

Supporting Information

for

Interplay of Protecting Groups and Side Chain Conformation in Glycopyranosides. Modulation of the Influence of Remote Substituents on Glycosylation?

Suresh Dharuman,[†] Harsha Amarasekara,[†] and David Crich *

Department of Chemistry, Wayne State University, 5101 Cass Avenue, Detroit, MI 48202, USA

dcrich@chem.wayne.edu

[†] These authors contributed equally

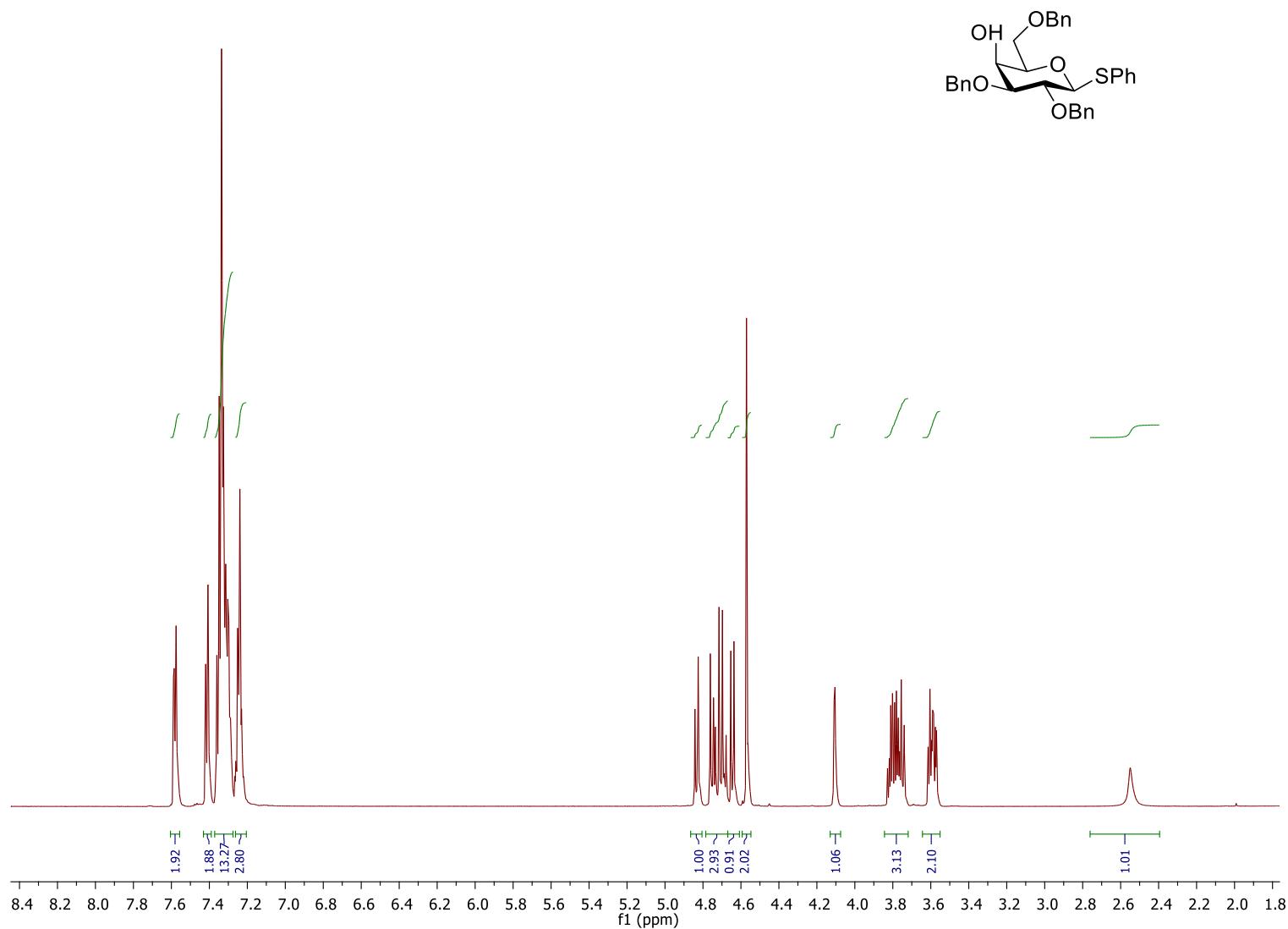
Table of Contents.

Compounds	Spectra
Phenyl 2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (1)	S5 – S6
Phenyl (6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-1)	S7 – S8
Phenyl 2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-glucopyranoside (2)	S9 – S10
Phenyl (6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-glucopyranoside (6S-D-2)	S11 – S12
Ethyl 2,3,4-tri- <i>O</i> -benzyl-1-thio- β -D-glucopyranoside (3)	S13 – S14
Ethyl (6 <i>S</i>)-[6- ² H]-2,3,4,6-tetra- <i>O</i> -acetyl-1-thio- β -D-glucopyranoside (6S-D-3)	S15
(6 <i>S</i>)-1,6-Anhydro-2,3,4-tri- <i>O</i> -acetyl-6-bromo- β -D-galactopyranose (5)	S16 – S17
(6 <i>S</i>)-[6- ² H]-1,6-Anhydro-2,3,4-tri- <i>O</i> -acetyl- β -D-galactopyranose (6)	S18 – S19
Phenyl (6 <i>S</i>)-[6- ² H]-2,3,4,6-tetra- <i>O</i> -acetyl-1-thio- β -D-galactopyranoside (8)	S20 – S21
Phenyl 2,3-di- <i>O</i> -benzyl-4,6- <i>O</i> -benzylidene-(6 <i>S</i>)-[6- ² H]-1-thio- β -D-galactopyranoside (10)	S22 – S23
Ethyl -(6 <i>S</i>)-[6- ² H]-2,3,4,6-tetra- <i>O</i> -acetyl-1-thio- β -D-glucopyranoside (12)	S24 – S25
Phenyl 4- <i>O</i> -acetyl-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (13)	S26 – S27
Phenyl 4- <i>O</i> -acetyl-(6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-13)	S28 – S29
Phenyl 4- <i>O</i> -pivoyl-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (14)	S30 – S32
Phenyl 4- <i>O</i> -pivaloyl-(6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-14)	S33 – S34
Phenyl 2,3,6-tri- <i>O</i> -benzyl-4- <i>O</i> -trifluoroacetyl -1-thio- β -D-galactopyranoside (15)	S35 – S39
Phenyl 4- <i>O</i> -trifluoroacetyl-(6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-15)	S40 – S41

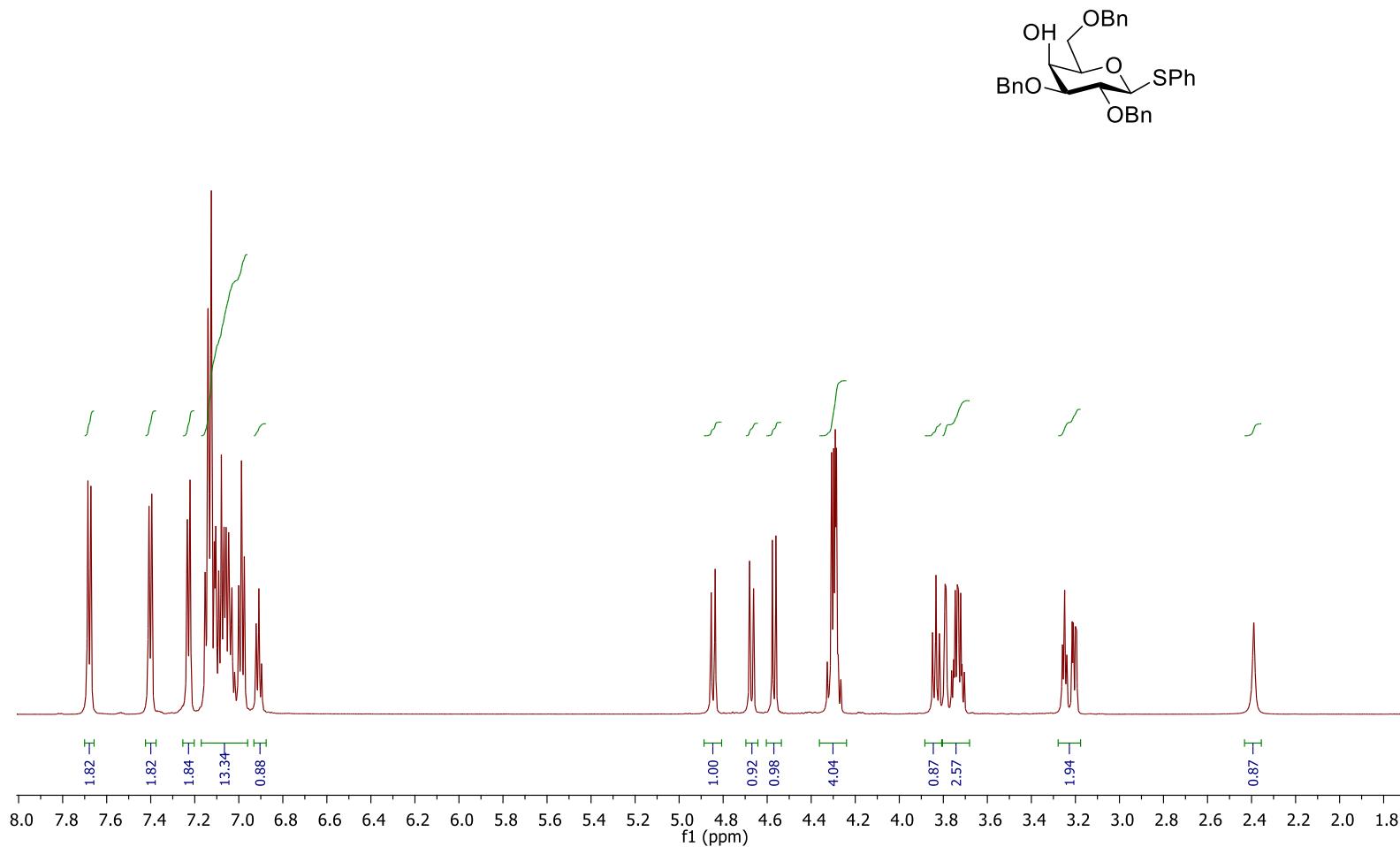
Phenyl 2,3,6-tri- <i>O</i> -benzyl-4- <i>O</i> -trichloroacetyl -1-thio- β -D-galactopyranoside (16)	S42 – S44
Phenyl 4- <i>O</i> -trichloroacetyl-(6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-16)	S45 – S46
Phenyl 4- <i>O</i> -benzoyl-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (17)	S47 – S48
Phenyl 4- <i>O</i> -benzoyl-(6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-17)	S49 – S50
Phenyl 4- <i>O</i> -(<i>p</i> -methylbenzoyl)-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (18)	S51 – S53
Phenyl 4- <i>O</i> -(<i>p</i> -methylbenzoyl)-(6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-18)	S54 – S55
Phenyl 4- <i>O</i> -(<i>p</i> -methoxybenzoyl)-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (19)	S56 – S57
Phenyl 4- <i>O</i> -(<i>p</i> -methoxybenzoyl)-(6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-19)	S58 – S59
Phenyl 4- <i>O</i> -(<i>p</i> -nitrobenzoyl)-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (20)	S60 – S62
Phenyl 4- <i>O</i> -(<i>p</i> -nitrobenzoyl)-(6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-20)	S63 – S64
Phenyl 2,3,4,6-tetra- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (21)	S65 – S66
Phenyl (6 <i>S</i>)-[6- ² H]-2,3,4,6-tetra- <i>O</i> -benzyl-1-thio- β -D-galactopyranoside (6S-D-21)	S67 – S68
Phenyl 2,3,6-tri- <i>O</i> -benzyl-4- <i>O</i> -(1',1',1'-trifluoroethyl)-1-thio- β -D-galactopyranoside (22)	S69 – S72
Phenyl (6 <i>S</i>)-[6- ² H]-2,3,6-tri- <i>O</i> -benzyl-4- <i>O</i> -(1',1',1'-trifluoroethyl)-1-thio- β -D-galactopyranoside (6S-D-22)	S73 – S74
Phenyl 4- <i>O</i> -acetyl-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-glucopyranoside (23)	S75 – S76
Phenyl 2,3,6-tri- <i>O</i> -benzyl-4- <i>O</i> -trifluoroacetyl-1-thio- β -D-glucopyranoside (24)	S77 – S80
Phenyl 4- <i>O</i> -benzoyl-2,3,6-tri- <i>O</i> -benzyl-1-thio- β -D-glucopyranoside (25)	S81 – S82

Phenyl 4- <i>O</i> -benzoyl-(6 <i>S</i>)-[6- ² H ₁]-2,3,6-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (6S-D-25)	S83 – S84
Spectrum of Phenyl 4- <i>O</i> -benzenesulfonyl-2,3,6-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (26)	S85 – S87
Phenyl 4- <i>O</i> -benzenesulfonyl-(6 <i>S</i>)-[6- ² H ₁]-2,3,6-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (6S-D-26)	S88 – S89
Phenyl 2,3,4,6-tetra- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (27)	S90 – S91
Phenyl (6 <i>S</i>)-[6- ² H ₁]-2,3,4,6-tetra- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (6S-D-27)	S92 – S93
Ethyl 6- <i>O</i> -acetyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (28)	S94 – S96
Ethyl 2,3,4-tri- <i>O</i> -benzyl-6- <i>O</i> -pivolyl-1-thio-β-D-glucopyranoside (29)	S97 – S99
Ethyl 2,3,4-tri- <i>O</i> -benzyl-6- <i>O</i> -trifluoroacetyl-1-thio-β-D-glucopyranoside (30)	S100 – S103
Ethyl 6- <i>O</i> -benzoyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (31)	S104 – S105
Ethyl (6 <i>S</i>)-[6- ² H ₁]-6- <i>O</i> -benzoyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (6S-D-31)	S106 – S107
Spectrum of Ethyl 6- <i>O</i> - <i>p</i> -methylbenzoyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (32)	S108 – S111
Ethyl (6 <i>S</i>)-[6- ² H ₁]-6- <i>O</i> - <i>p</i> -methylbenzoyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (6S-D-32)	S112 – S113
Ethyl 6- <i>O</i> - <i>p</i> -methoxybenzoyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (33)	S114 – S117
Ethyl (6 <i>S</i>)-[6- ² H ₁]-6- <i>O</i> - <i>p</i> -methoxybenzoyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (6S-D-33)	S118 – S119
Ethyl 6- <i>O</i> - <i>p</i> -nitrobenzoyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (34)	S120 – S122
Ethyl (6 <i>S</i>)-[6- ² H ₁]-6- <i>O</i> - <i>p</i> -nitrobenzoyl-2,3,4-tri- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (6S-D-34)	S123 – S124
Ethyl 2,3,4-tri- <i>O</i> -benzyl-6- <i>O</i> -(<i>N</i> -phenylcarbamoyl)-1-thio-β-D-glucopyranoside (35)	S125 – S127
Ethyl 2,3,4-tri- <i>O</i> -benzyl-(6 <i>S</i>)-[6- ² H ₁]-6- <i>O</i> -(<i>N</i> -phenylcarbamoyl)-1-thio-β-D-glucopyranoside (6S-D-35)	S128 – S129
Ethyl 2,3,4,6-tetra- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (36)	S130 – S131
Ethyl (6 <i>S</i>)-[6- ² H ₁]-2,3,4,6-tetra- <i>O</i> -benzyl-1-thio-β-D-glucopyranoside (6S-D-36)	S132 – S133

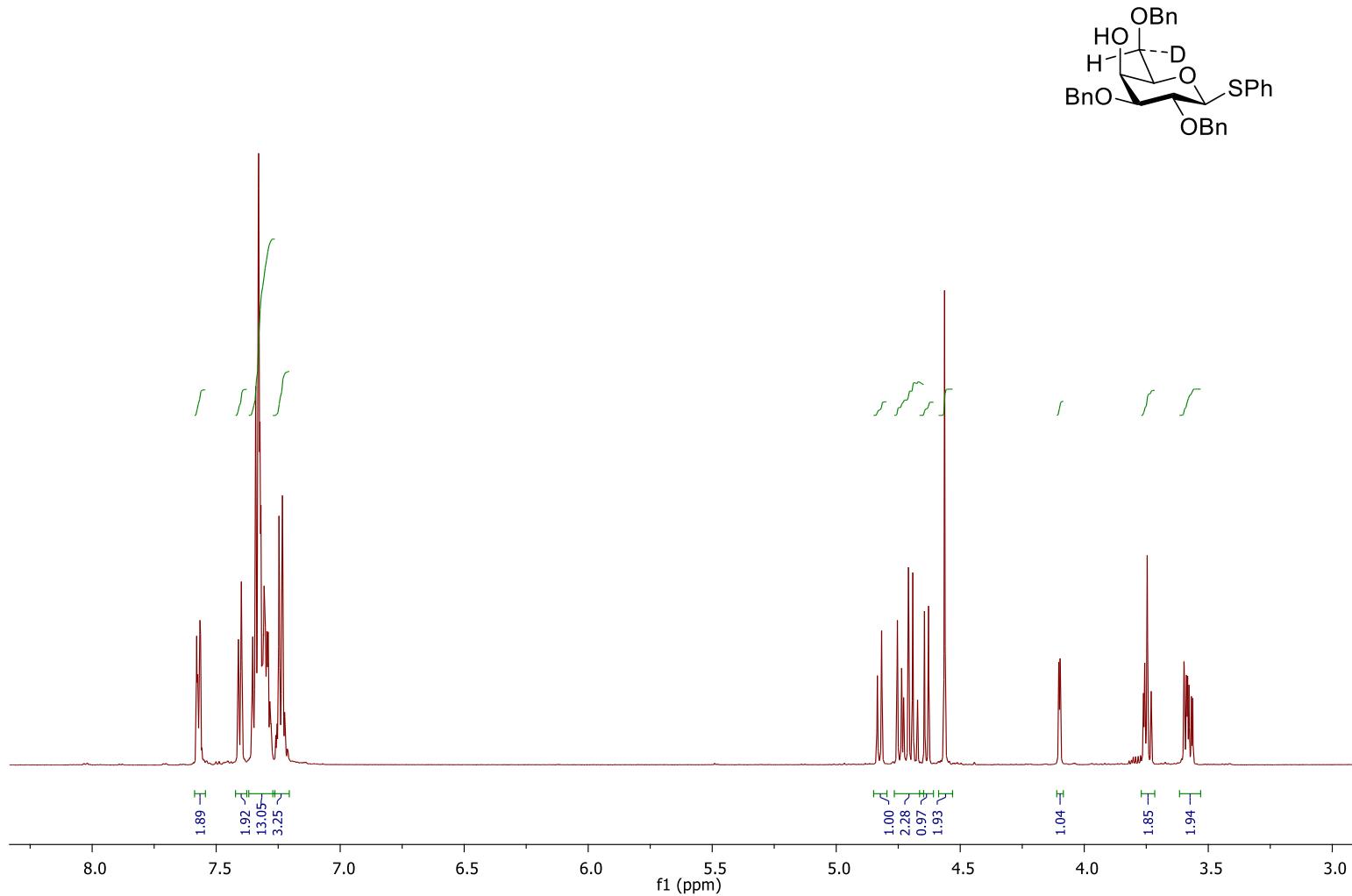
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**1**)



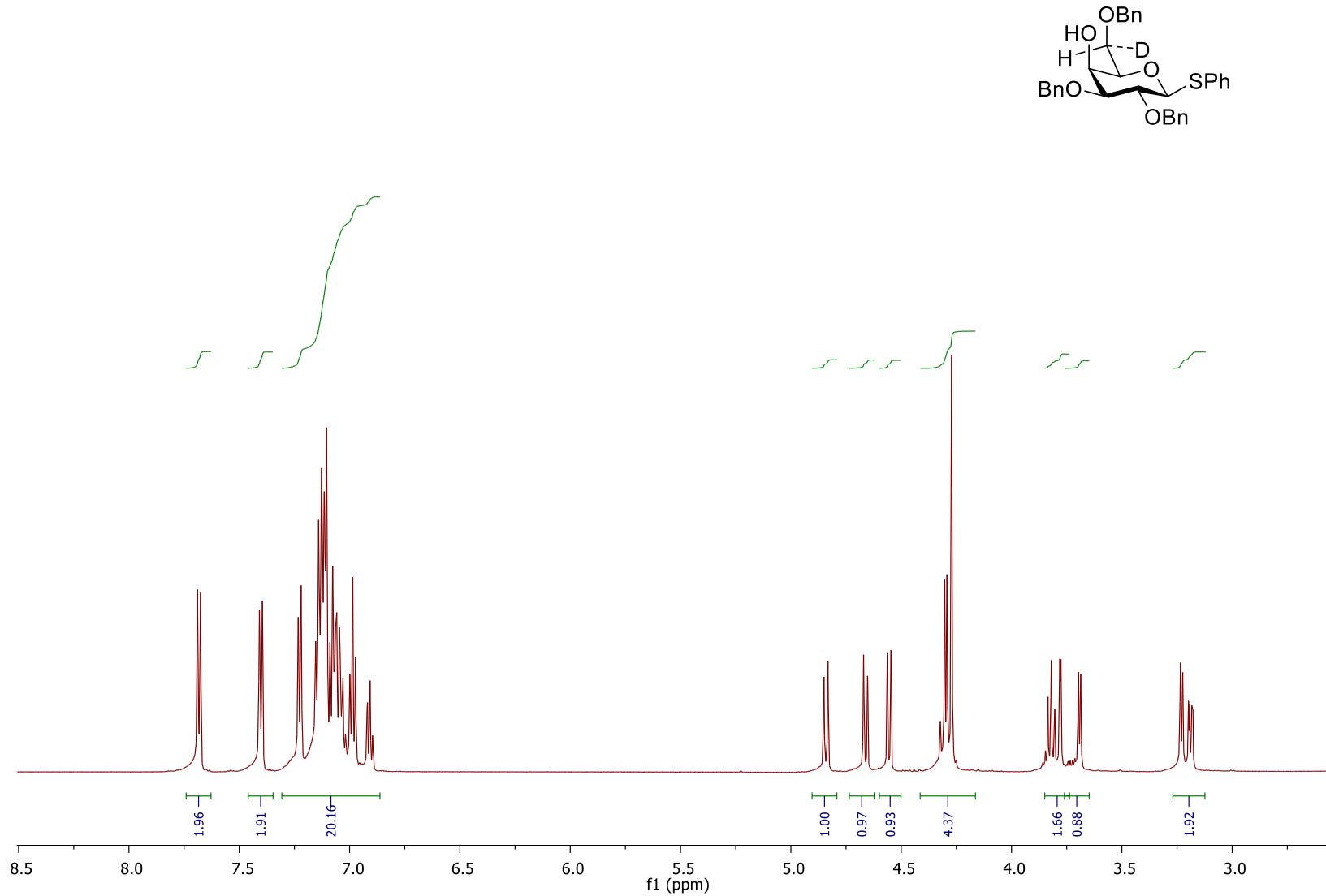
^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl 2,3,6-tri- O -benzyl-1-thio- β -D-galactopyranoside (**1**)



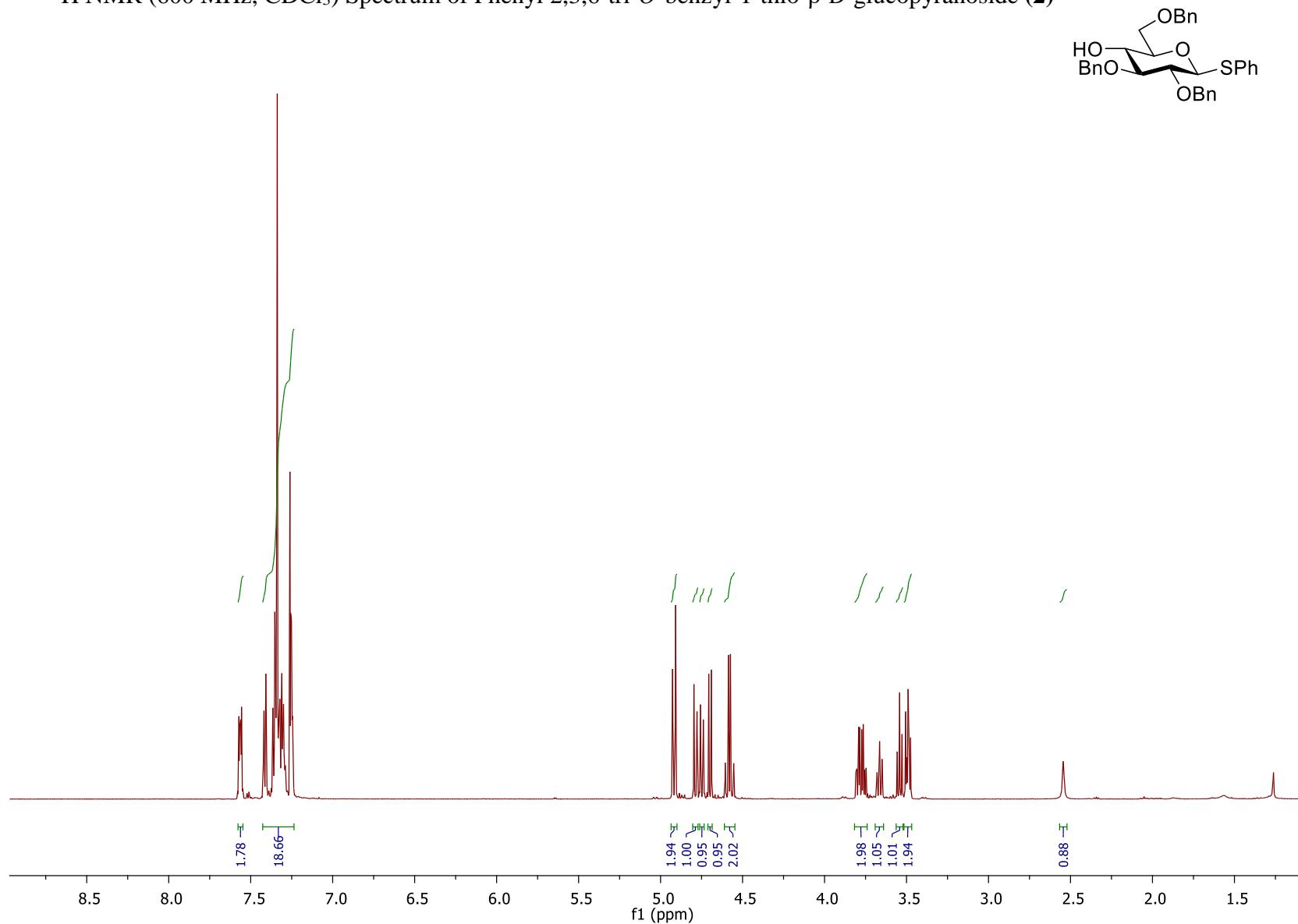
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl ($6S$)-[$6-^2\text{H}_1$]-2,3,6-tri- O -benzyl-1-thio- β -D-galactopyranoside (**6S-D-1**)



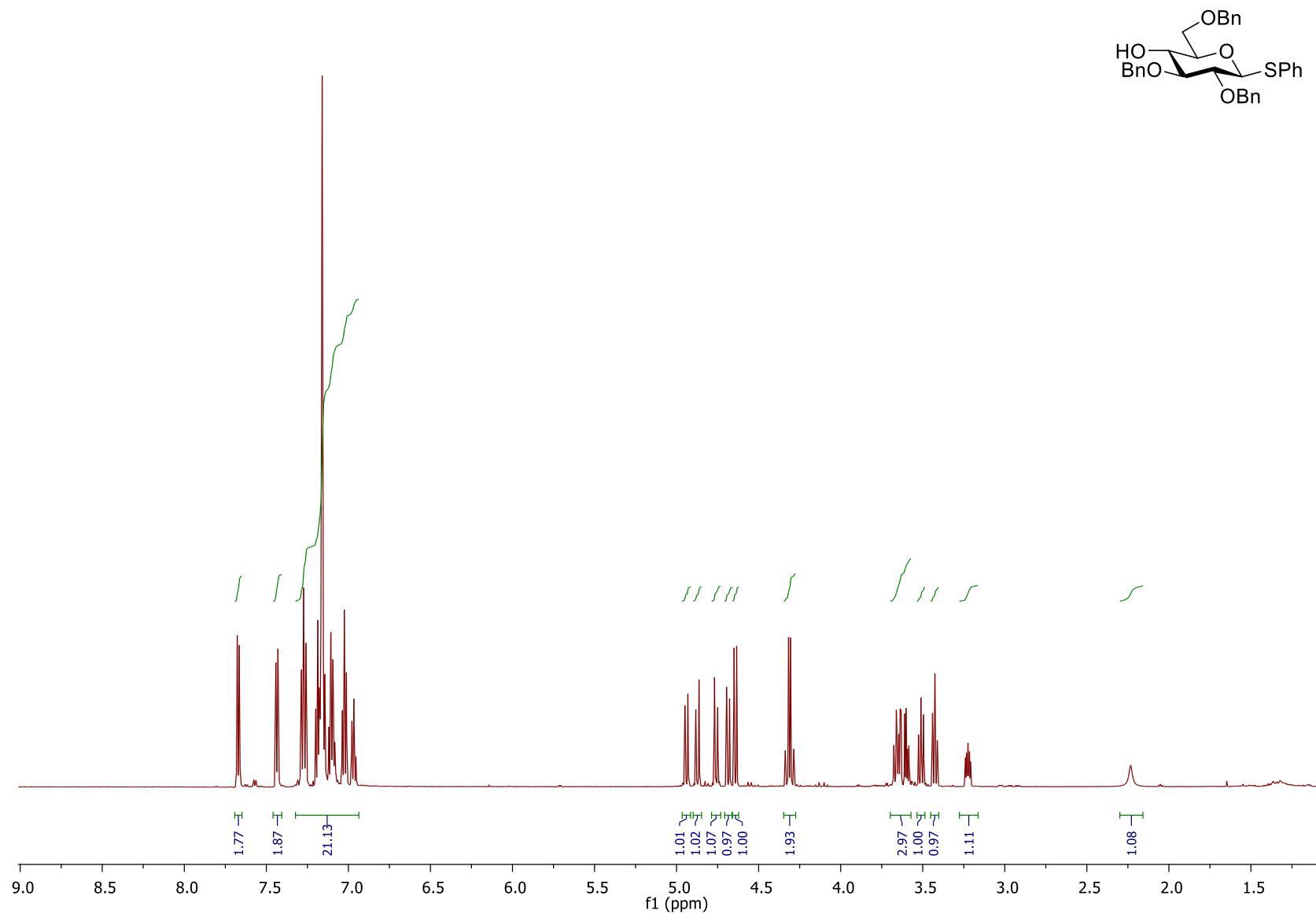
^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl (6*S*)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-1**)



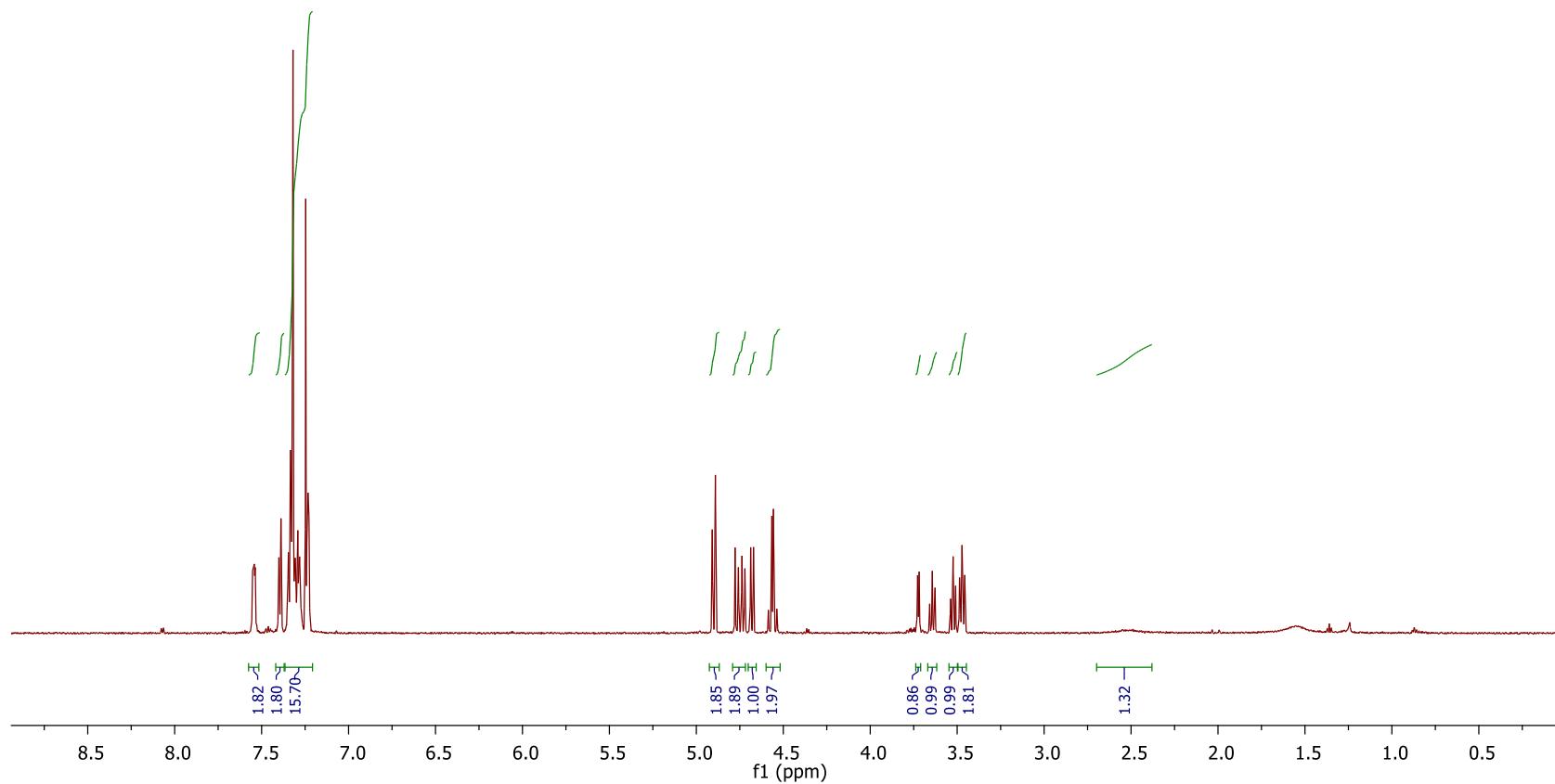
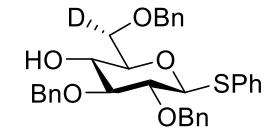
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**2**)



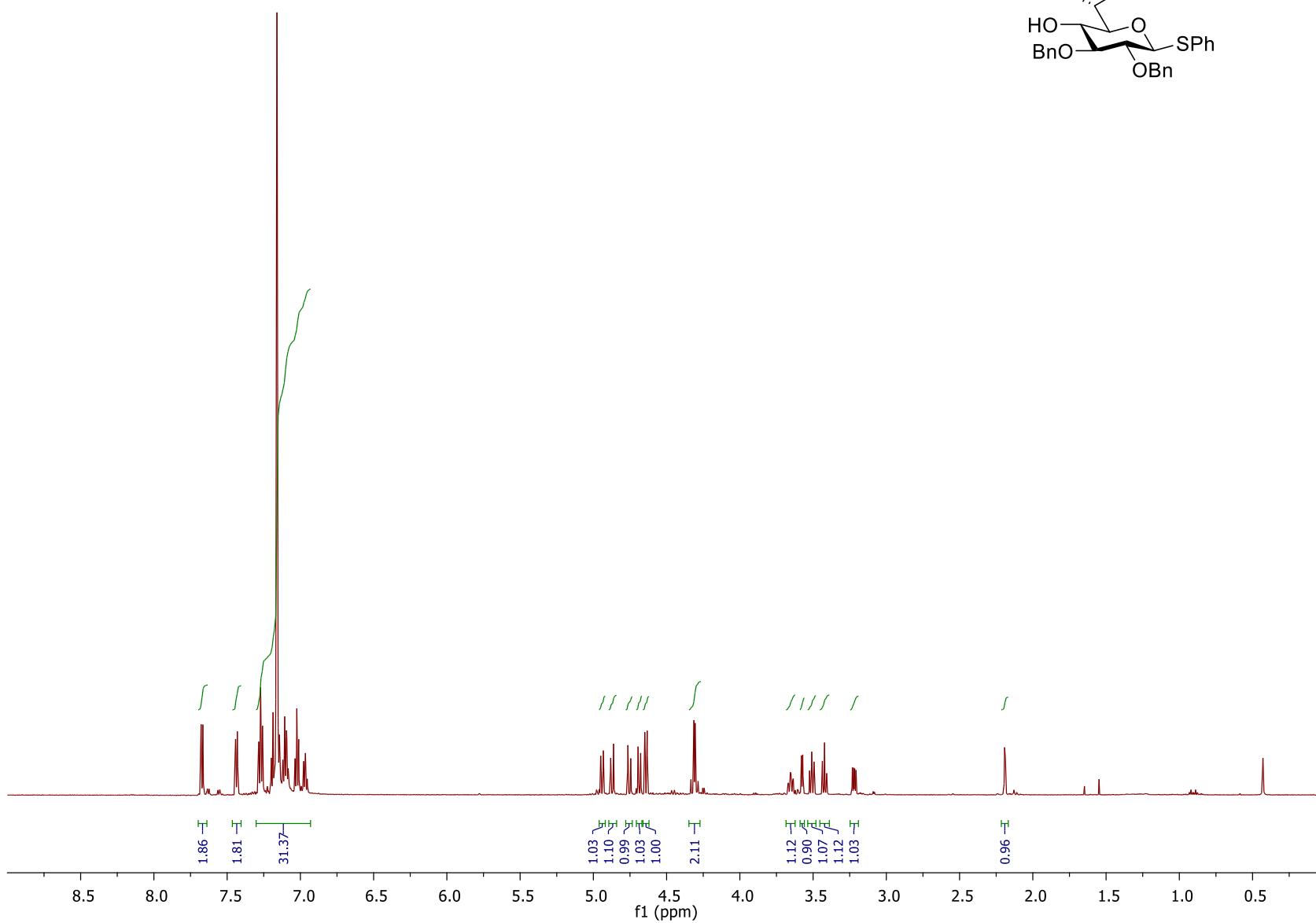
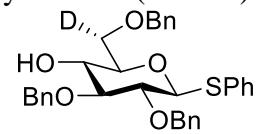
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 2,3,6-tri-O-benzyl-1-thio-β-D-glucopyranoside (**2**)



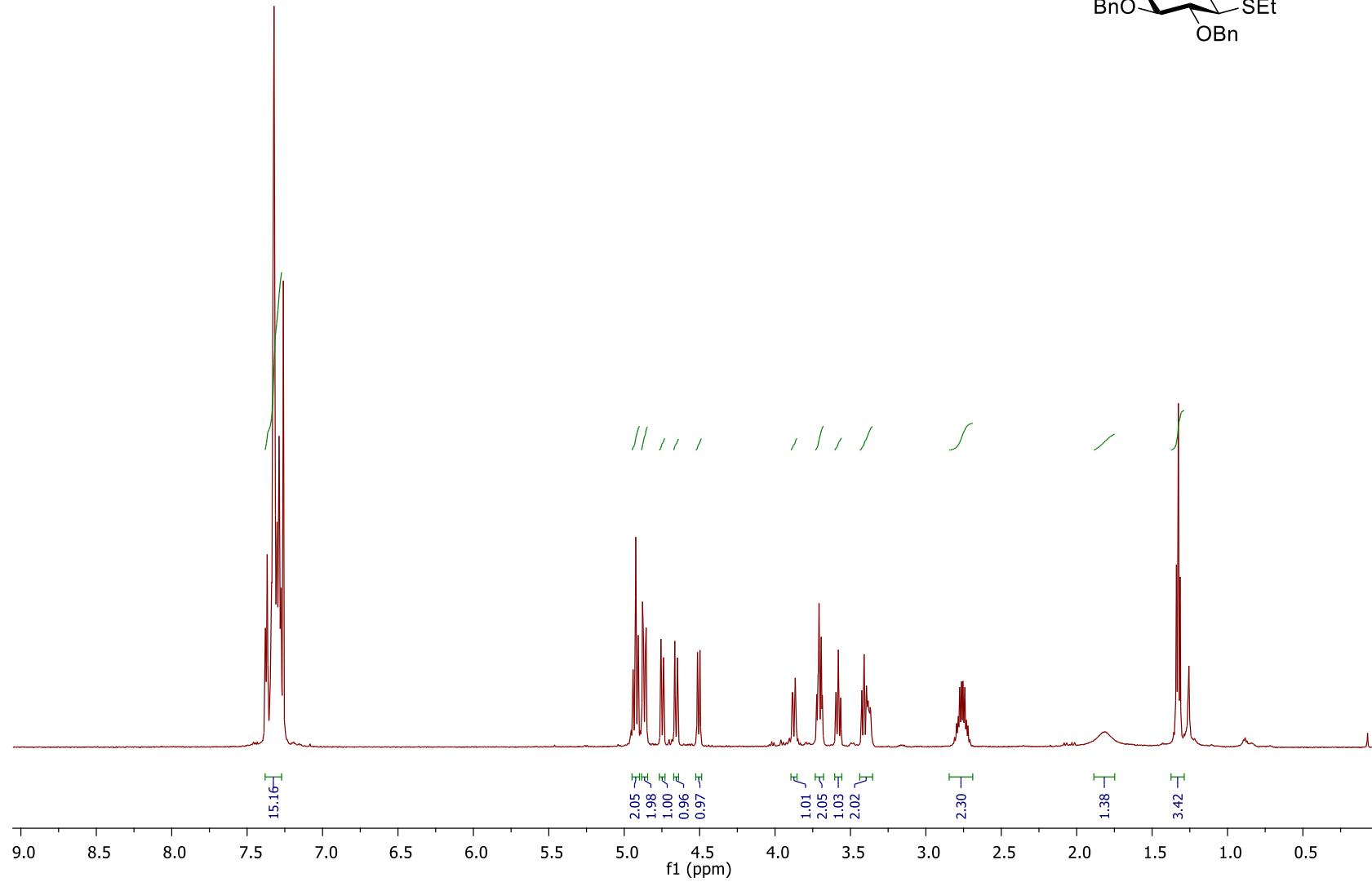
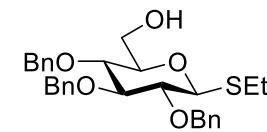
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl (6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside(**6S-D-2**)



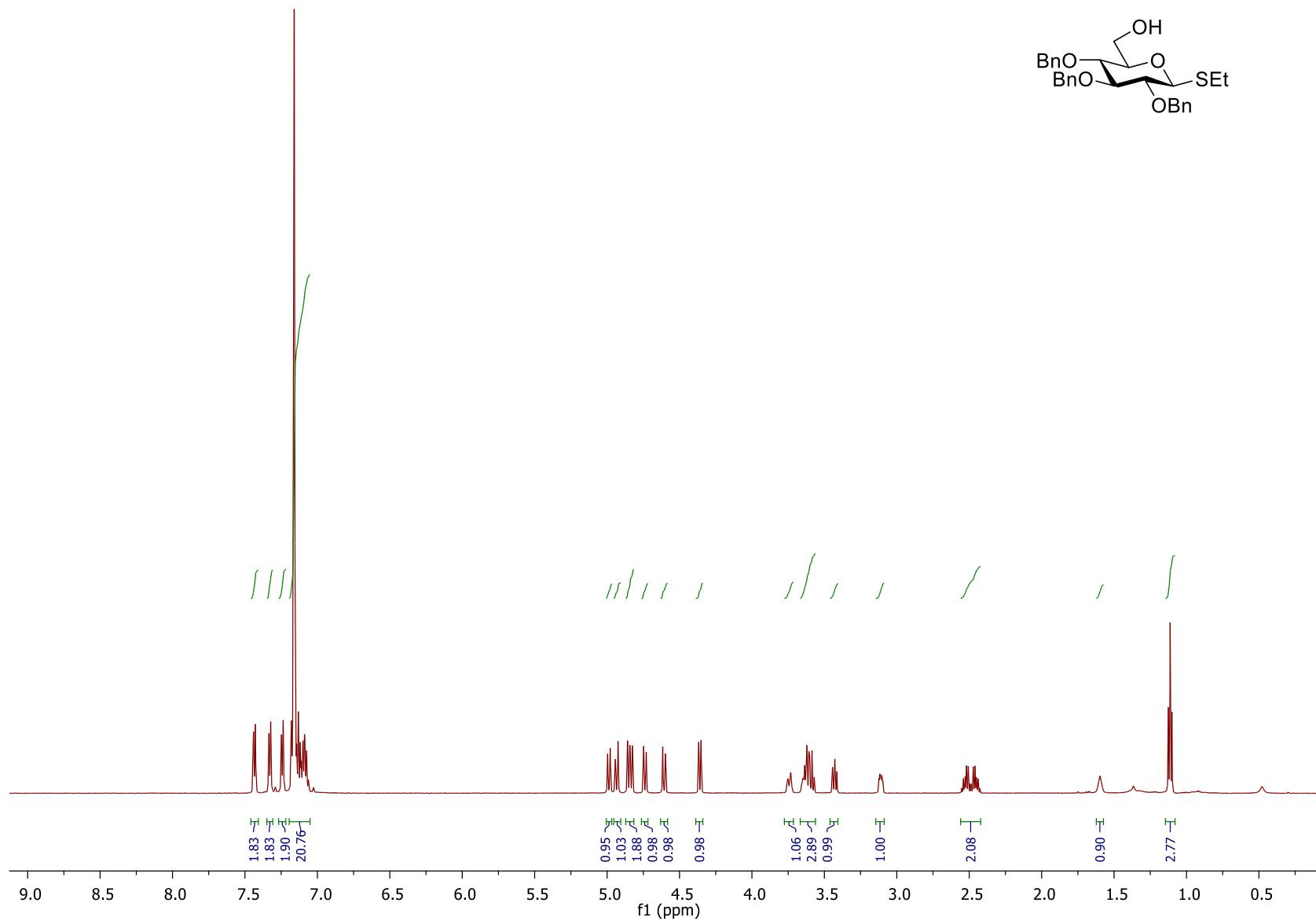
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl (6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**6S-D-2**)



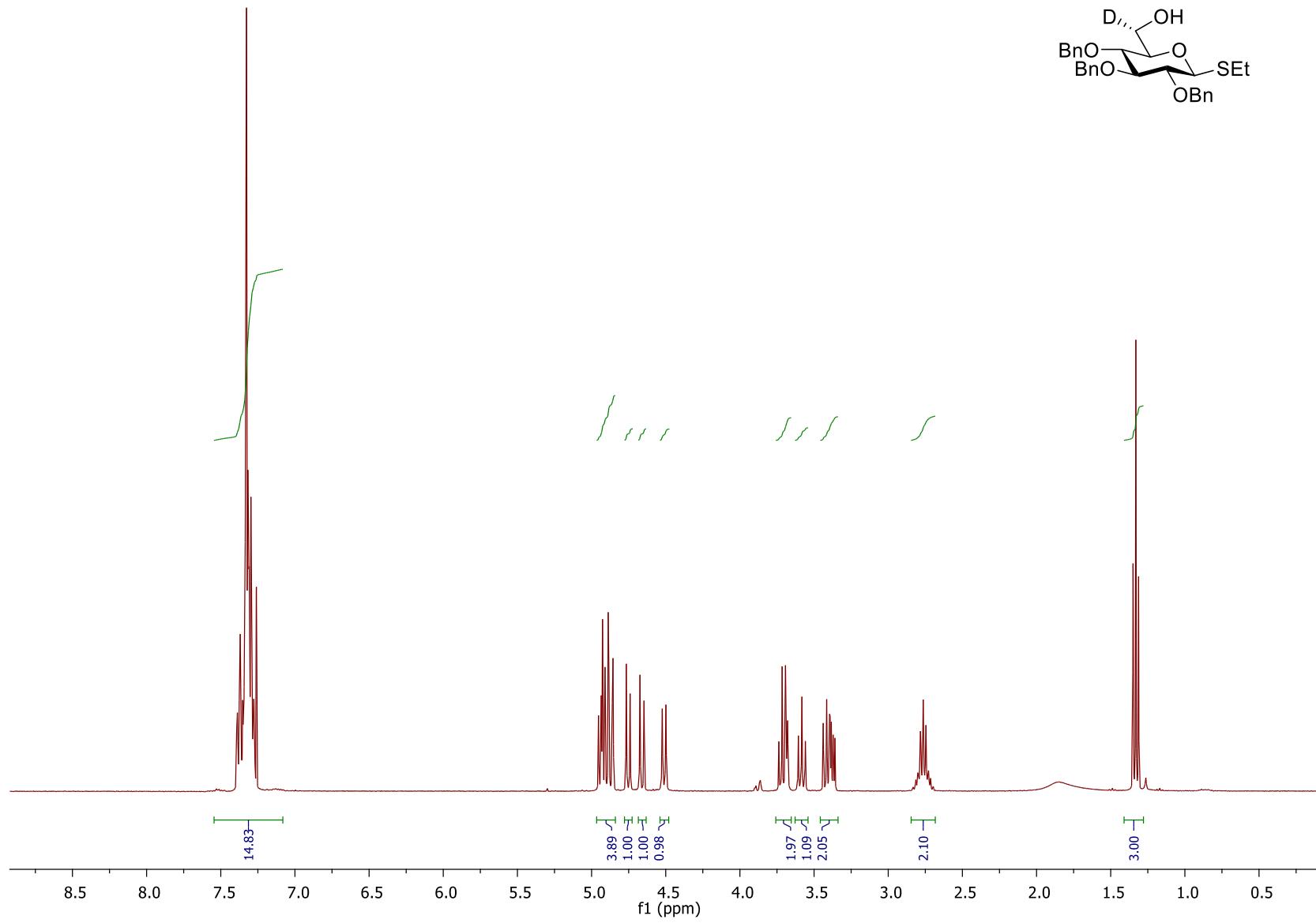
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**3**)



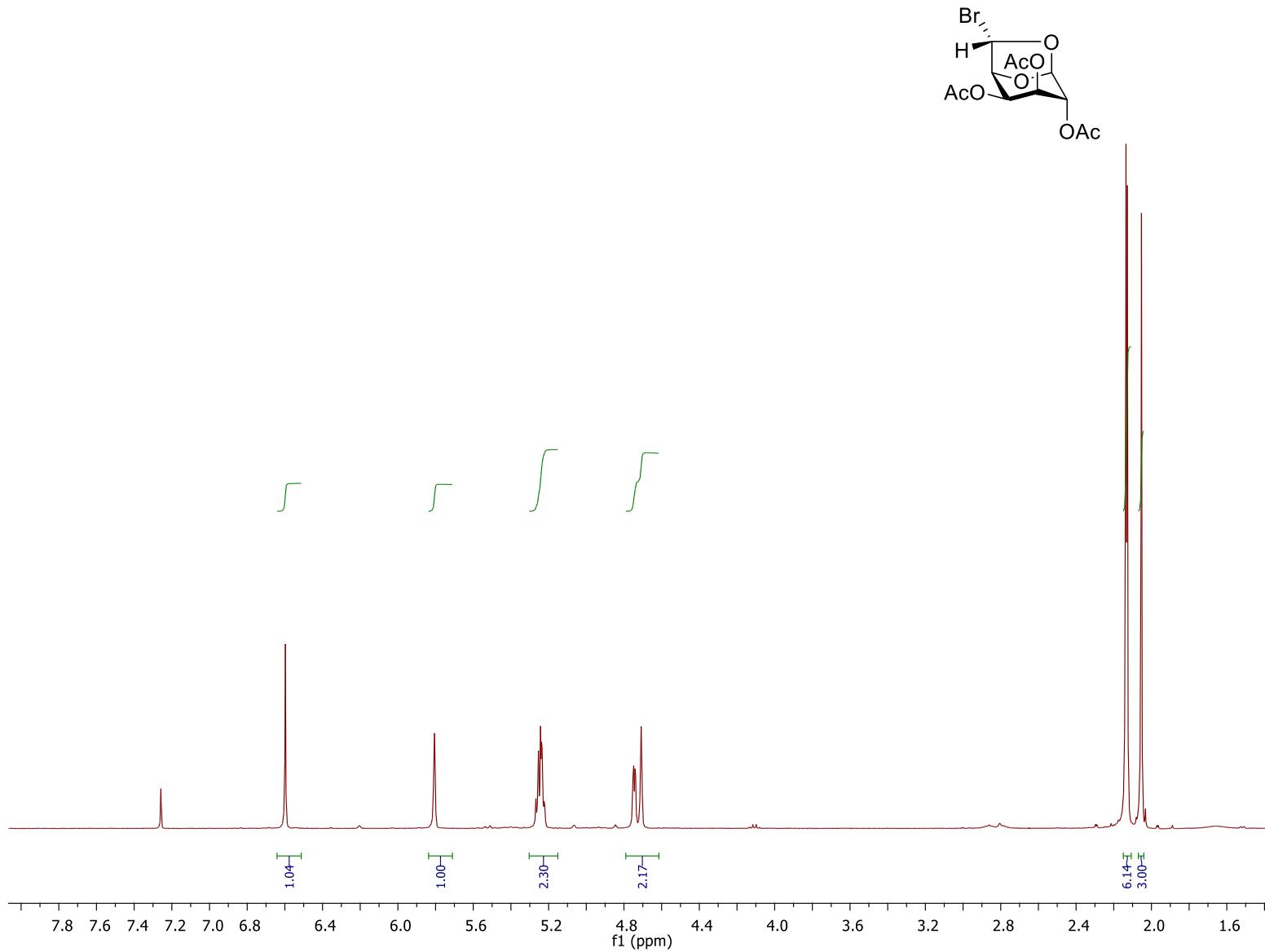
¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl 2,3,4-tri-O-benzyl-1-thio-β-D-glucopyranoside (**3**)



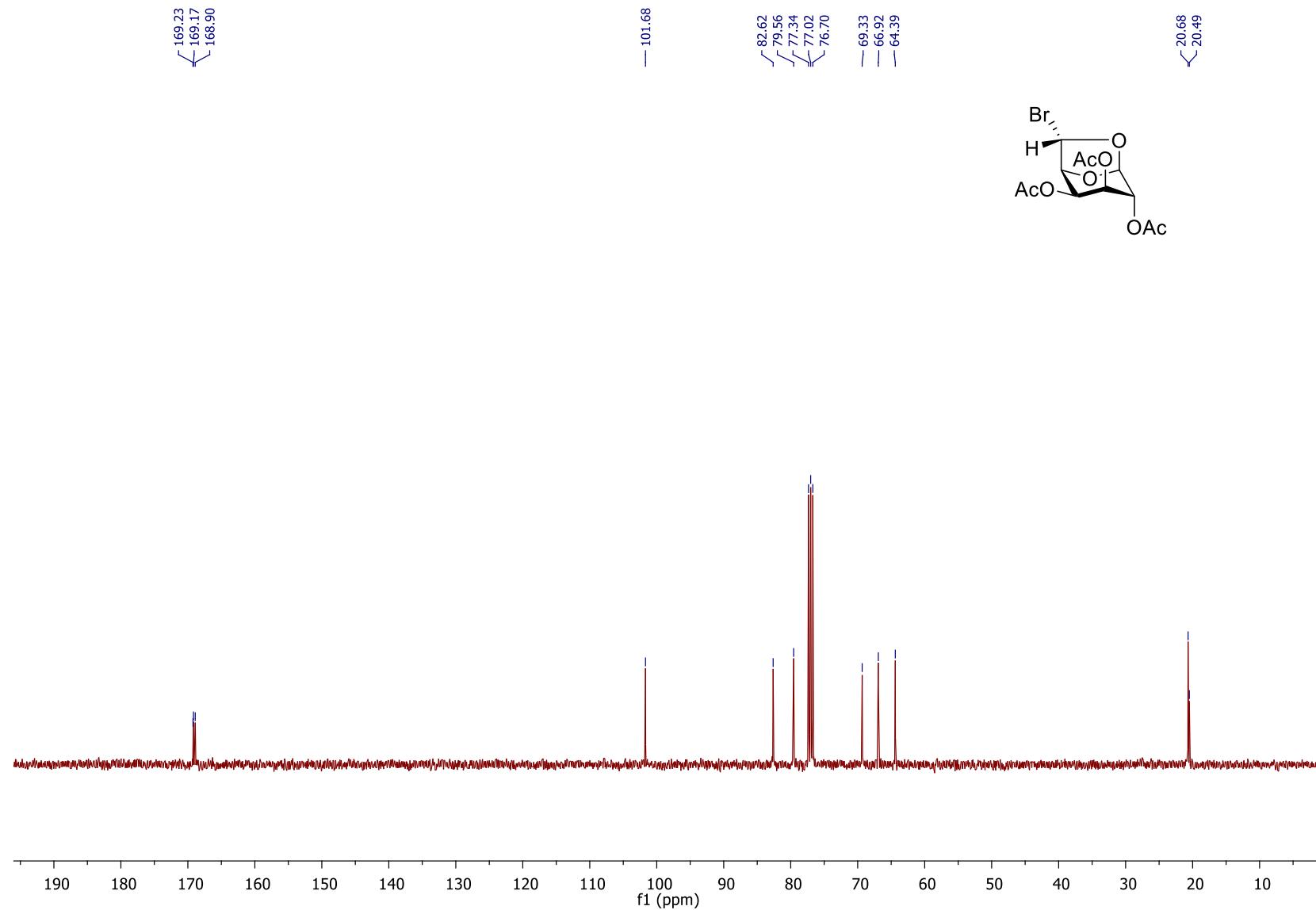
^1H NMR (400 MHz, CDCl_3) Spectrum of Ethyl ($6S$)-[$6-^2\text{H}_1$]-2,3,4,6-tetra- O -acetyl-1-thio- β -D-glucopyranoside (**6S-D-3**)



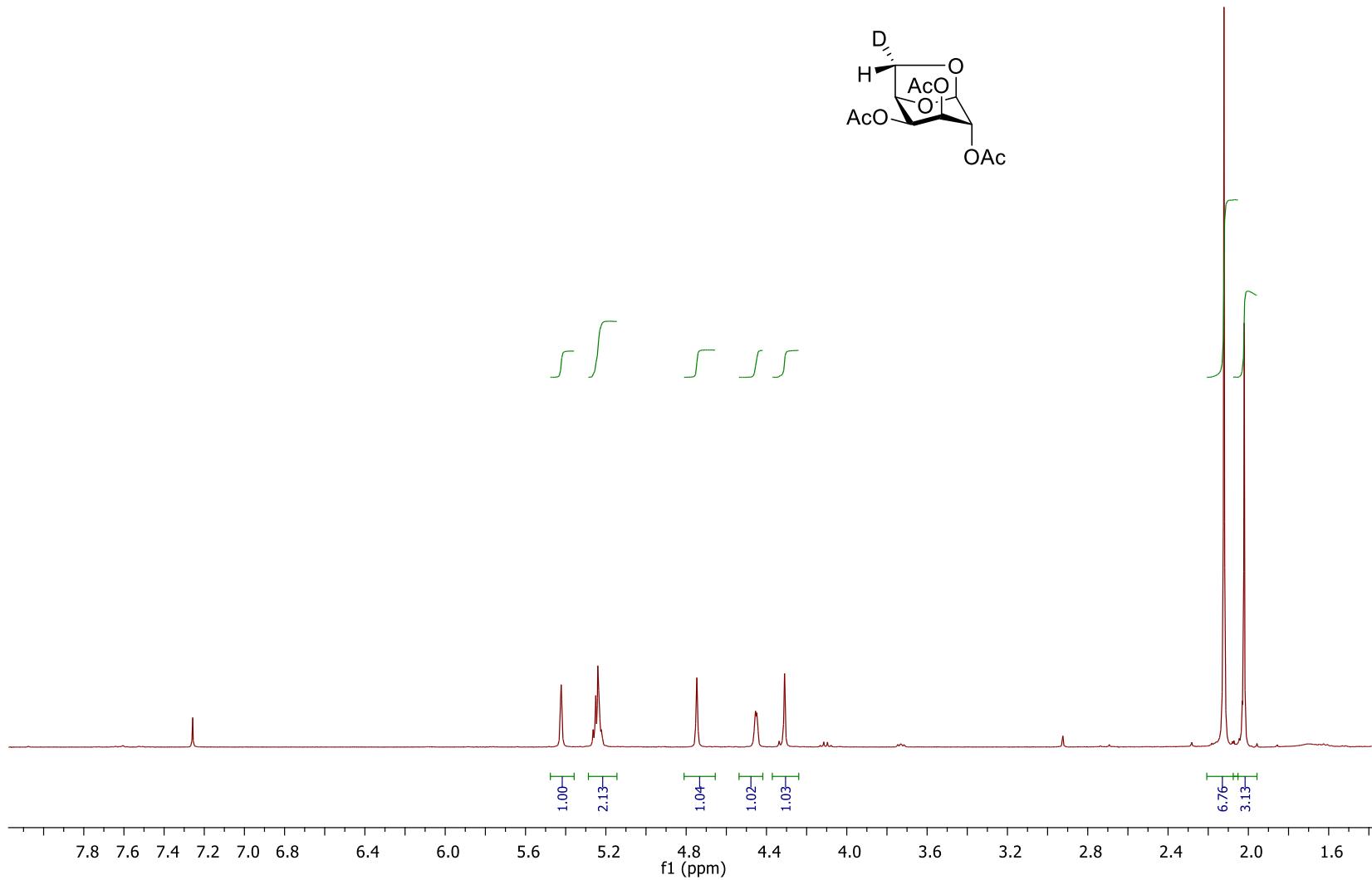
¹H NMR (400 MHz, CDCl₃) Spectrum of (6*S*) -1,6-Anhydro-2,3,4-tri-O-acetyl-6-bromo- β -D-galactopyranose (**5**)



