

Supplementary information for:

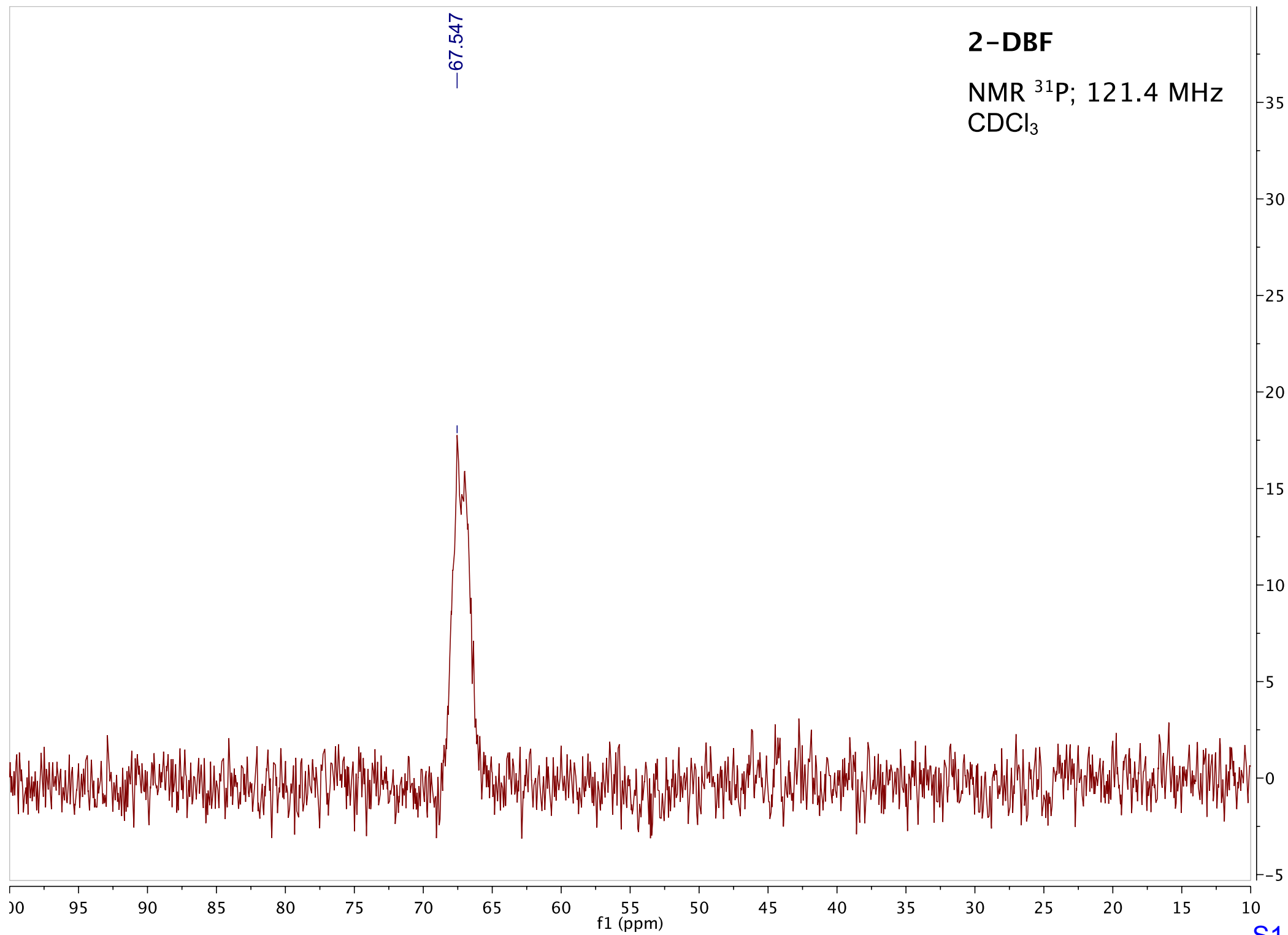
Ruthenium complexes of *P*-stereogenic phosphines with a heterocyclic substituent

Pau Clavero,^a Arnald Grabulosa,^{*a} Mercè Rocamora,^a Guillermo Muller,^a and Mercè
Font-Bardia^b

^aDepartament de Química Inorgànica i Orgànica, Secció d'Inorgànica, Universitat de Barcelona, Martí i
Franquès, 1-11, E-08028, Barcelona, Spain; ^bDepartament de Cristal·lografia, Mineralogia i Dipòsits
Minerals, Universitat de Barcelona, Martí i Franquès, s/n, E-08028, Barcelona, Spain

Table of contents

NMR spectra of 2	S1
NMR spectra of 3	S15
NMR spectra of 4	S27
NMR spectra of L	S54
NMR spectra of Ru	S91
NMR spectra of Ru*	S138
NMR spectra of Ru'	S151



2-DBF

NMR ^1H ; 400 MHz

CDCl_3

7.483
7.435
7.394
7.388
7.363
7.344
7.338
7.336
7.307
7.262
7.260
7.249

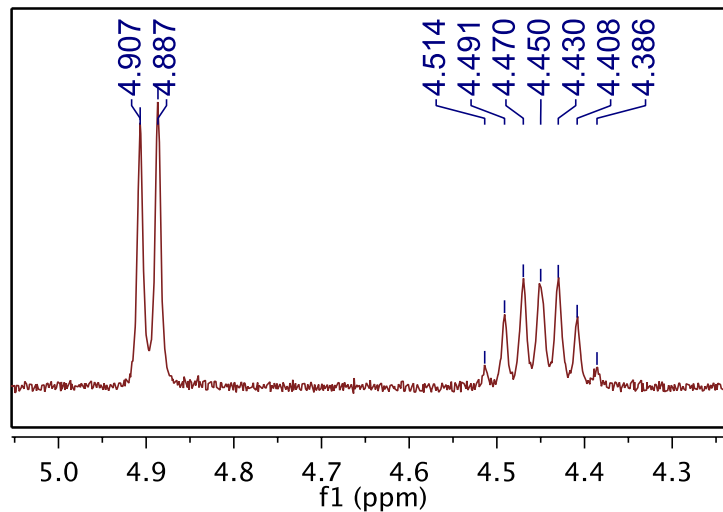
3.747

2.640
2.613

1.853

1.301
1.279

0.004
0.001



THF

THF

0.90
1.45
1.06
0.64
15.80

1.00
1.12

2.86

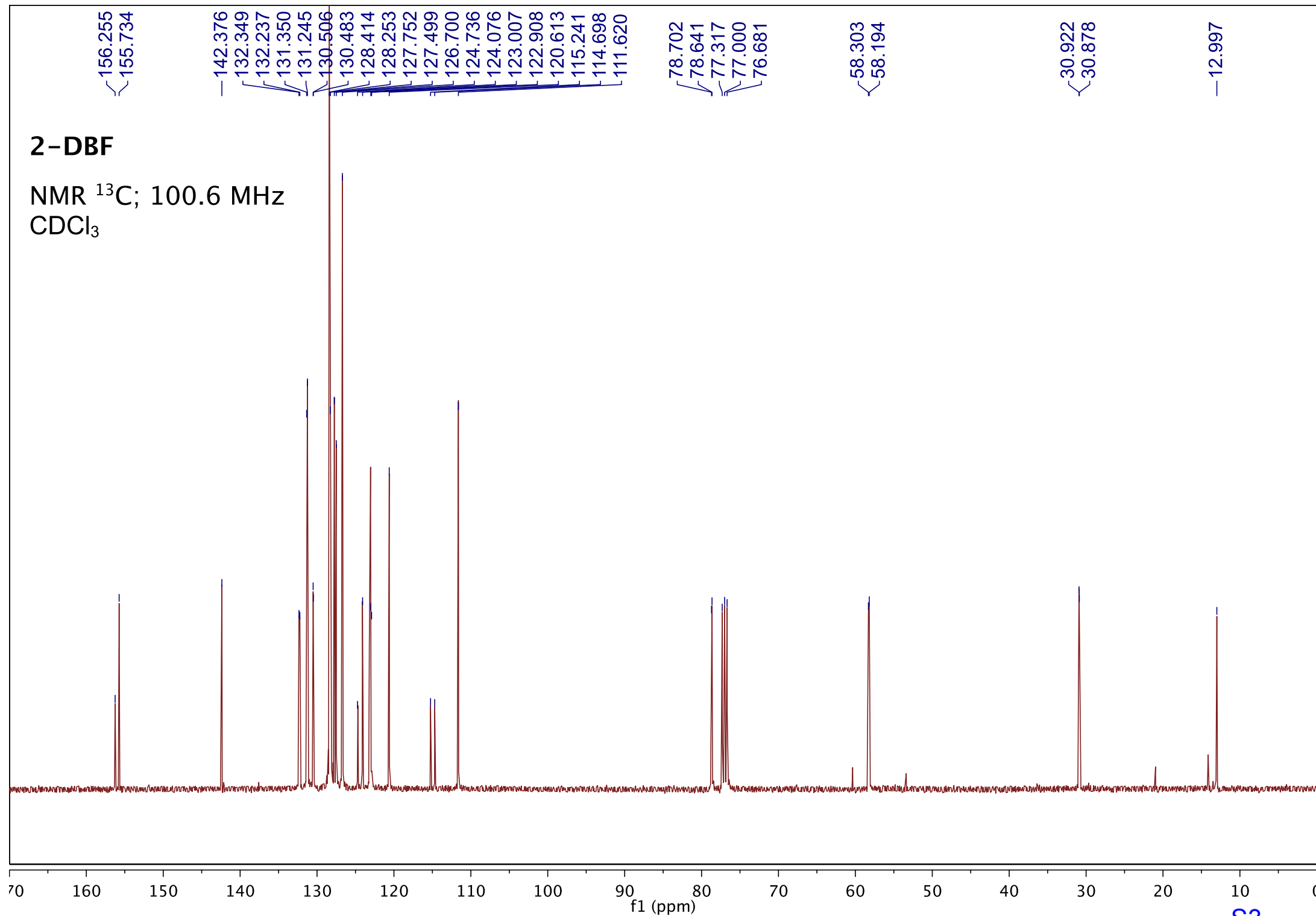
3.65

S2

2-DBF

NMR ^{13}C ; 100.6 MHz

CDCl_3



2-DBT

NMR ^{31}P ; 121.4 MHz

CDCl_3

—70.060

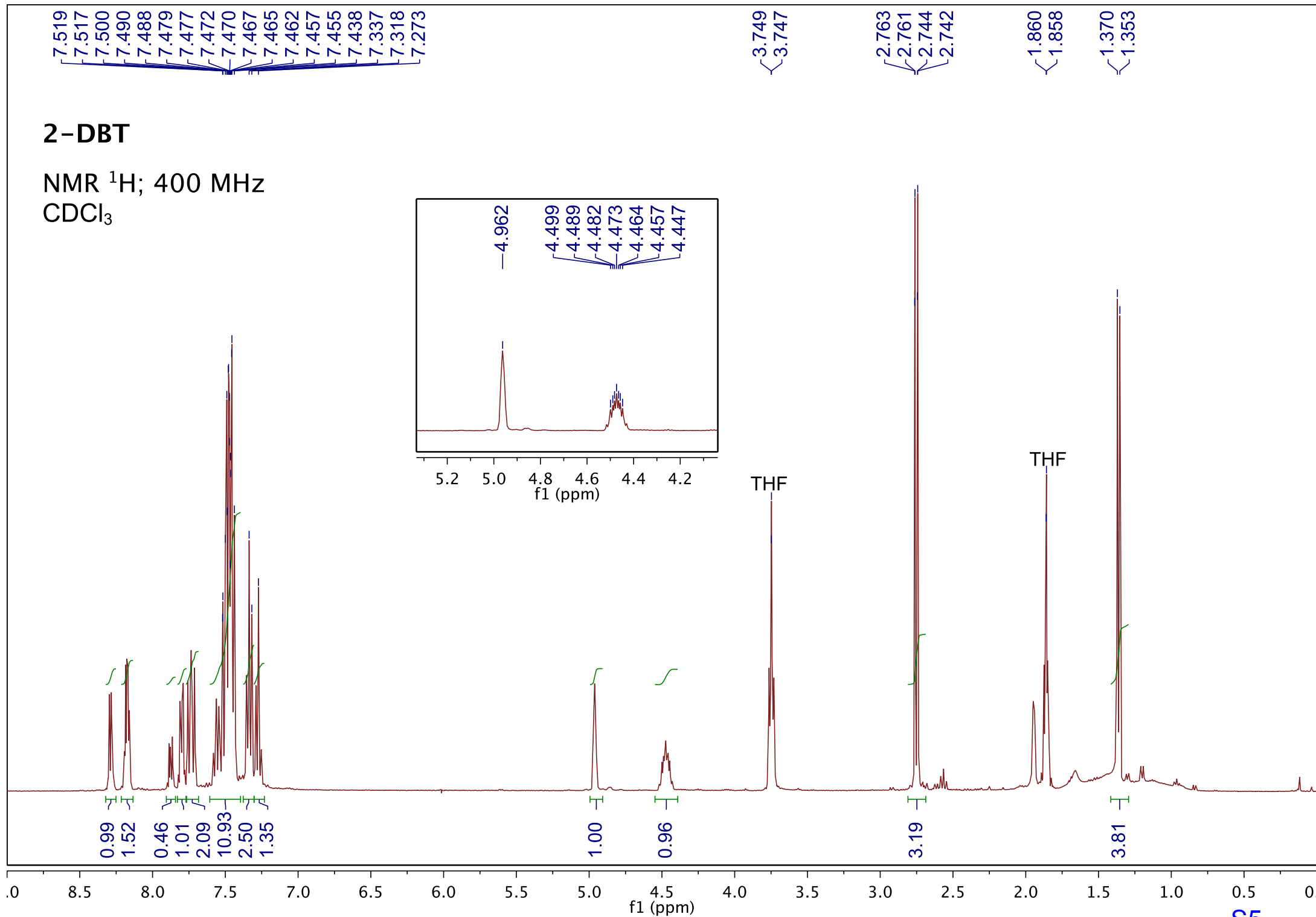
60 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)

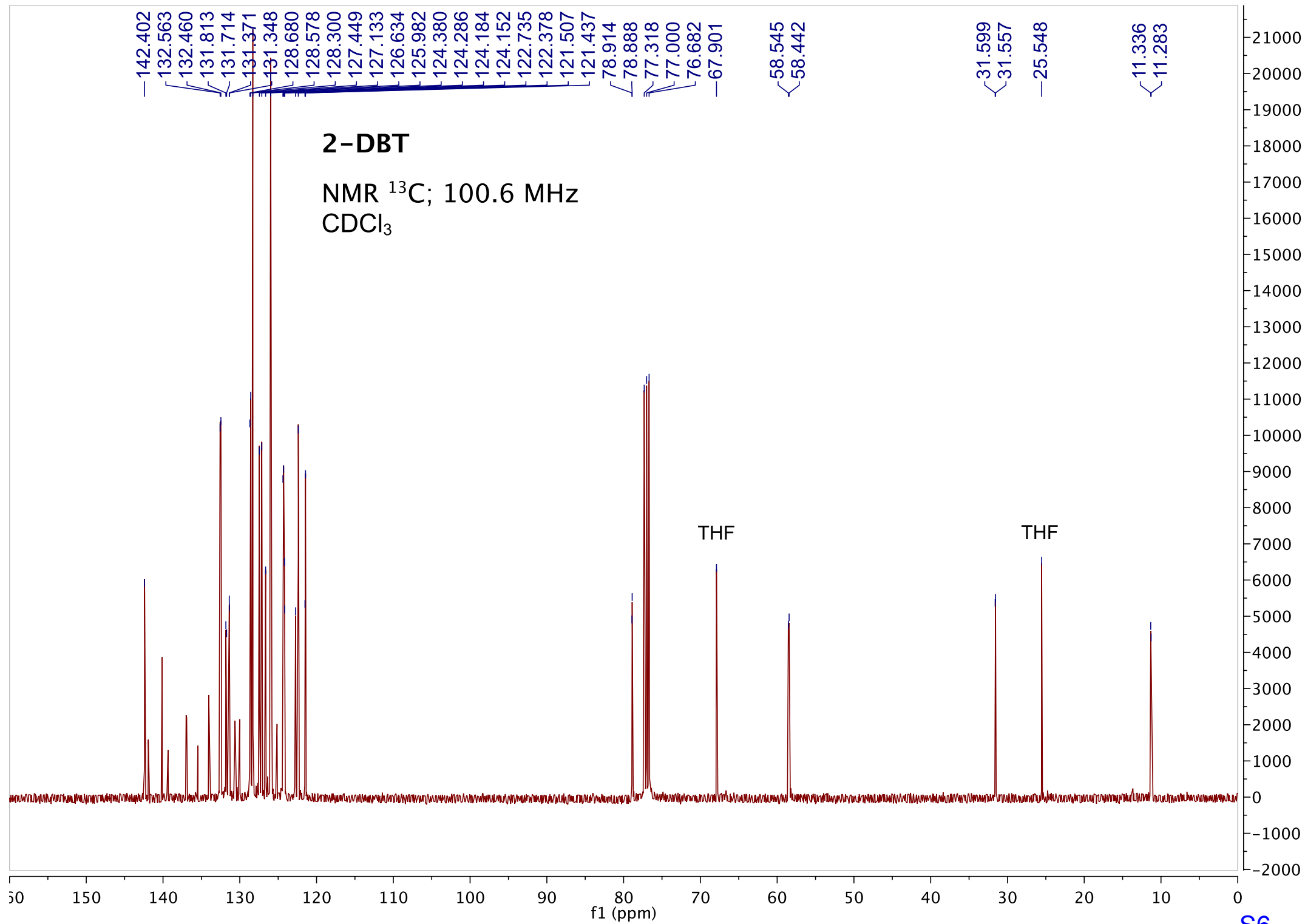
S4

2-DBT

NMR ^1H ; 400 MHz

CDCl_3

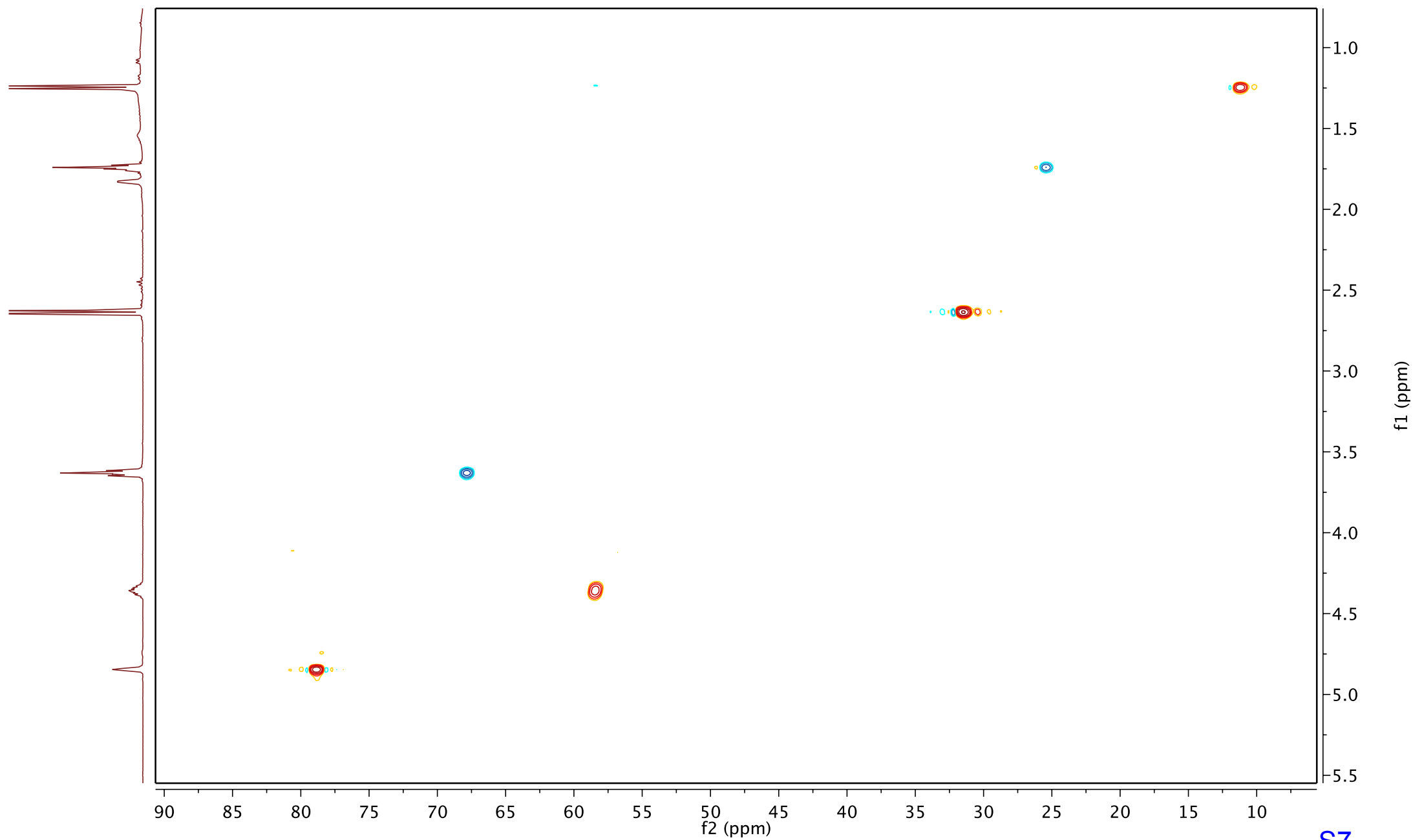




2-DBT

gHSQC 400MHz

CDCl₃

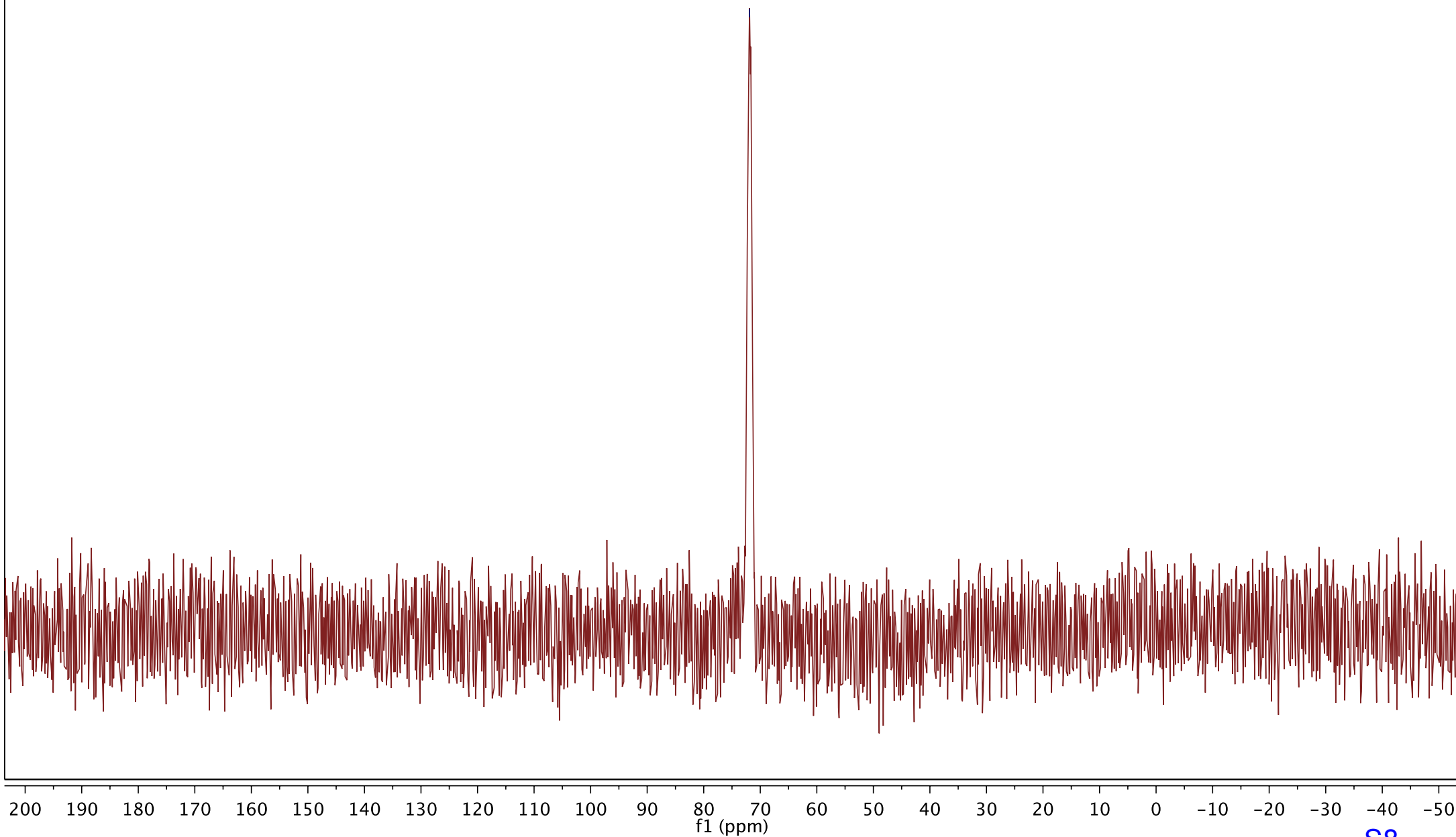


2-TA

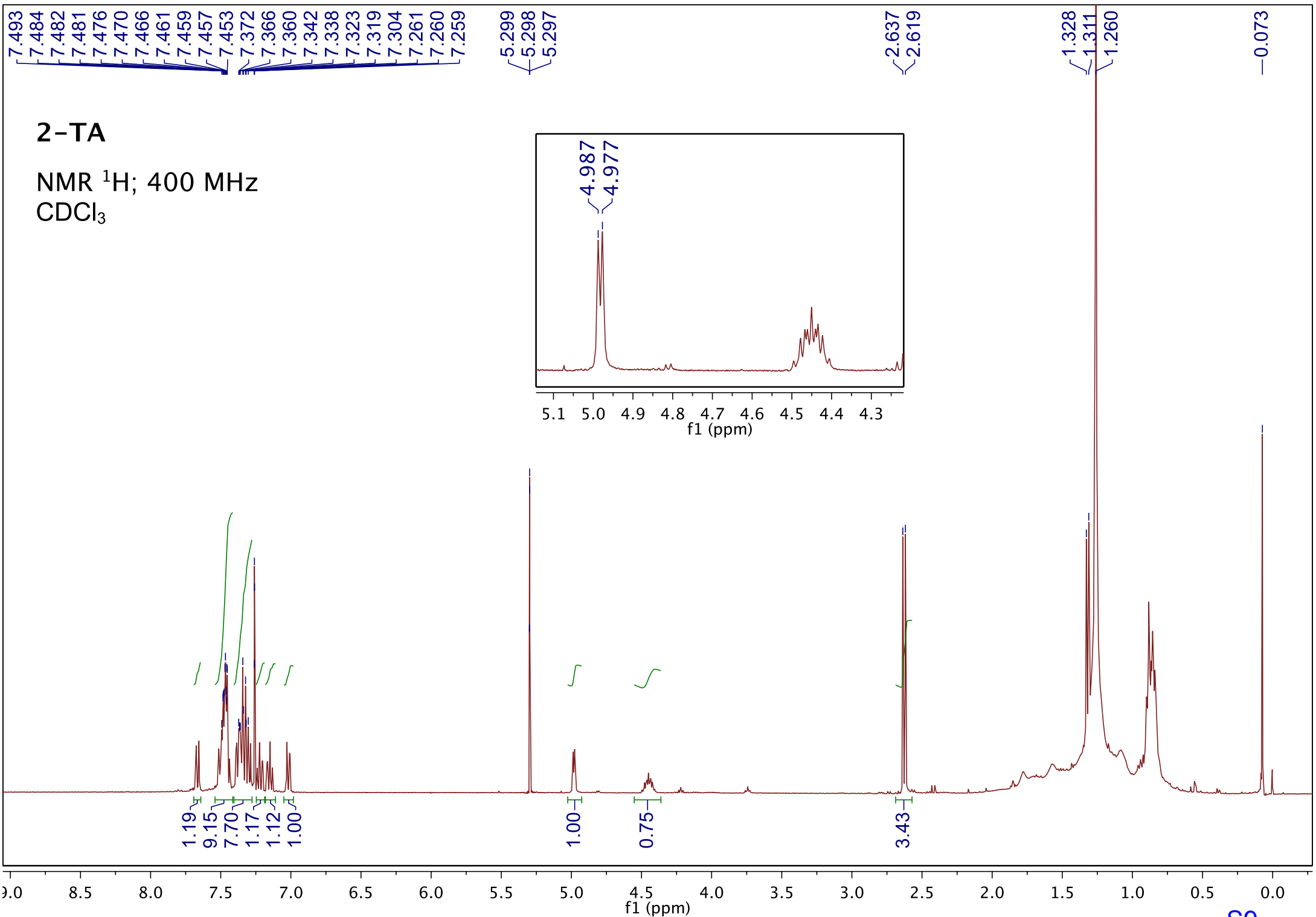
NMR ^{31}P ; 161.9 MHz

CDCl_3

-71.886



S8



2-TA

NMR ^{13}C ; 100.6 MHz

CDCl_3

142.469
131.802
131.698
131.644
130.723
129.438
128.633
128.529
128.395
127.911
127.716
127.573
126.168

