

Electronic Supplementary Information (ESI).

Evaluating *N*-benzylgalactonoamidines as putative transition state analogs for β -galactoside hydrolysis

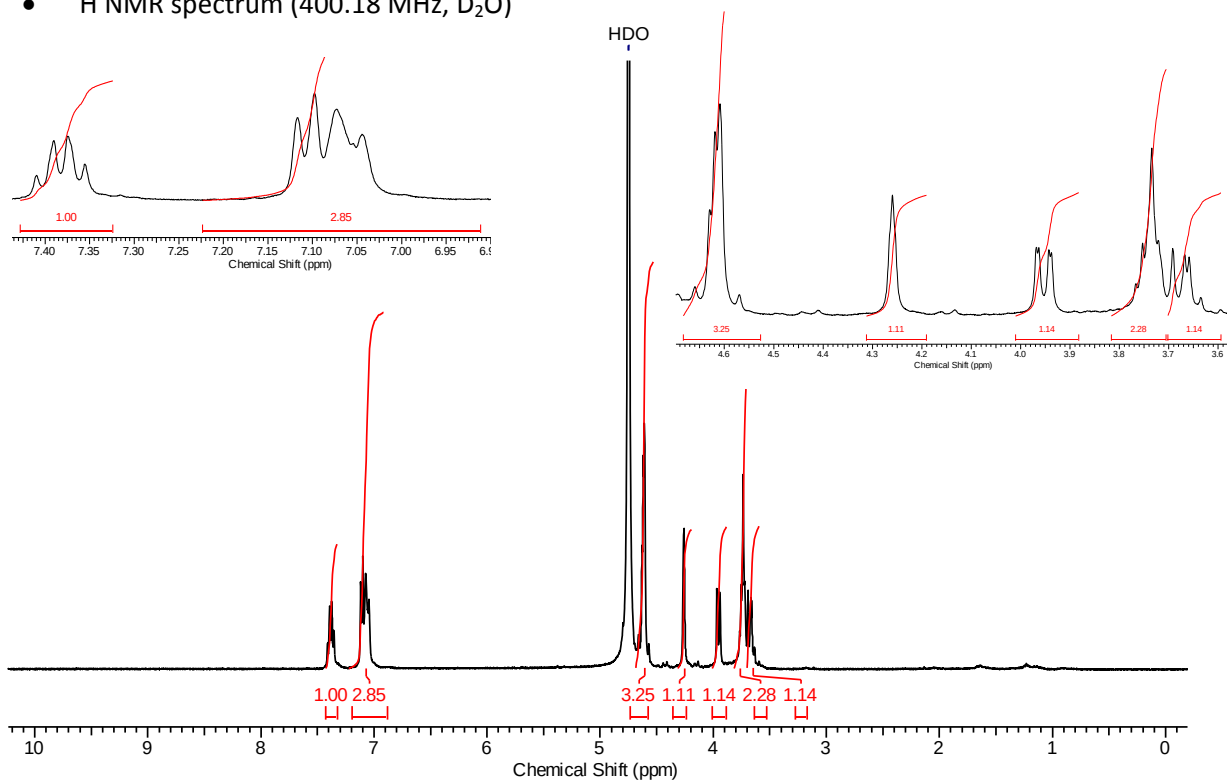
Qiu-Hua Fan, Susanne Striegler*, Rebekah G. Langston and James D. Barnett

¹H and ¹³C NMR spectra

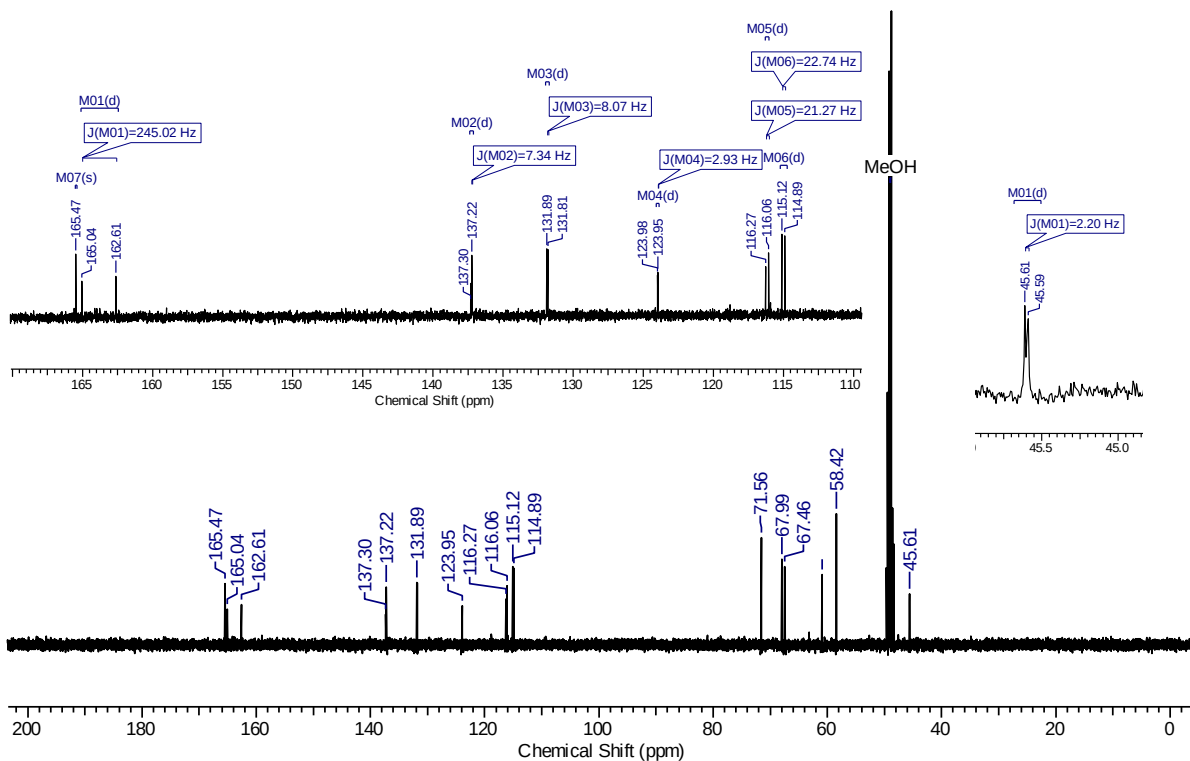
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3-fluorobenzyl-D-galactonoamidine (1f)	2
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3-fluorobenzyl- β -D-galactonoamidine (1f).

- ^1H NMR spectrum (400.18 MHz, D_2O)

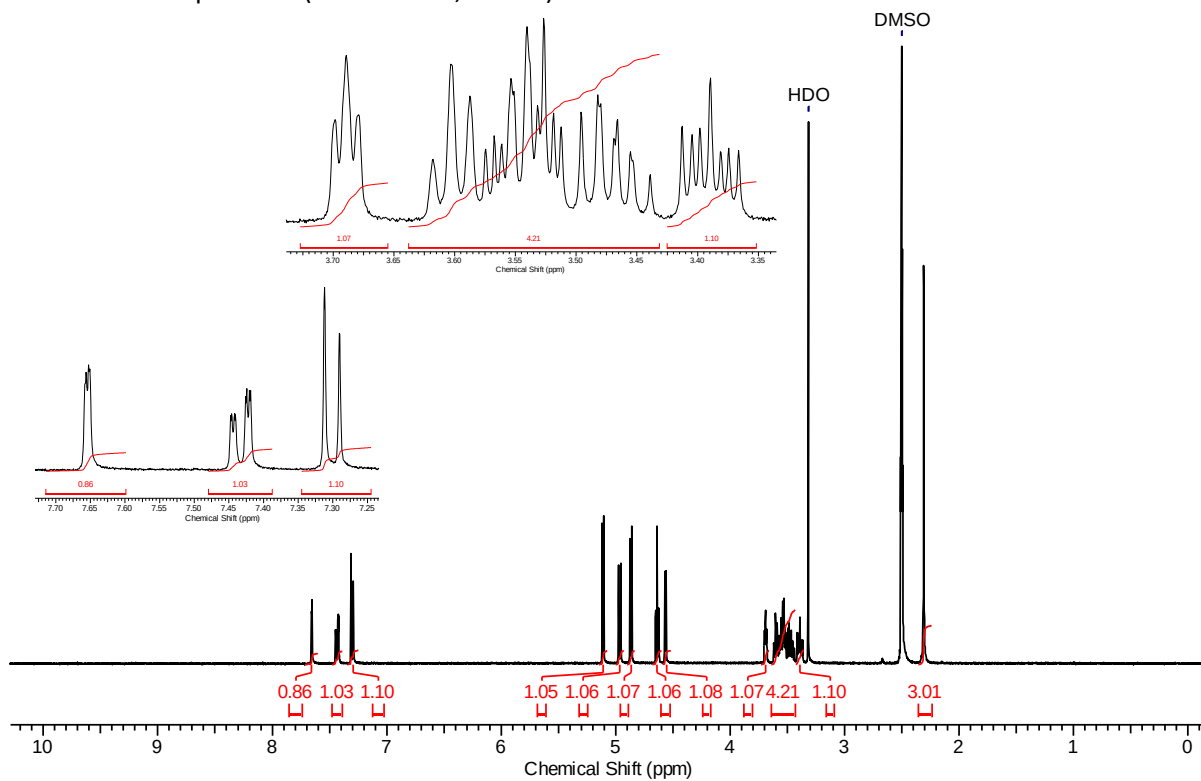


- ^{13}C NMR spectrum (100.6 MHz, $\text{D}_2\text{O}/\text{MeOH-d}_4$)

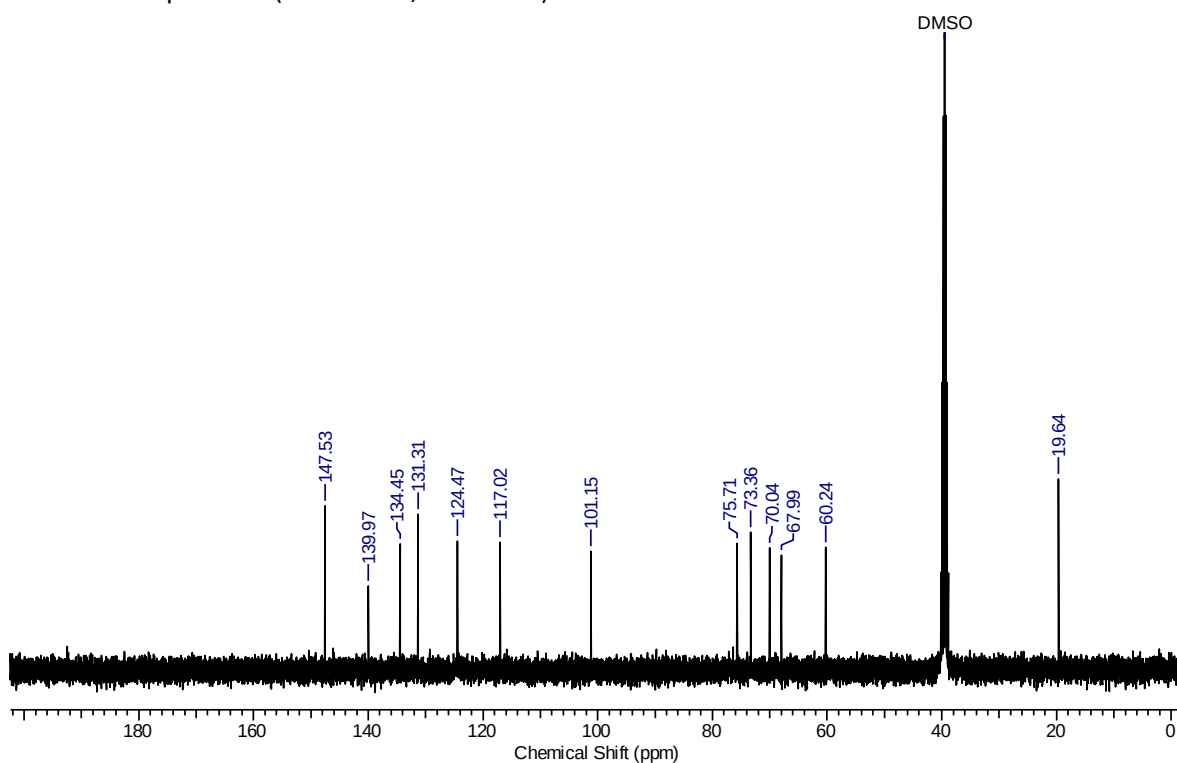


4-Methyl-2-nitrophenyl- β -D-galactopyranoside (2b).

- ^1H NMR spectrum (400.18 MHz, DMSO)

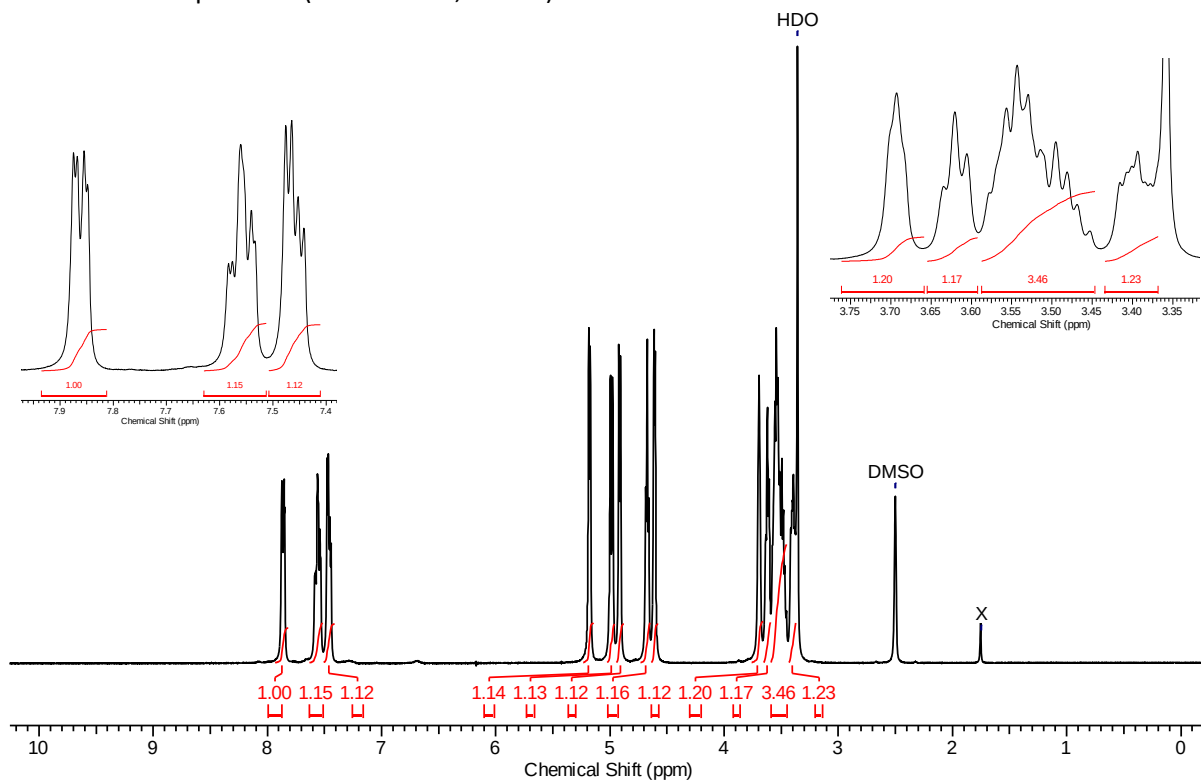


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

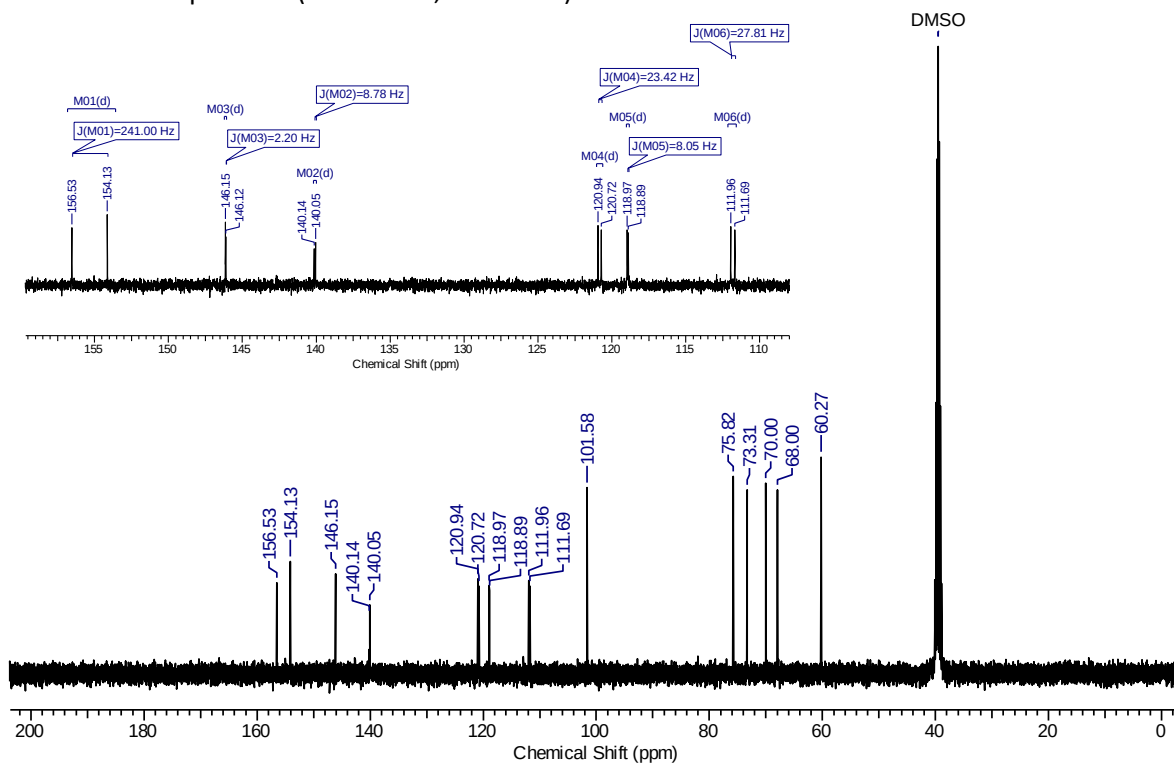


4-Fluoro-2-nitrophenyl- β -D-galactopyranoside (2c).

