# Synthesis of the enantiomers of XYLNAc and LYXNAc: comparison of β-*N*-acetyl hexosaminidase inhibition by the 8 stereoisomers of 2-*N*-acetylamino-1,2,4-trideoxy-1,4-iminopentitols

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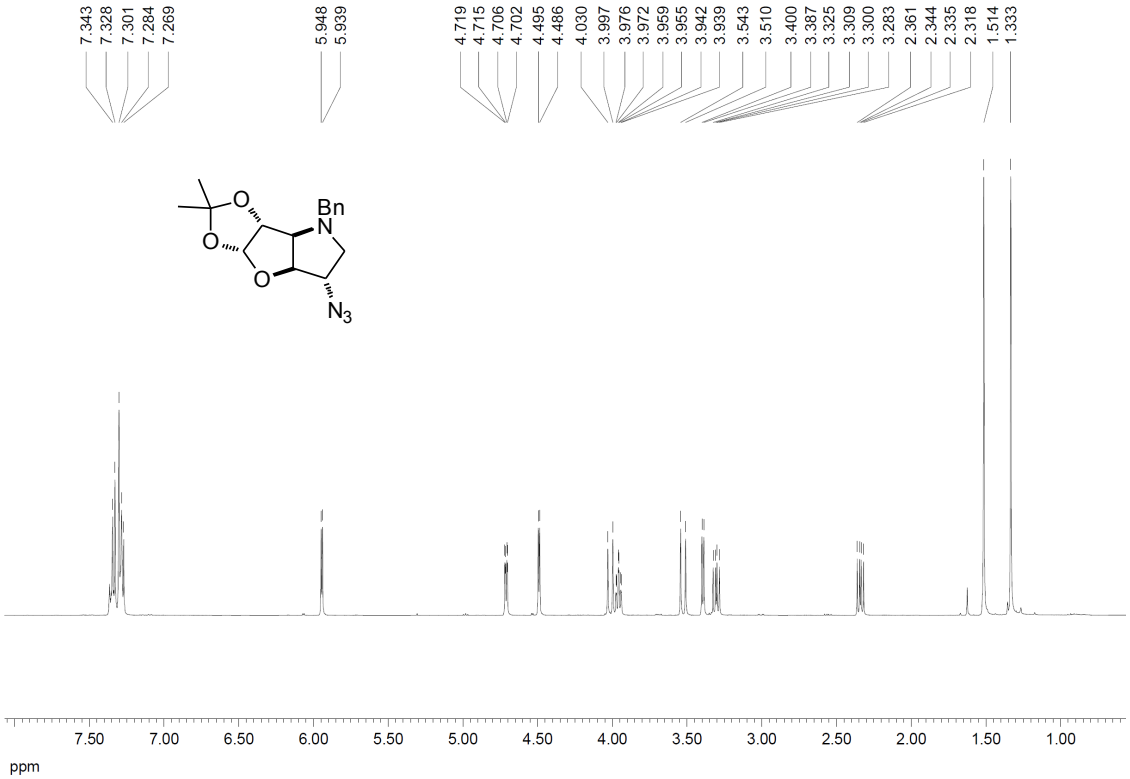
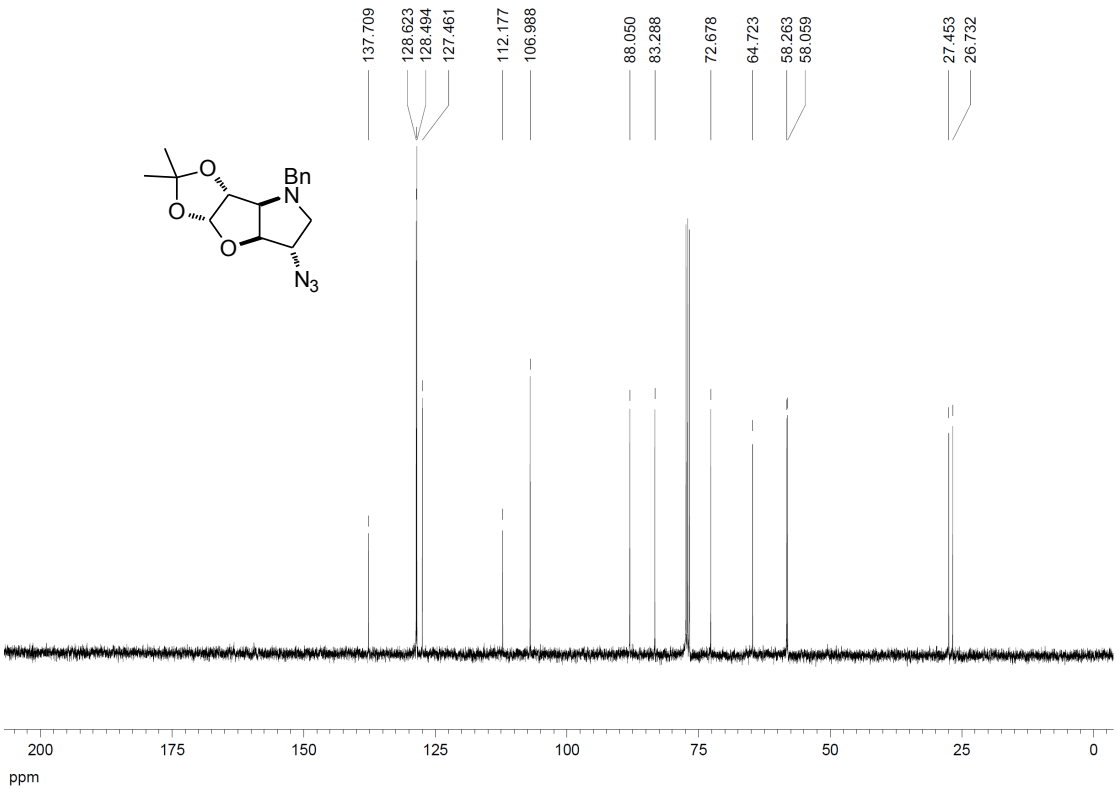
## Electronic Supplementary Information

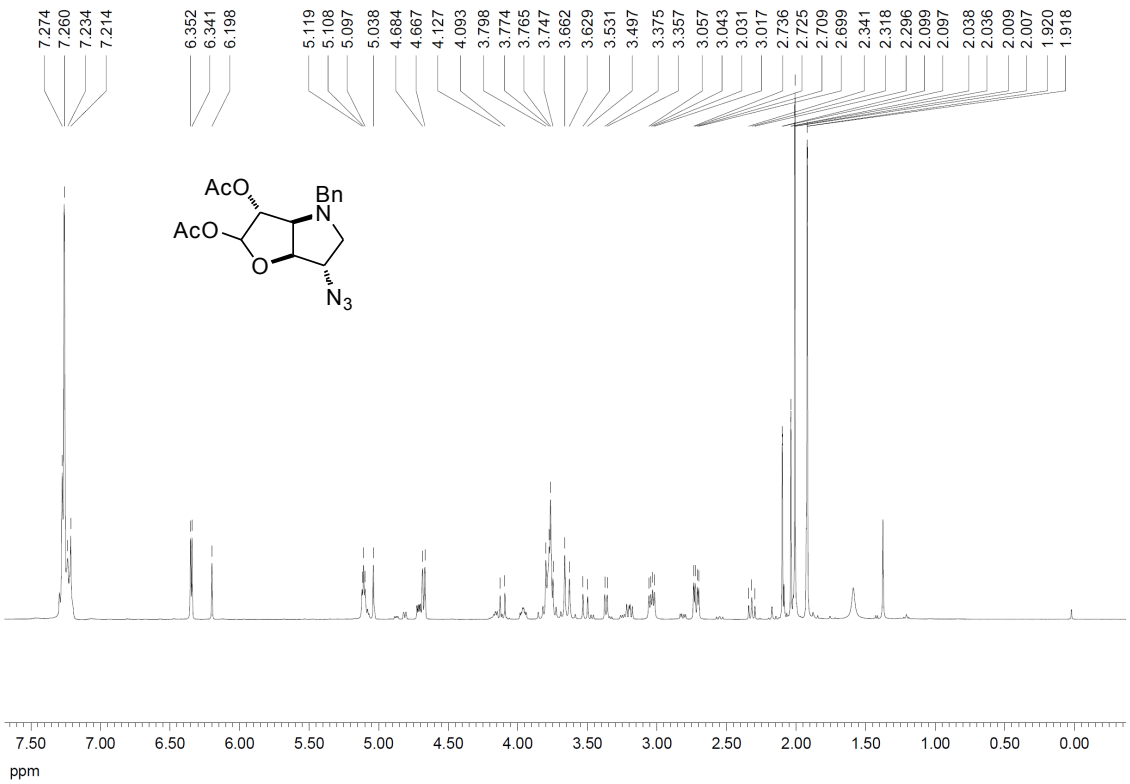
$^{1}$H NMR spectrum for **29L** (400 MHz, $CDCl_3$)



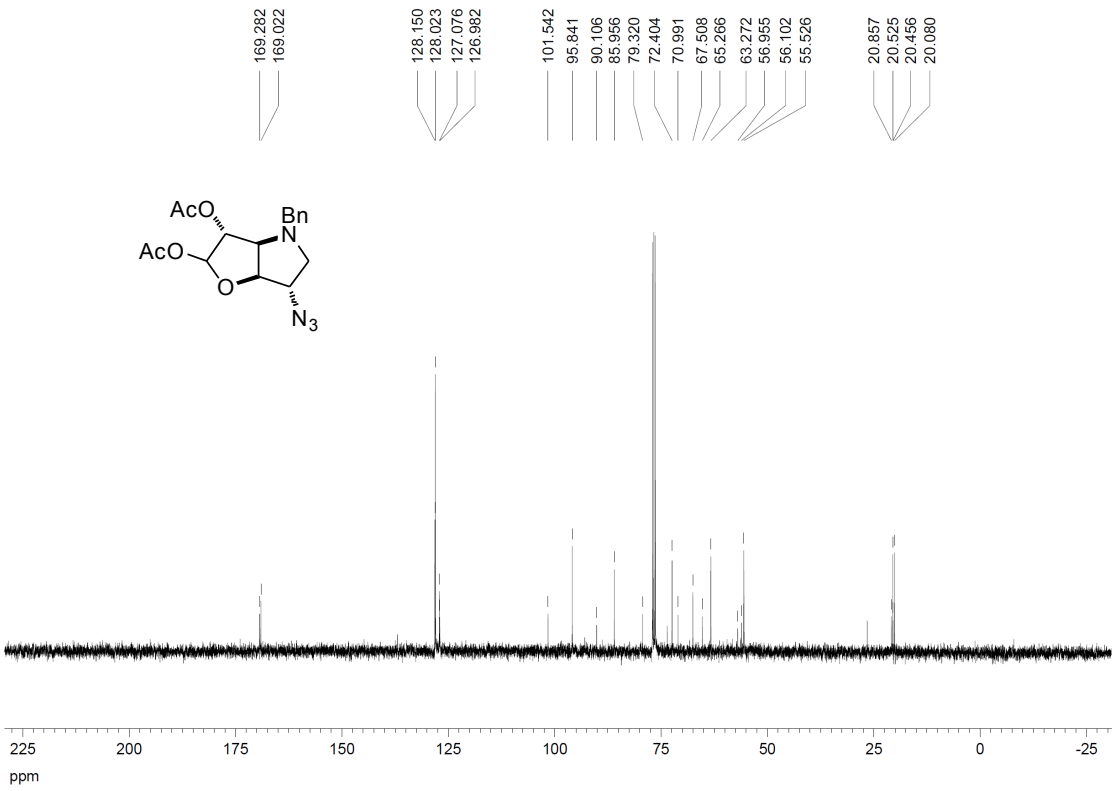

$^{13}$C NMR spectrum for **29L** (100 MHz, $CDCl_3$)



