

Supporting information

Synthesis and aromatisation of cyclic enediyne-containing amino acids

Jasper Kaiser,^a Bart C. J. van Esseveldt,^a Margot J. A. Segers,^a Floris L. van Delft,^a Jan M. M. Smits,^a Sam Butterworth^b and Floris P. J. T. Rutjes^{*a}

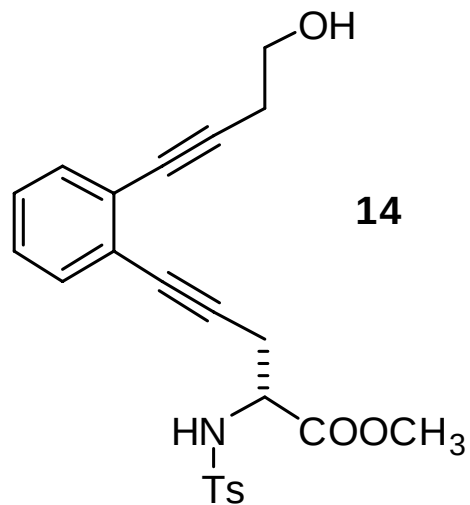
^a *Institute for Molecules and Materials, Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands. Fax: +31 24 365 3393; Tel: +31 24 365 3202; E-mail: F.Rutjes@science.ru.nl*

^b *AstraZeneca R&D, Alderley Park, Macclesfield, Cheshire SK10 4TG, United Kingdom.*

Contents

¹³C-NMR and / or ¹H-NMR spectra of compounds **14-19, 23-26, 28, 29, 31-36.**

75 MHz
CDCl₃



169.863

143.298

136.748

131.779

131.562

129.362

127.741

127.293

126.921

125.756

125.057

91.091

86.533

83.044

81.284

77.000

60.931

54.326

52.890

25.158

24.036

21.657

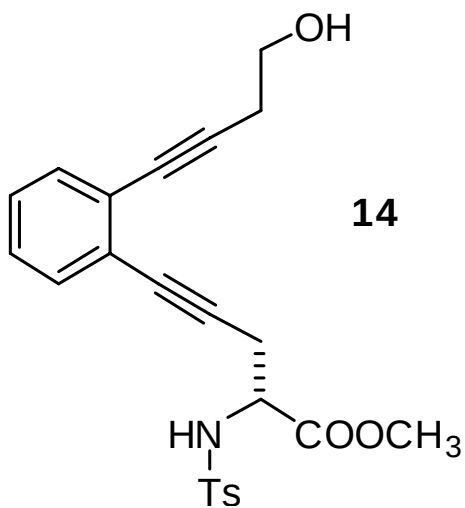
ppm (t1)

300 MHz
CDCl₃

7.751
7.724
7.384
7.354
7.294
7.139

6.135
6.106

4.205
4.188
4.172
4.158
4.141
3.890
3.885
3.870
3.865
3.850
3.845
3.830
3.825
3.615
3.001
2.713
2.574
2.553
2.533
2.342



2.05
0.97
5.42

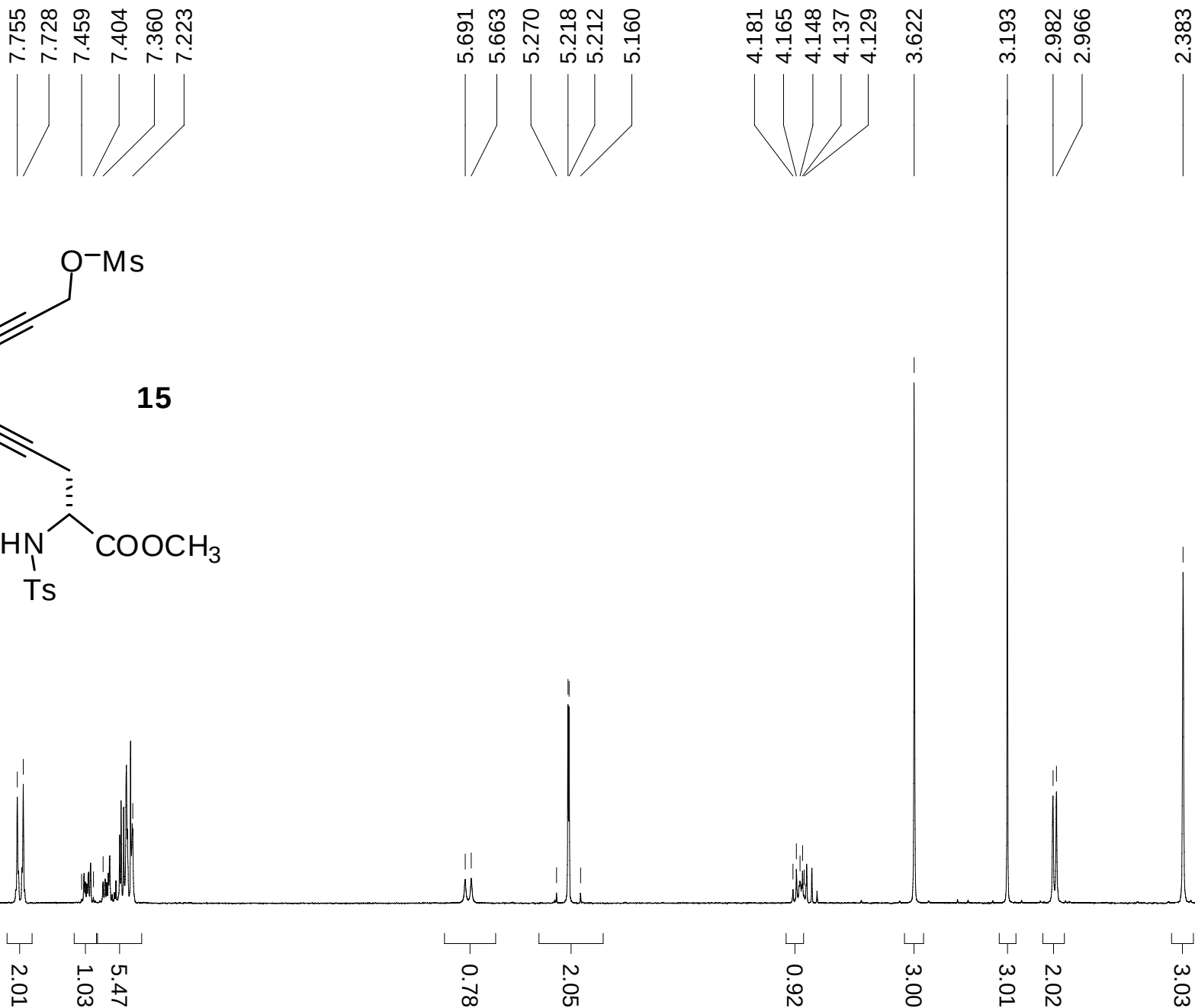
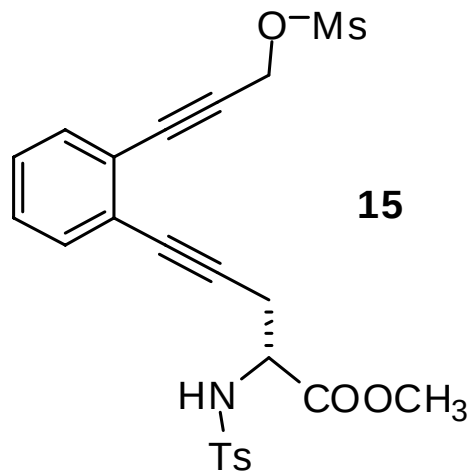
0.96

1.04
2.00
3.29

4.24
0.99
2.92

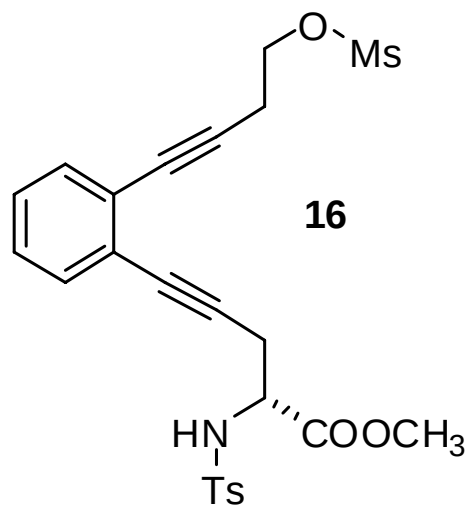
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300 MHz
CDCl₃



