Supplementary Material (ESI) for New Journal of Chemistry

Synthesis and screening of a small glycomimetic library for inhibitory activity on medically relevant galactoside-specific lectins in assays of increasing biorelevance

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Experimental

General

All reactions involving water-sensitive chemicals were carried out in flamedried glassware with magnetic stirring under a nitrogen atmosphere. Anhydrous DCM was distilled from CaH_2 and anhydrous THF were distilled from Na/K prior to use. All non-aqueous reactions were carried out under anhydrous conditions within an nitrogen atmosphere in distilled solvents. All other solvents and reagents were used as received. TLC was performed on aluminium plates (silica gel 60 F254) with detection by UV or by coloration with ammonium molybdate in acid solution. Column chromatography were performed on silica gel (230-400 mesh) with the indicated eluent. NMR spectra were recorded at 22 °C on Varian Gemini 300 MHz or Innova 600 MHz spectrometers. Proton and carbon chemical shifts are reported in ppm (δ) relative to $CDCl_3$ (δ 7.27 and 77.00 ppm for ^{1}H- and ^{13}C-NMR, respectively) or relative to the signal of D_2O (δ 4.81 ppm for ^{1}H) or CD_3OD (3.31 and 49.0 ppm for ^{1}H- and ^{13}C) or DMSO*d6* (2.49 and 39.5 ppm for ^{1}H- and ^{13}C-NMR, respectively) as internal standard. Coupling constants (*J*) are reported in Hertz (Hz), and the following abbreviations are used for signal multiplicities: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), multiplet (m), broad (b). Analysis of the spectra and assignments were made by COSY, DEPT, and HETCOR experiments. Optical rotations were measured on a Polarimeter JASCO P-1000, melting point on a Fisher-Johns Point Apparatus. High-resolution mass spectrometry (HRMS) was carried out in our analytical laboratory and by the analytical platform of UQAM (Université du Québec à Montréal, QC, Canada).

