

Glycoconjugation of Quinoline Derivatives Using the C-6 Position in Sugars as a Strategy for Improving the Selectivity and Cytotoxicity of Functionalized Compounds

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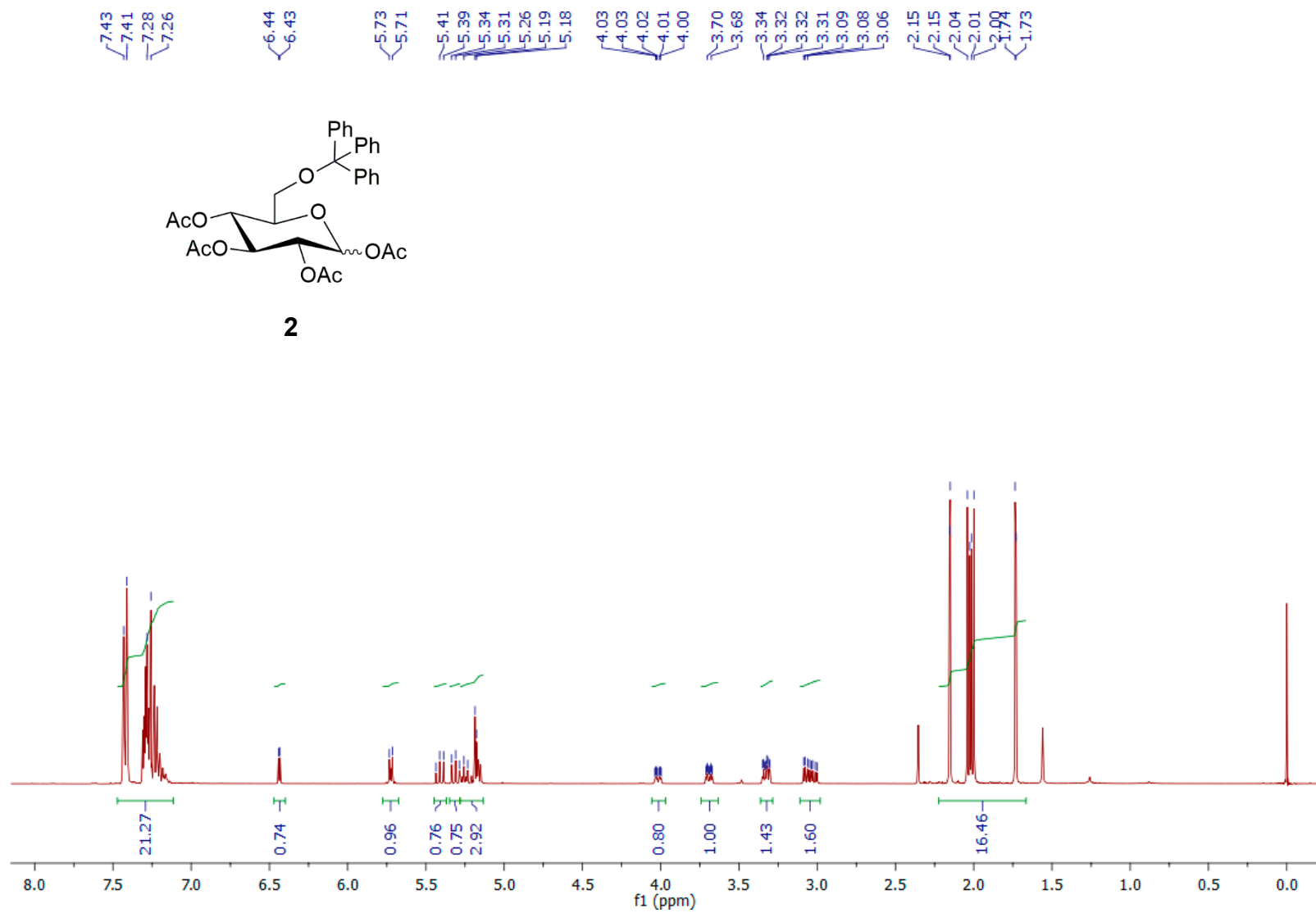


Fig. S1: ¹H NMR spectrum of 1,2,3,4-tetra-O-acetyl-6-O-triphenylmethyl-D-glucopyranose **2** (400 MHz/CDCl₃/TMS; δ (ppm)).

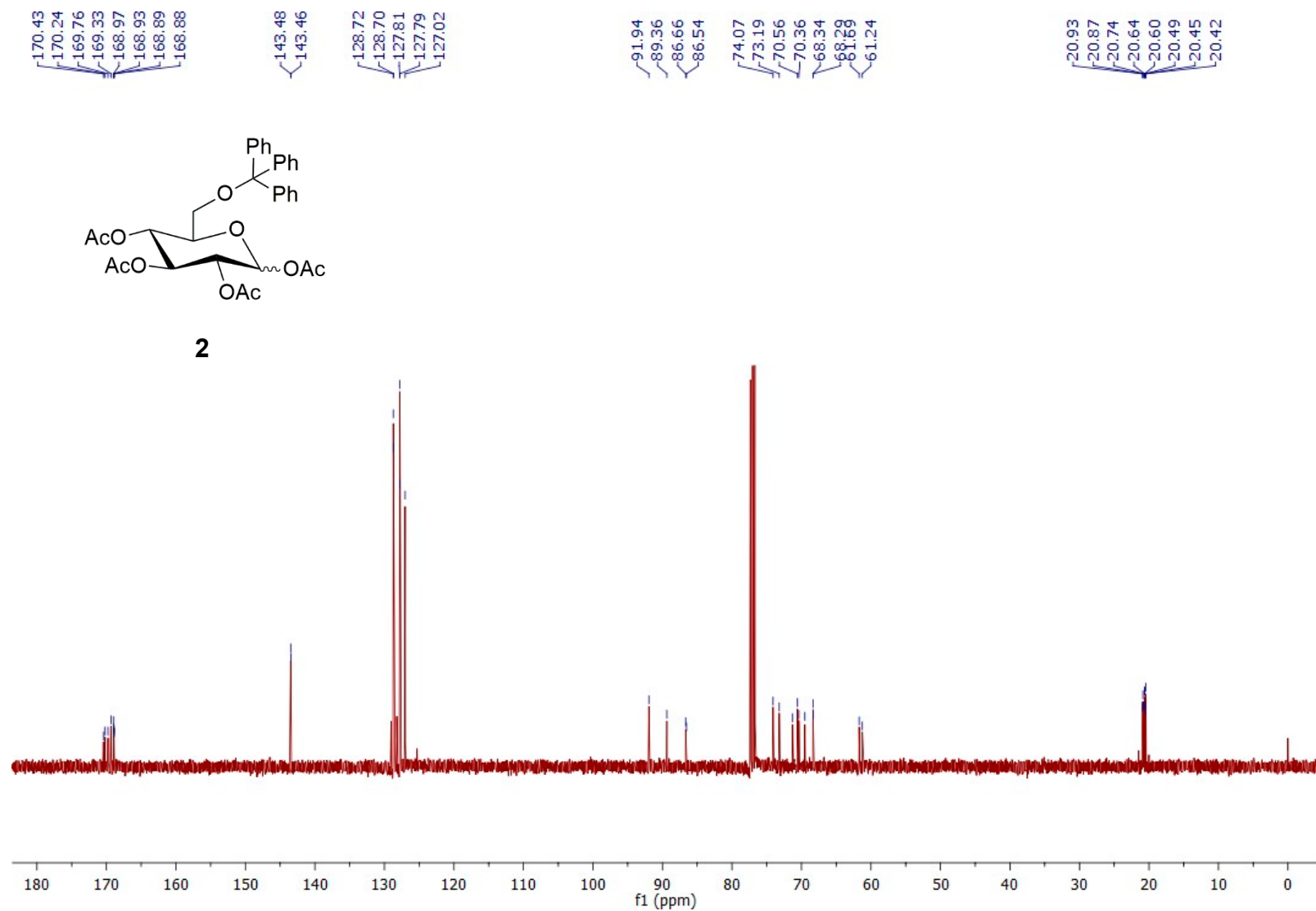


Fig. S2: ^{13}C NMR spectrum of 1,2,3,4-tetra-*O*-acetyl-6-*O*-triphenylmethyl-D-glucopyranose **2** (100 MHz/ CDCl_3 /TMS; δ (ppm)).

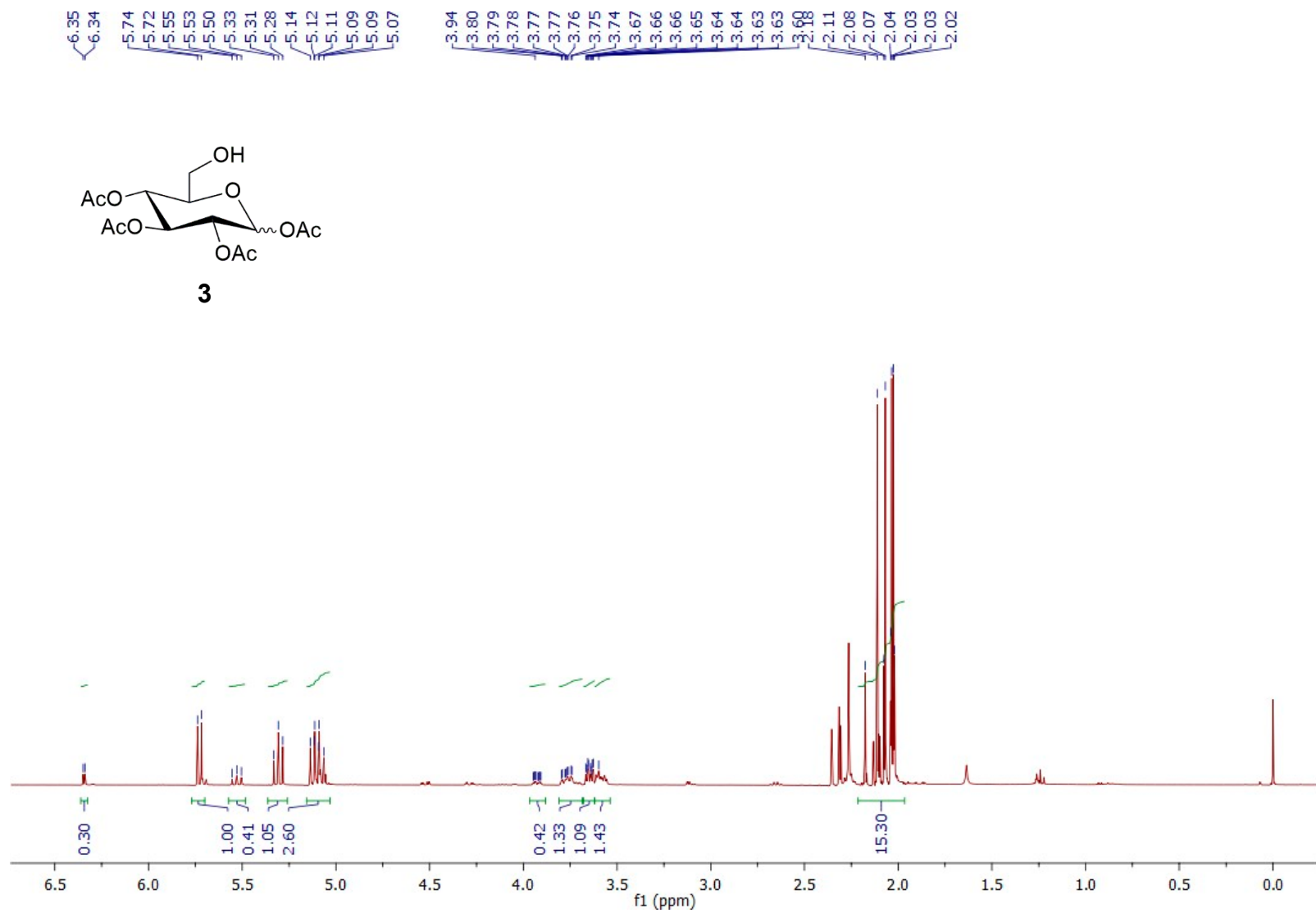


Fig. S3: ¹H NMR spectrum of 1,2,3,4-tetra-O-acetyl-D-glucopyranose **3** (400 MHz/CDCl₃/TMS; δ (ppm)).

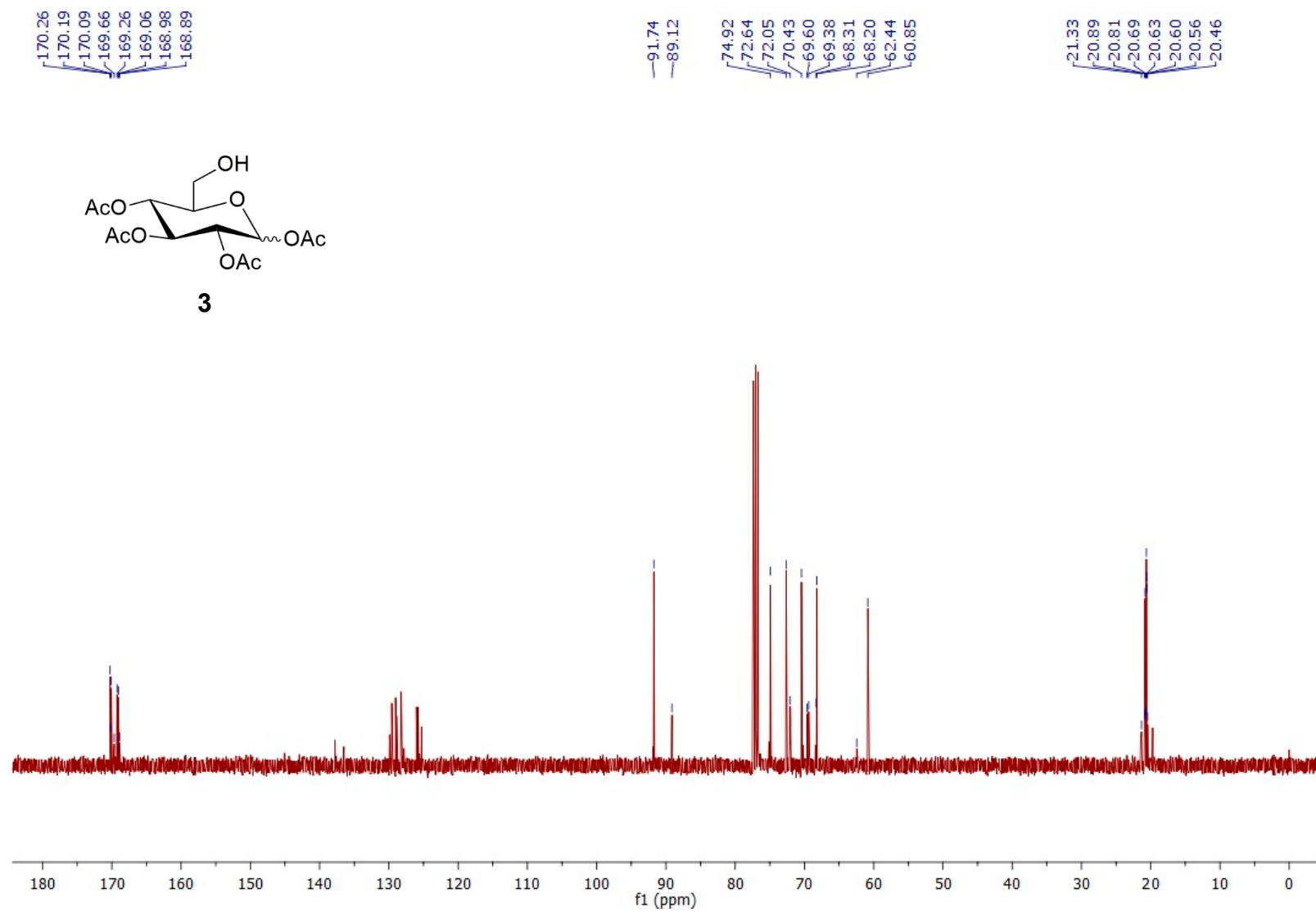


Fig. S4: ¹³C NMR spectrum of 1,2,3,4-tetra-*O*-acetyl-D-glucopyranose **3** (100 MHz/CDCl₃/TMS; δ (ppm)).

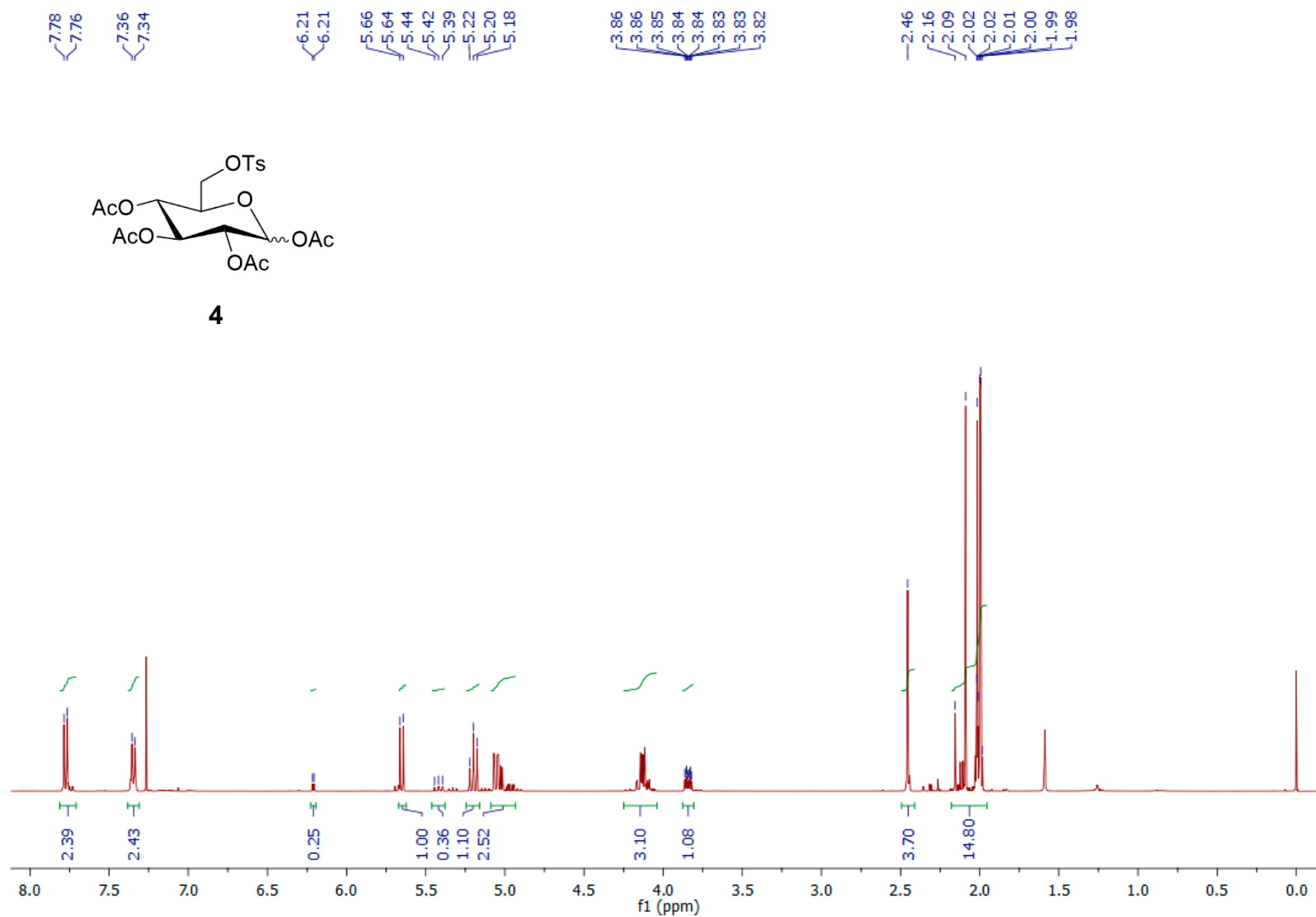


Fig. S5: ¹H NMR spectrum of 1,2,3,4-tetra-*O*-acetyl-6-*O*-*p*-toluenesulfonyl-D-glucopyranose **4** (400 MHz/CDCl₃/TMS; δ (ppm)).

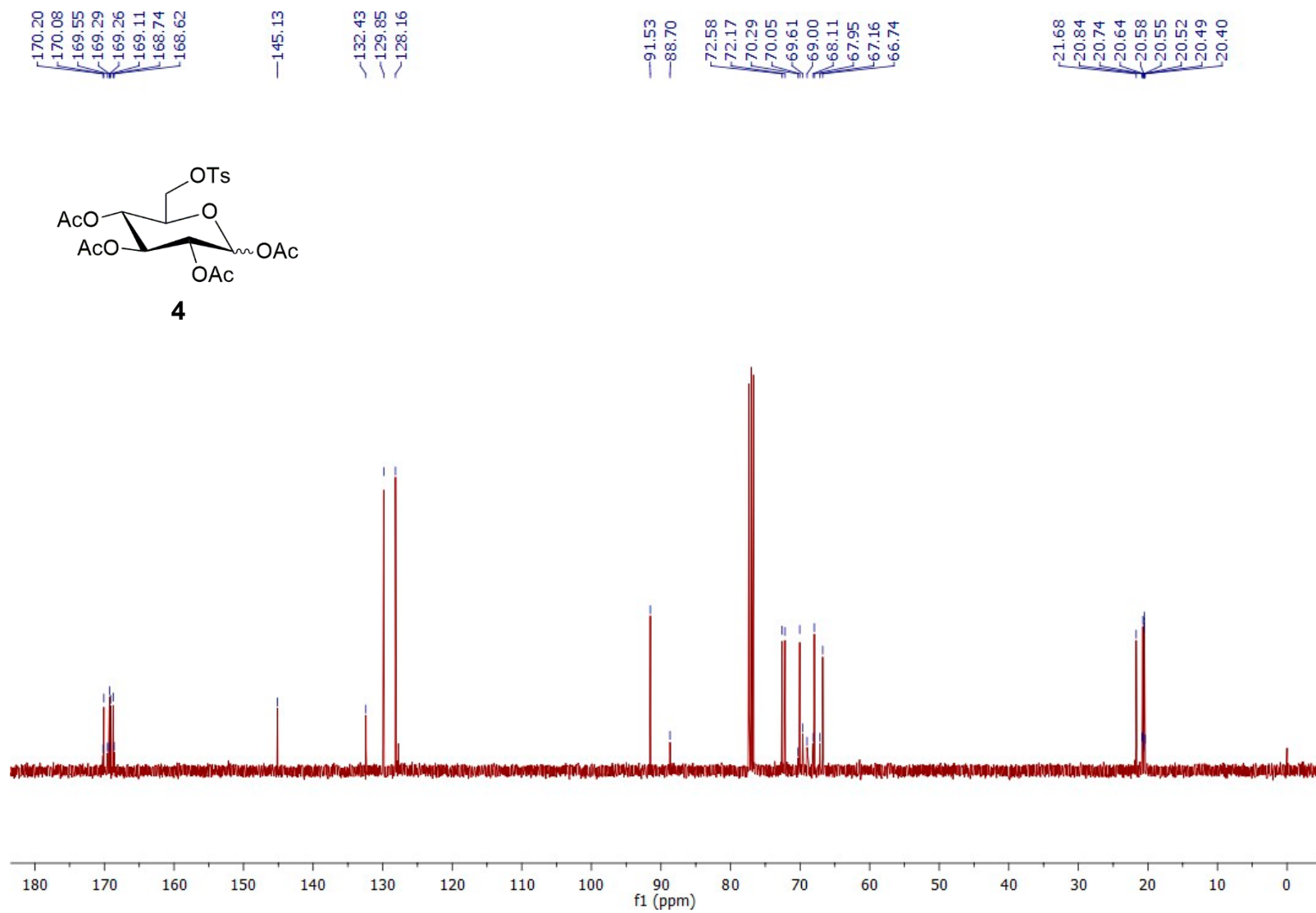


Fig. S6: ¹³C NMR spectrum of 1,2,3,4-tetra-*O*-acetyl-6-*O*-*p*-toluenesulfonyl-D-glucopyranose **4** (100 MHz/CDCl₃/TMS; δ (ppm)).

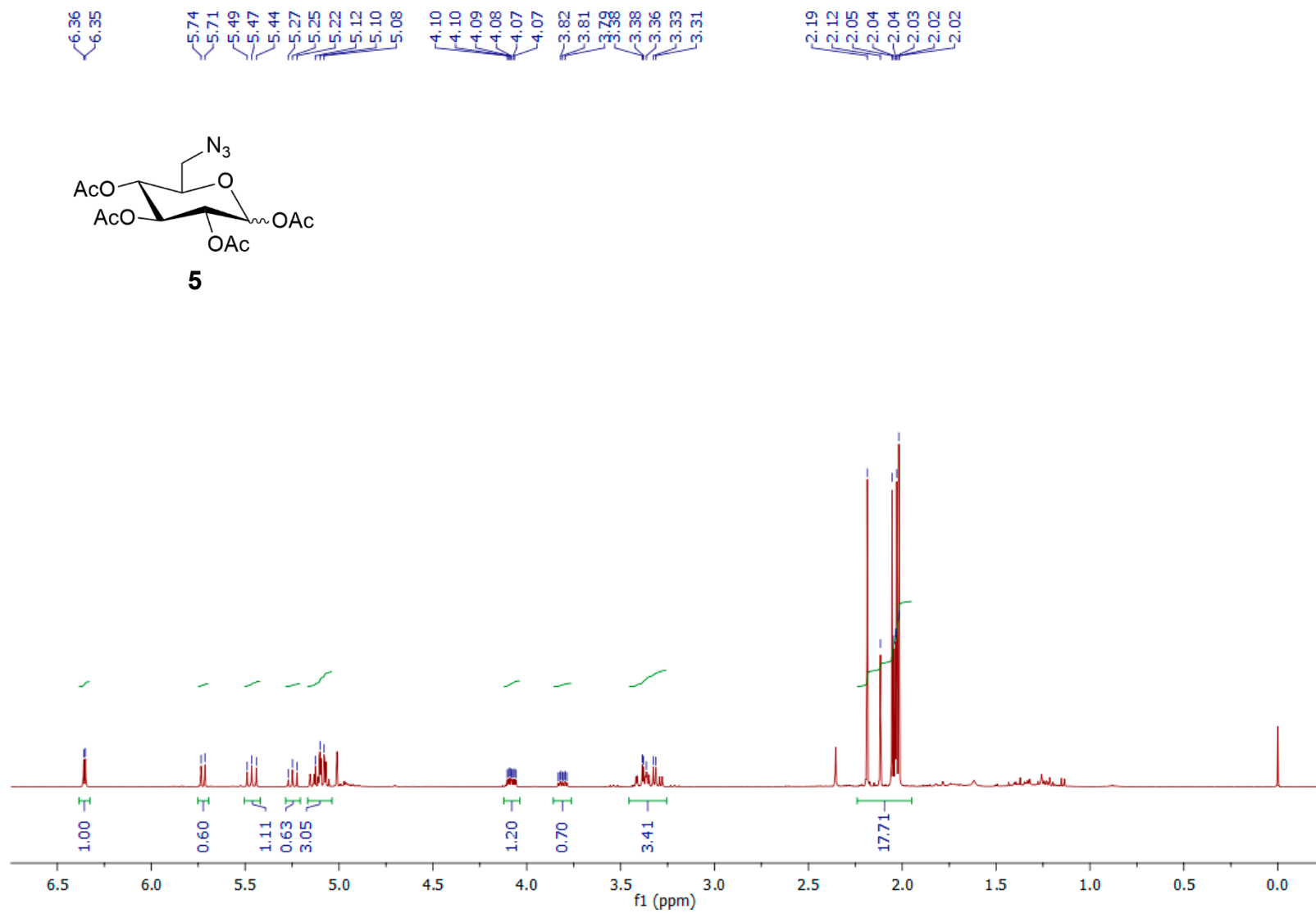


Fig. S7: ¹H NMR spectrum of 1,2,3,4-tetra-O-acetyl-6-azido-6-deoxy-D-glucopyranose **5** (400 MHz/CDCl₃/TMS; δ (ppm)).

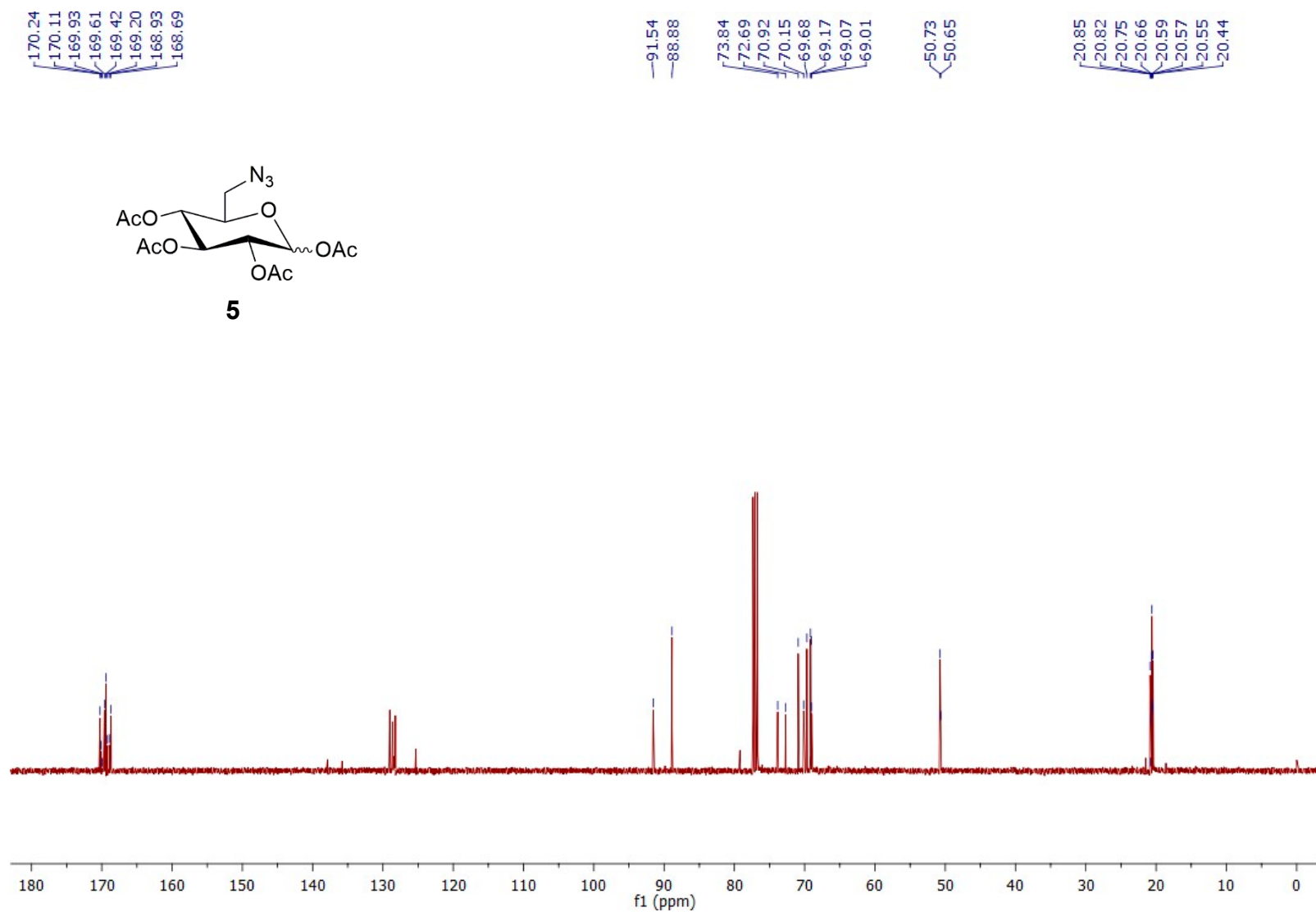


Fig. S8: ^{13}C NMR spectrum of 1,2,3,4-tetra-O-acetyl-6-azido-6-deoxy-D-glucopyranose **5** (100 MHz/ CDCl_3/TMS ; δ (ppm)).

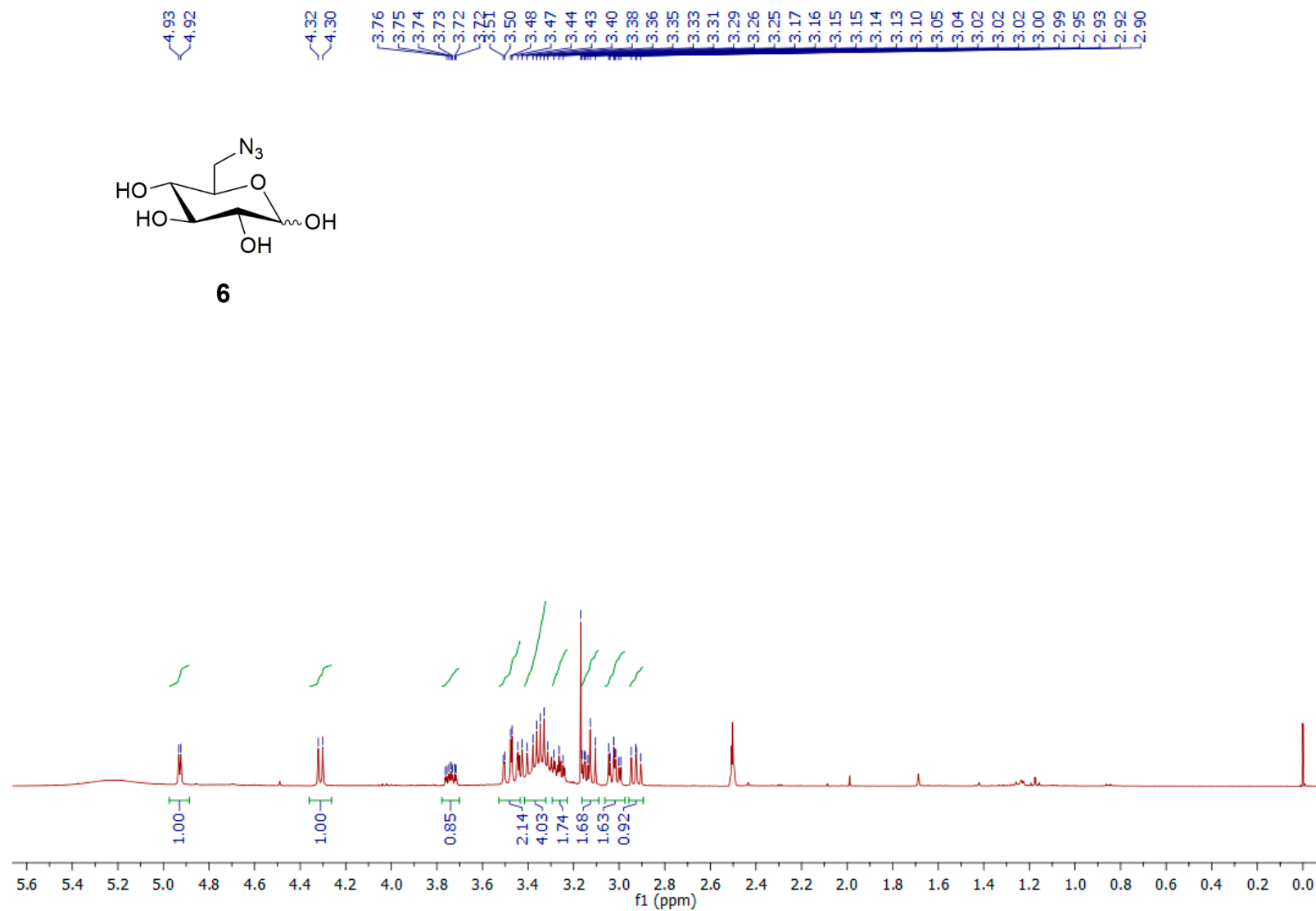


Fig. S9: ^1H NMR spectrum of 6-azido-6-deoxy-D-glucopyranose **6** (400 MHz/DMSO/TMS; δ (ppm)).