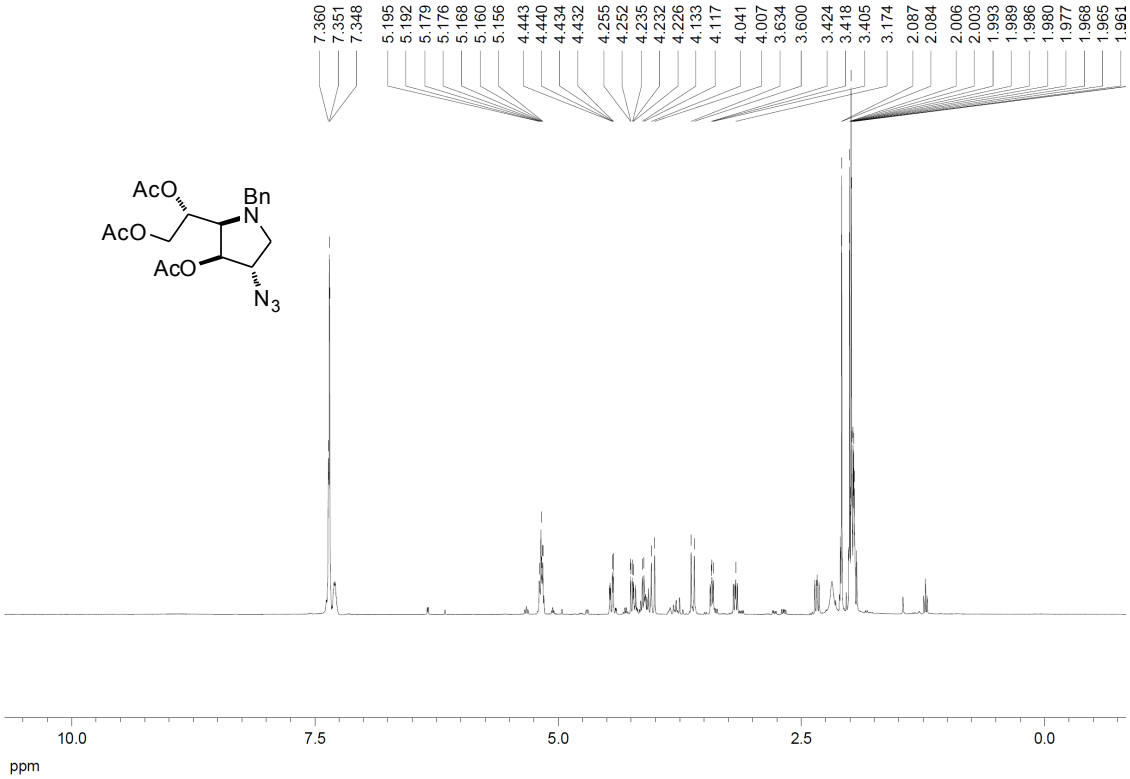
$^{1}$H NMR spectrum for **30L** (400 MHz, $CDCl_3$)



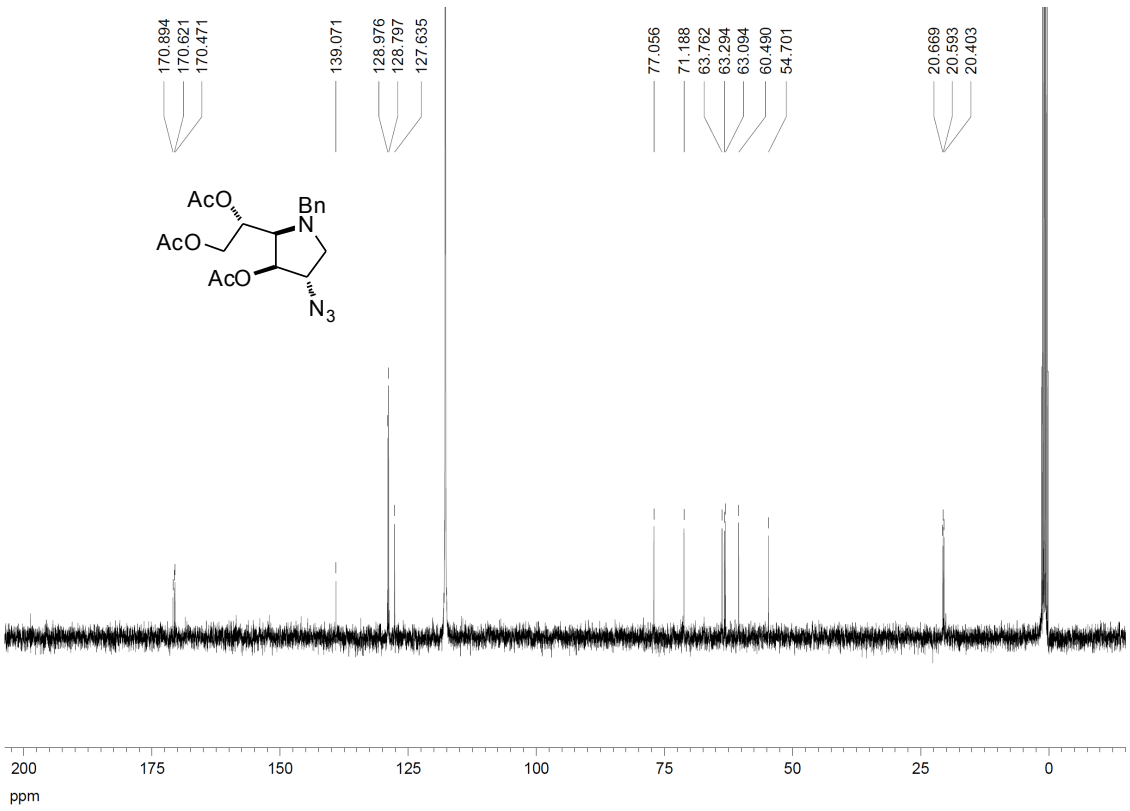

$^{13}$C NMR spectrum for **30L** (100 MHz, $CDCl_3$)



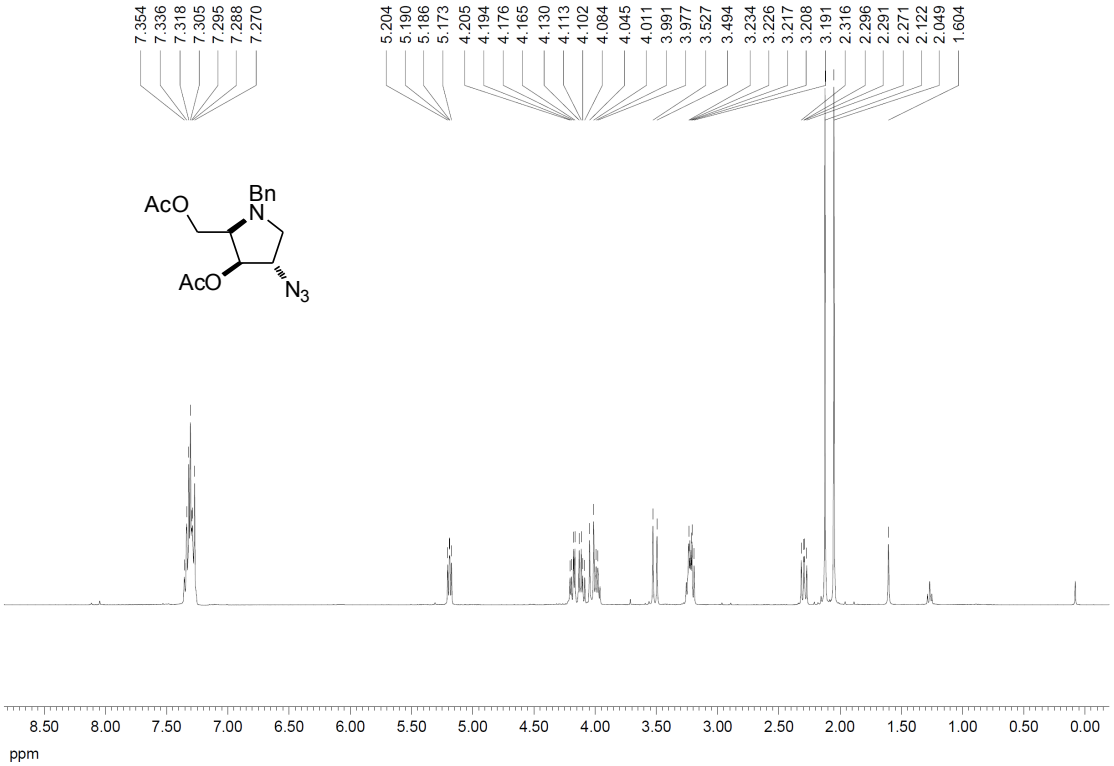
$^{1}$H NMR spectrum for **31L** (400 MHz, $CD_3CN$)



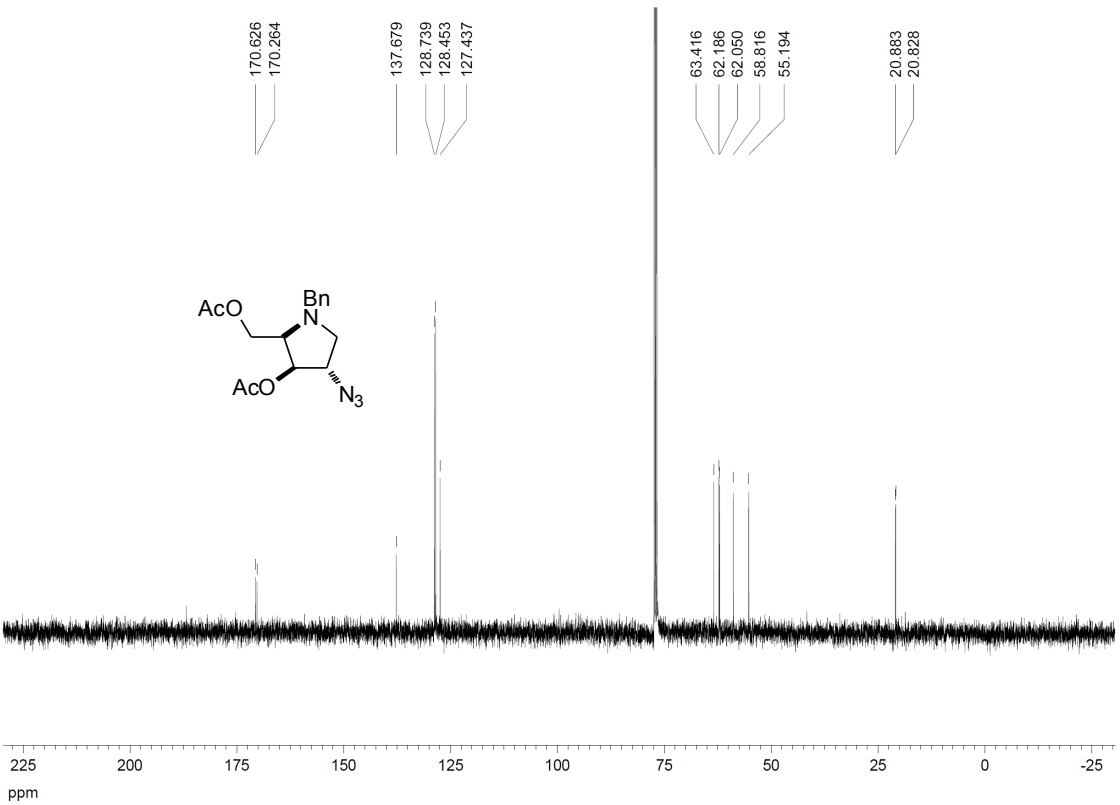

$^{13}$C NMR spectrum for **31L** (100 MHz, $CD_3CN$)



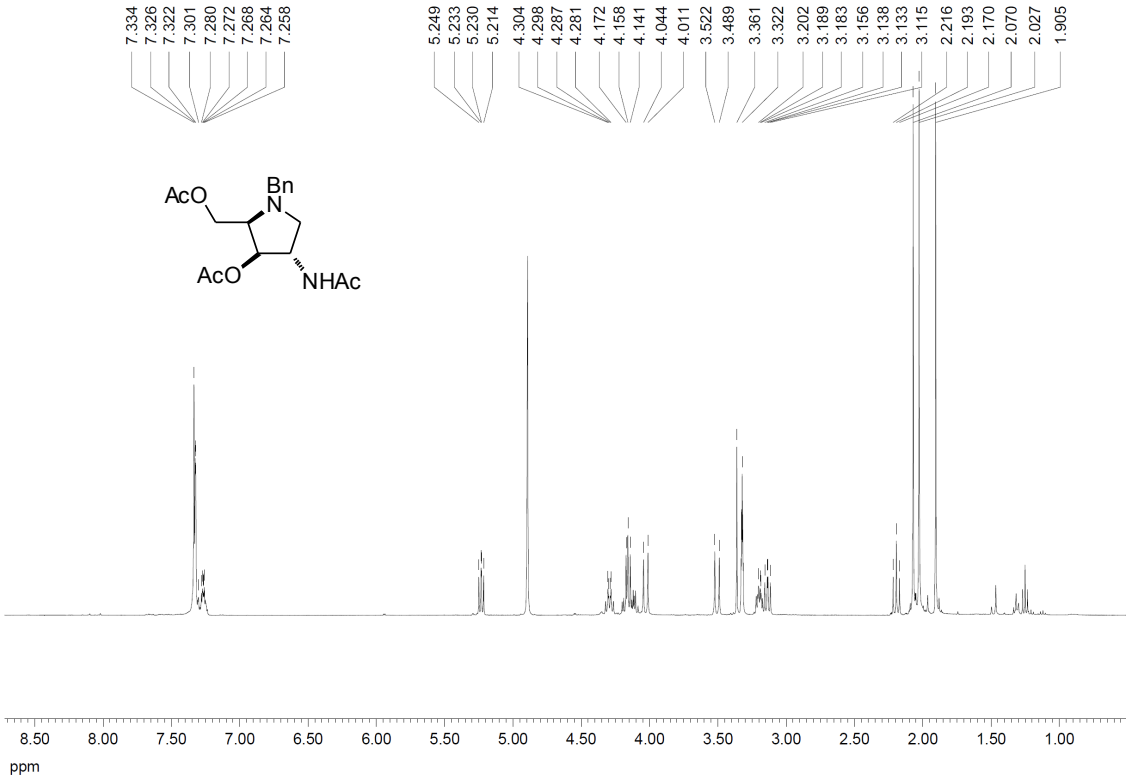
$^{1}$H NMR spectrum for **32D** (400 MHz, $CDCl_3$)