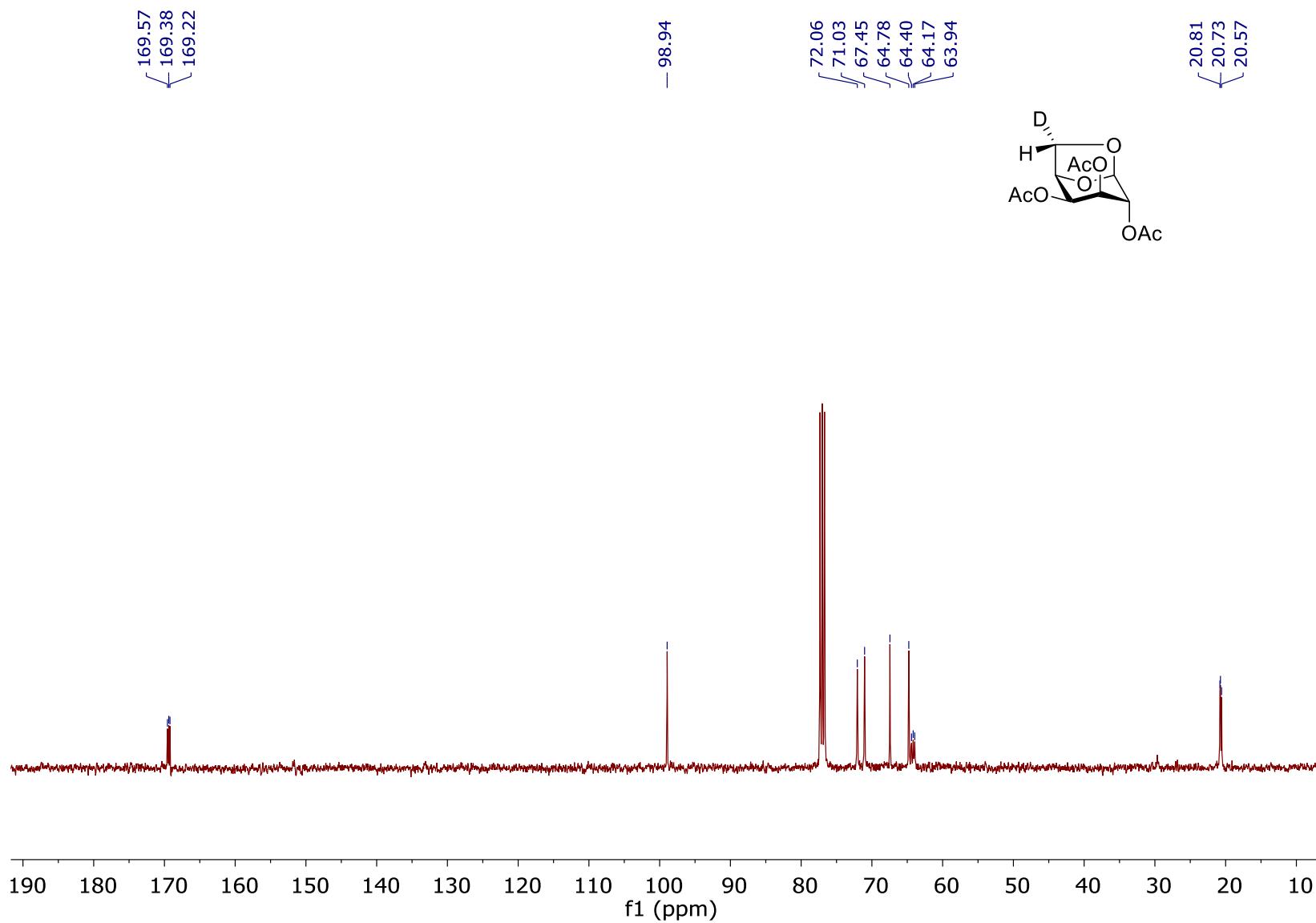
¹H NMR (100 MHz, CDCl₃) Spectrum of (6S)-1,6-Anhydro-2,3,4-tri-O-acetyl-6-bromo- β -D-galactopyranose (**5**)



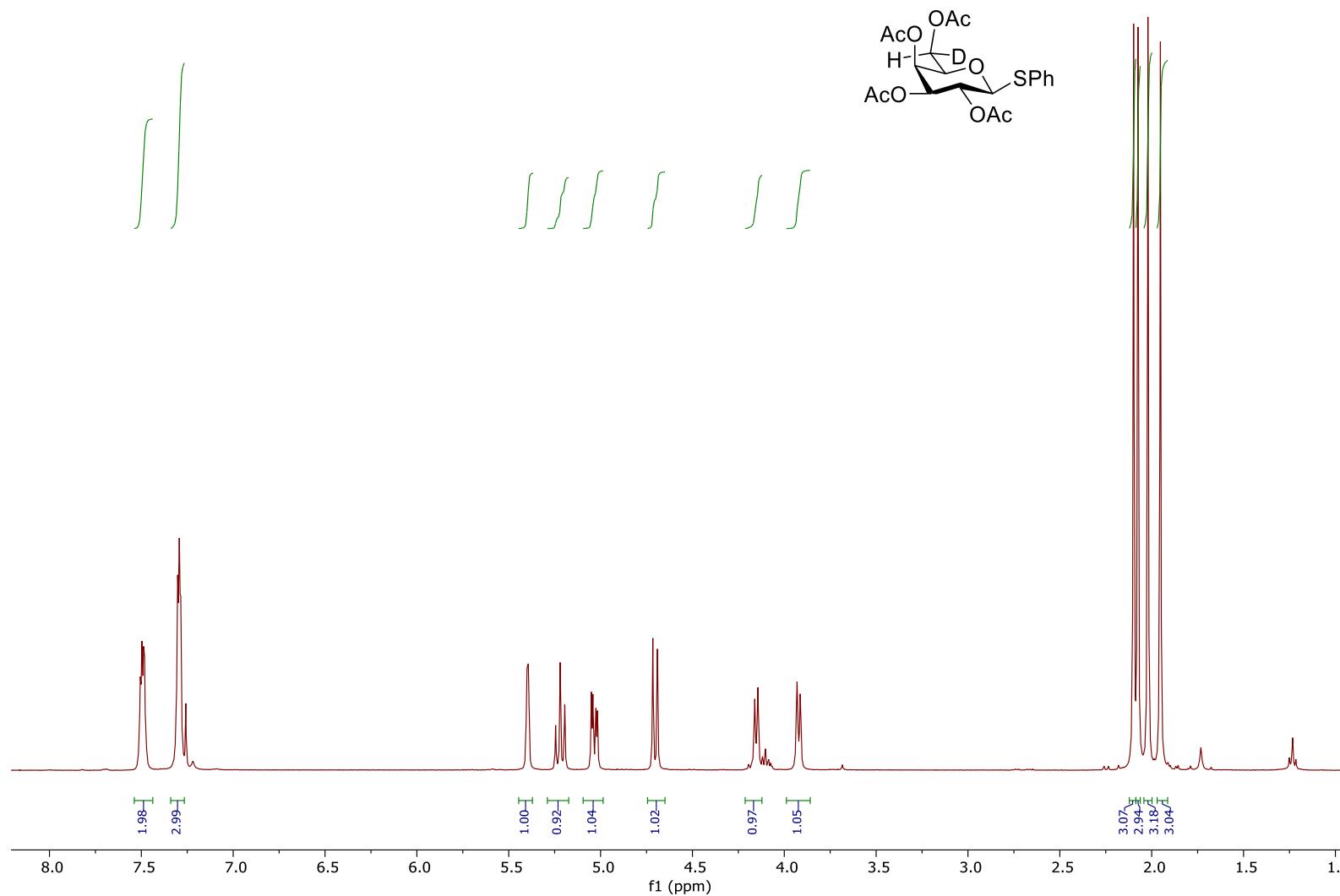
^1H NMR (400 MHz, CDCl_3) Spectrum of ($6S$)-[$6-^2\text{H}_1$]-1,6-Anhydro-2,3,4-tri-O-acetyl- β -D-galactopyranose (**6**)



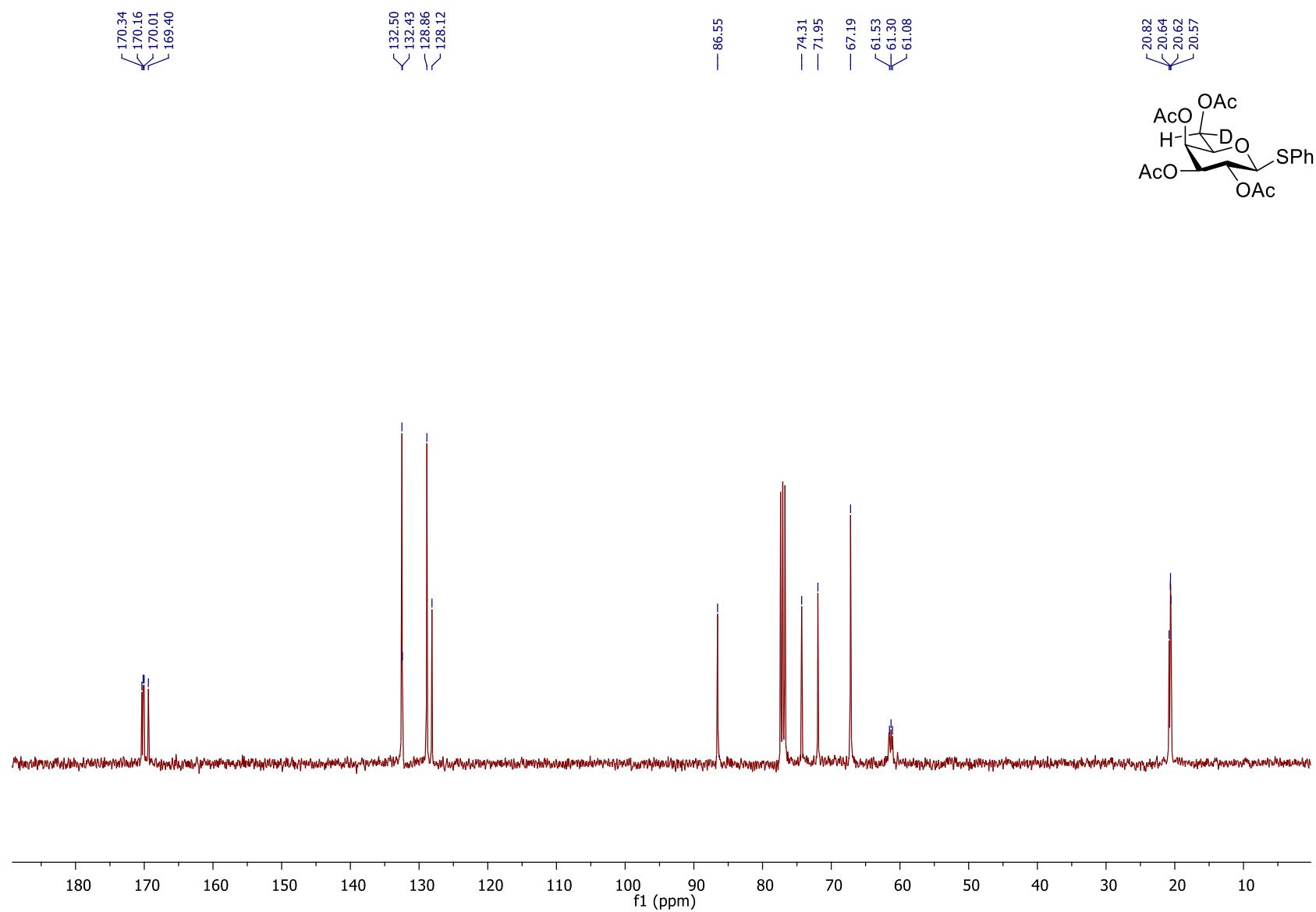
^{13}C NMR (100 MHz, CDCl_3) Spectrum of ($6S$)-[$6-^2\text{H}_1$]-1,6-Anhydro-2,3,4-tri-O-acetyl- β -D-galactopyranose (**6**)



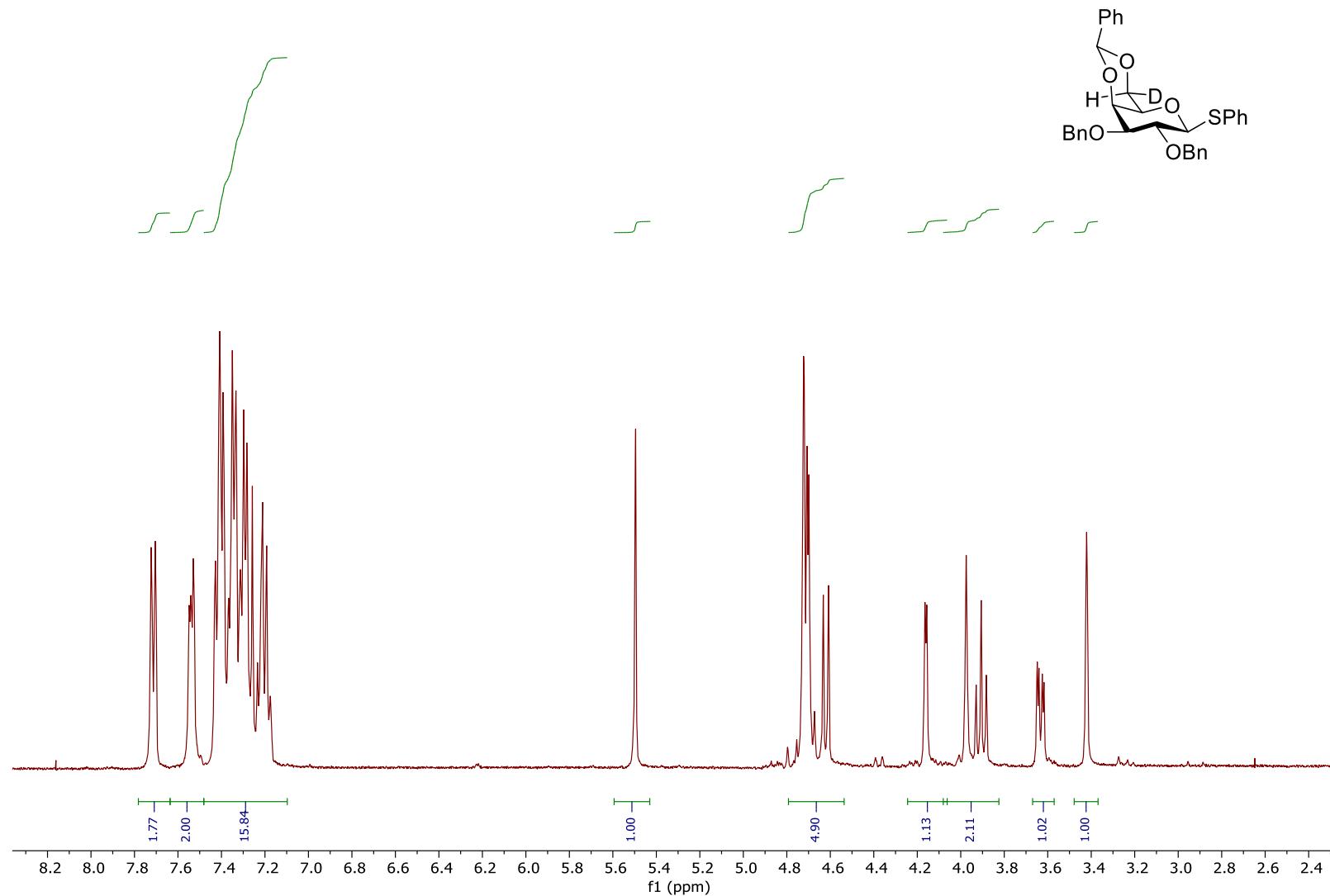
^1H NMR (400 MHz, CDCl_3) Spectrum of Phenyl (6S)-[6- $^2\text{H}_1$]-2,3,4,6-tetra- O -acetyl-1-thio- β -D-galactopyranoside (**8**)



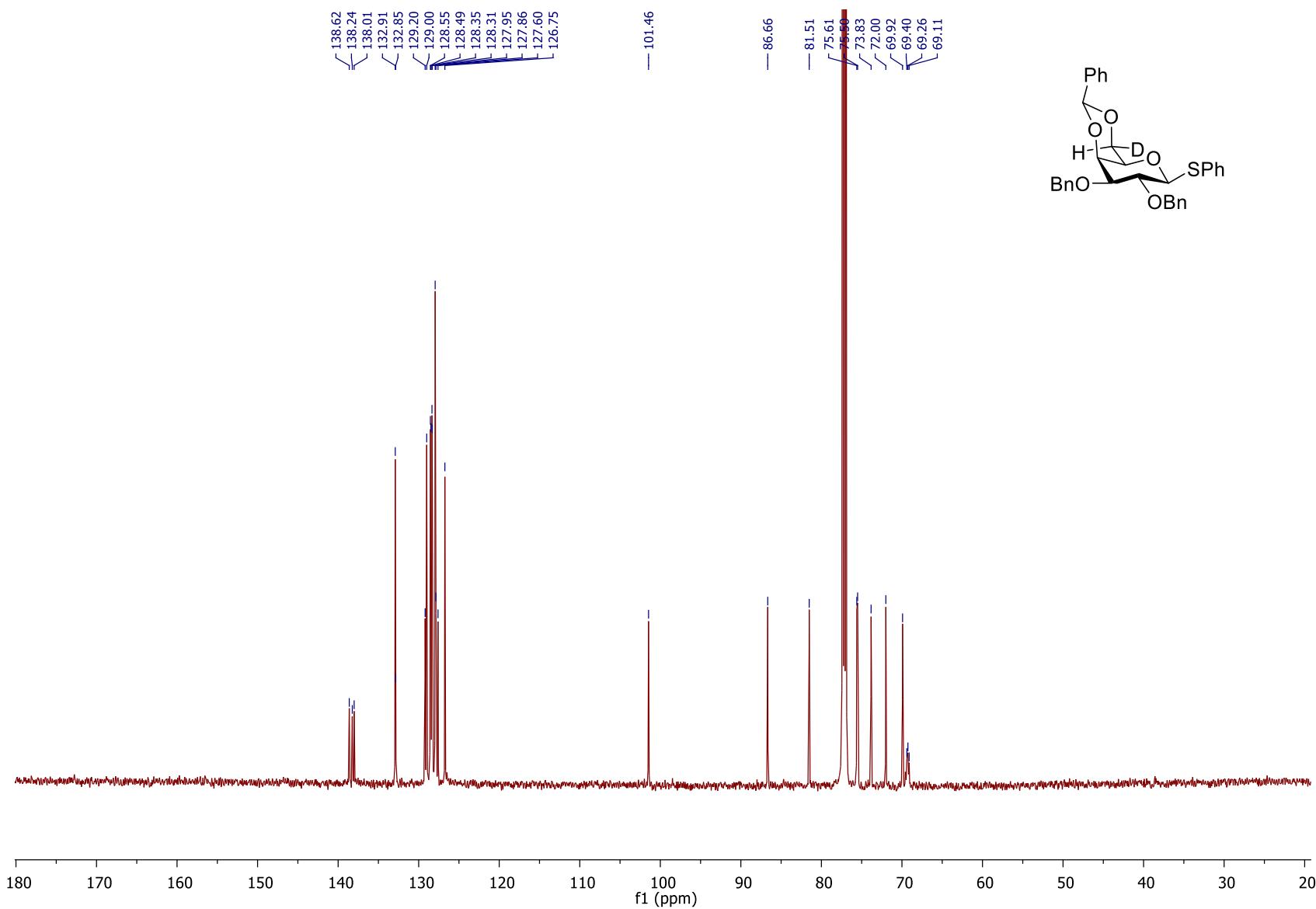
^{13}C NMR (100 MHz, CDCl_3) Spectrum of Phenyl ($6S$)-[$6-^2\text{H}_1$]-2,3,4,6-tetra- O -acetyl-1-thio- β -D-galactopyranoside (**8**)



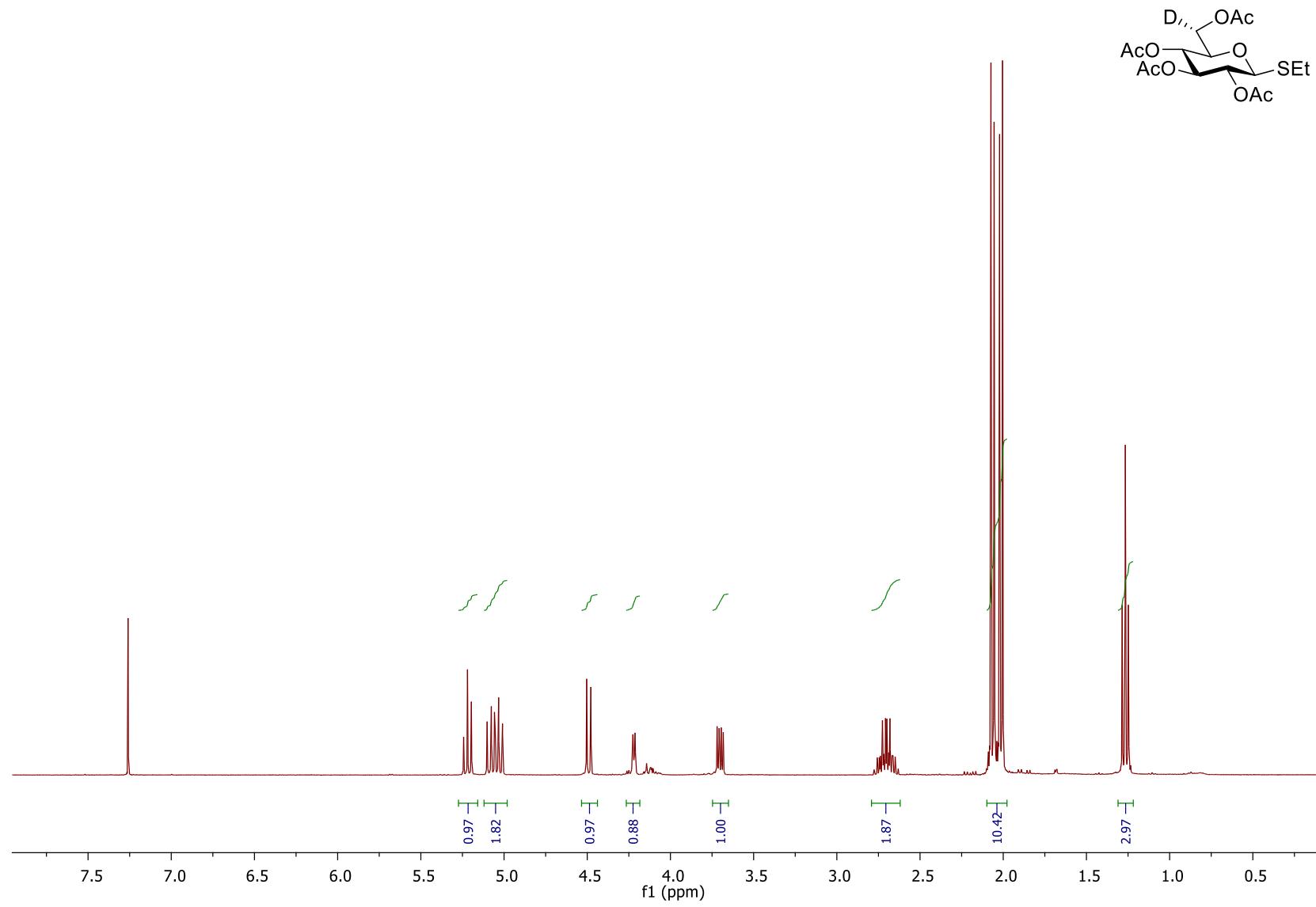
^1H NMR (400 MHz, CDCl_3) Spectrum of Phenyl 2,3-di-*O*-benzyl-4,6-*O*-benzylidene-(6*S*)-[6- $^2\text{H}_1$]-1-thio- β -D-galactopyranoside (**10**)



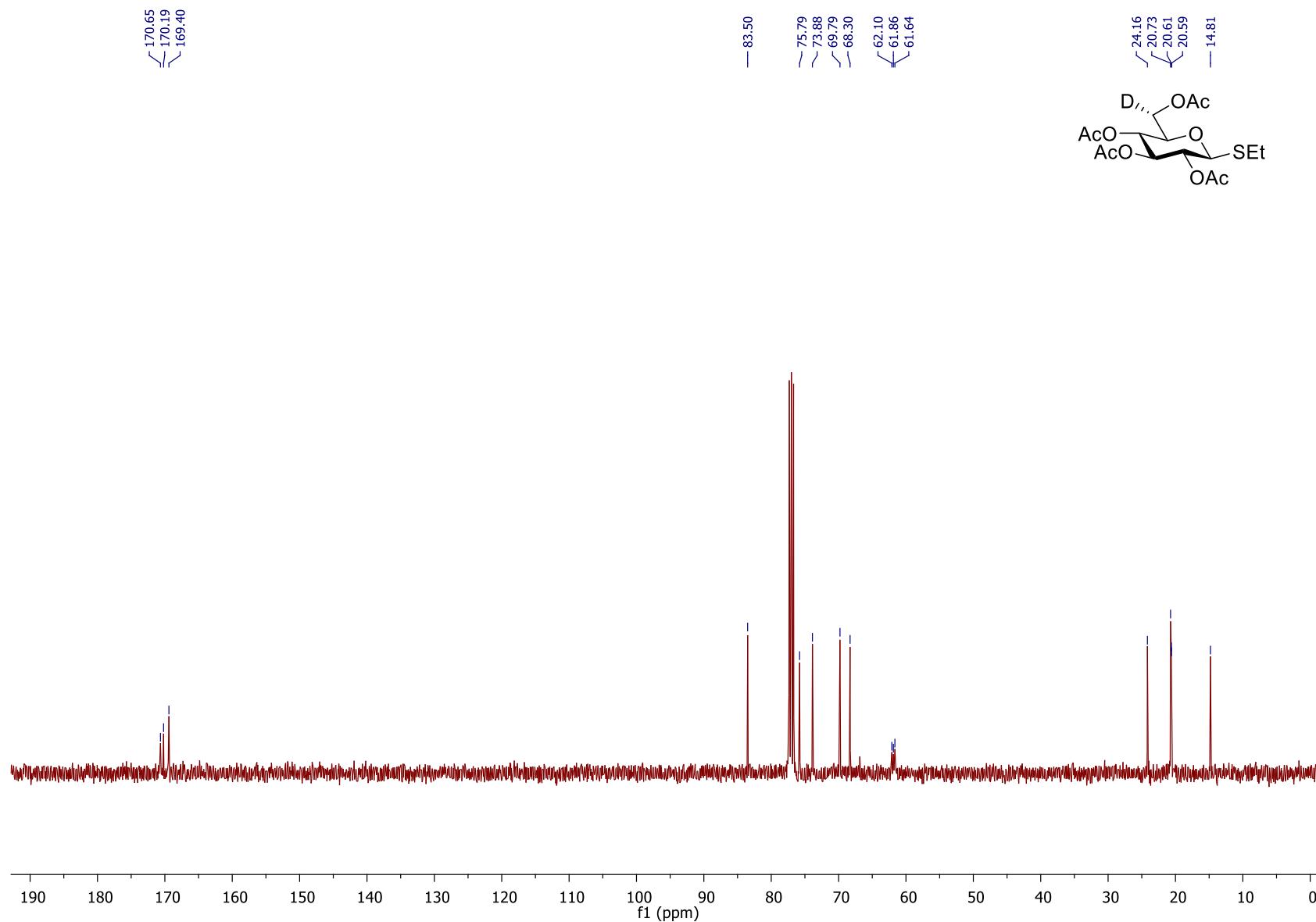
^{13}C NMR (150 MHz, CDCl_3) Spectrum of Phenyl 2,3-di- O -benzyl-4,6- O -benzylidene-(6*S*)-[6- $^2\text{H}_1$]-1-thio- β -D-galactopyranoside (**10**)



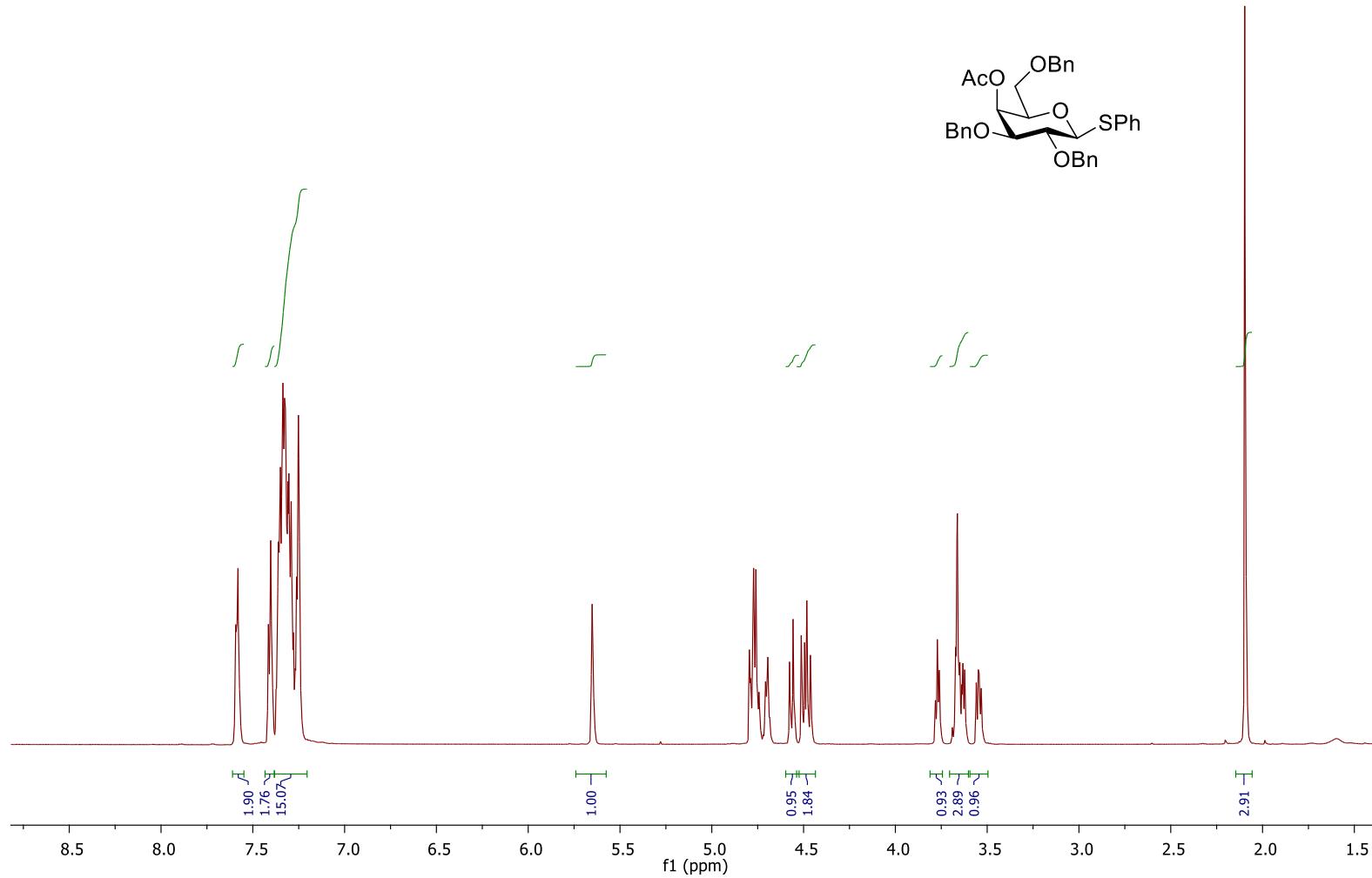
^1H NMR (400 MHz, CDCl_3) Spectrum of Ethyl -(6*S*)-[6- $^2\text{H}_1$]-2,3,4,6-tetra-*O*-acetyl-1-thio- β -D-glucopyranoside (**12**)



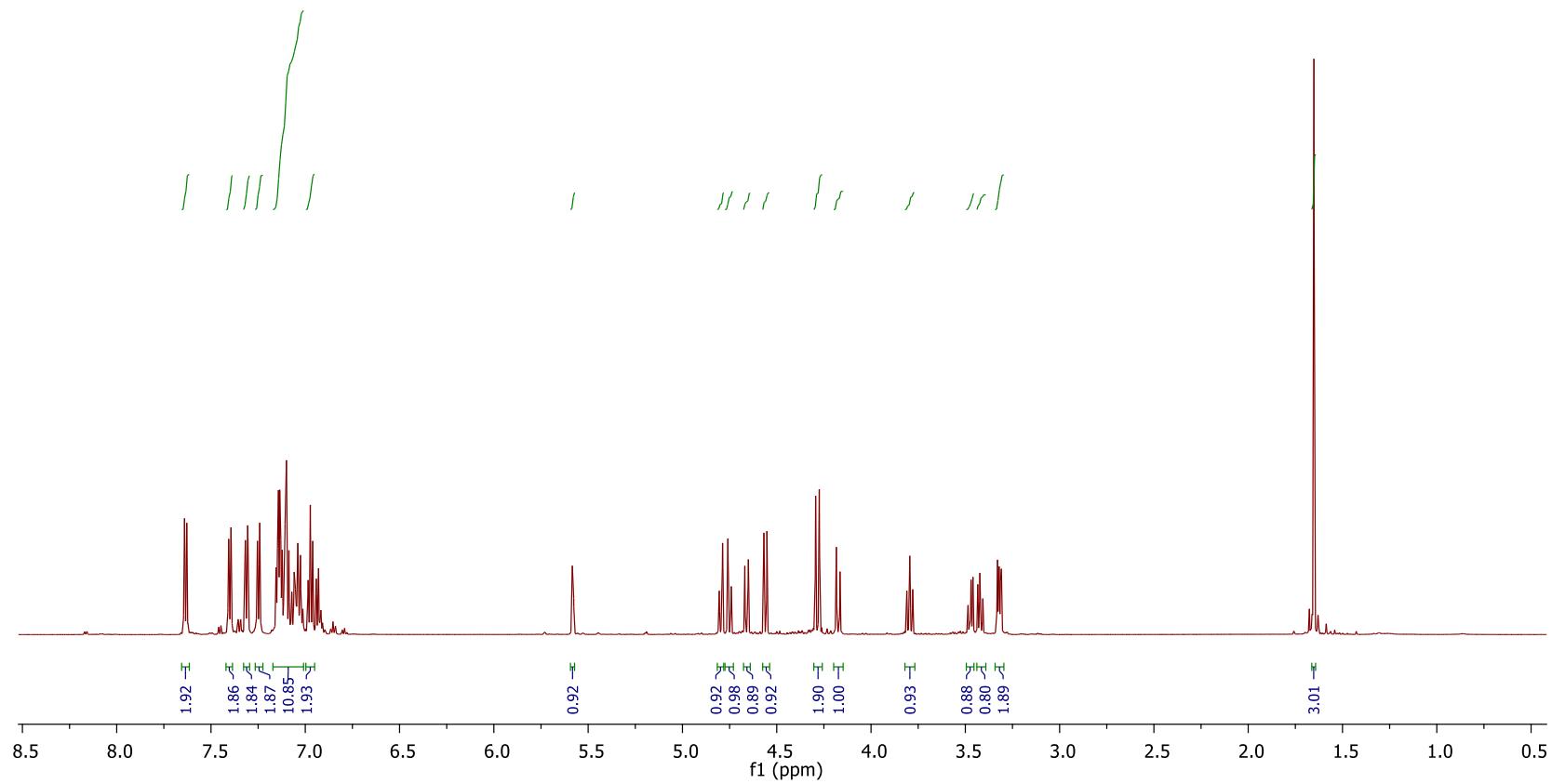
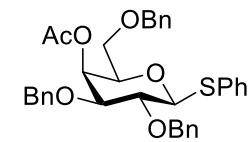
¹³C NMR (100 MHz, CDCl₃) Spectrum of Ethyl -(6*S*)-(6-²H₁)-2,3,4,6-tetra-*O*-acetyl-1-thio- β -D-glucopyranoside (**12**)



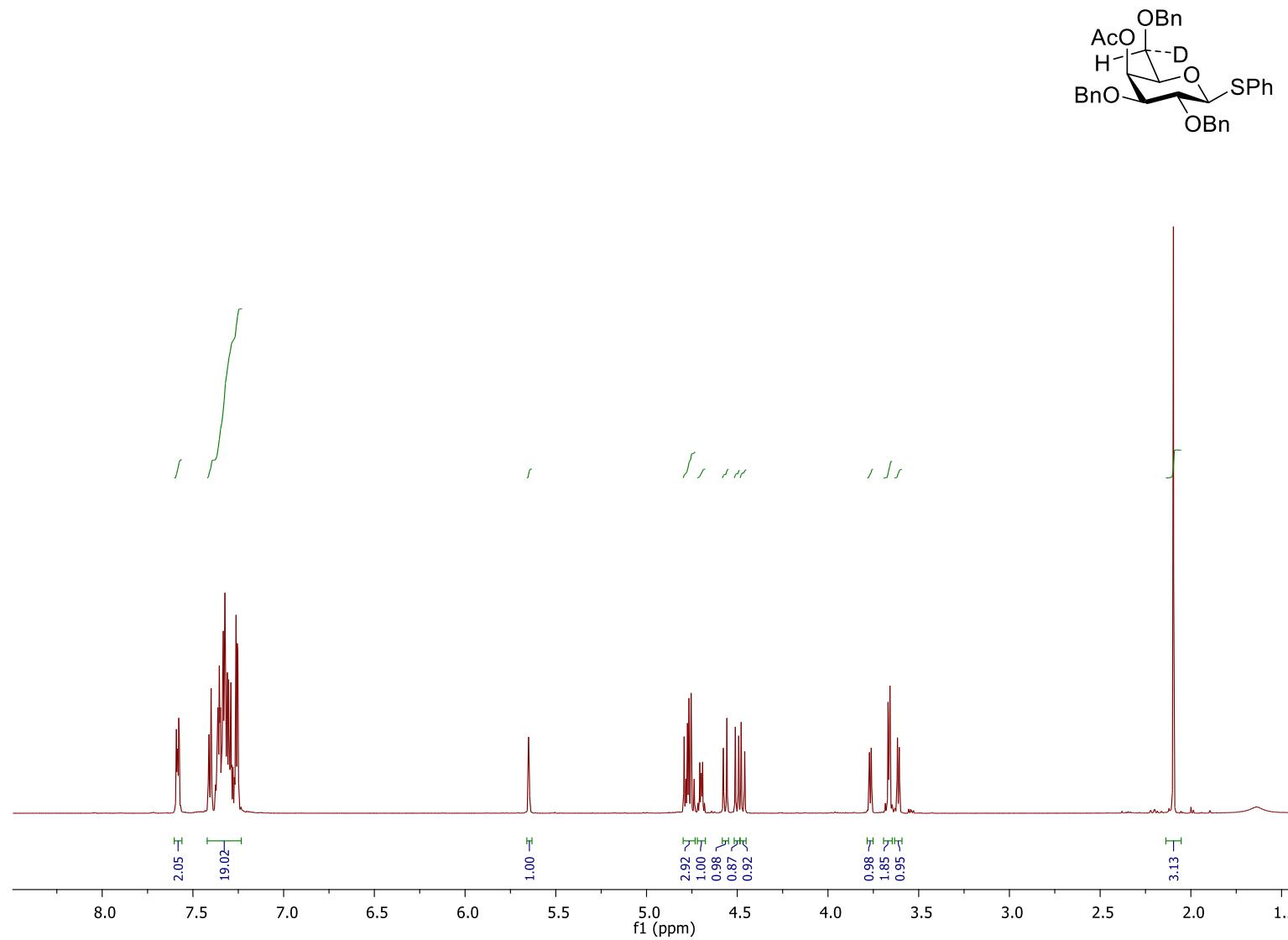
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 4-*O*-acetyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**13**)



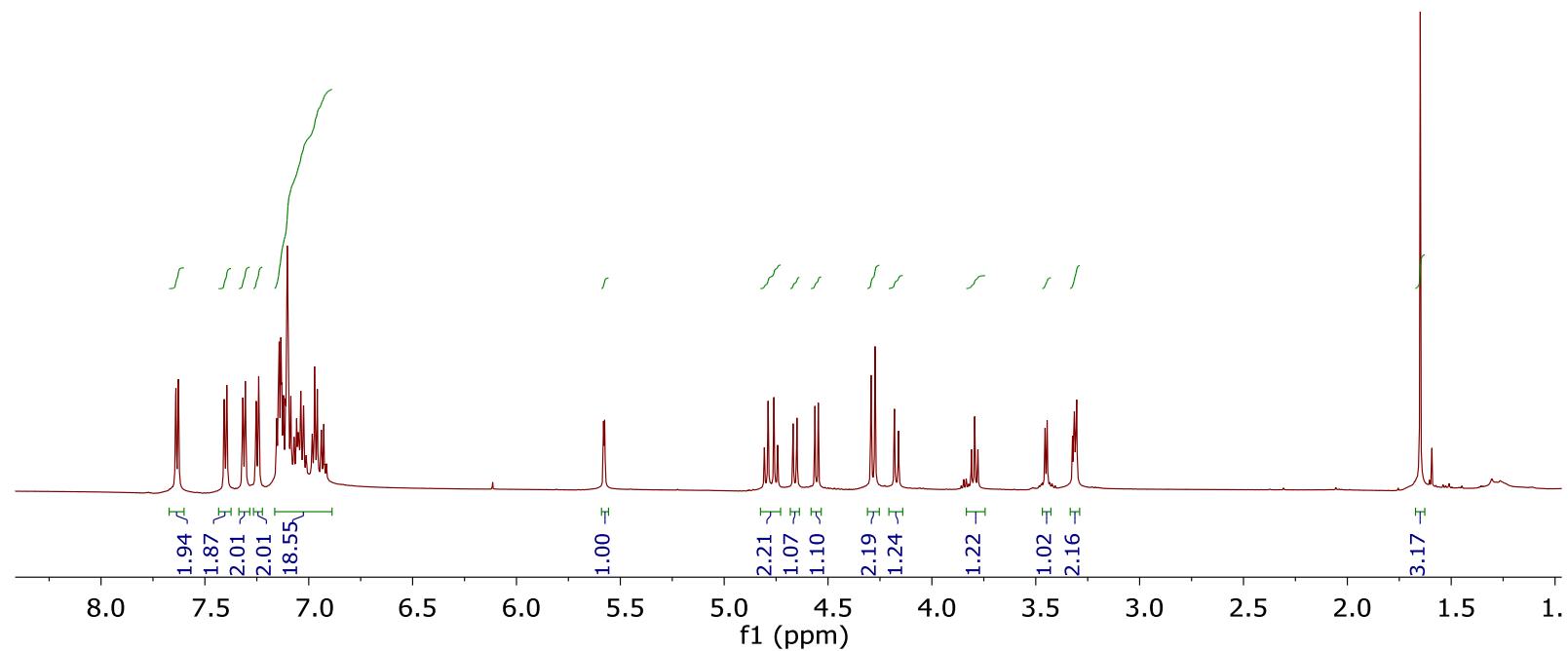
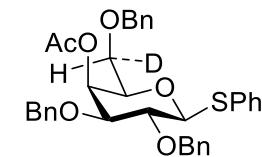
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-acetyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**13**)



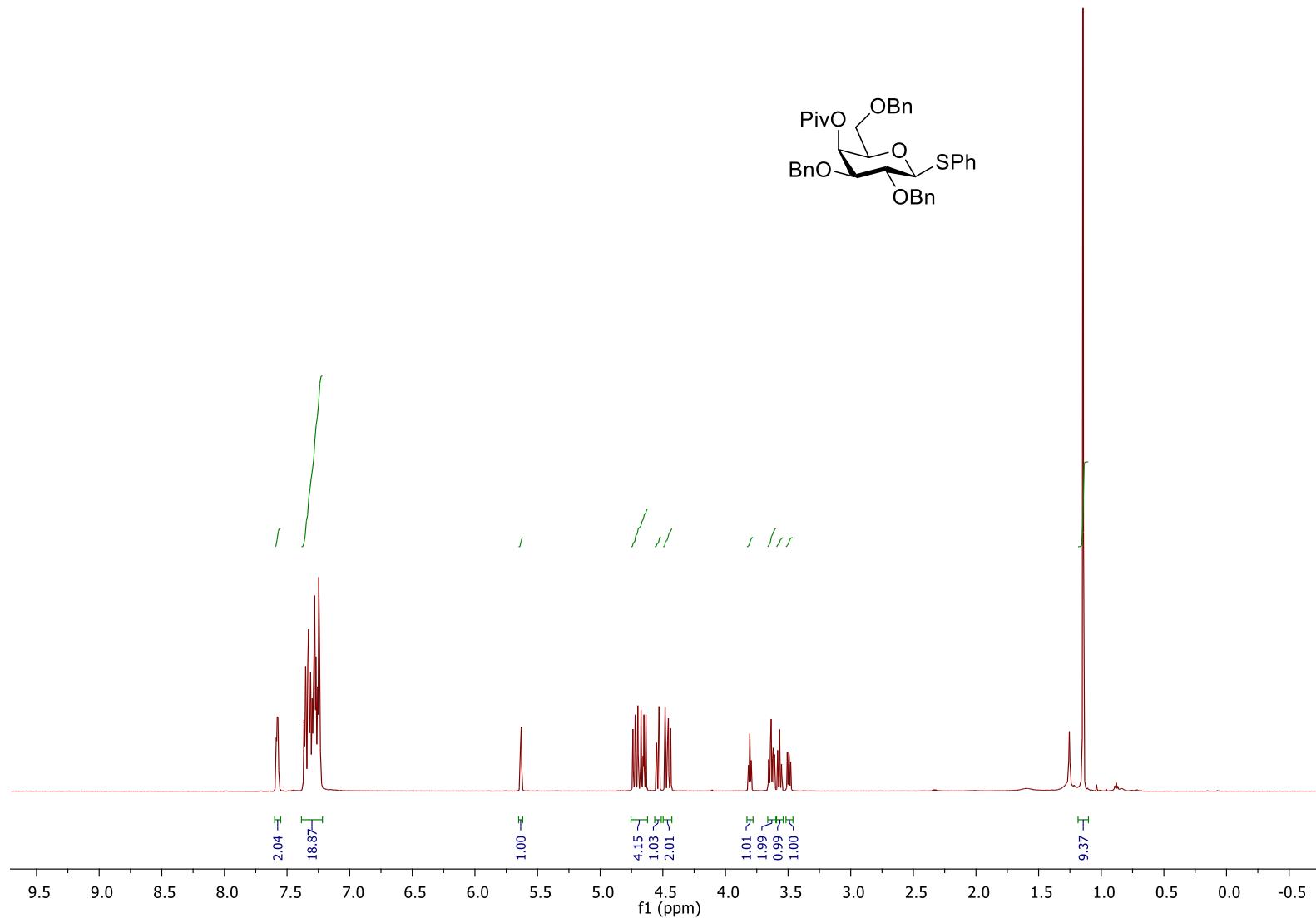
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 4-*O*-acetyl-(6*S*)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-13**)



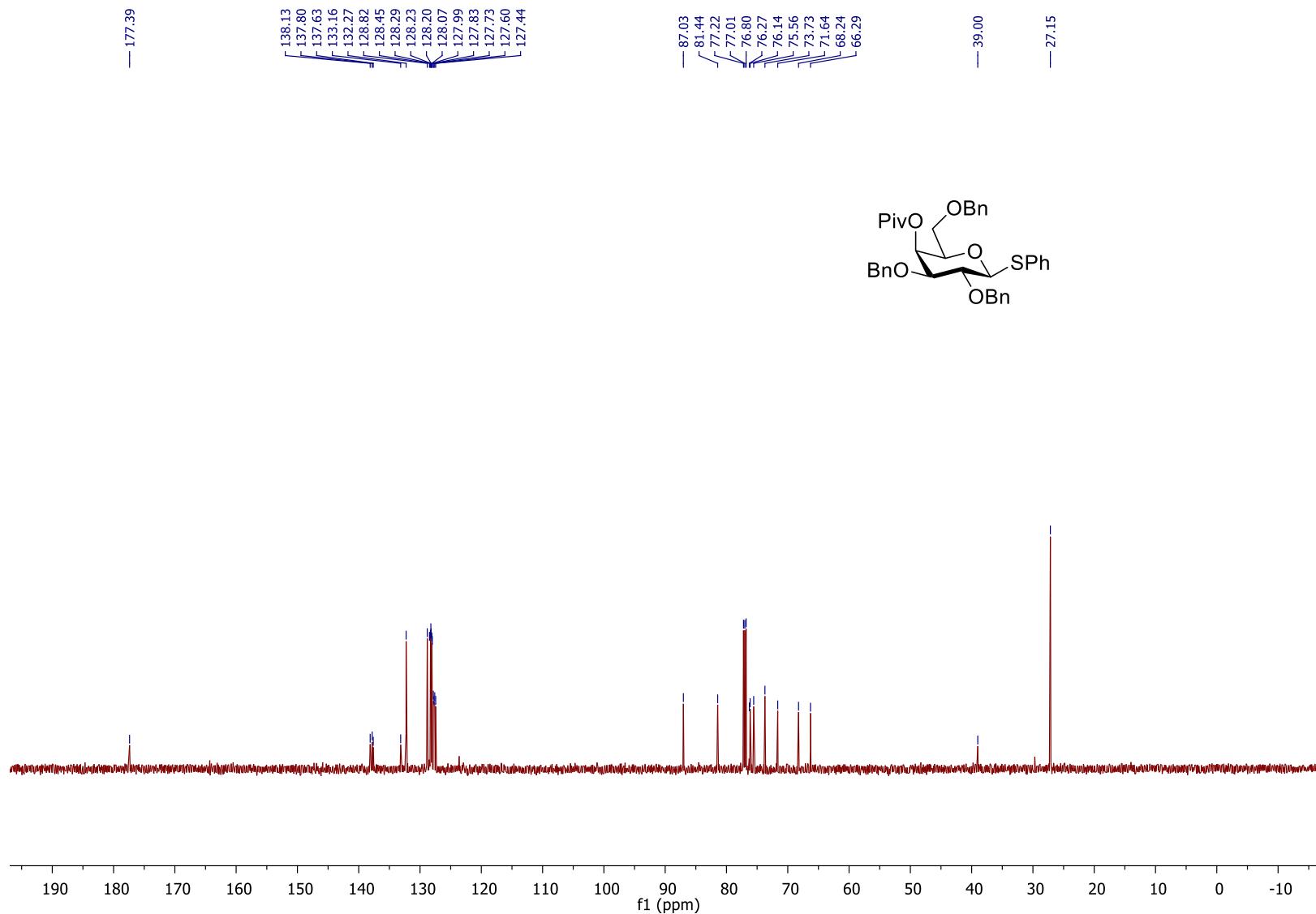
^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl 4-*O*-acetyl-(6*S*)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-13**)



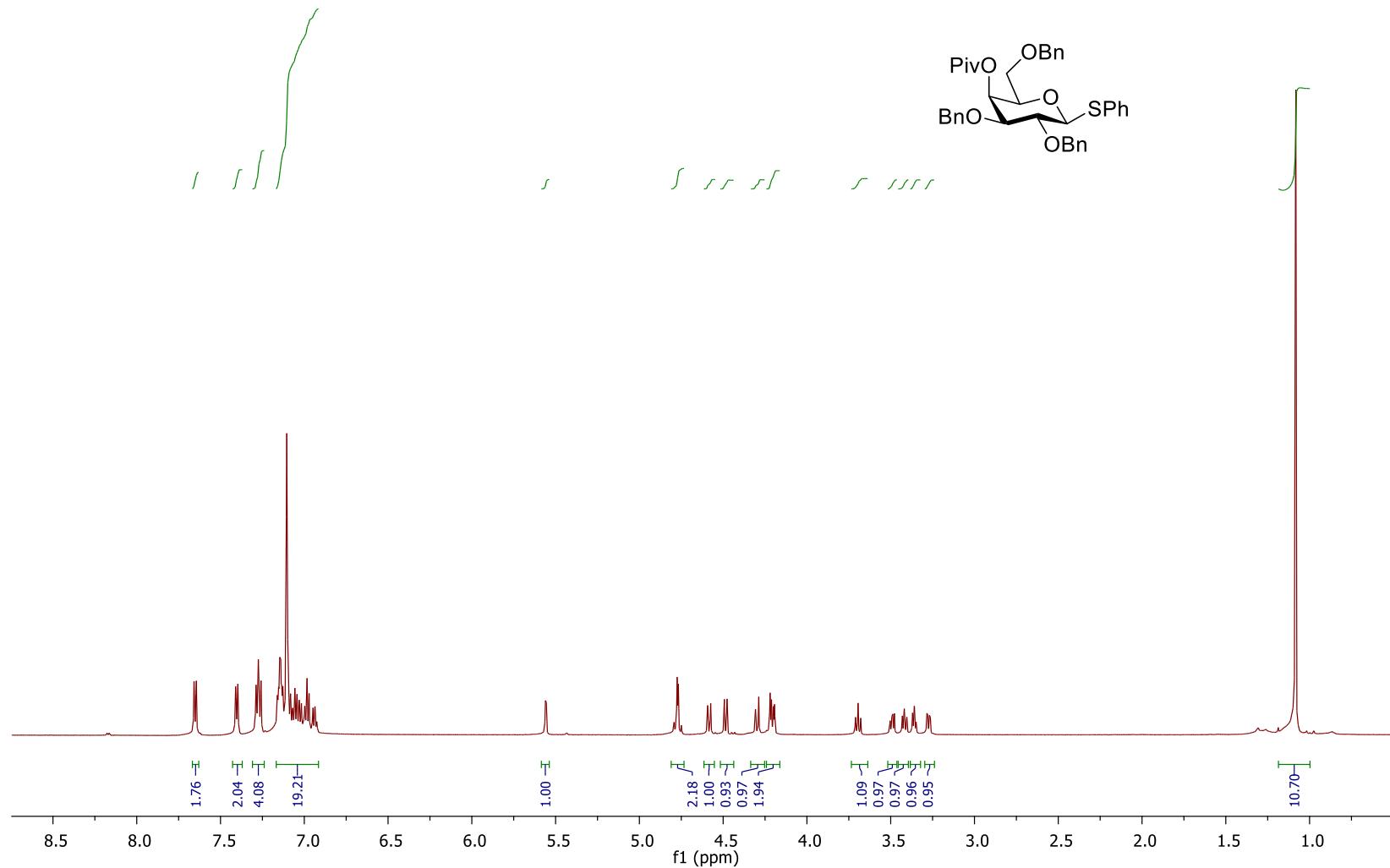
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-pivoyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**14**)



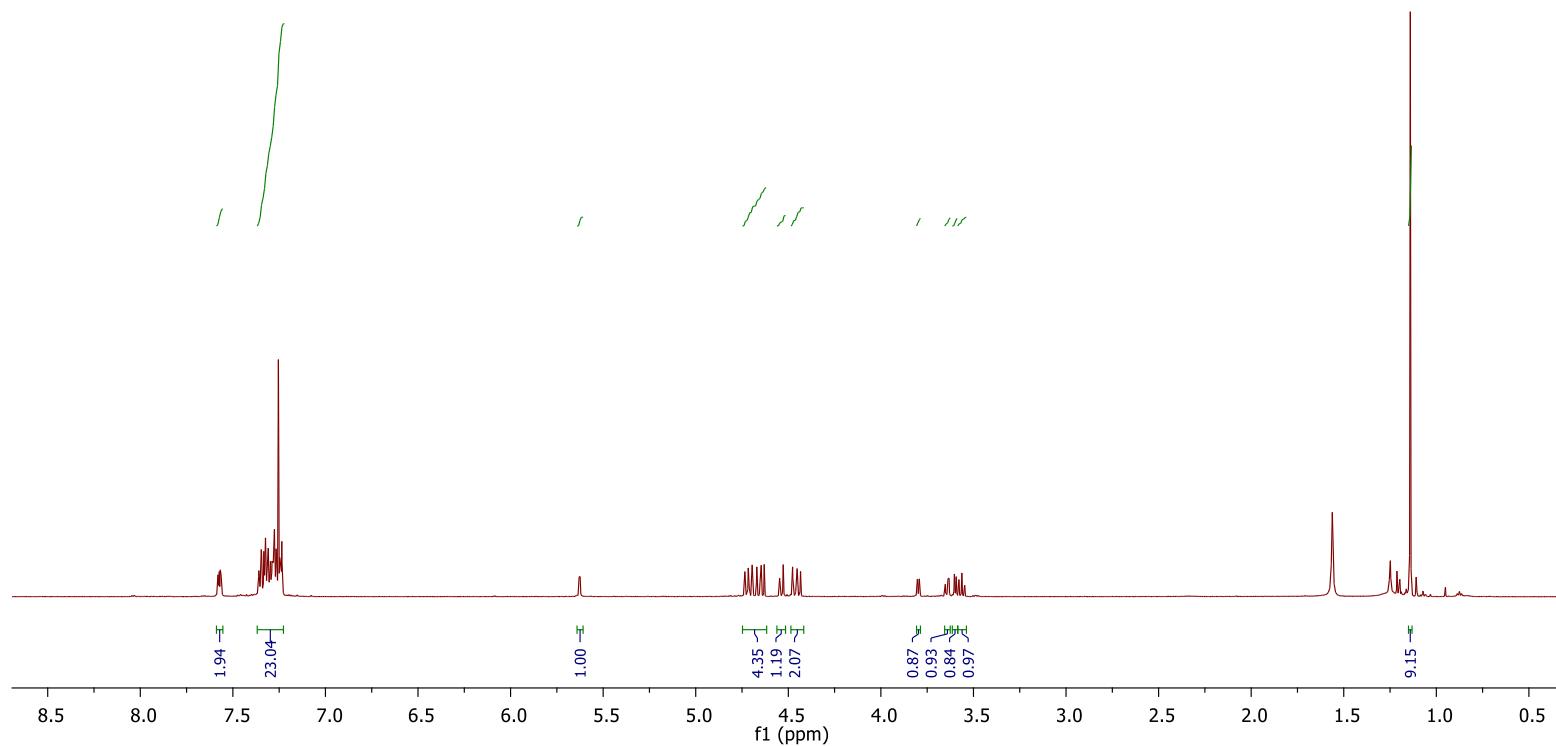
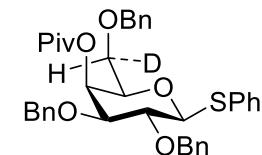
^{13}C NMR (150 MHz, CDCl_3) Spectrum of Phenyl 4-*O*-pivoyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**14**)



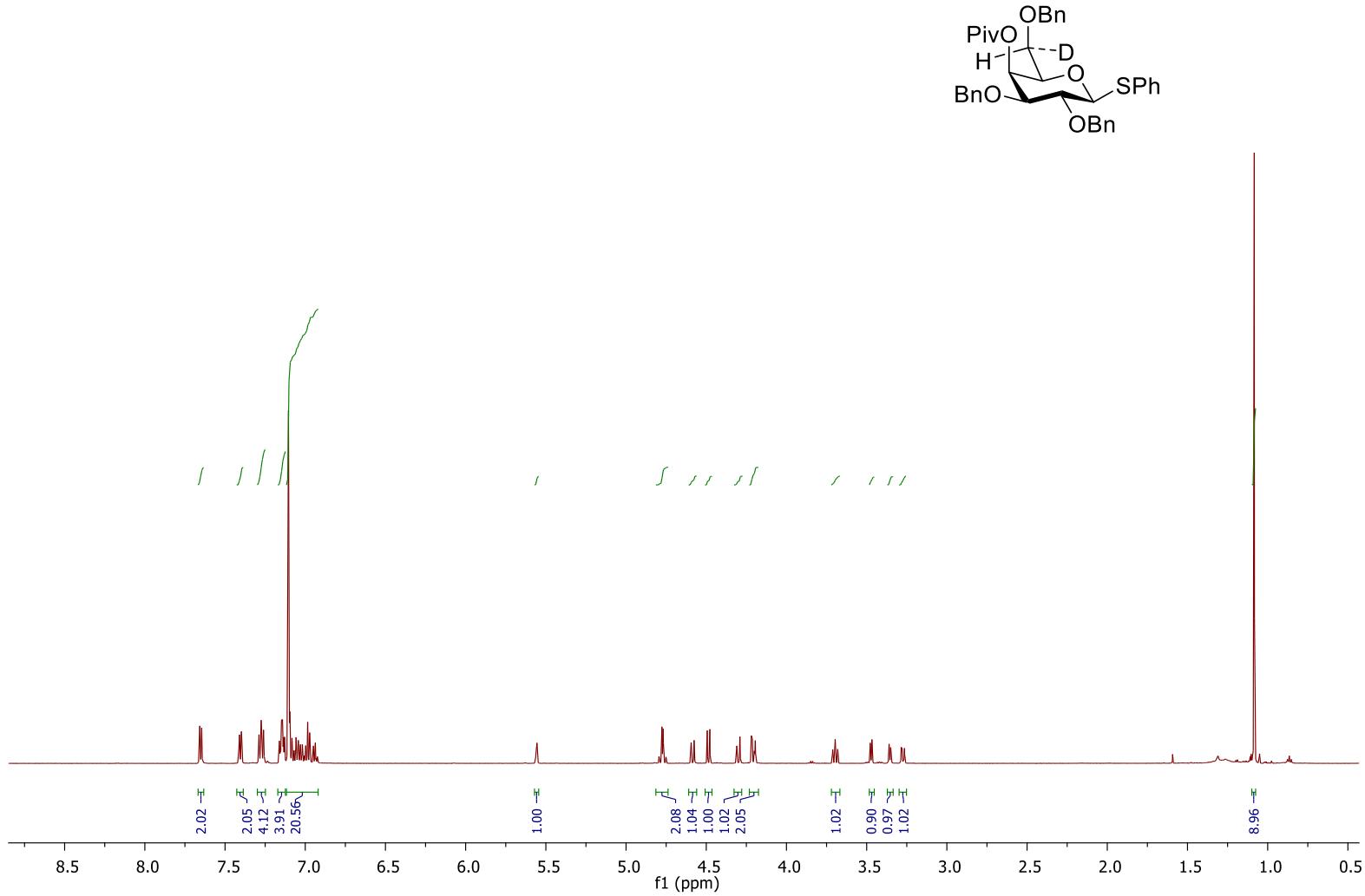
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-pivoyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**14**)



