

Supporting Information

Design of Configuration-Restricted Triazolylated β -D-Ribofuranosides: A Unique Family of Crescent-Shaped RNase A Inhibitors

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Kharagpur 721 302, West Bengal, India

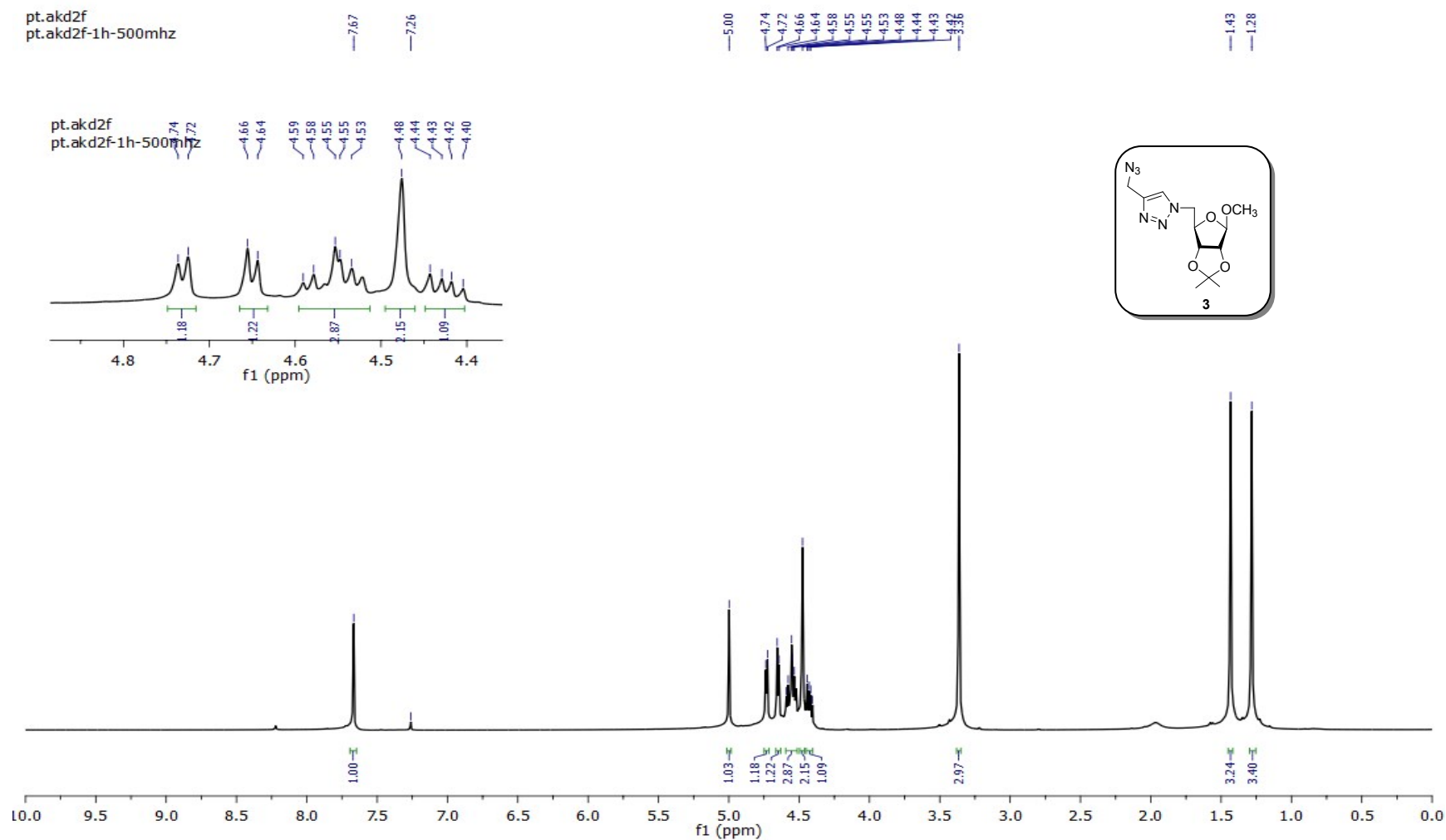
*Corresponding author. Tel.: +91-3222-283306; Tel.: +91-3222-283342; fax: +91-3222-255303; e-mail: swagata@chem.iitkgp.ac.in (S. Dasgupta.) tpathak@chem.iitkgp.ac.in (T. Pathak).

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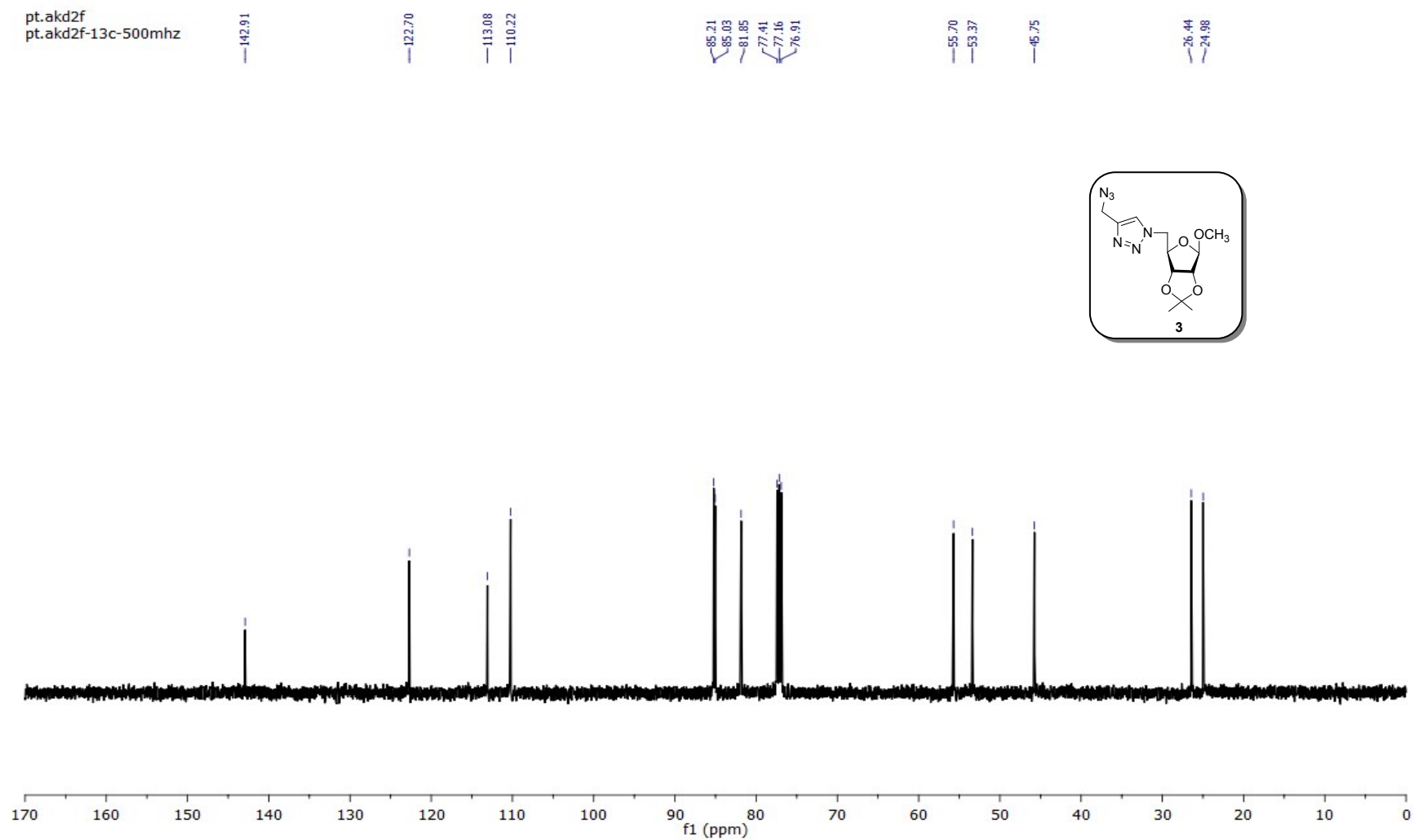
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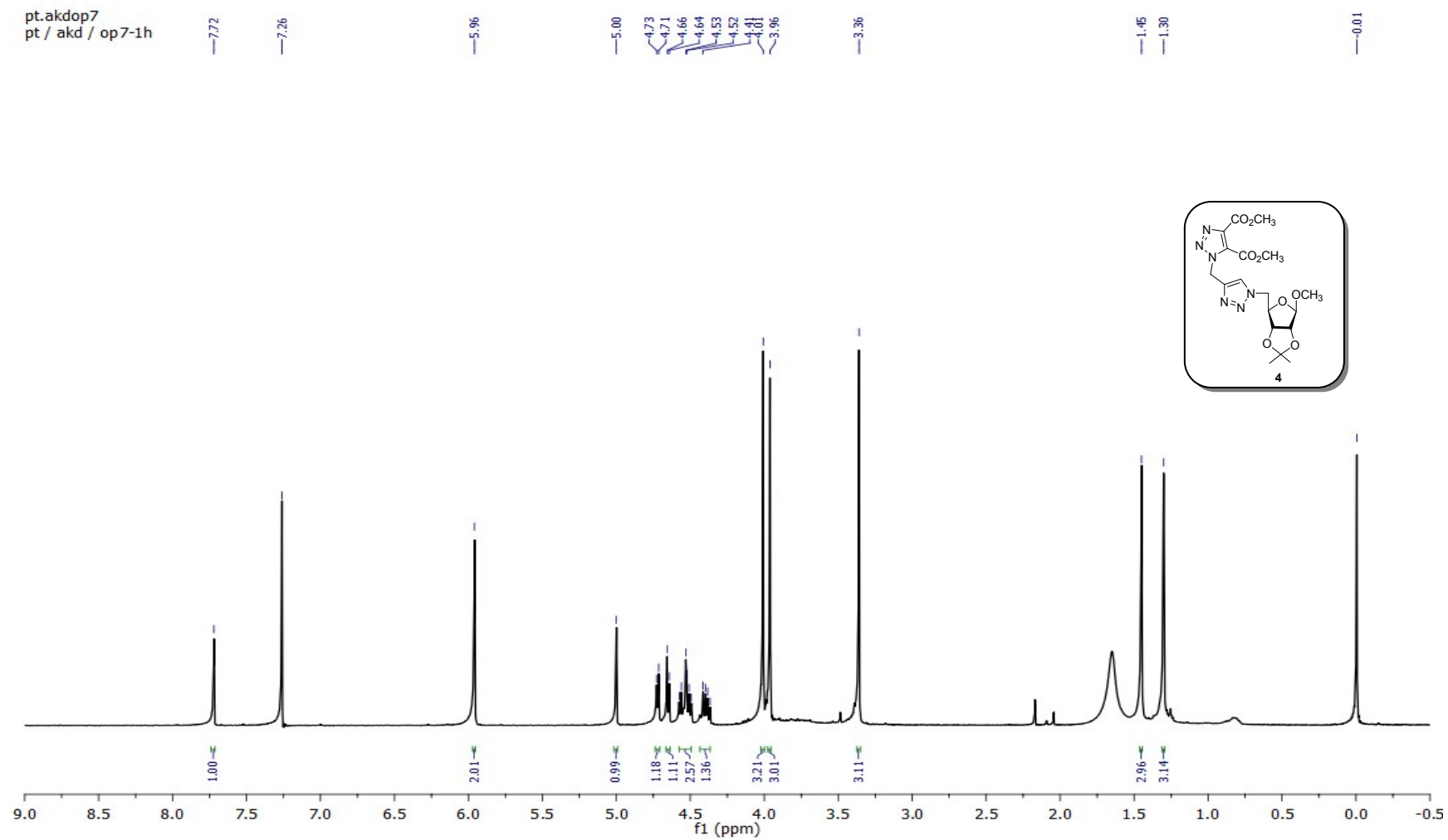
¹H -NMR spectra of compound 3



