

SUPPORTING INFORMATION

***N*-Acetyl Allolactosamine [Gal-(β 1 $\rightarrow$ 6)-GlcNAc]:** Both spectra were concordant with reference literature. ^1H -NMR (700 MHz, D_2O): 1.94 (s, 3H, Ac), 4.33 (d, 1H, $\text{H}_{1'}$, $J_{1',2'} = 7.91\text{Hz}$), 4.61 (d, 0.56H, $\text{H}_{1\beta}$, $J_{1\beta,2} = 8.47\text{Hz}$), 5.09 (d, 0.66H, $\text{H}_{1\alpha}$, $J_{1\alpha,2} = 3.58\text{Hz}$). ^{13}C -NMR: 21.81 (Me of Ac, α), 22.08 (Me of Ac, β), 53.95 (C-2 α), 56.52 (C-2 β), 60.94 (C-6'), 68.49 (C-4'), 68.57 (C-6 β), 68.59 (C-6 α), 69.62 (C-3 α), 69.77 (C-5 α), 70.52 (C-4 β), 70.56 (C-4 α), 70.56 (C-2'), 72.58 (C-3 β), 72.61 (C-3'), 74.85 (C-5 β), 75.11 (C-5'), 90.81 (C-1 α), 94.93 (C-1 β), 103.26 (C-1' β), 103.27 (C-1' α), 174.45 (C=O of Ac α), 174.70 (C=O of Ac β).