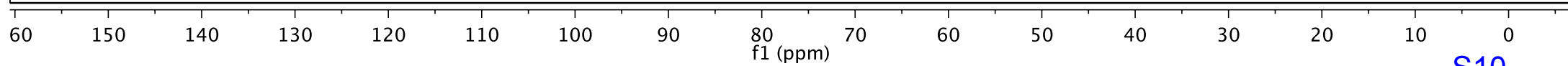
79.032
77.318
77.000
76.683

58.440
58.334

31.927
31.393
29.701
29.363

22.693

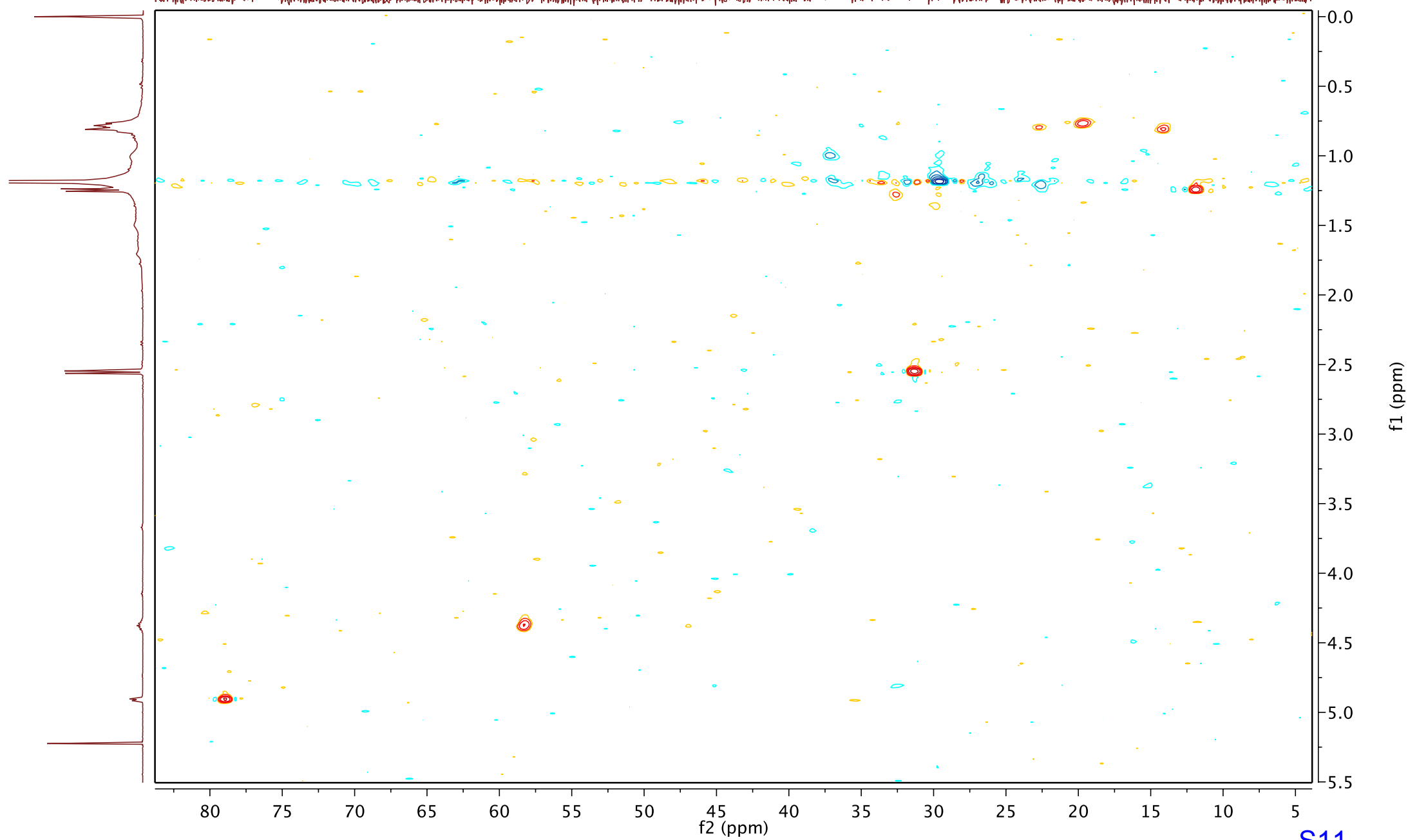
14.121
12.047



2-TA

gHSQC 400MHz

CDCl₃

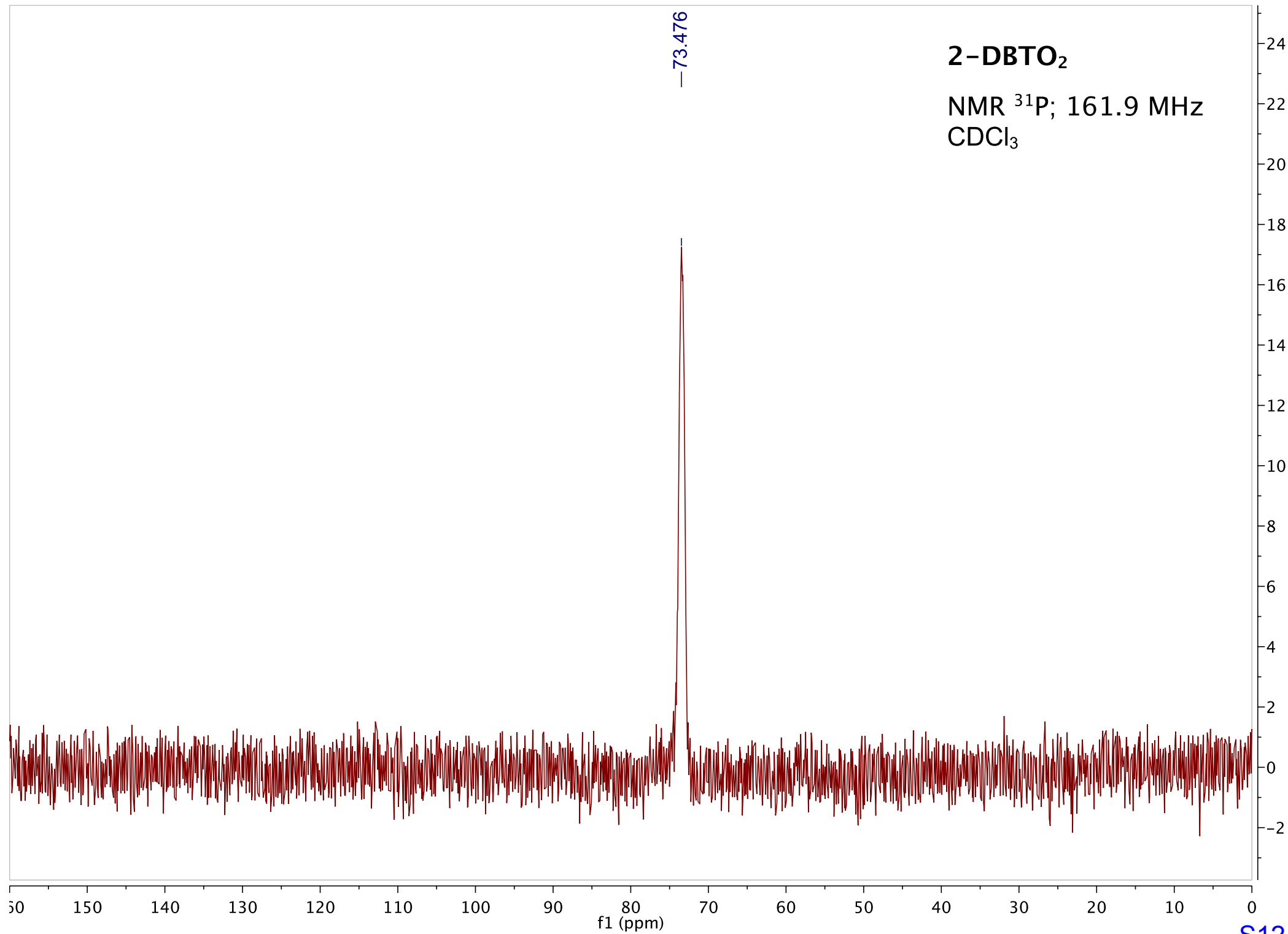


2-DBTO₂

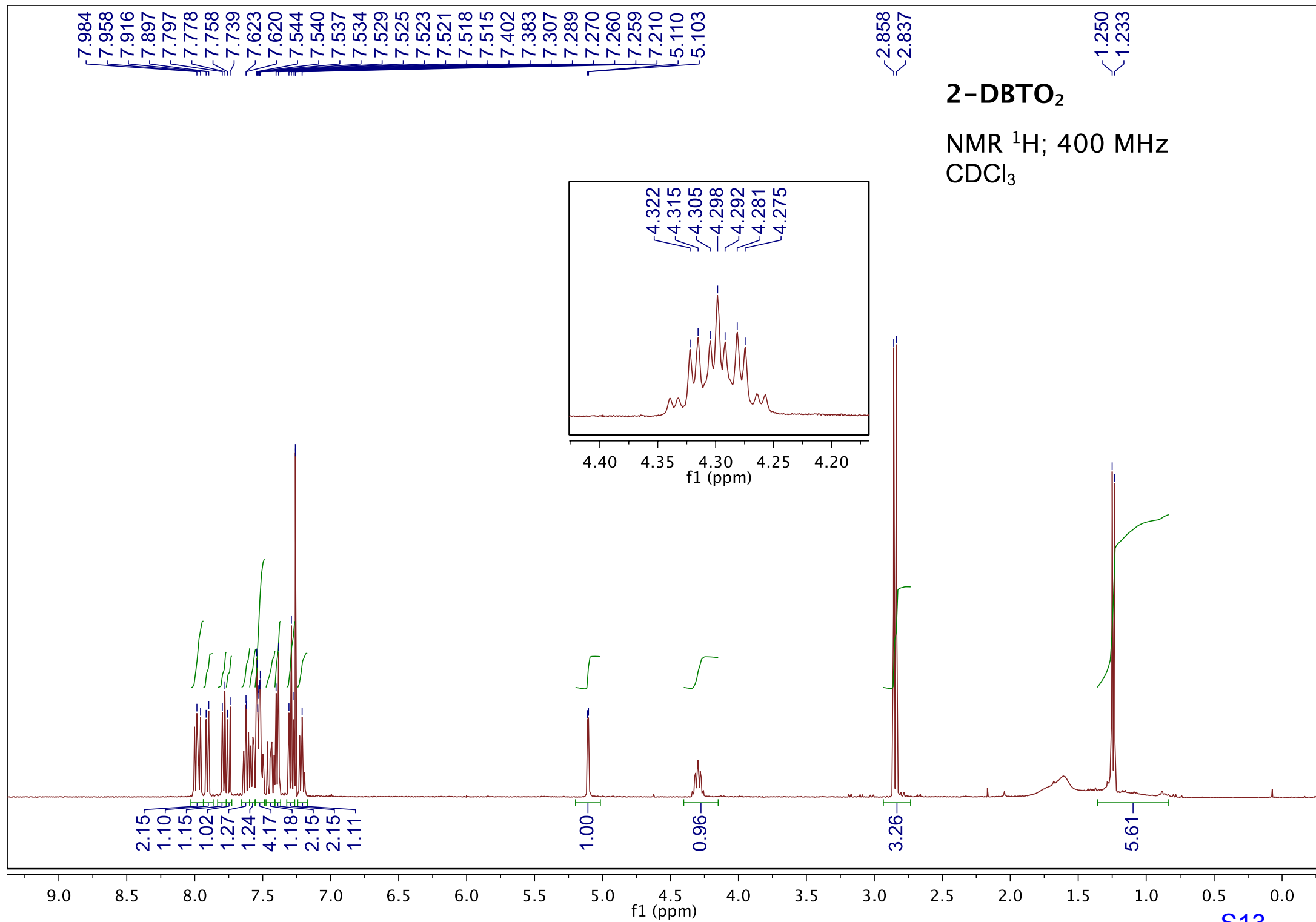
NMR ³¹P; 161.9 MHz

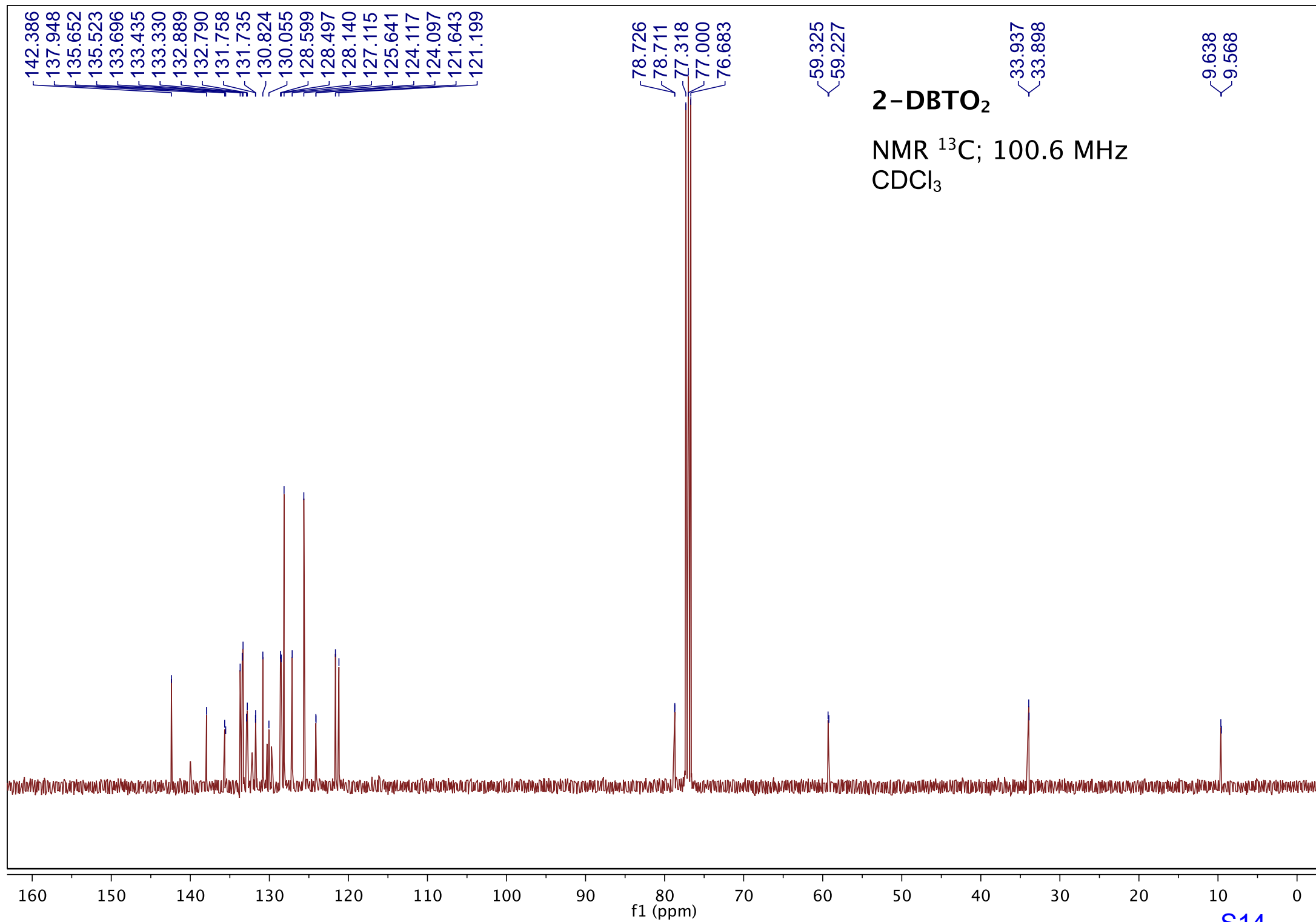
CDCl₃

-73.476



S12



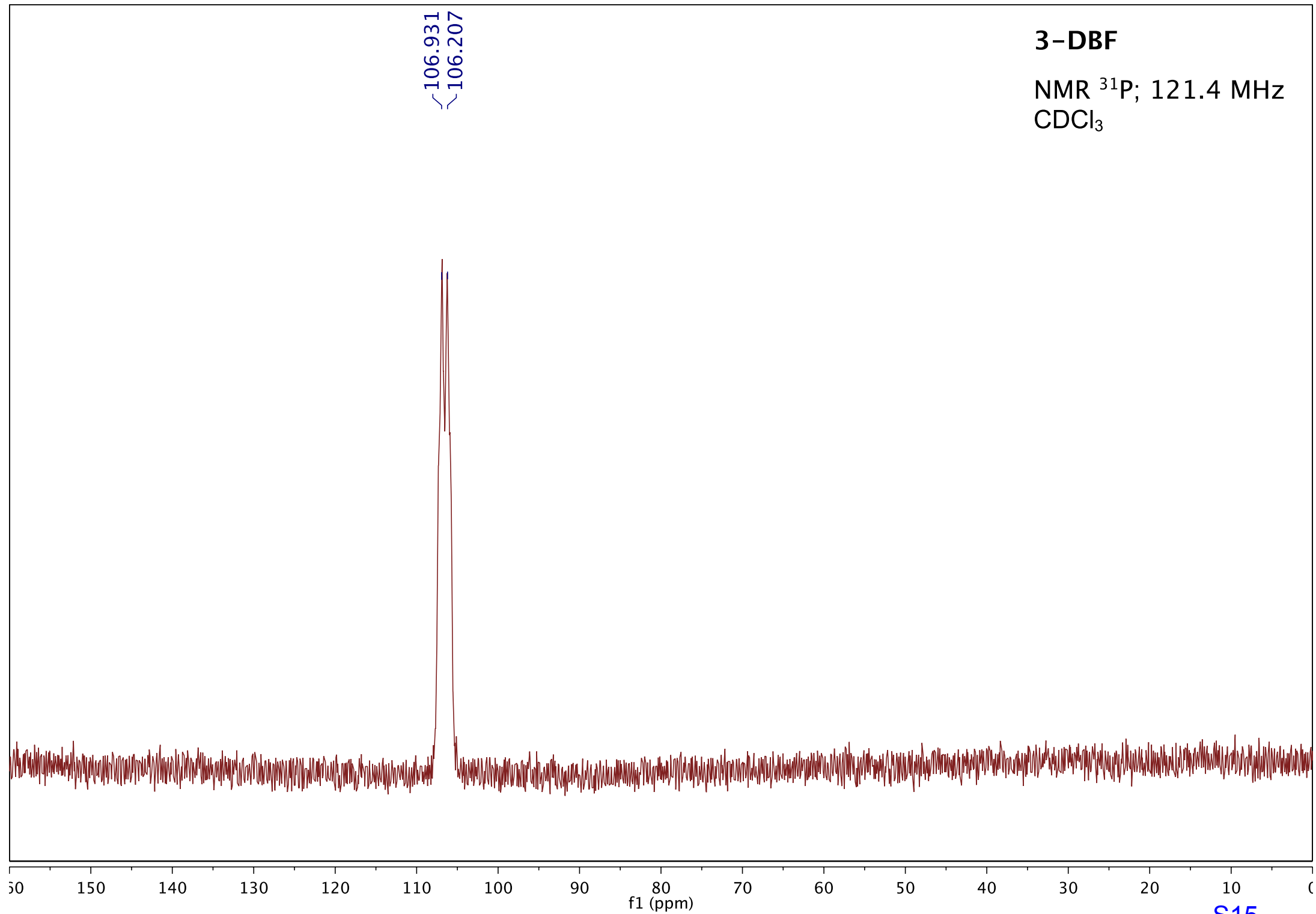


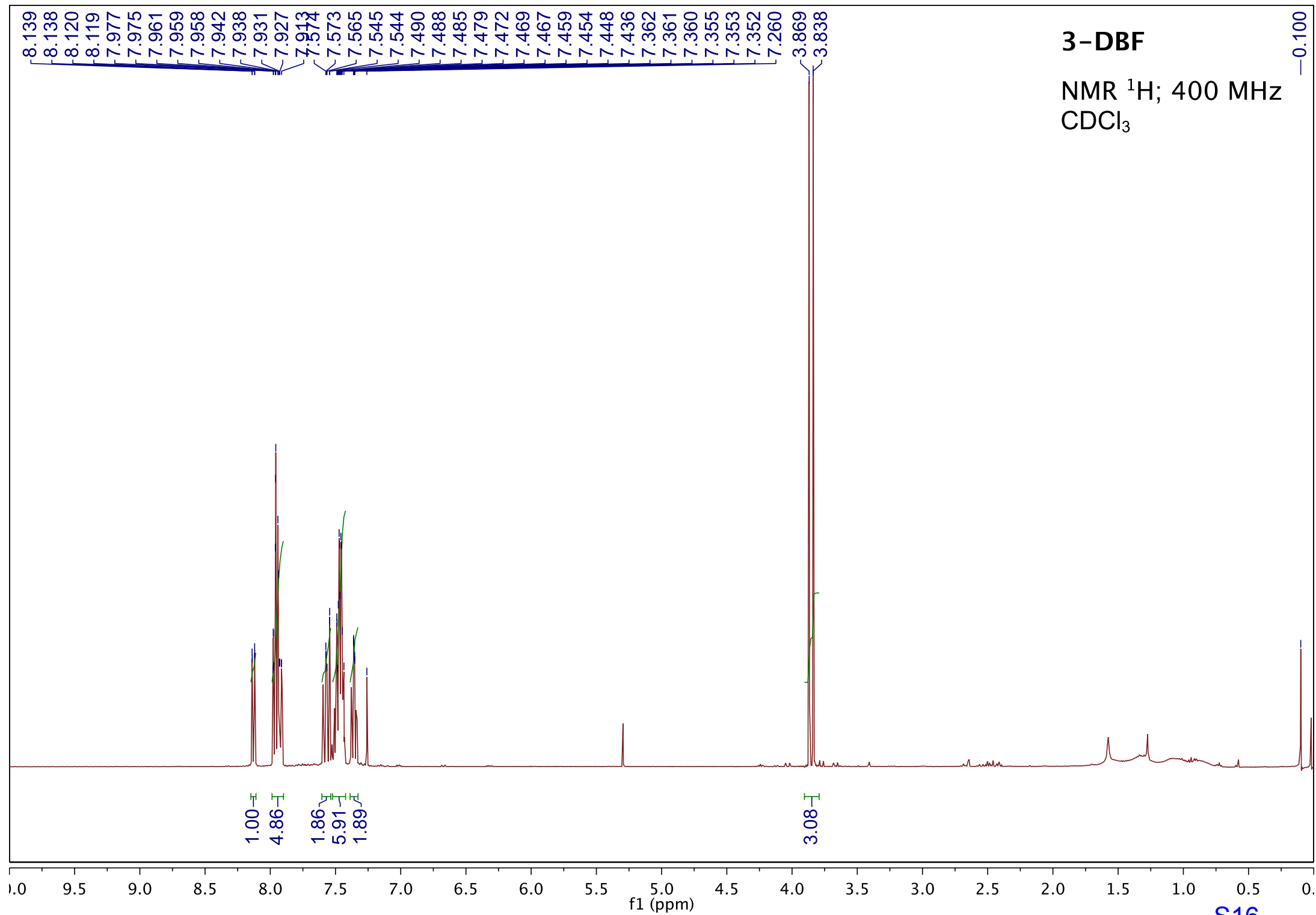
3-DBF

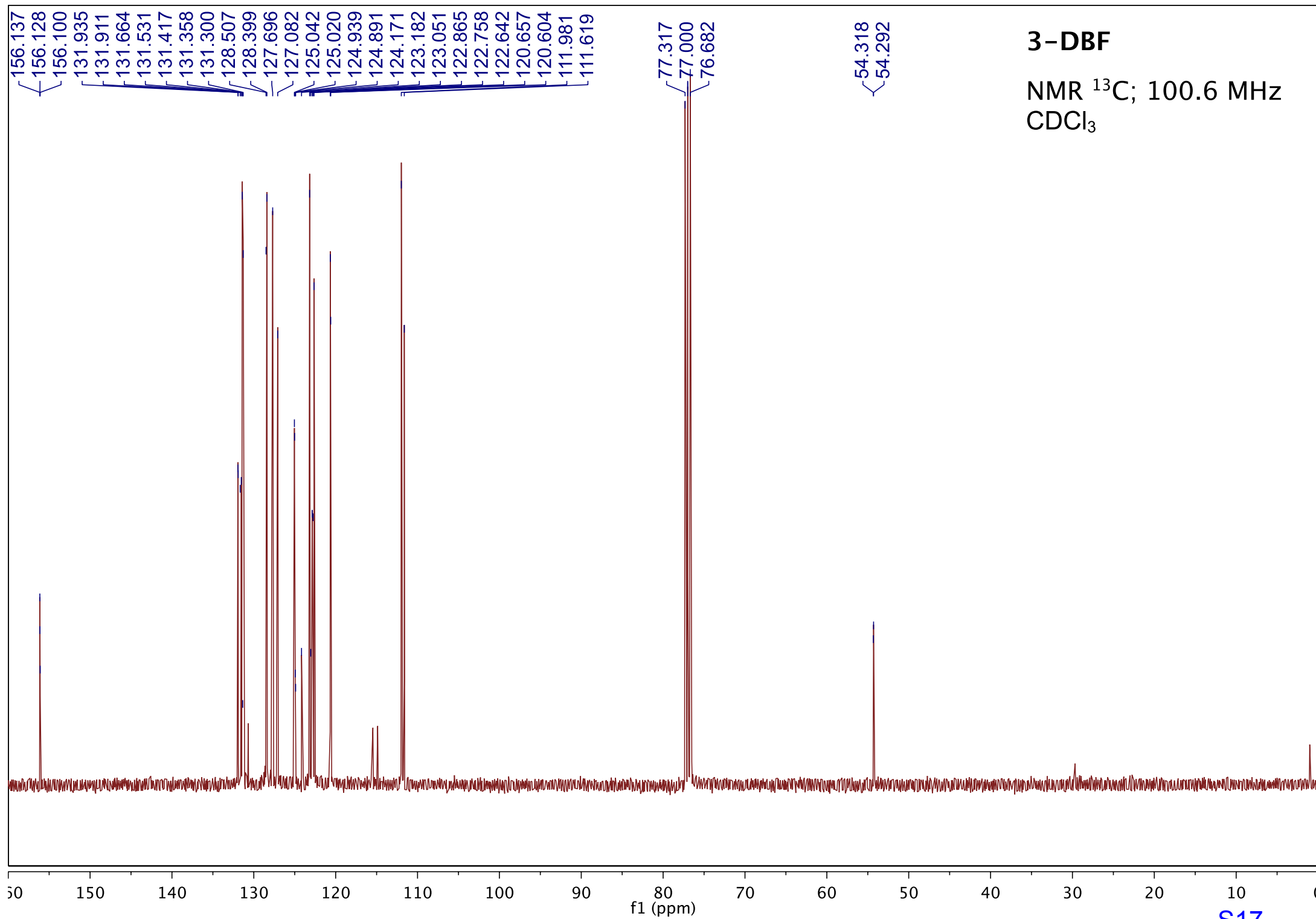
NMR ^{31}P ; 121.4 MHz

CDCl_3

106.931
106.207





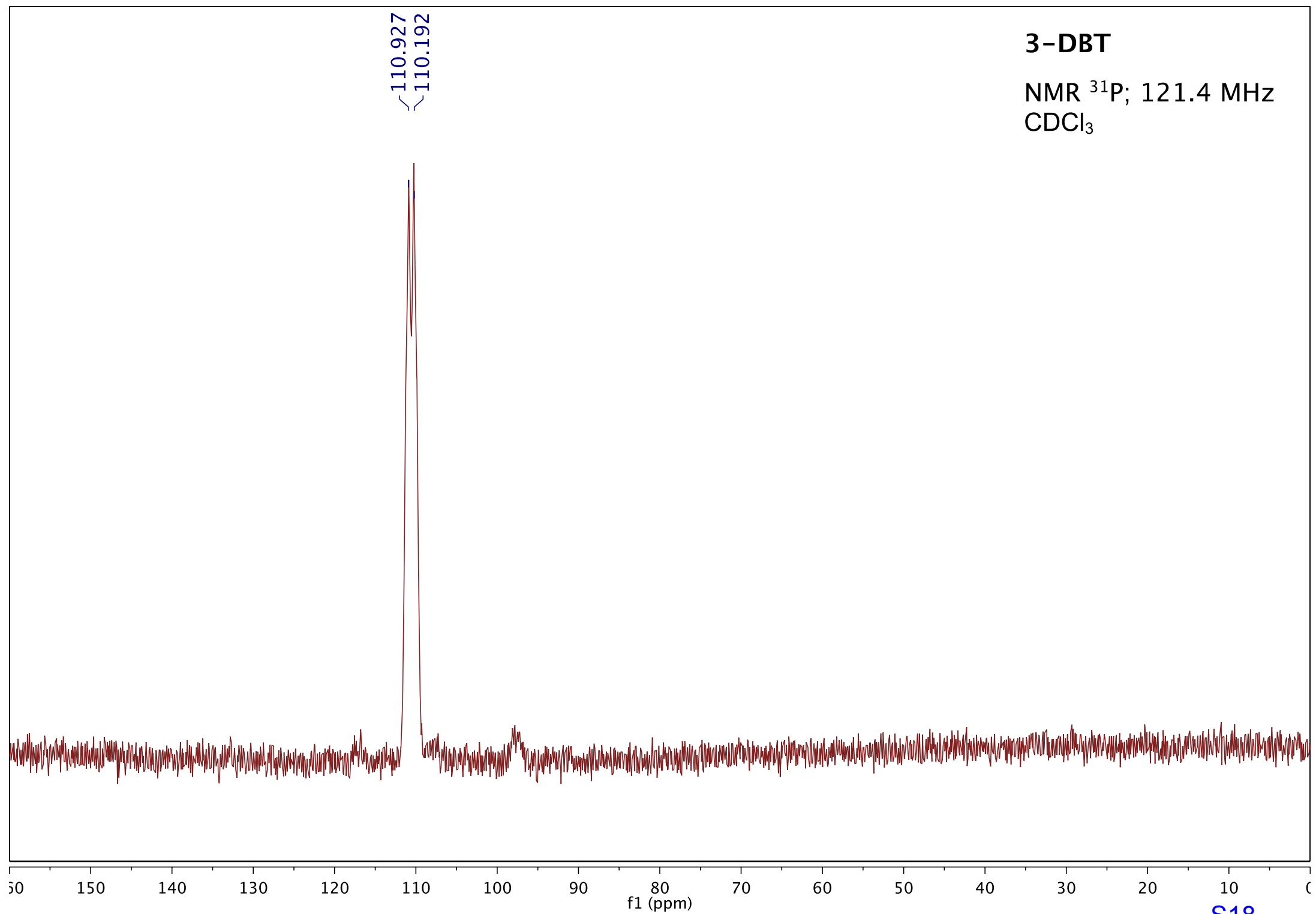


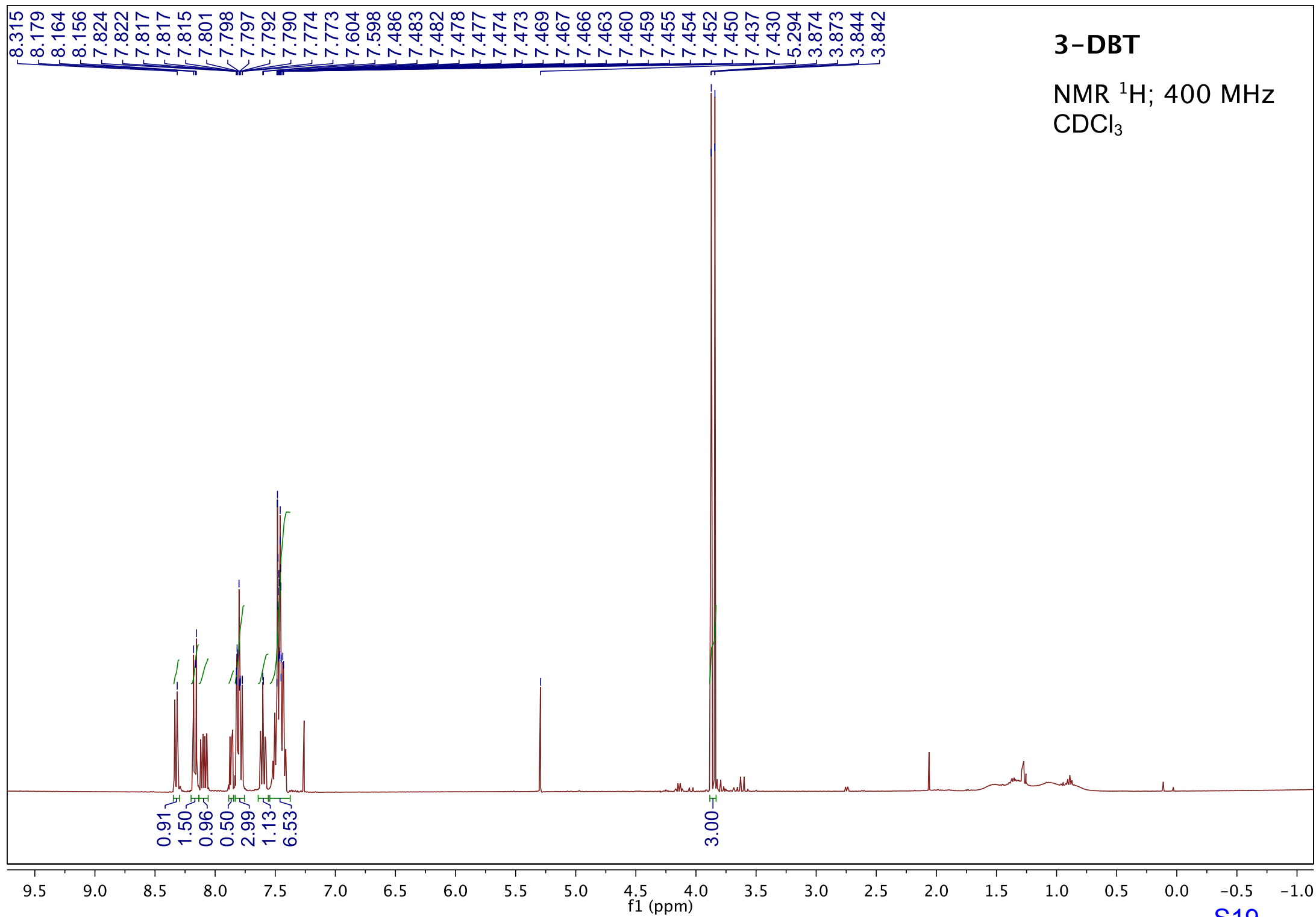
3-DBT

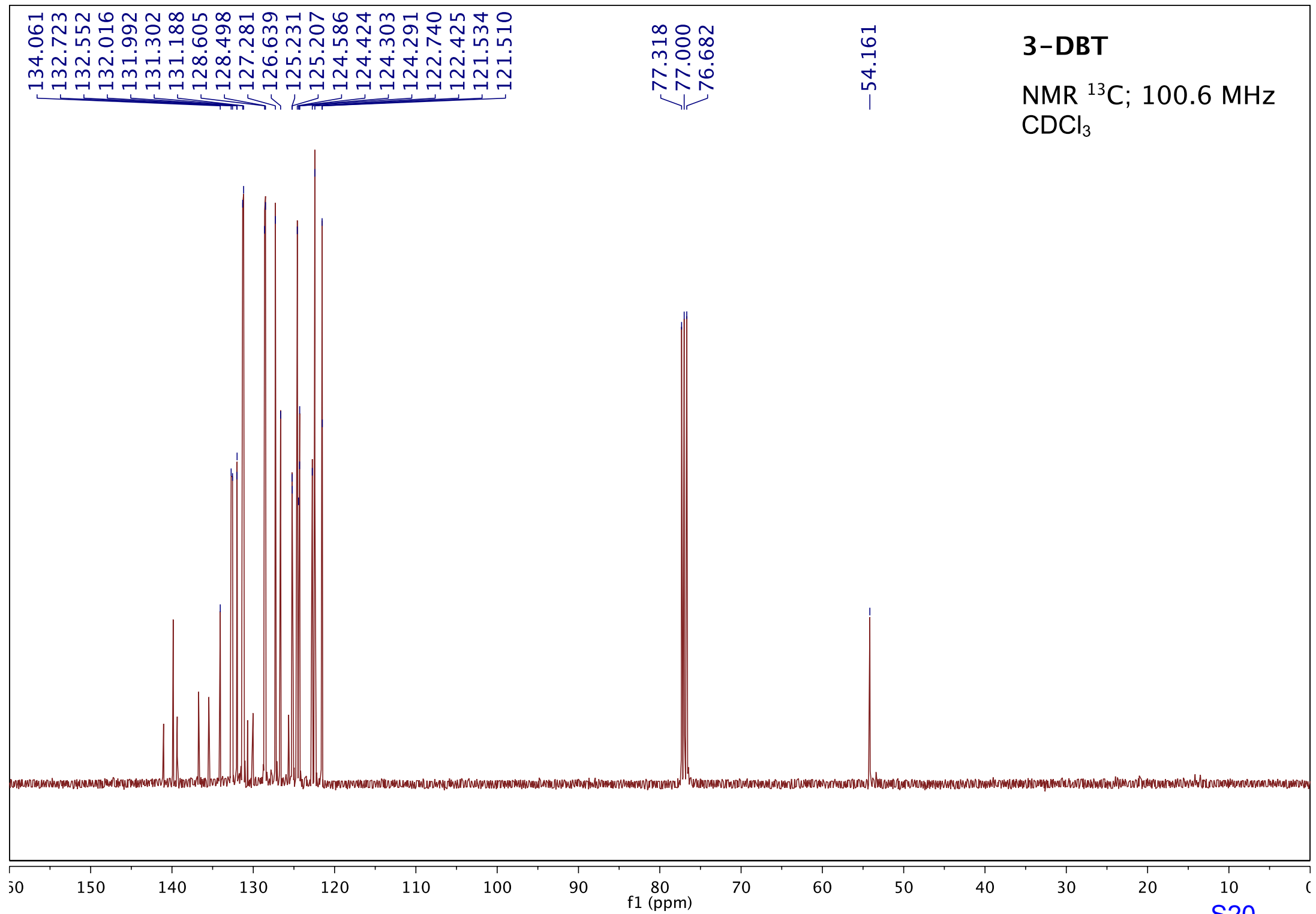
NMR ^{31}P ; 121.4 MHz

CDCl_3

110.927
110.192



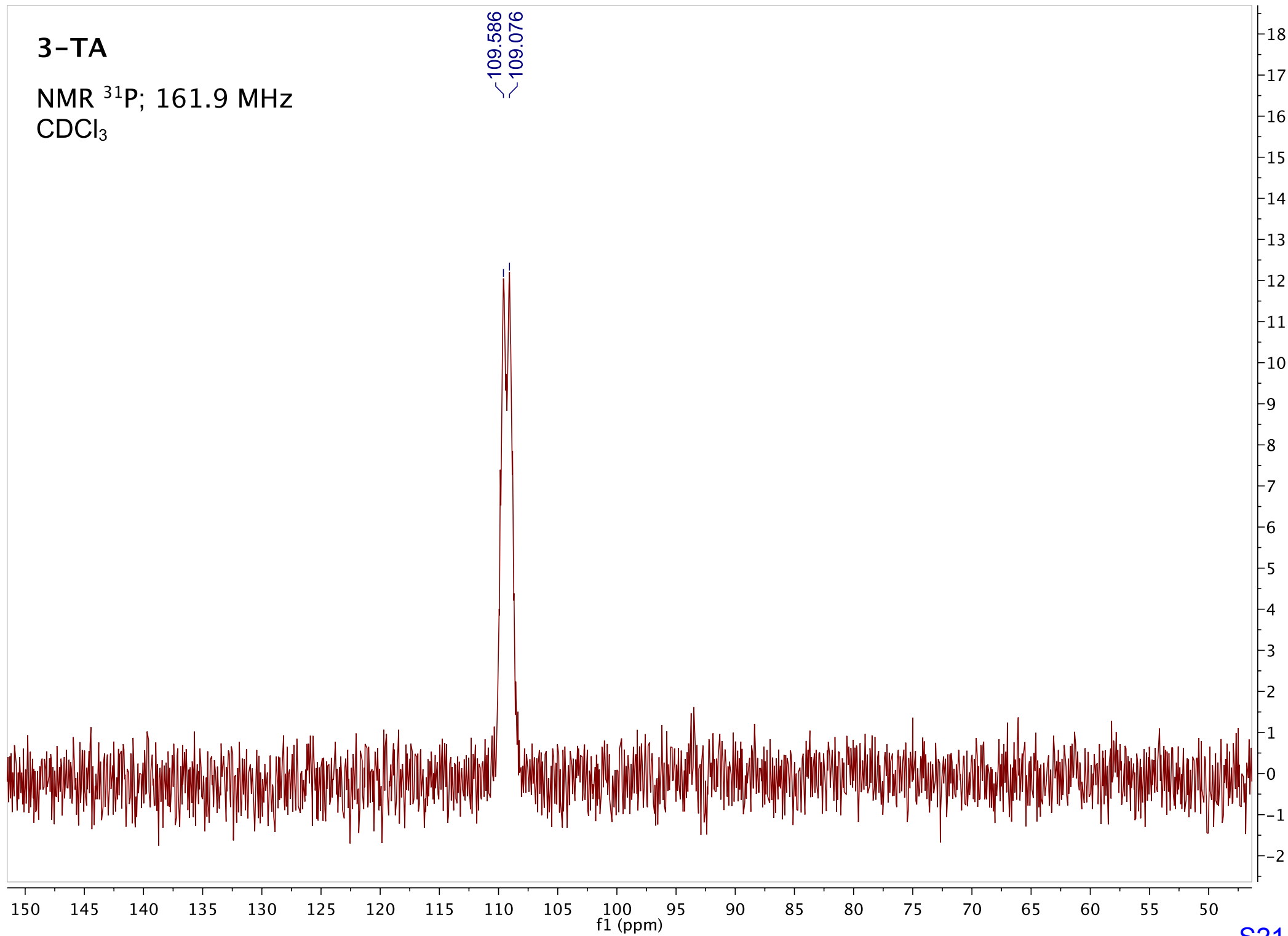


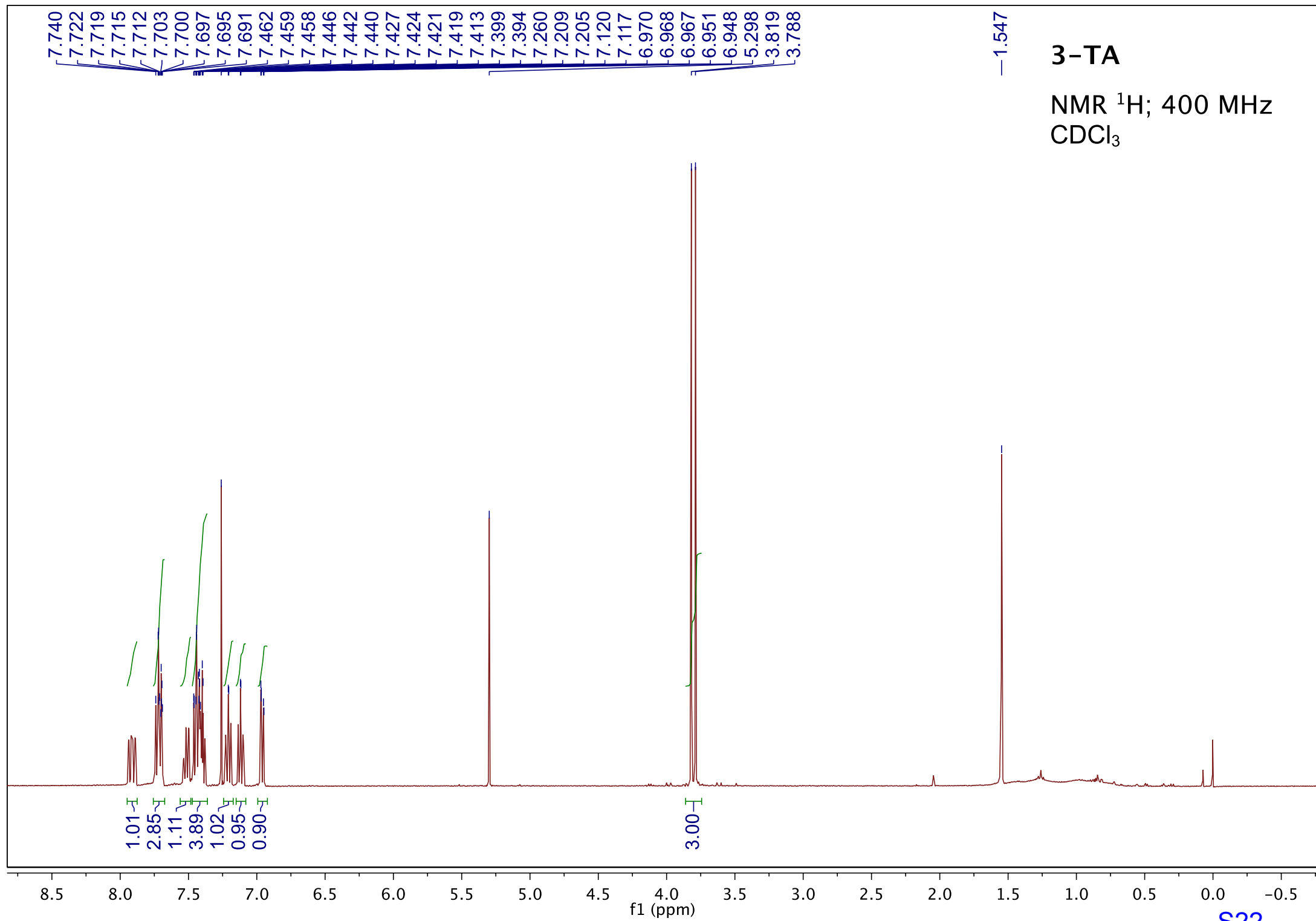


3-TA

NMR ^{31}P ; 161.9 MHz

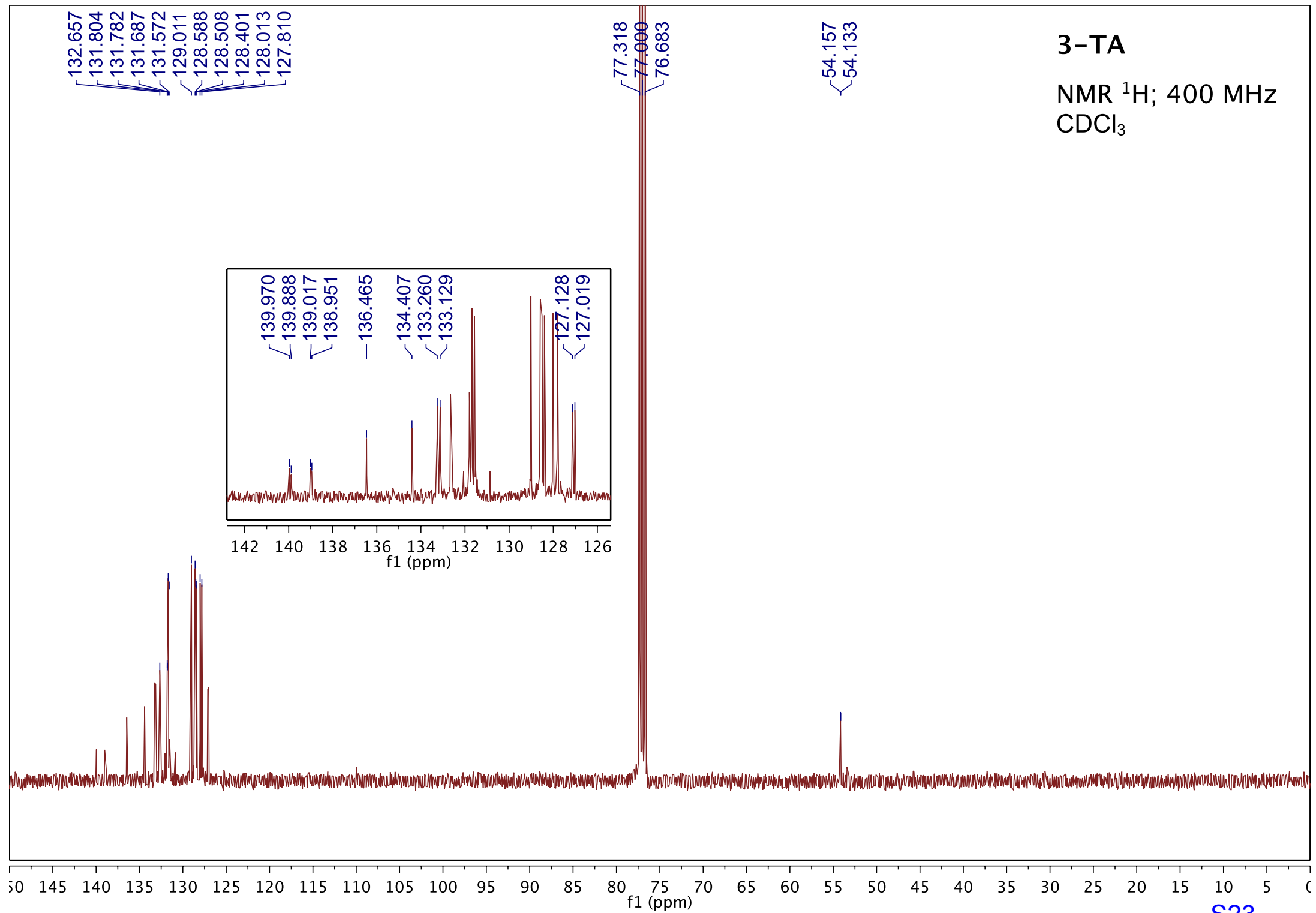
CDCl_3

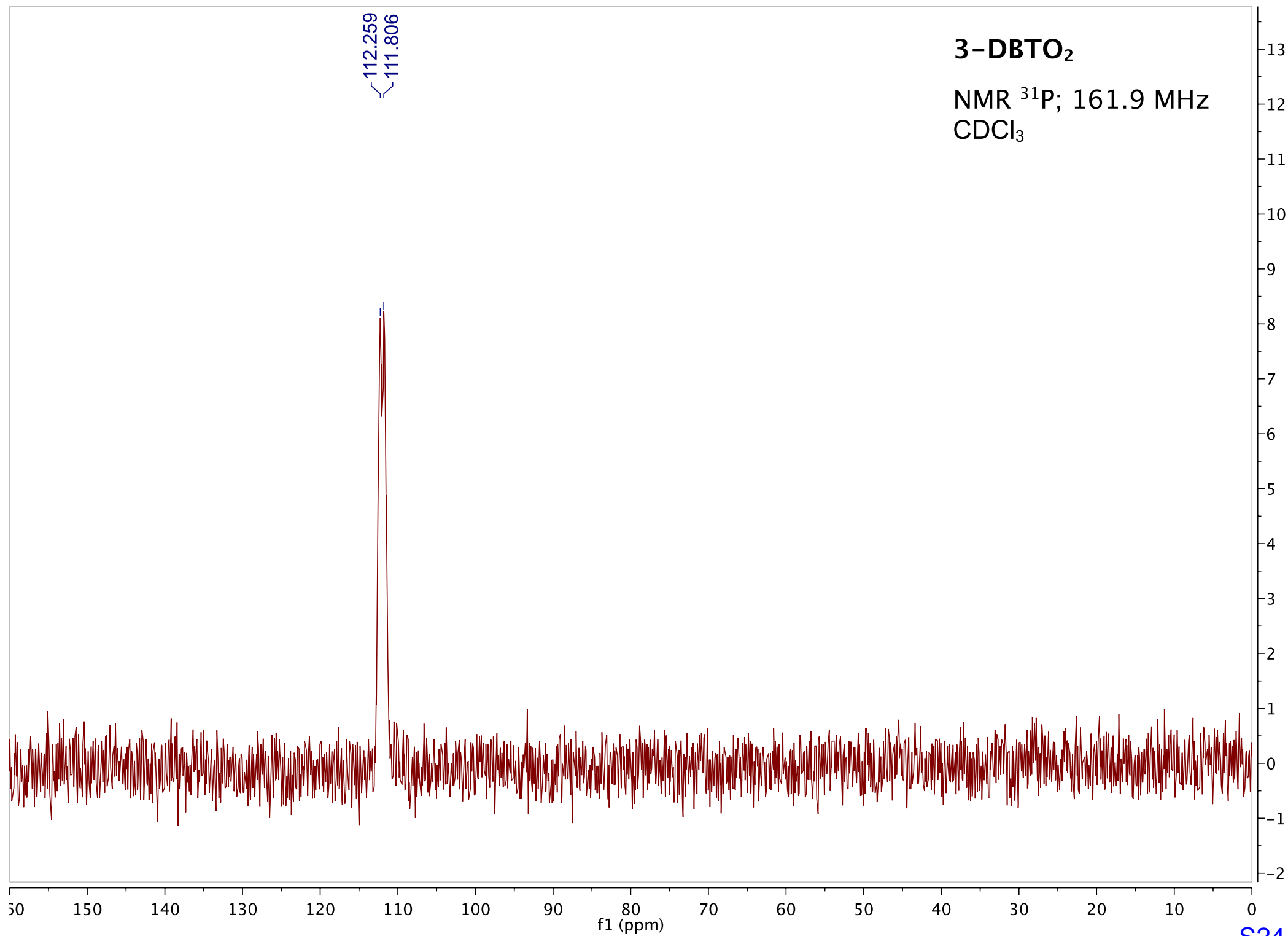


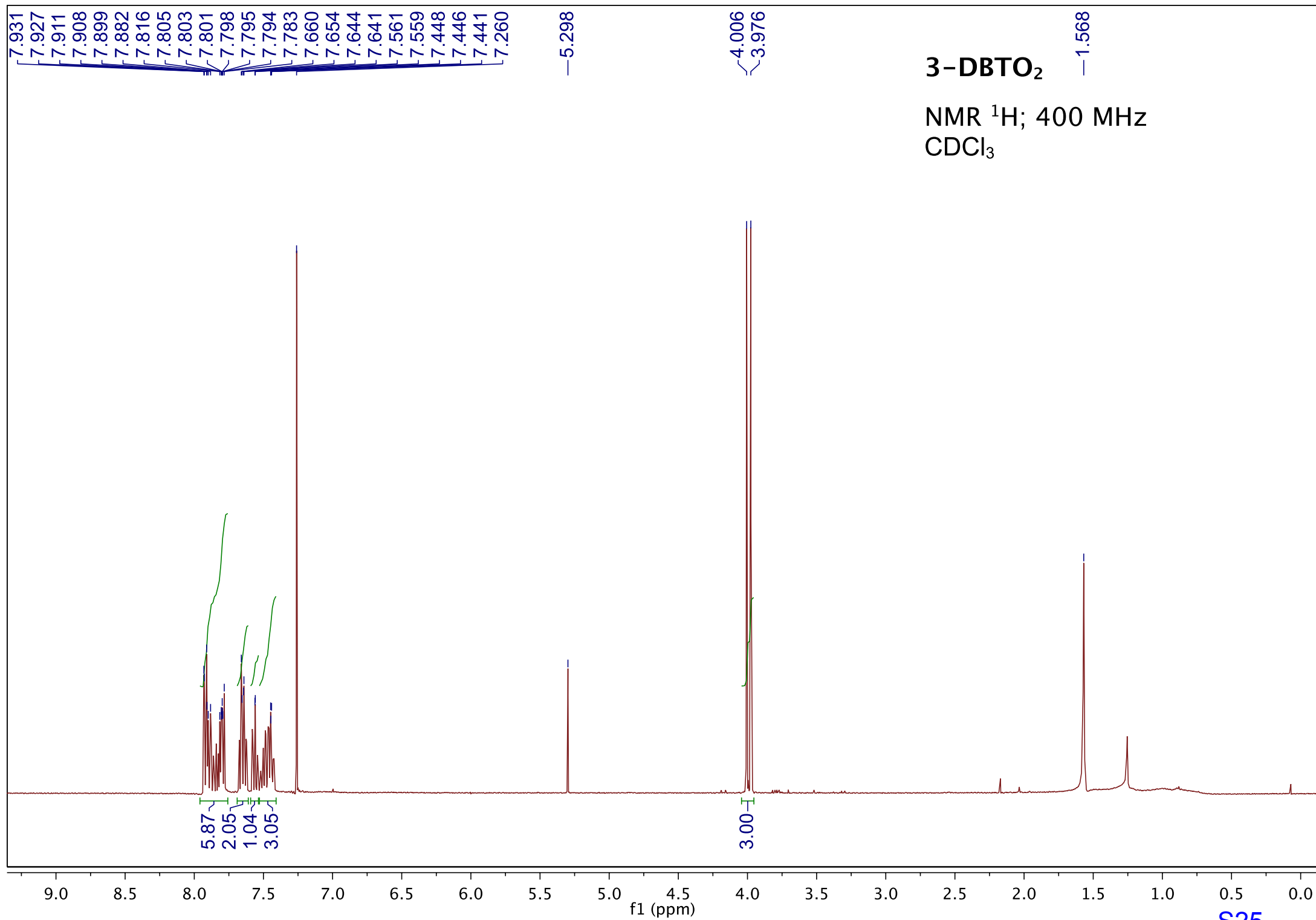


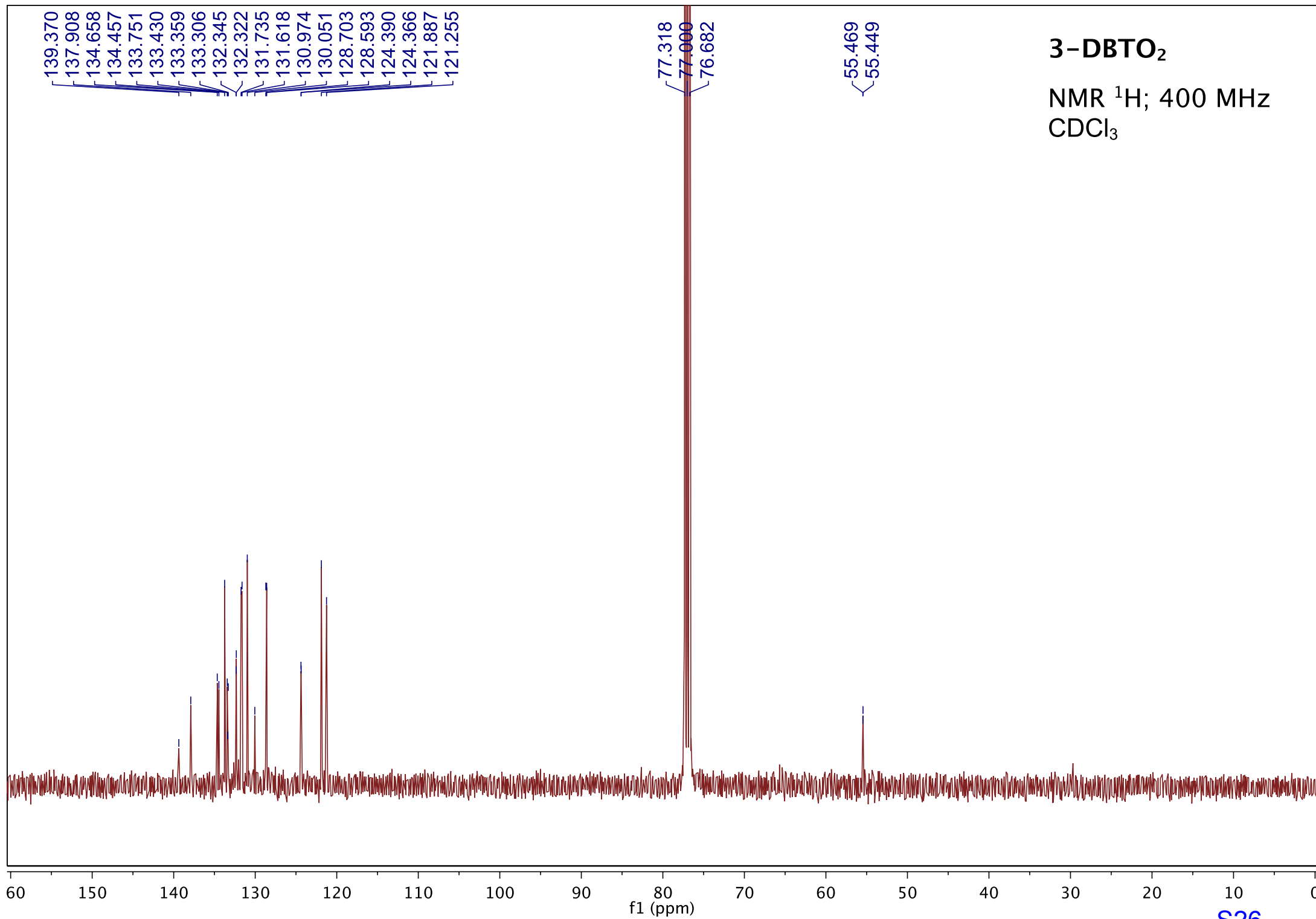
3-TA

NMR ^1H ; 400 MHz
 CDCl_3







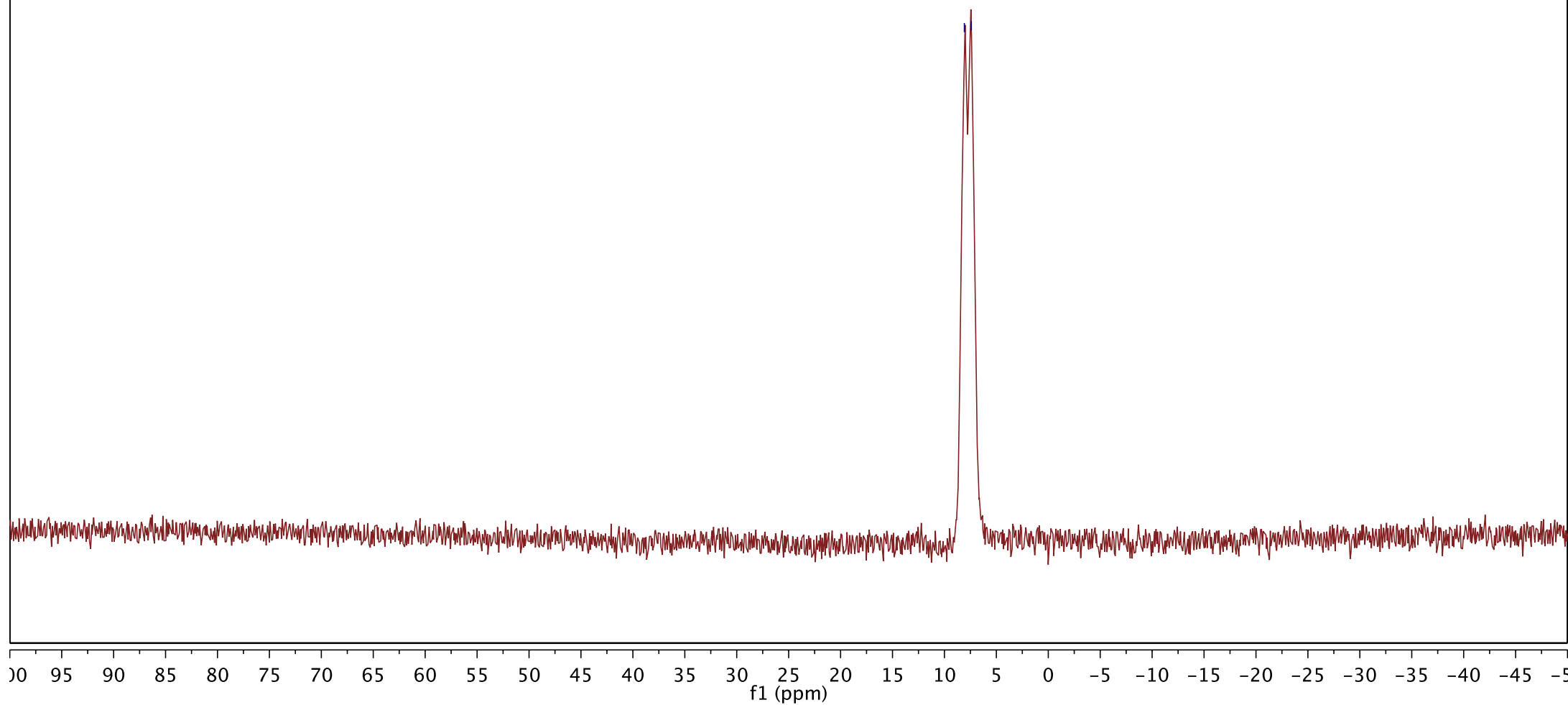


4-DBF-Me

NMR ^{31}P ; 121.4 MHz

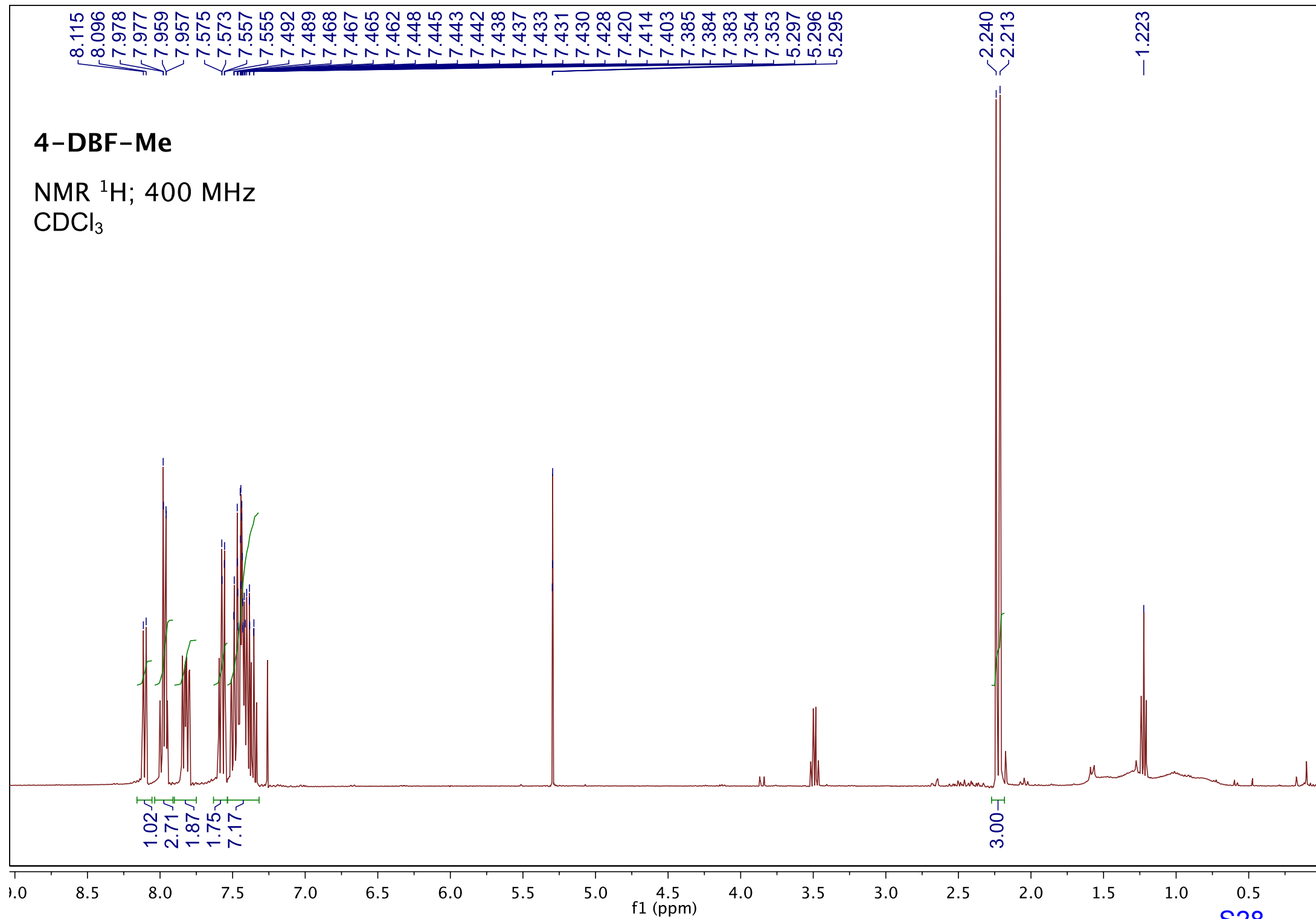
CDCl_3

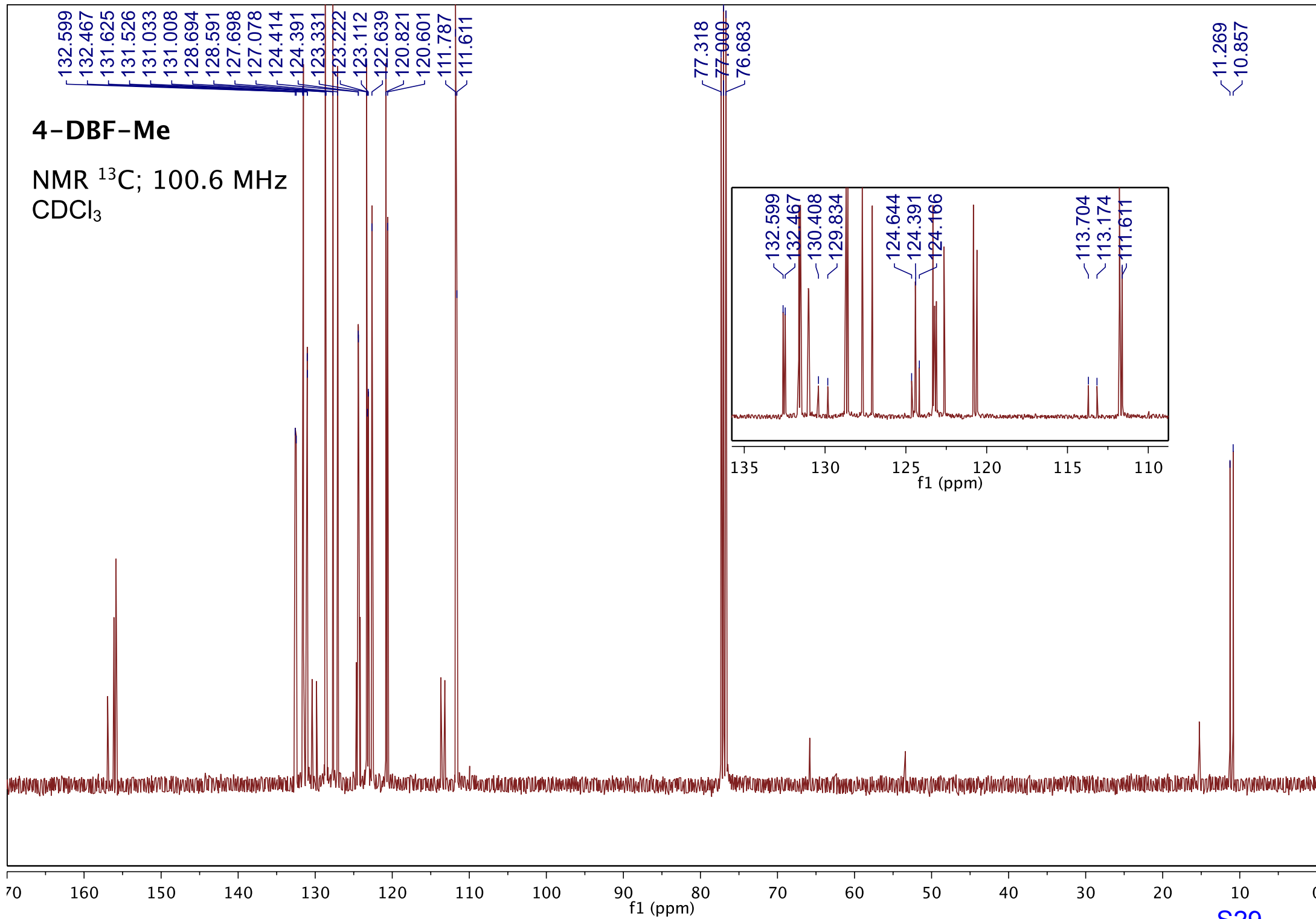
8.082
7.413



4-DBF-Me

NMR ^1H ; 400 MHz
 CDCl_3



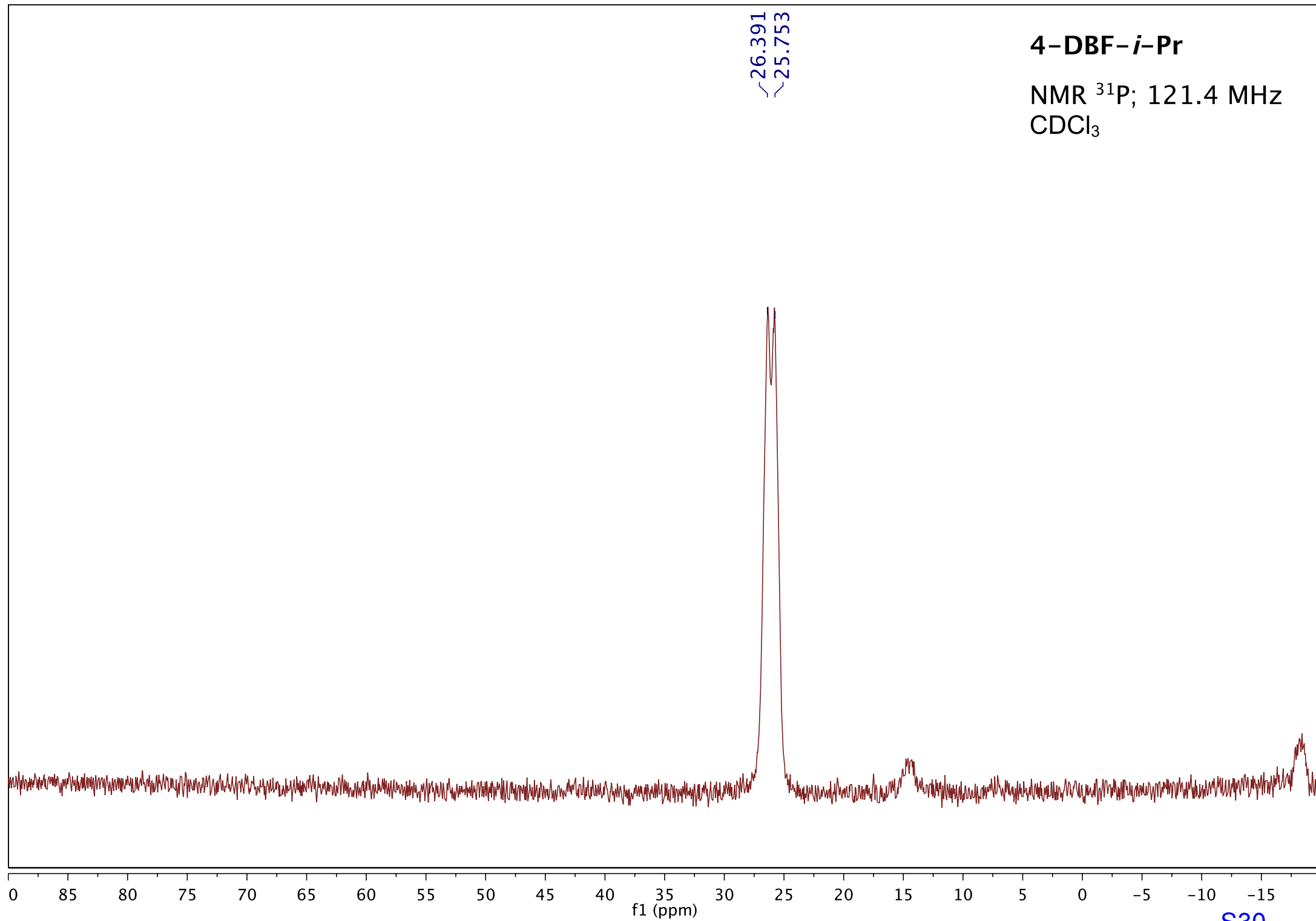


4-DBF-*i*-Pr

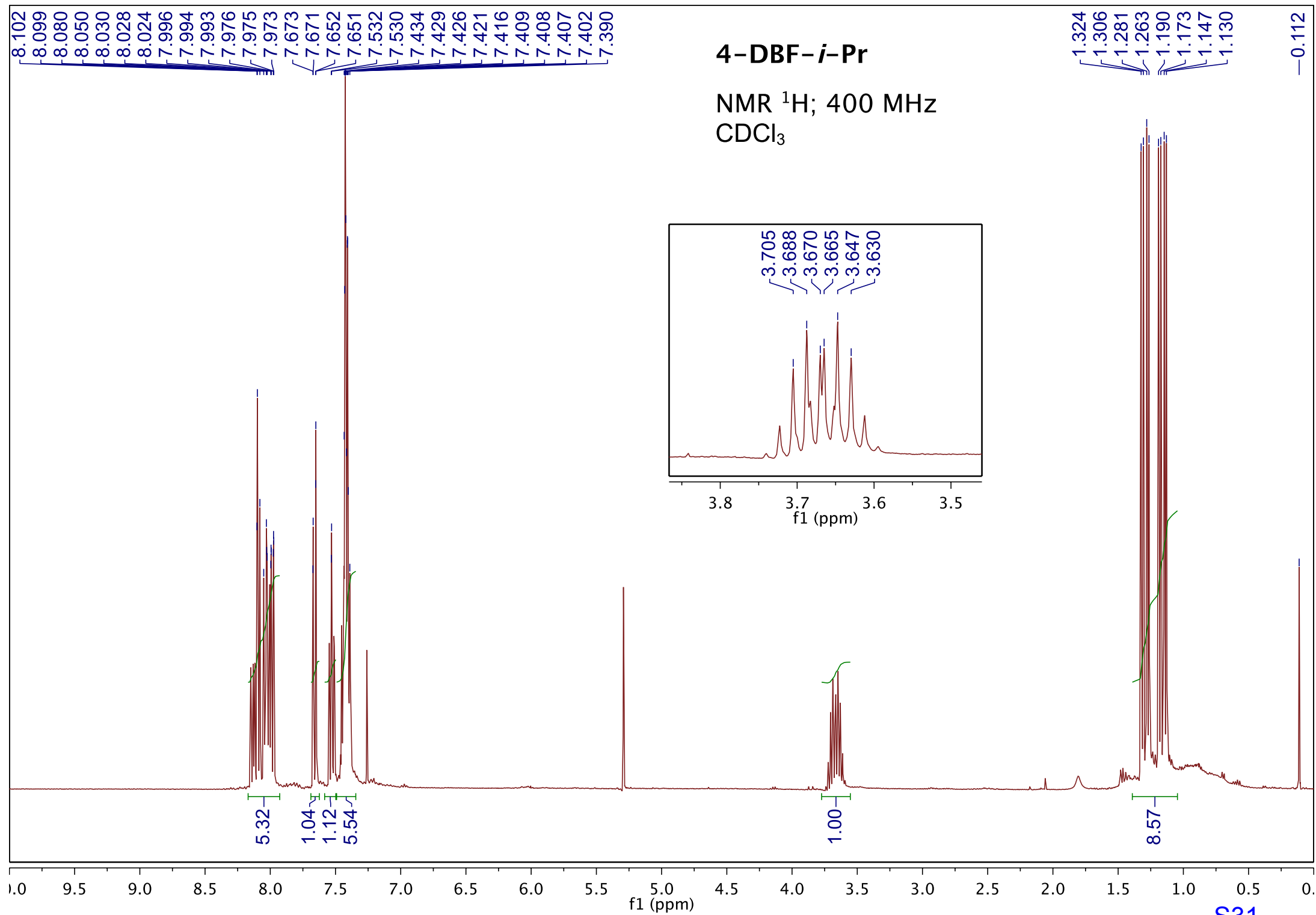
NMR ^{31}P ; 121.4 MHz

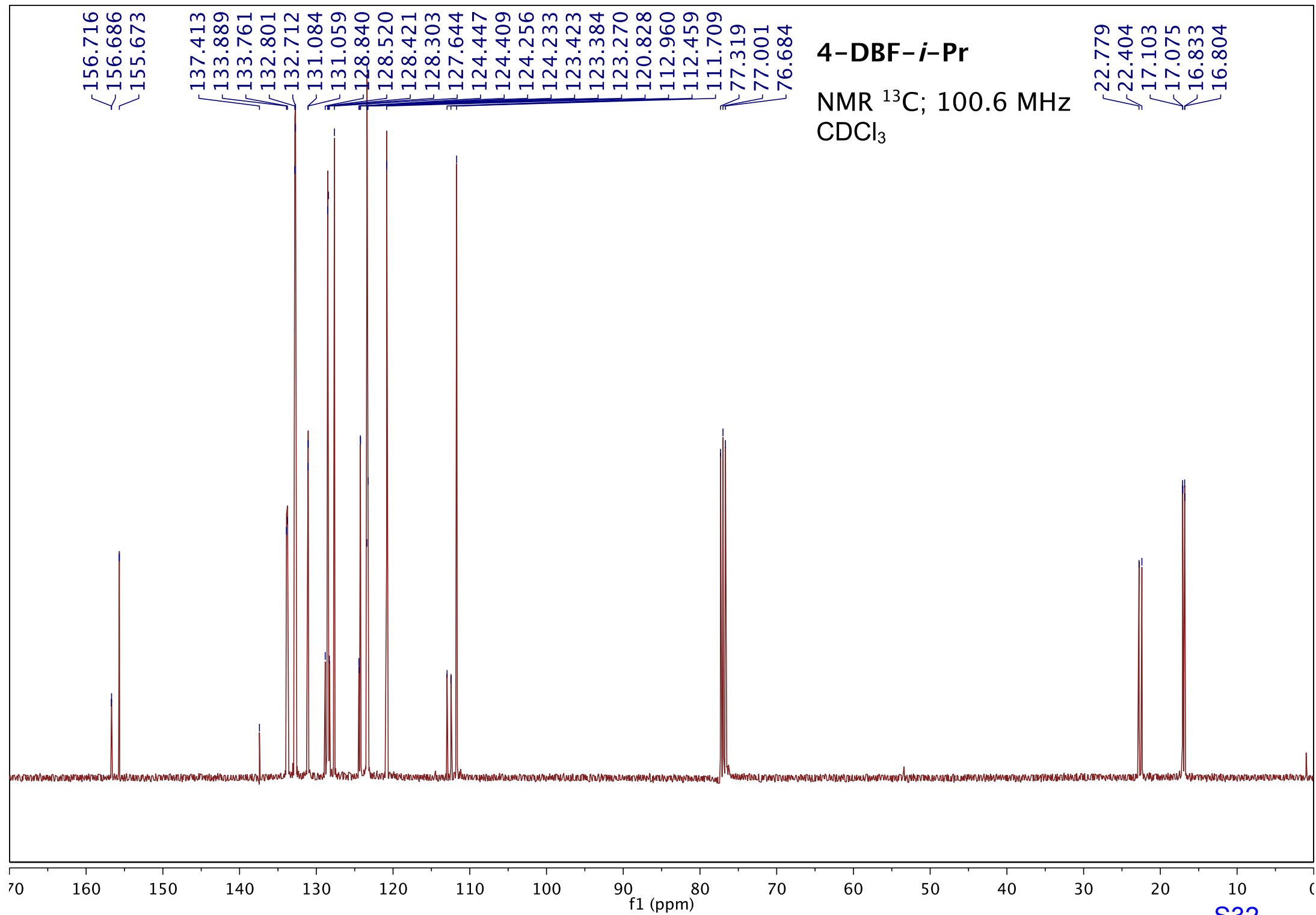
CDCl_3

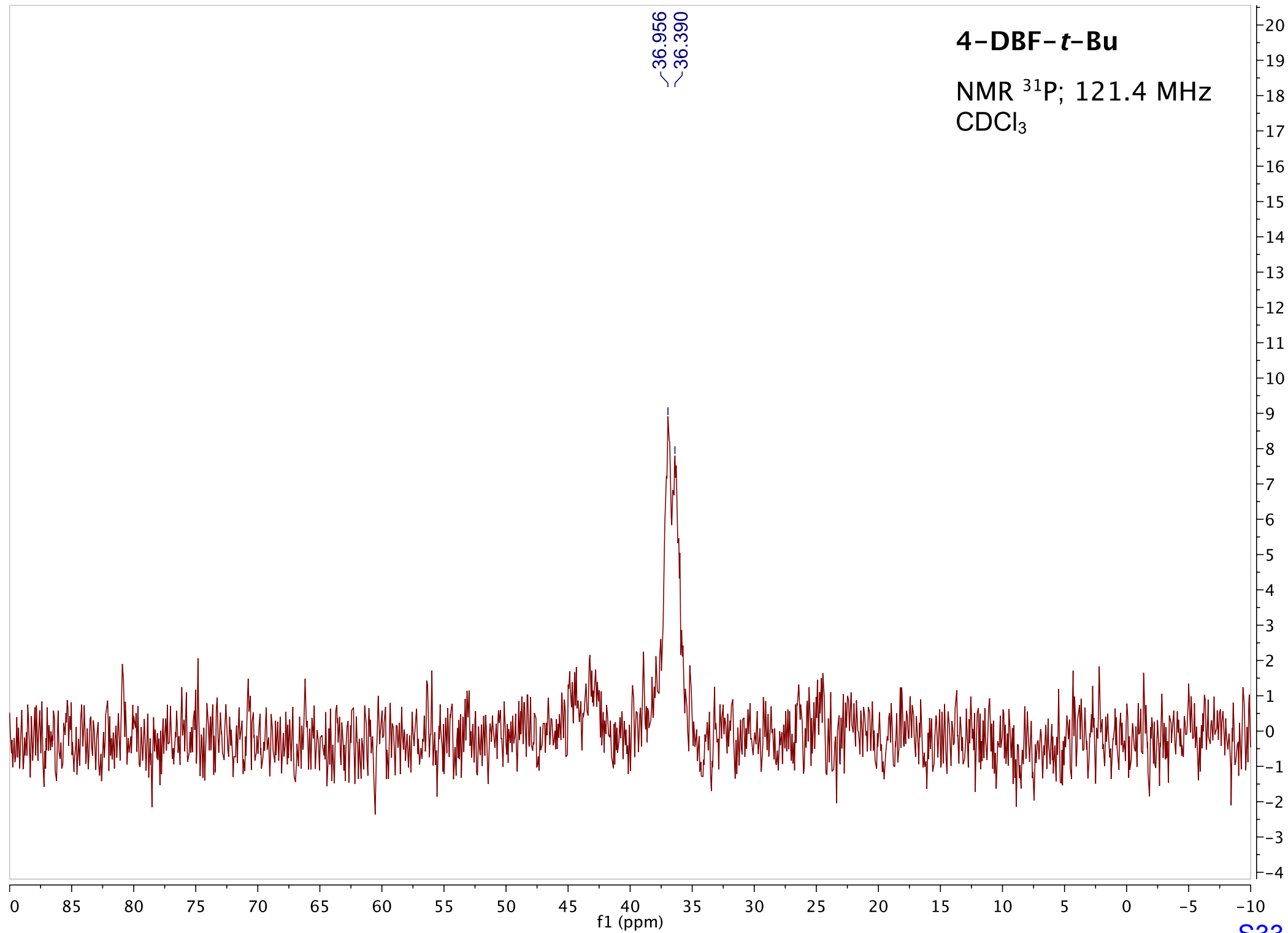
26.391
25.753

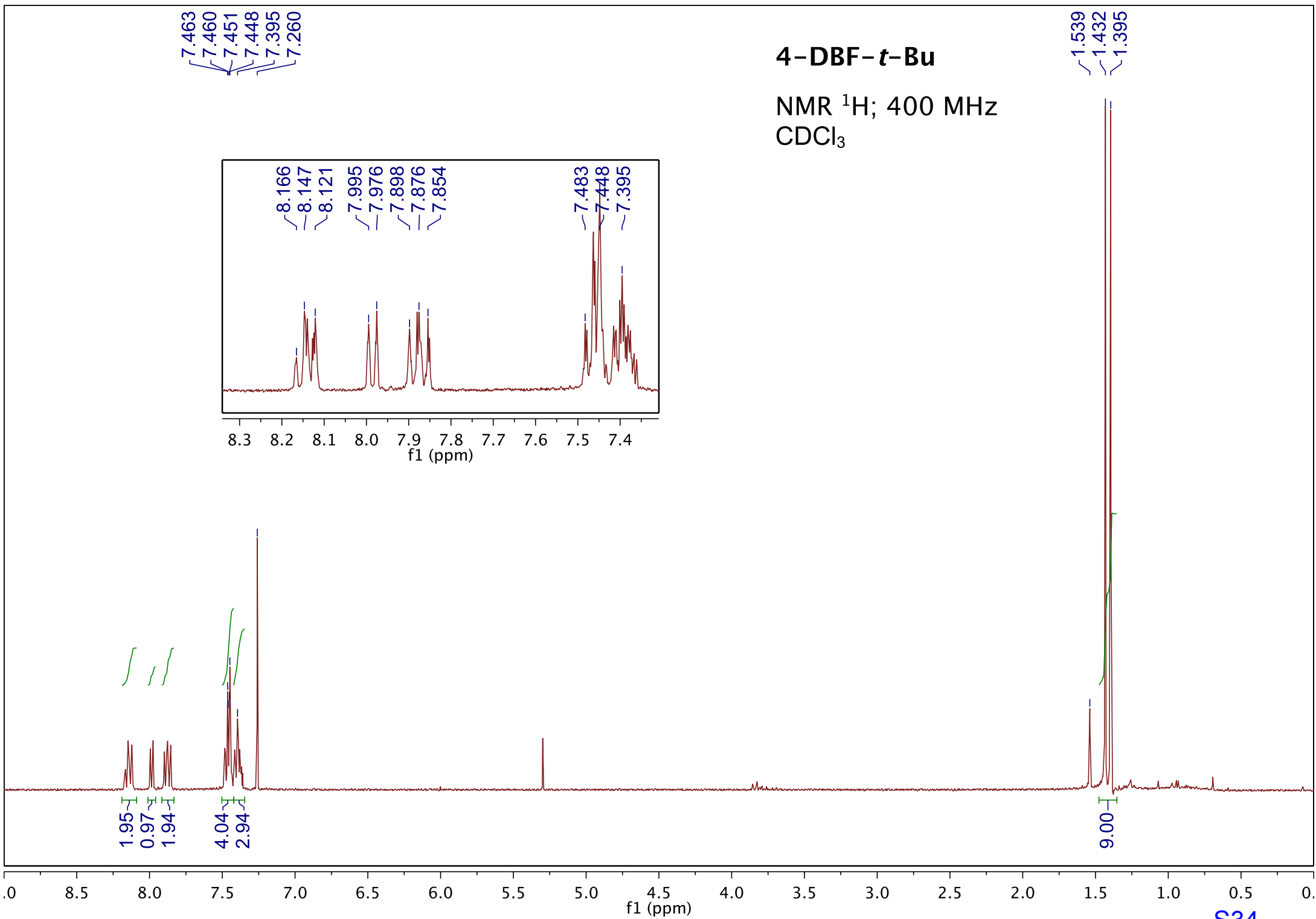


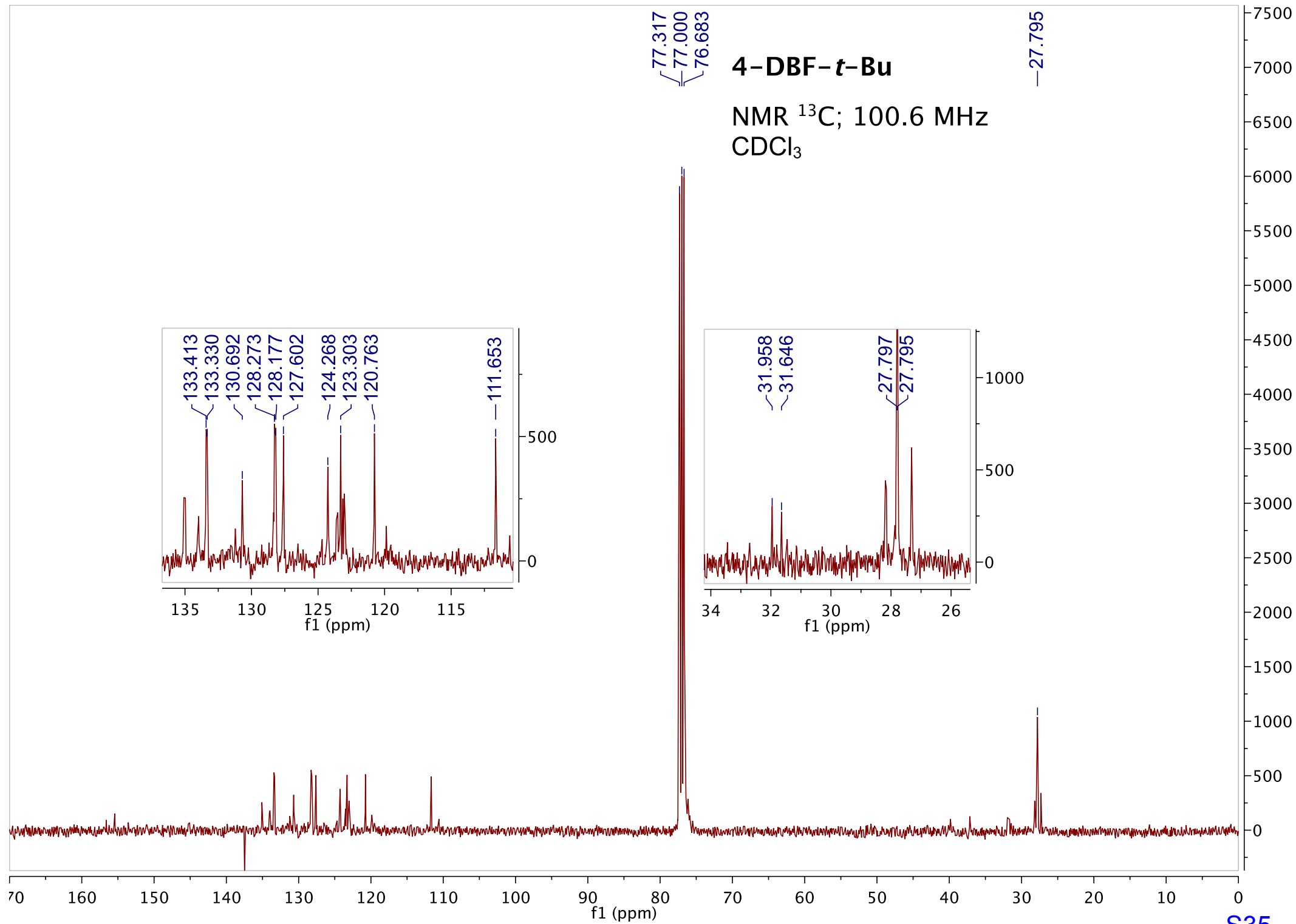
S30









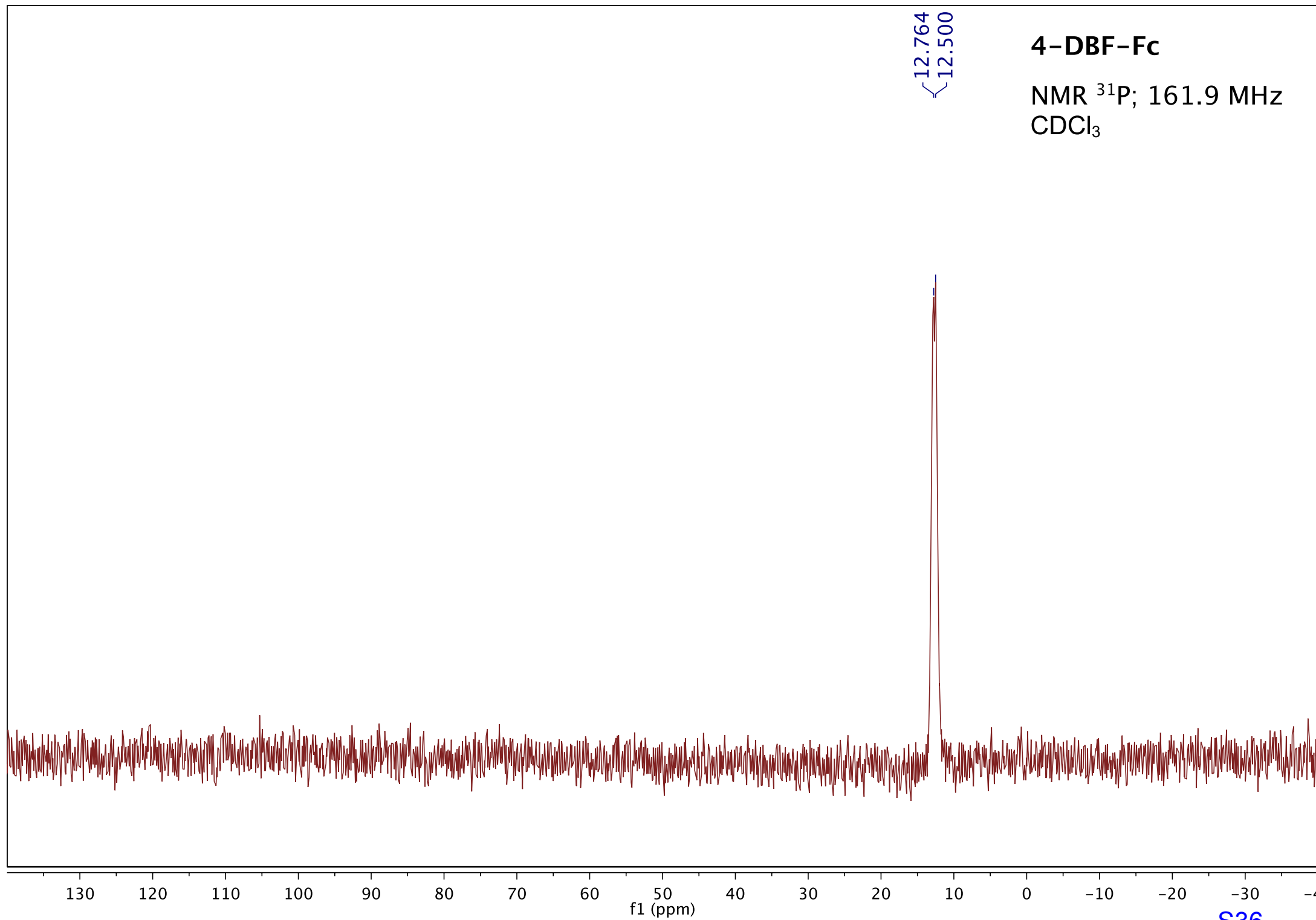


4-DBF-Fc

NMR ^{31}P ; 161.9 MHz

CDCl_3

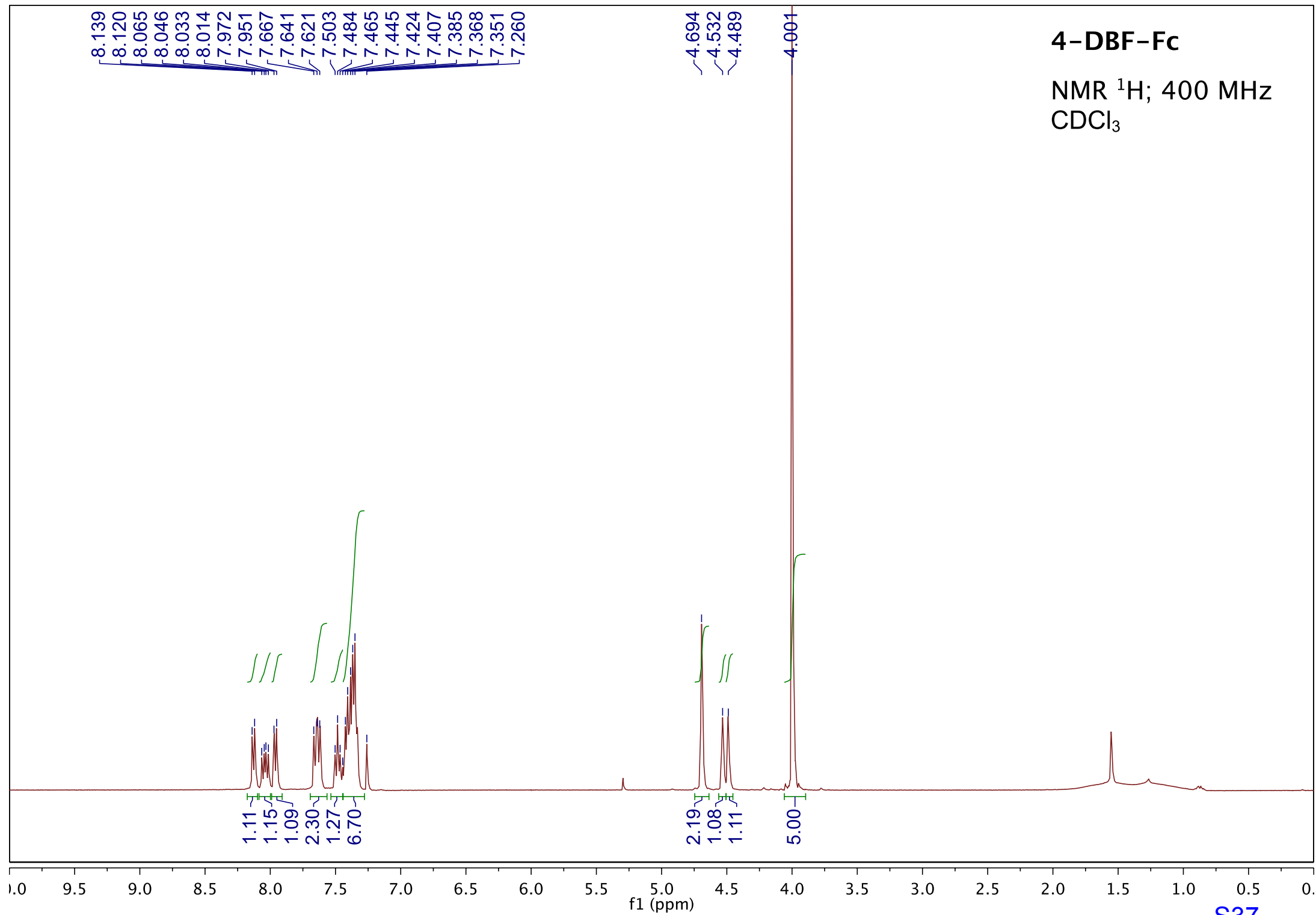
12.764
12.500

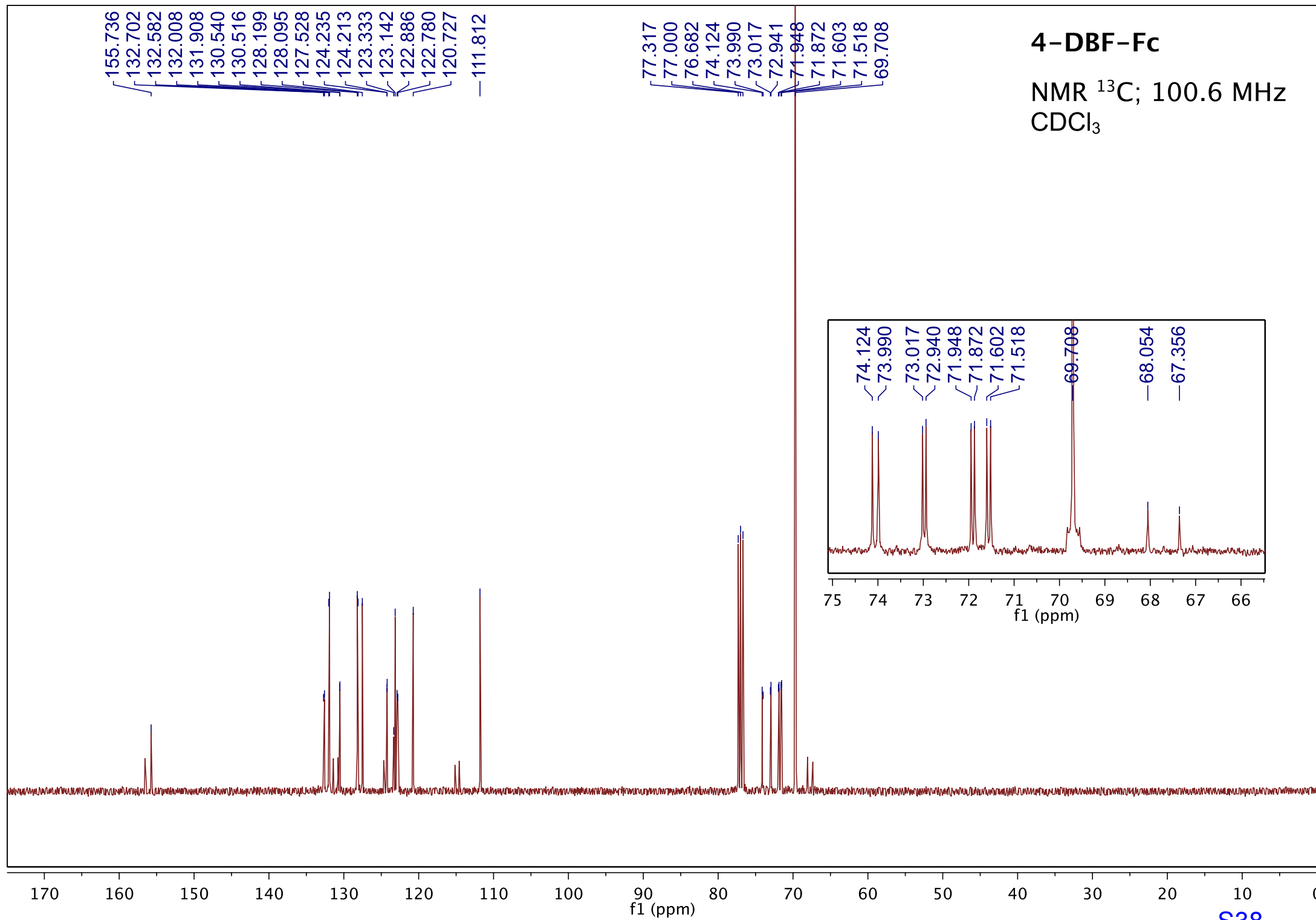


4-DBF-Fc

NMR ^1H ; 400 MHz

CDCl_3

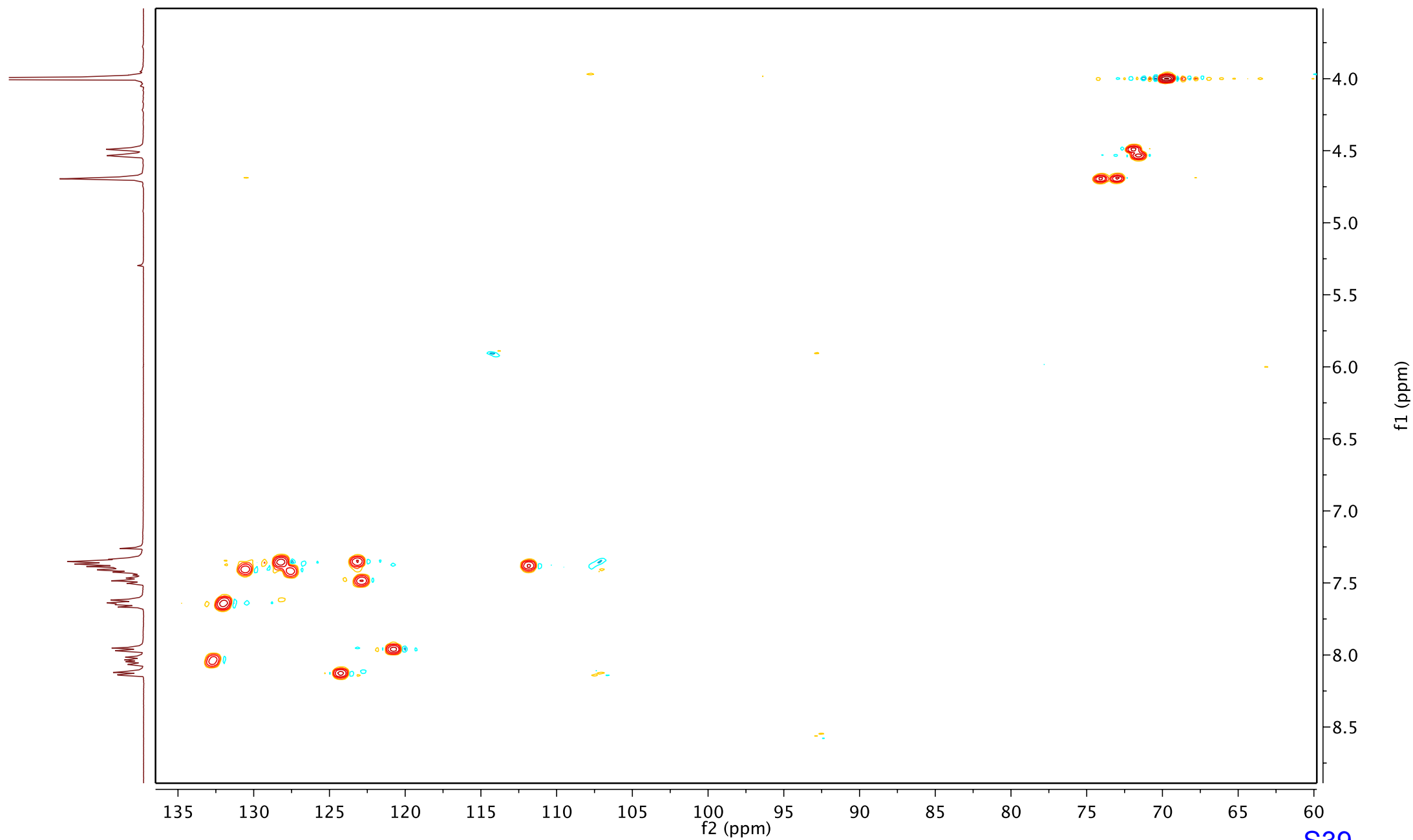




4-DBF-Fc

gHSQC 400MHz

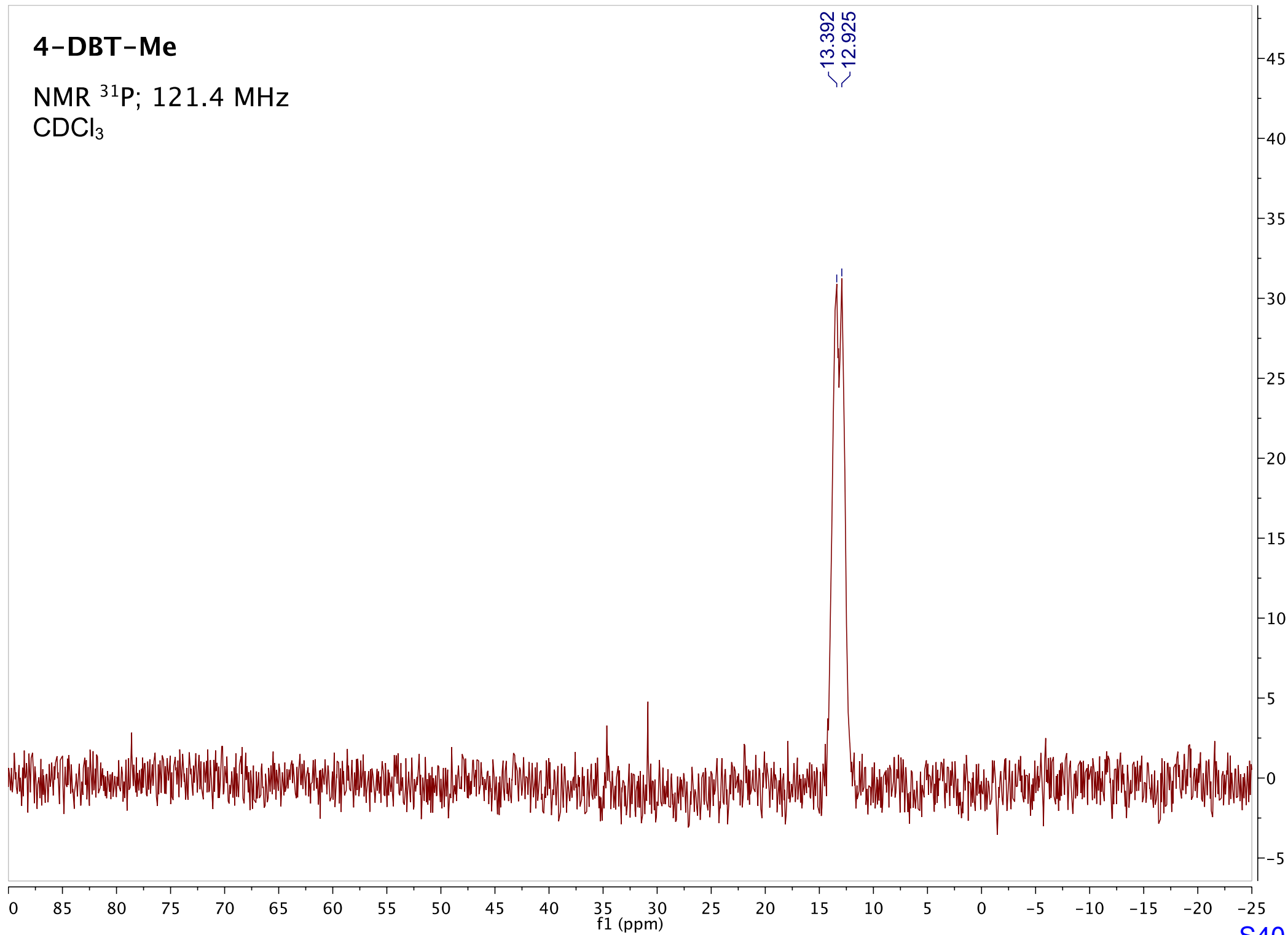
CDCl₃



4-DBT-Me

NMR ^{31}P ; 121.4 MHz

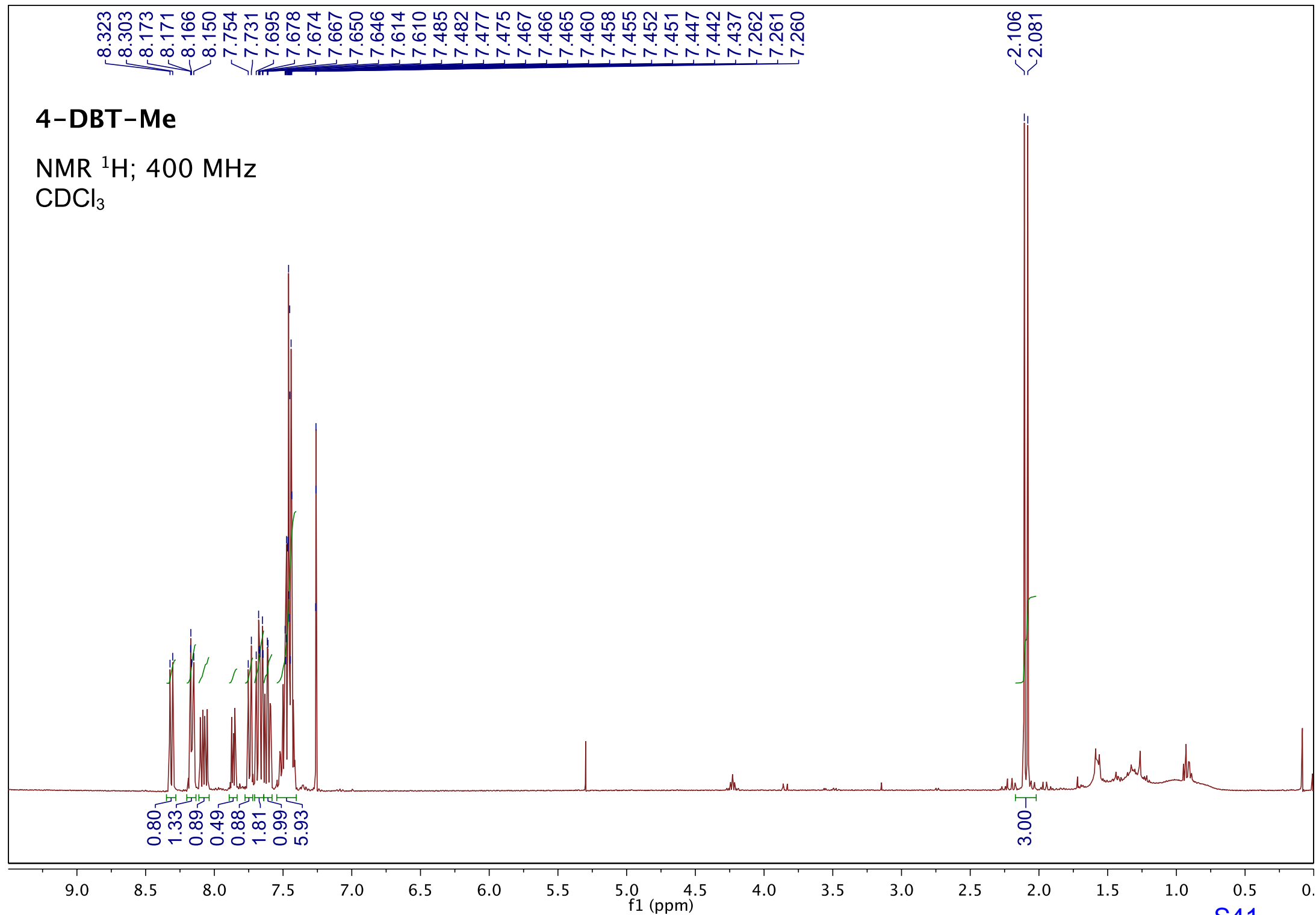
CDCl_3



4-DBT-Me

NMR ^1H ; 400 MHz

CDCl_3



4-DBT-Me

NMR ^{13}C ; 100.6 MHz

CDCl_3

139.303
132.771
132.638
131.895
131.799
131.301
131.276
128.947
128.845
127.293
126.673
124.723
124.692
124.633
124.522
124.324
122.781
122.467
121.672
121.545

