

8-Hydroxyquinoline glycoconjugates: modifications in the linker structure and their effect on the cytotoxicity of the obtained compounds

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1. Spectra

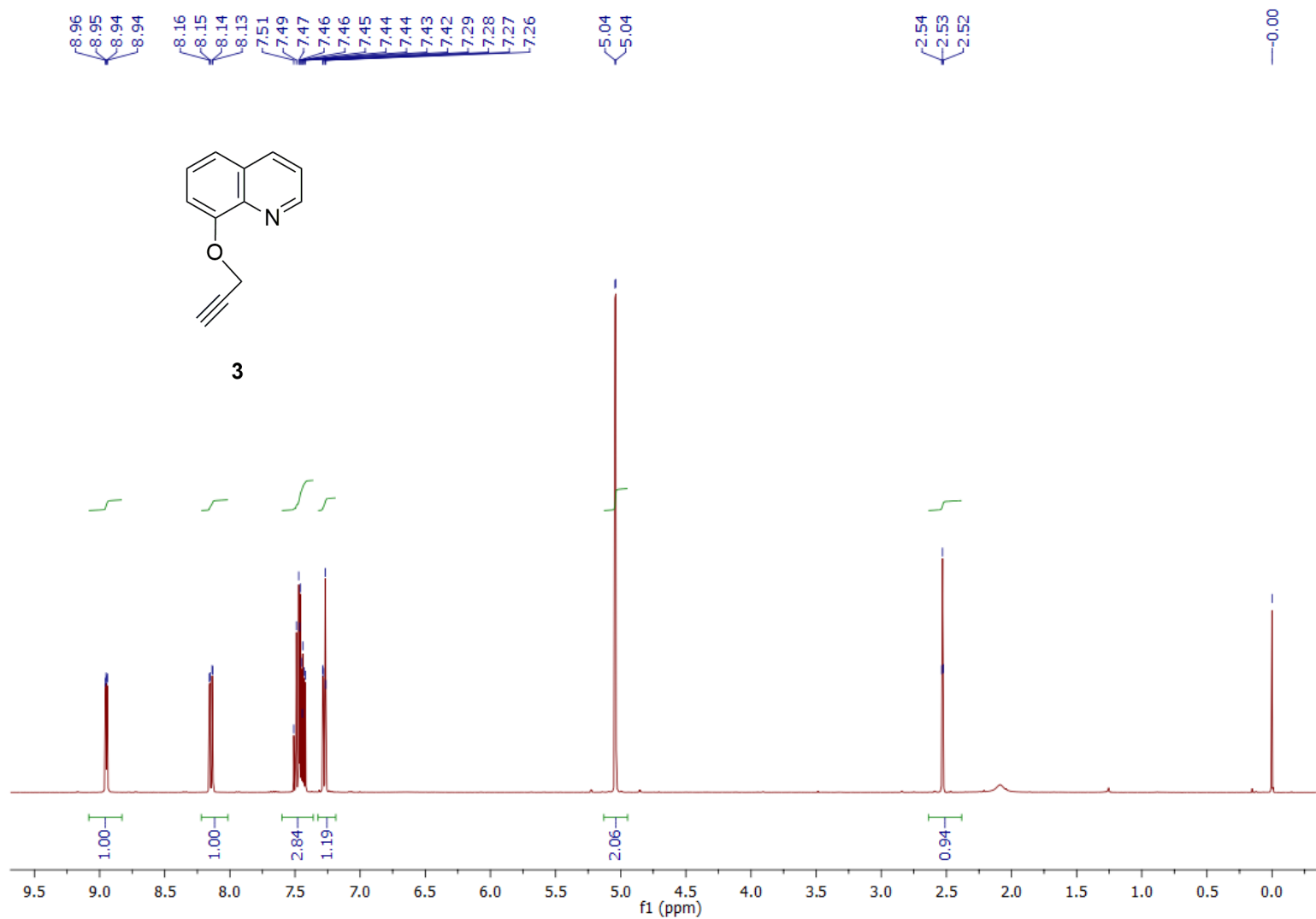


Fig. S1: ¹H NMR spectrum of compound 3.

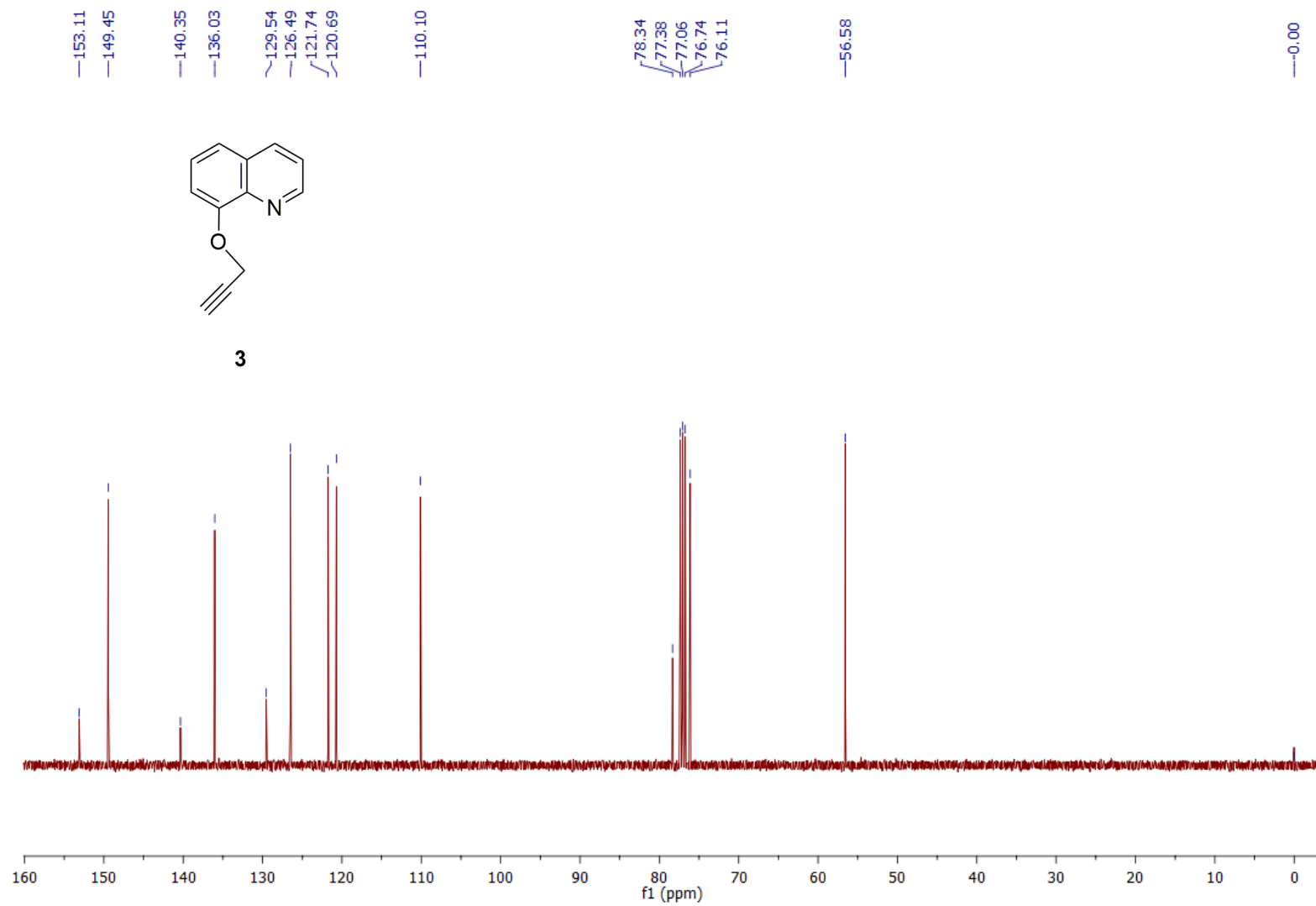


Fig. S2: ^{13}C NMR spectrum of compound **3**.

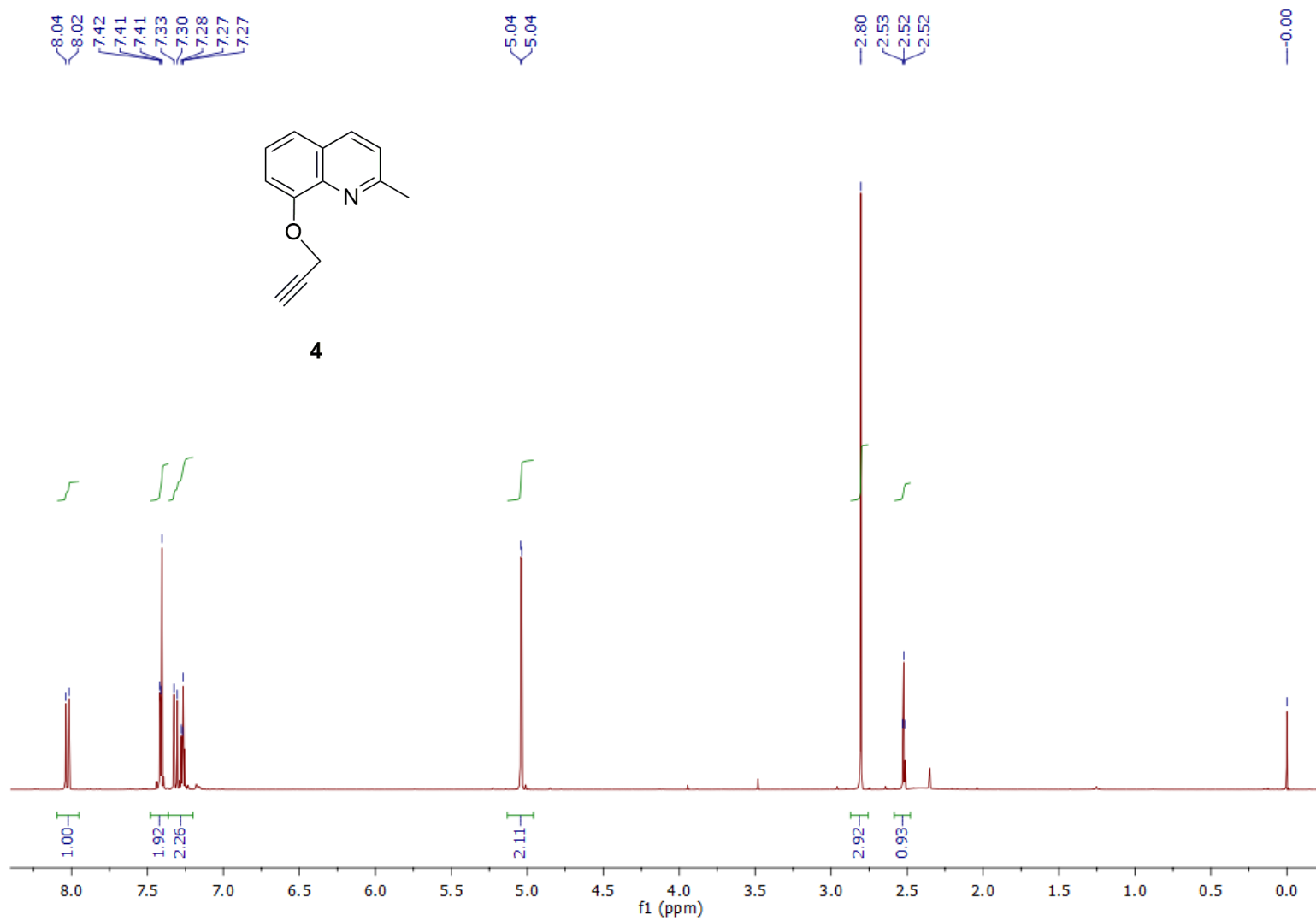


Fig. S3: ¹H NMR spectrum of compound 4.

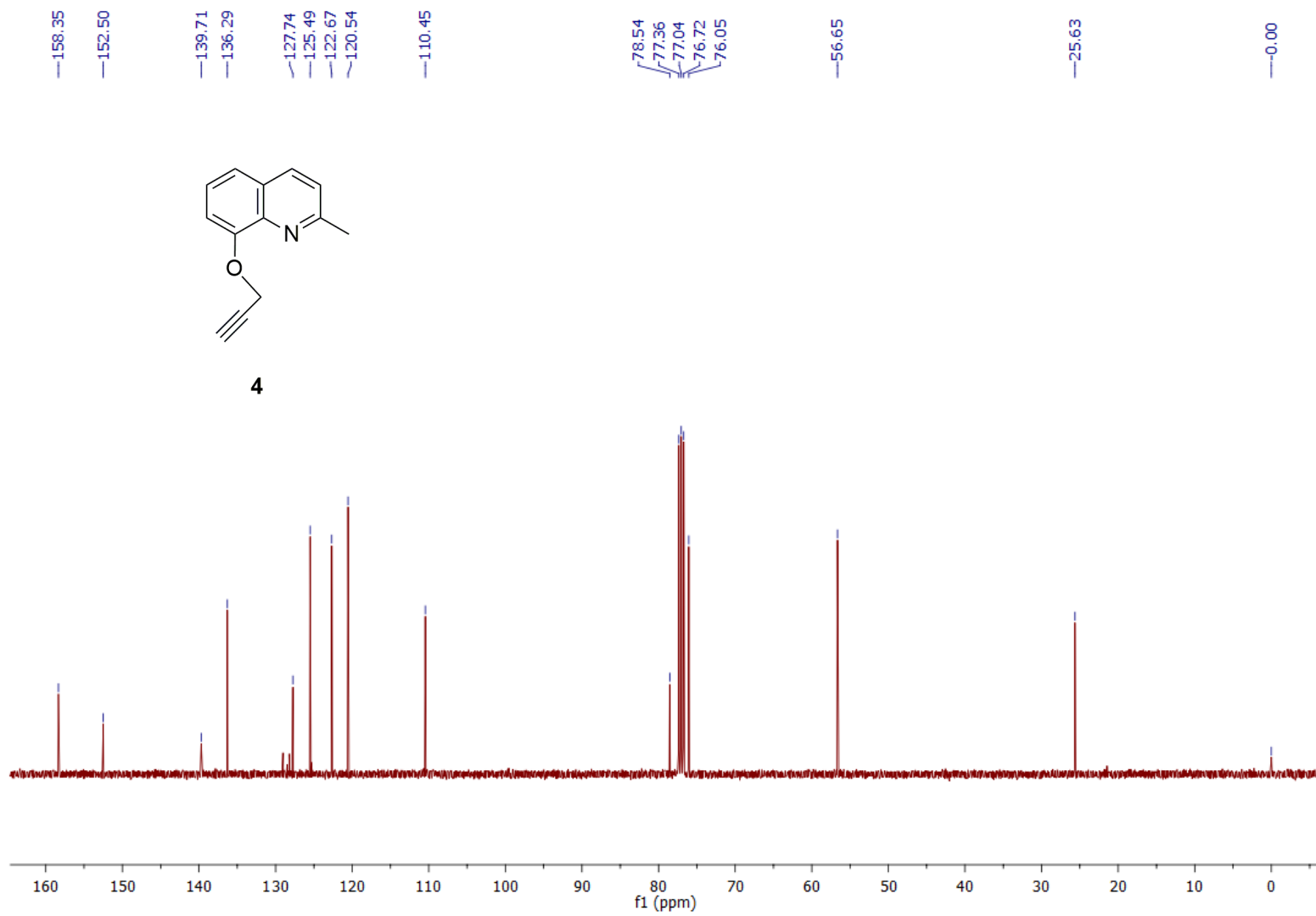


Fig. S4: ^{13}C NMR spectrum of compound 4.

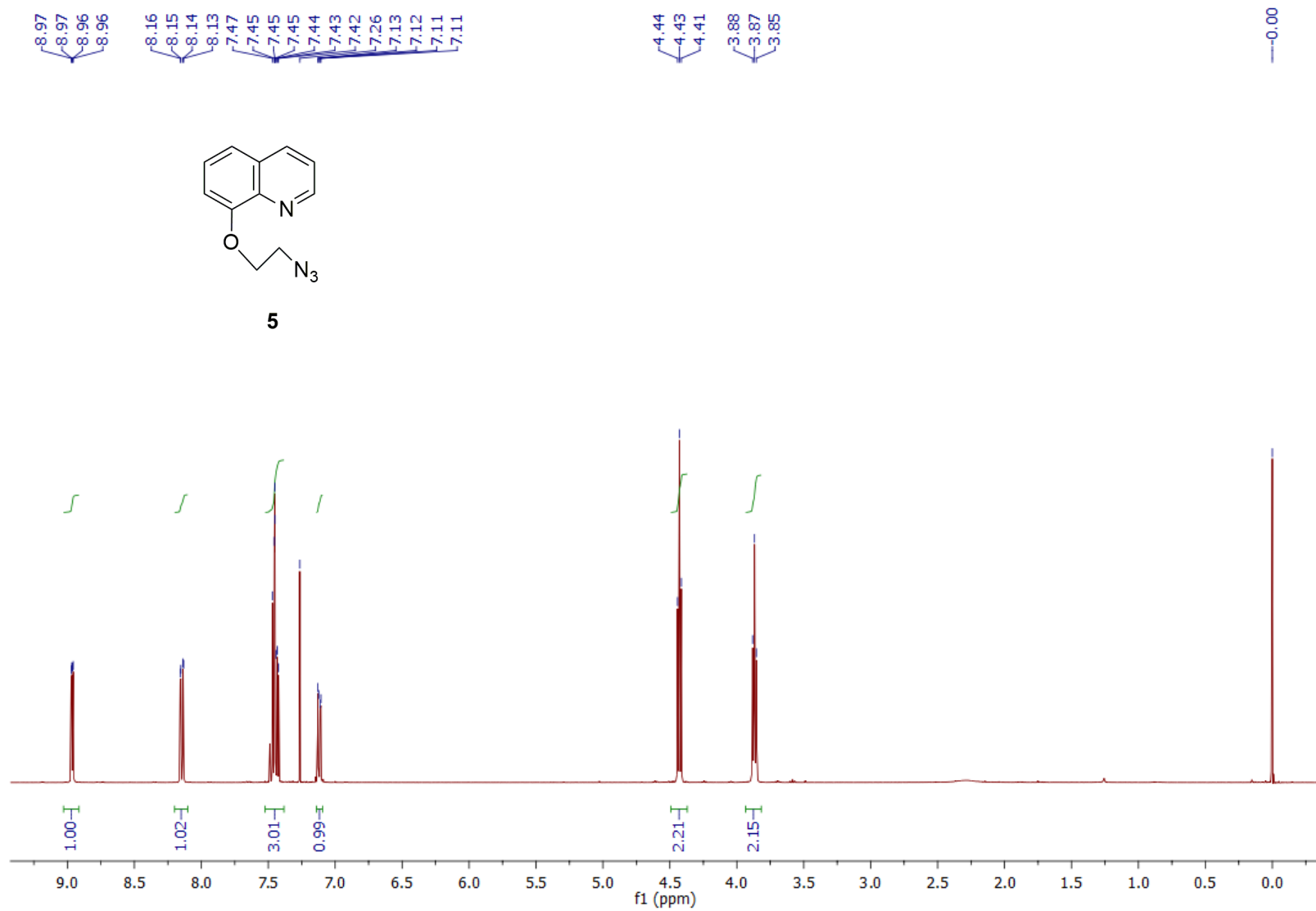


Fig. S5: ¹H NMR spectrum of compound 5.

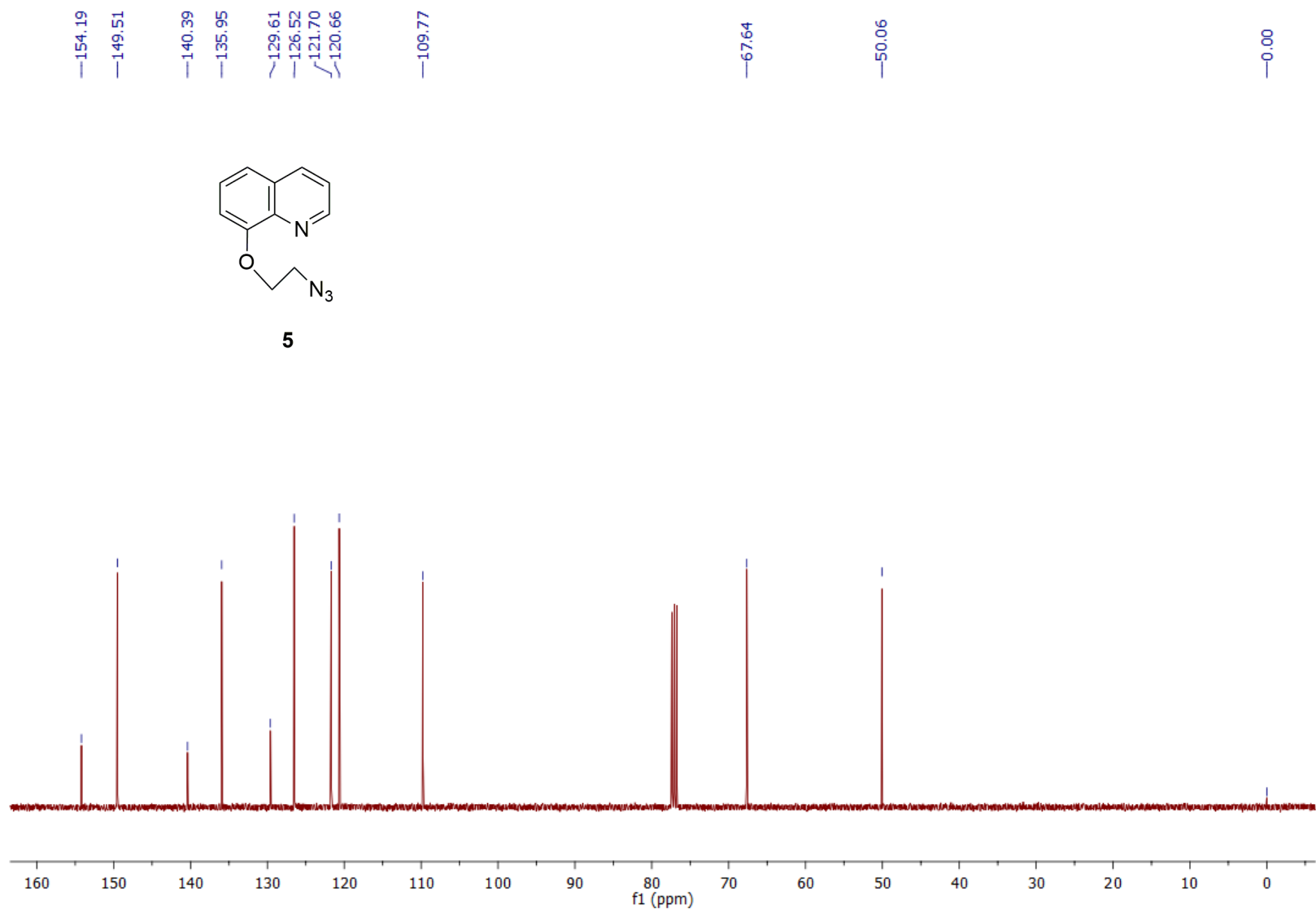


Fig. S6: ¹³C NMR spectrum of compound 5.

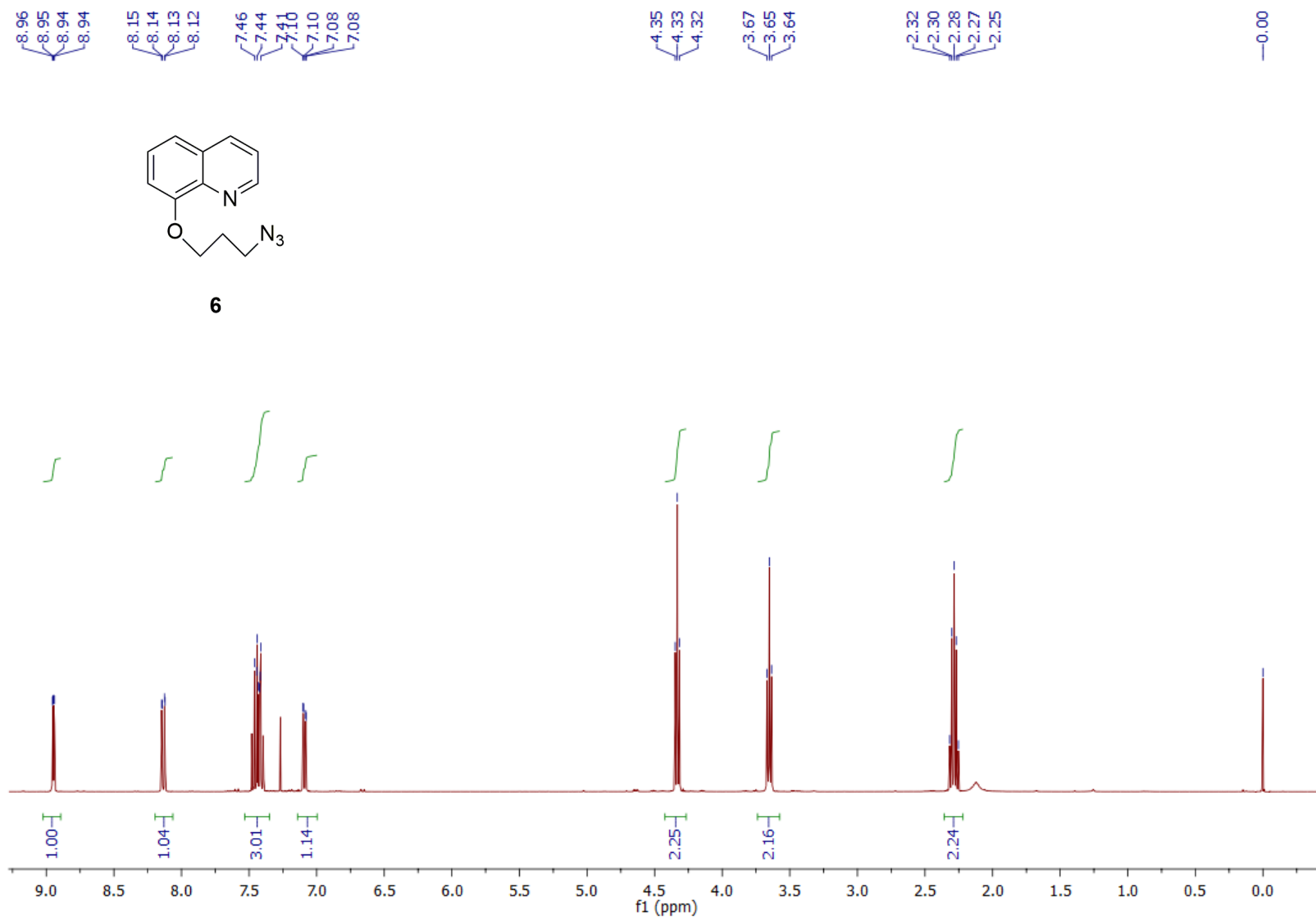


Fig. S7: ¹H NMR spectrum of compound **6**.

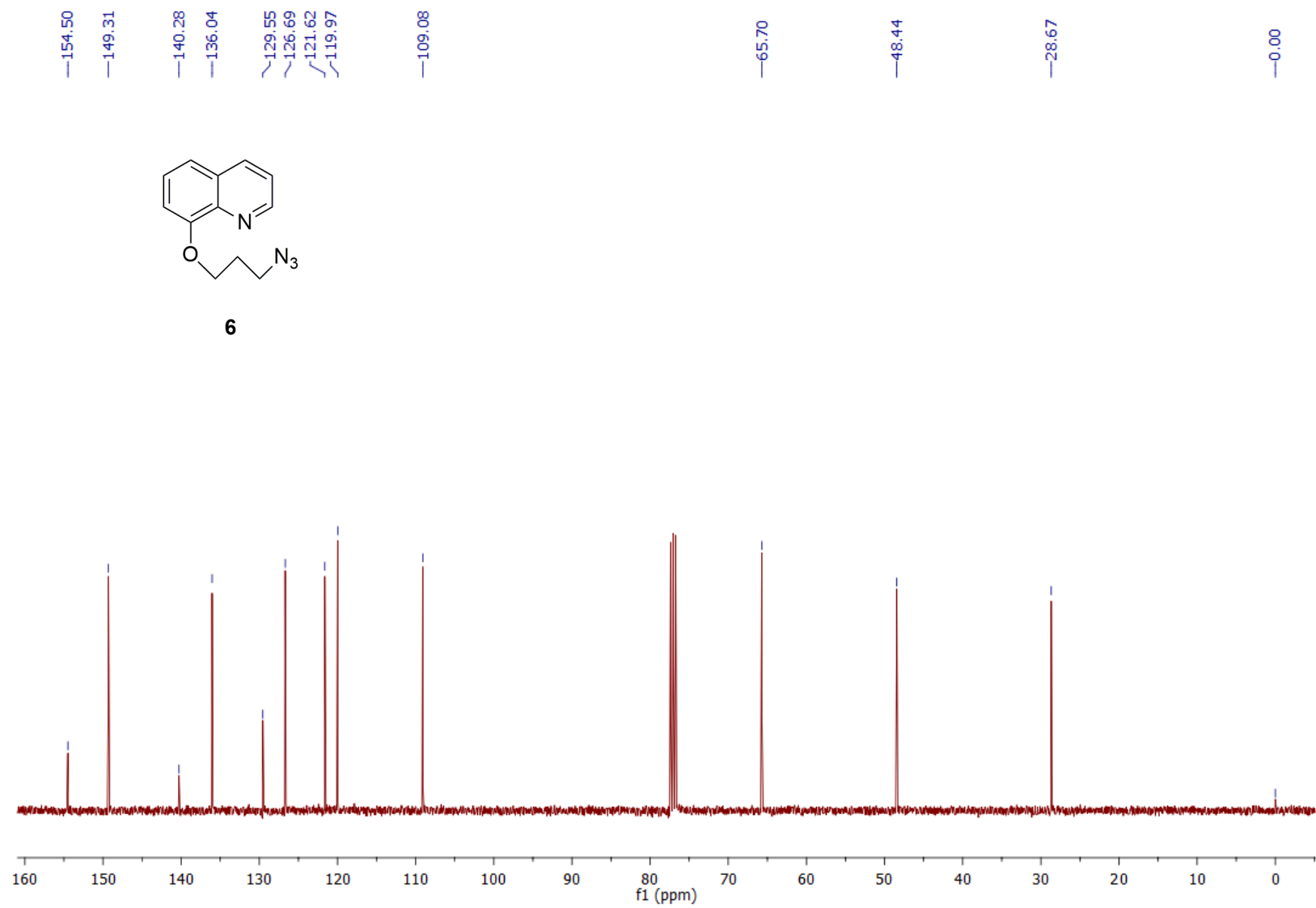


Fig. S8: ^{13}C NMR spectrum of compound **6**.

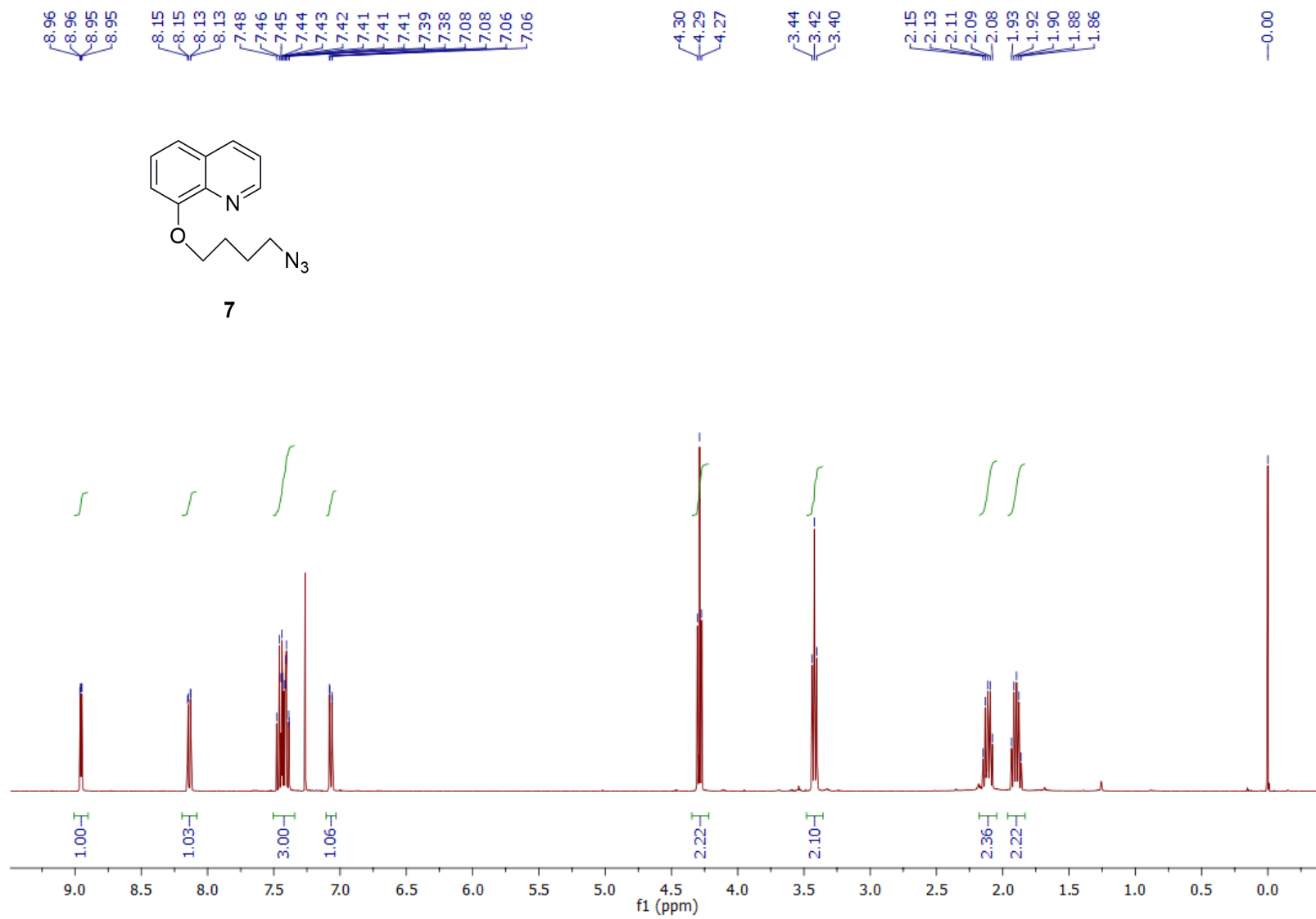


Fig. S9: ^1H NMR spectrum of compound 7.

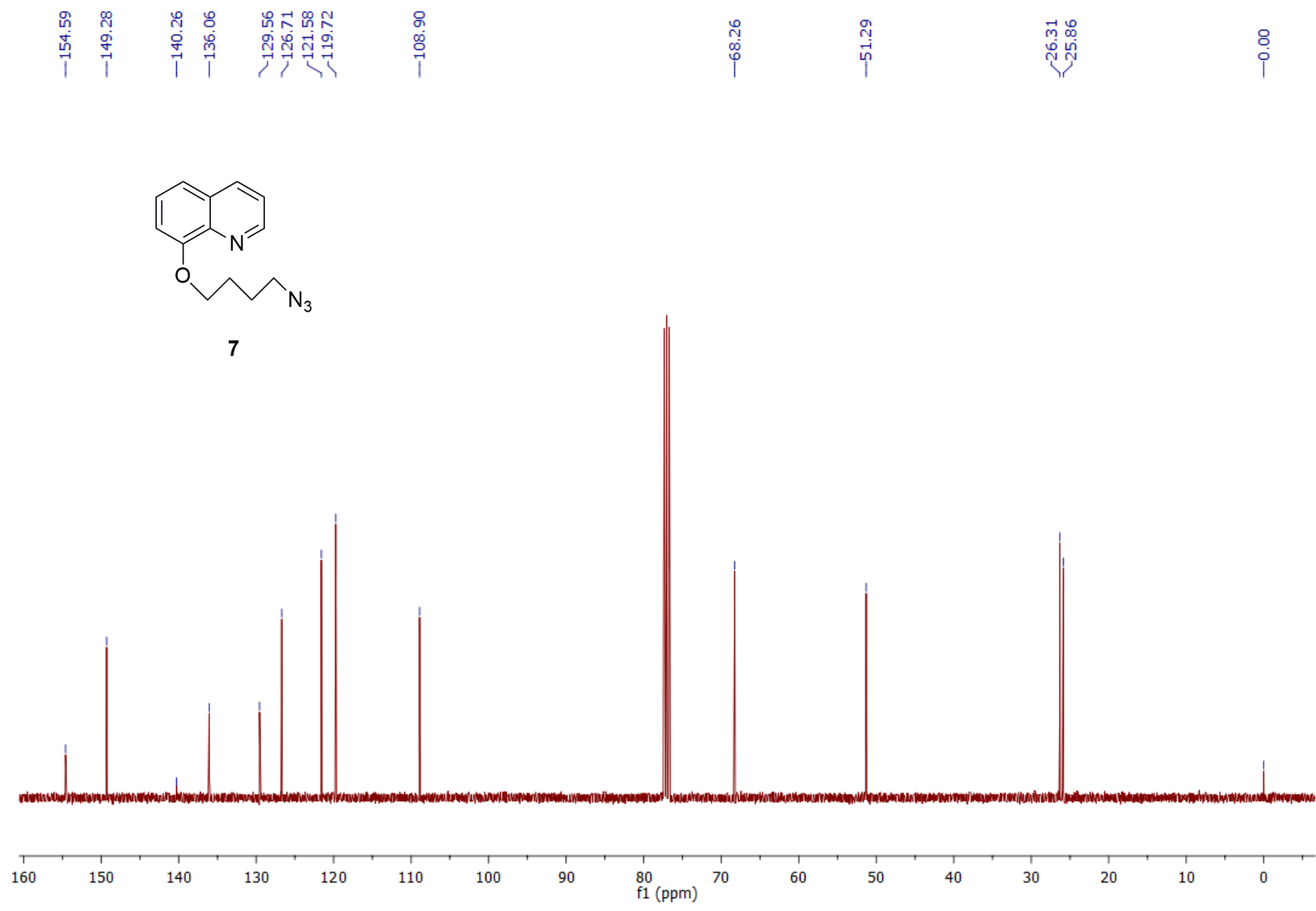


Fig. S10: ¹³C NMR spectrum of compound 7.

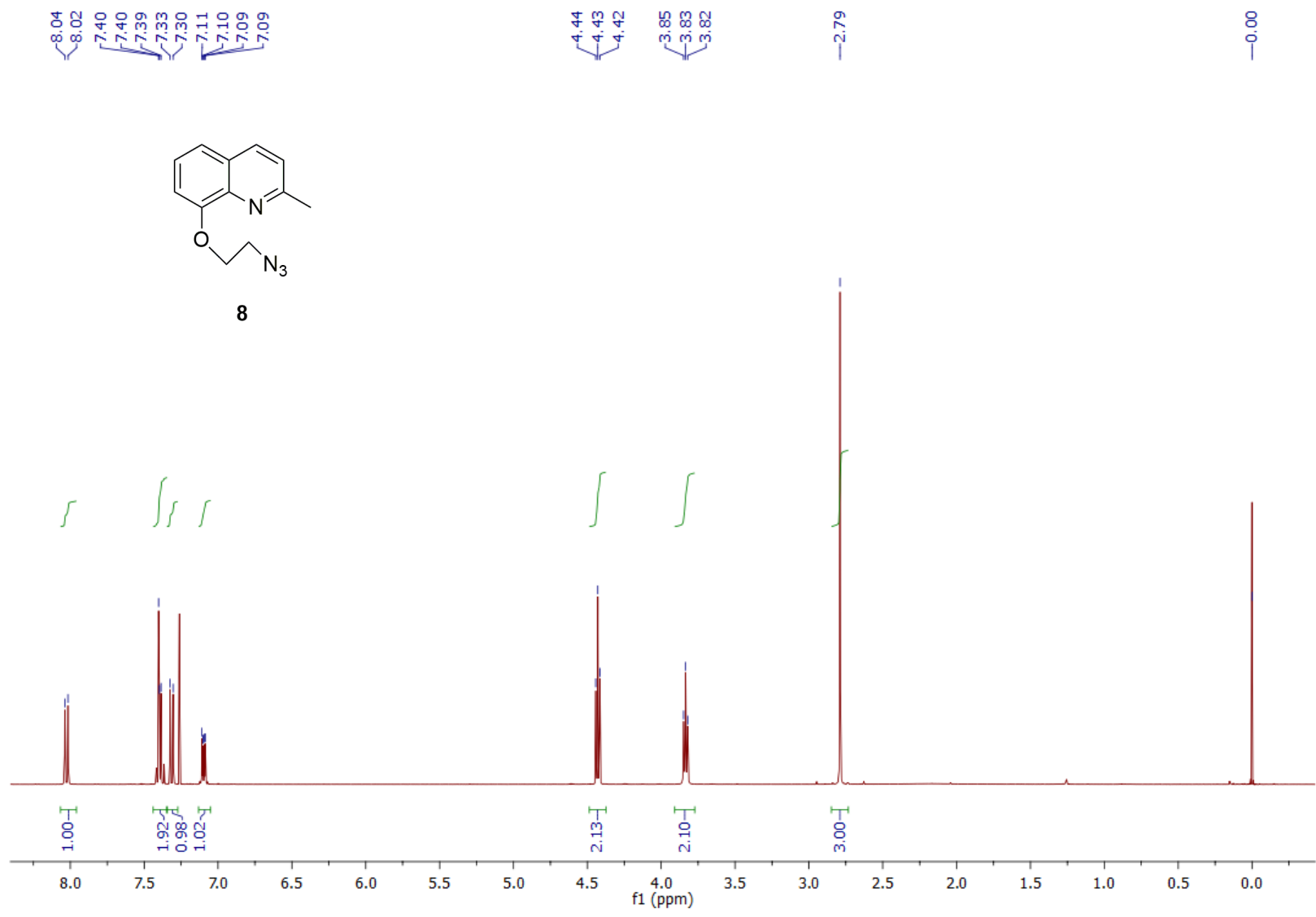


Fig. S11: ¹H NMR spectrum of compound **8**.

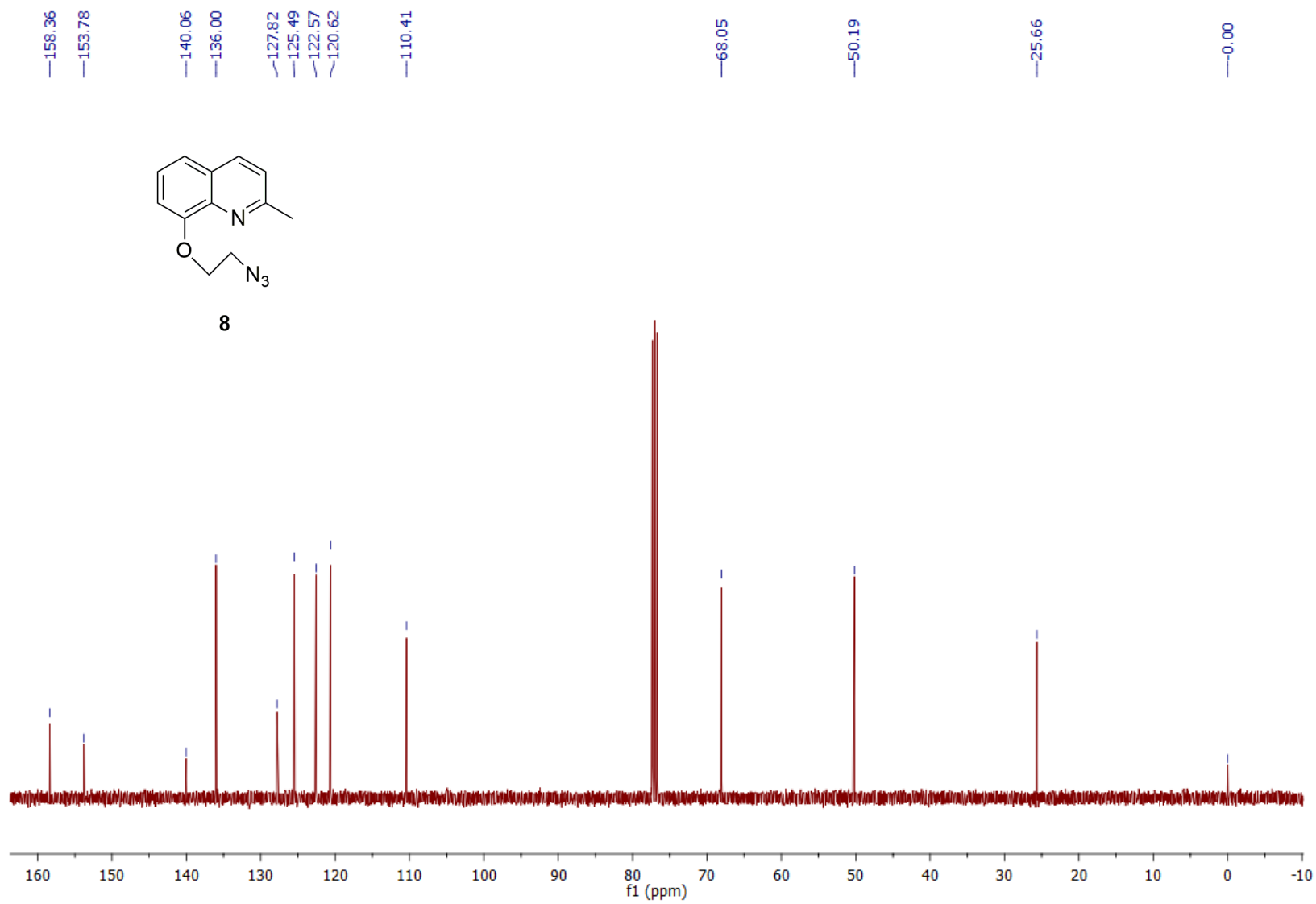


Fig. S12: ^{13}C NMR spectrum of compound **8**.

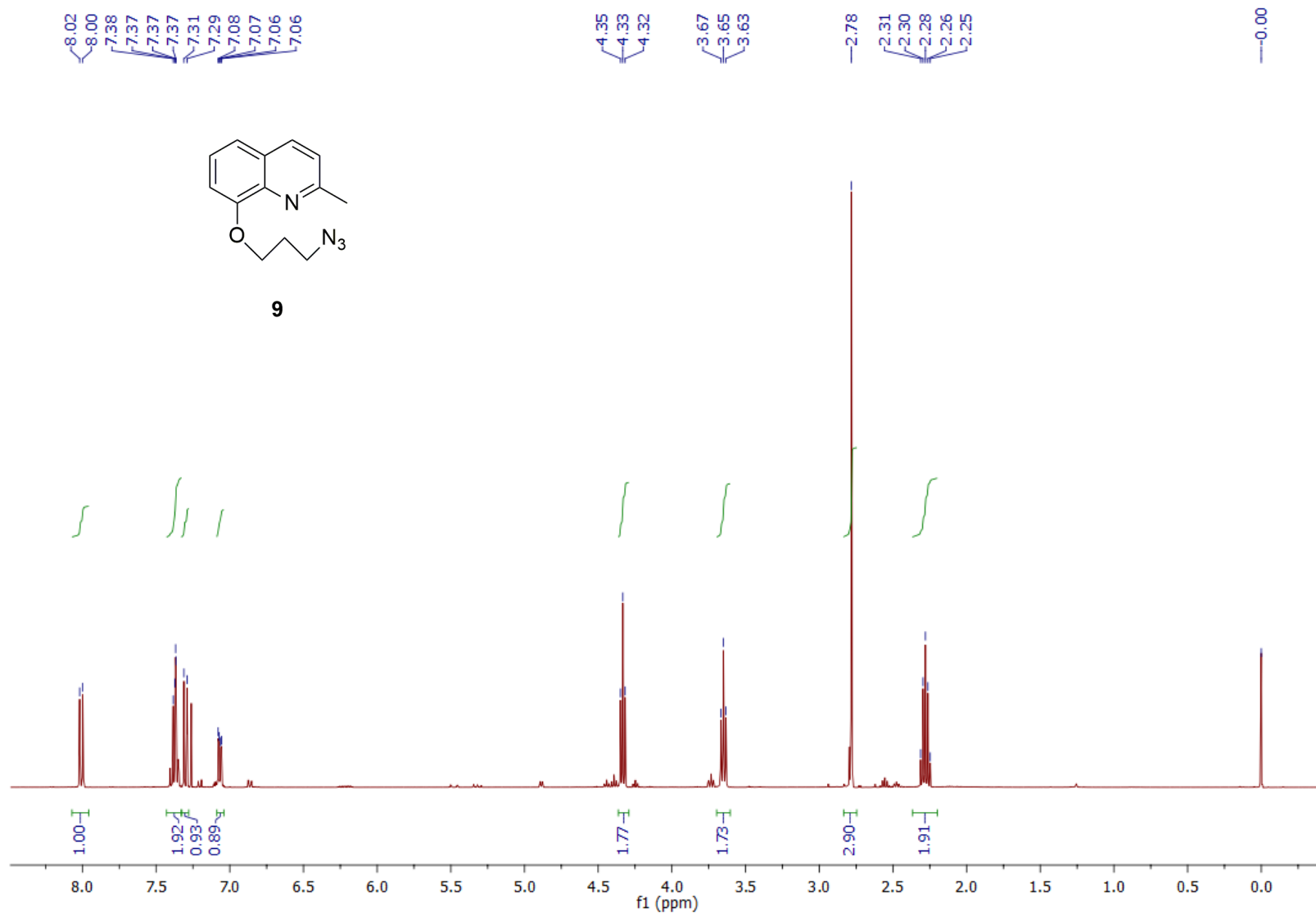


Fig. S13: ^1H NMR spectrum of compound **9**.

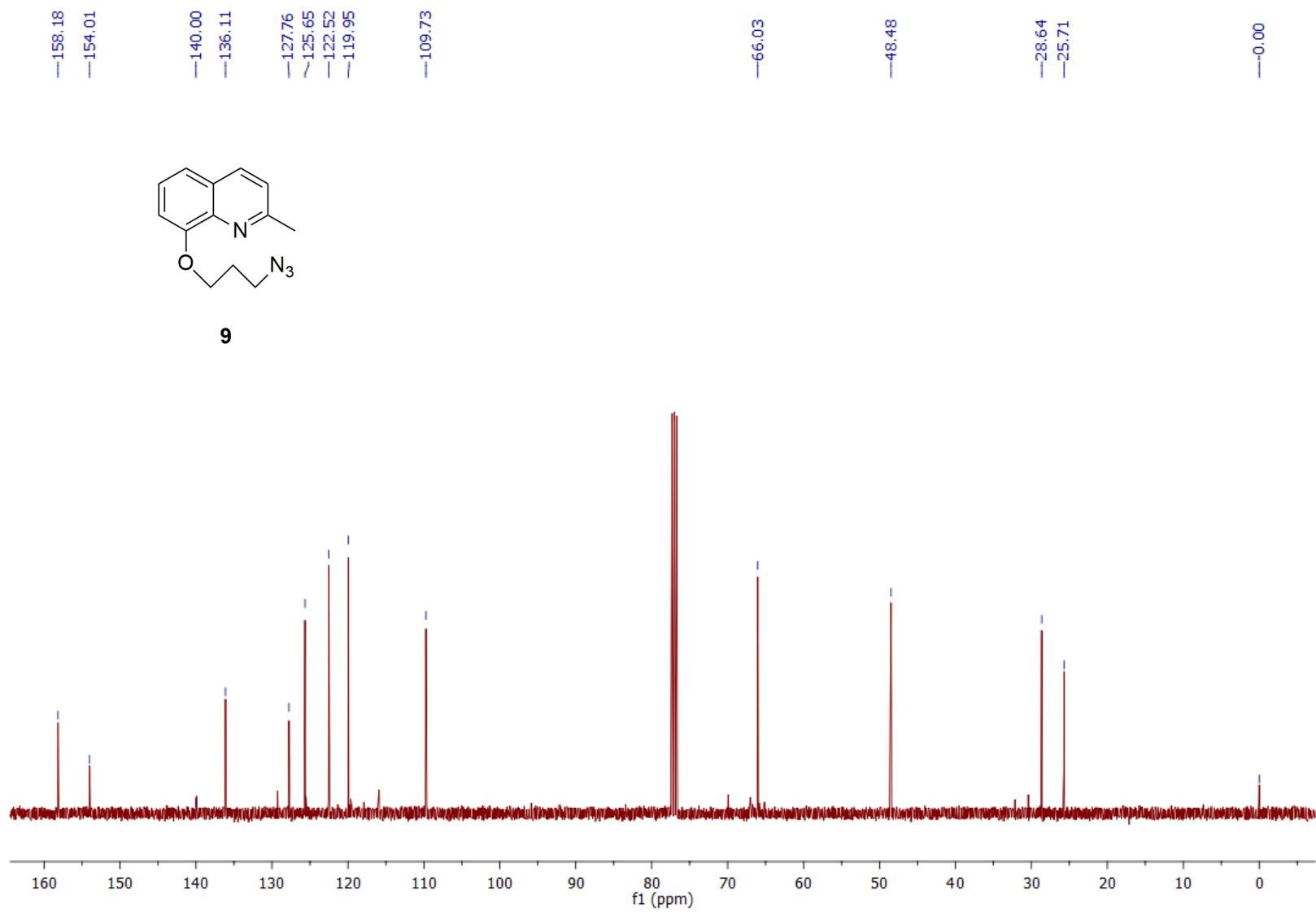


Fig. S14: ^{13}C NMR spectrum of compound **9**.

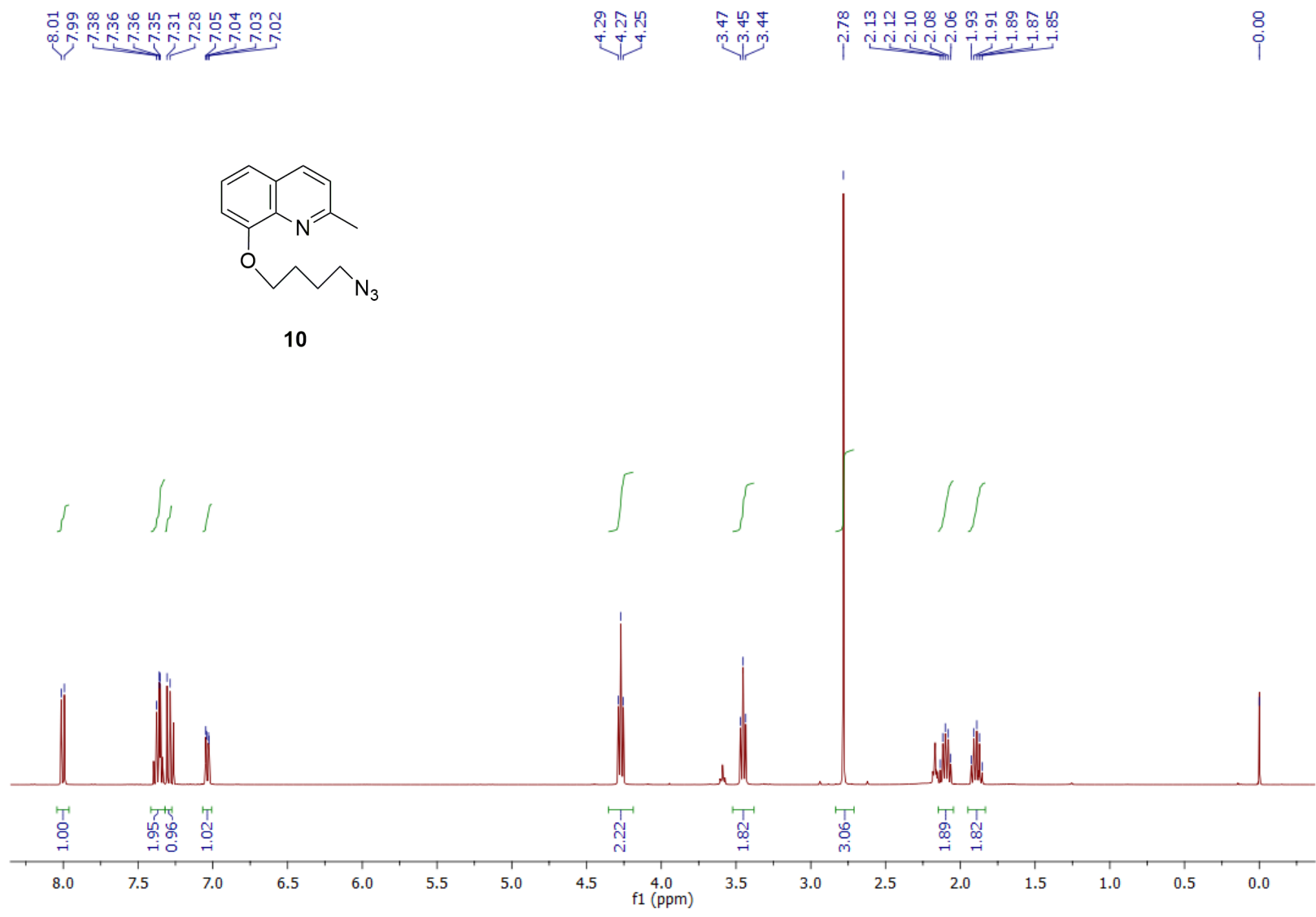


Fig. S15: ^1H NMR spectrum of compound **10**.

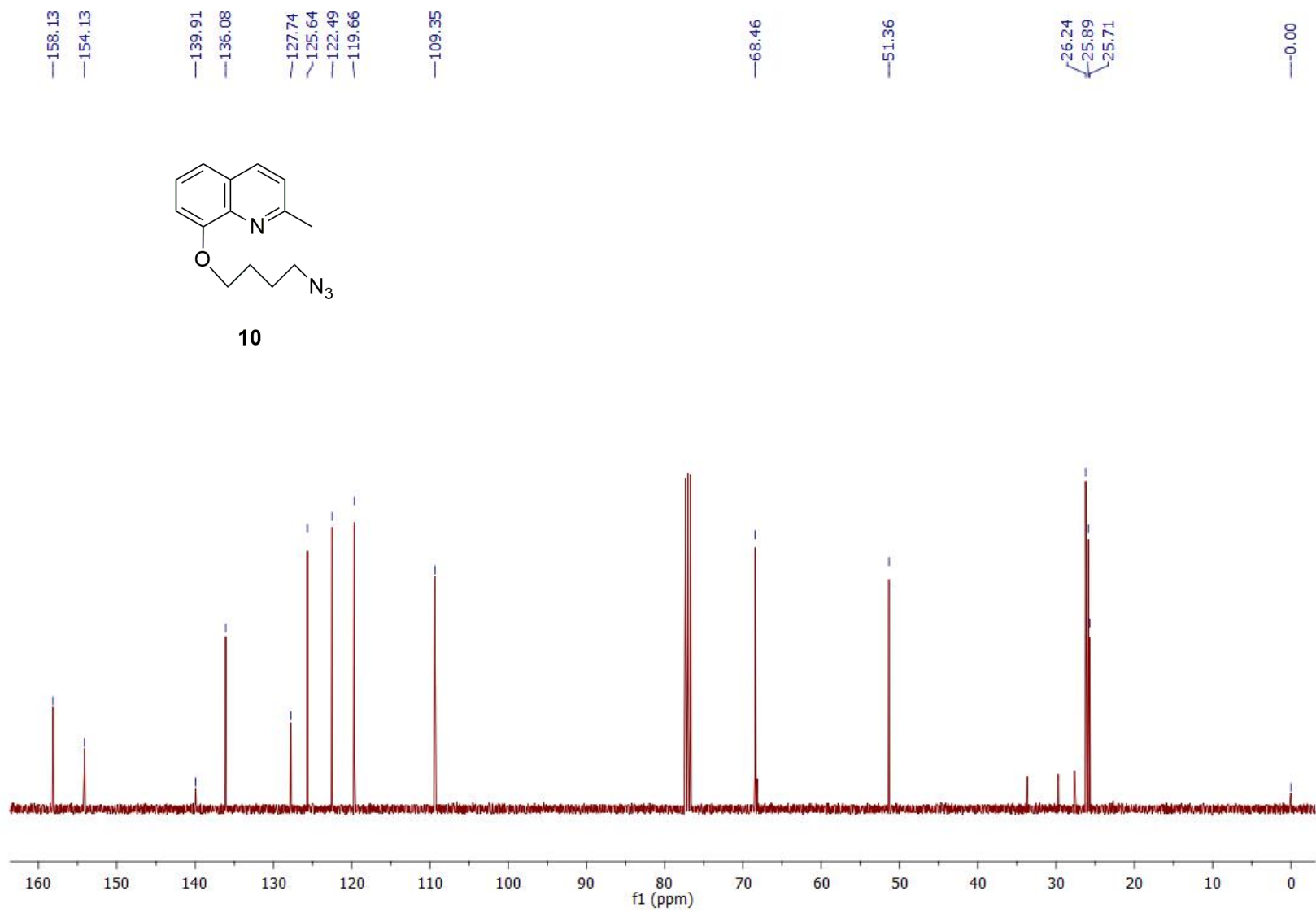


Fig. S16: ^{13}C NMR spectrum of compound **10**.

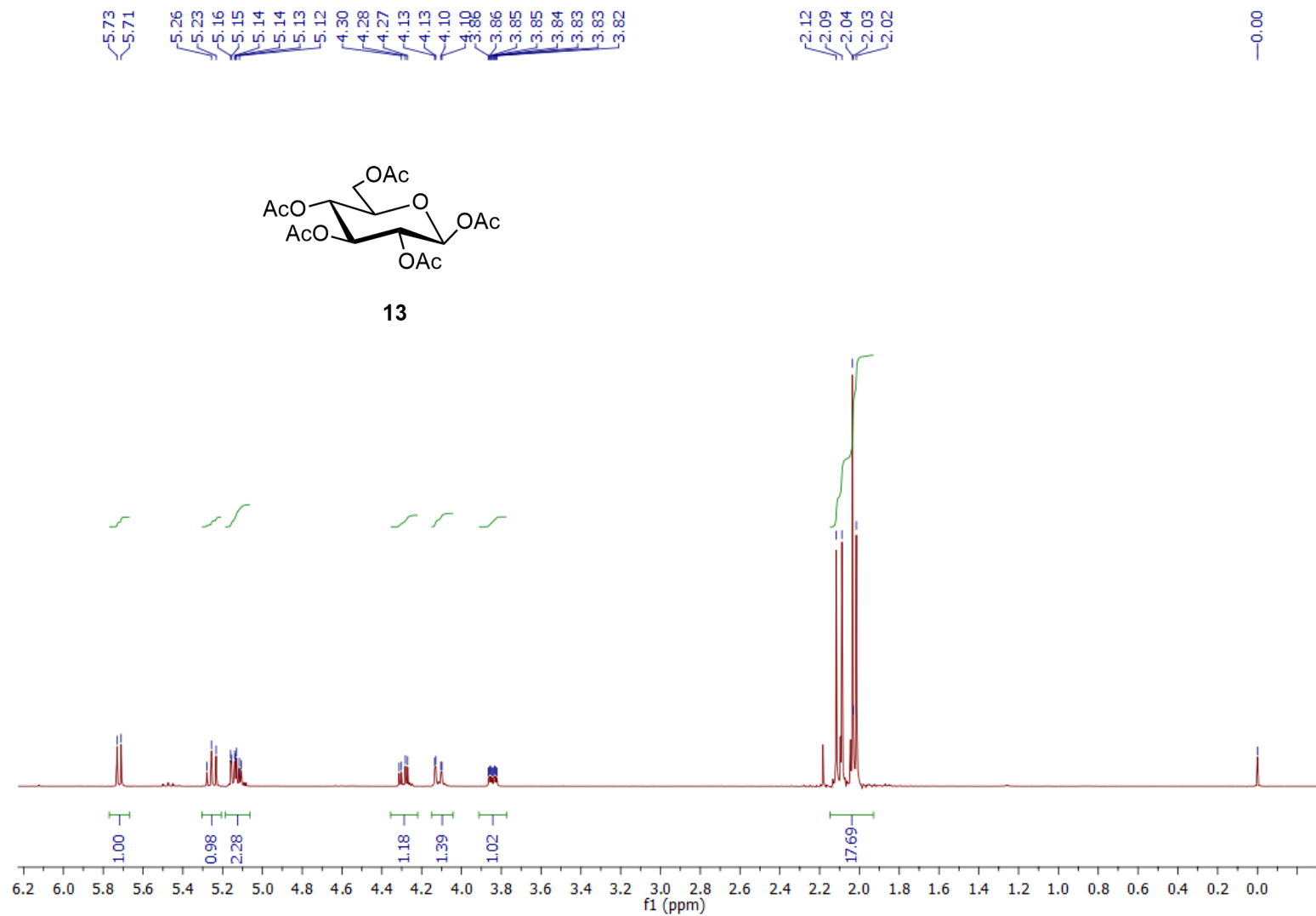


Fig. S17: ^1H NMR spectrum of compound **13**.

170.59
170.08
169.38
169.23
168.94

91.72
77.35
77.04
76.72
72.81
72.75
70.26
67.79
61.48

20.81
20.70
20.56
20.55

0.00

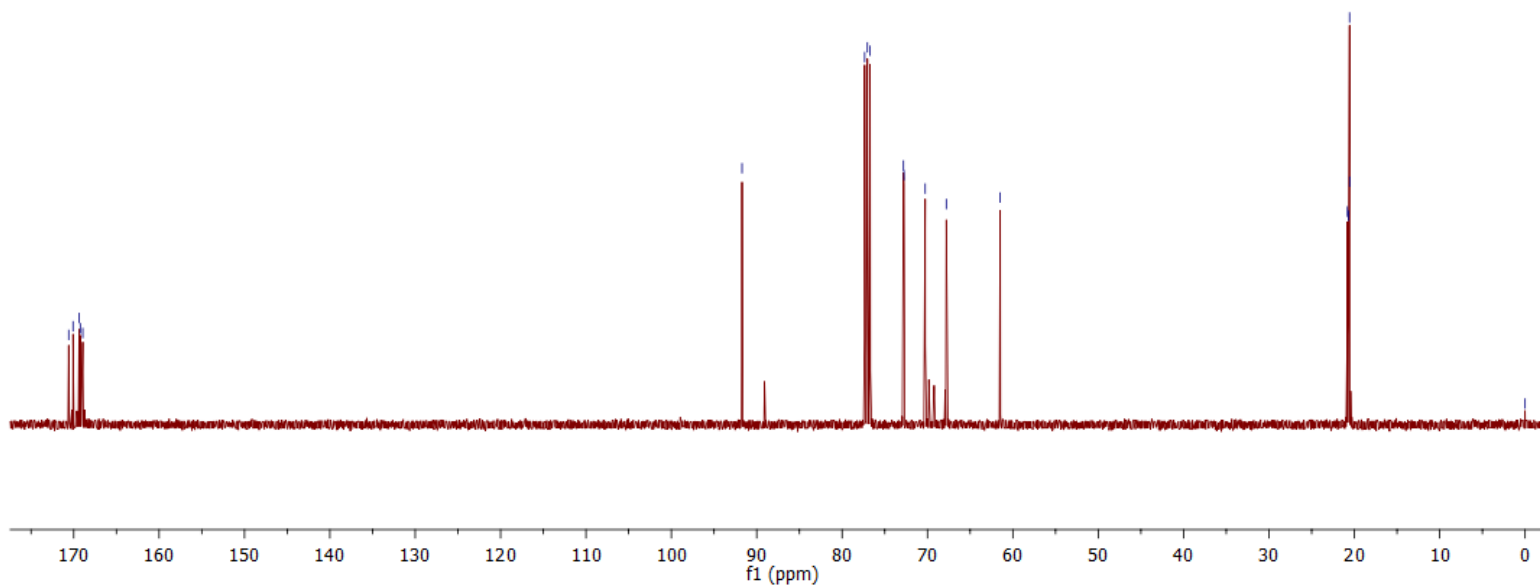
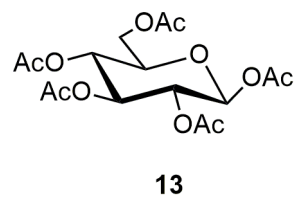


Fig. S18: ¹³C NMR spectrum of compound **13**.

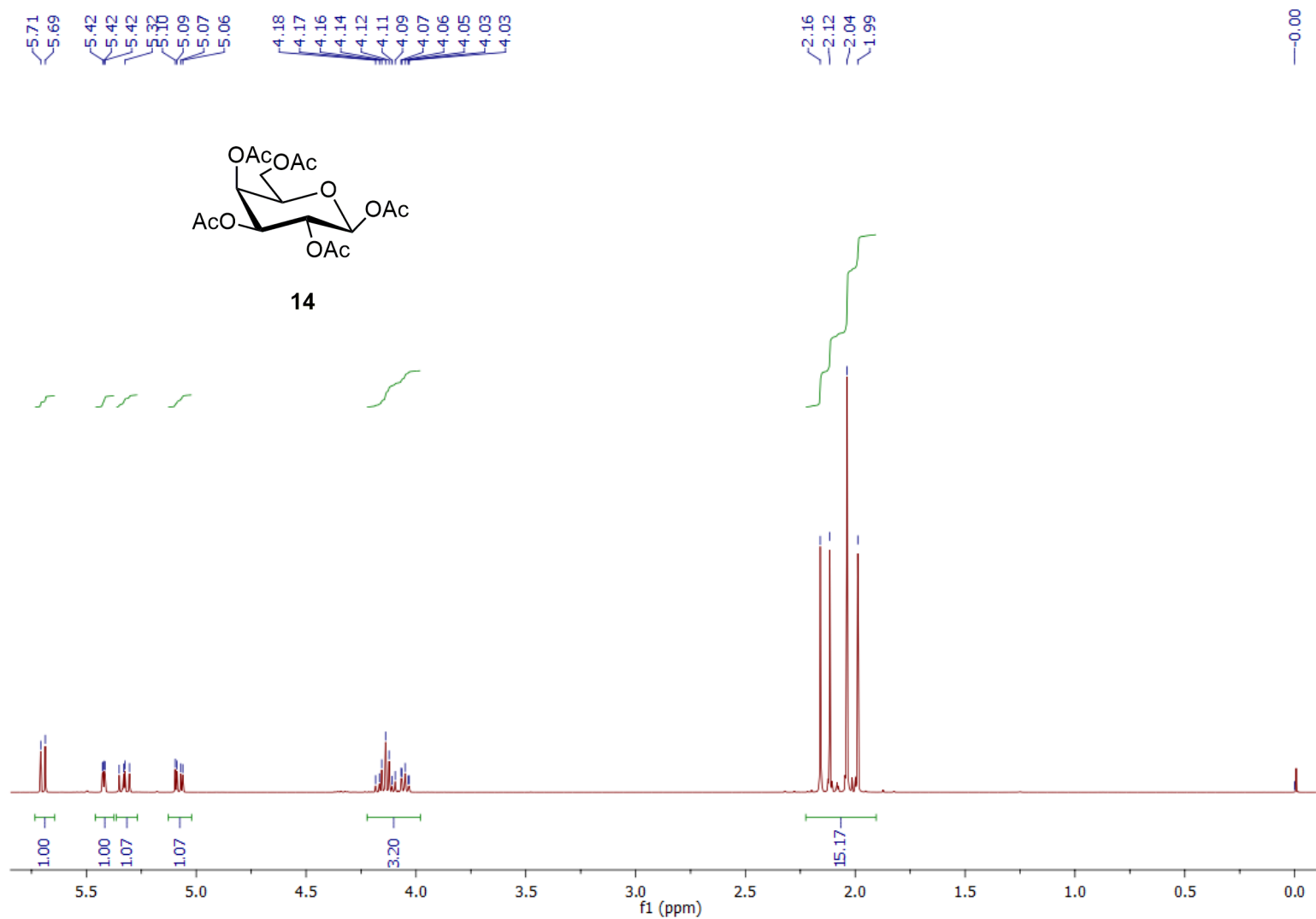


Fig. S19: ¹H NMR spectrum of compound **14**.

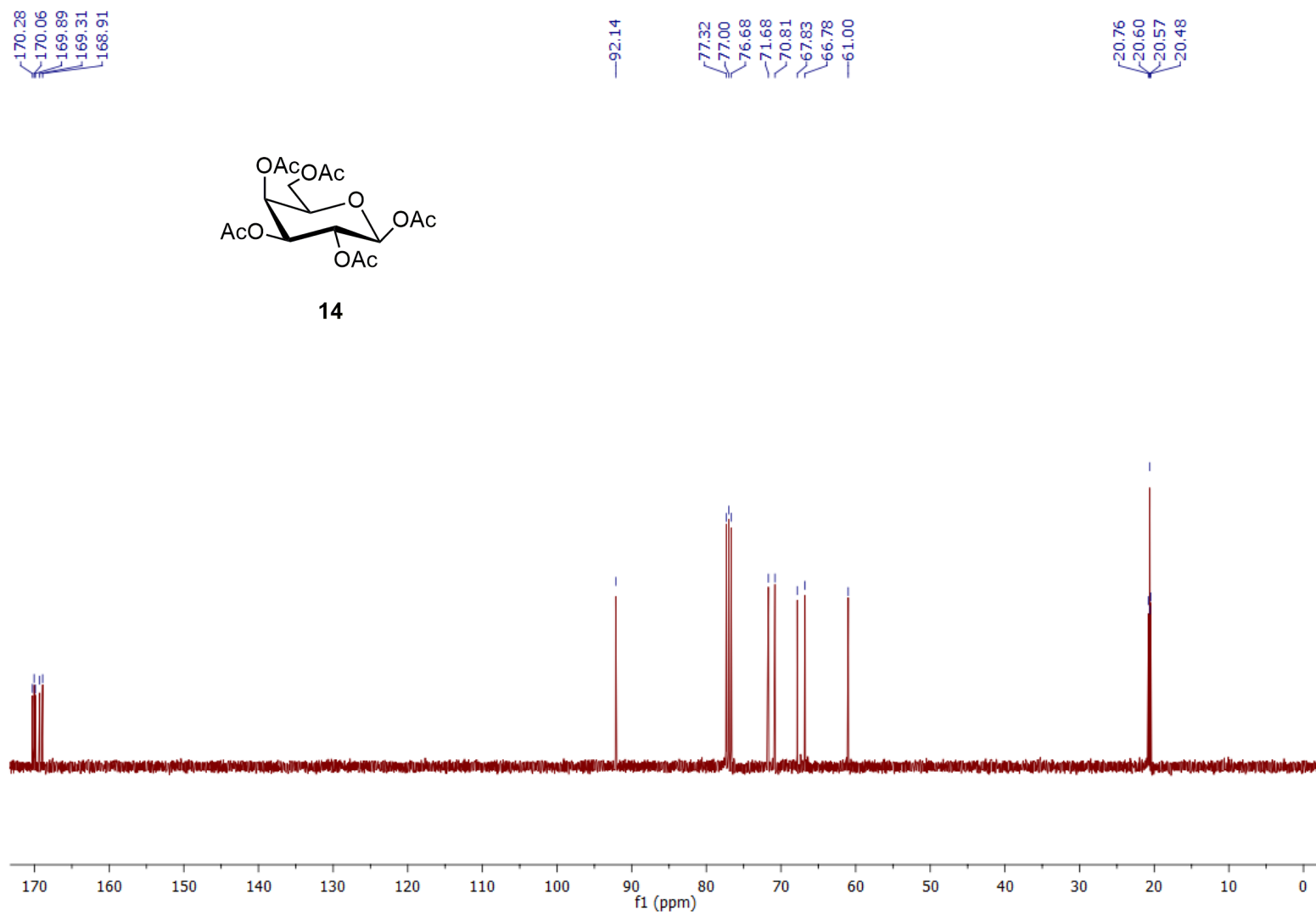


Fig. S20: ¹³C NMR spectrum of compound **14**.

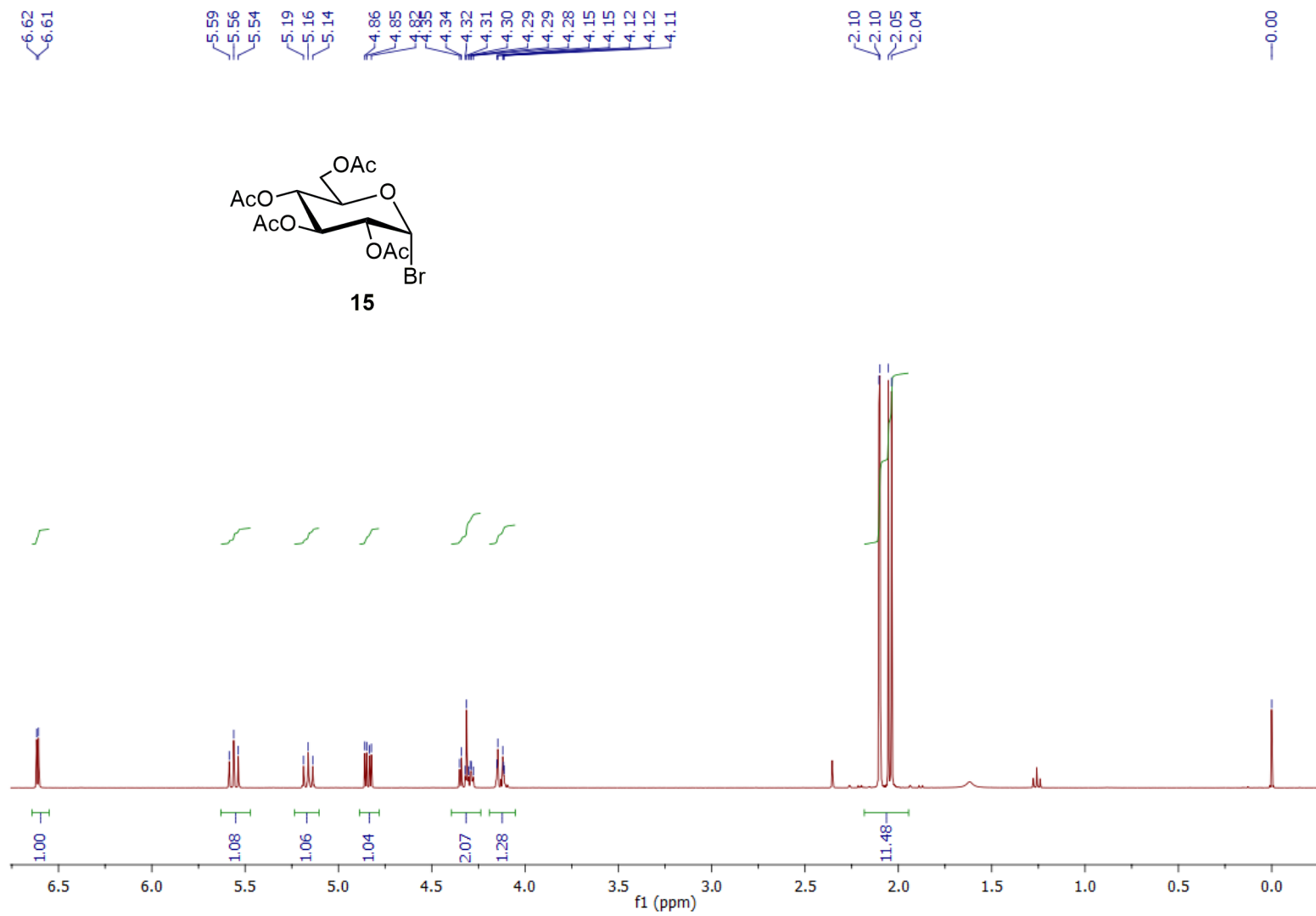


Fig. S21: ¹H NMR spectrum of compound **15**.

170.48
169.82
169.77
169.45

86.57
77.34
77.03
76.71
72.16
70.63
70.19
67.21
60.97

20.66
20.64
20.61
20.55

0.00

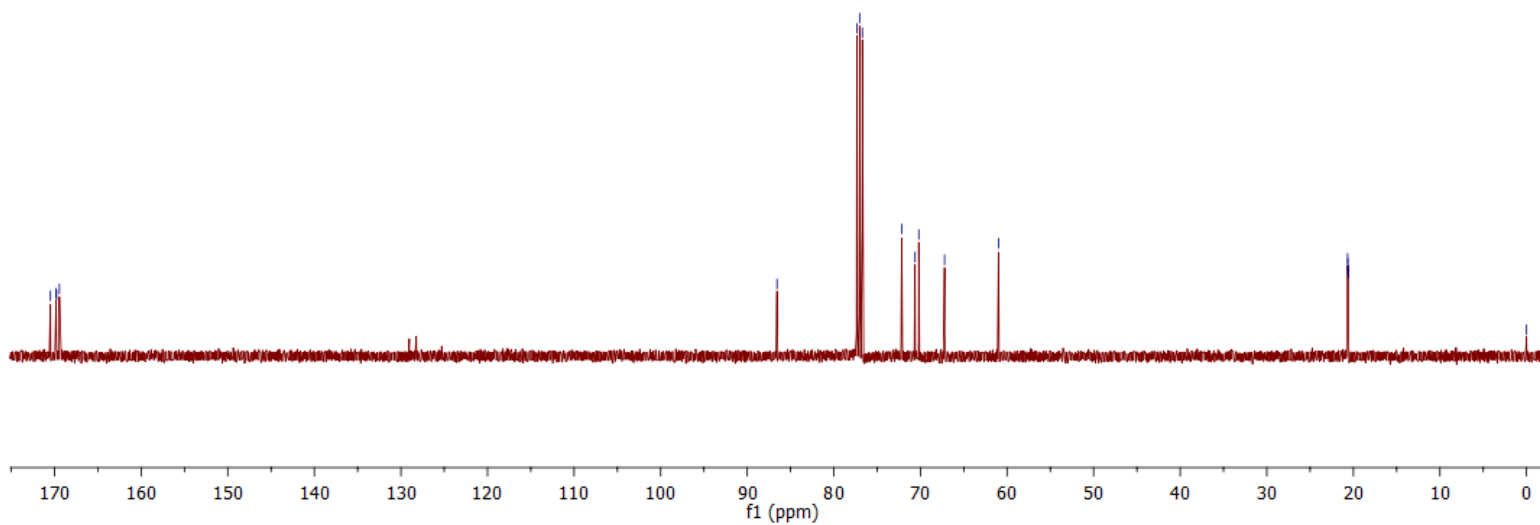
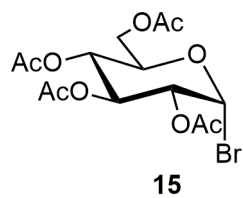


Fig. S22: ^{13}C NMR spectrum of compound **15**.

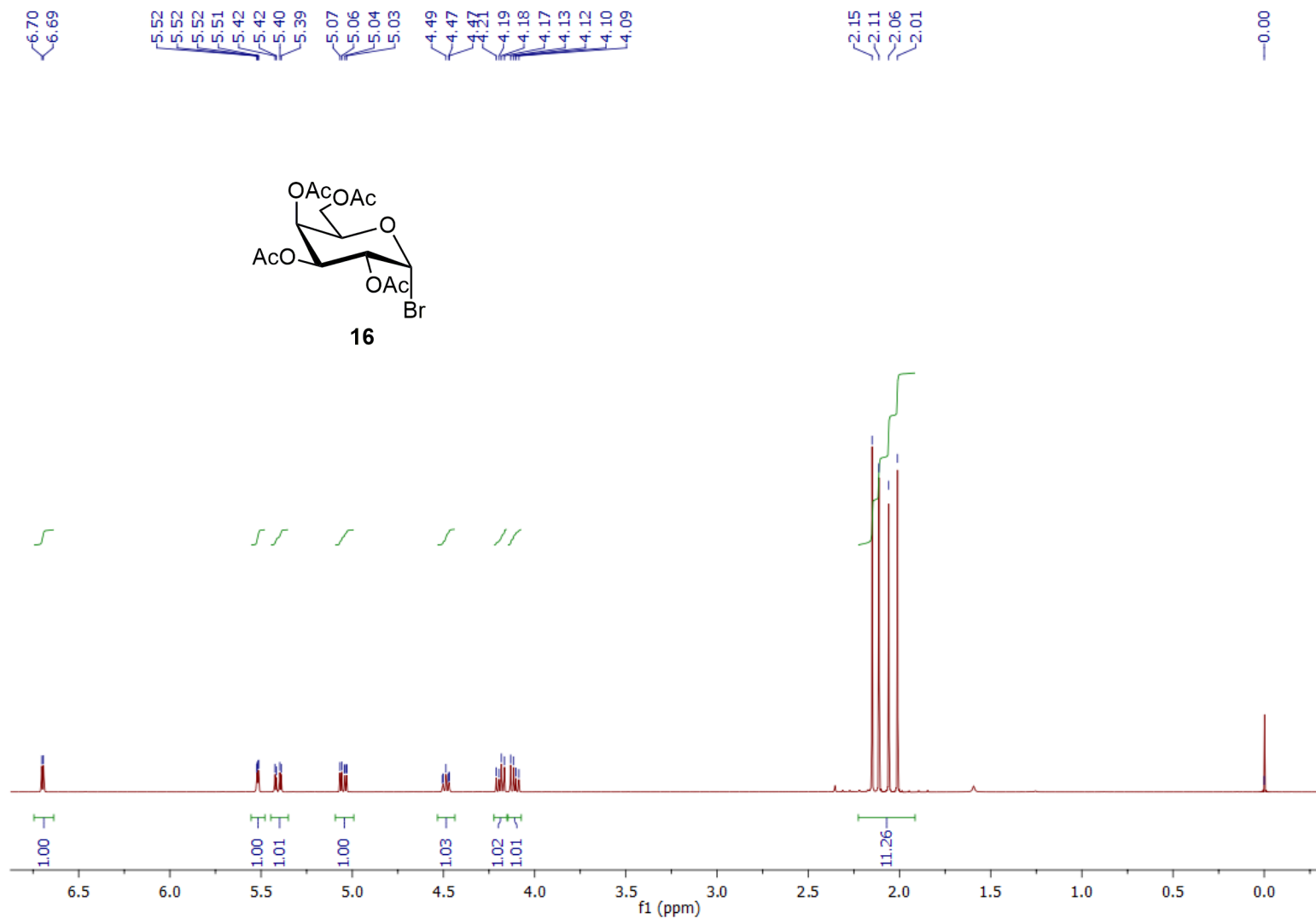


Fig. S23: ^1H NMR spectrum of compound **16**.

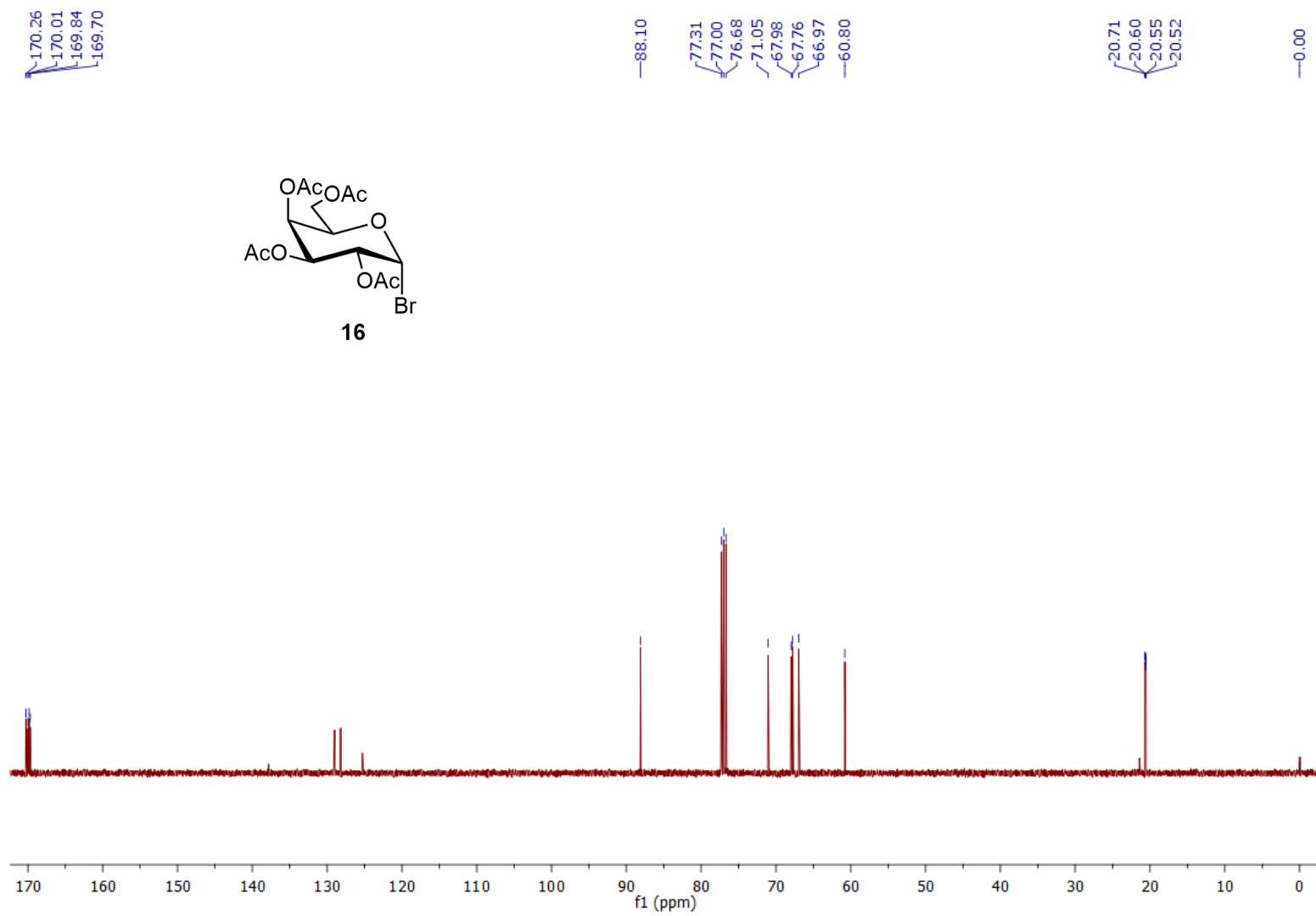


Fig. S24: ^{13}C NMR spectrum of compound **16**.

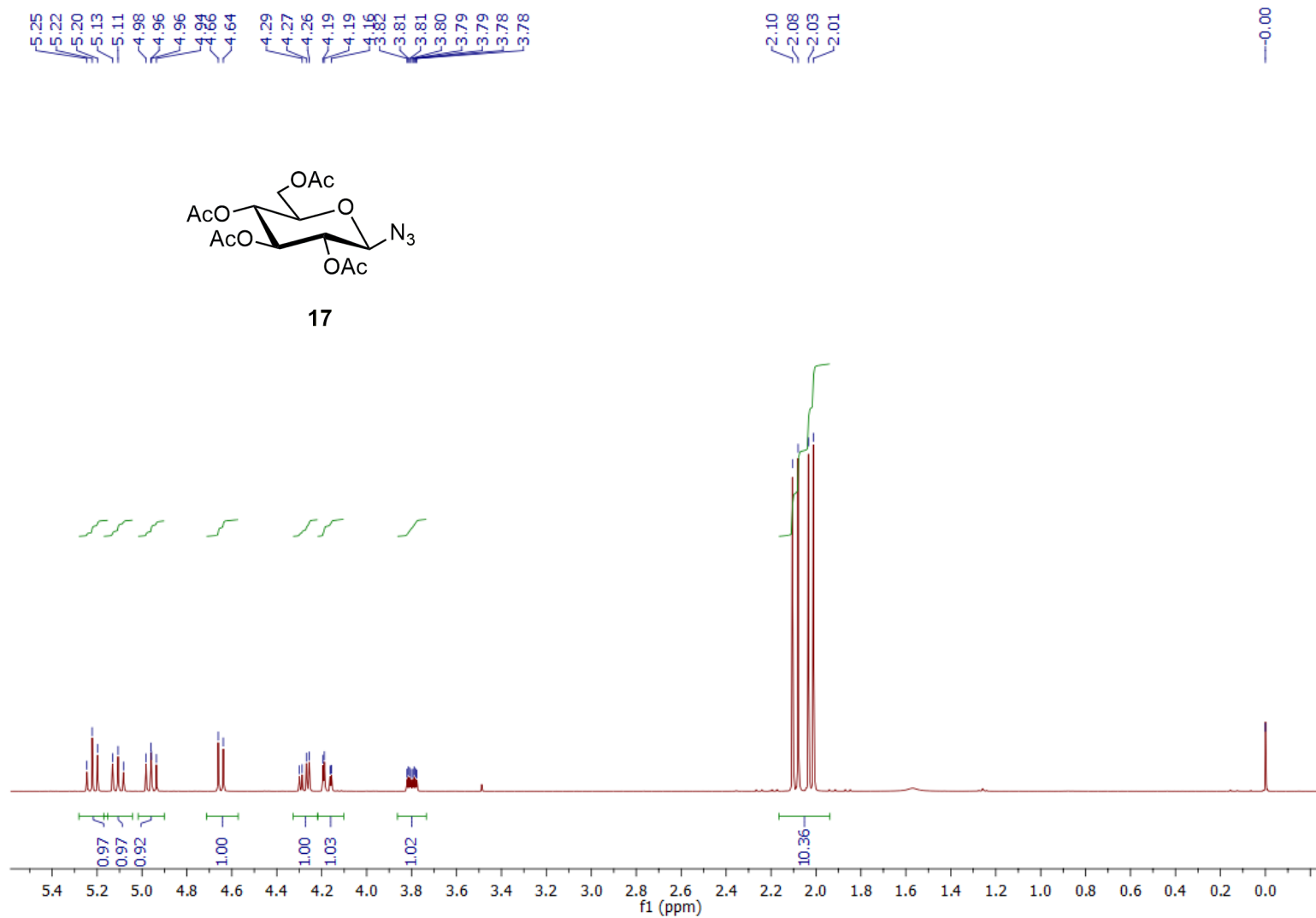


Fig. S25: 1H NMR spectrum of compound **17**.

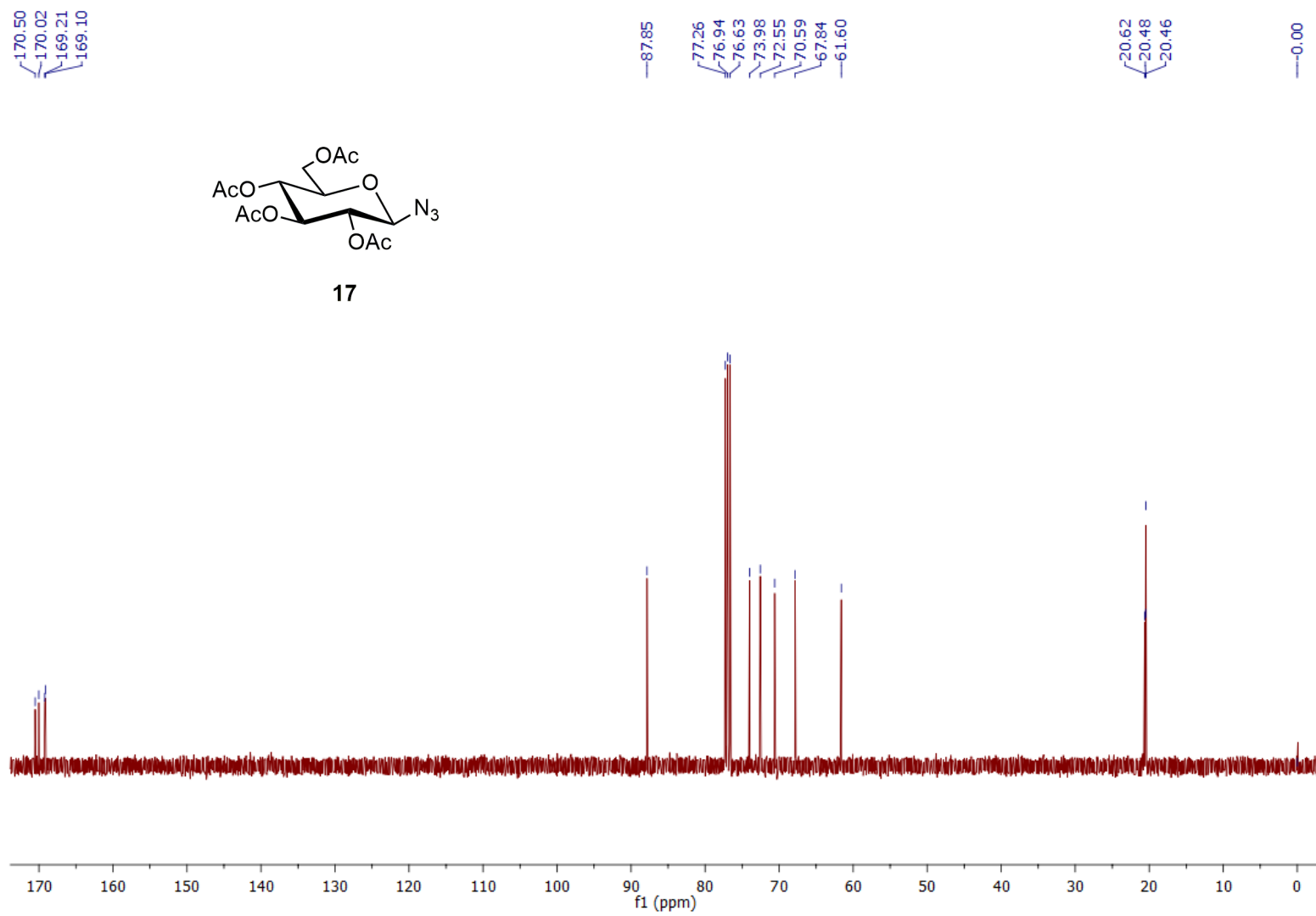


Fig. S26: ¹³C NMR spectrum of compound **17**.

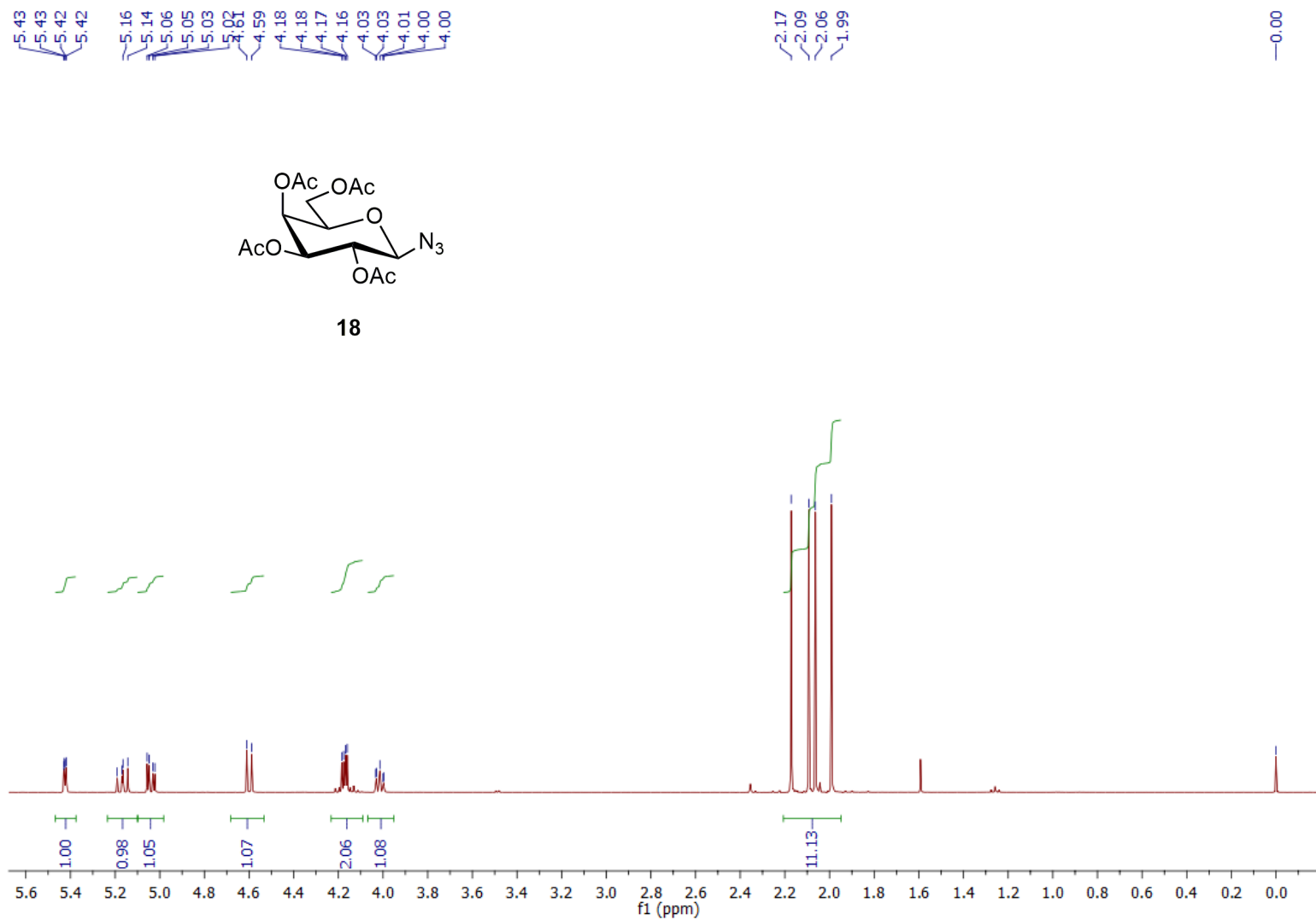
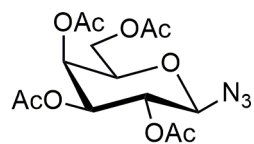


Fig. S27: ^1H NMR spectrum of compound **18**.

