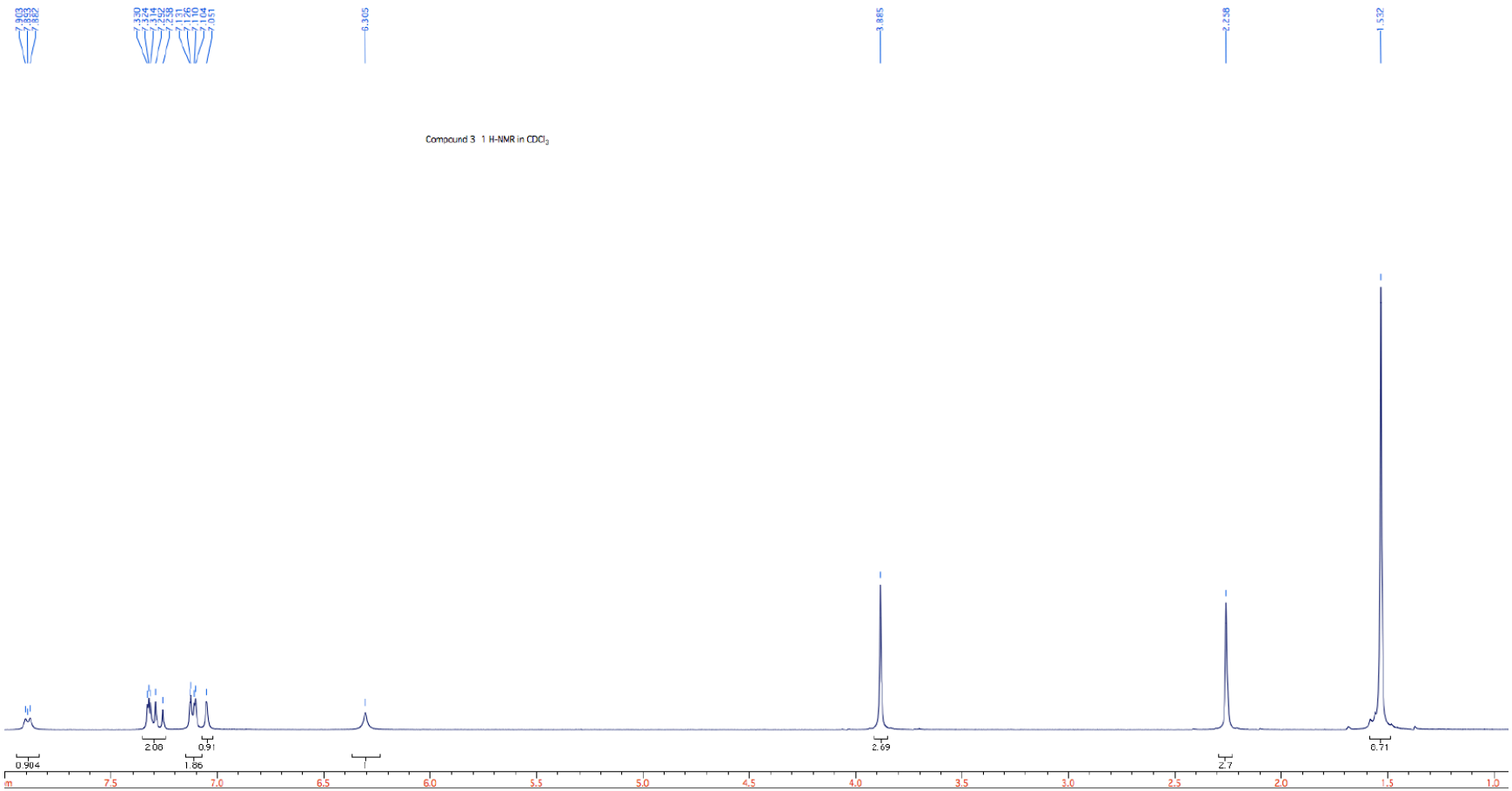
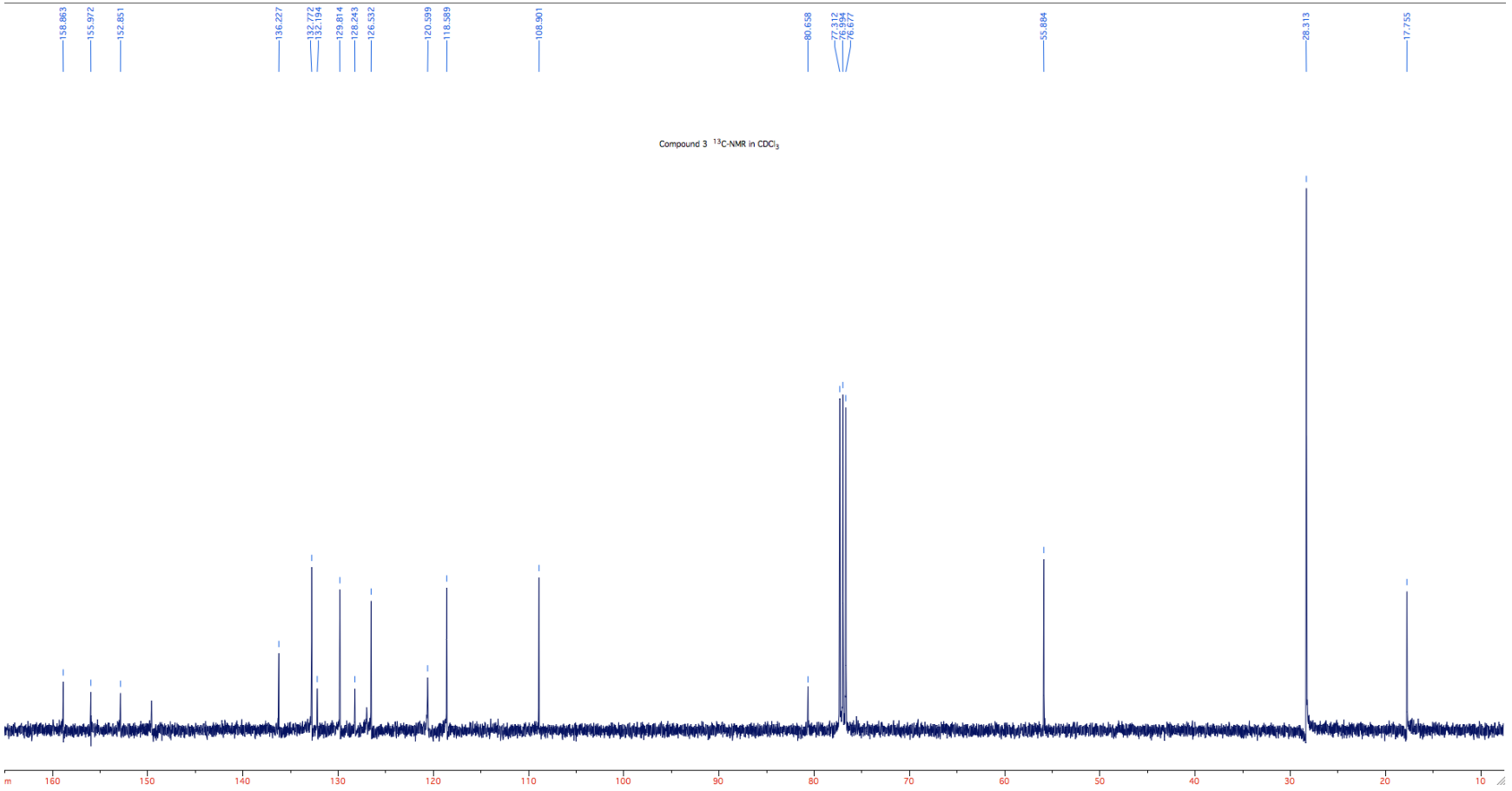
SUPPORTING INFORMATION