77.326
77.008
76.690

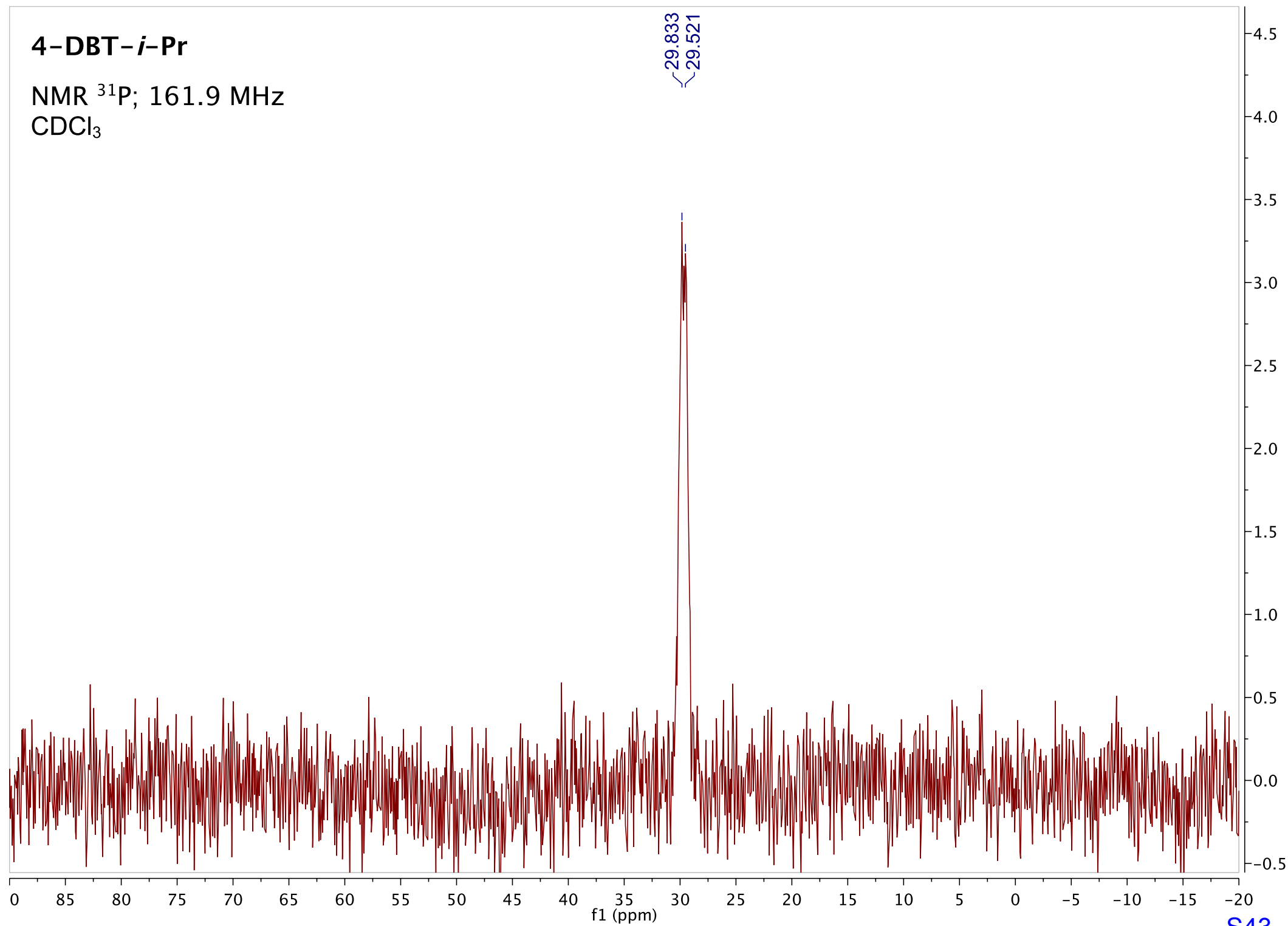
10.190
9.792

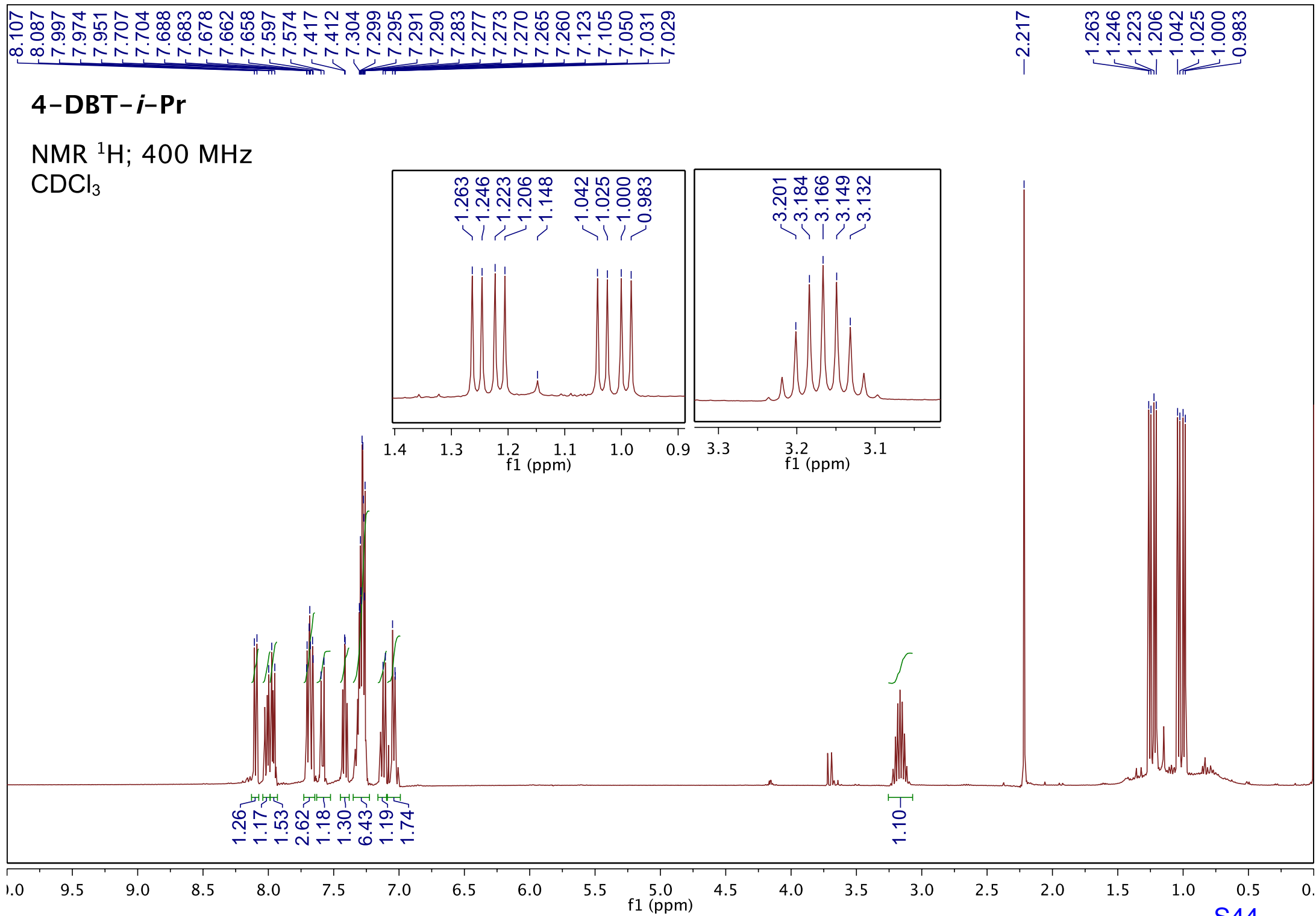
50 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