170.32
170.07
169.94
169.32

88.29
77.32
77.00
76.68
72.87
70.72
68.06
66.84
61.21

20.65
20.63
20.59
20.49



18

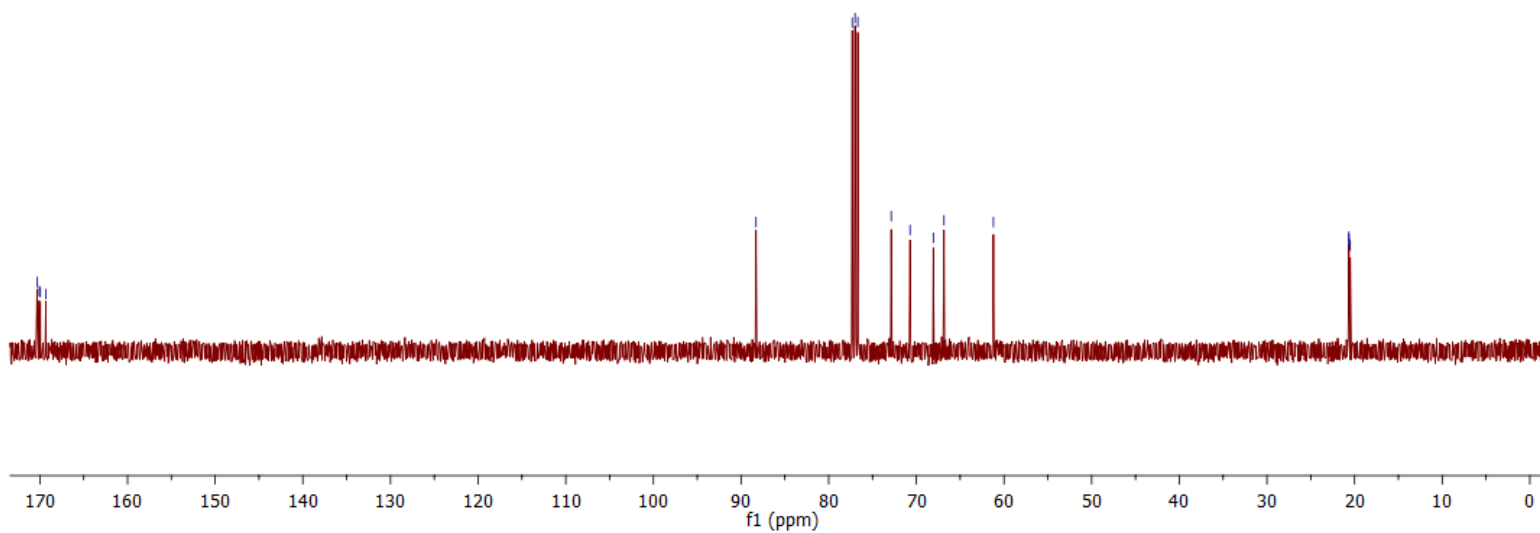


Fig. S28: ¹³C NMR spectrum of compound 18.

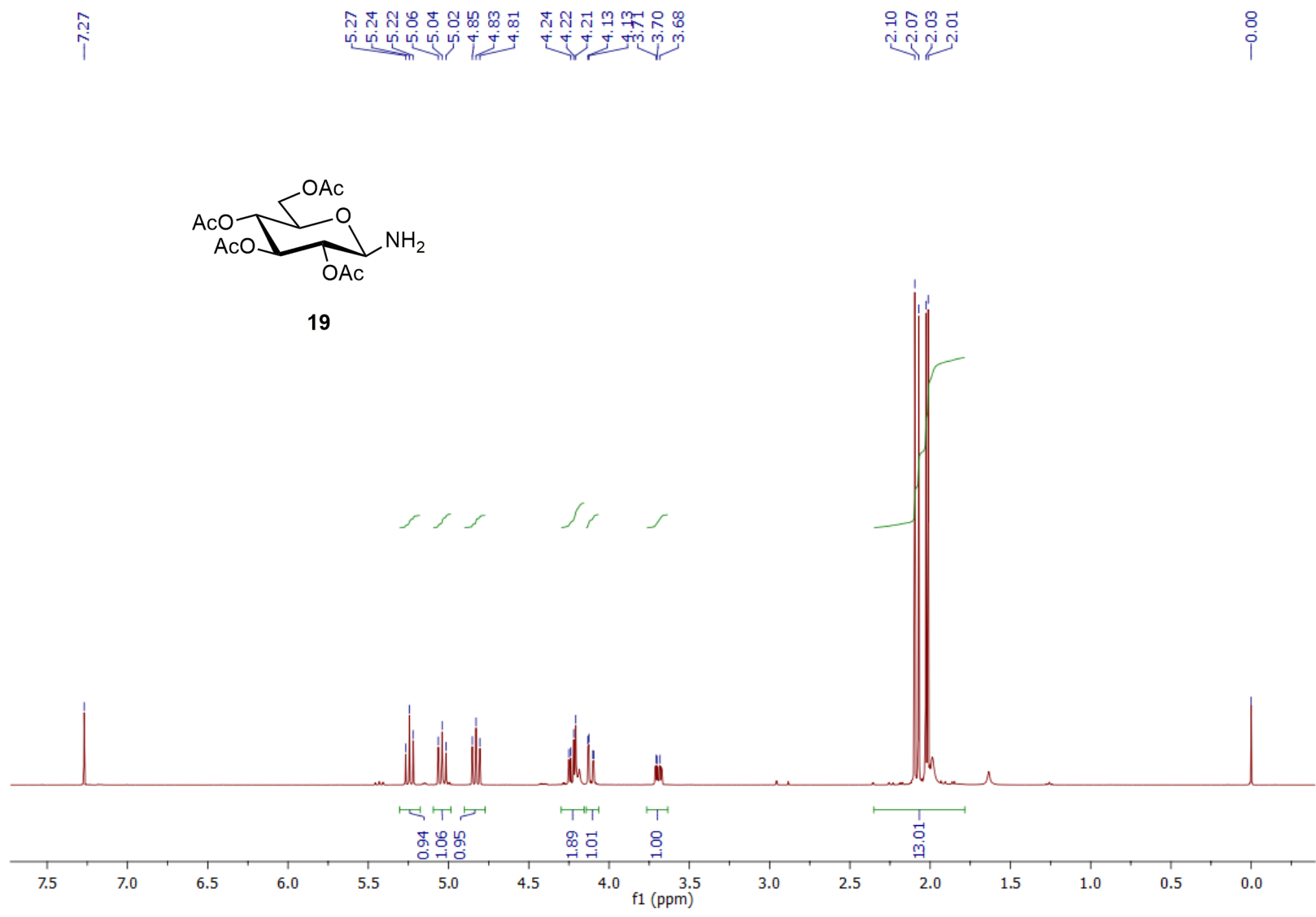


Fig. S29: ¹H NMR spectrum of compound **19**.

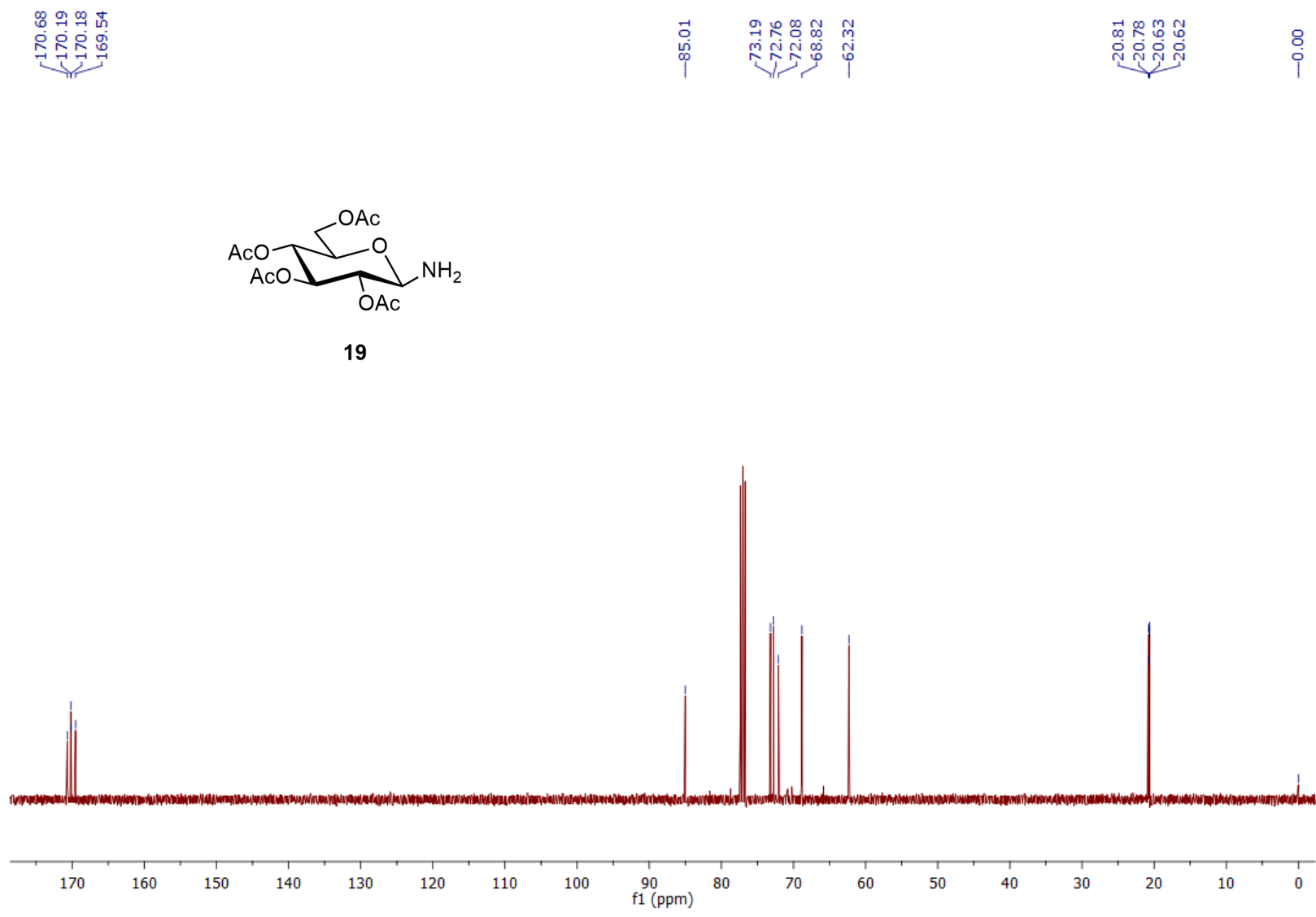


Fig. S30: ¹³C NMR spectrum of compound **19**.

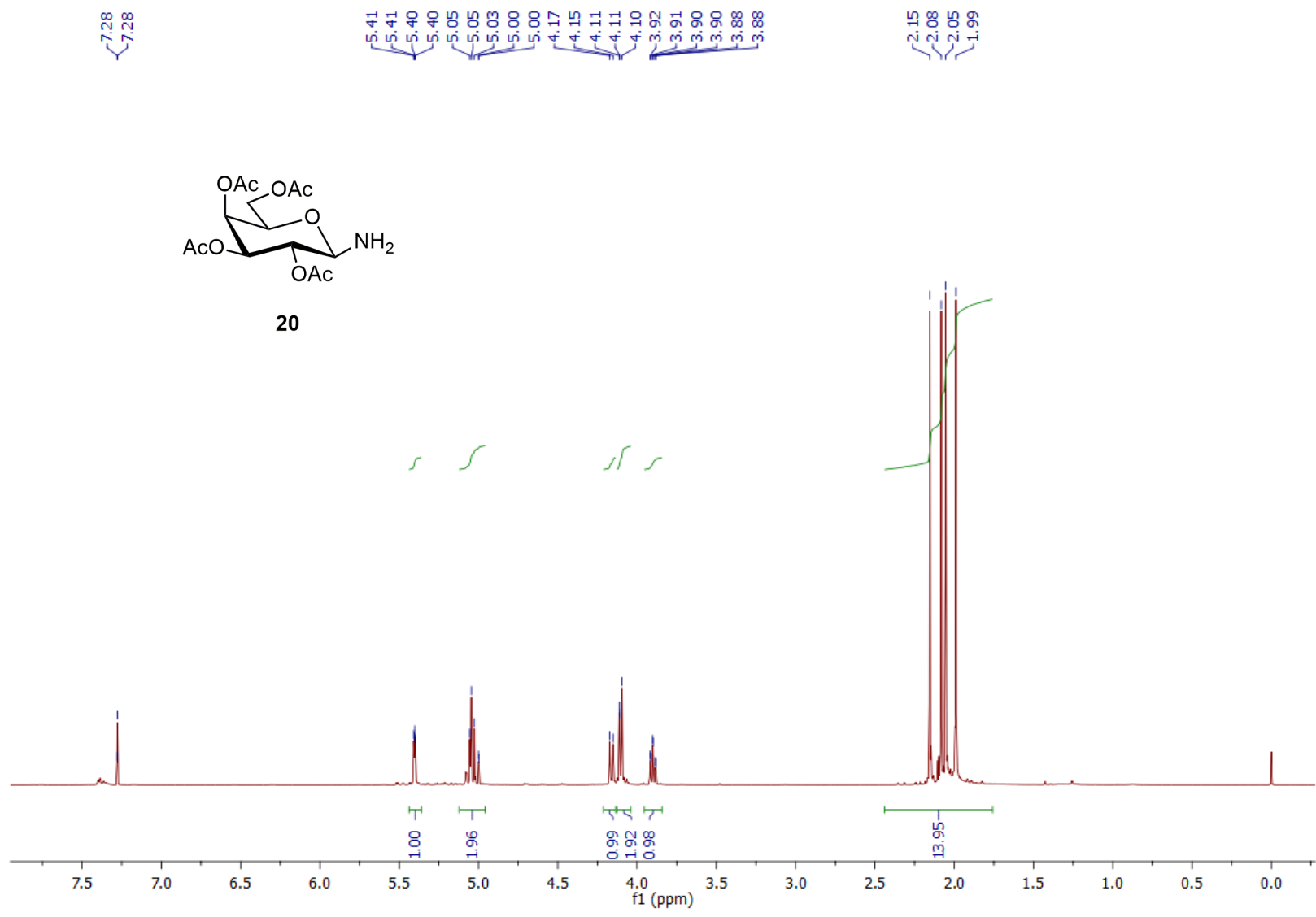


Fig. S31: ¹H NMR spectrum of compound **20**.

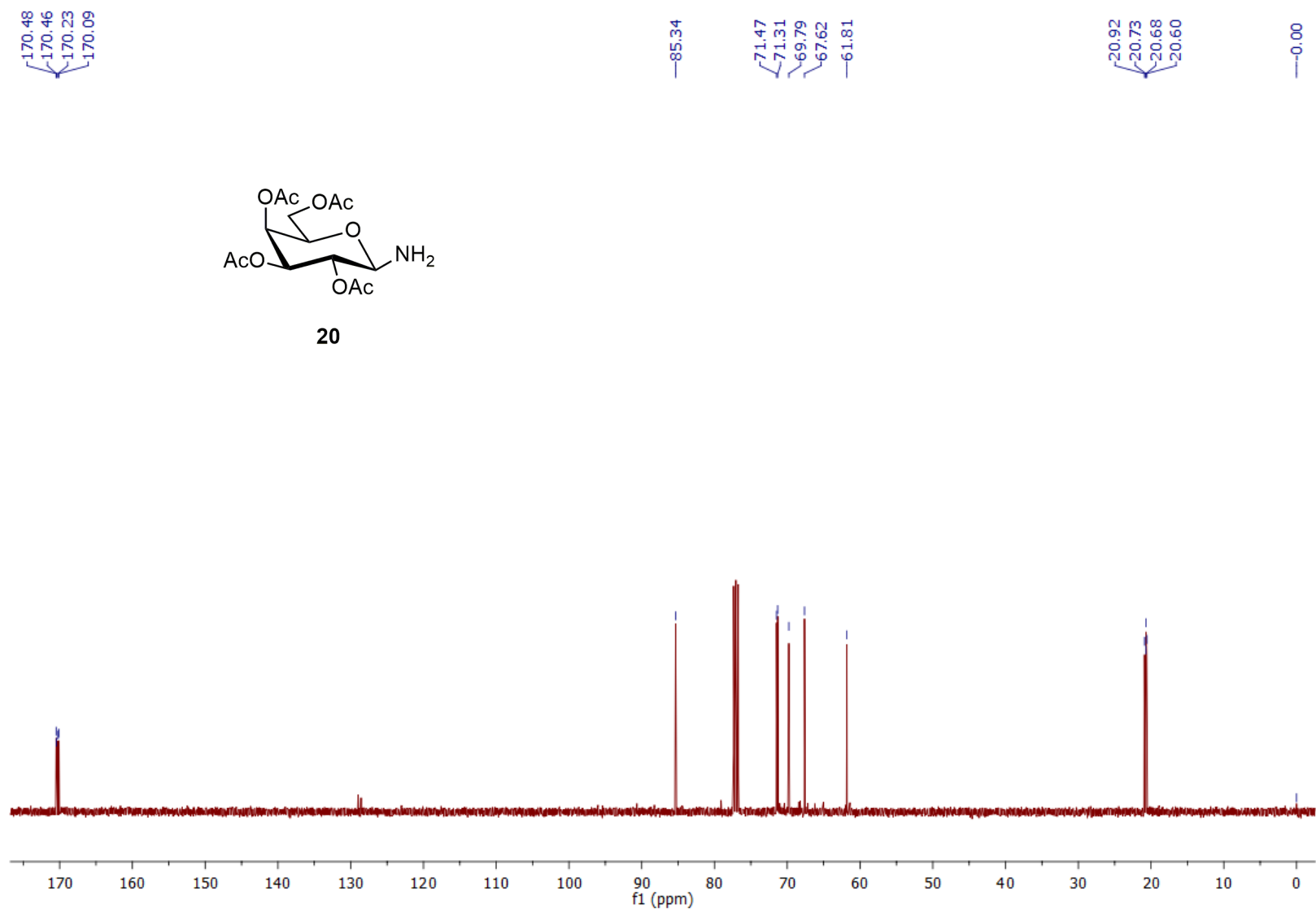


Fig. S32: ¹³C NMR spectrum of compound **20**.

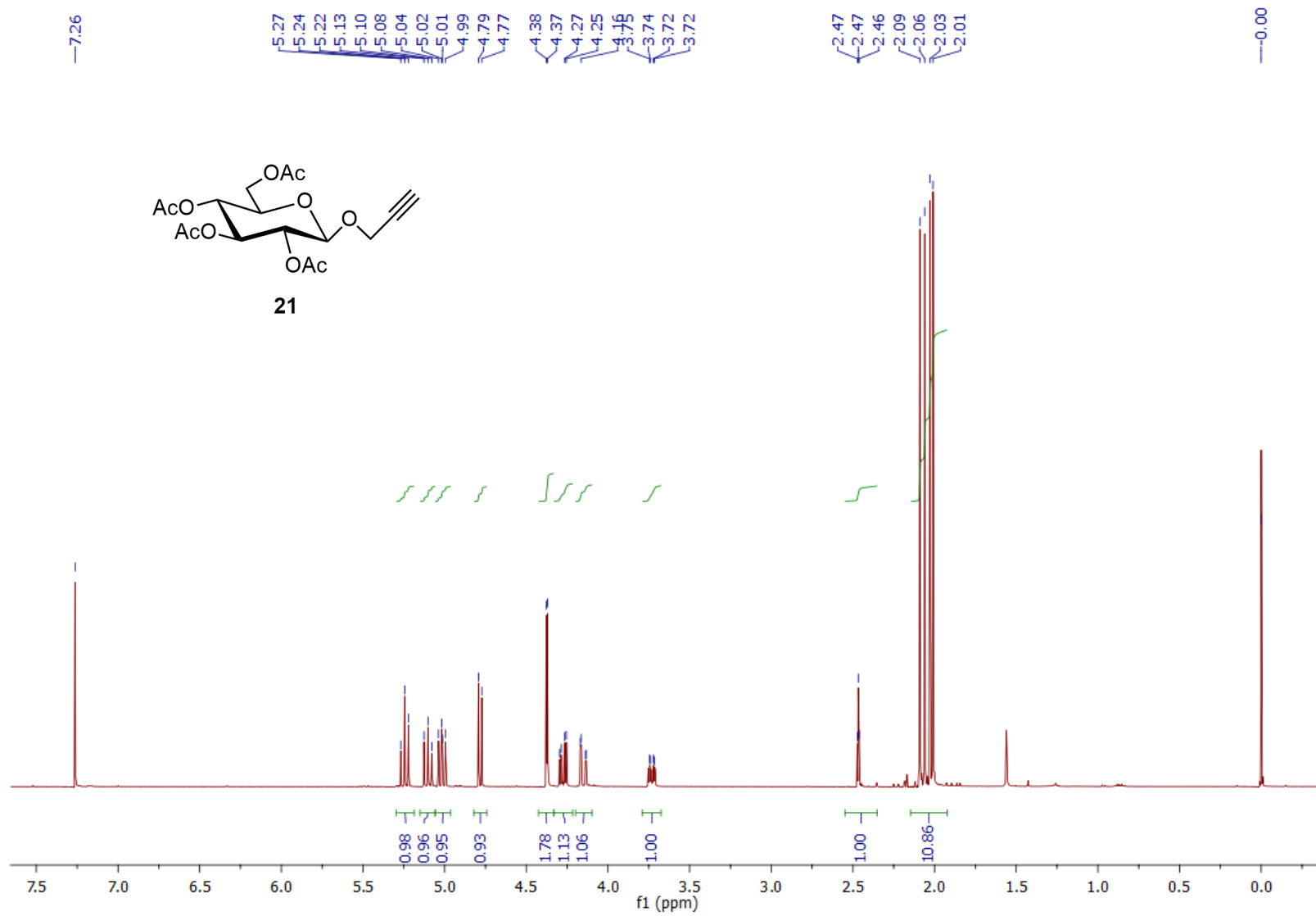


Fig. S33: ^1H NMR spectrum of compound **21**.

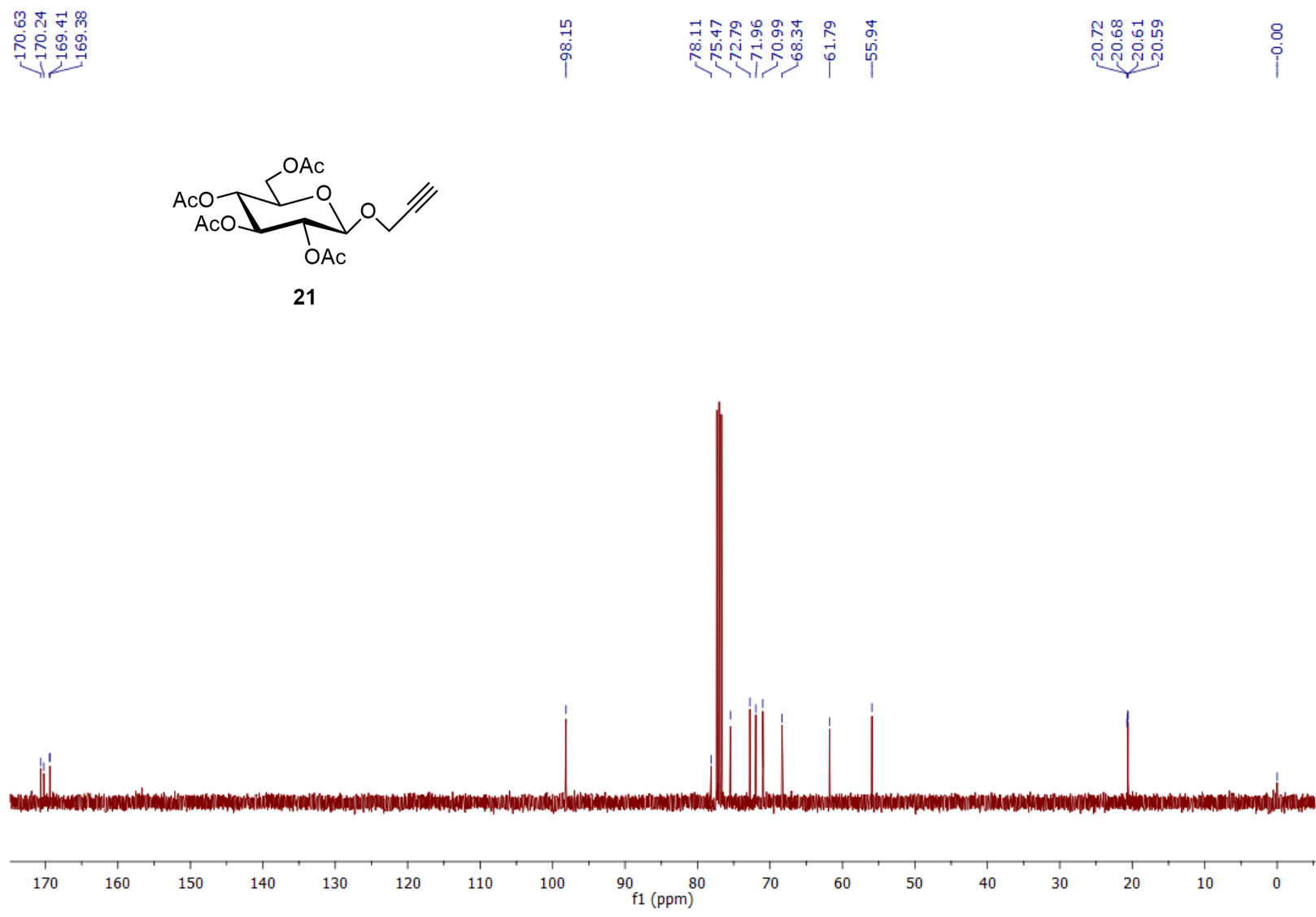


Fig. S34: ¹³C NMR spectrum of compound 21.

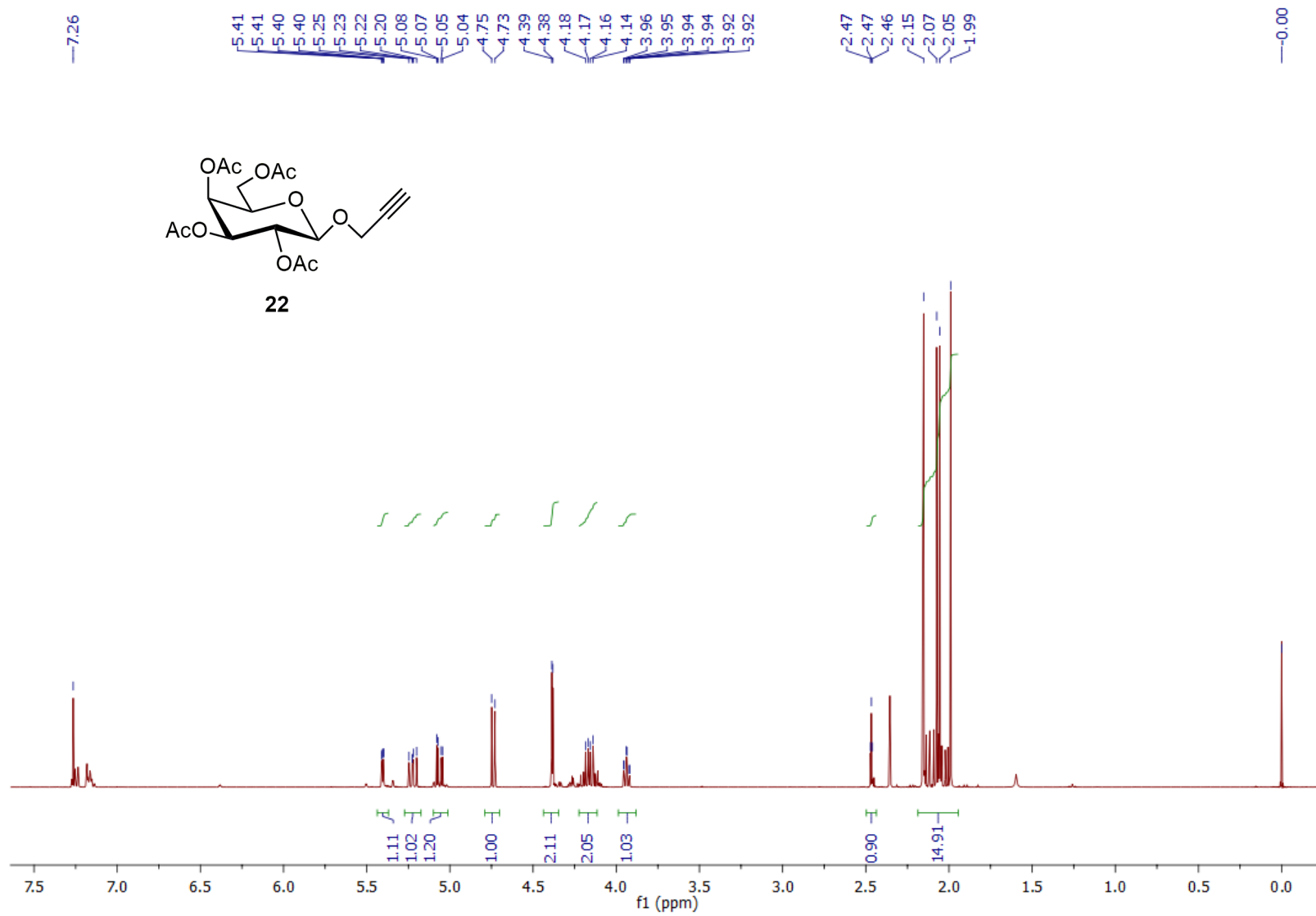


Fig. S35: ^1H NMR spectrum of compound **22**.

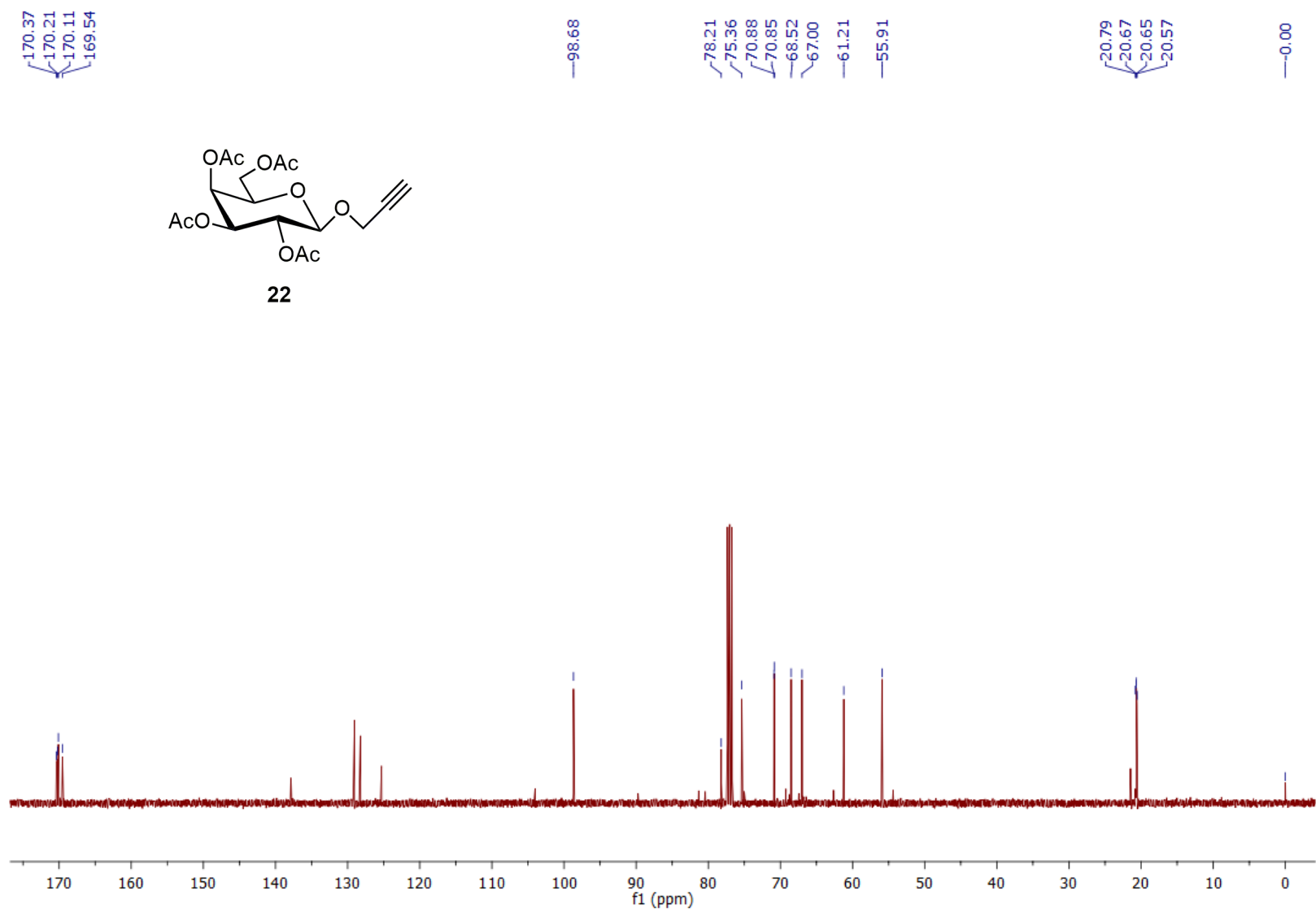


Fig. S36: ¹³C NMR spectrum of compound **22**.

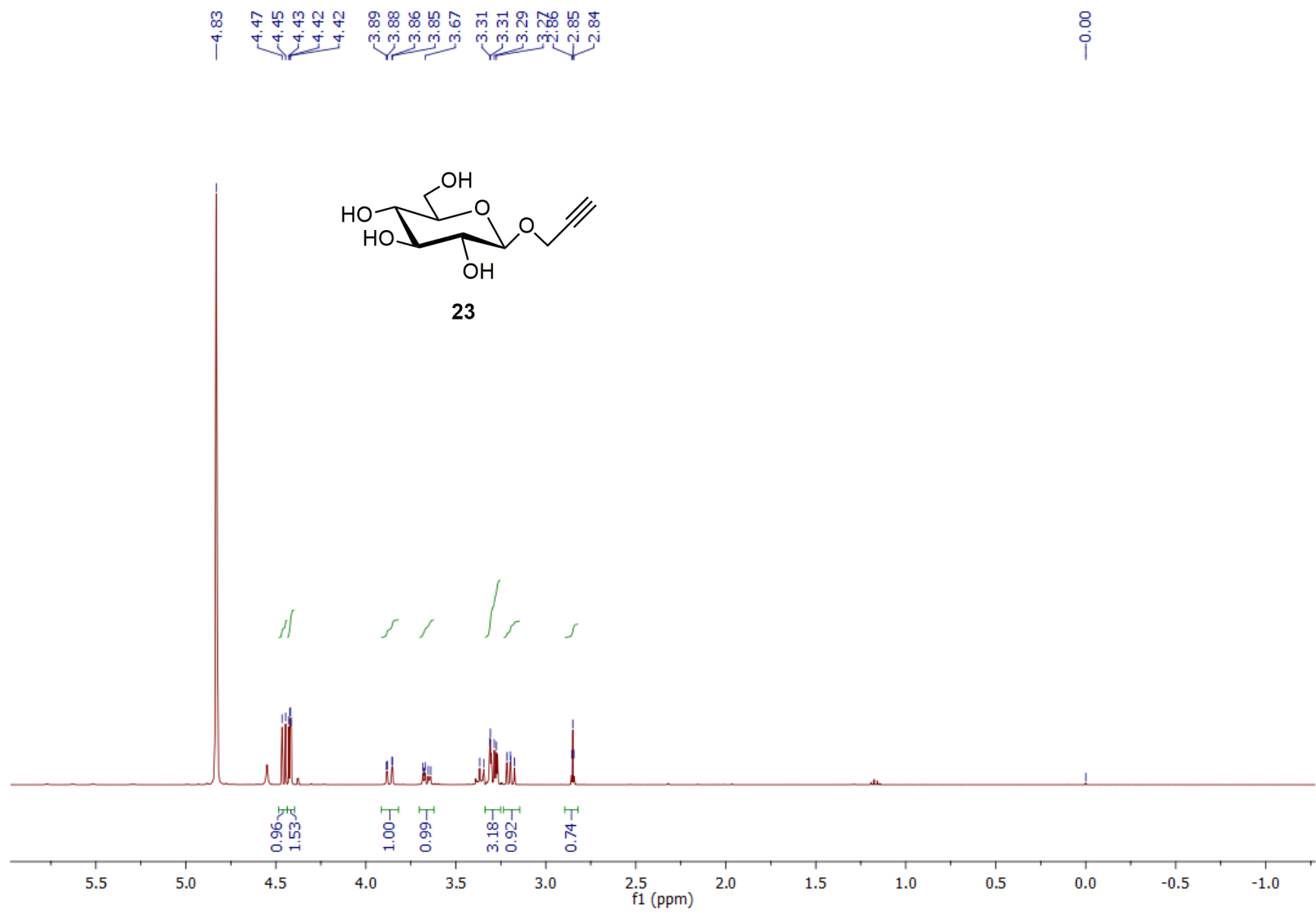


Fig. S37: ^1H NMR spectrum of compound **23**.

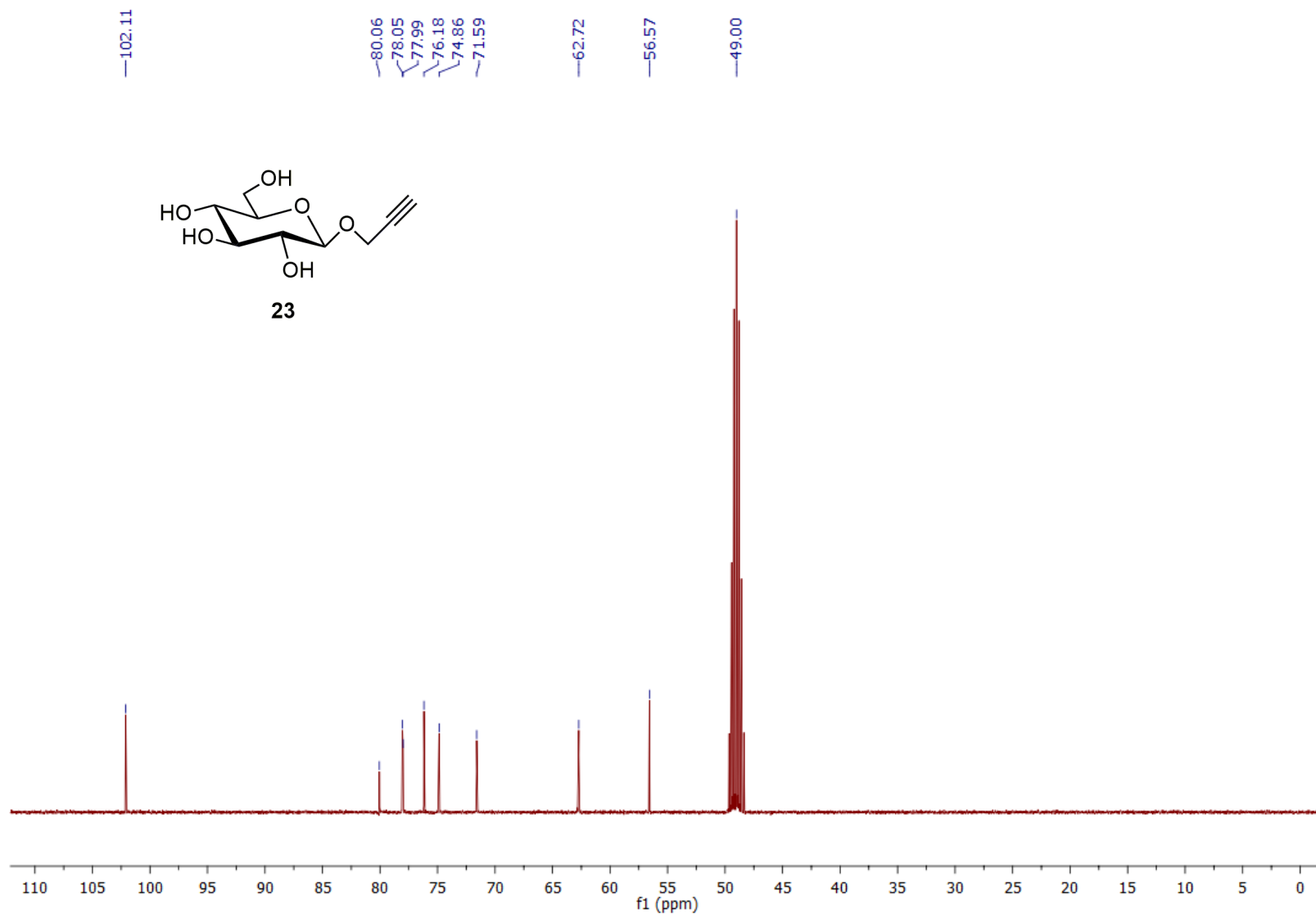


Fig. S38: ^{13}C NMR spectrum of compound **23**.

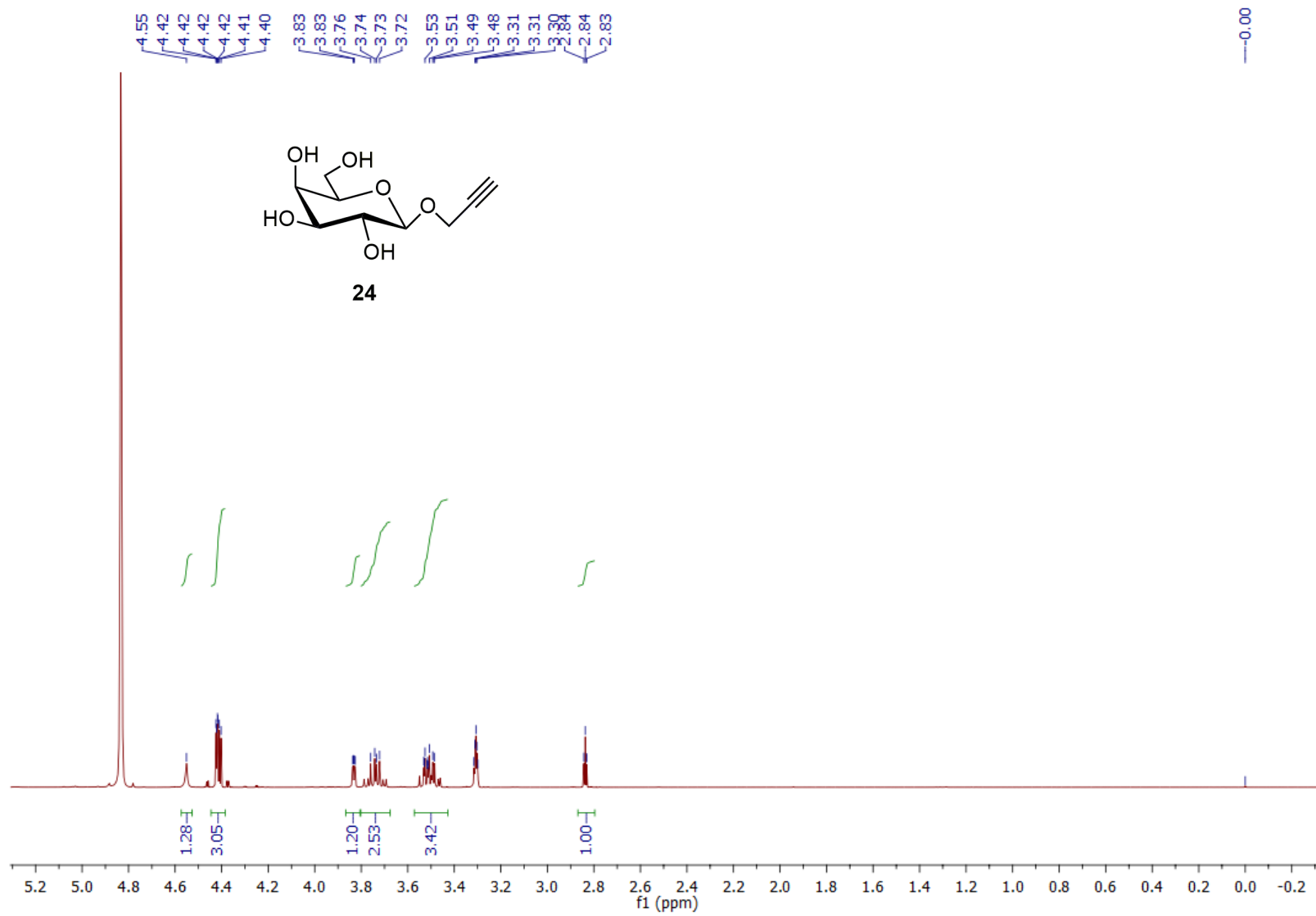


Fig. S39: ¹H NMR spectrum of compound **24**.

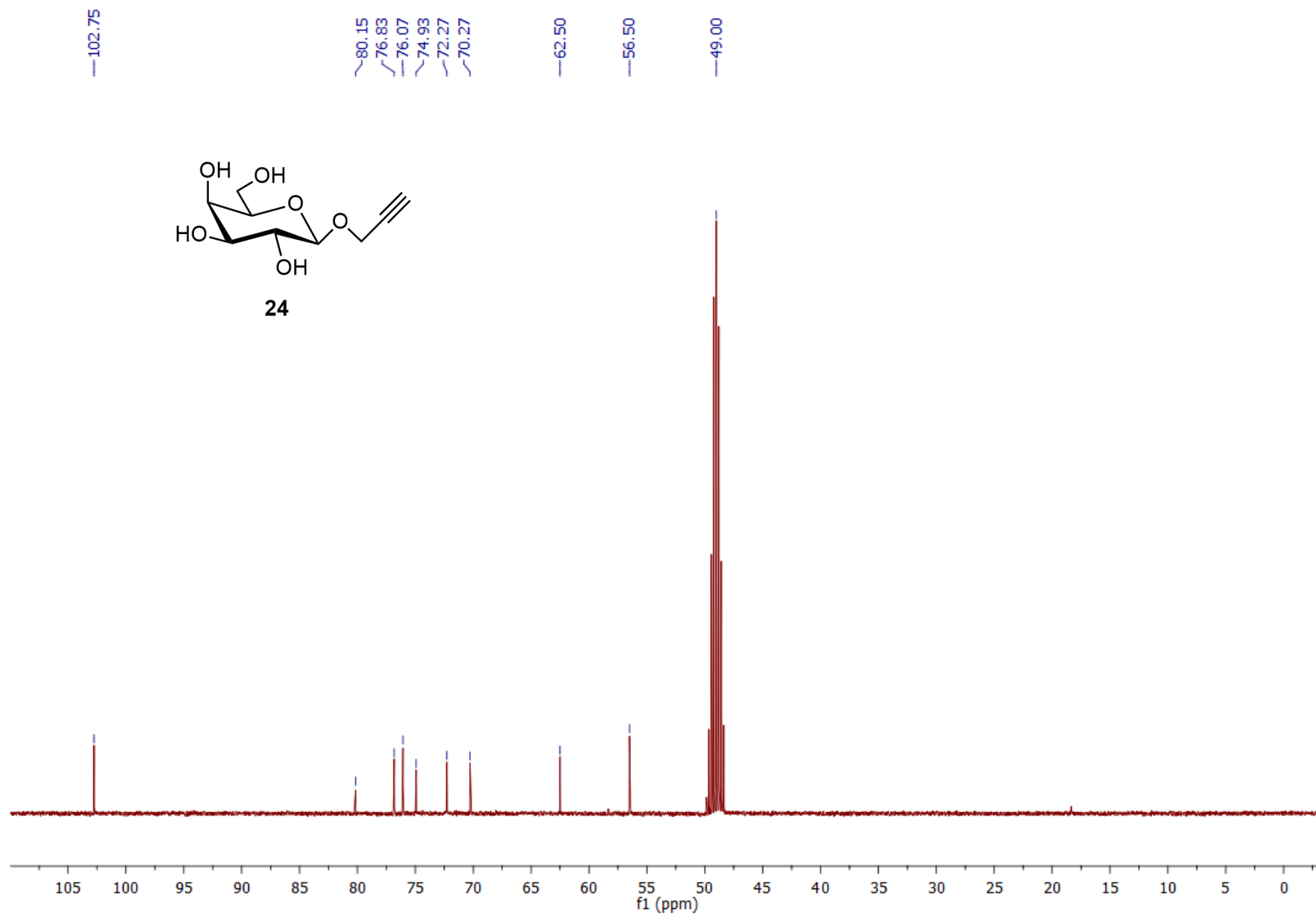


Fig. S40: ¹³C NMR spectrum of compound **24**.

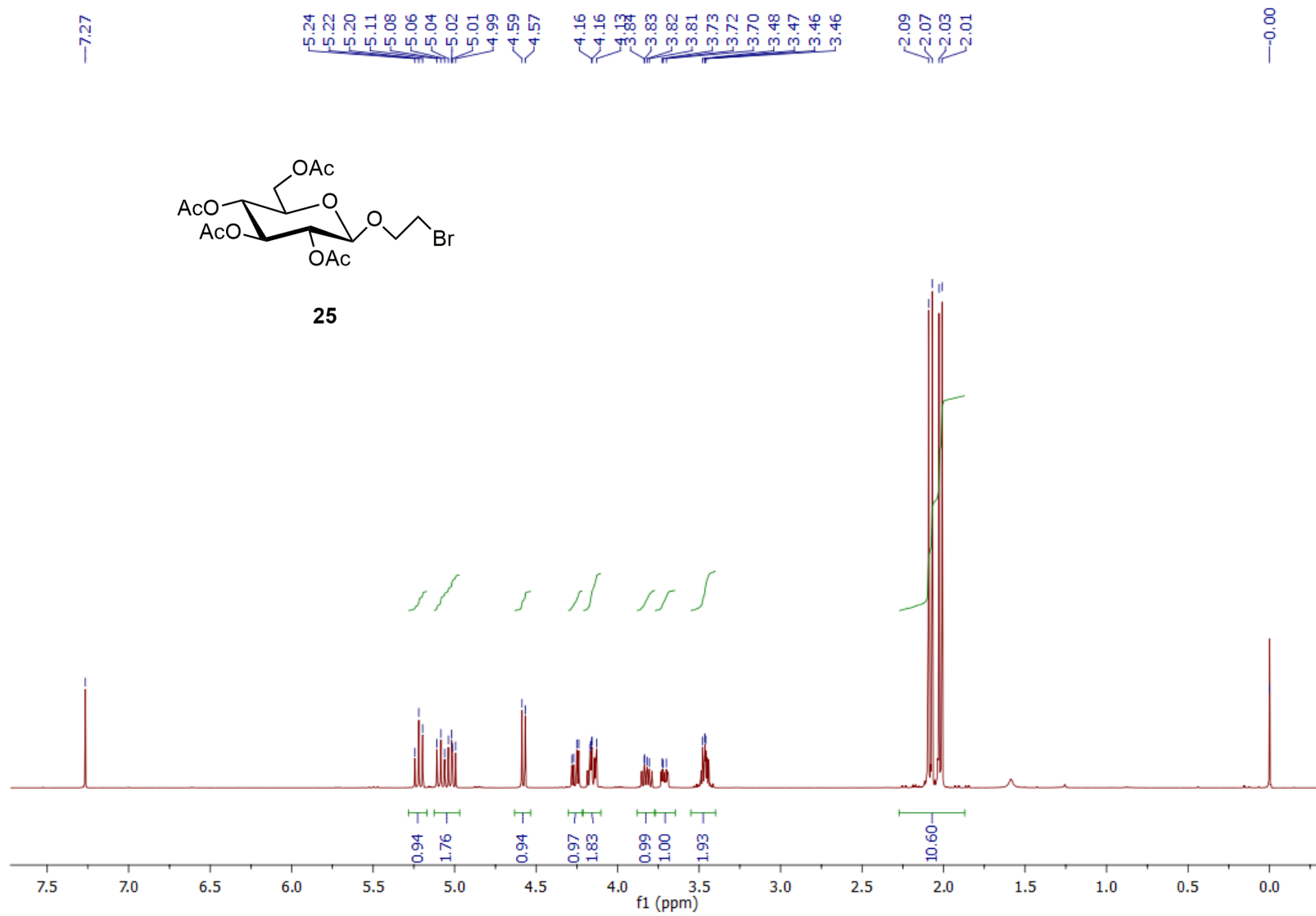


Fig. S41: ^1H NMR spectrum of compound **25**.

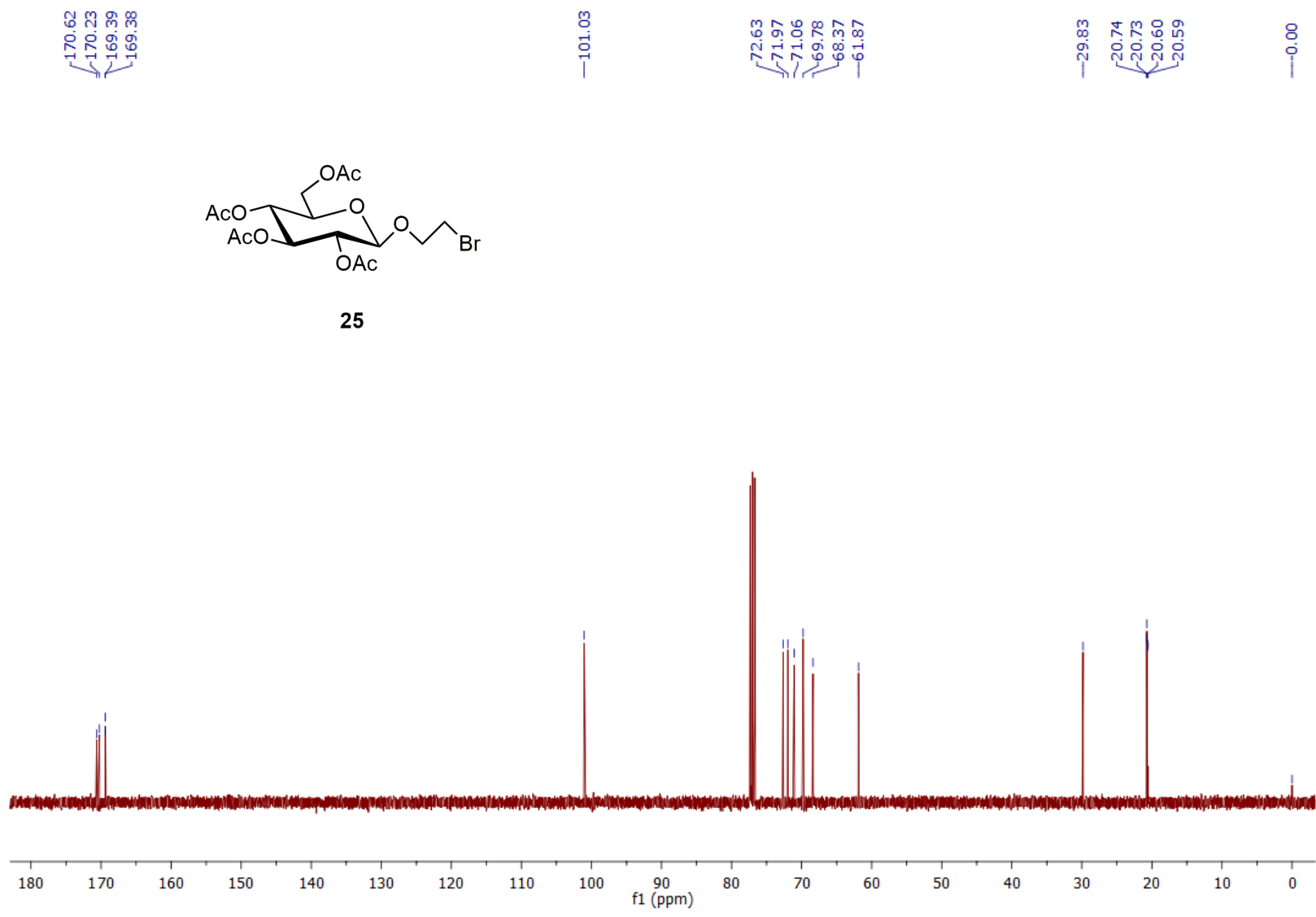


Fig. S42: ¹³C NMR spectrum of compound 25.

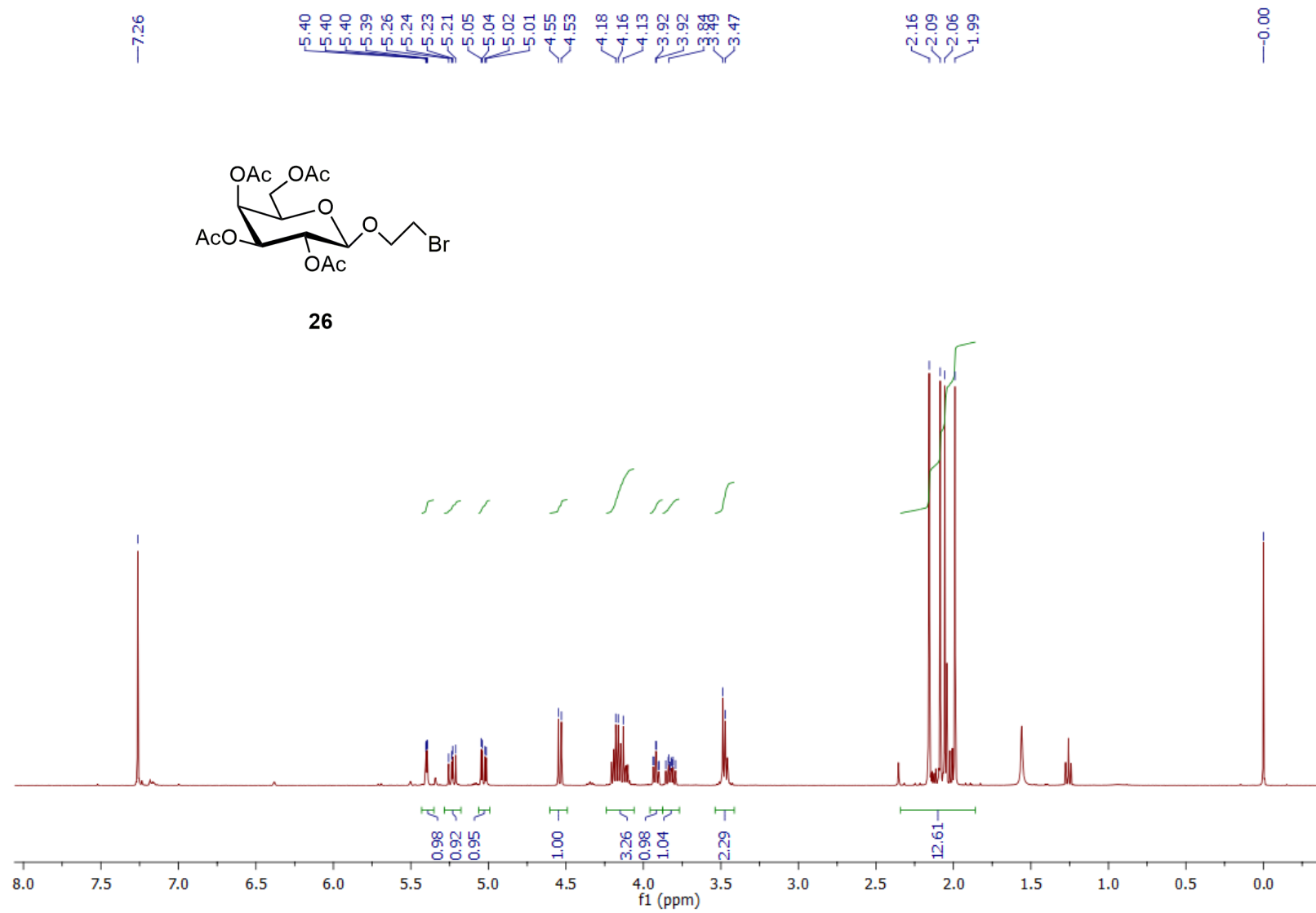


Fig. S43: ^1H NMR spectrum of compound **26**.

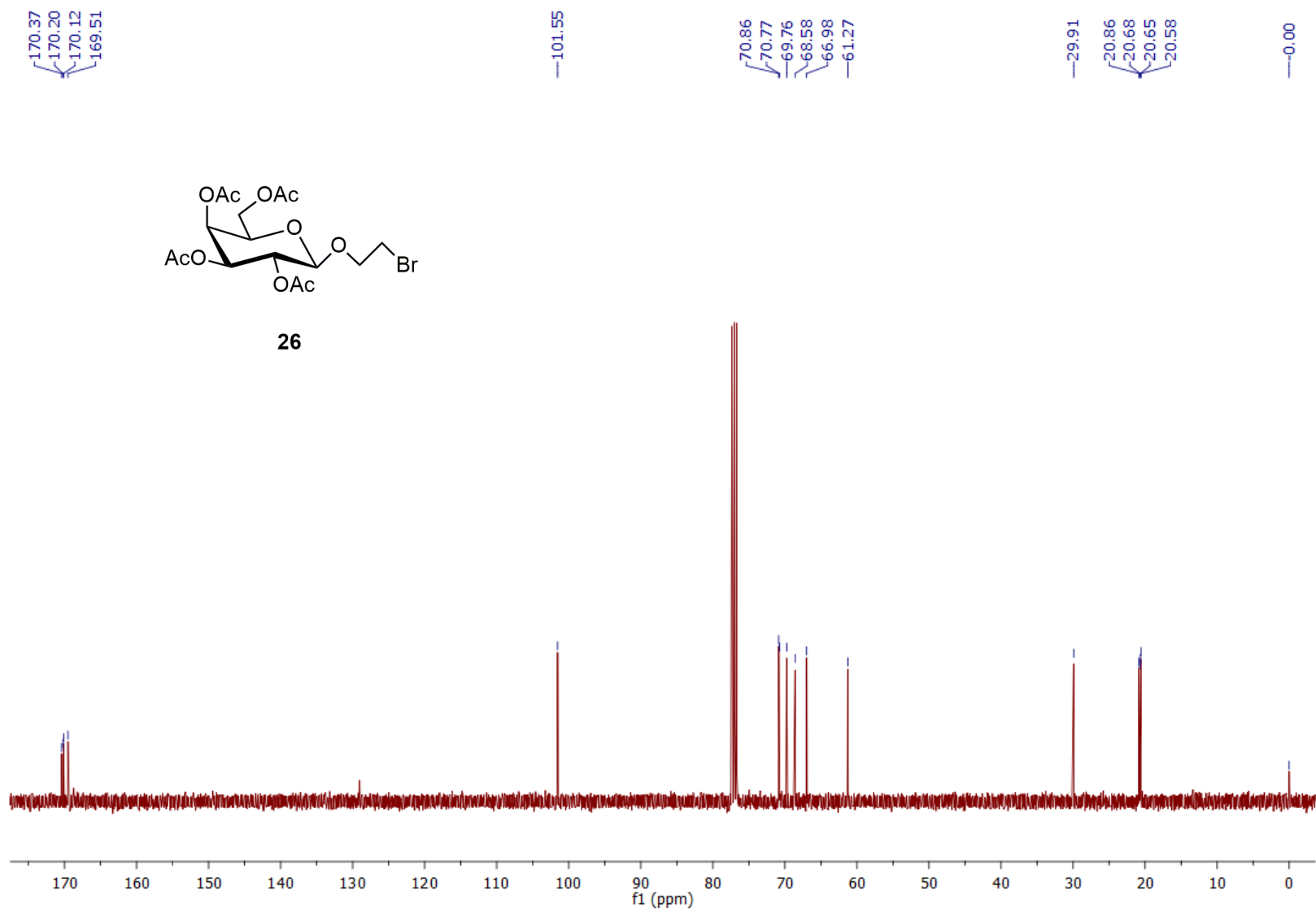


Fig. S44: ¹³C NMR spectrum of compound 26.

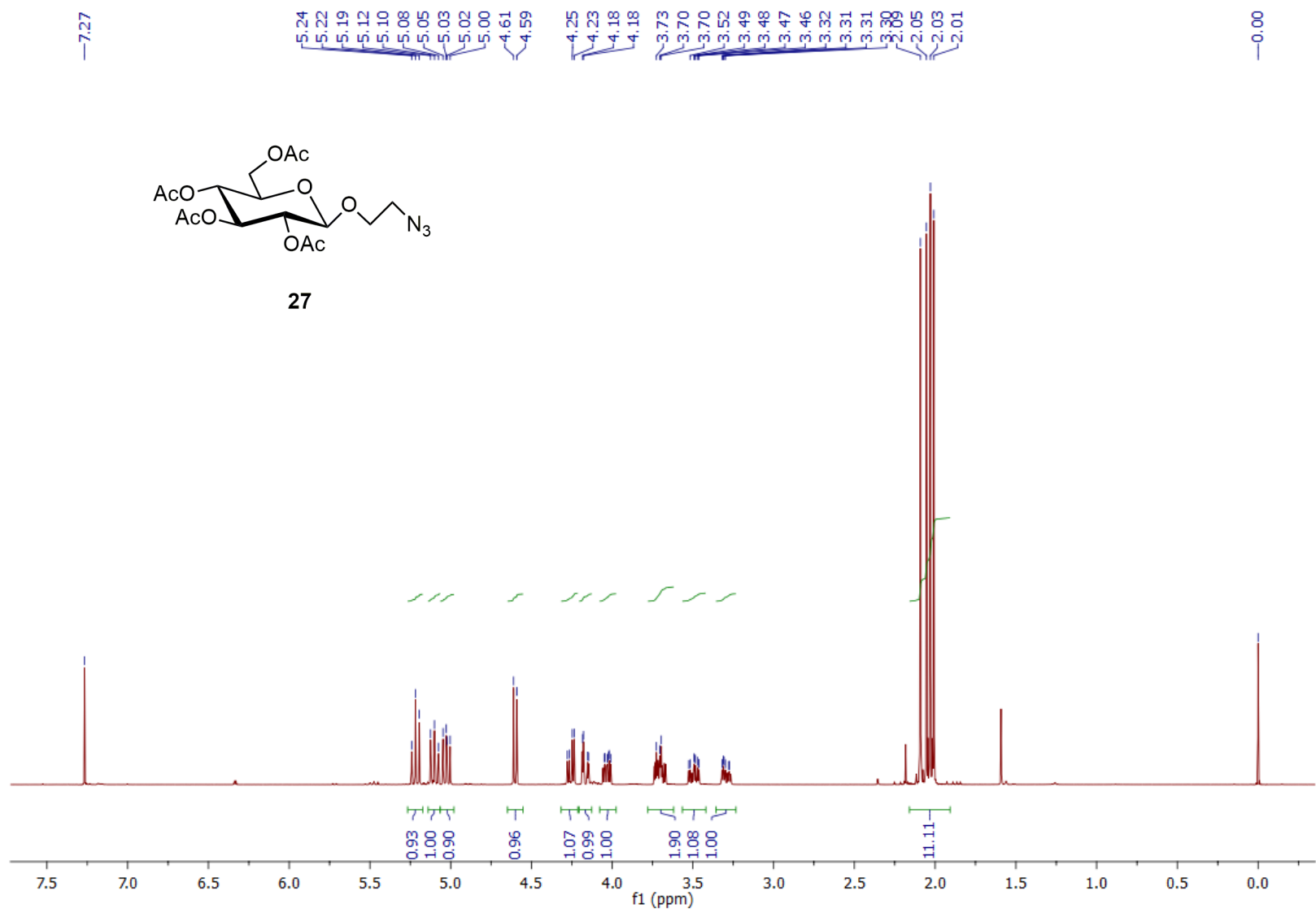


Fig. S45: ¹H NMR spectrum of compound **27**.

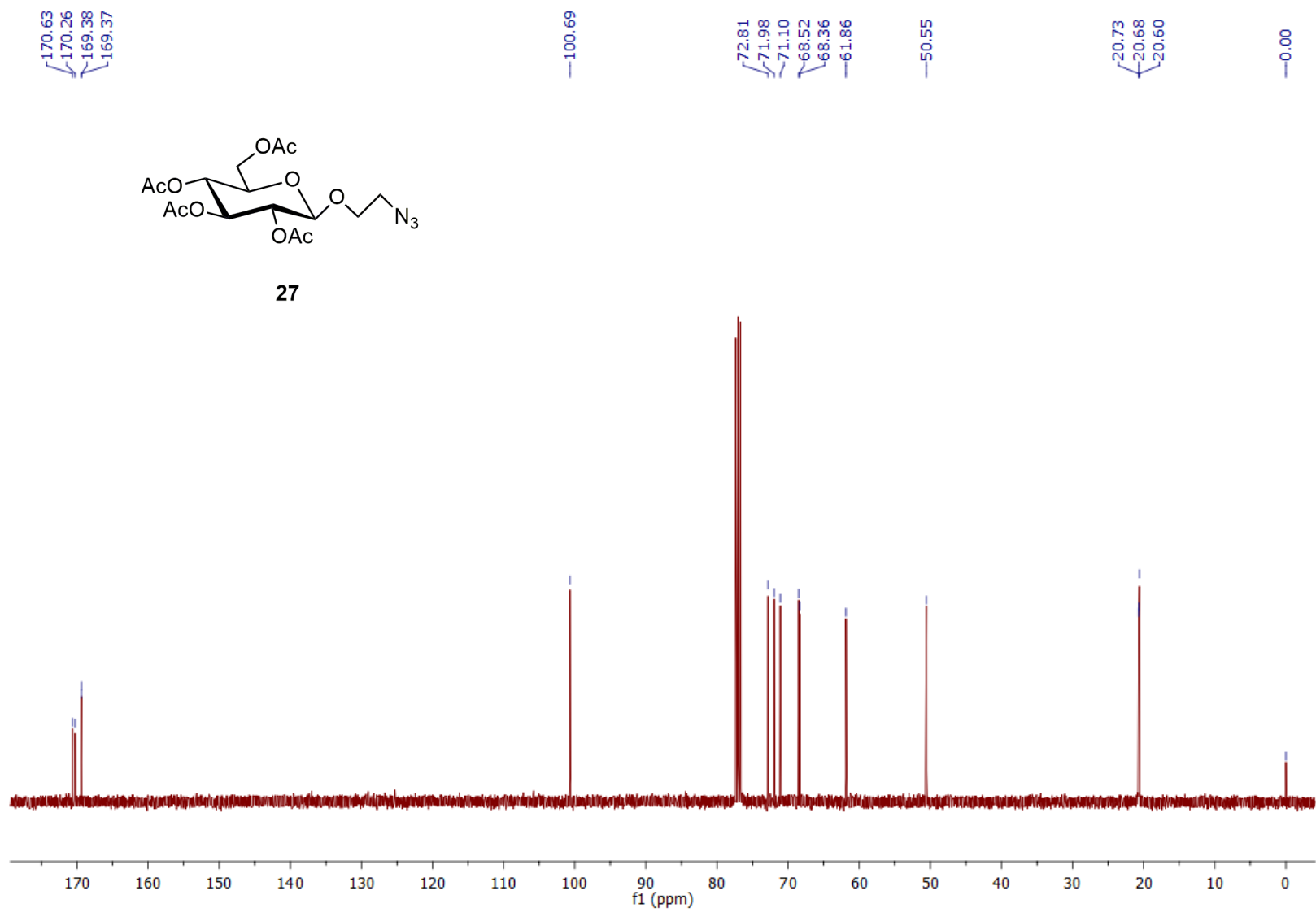


Fig. S46: ¹³C NMR spectrum of compound 27.

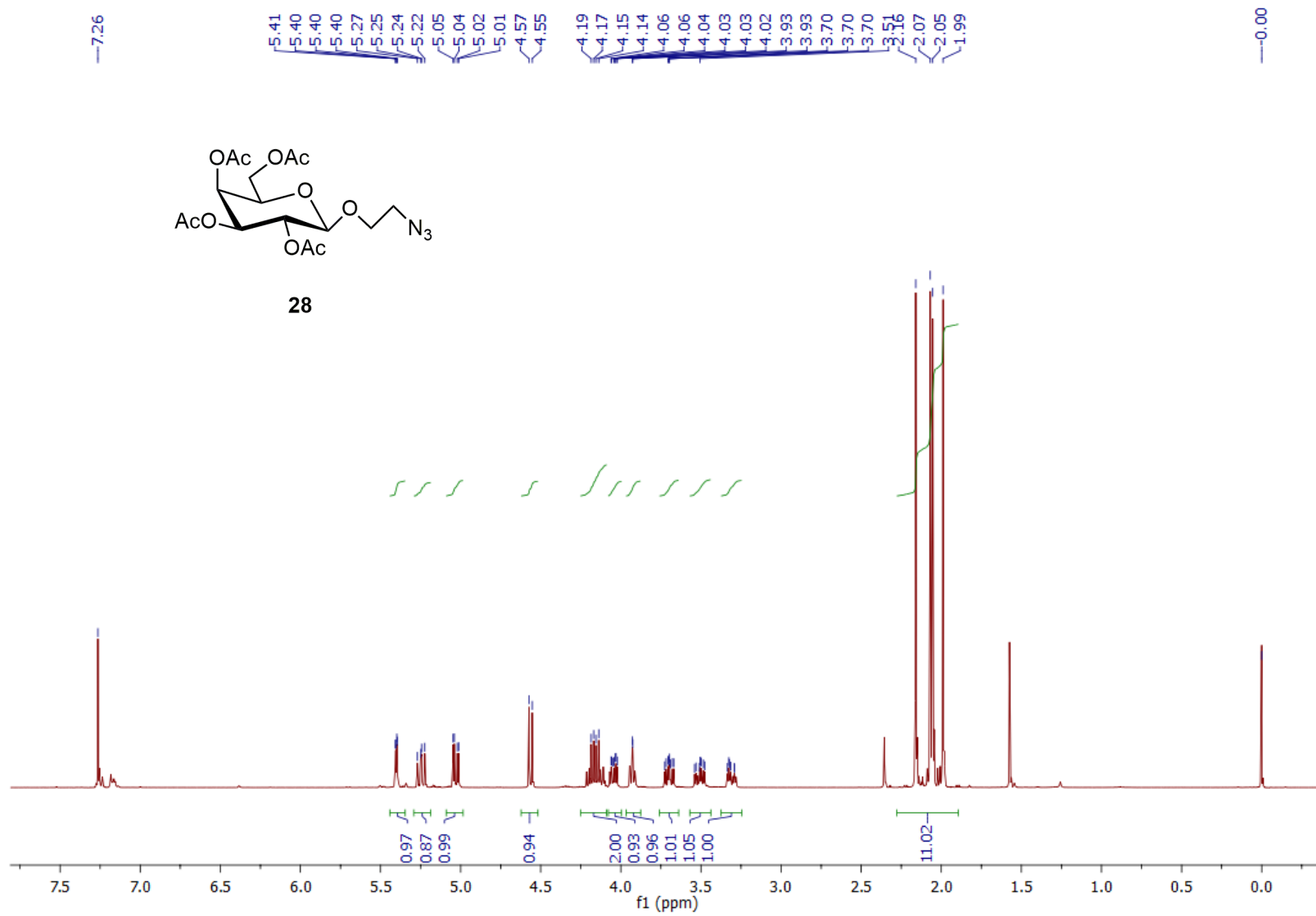


Fig. S47: ^1H NMR spectrum of compound **28**.

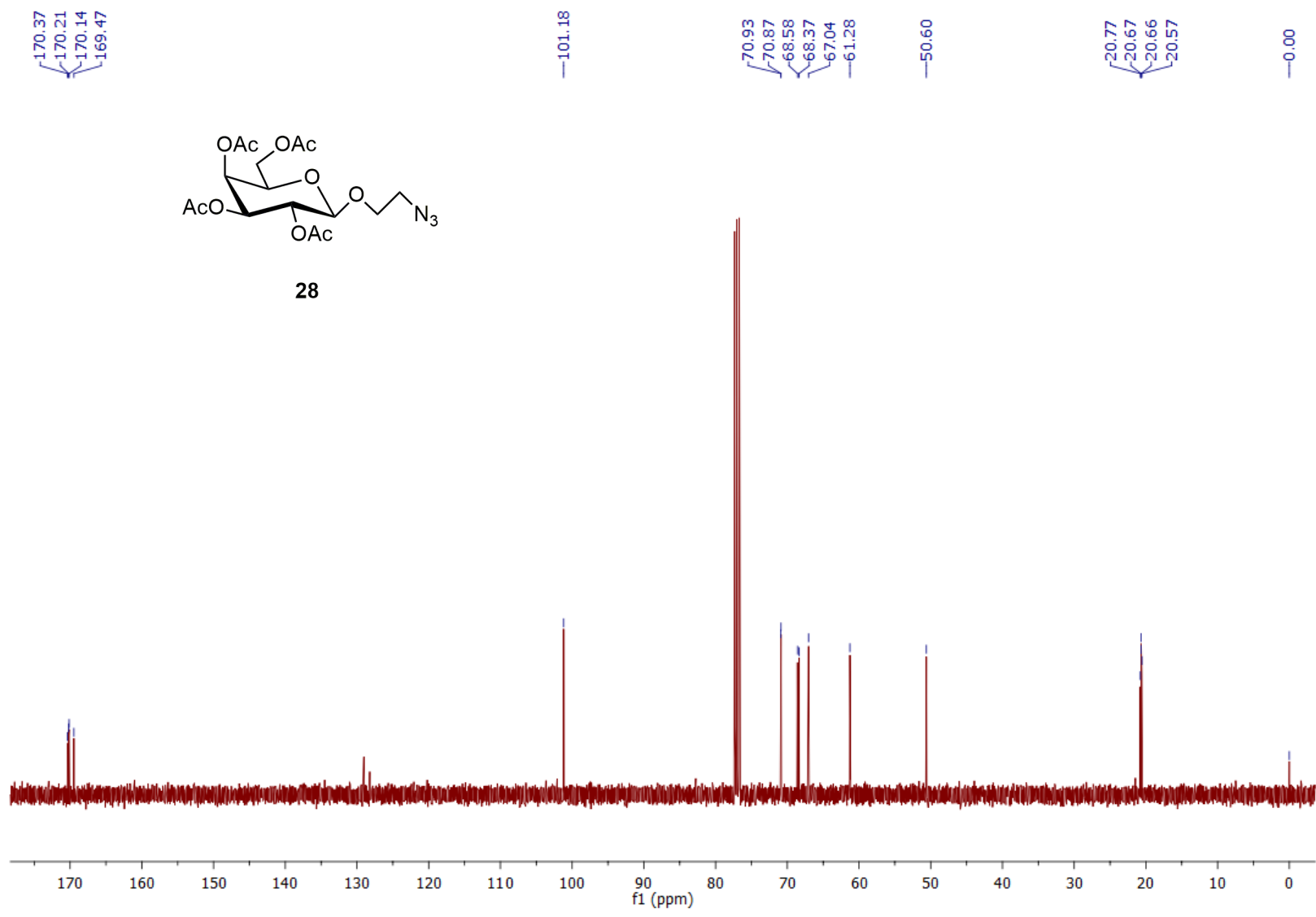


Fig. S48: ¹³C NMR spectrum of compound **28**.

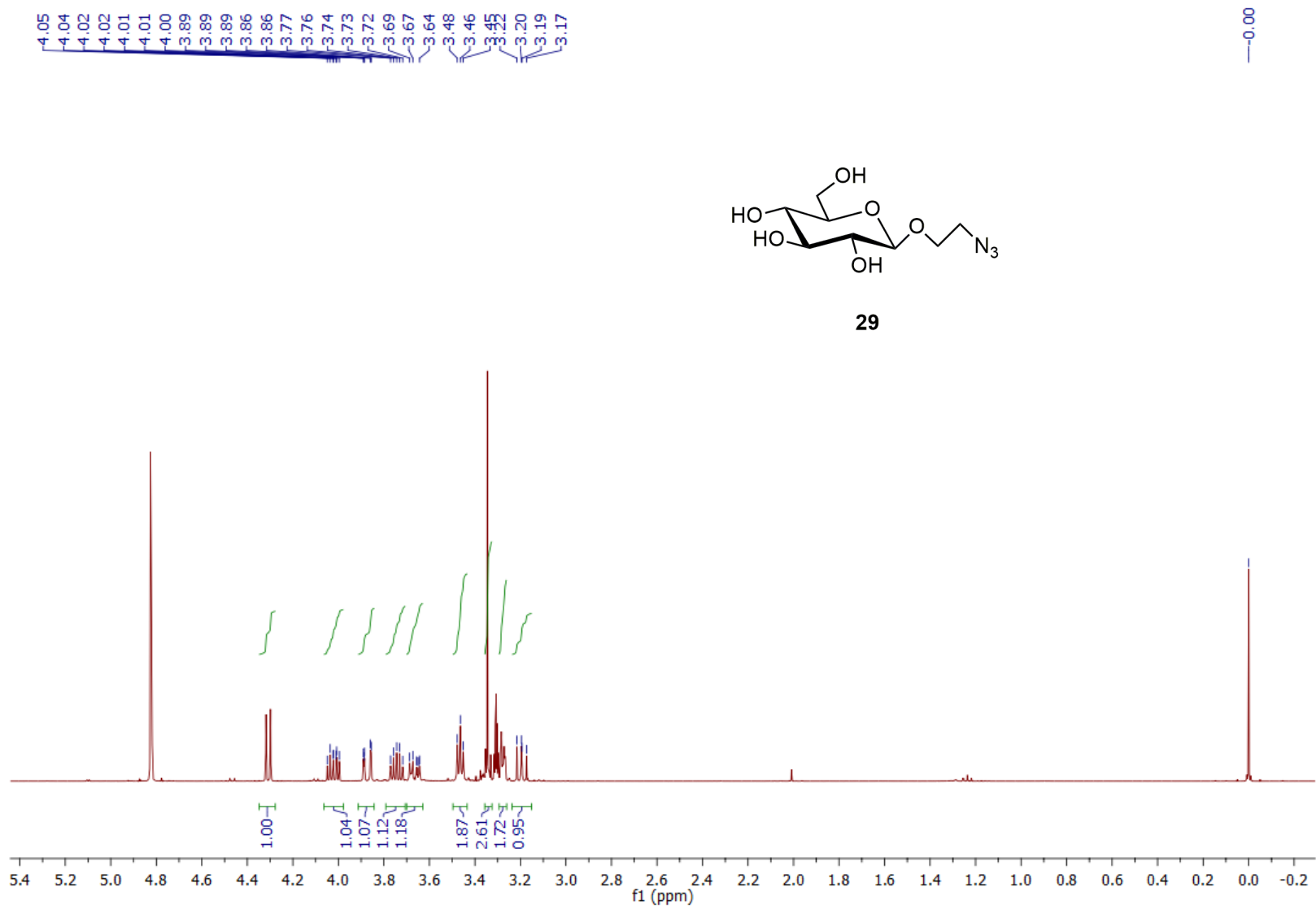


Fig. S49: ^1H NMR spectrum of compound **29**.

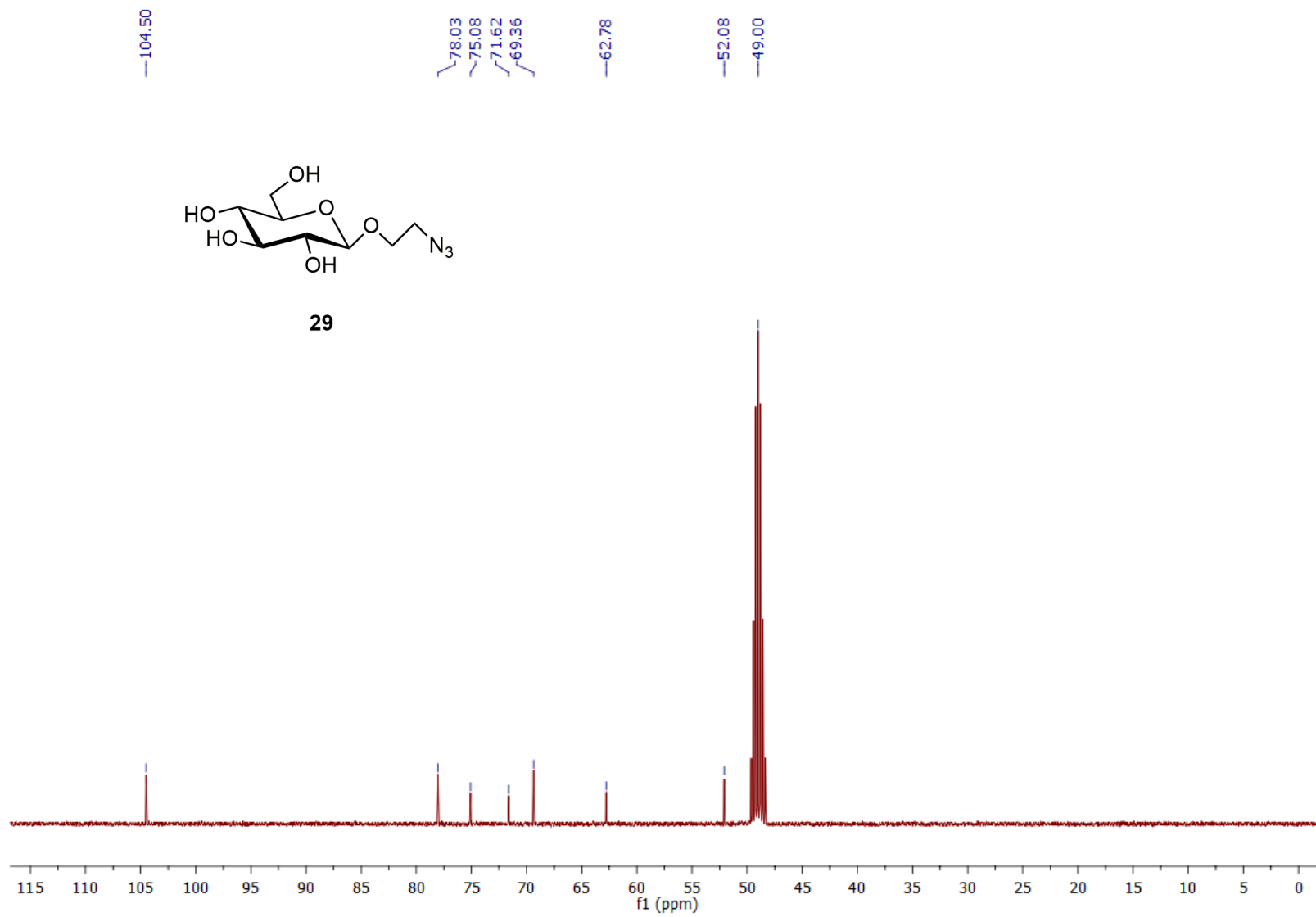


Fig. S50: ¹³C NMR spectrum of compound **29**.

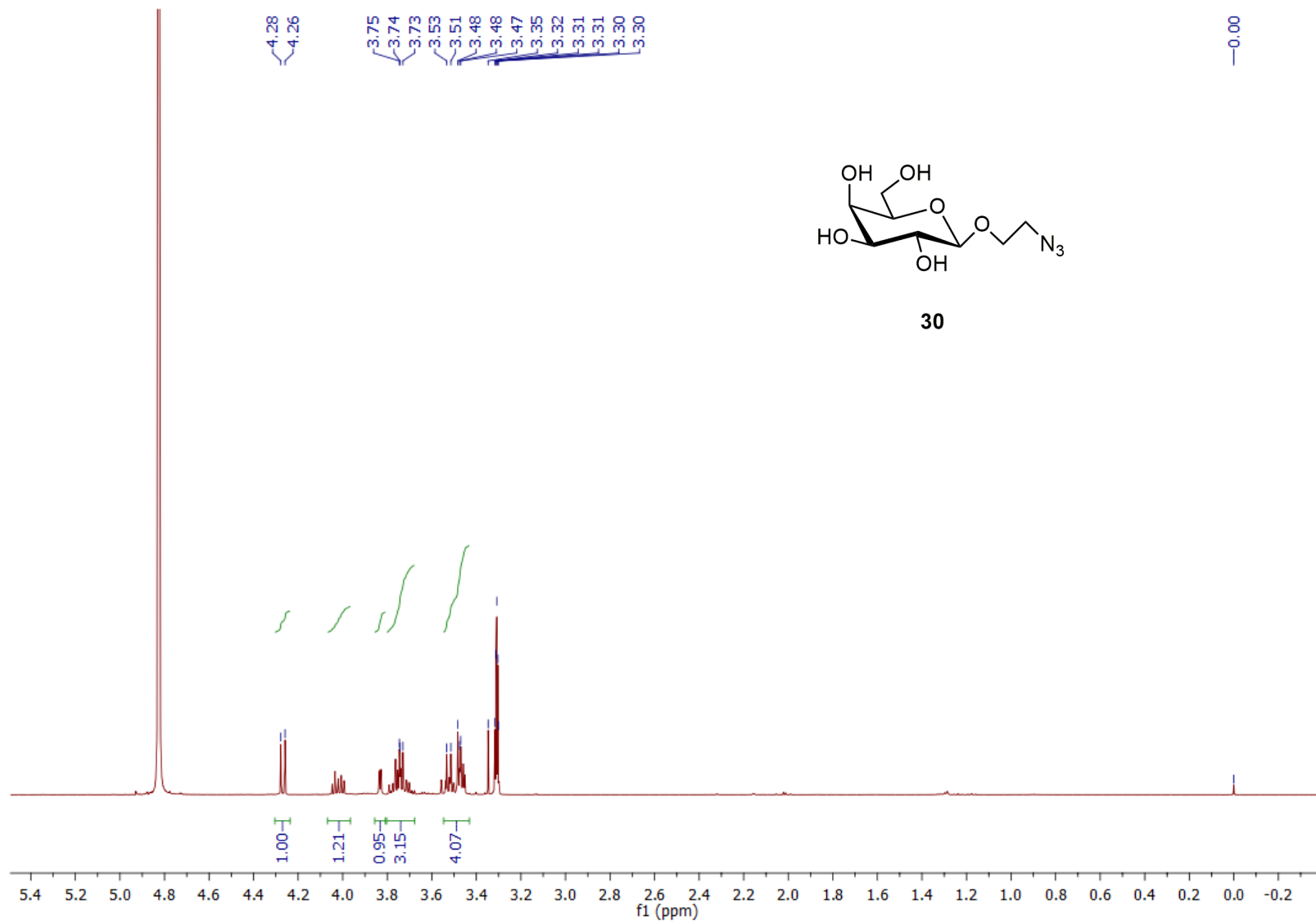


Fig. S51: ^1H NMR spectrum of compound **30**.

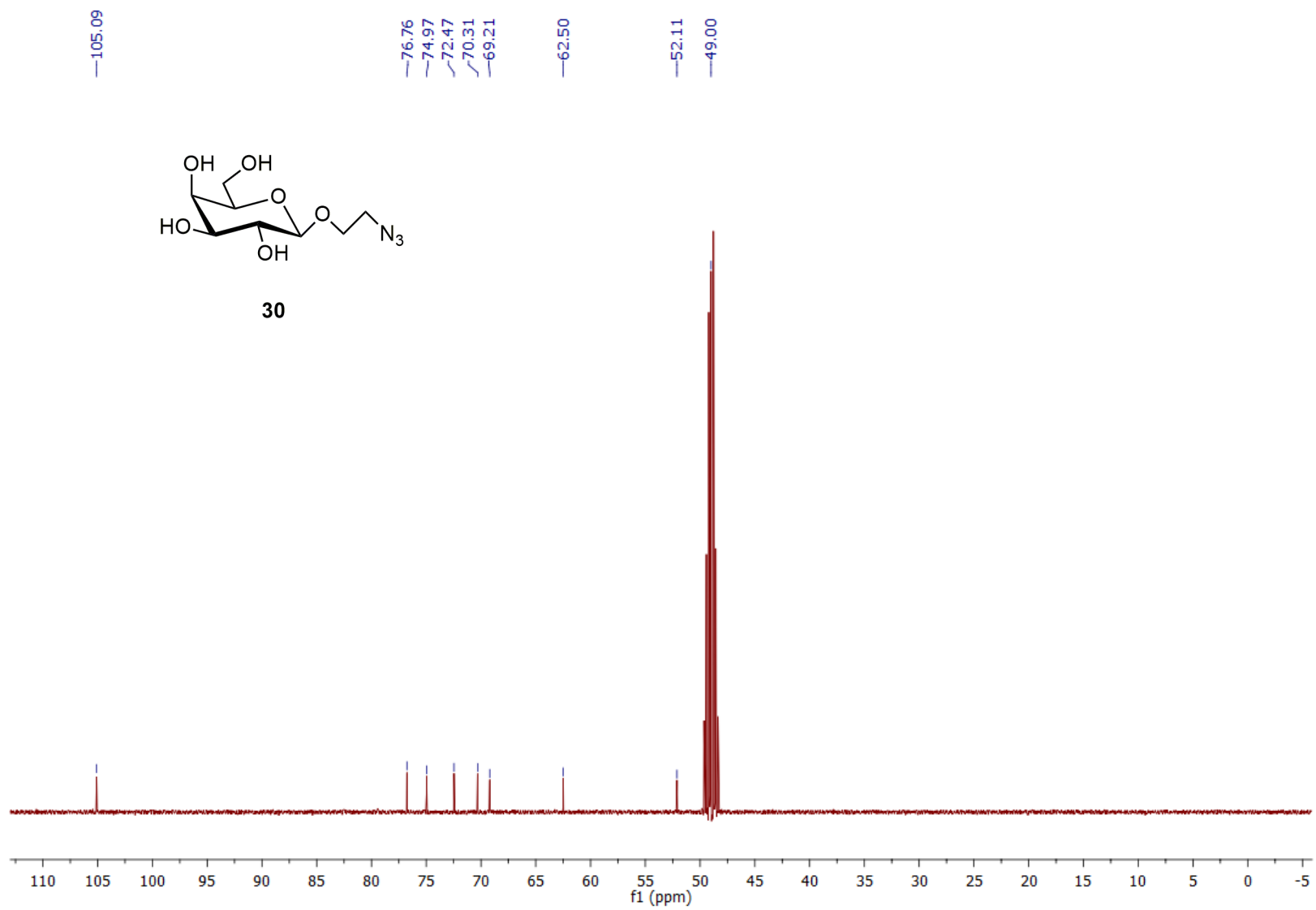


Fig. S52: ^{13}C NMR spectrum of compound **30**.

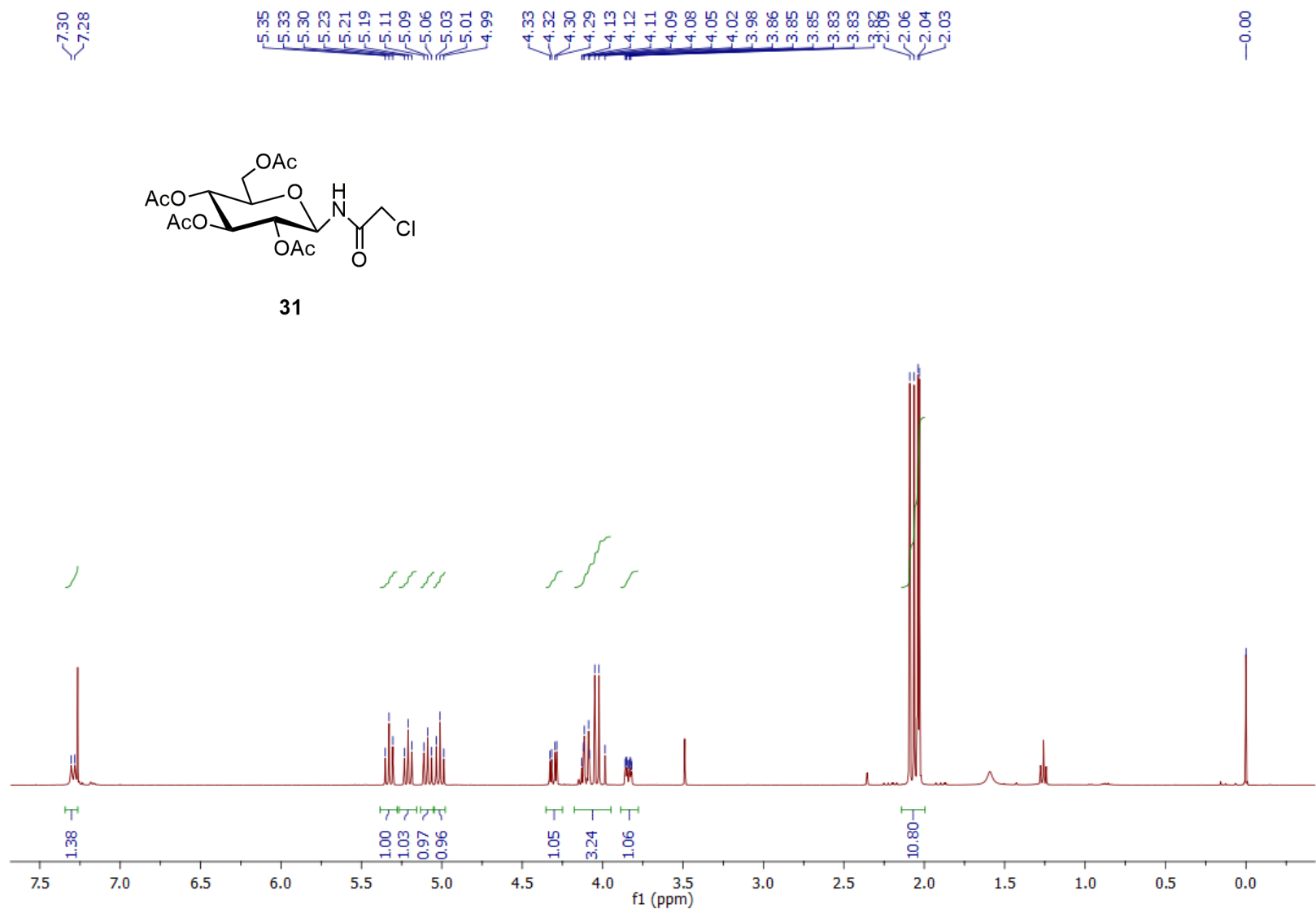


Fig. S53: ¹H NMR spectrum of compound **31**.

