Electronic Supplementary Information (ESI).

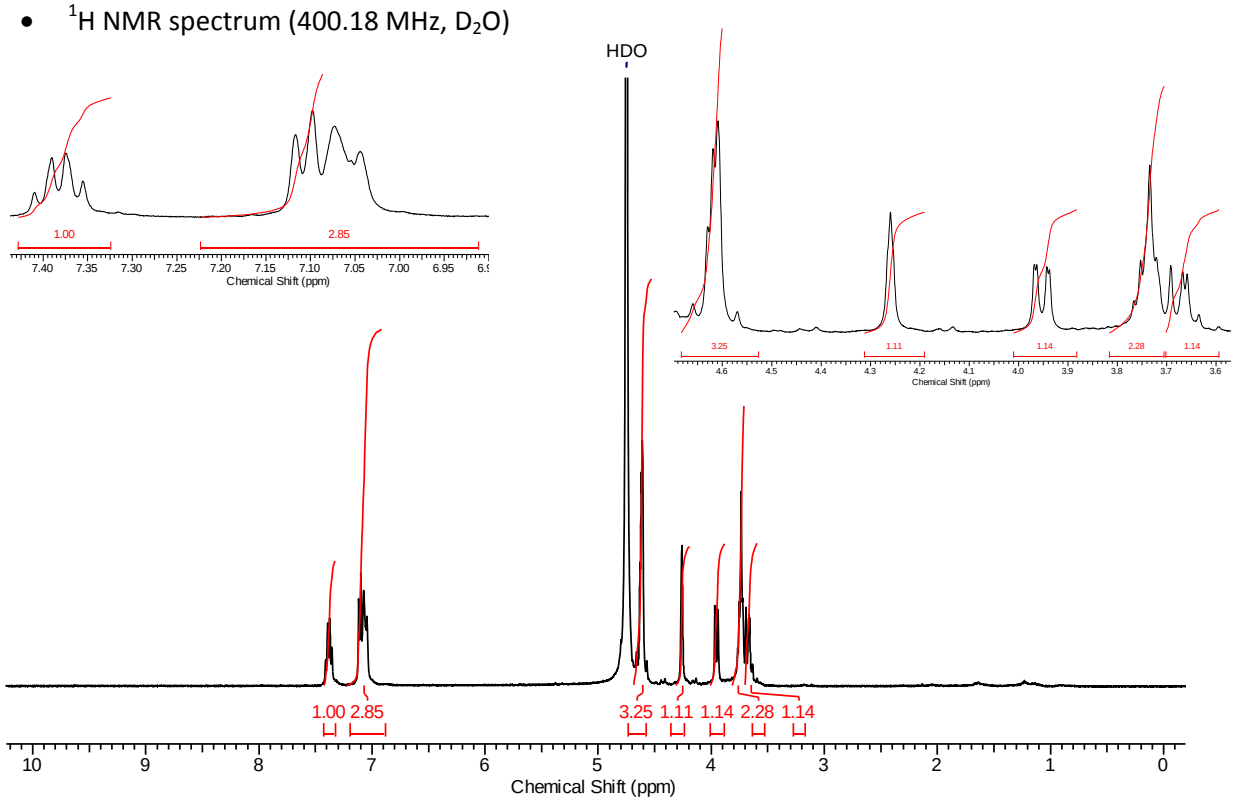
Evaluating *N*-benzylgalactonoamidines as putative transition state analogs for β-galactoside hydrolysis

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

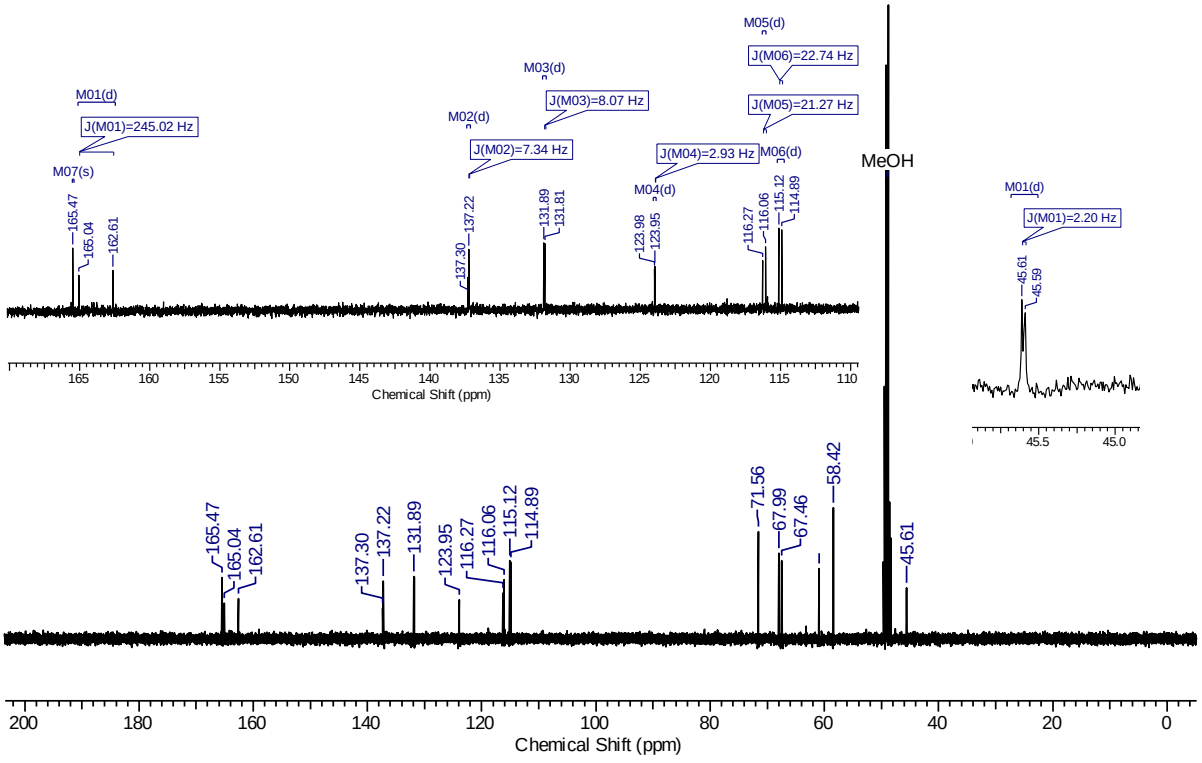
^{1}H and ^{13}C NMR spectra

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

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

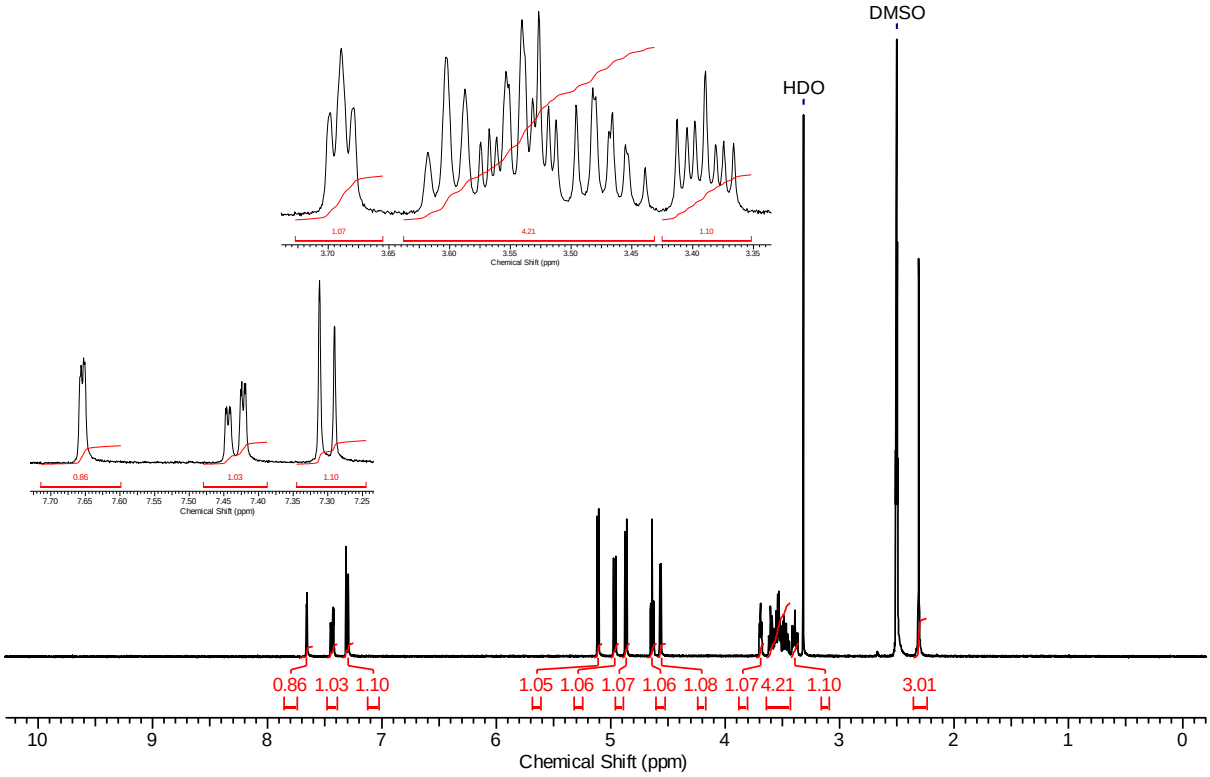


- ^{13}C NMR spectrum (100.6 MHz, D_2O/MeOH-d4)

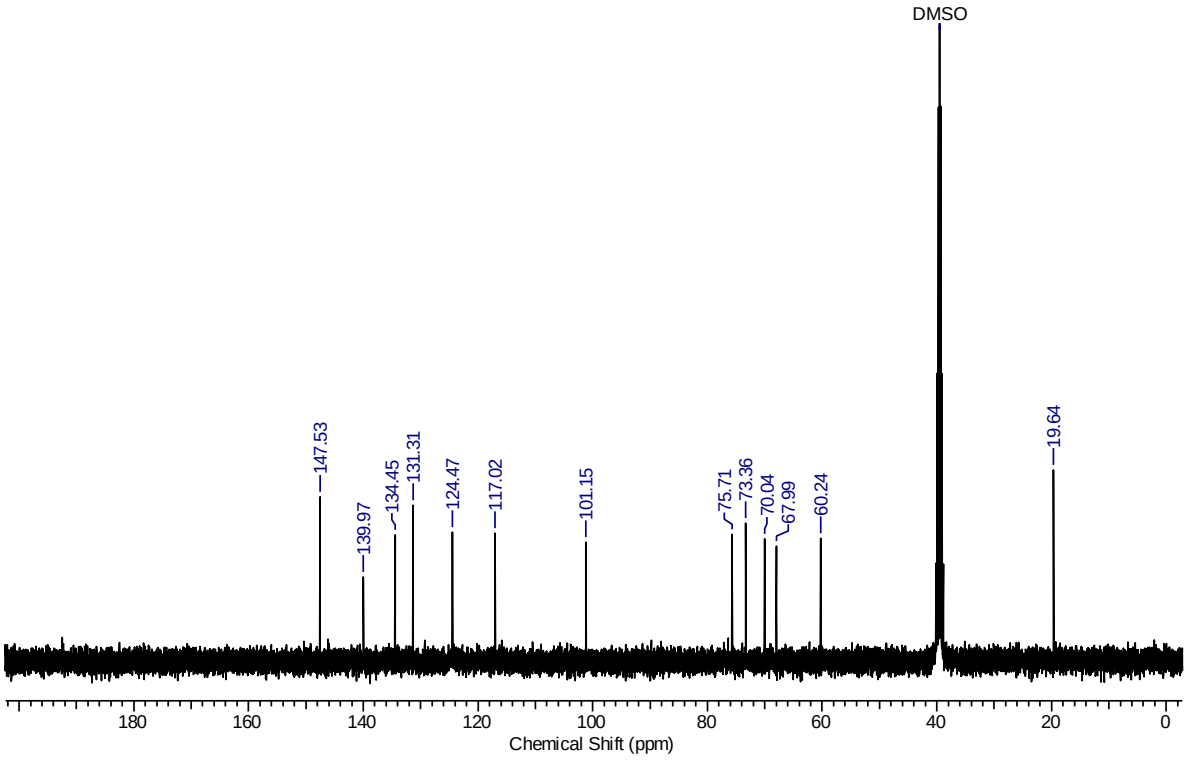


4-Methyl-2-nitrophenyl-β-D-galactopyranoside (2b).

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

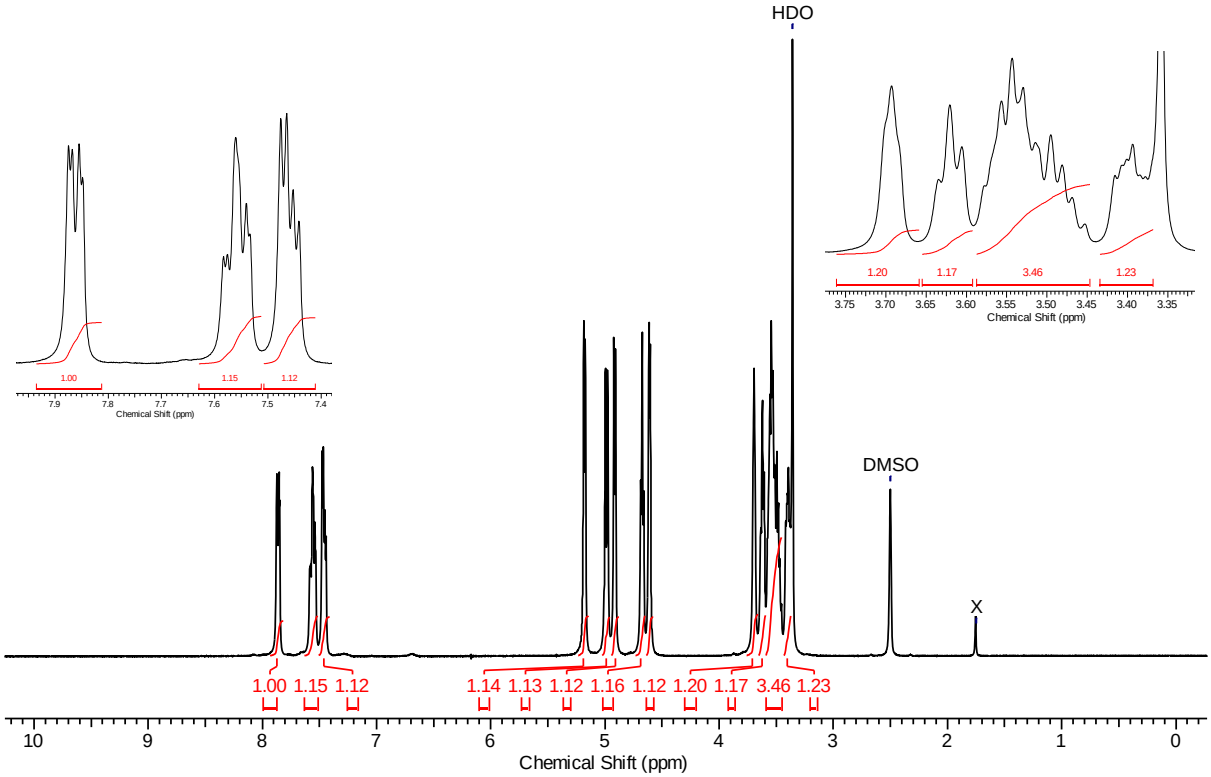


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

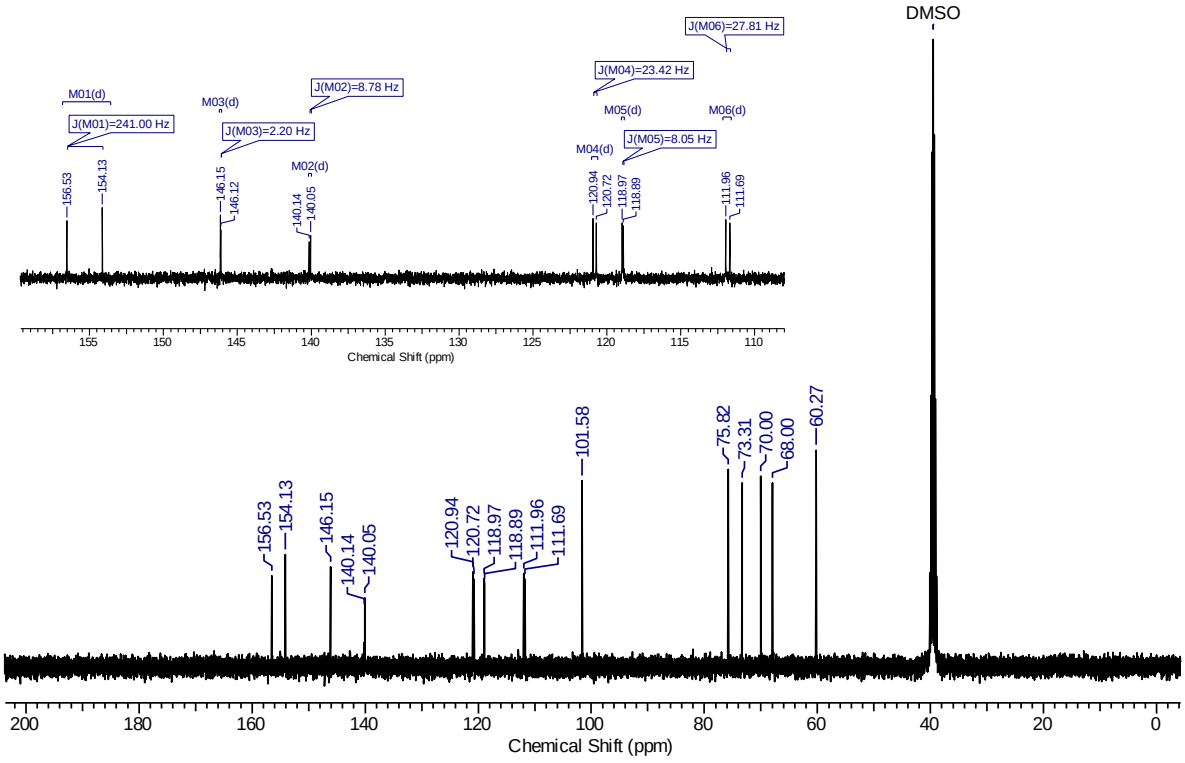


4-Fluoro-2-nitrophenyl-β-D-galactopyranoside (2c).