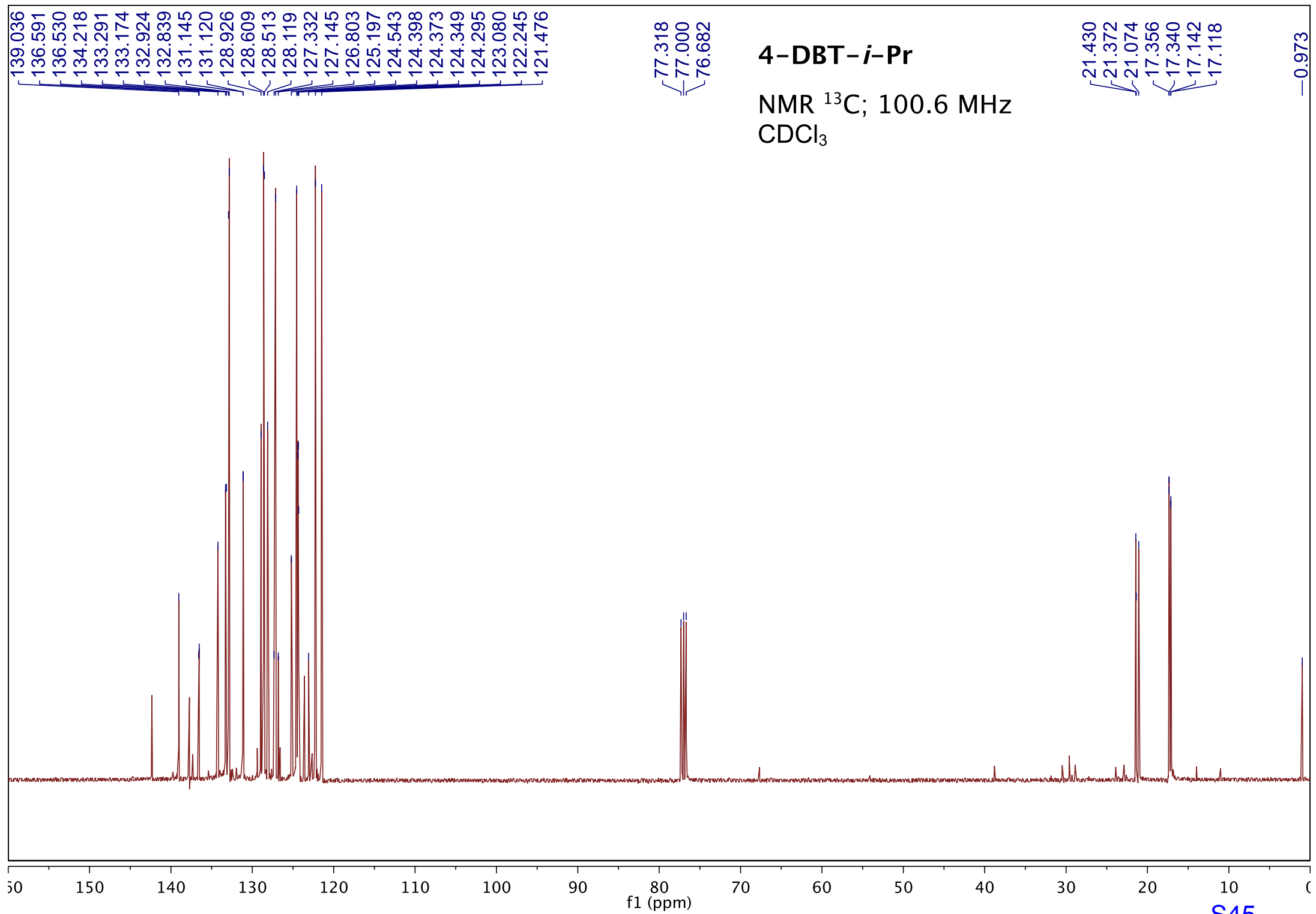
4-DBT-*i*-Pr

NMR ^{31}P ; 161.9 MHz

CDCl_3



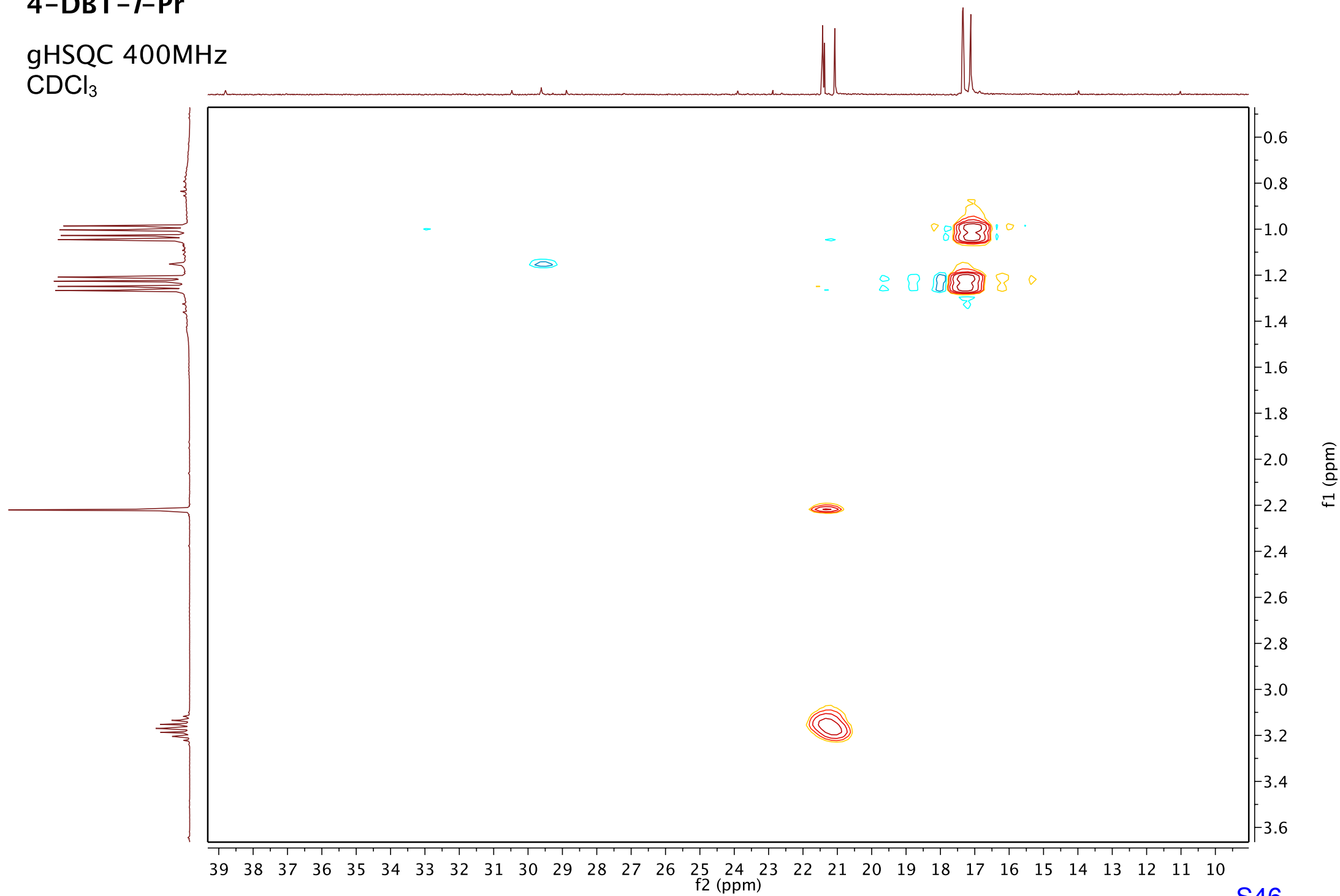




4-DBT-*i*-Pr

gHSQC 400MHz

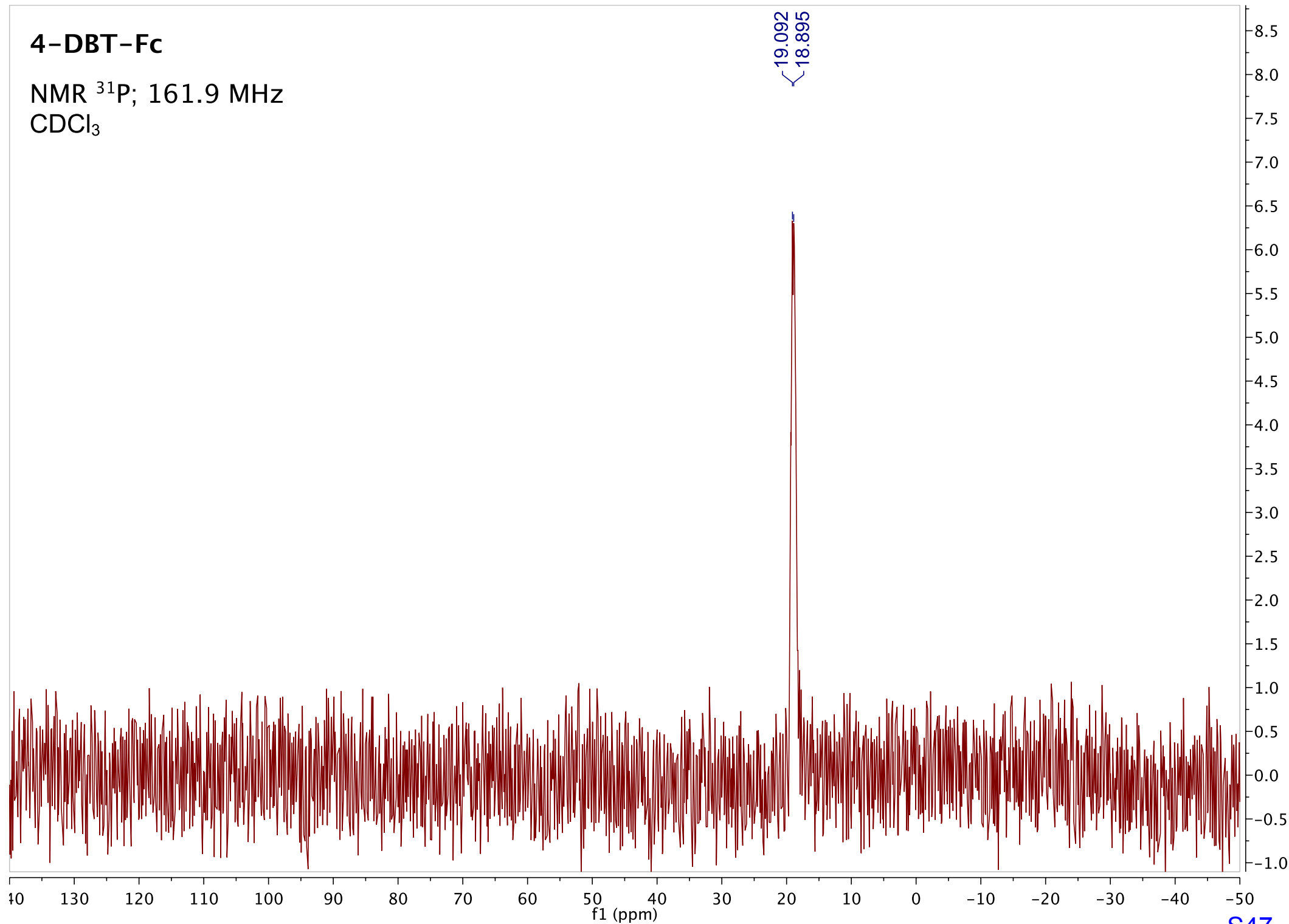
CDCl₃

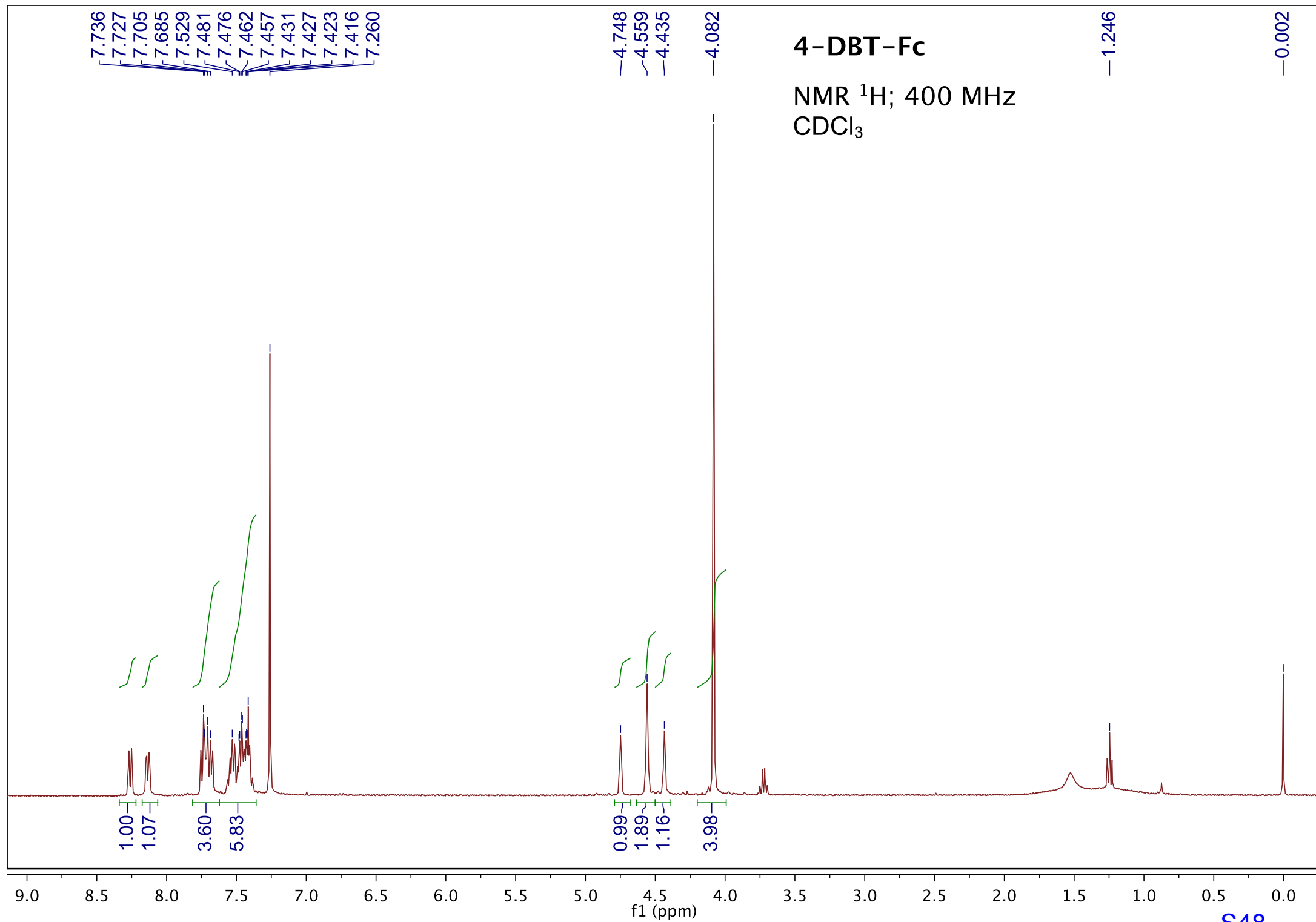


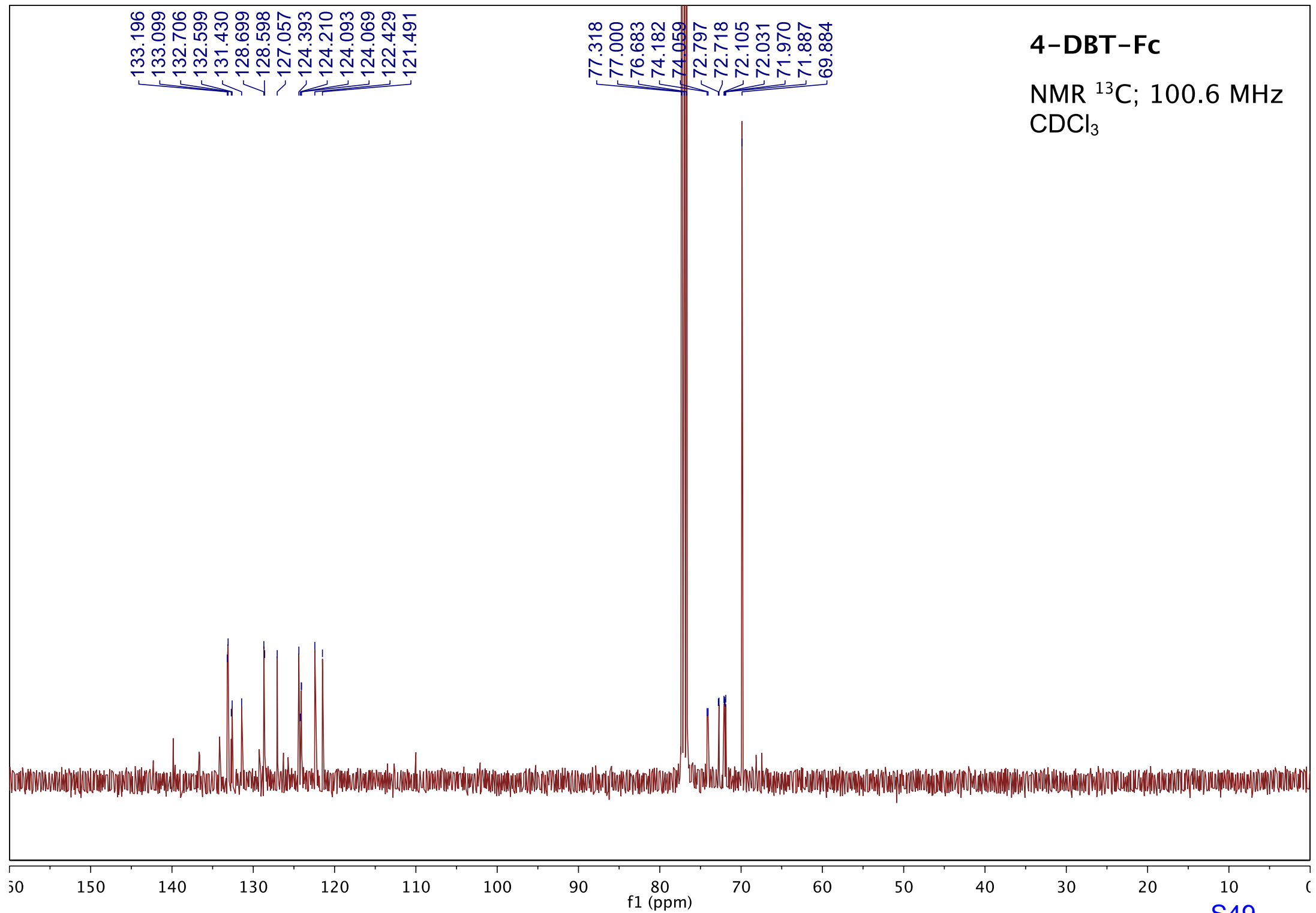
4-DBT-Fc

NMR ^{31}P ; 161.9 MHz

CDCl_3



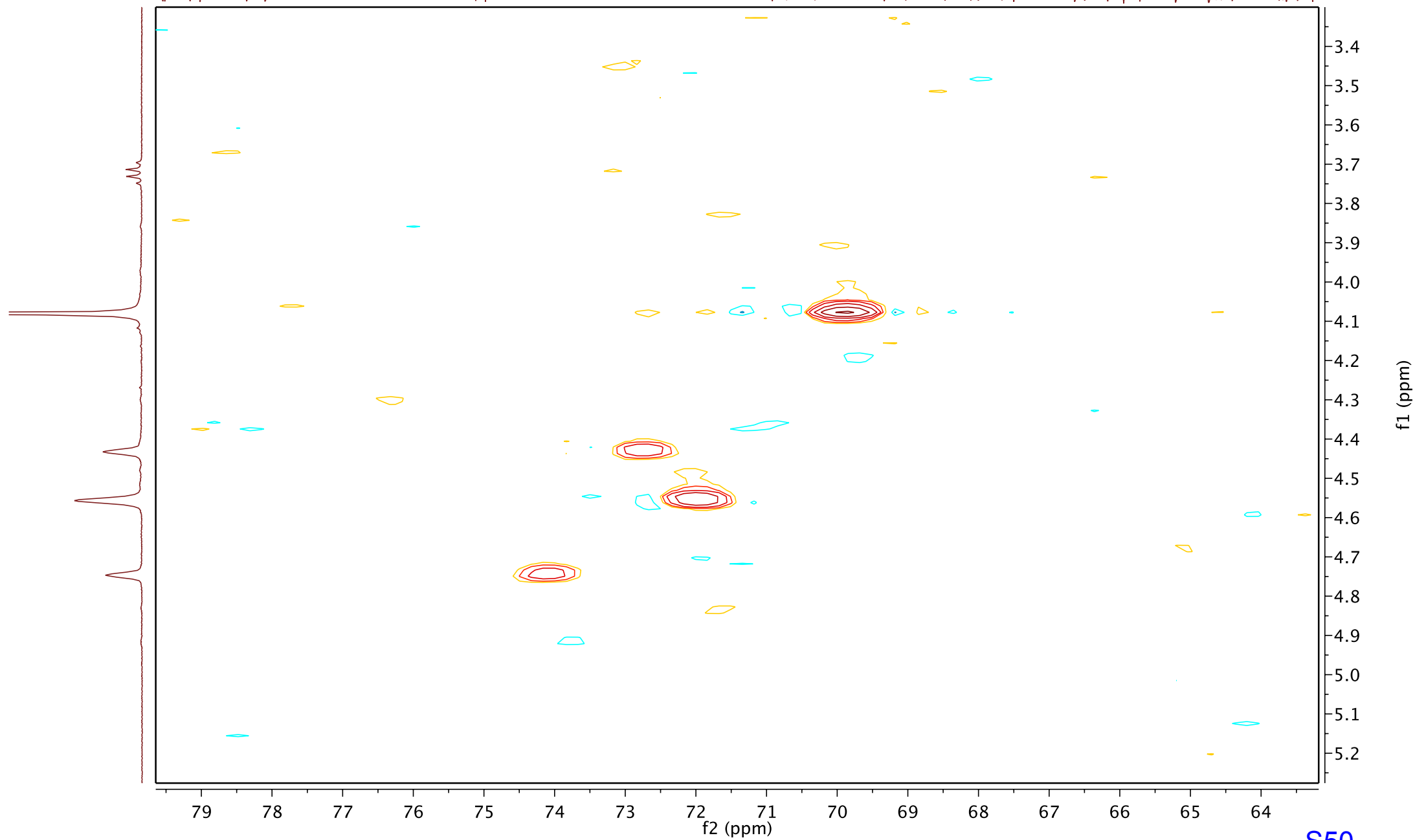




4-DBT-Fc

gHSQC 400MHz

CDCl₃

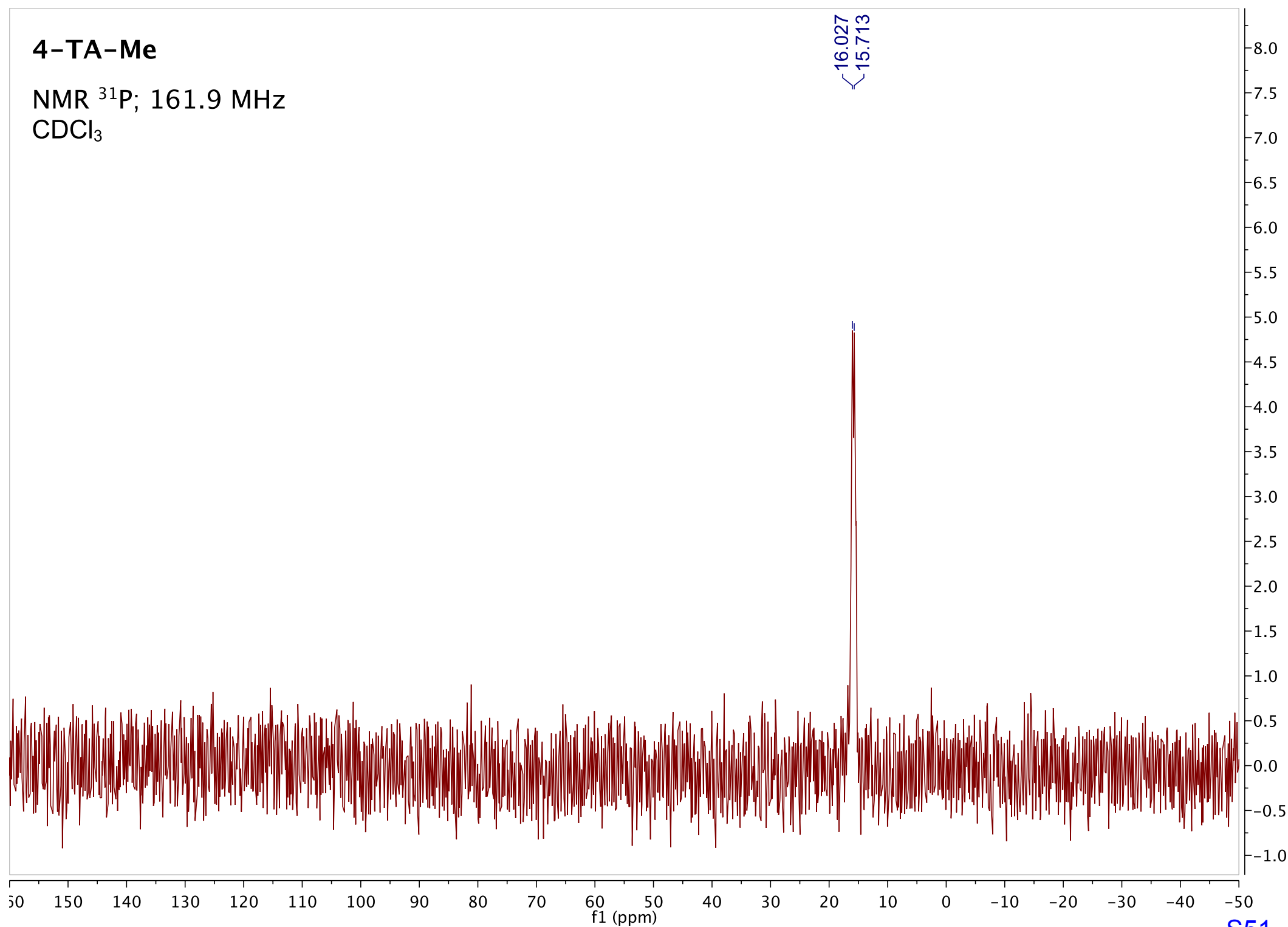


4-TA-Me

NMR ^{31}P ; 161.9 MHz

CDCl_3

16.027
15.713

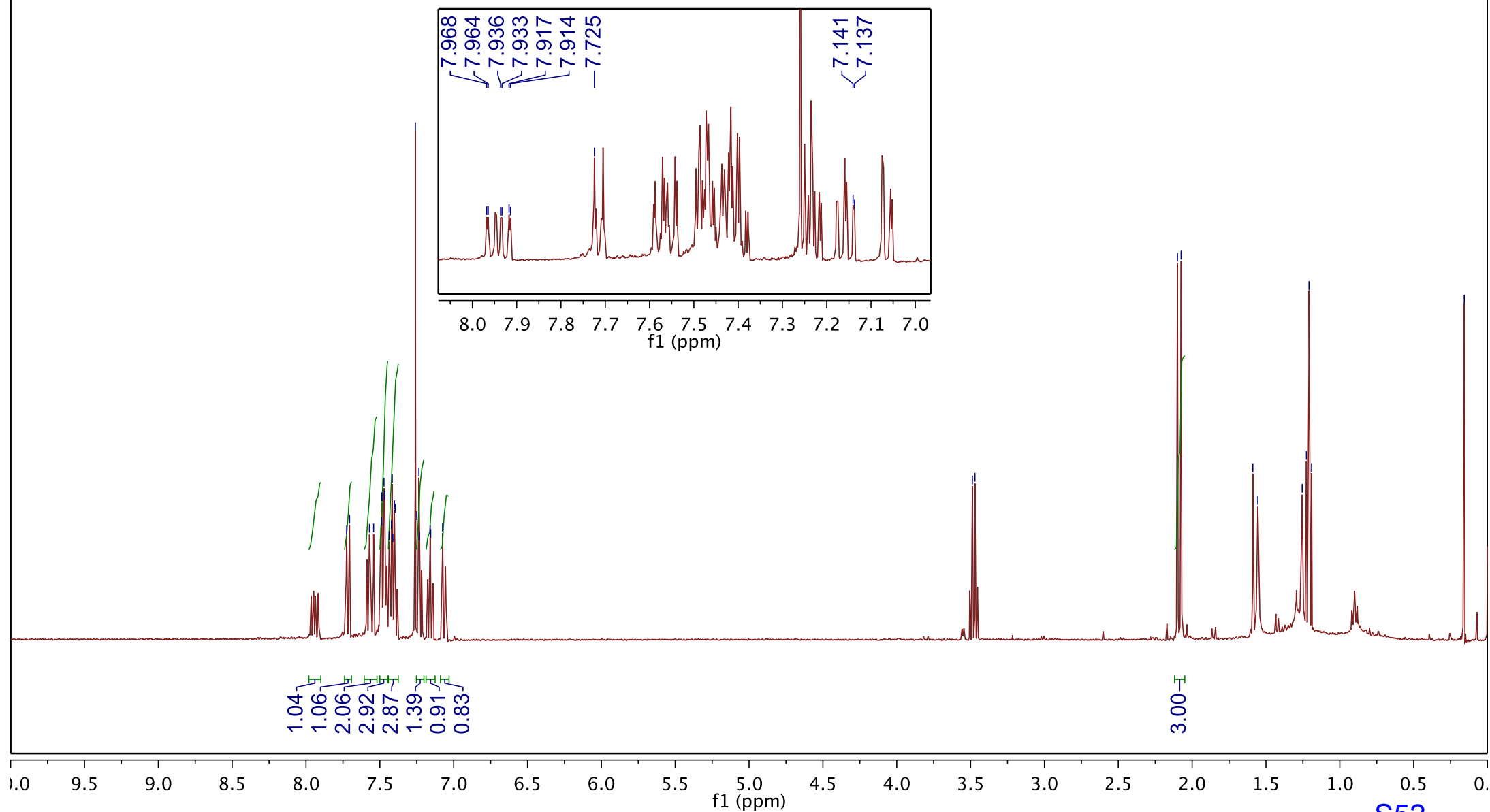


S51

4-TA-Me

NMR ^1H ; 400 MHz

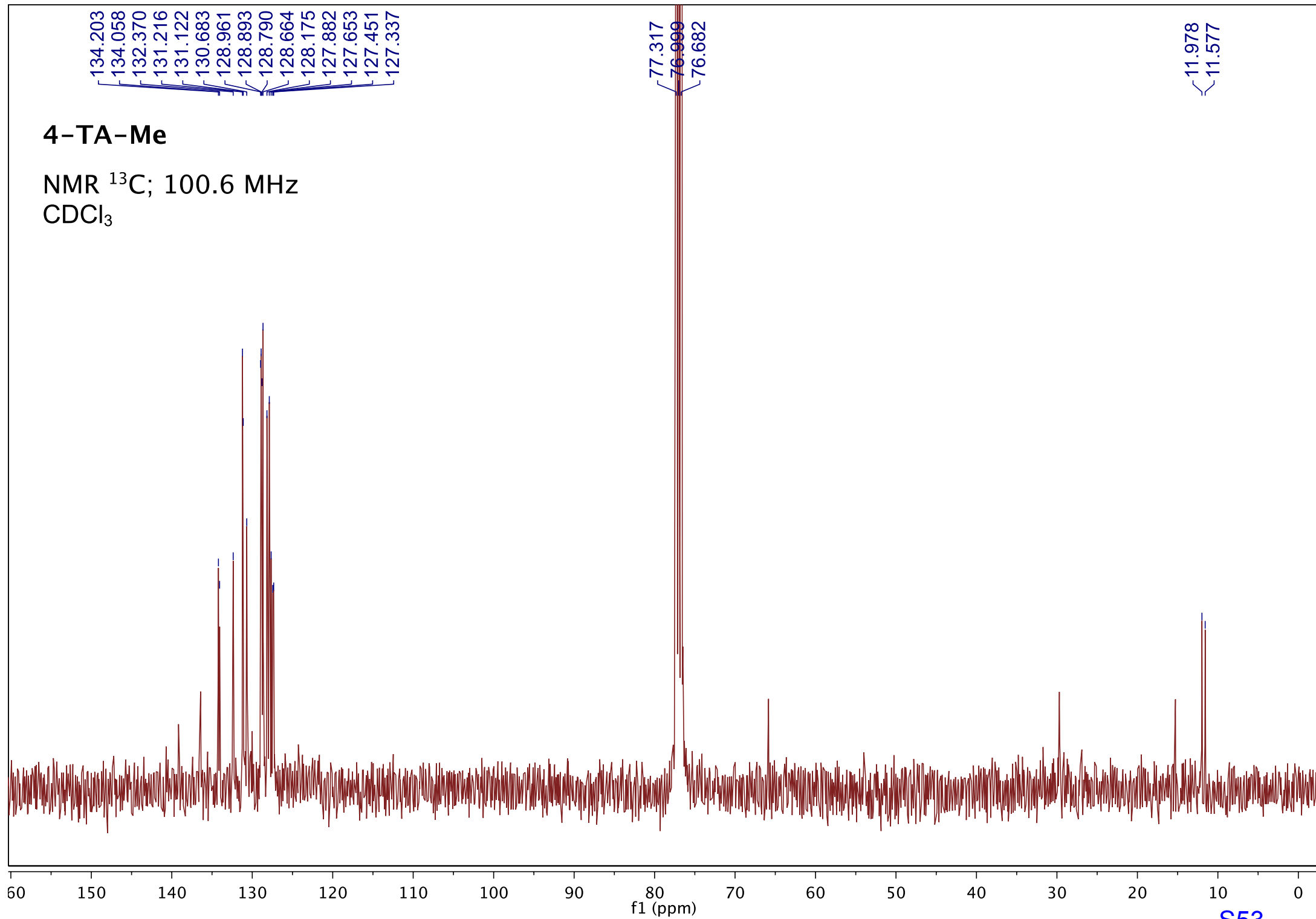
CDCl_3



4-TA-Me

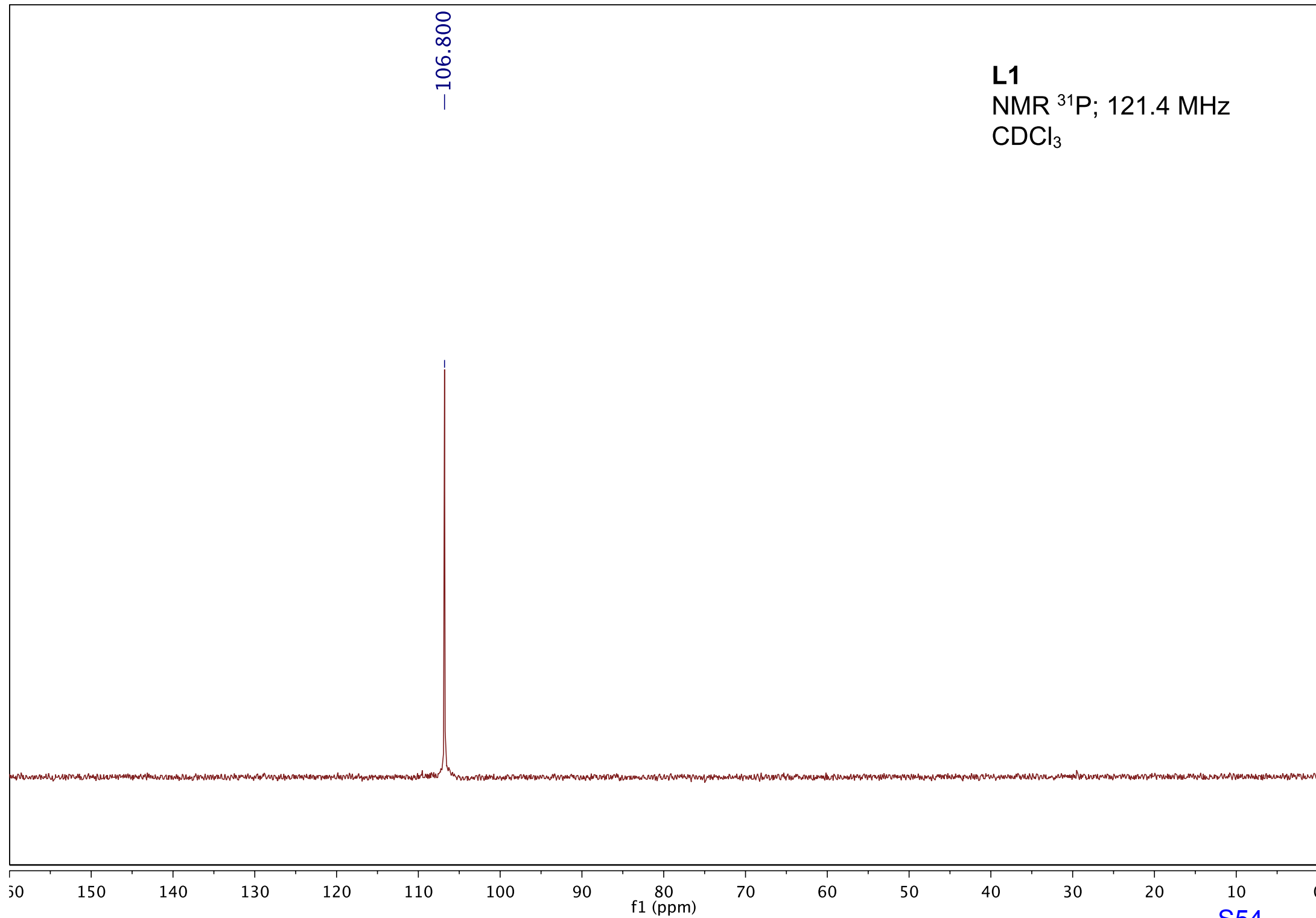
NMR ^{13}C ; 100.6 MHz

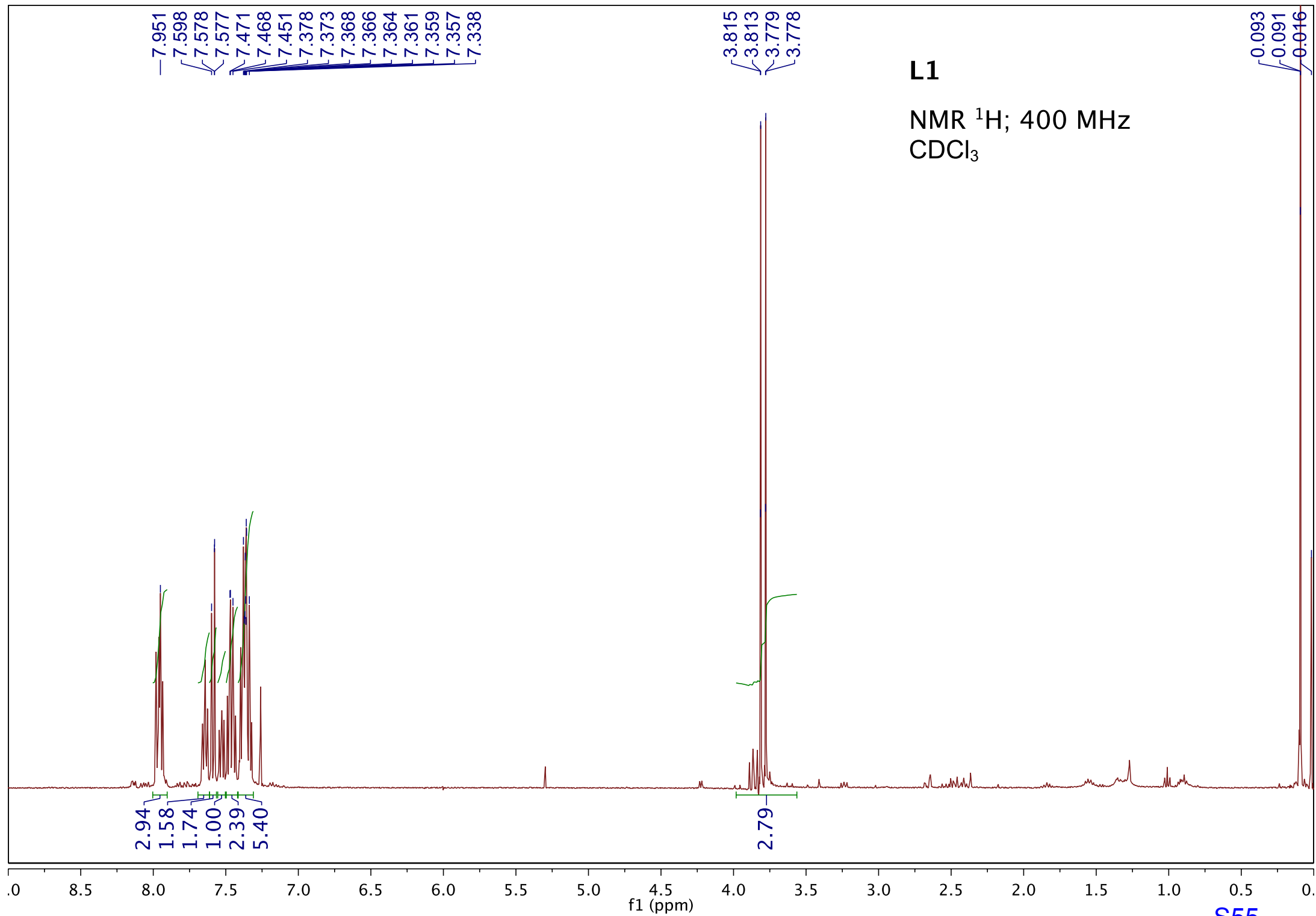
CDCl_3

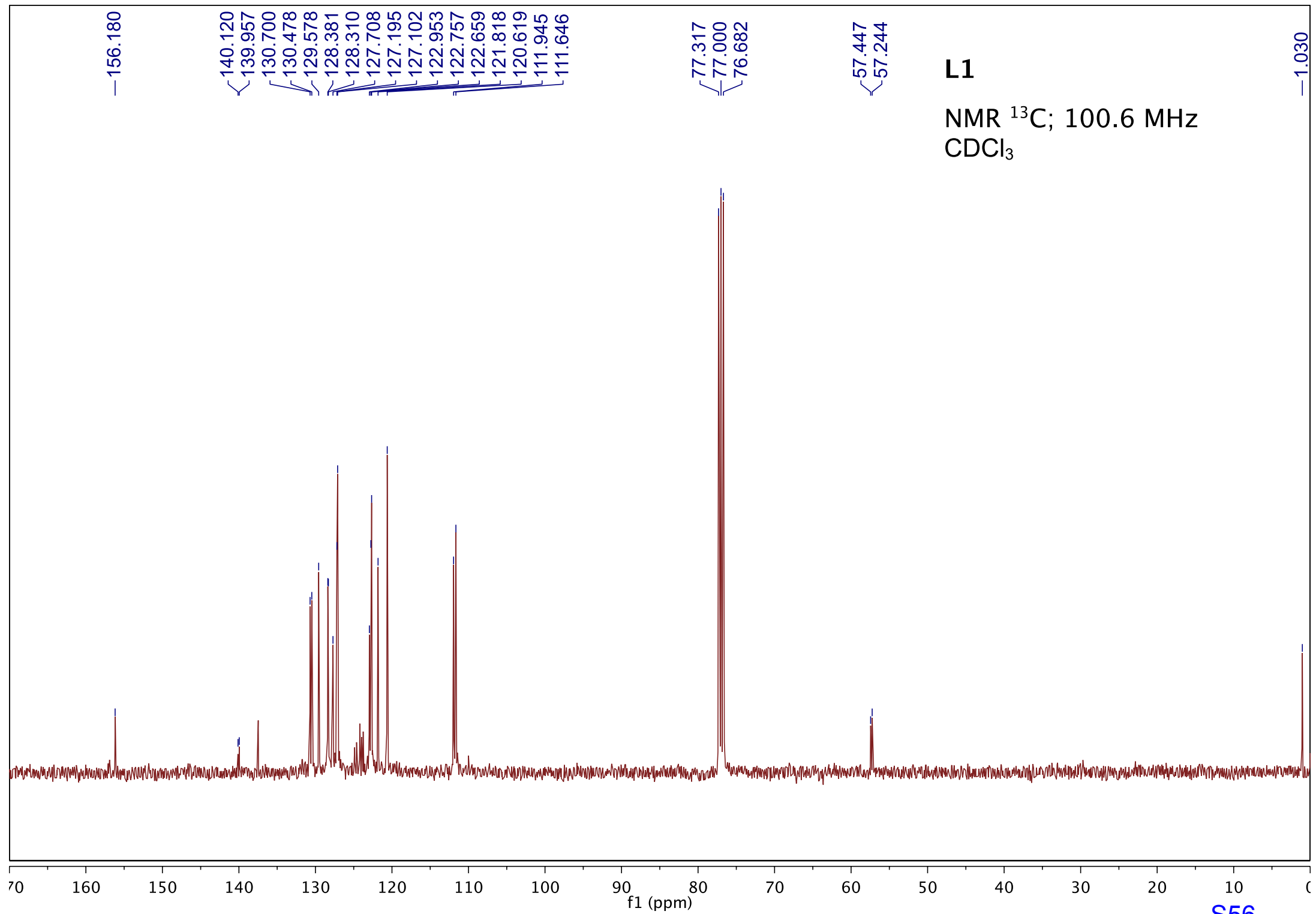


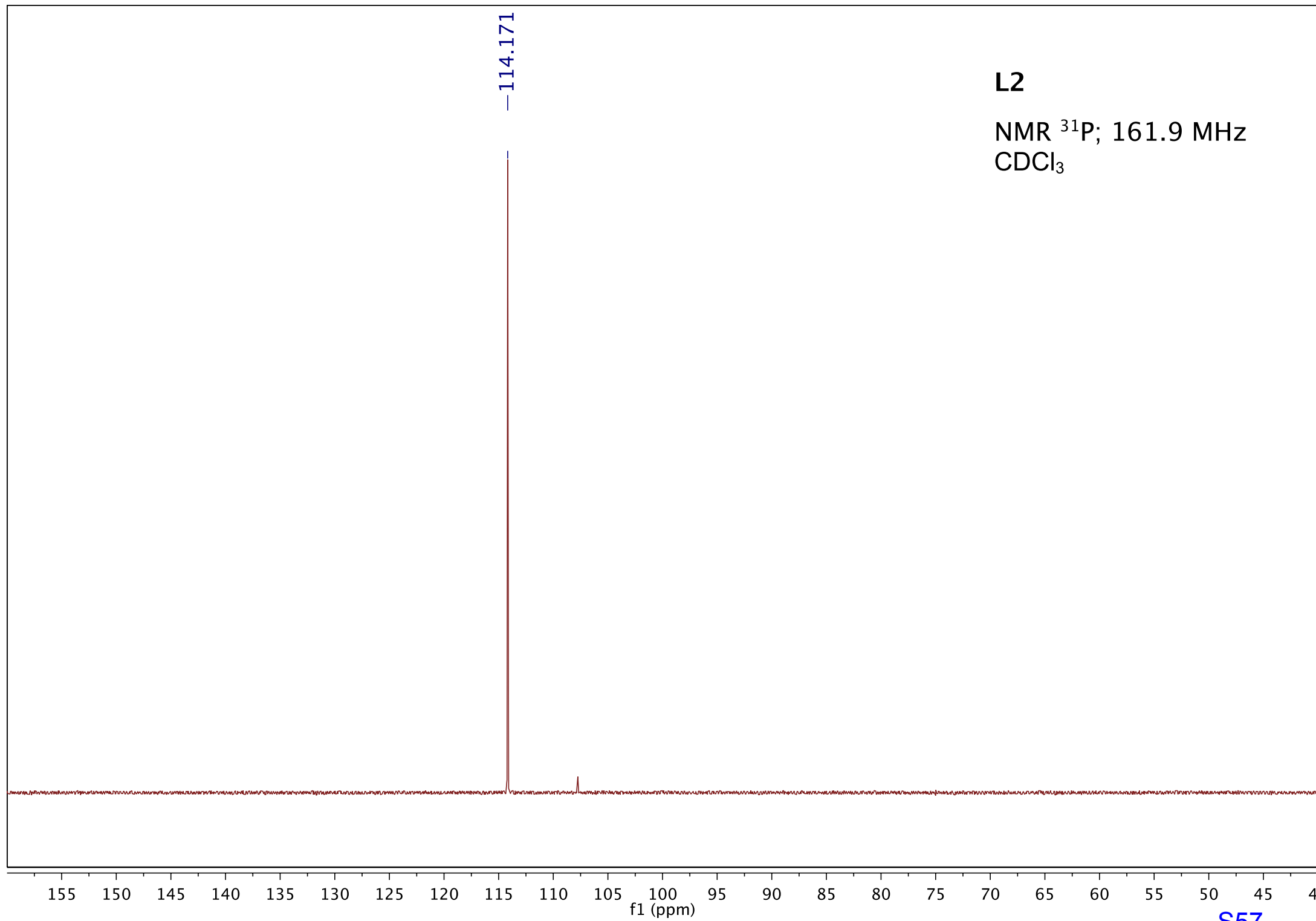
L1
NMR ^{31}P ; 121.4 MHz
 CDCl_3

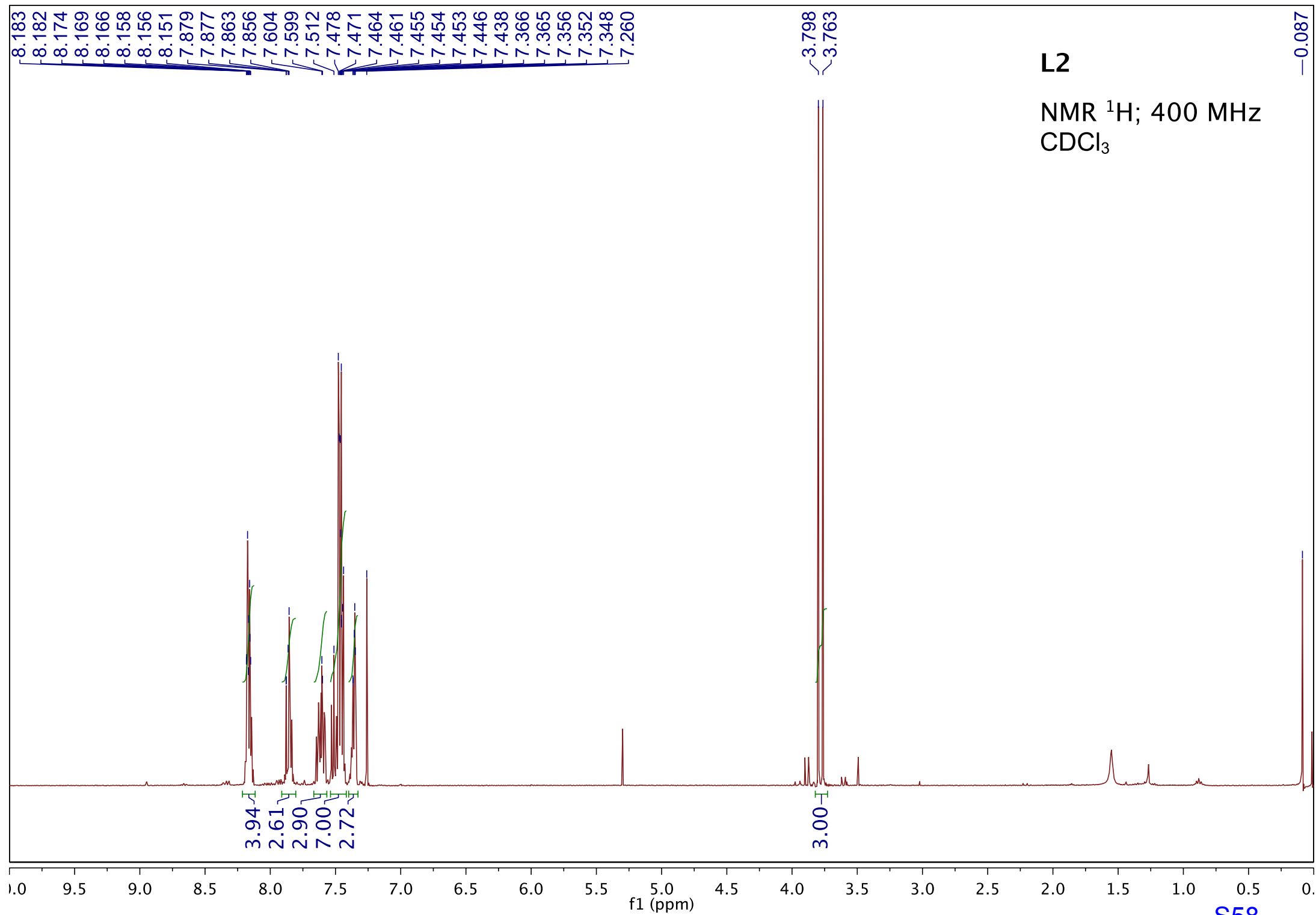
—106.800

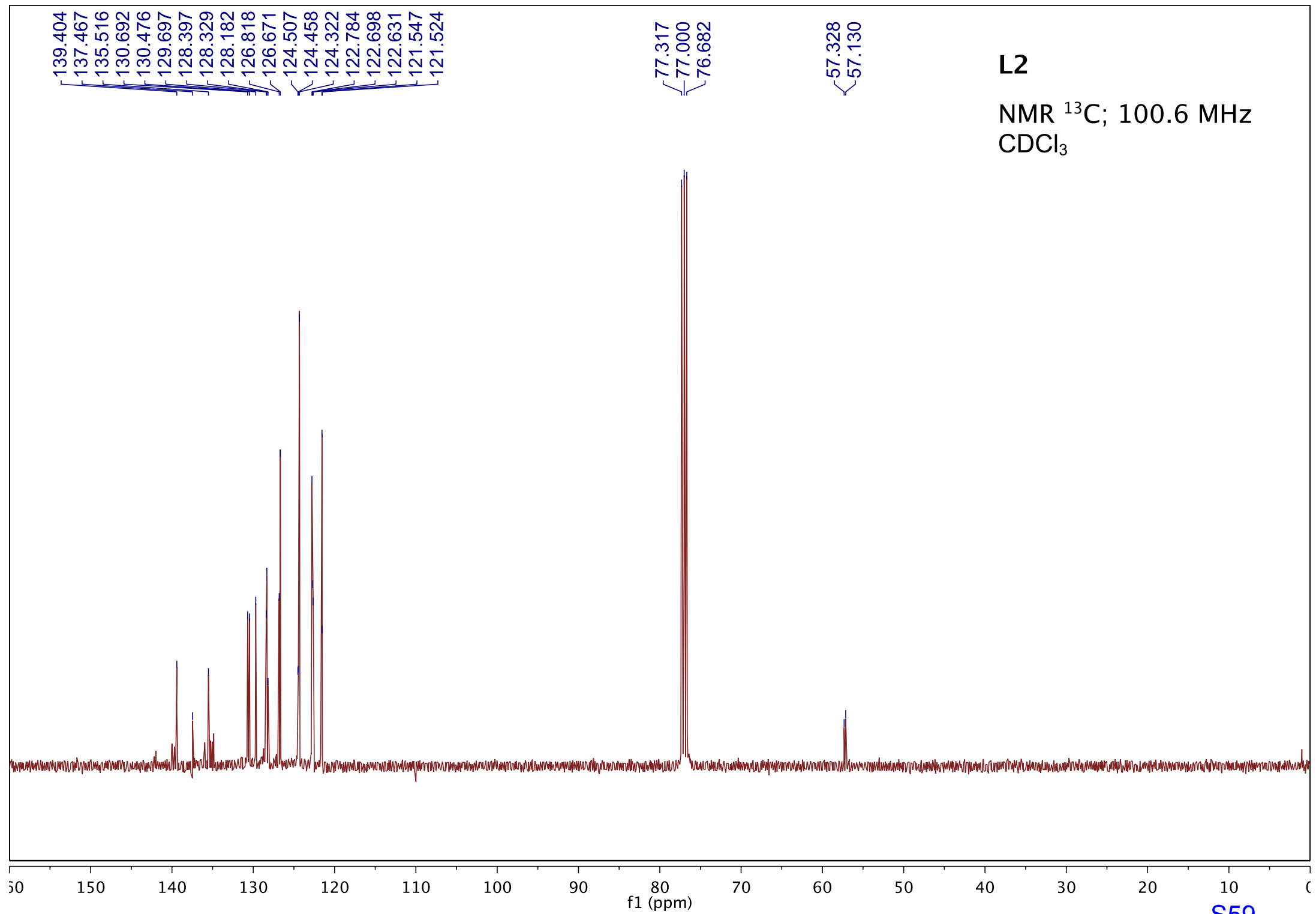








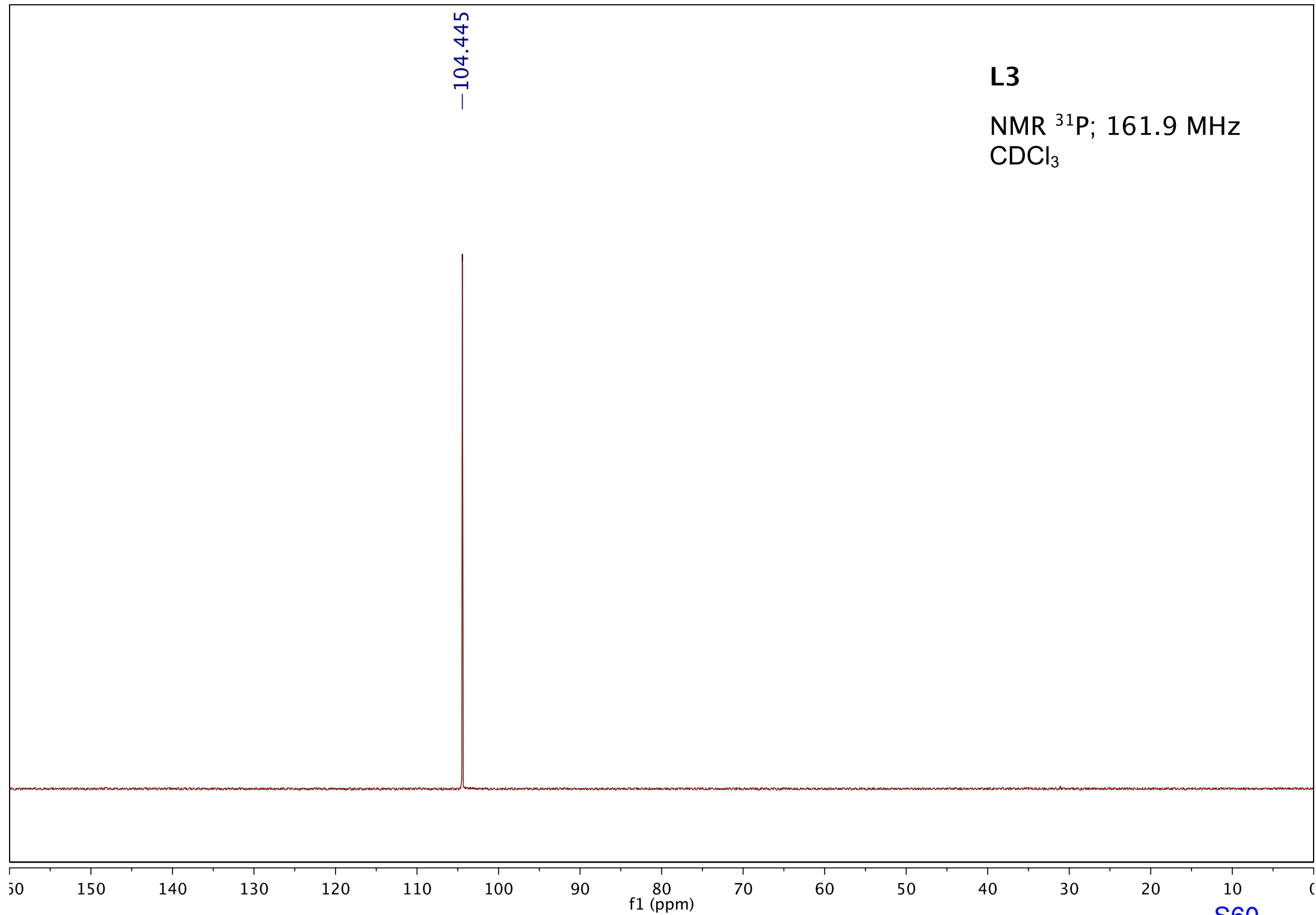




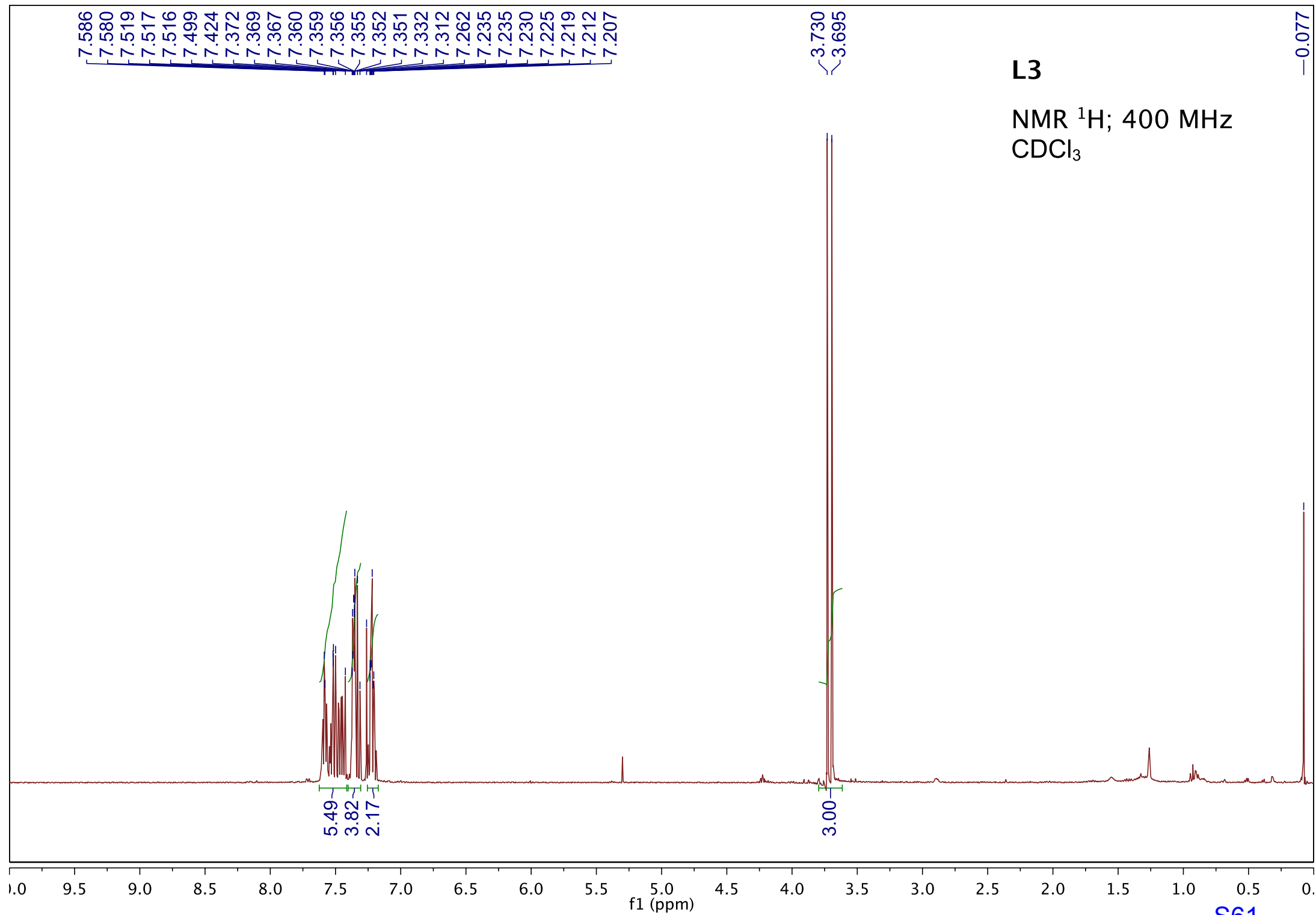
L3

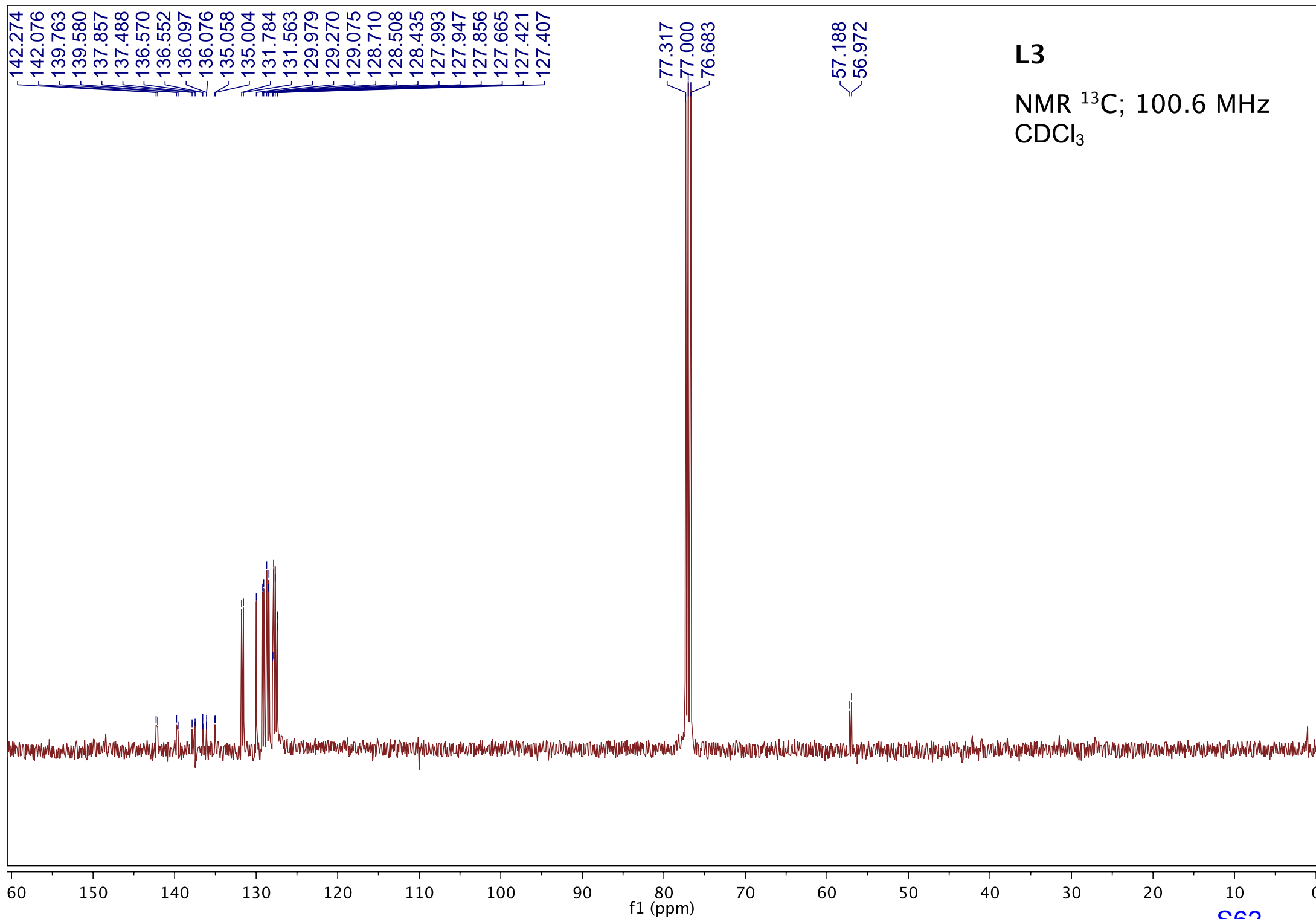
NMR ^{31}P ; 161.9 MHz
 CDCl_3

—104.445



S60

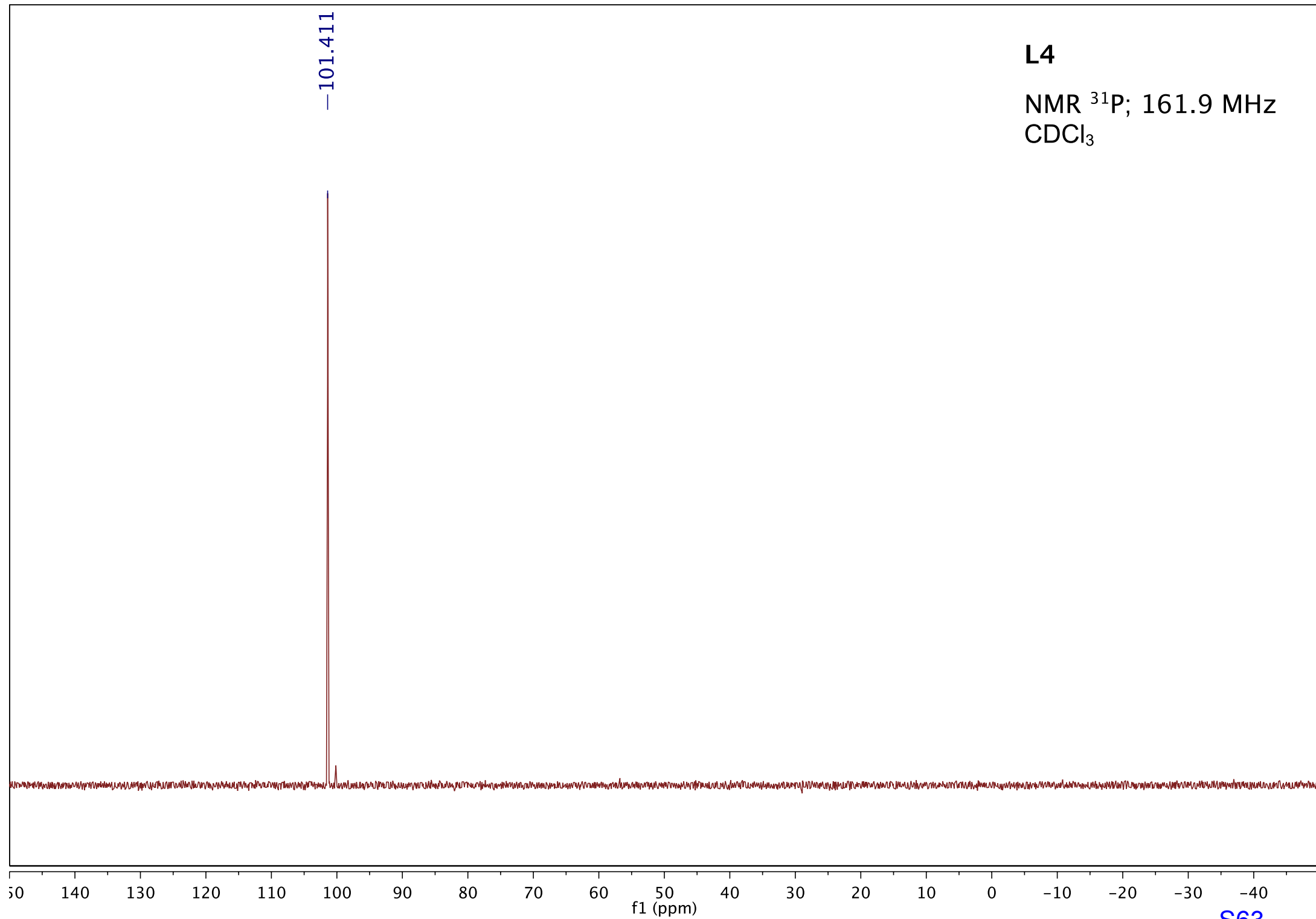




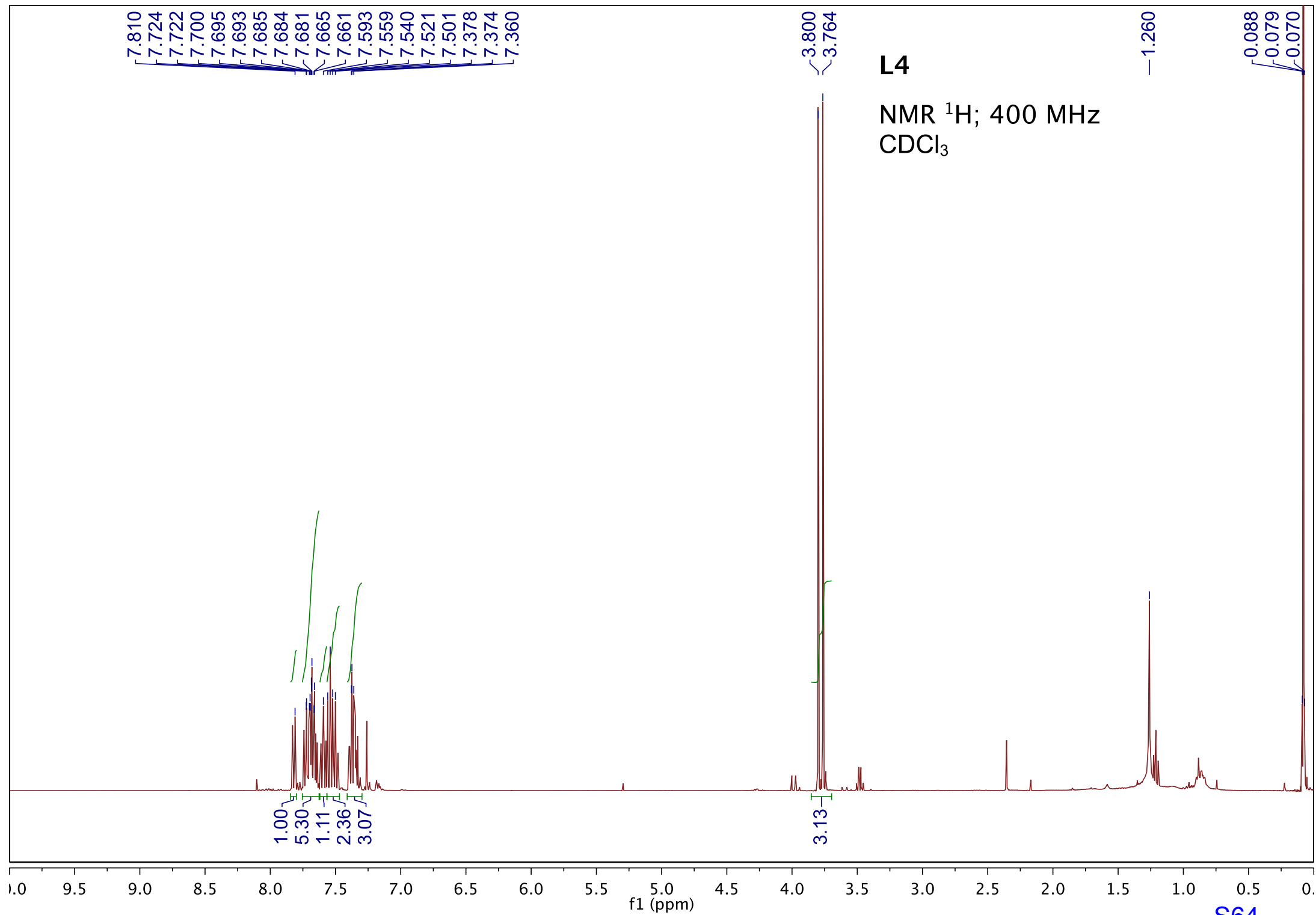
L4

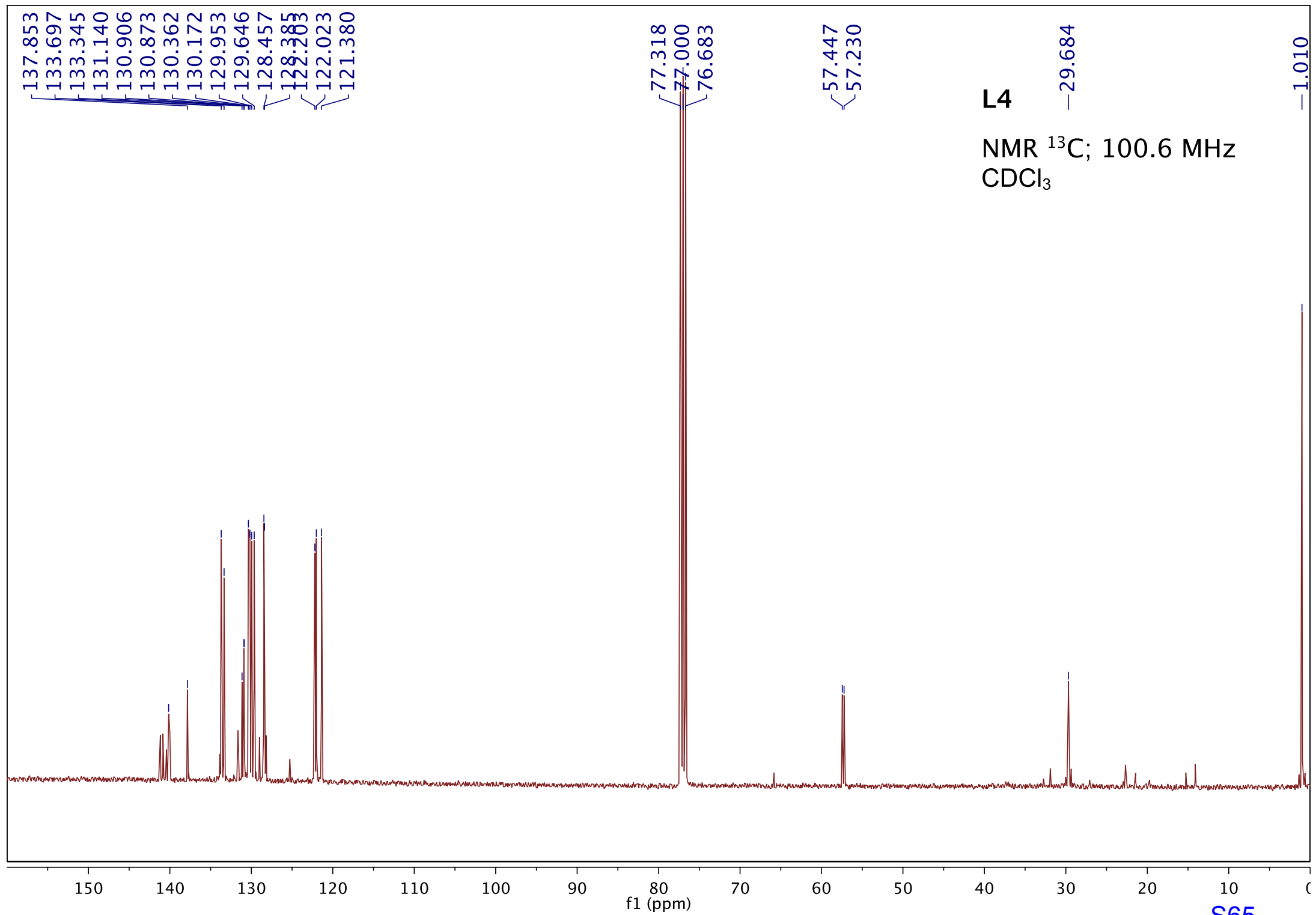
NMR ^{31}P ; 161.9 MHz
 CDCl_3

—101.411



S63





L5

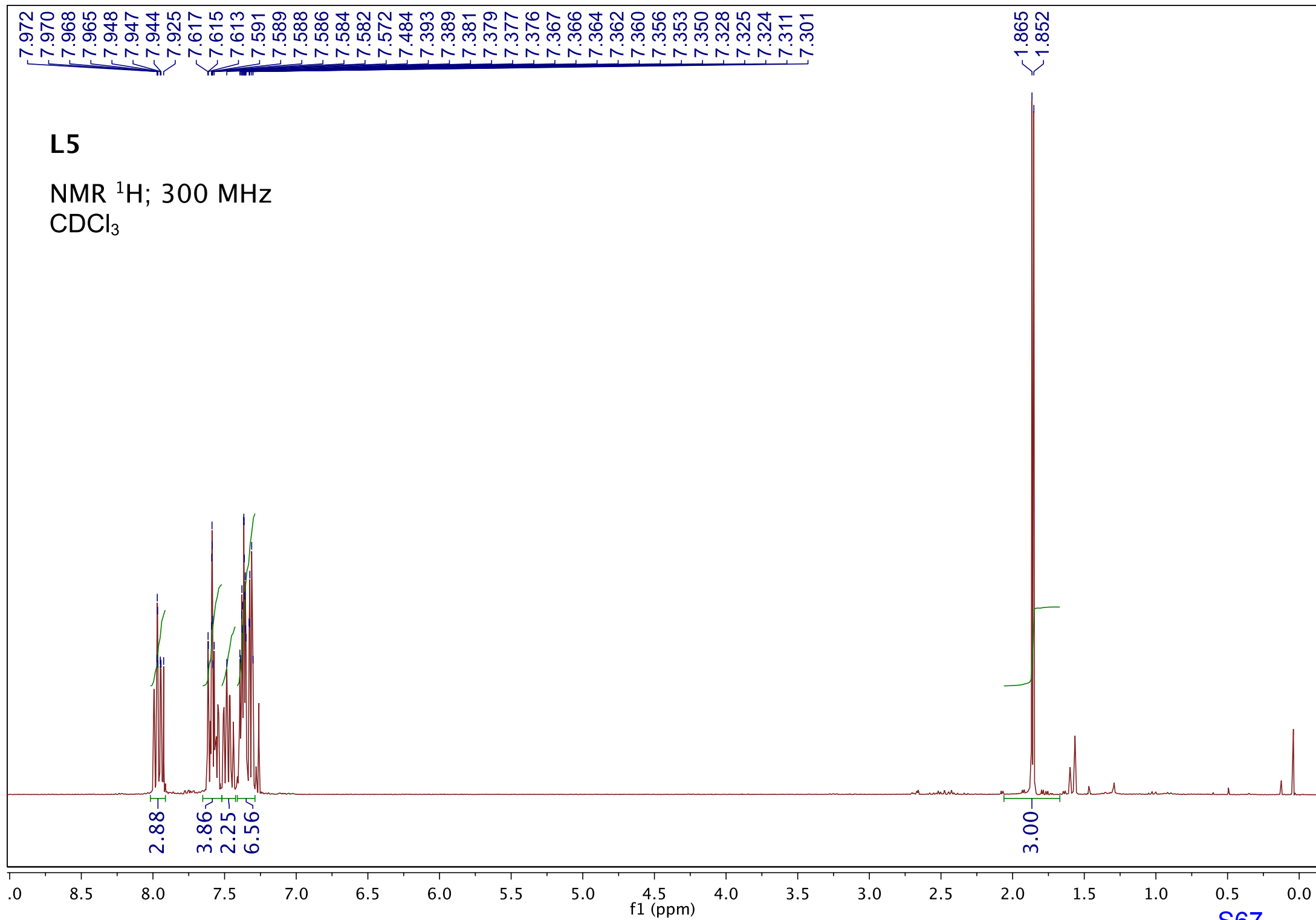
NMR ^{31}P ; 121.4 MHz

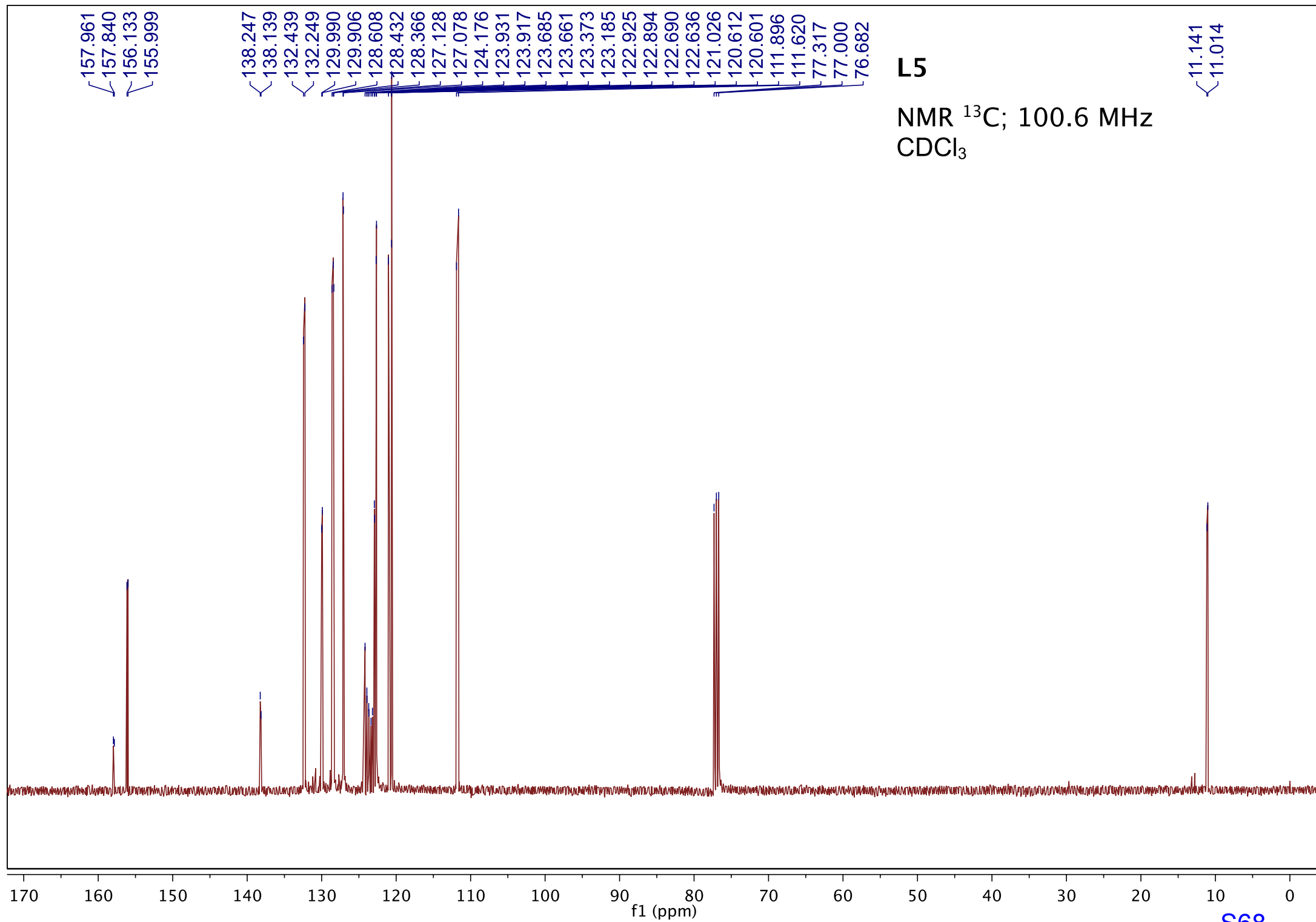
CDCl_3

--37.017

0 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -5
f1 (ppm)

S66





L6

NMR ^{31}P ; 121.4 MHz

CDCl_3

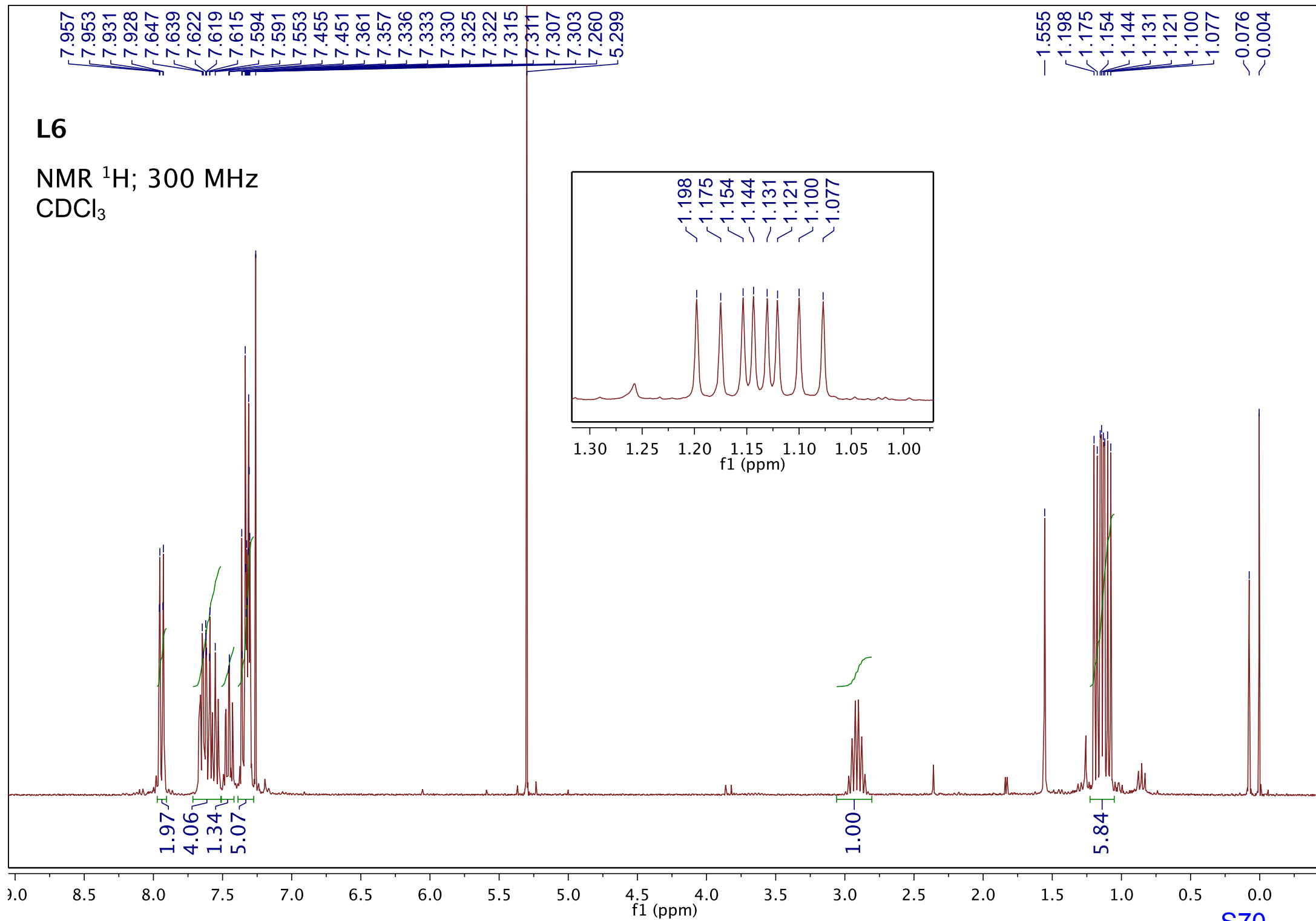
10.713

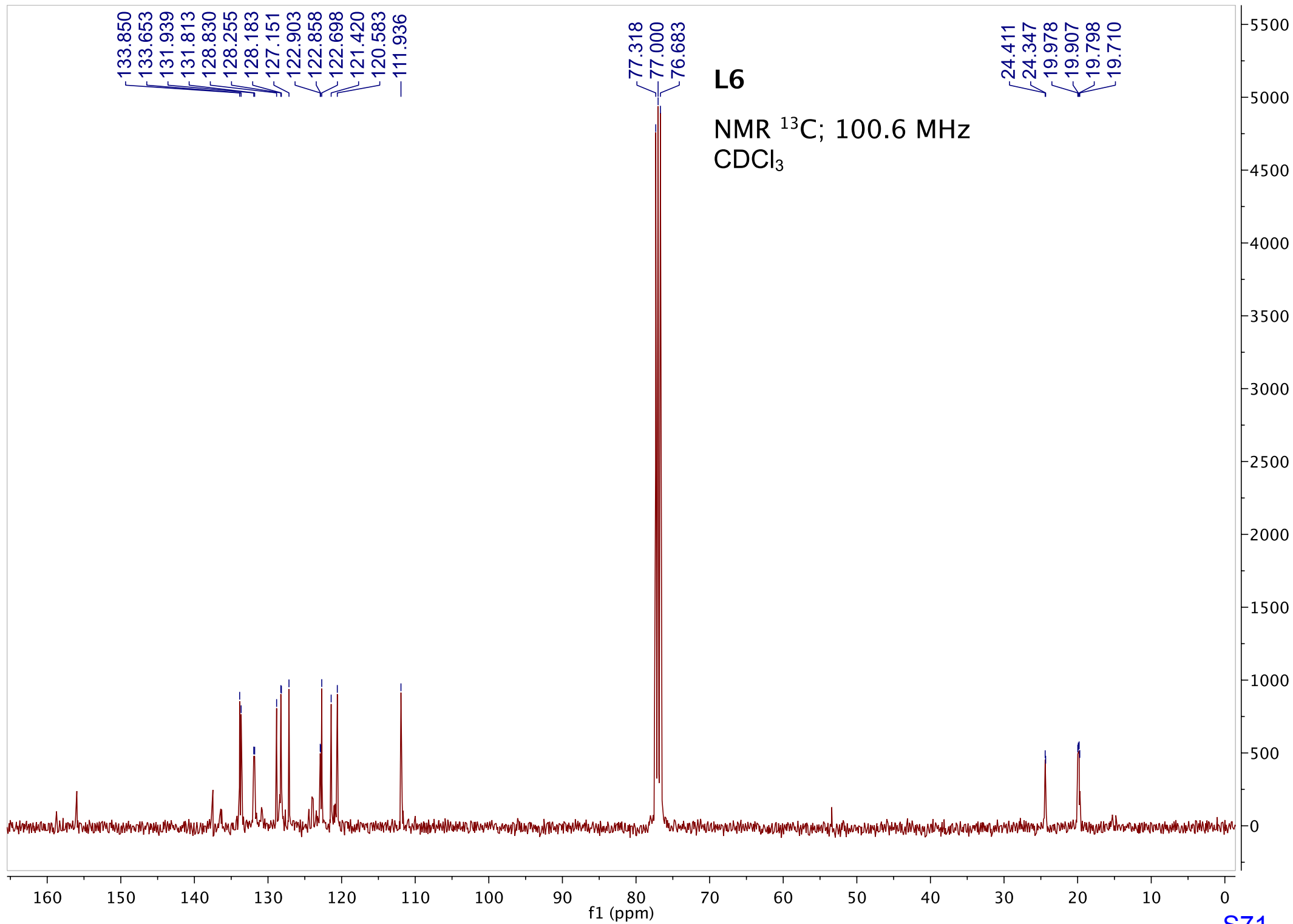
f1 (ppm)

S69

L6

NMR ^1H ; 300 MHz
 CDCl_3





L7

NMR ^{31}P ; 121.4 MHz

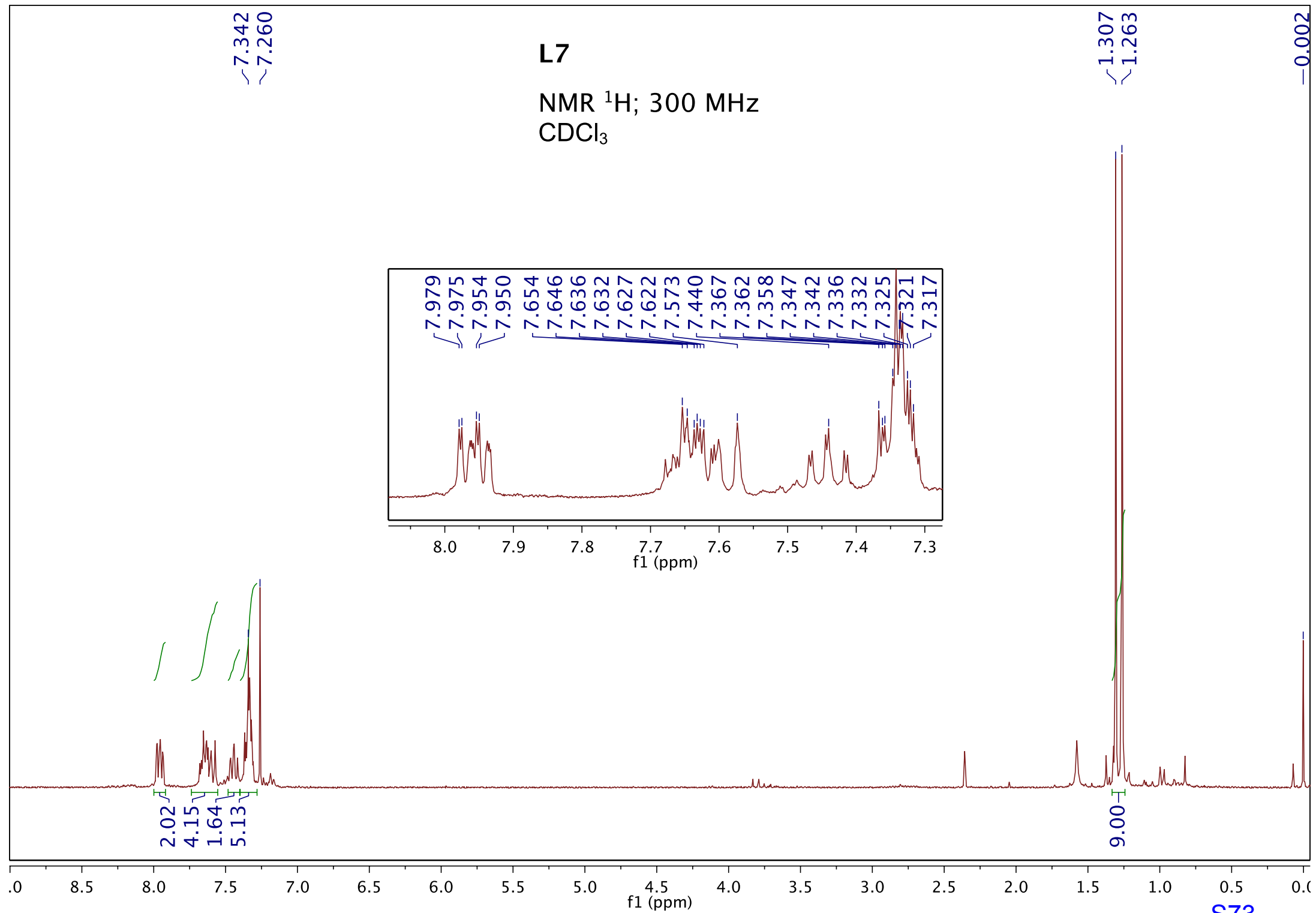
CDCl_3

—0.651

100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45 -50

f1 (ppm)

S72

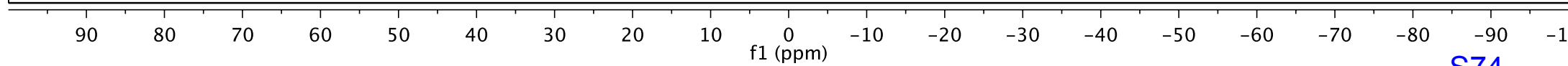


L8

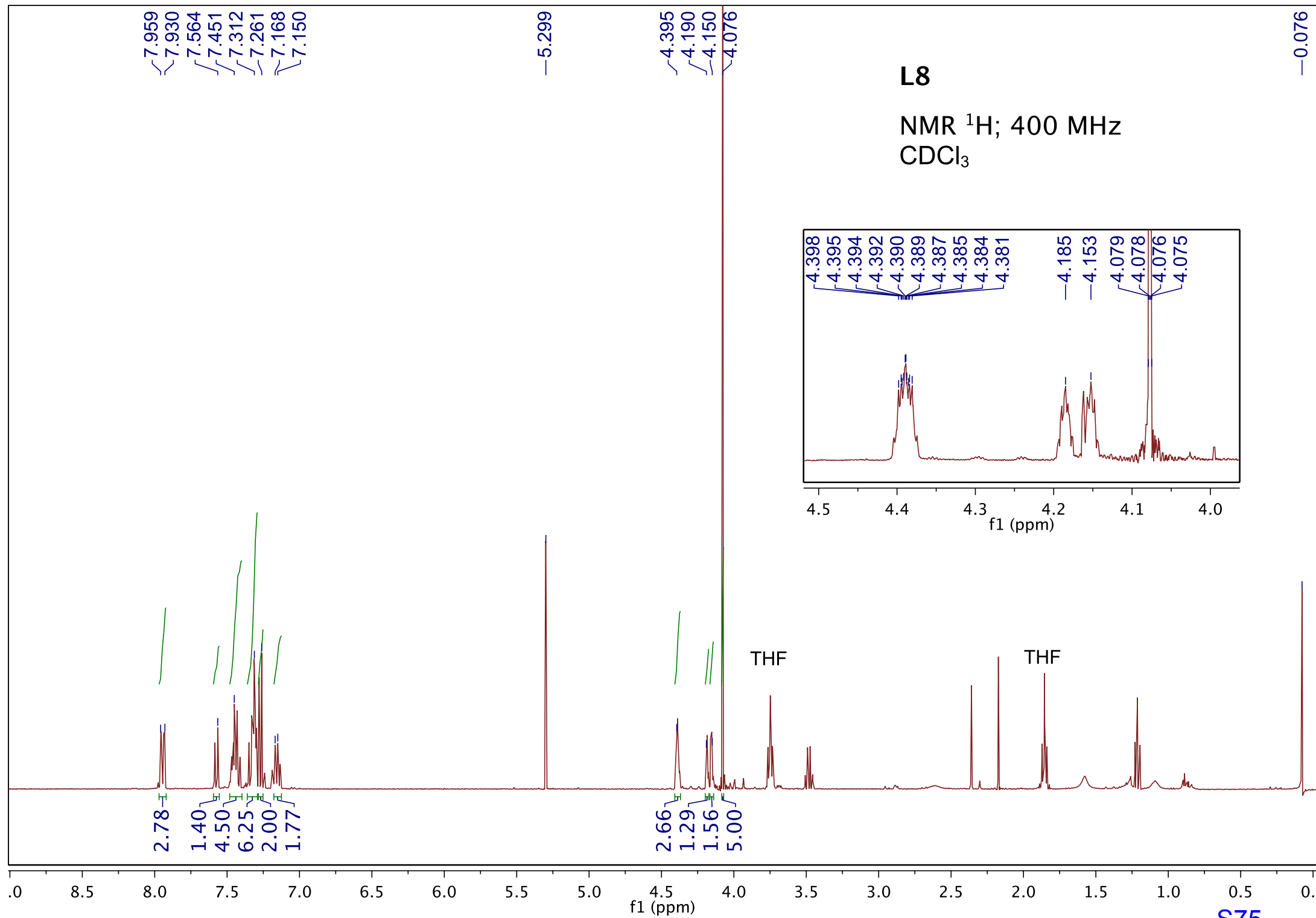
NMR ^{31}P ; 161.9 MHz

CDCl_3

--32.128

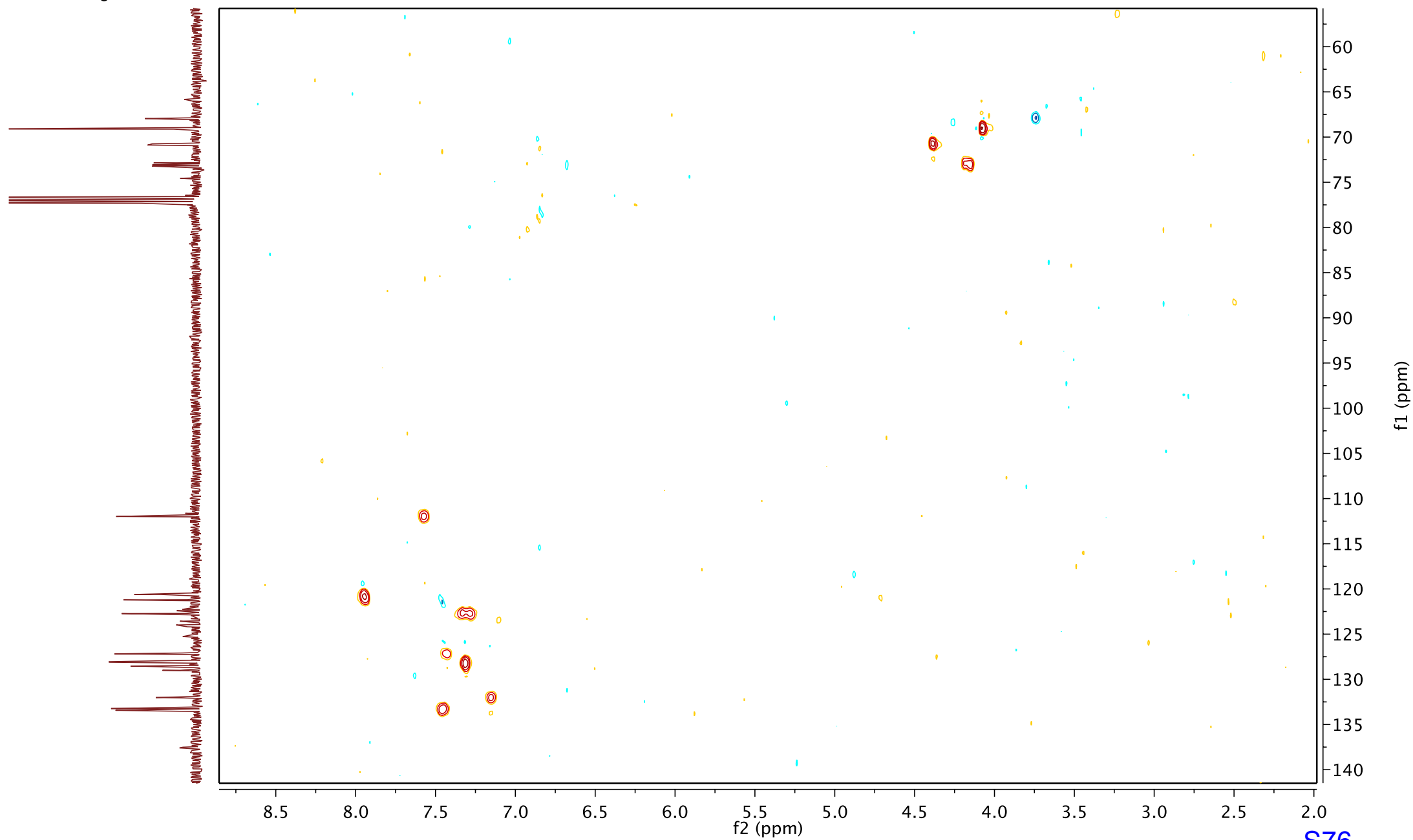


S74



L8

gHSQC 400MHz
CDCl₃



L9

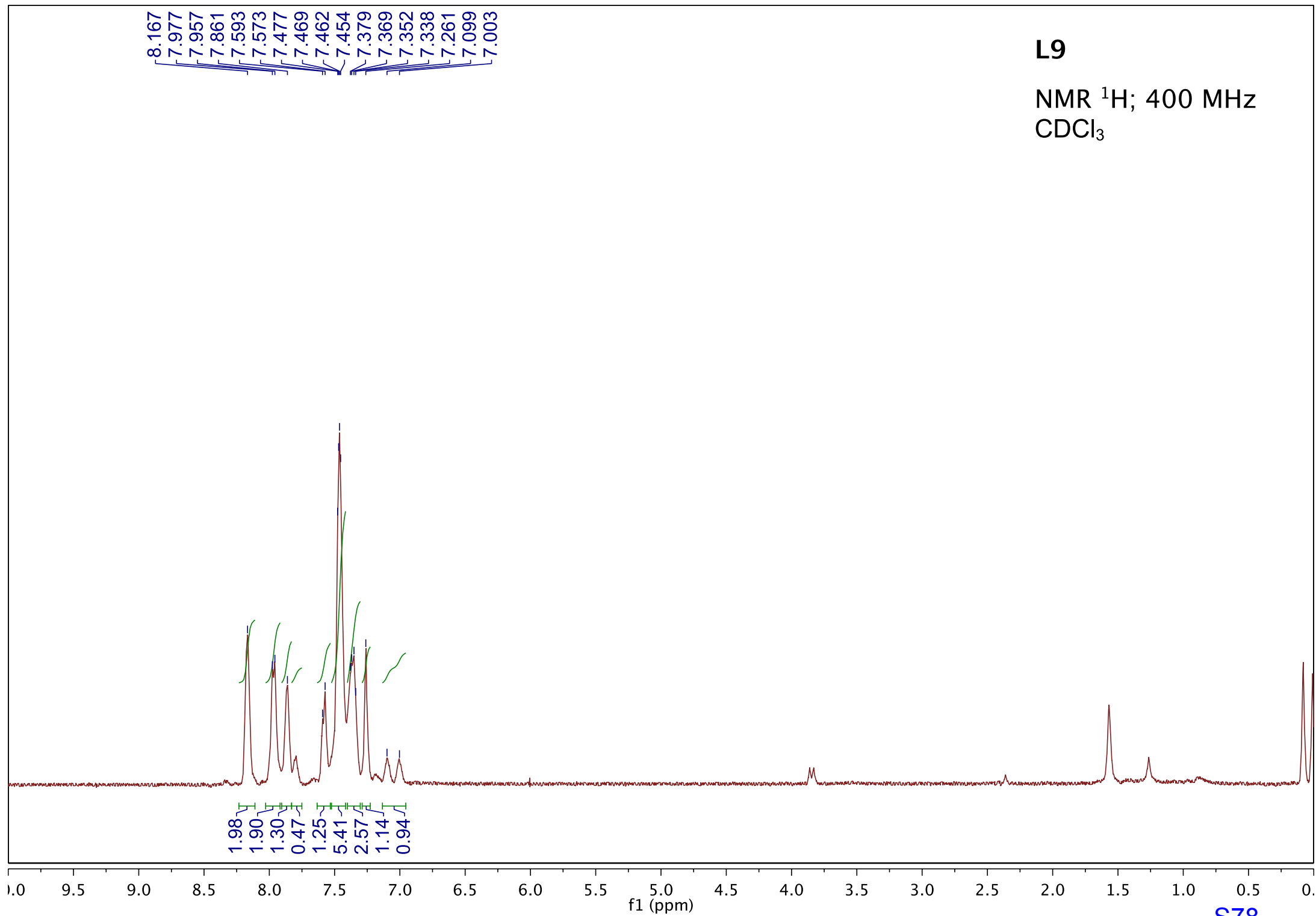
NMR ^{31}P ; 161.9 MHz

CDCl_3

--23.083

40 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -5
f1 (ppm)