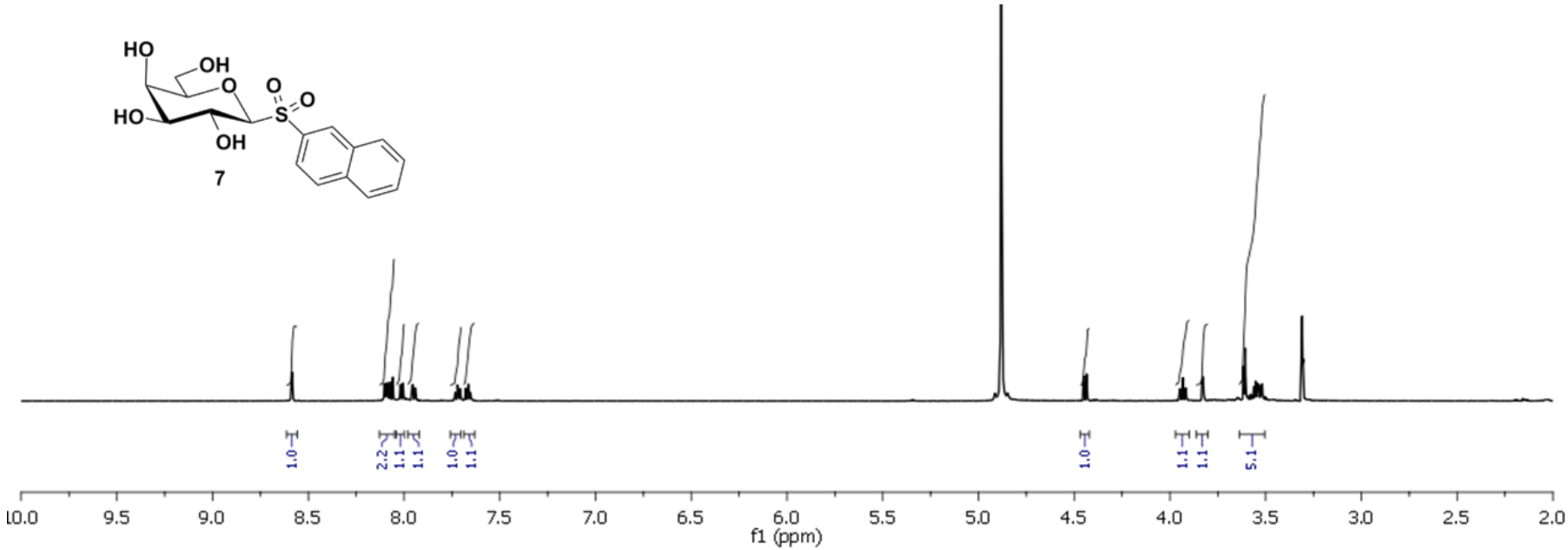

Figure 1. ^{1}H NMR of β-Naphthyl 1-sulfonyl-β-D-galactopyranoside **(7)**

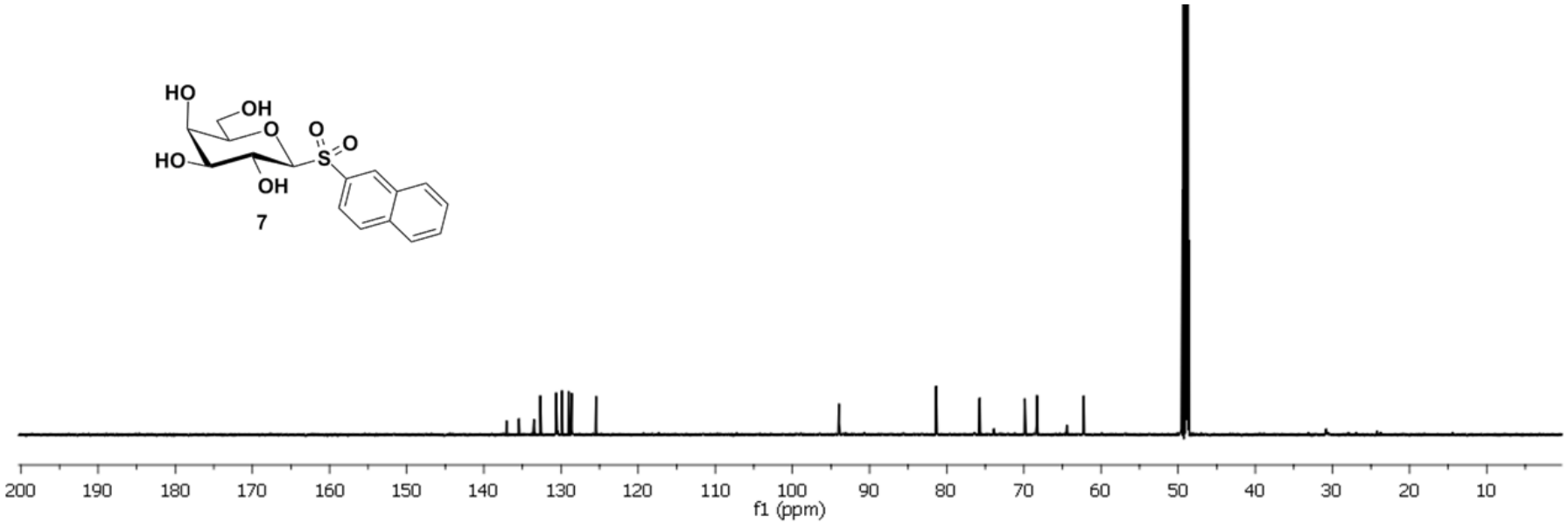

Figure 2. ^{13}C NMR of β-Naphthyl 1-sulfonyl-β-D-galactopyranoside **(7)**

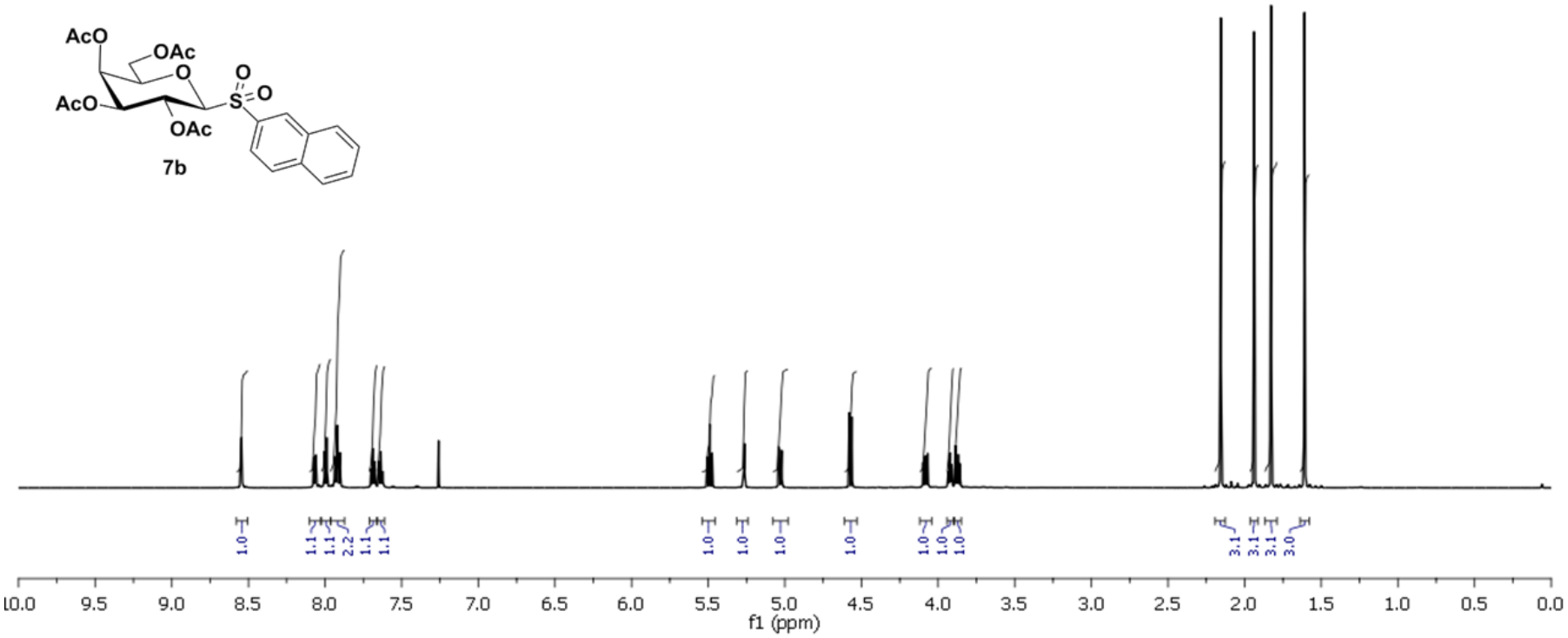

Figure 3. ^{1}H NMR of β-Naphthyl 2,3,4,6-tetra-O-acetyl-1-sulfonyl-β-D-galactopyranoside **(7b)**

