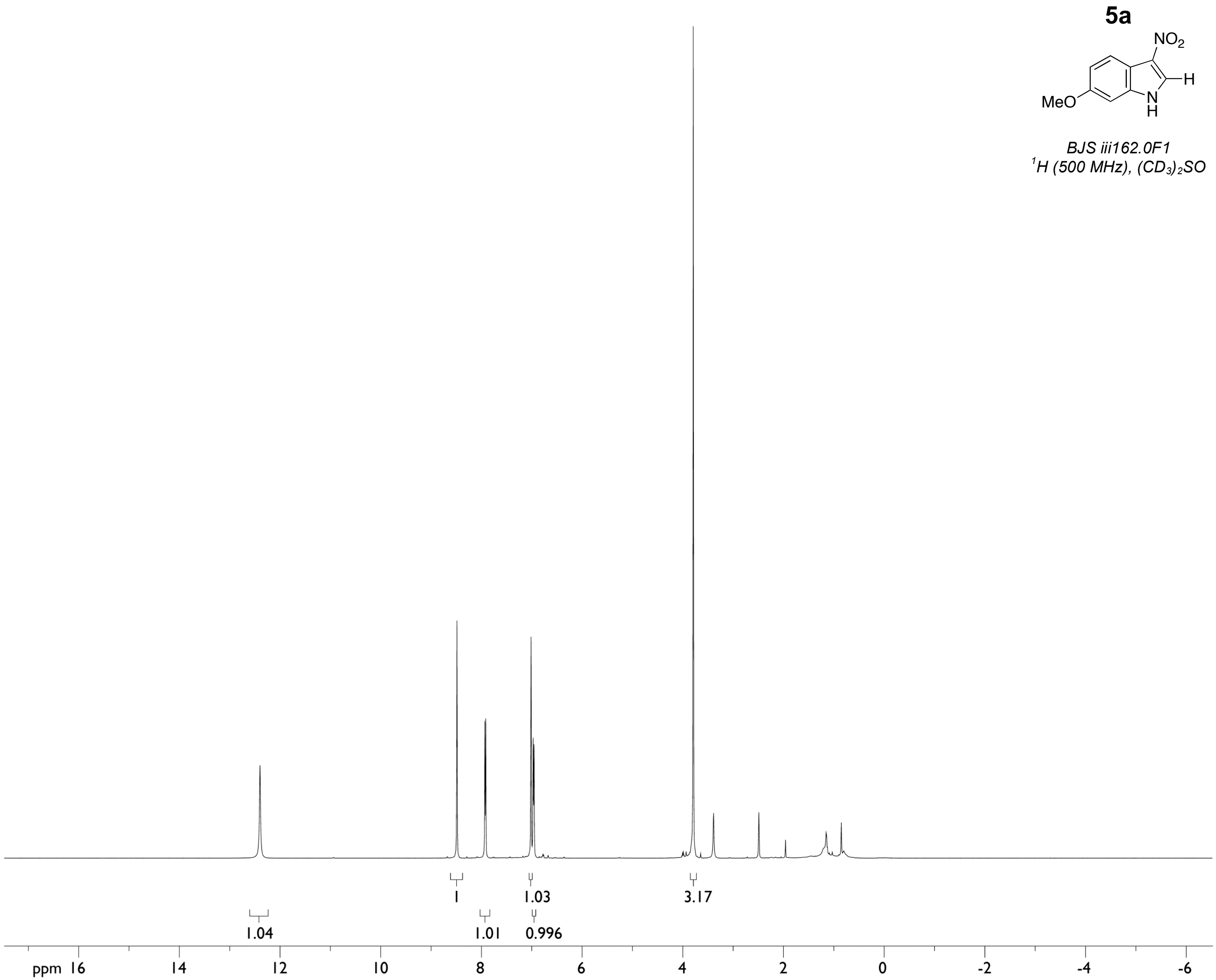

Bz
NO2
N3
BJS iv146.0F1
13C (125 MHz), CDCl3
129.5
129.0
128.5
ppm 220
200
180
160
140
120
100
80
60
40
20
0

3

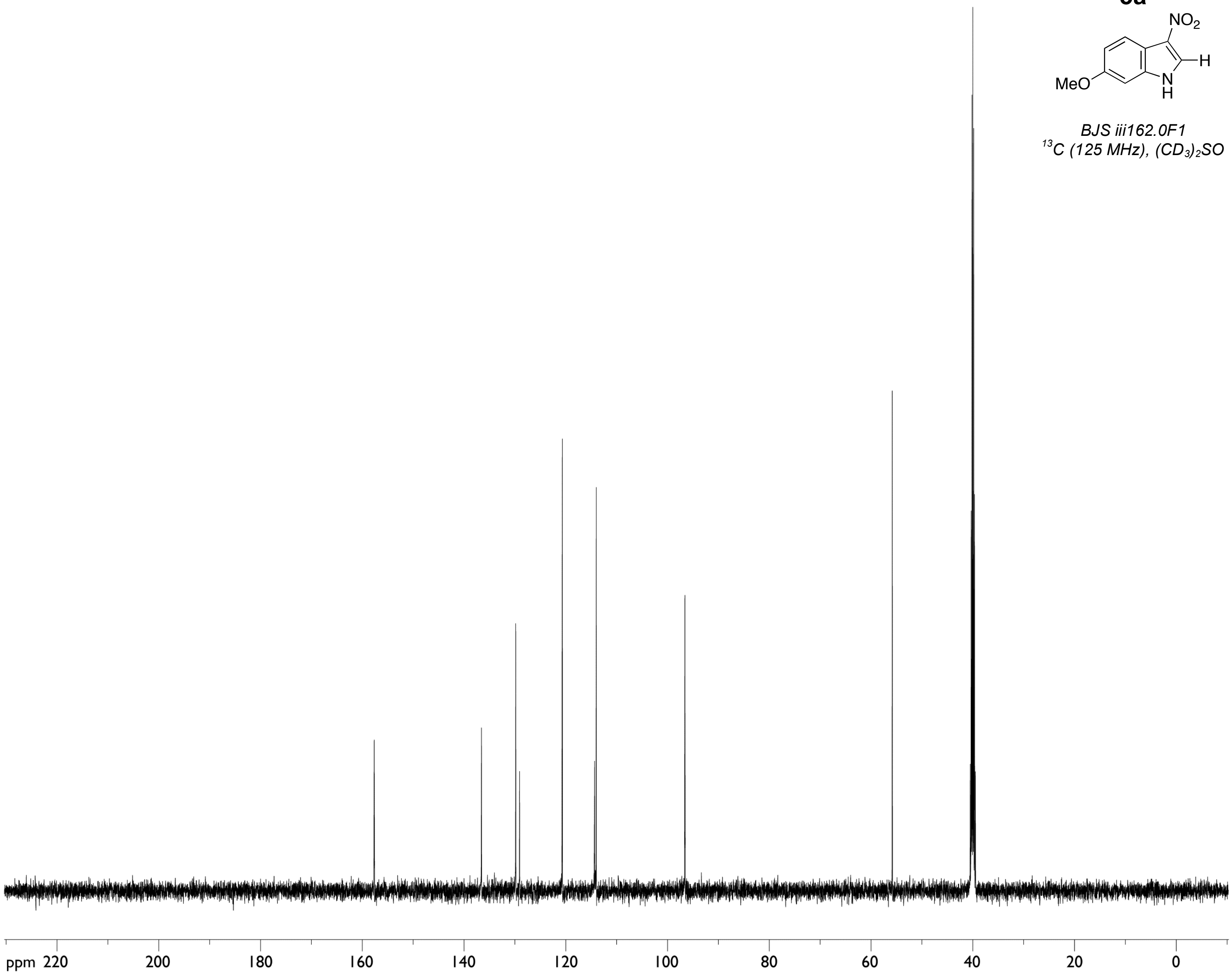


BJS iii145.0F1
^{1}H (500 MHz), $(CD_3)_2SO$

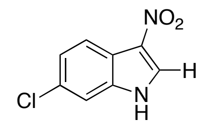

3
NO_2
H
N
H
BJS iii145.0F1
^{13}C (125 MHz), $(CD_3)_2SO$
ppm 220
200
180
160
140
120
100
80
60
40
20
0


5a
NO2
H
MeO
N
H
BJS iii162.0F1
1H (500 MHz), (CD3)2SO
1
1.03
3.17
1.04
1.01
0.996
ppm 16
14
12
10
8
6
4
2
0
-2
-4
-6

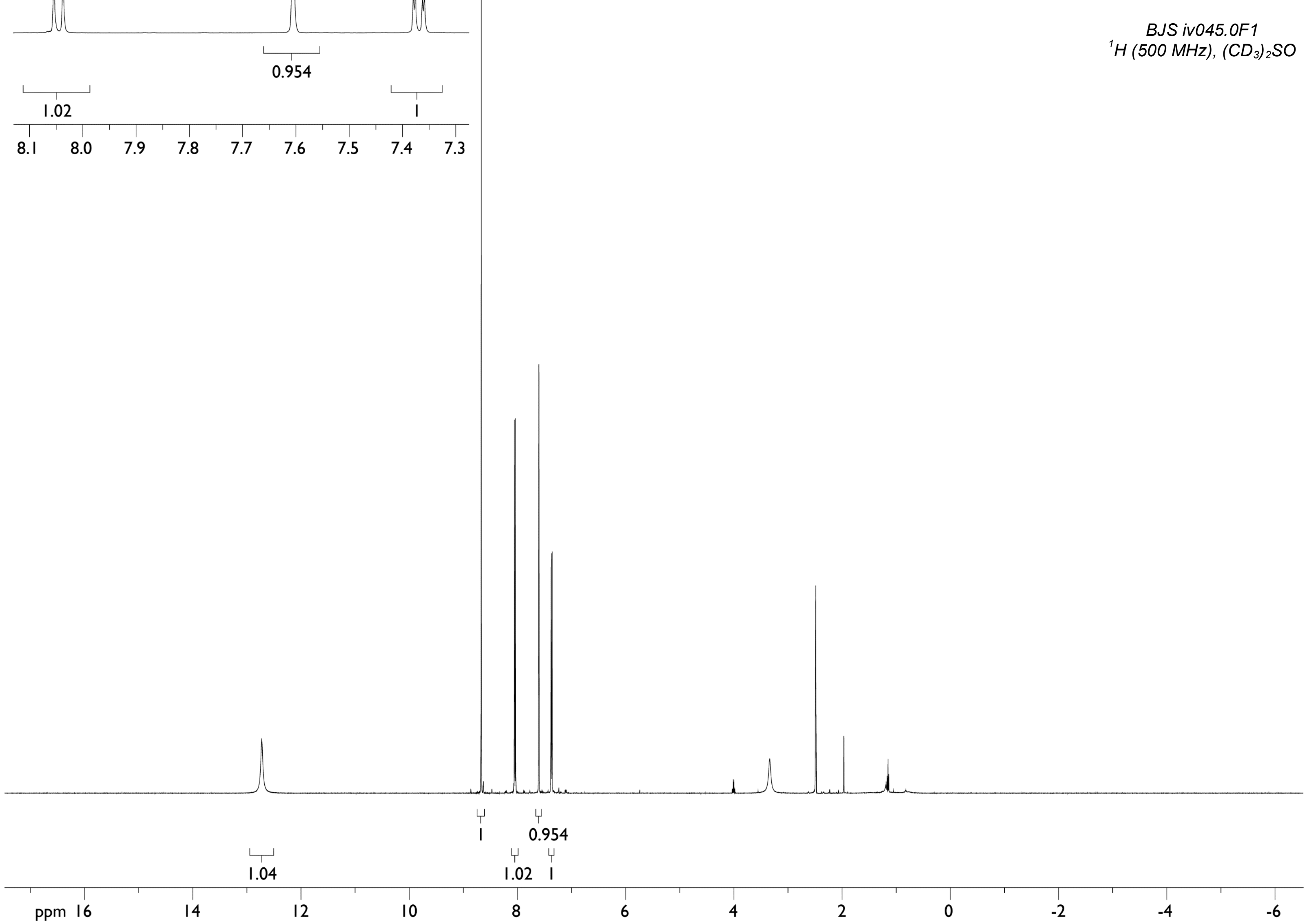
5a


NO2
H
MeO
N
H
BJS iii162.0F1
13C (125 MHz), (CD3)2SO
ppm 220
200
180
160
140
120
100
80
60
40
20
0

5b



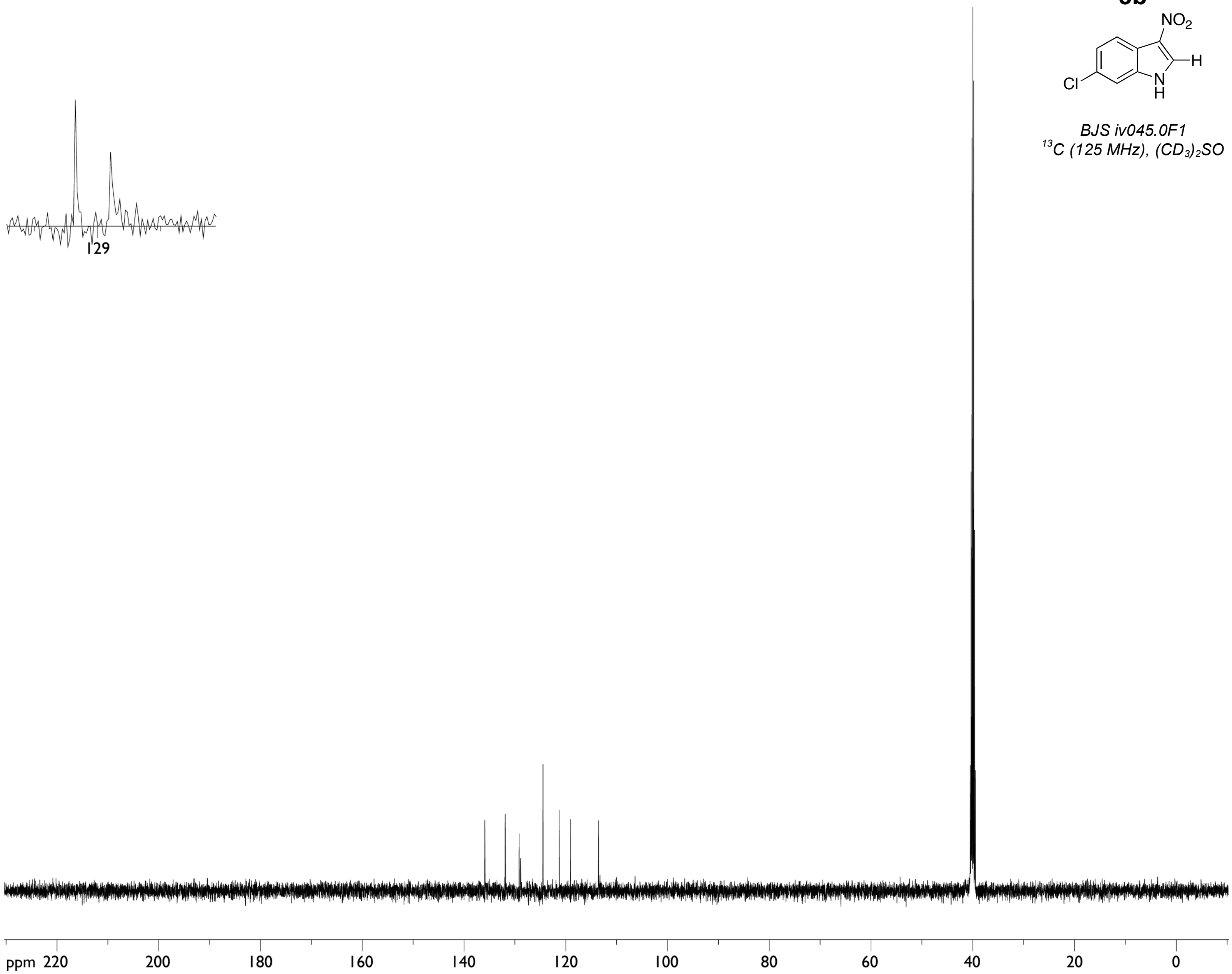
BJS iv045.0F1
[1]H (500 MHz), $(CD_3)_2SO$



5b

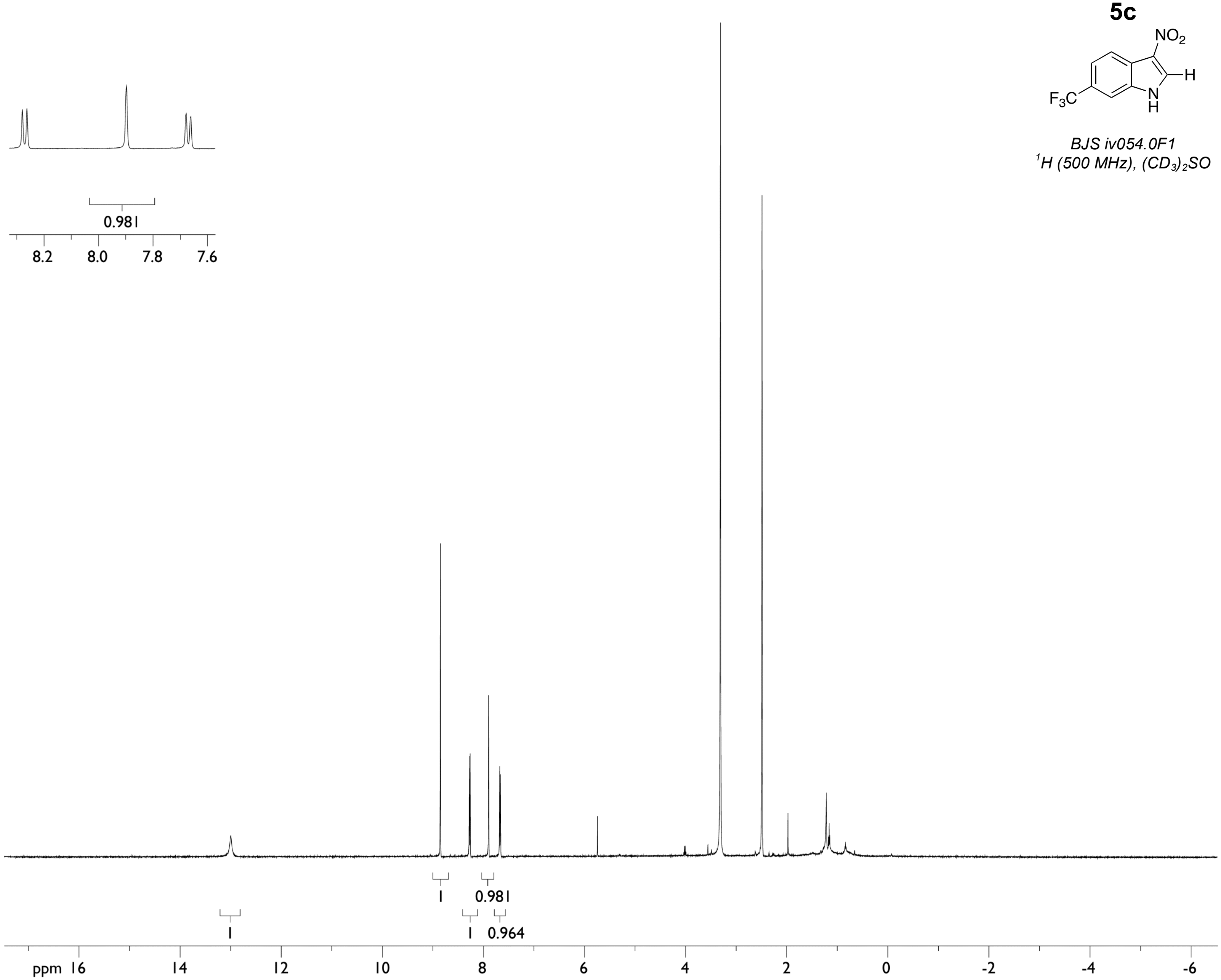
BJS iv045.0F1

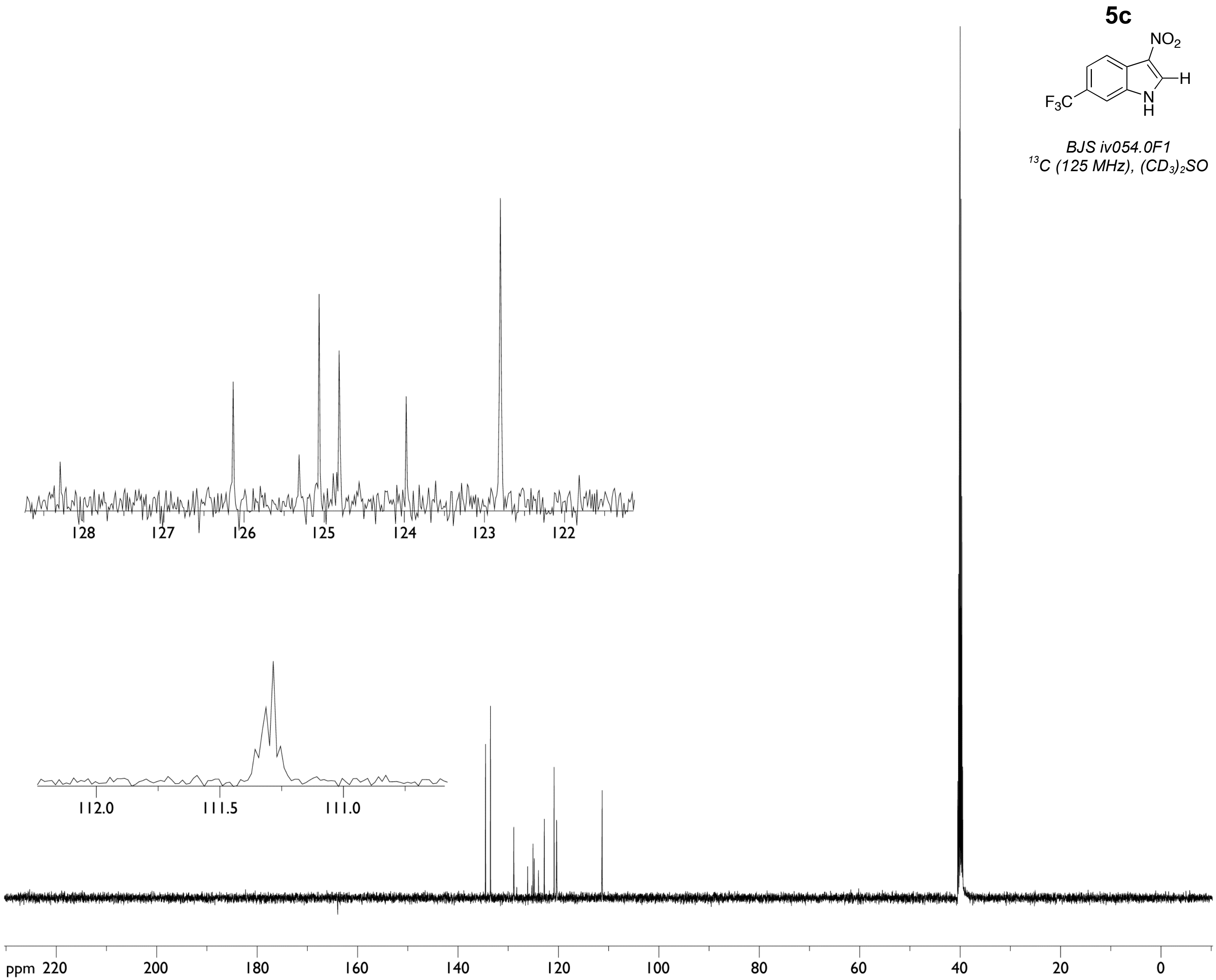
^{13}C (125 MHz), $(CD_3)_2SO$



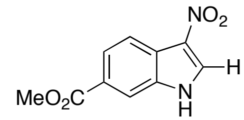
5c

BJS iv054.0F1
^{1}H (500 MHz), $(CD_3)_2SO$

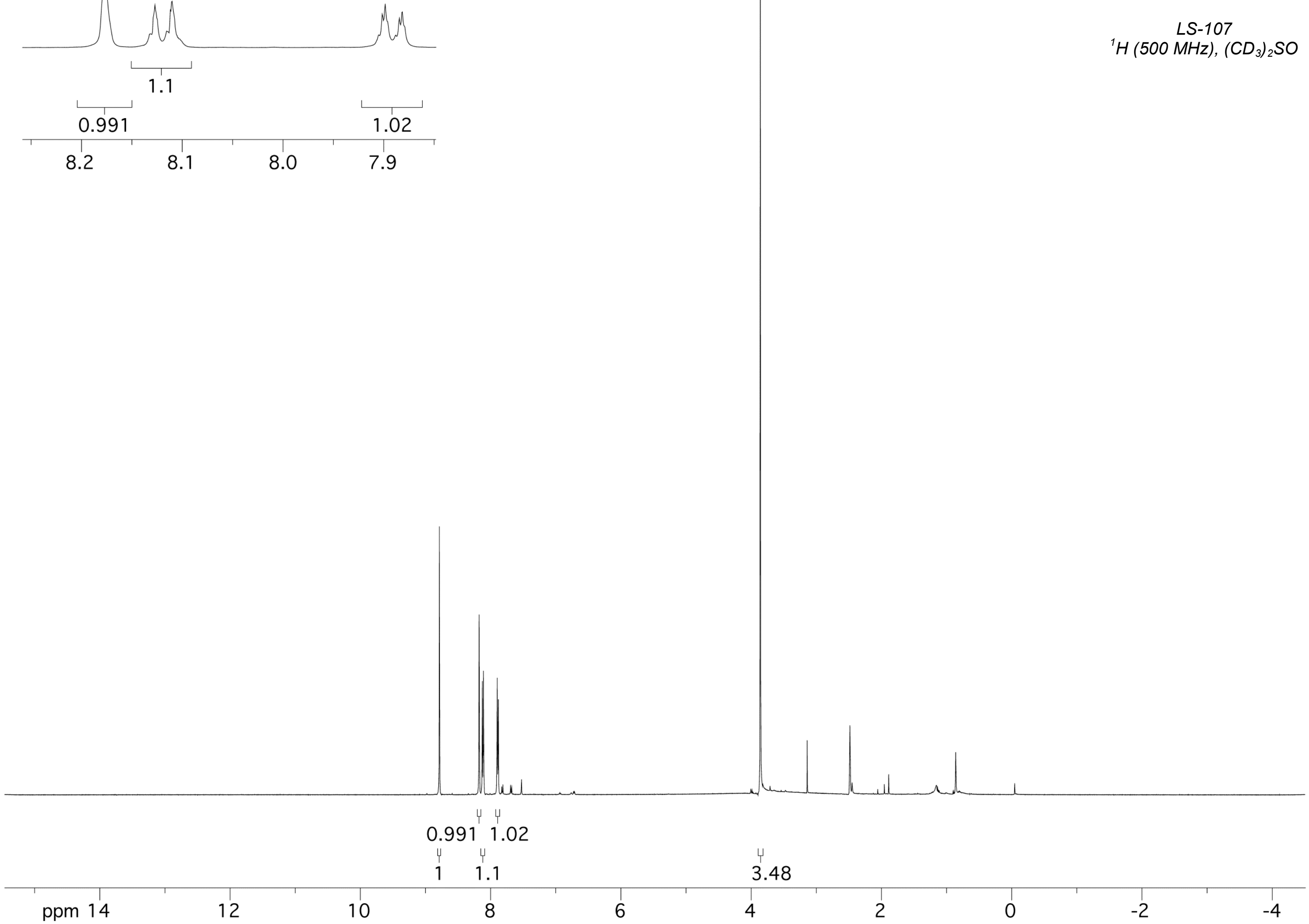


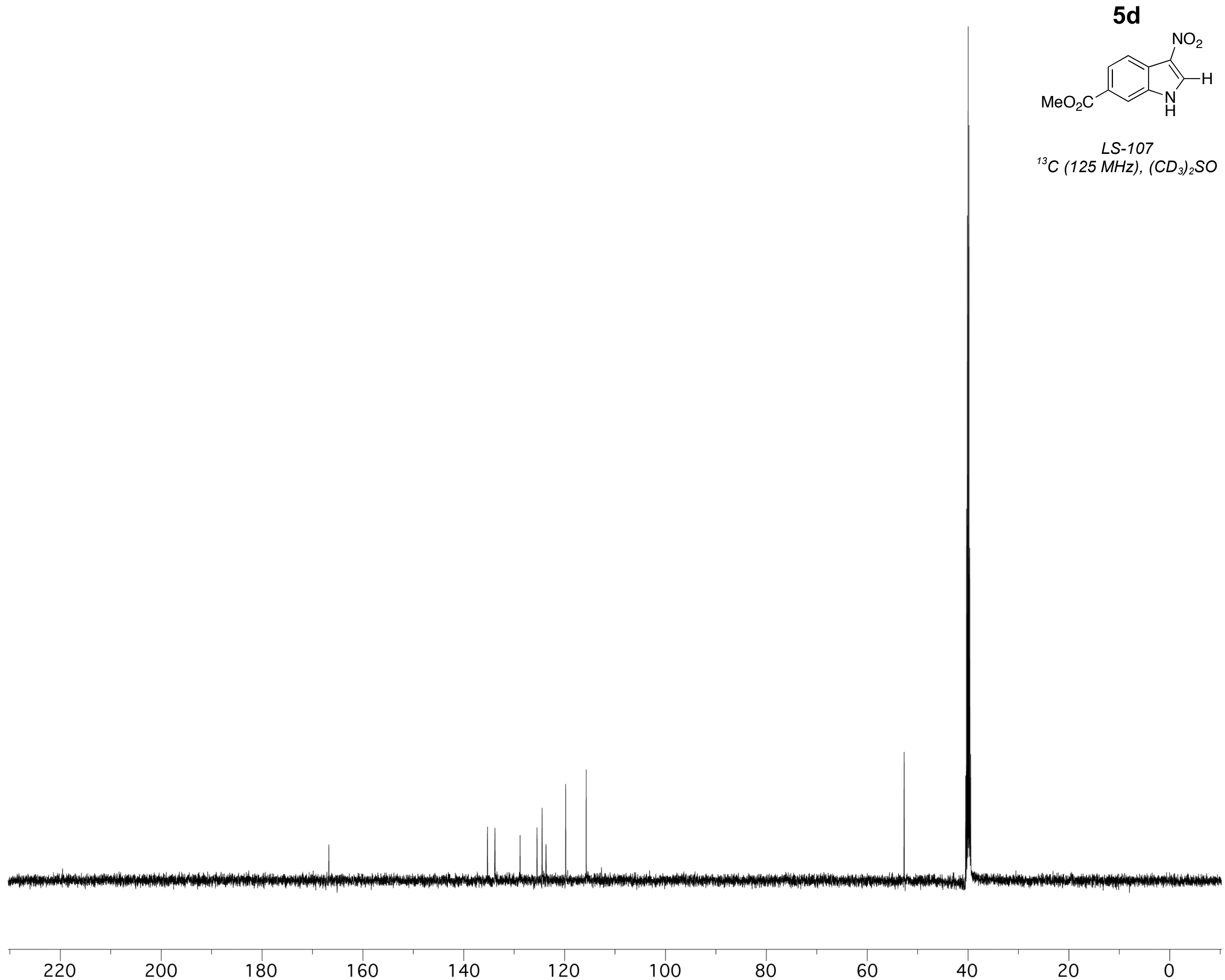

5c
NO_2
H
F_3C
N
H
BJS iv054.0F1
^{13}C (125 MHz), $(CD_3)_2SO$
128
127
126
125
124
123
122
112.0
111.5
111.0
ppm 220
200
180
160
140
120
100
80
60
40
20
0

