Supporting information

Trehalose-Modified Silver Nanoparticles as Antibacterial Agents with Reduced Cytotoxicity and Enhanced Uptake by Mycobacteria

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Characterization of ≥ 15 nm AuNPs and AgNPs synthesized by seeded-growth method

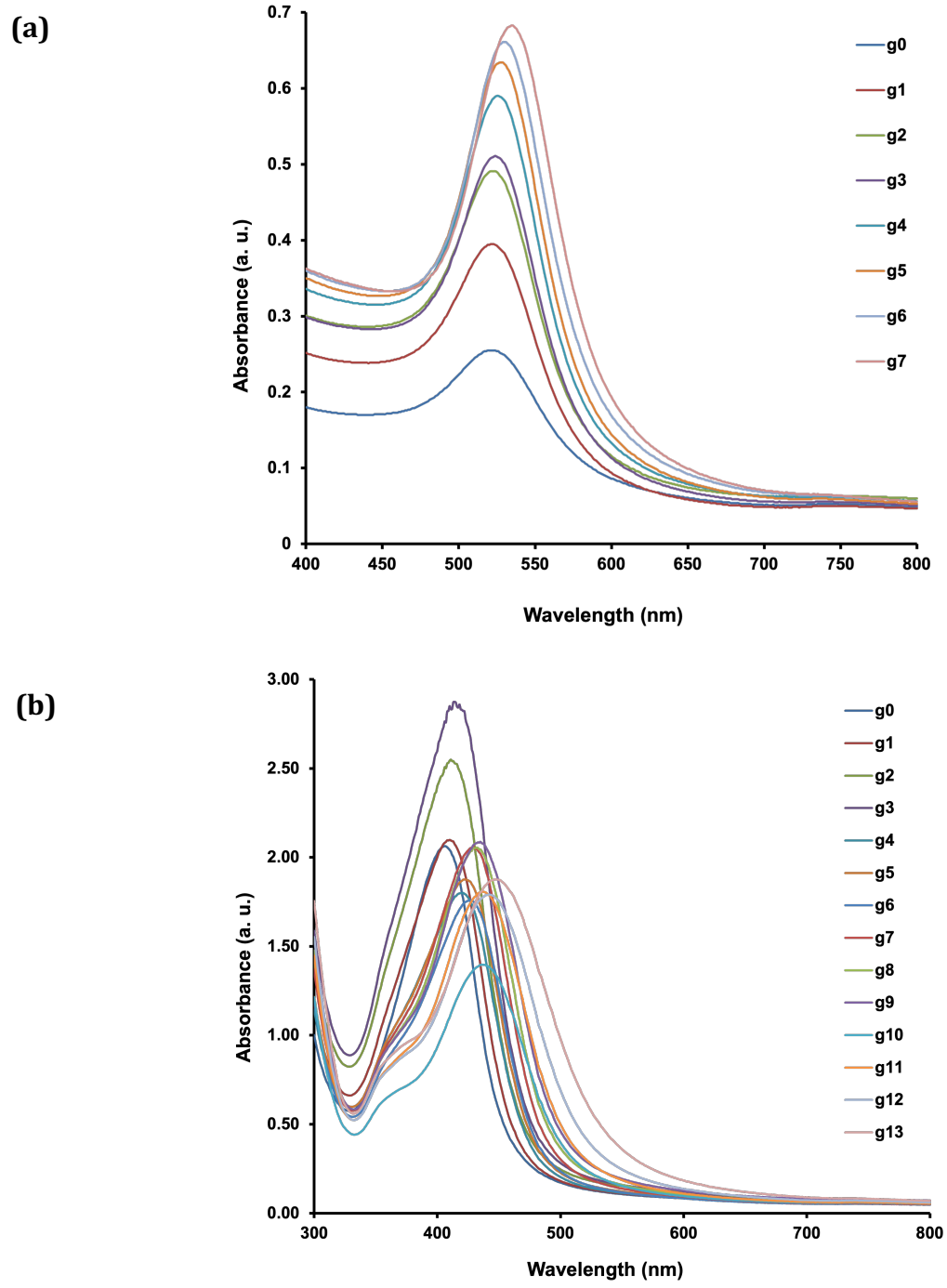


Figure S1. UV-Vis spectra of (a) AuNPs, and (b) AgNPs at each growth step during the seeded growth synthesis. The λ_{max} from g0-g13 are as follows: 406, 410, 411, 414, 419, 423, 427, 429, 432, 435, 436, 437, 442, 447 nm.

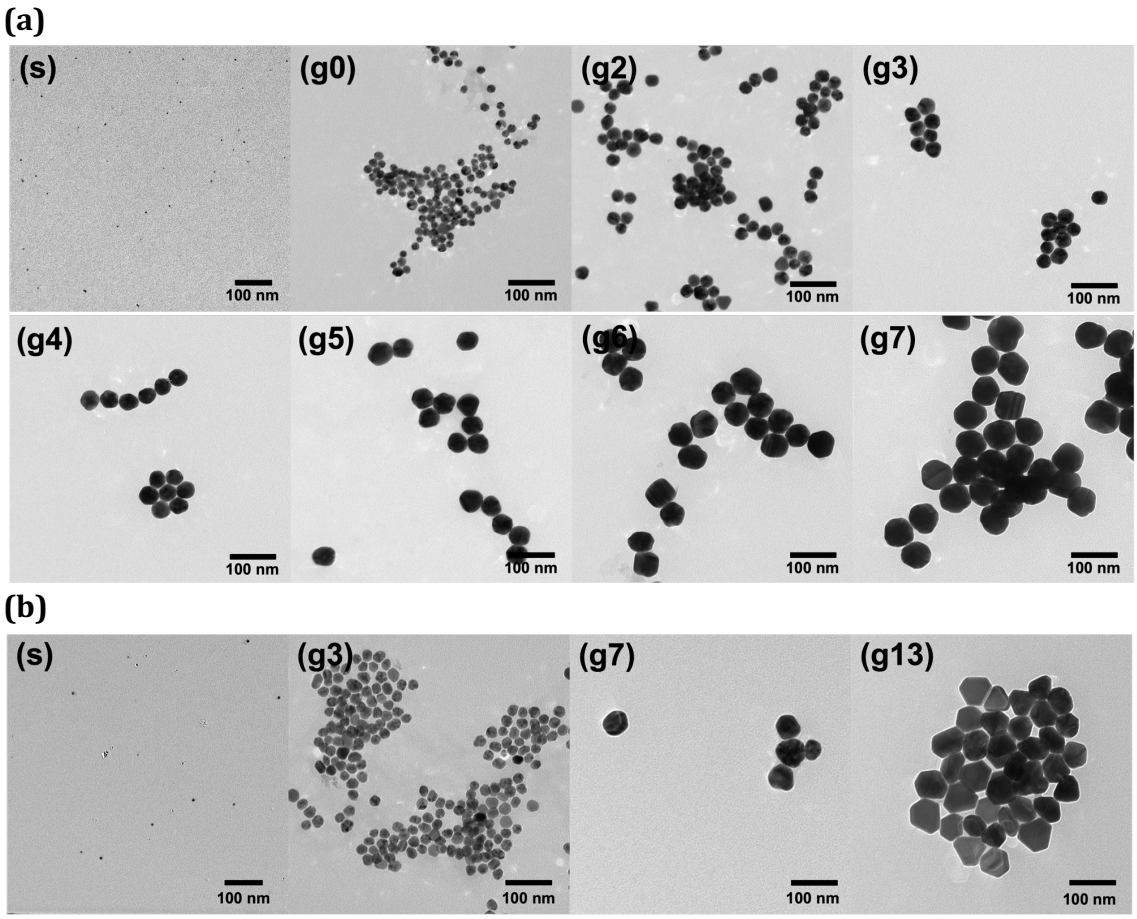


Figure S2. TEM images of (a) AuNPs, s: ~5 nm seeds, (b) AgNPs, s: ~7 nm seeds, at various stages of the seeded growth synthesis. The 'n' in (gn) represents the corresponding growth step.

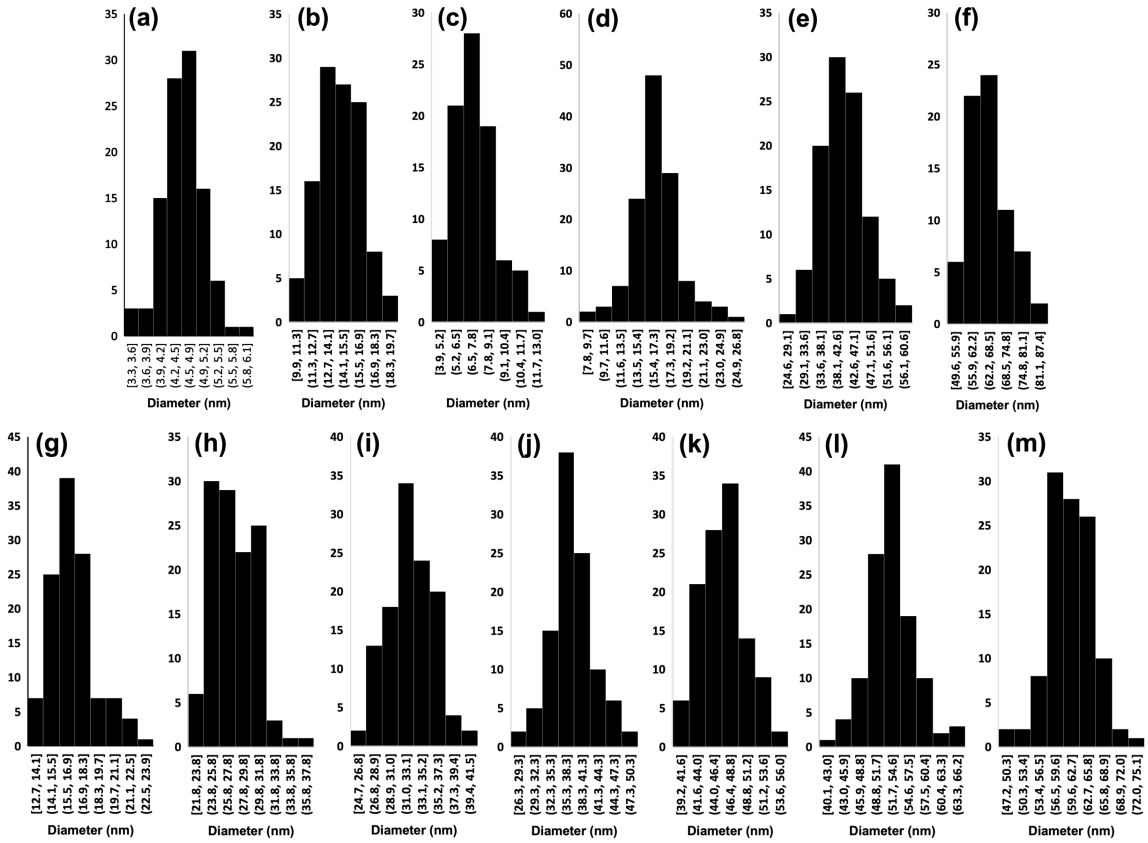


Figure S3. Particle size distributions of AuNPs of (a) 4.5 ±0.4 nm, (b) 14.5 ± 2.0 nm and AgNPs of (c) 7.2 ± 1.9 nm, (d) 16.2 ± 2.0 nm, (e) 42.0 ± 4.3 nm, (f) 65.2 ± 7.5 nm. Particle size distributions of AuNPs synthesized using growth method: (g) g0, 16.7 ± 2.0 nm, (h) g2, 27.6 ± 2.8 nm, (i) g3, 32.7 ± 3.0 nm, (j) g4, 38.2 ± 4.1 nm, (k) g5, 46.5 ± 3.4 nm, (l) g6, 53.1 ± 4.1 nm, (m) g7, 61.0 ±4.3 nm. Particle diameters were measured from about 100 nanoparticles from the TEM images.