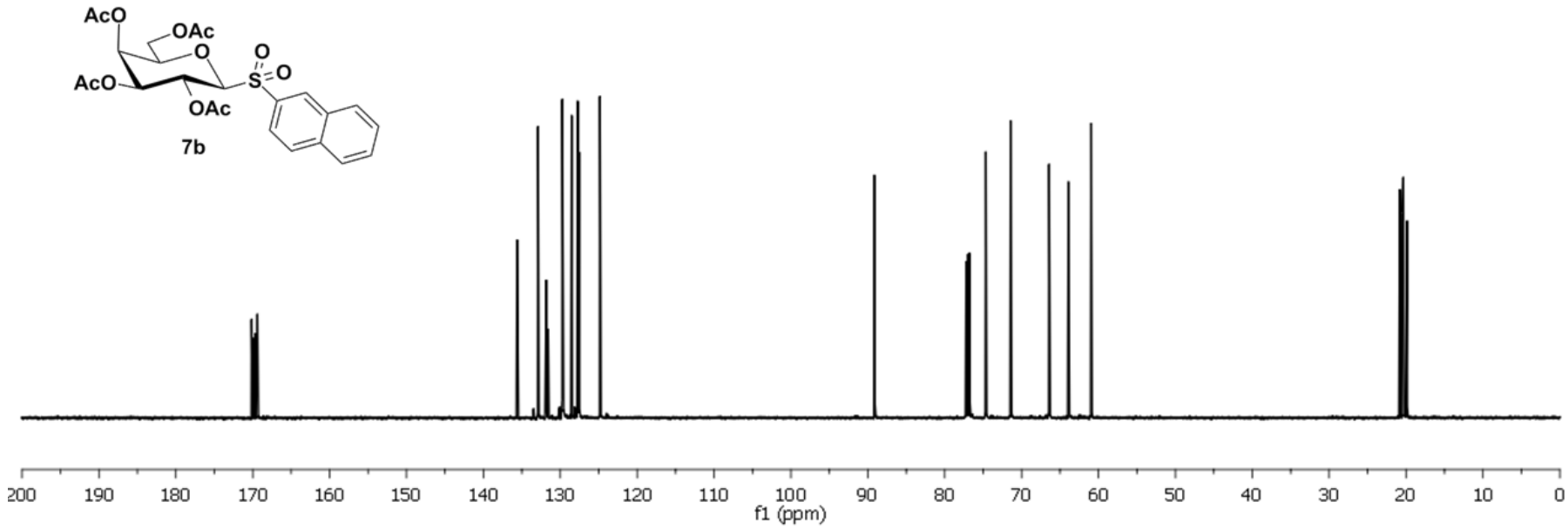

Figure 4. ^{13}C NMR of β-Naphthyl 2,3,4,6-tetra-O-acetyl-1-sulfonyl-β-D-galactopyranoside **(7b)**