- ^1H NMR spectrum (400.18 MHz, DMSO)

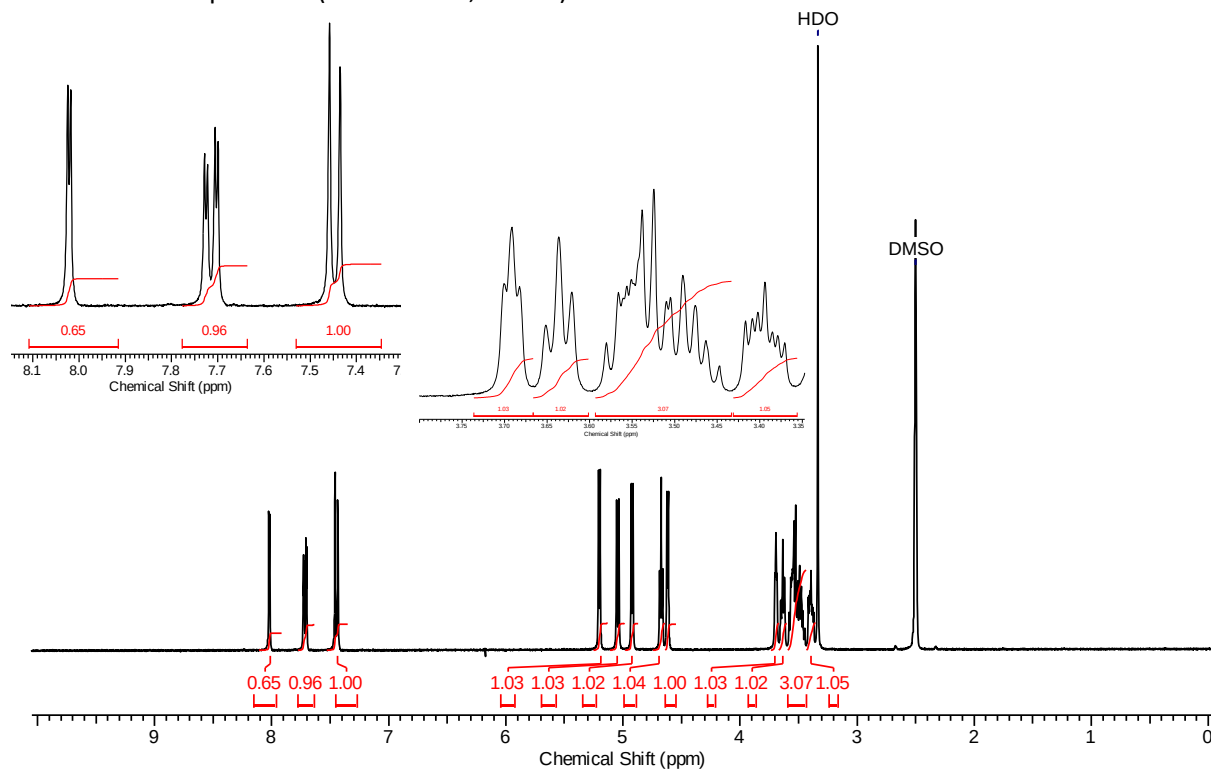


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

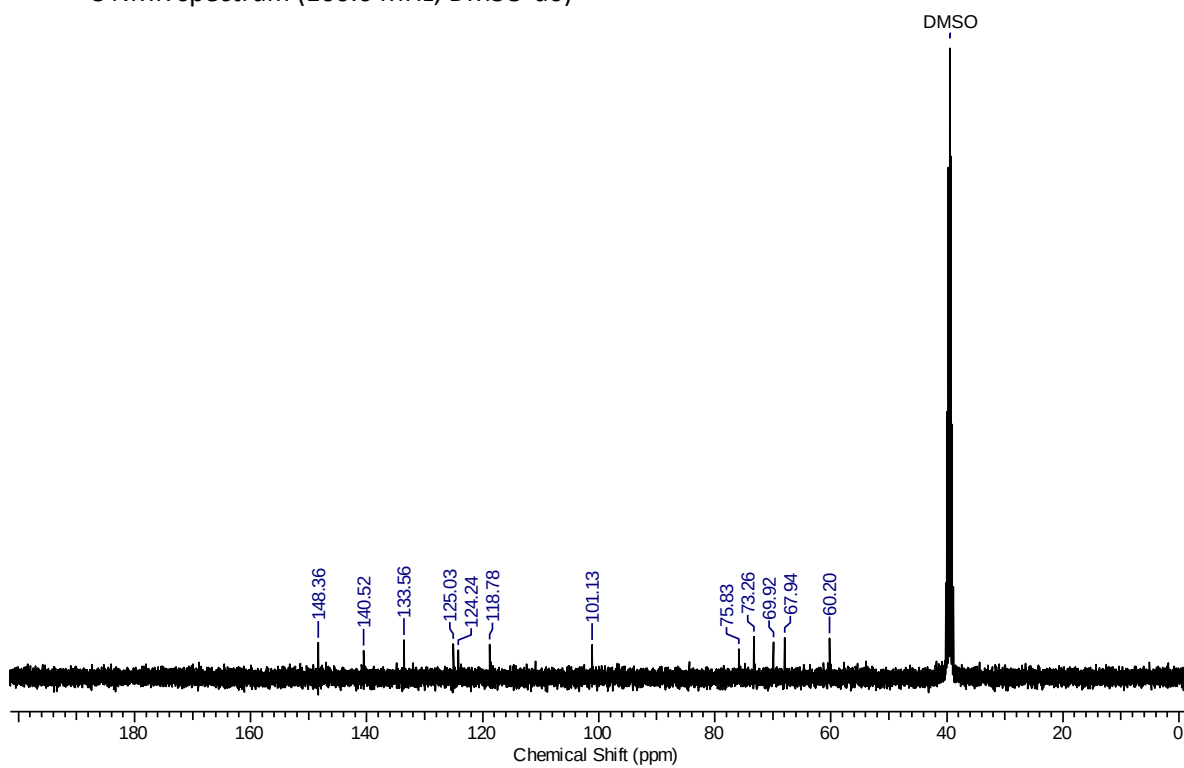


4-Chloro-2-nitrophenyl- β -D-galactopyranoside (2d).

- ^1H NMR spectrum (400.18 MHz, DMSO)

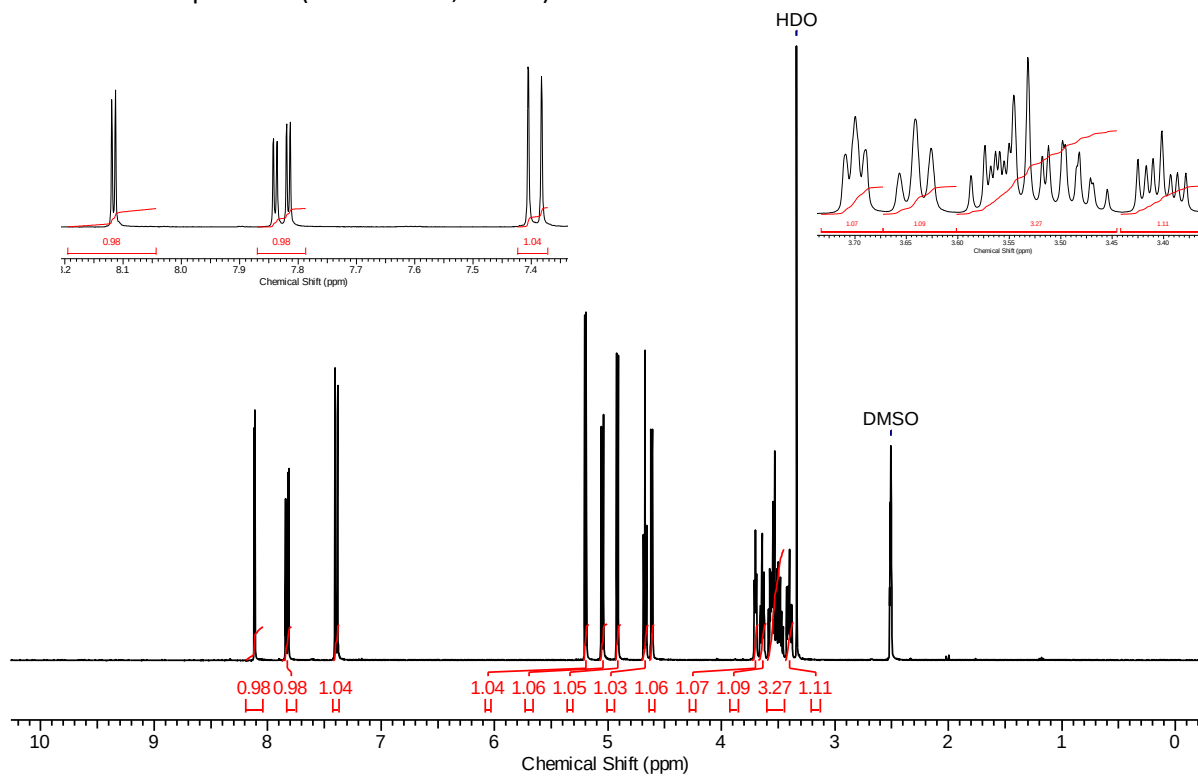


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d₆)

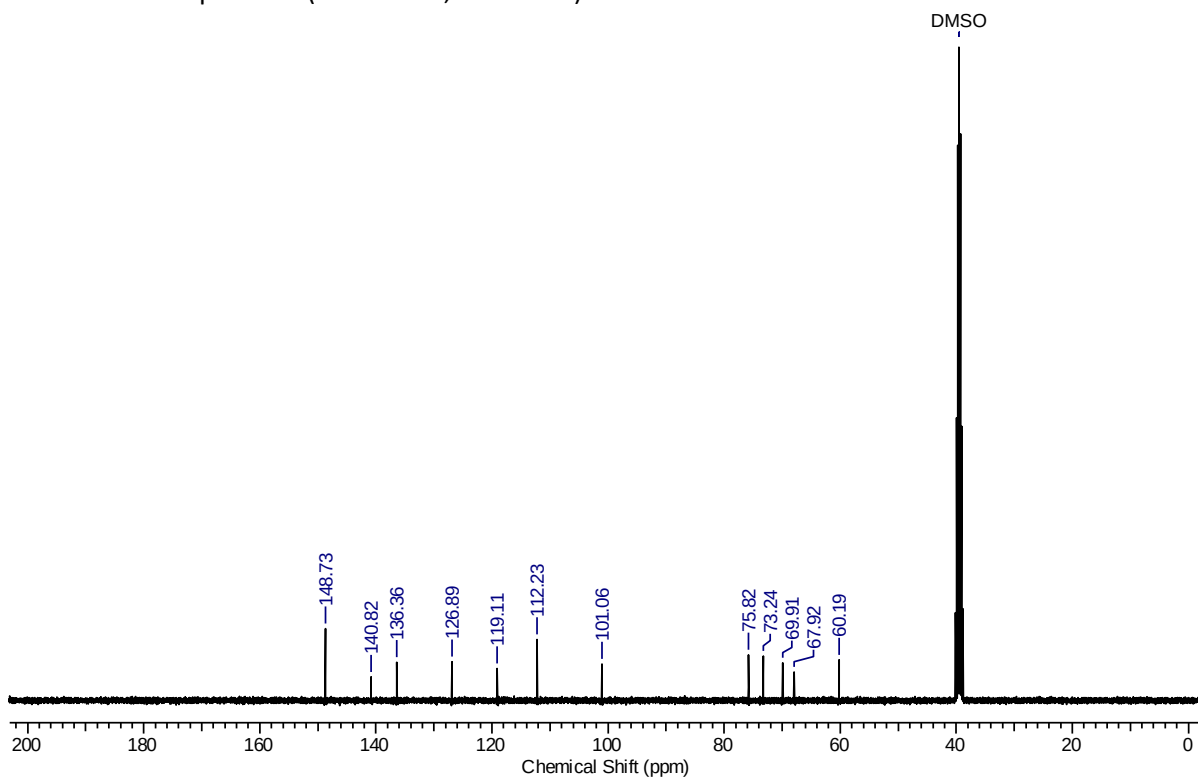


4-Bromo-2-nitrophenyl- β -D-galactopyranoside (2e).

- ^1H NMR spectrum (400.18 MHz, DMSO)

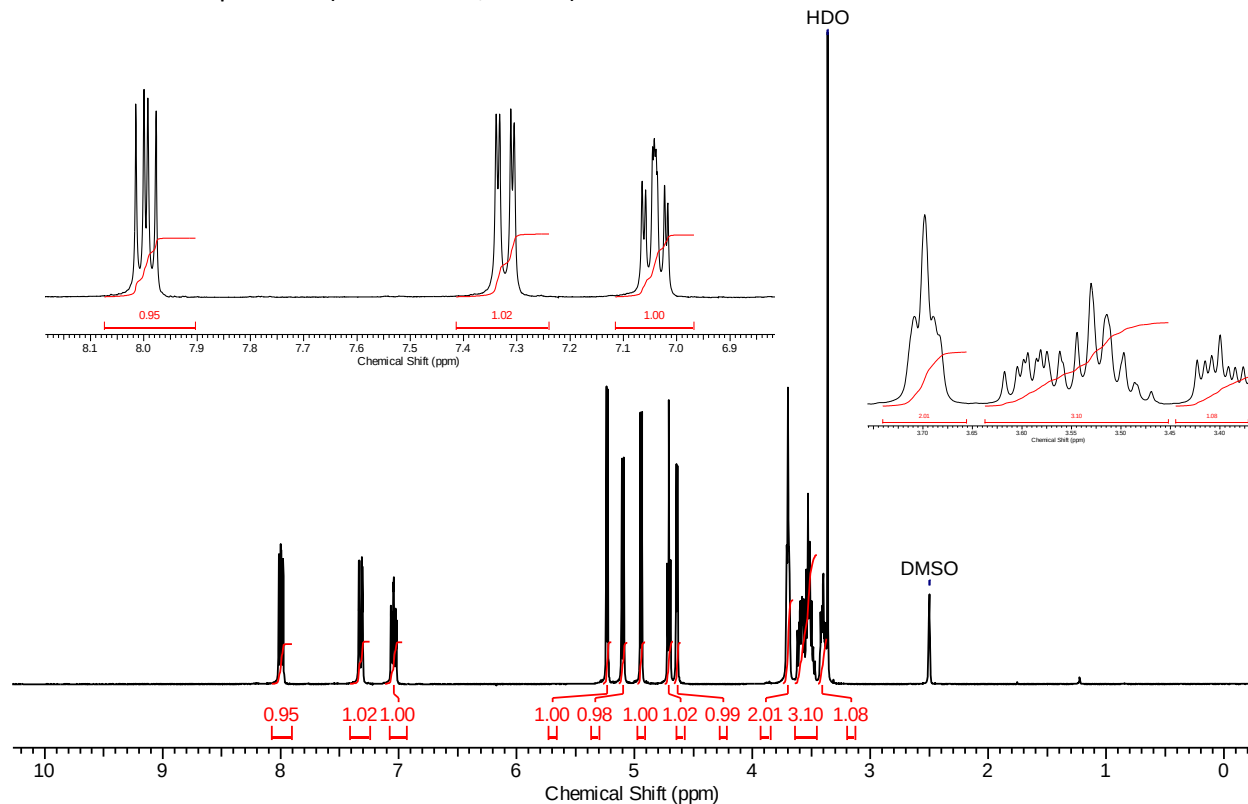


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

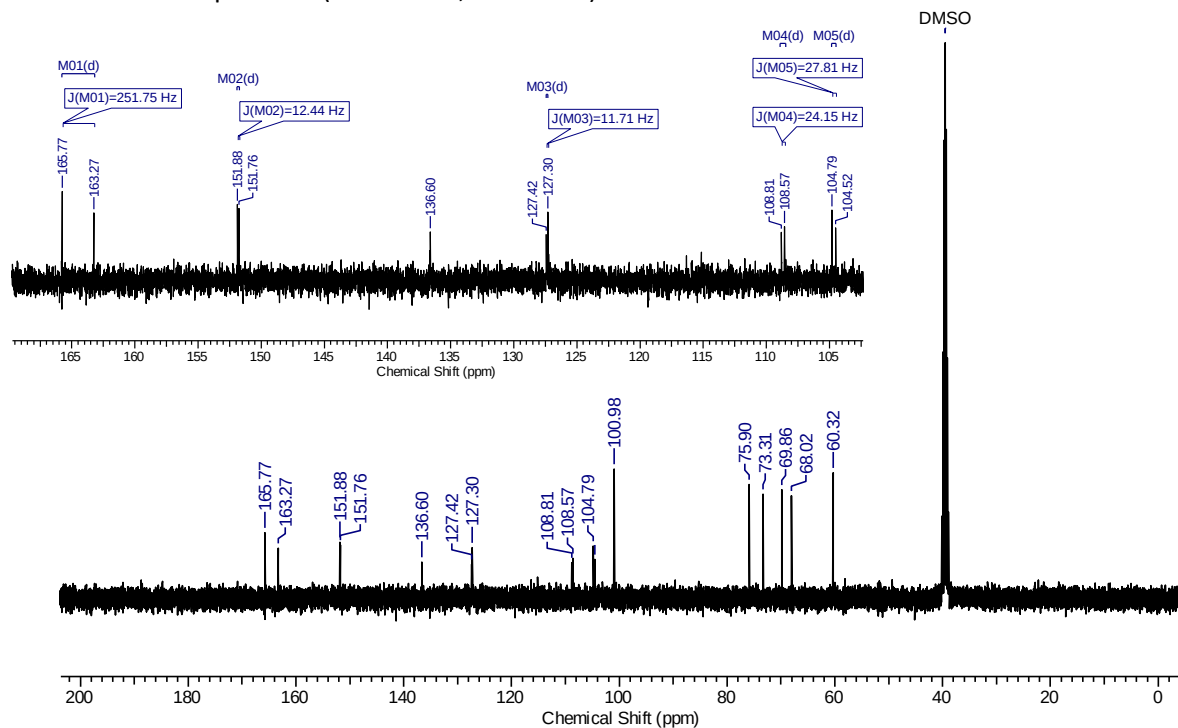


5-Fluoro-2-nitrophenyl- β -D-galactopyranoside (2f).

- ^1H NMR spectrum (400.18 MHz, DMSO)

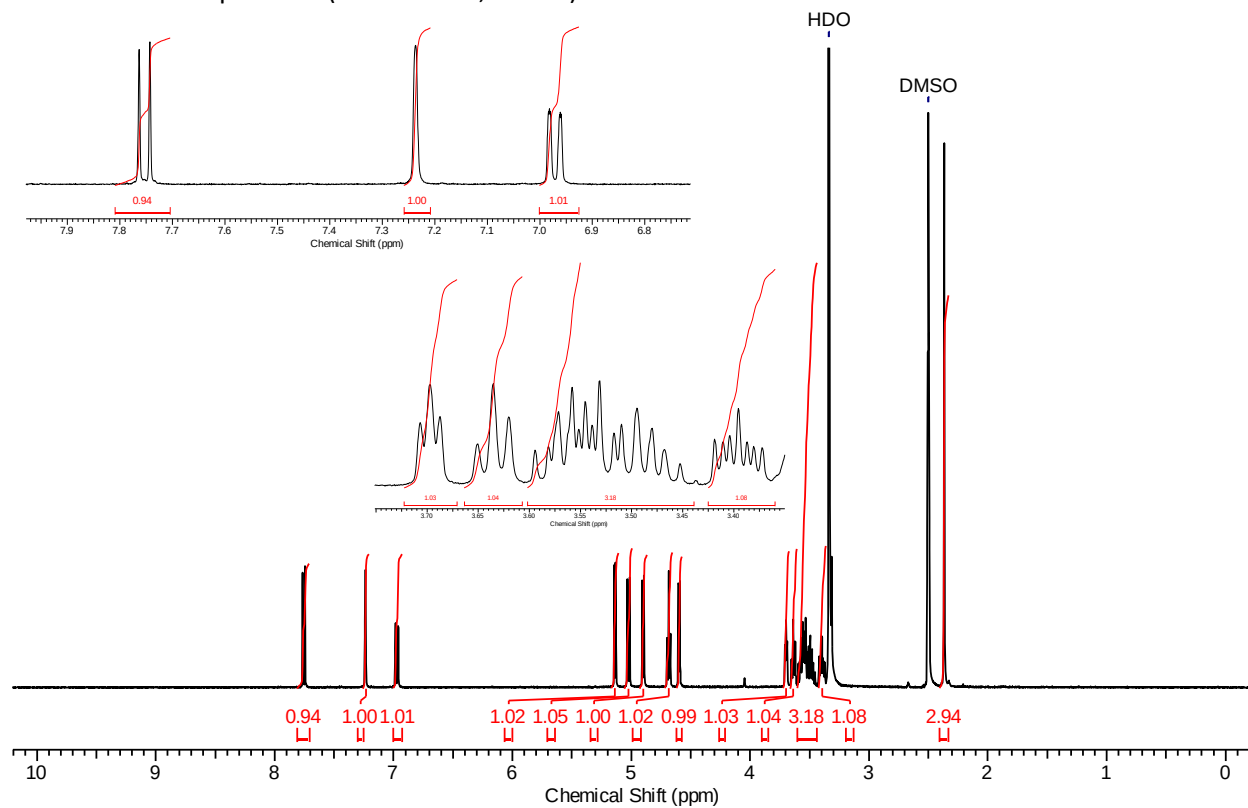


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

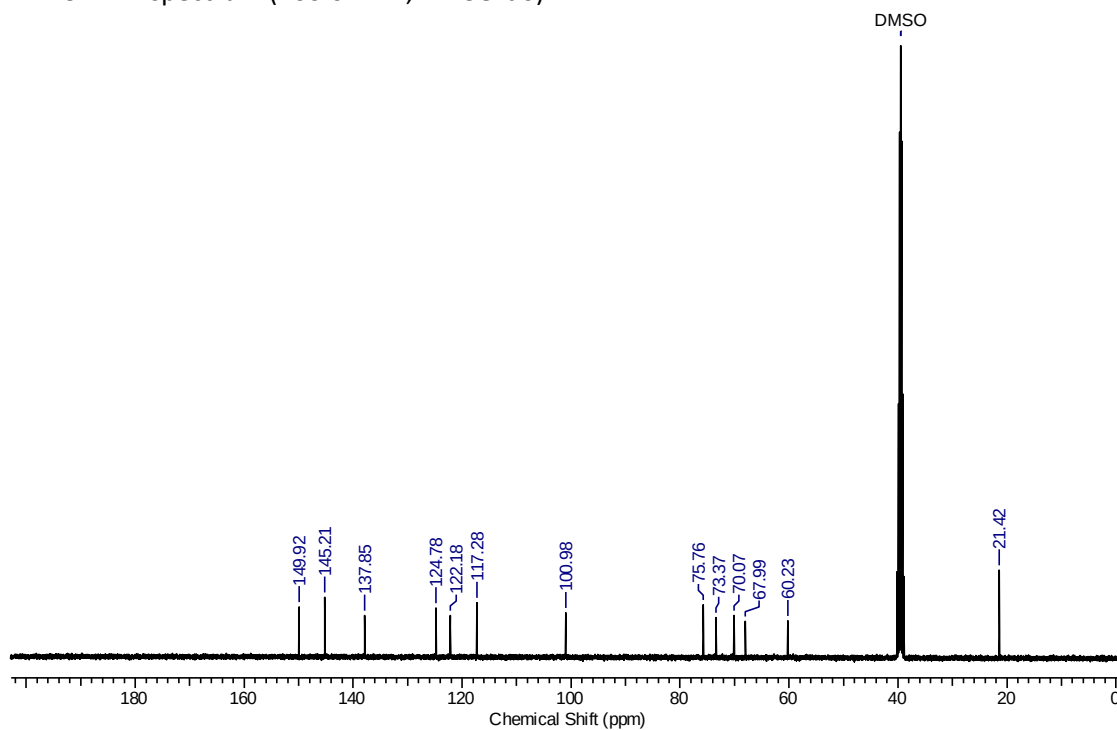


5-Methyl-2-nitrophenyl- β -D-galactopyranoside (2g).