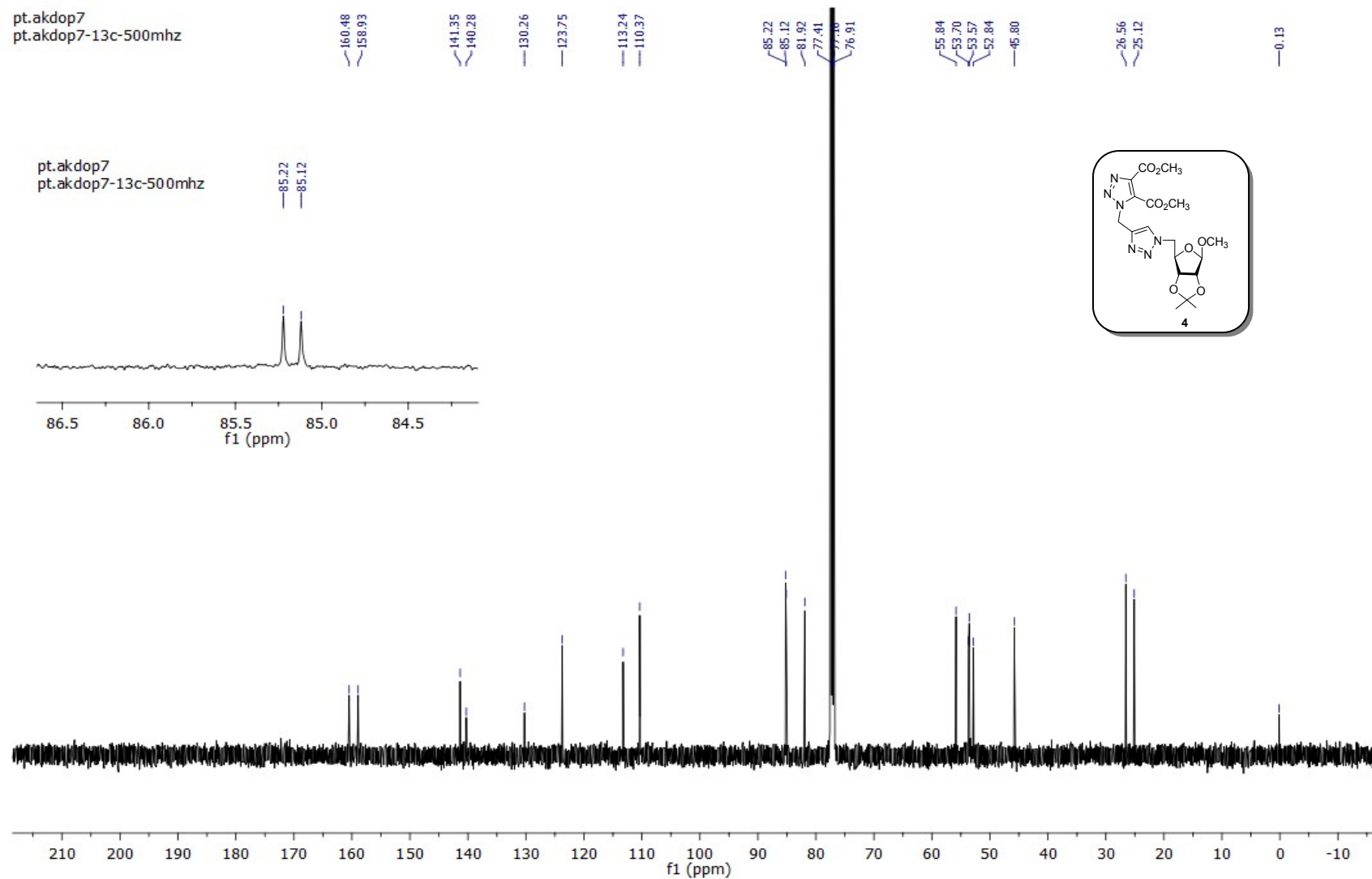
^{13}C -NMR spectra of compound **3**



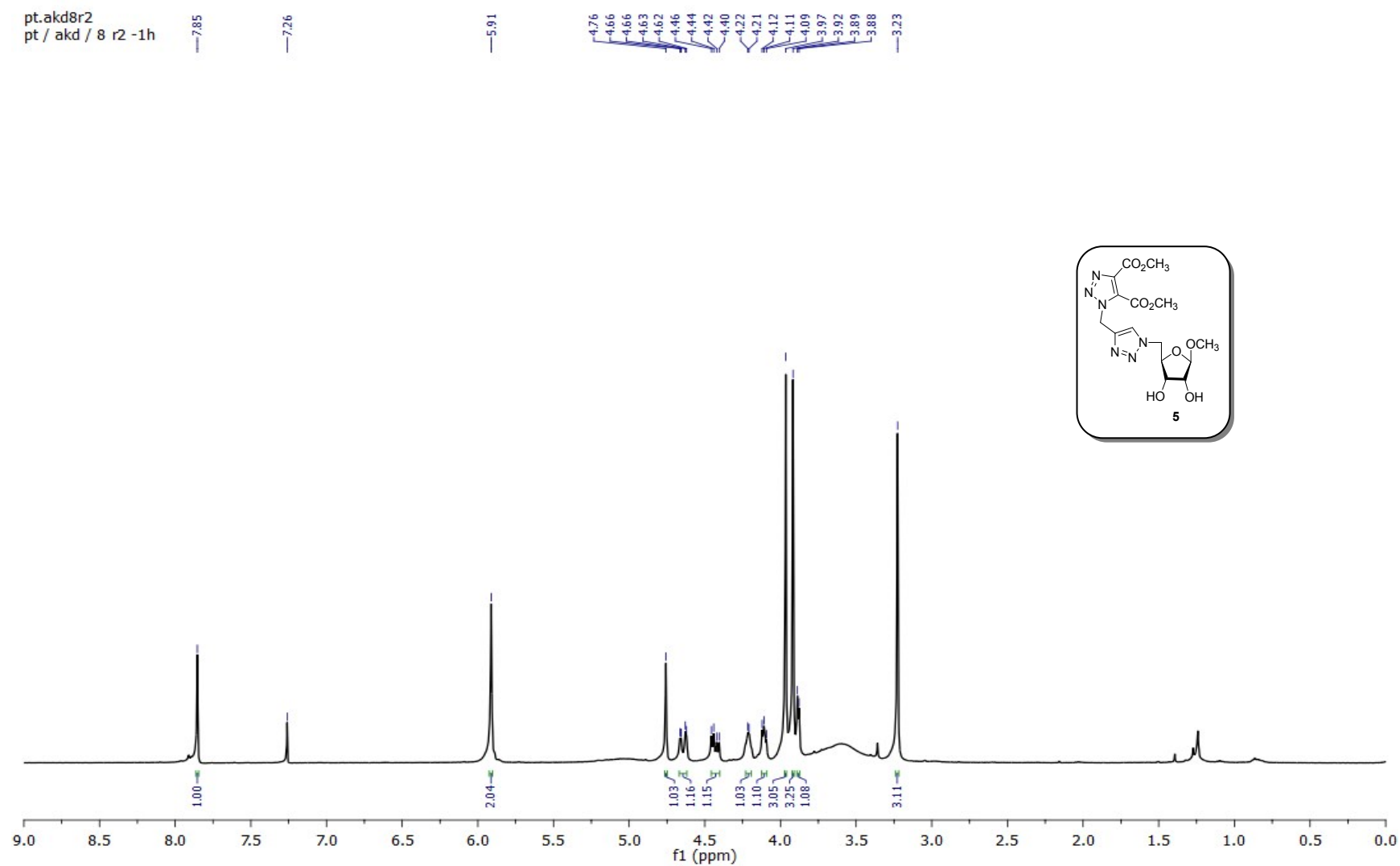
¹H -NMR spectra of compound 4



¹³C -NMR spectra of compound 4

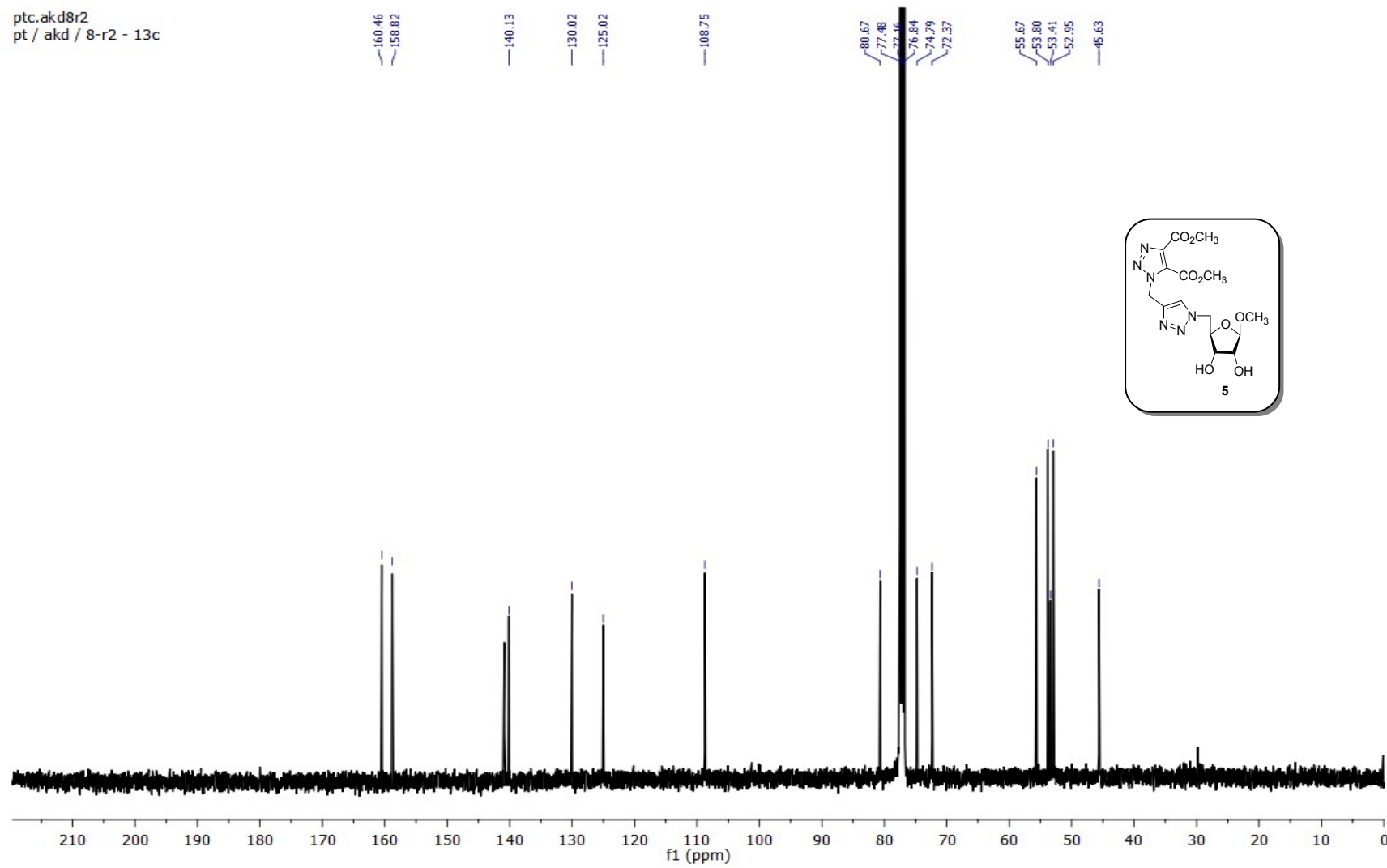


¹H -NMR spectra of compound **5**

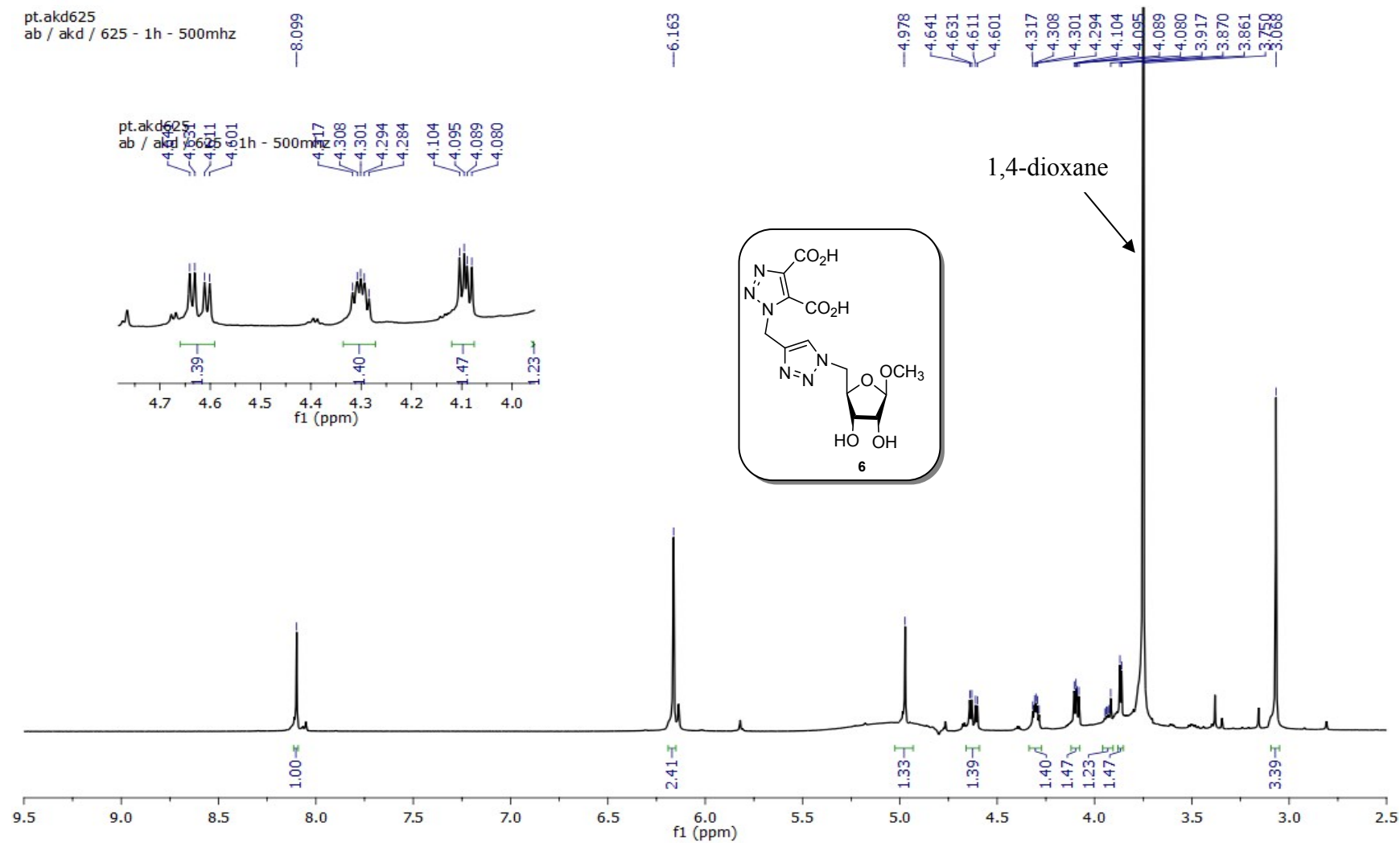


^{13}C -NMR spectra of compound **5**

ptc.akd8r2
pt / akd / 8-r2 - 13c



¹H -NMR spectra of compound 6



^{13}C -NMR spectra of compound 6

pt.akd625
pt / akd / 625 - 13c - 500mhz

164.736
161.715

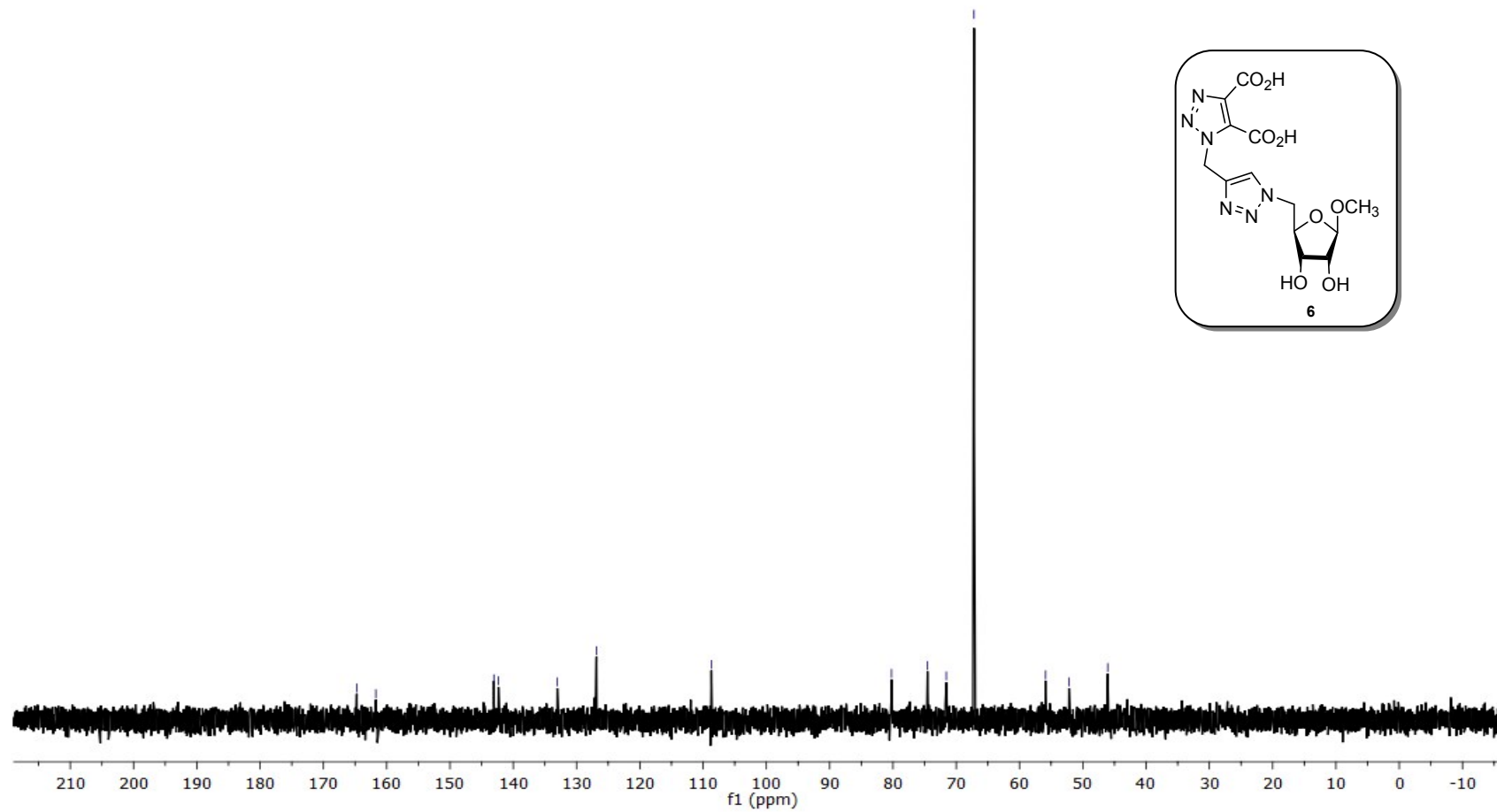
143.065
142.342

133.075
126.849

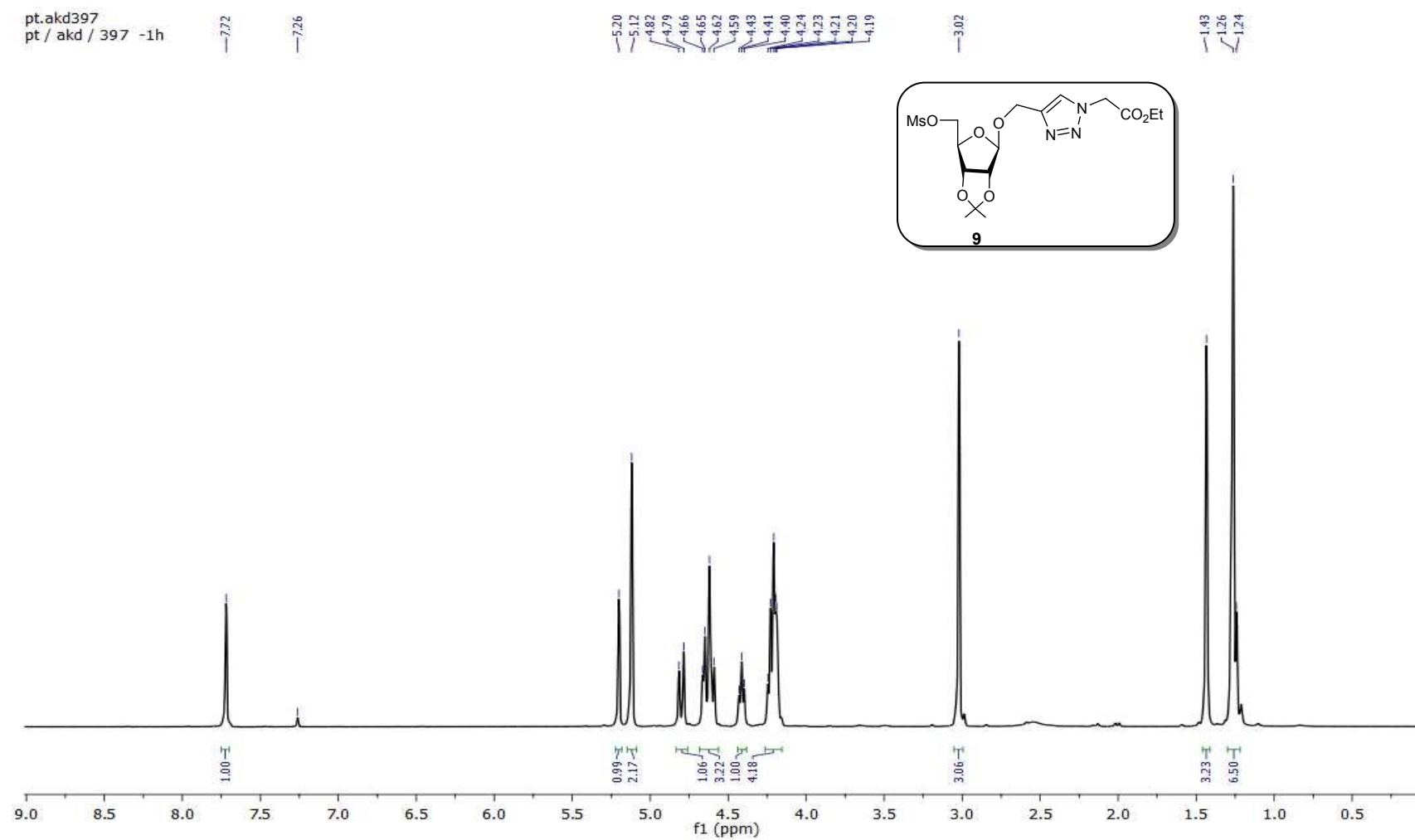
108.692

80.230
74.539
71.566
67.190

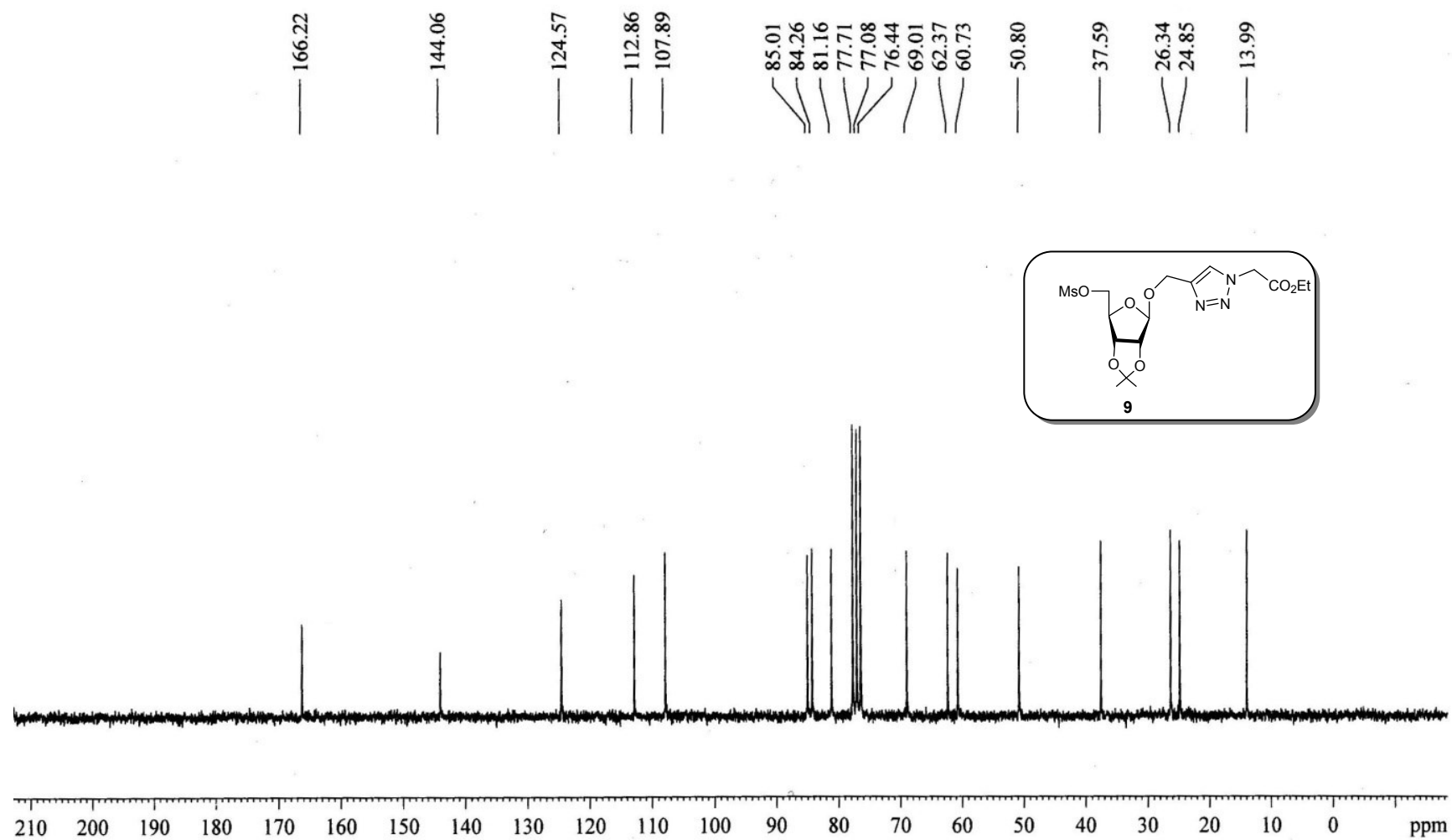
55.879
52.176
46.058



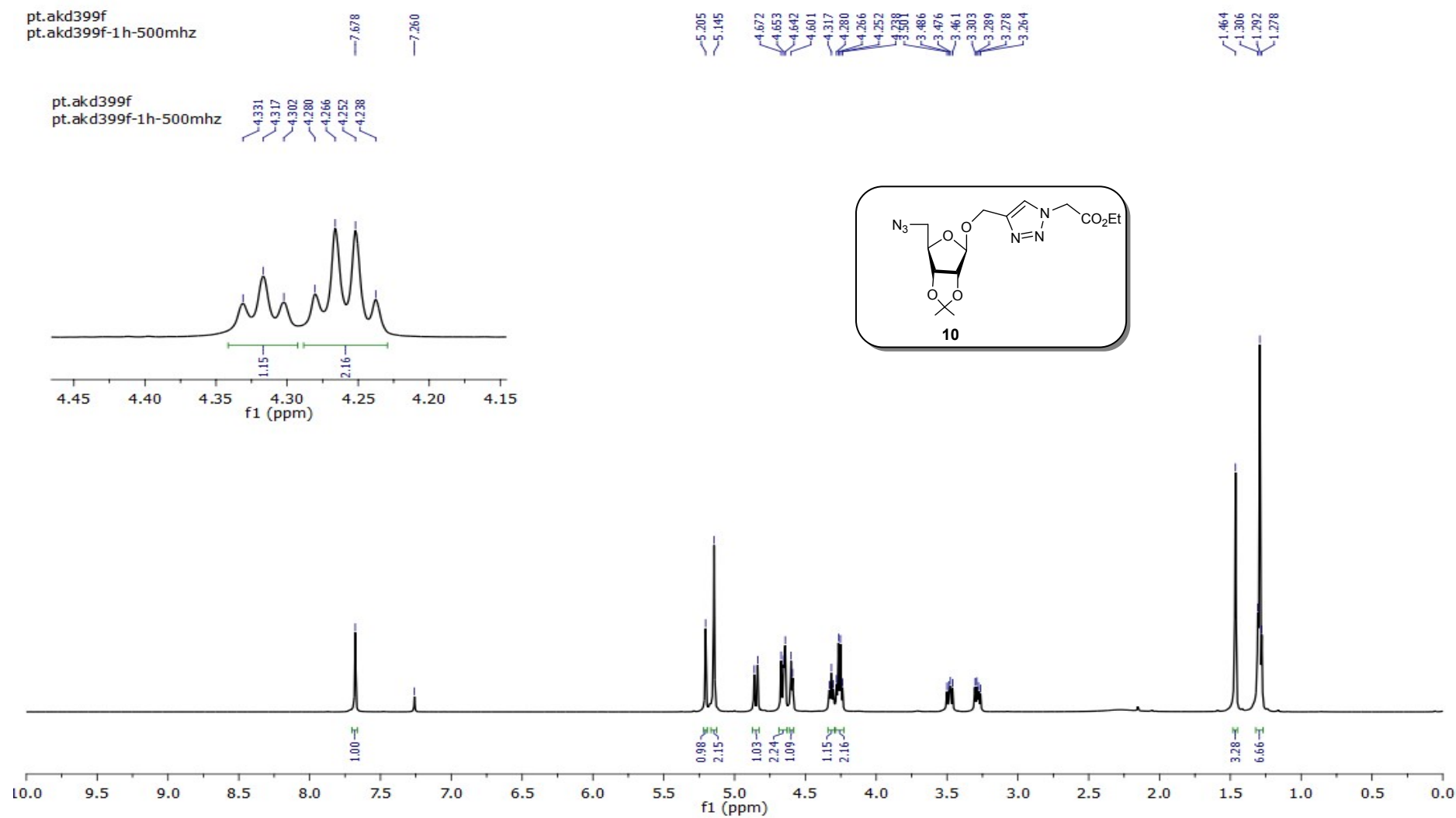
^{13}C -NMR spectra of compound **9**



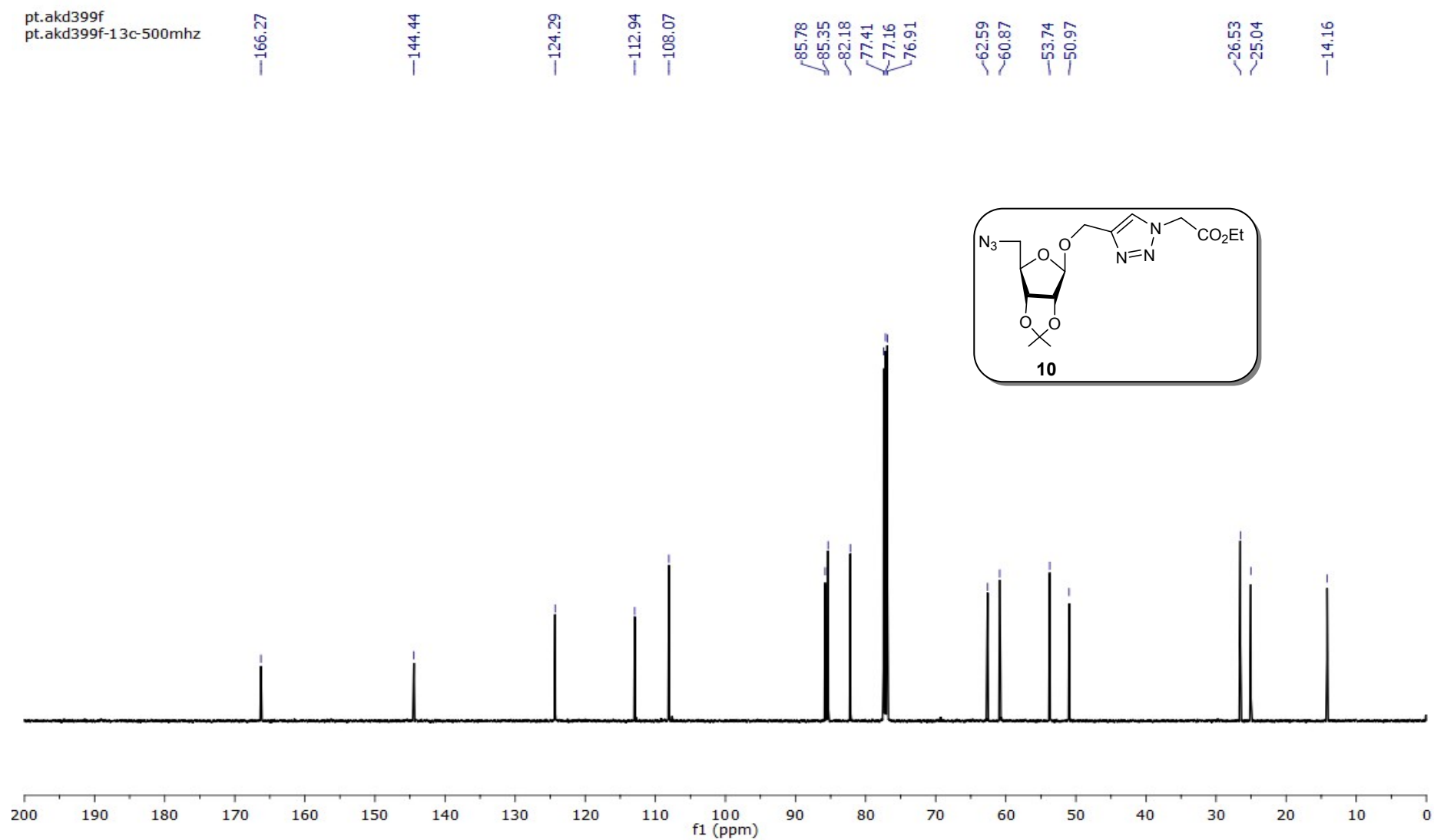
^{13}C -NMR spectra of compound **9**



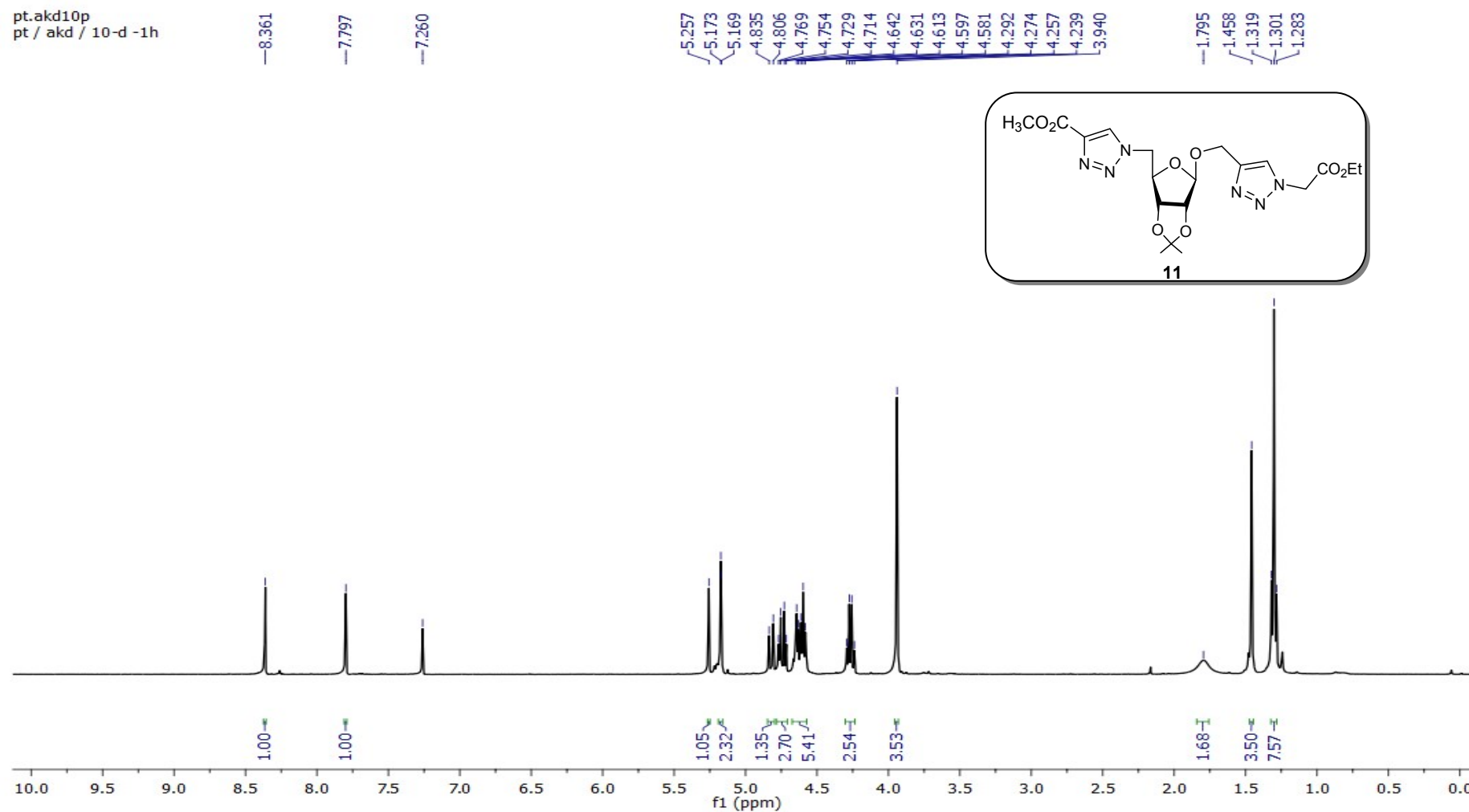
¹H -NMR spectra of compound **10**



^{13}C -NMR spectra of compound **10**



¹H -NMR spectra of compound **11**



¹³C -NMR spectra of compound **11**

pt.akd10p
pt.akd10p-13c-500mhz

—166.337
—161.230

—144.089
—140.196

—128.459
—124.769

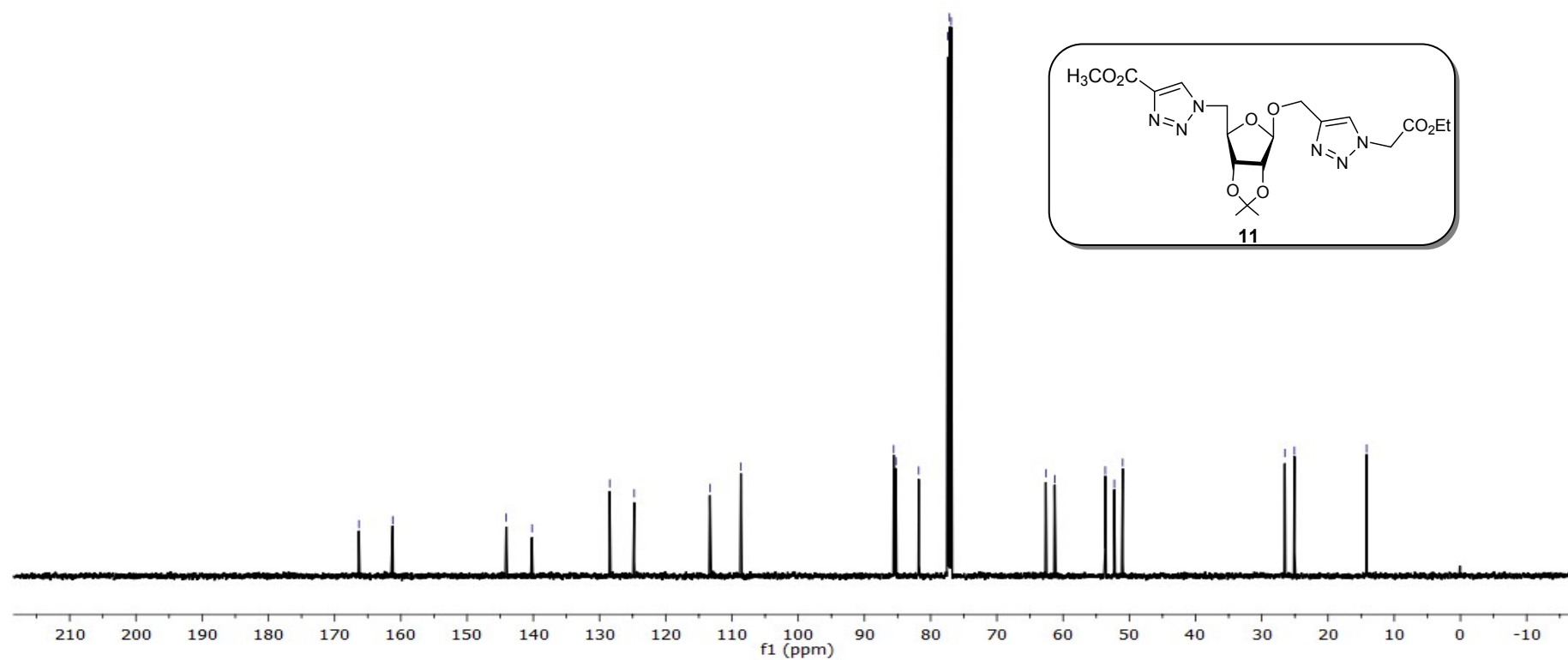
—113.340
—108.653

85.579
85.254
81.808
77.415
77.160
76.907

62.616
61.277
53.630
52.273
51.002

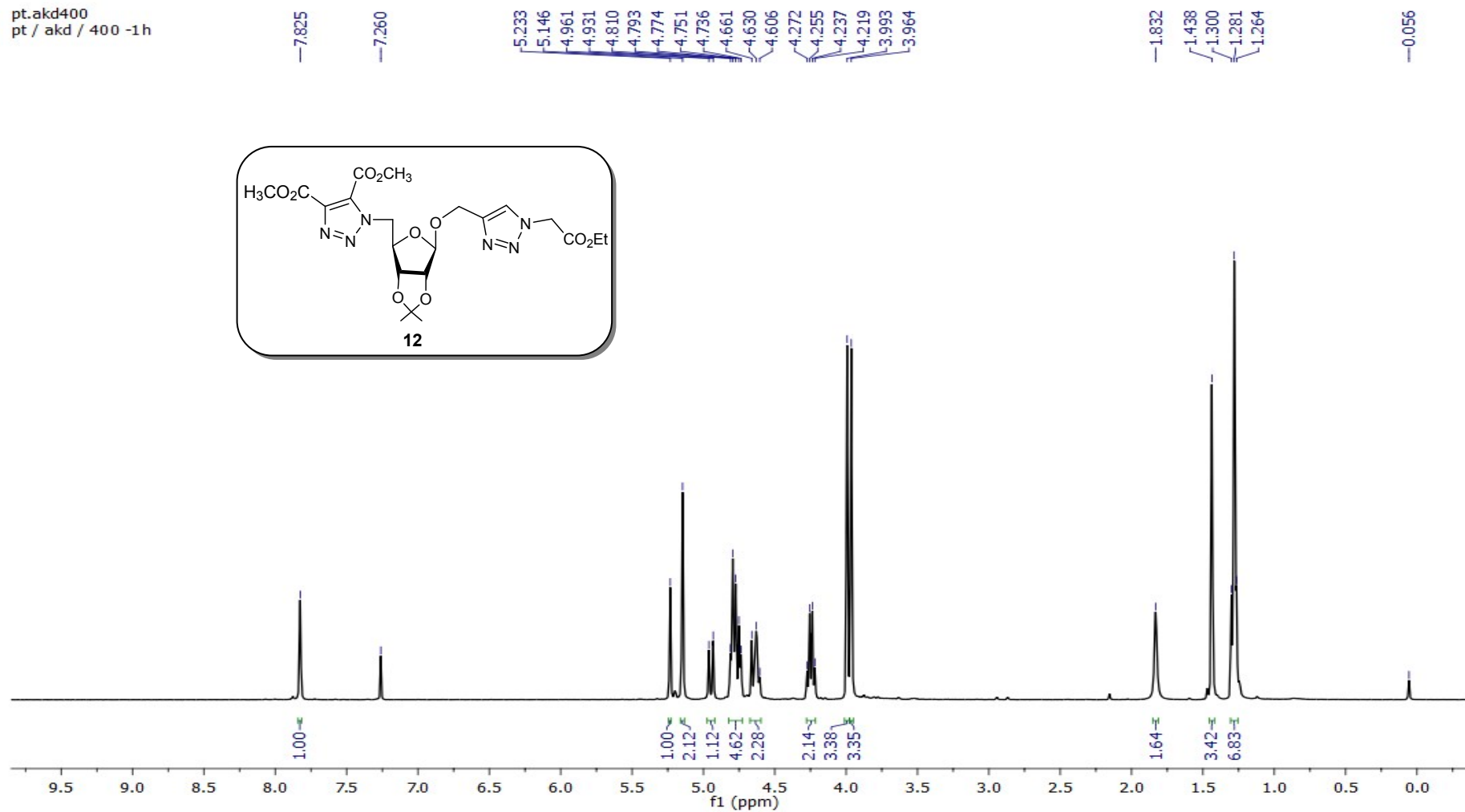
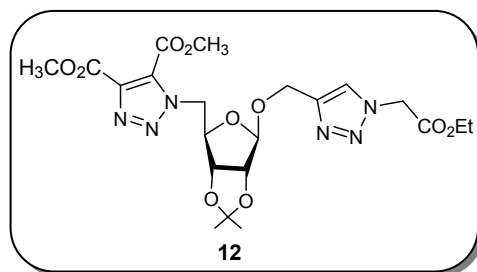
26.521
25.075