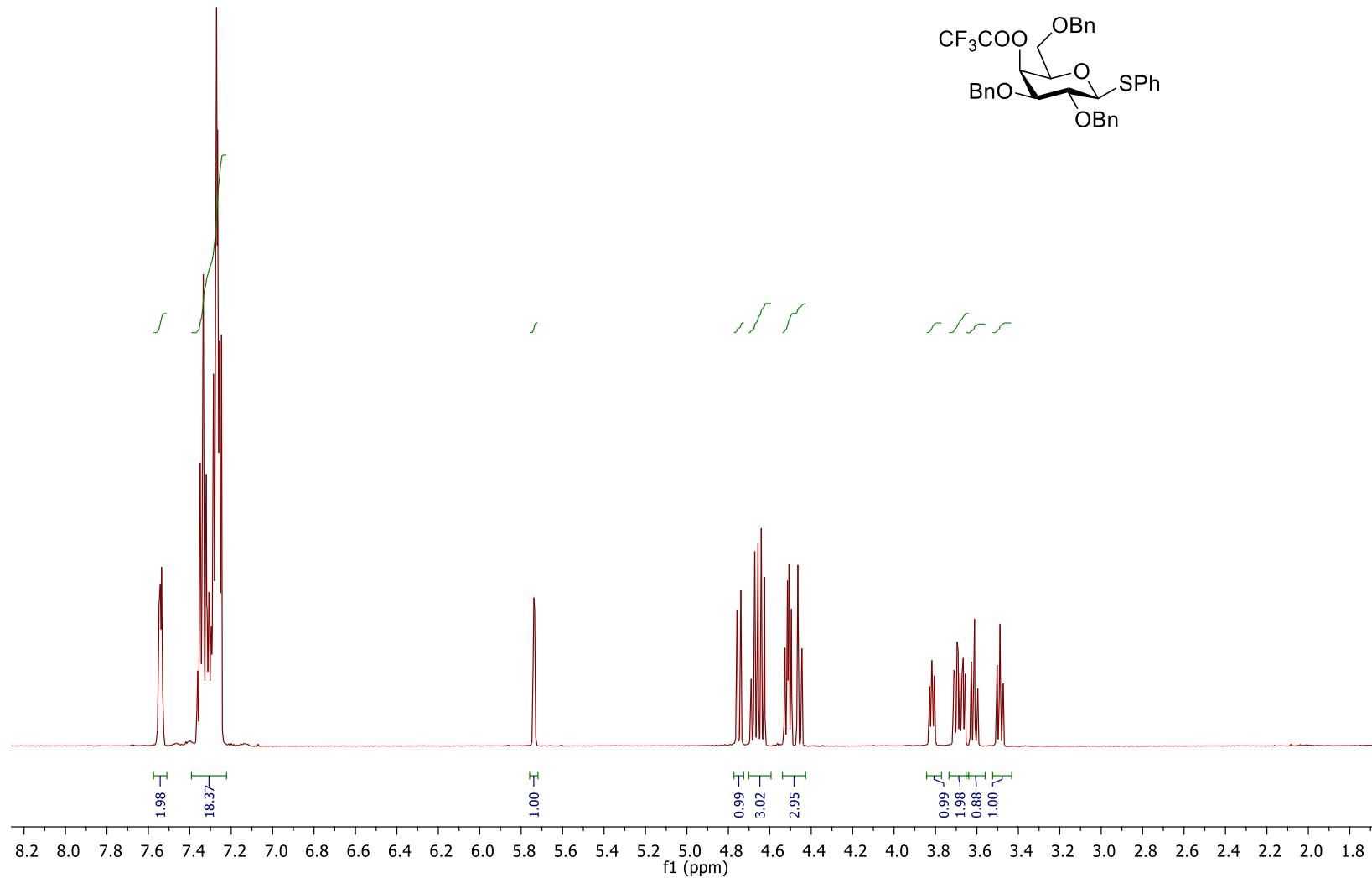
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-O-pivaloyl-(6S)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio-β-D-galactopyranoside (**6S-D-14**)



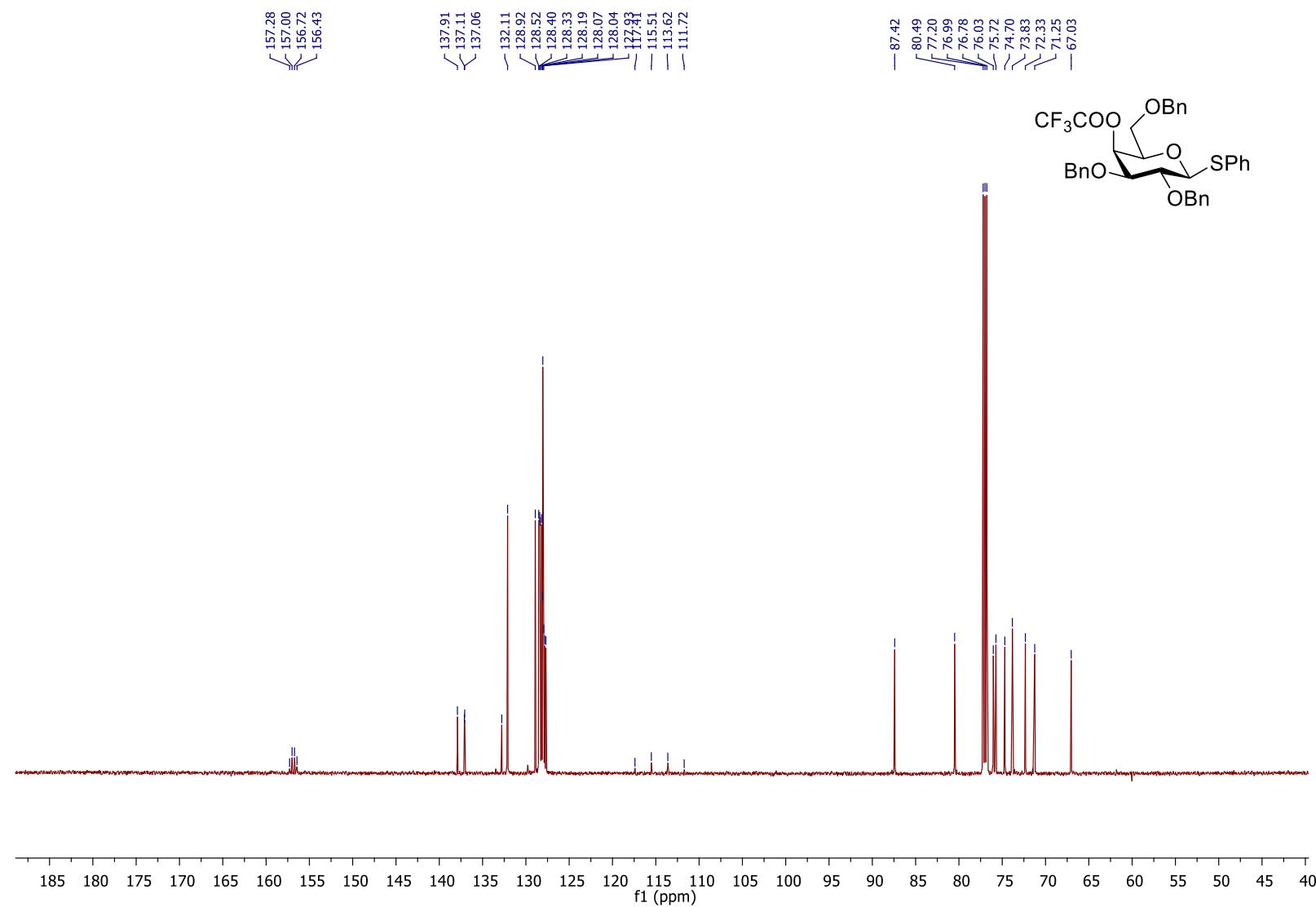
^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl 4-*O*-pivaloyl-(6*S*)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-14**)



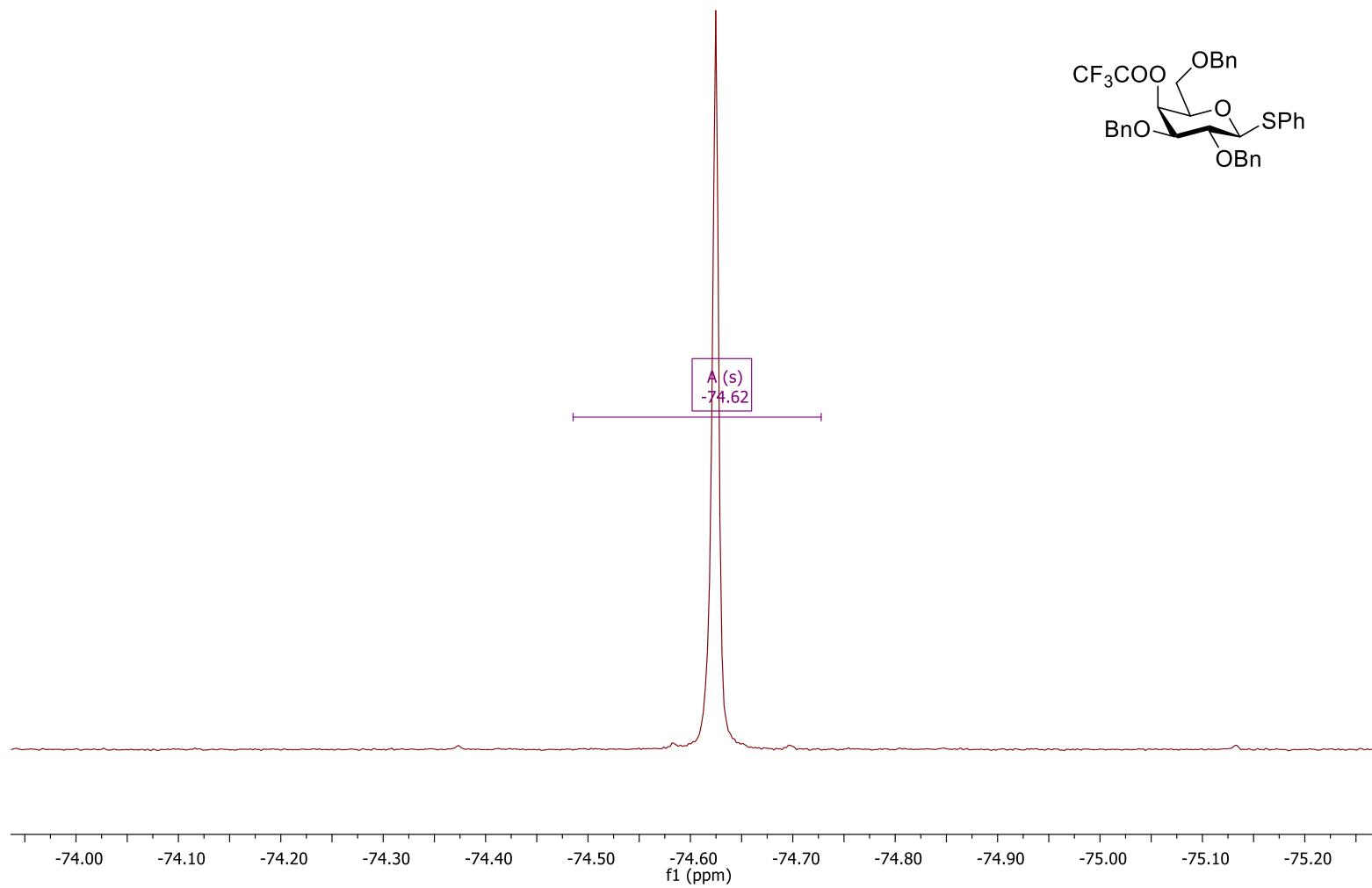
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-trifluoroacetyl -1-thio- β -D-galactopyranoside (**15**)



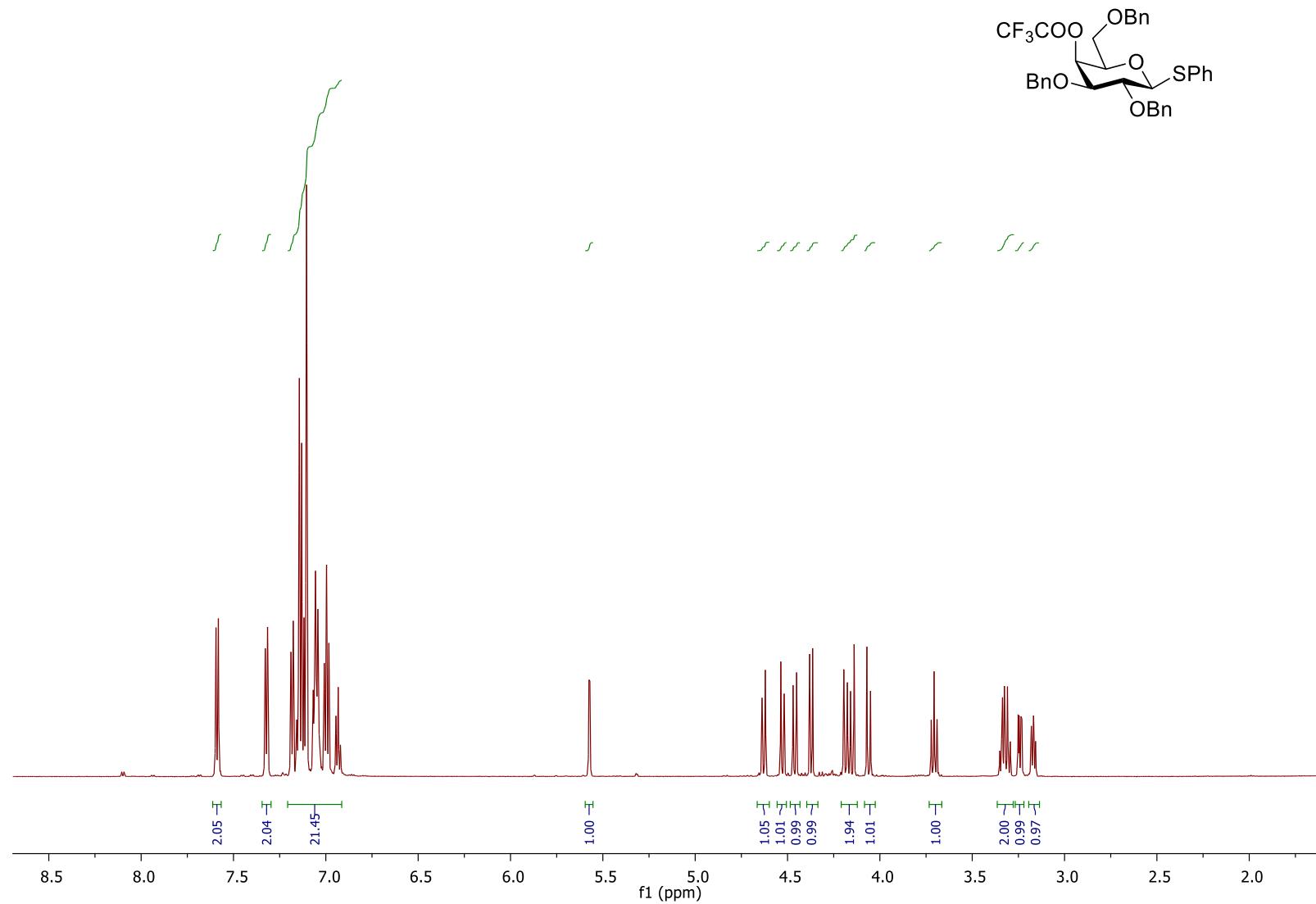
¹³C NMR (150 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-trifluoroacetyl -1-thio- β -D-galactopyranoside (**15**)



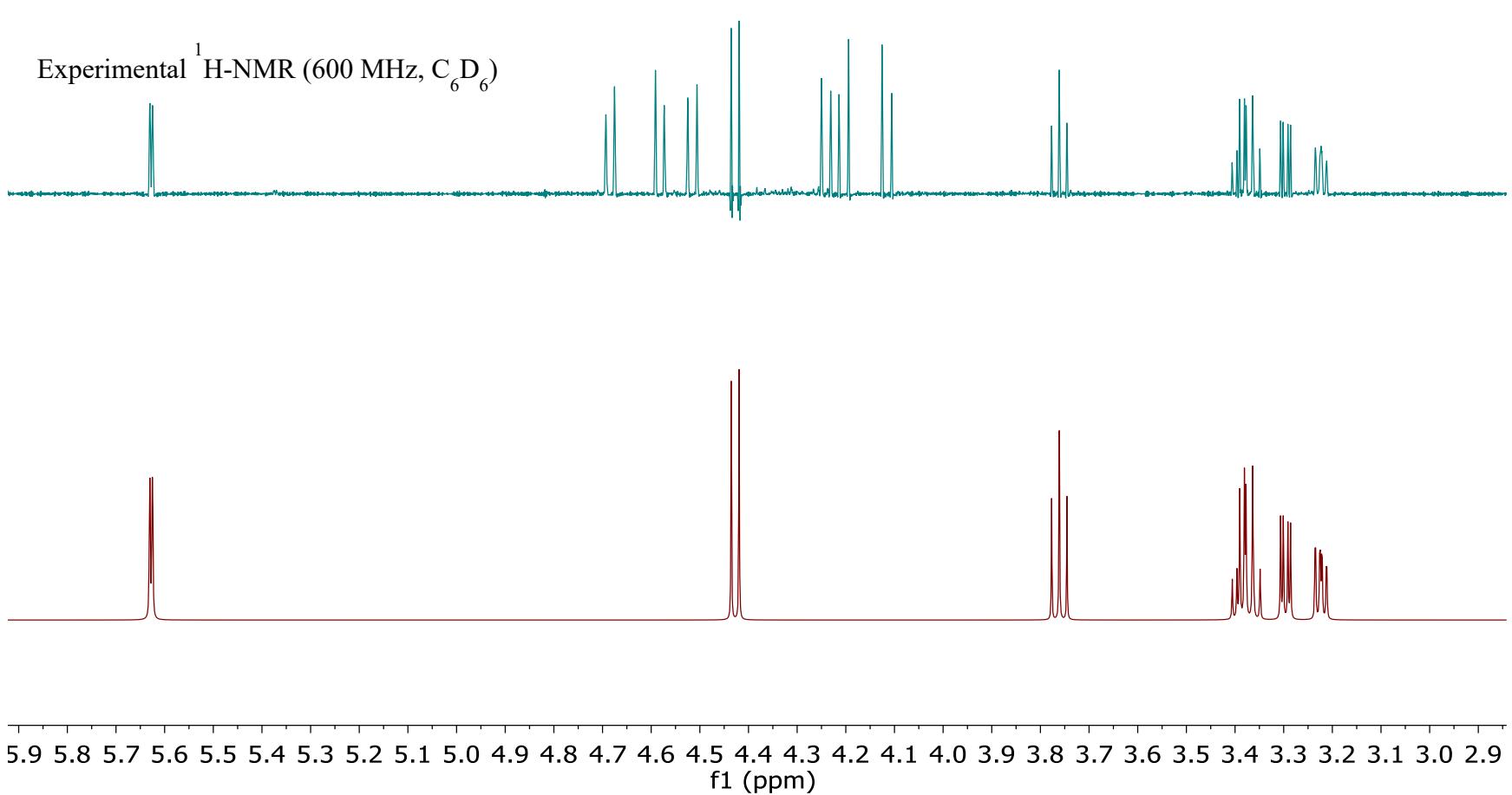
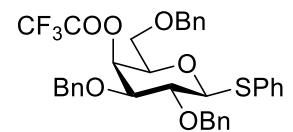
¹⁹F NMR (375 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-trifluoroacetyl -1-thio- β -D-galactopyranoside (**15**)



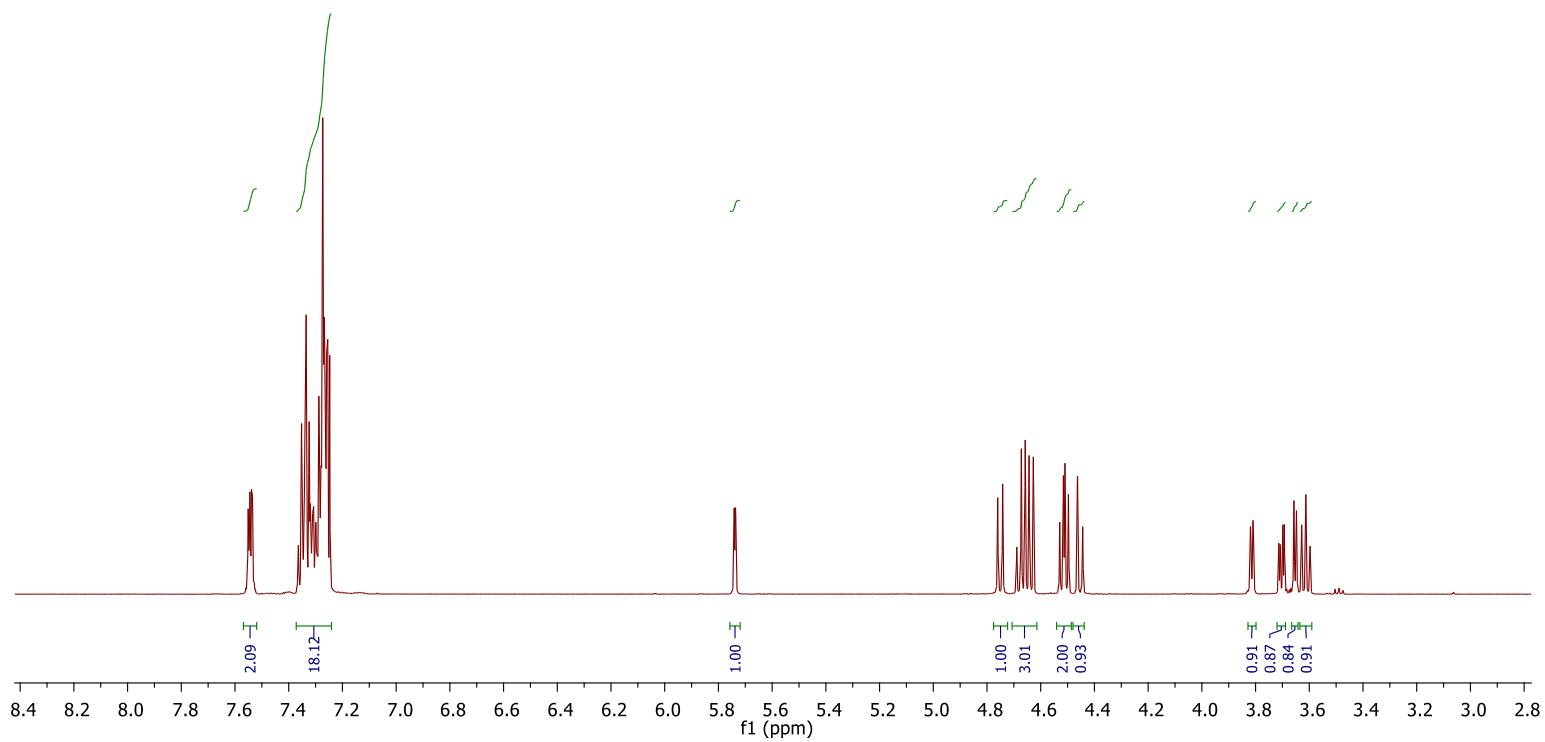
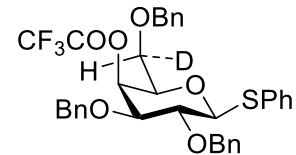
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 2,3,6-tri-O-benzyl-4-O-trifluoroacetyl -1-thio-β-D-galactopyranoside (**15**)



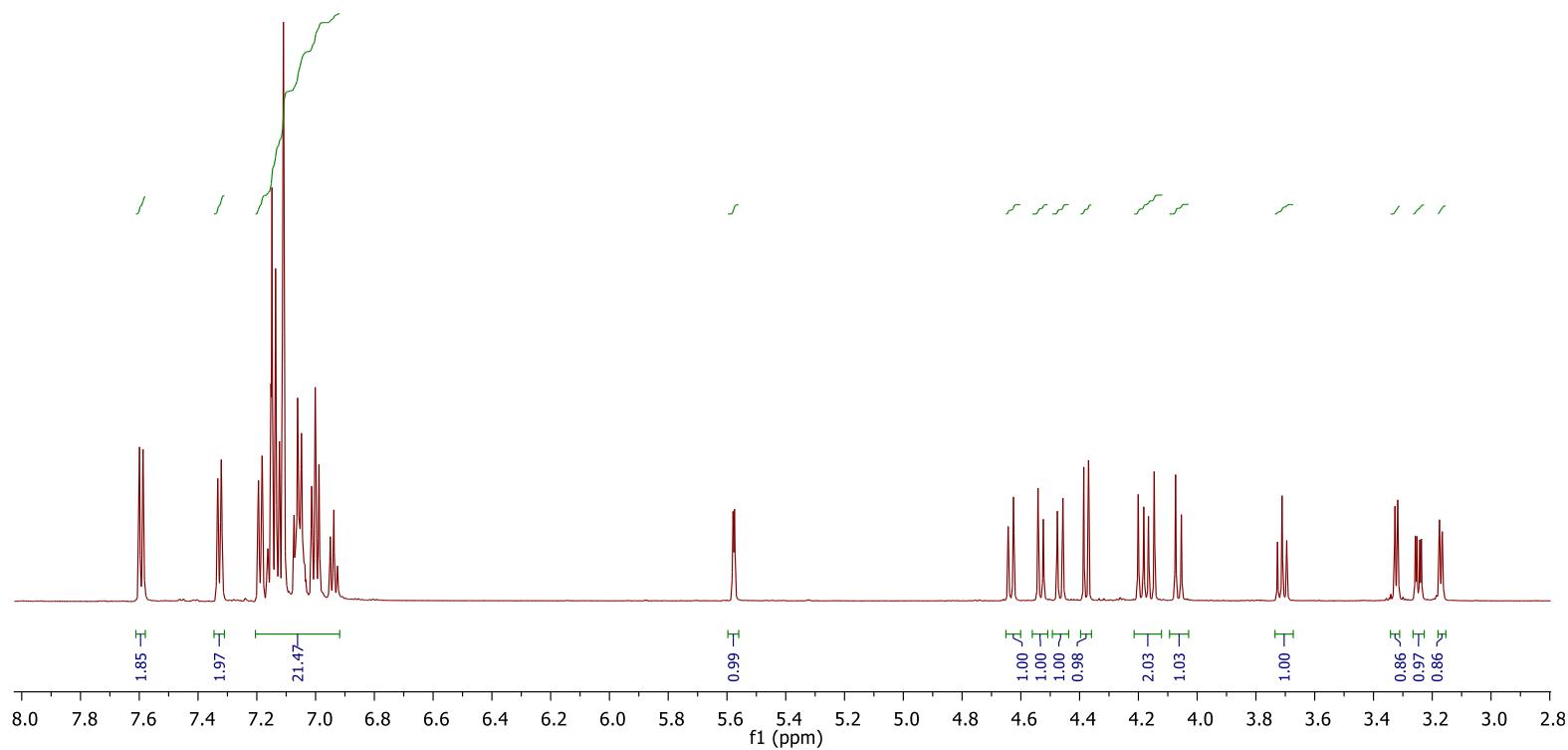
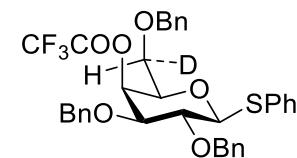
Simulated ^1H NMR and ^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl 2,3,6-tri- O -benzyl-4- O -trifluoroacetyl -1-thio- β -D-galactopyranoside (**15**)



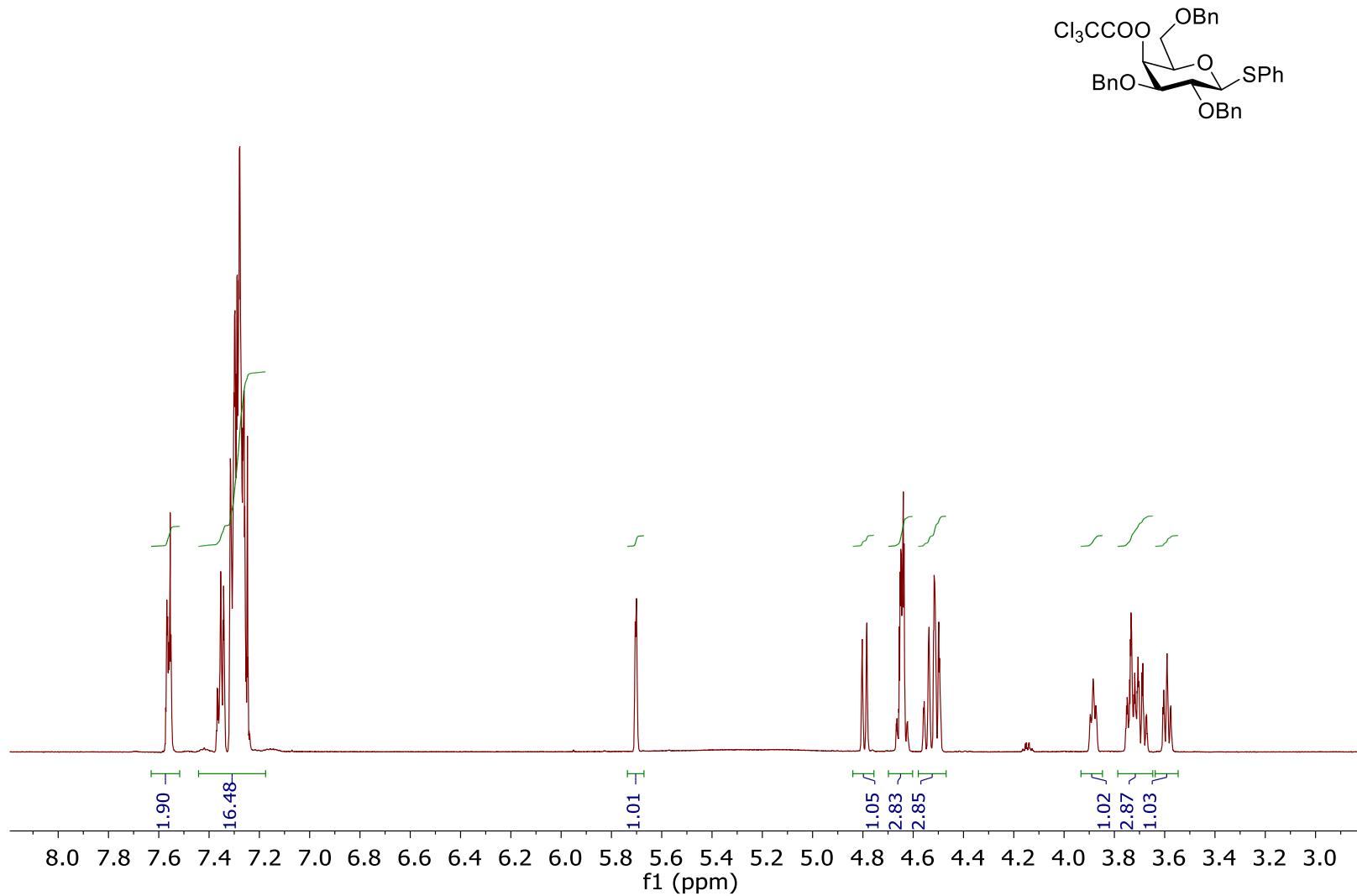
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-O-trifluoroacetyl-(6S)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside
(6S-D-15)



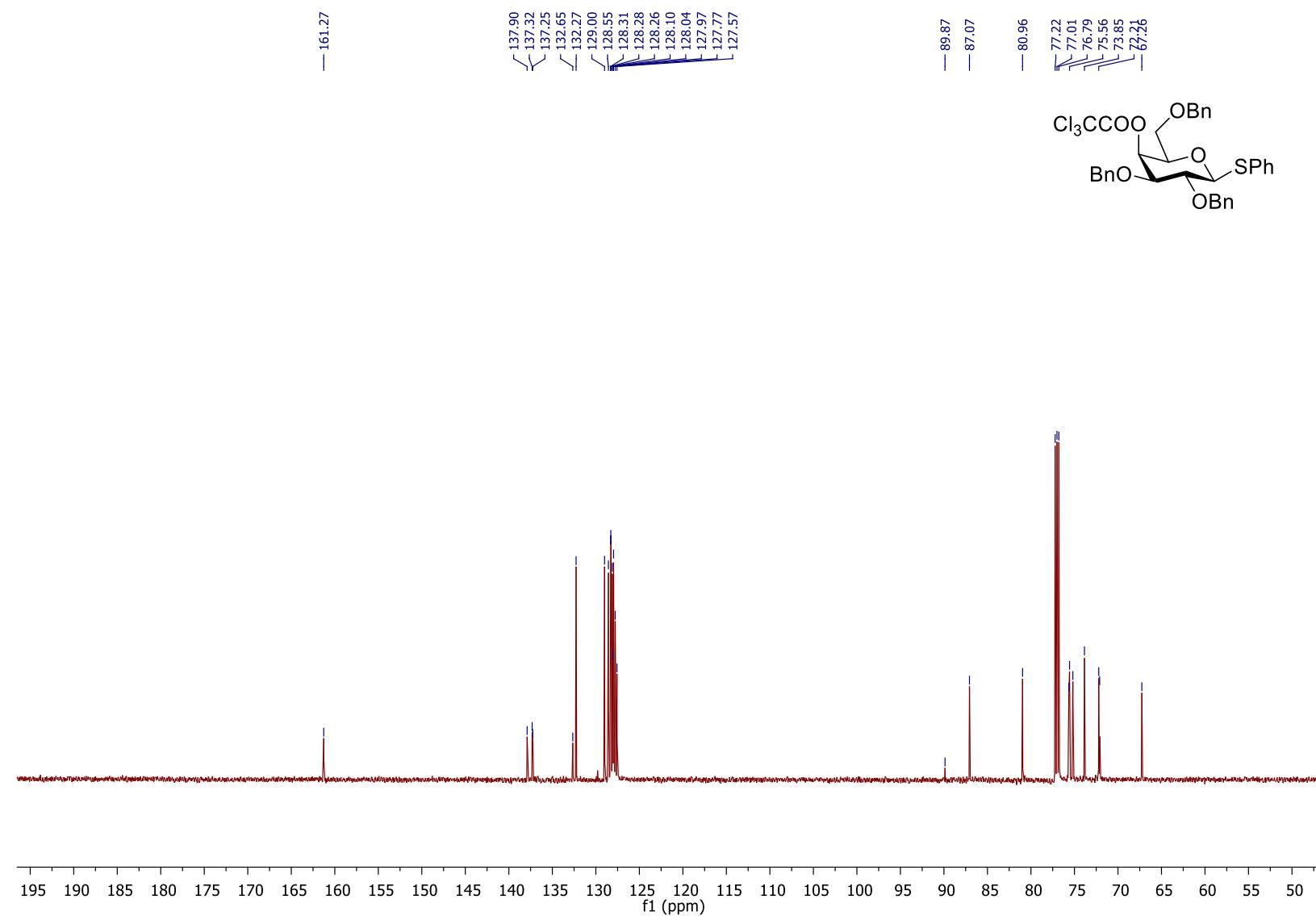
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-trifluoroacetyl-(6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-15**)



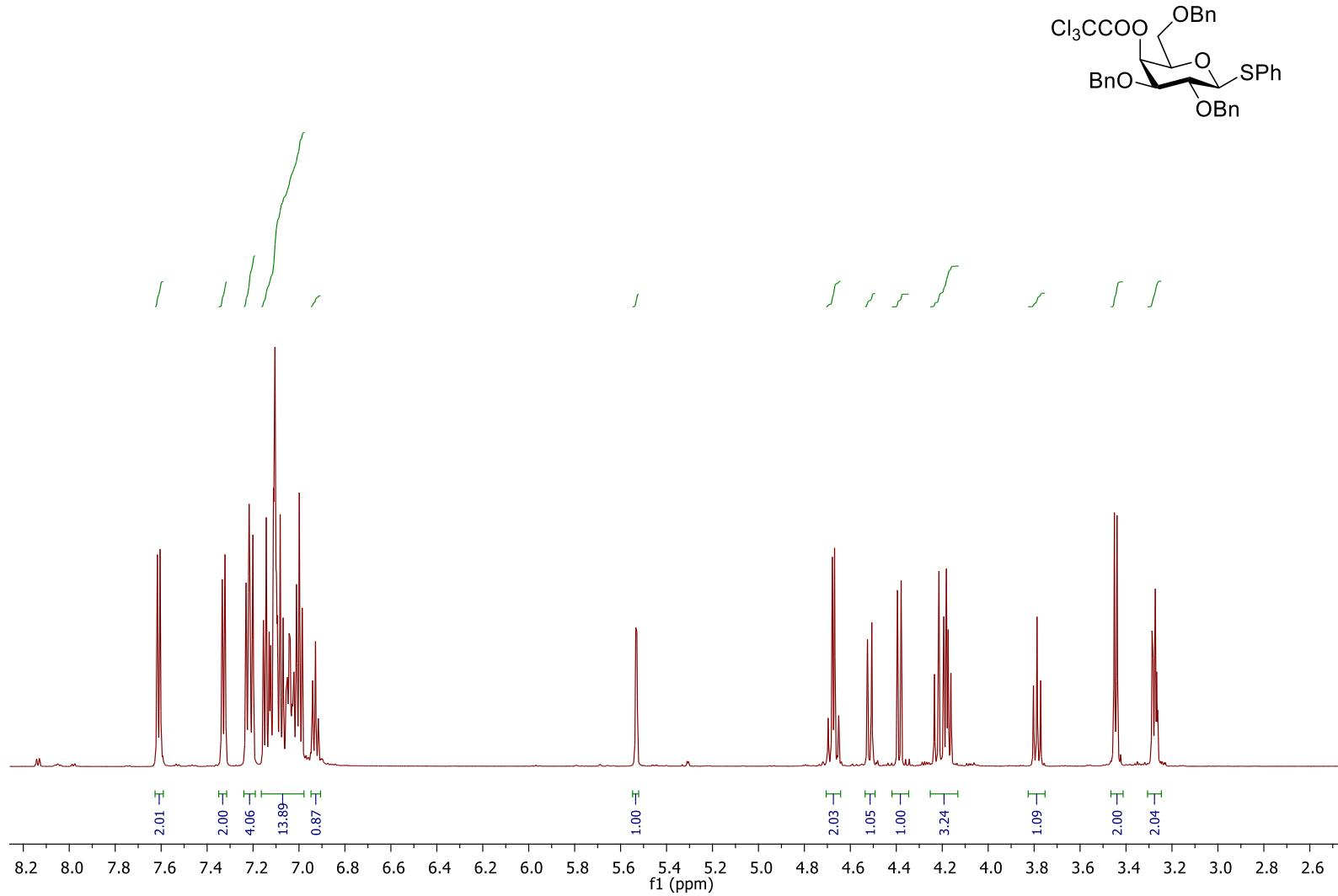
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 2,3,6-tri- O -benzyl-4- O -trichloroacetyl -1-thio- β -D-galactopyranoside (**16**)



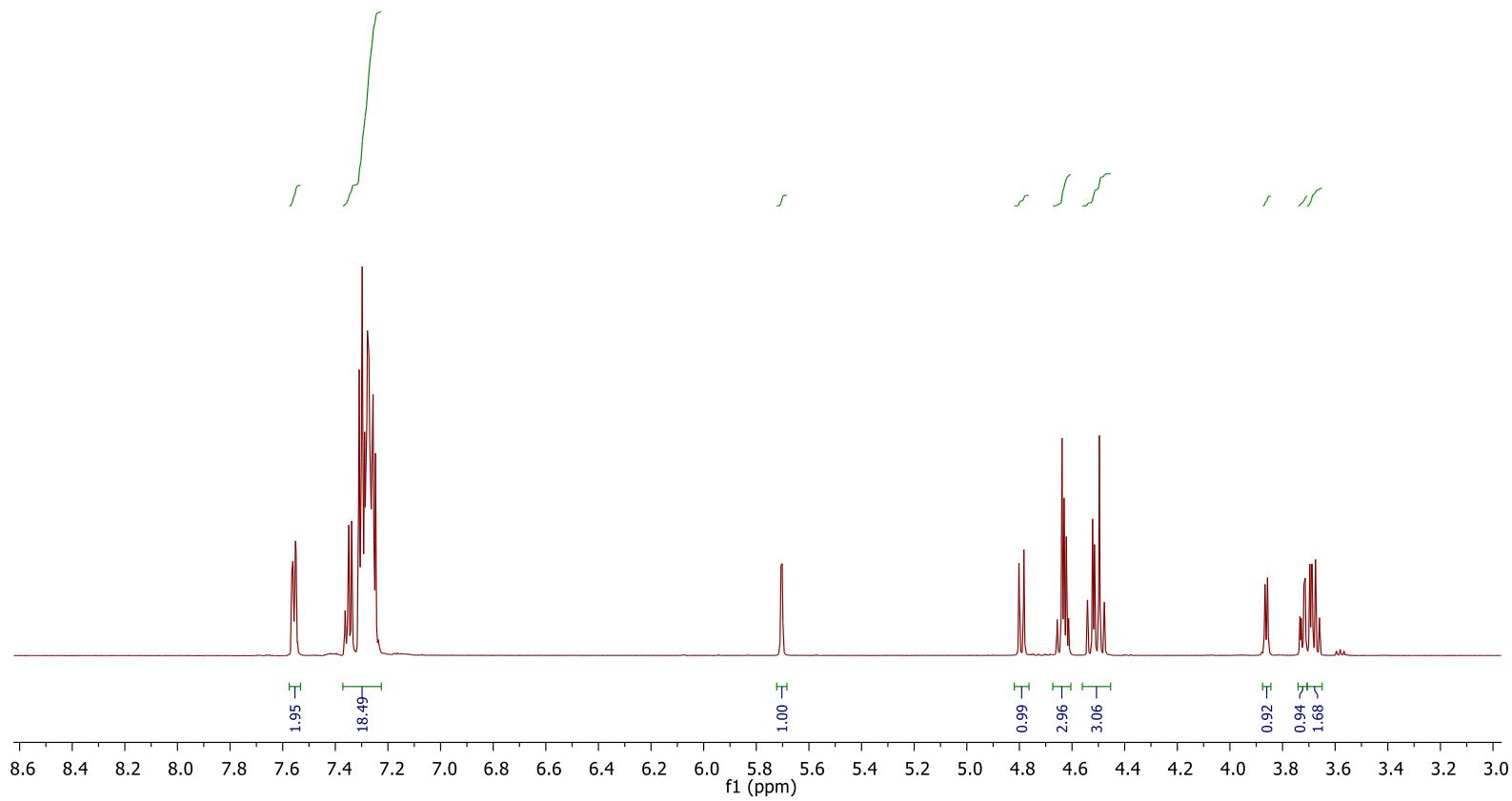
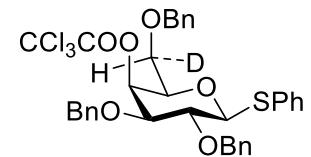
¹³C NMR (150 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-O-benzyl-4-O-trichloroacetyl -1-thio- β -D-galactopyranoside (**16**)



¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 2,3,6-tri-O-benzyl-4-O-trichloroacetyl -1-thio-β-D-galactopyranoside (**16**)

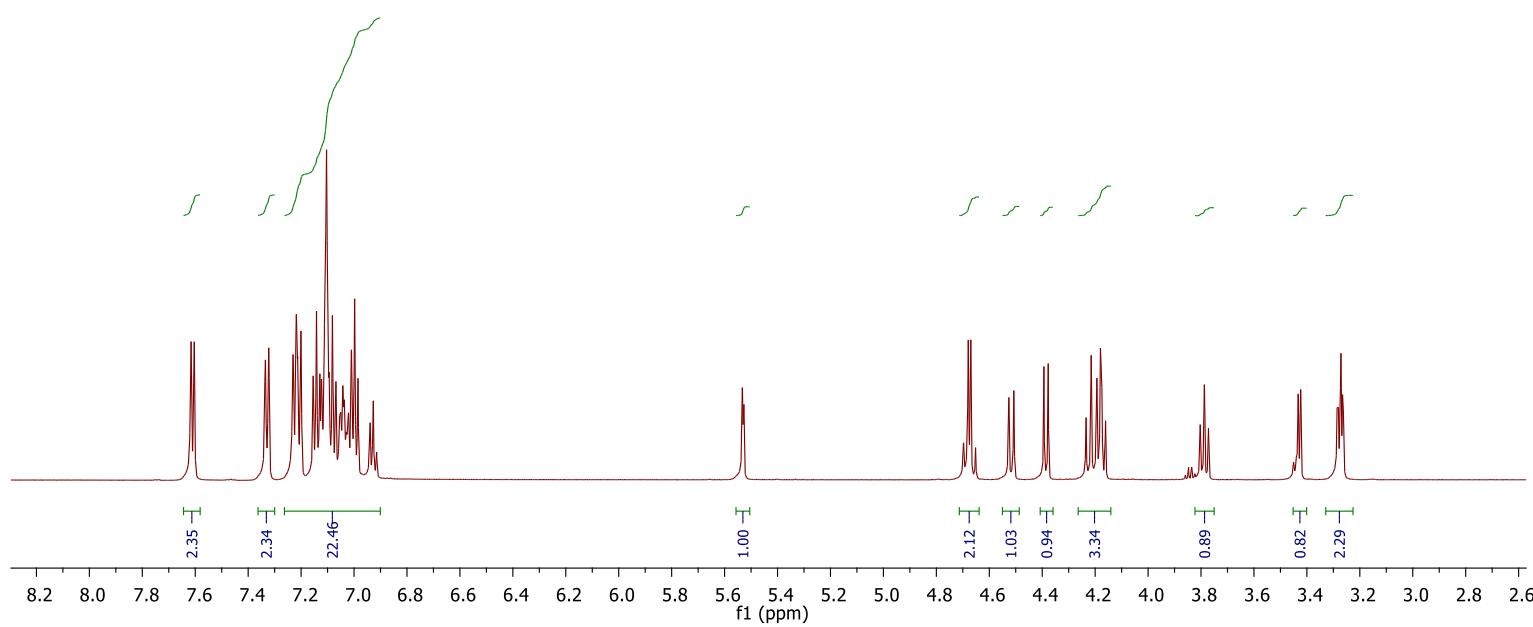
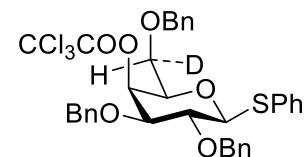


¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-O-trichloroacetyl-(6S)-[6-²H₁]-2,3,6-tri-O-benzyl-1-thio-β-D-galactopyranoside
(6S-D-16)

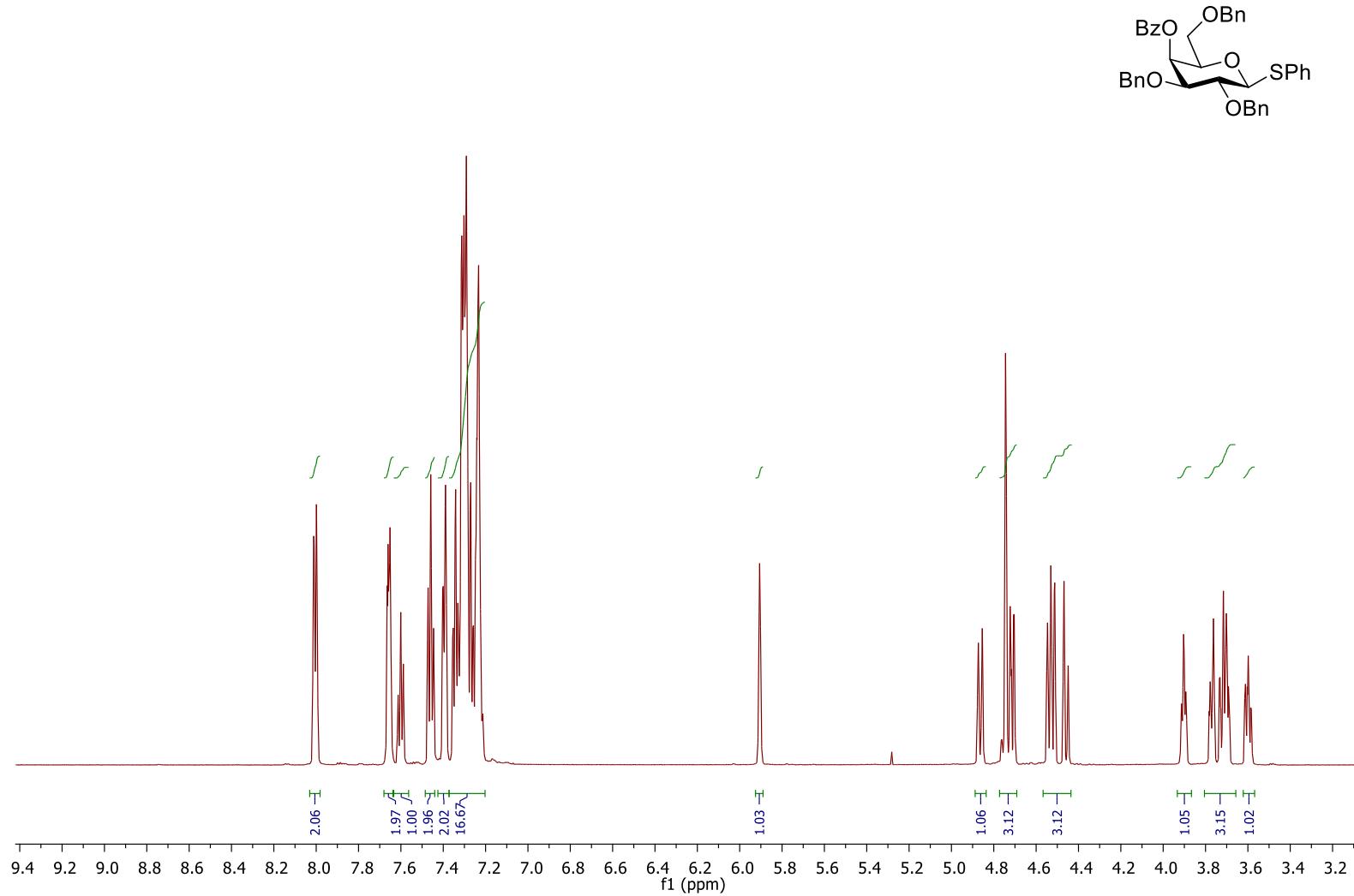


¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-O-trichloroacetyl-(6*S*)-[6-²H]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside

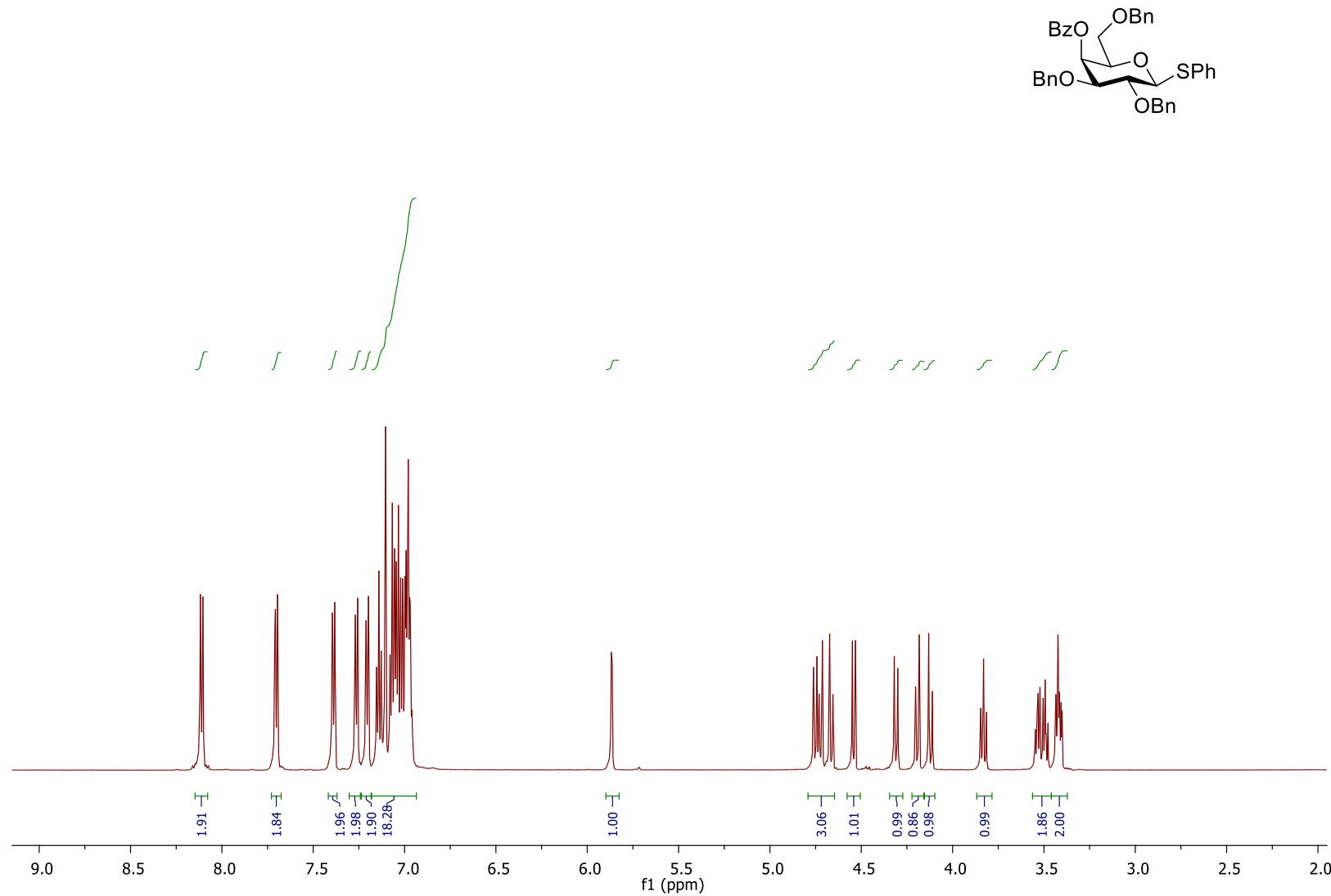
(6*S*-D-16)



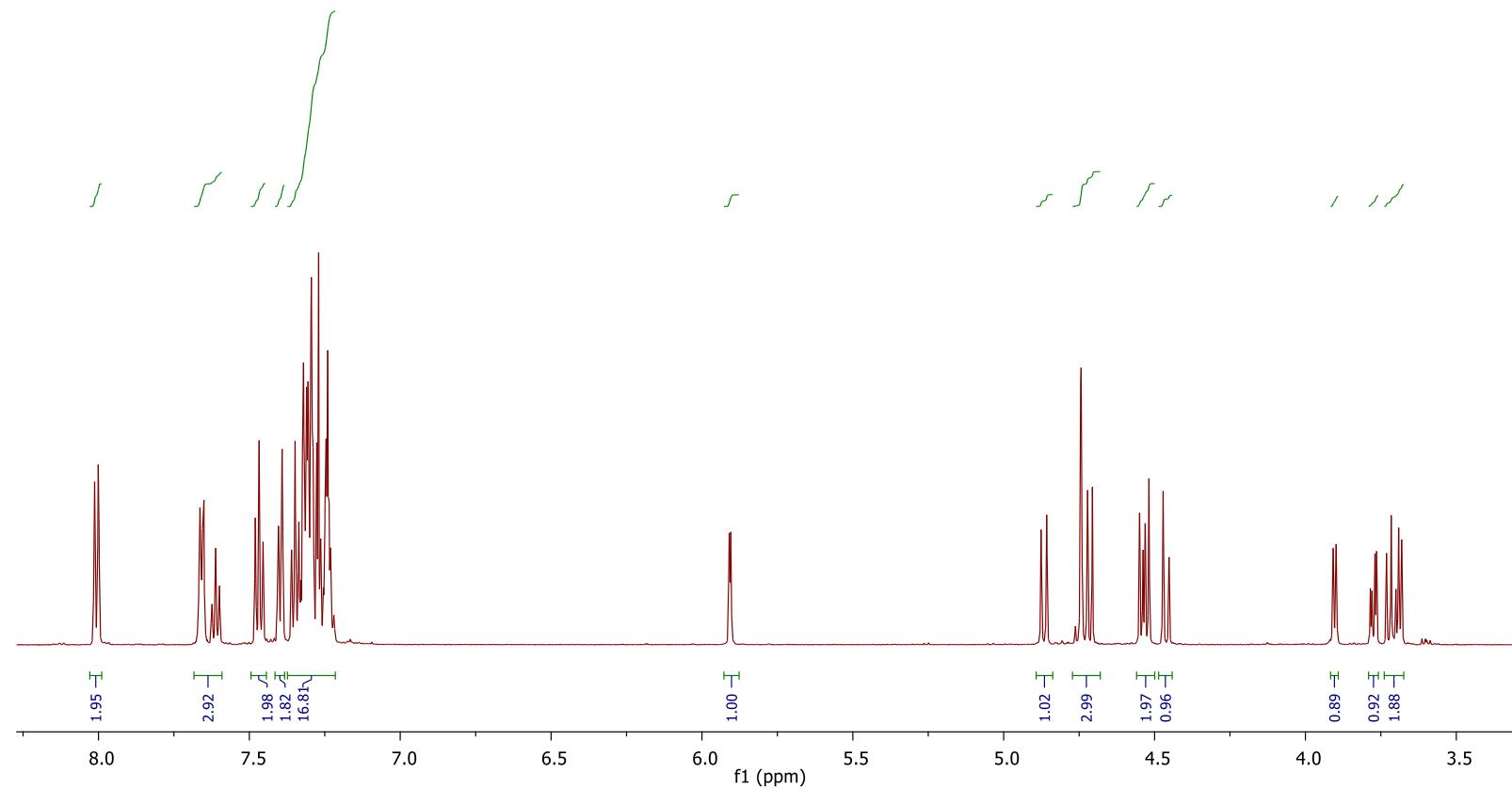
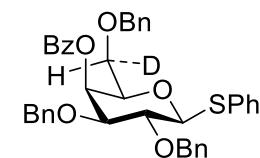
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 4-*O*-benzoyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**17**)



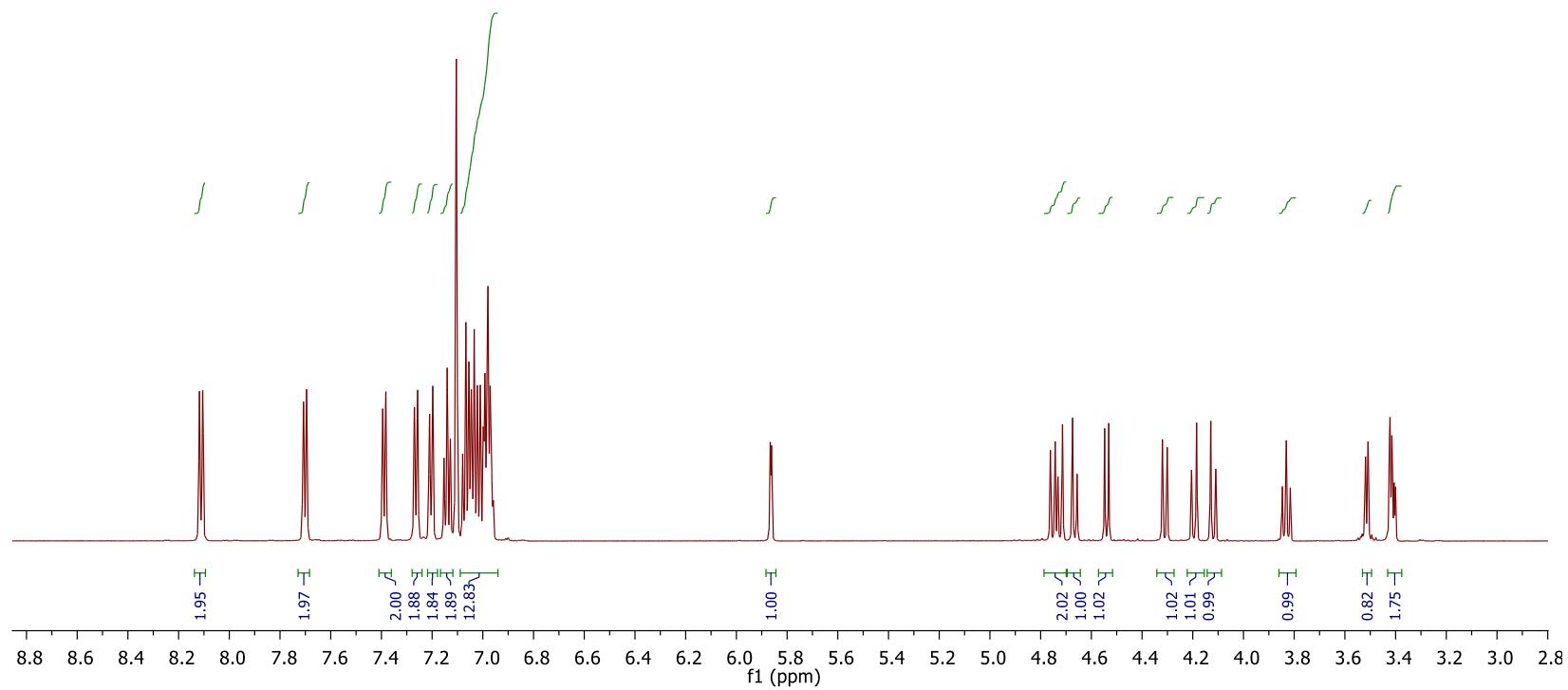
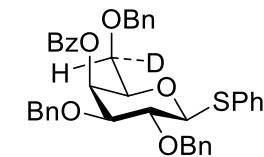
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-benzoyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**17**)



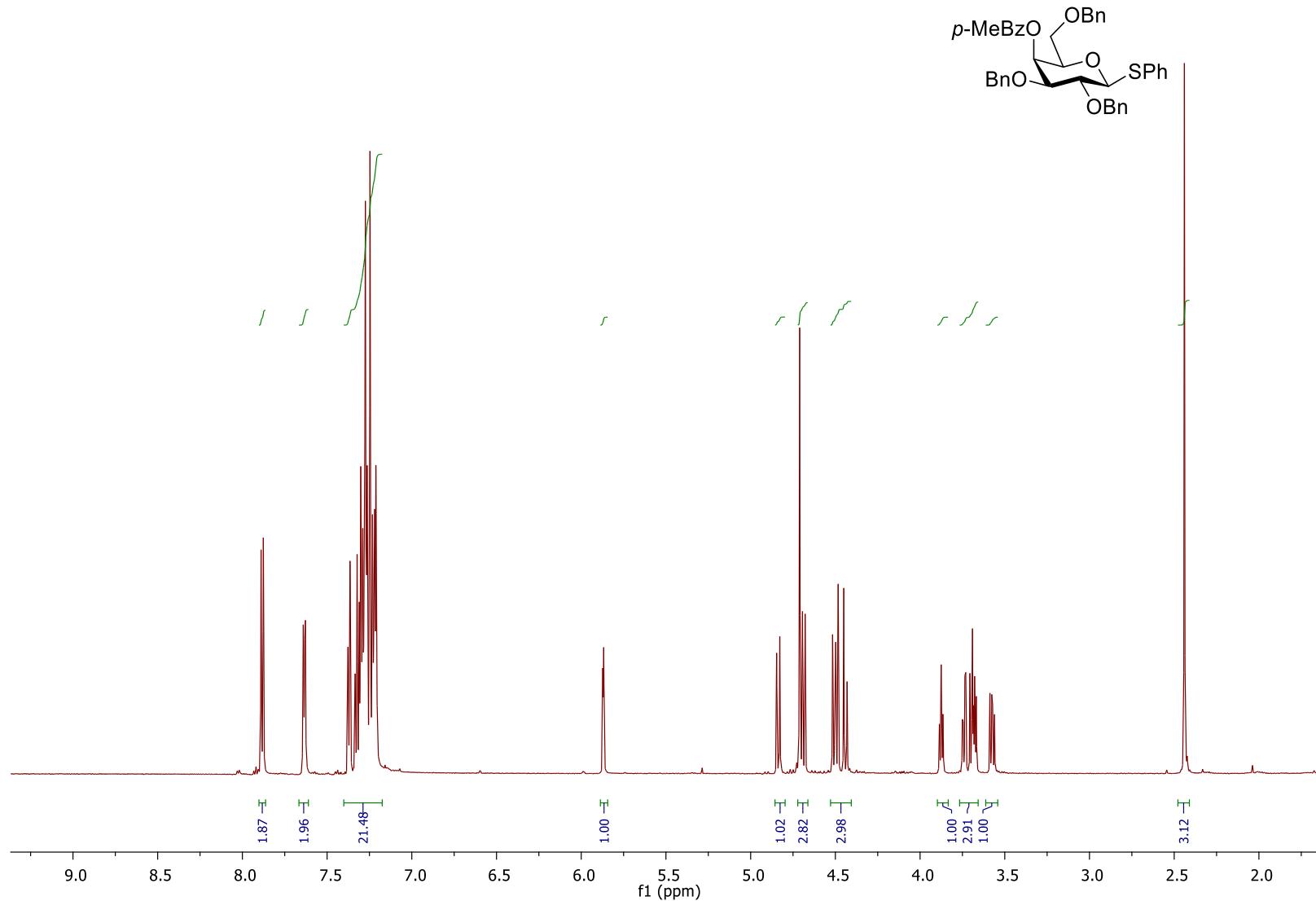
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-benzoyl-(6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio-β-D-galactopyranoside (**6S-D-17**)