Table S1. Particle diameter and polydispersity index (Đ) of ≥ 15 nm AuNP and AgNP measured by TEM and DLS.

	TEM (nm)[a]	DLS (nm)[b]	Đ[b]
AuNP	15 ±2.0	18 ± 0.4	0.155 ± 0.096
AgNP	16 ±2.0	19 ±0.1	0.521 ± 0.014
	22 ±4.3	24 ±0.3	0.326 ± 0.055
	42 ±6.0	44 ±0.2	0.284 ± 0.026
	65 ±7.5	57 ±0.8	0.435 ± 0.047

[a] Average ± standard deviation (S.D.) obtained from about 100 nanoparticles.

[b] Average ± S.D. obtained from 3 repetitions.

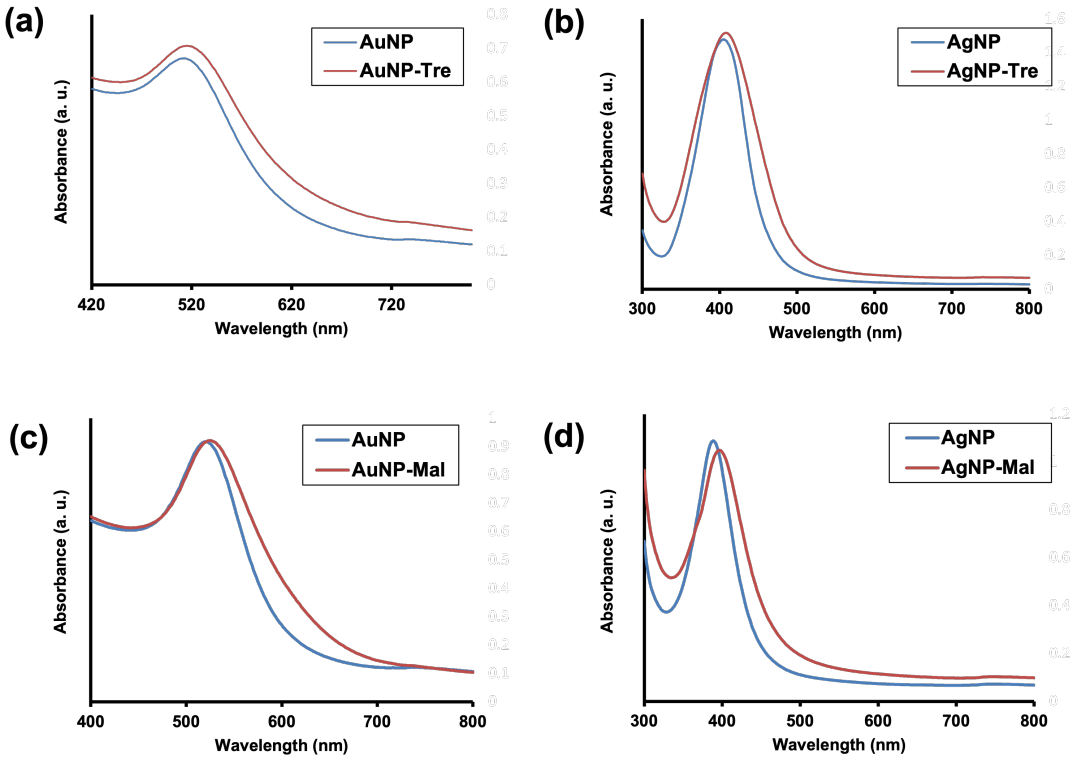


Figure S4. UV-Vis spectra of 15 nm AuNPs and 16 nm AgNPs before and after functionalized with (a, b) trehalose-thiol **5** or (c, d) maltose-thiol **10**.

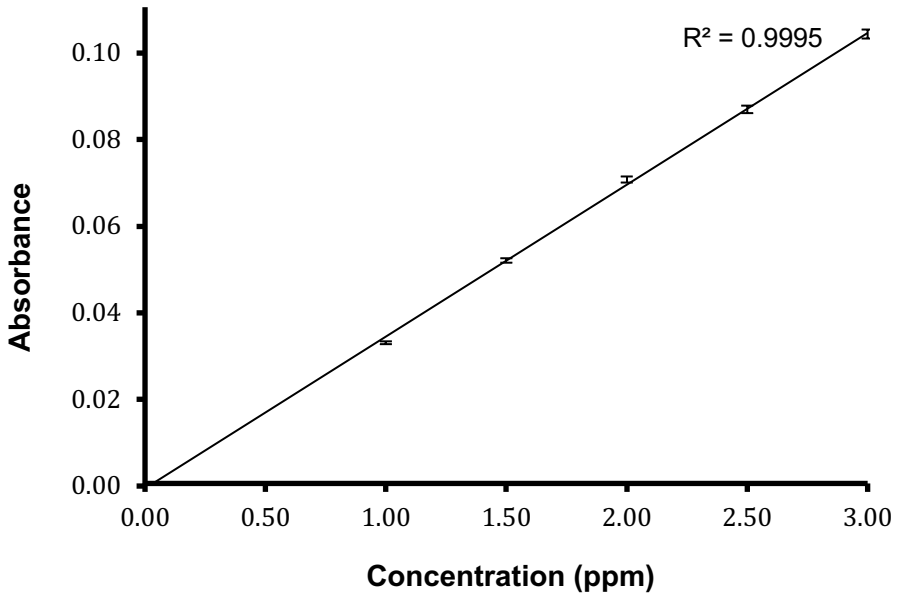
Determination of the concentration of Ag in AgNPs and Au in AuNPs by atomic absorption spectroscopy (AAS)

A stock solution of $AgNO_3$ (1000 ppm) was prepared by dissolving $AgNO_3$ (Fisher Scientific, 1000 ppm ±1%, certified) in Milli-Q water. The calibration series were prepared by diluting the stock solution with Milli-Q water to give concentrations of 1.0, 1.5, 2.0, 2.5 and 3.0 ppm. The absorbances of the solutions were measured using a flame atomic absorption spectrometer (Agilent 200 Series AA spectrometer), equipped with a silver hollow cathode lamp (HCL, Agilent, Multi-Element UltraAA) at the excitation wavelength of 328.1 nm. The data were plotted against the concentration of $AgNO_3$ to construct the calibration curve (**Fig. S5a**).

To determine the concentrations of Ag in AgNPs, 100 µL of the AgNP samples was dissolved in 900 µL of conc. HNO_3, and the solution was subsequently topped to 5.0 mL with Milli-Q water. The solutions were analyzed by AAS, and the absorbances were compared to the standard calibration curve to determine the concentration. Dilutions were made when concentrations were out of the range of the calibration curve.

The concentrations of Au in AuNPs were determined in a similar manner from AuNP samples dissolved in conc. HNO_3 and Milli-Q water using AAS and a gold HCL (242.8 nm, Agilent Single element Au), and comparing the results with the standard calibration curve constructed from a concentration series (1.0, 1.5, 2.0, 2.5, 3.0 ppm) prepared from the stock solution of $HAuCl_4$ (1000 ppm) (**Fig. S5b**).

(a)



(b)

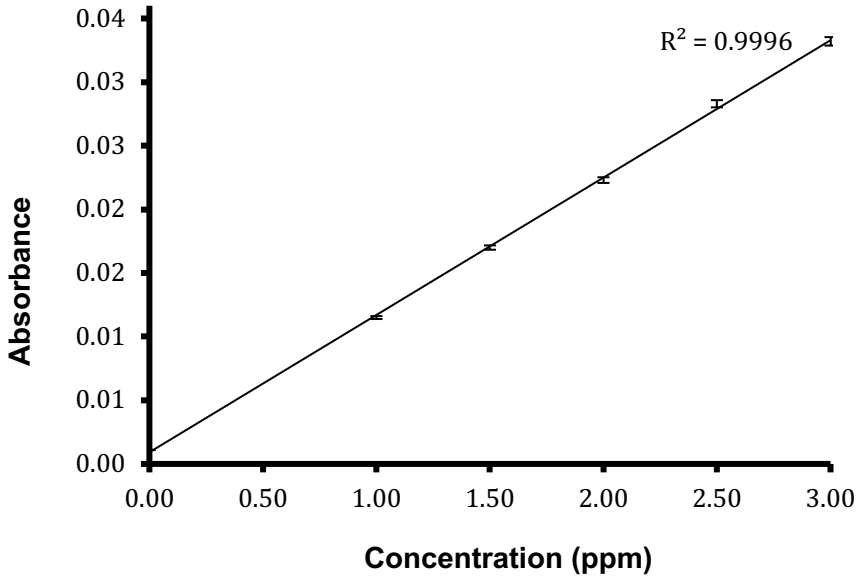


Figure S5. (**A**) Standard calibration curve for Ag^{+} obtained from a series of $AgNO_3$ solutions using AAS. **(B)** Standard calibration curve for Au^{3+} obtained from $HAuCl_4$ solutions using AAS.