9.00 (t1) 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00

300 MHz
CDCl₃



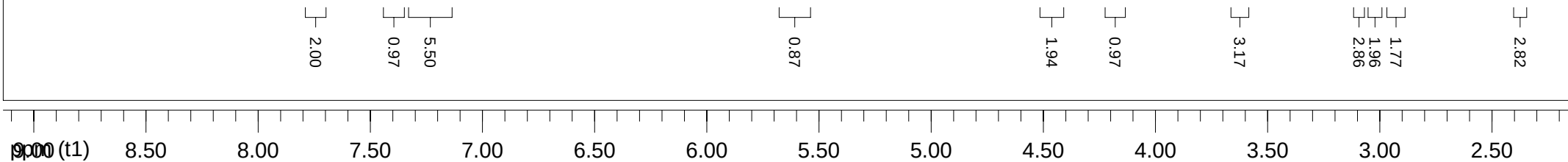
7.740
7.712
7.397
7.367
7.308
7.160

5.618
5.587

4.478
4.456
4.433
4.197
4.134

3.618

3.085
3.046
3.023
3.001
2.945
2.930
2.913
2.381



75 MHz
CDCl₃

169.910

143.587

136.904

132.057

131.923

129.586

127.924

127.864

127.593

127.108

125.607

124.918

117.200

91.978

88.673

86.911

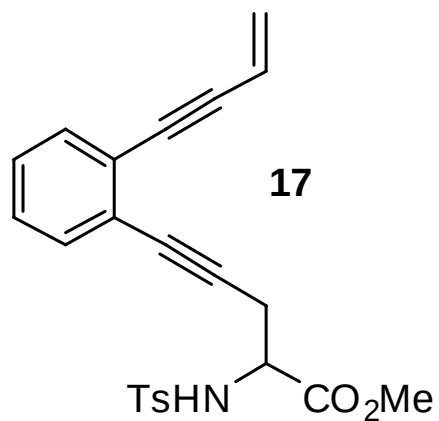
82.994

54.537

53.068

25.491

21.861



ppm (t1)

200

175

150

125

100

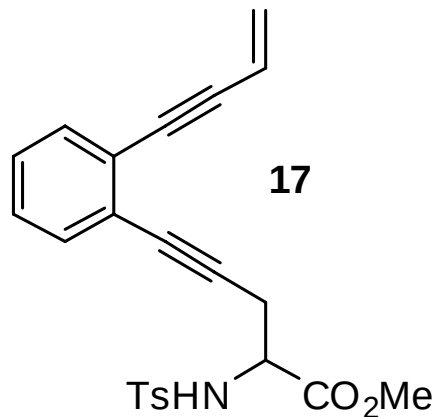
75

50

25

0

300 MHz
CDCl₃



7.741
7.713

6.157
6.120
6.099
6.062
5.814
5.807
5.755
5.748
5.606
5.599
5.569
5.562
5.525
5.495

4.235
4.217
4.202
4.187
4.172

3.610

3.018
3.003
2.961
2.946
2.925
2.907
2.869
2.851
2.378

2.13

1.11
5.70

0.87

1.06

1.00
0.85

0.97

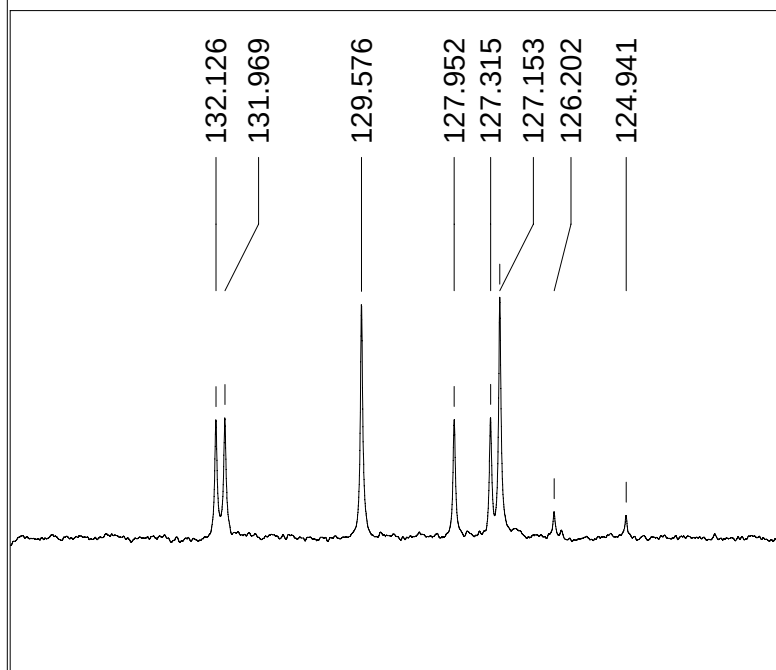
3.00

2.42

3.02

ppm (t1) 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00

75 MHz
CDCl₃



135.0
ppm (t1)

130.0

125.0

ppm (t1)

170.374

143.575

136.956

132.126

131.969

129.576

127.952

127.315

127.153

126.202

124.941

93.826

86.470

83.009

80.109

77.000

61.865

54.325

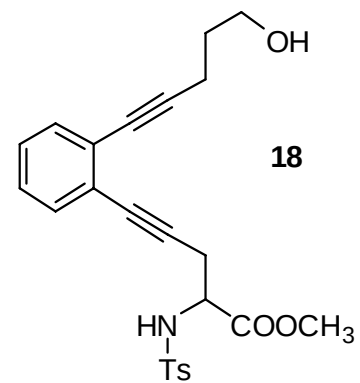
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31.070

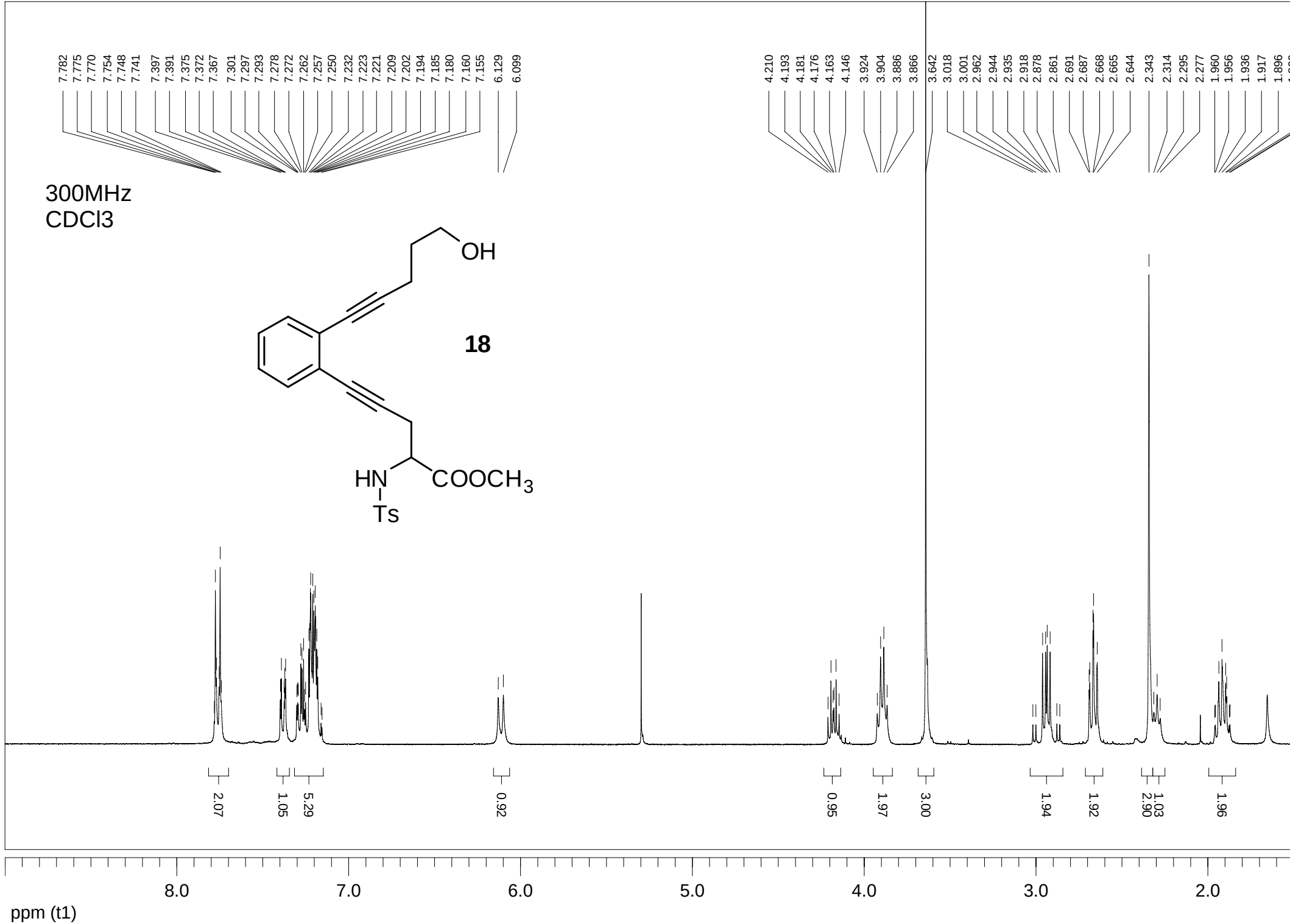
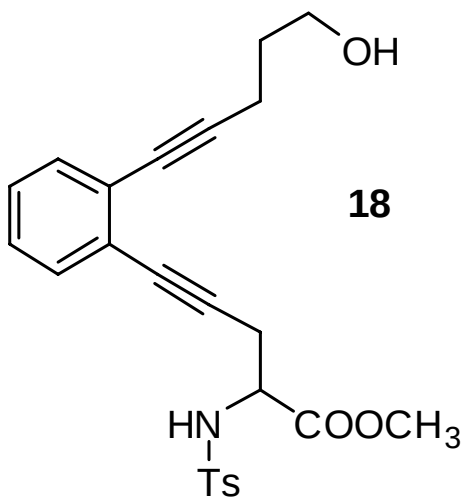
24.886