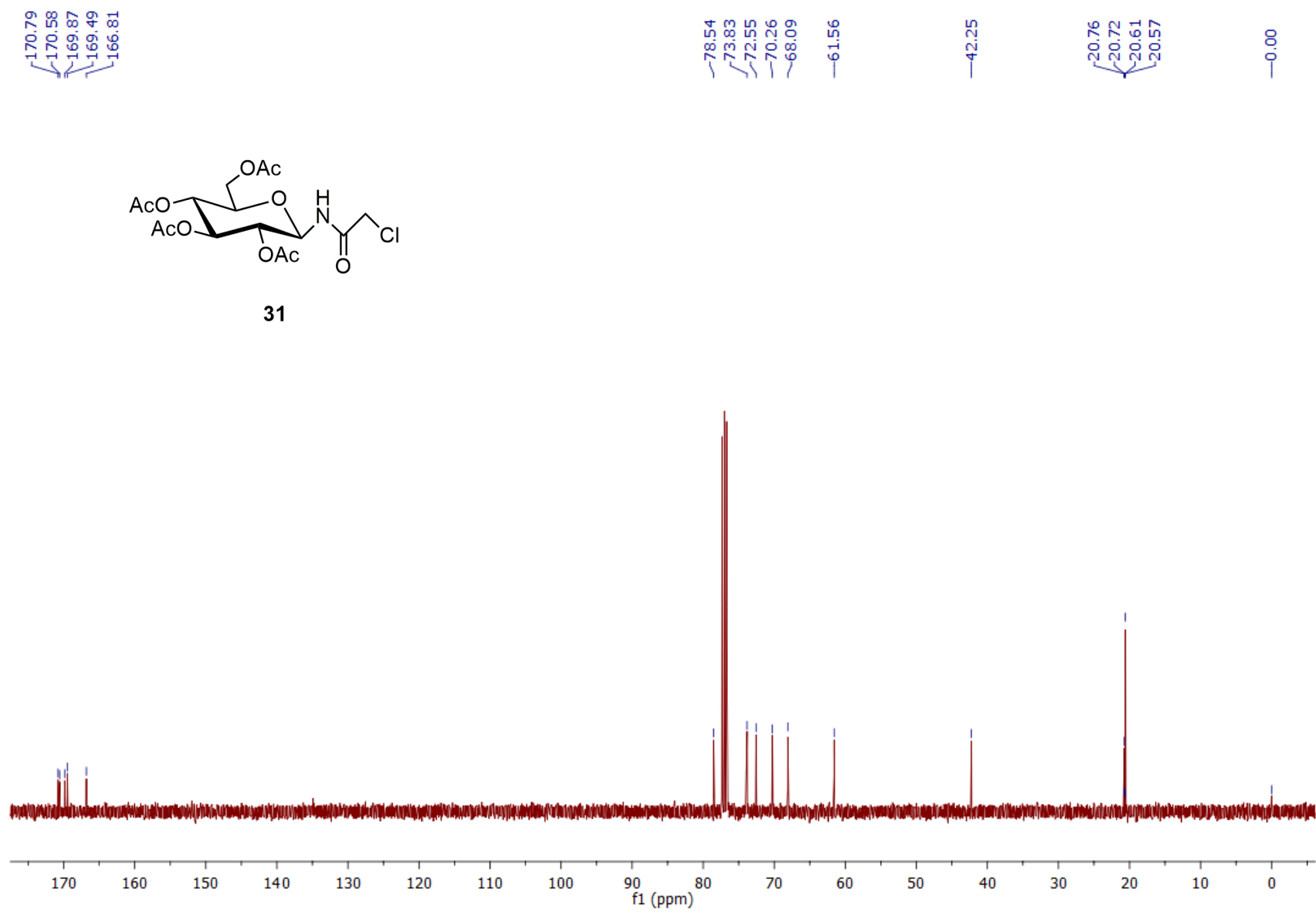


Fig. S54: ¹³C NMR spectrum of compound **31**.

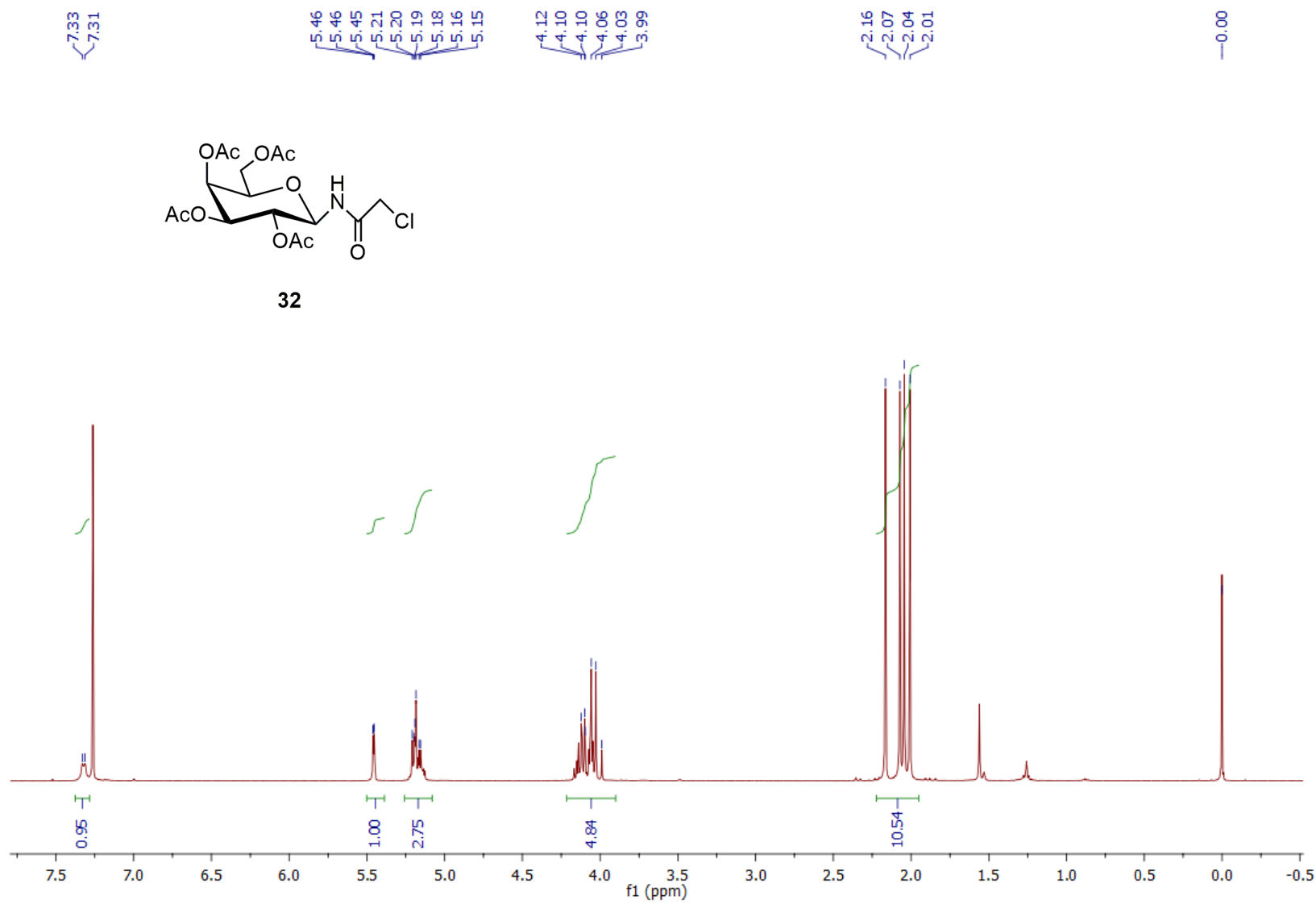


Fig. S55: ¹H NMR spectrum of compound **32**.

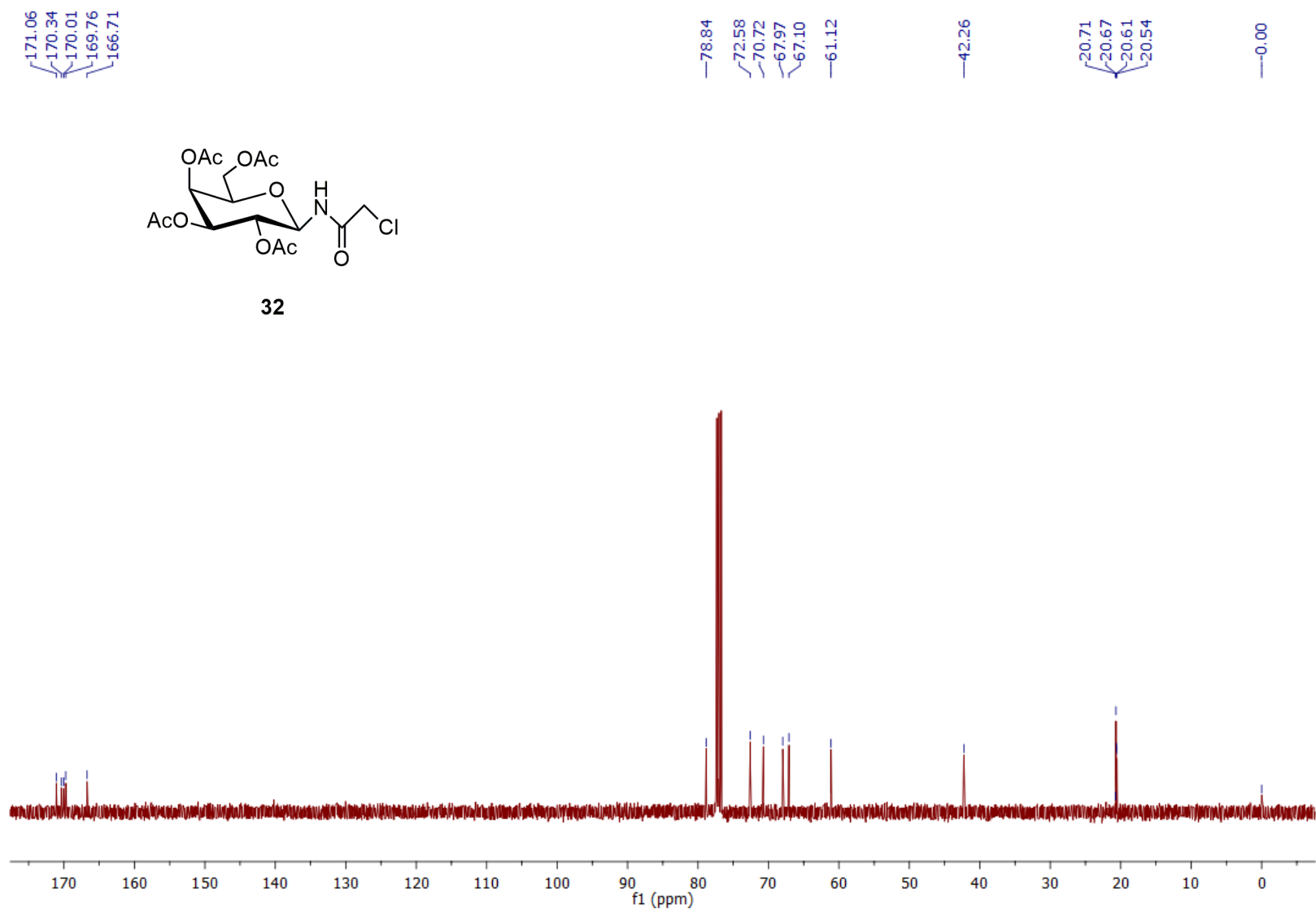


Fig. S56: ¹³C NMR spectrum of compound **32**.

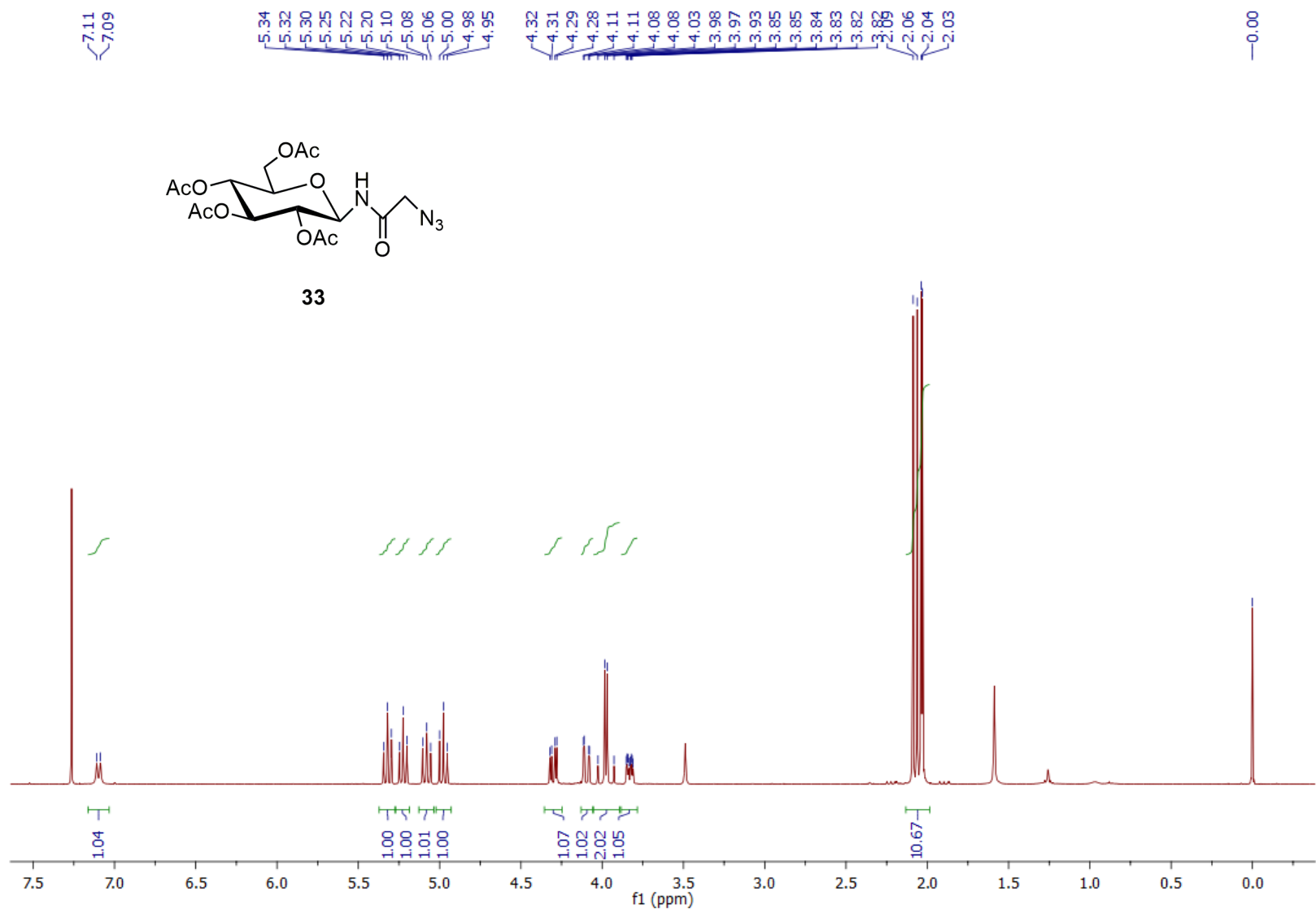


Fig. S57: ¹H NMR spectrum of compound **33**.

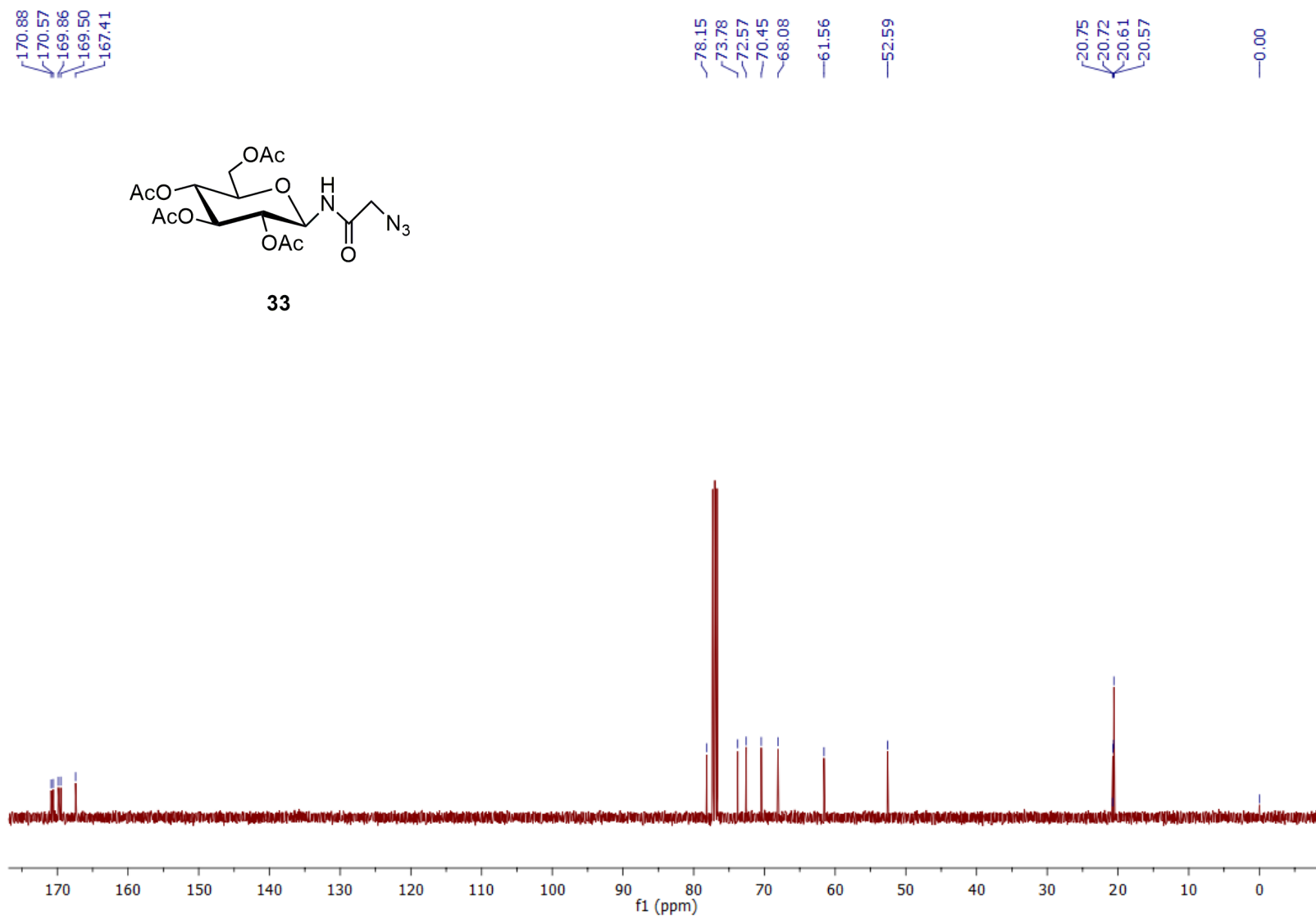


Fig. S58: ¹³C NMR spectrum of compound **33**.

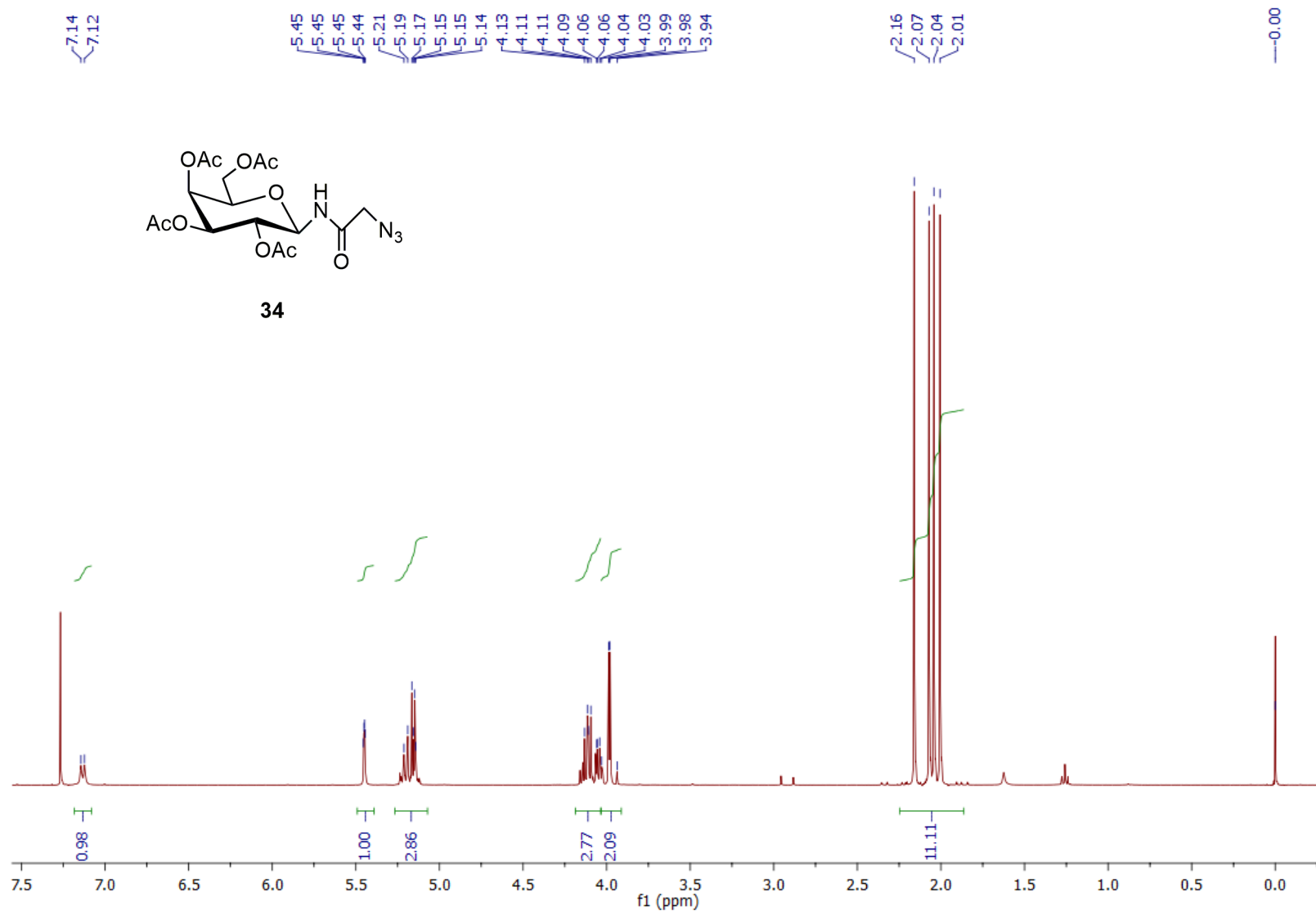


Fig. S59: ^1H NMR spectrum of compound **34**.

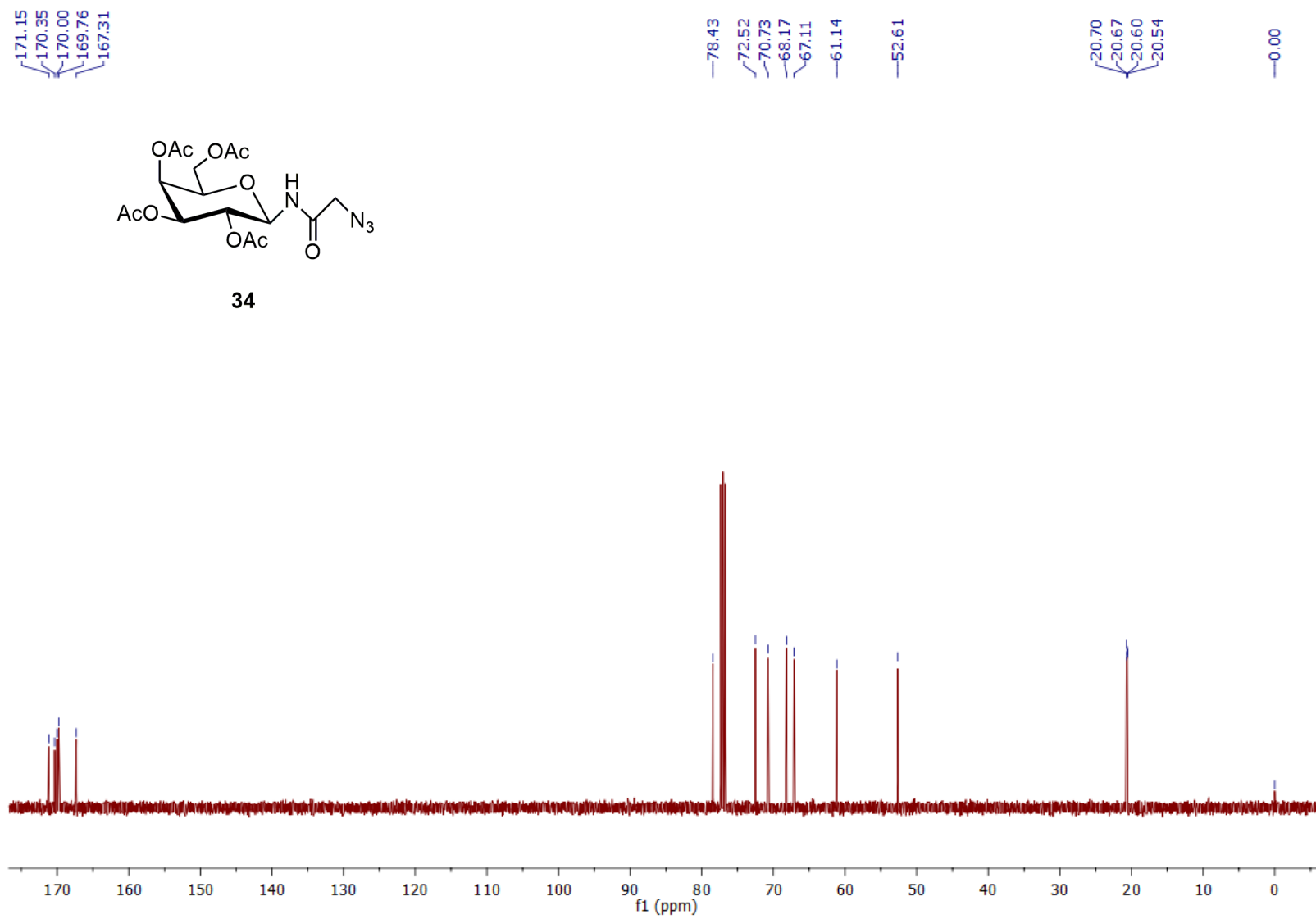


Fig. S60: ^{13}C NMR spectrum of compound **34**.

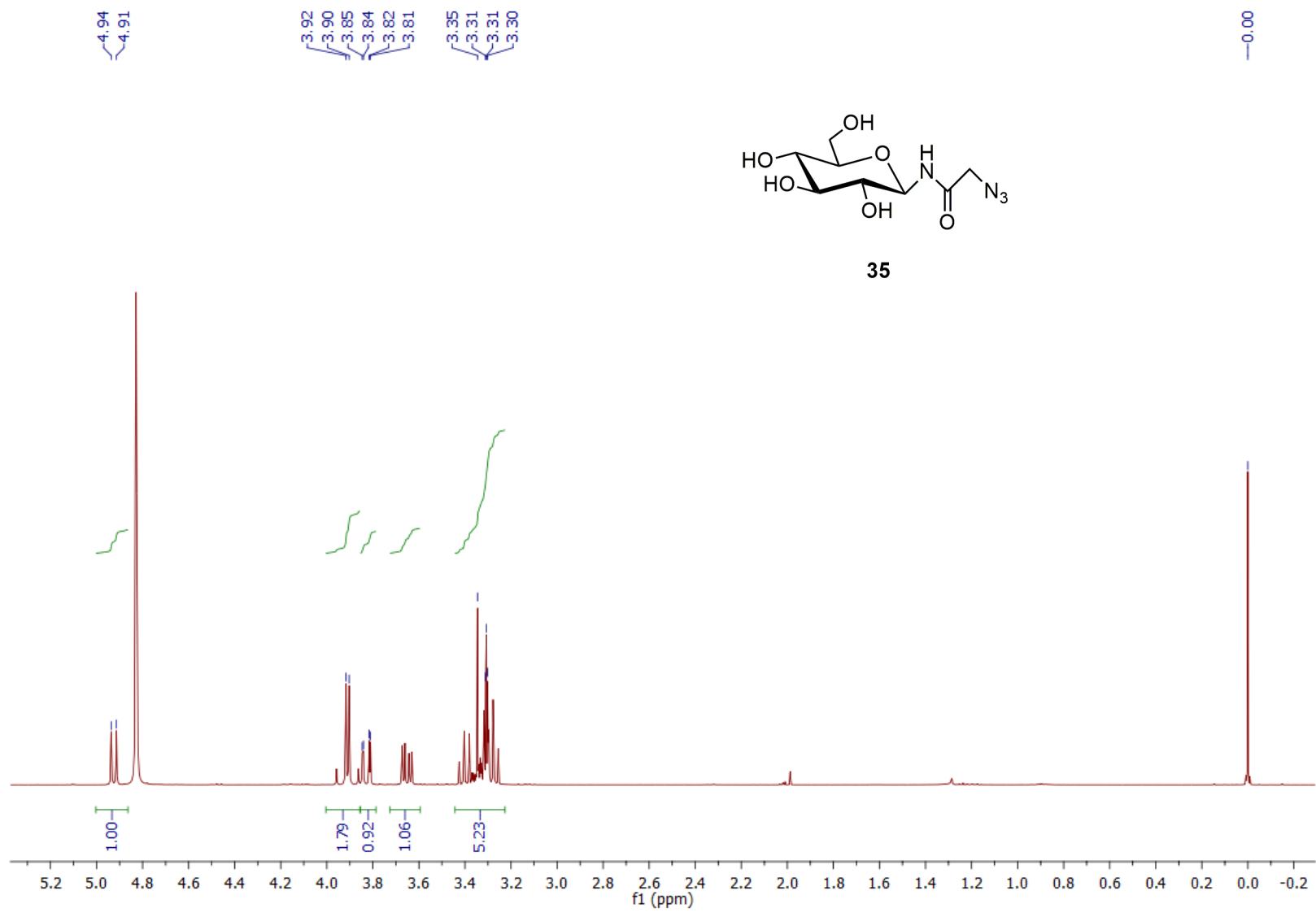


Fig. S61: ¹H NMR spectrum of compound 35.

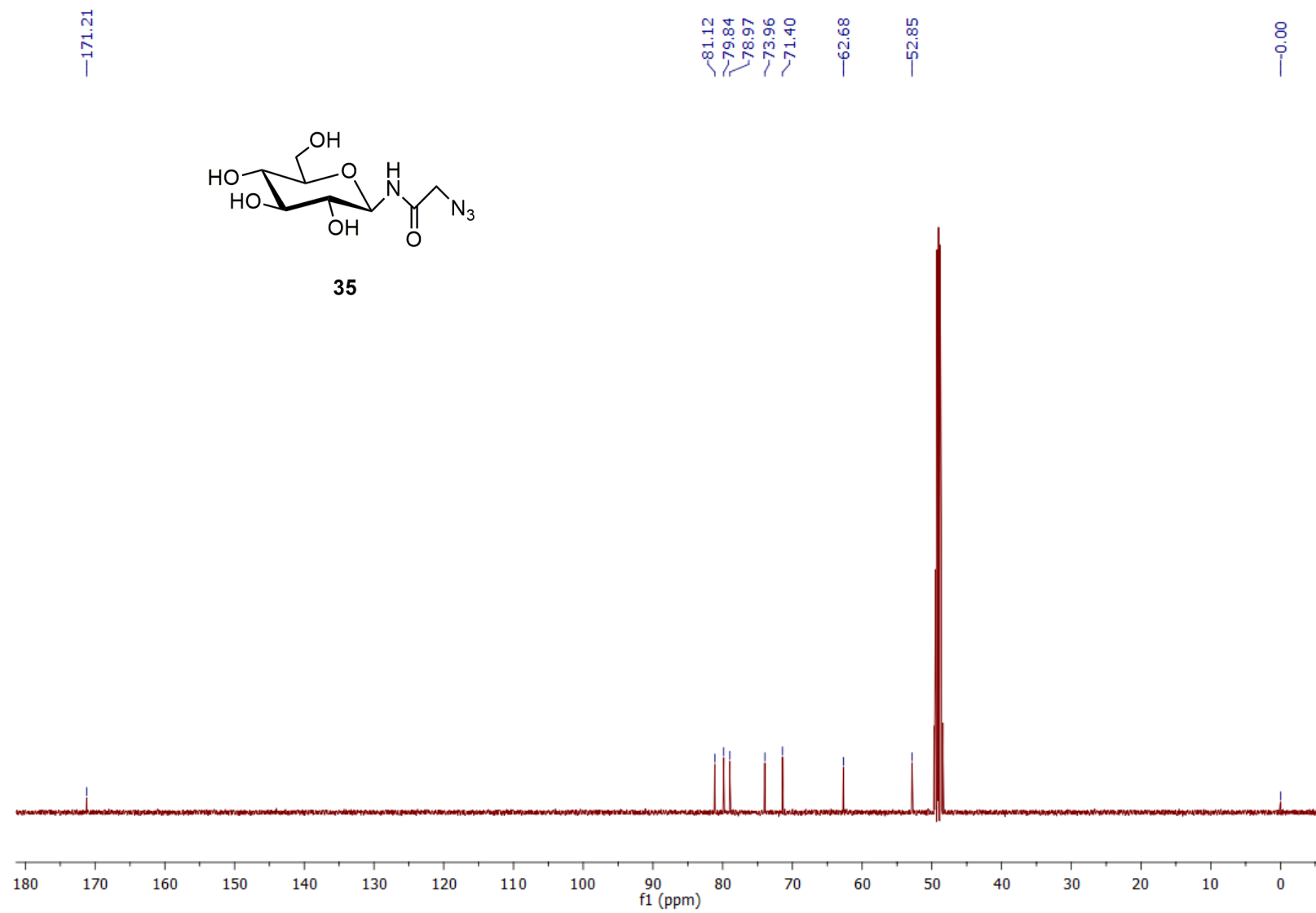


Fig. S62: ^{13}C NMR spectrum of compound **35**.

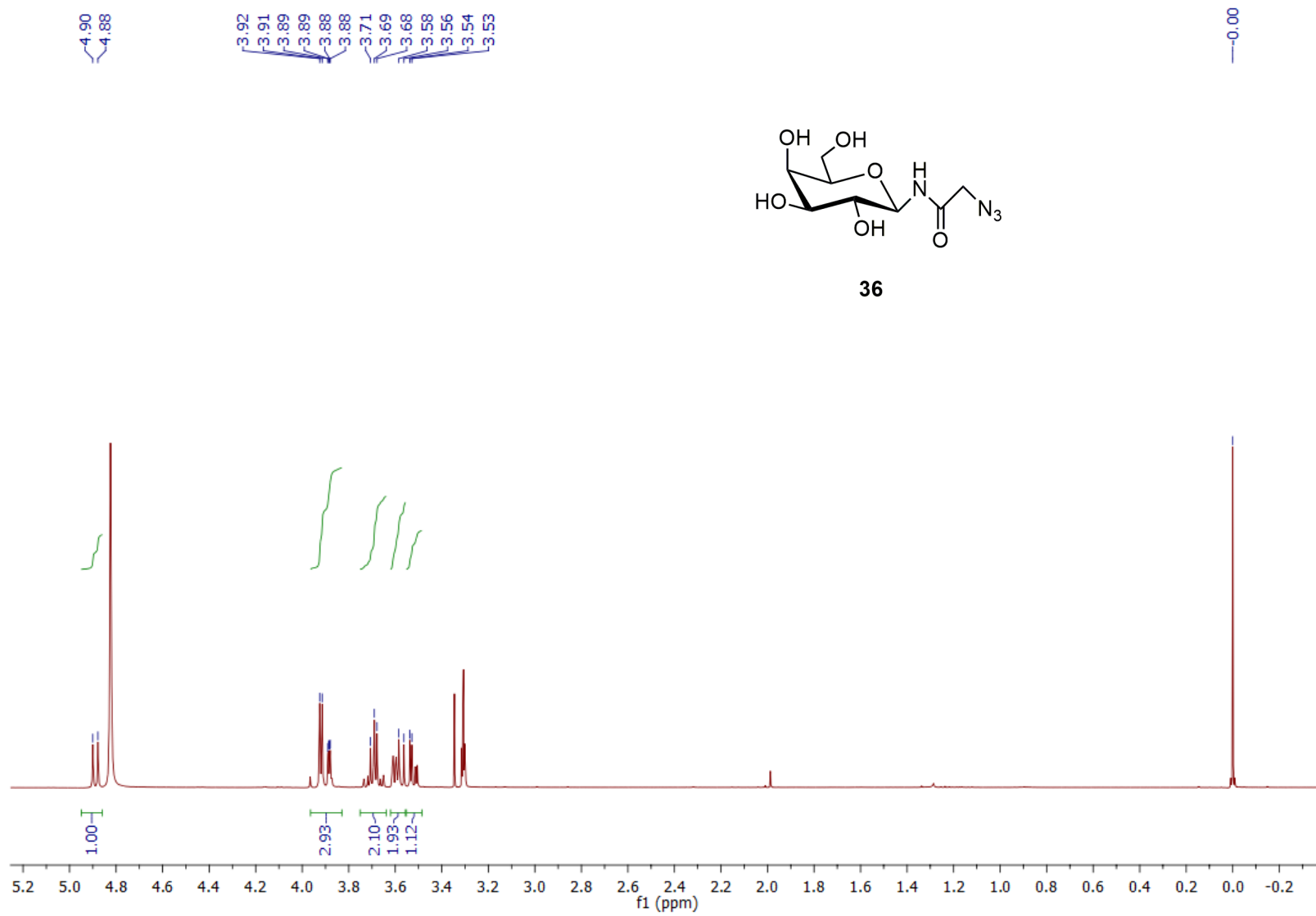


Fig. S63: ^1H NMR spectrum of compound **36**.

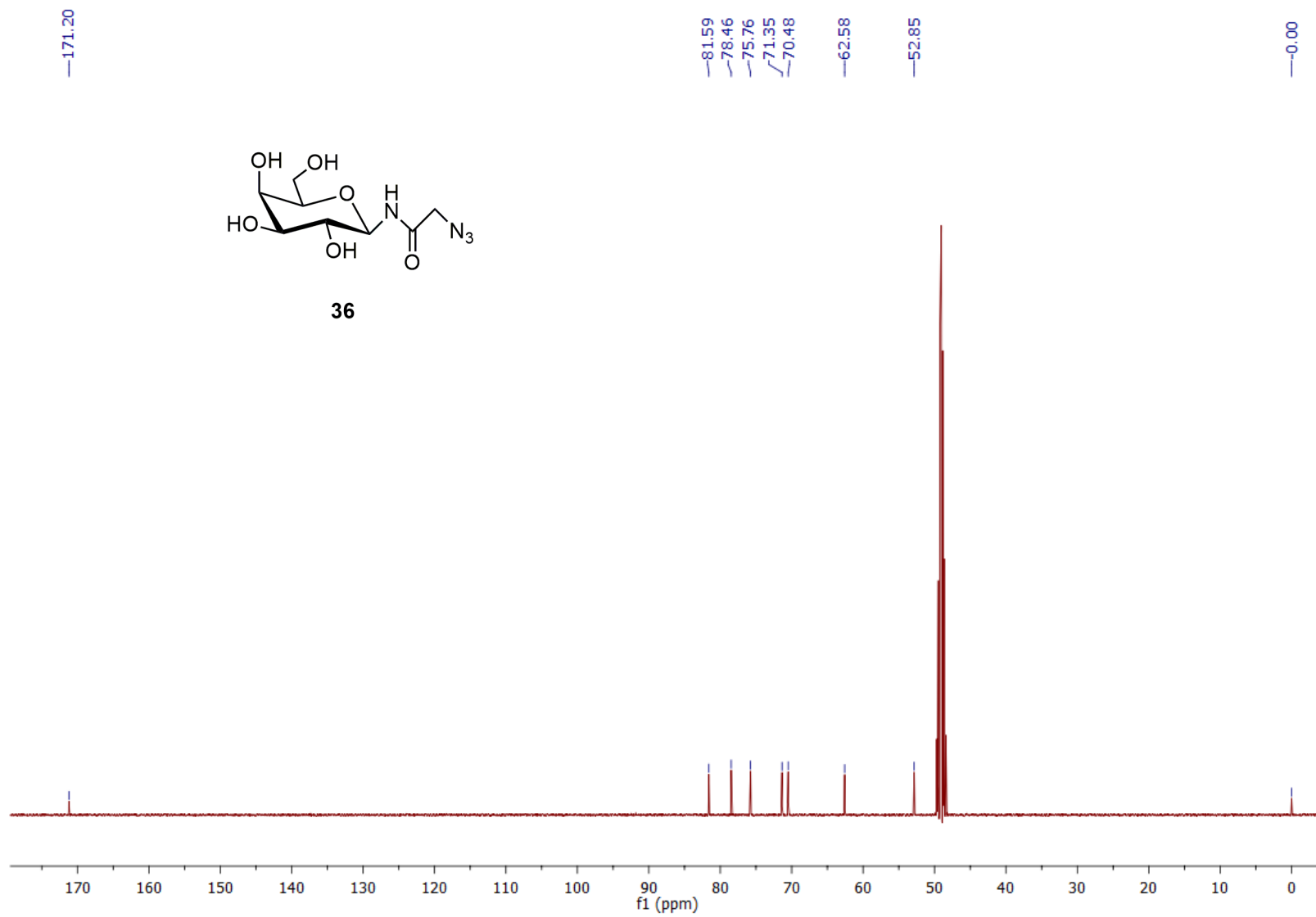


Fig. S64: ^{13}C NMR spectrum of compound **36**.

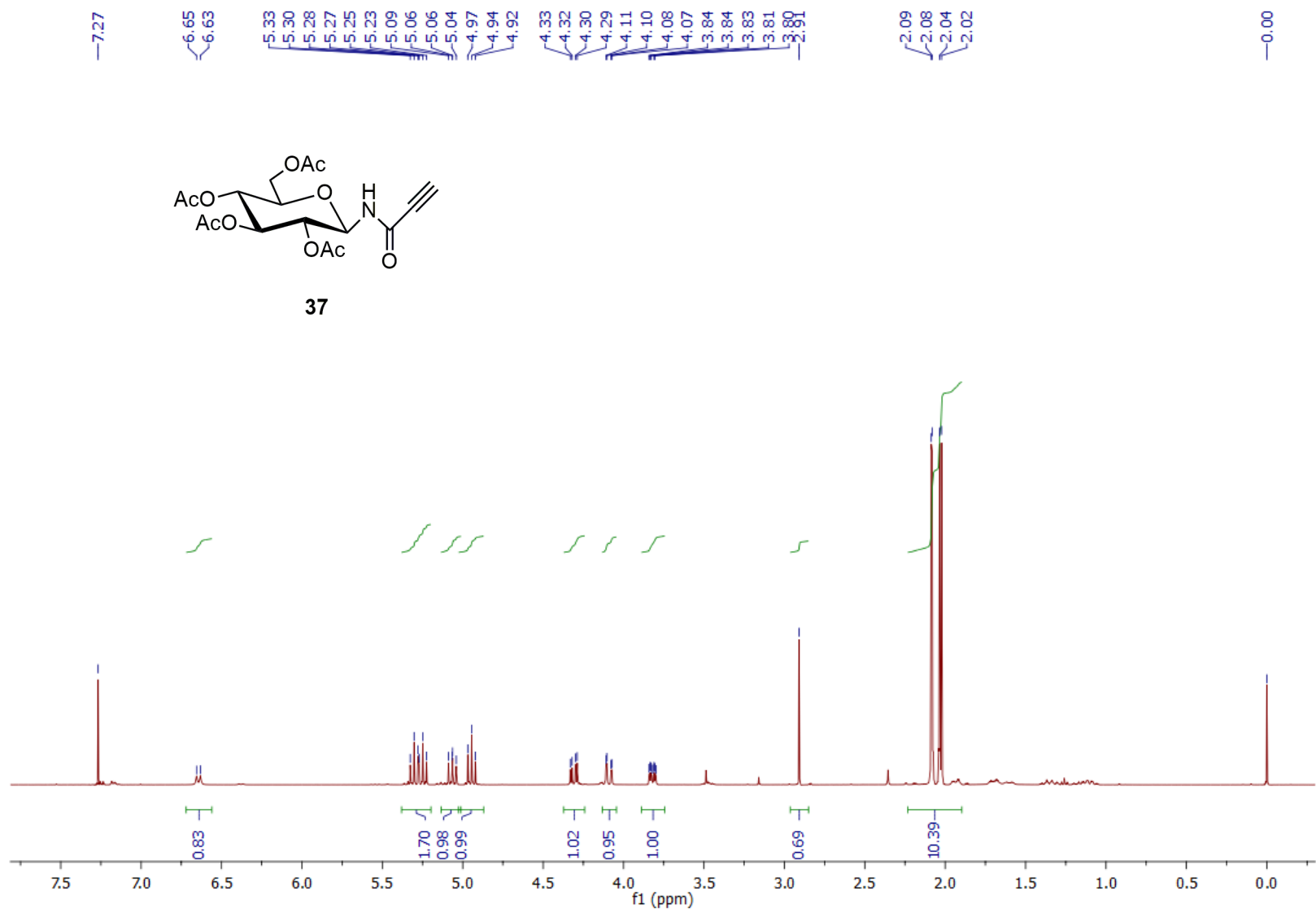


Fig. S65: ^1H NMR spectrum of compound **37**.

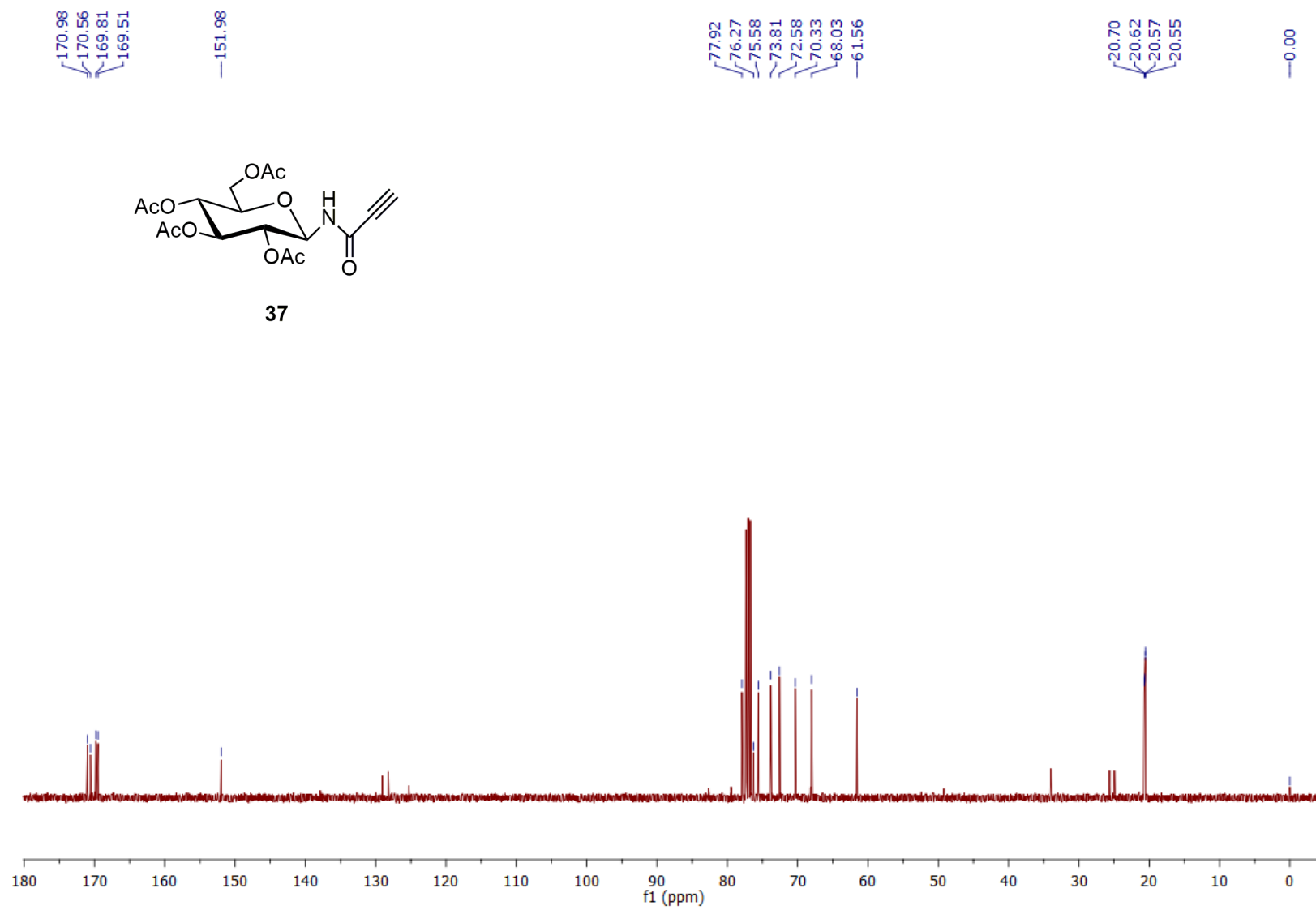


Fig. S66: ^{13}C NMR spectrum of compound **37**.

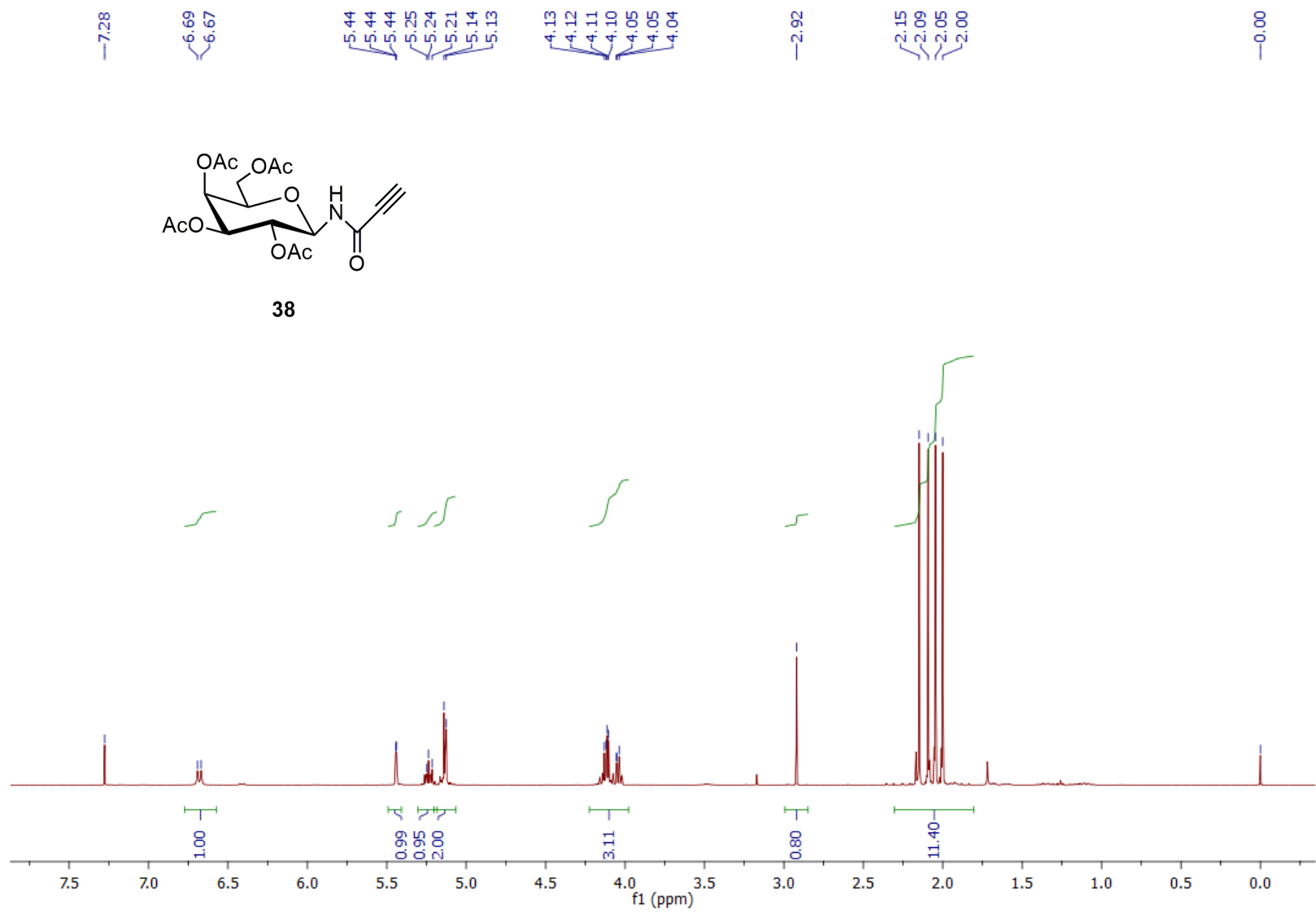


Fig. S67: ^1H NMR spectrum of compound **38**.

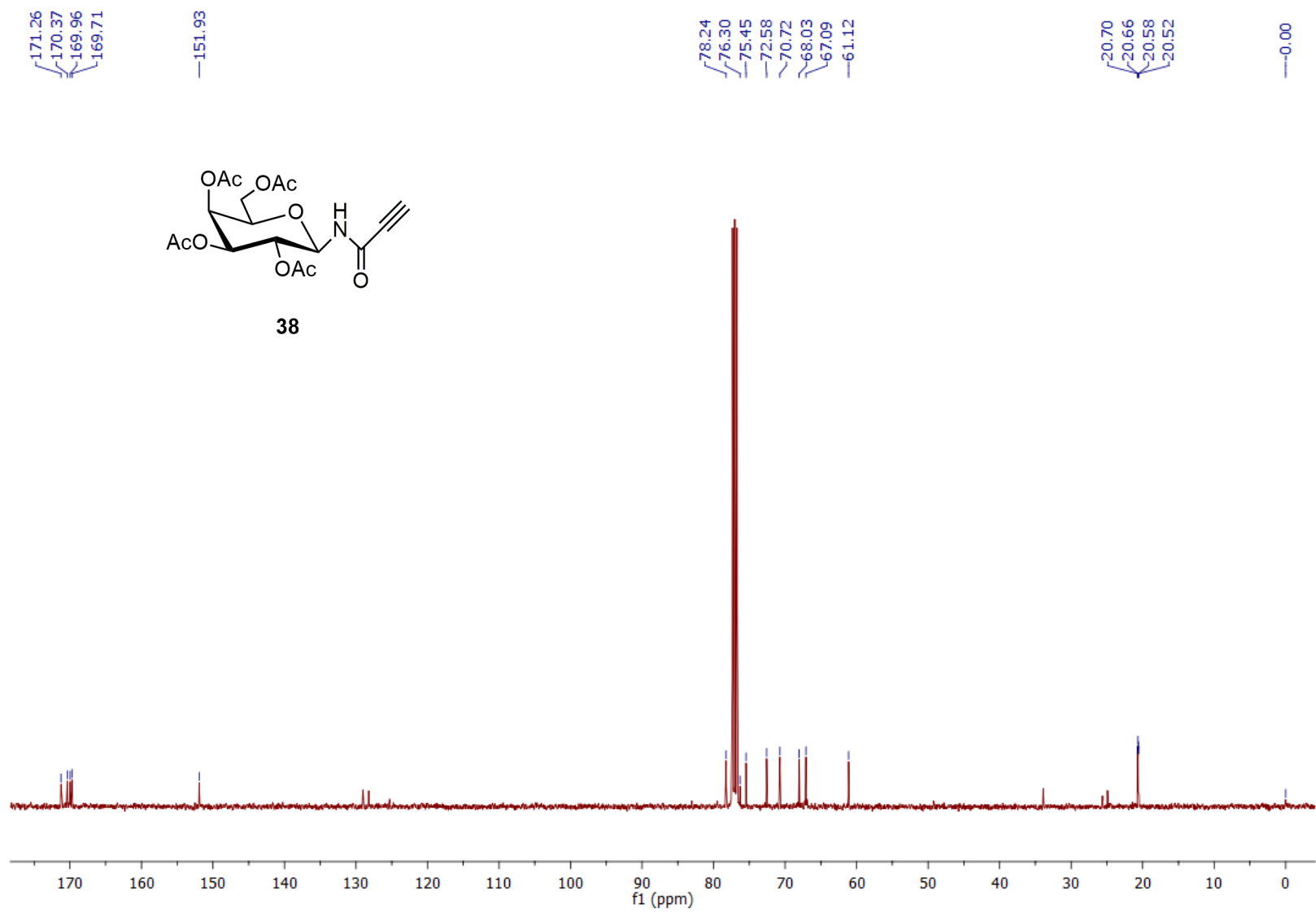


Fig. S68: ^{13}C NMR spectrum of compound **38**.

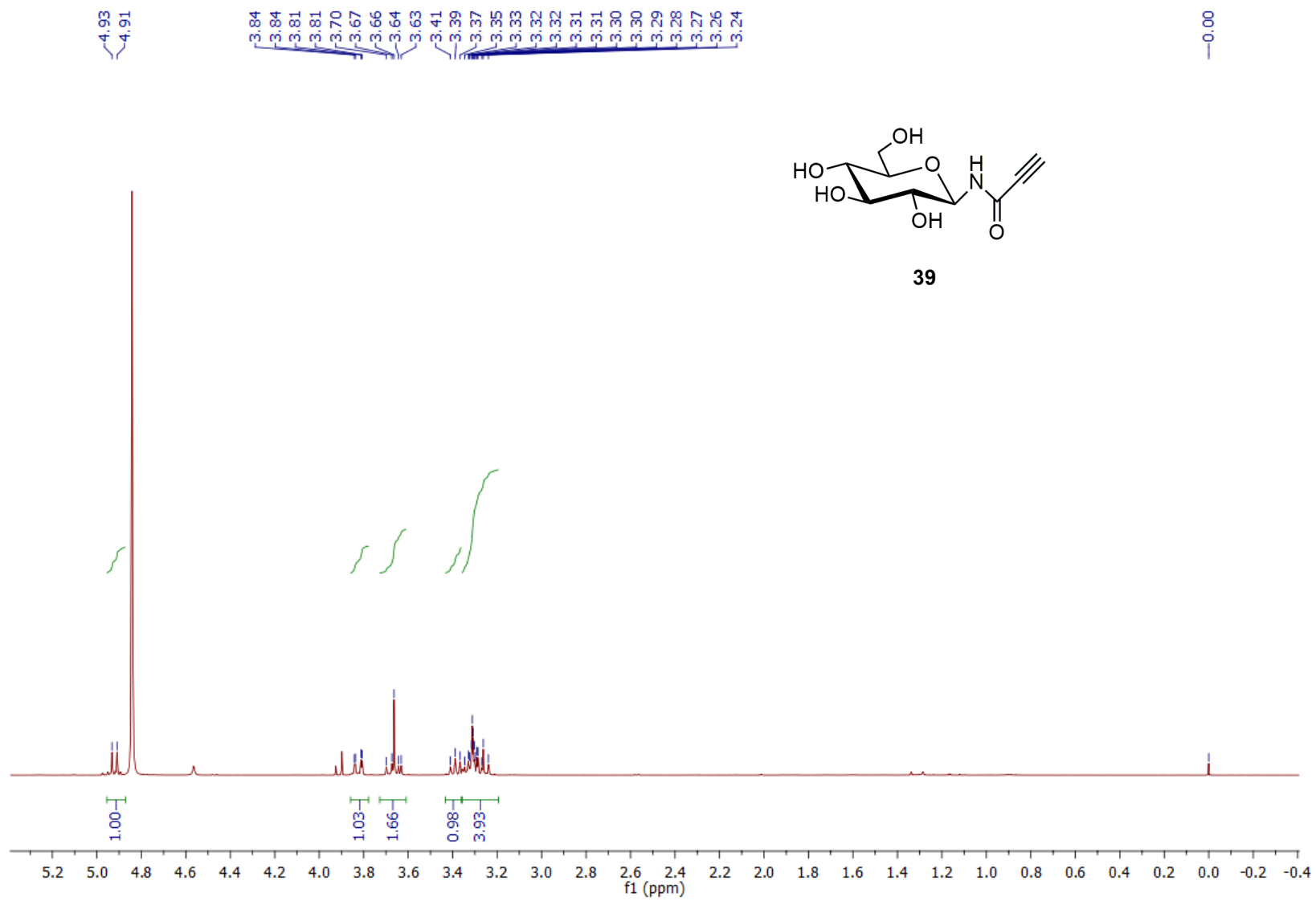


Fig. S69: ^1H NMR spectrum of compound **39**.

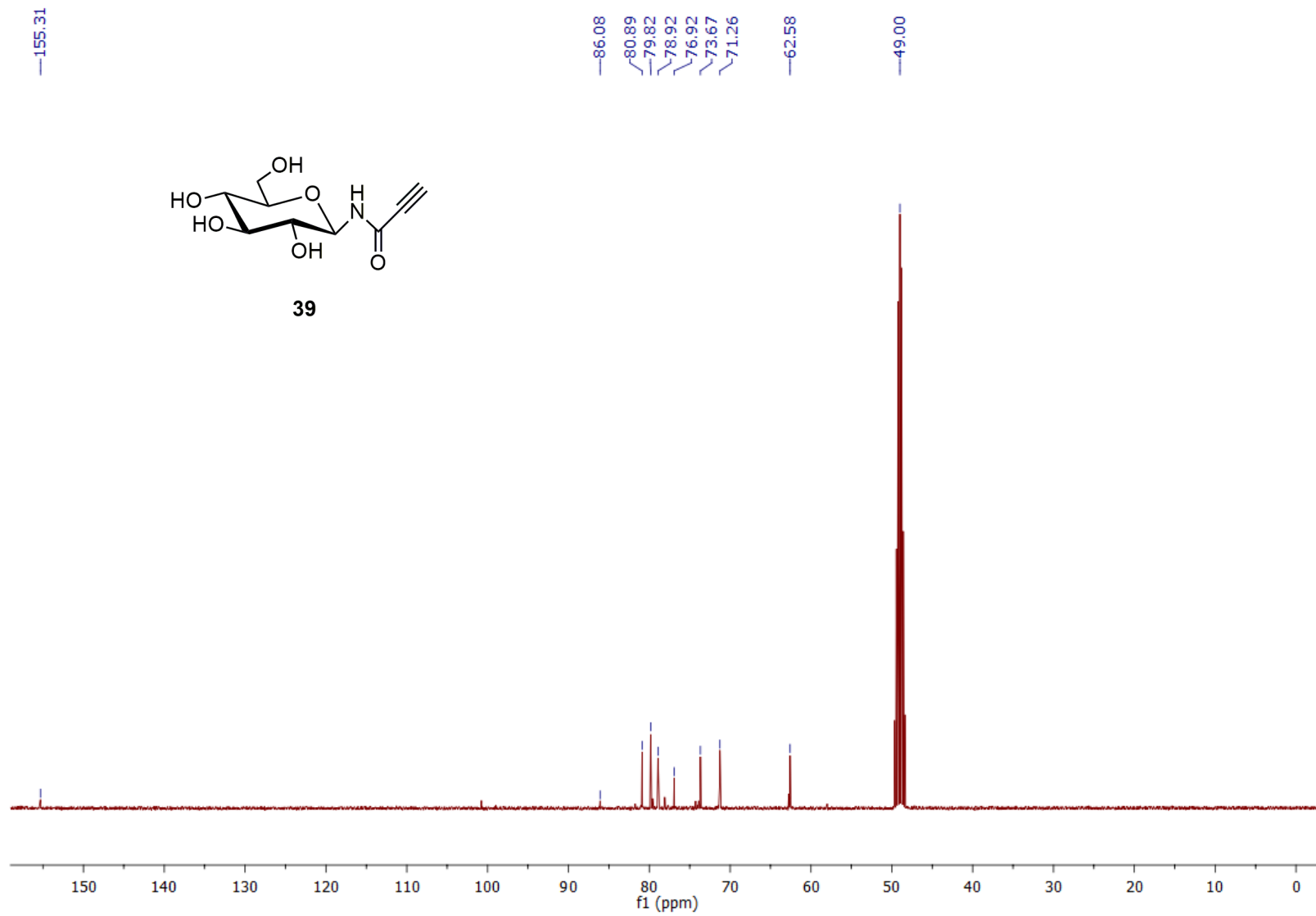


Fig. S70: ^{13}C NMR spectrum of compound **39**.

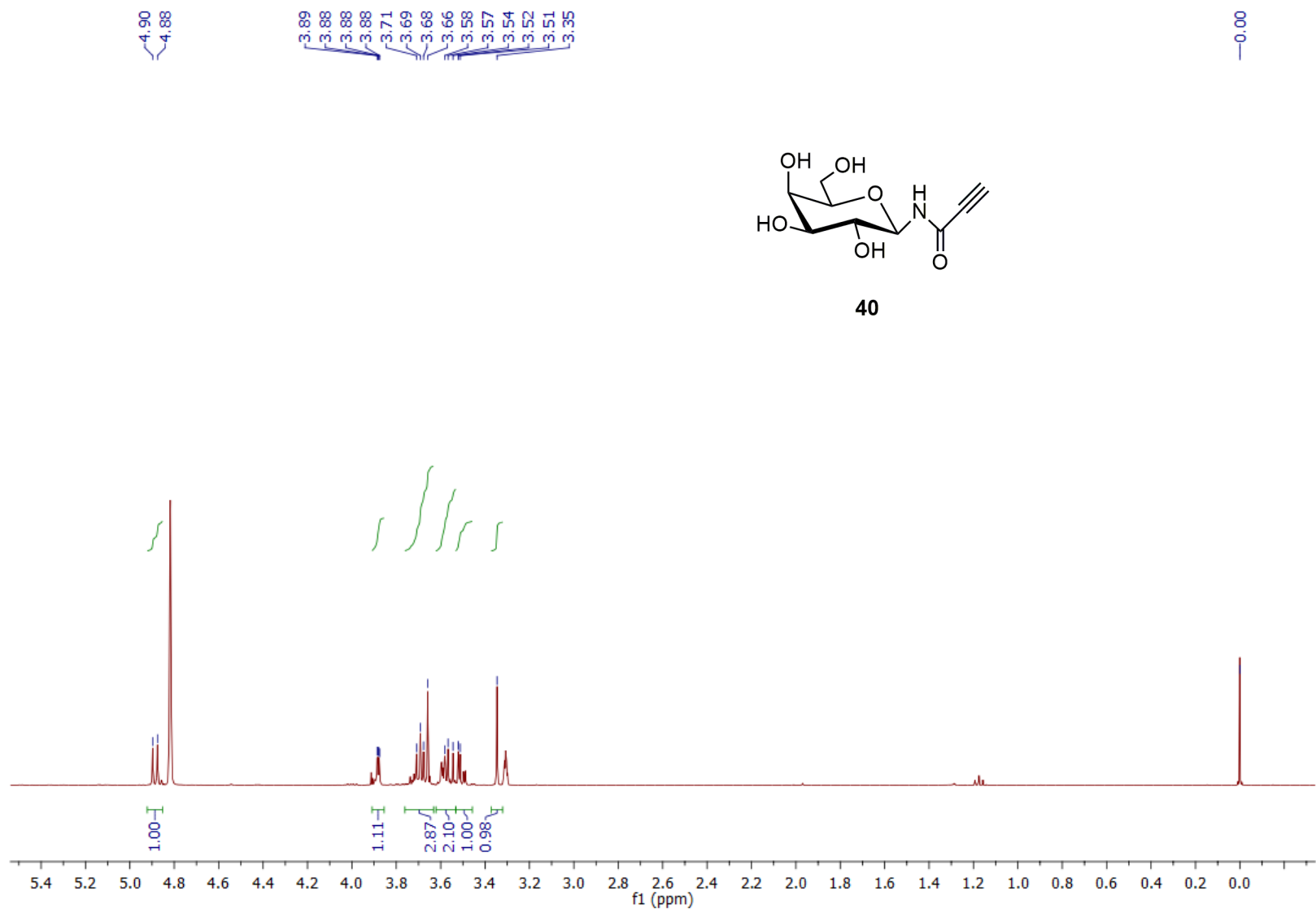


Fig. S71: ¹H NMR spectrum of compound **40**.

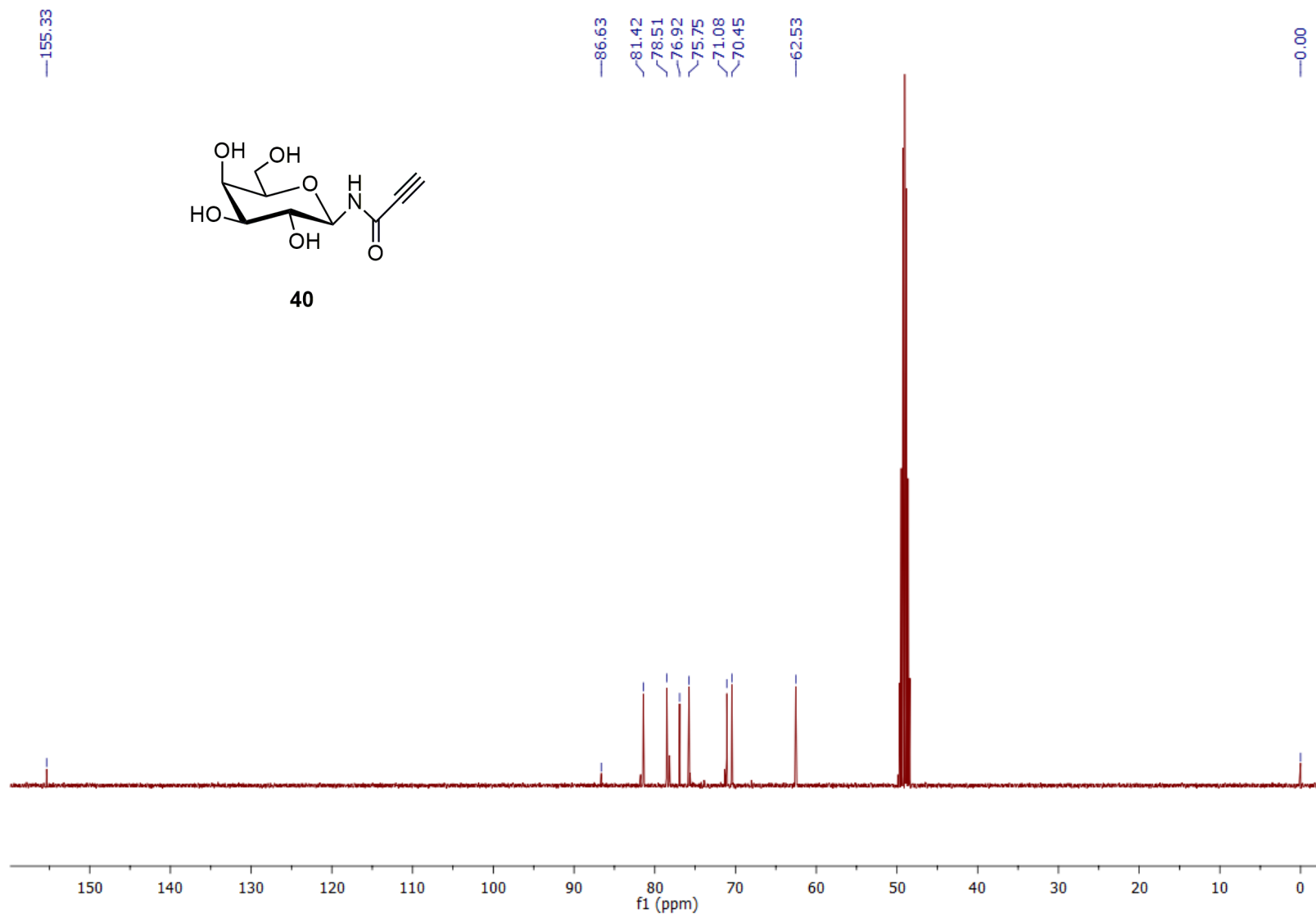


Fig. S72: ^{13}C NMR spectrum of compound **40**.

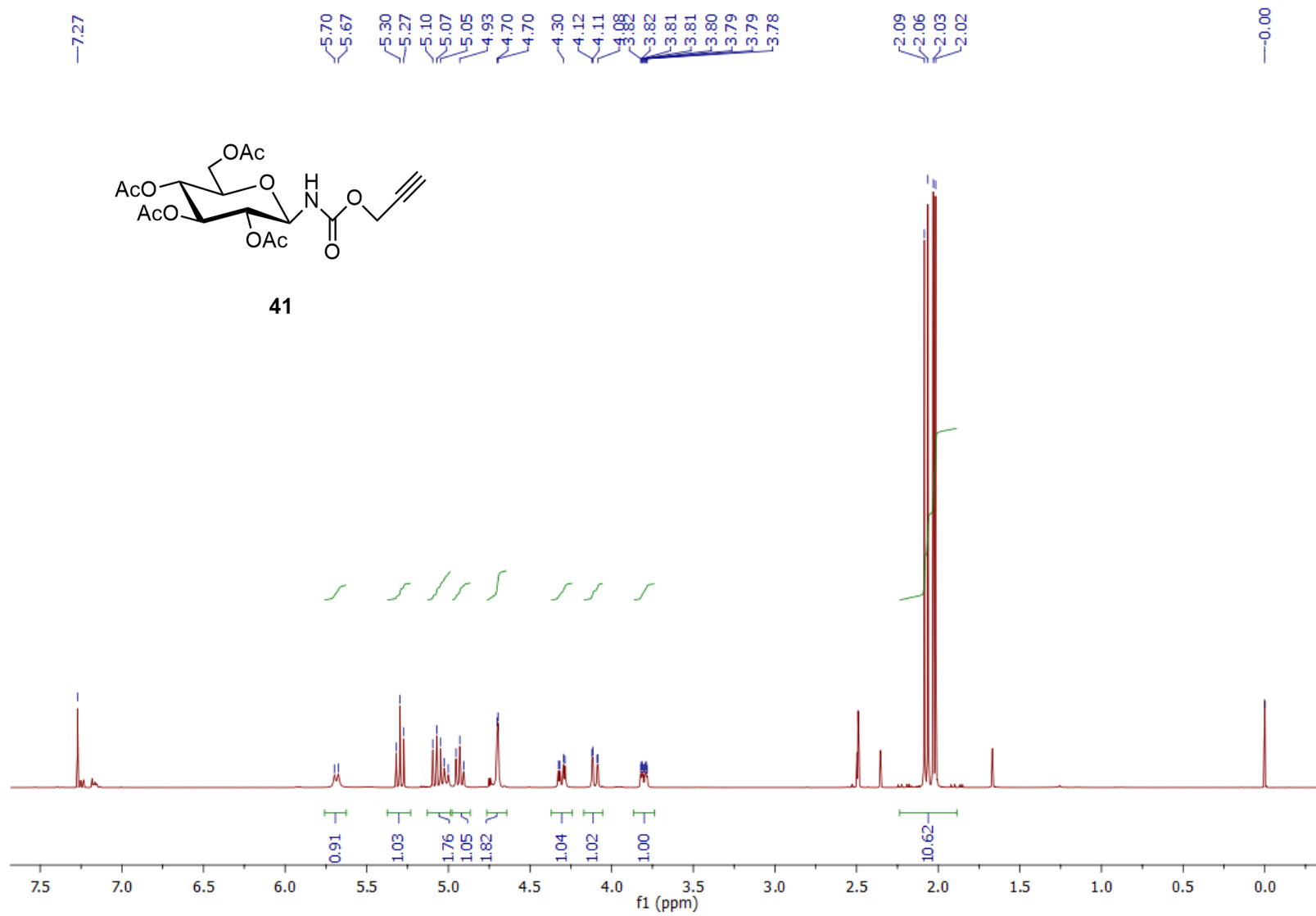


Fig. S73: ^1H NMR spectrum of compound **41**.

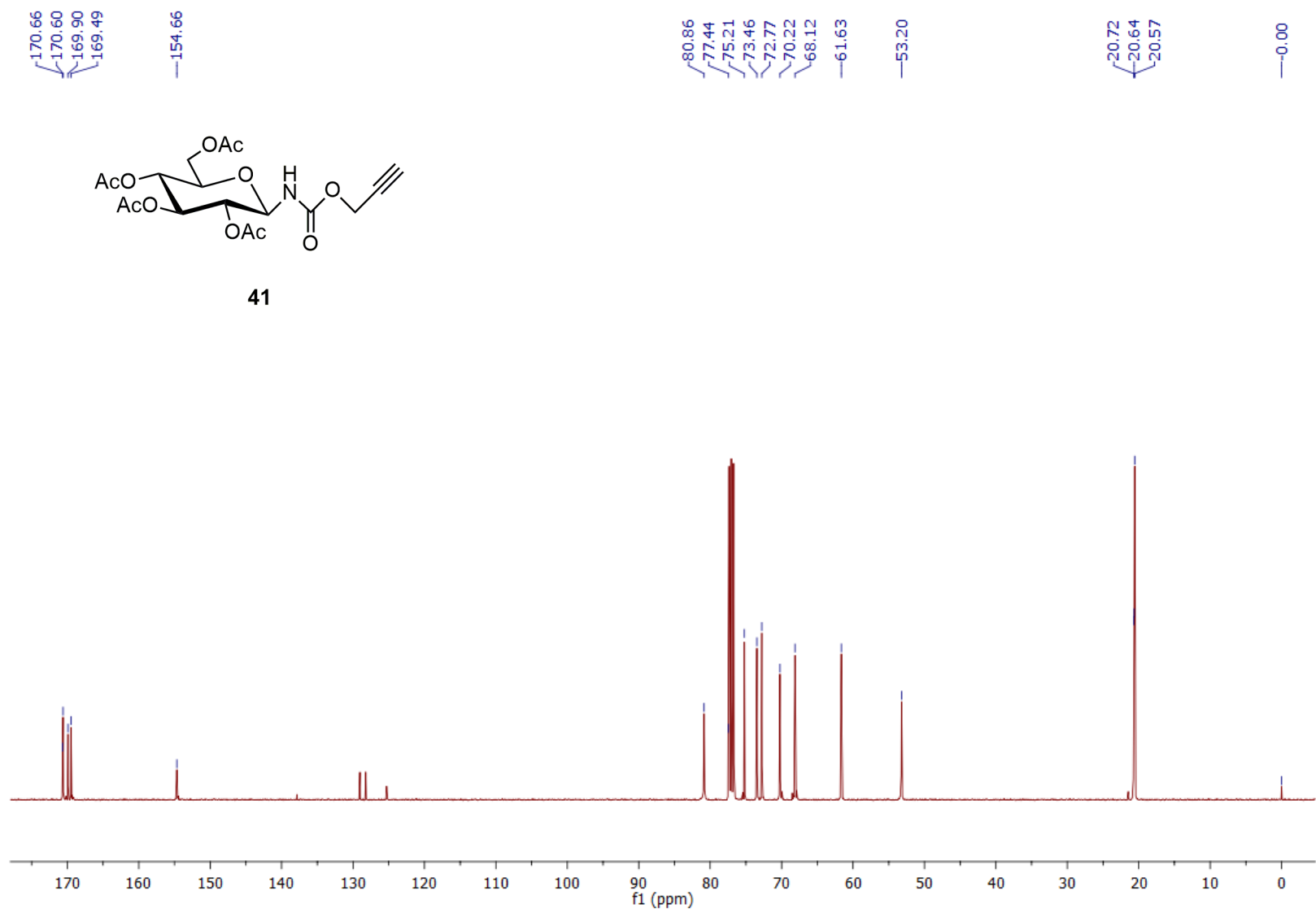


Fig. S74: ¹³C NMR spectrum of compound **41**.

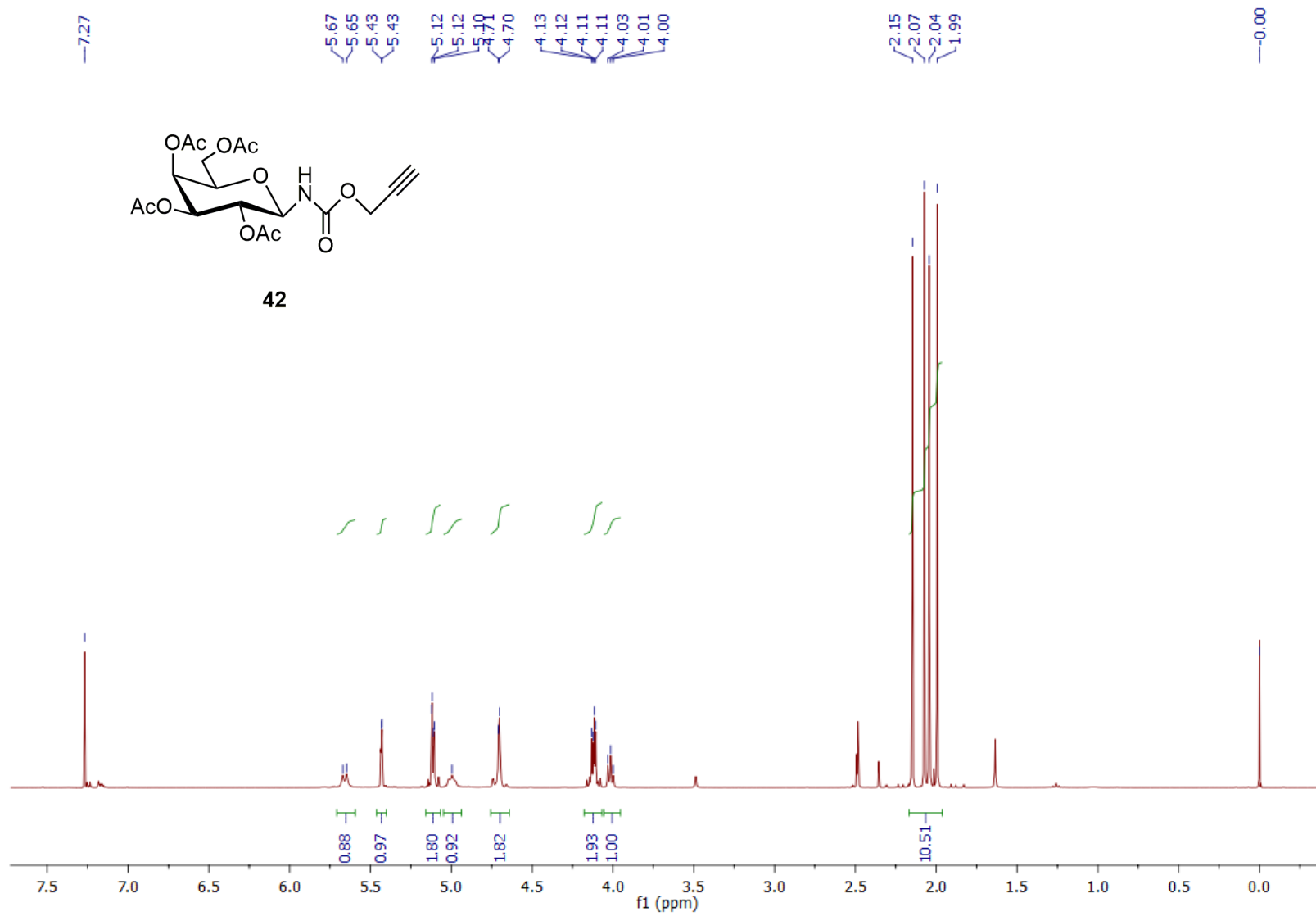


Fig. S75: ^1H NMR spectrum of compound **42**.

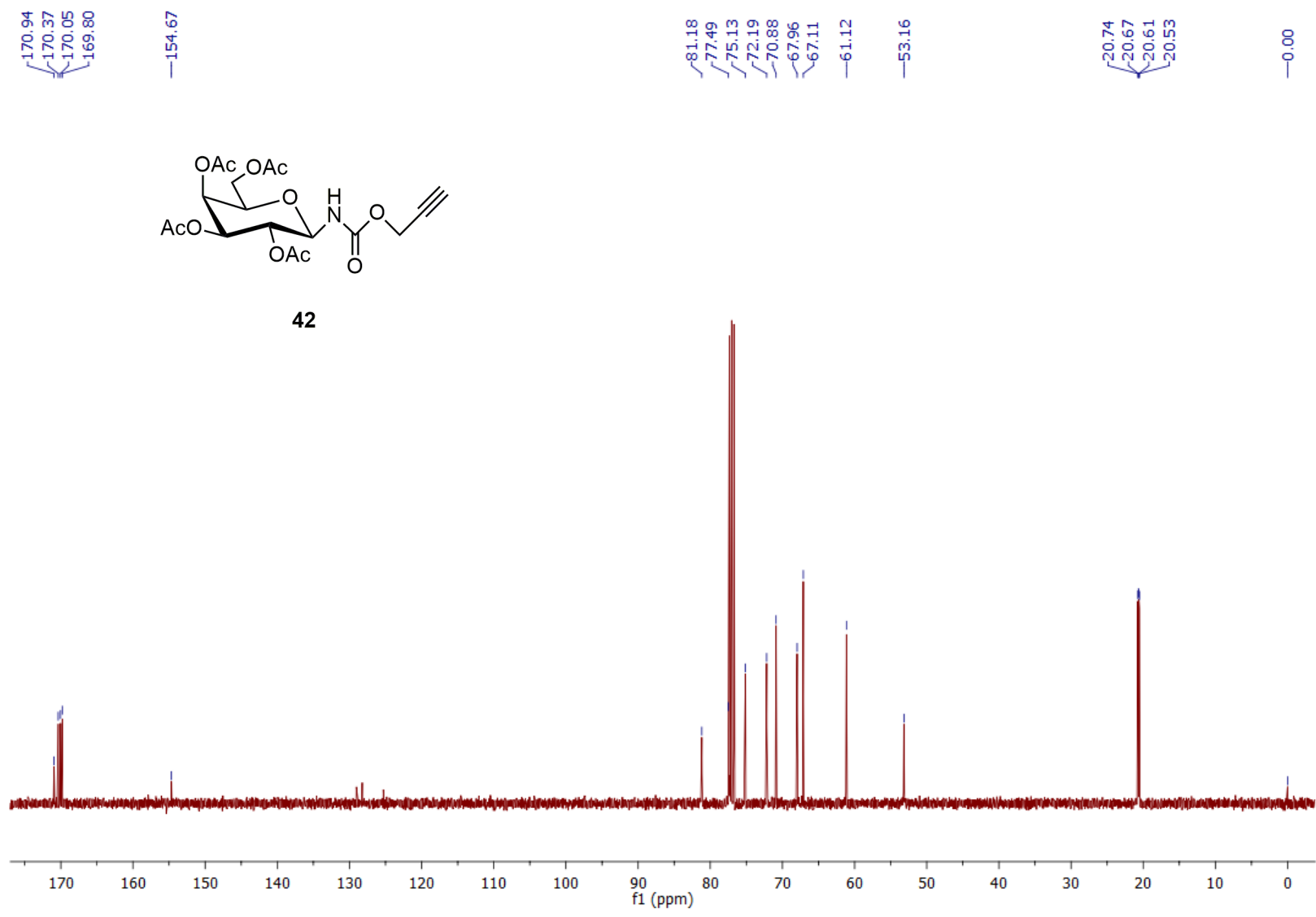


Fig. S76: ¹³C NMR spectrum of compound 42.

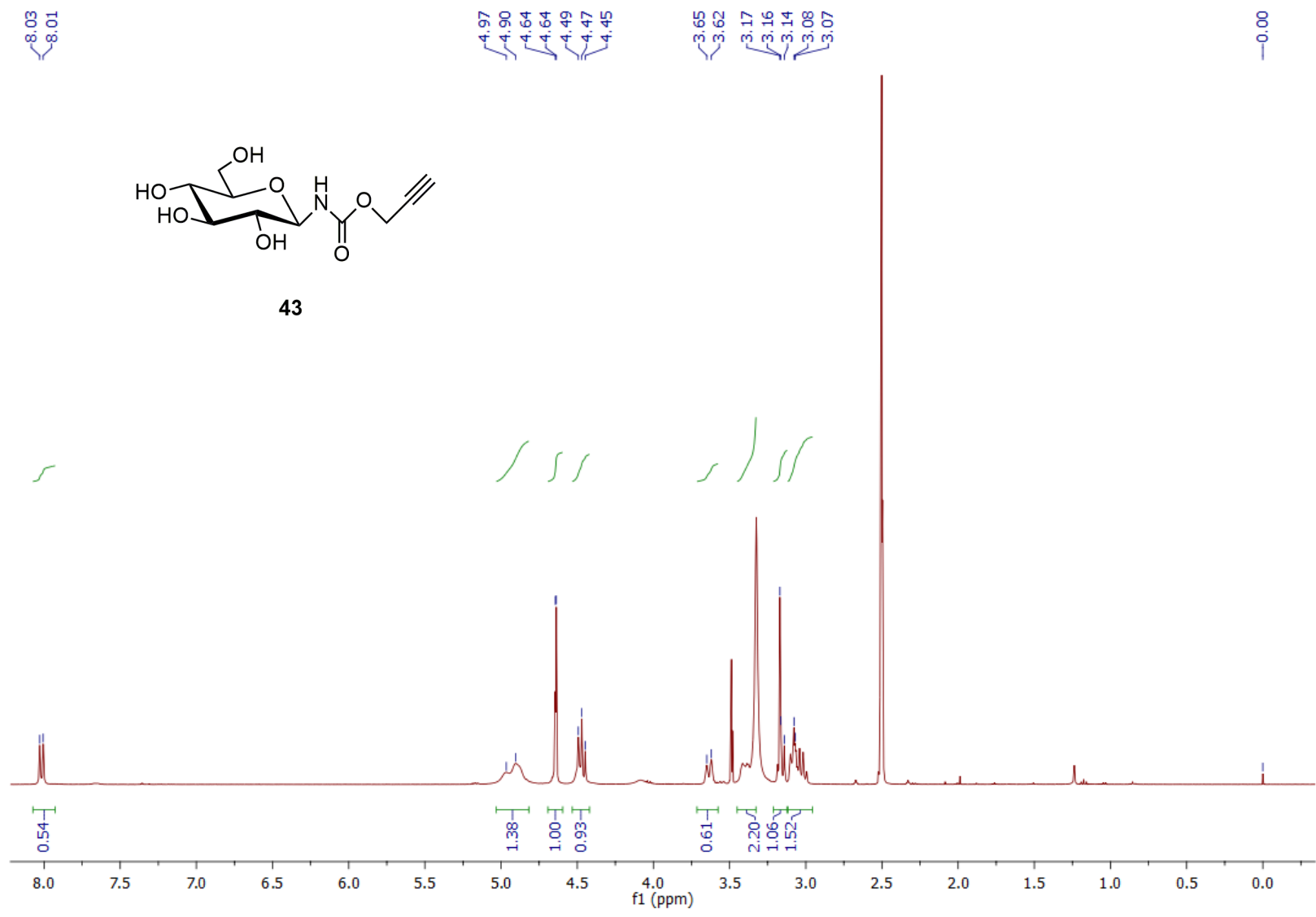


Fig. S77: ¹H NMR spectrum of compound **43**.

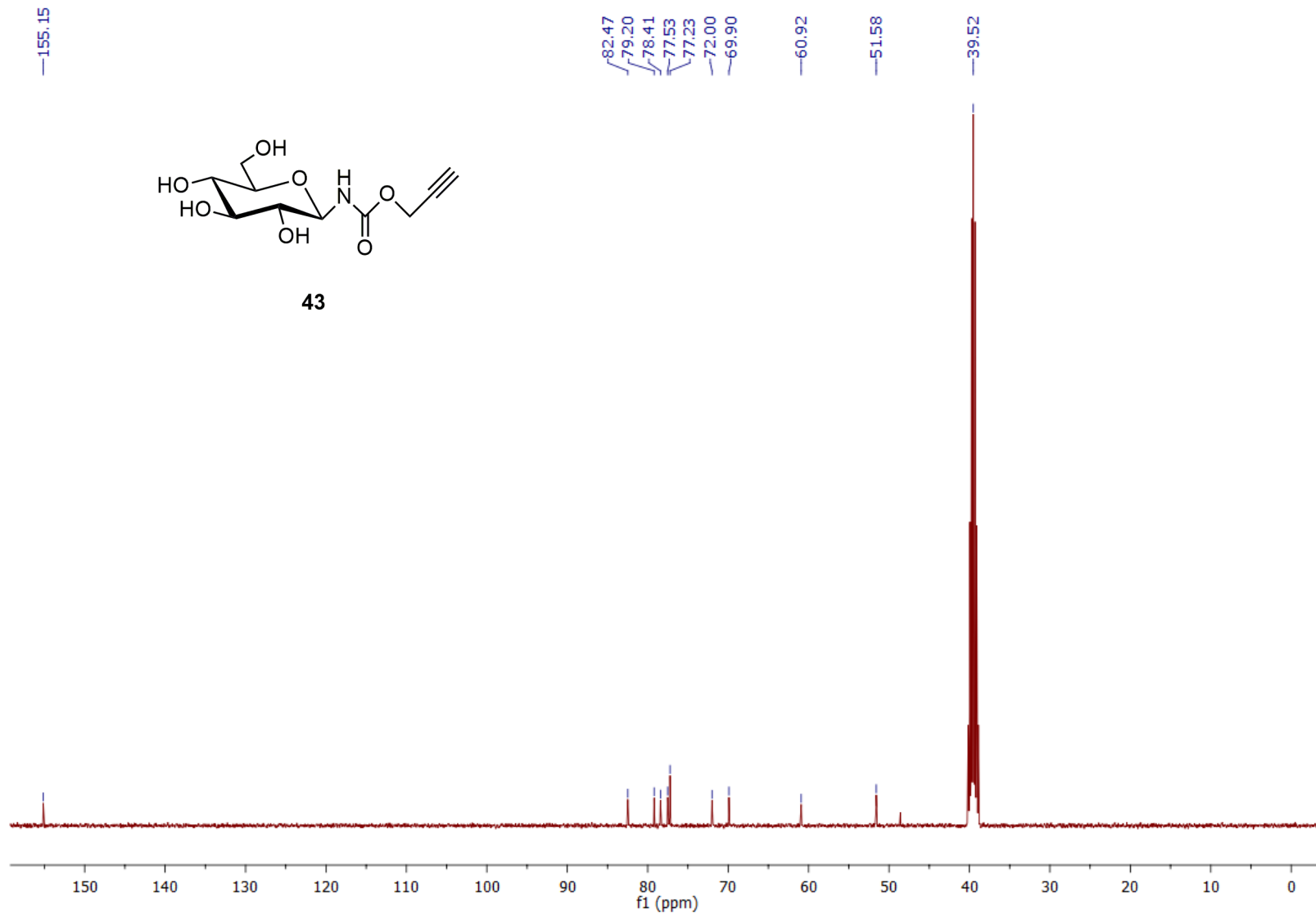


Fig. S78: ^{13}C NMR spectrum of compound **43**.

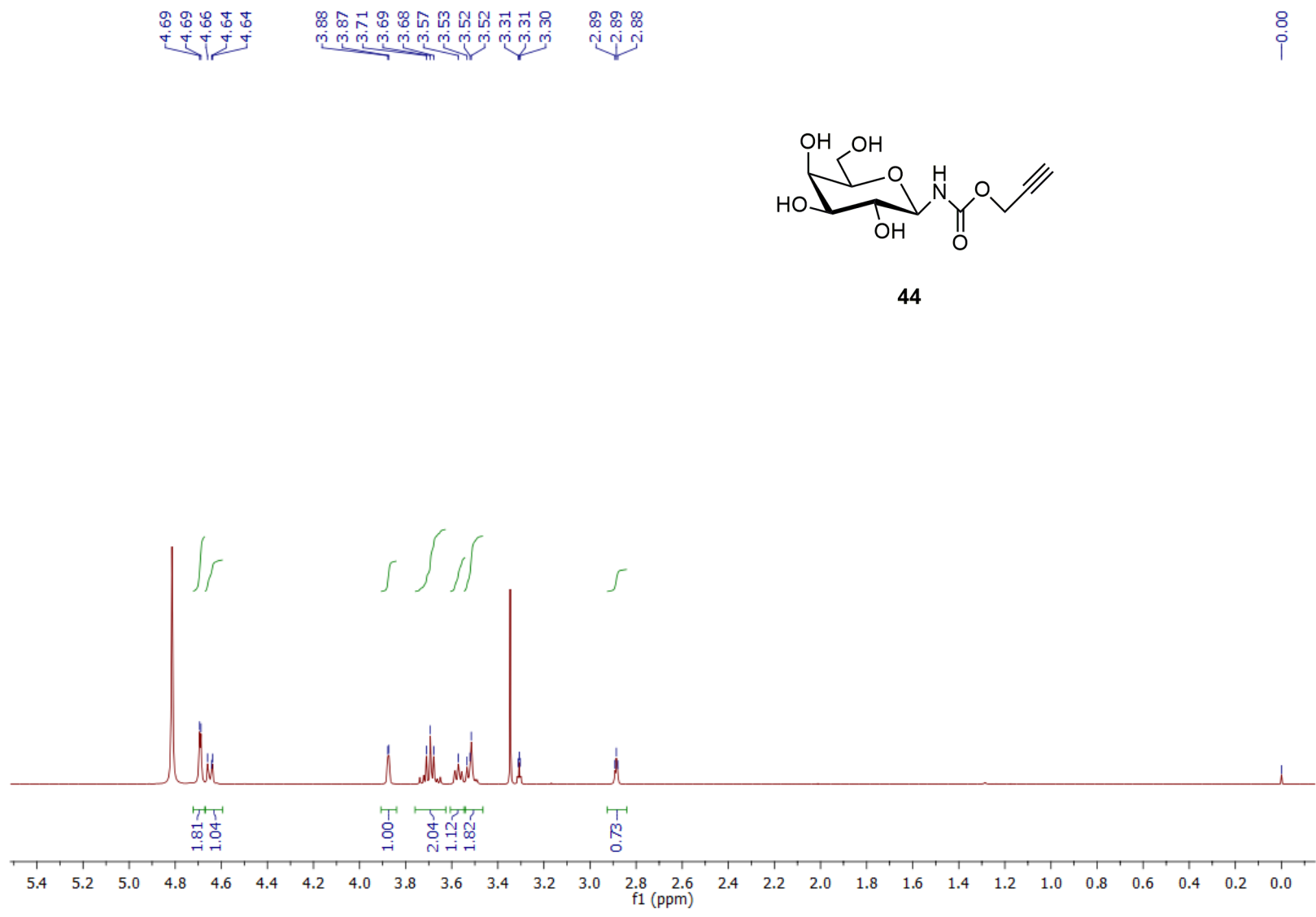


Fig. S79: ¹H NMR spectrum of compound **44**.