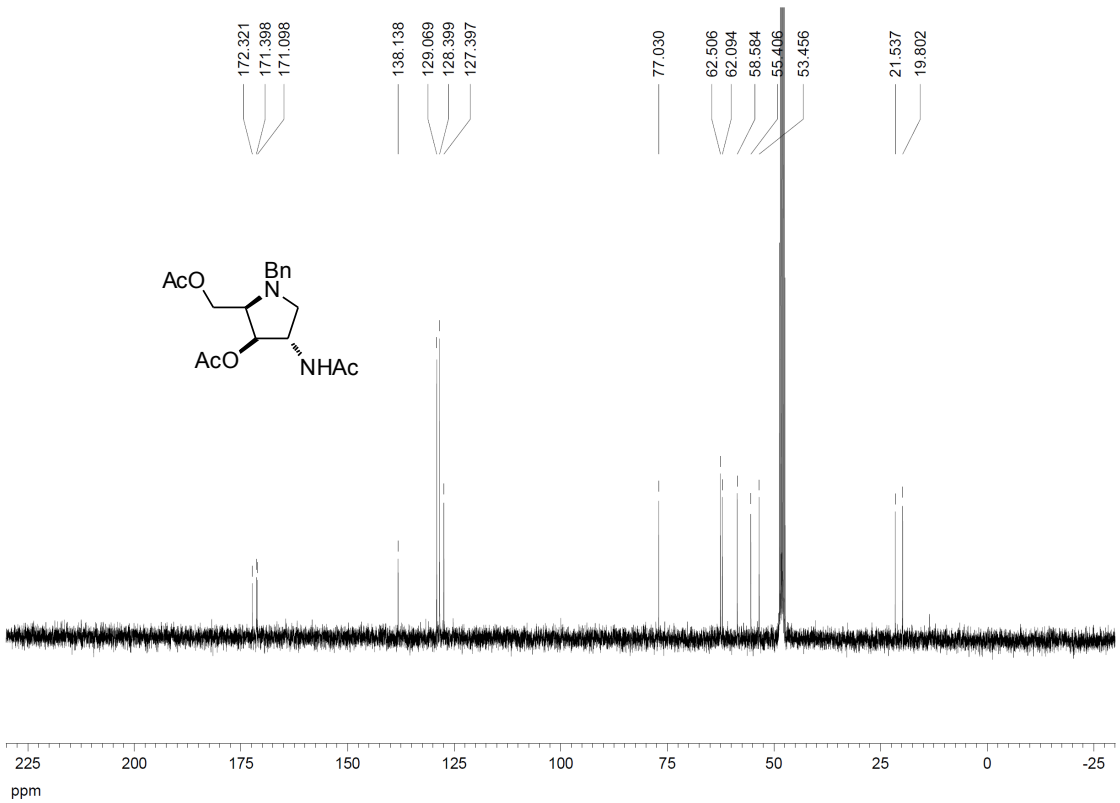

$^{13}$C NMR spectrum for **32D** (100 MHz, $CDCl_3$)



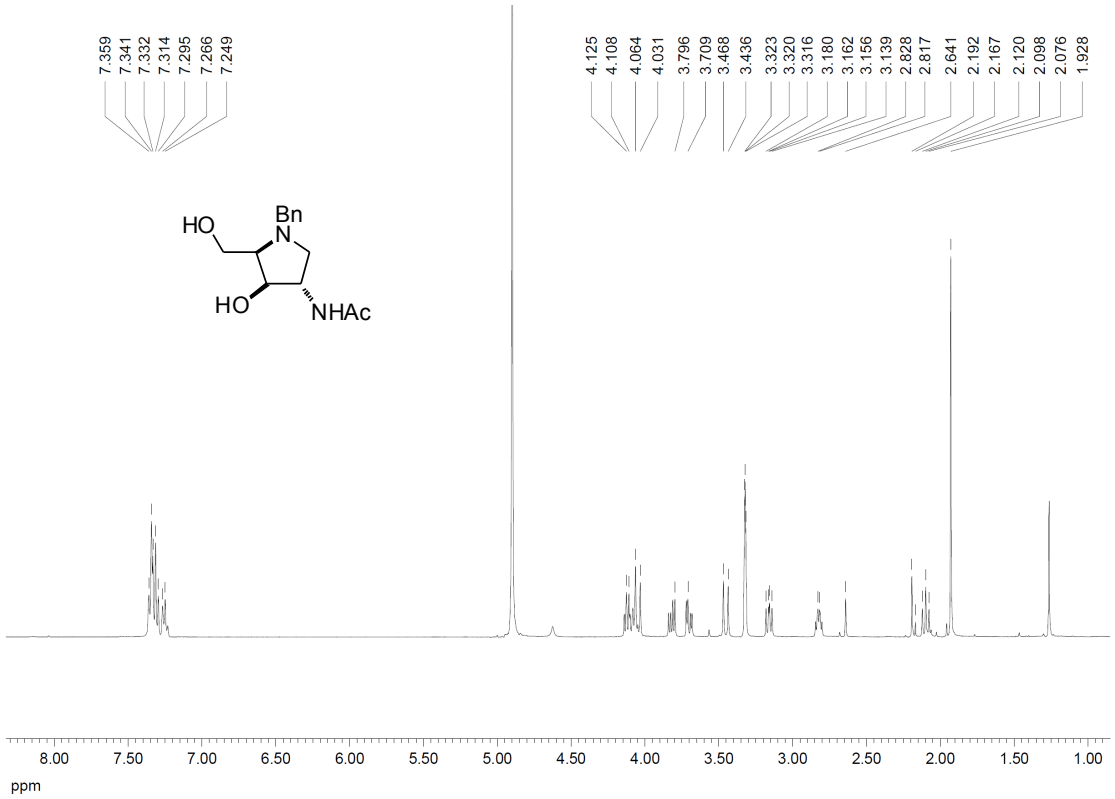
$^{1}$H NMR spectrum for **33D** (400 MHz, MeOD)



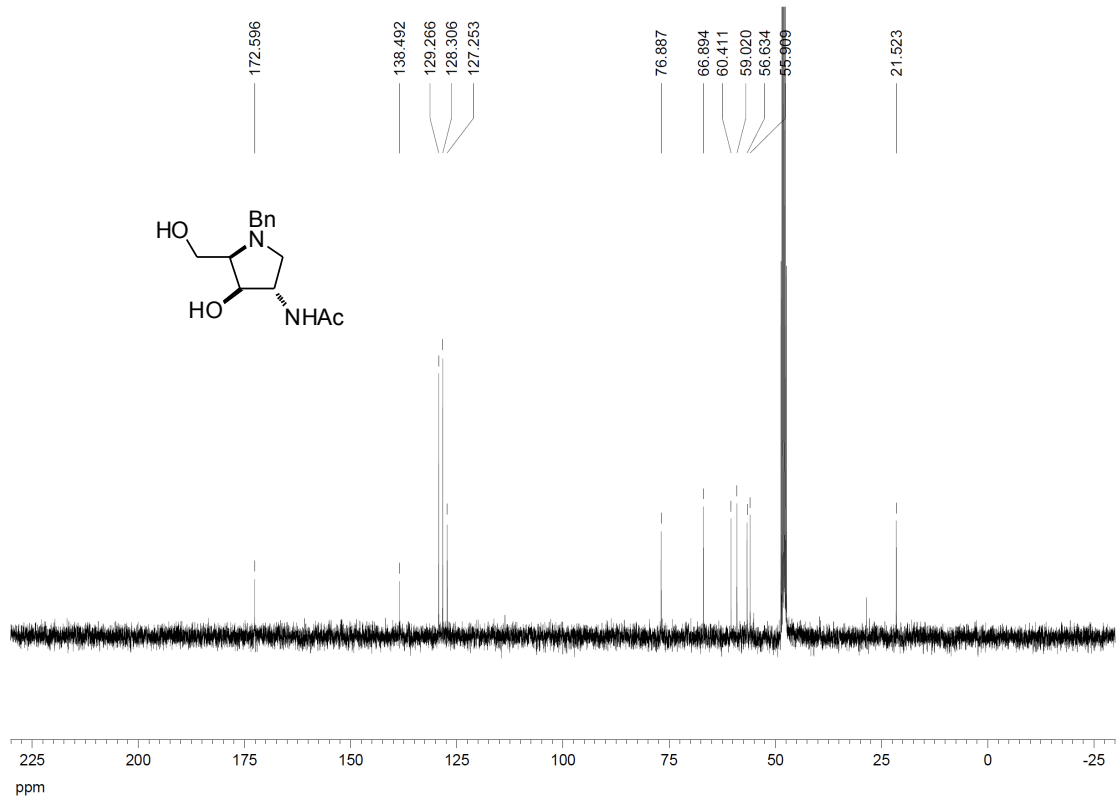

$^{13}$C NMR spectrum for **33D** (100 MHz, MeOD)



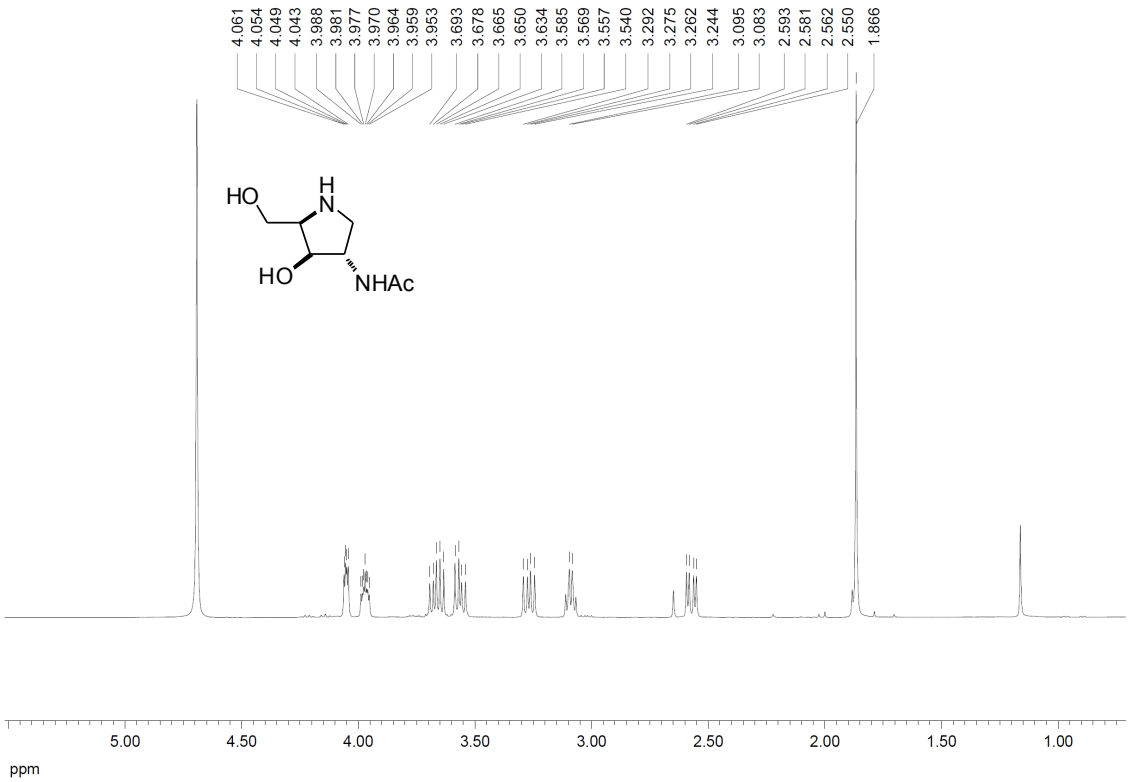
$^{1}$H NMR spectrum for **21D** (400 MHz, MeOD)