- ^1H NMR spectrum (400.18 MHz, DMSO)

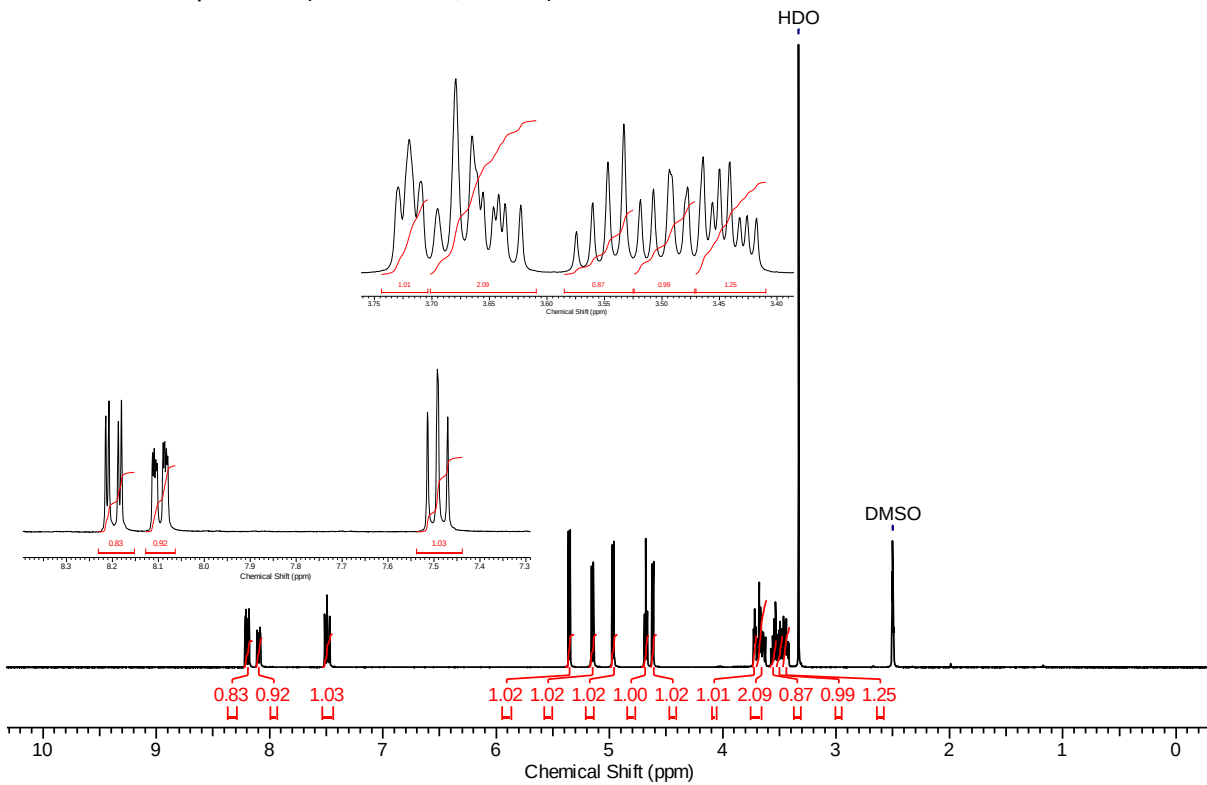


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

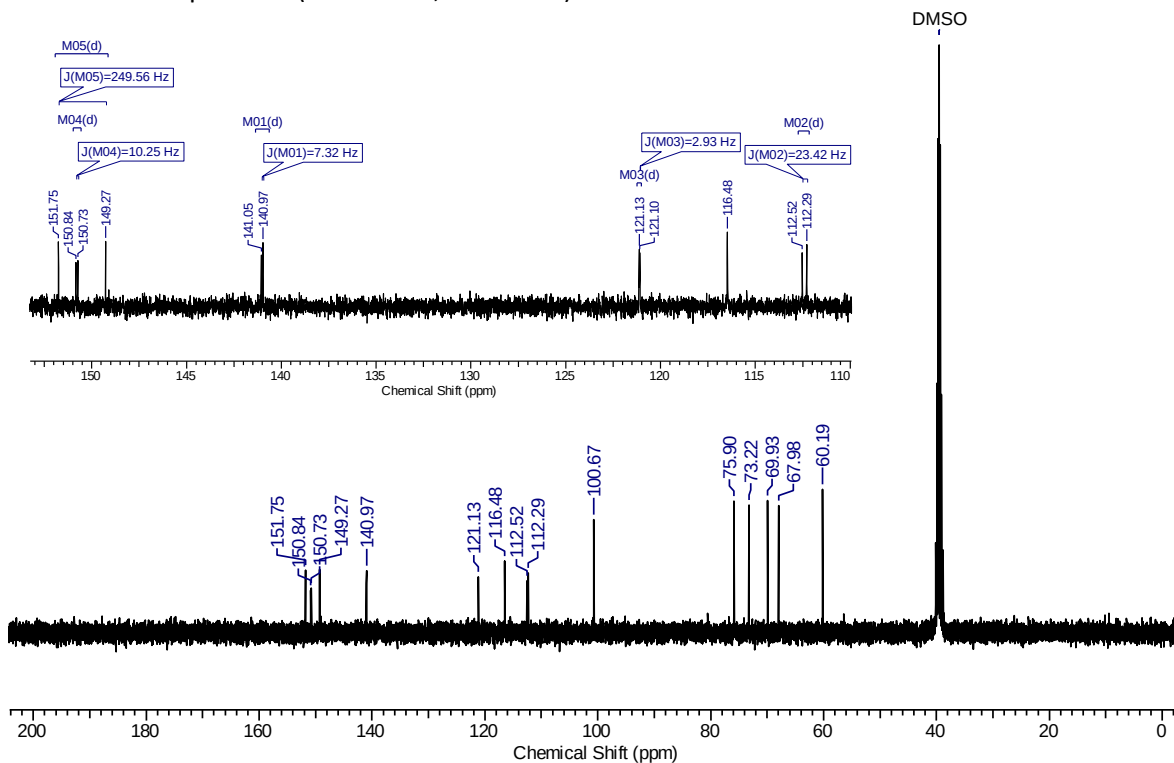


2-Fluoro-4-nitrophenyl- β -D-galactopyranoside (2i).

- ^1H NMR spectrum (400.18 MHz, DMSO)

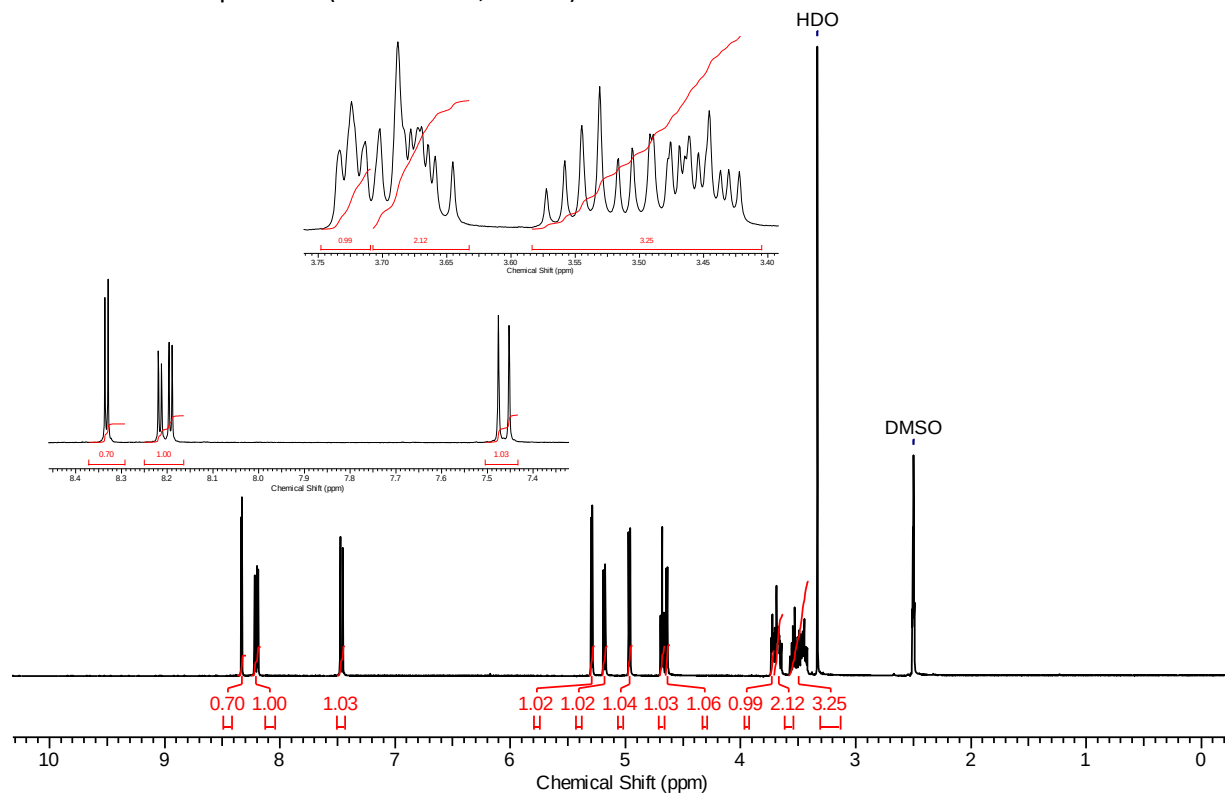


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

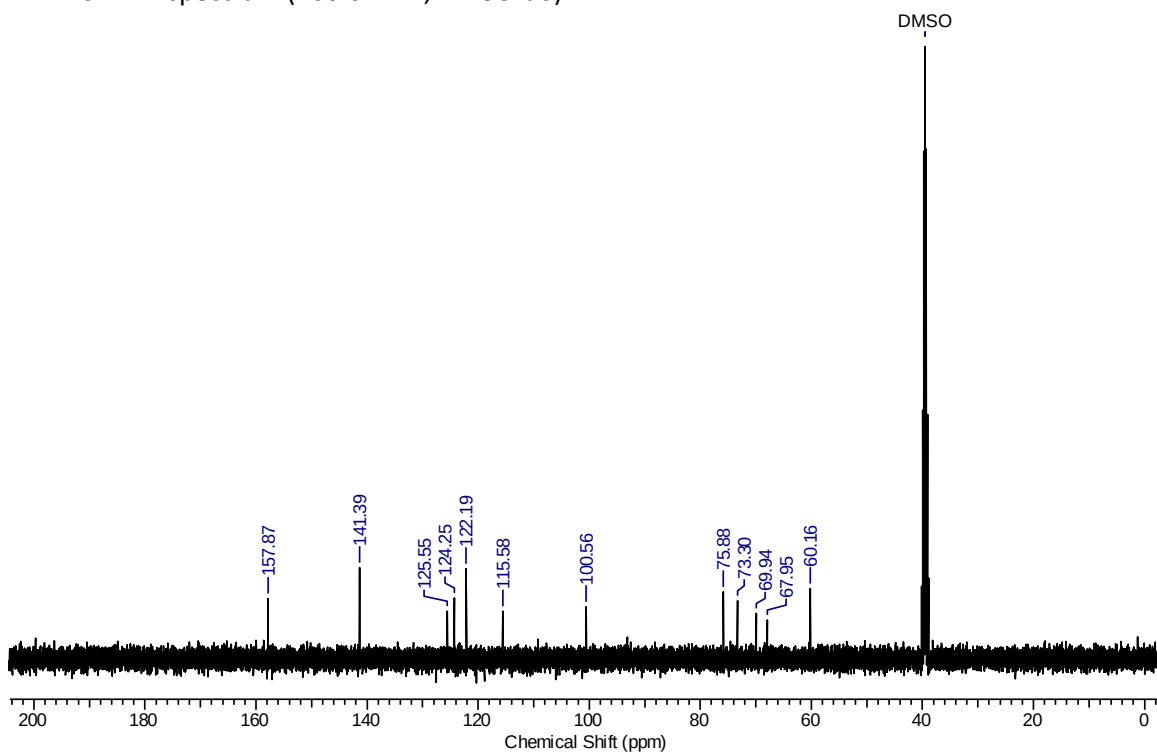


2-Chloro-4-nitrophenyl- β -D-galactopyranoside (2k).

- ^1H NMR spectrum (400.18 MHz, DMSO)

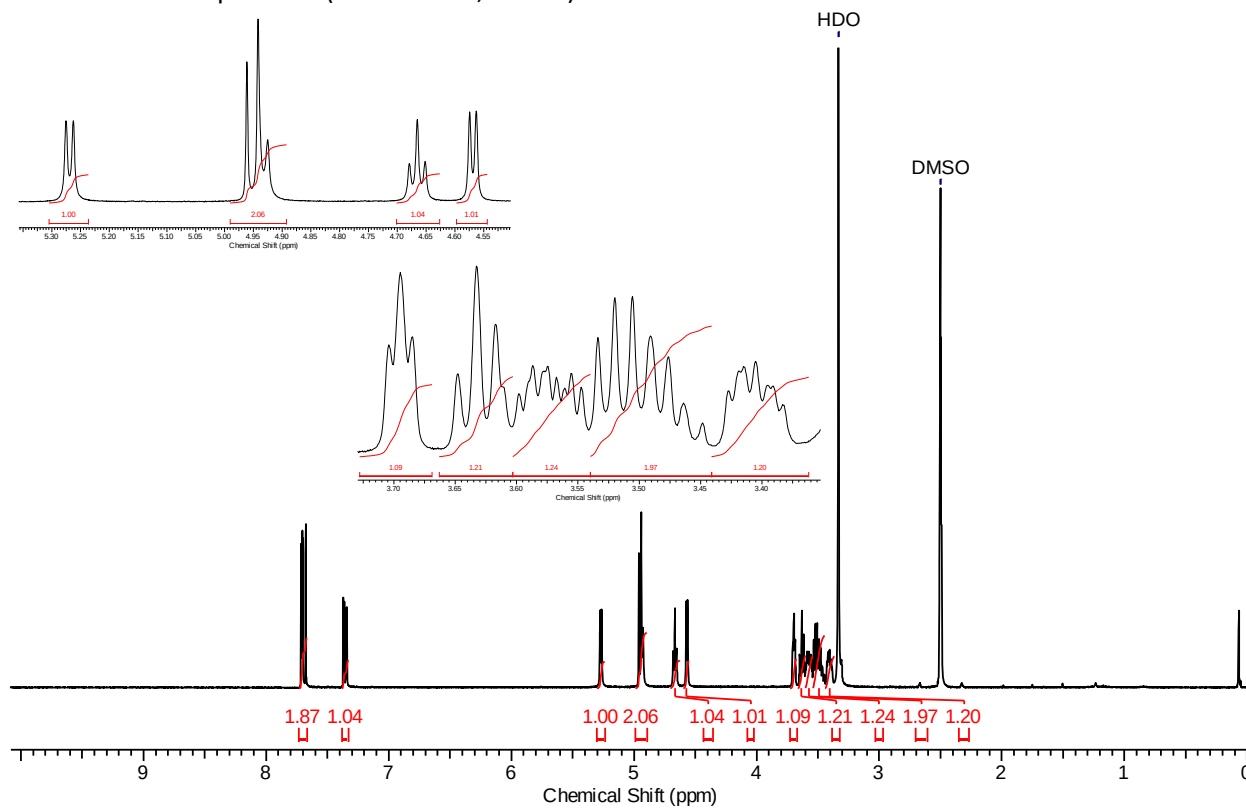


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

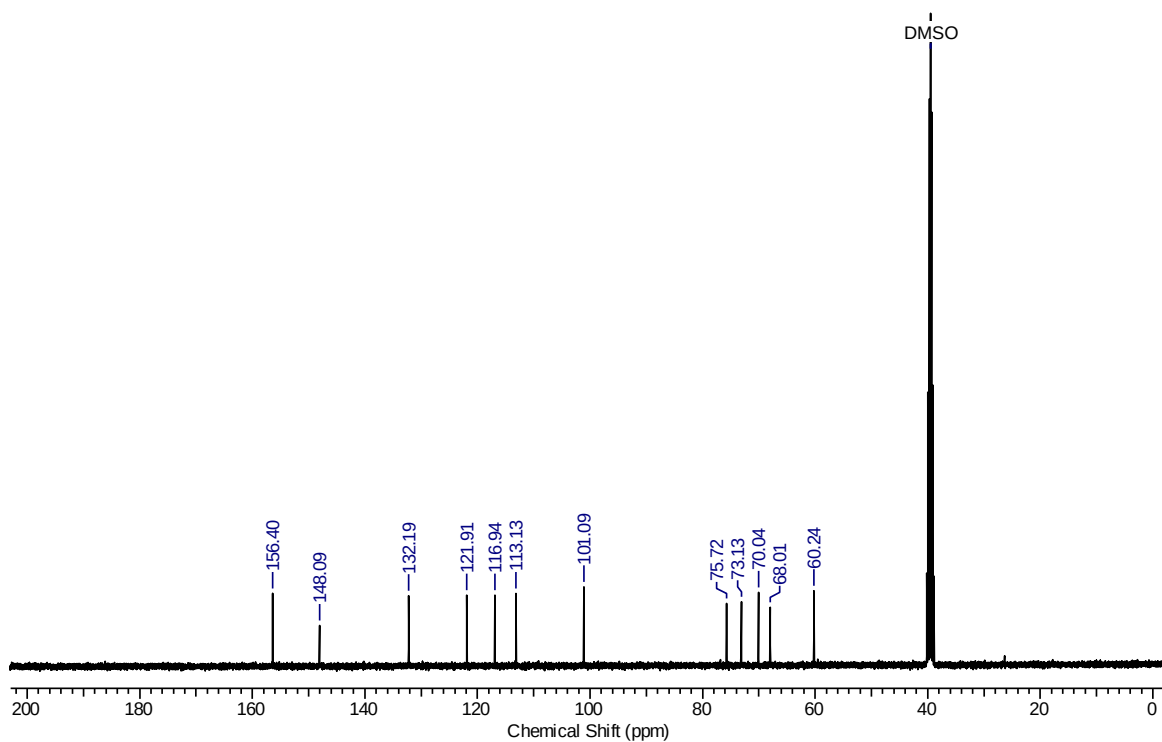


4-Chloro-3-nitrophenyl- β -D-galactopyranoside (2m).

- ^1H NMR spectrum (400.18 MHz, DMSO)

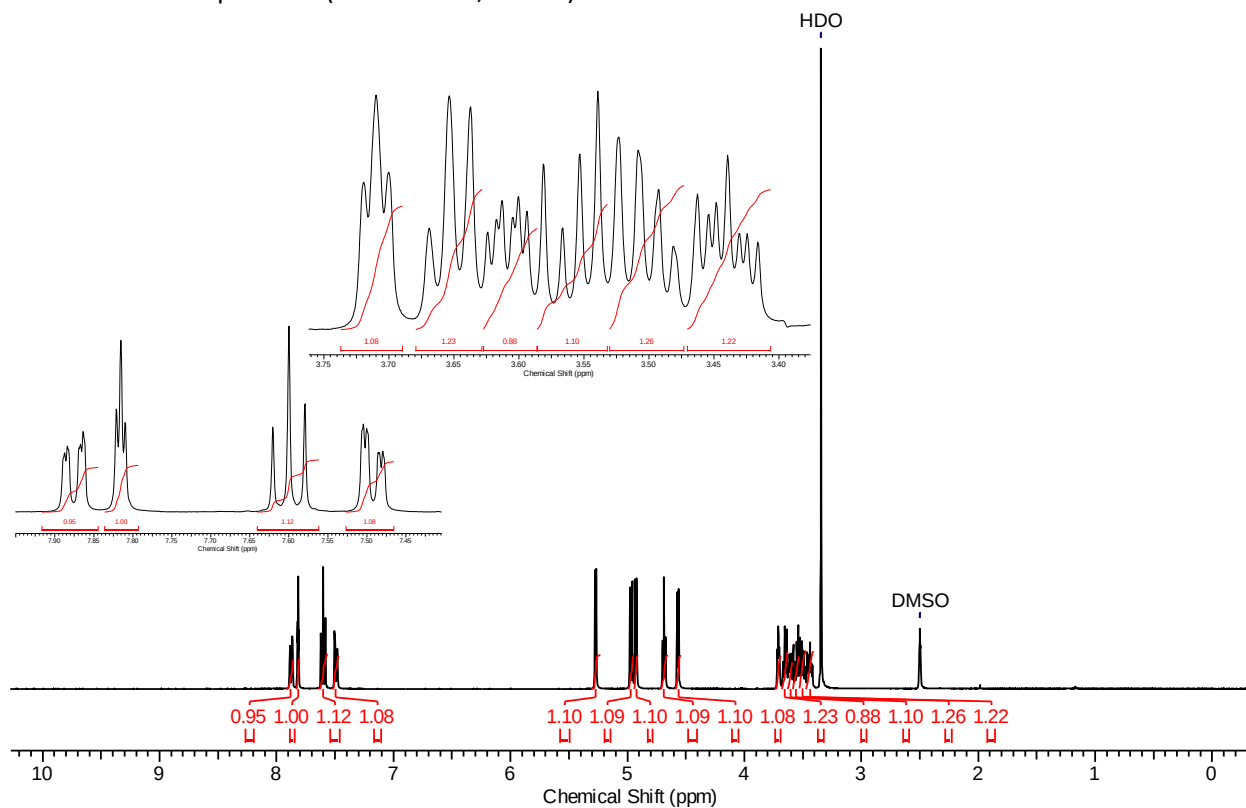


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

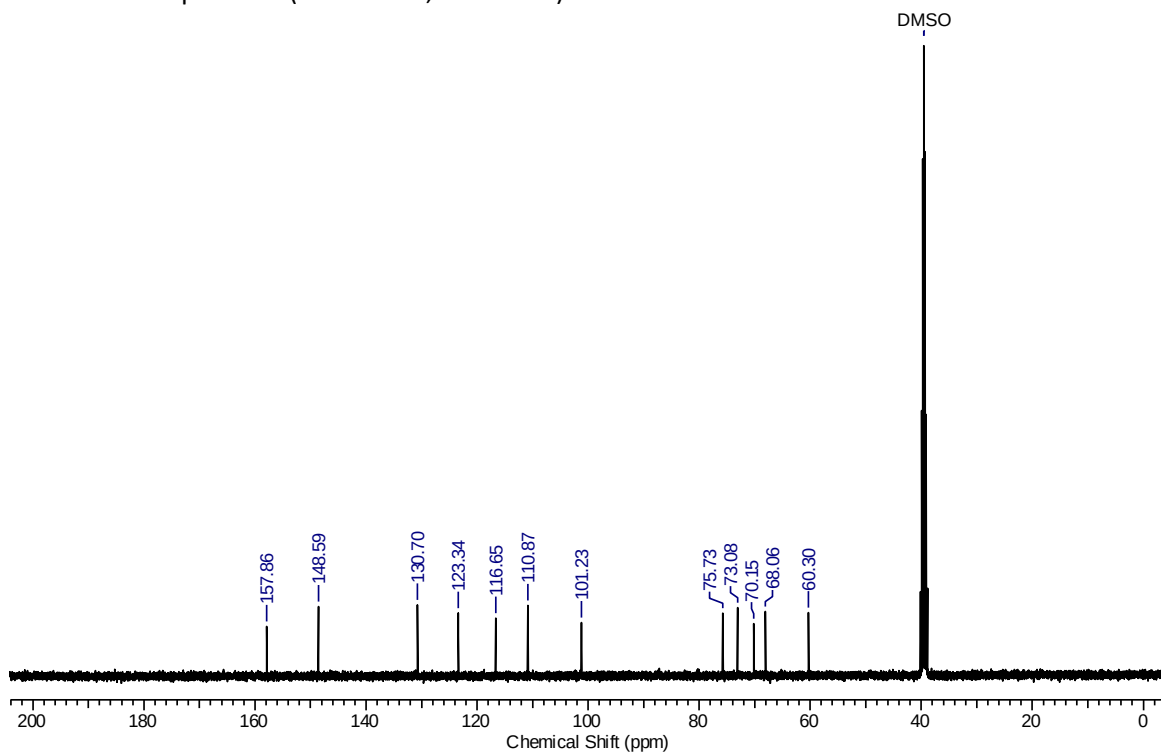


3-Nitrophenyl- β -D-galactopyranoside (2n).