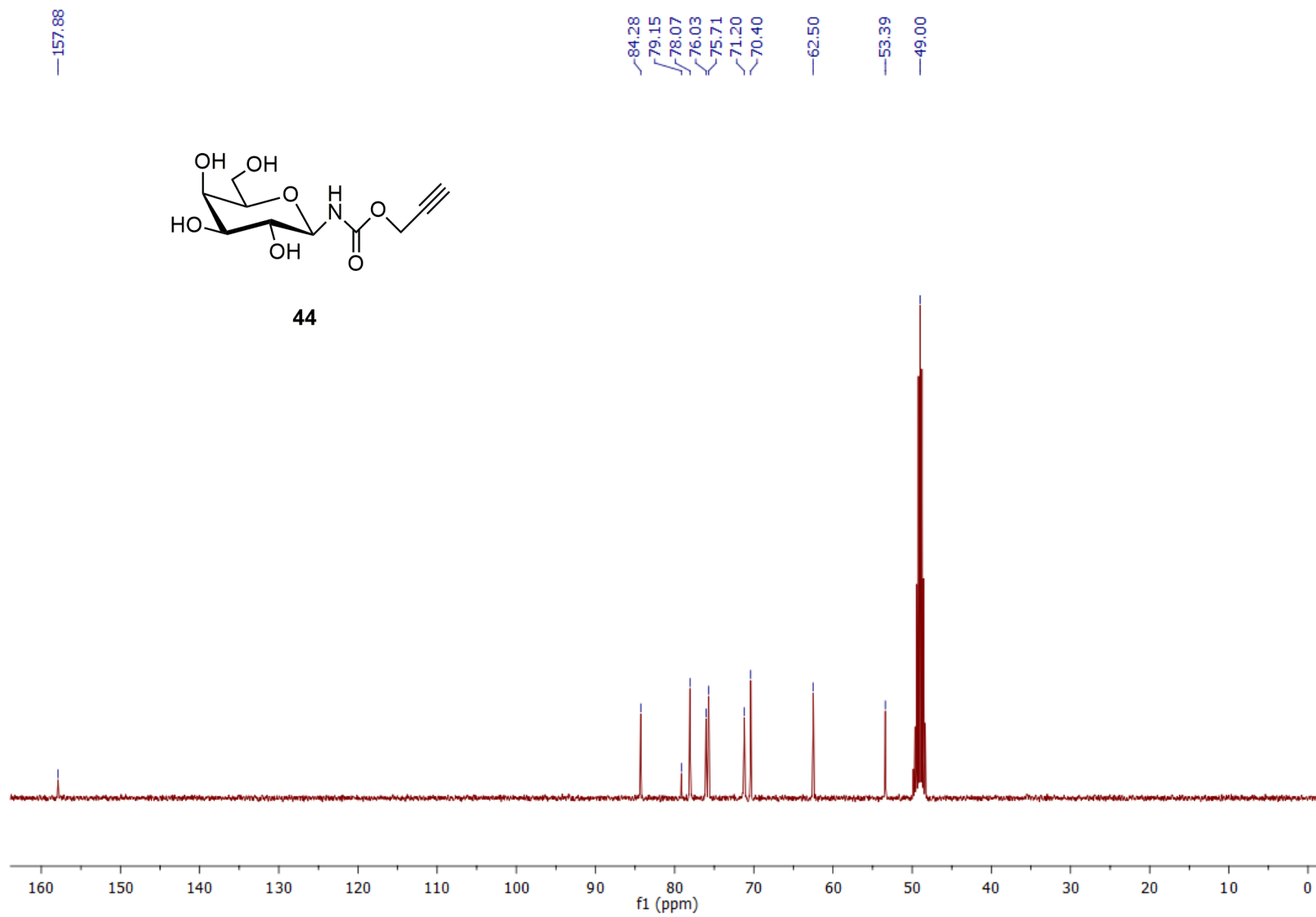


Fig. S80: ^{13}C NMR spectrum of compound **44**.

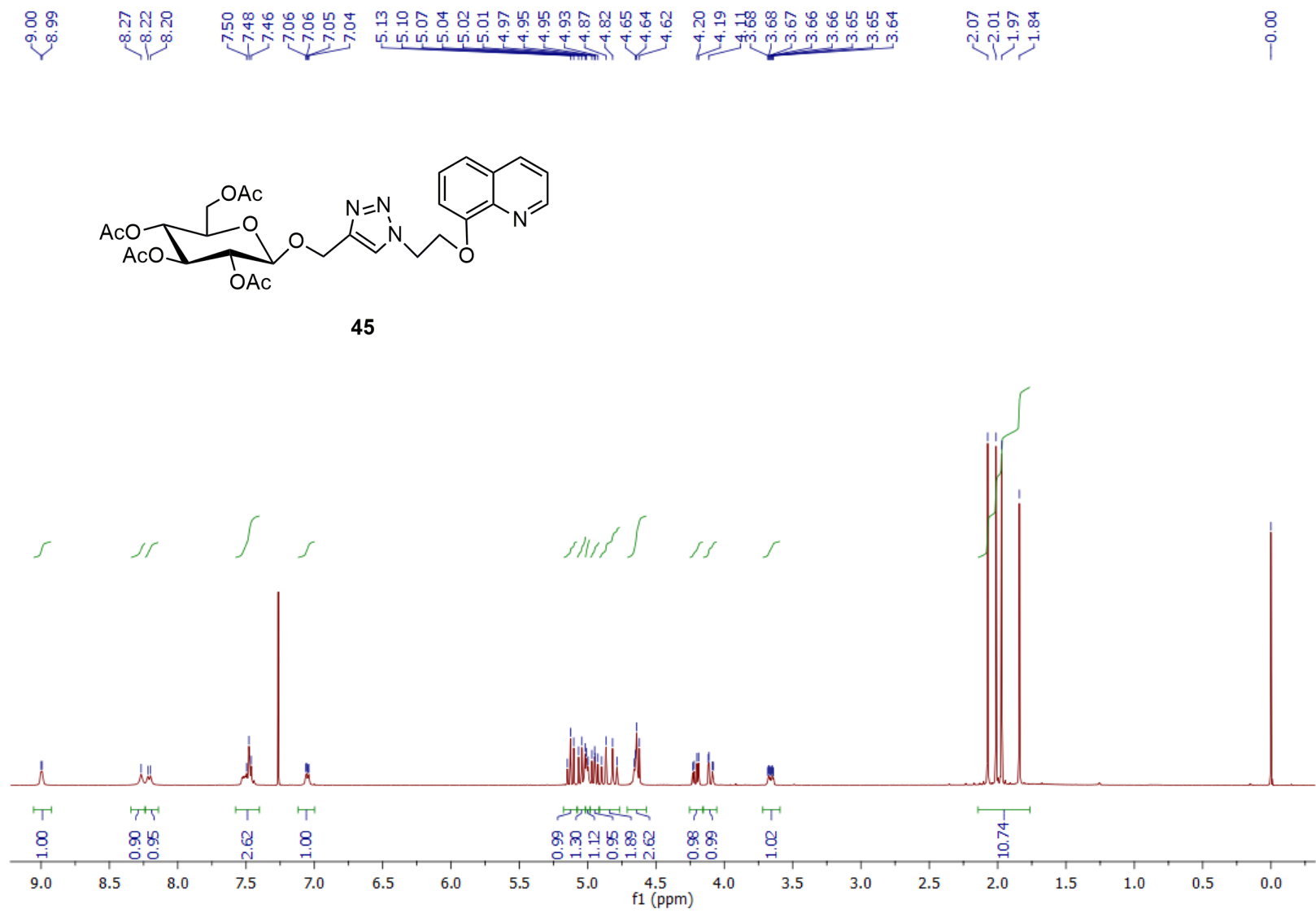


Fig. S81: ^1H NMR spectrum of glycoconjugate **45**.

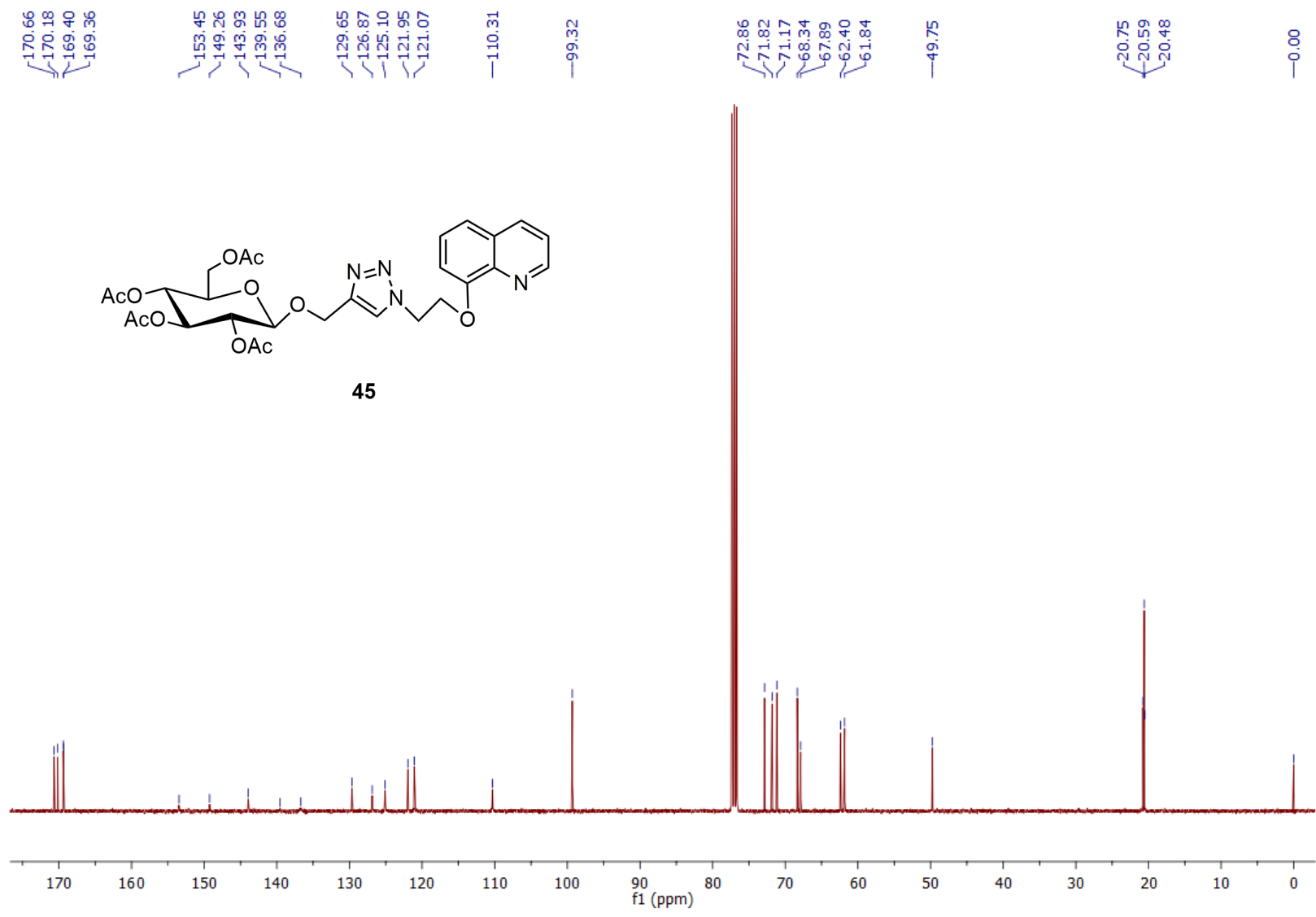


Fig. S82: ^{13}C NMR spectrum of glycoconjugate **45**.

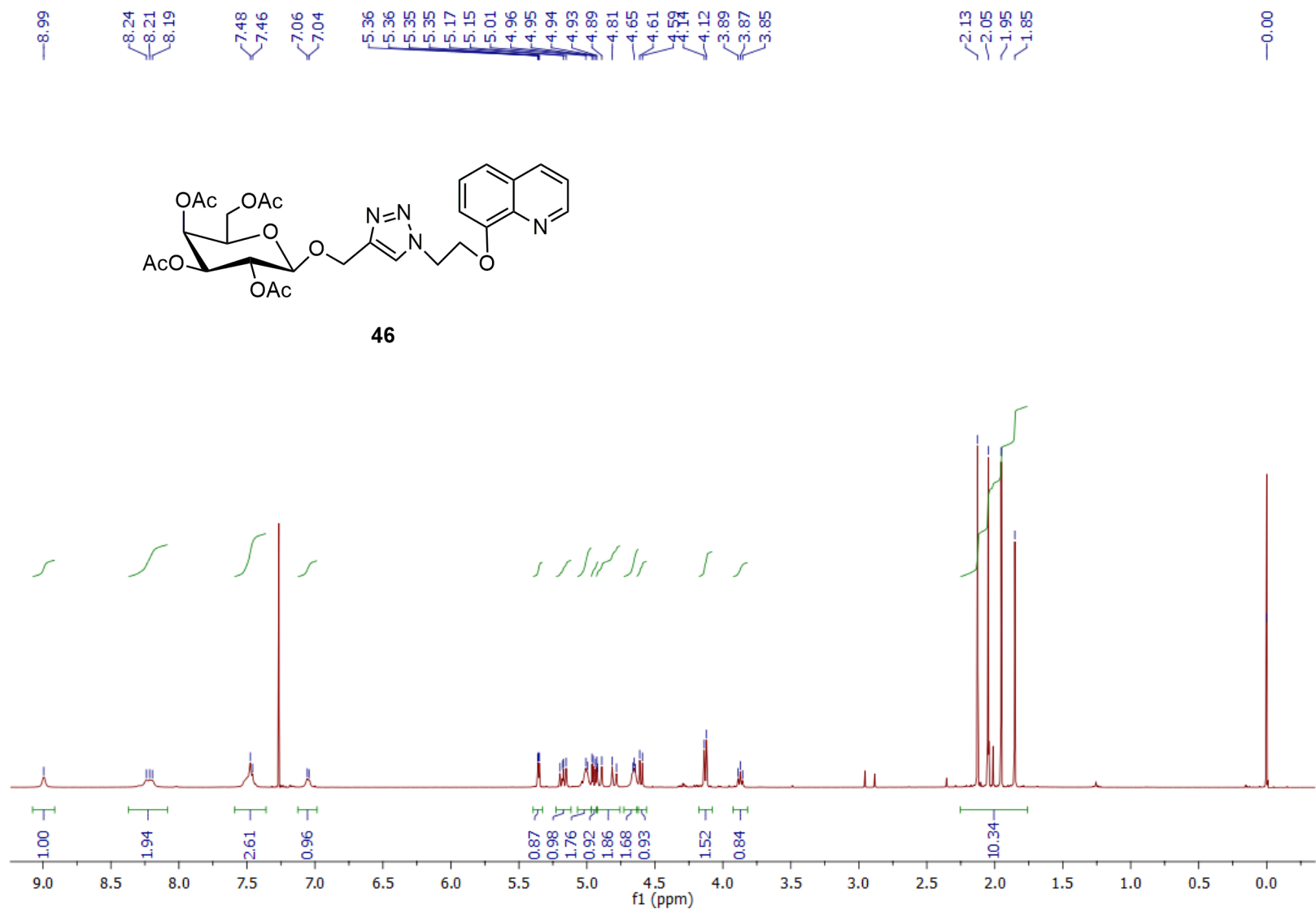


Fig. S83: ¹H NMR spectrum of glycoconjugate **46**.

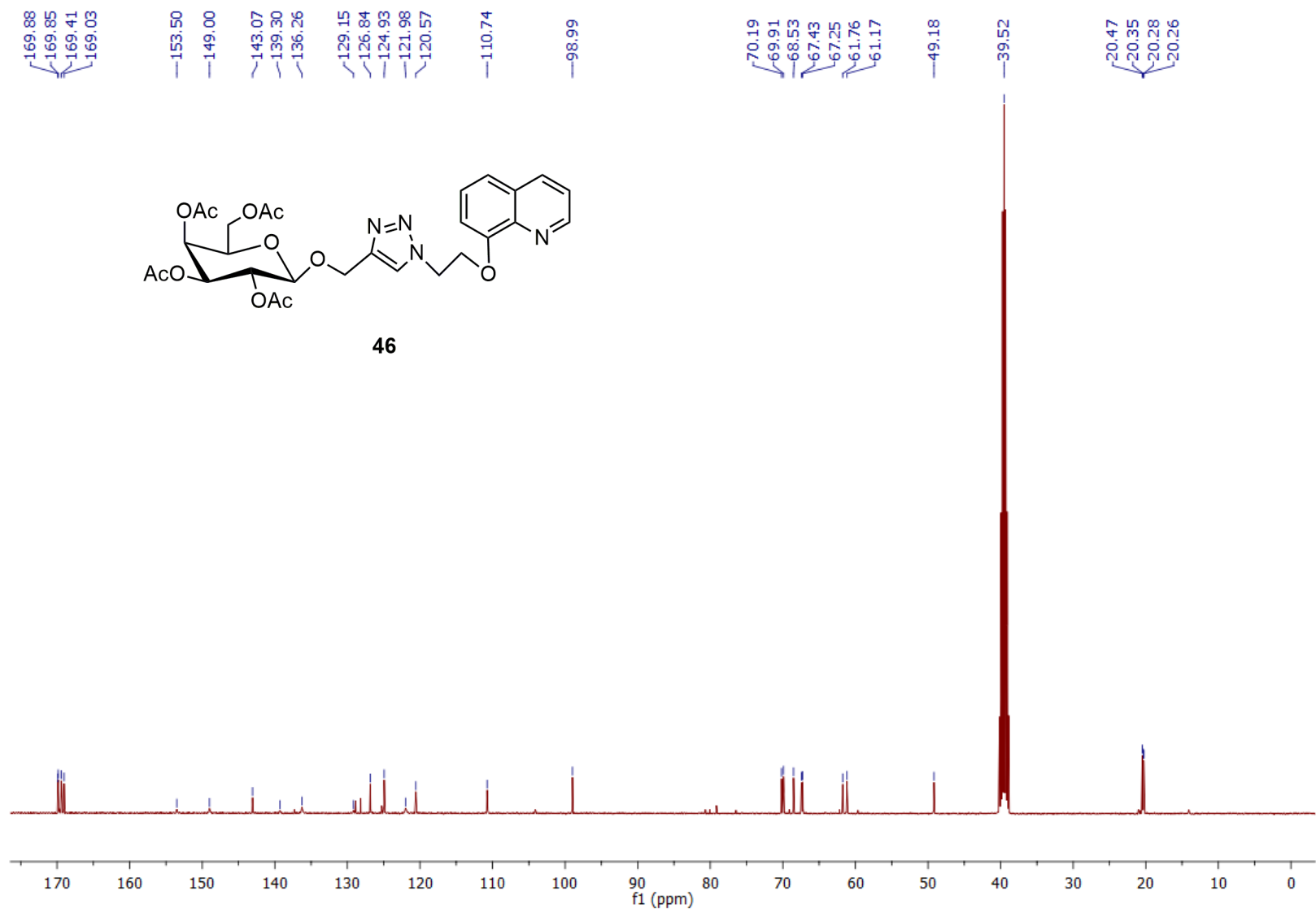


Fig. S84: ^{13}C NMR spectrum of glycoconjugate **46**.

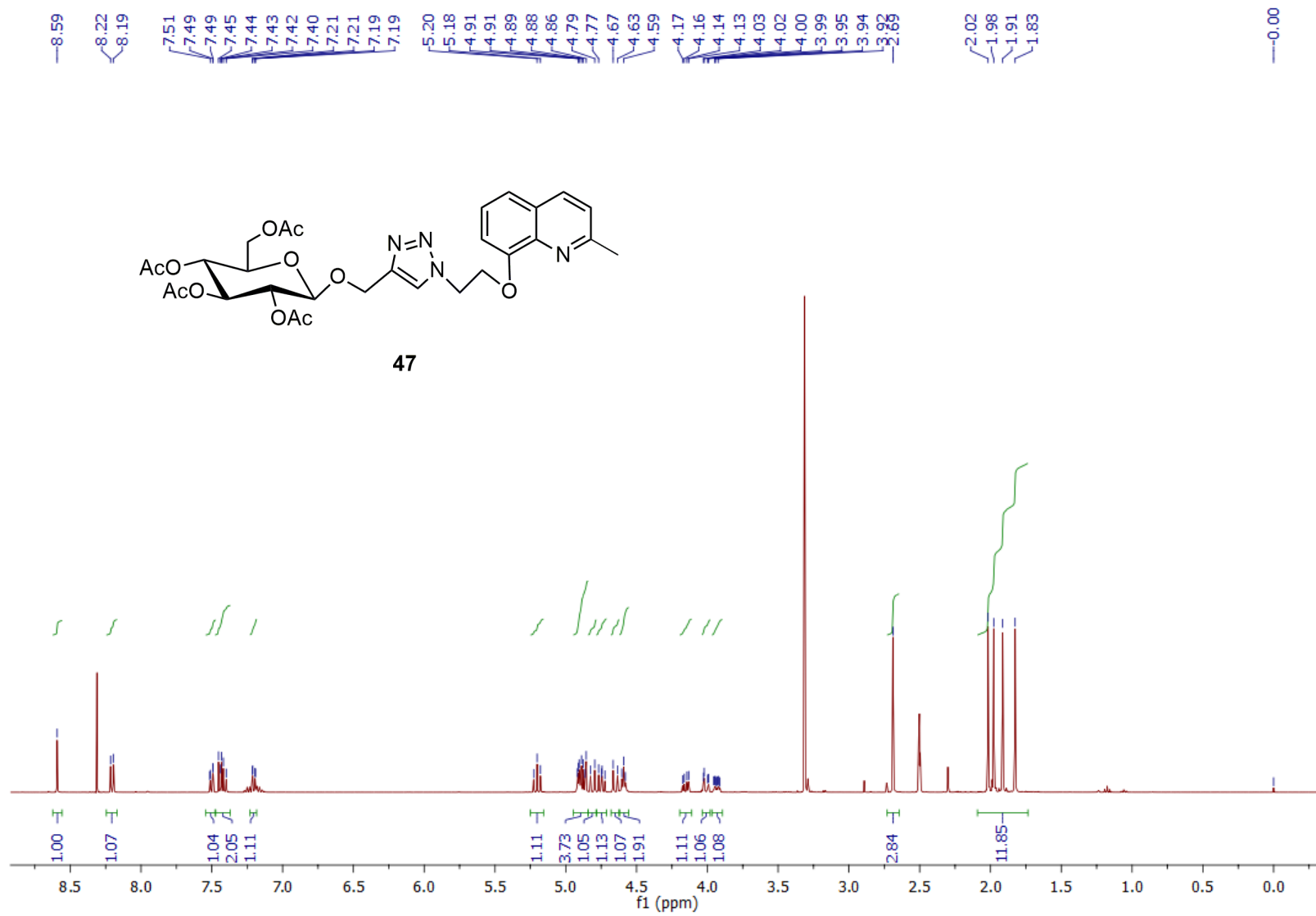


Fig. S85: ^1H NMR spectrum of glycoconjugate **47**.

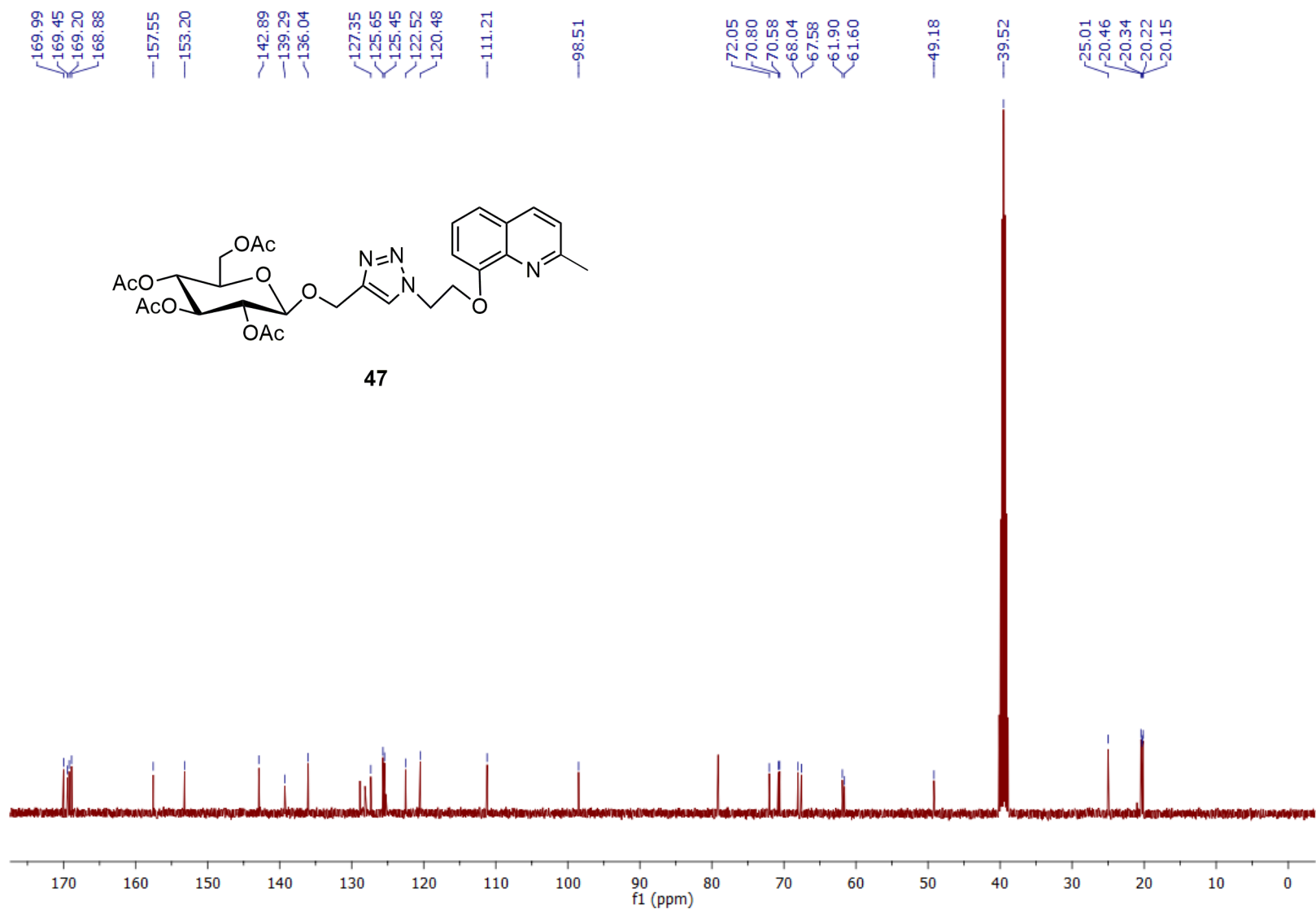


Fig. S86: ^{13}C NMR spectrum of glycoconjugate **47**.

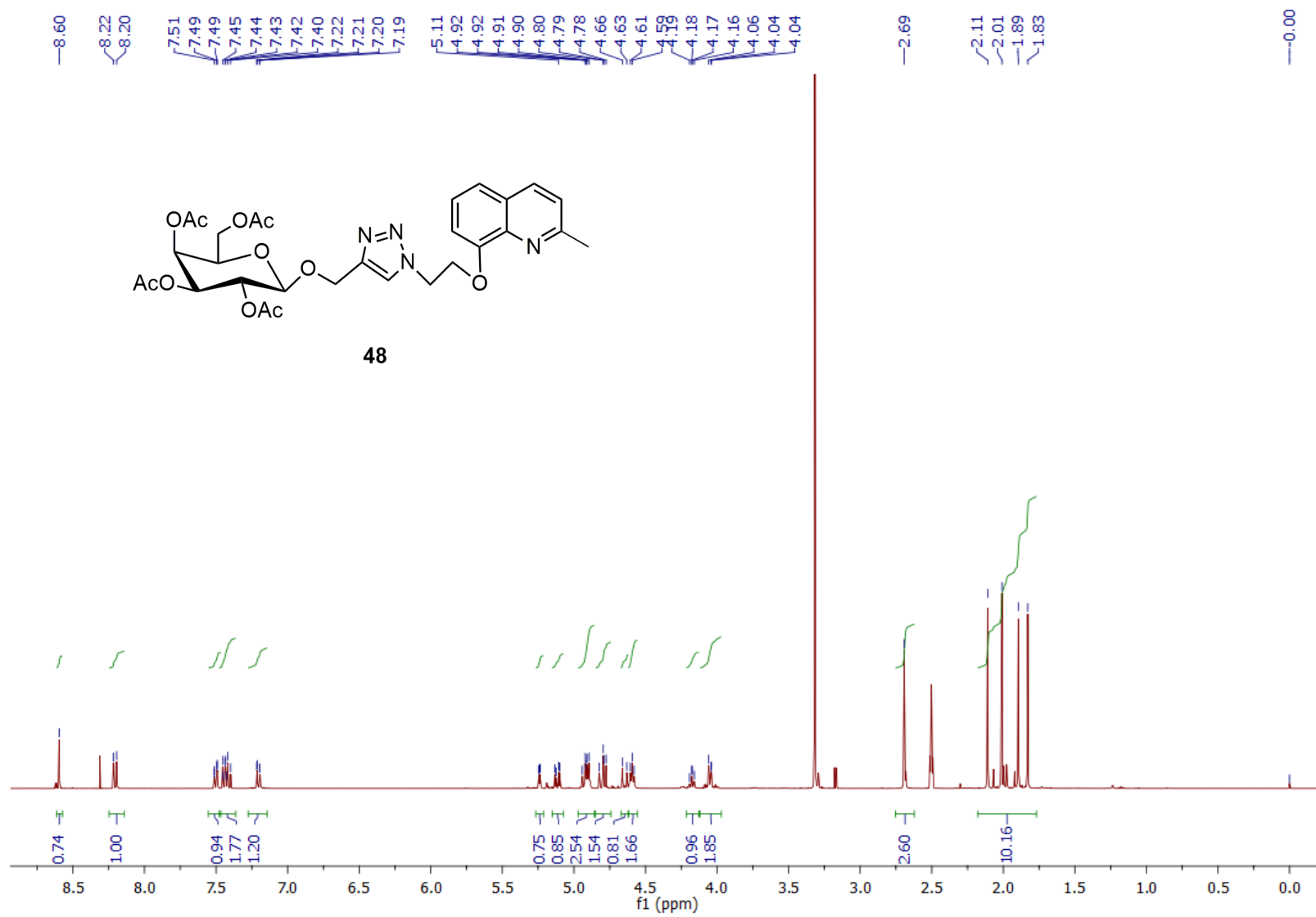


Fig. S87: ^1H NMR spectrum of glycoconjugate **48**.

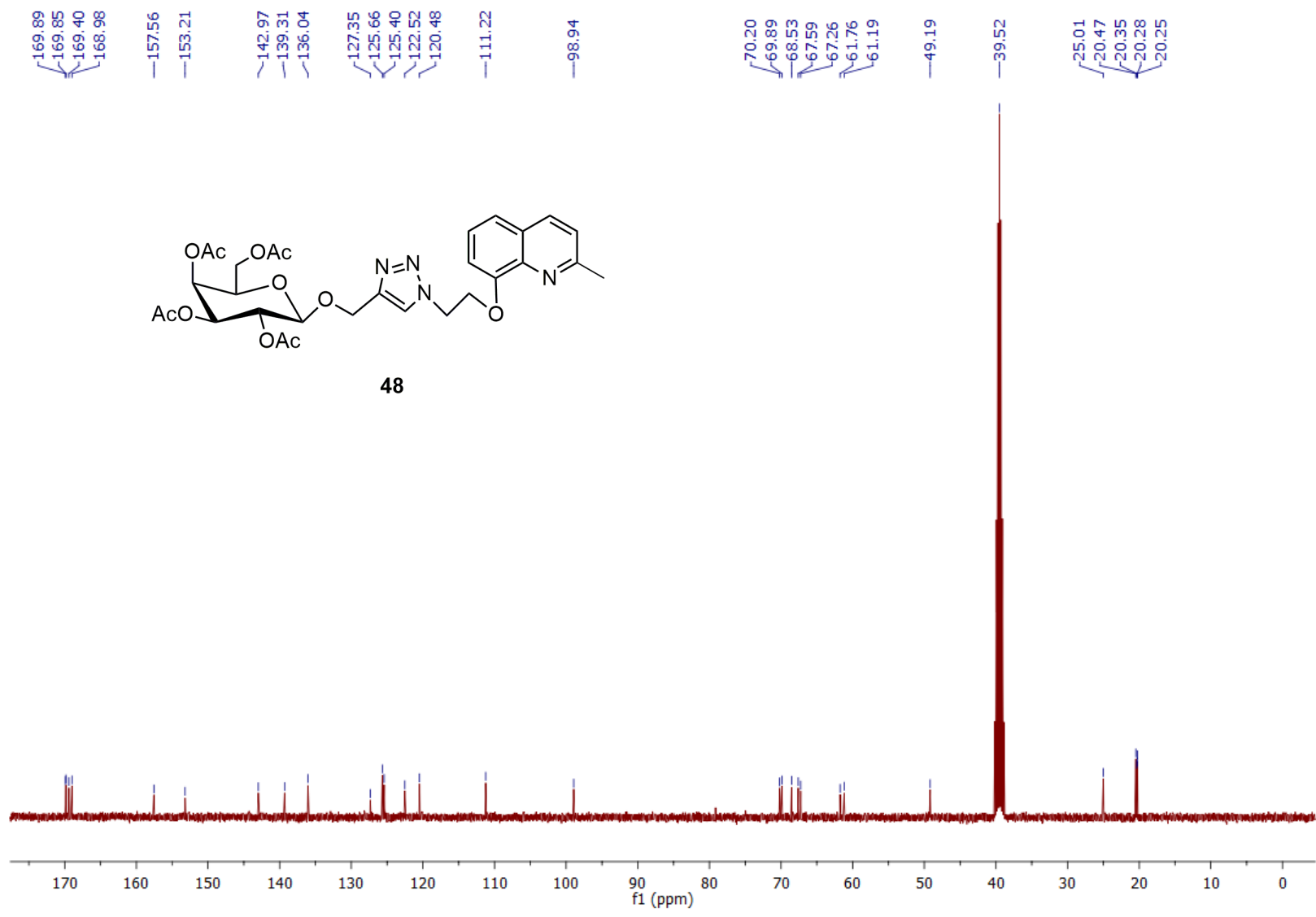


Fig. S88: ^{13}C NMR spectrum of glycoconjugate **48**.

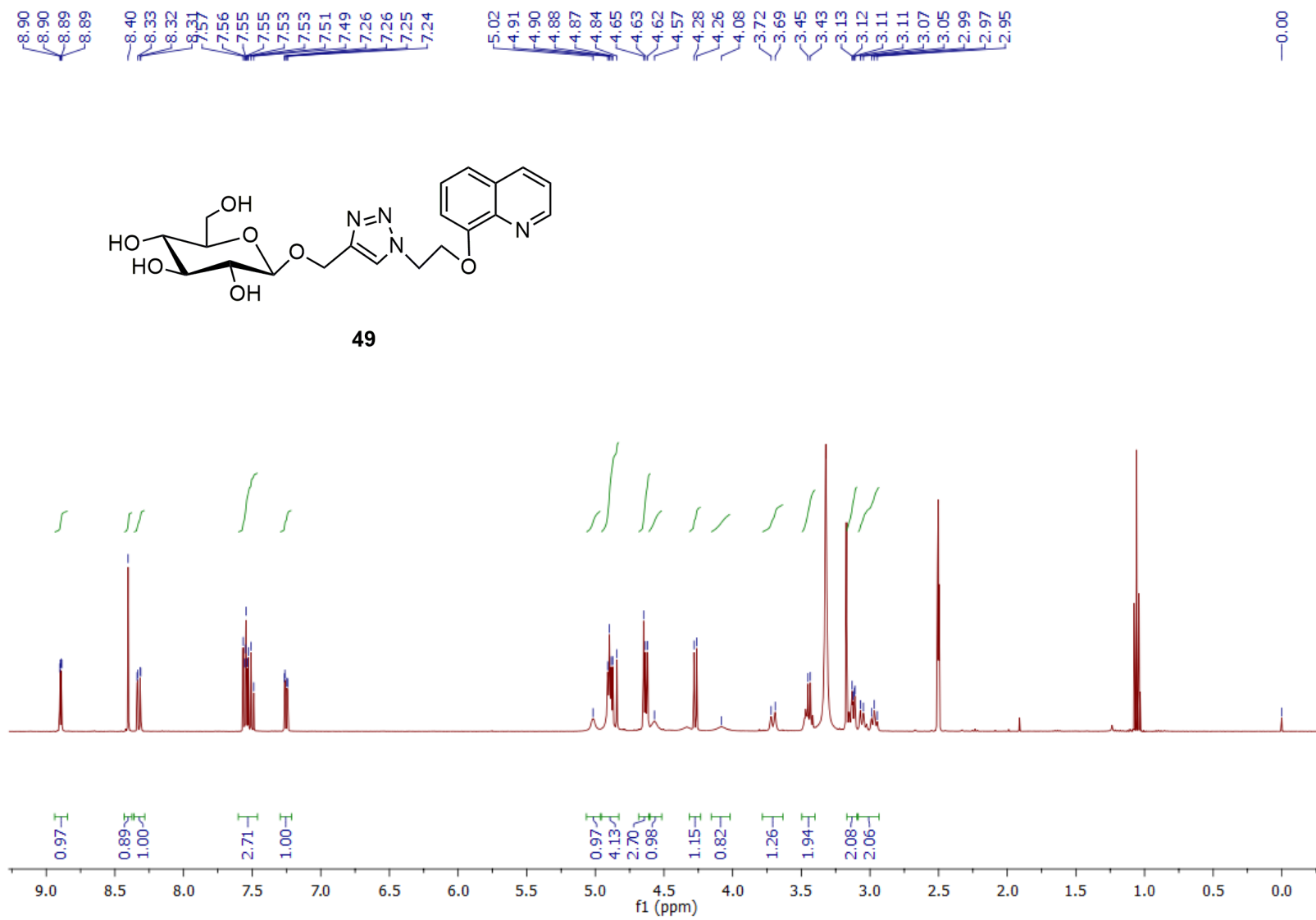


Fig. S89: ^1H NMR spectrum of glycoconjugate **49**.

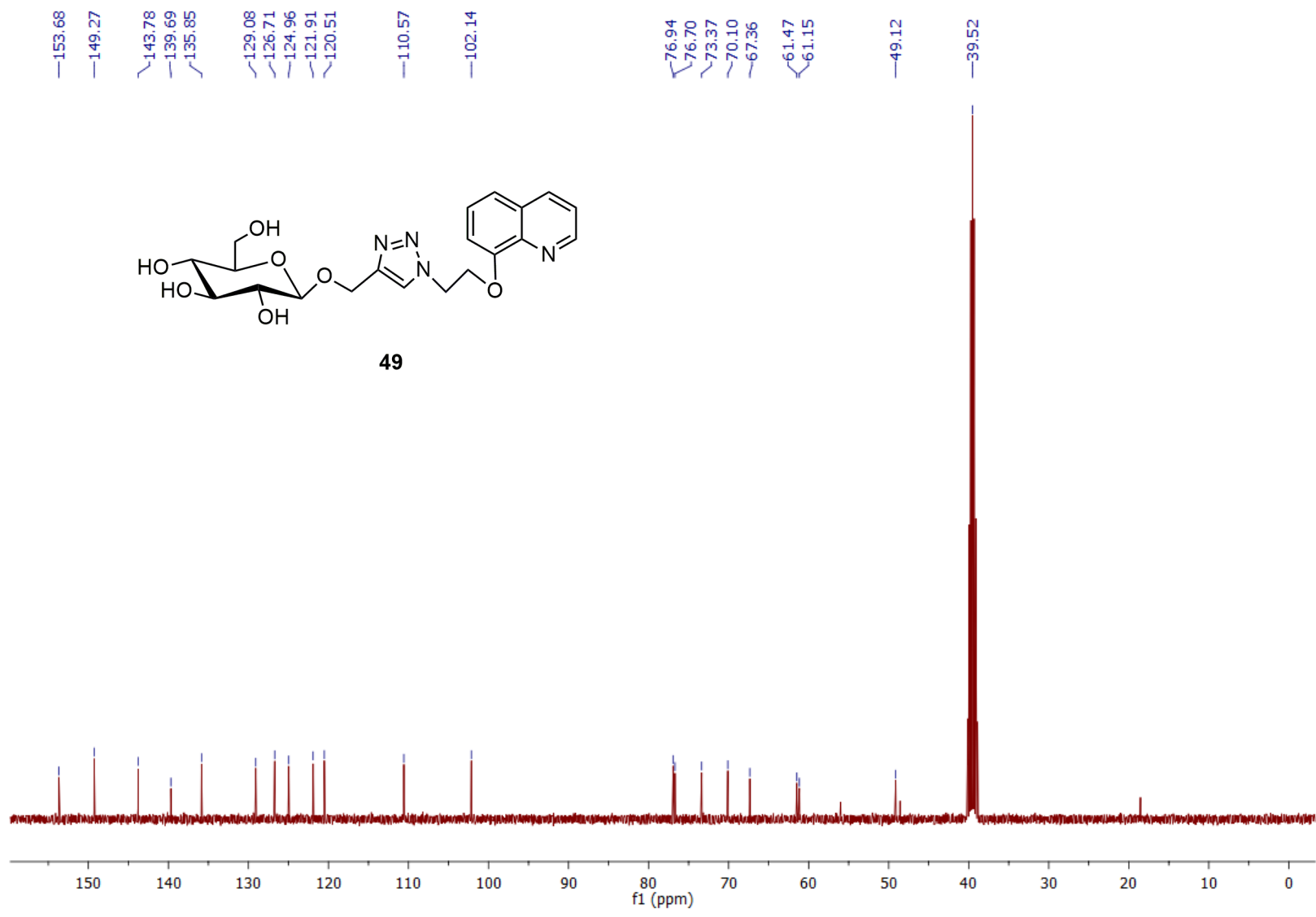


Fig. S90: ^{13}C NMR spectrum of glycoconjugate **49**.

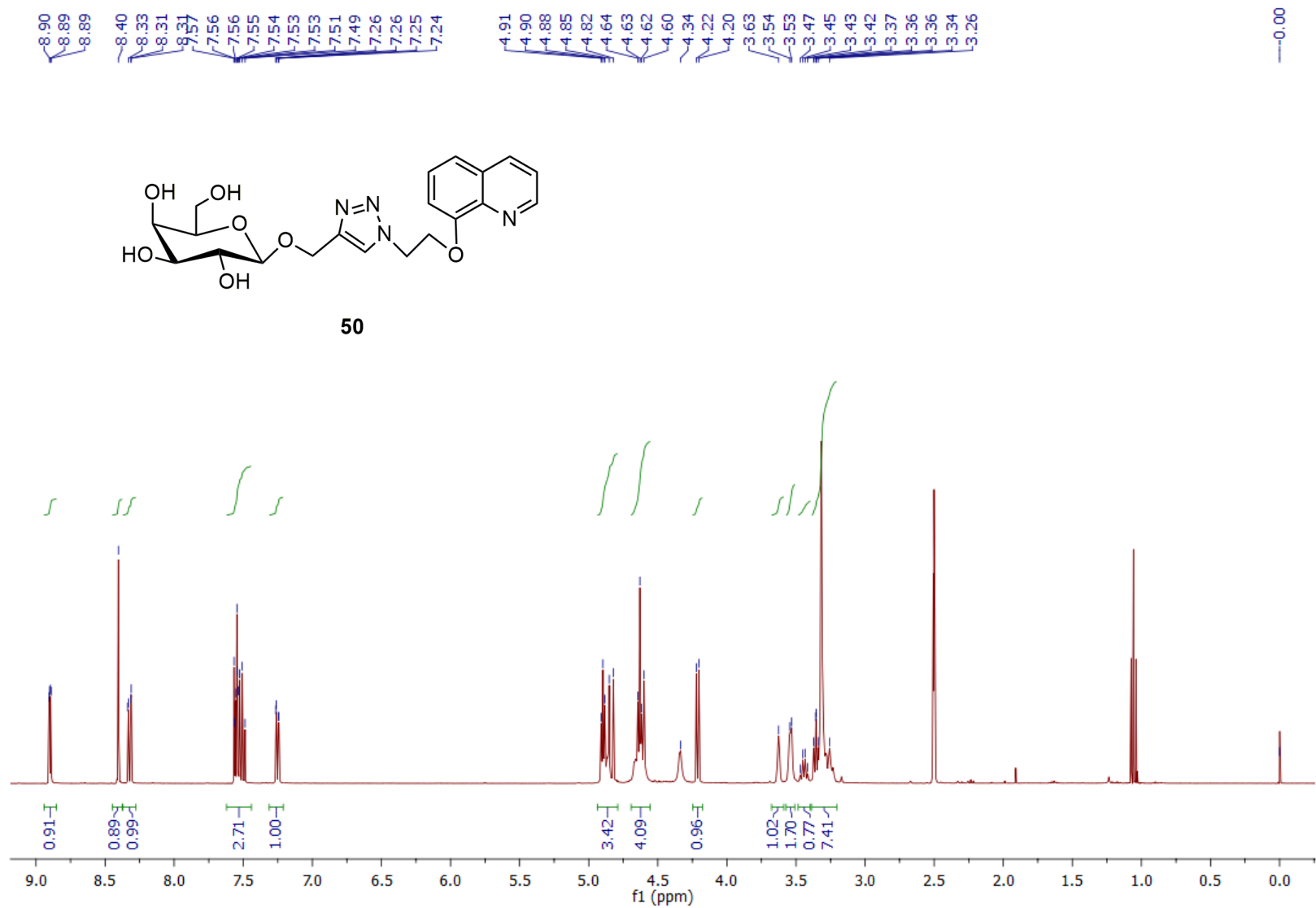


Fig. S91: ¹H NMR spectrum of glycoconjugate **50**.

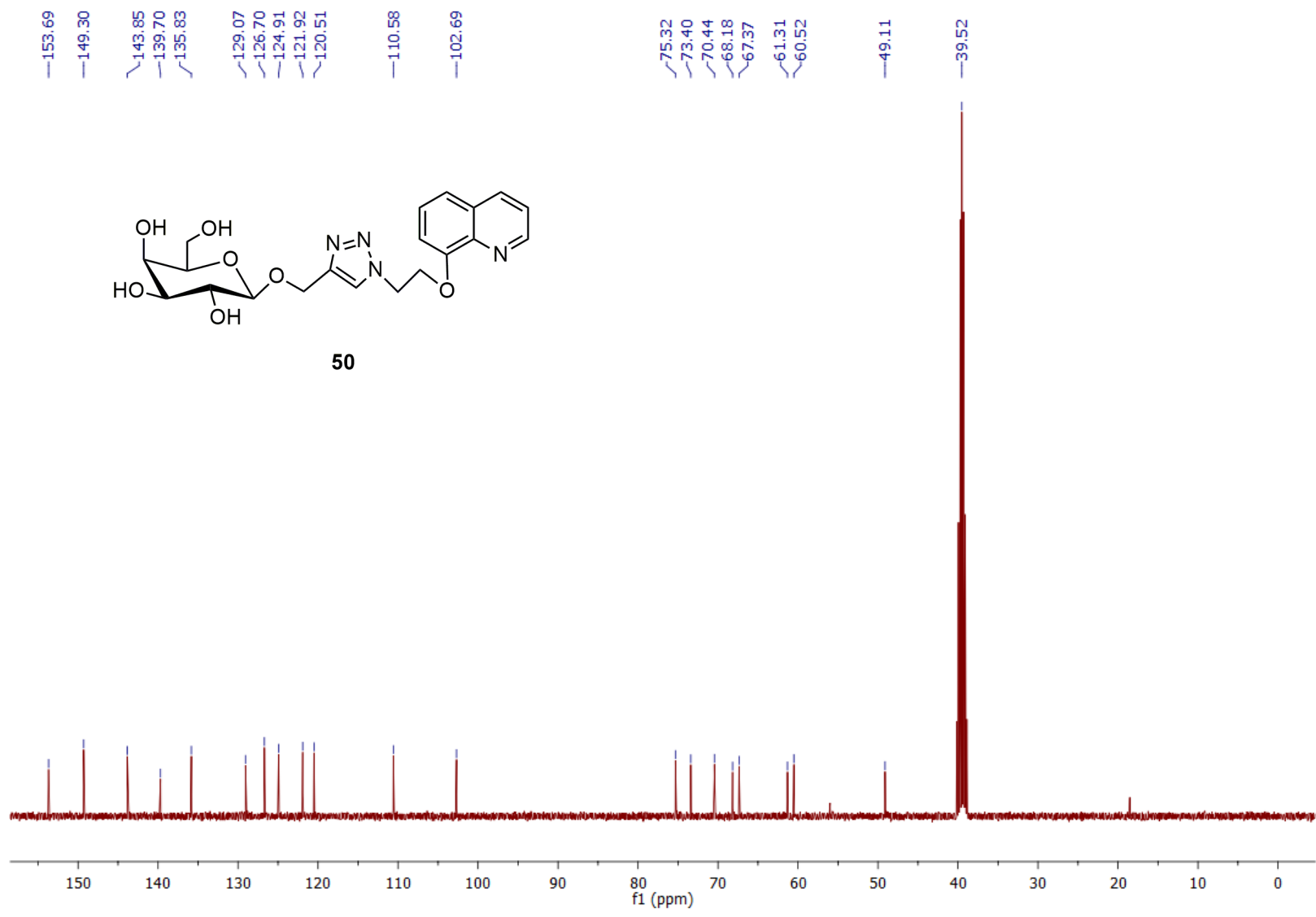


Fig. S92: ^{13}C NMR spectrum of glycoconjugate **50**.

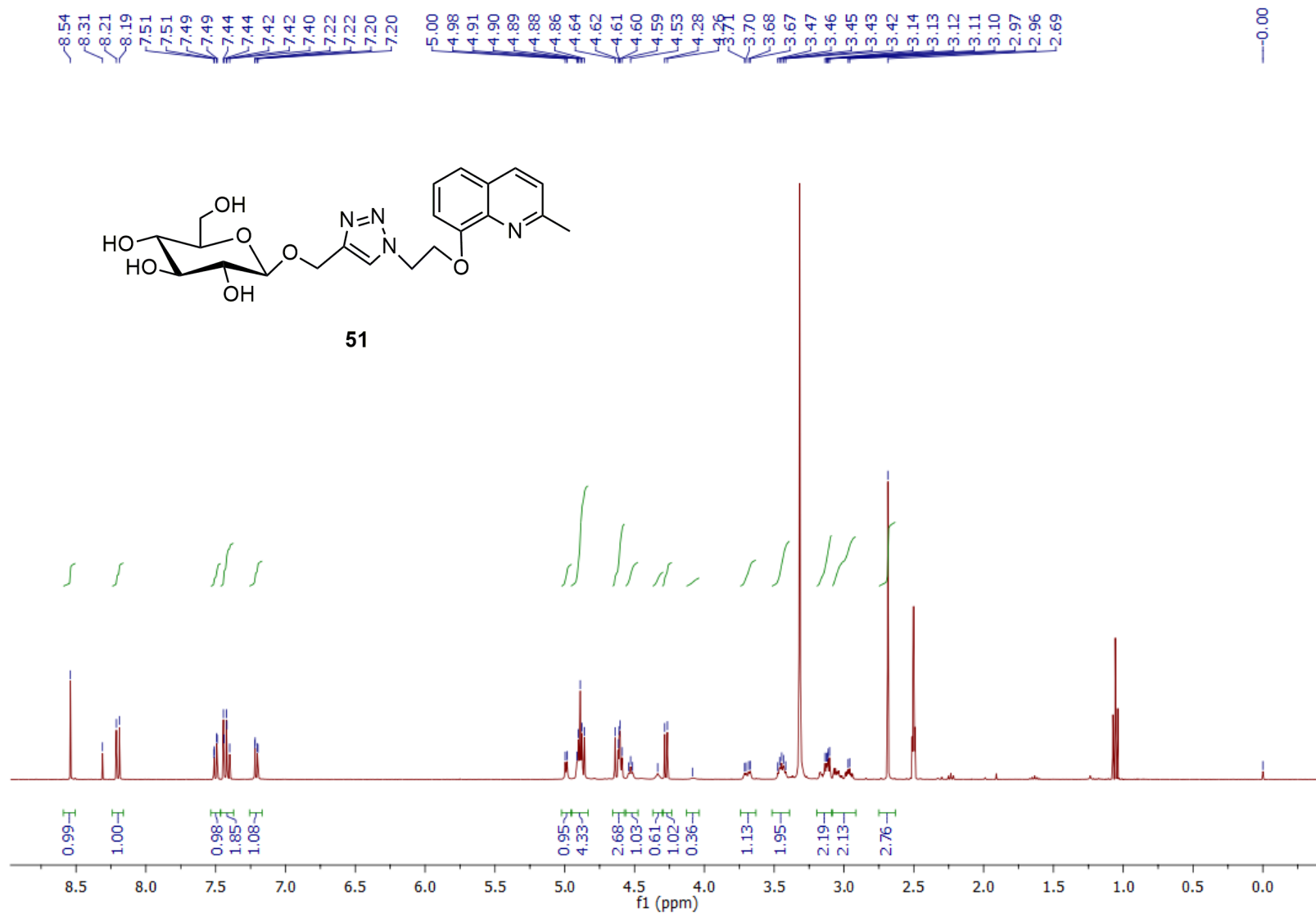


Fig. S93: ^1H NMR spectrum of glycoconjugate **51**.

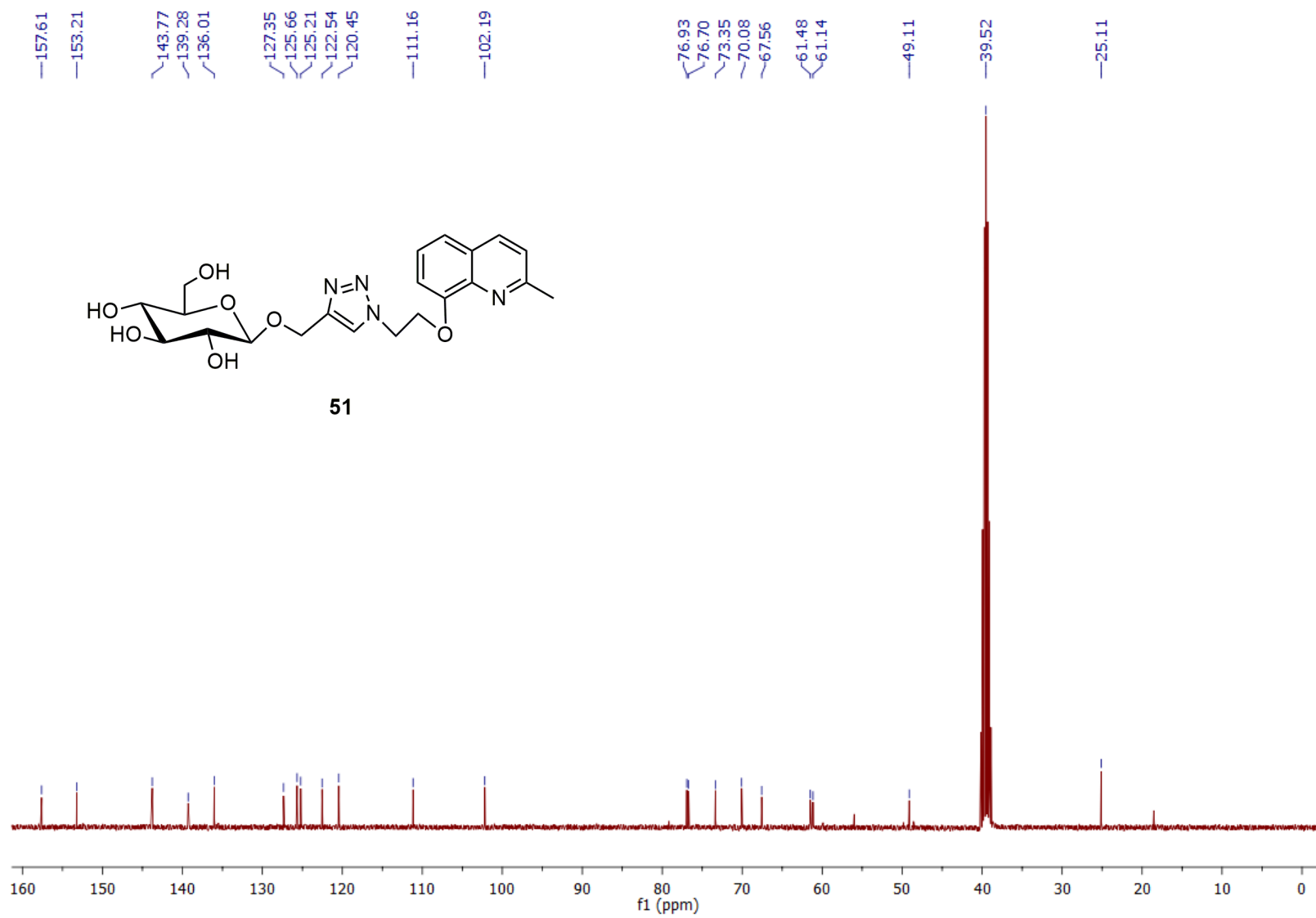


Fig. S94: ^{13}C NMR spectrum of glycoconjugate **51**.

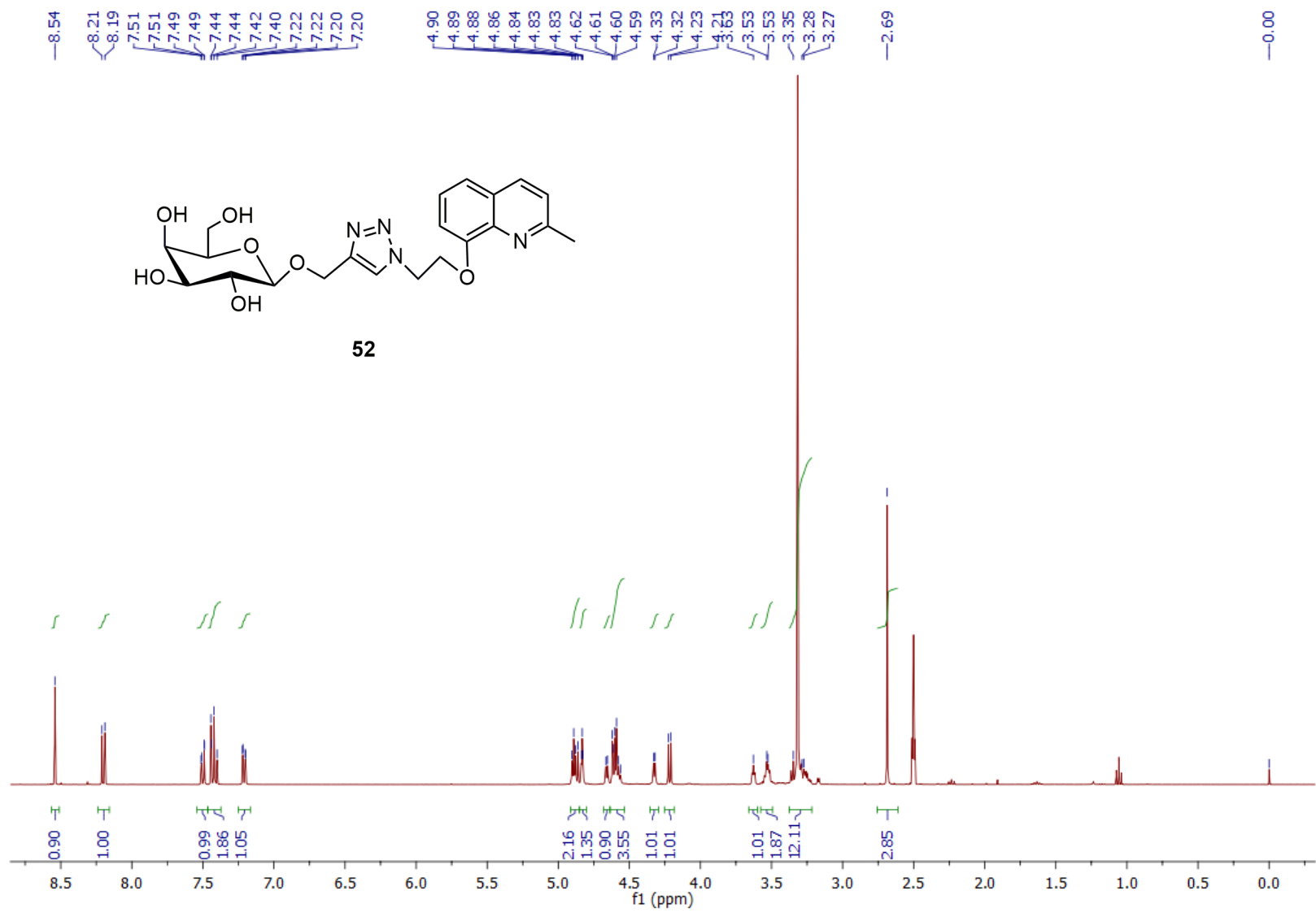


Fig. S95: ^1H NMR spectrum of glycoconjugate **52**.

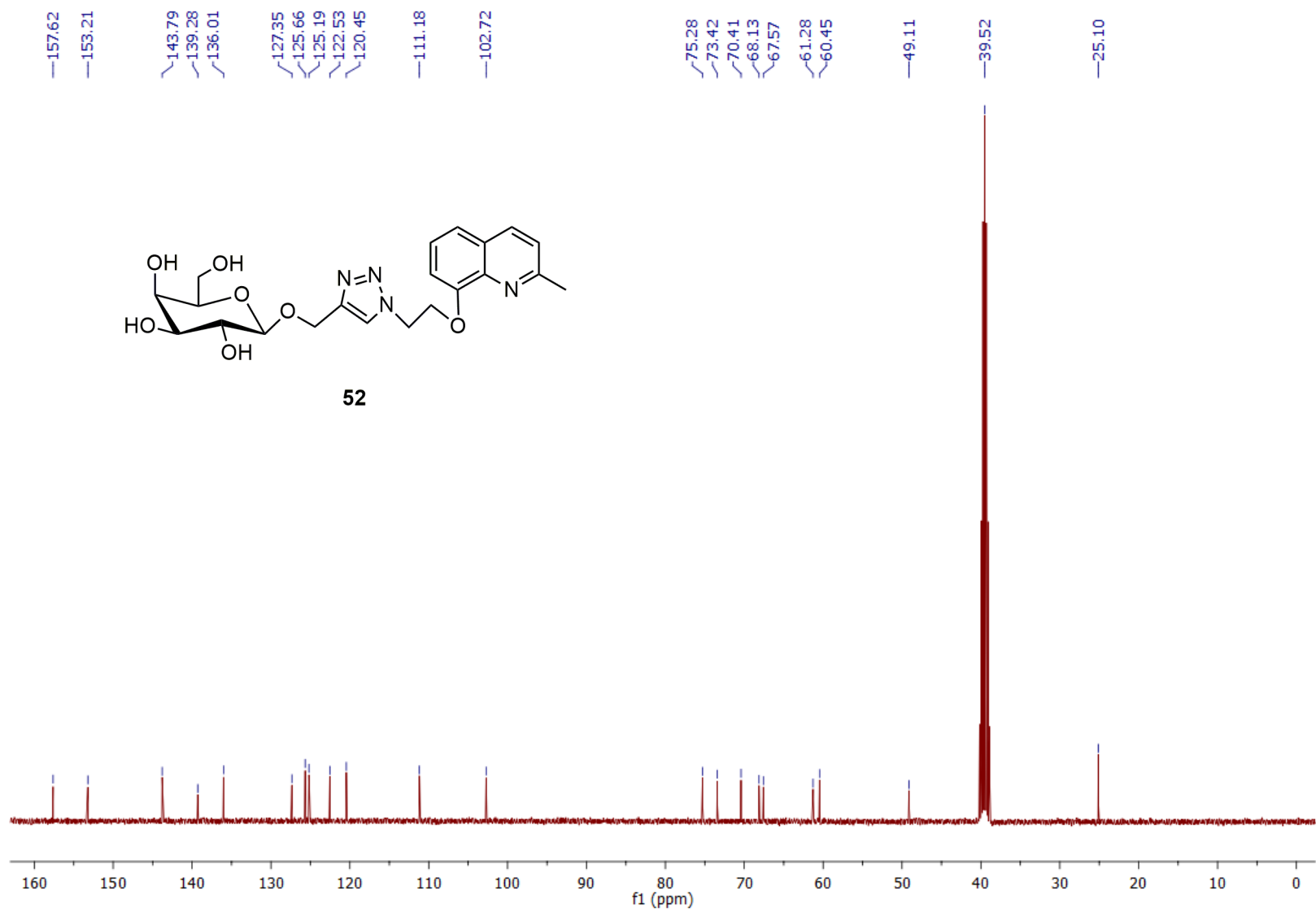


Fig. S96: ^{13}C NMR spectrum of glycoconjugate **52**.

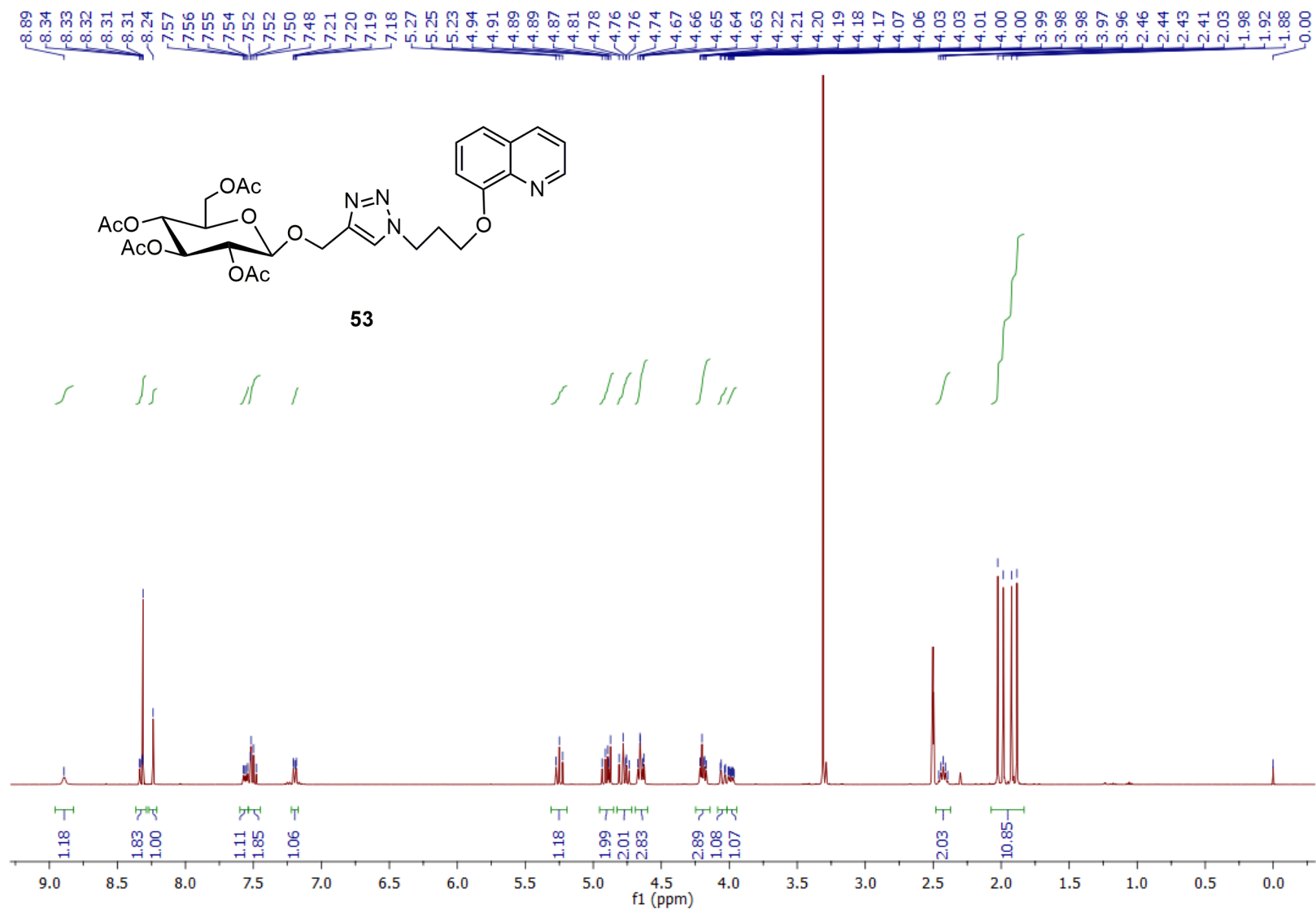


Fig. S97: ^1H NMR spectrum of glycoconjugate **53**.

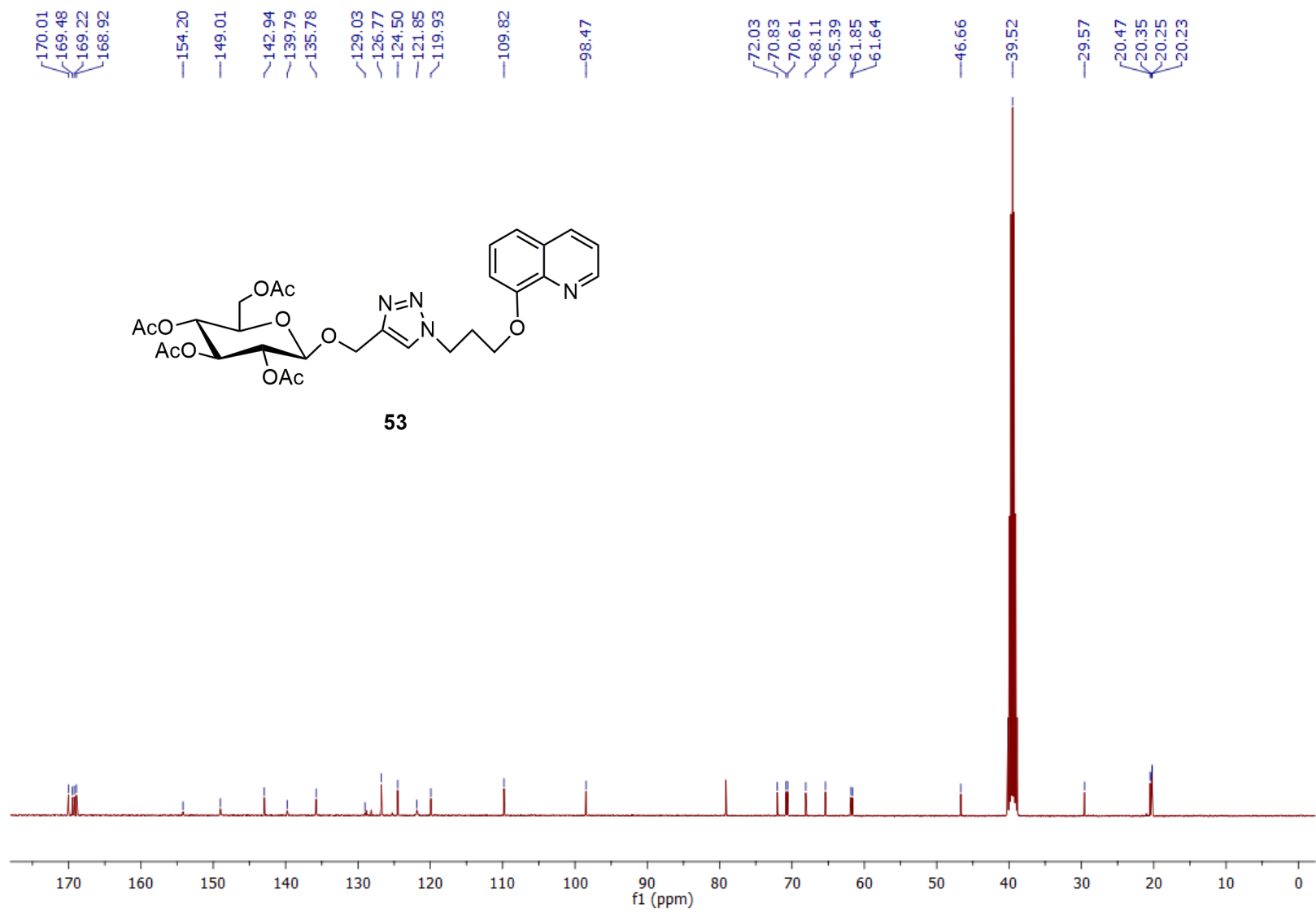


Fig. S98: ^{13}C NMR spectrum of glycoconjugate **53**.

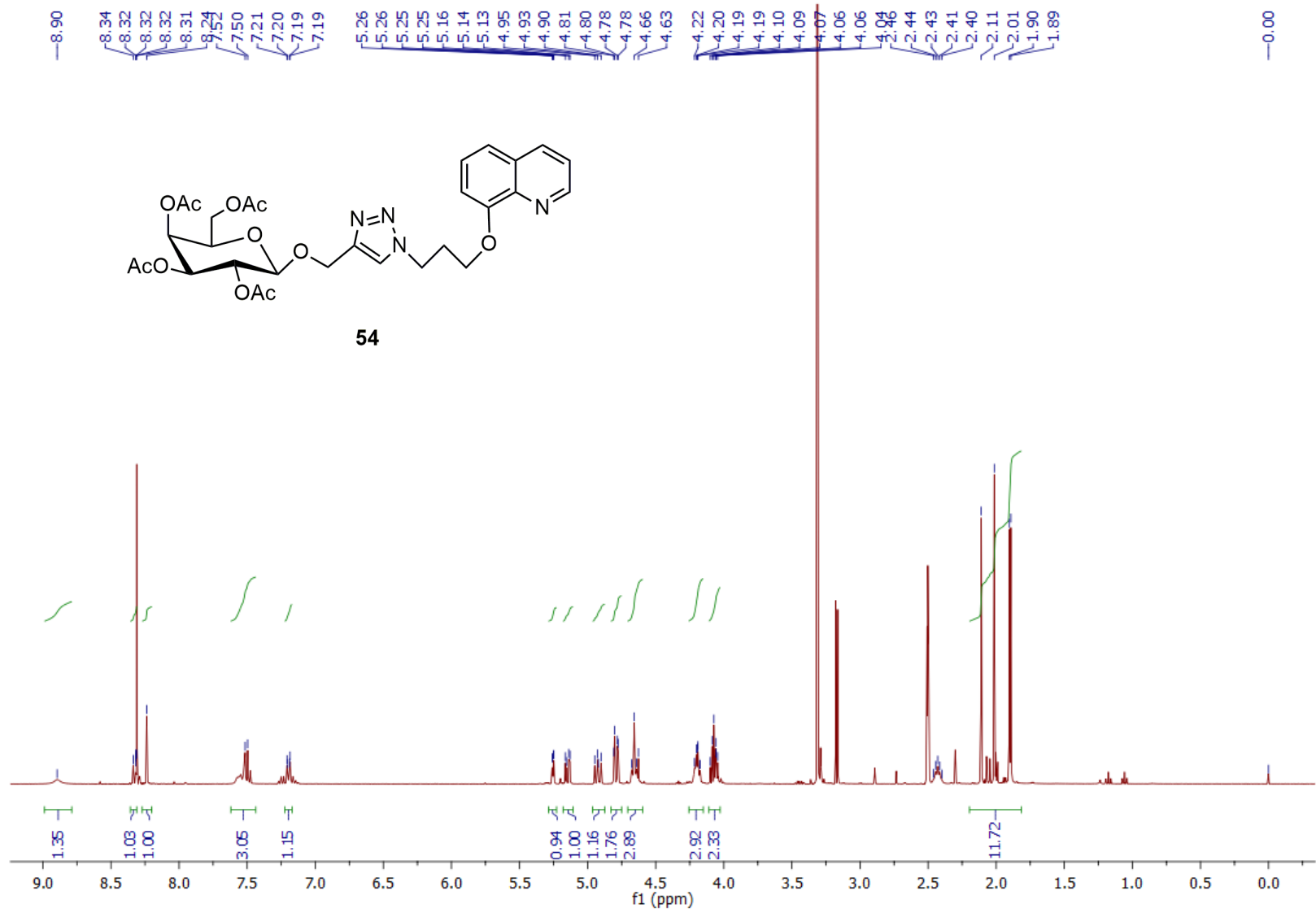


Fig. S99: ^1H NMR spectrum of glycoconjugate **54**.

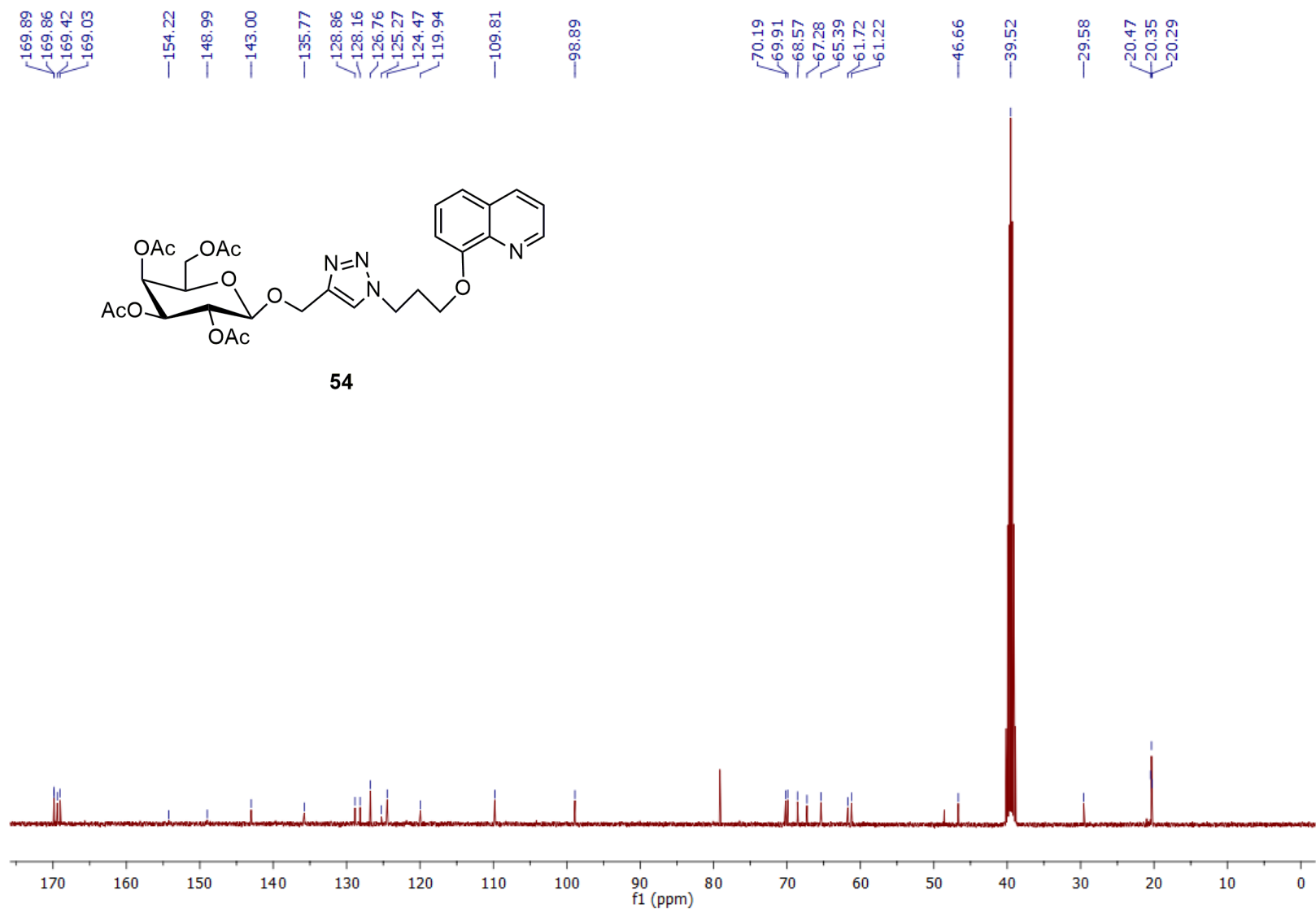


Fig. S100: ^{13}C NMR spectrum of glycoconjugate **54**.

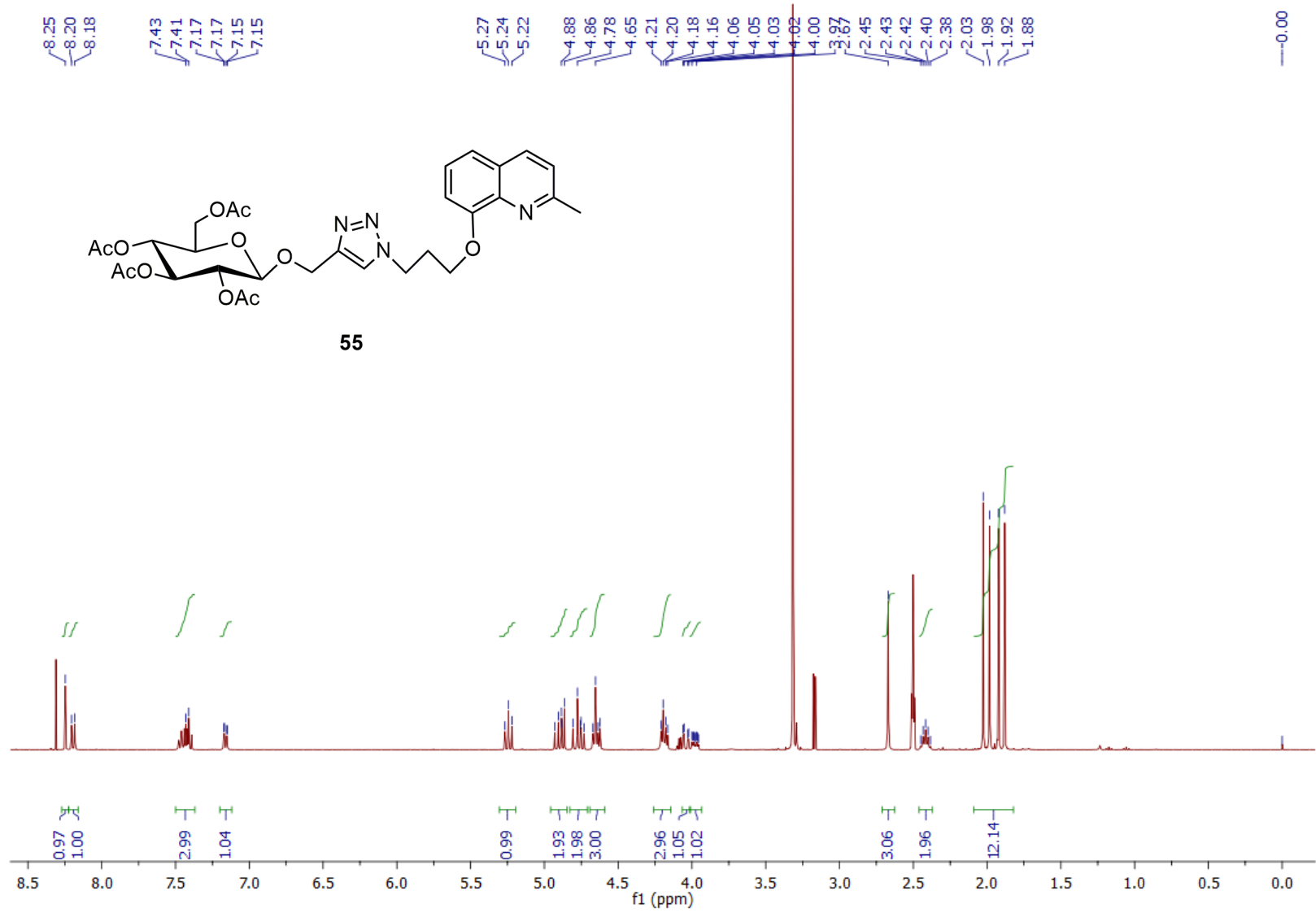


Fig. S101: ^1H NMR spectrum of glycoconjugate **55**.

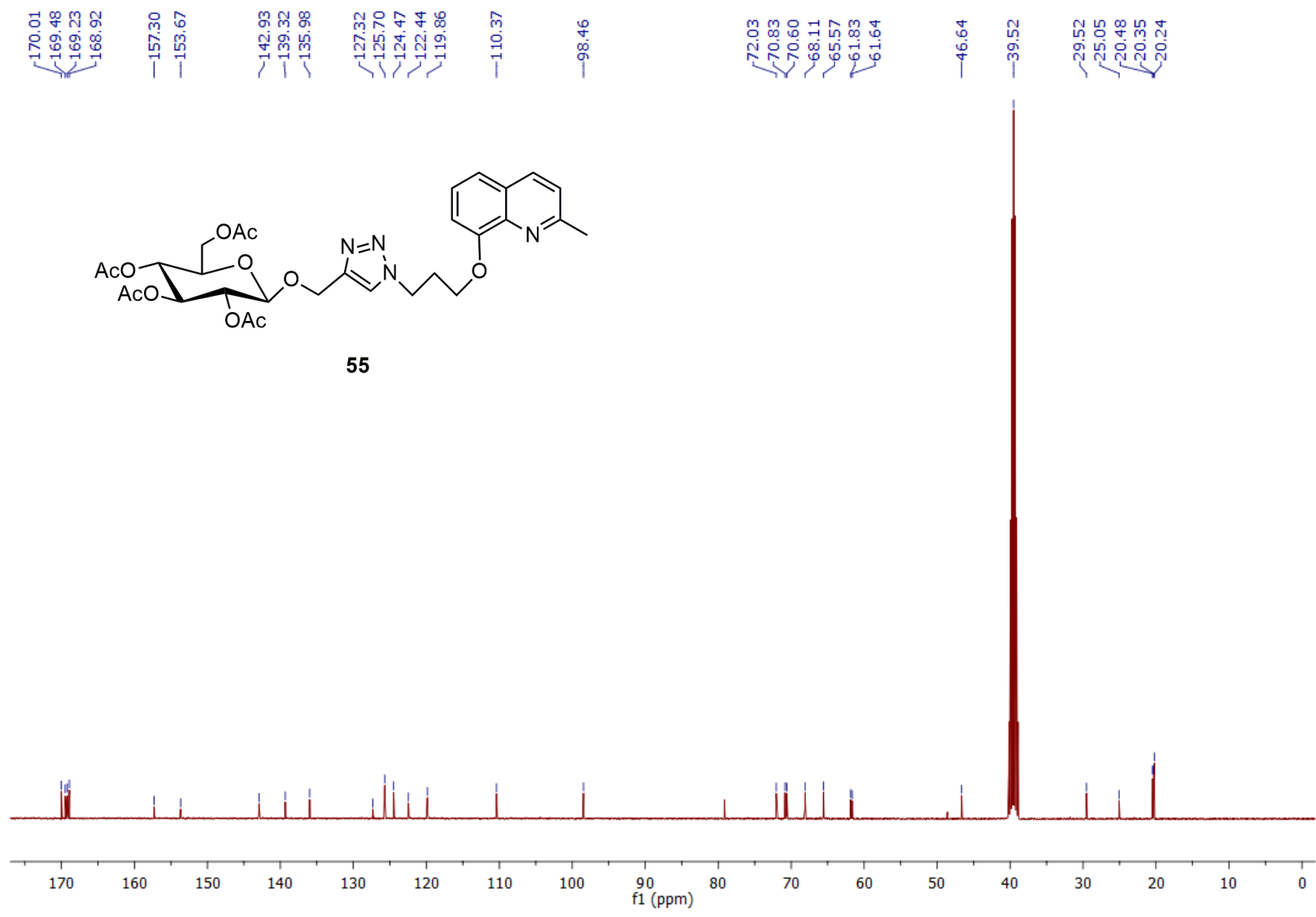


Fig. S102: ¹³C NMR spectrum of glycoconjugate **55**.

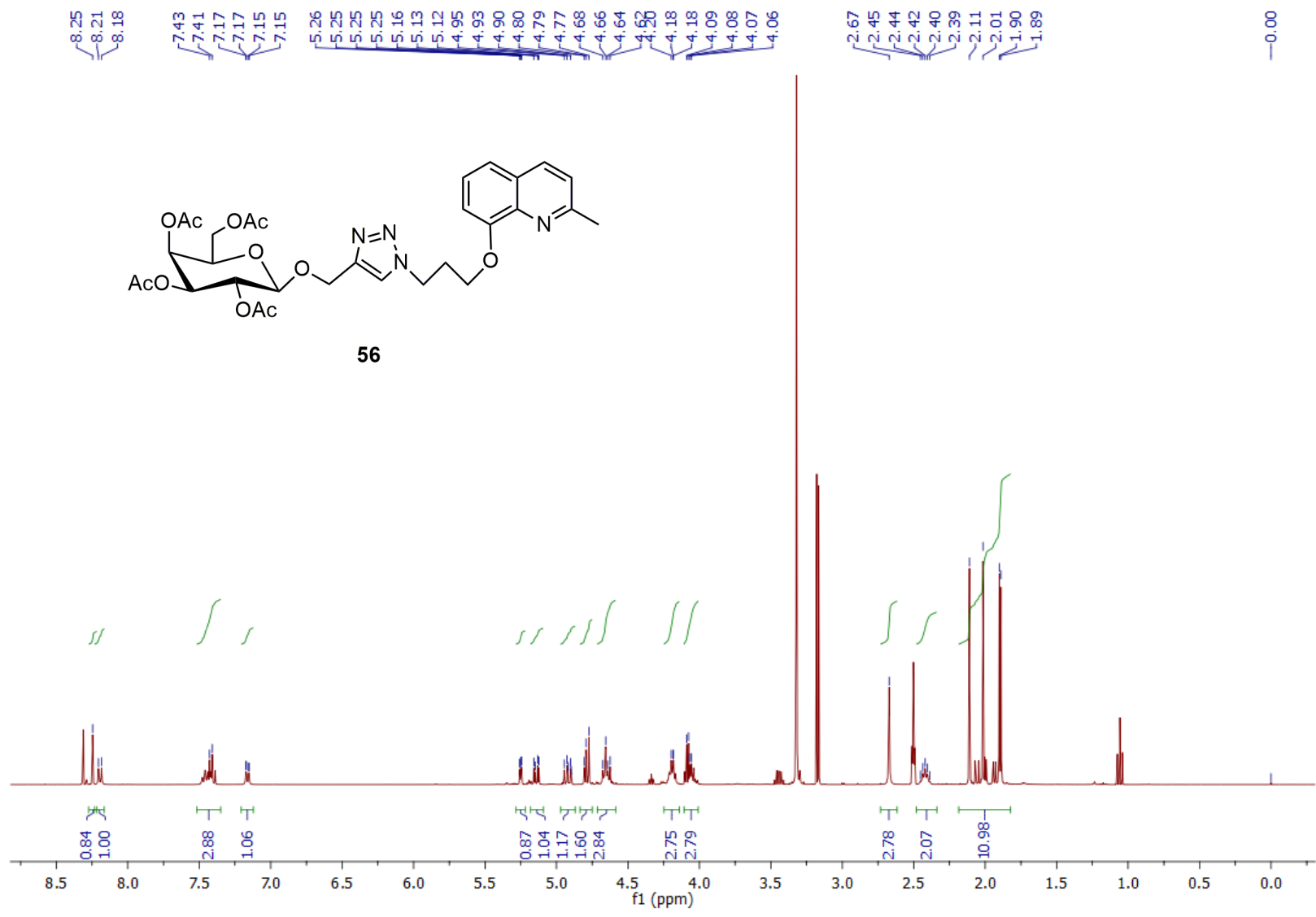


Fig. S103: ¹H NMR spectrum of glycoconjugate **56**.

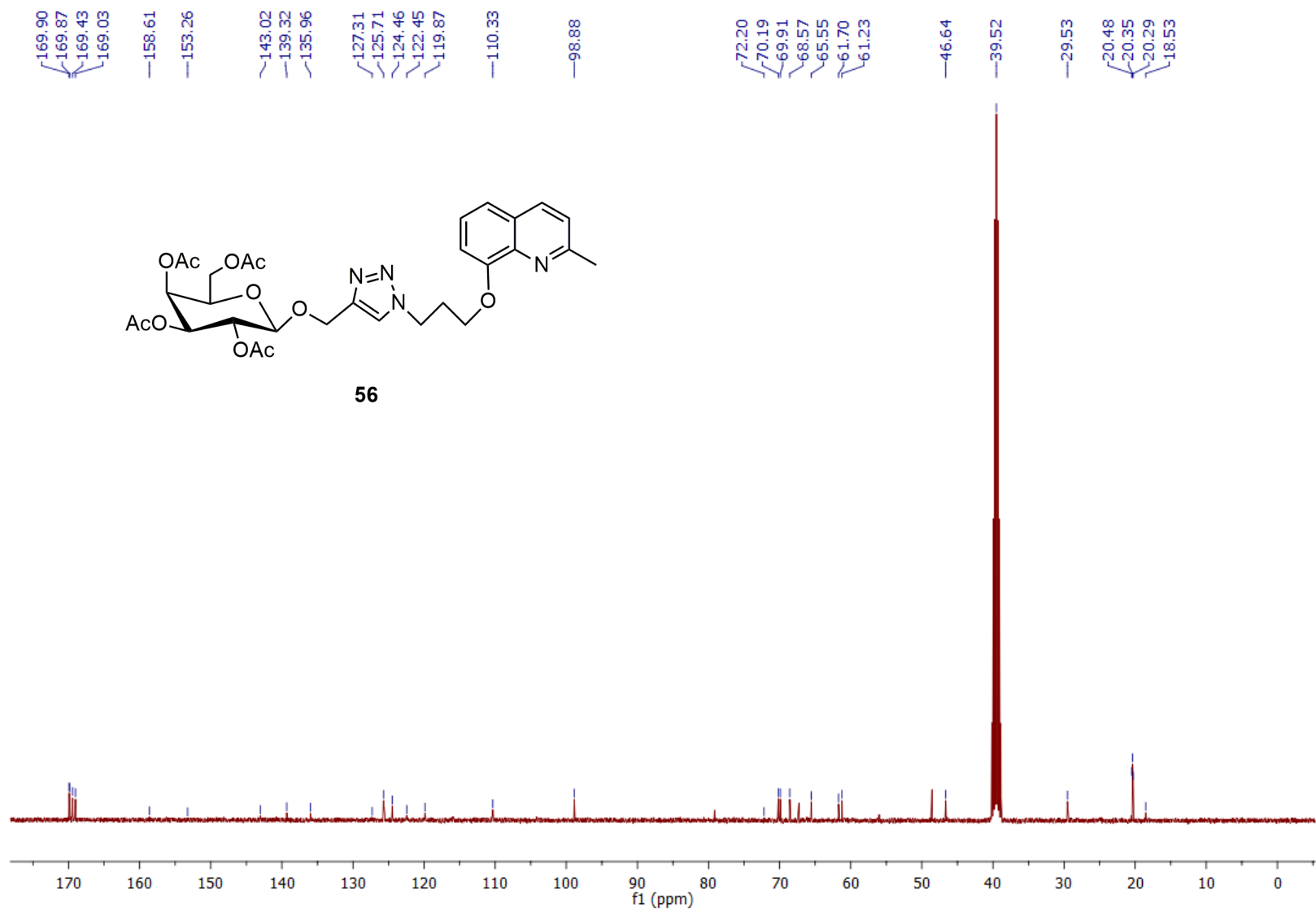


Fig. S104: ^{13}C NMR spectrum of glycoconjugate **56**.

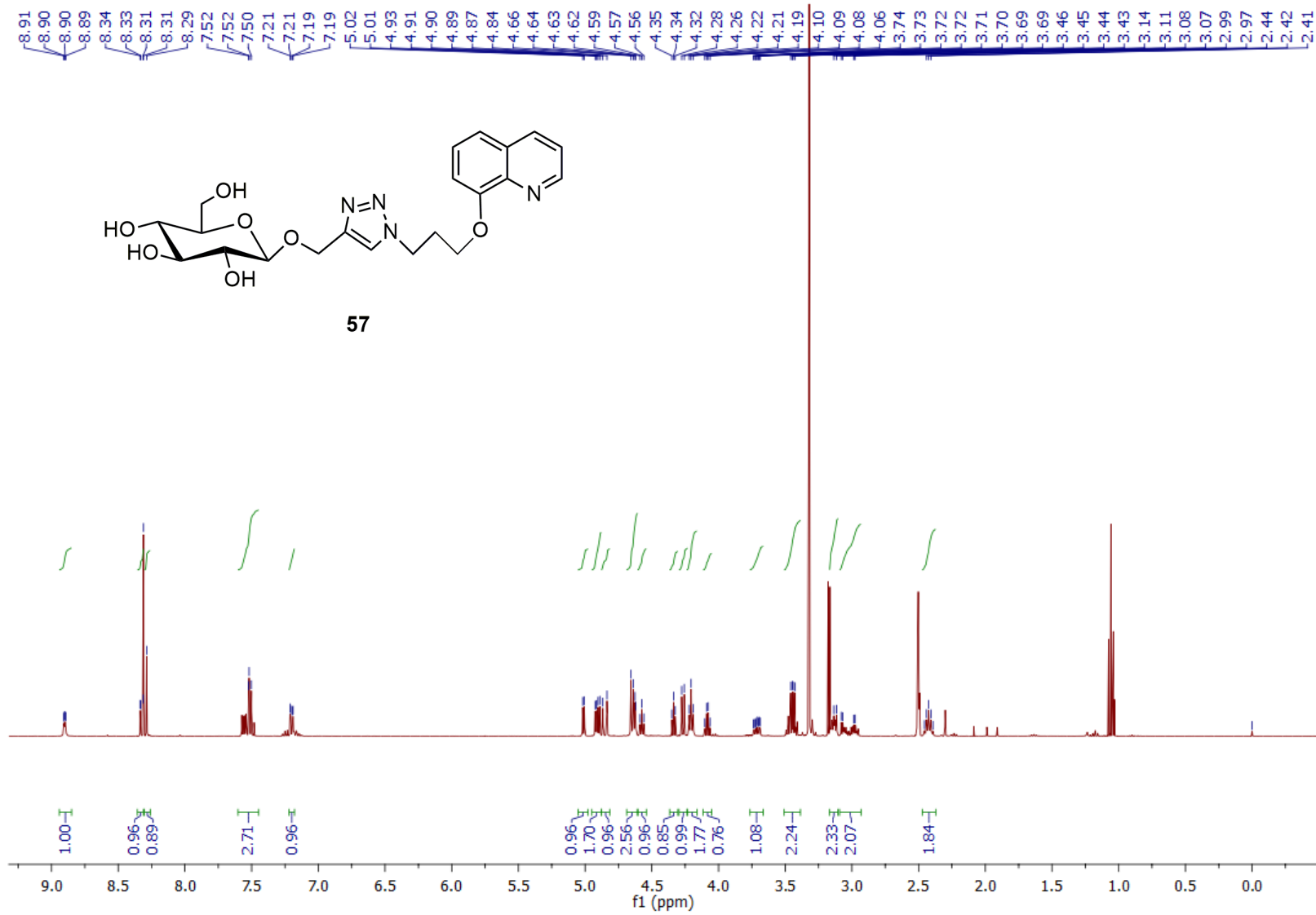


Fig. S105: ^1H NMR spectrum of glycoconjugate **57**.