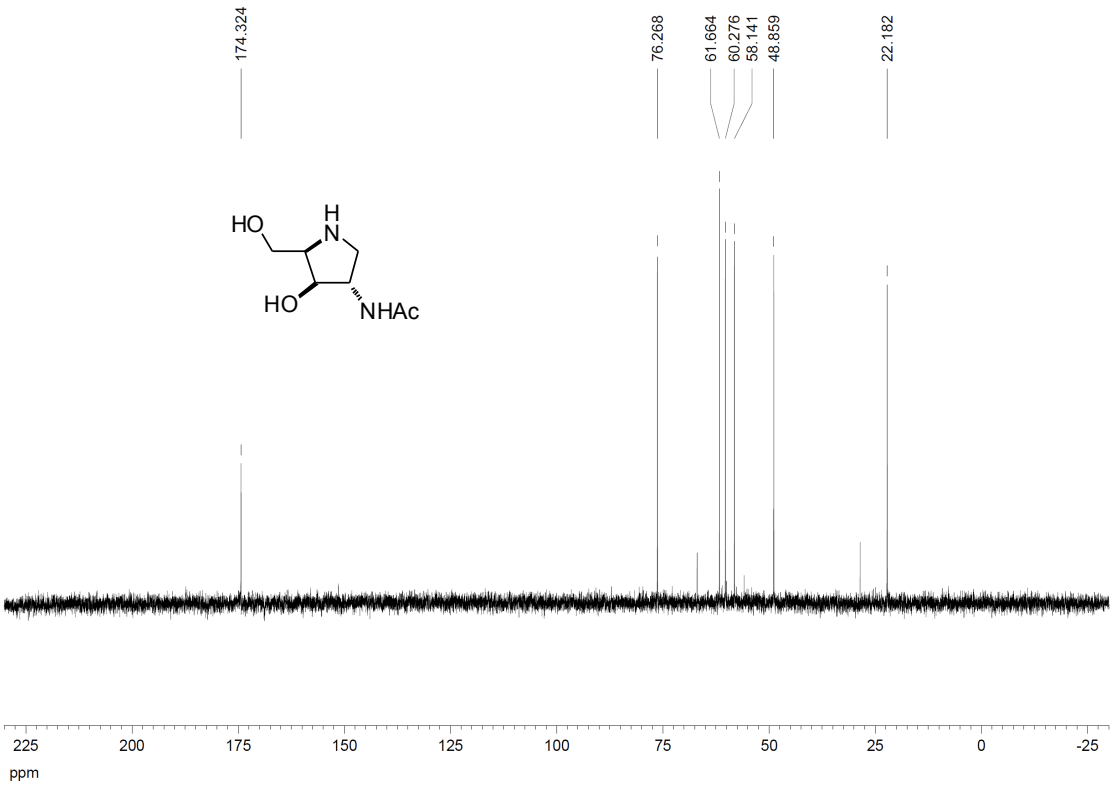

$^{13}$C NMR spectrum for **21D** (100 MHz, MeOD)



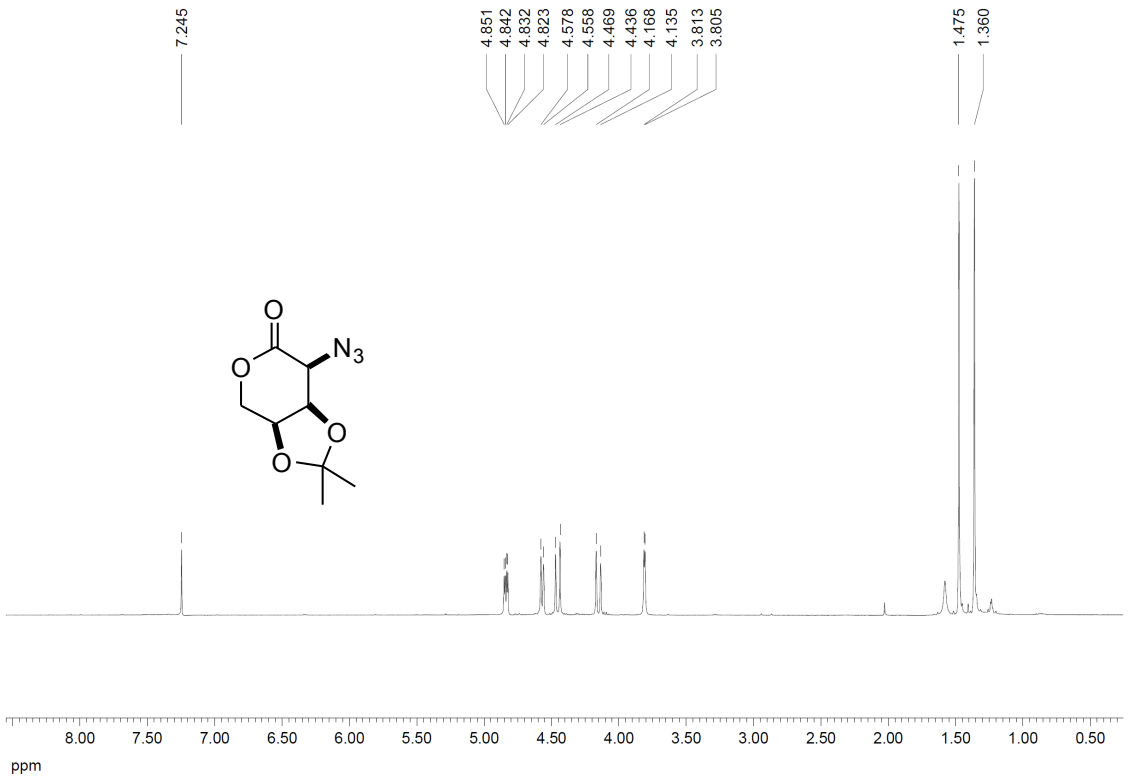
$^{1}$H NMR spectrum for **20D** (400 MHz, $D_2O$)



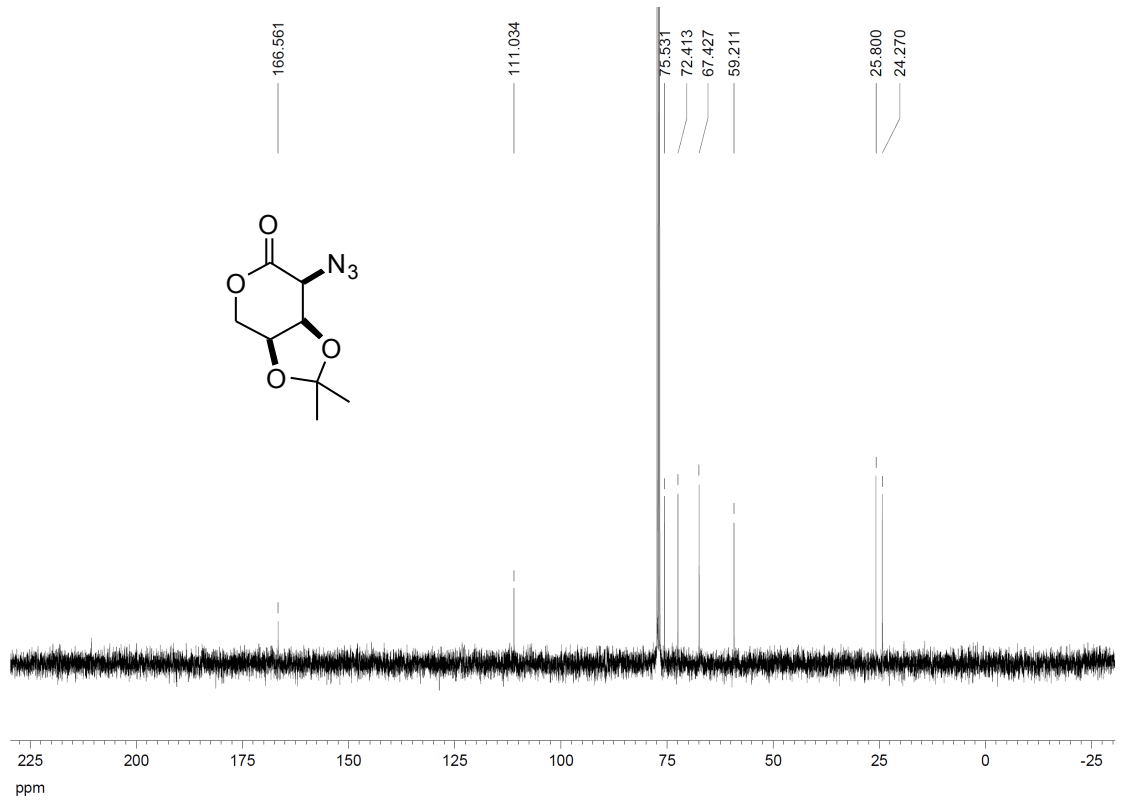

$^{13}$C NMR spectrum for **20D** (100 MHz, $D_2O$)



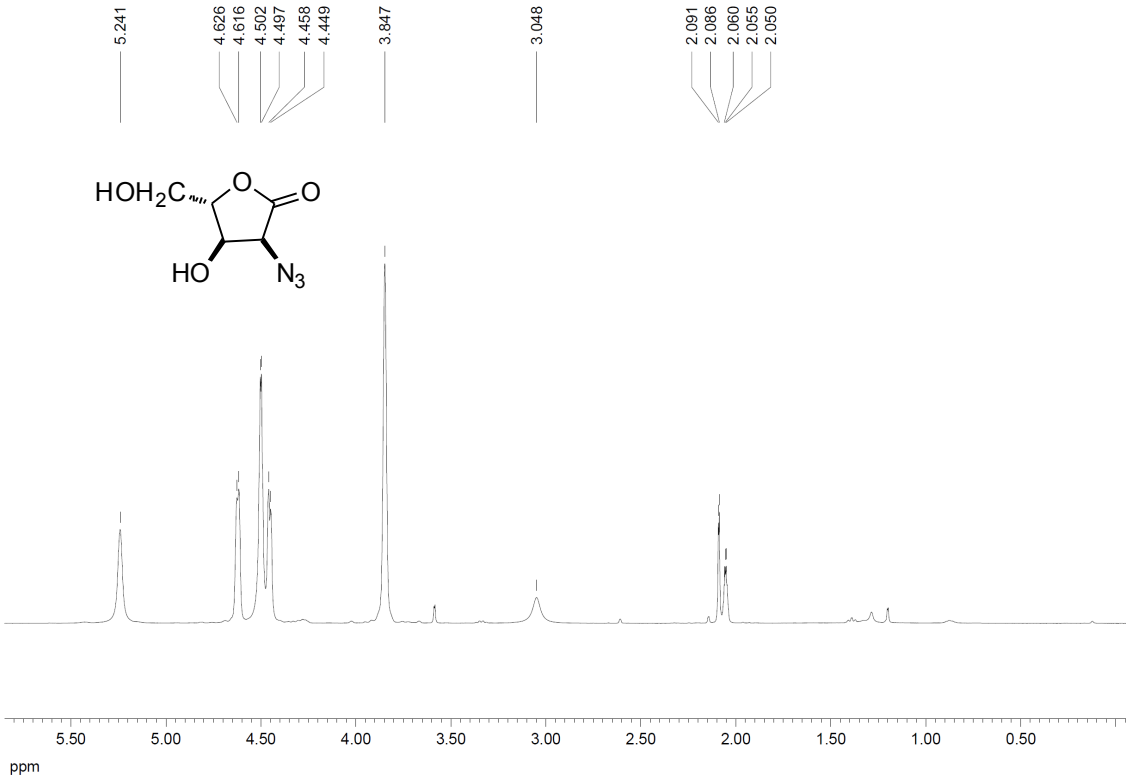
$^{1}$H NMR spectrum for **40L** (400 MHz, $CDCl_3$)



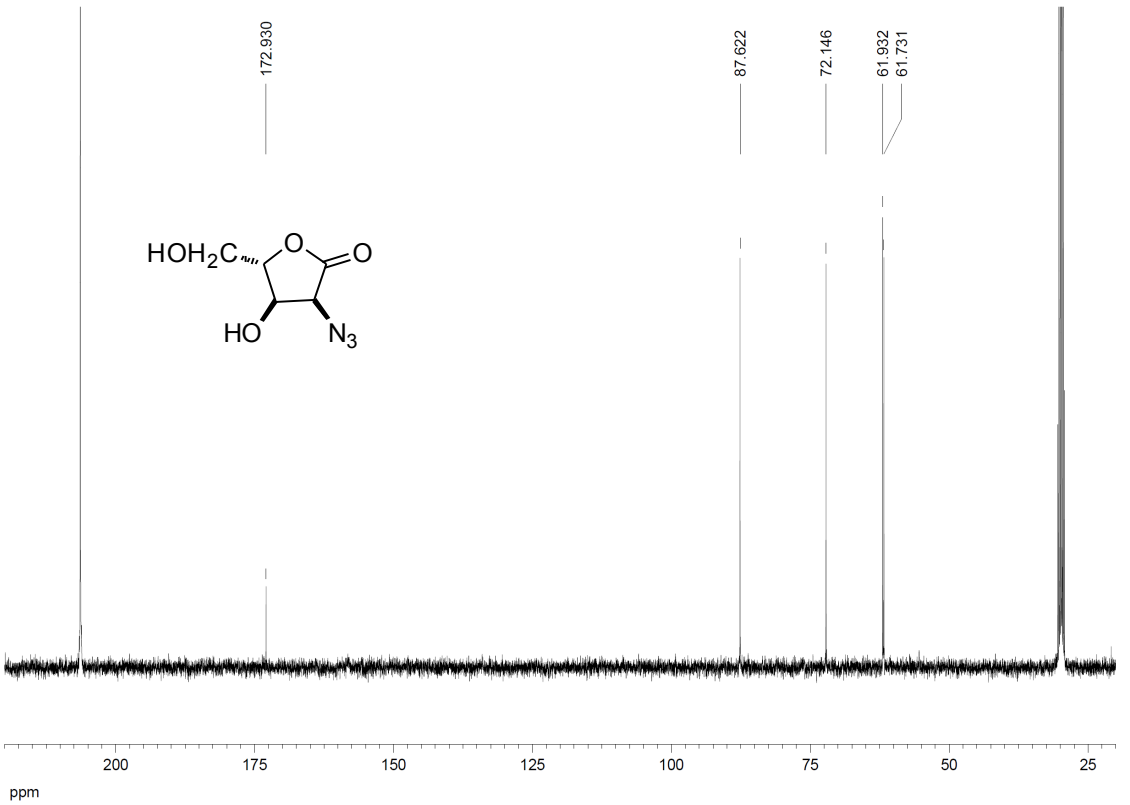

$^{13}$C NMR spectrum for **40L** (100 MHz, $CDCl_3$)