S77

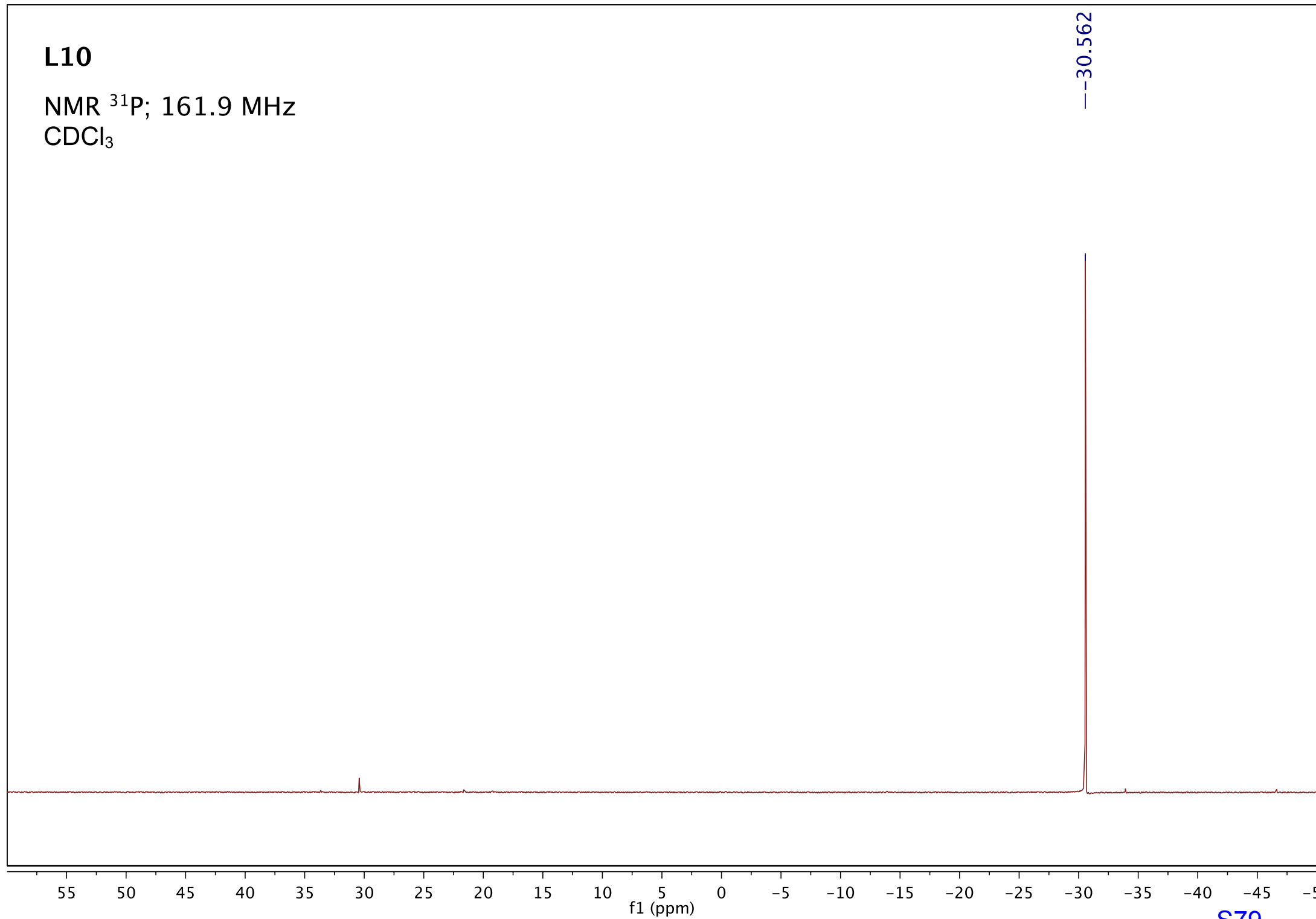


L10

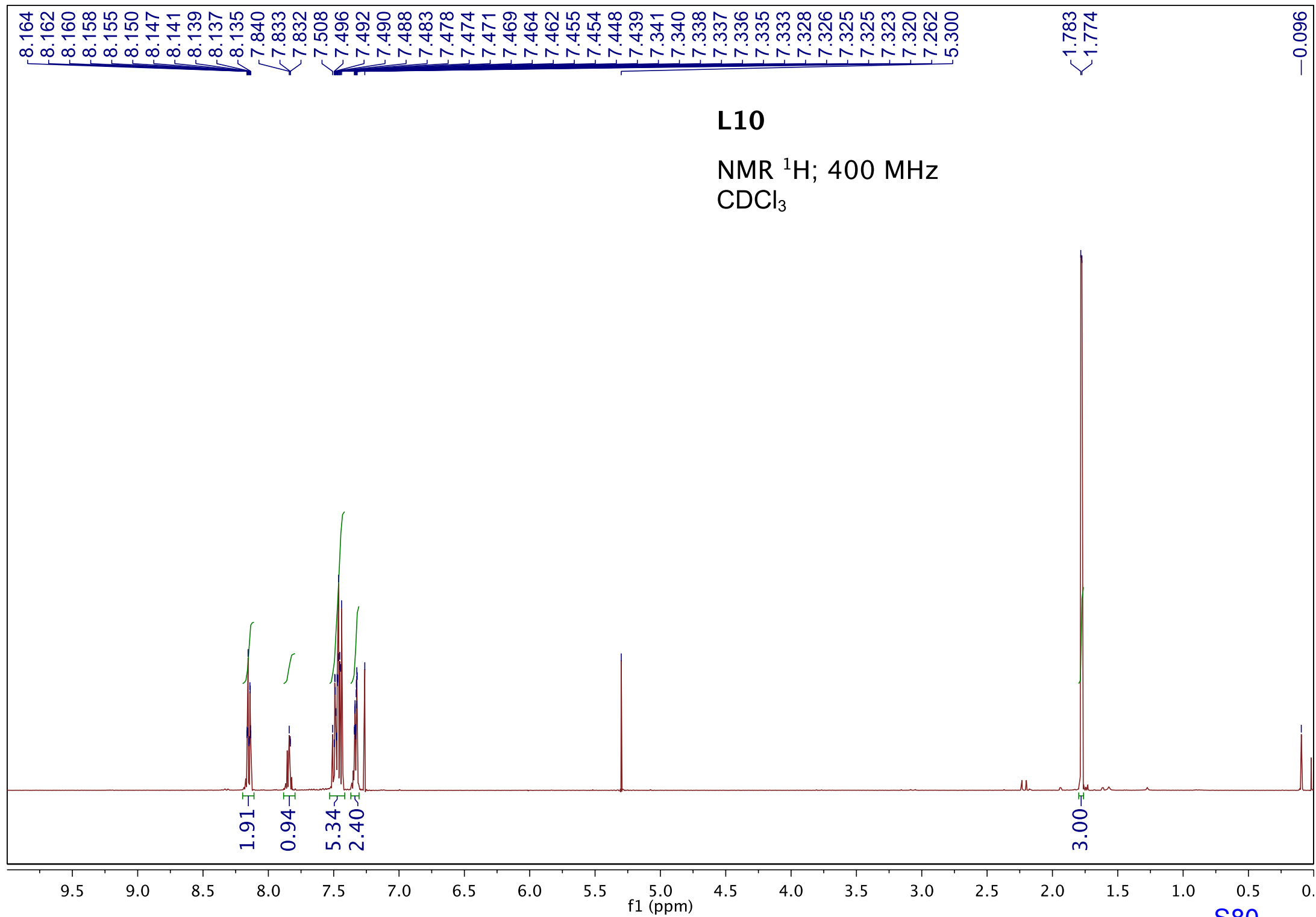
NMR ^{31}P ; 161.9 MHz

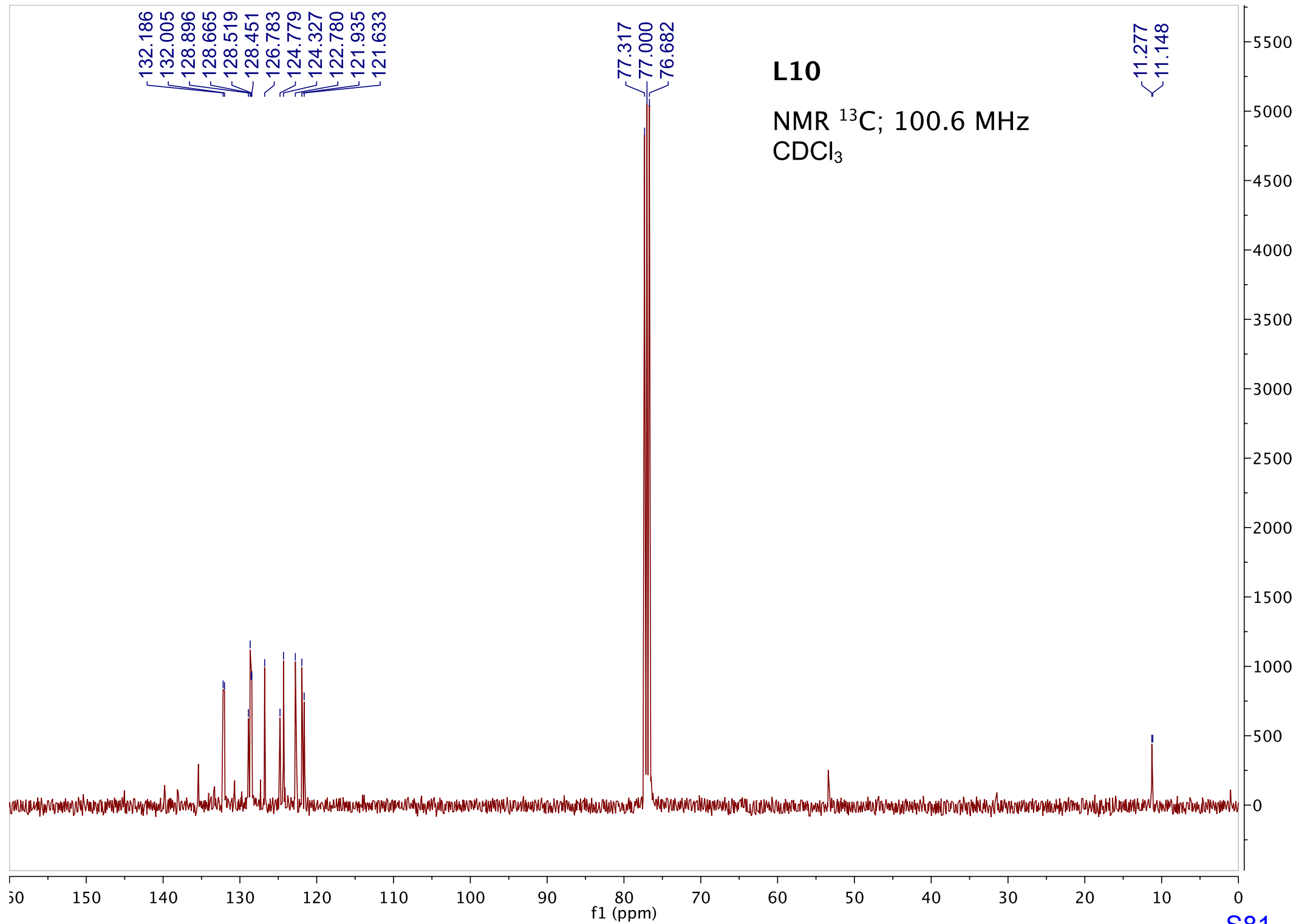
CDCl_3

--30.562



S79





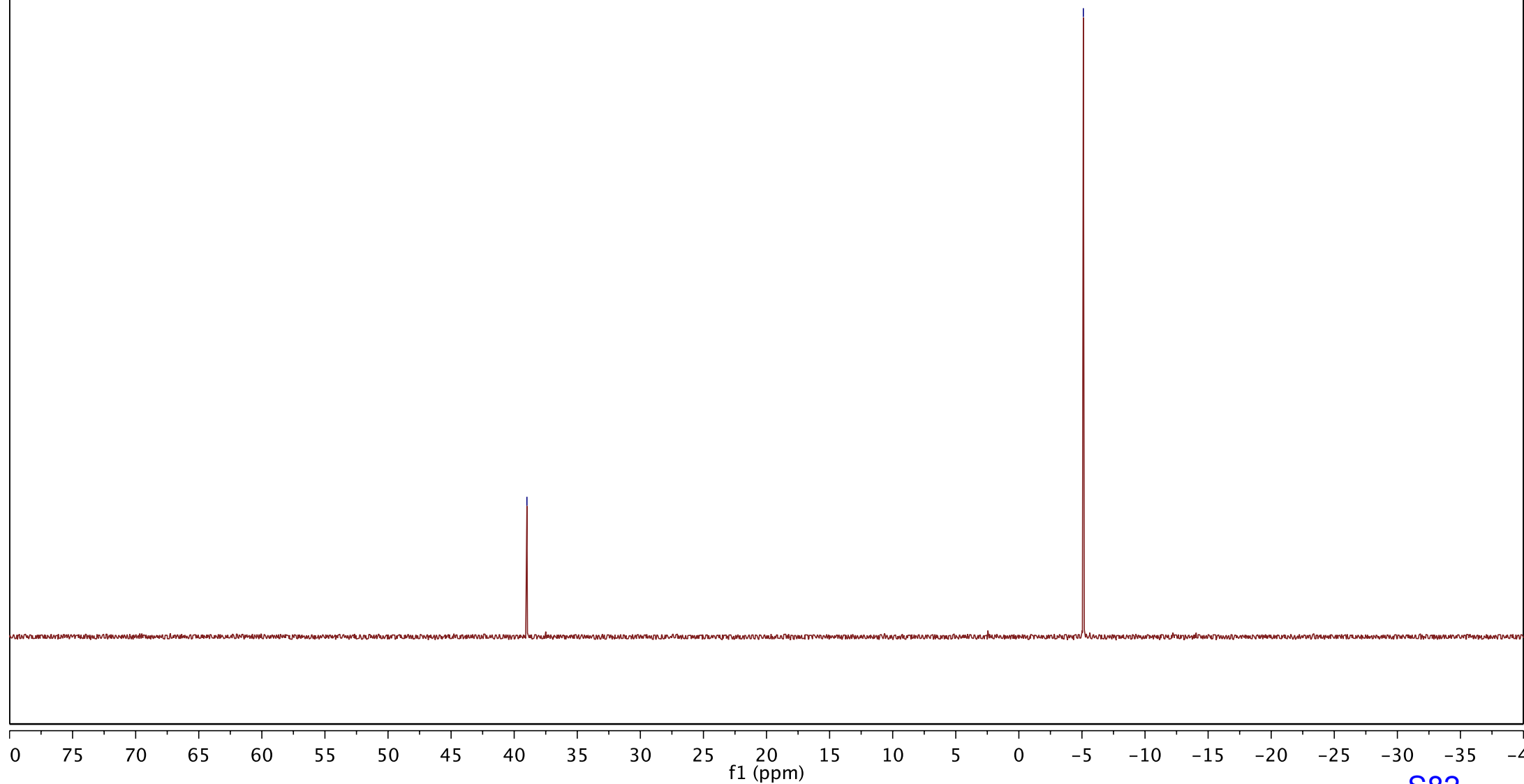
L11

NMR ^{31}P ; 161.9 MHz

CDCl_3

—38.990

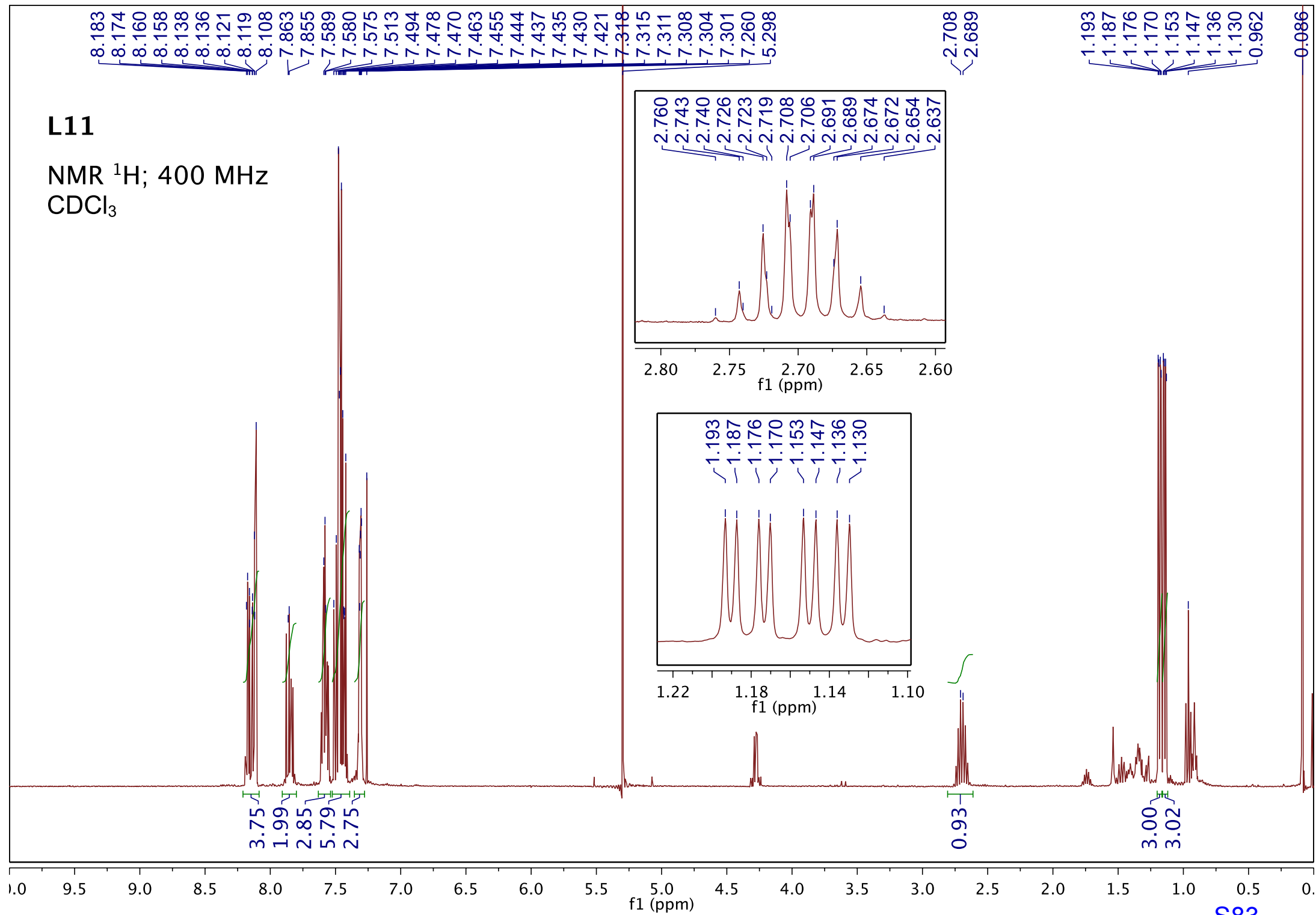
—5.111

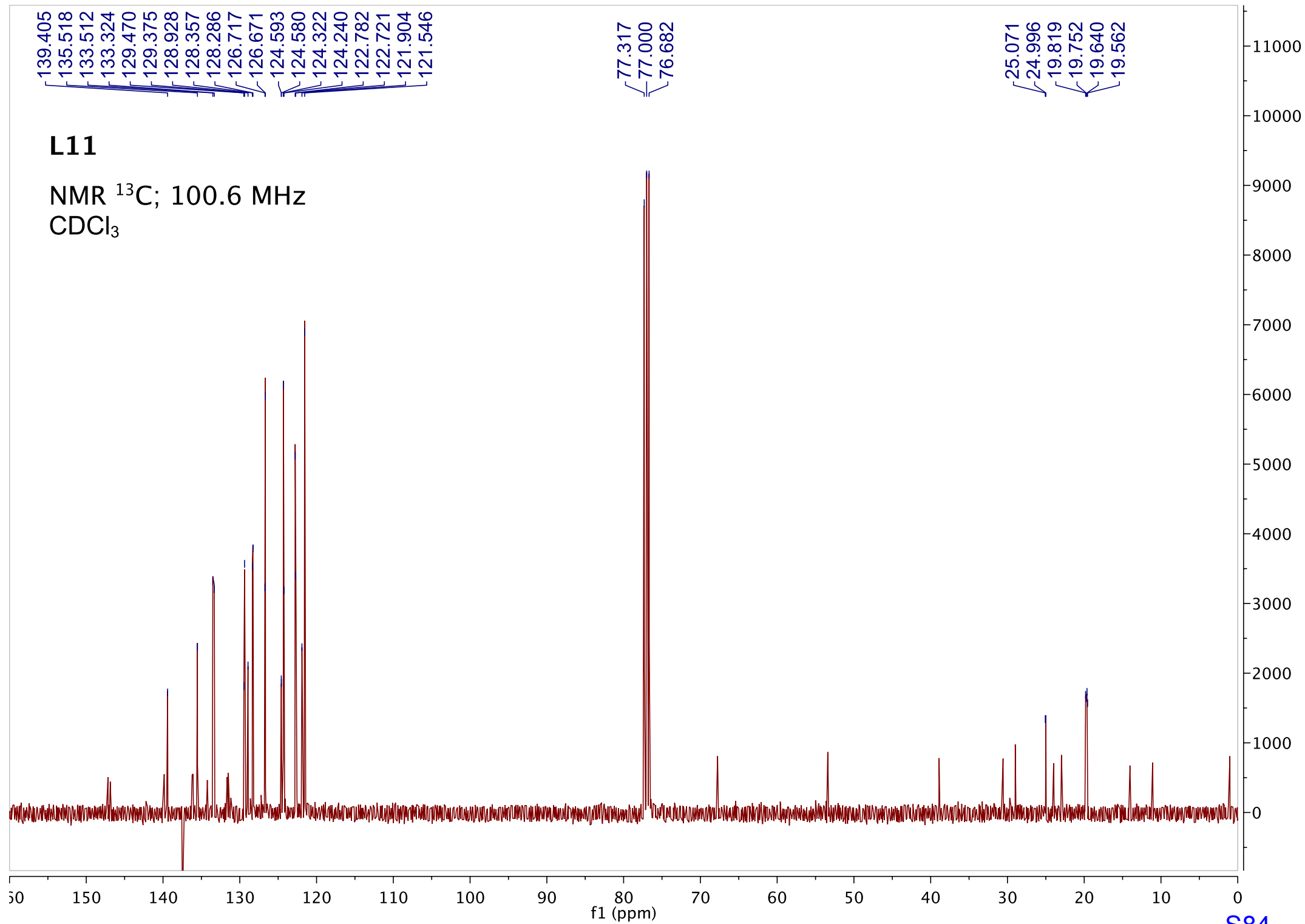


S82

L11

NMR ^1H ; 400 MHz
 CDCl_3





L12

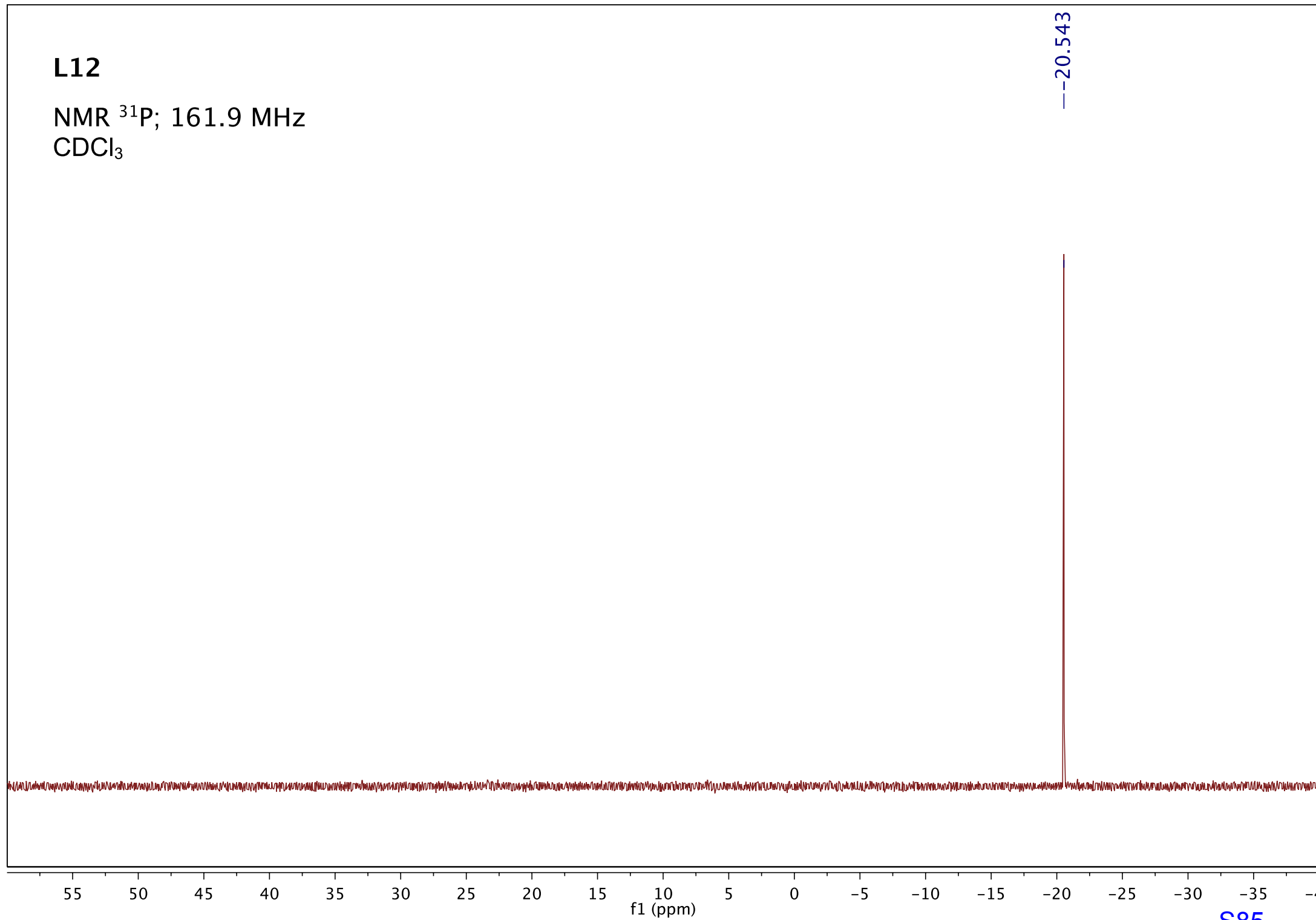
NMR ^{31}P ; 161.9 MHz

CDCl_3

--20.543

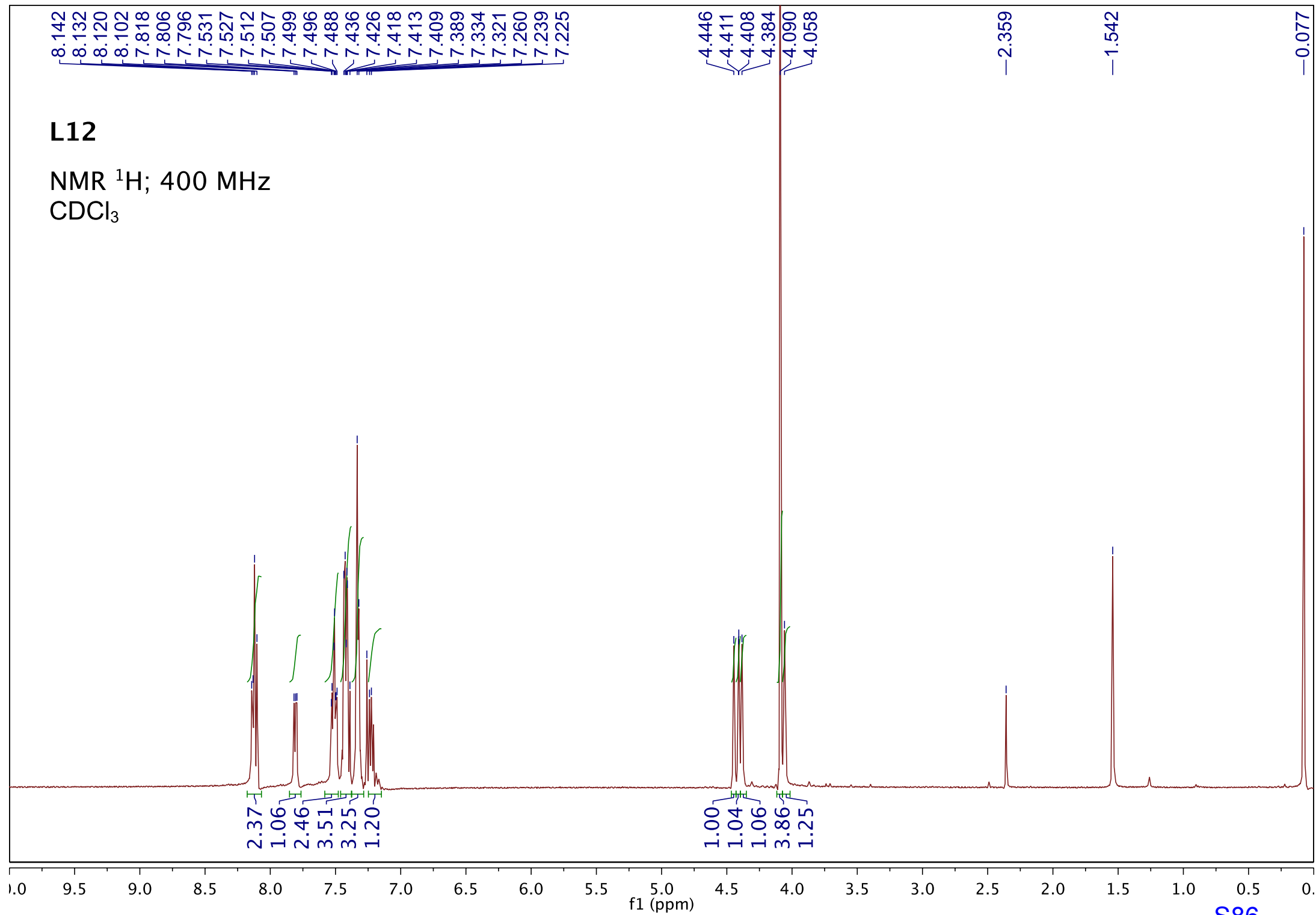
f1 (ppm)

S85



L12

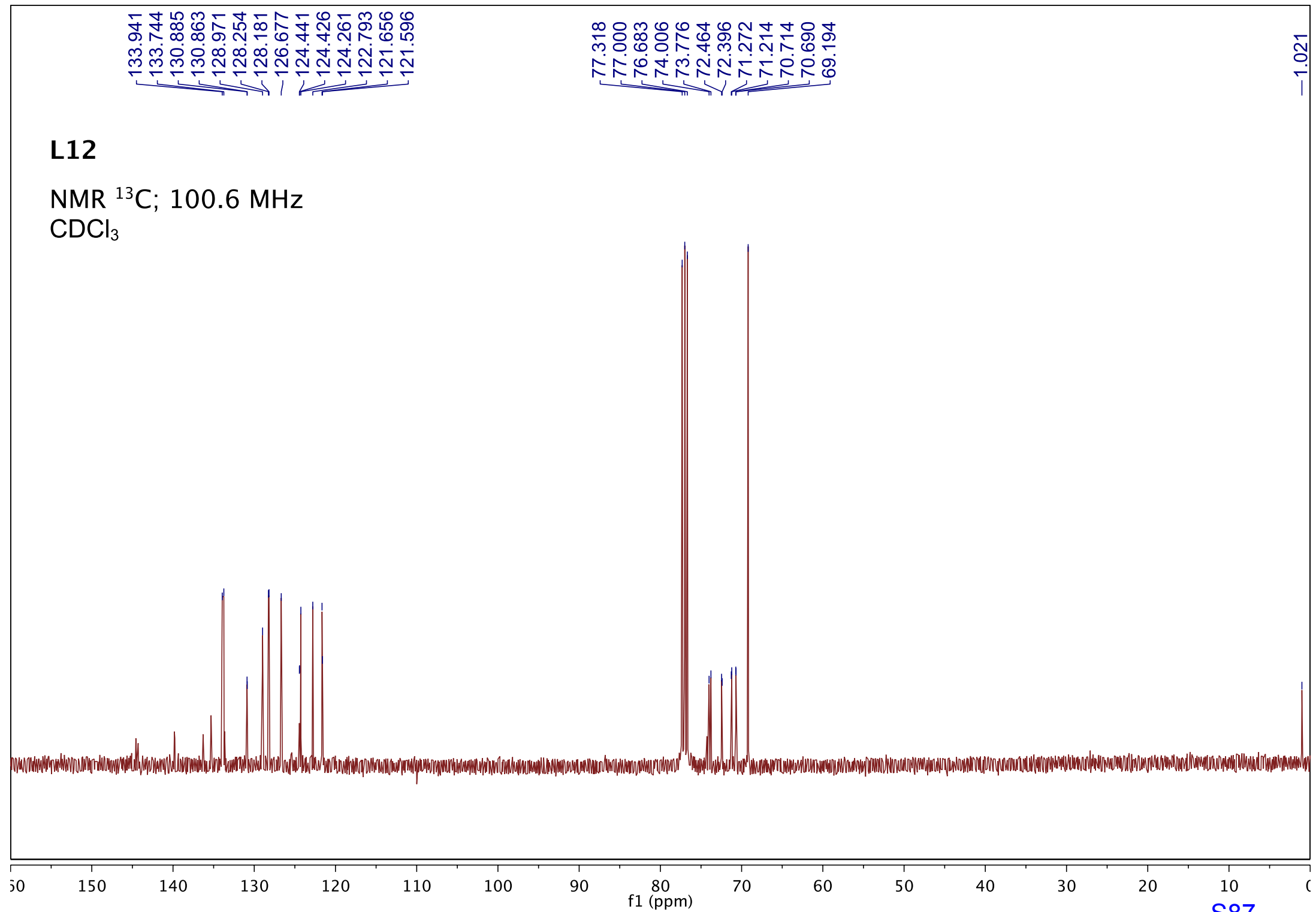
NMR ^1H ; 400 MHz
 CDCl_3



L12

NMR ^{13}C ; 100.6 MHz

CDCl_3



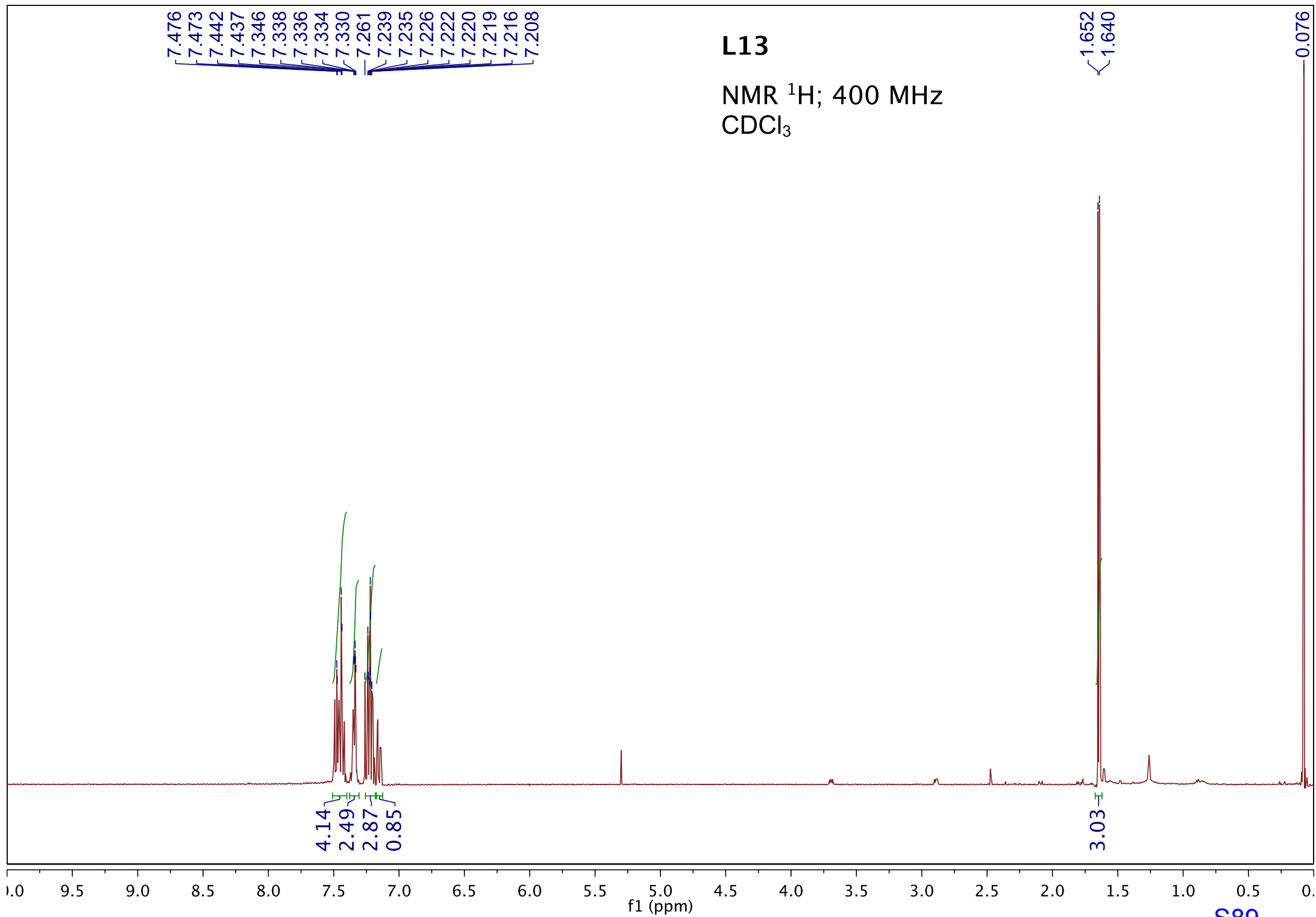
L13

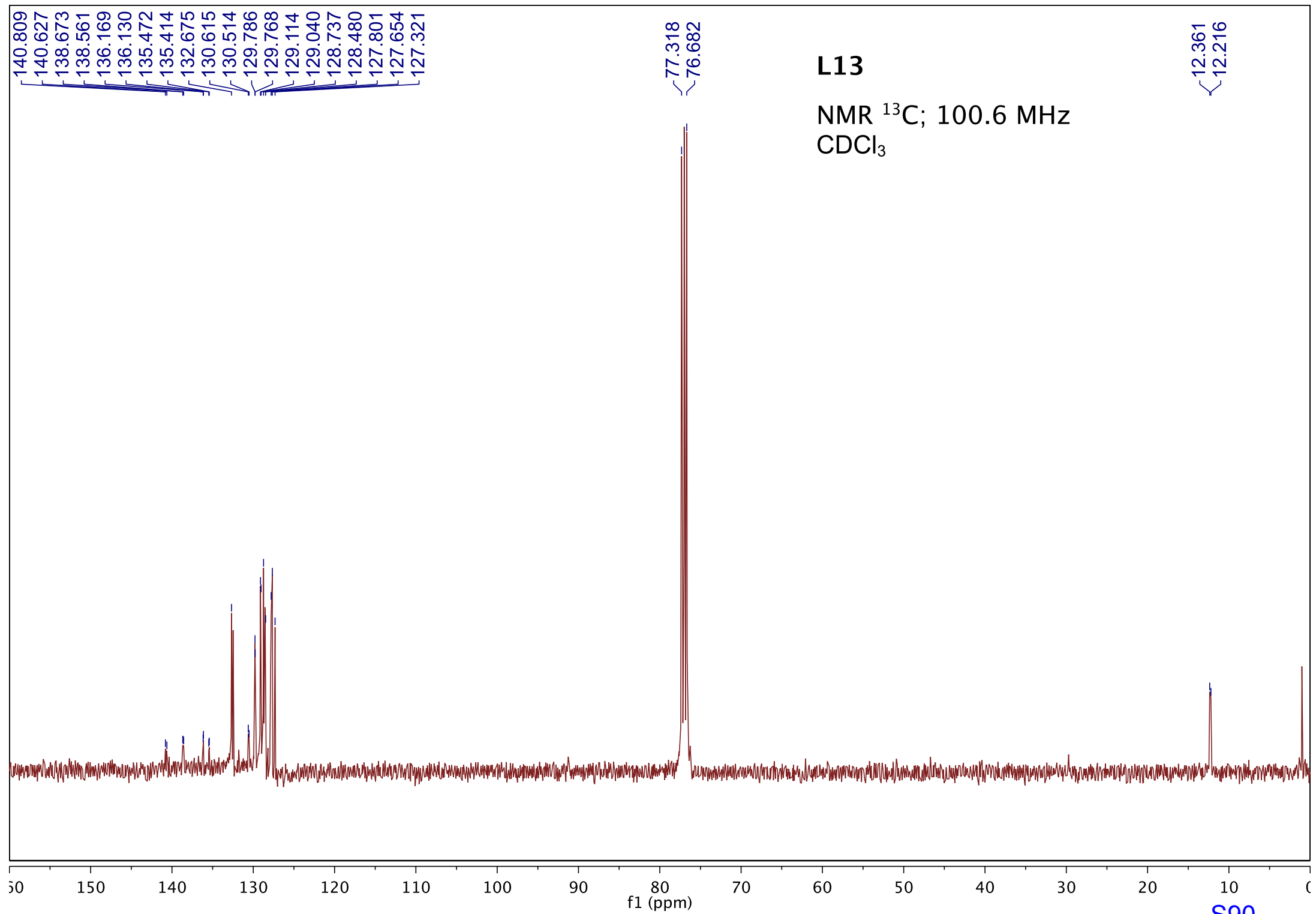
NMR ^{31}P ; 161.9
MHz CDCl_3

--32.049

0 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40 -45
f1 (ppm)

S88





Ru1

NMR ^{31}P ; 121.4 MHz
 CDCl_3

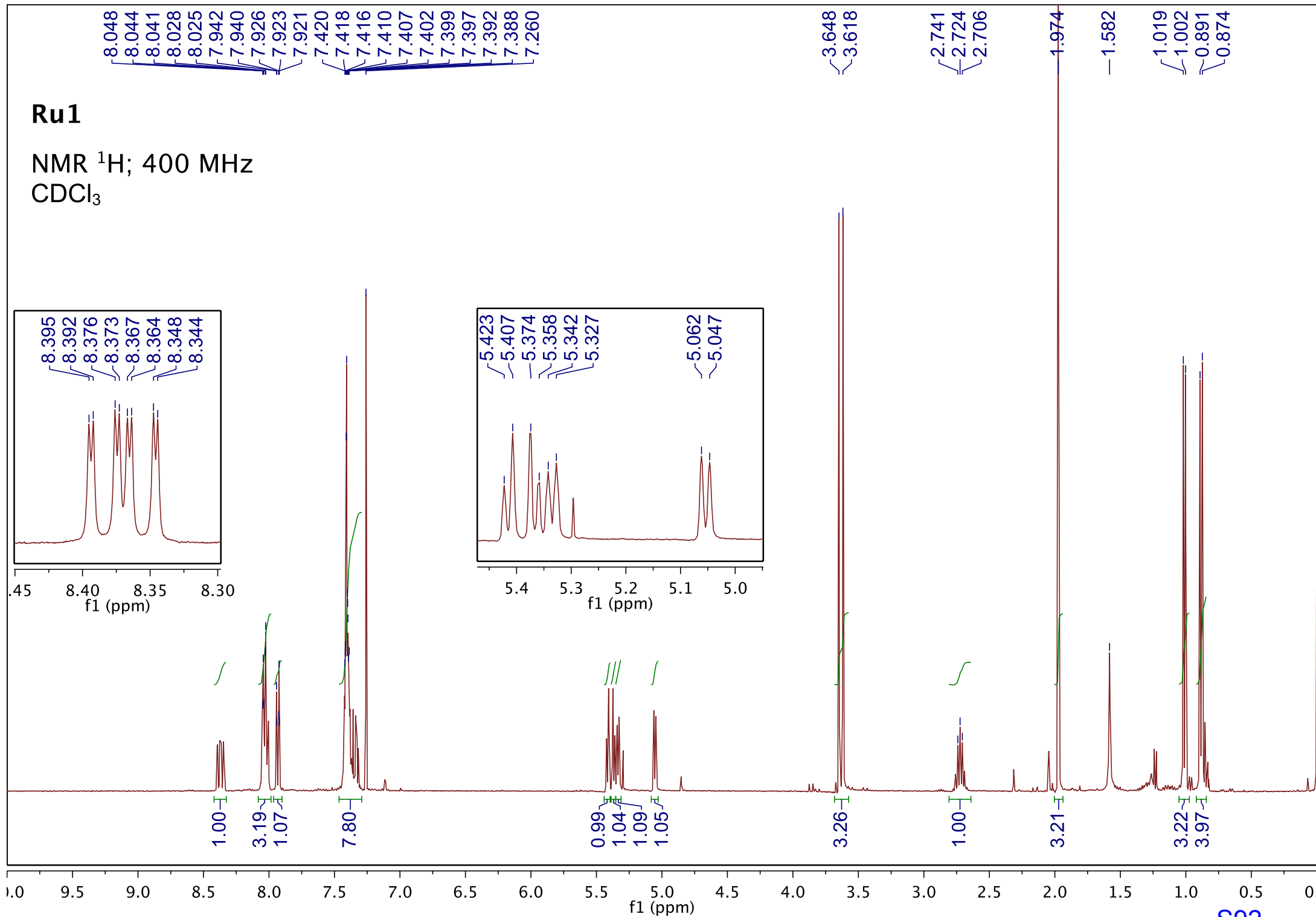
112.651

170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

S91

Ru1

NMR ^1H ; 400 MHz
 CDCl_3



Ru1

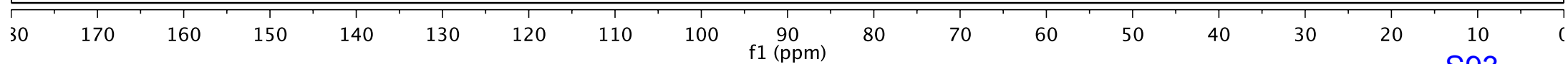
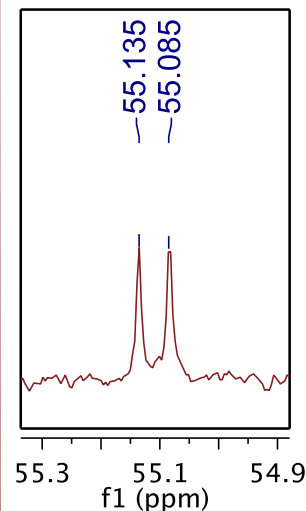
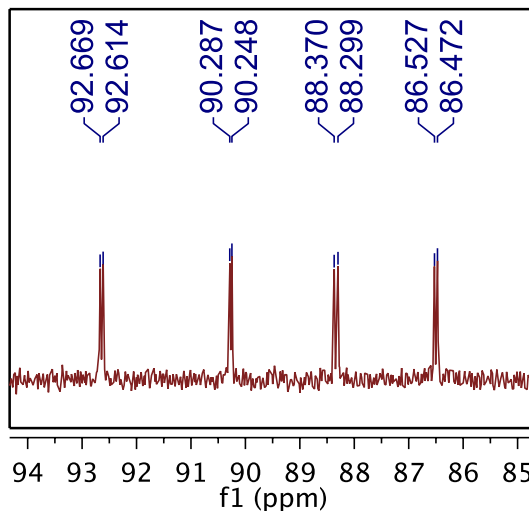
NMR ^{13}C ; 100.6 MHz
 CDCl_3

155.628
155.041
135.384
135.254
131.887
131.772
127.831
127.725
127.267
124.085
124.063
123.446
123.099
122.564
122.462
120.595
111.559
110.958
110.941
—96.507

55.135
55.085

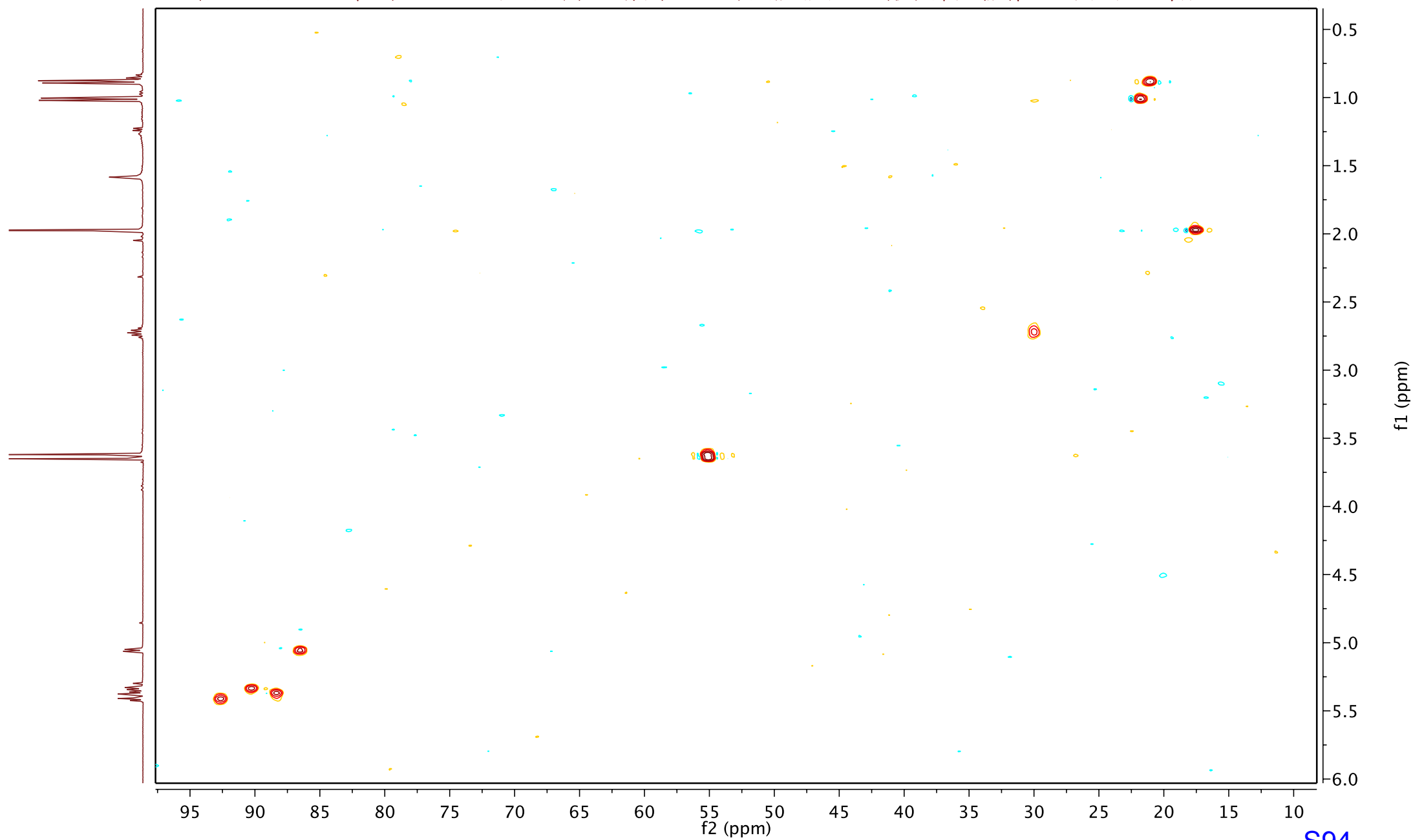
—29.979

21.833
21.040
17.577



Ru1

gHSQC 400MHz
CDCl₃

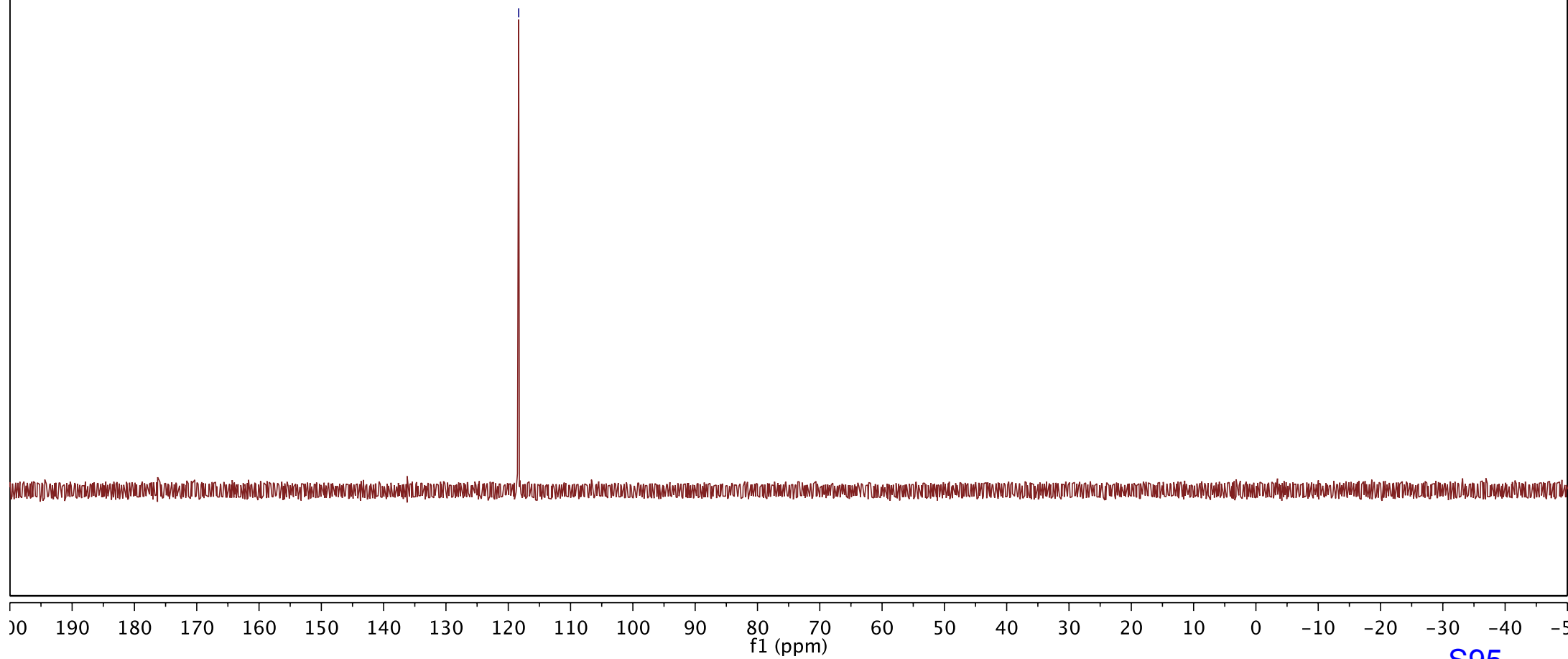


Ru2

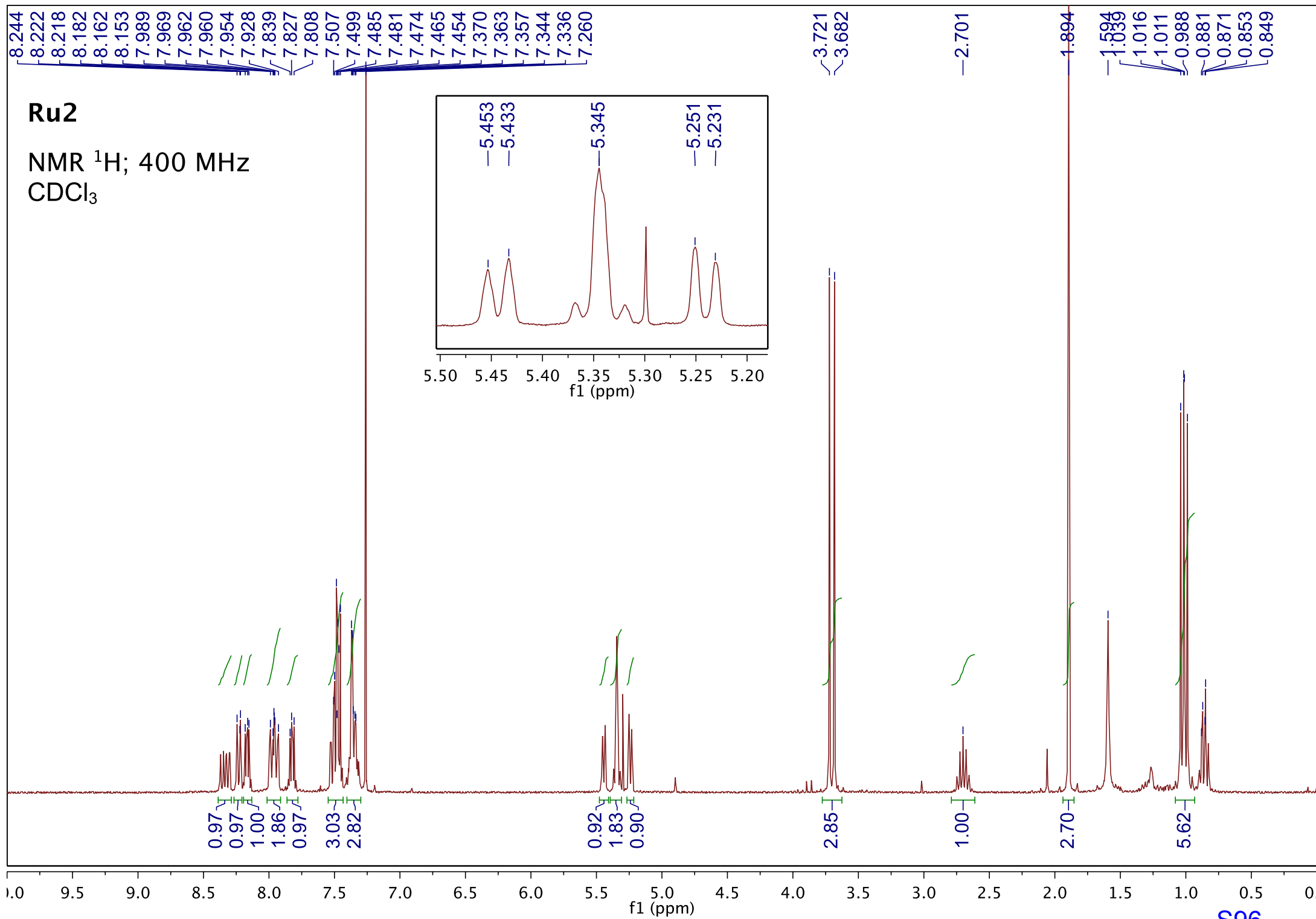
NMR ^{31}P ; 121.4 MHz

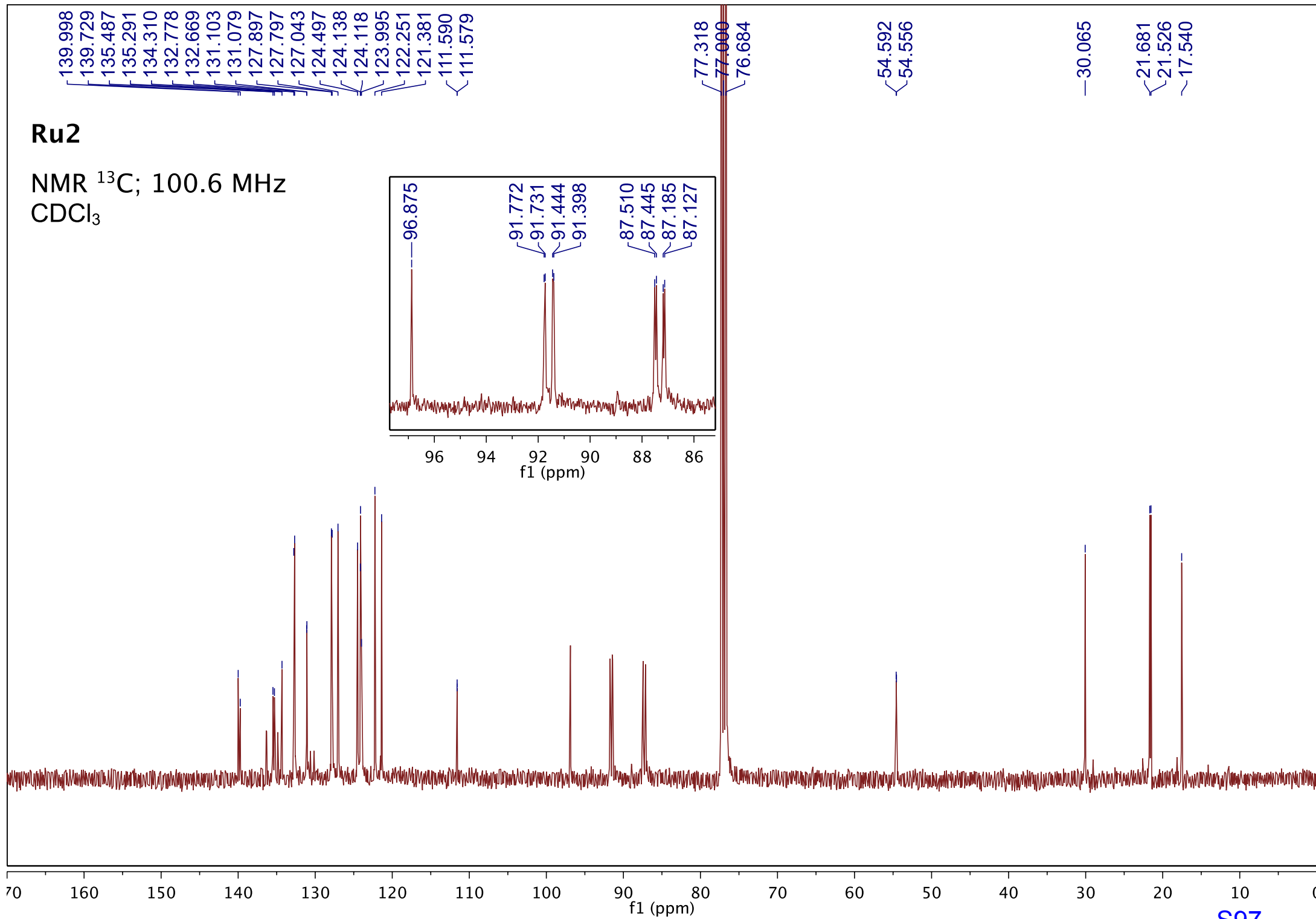
CDCl_3

—118.326



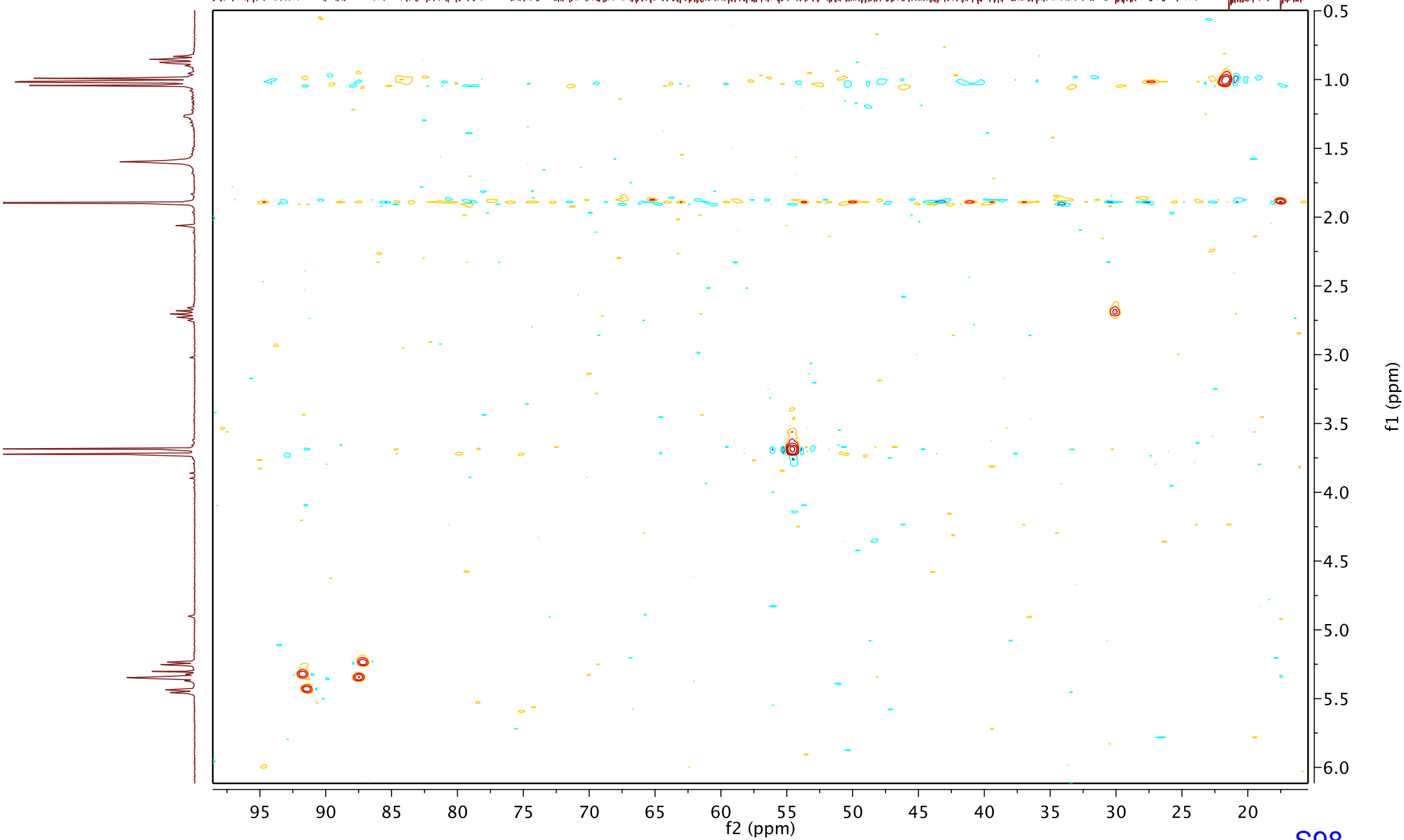
S95





Ru2

gHSQC 400MHz
CDCl₃



Ru3

NMR ^{31}P ; 161.9 MHz

CDCl_3

—140.101

—110.196

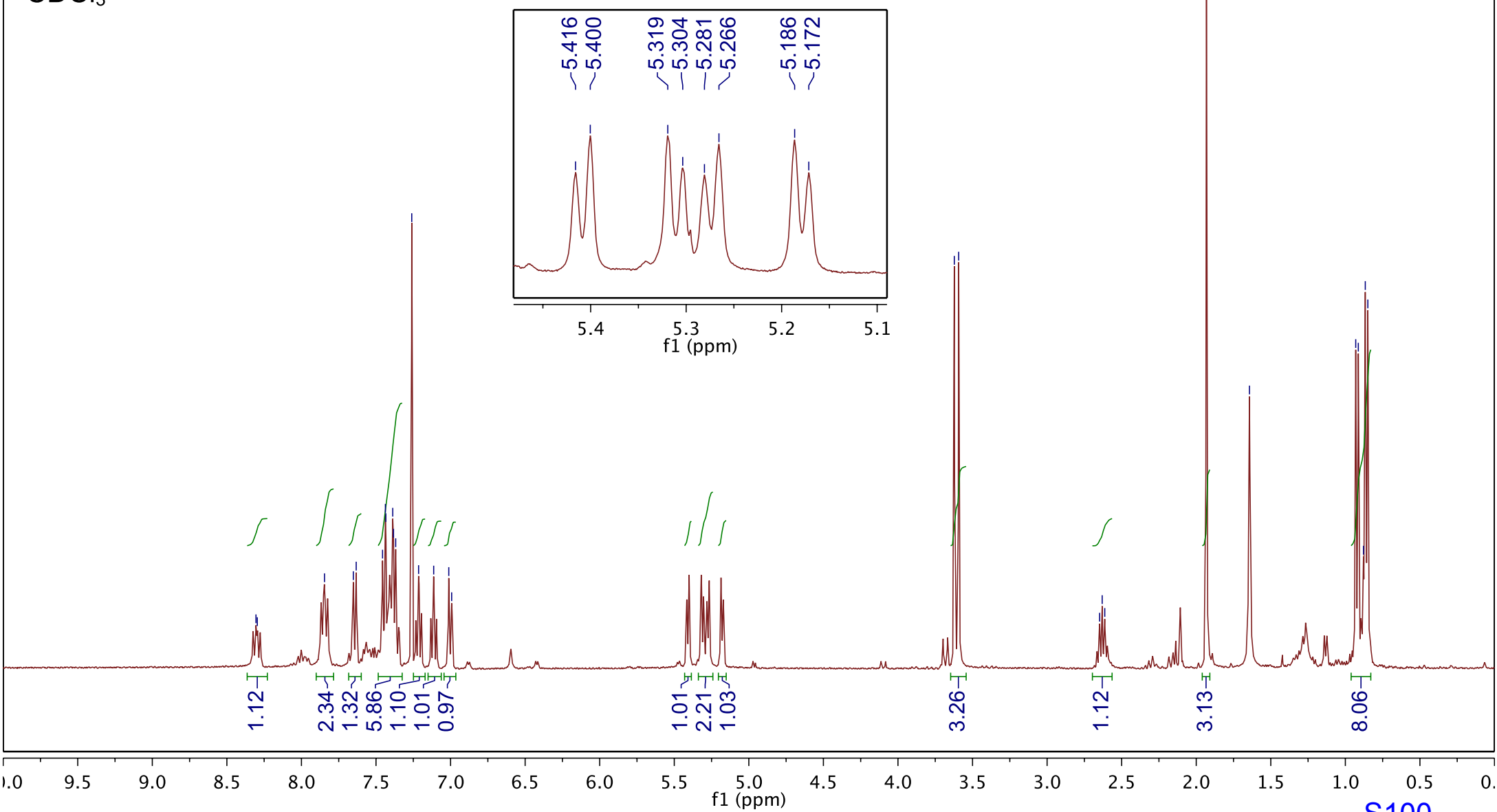
55 160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 2
f1 (ppm)