- ^1H NMR spectrum (400.18 MHz, DMSO)

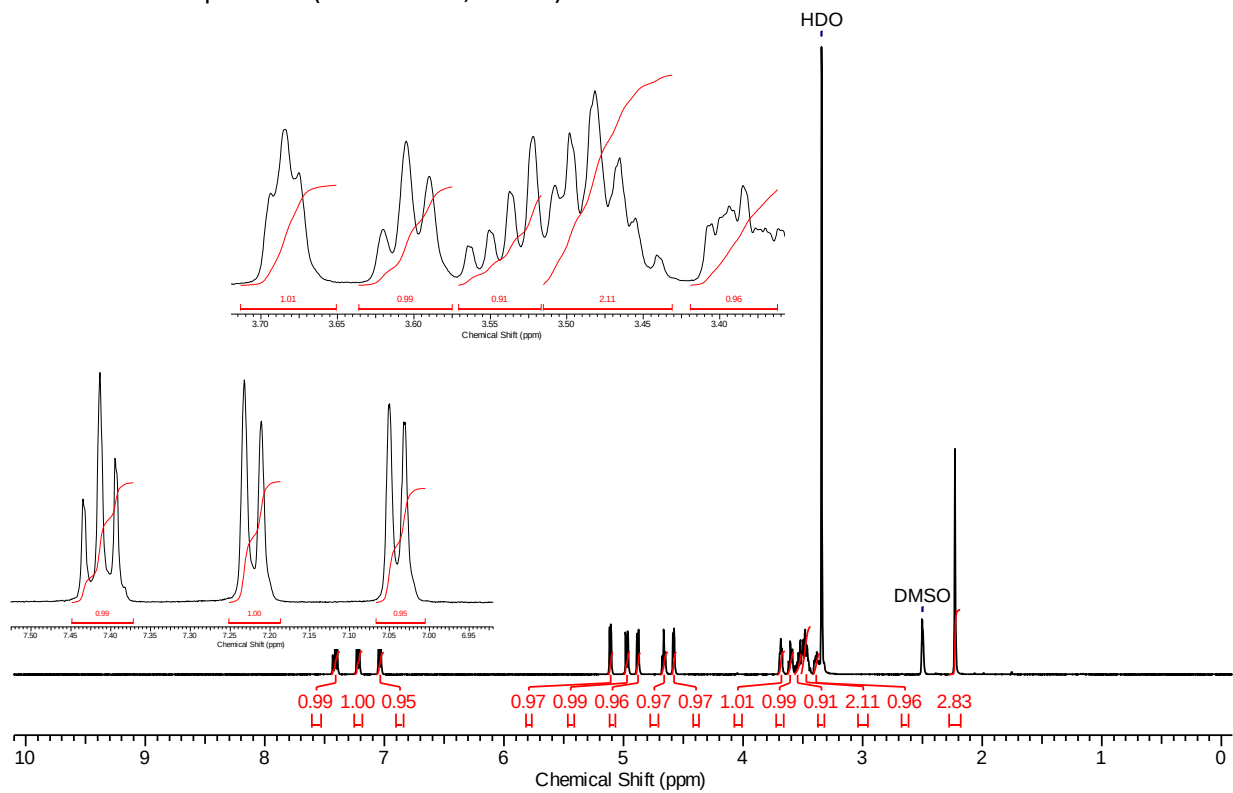


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

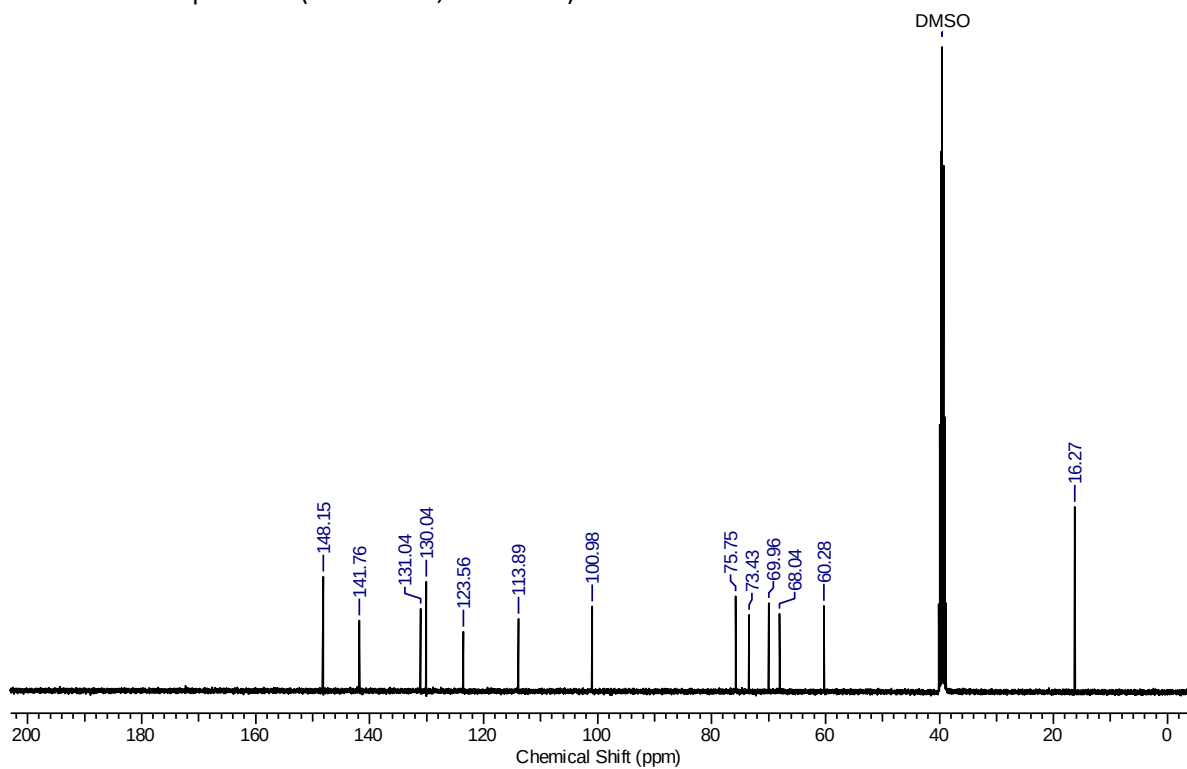


3-Methyl-2-nitrophenyl- β -D-galactopyranoside (2o).

- ^1H NMR spectrum (400.18 MHz, DMSO)

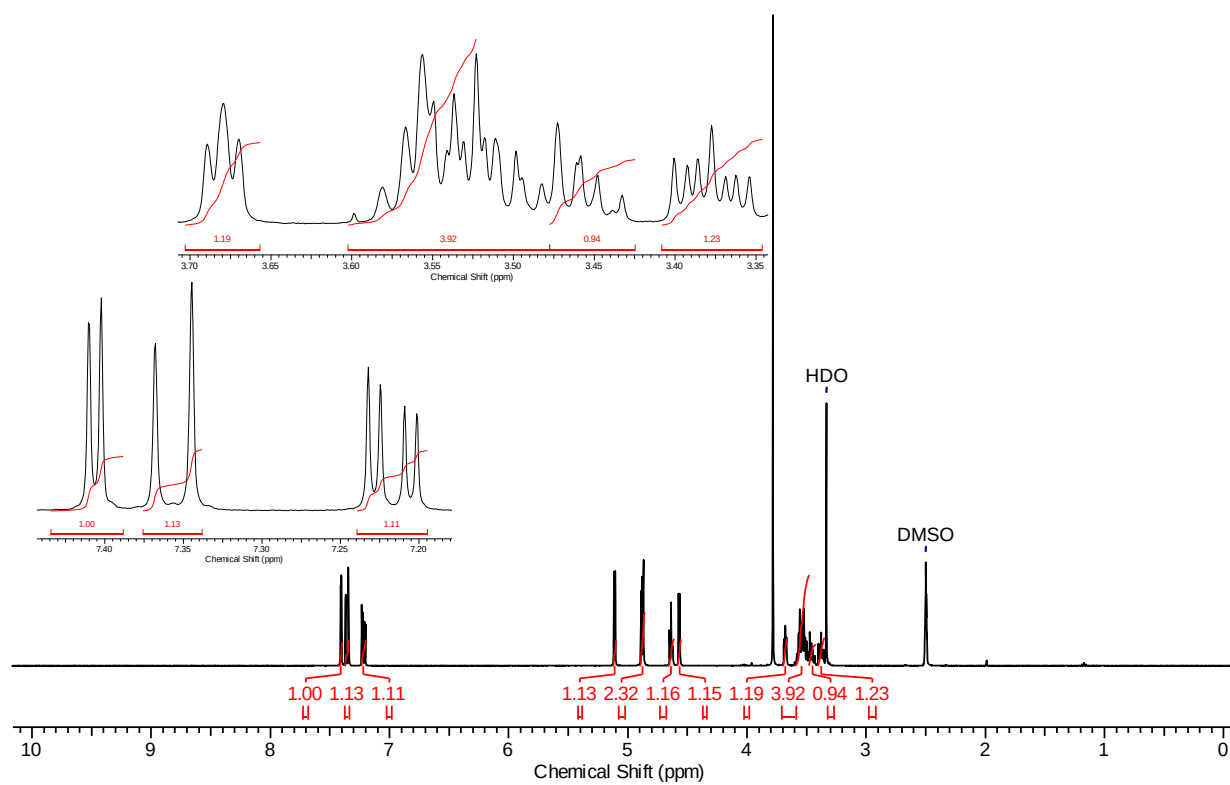


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

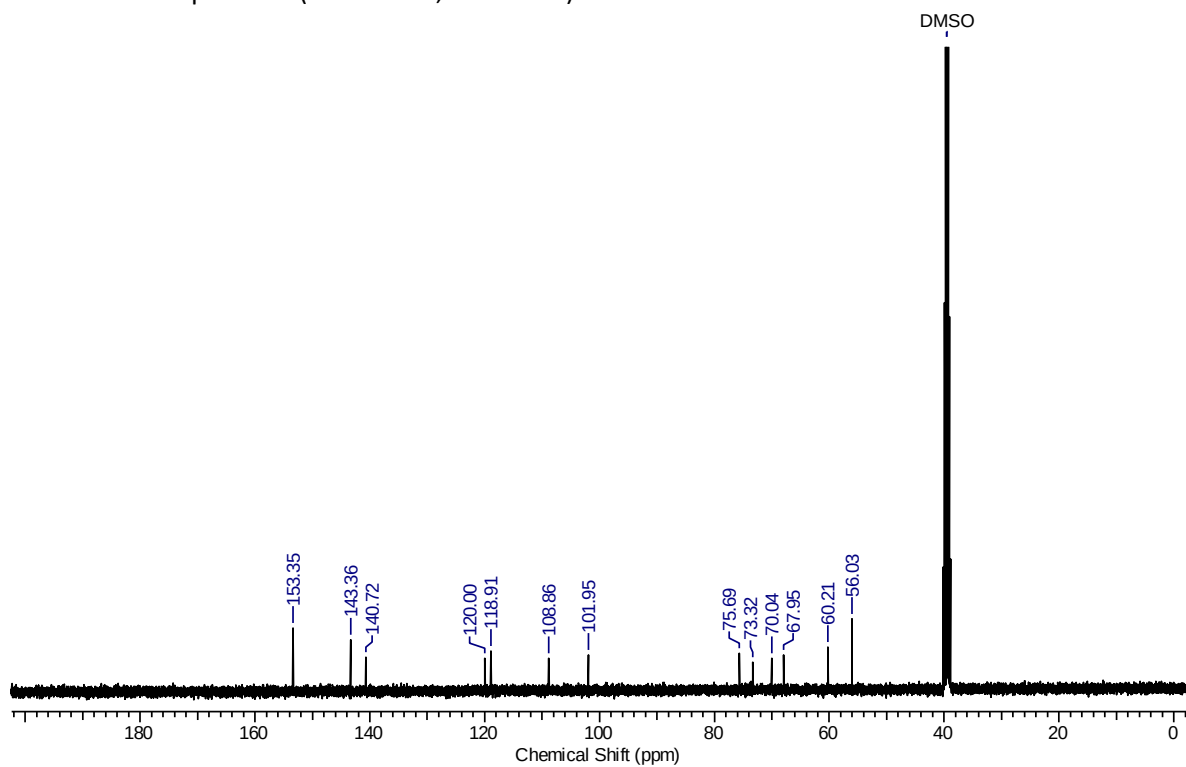


4-Methoxy-2-nitrophenyl- β -D-galactopyranoside (2p).

- ^1H NMR spectrum (400.18 MHz, DMSO)

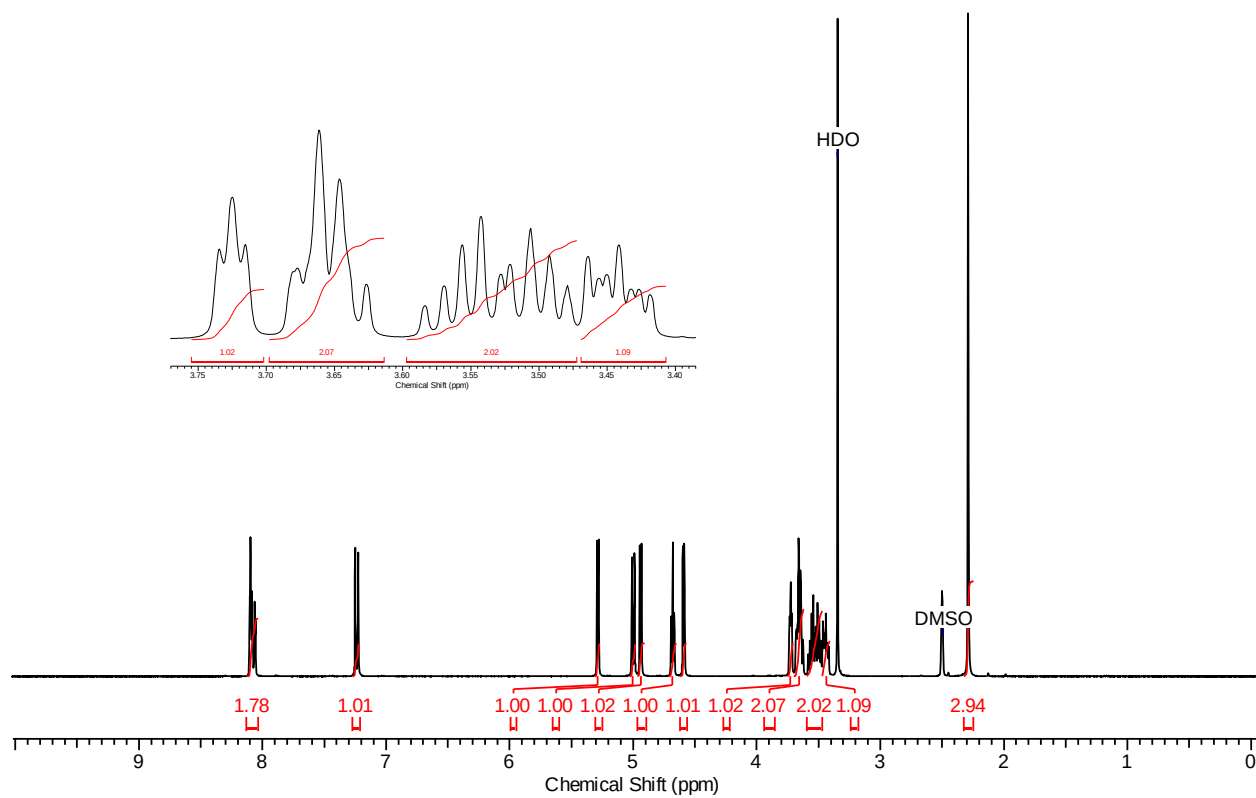


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d₆)

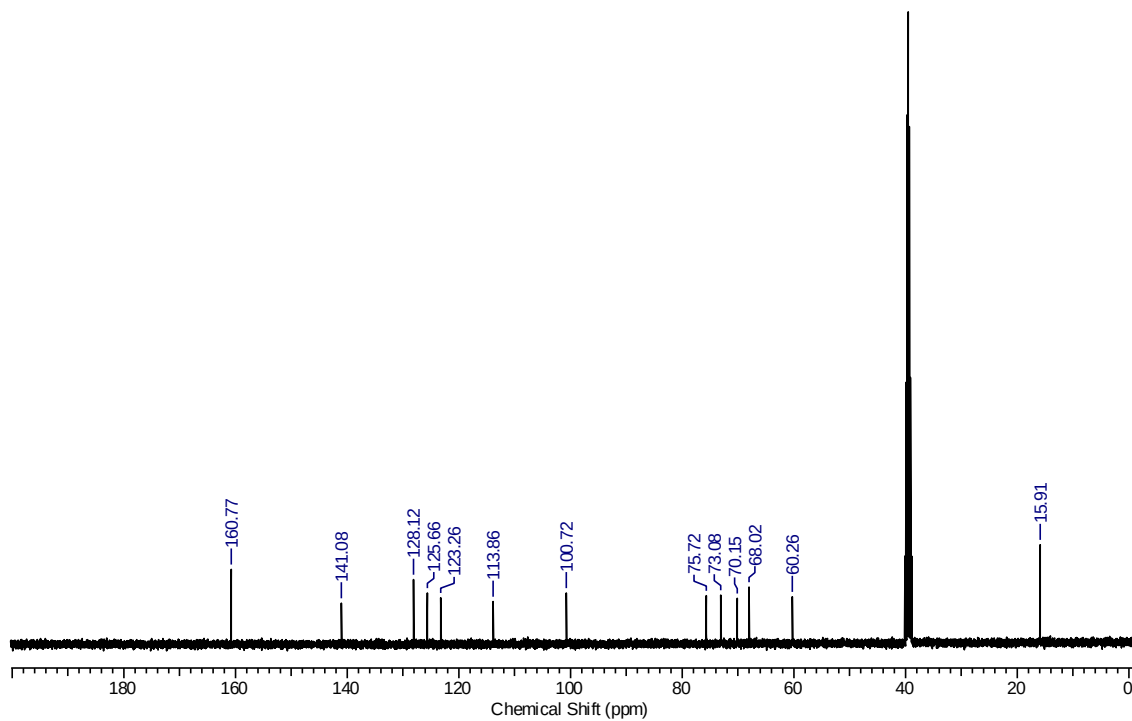


2-Methyl-4-nitrophenyl- β -D-galactopyranoside (2q).