5d

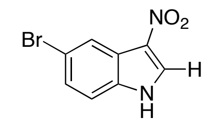


LS-107
^{1}H (500 MHz), $(CD_3)_2SO$

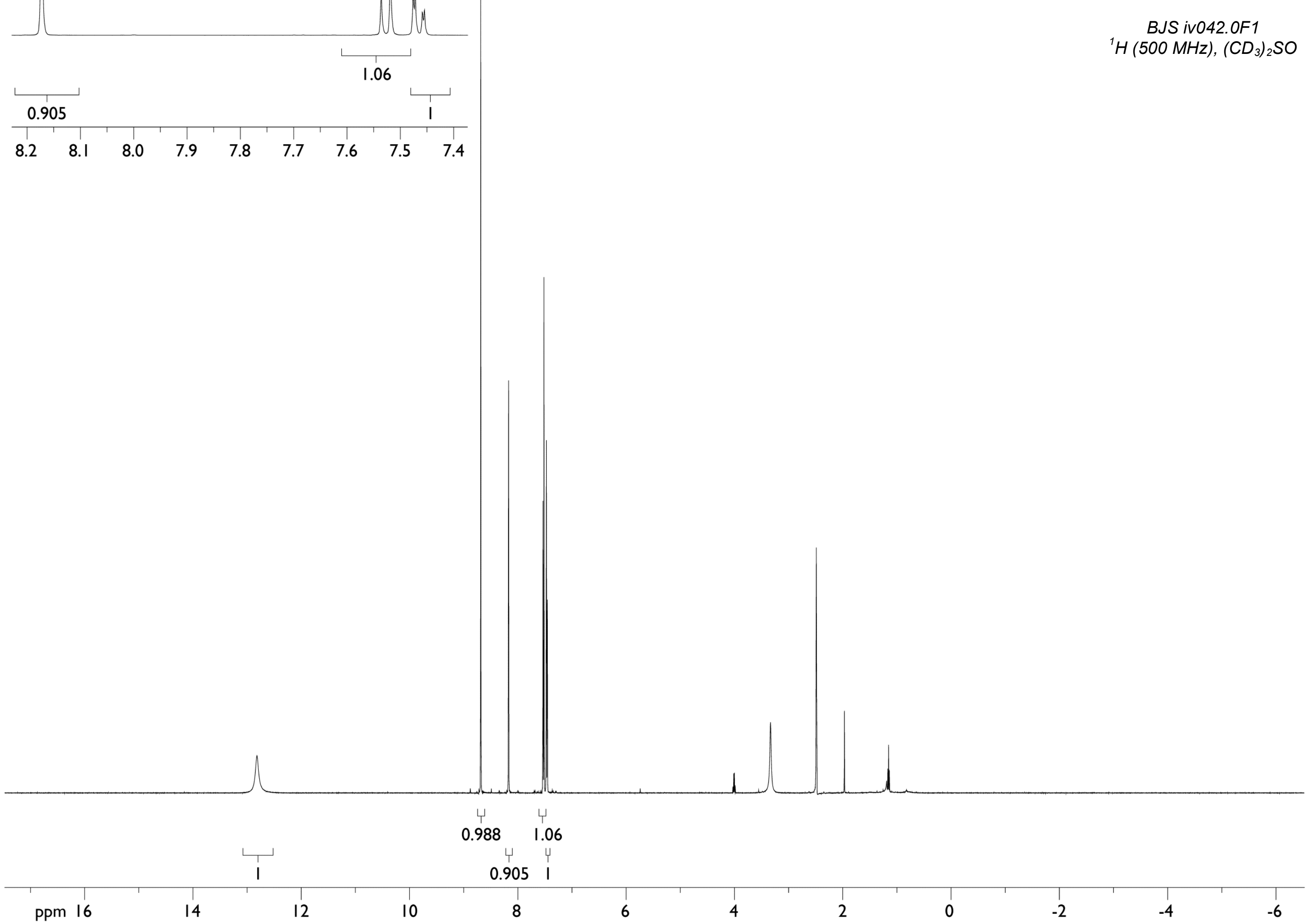


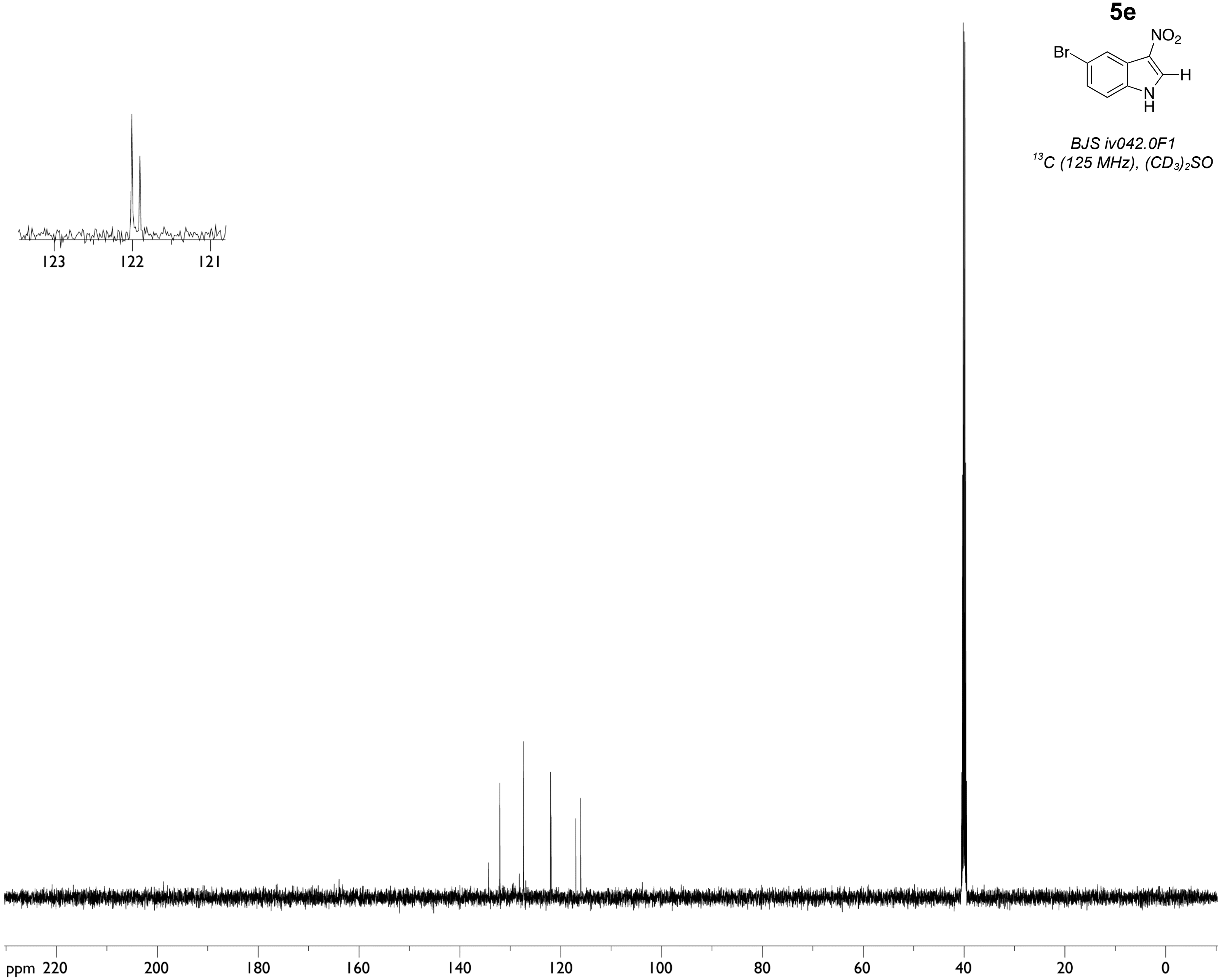

5d
NO2
H
MeO2C
N
H
LS-107
13C (125 MHz), (CD3)2SO
220
200
180
160
140
120
100
80
60
40
20
0

5e

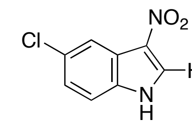


BJS iv042.0F1
^1H (500 MHz), $(CD_3)_2SO$

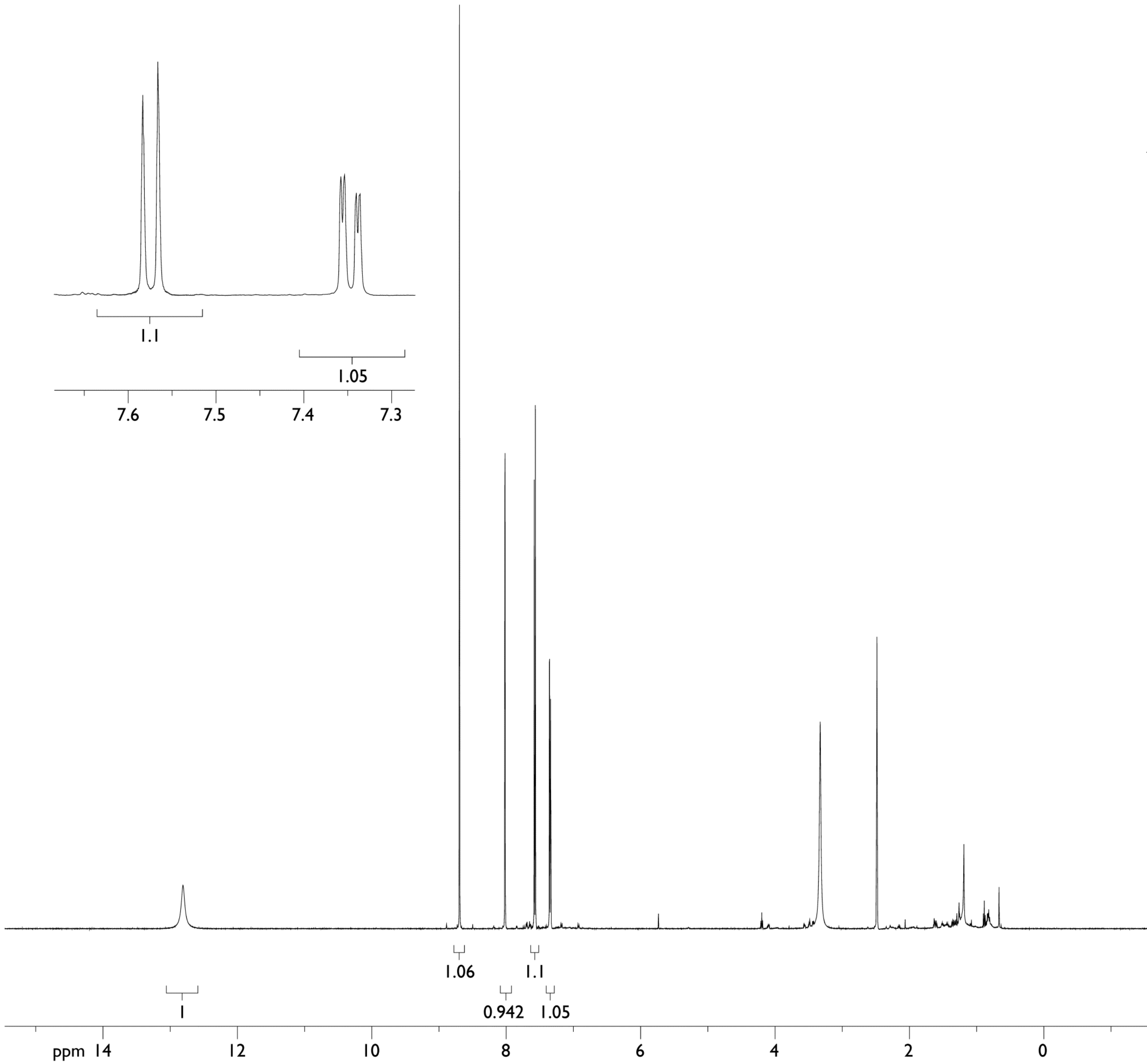



5e
NO2
Br
H
N
H
BJS iv042.0F1
13C (125 MHz), (CD3)2SO
123
122
121
ppm 220
200
180
160
140
120
100
80
60
40
20
0

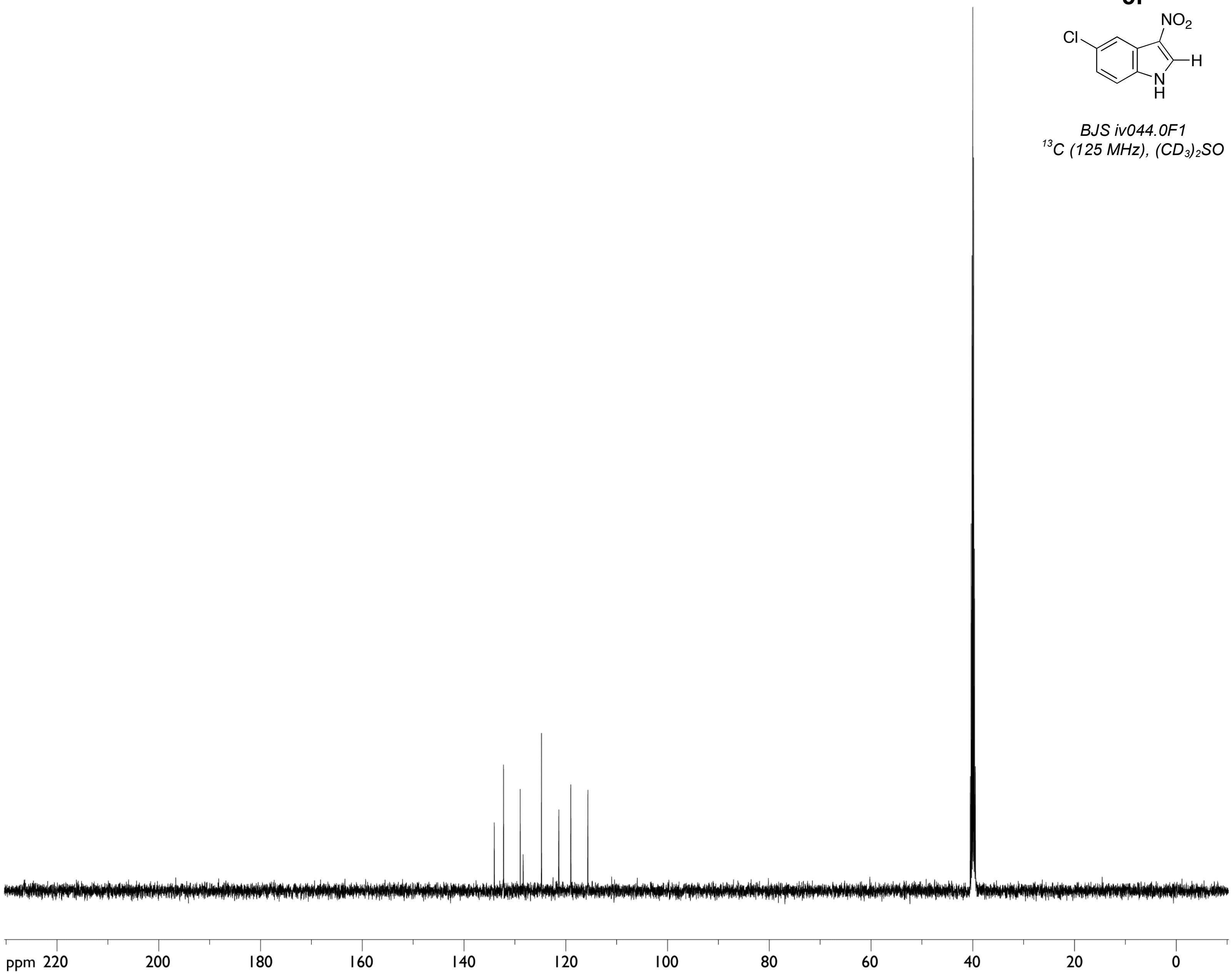
5f



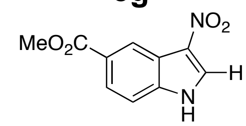
BJS iv044.0F1
^1H (500 MHz), $(CD_3)_2SO$



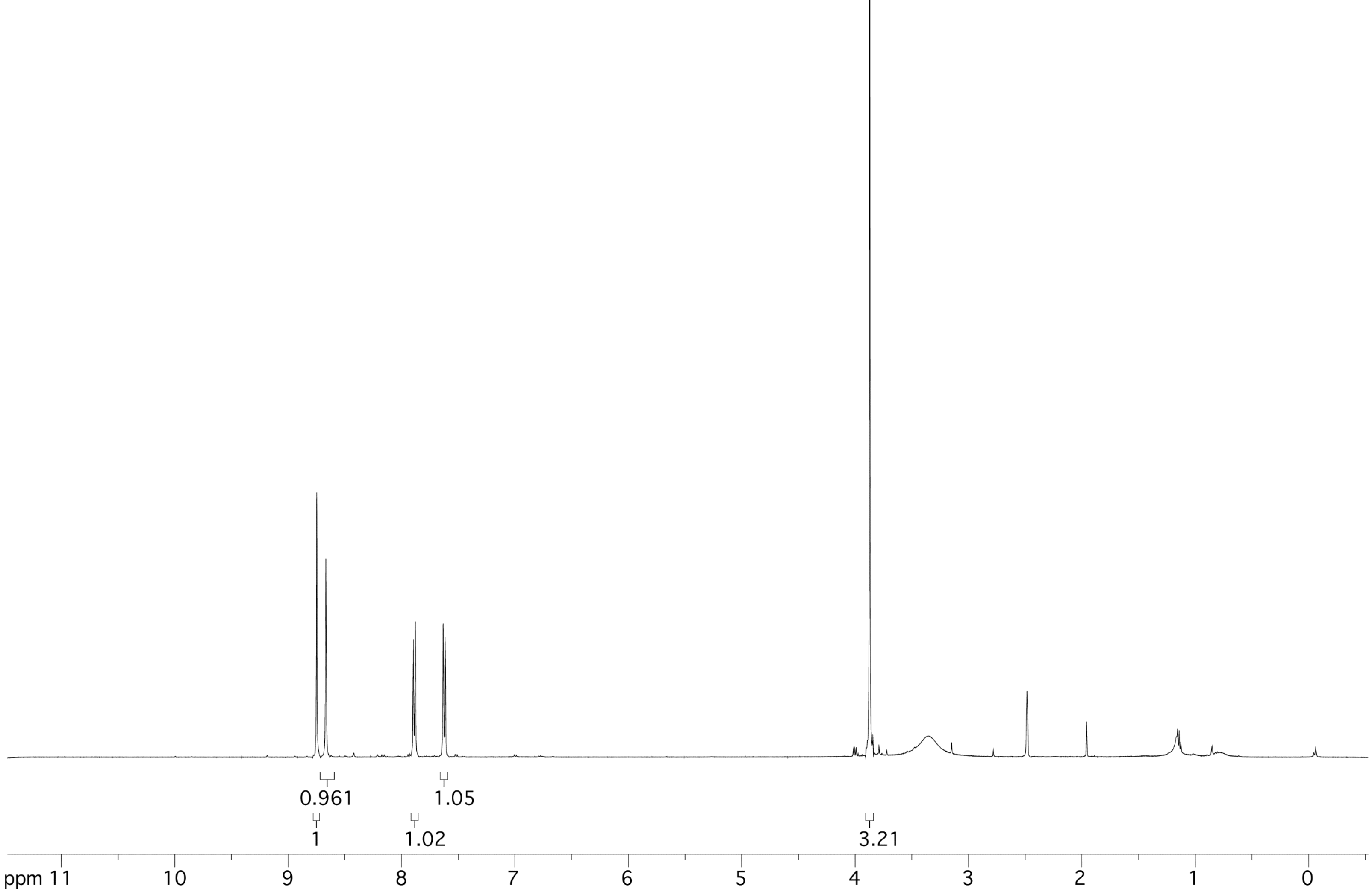
5f


NO2
Cl
H
N
H
BJS iv044.0F1
13C (125 MHz), (CD3)2SO
ppm 220
200
180
160
140
120
100
80
60
40
20
0