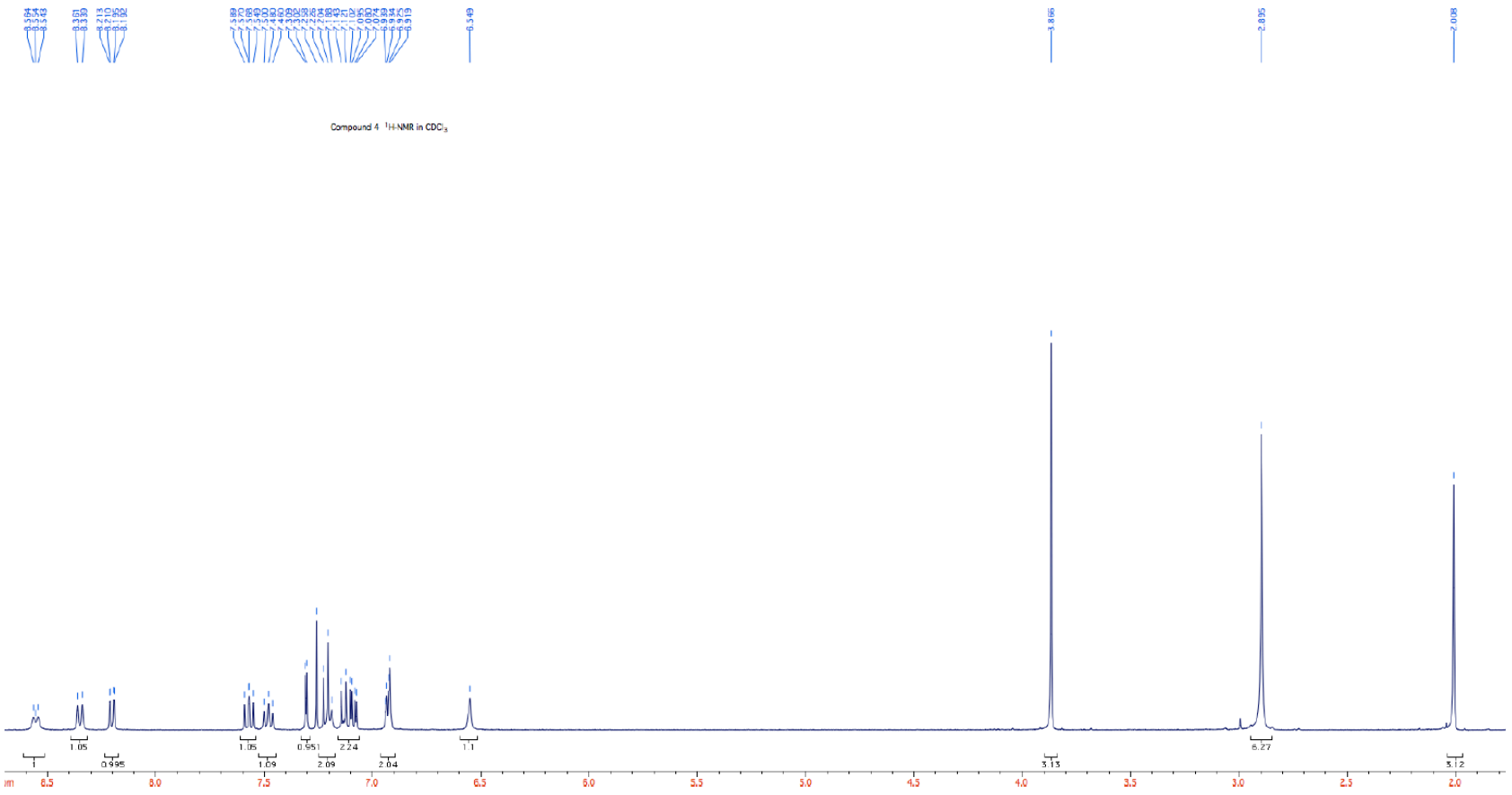
Novel Carbazole Inhibits Phospho-STAT3 Through Induction of Protein Tyrosine Phosphatase PTPN6