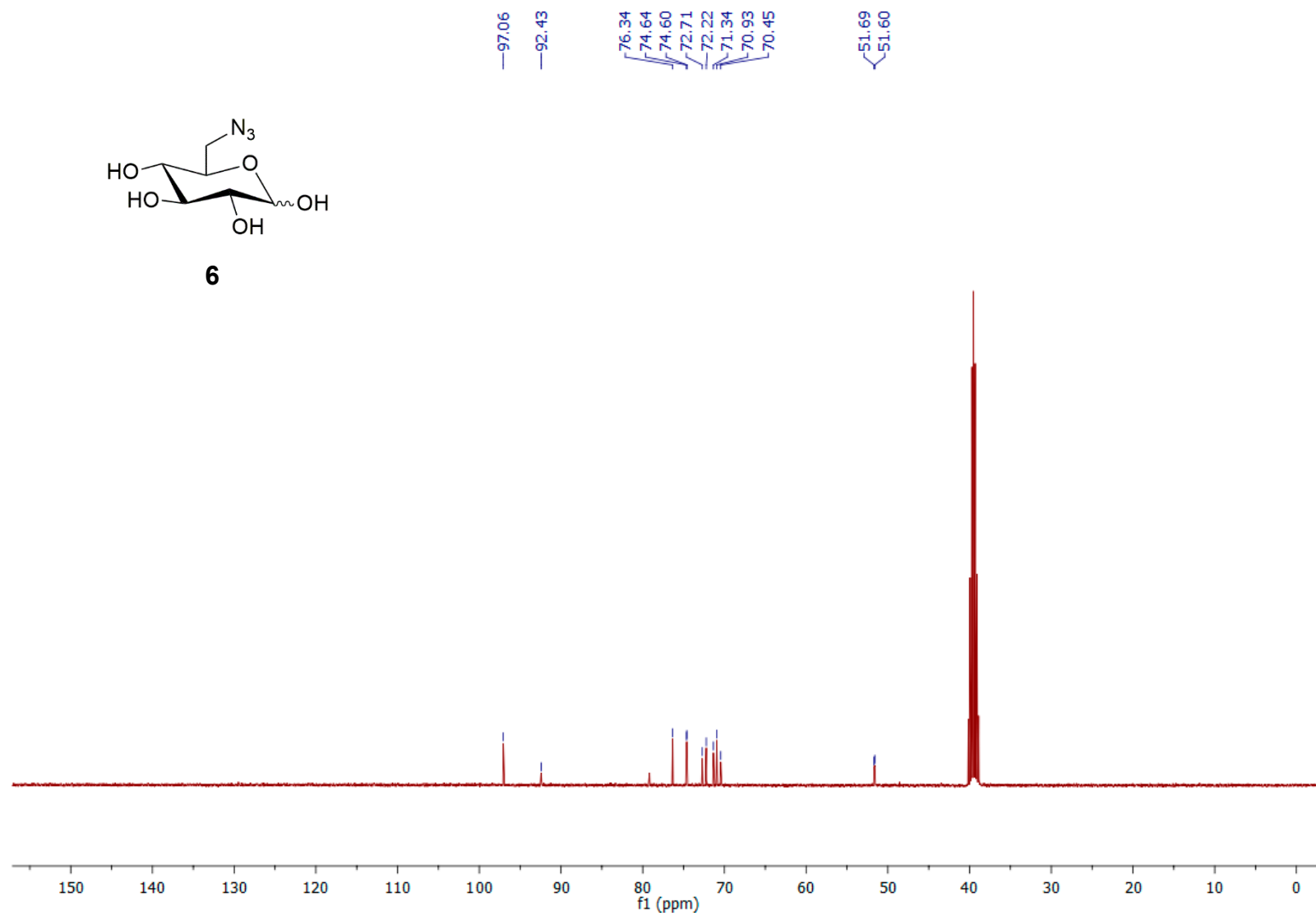


Fig. S10: ¹³C NMR spectrum of 6-azido-6-deoxy-D-glucopyranose **6** (100 MHz/DMSO/TMS; δ (ppm)).

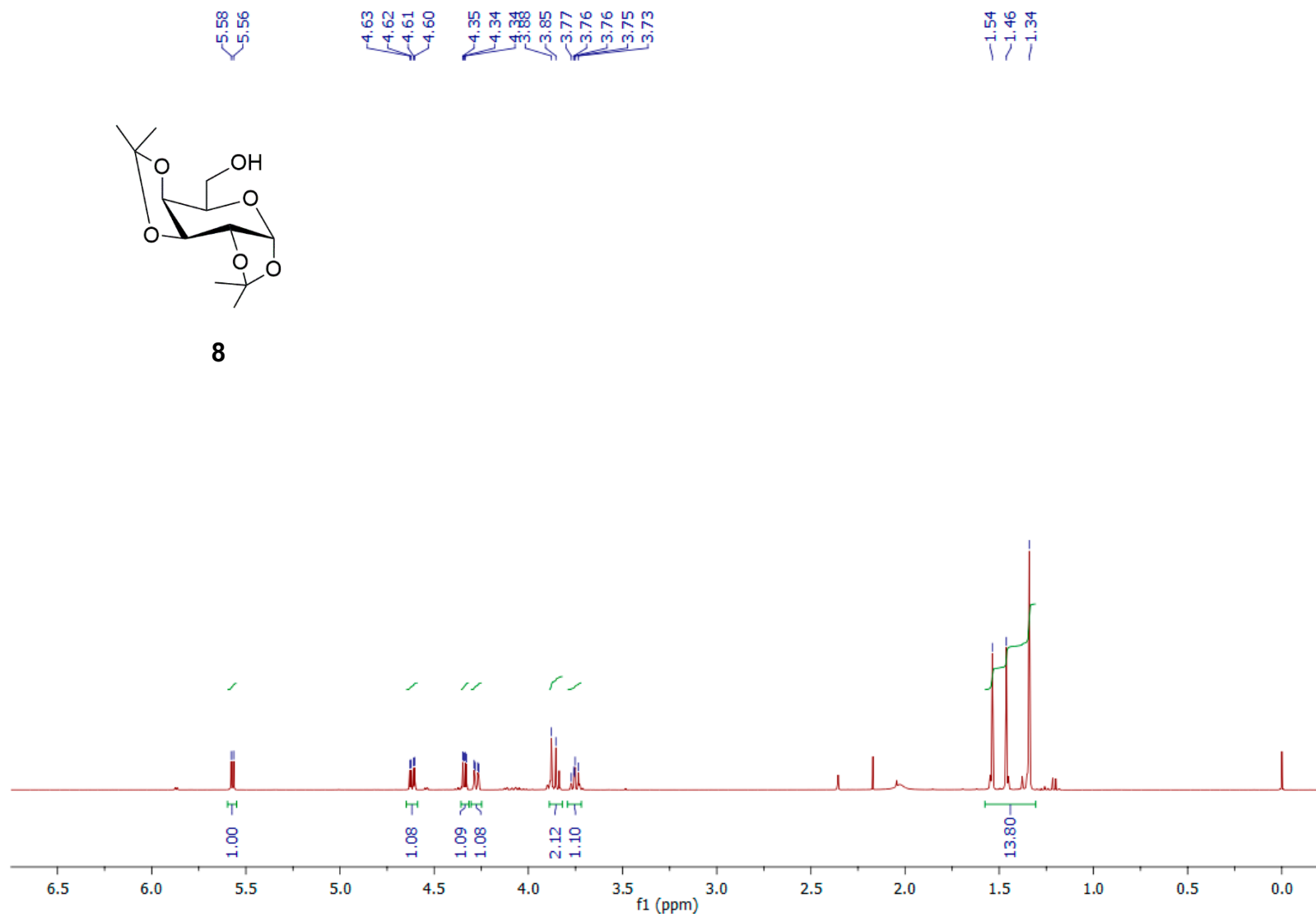
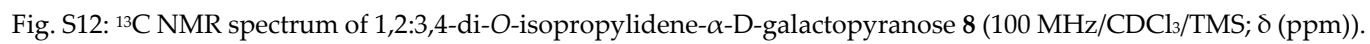


Fig. S11: ^1H NMR spectrum of 1,2:3,4-di-O-isopropylidene- α -D-galactopyranose **8** (400 MHz/ CDCl_3 /TMS; δ (ppm)).



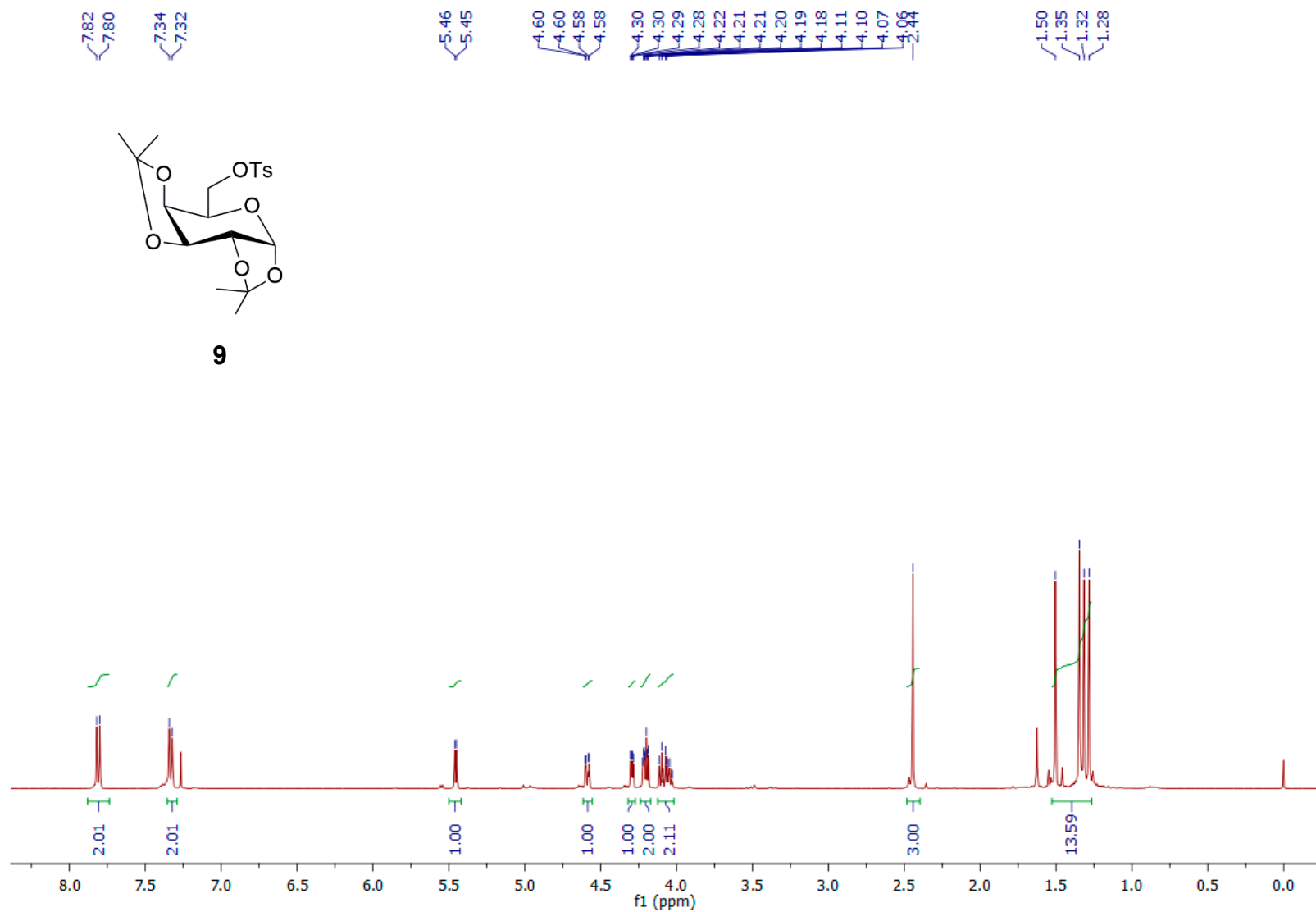


Fig. S13: ¹H NMR spectrum of 1,2:3,4-di-O-isopropylidene-6-O-*p*-toluenesulfonyl- α -D-galactopyranose **9** (400 MHz/CDCl₃/TMS; δ (ppm)).

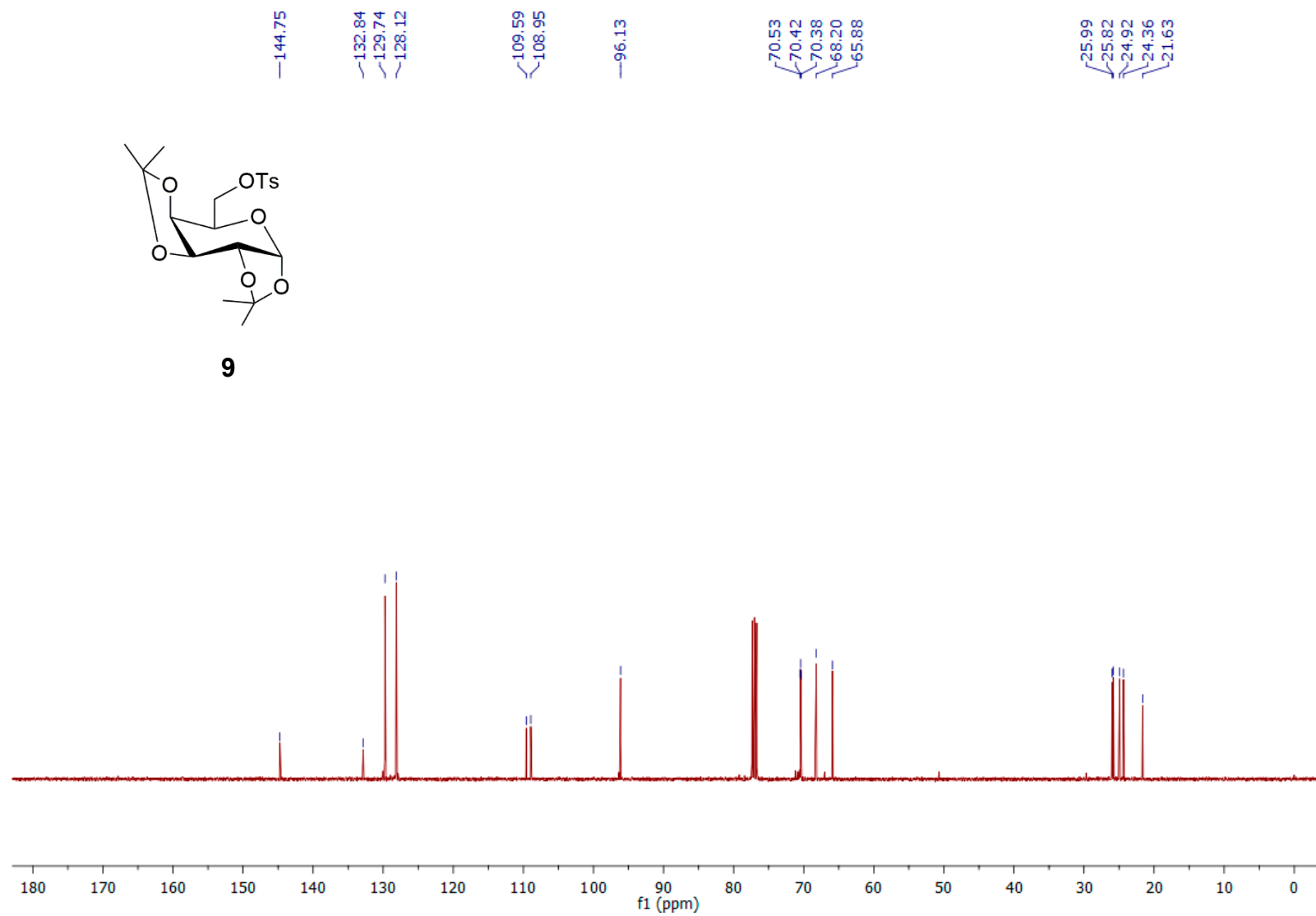


Fig. S14: ^{13}C NMR spectrum of 1,2:3,4-di-*O*-isopropylidene-6-*O*-*p*-toluenesulfonyl- α -D-galactopyranose **9** (100 MHz/ CDCl_3 /TMS; δ (ppm)).

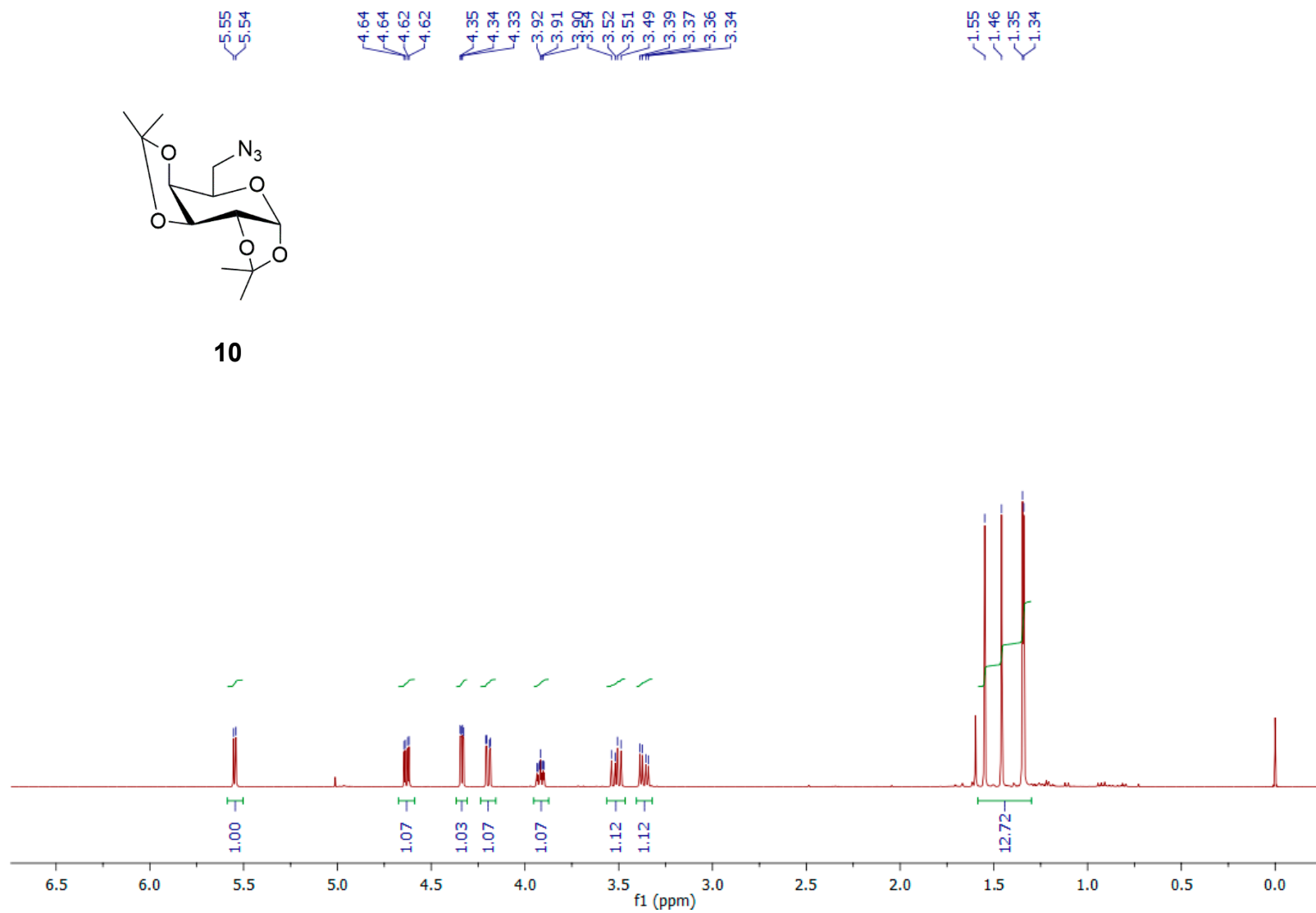


Fig. S15: ^1H NMR spectrum of 1,2,3,4-di-O-isopropylidene-6-azido-6-deoxy- α -D-galactopyranose **10** (400 MHz/ CDCl_3 /TMS; δ (ppm)).

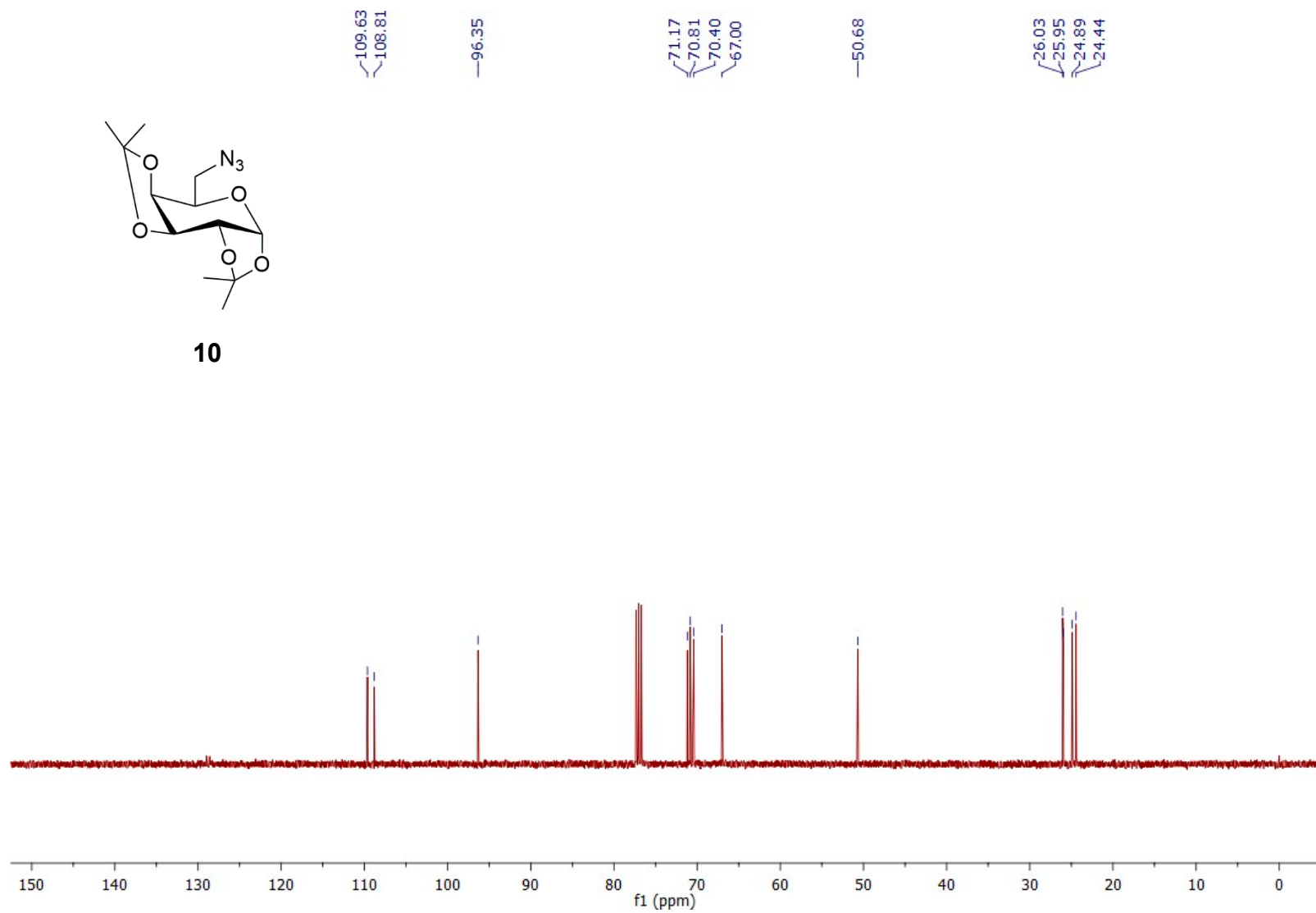


Fig. S16: ^{13}C NMR spectrum of 1,2:3,4-di-O-isopropylidene-6-azido-6-deoxy- α -D-galactopyranose **10** (100 MHz/ CDCl_3 /TMS; δ (ppm)).

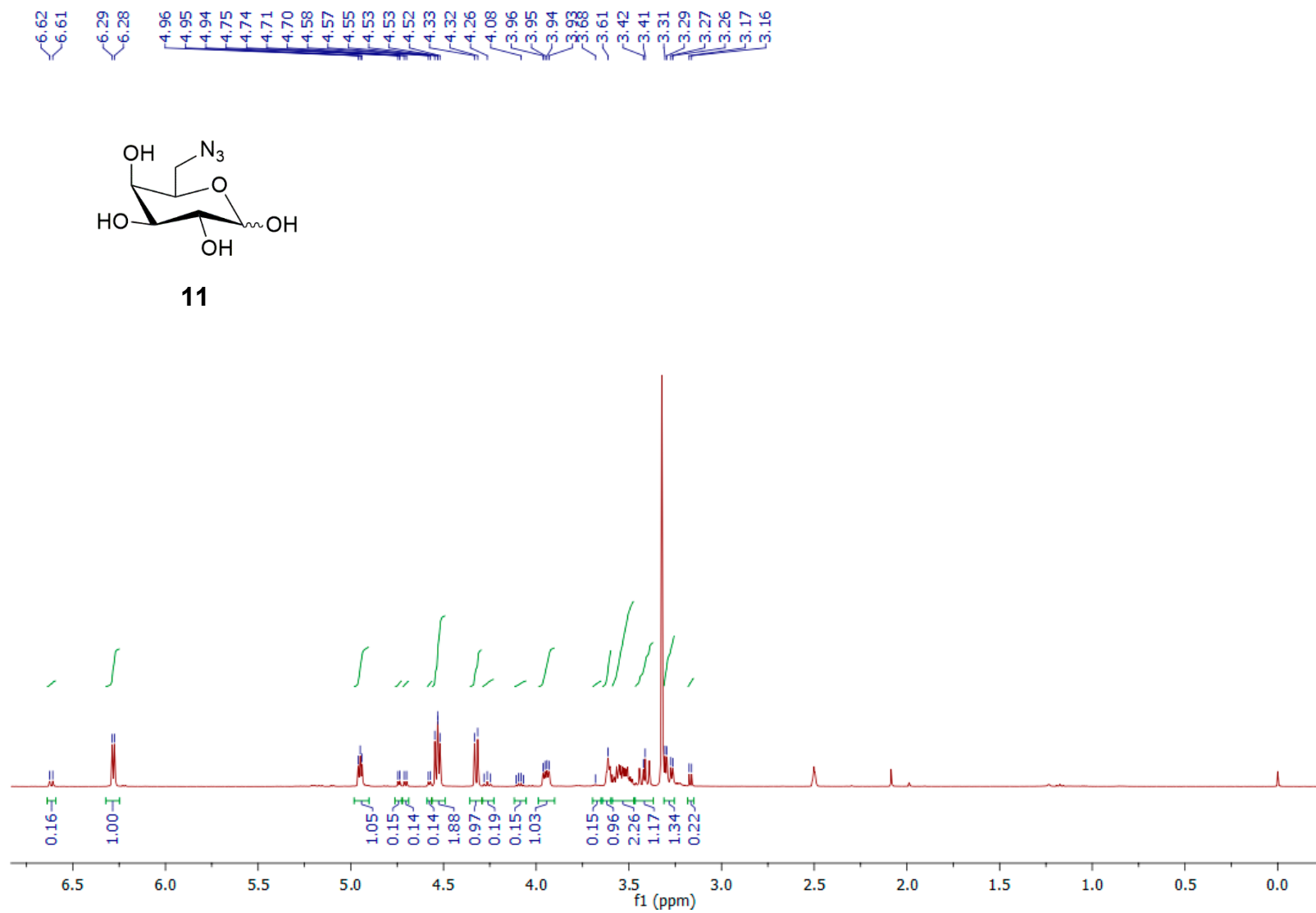


Fig. S17: ¹H NMR spectrum of 6-azido-6-deoxy-D-galactopyranose **11** (400 MHz/DMSO/TMS; δ (ppm)).

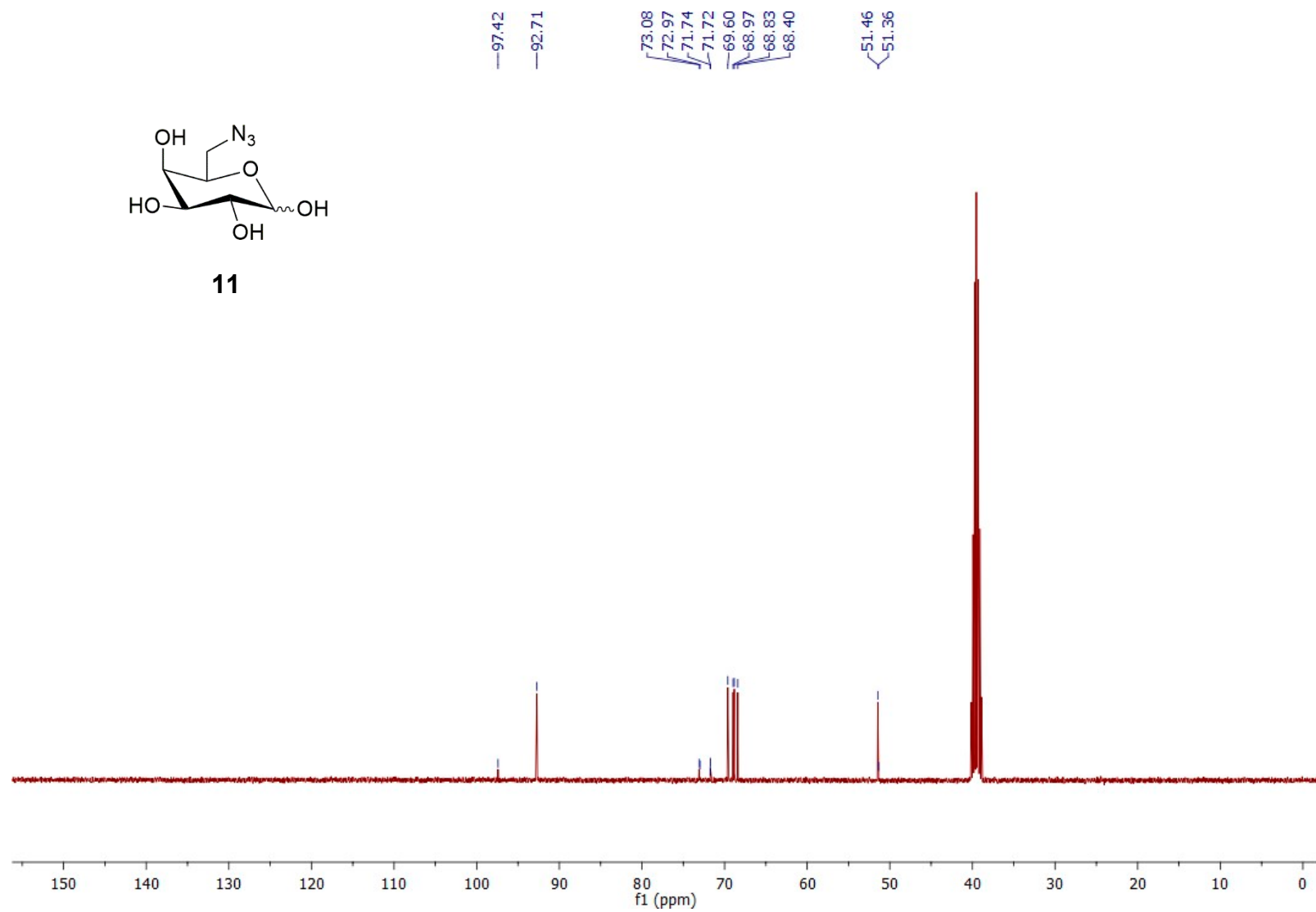


Fig. S18: ^{13}C NMR spectrum of 6-azido-6-deoxy-D-galactopyranose **11** (100 MHz/DMSO/TMS; δ (ppm)).

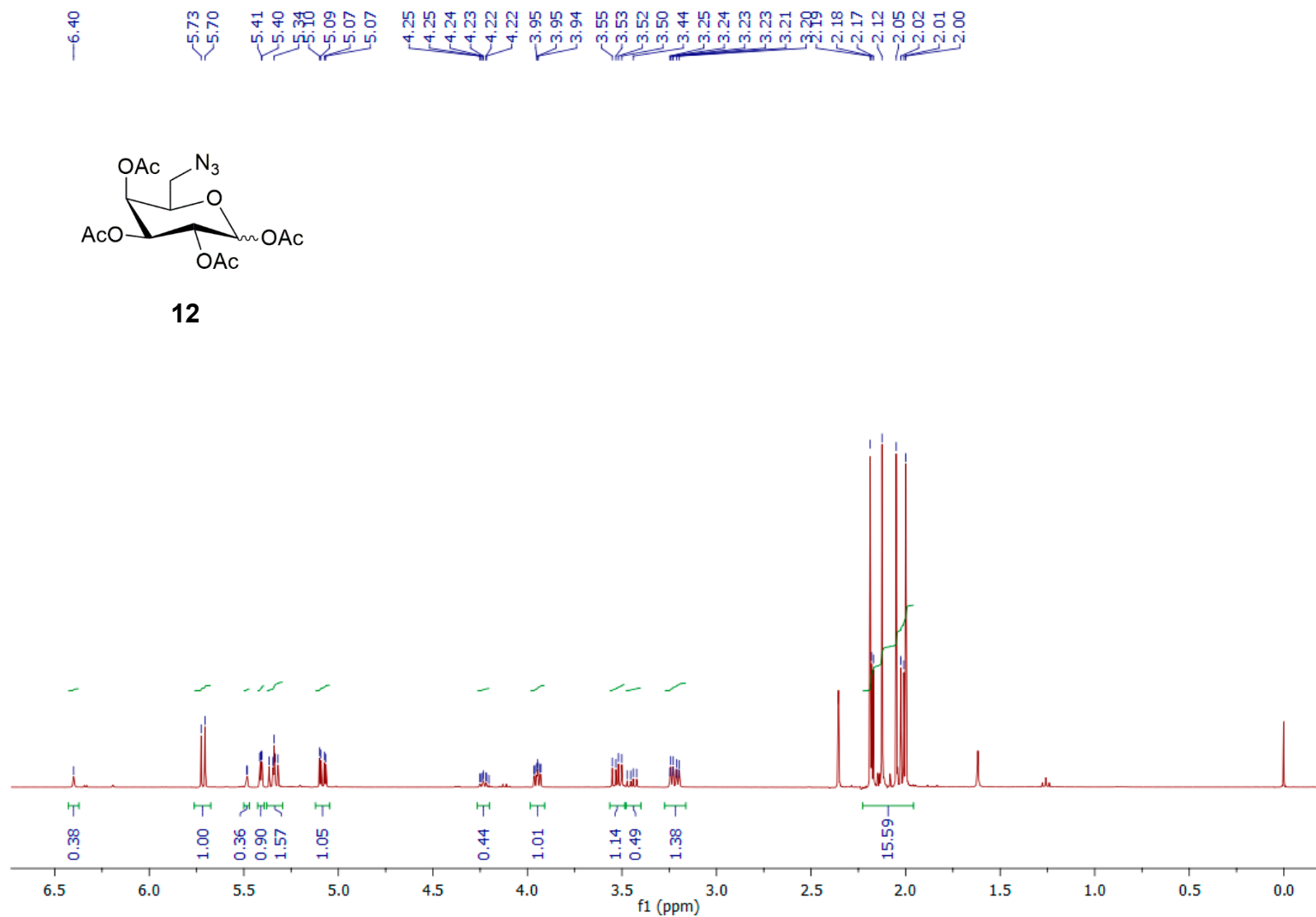


Fig. S19: ¹H NMR spectrum of 1,2,3,4-tetra-*O*-acetyl-6-azido-6-deoxy-*D*-galactopyranose **12** (400 MHz/CDCl₃/TMS; δ (ppm)).