- ^1H NMR spectrum (400.18 MHz, DMSO)

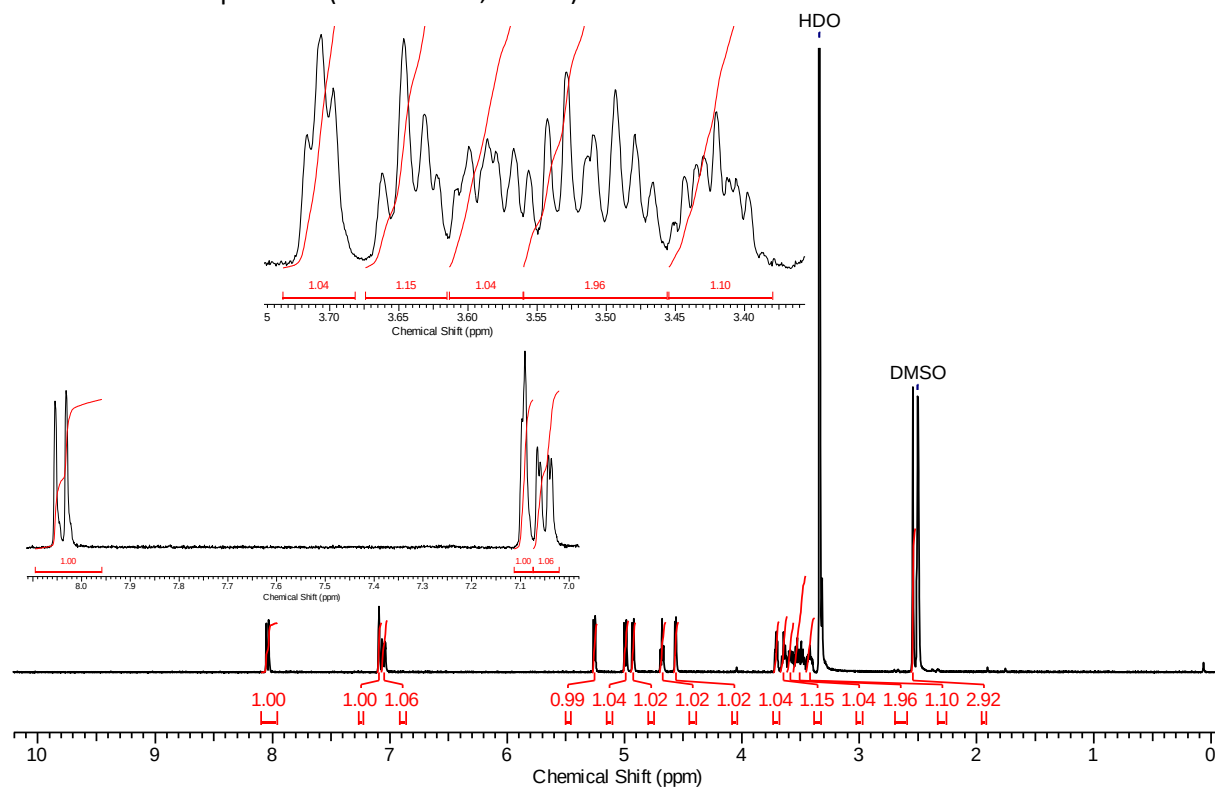


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

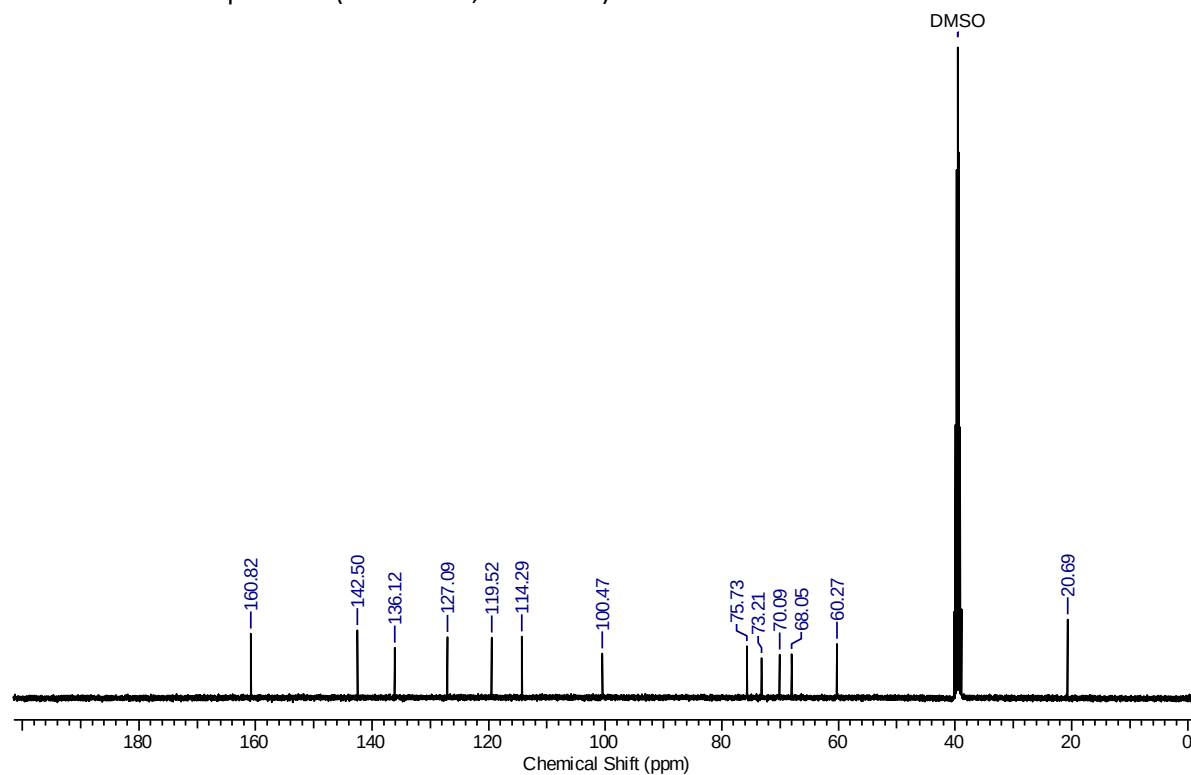


3-Methyl-4-nitrophenyl- β -D-galactopyranoside (2r).

- ^1H NMR spectrum (400.18 MHz, DMSO)

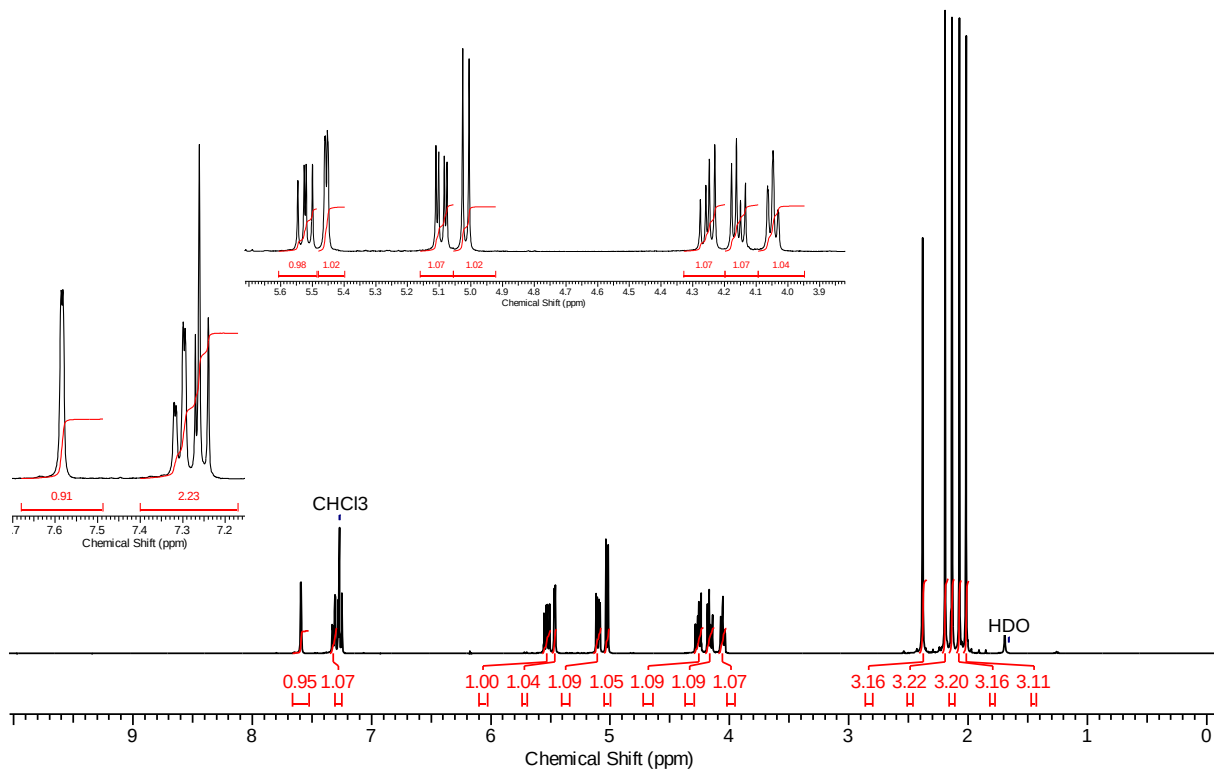


- ^{13}C NMR spectrum (100.6 MHz, DMSO- d_6)

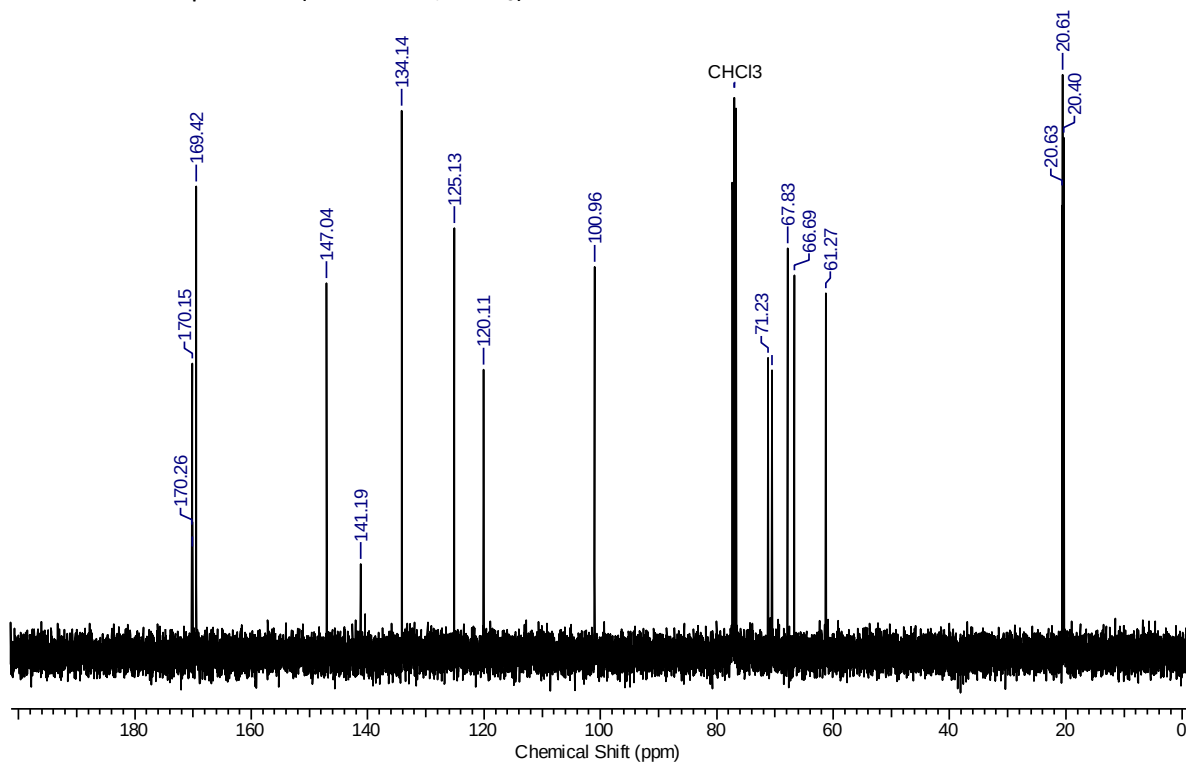


4-Methyl-2-nitrophenyl-tetra-*O*-acetyl β -D-galactopyranoside (4b).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

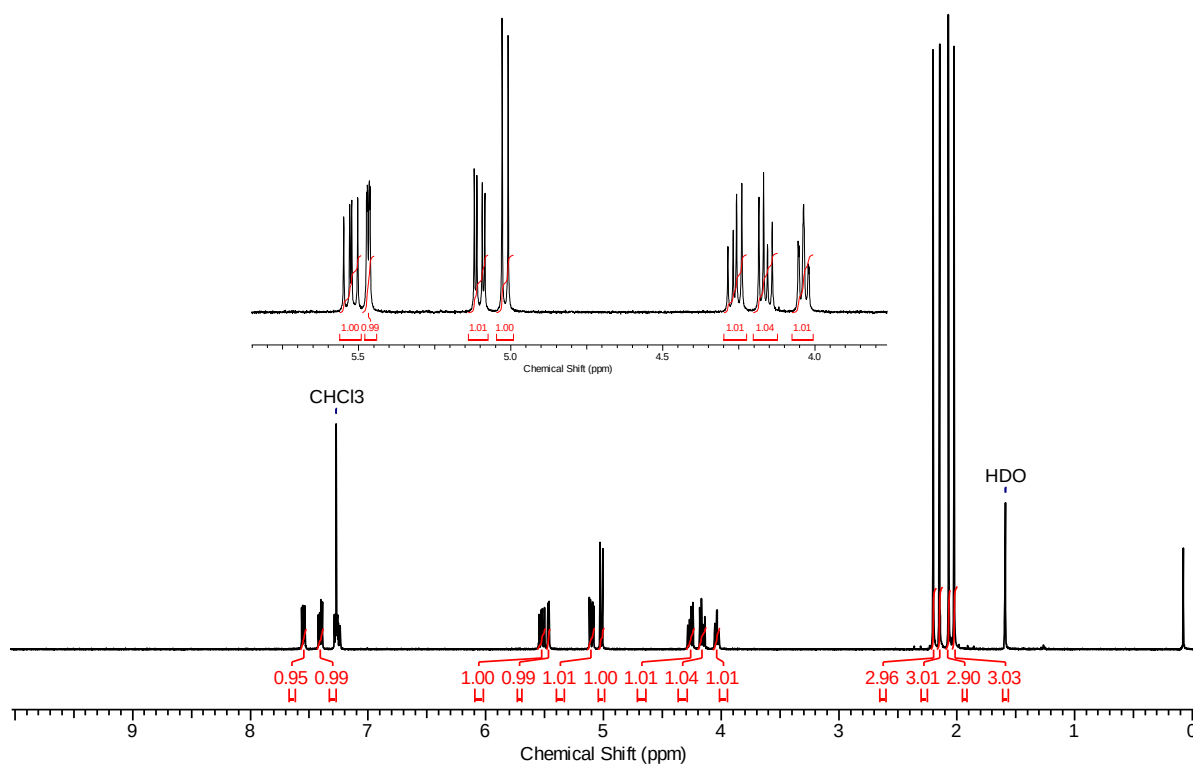


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

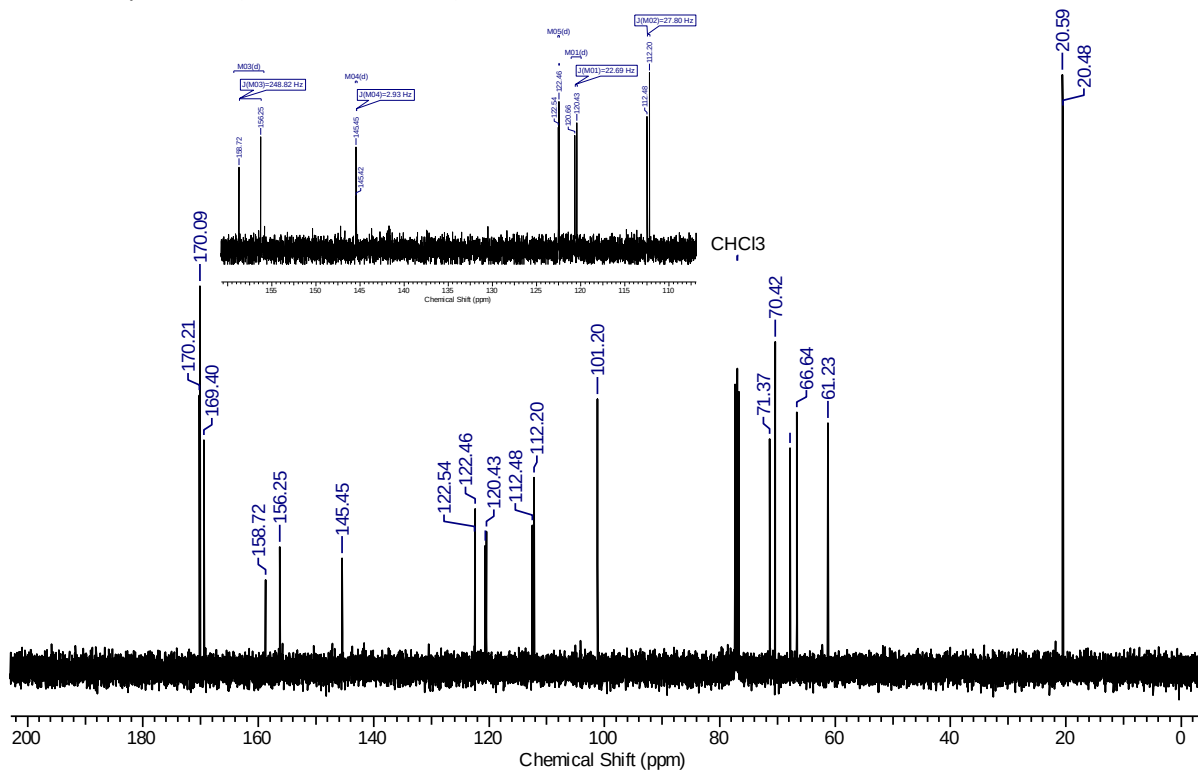


4-Fluoro-2-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4c).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

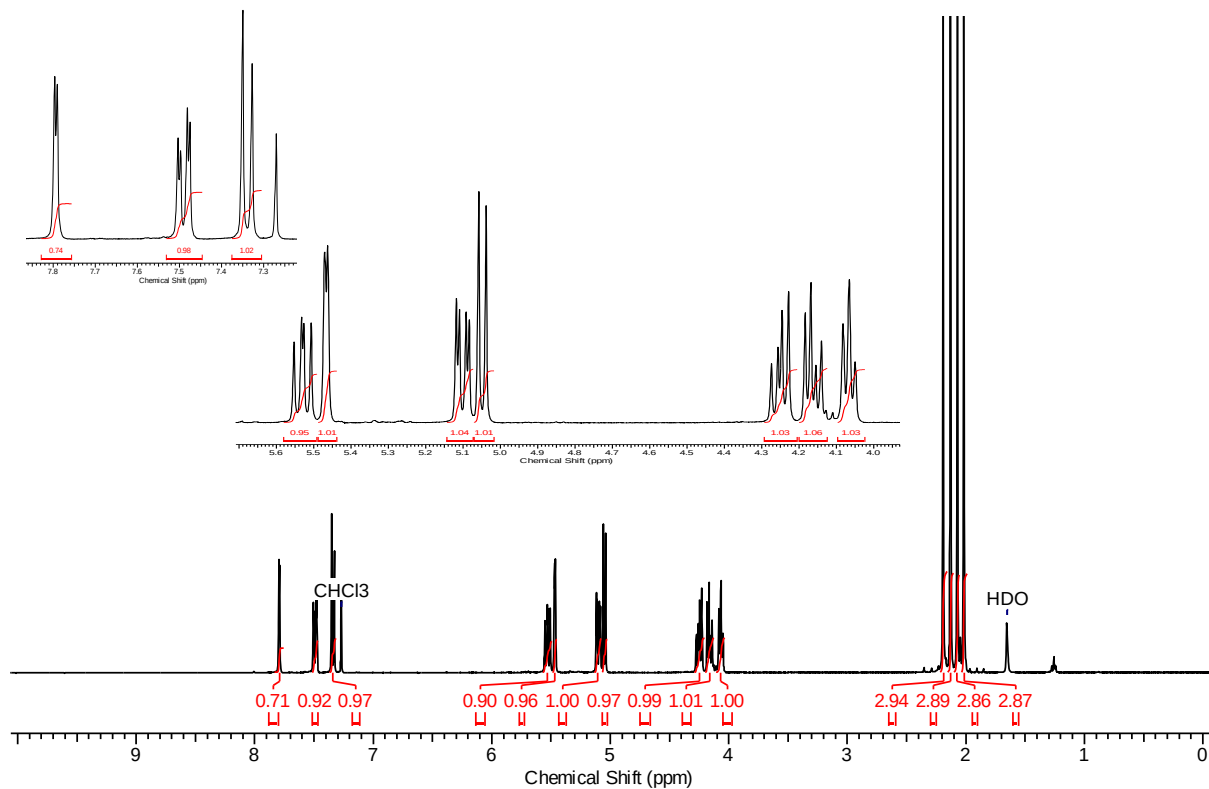


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

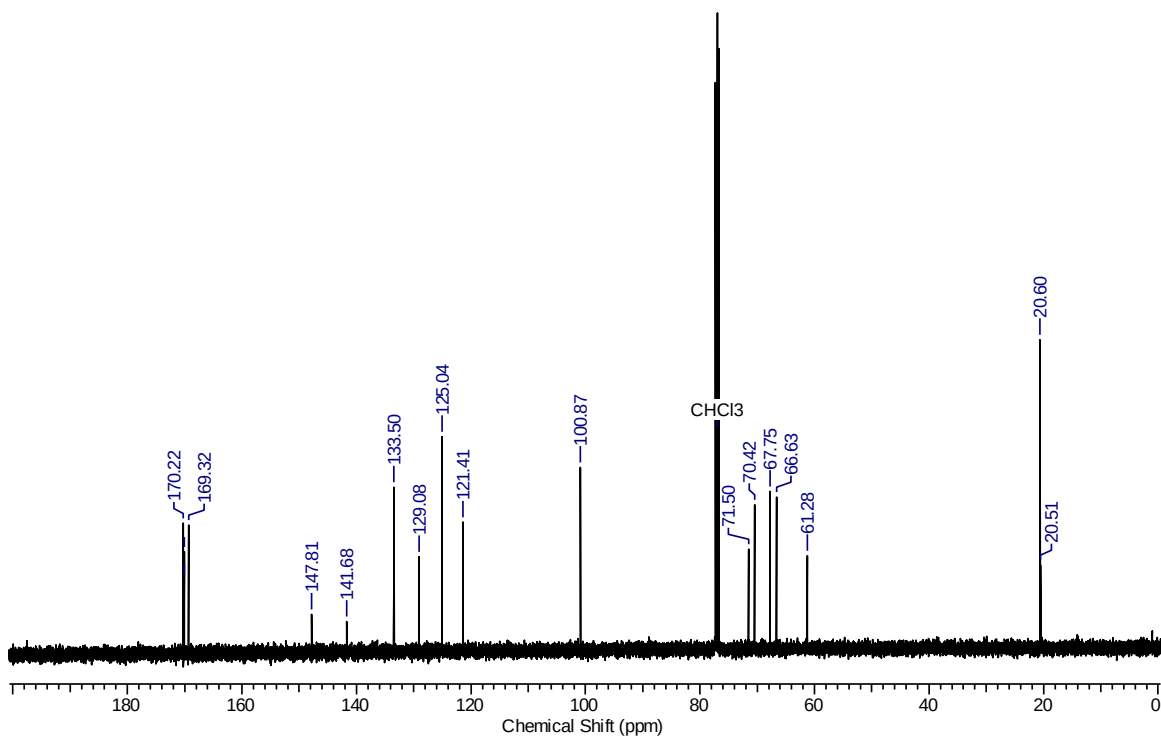


4-Chloro-2-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4d).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