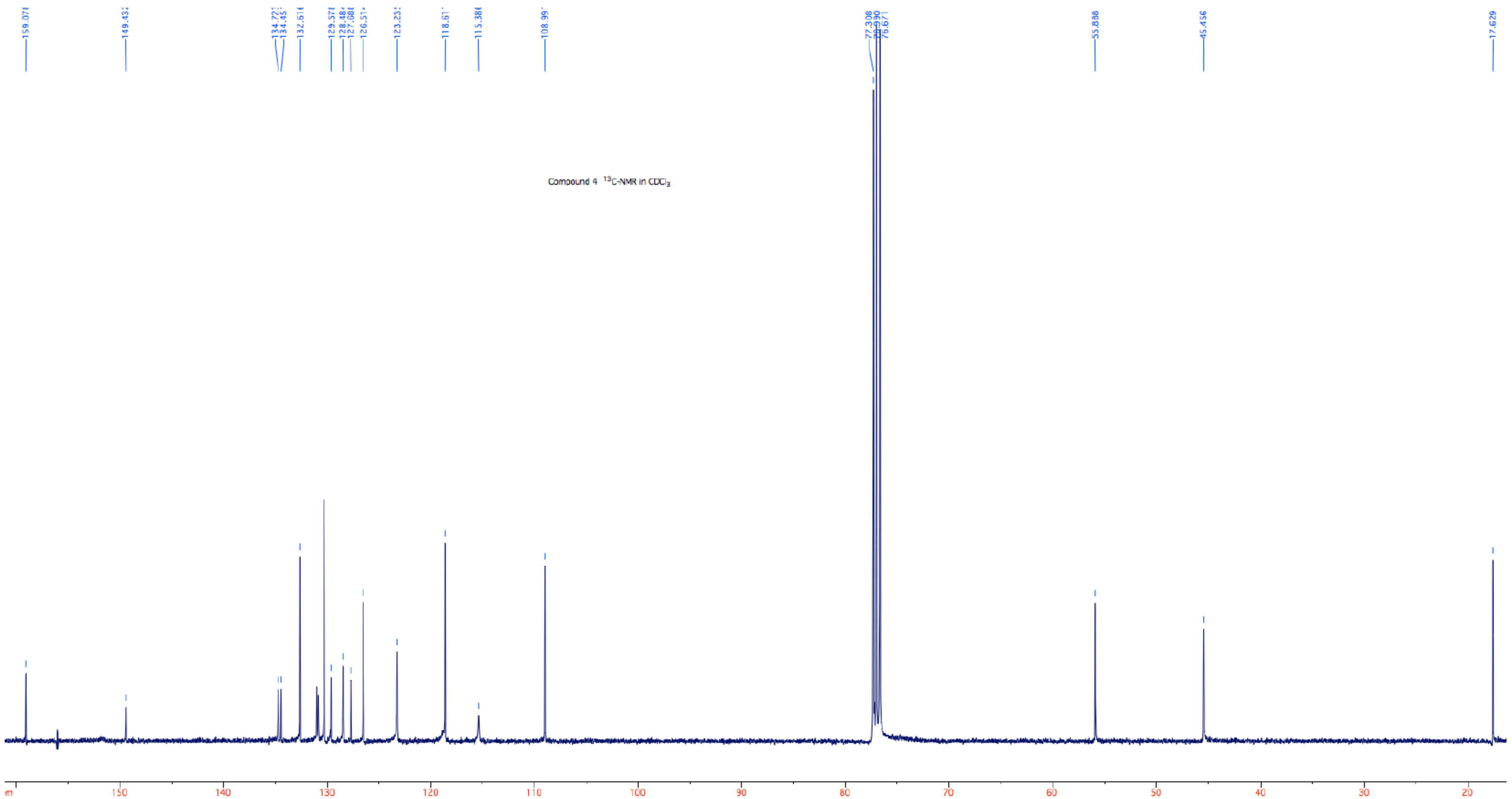
Shujie Hou, Yong Weon Yi , Hyo Jin Kang , Li Zhang, Hee Jeong Kim, Yali Kong, Yong Liu, Kan Wang, Hye-Sik Kong, Scott Grindrod, Insoo Bae *, Milton L. Brown *