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

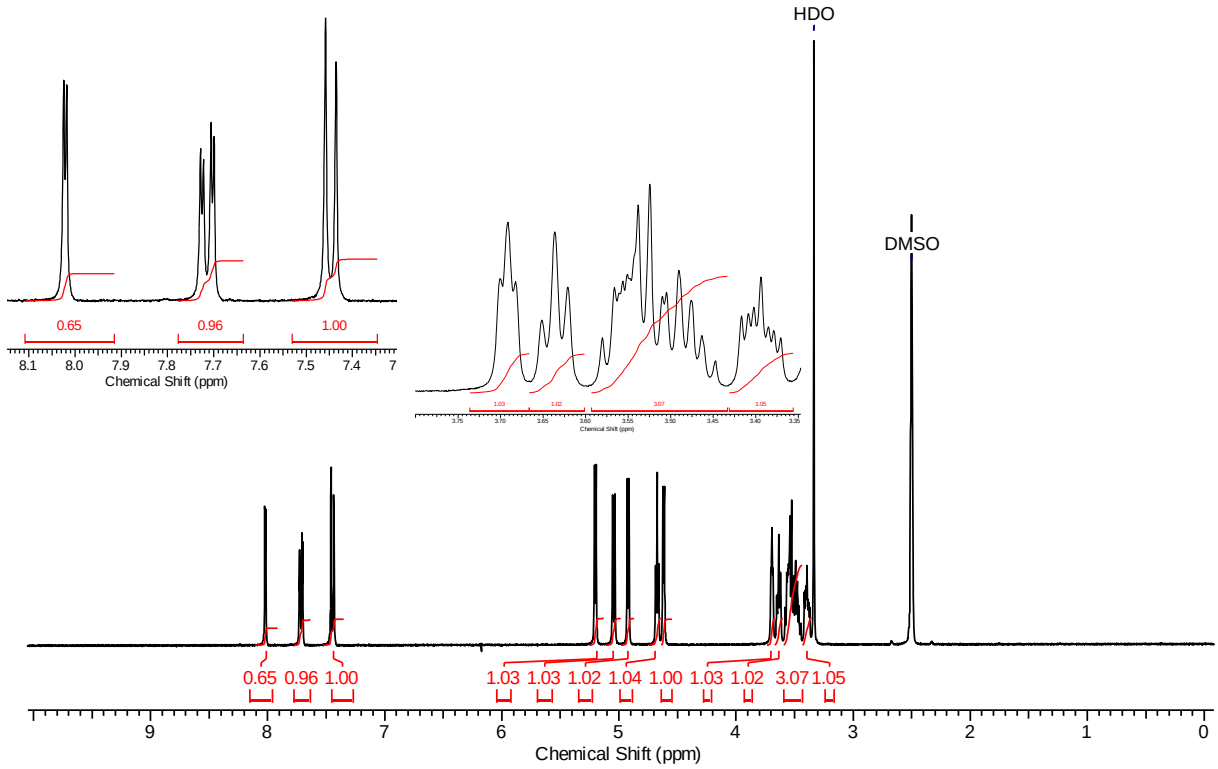


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

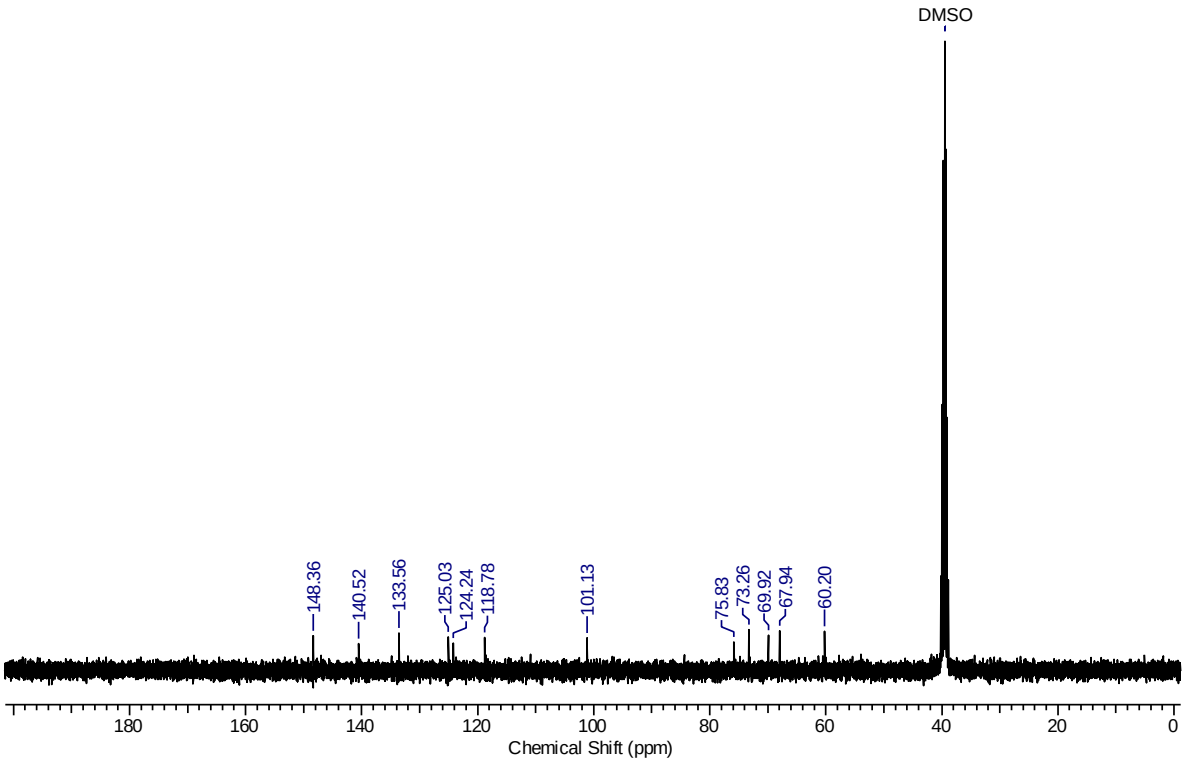


4-Chloro-2-nitrophenyl-β-D-galactopyranoside (2d).

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

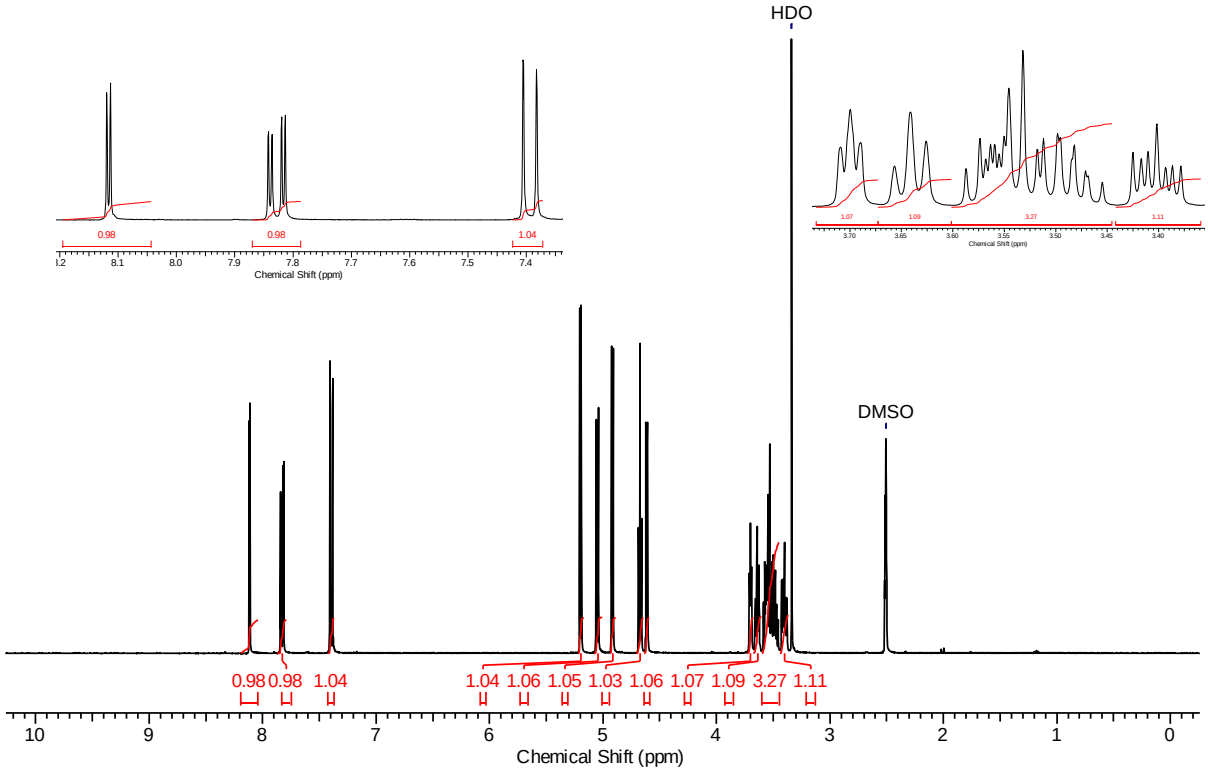


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

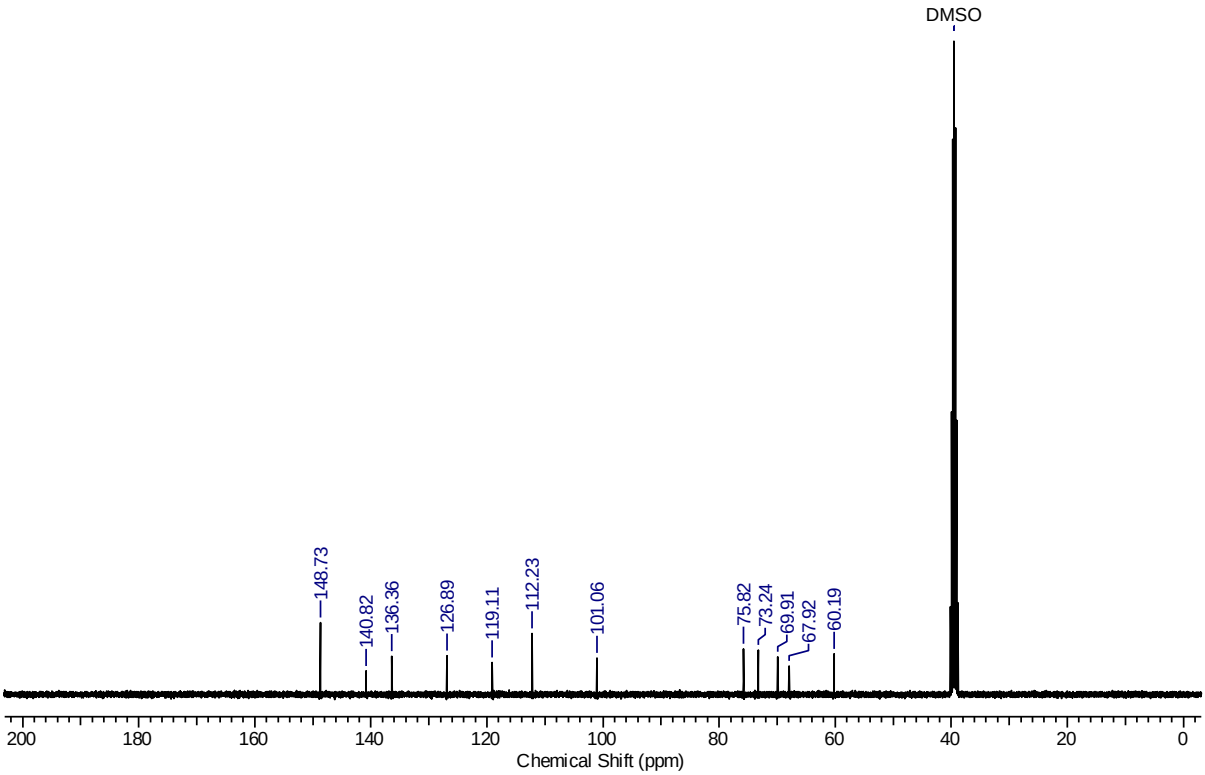


4-Bromo-2-nitrophenyl-β-D-galactopyranoside (2e).

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

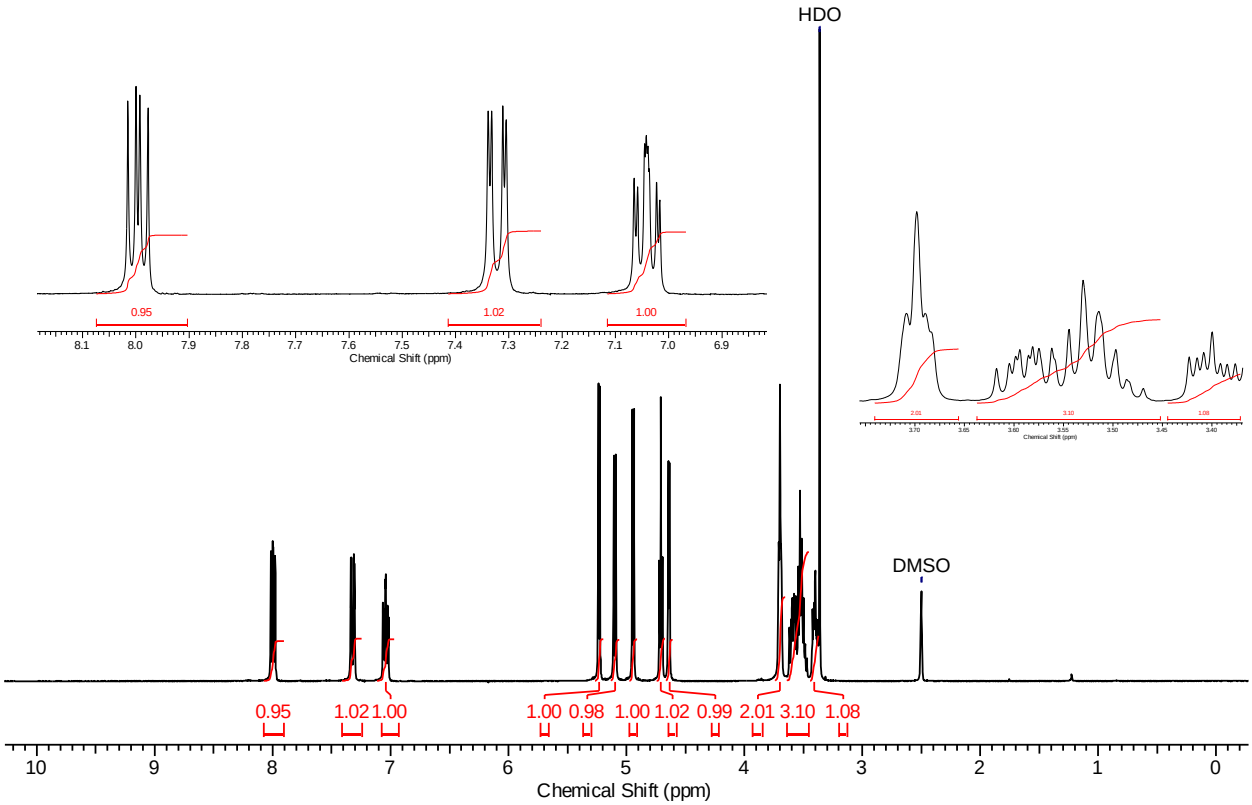


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

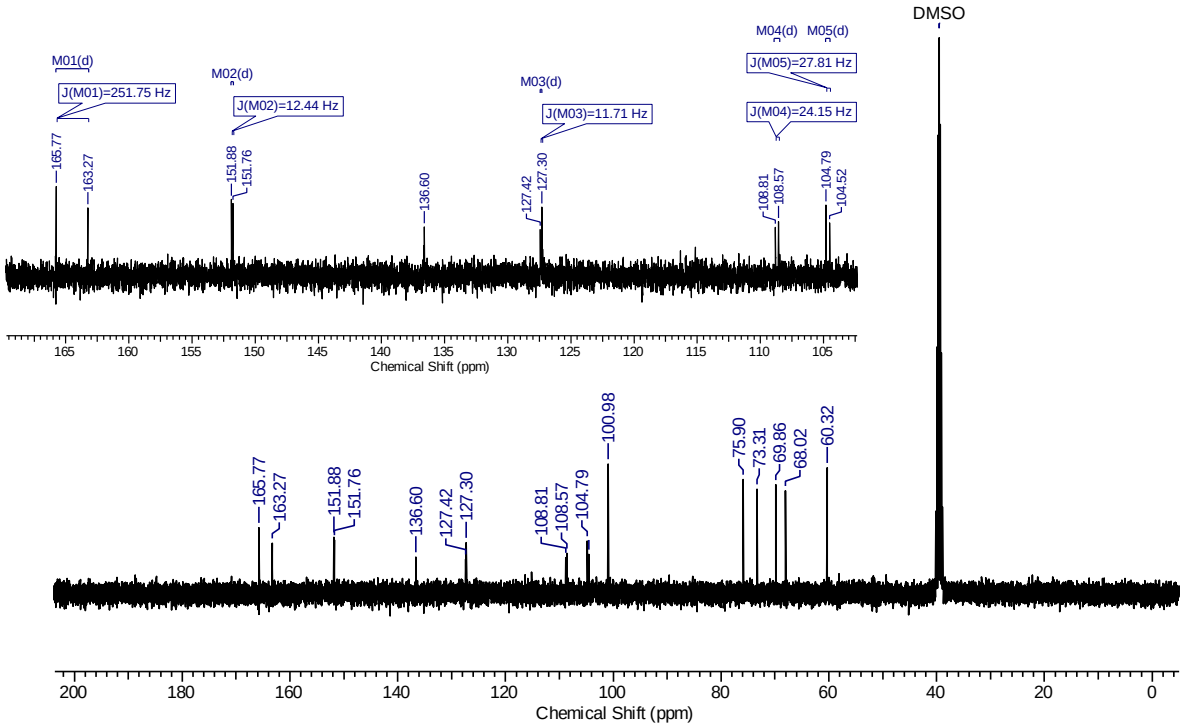


5-Fluoro-2-nitrophenyl-β-D-galactopyranoside (2f).

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

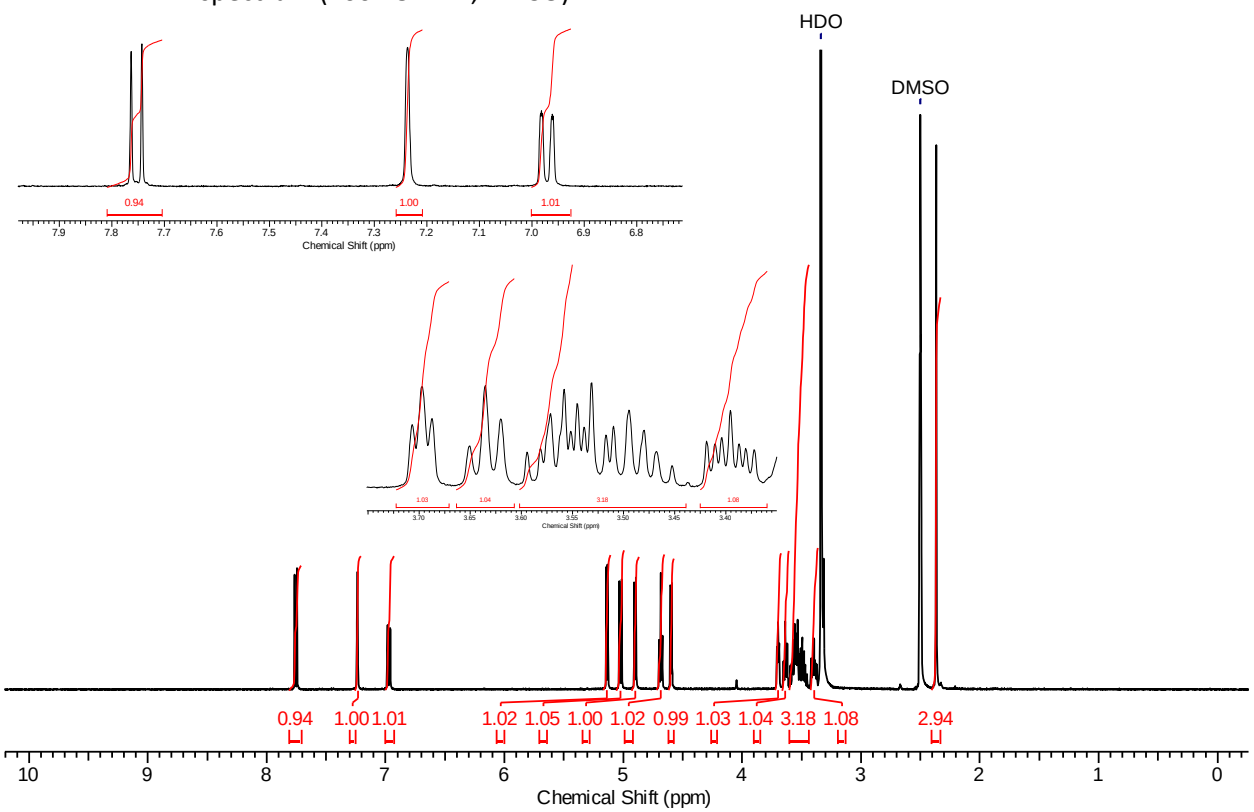


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

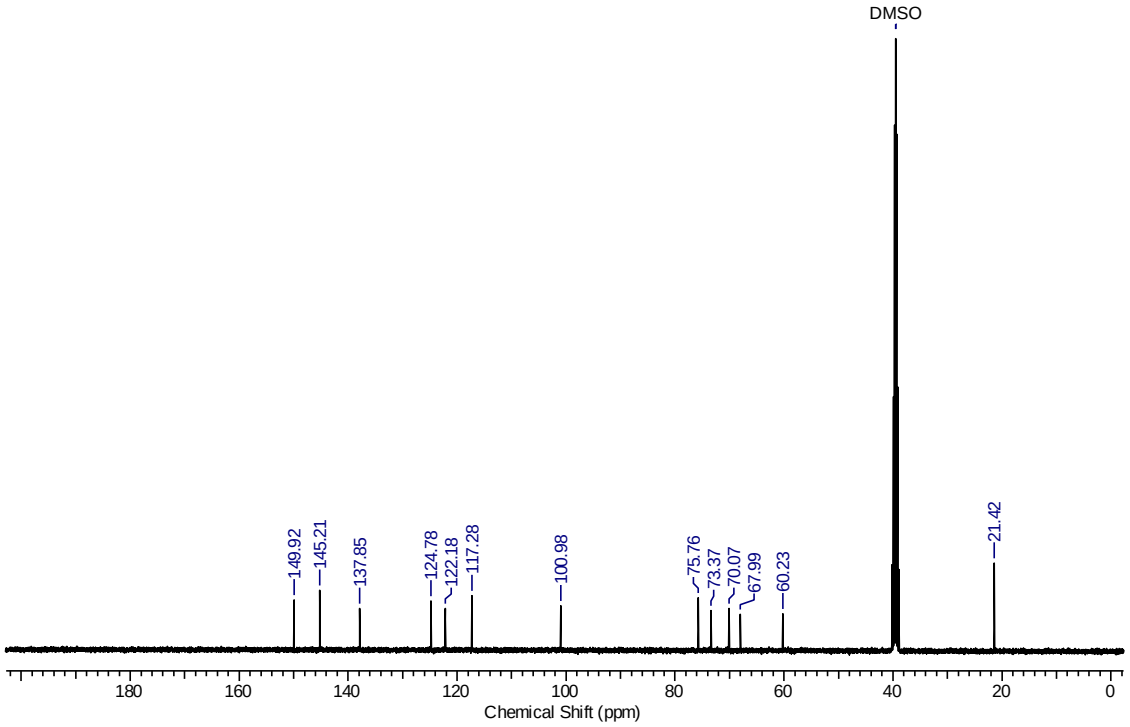


5-Methyl-2-nitrophenyl-β-D-galactopyranoside (2g).