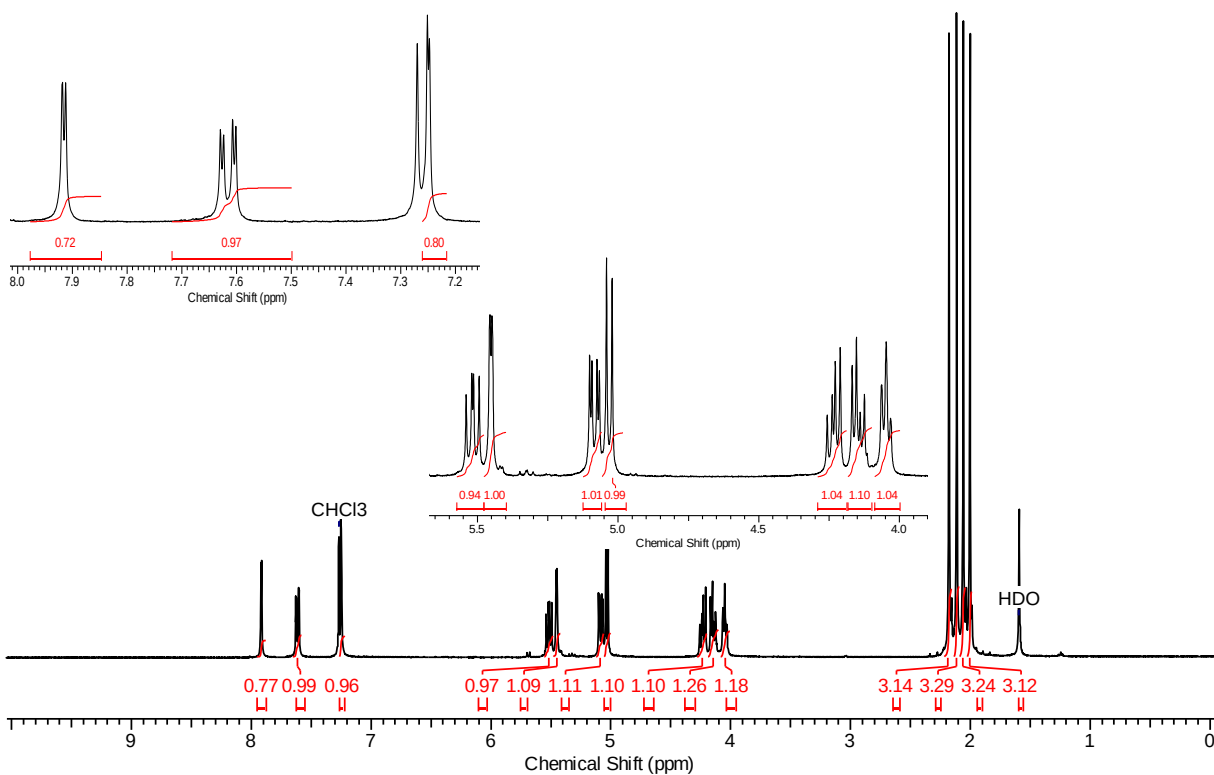


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

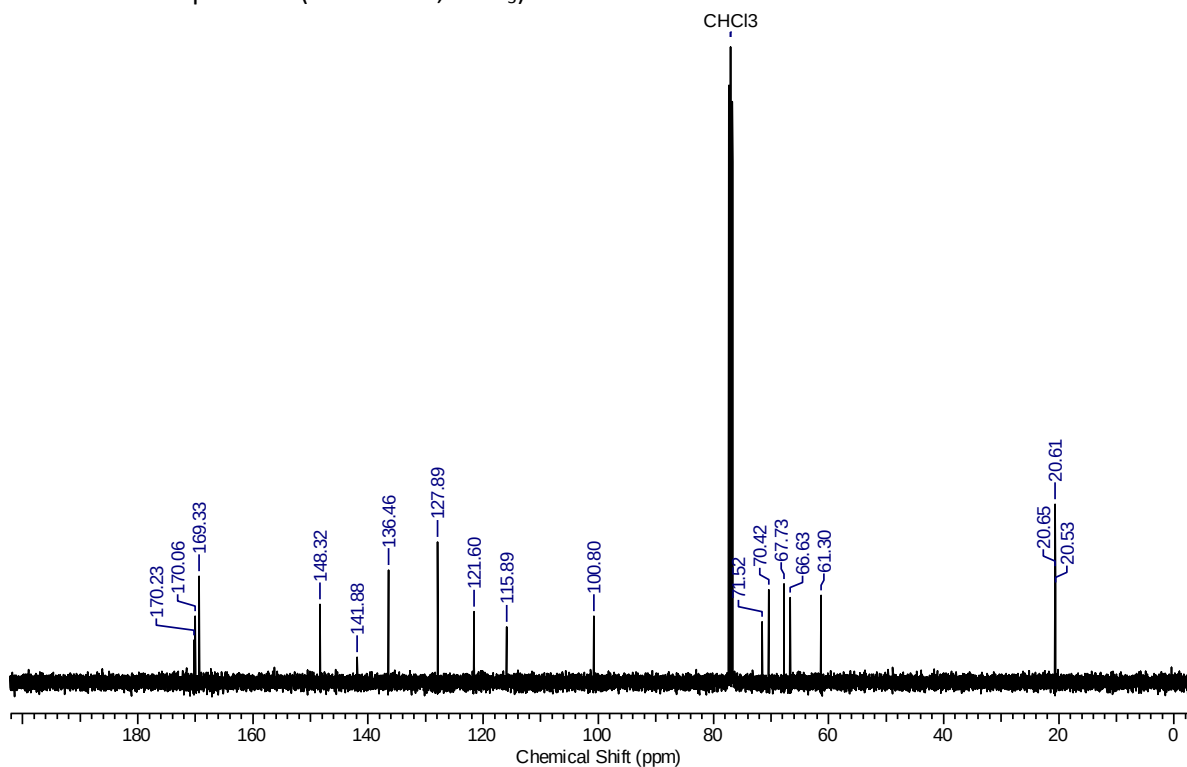


4-Bromo-2-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4e).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

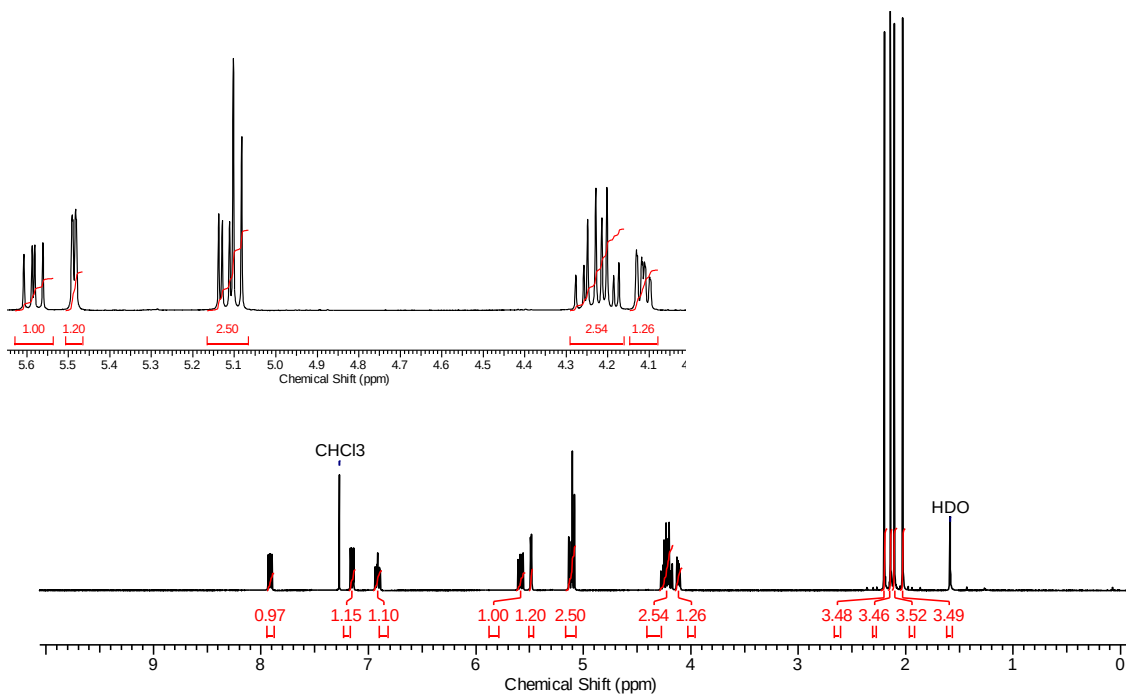


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

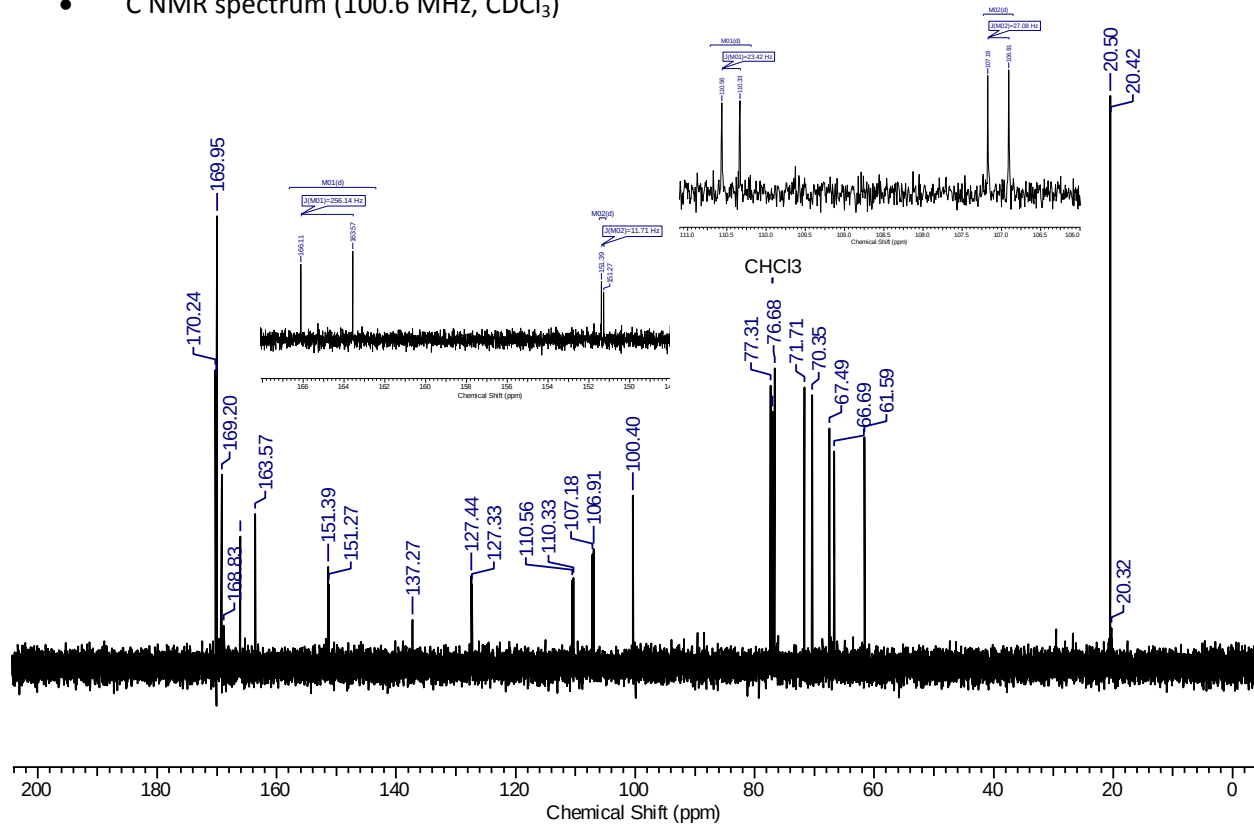


5-Fluoro-2-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4f).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

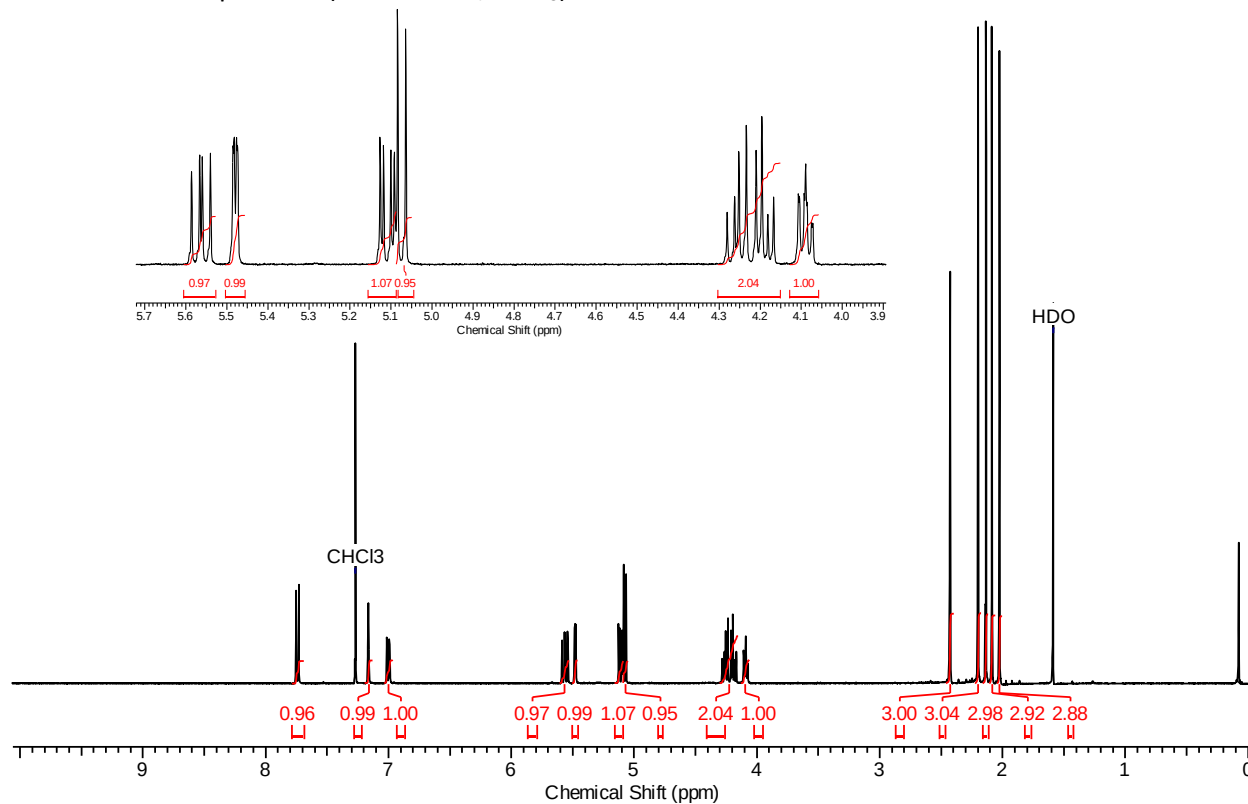


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

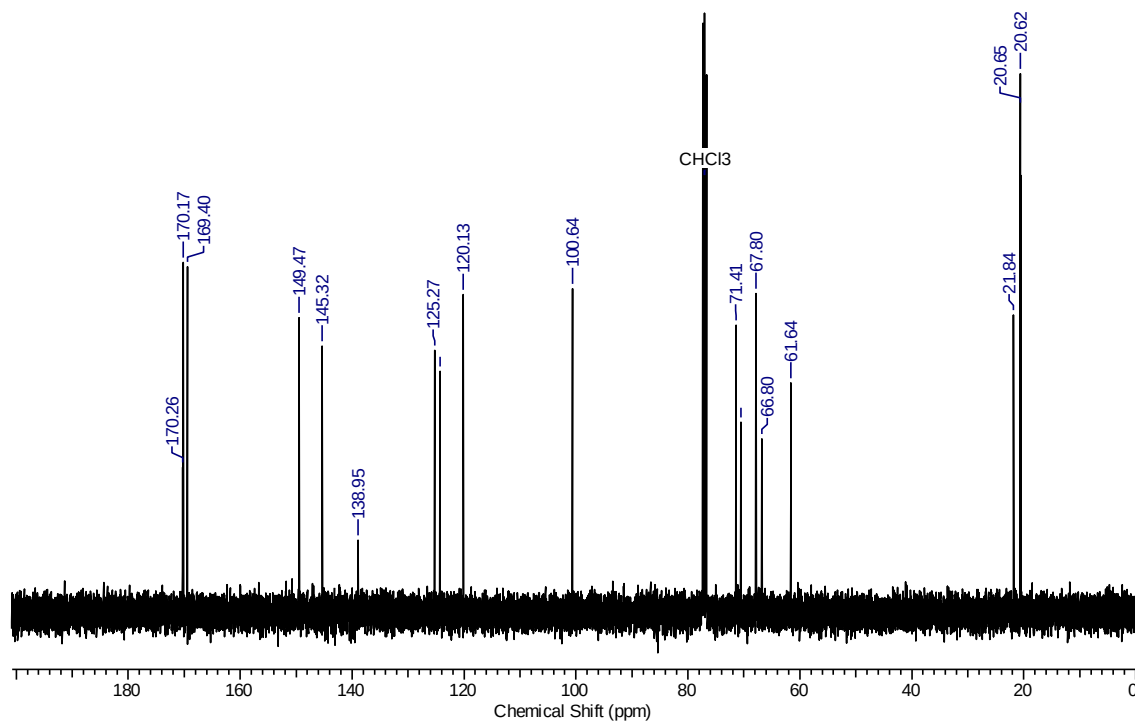


5-Methyl-2-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4g).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