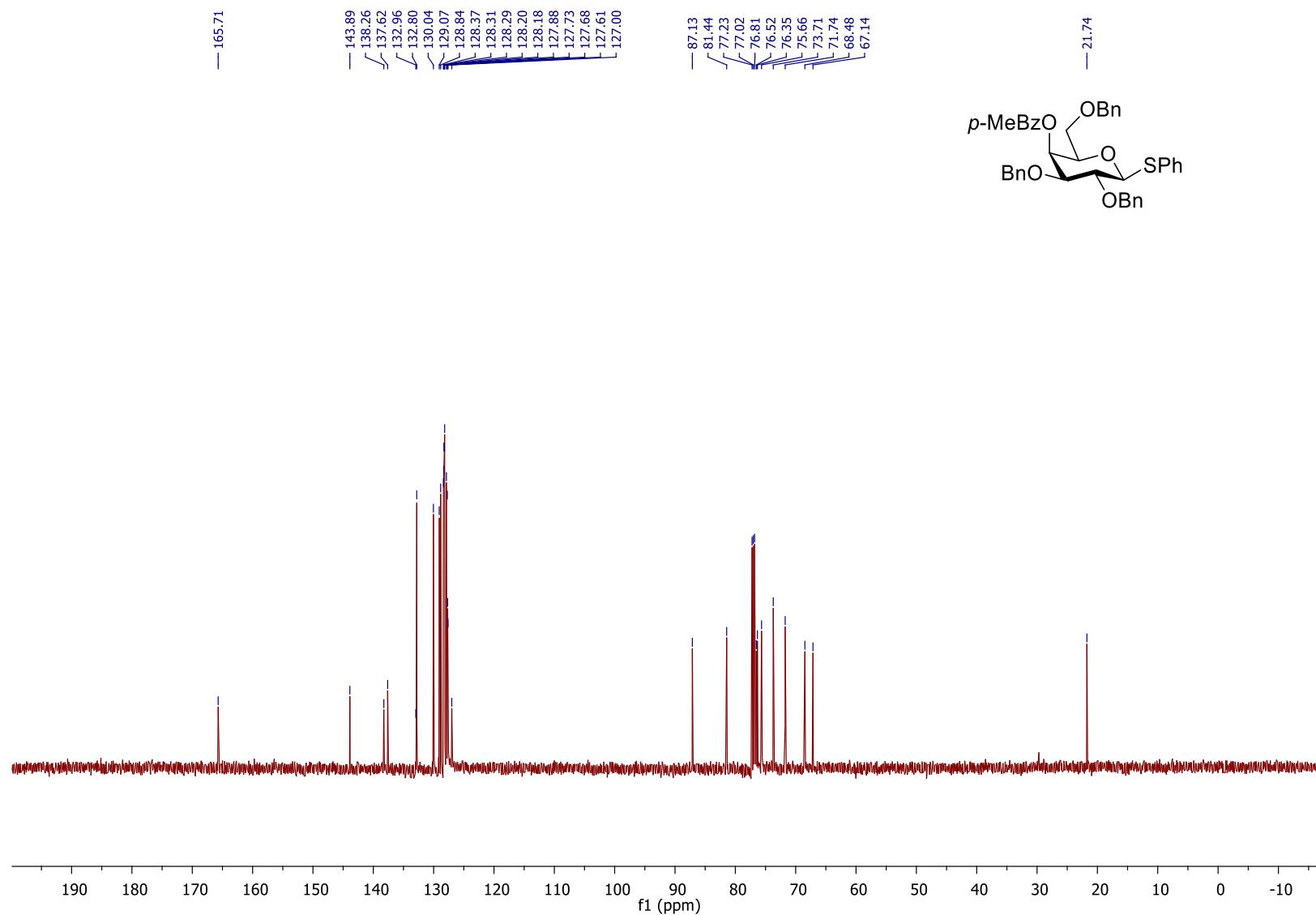
^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl 4-*O*-benzoyl-(6*S*)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-17**)



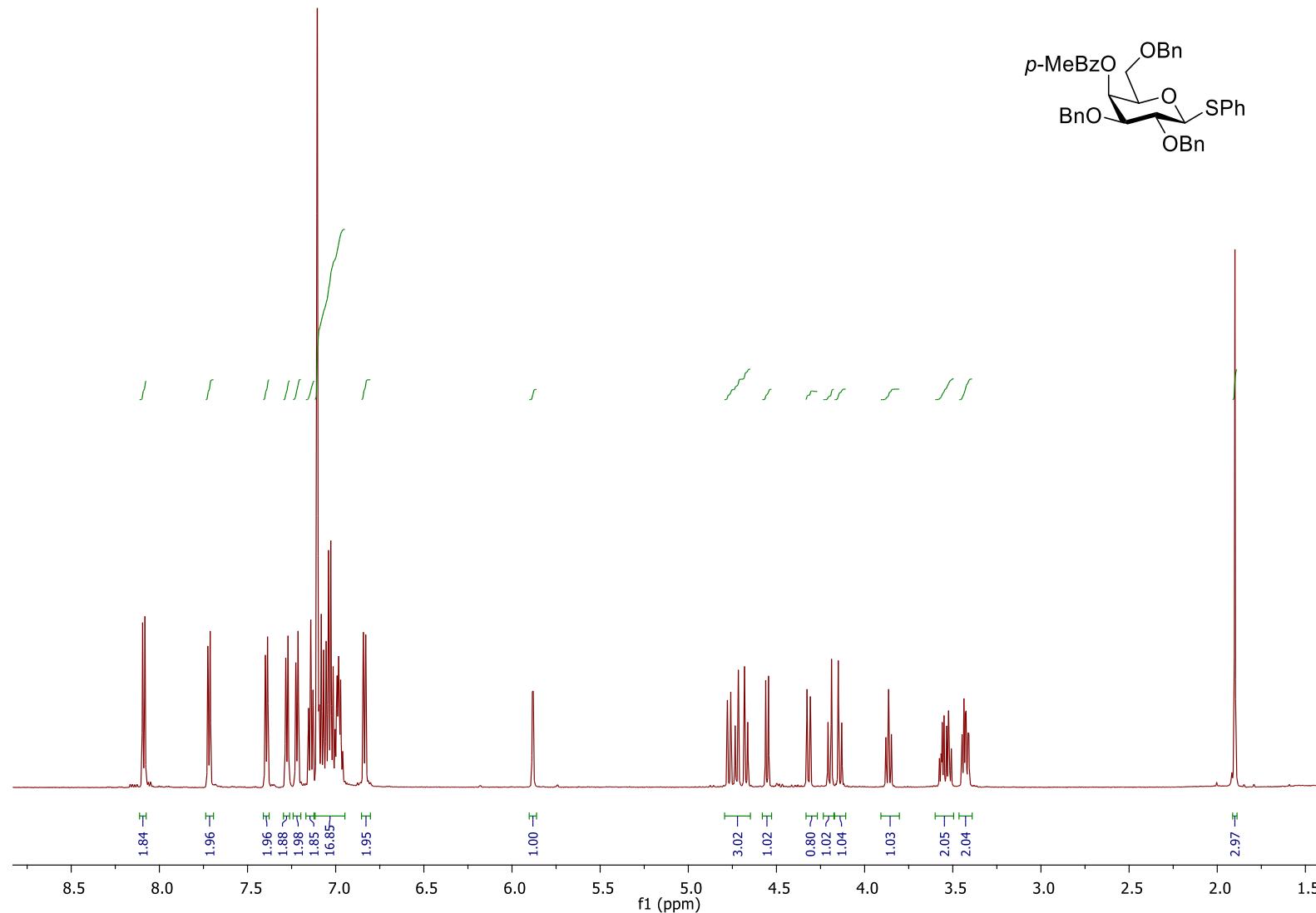
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 4-*O*-(*p*-methylbenzoyl)-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**18**)



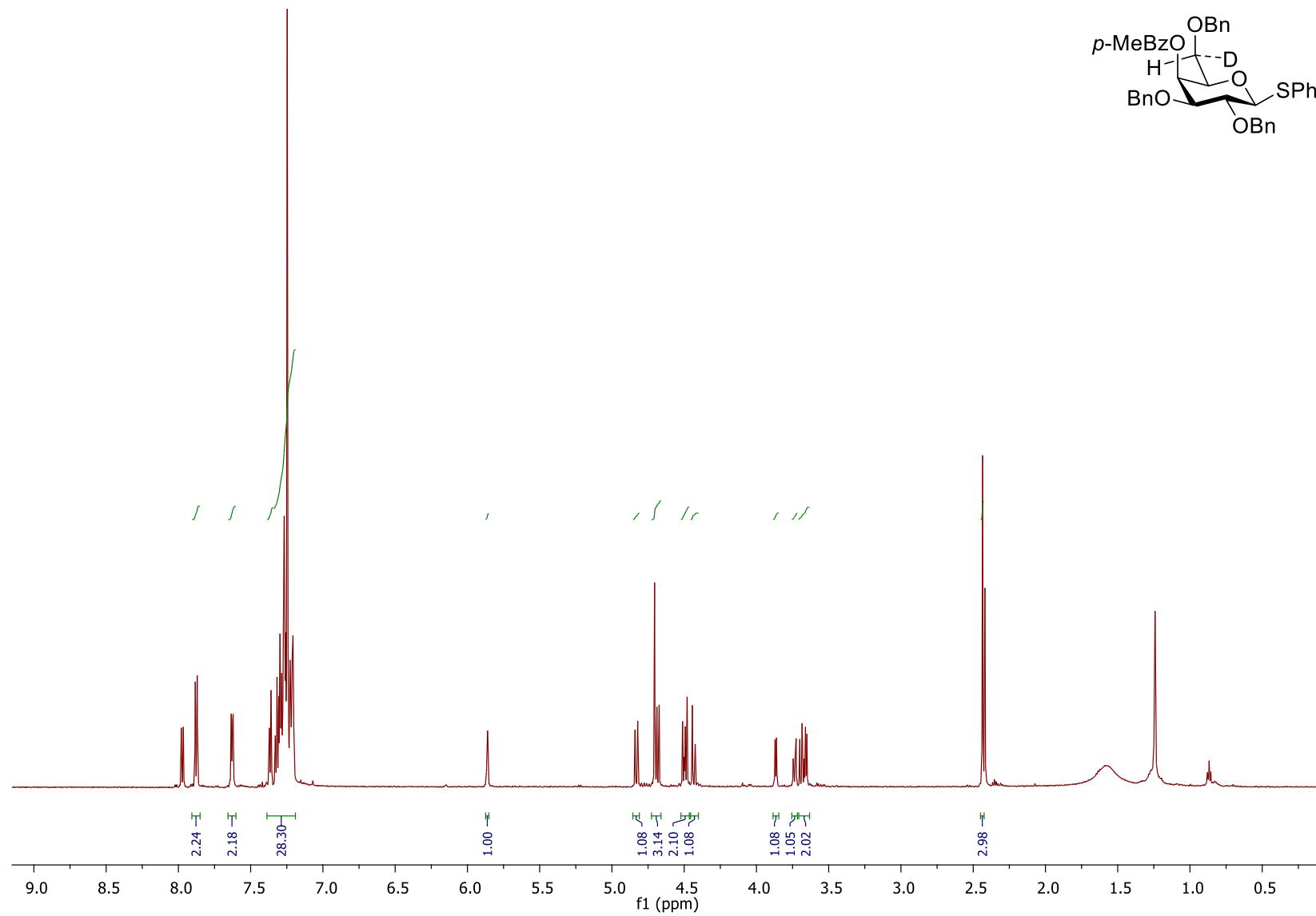
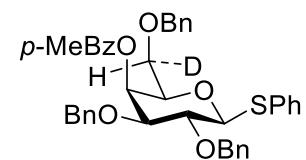
¹³C NMR (150 MHz, CDCl₃) Spectrum of Phenyl 4-O-(*p*-methylbenzoyl)-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**18**)



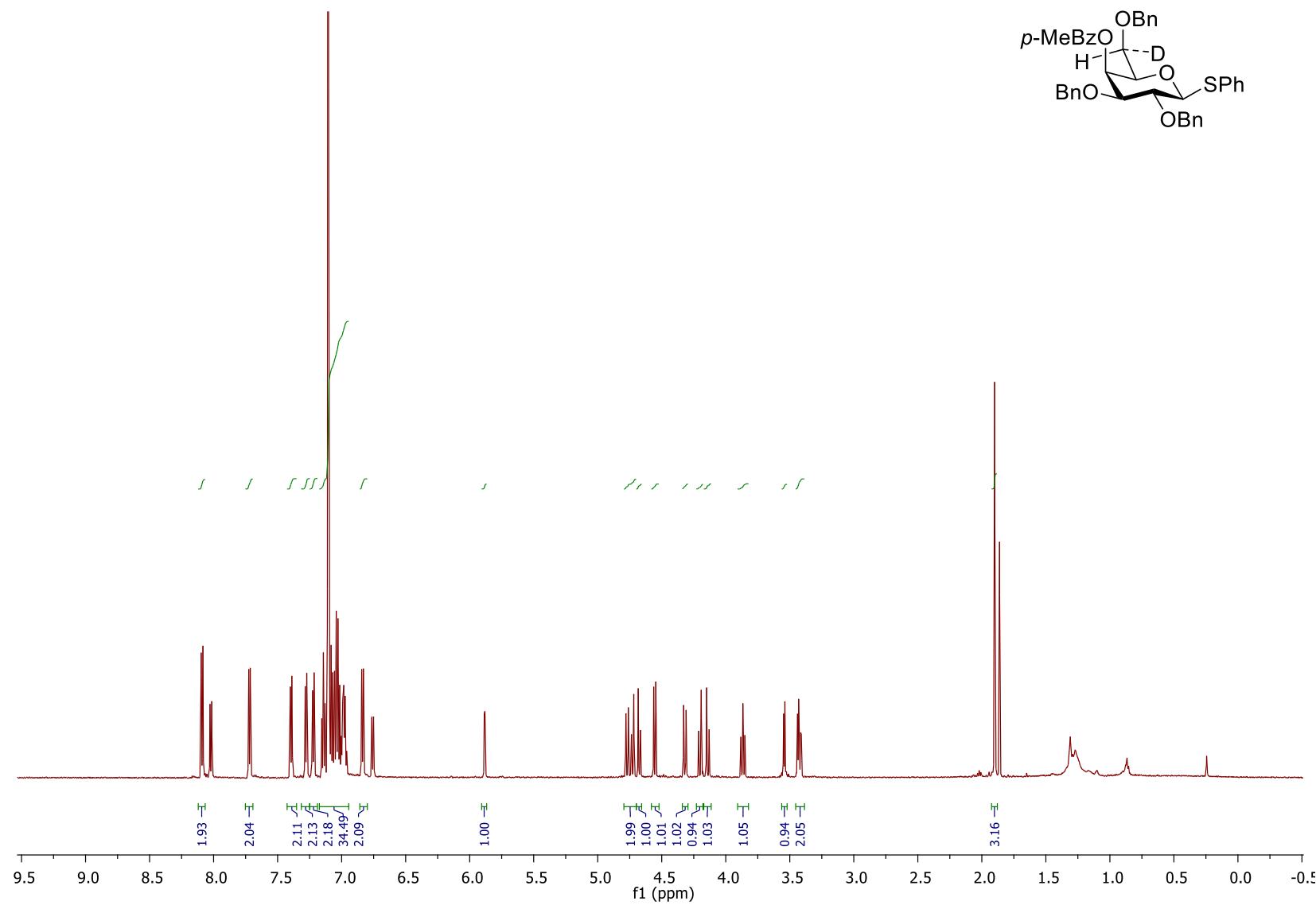
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-(*p*-methylbenzoyl)-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**18**)



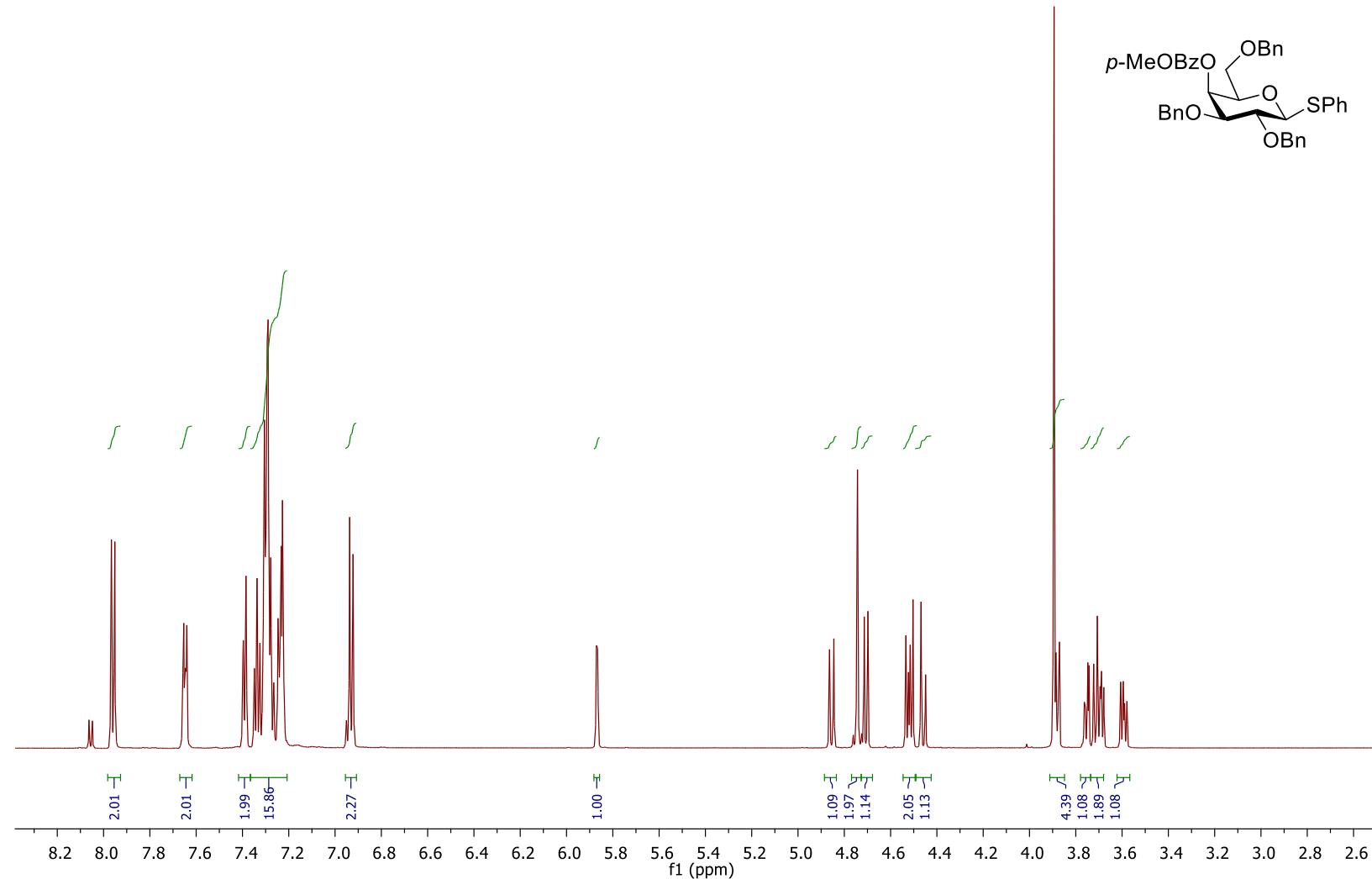
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-(*p*-methylbenzoyl)-(6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside
(6S-D-18)



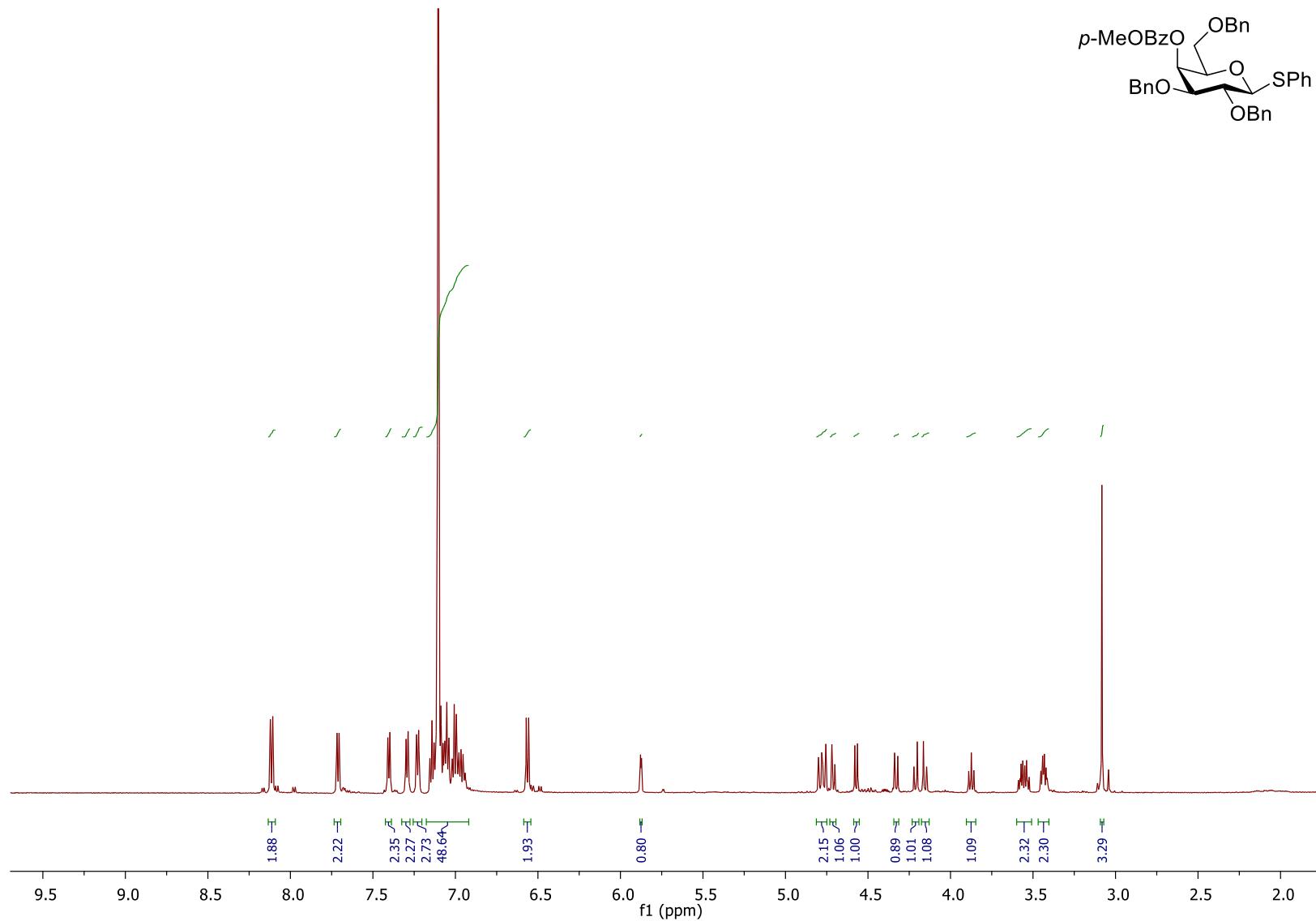
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-(*p*-methylbenzoyl)-(*6S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside
(6S-D-18)



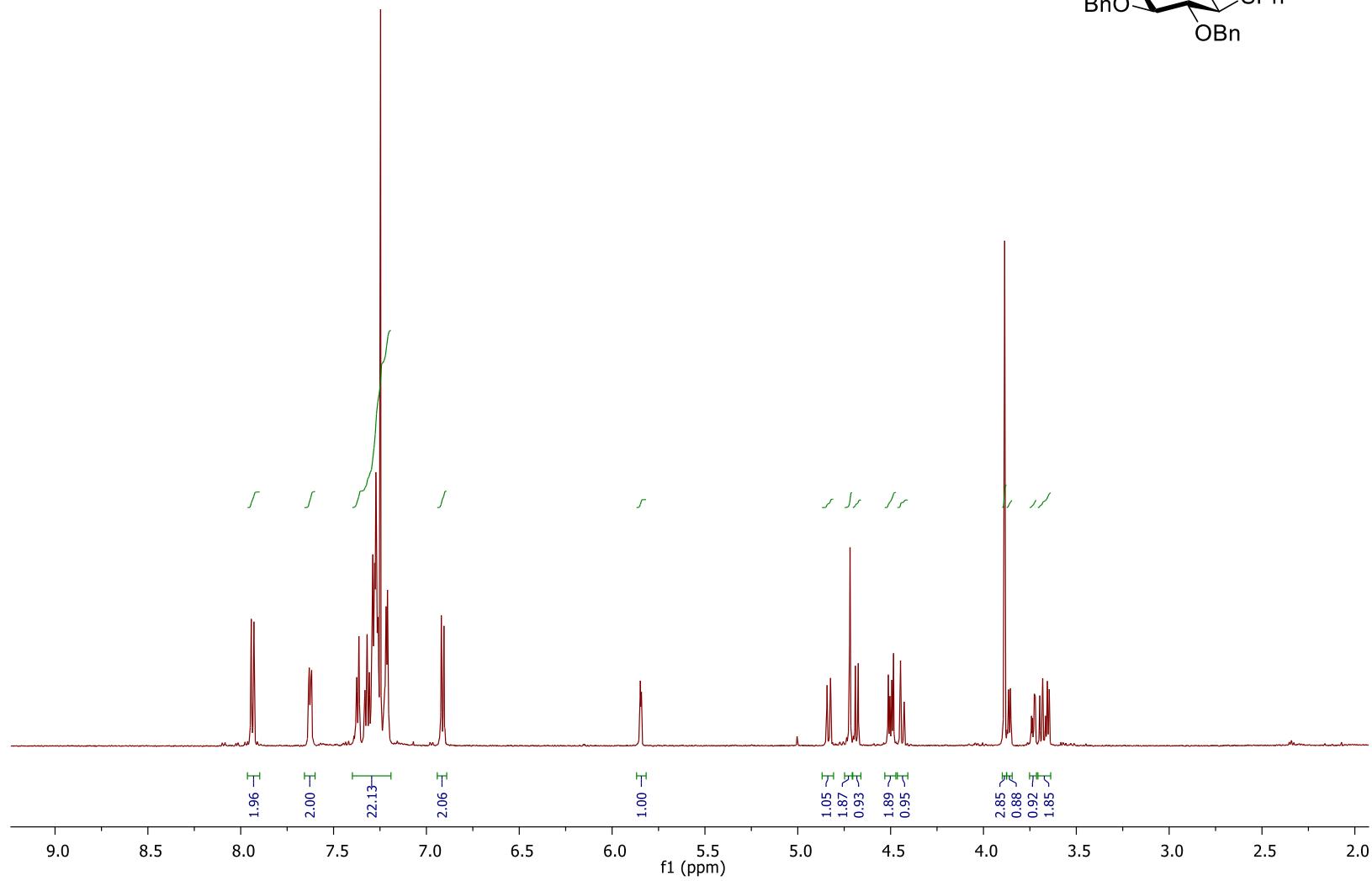
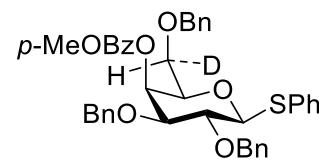
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-(*p*-methoxybenzoyl)-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**19**)



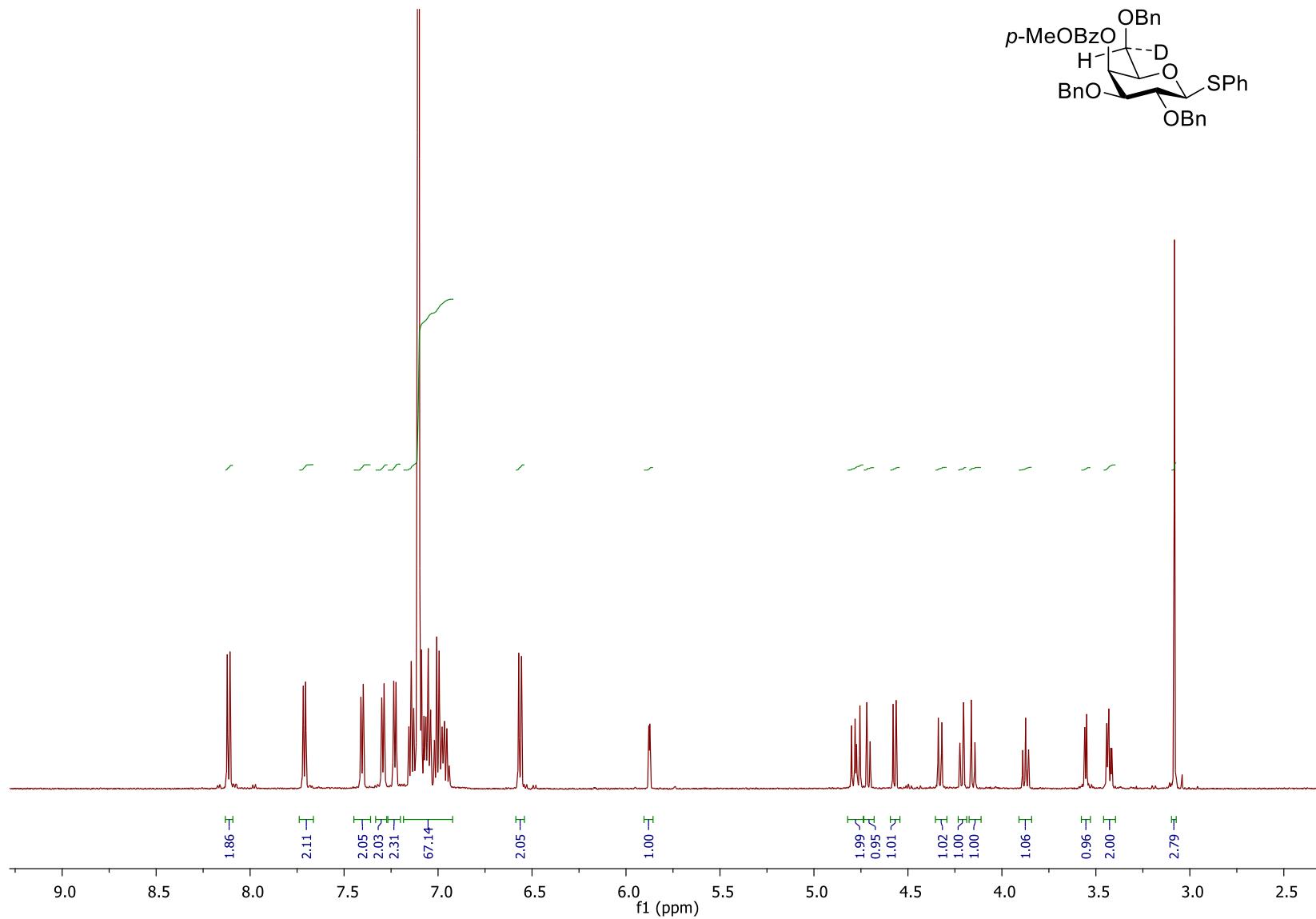
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-(*p*-methoxybenzoyl)-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**19**)



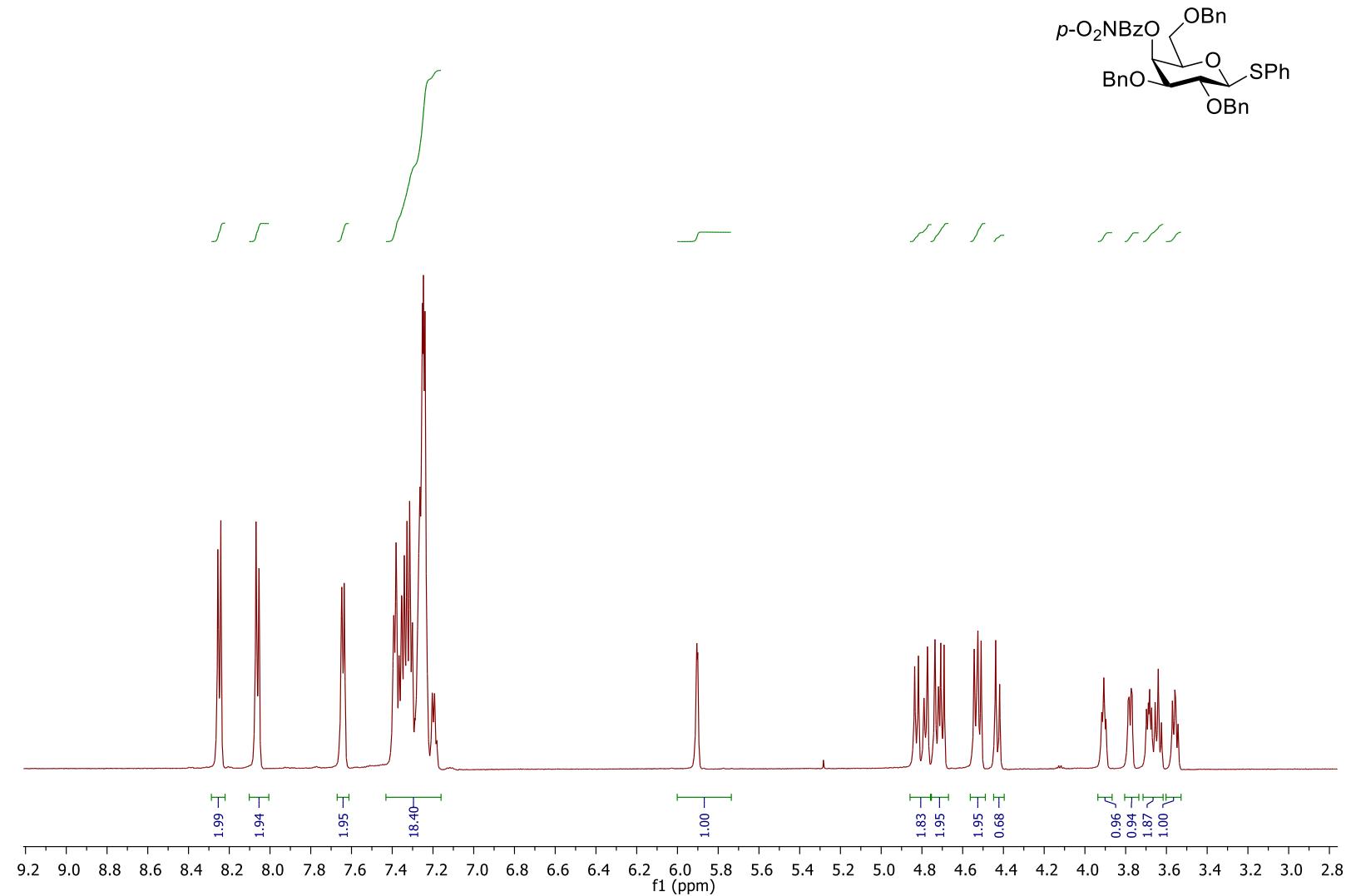
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 4-*O*-(*p*-methoxybenzoyl)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-19**)



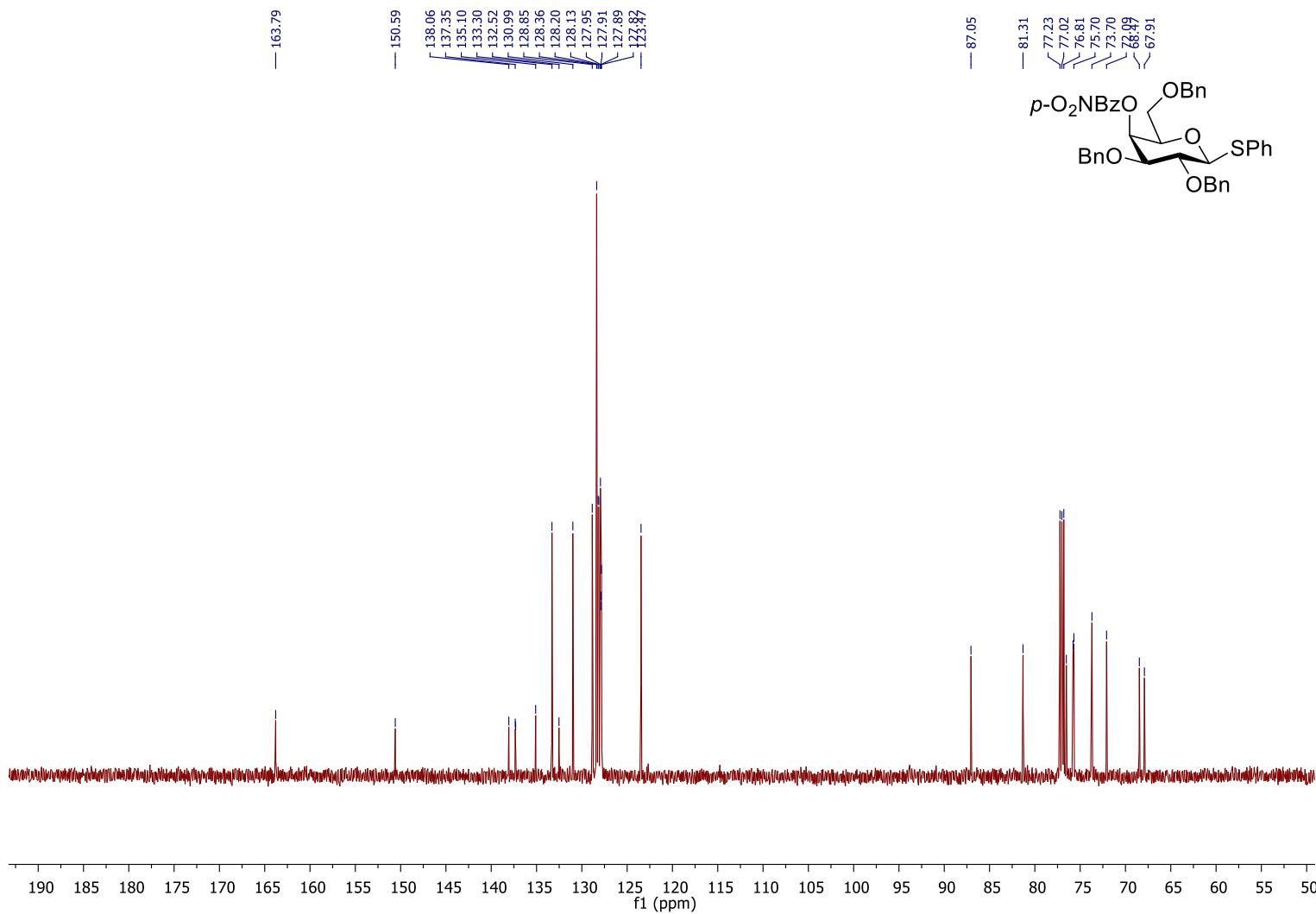
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-O-(*p*-methoxybenzoyl)-(6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-19**)



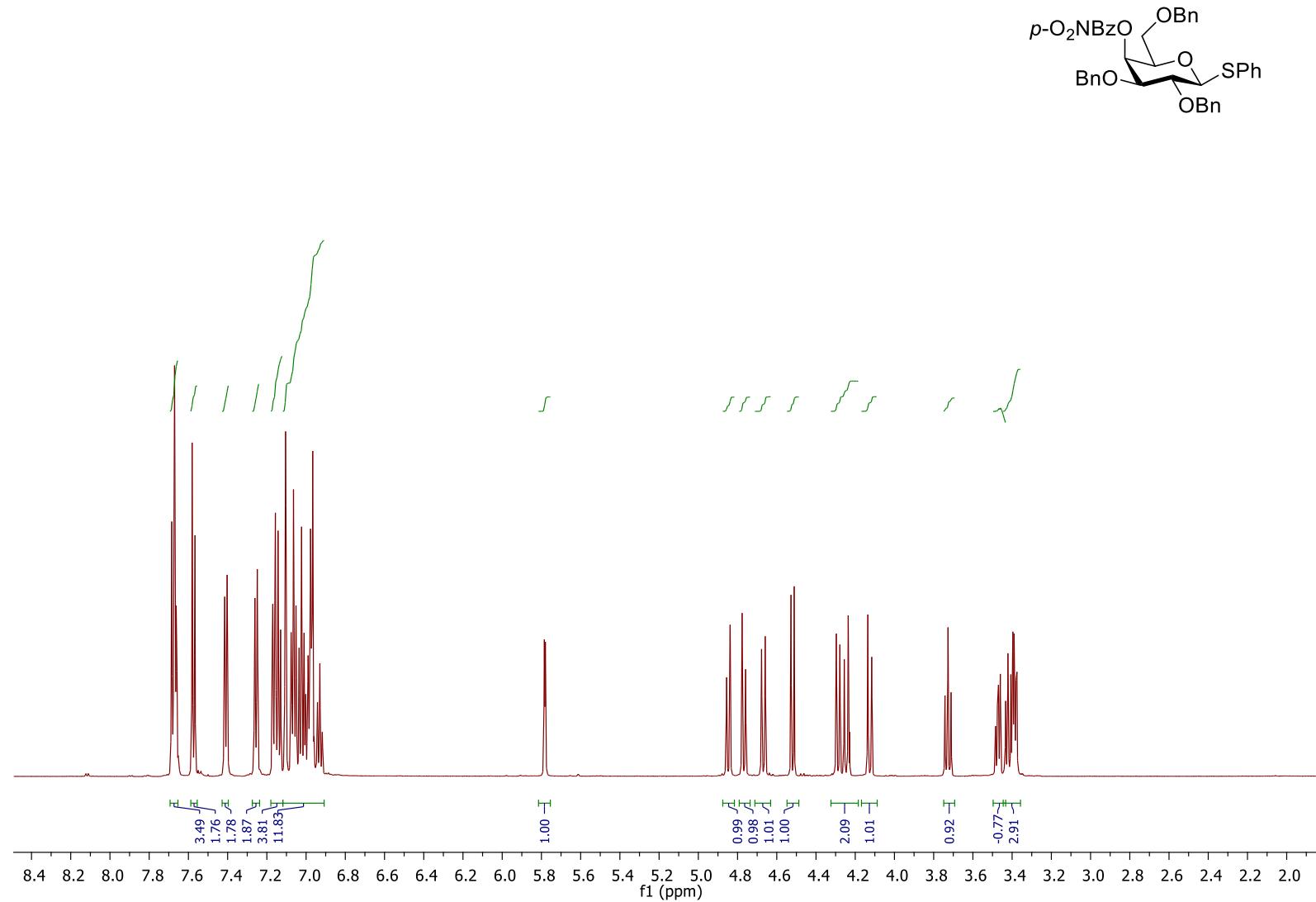
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-(*p*-nitrobenzoyl)-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**20**)



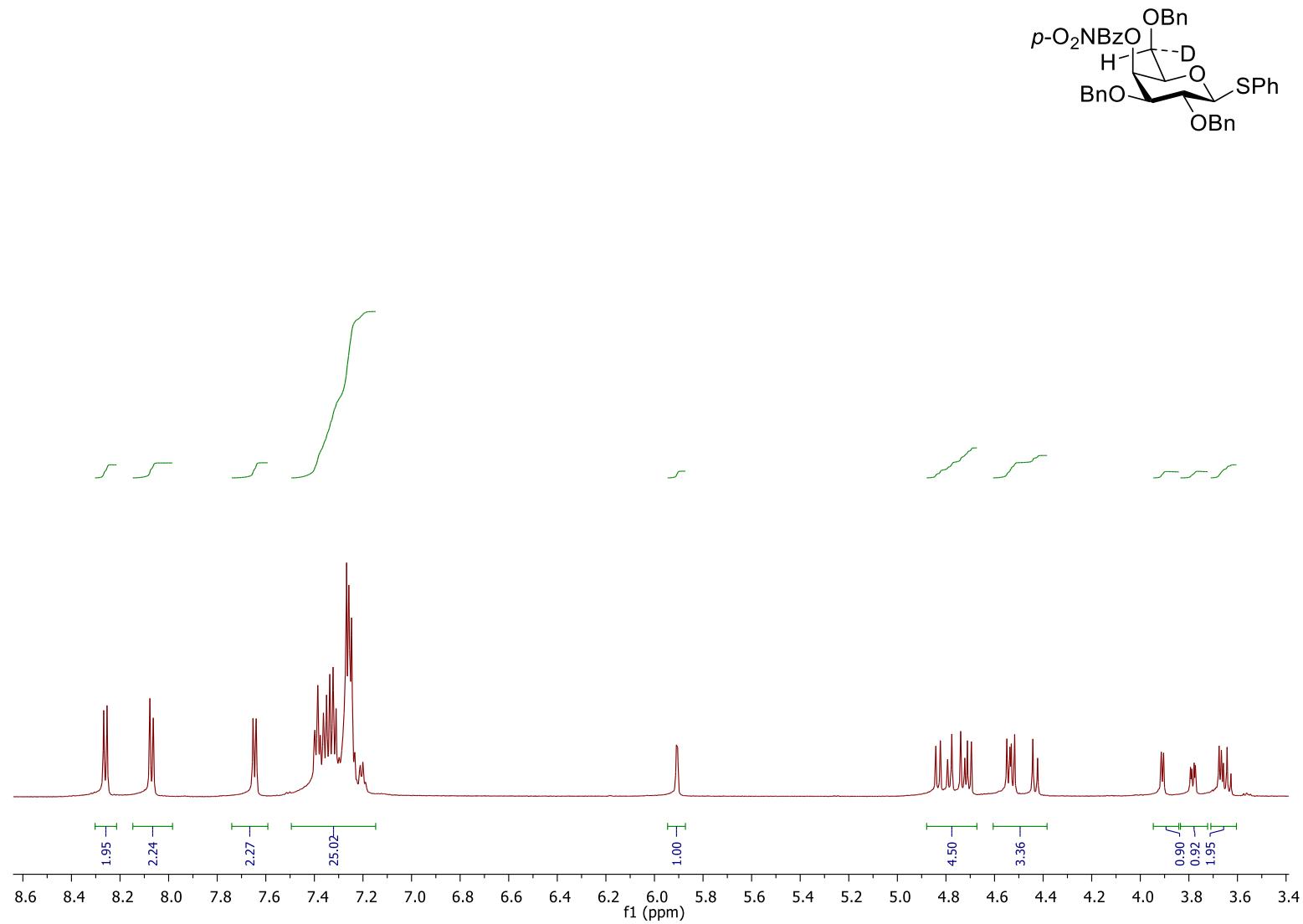
¹³C NMR (150 MHz, CDCl₃) Spectrum of Phenyl 4-O-(*p*-nitrobenzoyl)-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**20**)



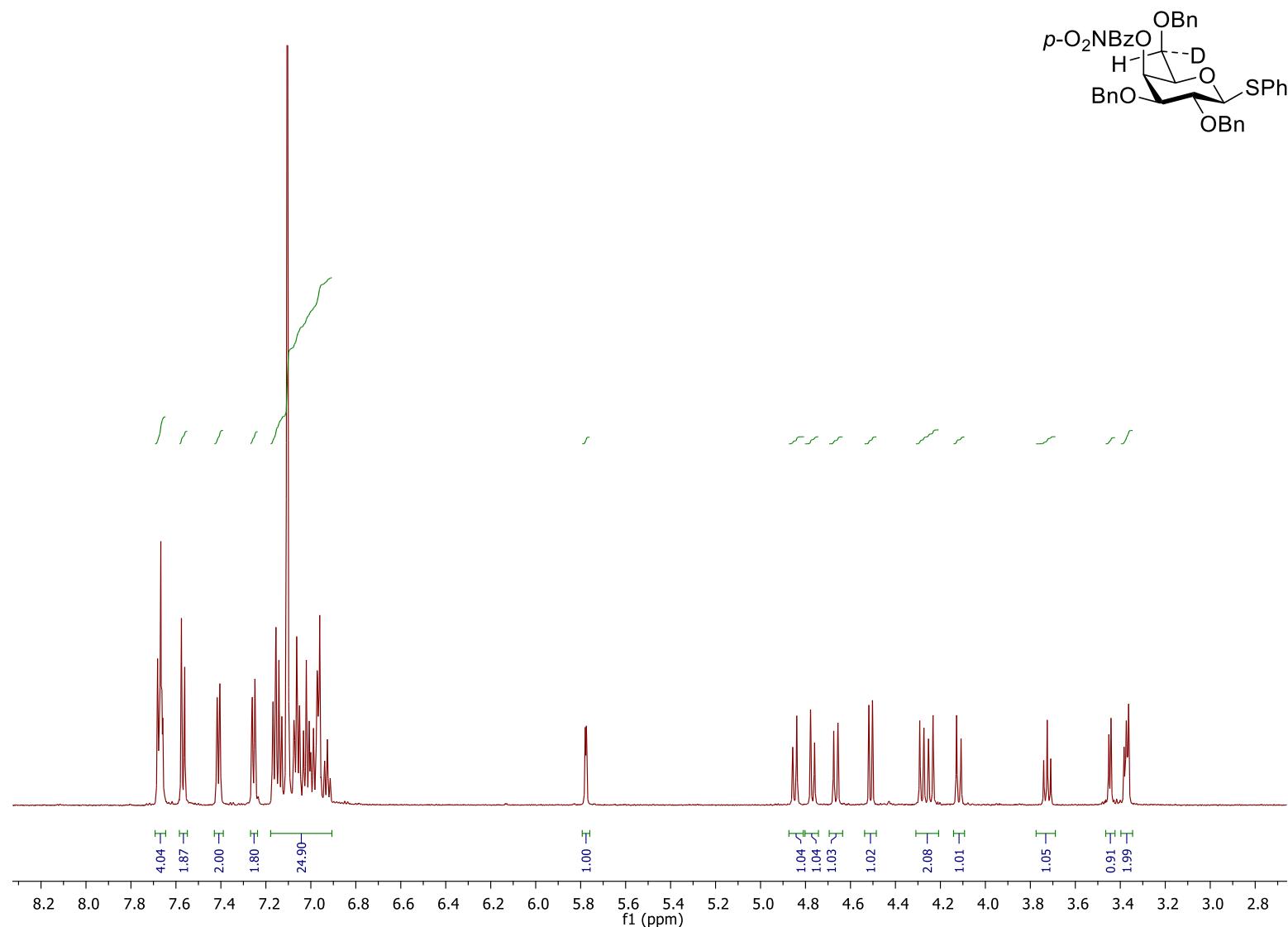
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-O-(*p*-nitrobenzoyl)-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**20**)



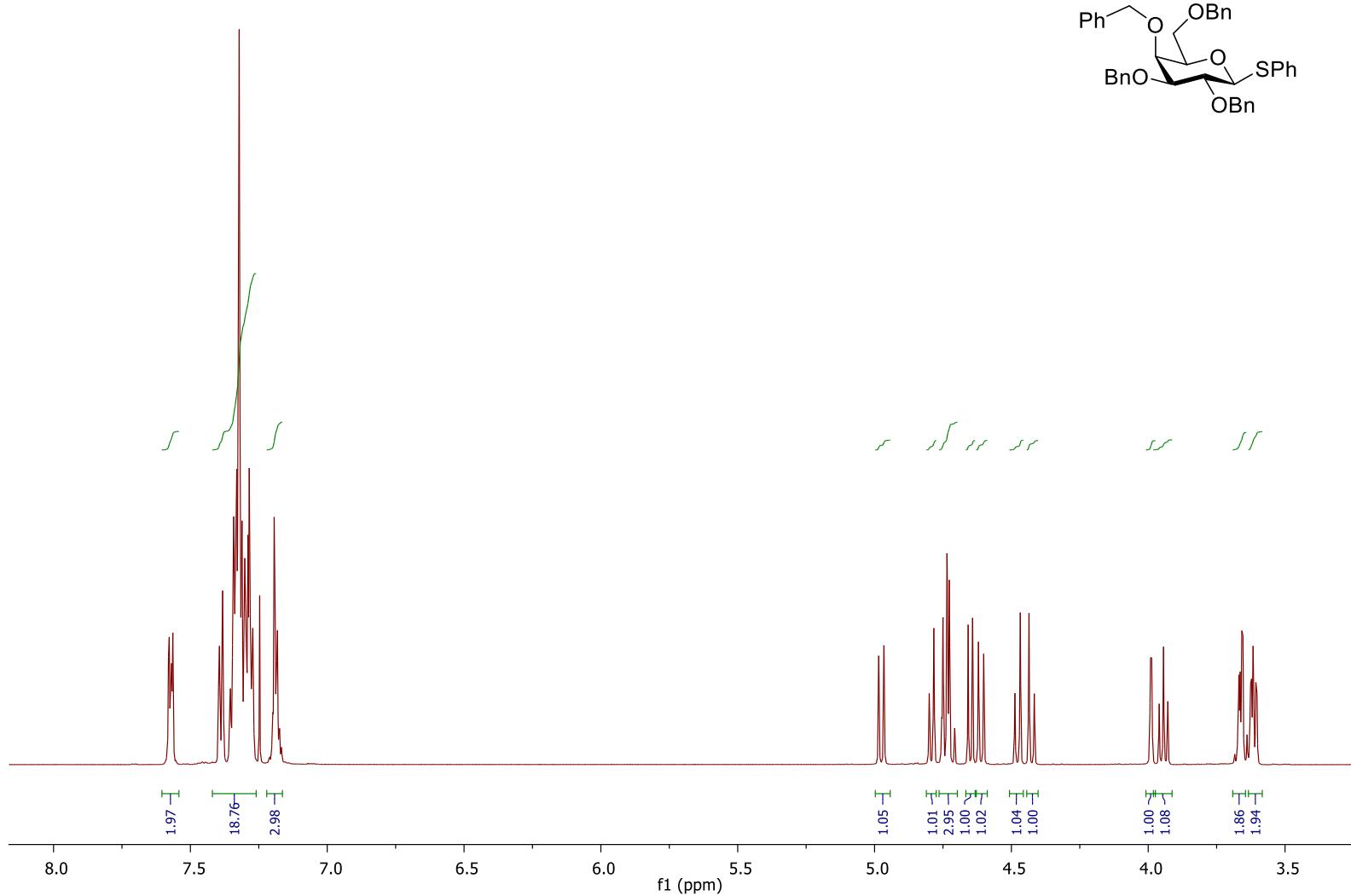
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-O-(*p*-nitrobenzoyl)-(6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-20**)



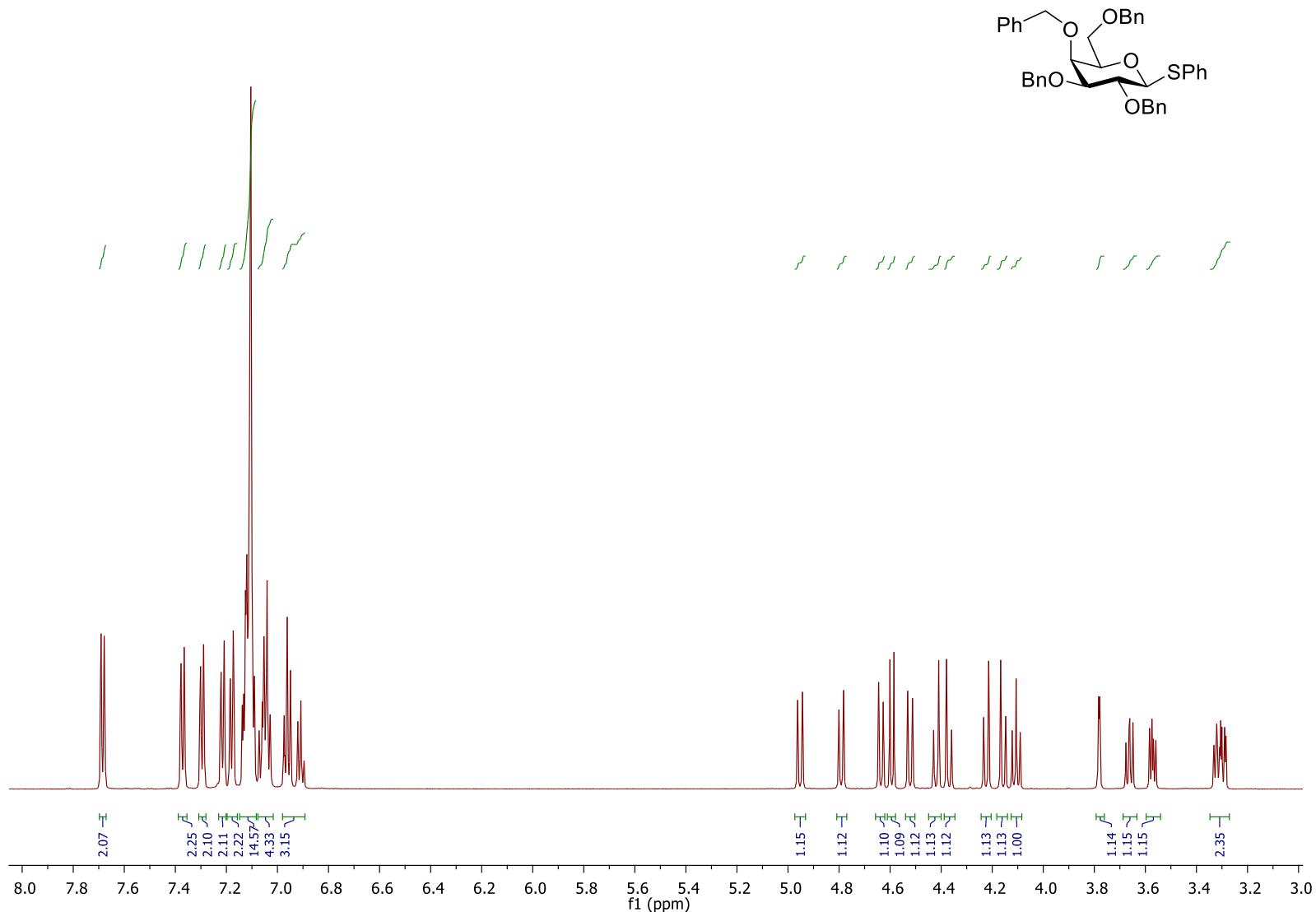
^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl 4-*O*-(*p*-nitrobenzoyl)-(*6S*)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-20**)



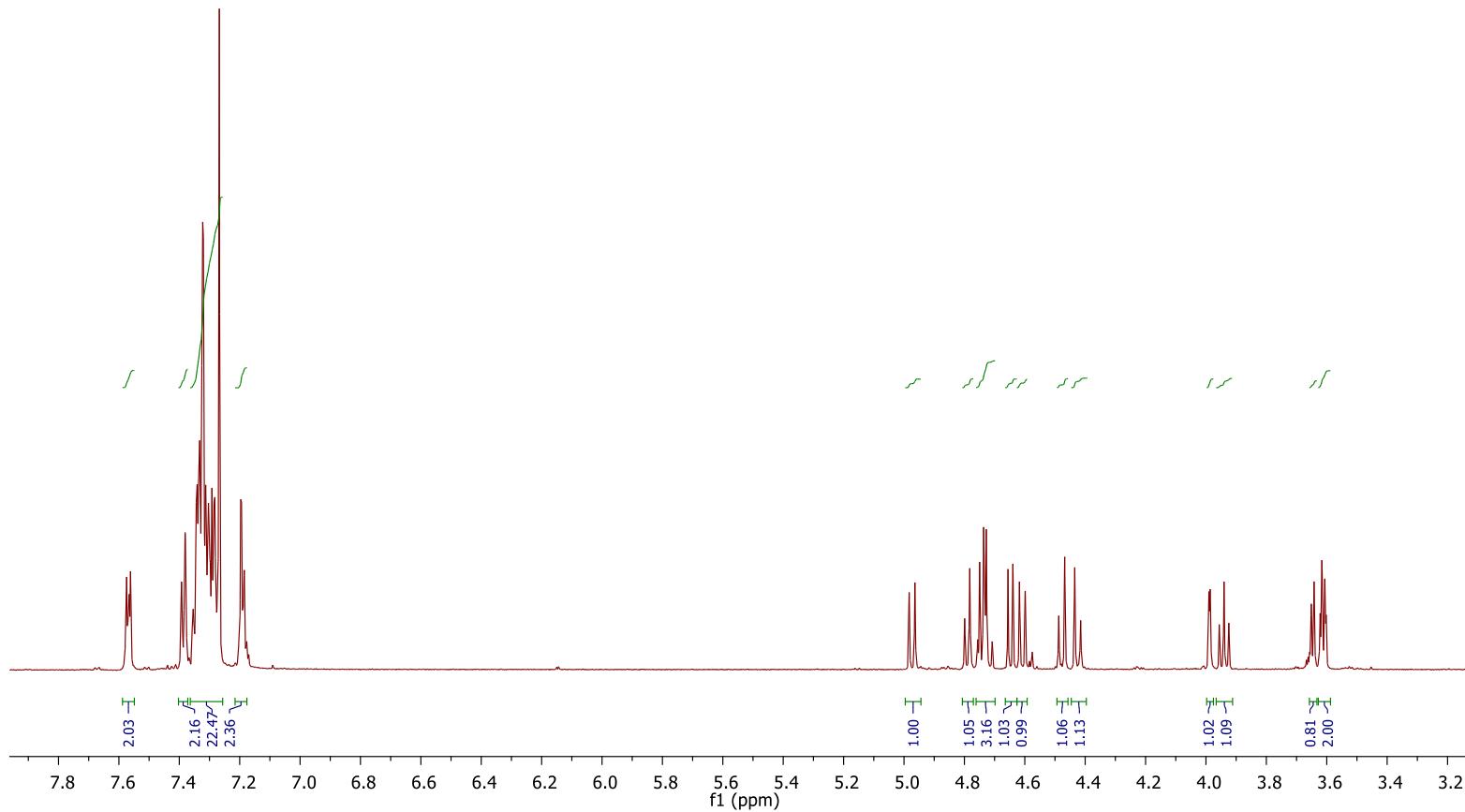
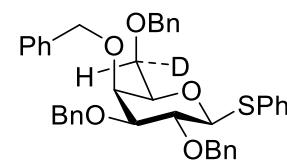
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 2,3,4,6-tetra- O -benzyl-1-thio- β -D-galactopyranoside (**21**)