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

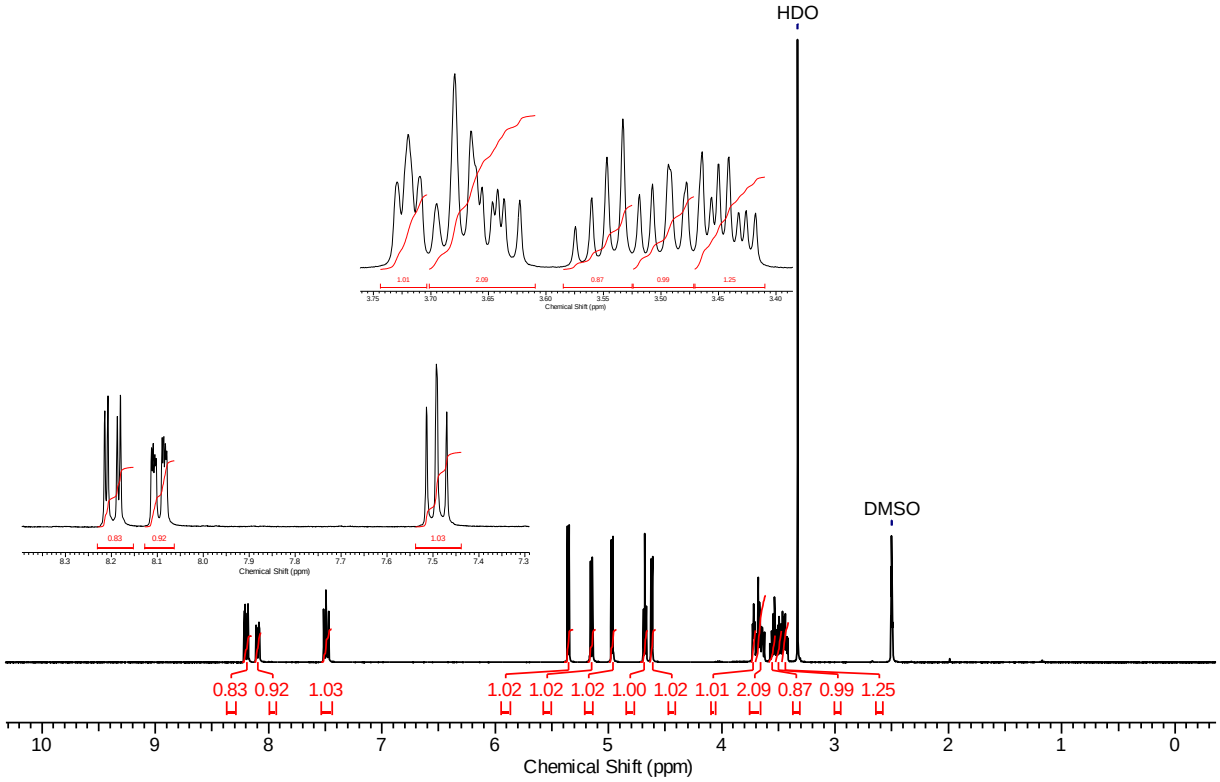


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

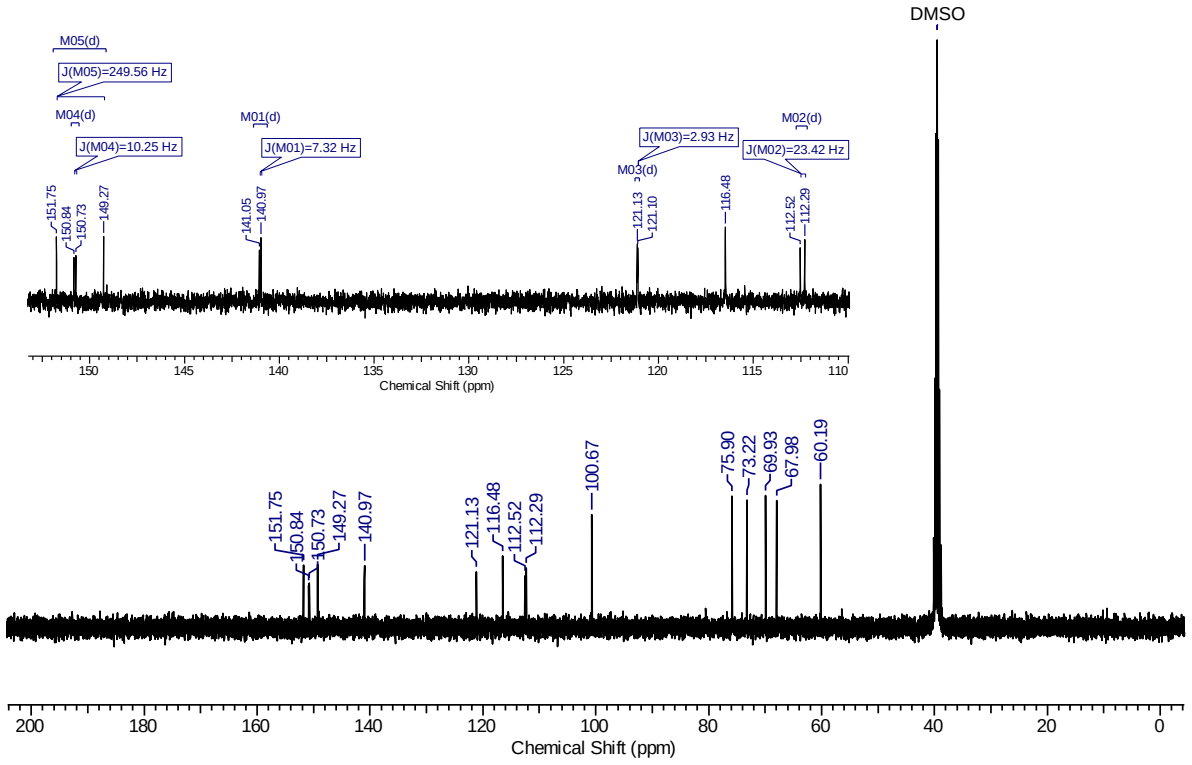


2-Fluoro-4-nitrophenyl-β-D-galactopyranoside (2i).

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

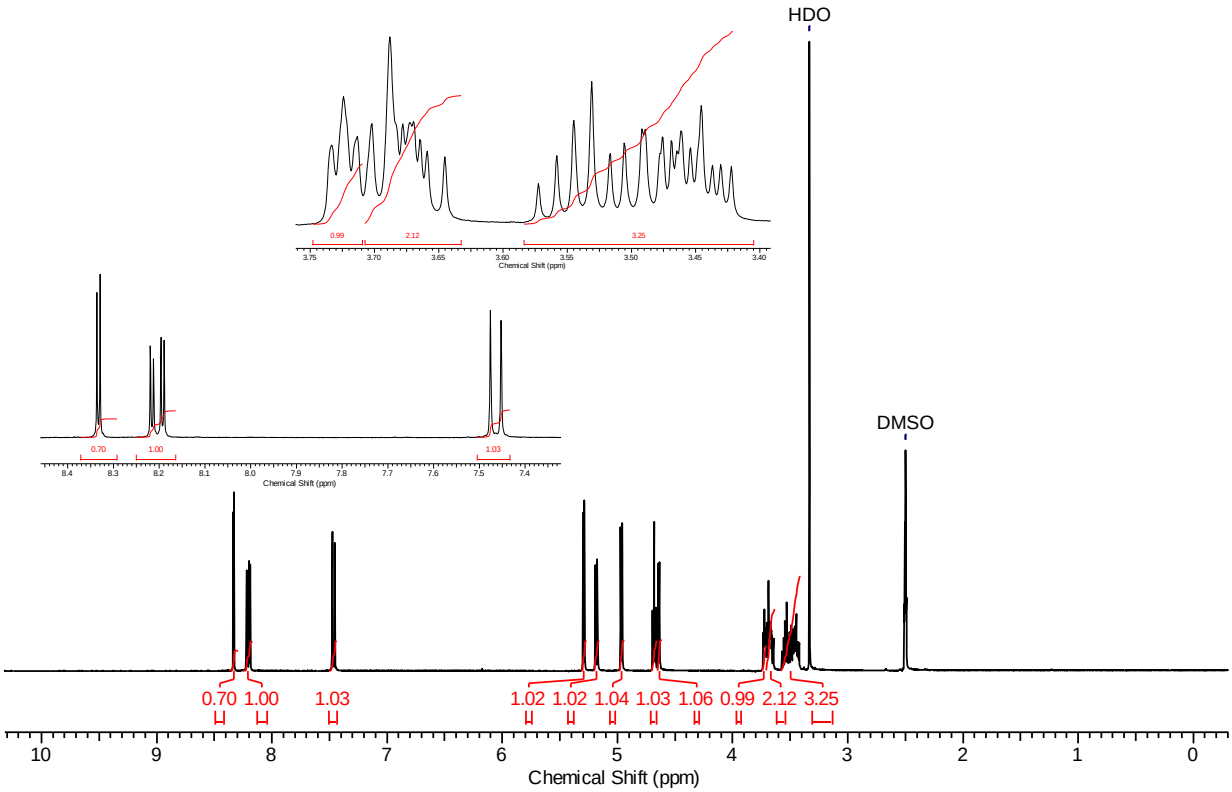


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

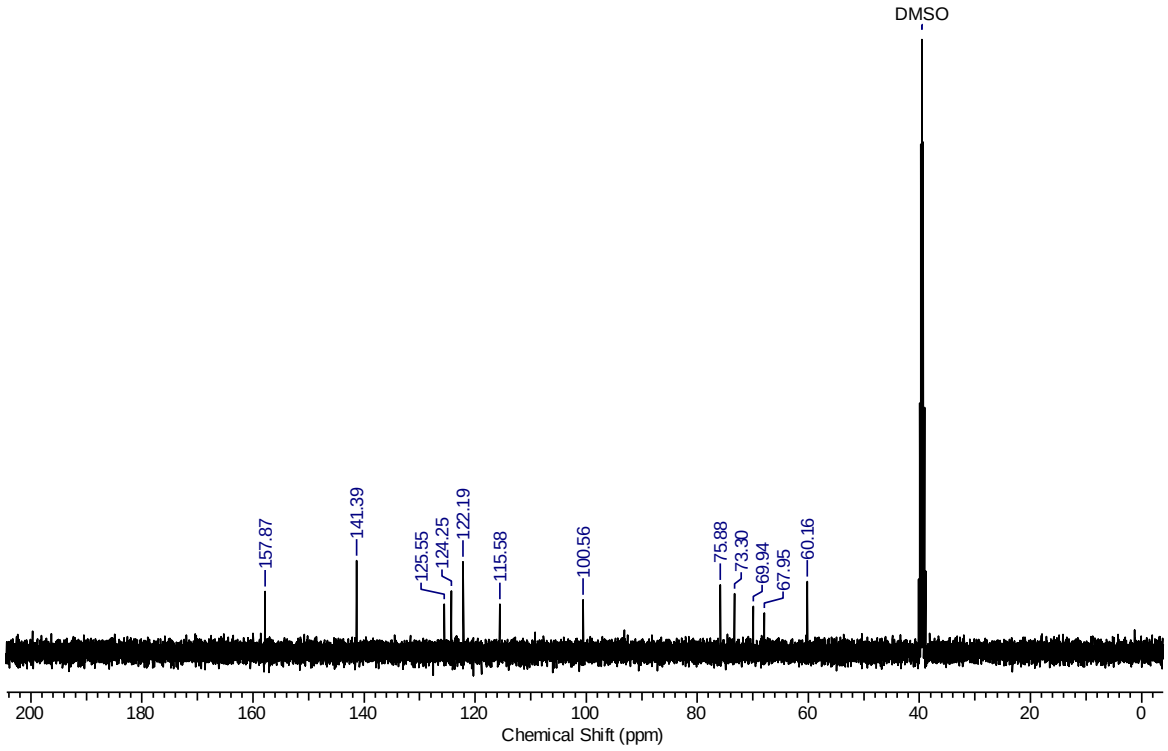


2-Chloro-4-nitrophenyl-β-D-galactopyranoside (2k).

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

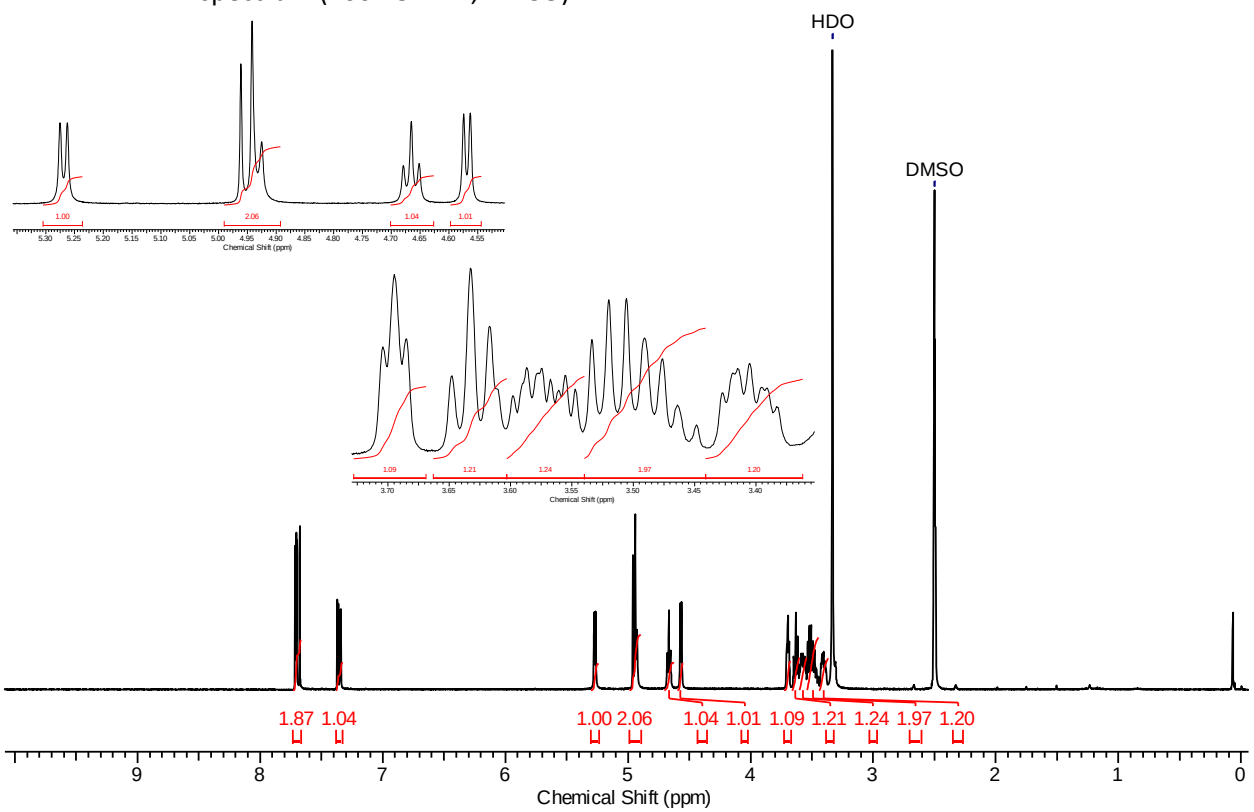


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

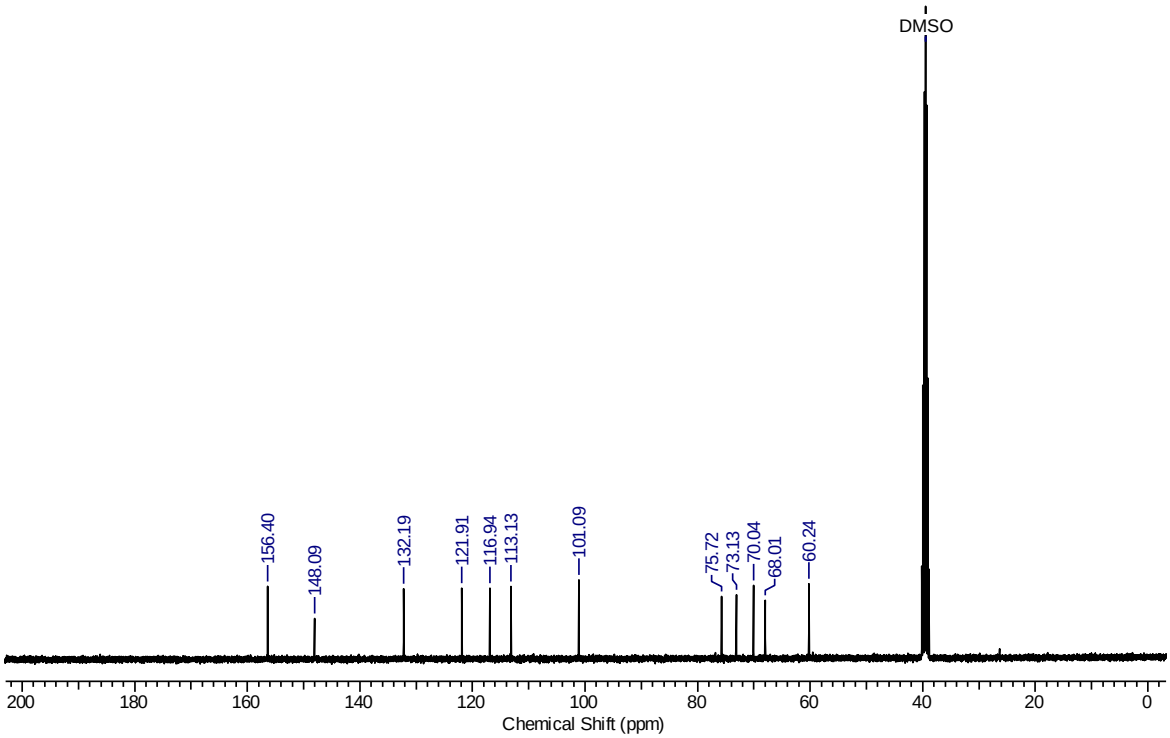


4-Chloro-3-nitrophenyl-β-D-galactopyranoside (2m).

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

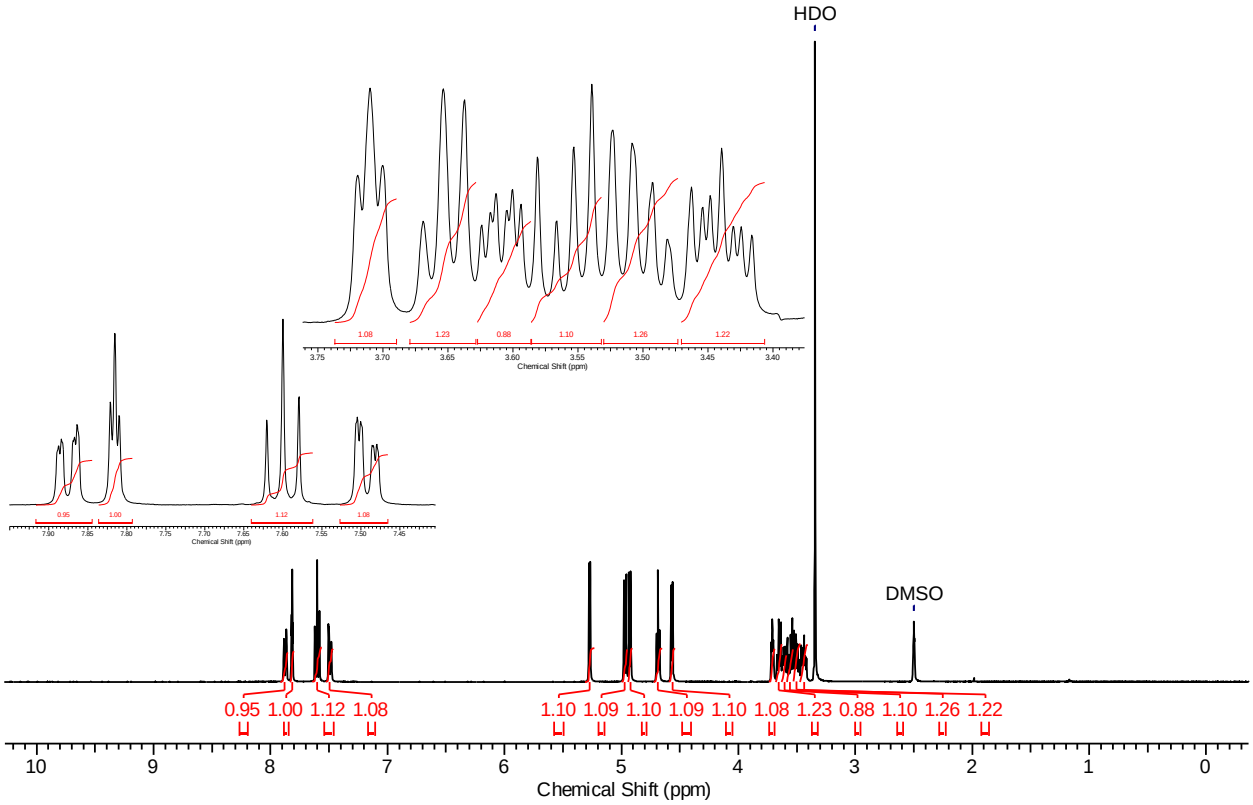


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

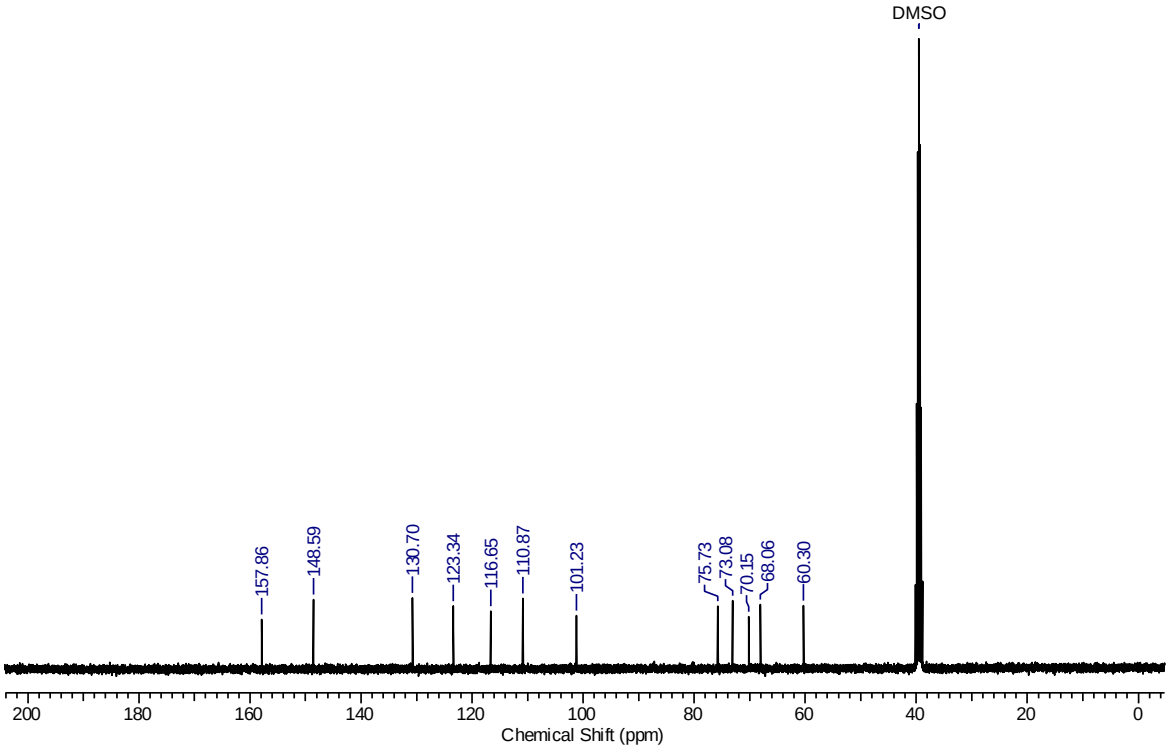


3-Nitrophenyl-β-D-galactopyranoside (2n).