21.469

16.325



300MHz
CDCl₃



100MHz
cdcl3

169.129

143.438

136.173

131.138

129.453

127.938

127.160

126.831

126.677

94.483

88.163

82.828

81.382

77.000

57.779

52.141

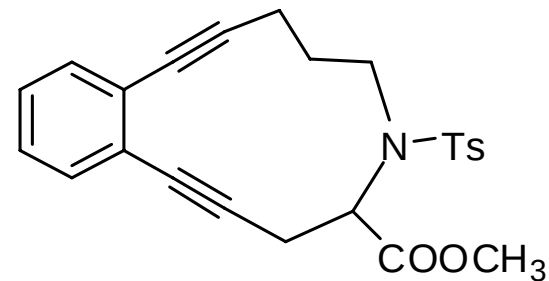
45.756

30.855

23.895

21.405

17.037



19

ppm (t1)

175

150

125

100

75

50

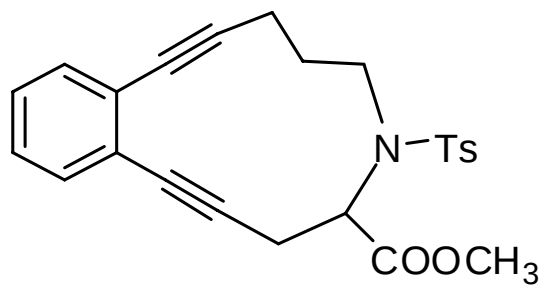
25

0

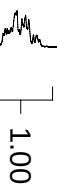
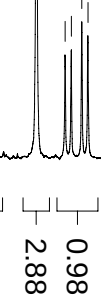
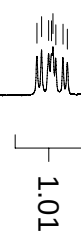
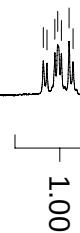
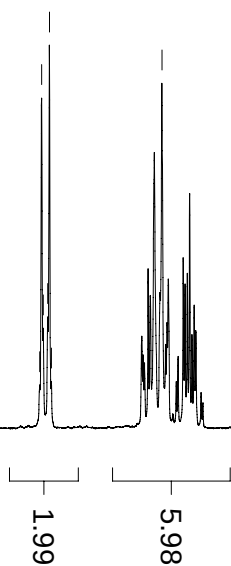
300MHz
CDCl₃

7.691
7.684
7.678
7.662
7.656
7.650
7.260

4.884
4.876
4.862
4.855
4.147
4.134
4.106
4.096
4.083
4.056
4.042
3.774
3.758
3.733
3.723
3.718
3.708
3.683
3.667
3.494
3.393
3.372
3.334
3.313
2.855
2.847
2.796
2.788
2.394

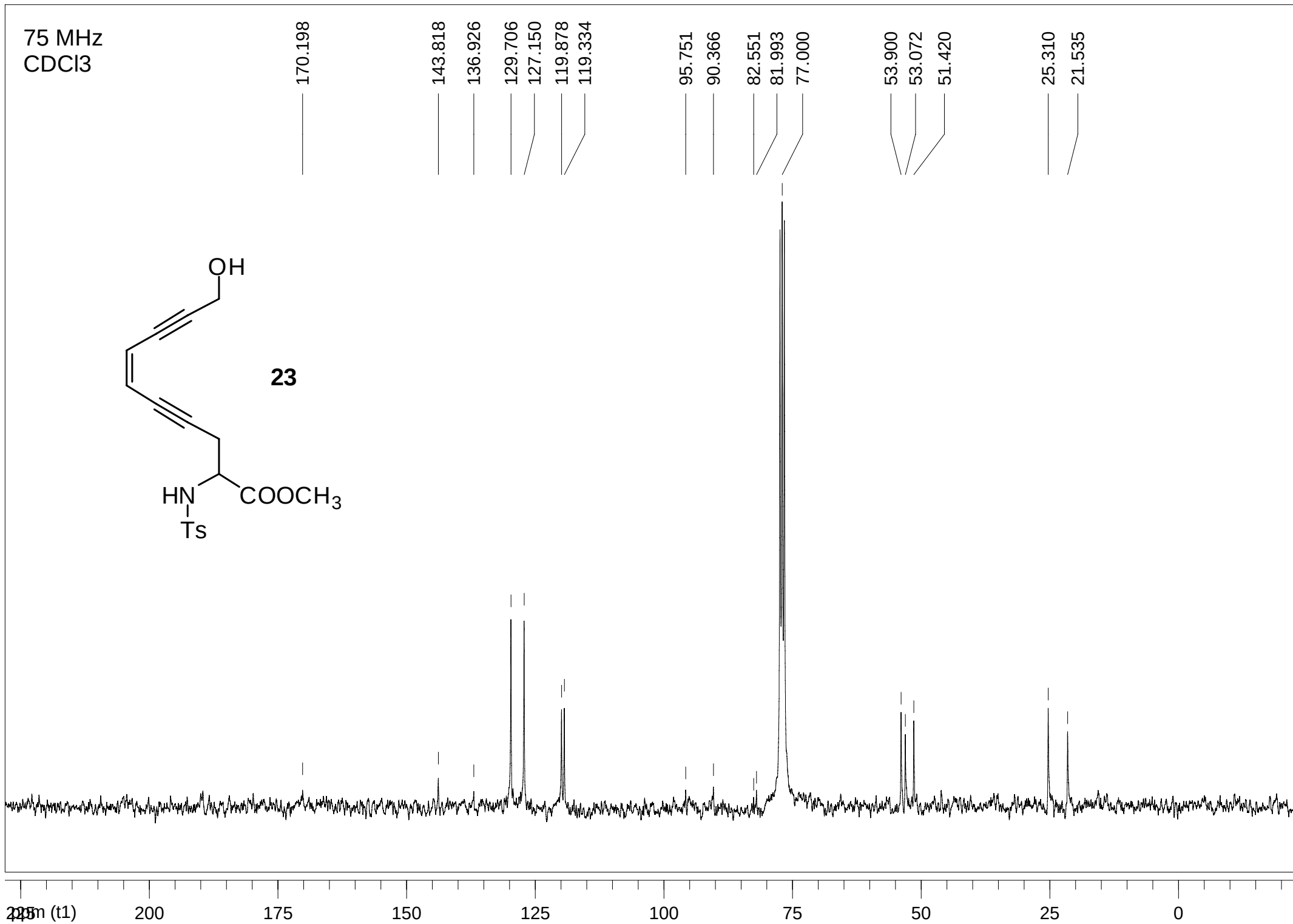


19



ppm (t1) 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00

75 MHz
CDCl₃



300MHz
CDCl₃

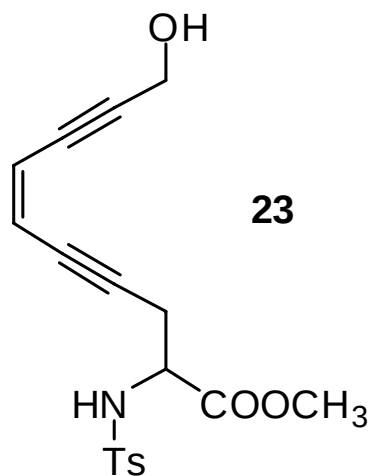
7.782
7.754

7.308
7.279
7.260

5.959
5.929
5.878
5.872
5.867
5.842
5.836
5.831
5.767
5.761
5.755
5.731
5.725
5.720

4.581
4.576
4.559
4.553
4.520
4.499
4.465
4.459
4.444
4.438
4.206
4.146

3.652
3.068
3.046
3.024
2.961
2.955
2.948
2.941
2.904
2.891
2.885
2.875
2.869
2.834
2.828
2.818
2.812
2.419



2.01

2.05

0.94
1.99

2.06

1.00

3.00

1.00

2.09

3.09

ppm (t1) 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00

75 MHz
CDCl₃

169.924 143.462 136.781 129.444 126.913 120.122 118.324 95.263 90.064 81.462 79.505 77.000 60.572 53.966 52.597 24.842 23.740 21.289