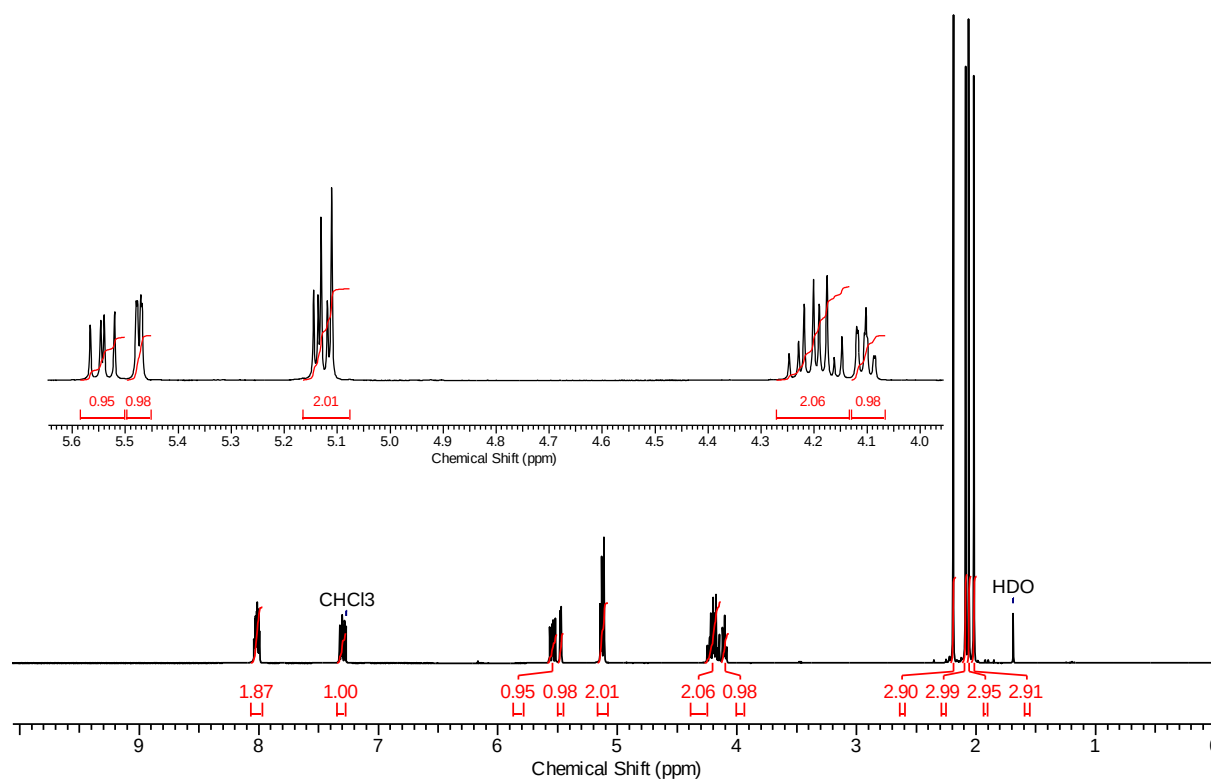


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

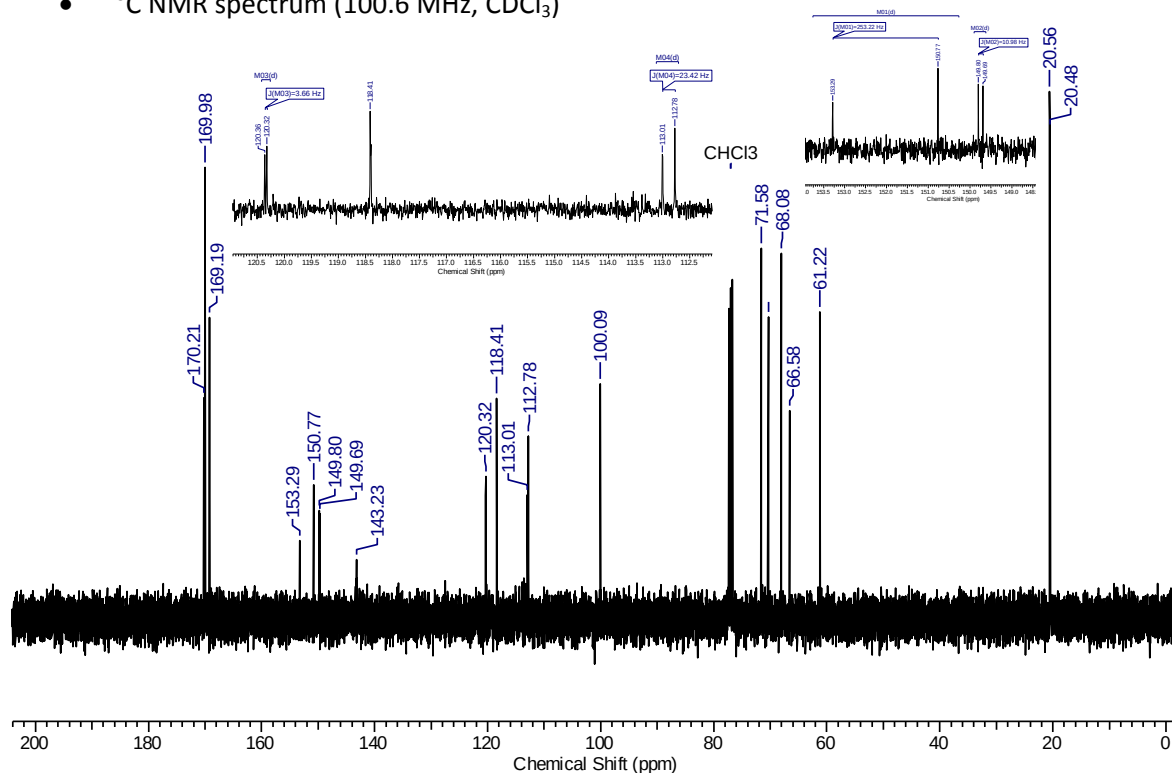


2-Fluoro-4-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4i).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

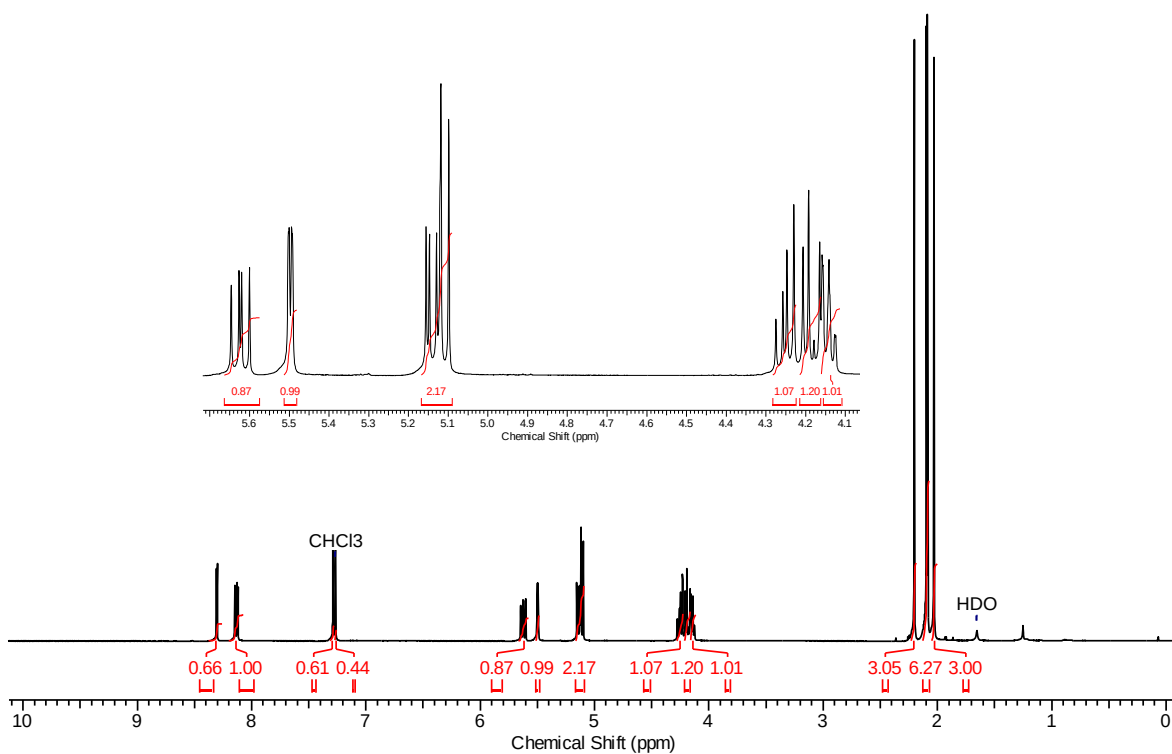


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

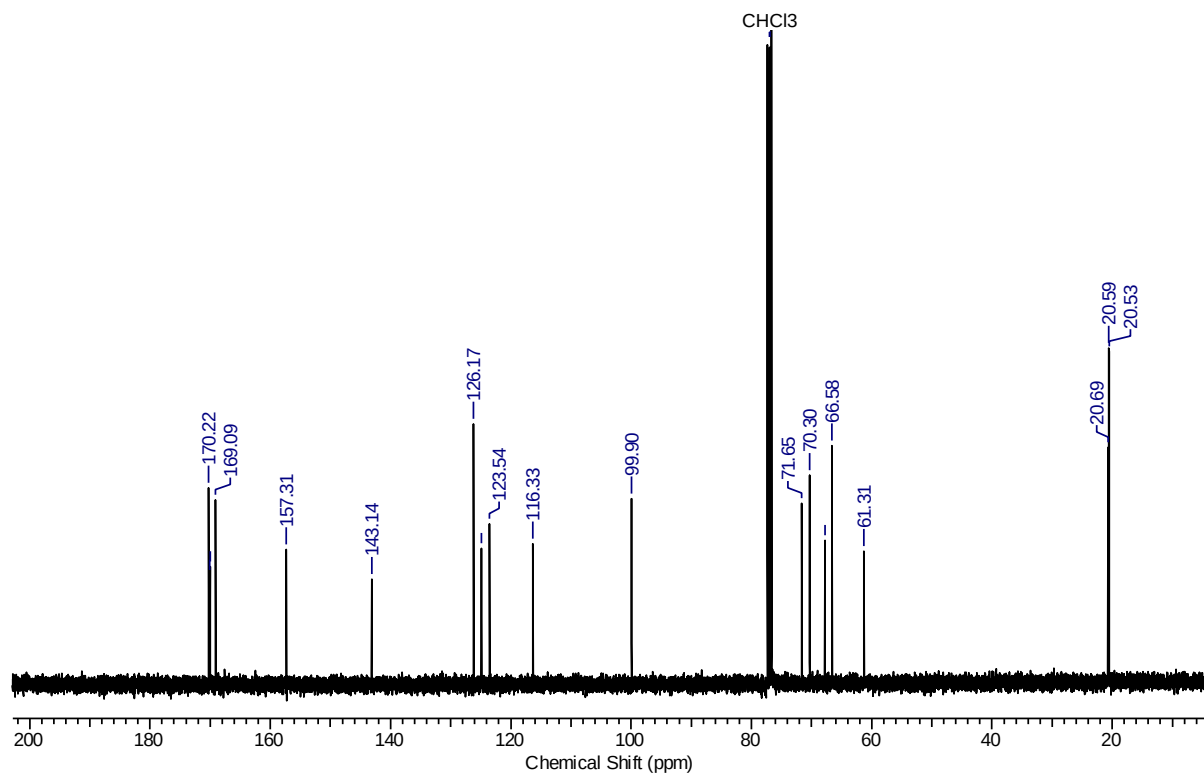


2-Chloro-4-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4k).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

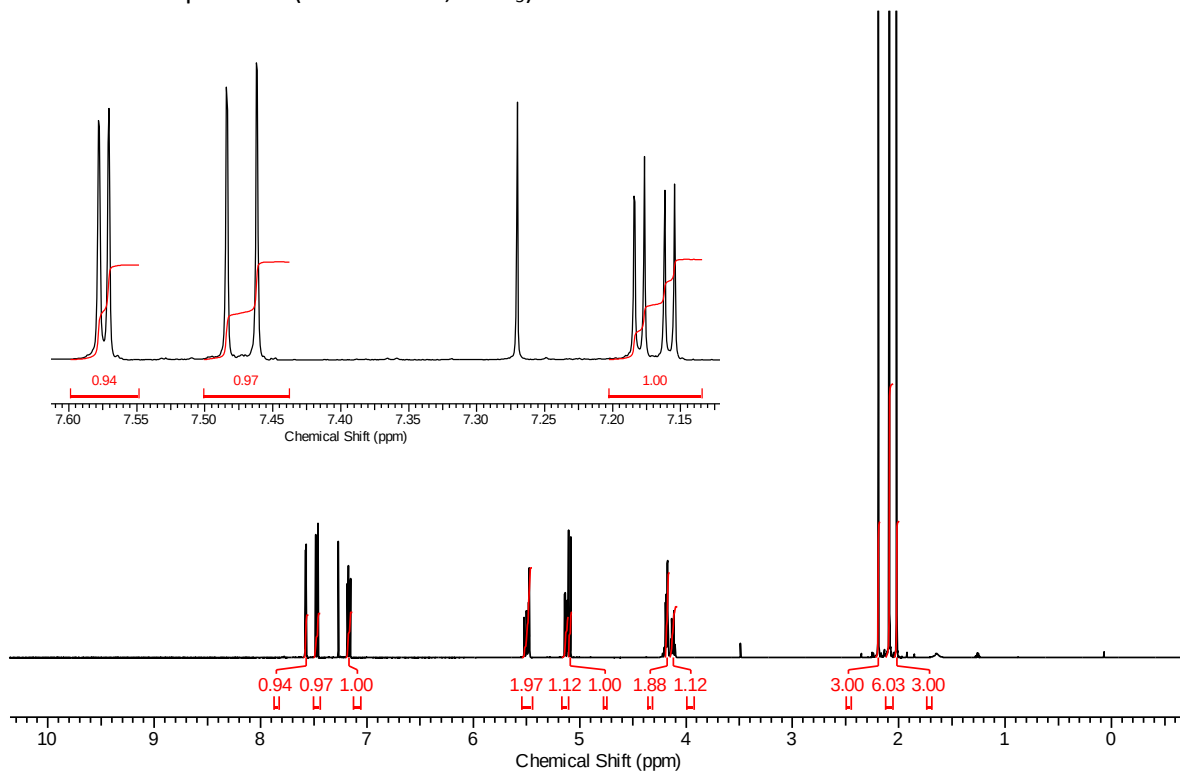


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

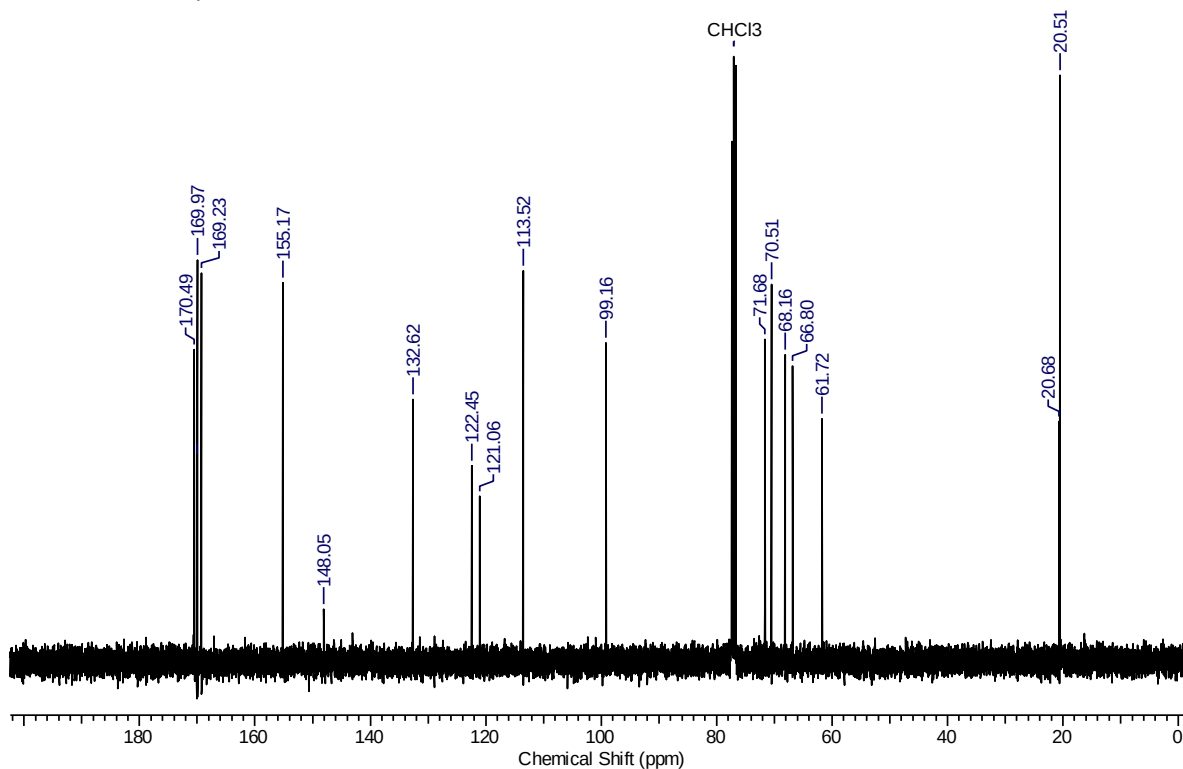


4-Chloro-3-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4m).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

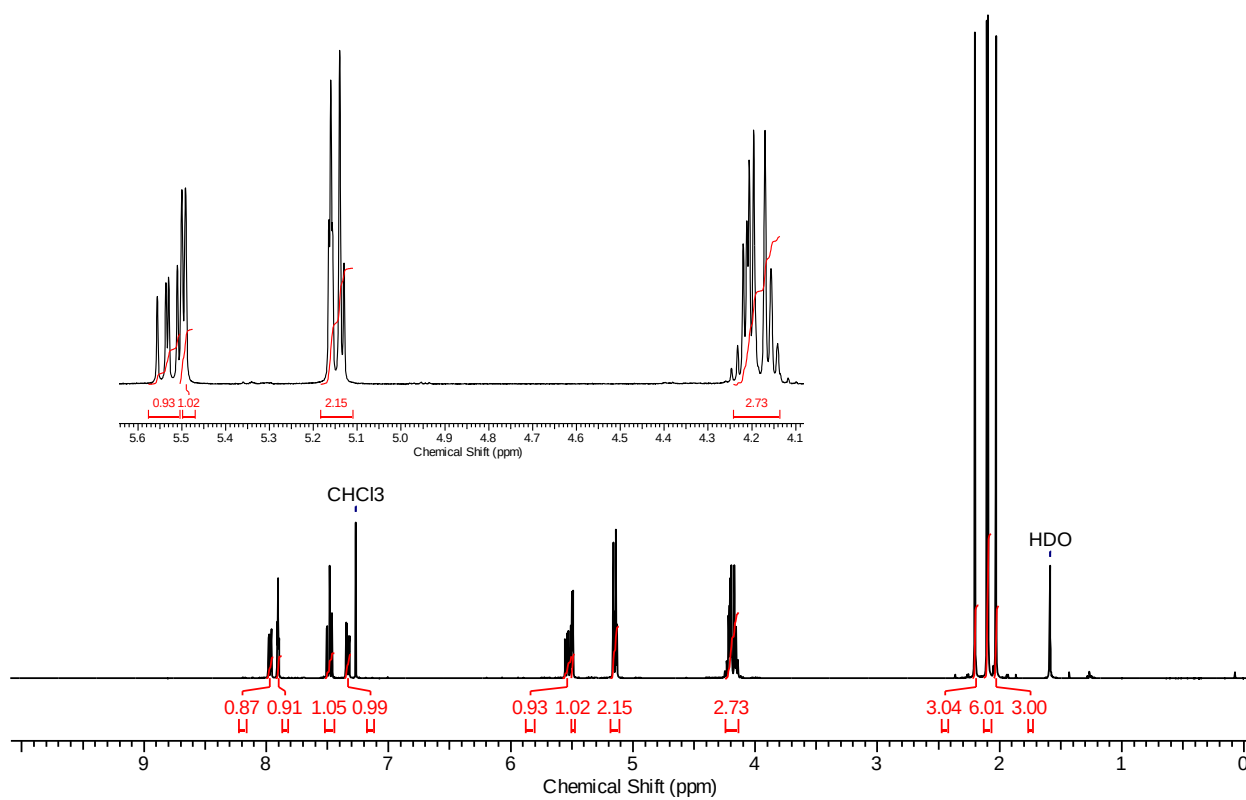


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

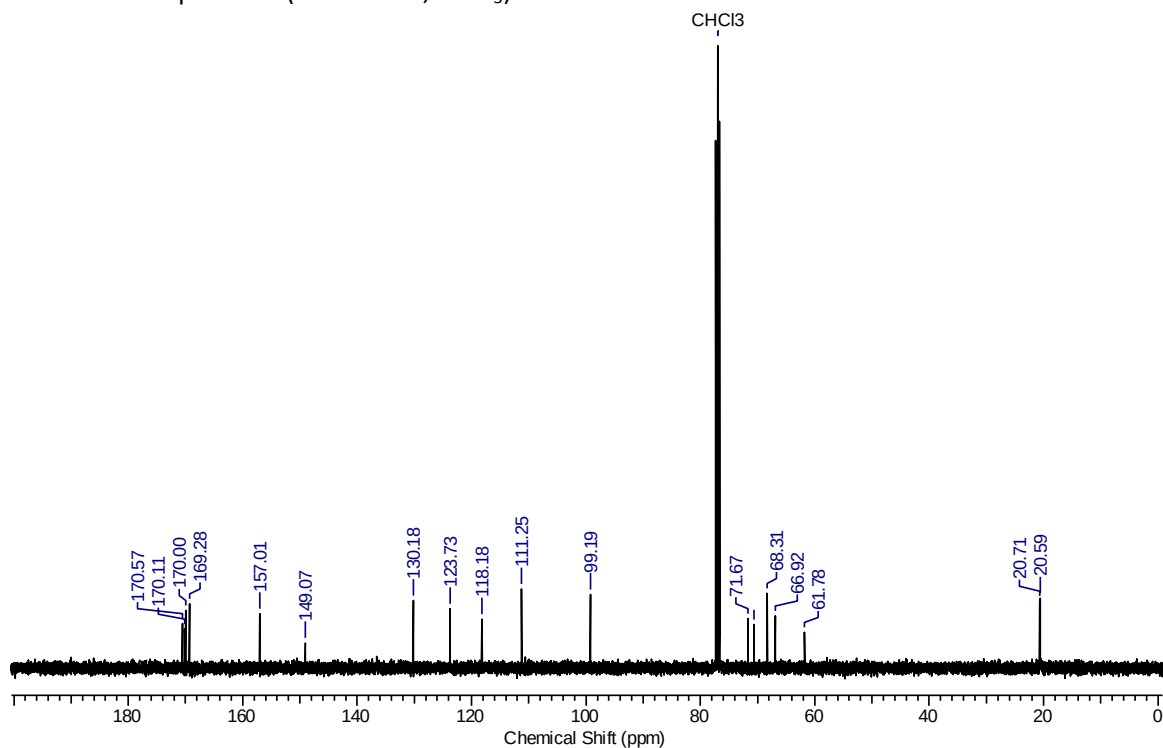


3-Nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4n).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