—14.170

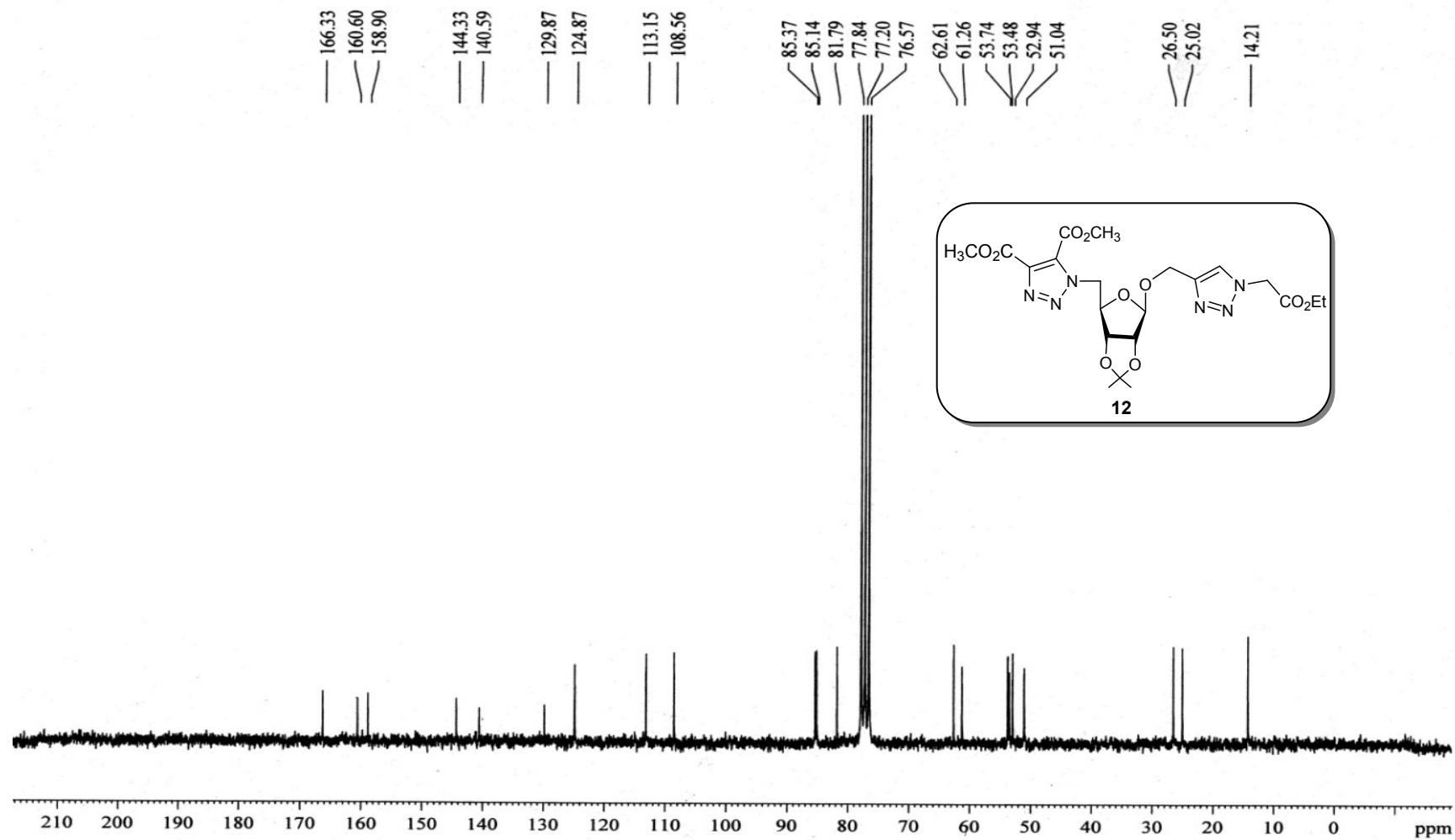


¹H -NMR spectra of compound **12**

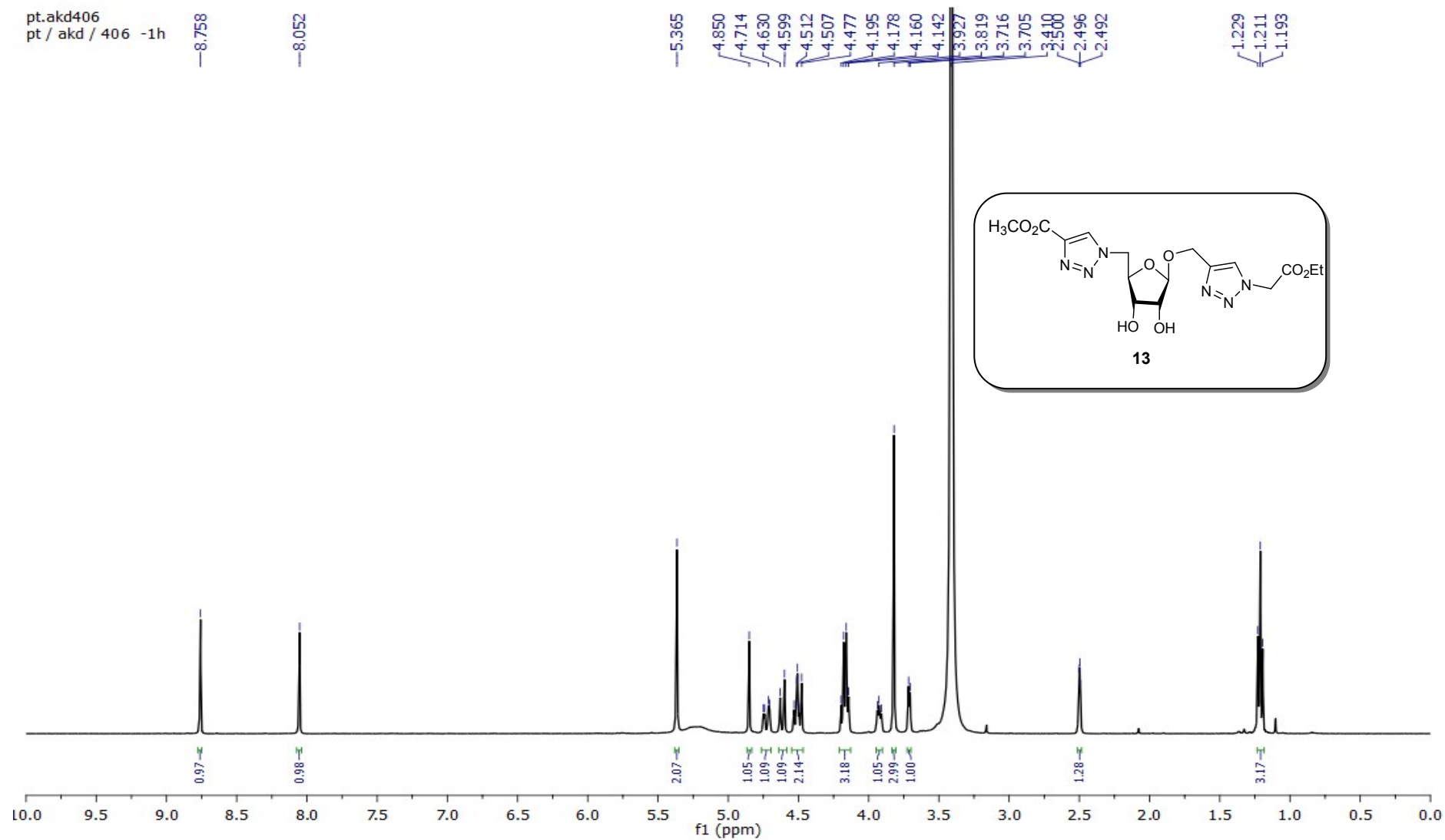
pt.akd400
pt / akd / 400 -1h



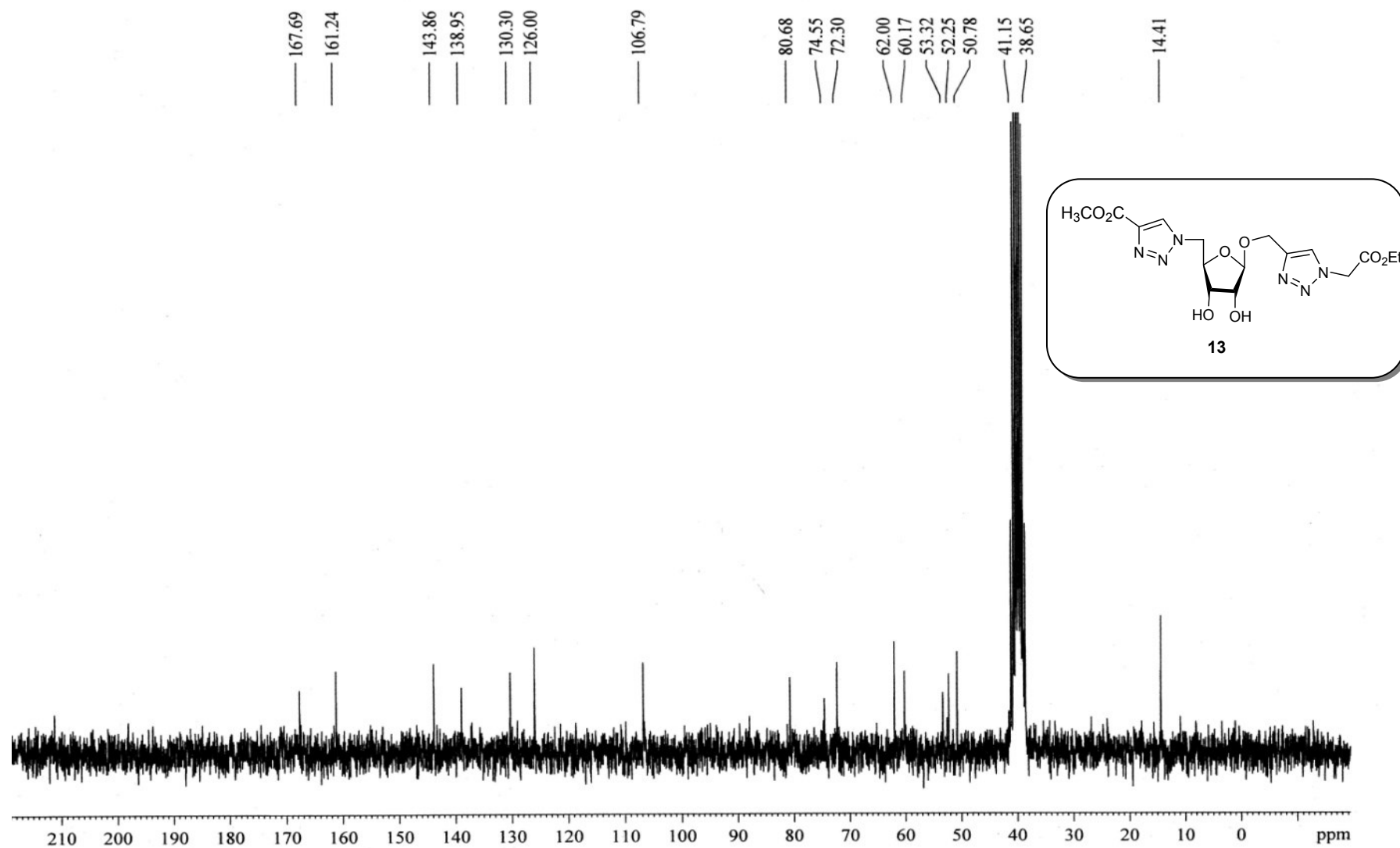
^{13}C -NMR spectra of compound **12**



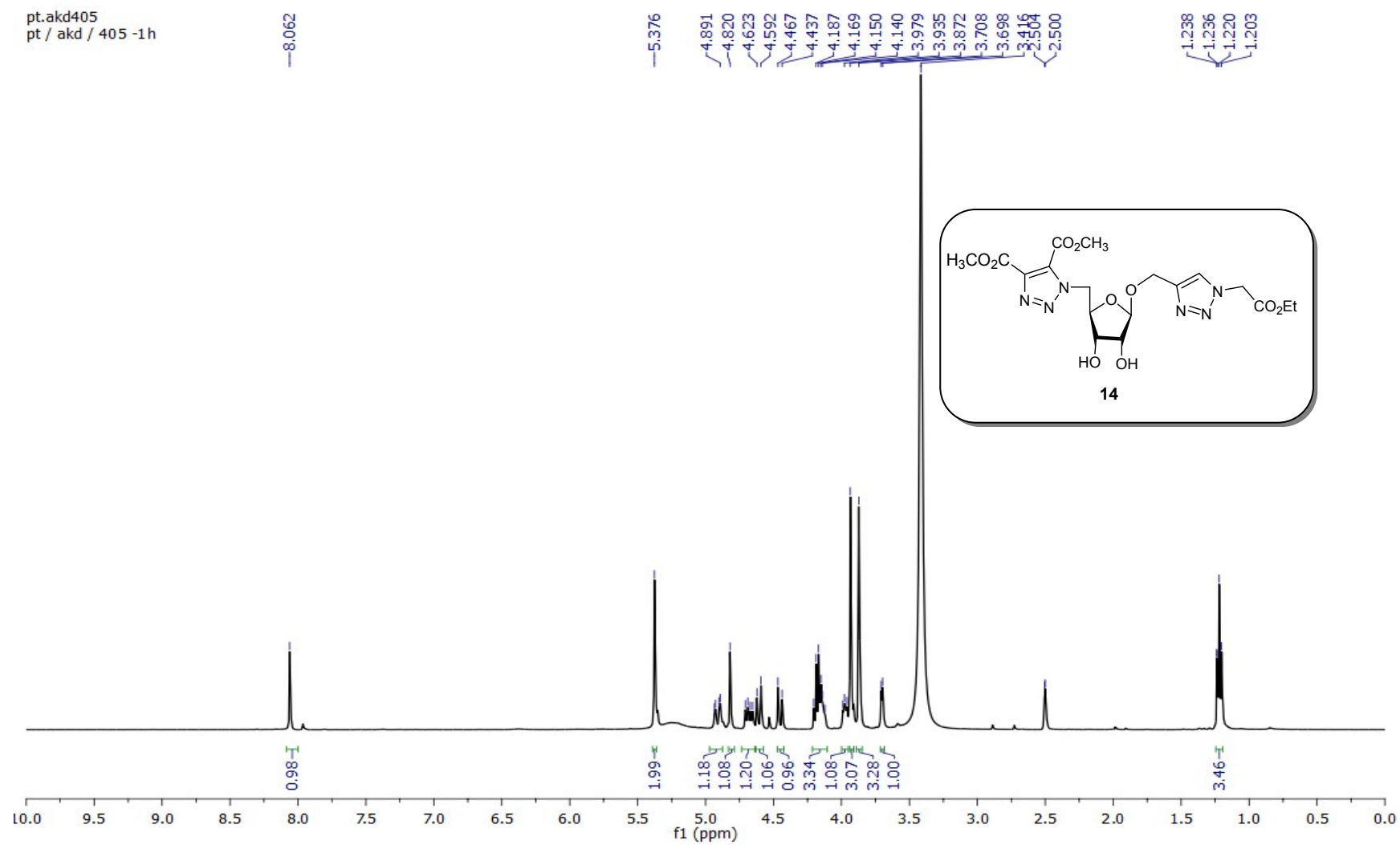
¹H -NMR spectra of compound **13**



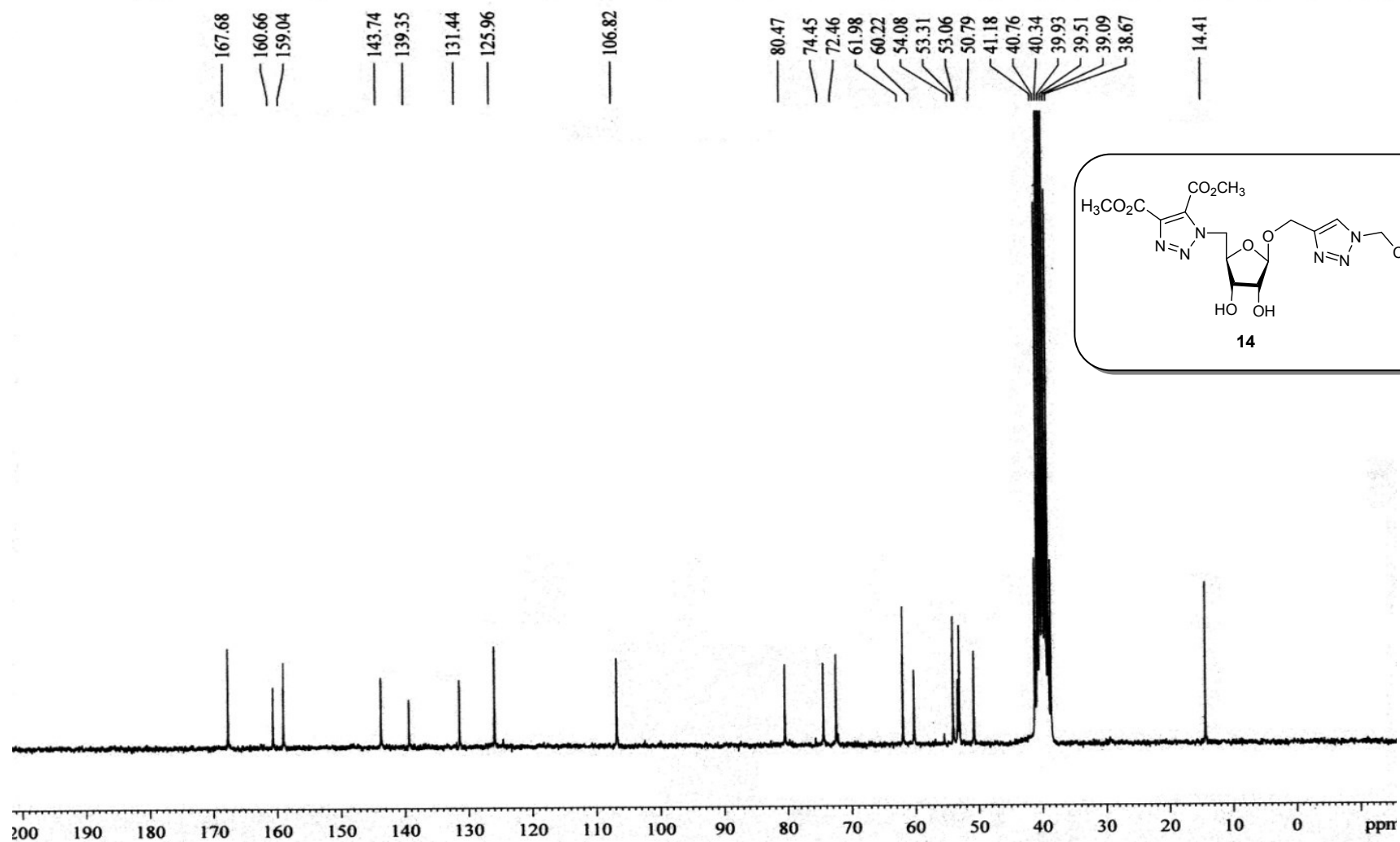
^{13}C -NMR spectra of compound **13**



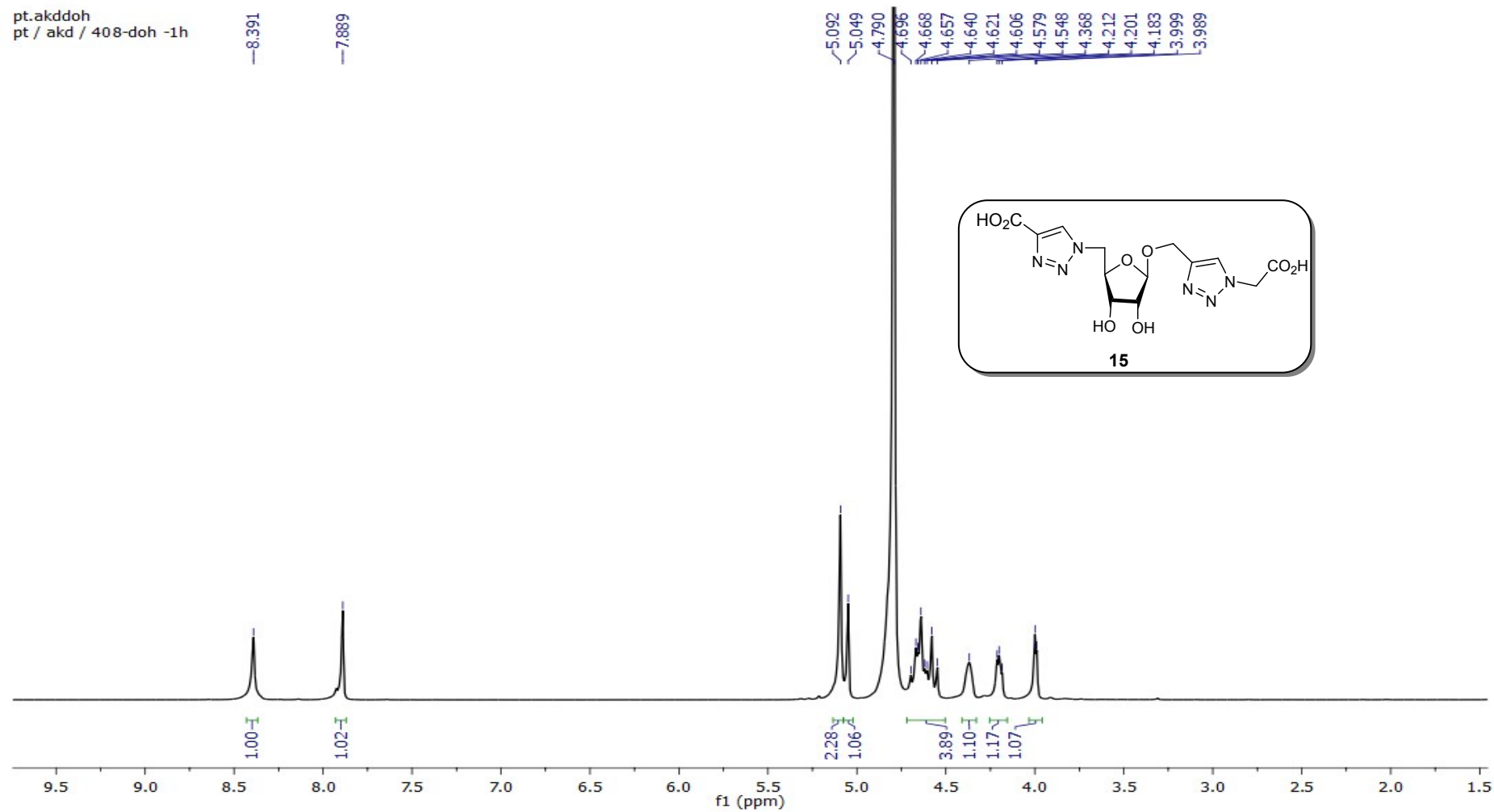
¹H -NMR spectra of compound **14**



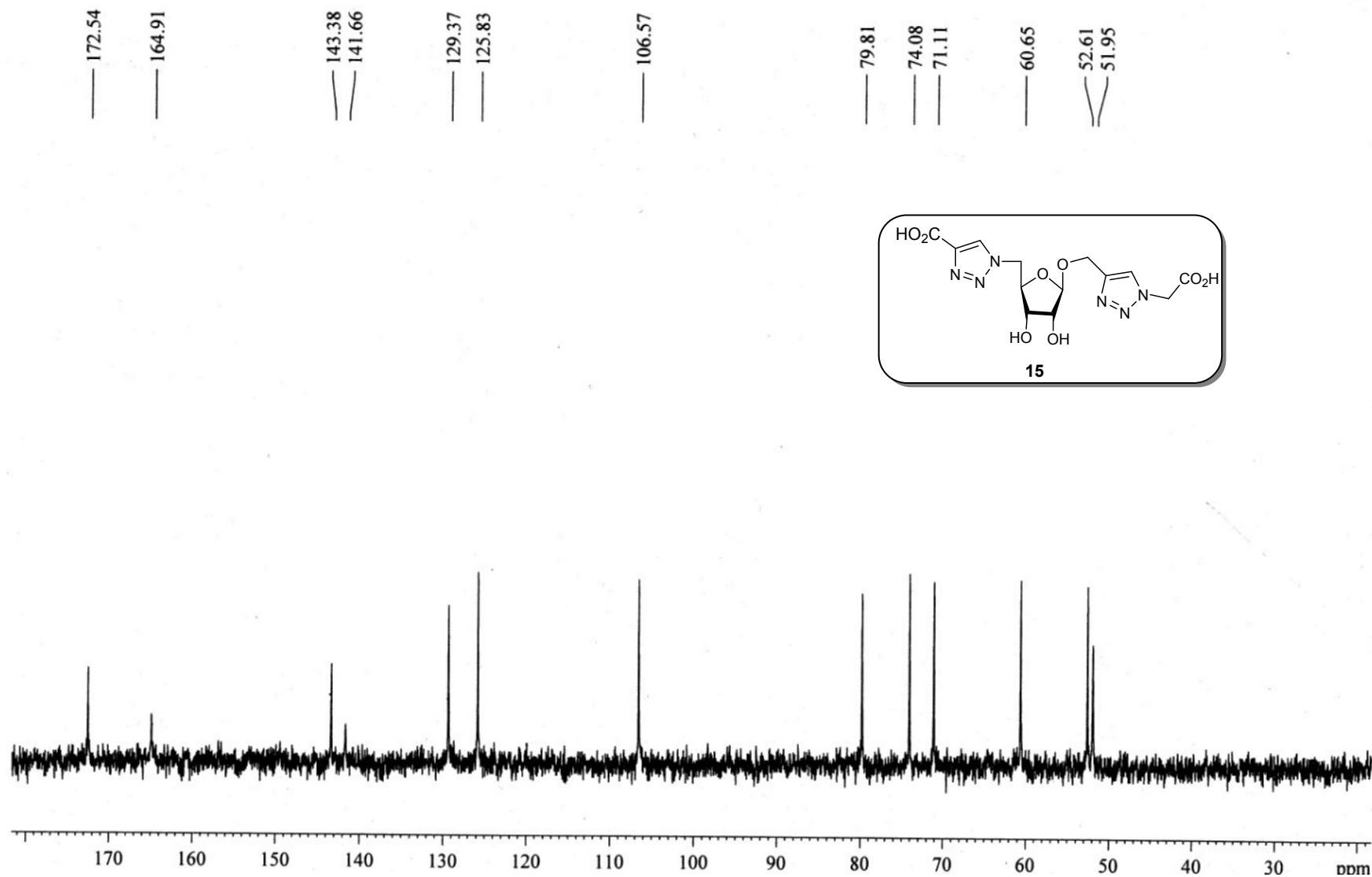
^{13}C -NMR spectra of compound **14**



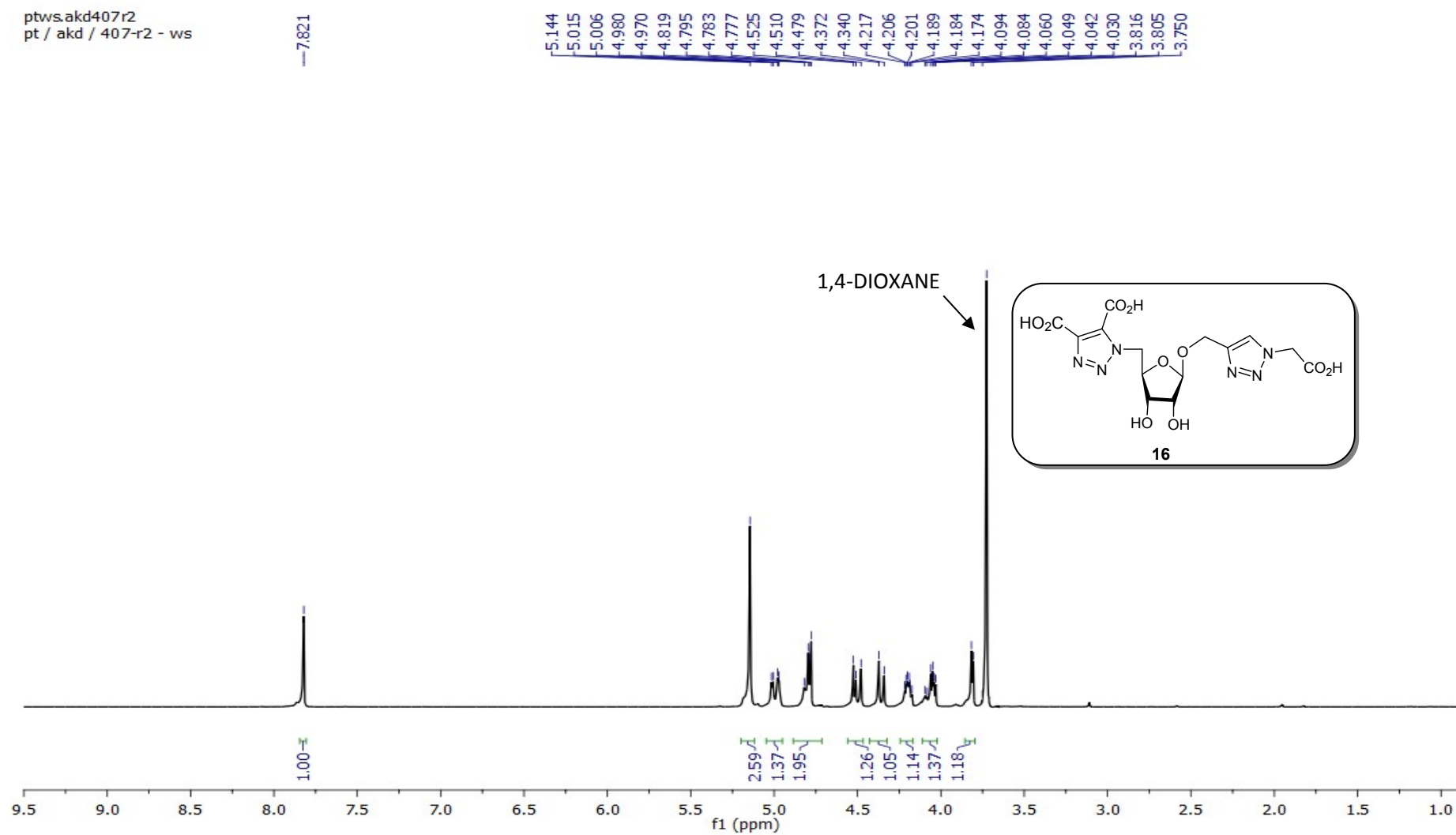
^1H -NMR spectra of compound **15**



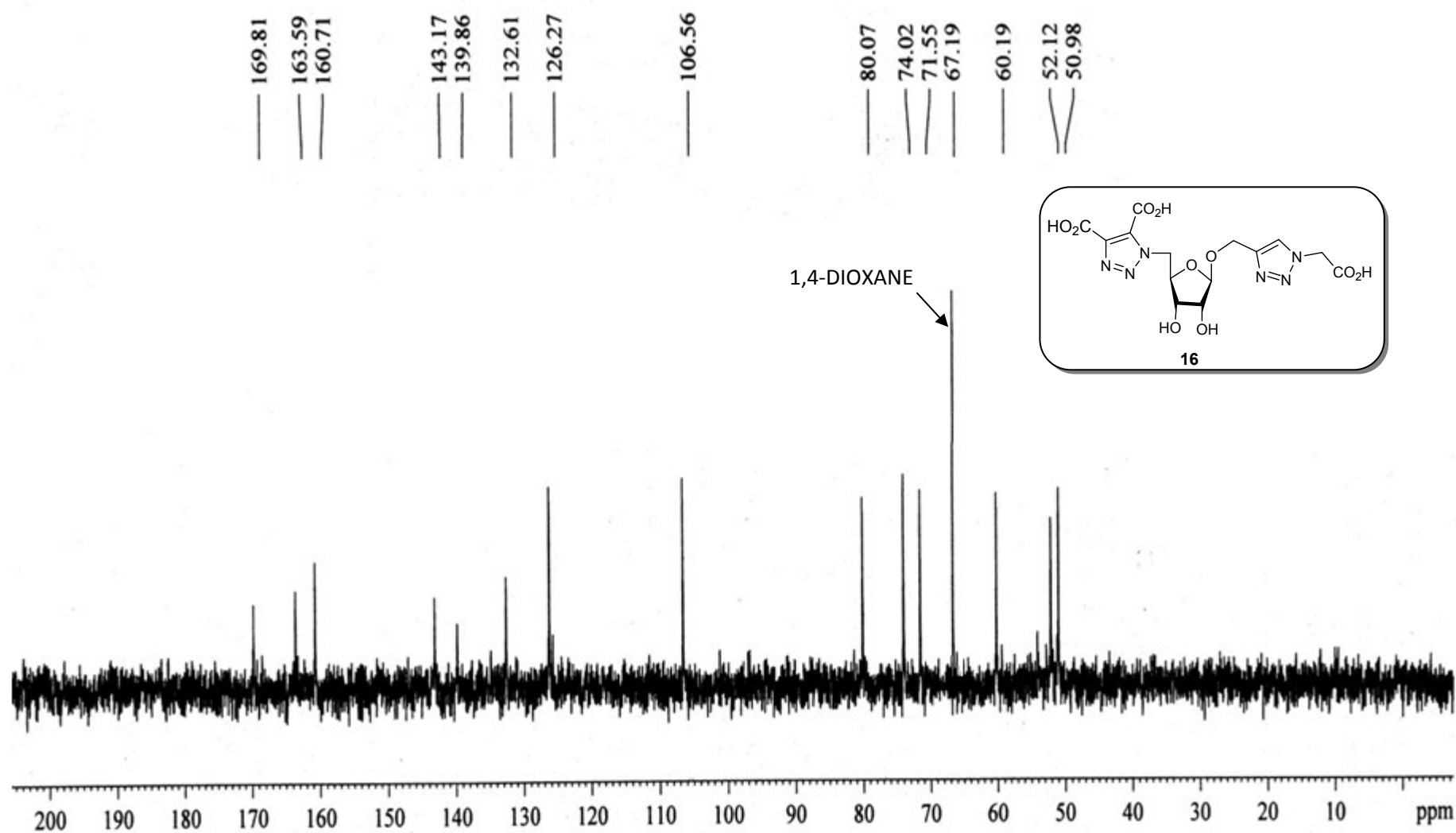
^{13}C -NMR spectra of compound **15**



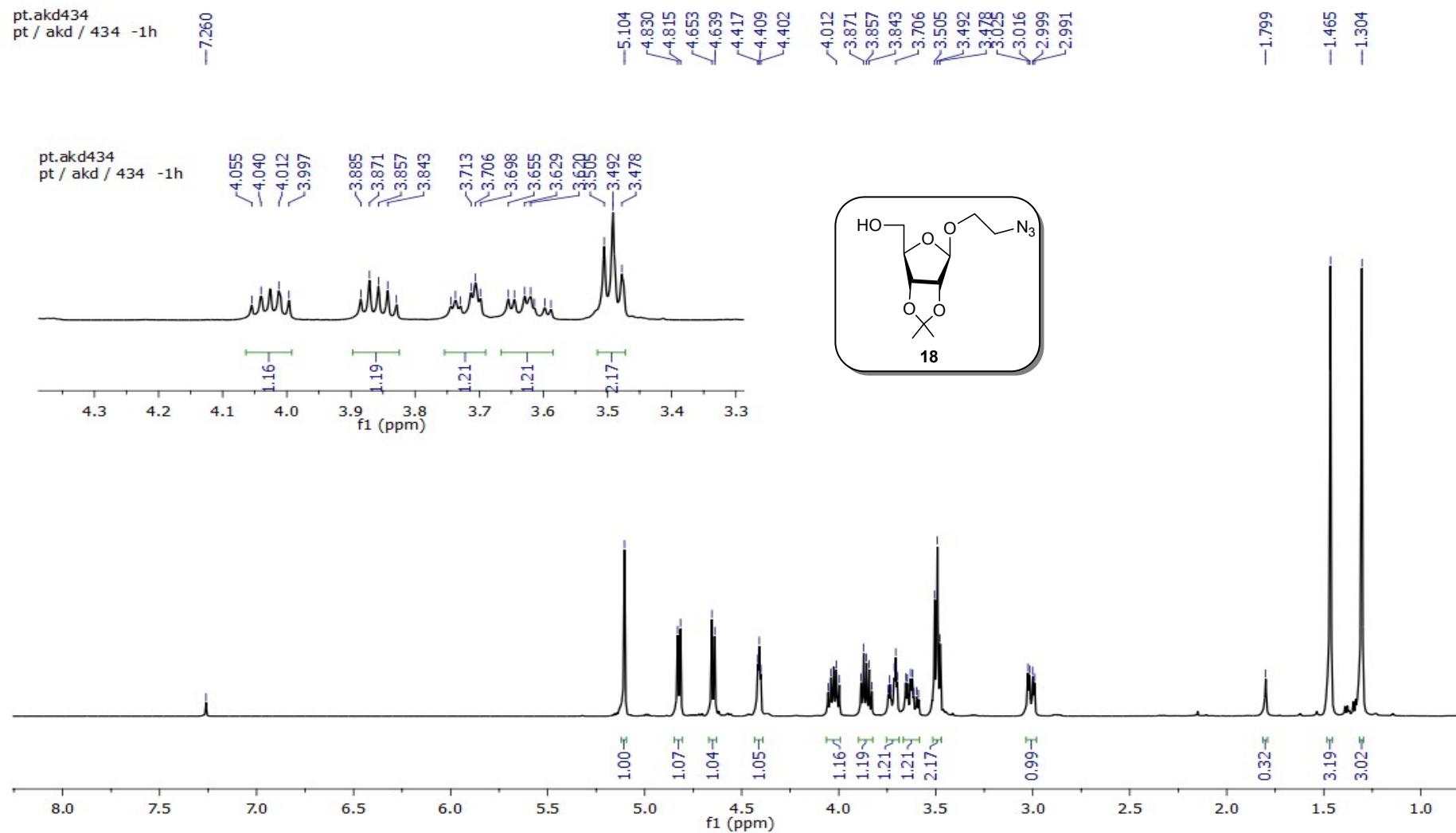
^1H -NMR spectra of compound **16**



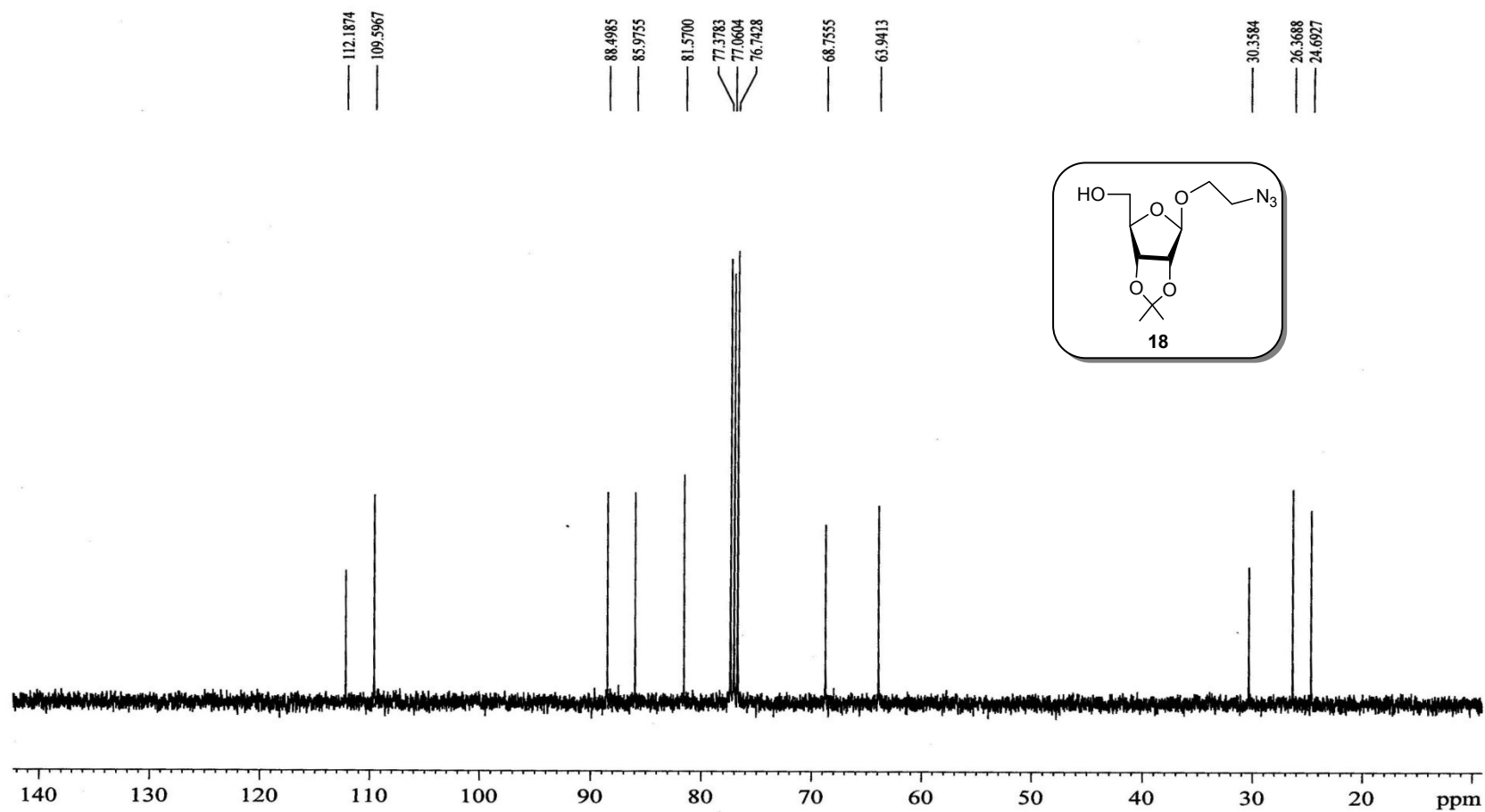
^{13}C -NMR spectra of compound **16**



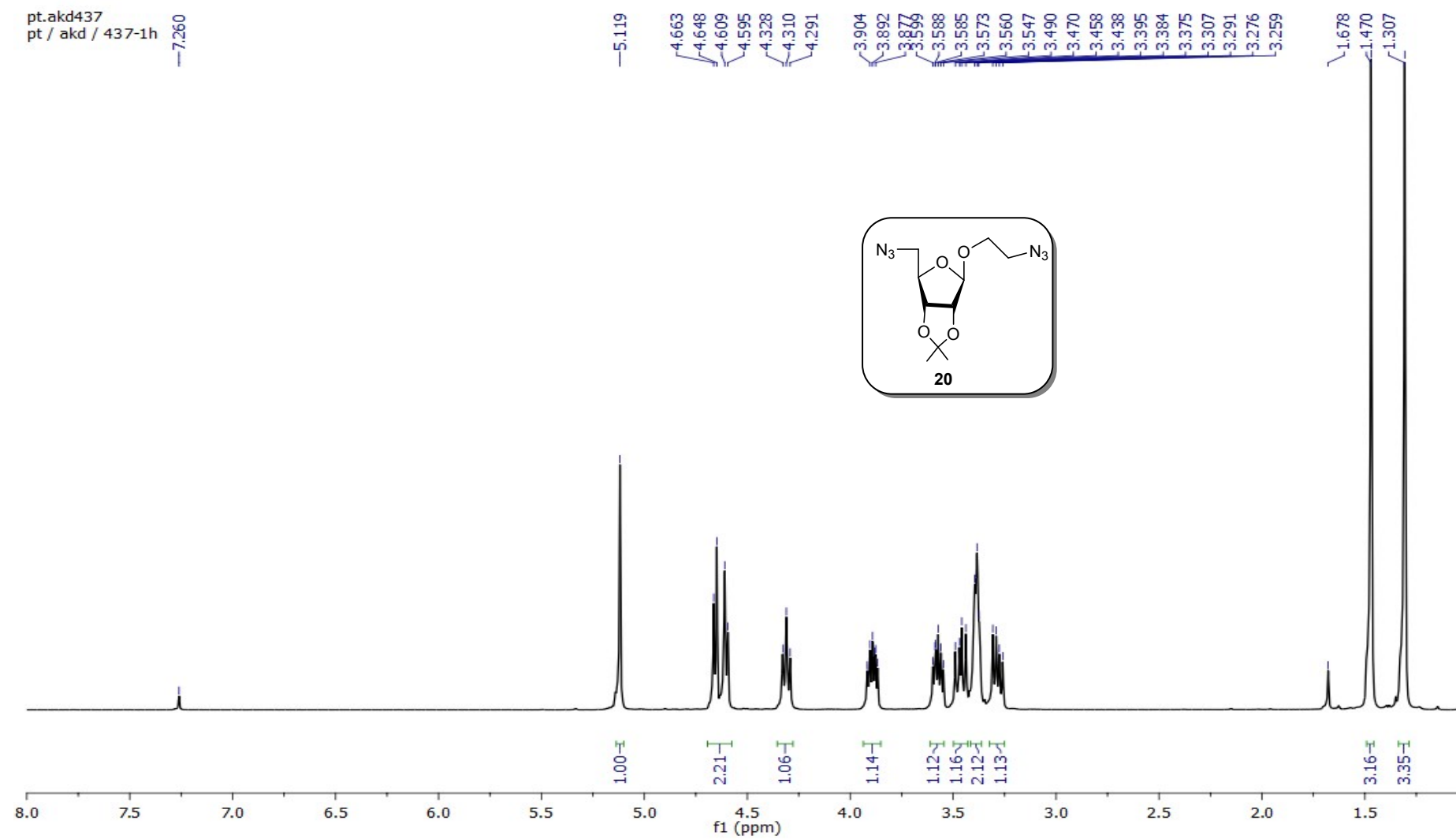
¹H -NMR spectra of compound **18**



^{13}C -NMR spectra of compound **18**



¹H -NMR spectra of compound **20**



^{13}C -NMR spectra of compound **20**

ptc.akd437
pt / akd / 437 - 13c

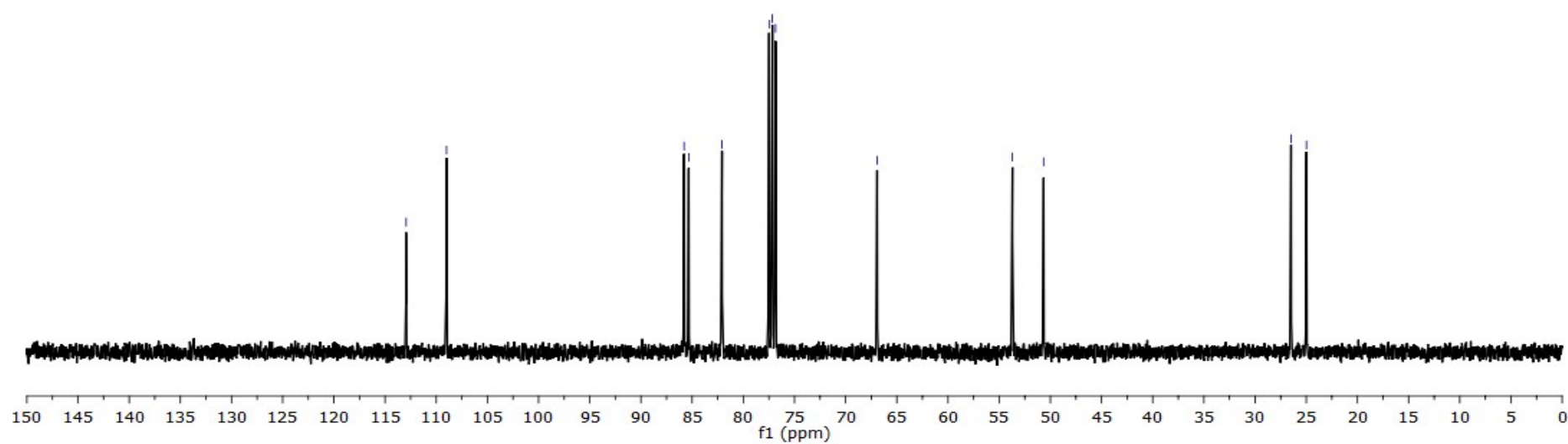
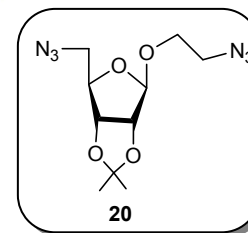
—112.943
—108.992

—85.786
—85.330
—82.082
—77.478
—77.160
—76.842