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

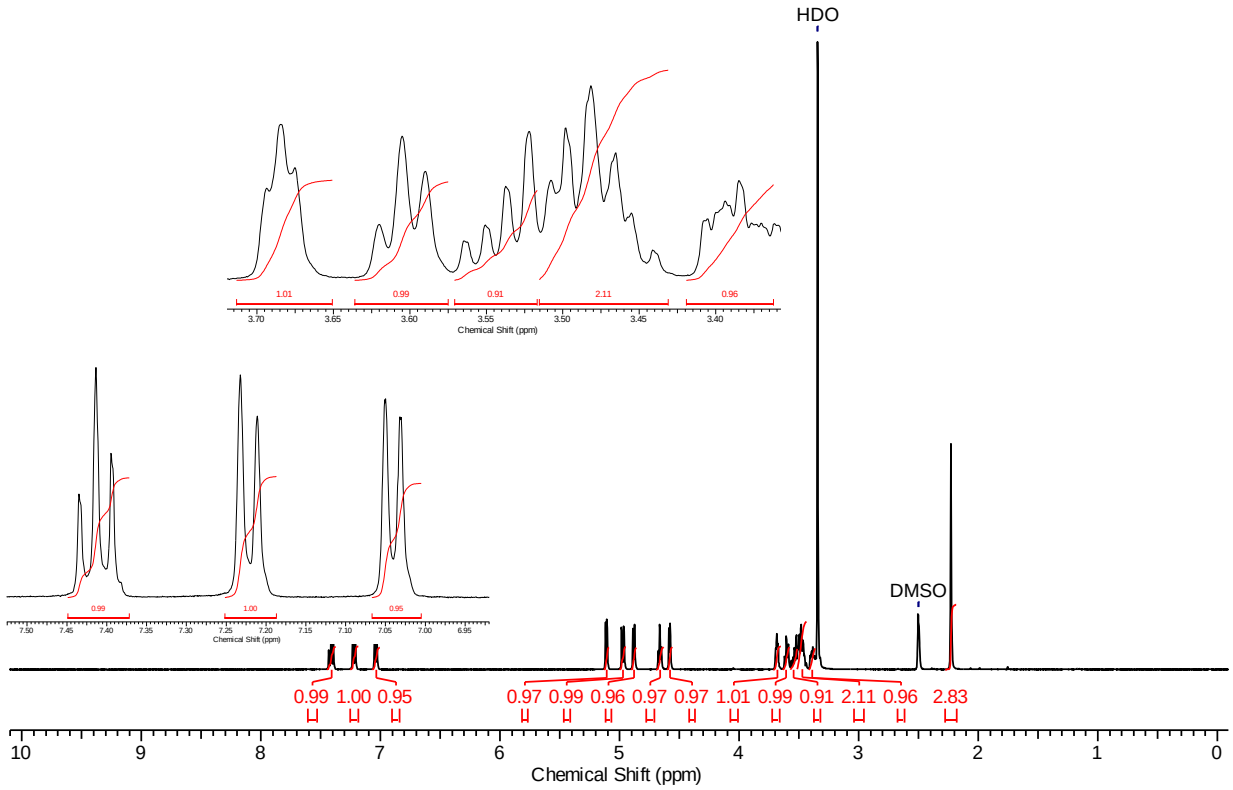


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

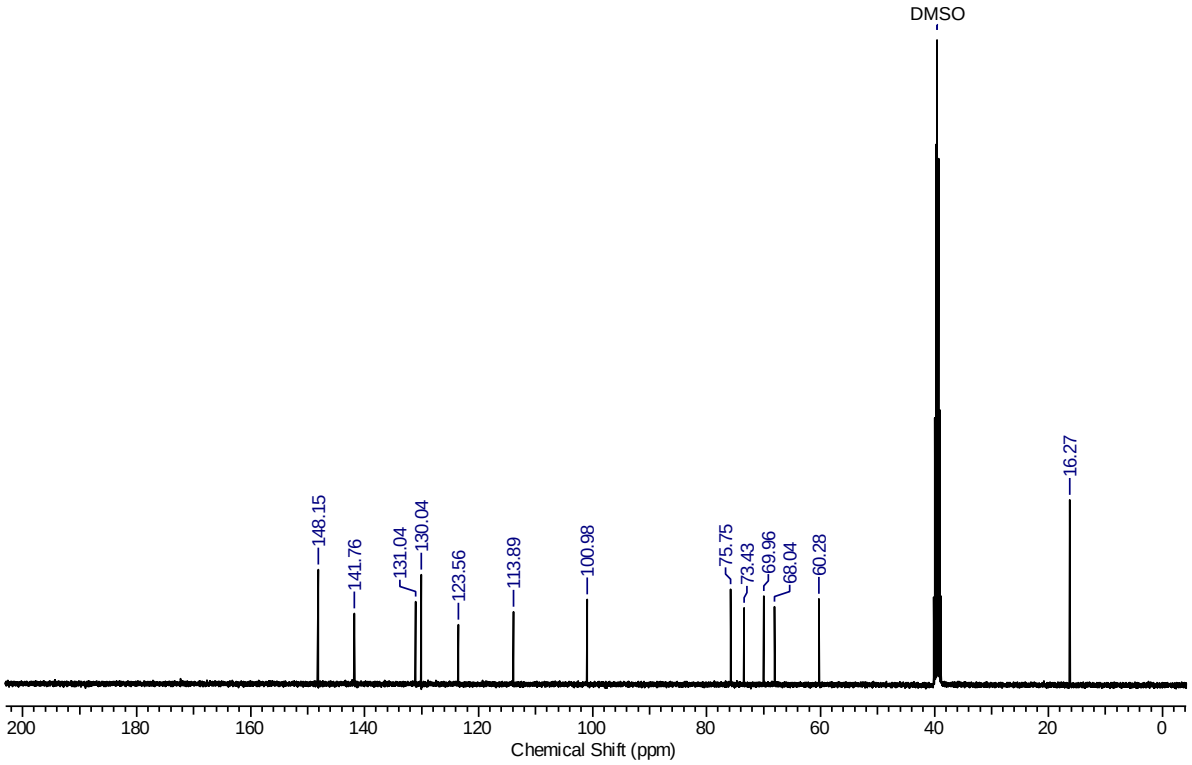


3-Methyl-2-nitrophenyl-β-D-galactopyranoside (2o).

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

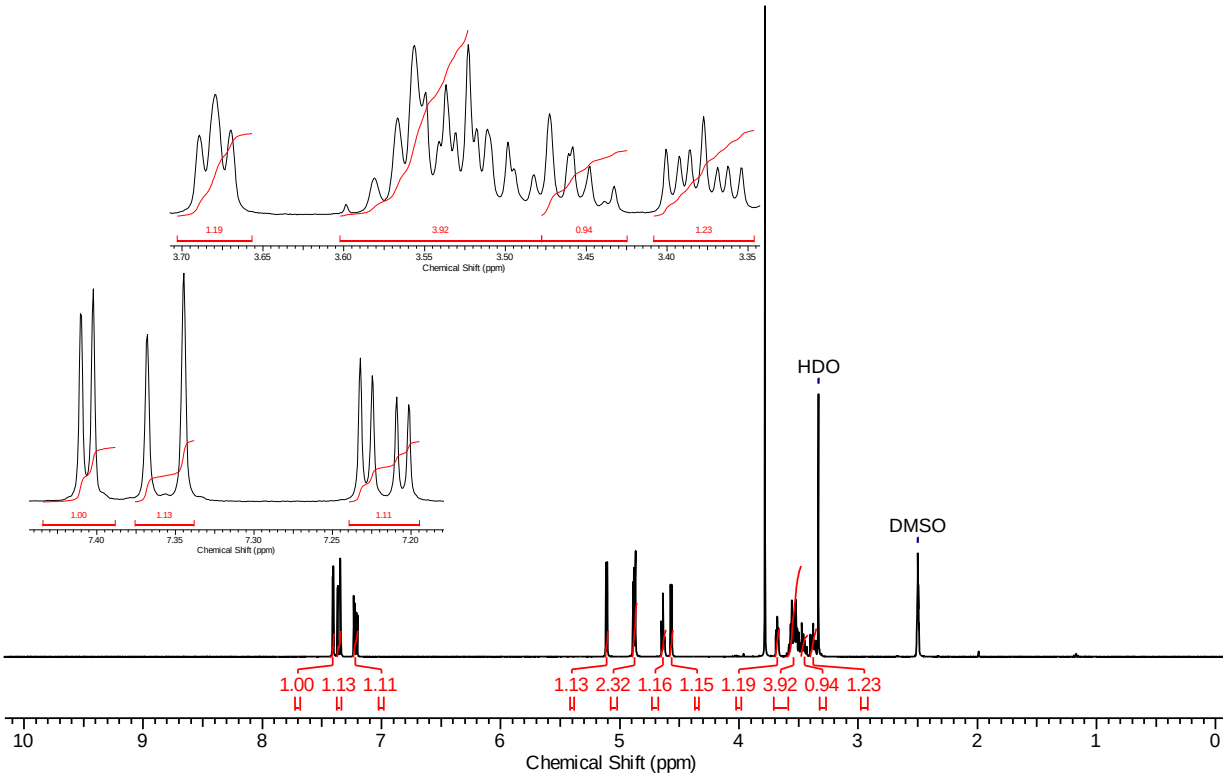


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

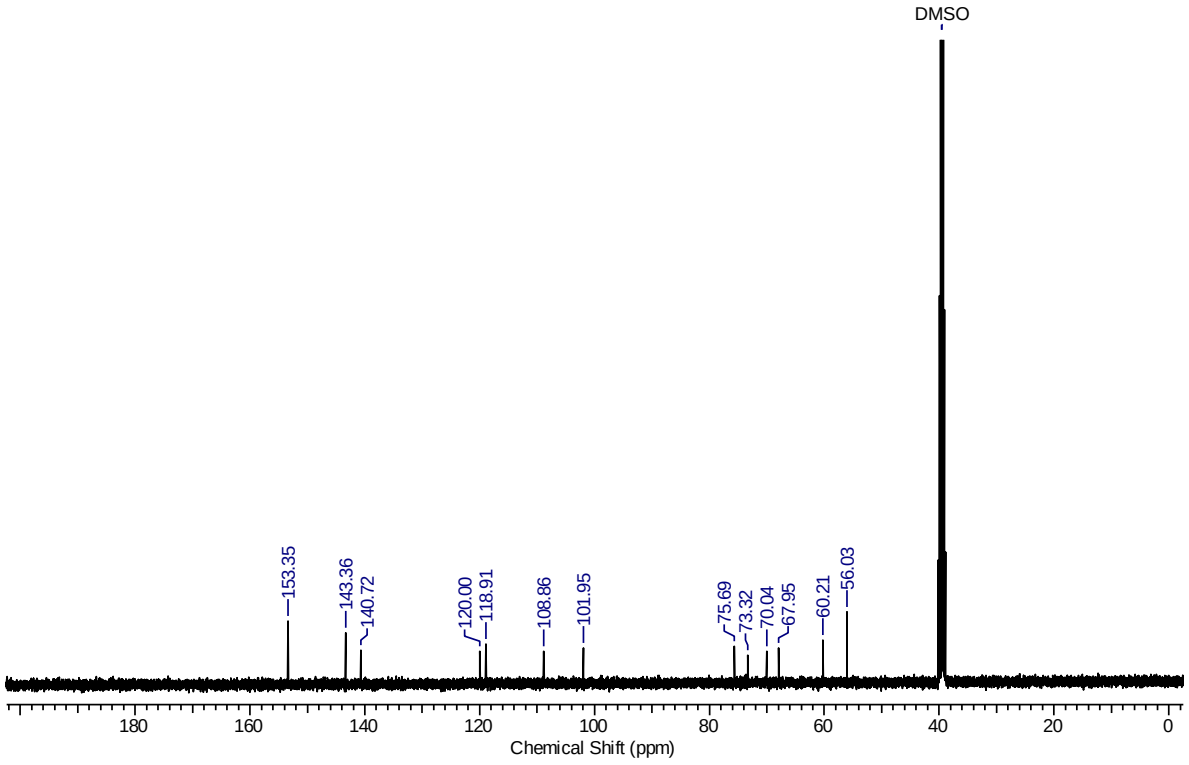


4-Methoxy-2-nitrophenyl-β-D-galactopyranoside (2p).

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

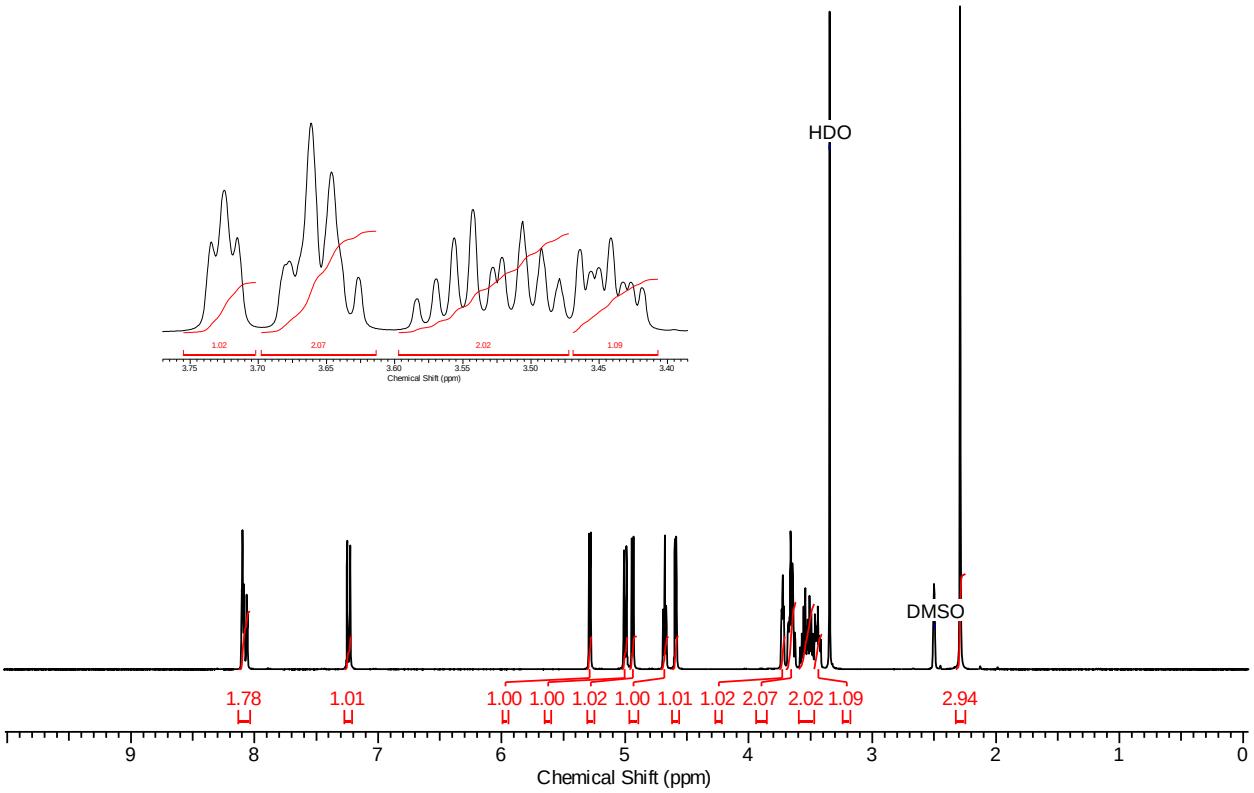


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

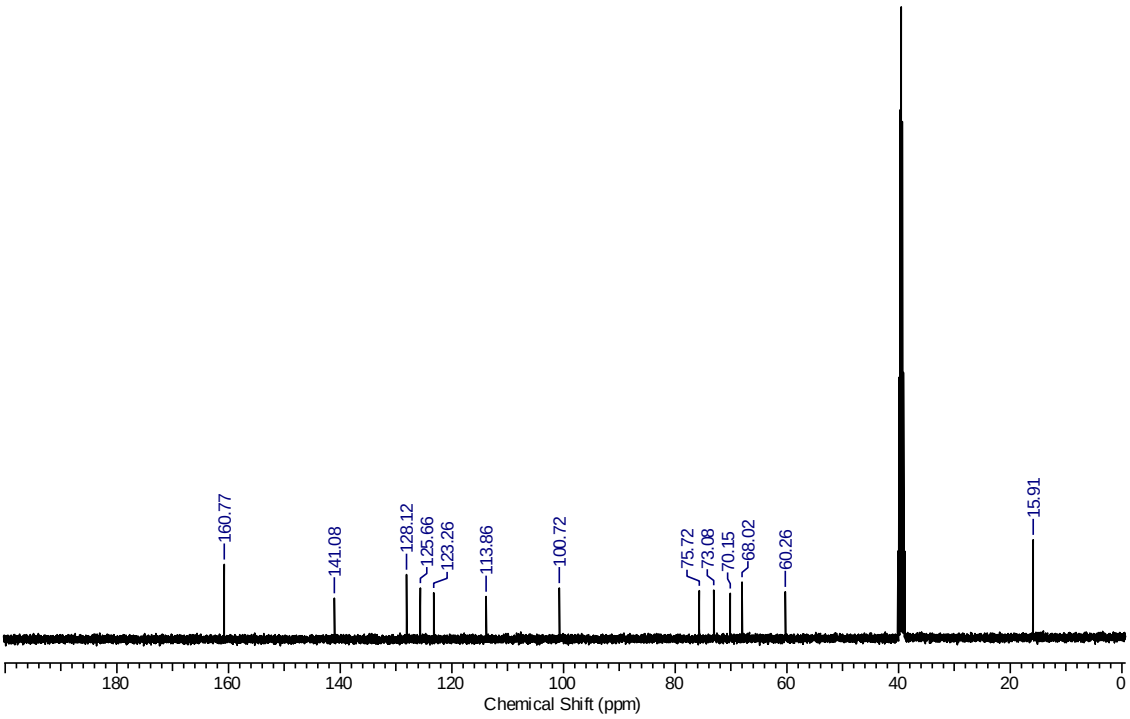


2-Methyl-4-nitrophenyl-β-D-galactopyranoside (2q).