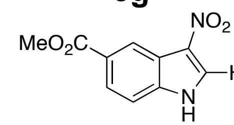
5g



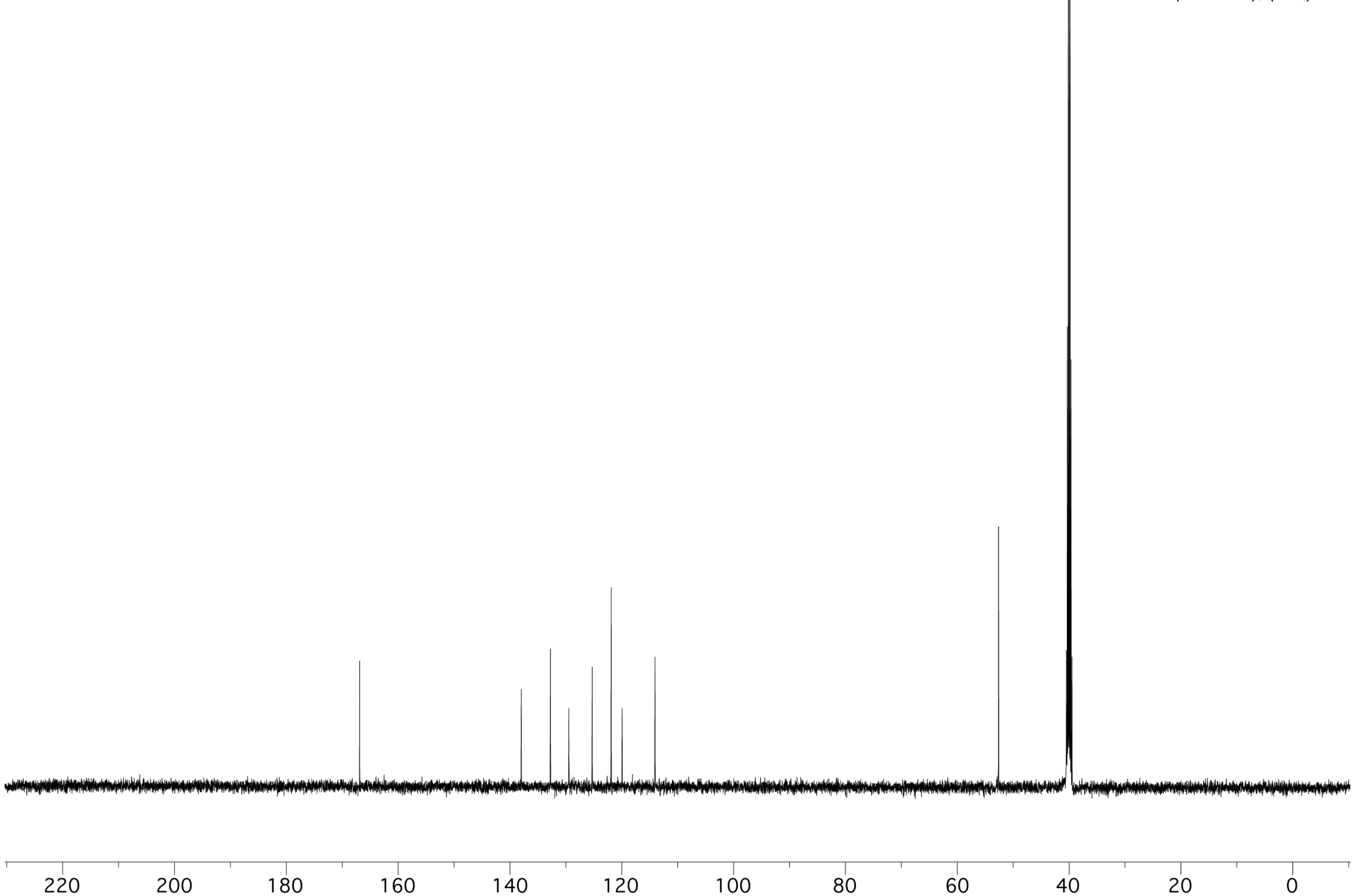
LS-108
[1]H (500 MHz), $(CD_3)_2SO$



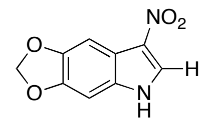
5g



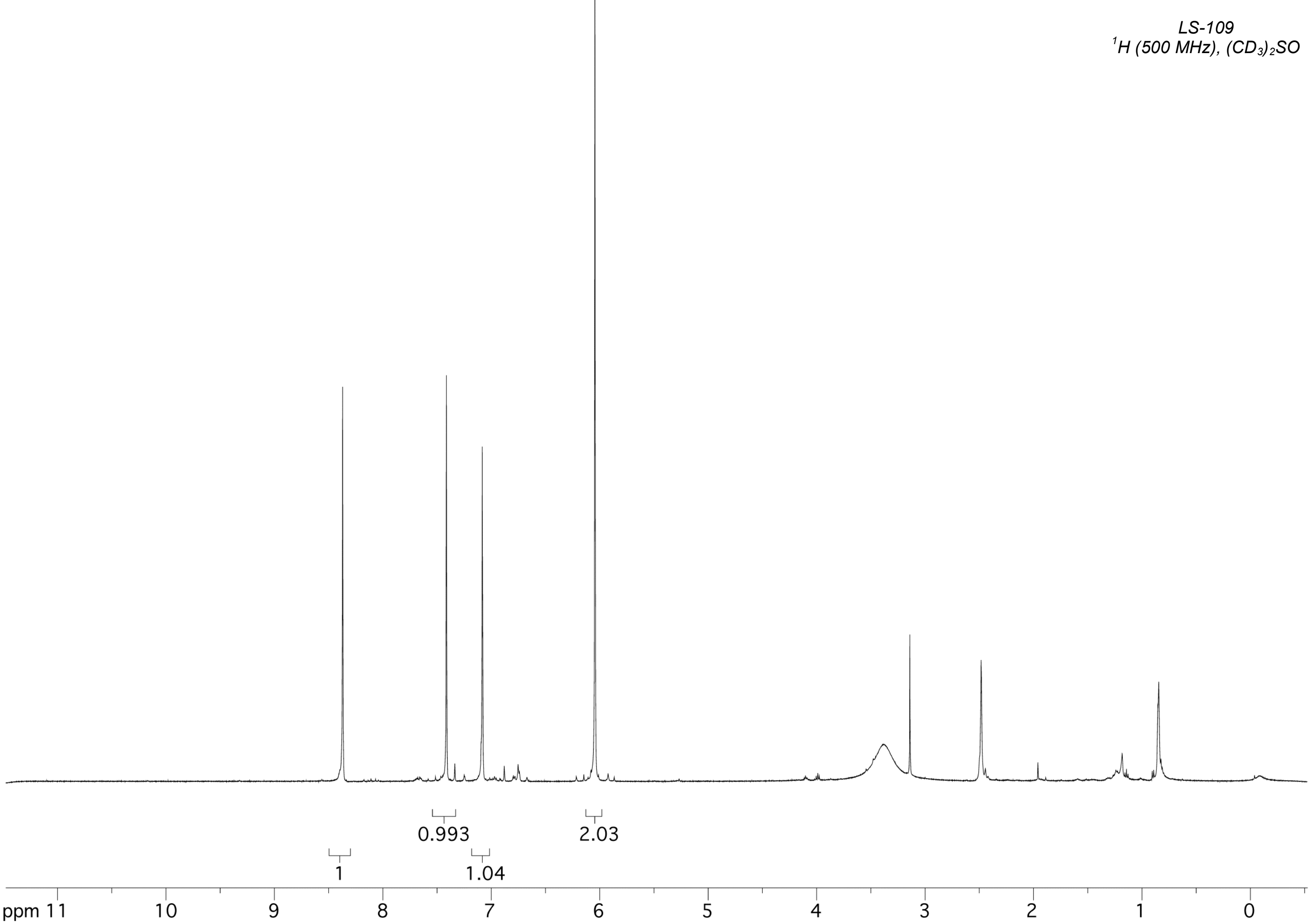
LS-108
^{13}C (125 MHz), $(CD_3)_2SO$

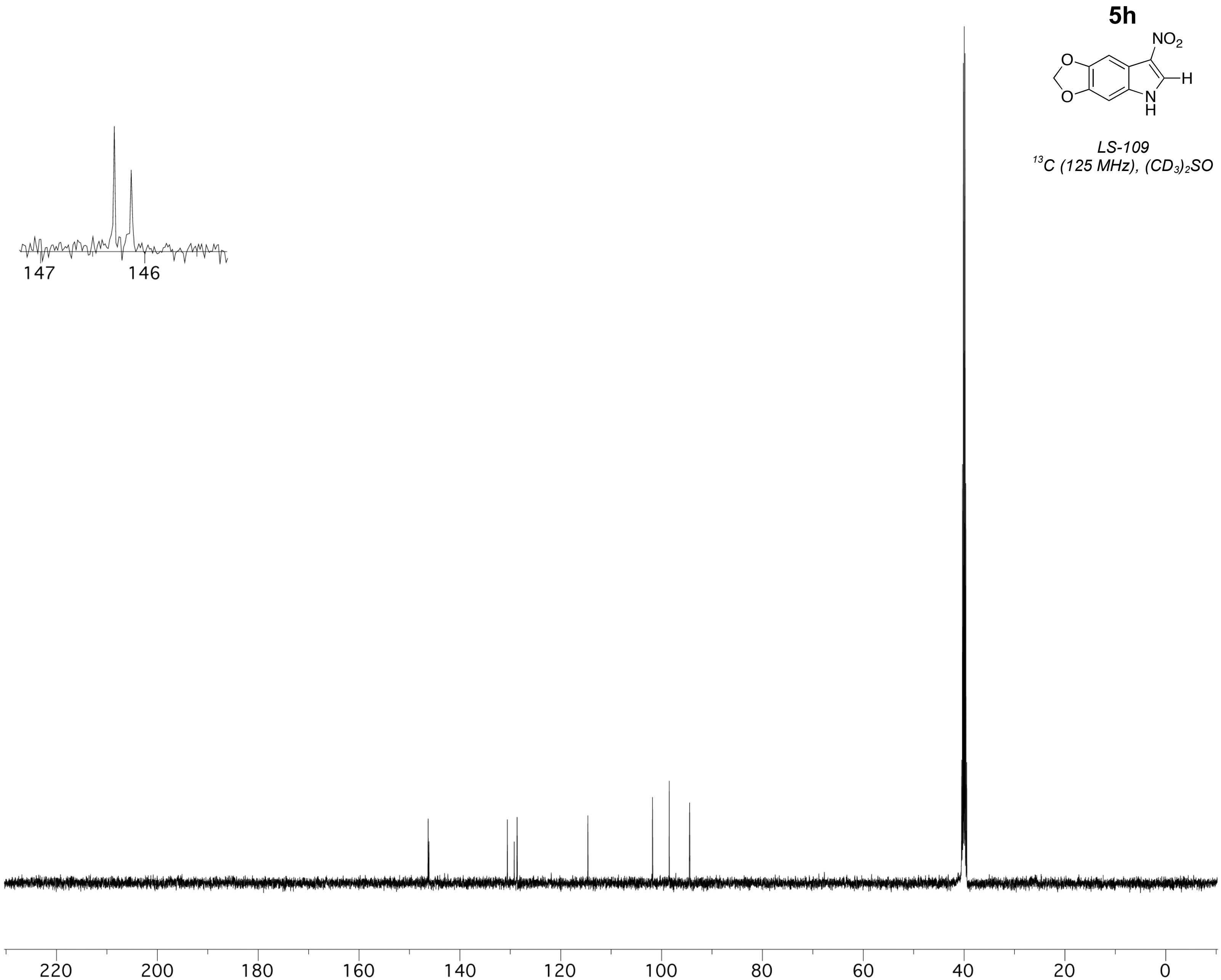


5h



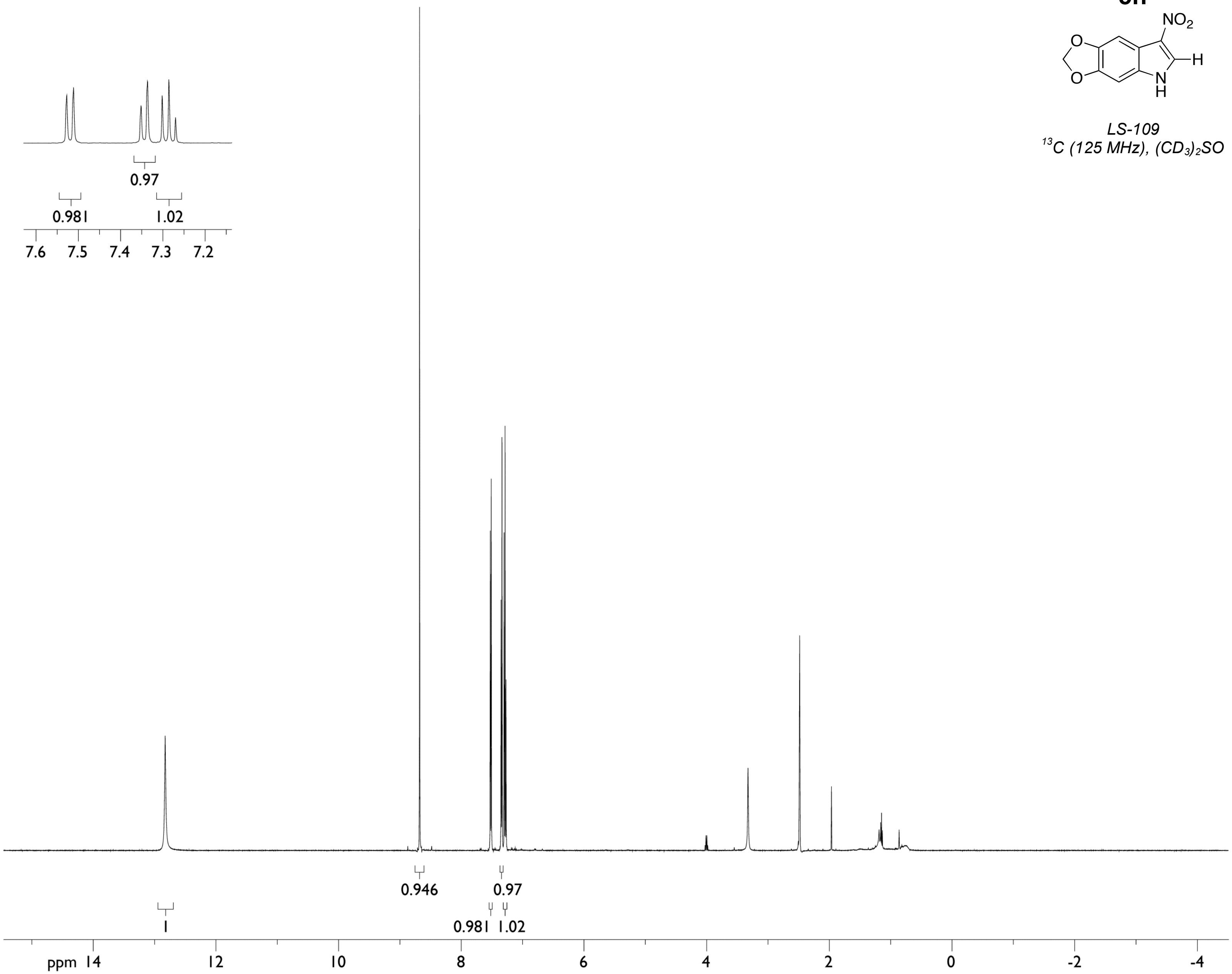
LS-109
^{1}H (500 MHz), $(CD_3)_2SO$

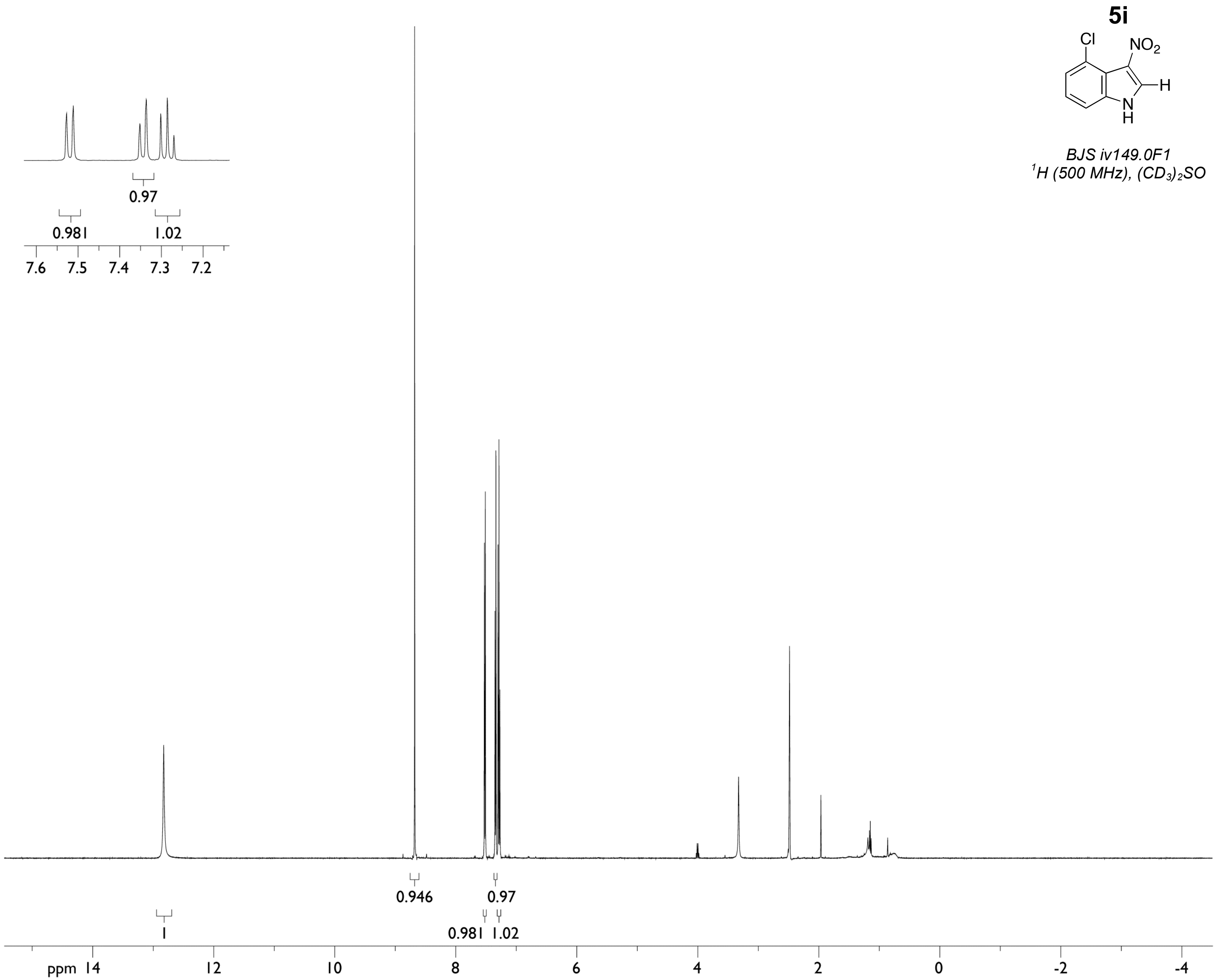



5h
NO_2
O
O
H
N
H
LS-109
^{13}C (125 MHz), $(CD_3)_2SO$
147
146
220
200
180
160
140
120
100
80
60
40
20
0

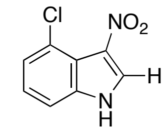
5h

LS-109
^{13}C (125 MHz), $(CD_3)_2SO$

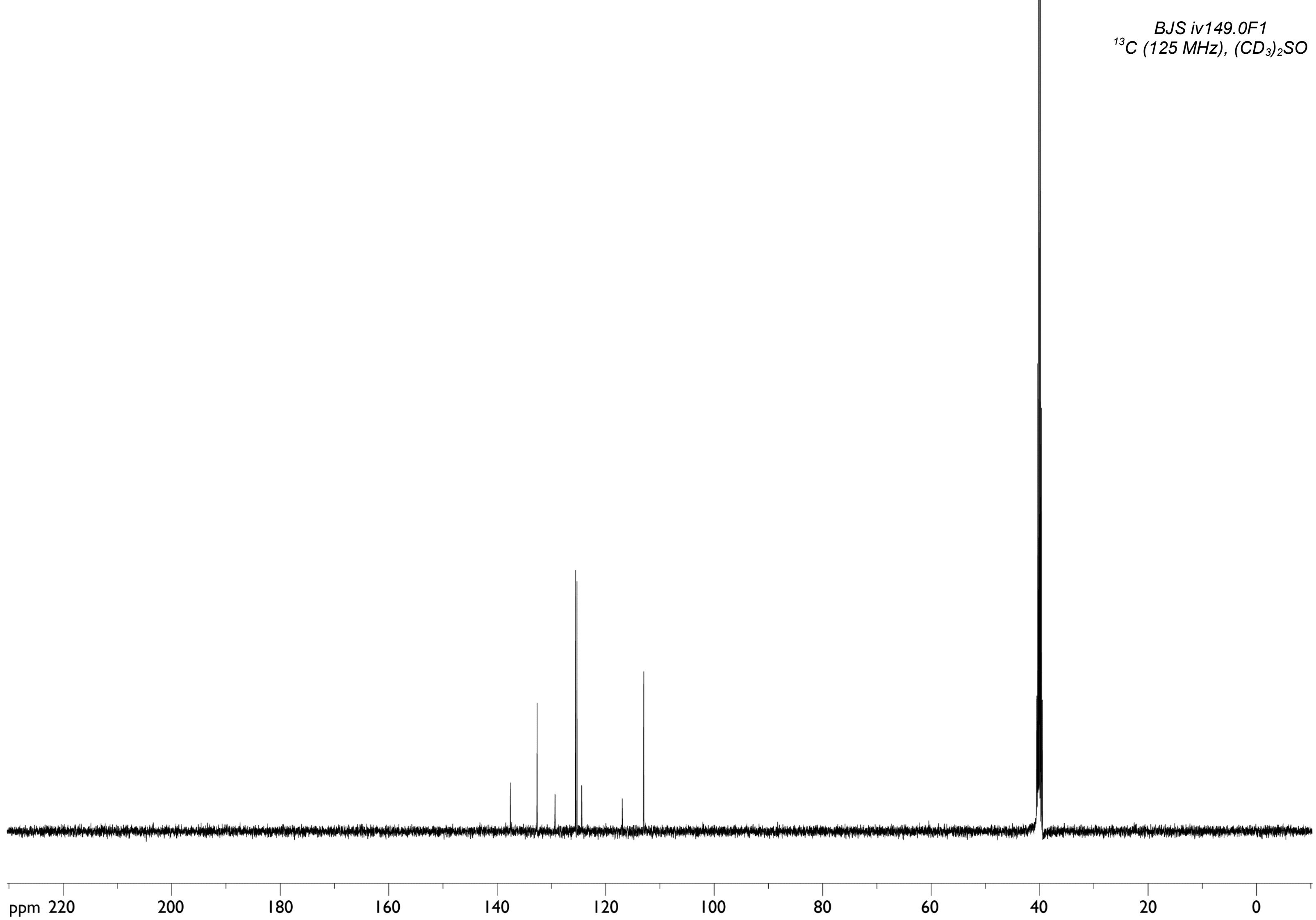


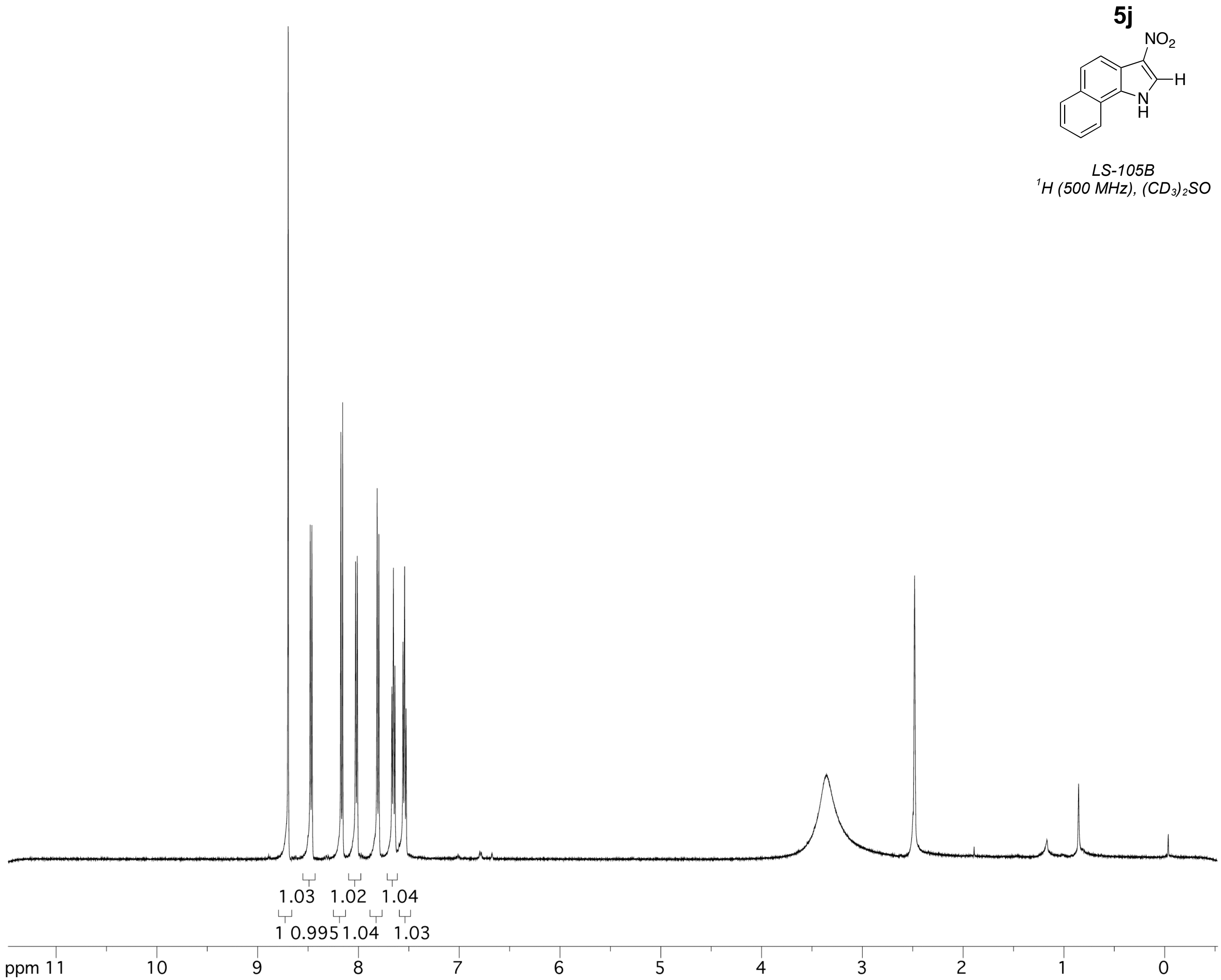

5i
Cl
NO_2
H
N
H
BJS iv149.0F1
^{1}H (500 MHz), $(CD_3)_2SO$
0.97
0.981
1.02
7.6 7.5 7.4 7.3 7.2
0.946
0.97
1
0.981 1.02
ppm 14 12 10 8 6 4 2 0 -2 -4

5i

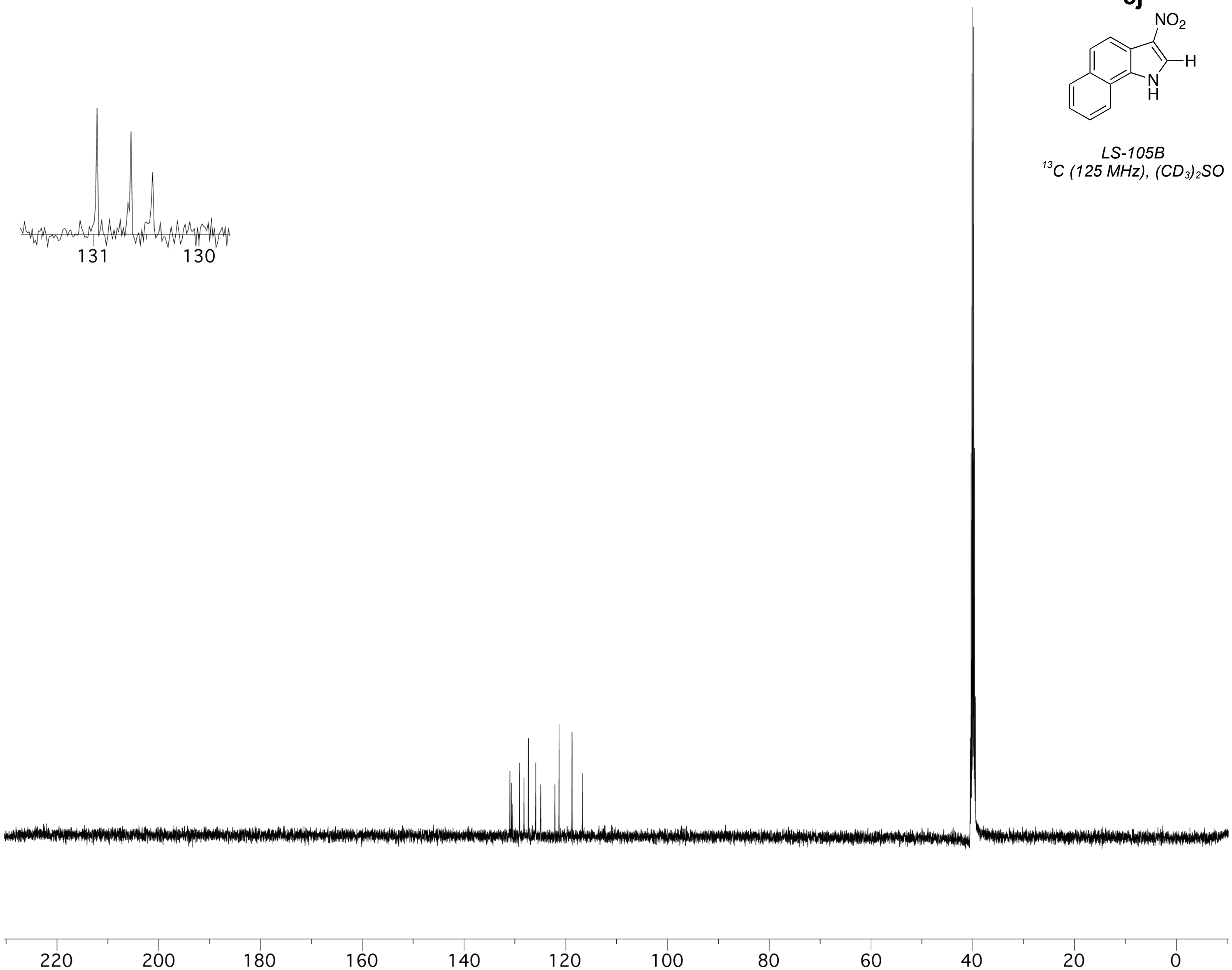


BJS iv149.0F1
^{13}C (125 MHz), $(CD_3)_2SO$



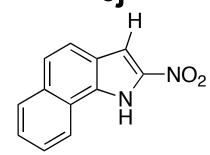

5j
NO_2
H
N
H
LS-105B
^1H (500 MHz), $(CD_3)_2SO$
1.03
1.02
1.04
1
0.995
1.04
1.03
ppm 11
10
9
8
7
6
5
4
3
2
1
0