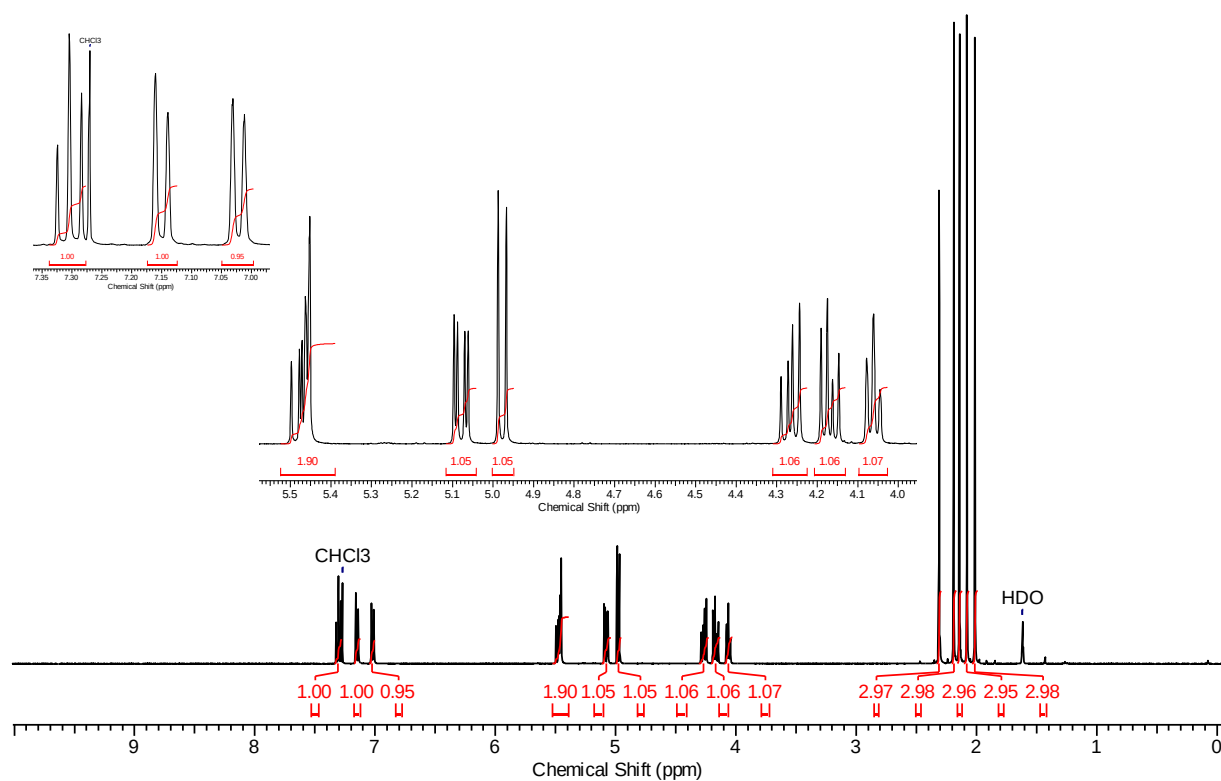


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

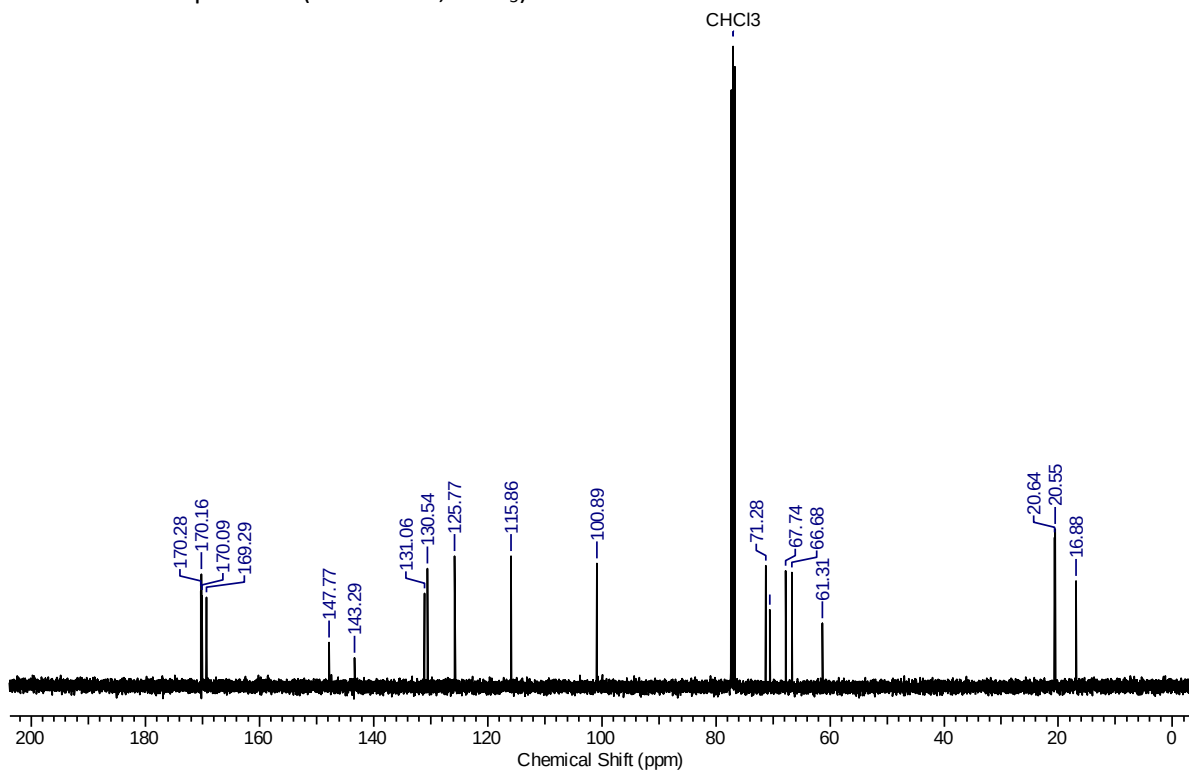


3-Methyl-2-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4o).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

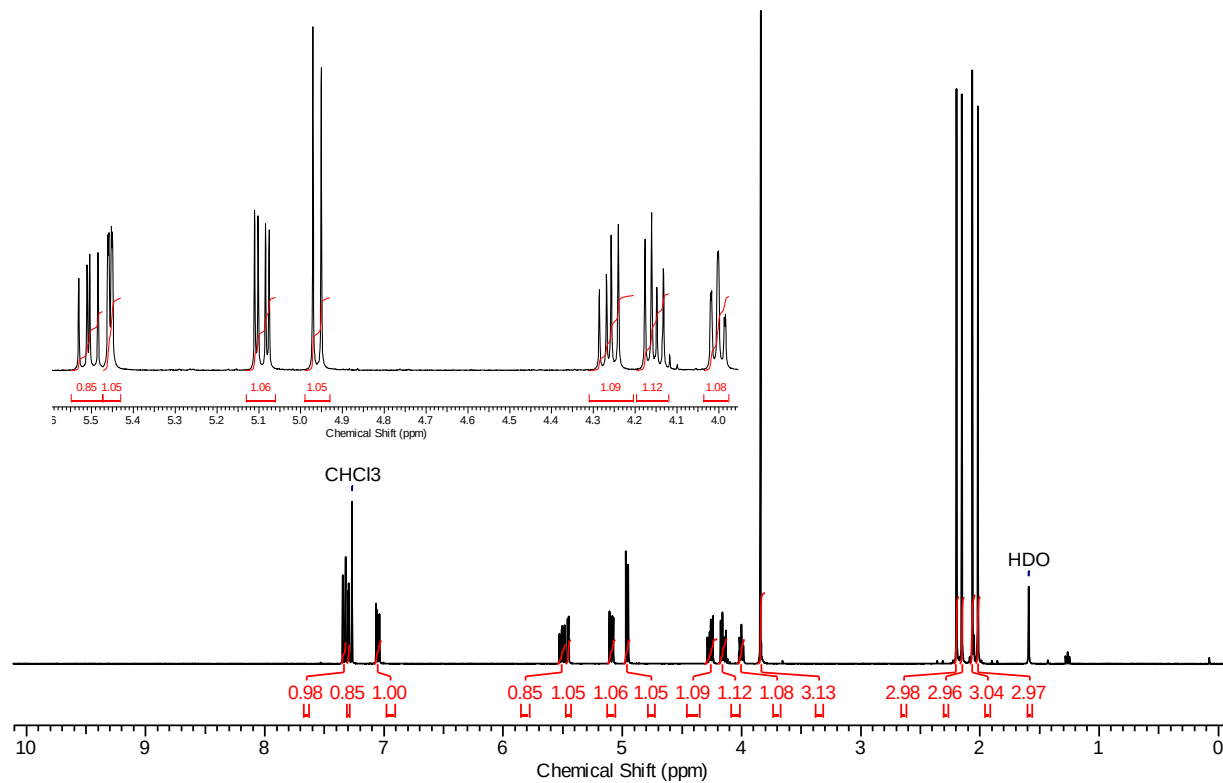


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

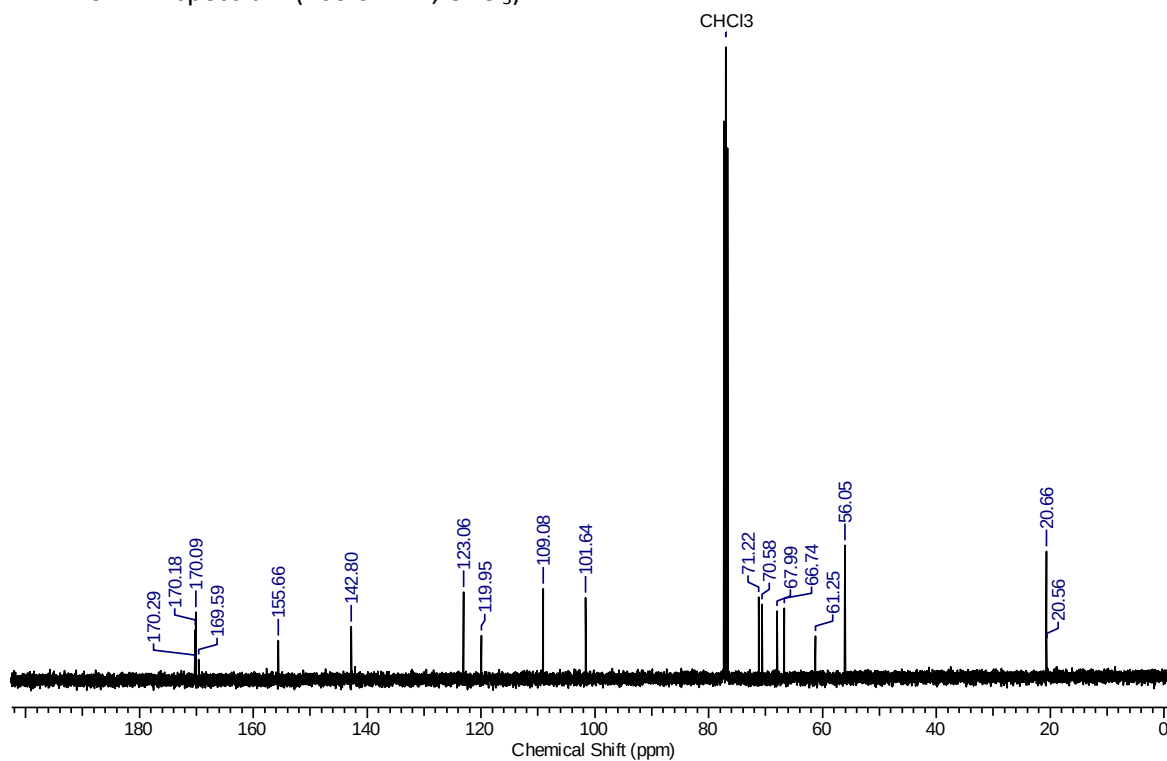


4-Methoxy-2-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4p).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

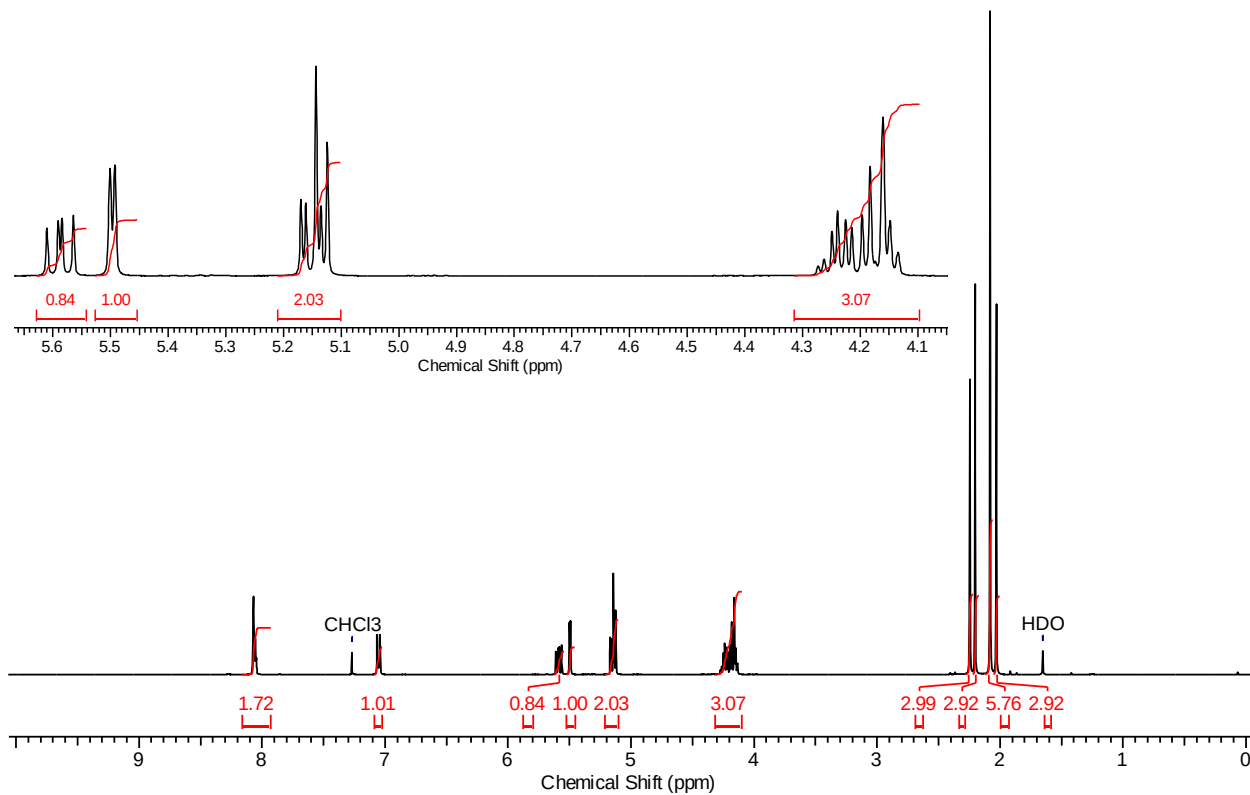


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

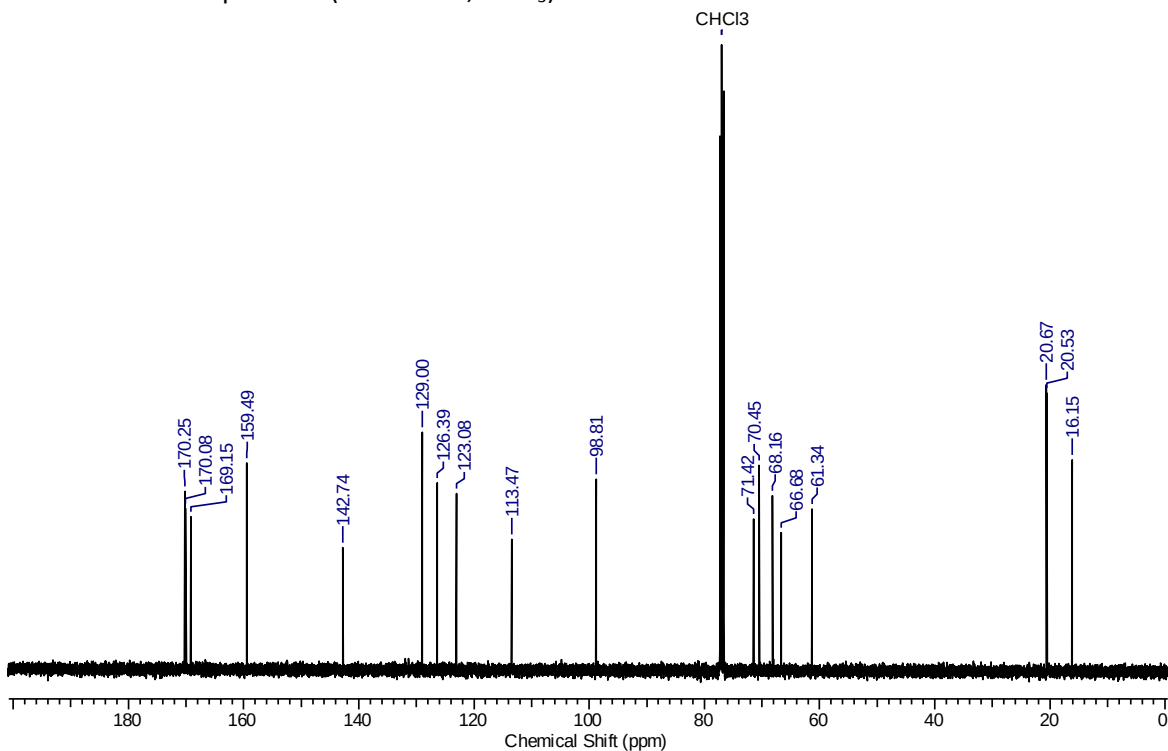


2-Methyl-4-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4q).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)

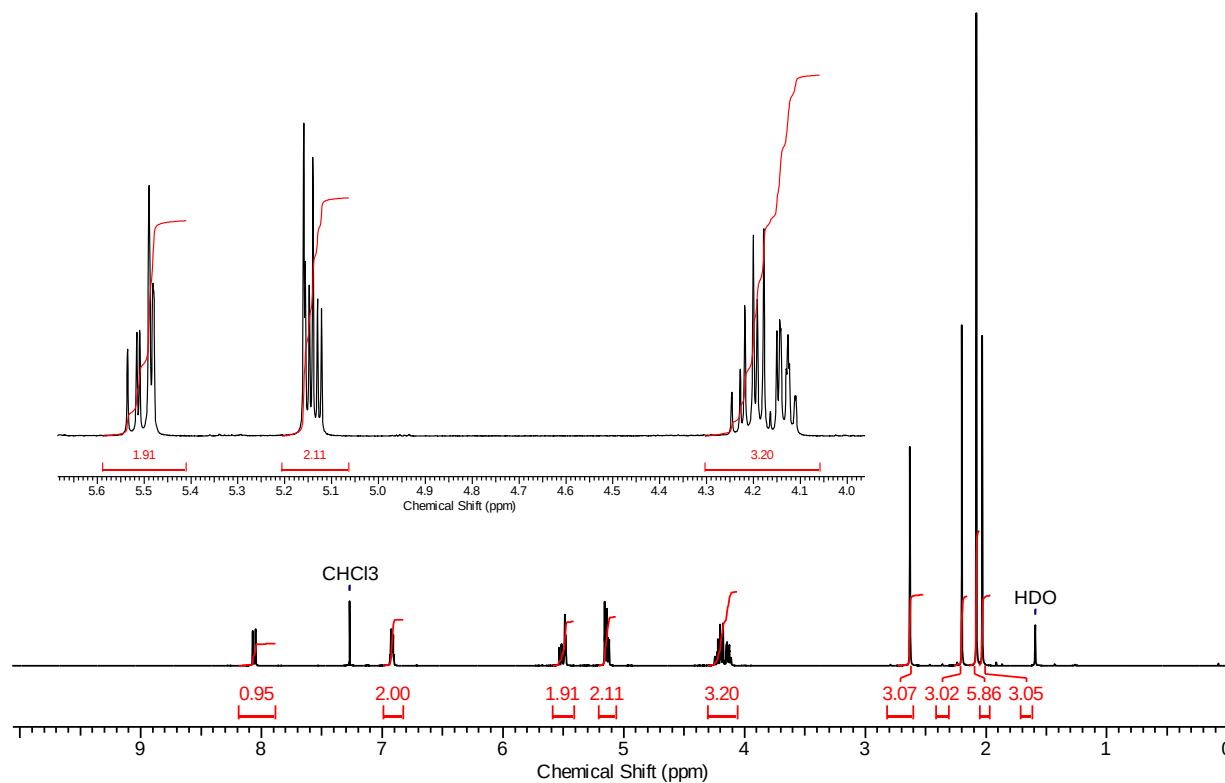


- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)



3-Methyl-4-nitrophenyl-tetra-*O*-acetyl- β -D-galactopyranoside (4r).

- ^1H NMR spectrum (400.18 MHz, CDCl_3)



- ^{13}C NMR spectrum (100.6 MHz, CDCl_3)