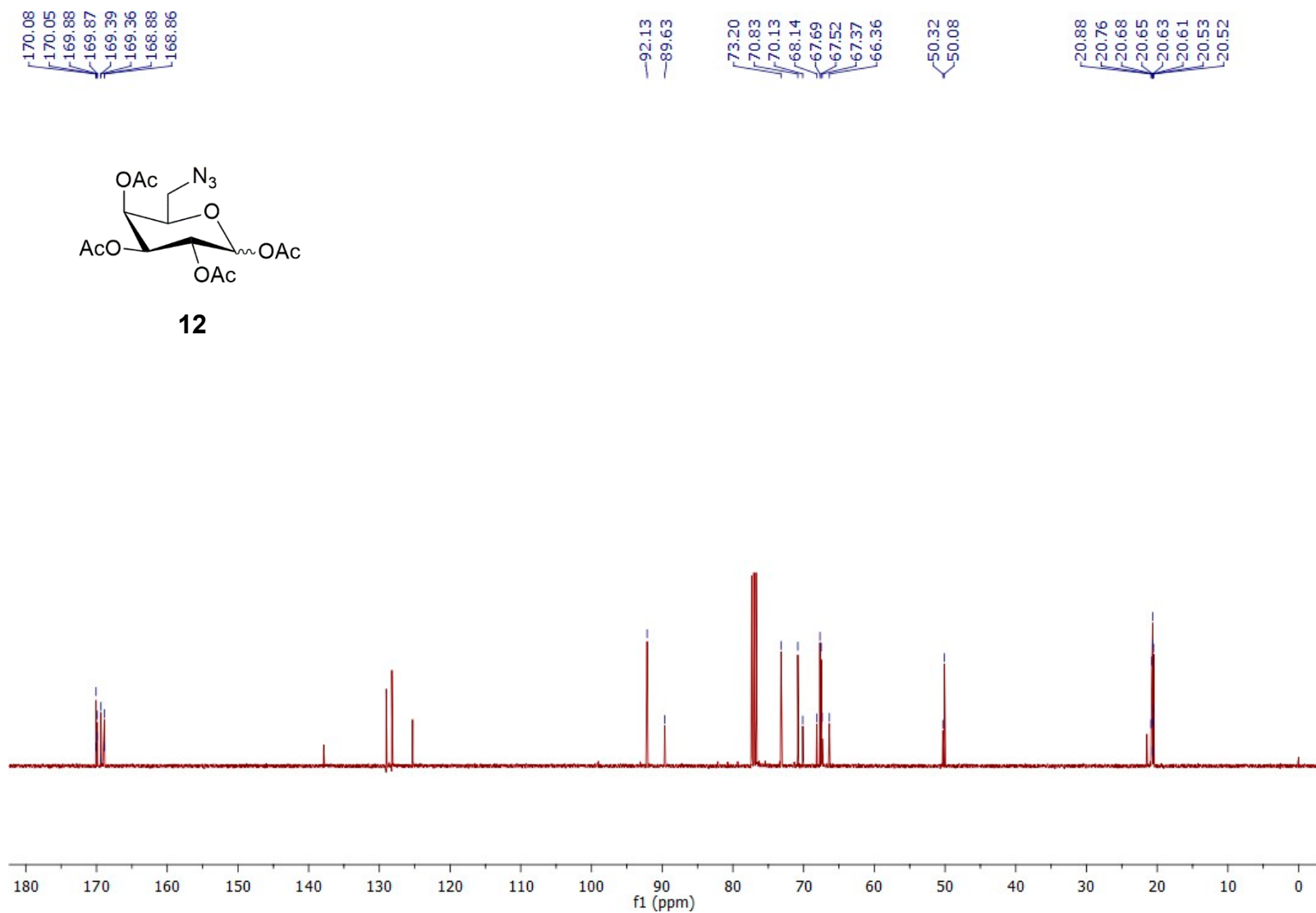


Fig. S20: ¹³C NMR spectrum of 1,2,3,4-tetra-O-acetylo-6-azido-6-deoxy-D-galactopyranose **12** (100 MHz/CDCl₃/TMS; δ (ppm)).

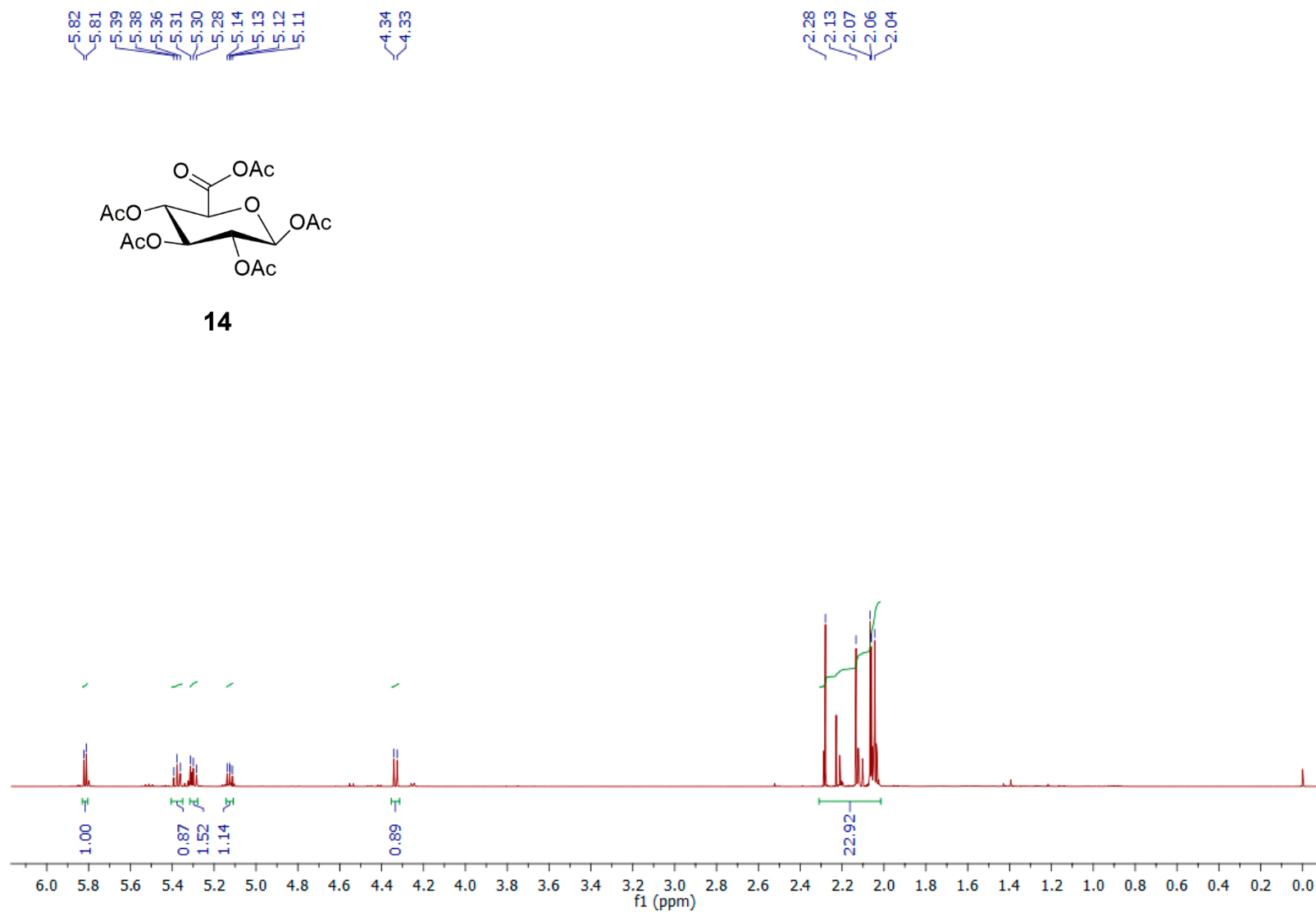


Fig. S21: ^1H NMR spectrum of 1,2,3,4-tetra-*O*-acetyl- β -D-glucopyranuronic acetic anhydride **14** (400 MHz/ CDCl_3 /TMS; δ (ppm)).

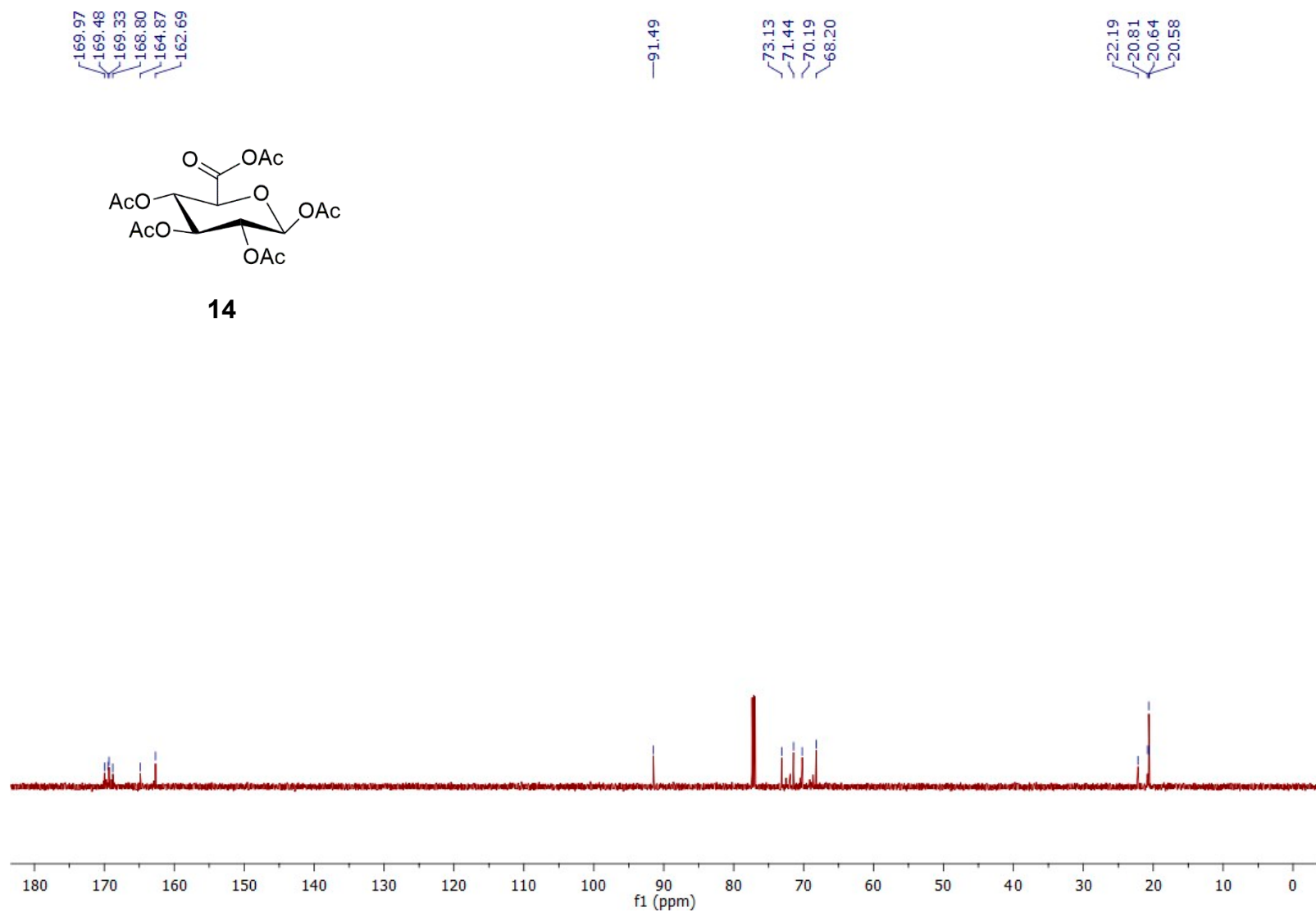


Fig. S22: ¹³C NMR spectrum of 1,2,3,4-tetra-O-acetyl-β-D-glucopyranuronic acetic anhydride **14** (100 MHz/CDCl₃/TMS; δ (ppm)).

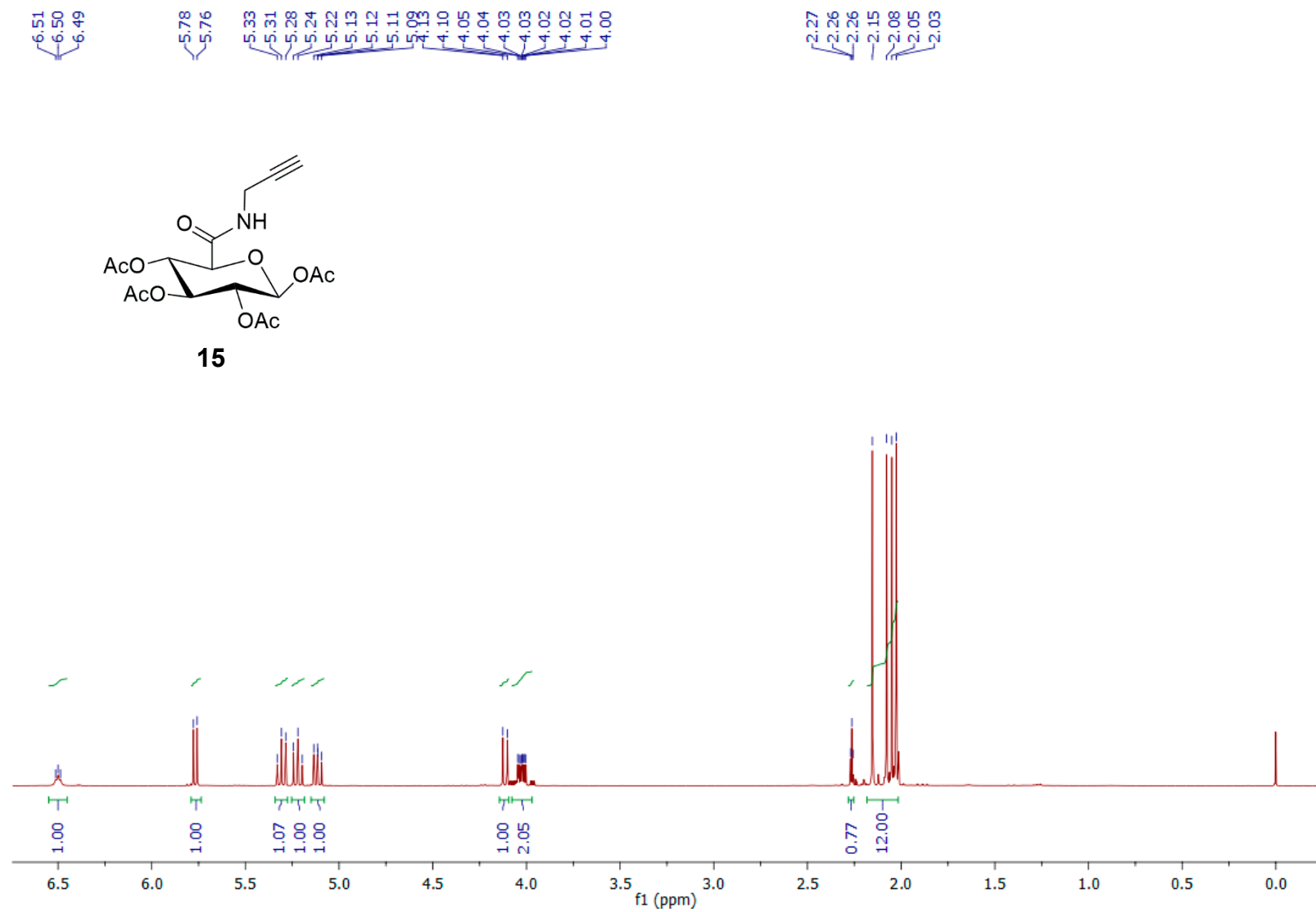


Fig. S23: ^1H NMR spectrum of 1,2,3,4-tetra-*O*-acetyl-*N*-(prop-2-yn-1-yl)- β -D-glucopyranuronic acid amide **15** (400 MHz/ CDCl_3 /TMS; δ (ppm)).

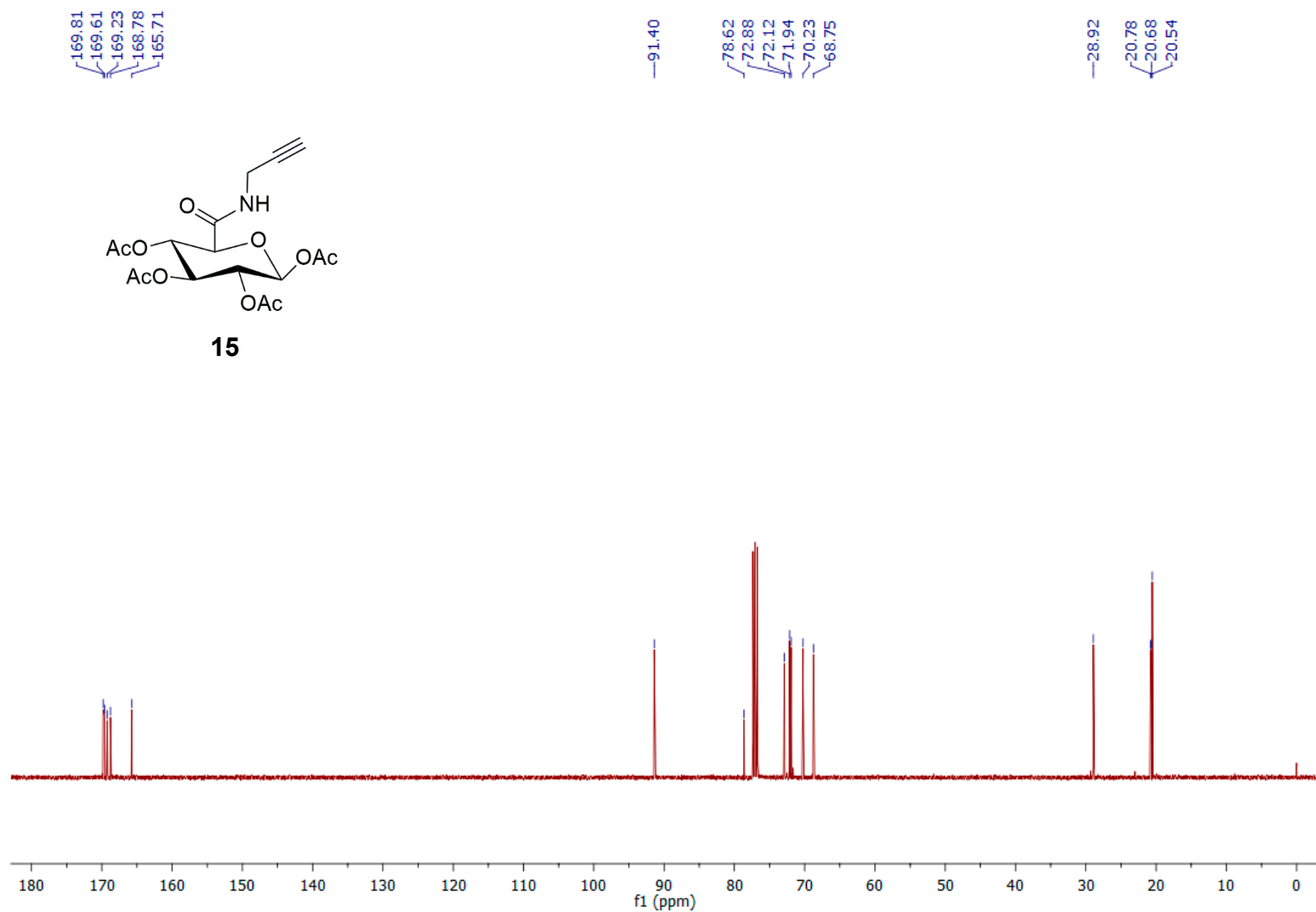


Fig. S24: ^{13}C NMR spectrum of 1,2,3,4-tetra-*O*-acetyl-*N*-(prop-2-yn-1-yl)- β -D-glucopyranuronic acid amide **15** (100 MHz/ CDCl_3 /TMS; δ (ppm)).

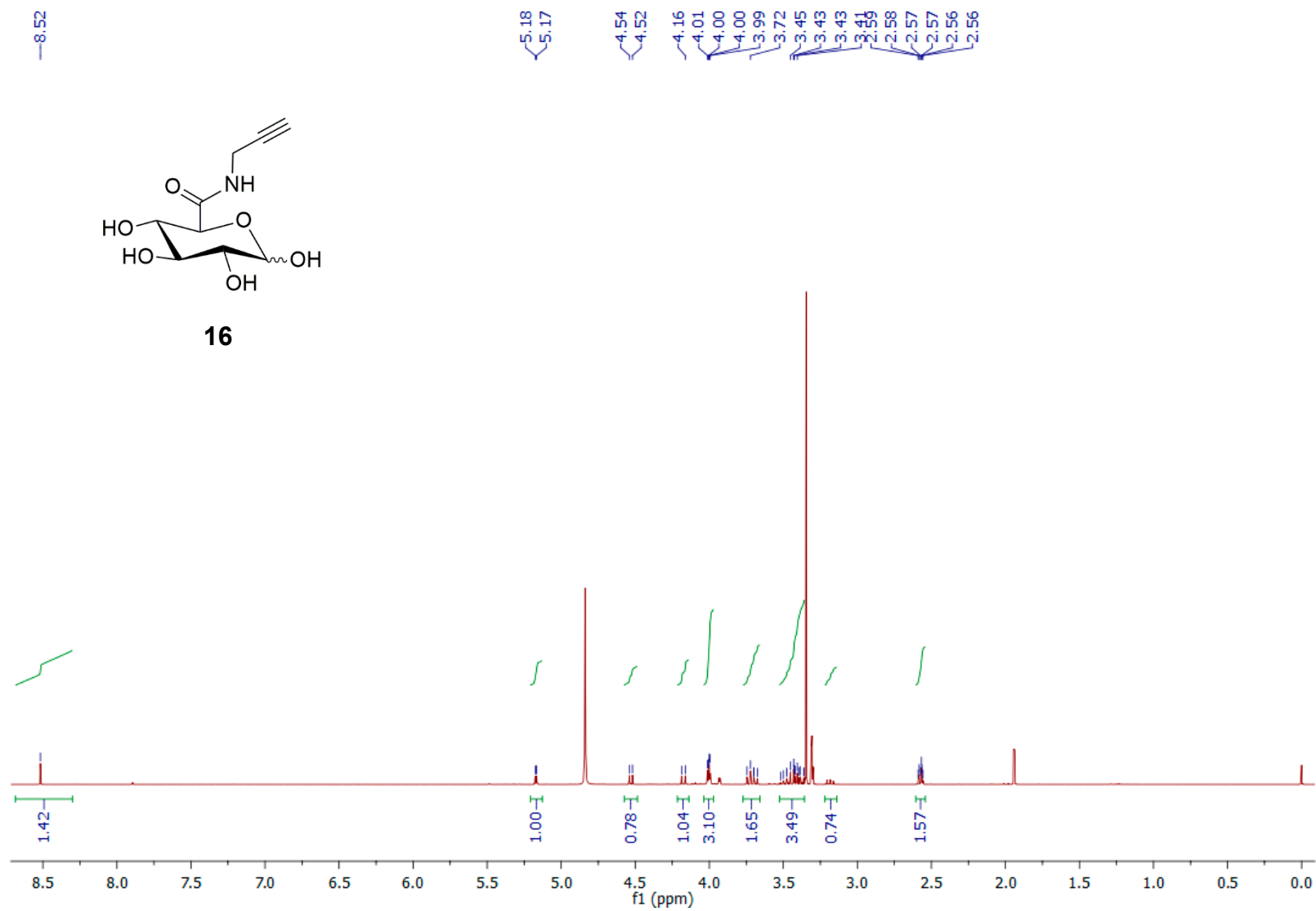


Fig. S25: ¹H NMR spectrum of *N*-(prop-2-yn-1-yl)-D-glucopyranuronic acid amide **16** (400 MHz/CD₃OD/TMS; δ (ppm)).

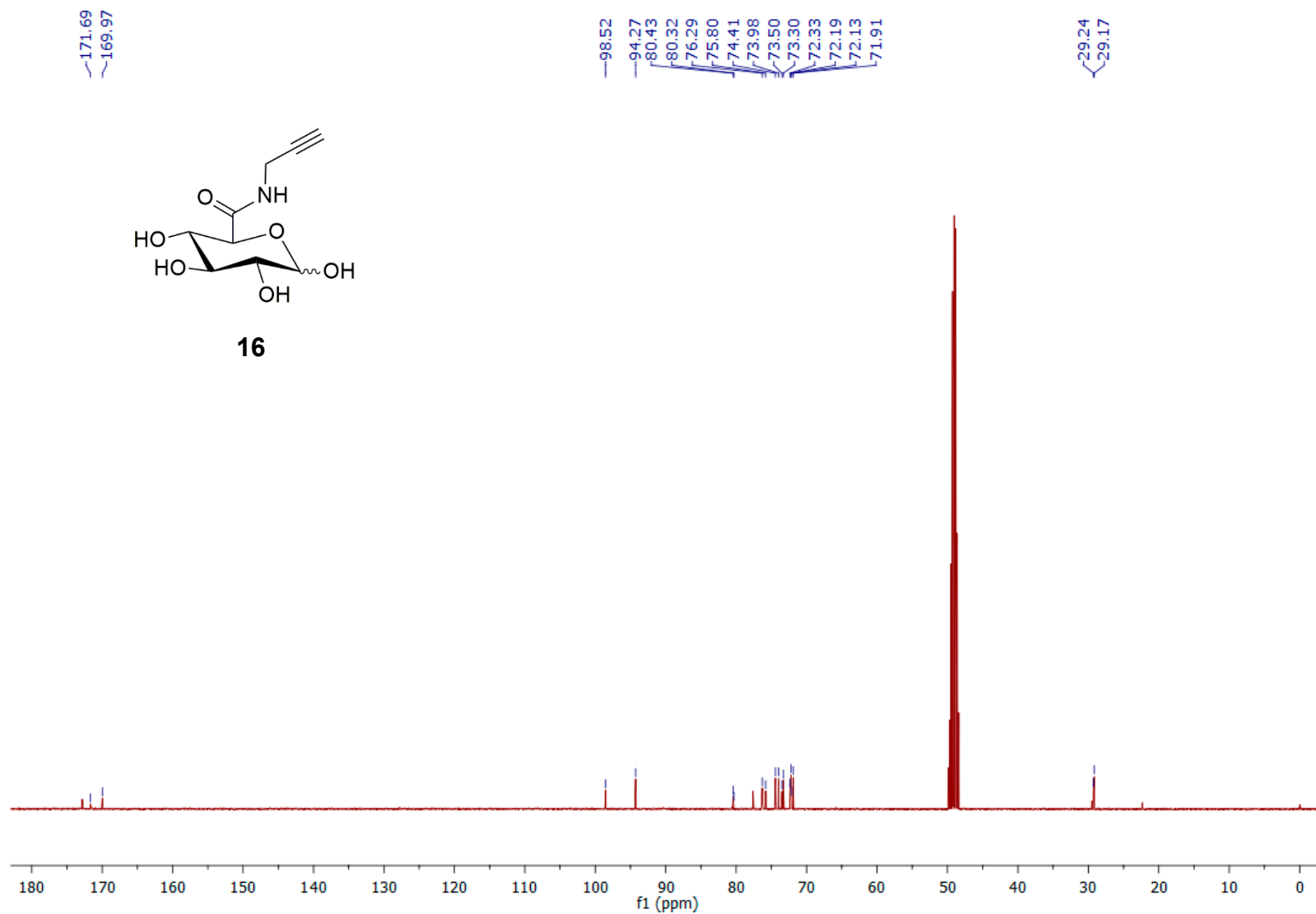


Fig. S26: ^{13}C NMR spectrum of *N*-(prop-2-yn-1-yl)-D-glucopyranuronic acid amide **16** (100 MHz/ CD_3OD /TMS; δ (ppm)).

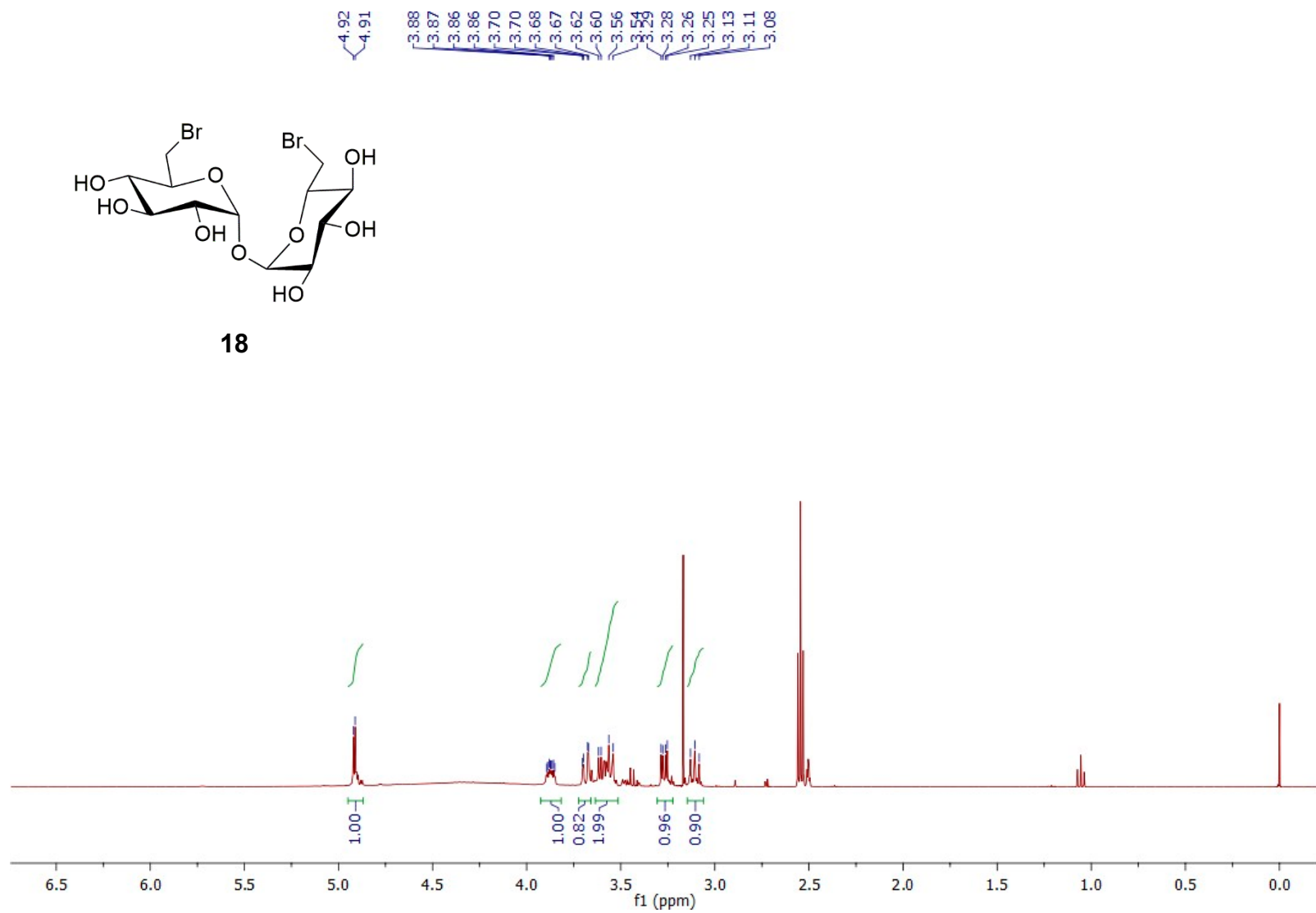


Fig. S27: ¹H NMR spectrum of 6,6'-dibromo-6,6'-dideoxy-D-trehalose **18** (400 MHz/DMSO/TMS; δ (ppm)).

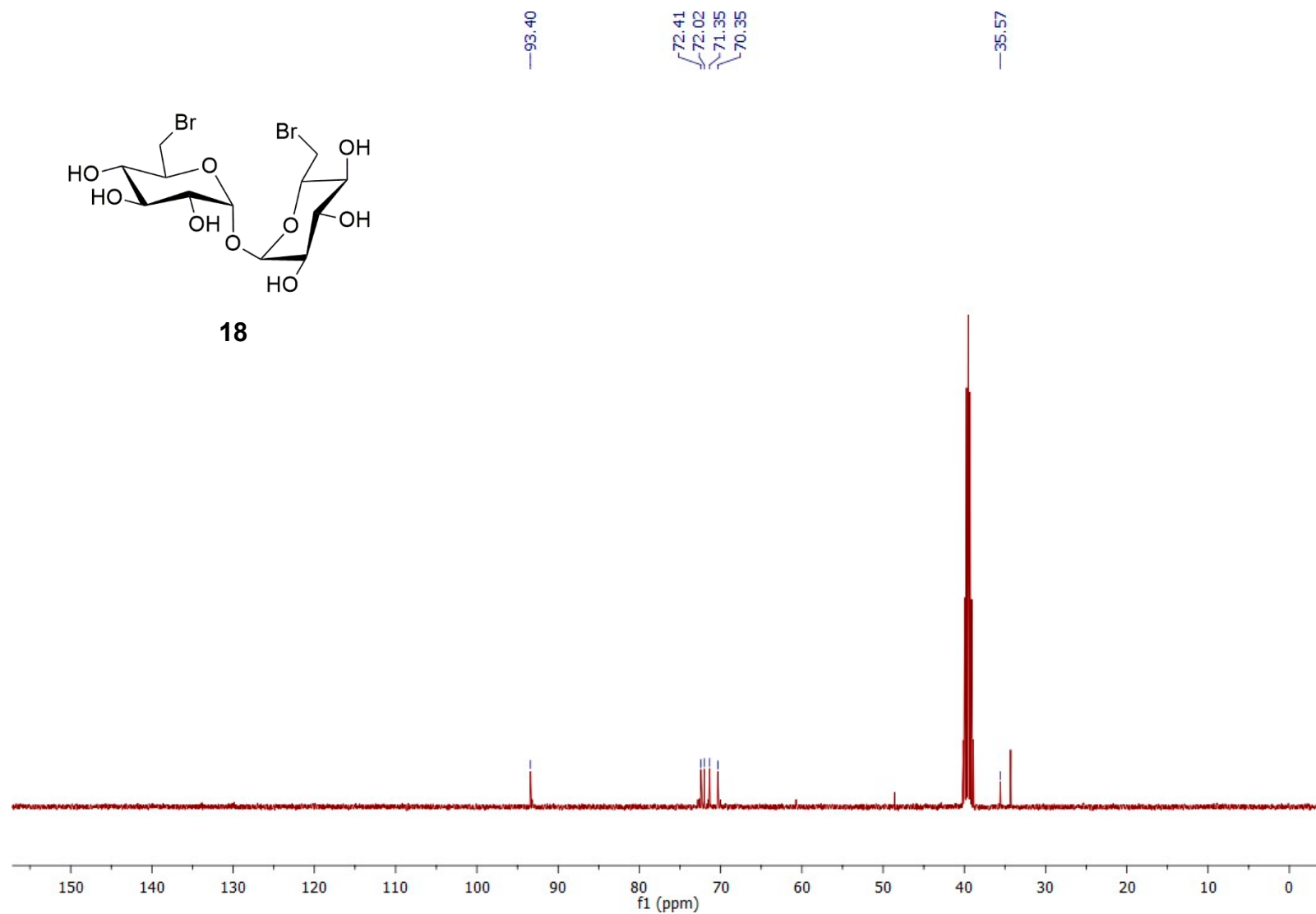


Fig. S28: ^{13}C NMR spectrum of 6,6'-dibromo-6,6'-dideoxy-D-trehalose **18** (100 MHz/DMSO/TMS; δ (ppm)).

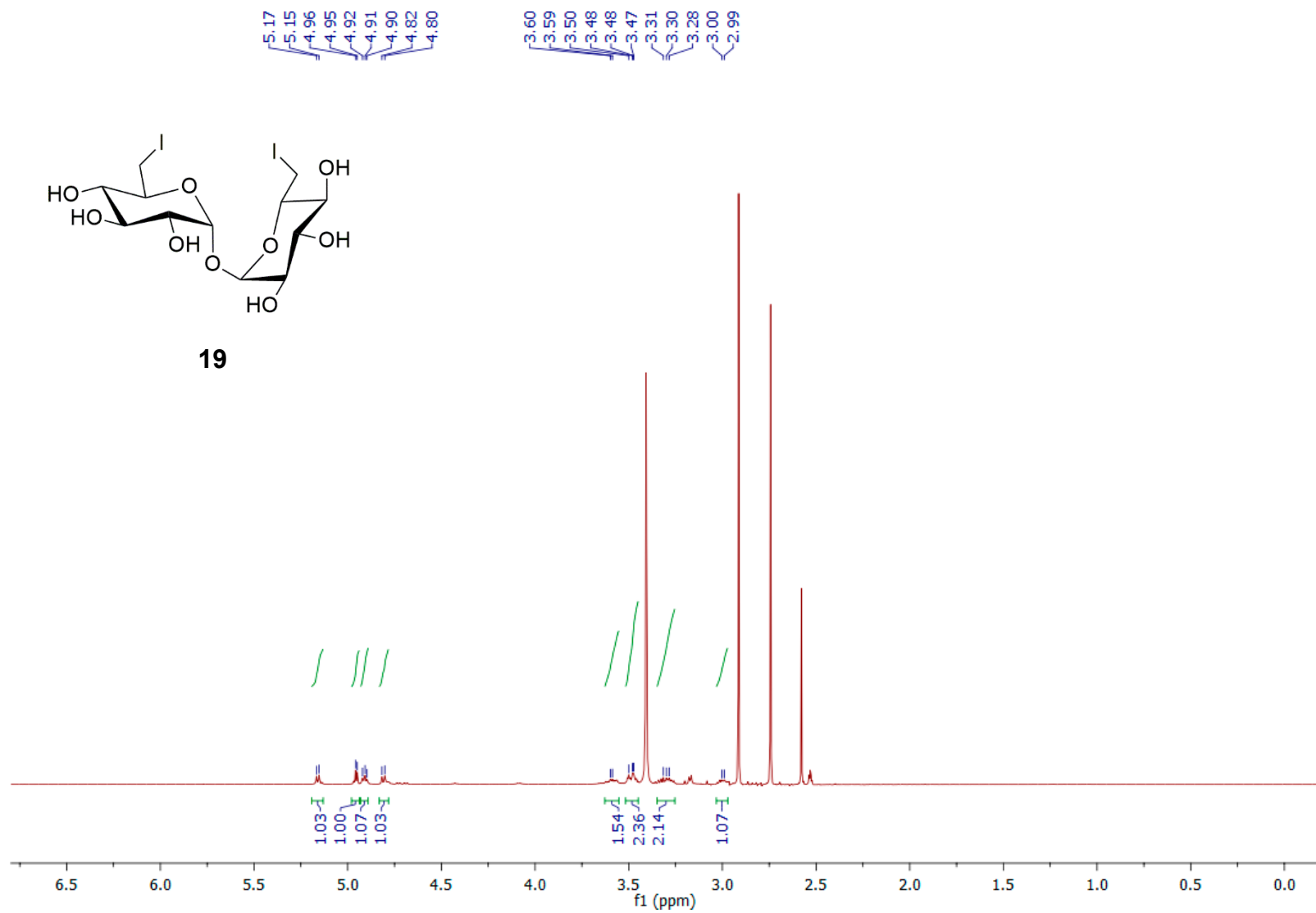


Fig. S29: ^1H NMR spectrum of 6,6'-diiodo-6,6'-dideoxy-D-trehalose **19** (400 MHz/DMSO/TMS; δ (ppm)).