5j

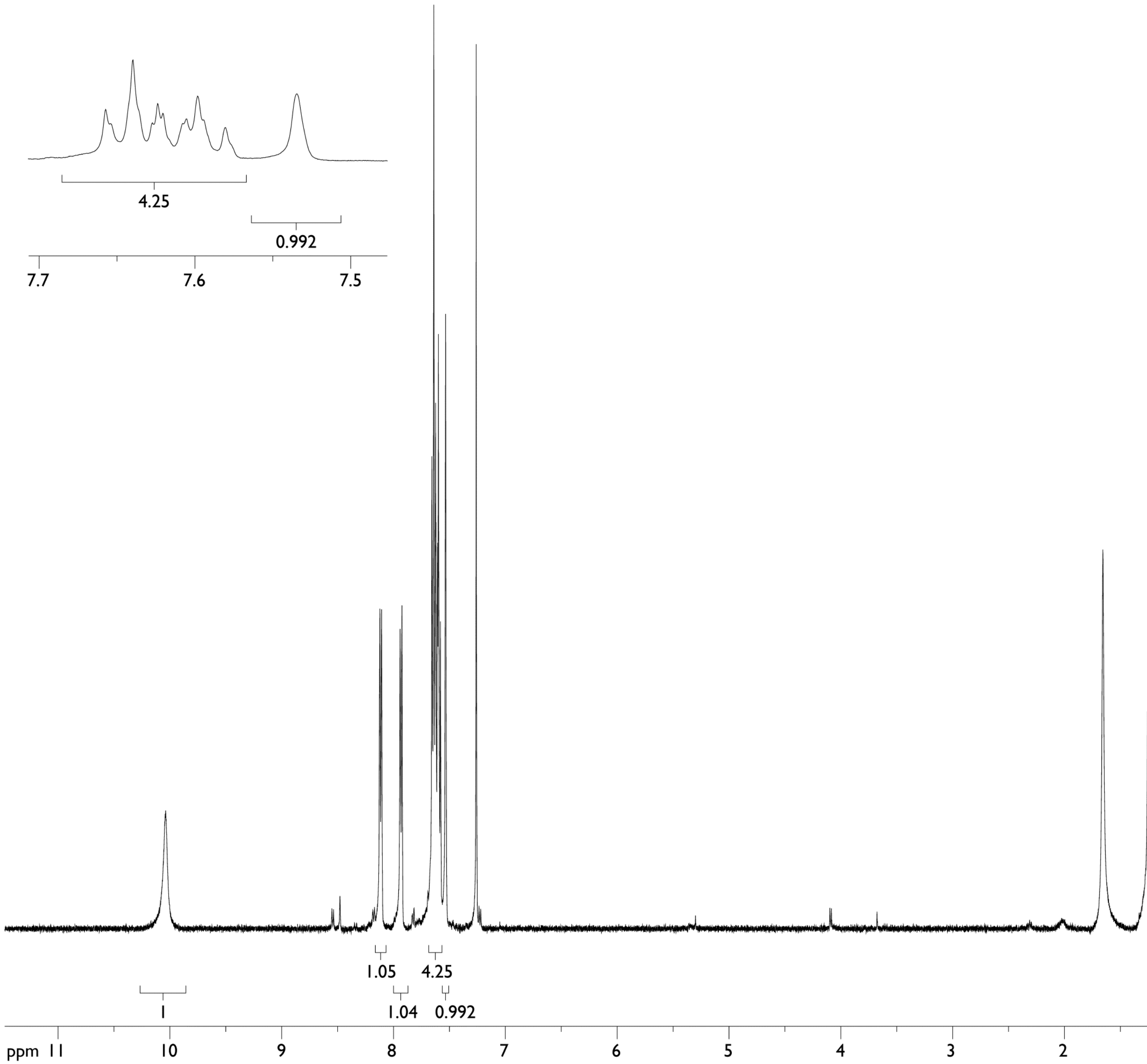


LS-105B
^{13}C (125 MHz), $(CD_3)_2SO$

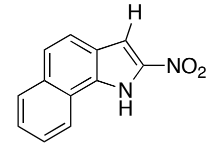
6j



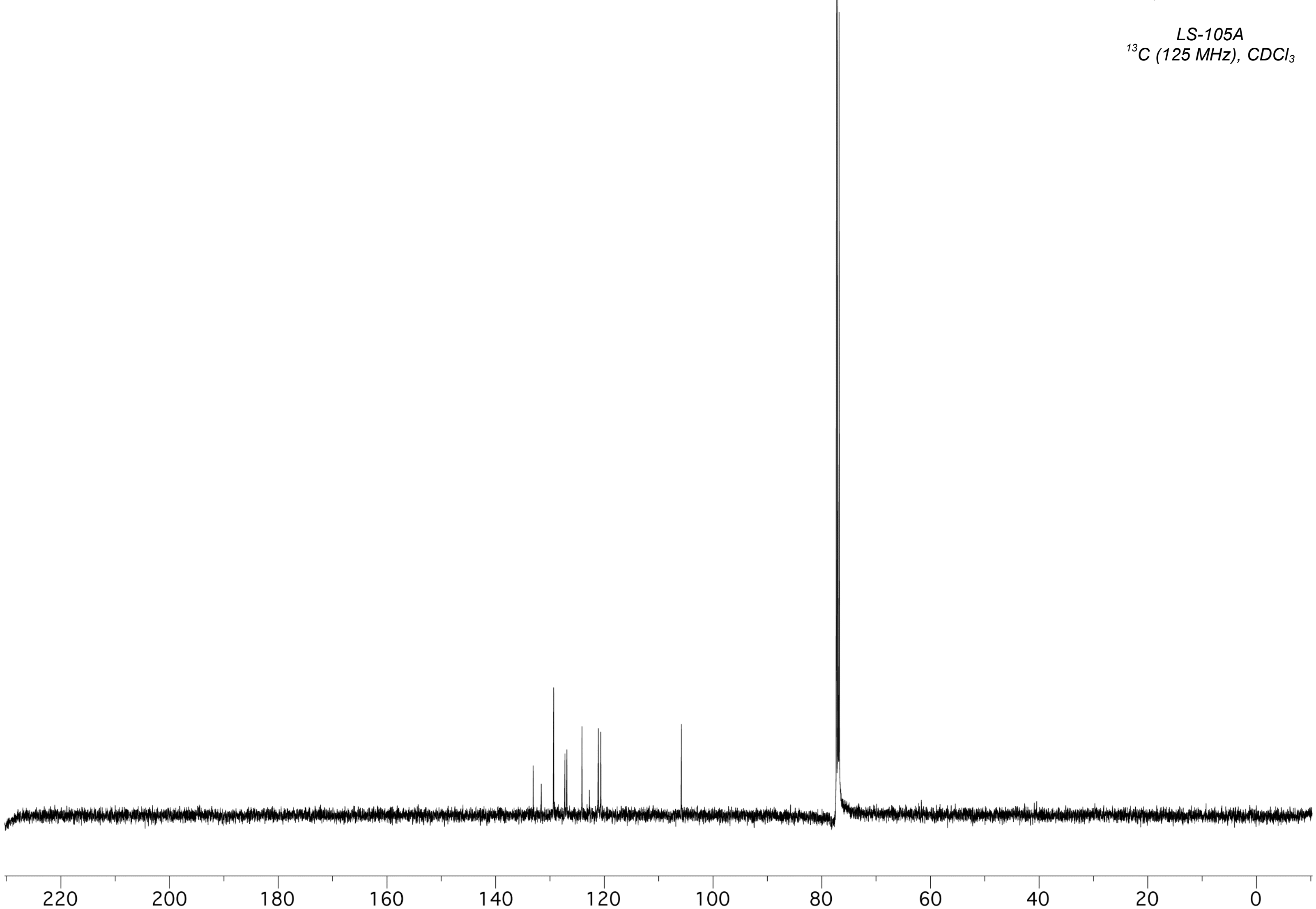
LS-105A
^1H (500 MHz), $CDCl_3$



6j



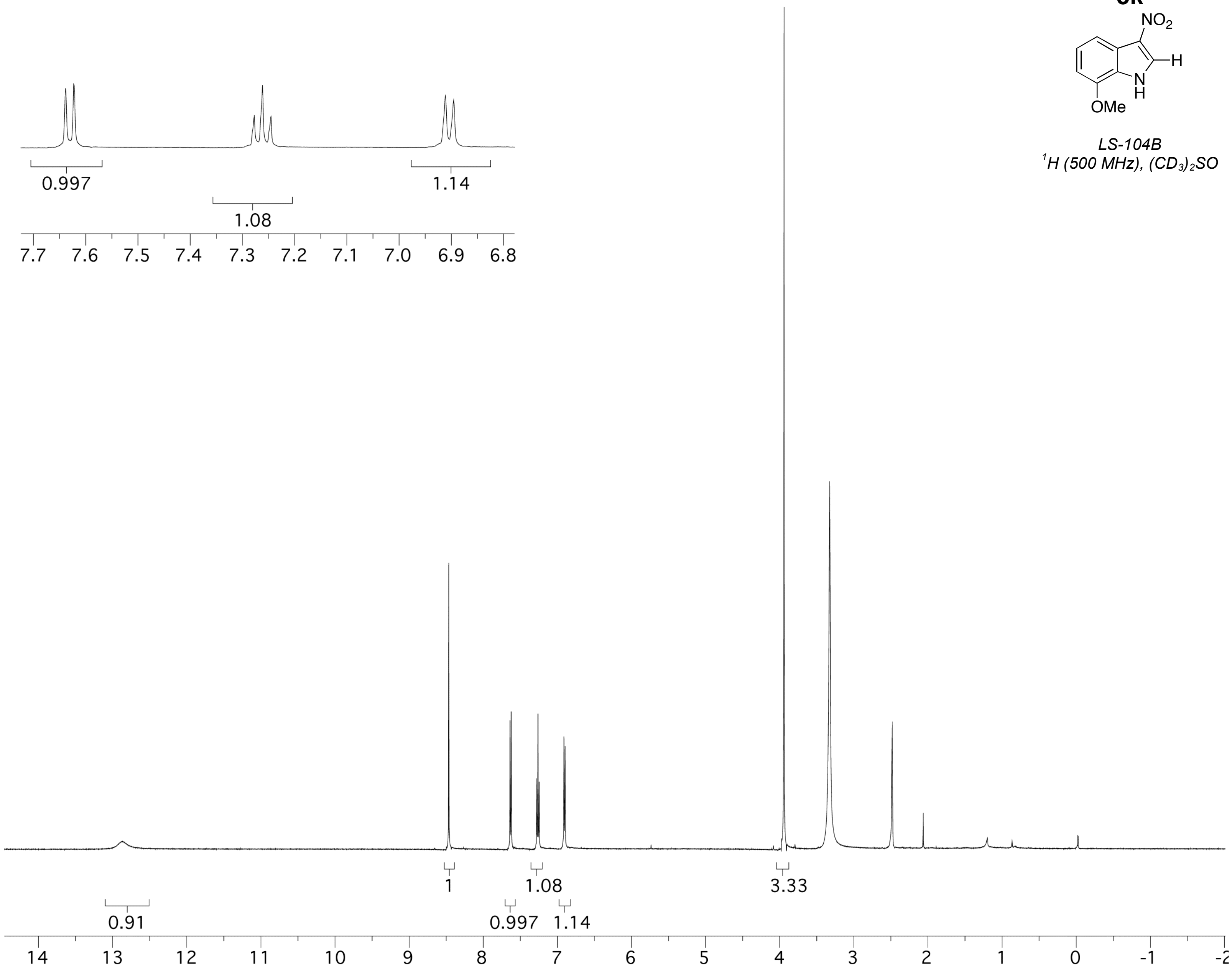
LS-105A
^{13}C (125 MHz), $CDCl_3$



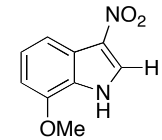
5k

LS-104B

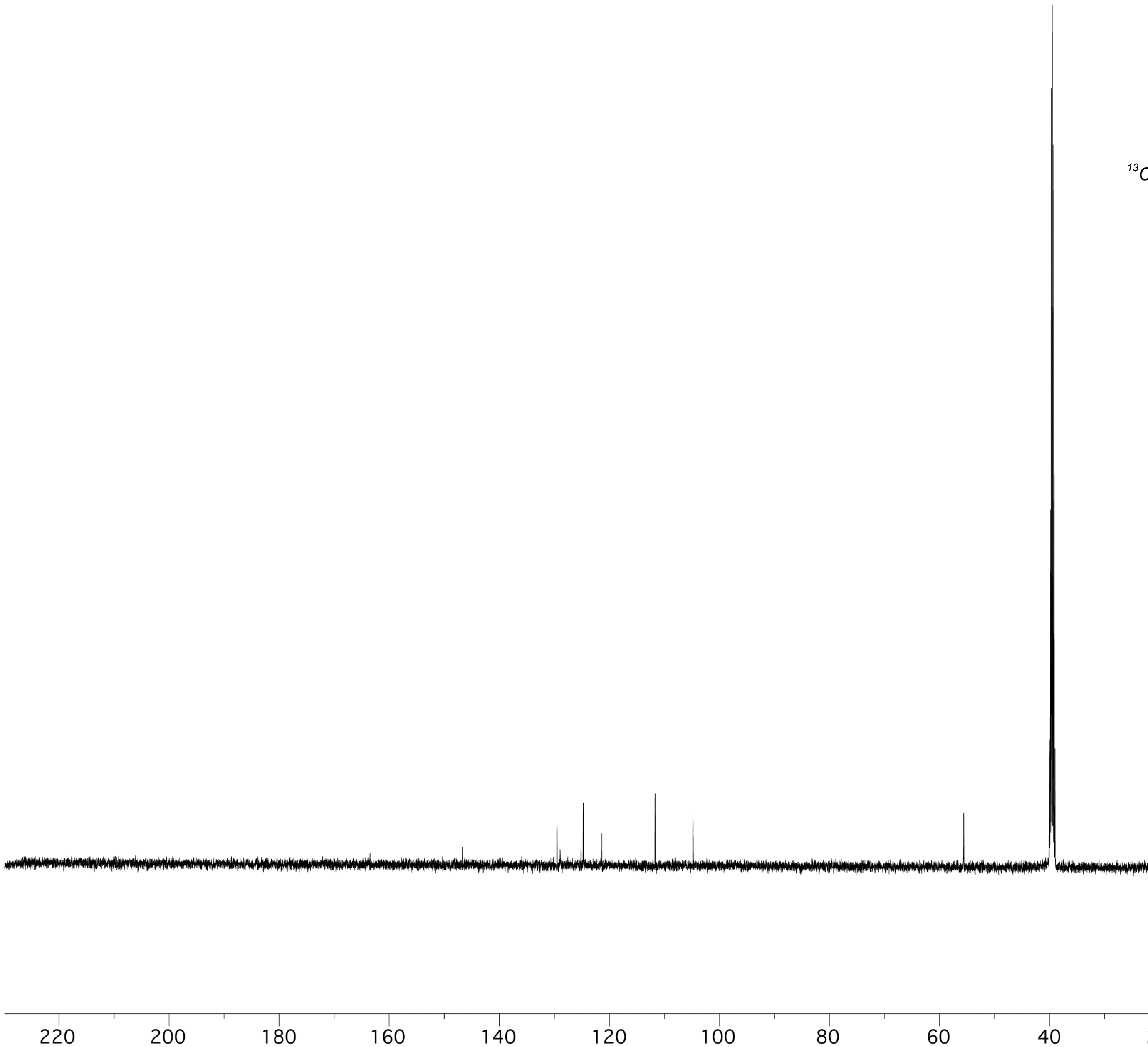
^{1}H (500 MHz), $(CD_3)_2SO$



5k

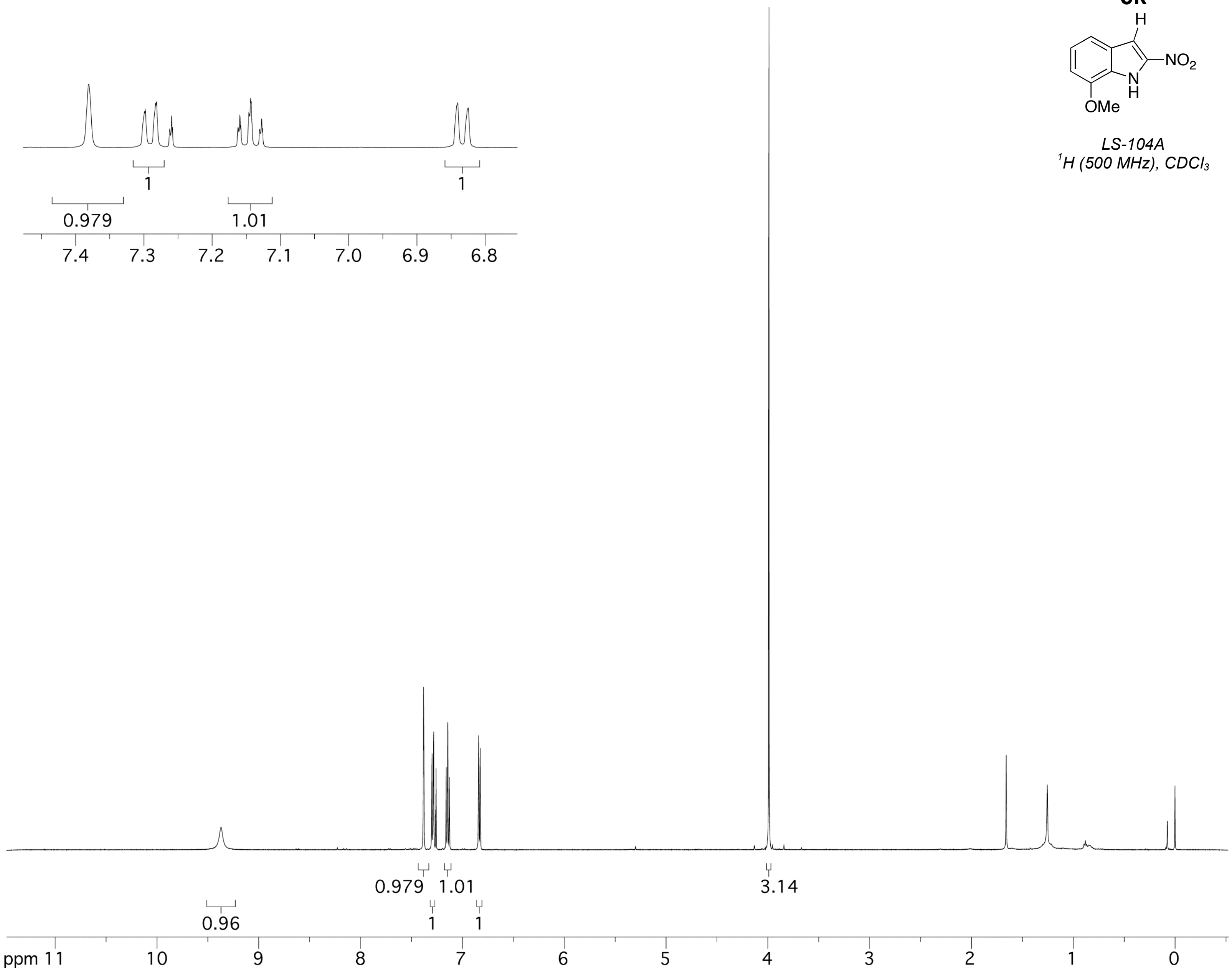


LS-104B
^{13}C (125 MHz), $(CD_3)_2SO$

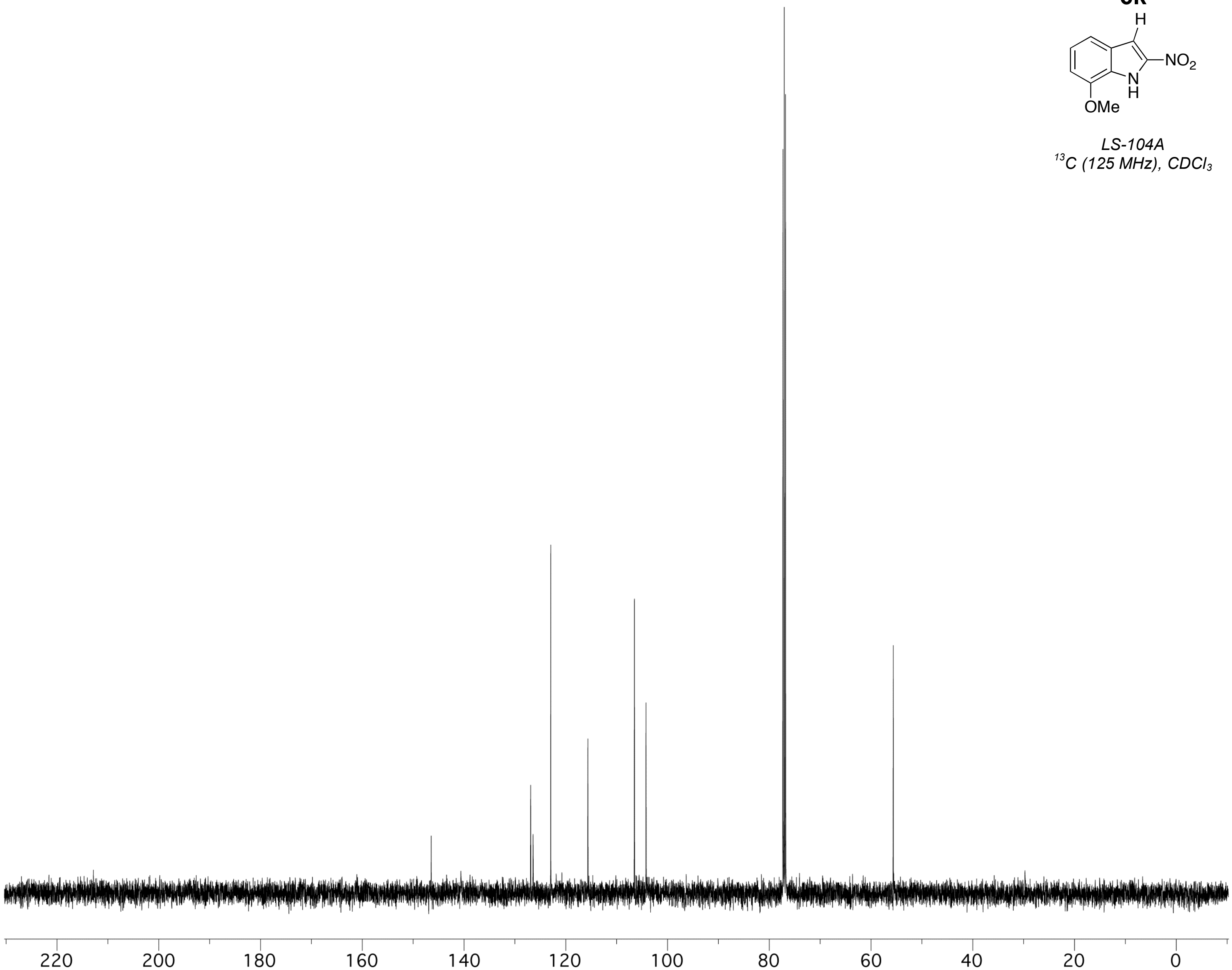


6k

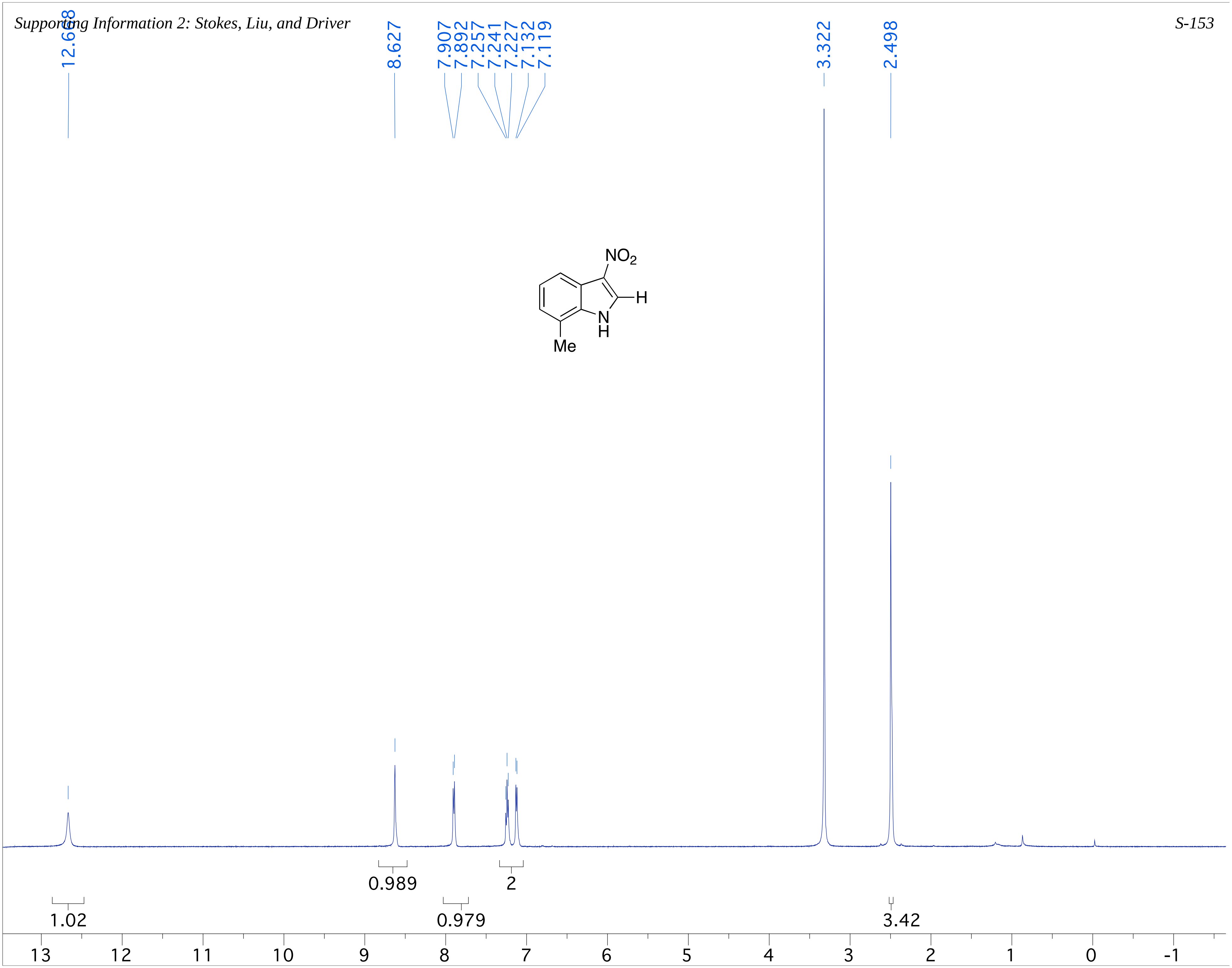
LS-104A
^{1}H (500 MHz), $CDCl_3$

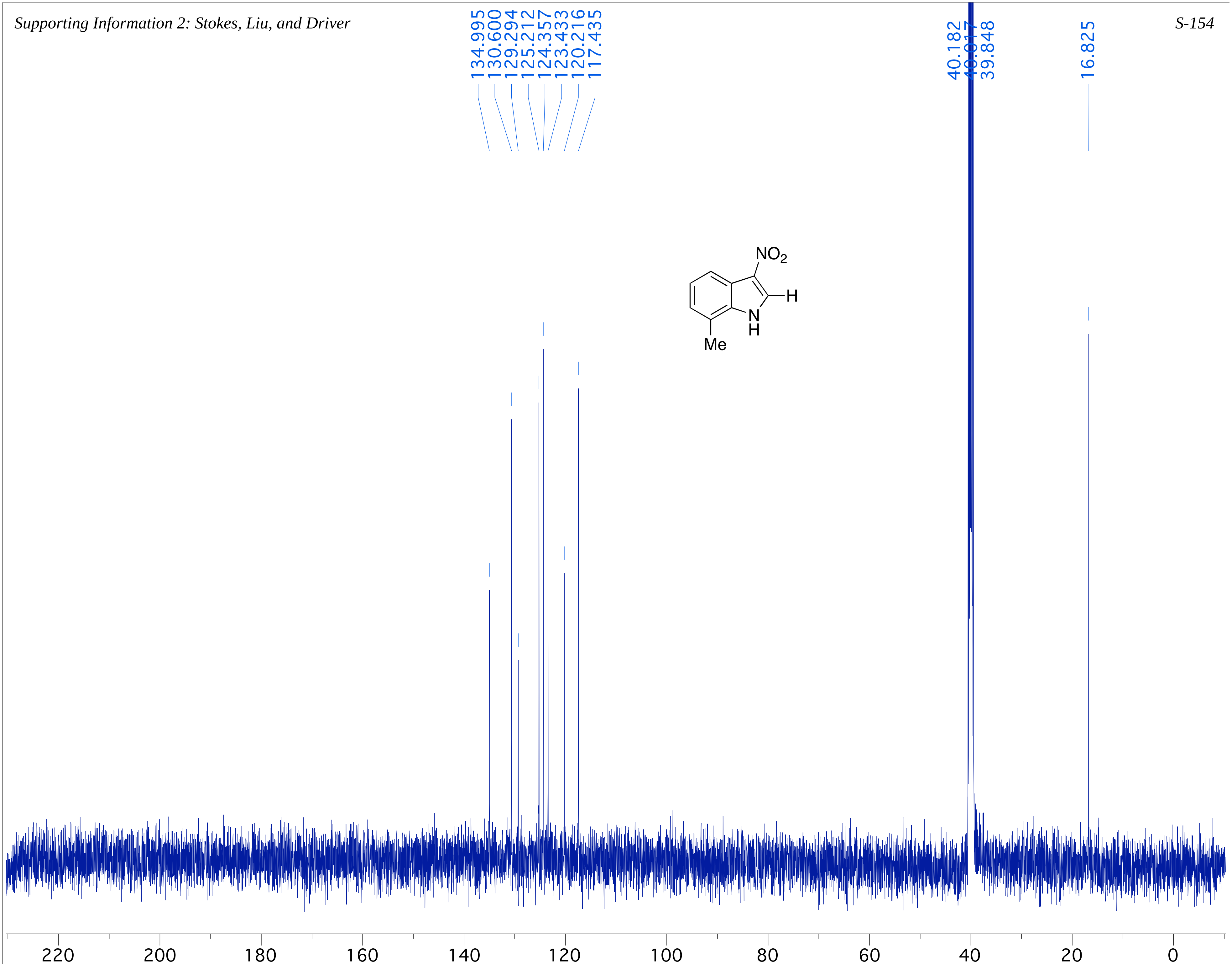


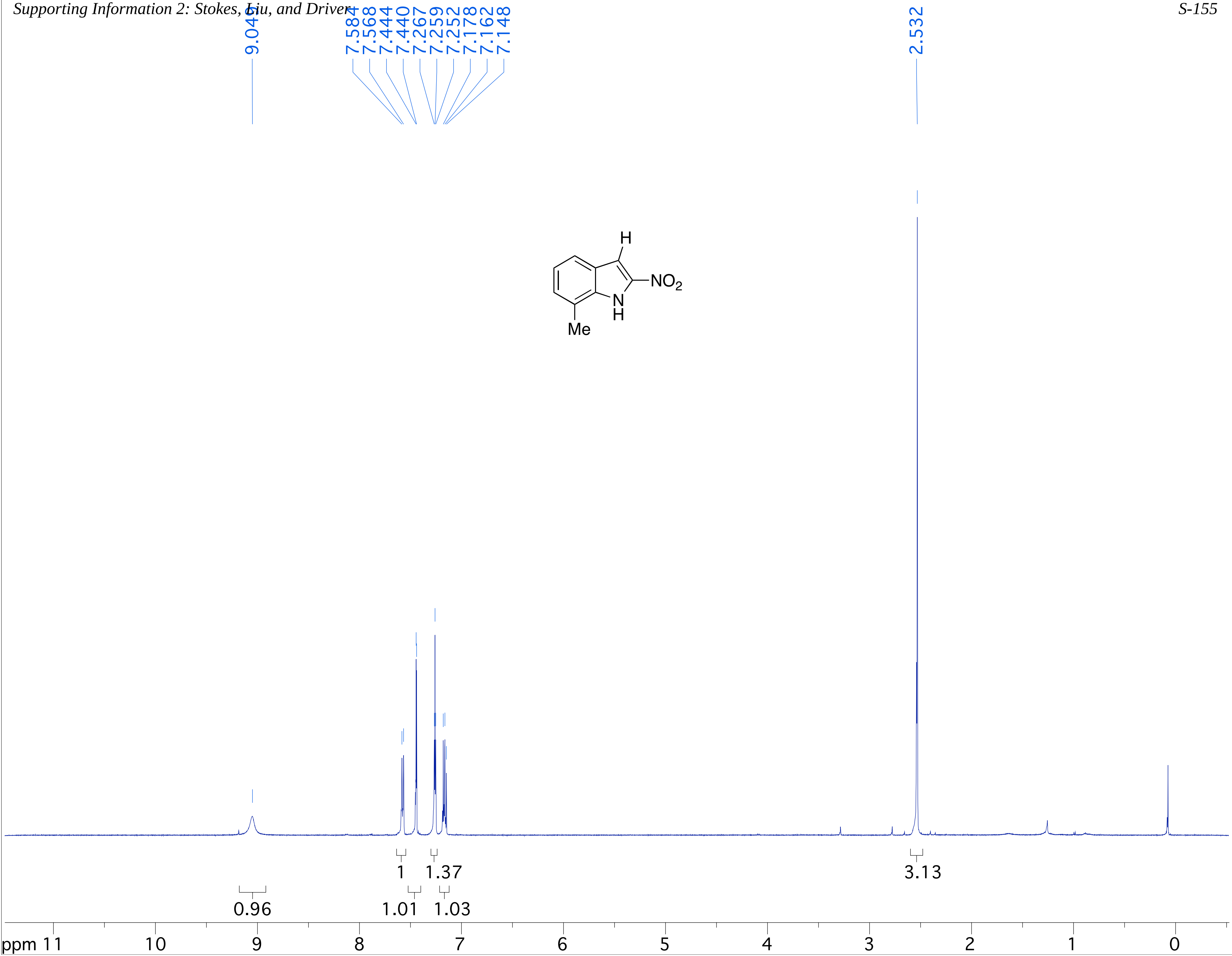
6k

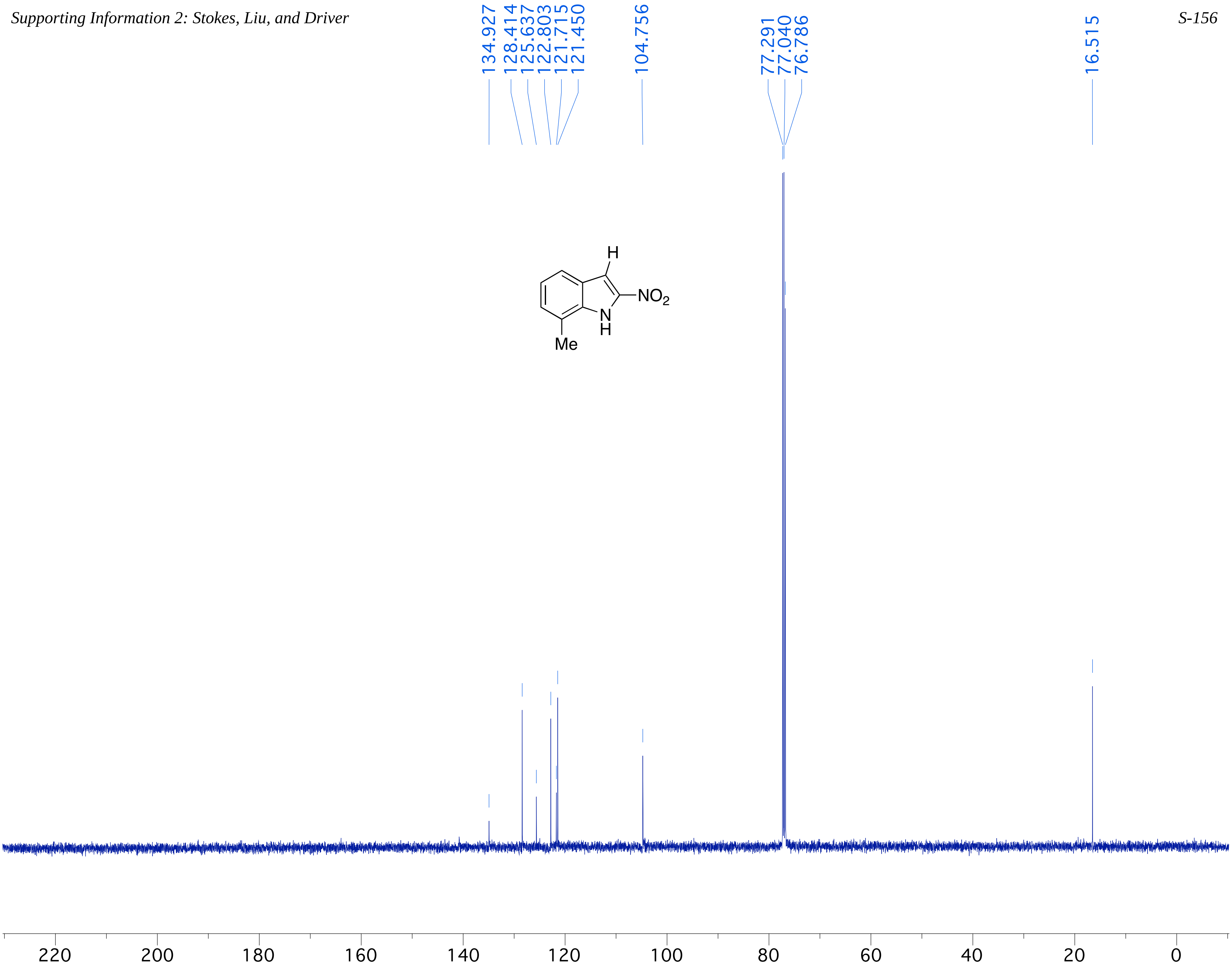


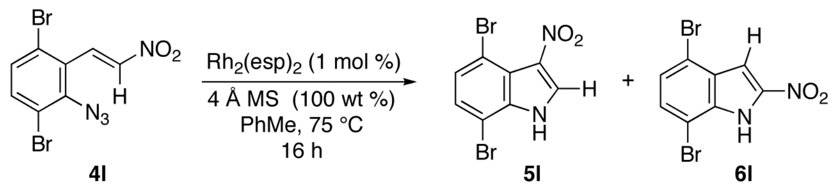
LS-104A
^{13}C (125 MHz), $CDCl_3$


12.668
8.627
7.907
7.892
7.257
7.241
7.227
7.132
7.119
3.322
2.498
NO2
H
N
H
Me
1.02
0.989
0.979
2
3.42
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1

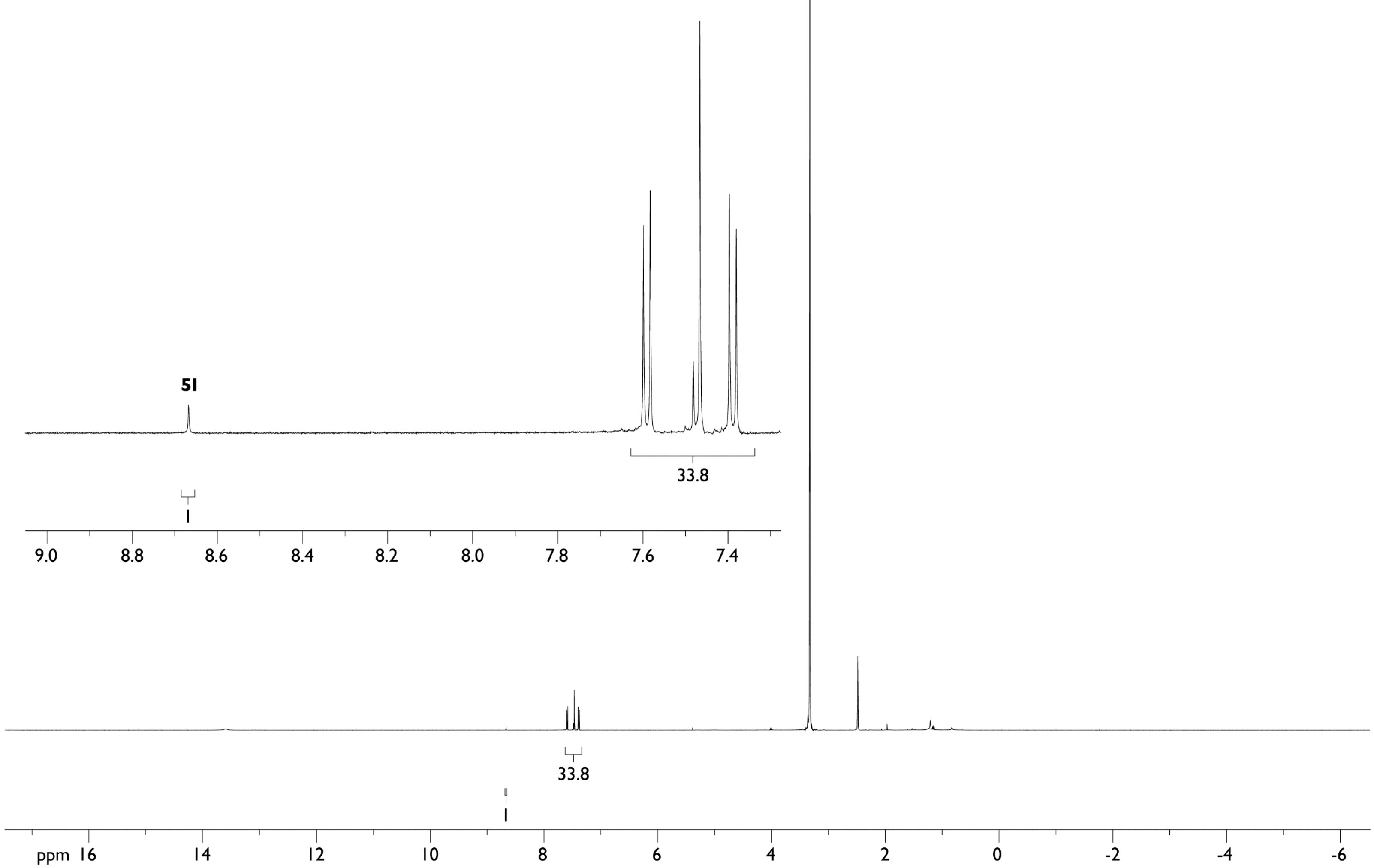

134.995
130.600
129.294
125.212
124.357
123.433
120.216
117.435
40.182
40.017
39.848
16.825
NO_2
H
N
H
Me
220
200
180
160
140
120
100
80
60
40
20
0


9.049
7.584
7.568
7.444
7.440
7.267
7.259
7.252
7.178
7.162
7.148
2.532
H
NO_2
N
H
Me
1
1.37
3.13
0.96
1.01
1.03
ppm 11
10
9
8
7
6
5
4
3
2
1
0

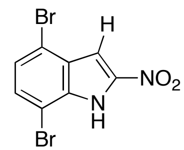

134.927
128.414
125.637
122.803
121.715
121.450
104.756
77.291
77.040
76.786
16.515
H
NO_2
N
H
Me
220
200
180
160
140
120
100
80
60
40
20
0



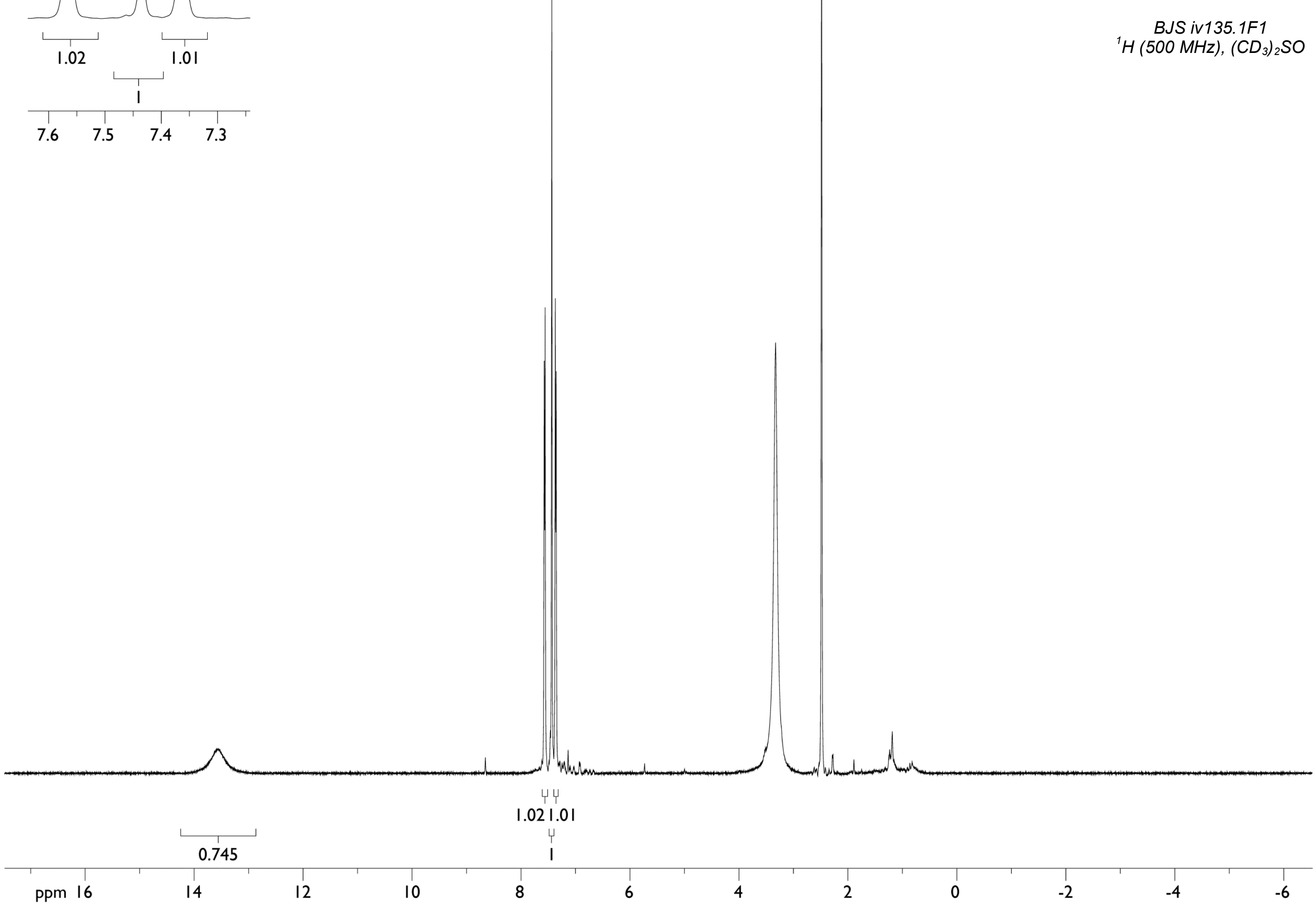
BJS iv135.0F1
[1]H (500 MHz), $(CD_3)_2SO$



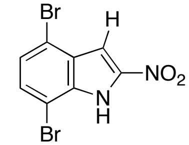
6l



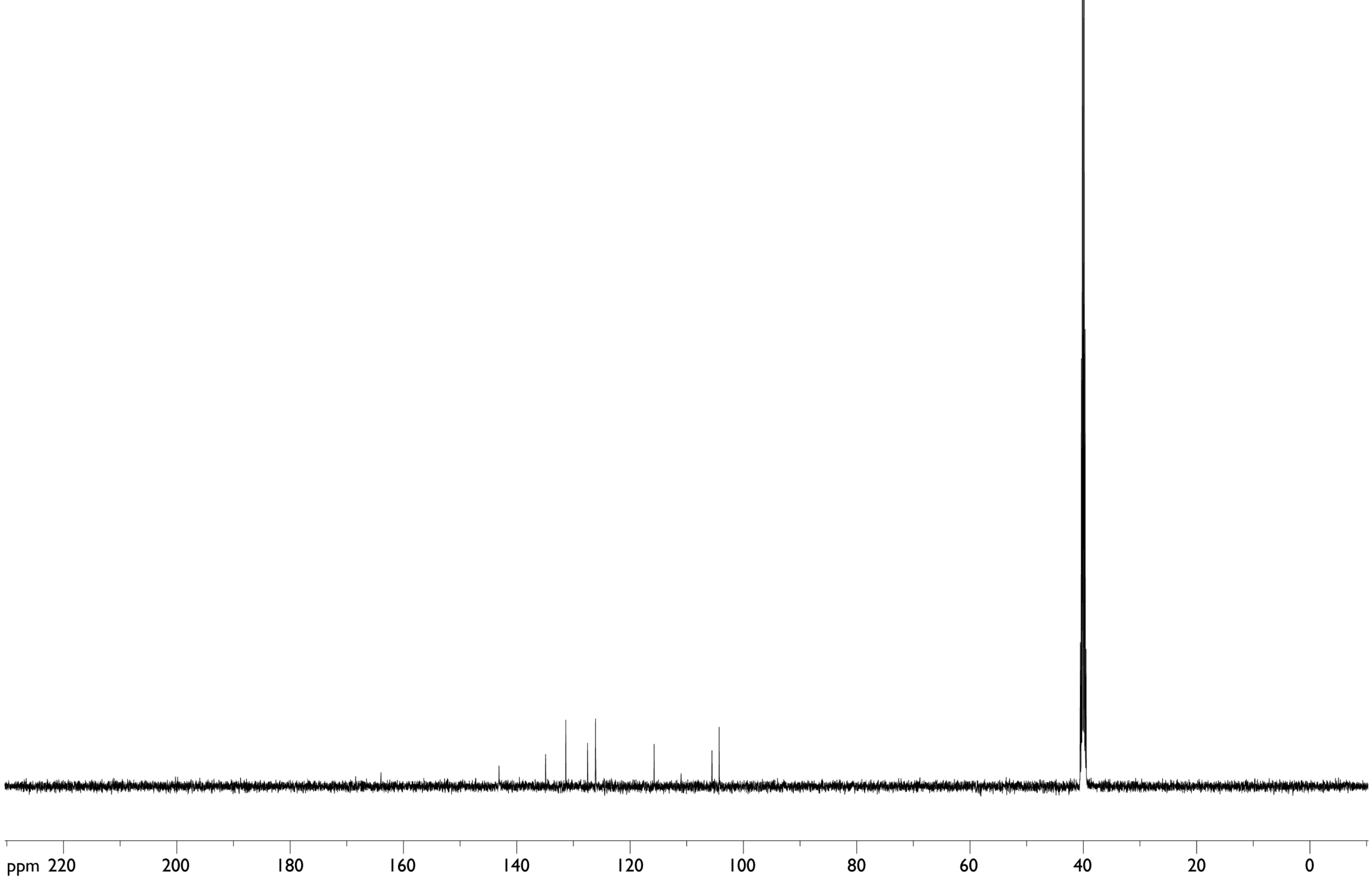
BJS iv135.1F1
^{1}H (500 MHz), $(CD_3)_2SO$