S99

Ru3

NMR ^1H ; 400 MHz

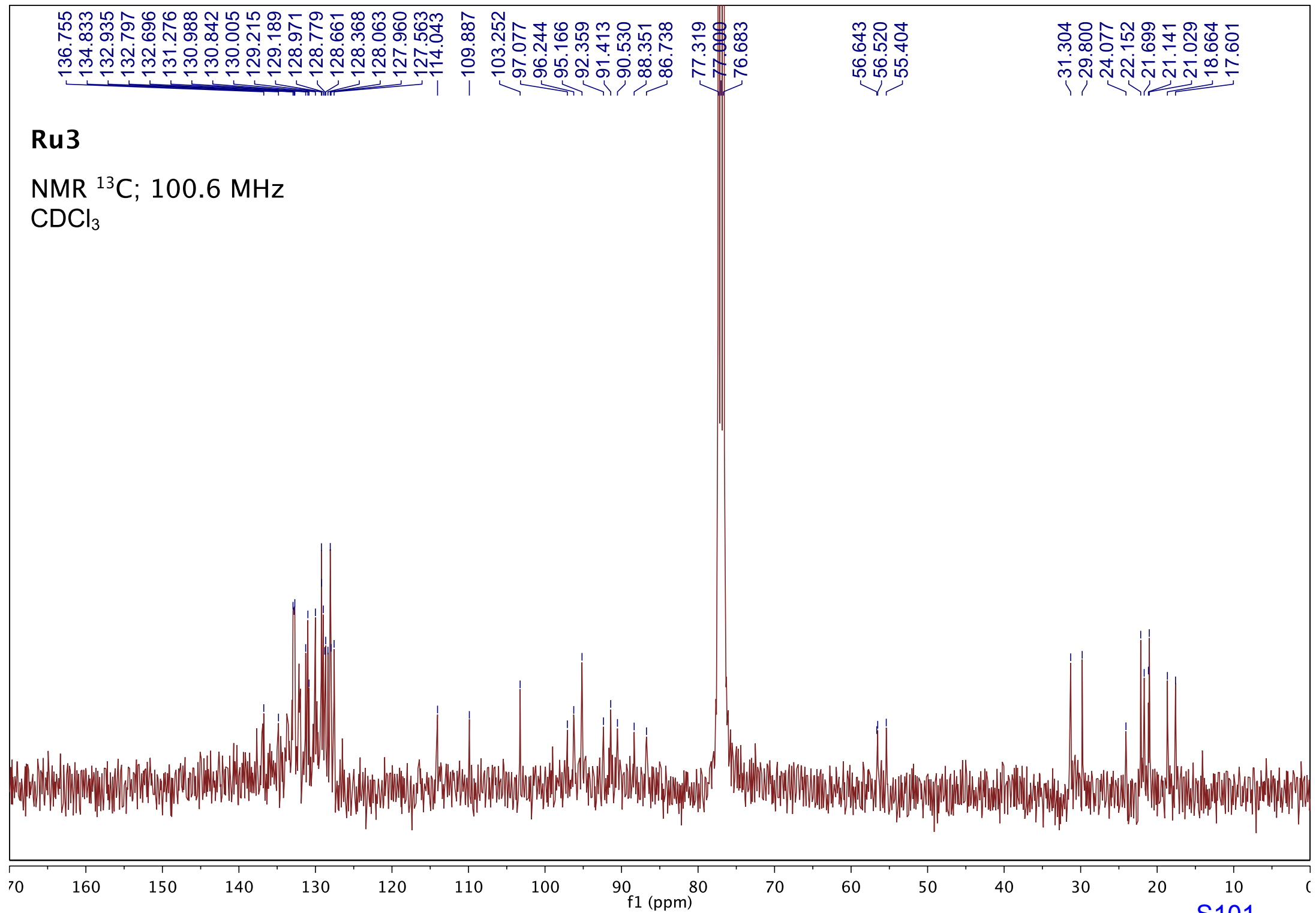
CDCl_3



Ru3

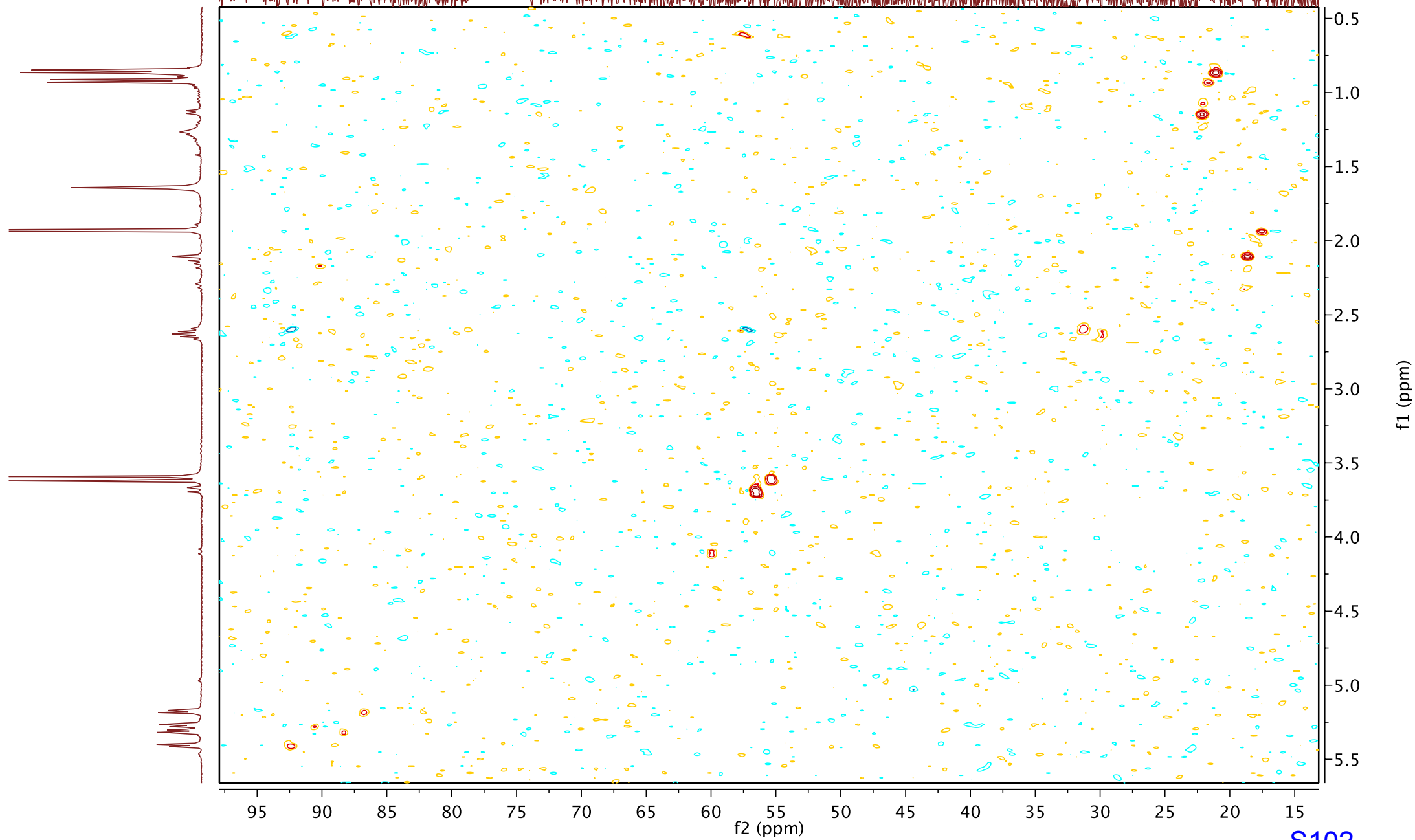
NMR ^{13}C ; 100.6 MHz

CDCl_3



S101

gHSQC
400MHz CDCl₃



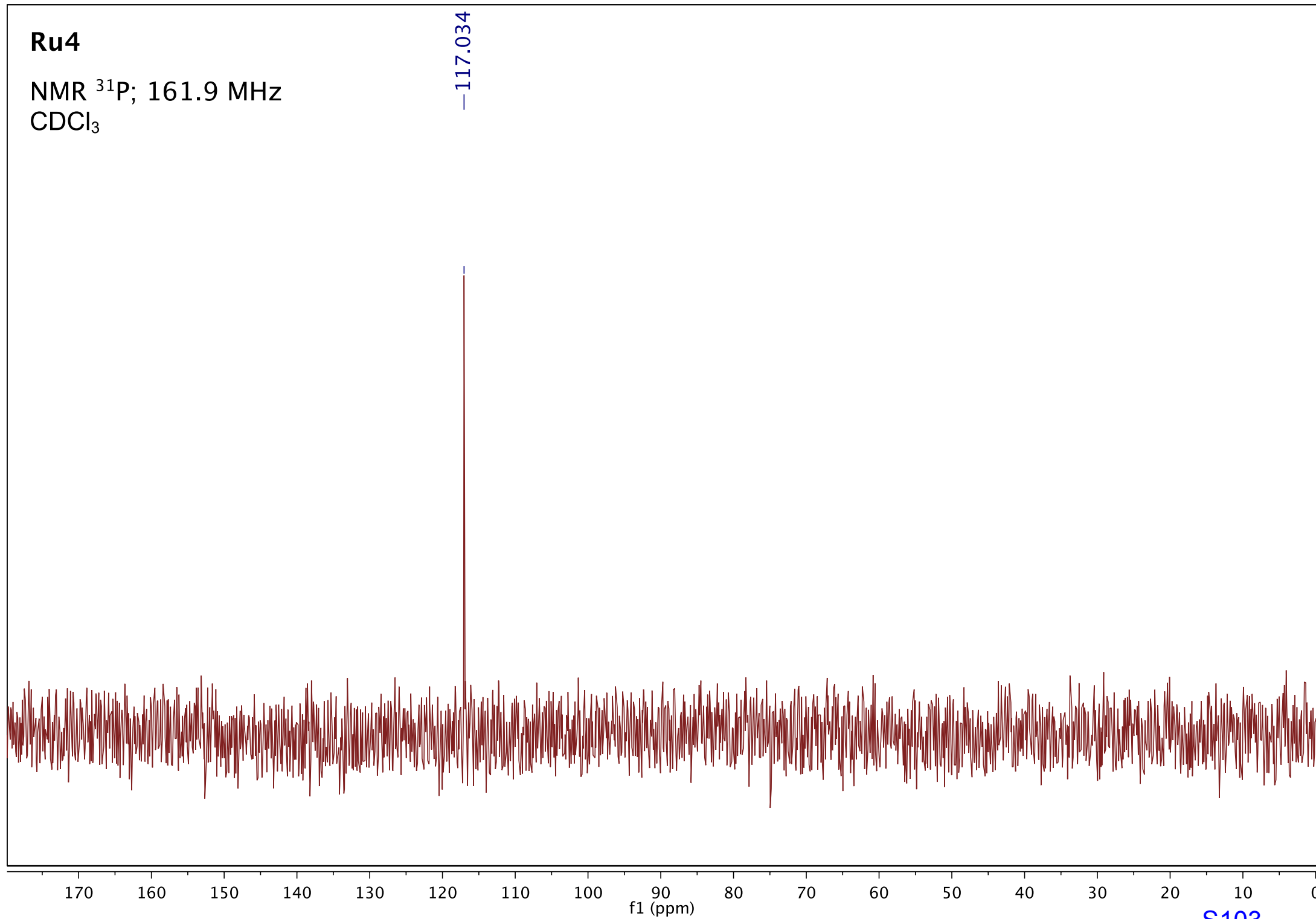
S102

Ru4

NMR ^{31}P ; 161.9 MHz

CDCl_3

—117.034

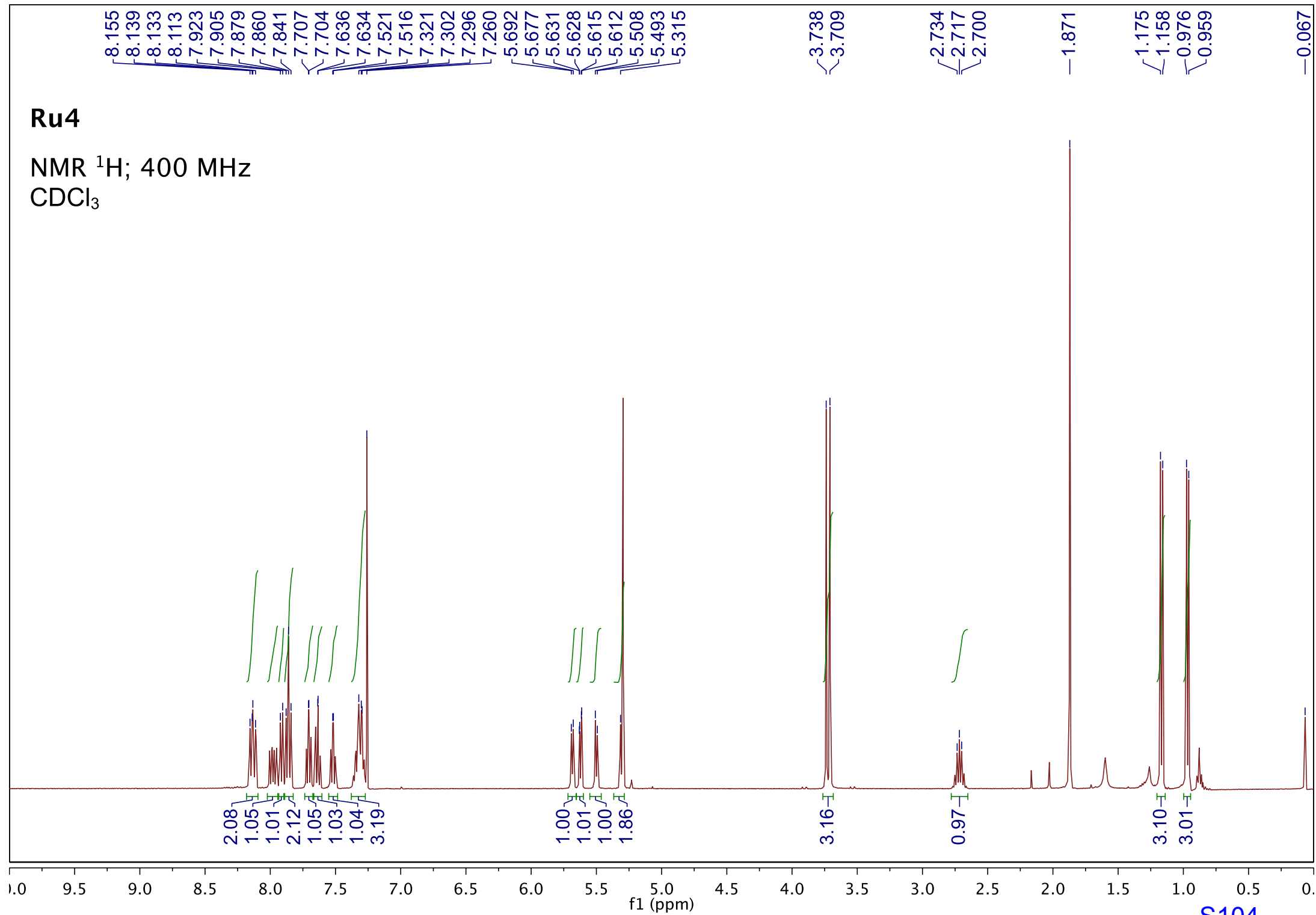


S103

Ru4

NMR ^1H ; 400 MHz

CDCl_3



Ru4

NMR ^{13}C ; 100.6 MHz

CDCl_3

141.861
141.366

121.241

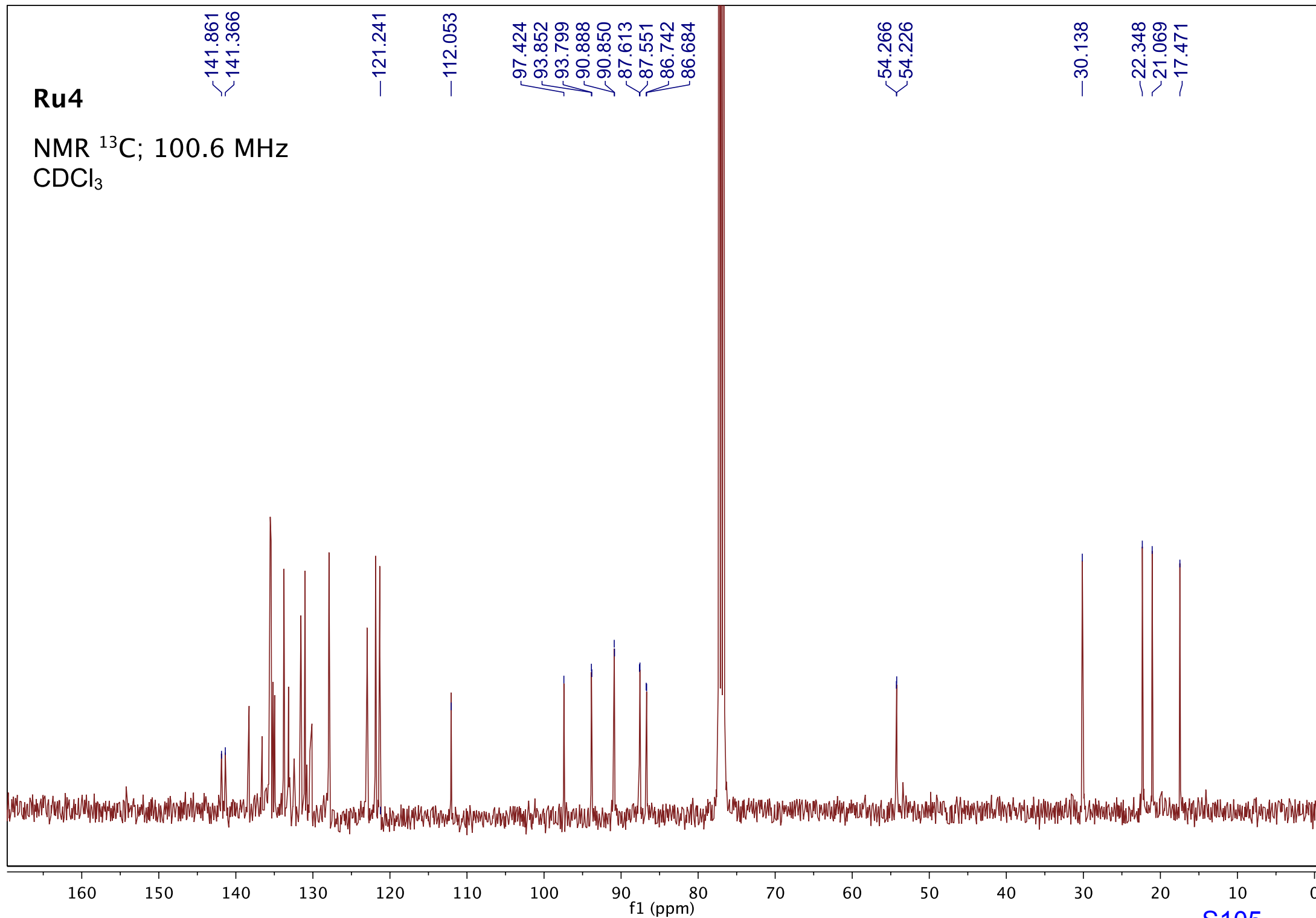
112.053

97.424
93.852
93.799
90.888
90.850
87.613
87.551
86.742
86.684

54.266
54.226

30.138

22.348
21.069
17.471

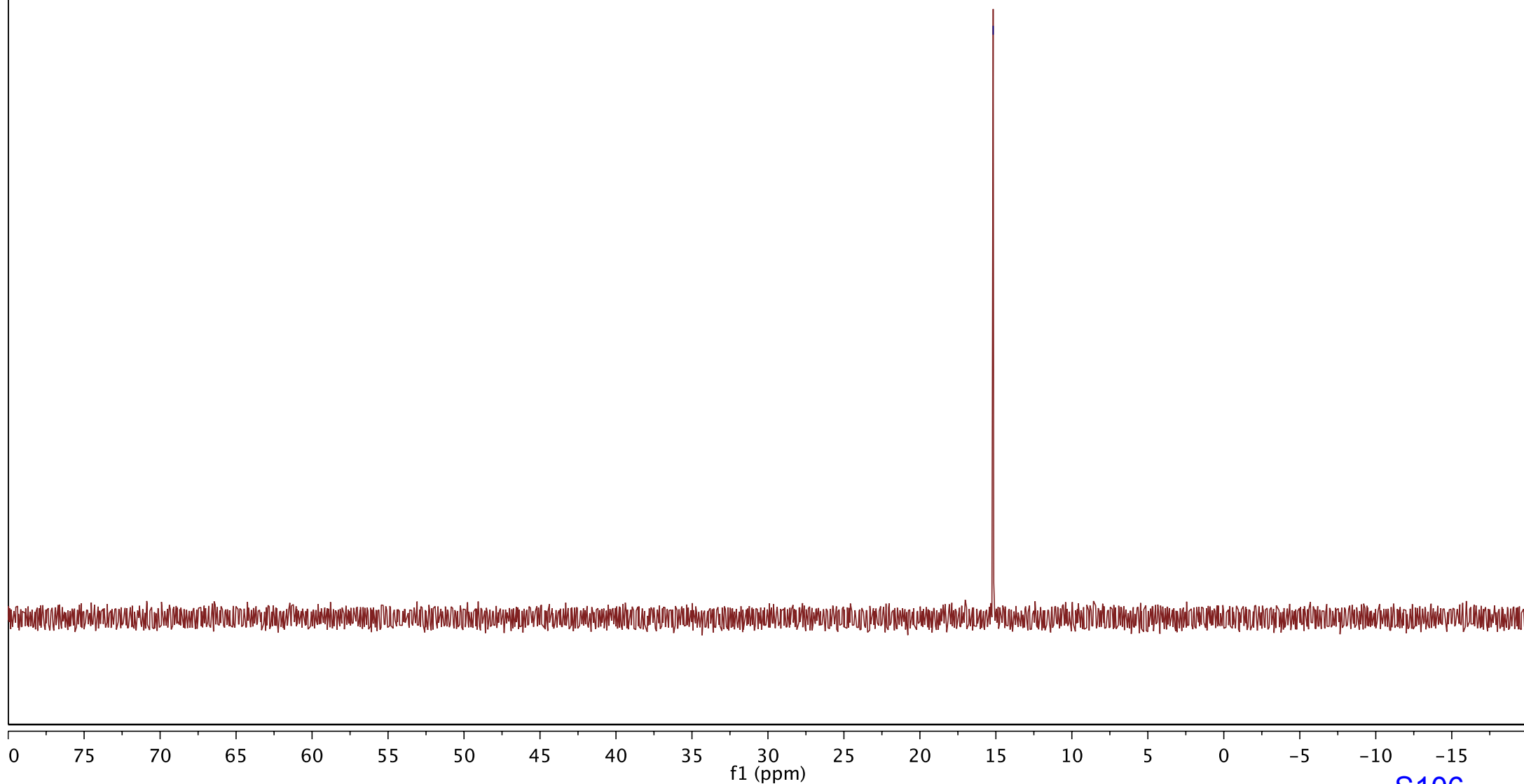


Ru5

NMR ^{31}P ; 121.4 MHz

CDCl_3

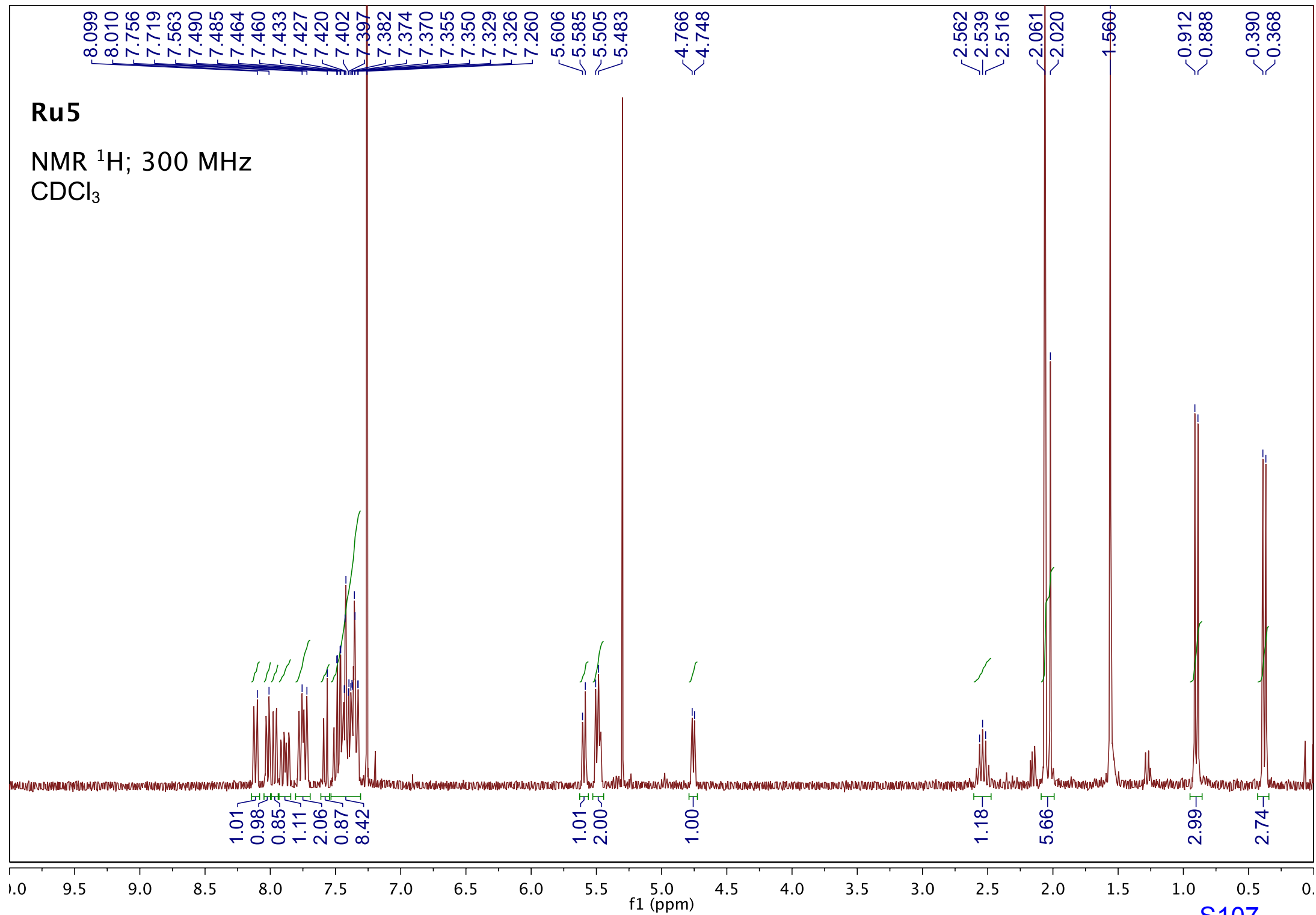
-15.178



S106

Ru5

NMR ^1H ; 300 MHz
 CDCl_3

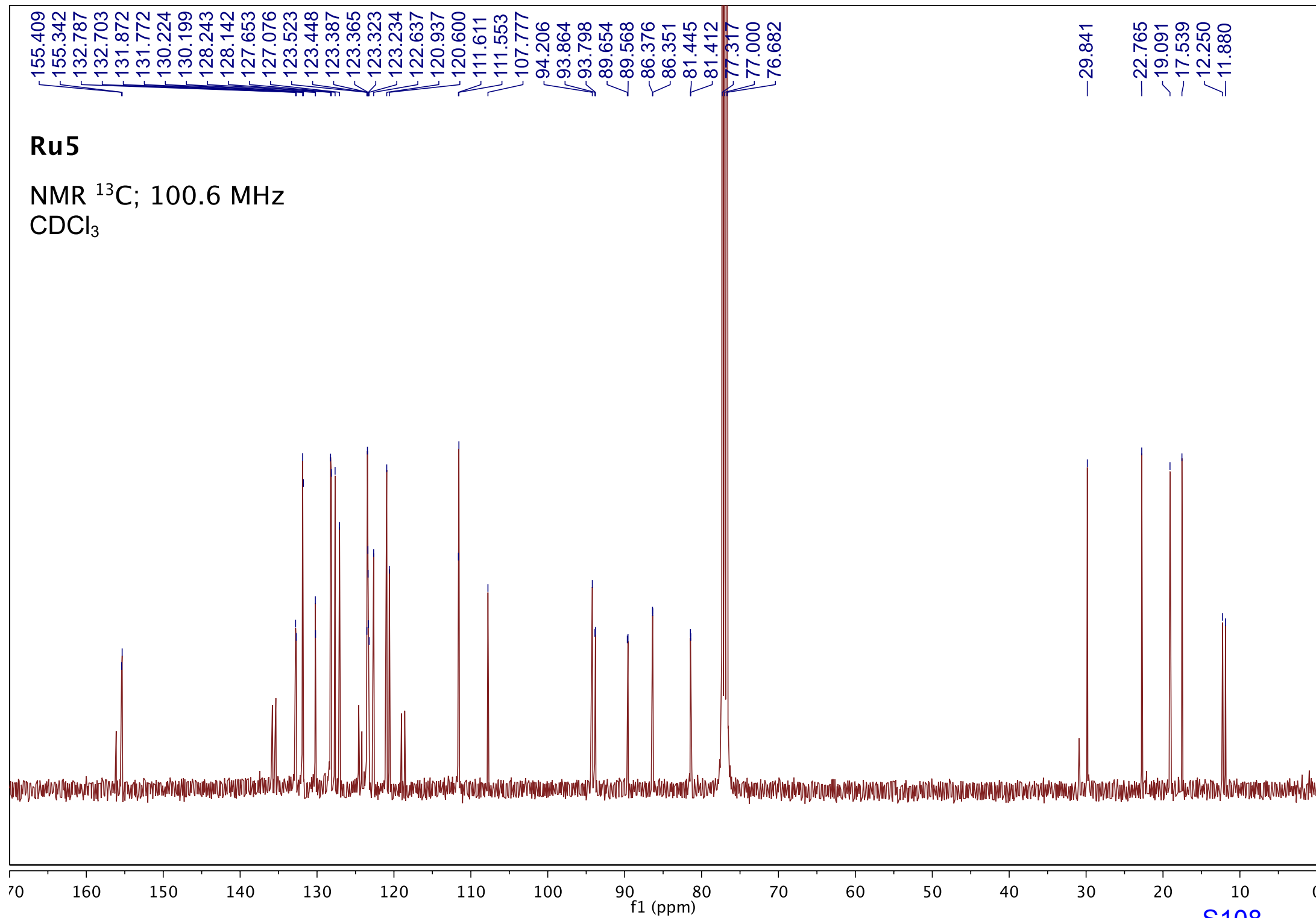


S107

Ru5

NMR ^{13}C ; 100.6 MHz

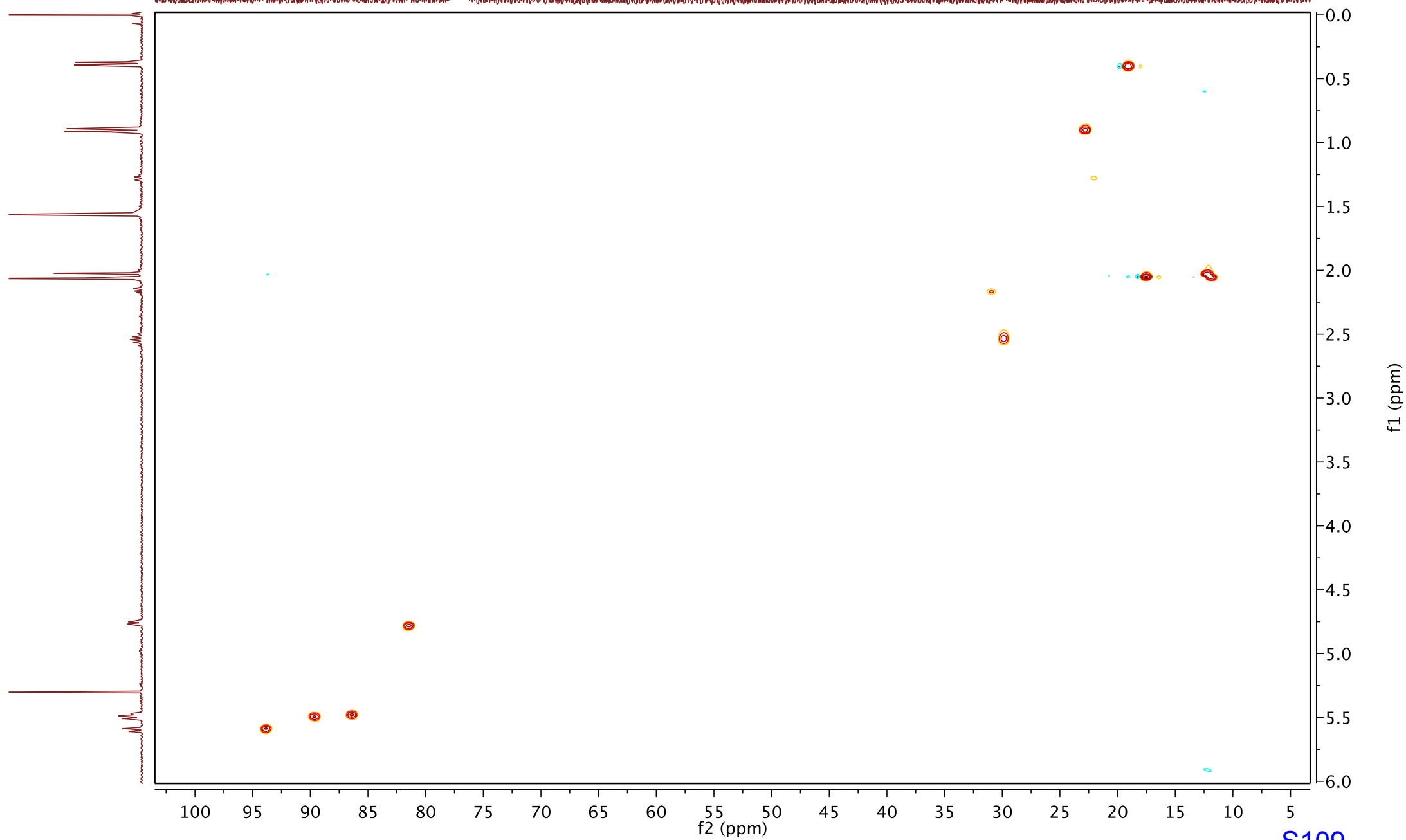
CDCl_3



Ru5

gHSQC 400MHz

CDCl₃



S109

Ru6

NMR ^{31}P ; 121.4 MHz

CDCl_3

-21.538

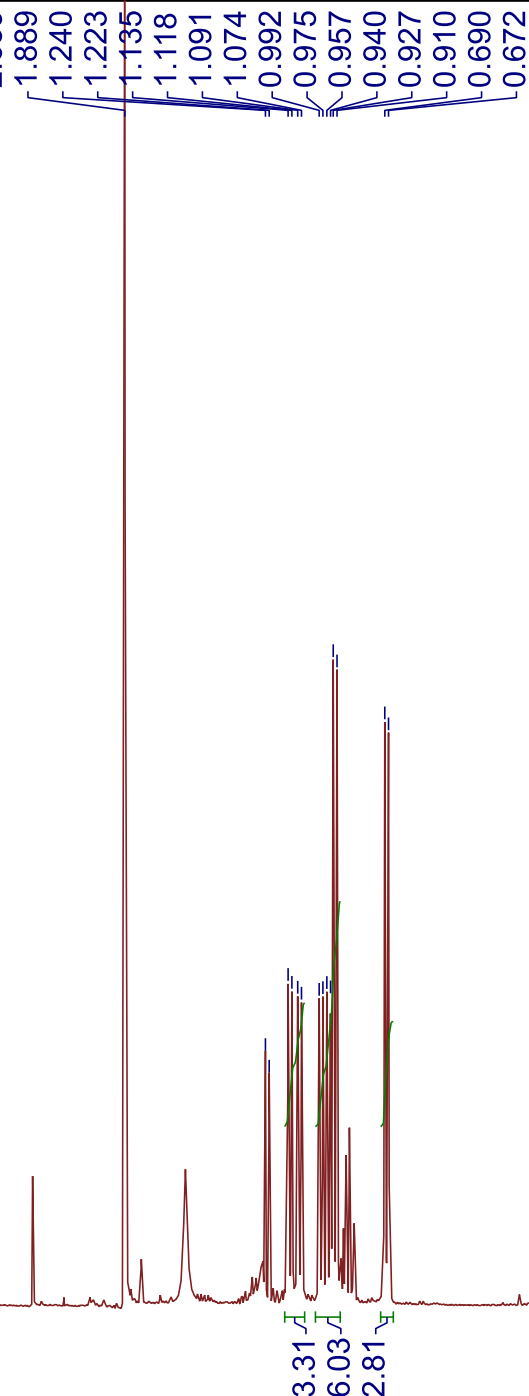
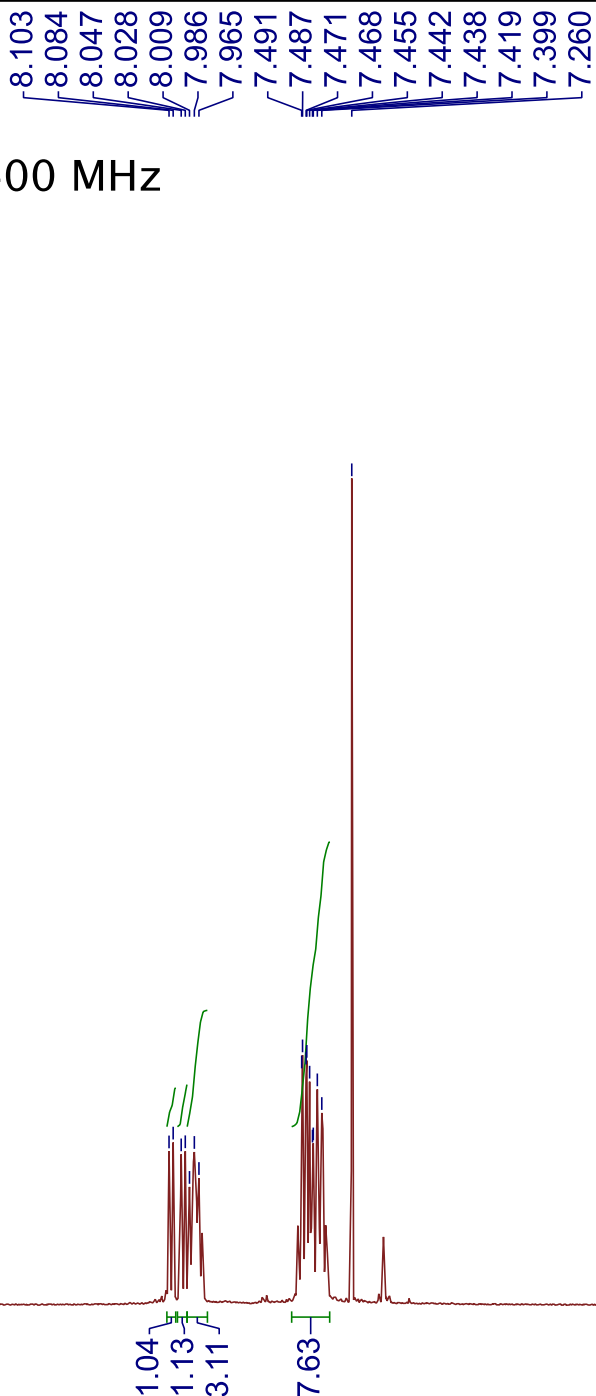
0 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30
f1 (ppm)

S110

Ru6

NMR ^1H ; 400 MHz

CDCl_3

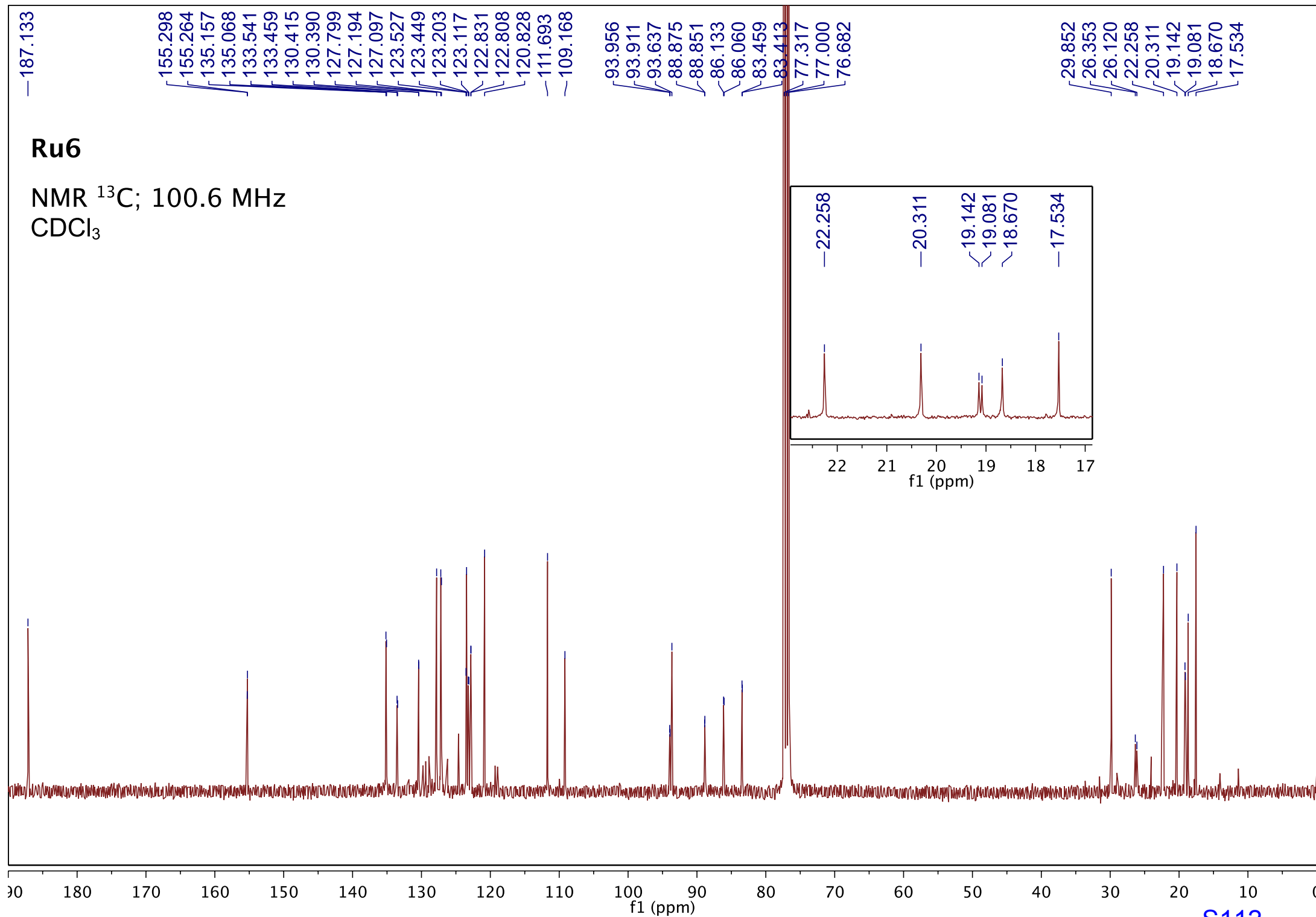


S111

Ru6

NMR ^{13}C ; 100.6 MHz

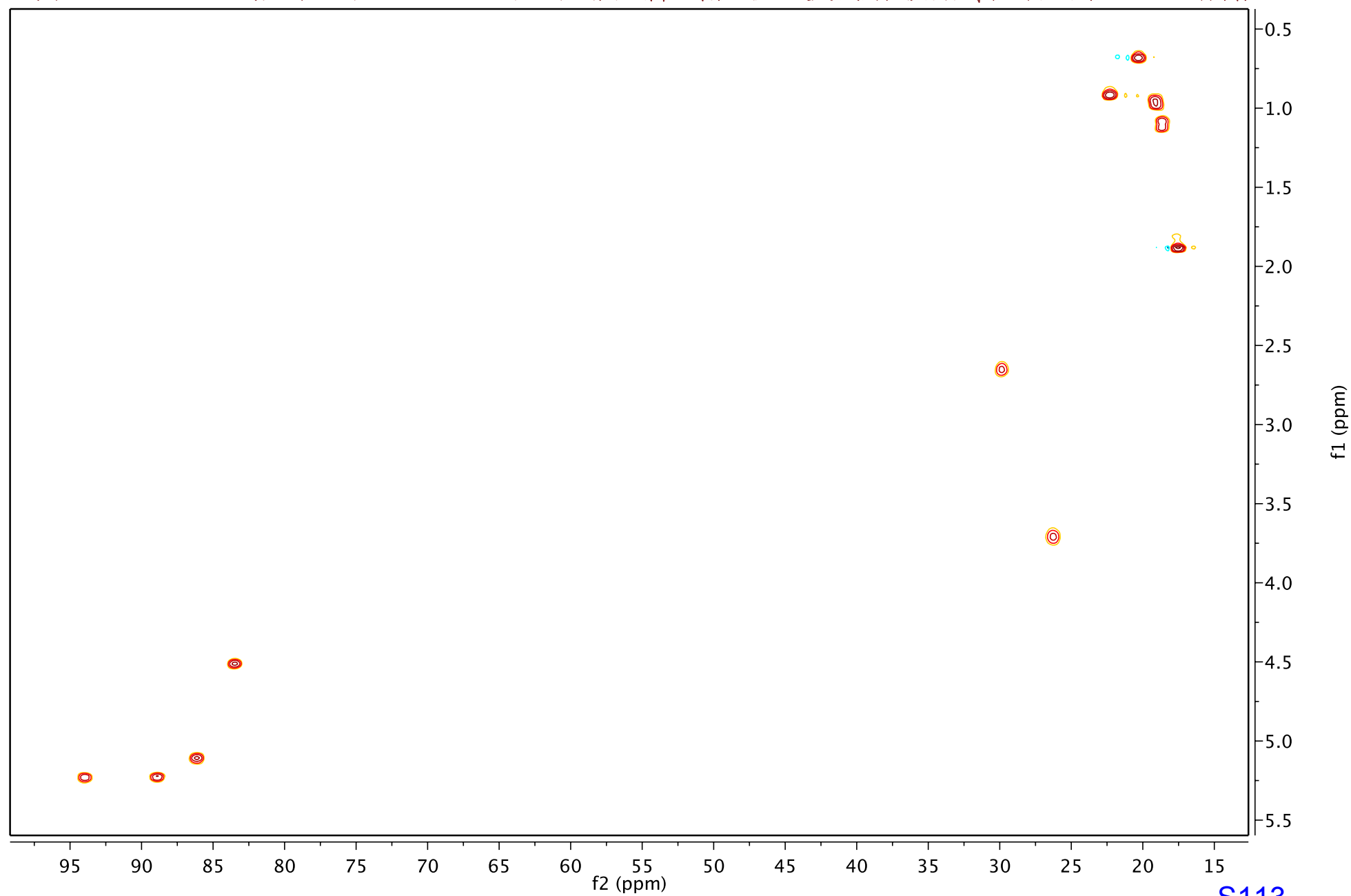
CDCl_3



Ru6

gHSQC 400MHz

CDCl₃



Ru8

NMR ^{31}P ; 161.9 MHz

CDCl_3

—15.802

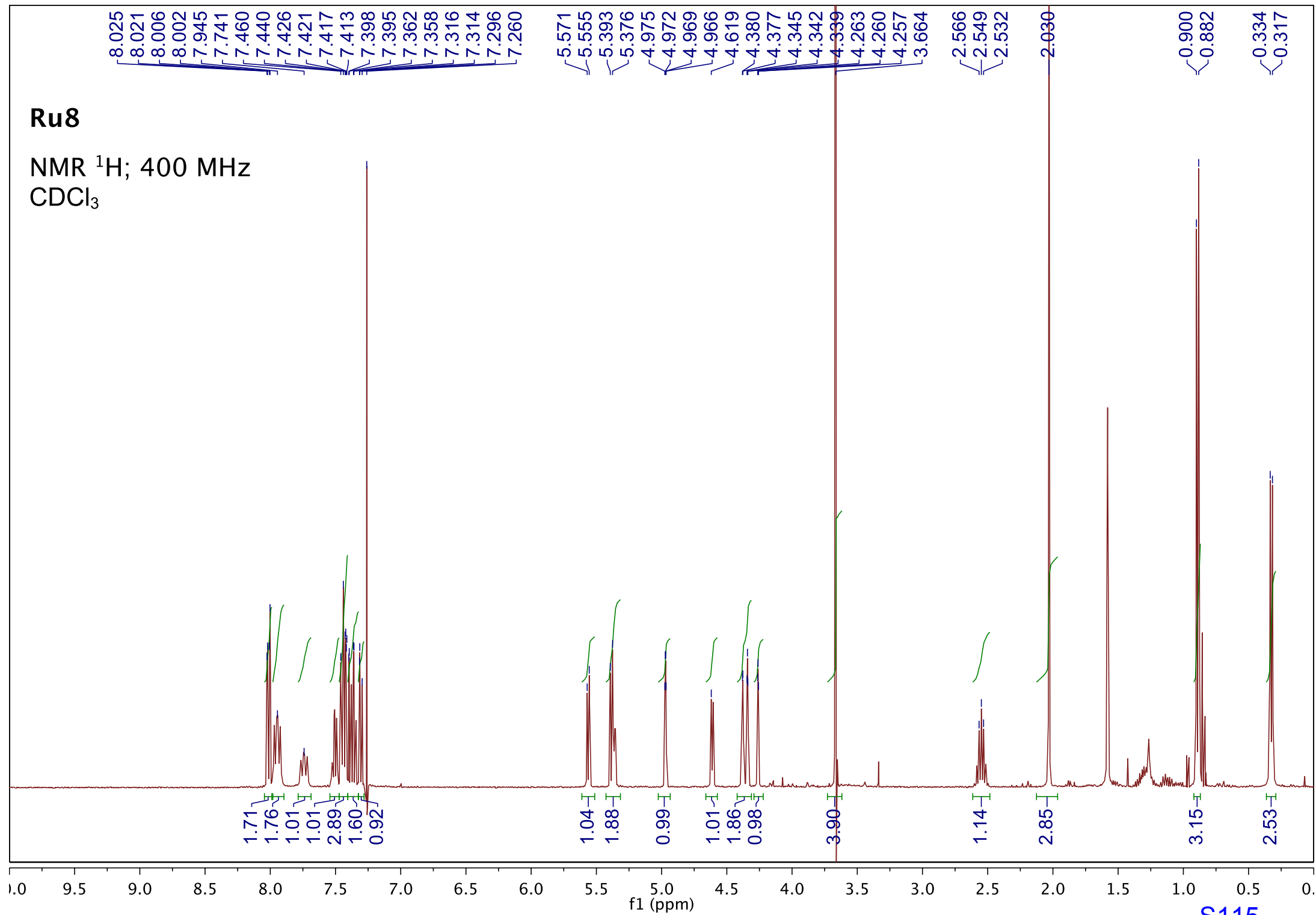
100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30
f1 (ppm)

S114

Ru8

NMR ^1H ; 400 MHz

CDCl_3

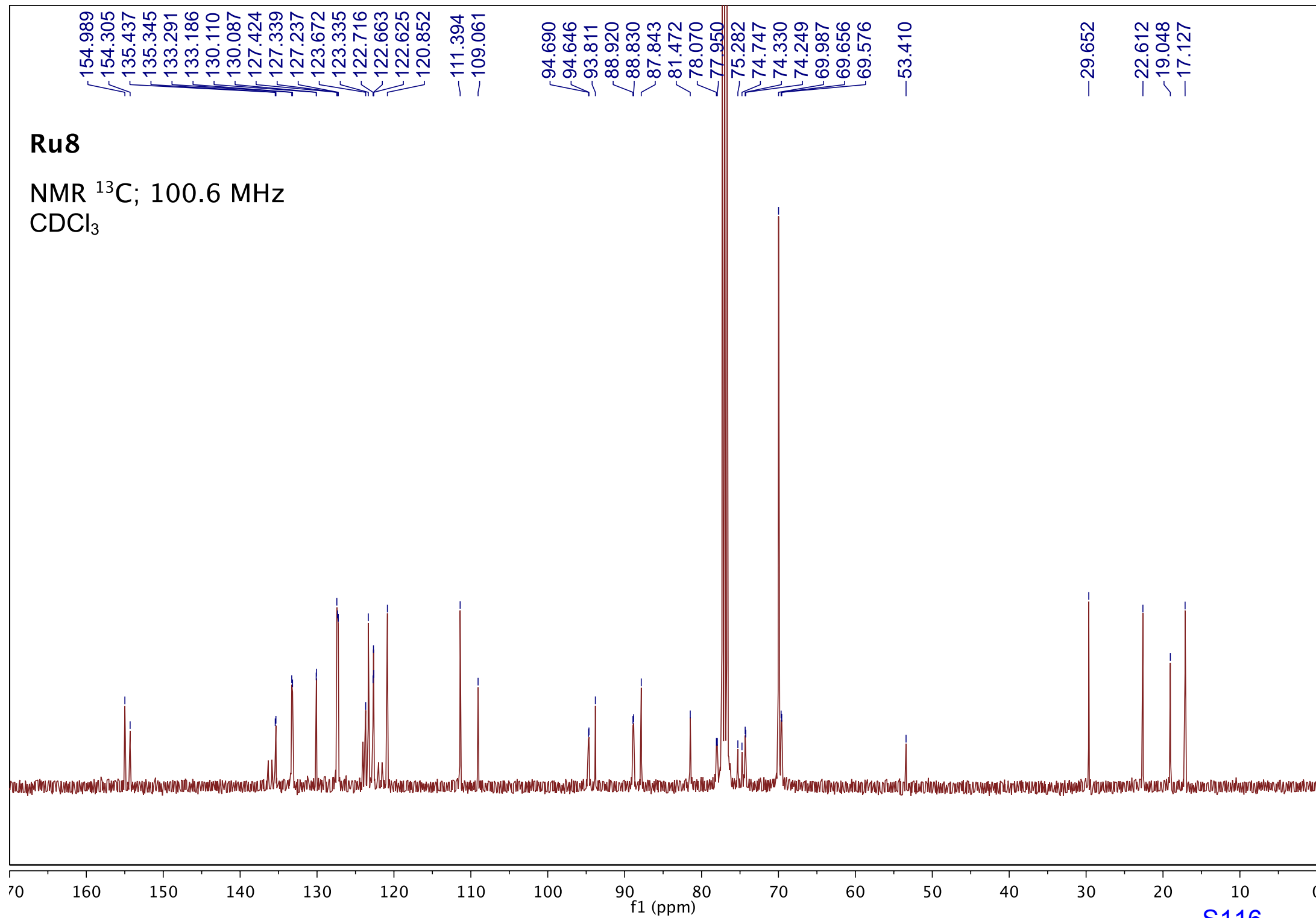


S115

Ru8

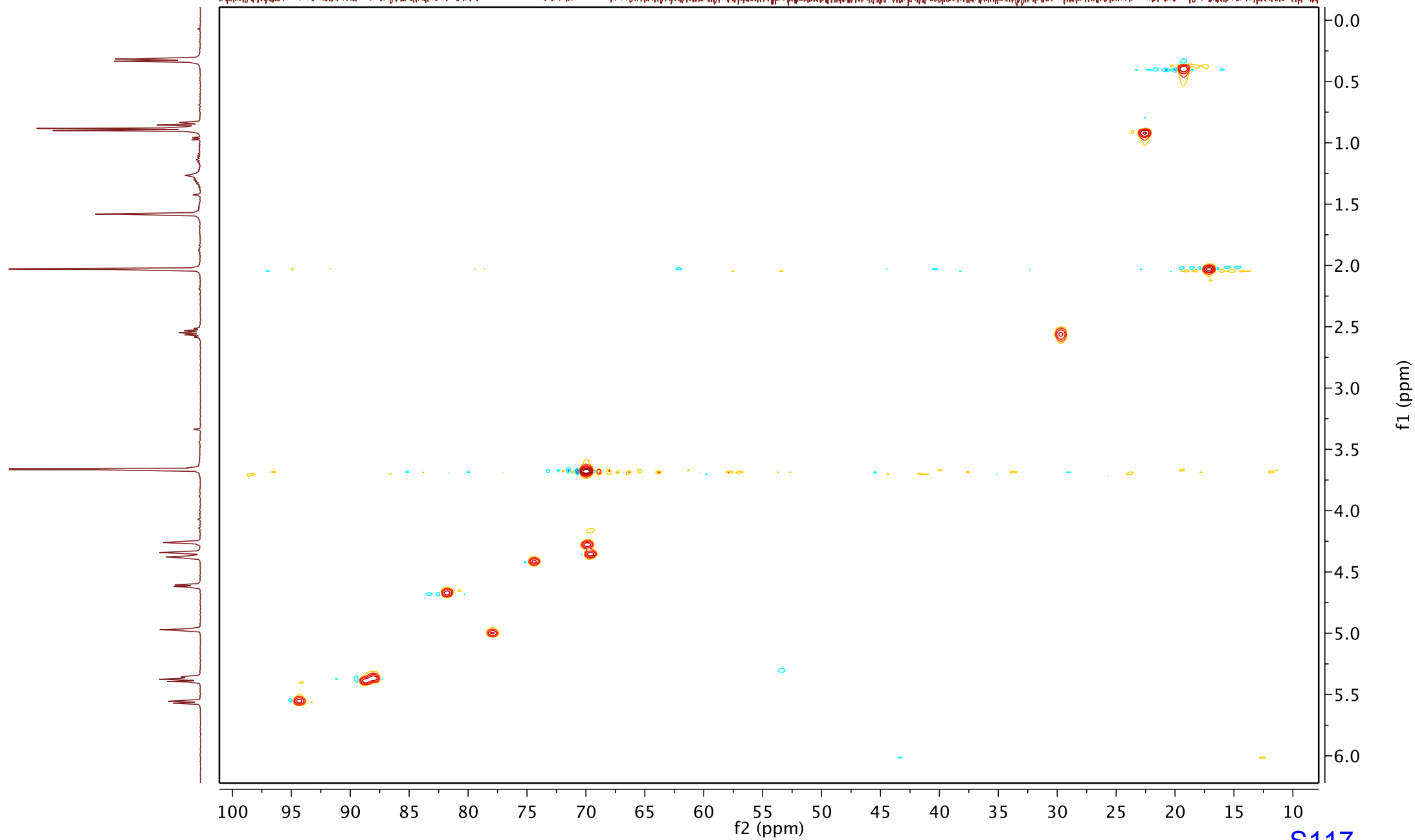
NMR ^{13}C ; 100.6 MHz

CDCl_3



Ru8

gHSQC 400MHz
CDCl₃



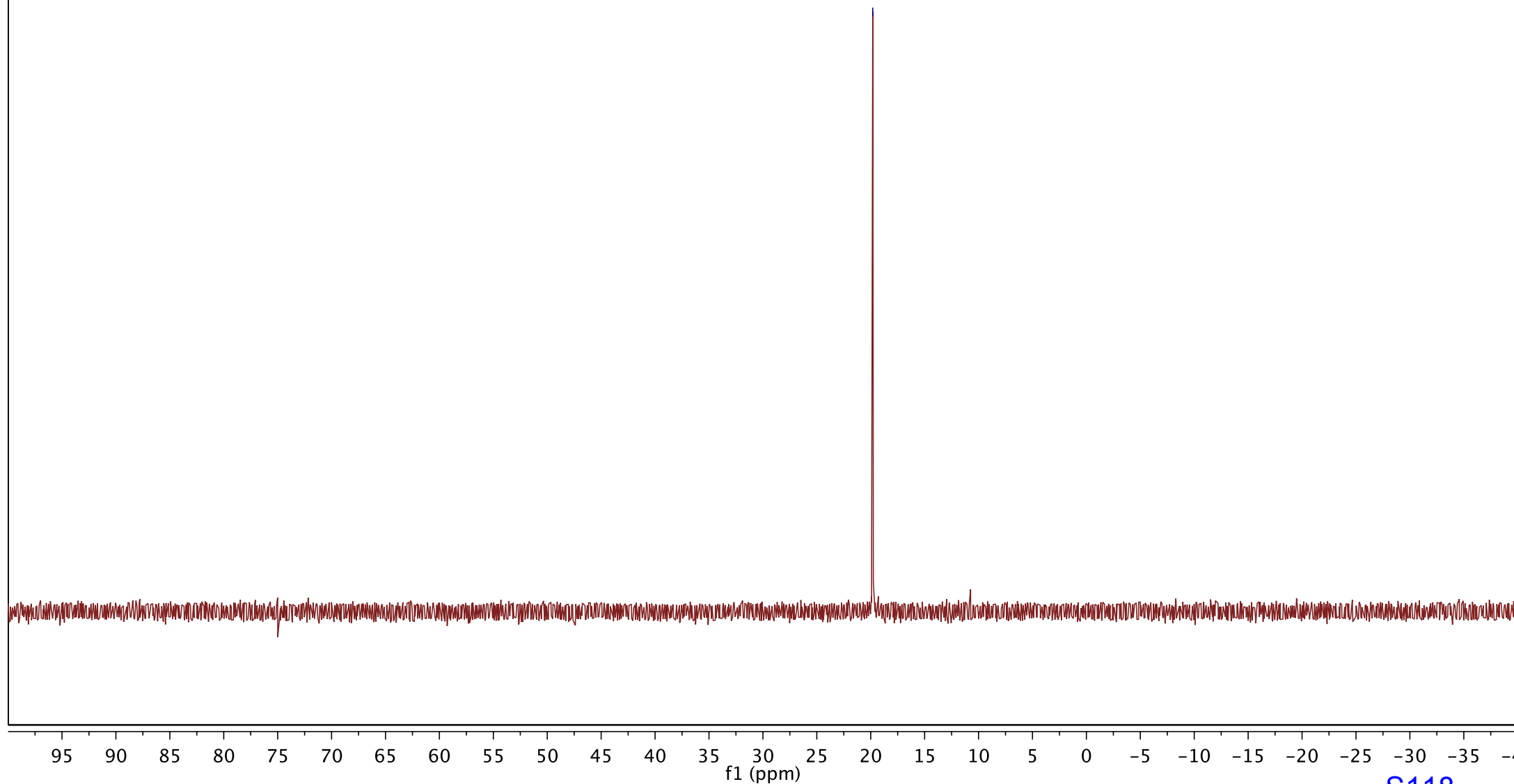
S117

Ru9

NMR ^{31}P ; 161.9 MHz

CDCl_3

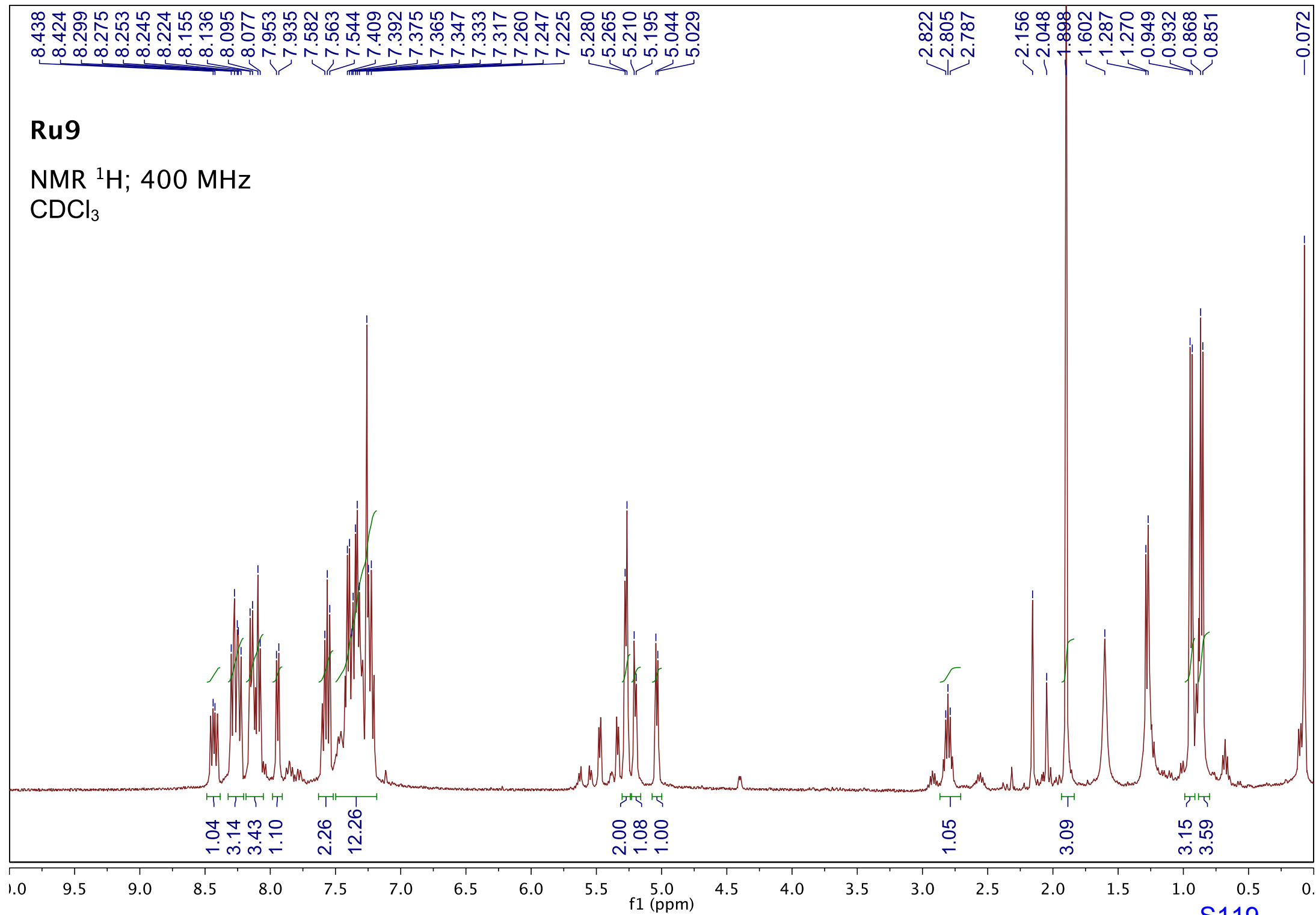
—19.814



S118

Ru9

NMR ^1H ; 400 MHz
 CDCl_3

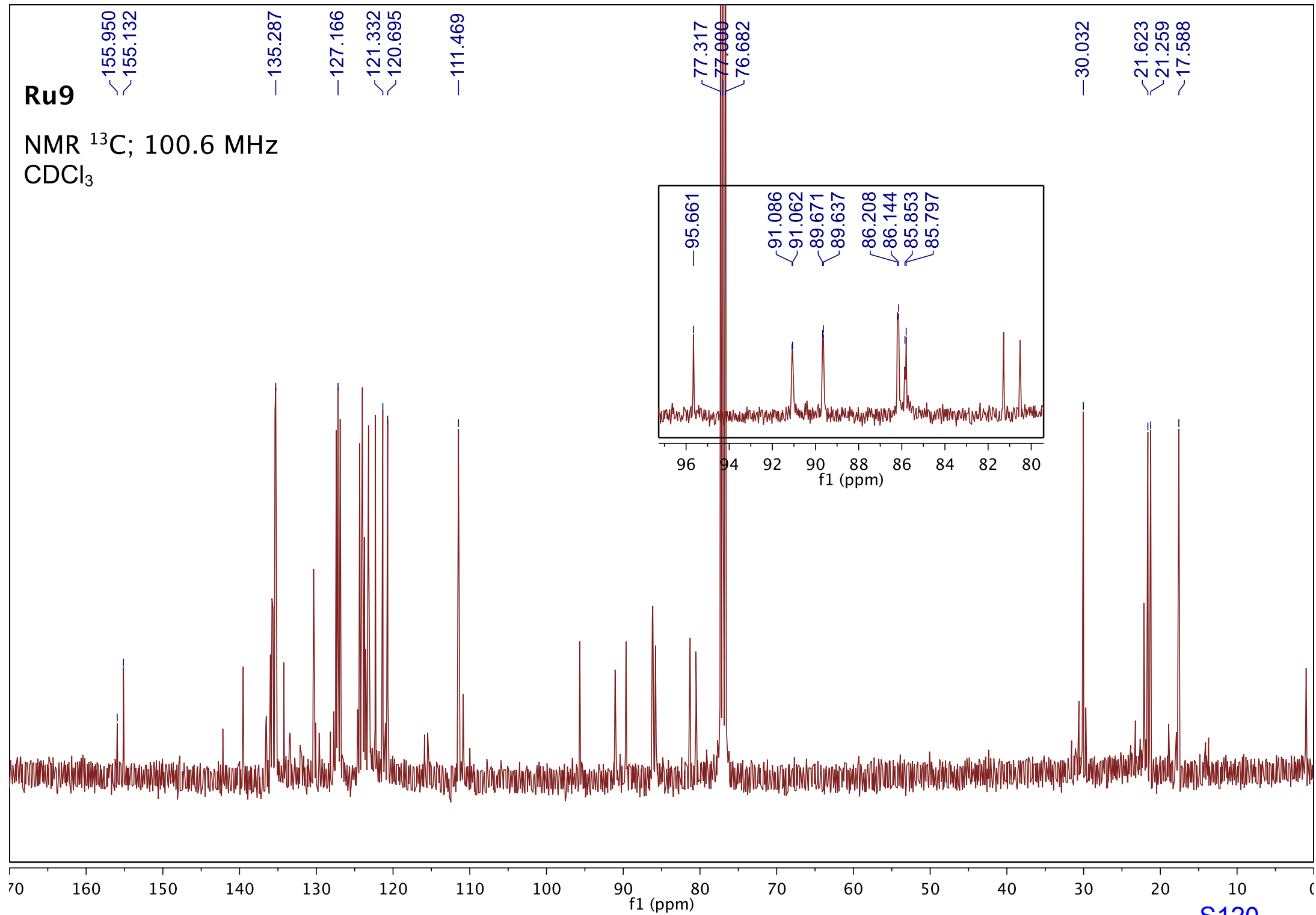


S119

Ru9

NMR ^{13}C ; 100.6 MHz

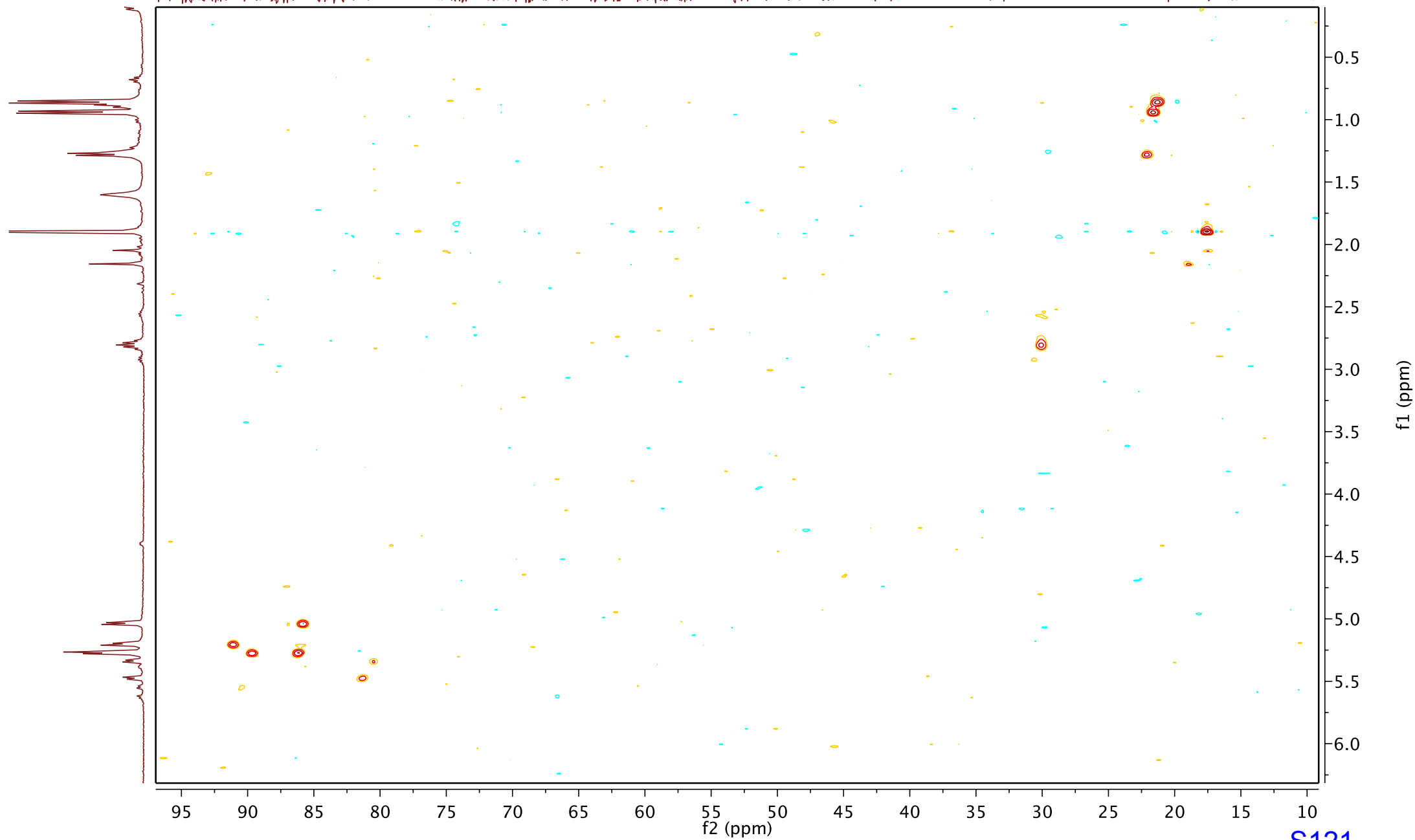
CDCl_3



Ru9

gHSQC 400MHz

CDCl₃

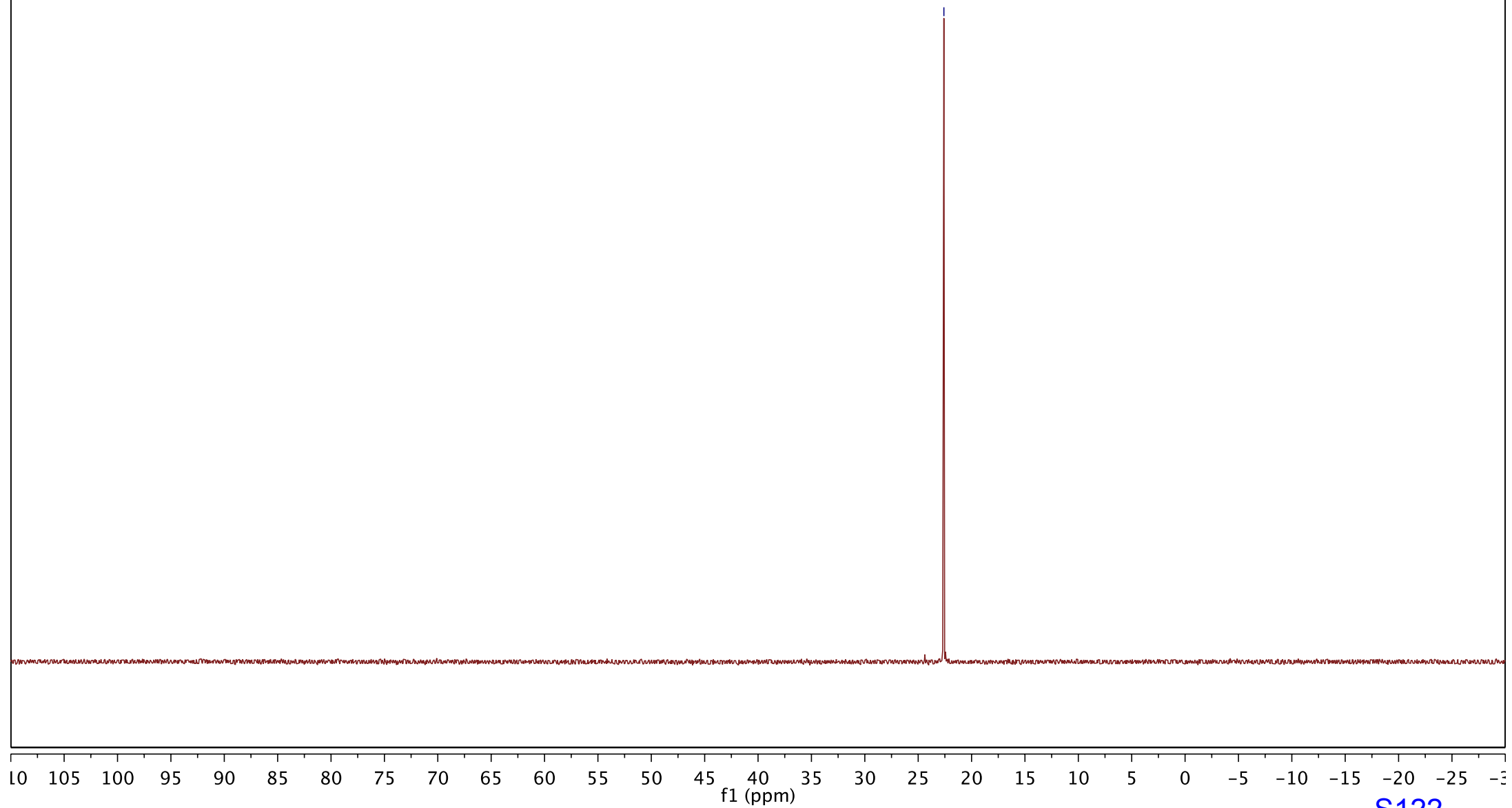


Ru10

NMR ^{31}P ; 161.9 MHz

CDCl_3

—22.592

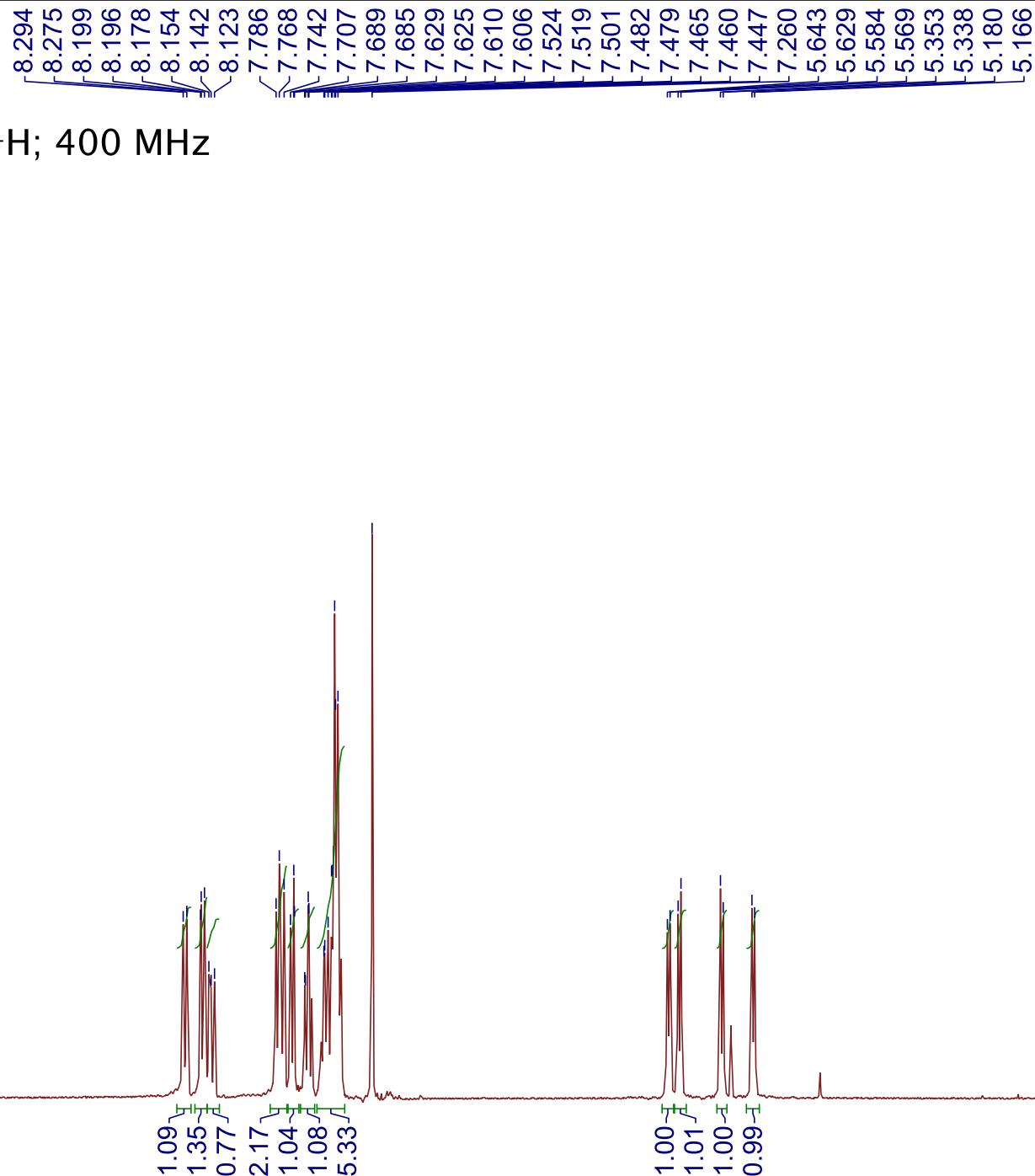


S122

Ru10

NMR ^1H ; 400 MHz

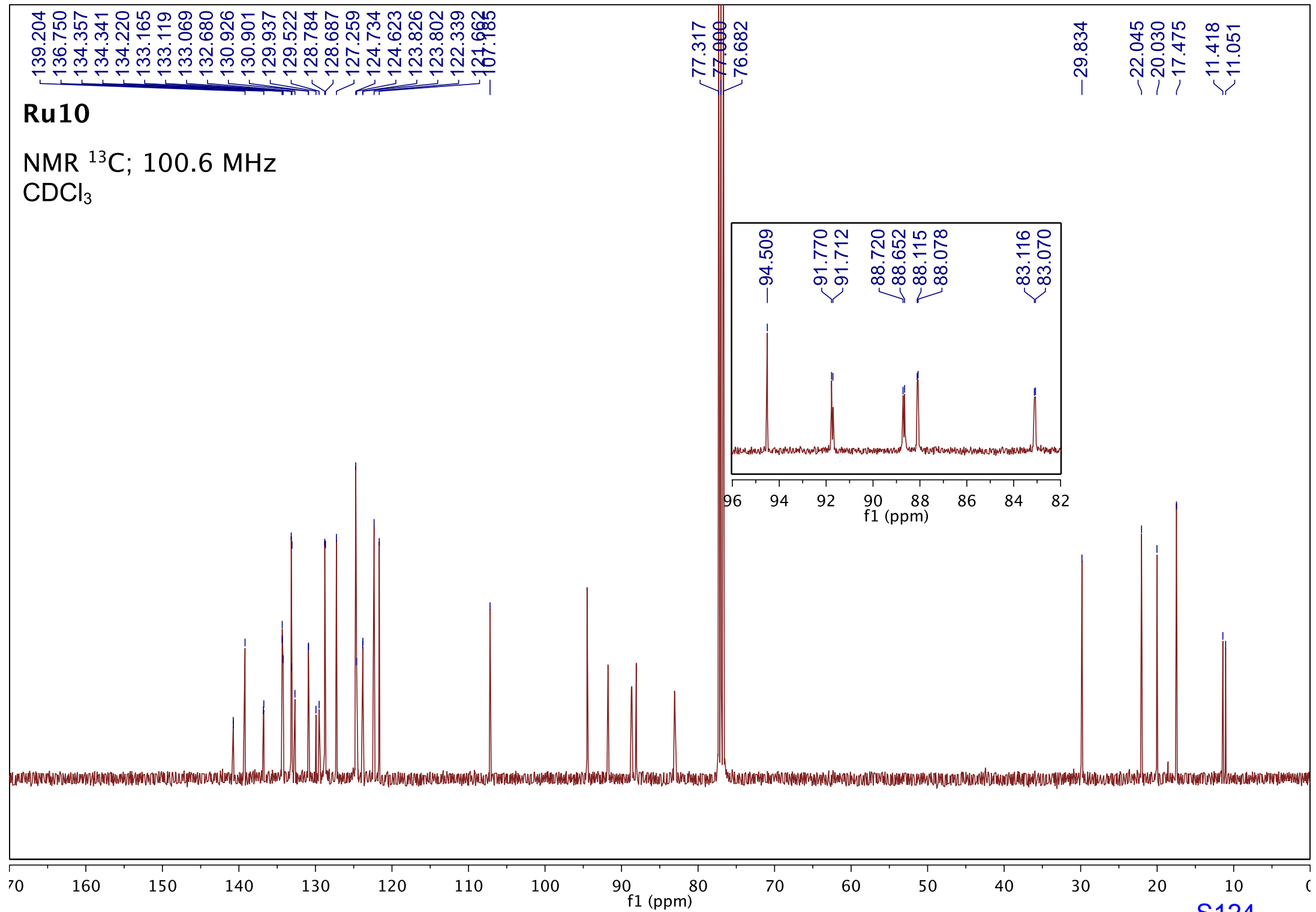
CDCl_3



Ru10

NMR ^{13}C ; 100.6 MHz

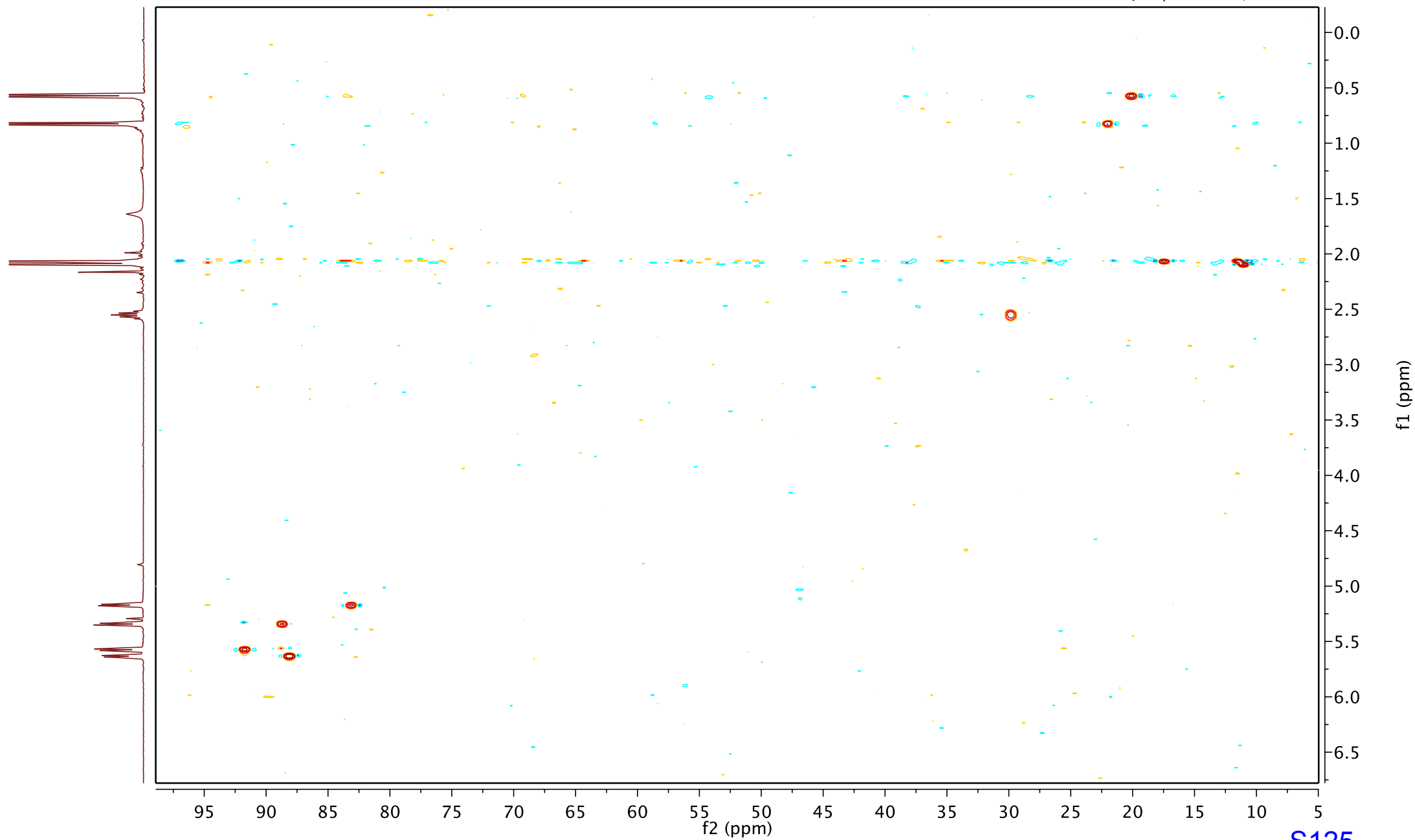
CDCl_3



Ru10

gHSQC 400MHz

CDCl₃



Ru11

NMR ^{31}P ; 161.9 MHz

CDCl_3

—25.437

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40 -50
f1 (ppm)