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

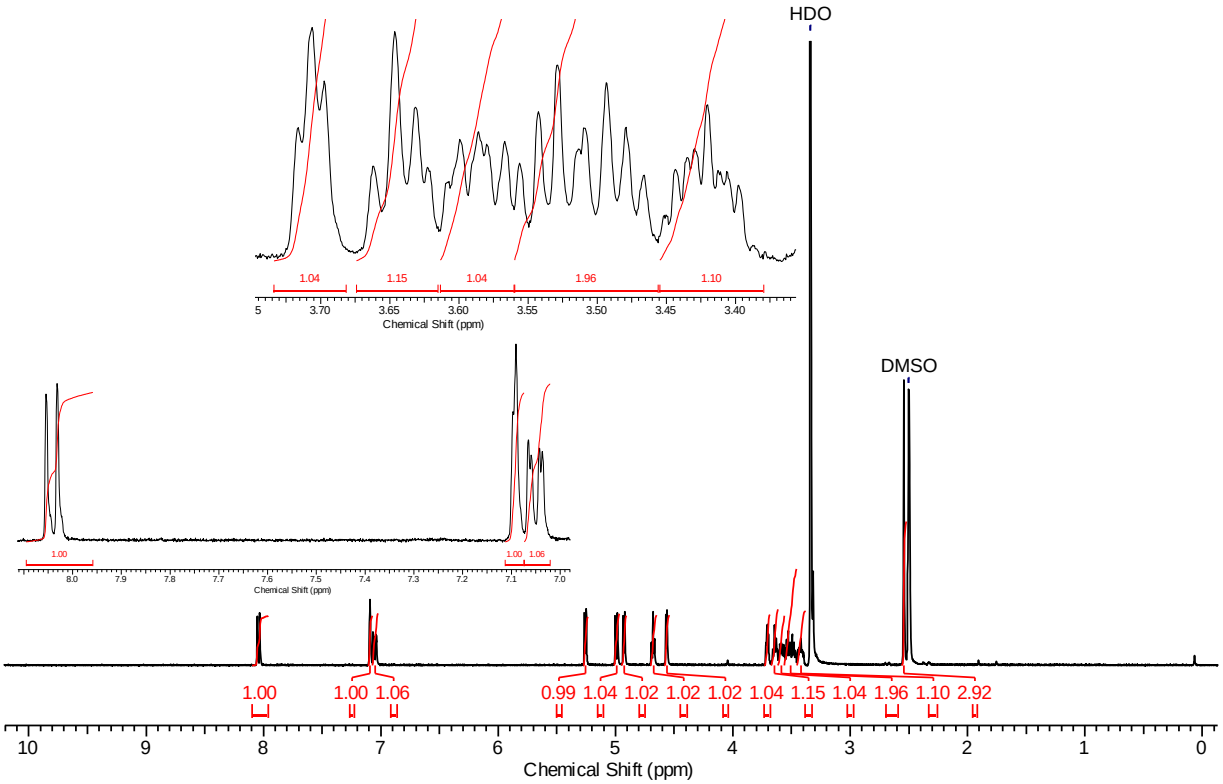


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

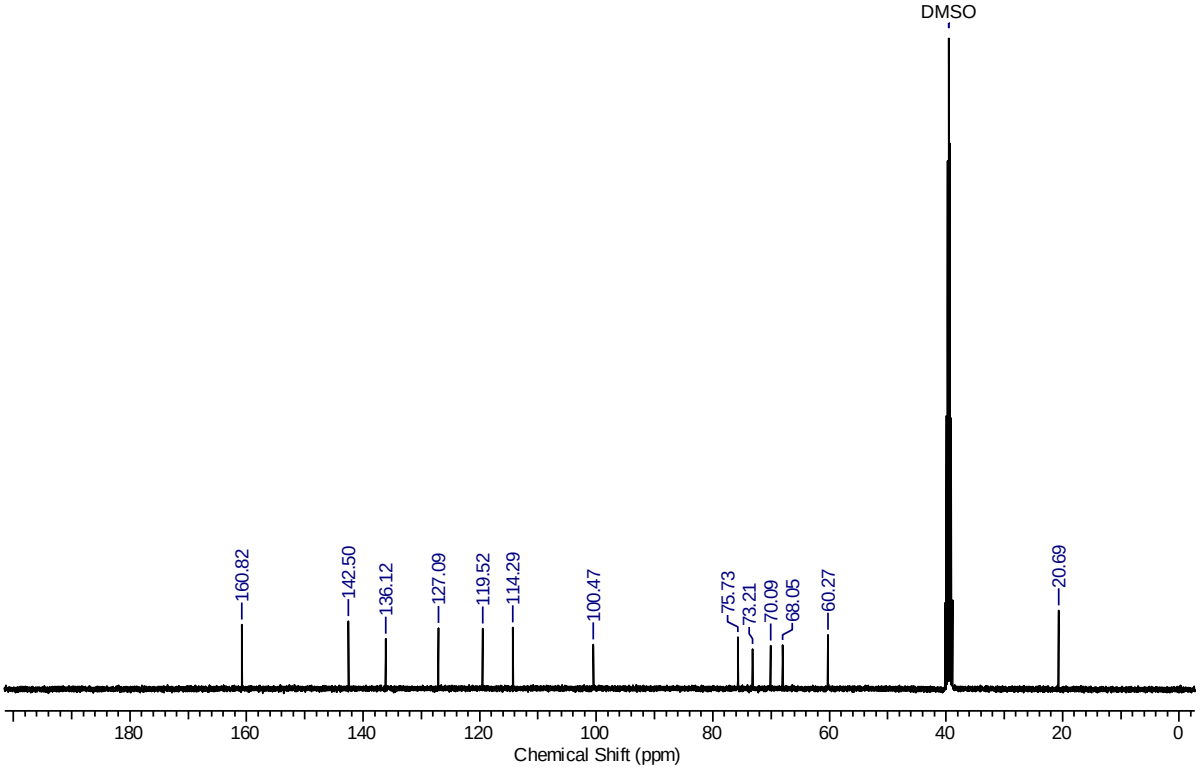


3-Methyl-4-nitrophenyl-β-D-galactopyranoside (2r).

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

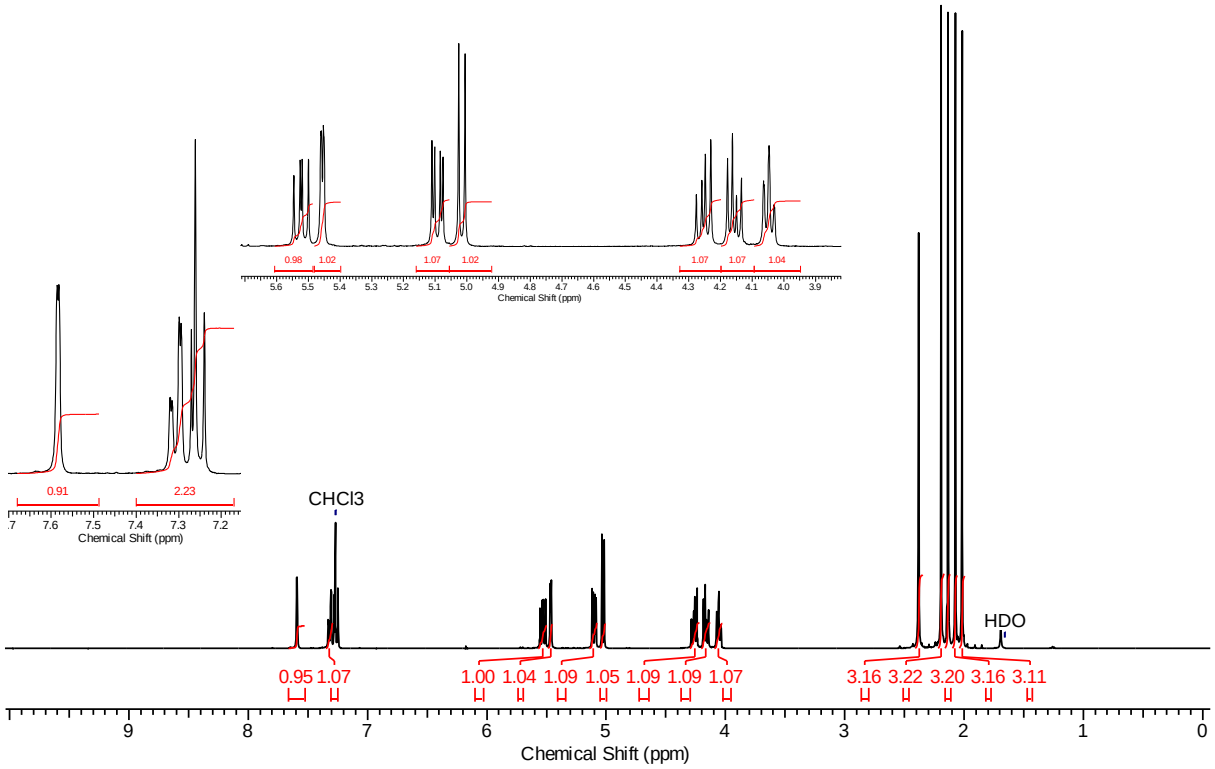


- ^{13}C NMR spectrum (100.6 MHz, DMSO-d6)

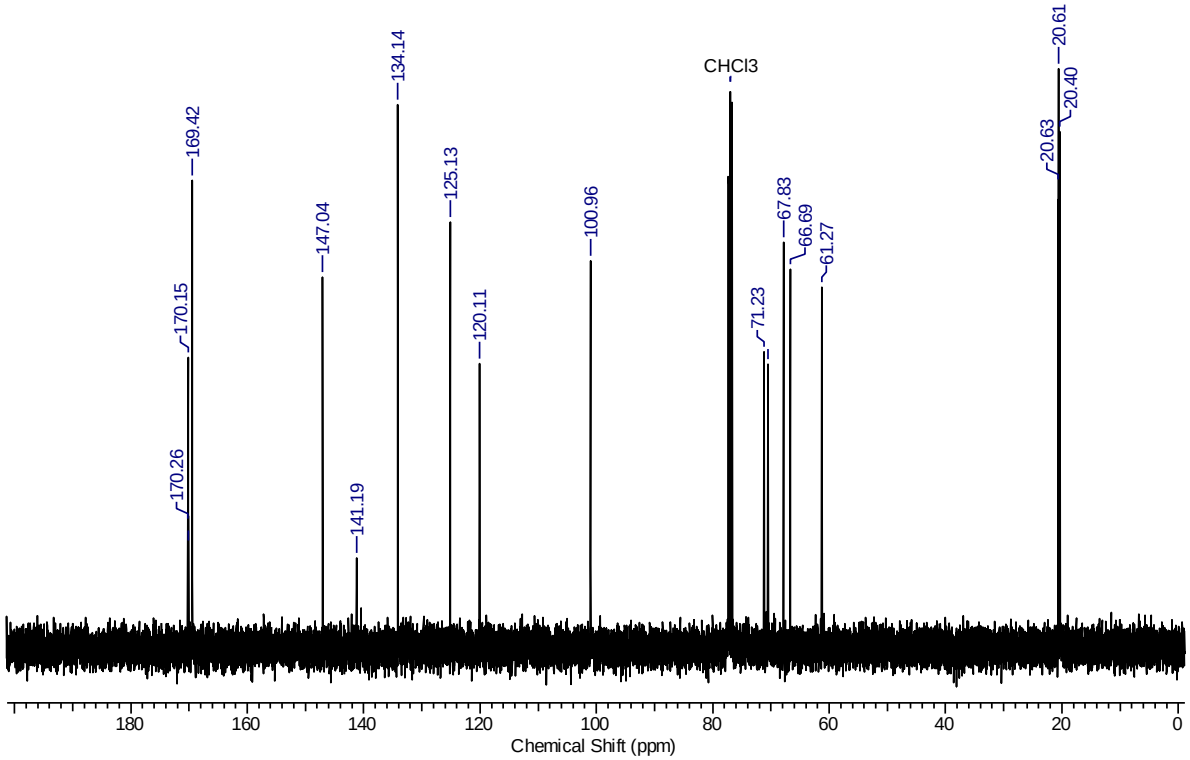


4-Methyl-2-nitrophenyl-tetra-*O*-acetylβ-D-galactopyranoside (4b).

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

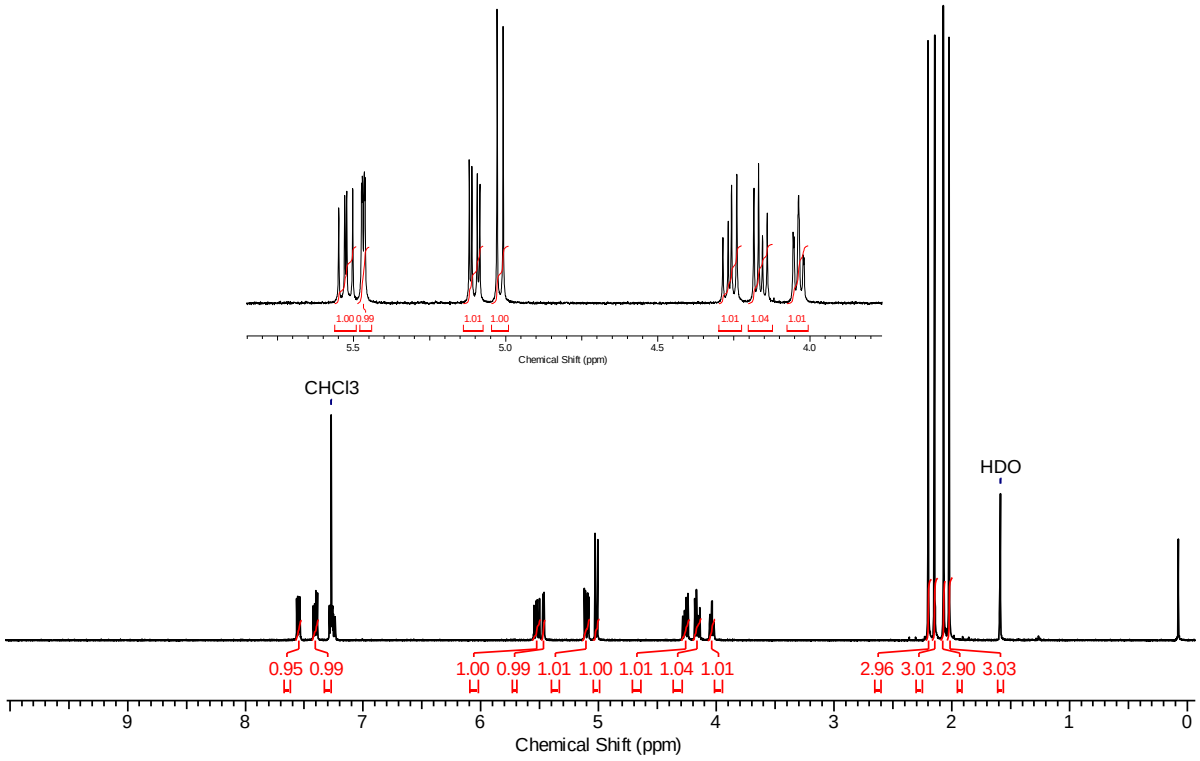


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

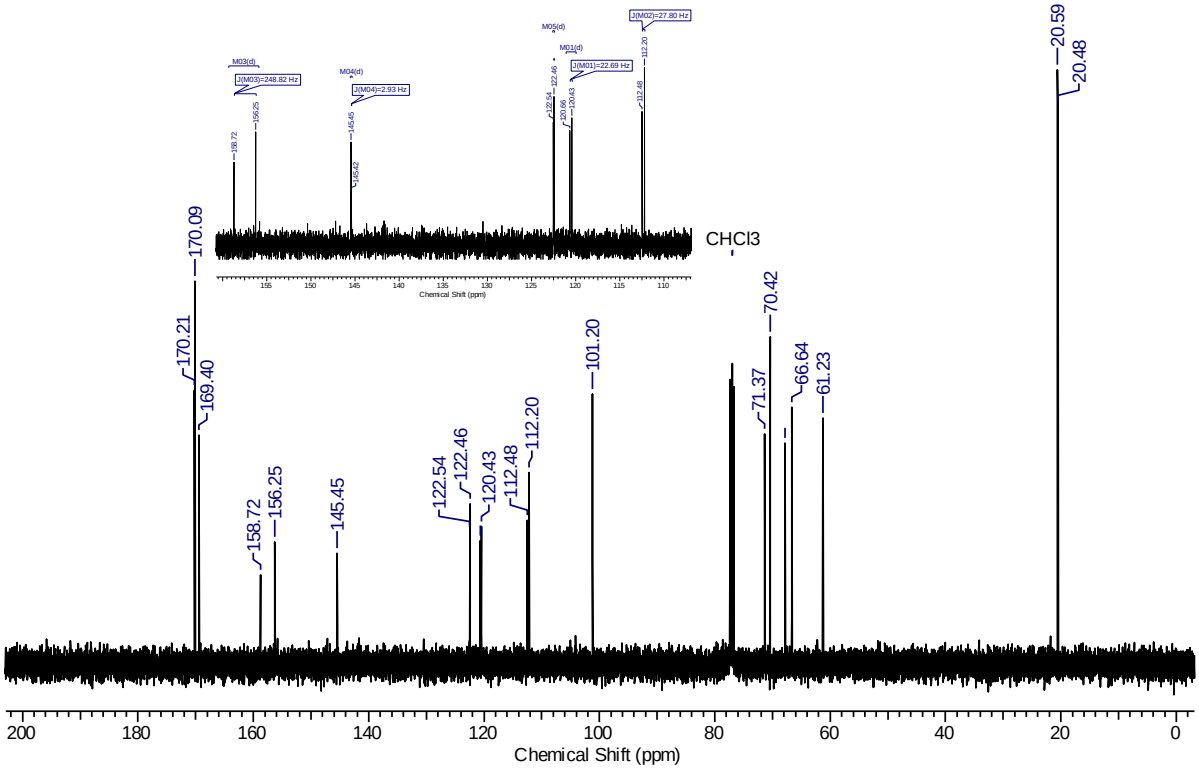


4-Fluoro-2-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4c).

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

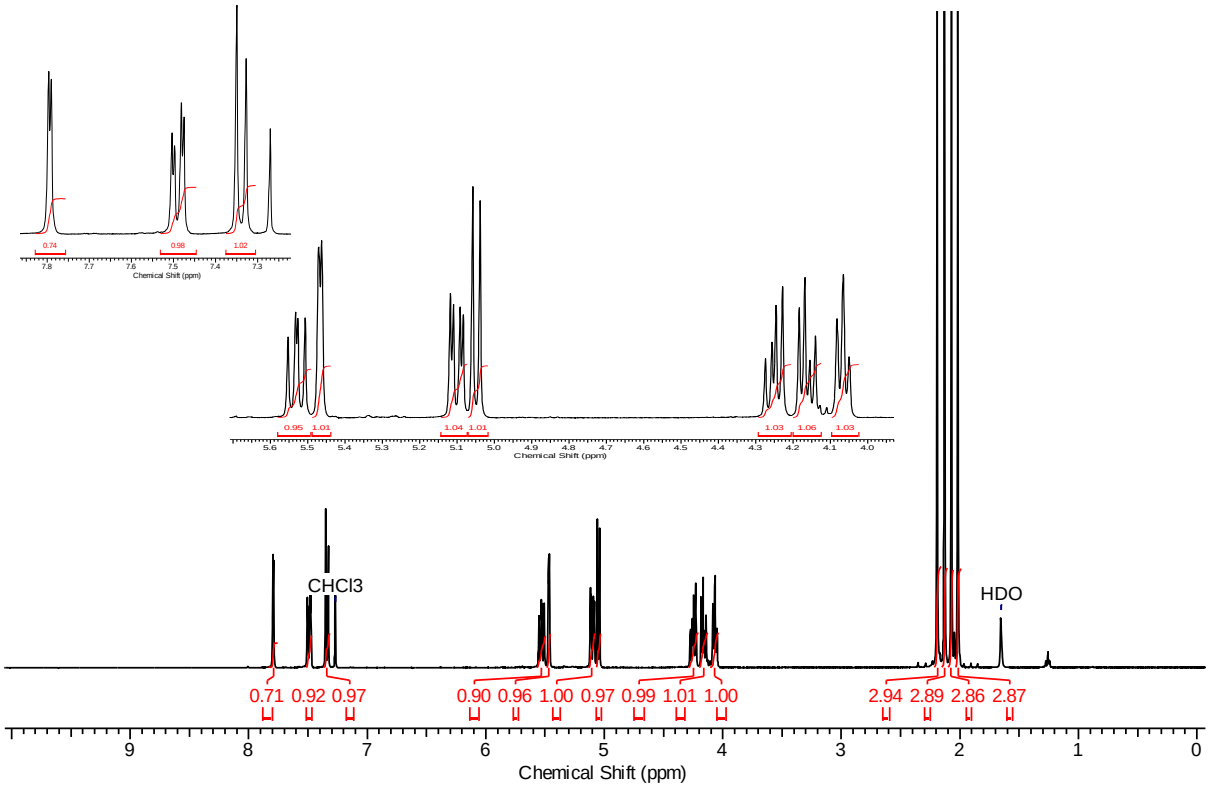


^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

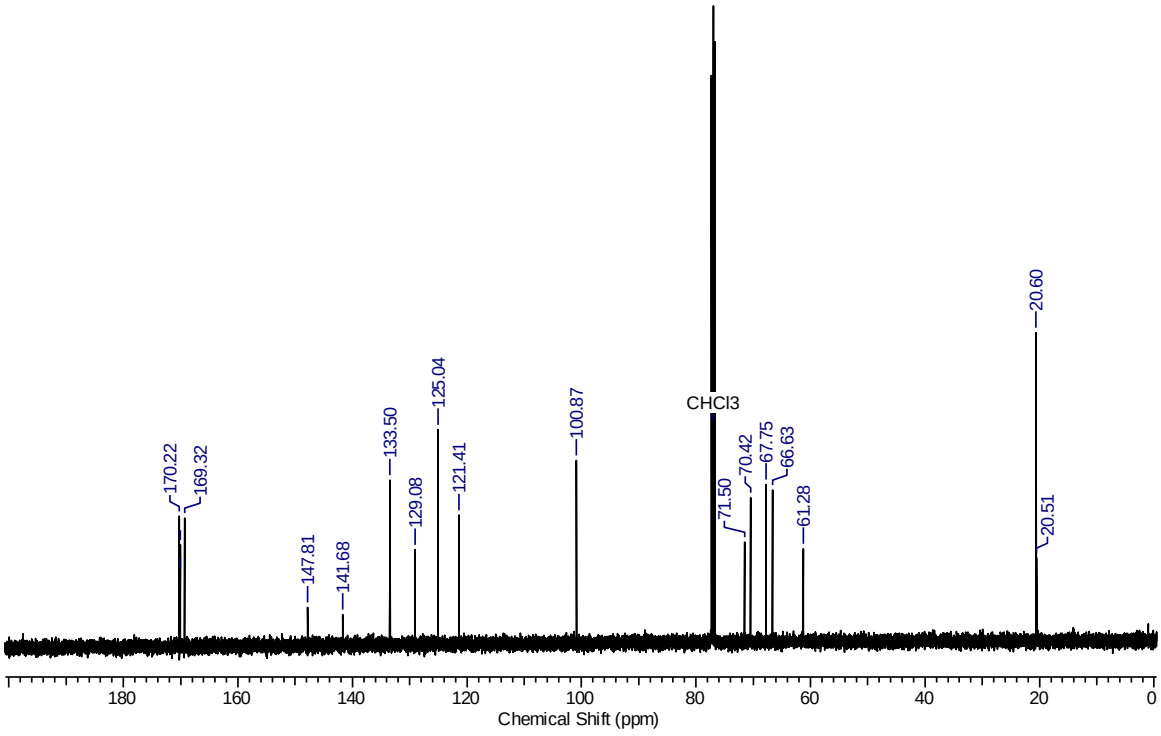


4-Chloro-2-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4d).