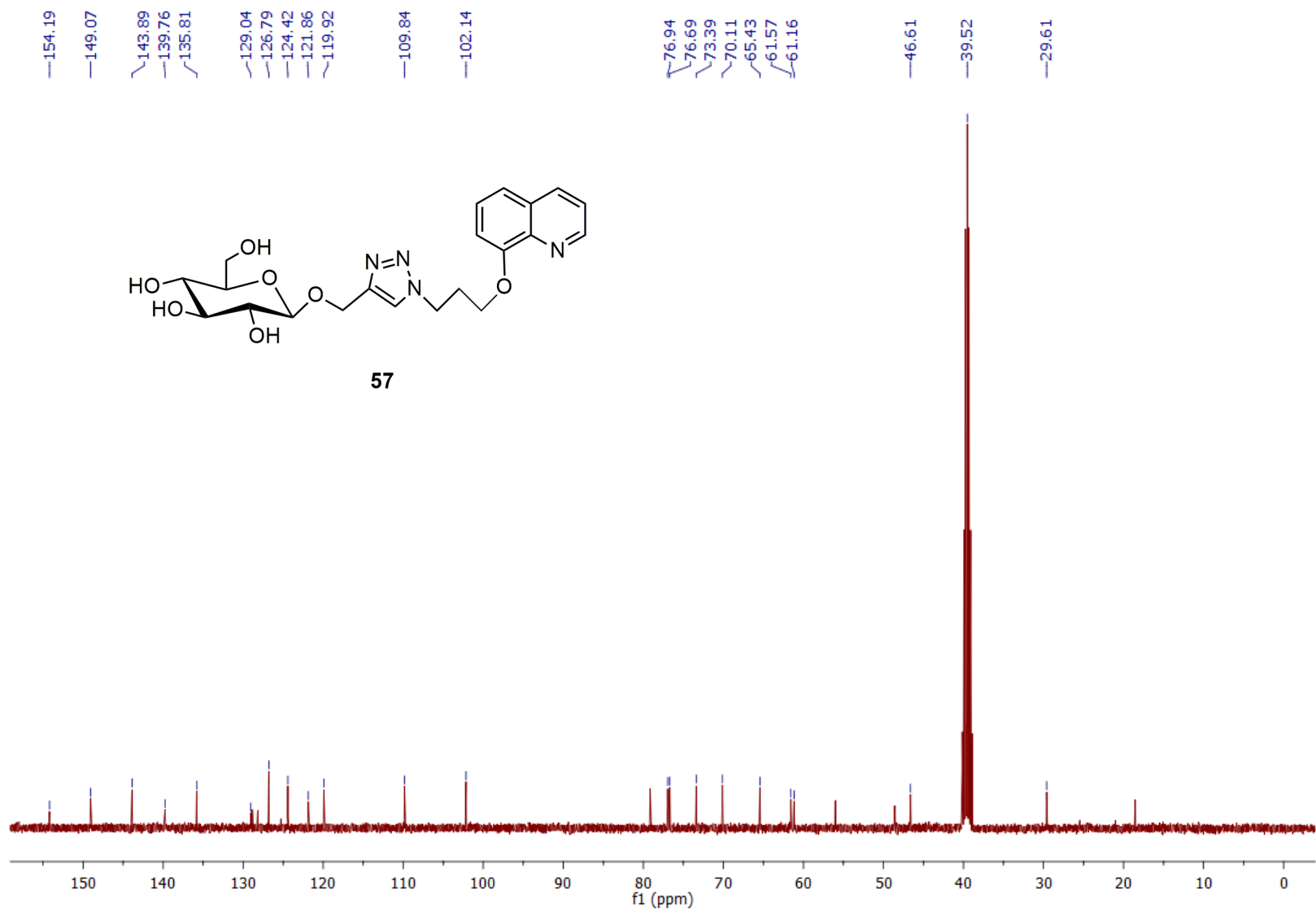


Fig. S106: ¹³C NMR spectrum of glycoconjugate **57**.

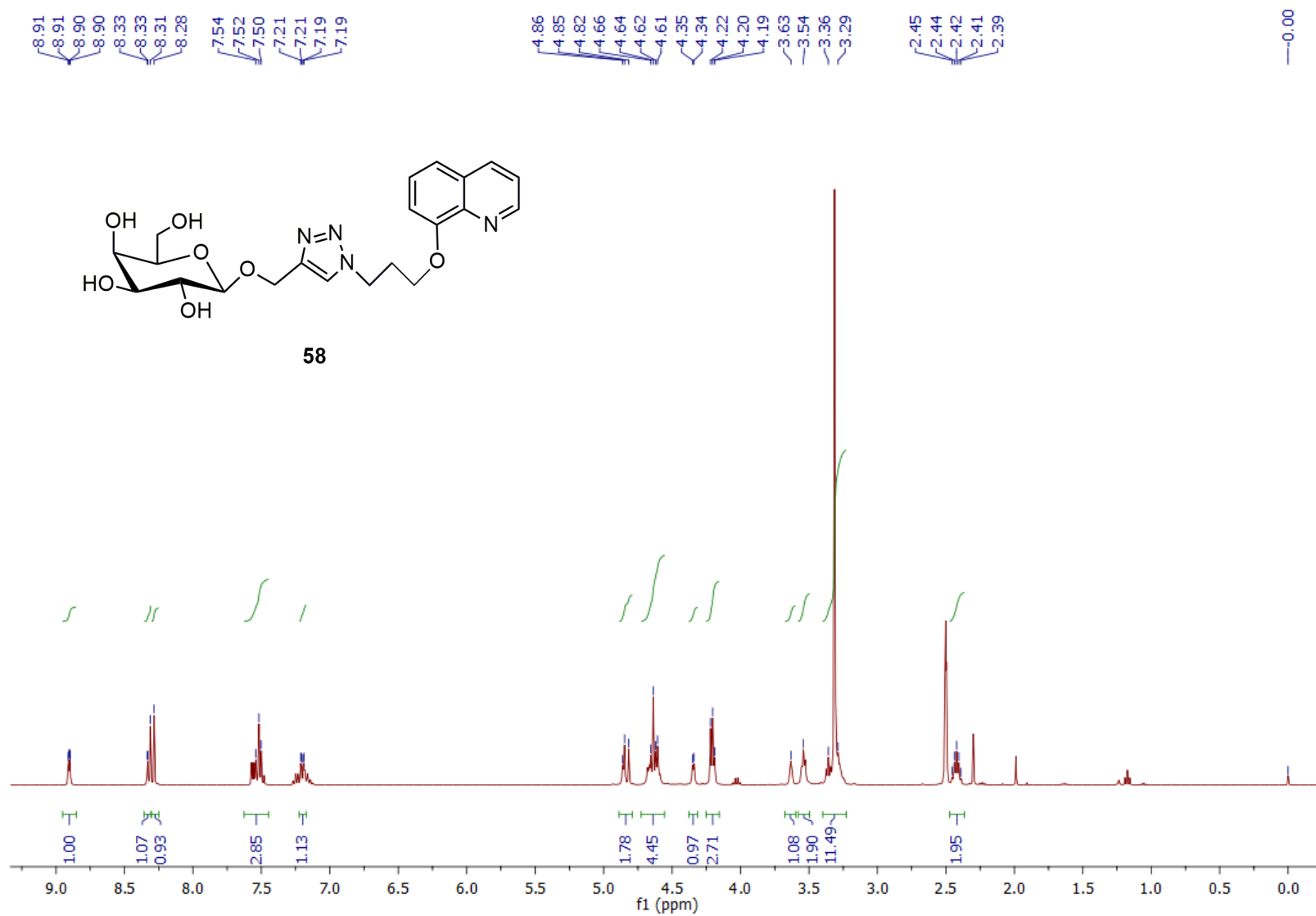


Fig. S107: ^1H NMR spectrum of glycoconjugate **58**.

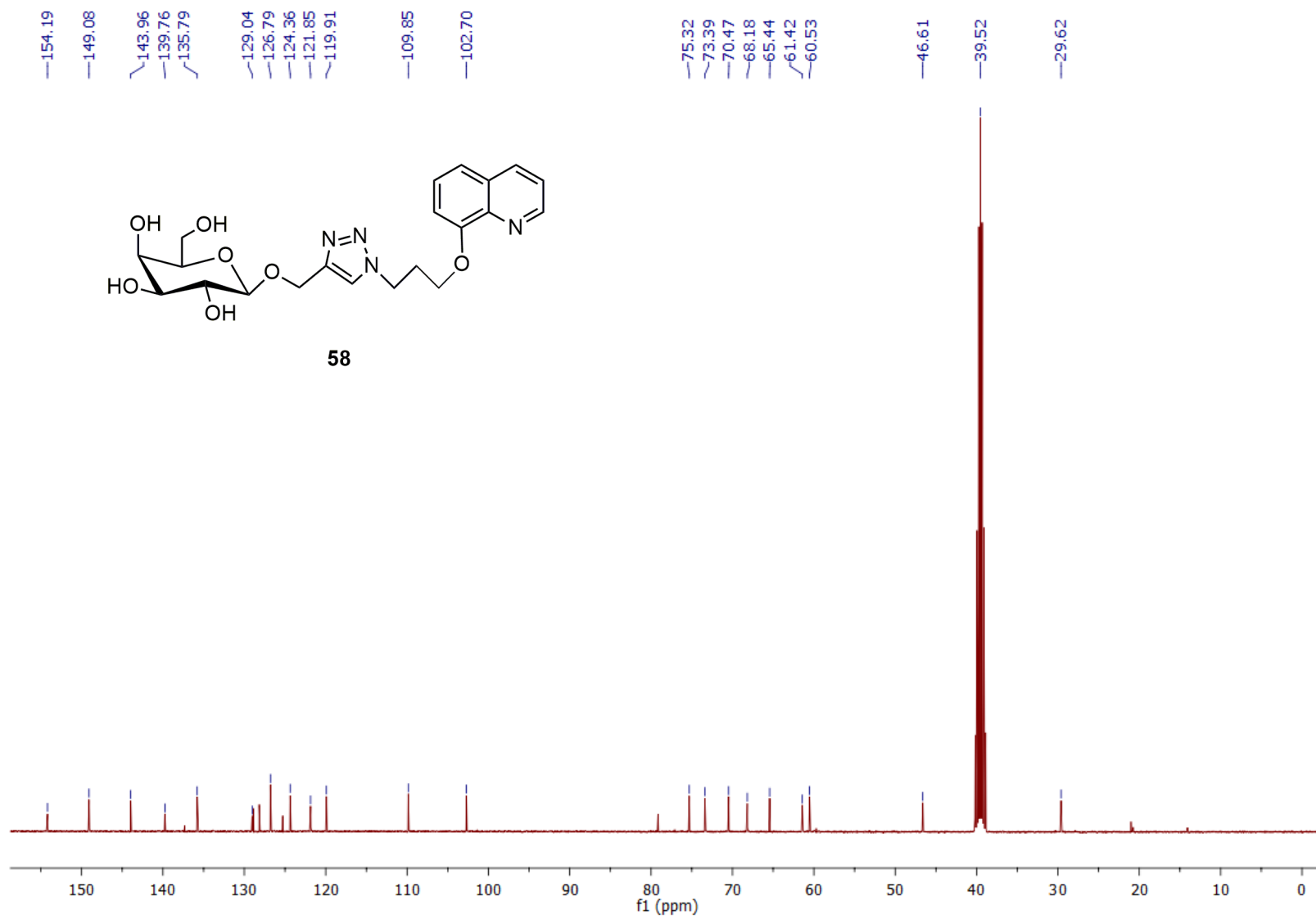


Fig. S108: ^{13}C NMR spectrum of glycoconjugate **58**.

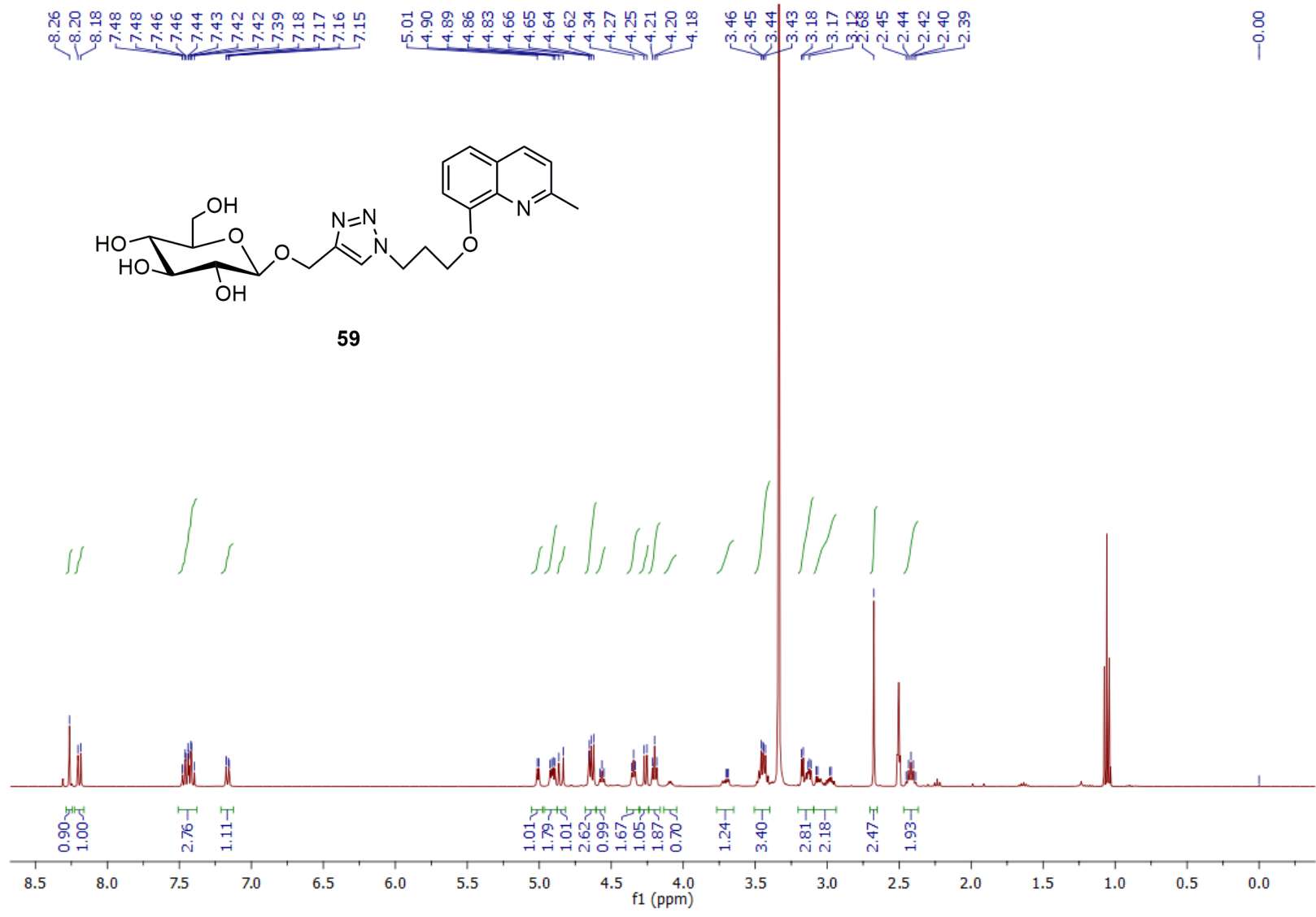


Fig. S109: ^1H NMR spectrum of glycoconjugate **59**.

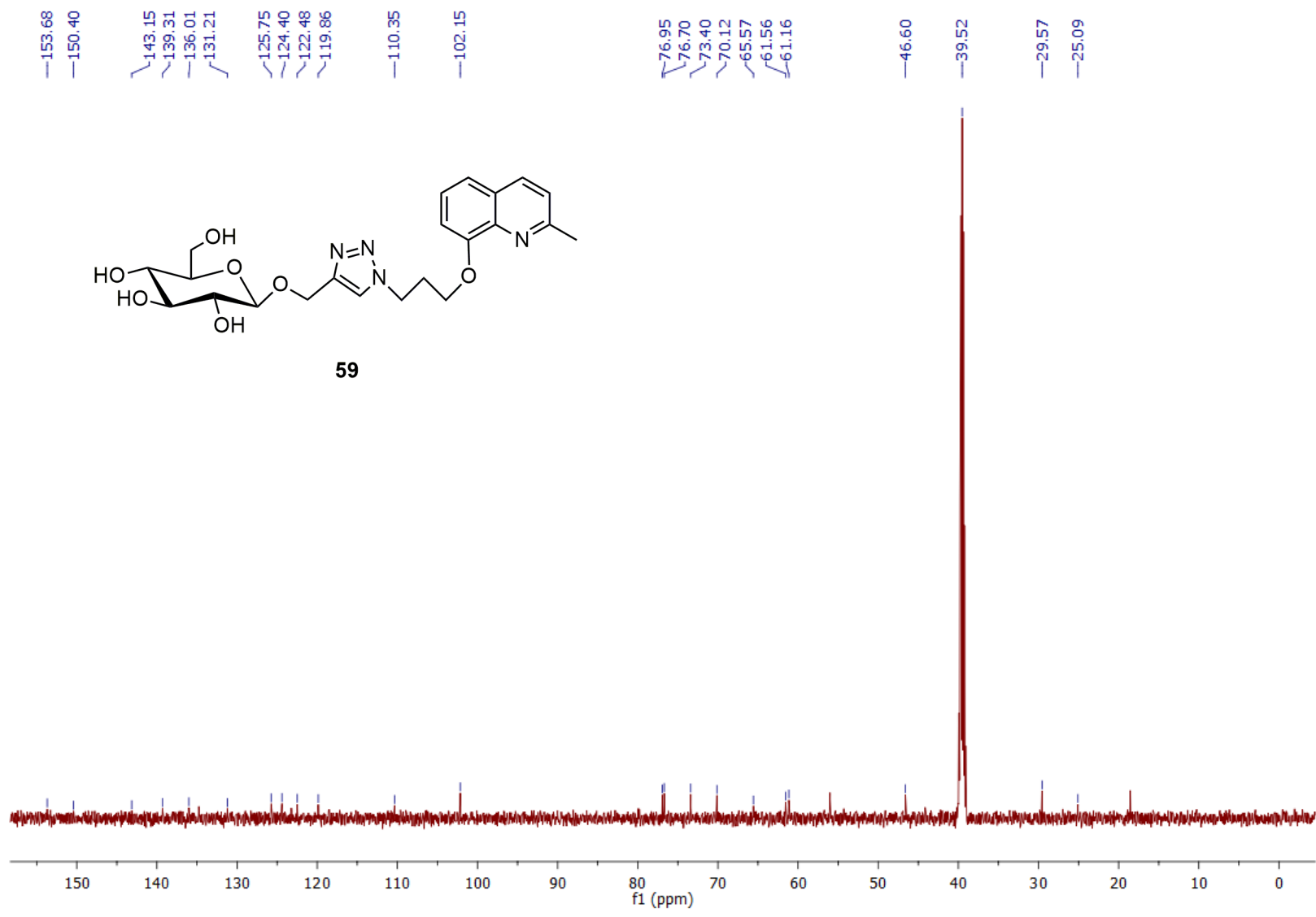


Fig. S110: ^{13}C NMR spectrum of glycoconjugate **59**.

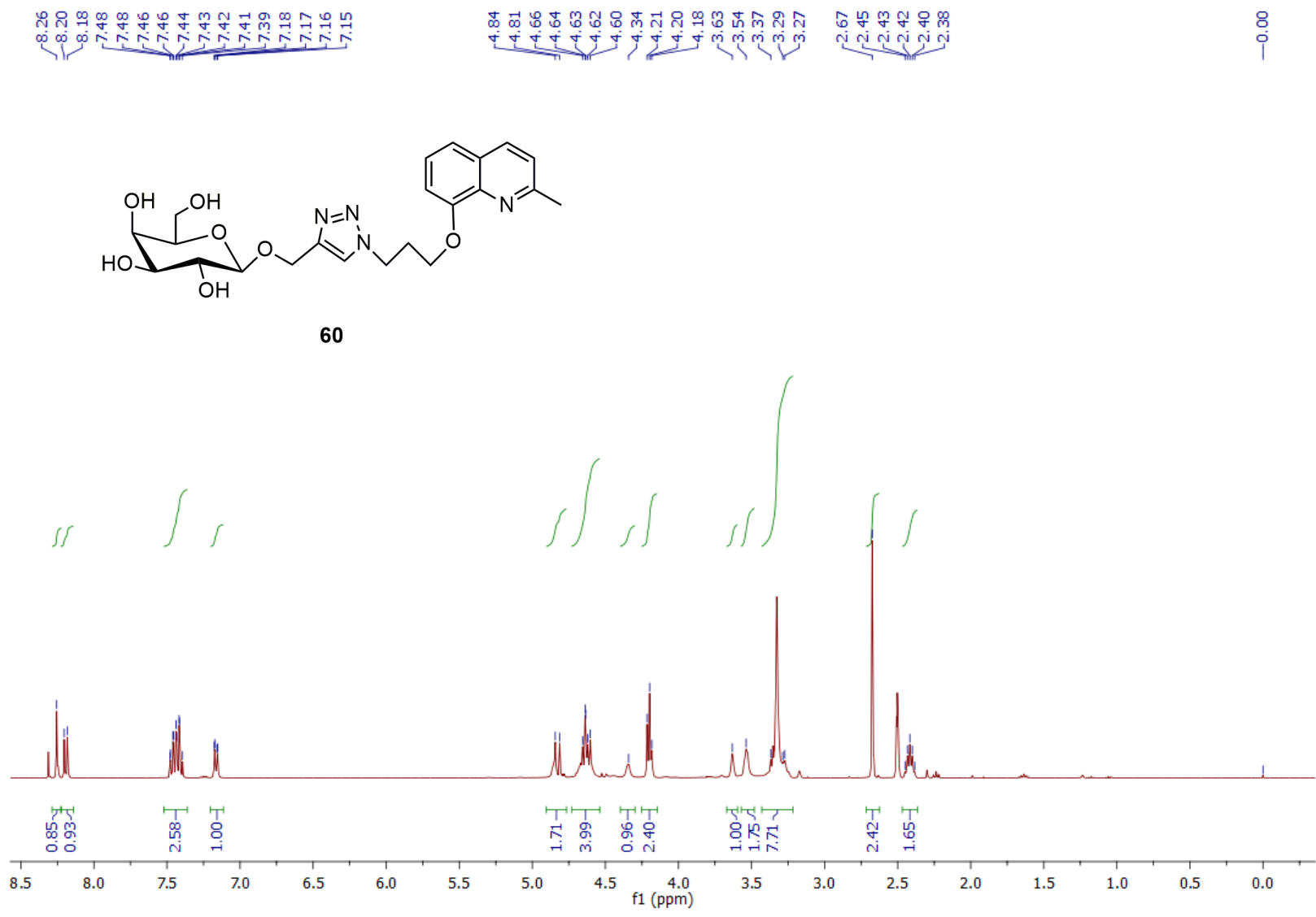


Fig. S111: ^1H NMR spectrum of glycoconjugate **60**.

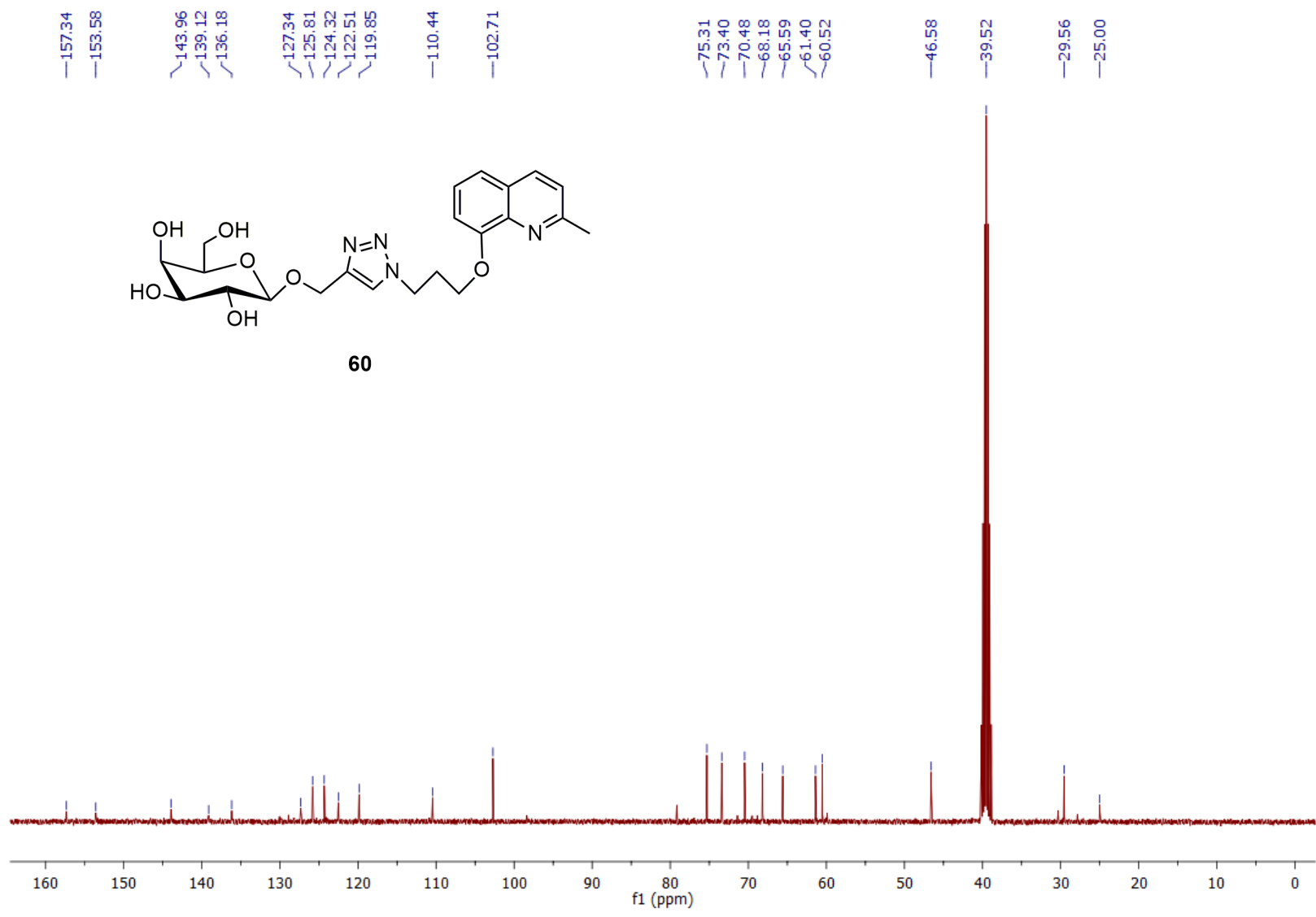


Fig. S112: ^{13}C NMR spectrum of glycoconjugate **60**.

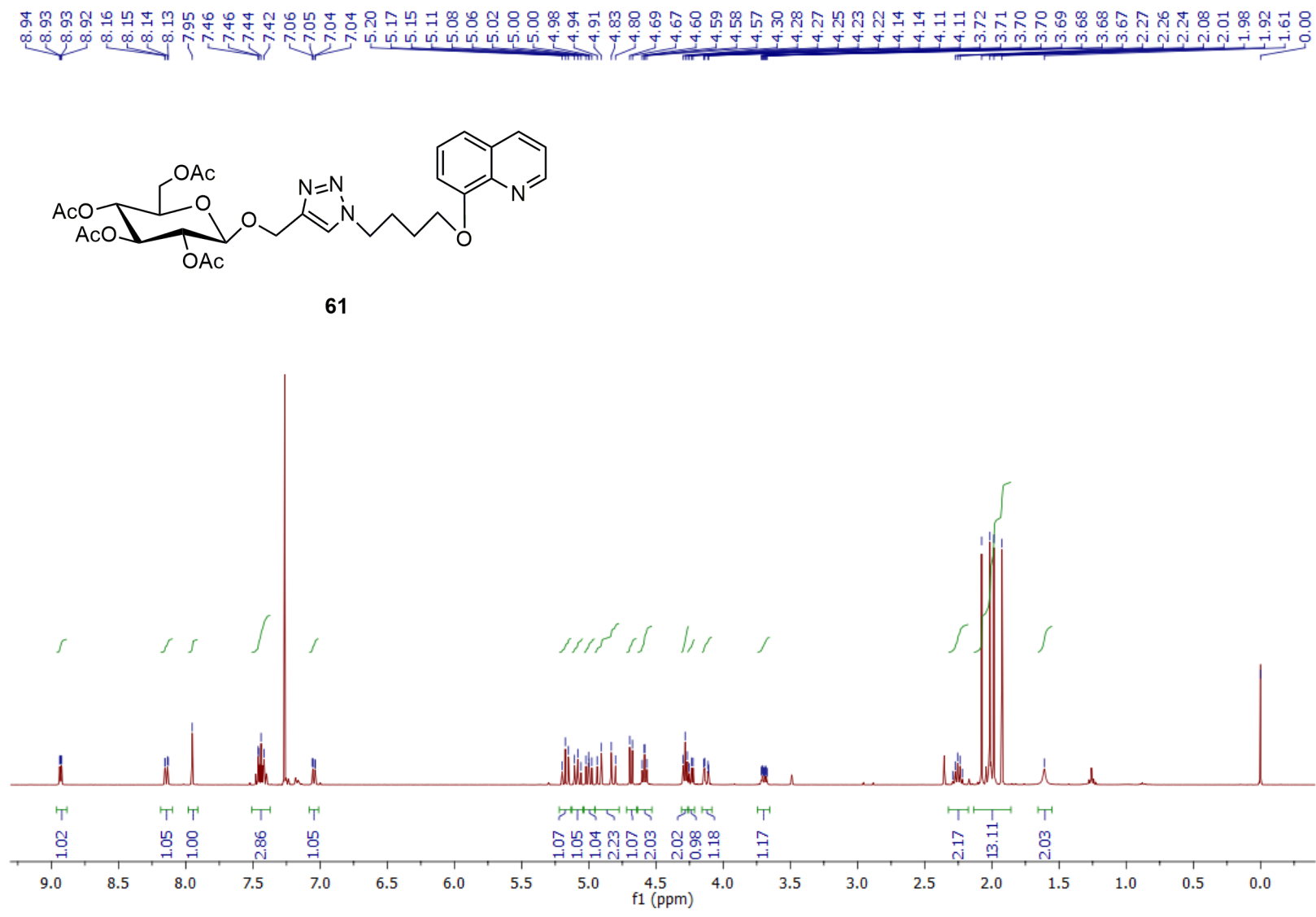


Fig. S113: ¹H NMR spectrum of glycoconjugate **61**.

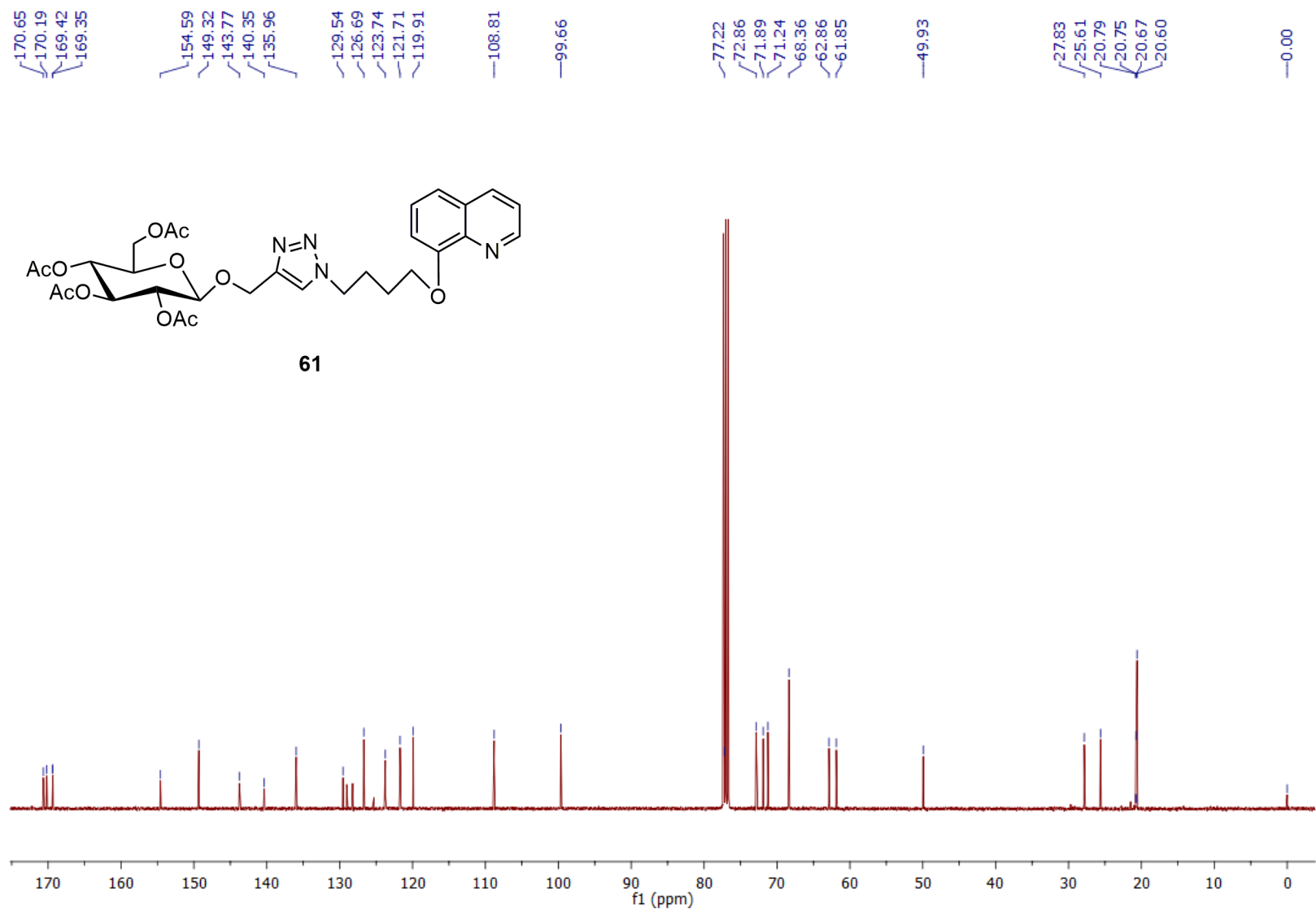


Fig. S114: ¹³C NMR spectrum of glycoconjugate **61**.

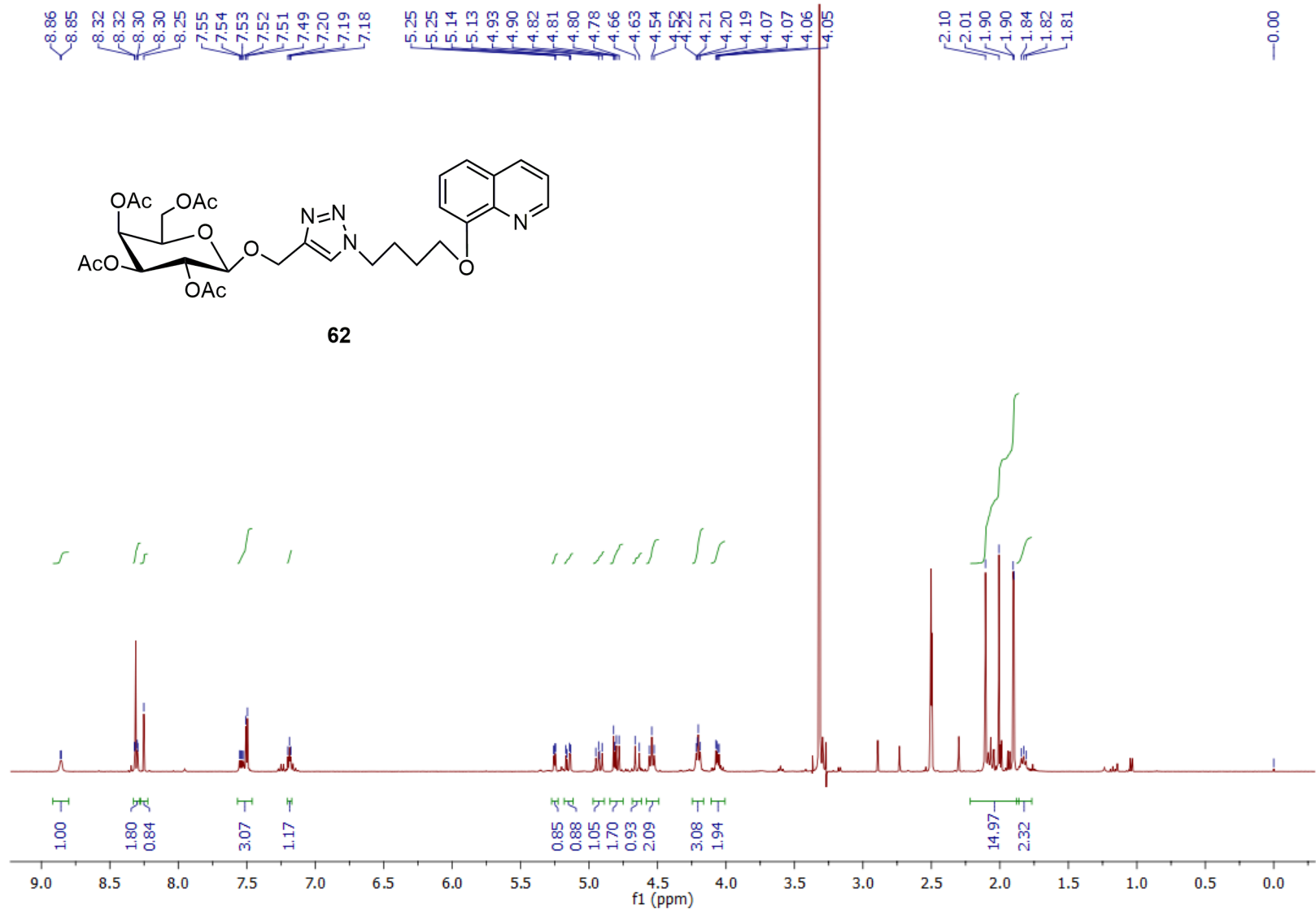


Fig. S115: ^1H NMR spectrum of glycoconjugate **62**.

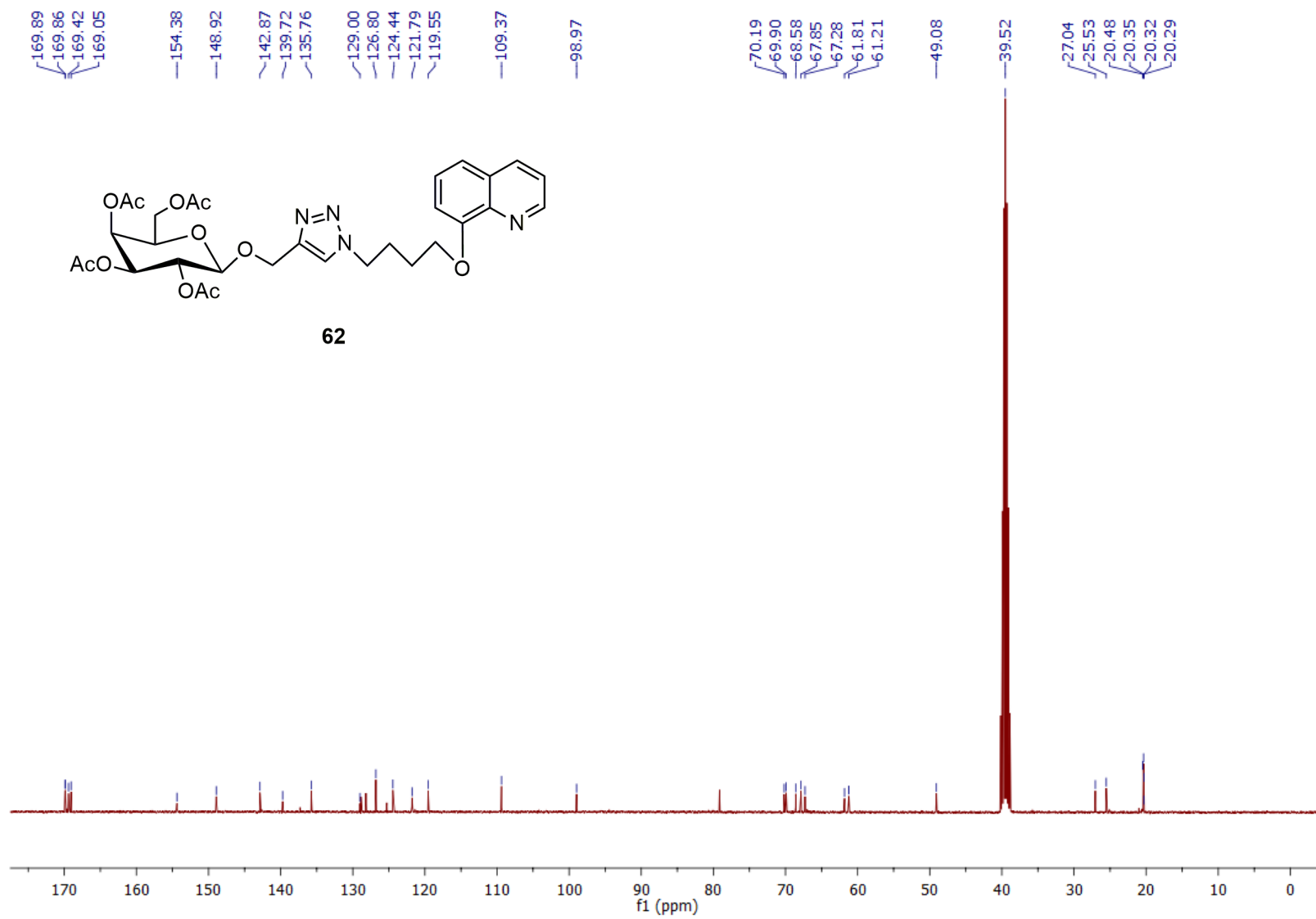


Fig. S116: ^{13}C NMR spectrum of glycoconjugate **62**.

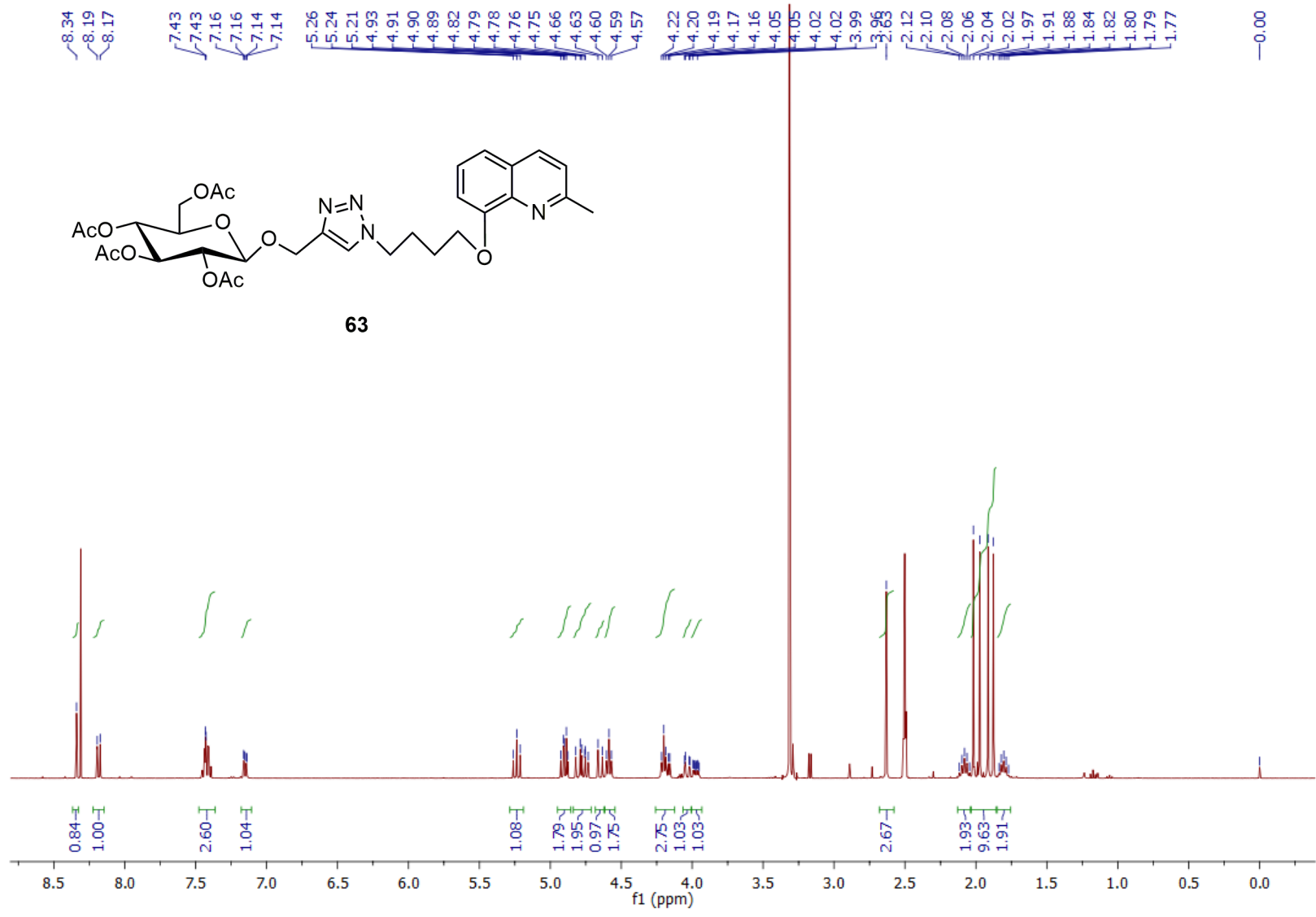


Fig. S117: ^1H NMR spectrum of glycoconjugate **63**.

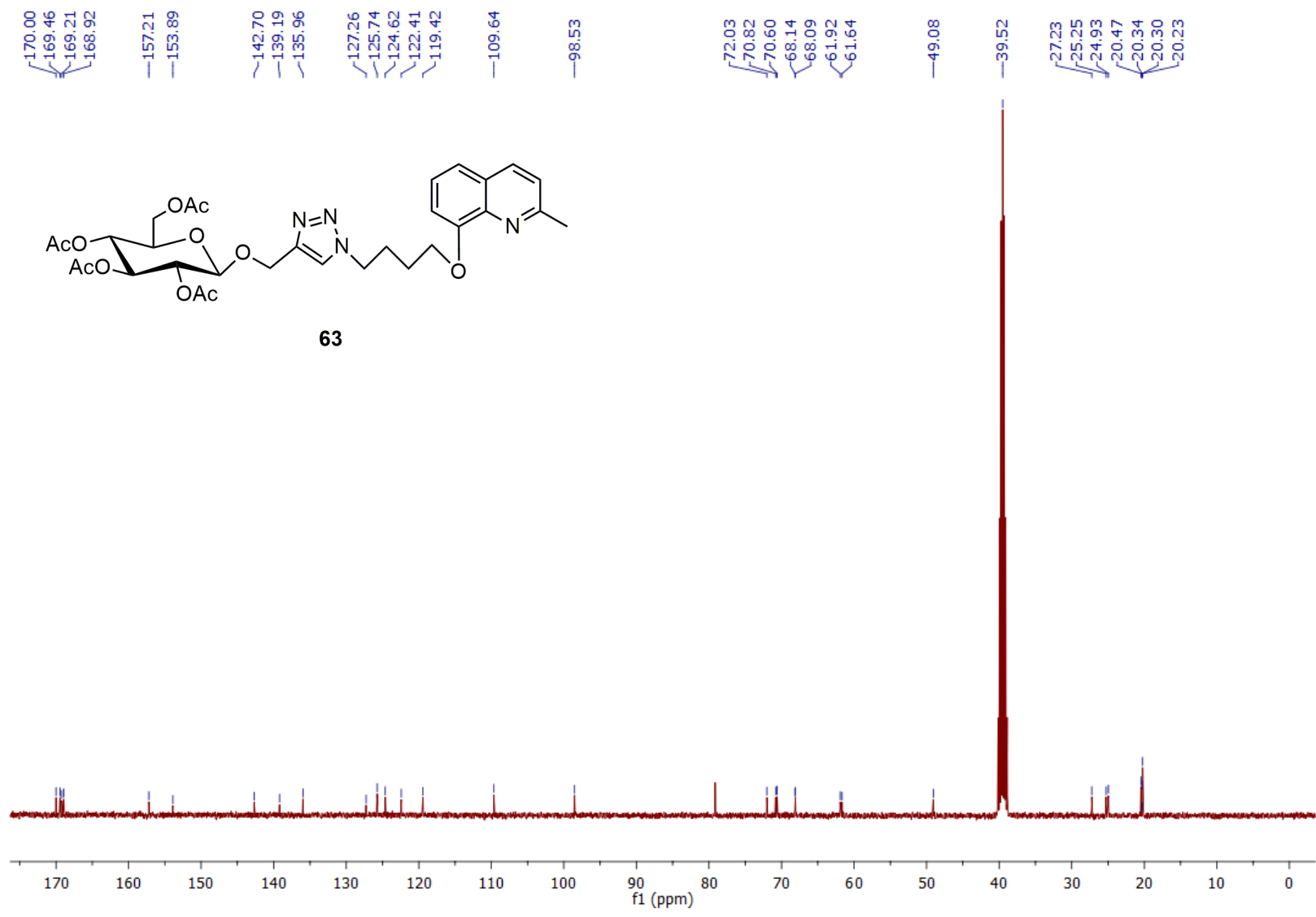


Fig. S118: ^{13}C NMR spectrum of glycoconjugate **63**.

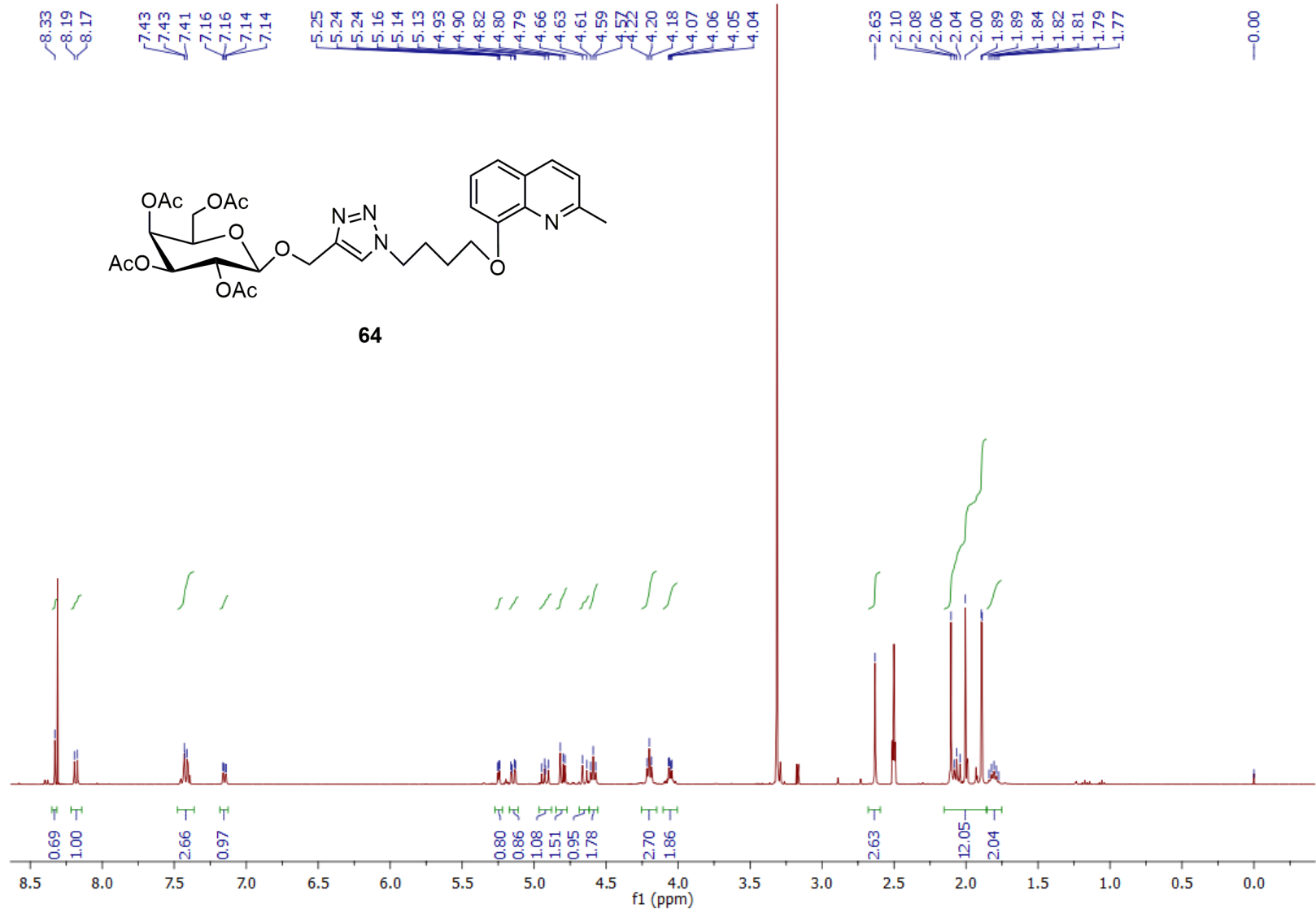


Fig. S119: ¹H NMR spectrum of glycoconjugate **64**.

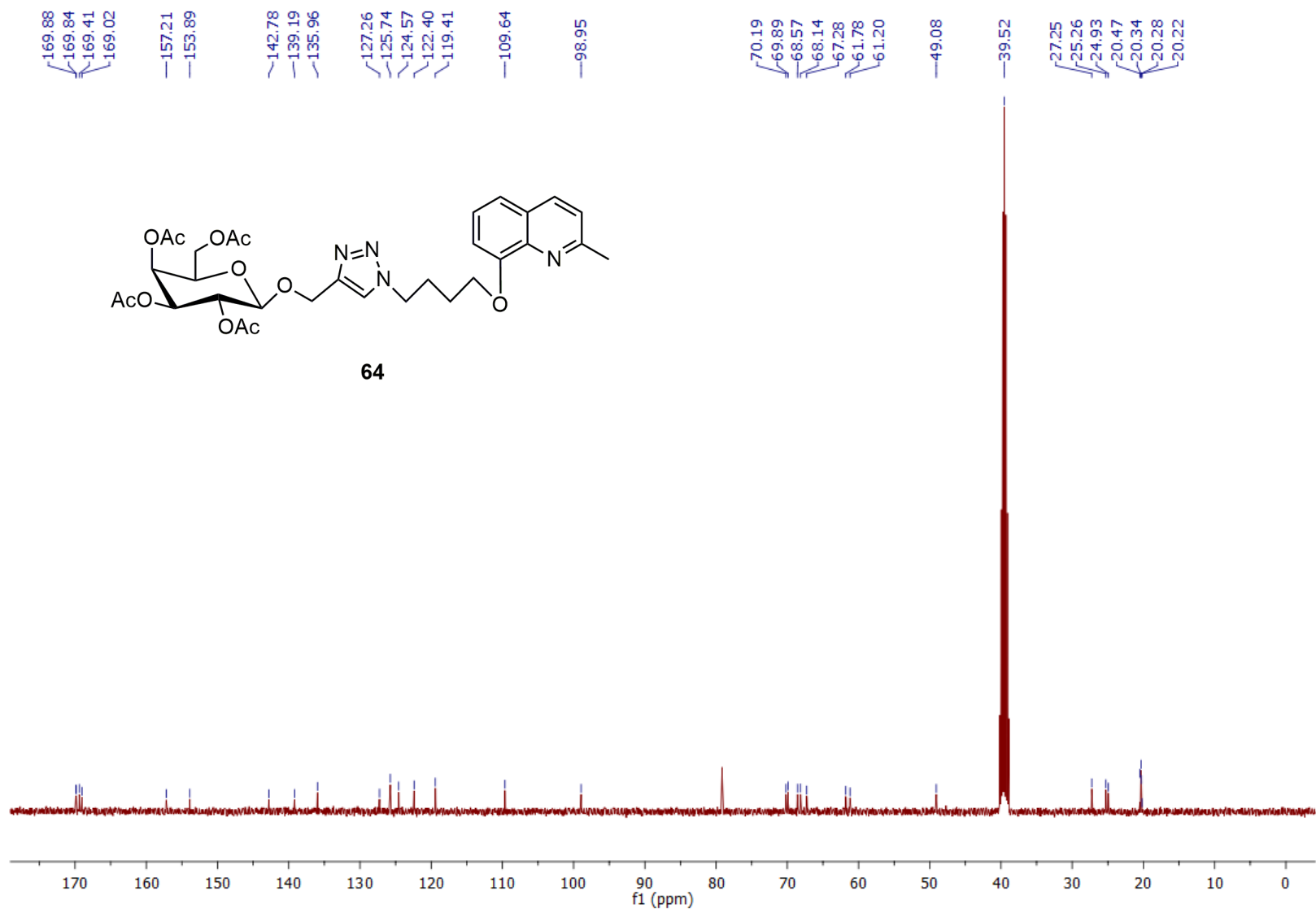


Fig. S120: ^{13}C NMR spectrum of glycoconjugate **64**.

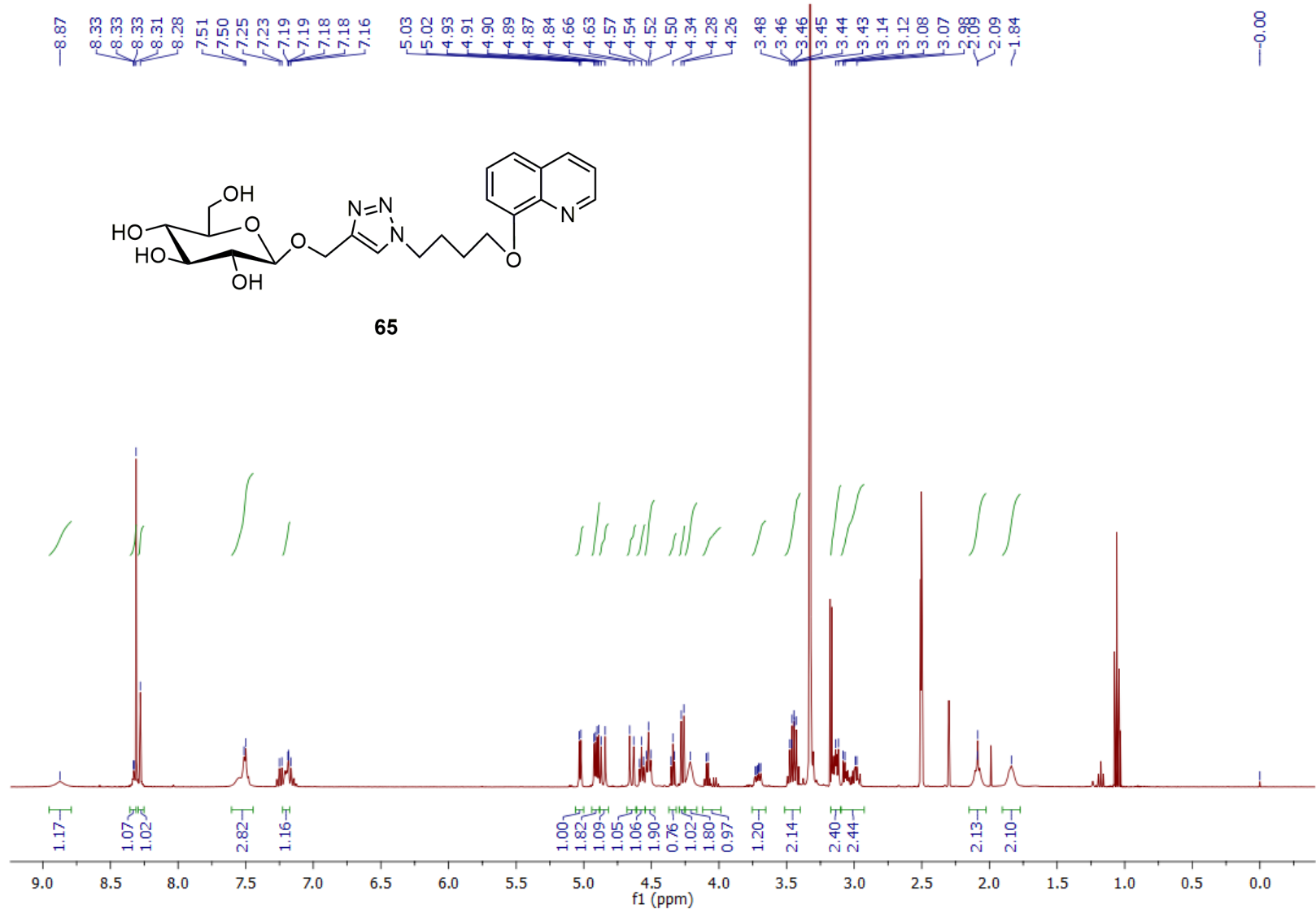


Fig. S121: ^1H NMR spectrum of glycoconjugate **65**.

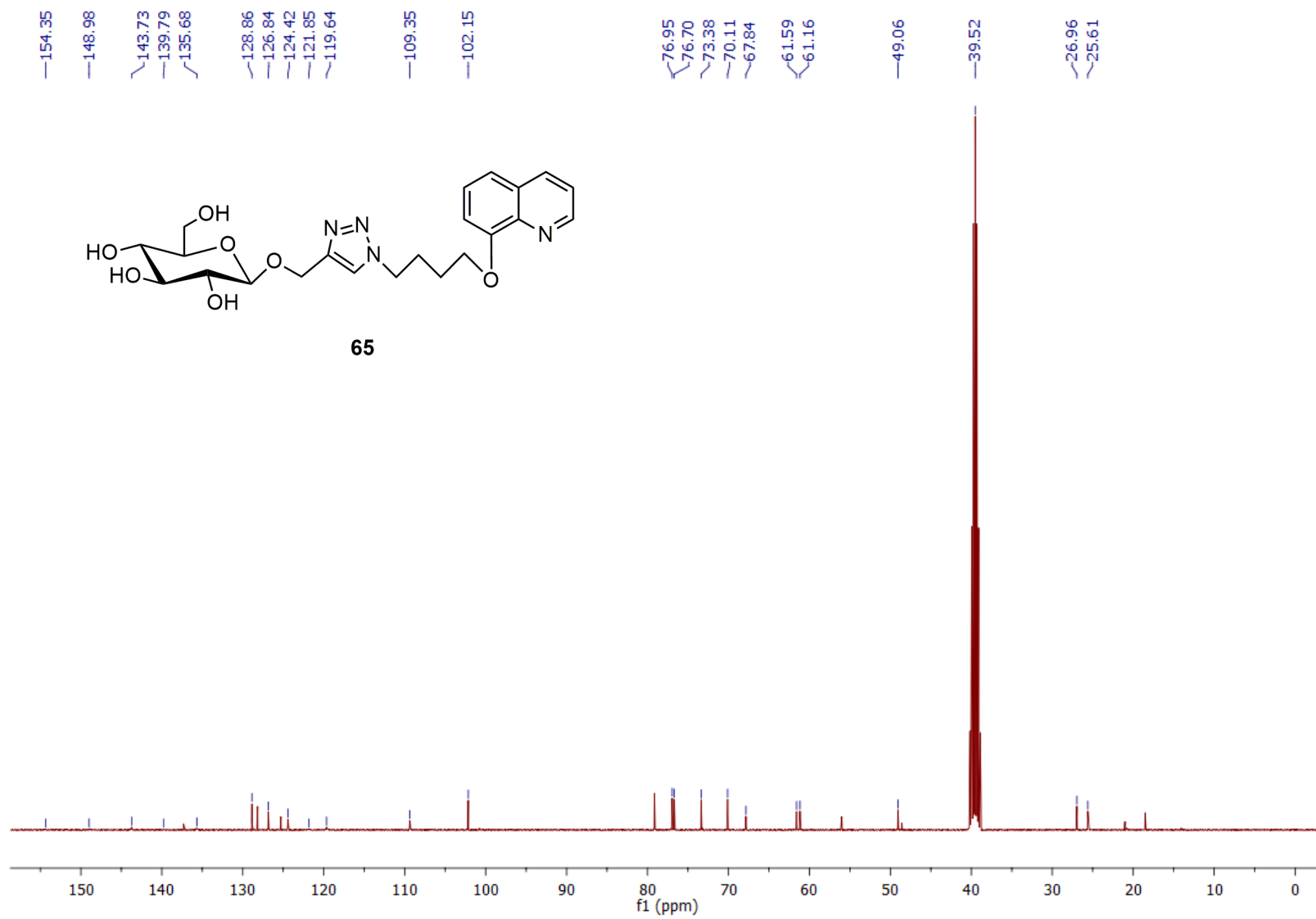


Fig. S122: ^{13}C NMR spectrum of glycoconjugate **65**.

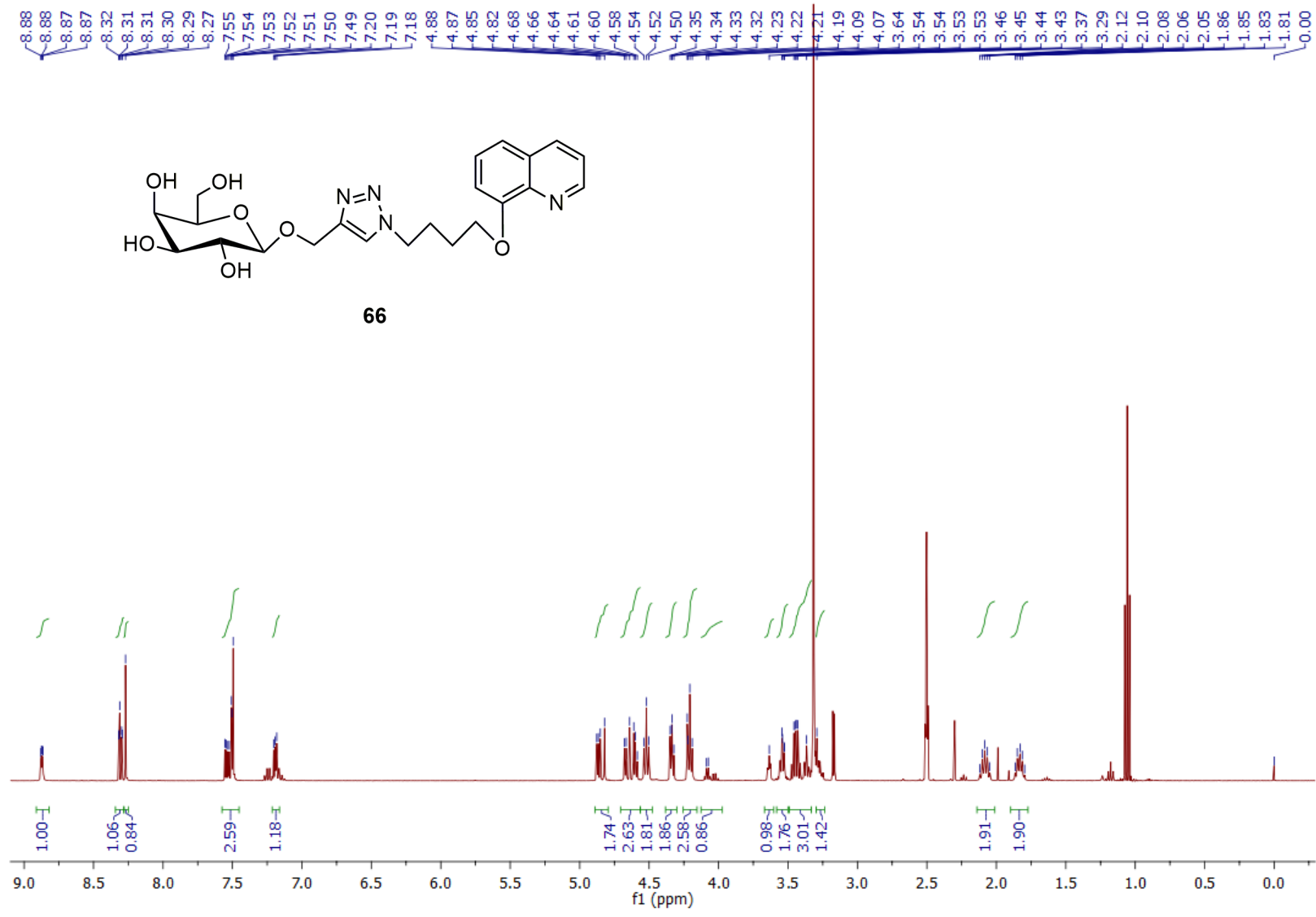


Fig. S123: ^1H NMR spectrum of glycoconjugate **66**.

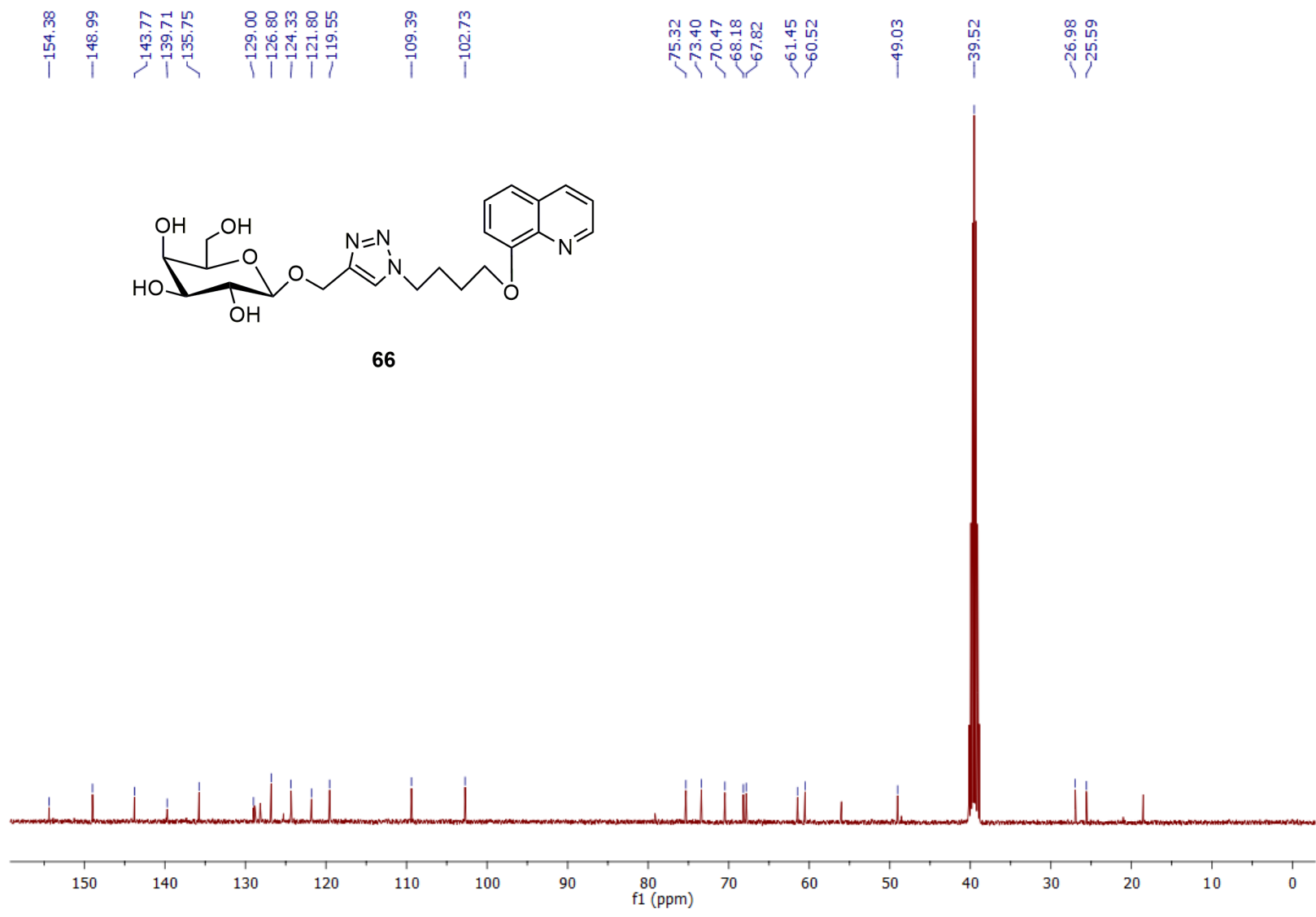


Fig. S124: ^{13}C NMR spectrum of glycoconjugate **66**.

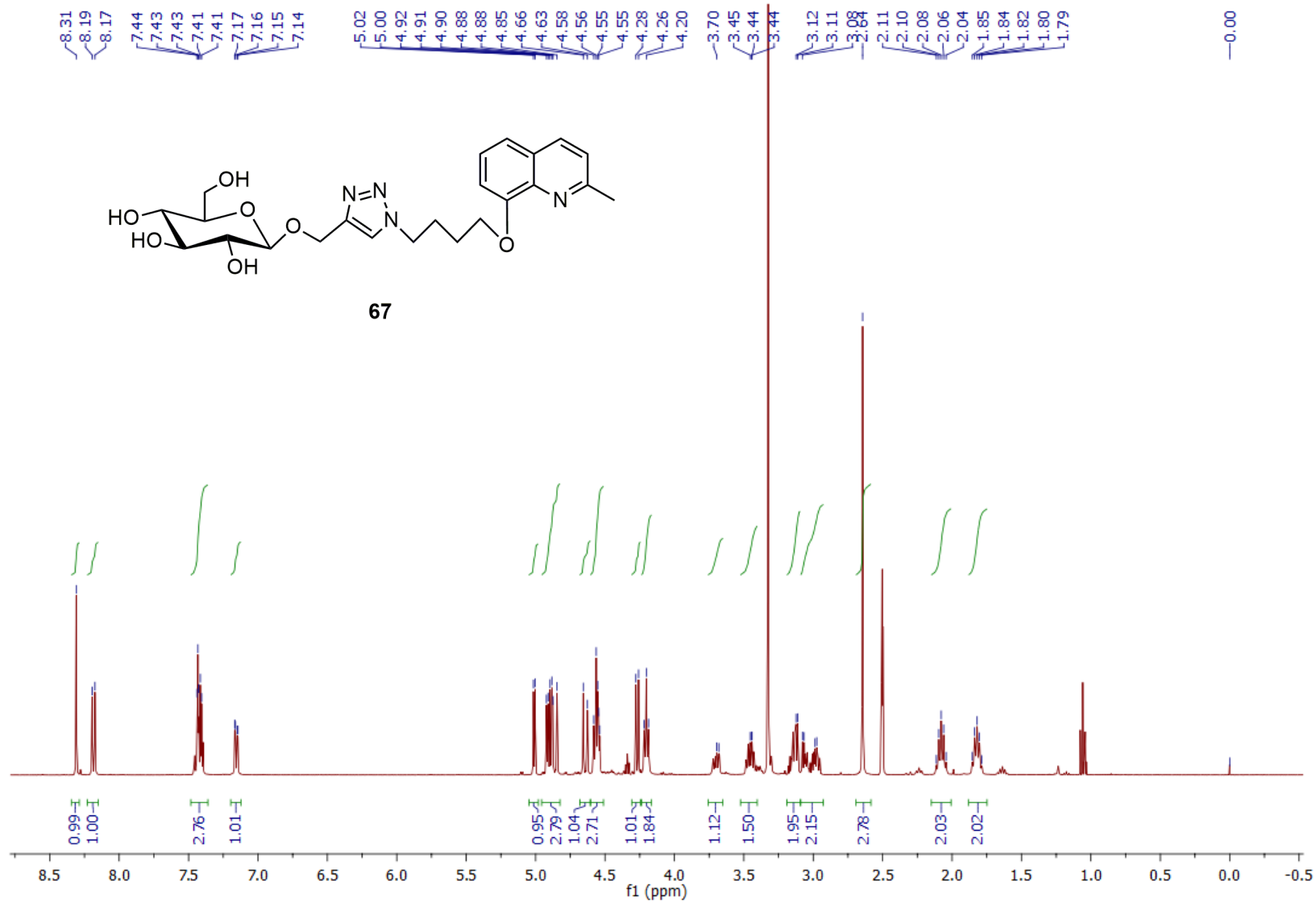


Fig. S125: ^1H NMR spectrum of glycoconjugate **67**.

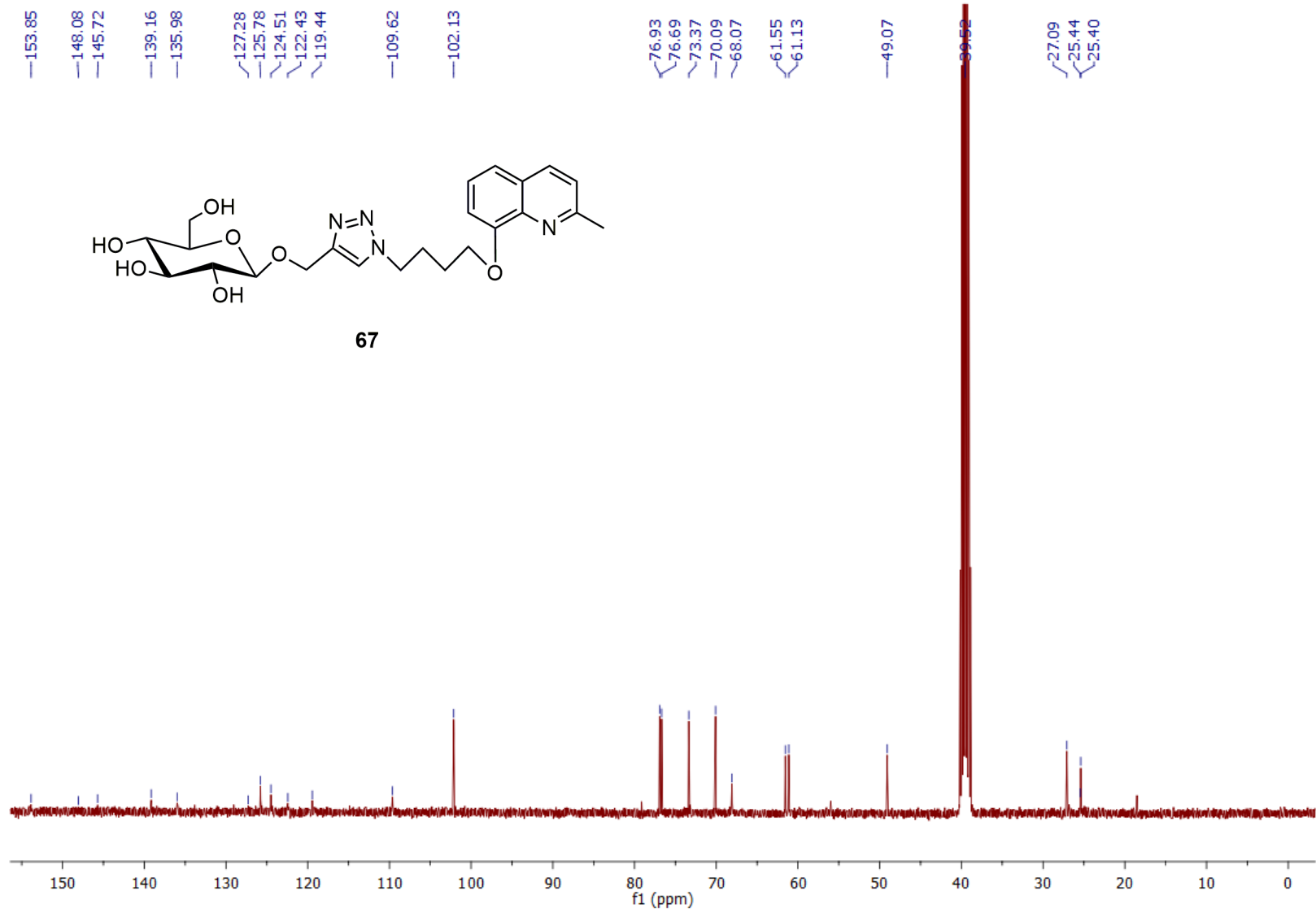


Fig. S126: ^{13}C NMR spectrum of glycoconjugate **67**.

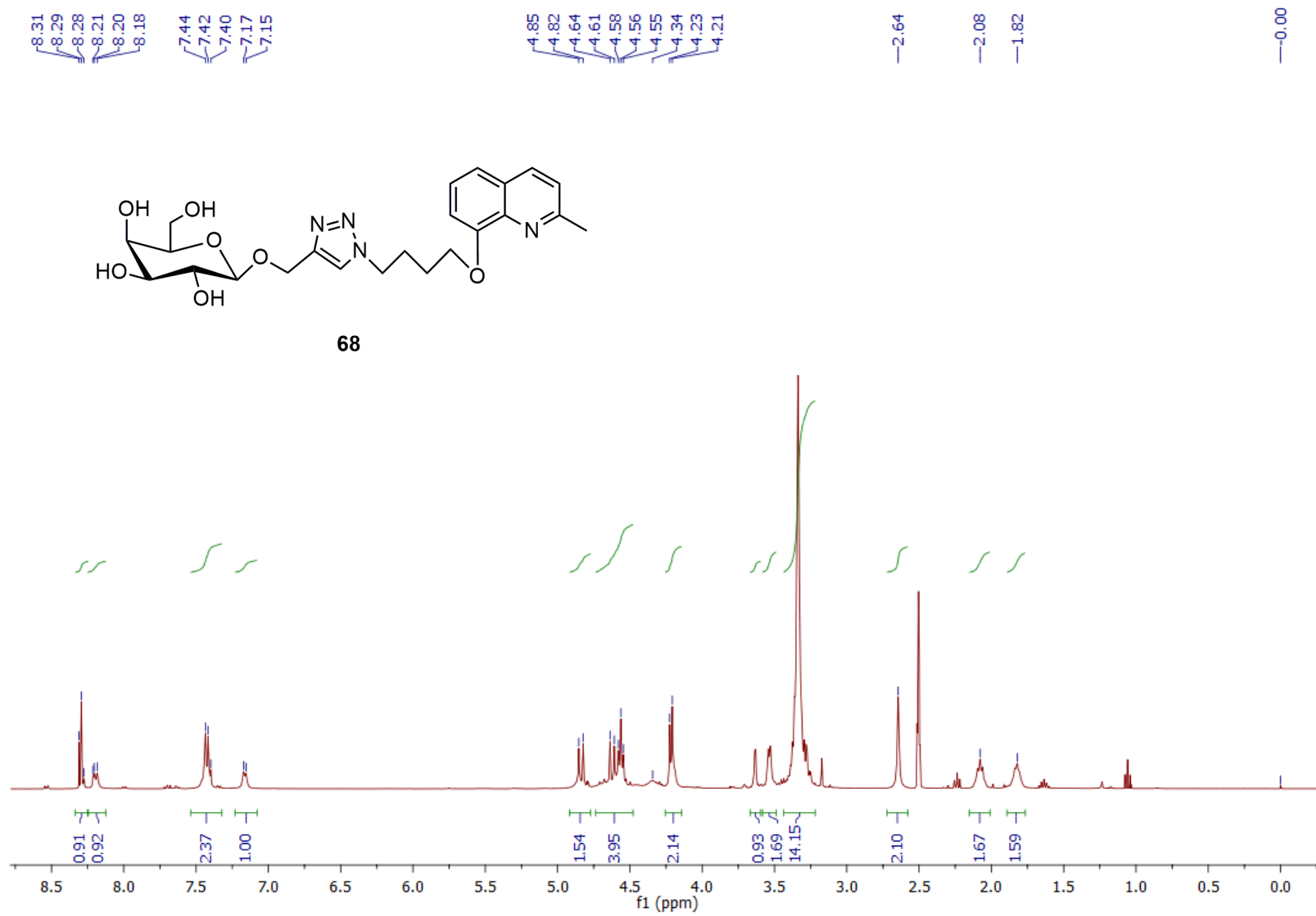


Fig. S127: ^1H NMR spectrum of glycoconjugate **68**.

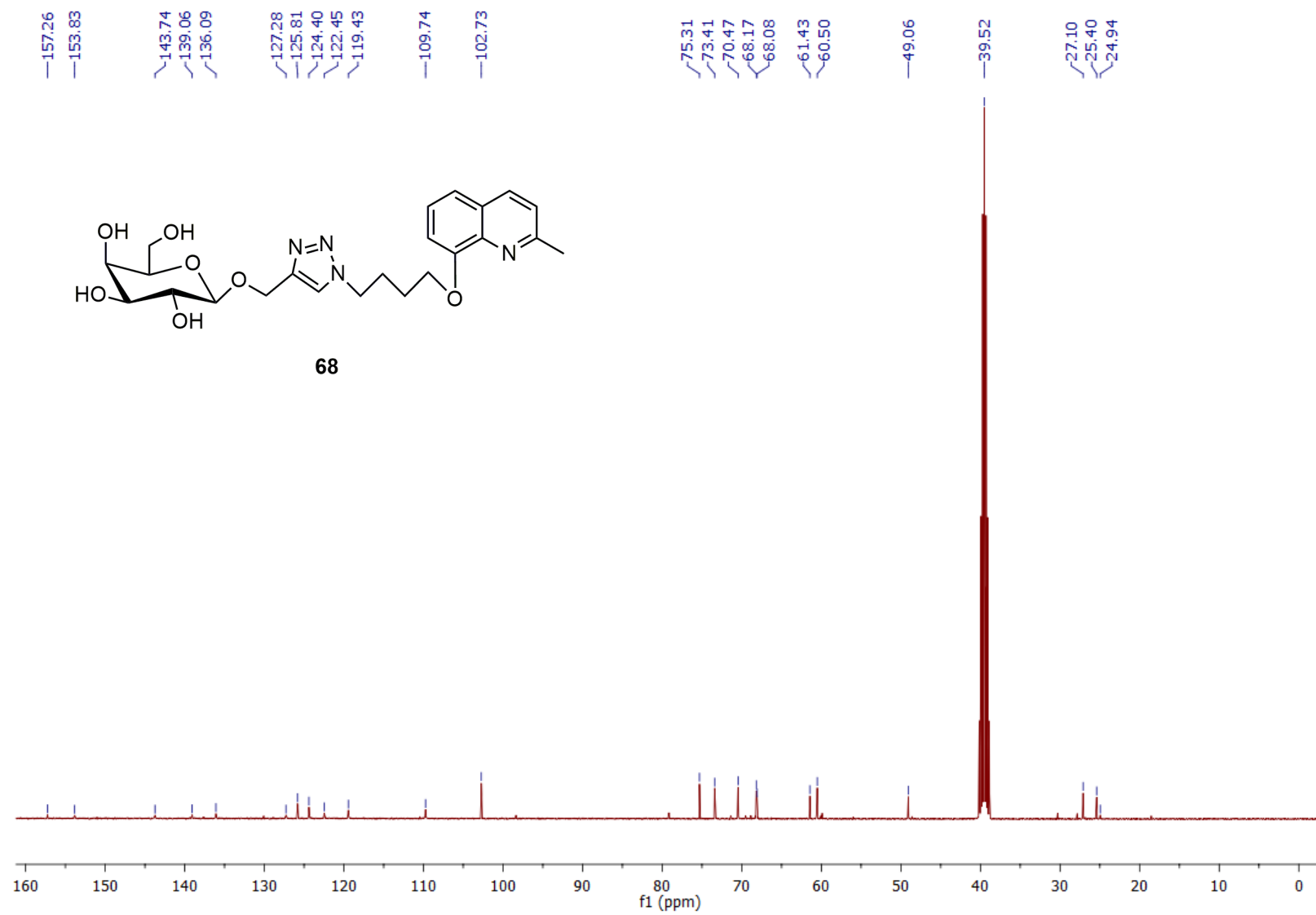


Fig. S128: ^{13}C NMR spectrum of glycoconjugate **68**.

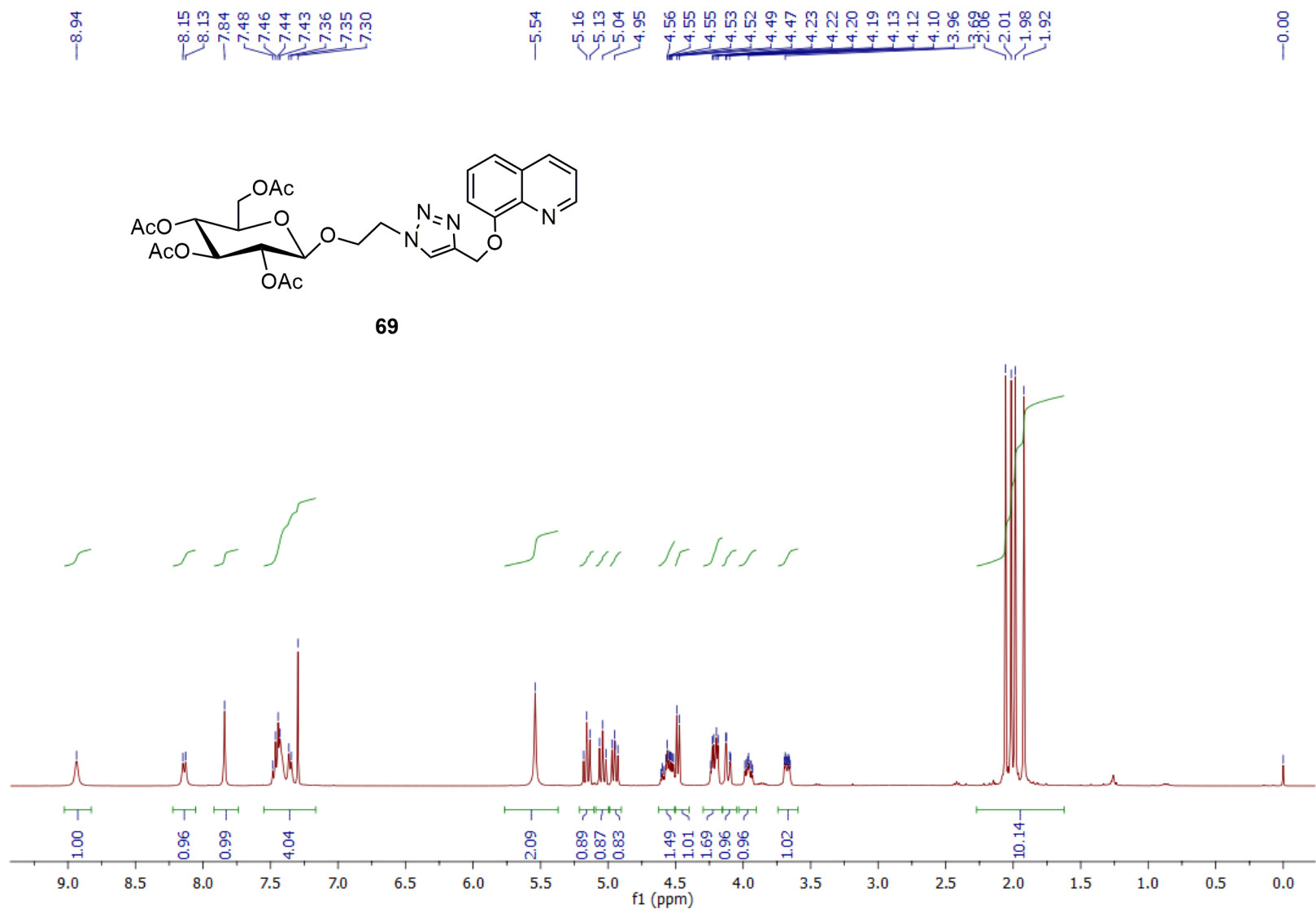


Fig. S129: ¹H NMR spectrum of glycoconjugate **69**.

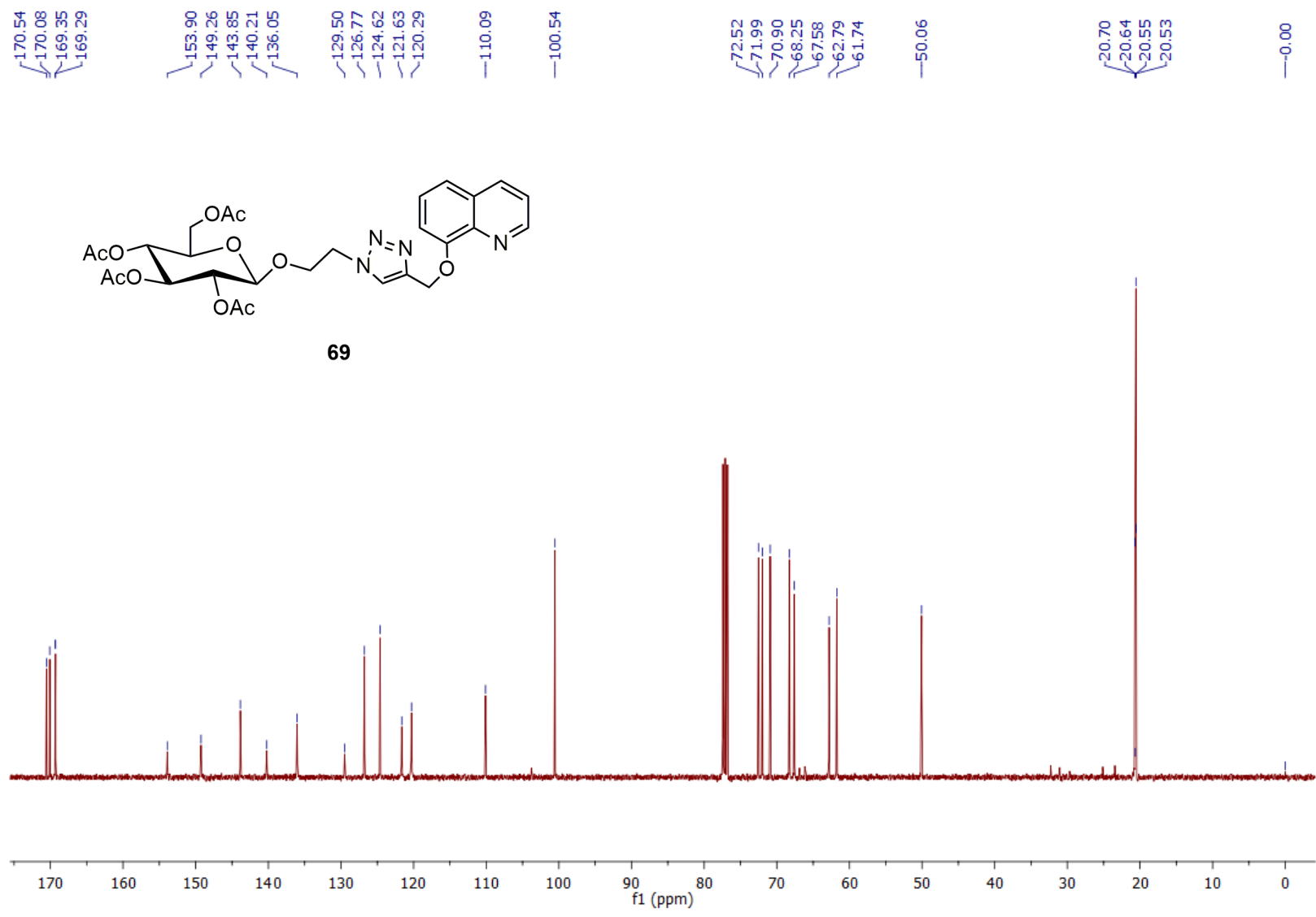


Fig. S130: ¹³C NMR spectrum of glycoconjugate **69**.

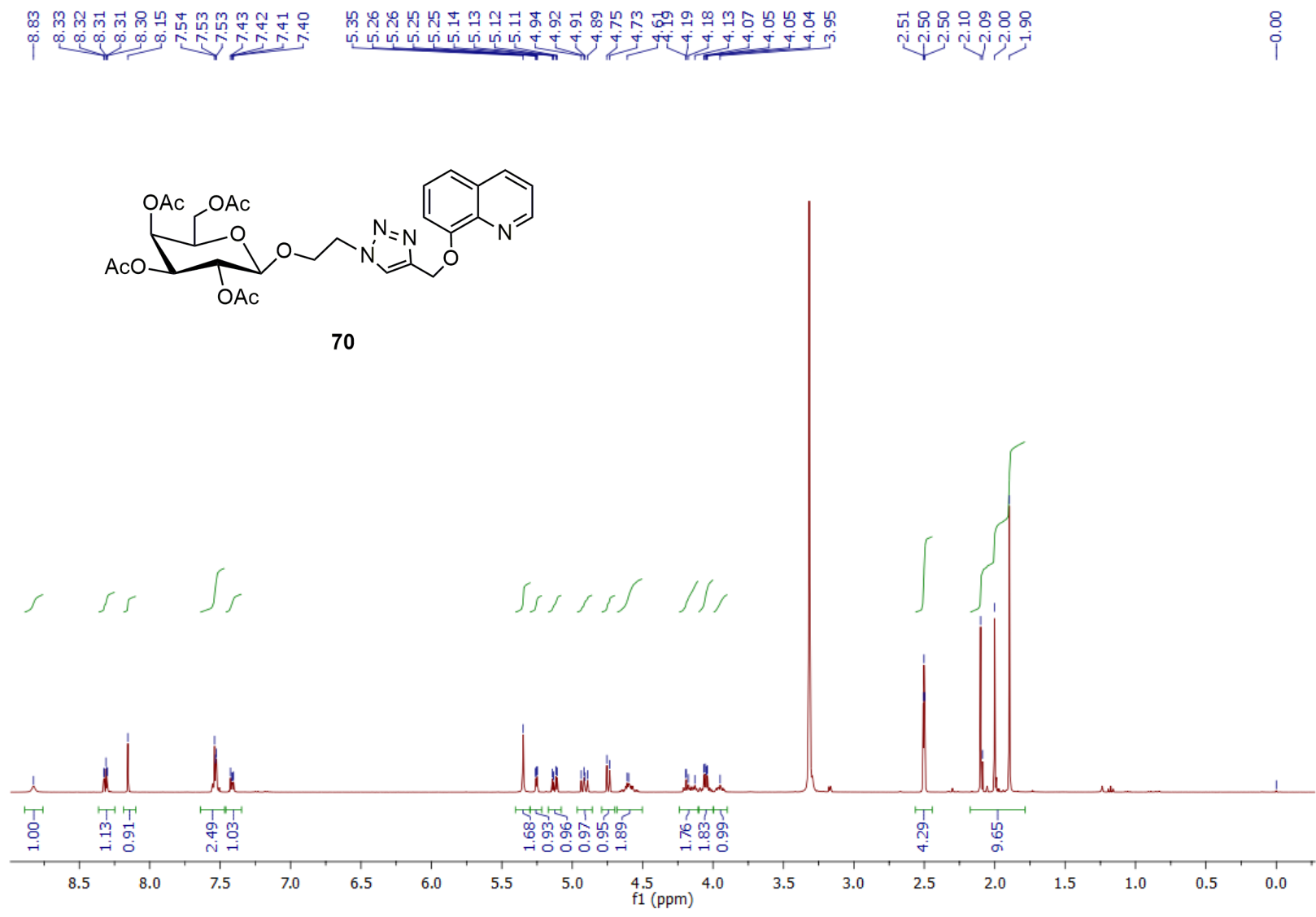


Fig. S131: ^1H NMR spectrum of glycoconjugate **70**.

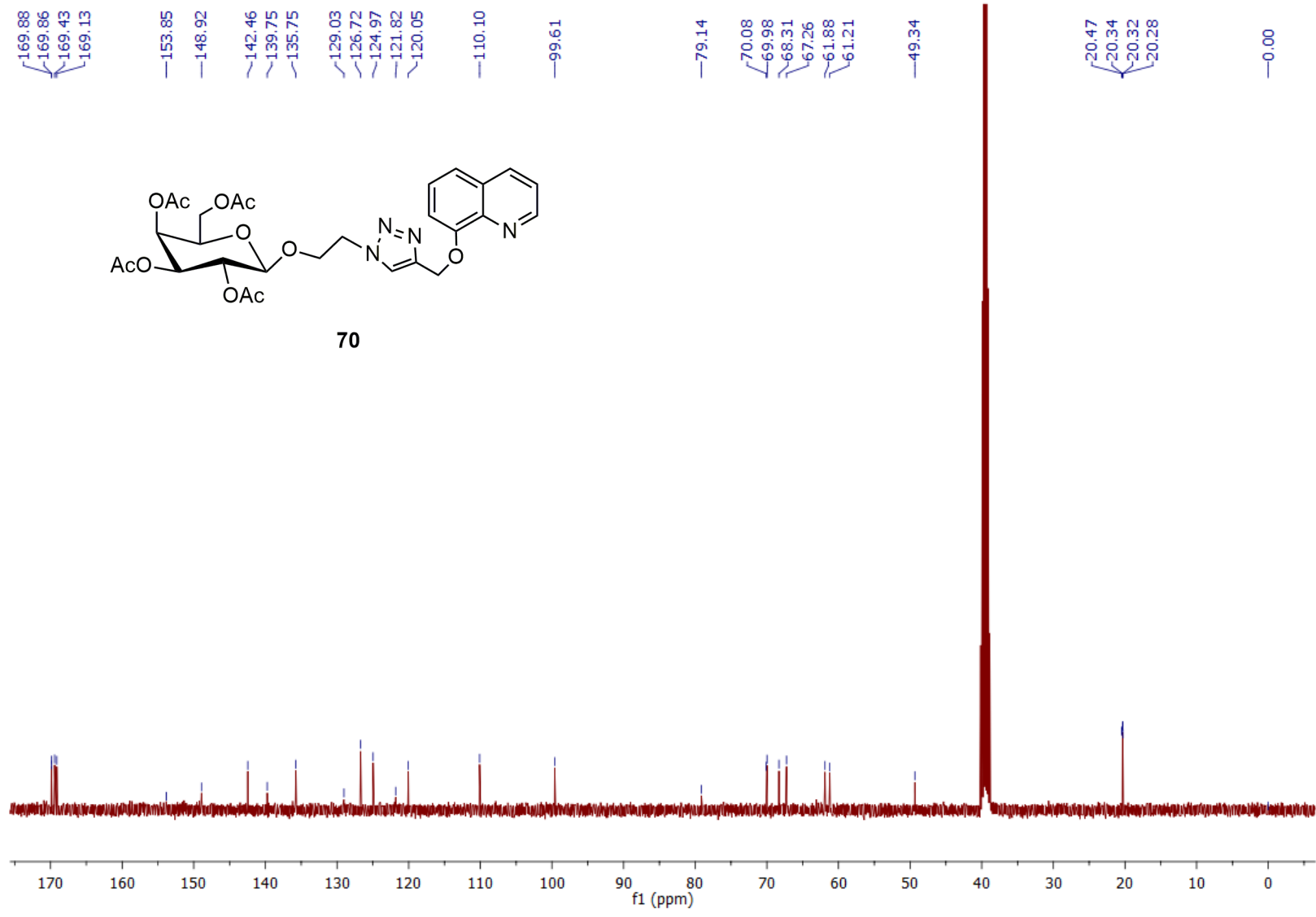


Fig. S132: ^{13}C NMR spectrum of glycoconjugate **70**.