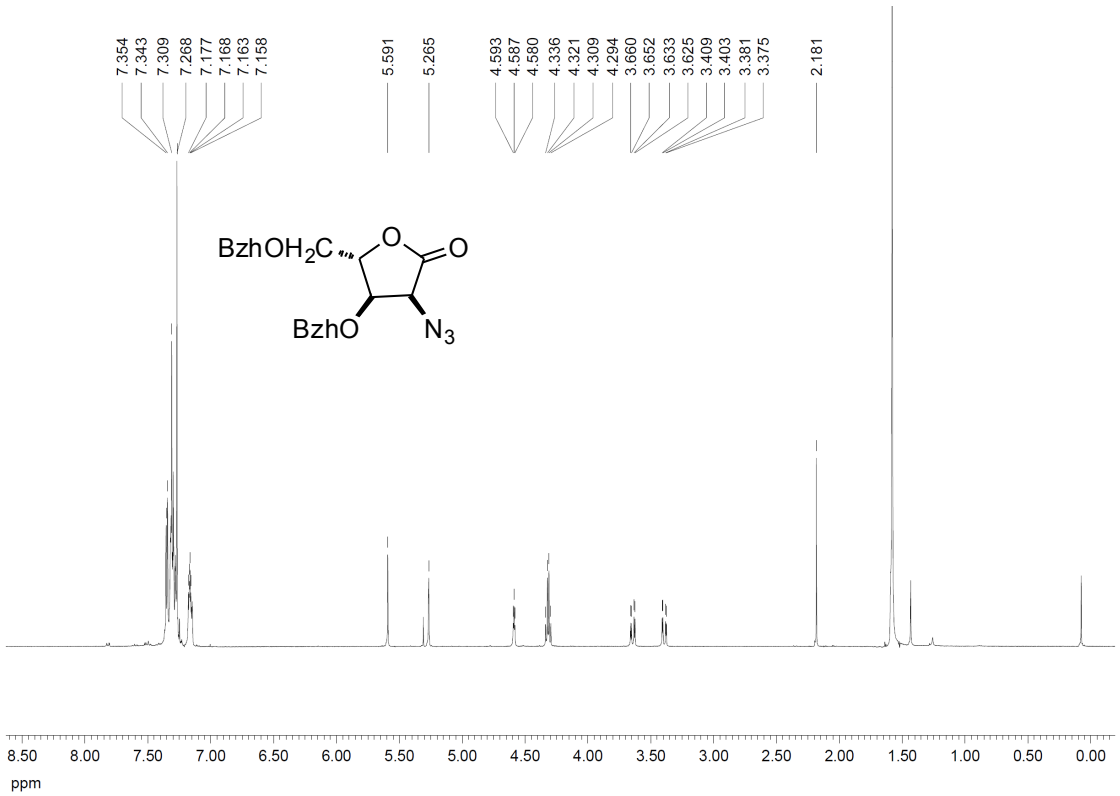
$^{1}$H NMR spectrum for **36L** (400 MHz, $(CD_3)_2CO$)



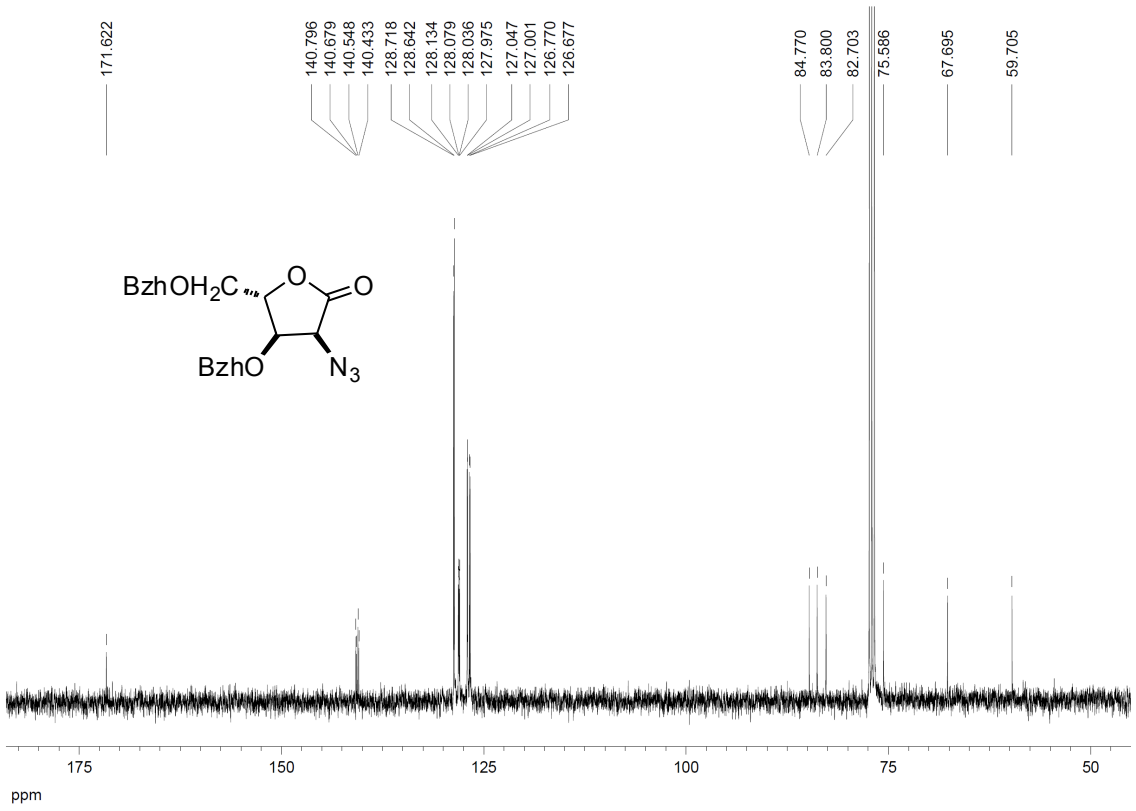

$^{13}$C NMR spectrum for **36L** (100 MHz, $(CD_3)_2CO$)



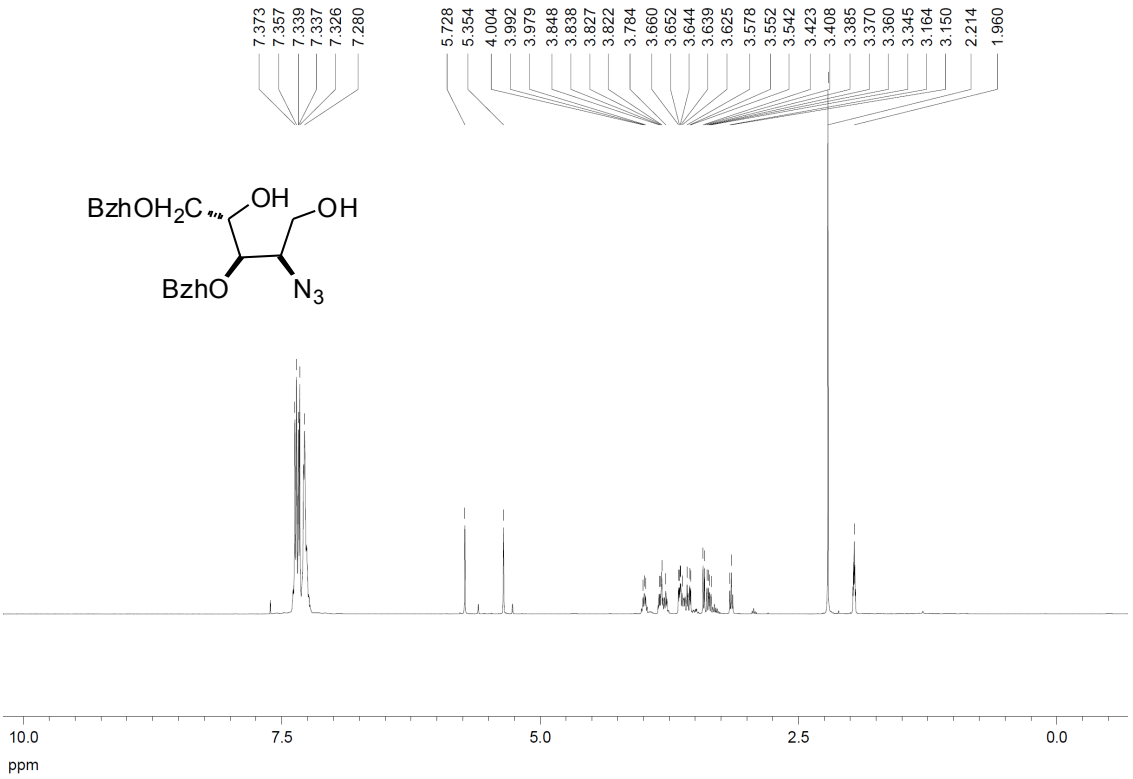
$^{1}$H NMR spectrum for **41L** (400 MHz, $CDCl_3$)



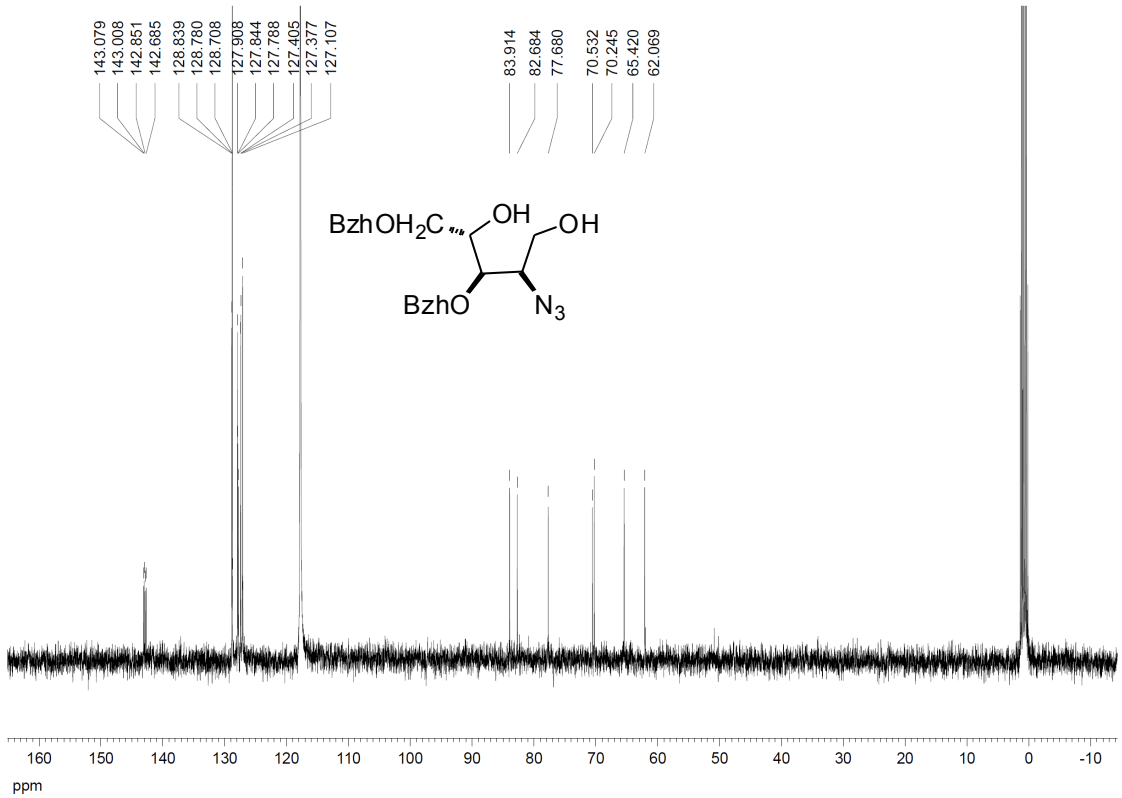

$^{13}$C NMR spectrum for **41L** (100 MHz, $CDCl_3$)