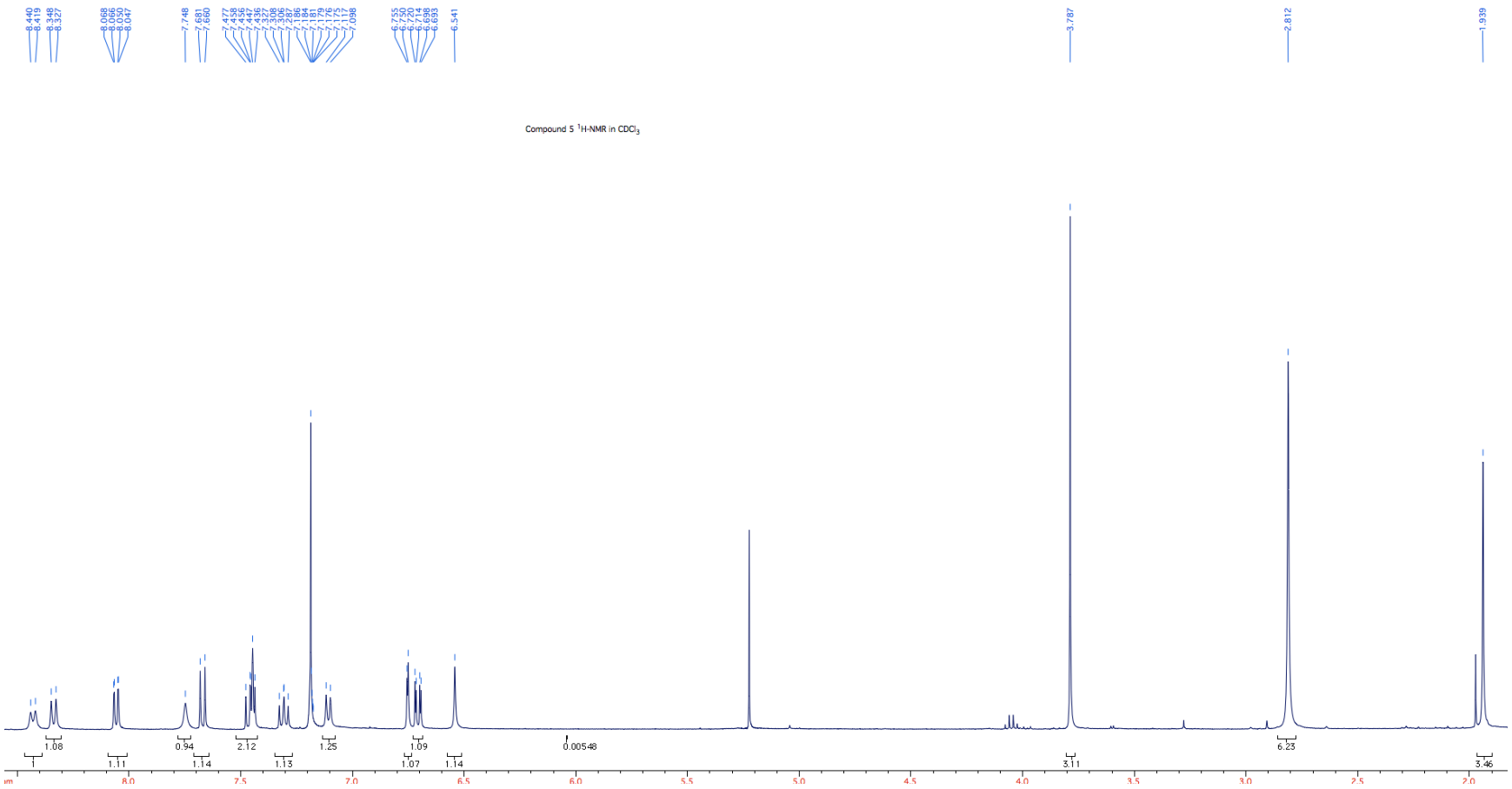
Contents

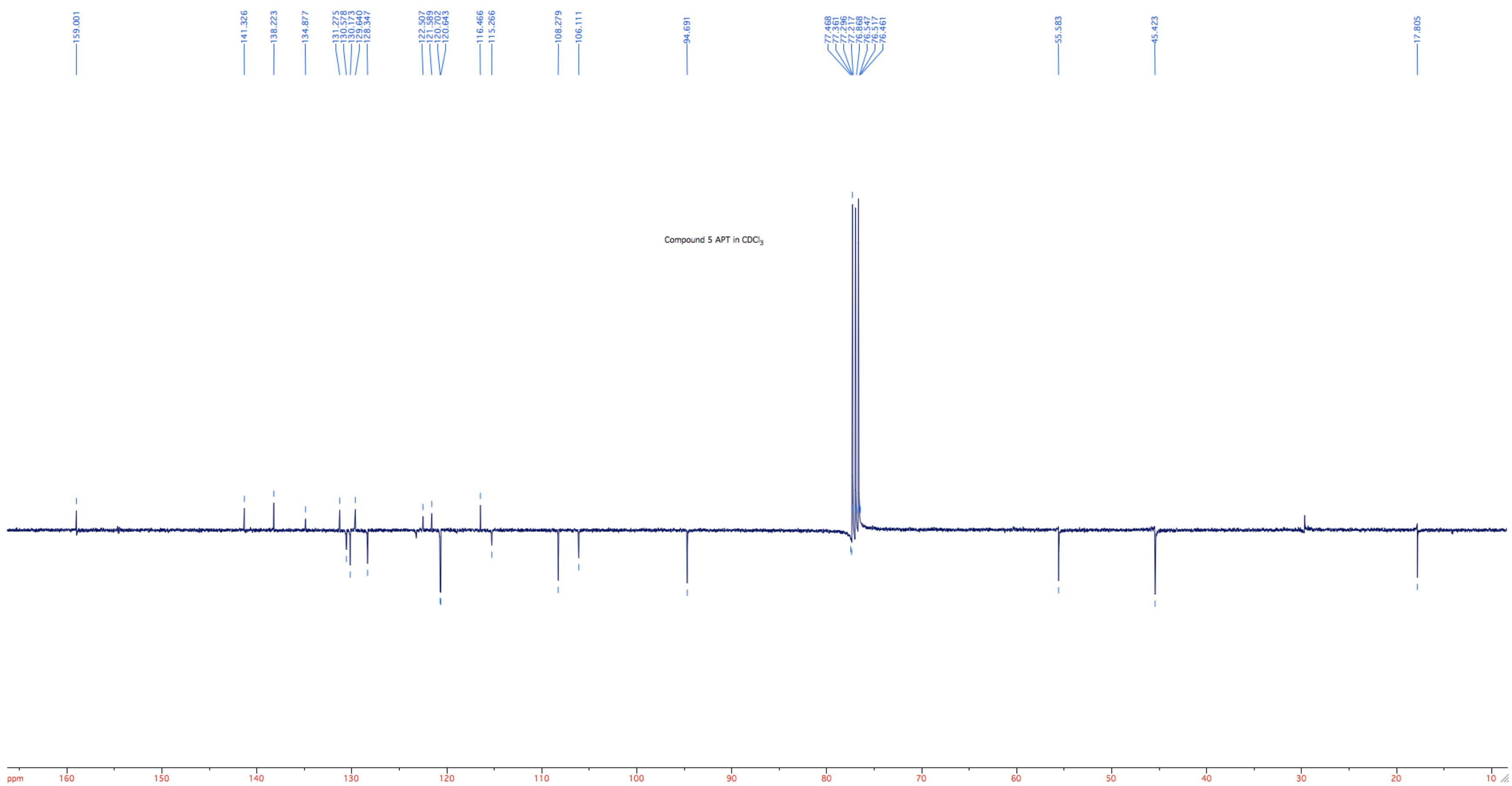

7.903
7.893
7.882
7.330
7.324
7.314
7.292
7.258
7.251
7.126
7.110
7.064
7.051
6.305
3.885
2.258
1.532
Compound 3 1 H-NMR in CDCl3
0.904
2.08
0.91
1.86
1
2.69
2.7
0.71
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0