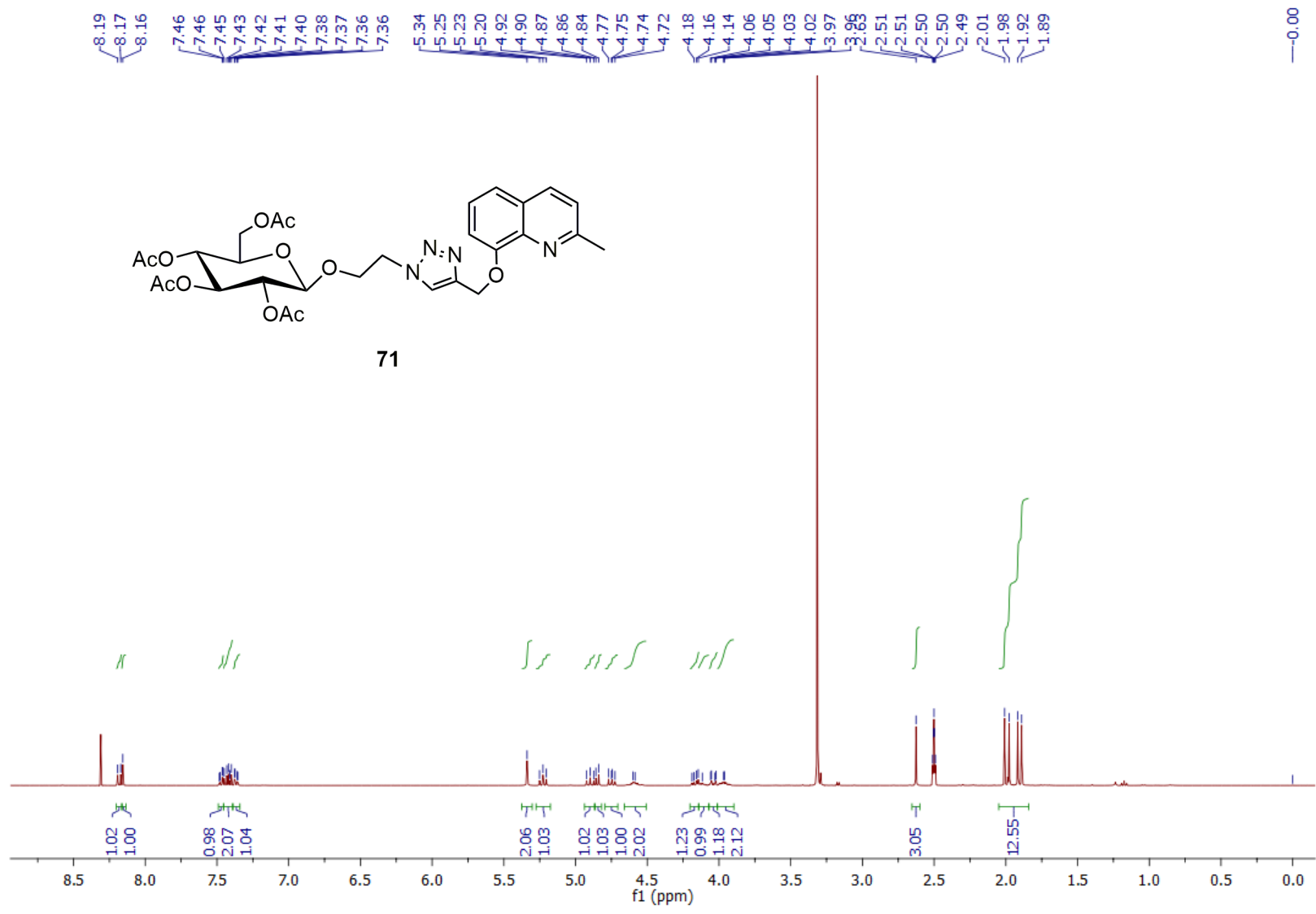


Fig. S133: ^1H NMR spectrum of glycoconjugate **71**.

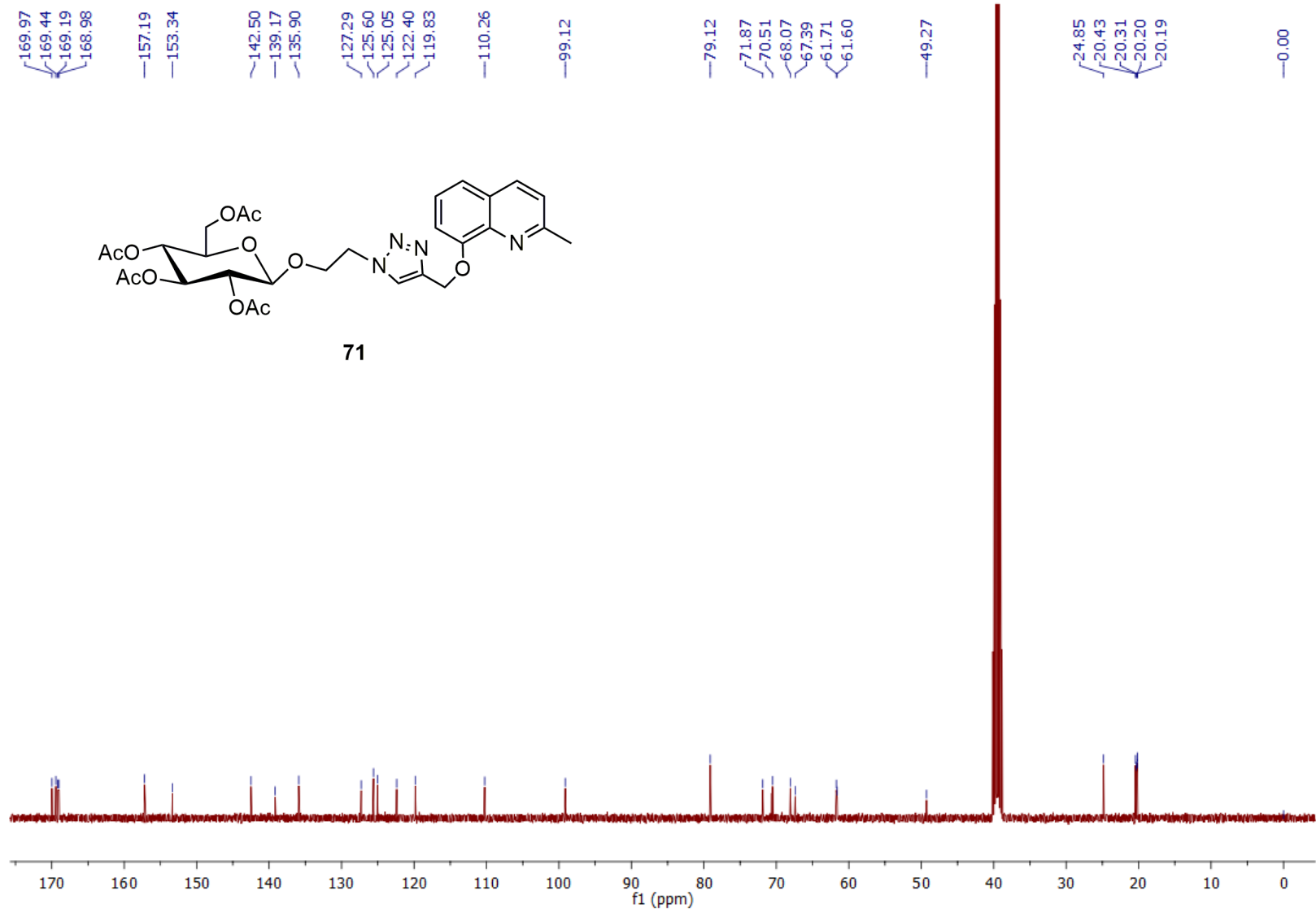


Fig. S134: ^{13}C NMR spectrum of glycoconjugate **71**.

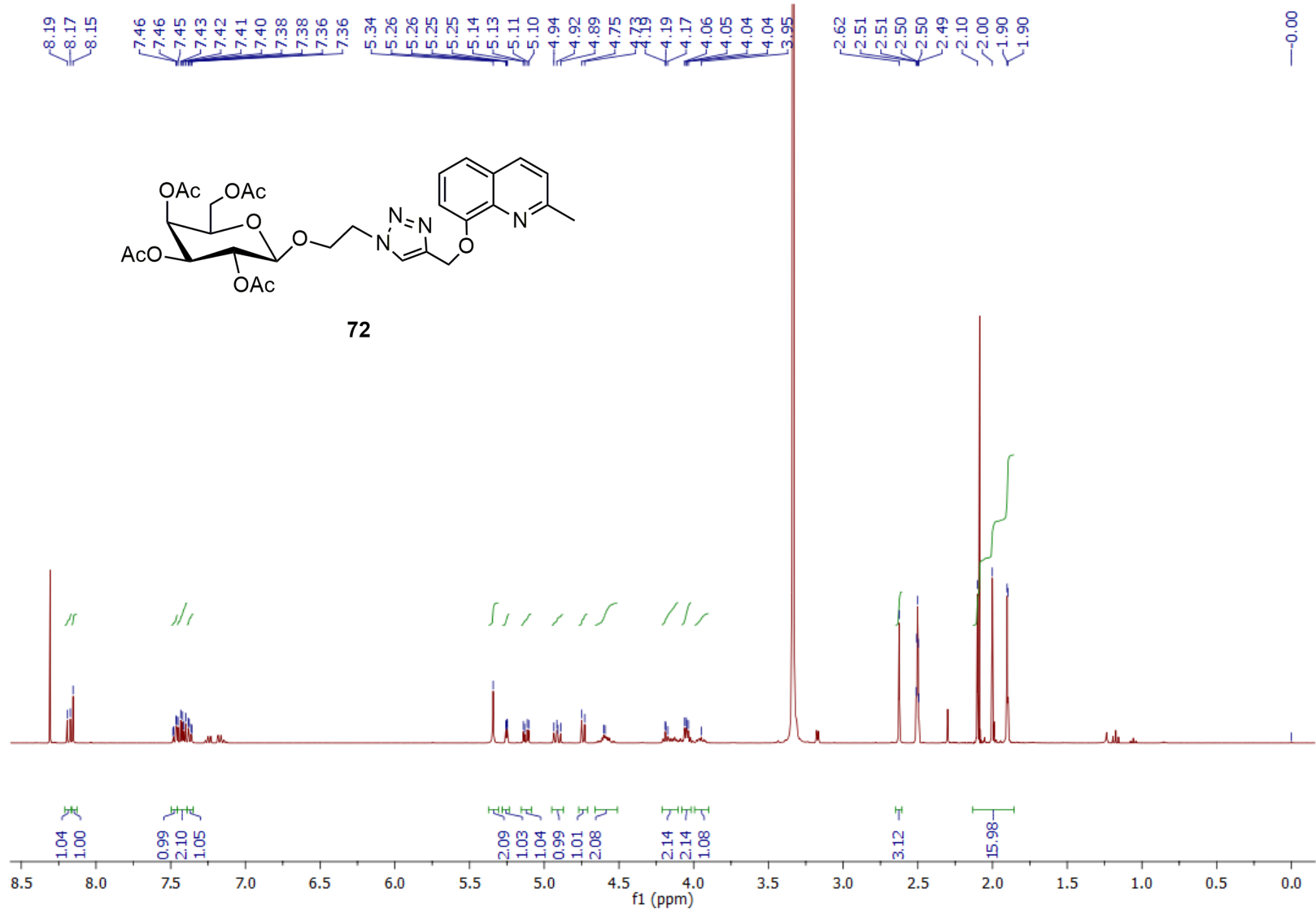


Fig. S135: ¹H NMR spectrum of glycoconjugate **72**.

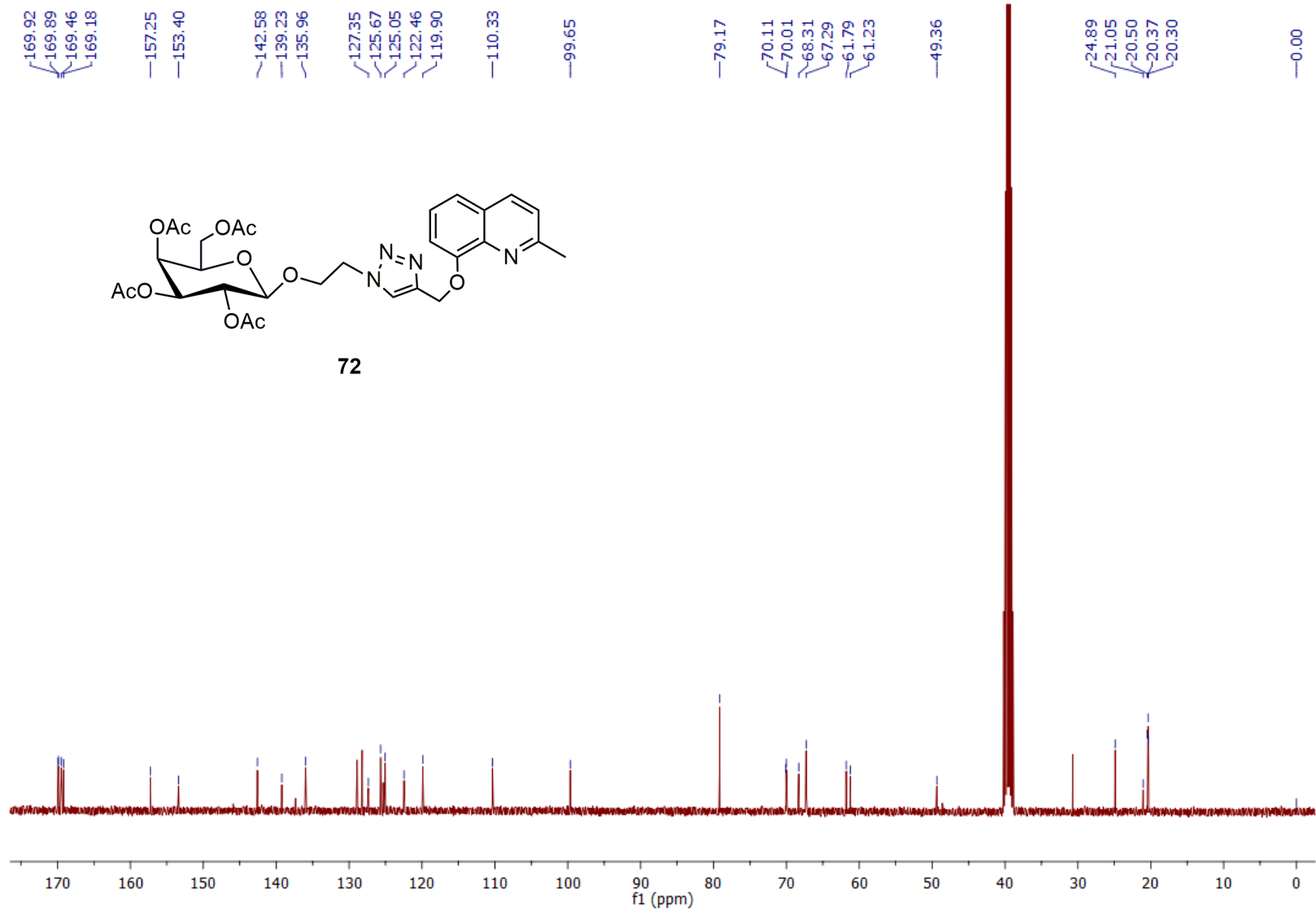


Fig. S136: ^{13}C NMR spectrum of glycoconjugate **72**.

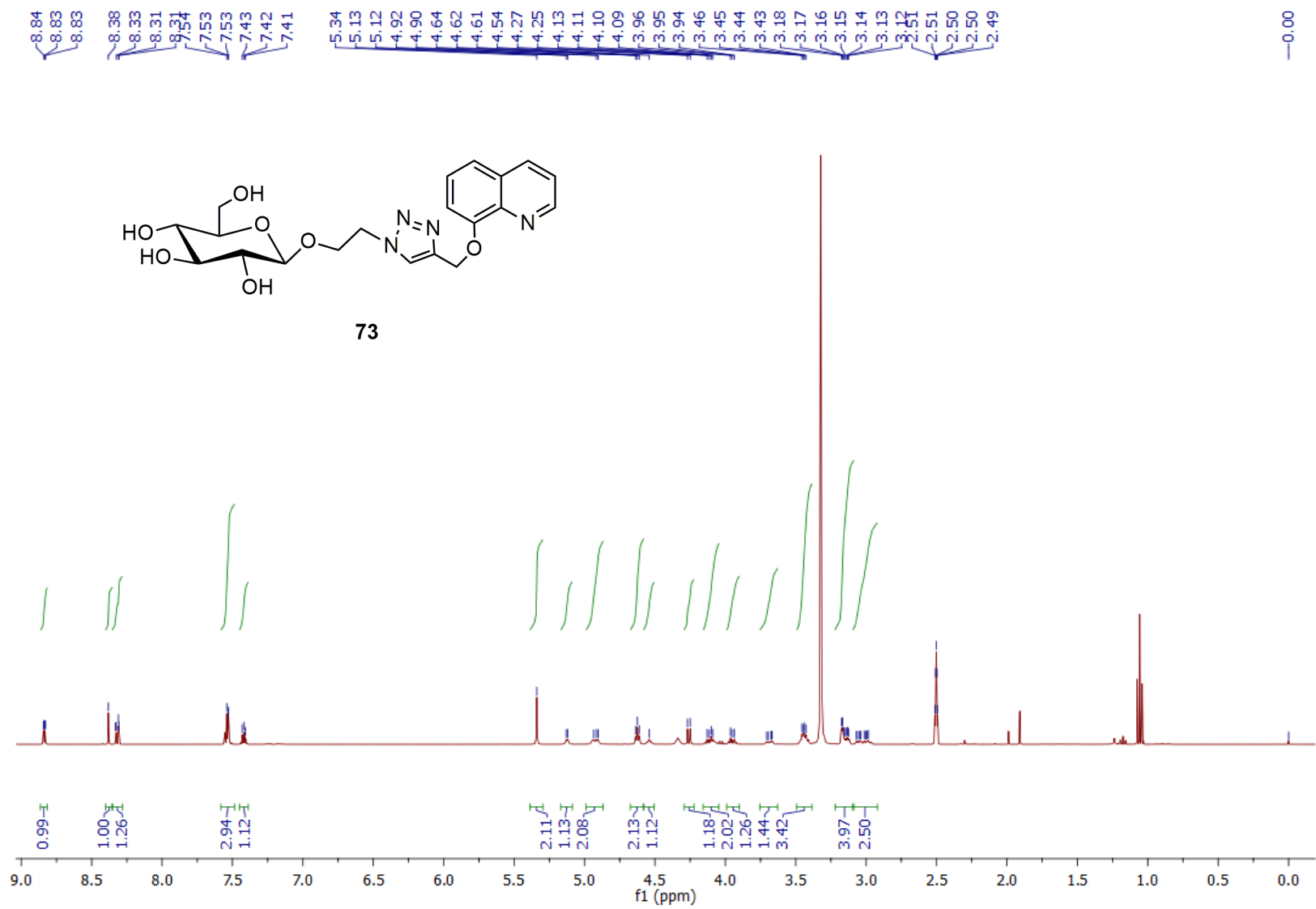


Fig. S137: ^1H NMR spectrum of glycoconjugate **73**.

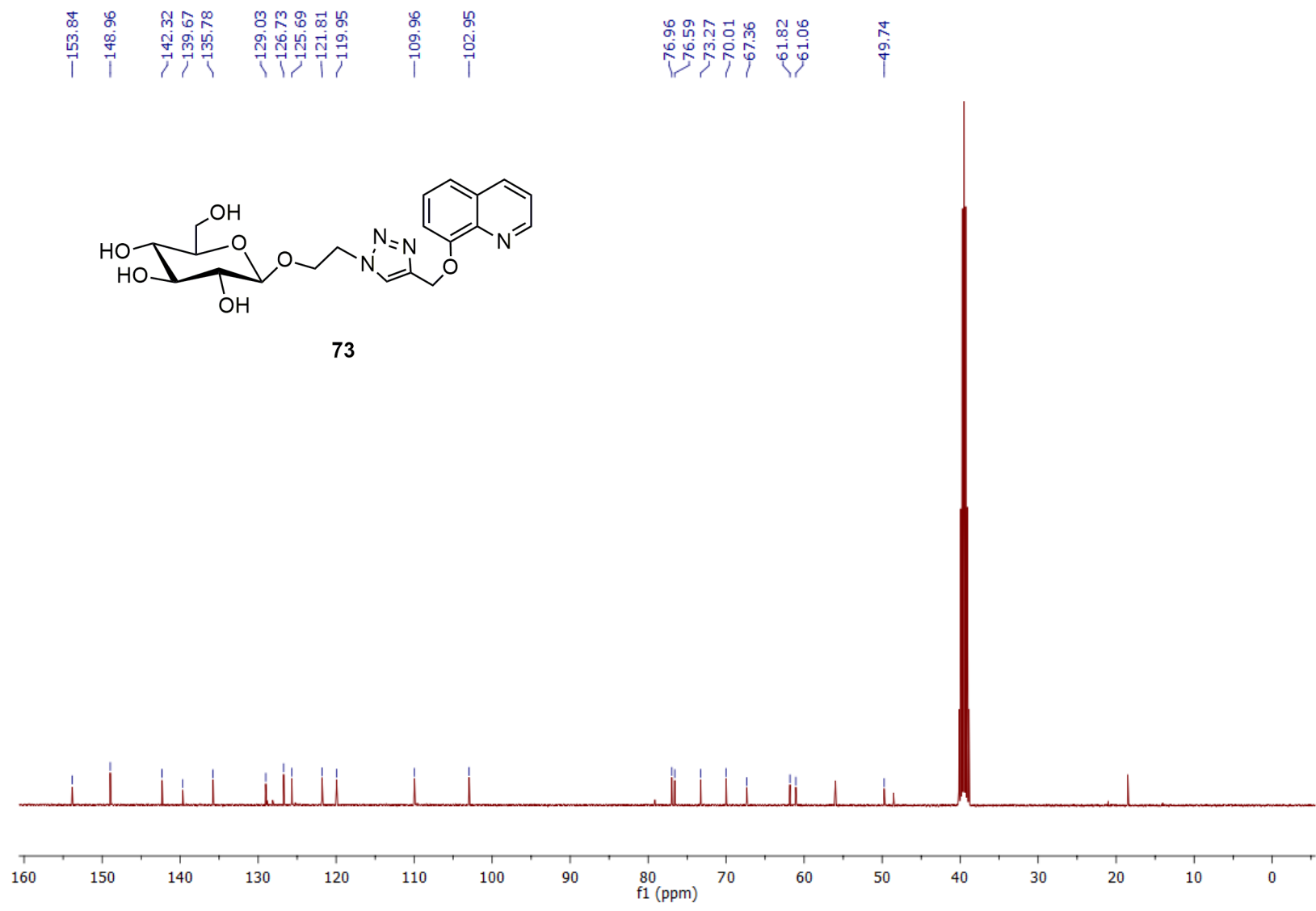


Fig. S138: ¹³C NMR spectrum of glycoconjugate **73**.

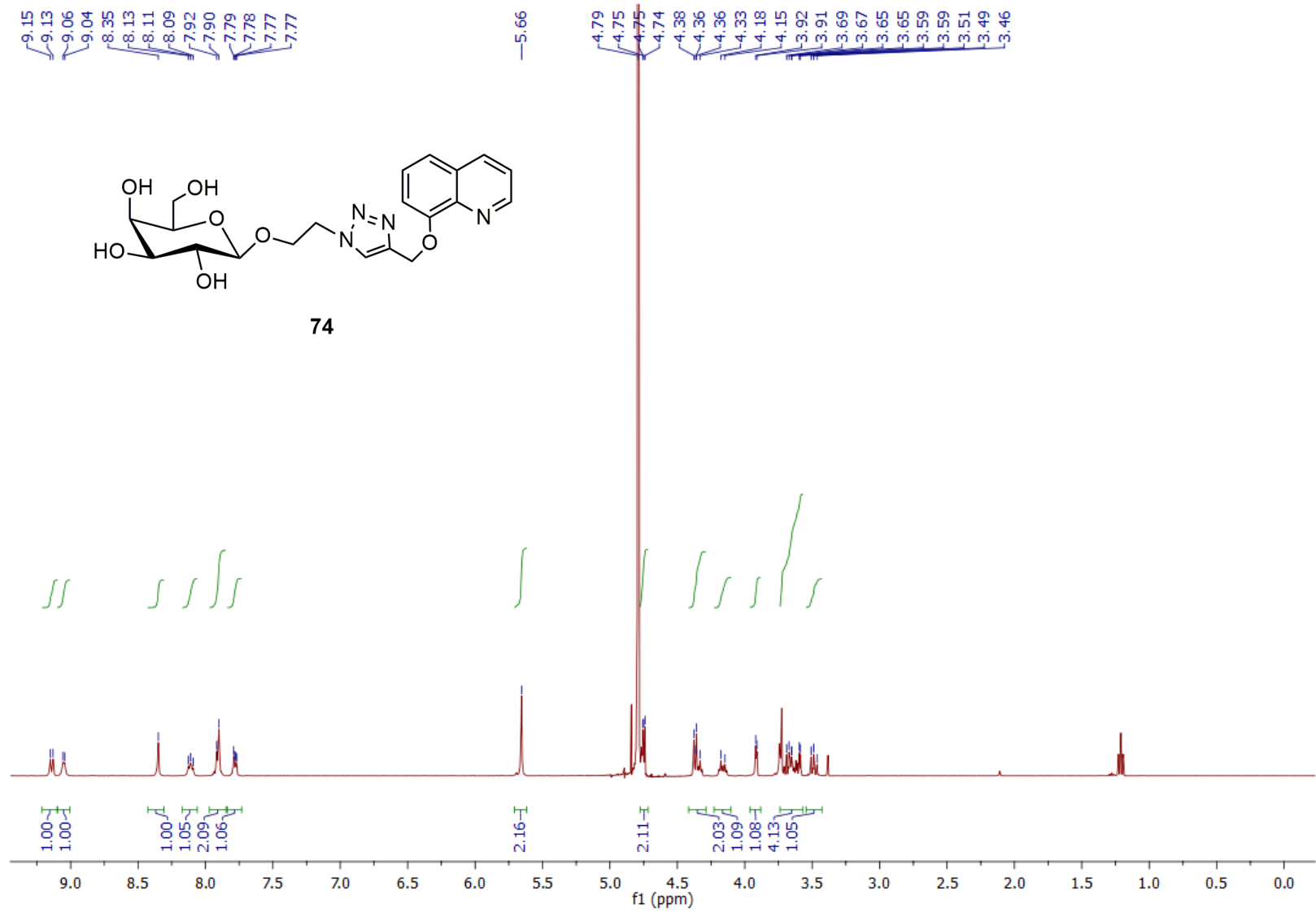


Fig. S139: ^1H NMR spectrum of glycoconjugate **74**.

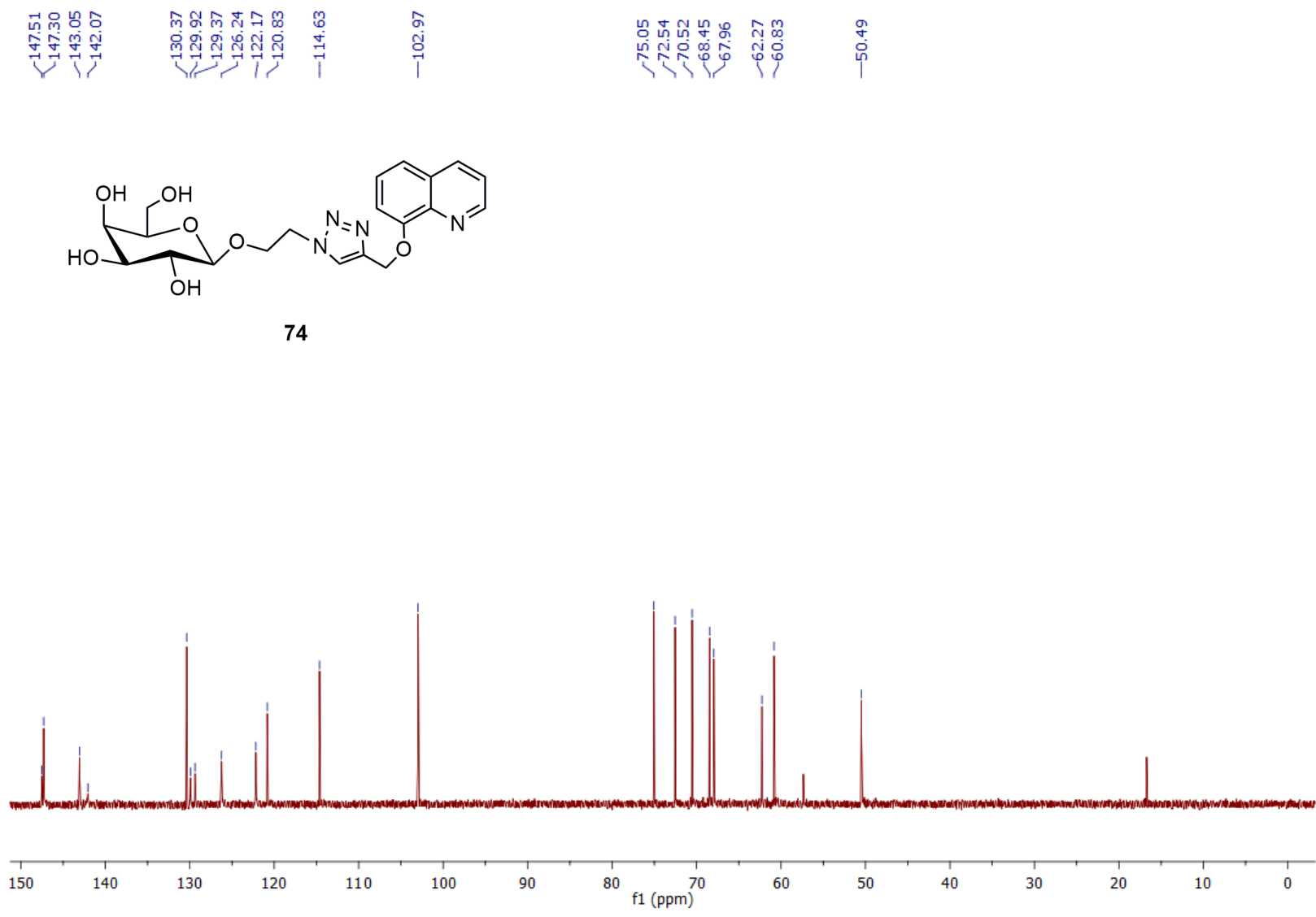


Fig. S140: ^{13}C NMR spectrum of glycoconjugate **74**.

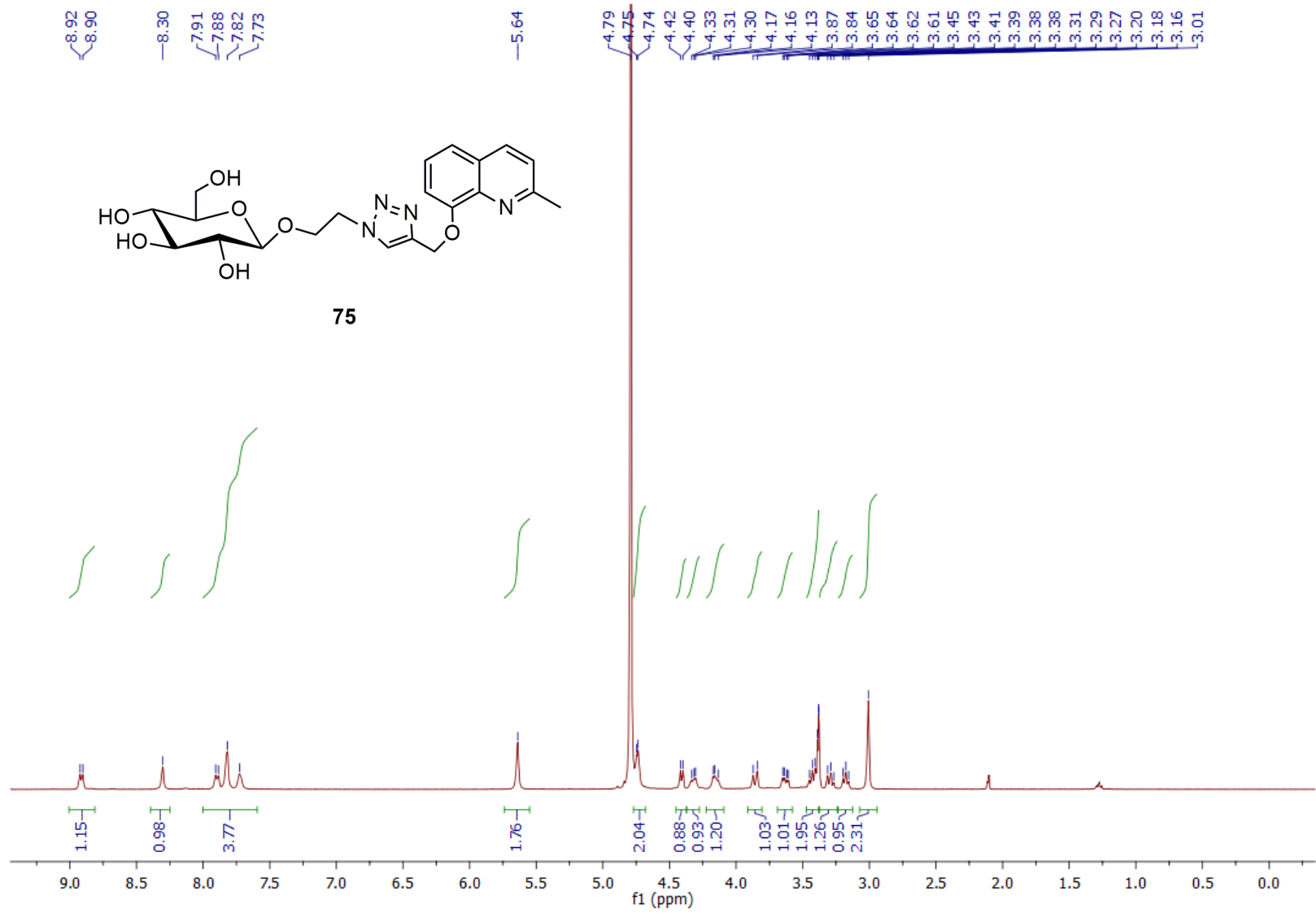


Fig. S141: ¹H NMR spectrum of glycoconjugate **75**.

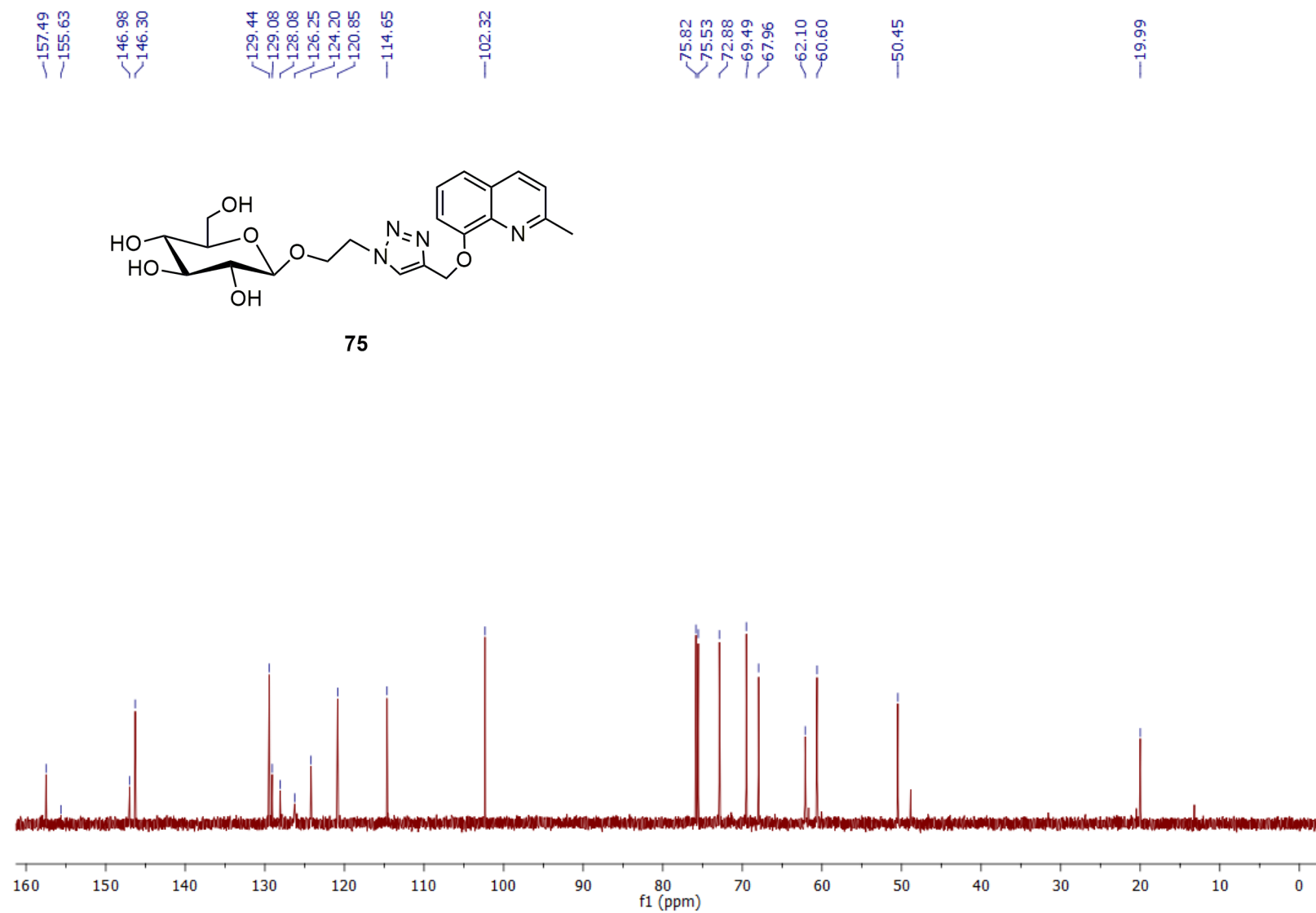


Fig. S142: ^{13}C NMR spectrum of glycoconjugate **75**.

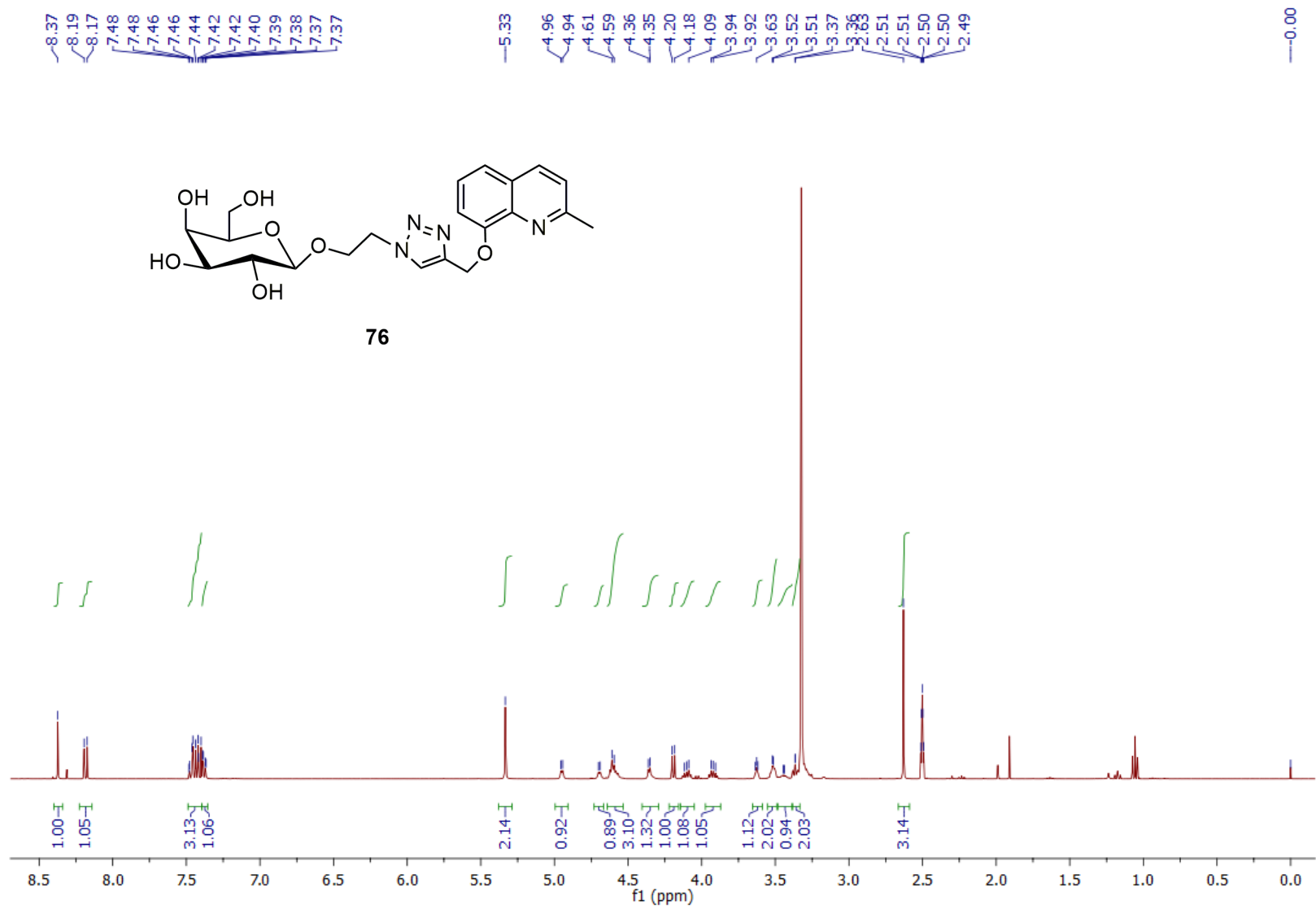


Fig. S143: ^1H NMR spectrum of glycoconjugate **76**.

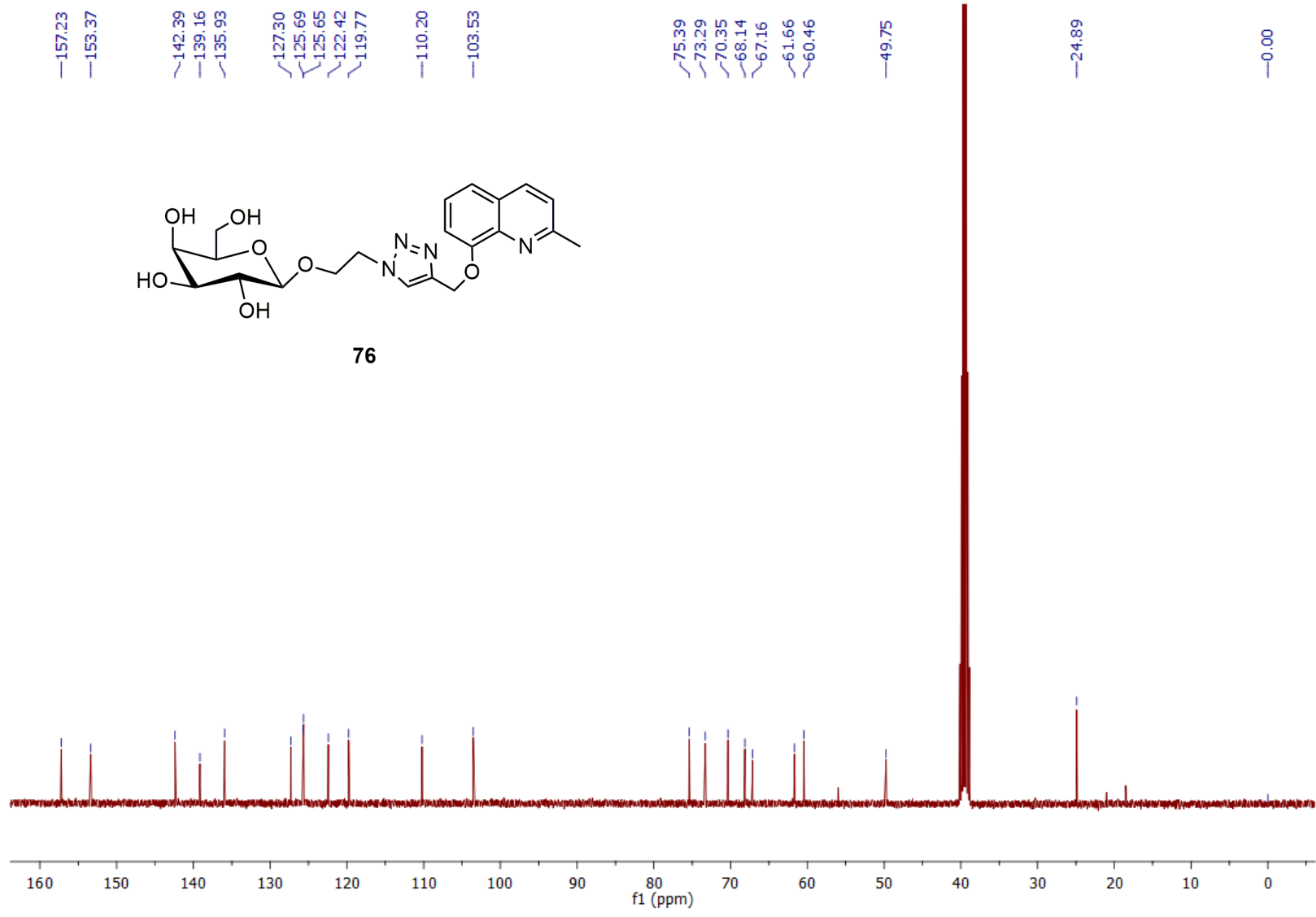


Fig. S144: ^{13}C NMR spectrum of glycoconjugate **76**.

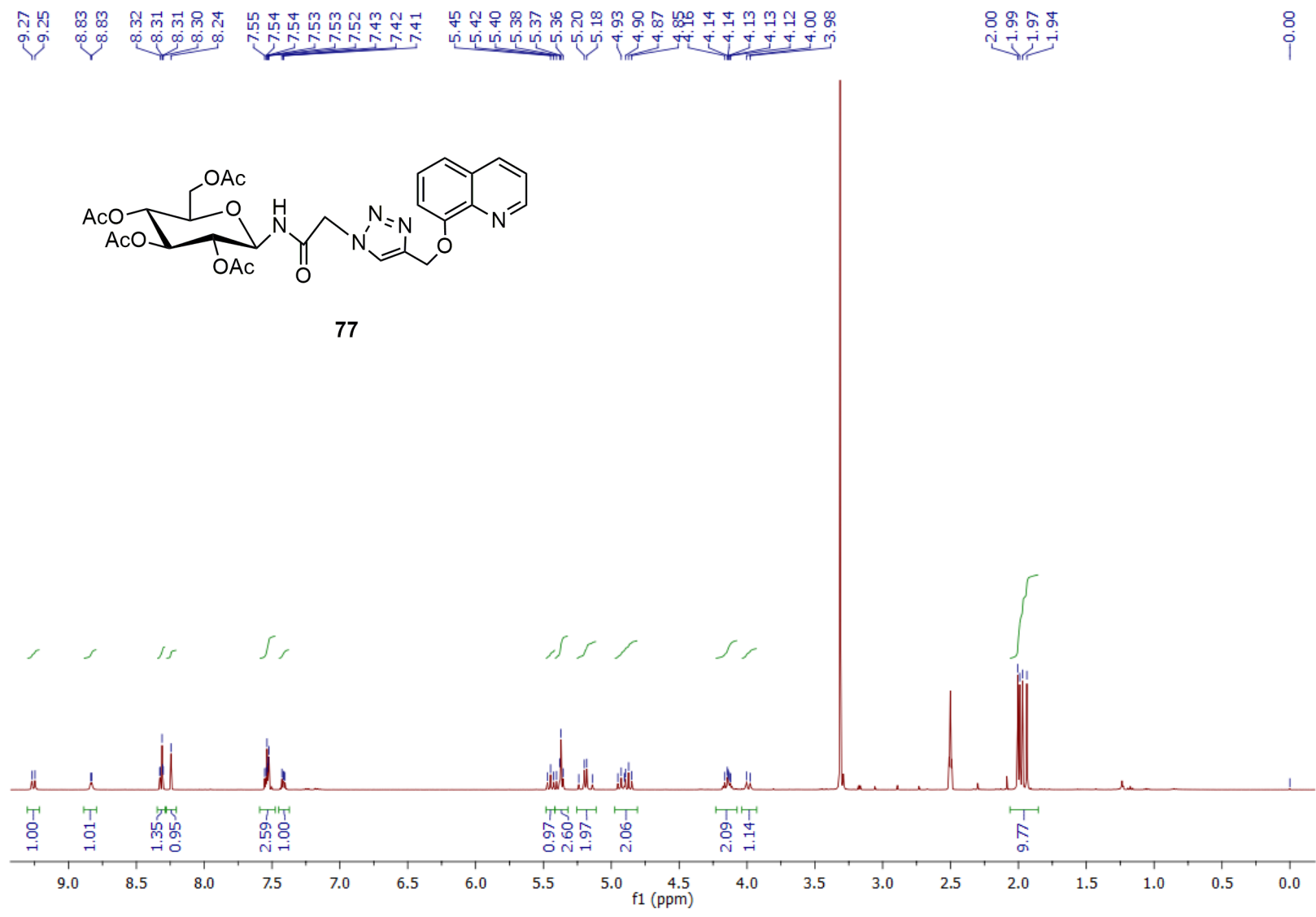


Fig. S145: ¹H NMR spectrum of glycoconjugate **77**.

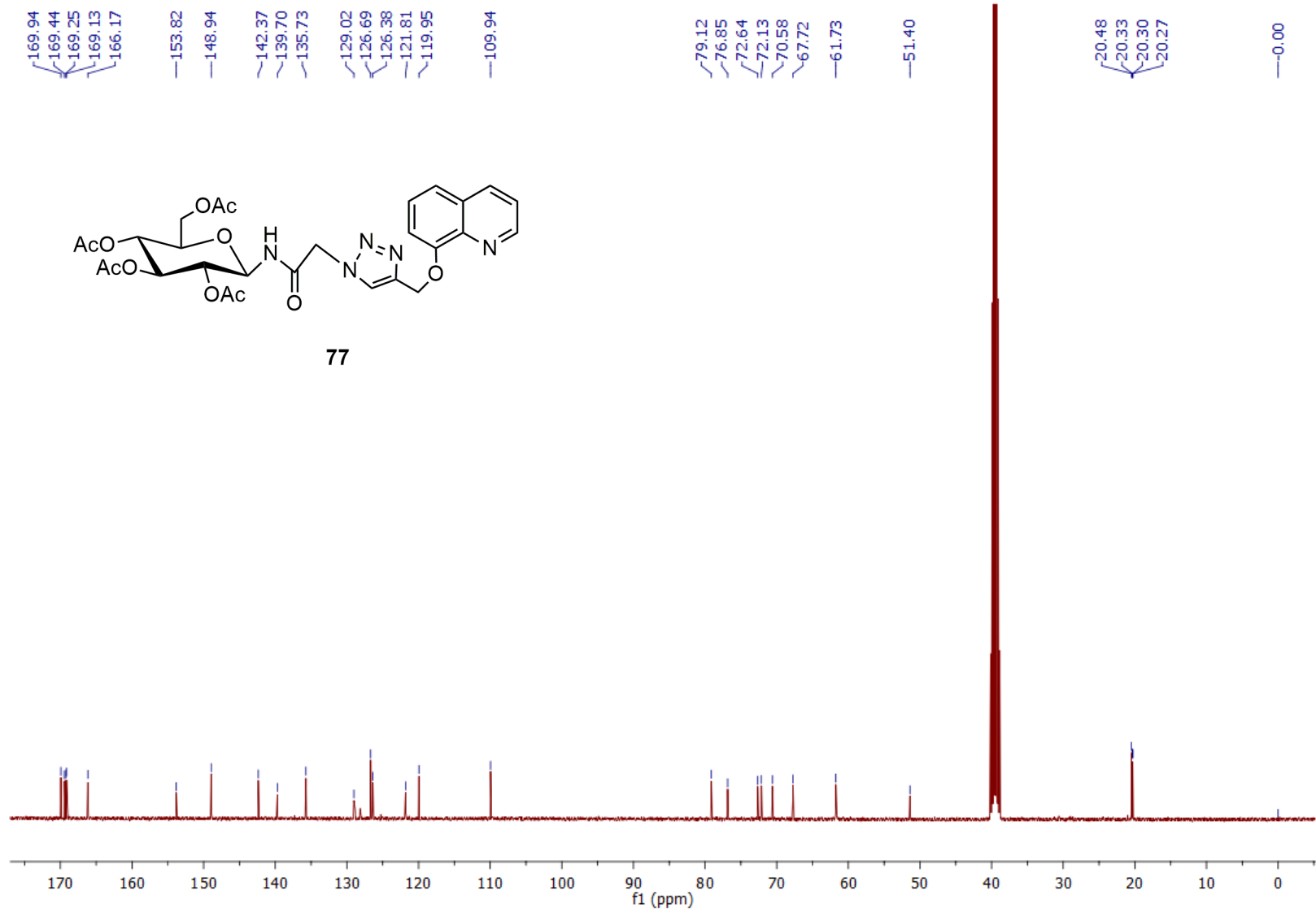


Fig. S146: ^{13}C NMR spectrum of glycoconjugate **77**.

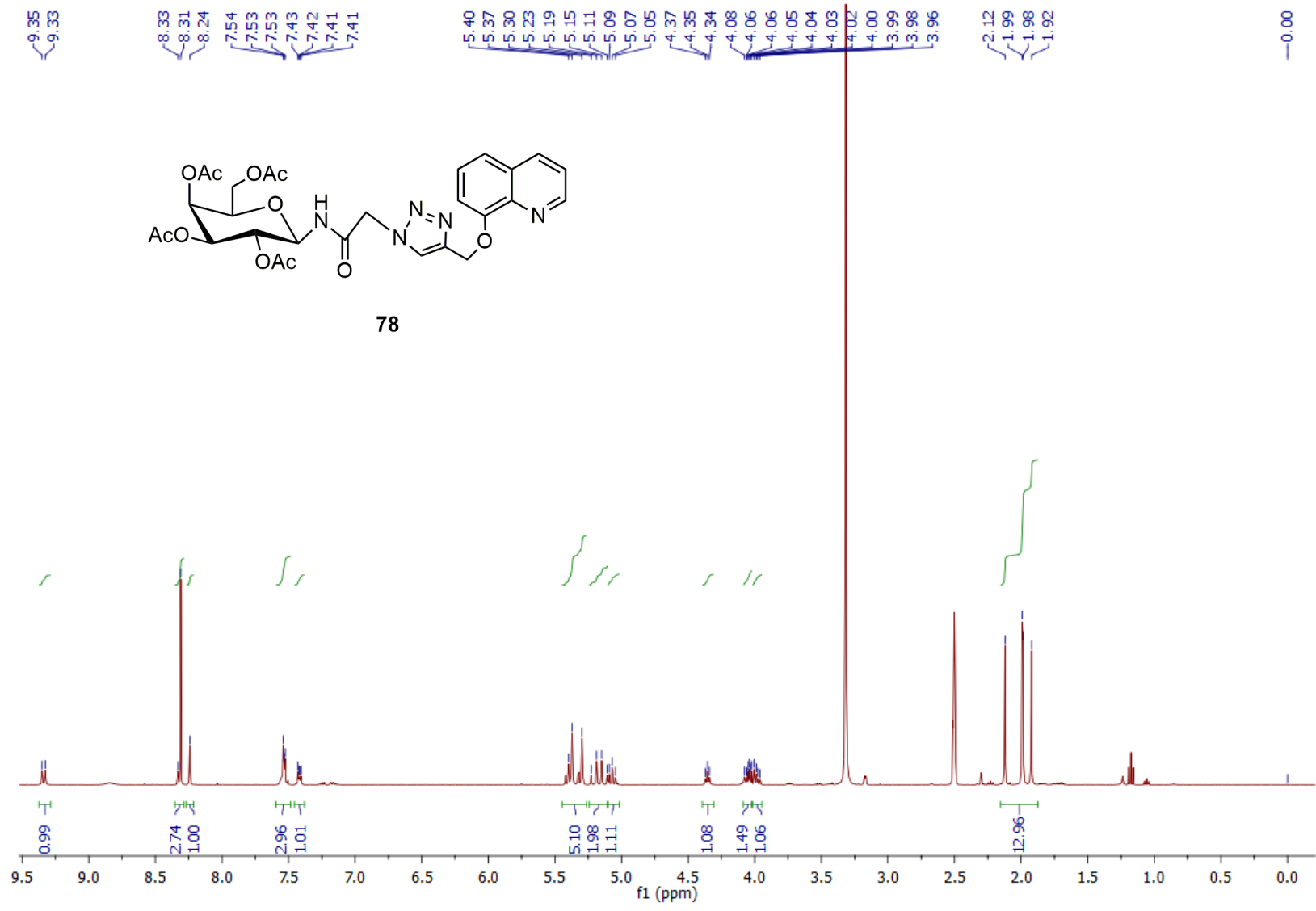


Fig. S147: ¹H NMR spectrum of glycoconjugate **78**.

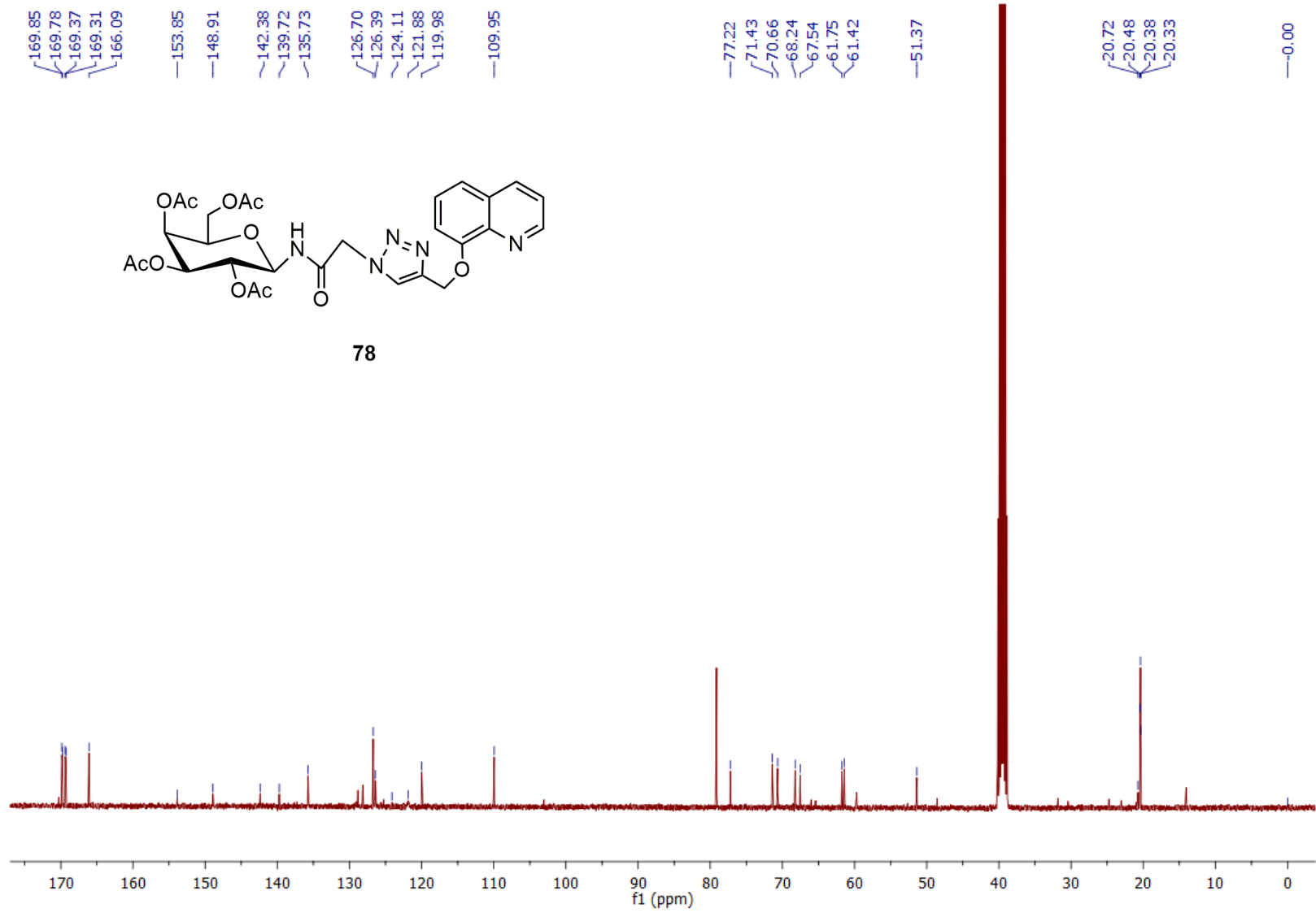


Fig. S148: ^{13}C NMR spectrum of glycoconjugate **78**.

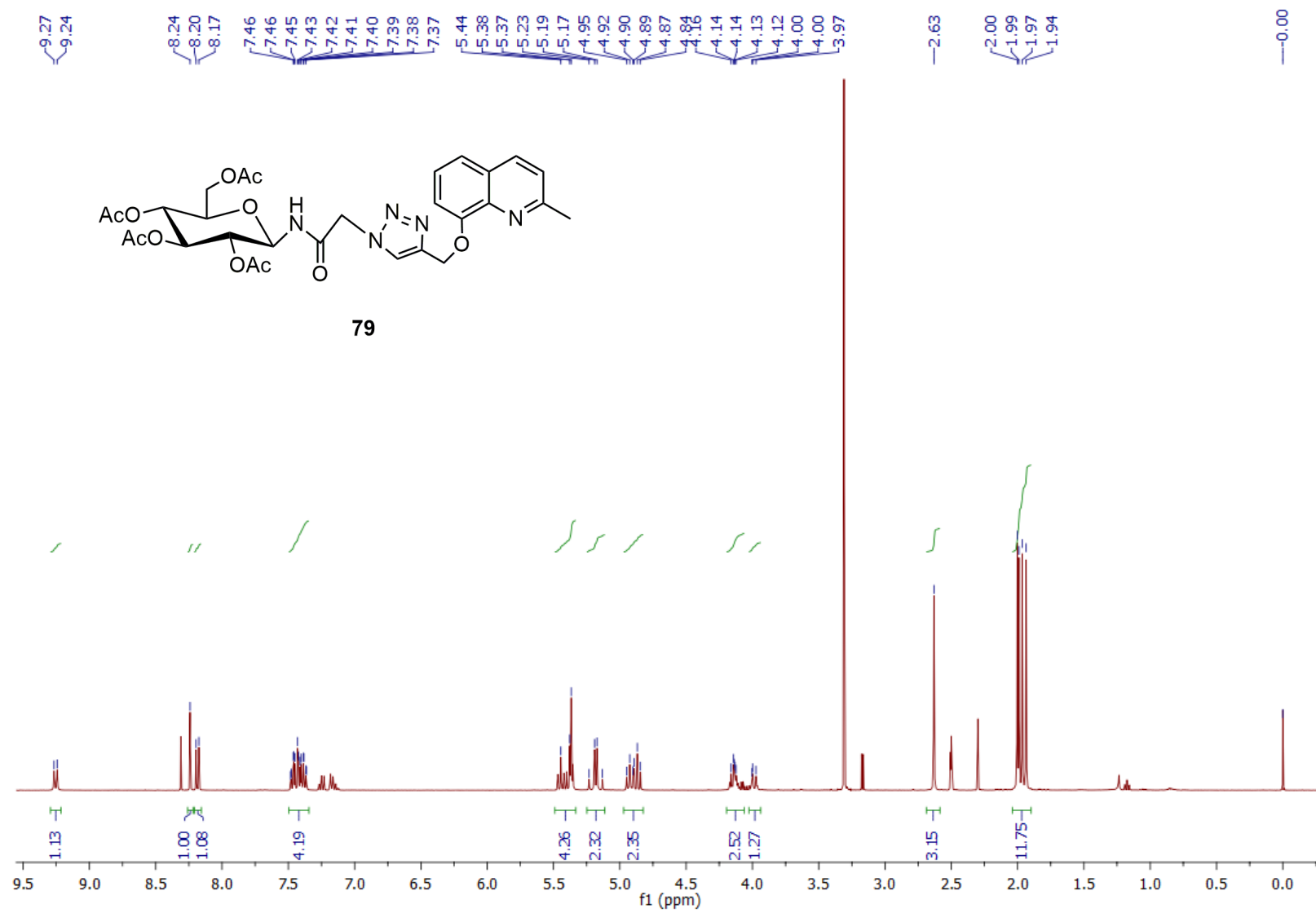


Fig. S149: ^1H NMR spectrum of glycoconjugate **79**.

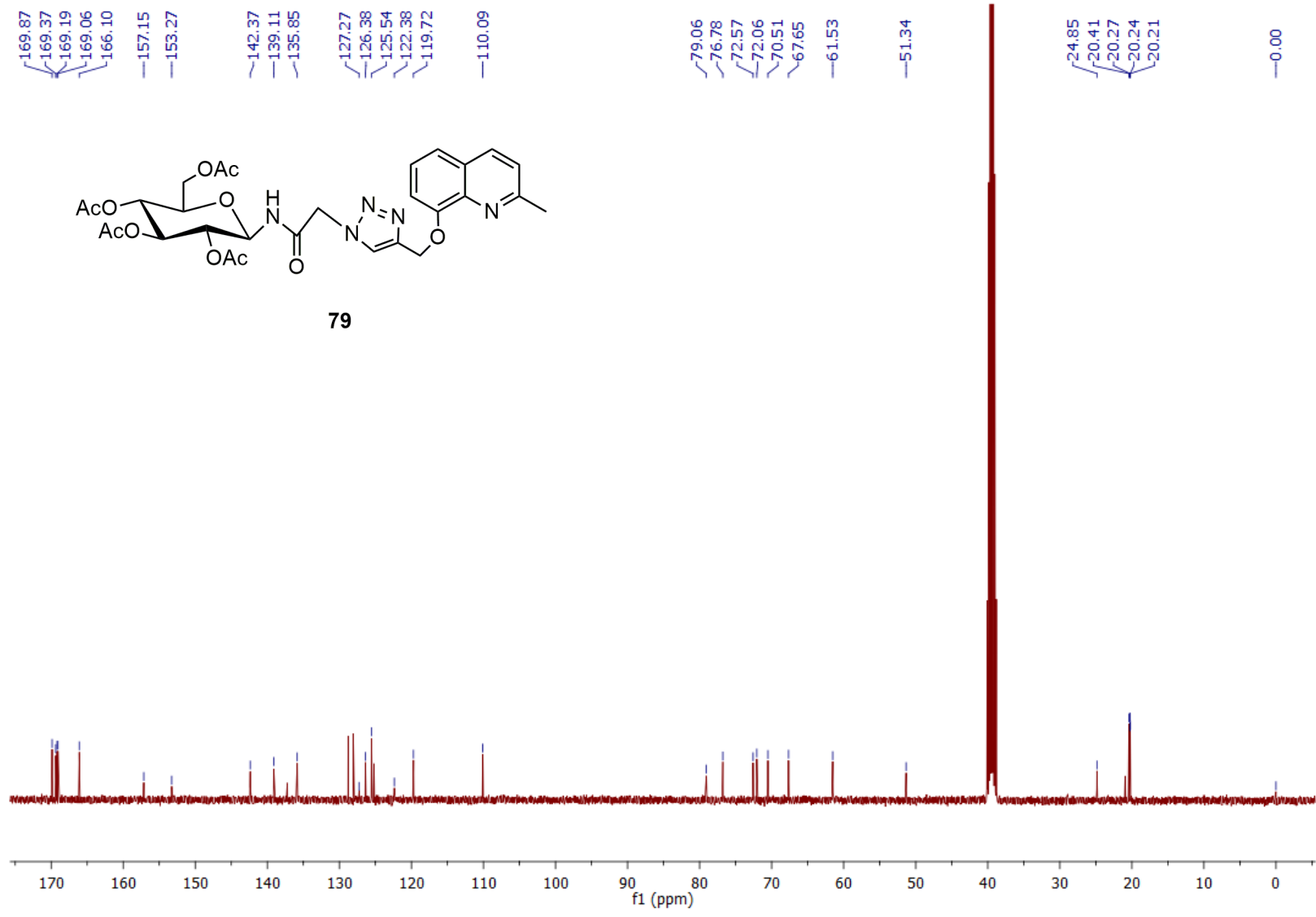


Fig. S150: ^{13}C NMR spectrum of glycoconjugate **79**.

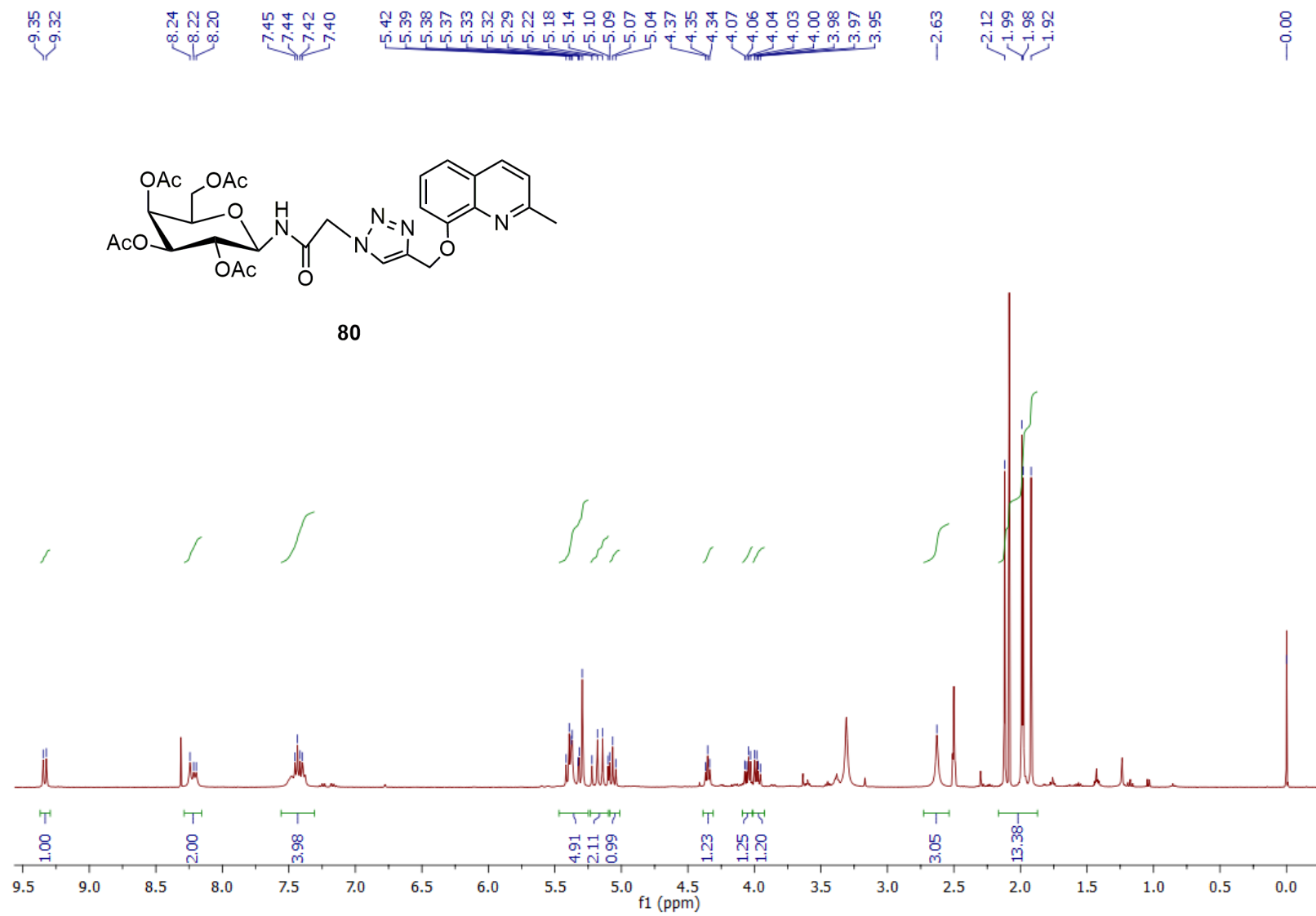


Fig. S151: ^1H NMR spectrum of glycoconjugate **80**.

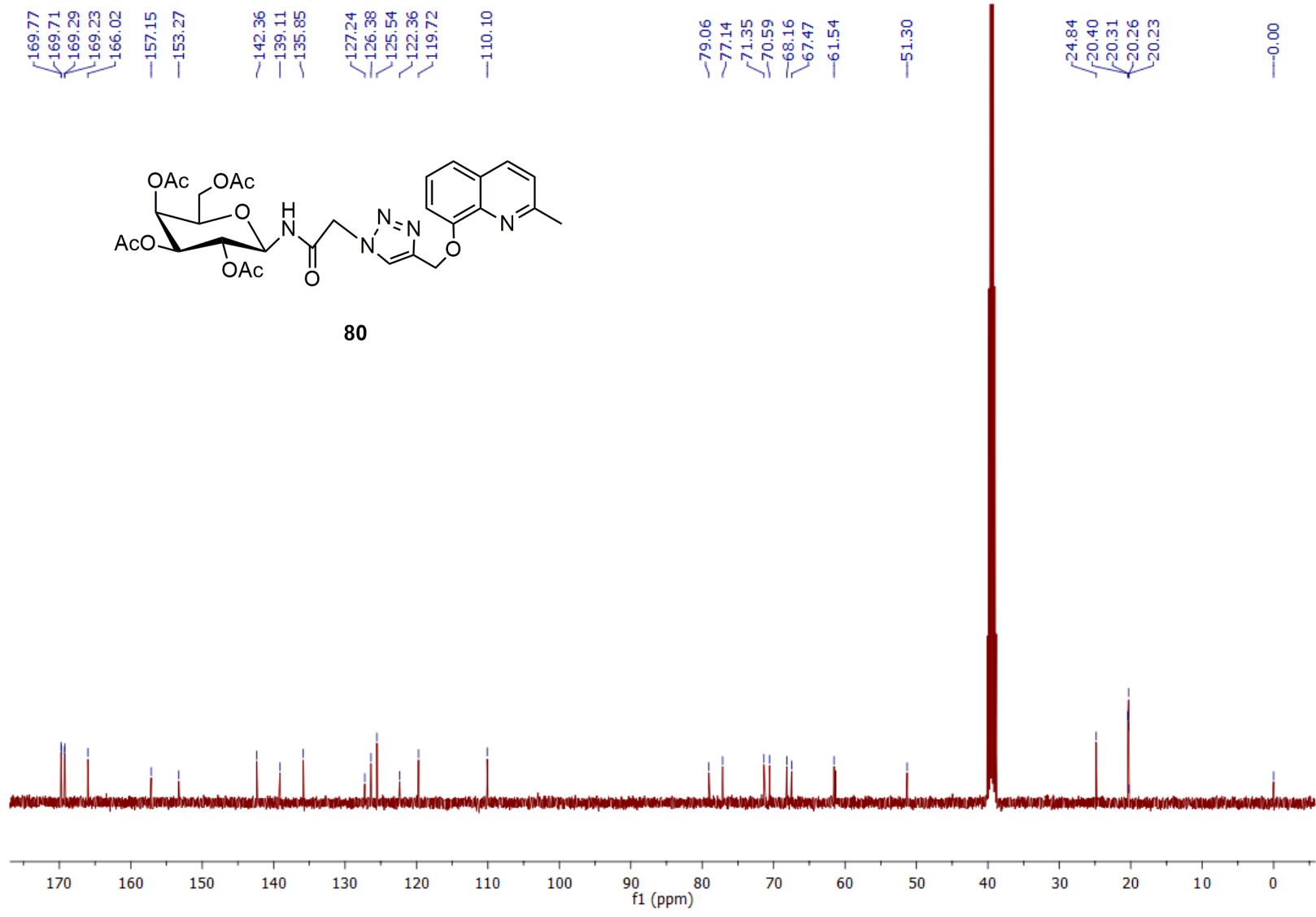


Fig. S152: ^{13}C NMR spectrum of glycoconjugate **80**.

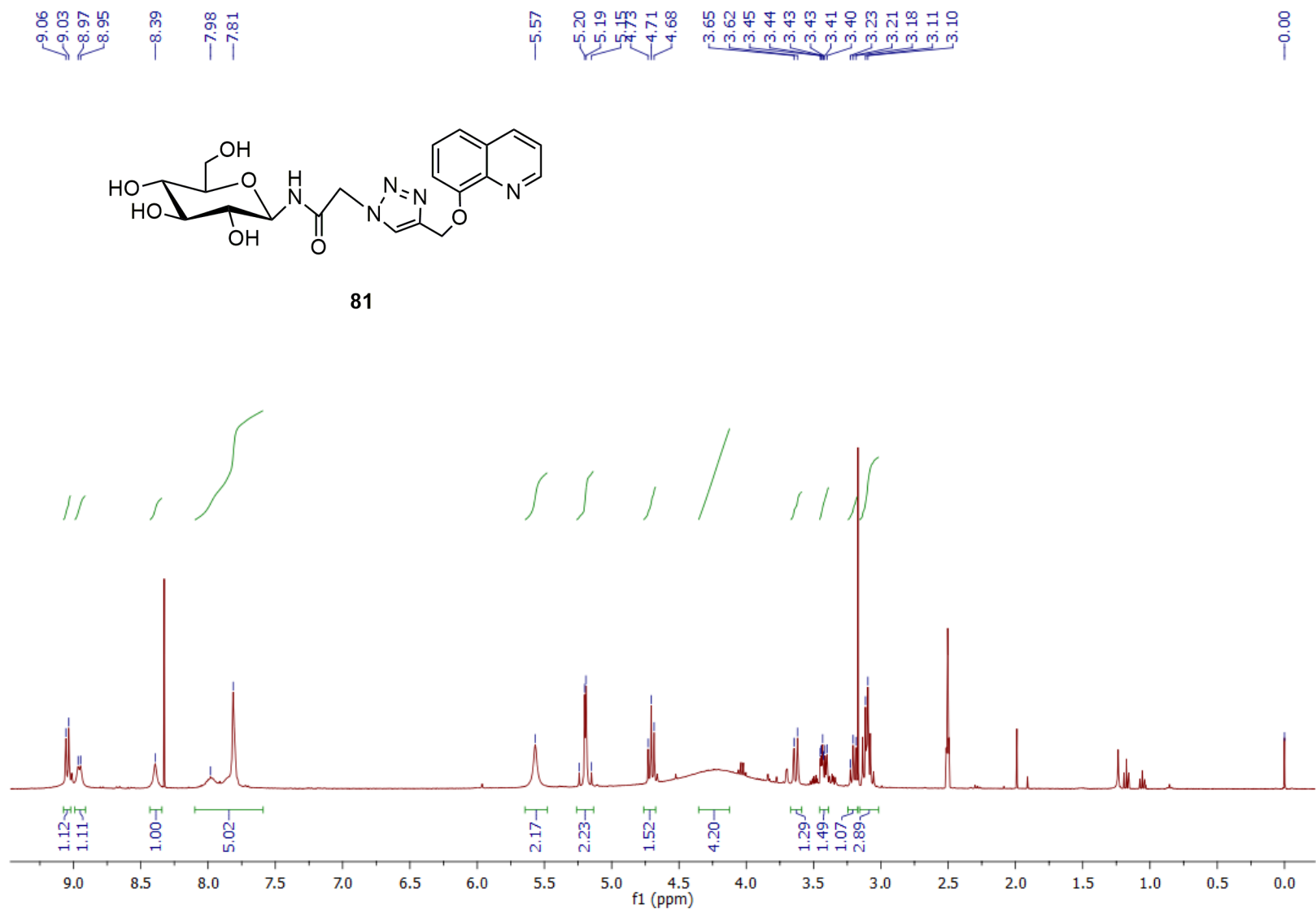


Fig. S153: ^1H NMR spectrum of glycoconjugate **81**.

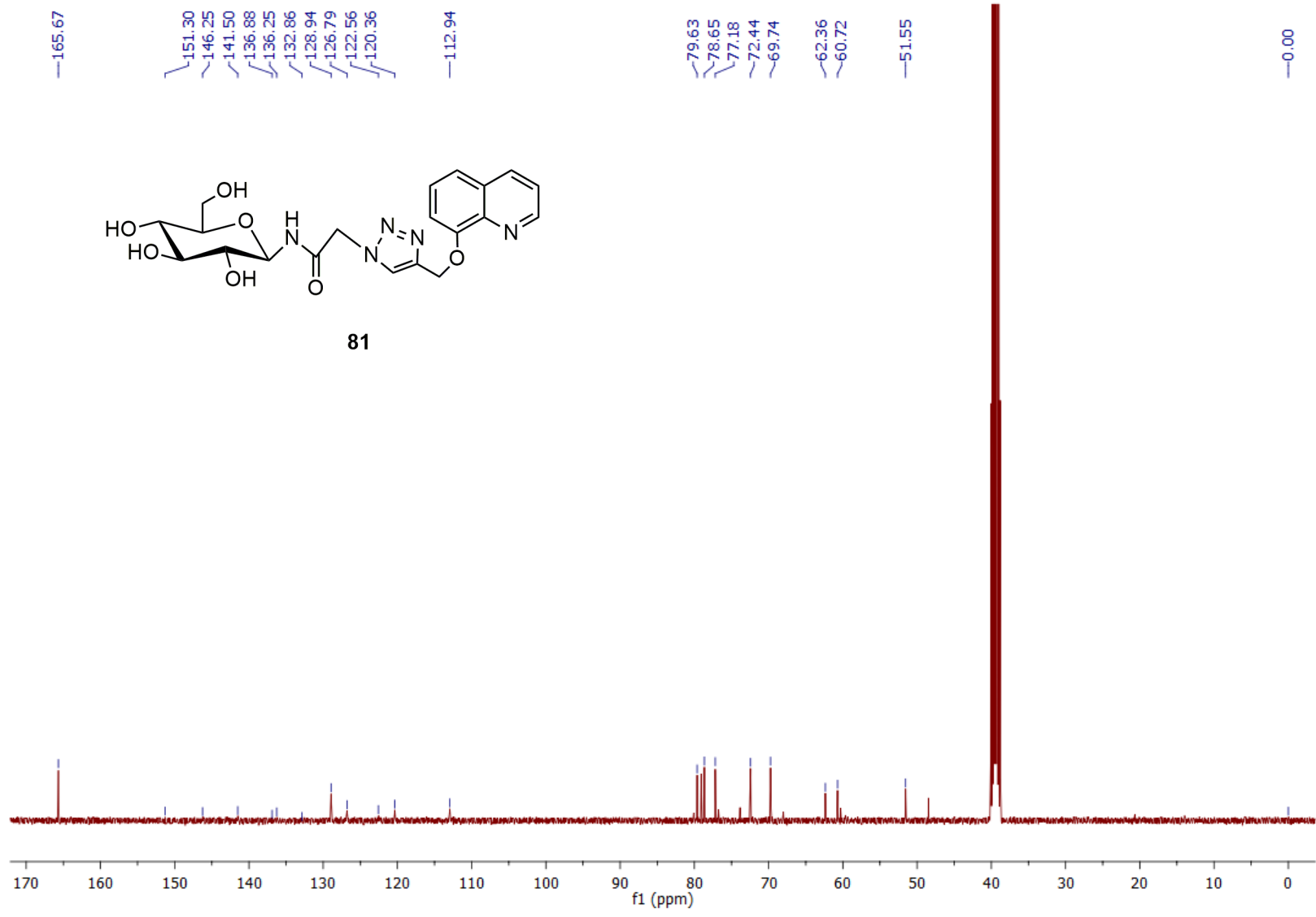


Fig. S154: ¹³C NMR spectrum of glycoconjugate **81**.

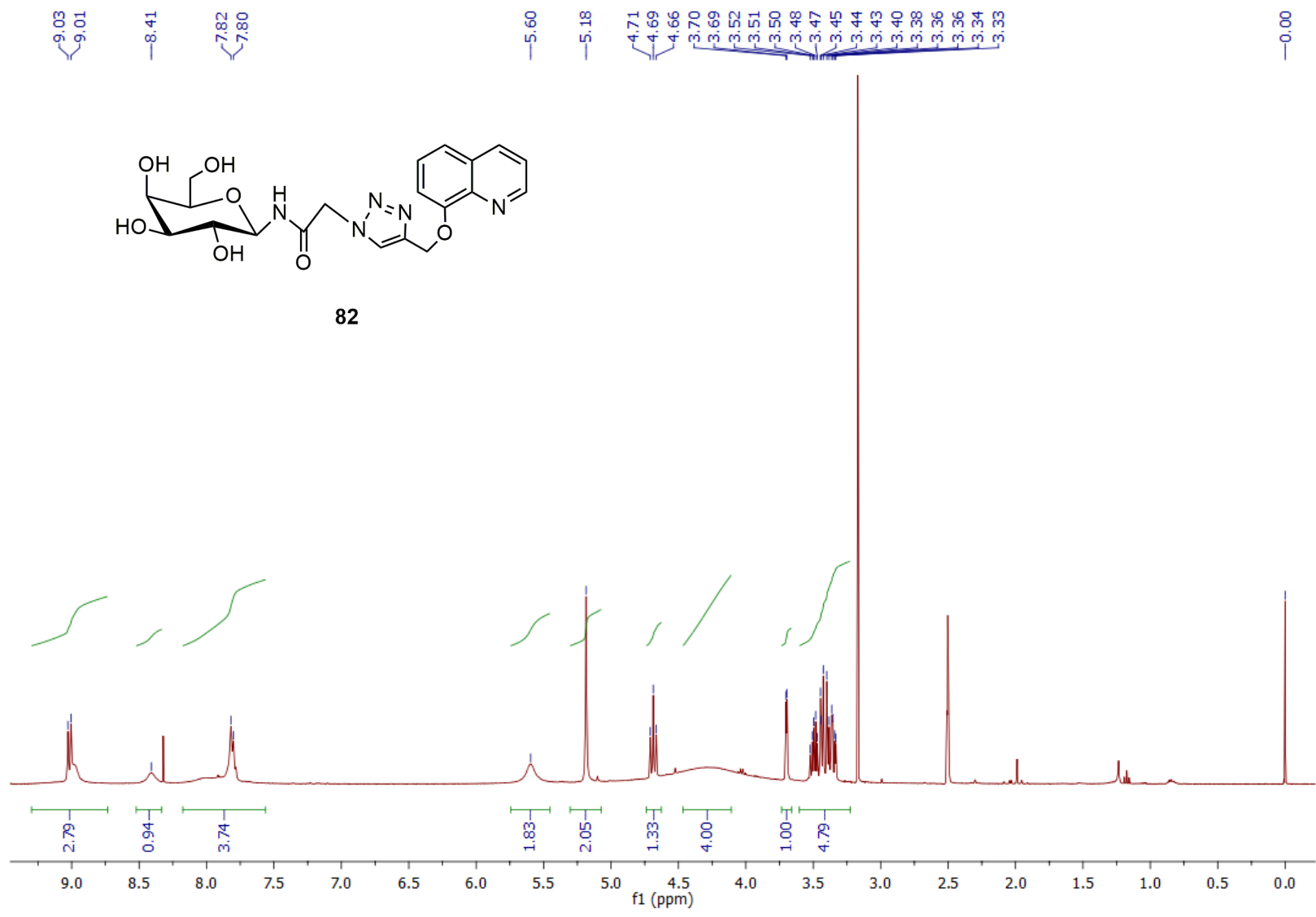


Fig. S155: ^1H NMR spectrum of glycoconjugate **82**.

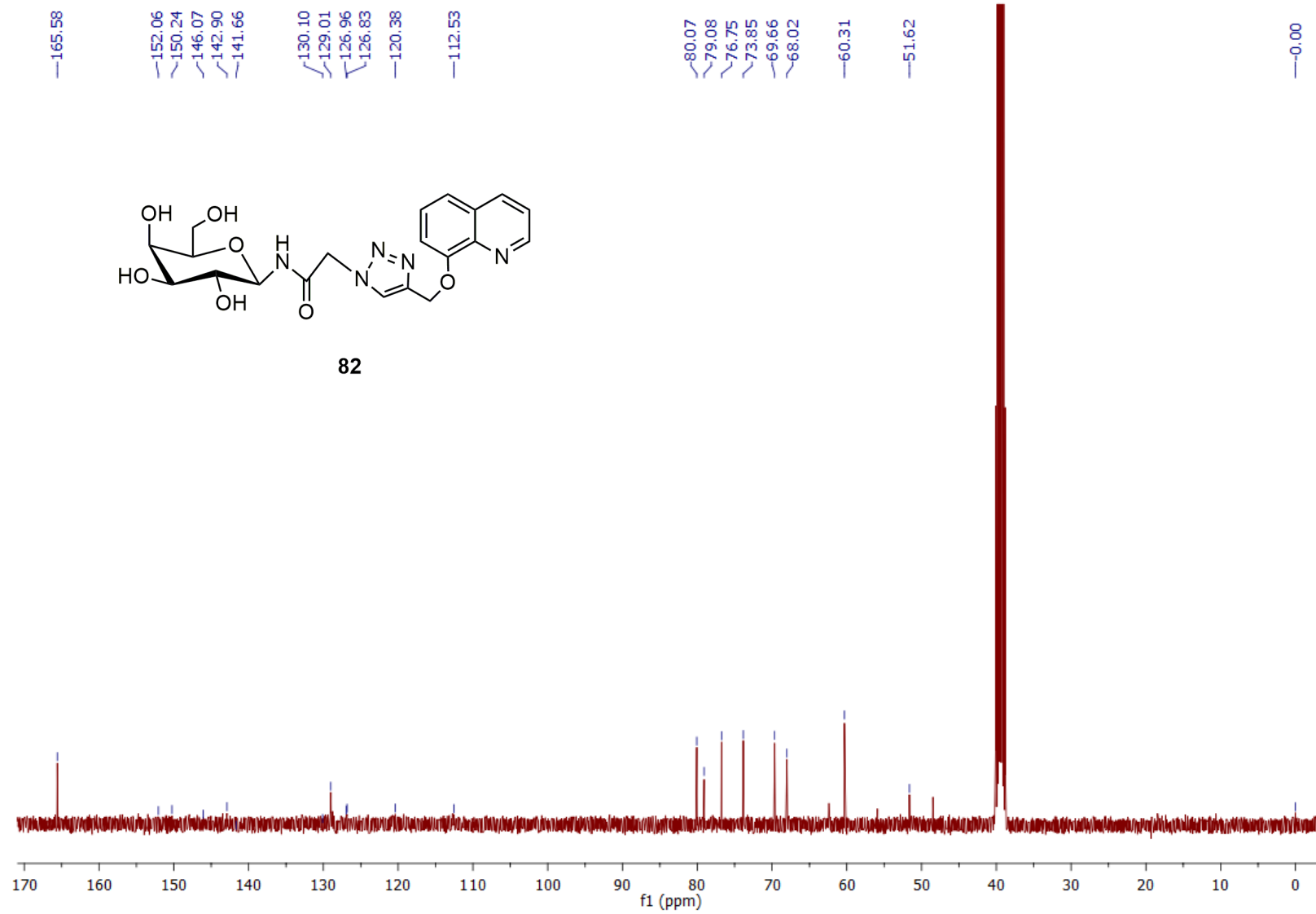


Fig. S156: ^{13}C NMR spectrum of glycoconjugate **82**.

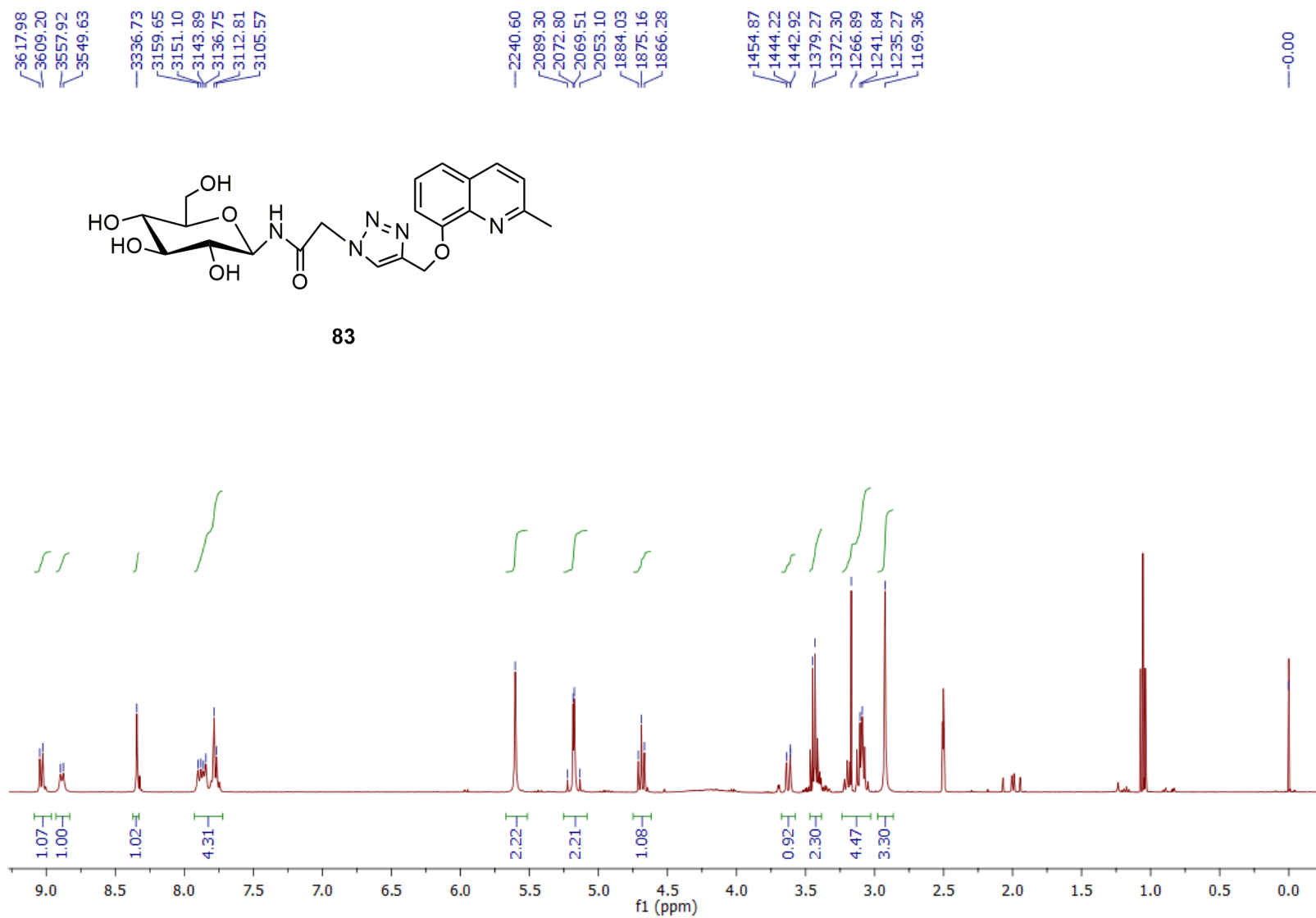


Fig. S157: ^1H NMR spectrum of glycoconjugate **83**.

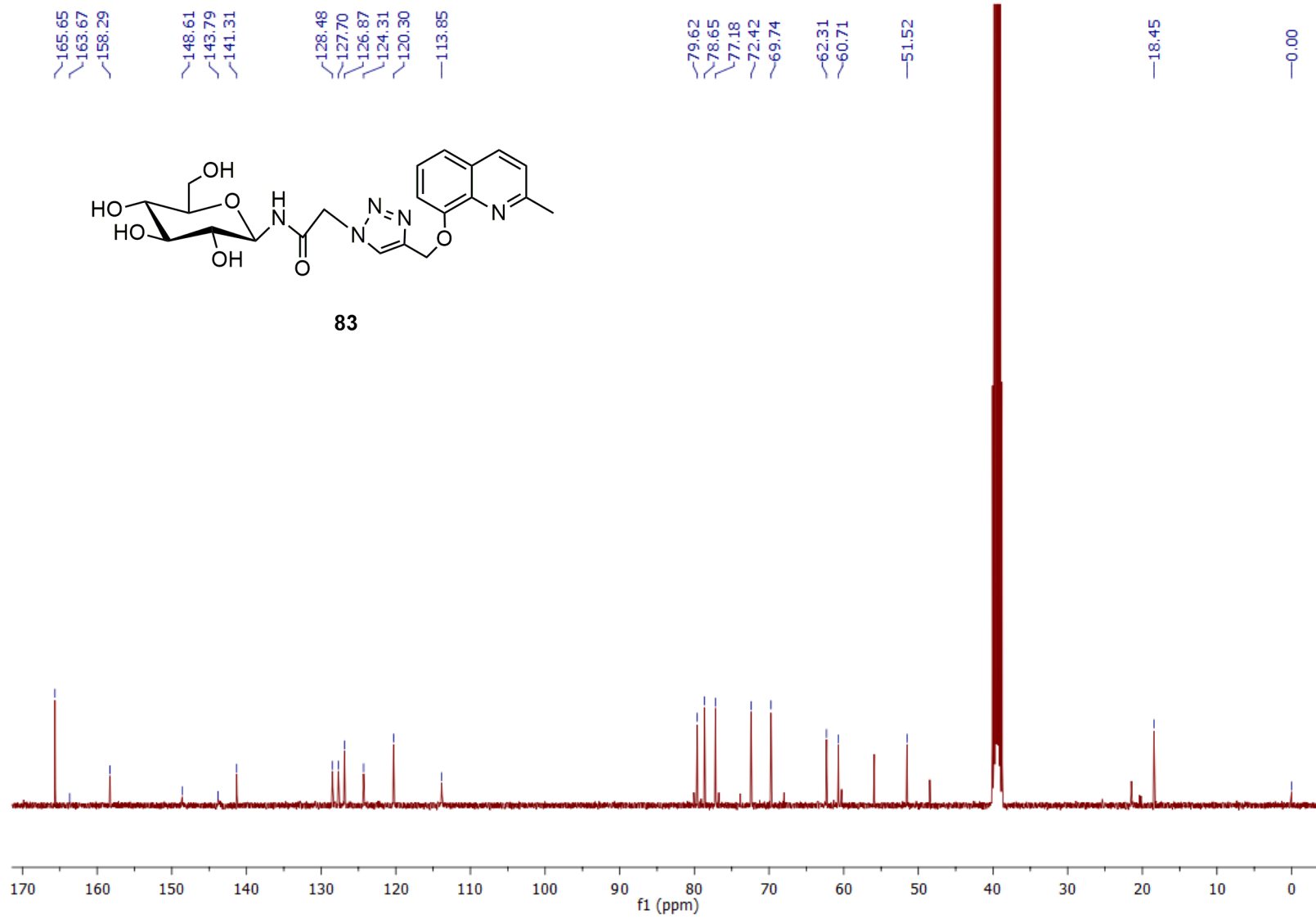


Fig. S158: ^{13}C NMR spectrum of glycoconjugate **83**.