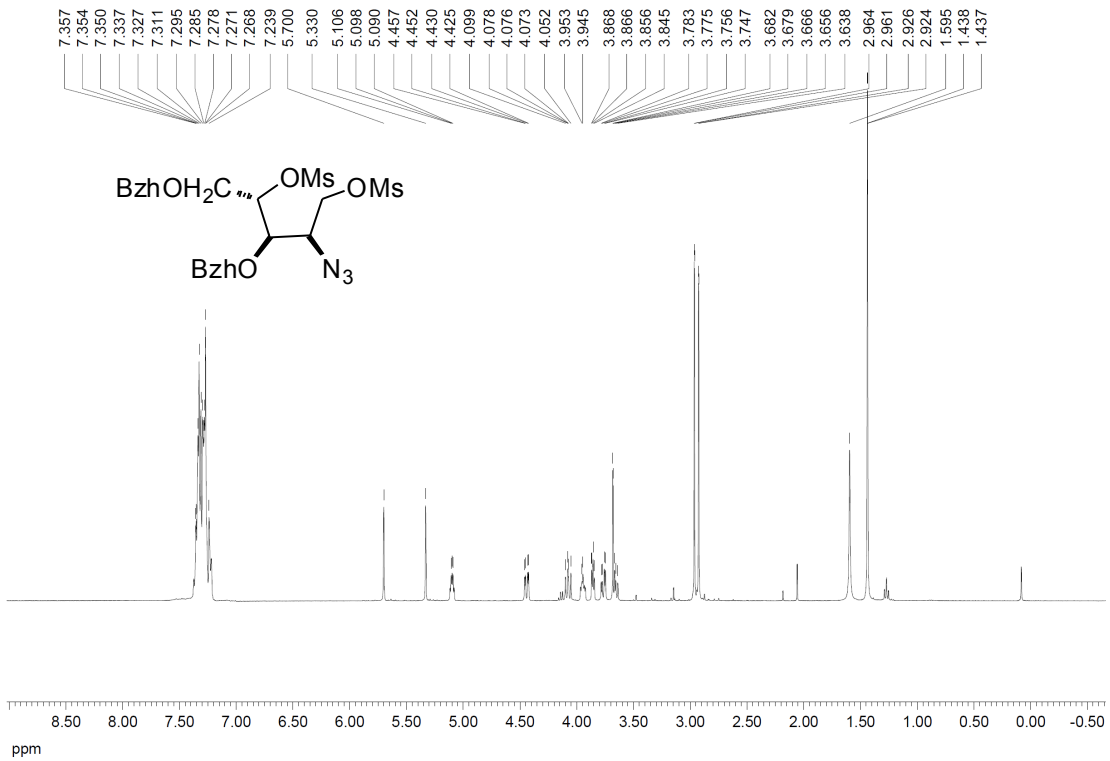
$^{1}$H NMR spectrum for **42L** (400 MHz, $CD_3CN$)



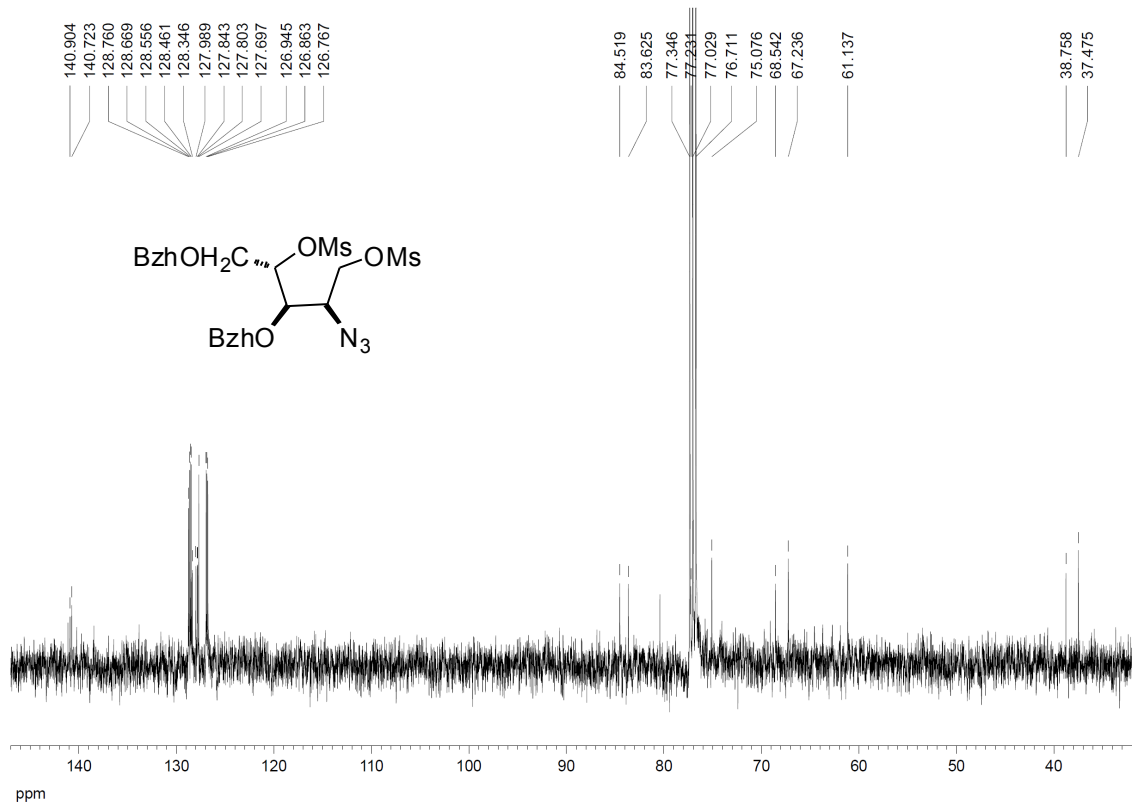

$^{13}$C NMR spectrum for **42L** (100 MHz, $CD_3CN$)



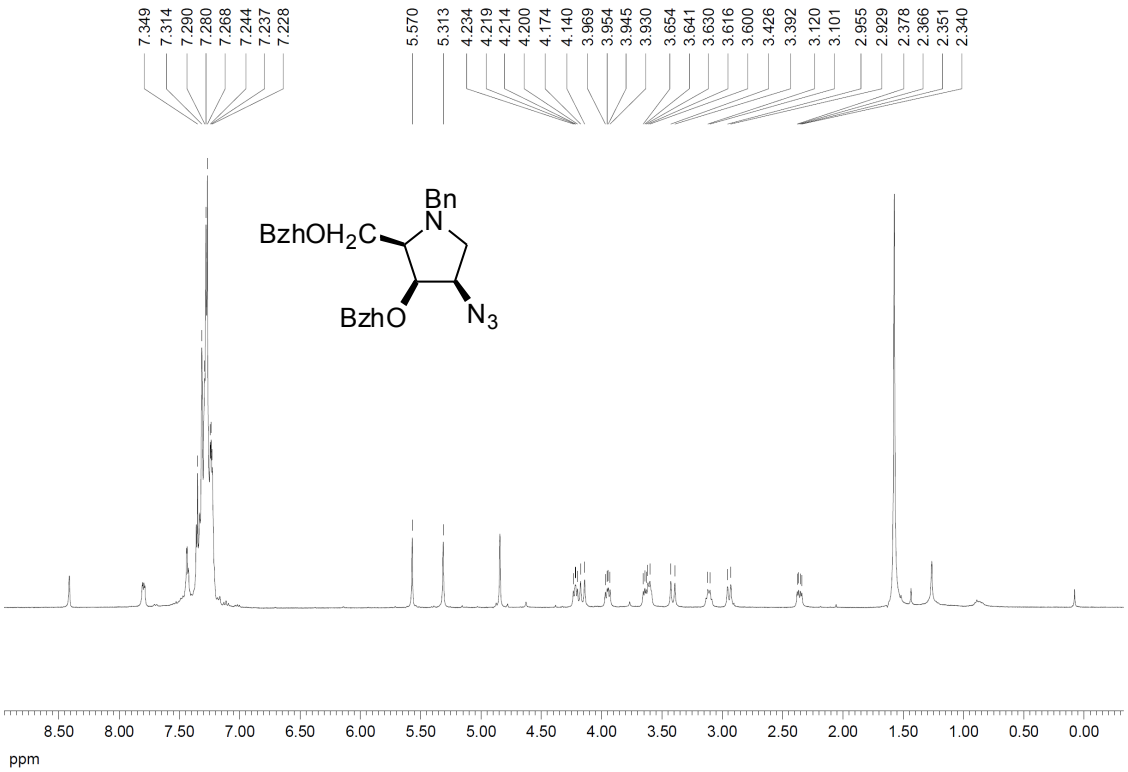
$^{1}$H NMR spectrum for **43L** (400 MHz, $CDCl_3$)



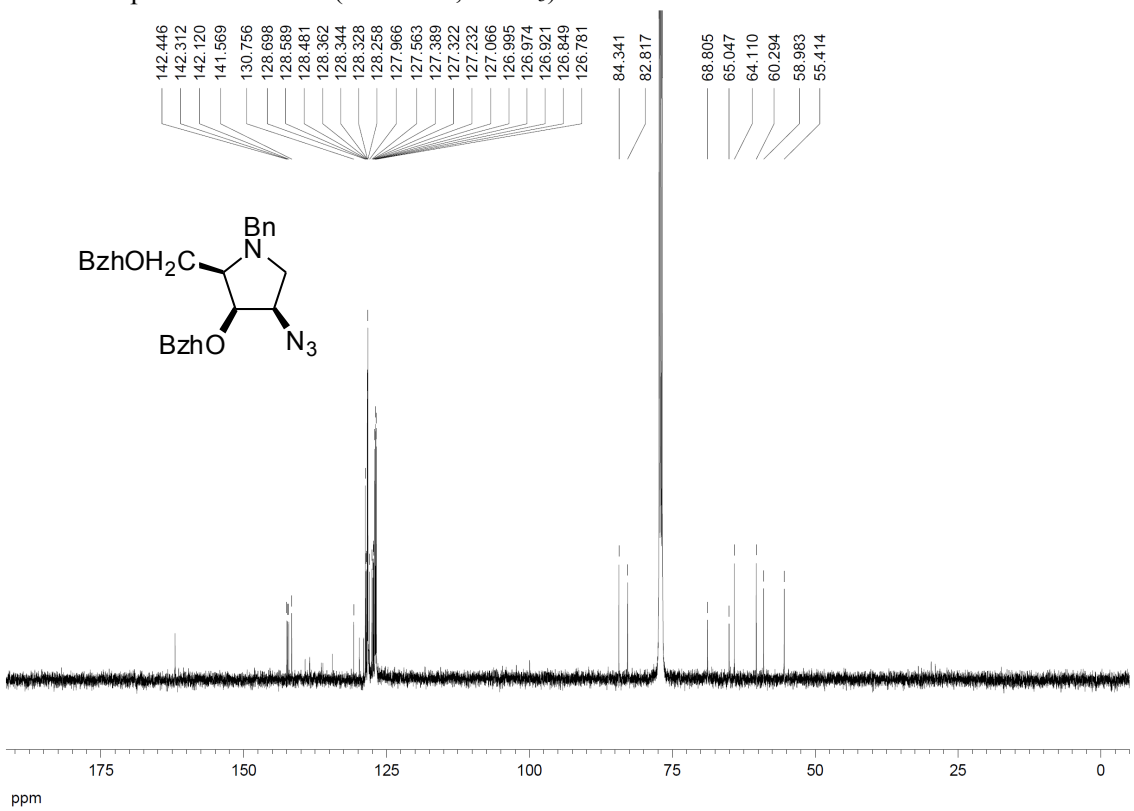

$^{13}$C NMR spectrum for **43L** (100 MHz, $CDCl_3$)



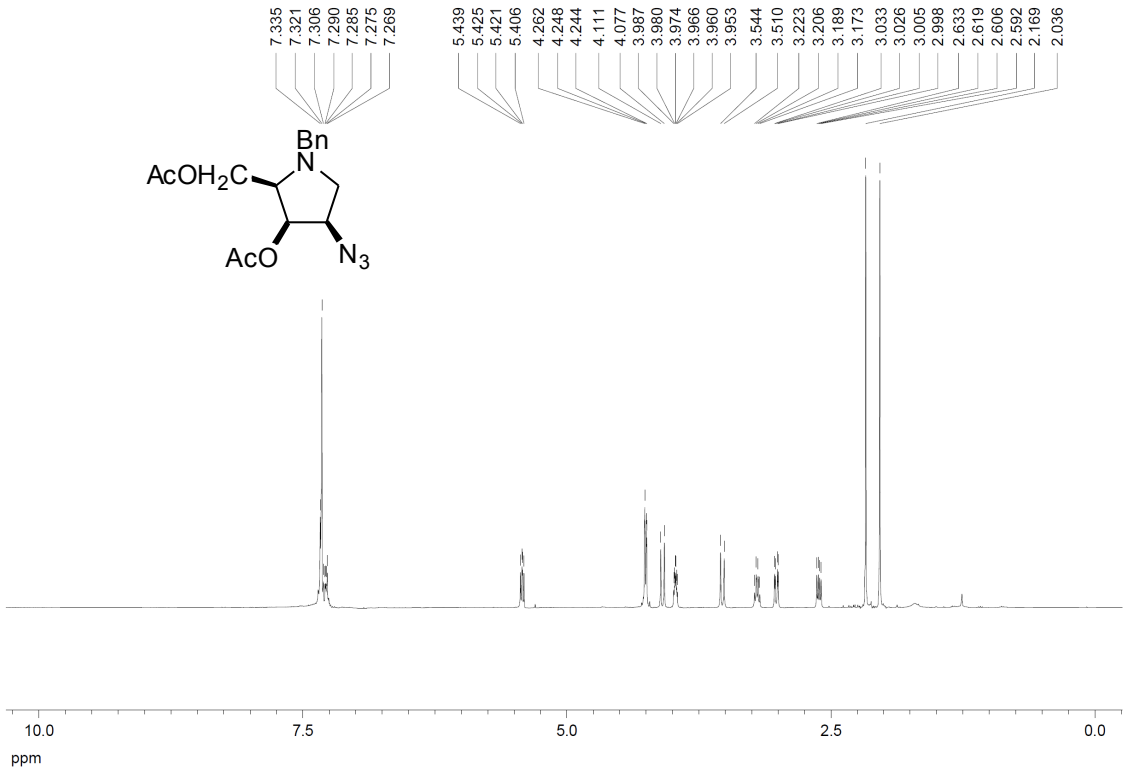
$^{1}$H NMR spectrum for **44D** (400 MHz, $CDCl_3$)