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

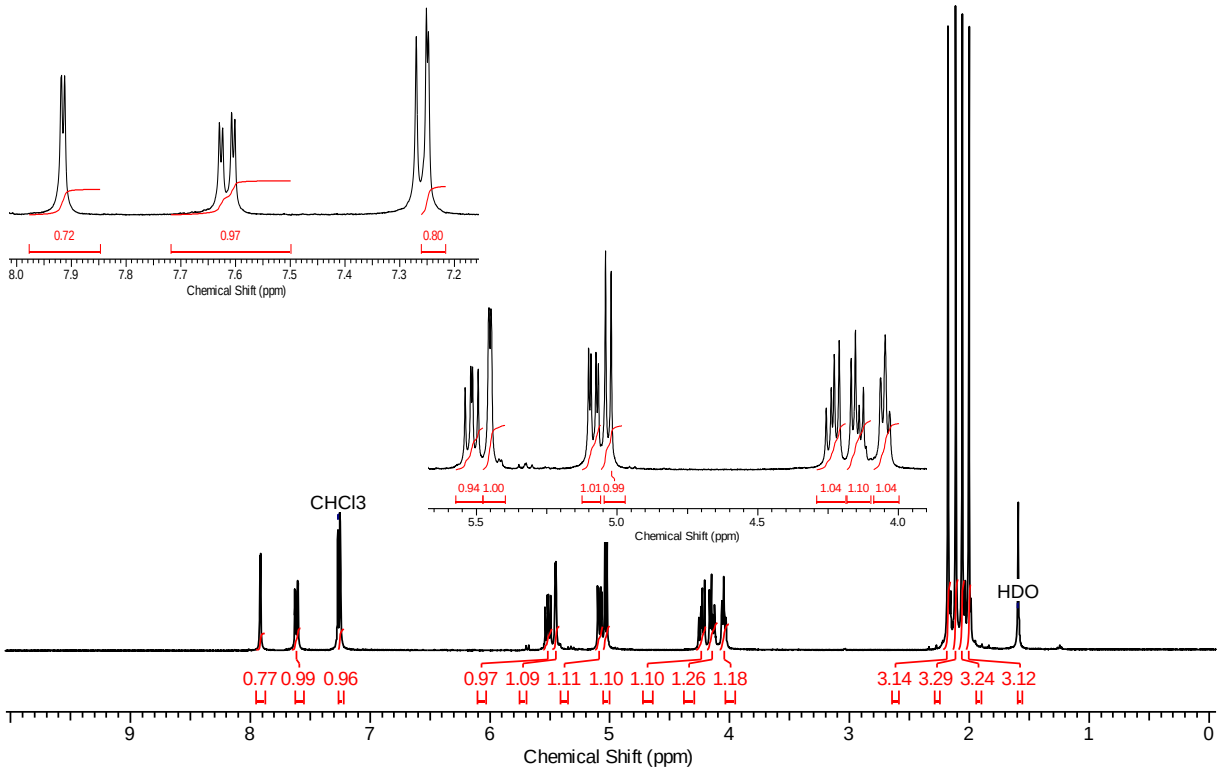


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

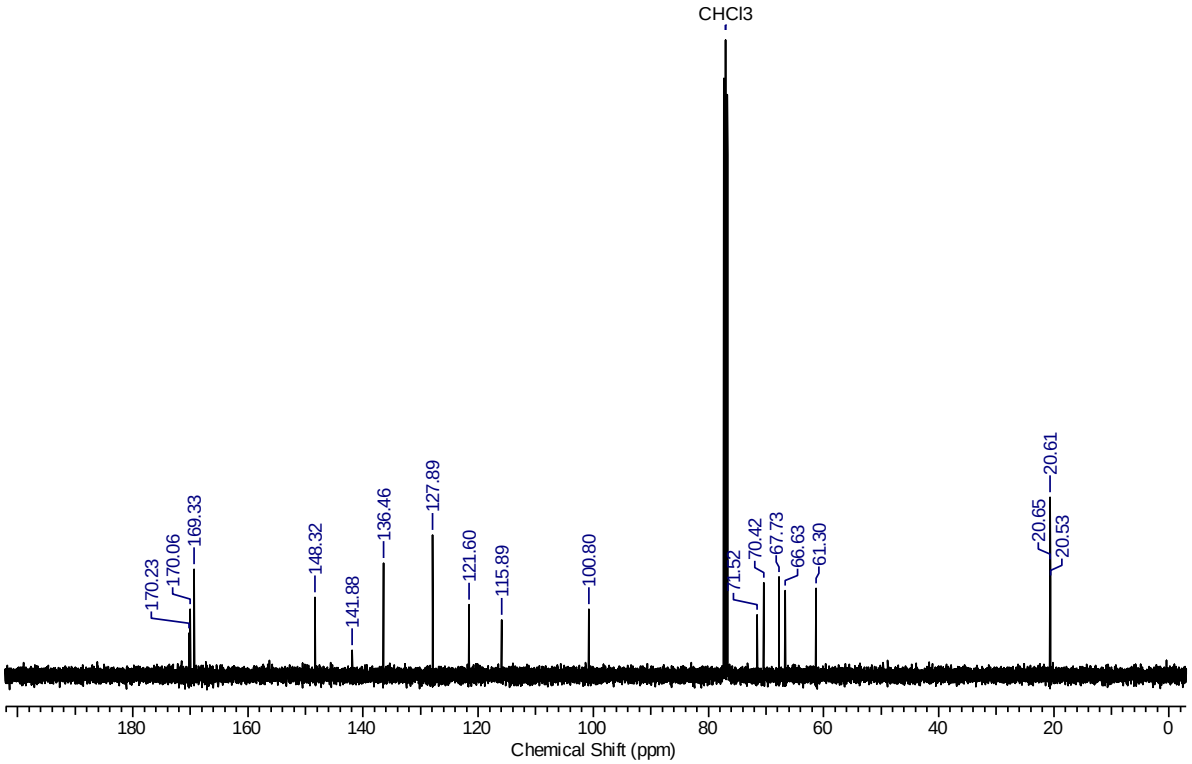


4-Bromo-2-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4e).

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

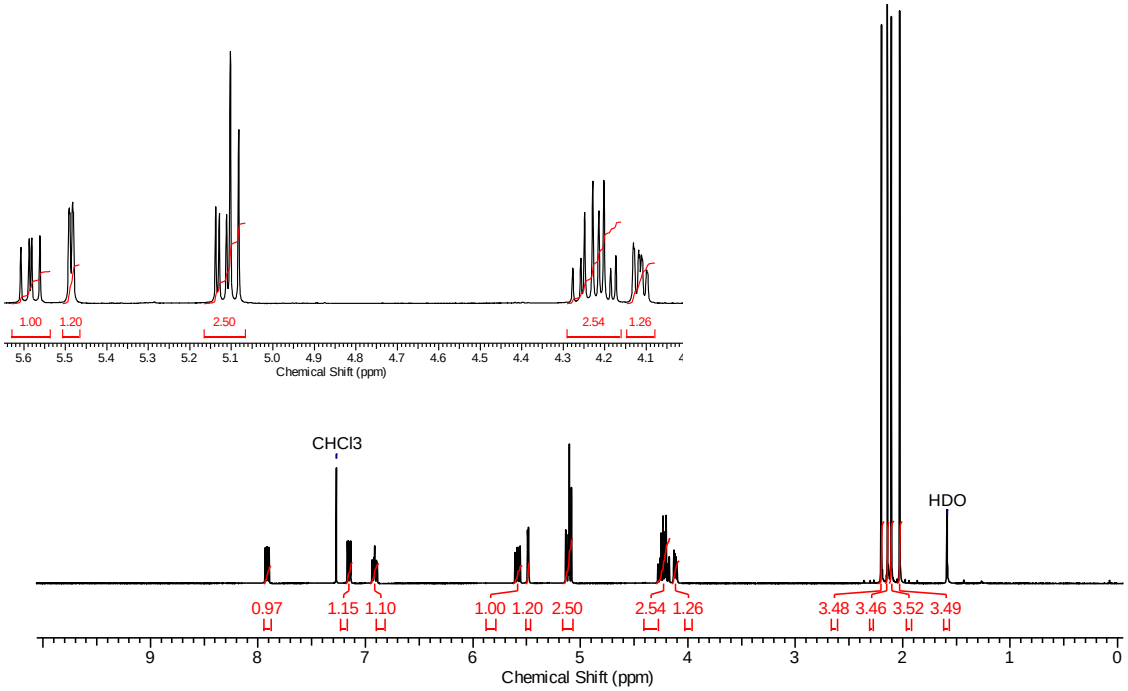


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

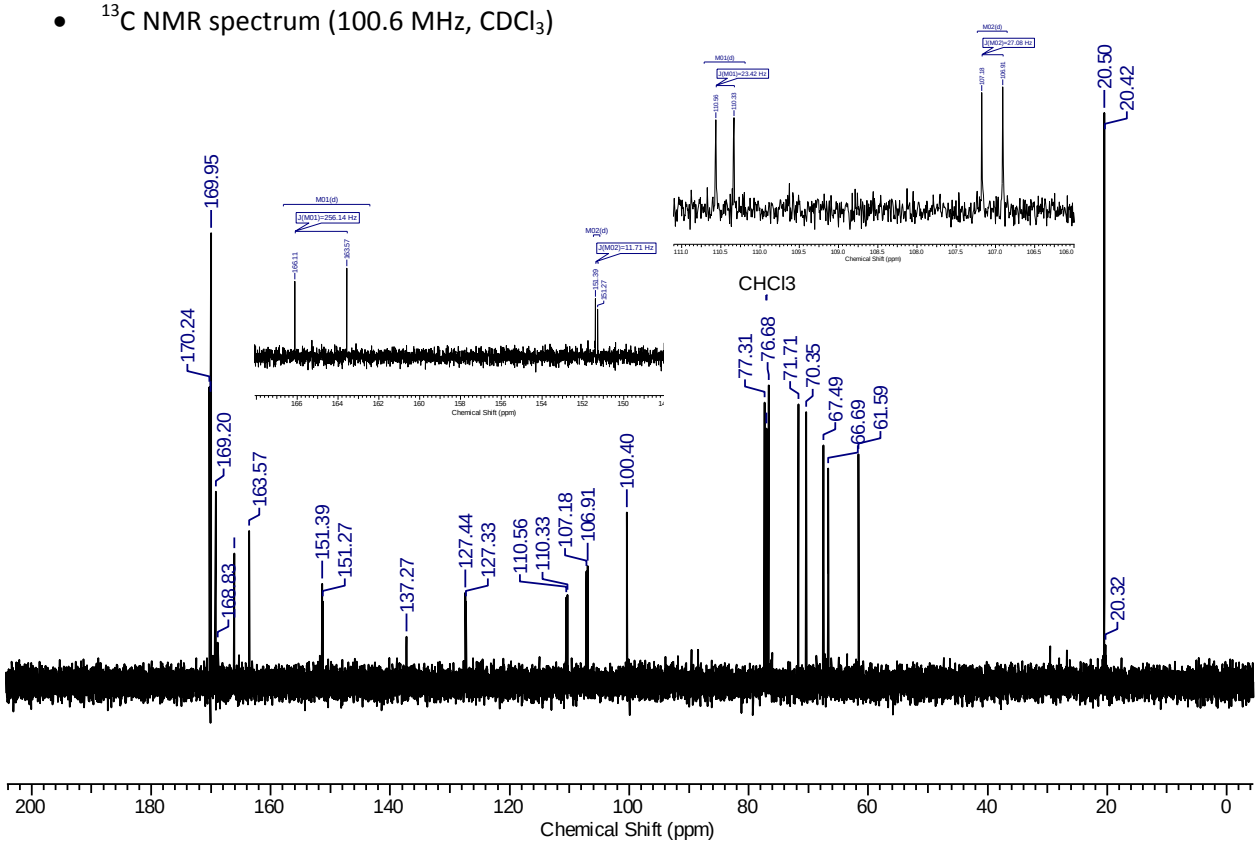


5-Fluoro-2-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4f).

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

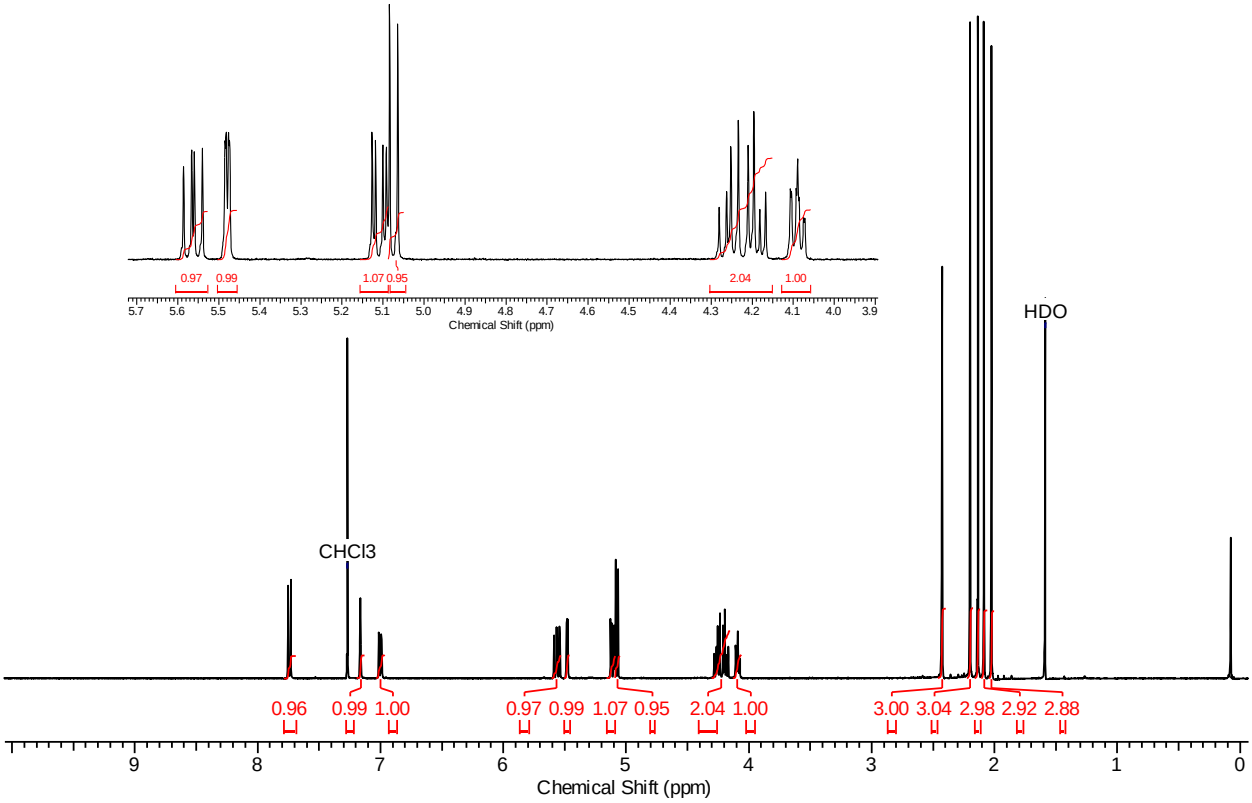


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

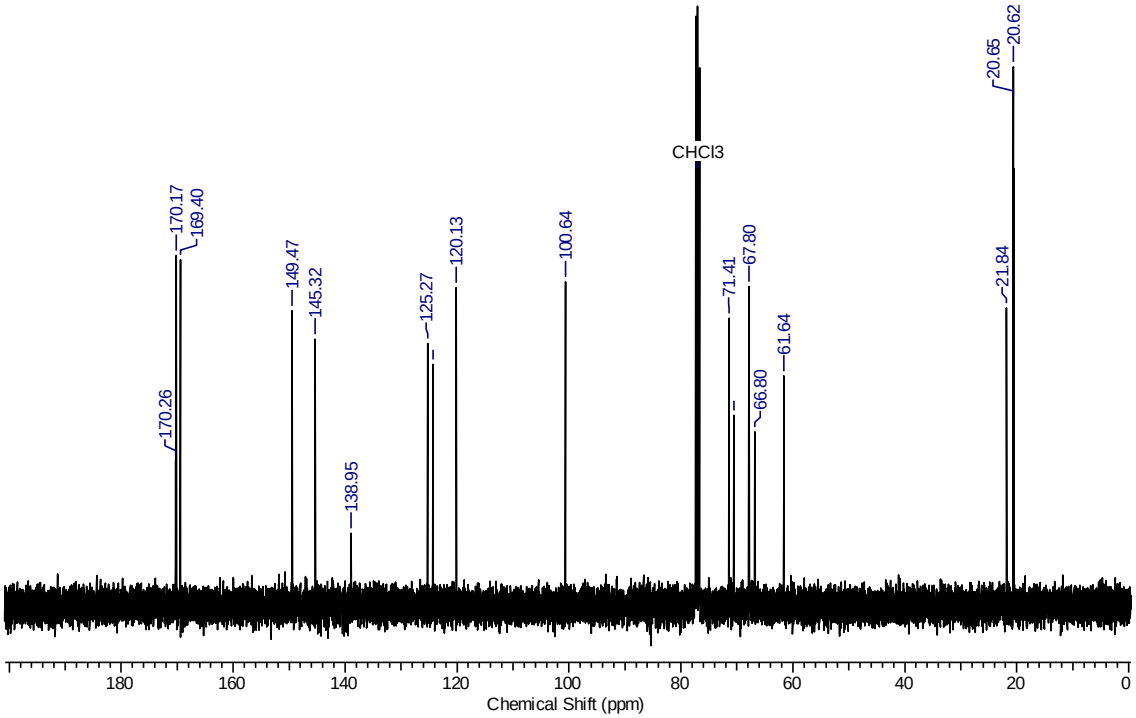


5-Methyl-2-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4g).