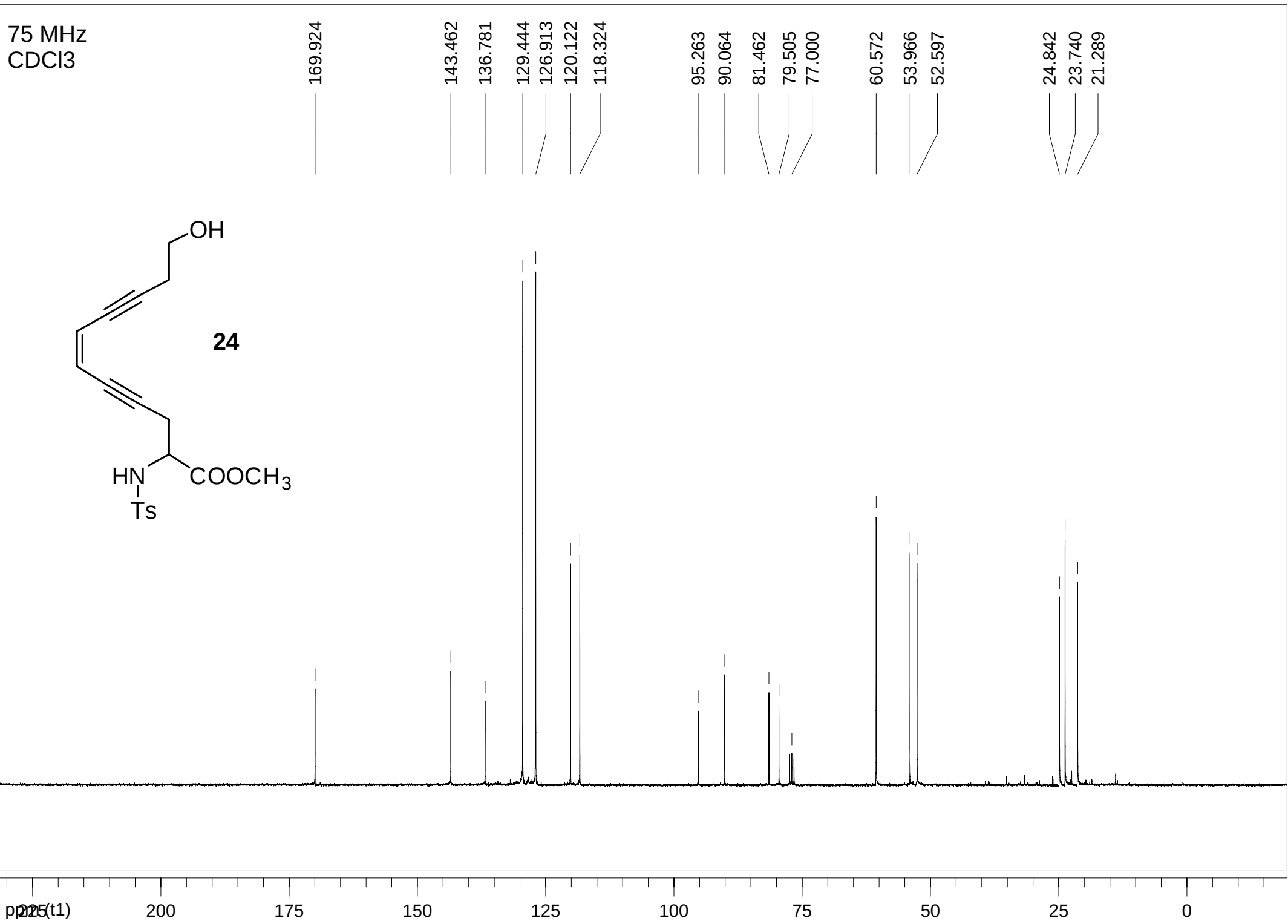
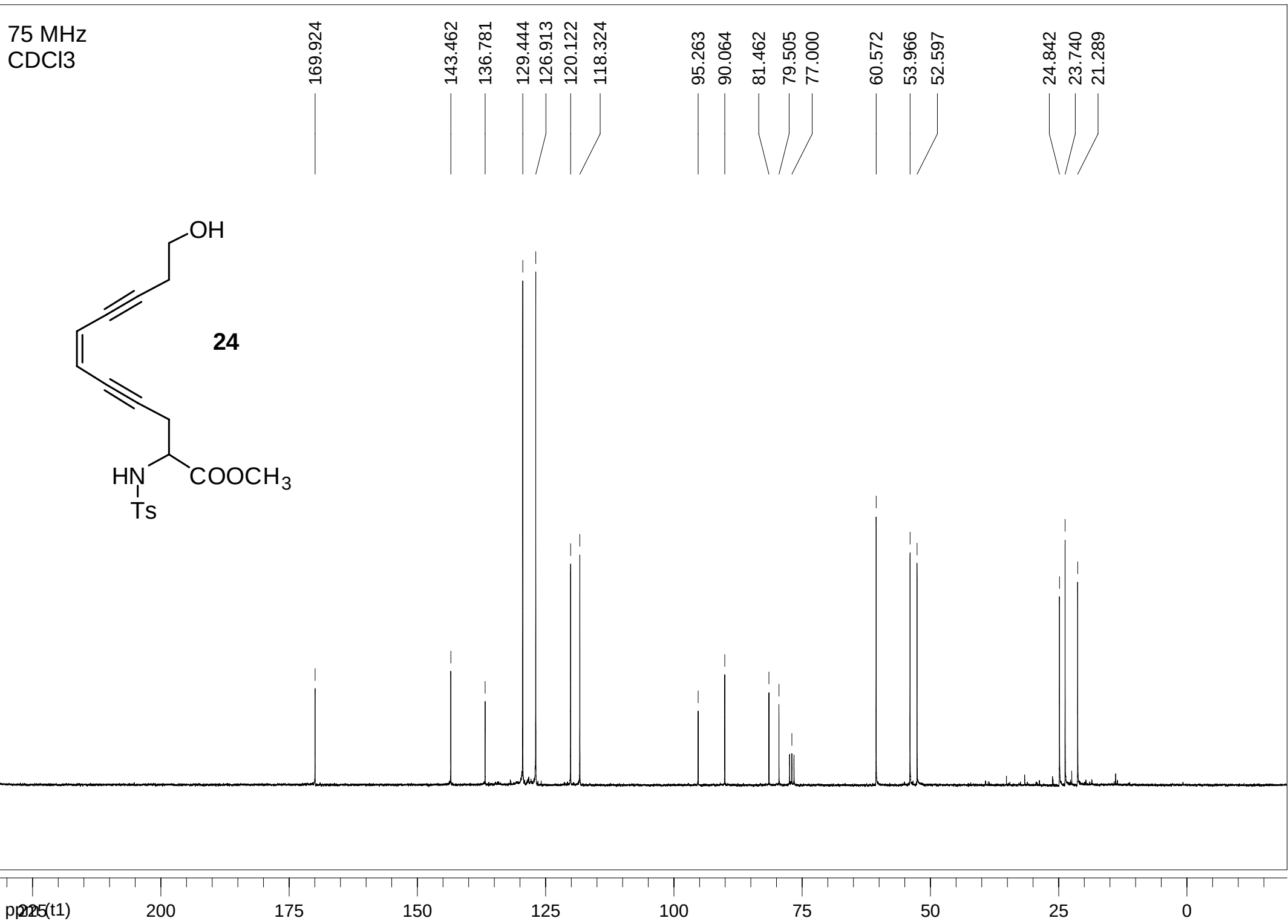
24

HN
Ts

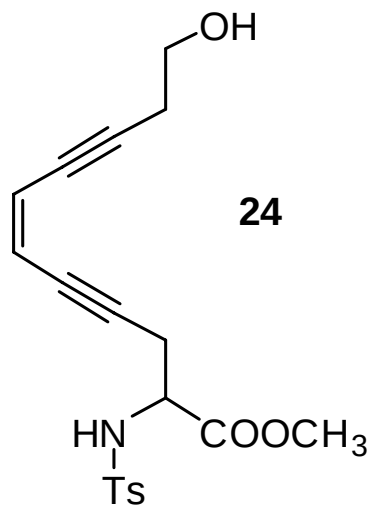
COOCH₃

OH

ppm (t1)



300 MHz
CDCl₃



7.720
7.692

7.241
7.214

6.121
5.761
5.754
5.747
5.725
5.718
5.711
5.644
5.638
5.632
5.608
5.602
5.596

4.106
4.091
4.075
3.762
3.742
3.721
3.544
2.885
2.863
2.828
2.779
2.746
2.722
2.674
2.633
2.345