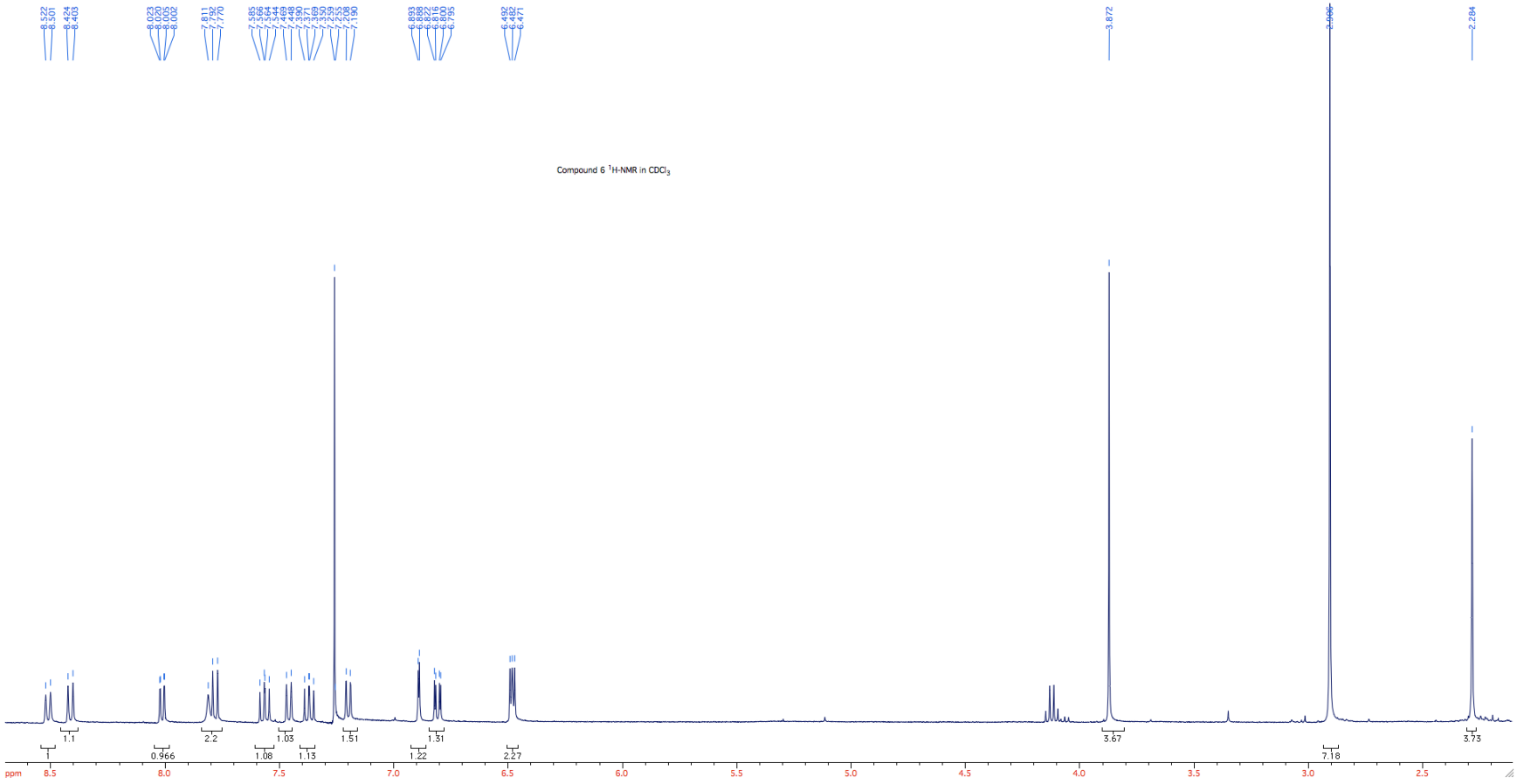

158.863
155.972
152.851
136.227
132.772
132.194
129.814
128.243
126.532
120.599
118.589
108.901
80.658
77.312
76.994
76.677
55.884
28.313
17.755
Compound 3 13C-NMR in CDCl3
m
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

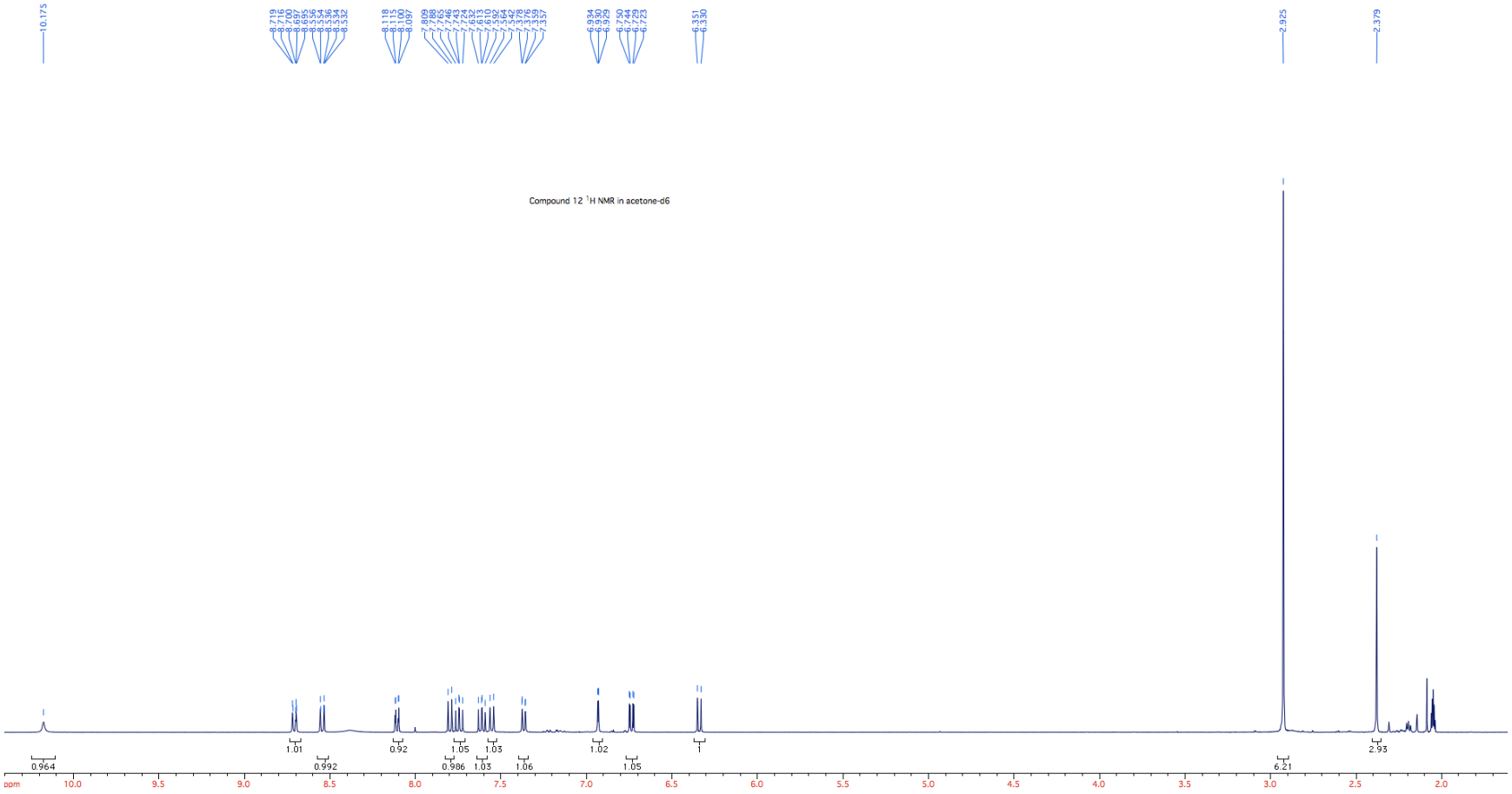

Compound 4 ¹H-NMR in CDCl₃
3.866
2.895
2.008
6.349
1.05
0.995
1.05
1.09
0.951
2.09
2.24
2.04
1.1
3.13
6.27
3.12
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0