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

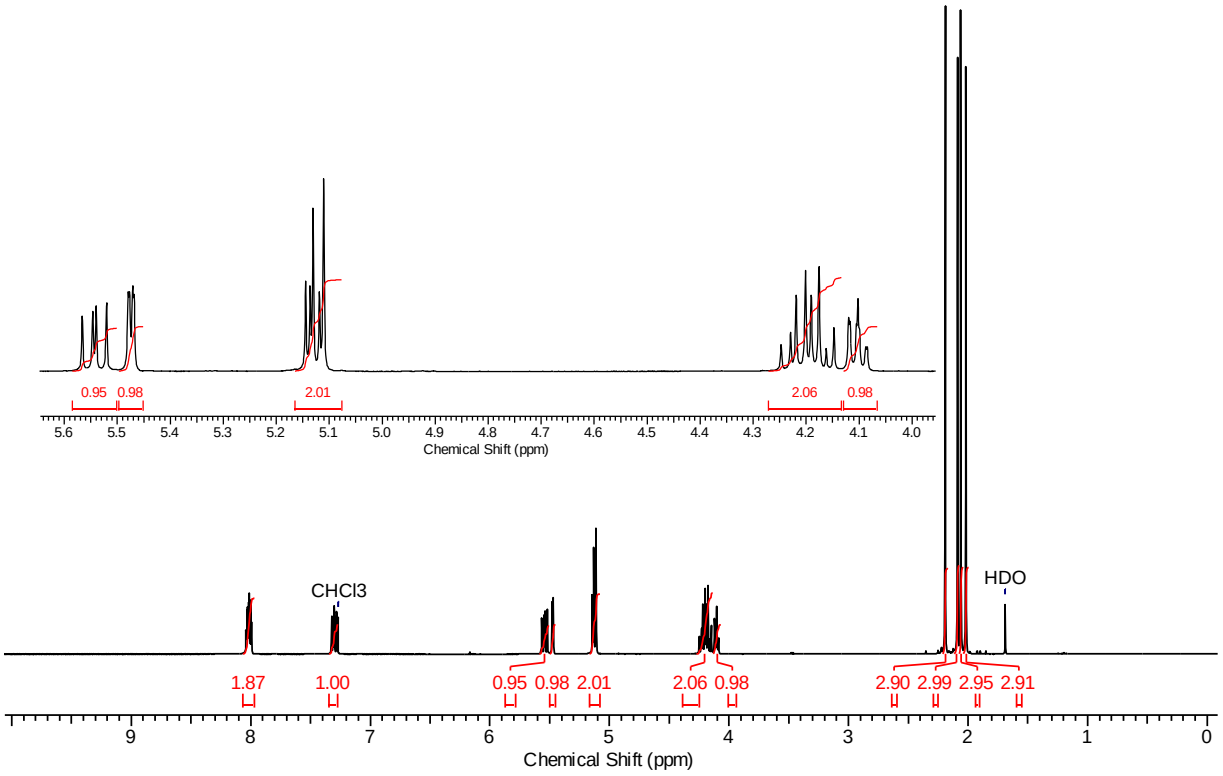


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

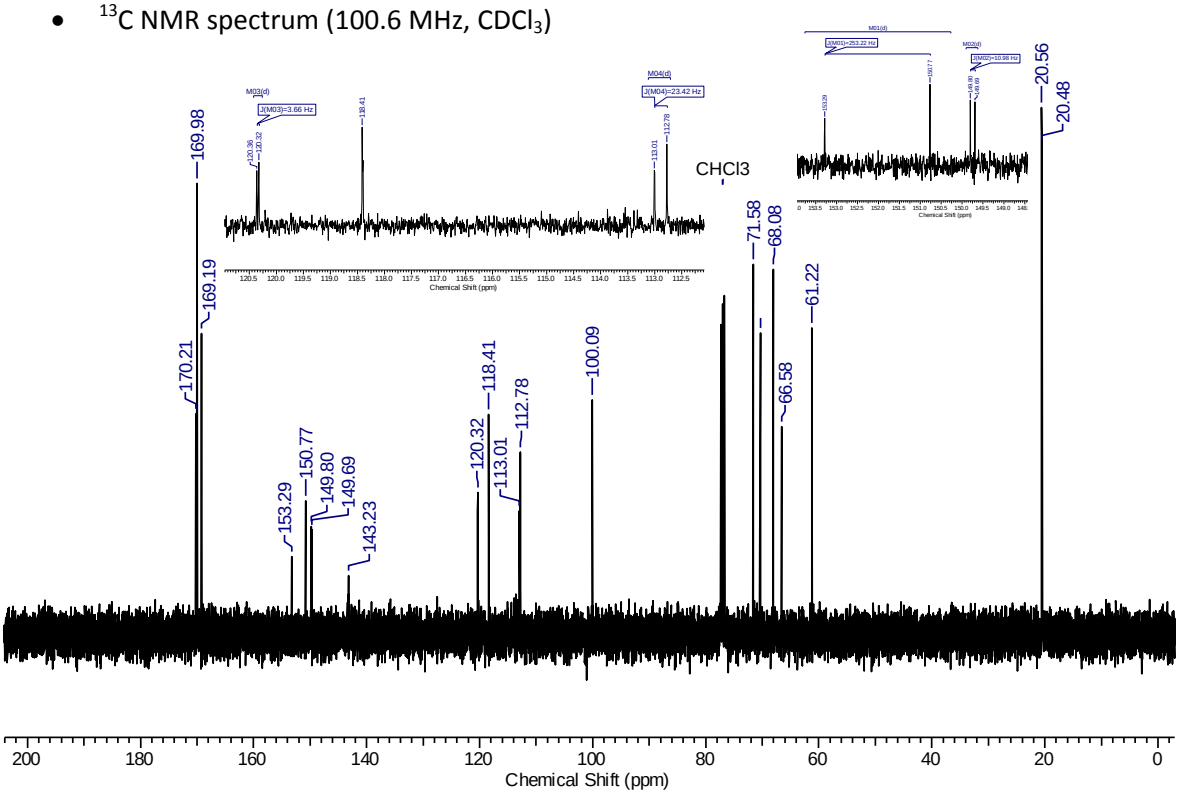


2-Fluoro-4-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4i).

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

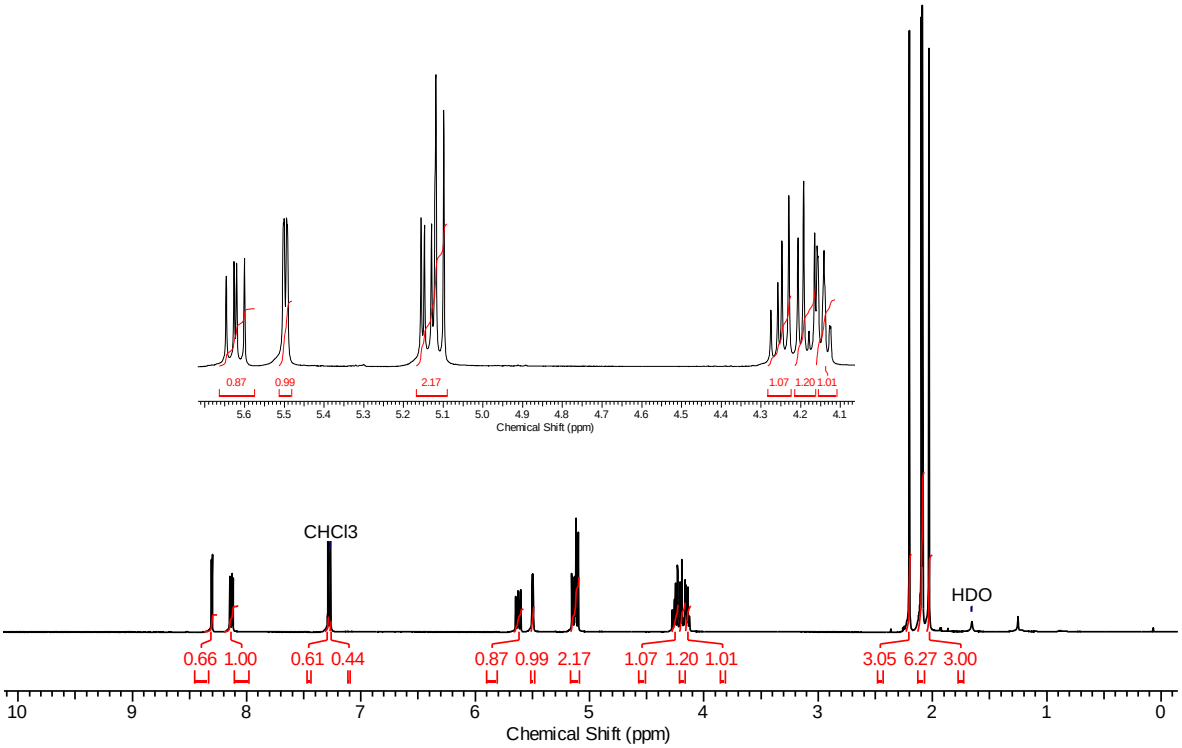


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

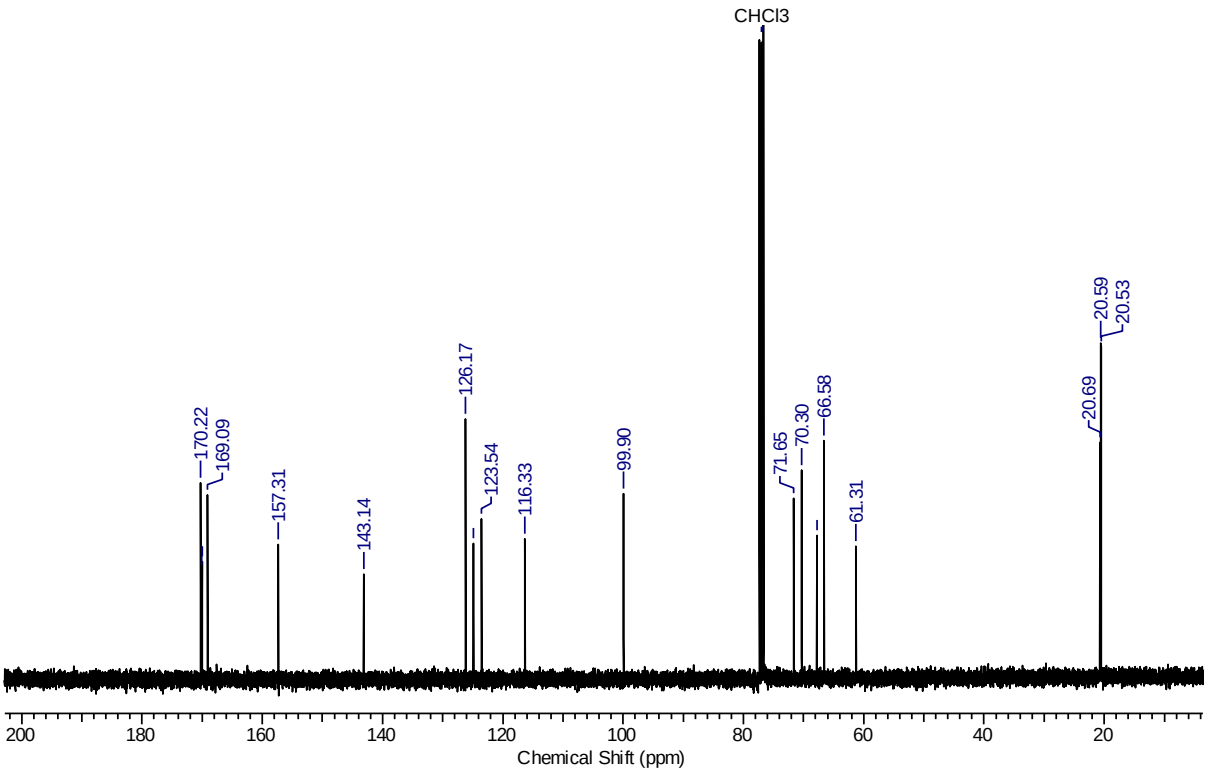


2-Chloro-4-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4k).

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

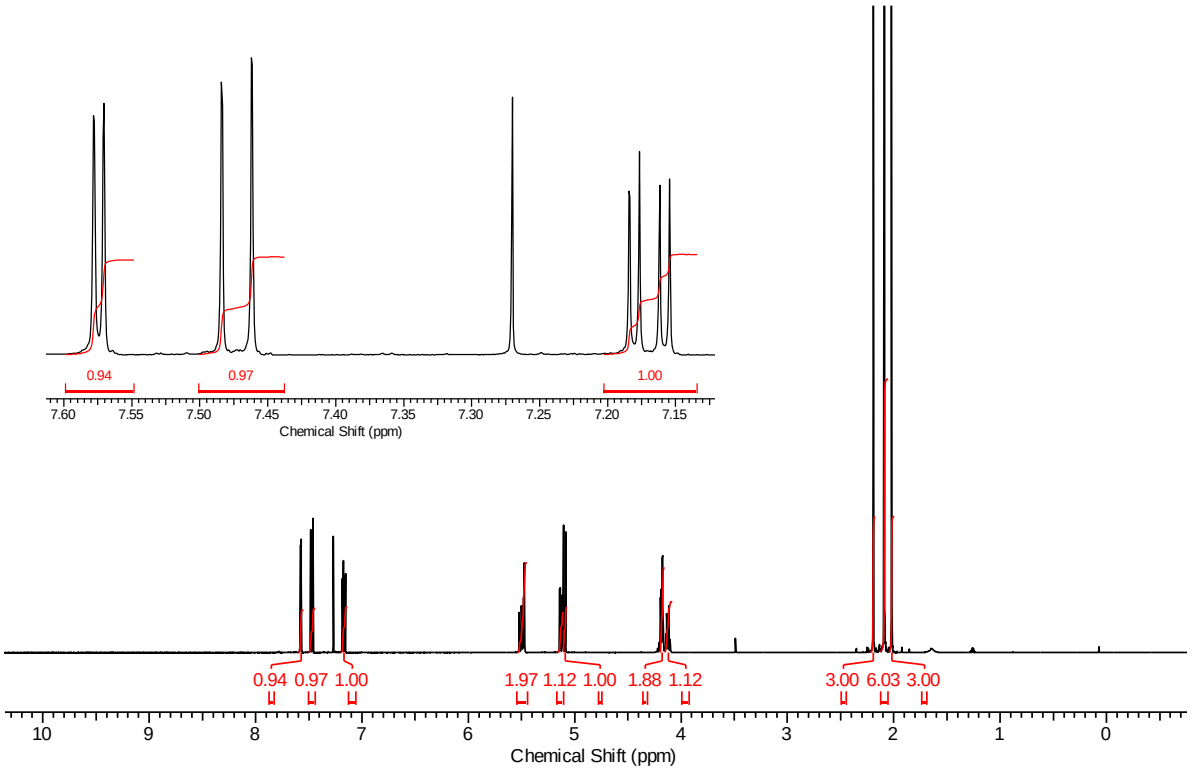


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

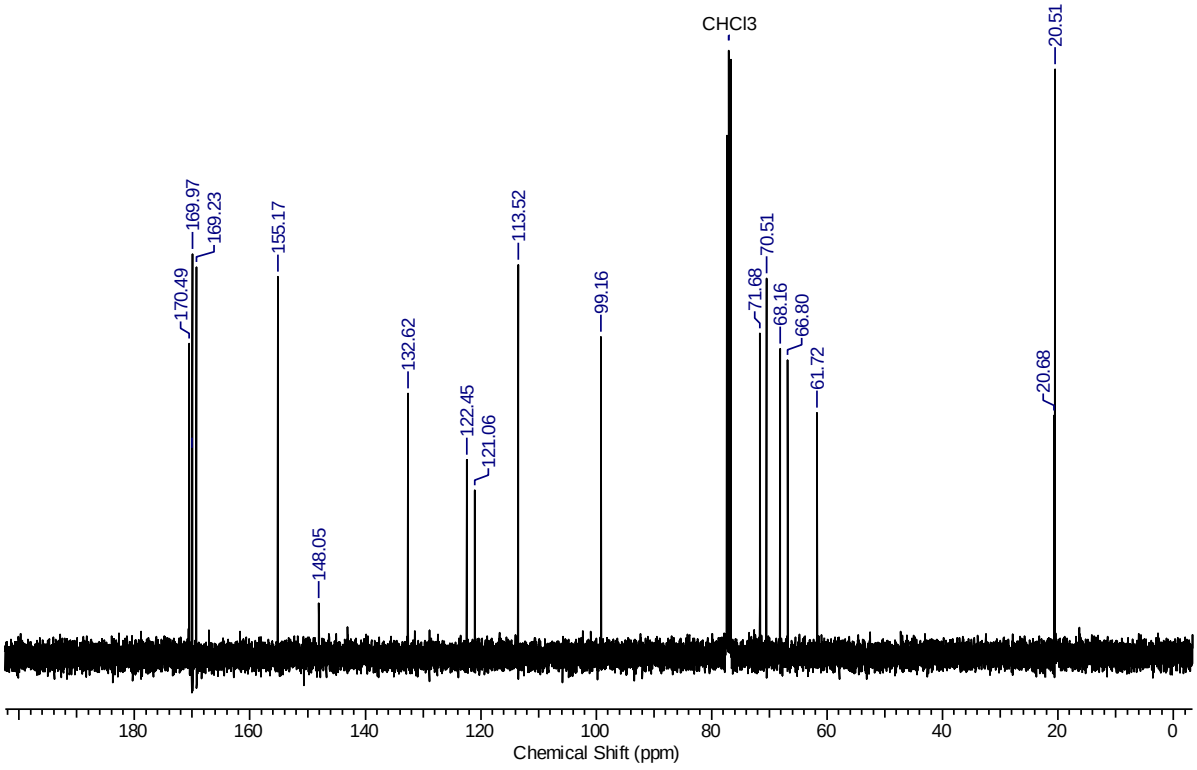


4-Chloro-3-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4m).

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

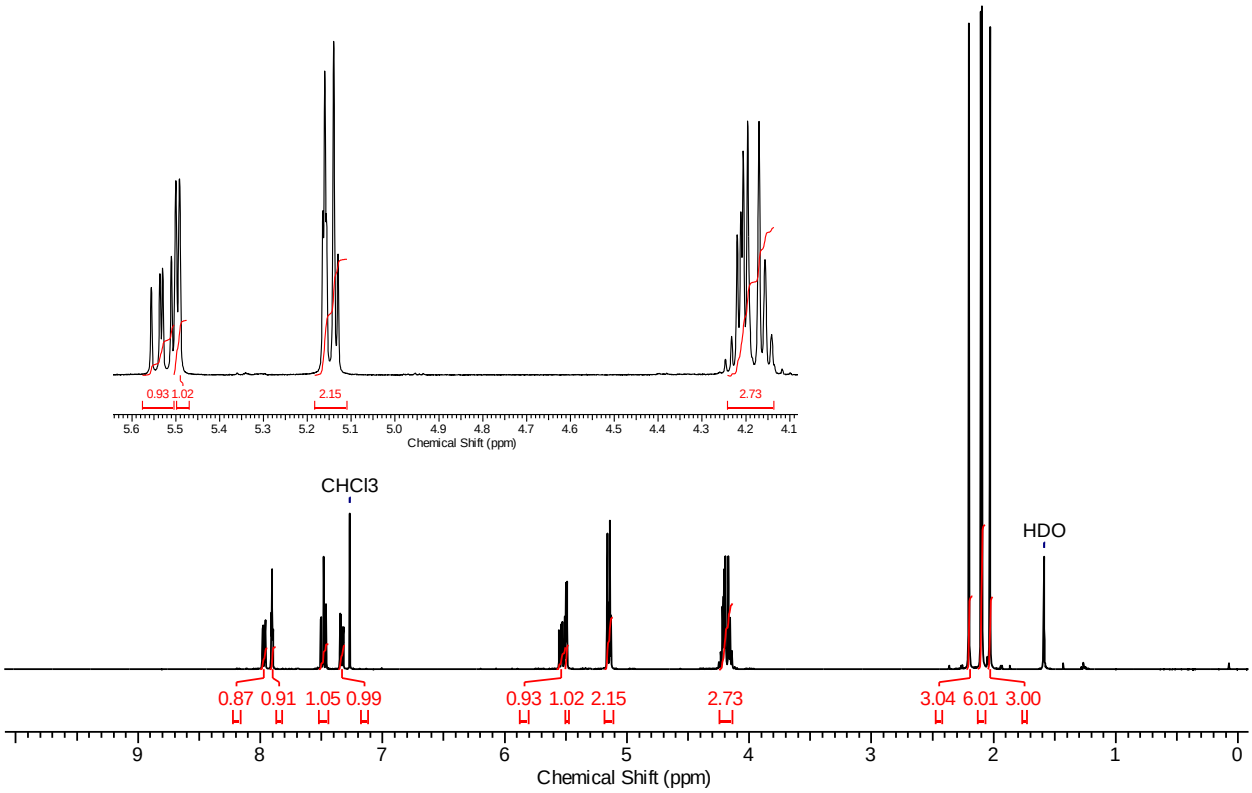


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

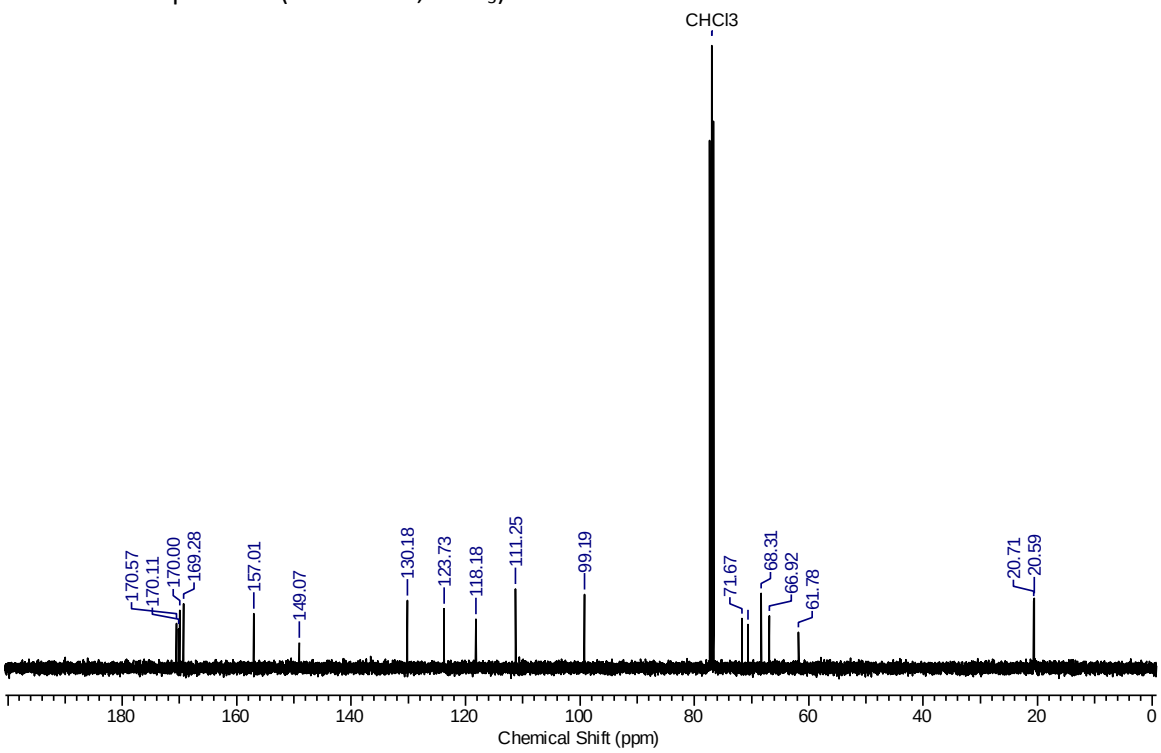


3-Nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4n).