Characterization spectra

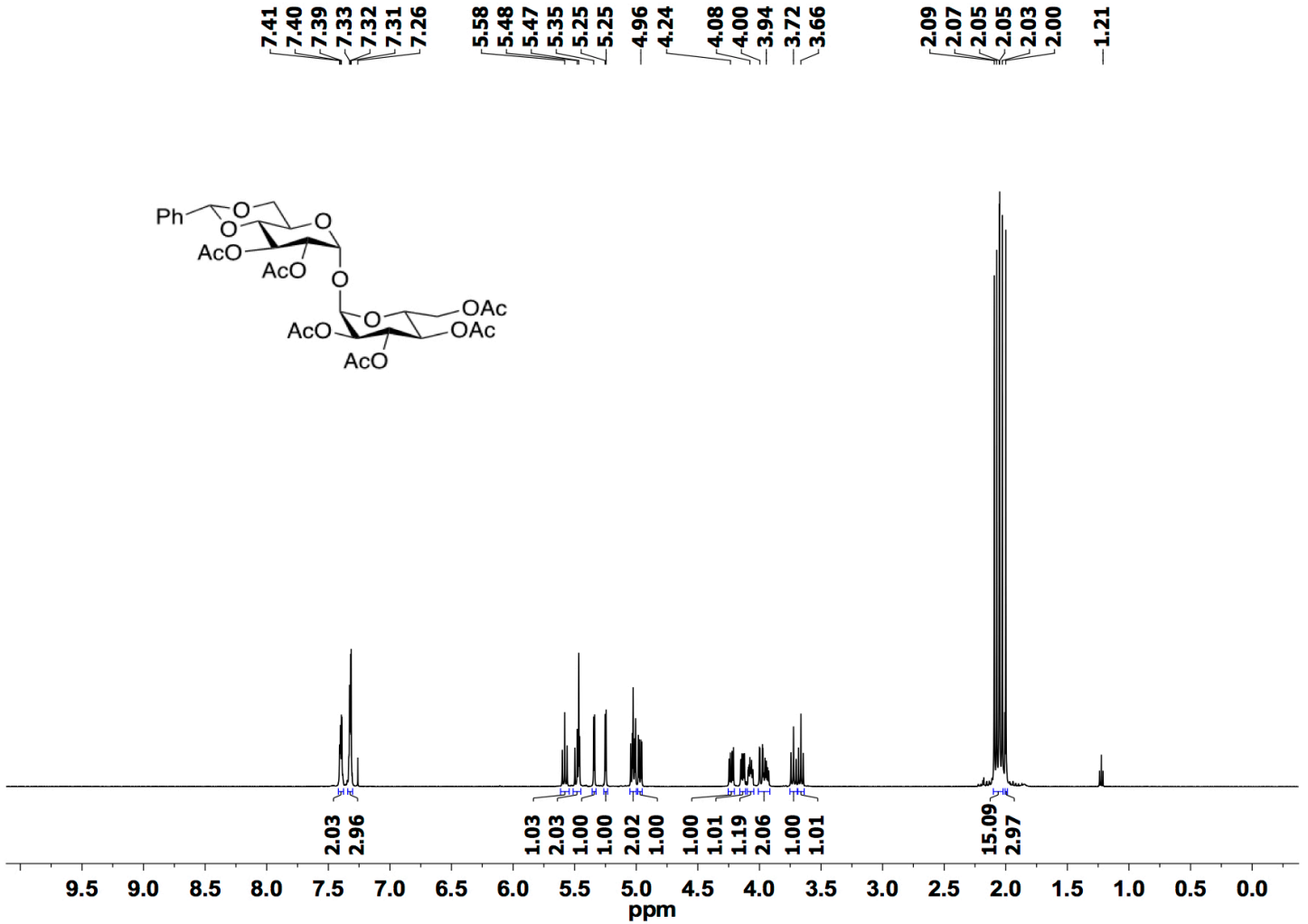


Figure S6. ^{1}H NMR spectrum of compound 2 in $CDCl_3$, δ 1.21 ppm: from ethyl acetate.

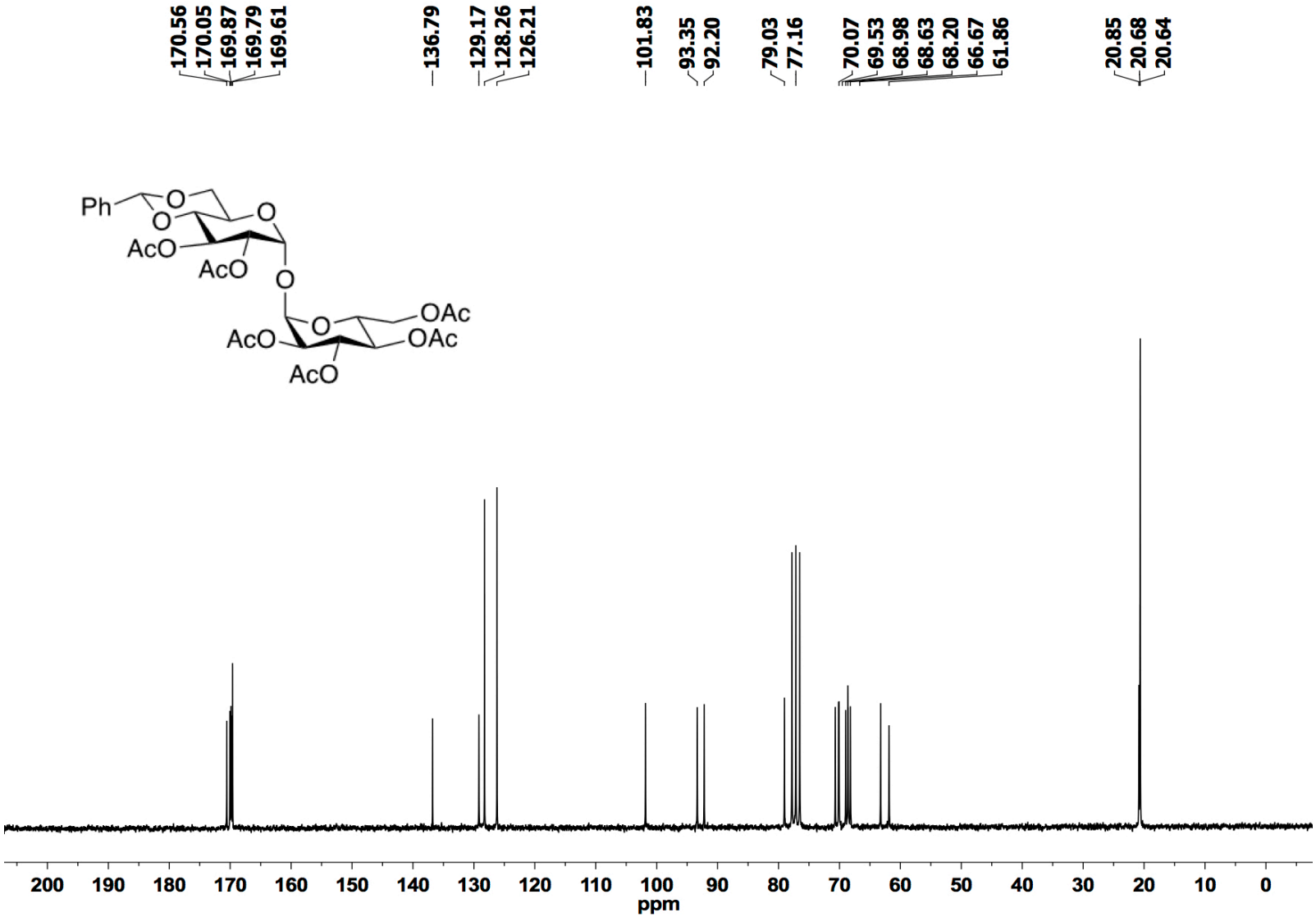


Figure S7. ^{13}C NMR spectrum of compound 2 in $CDCl_3$.

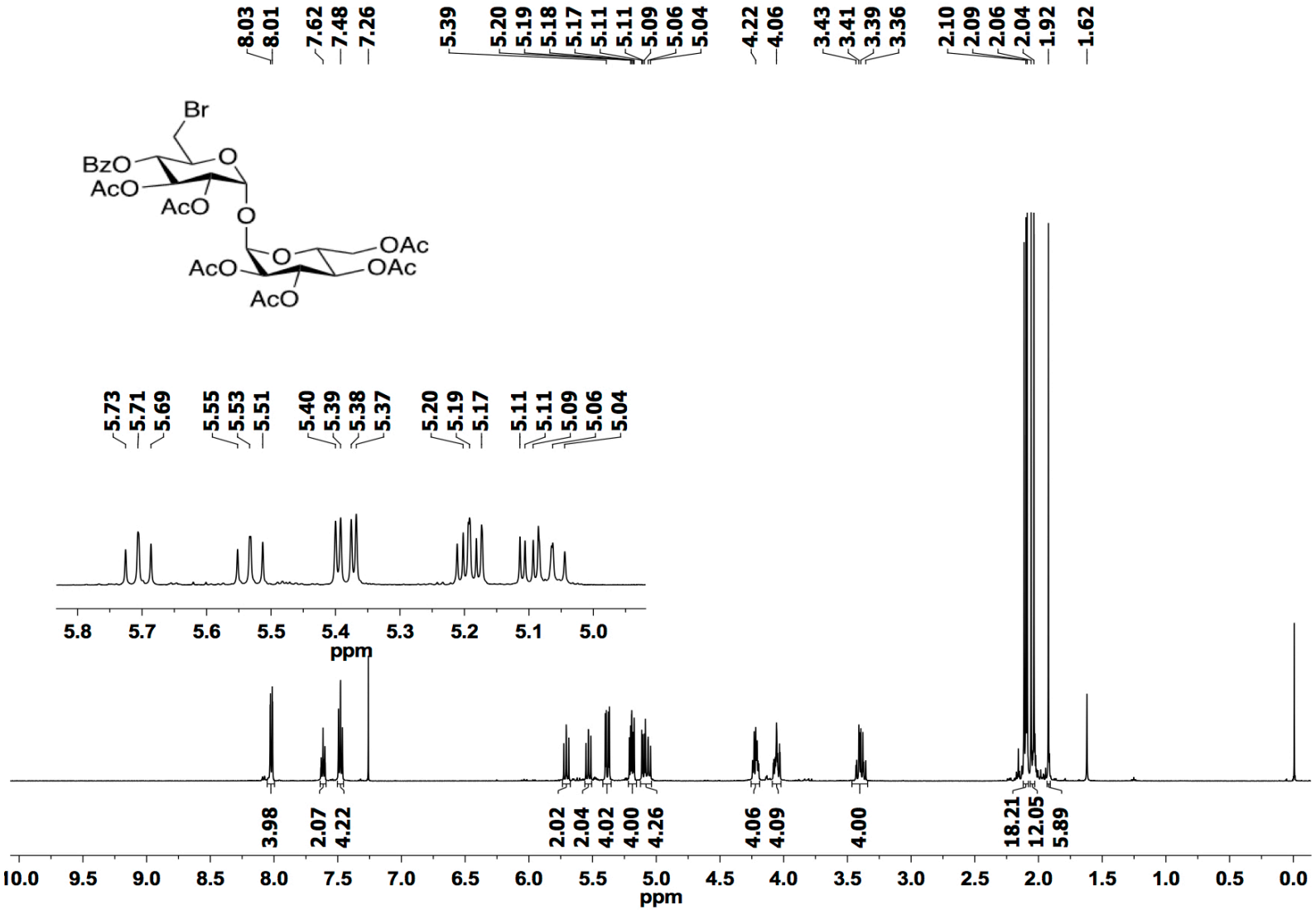


Figure S8. ^{1}H NMR spectrum of compound 3 in $CDCl_3$.