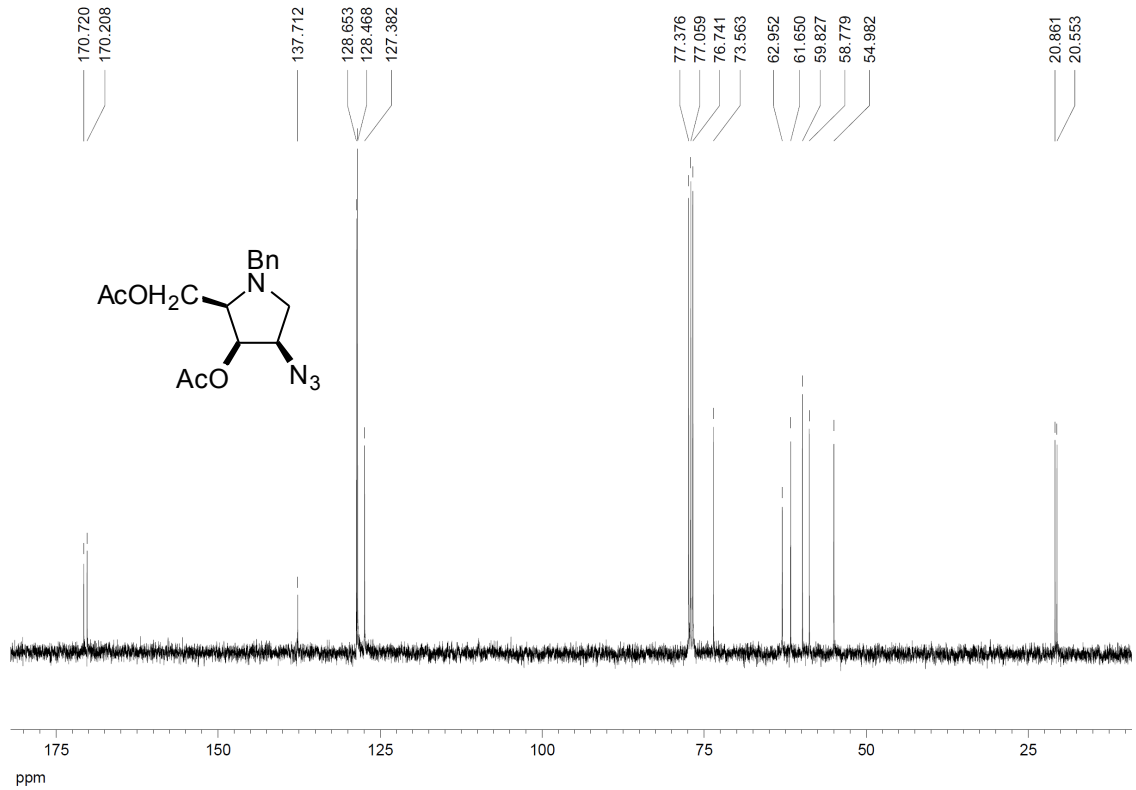

$^{13}$C NMR spectrum for **44D** (100 MHz, $CDCl_3$)



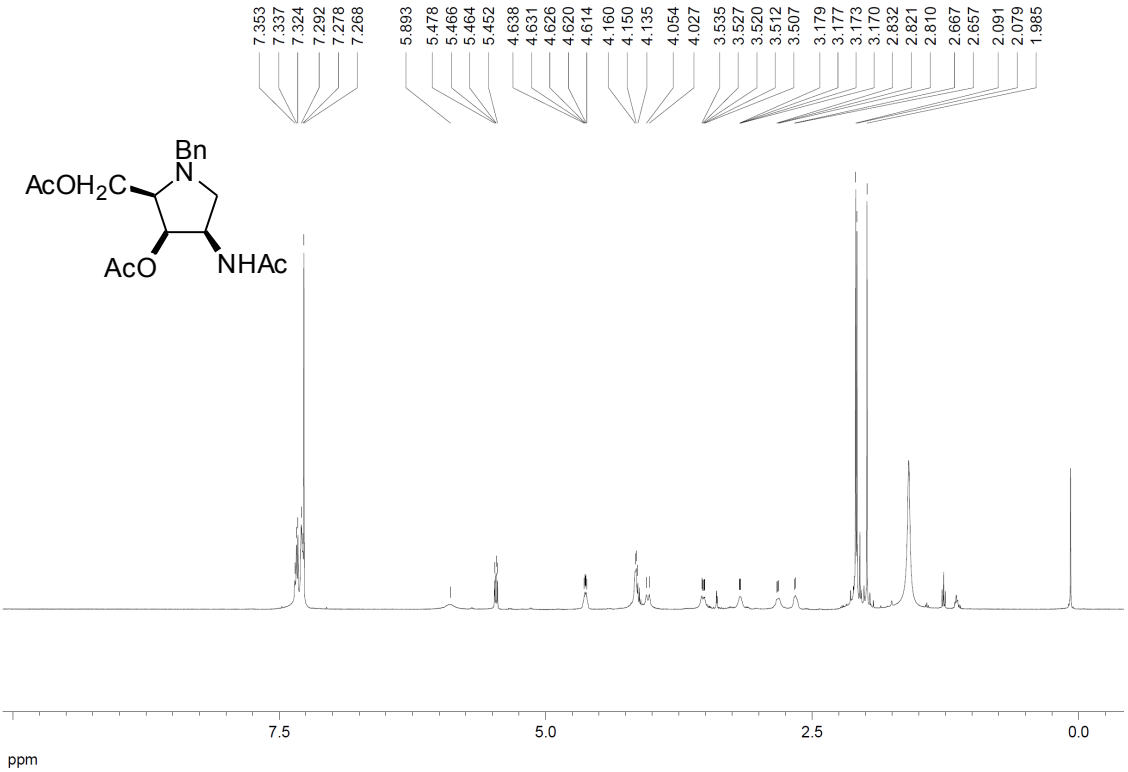
$^{1}$H NMR spectrum for **45D** (400 MHz, $CDCl_3$)



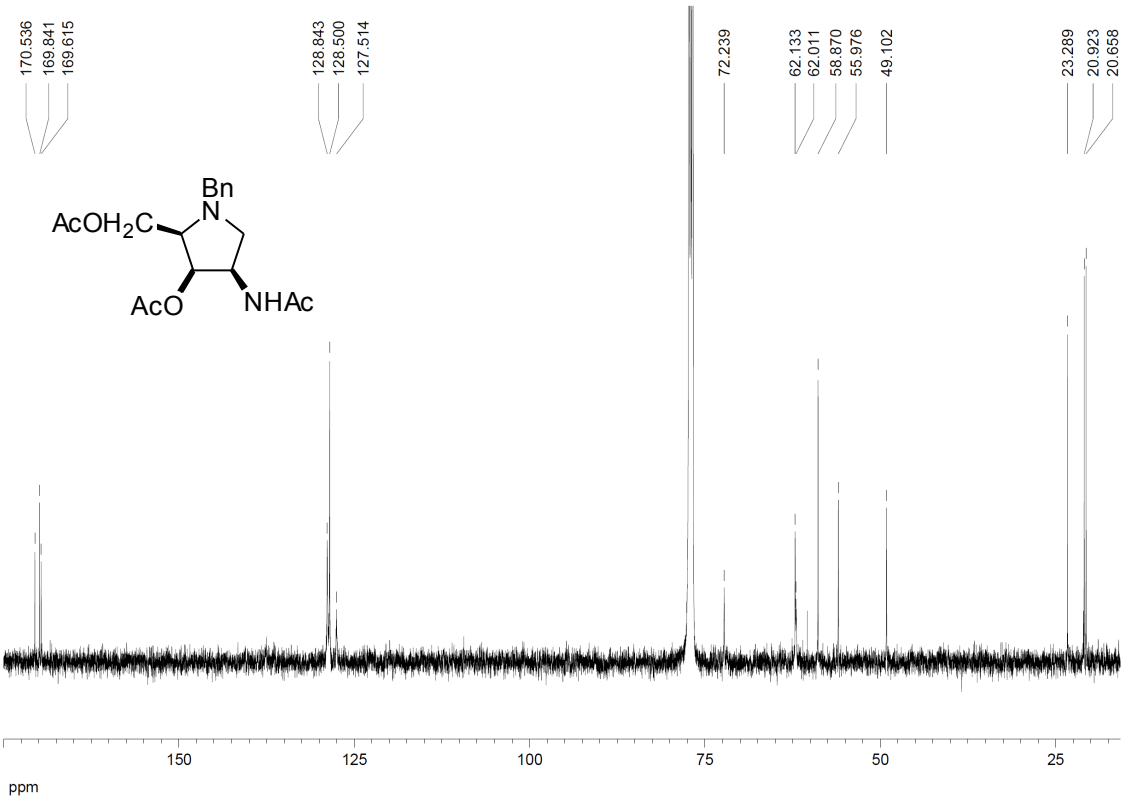

$^{13}$C NMR spectrum for **45D** (100 MHz, $CDCl_3$)



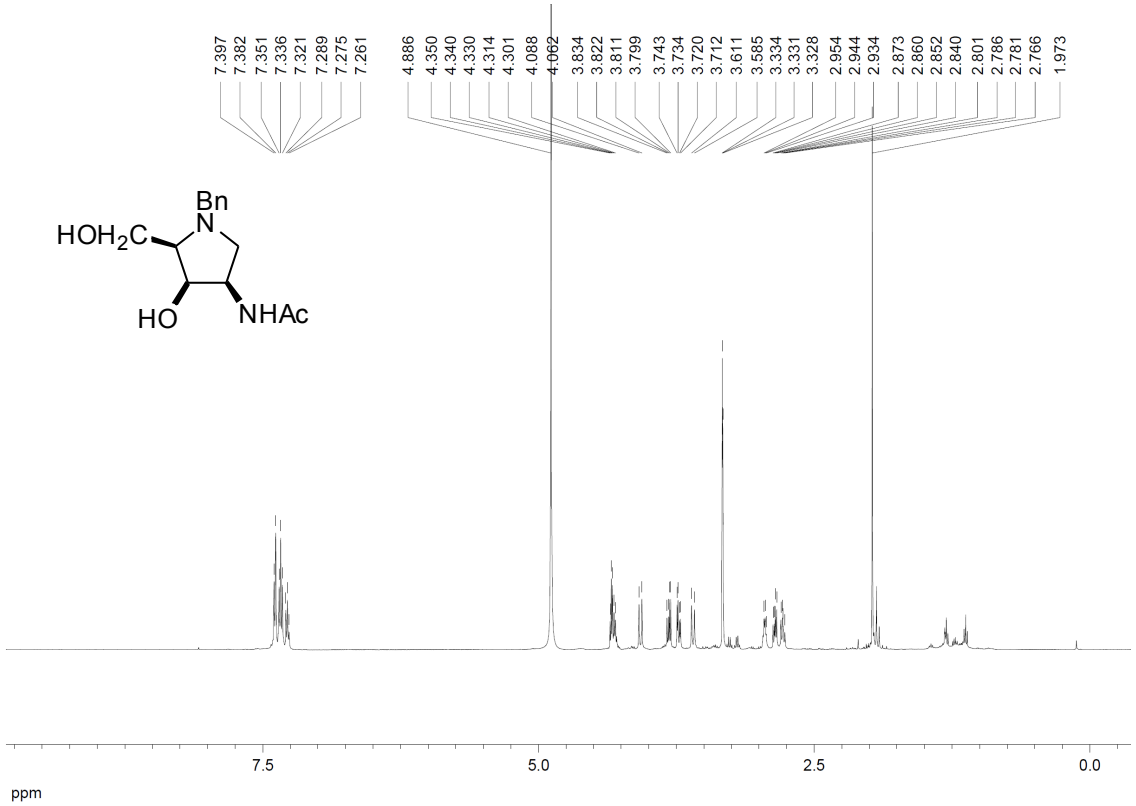
$^{1}$H NMR spectrum for **46D** (400 MHz, $CDCl_3$)