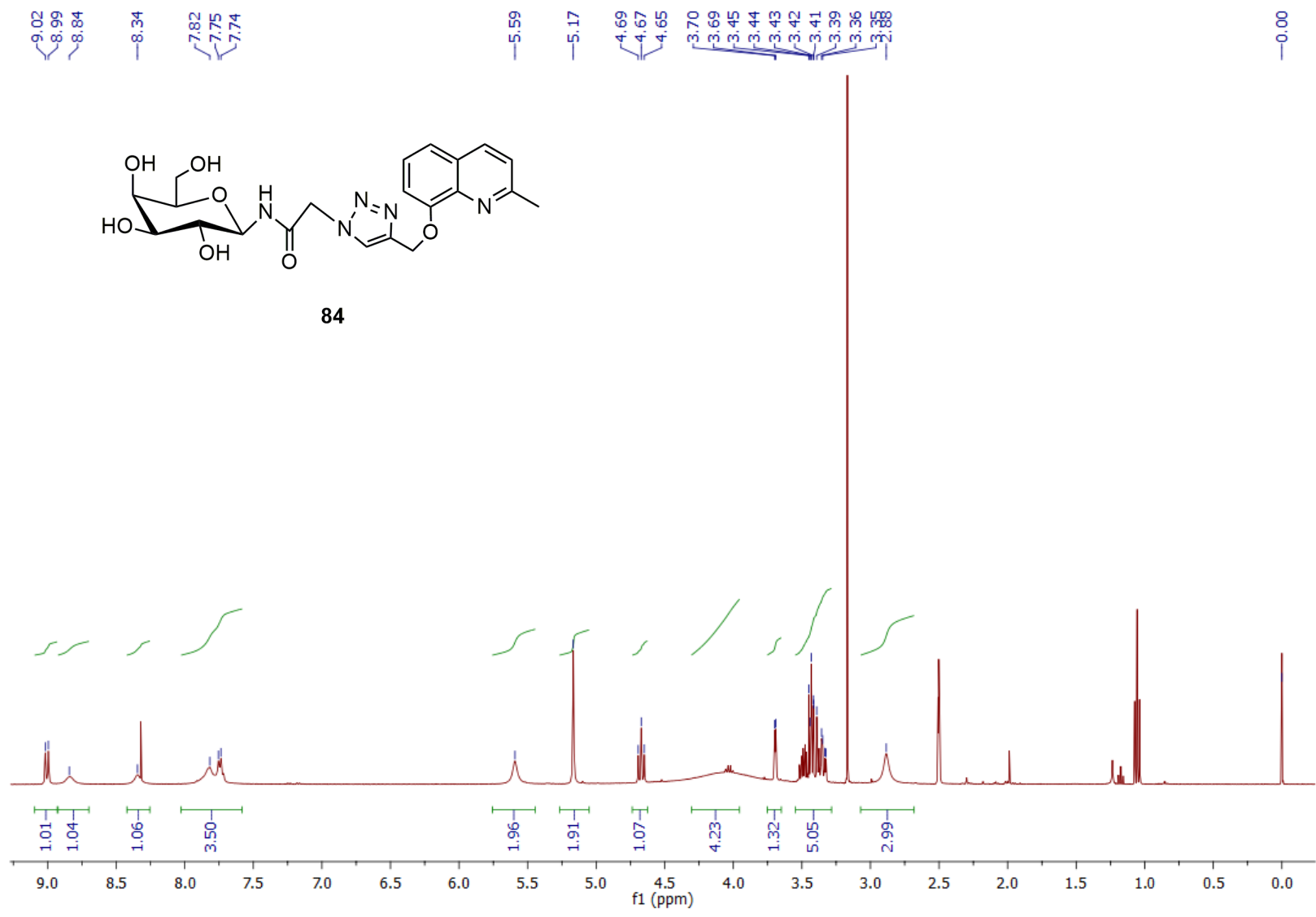


Fig. S159: ^1H NMR spectrum of glycoconjugate **84**.

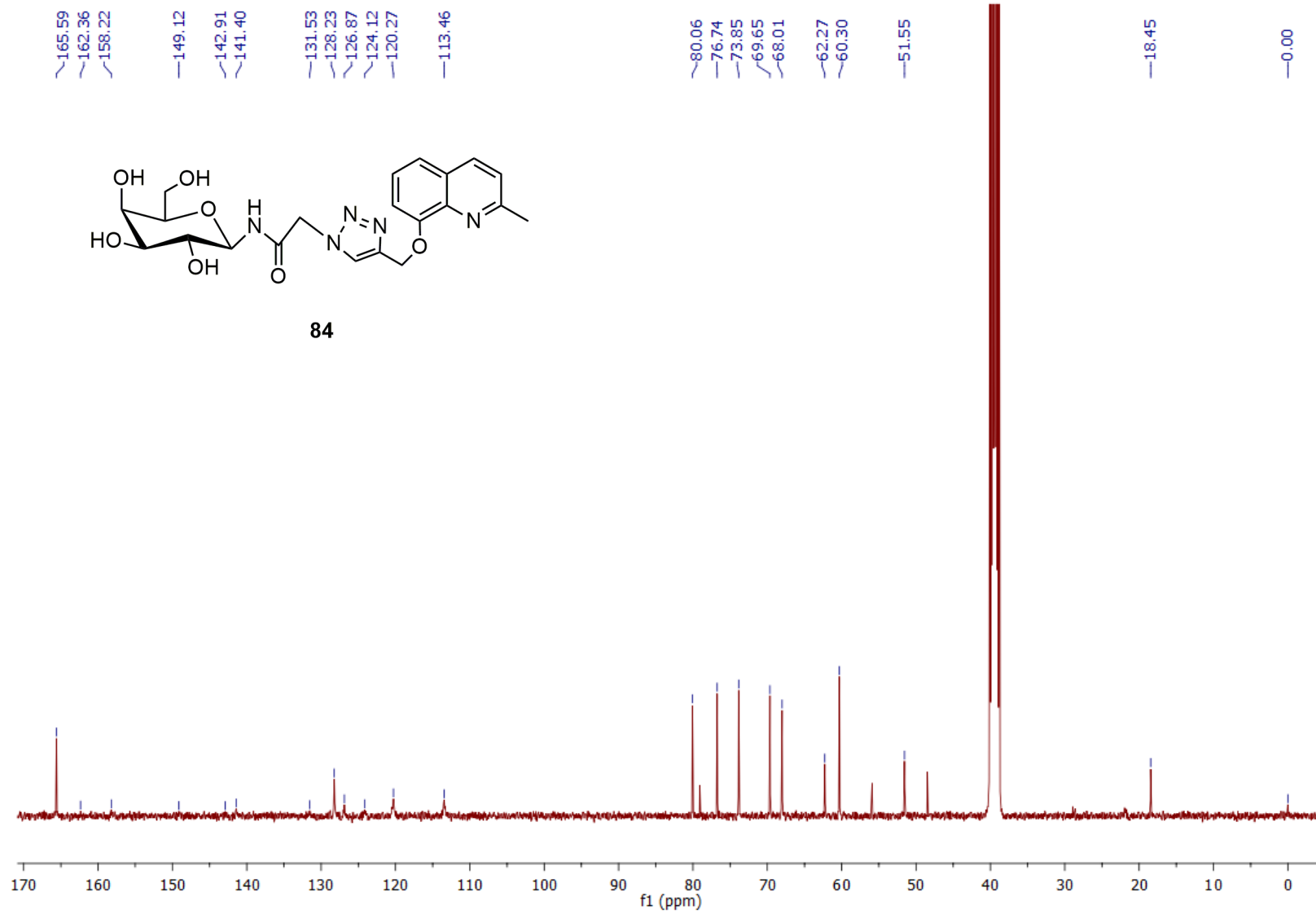


Fig. S160: ^{13}C NMR spectrum of glycoconjugate **84**.

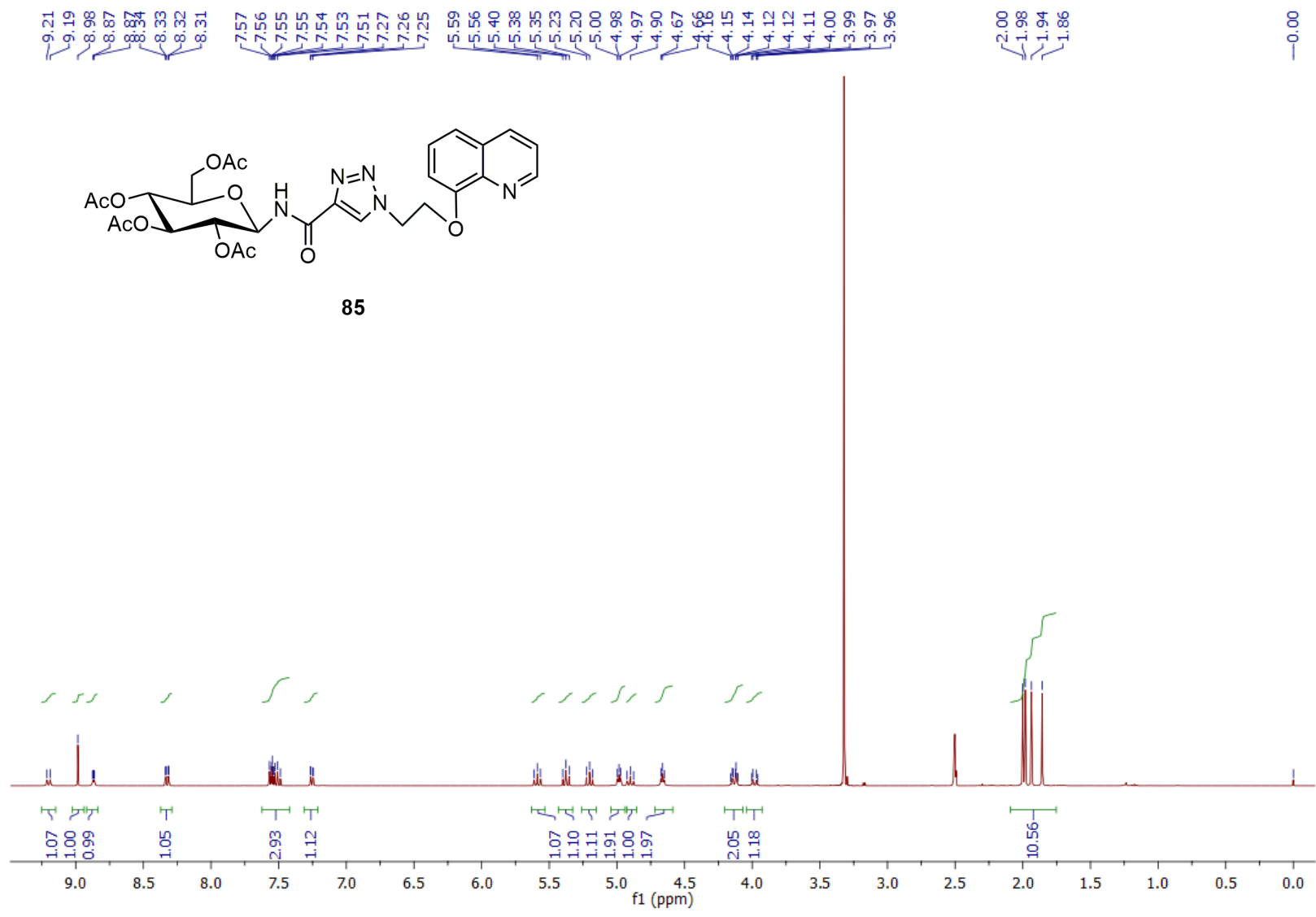


Fig. S161: ¹H NMR spectrum of glycoconjugate **85**.

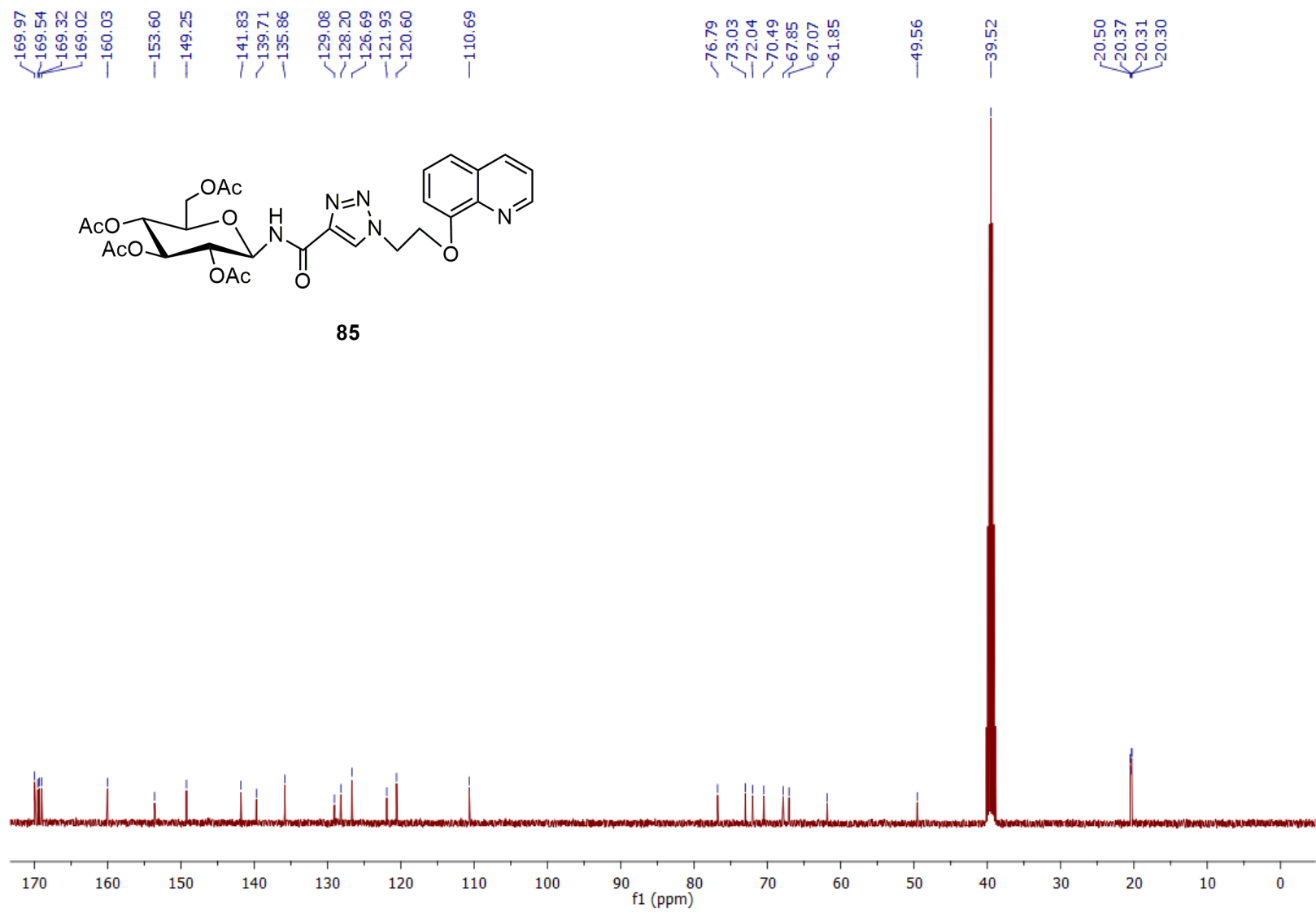


Fig. S162: ^{13}C NMR spectrum of glycoconjugate **85**.

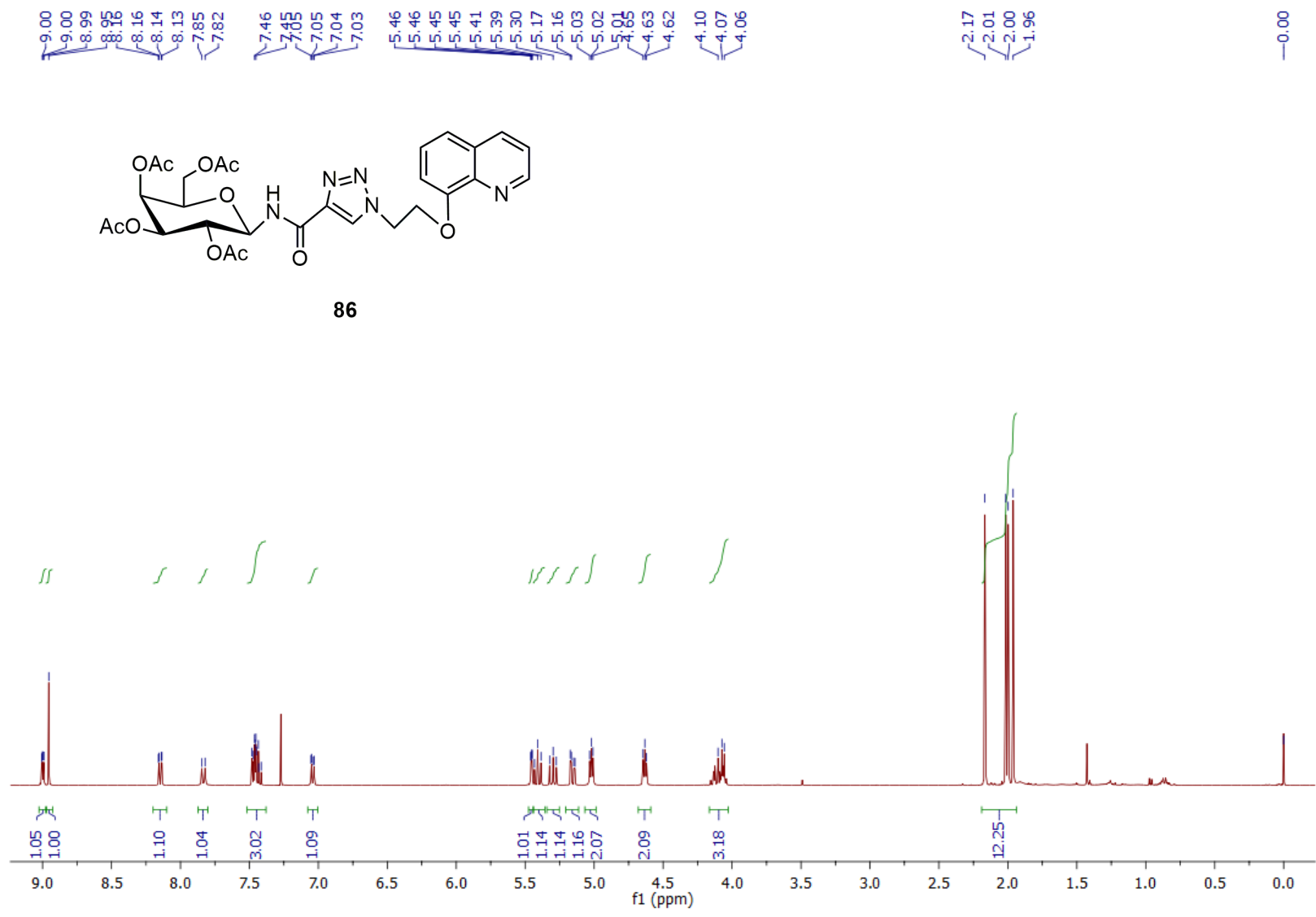


Fig. S163: ^1H NMR spectrum of glycoconjugate **86**.

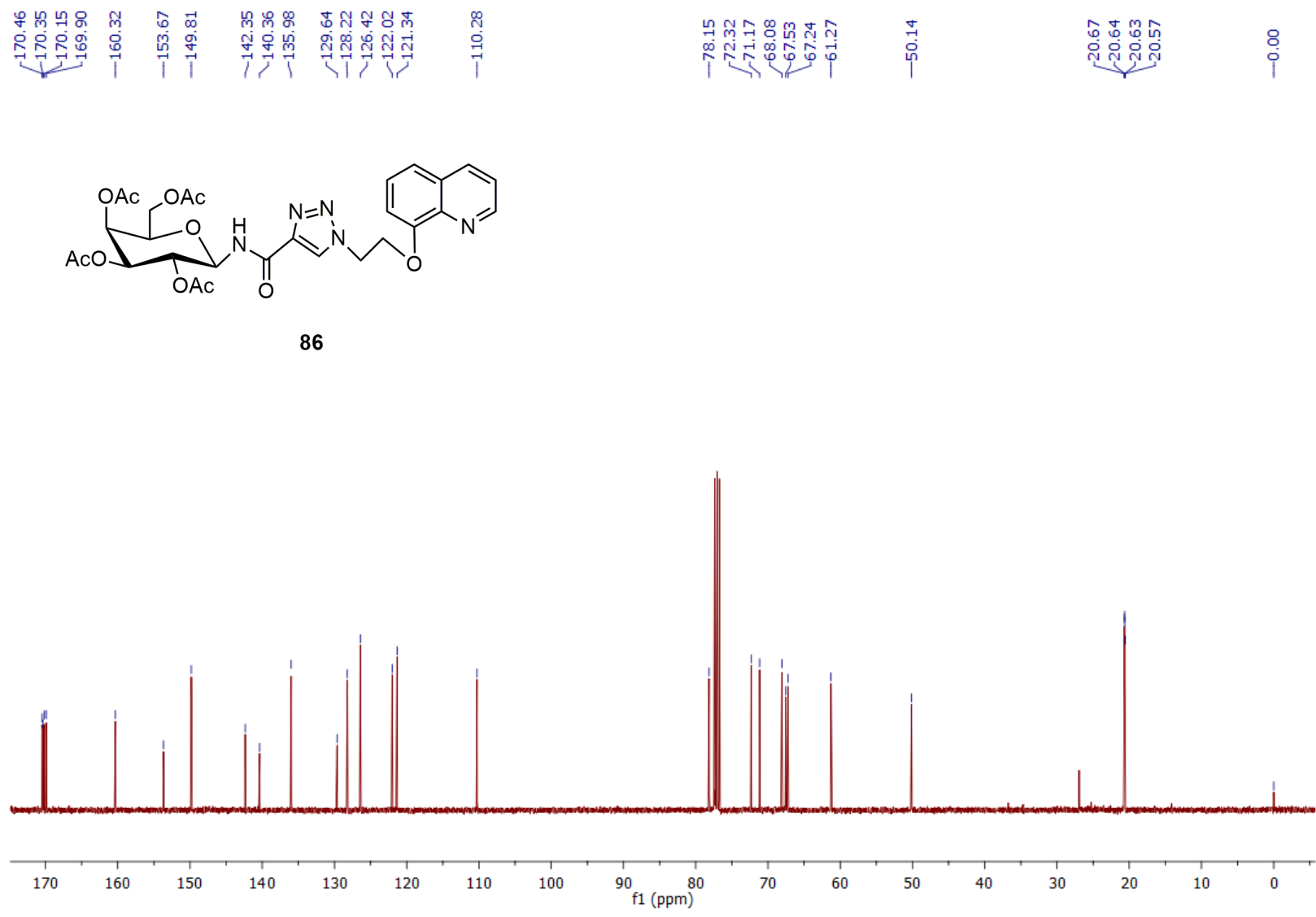


Fig. S164: ¹³C NMR spectrum of glycoconjugate **86**.

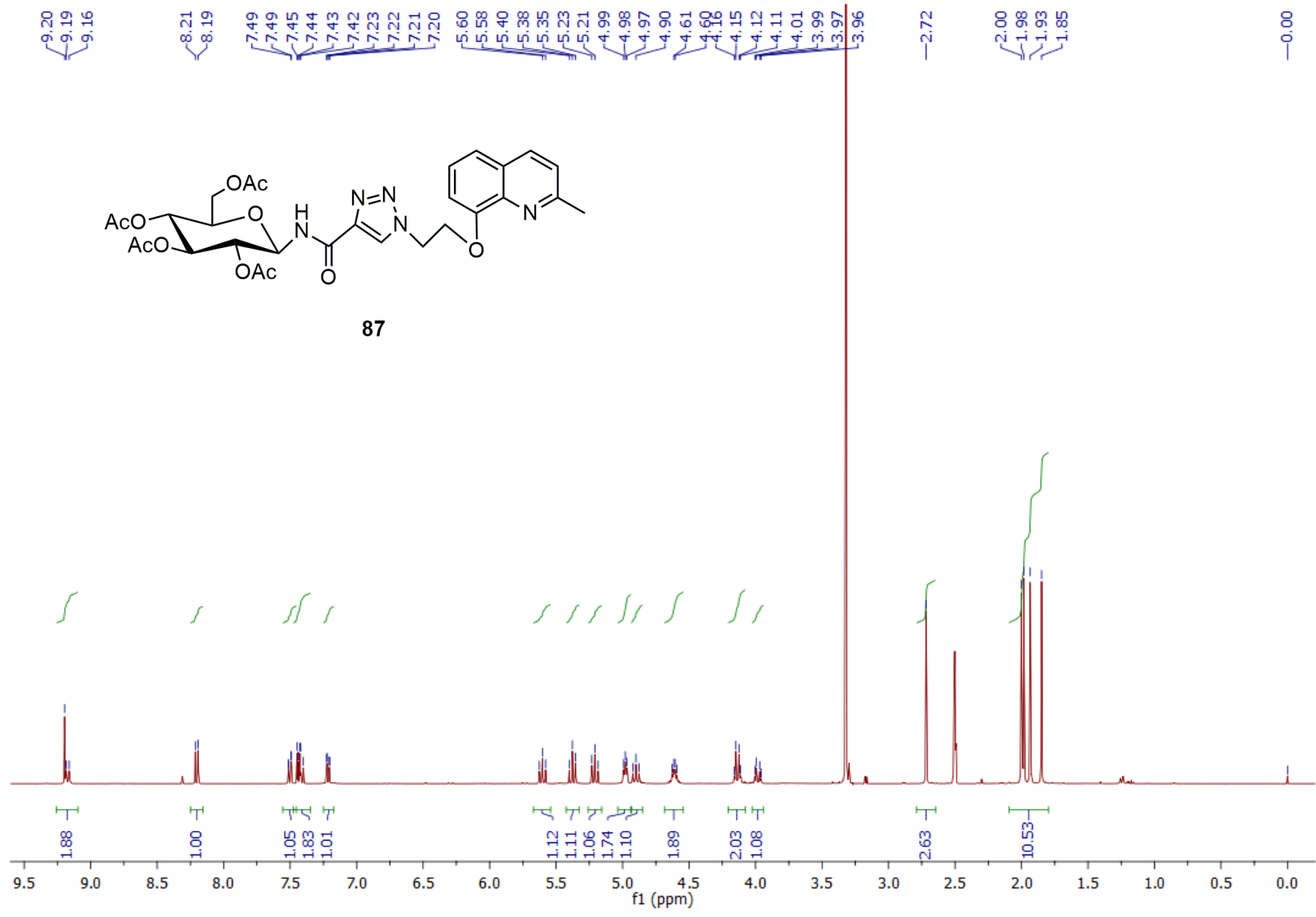


Fig. S165: ¹H NMR spectrum of glycoconjugate **87**.

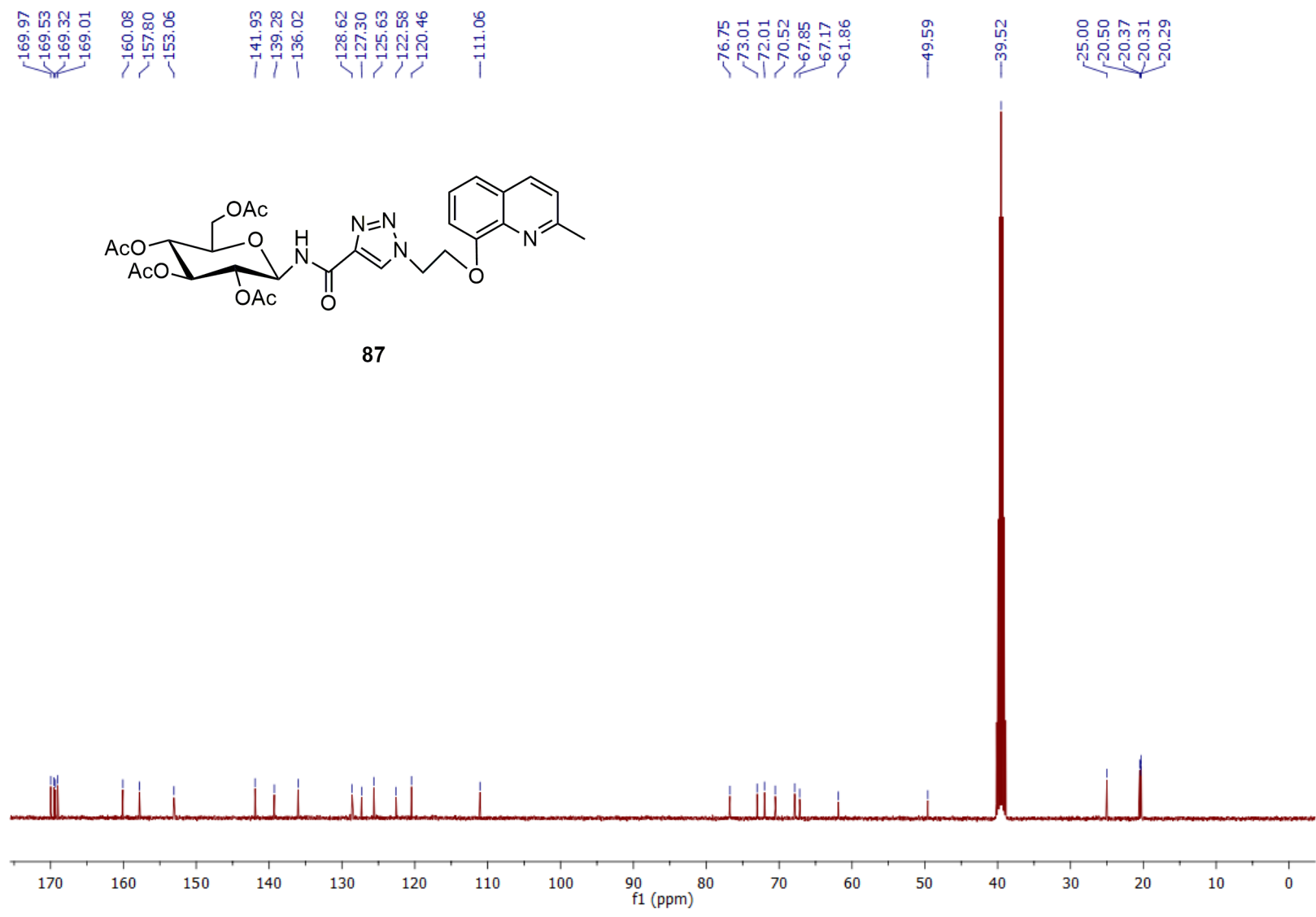


Fig. S166: ¹³C NMR spectrum of glycoconjugate **87**.

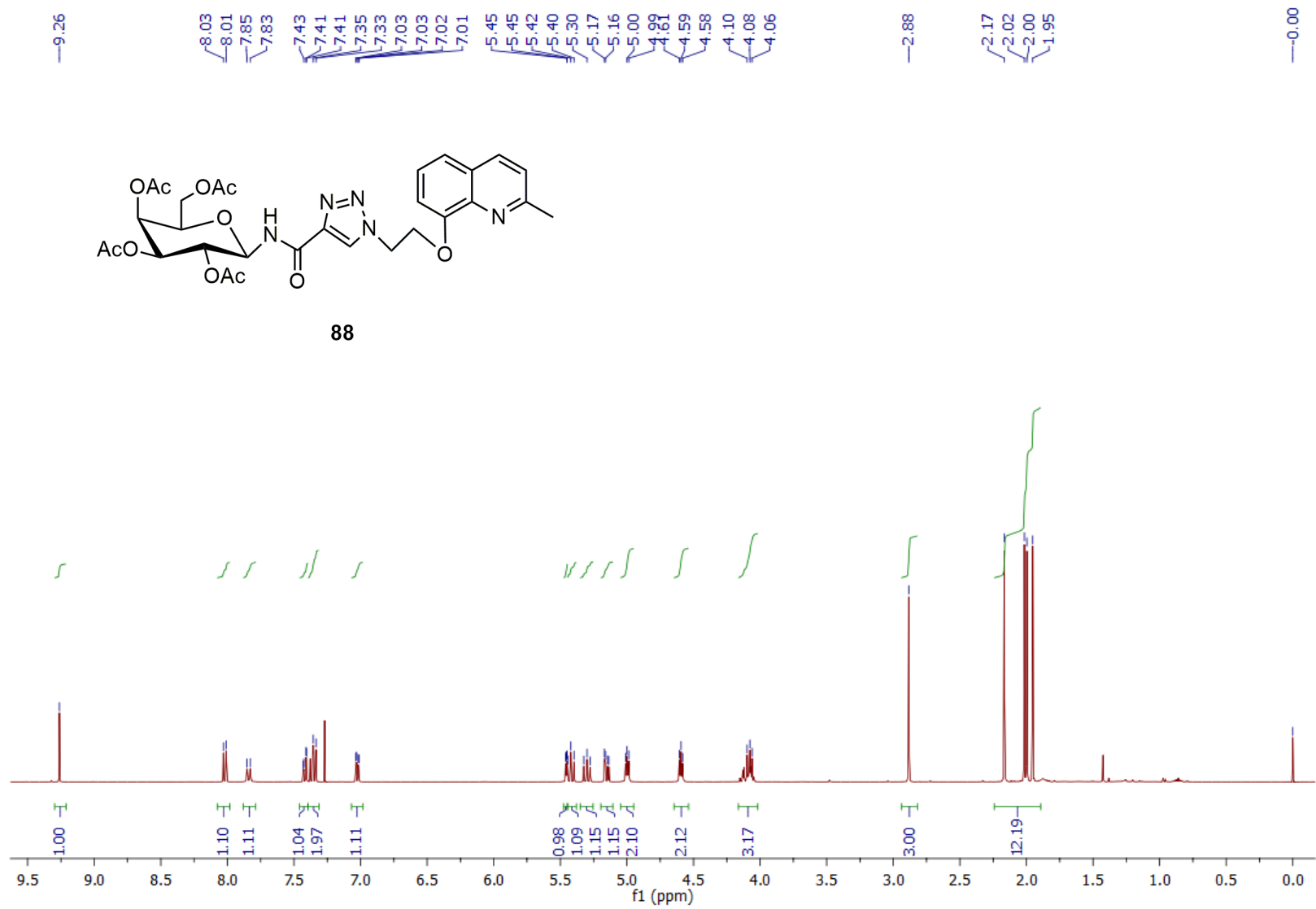


Fig. S167: ^1H NMR spectrum of glycoconjugate **88**.

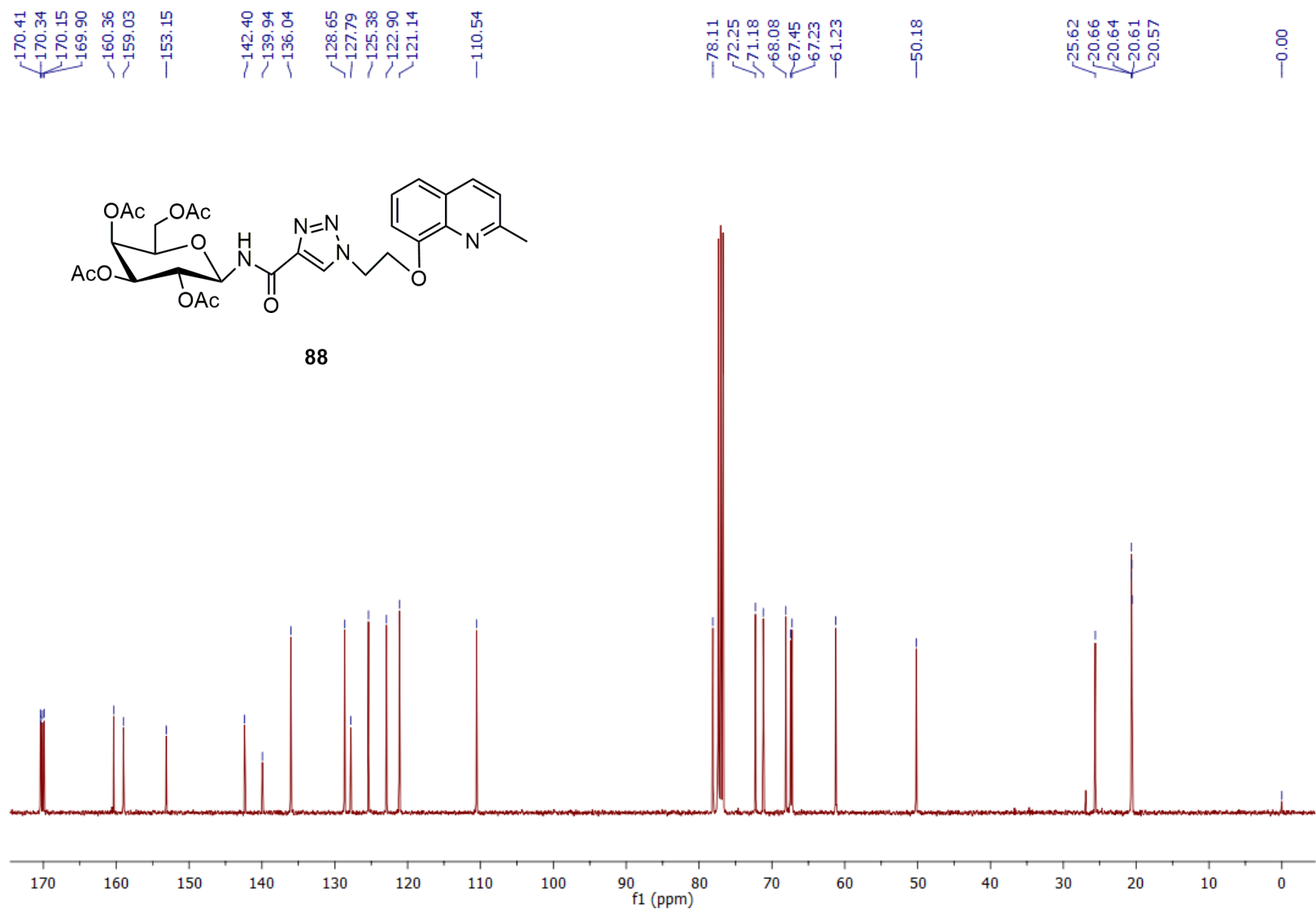


Fig. S168: ^{13}C NMR spectrum of glycoconjugate **88**.

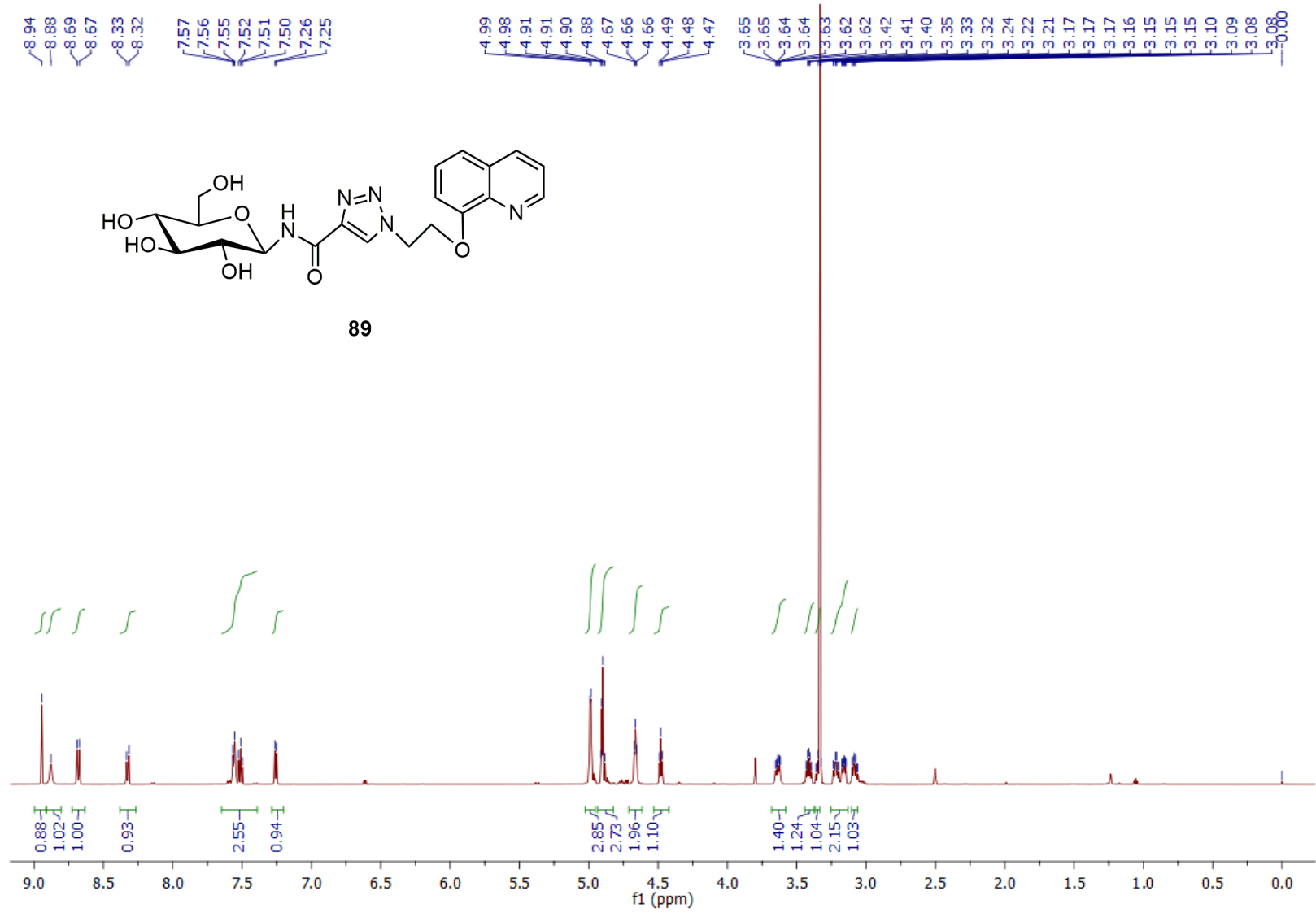


Fig. S169: ¹H NMR spectrum of glycoconjugate **89**.

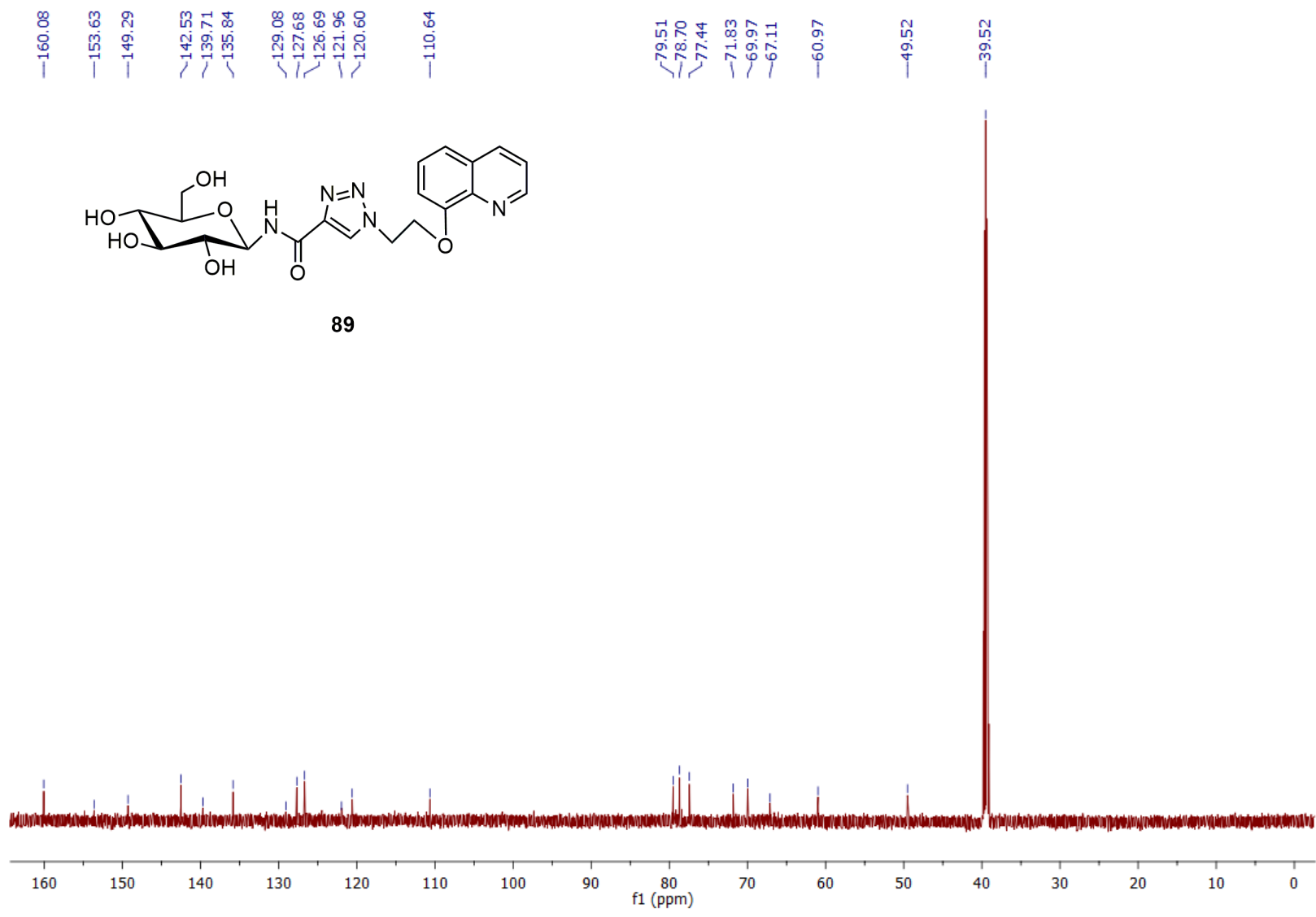


Fig. S170: ^{13}C NMR spectrum of glycoconjugate **89**.

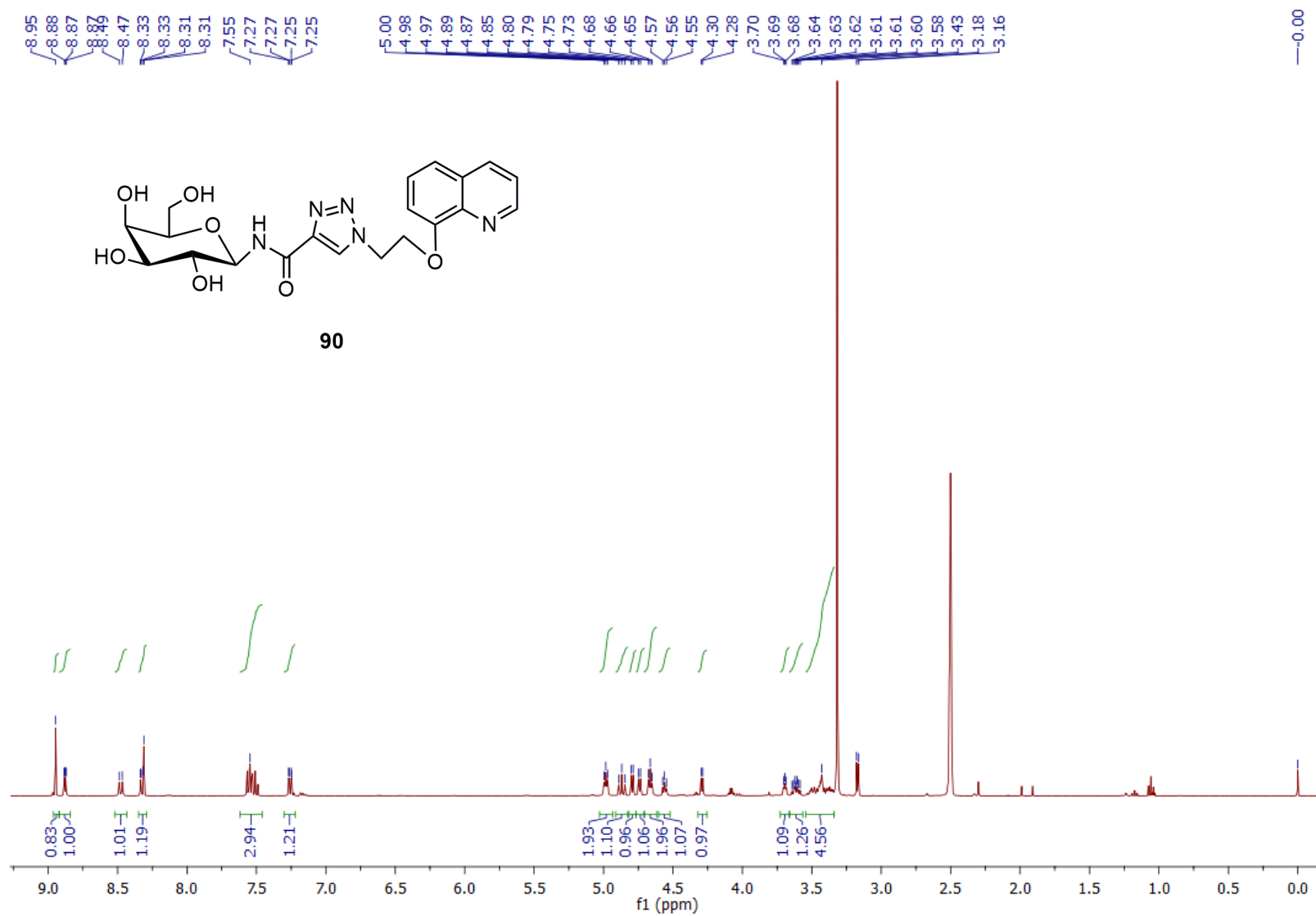


Fig. S171: ^1H NMR spectrum of glycoconjugate **90**.

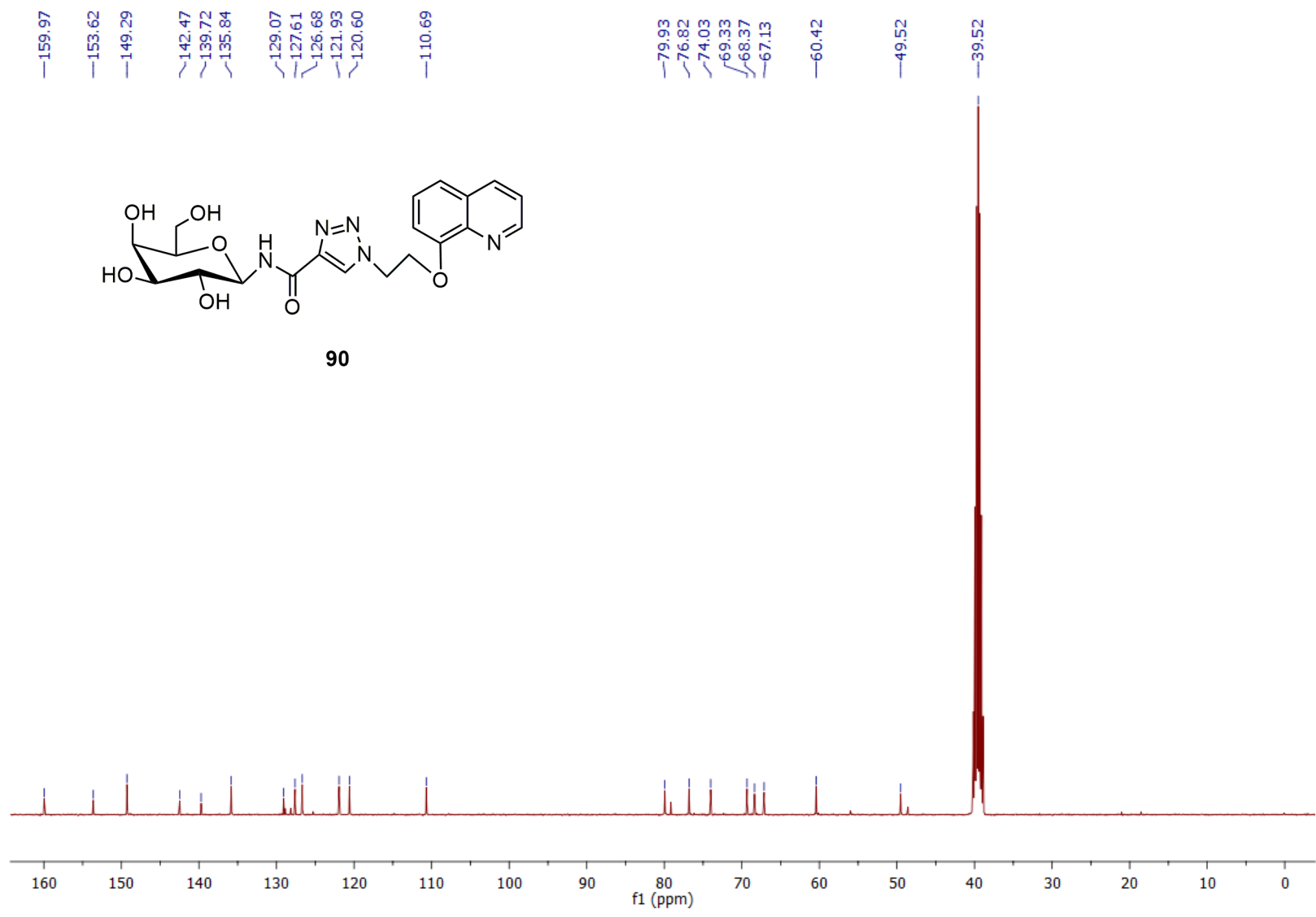


Fig. S172: ^{13}C NMR spectrum of glycoconjugate **90**.

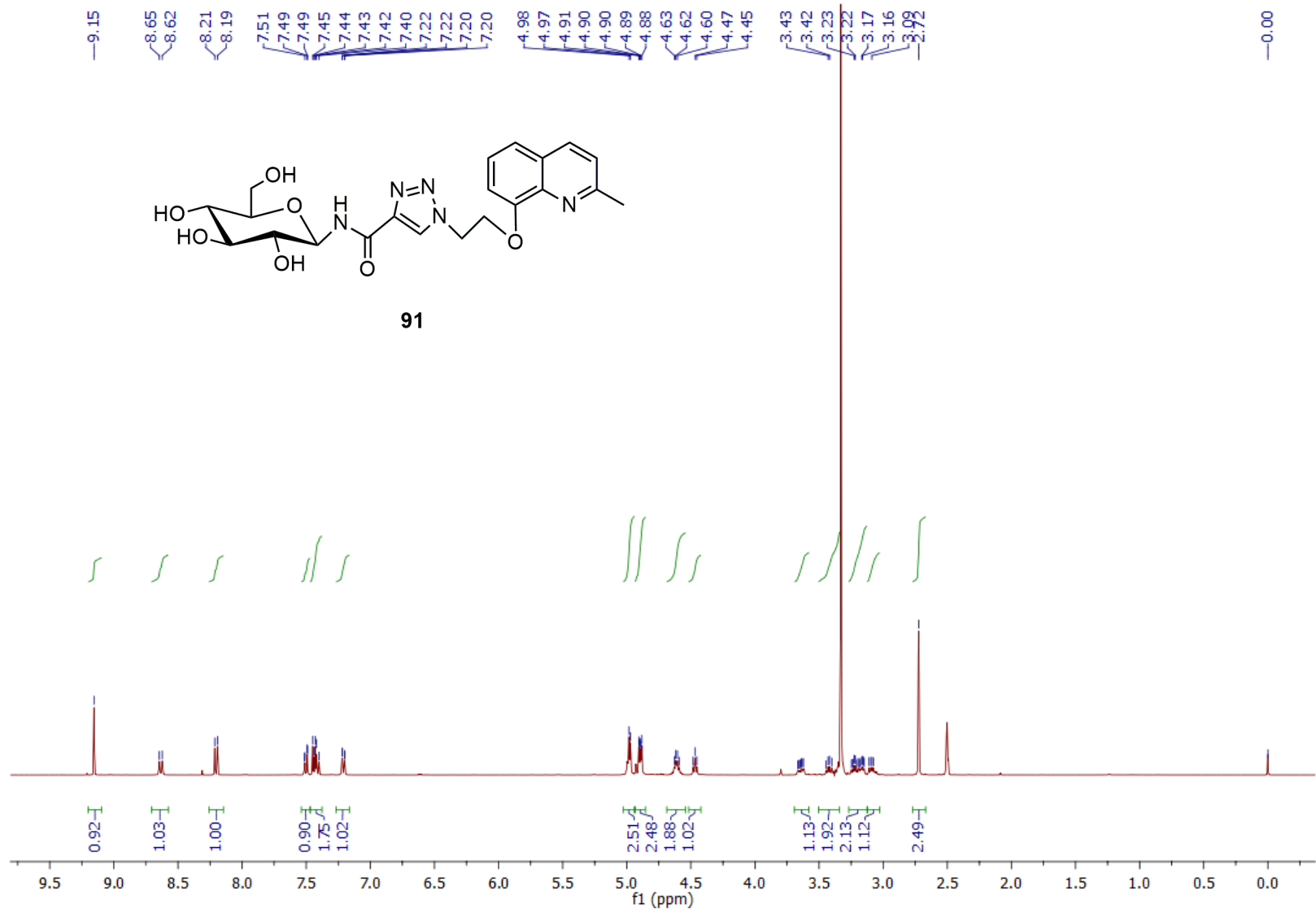


Fig. S173: ¹H NMR spectrum of glycoconjugate **91**.

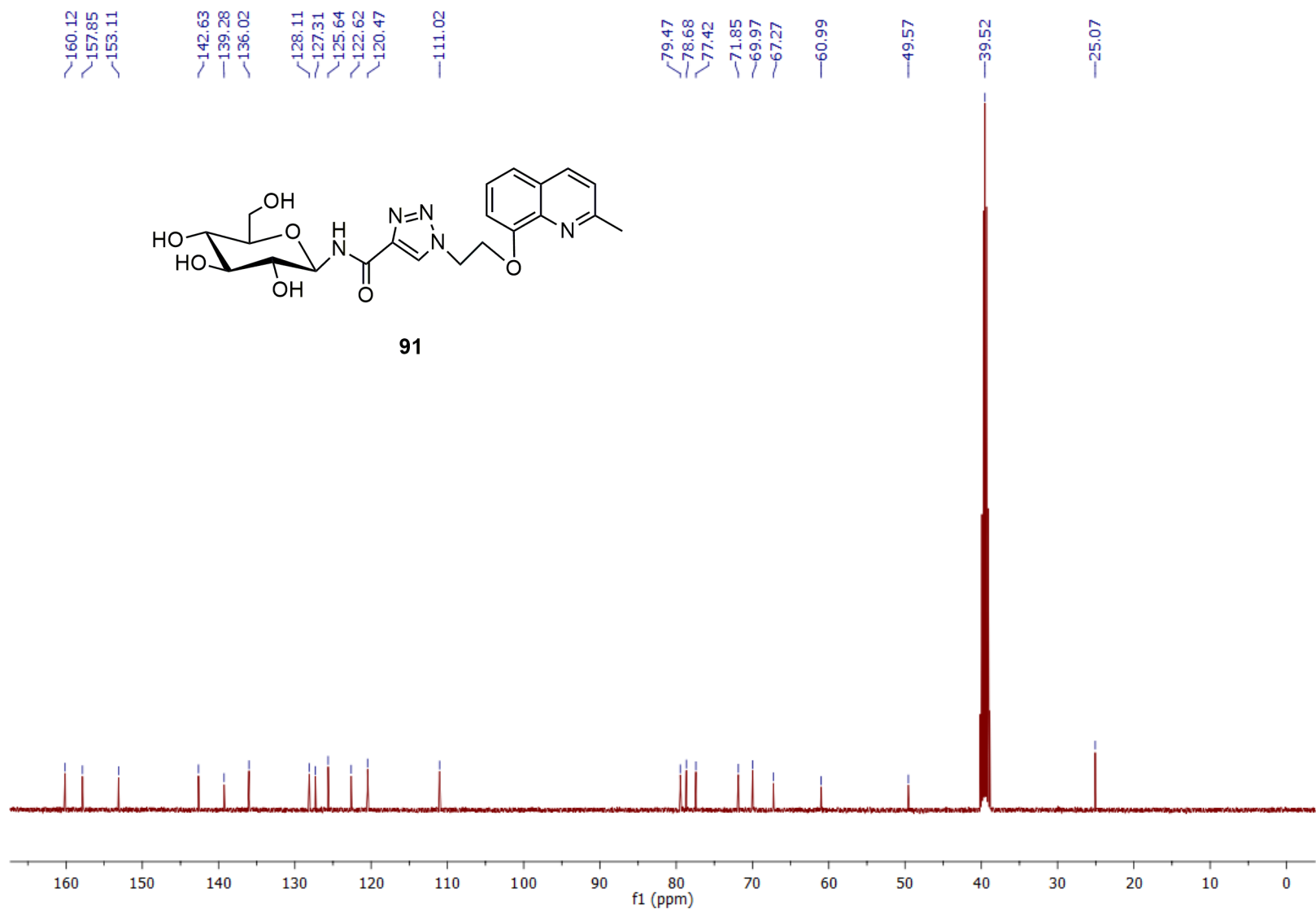


Fig. S174: ¹³C NMR spectrum of glycoconjugate **91**.

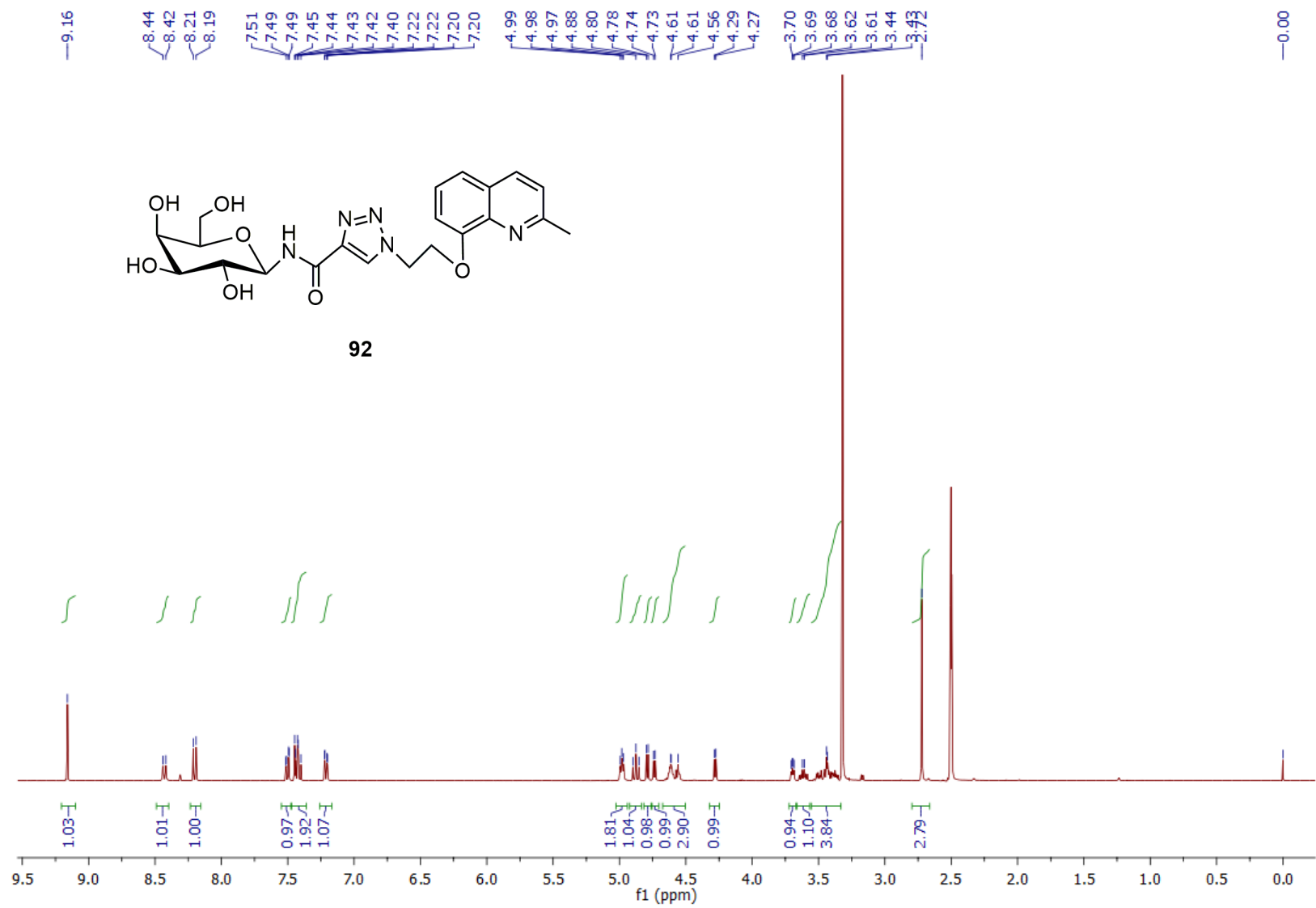


Fig. S175: ^1H NMR spectrum of glycoconjugate **92**.

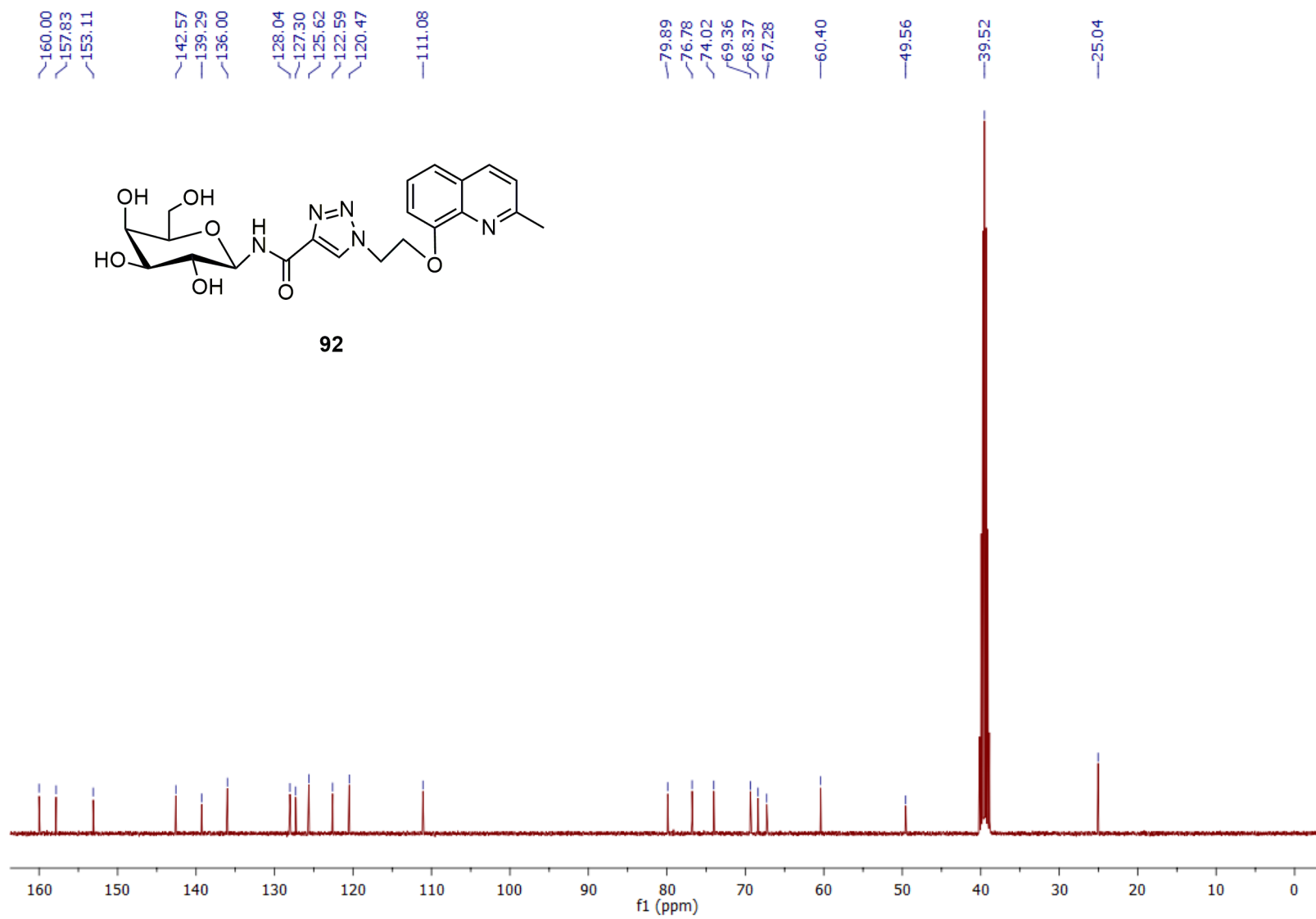


Fig. S176: ^{13}C NMR spectrum of glycoconjugate **92**.

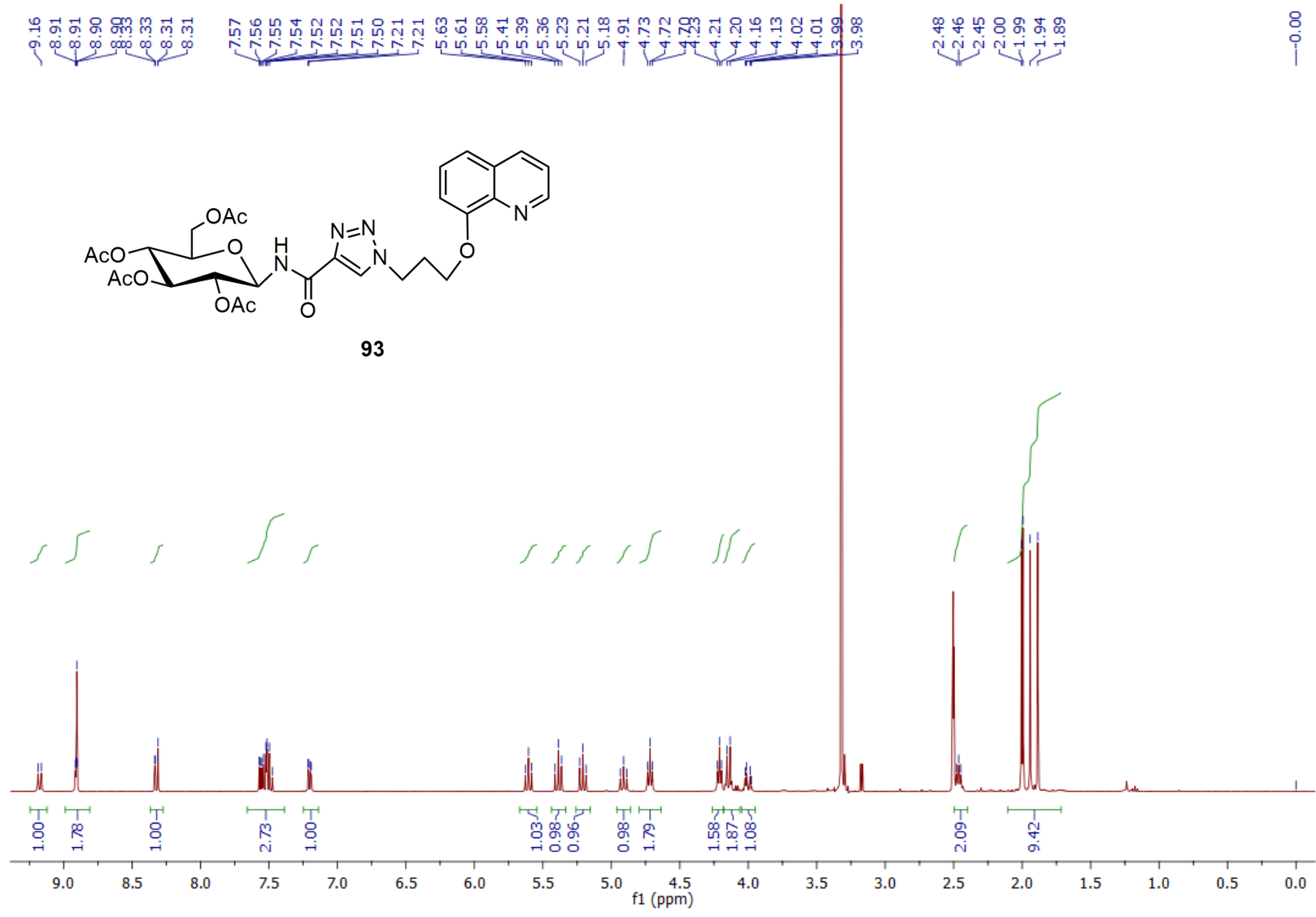


Fig. S177: ^1H NMR spectrum of glycoconjugate **93**.

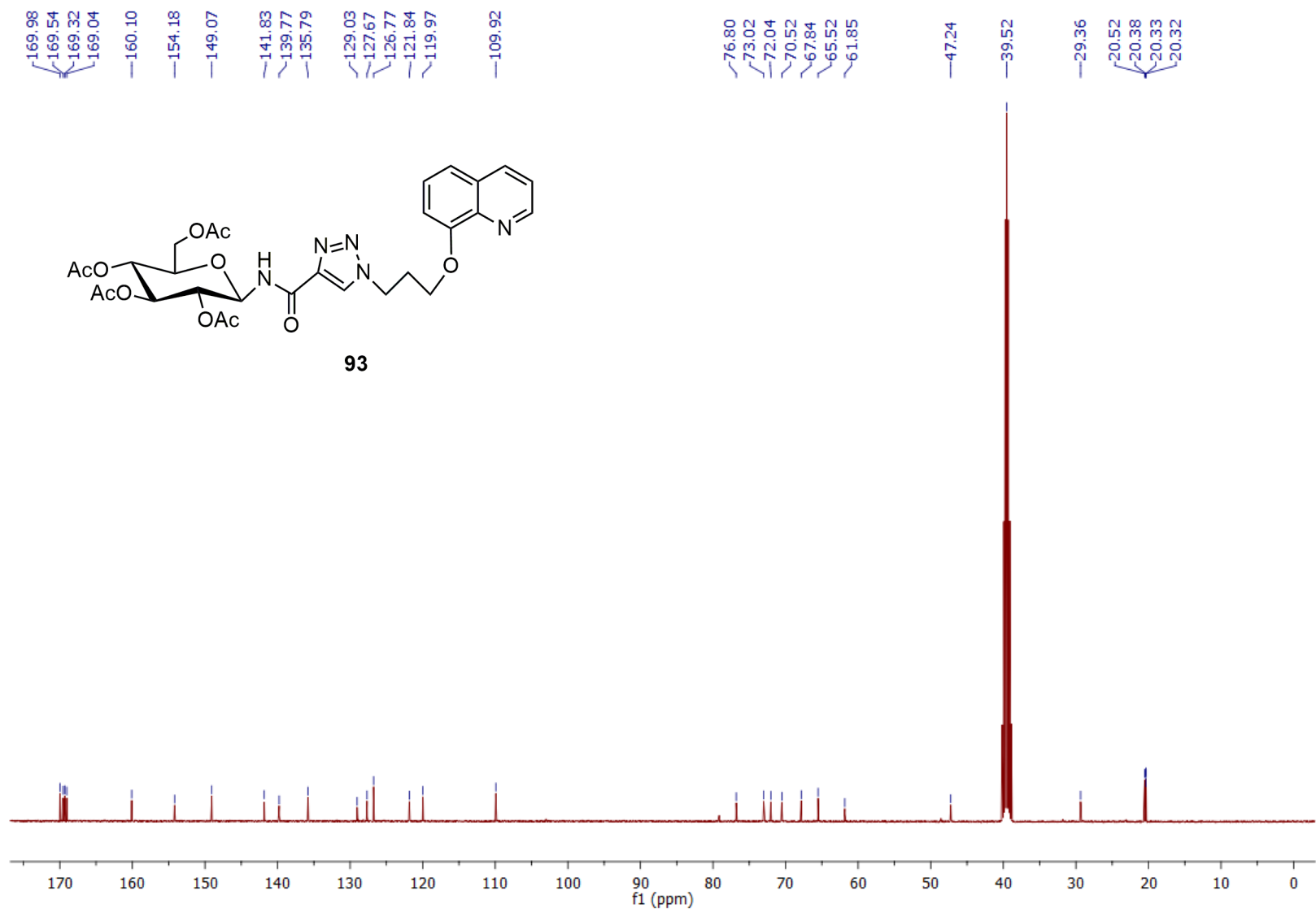


Fig. S178: ¹³C NMR spectrum of glycoconjugate **93**.

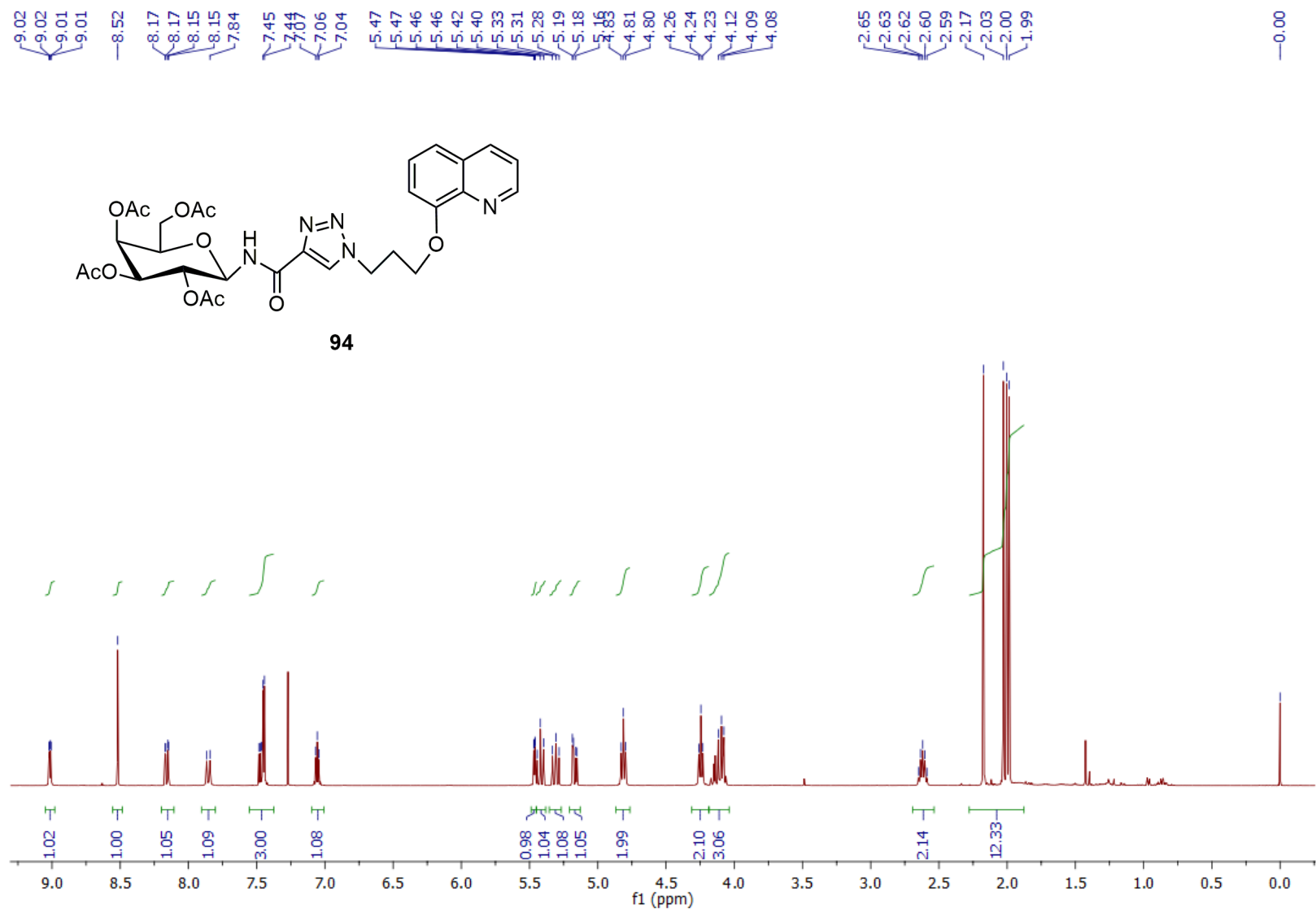


Fig. S179: ^1H NMR spectrum of glycoconjugate **94**.

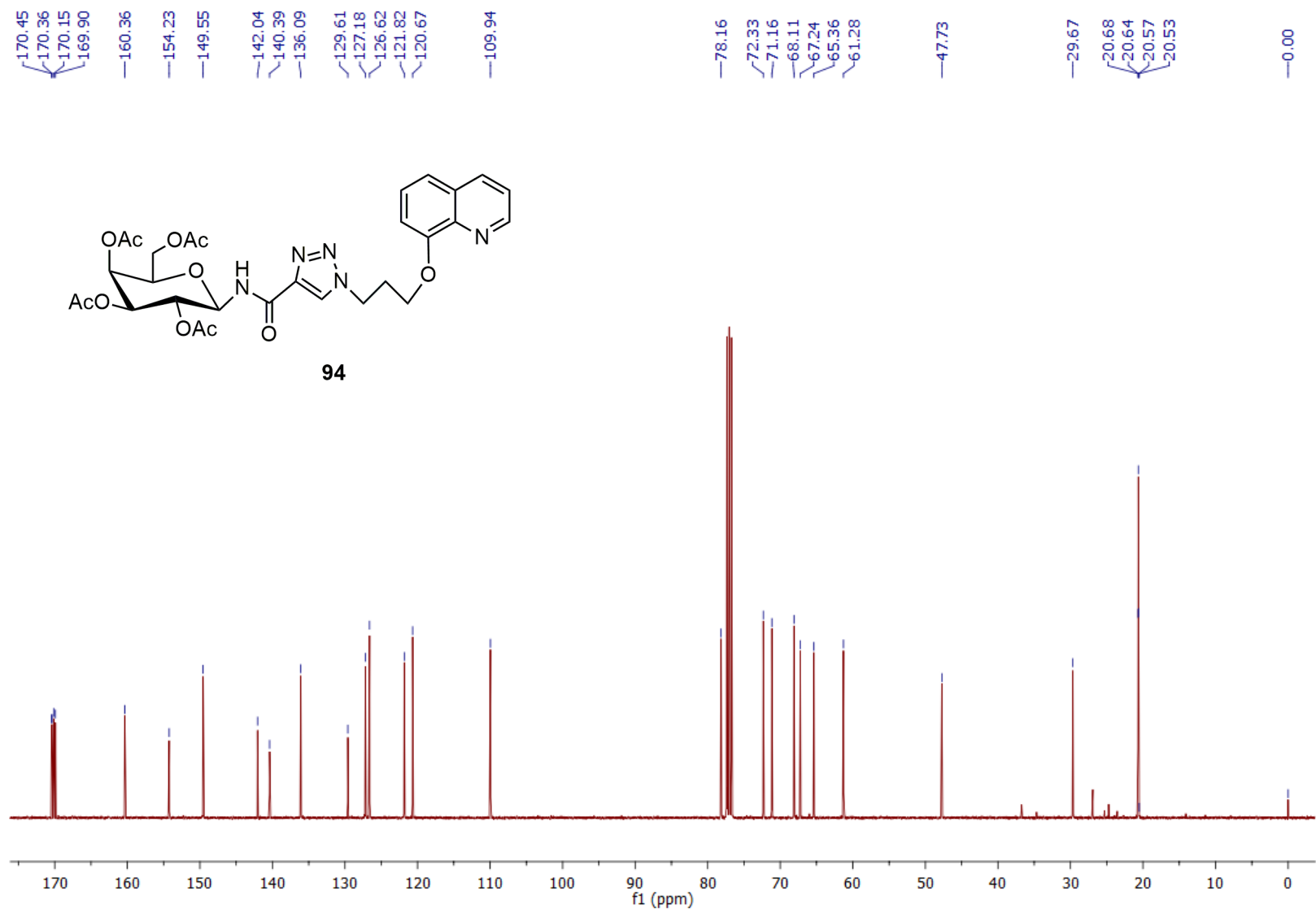


Fig. S180: ^{13}C NMR spectrum of glycoconjugate **94**.

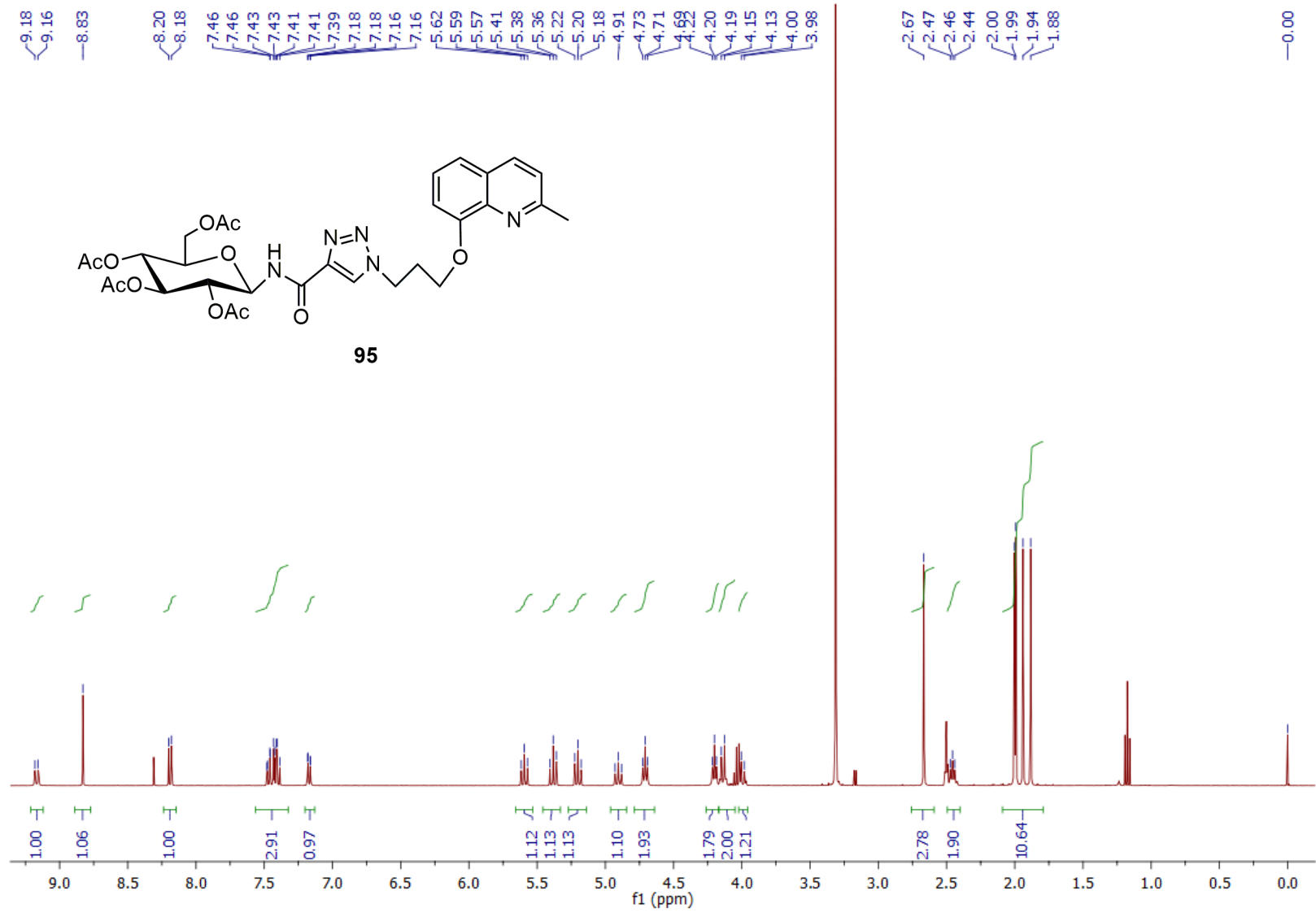


Fig. S181: ¹H NMR spectrum of glycoconjugate **95**.

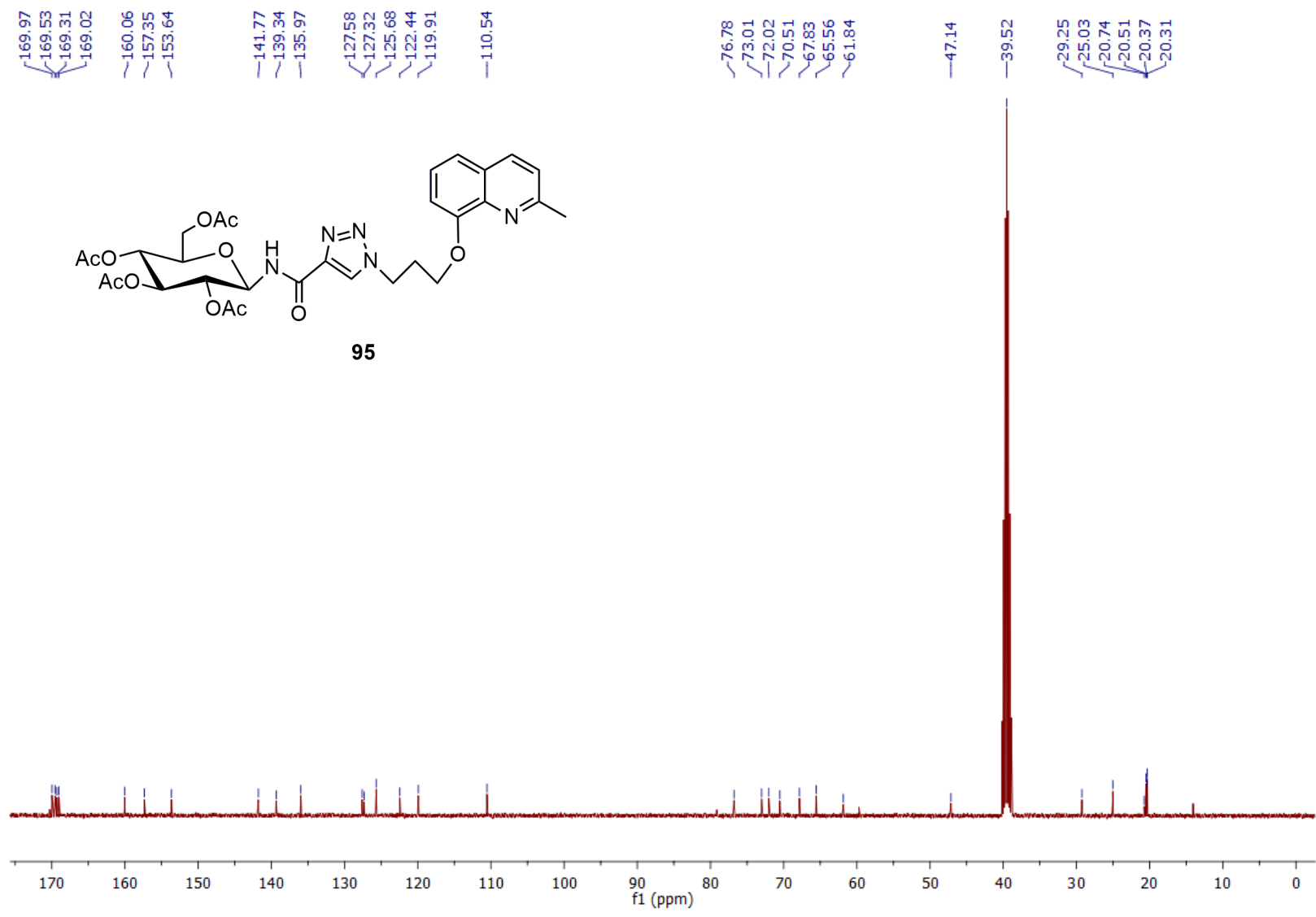


Fig. S182: ¹³C NMR spectrum of glycoconjugate **95**.

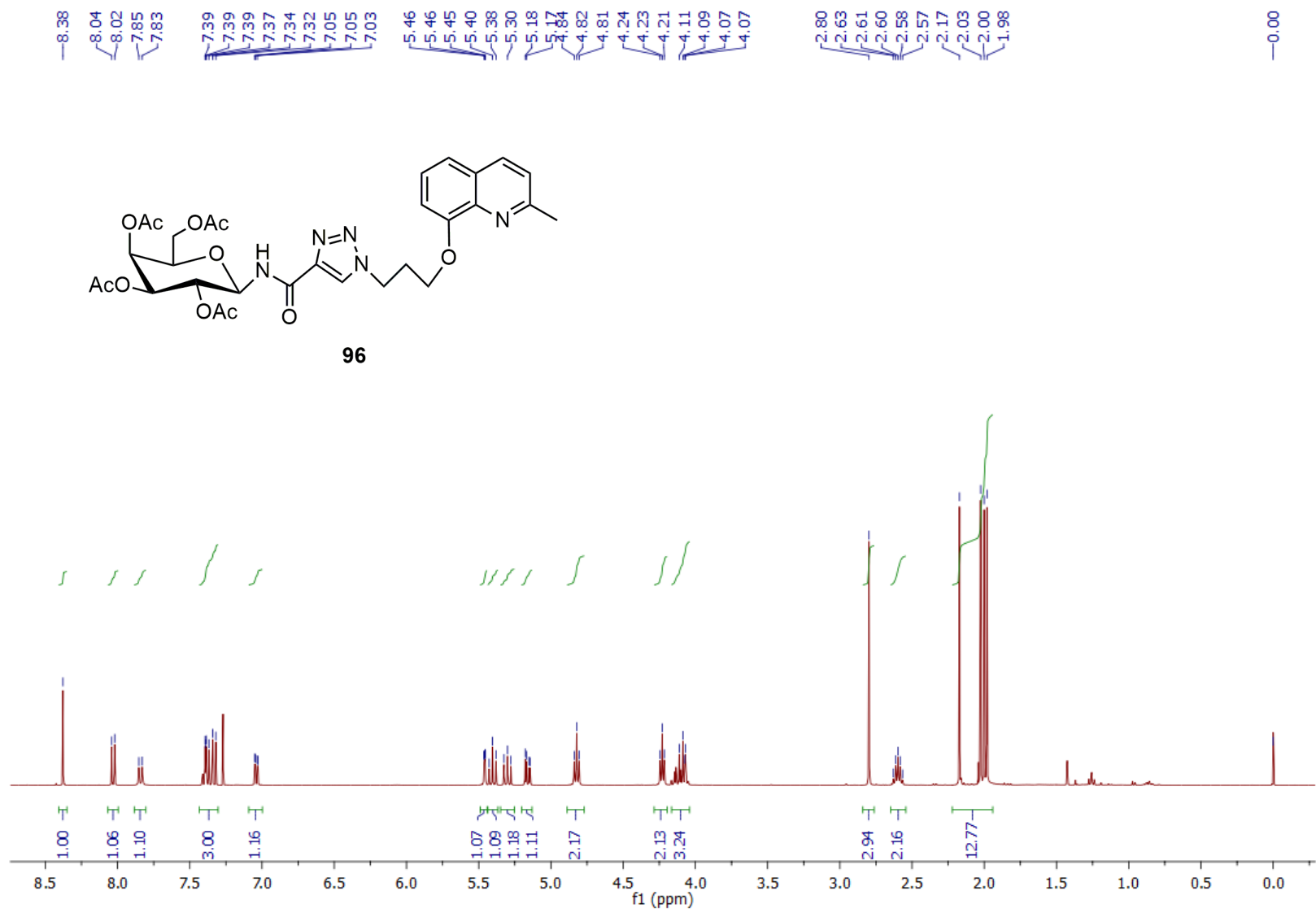


Fig. S183: ^1H NMR spectrum of glycoconjugate **96**.

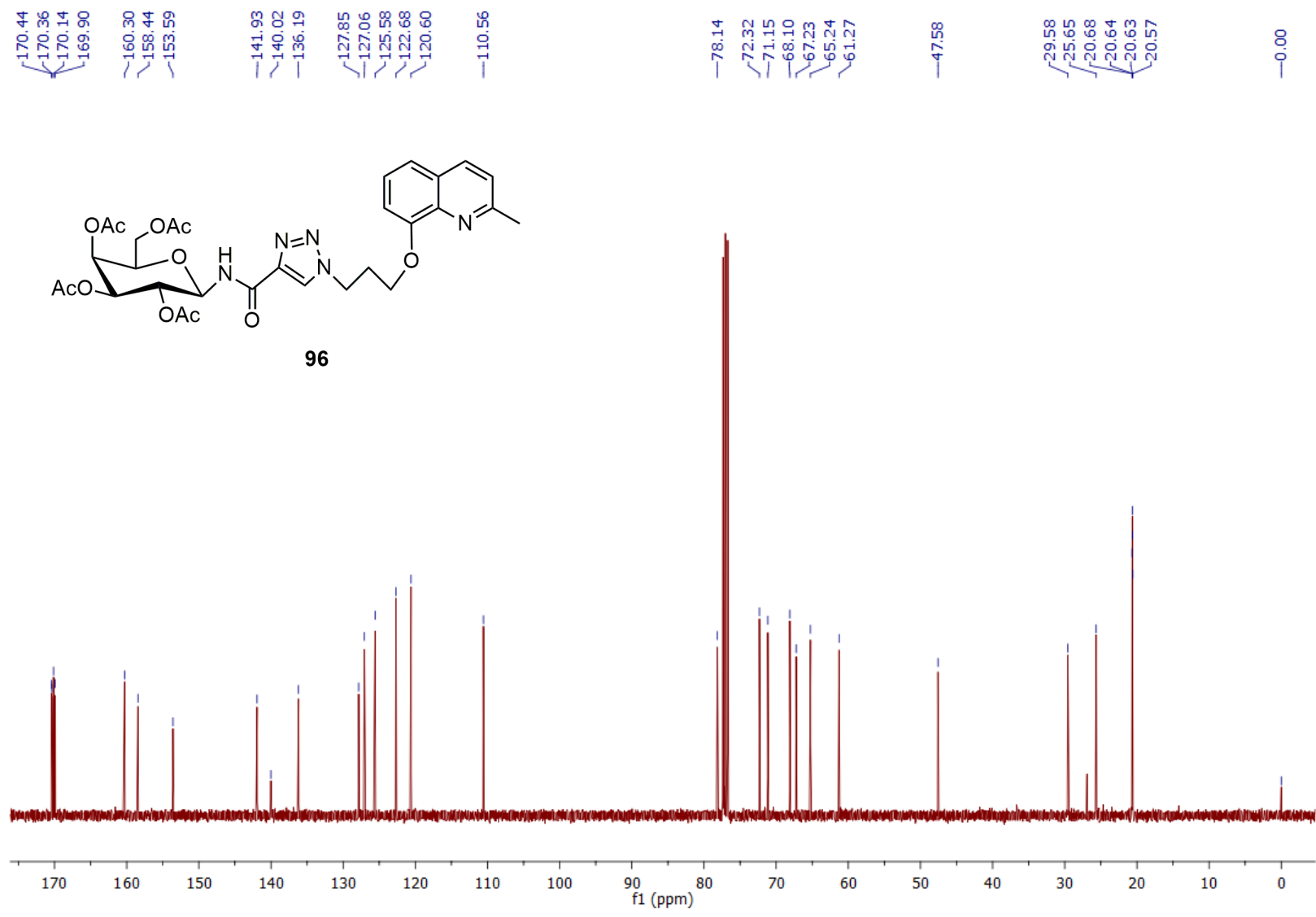


Fig. S184: ^{13}C NMR spectrum of glycoconjugate **96**.