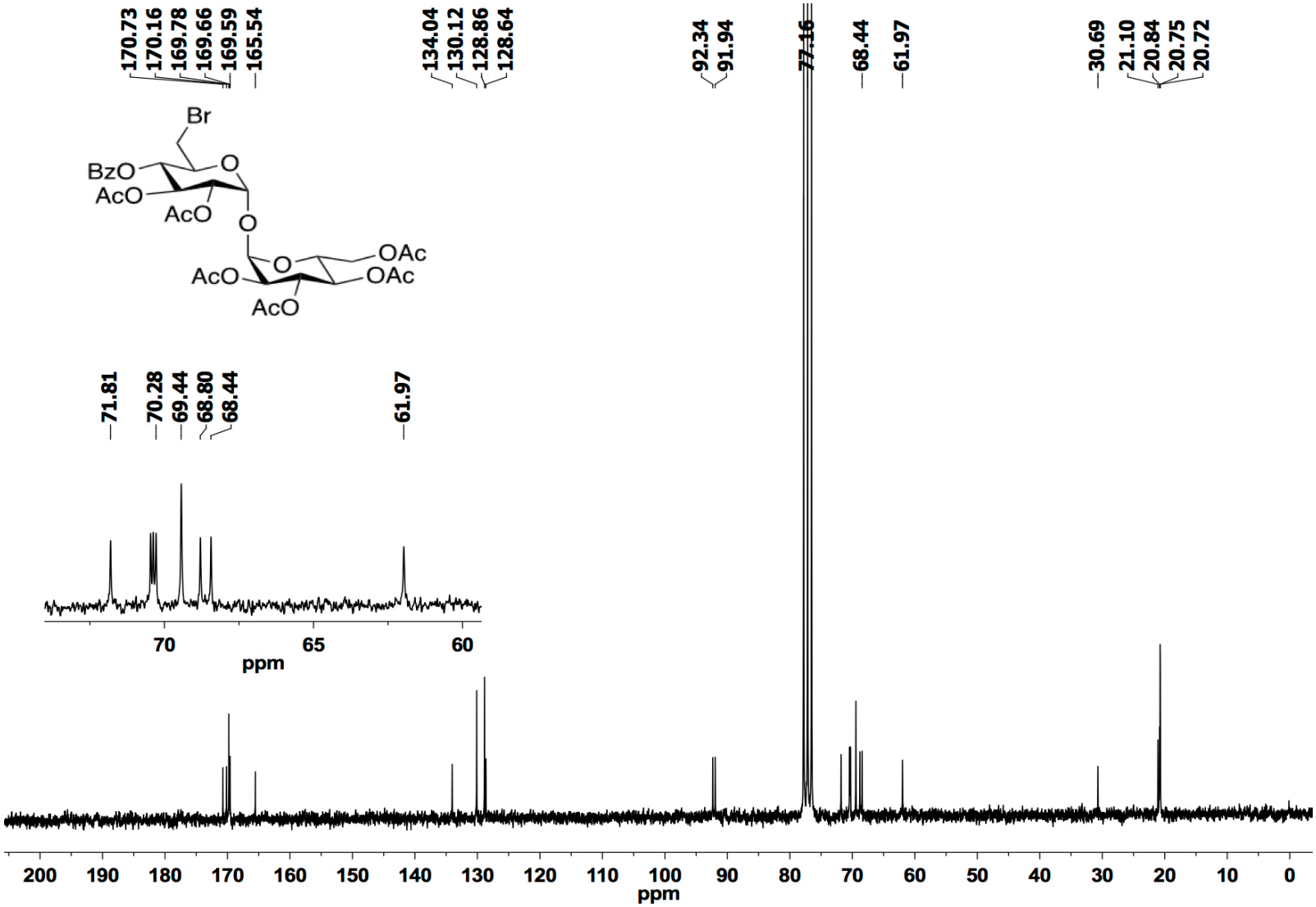


Figure S9. ^{13}C NMR spectrum of compound **3** in $CDCl_3$.

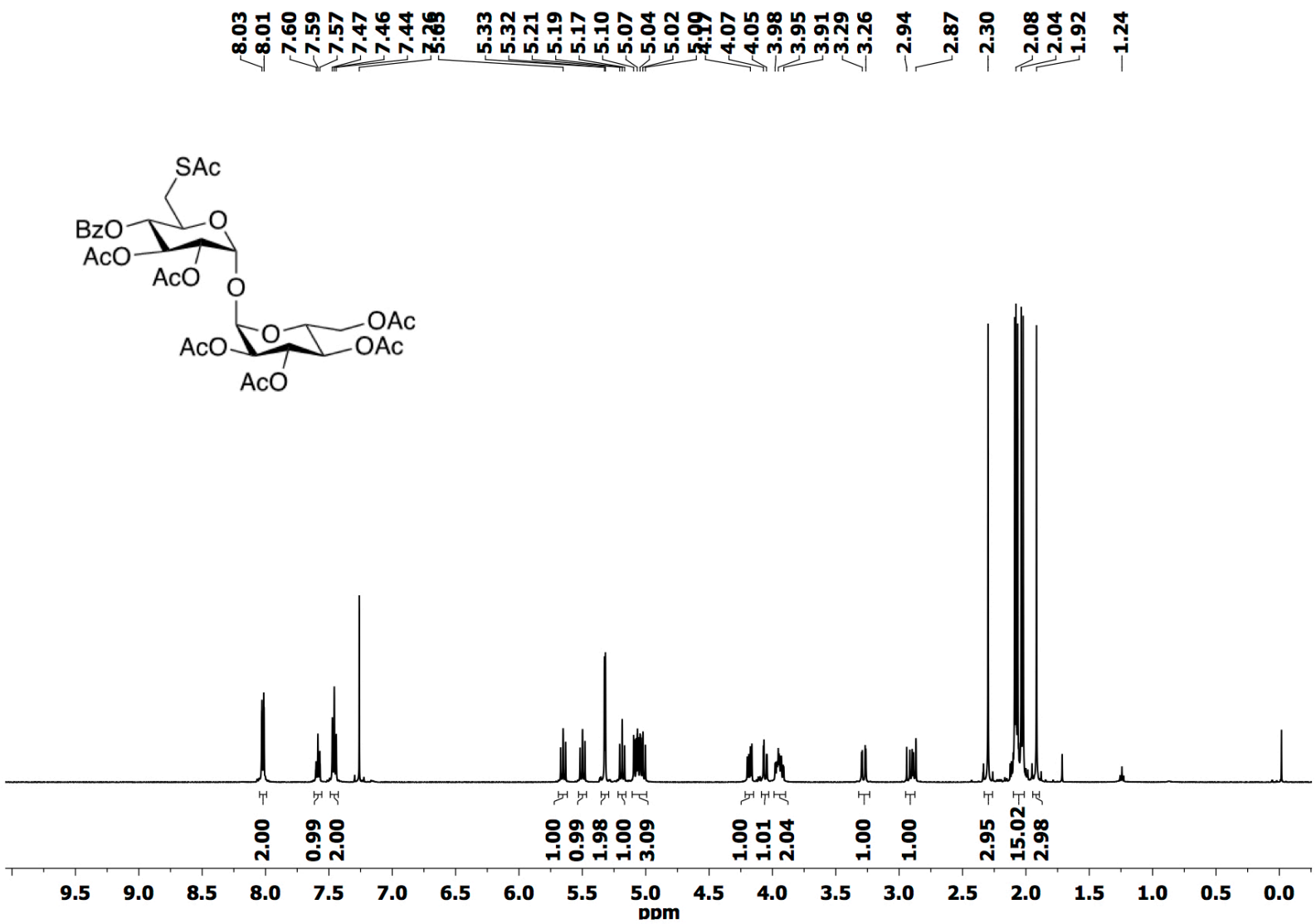


Figure S10. ^{1}H NMR spectrum of compound 4 in $CDCl_3$.

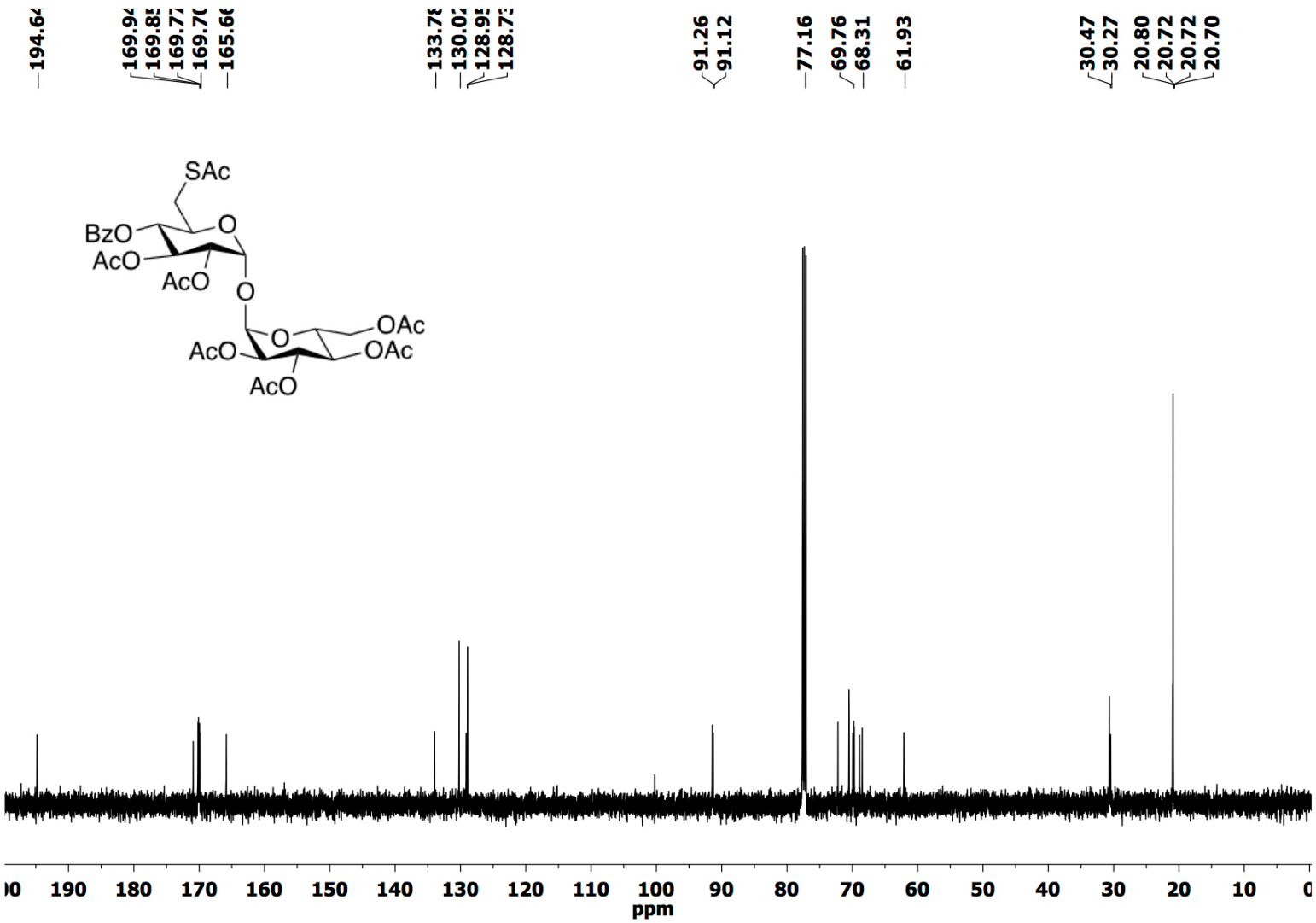


Figure S11. ^{13}C NMR spectrum of compound 4 in $CDCl_3$.