2.00

1.90

0.84

1.75

0.97

1.80

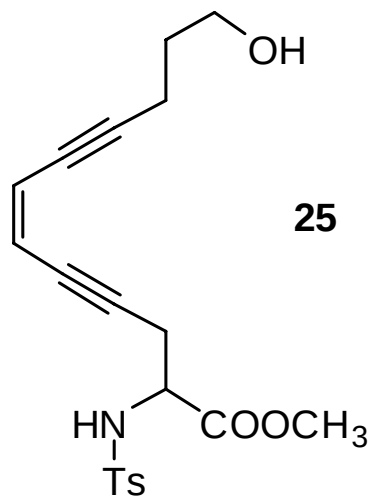
2.53

4.29

3.02

ppm (t1) 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00

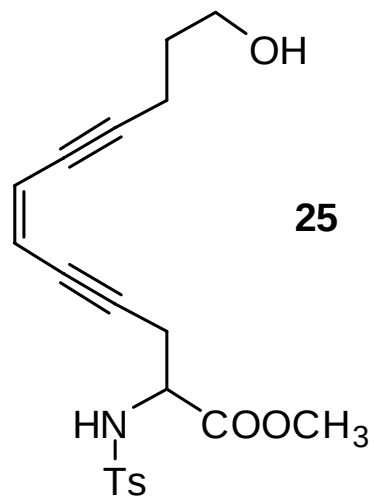
75 MHz
CDCl₃



170.065
143.476
136.770
129.464
126.932
120.279
117.860
97.944
89.907
81.382
78.545
77.000
61.349
54.037
52.601
30.814
24.767
21.321
16.207

ppm (1)

300 MHz
CDCl₃



7.722
7.695

7.260
7.251
7.224

6.175
6.144
5.755
5.747
5.740
5.719
5.711
5.704
5.624
5.617
5.609
5.588
5.581
5.573

4.118
4.101
4.088
4.084
4.071
4.054
3.780
3.760
3.739
3.558

2.900
2.733
2.650
2.540
2.533
2.518
2.510
2.495
2.488
2.357

1.832
1.810
1.789
1.768
1.746

2.13

2.38

0.98

1.03
0.98

1.11

2.09

3.00

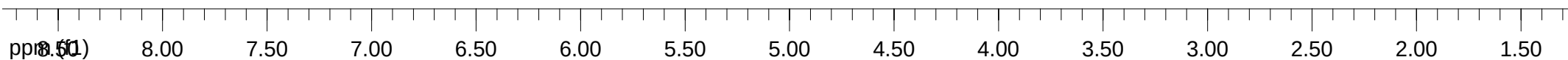
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0.99

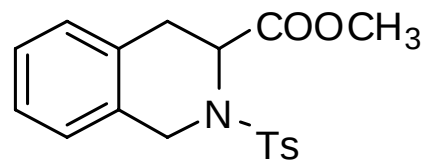
2.18

3.34

1.97



75 MHz
CDCl₃



26

170.737

143.482

136.038

131.435

130.664

129.510

128.729

127.348

126.793

126.121

77.000

53.767

52.190

44.378

31.896

21.509

ppm (t1)

200

175

150

125

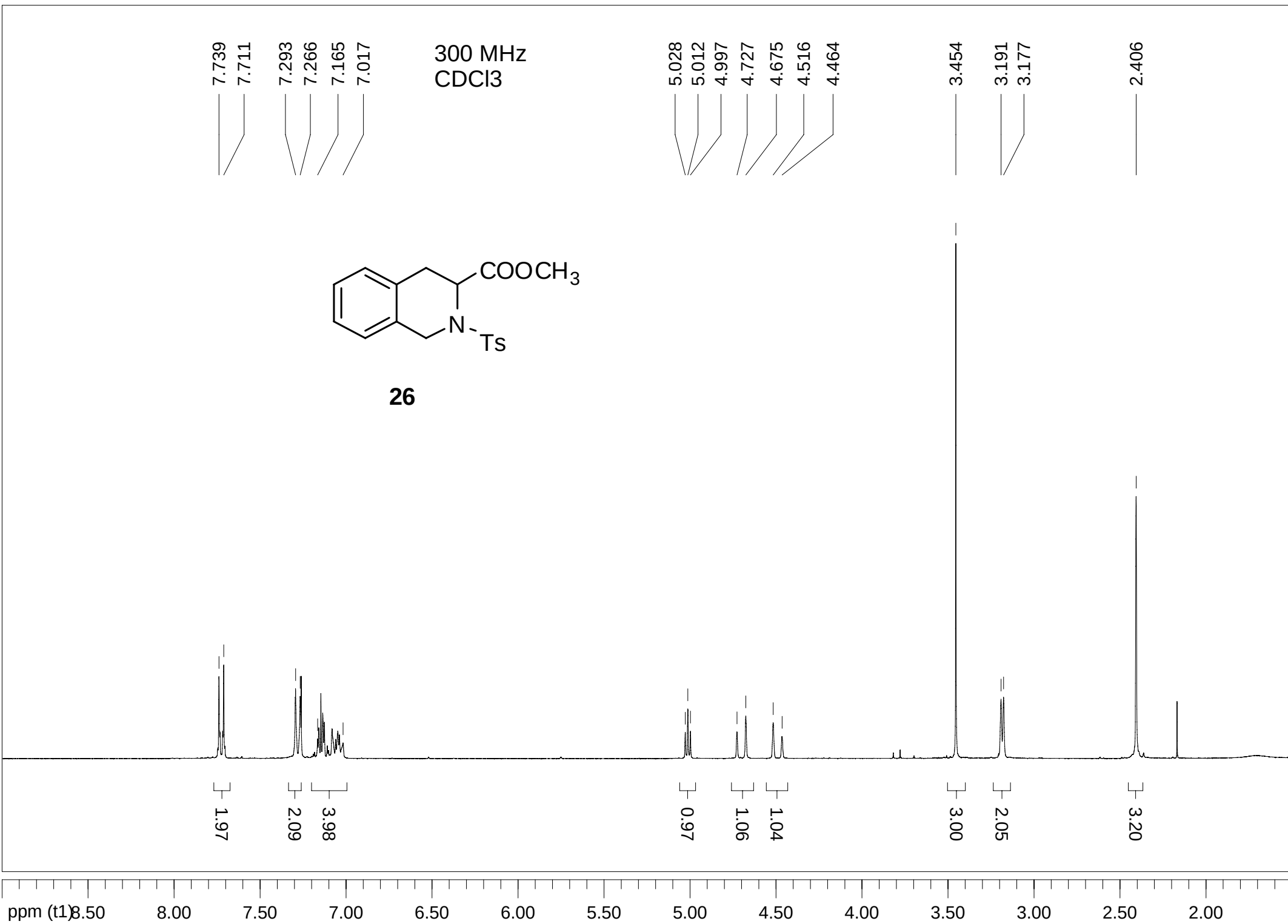
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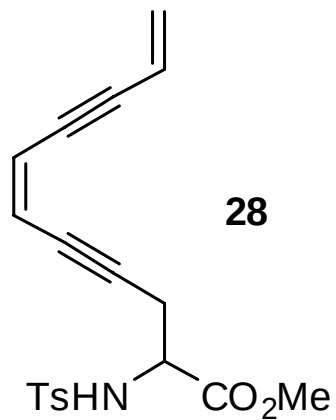
50

25

0



75 MHz
CDCl₃



169.963

143.718

136.944

129.650

128.000

127.145

119.816

118.780

117.046

95.665

90.906

87.221

81.649

77.000

54.081

52.826

25.295

21.518

ppm (t1)