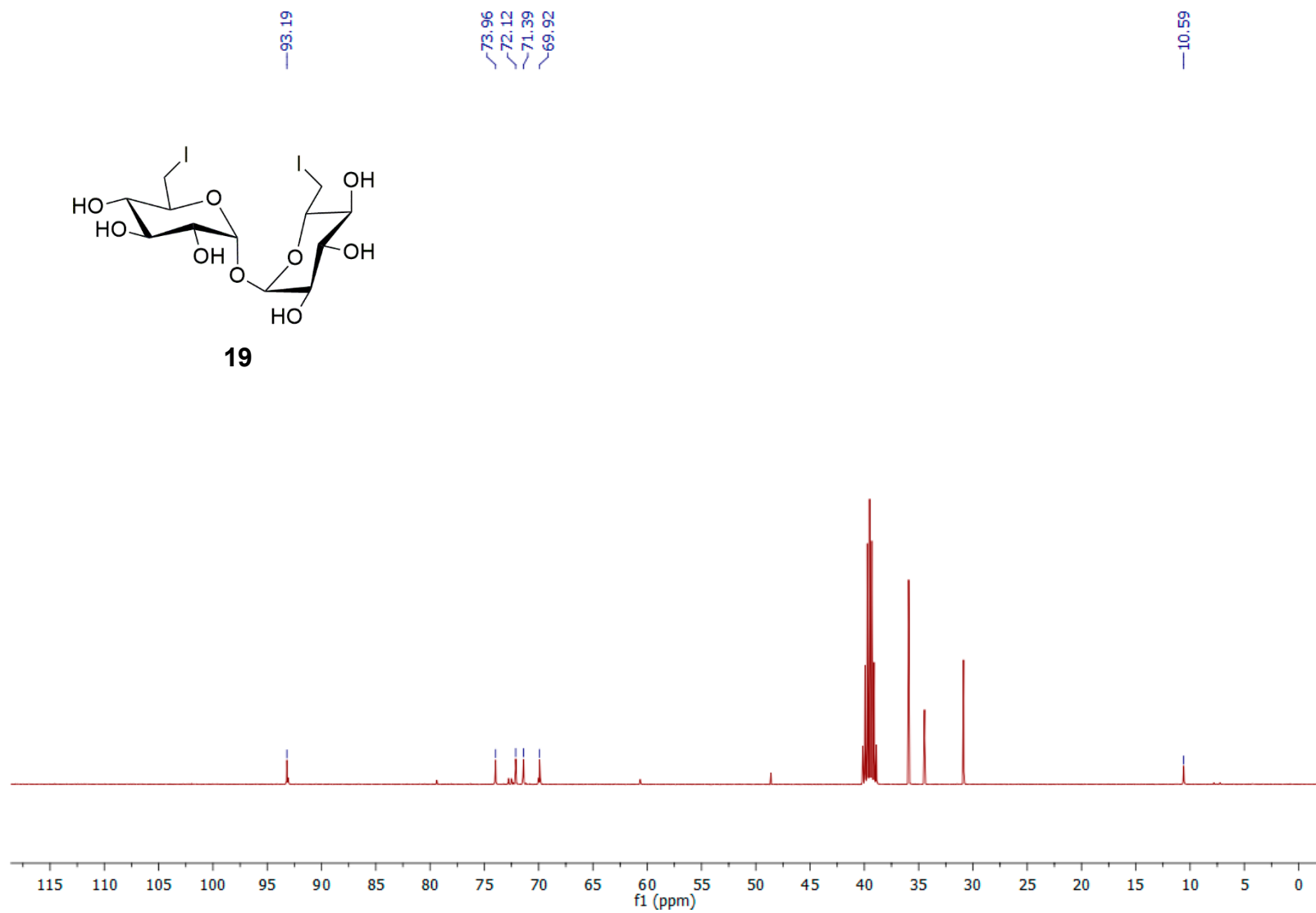


Fig. S30: ¹³C NMR spectrum of 6,6'-diiodo-6,6'-dideoxy-D-trehalose **19** (100 MHz/DMSO/TMS; δ (ppm)).

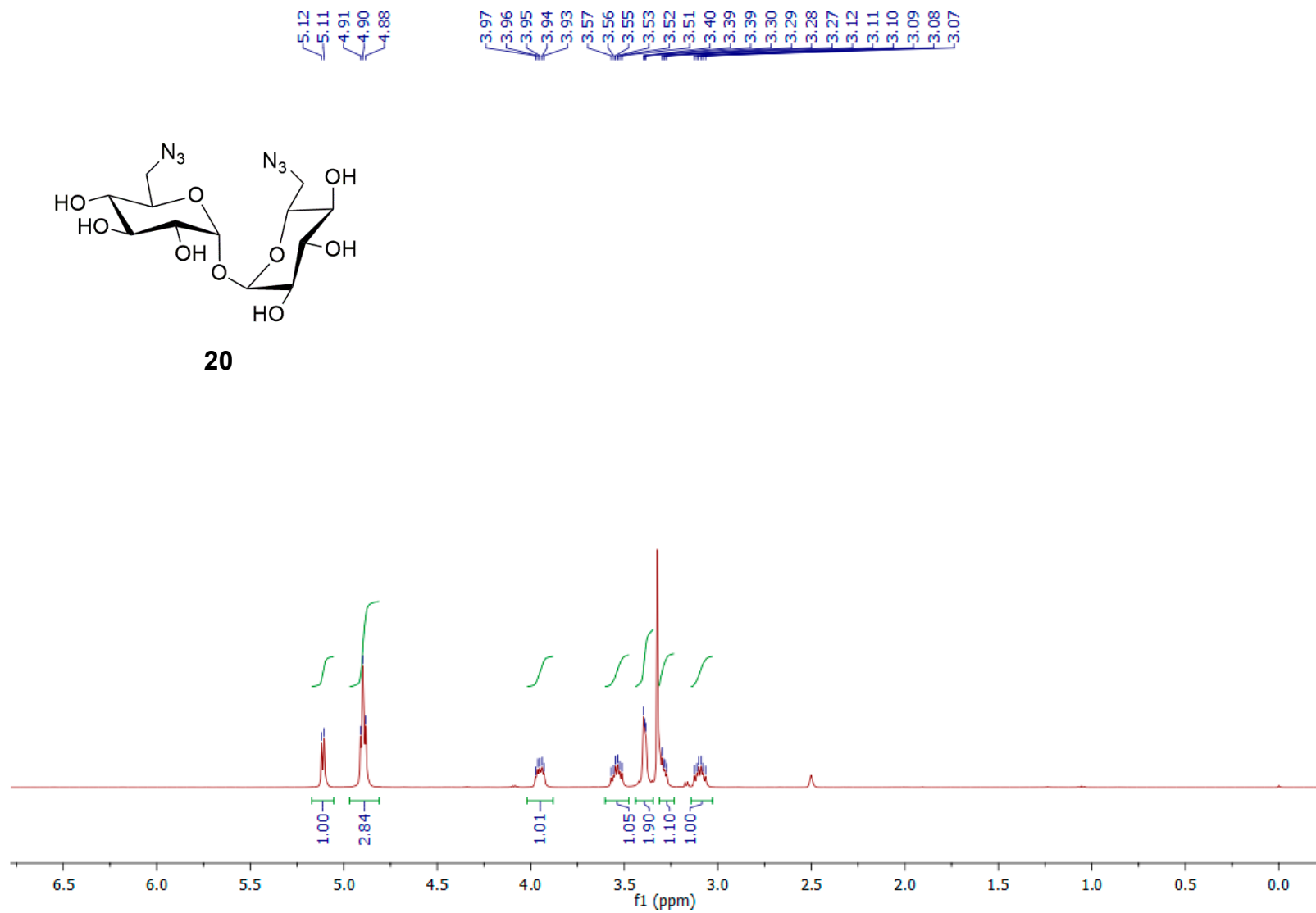


Fig. S31: ^1H NMR spectrum of 6,6'-diazido-6,6'-dideoxy-D-trehalose **20** (400 MHz/DMSO/TMS; δ (ppm)).

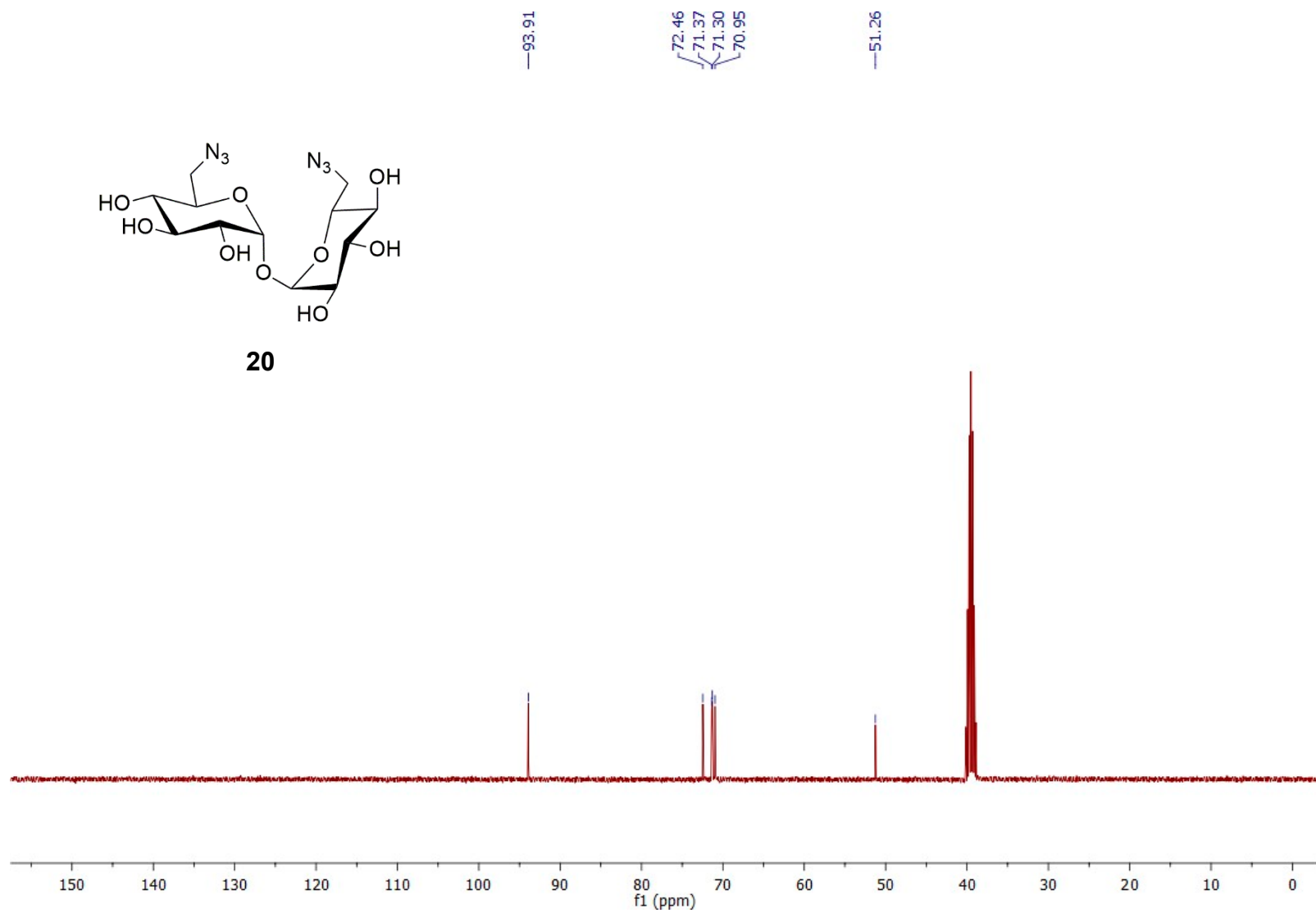


Fig. S32: ^{13}C NMR spectrum of 6,6'-diazido-6,6'-dideoxy-D-trehalose **20** (100 MHz/DMSO/TMS; δ (ppm)).

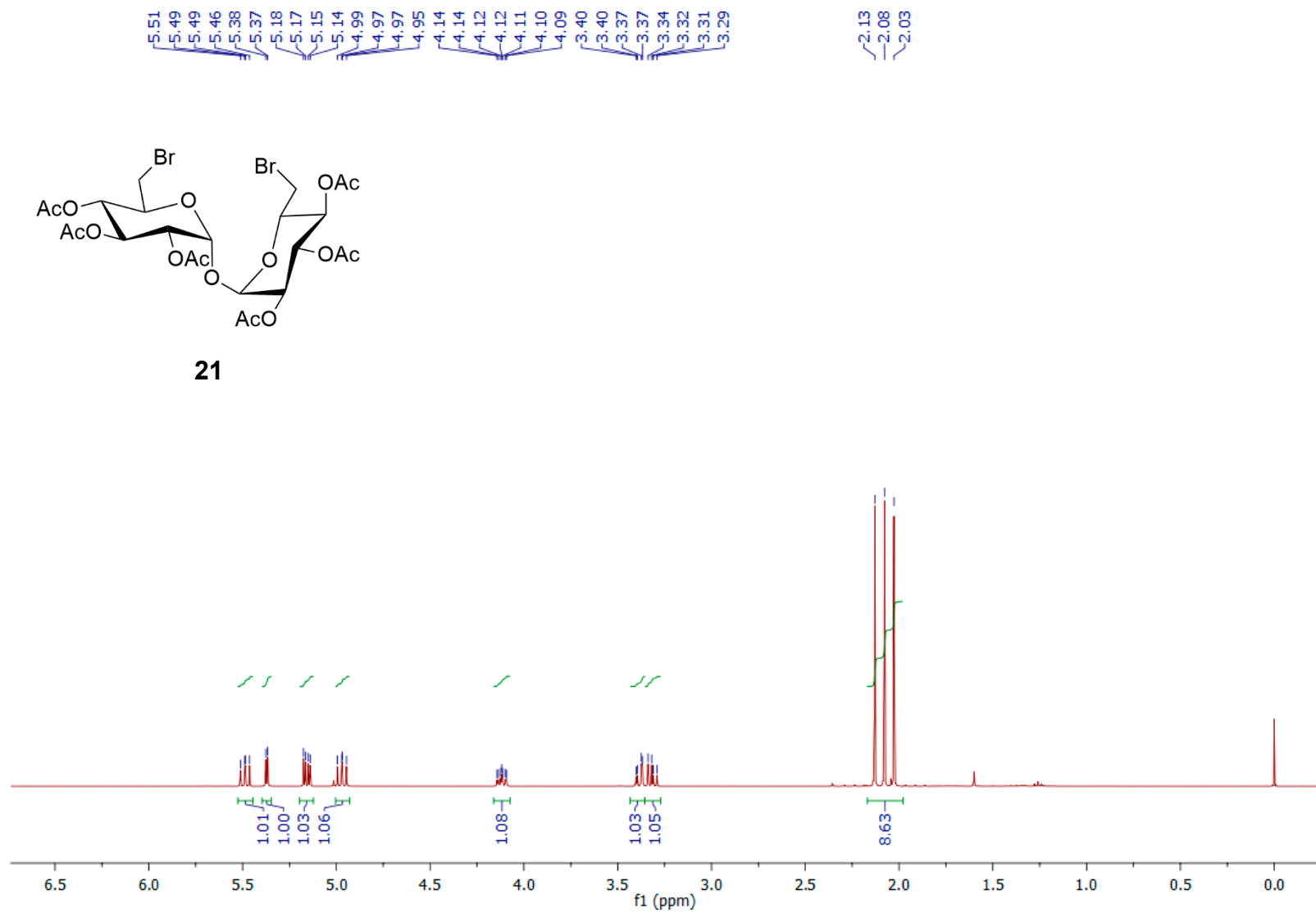


Fig. S33: ^1H NMR spectrum of 2,3,4,2',3',4'-hexa-*O*-acetyl-6,6'-dibromo-6,6'-dideoxy-D-trehalose **21** (400 MHz/ CDCl_3/TMS ; δ (ppm)).

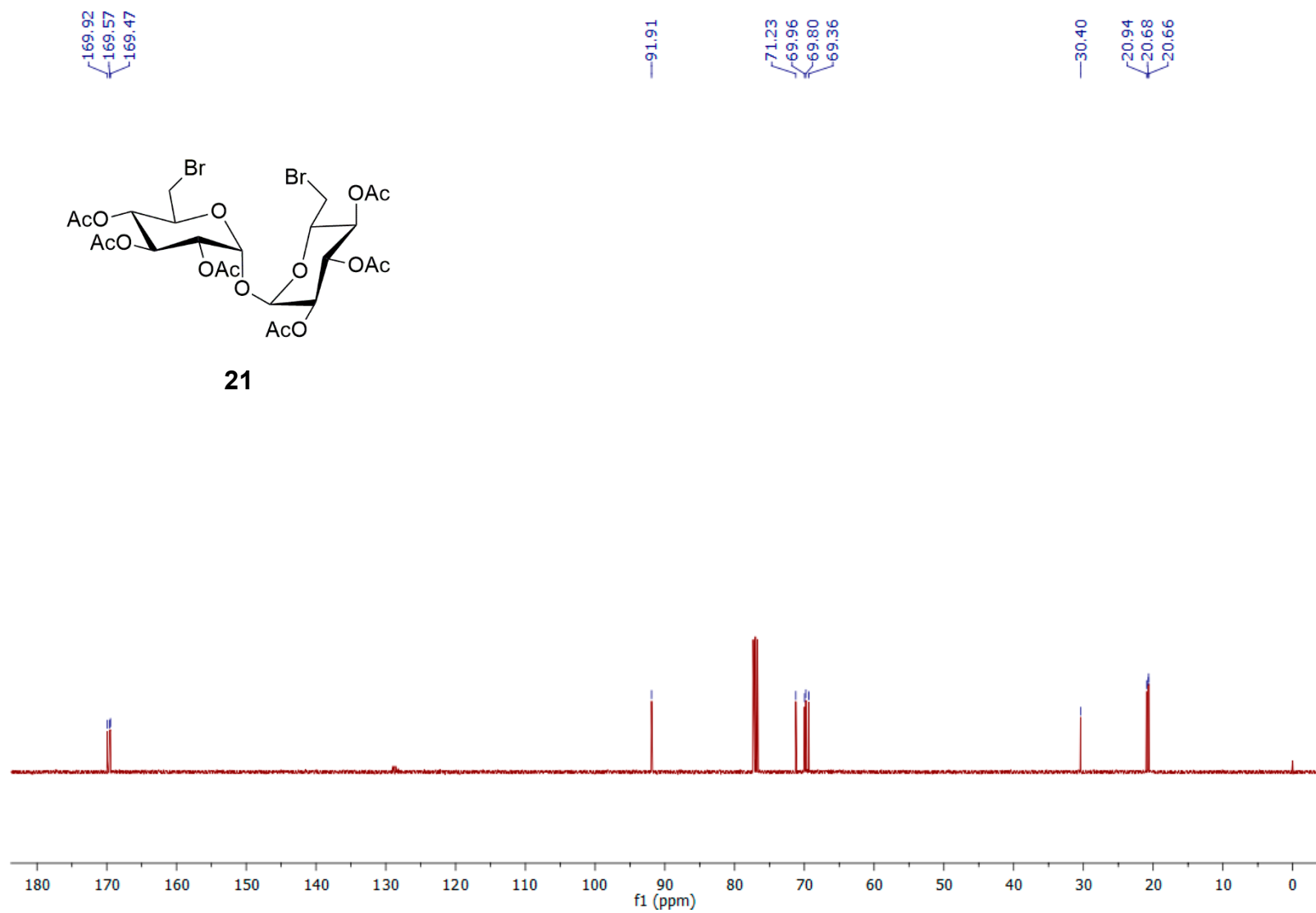


Fig. S34: ¹³C NMR spectrum of 2,3,4,2',3',4'-hexa-*O*-acetyl-6,6'-dibromo-6,6'-dideoxy-D-trehalose **21** (100 MHz/CDCl₃/TMS; δ (ppm)).

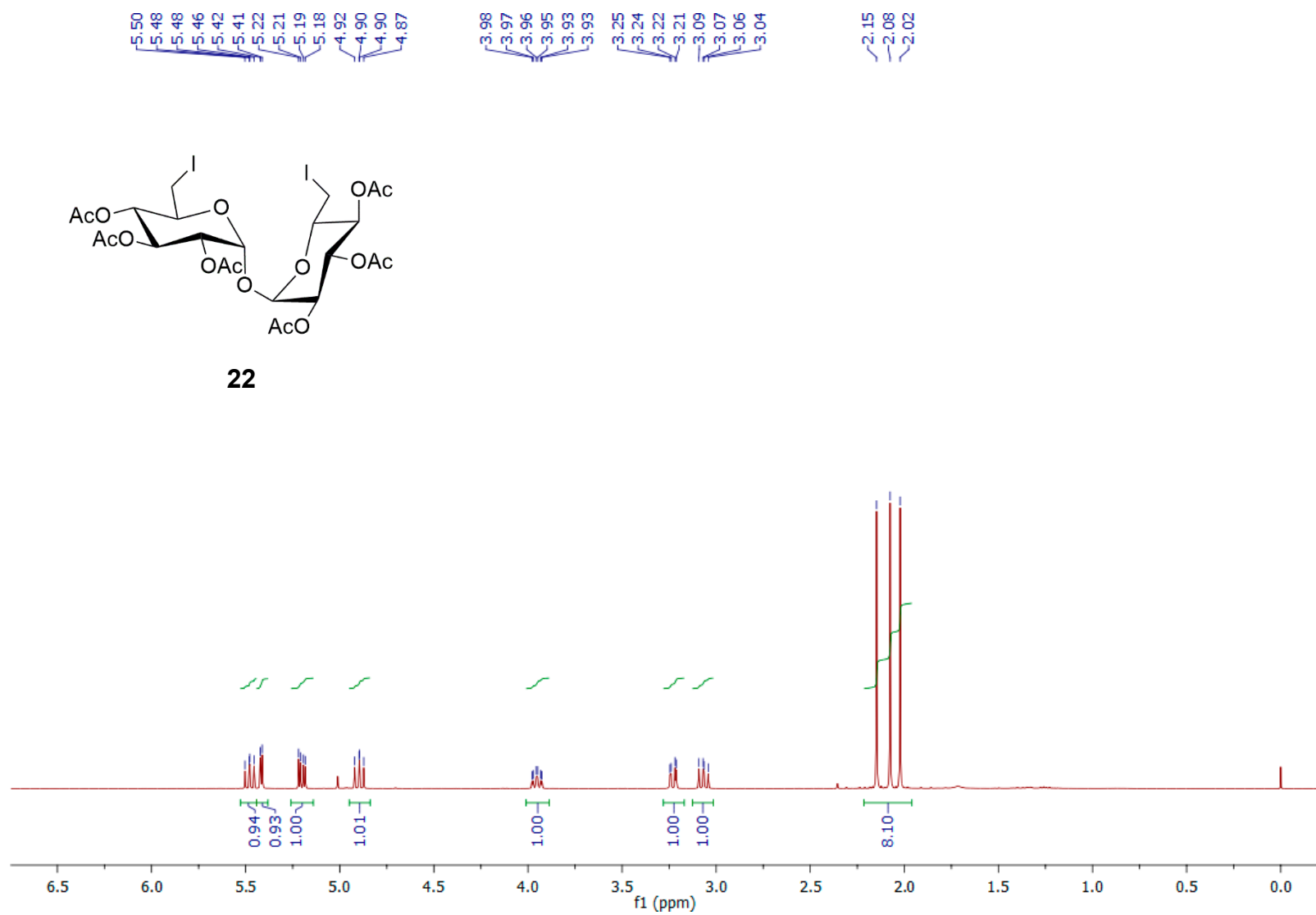


Fig. S35: ¹H NMR spectrum of 2,3,4,2',3',4'-hexa-O-acetyl-6,6'-diiodo-6,6'-dideoxy-D-trehalose **22** (400 MHz/CDCl₃/TMS; δ (ppm)).

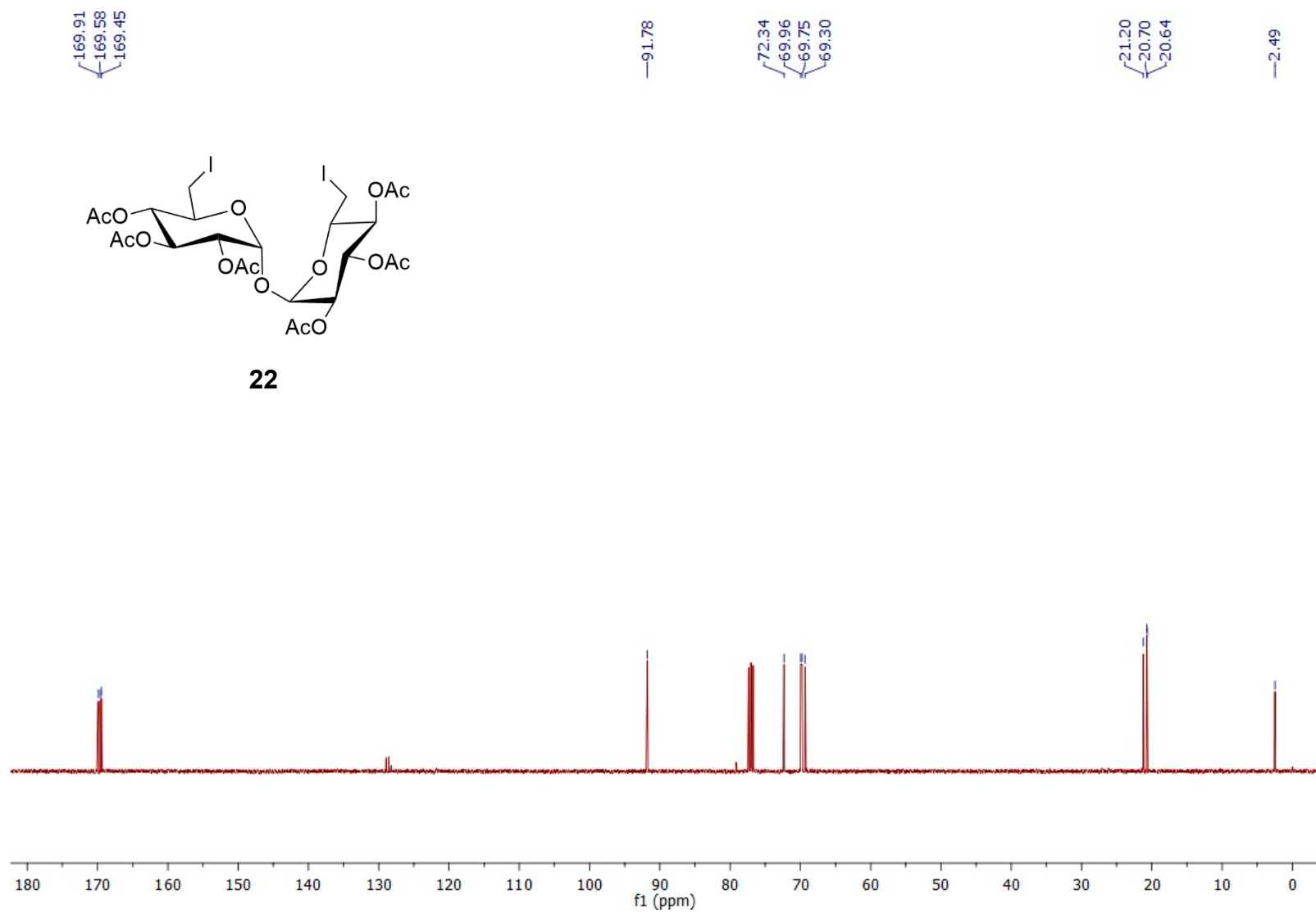


Fig. S36: ¹³C NMR spectrum of 2,3,4,2',3',4'-hexa-*O*-acetyl-6,6'-diiodo-6,6'-dideoxy-D-trehalose **22** (100 MHz/CDCl₃/TMS; δ (ppm)).

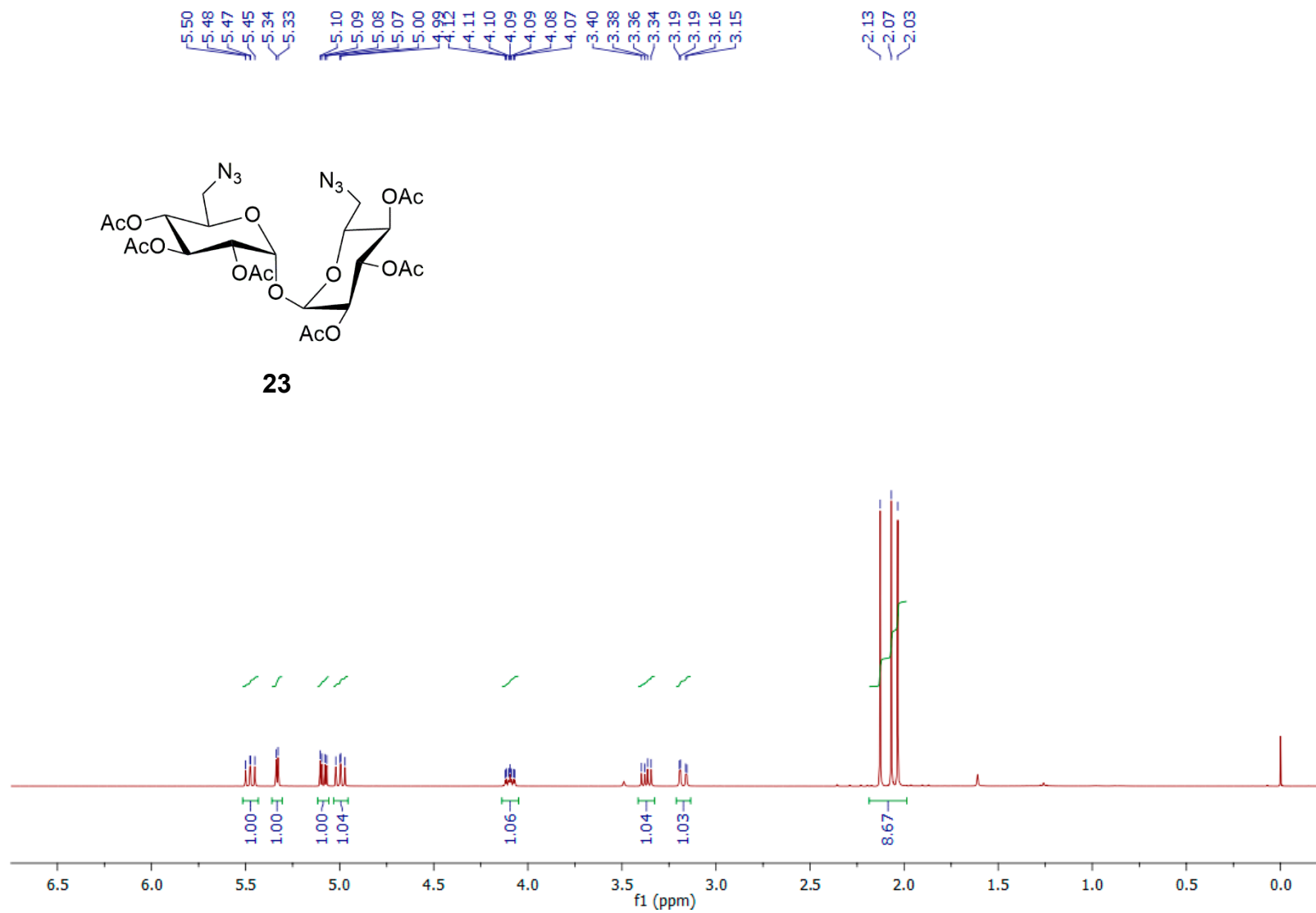


Fig. S37: ¹H NMR spectrum of 2,3,4,2',3',4'-hexa-*O*-acetyl-6,6'-diazido-6,6'-dideoxy-D-trehalose **23** (400 MHz/CDCl₃/TMS; δ (ppm)).

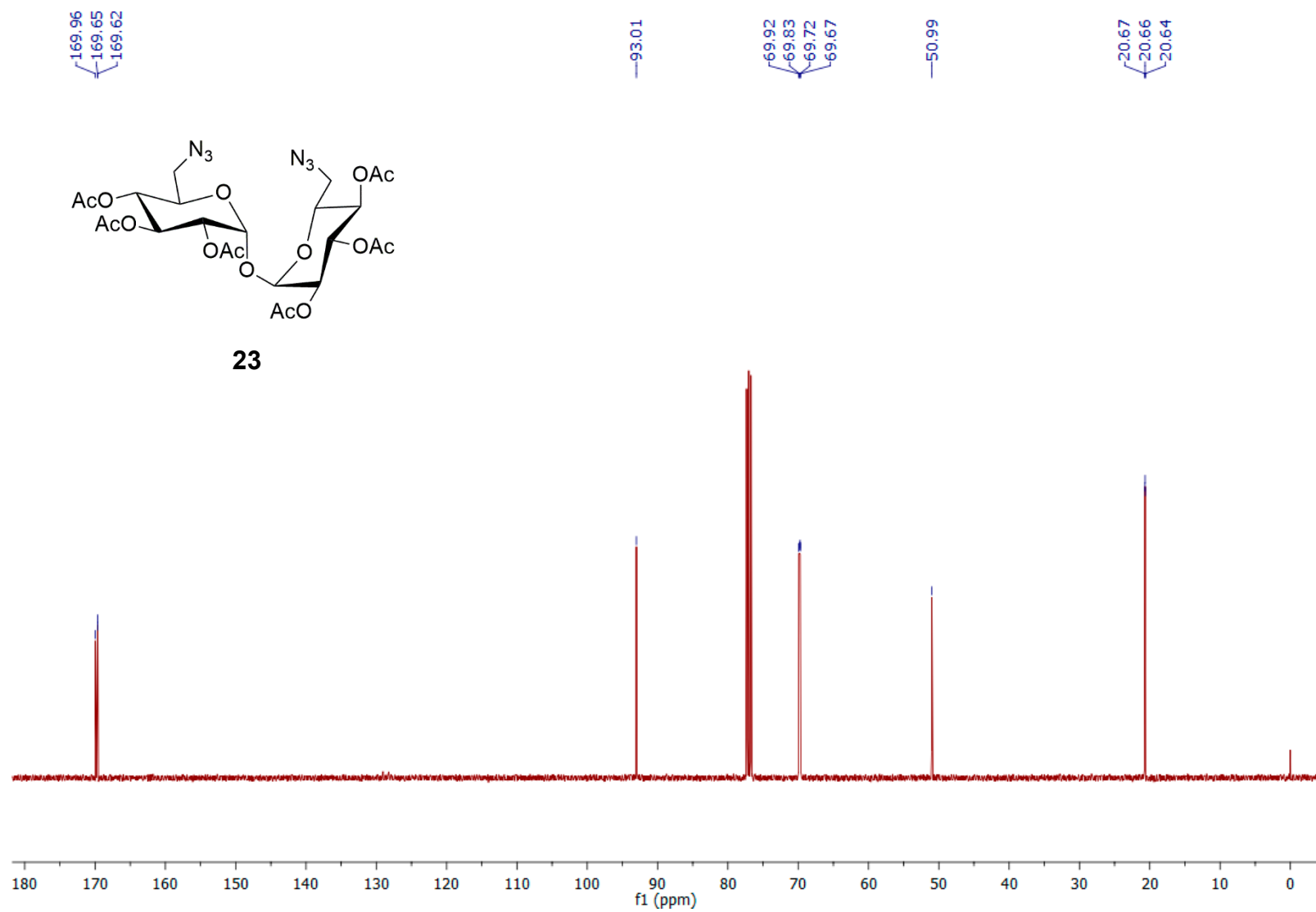


Fig. S38: ^{13}C NMR spectrum of 2,3,4,2',3',4'-hexa-*O*-acetyl-6,6'-diazido-6,6'-dideoxy-D-trehalose **23** (100 MHz/ CDCl_3/TMS ; δ (ppm)).