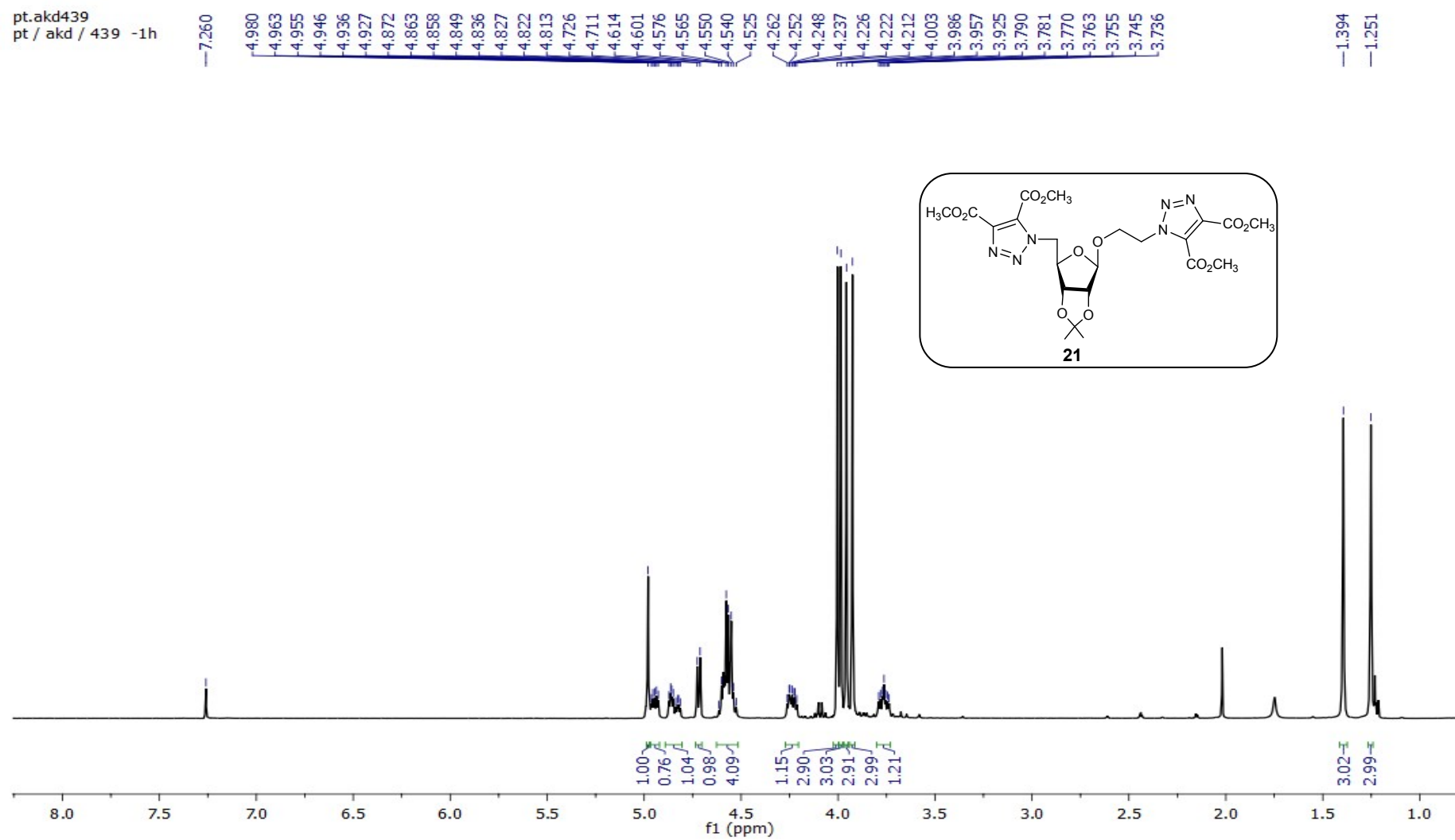
—66.926

—53.712
—50.658

—26.484
—24.982



¹H -NMR spectra of compound **21**



¹³C -NMR spectra of compound **21**

ptc.akd439
pt / akd / 439 - 13c

160.501
160.486
159.210
158.781

140.596
139.899
131.109
129.373

113.155
108.910

85.039
84.988
81.506
77.478
77.160
76.843

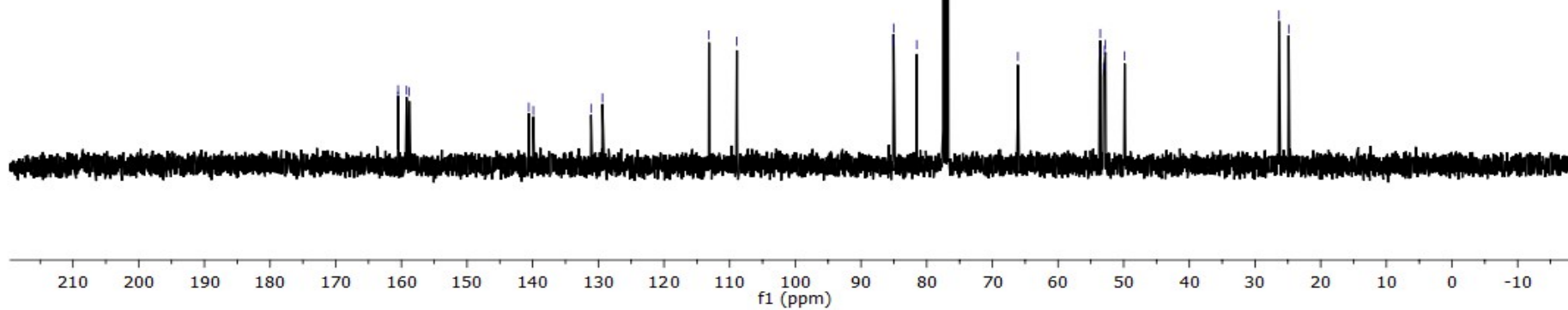
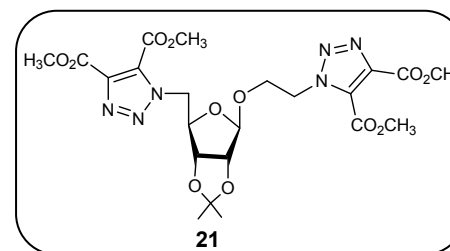
66.116
53.676
53.571
53.076
52.907
52.784
49.860

26.351
24.871

ptc.akd439
pt / akd / 439 - 13c

160.501
160.486

161.0 160.8 160.6 160.4
f1 (ppm)

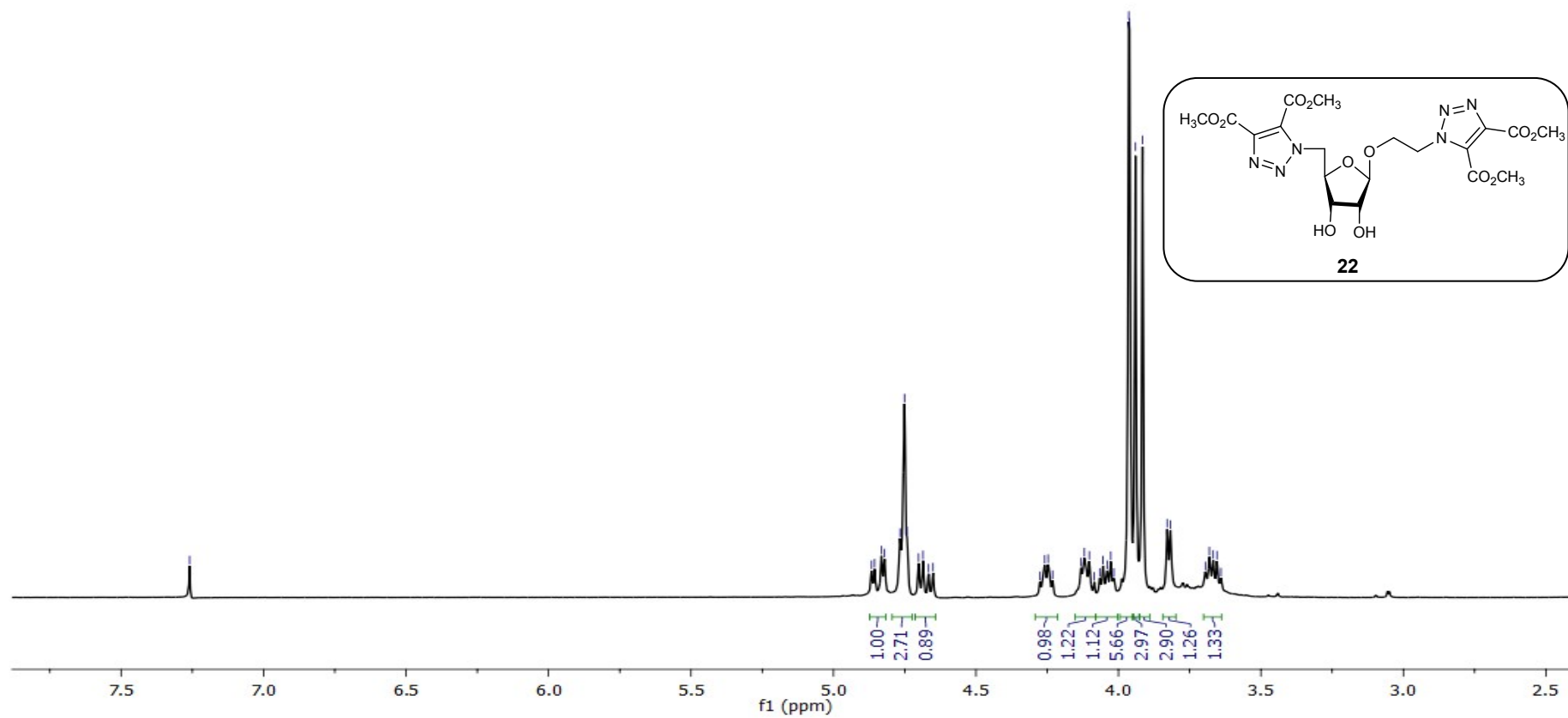


¹H -NMR spectra of compound **22**

pt.akddp
pt / akd / dp -1h

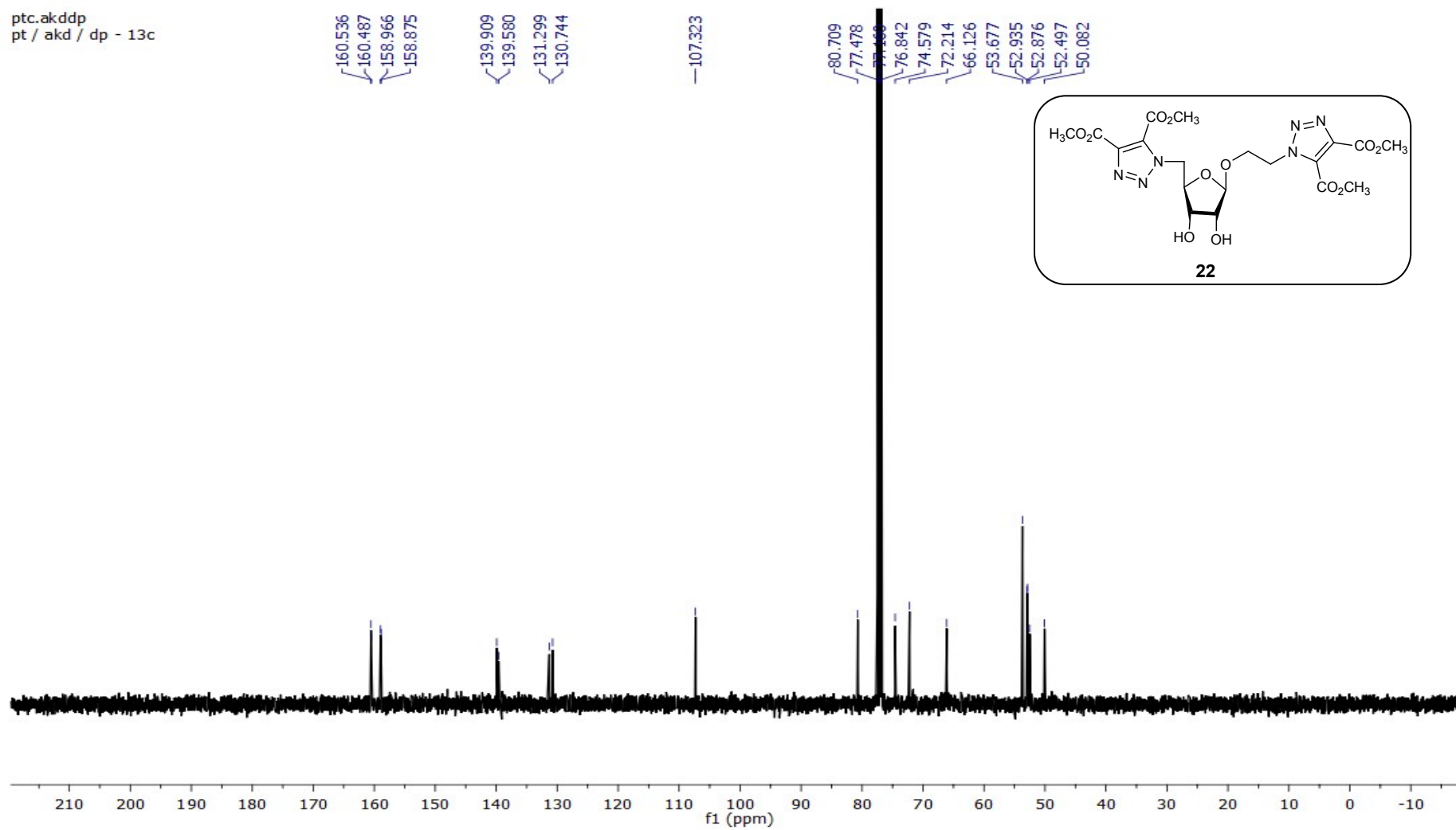
7.260

4.866
4.856
4.831
4.821
4.766
4.751
4.742
4.701
4.686
4.666
4.651
4.275
4.259
4.247
4.231
4.131
4.120
4.102
4.085
4.066
4.054
4.040
4.027
4.016
3.964
3.961
3.940
3.915
3.829
3.818
3.695
3.681
3.667
3.654
3.640



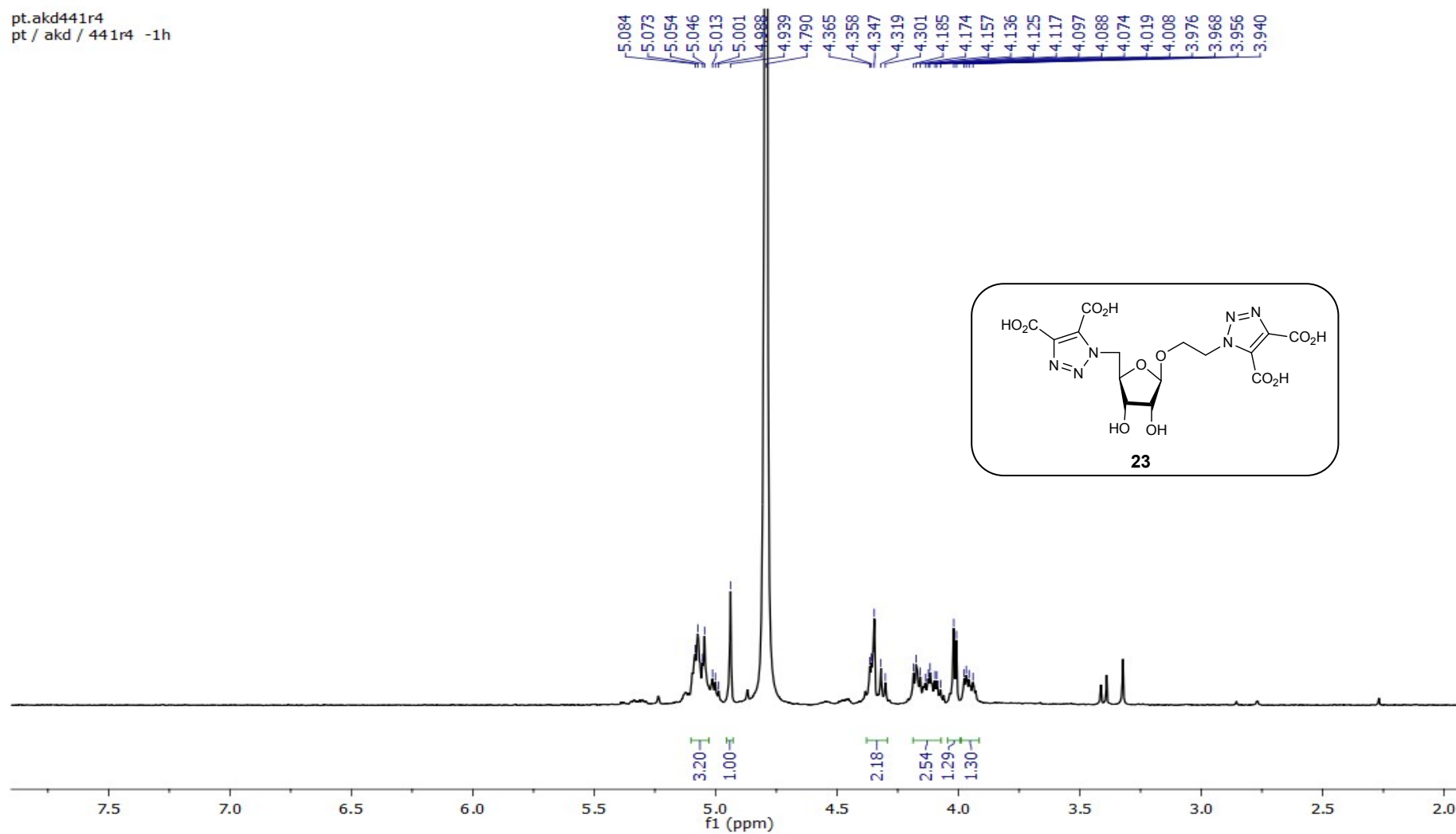
¹³C -NMR spectra of compound **22**

ptc.akddp
pt / akd / dp - 13c



¹H -NMR spectra of compound **23**

pt.akd441r4
pt / akd / 441r4 -1h



^{13}C -NMR spectra of compound **23**

ptc.akd441r4
pt / akd / 441-r4 - 13c

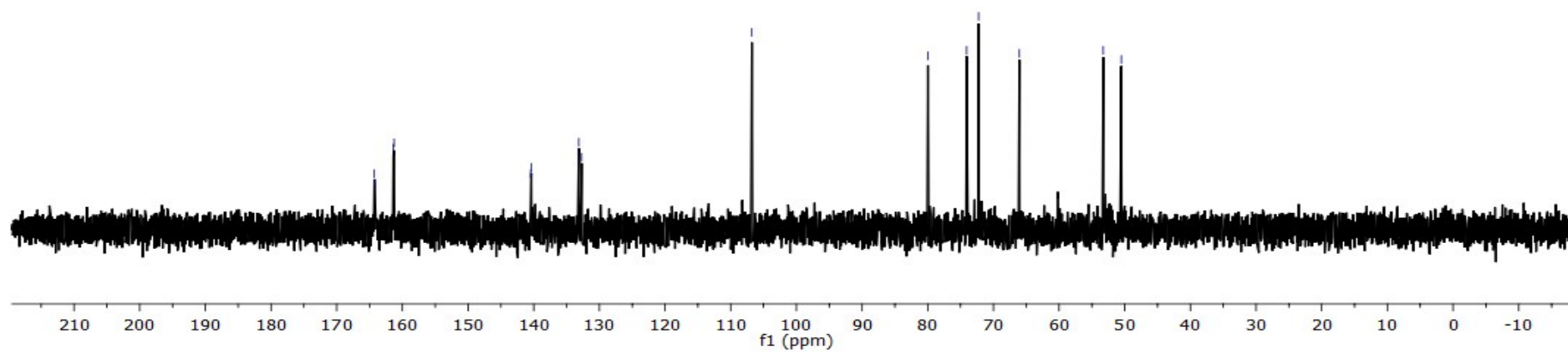
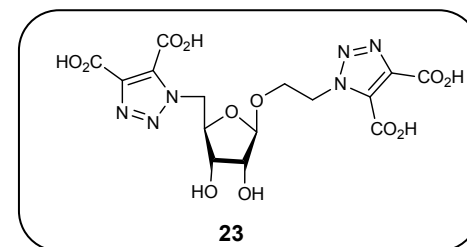
164.273
164.196
161.383
161.264