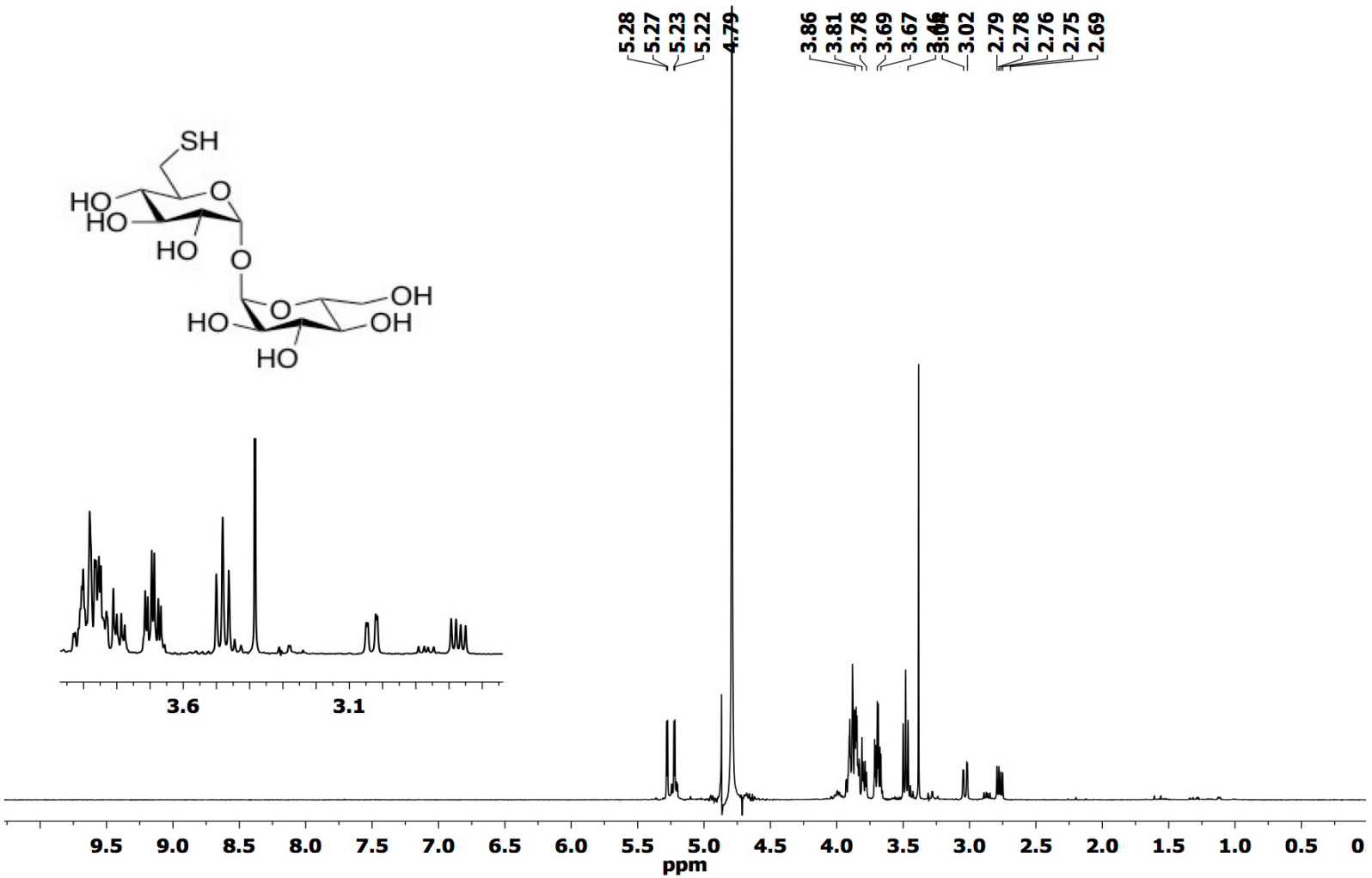


Figure S12. ^{1}H NMR spectrum of compound **5** in D_2O.

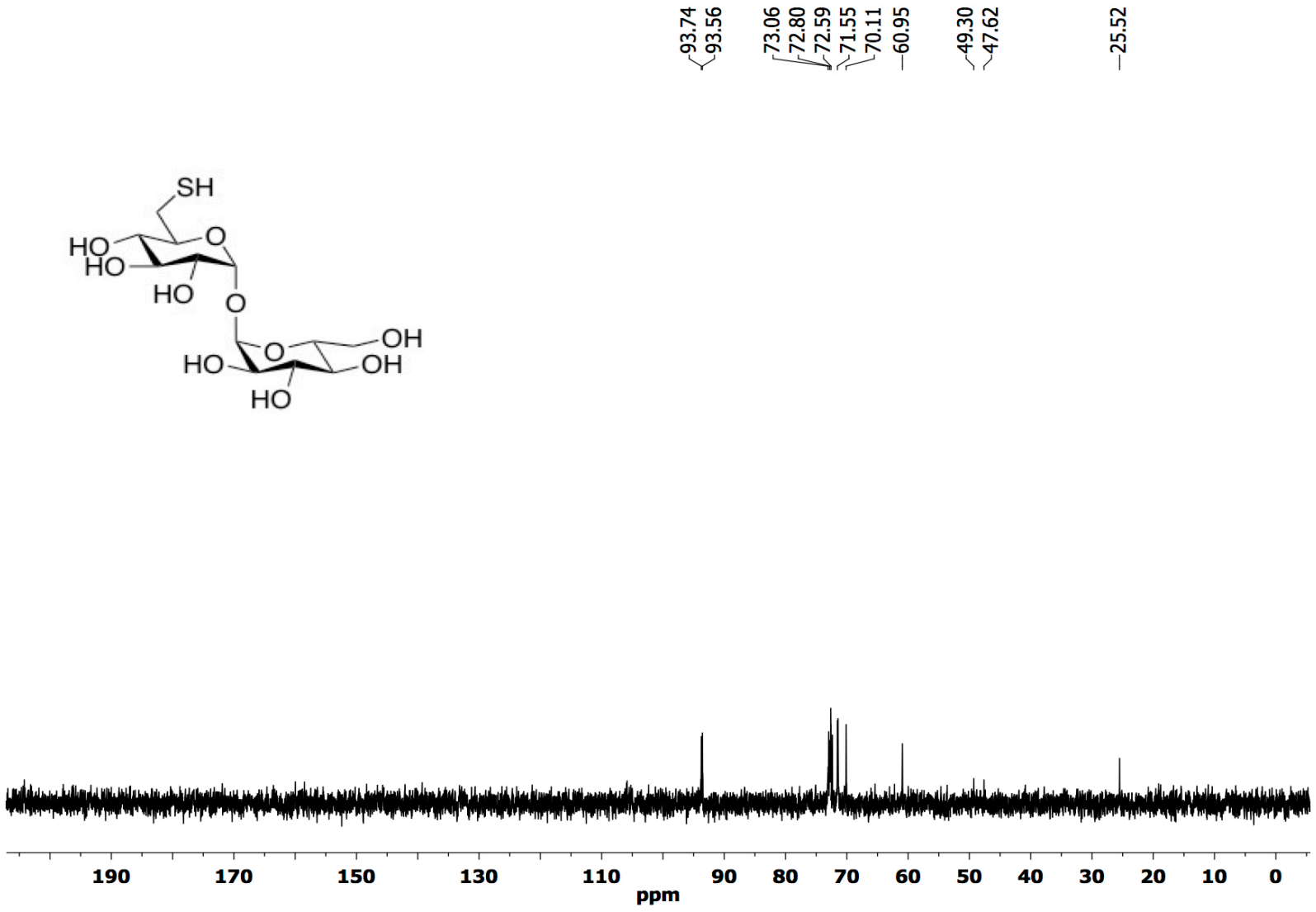


Figure S13. ^{13}C NMR spectrum of compound 5 in D_2O.

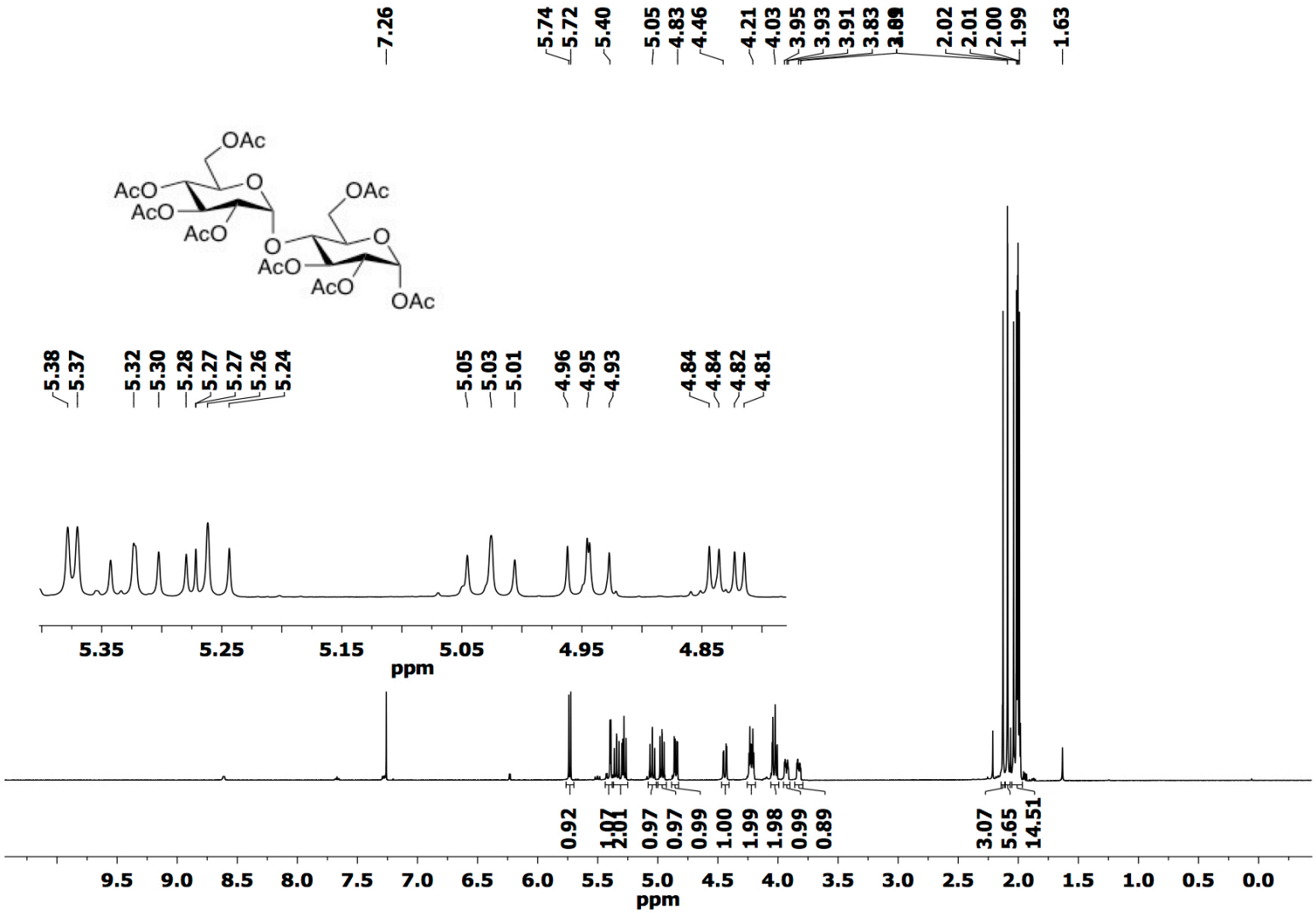


Figure S14. ^{1}H NMR spectrum of compound 7 in $CDCl_3$.