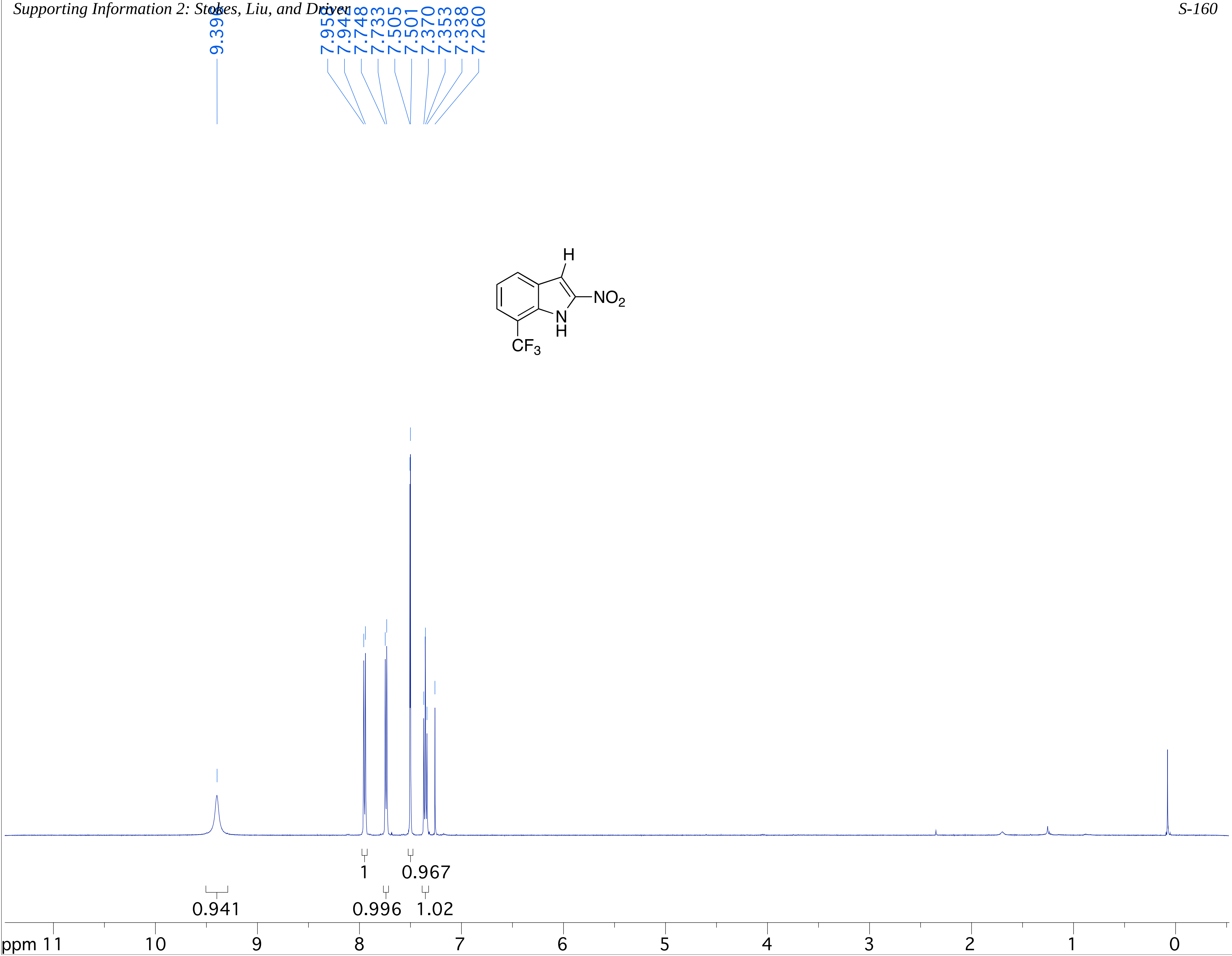


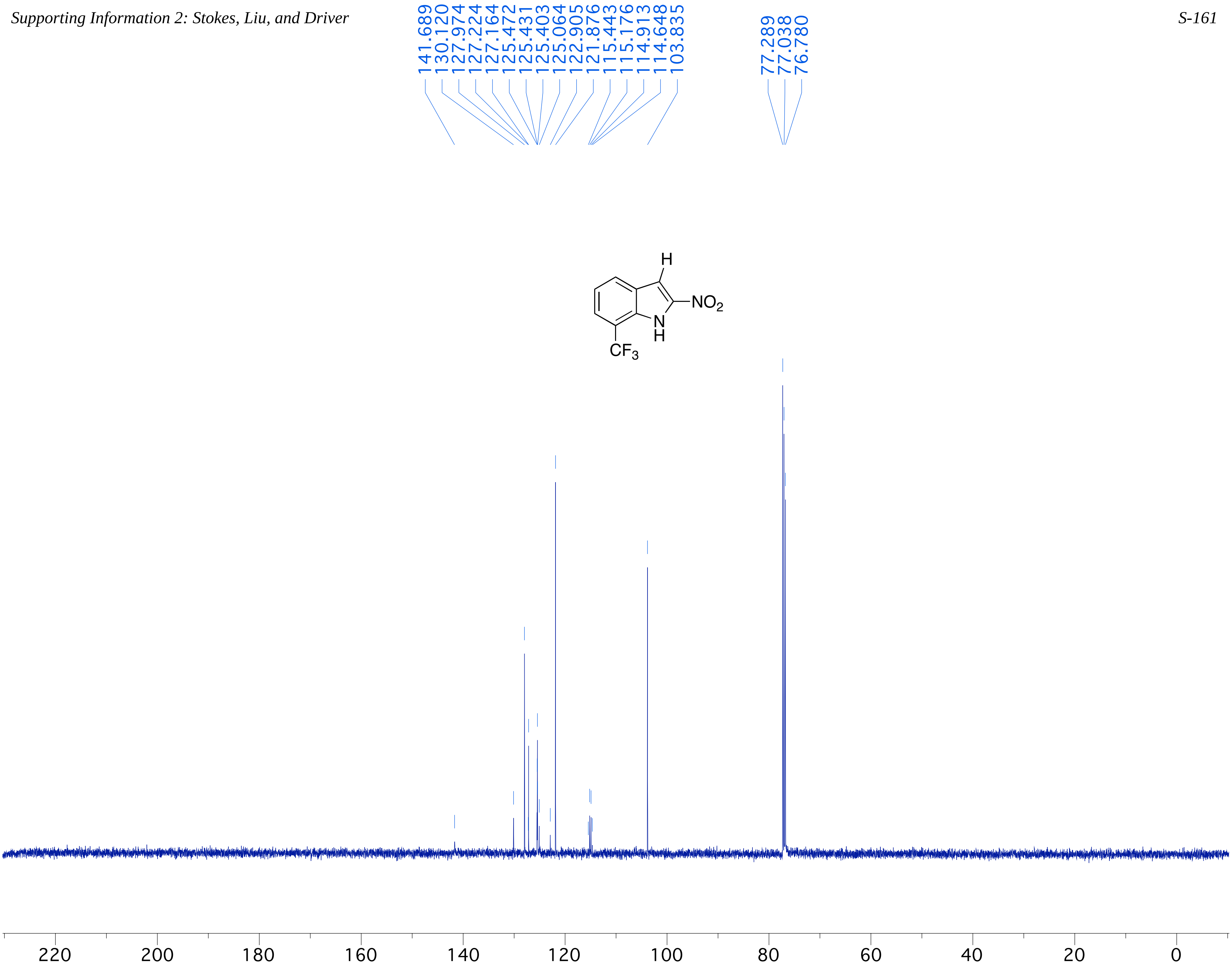
6l



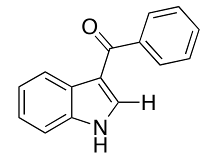
BJS iv135.1F1
^{13}C (125 MHz), $(CD_3)_2SO$



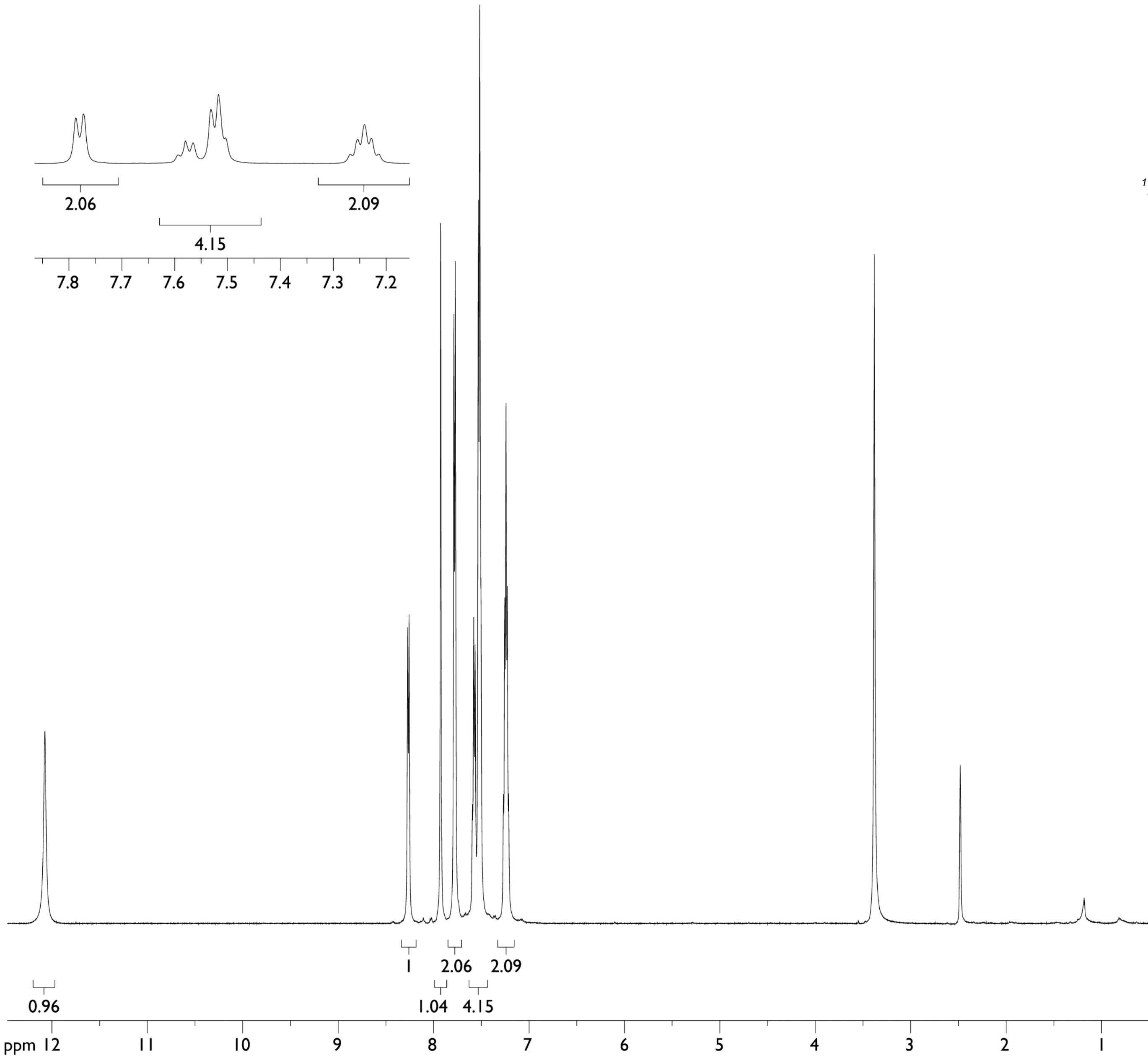

9.396
7.958
7.941
7.748
7.733
7.505
7.501
7.370
7.353
7.338
7.260
H
NO2
N
H
CF3
1
0.967
0.941
0.996
1.02
ppm 11
10
9
8
7
6
5
4
3
2
1
0


141.689
130.120
127.974
127.224
127.164
125.472
125.431
125.403
125.064
122.905
121.876
115.443
115.176
114.913
114.648
103.835
77.289
77.038
76.780
H
NO2
N
H
CF3
220
200
180
160
140
120
100
80
60
40
20
0

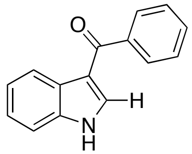
8a



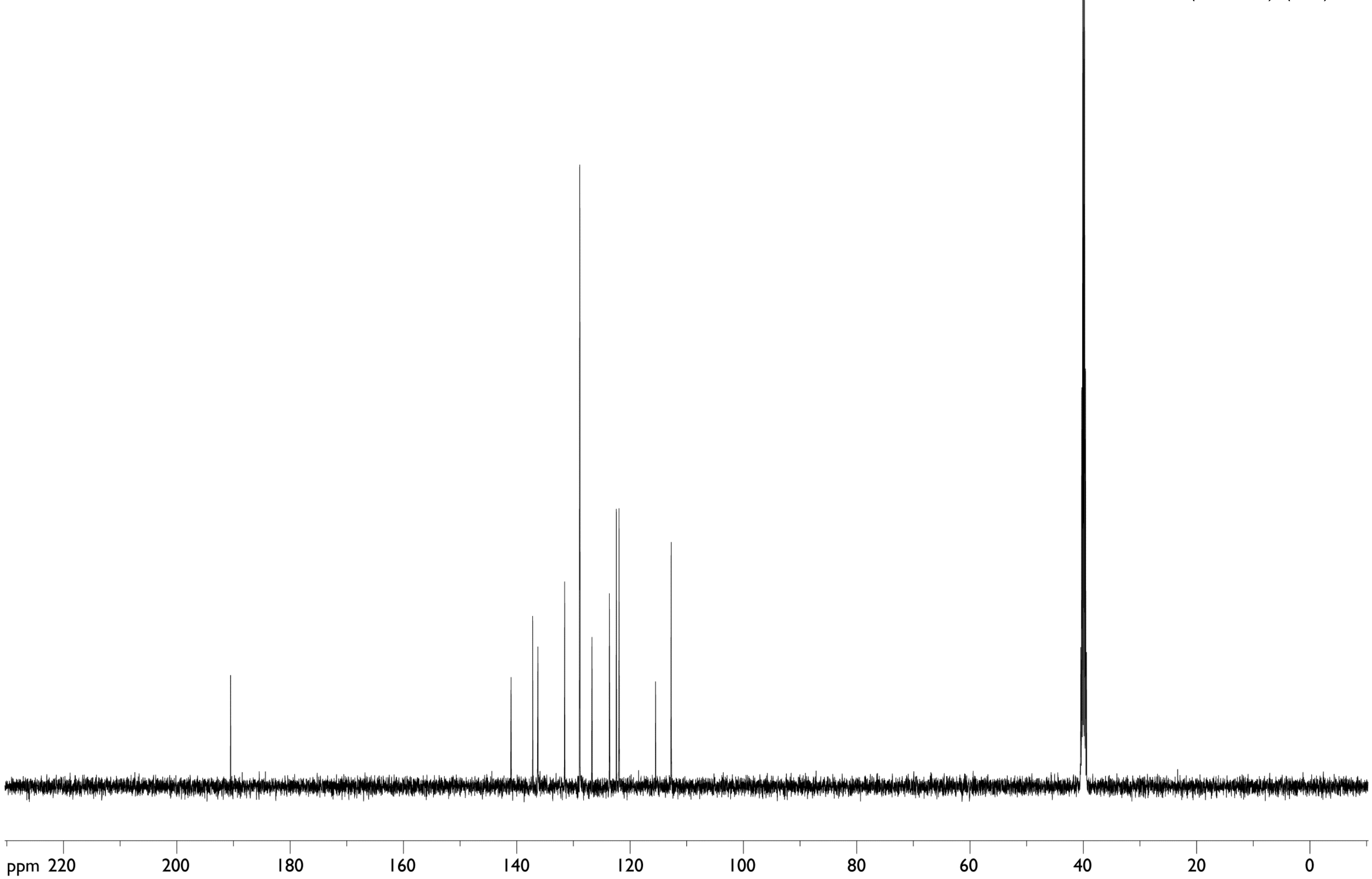
BJS iv105.0F1
[1]H (500 MHz), $(CD_3)_2SO$



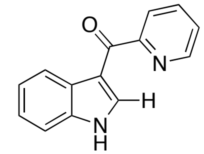
8a



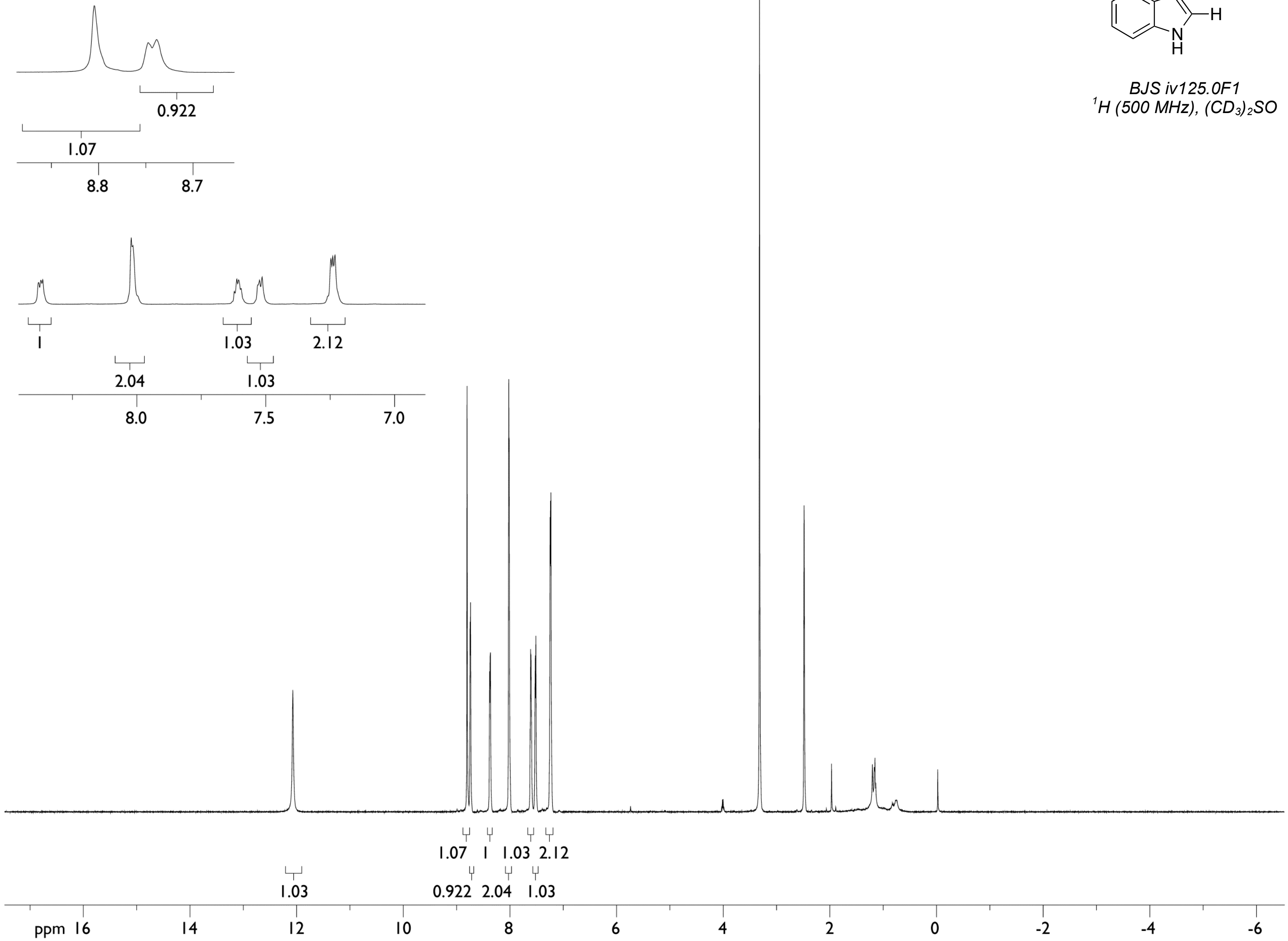
BJS iv105.0F1
^{13}C (125 MHz), $(CD_3)_2SO$



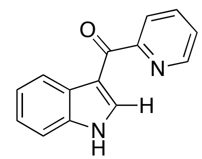
8b



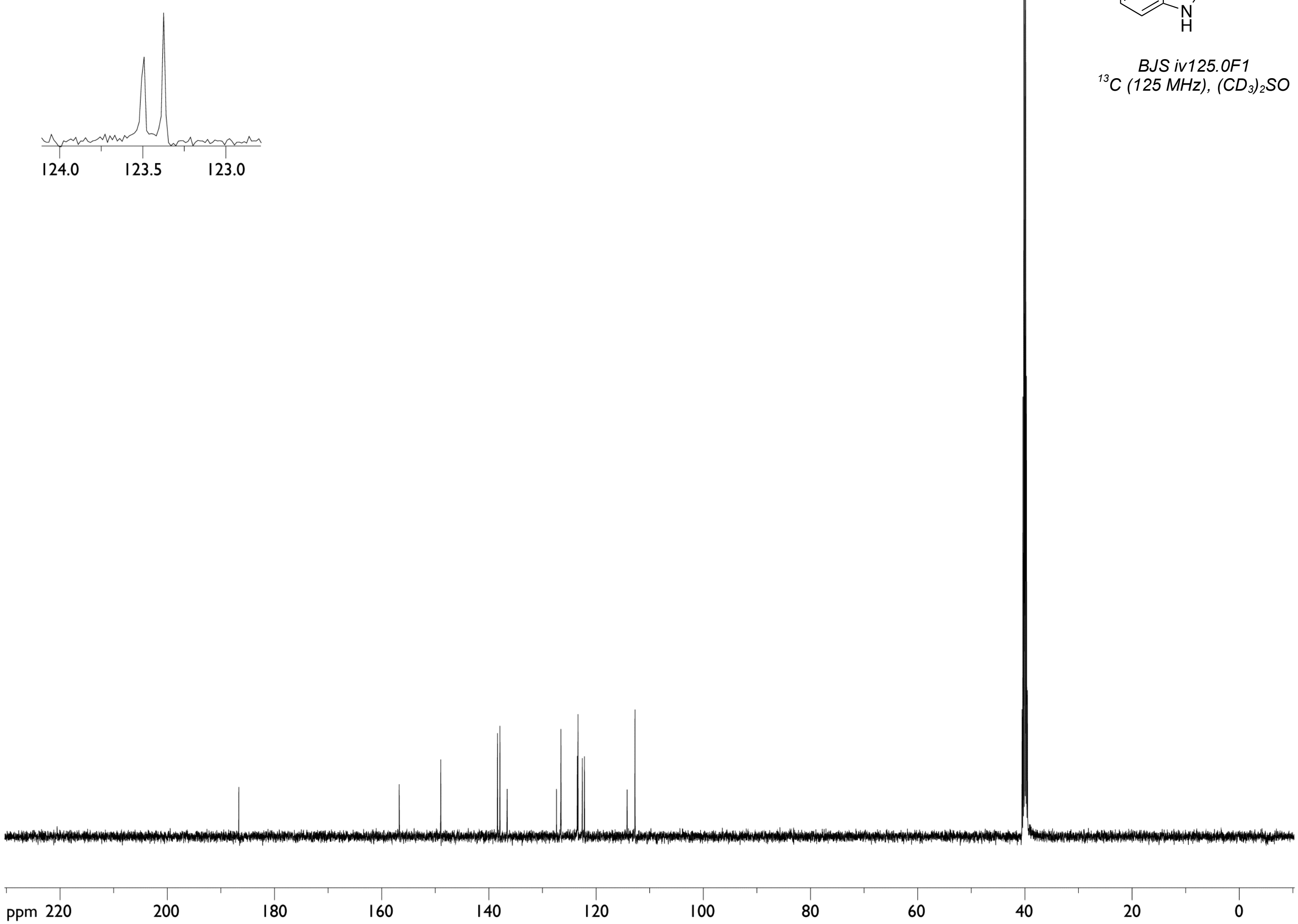
BJS iv125.0F1
^{1}H (500 MHz), $(CD_3)_2SO$



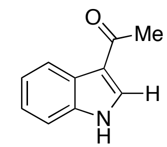
8b



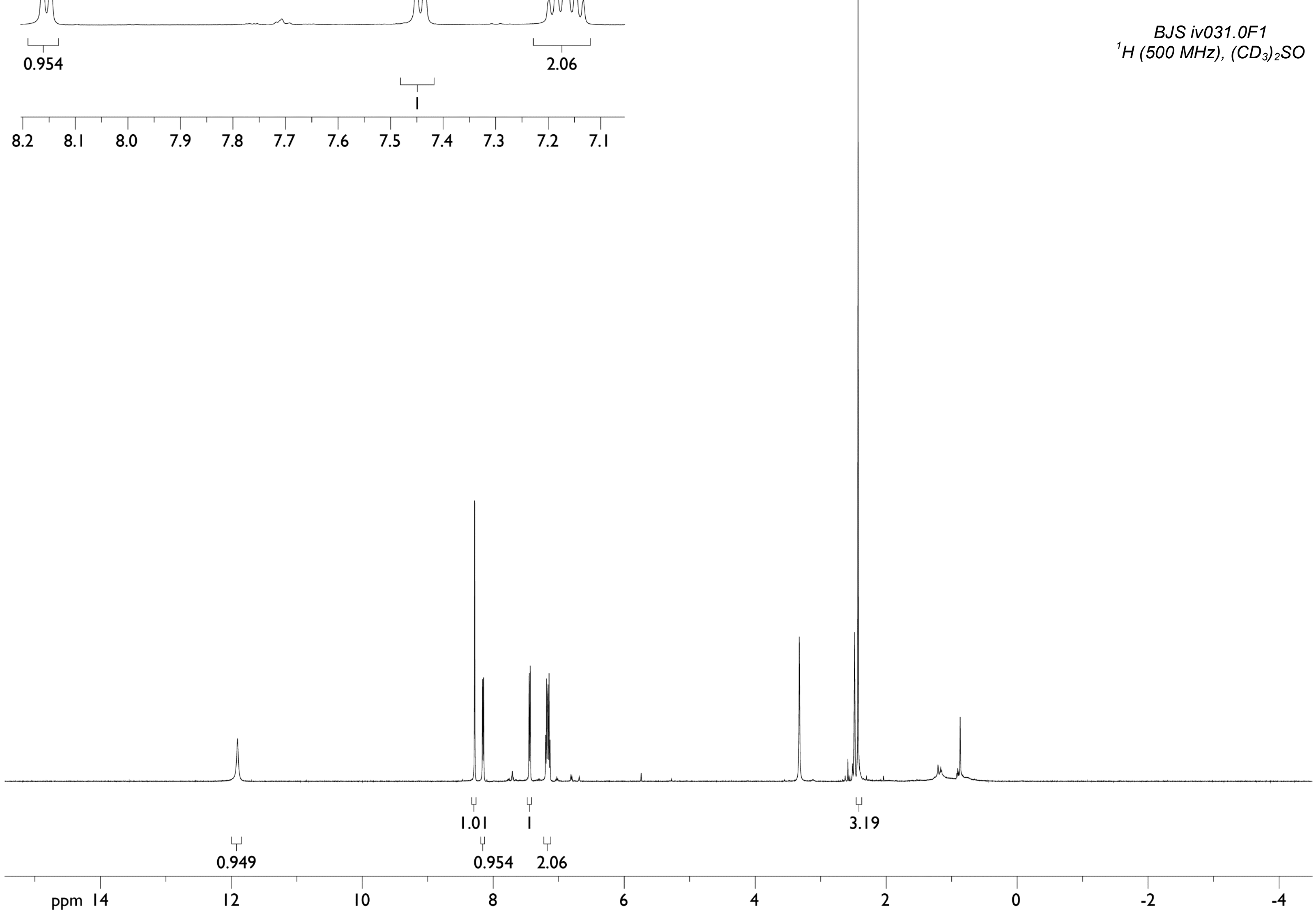
BJS iv125.0F1
^{13}C (125 MHz), $(CD_3)_2SO$

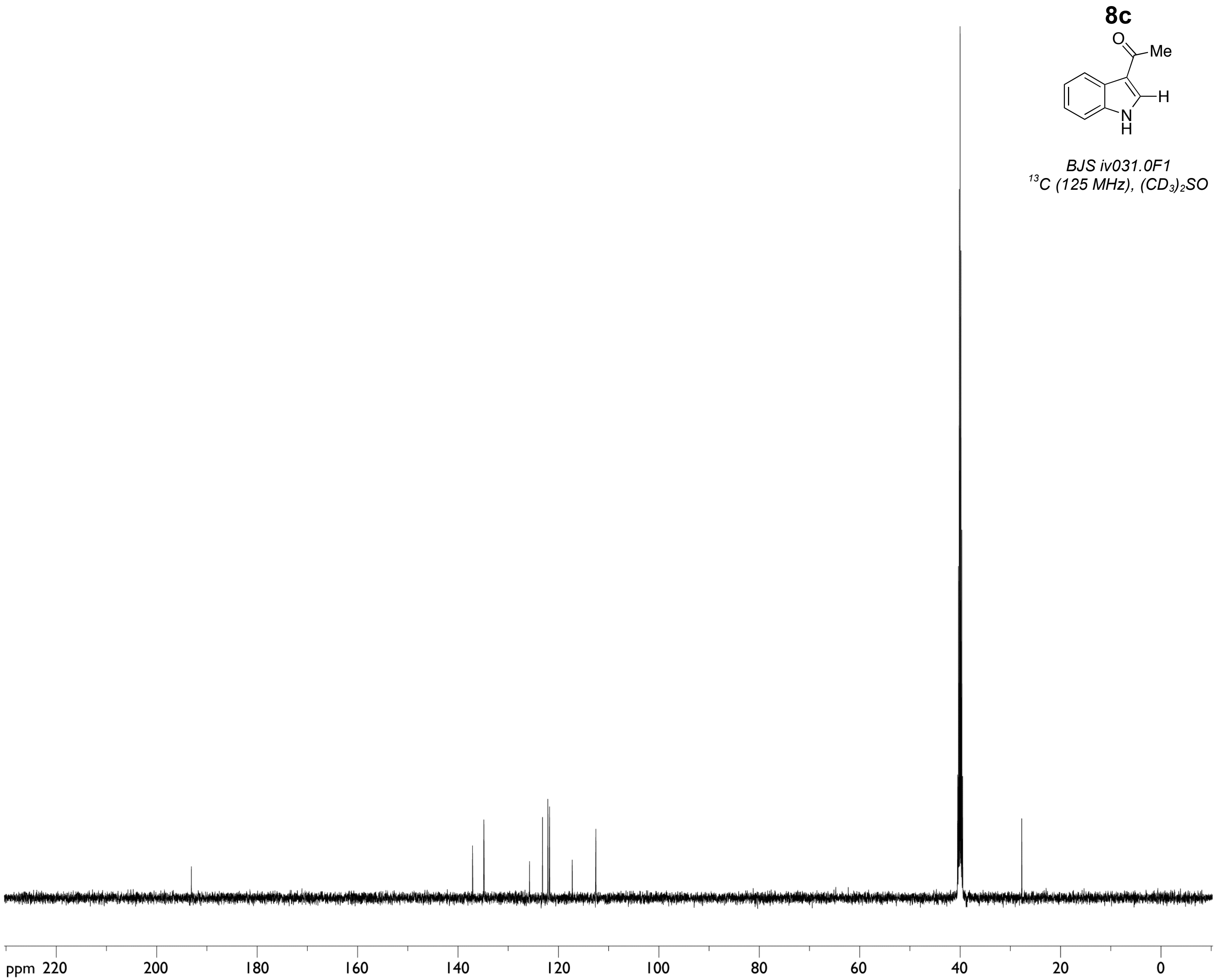


8c



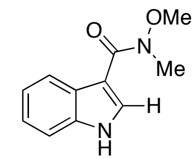
BJS iv031.0F1
^{1}H (500 MHz), $(CD_3)_2SO$



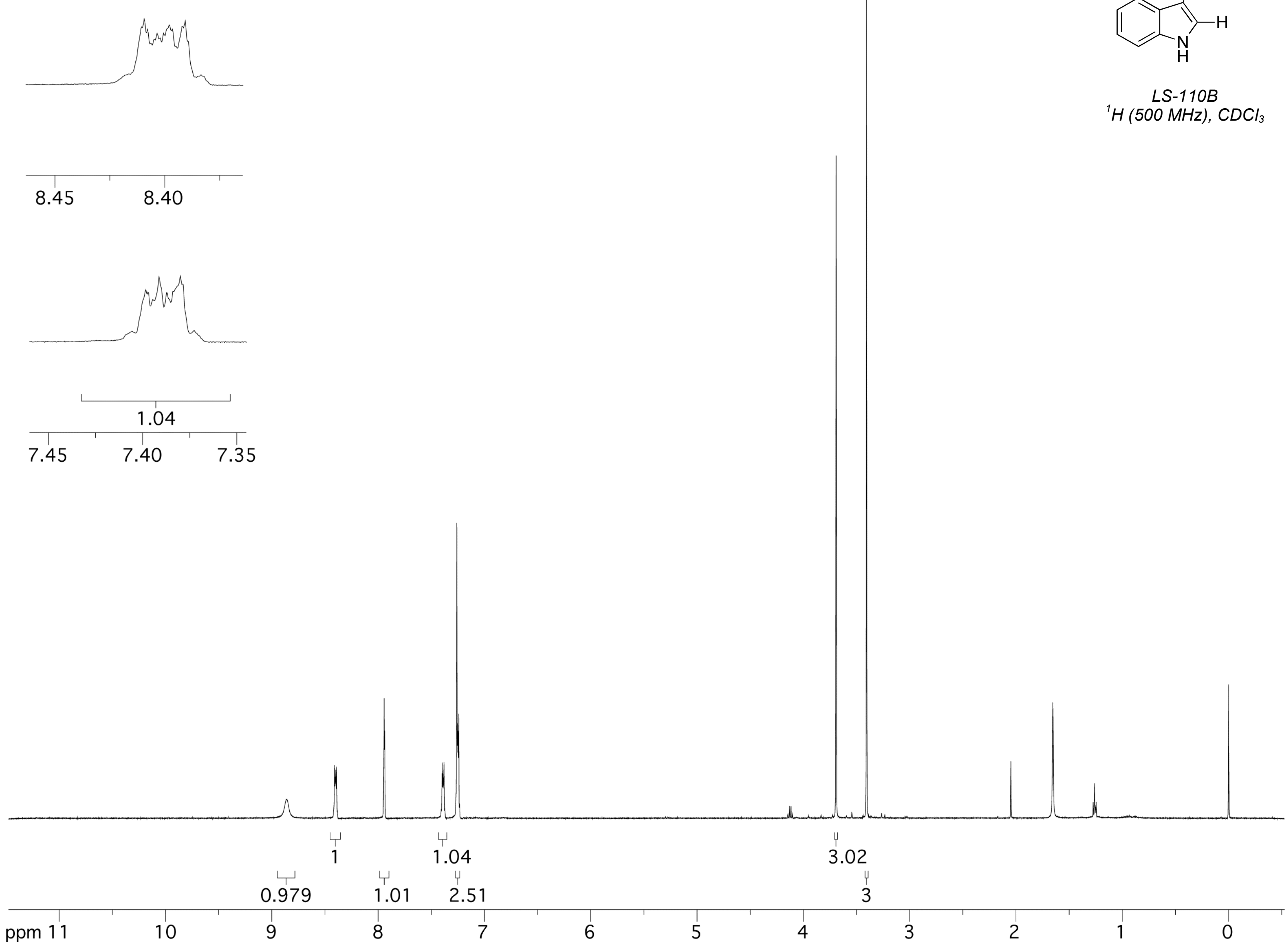


8c
O
Me
H
N
H
BJS iv031.0F1
^{13}C (125 MHz), $(CD_3)_2SO$
ppm 220
200
180
160
140
120
100
80
60
40
20
0