140.457
140.364
133.131
132.700

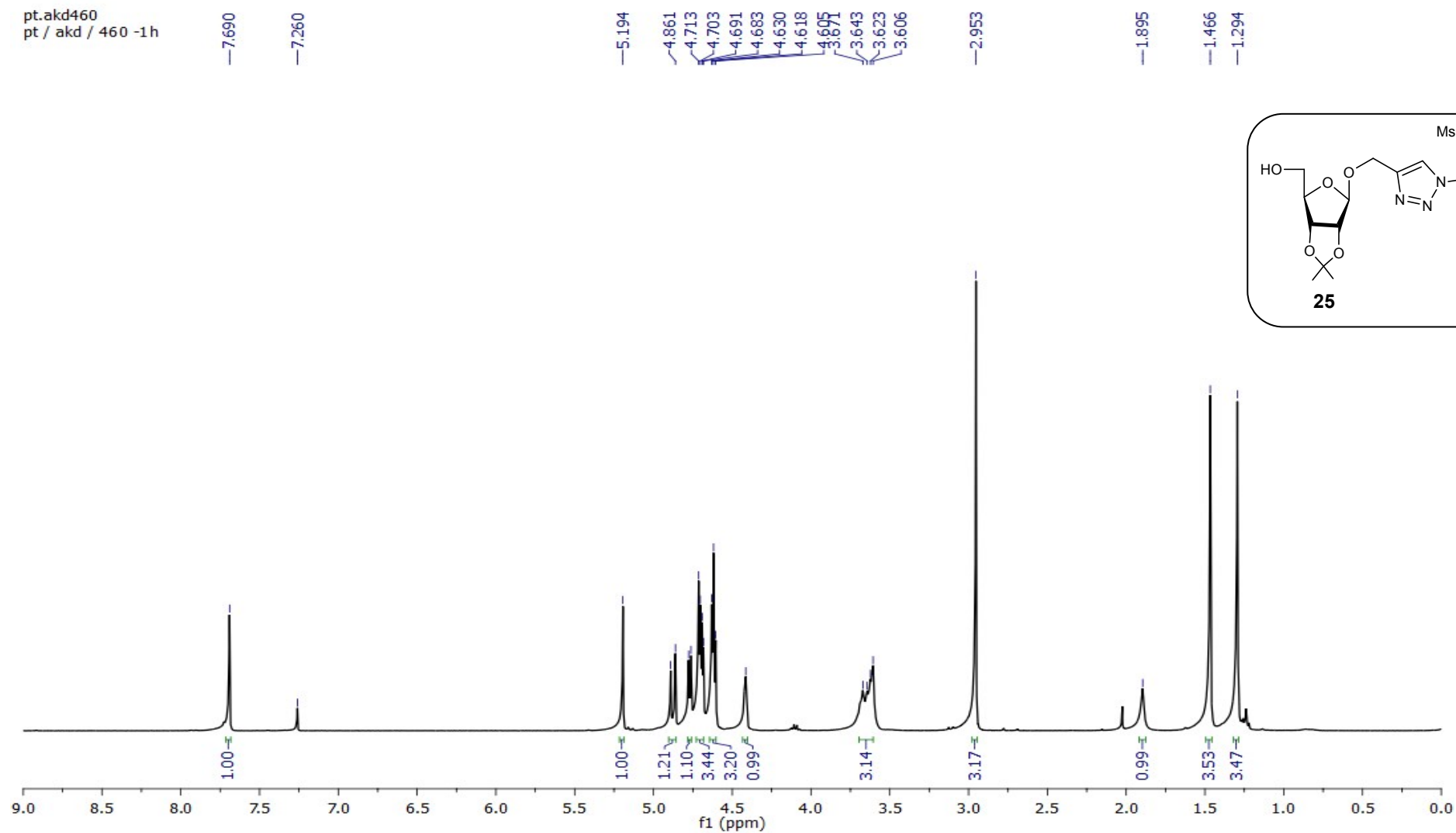
106.776

79.966
74.071
72.249
66.051

53.277
50.525



¹H -NMR spectra of compound **25**



^{13}C -NMR spectra of compound **25**

pt.akd460p
pt.akd460p-13c-500mhz

—144.305

—124.073

—112.329

—108.421

88.551

85.903

81.508

77.415

77.160

76.906

67.179

63.783

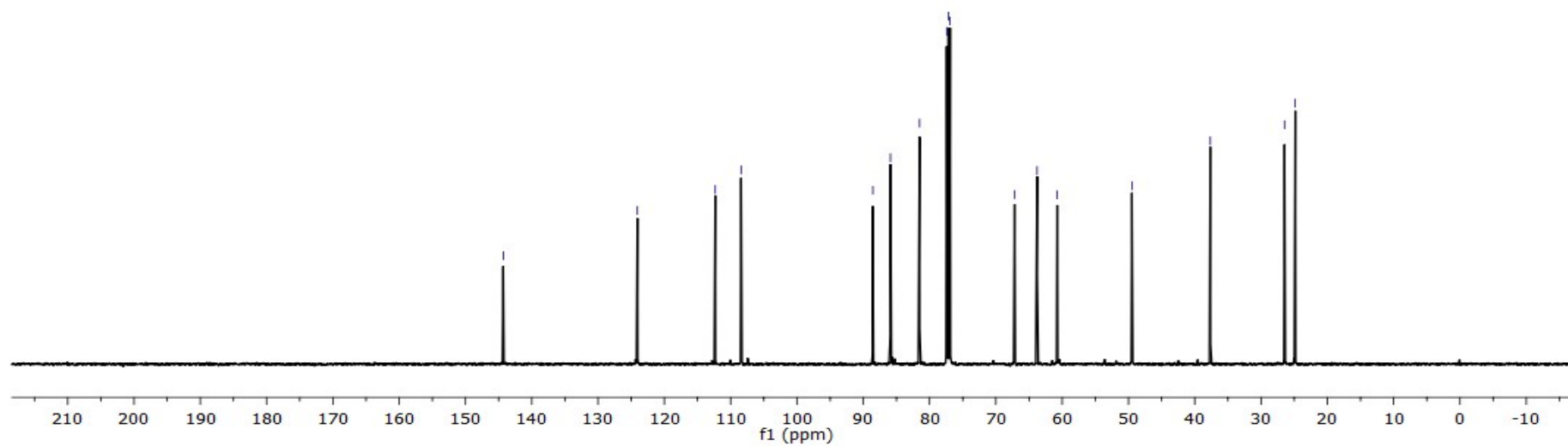
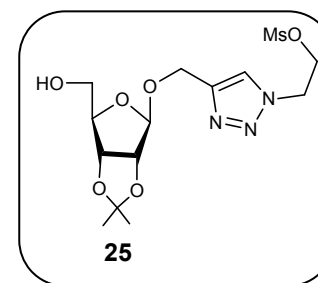
60.741

—49.485

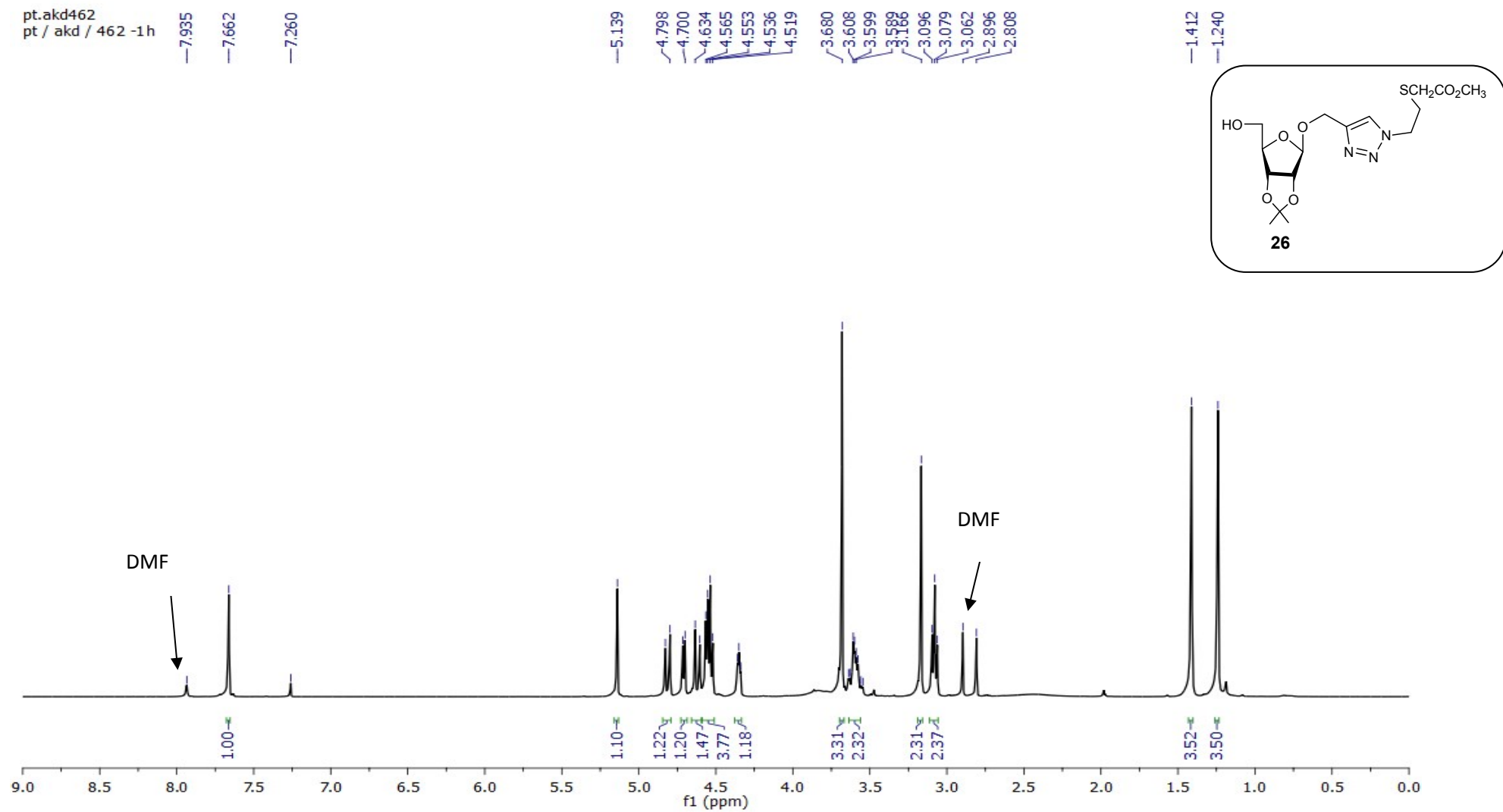
—37.654

26.464

24.843



¹H -NMR spectra of compound **26**



¹³C -NMR spectra of compound **26**

ptc.akd462
ptc / akd / 462 - 13c

—170.572

—143.713

—123.447

—112.135

—108.121

88.341

85.736

81.399

77.478

77.160

76.841

63.607

60.543

52.593

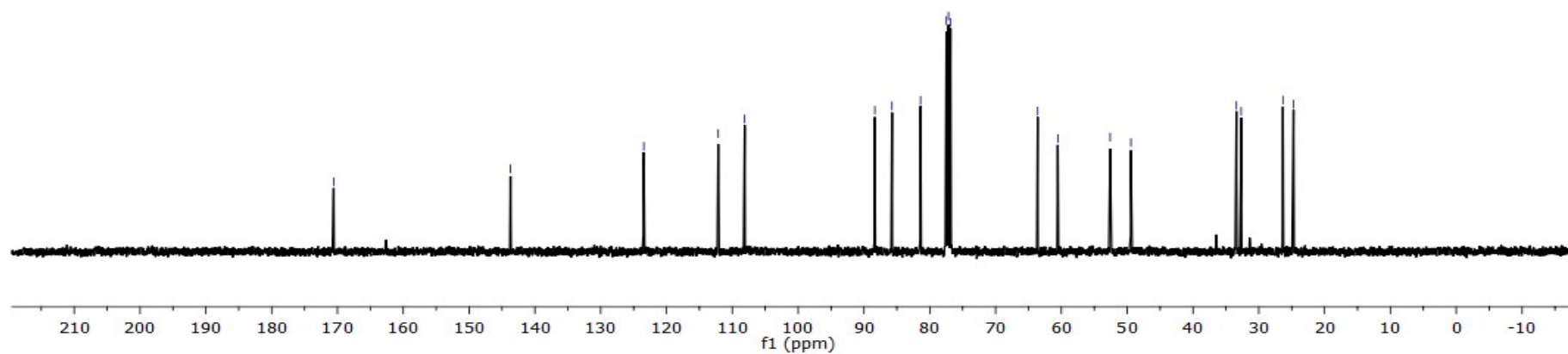
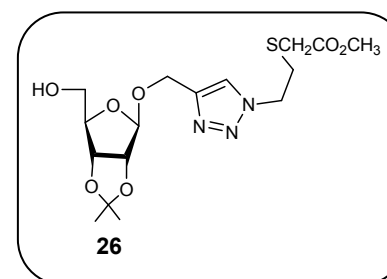
49.430