200

175

150

125

100

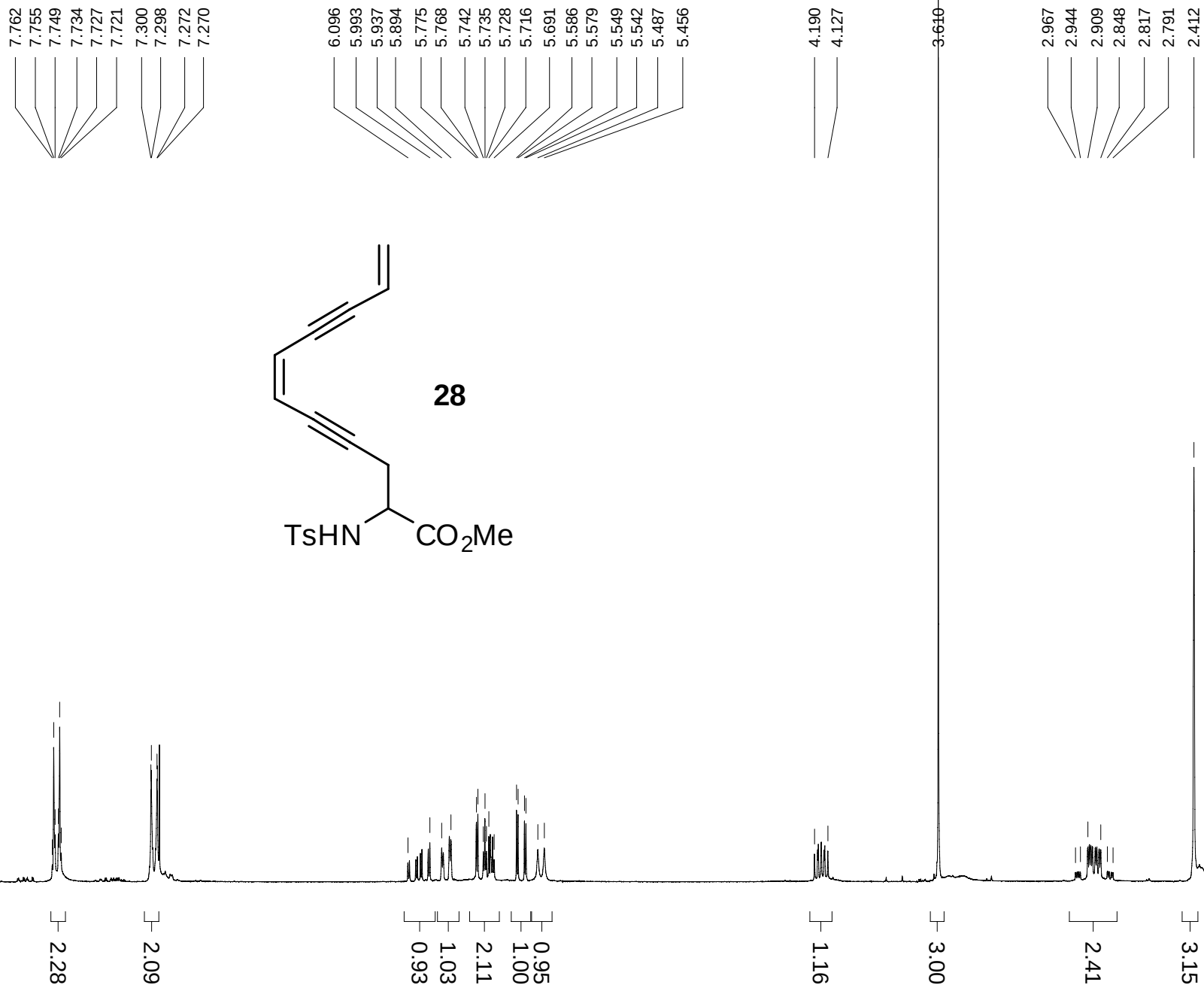
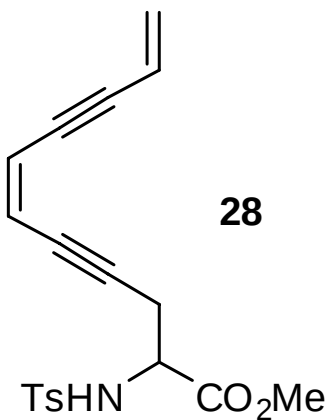
75

50

25

0

300 MHz
CDCl₃



75 MHz
CDCl₃

169.102

143.488

136.201

129.490

127.151

121.847

120.579

98.430

91.837

82.061

81.206

77.000

57.632

52.175

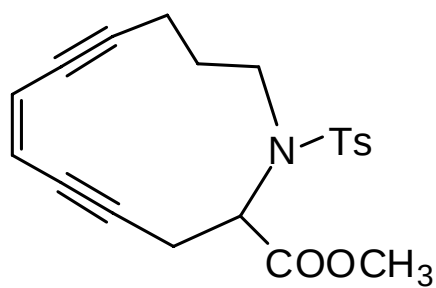
45.557

30.703

23.835

21.415

17.294



29

225 (t1)

200

175

150

125

100

75

50

25

0

300 MHz
CDCl₃

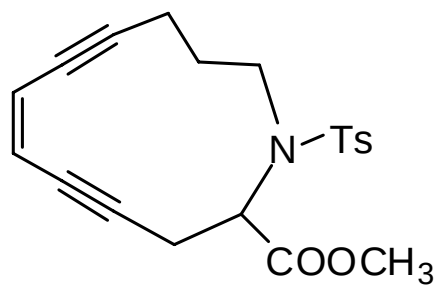
7.665
7.658
7.652
7.636
7.630
7.624
7.280
7.255

5.690
5.685

4.832
4.824
4.811
4.803

4.015
3.910
3.811
3.705
3.533
3.263
3.258
3.253

3.242
3.237
3.232
3.204
3.199
3.194
3.183
3.178
3.173
2.734
2.726
2.675
2.668
2.474
2.416
2.394
2.368
2.180
2.037
1.904



29

2.02

2.12

1.97

1.00

1.01

1.04

3.00

1.01

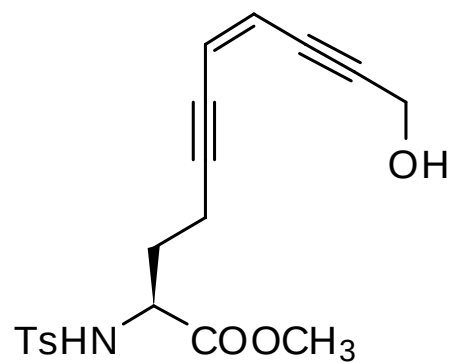
1.00

6.23

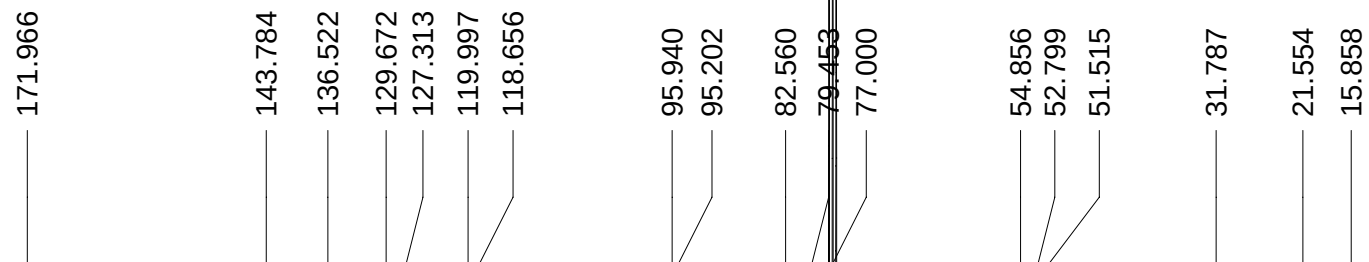
1.38

ppm (δ)

75 MHz
CDCl₃



31



ppm (1)

300 MHz
CDCl₃

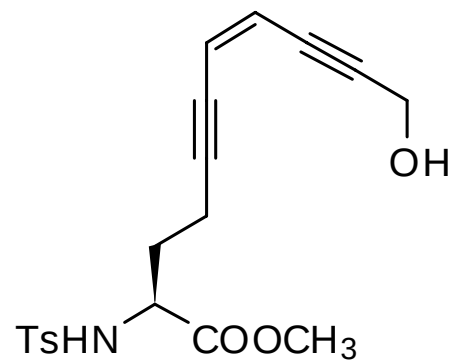
7.772
7.744

7.300
7.273

5.848
5.842
5.836
5.812
5.806
5.800
5.785
5.779
5.772
5.749
5.743
5.736
5.358
5.327

4.477
4.471
4.456
4.450
4.187
4.170
4.160
4.157
4.143
4.140
4.130
4.113
4.109
3.594

2.604
2.582
2.560
2.513
2.506
2.491
2.484
2.469
2.462
2.416
2.078
1.969
1.934
1.820



31

2.04

1.98

1.91

0.94

1.92

1.15

2.83

1.00
2.02
3.01

1.30
1.09

ppm 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00 1.50

75 MHz
CDCl₃

172.125

143.604

136.447

132.064

131.729

129.511

127.938

127.506

127.221

125.814

125.069

91.775

91.585

83.851

80.580

77.000

54.882

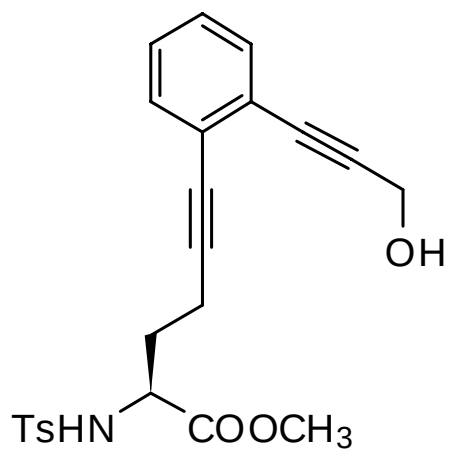
52.682

51.350

31.643

21.384

15.708



32

ppm (t1)