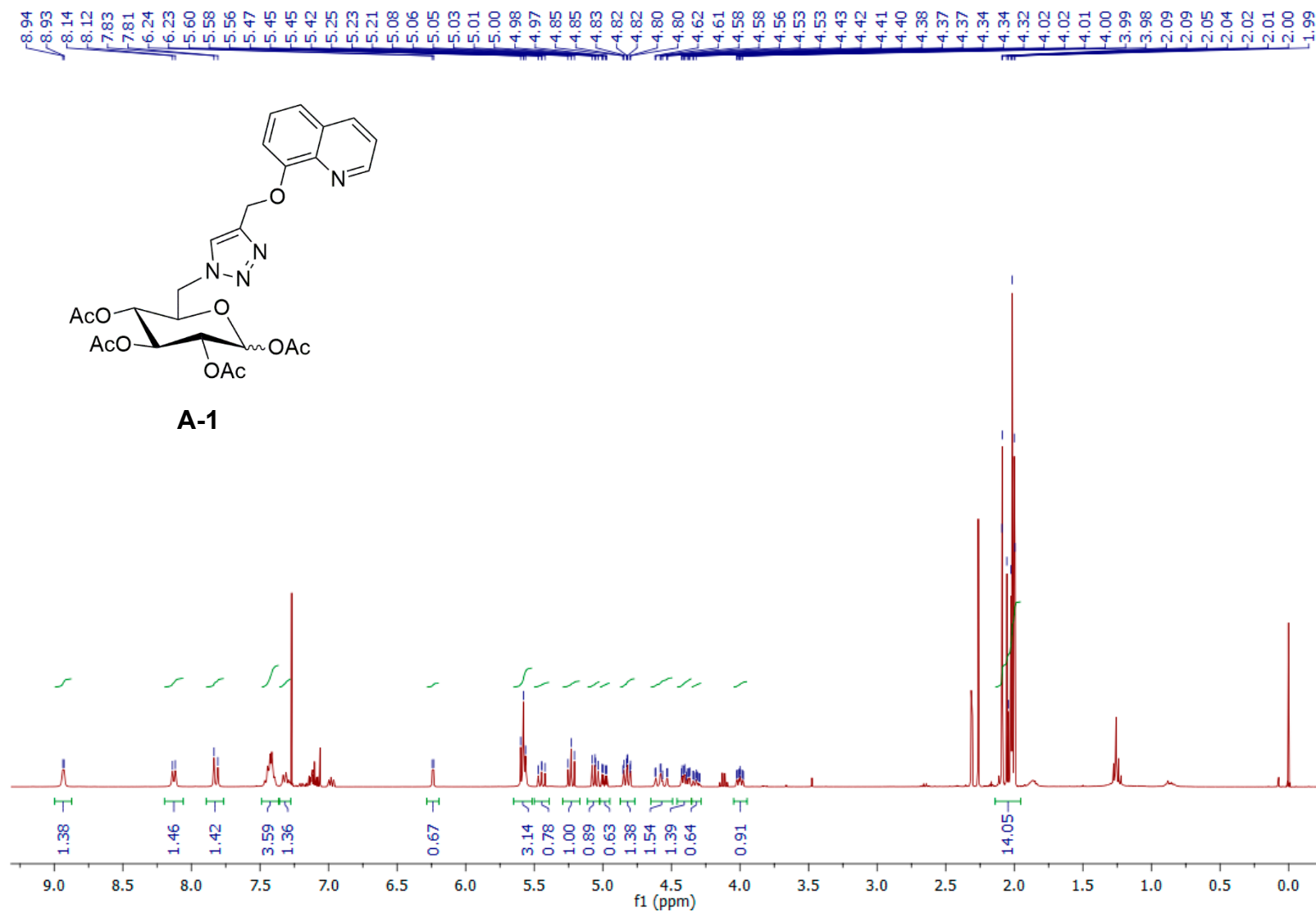


Fig. S39: ¹H NMR spectrum of glycoconjugates **A-1** (400 MHz/CDCl₃/TMS; δ (ppm)).

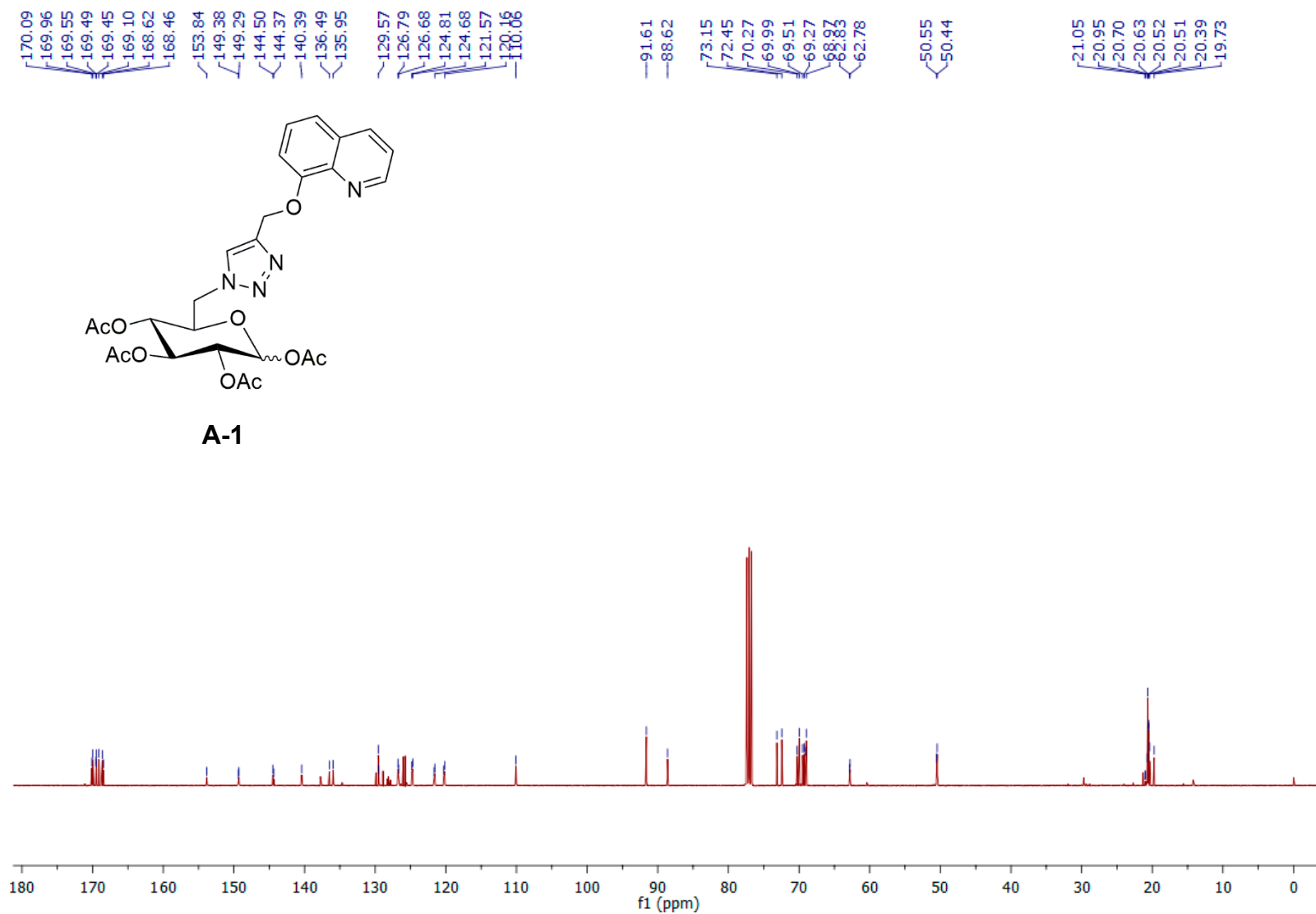


Fig. S40: ^{13}C NMR spectrum of glycoconjugates **A-1** (100 MHz/ CDCl_3/TMS ; δ (ppm)).

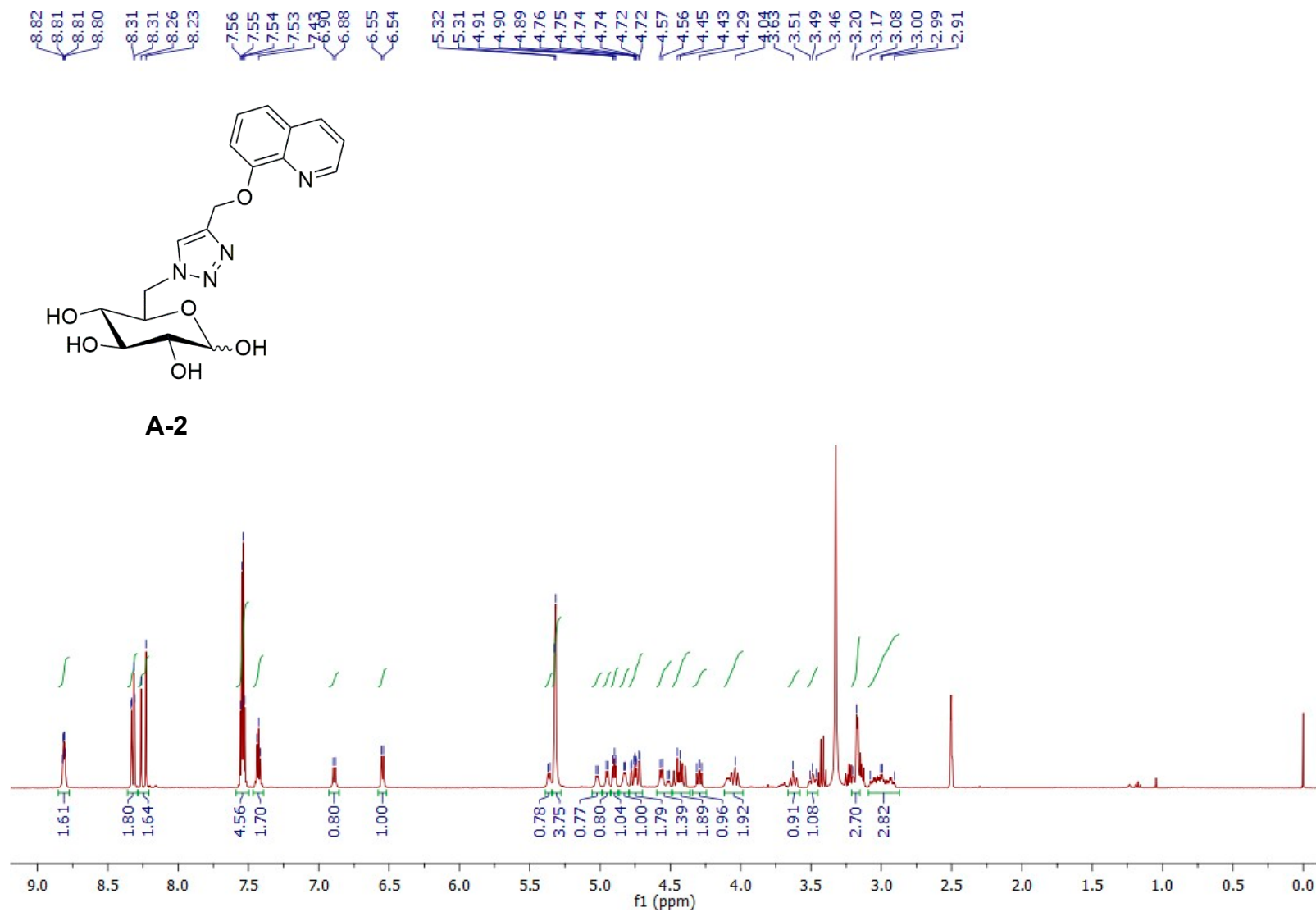


Fig. S41: ^1H NMR spectrum of glycoconjugates **A-2** (400 MHz/DMSO/TMS; δ (ppm)).

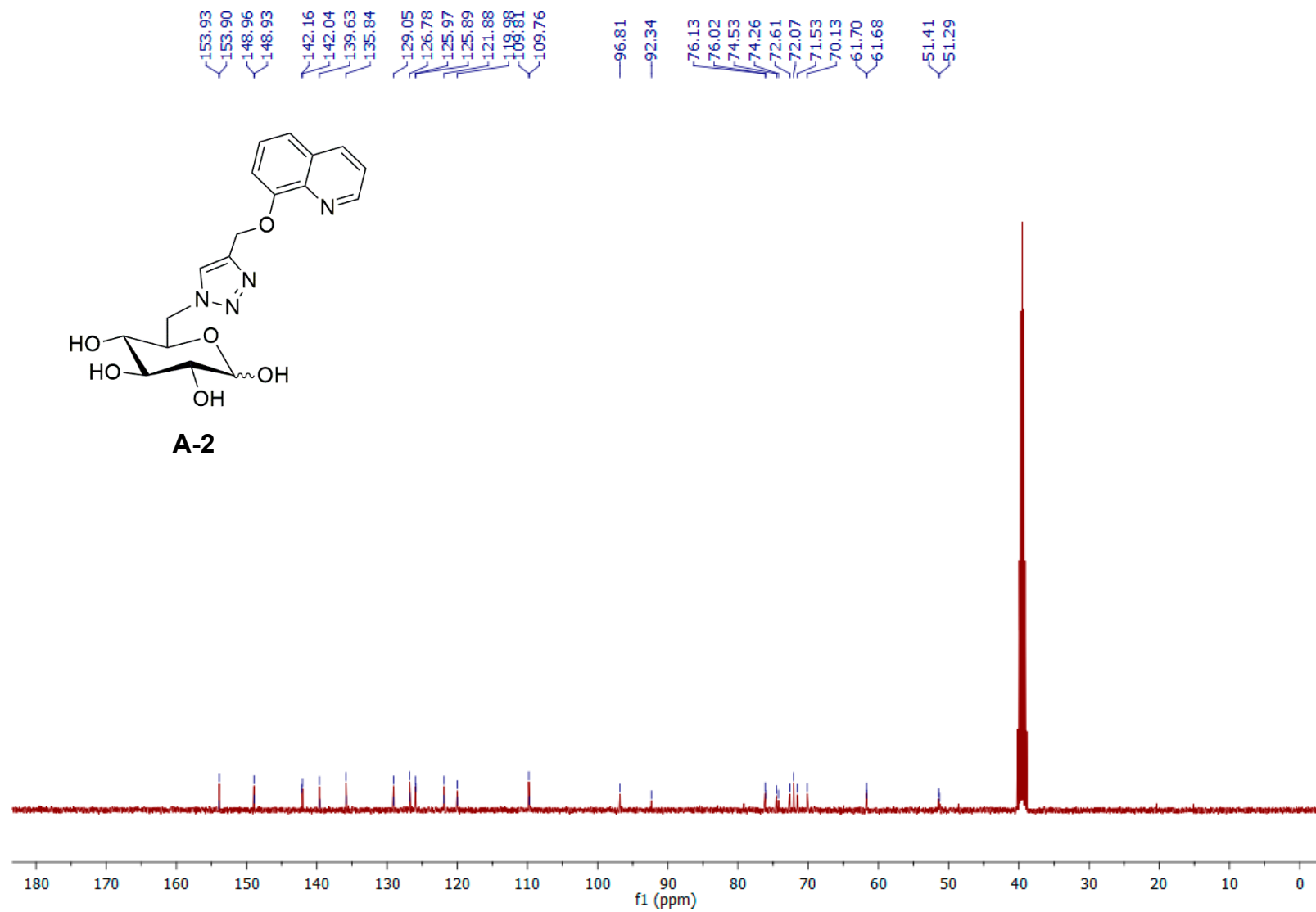


Fig. S42: ¹³C NMR spectrum of glycoconjugates **A-2** (100 MHz/DMSO/TMS; δ (ppm)).

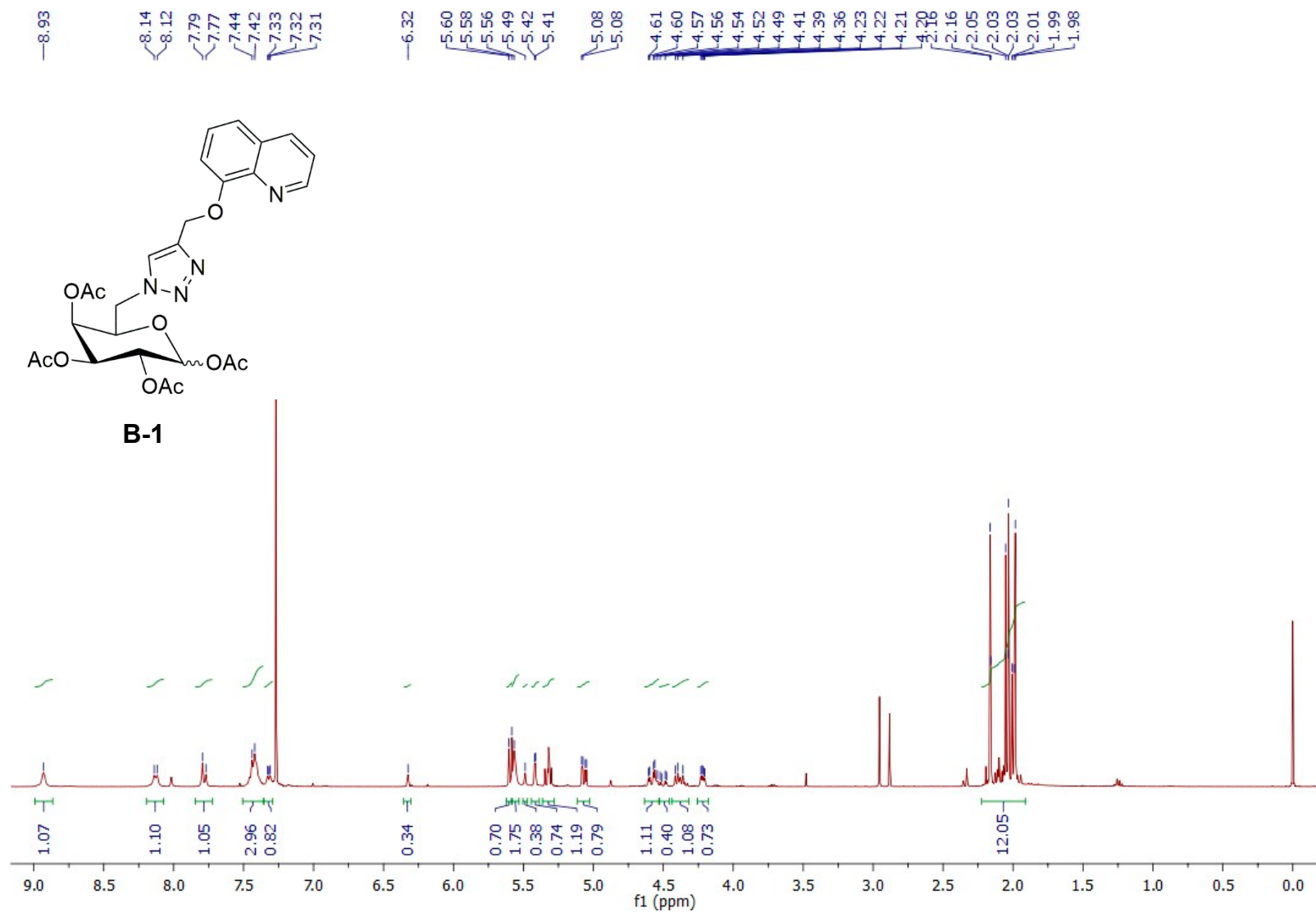


Fig. S43: ¹H NMR spectrum of glycoconjugates **B-1** (400 MHz/CDCl₃/TMS; δ (ppm)).

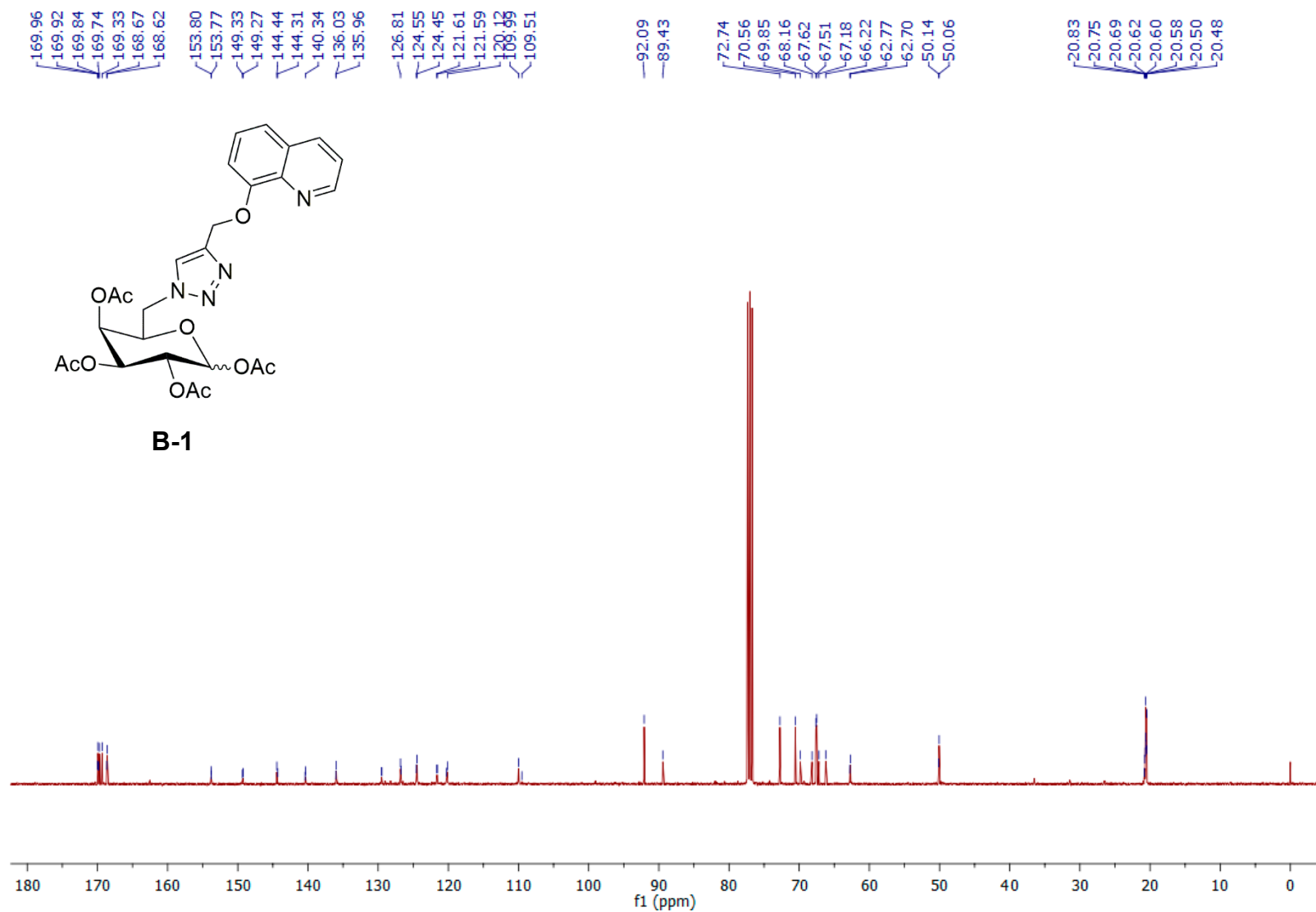


Fig. S44: ¹³C NMR spectrum of glycoconjugates **B-1** (100 MHz/CDCl₃/TMS; δ (ppm)).

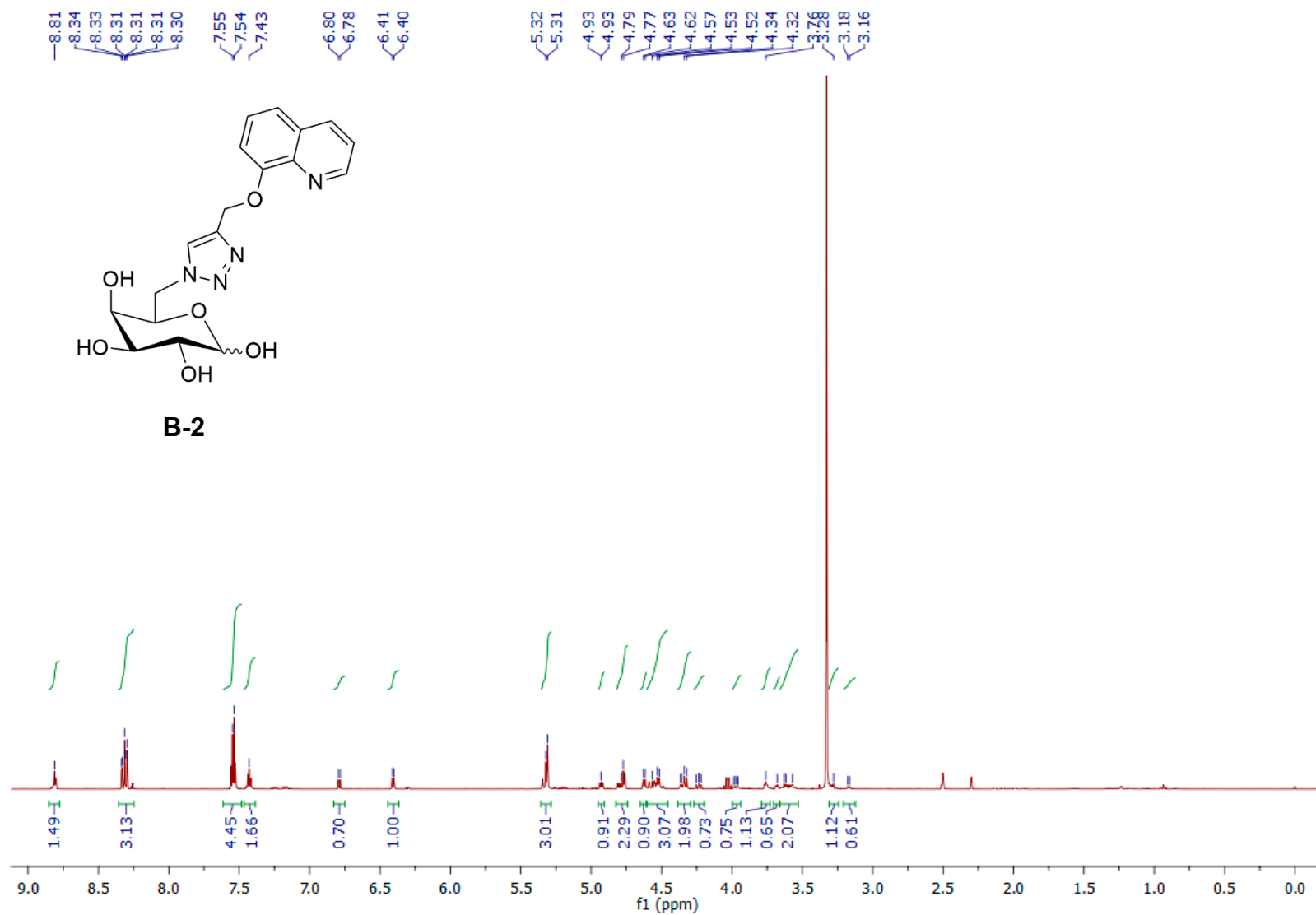


Fig. S45: ¹H NMR spectrum of glycoconjugates **B-2** (400 MHz/DMSO/TMS; δ (ppm)).

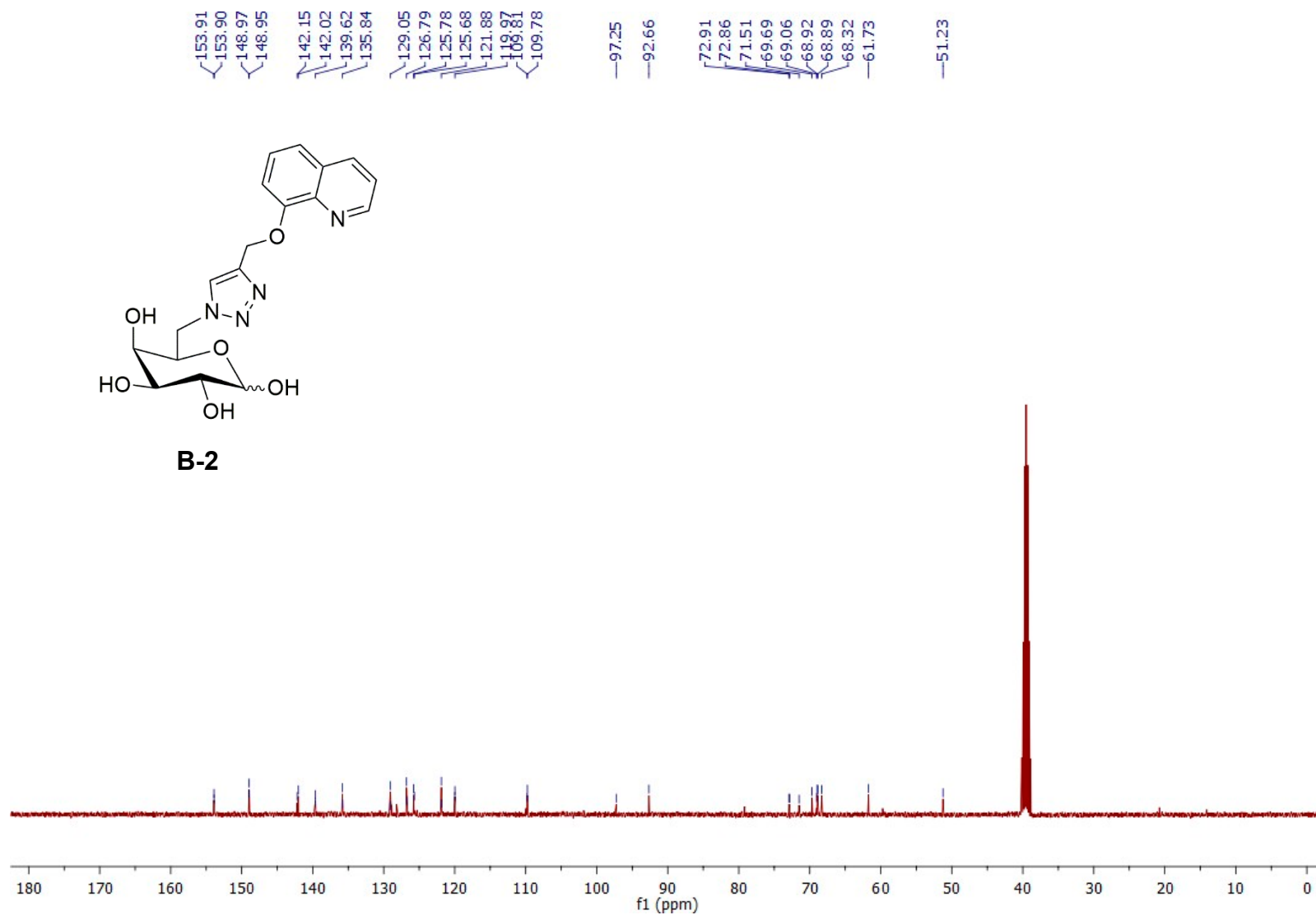


Fig. S46: ¹³C NMR spectrum of glycoconjugates **B-2** (100 MHz/DMSO/TMS; δ (ppm)).

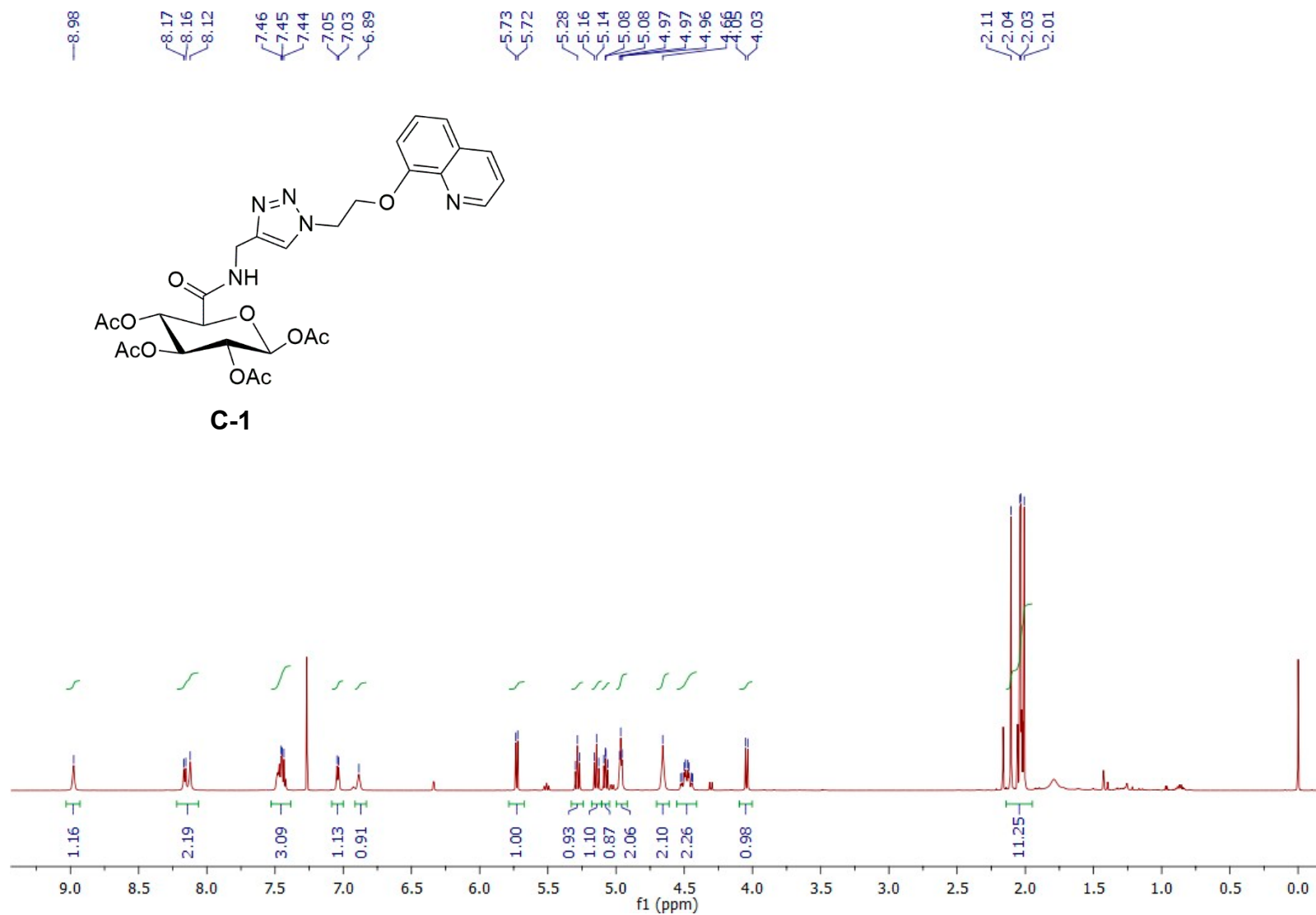


Fig. S47: ^1H NMR spectrum of glycoconjugates **C-1** (400 MHz/ CDCl_3/TMS ; δ (ppm)).