33.406

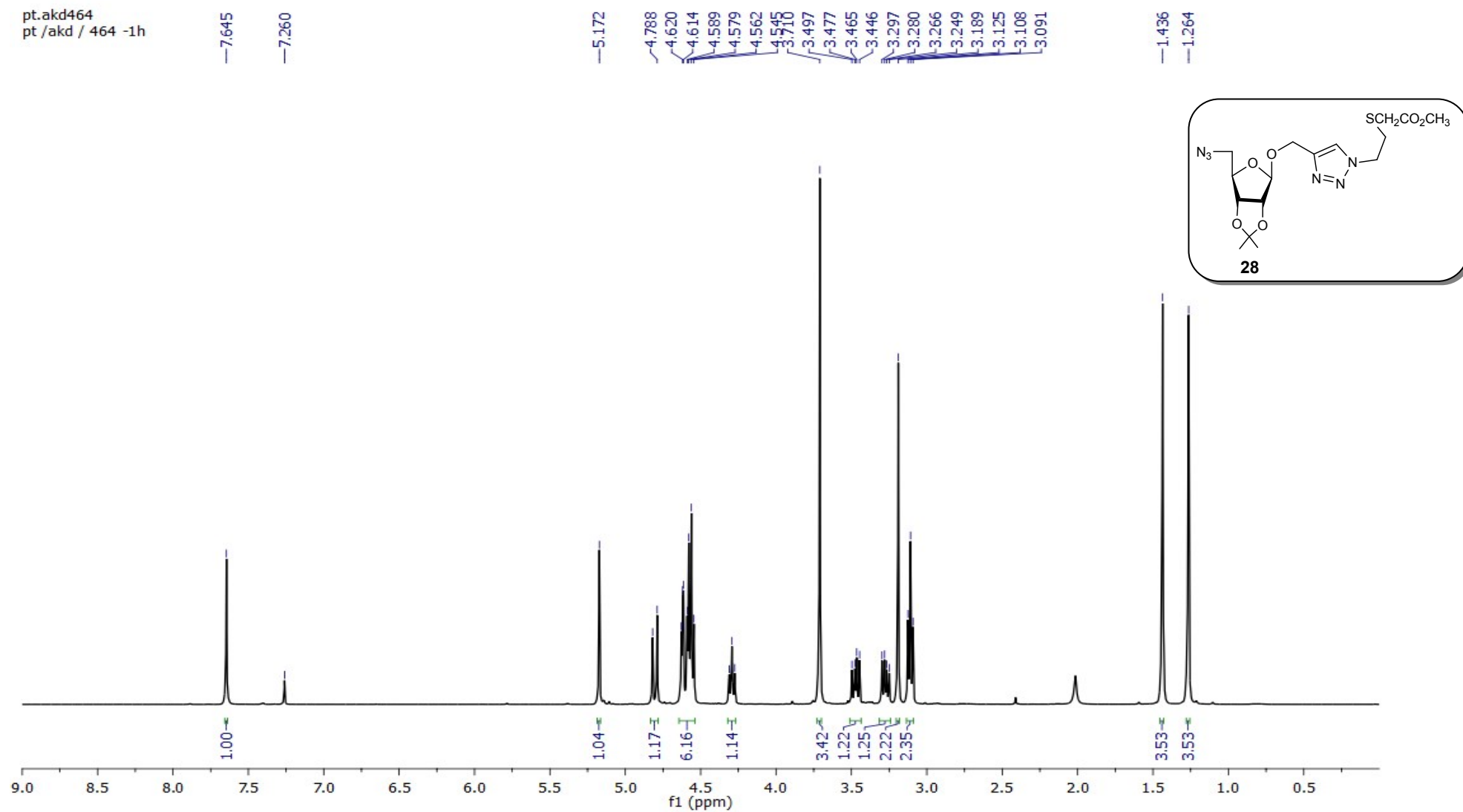
32.685

26.332

24.721

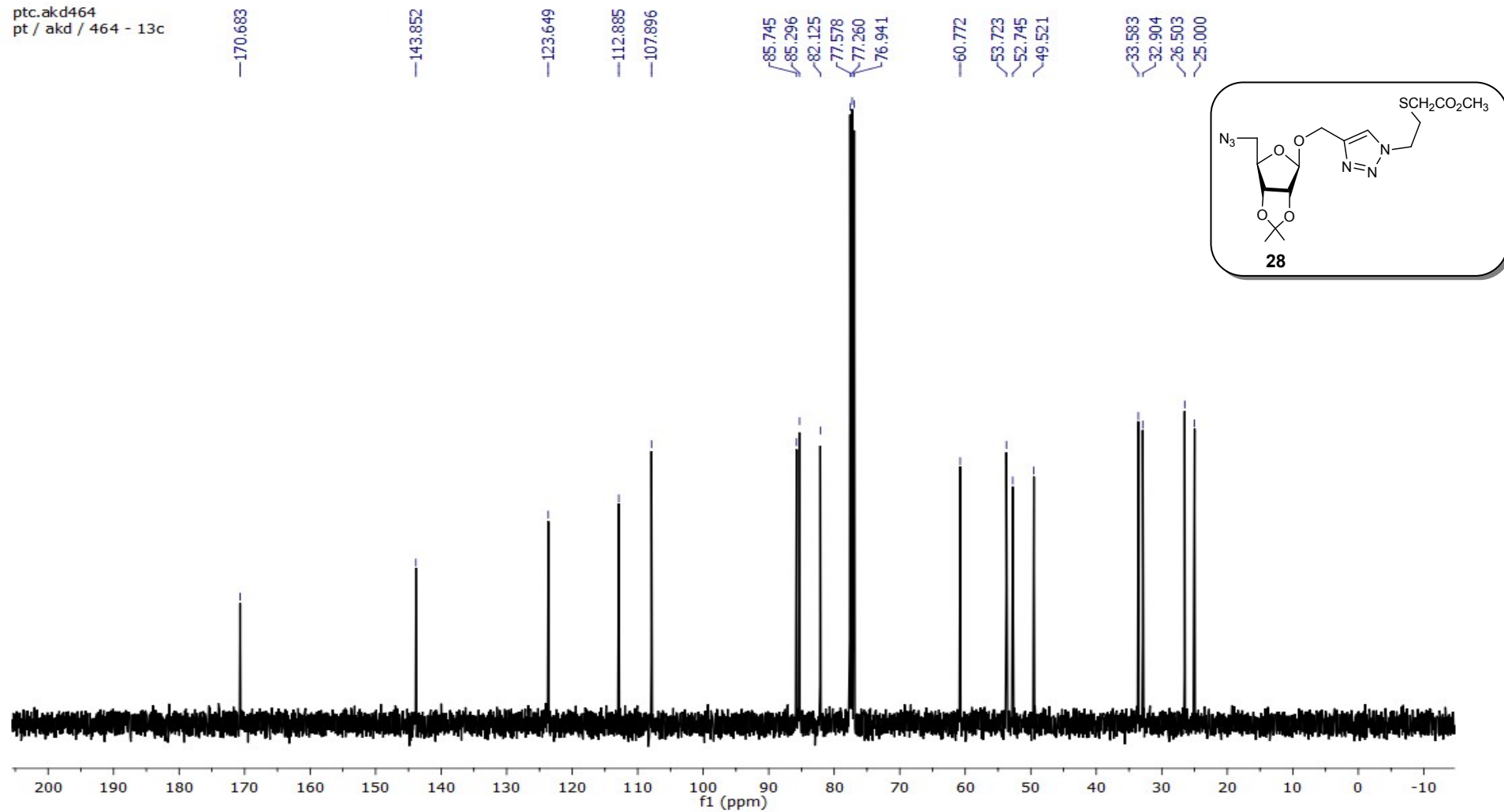


¹H -NMR spectra of compound **28**

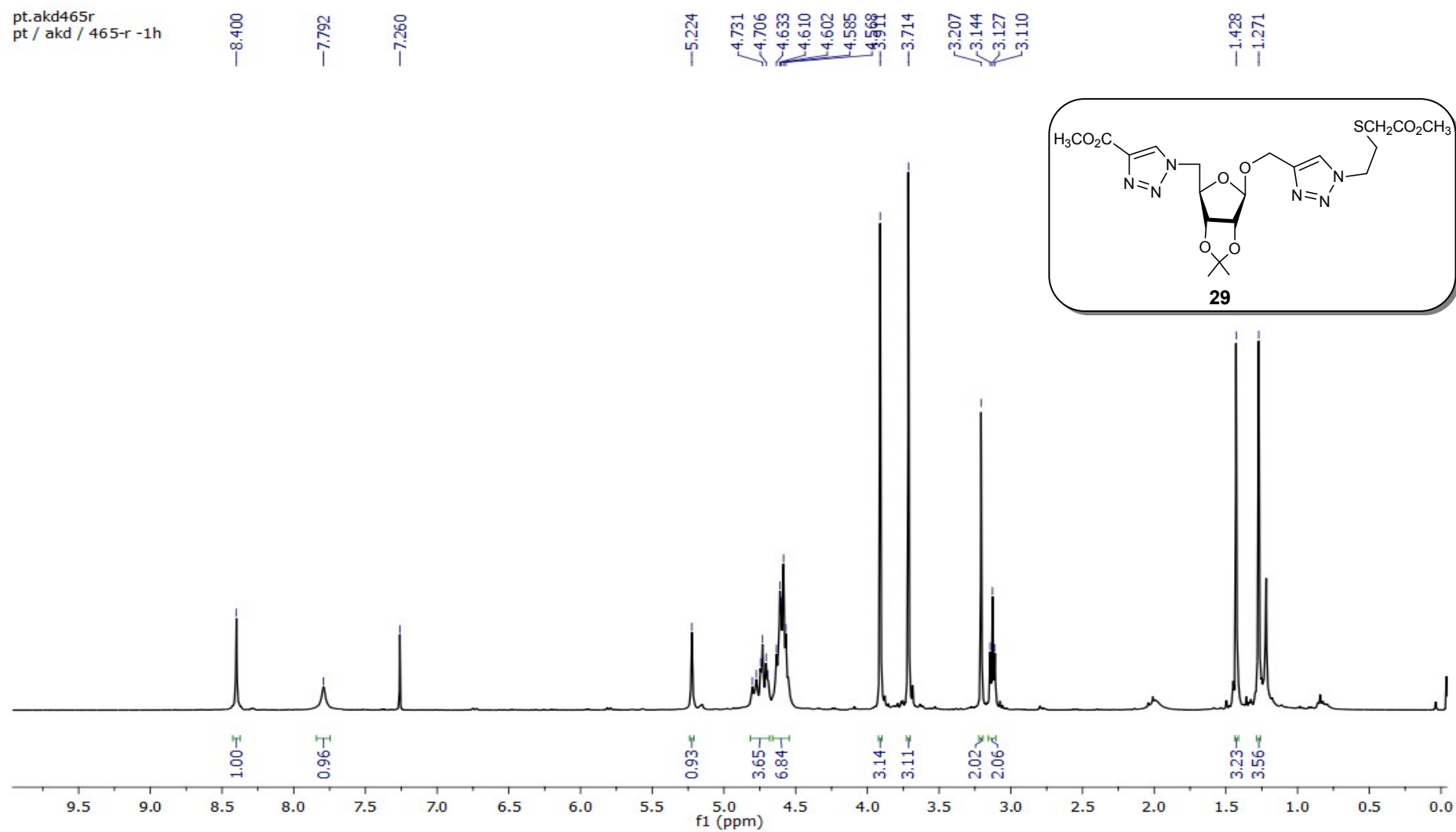


^{13}C -NMR spectra of compound **28**

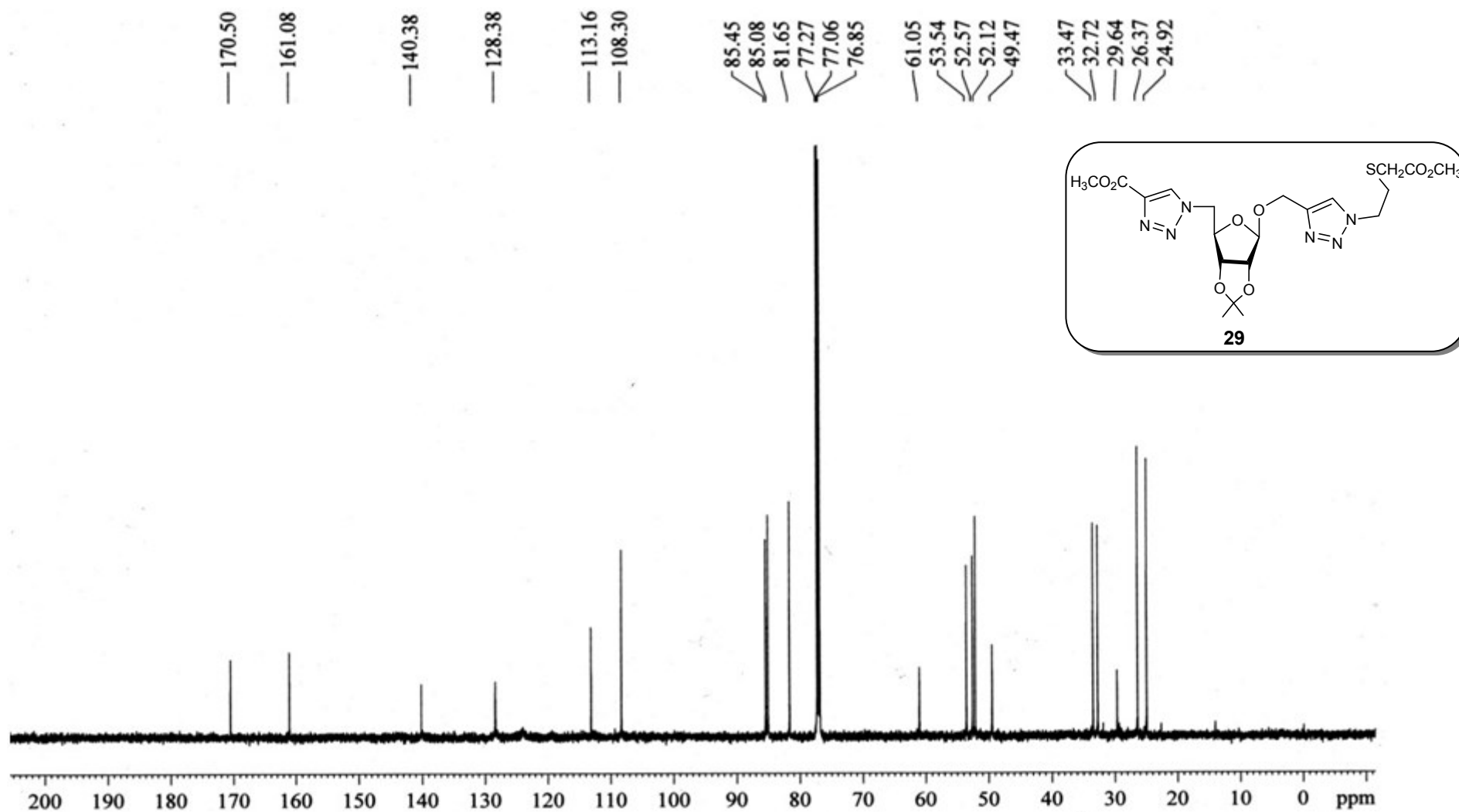
ptc.akd464
pt / akd / 464 - 13c



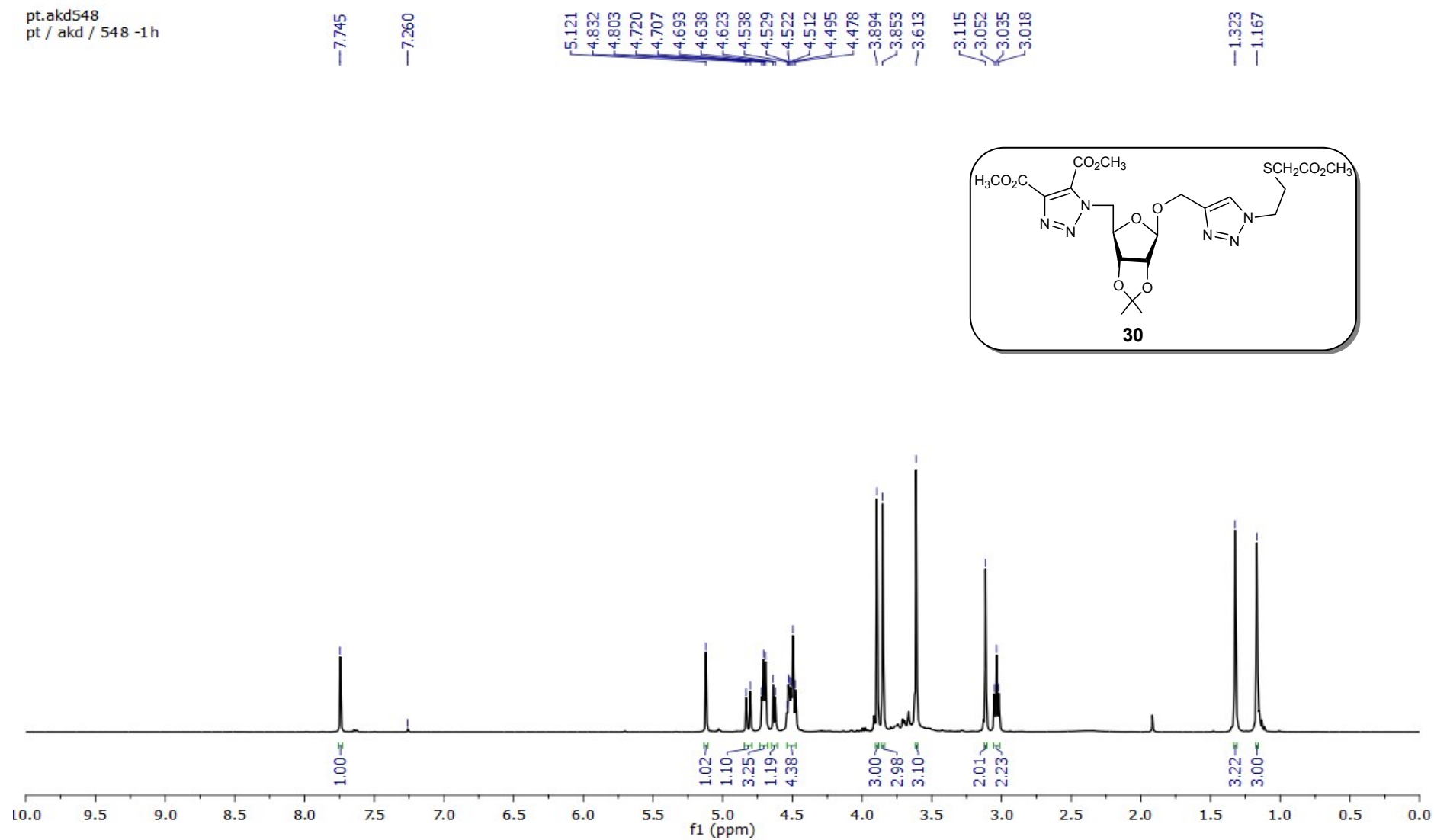
¹H -NMR spectra of compound **29**



^{13}C -NMR spectra of compound **29**



¹H -NMR spectra of compound **30**



¹³C -NMR spectra of compound **30**

pt.akd548
pt / akd / 548- 13C-500MHz

170.371

160.279

158.547

143.477

140.203

129.537

123.839

112.725

108.016

84.999

84.761

81.449

77.416

77.160

76.905

60.821

53.434

53.131

52.592

52.385

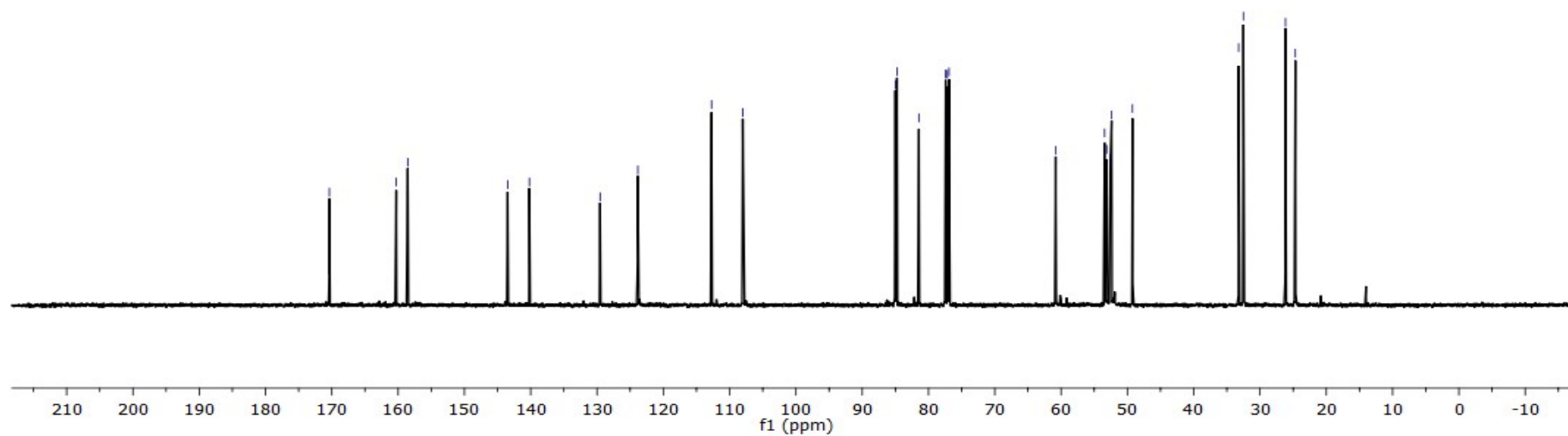
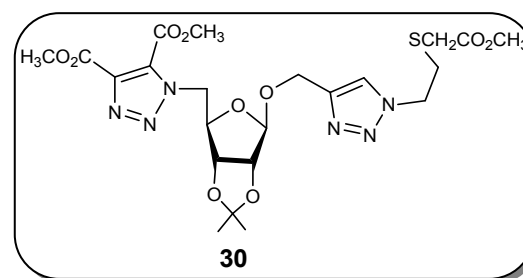
49.238

33.222

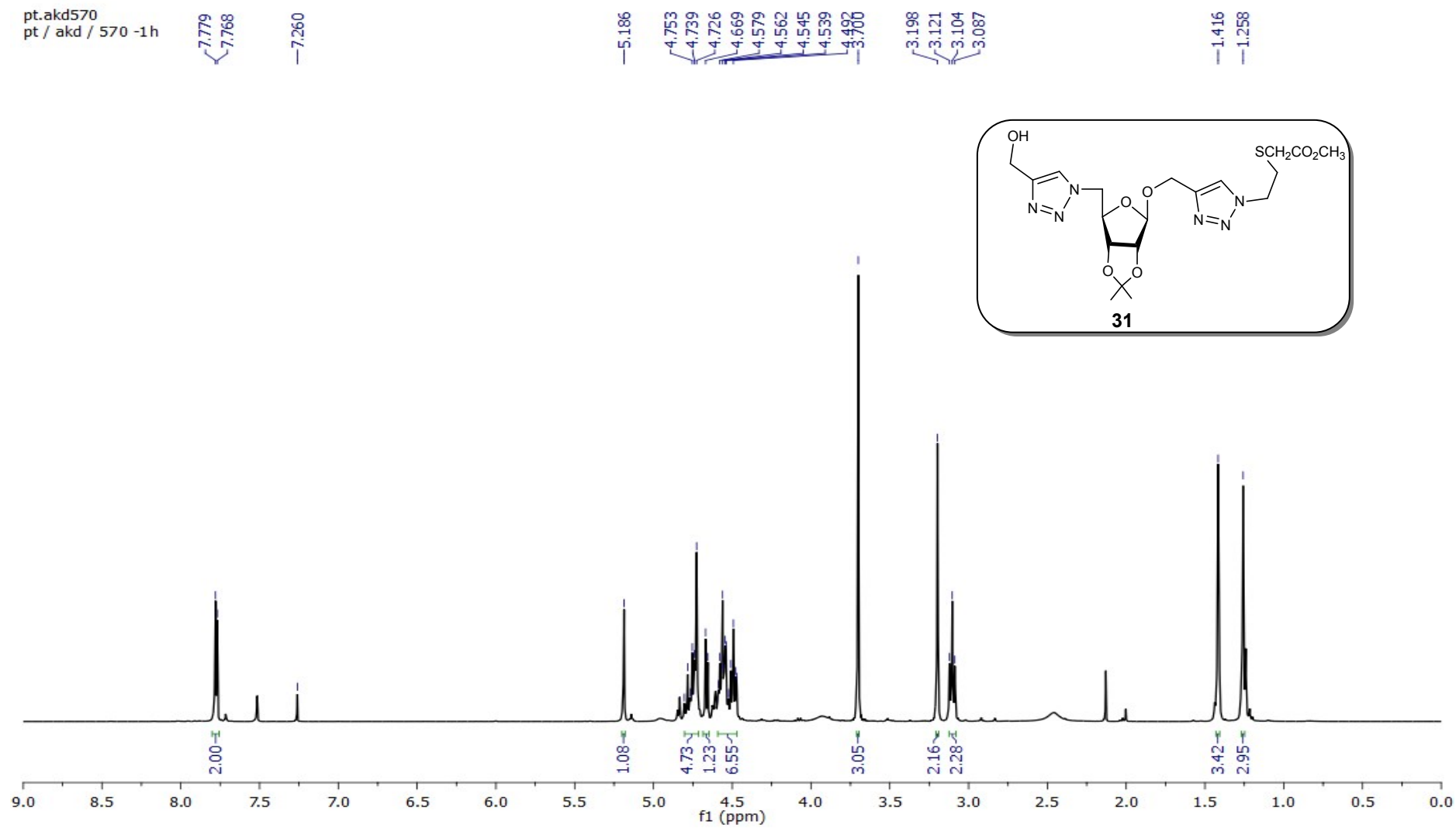
32.509

26.155

24.666

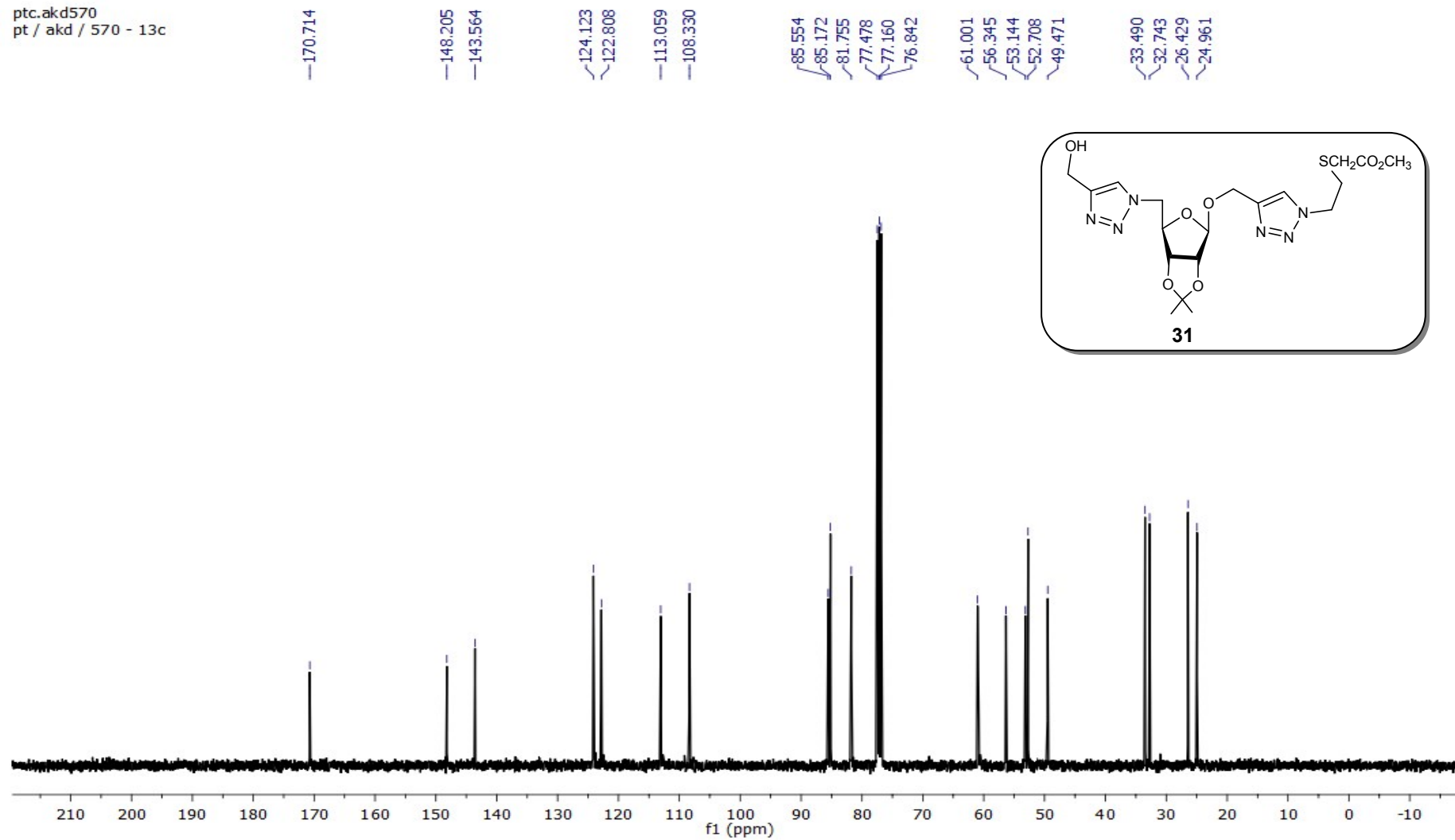


¹H -NMR spectra of compound **31**

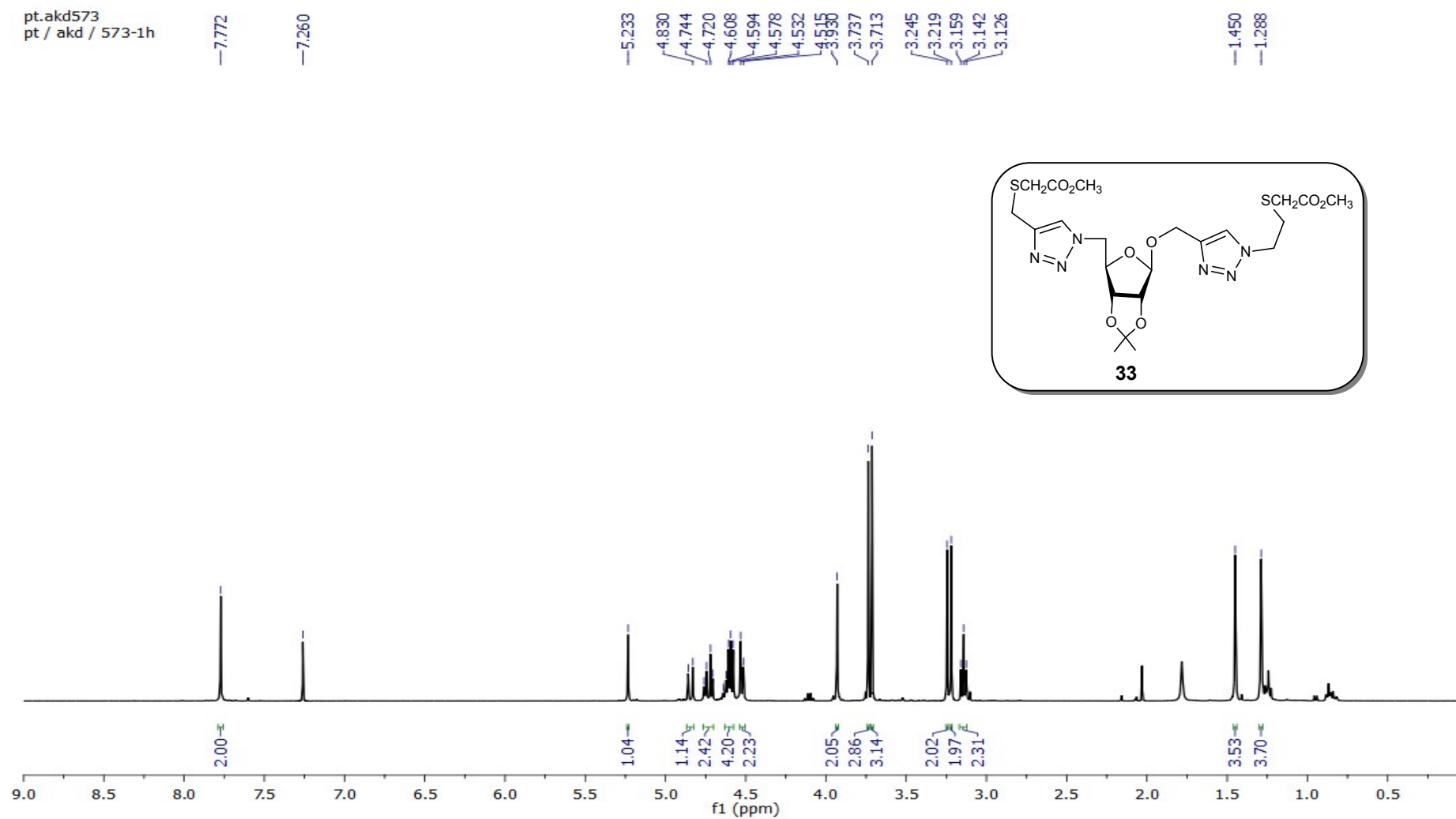


^{13}C -NMR spectra of compound **31**

ptc.akd570
pt / akd / 570 - 13c

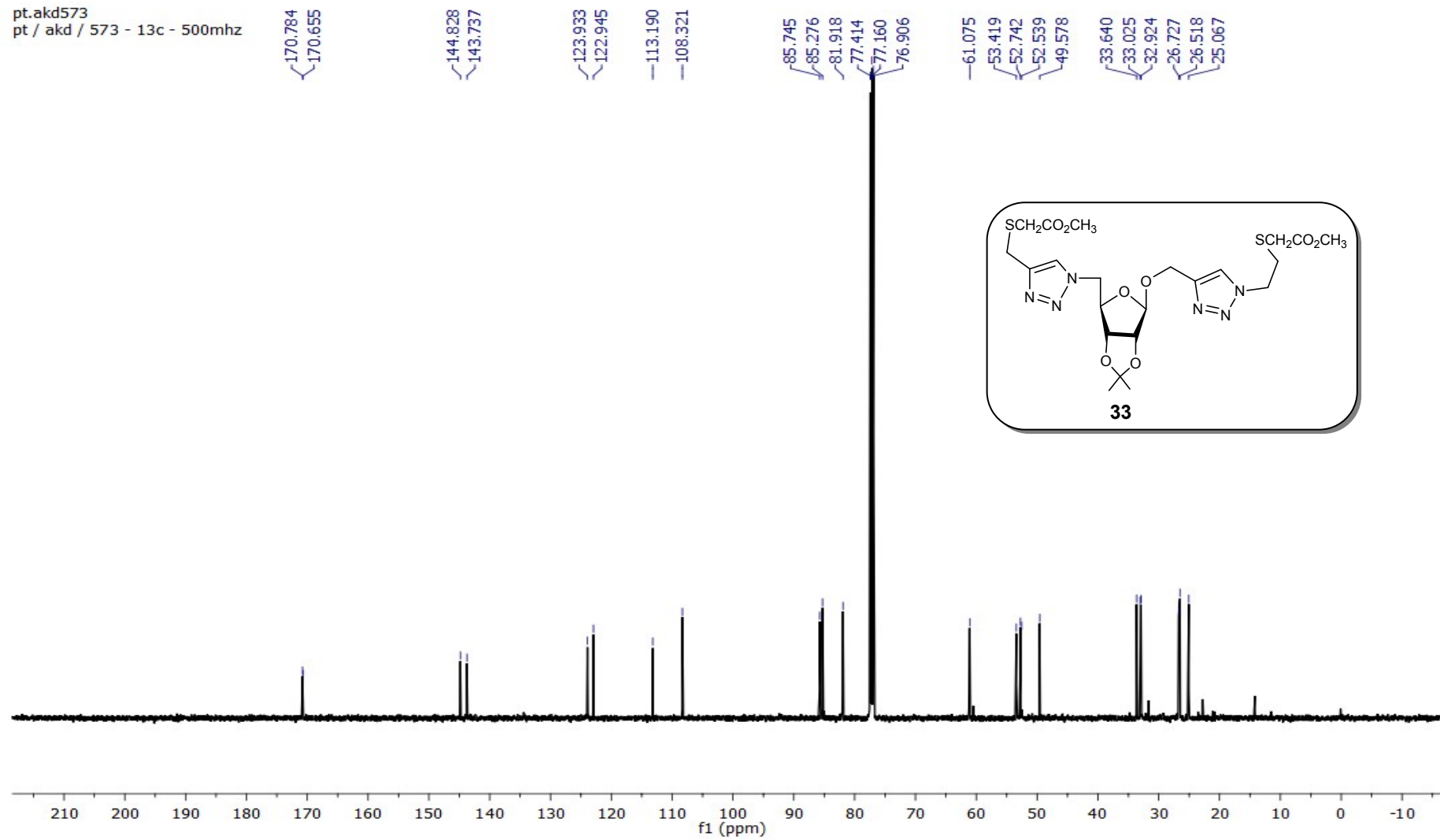


¹H -NMR spectra of compound **33**

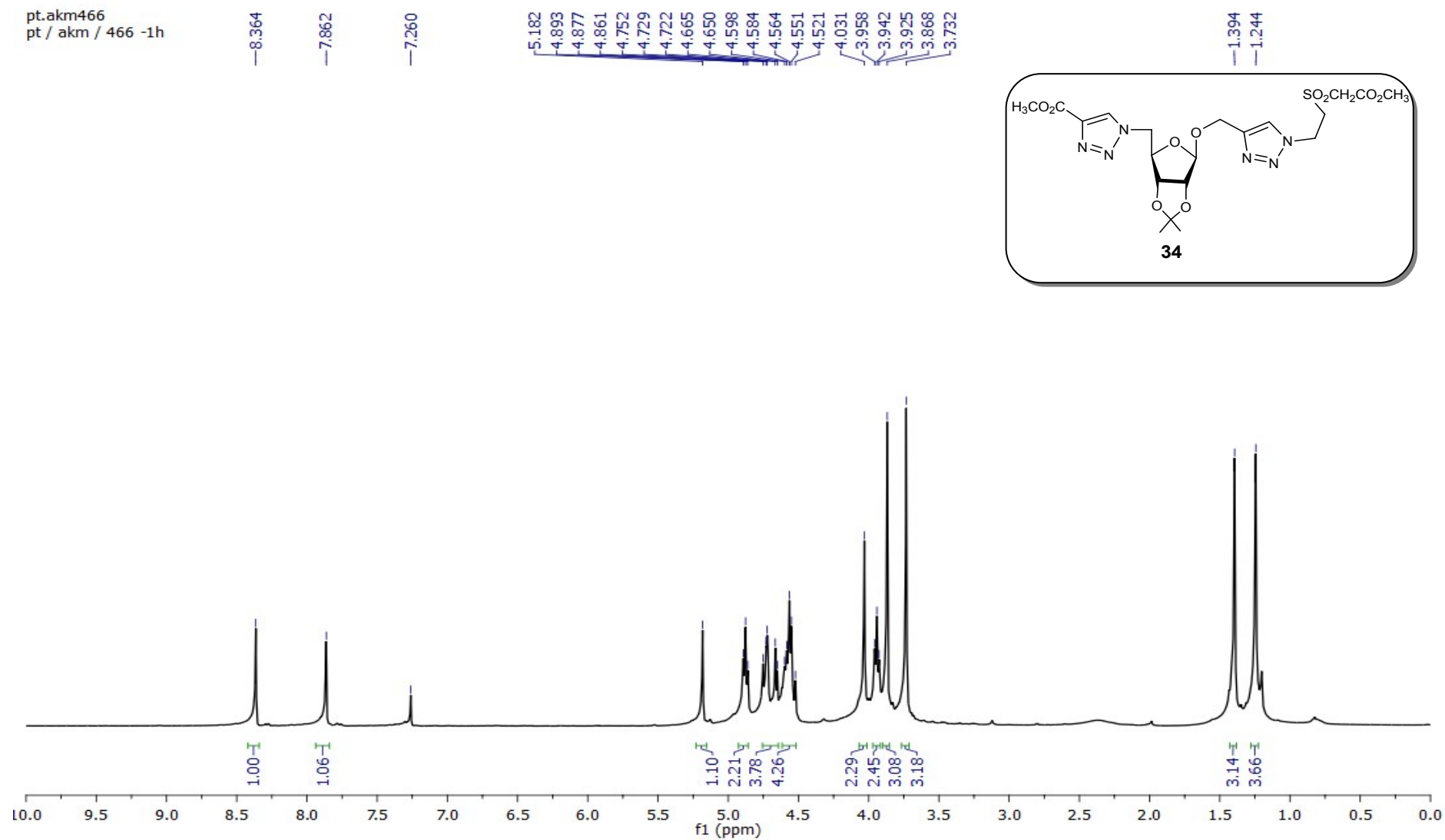


^{13}C -NMR spectra of compound **33**

pt.akd573
pt / akd / 573 - ^{13}C - 500mhz



¹H -NMR spectra of compound **34**



^{13}C -NMR spectra of compound **34**

ptc.akd466
pt / akd / 466 - 13c

163.290
161.164

143.931
139.949

128.521
124.697

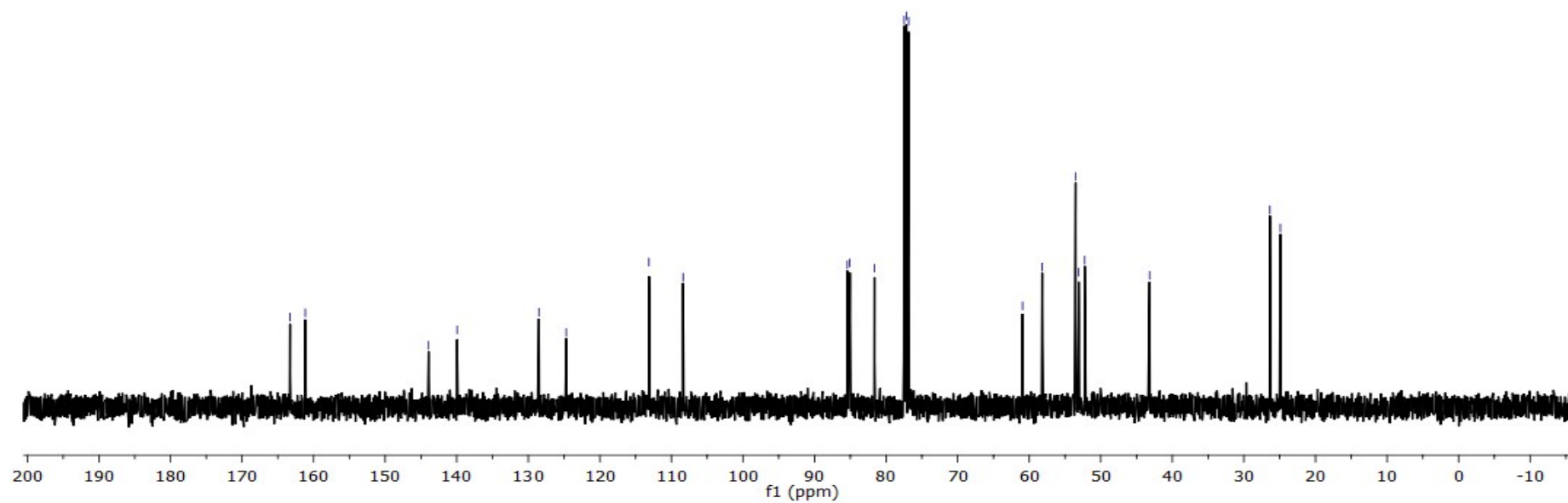
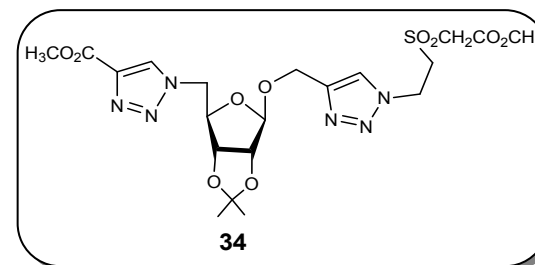
113.138
108.373