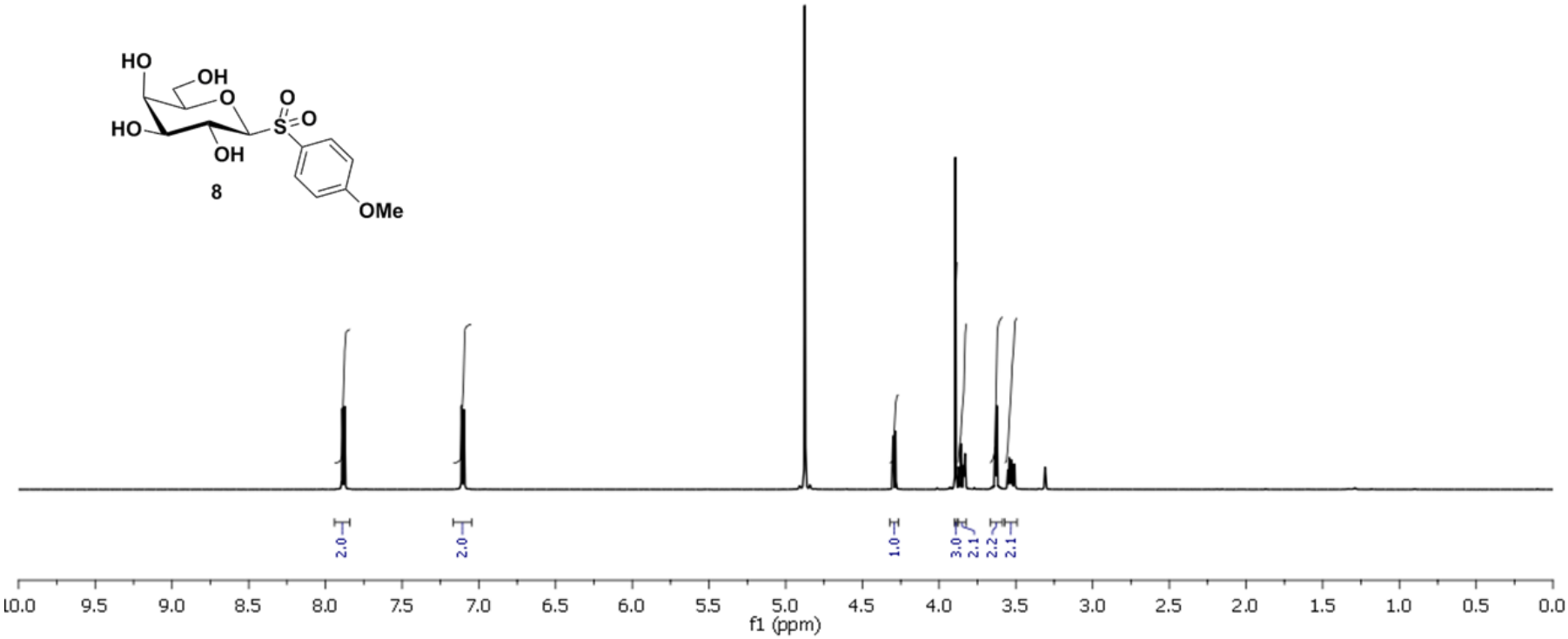

Figure 5. ^{1}H NMR of 4-Methoxyphenyl 1-sulfonyl-β-D-galactopyranoside **(8)**

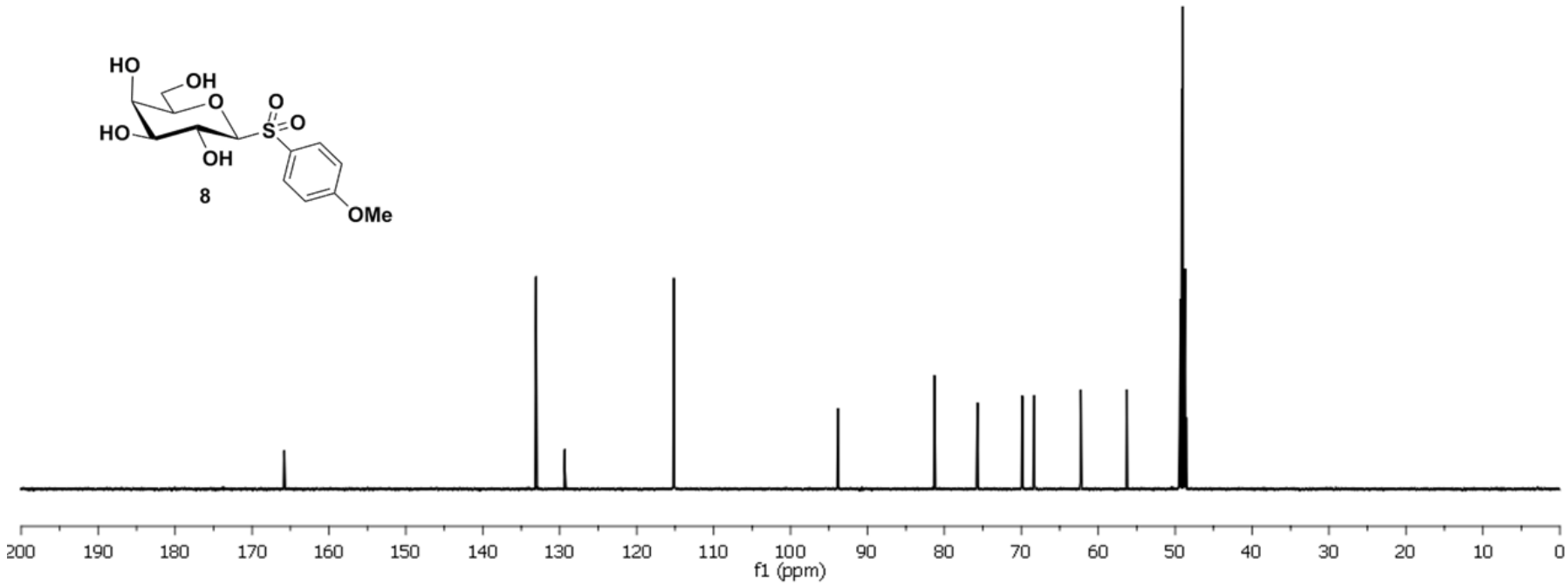

Figure 6. ^{13}C NMR of 4-Methoxyphenyl 1-sulfonyl-β-D-galactopyranoside **(8)**

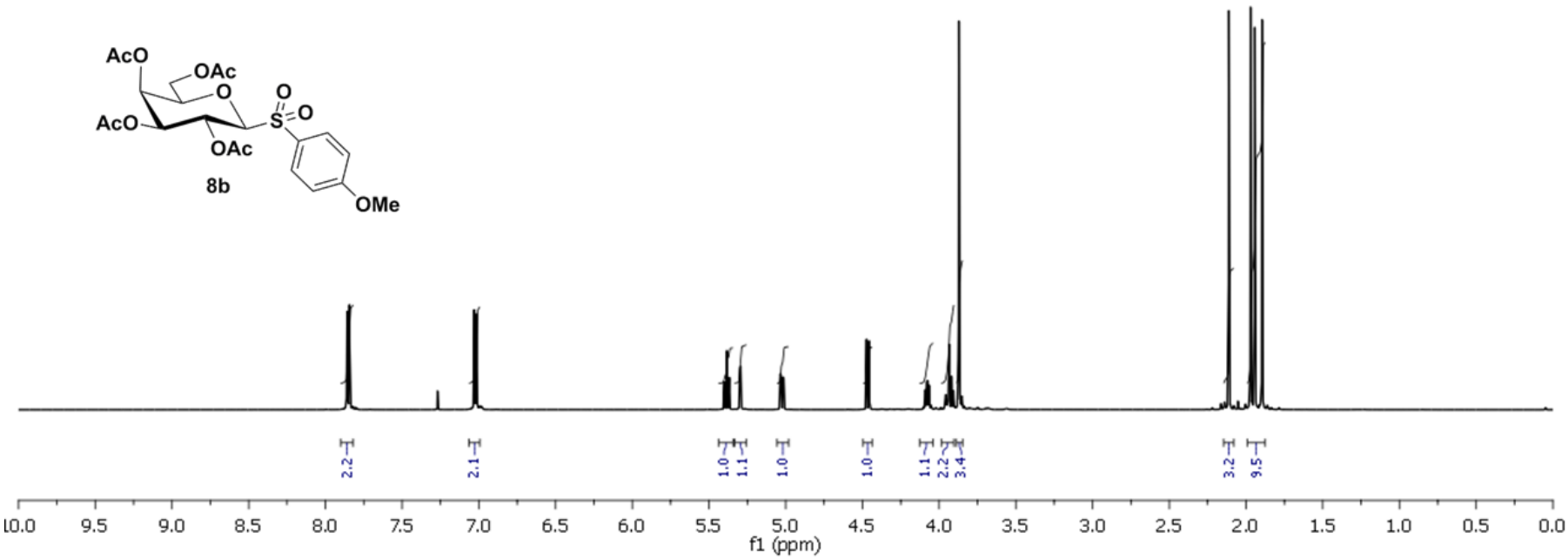

Figure 7. ^{1}H NMR of 4-Methoxyphenyl 2,3,4,6-tetra-*O*-acetyl-1-sulfonyl-β-D-galactopyranoside **(8b)**