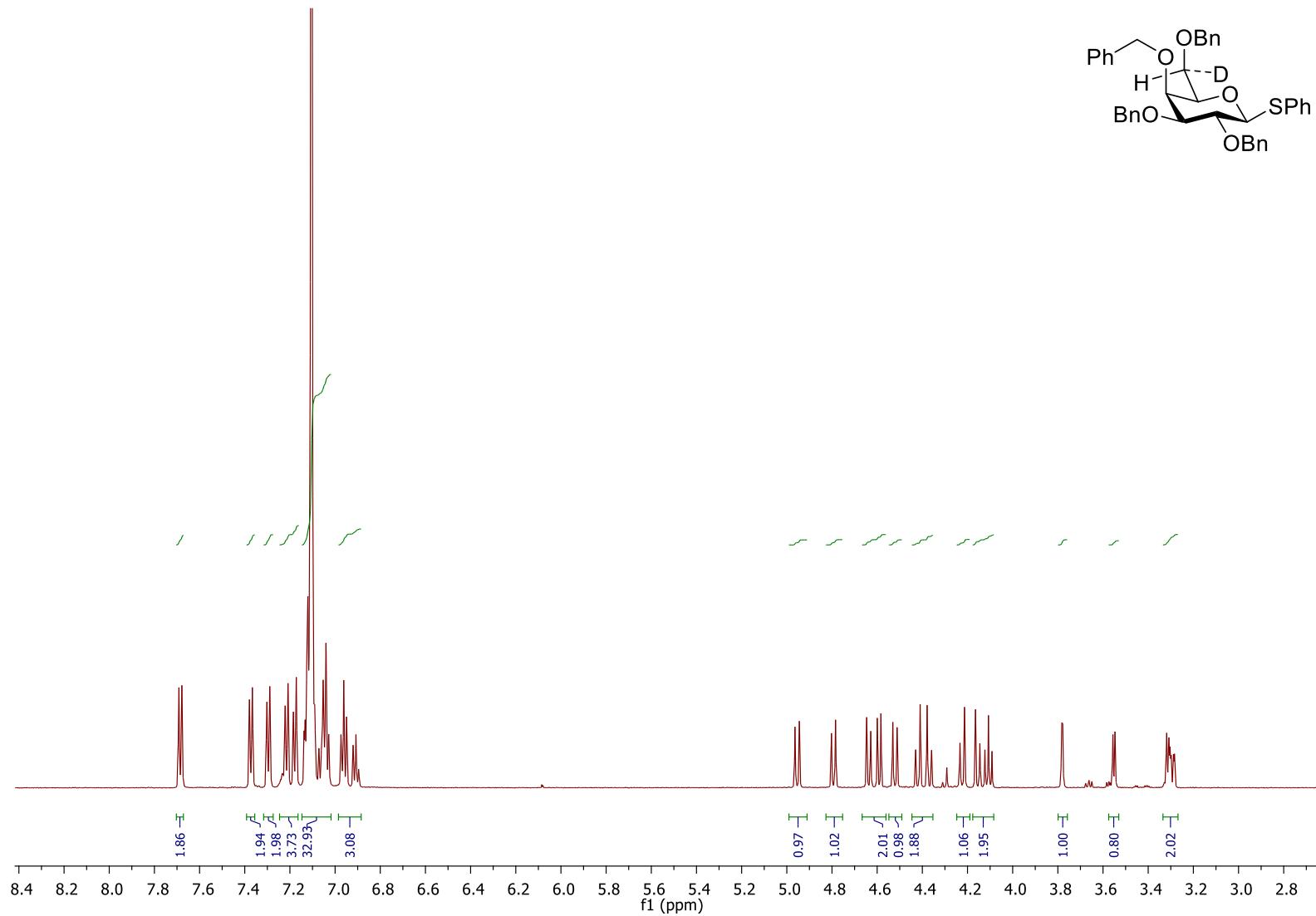
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 2,3,4,6-tetra-O-benzyl-1-thio-β-D-galactopyranoside (**21**)



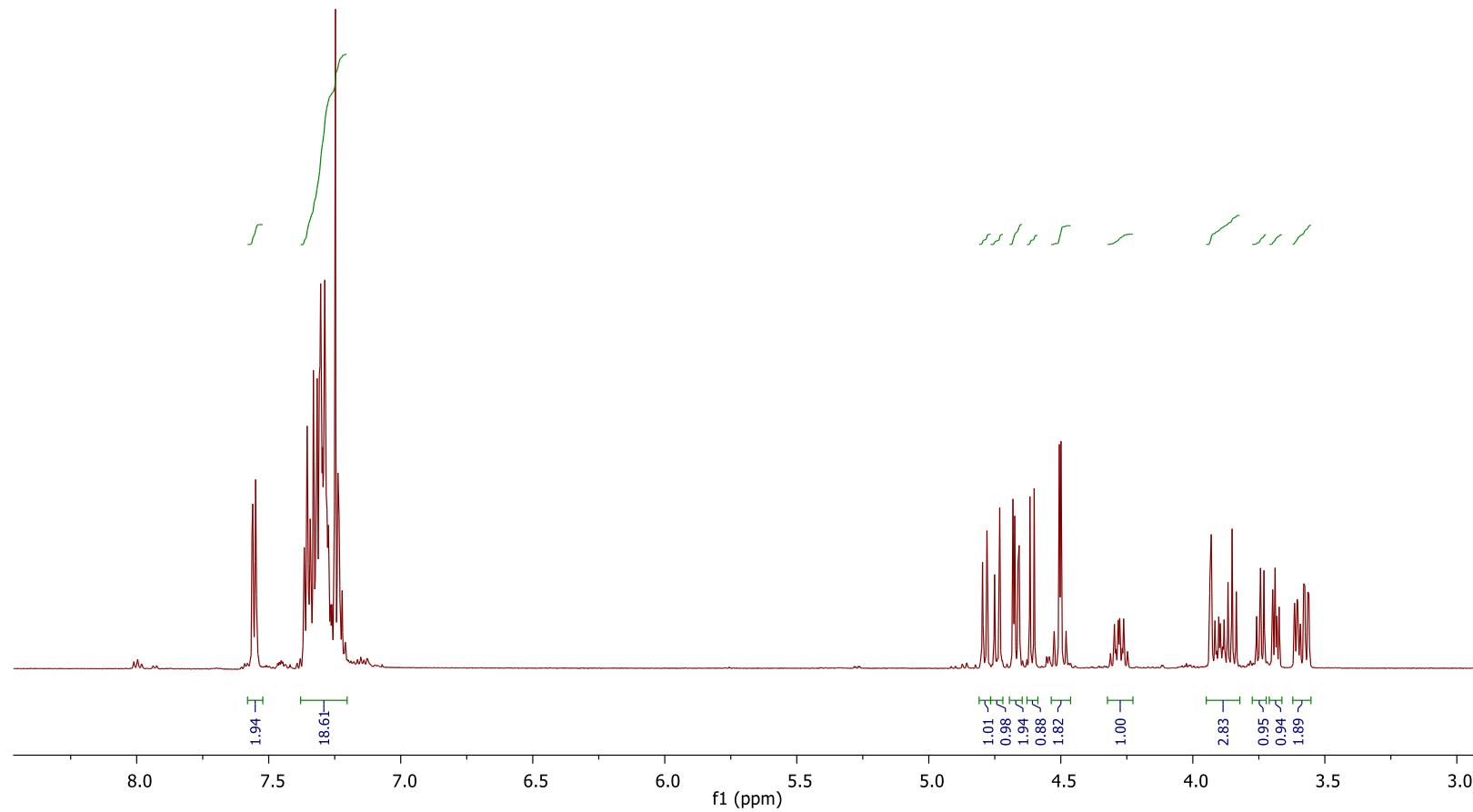
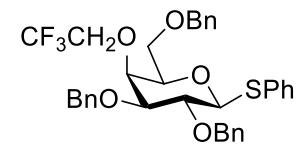
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl (6*S*)-[6- $^2\text{H}_1$]-2,3,4,6-tetra-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-21**)



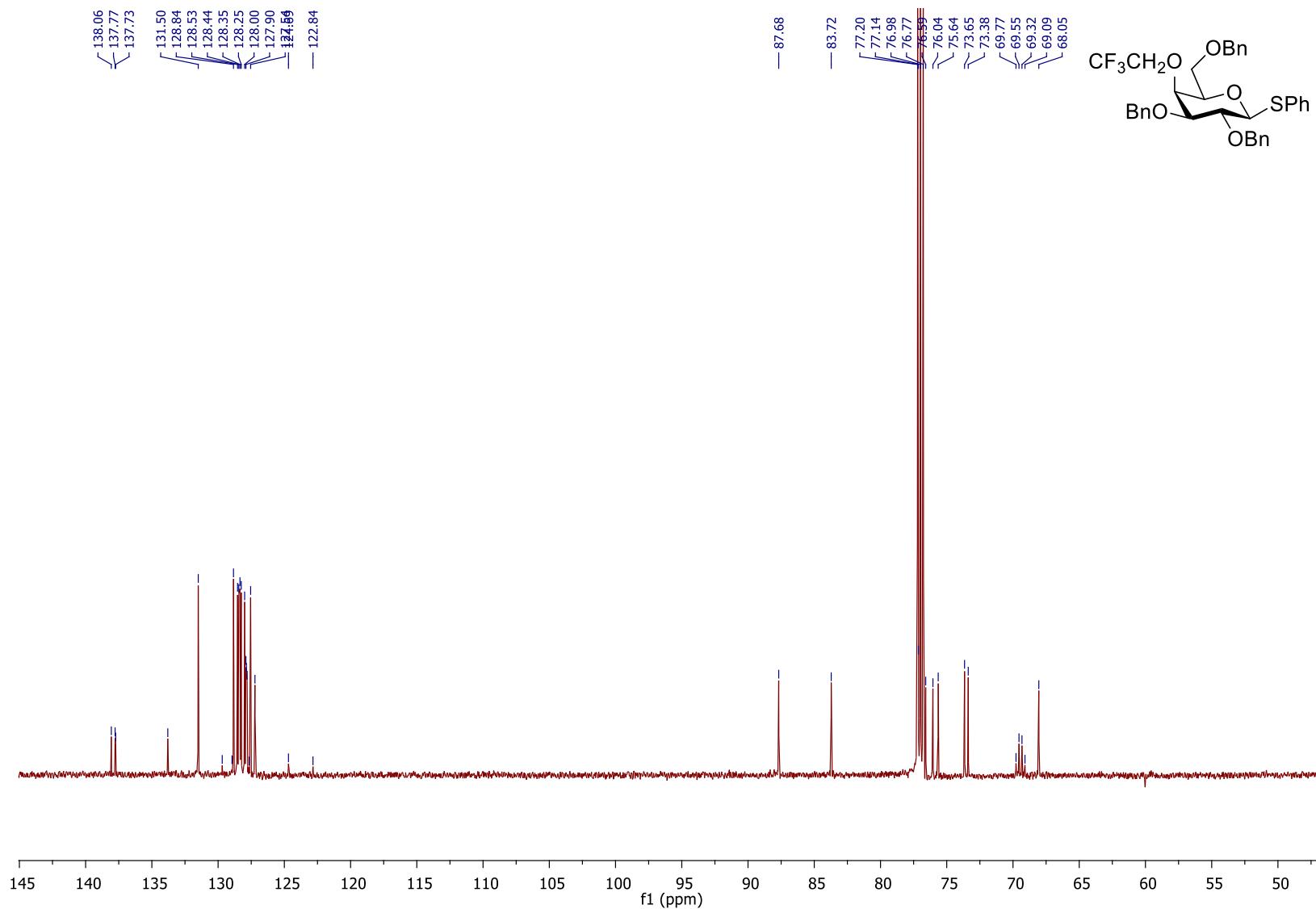
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl (6*S*)-[6-²H₁]-2,3,4,6-tetra-*O*-benzyl-1-thio- β -D-galactopyranoside (**6S-D-21**)



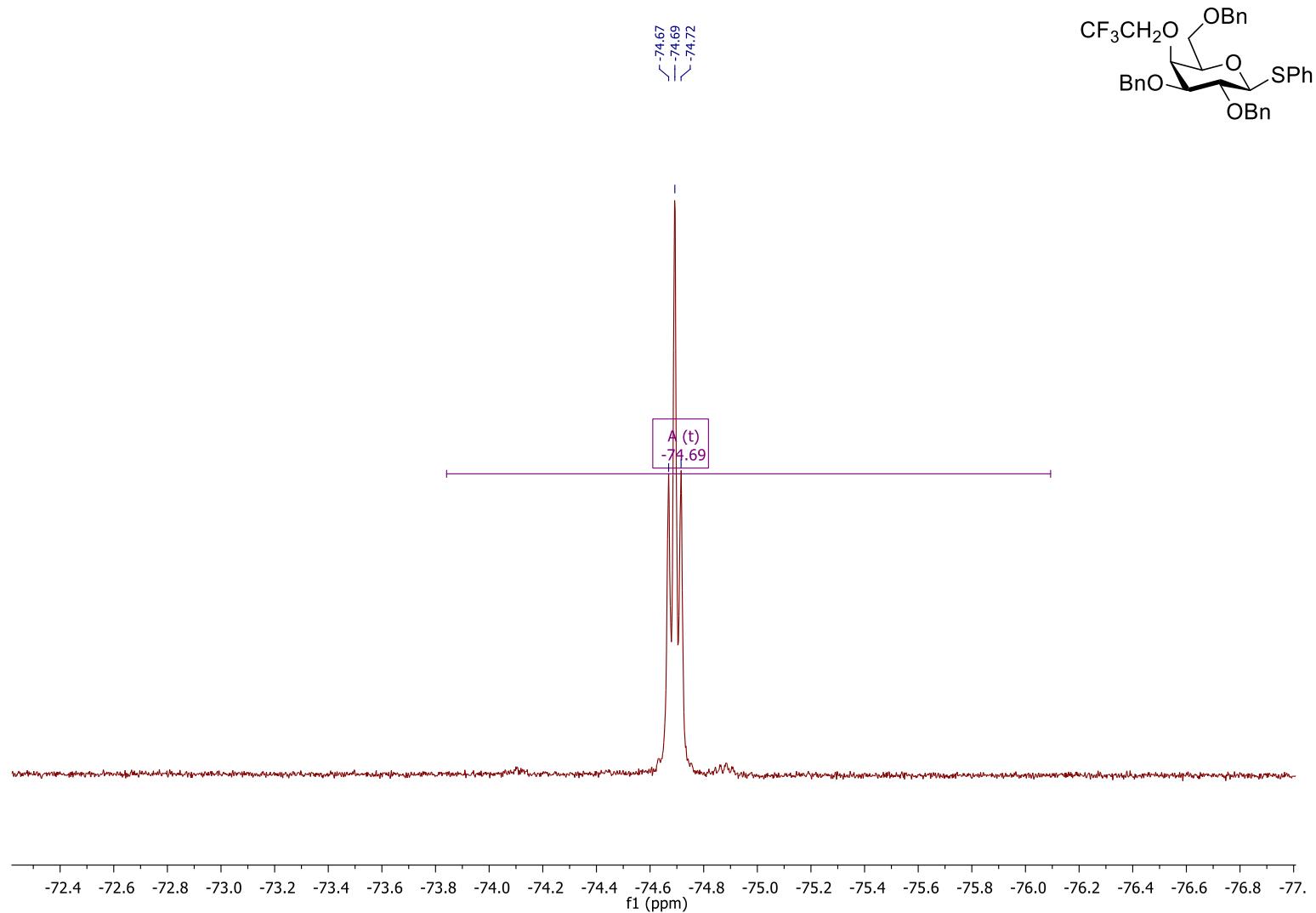
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-(1',1',1'-trifluoroethyl)-1-thio- β -D-galactopyranoside (**22**)



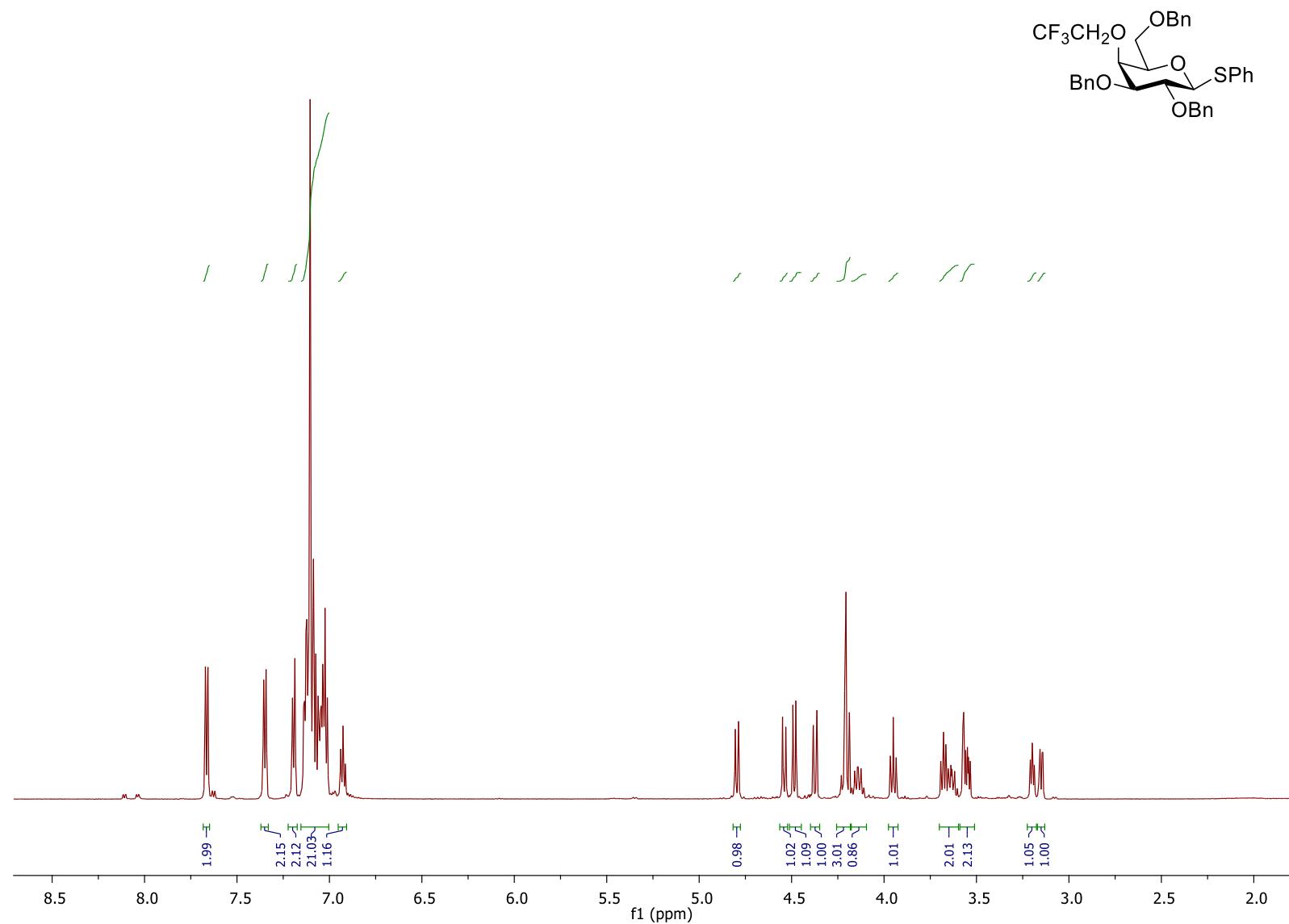
¹³C NMR (150 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-(1',1',1'-trifluoroethyl)-1-thio- β -D-galactopyranoside (**22**)



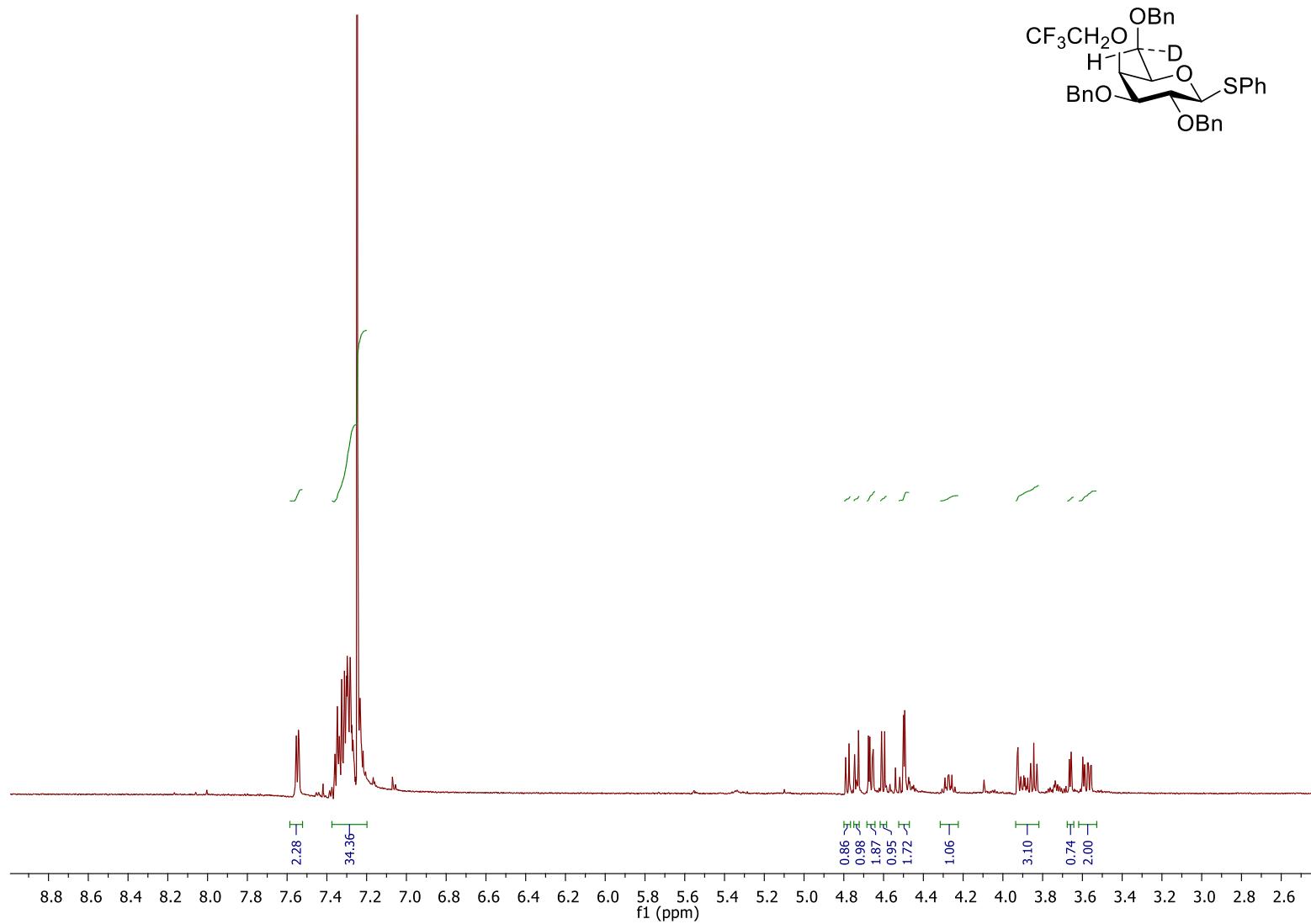
¹⁹F NMR (375 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-(1',1',1'-trifluoroethyl)-1-thio- β -D-galactopyranoside (**22**)



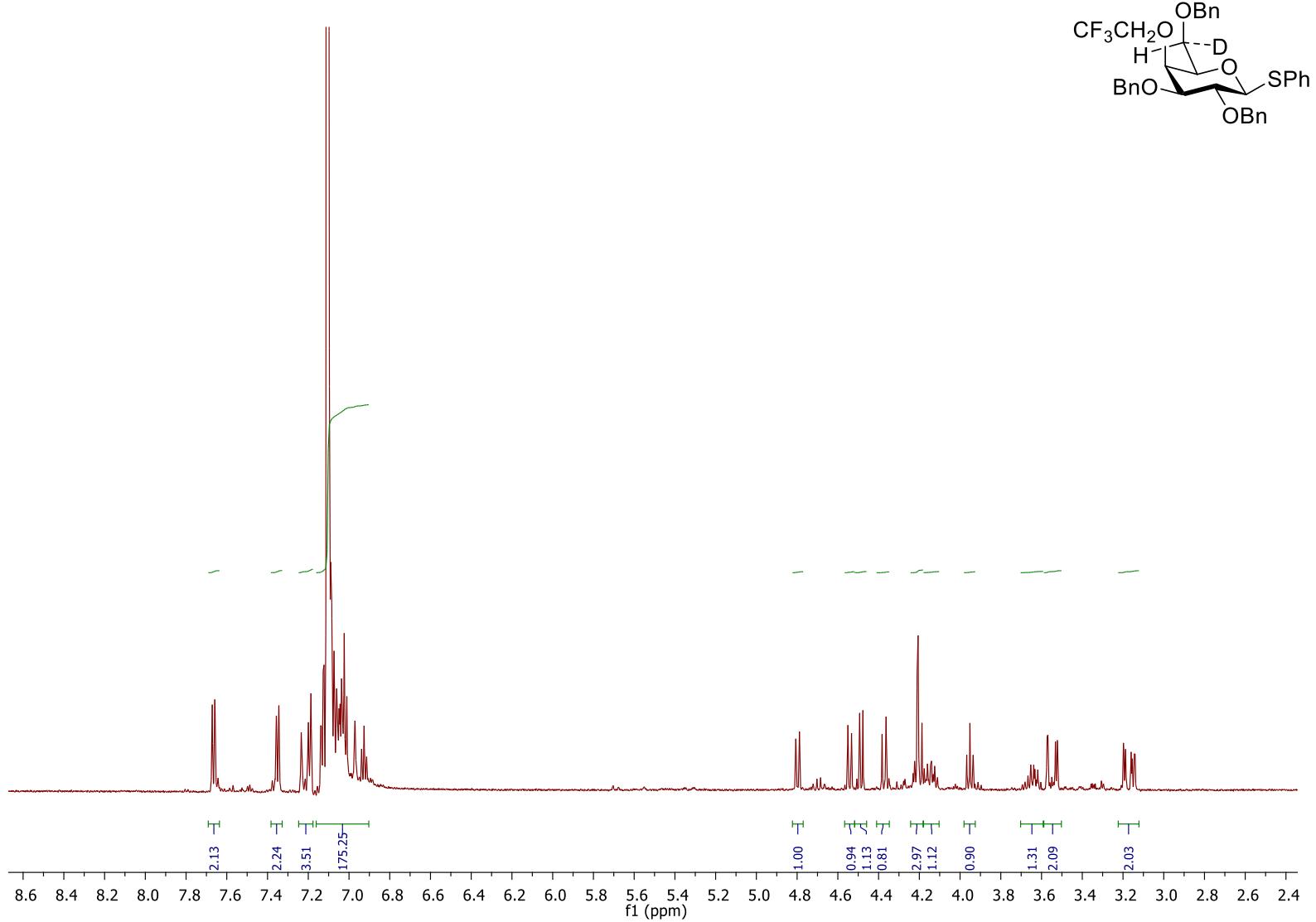
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 2,3,6-tri-O-benzyl-4-O-(1',1',1'-trifluoroethyl)-1-thio-β-D-galactopyranoside (**22**)



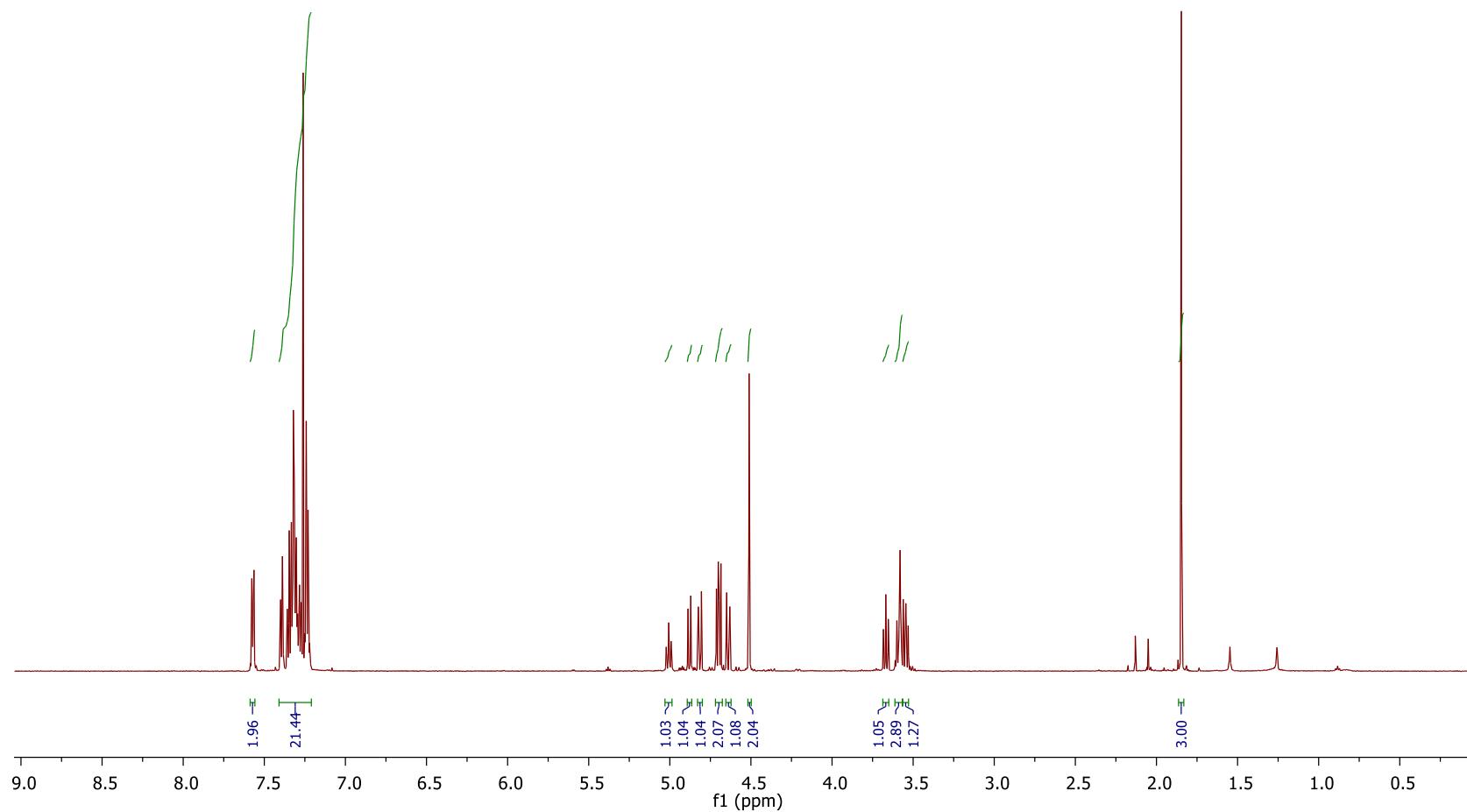
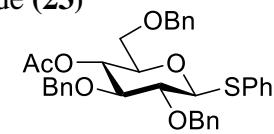
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl (6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-4-*O*-(1',1',1'-trifluoroethyl)-1-thio- β -D-galactopyranoside (**6S-D-22**)



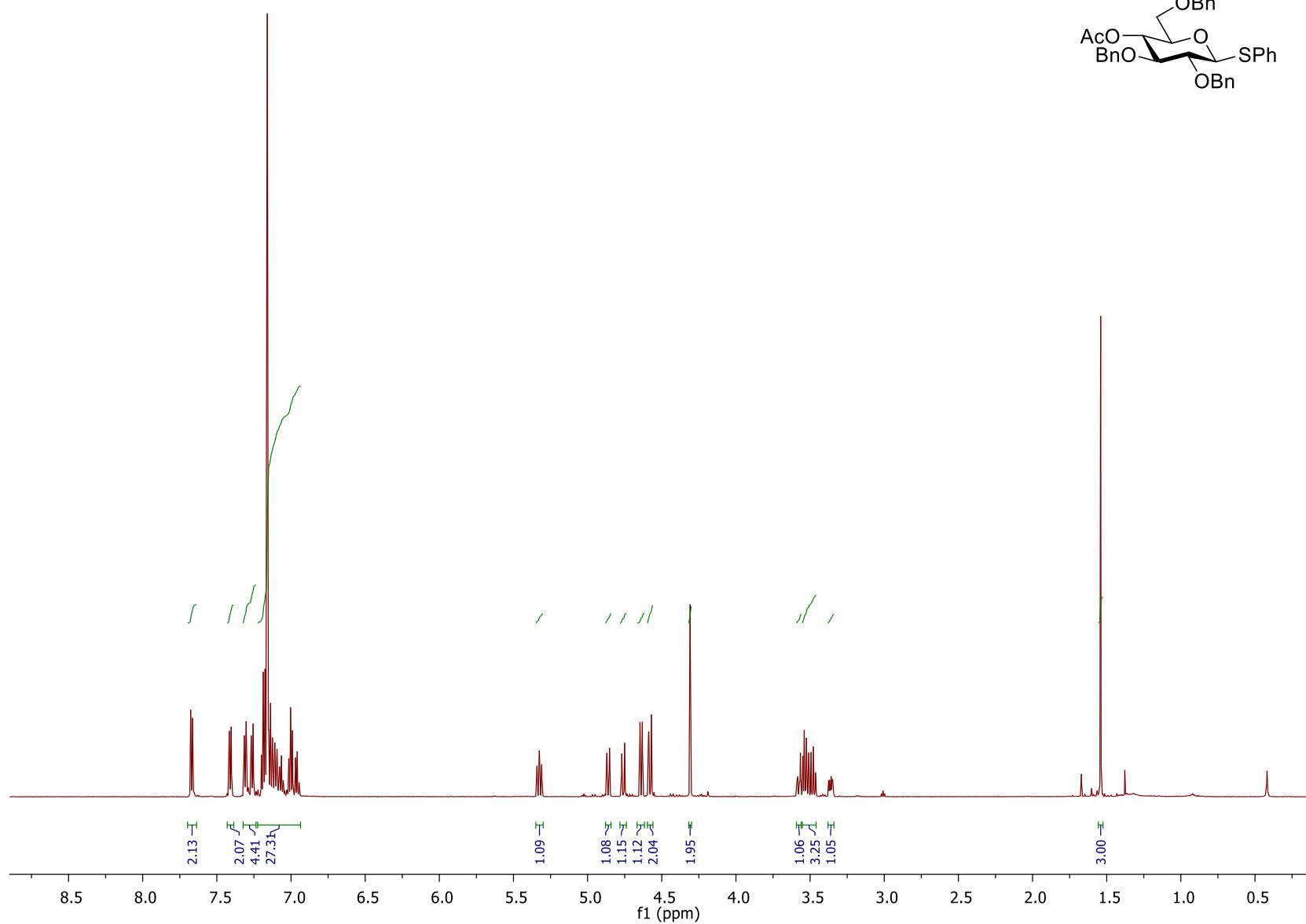
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl (6S)-[6-²H₁]-2,3,6-tri-O-benzyl-4-O-(1',1',1'-trifluoroethyl)-1-thio-β-D-galactopyranoside (**6S-D-22**)



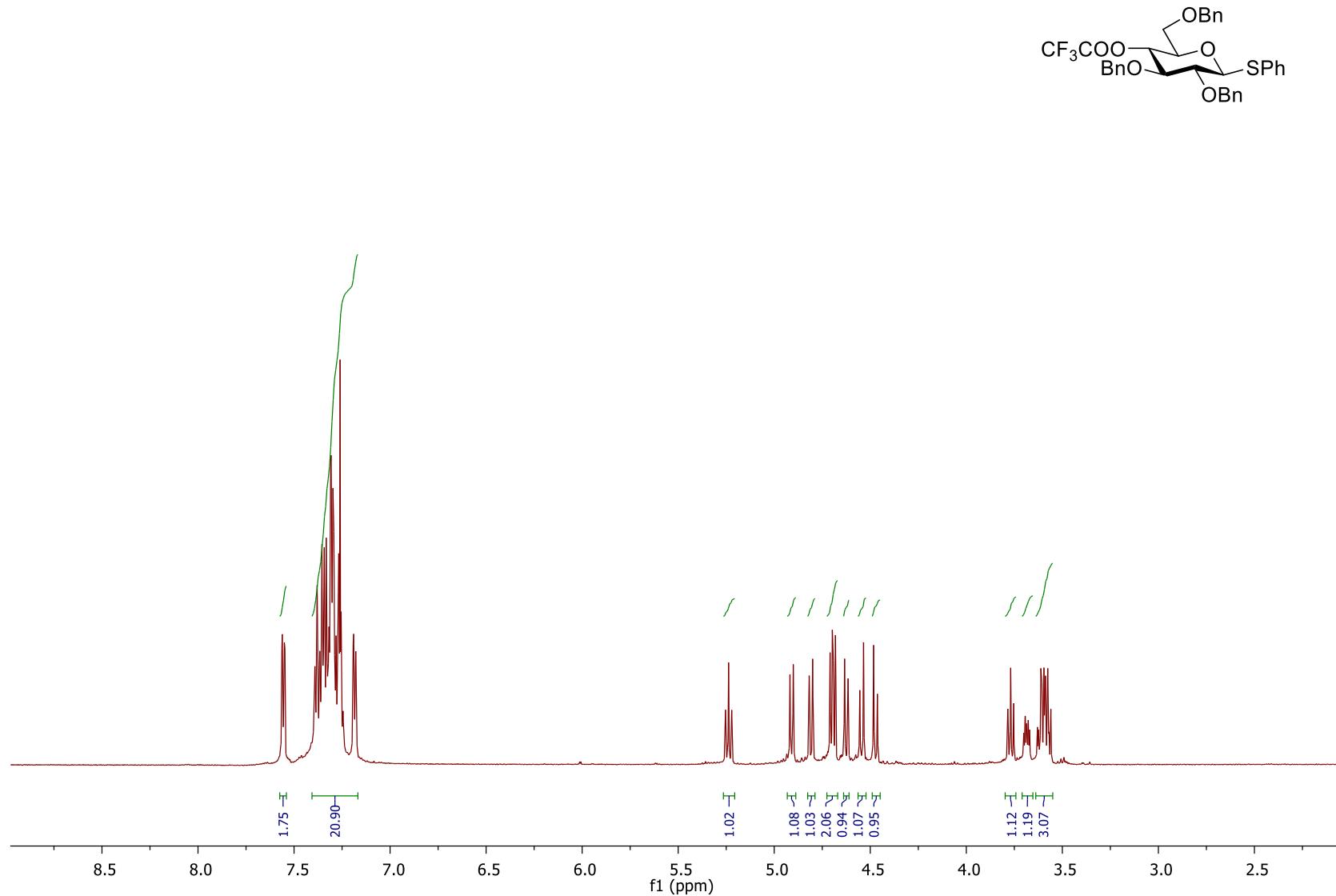
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-acetyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**23**)



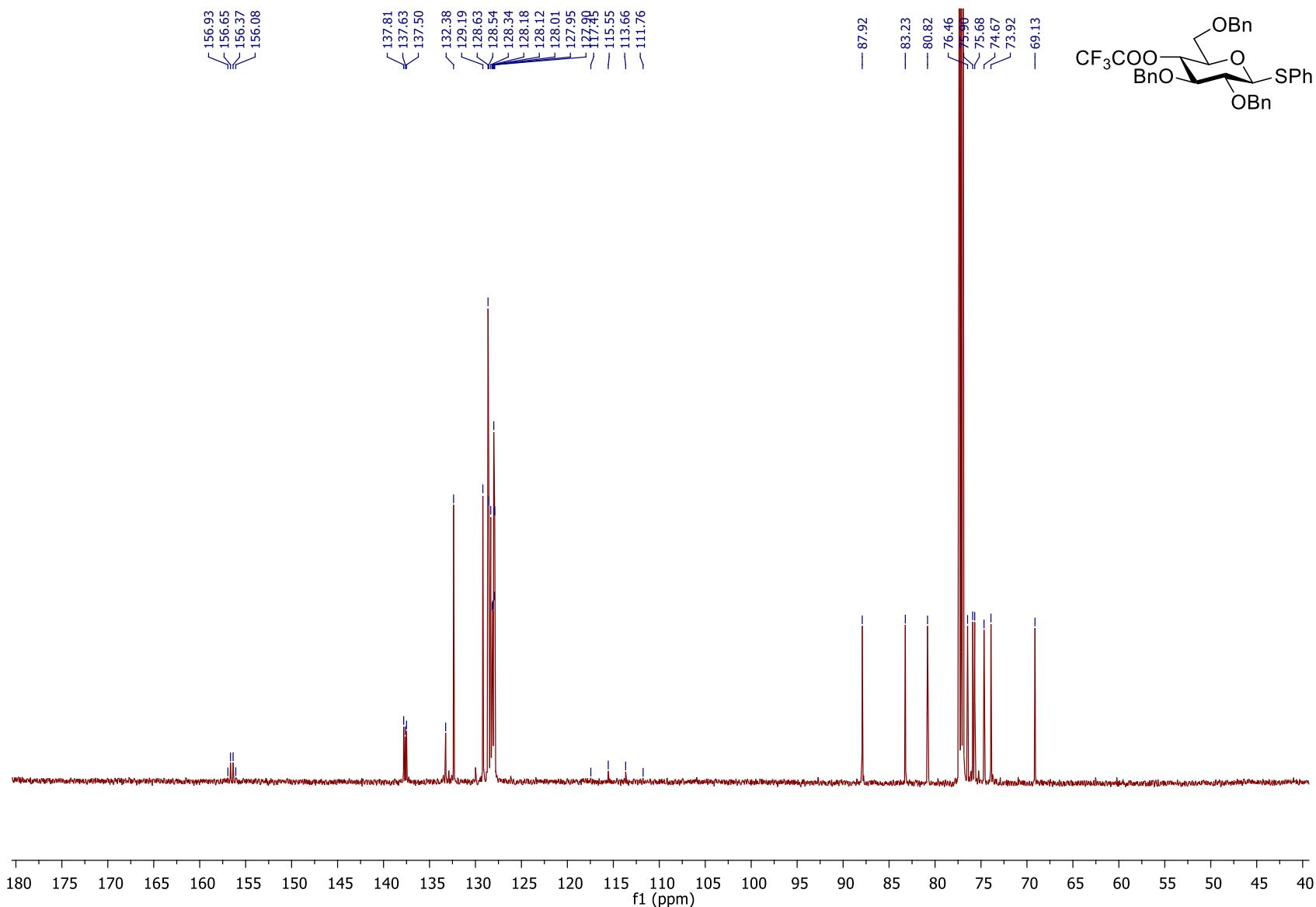
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-acetyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**23**)



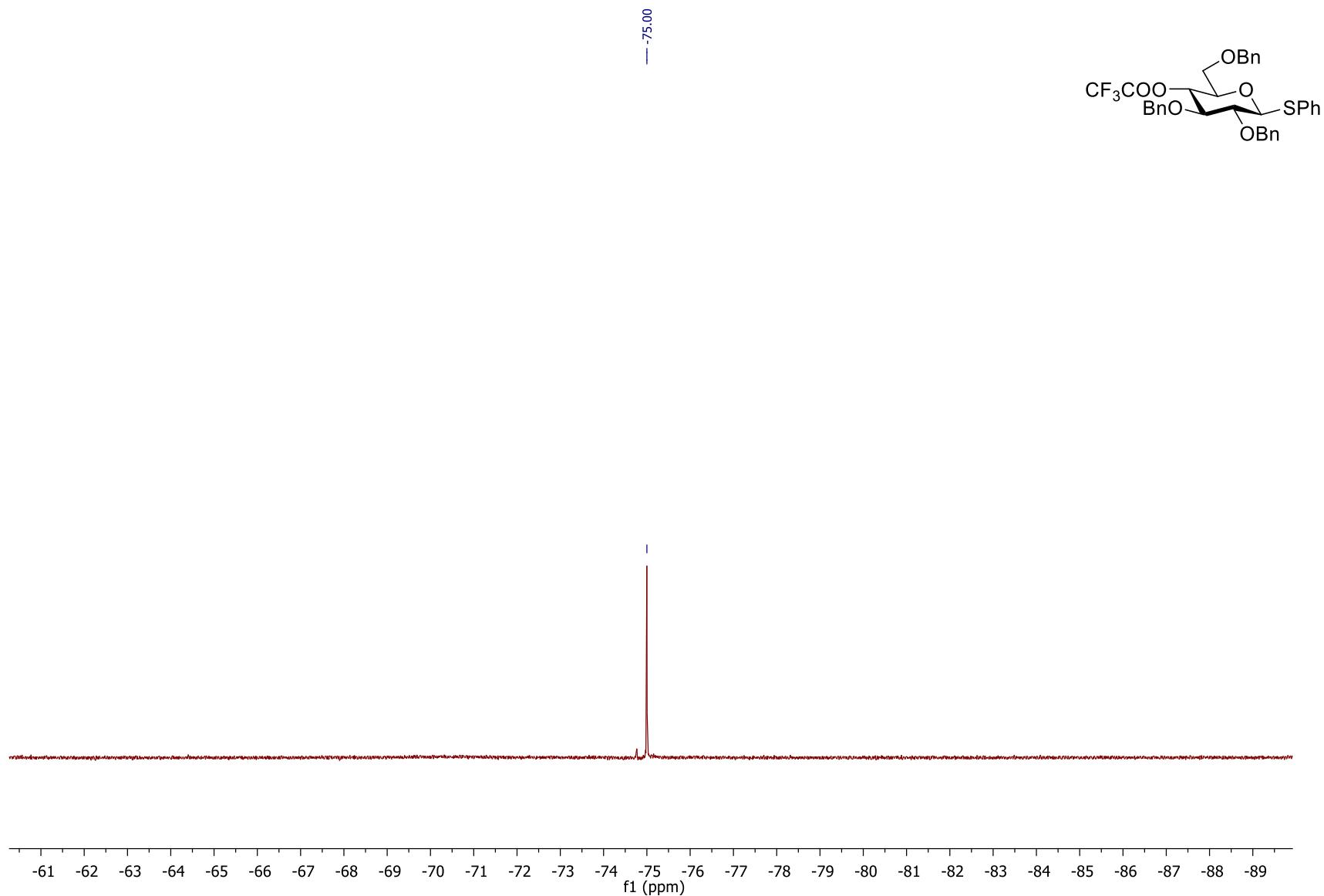
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 2,3,6-tri- O -benzyl-4- O -trifluoroacetyl-1-thio- β -D-glucopyranoside (**24**)



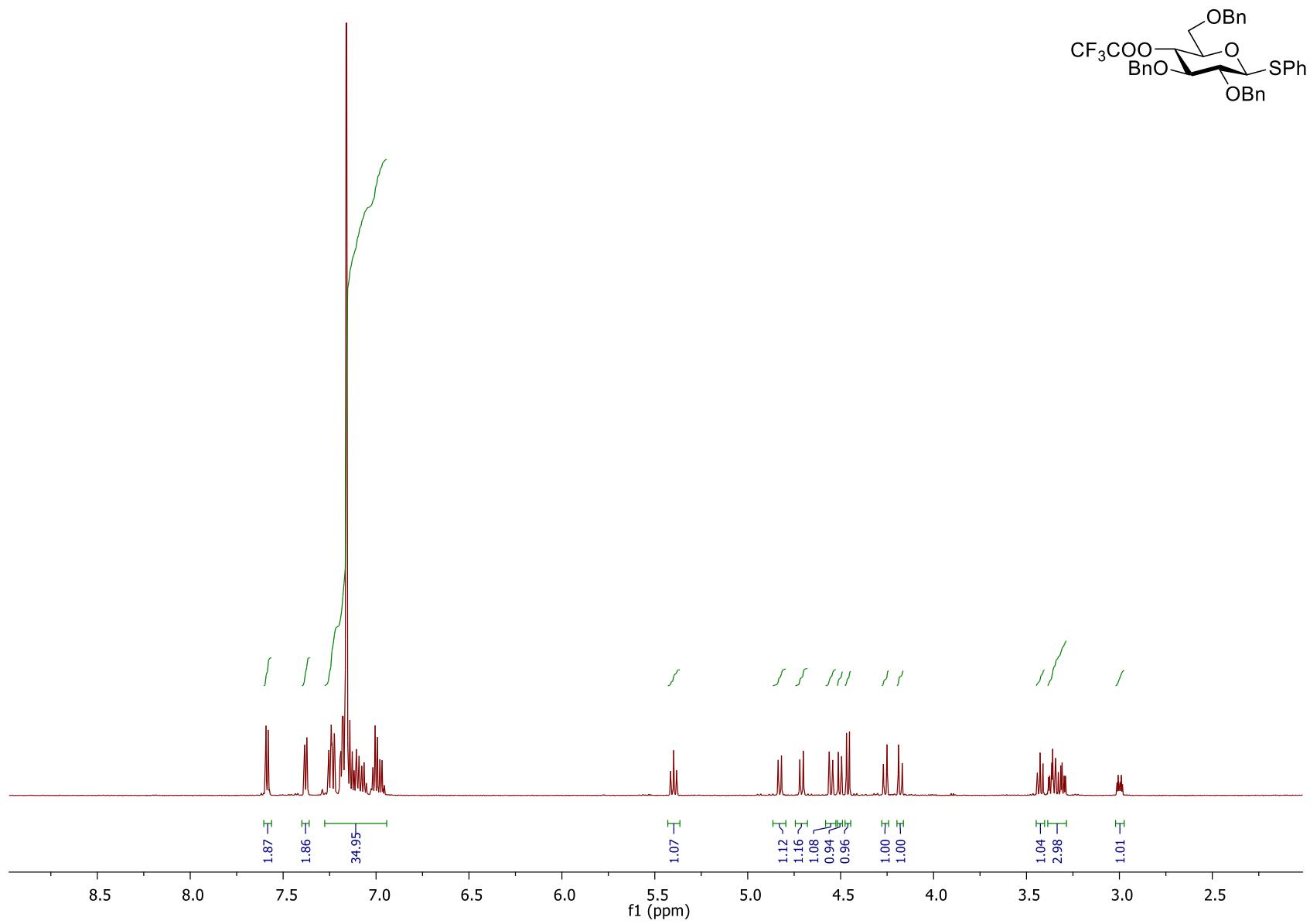
¹³C NMR (150 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-trifluoroacetyl-1-thio- β -D-glucopyranoside (**24**)



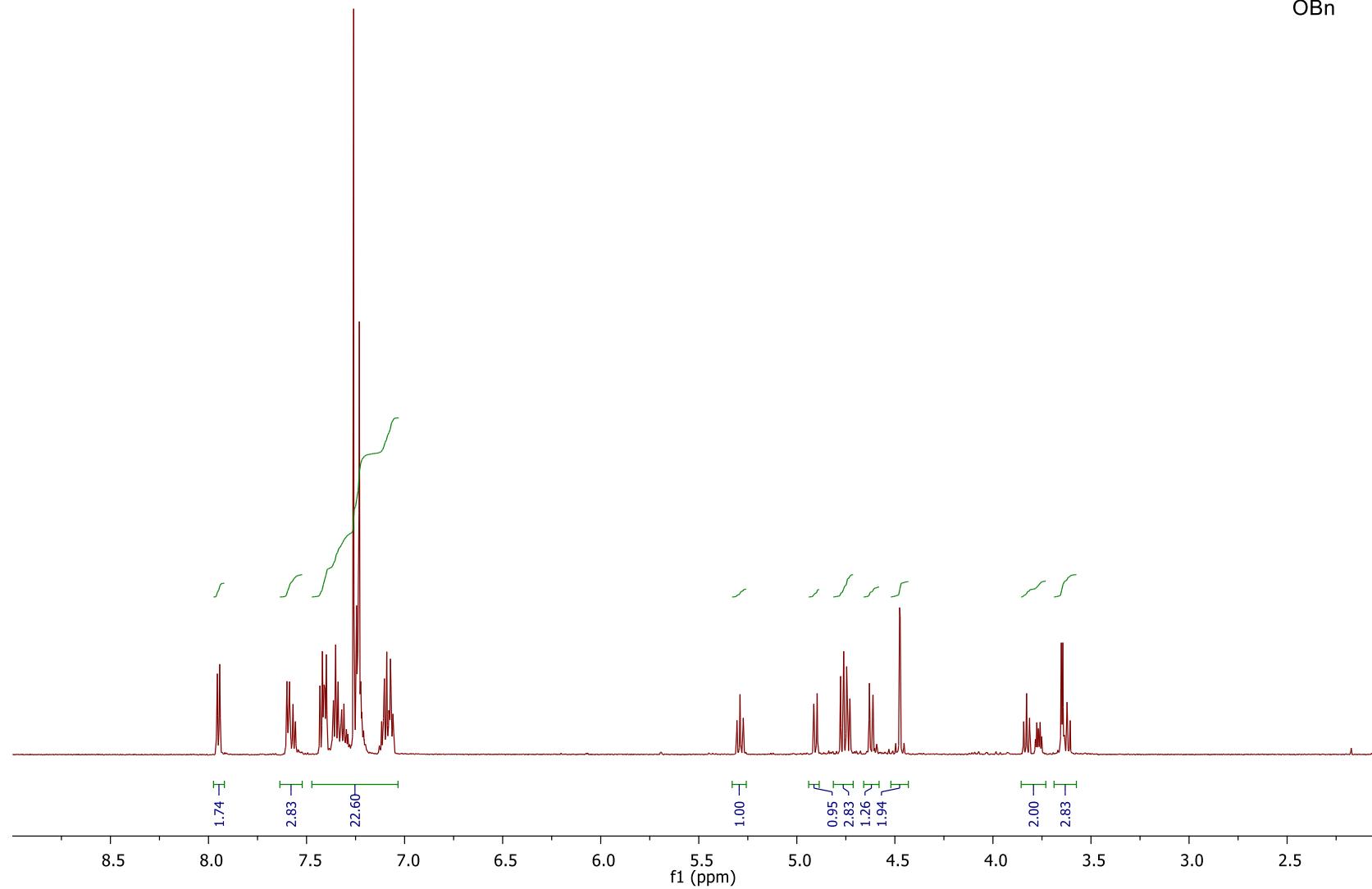
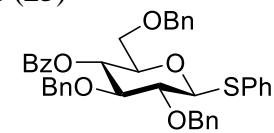
¹⁹F NMR (376 MHz, CDCl₃) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-trifluoroacetyl-1-thio- β -D-glucopyranoside (**24**)



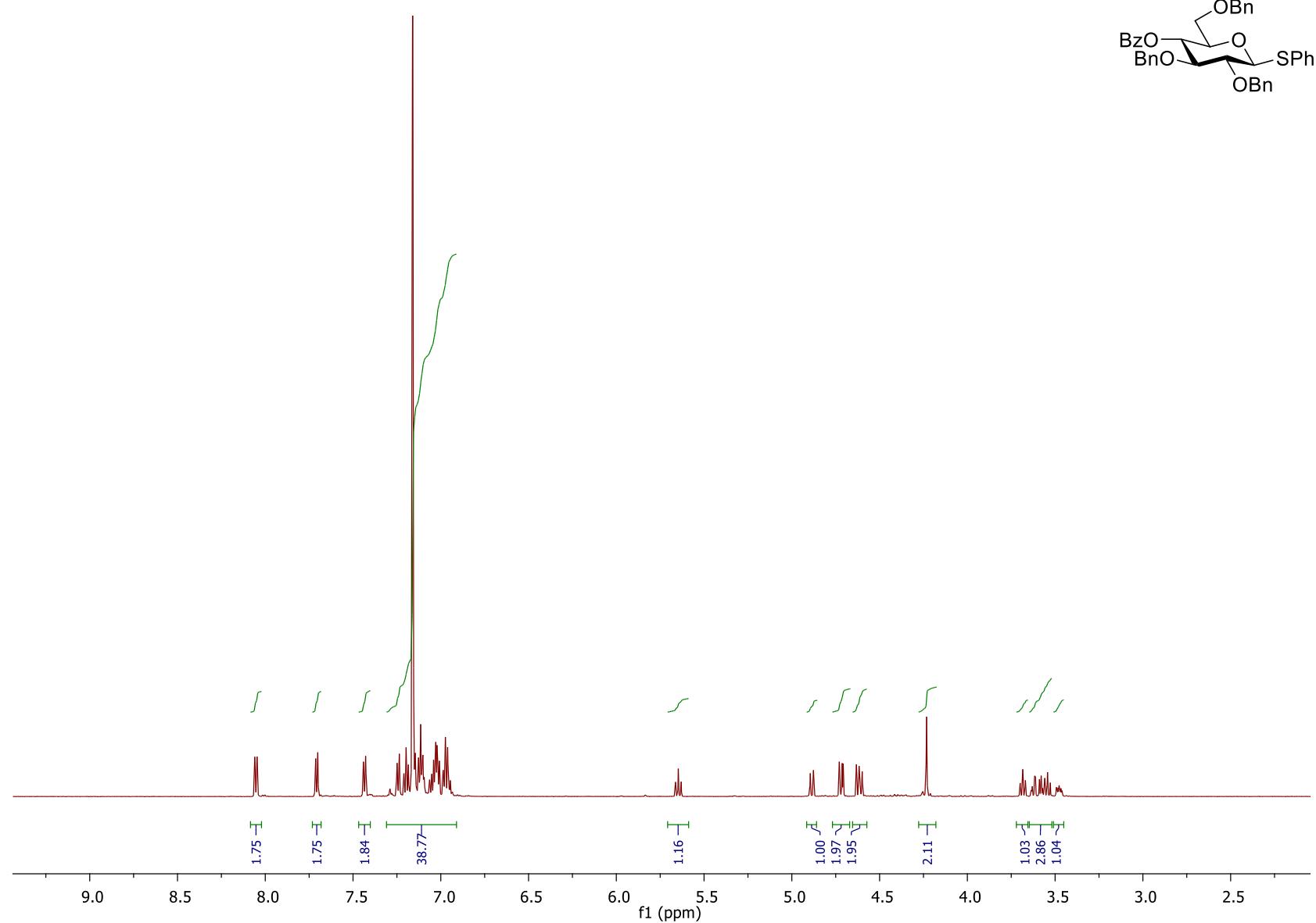
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 2,3,6-tri-*O*-benzyl-4-*O*-trifluoroacetyl-1-thio- β -D-glucopyranoside (**24**)



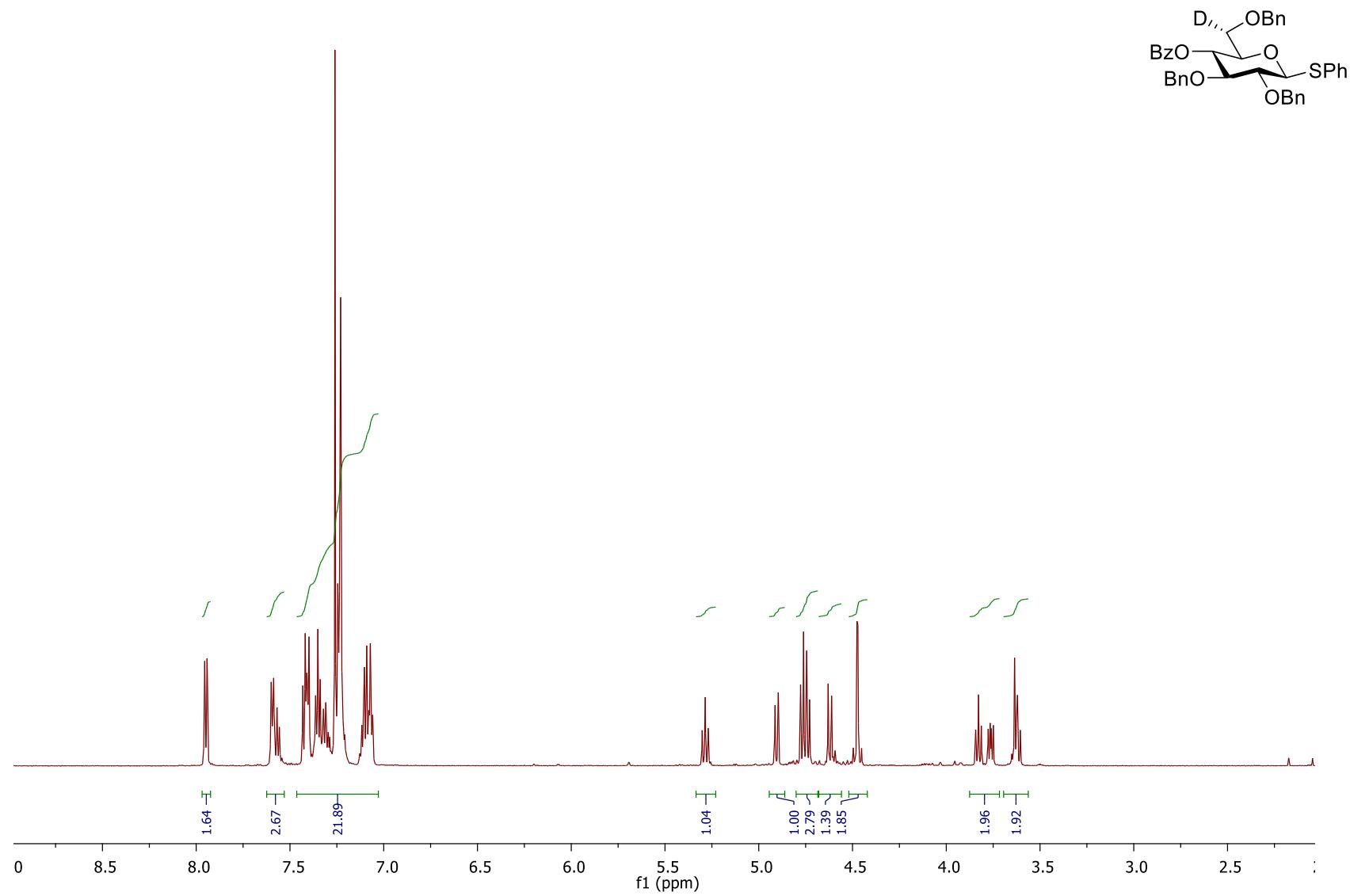
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-benzoyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**25**)