85.427
85.064
81.623
77.478
77.160
76.842

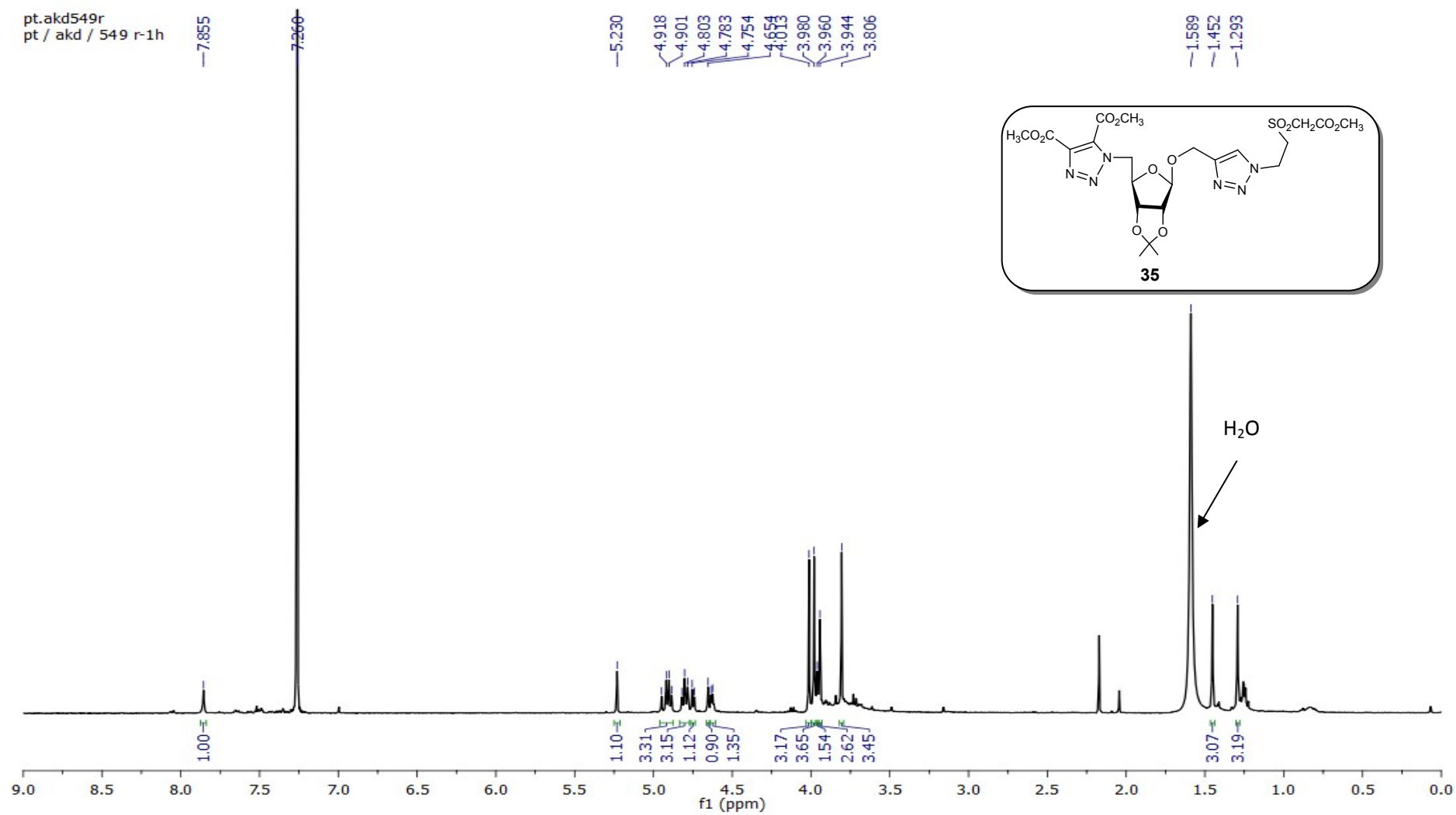
60.938
58.186
53.518
53.085
52.242

43.188

26.373
24.907



¹H -NMR spectra of compound **35**



^{13}C -NMR spectra of compound **35**

pt.akd549r

pt / akd / 549 r - 13c - 500mhz

~163.252
 ~160.555
 ~158.844

—144.385
—140.524

—129.753

—124.671

—113.122

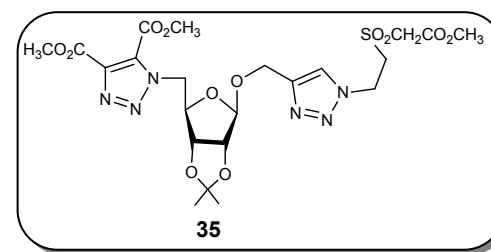
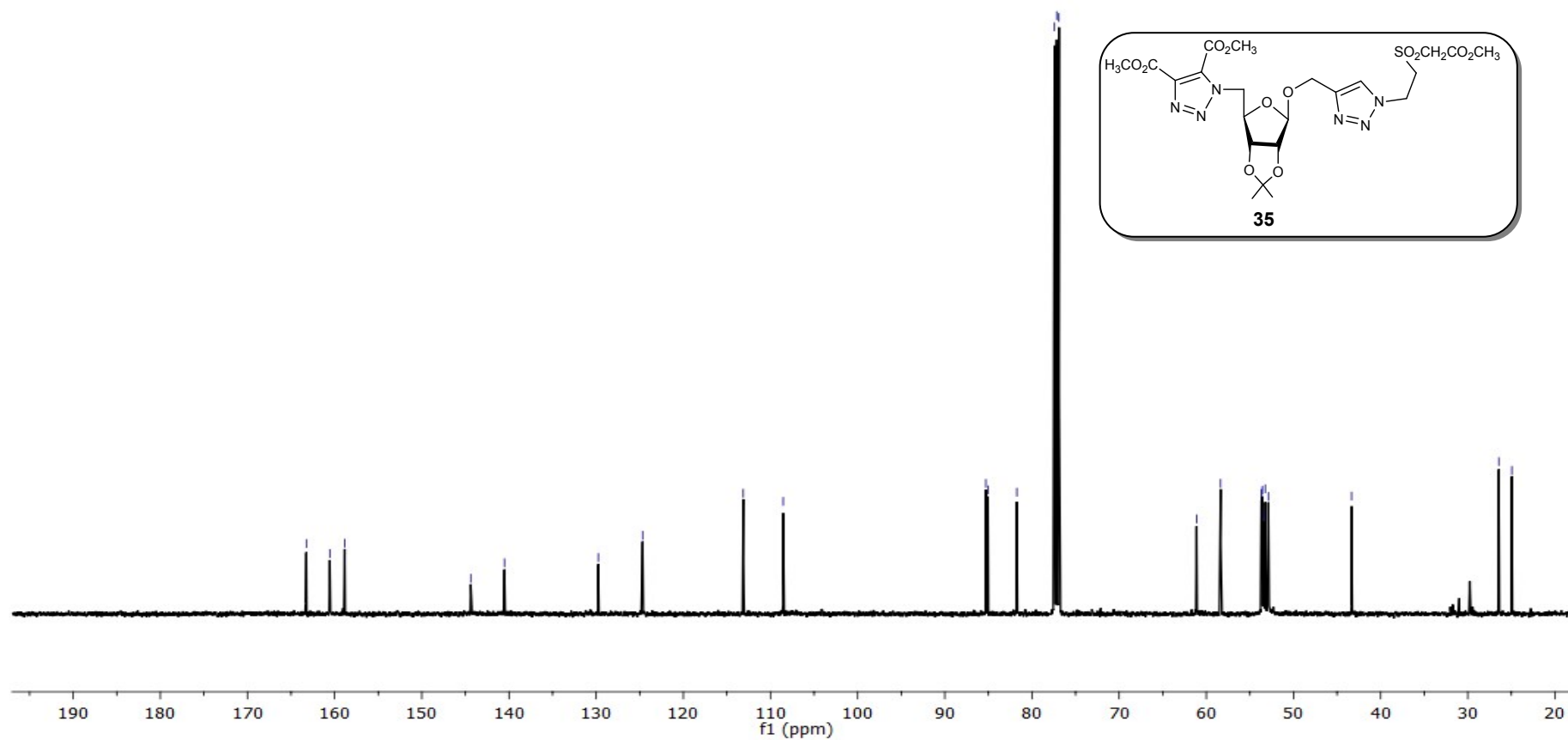
—108.541

85.288
85.059
81.734
77.415
77.160
76.906

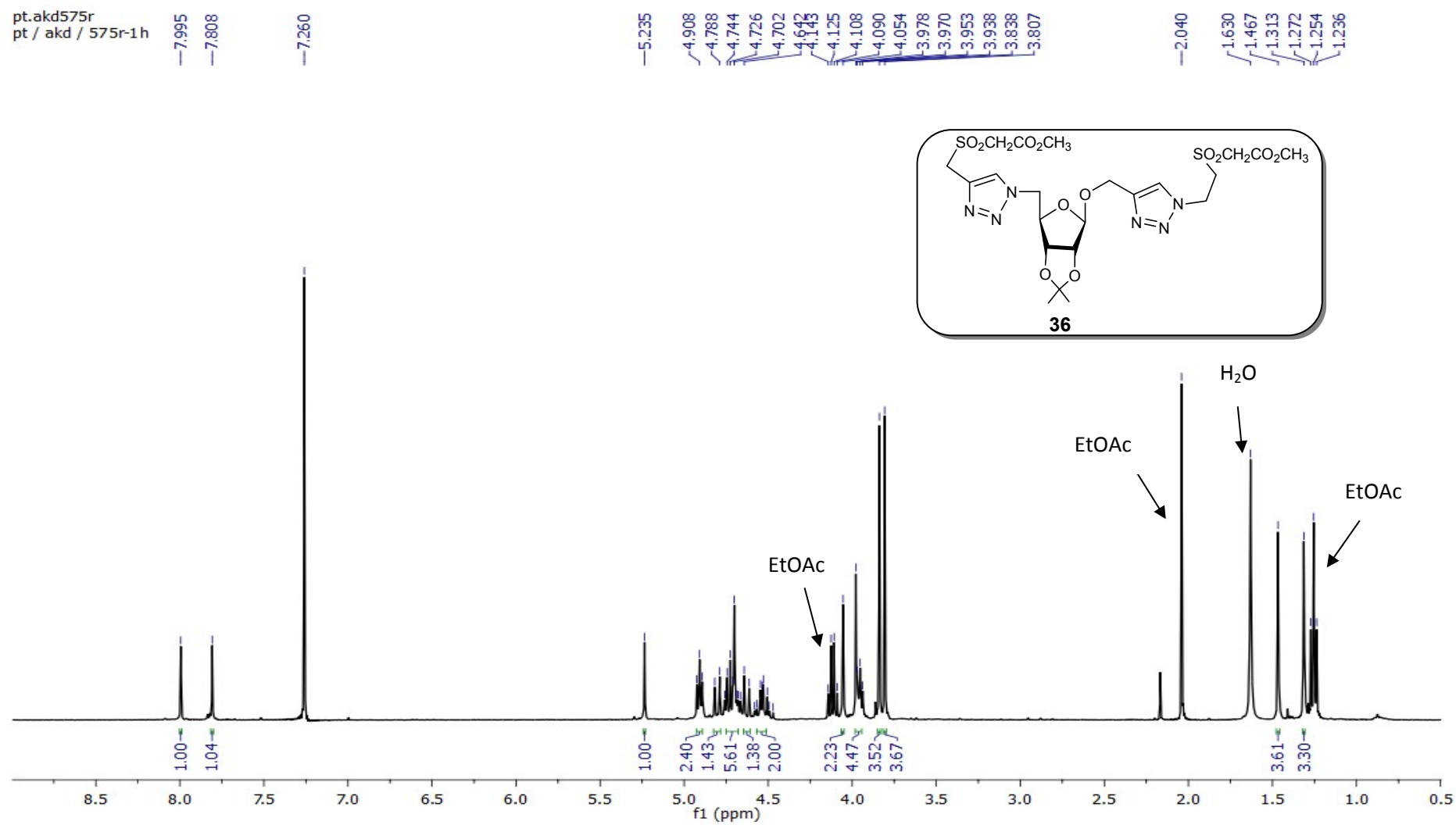
61.119
58.359
53.687
53.577
53.431
53.235
52.884

43.325

26.436
24.943

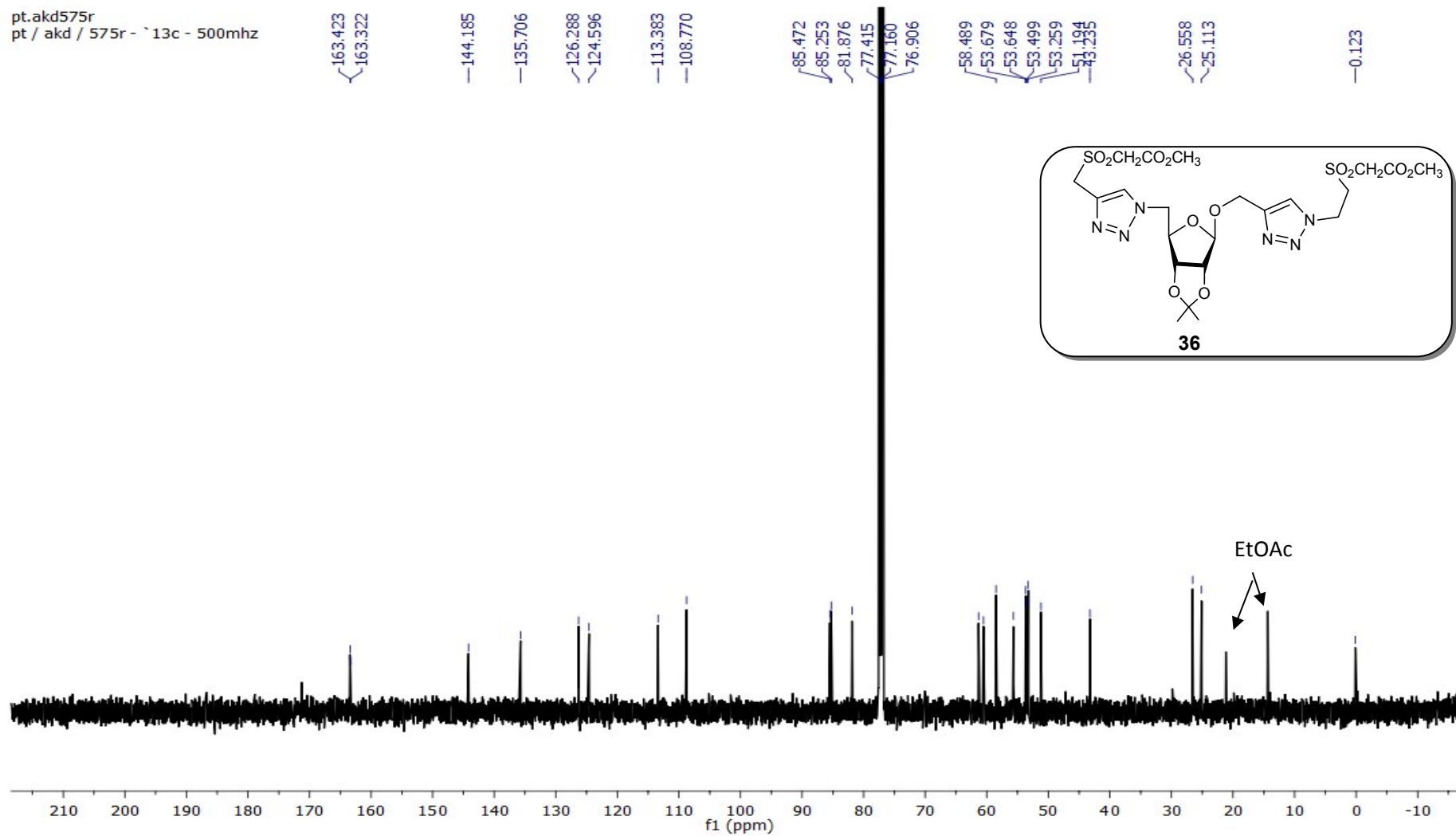


¹H -NMR spectra of compound **36**

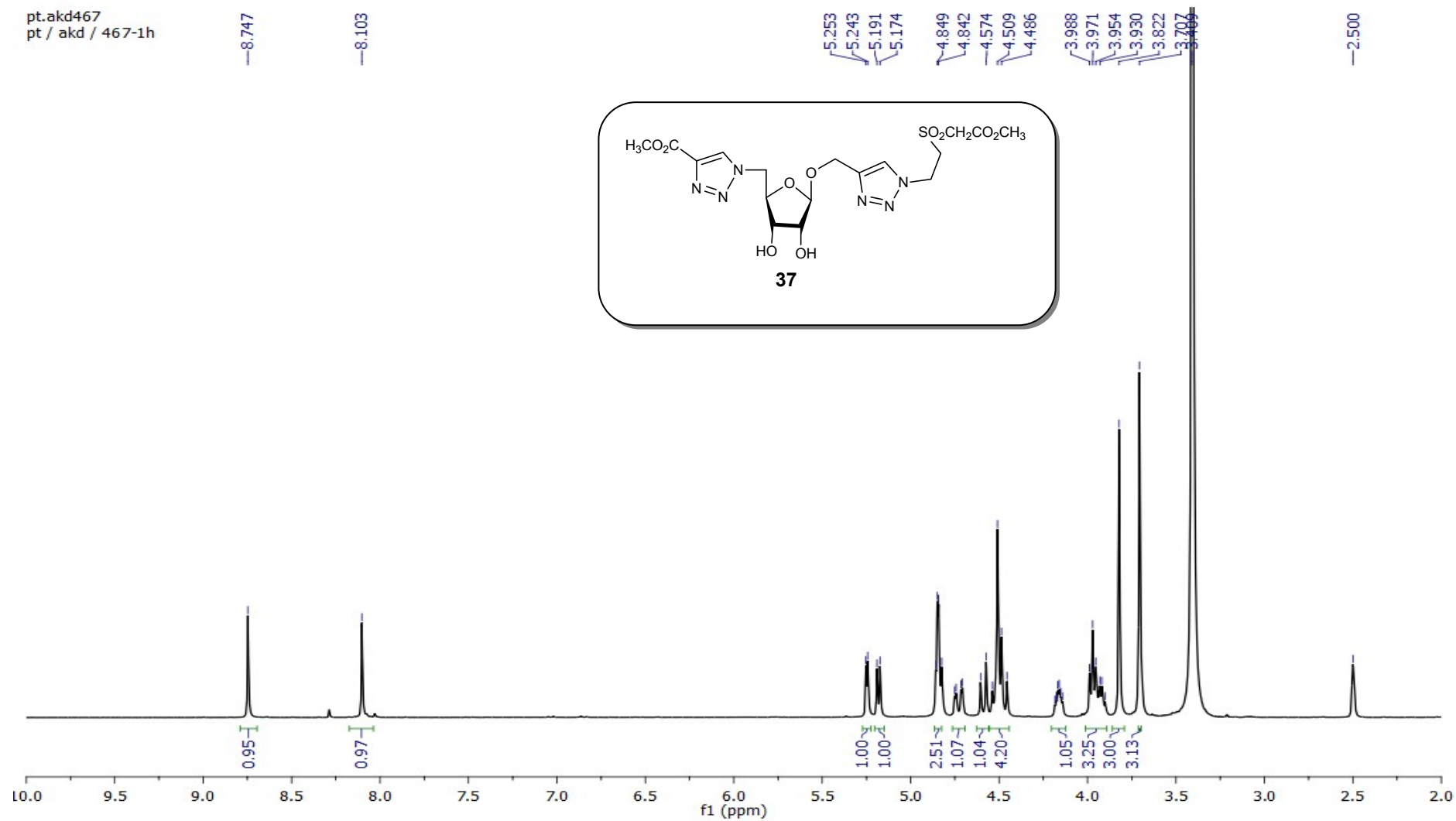


¹³C -NMR spectra of compound **36**

pt.akd575r
pt / akd / 575r - ¹³C - 500mhz

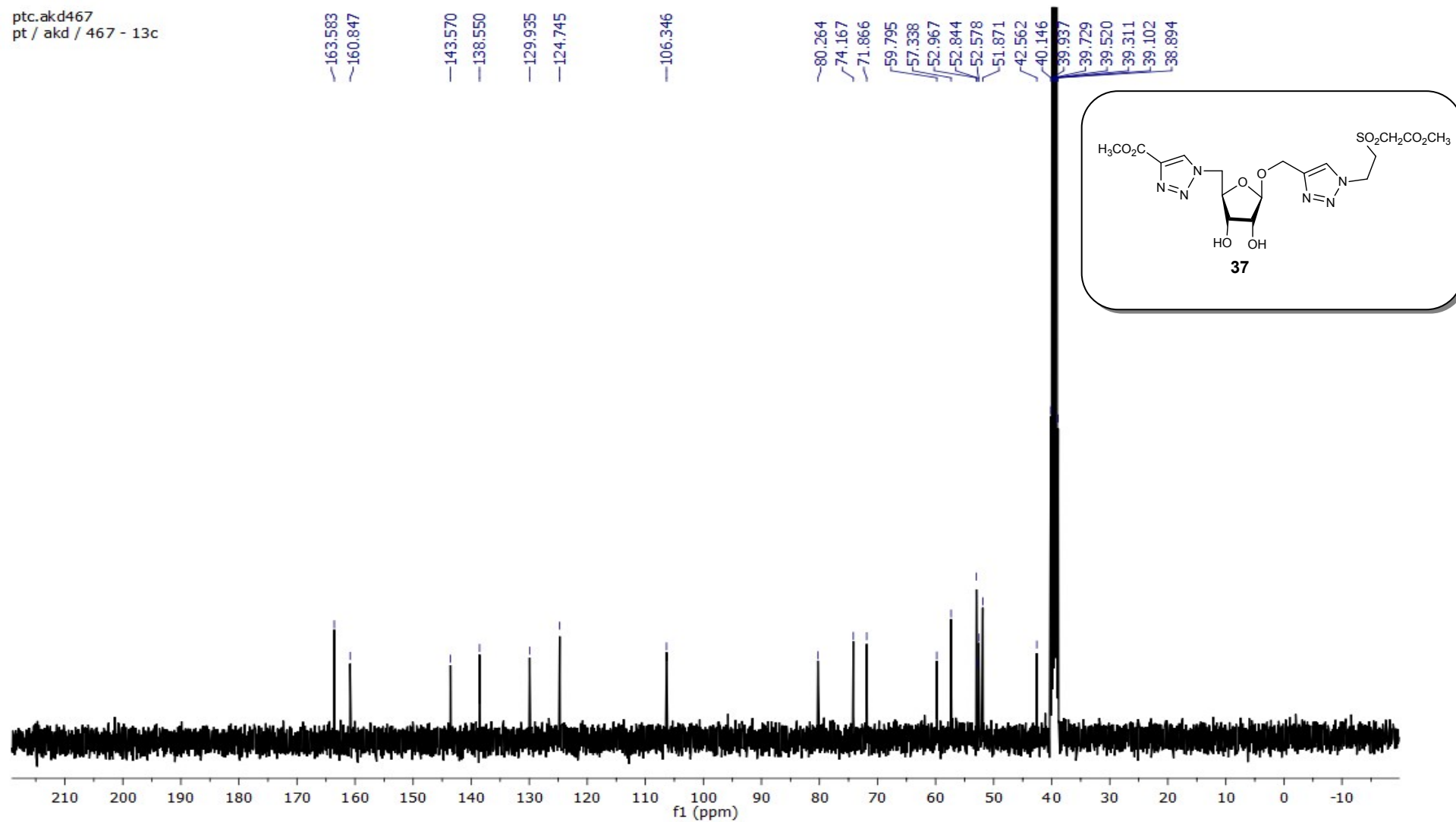


¹H -NMR spectra of compound **37**



^{13}C -NMR spectra of compound **37**

ptc.akd467
pt / akd / 467 - 13c



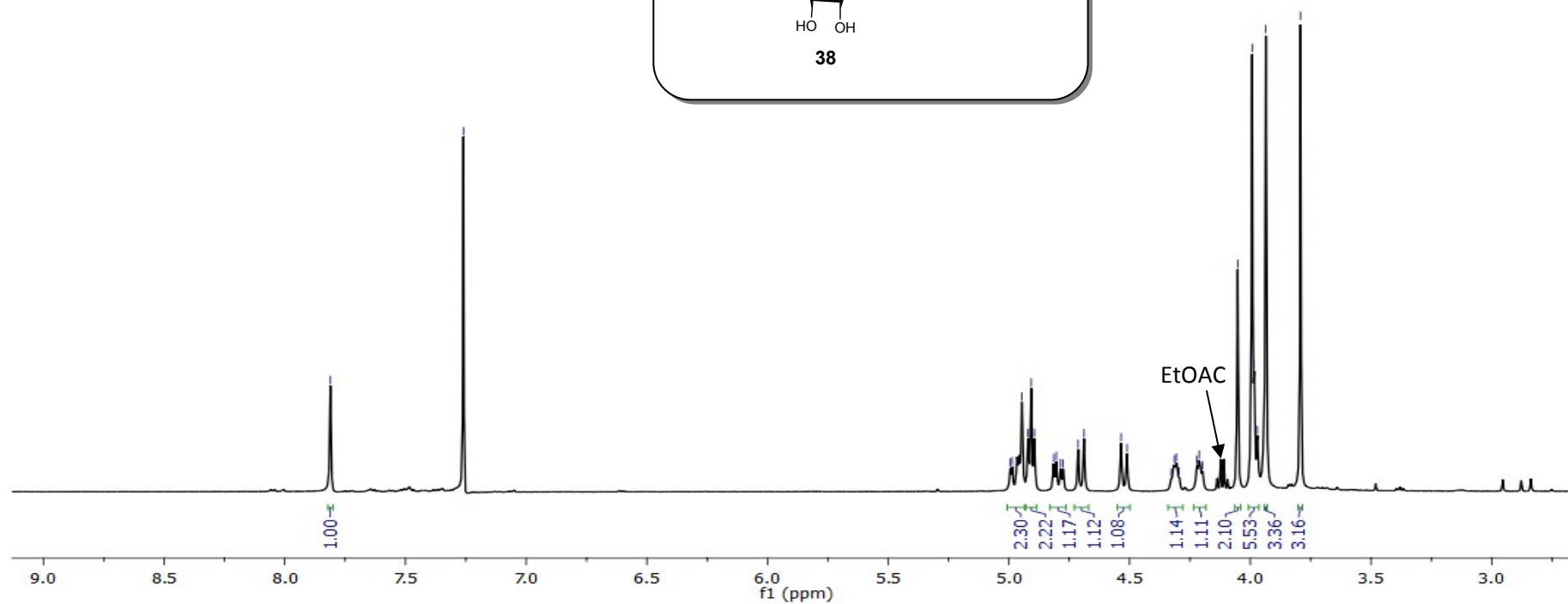
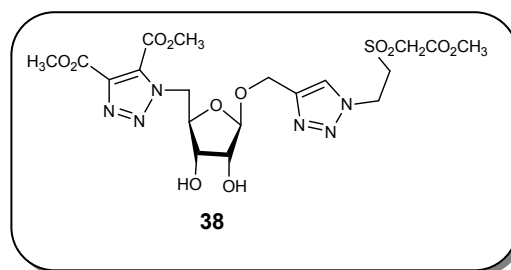
¹H -NMR spectra of compound **38**

pt.akd565
pt / akd / 565 - 1h - 500mhz

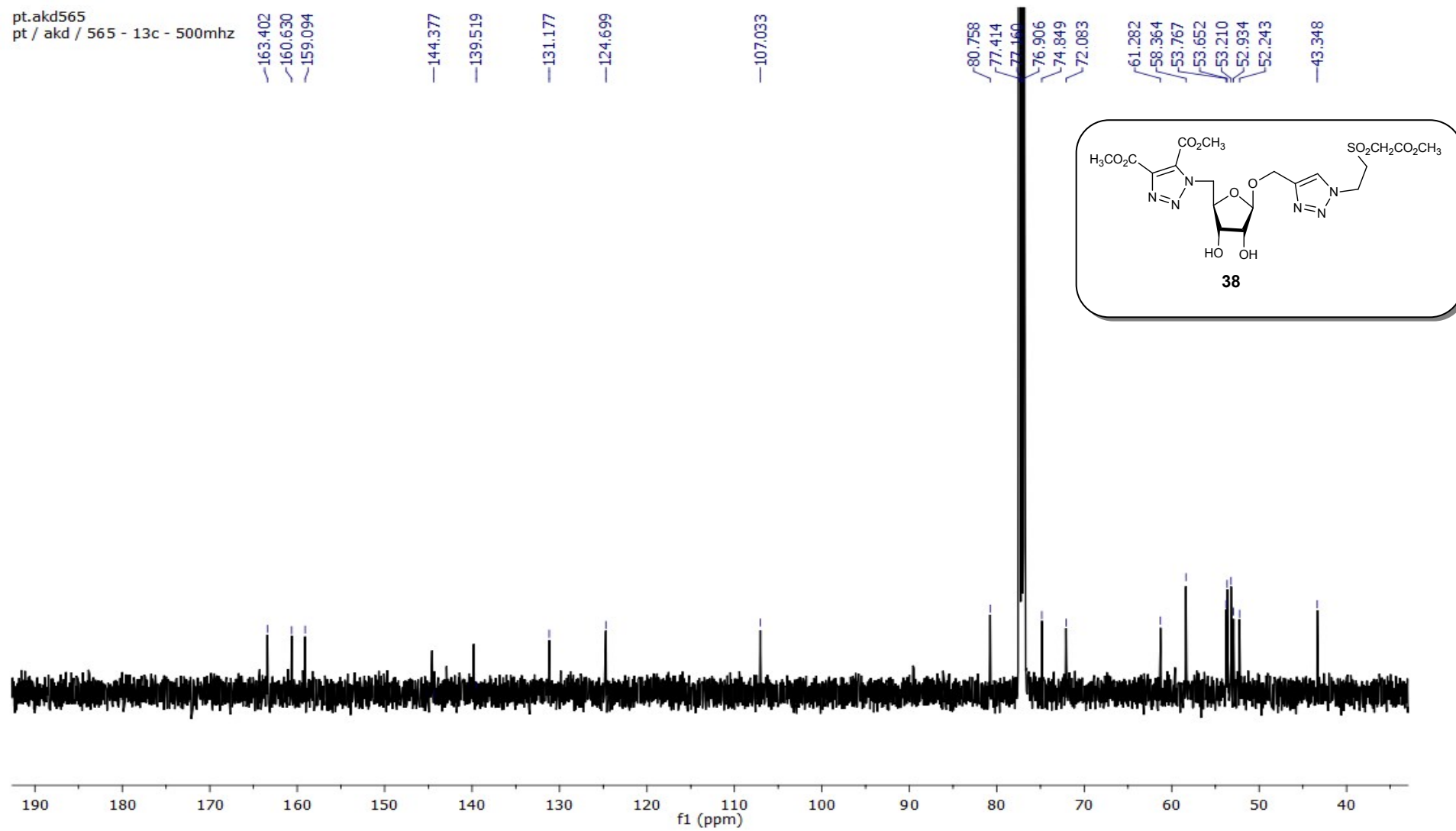
7.811

7.260

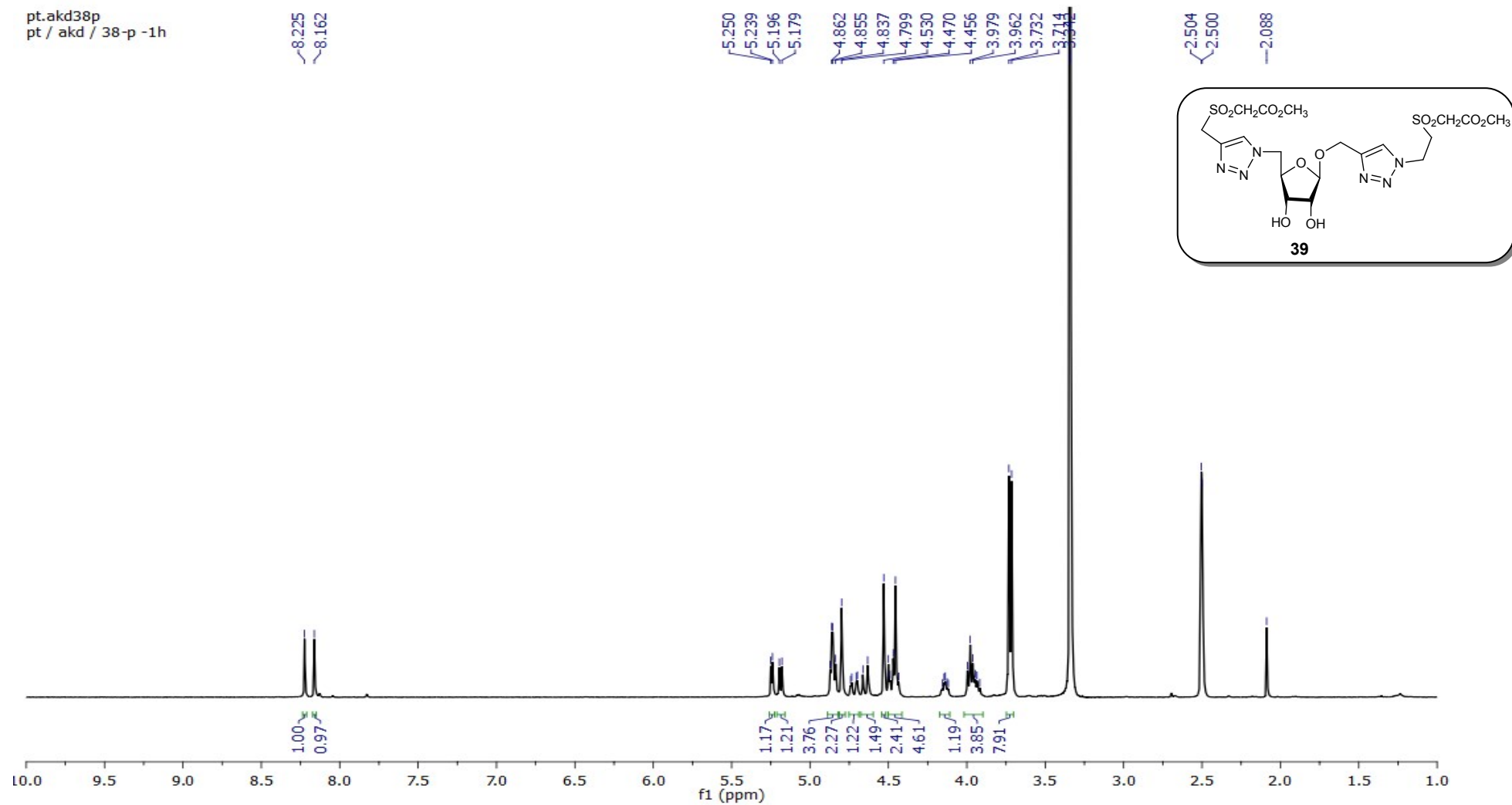
4.994
4.986
4.946
4.921
4.907
4.894
4.815
4.803
4.786
4.775
4.713
4.689
4.535
4.511
4.328
4.315
4.305
4.295
4.221
4.212
4.198
4.052
3.992
3.984
3.970
3.935
3.792