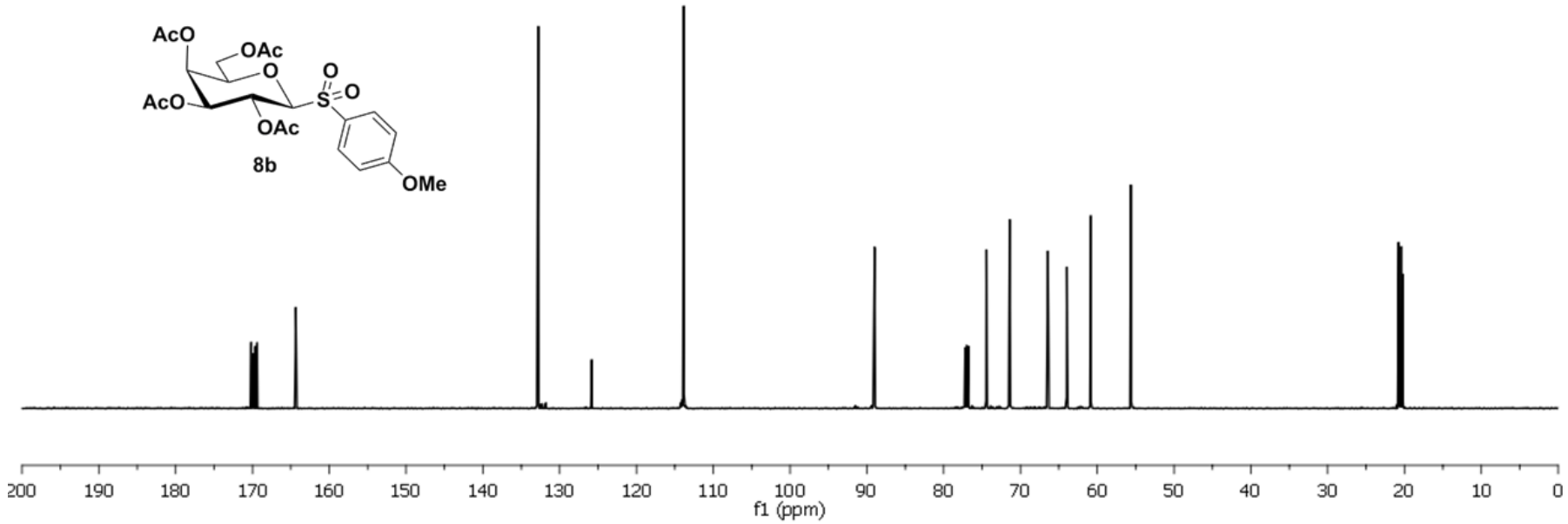

Figure 8. ^{13}C NMR of 4-Methoxyphenyl 2,3,4,6-tetra-*O*-acetyl-1-sulfonyl-β-D-galactopyranoside **(8b)**