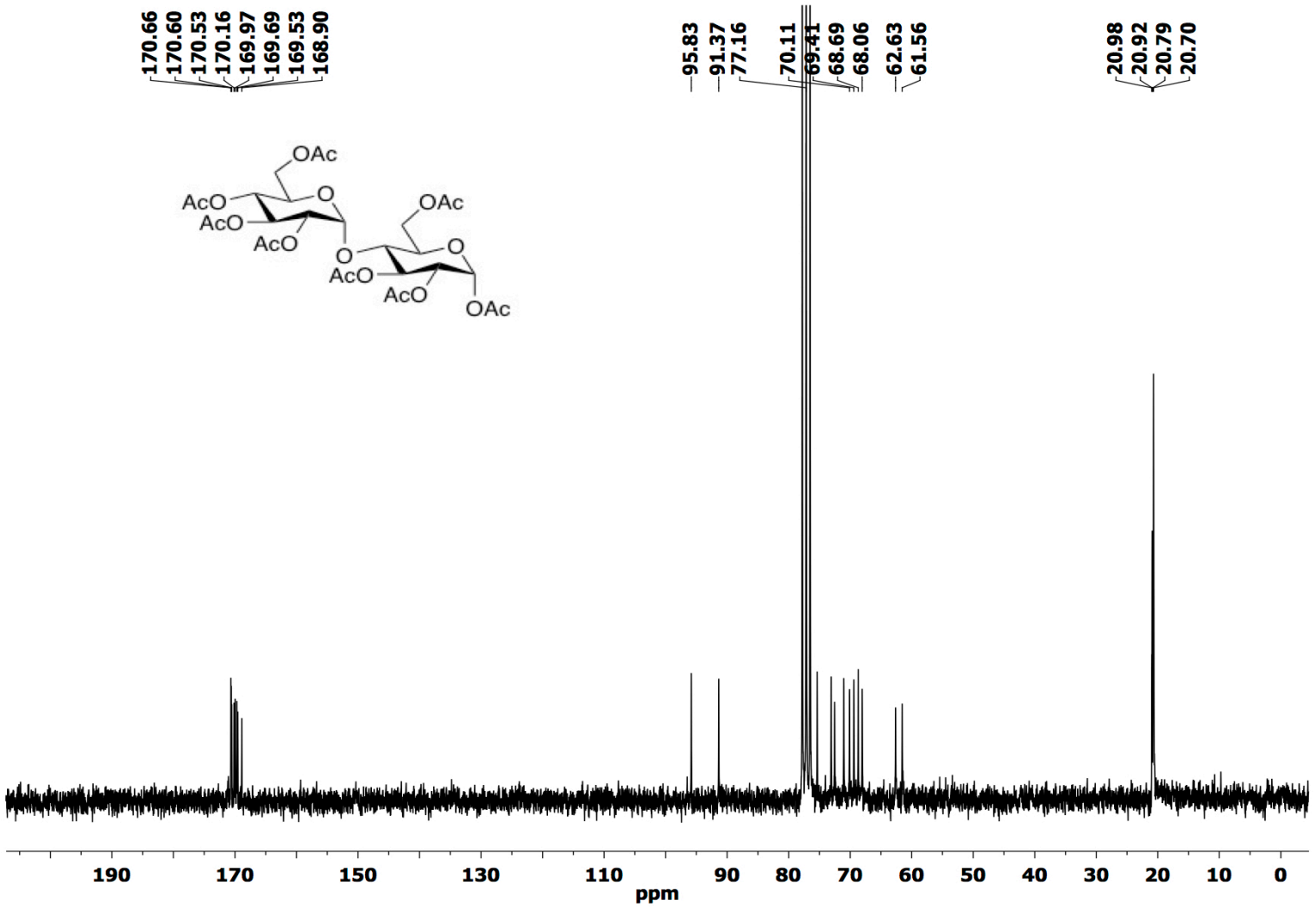


Figure S15. ^{13}C NMR spectrum of compound 7 in $CDCl_3$.

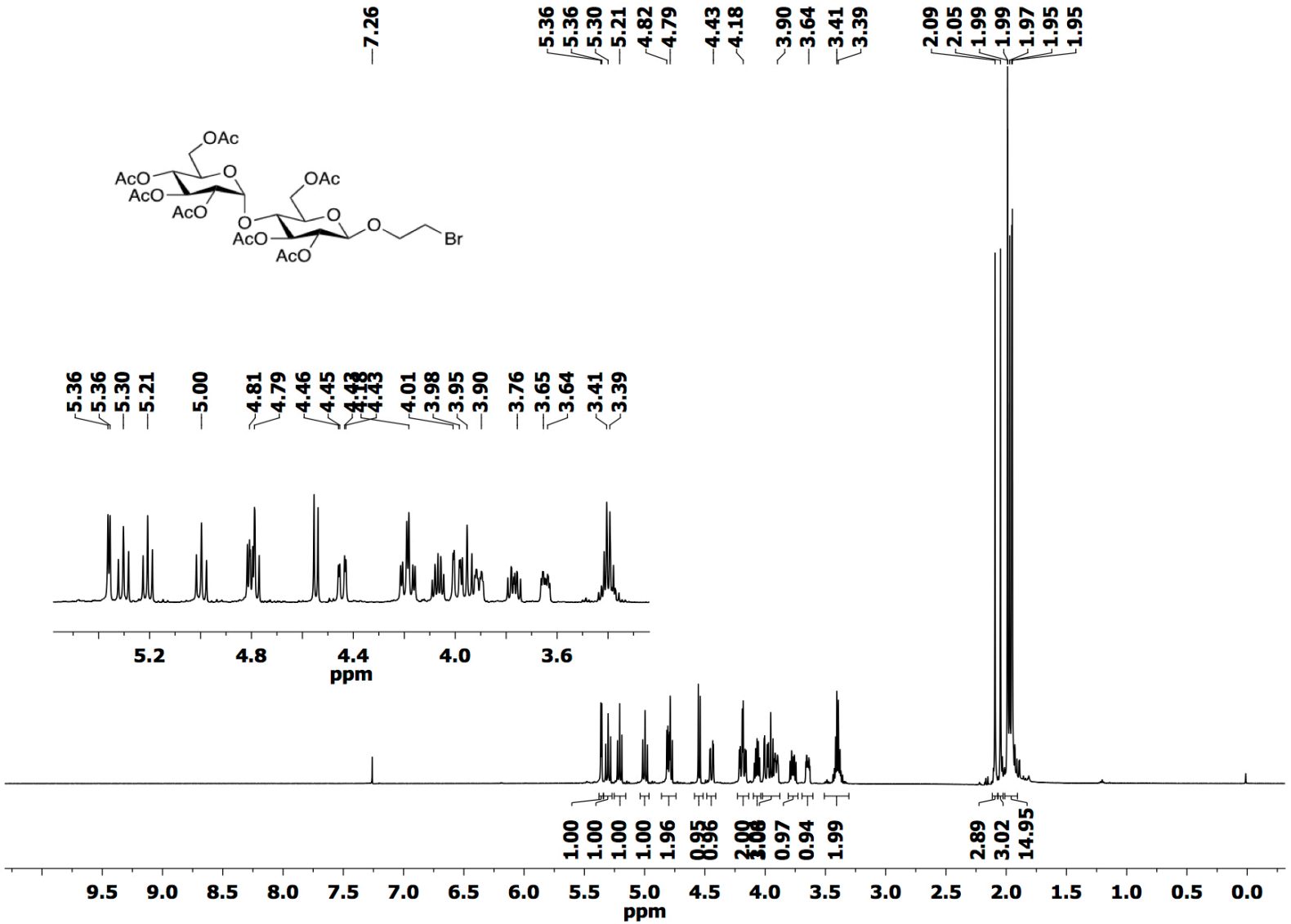


Figure S16. ^{1}H NMR spectrum of compound 8 in $CDCl_3$.