^{13}C -NMR spectra of compound **38**



¹H -NMR spectra of compound **39**



¹³C -NMR spectra of compound **39**

pt.akd38p r
pt.akd38p r-135dept-500mhz

163.499
163.474

143.476

134.501

126.587

124.735

106.218

80.537

74.073

71.943

59.549

57.251

56.055

52.940

52.841

52.807

52.500

50.500

42.444

40.021

39.654

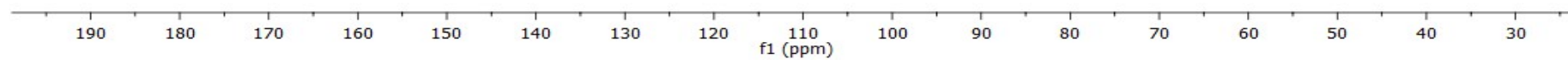
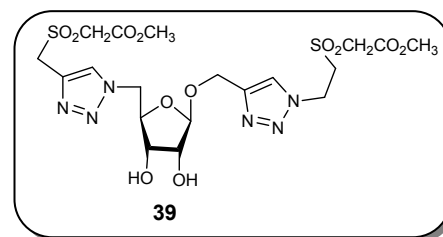
39.687

39.520

39.353

39.186

39.019



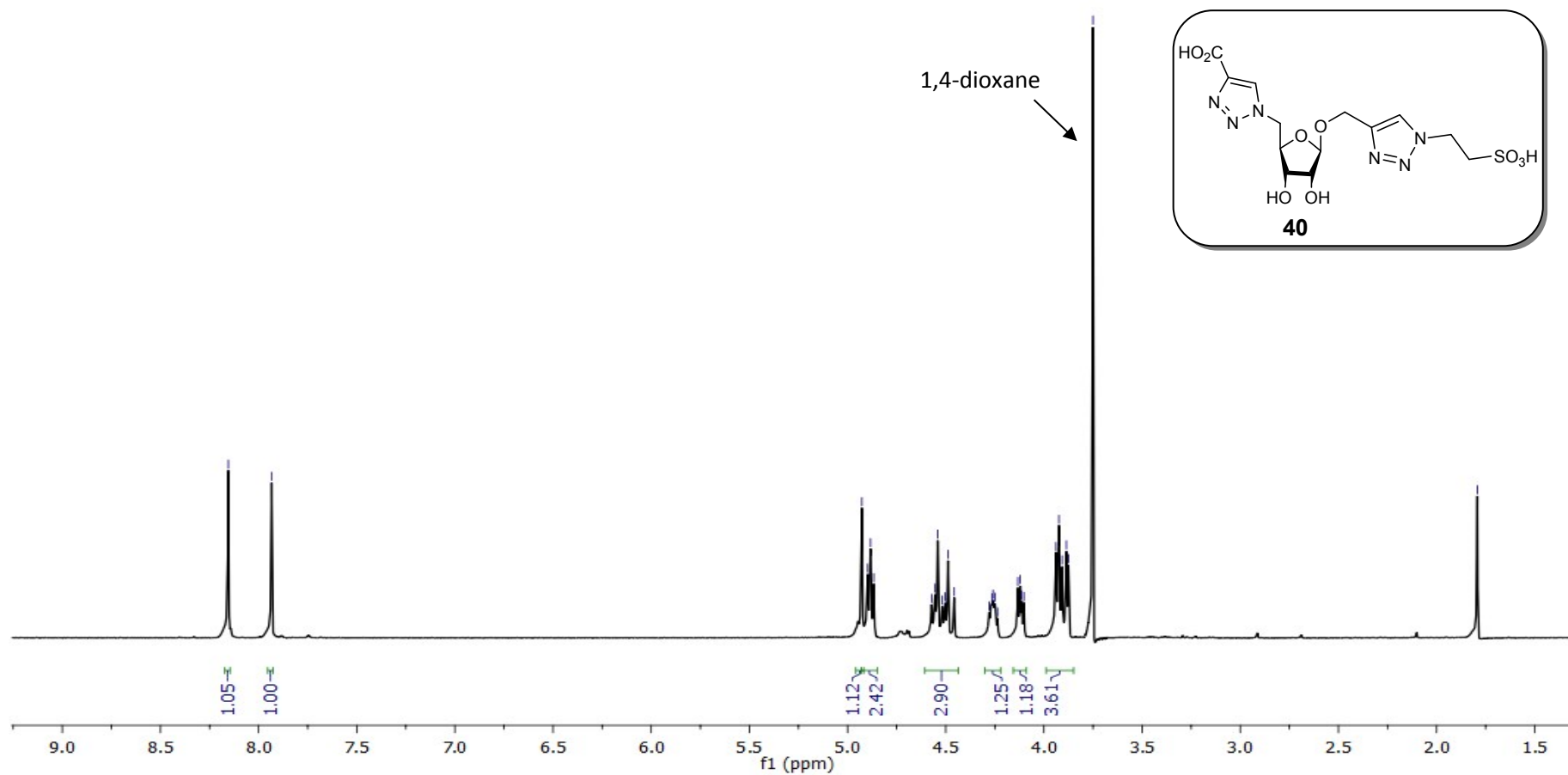
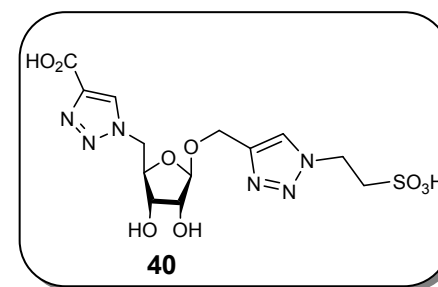
¹H -NMR spectra of compound **40**

ptws.akd468r
pt / akd / 468r - ws

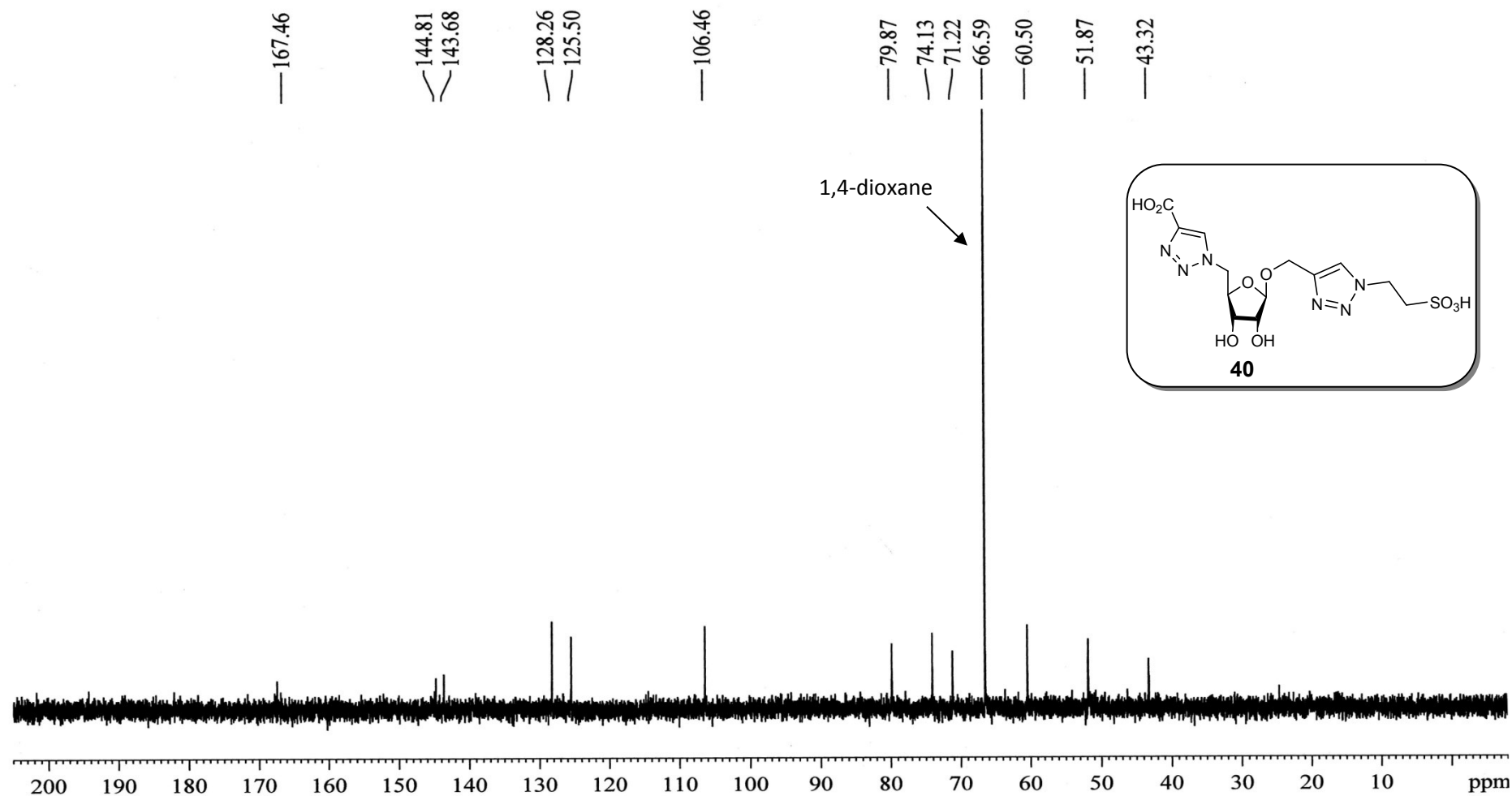
—8.154
—7.934

4.927
4.898
4.883
4.866
4.572
4.554
4.541
4.517
4.503
4.488
4.457
4.279
4.265
4.259
4.250
4.236
4.133
4.121
4.113
4.102
3.939
3.923
3.907
3.886
3.875
3.758
—1.793

1,4-dioxane

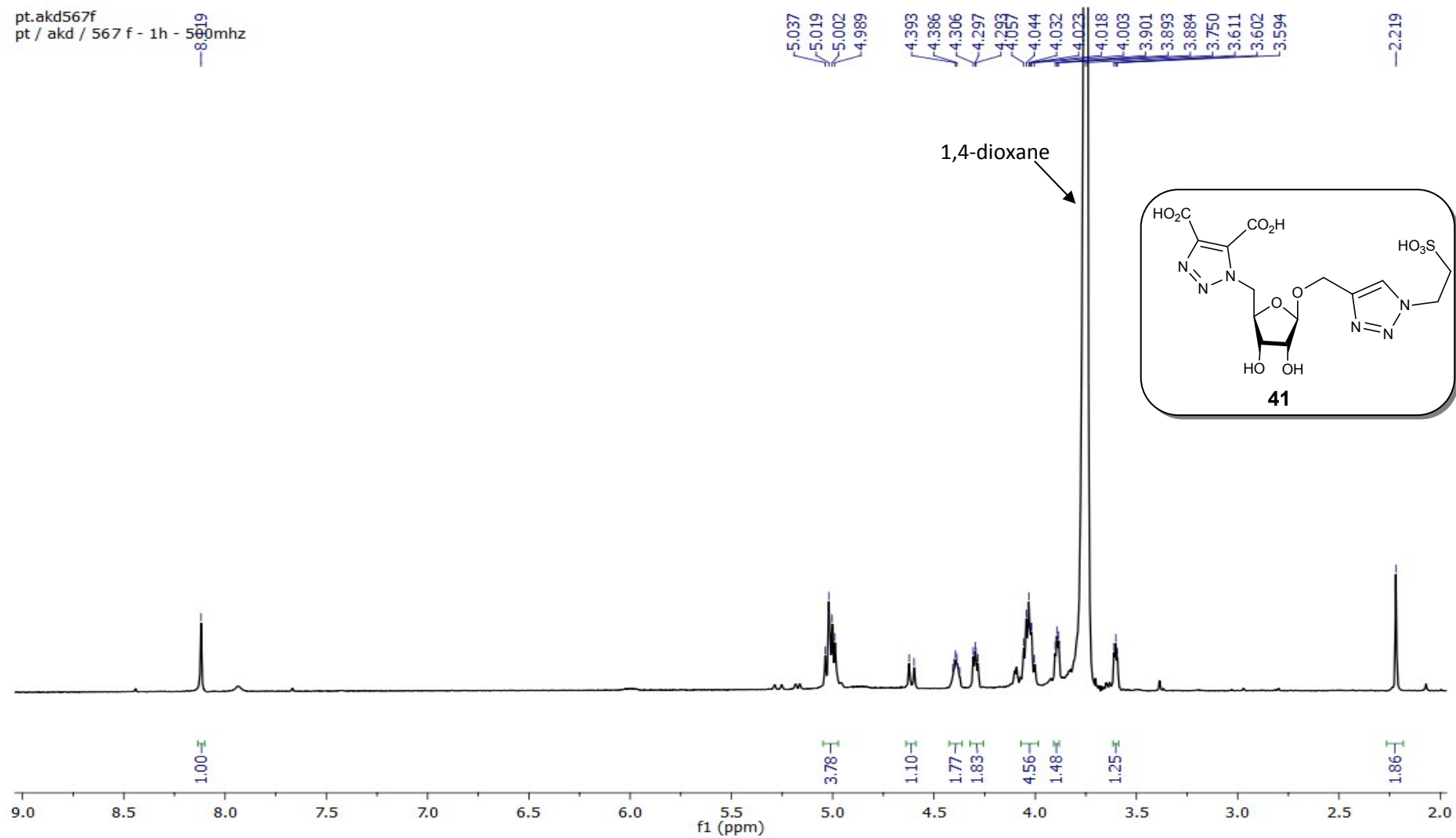


^{13}C -NMR spectra of compound **40**

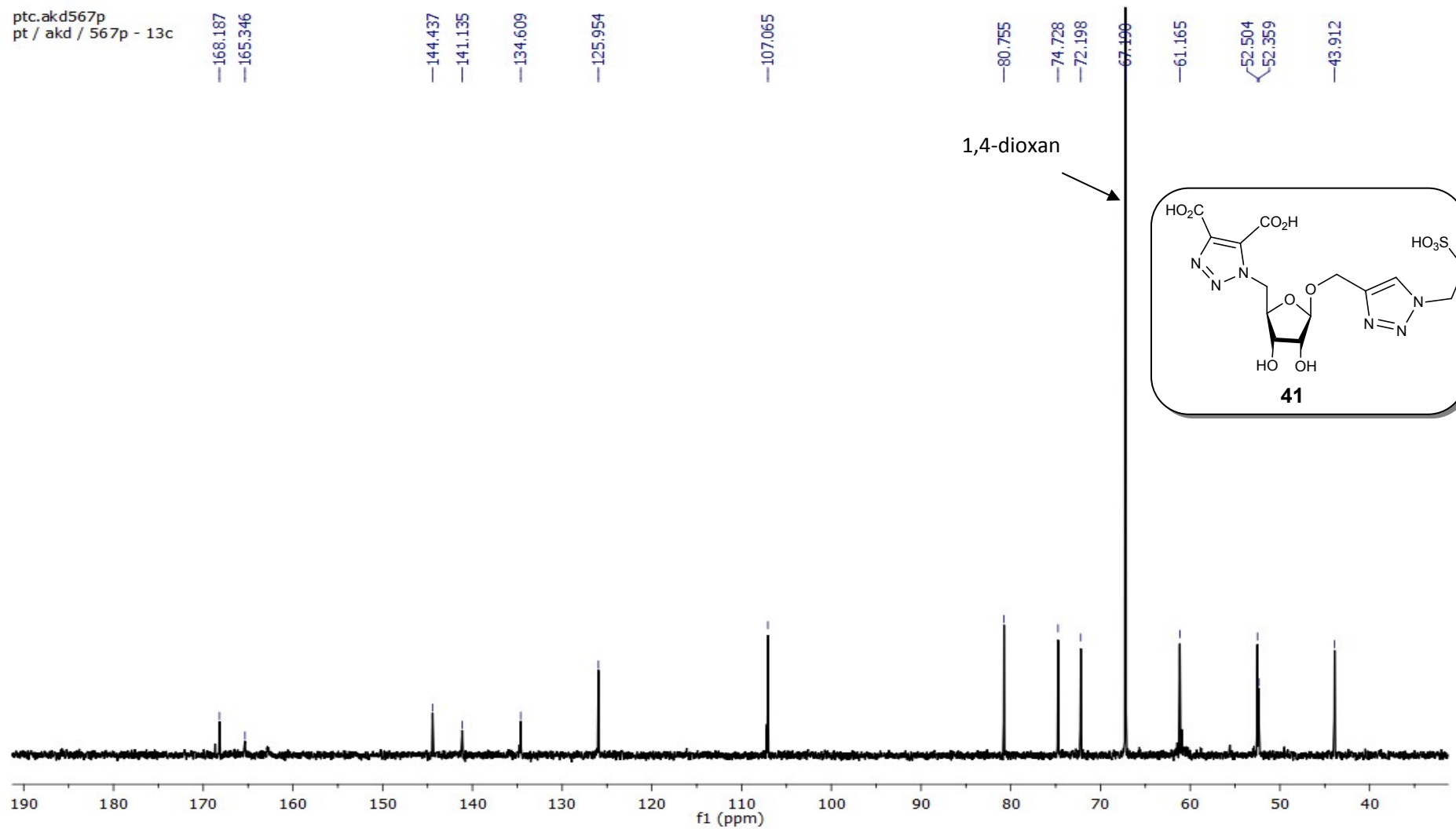


¹H -NMR spectra of compound **41**

pt.akd567f
pt / akd / 567 f - 1h - 500mhz



^{13}C -NMR spectra of compound **41**



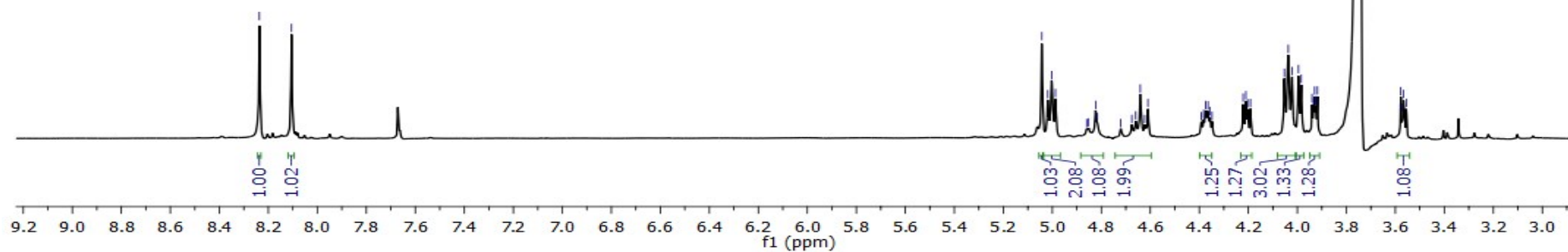
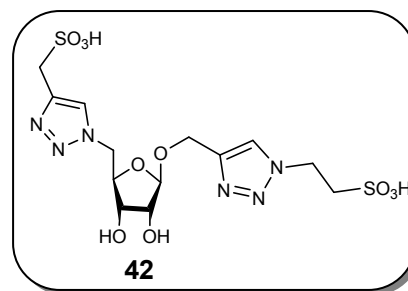
¹H -NMR spectra of compound **42**

ptws.akd581
pt / akd / 581 -1h

—8.237
—8.105

5.043 5.019 5.003 4.987 4.860 4.852 4.823 4.816 4.721 4.676 4.660 4.641 4.623 4.610 4.053 4.037 4.022 3.995 3.984 3.929 3.918 3.578 3.571 3.566 3.555

1,4-dioxane



^{13}C -NMR spectra of compound **42**

pt.akd579
pt / akd / 579 - ^{13}C - 500mhz

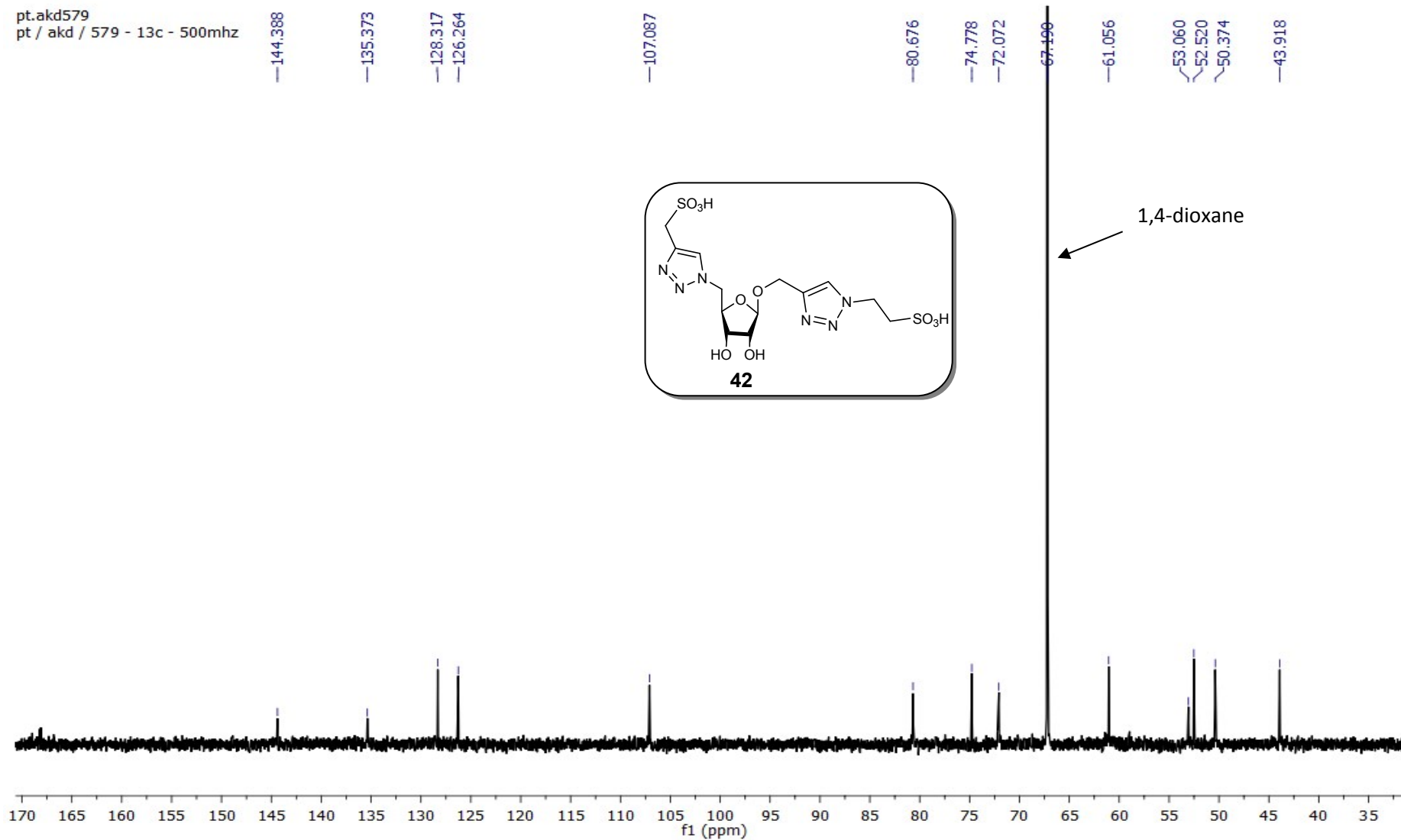
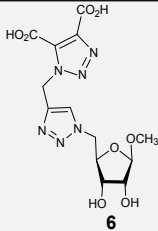
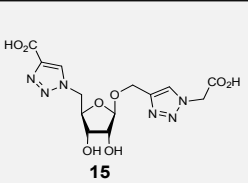
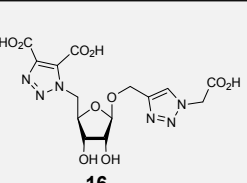
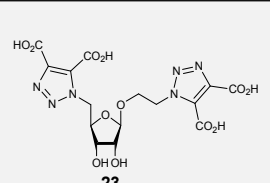
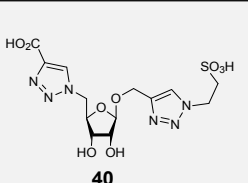
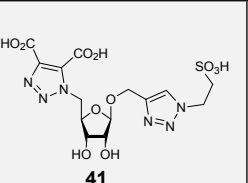
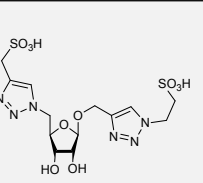


Table S1: H-bonding Distance (Å) measurement from Docking Studies

RNase A (PDB ID: 1FS3) Amino acid residues							
Lys7 NHζ			2.2 [CO]of CO ₂ H	1.9 [OH] of CO ₂ H 2.2 [3'-OH] of sugar	2.1 [OH] of SO ₃ H 2.2 [O] of SO ₃ H	2.5 [OH] of CO ₂ H 2.5 [3'-OH] of sugar	1.9 [O] of SO ₃ H
Gln11 COϵ^1				2.3[OH] of CO ₂ H		2.3 [OH] of CO ₂ H	
Gln11 NHϵ^2	3.0 [OCH ₃]	2.5 [OH] of CO ₂ H	2.7 [N] of triazole	1.6 [O] of sugar	2.1 [OH] of SO ₃ H 2.7 [O] of SO ₃ H	1.9 [O] of sugar ring	2.4 [O] of SO ₃ H 2.0 [N] of nitrogen ring
His12 NHϵ^2		1.9 [OH] of CO ₂ H	2.2 [N] of triazole		3.1 [N] of triazole ring	2.7 [O] of glycoside ring	2.6 [N] of triazole ring 3.2 [N] of triazole ring
Arg39 Nη^1				1.6 [CO] of CO ₂ H		2.0 [CO] of CO ₂ H	
Arg39 Nη^2				2.1 [OH] of CO ₂ H			
Lys41 NHζ	2.3 [O] of sugar ring	2.3 [N] of triazole 2.2 [N] of triazole	2.3 [N] of triazole 1.8 [N] of triazole		1.7 [N] of triazole ring 2.0 [N] of triazole ring	2.3 [OH] of CO ₂ H 2.3 [N] of triazole 1.9 [O] of glycoside	2.3 [N] of triazole
Asn44 δ^1							3.2 [3'-OH] of sugar ring
Thr45 OHγ^1		2.0 [O] of sugar 2.3 [O] of glycoside	3.3 [O] of sugar	2.4 [CO] of CO ₂ H		2.5 [O] of SO ₃ H 3.1 [O] of SO ₃ H	2.4 [2'-OH] of sugar ring
Thr45 amide NH							1.8 [3'-OH] of sugar ring
Asp83 CO₂γ		3.2 [O] of sugar ring				2.8 [O] of SO ₃ H	
Arg85	3.1 [CO]of	2.9 [3'-OH] of sugar					

NHη^1	CO ₂ H						
Arg85 NHϵ^1	2.8 [CO] of CO ₂ H						
Lys104 NHζ					2.7 [OH] of CO ₂ H		2.7 [O] of SO ₃ H
Val118 amide CO				2.5 [2'-OH] of sugar			2.1 [OH] of SO ₃ H 3.0 [O] of SO ₃ H
His119 NHδ^1	1.9 [3'-OH] of sugar	2.1 [CO] of CO ₂ H	2.1 [OH] of CO ₂ H		2.8 [O] of SO ₃ H	2.2[2'-OH] of sugar	
Phe120 amide NH	2.9 [3'-OH] of sugar			2.7 [2'-OH] of sugar		2.4 [2'-OH] of sugar	
Phe120 amide CO	1.9 [3'-OH] of sugar						
Asp121 CO₂-δ							
Asp121 amide CO			1.9 [OH] of CO ₂ H	2.1 [OH] of CO ₂ H 2.2 [OH] of CO ₂ H	1.9 [2'-OH] of sugar ring 2.0 [3'-OH] of sugar ring		
Ser123 OHγ	3.2 [CO] of CO ₂ H		2.0 [OH] of CO ₂ H		2.2 [OH] of CO ₂ H		3.0 [O] of SO ₃ H
Ser123 amide CO		2.2 [OH] of CO ₂ H					2.8 [O] of SO ₃ H 3.1 [O] of SO ₃ H
Ser123 amide NH	3.3 [CO] of CO ₂ H	2.2 [N] of triazole	2.2 [CO] of CO ₂ H				1.9 [O] of SO ₃ H