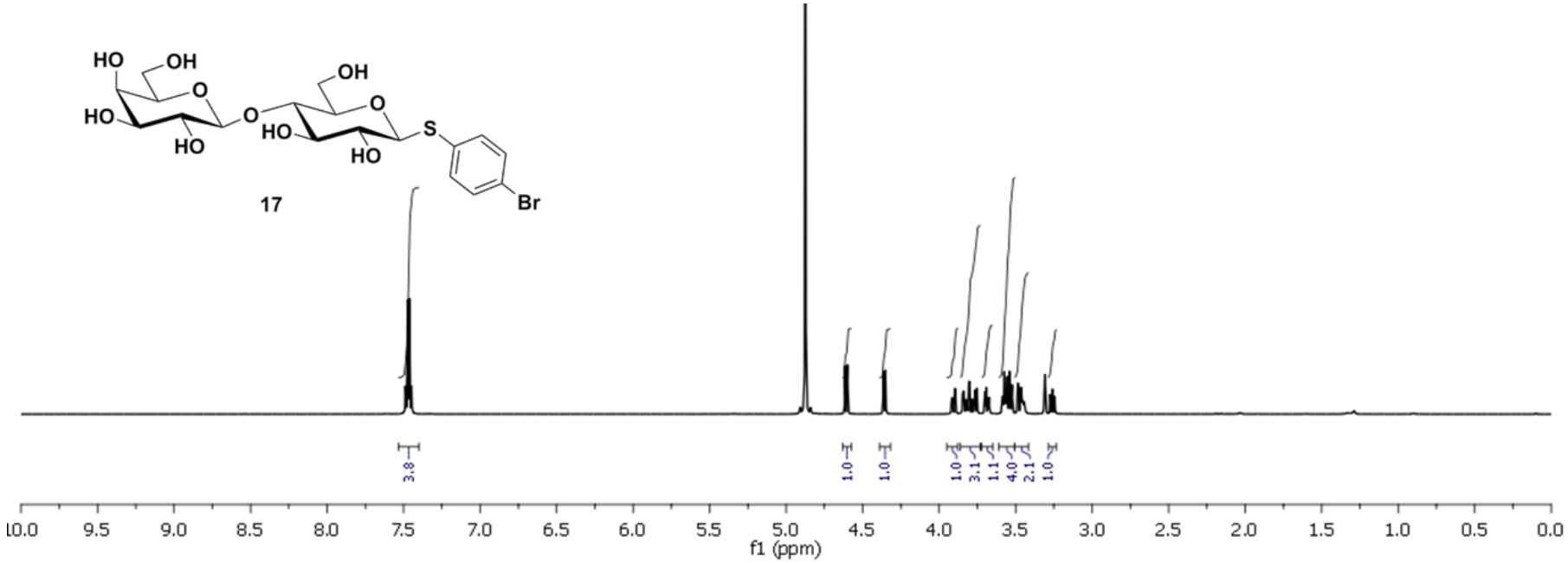

Figure 9. ^{1}H NMR of *p*-Bromophenyl 1-thio-β-D-lactoside **(17)**

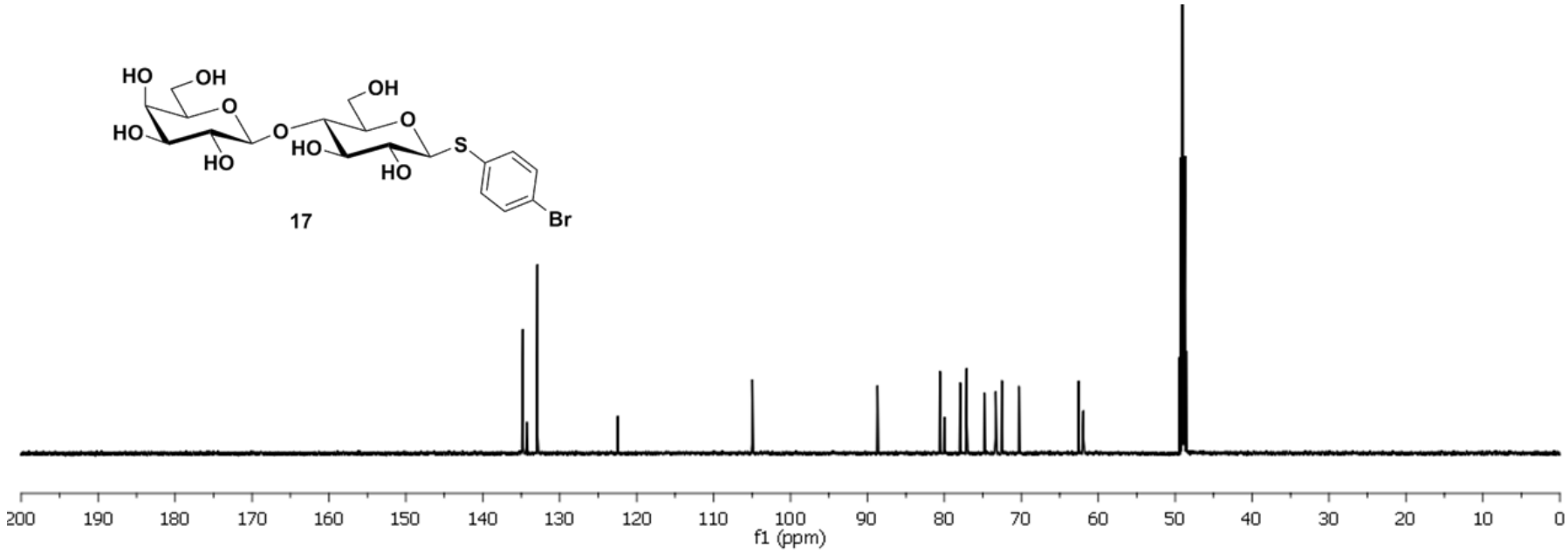

Figure 10. ^{13}C NMR of *p*-Bromophenyl 1-thio-β-D-lactoside **(17)**

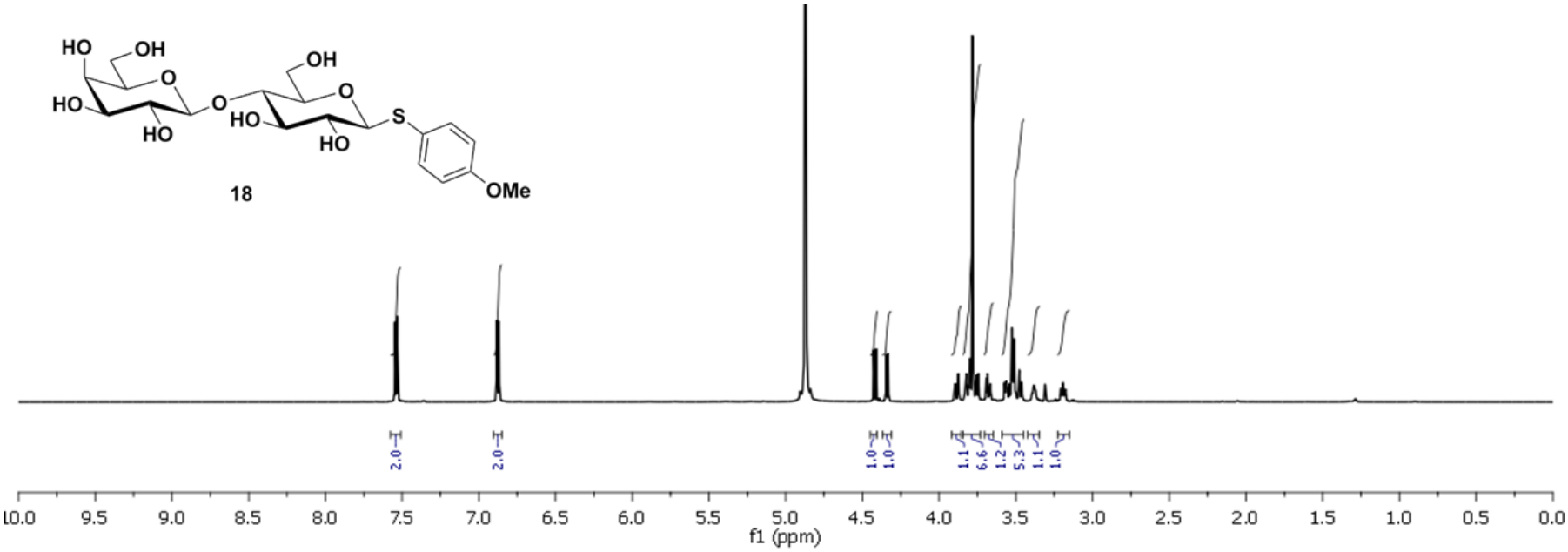