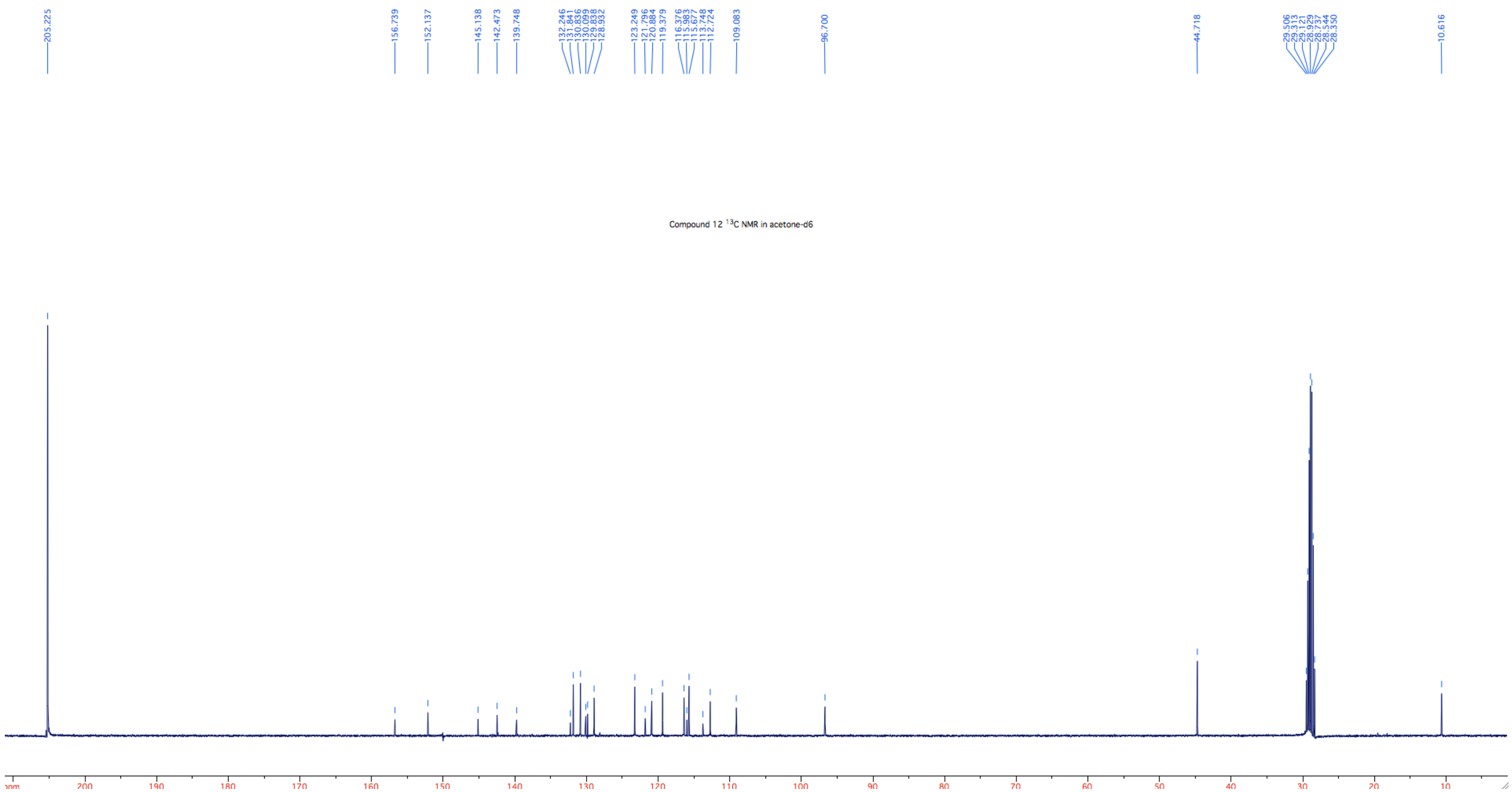

159.078
149.432
134.723
134.453
132.610
129.578
128.484
127.688
126.514
123.233
118.617
115.388
108.991
77.308
76.990
76.671
55.888
45.456
17.629
Compound 4 ^{13}C-NMR in $CDCl_3$
150
140
130
120
110
100
90
80
70
60
50
40
30
20