200

175

150

125

100

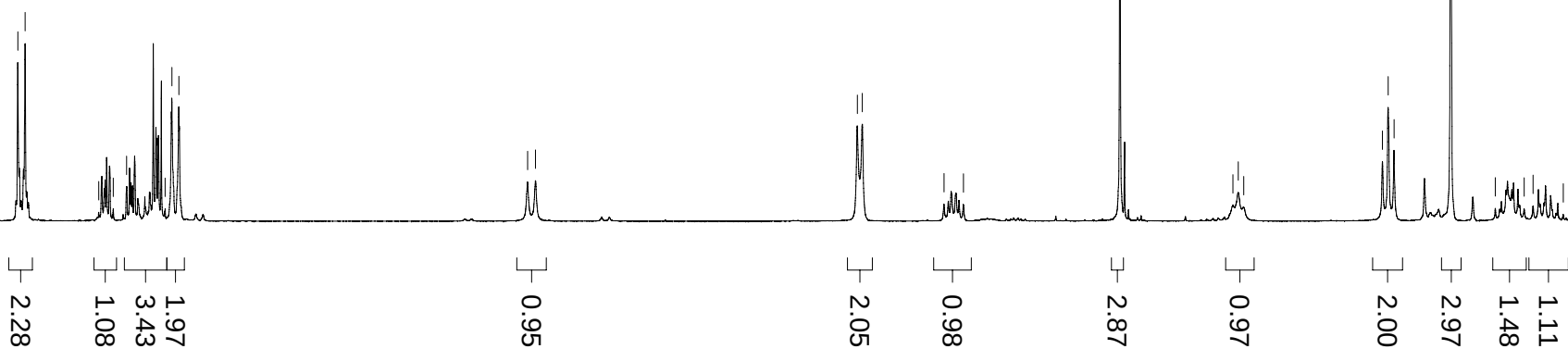
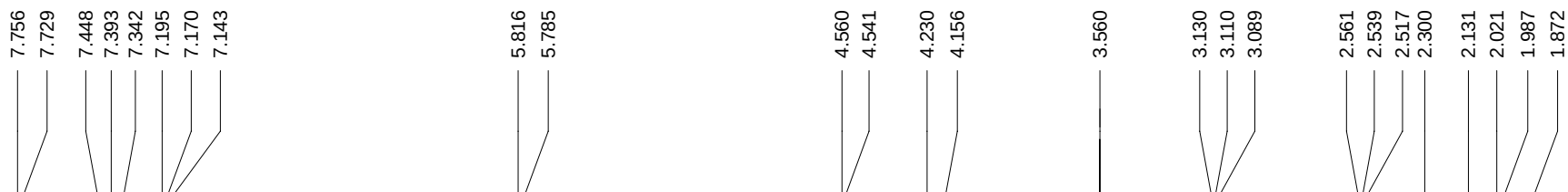
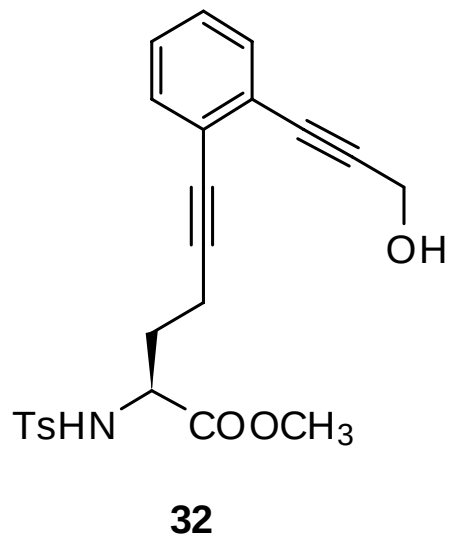
75

50

25

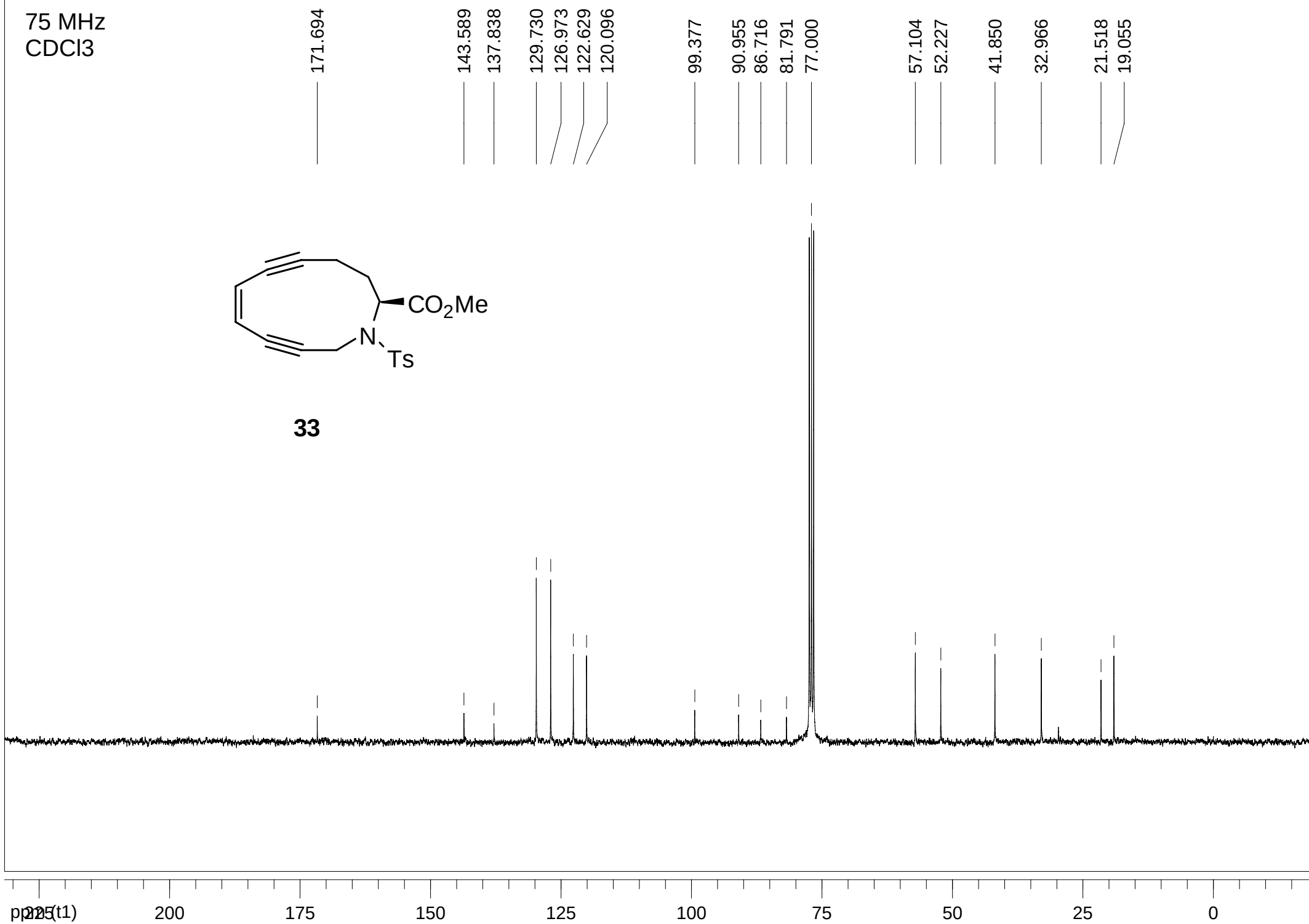
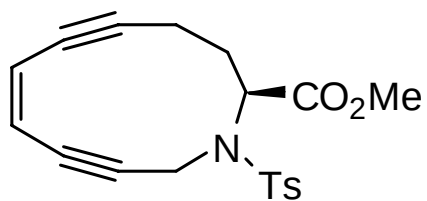
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300 MHz
CDCl₃