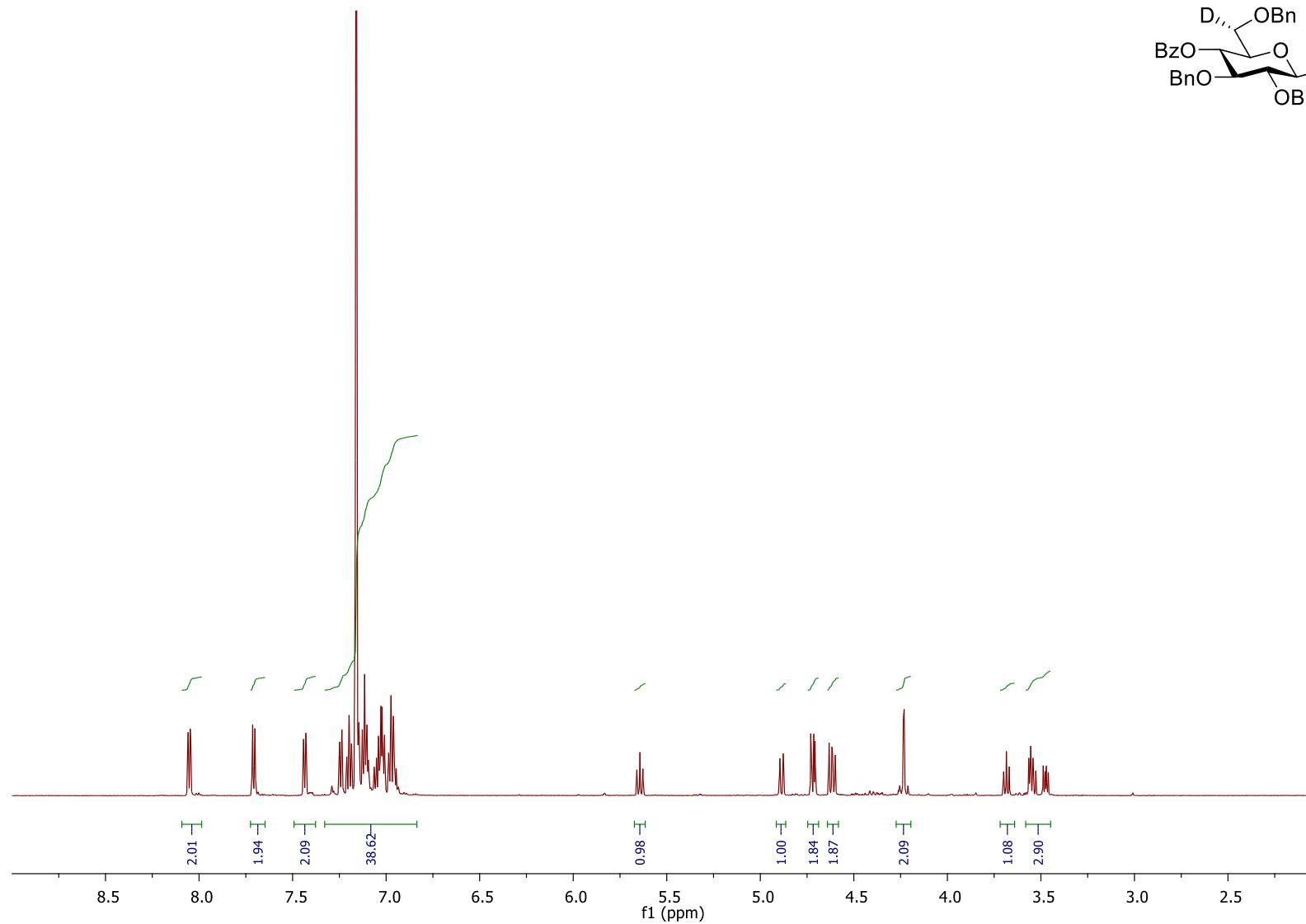
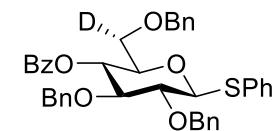
^1H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-benzoyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**25**)



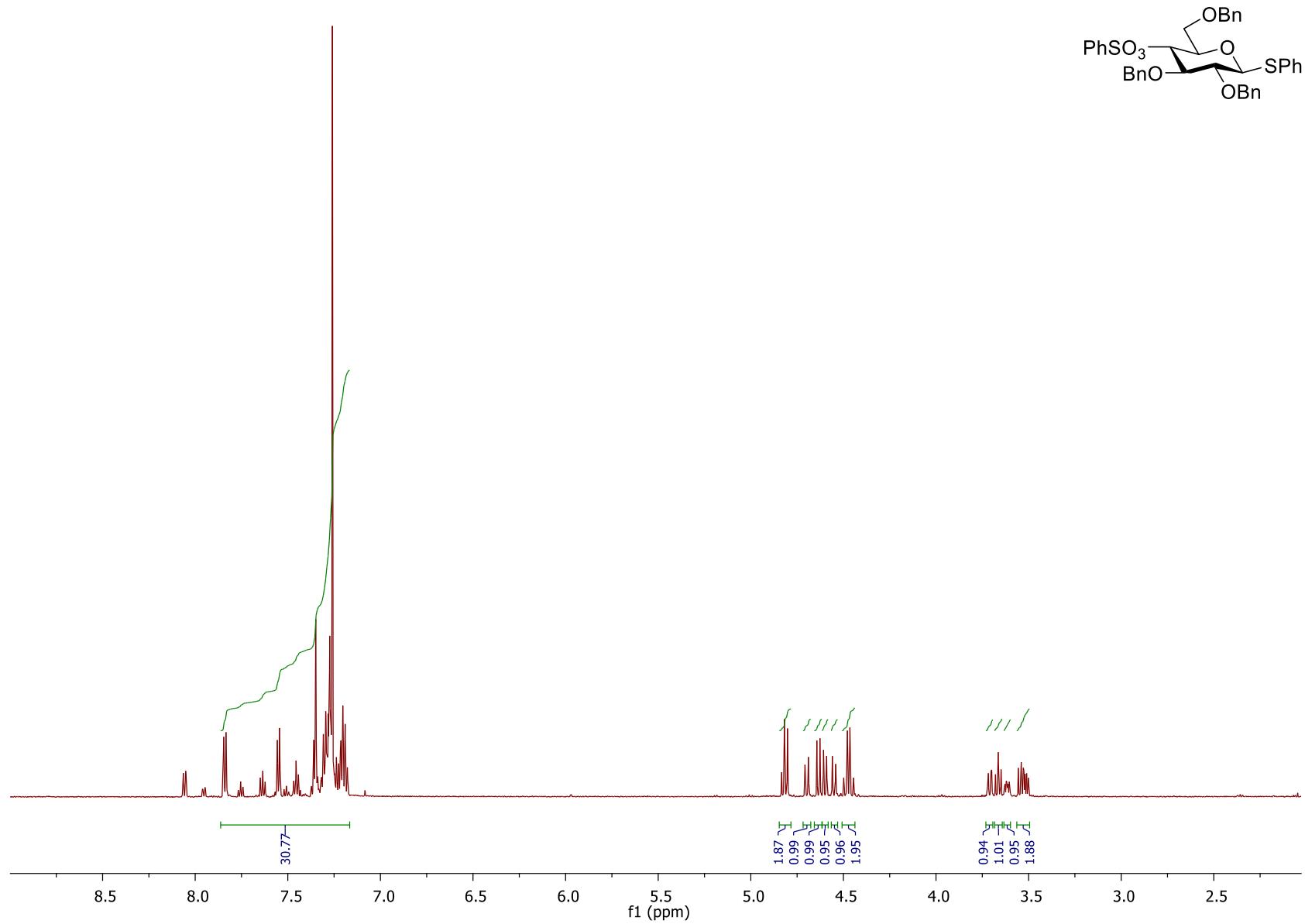
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 4-*O*-benzoyl-(6*S*)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**6S-D-25**)



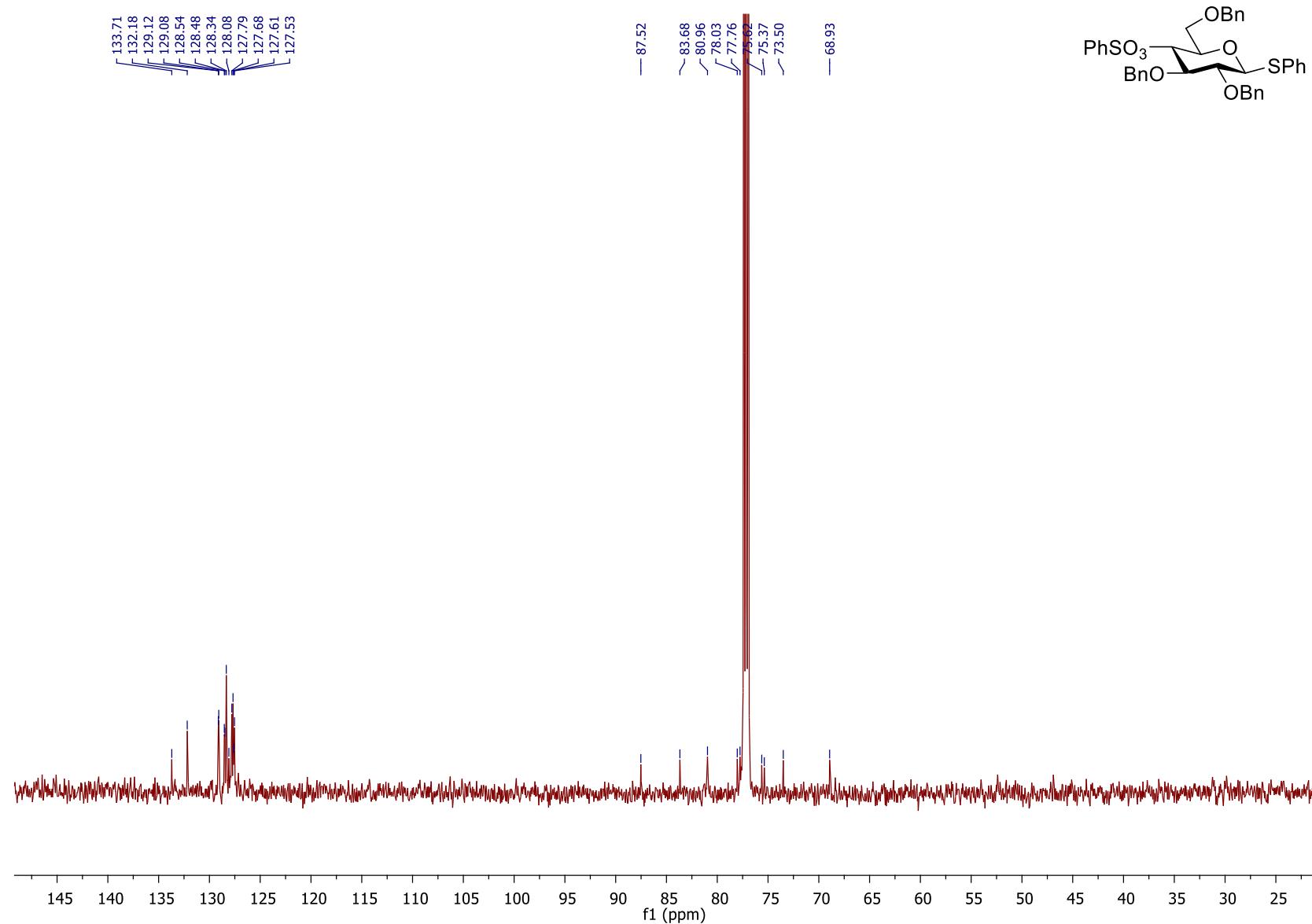
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-benzoyl-(6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-(6*S*-²H)-glucopyranoside
(6*S*-D-25)



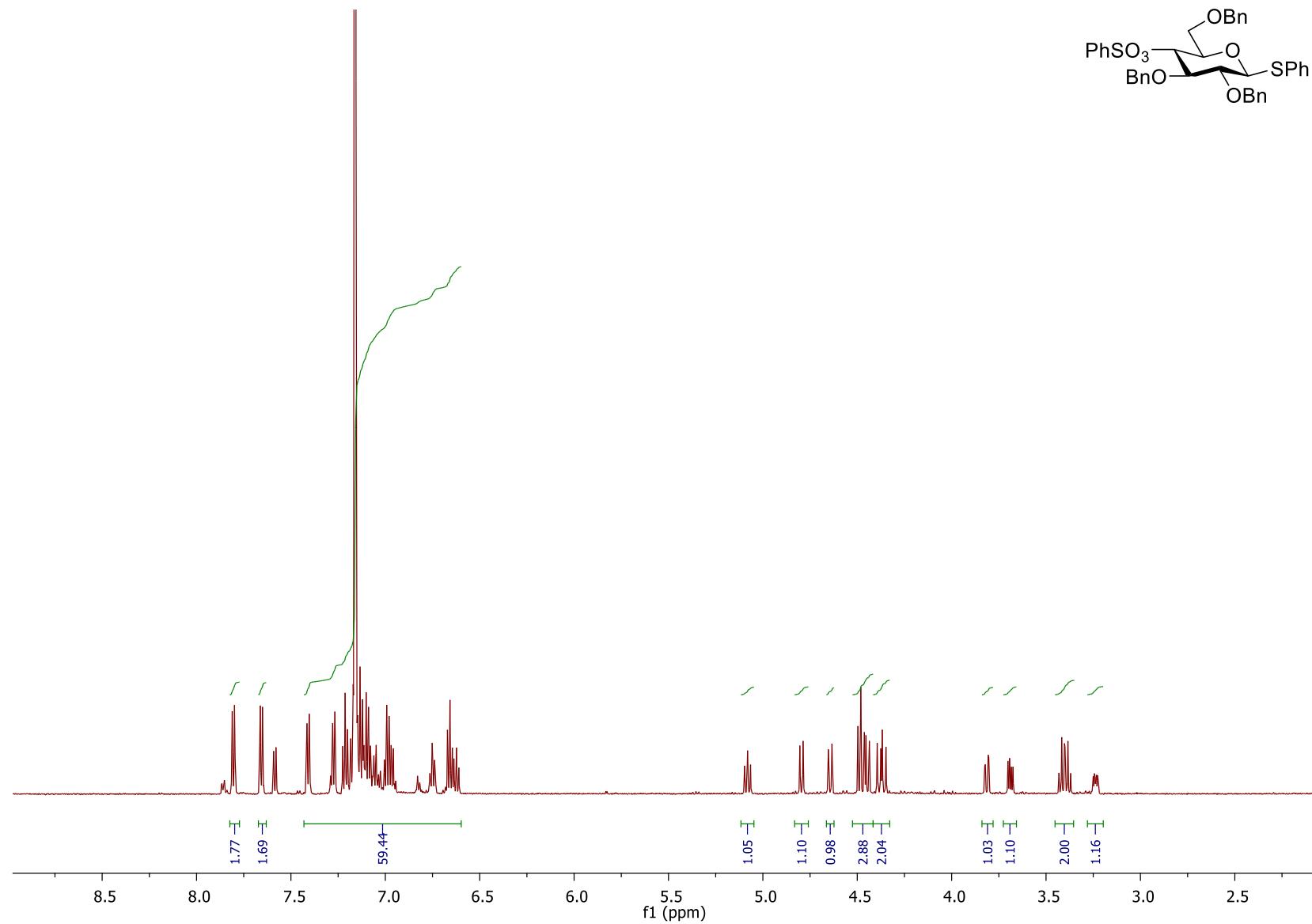
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 4-*O*-benzenesulfonyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**26**)



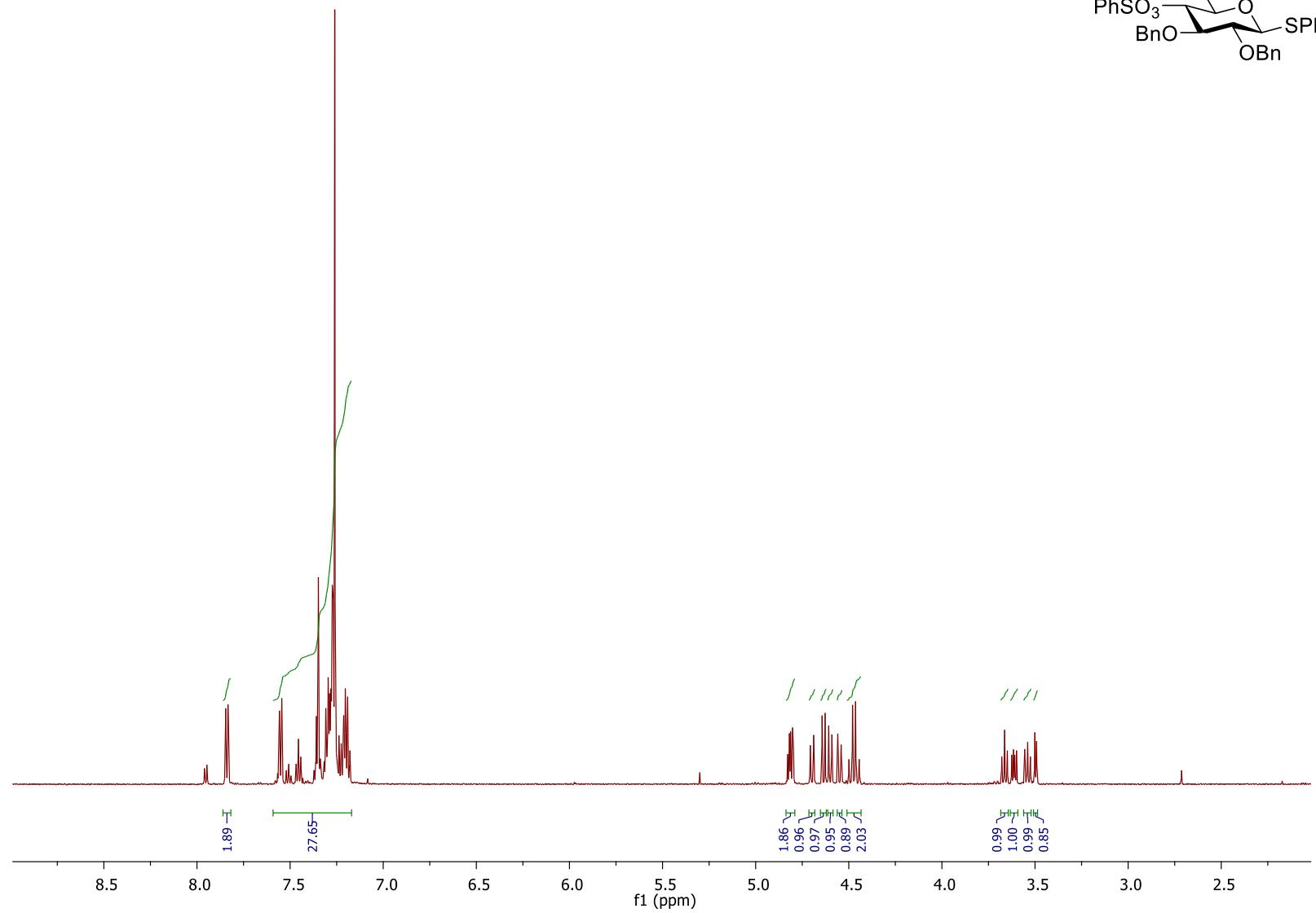
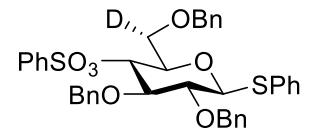
¹³C NMR (150 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-benzenesulfonyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**26**)



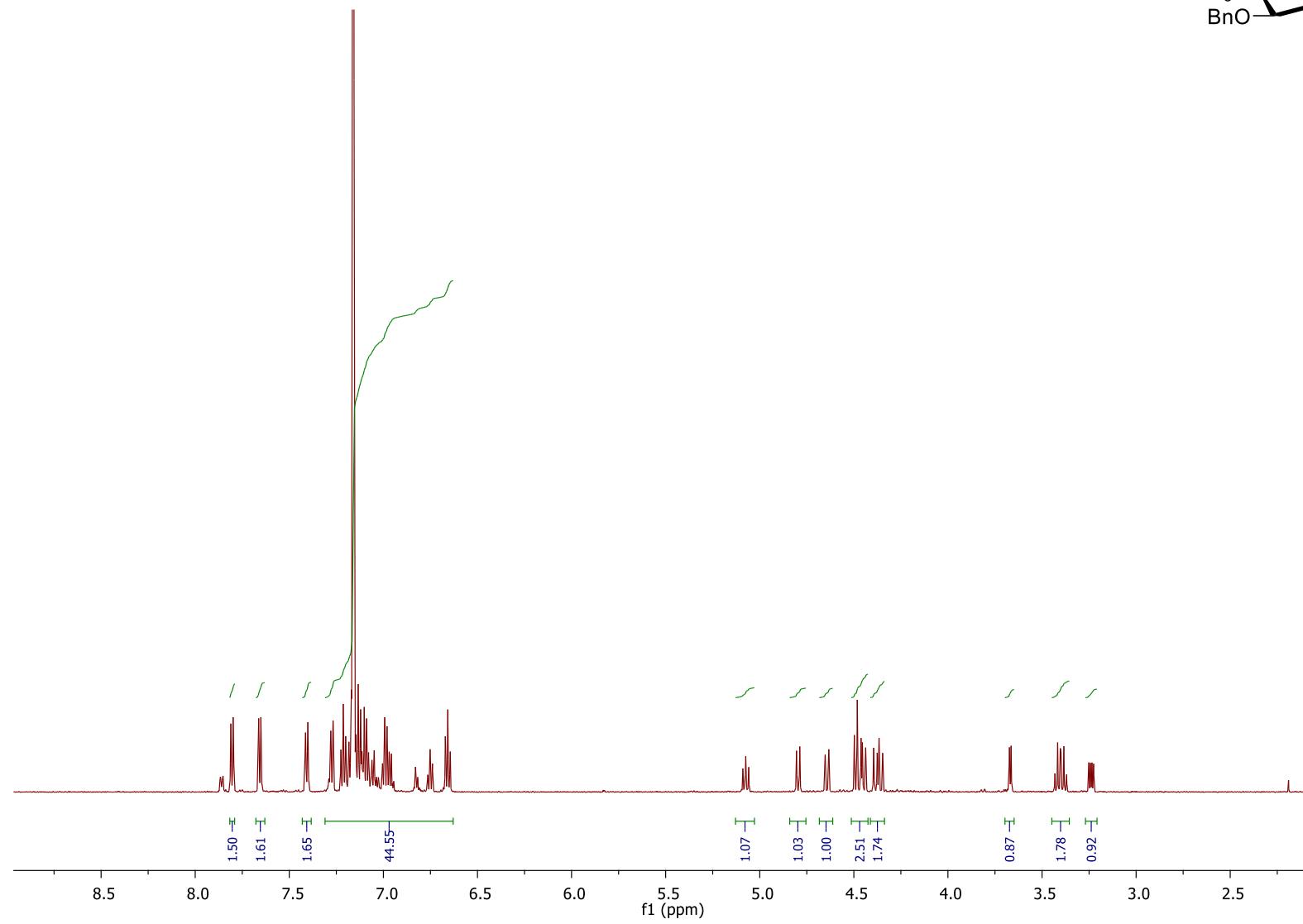
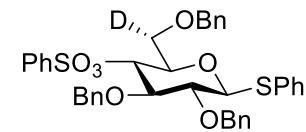
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 4-*O*-benzenesulfonyl-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**26**)



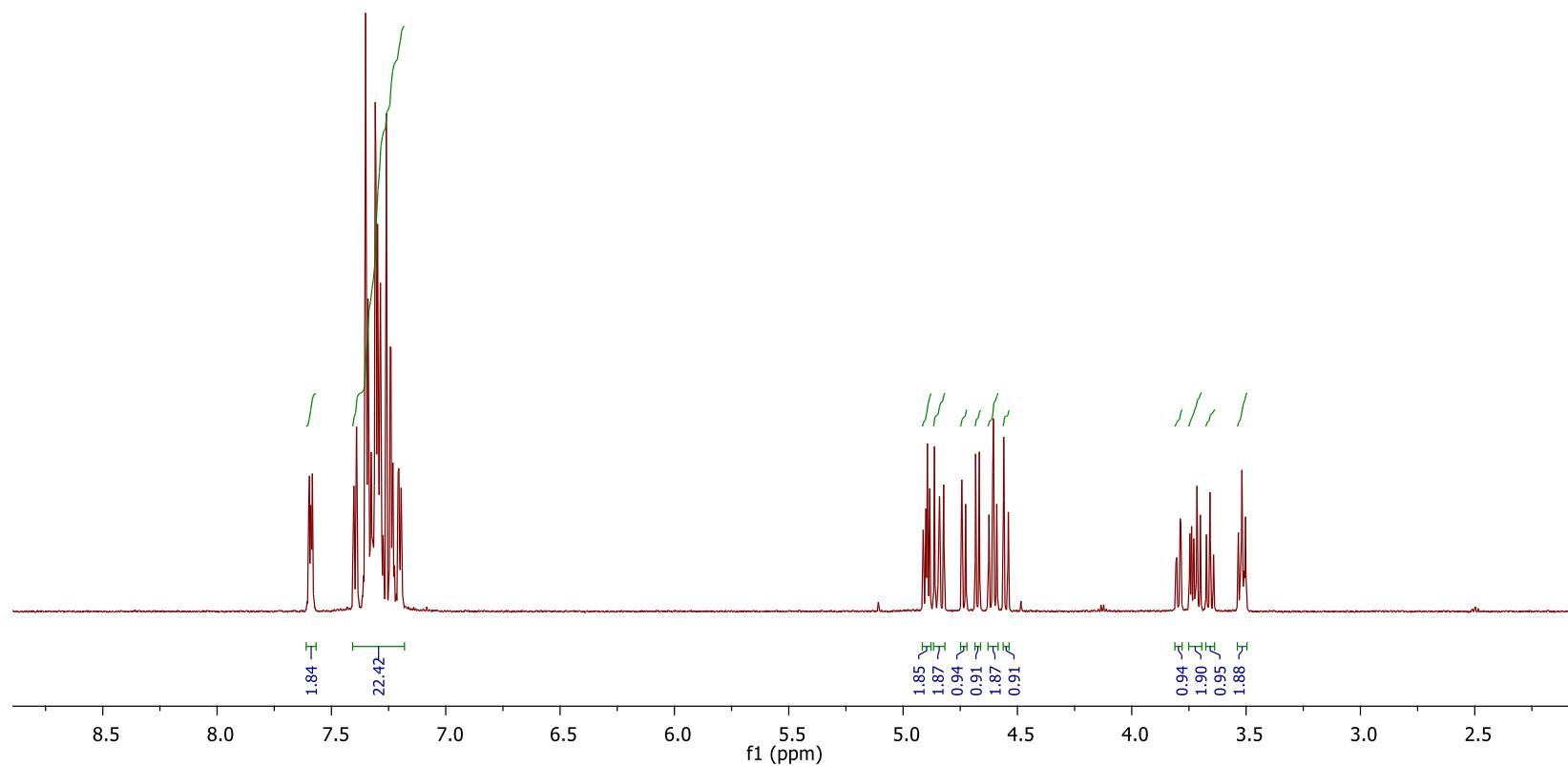
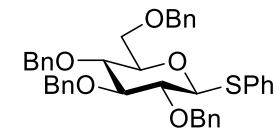
¹H NMR (600 MHz, CDCl₃) Spectrum of Phenyl 4-*O*-benzenesulfonyl-(6*S*)-[6-²H₁]-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside
(6S-D-26)



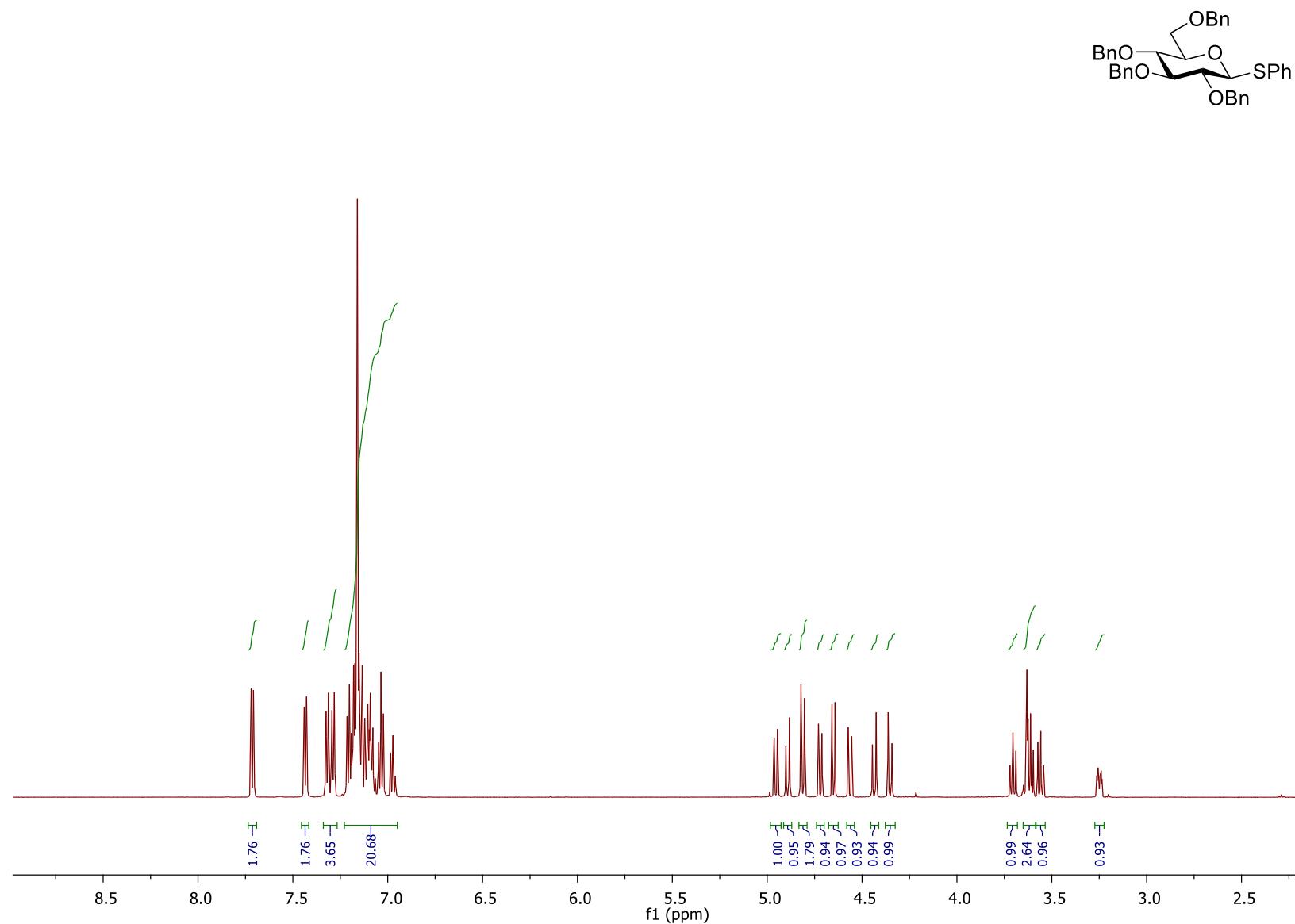
^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl 4-*O*-benzenesulfonyl-(6*S*)-[6- $^2\text{H}_1$]-2,3,6-tri-*O*-benzyl-1-thio- β -D-glucopyranoside
(6*S*-D-26)



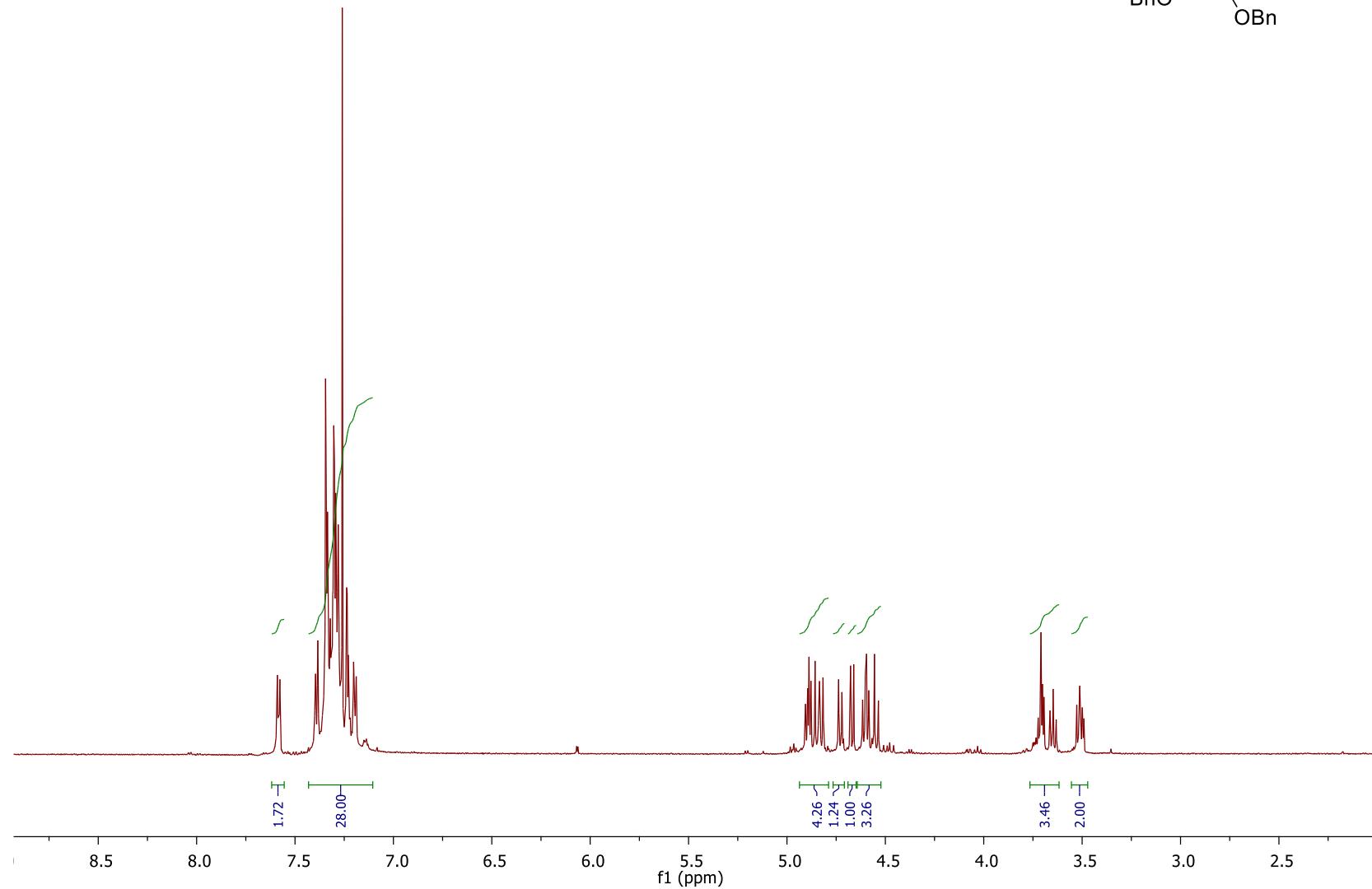
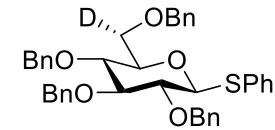
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl 2,3,4,6-tetra- O -benzyl-1-thio- β -D-glucopyranoside (**27**)



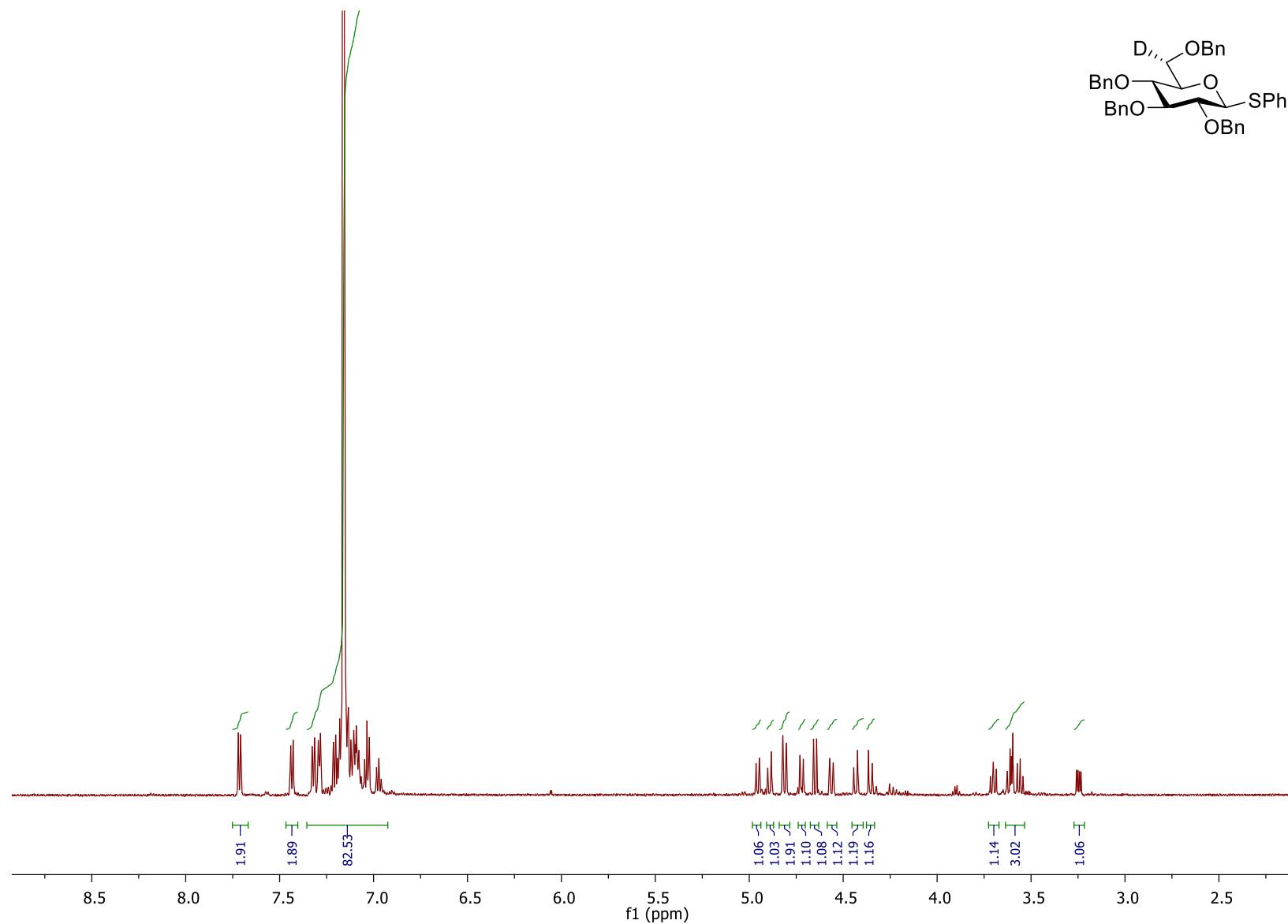
¹H NMR (600 MHz, C₆D₆) Spectrum of Phenyl 2,3,4,6-tetra-O-benzyl-1-thio-β-D-glucopyranoside (**27**)



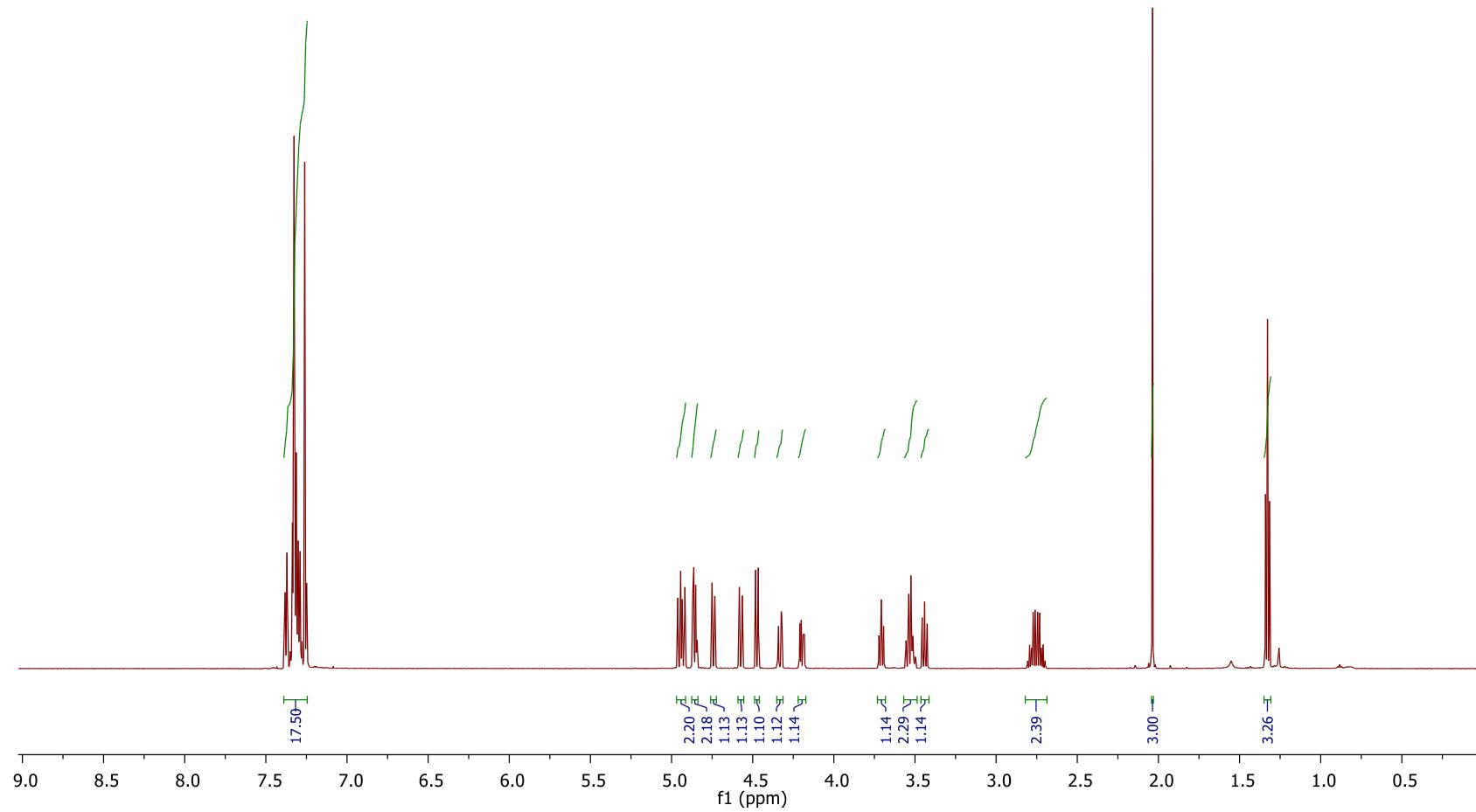
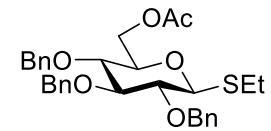
^1H NMR (600 MHz, CDCl_3) Spectrum of Phenyl ($6S$)-[$6-^2\text{H}_1$]-2,3,4,6-tetra- O -benzyl-1-thio- β -D-glucopyranoside (**6S-D-27**)



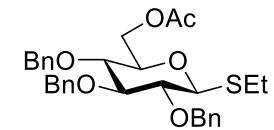
^1H NMR (600 MHz, C_6D_6) Spectrum of Phenyl (6*S*)-[6- $^2\text{H}_1$]-2,3,4,6-tetra-*O*-benzyl-1-thio- β -D-glucopyranoside (**6S-D-27**)



^1H NMR (600 MHz, CDCl_3) Spectrum of Ethyl 6-*O*-acetyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**28**)



Simulated ^1H NMR and Experimental ^1H NMR (600 MHz, CDCl_3) Spectrum of Ethyl 6-*O*-acetyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (28)



Experimental ^1H NMR (600 MHz, CDCl_3)

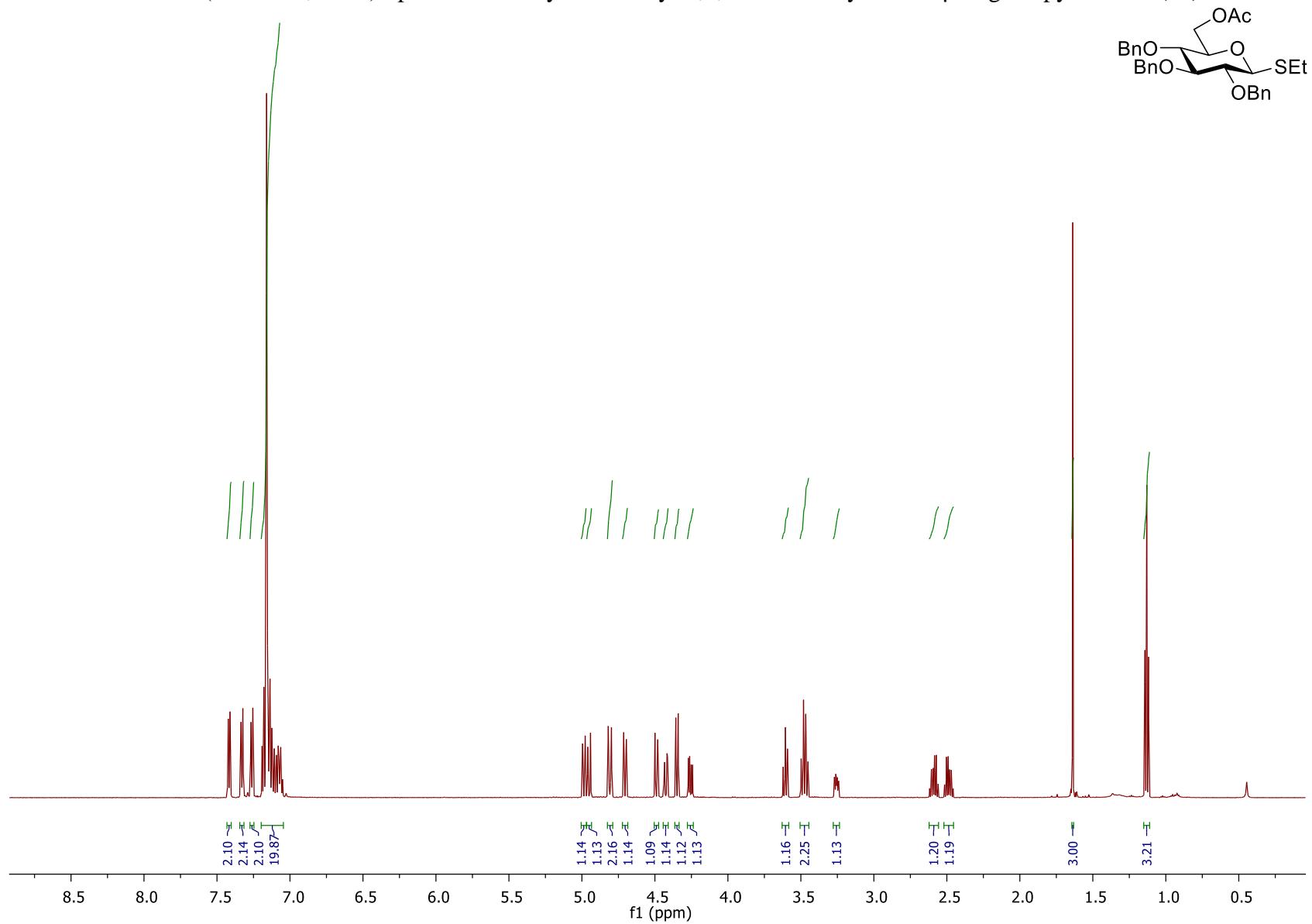


Simulated ^1H NMR

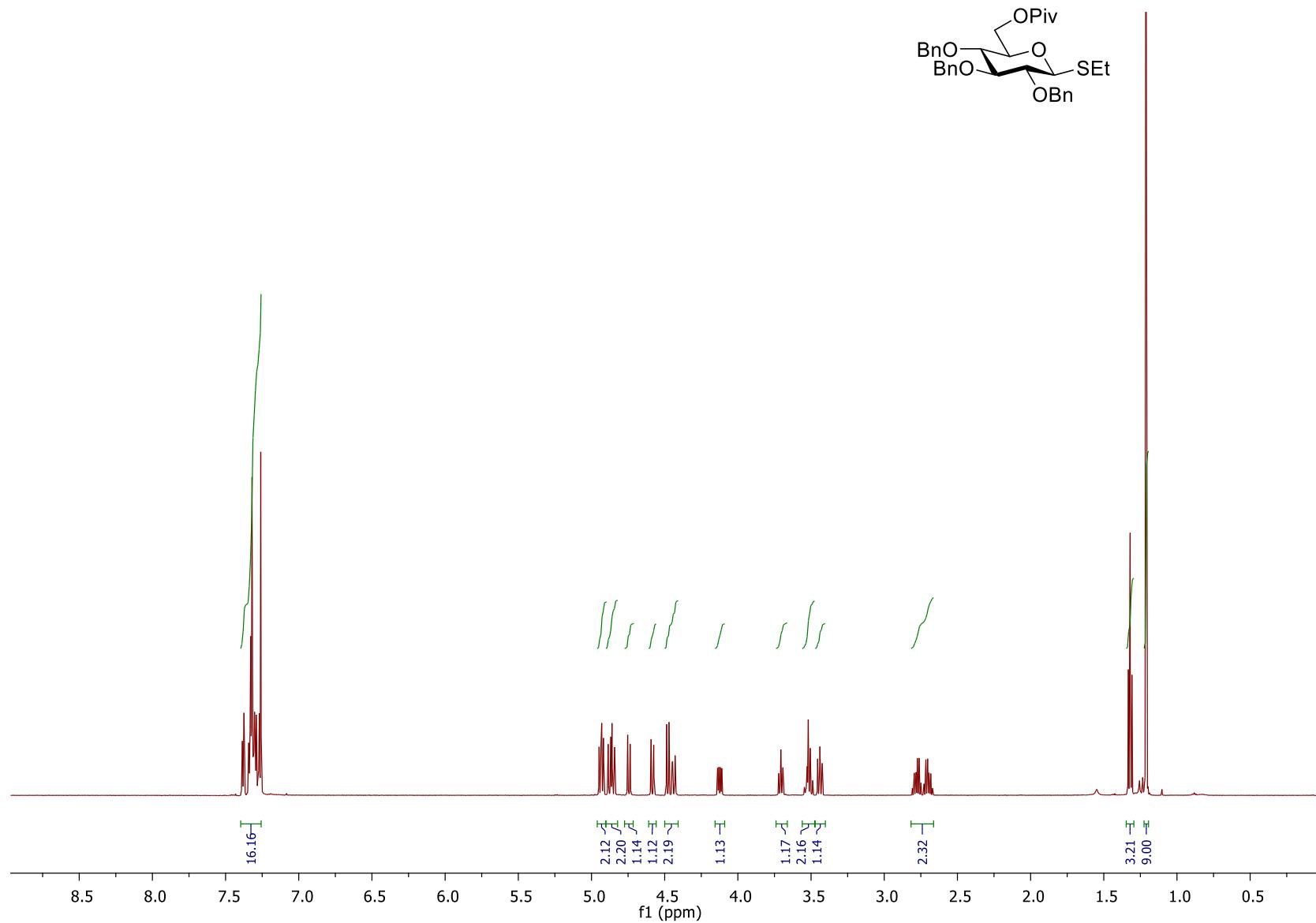


4.50 4.45 4.40 4.35 4.30 4.25 4.20 4.15 4.10 4.05 4.00 3.95 3.90 3.85 3.80 3.75 3.70 3.65 3.60 3.55 3.50 3.45 3.40
f1 (ppm)
S95

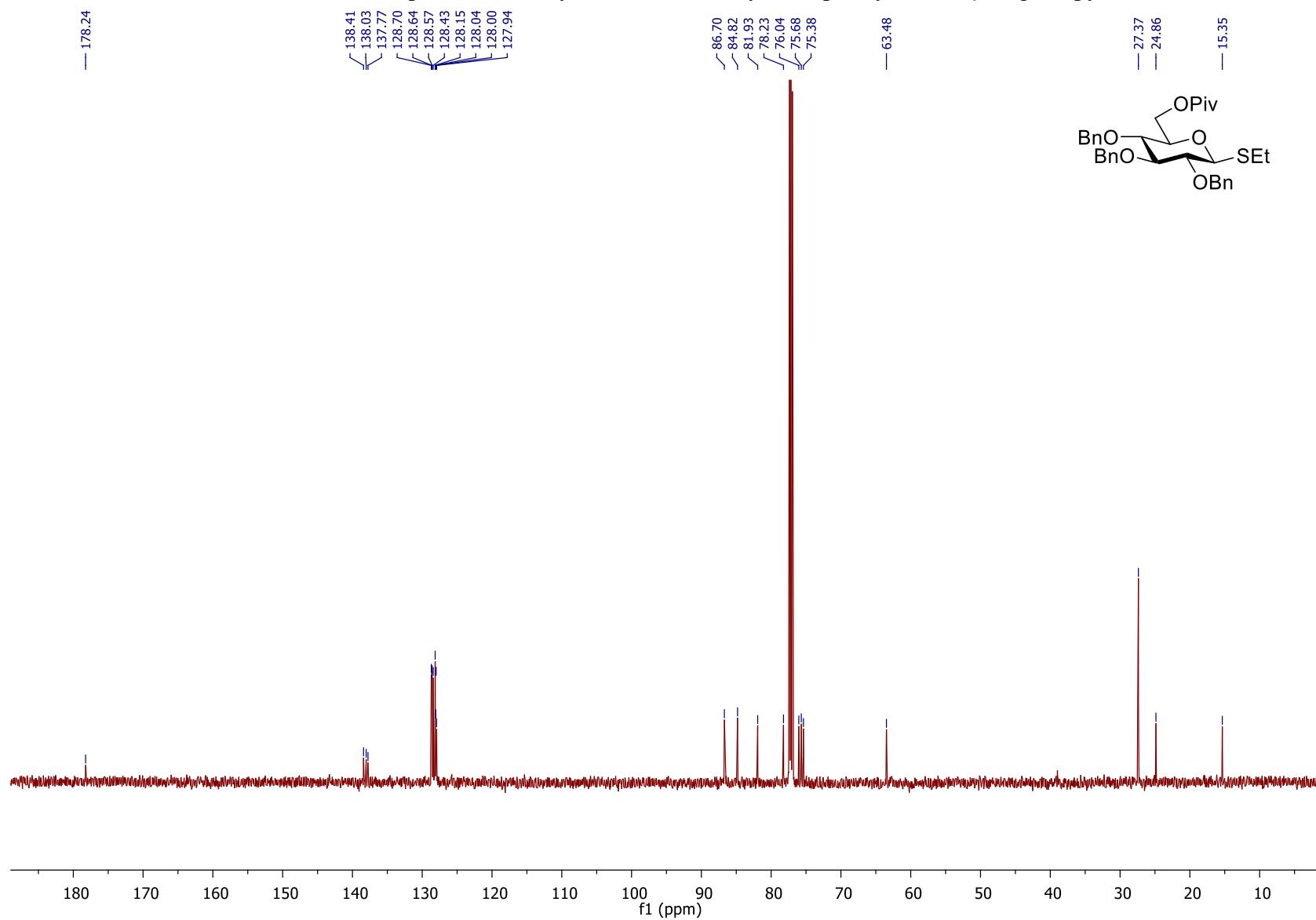
^1H NMR (600 MHz, C_6D_6) Spectrum of Ethyl 6-*O*-acetyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**28**)



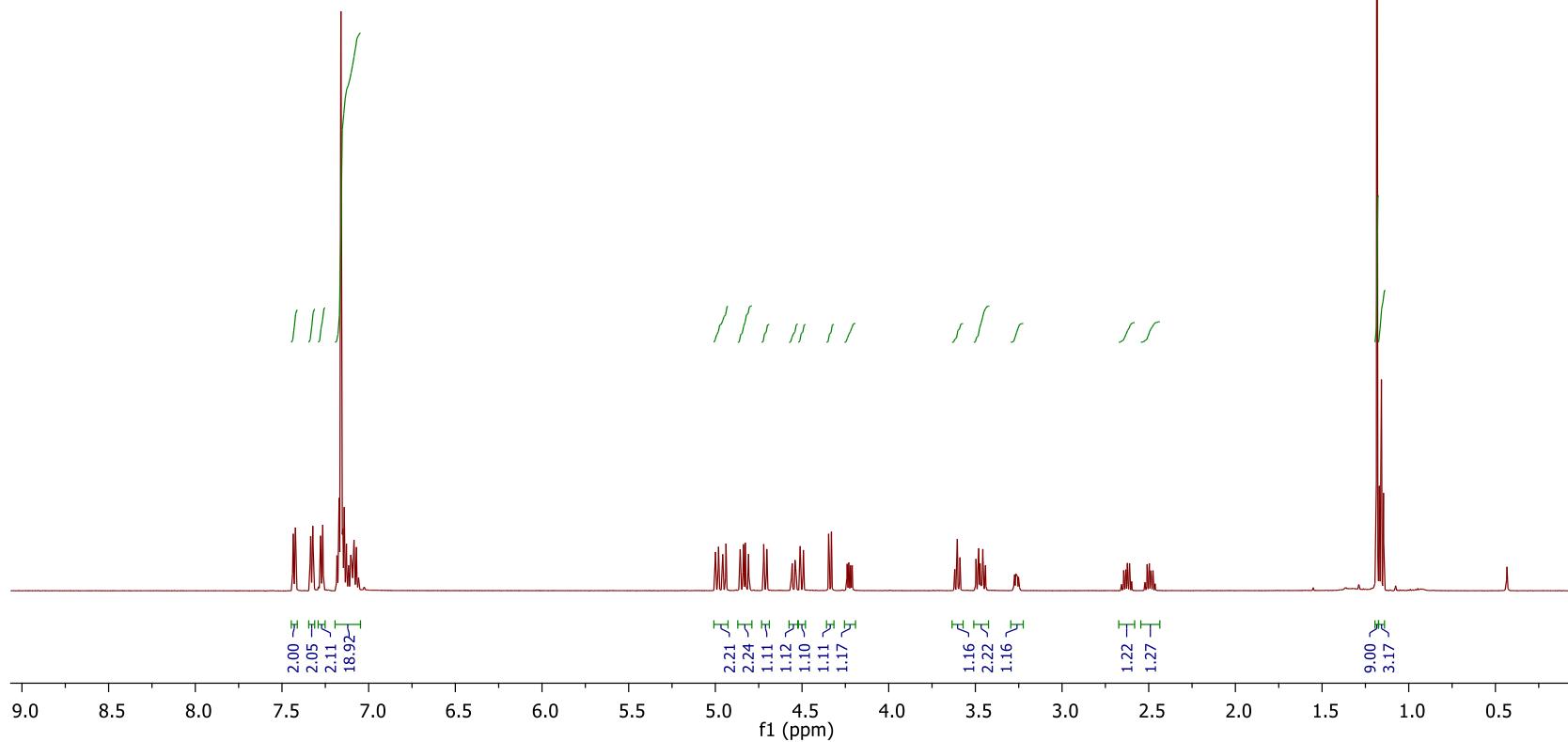
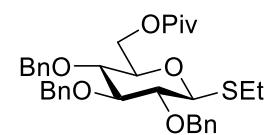
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 2,3,4-tri-O-benzyl-6-O-pivoyl-1-thio-β-D-glucopyranoside (**29**)



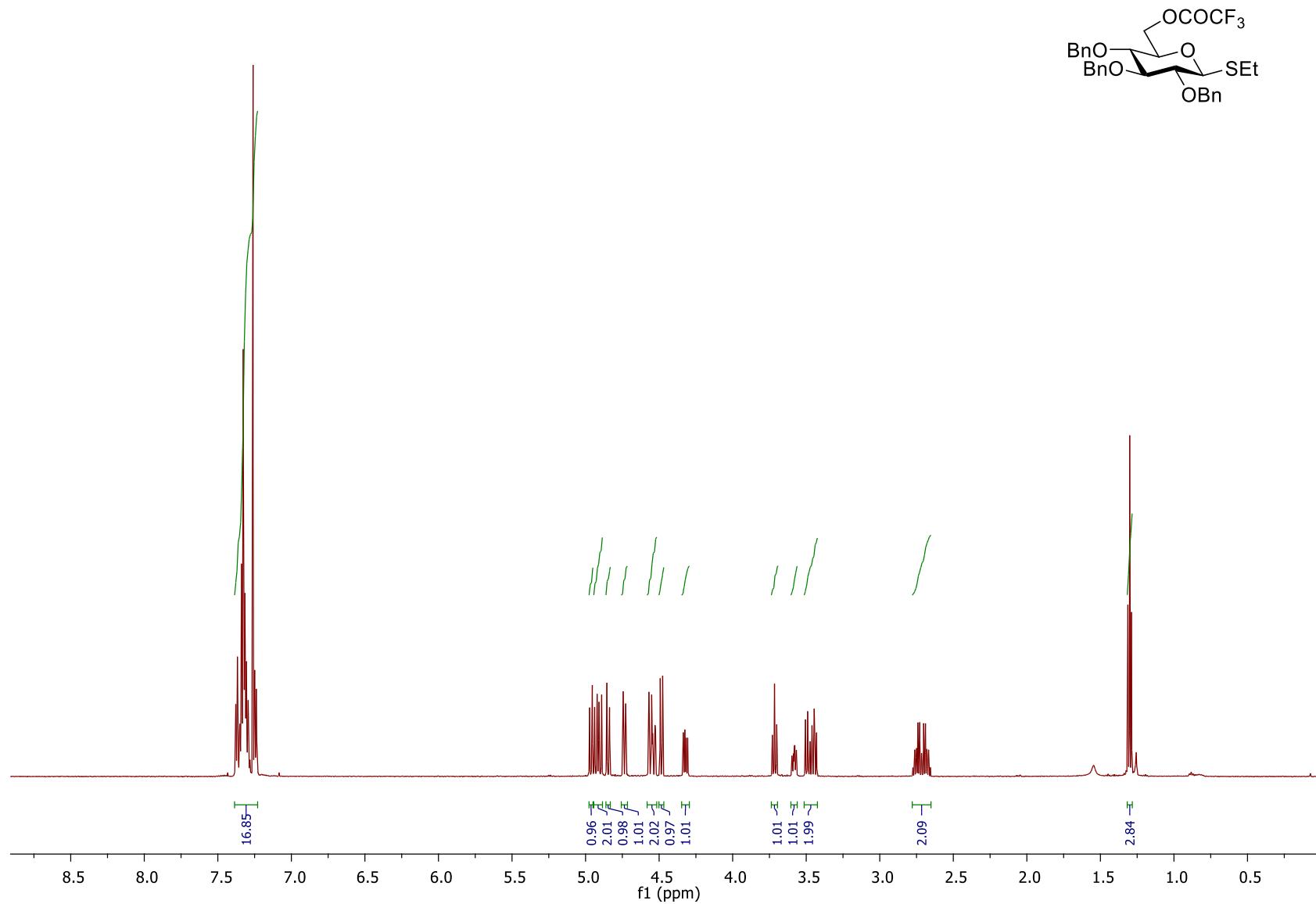
^{13}C NMR (150 MHz, CDCl_3) Spectrum of Ethyl 2,3,4-tri-*O*-benzyl-6-*O*-pivoyl-1-thio- β -D-glucopyranoside (**29**)



¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl 2,3,4-tri-O-benzyl-6-O-pivoyl-1-thio-β-D-glucopyranoside (**29**)

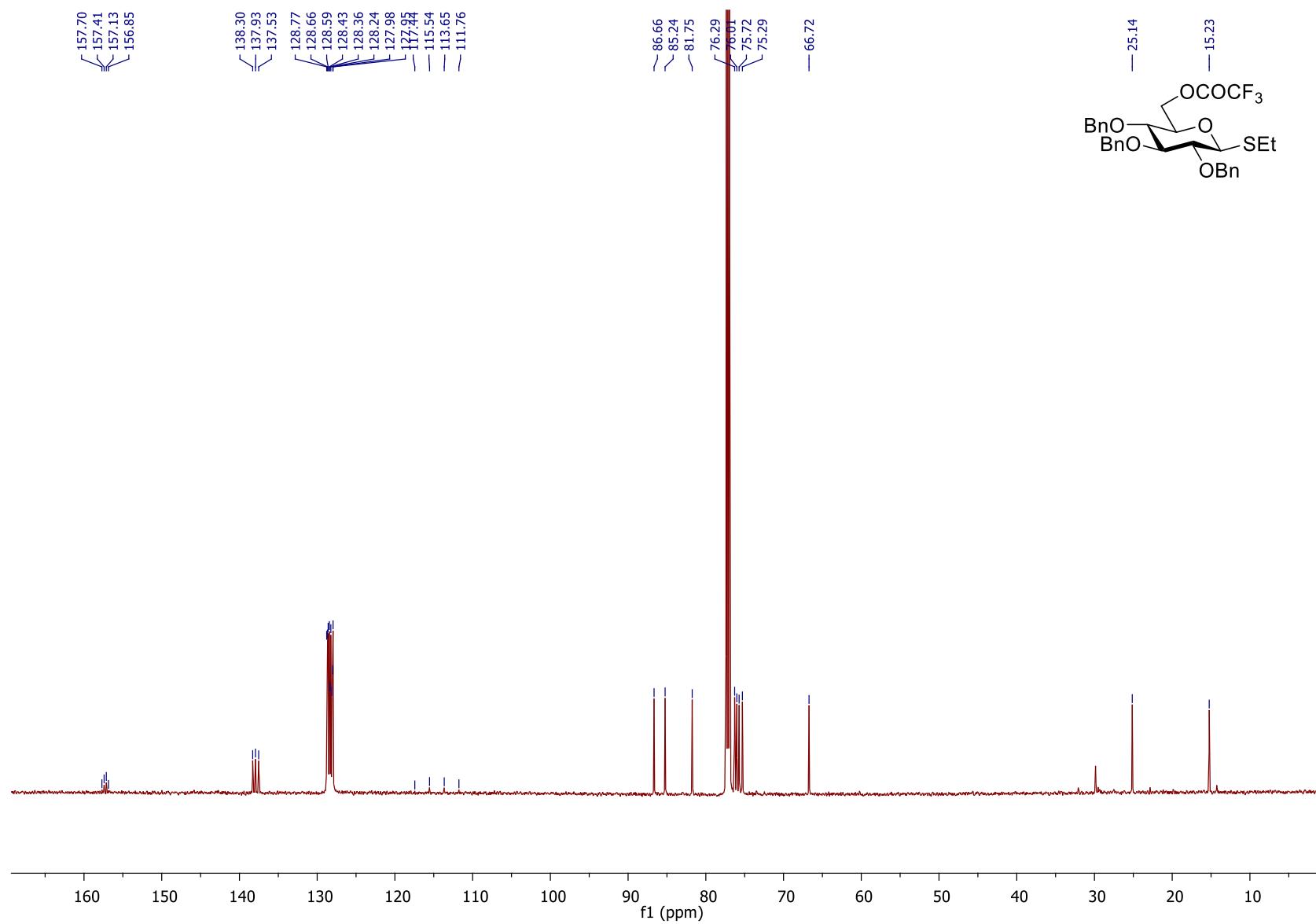


¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 2,3,4-tri-*O*-benzyl-6-*O*-trifluoroacetyl-1-thio- β -D-glucopyranoside (**30**)

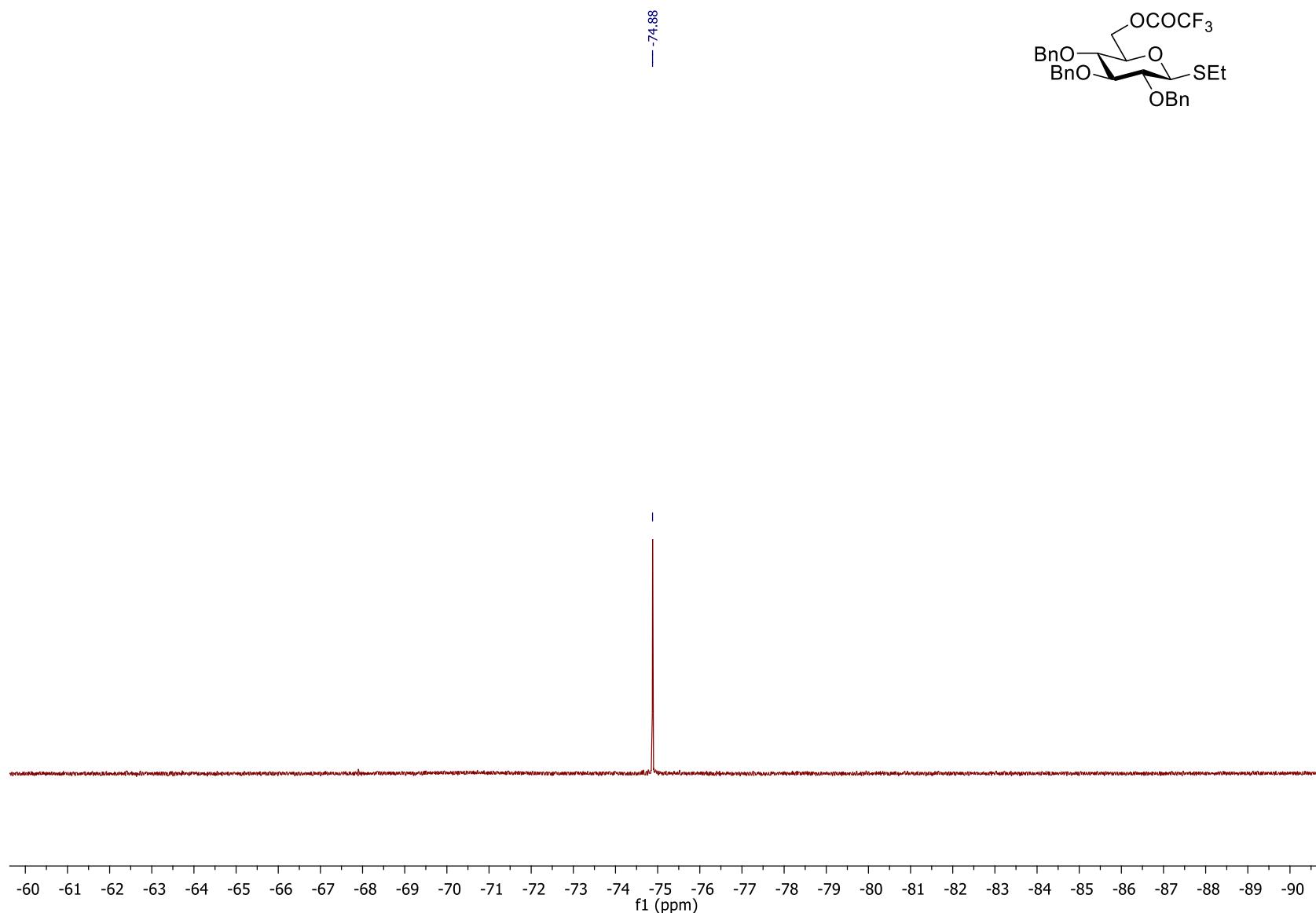


S100

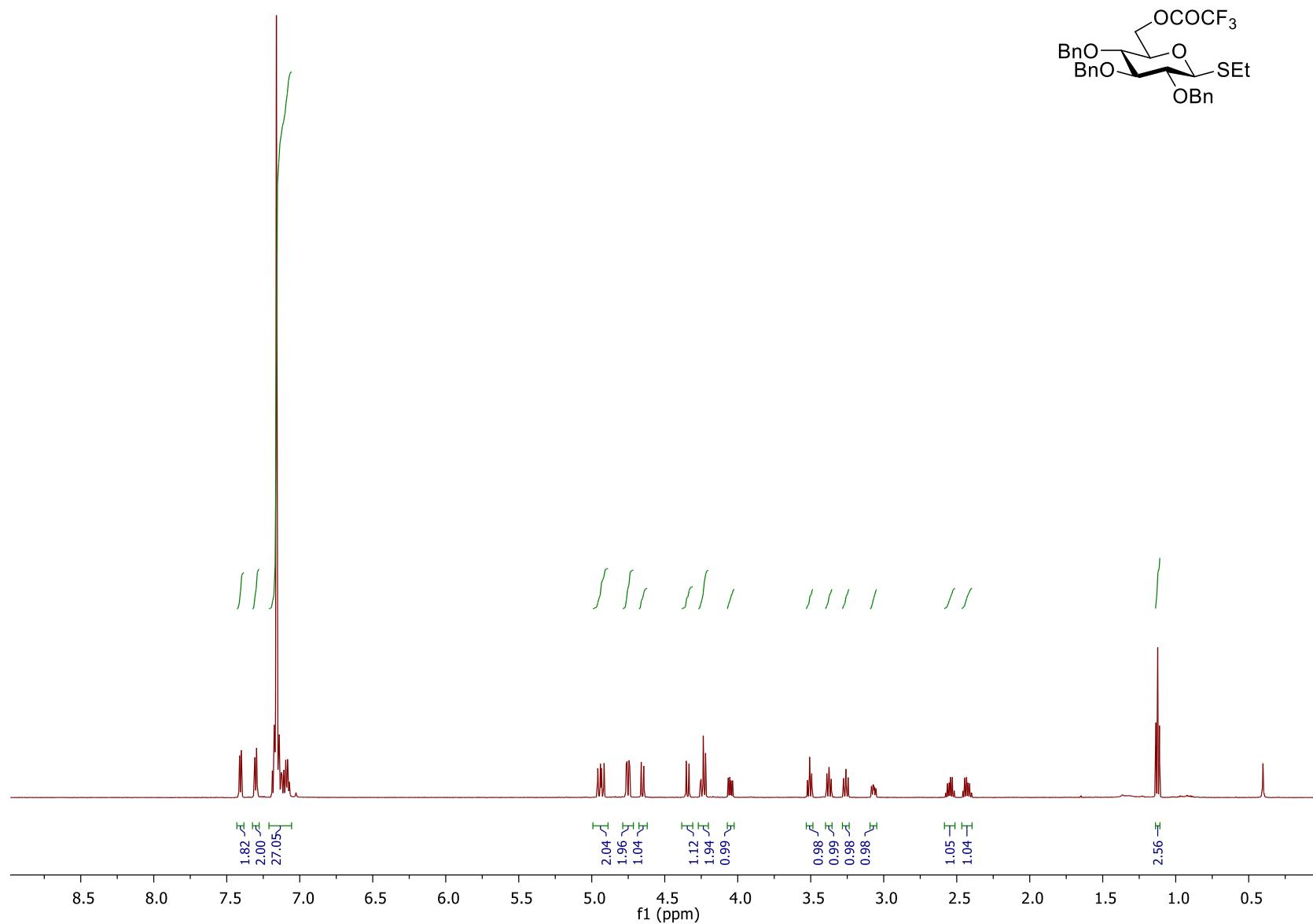
^{13}C NMR (150 MHz, CDCl_3) Spectrum of Ethyl 2,3,4-tri-*O*-benzyl-6-*O*-trifluoroacetyl-1-thio- β -D-glucopyranoside (**30**)



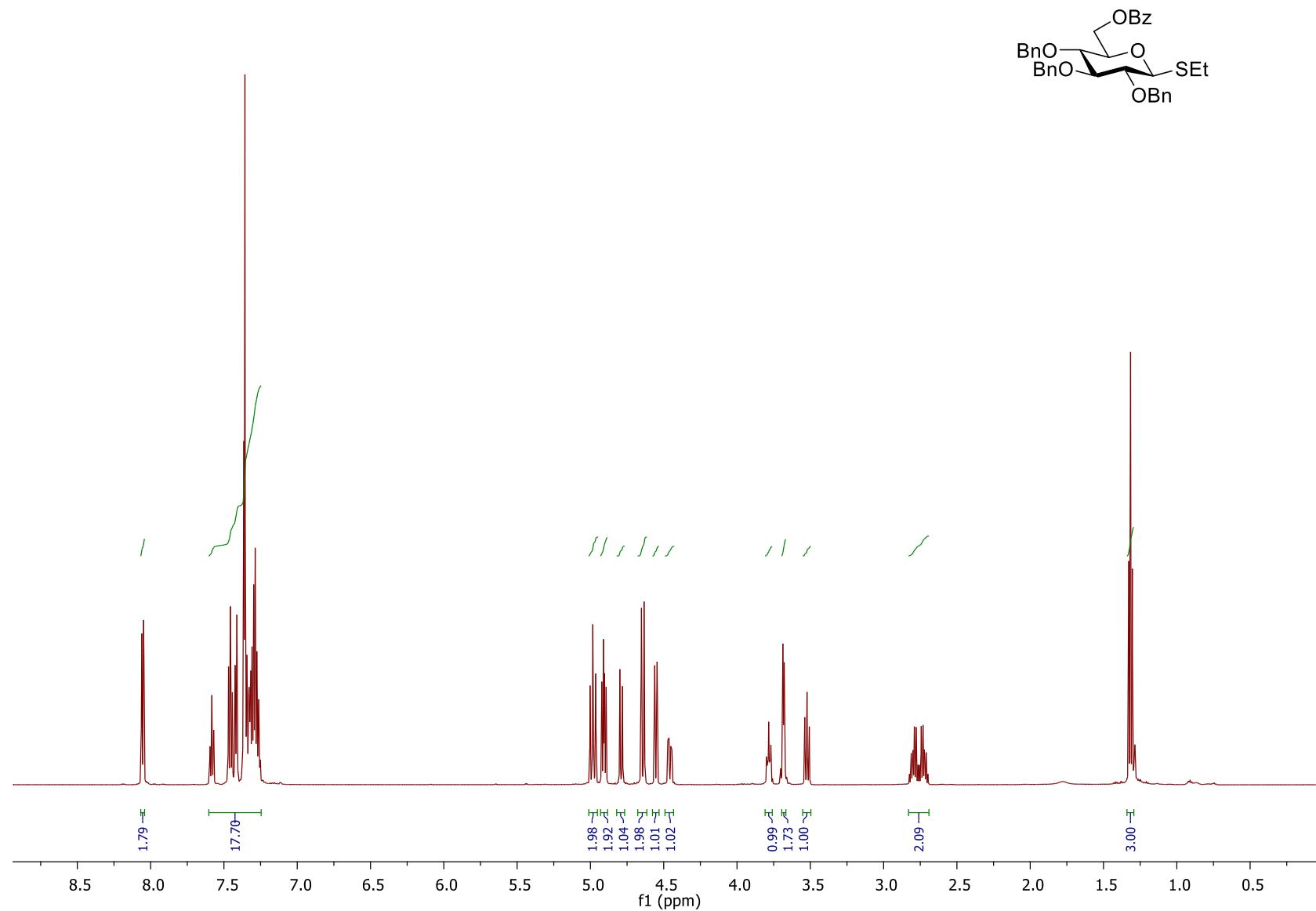
¹⁹F NMR (376 MHz, CDCl₃) Spectrum of Ethyl 2,3,4-tri-*O*-benzyl-6-*O*-trifluoroacetyl-1-thio- β -D-glucopyranoside (**30**)



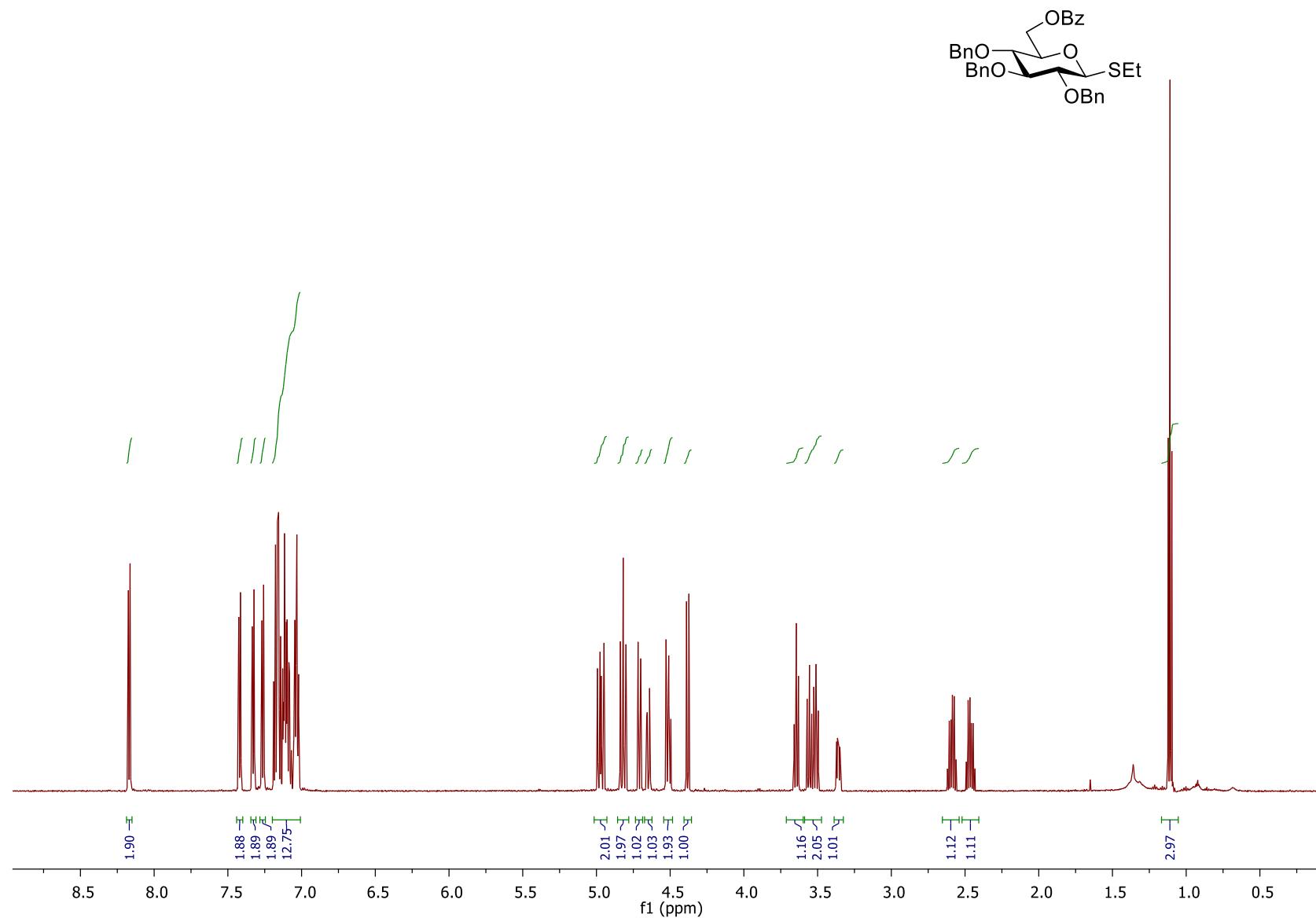
¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl 2,3,4-tri-O-benzyl-6-O-trifluoroacetyl-1-thio-β-D-glucopyranoside (**30**)



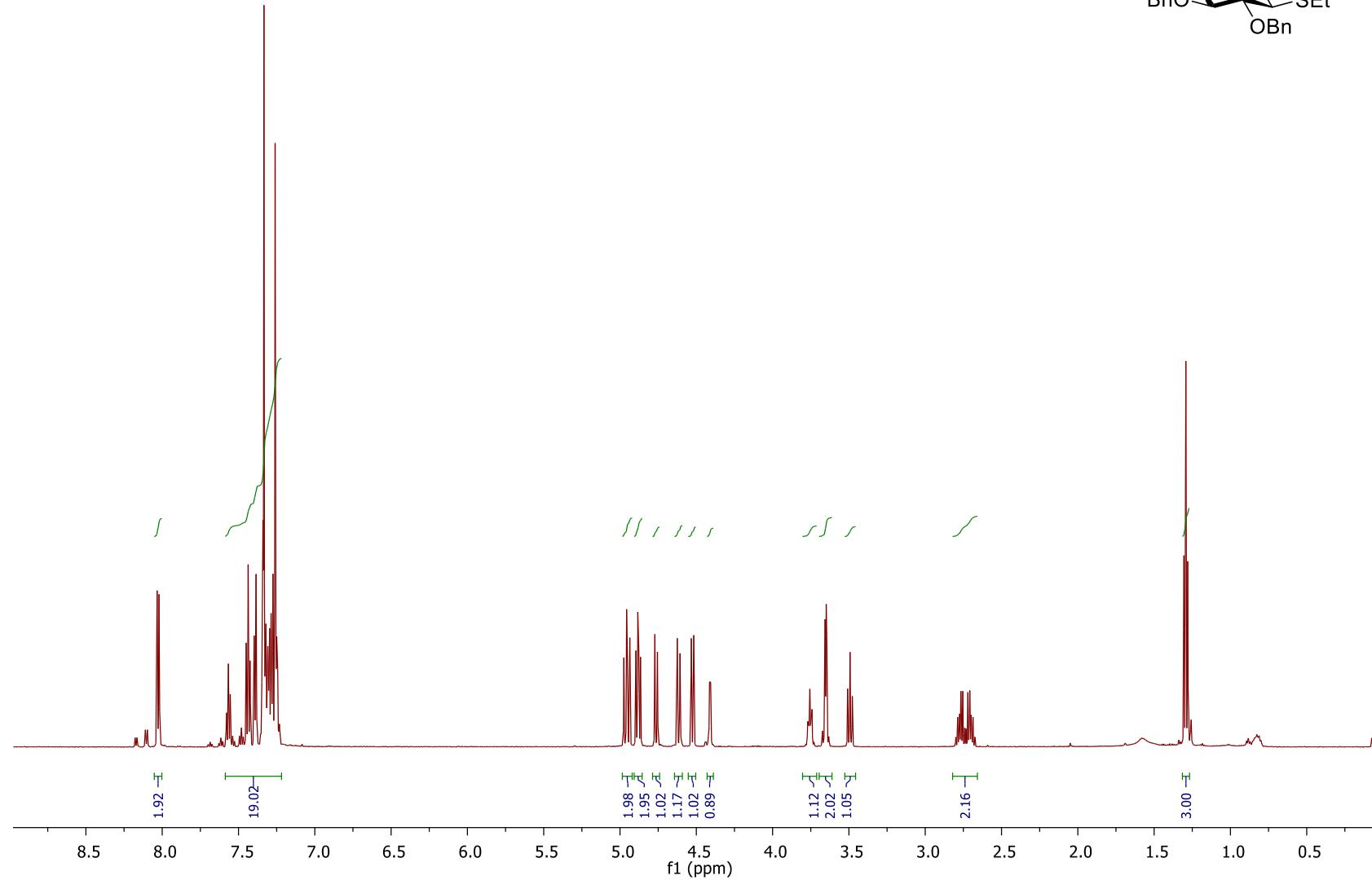
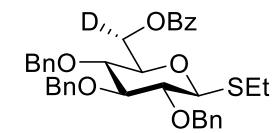
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 6-*O*-benzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**31**)



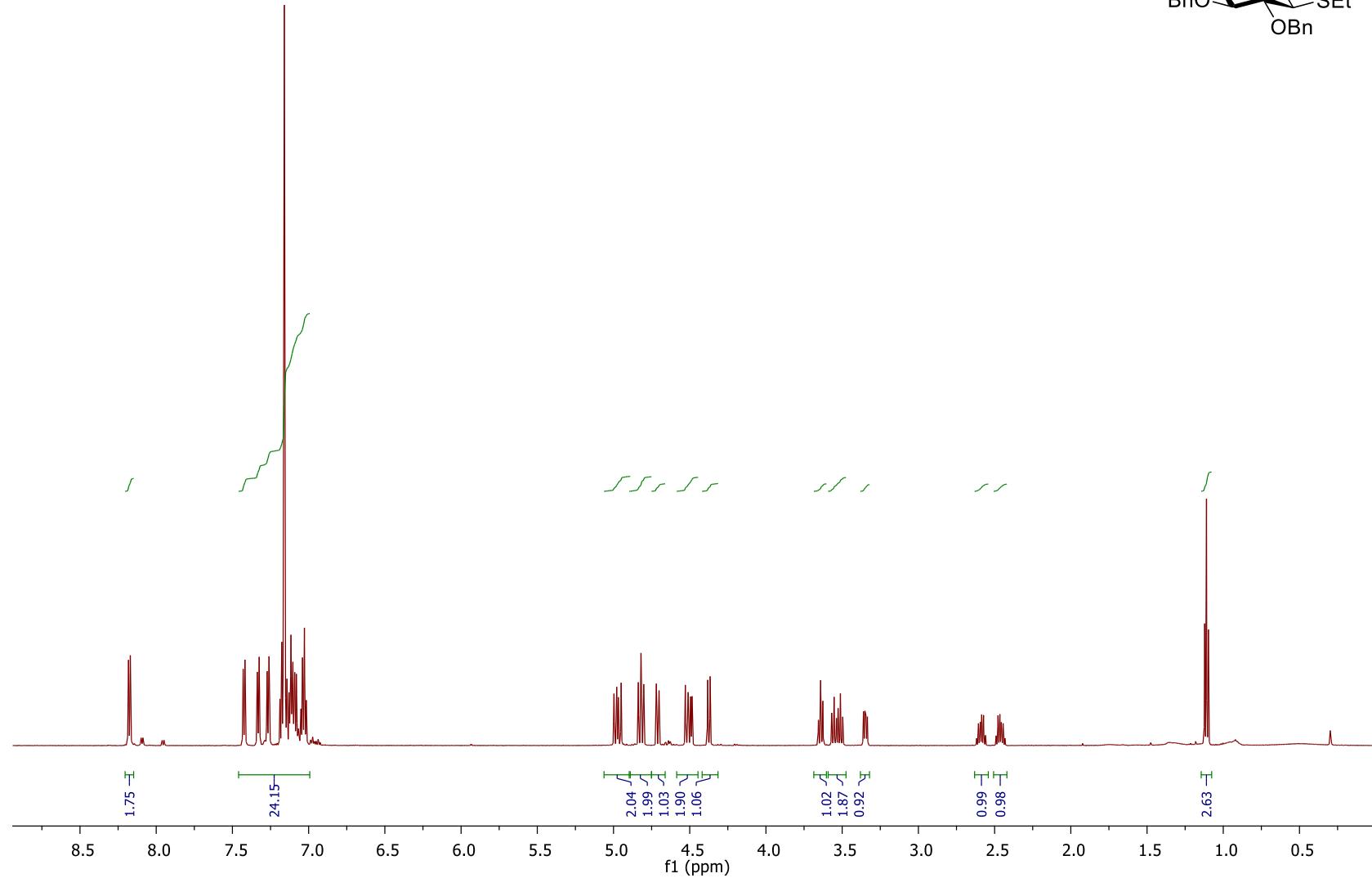
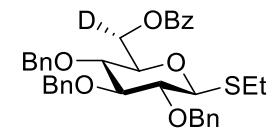
^1H NMR (600 MHz, C_6D_6) Spectrum of Ethyl 6-*O*-benzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**31**)



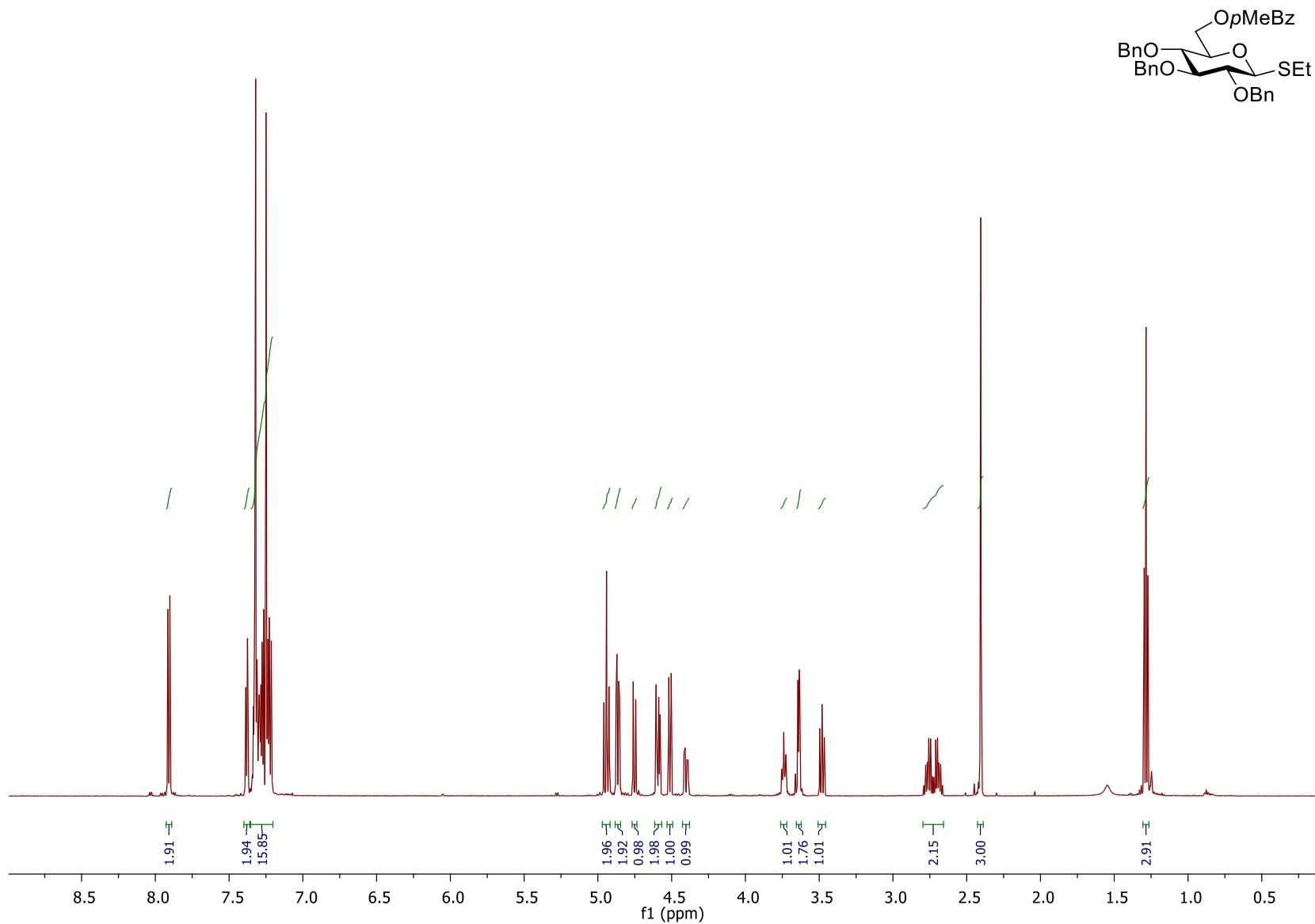
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl (6*S*)-[6-²H₁]-6-*O*-benzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**6S-D-31**)



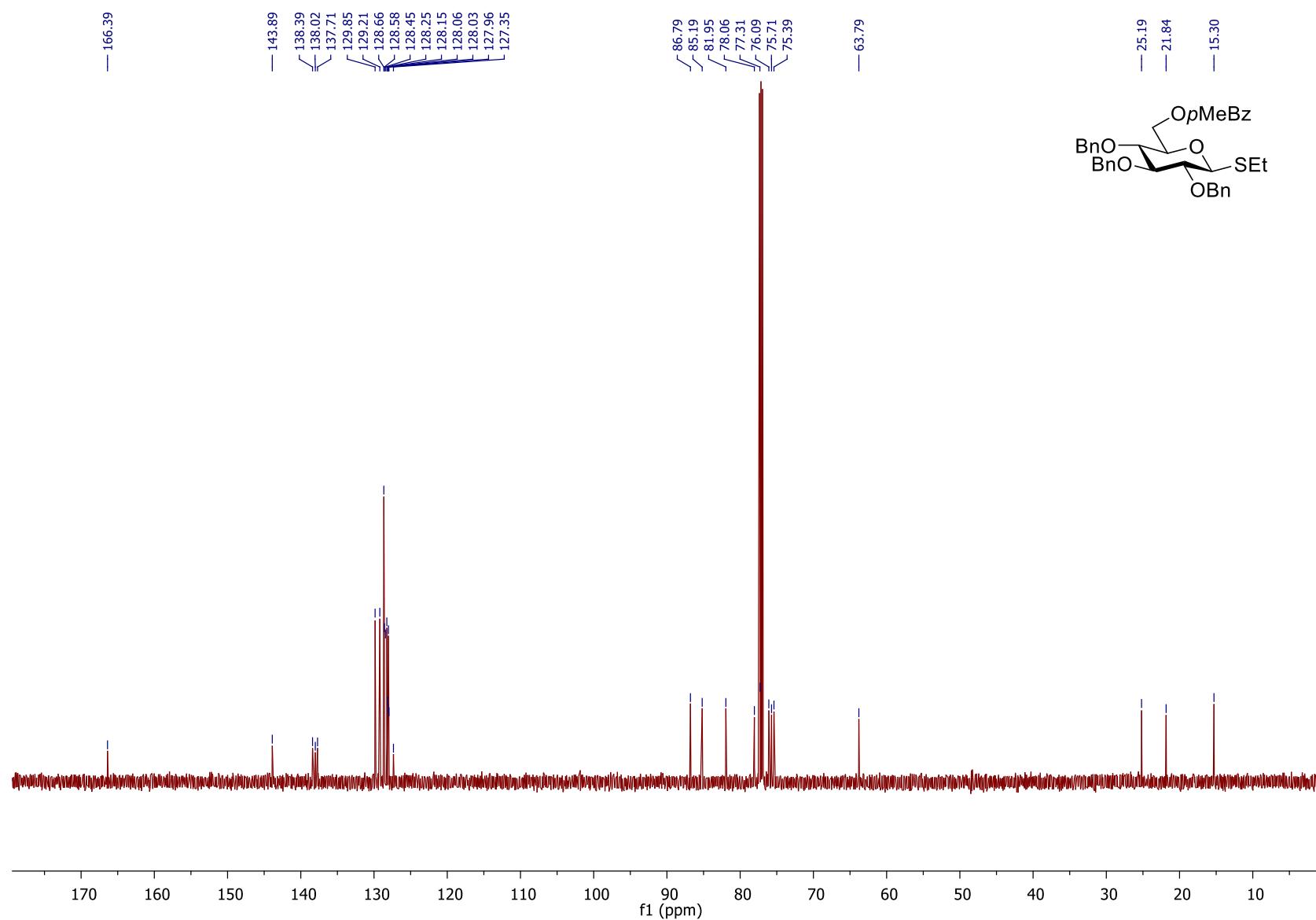
¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl (6*S*)-[6-²H₁]-6-*O*-benzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**6S-D-31**)



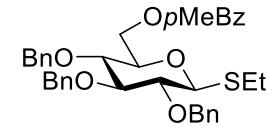
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 6-*O*-*p*-methylbenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**32**)



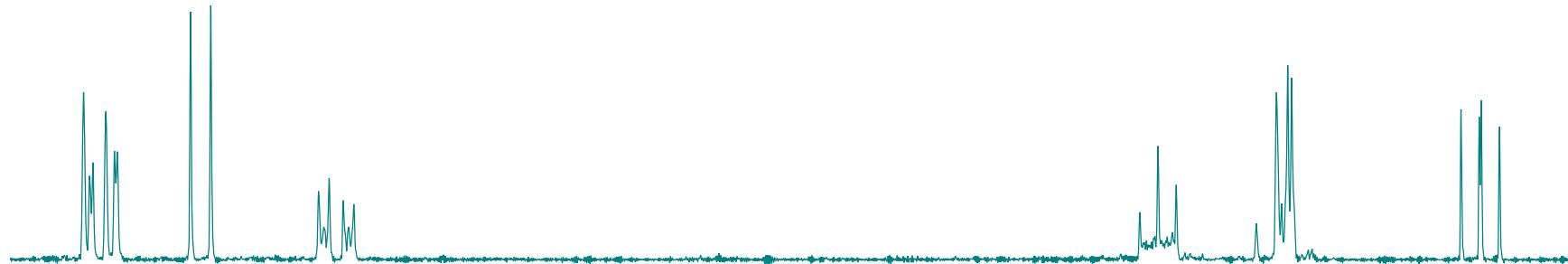
¹³C NMR (150 MHz, CDCl₃) Spectrum of Ethyl 6-*O*-*p*-methylbenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**32**)



Simulated ^1H NMR and ^1H NMR (600 MHz, CDCl_3) Spectrum of Ethyl 6-*O*-*p*-methylbenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**32**)



Experimental $^1\text{H-NMR}$ (600 MHz, CDCl_3)

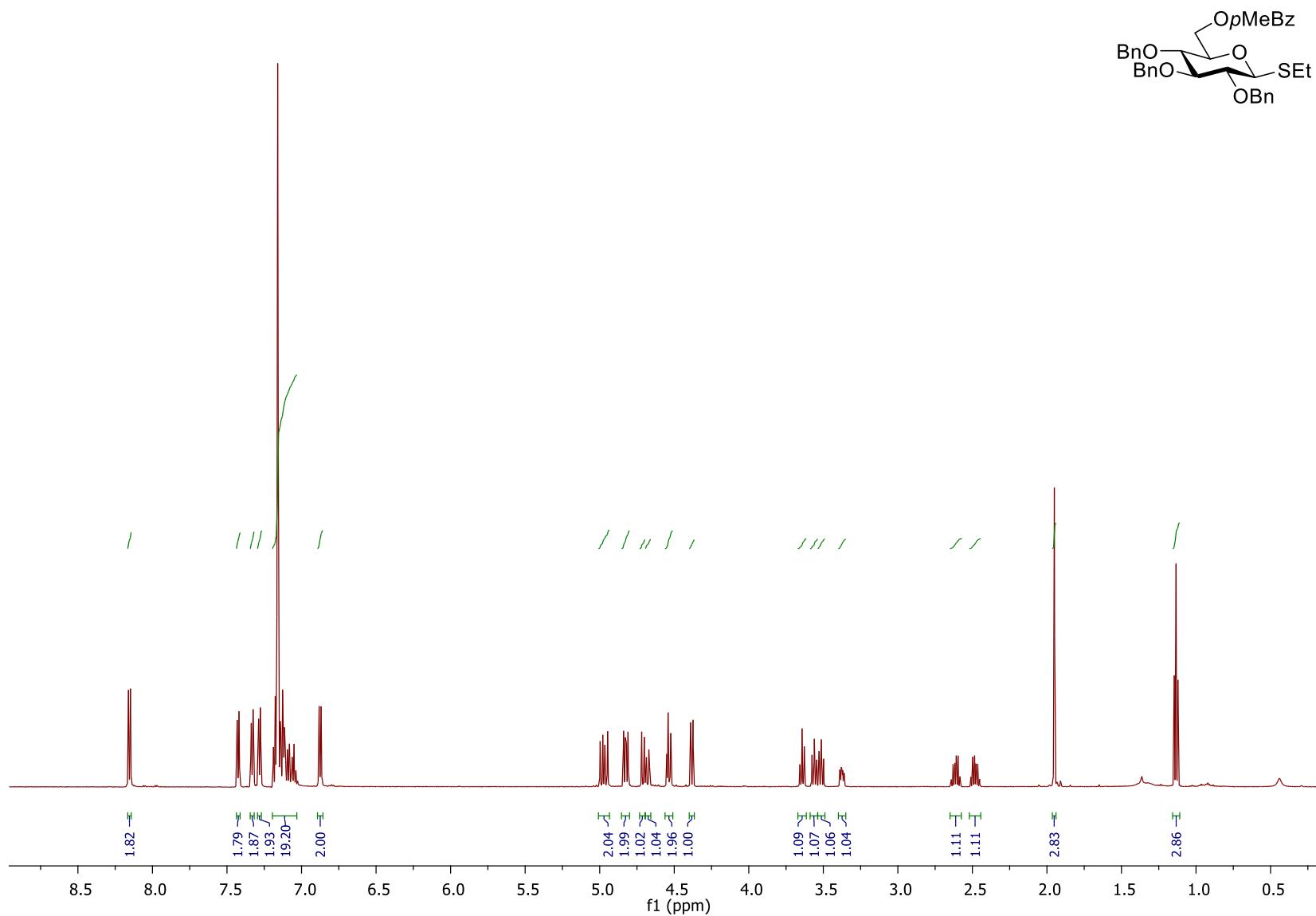


Simulated $^1\text{H-NMR}$

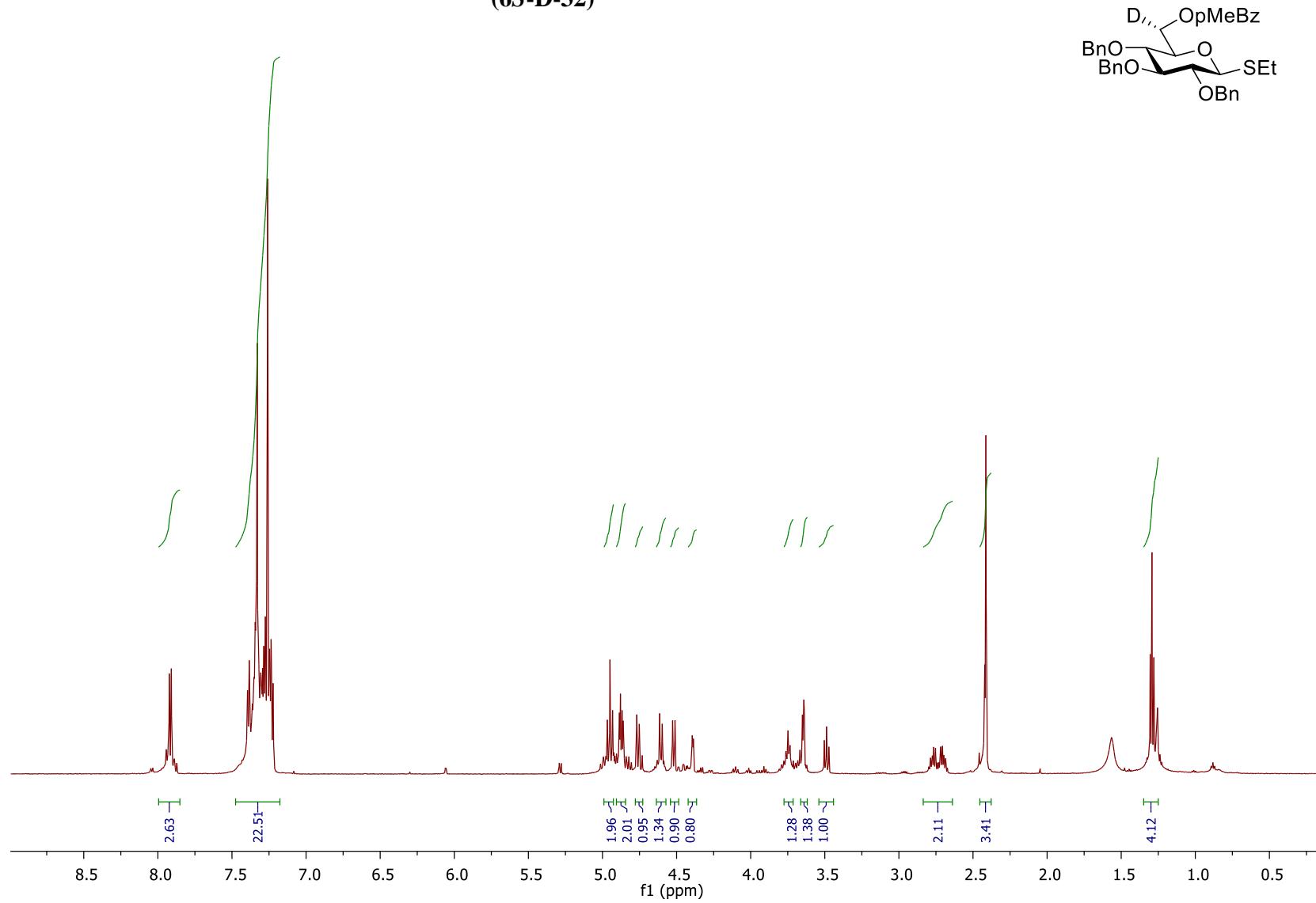


4.65 4.60 4.55 4.50 4.45 4.40 4.35 4.30 4.25 4.20 4.15 4.10 4.05 4.00 3.95 3.90 3.85 3.80 3.75 3.70 3.65 3.60 3.55 3.50 3.45
 $f1s(\text{ppm})$

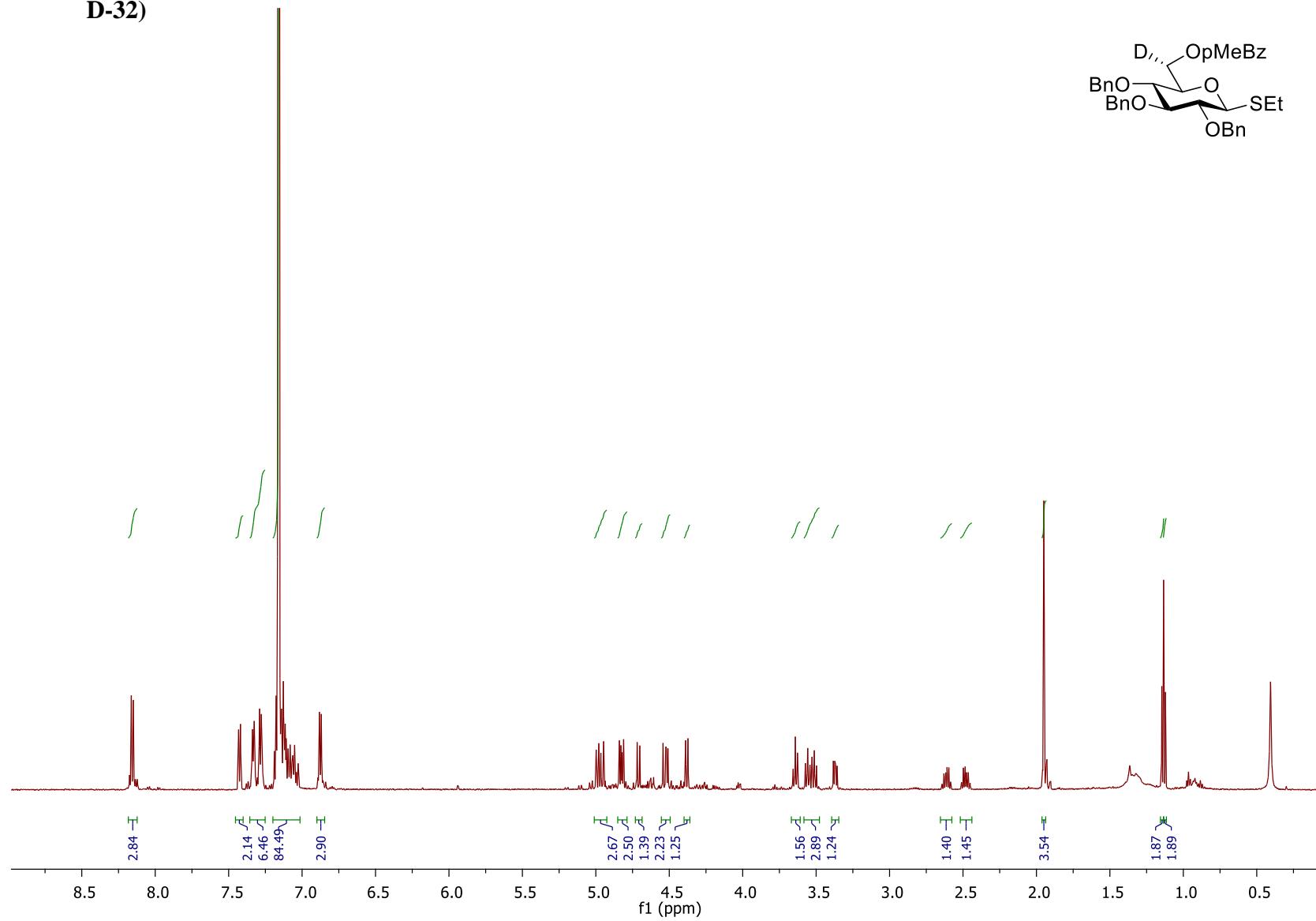
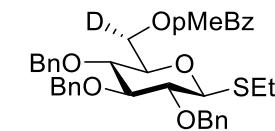
^1H NMR (600 MHz, C_6D_6) Spectrum of Ethyl 6-*O*-*p*-methylbenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**32**)



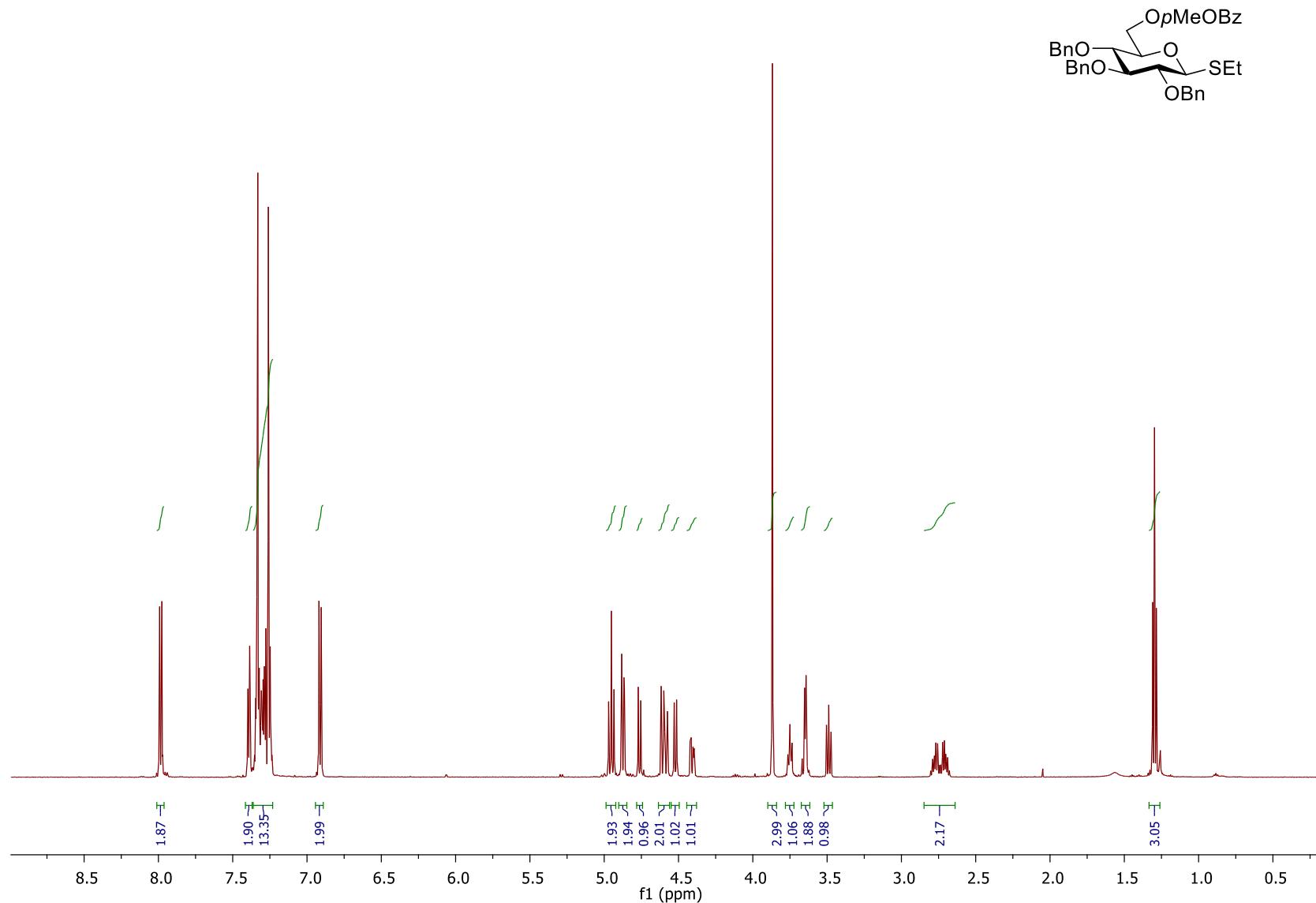
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl (6*S*)-[6-²H₁]-6-*O*-*p*-methylbenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside
(6*S*-D-32)



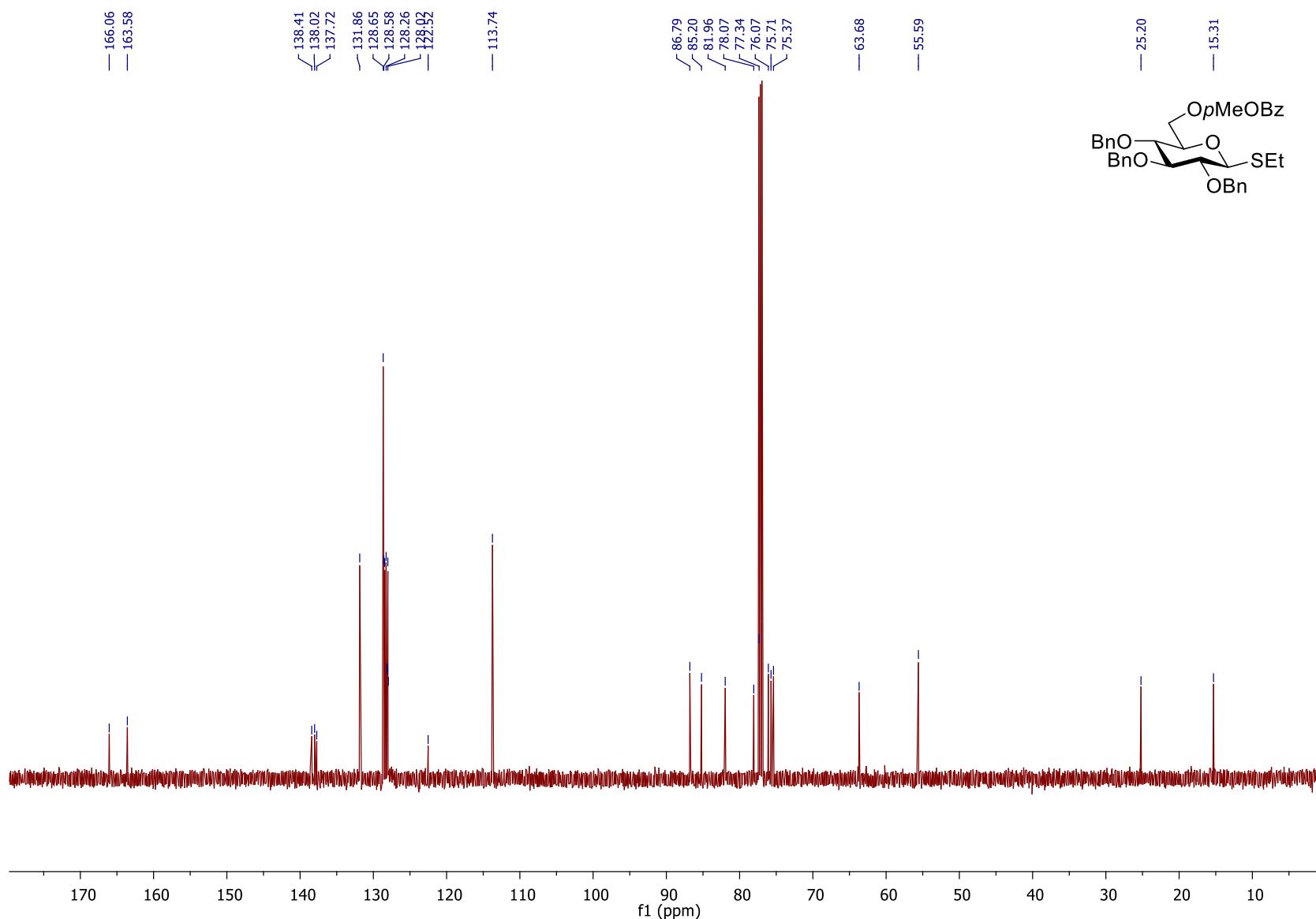
¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl (6S)-[6-²H₁]-6-O-p-methylbenzoyl-2,3,4-tri-O-benzyl-1-thio-β-D-glucopyranoside (**6S-D-32**)



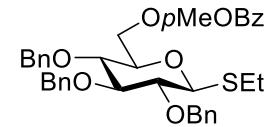
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 6-*O*-*p*-methoxybenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**33**)



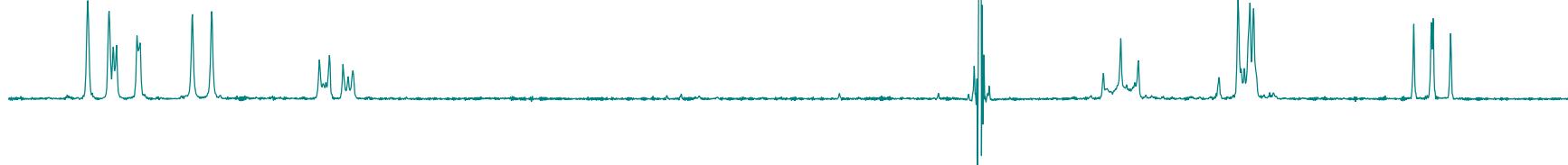
^{13}C NMR (150 MHz, CDCl_3) Spectrum of Ethyl 6-*O*-*p*-methoxybenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**33**)



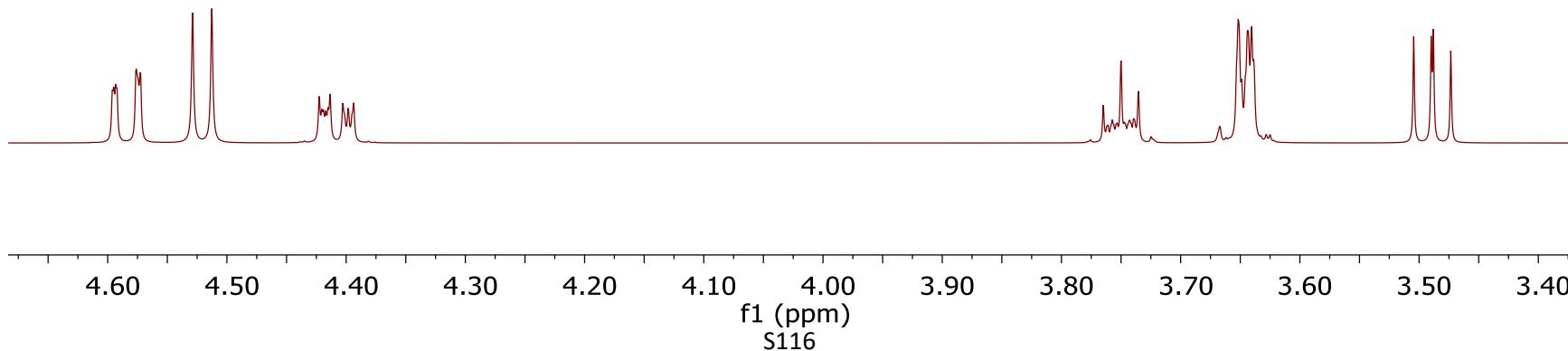
Simulated ^1H NMR and Experimental ^1H NMR (600 MHz, CDCl_3) Spectrum of Ethyl 6-*O*-*p*-methoxybenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**33**)



Experimental ^1H -NMR (600 MHz, CDCl_3)