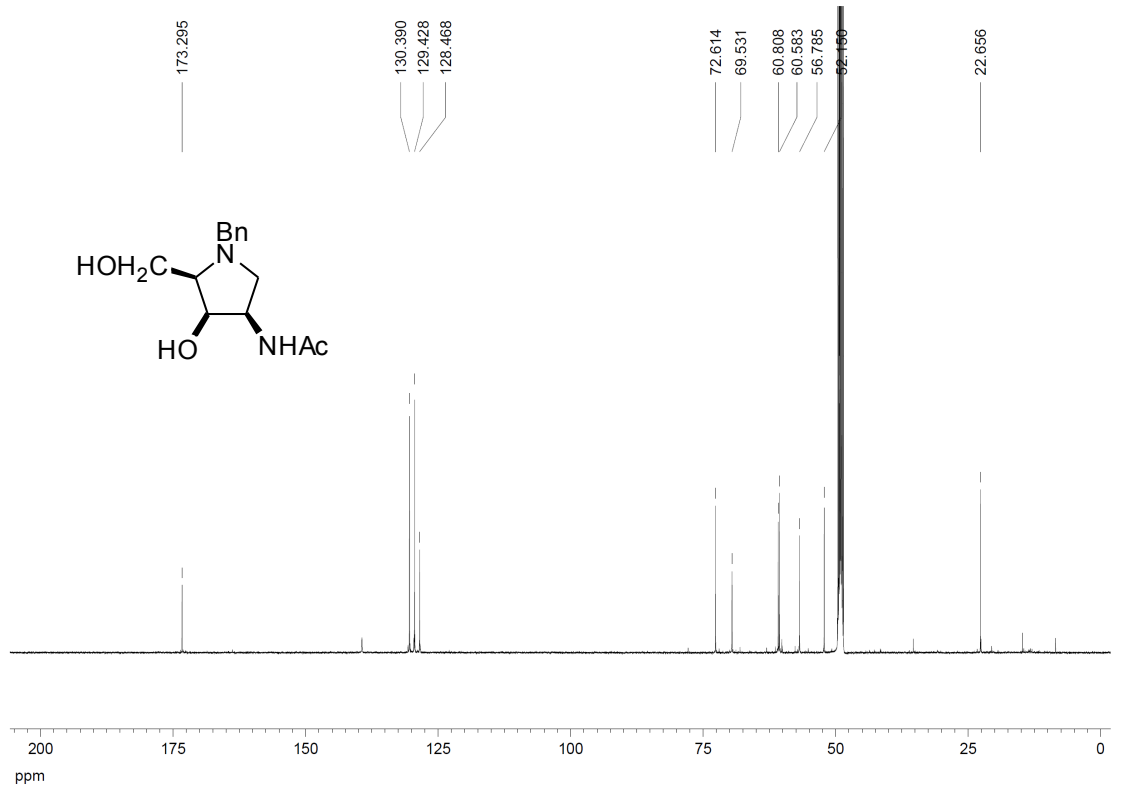

$^{13}$C NMR spectrum for **46D** (100 MHz, $CDCl_3$)



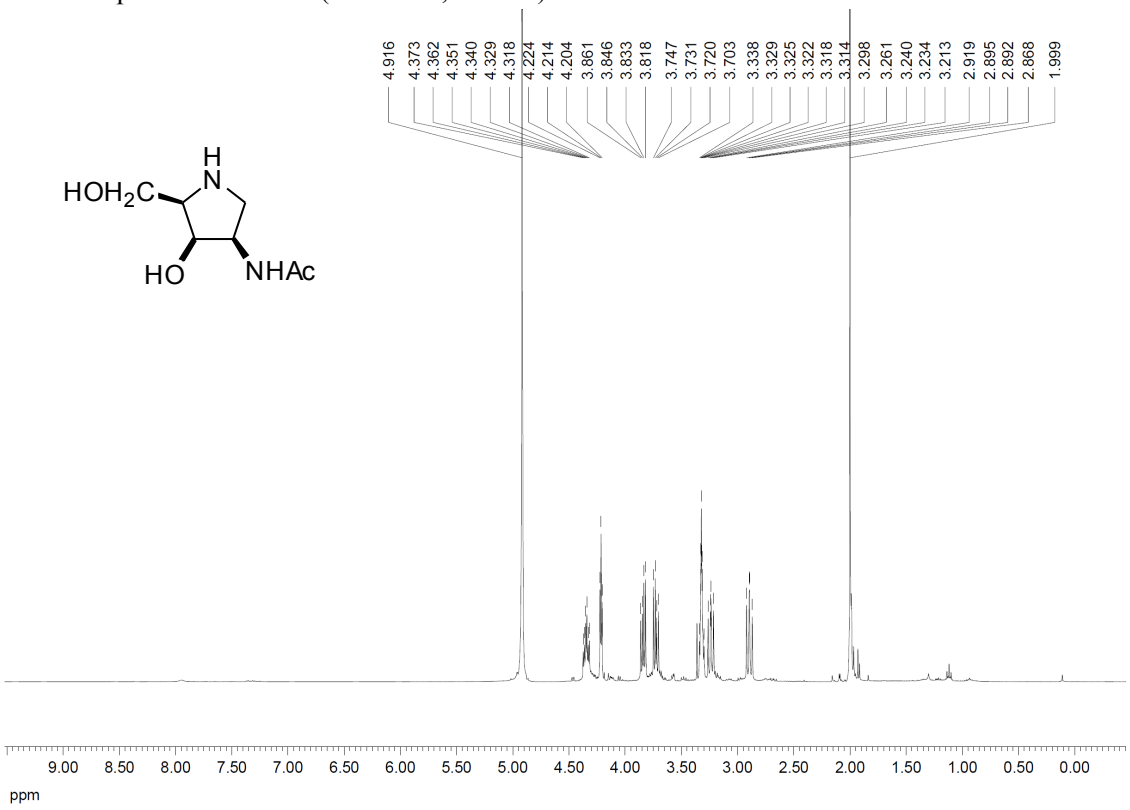
$^{1}$H NMR spectrum for **23D** (400 MHz, MeOD)




$^{13}$C NMR spectrum for **23D** (100 MHz, MeOD)



$^{1}$H NMR spectrum for **22D** (400 MHz, MeOD)




$^{13}$C NMR spectrum for **22D** (100 MHz, MeOD)

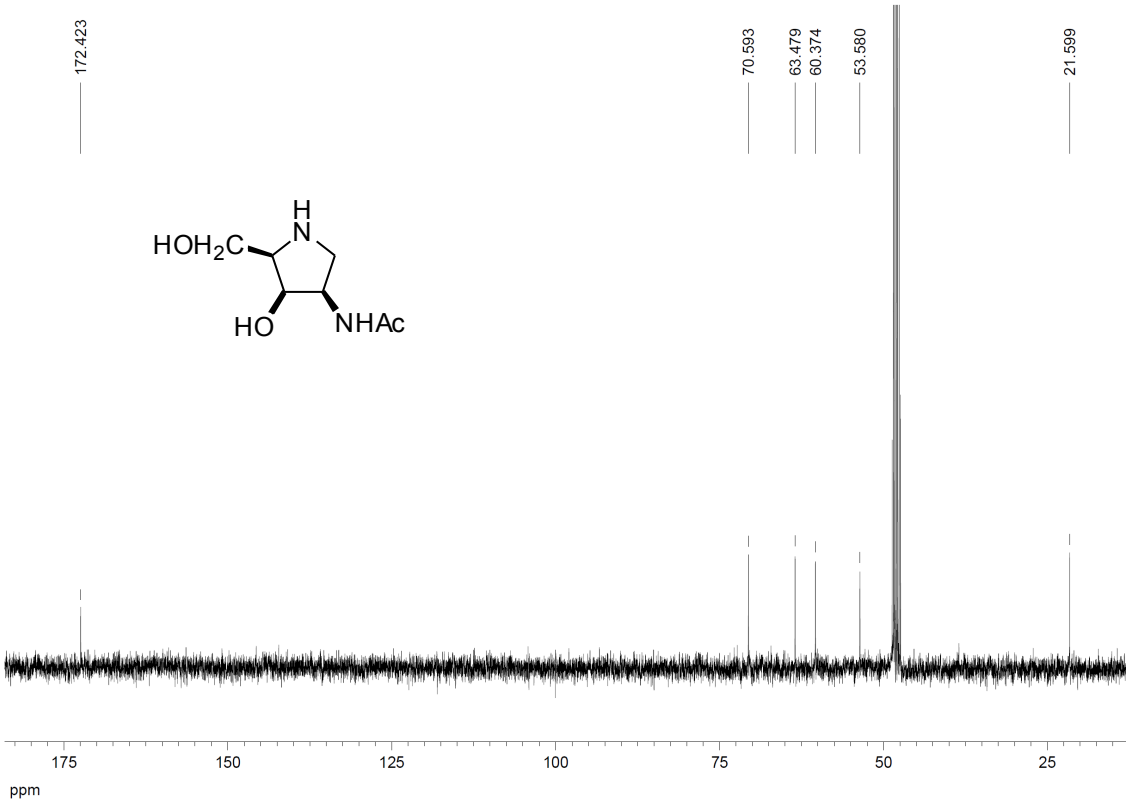
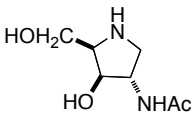
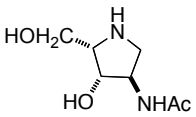
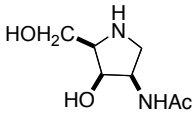
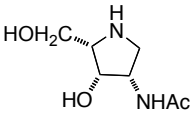


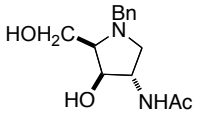
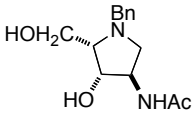
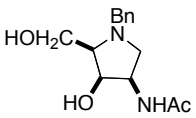
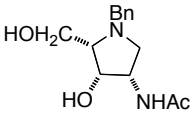
**Table S1**. Concentration of iminosugars giving 50 % inhibition of various glycosidases

| | $IC_{50}$ (μM) | | | |
|---|---|---|---|---|
| |  |  |  |  |
| | **20D** | **20L** | **22D** | **22L** |
| Enzyme | D-*xylo* | L-*xylo* | D-*lyxo* | L-*lyxo* |
| α-Glucosidase | | | | |
| Yeast | NI (4.0%) | NI (15.4%) | NI (14.1%) | NI (0.8%) |
| β-Glucosidase | | | | |
| Almond | NI (19.7%) | NI (8.8%) | NI (9.0%) | NI (0.9%) |
| α-Galactosidase | | | | |
| Coffee beans | NI (27.1%) | NI (9.6%) | NI (11.7%) | NI (11.9%) |
| β-Galactosidase | | | | |
| Bovine liver | NI (7.4%) | NI (3.7%) | NI (2.7%) | NI (12.6%) |
| α-Mannosidase | | | | |
| Jack beans | NI (1.3%) | NI (0%) | NI (0%) | NI (0%) |
| β-Mannosidase | | | | |
| Snail | NI (0%) | NI (0%) | NI (0%) | NI (1.7%) |
| α-L-Rhamnosidase | | | | |
| *P. decumbens* | NI (0%) | NI (2.3%) | NI (1.2%) | NI (6.2%) |

[a] NI : No inhibition (less than 50% inhibition at 1000 μM).

[b] ( ) : inhibition % at 1000 μM

**Table S2**. Concentration of iminosugars giving 50 % inhibition of various glycosidases

| | $IC_{50}$ (μM) | | | |
|---|---|---|---|---|
| |  |  |  |  |
| Enzyme | **21D** *N*Bn-D-*xylo* | **21L** *N*Bn-L-*xylo* | **23D** *N*Bn-D-*lyxo* | **23L** *N*Bn-L-*lyxo* |
| α-Glucosidase | | | | |
| Yeast | NI [a] (4.7%)[b] | NI (10.1%) | NI (0%) | NI (0.8%) |
| β-Glucosidase | | | | |
| Almond | NI (4.4%) | NI (6.0%) | NI (4.1%) | NI (0%) |
| α-Galactosidase | | | | |
| Coffee beans | NI (27.1%) | NI (4.4%) | NI (0%) | NI (2.2%) |
| β-Galactosidase | | | | |
| Bovine liver | NI (16.0%) | NI (22.2%) | NI (40.2%) | NI (16.1%) |
| α-Mannosidase | | | | |
| Jack bean | NI (1.8%) | NI (0%) | NI (6.3%) | NI (2.6%) |
| β-Mannosidase | | | | |
| Snail | NI (0%) | NI (5.2%) | NI (0%) | NI (3.0%) |
| α-L-Rhamnosidase | | | | |
| *P. decumbens* | NI (1.8%) | NI (0%) | NI (13.7%) | NI (0%) |

[a] NI : No inhibition (less than 50% inhibition at 1000 μM).

[b] ( ) : inhibition % at 1000 μM