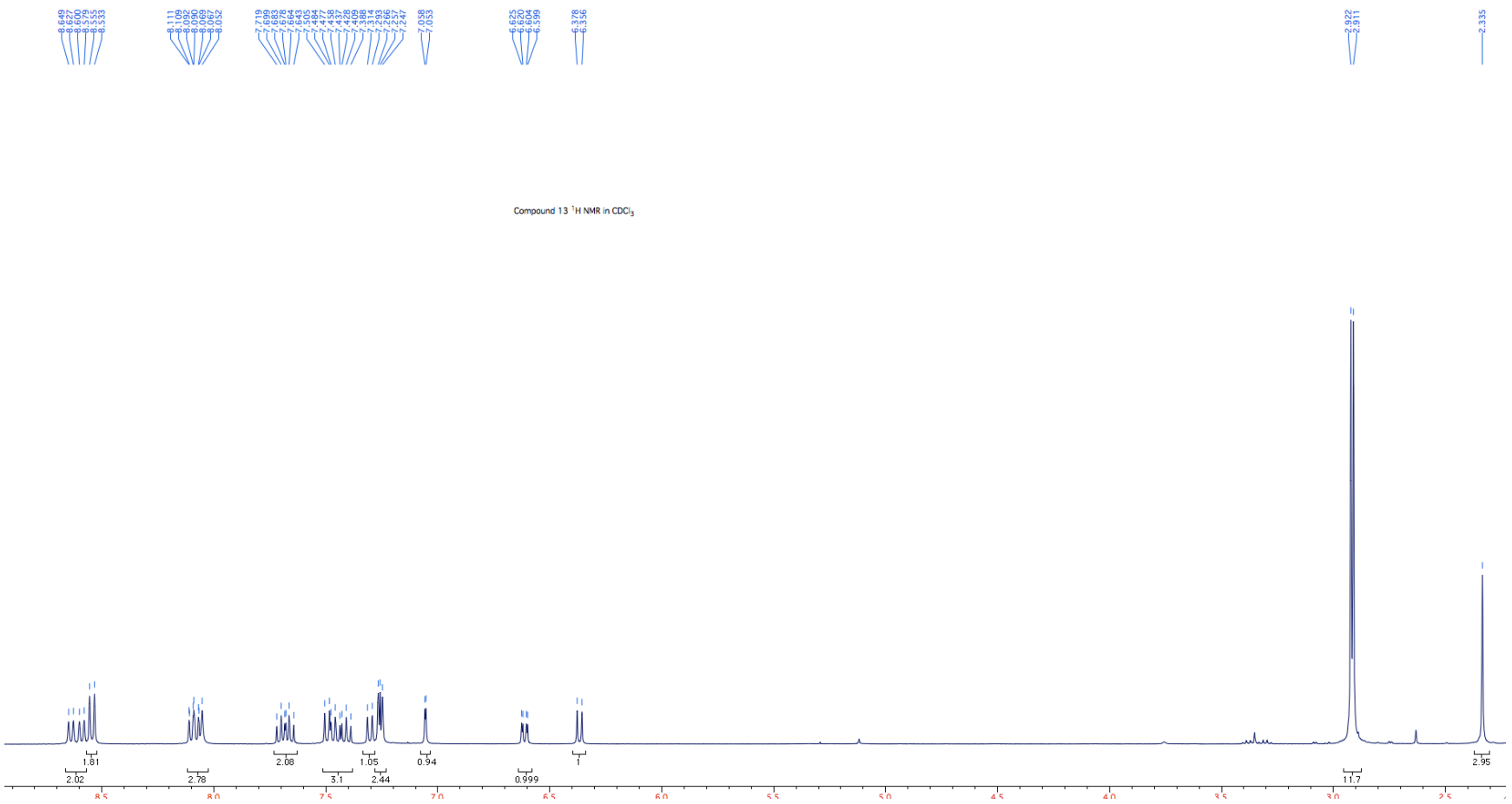

8.440
8.419
8.348
8.327
8.068
8.066
8.050
8.049
8.047
7.748
7.681
7.660
7.477
7.458
7.456
7.447
7.436
7.327
7.306
7.187
7.186
7.184
7.181
7.179
7.176
7.175
7.117
7.098
6.755
6.750
6.717
6.714
6.698
6.693
6.541
3.787
2.812
1.939
Compound 5 ^{1}H-NMR in $CDCl_3$
1.08
0.94
2.12
1.25
1.09
0.00548
6.23
1
1.11
1.14
1.13
1.07
1.14
3.11
3.46

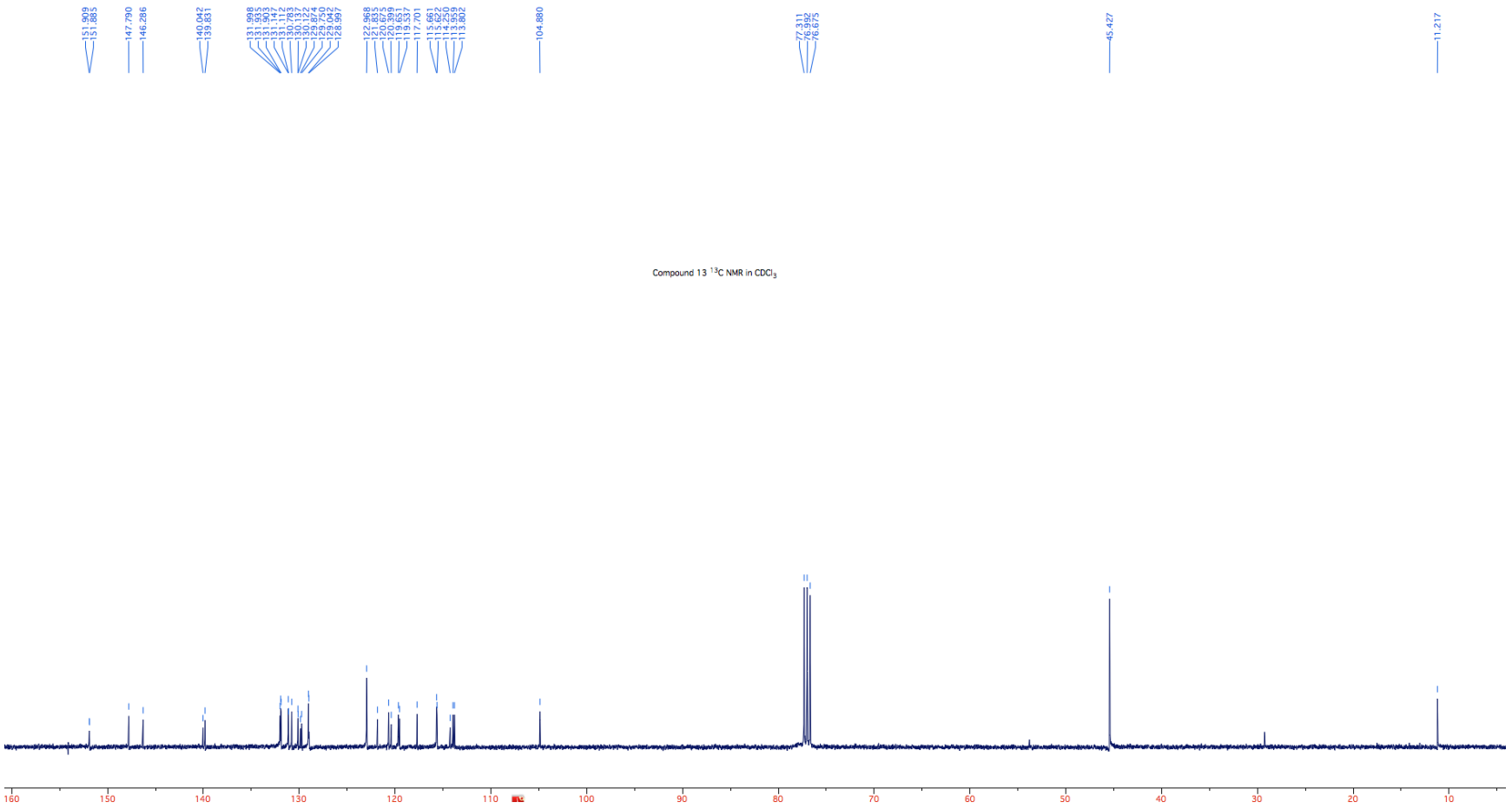

159.001
141.326
138.223
134.877
131.275
130.578
130.173
129.640
128.347
122.507
121.589
120.702
120.643
116.466
115.266
108.279
106.111
94.691
77.468
77.361
77.296
77.217
76.868
76.547
76.517
76.461
55.583
45.423
17.805
Compound 5 APT in $CDCl_3$
ppm 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10