S126

Ru11

NMR ^1H ; 400 MHz

CDCl_3

8.290
8.270
8.226
8.203
7.993
7.794
7.773
7.600
7.507
7.498
7.489
7.260

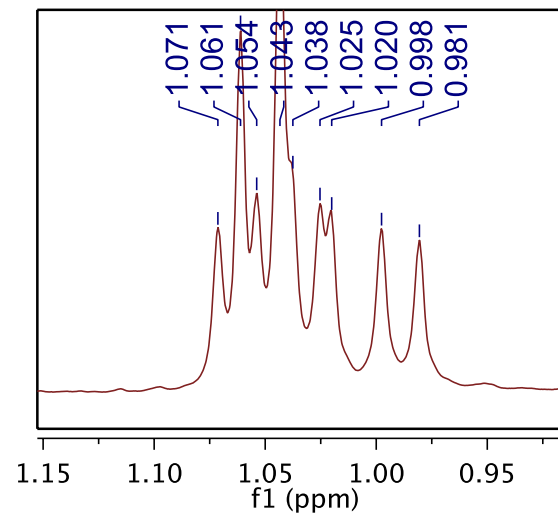
5.425
5.410
4.948
4.934
4.674
4.659

3.778
3.763

2.729
2.712
2.695

1.856

1.071
1.061
1.054
1.043
1.025
1.020



1.39
1.64
1.98
1.28
2.70
5.60

2.06

1.12

1.15

0.94

0.94

4.10

9.42

2.23

3.70

S127

Ru11

NMR ^{13}C ; 100.6 MHz

CDCl_3

141.017
139.147
136.890
136.833
134.200
133.373
131.369
131.343
127.649
127.429
127.077
126.709
124.778
123.115
123.092
122.352
121.552
108.469

94.420
93.209
88.324
88.288
85.527
85.006
77.317
77.000
76.682

29.833
25.229
25.004
22.223
21.008
19.010
18.938
17.601

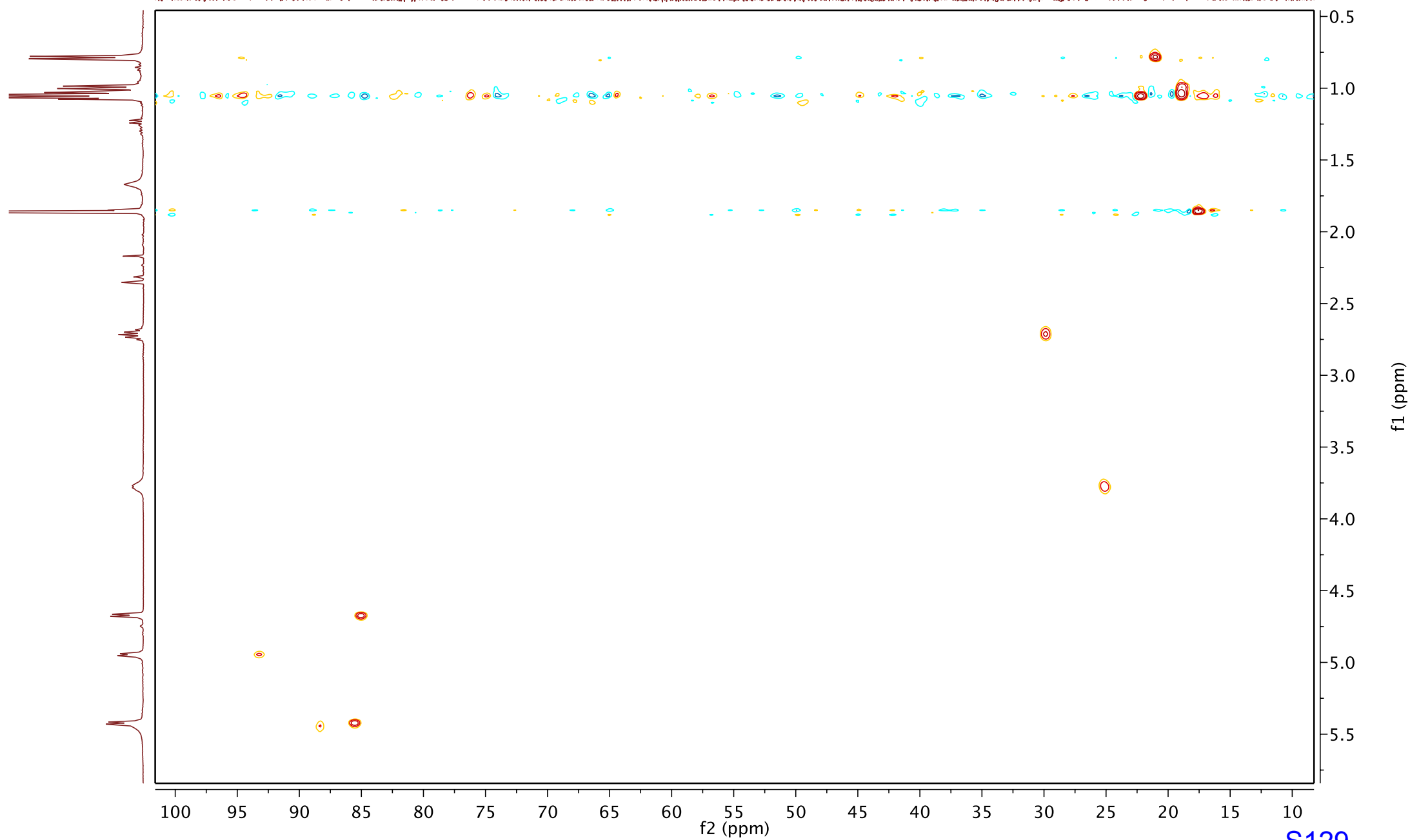
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

Ru11

gHSQC 400MHz

CDCl₃



Ru12

NMR ^{31}P ; 161.9 MHz

CDCl_3

-20.628

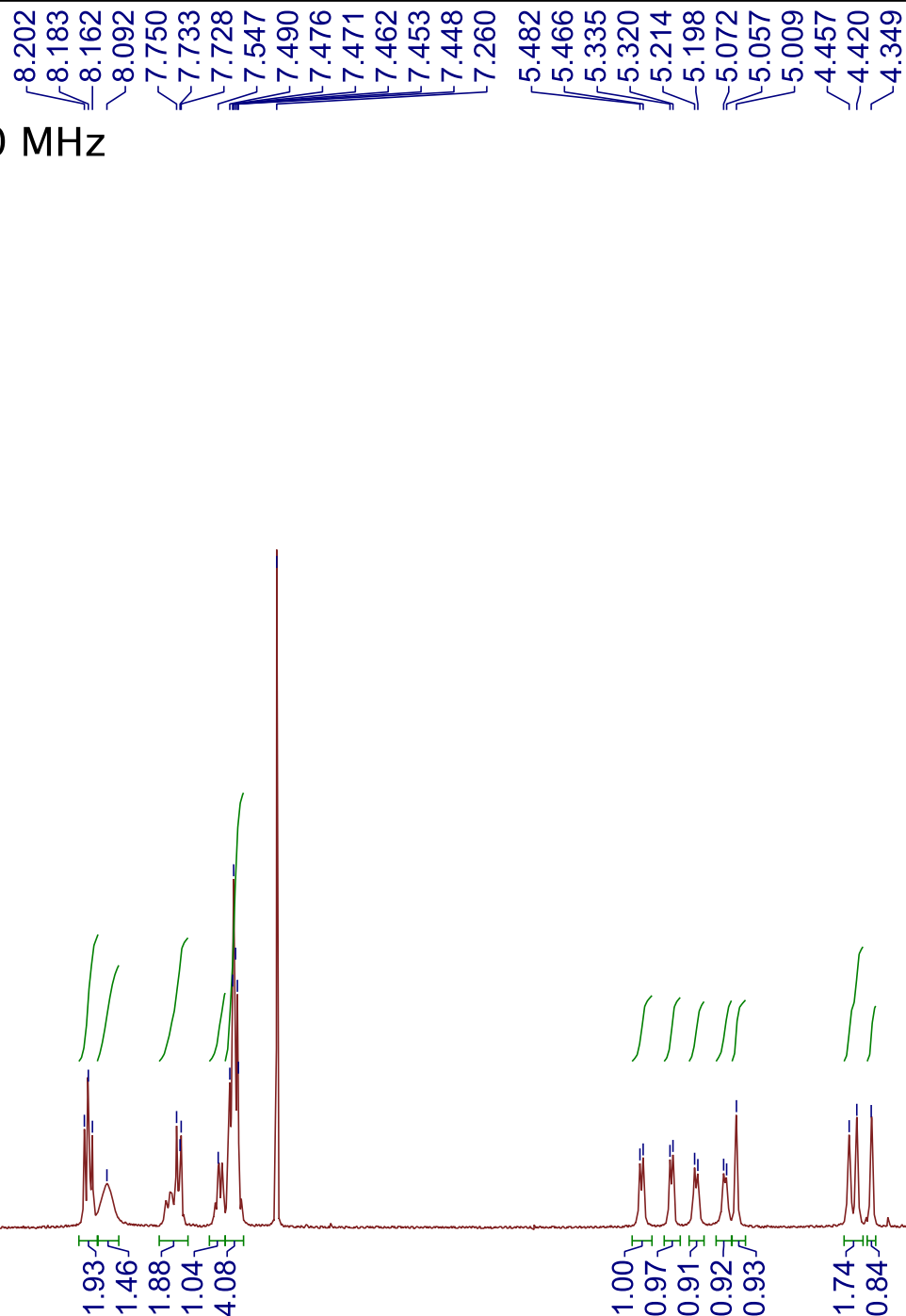
f1 (ppm)

S130

Ru12

NMR ^1H ; 400 MHz

CDCl_3



Ru12

NMR ^{13}C ; 100.6 MHz
 CDCl_3

—140.512

—121.483

—108.909

—94.958

—92.832

—88.711

—88.279

—82.644

—79.180

—79.023

—74.051

—70.646

—70.325

—69.785

—69.708

—69.609

—29.701

—22.441

—19.899

—17.224

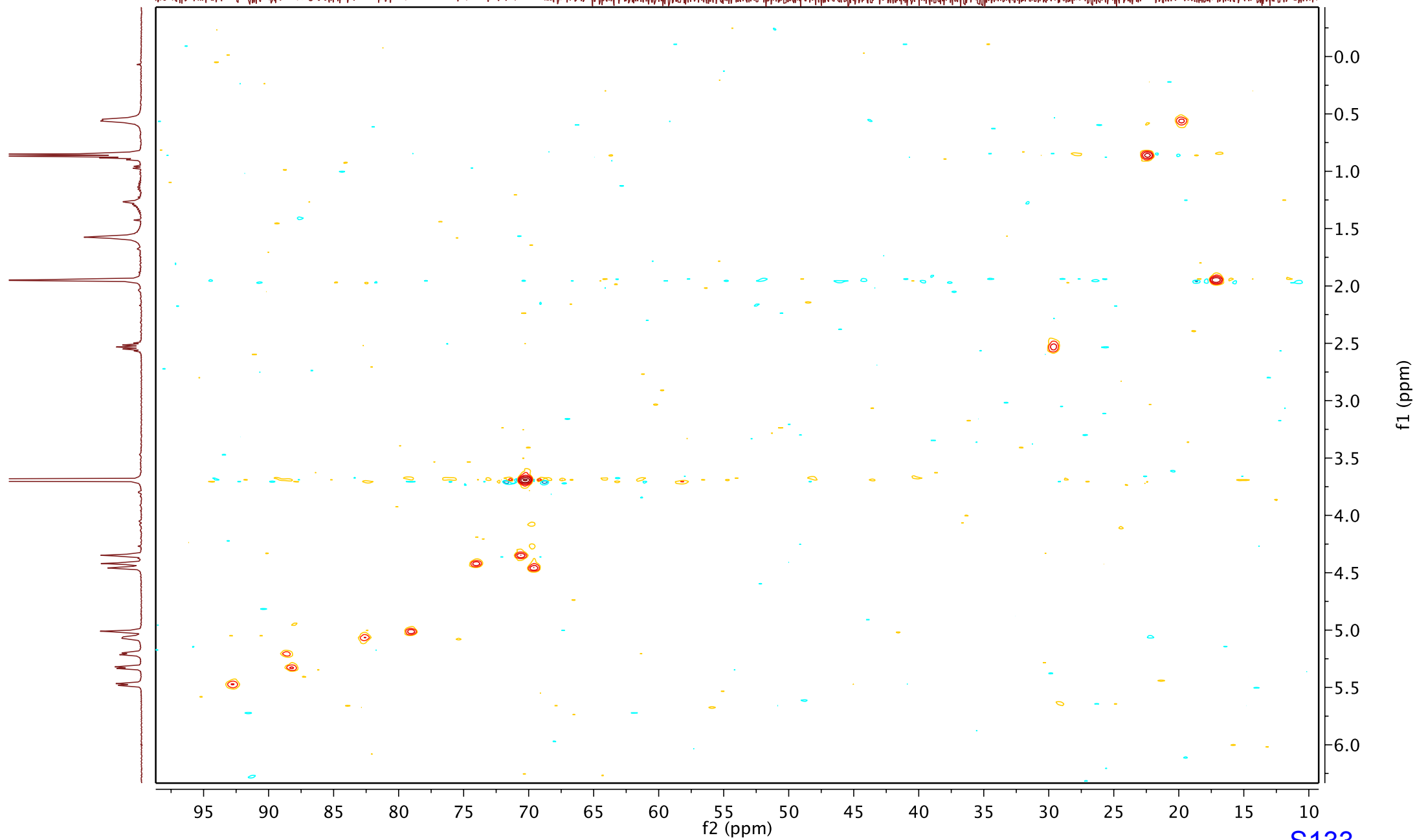
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

S132

Ru12

gHSQC 400MHz

CDCl₃

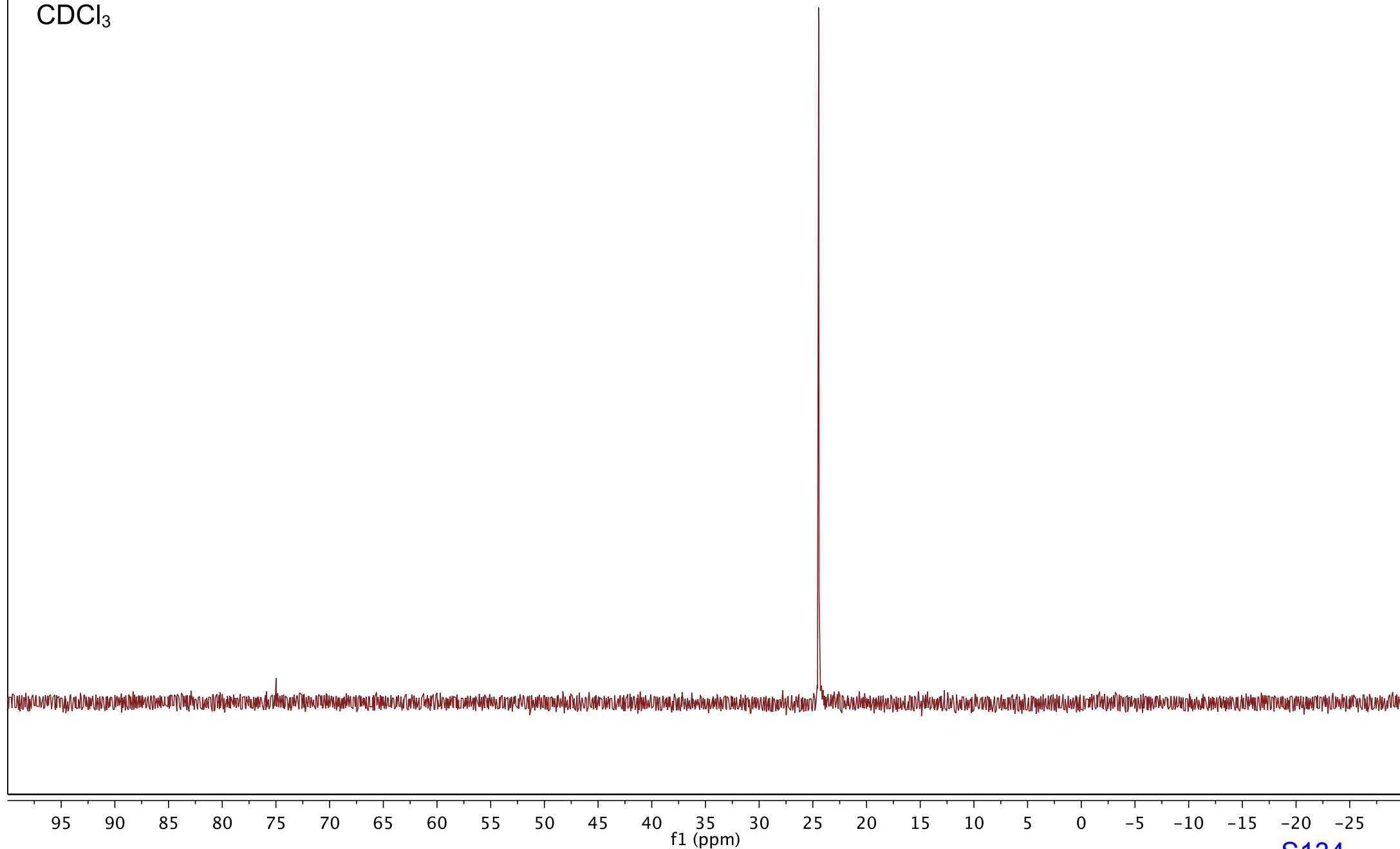


Ru13

NMR ^{31}P ; 161.9 MHz

CDCl_3

-24.458



S134

Ru13

NMR ^1H ; 400 MHz

CDCl_3

7.975
7.683
7.663
7.520
7.501
7.476
7.374
7.272
7.260
7.184
7.128

5.634
5.619
5.458
5.443
5.194
5.181

2.493
2.475
2.458
2.153
2.027
2.000

0.824
0.806

0.303
0.286

1.13
2.89
4.24
1.21
1.99
1.21
1.15

1.86
1.01
1.00

1.37
2.95
3.33

3.17

2.97

f1 (ppm)

S135

Ru13

NMR ^{13}C ; 100.6 MHz

CDCl_3

138.943

126.204

106.487

95.102

93.689

90.992

85.642

81.295

77.318

77.000

76.683

29.619

22.719

19.105

17.651

13.725

13.357

70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

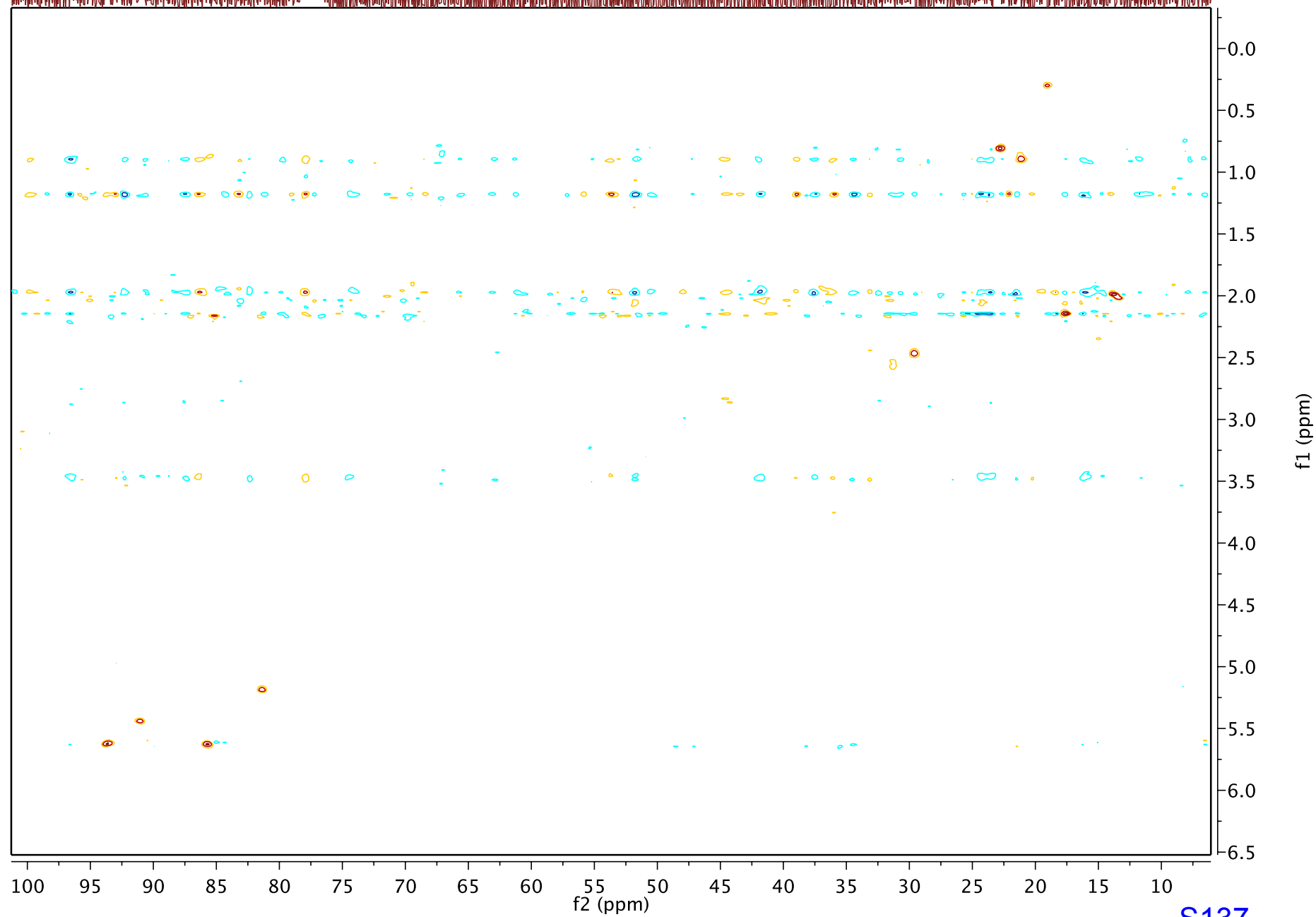
f1 (ppm)

S136

Ru13

gHSQC 400MHz

CDCl₃



S137

Ru6*

NMR ^{31}P ; 161.9 MHz

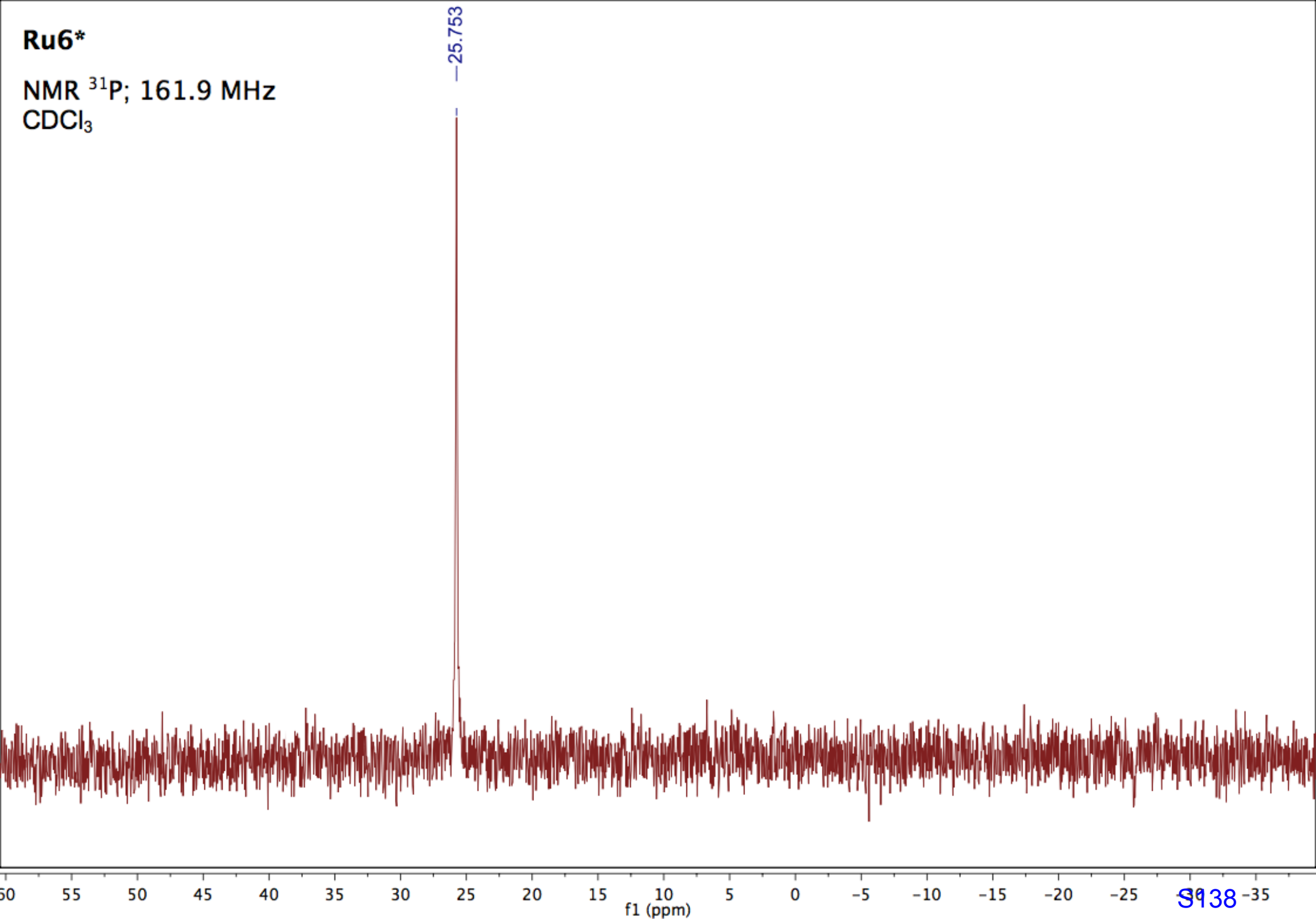
CDCl_3

—25.753

60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35

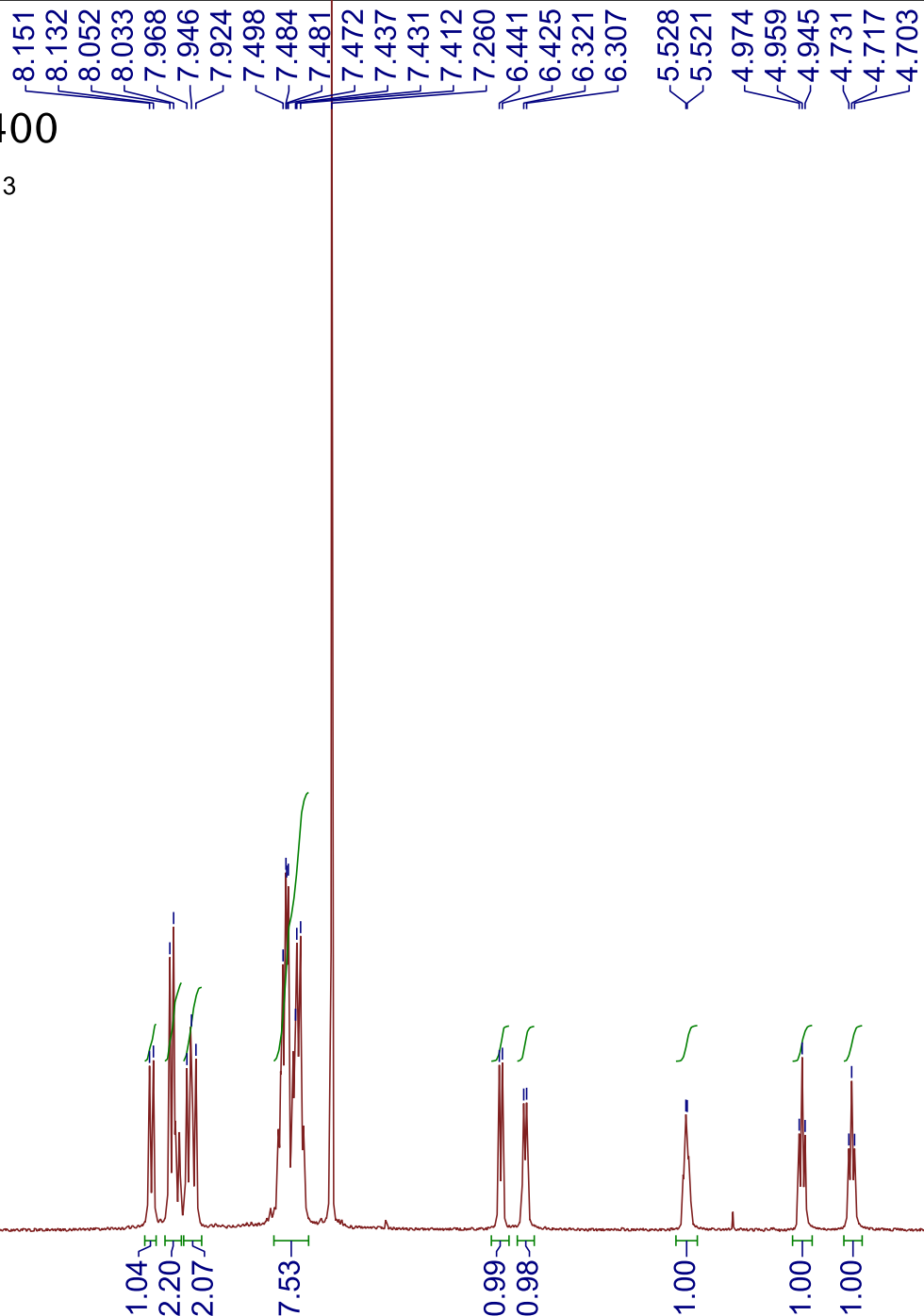
f1 (ppm)

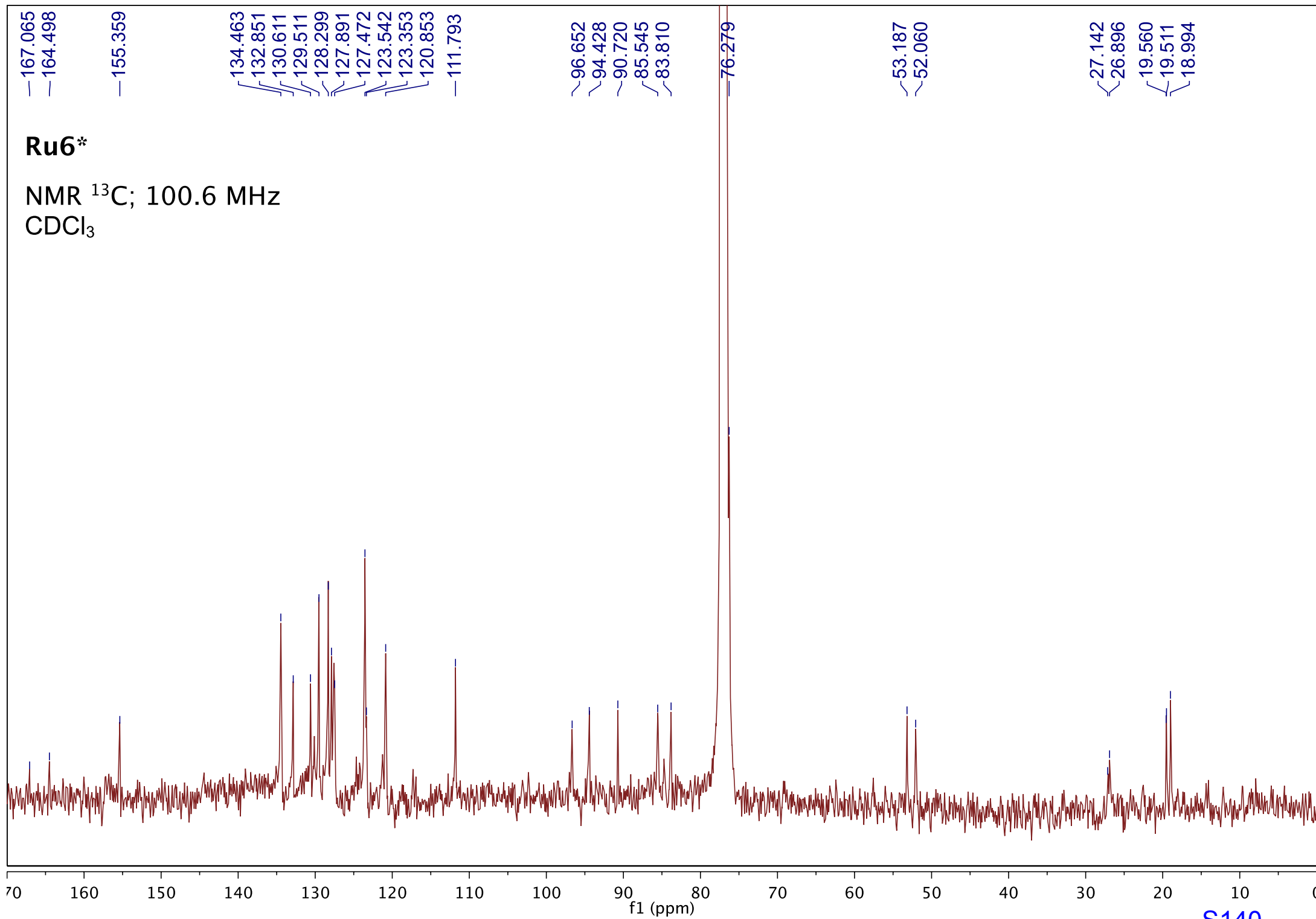
S138



Ru6*

NMR ^1H ; 400
MHz CDCl_3



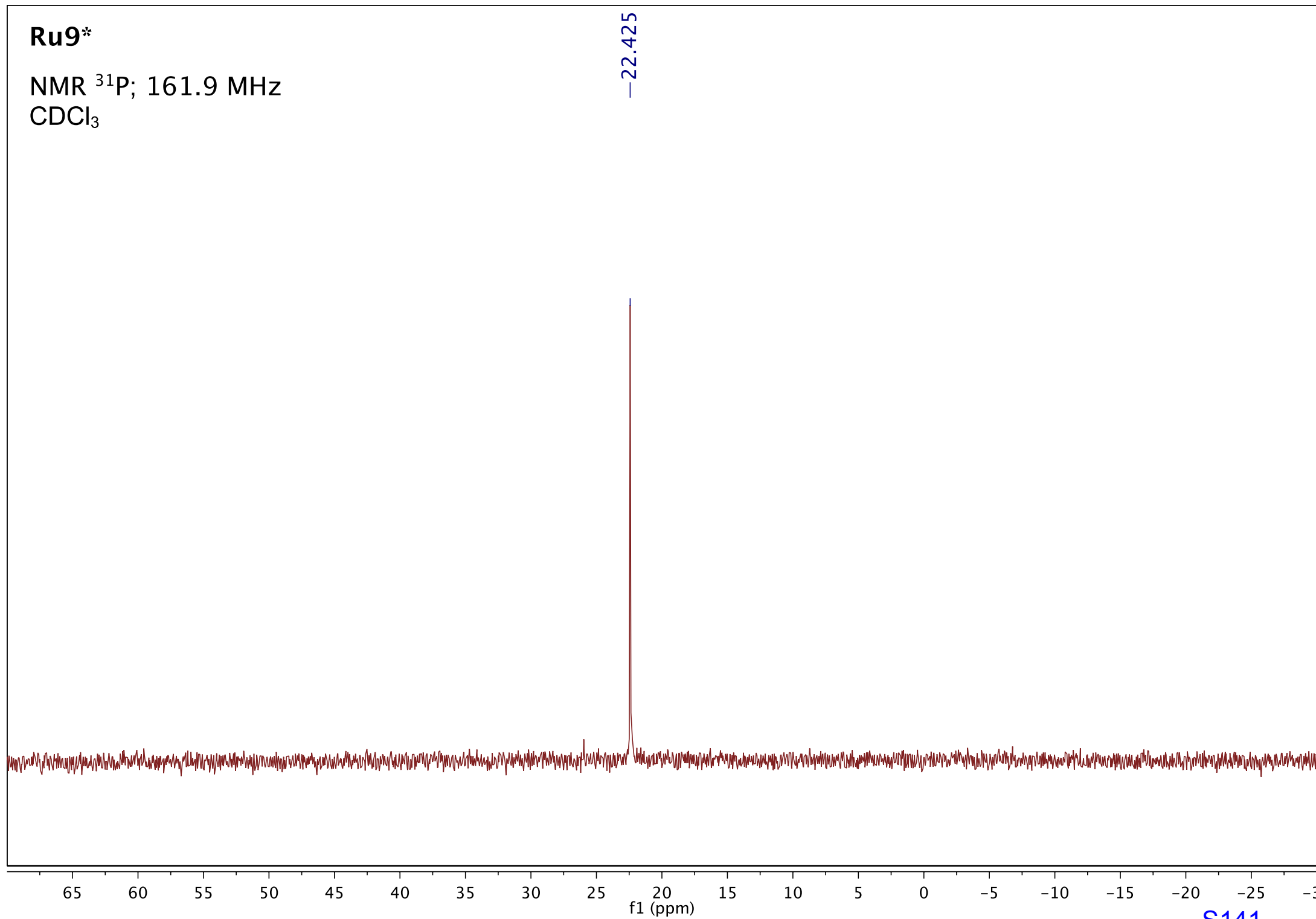


Ru9*

NMR ^{31}P ; 161.9 MHz

CDCl_3

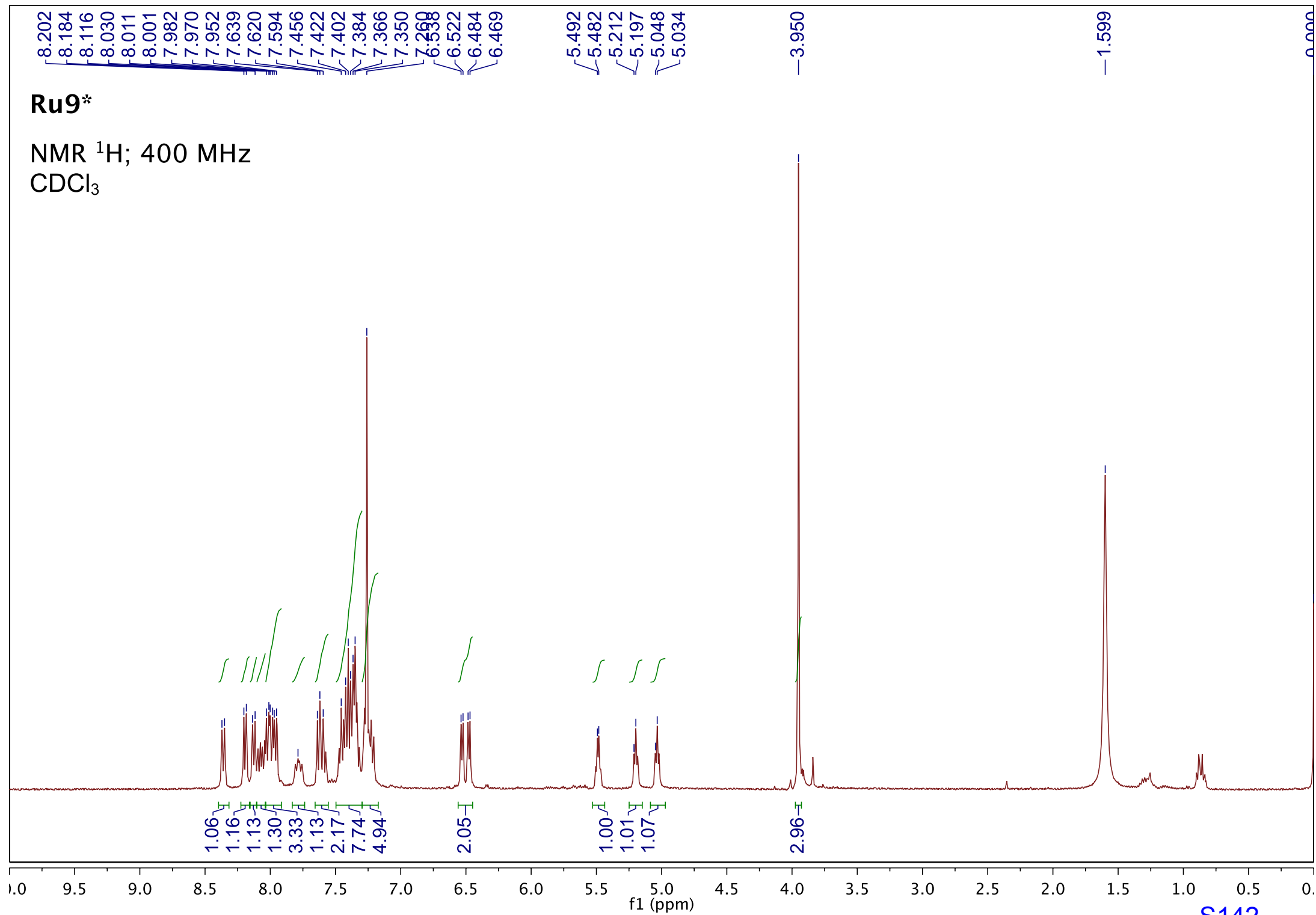
-22.425



Ru9*

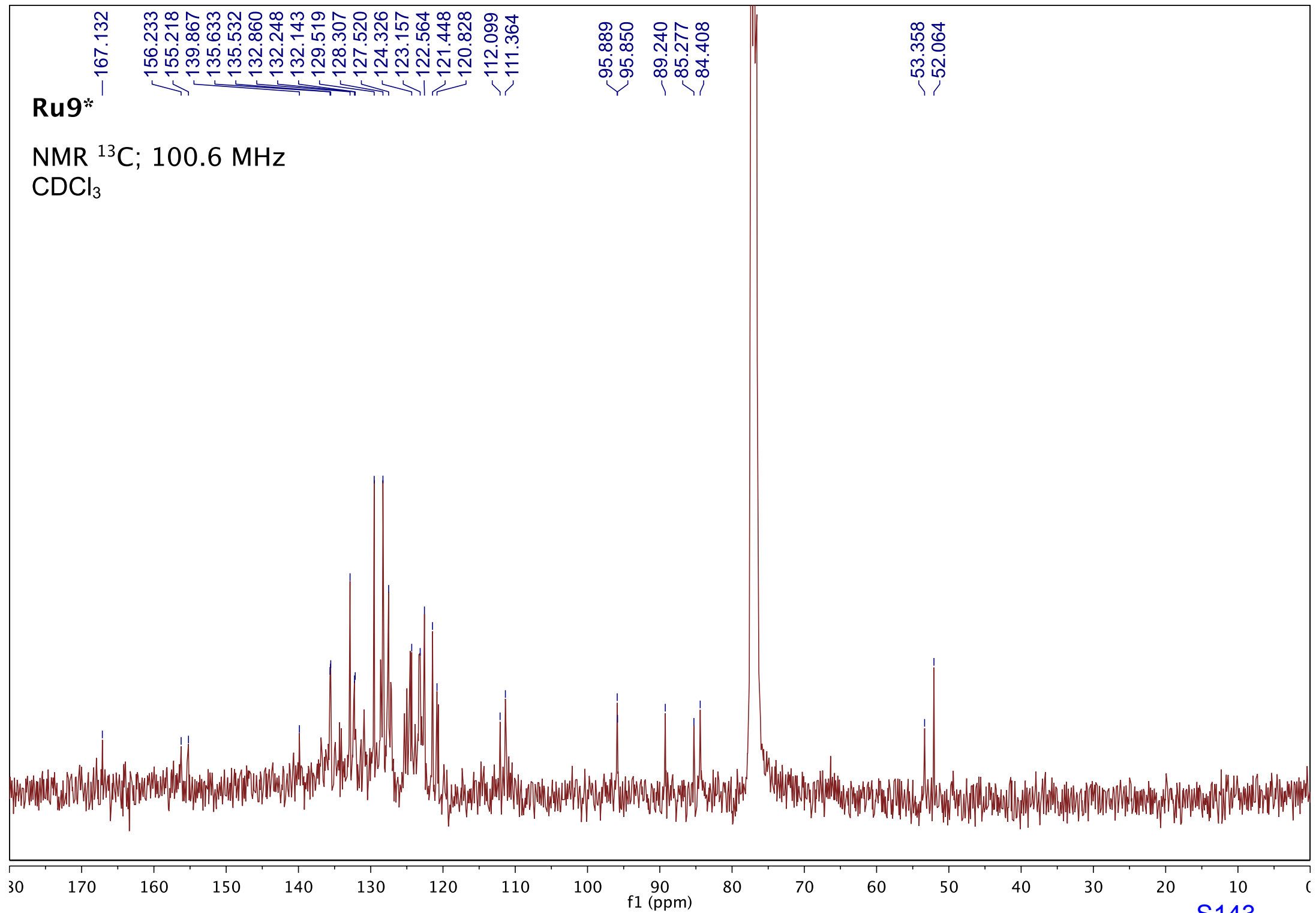
NMR ^1H ; 400 MHz

CDCl_3



Ru9*

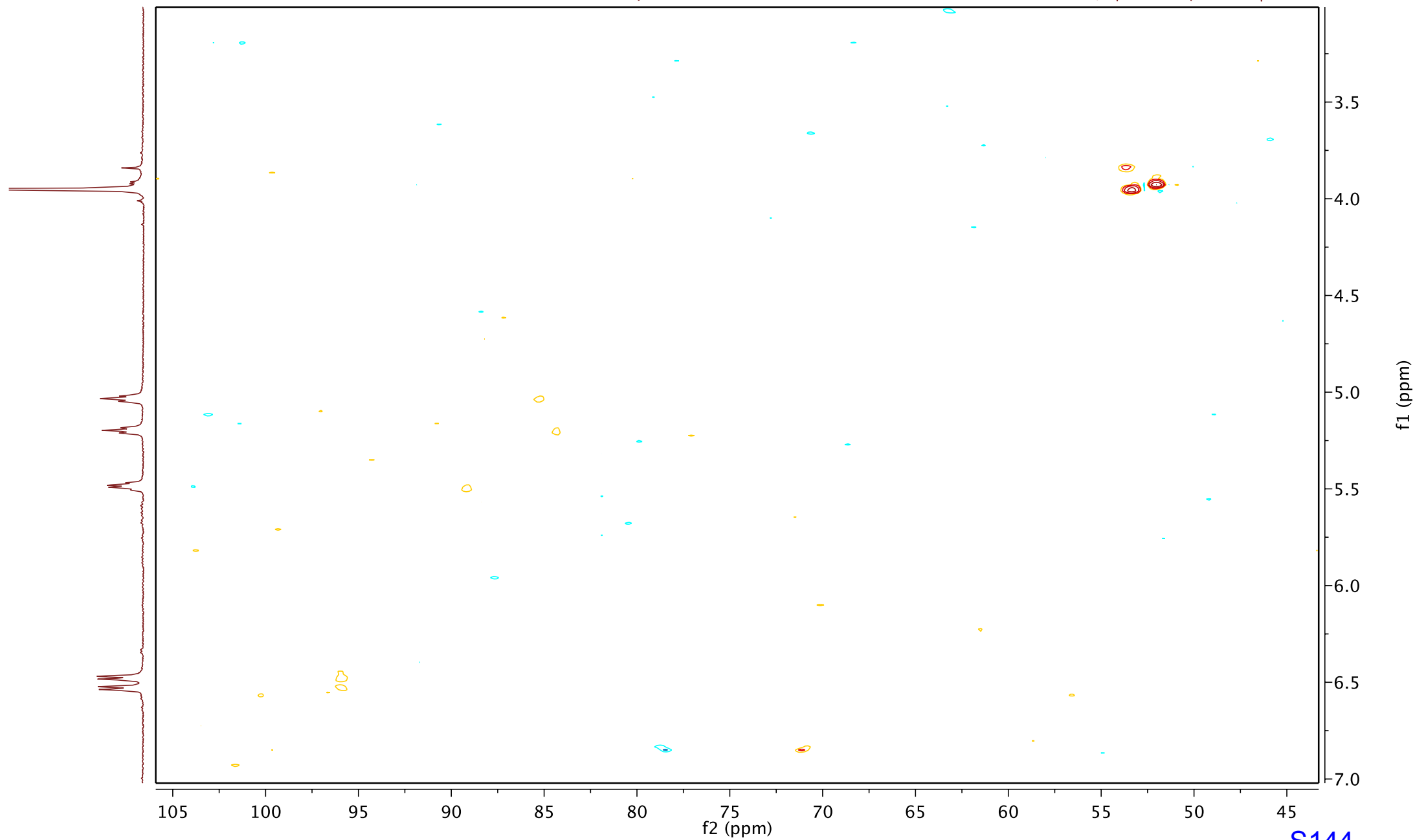
NMR ^{13}C ; 100.6 MHz
 CDCl_3



Ru9*

gHSQC 400MHz

CDCl₃



Ru11*

NMR ^{31}P ; 161.9 MHz

CDCl_3

—31.347

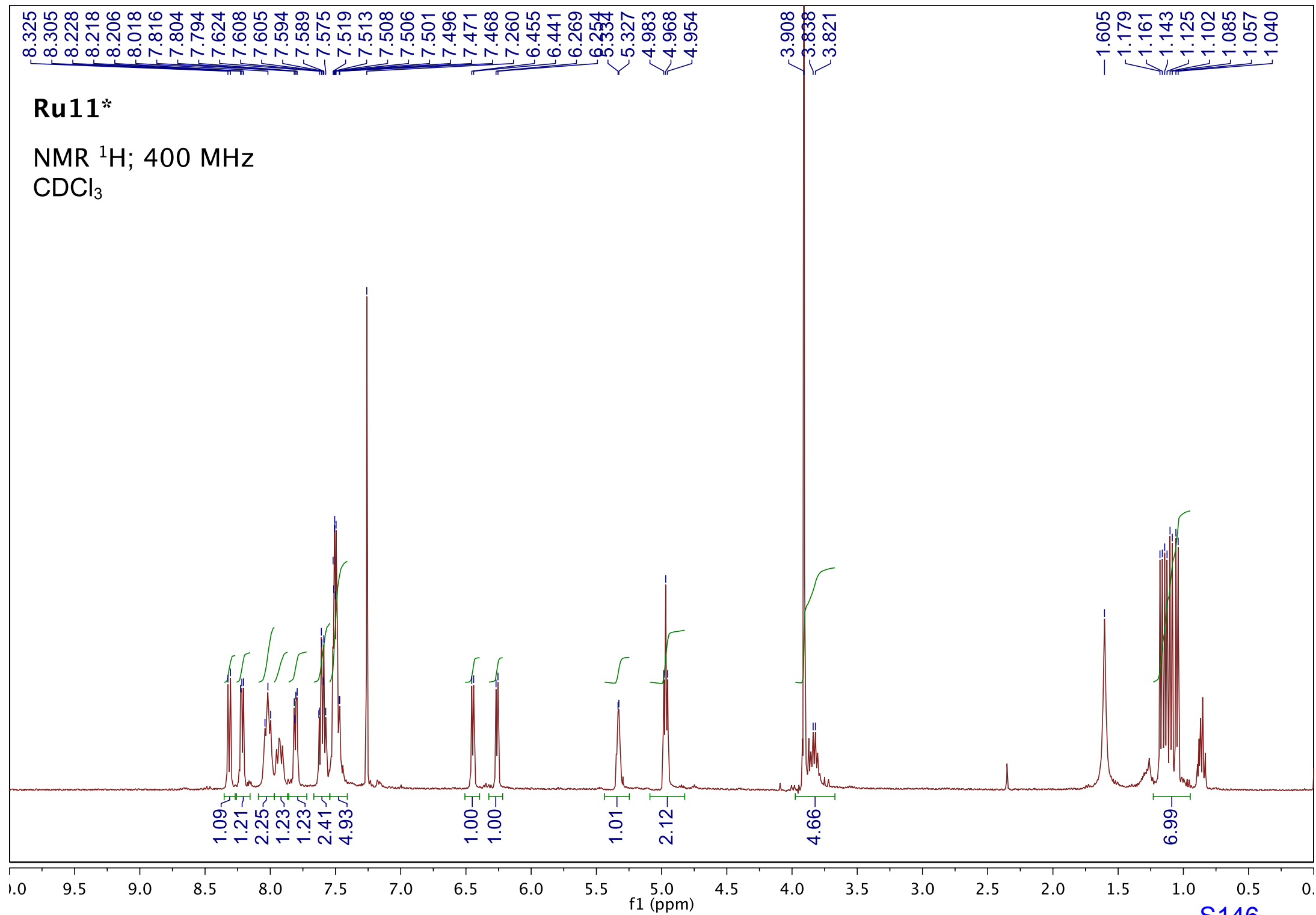
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20 -30 -40
f1 (ppm)

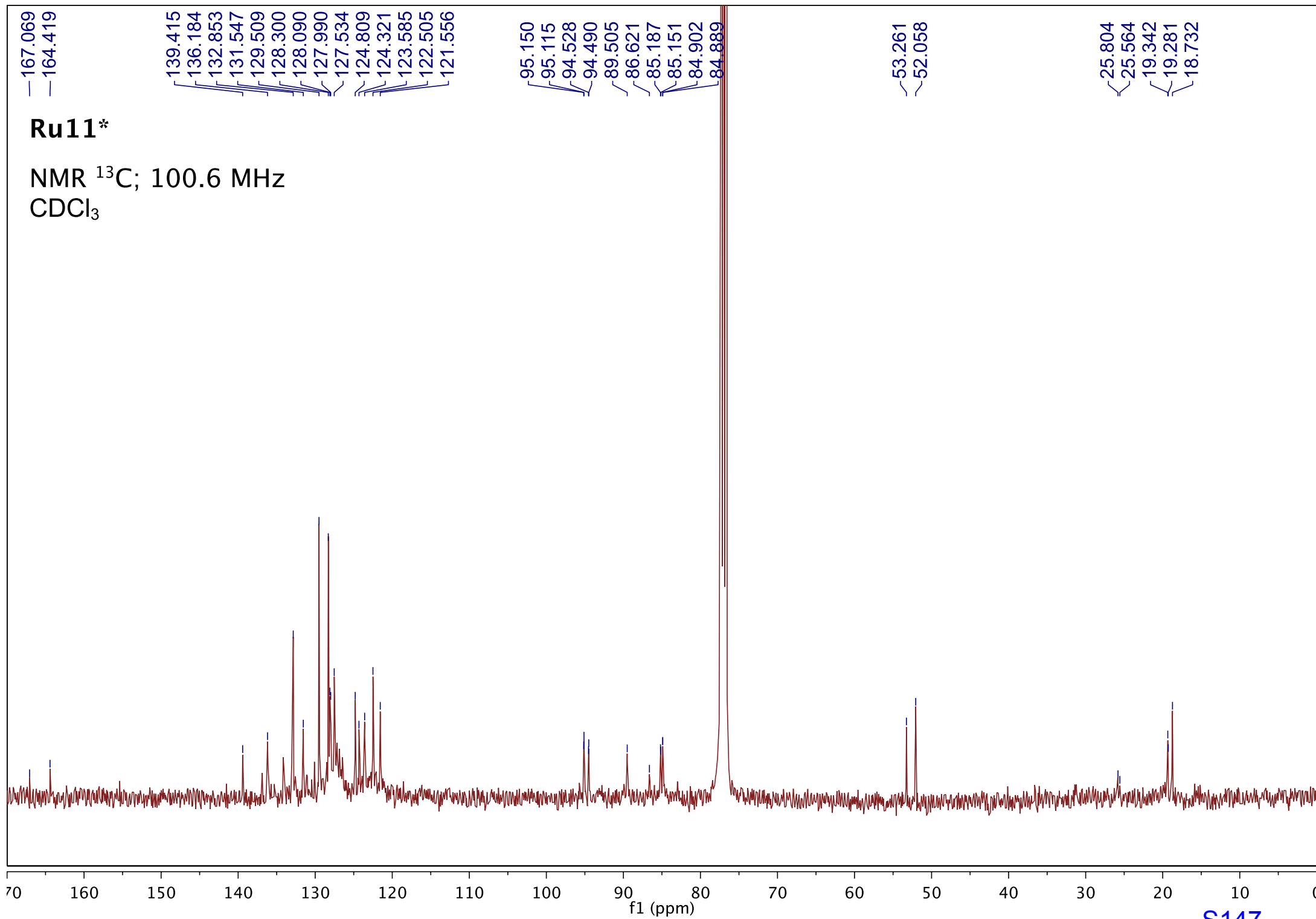
S145

Ru11*

NMR ^1H ; 400 MHz

CDCl_3

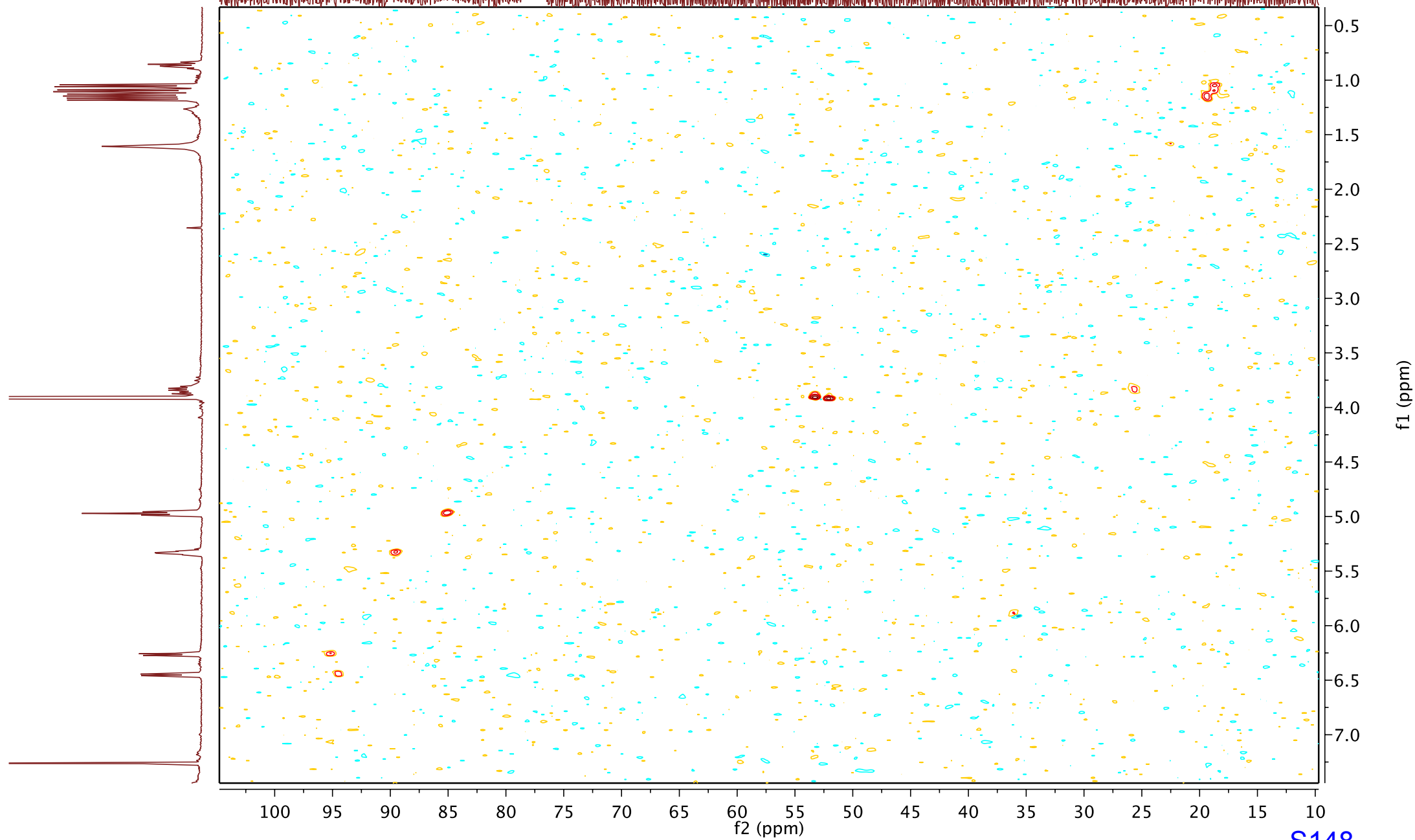




Ru11*

gHSQC 400MHz

CDCl₃



Ru13*

NMR ^{31}P ; 161.9 MHz

CDCl_3

—25.384

10 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30
f1 (ppm)

S149

Ru13*

NMR ^1H ; 400 MHz

CDCl_3

8.005
7.993
7.746
7.727
7.664
7.518
7.498
7.484
7.470
7.452
7.433
7.267
7.260
7.185
7.150
6.419
6.404
6.352
6.338
5.539
5.426
5.412
5.398

3.832

2.156
2.127

1.29
1.11
2.16
5.58
2.12
2.27

1.00
1.06

1.01
1.87

2.85

3.01

f1 (ppm)

S150

Ru2'

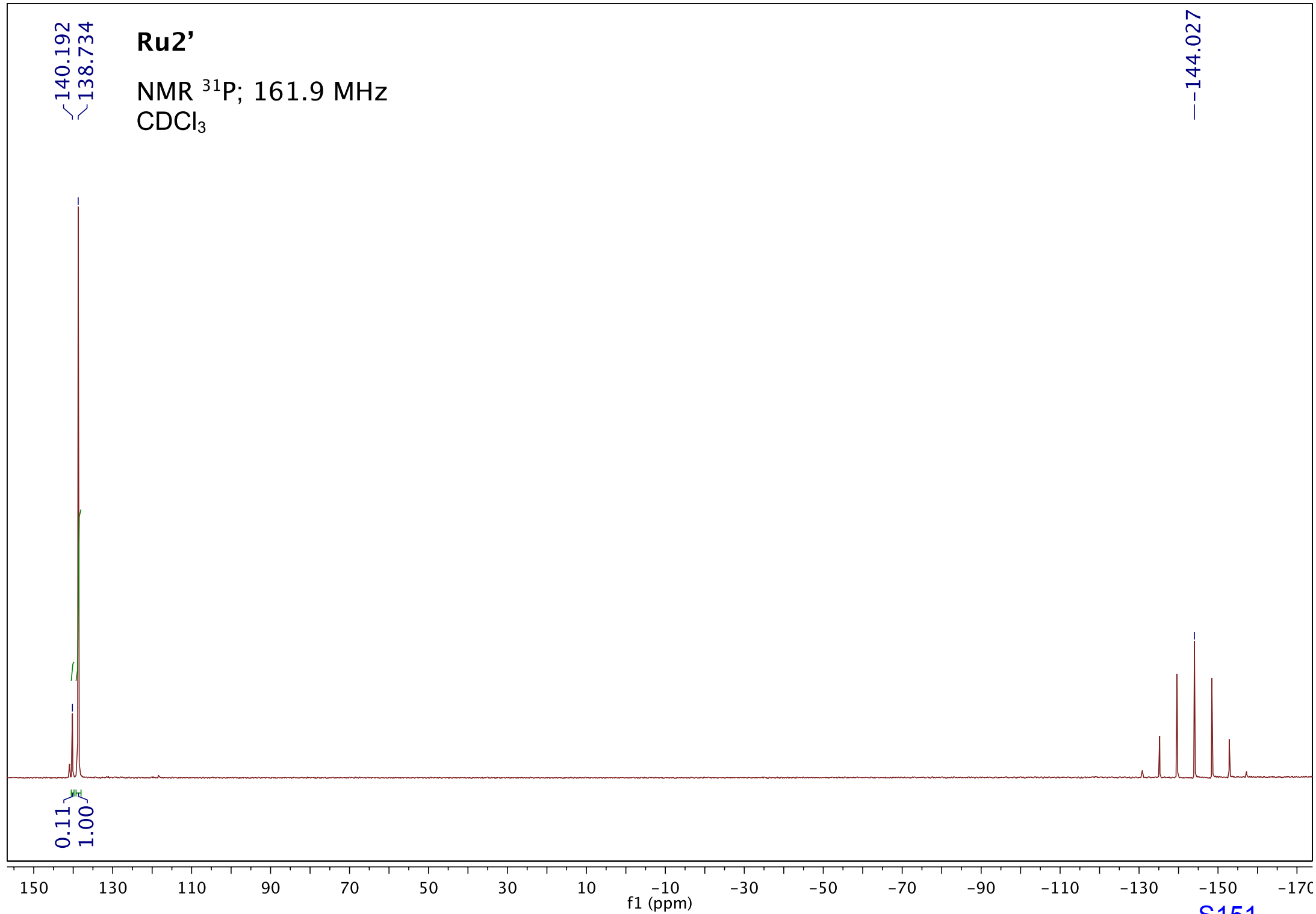
NMR ^{31}P ; 161.9 MHz

CDCl_3

140.192
138.734

144.027

0.11
1.00

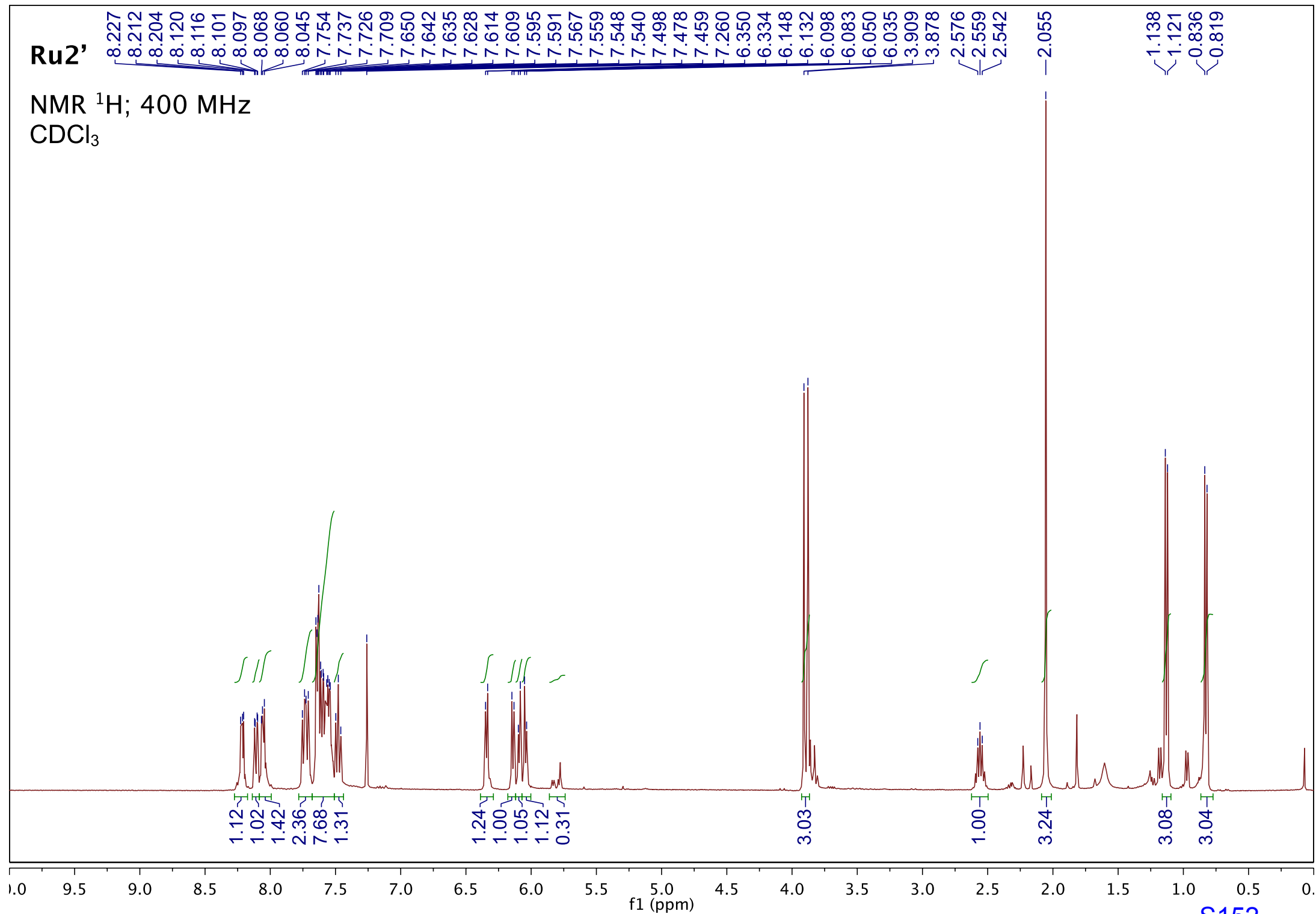


S151

Ru2'