8d

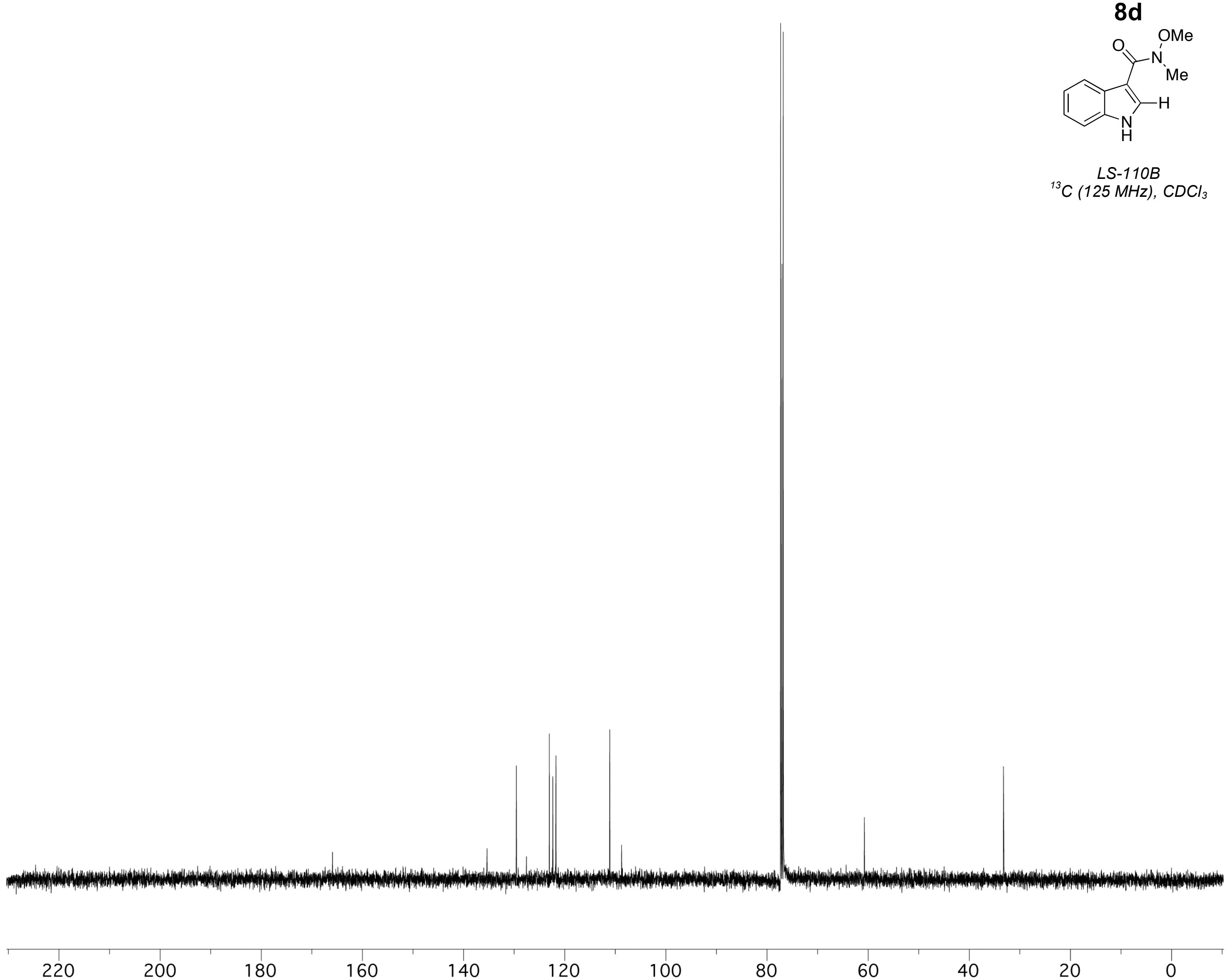


LS-110B
^{1}H (500 MHz), $CDCl_3$



8d

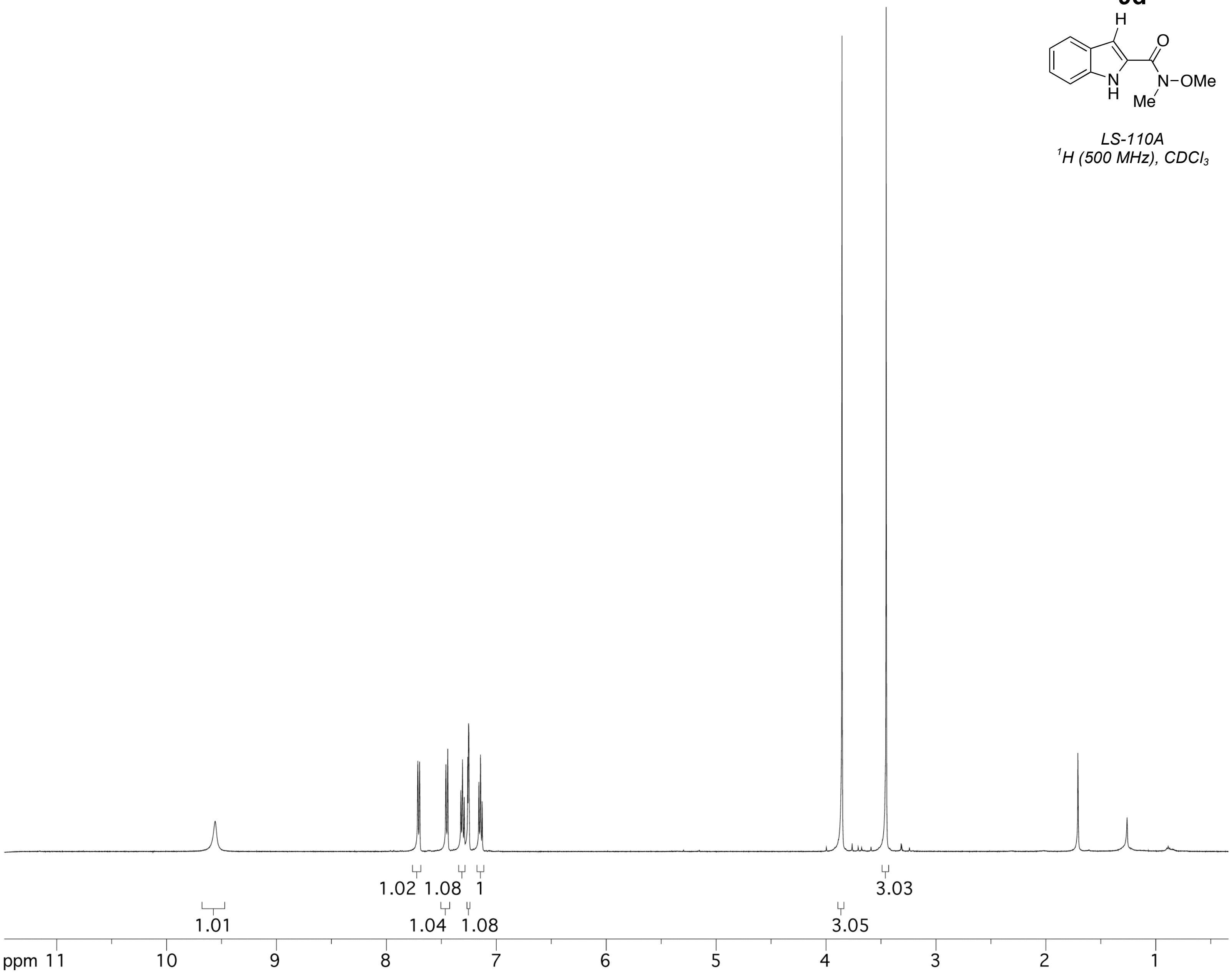
LS-110B
^{13}C (125 MHz), $CDCl_3$



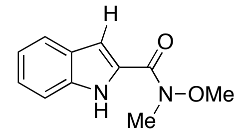
9d

LS-110A

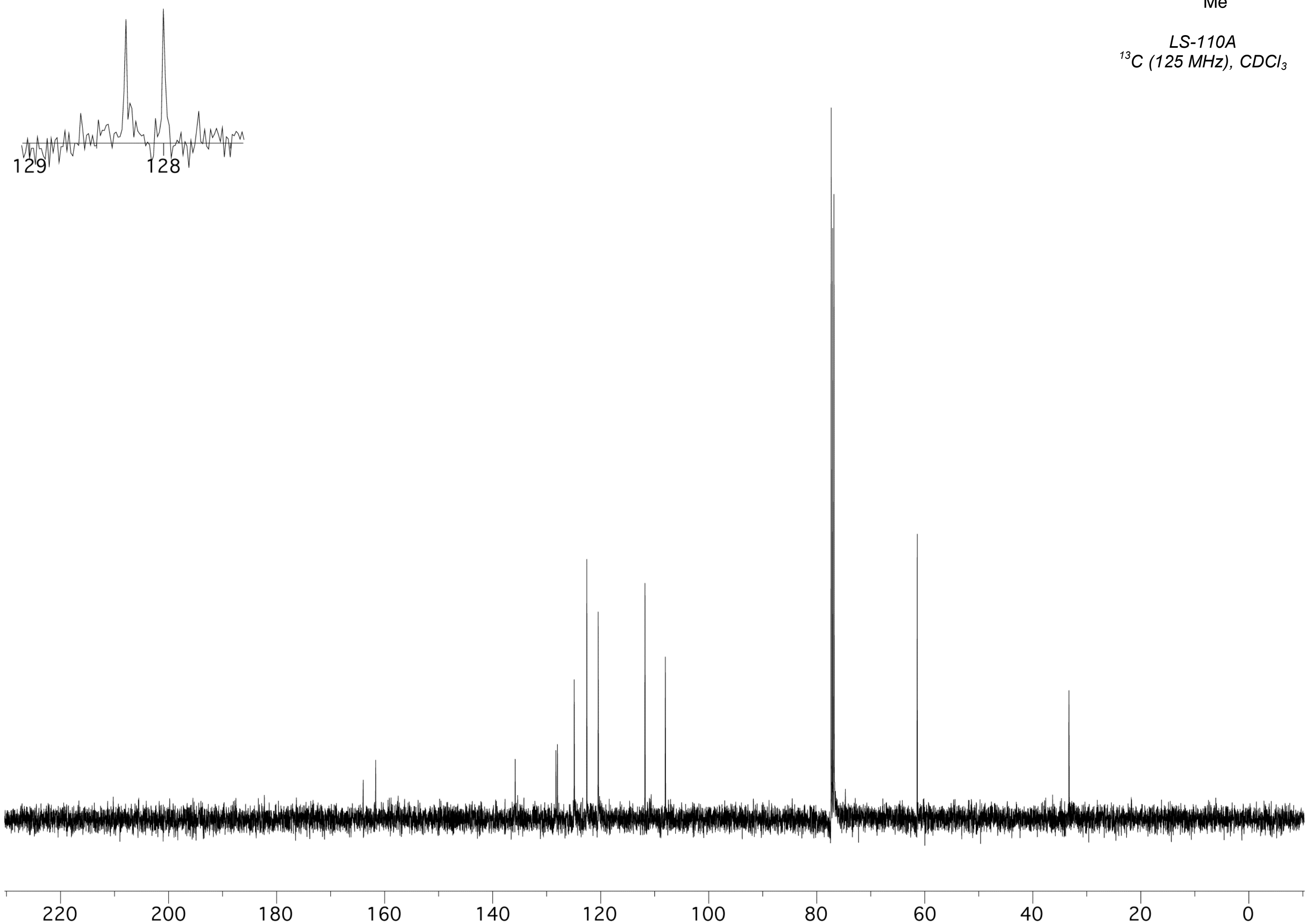
^{1}H (500 MHz), $CDCl_3$



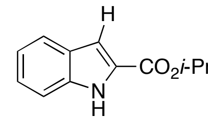
9d



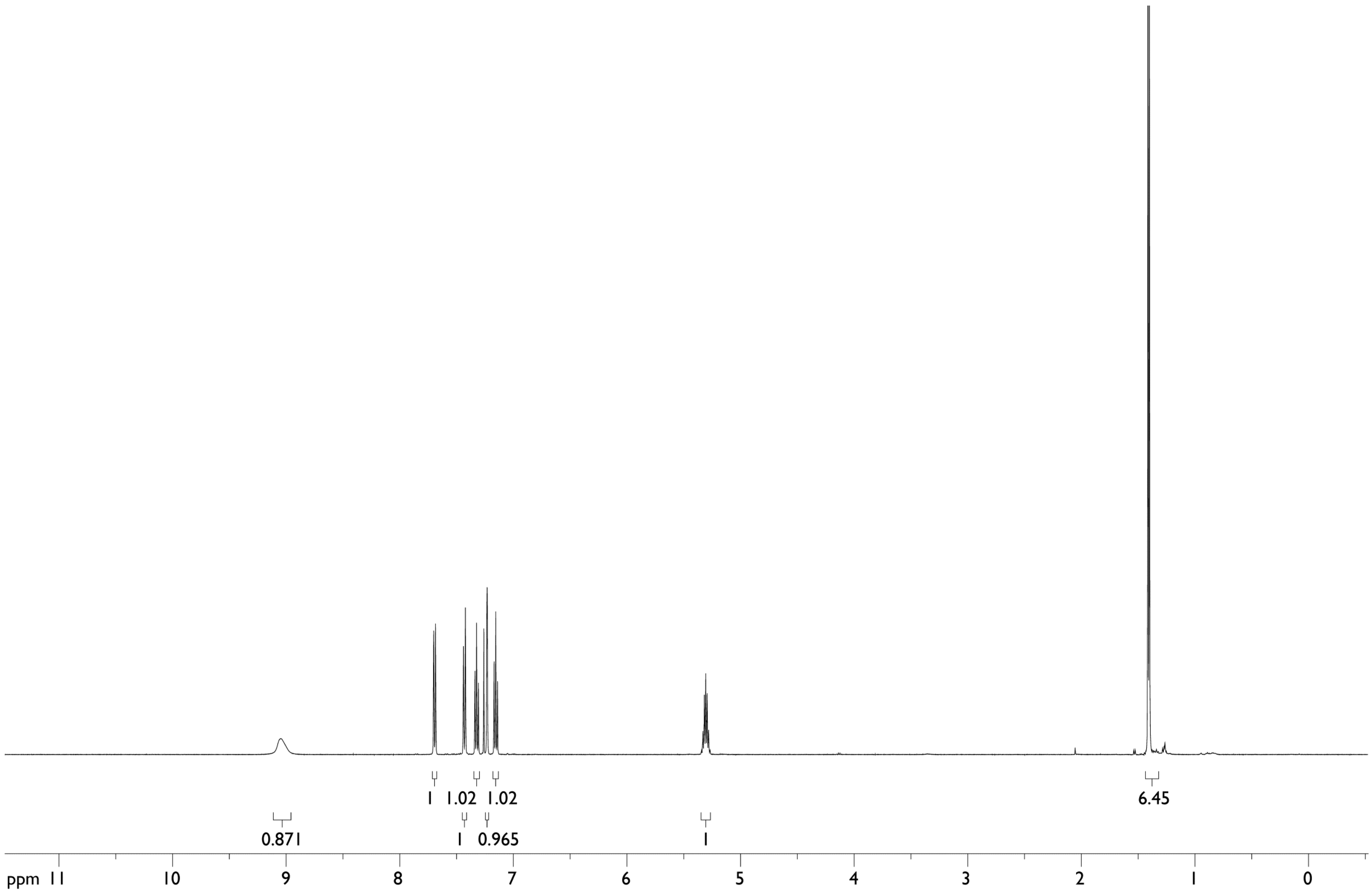
LS-110A
^{13}C (125 MHz), $CDCl_3$

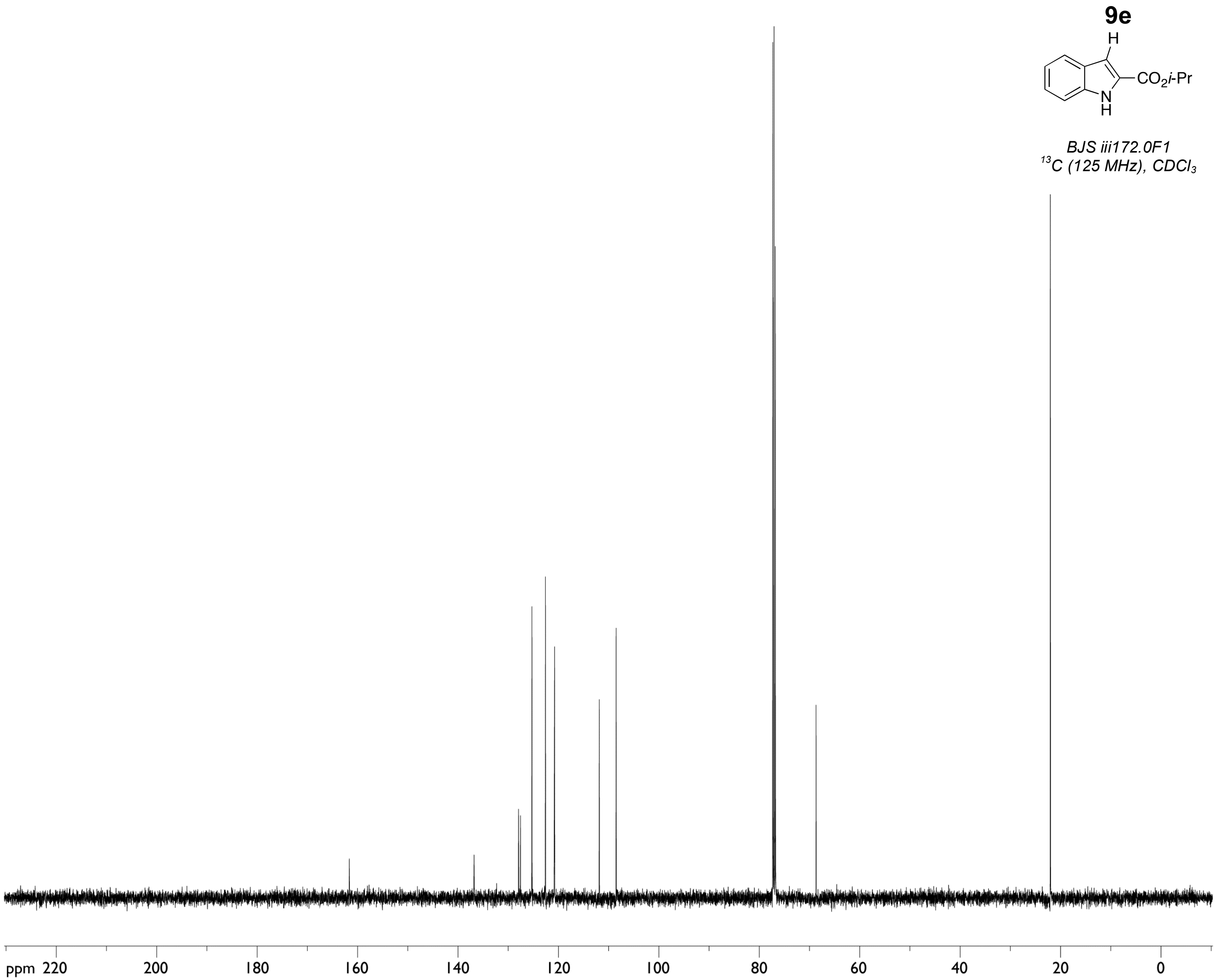


9e

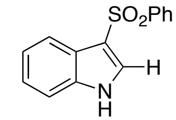


BJS iii172.0F1
^{1}H (500 MHz), $CDCl_3$

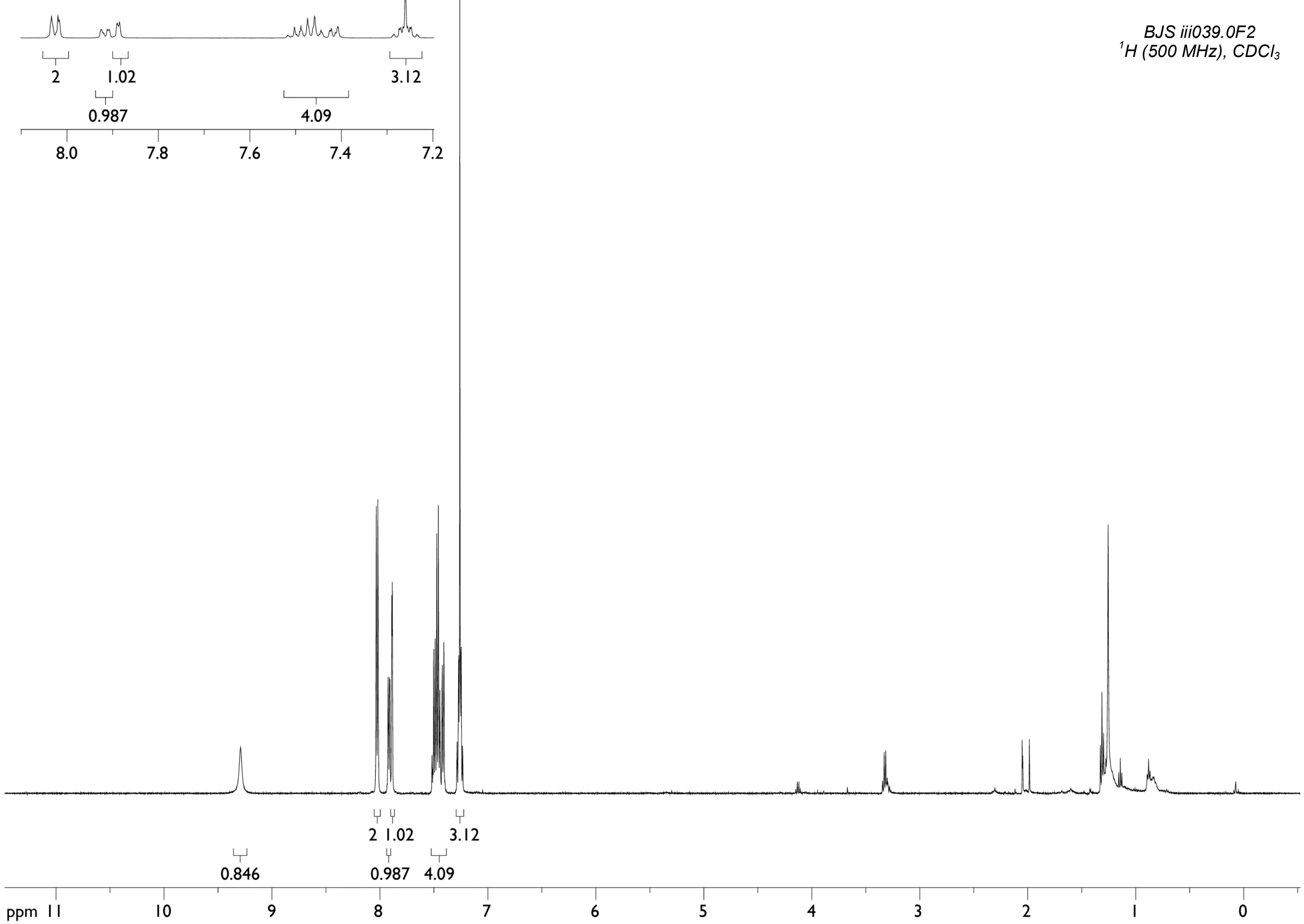



9e
H
CO2i-Pr
N
H
BJS iii172.0F1
13C (125 MHz), CDCl3
ppm 220
200
180
160
140
120
100
80
60
40
20
0

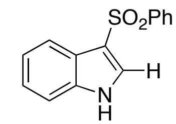
8f



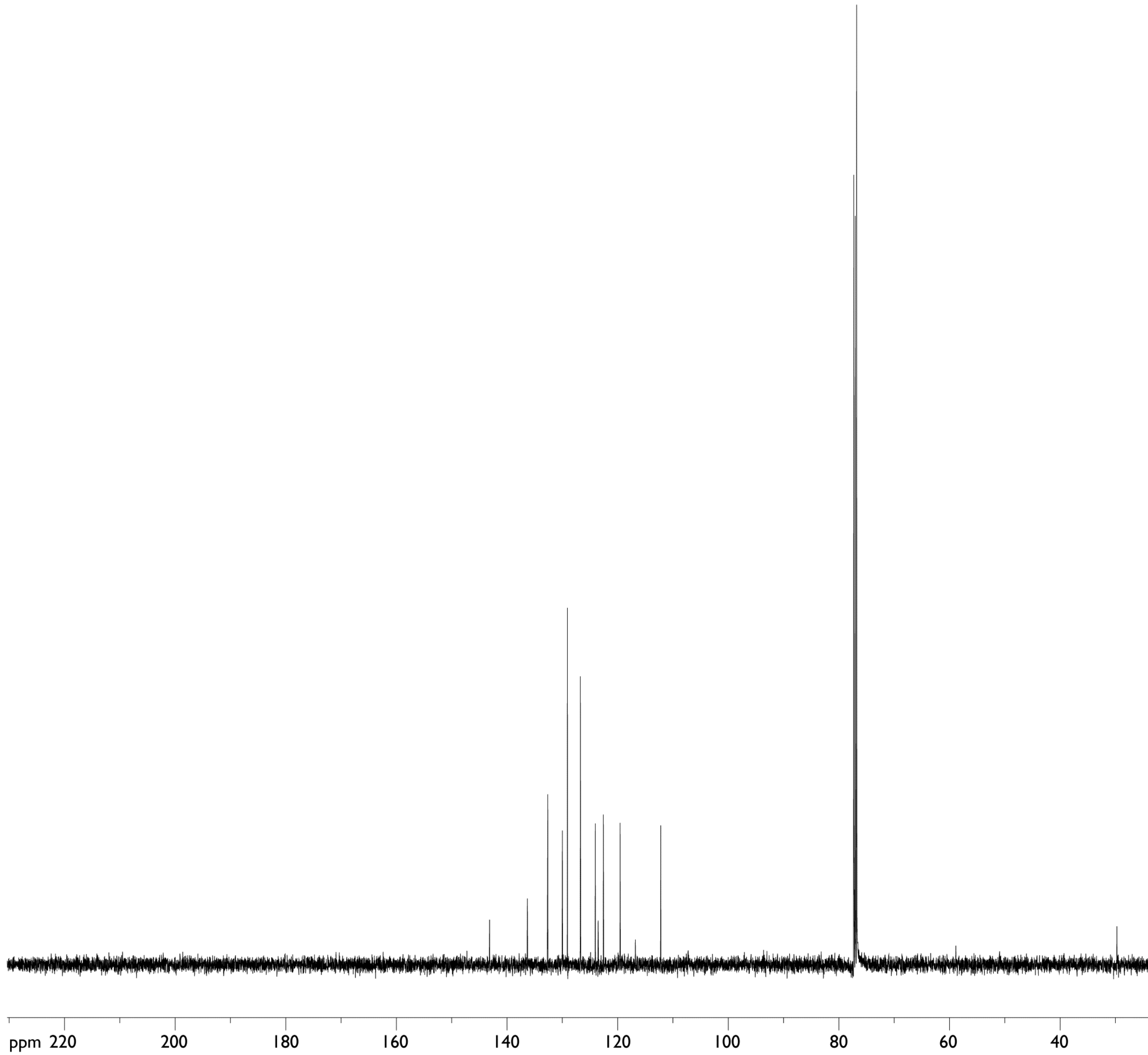
BJS iii039.0F2
^{1}H (500 MHz), $CDCl_3$



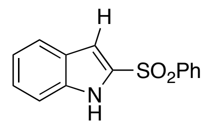
8f



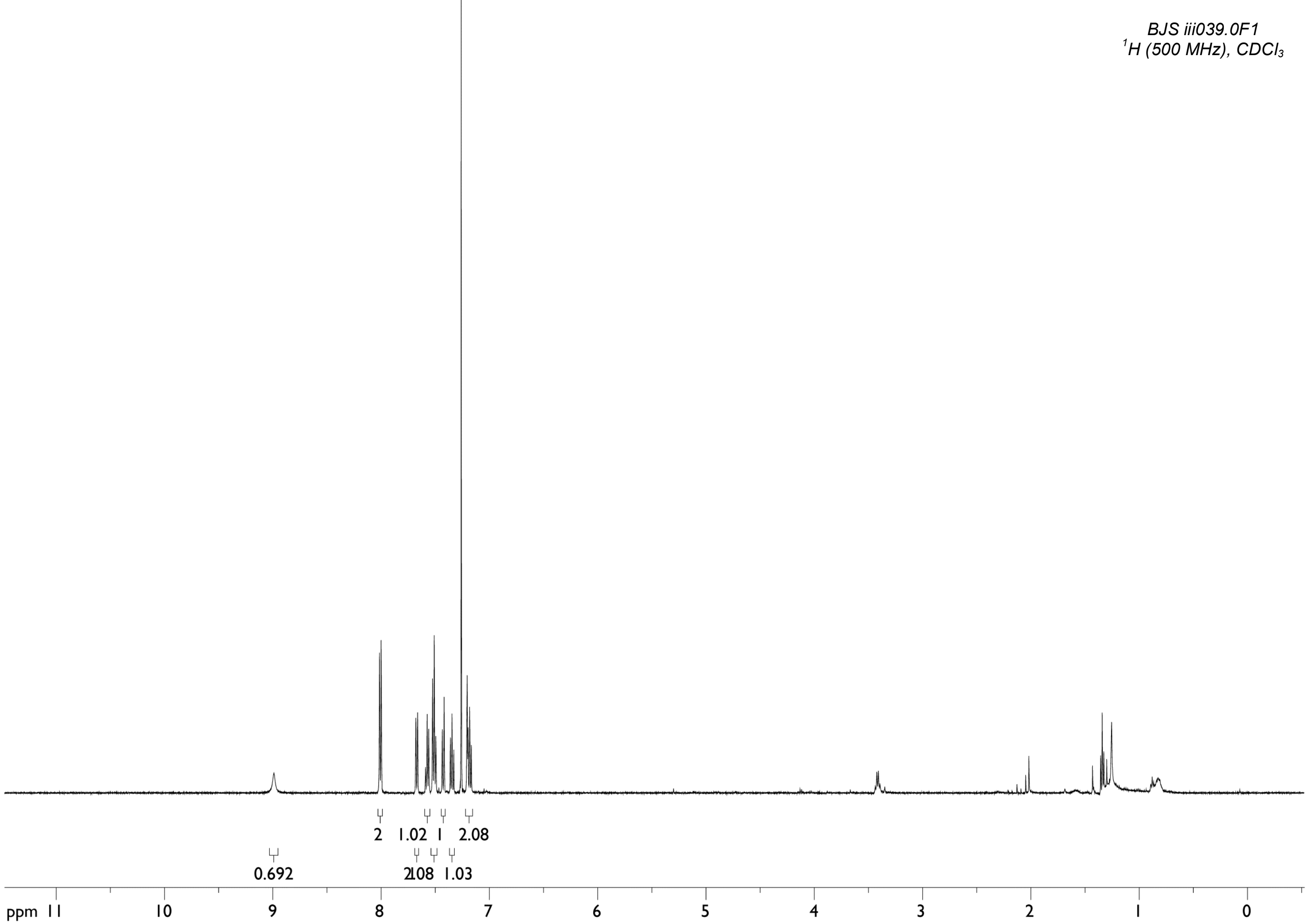
BJS iii039.0F2
^{13}C (125 MHz), $CDCl_3$