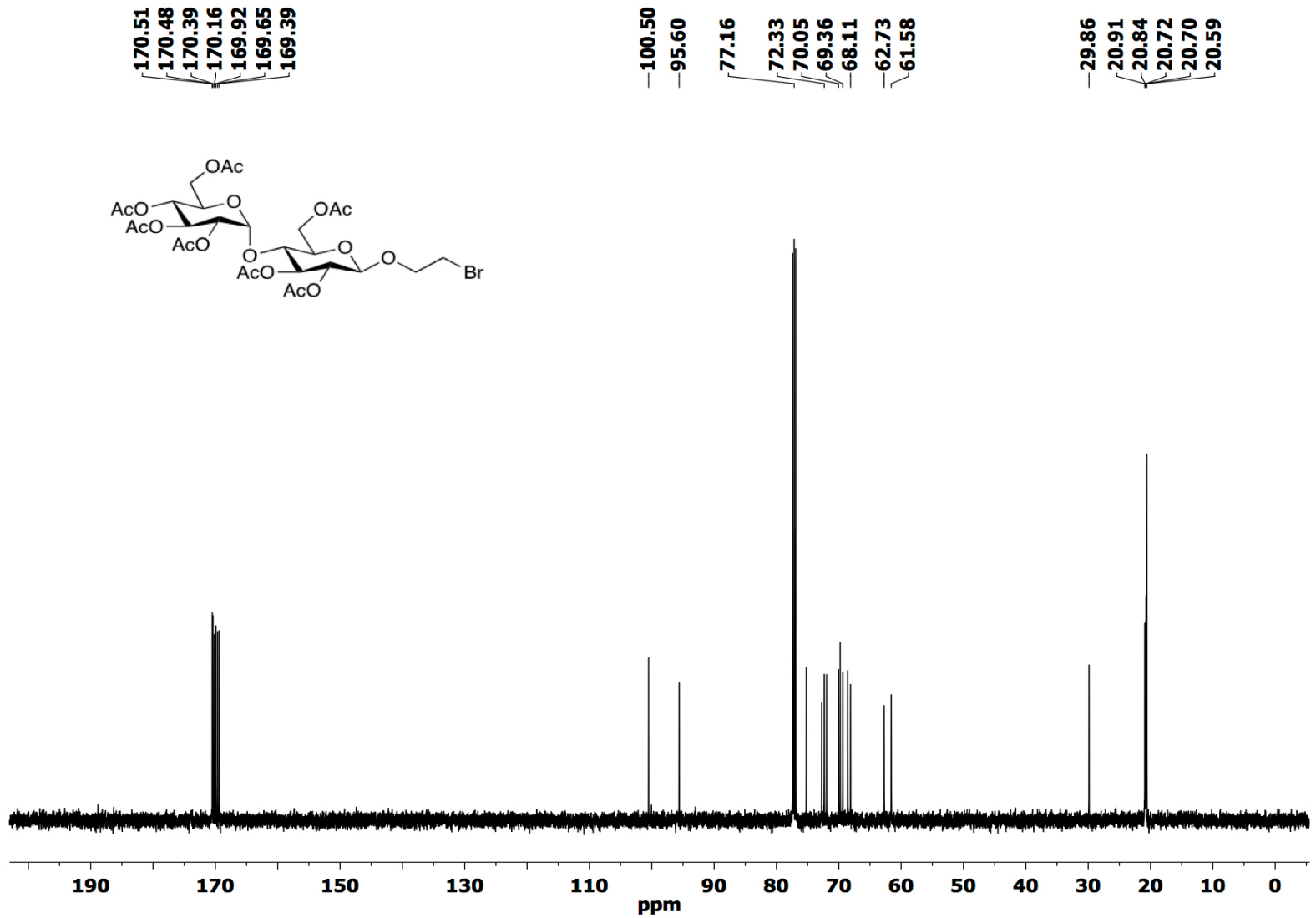


Figure S17. ^{13}C NMR spectrum of compound 8 in $CDCl_3$.

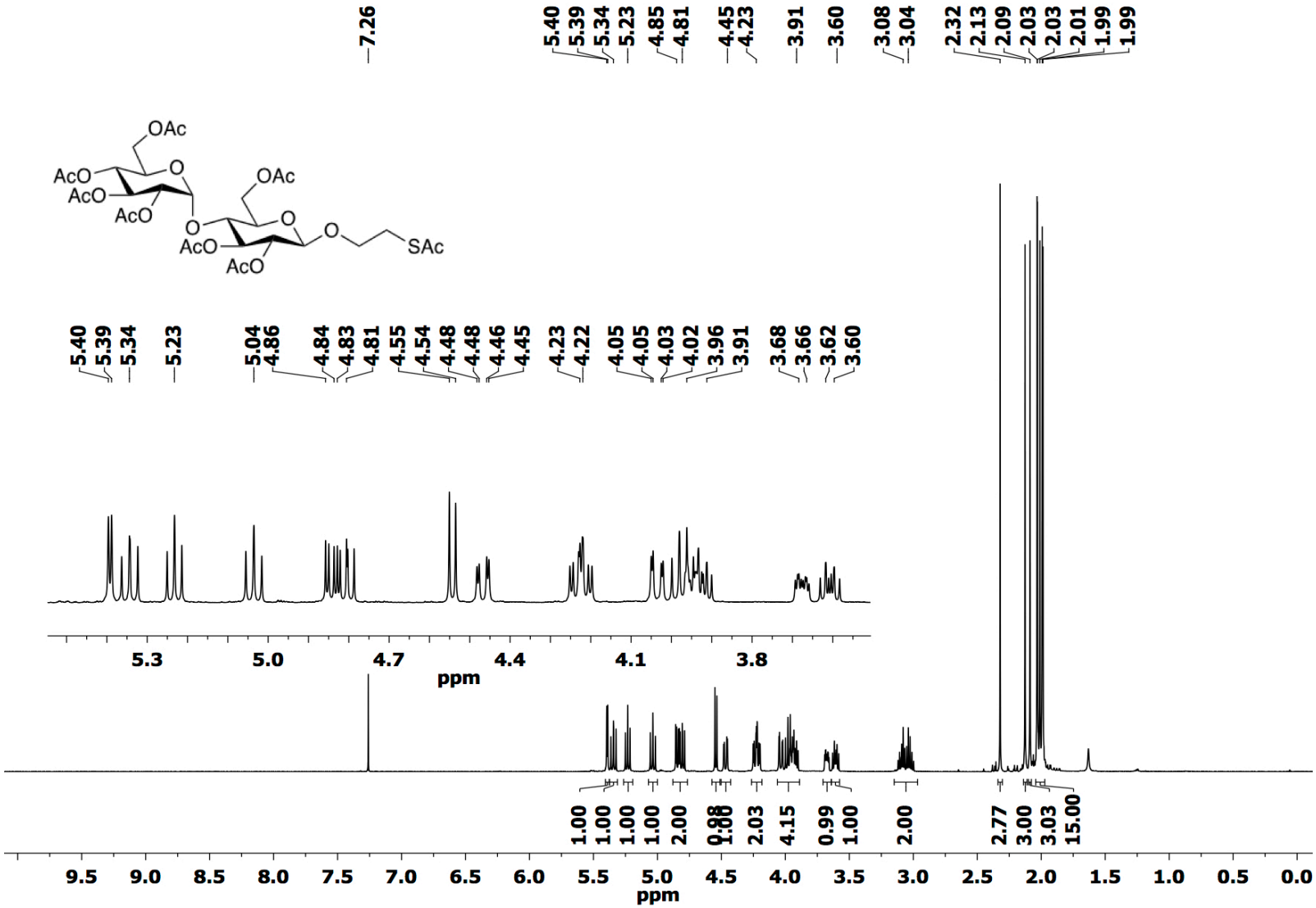


Figure S18. ^{1}H NMR spectrum of compound 9 in $CDCl_3$.

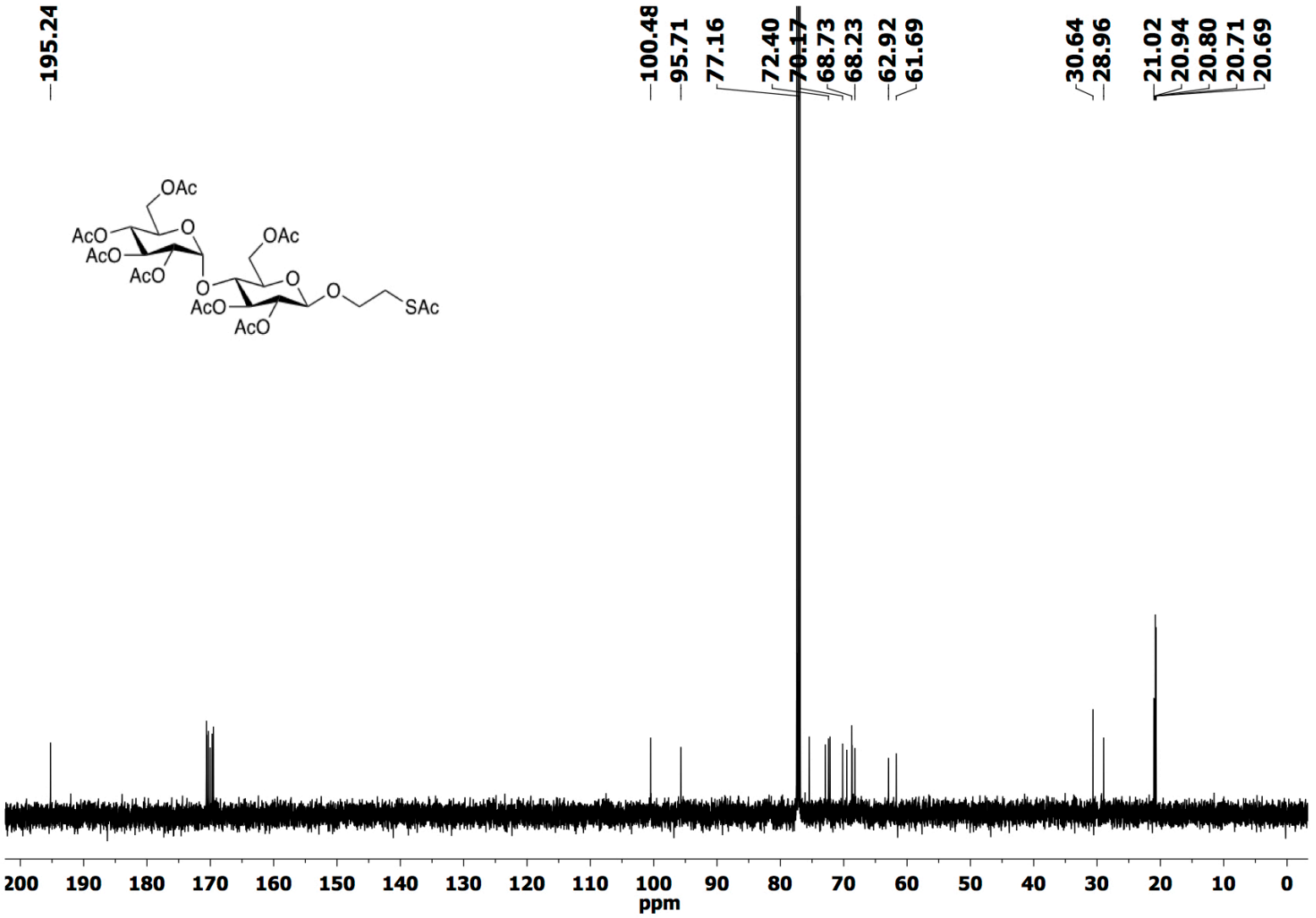


Figure S19. ^{13}C NMR spectrum of compound **9** in $CDCl_3$.