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

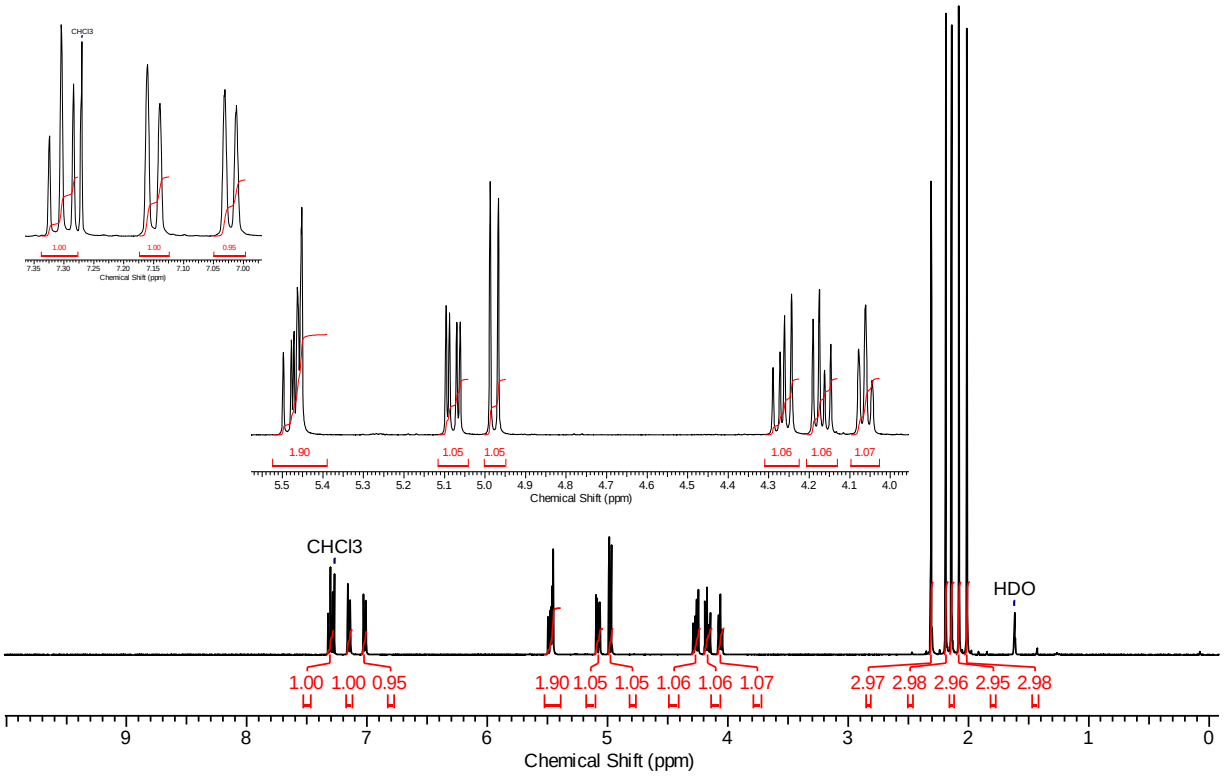


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

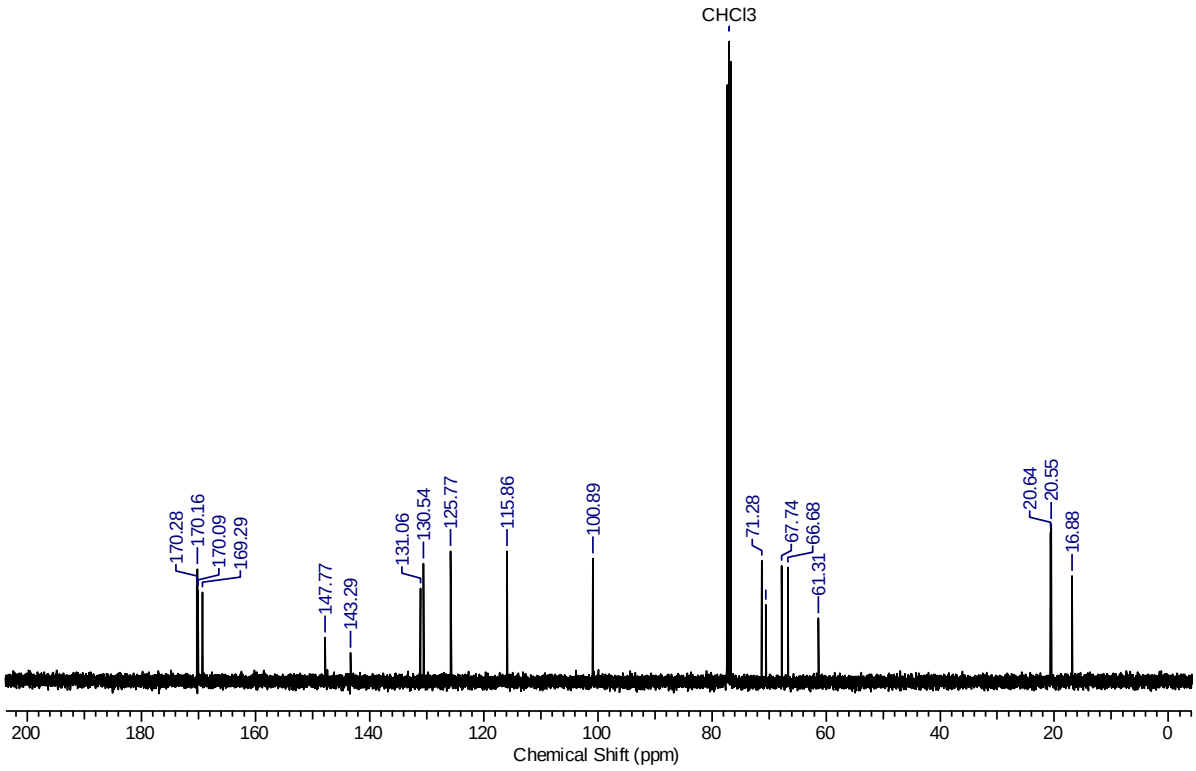


3-Methyl-2-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4o).

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

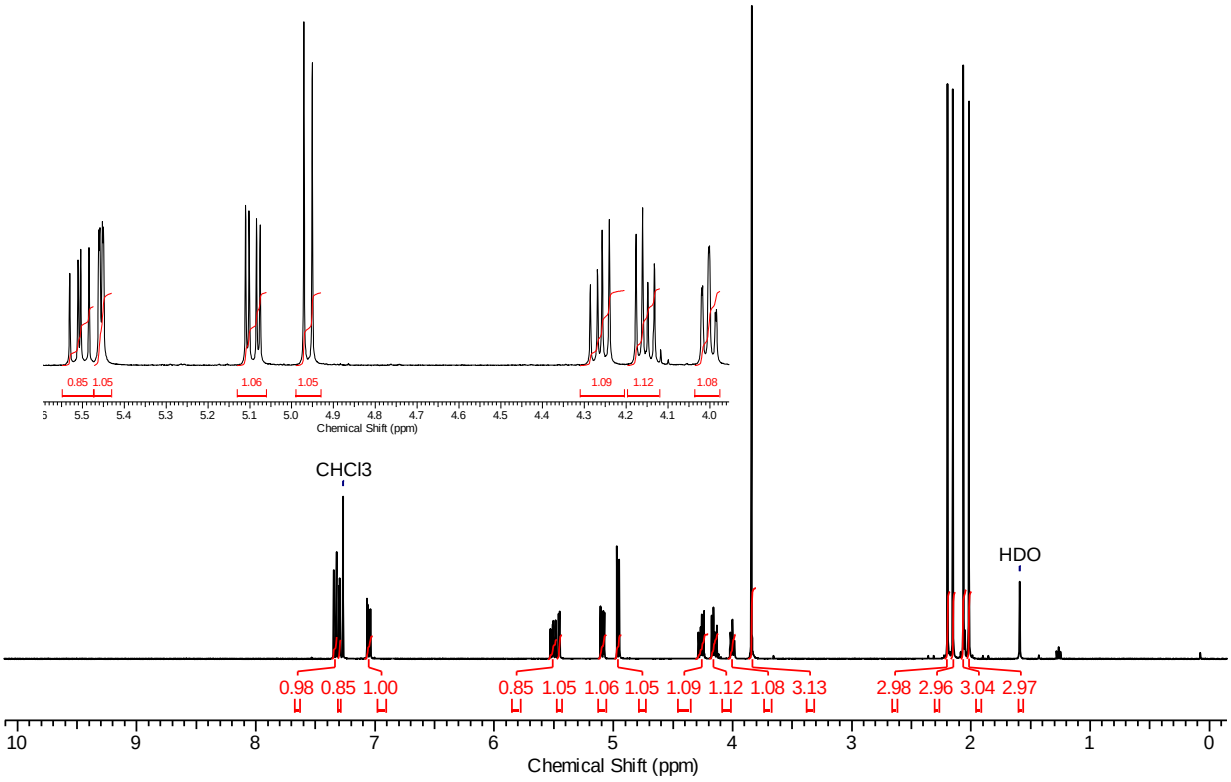


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

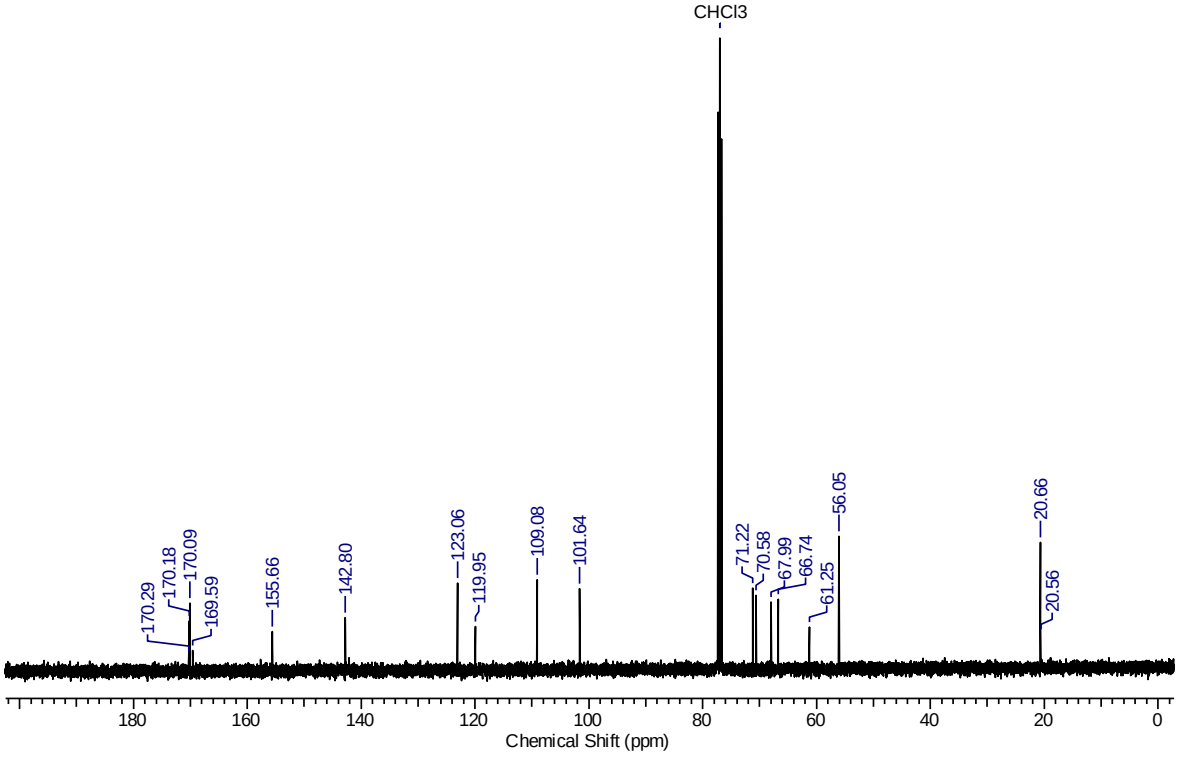


4-Methoxy-2-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4p).

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

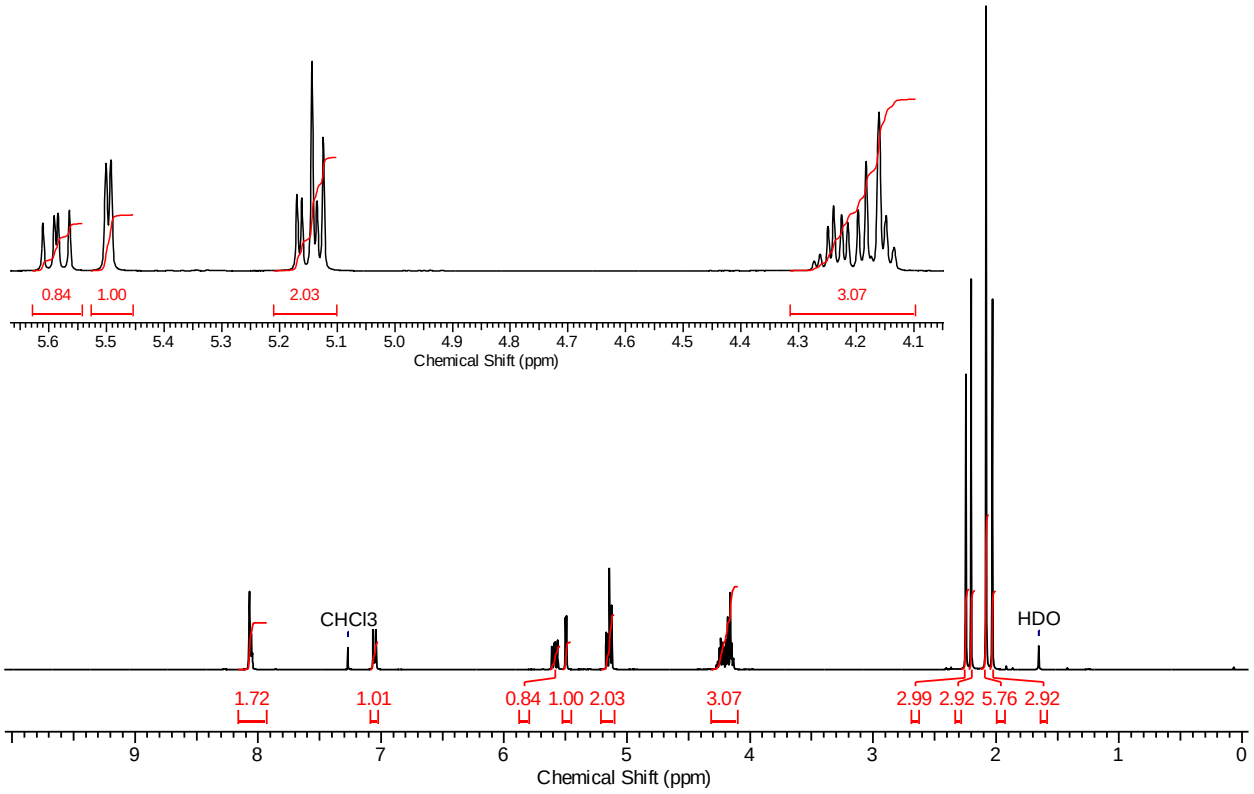


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)

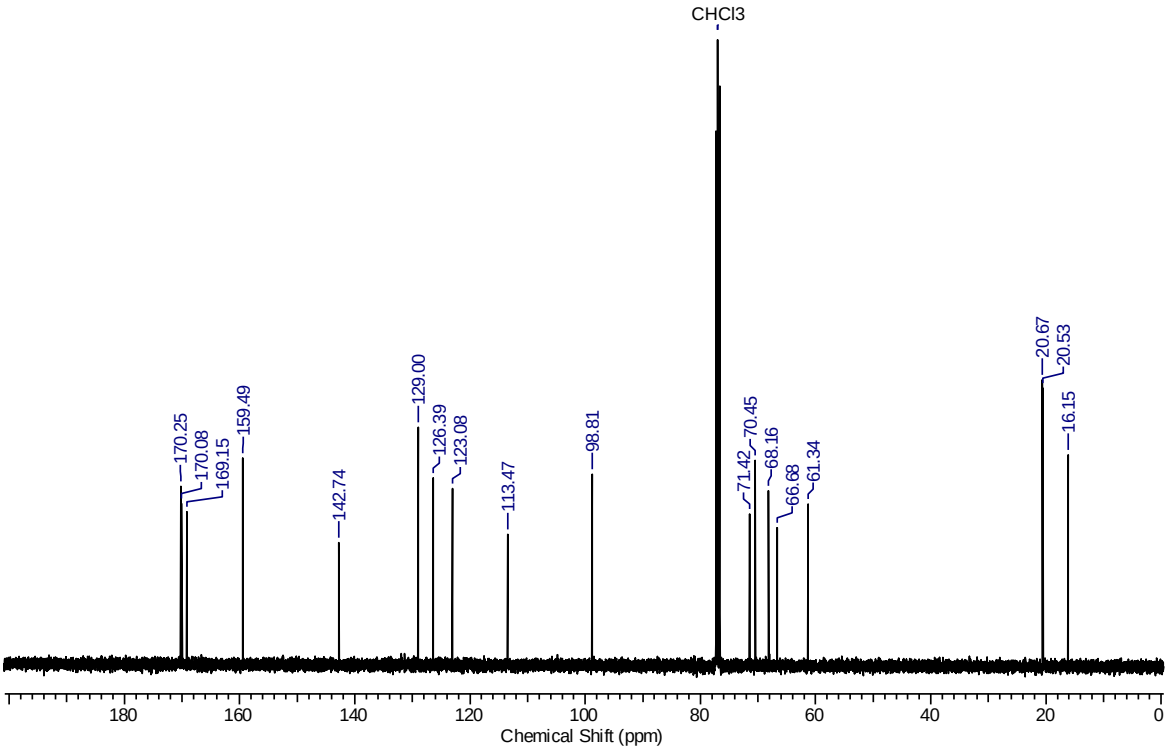


2-Methyl-4-nitrophenyl-tetra-*O*-acetyl-β-D-galactopyranoside (4q).

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

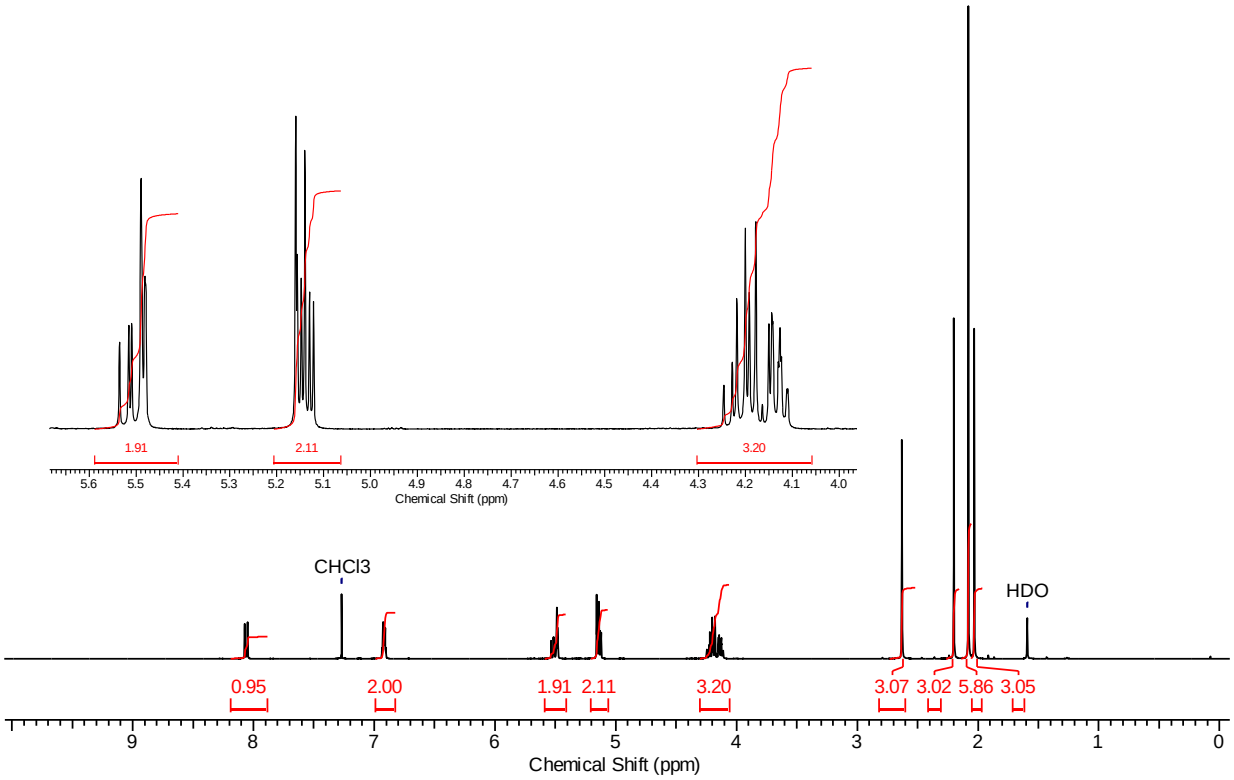


- ^{13}C NMR spectrum (100.6 MHz, $CDCl_3$)



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

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



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