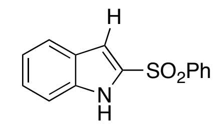
9f



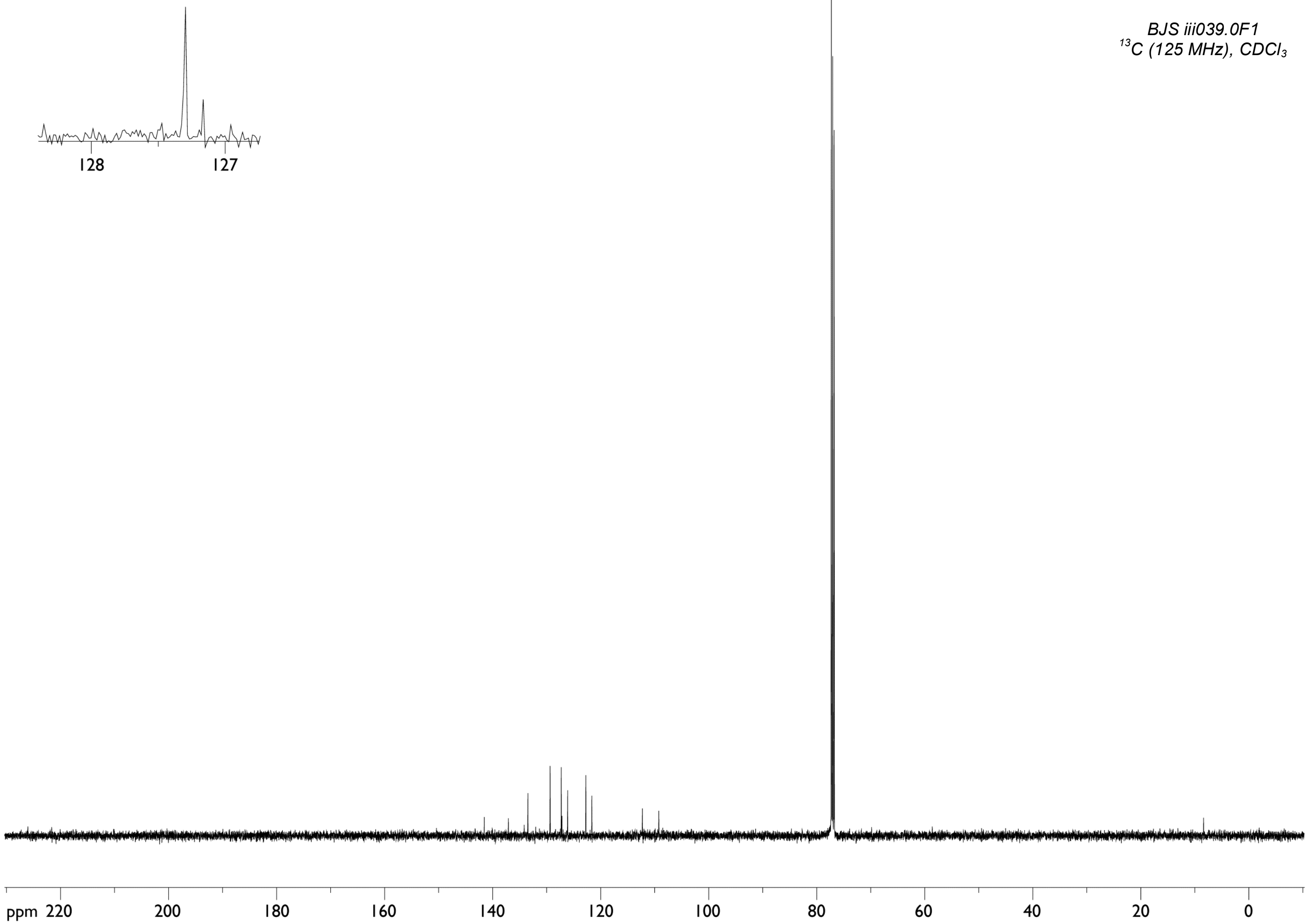
BJS iii039.0F1
[1]H (500 MHz), CDCl3



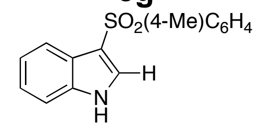
9f



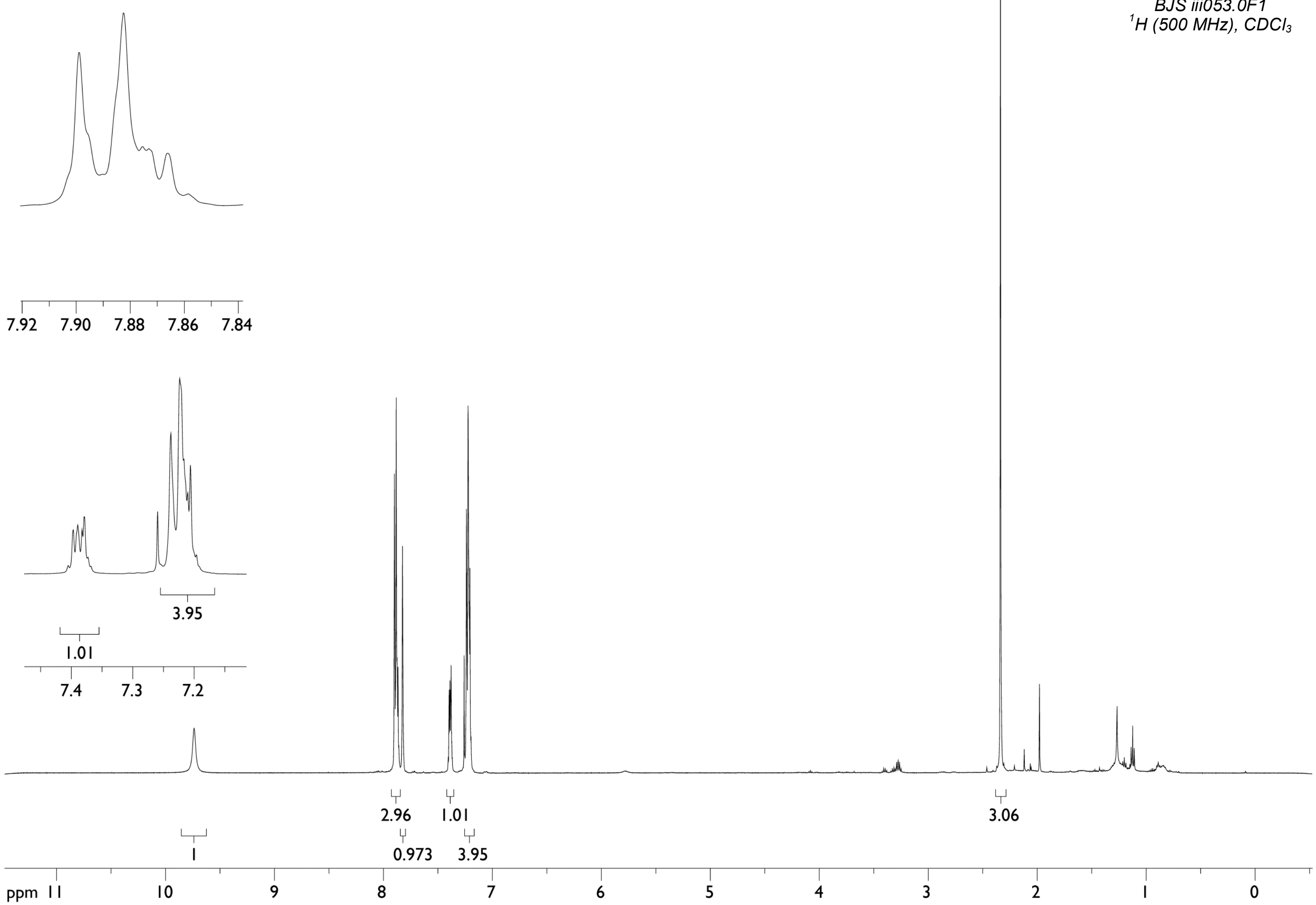
BJS iii039.0F1
^{13}C (125 MHz), $CDCl_3$



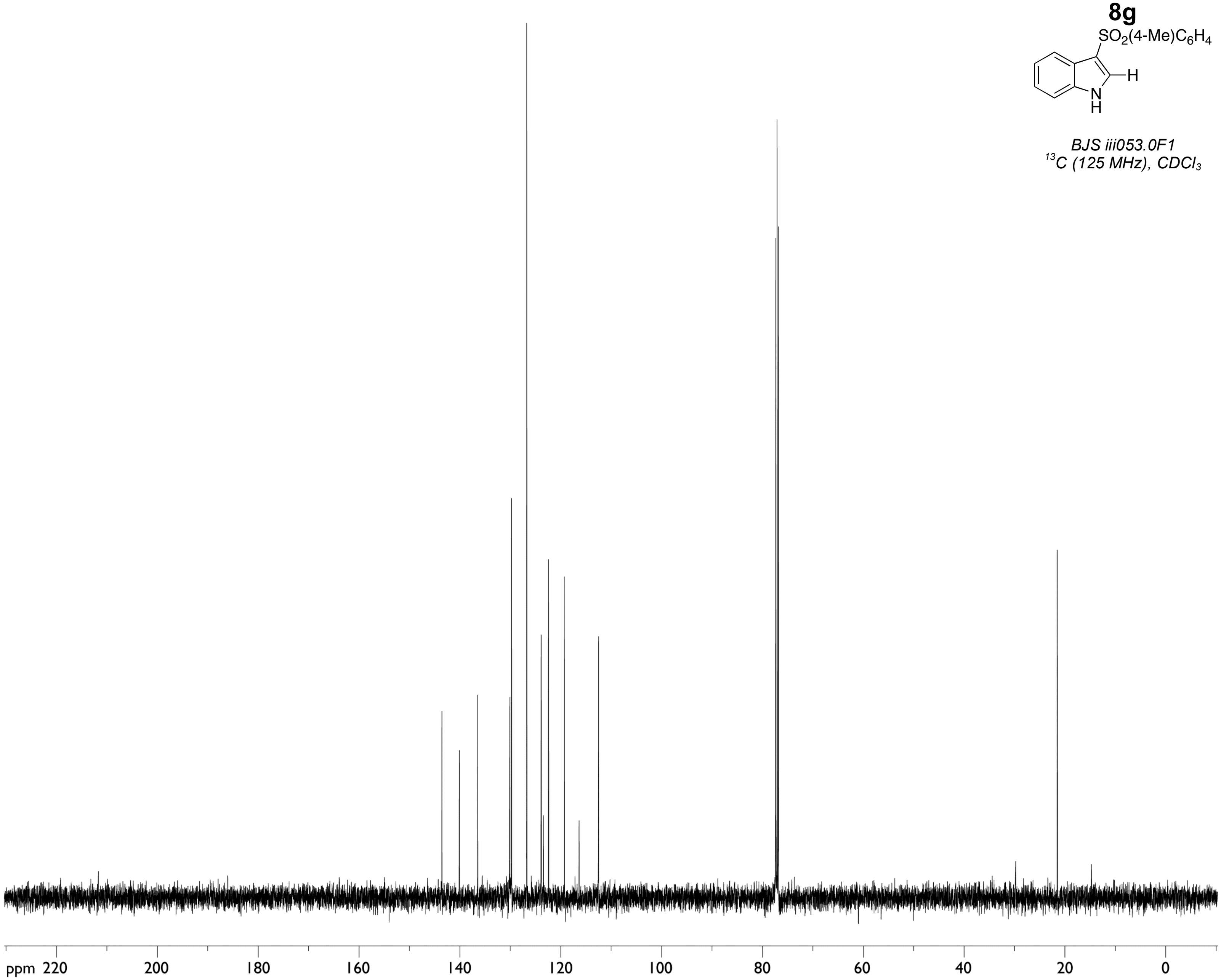
8g



BJS iii053.0F1
^{1}H (500 MHz), CDCl$_3$

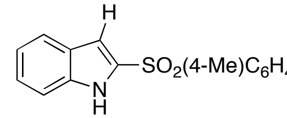


8g

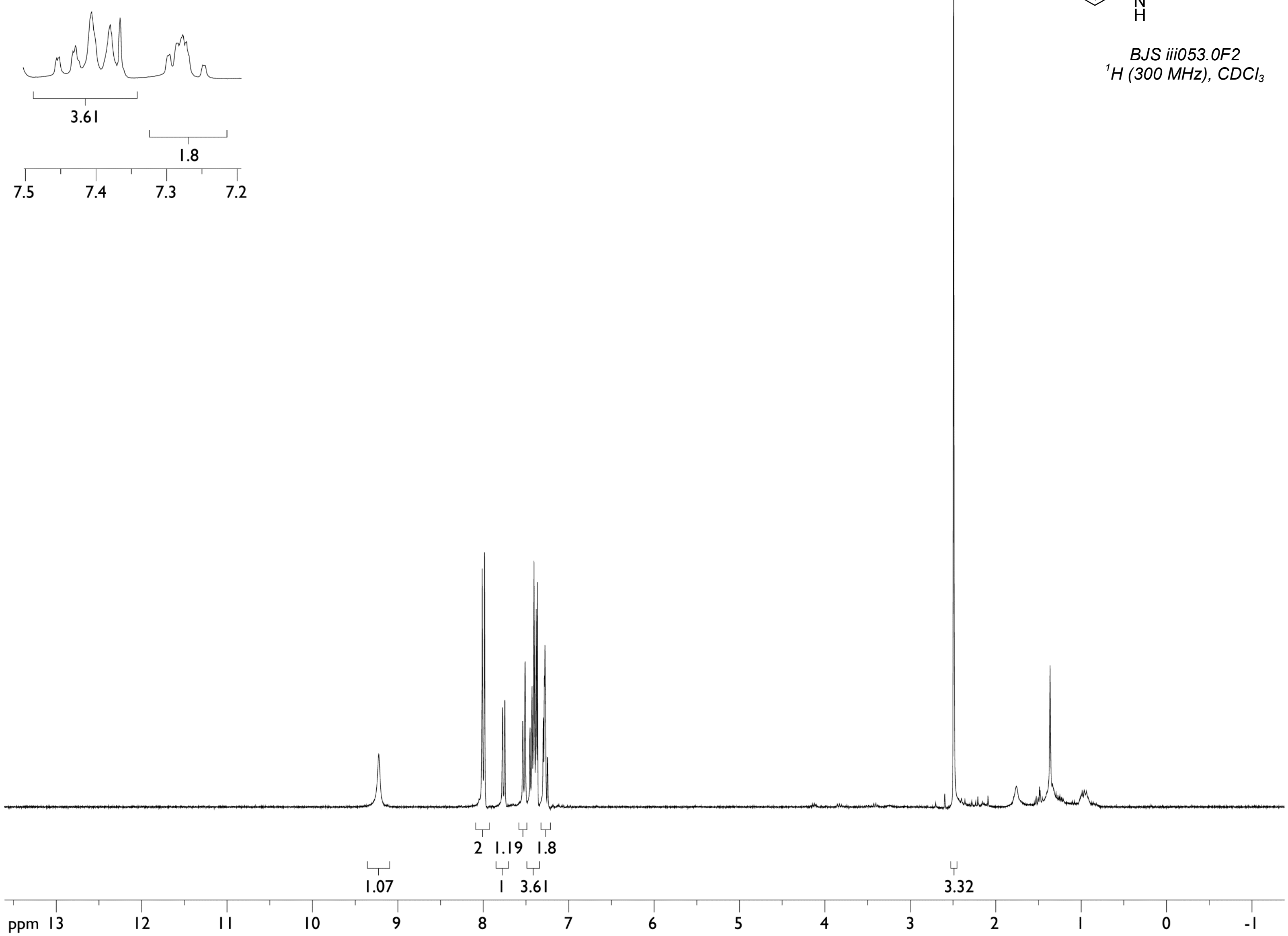


BJS iii053.0F1
^{13}C (125 MHz), CDCl$_3$

9g

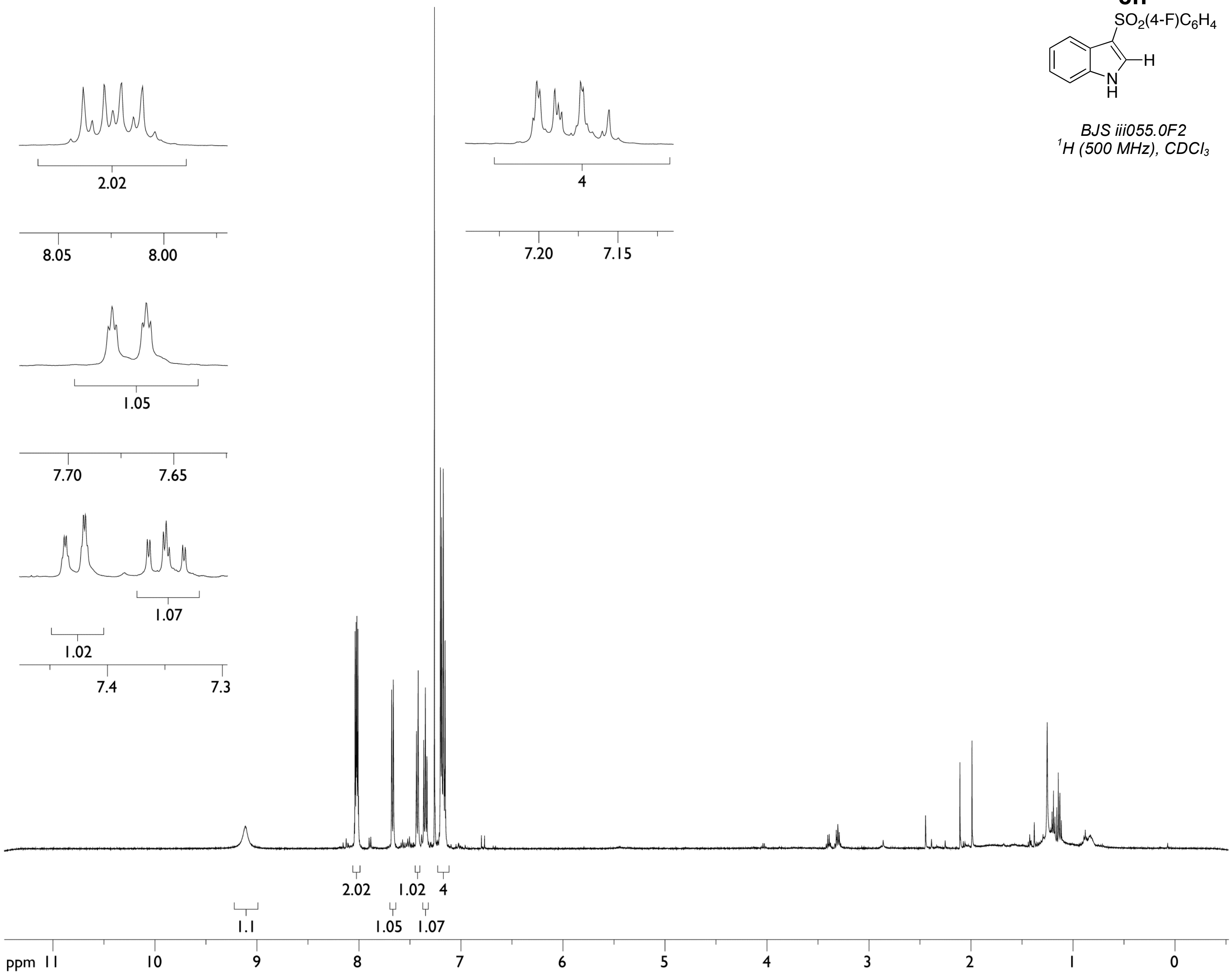


BJS iii053.0F2
^{1}H (300 MHz), CDCl$_3$

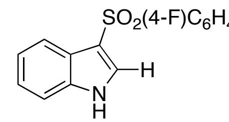


8h

BJS iii055.0F2
^{1}H (500 MHz), $CDCl_3$

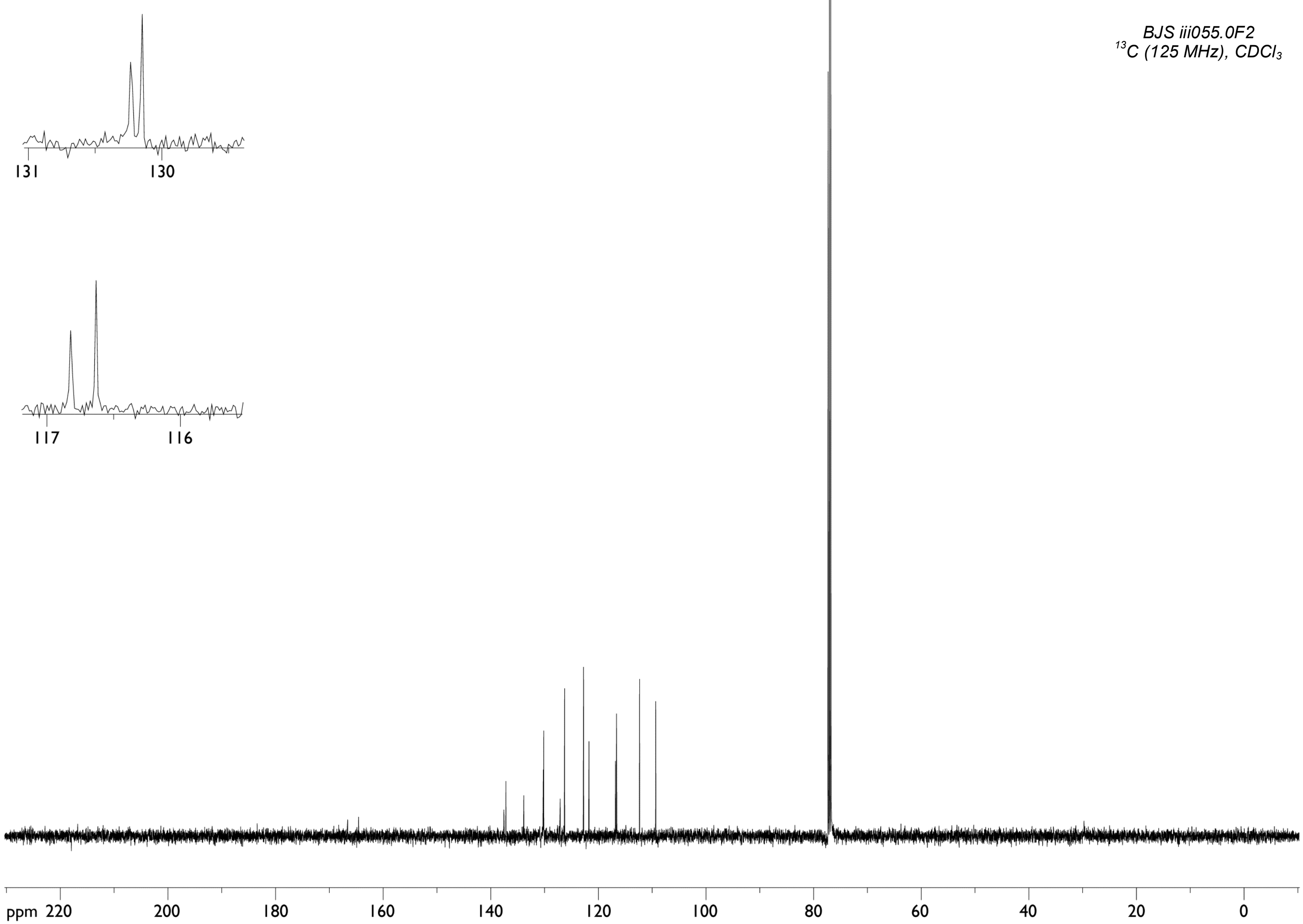


8h



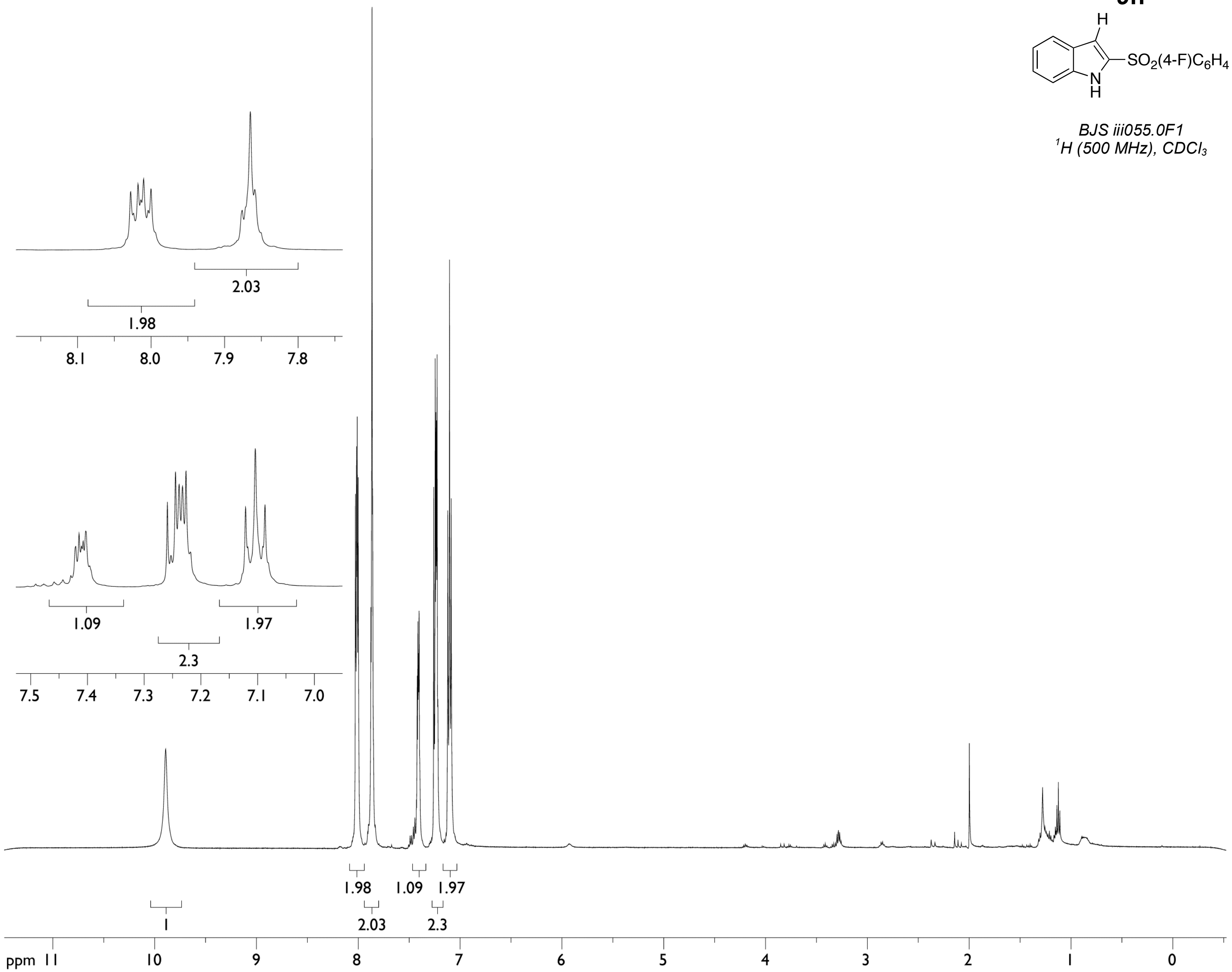
BJS iii055.0F2

^{13}C (125 MHz), $CDCl_3$

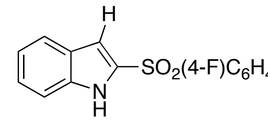


9h

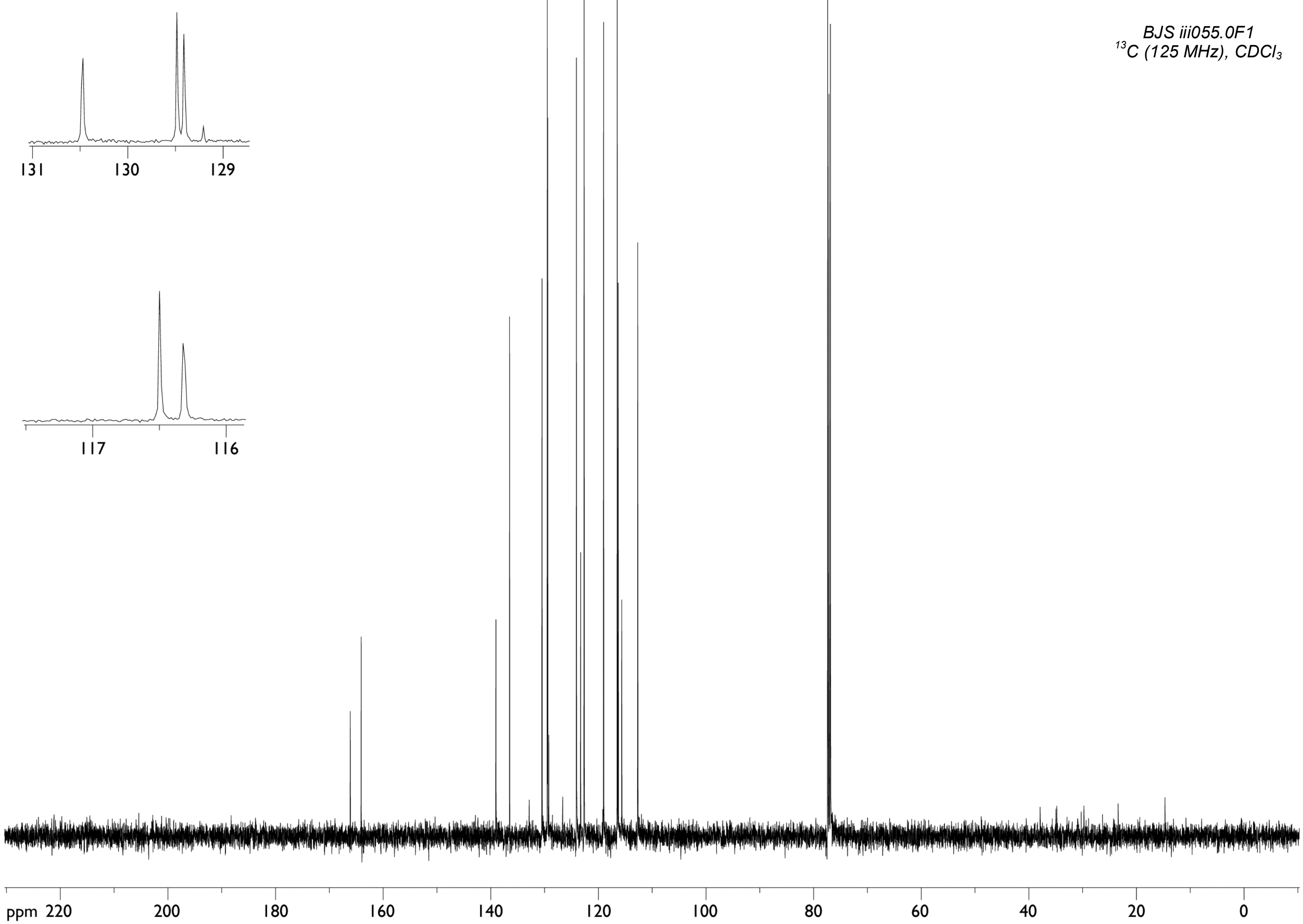
BJS iii055.0F1
^{1}H (500 MHz), CDCl$_3$



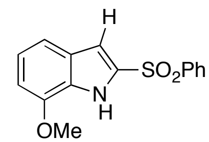
9h



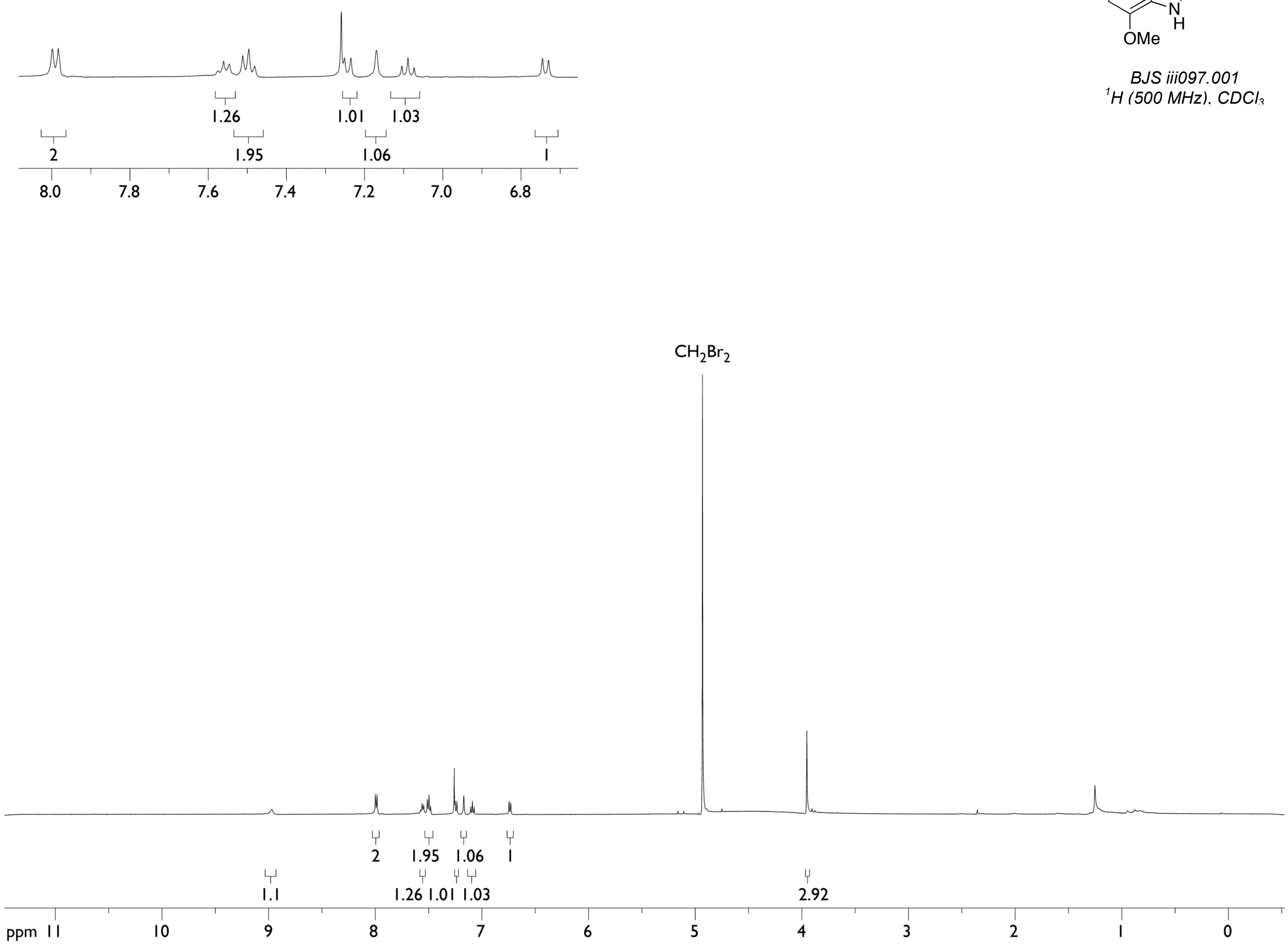
BJS iii055.0F1
^{13}C (125 MHz), $CDCl_3$