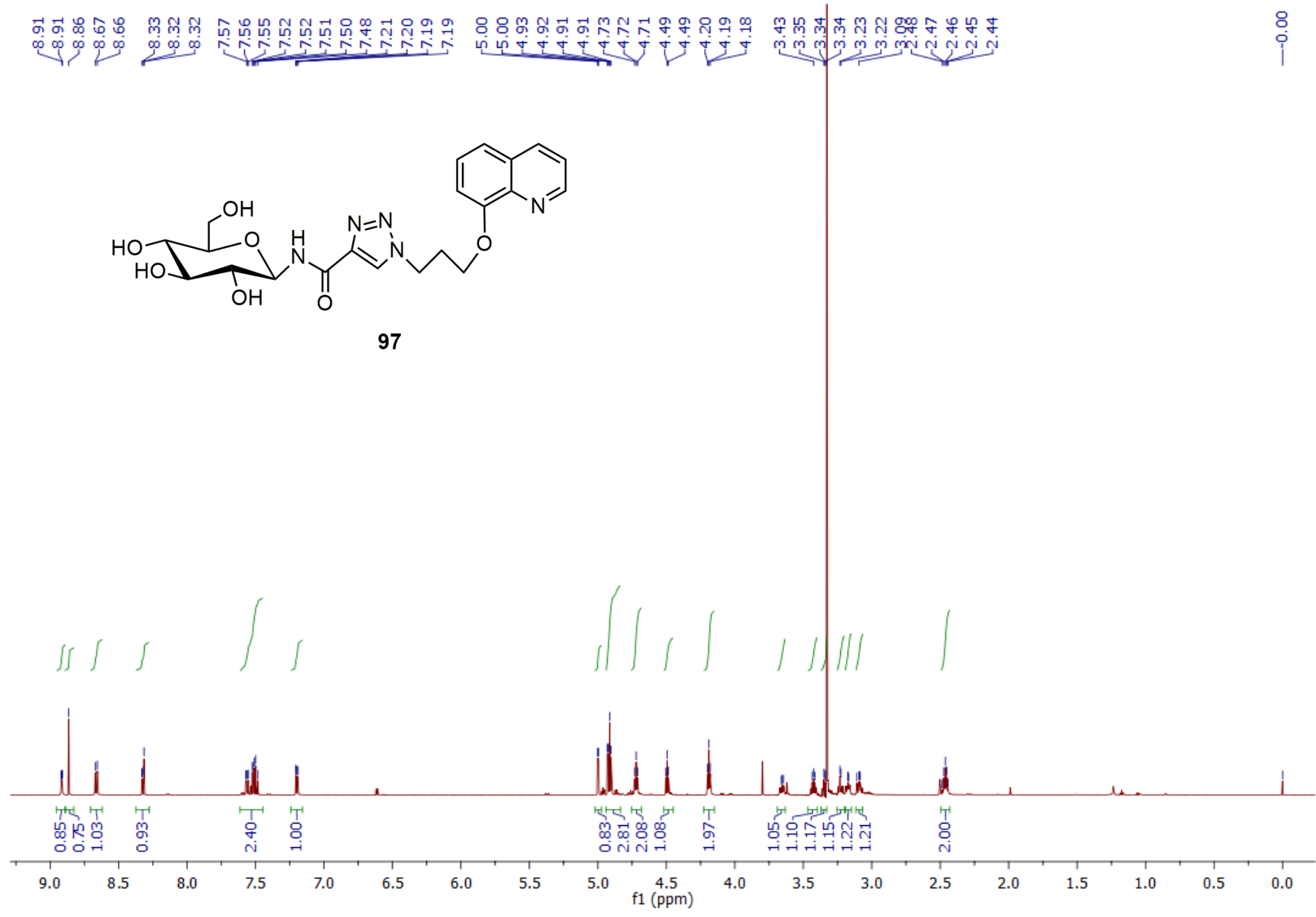


Fig. S185: ^1H NMR spectrum of glycoconjugate **97**.

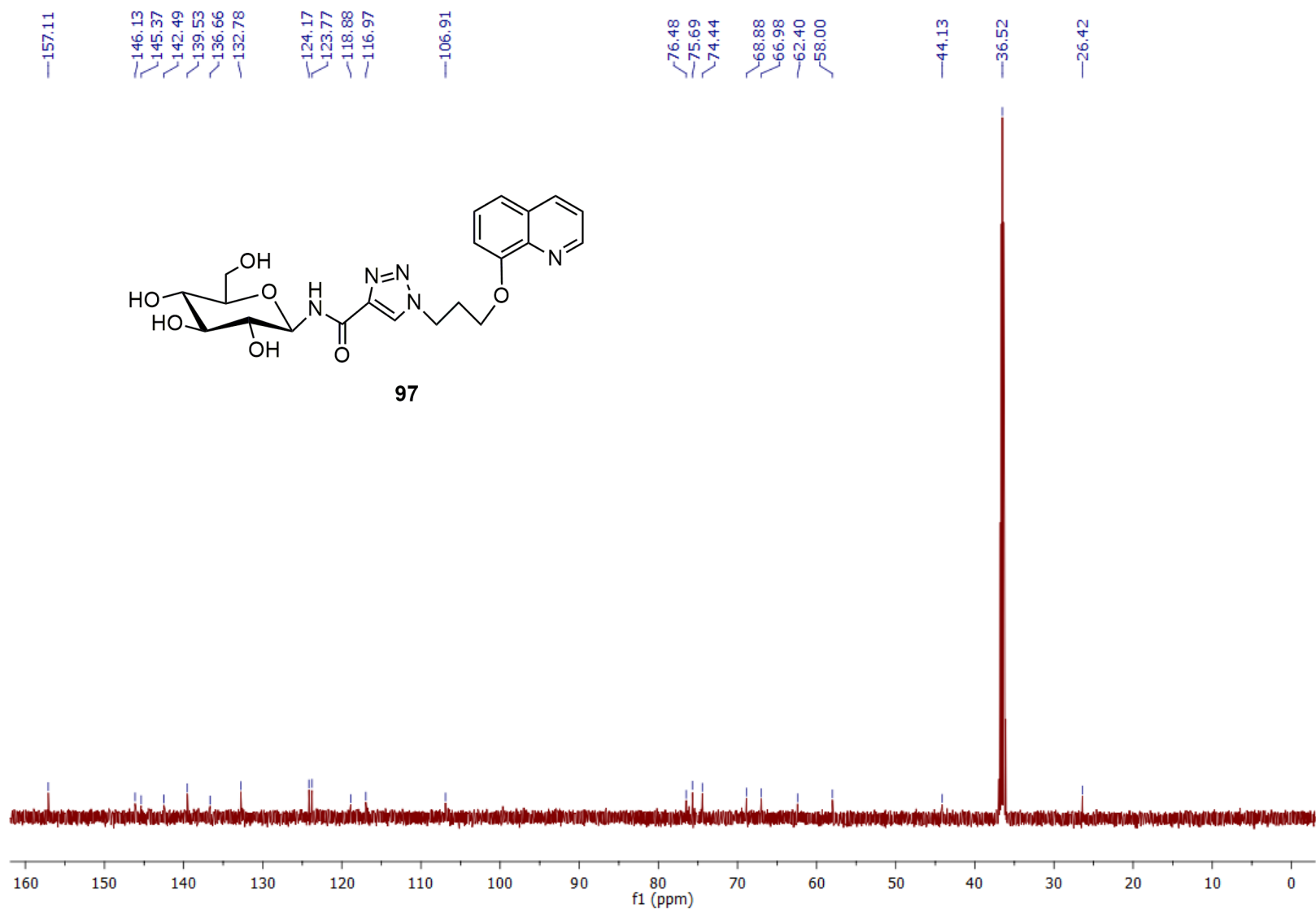


Fig. S186: ¹³C NMR spectrum of glycoconjugate **97**.

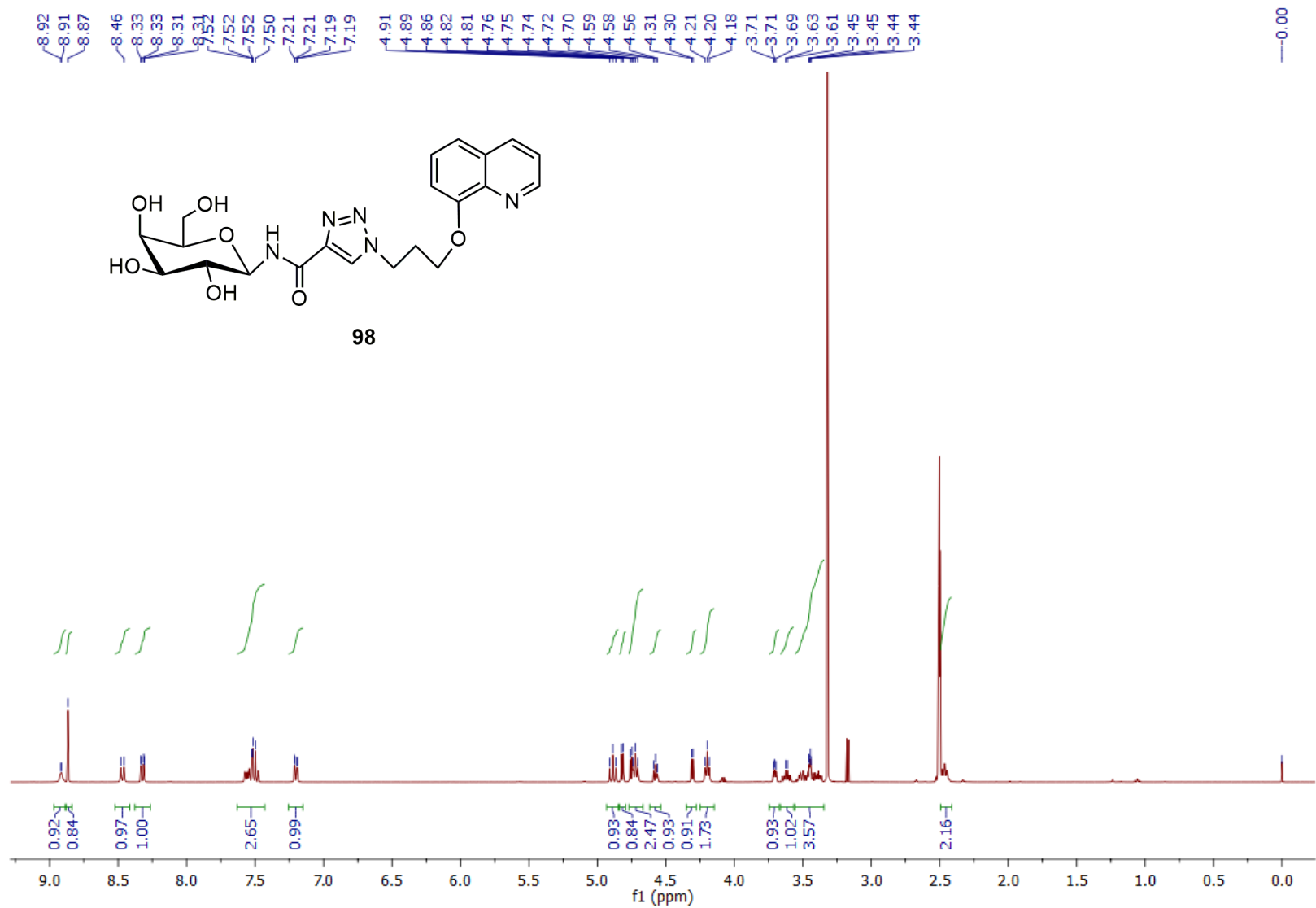


Fig. S187: ^1H NMR spectrum of glycoconjugate **98**.

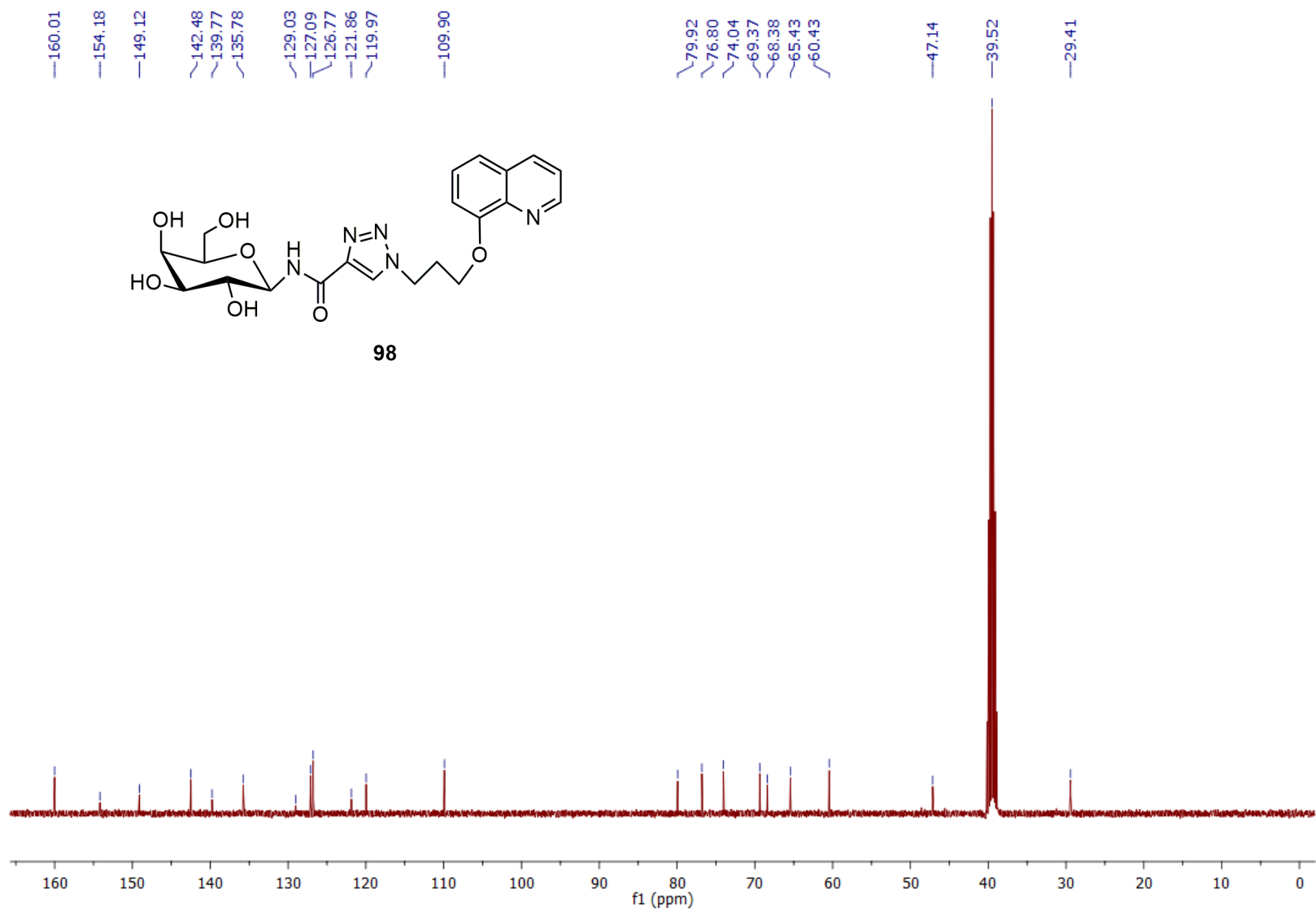


Fig. S188: ^{13}C NMR spectrum of glycoconjugate **98**.

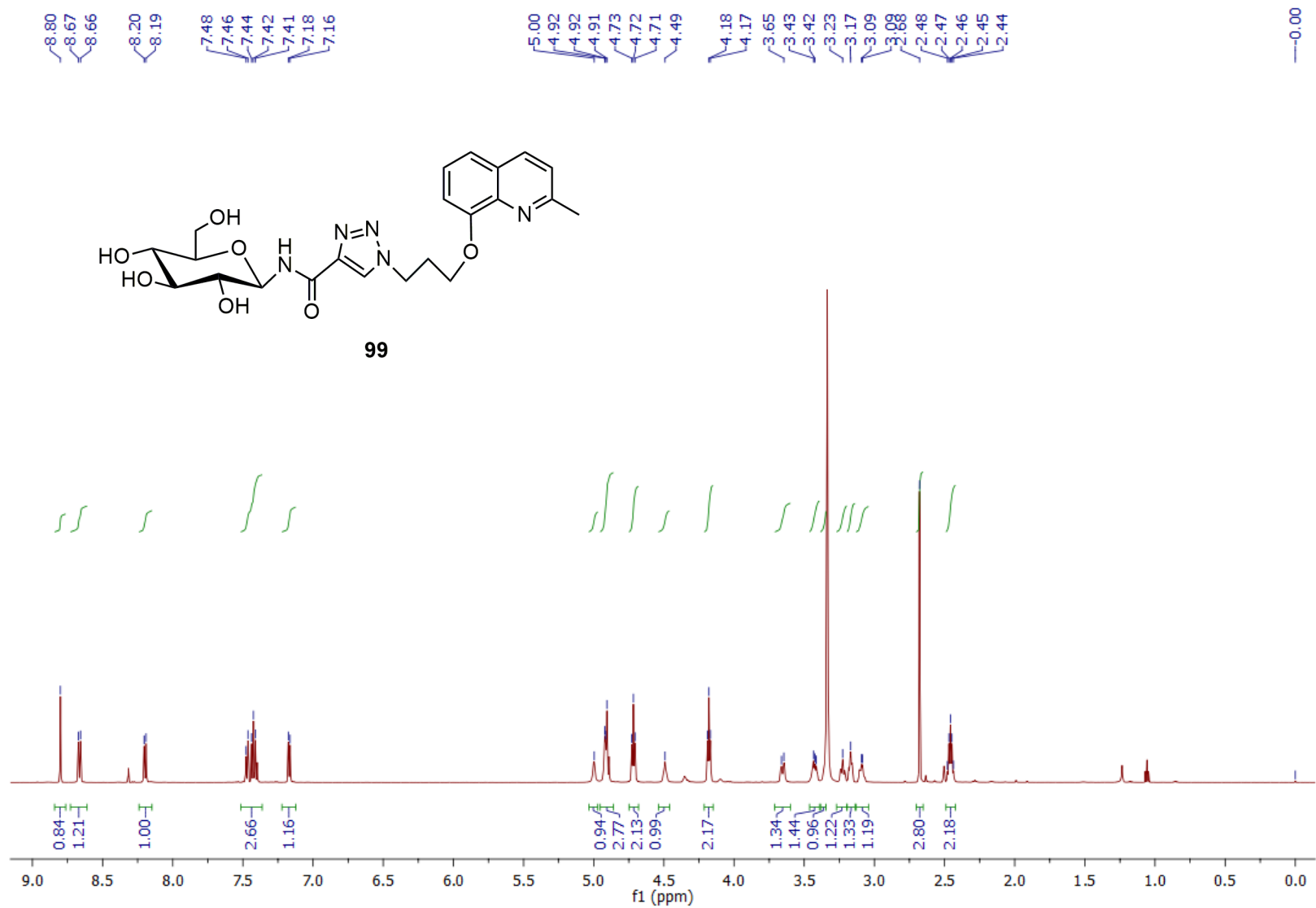


Fig. S189: ^1H NMR spectrum of glycoconjugate **99**.

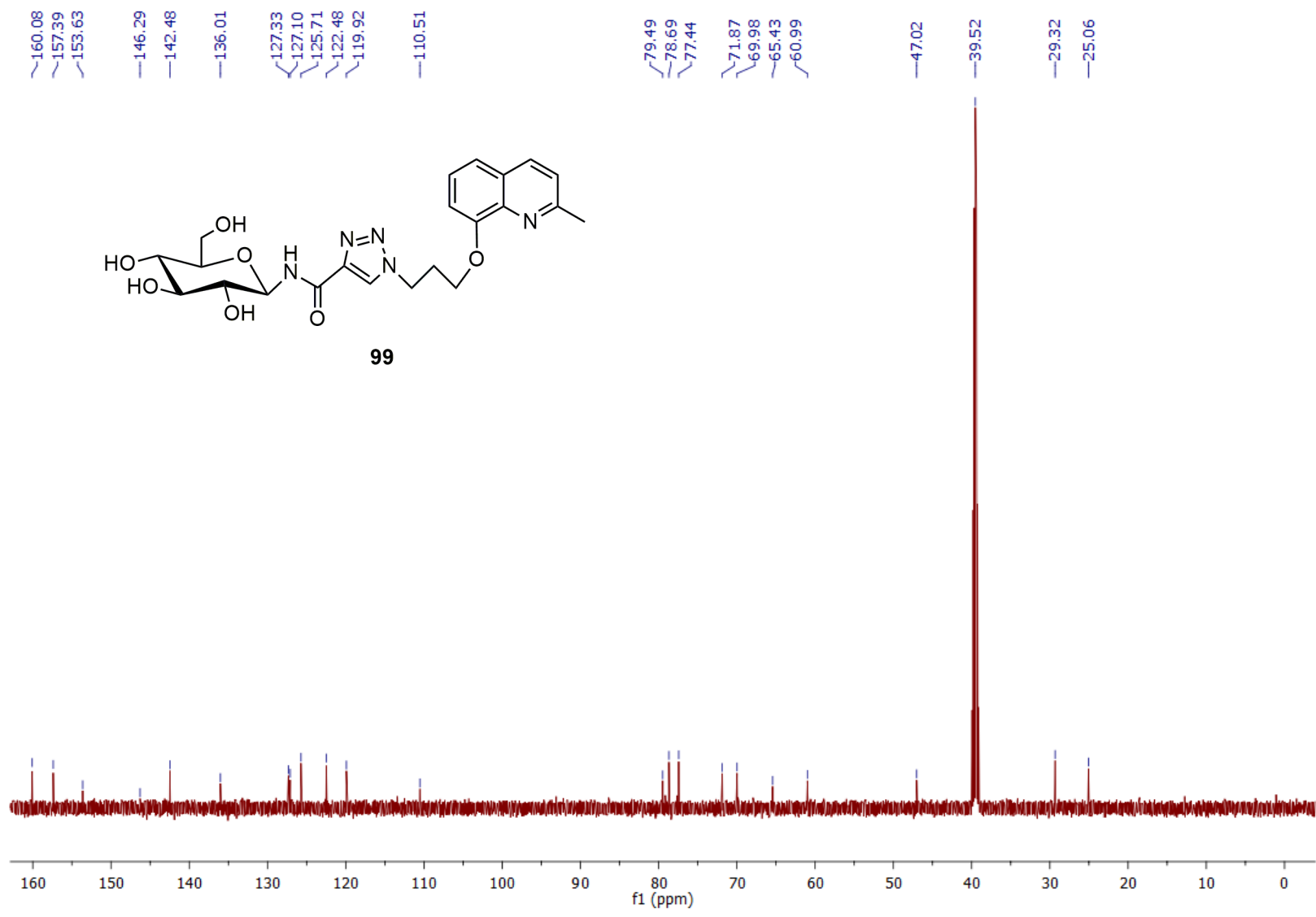


Fig. S190: ¹³C NMR spectrum of glycoconjugate **99**.

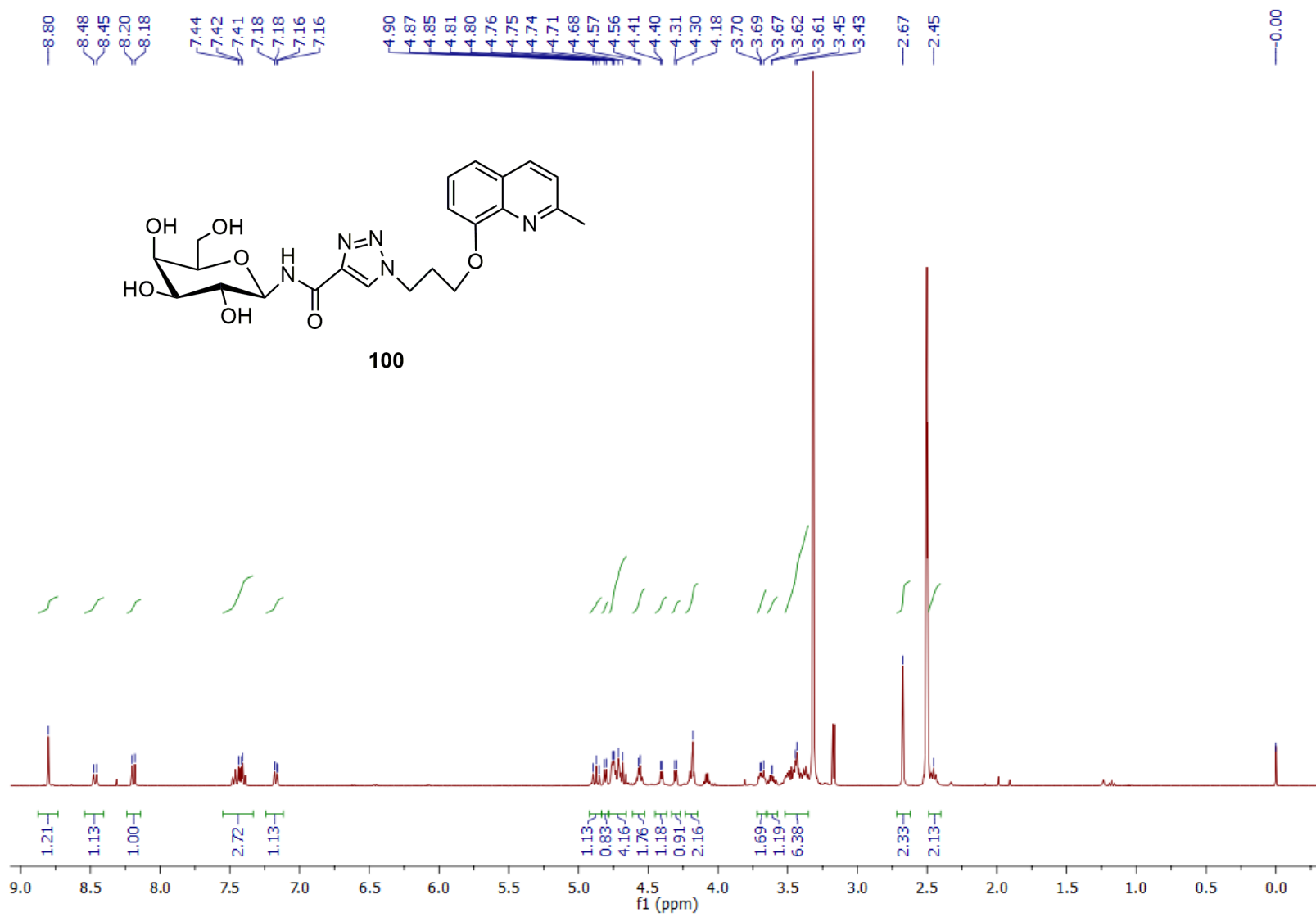


Fig. S191: ^1H NMR spectrum of glycoconjugate **100**.

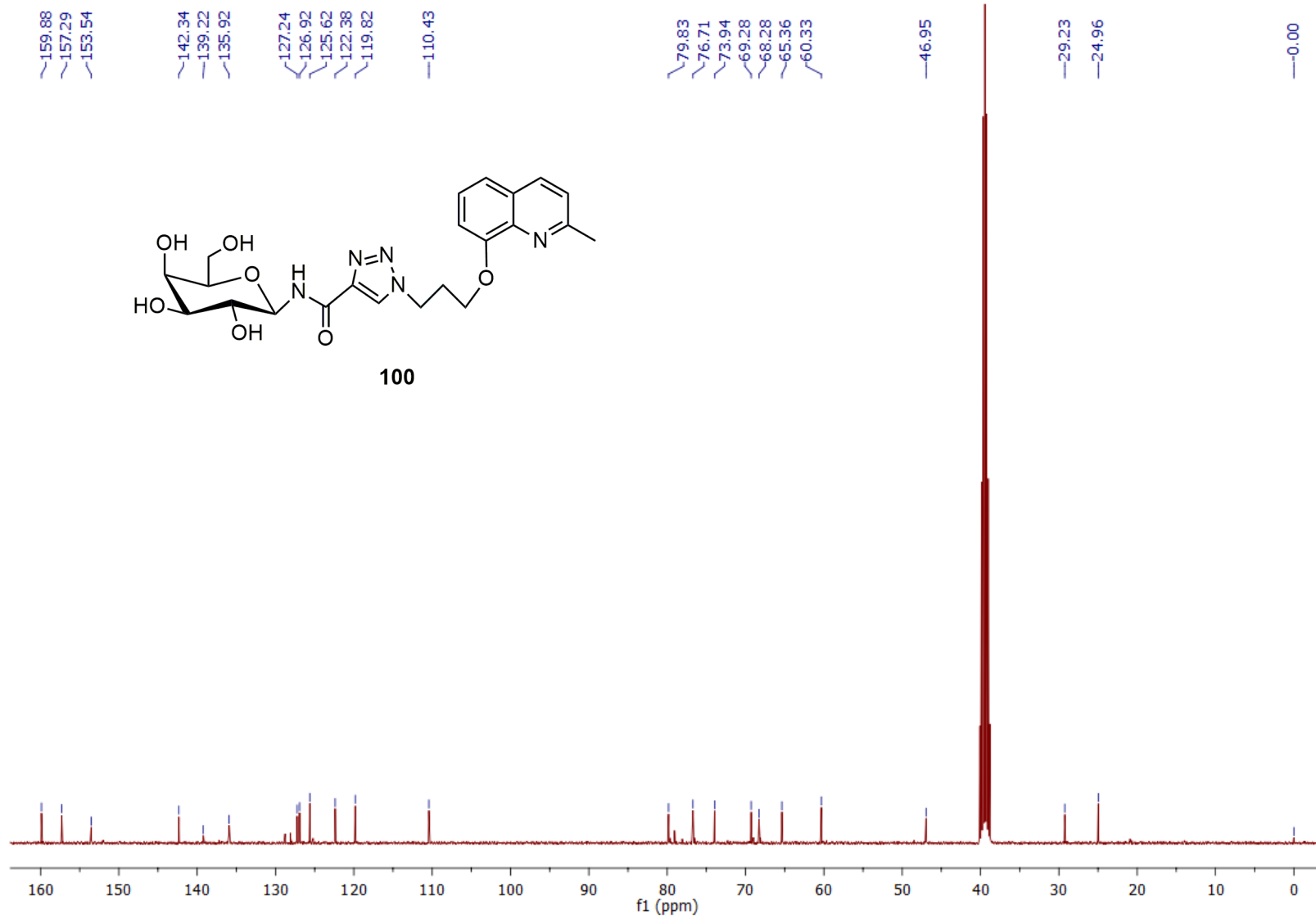


Fig. S192: ¹³C NMR spectrum of glycoconjugate **100**.

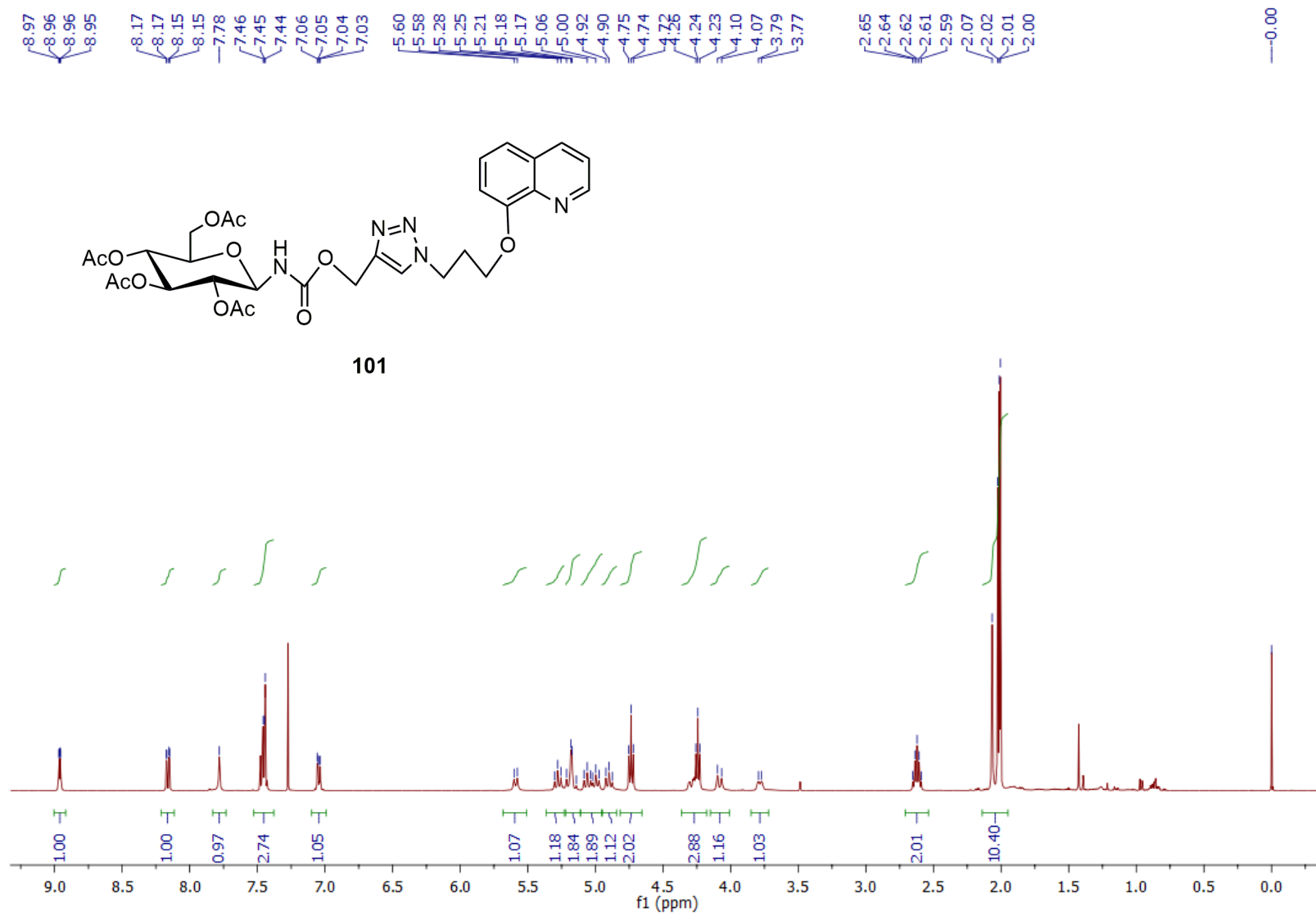


Fig. S193: ^1H NMR spectrum of glycoconjugate **101**.

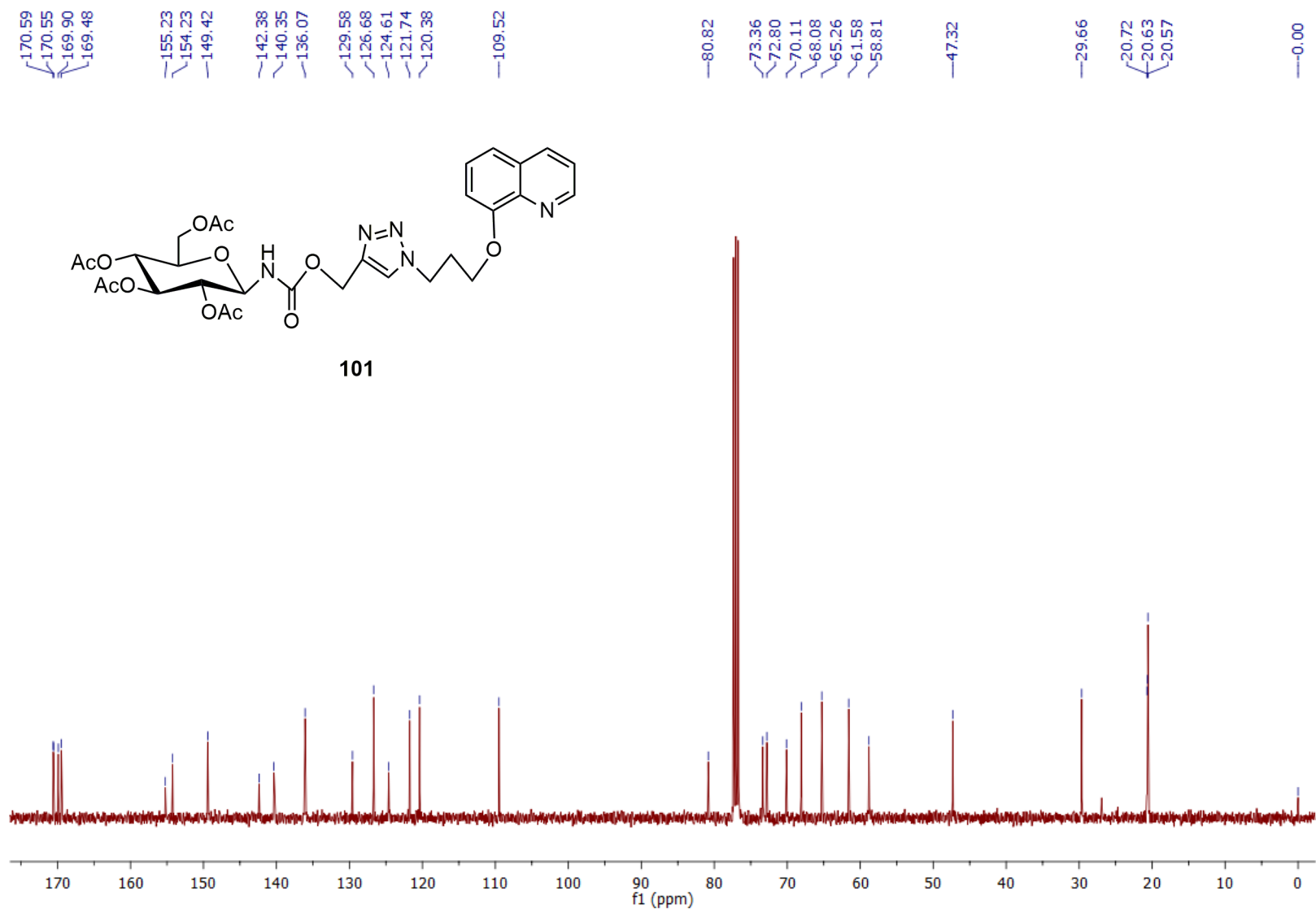


Fig. S194: ^{13}C NMR spectrum of glycoconjugate **101**.

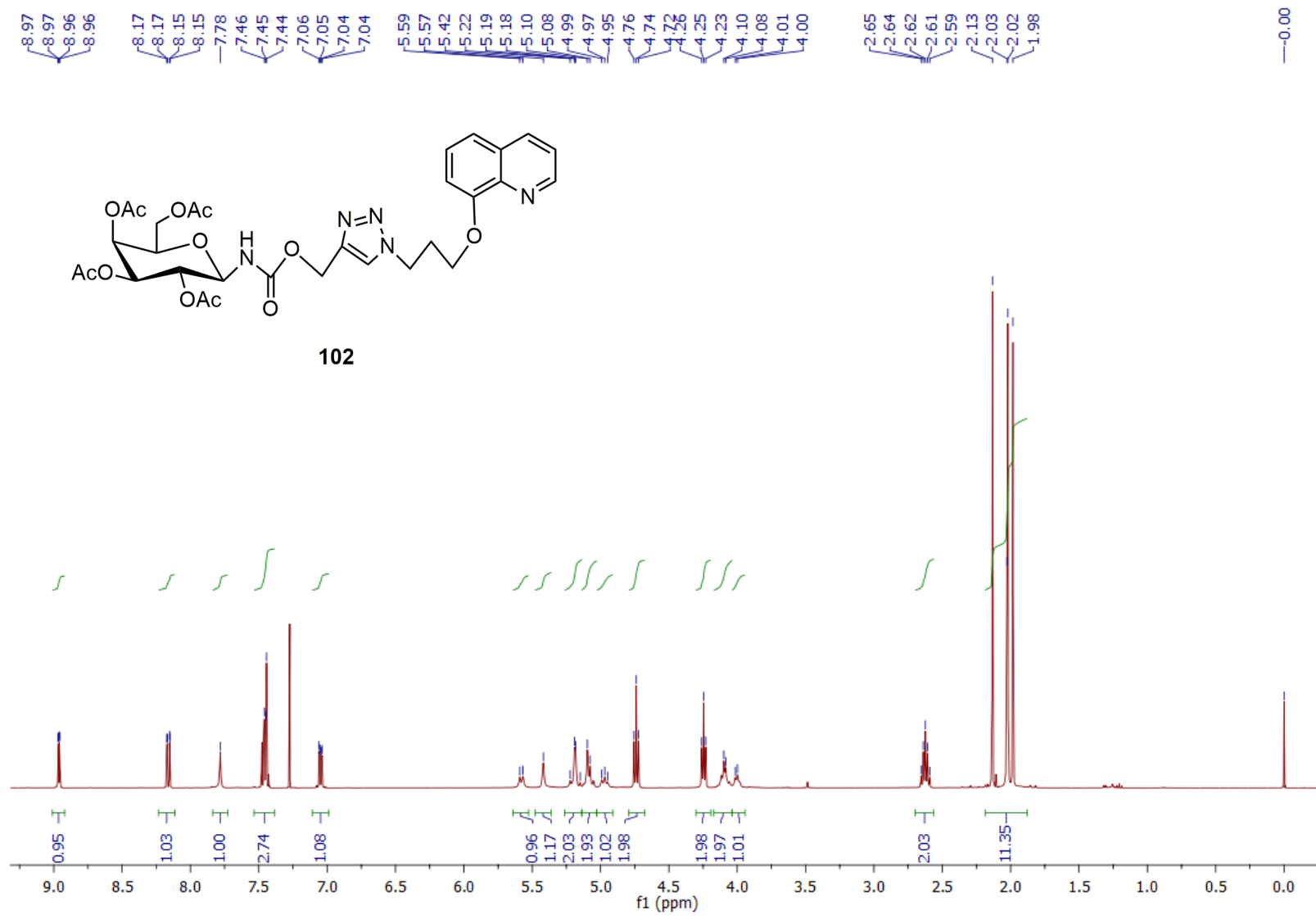


Fig. S195: ¹H NMR spectrum of glycoconjugate **102**.

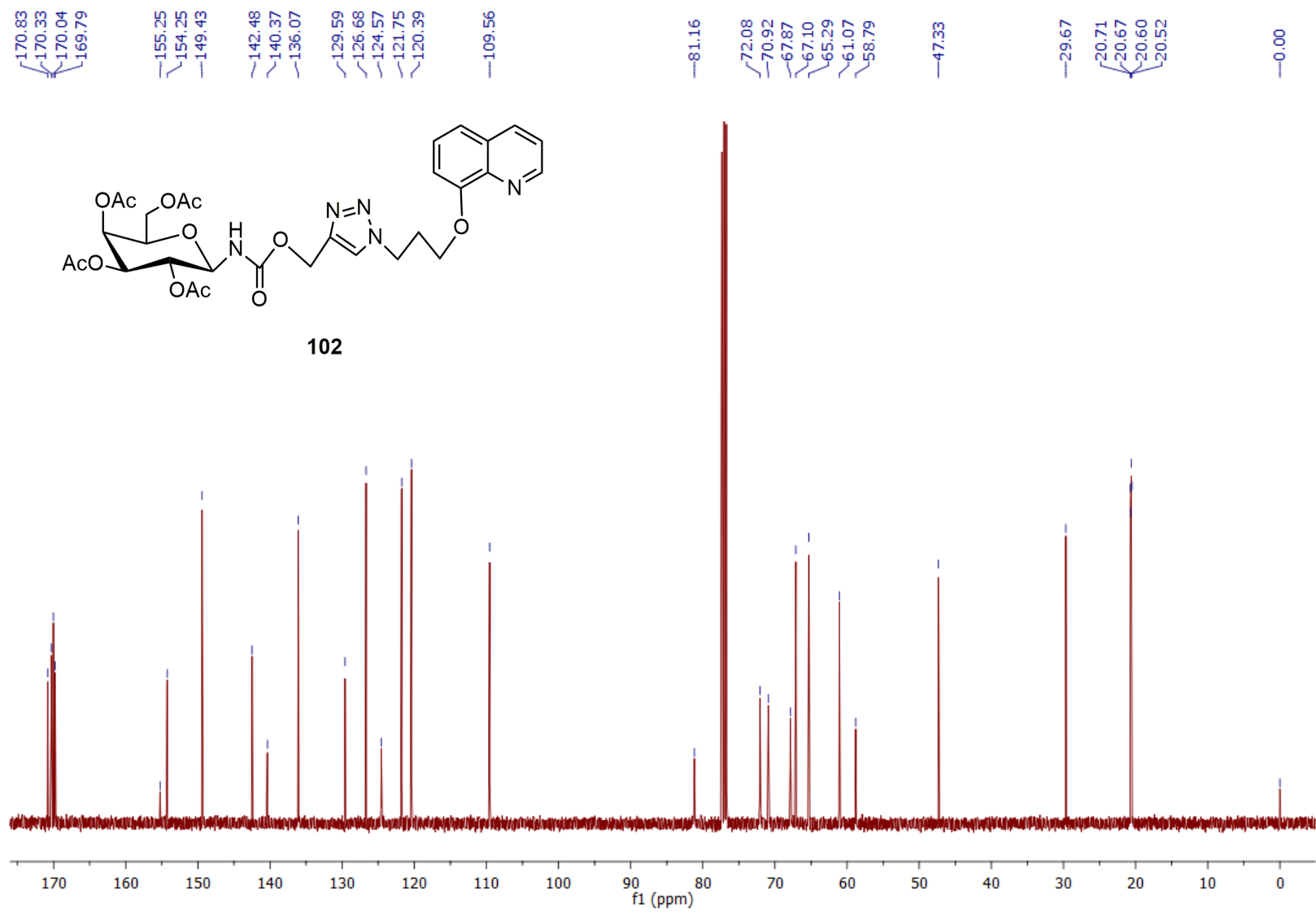


Fig. S196: ¹³C NMR spectrum of glycoconjugate **102**.

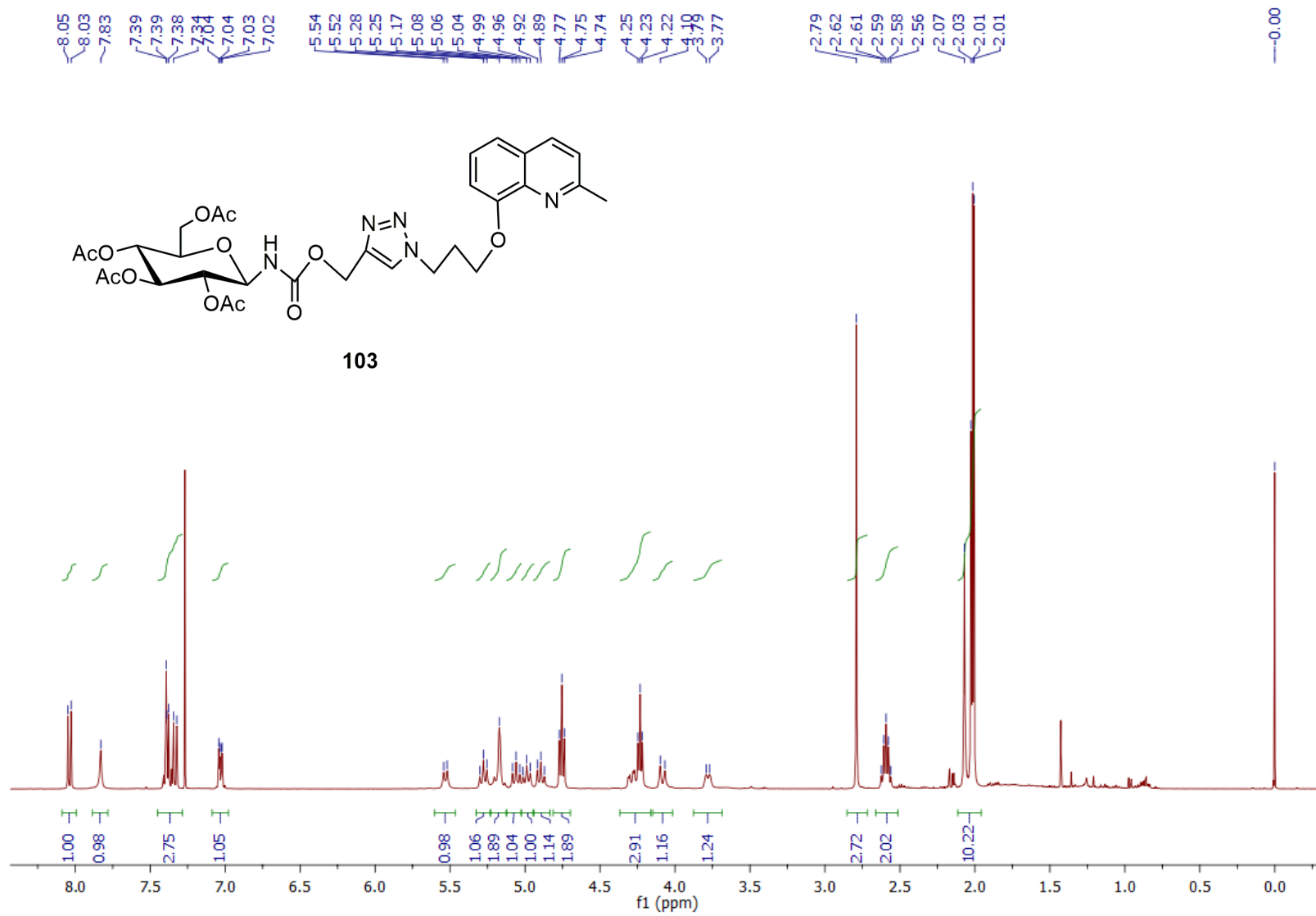


Fig. S197: ^1H NMR spectrum of glycoconjugate **103**.

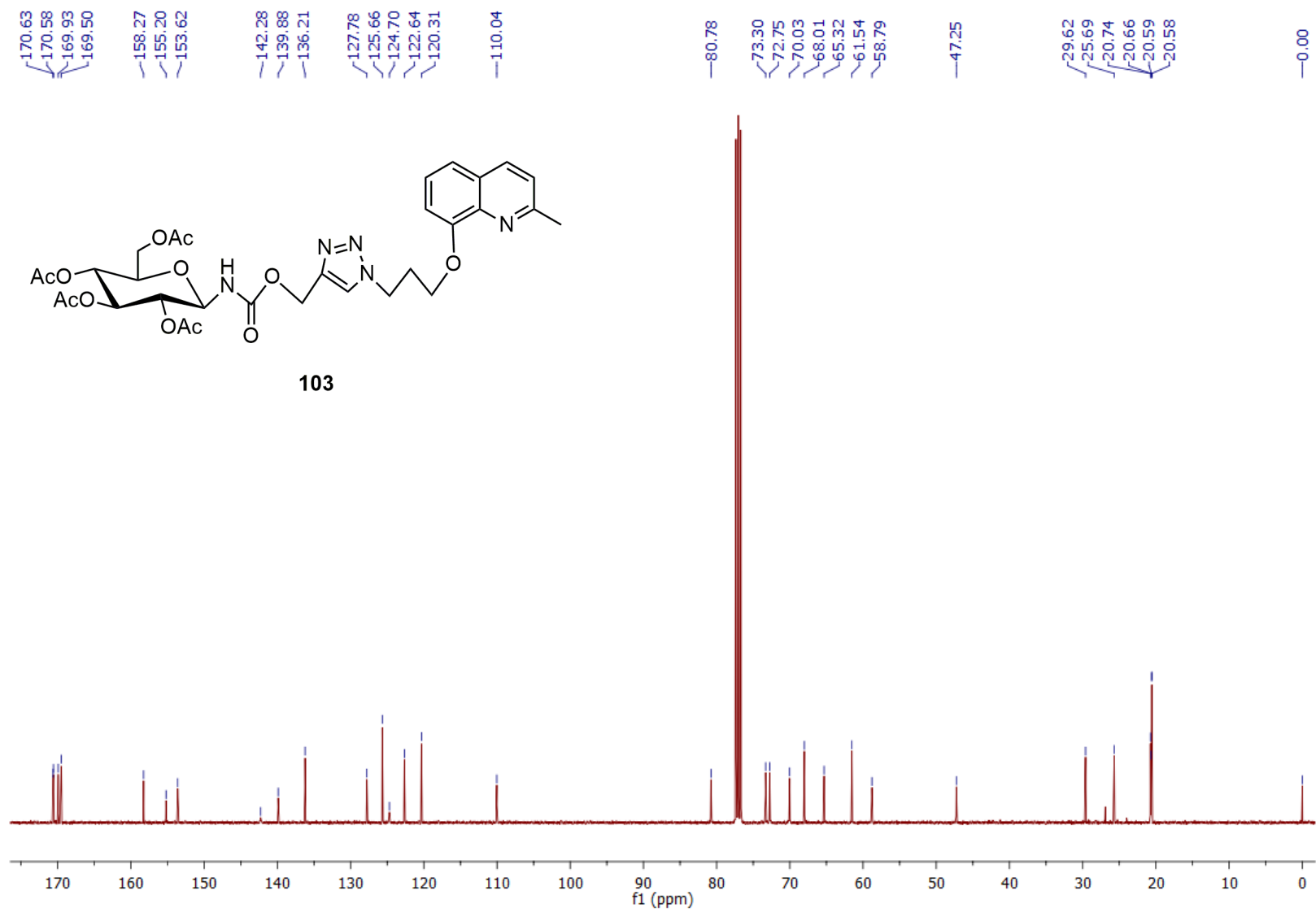


Fig. S198: ¹³C NMR spectrum of glycoconjugate **103**.

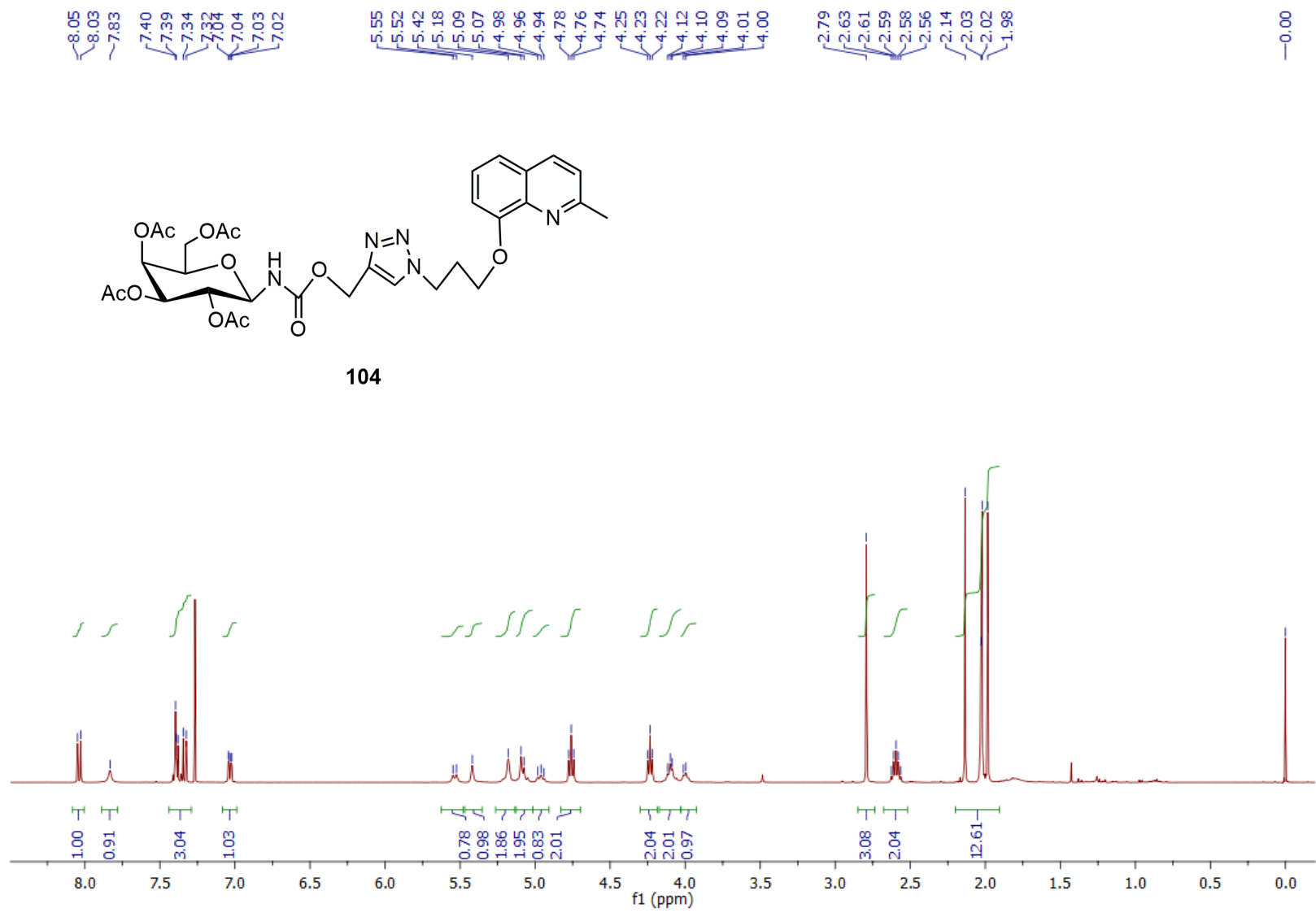


Fig. S199: ^1H NMR spectrum of glycoconjugate **104**.

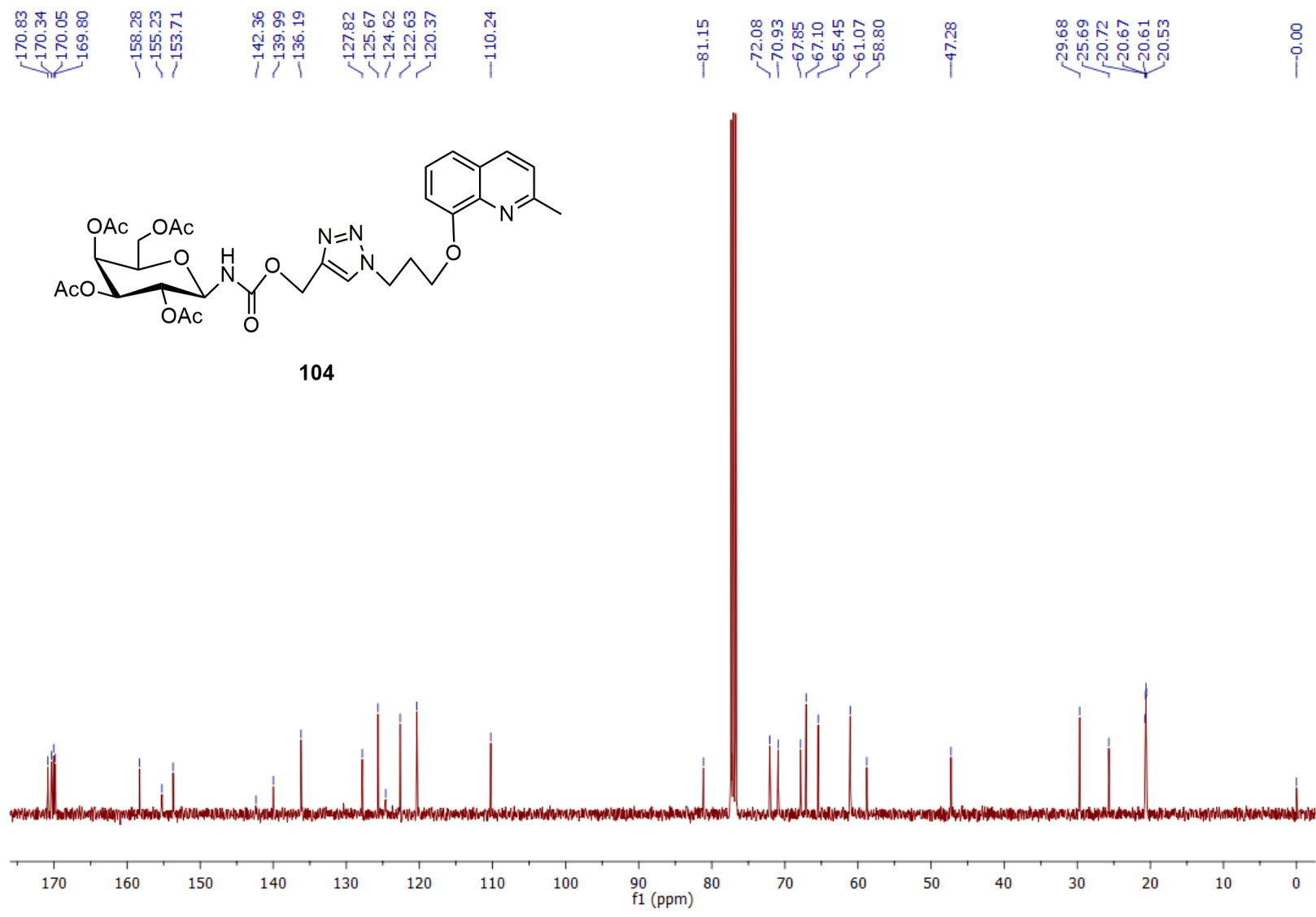


Fig. S200: ^{13}C NMR spectrum of glycoconjugate **104**.

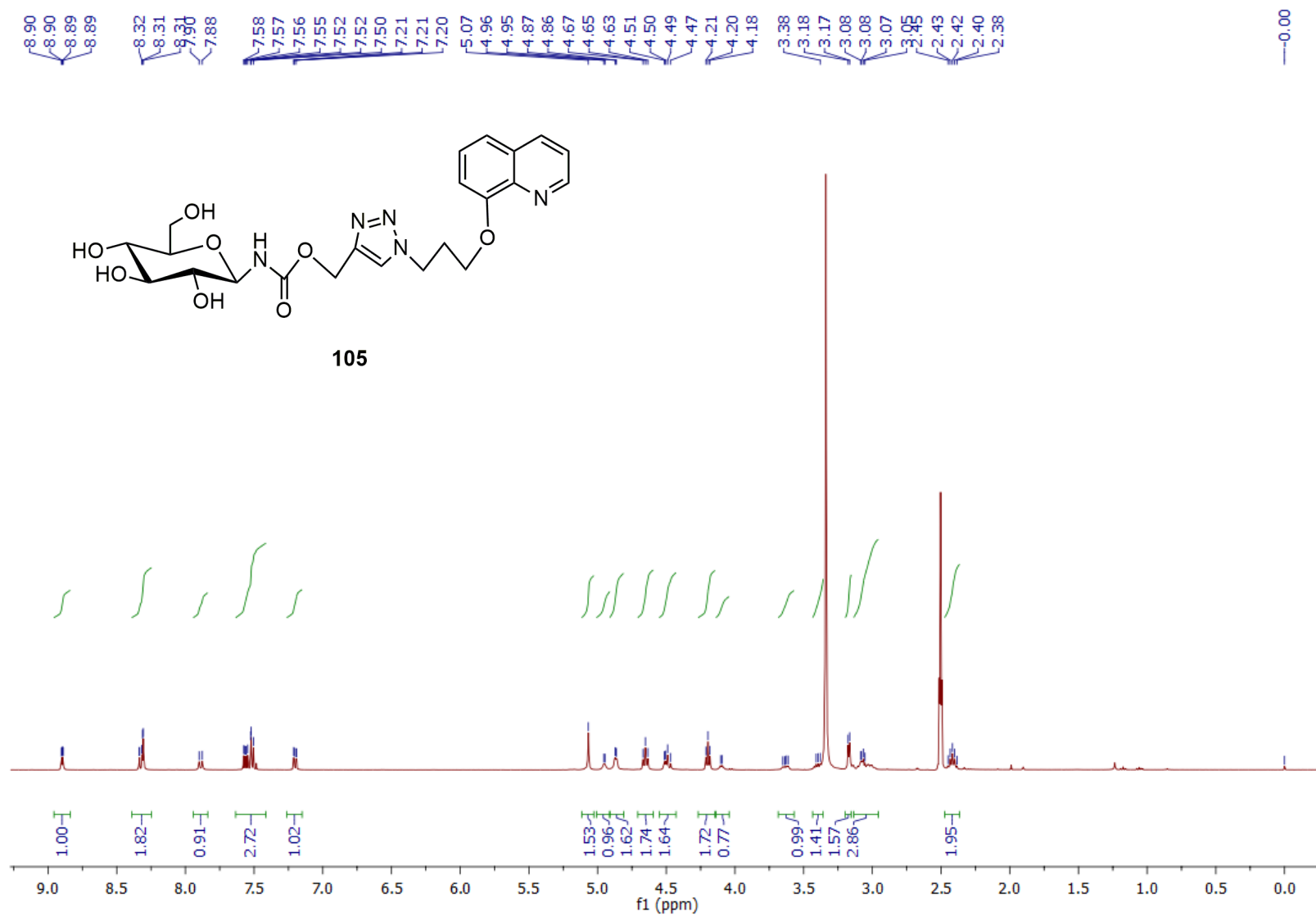


Fig. S201: ^1H NMR spectrum of glycoconjugate **105**.

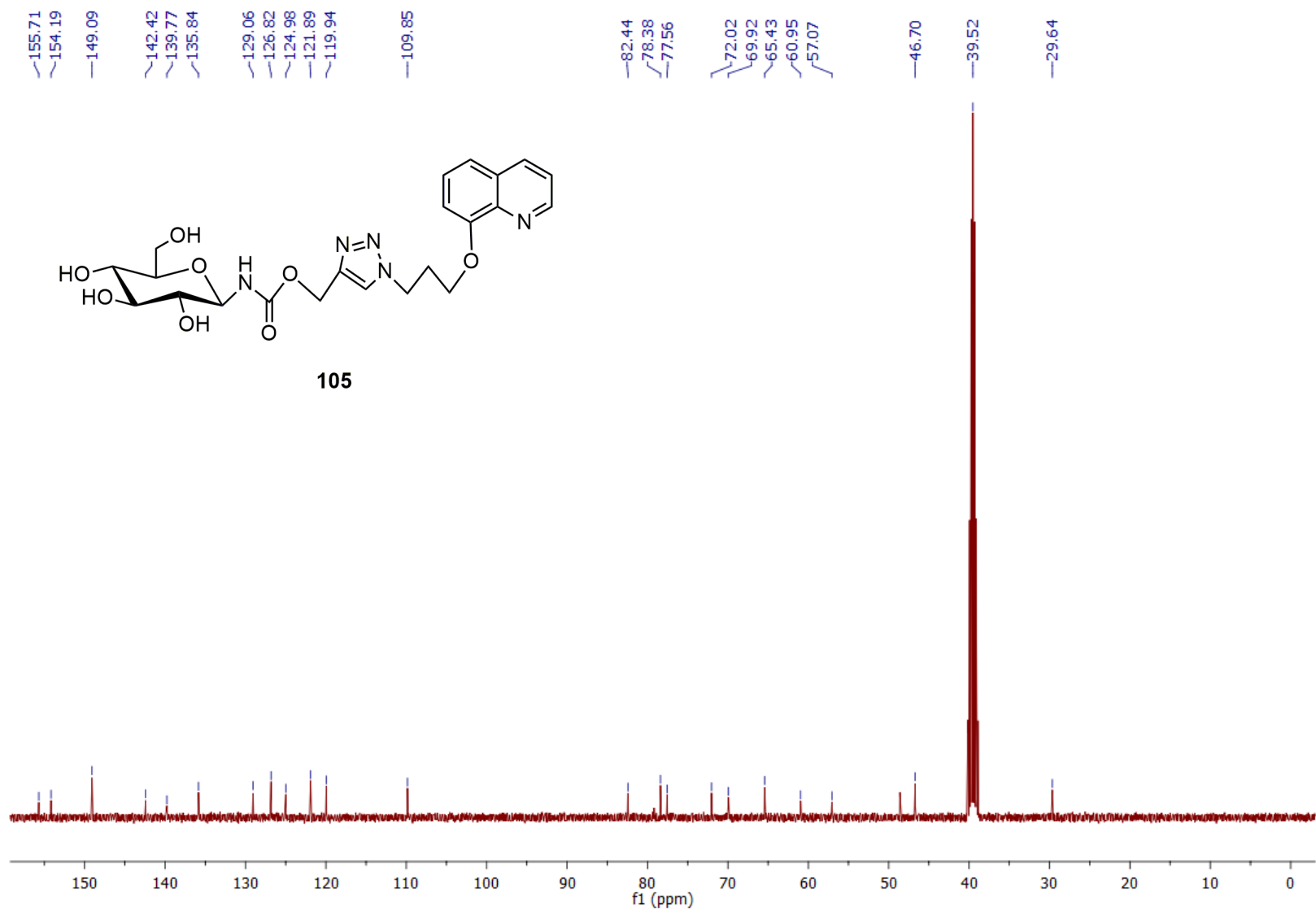


Fig. S202: ^{13}C NMR spectrum of glycoconjugate **105**.

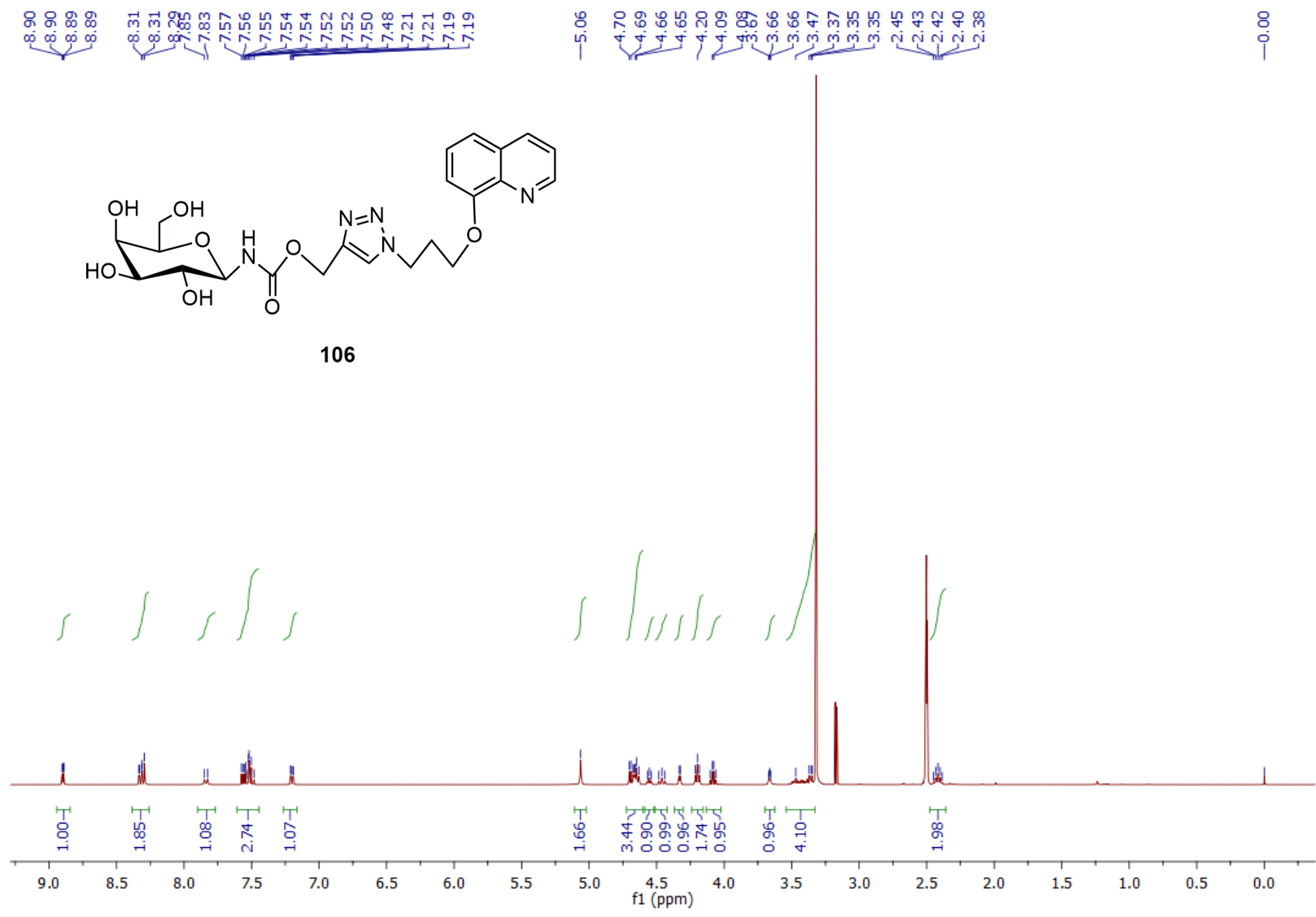


Fig. S203: ^1H NMR spectrum of glycoconjugate **106**.

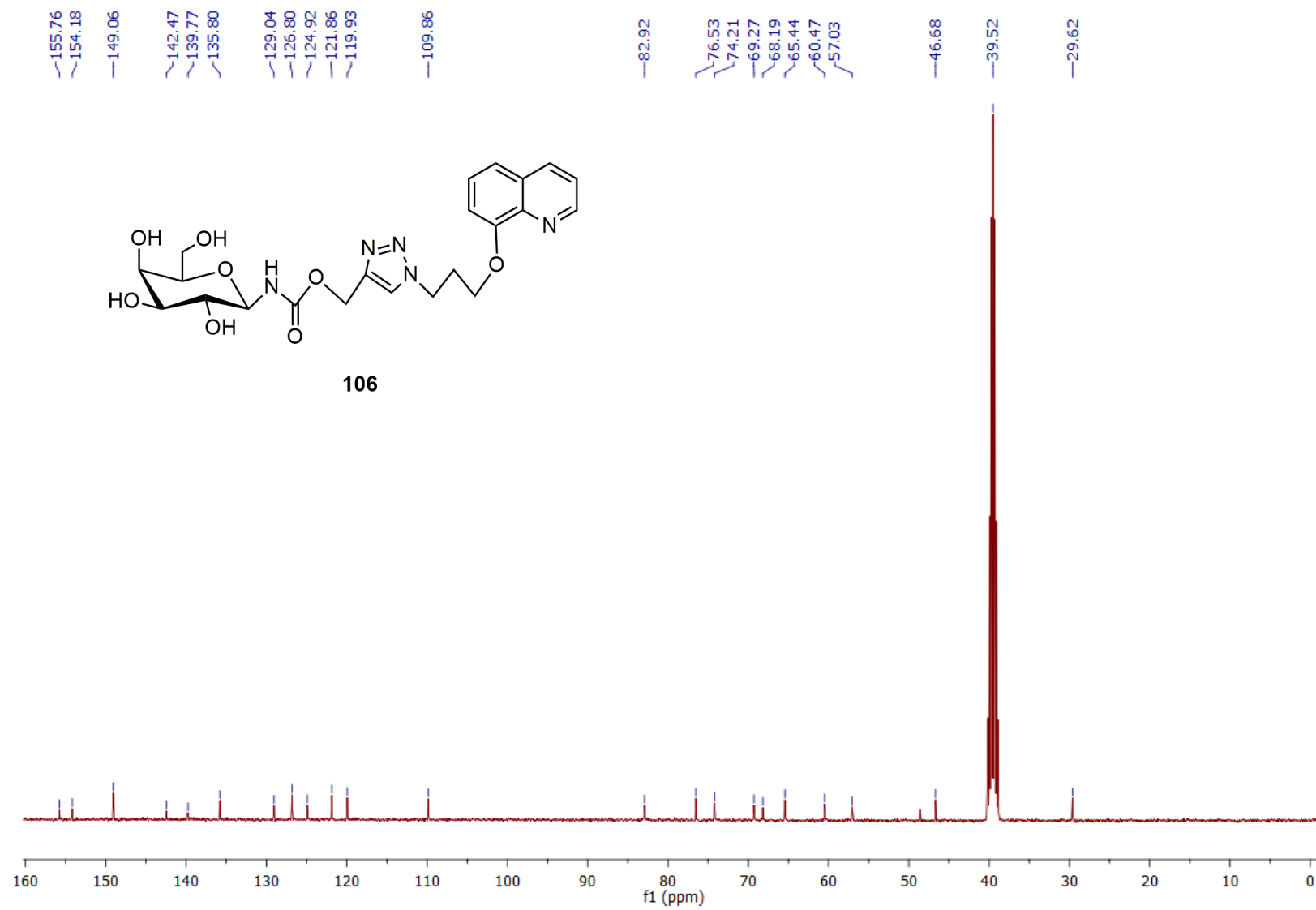


Fig. S204: ^{13}C NMR spectrum of glycoconjugate **106**.

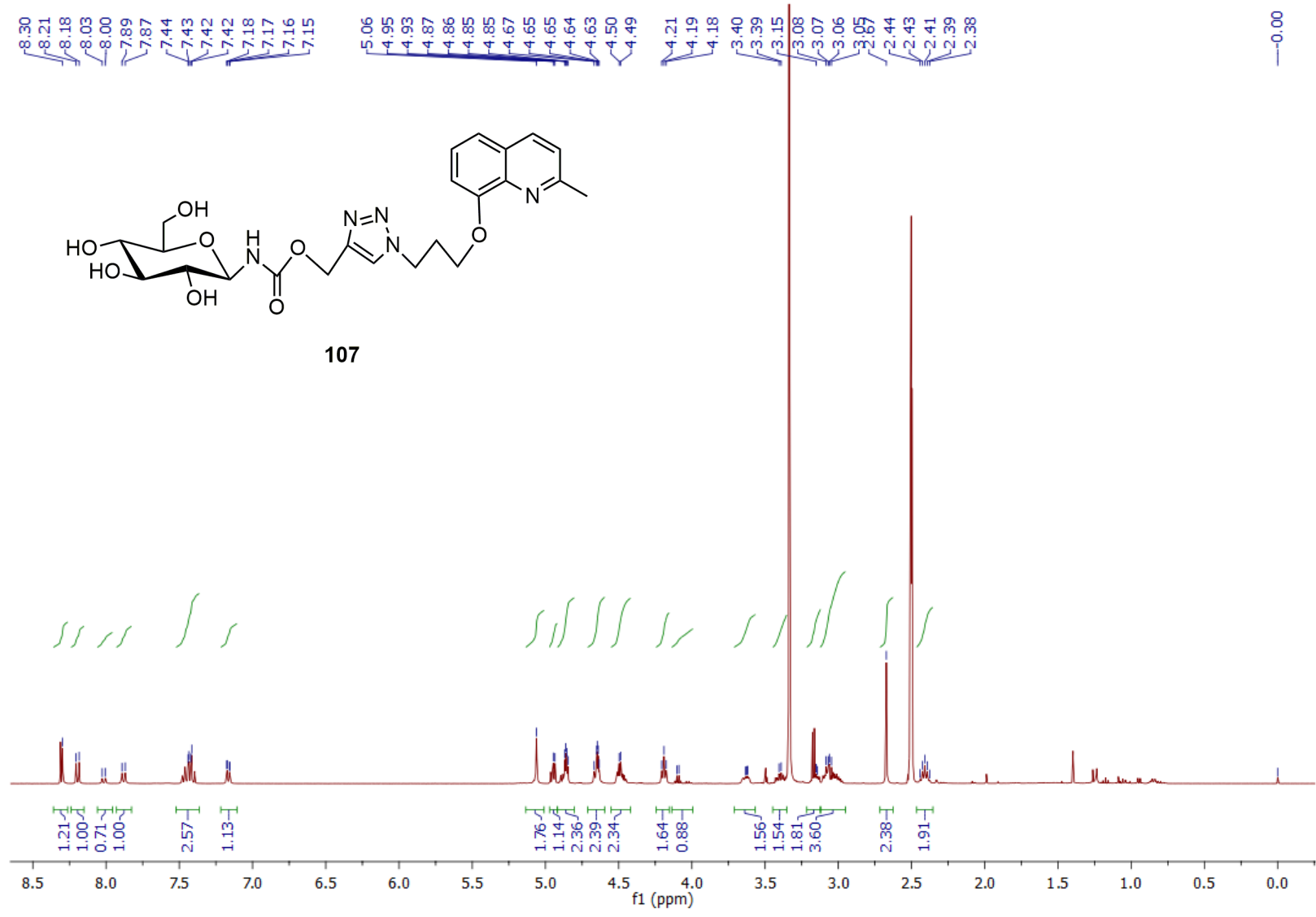


Fig. S205: ¹H NMR spectrum of glycoconjugate **107**.

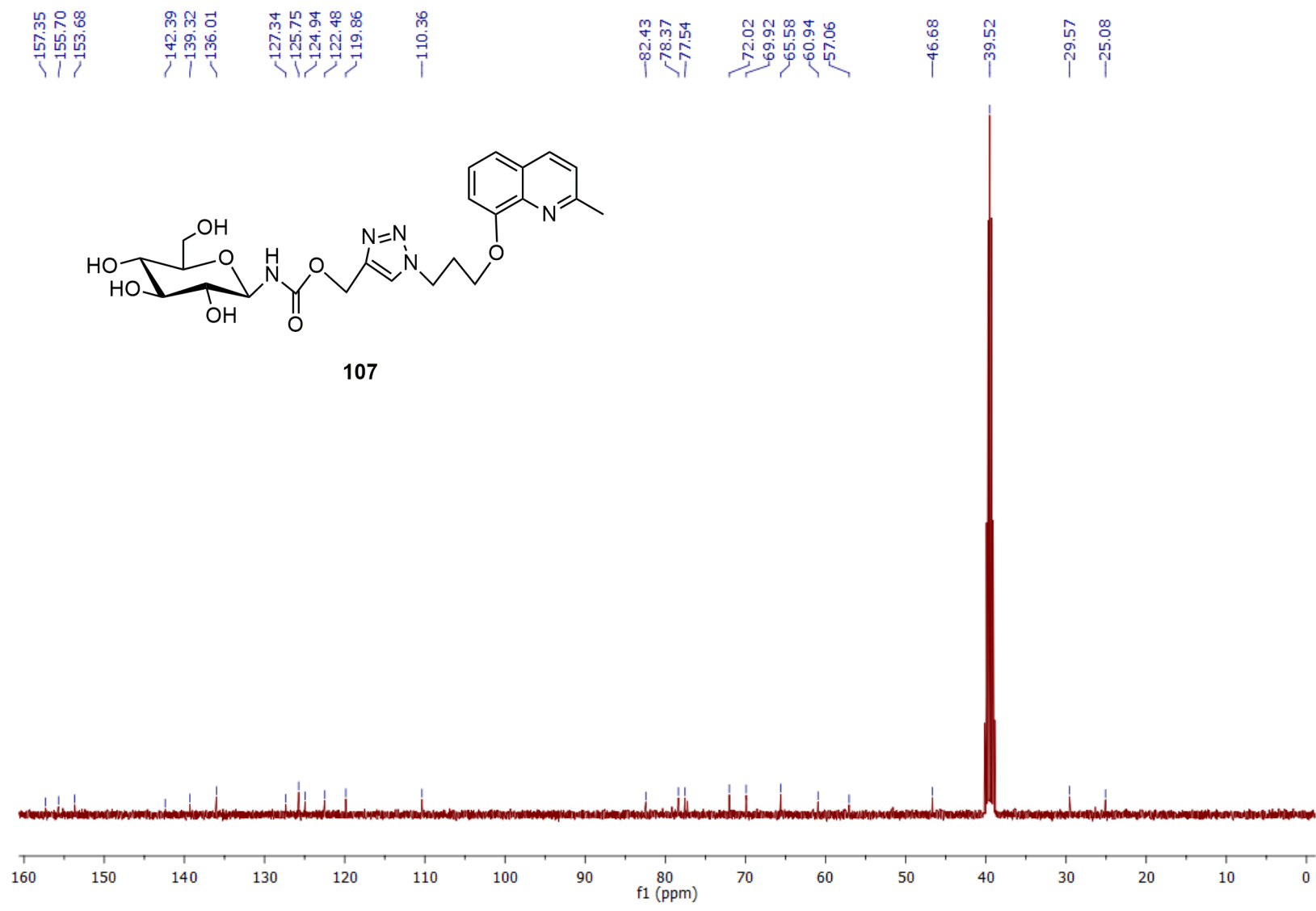


Fig. S206: ^{13}C NMR spectrum of glycoconjugate **107**.

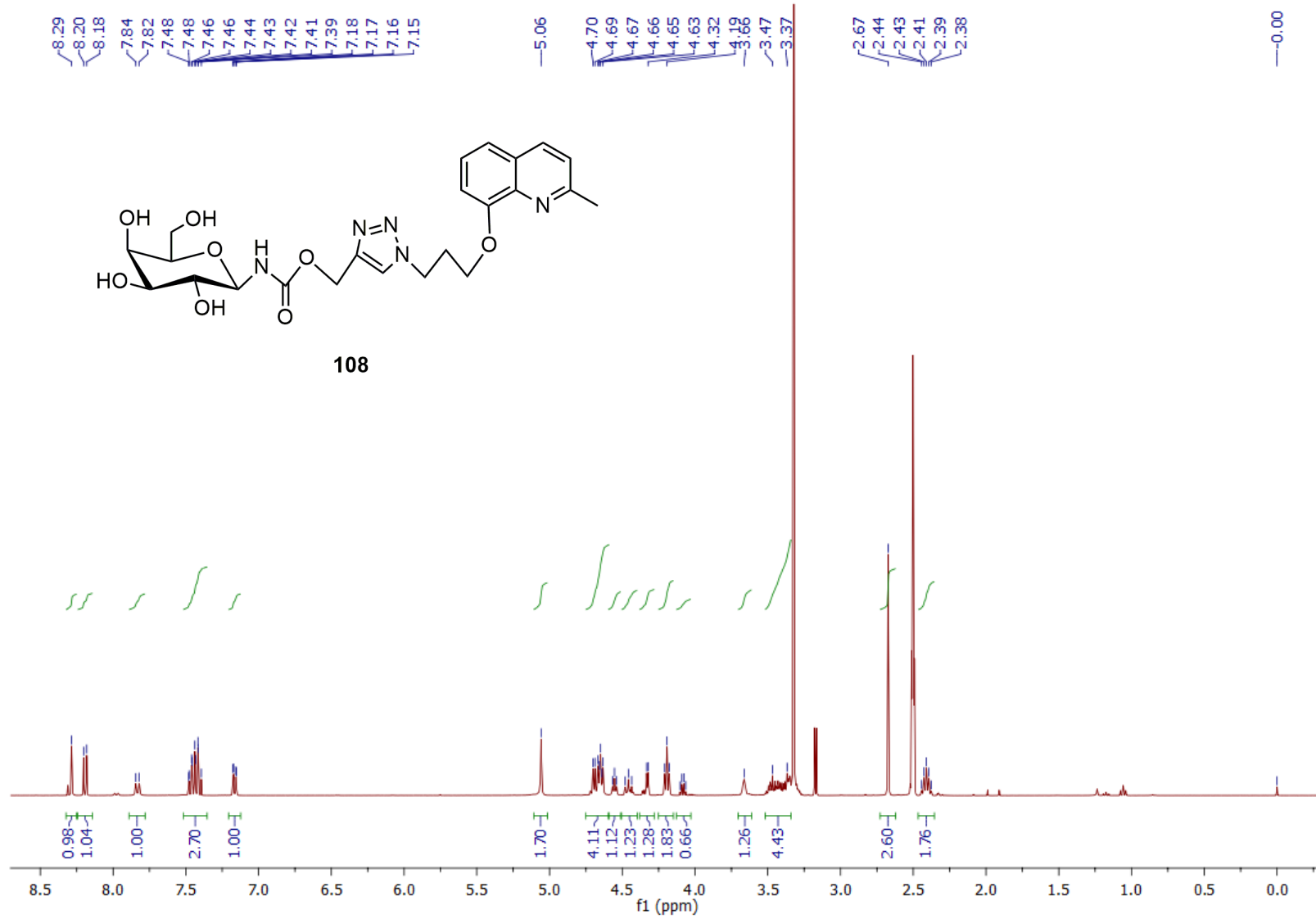


Fig. S207: ^1H NMR spectrum of glycoconjugate **108**.

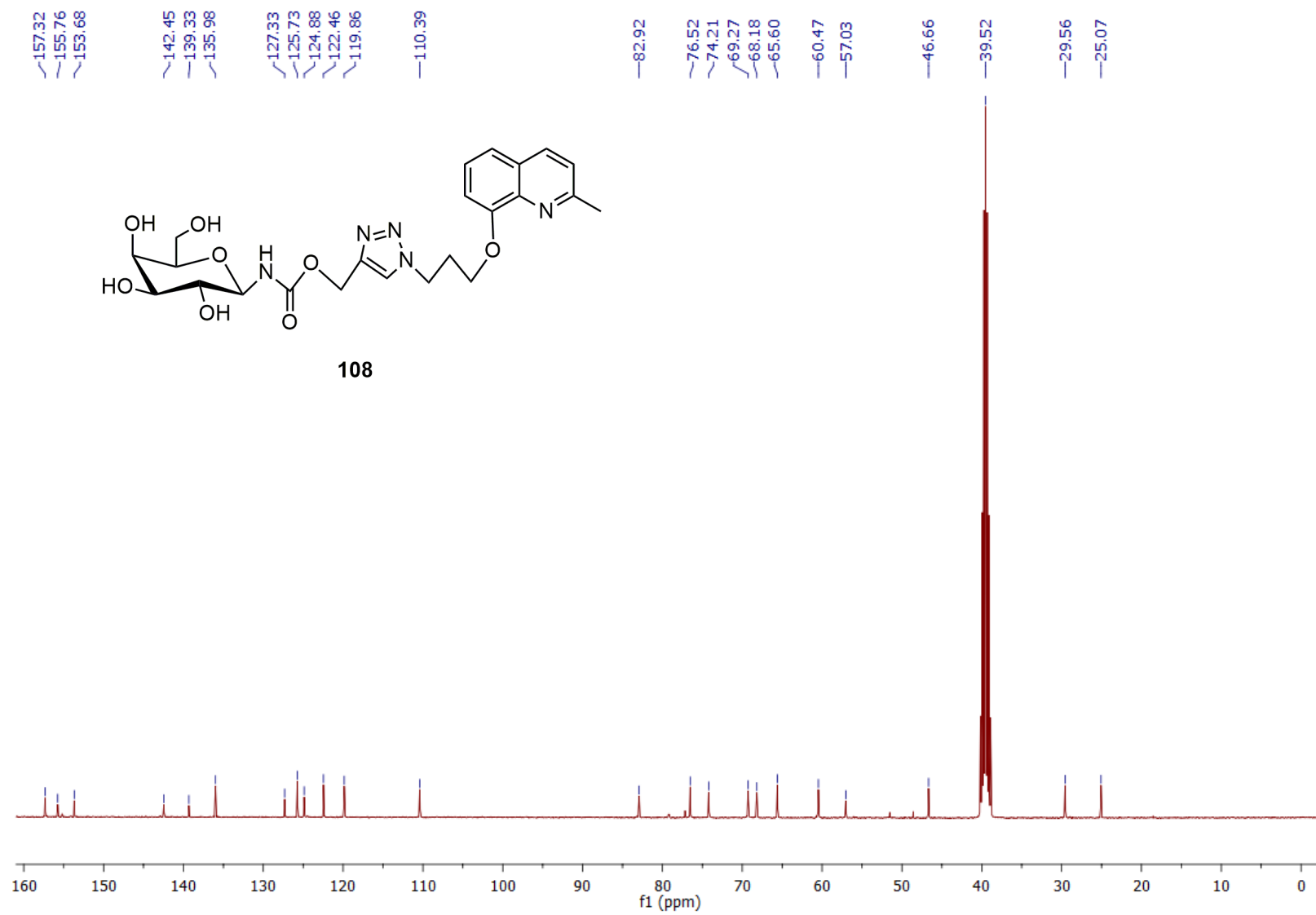


Fig. S208: ^{13}C NMR spectrum of glycoconjugate **108**.

2. Metal complexing properties of compound **93**

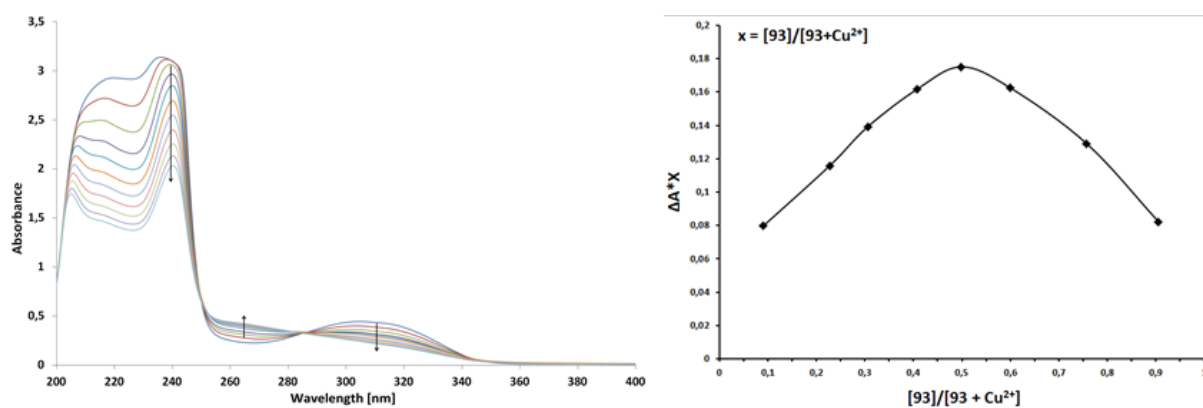
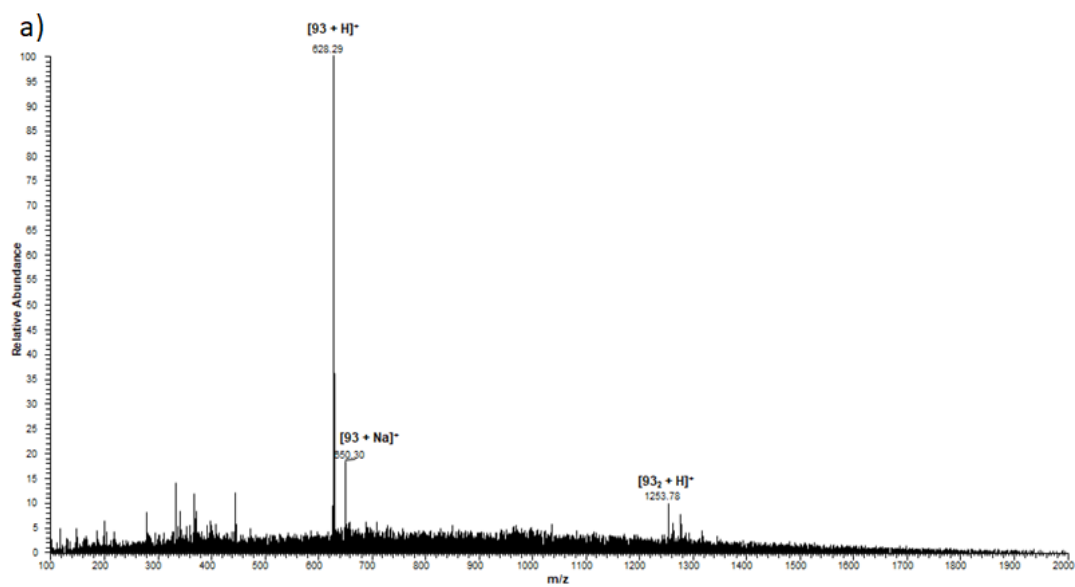


Figure S209: (a) UV spectrum of compound **93** with the addition of copper sulfate pentahydrate in methanol; (b) Job's plot of **93** with Cu^{2+} . The absorbance was monitored at 265 nm.



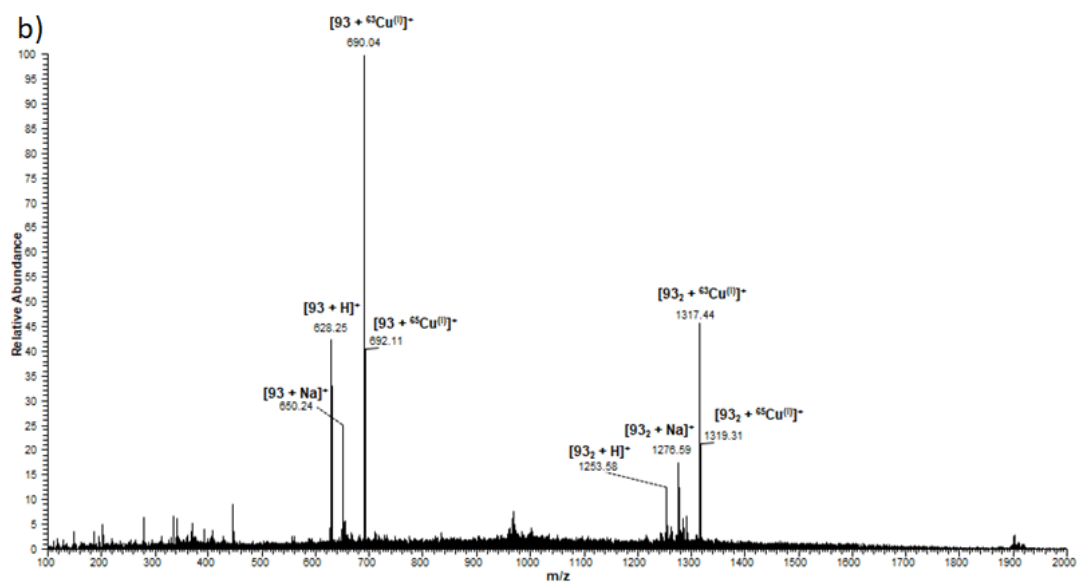


Figure S210: ESI-MS (positive-ion mode) spectrum of (a) **93** compound and (b) **93** after addition of Cu^{2+} ions into **93** solution.

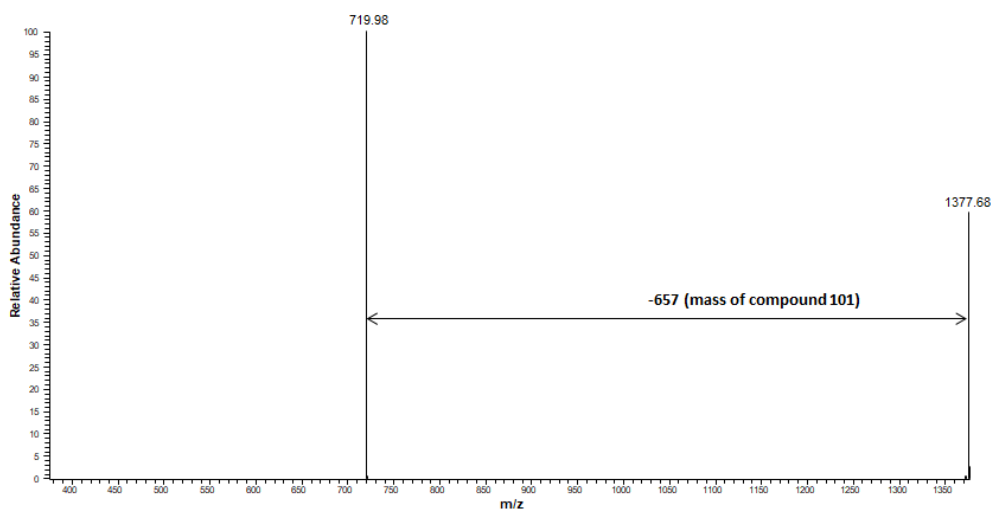


Figure S211: ESI-MS/MS fragmentation spectrum (positive-ion mode) of corresponding parent ion $m/z = 1377.68$.