Figure 11. ^{1}H NMR of *p*-Methoxyphenyl 1-thio-β-D-lactoside **(18)**

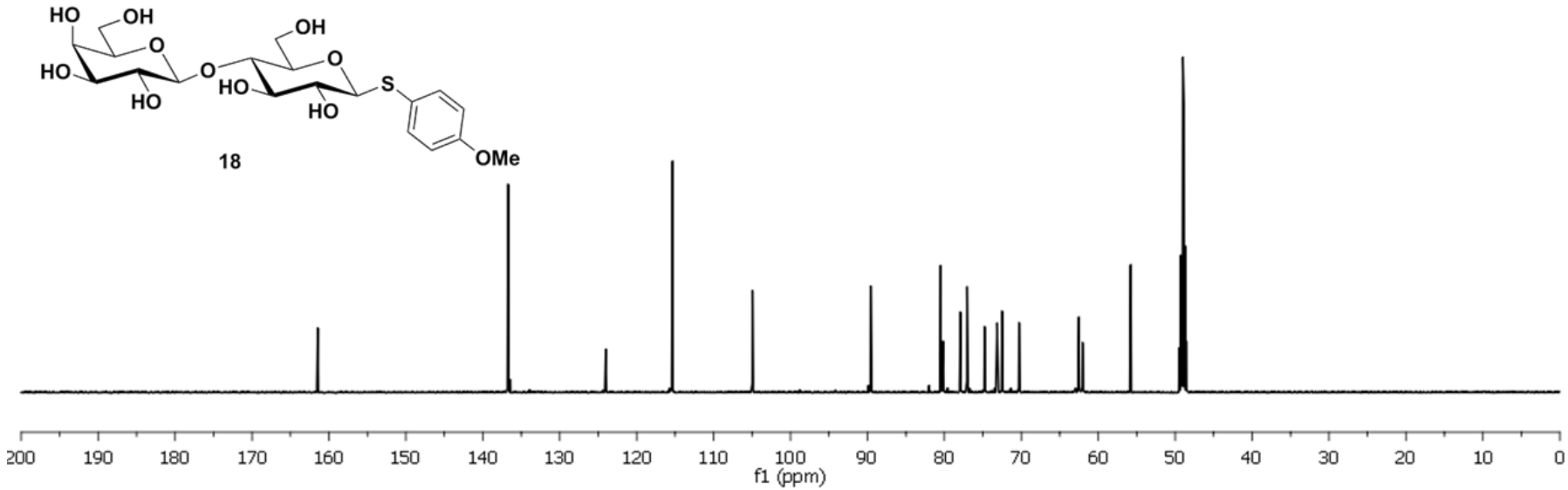

Figure 12. ^{13}C NMR of *p*-Bromophenyl 1-thio-β-D-lactoside **(18)**

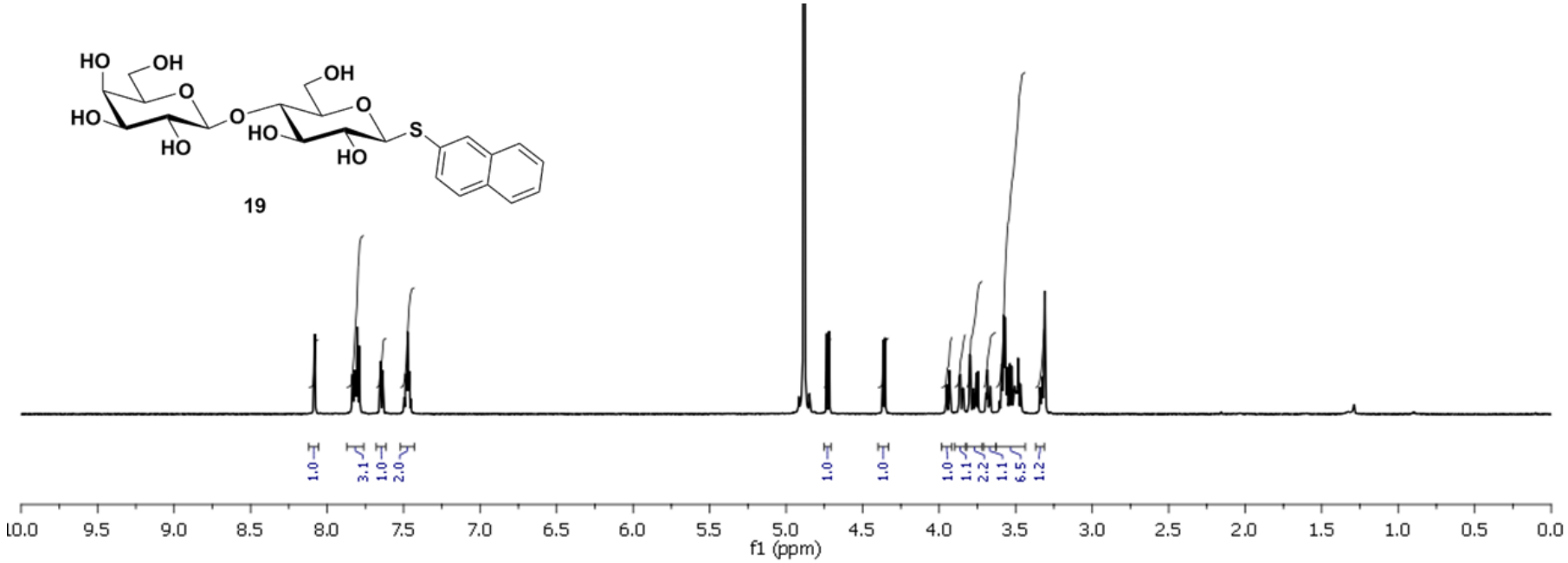

Figure 13. ^{1}H NMR of β-Naphthyl 1-thio-β-D-lactoside **(19)**

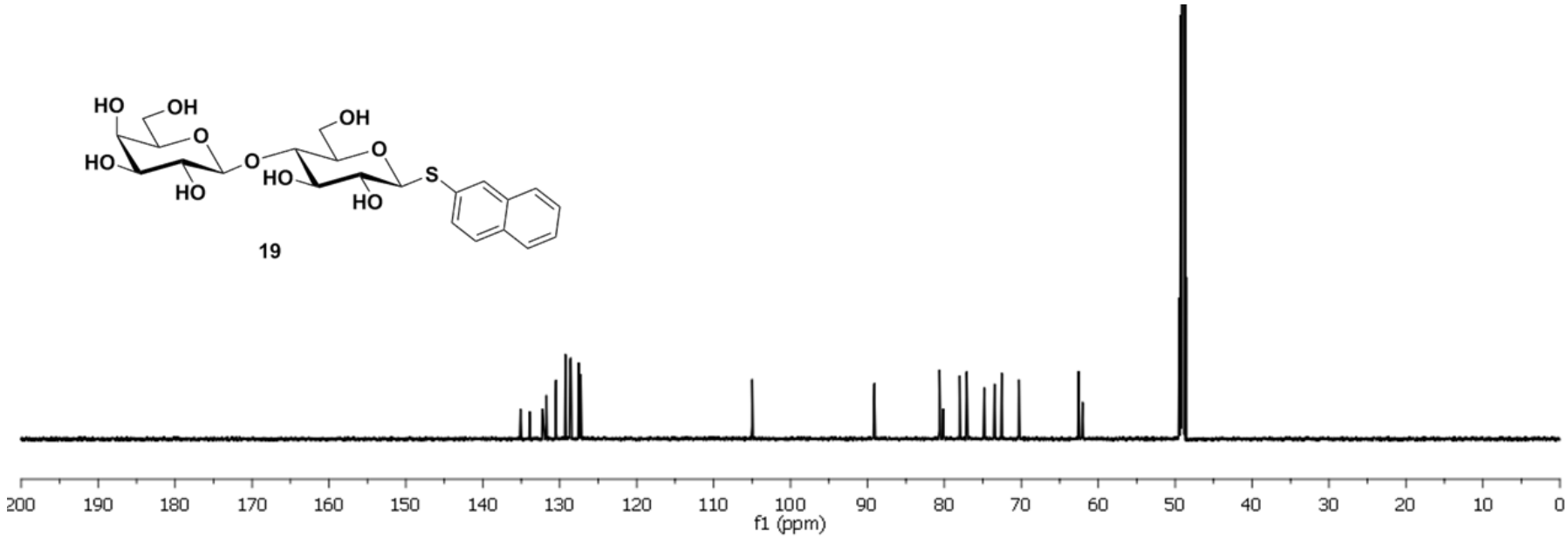