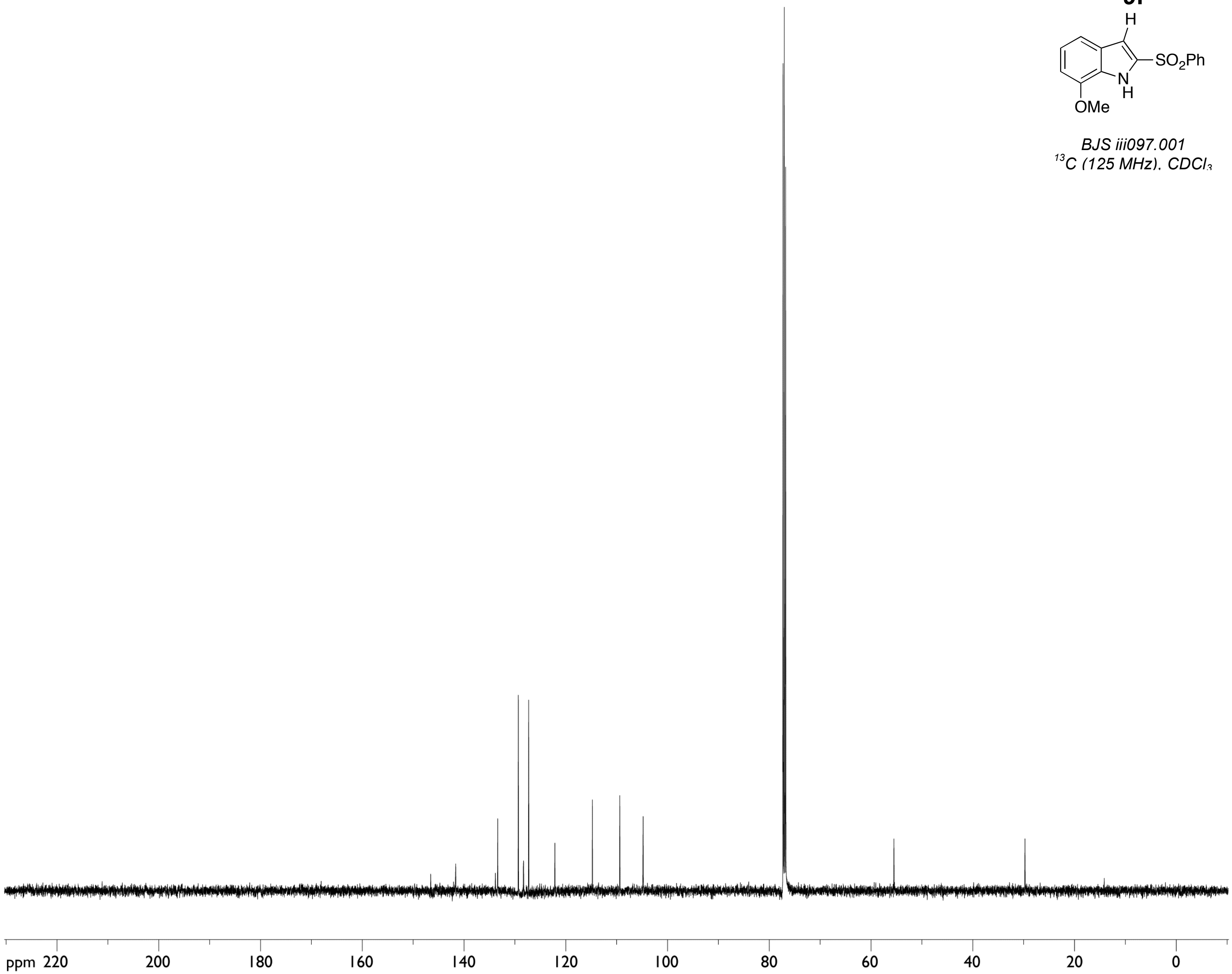
9i

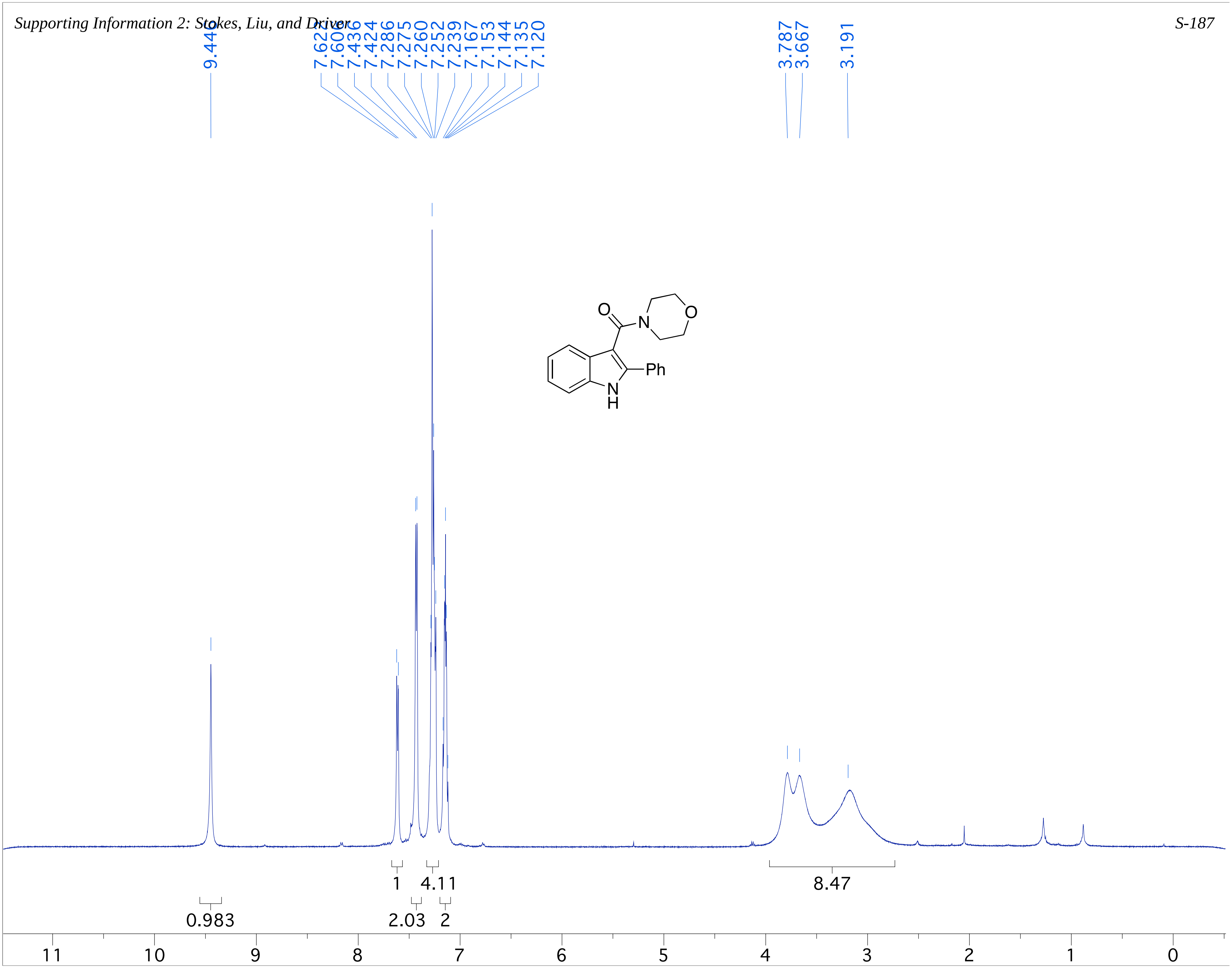


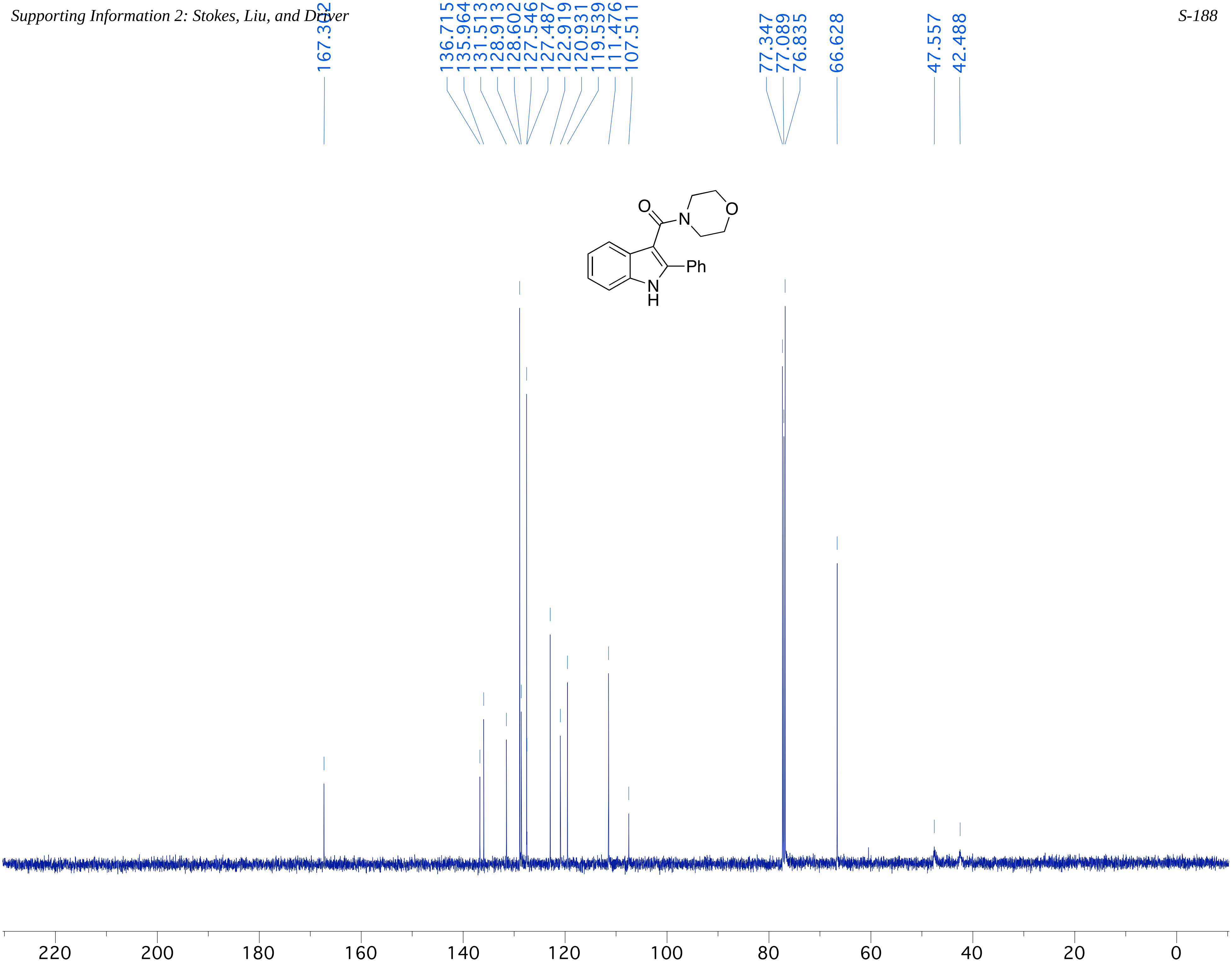
BJS iii097.001
^{1}H (500 MHz), CDCl$_3$



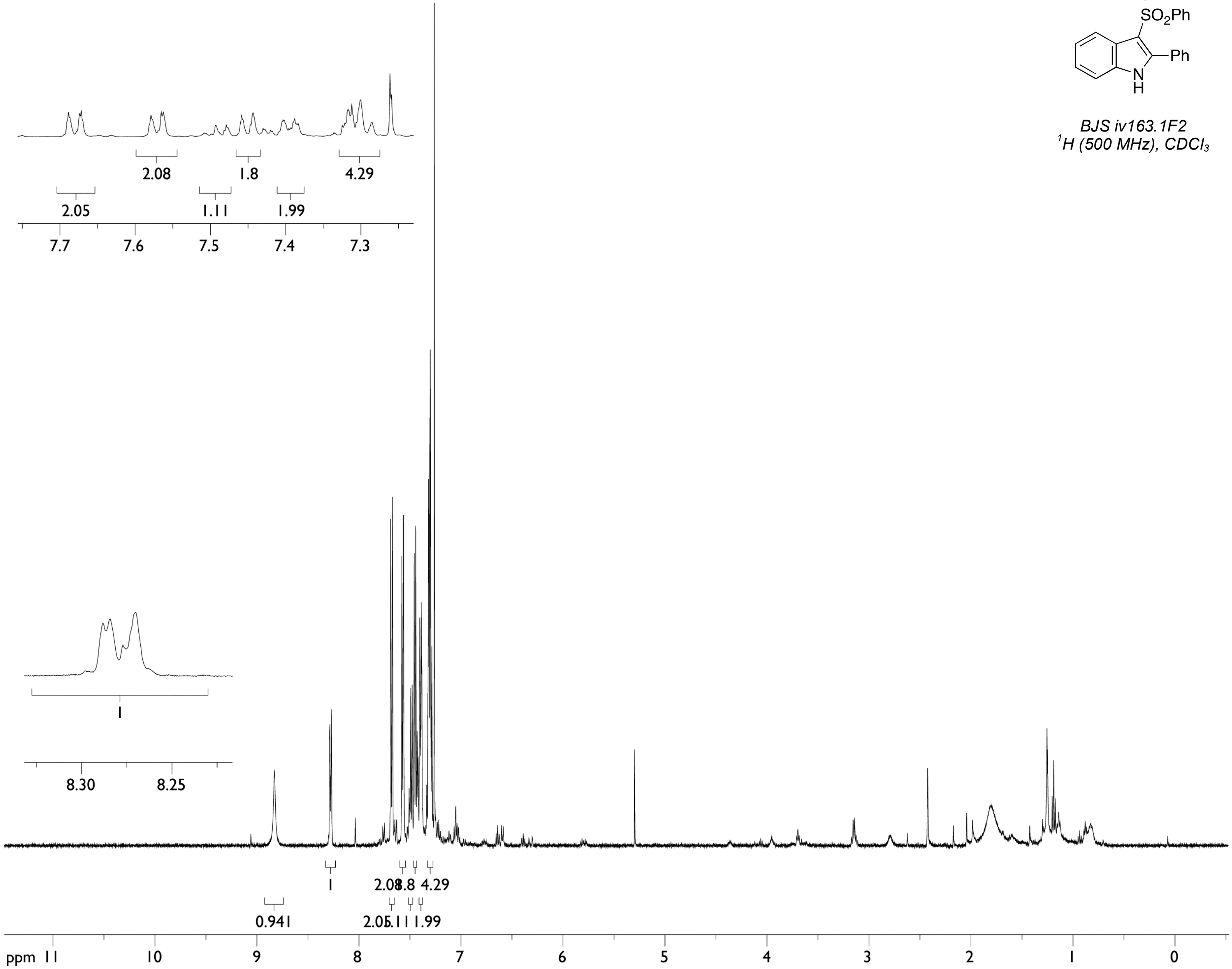
9i


H
SO2Ph
N
H
OMe
BJS iii097.001
13C (125 MHz), CDCl3
ppm 220 200 180 160 140 120 100 80 60 40 20 0

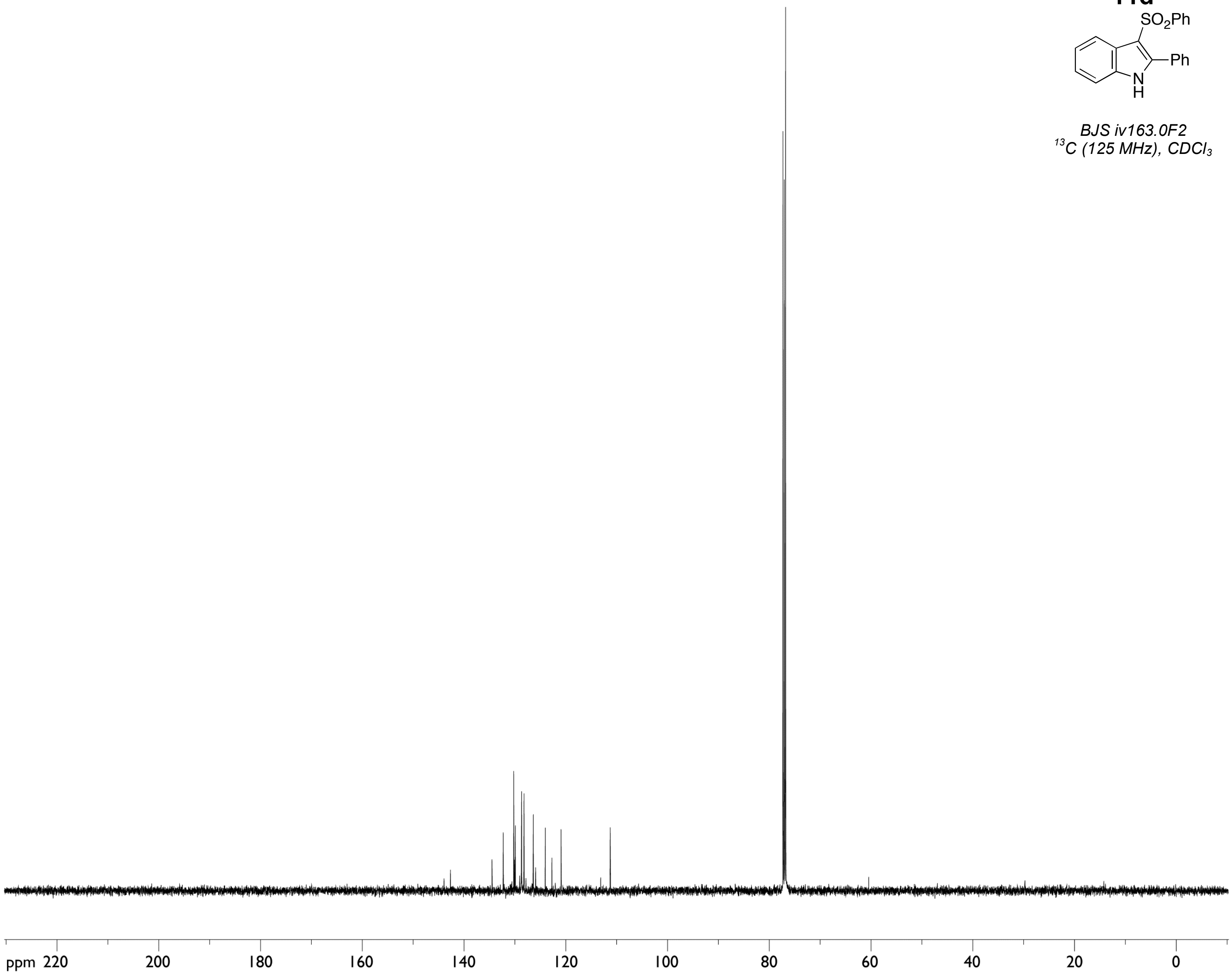

9.446
7.622
7.608
7.436
7.424
7.286
7.275
7.260
7.252
7.239
7.167
7.153
7.144
7.135
7.120
3.787
3.667
3.191
O
N
O
Ph
N
H
1
4.11
8.47
0.983
2.03
2
11
10
9
8
7
6
5
4
3
2
1
0


167.302
136.715
135.964
131.513
128.913
128.602
127.546
127.487
122.919
120.931
119.539
111.476
107.511
77.347
77.089
76.835
66.628
47.557
42.488
O
N
O
Ph
N
H
220
200
180
160
140
120
100
80
60
40
20
0

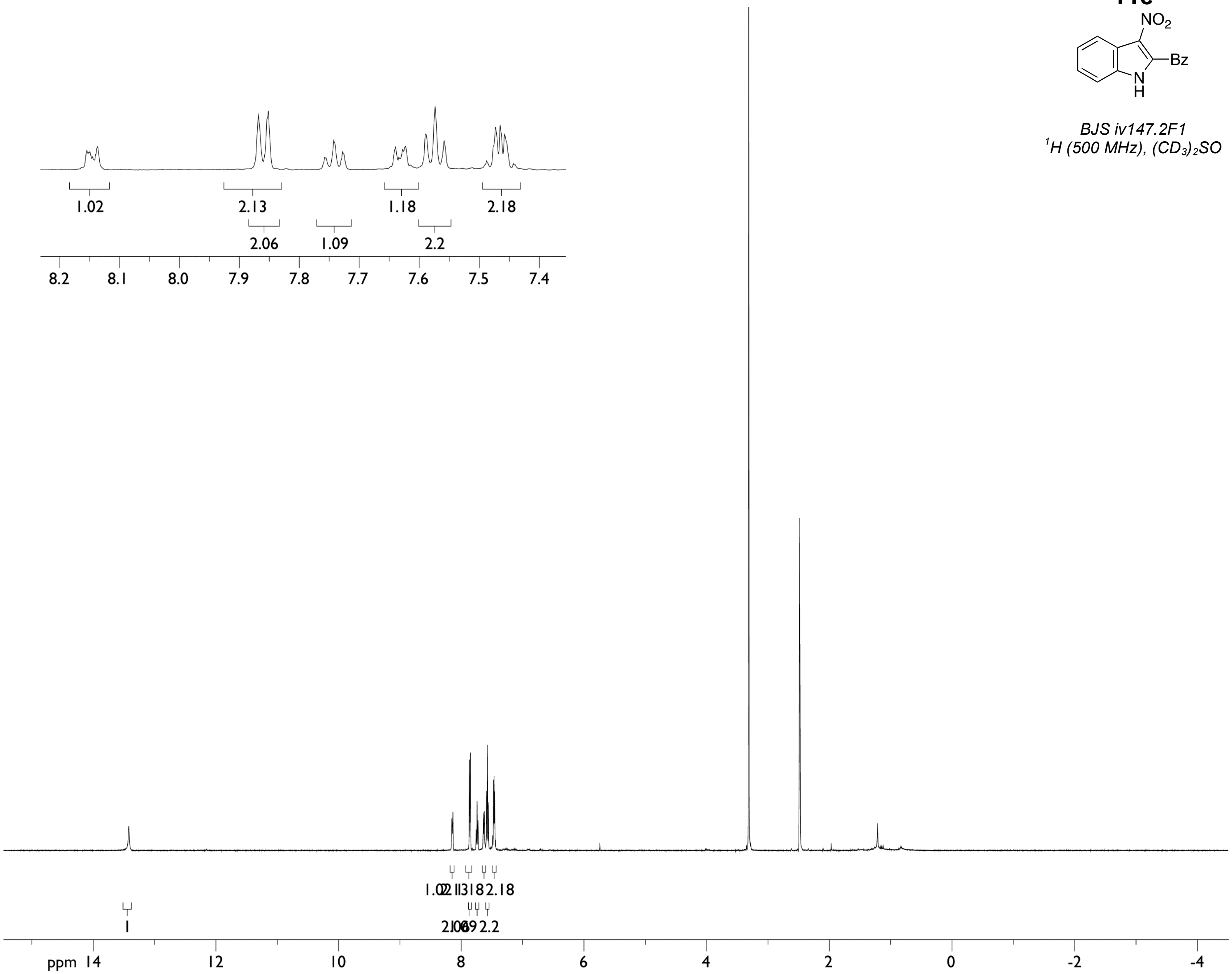
11d

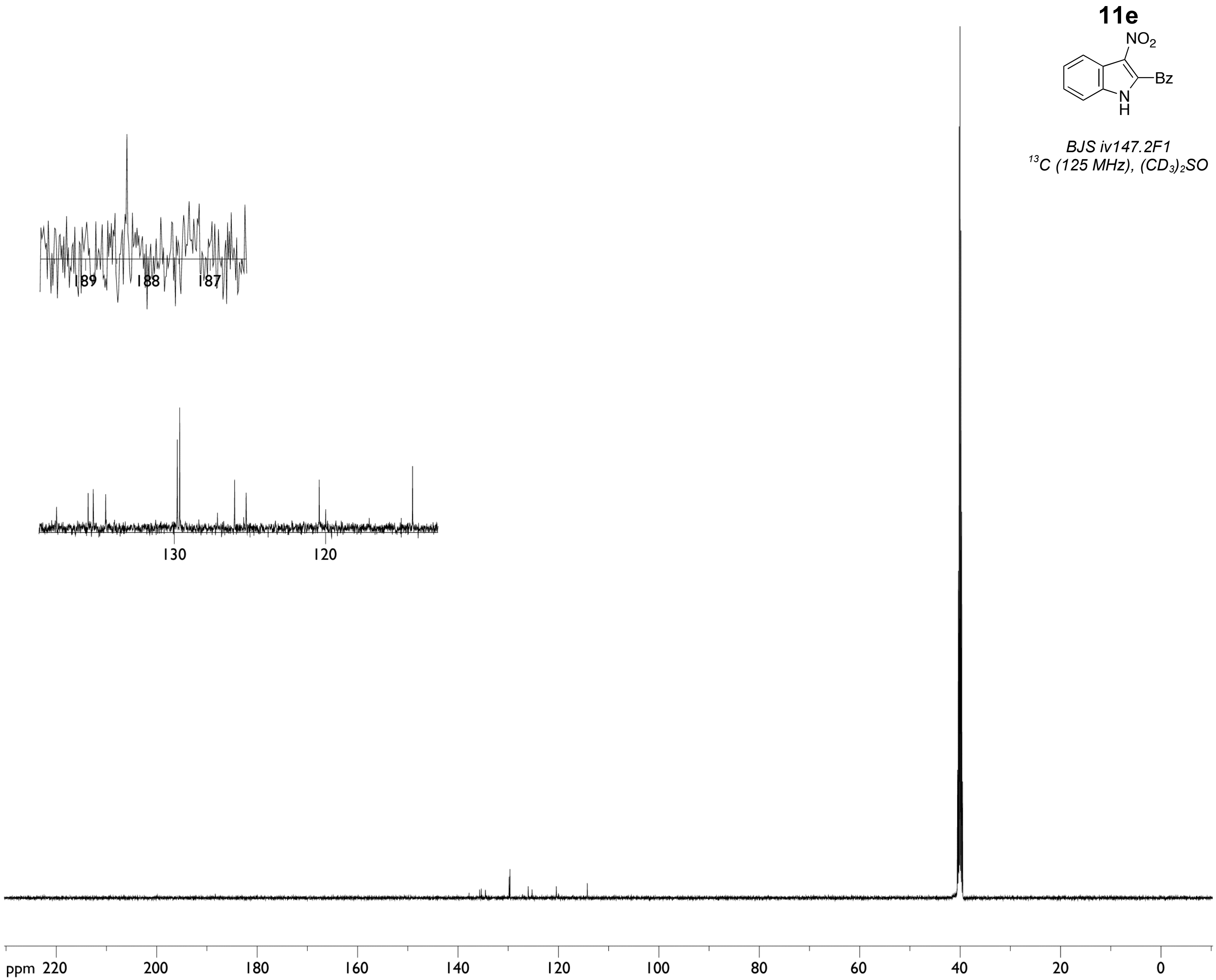

SO2Ph
Ph
N
H
BJS iv163.1F2
1H (500 MHz), CDCl3
2.08
1.8
4.29
2.05
1.11
1.99
7.7
7.6
7.5
7.4
7.3
1
8.30
8.25
0.941
ppm 11
10
9
8
7
6
5
4
3
2
1
0

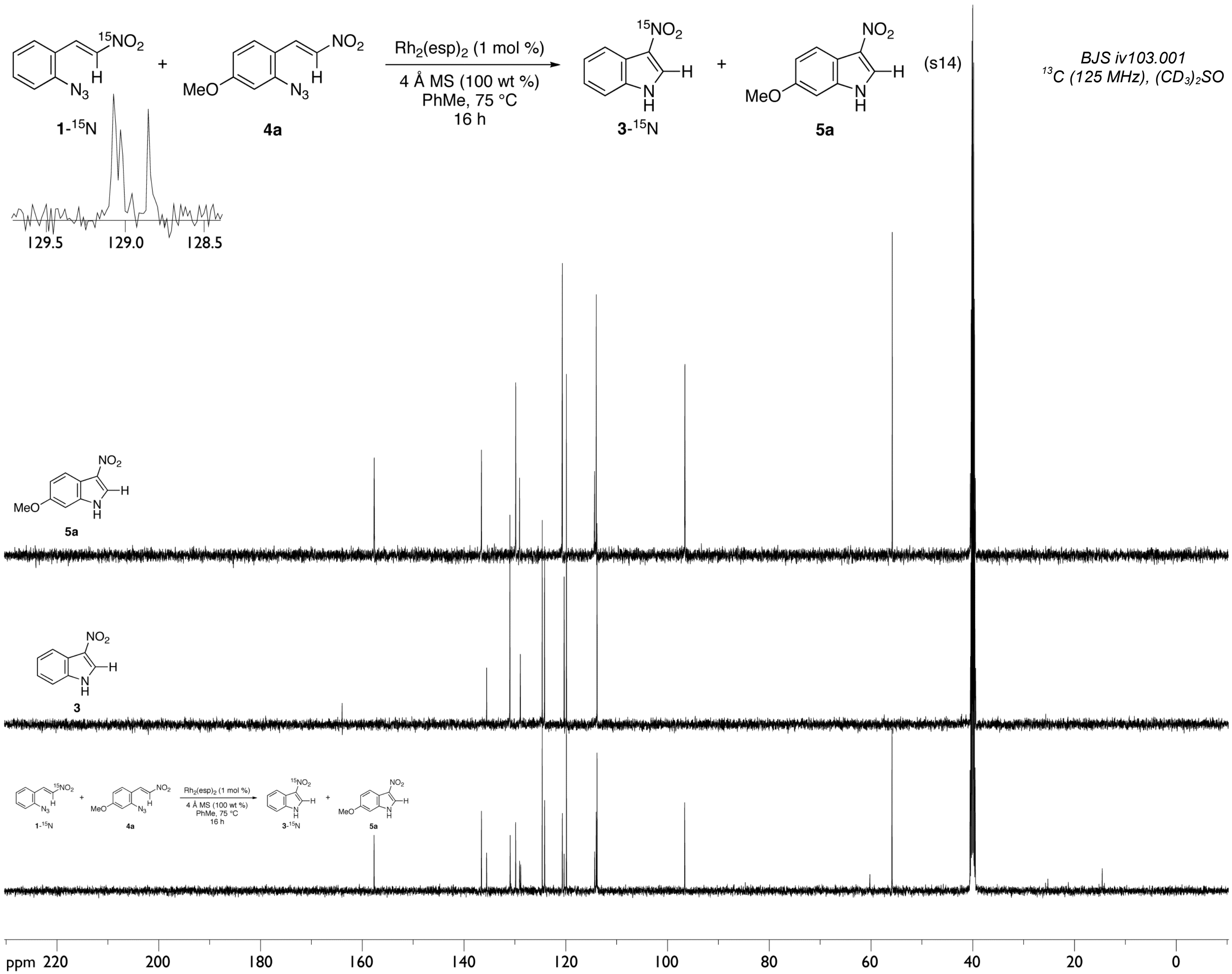
11d


SO2Ph
Ph
N
H
BJS iv163.0F2
13C (125 MHz), CDCl3
ppm 220
200
180
160
140
120
100
80
60
40
20
0

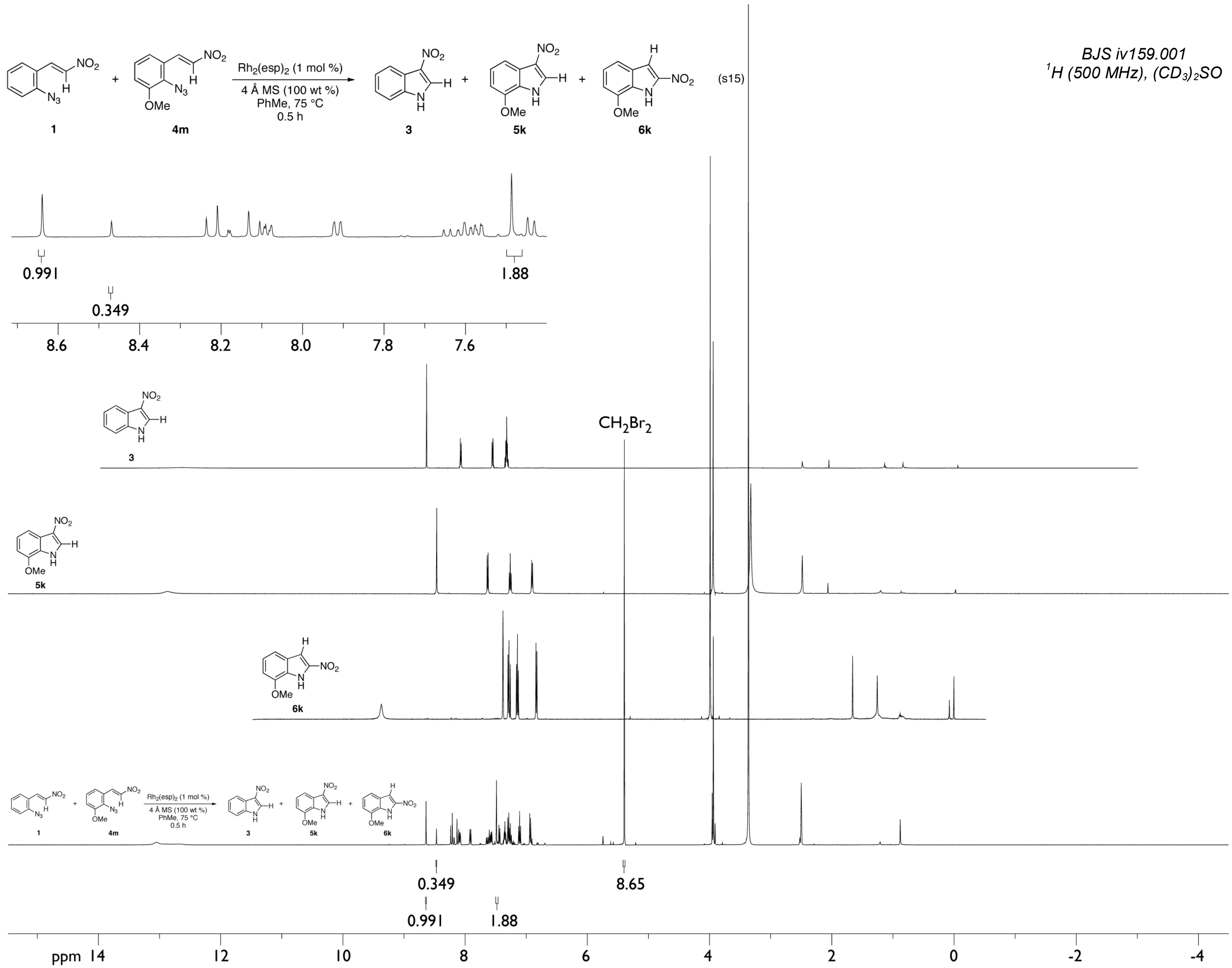
11e


NO2
Bz
N
H
BJS iv147.2F1
1H (500 MHz), (CD3)2SO
1.02
2.13
1.18
2.18
2.06
1.09
2.2
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
1
ppm 14
12
10
8
6
4
2
0
-2
-4


11e
NO2
Bz
N
H
BJS iv147.2F1
13C (125 MHz), (CD3)2SO
189
188
187
130
120
ppm 220
200
180
160
140
120
100
80
60
40
20
0



15NO2
NO2
Rh2(esp)2 (1 mol %)
4 Å MS (100 wt %)
PhMe, 75 °C
16 h
MeO
N3
H
1-15N
4a
3-15N
5a
(s14)
BJS iv103.001
13C (125 MHz), (CD3)2SO
129.5
129.0
128.5
5a
3
ppm 220
200
180
160
140
120
100
80
60
40
20
0



Rh2(esp)2 (1 mol %)
4 Å MS (100 wt %)
PhMe, 75 °C
0.5 h
(s15)
BJS iv159.001
1H (500 MHz), (CD3)2SO
0.991
0.349
1.88
CH2Br2
8.65
ppm