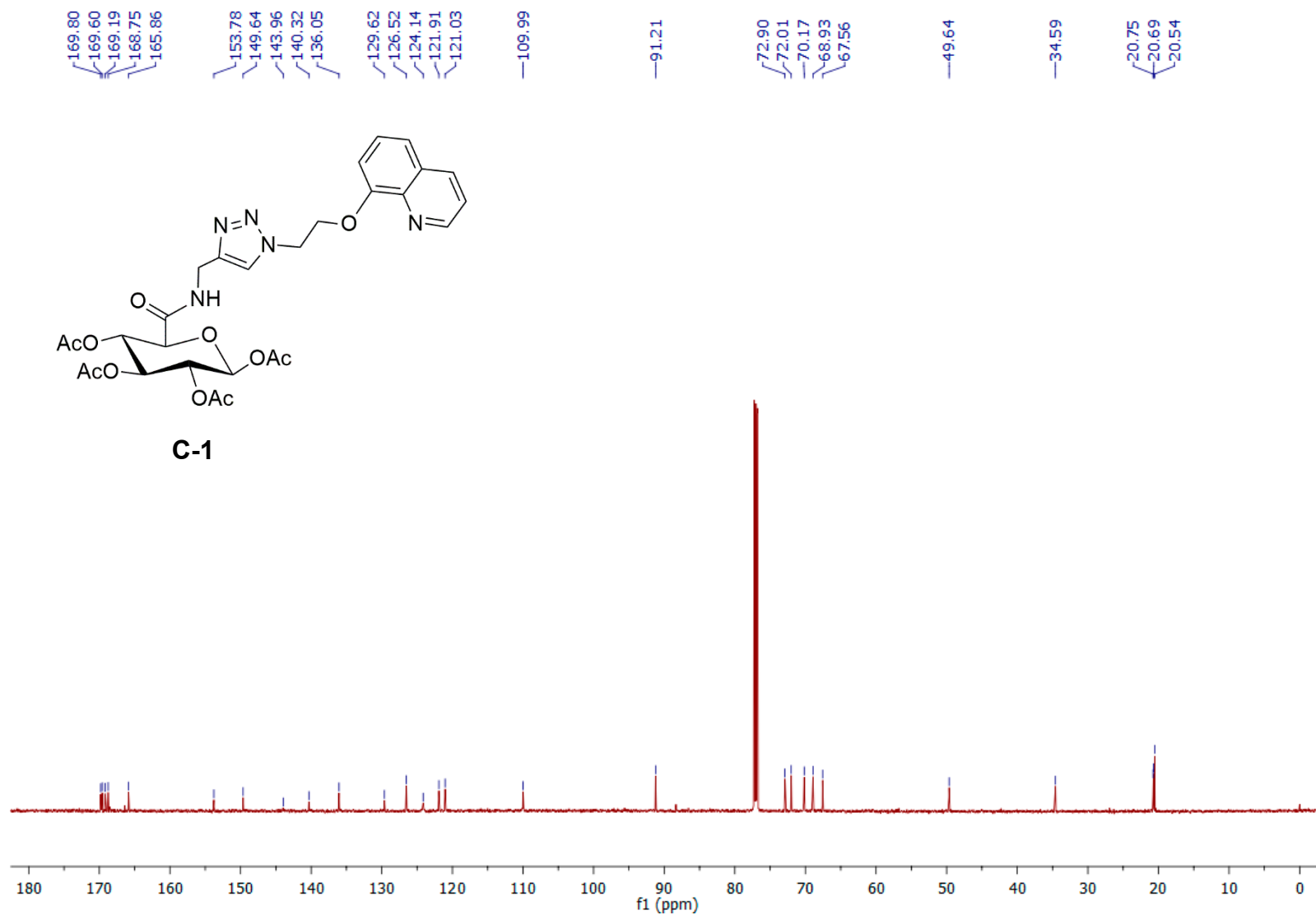


Fig. S48: ¹³C NMR spectrum of glycoconjugates C-1 (100 MHz/CDCl₃/TMS; δ (ppm)).

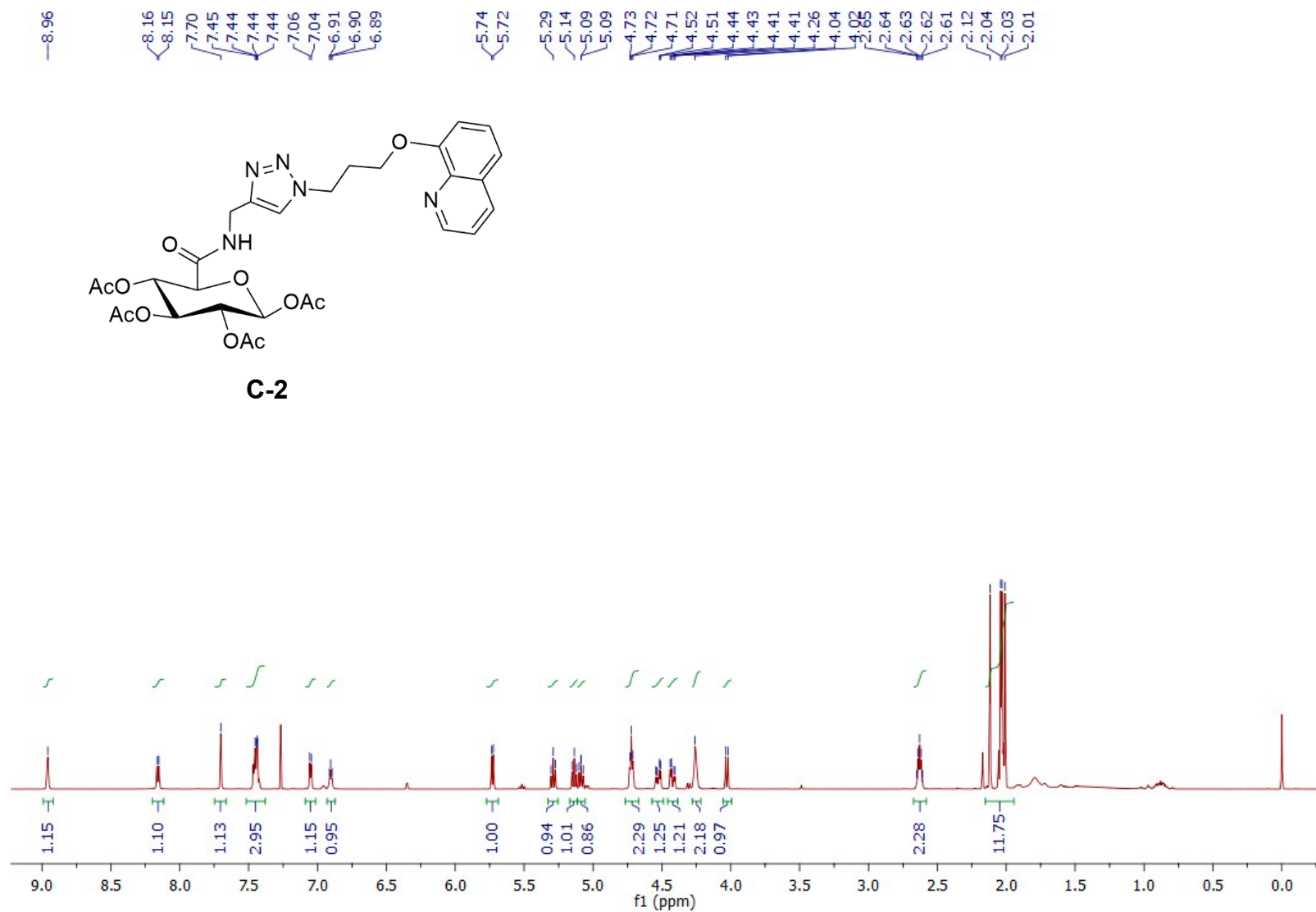


Fig. S49: ¹H NMR spectrum of glycoconjugates C-1 (400 MHz/CDCl₃/TMS; δ (ppm)).

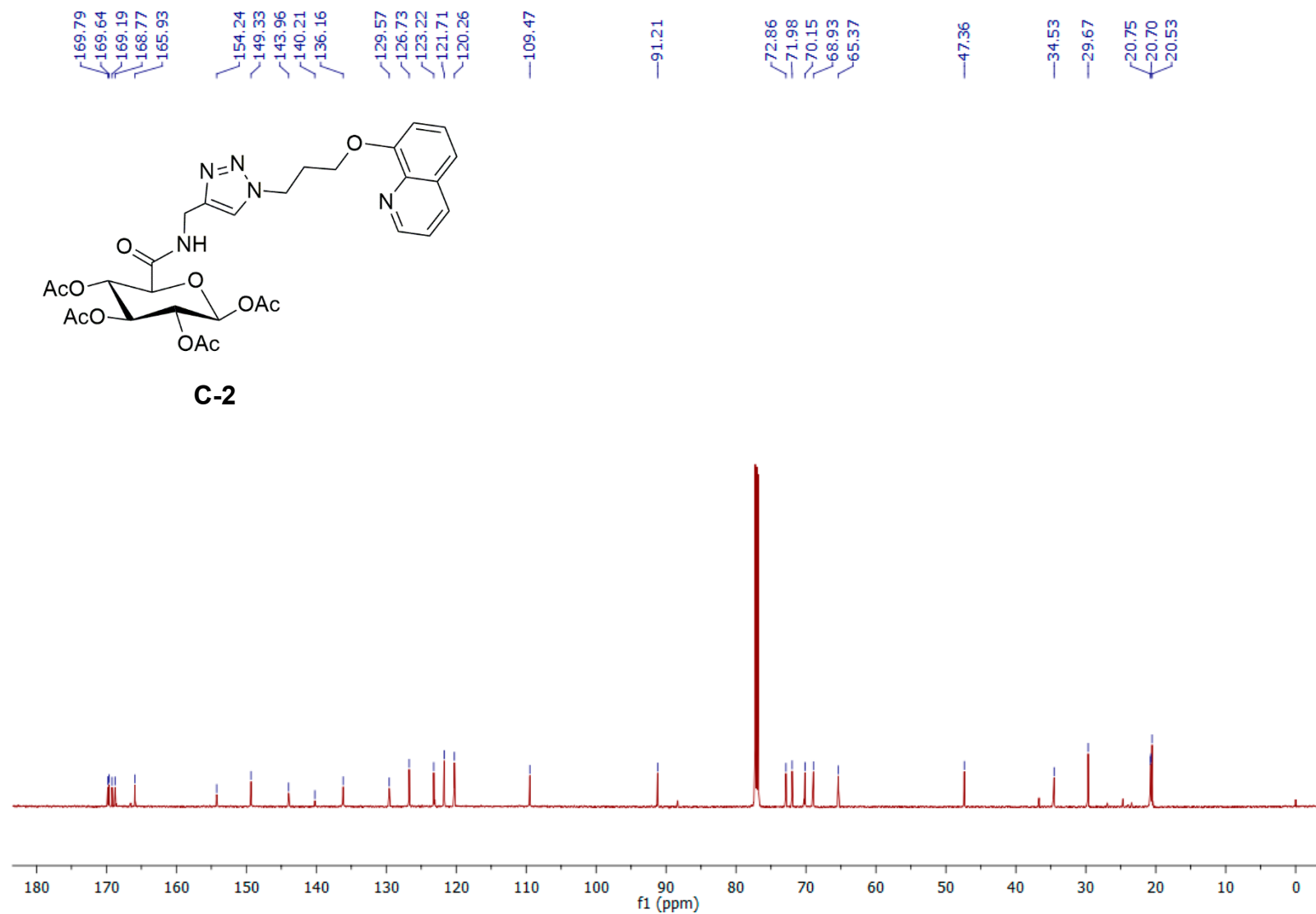


Fig. S50: ^{13}C NMR spectrum of glycoconjugates C-1 (100 MHz/ CDCl_3/TMS ; δ (ppm)).

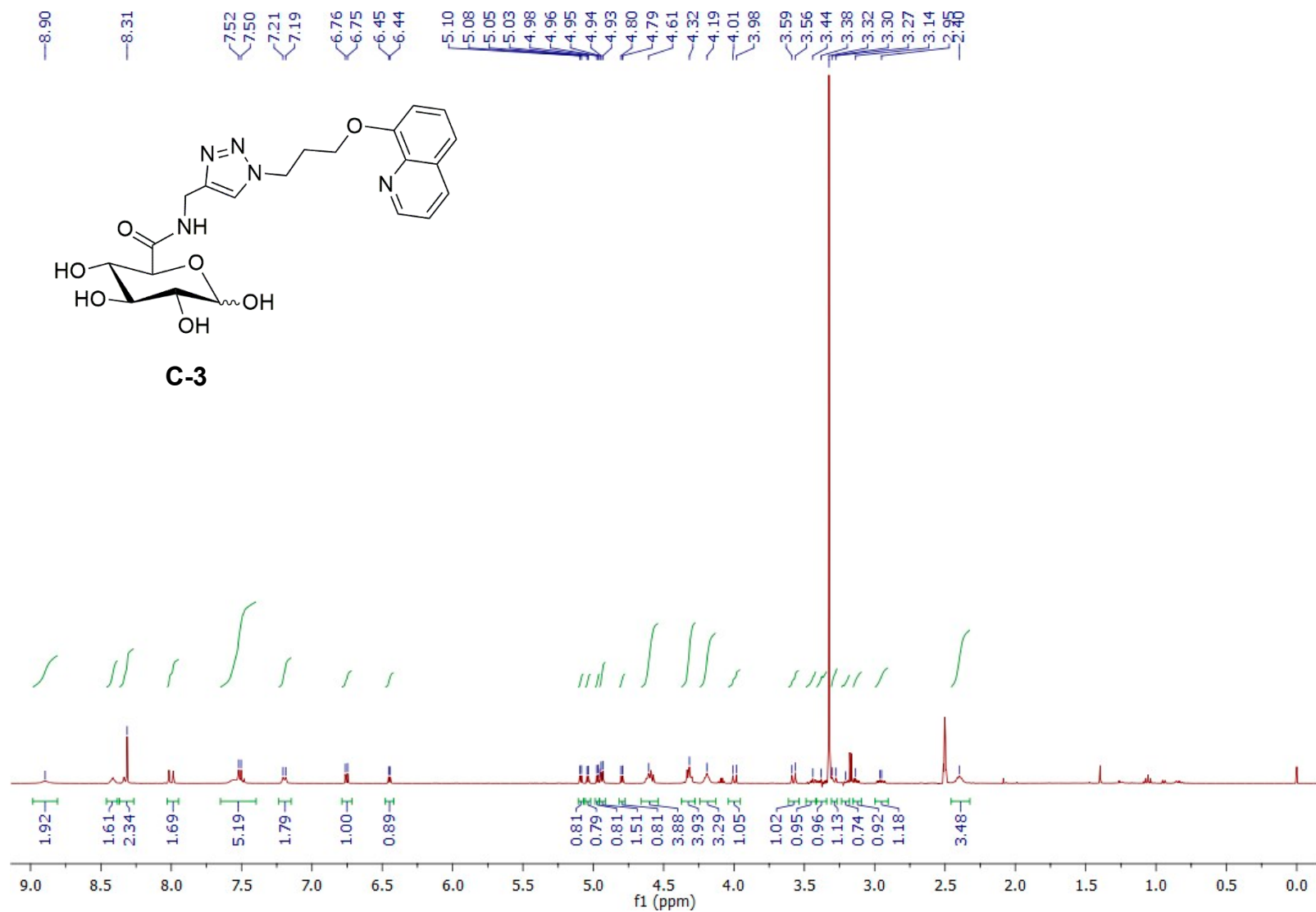


Fig. S51: ¹H NMR spectrum of glycoconjugates **C-3** (400 MHz/DMSO/TMS; δ (ppm)).

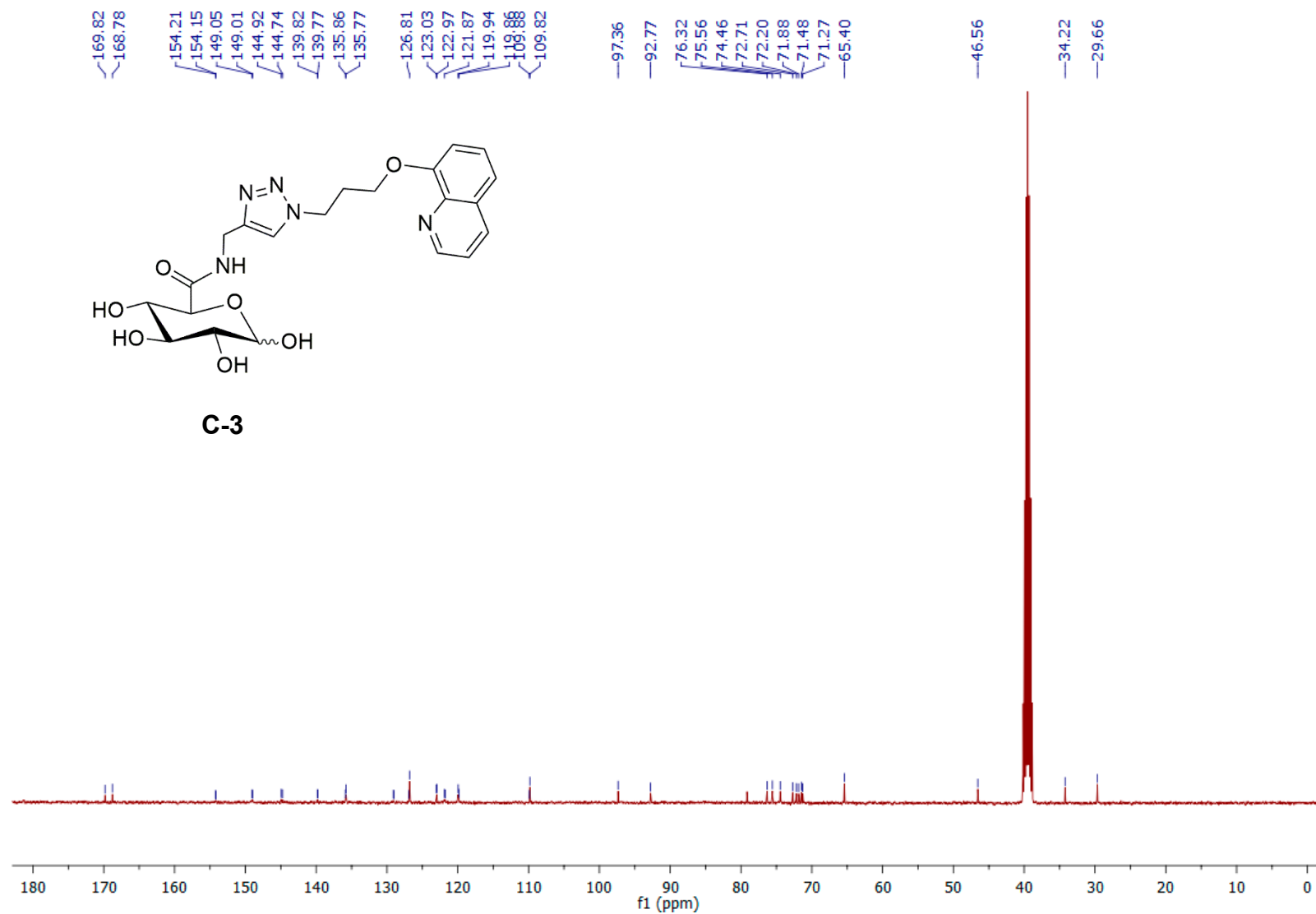


Fig. S52: ¹³C NMR spectrum of glycoconjugates C-3 (100 MHz/DMSO/TMS; δ (ppm)).

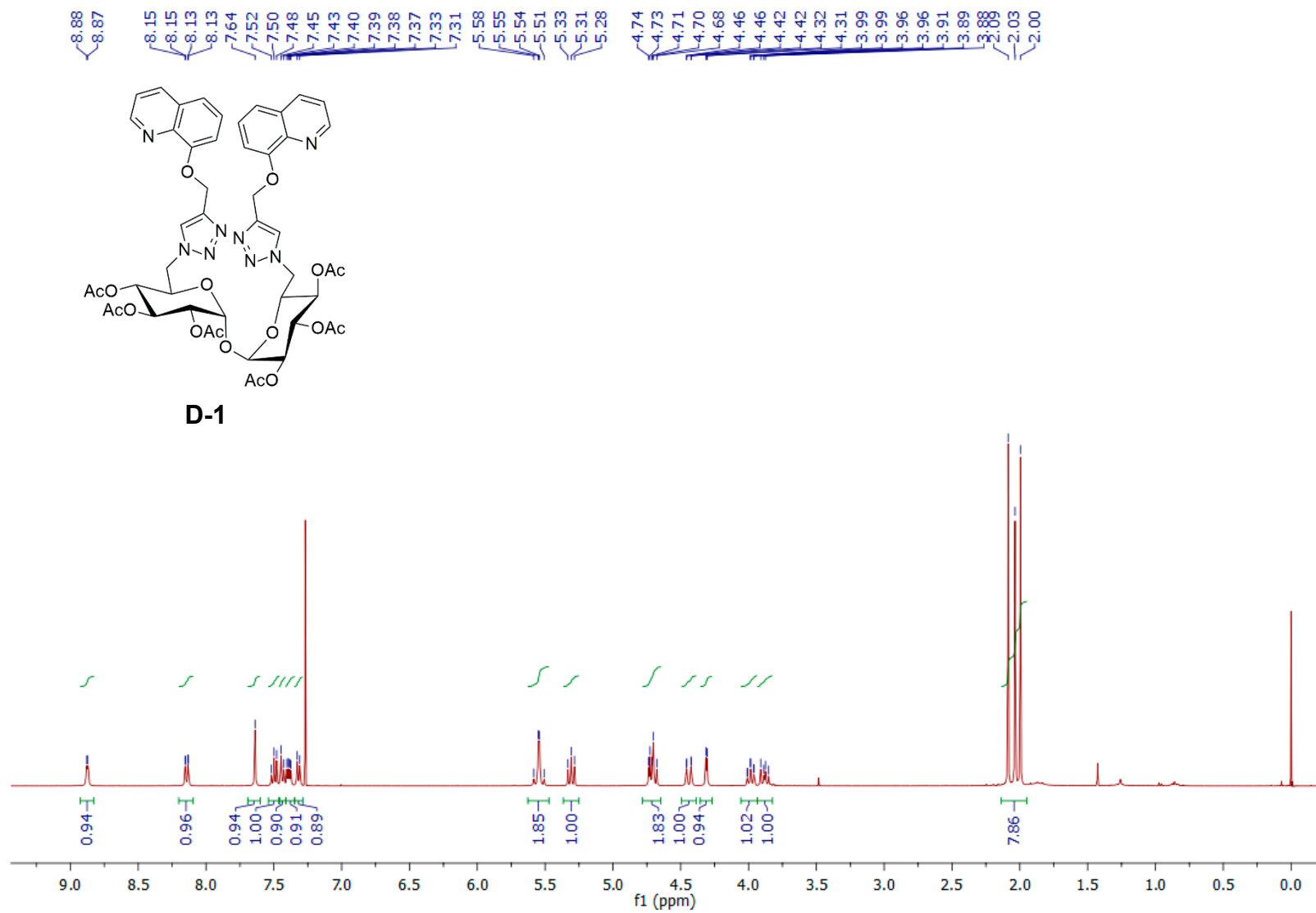


Fig. S53: ¹H NMR spectrum of glycoconjugates **D-1** (400 MHz/CDCl₃/TMS; δ (ppm)).

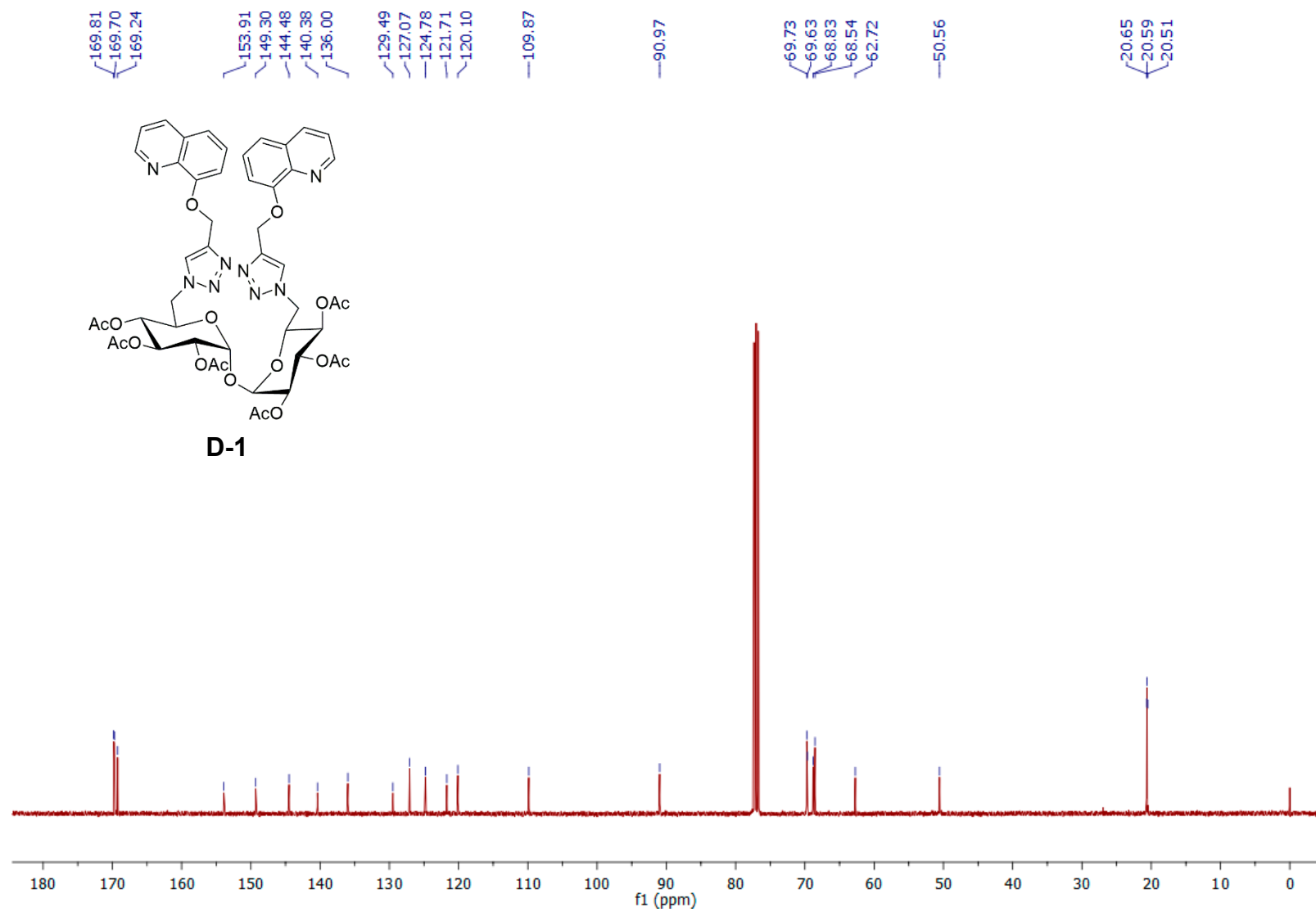


Fig. S54: ¹³C NMR spectrum of glycoconjugates **D-1** (100 MHz/CDCl₃/TMS; δ (ppm)).

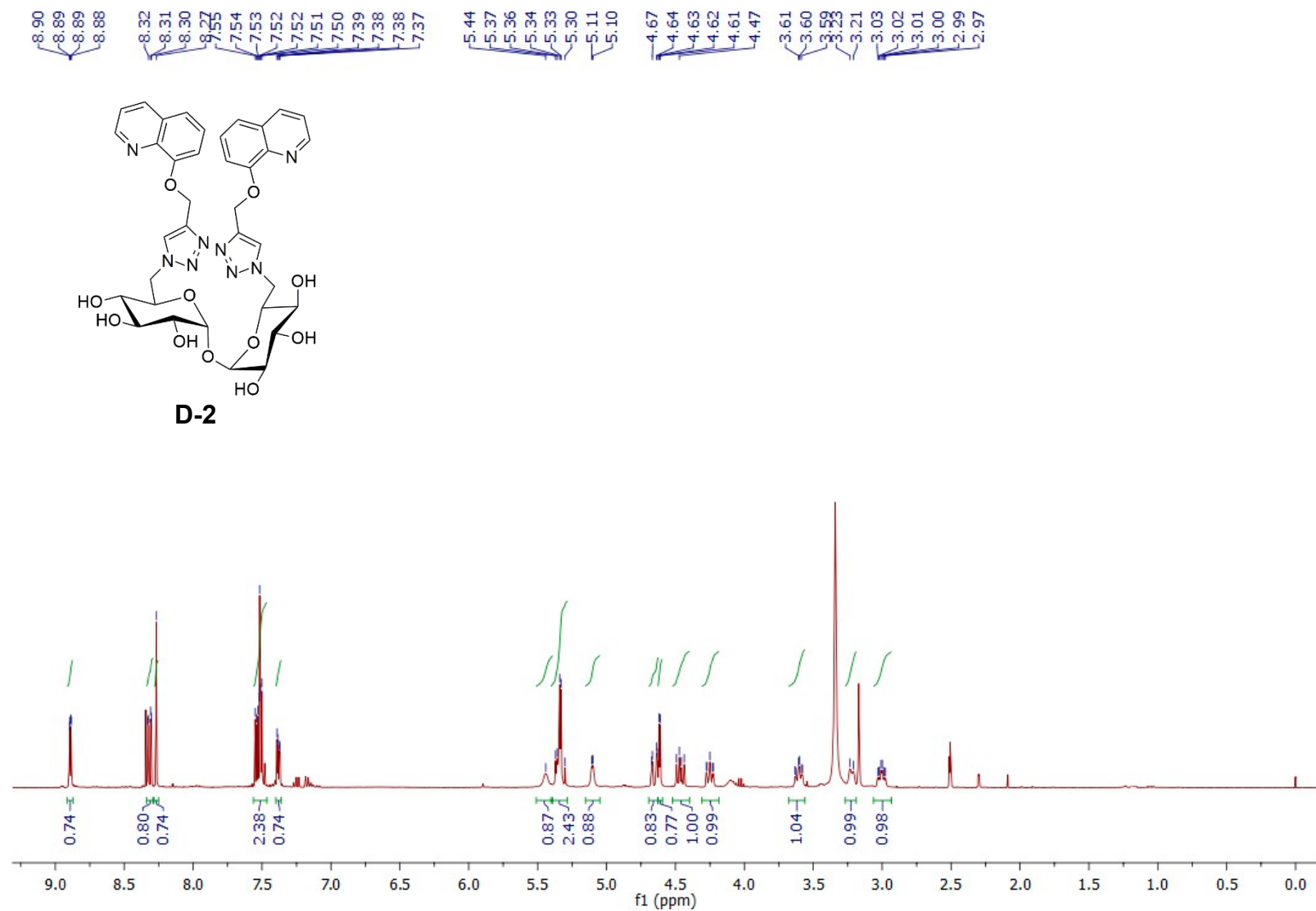


Fig. S55: ¹H NMR spectrum of glycoconjugates **D-2** (400 MHz/DMSO/TMS; δ (ppm)).

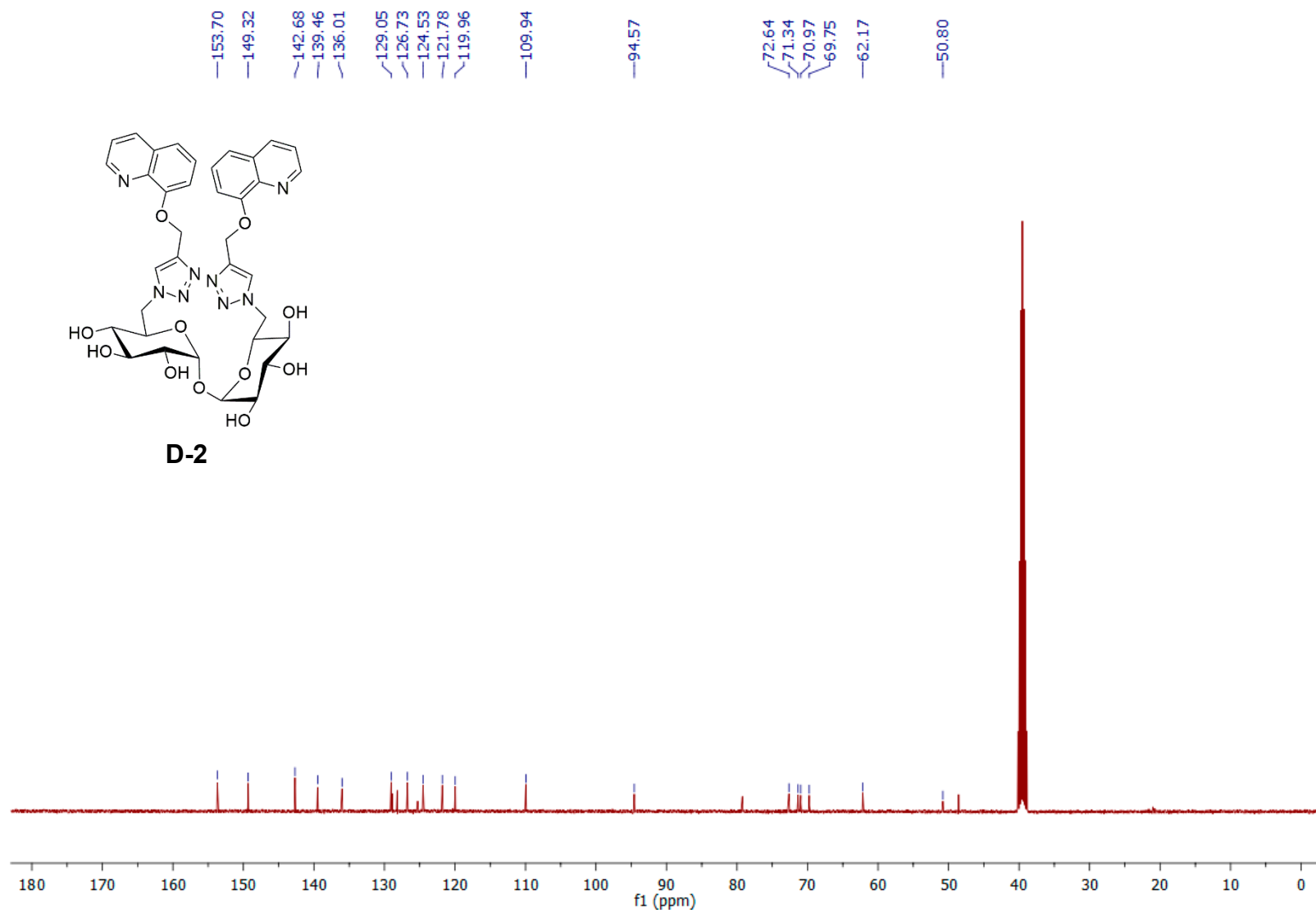


Fig. S56: ^{13}C NMR spectrum of glycoconjugates **D-2** (100 MHz/DMSO/TMS; δ (ppm)).

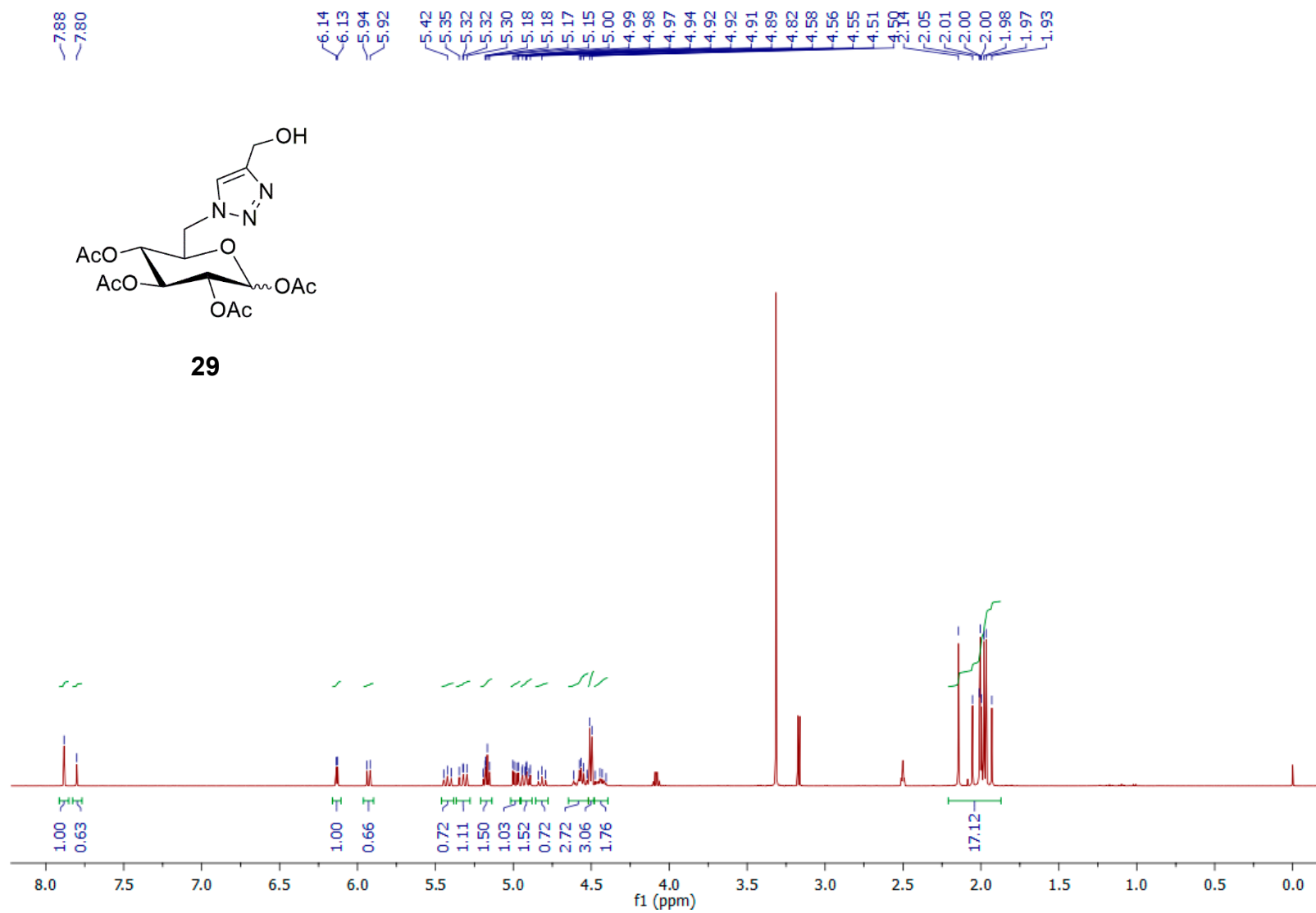


Fig. S57: ^1H NMR spectrum of metabolite **29** (400 MHz/DMSO/TMS; δ (ppm)).