Compound 6 ^{1}H-NMR in $CDCl_3$
8.522
8.501
8.424
8.403
8.023
8.020
8.005
8.002
7.811
7.792
7.770
7.585
7.566
7.564
7.544
7.469
7.446
7.390
7.371
7.359
7.255
7.253
7.208
7.190
6.893
6.888
6.822
6.815
6.800
6.795
6.492
6.482
6.471
3.872
3.086
2.284
1
1.1
0.966
2.2
1.08
1.03
1.13
1.51
1.22
1.31
2.27
3.67
7.18
3.73
ppm
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5

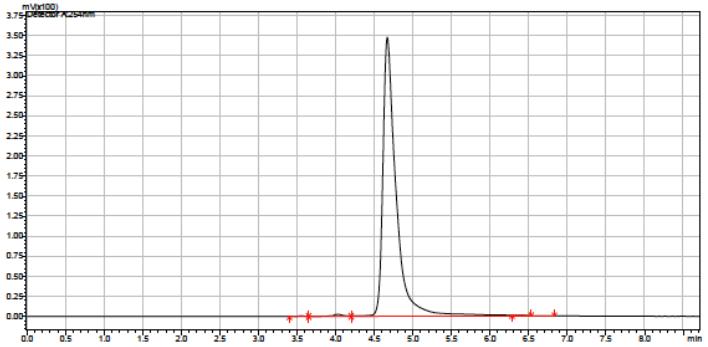

Compound 12 ¹H NMR in acetone-d6
10.175
8.719
8.716
8.707
8.700
8.695
8.556
8.554
8.536
8.534
8.532
8.118
8.115
8.100
8.097
7.809
7.788
7.765
7.746
7.745
7.724
7.612
7.611
7.610
7.599
7.564
7.542
7.378
7.376
7.359
7.357
6.934
6.930
6.929
6.750
6.744
6.729
6.723
6.351
6.330
2.925
2.379
0.964
1.01
0.992
0.92
0.986
1.05
1.03
1.03
1.06
1.02
1.05
1
6.21
2.93
ppm
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0


205.225
156.739
152.137
145.138
142.473
139.748
132.246
131.841
130.836
130.099
129.838
128.932
123.249
121.796
120.884
119.379
116.376
115.983
115.677
113.748
112.724
109.083
96.700
44.718
29.506
29.313
29.121
28.929
28.737
28.544
28.350
10.616
Compound 12 ^{13}C NMR in acetone-d6


8.649
8.617
8.607
8.579
8.565
8.533
8.111
8.102
8.092
8.090
8.069
8.067
8.052
7.719
7.689
7.683
7.678
7.664
7.648
7.505
7.464
7.457
7.458
7.437
7.430
7.409
7.308
7.314
7.293
7.266
7.257
7.247
7.058
7.053
6.625
6.620
6.604
6.599
6.378
6.356
2.922
2.911
2.335
Compound 13 ^{1}H NMR in CDCl$_3$
1.81
2.02
2.78
2.08
3.1
1.05
2.44
0.94
0.999
1
11.7
2.95

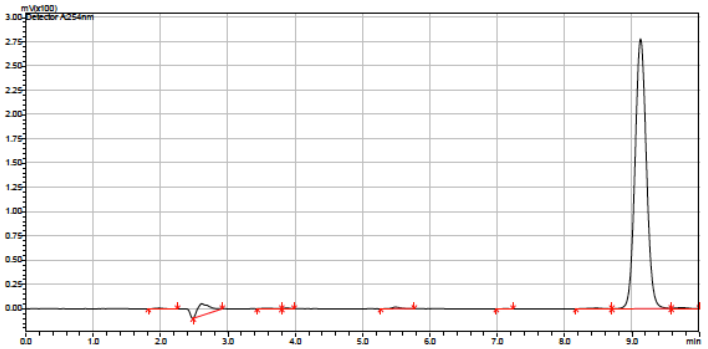

151.909
151.885
147.790
146.286
140.042
139.831
131.998
131.935
131.903
131.147
131.112
130.783
130.137
130.122
129.874
129.750
129.042
128.997
122.968
121.855
120.675
120.399
119.657
119.537
117.701
115.661
115.622
114.750
113.959
113.802
104.880
77.311
77.000
76.692
76.675
45.427
11.217
Compound 13 13C NMR in CDCl3
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10

Mobile phase :
H2O (0.1 % Acetic acid) : Acetonitrile = 20 : 80
Retention Time : 4.7 min
Flow rate : 1.0 ml/min
UV 254 nm



Purity 97.69 %

Mobile phase :
H2O (0.1 % Acetic acid) : Acetonitrile = 30 : 70
Retention Time : 9.0 min
Flow rate : 1.0 ml/min
UV 254 nm



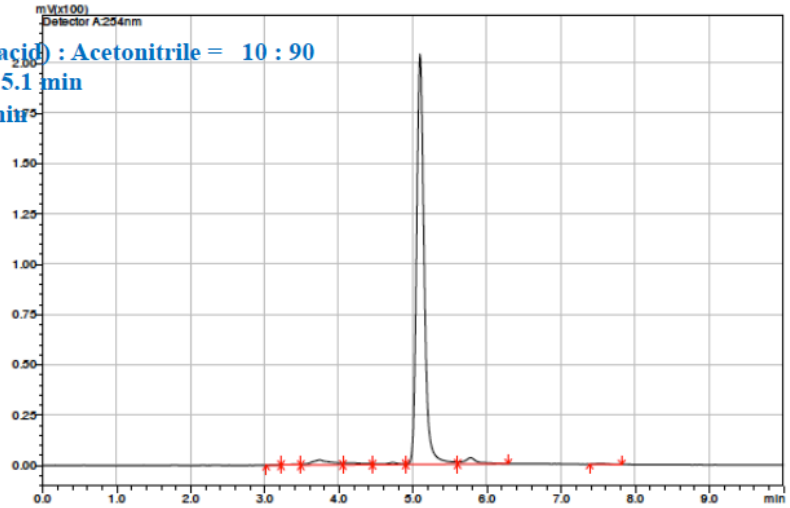
Mobile phase :

H2O (0.1 % Acetic acid) : Acetonitrile = 10 : 90

Retention Time : 5.1 min

Flow rate : 1.0 ml/min

UV 254 nm



Purity >95 %

Purity analysis of Compound 13

Mobile phase :

H2O (0.1 % Acetic acid) : Acetonitrile = 30 : 70

Retention Time : 6.4 min

Flow rate : 1.0 ml/min

UV 254 nm