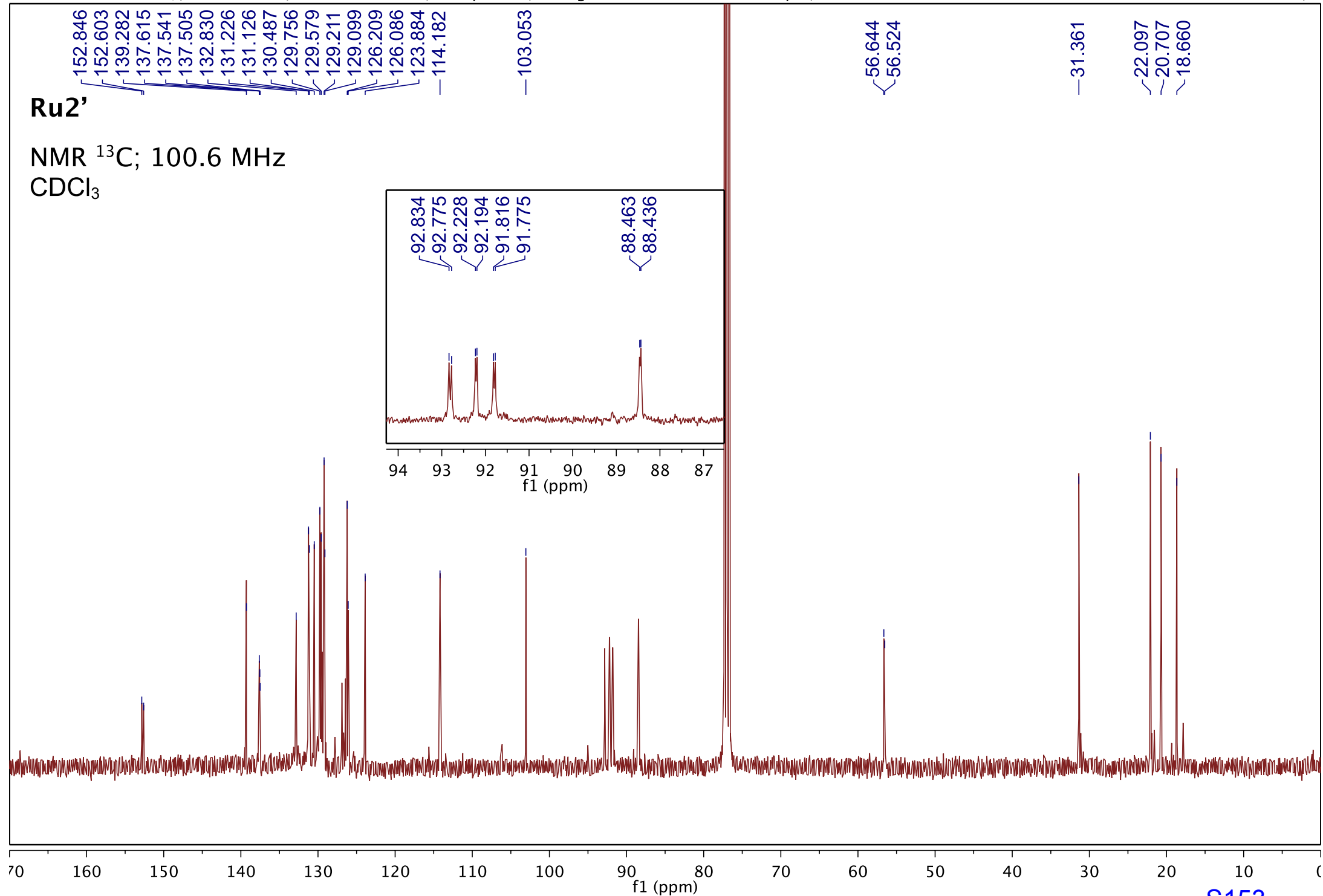
NMR ^1H ; 400 MHz

CDCl_3



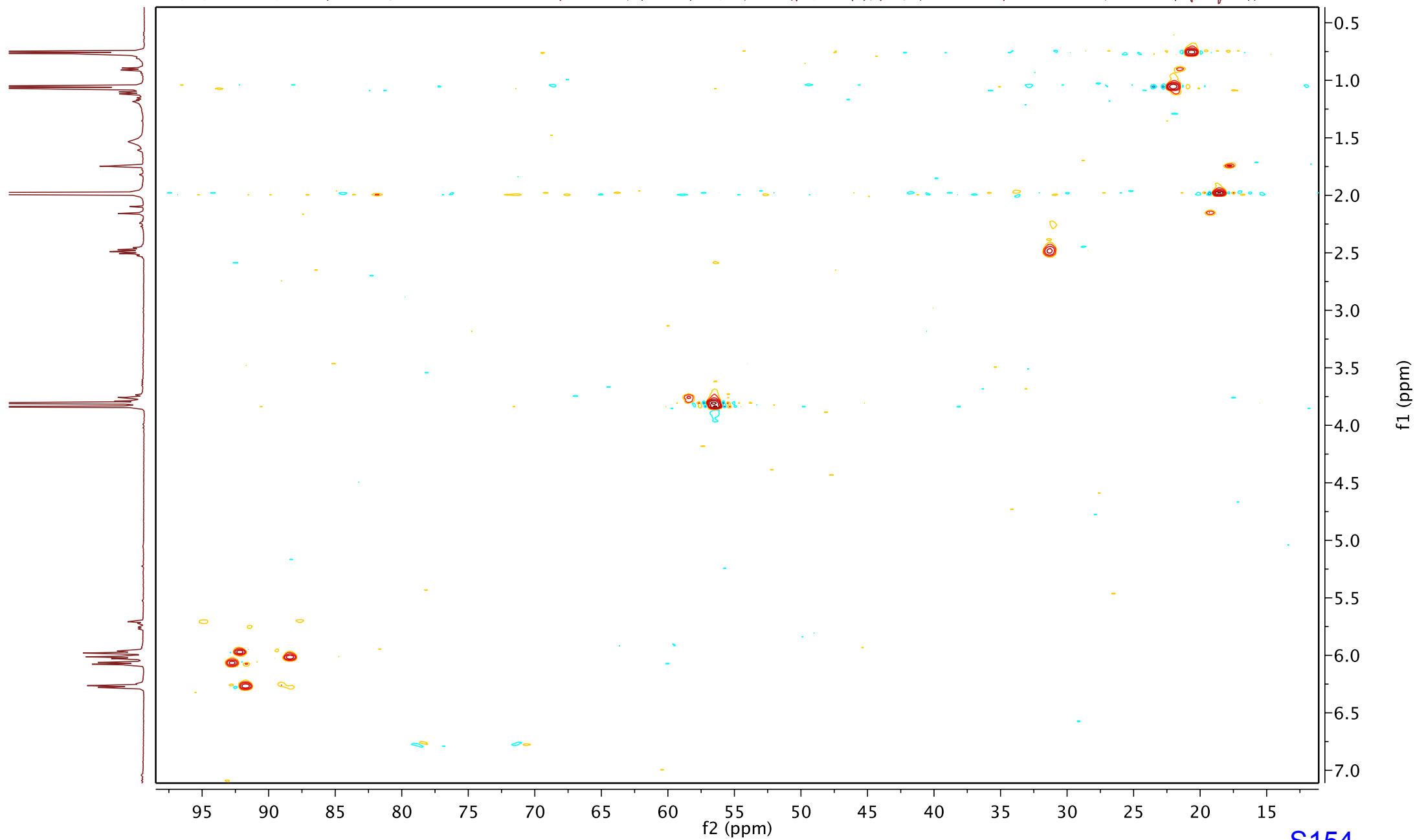
Ru2'

NMR ^{13}C ; 100.6 MHz
 CDCl_3



Ru2'

gHSQC 400MHz
CDCl₃

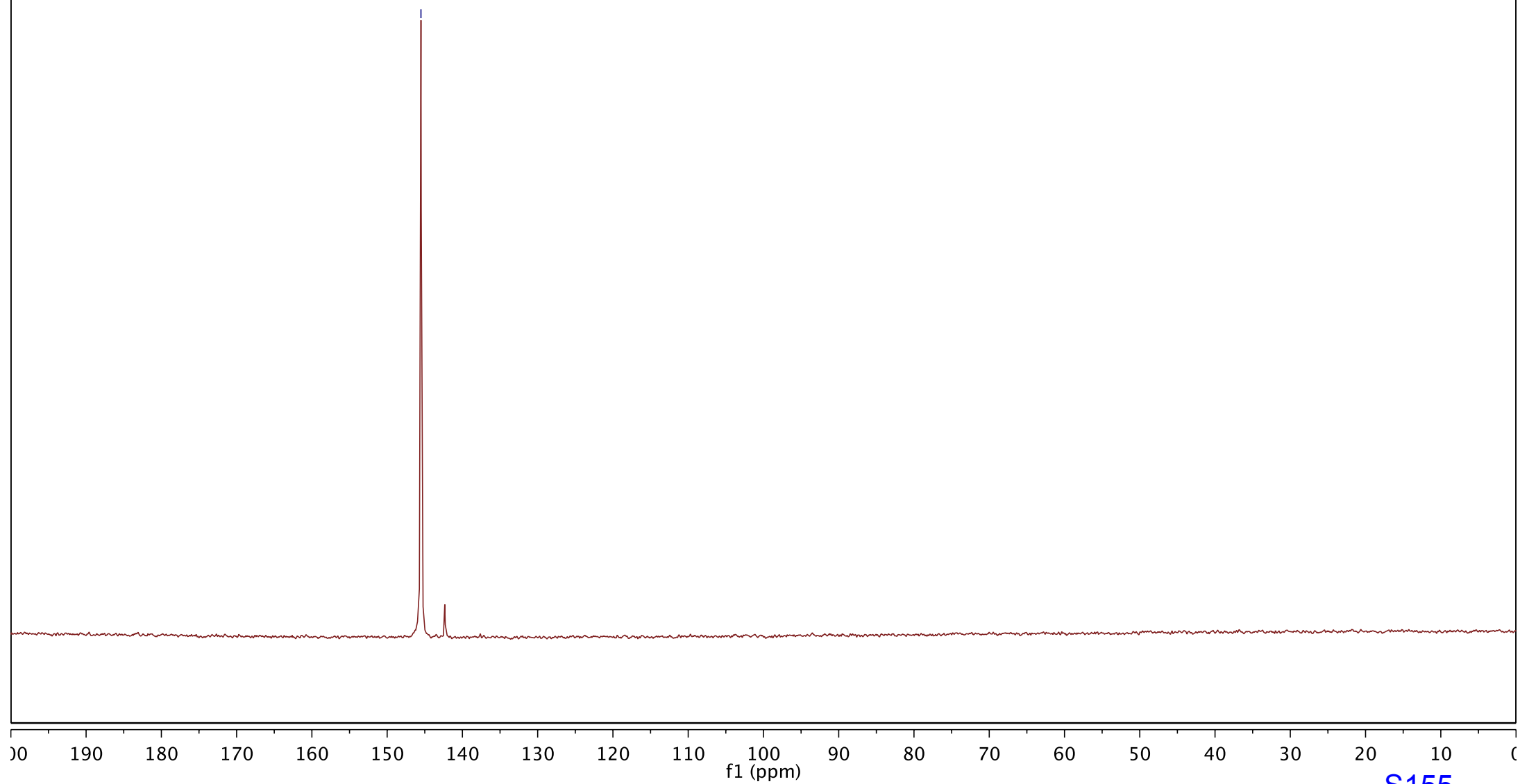


Ru3'

NMR ^{31}P ; 161.9 MHz

CDCl_3

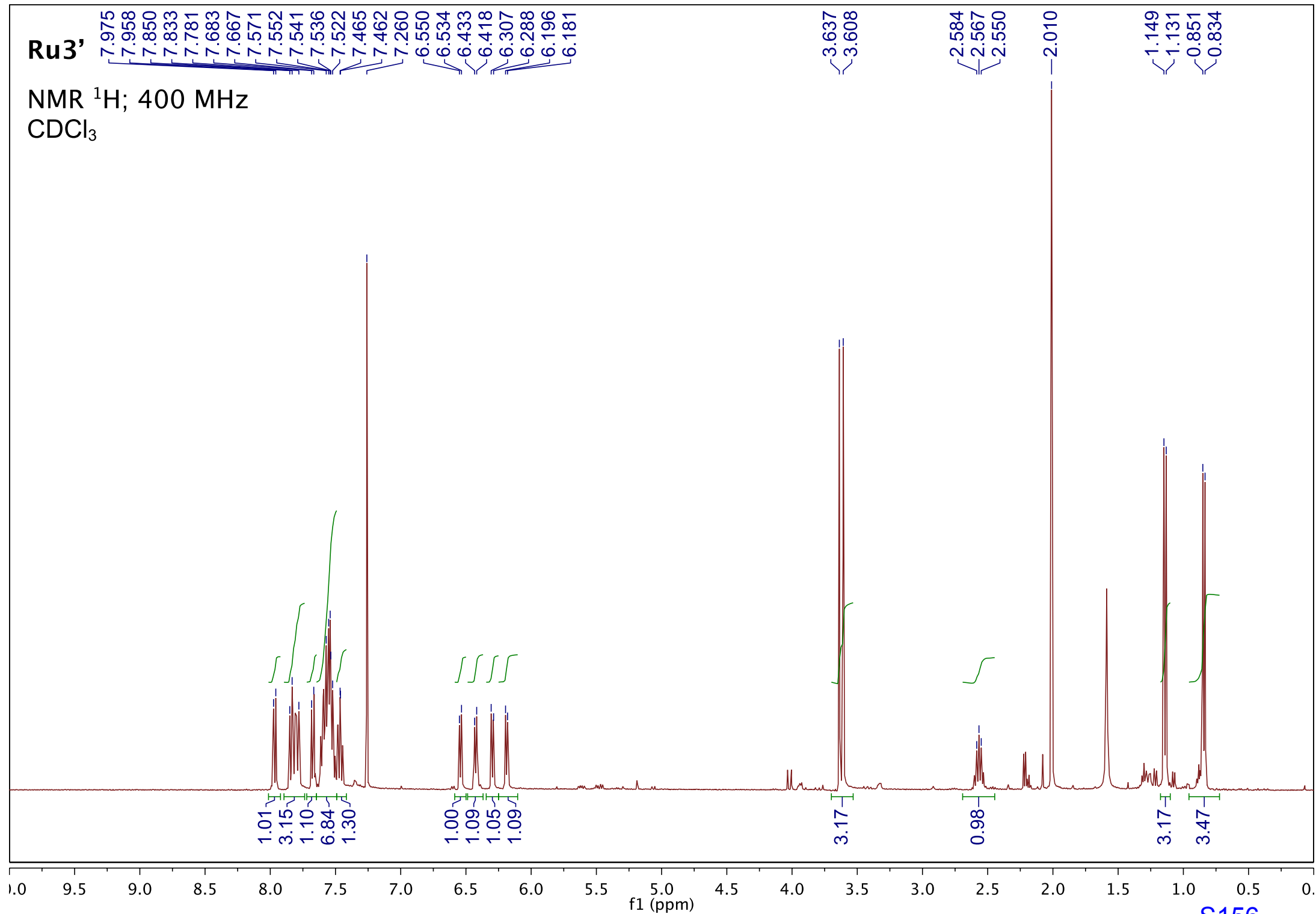
—145.507



Ru3'

NMR ^1H ; 400 MHz

CDCl_3



Ru3'

NMR ^{13}C ; 100.6 MHz

CDCl_3

140.490
133.607
133.117
132.844
132.283
131.514
130.907
130.106
129.815
129.210
128.793
127.379

— 114.157

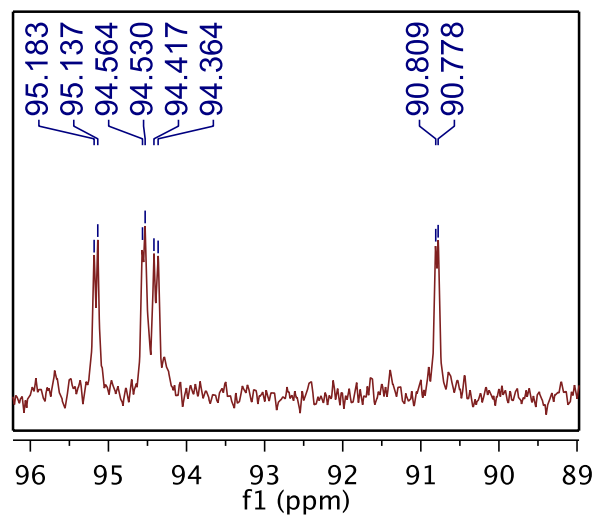
— 103.249

77.318
77.000
76.683

56.258
56.134

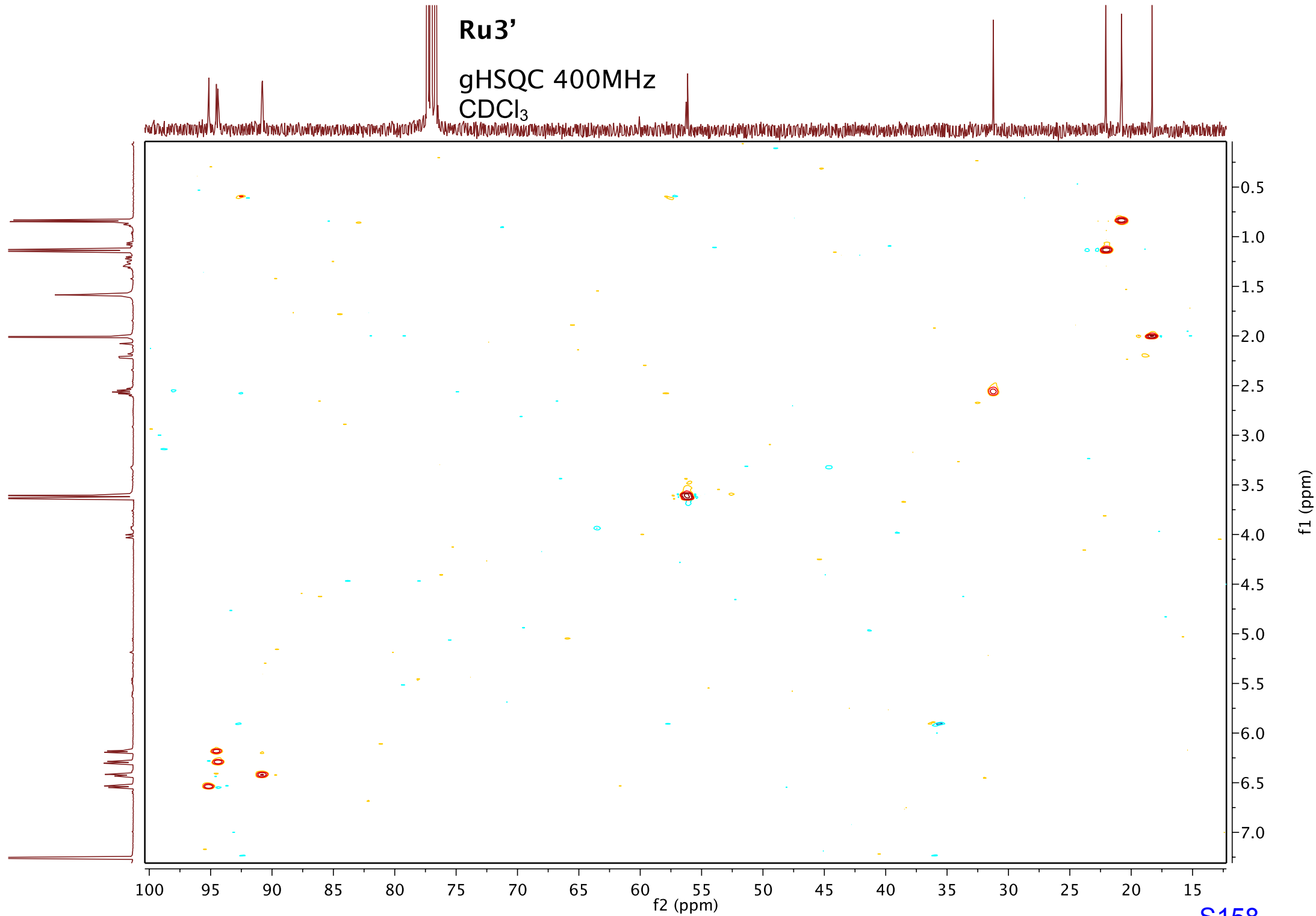
— 31.237

~ 22.075
~ 20.800
~ 18.309



70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)



Ru9'

NMR ^{31}P ; 161.9 MHz

CDCl_3

— 50.160

— 44.410

1.00

4.06

f1 (ppm)

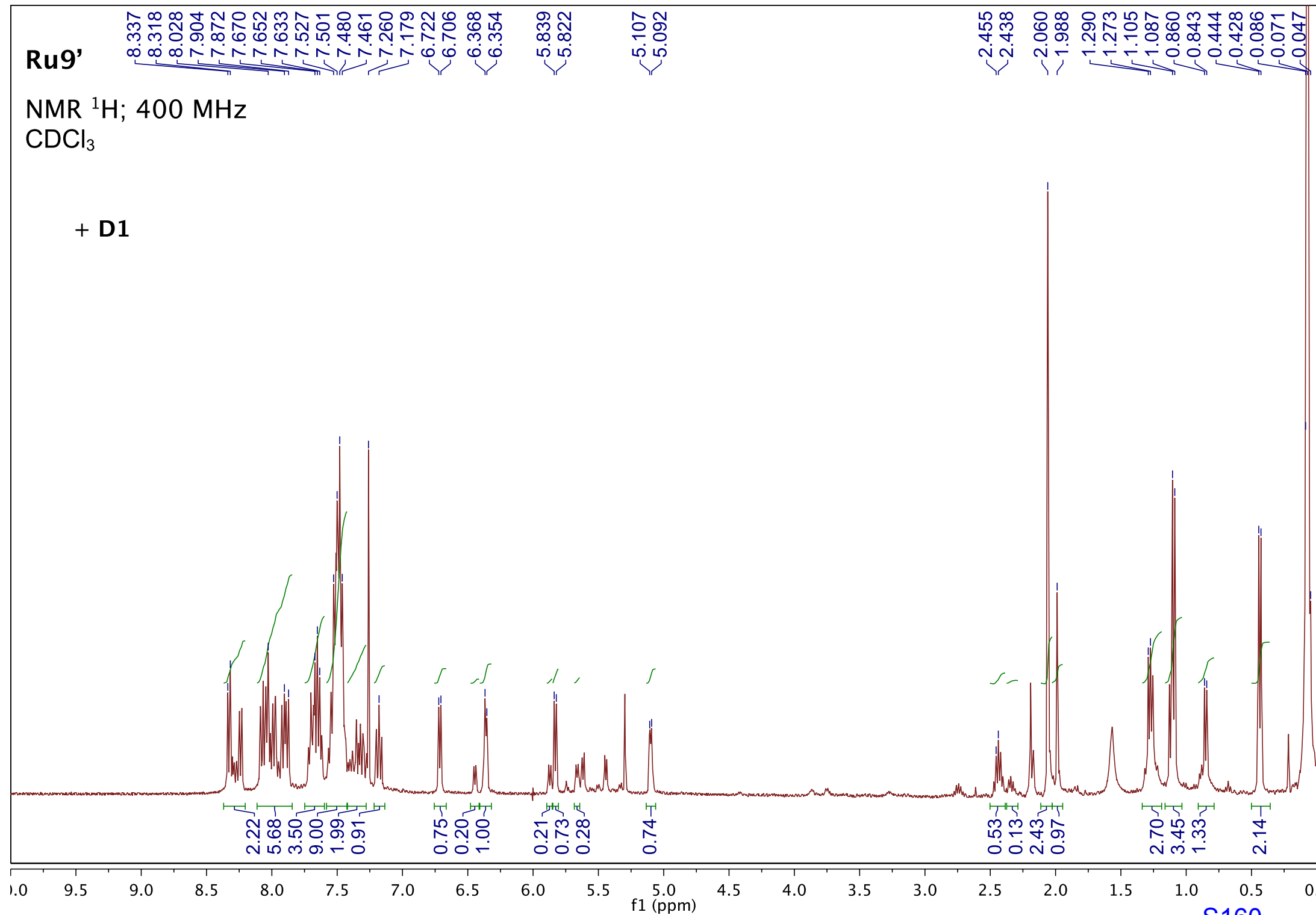
S159

Ru9'

NMR ^1H ; 400 MHz

CDCl_3

+ D1



S160

Ru9'

NMR ^{13}C ; 100.6 MHz
 CDCl_3

—155.616

—121.448

—112.000

—105.292

96.960

96.885

89.069

89.018

86.945

86.586

77.319

77.000

76.683

—31.319

—23.242

18.814

18.281

70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

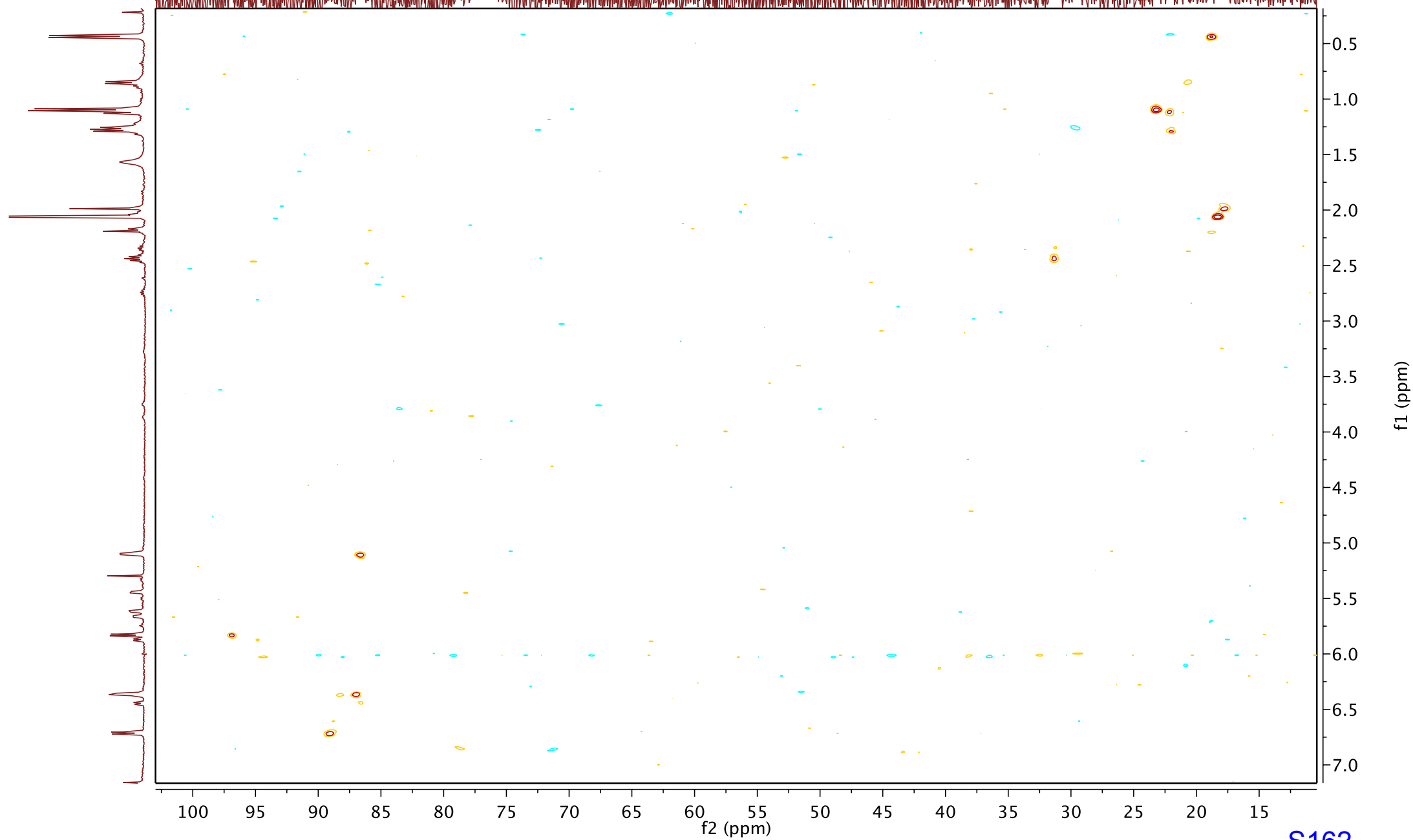
f1 (ppm)

S161

Ru9'

gHSQC 400MHz

CDCl₃



Ru10'

NMR ^{31}P ; 161.9 MHz

CDCl_3

—47.390

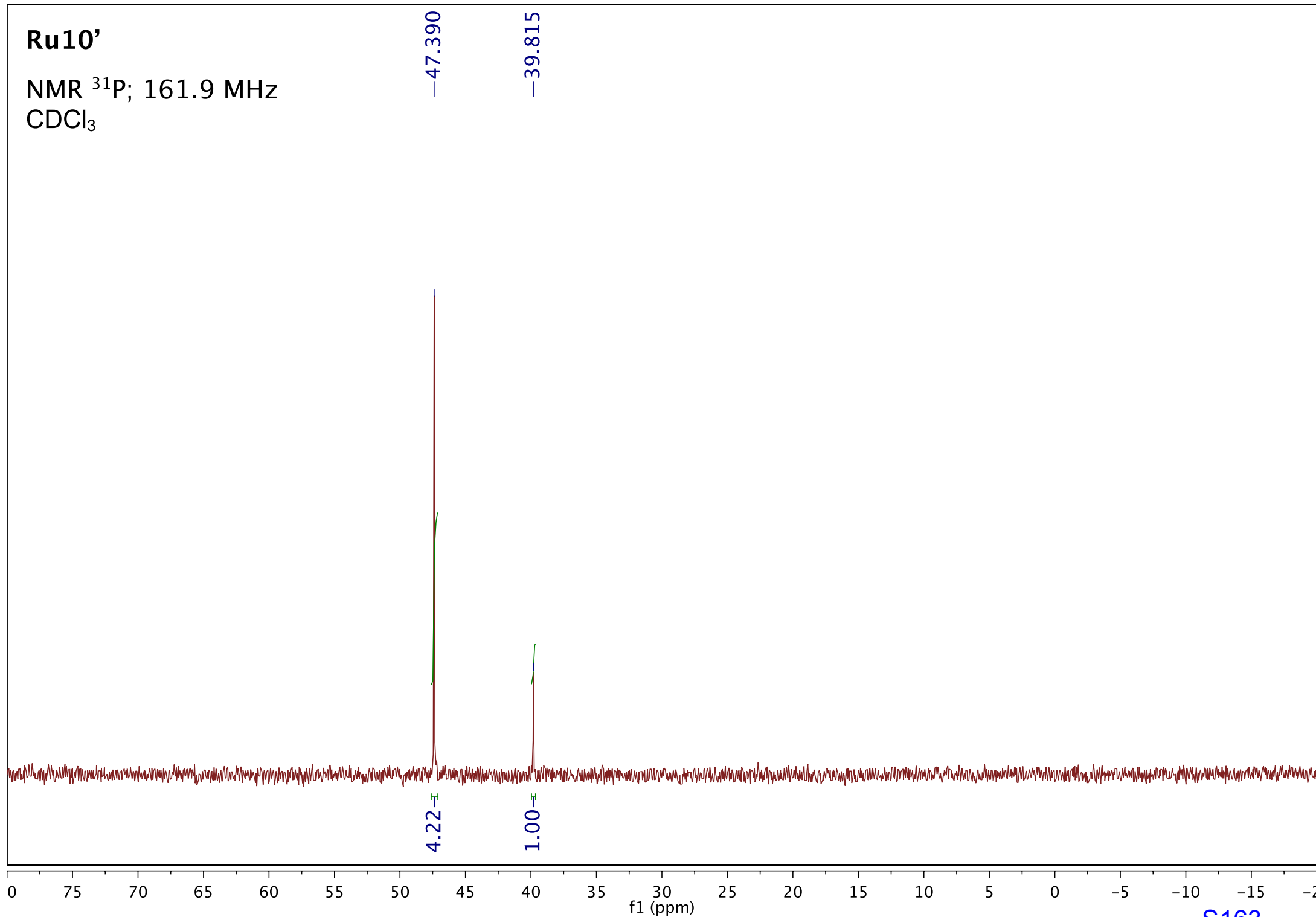
—39.815

4.22

1.00

f1 (ppm)

S163



Ru10'

NMR ^1H ; 400 MHz

CDCl_3

8.185
8.167
8.067
8.018
7.821
7.802
7.772
7.653
7.630
7.611
7.555
7.264
7.262
7.260
6.457
6.442
6.363
6.347
5.748
5.733
5.645
5.630

2.714
2.688
2.463
2.433
2.316
2.298
1.969
1.885

1.189
1.172
0.956
0.938

0.96
2.48
2.41
8.30
0.31

0.89
0.93
0.20

0.89
1.00

0.51
2.85
1.00

2.81

3.19
2.69

f1 (ppm)

S164

Ru10'

NMR ^{13}C ; 100.6 MHz

CDCl_3

151.980
151.786

123.999

112.868

104.293

94.521

94.464

89.808

89.763

88.013

87.993

86.264

86.230

31.136

22.020

21.445

17.943

12.376

12.011

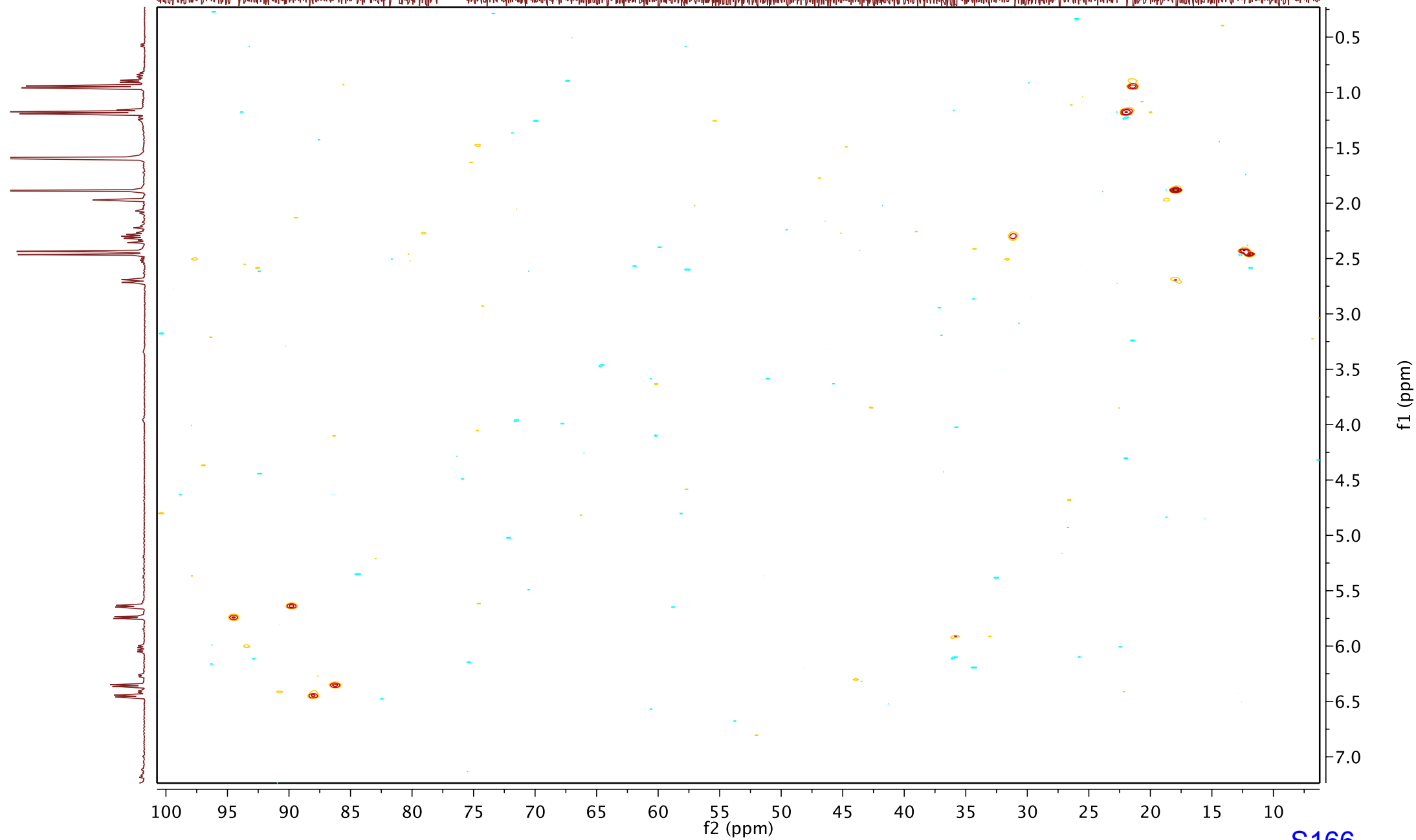
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

Ru10'

gHSQC 400MHz

CDCl₃



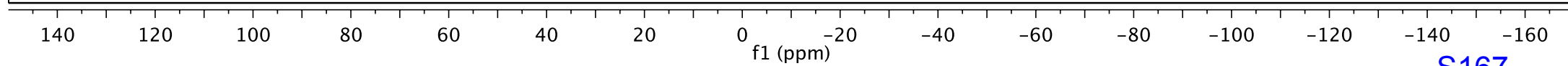
Ru11'

NMR ^{31}P ; 161.9 MHz

CDCl_3

68.130

--144.026



S167

Ru11'

NMR ^1H ; 400 MHz

CDCl_3

8.085
8.068
8.066
8.048
8.010
7.991
7.686
7.670
7.649
7.630
7.611
7.485
7.260
6.585
6.568
6.091
6.076
6.042
6.027
5.878
5.862

3.758
3.750
3.742

2.374
2.357
2.340
2.075
1.457
1.441
1.421
1.404
1.382
1.364
1.331
1.314
1.118
1.100
0.566
0.549

2.14

1.13

5.89

4.42

0.97

1.98

1.01

0.96

1.17

6.78

3.30

2.79

f1 (ppm)

S168

Ru11'

NMR ^{13}C ; 100.6 MHz
 CDCl_3

—153.022

—123.233

—113.273

97.902

93.689

93.627

91.665

91.609

91.286

85.713

77.318

77.000

76.683

31.404

29.390

29.123

23.118

19.424

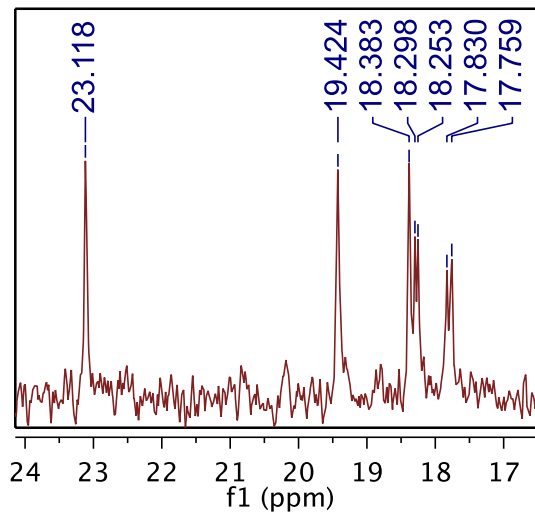
18.383

18.298

18.253

17.830

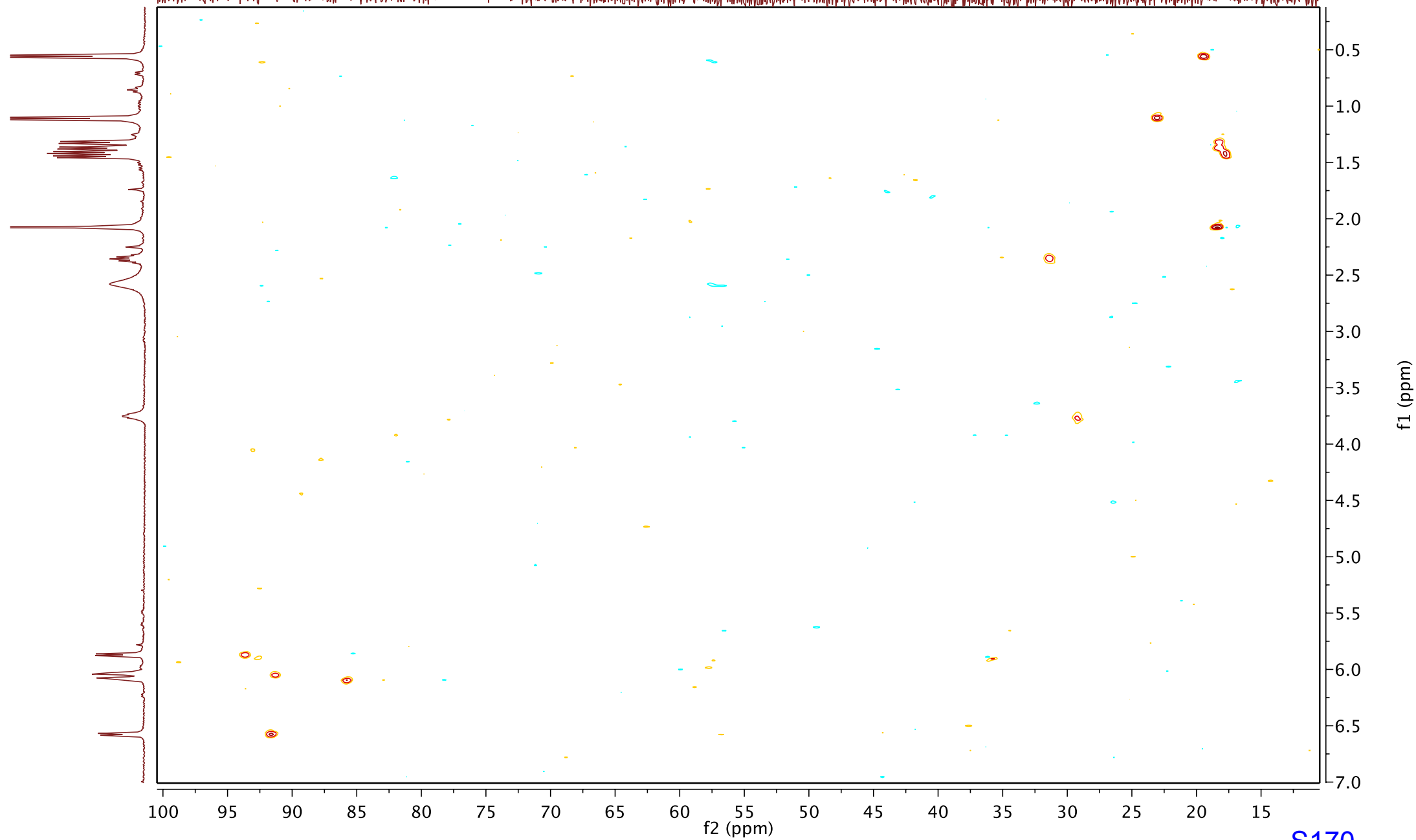
17.759



Ru11'

gHSQC 400MHz

CDCl₃

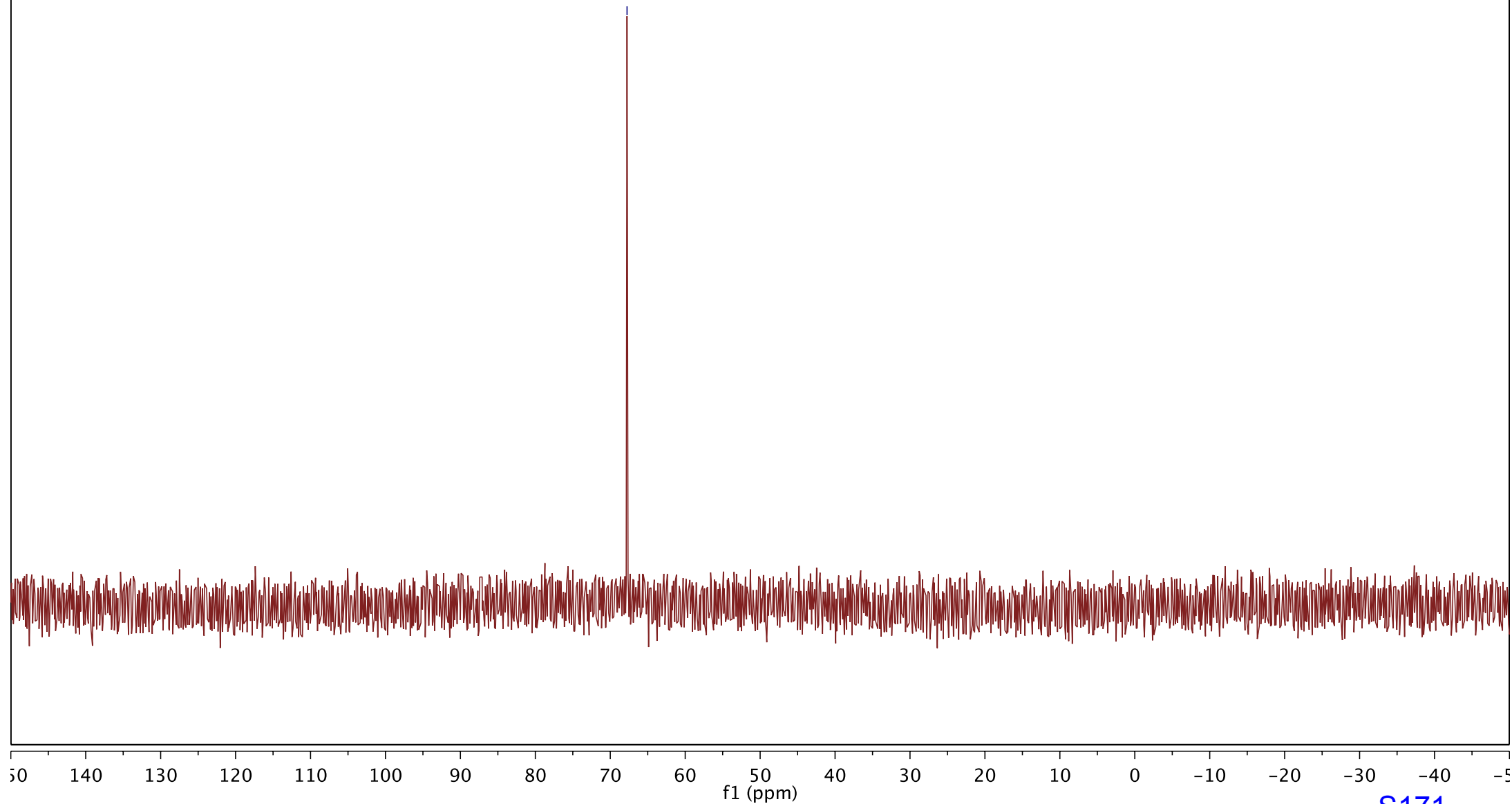


Ru11*

NMR ^{31}P ; 161.9 MHz

CDCl_3

—67.761



S171

Ru11*

NMR ^1H ; 400 MHz

CDCl_3

8.195
8.176
8.049
8.031
7.668
7.649
7.620
7.601
7.515
7.455
7.260
7.214
7.201
6.759
6.744
6.486

5.842

3.725

1.427
1.411
1.398
1.390
1.381
1.373
1.347
1.330

1.07

1.82

5.05

4.45

1.06

1.00

1.81

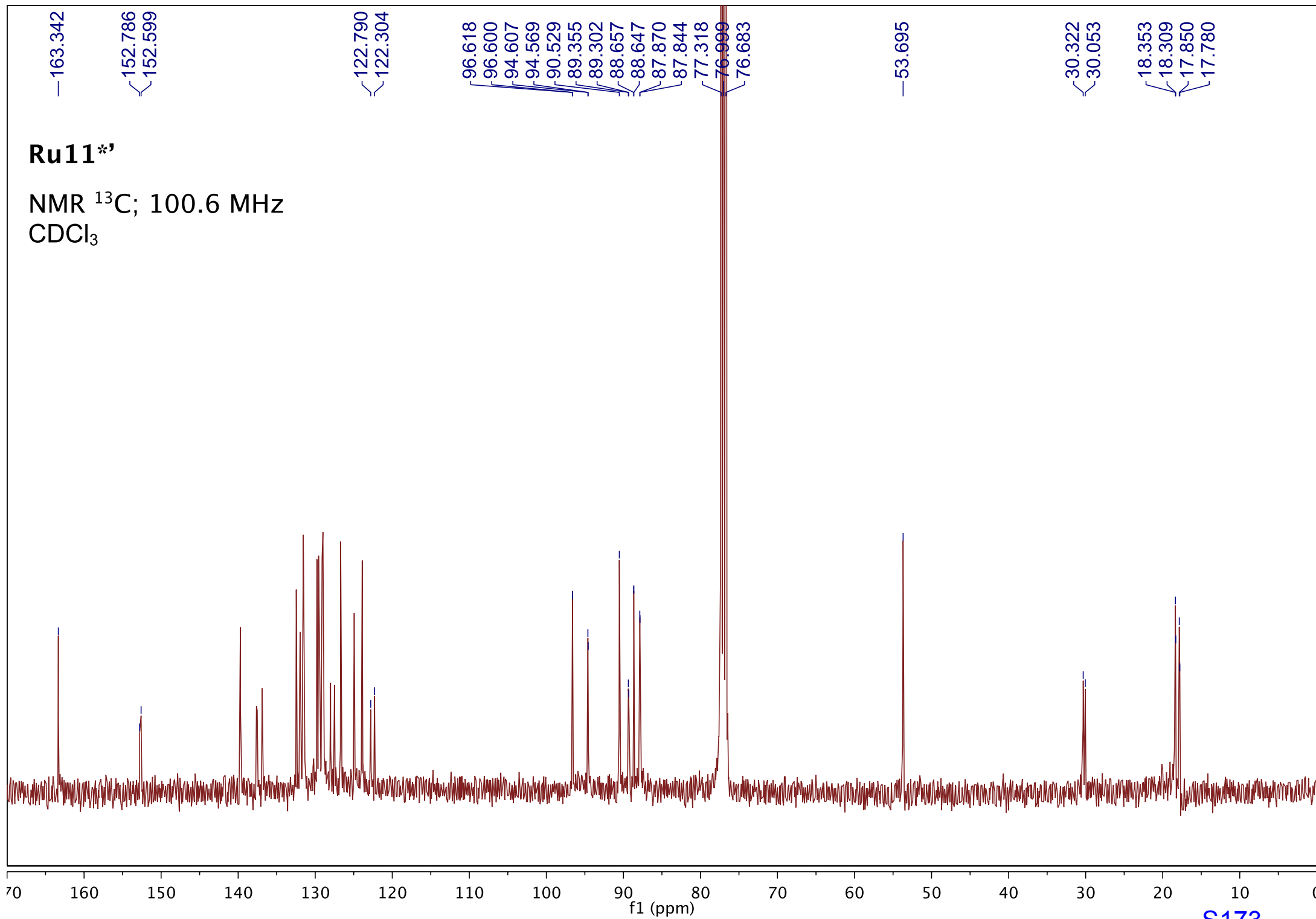
1.12

4.53

7.21

f1 (ppm)

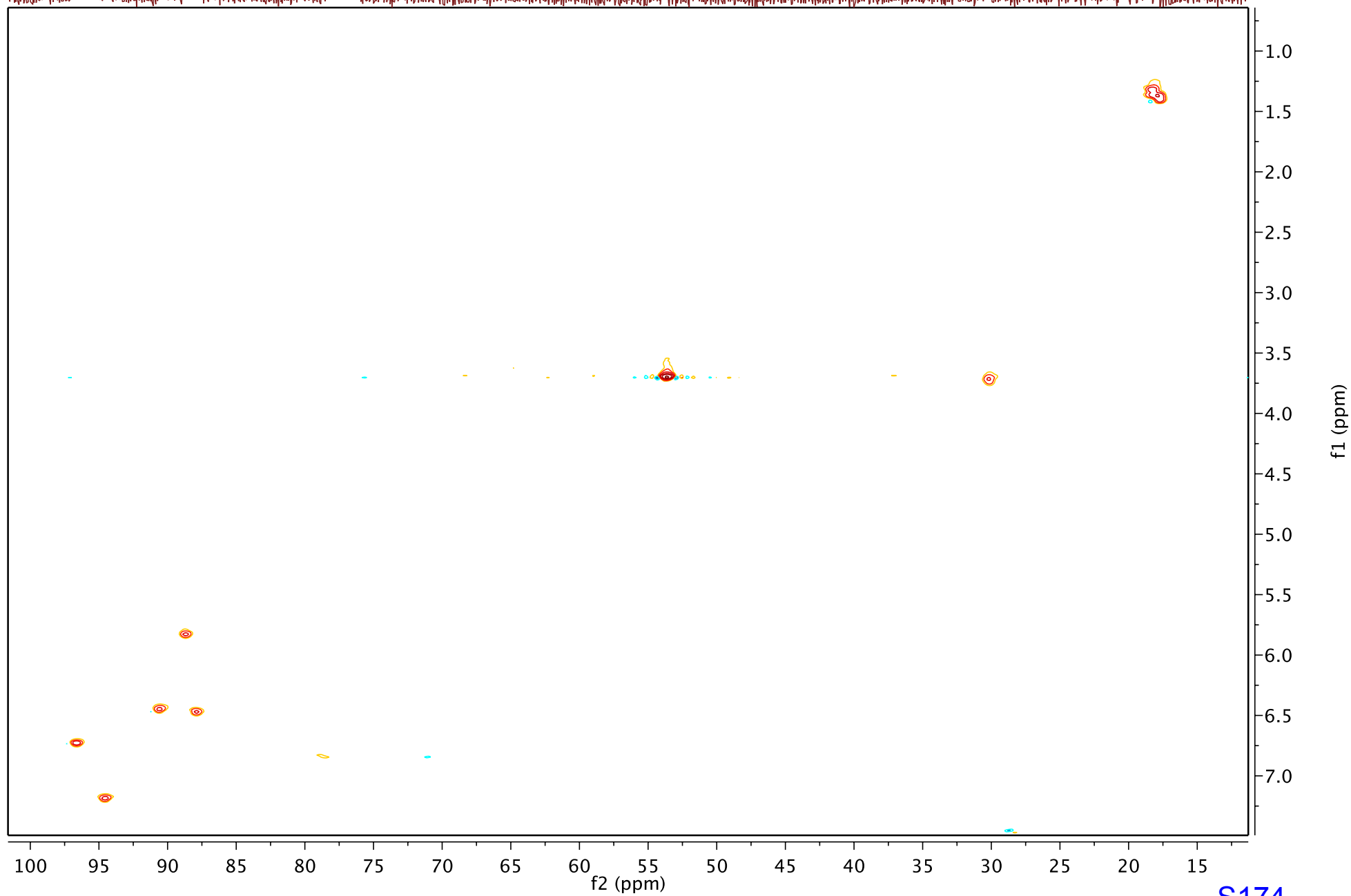
S172



Ru11*

gHSQC 400MHz

CDCl₃



Ru12'

NMR ^{31}P ; 161.9 MHz

CDCl_3

—52.953

—48.778

1.00

1.83

Ru12'

NMR ^1H ; 400 MHz

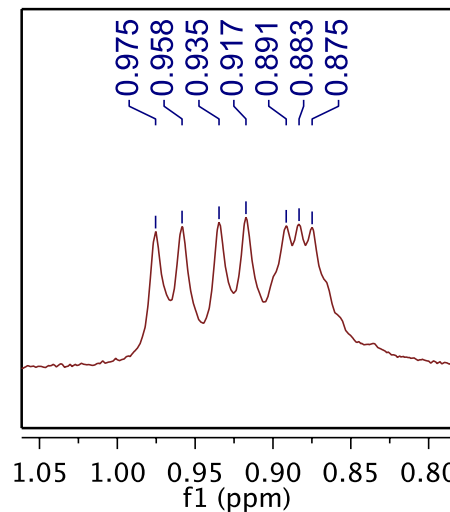
CDCl_3

—8.096
7.690
7.680
7.603
7.560
7.260

—6.249
—6.065
5.535
5.521
5.178
4.943
4.708
4.661
4.574
4.362
4.169
4.005

1.773
1.711
1.584

1.254
0.975
0.958
0.935
0.917
0.891
0.883
0.875



Arene

Ferrocene

5.74
3.96
6.89

1.89
1.02
0.87
0.89
1.55
1.05
1.10
0.82
1.18
1.13
0.82
3.16
3.05

1.52
1.58
1.26
1.25
2.71

1.91
8.27

Ru12'

NMR ^{13}C ; 100.6 MHz
 CDCl_3

—151.675

—123.893

—113.063

—111.832

—104.481

—100.234

—70.912

—70.327

—31.561

—31.153

—22.363

—21.744

—21.158

—20.856

—18.101

—17.638

95.279

95.245

94.879

94.824

90.495

90.457

90.148

90.114

89.228

89.189

88.379

86.840

86.802

86.738

86.703

74.603

74.523

73.089

73.005

72.656

72.551

72.240

72.097

71.550

71.457

71.323

71.206

70.807

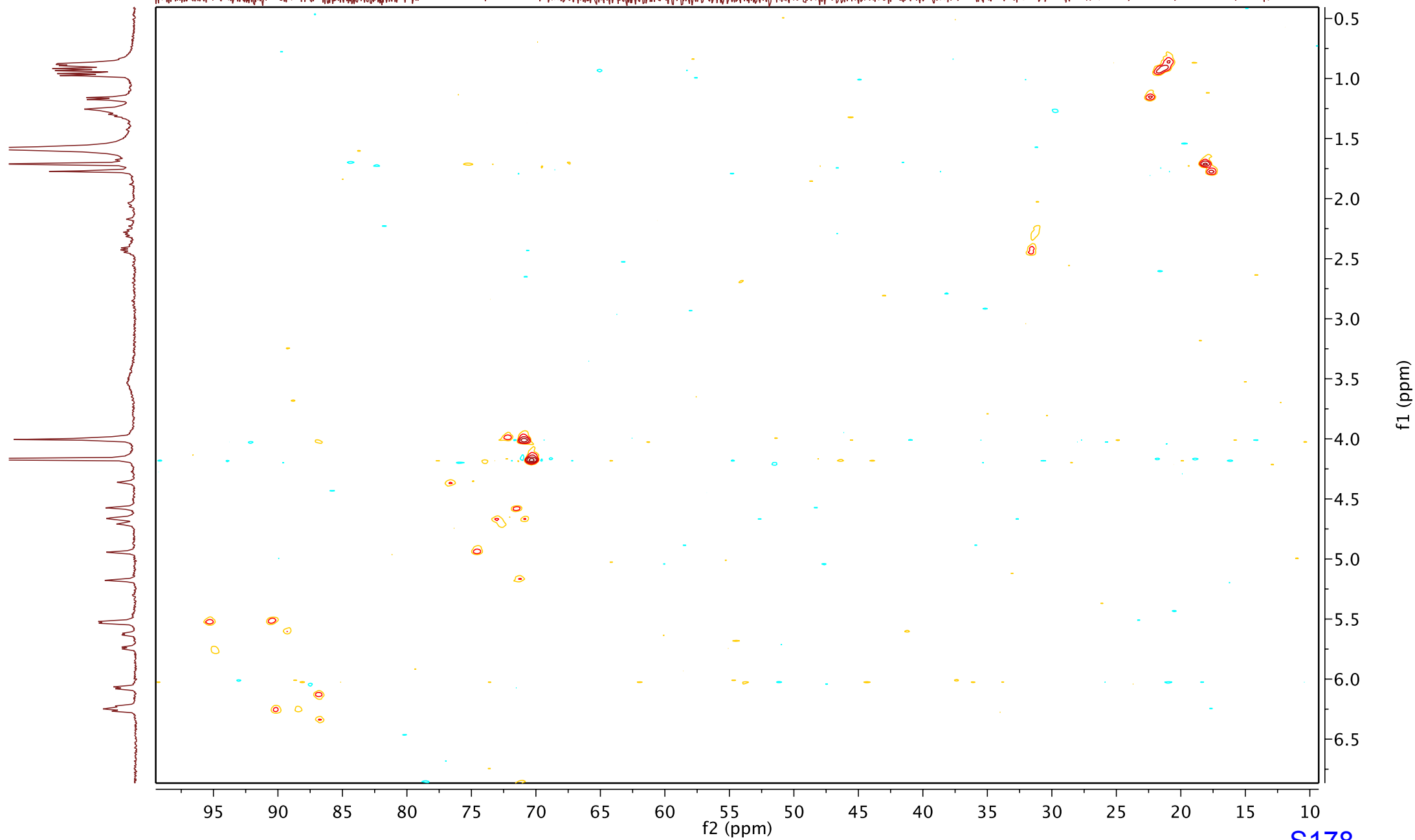
70 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0

f1 (ppm)

Ru12'

gHSQC 400MHz

CDCl₃



Ru13'

NMR ^{31}P ; 161.9 MHz

CDCl_3

—54.933

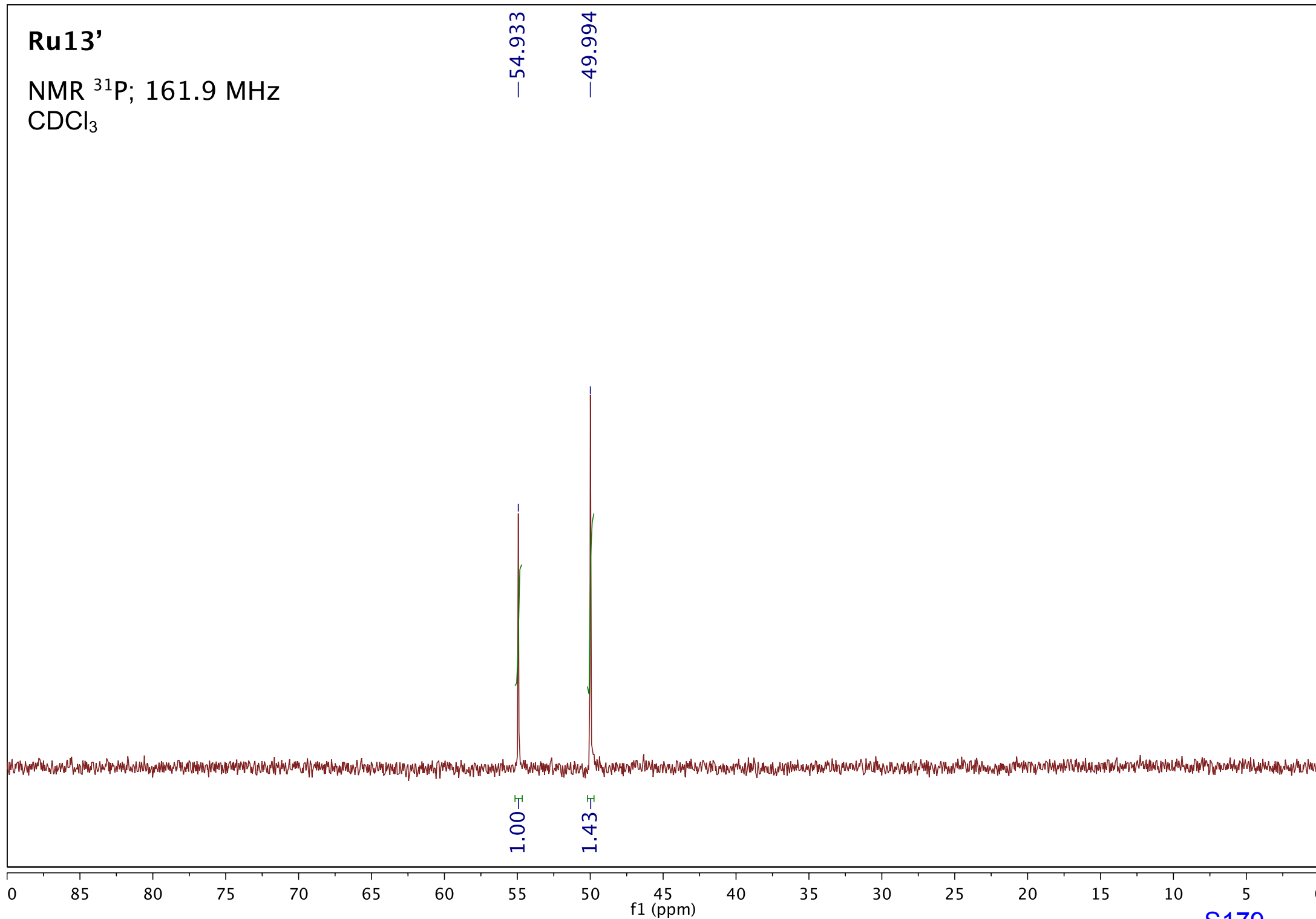
—49.994

1.00

1.43

f1 (ppm)

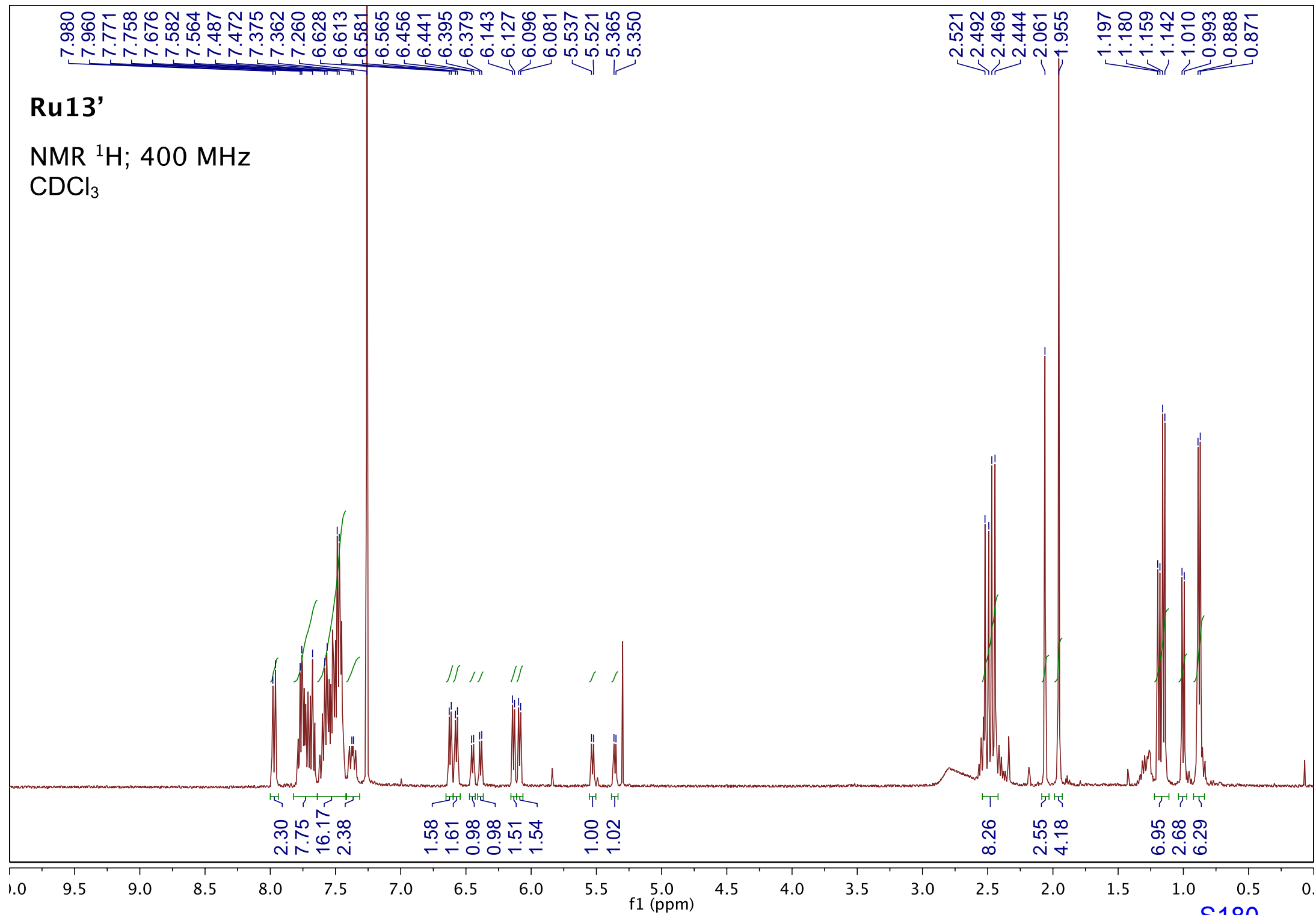
S179



Ru13'

NMR ^1H ; 400 MHz

CDCl_3



S180

Ru13'

NMR ^{13}C ; 100.6 MHz

CDCl_3

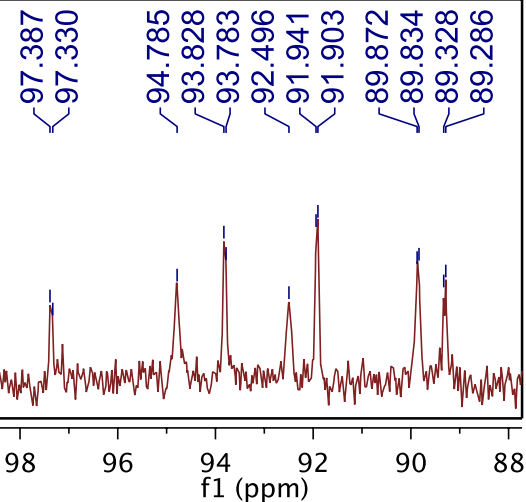
—146.213

—127.708

—113.356
—113.062

—104.004
—101.382

31.223
30.915
21.909
21.847
21.641
21.298
20.988
18.139
17.995
12.019
11.621



Ru13'

gHSQC 400MHz

CDCl₃