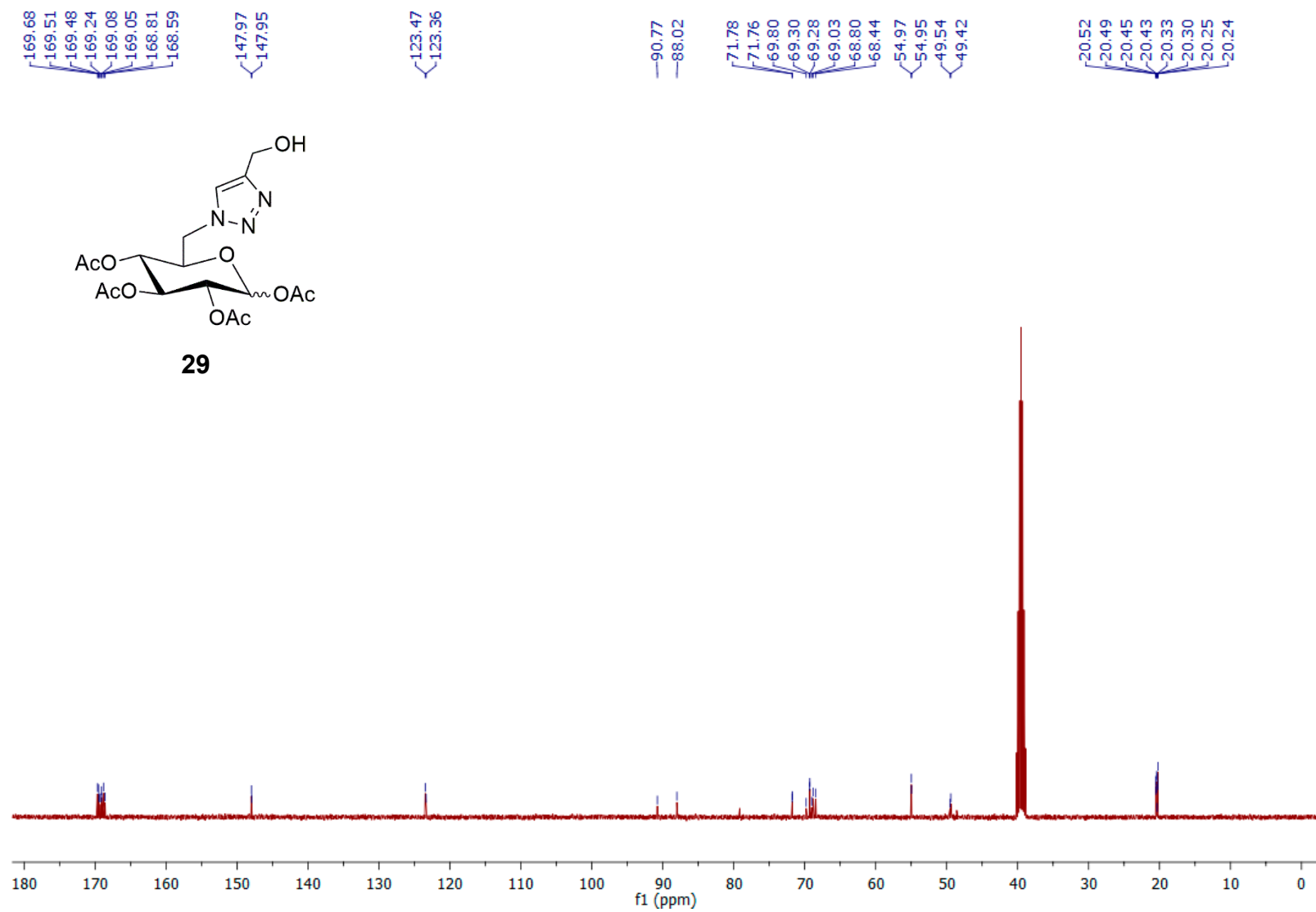


Fig. S58: ^{13}C NMR spectrum of metabolite **29** (100 MHz/DMSO/TMS; δ (ppm)).

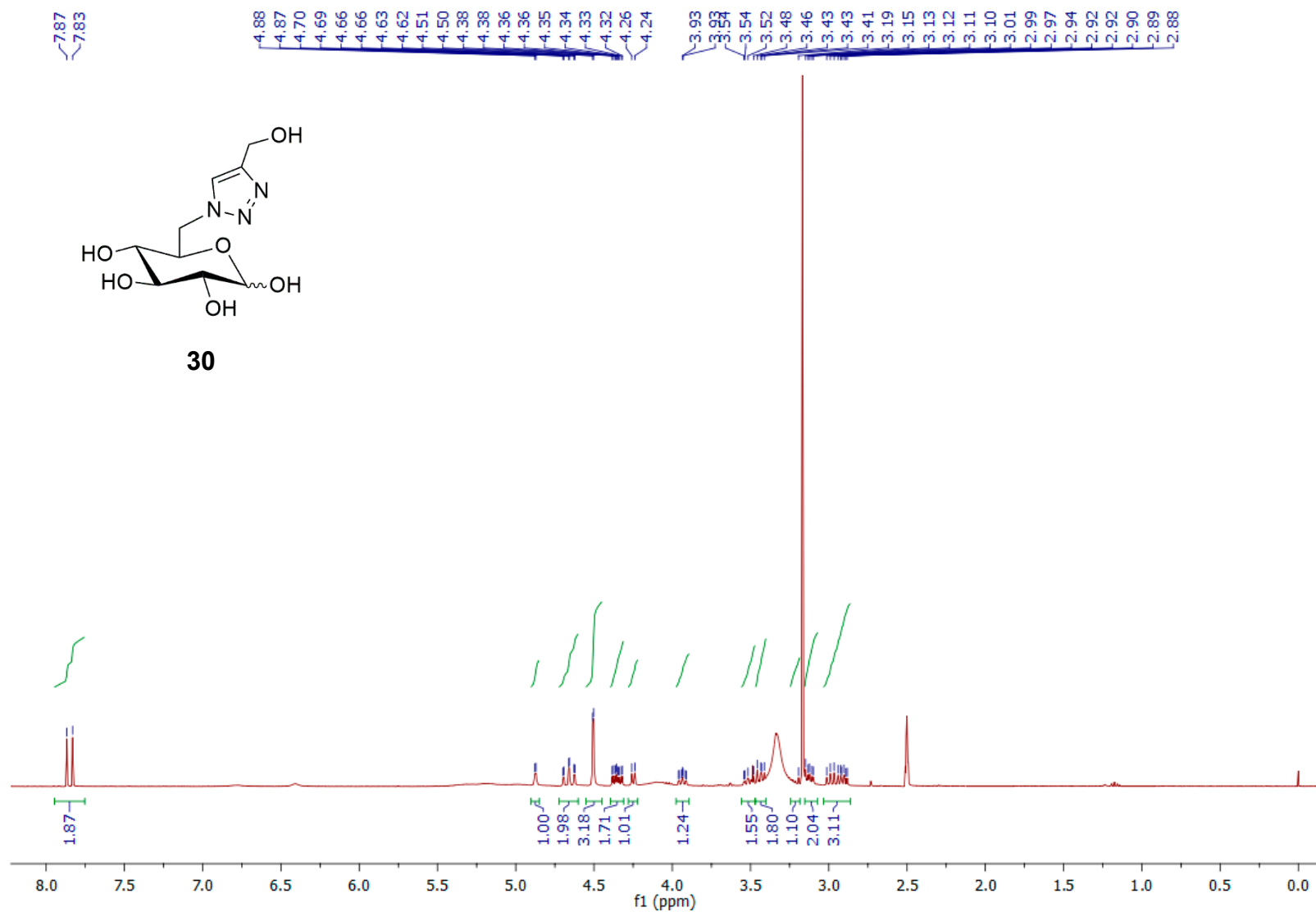


Fig. S59: ¹H NMR spectrum of metabolite **29** (400 MHz/DMSO/TMS; δ (ppm)).

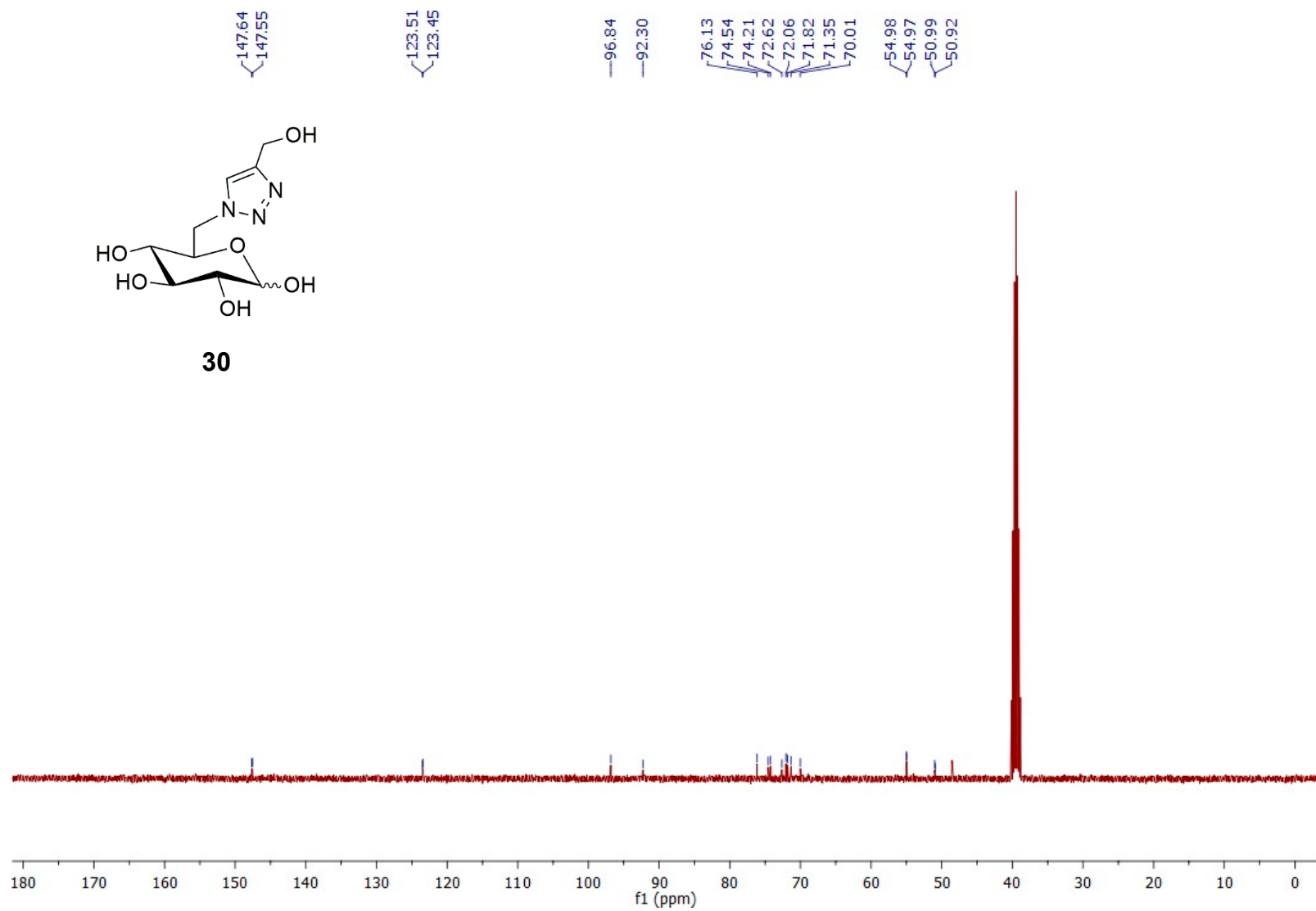


Fig. S60: ¹³C NMR spectrum of metabolite **29** (100 MHz/DMSO/TMS; δ (ppm)).

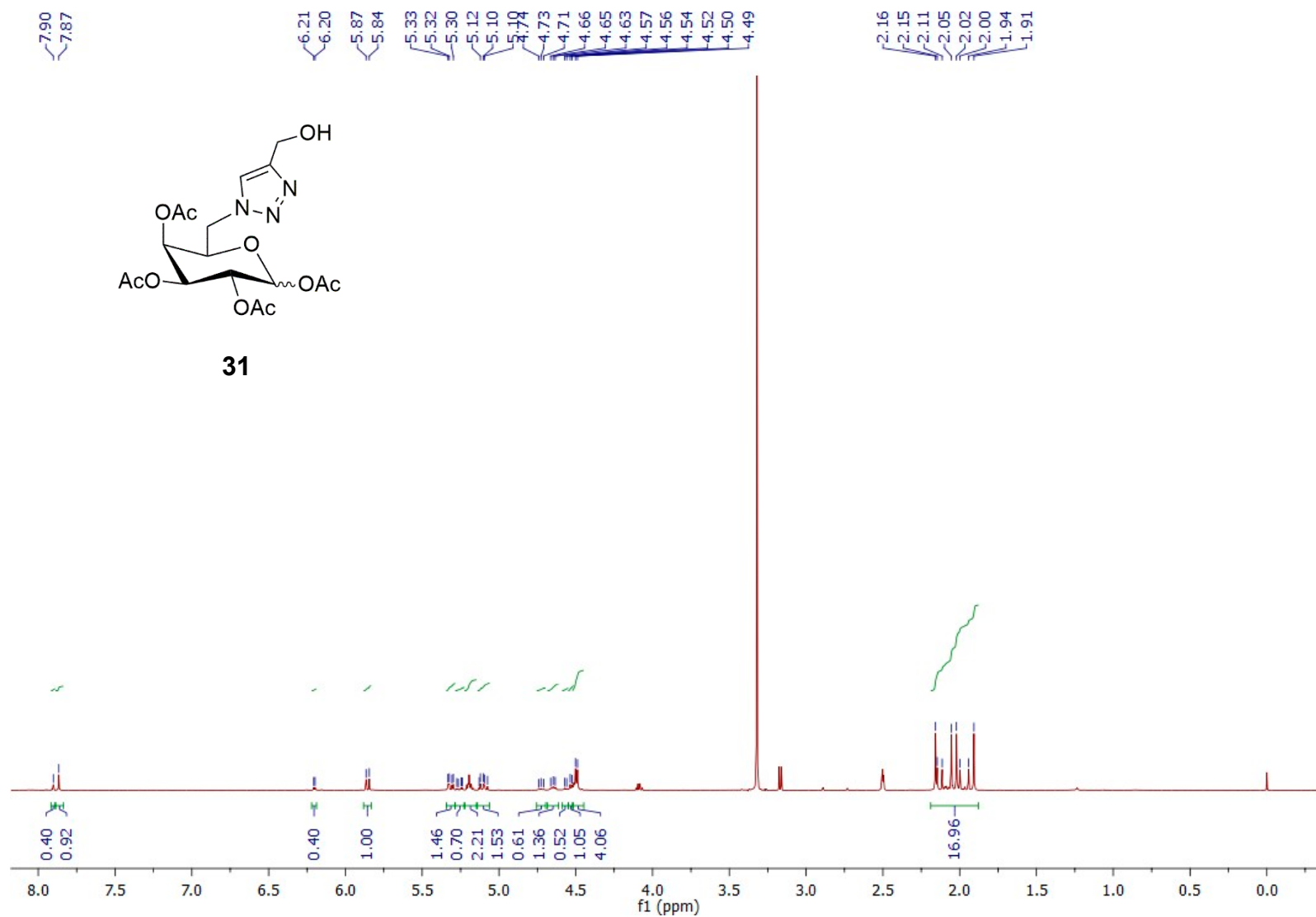


Fig. S61: ^1H NMR spectrum of metabolite **32** (400 MHz/DMSO/TMS; δ (ppm)).

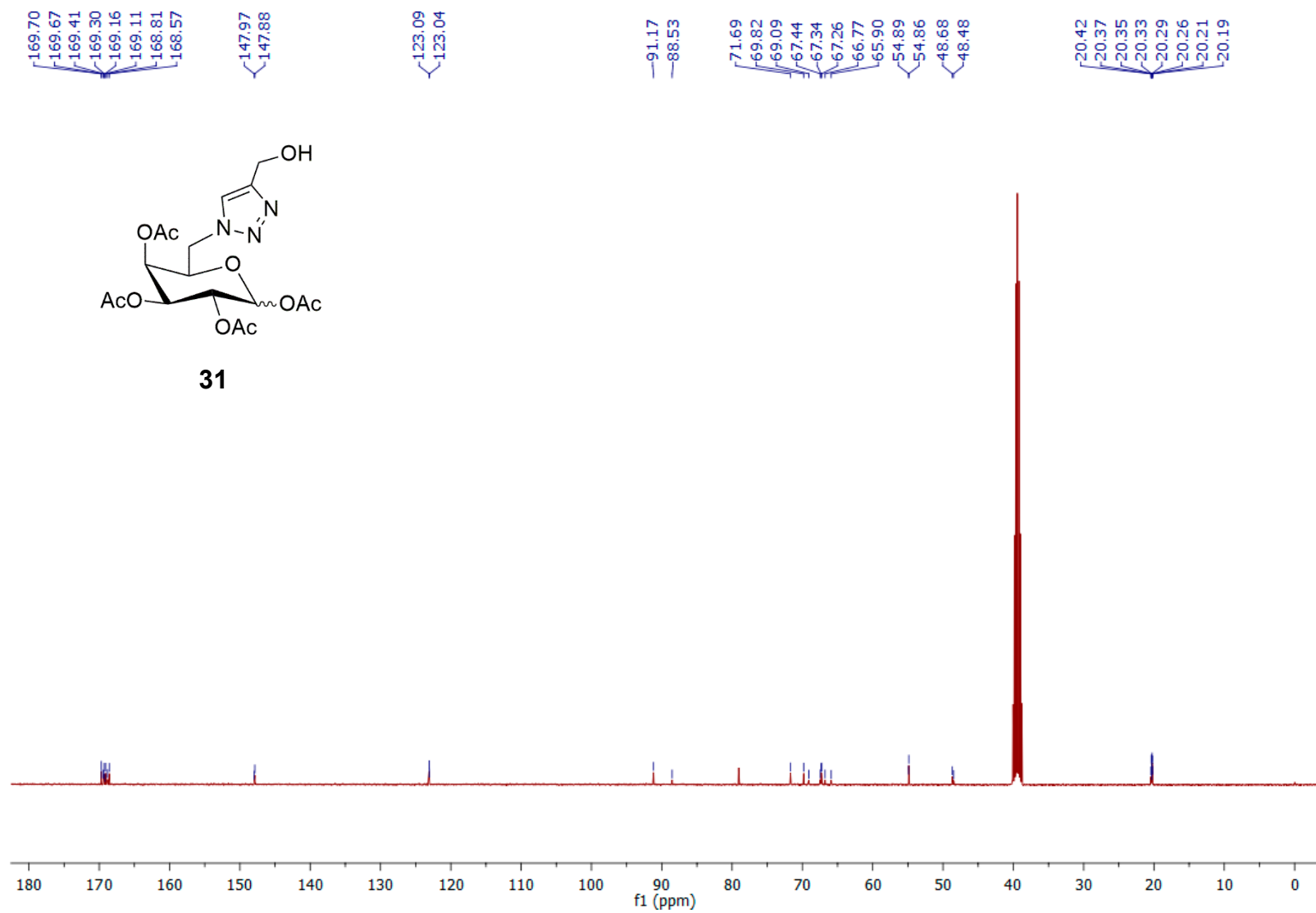


Fig. S62: ¹³C NMR spectrum of metabolite **31** (100 MHz/DMSO/TMS; δ (ppm)).

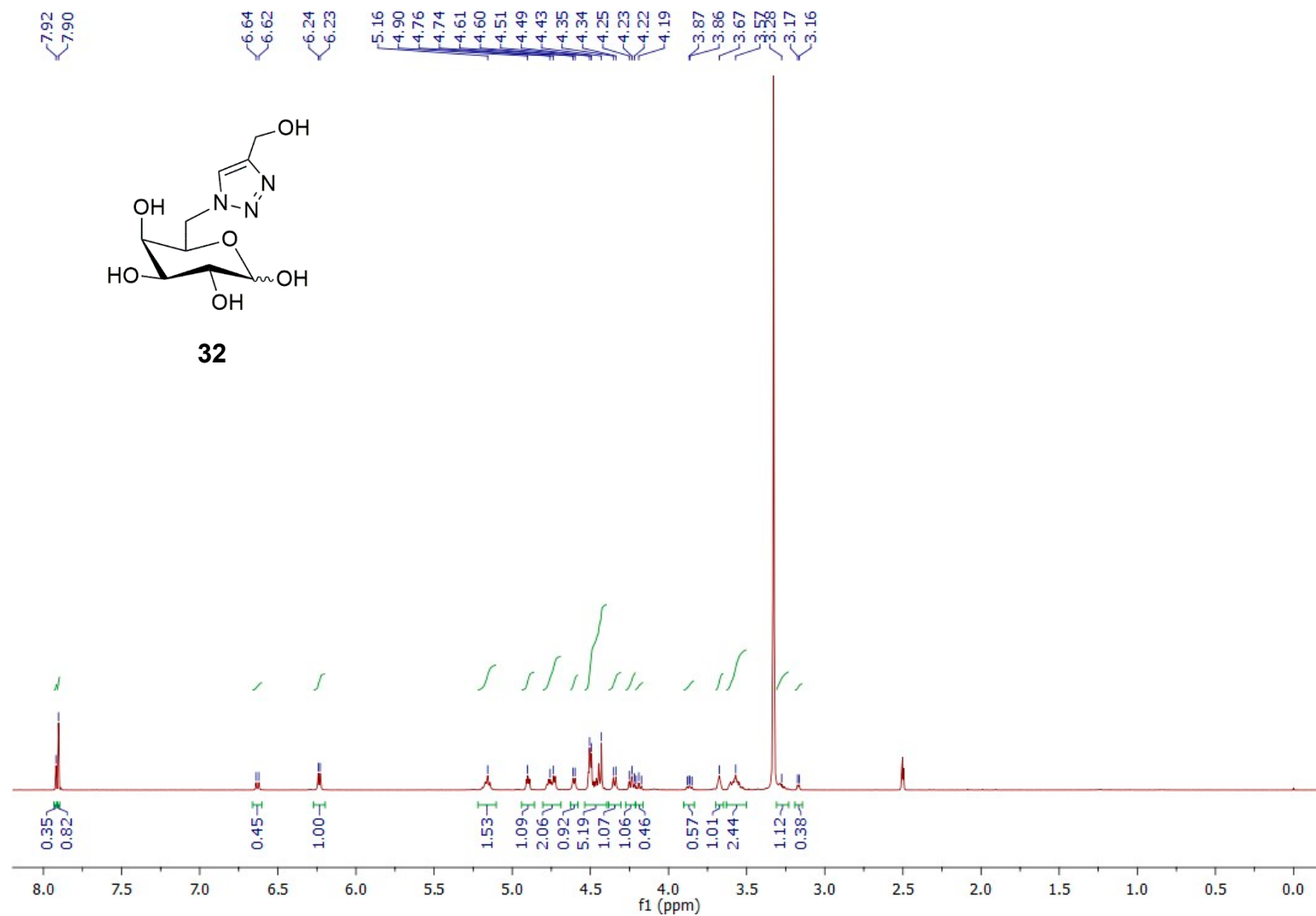


Fig. S63: ¹H NMR spectrum of metabolite **32** (400 MHz/DMSO/TMS; δ (ppm)).

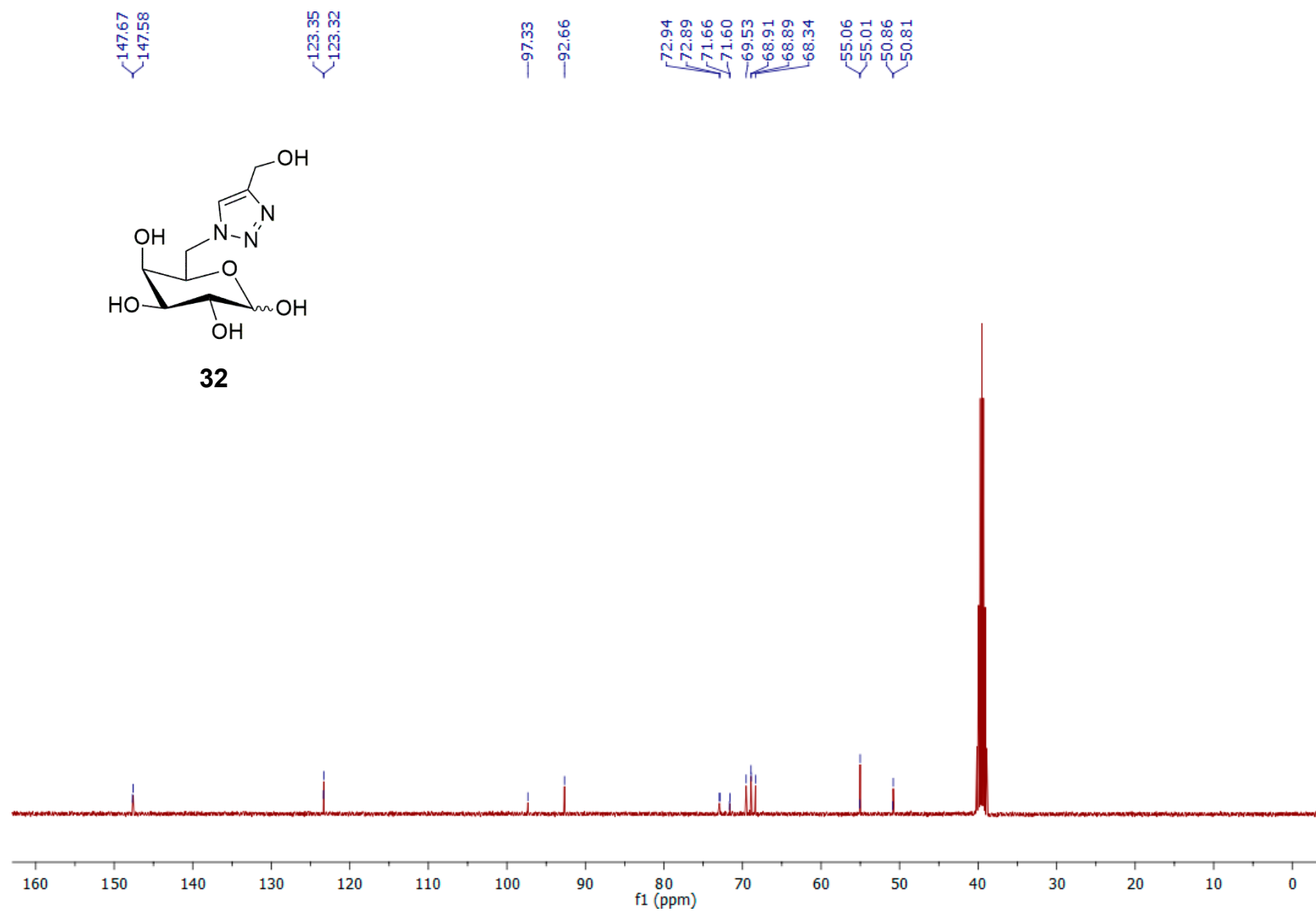


Fig. S64: ¹³C NMR spectrum of metabolite **31** (100 MHz/DMSO/TMS; δ (ppm)).

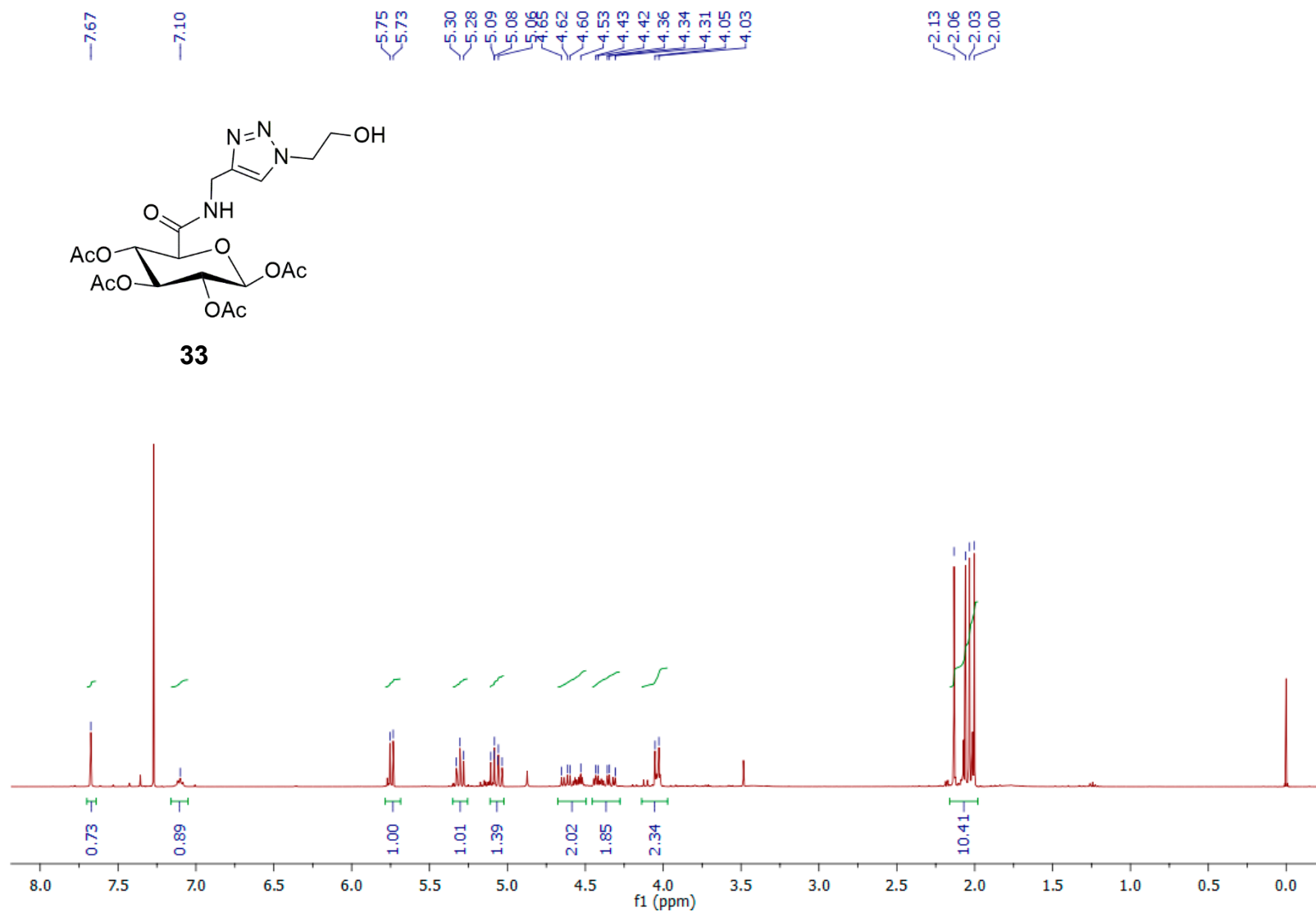


Fig. S65: ^1H NMR spectrum of metabolite **33** (400 MHz/ CDCl_3 /TMS; δ (ppm)).

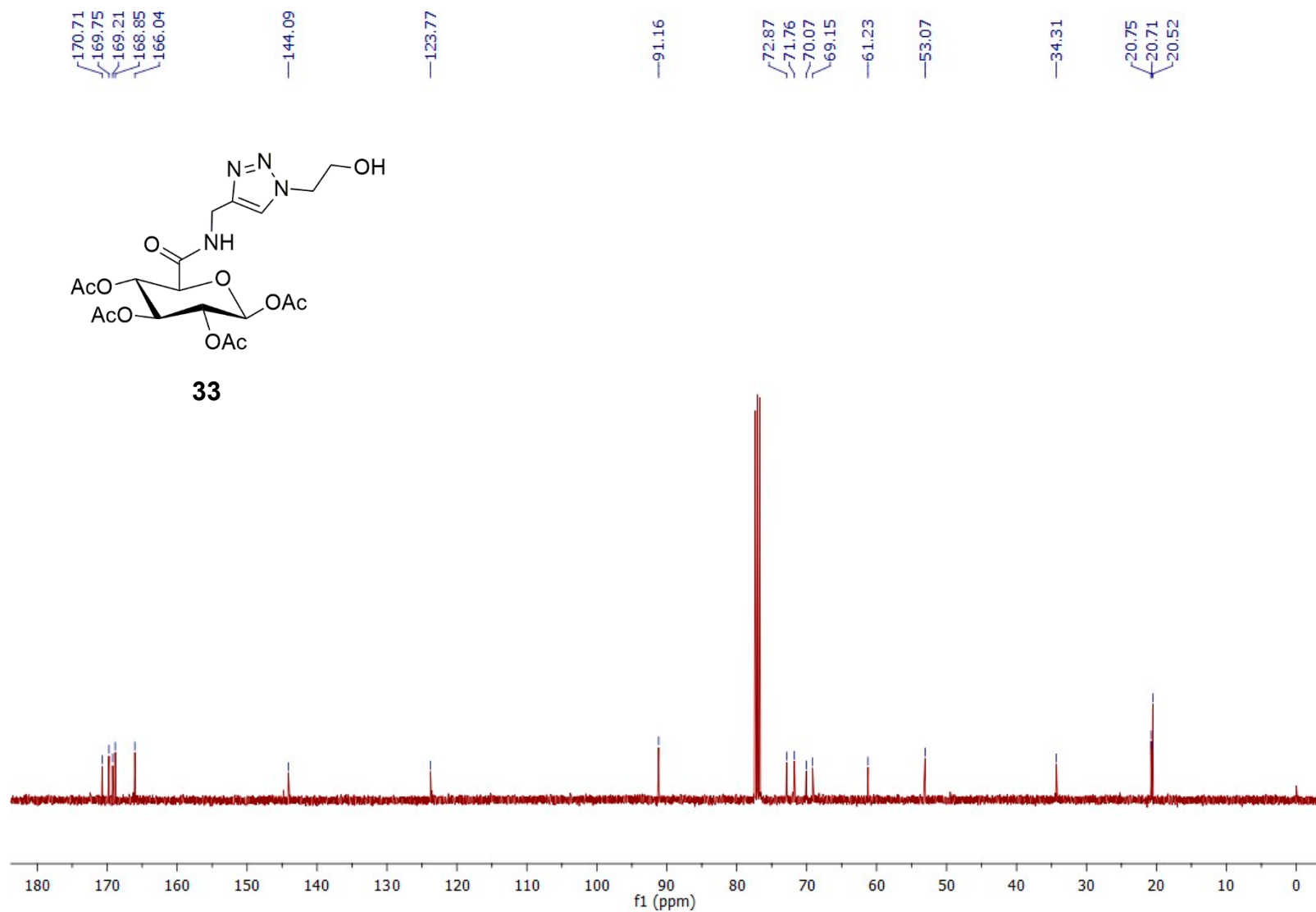


Fig. S66: ^{13}C NMR spectrum of metabolite **33** (100 MHz/ CDCl_3/TMS ; δ (ppm)).