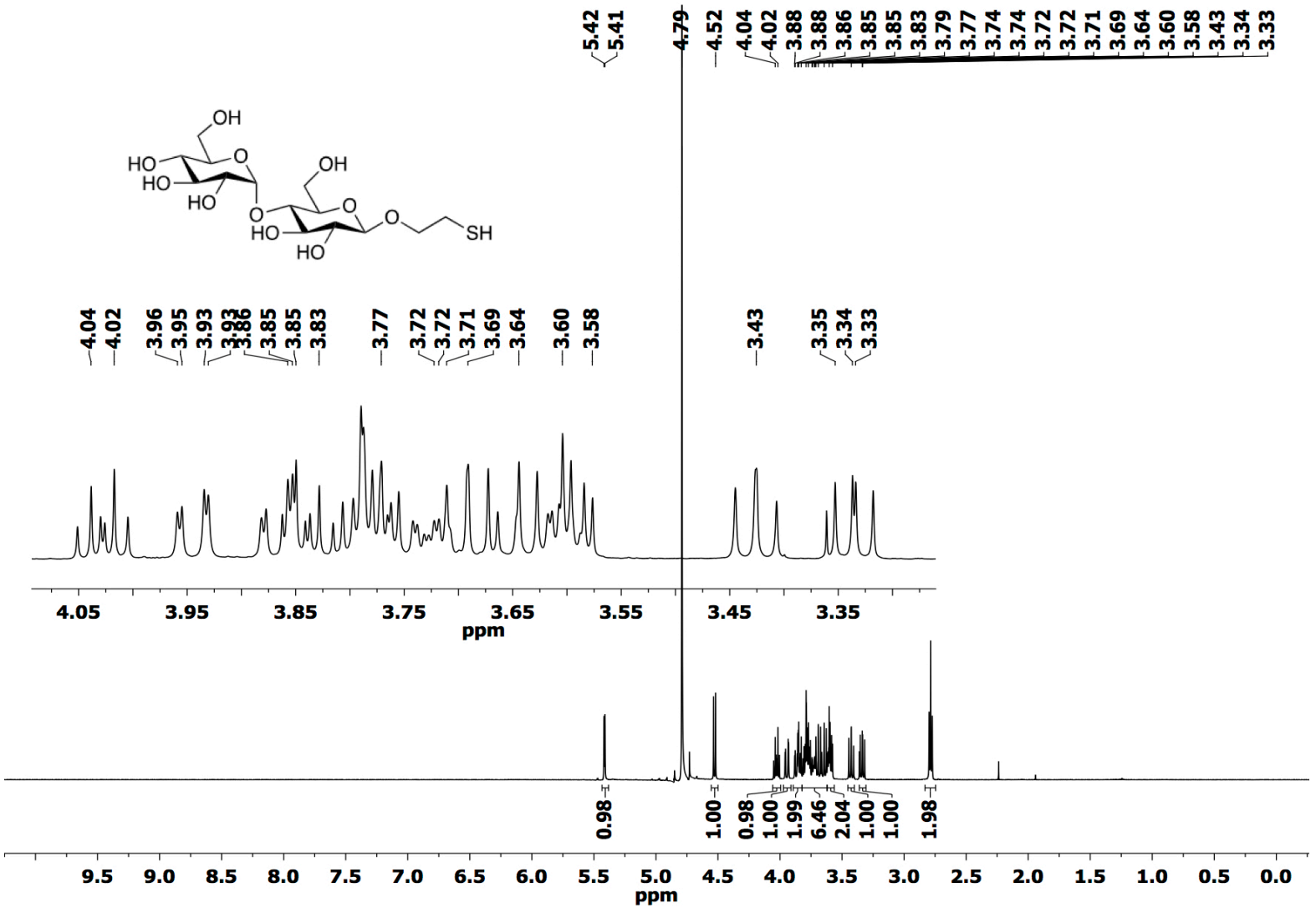


Figure S20. ^{1}H NMR spectrum of compound 10 in D_2O.

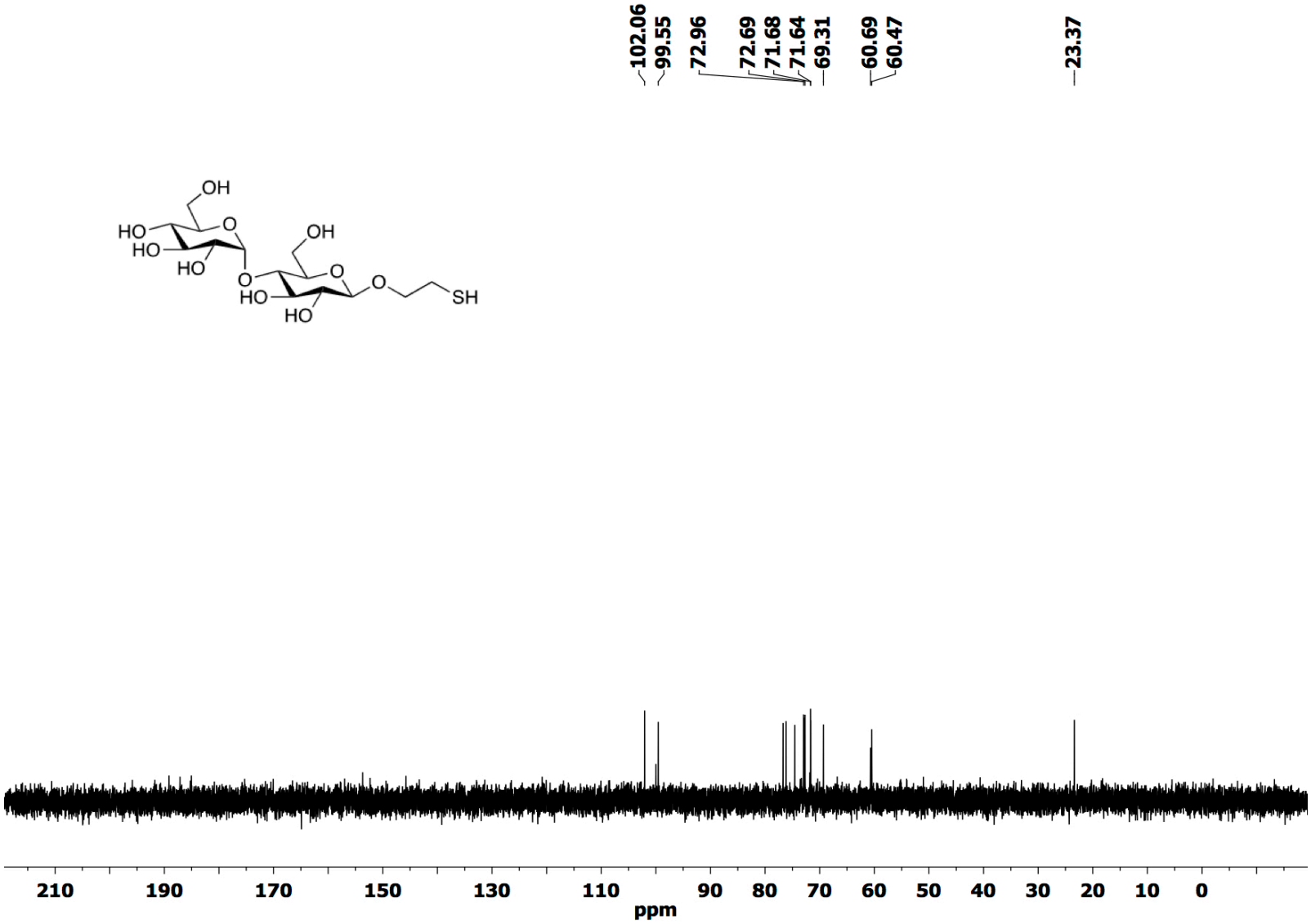


Figure S21. ^{13}C NMR spectrum of compound 10 in D_2O.

IR spectra

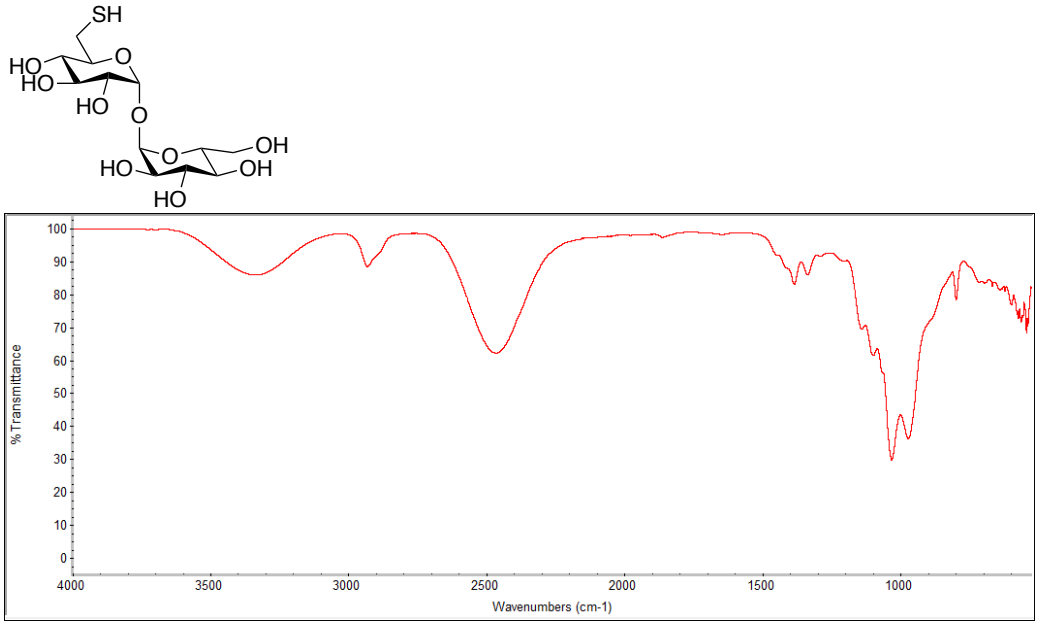


Figure S22. FT-IR spectrum of compound 5 (neat).

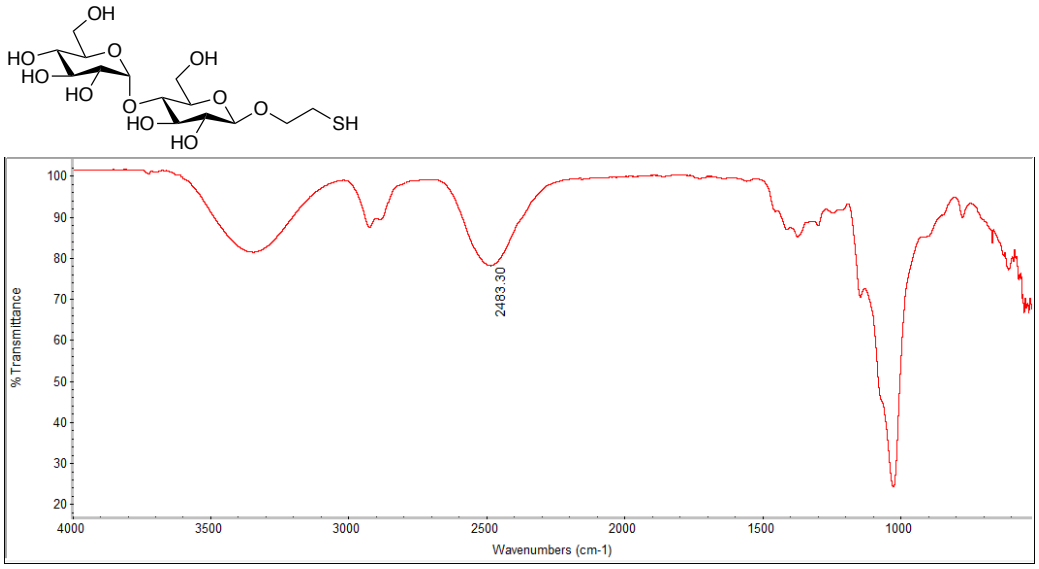


Figure S23. FT-IR spectrum of compound 10 (neat).