Figure 14. ^{13}C NMR of β-Naphthyl 1-thio-β-D-lactoside **(19)**

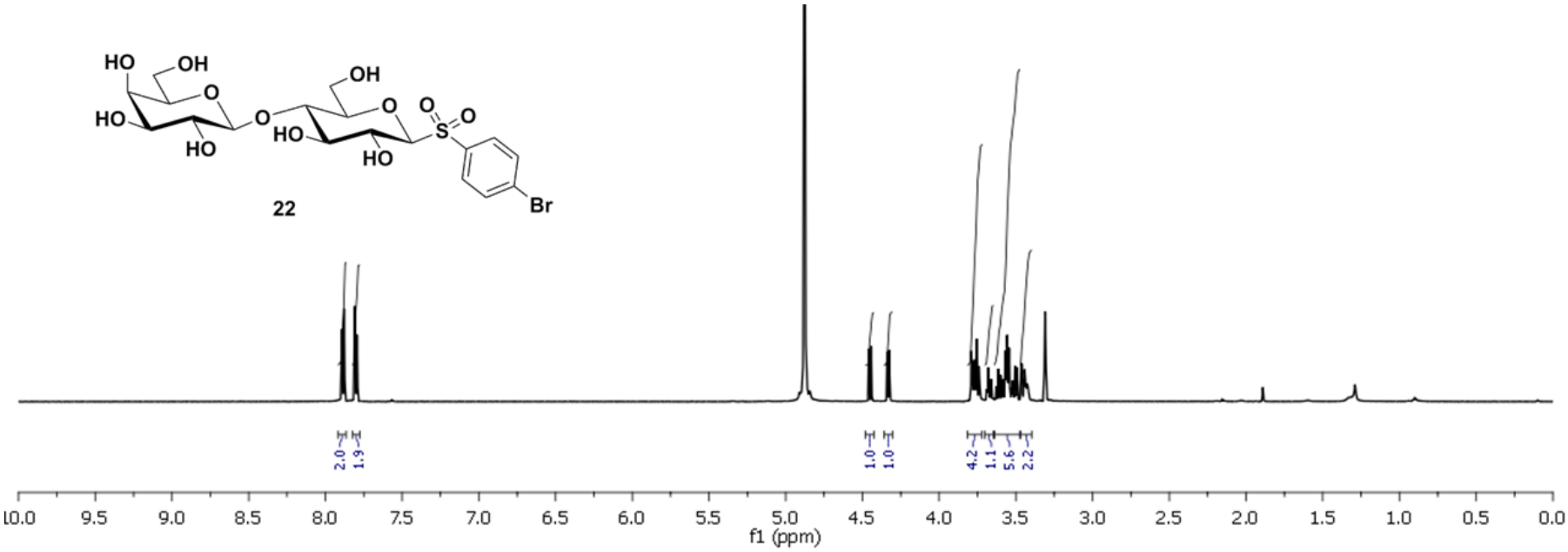

Figure 15. ^{1}H NMR of *p*-Bromophenyl 1-sulfonyl-β-D-lactoside **(22)**

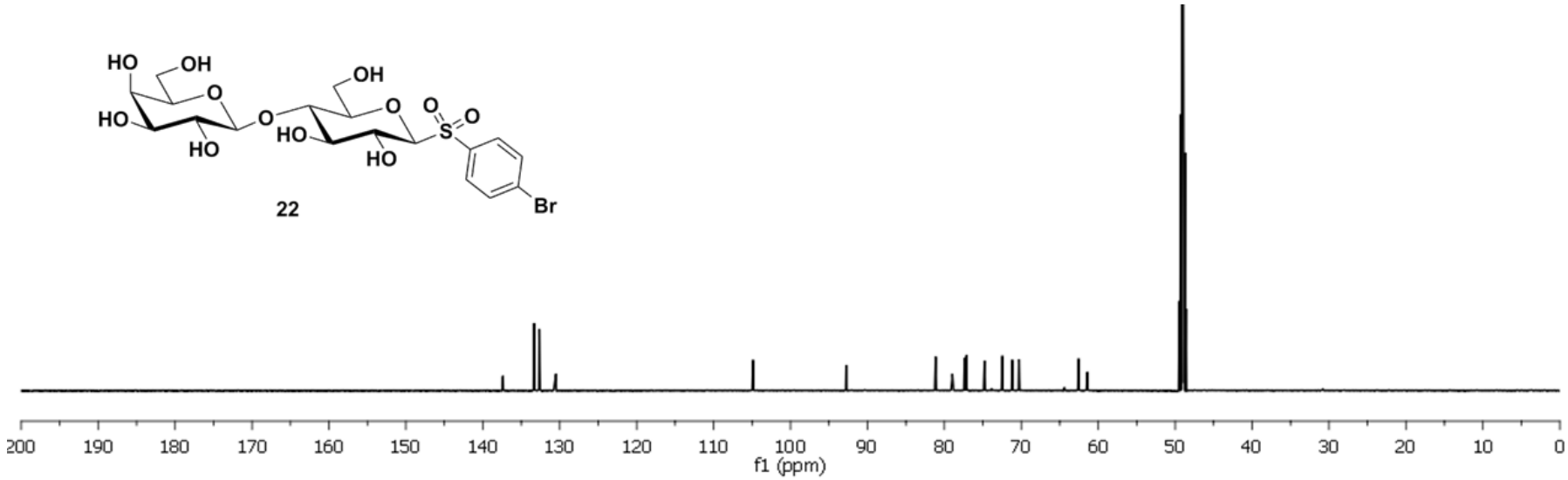

Figure 16. ^{13}C NMR of *p*-Bromophenyl 1-sulfonyl-β-D-lactoside **(22)**