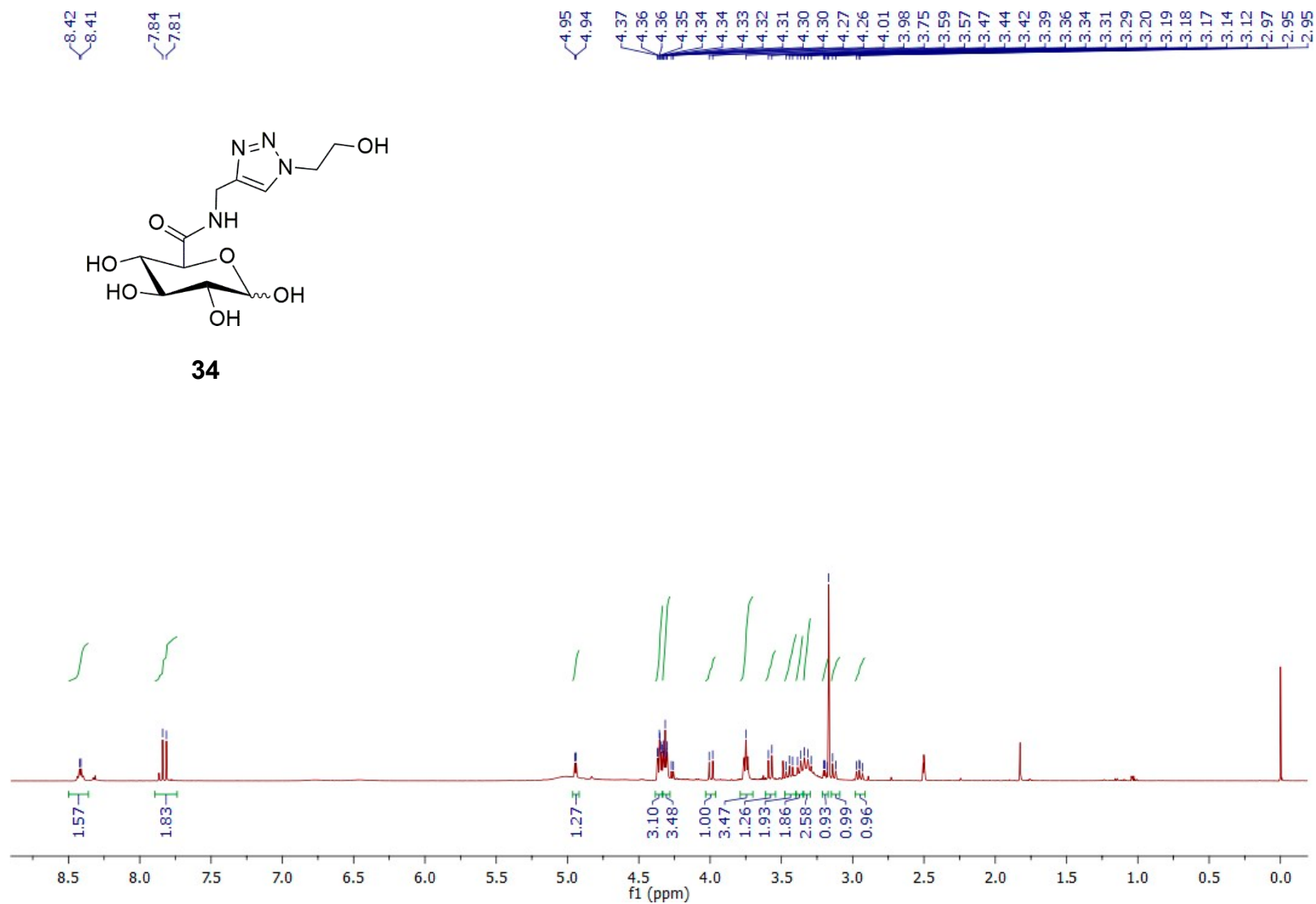


Fig. S67: ¹H NMR spectrum of metabolite **35** (400 MHz/DMSO/TMS; δ (ppm)).

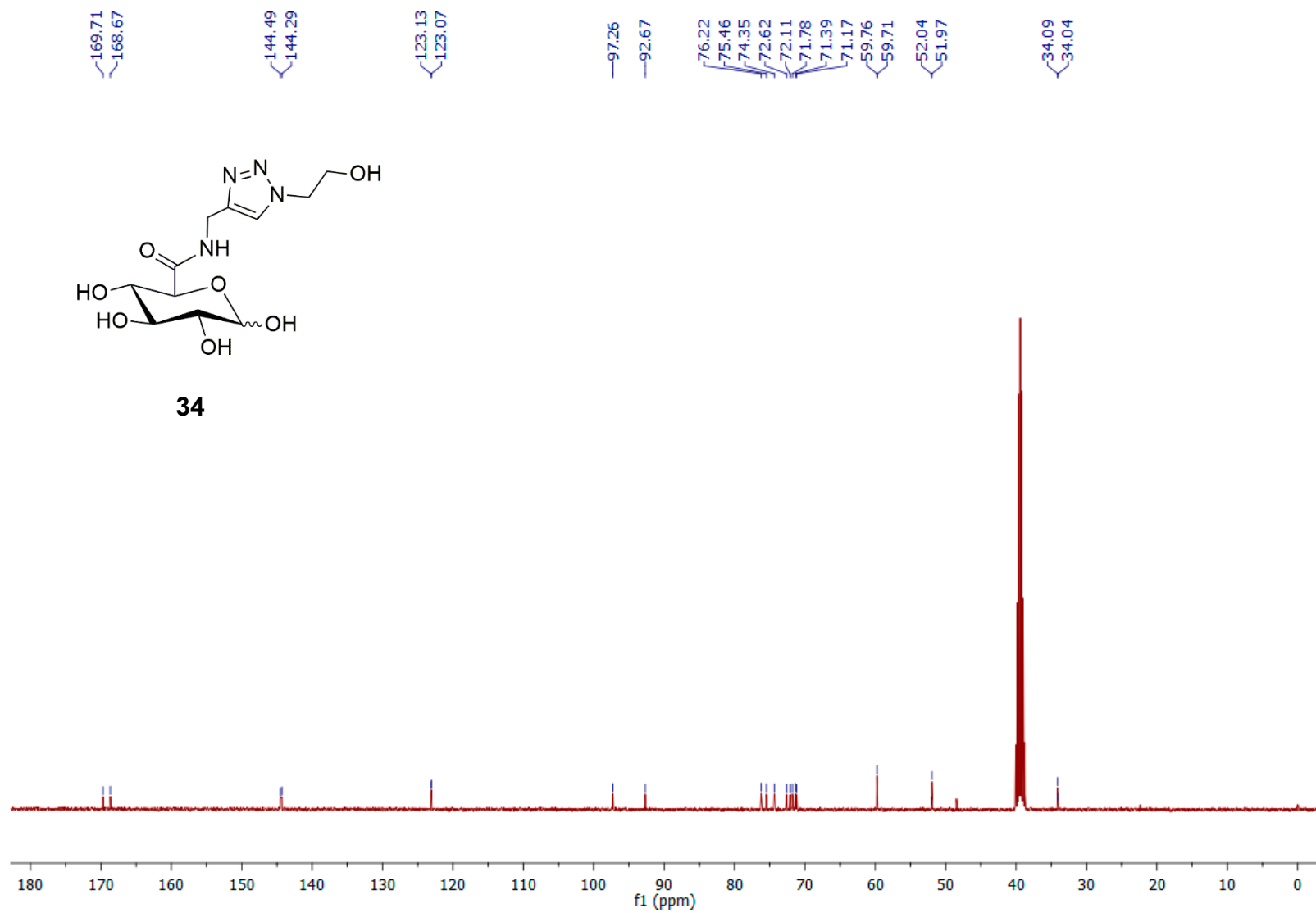


Fig. S68: ^{13}C NMR spectrum of metabolite **34** (100 MHz/DMSO/TMS; δ (ppm)).

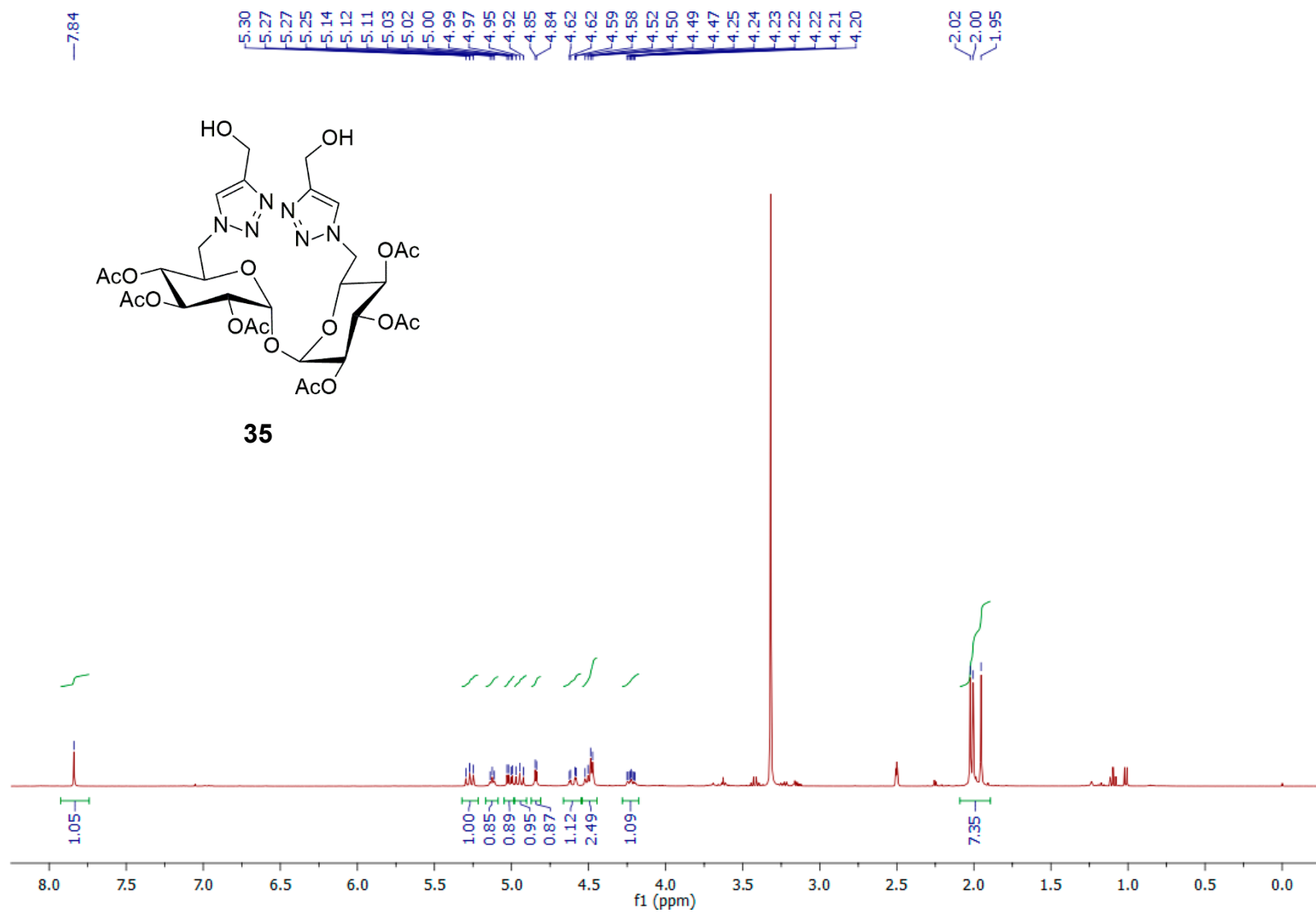


Fig. S69: ^1H NMR spectrum of metabolite **35** (400 MHz/DMSO/TMS; δ (ppm)).

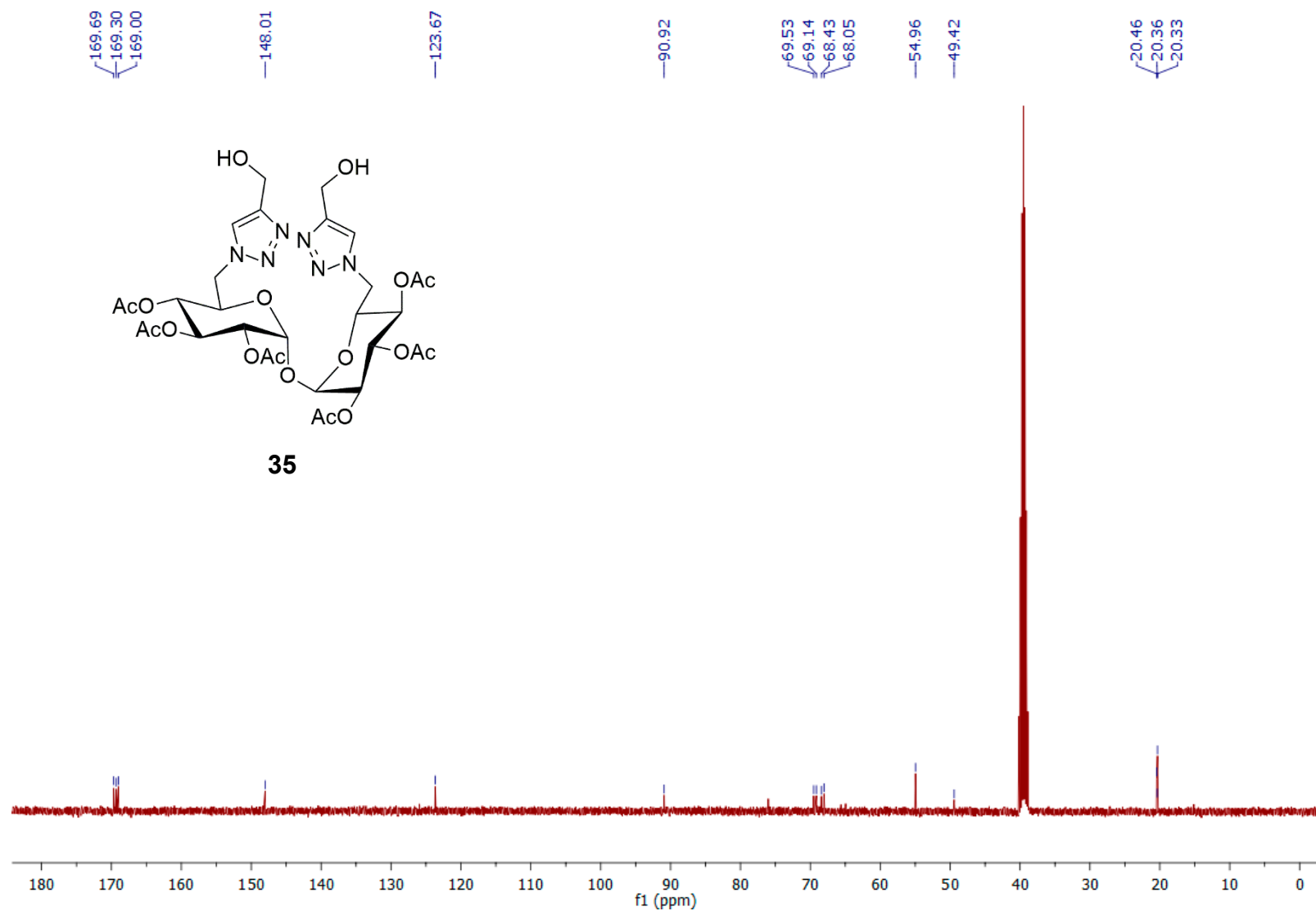


Fig. S70: ^{13}C NMR spectrum of metabolite **35** (100 MHz/DMSO/TMS; δ (ppm)).

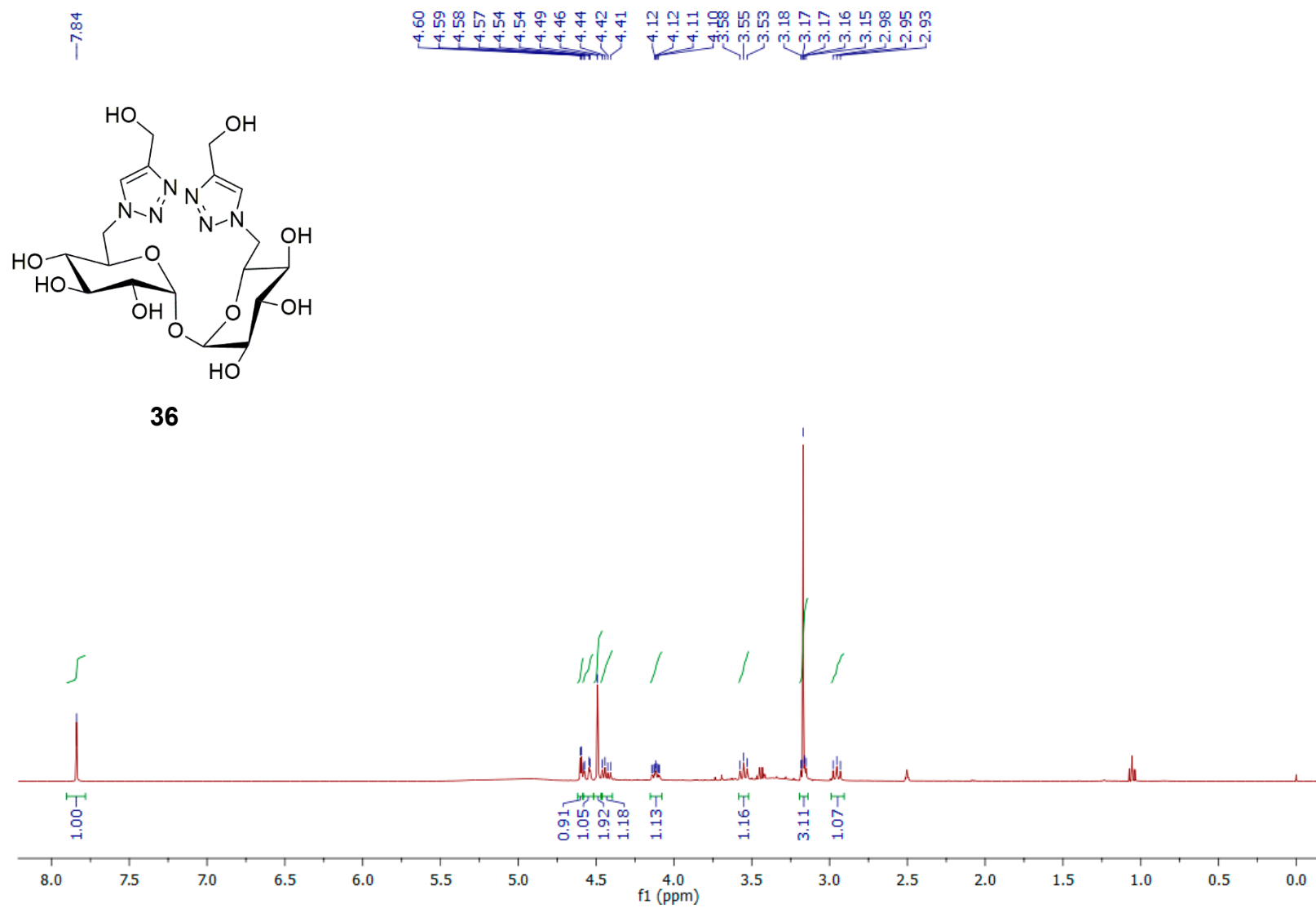


Fig. S71: ^1H NMR spectrum of metabolite **36** (400 MHz/DMSO/TMS; δ (ppm)).

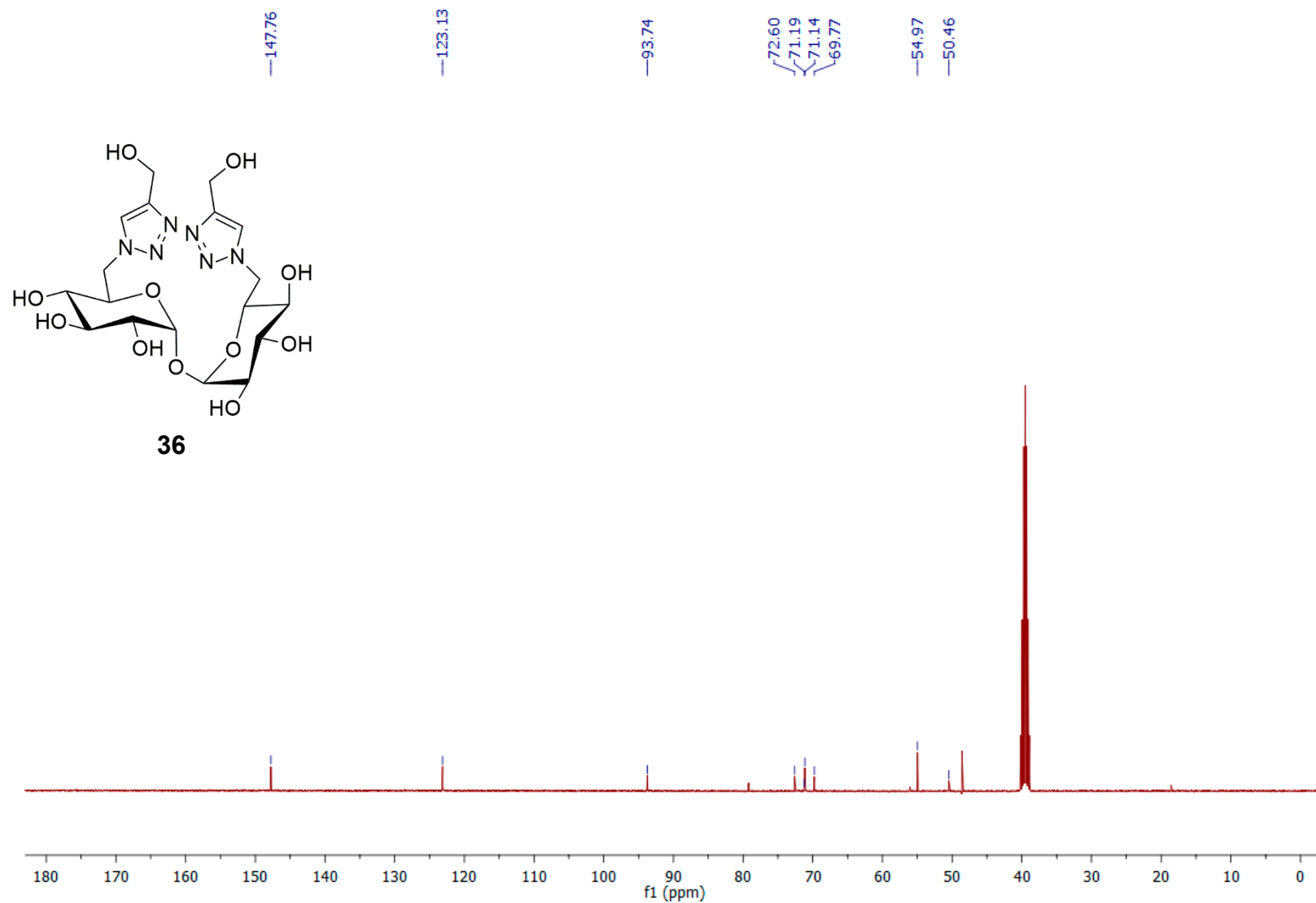


Fig. S72: ^{13}C NMR spectrum of metabolite **36** (100 MHz/DMSO/TMS; δ (ppm))

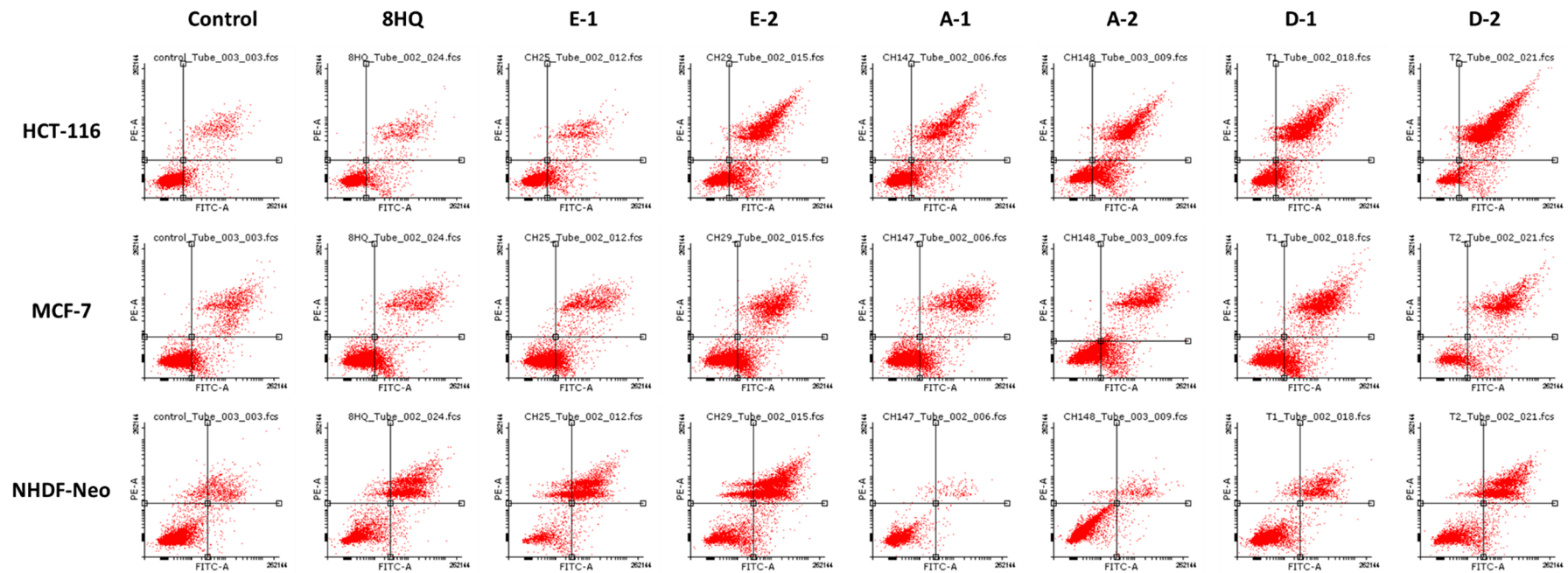


Fig. S73: Representative graphs of Annexin V/PI double staining apoptosis assay.

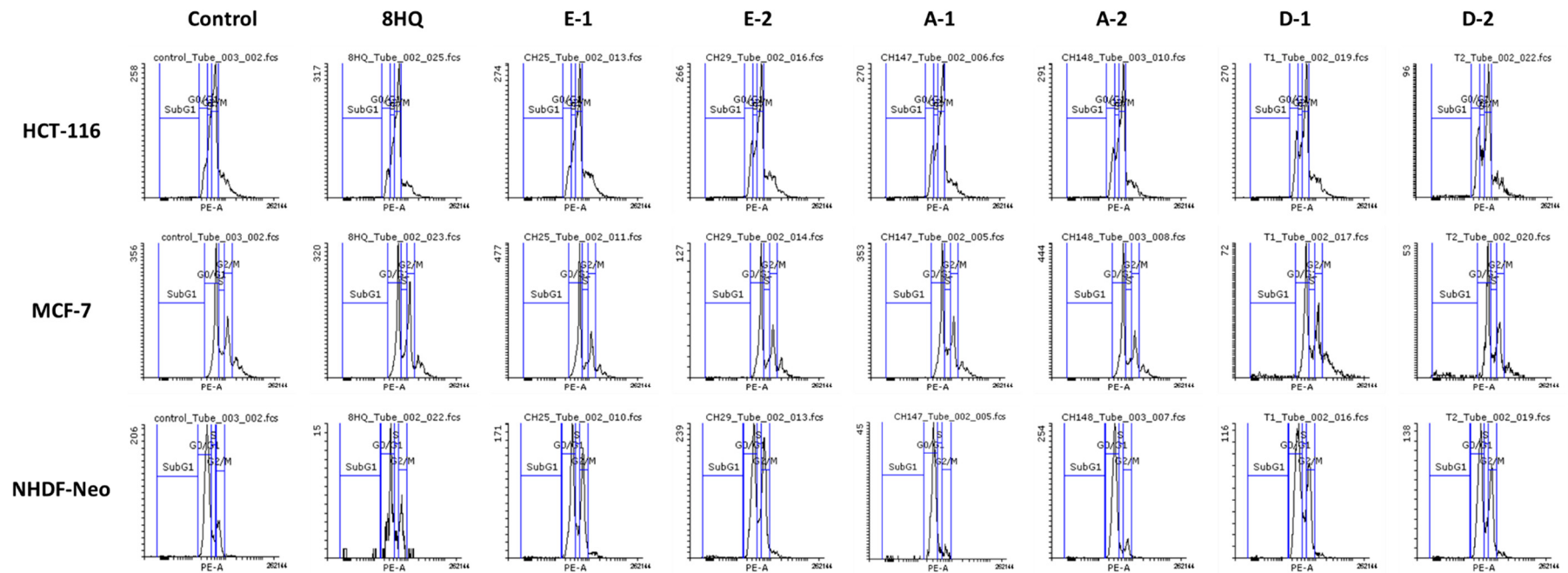


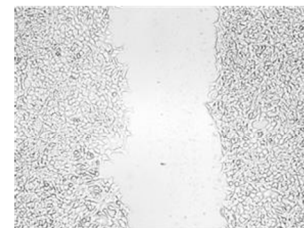
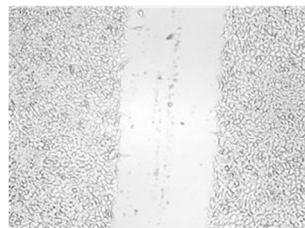
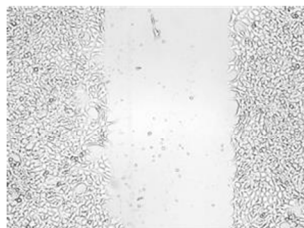
Fig. S74: Representative histograms of PI-stained DNA content.

A) HCT-116

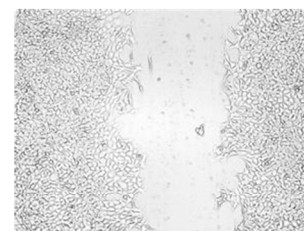
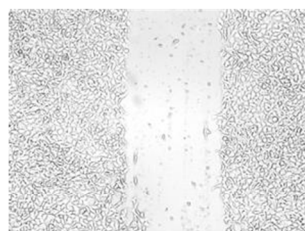
Control

A-1

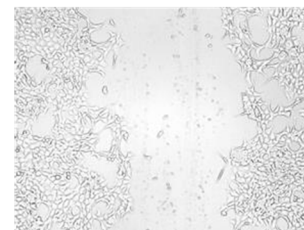
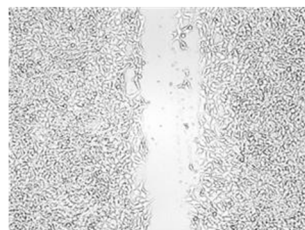
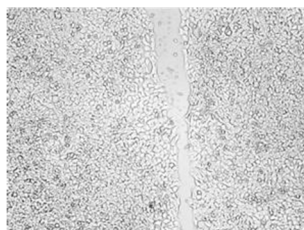
A-2



0 h



24 h



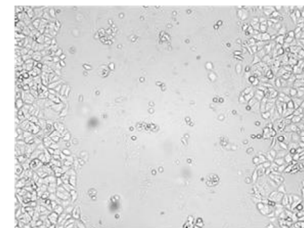
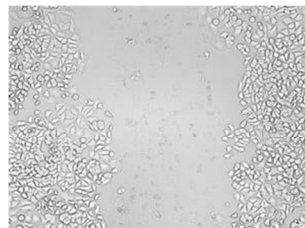
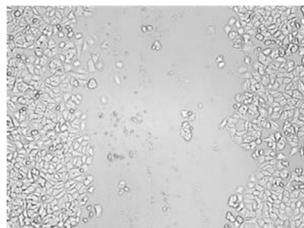
72h

B) MCF-7

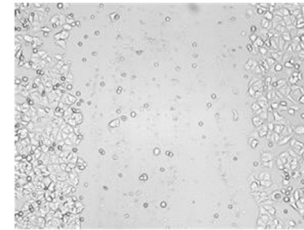
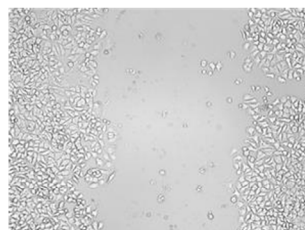
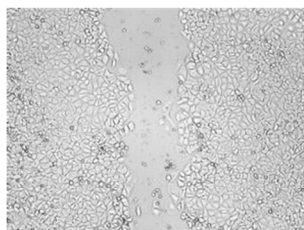
Control

A-1

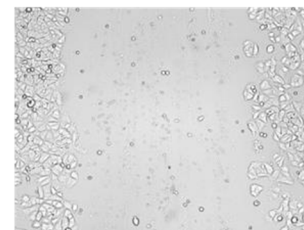
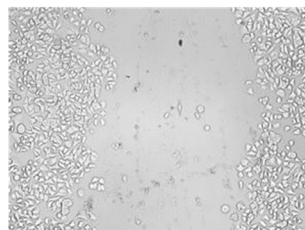
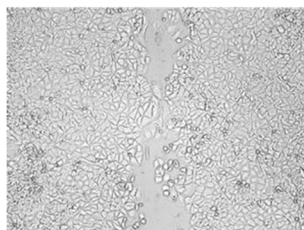
A-2



0 h



24 h



72h

C) NHDF-Neo

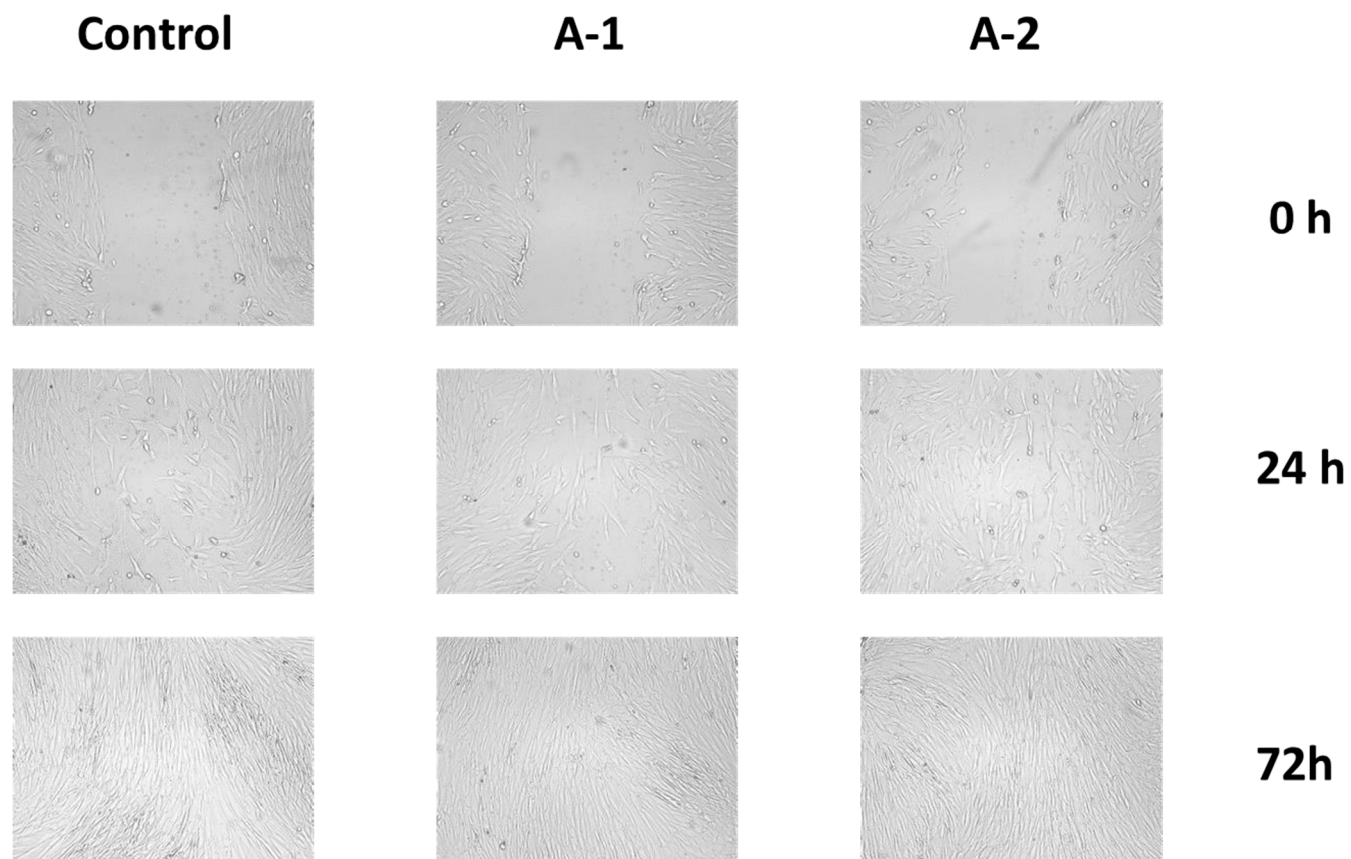


Fig. S75: Representative images of HCT-116 cancer cells (A), MCF-7 cancer cells (B), and NHDF-Neo healthy cells (C) were acquired at time 0 and after 24 h and 72 h incubation with compounds A-1 and A-2 in wound healing assay.