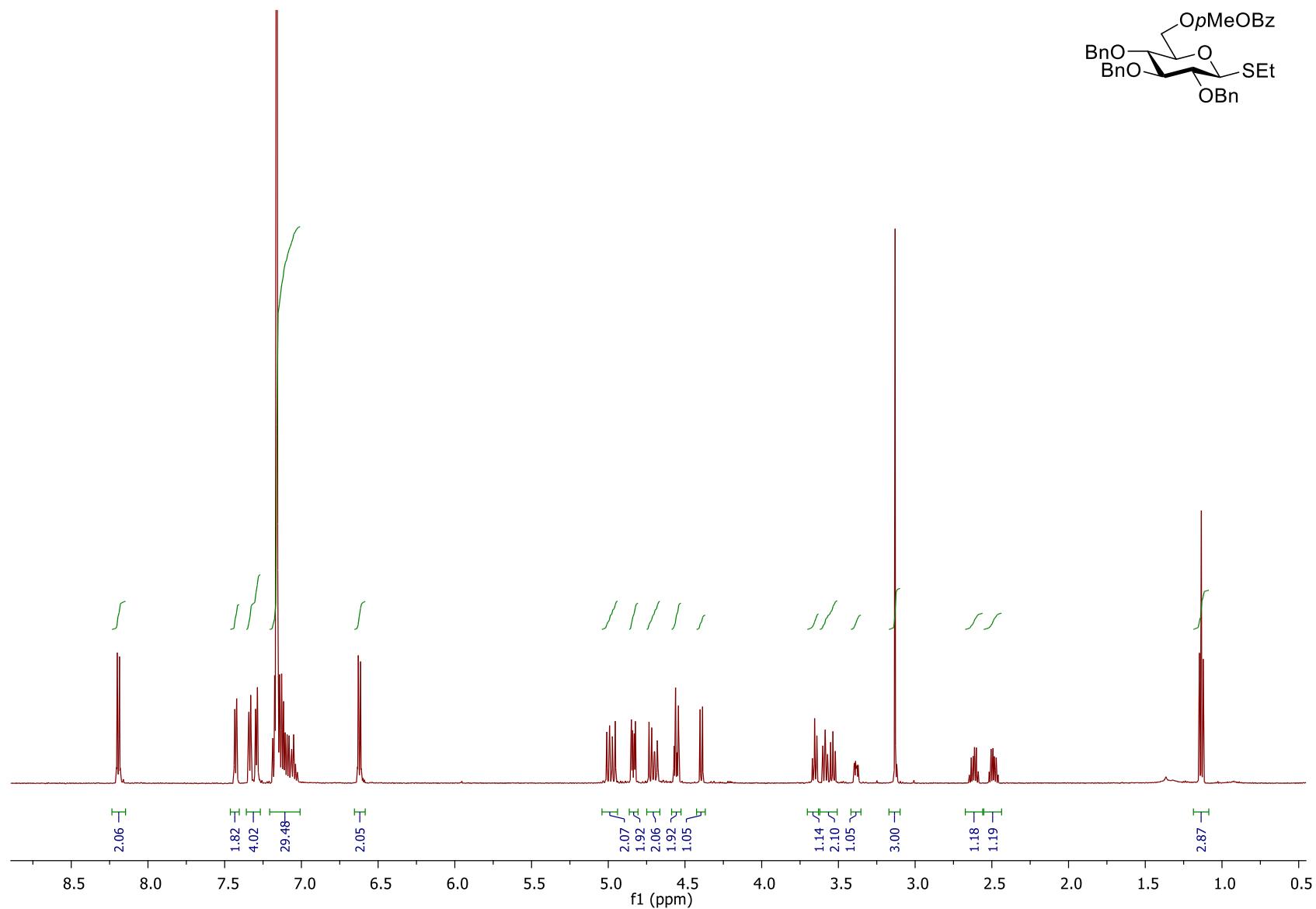


Simulated ^1H -NMR

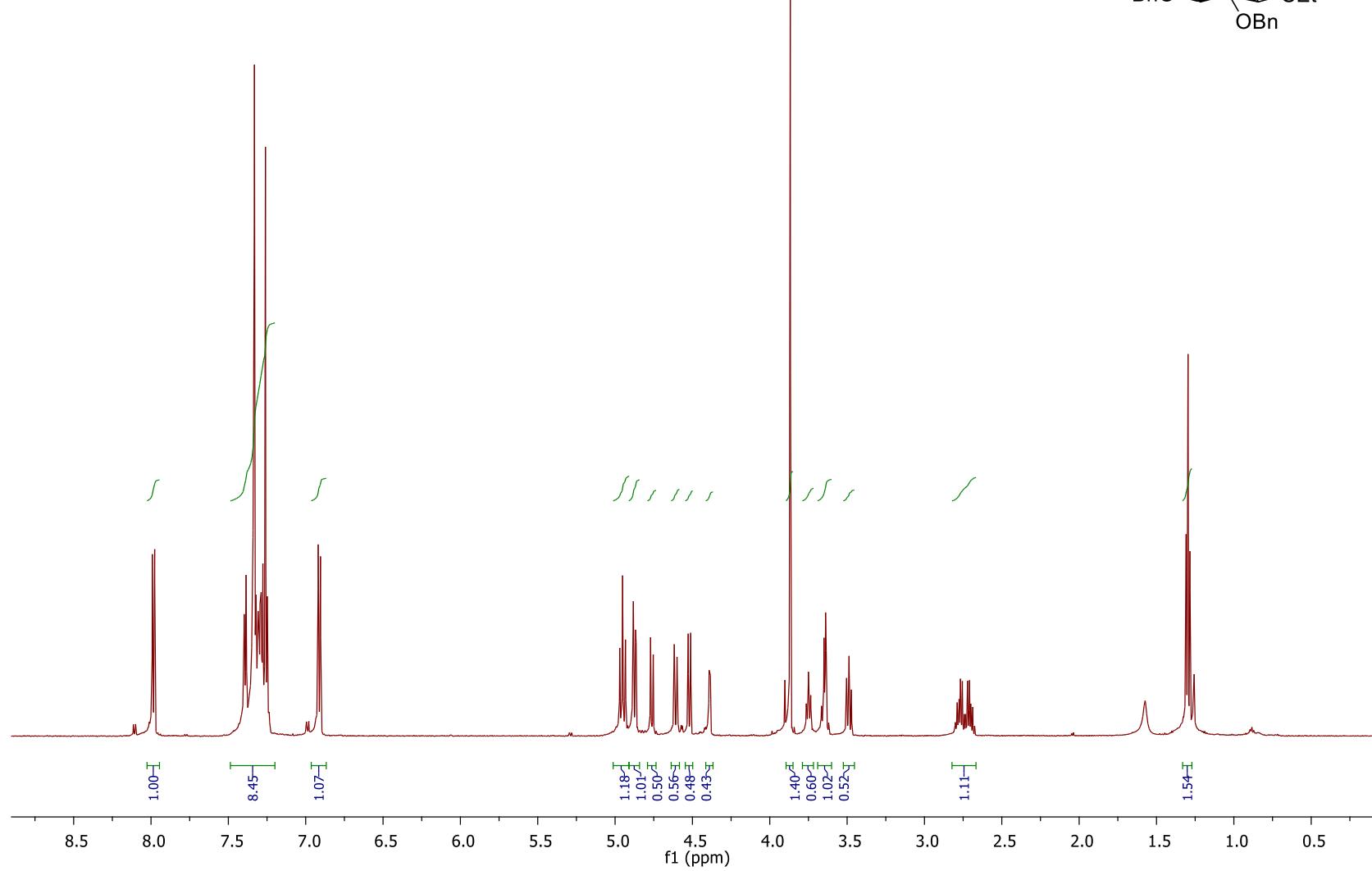
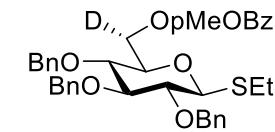


f1 (ppm)
S116

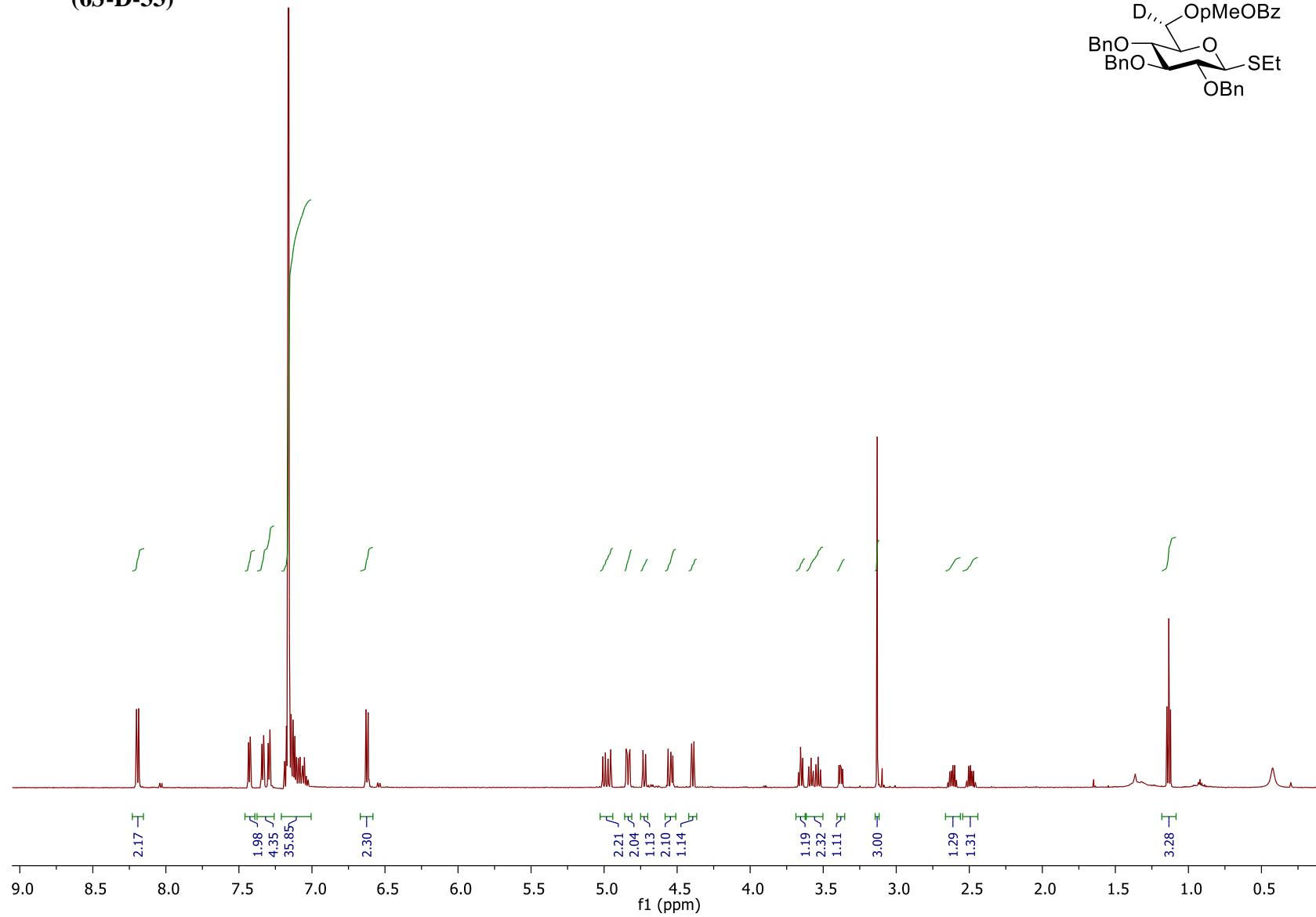
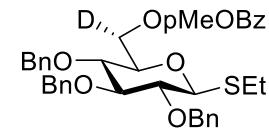
¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl 6-*O*-*p*-methoxybenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**33**)



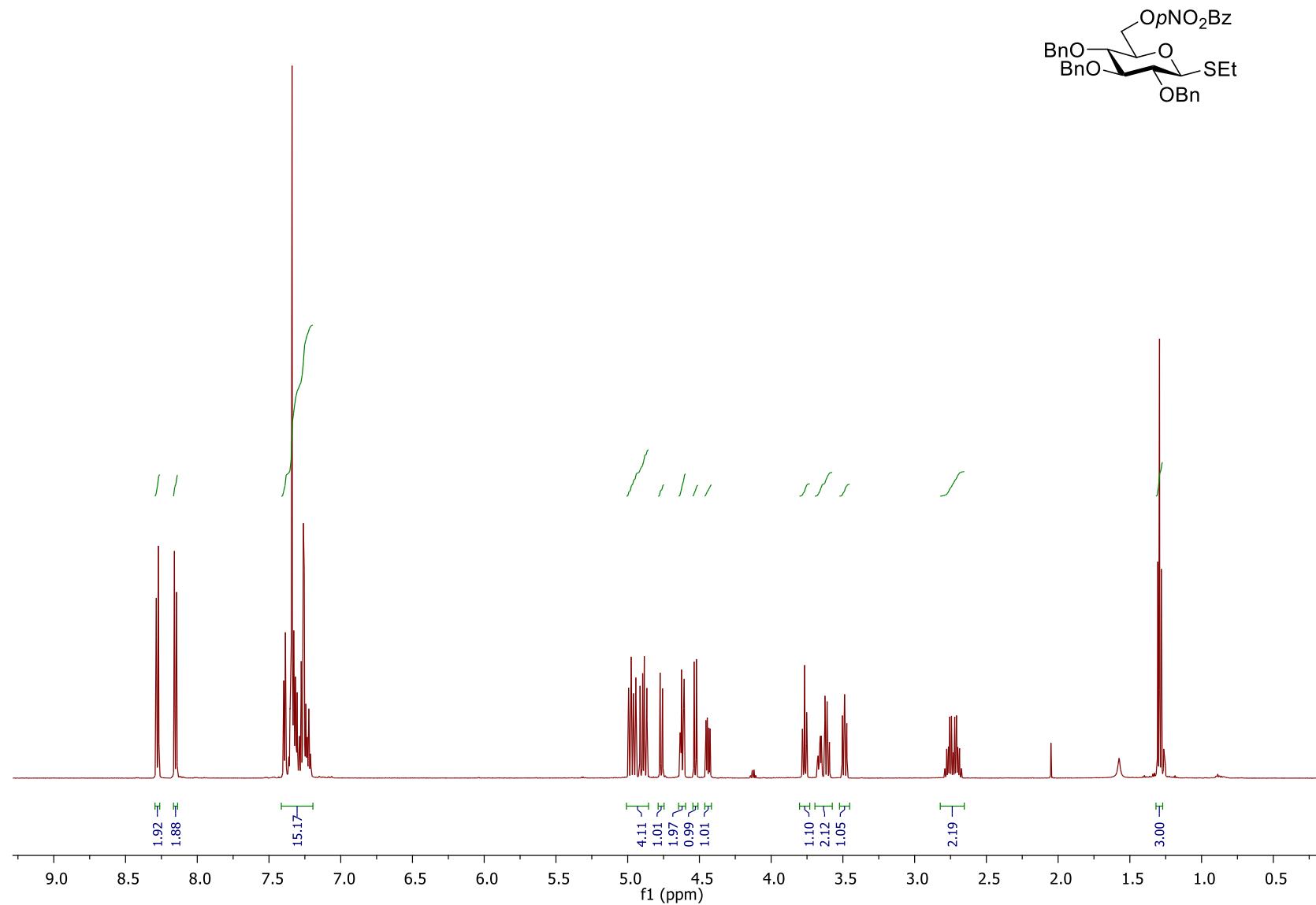
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl (6*S*)-[6-²H₁]-6-*O*-*p*-methoxybenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside
(6*S*-D-33)



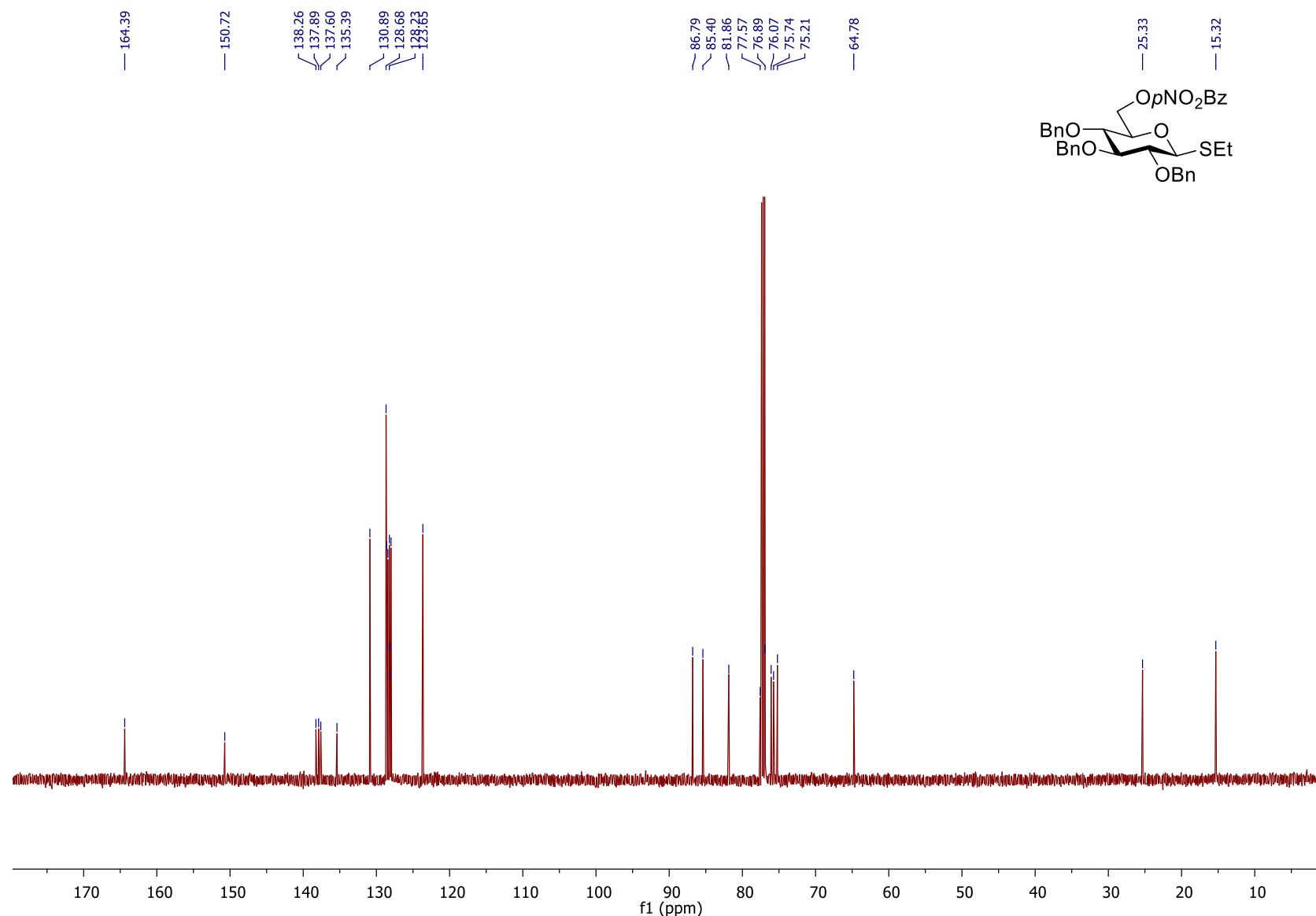
¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl (6*S*)-[6-²H₁]-6-*O*-*p*-methoxybenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside
(6*S*-D-33)



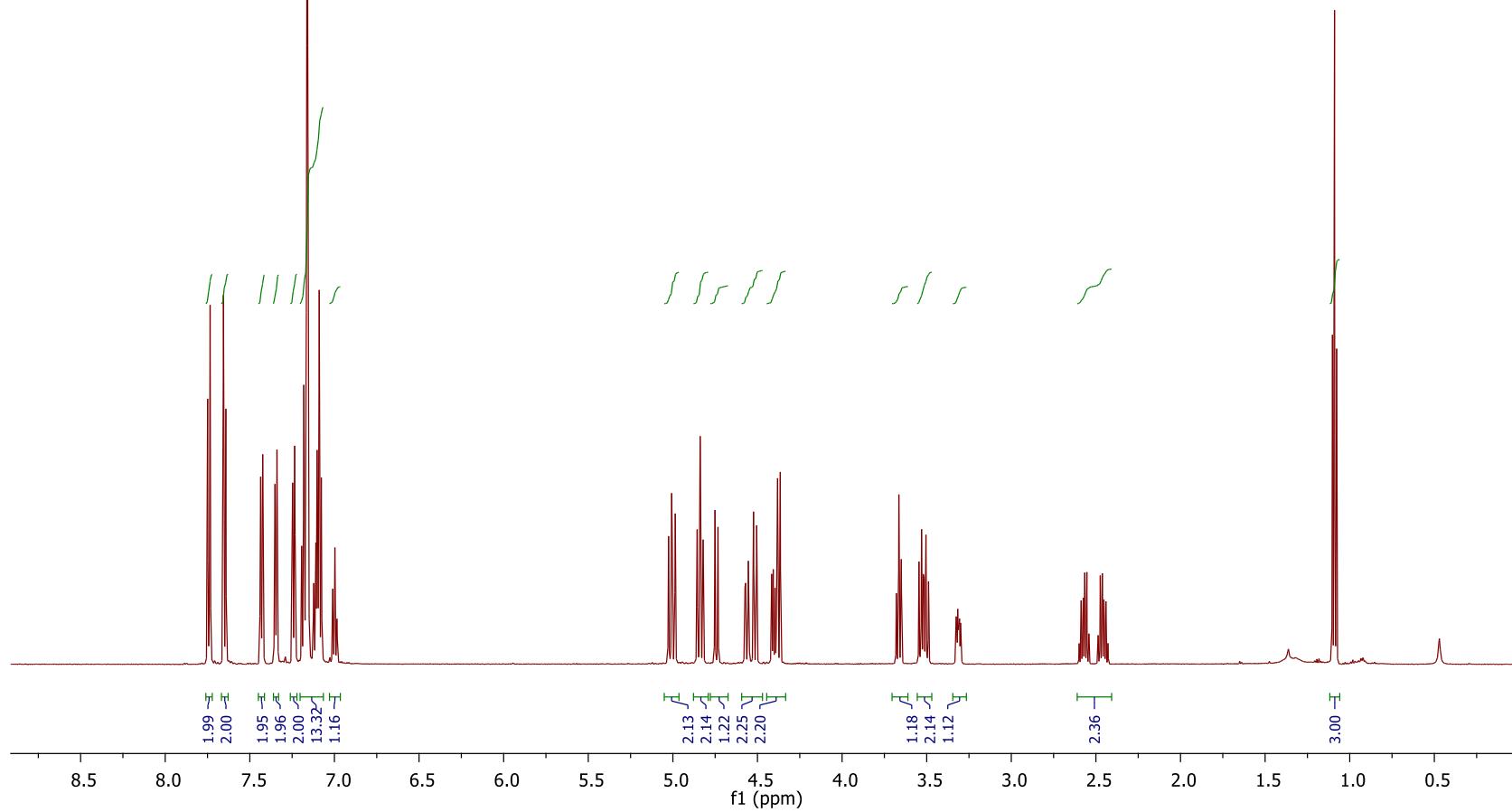
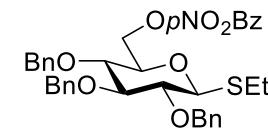
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 6-*O*-*p*-nitrobenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**34**)



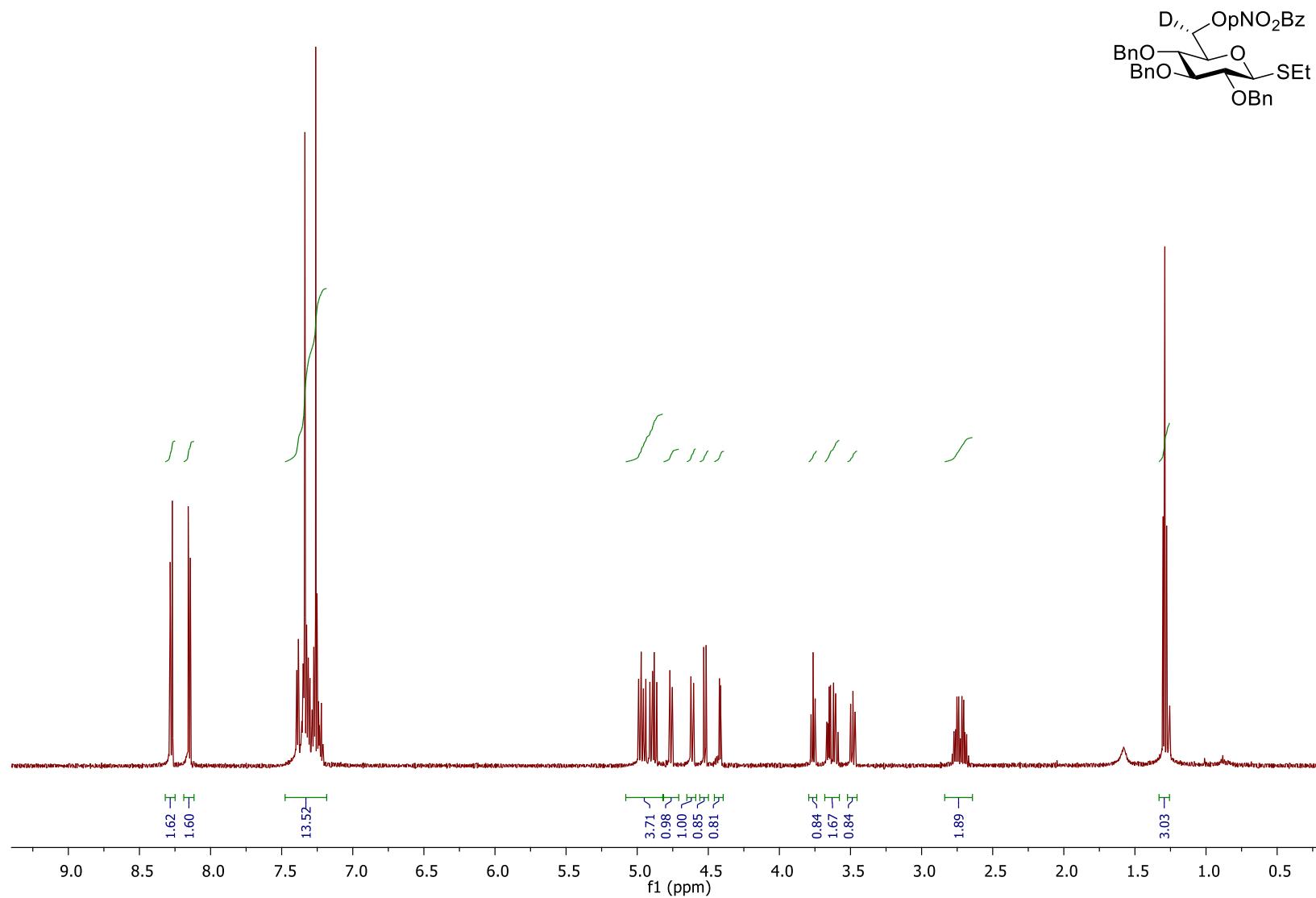
¹³C NMR (150 MHz, CDCl₃) Spectrum of Ethyl 6-*O*-*p*-nitrobenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**34**)



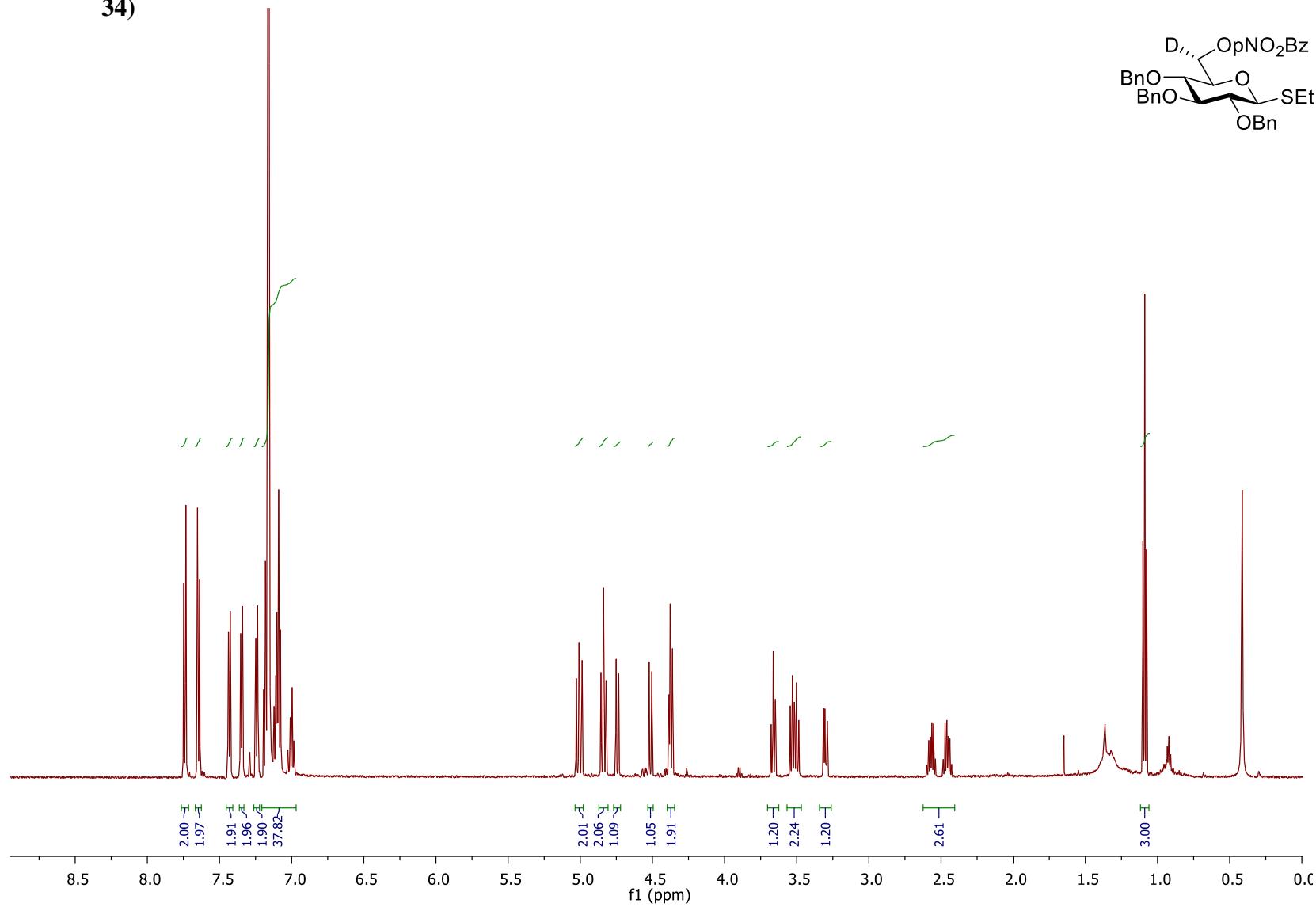
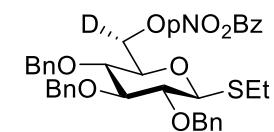
¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl 6-*O*-*p*-nitrobenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**34**)



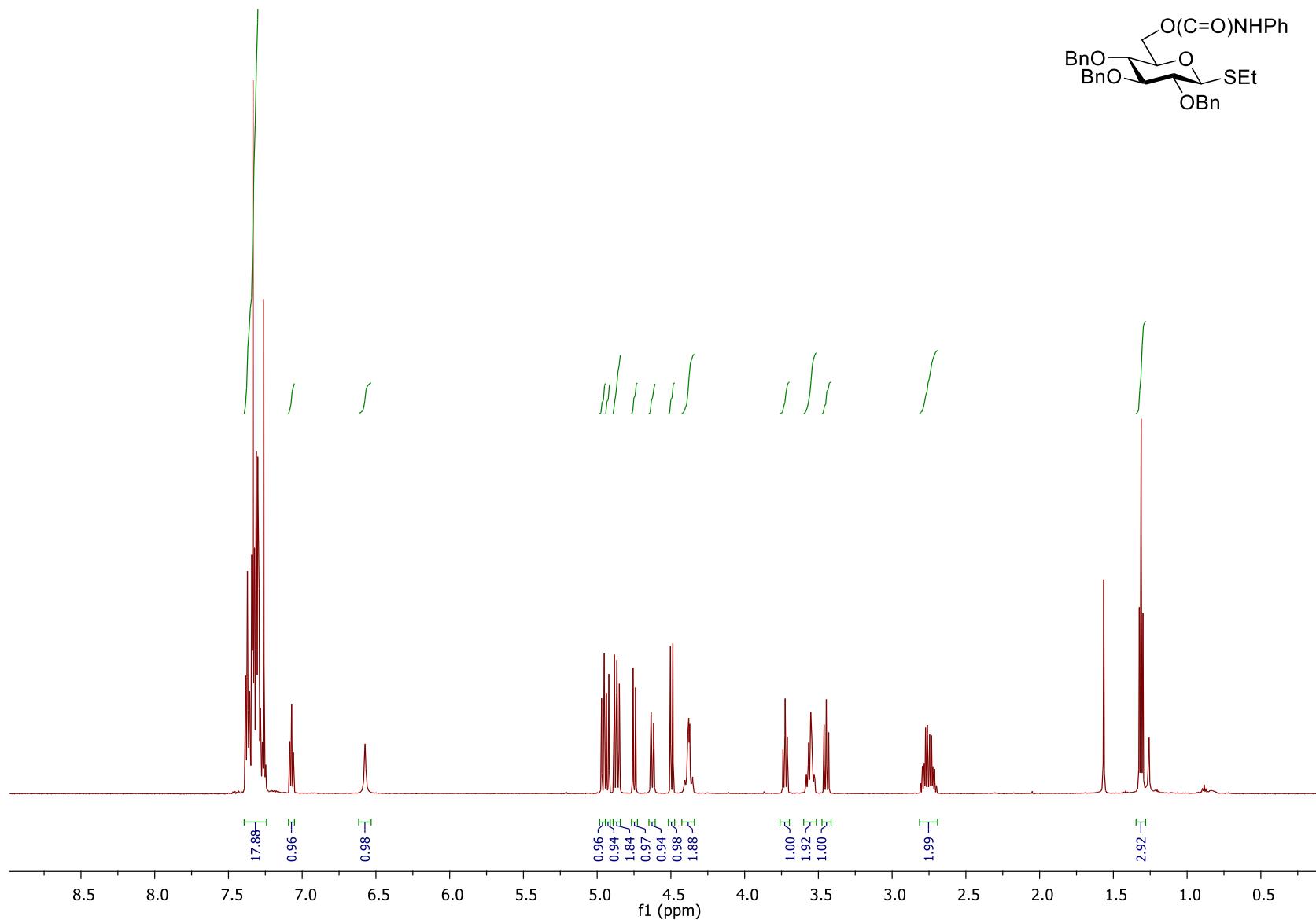
^1H NMR (600 MHz, CDCl_3) Spectrum of Ethyl (6*S*)-[6- $^2\text{H}_1$]-6-*O*-*p*-nitrobenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β D-glucopyranoside (**6S-D-34**)



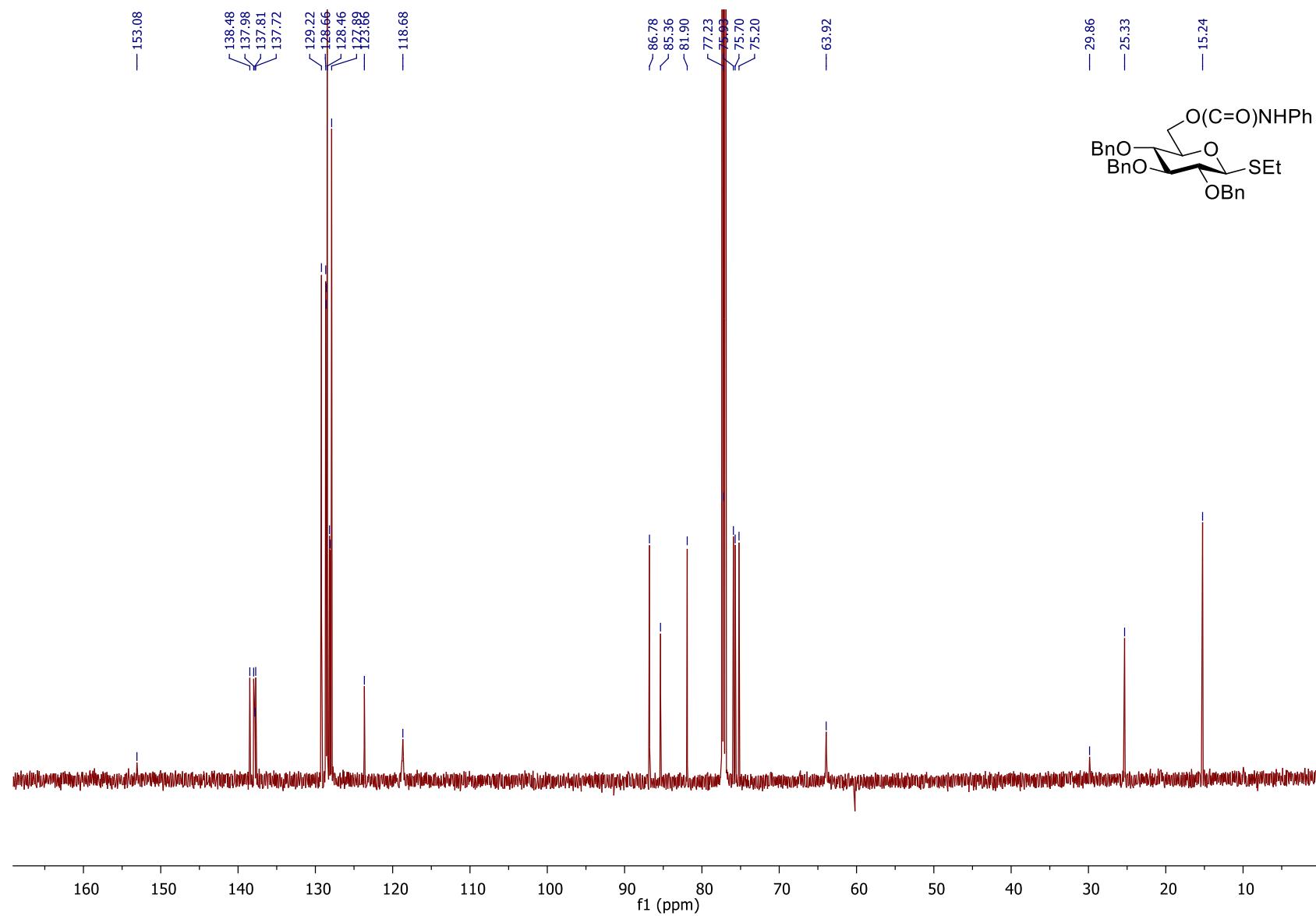
¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl (6*S*)-[6-²H₁]-6-*O*-*p*-nitrobenzoyl-2,3,4-tri-*O*-benzyl-1-thio- β -D-glucopyranoside (**6S-D-34**)



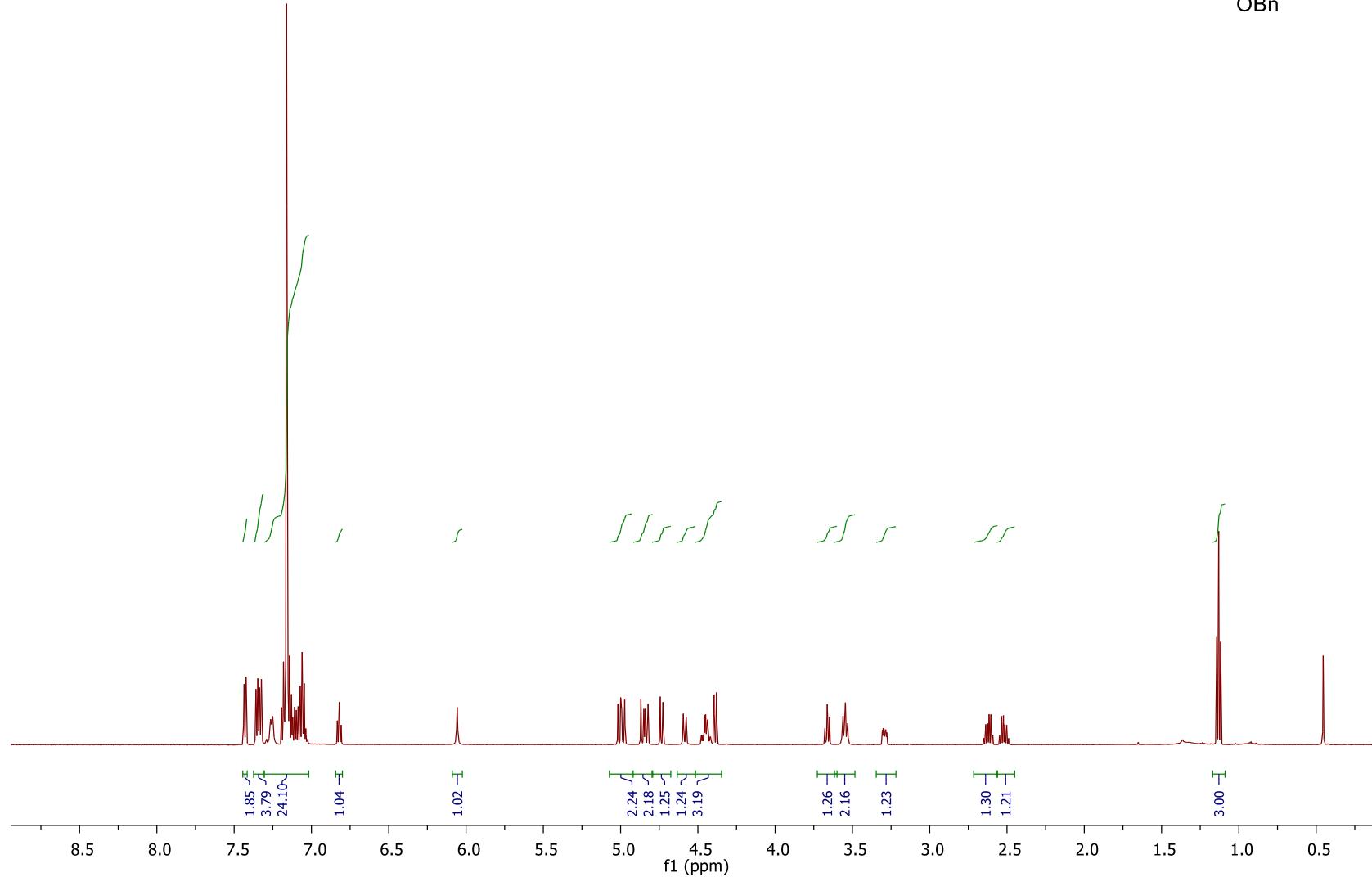
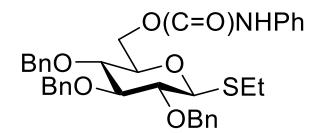
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 2,3,4-tri-*O*-benzyl-6-*O*-(*N*-phenylcarbamoyl)-1-thio- β -D-glucopyranoside (**35**)



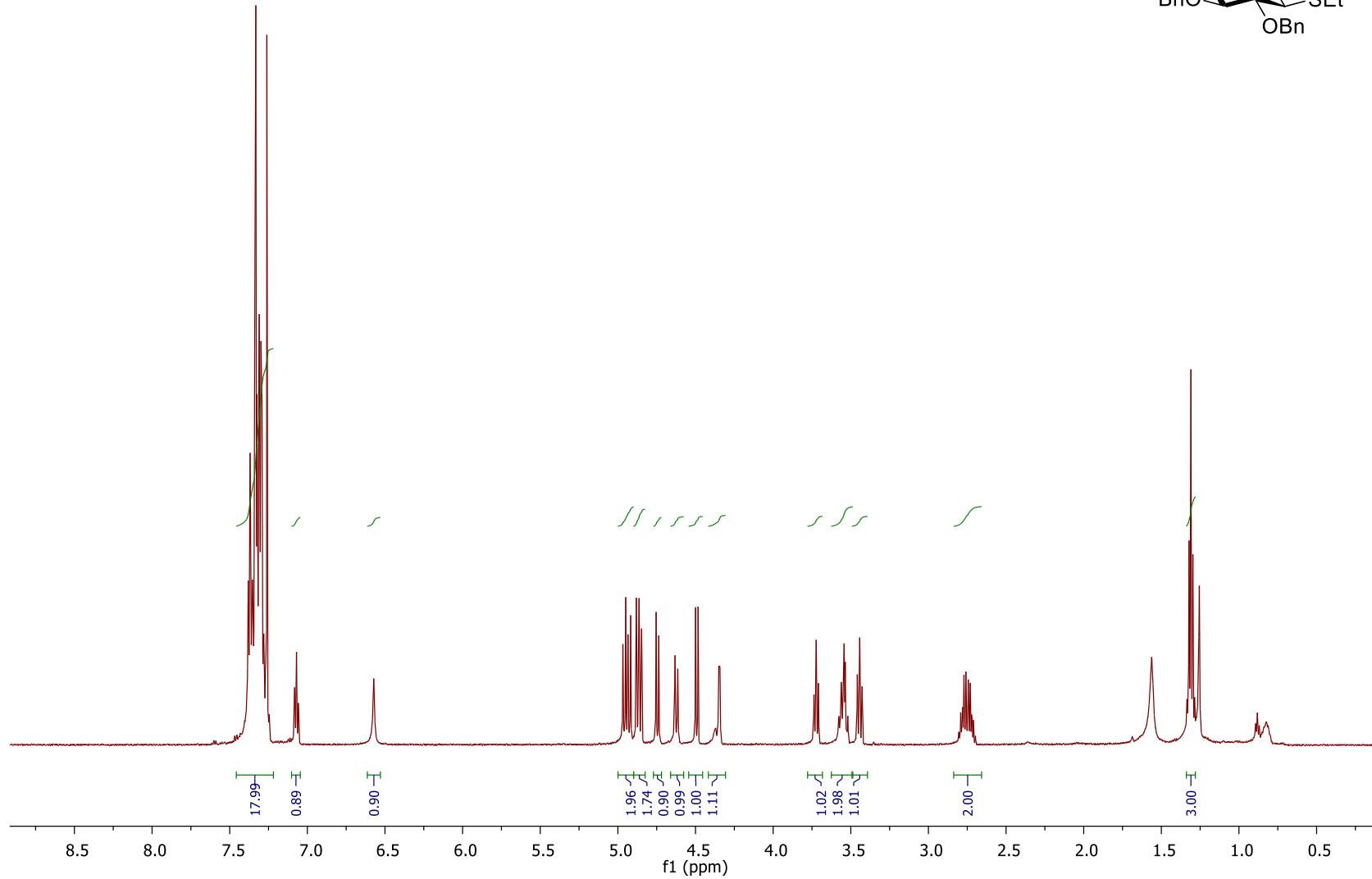
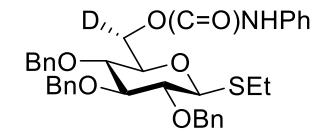
^{13}C NMR (150 MHz, CDCl_3) Spectrum of Ethyl 2,3,4-tri- O -benzyl-6- O -(*N*-phenylcarbamoyl)-1-thio- β -D-glucopyranoside (**35**)



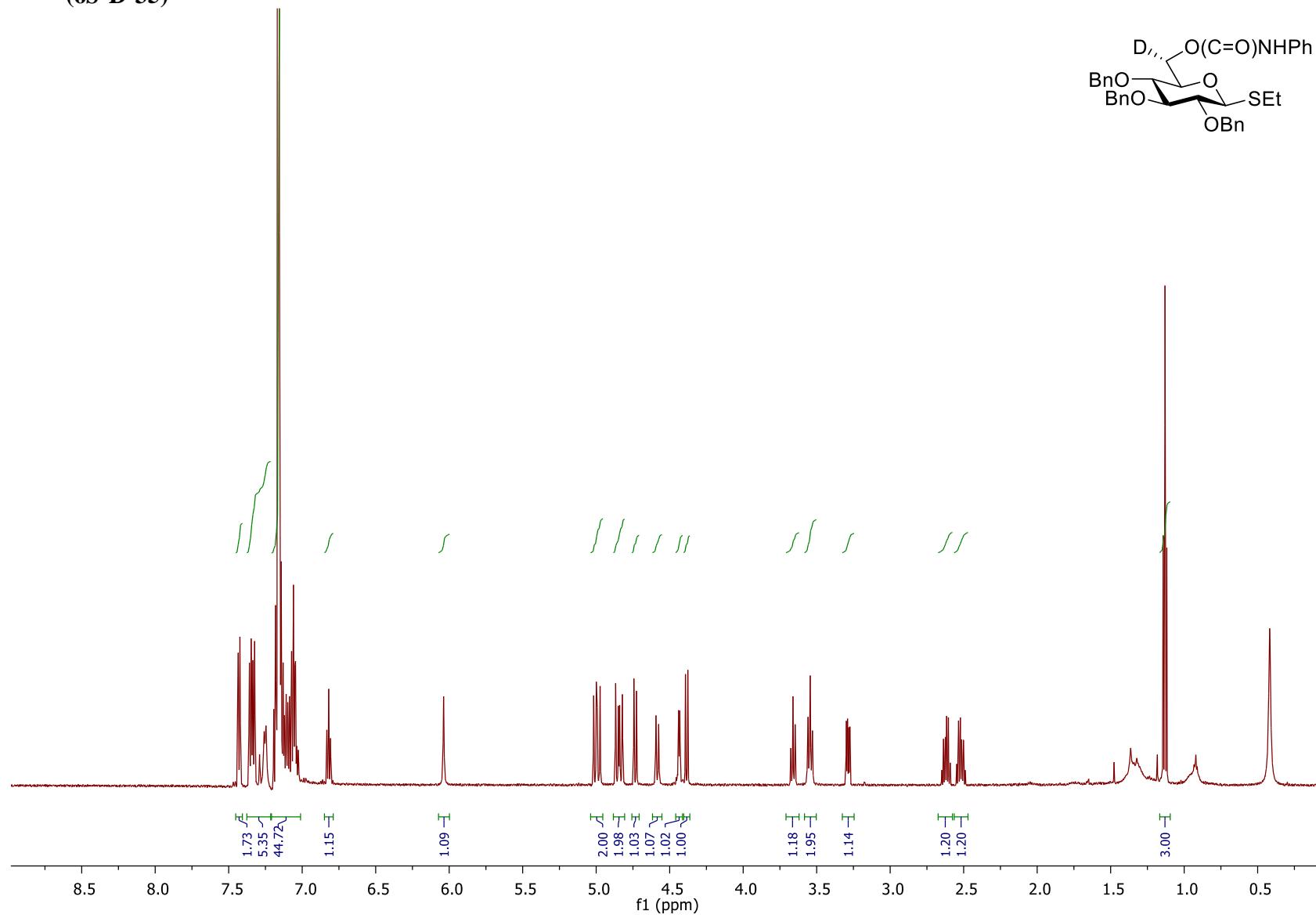
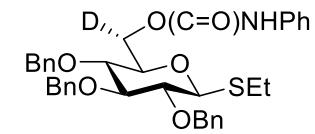
^1H NMR (600 MHz, C_6D_6) Spectrum of Ethyl 2,3,4-tri- O -benzyl-6- O -(*N*-phenylcarbamoyl)-1-thio- β -D-glucopyranoside (**35**)



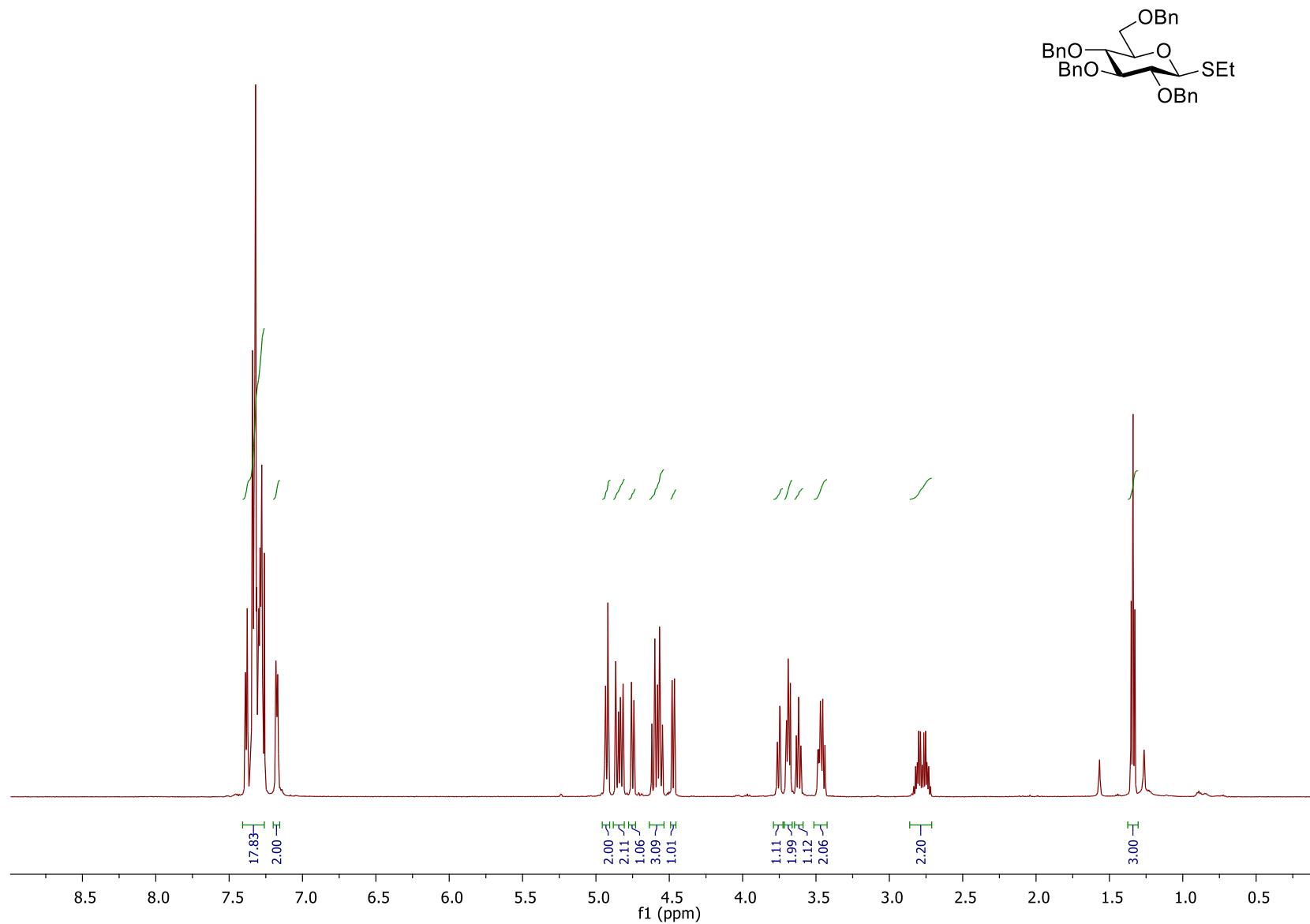
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 2,3,4-tri-O-benzyl-(6*S*)-[6-²H]-6-*O*-(*N*-phenylcarbamoyl)-1-thio-β-D-glucopyranoside (**6S-D-35**)



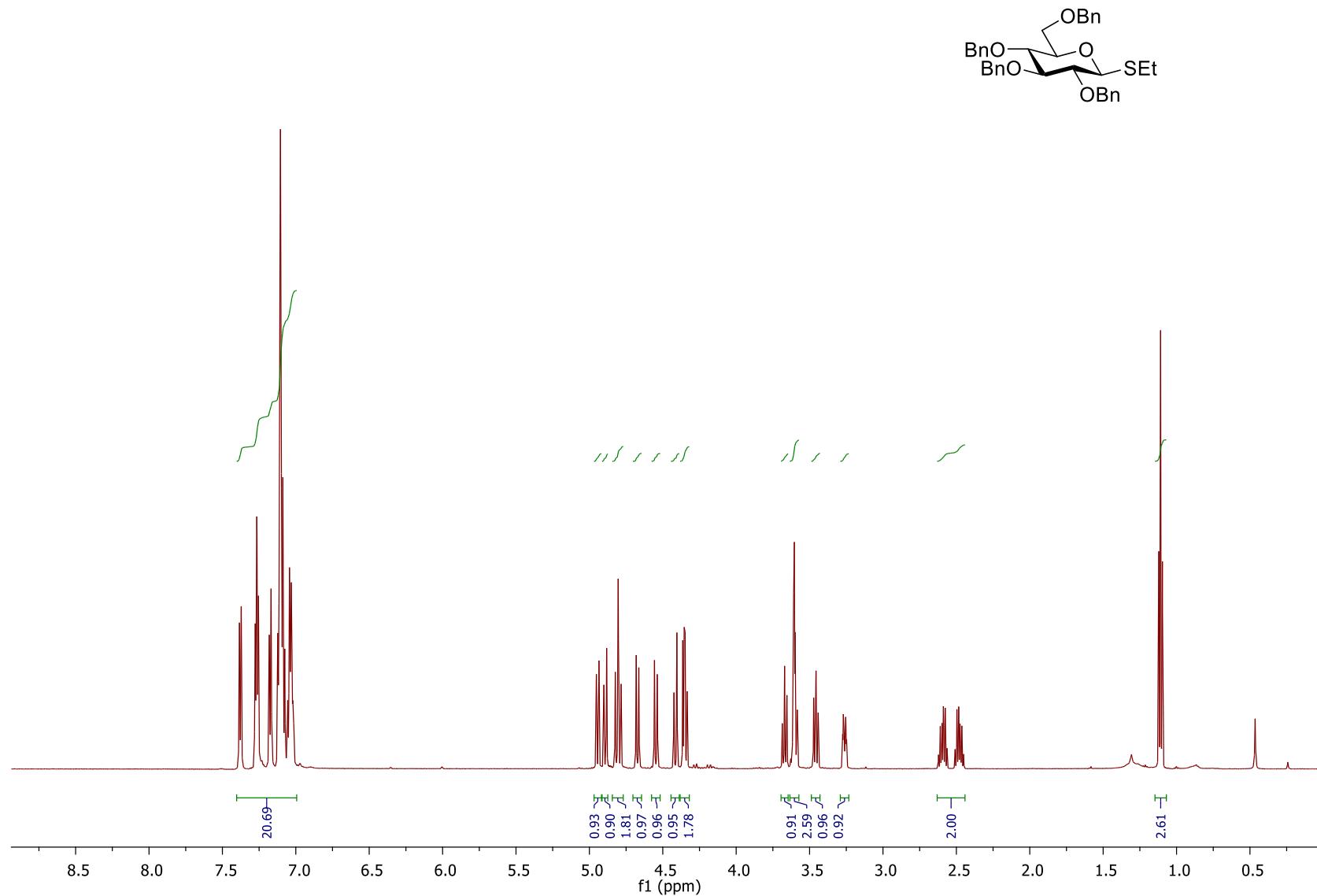
^1H NMR (600 MHz, C_6D_6) Spectrum of Ethyl 2,3,4-tri- O -benzyl-(6*S*)-[6- $^2\text{H}_1$]-6- O -(*N*-phenylcarbamoyl)-1-thio- β -D-glucopyranoside
(6*S*-D-35)



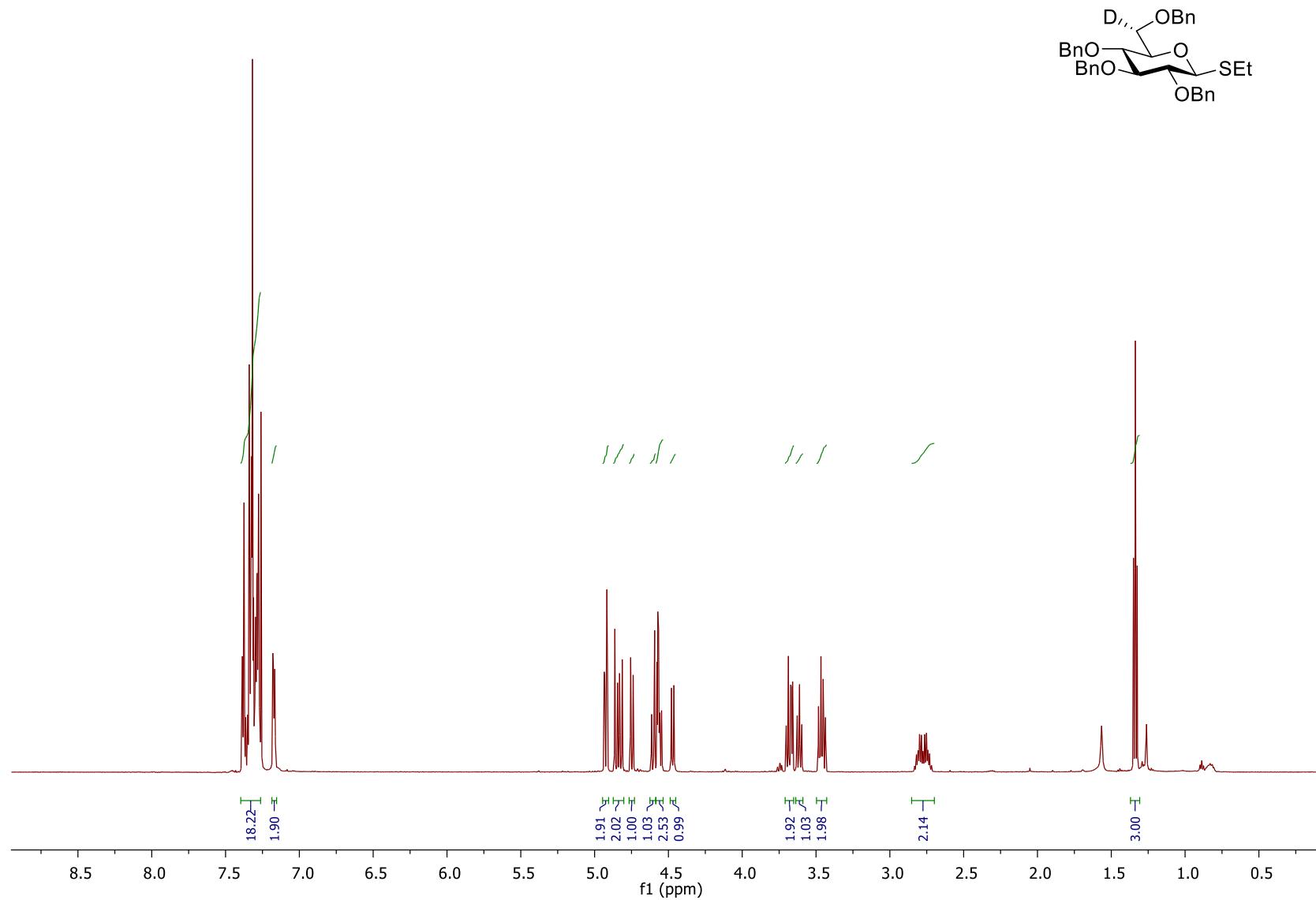
¹H NMR (600 MHz, CDCl₃) Spectrum of Ethyl 2,3,4,6-tetra-O-benzyl-1-thio-β-D-glucopyranoside (**36**)



¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl 2,3,4,6-tetra-O-benzyl-1-thio-β-D-glucopyranoside (**36**)



^1H NMR (600 MHz, CDCl_3) Spectrum of Ethyl (6*S*)-[6- $^2\text{H}_1$]-2,3,4,6-tetra-*O*-benzyl-1-thio- β -D-glucopyranoside (**6S-D-36**)



¹H NMR (600 MHz, C₆D₆) Spectrum of Ethyl (6*S*)-[6-²H₁]-2,3,4,6-tetra-*O*-benzyl-1-thio- β -D-glucopyranoside (**6S-D-36**)