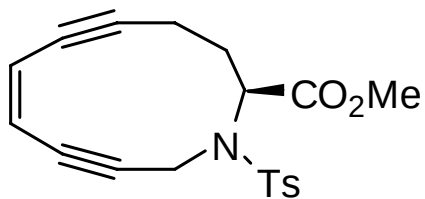


ppm (t1) 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00

75 MHz
CDCl₃



300 MHz
CDCl₃



7.697
7.670
7.312
7.286
7.260

5.840
5.806
5.796
5.762
5.255
5.247
5.226
5.217

4.514
4.455
4.396
4.336

3.636

2.781
2.680
2.625
2.491
2.415
2.107
2.001

2.00

1.99

1.87

0.92

1.00

0.99

2.88

1.02

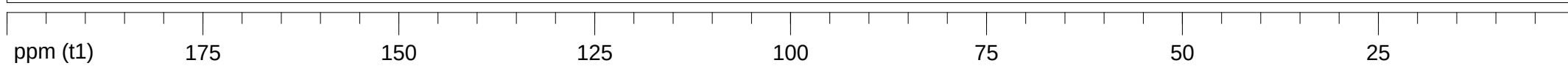
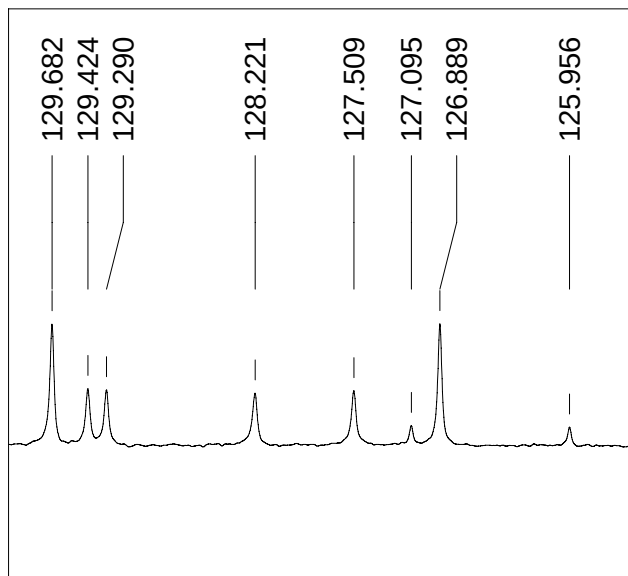
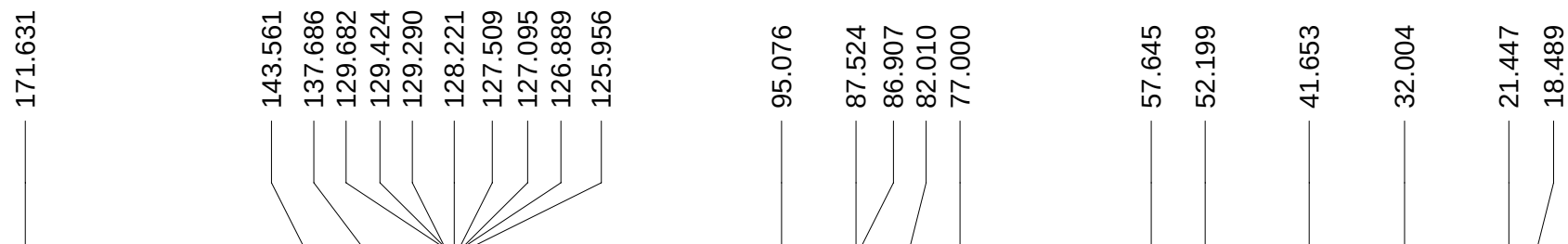
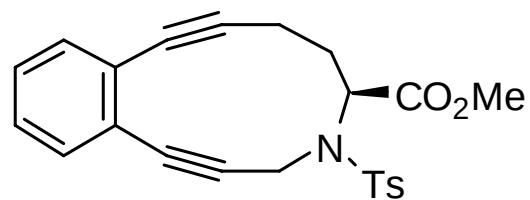
1.97

3.00

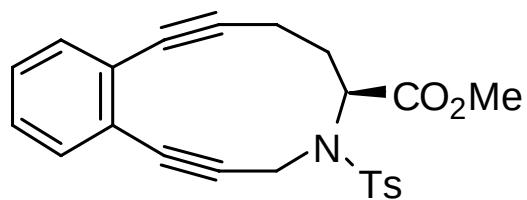
1.00

ppm (t1) 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00

50 MHz
CDCl₃



300 MHz
CDCl₃



7.728
7.701
7.336
7.306
7.280
7.179

5.250
5.239
5.223
5.211

4.604
4.546
4.471
4.413

3.650

2.761
2.659
2.633
2.590
2.402
2.209
2.104

1.94

5.88

0.94

0.98

0.98

2.86

1.06

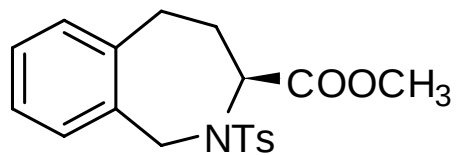
1.93

3.00

1.03

ppm (t1) 8.50 8.00 7.50 7.00 6.50 6.00 5.50 5.00 4.50 4.00 3.50 3.00 2.50 2.00

75 MHz
CDCl₃



171.422

143.027

139.875

137.182

136.701

129.399

129.186

128.679

127.619

127.138

126.331

77.000

59.177

52.308

48.565

31.420

29.345

21.429

129.399

129.186

128.679

127.619

127.138

126.331

ppm (1)

200

175

150

125

100

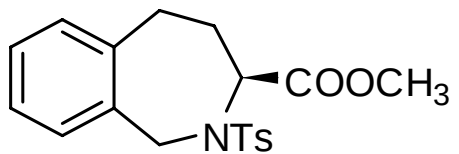
75

50

25

0

400 MHz
CDCl₃



35

7.496
7.475
7.207
7.185
7.160
7.128
7.109
7.005
6.964

4.806
4.803
4.761
4.744
4.729
4.655
4.614

3.668

2.932
2.908
2.892
2.869
2.615
2.594
2.576
2.555
2.352
2.335
2.255
1.994
1.916

1.96

4.02
1.00

1.01

1.97

0.97

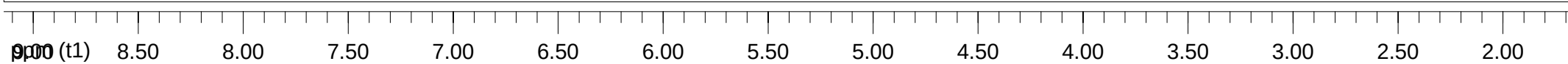
3.00

1.04

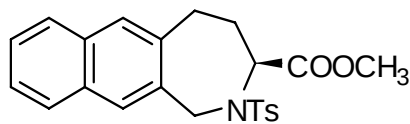
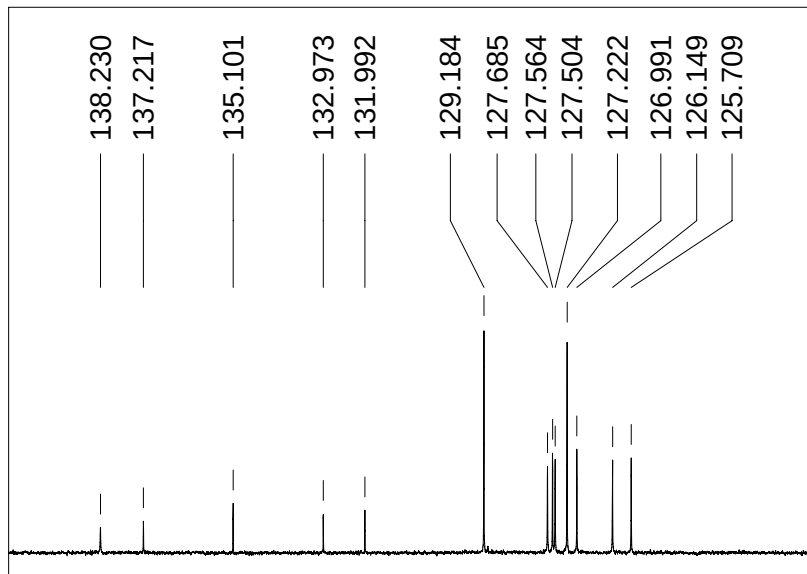
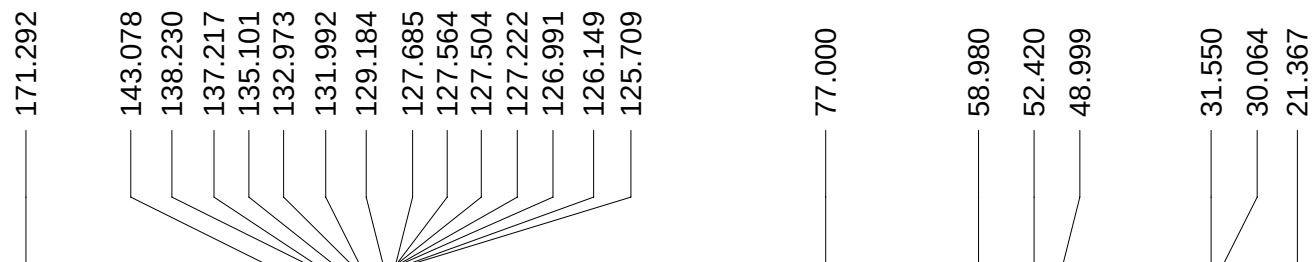
1.01

3.08
0.94

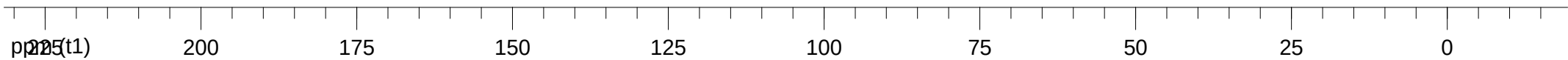
1.13



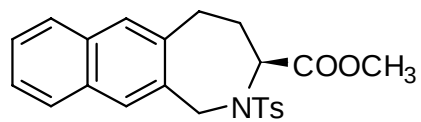
75 MHz
CDCl₃



36



400 MHz
CDCl₃



36