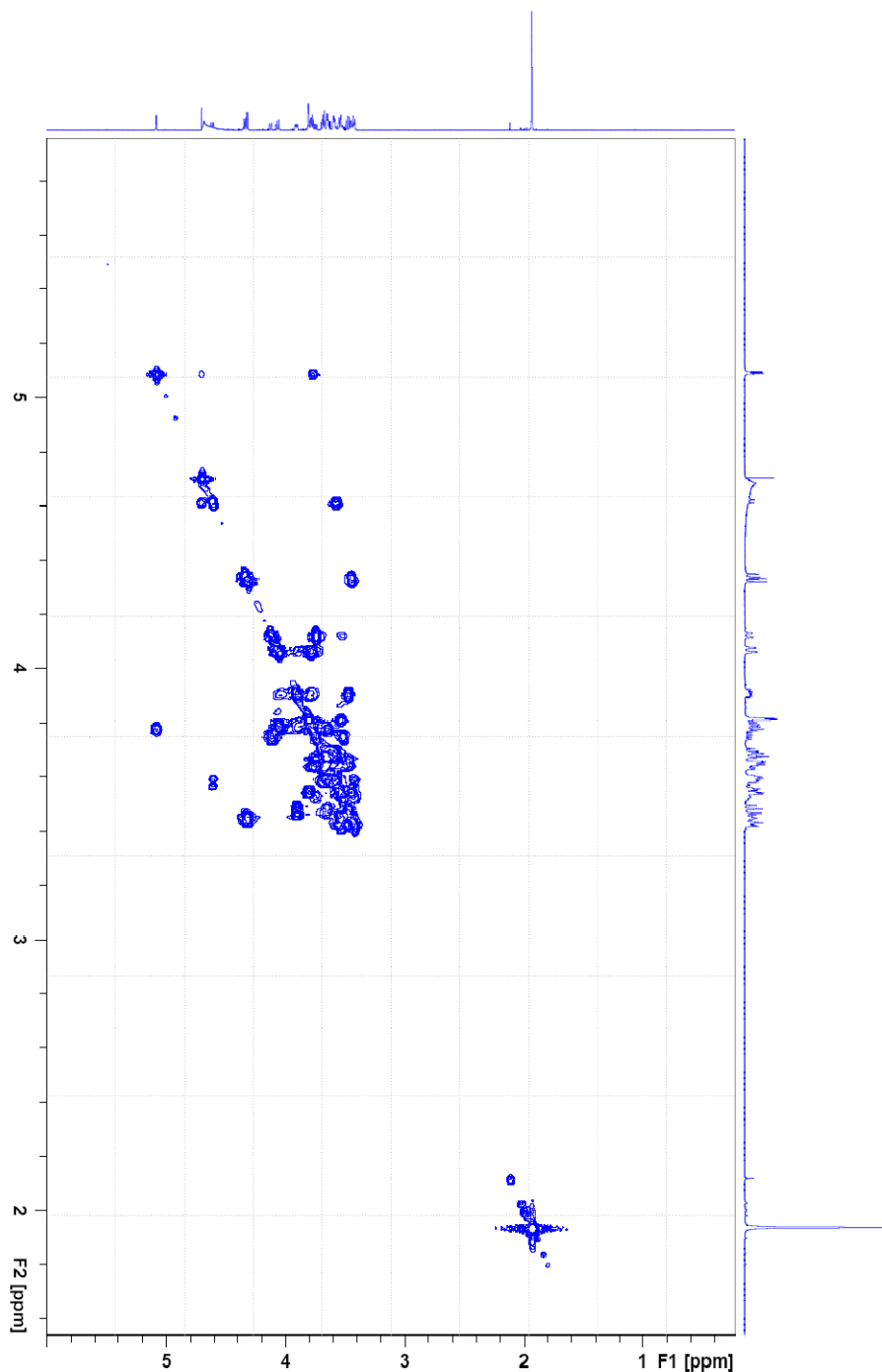


Figure 1: COSY experiment for Gal-(β 1 $\rightarrow$ 6)-GlcNAc

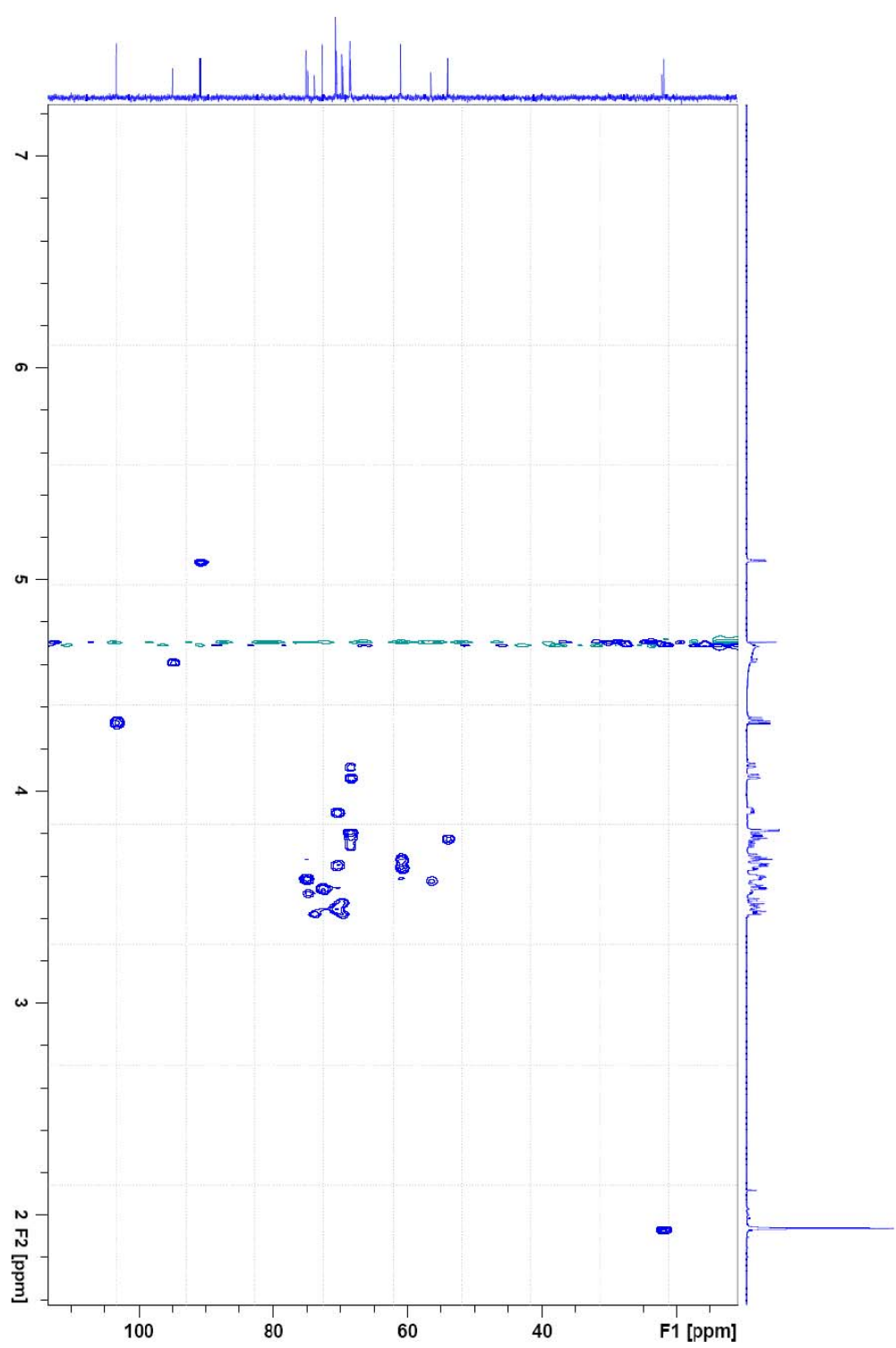


Figure 2: HSQC experiment for Gal-(β1→6)-GlcNAc

***N*-Acetyl Lactosamine [Gal-(β 1 $\rightarrow$ 4)-GlcNAc]:** Both spectra were concordant with reference literature. ^1H -NMR (700 MHz, D_2O): 1.93 (s, 3H, Ac), 4.37 (d, 1H, $\text{H}_{1'}$, $J_{1',2'} = 7.84$ Hz), 4.62 (d, 0.37H, $\text{H}_{1\beta}$, $J_{1\beta,2} = 8.06$ Hz), 5.10 (d, 0.57H, $\text{H}_{1\alpha}$, $J_{1\alpha,2} = 2.24$ Hz). ^{13}C -NMR: 21.80 (Me of Ac, α), 22.10 (Me of Ac, β), 53.65 (C-2 α), 56.13 (C-2 β), 59.86 (C-6 α), 59.99 (C-6 β), 60.96 (C-6'), 68.48 (C-4'), 69.21 (C-3 α), 70.20 (C-5 α), 70.90 (C-2'), 72.43 (C-3 β , C-3'), 74.79 (C-5 β), 75.29 (C-5'), 78.24 (C-4 β), 78.68 (C-4 α), 90.46 (C-1 α), 94.80 (C-1 β), 102.80 (C-1' β), 102.86 (C-1' α), 174.40 (C=O of Ac α), 174.66 (C=O of Ac β).

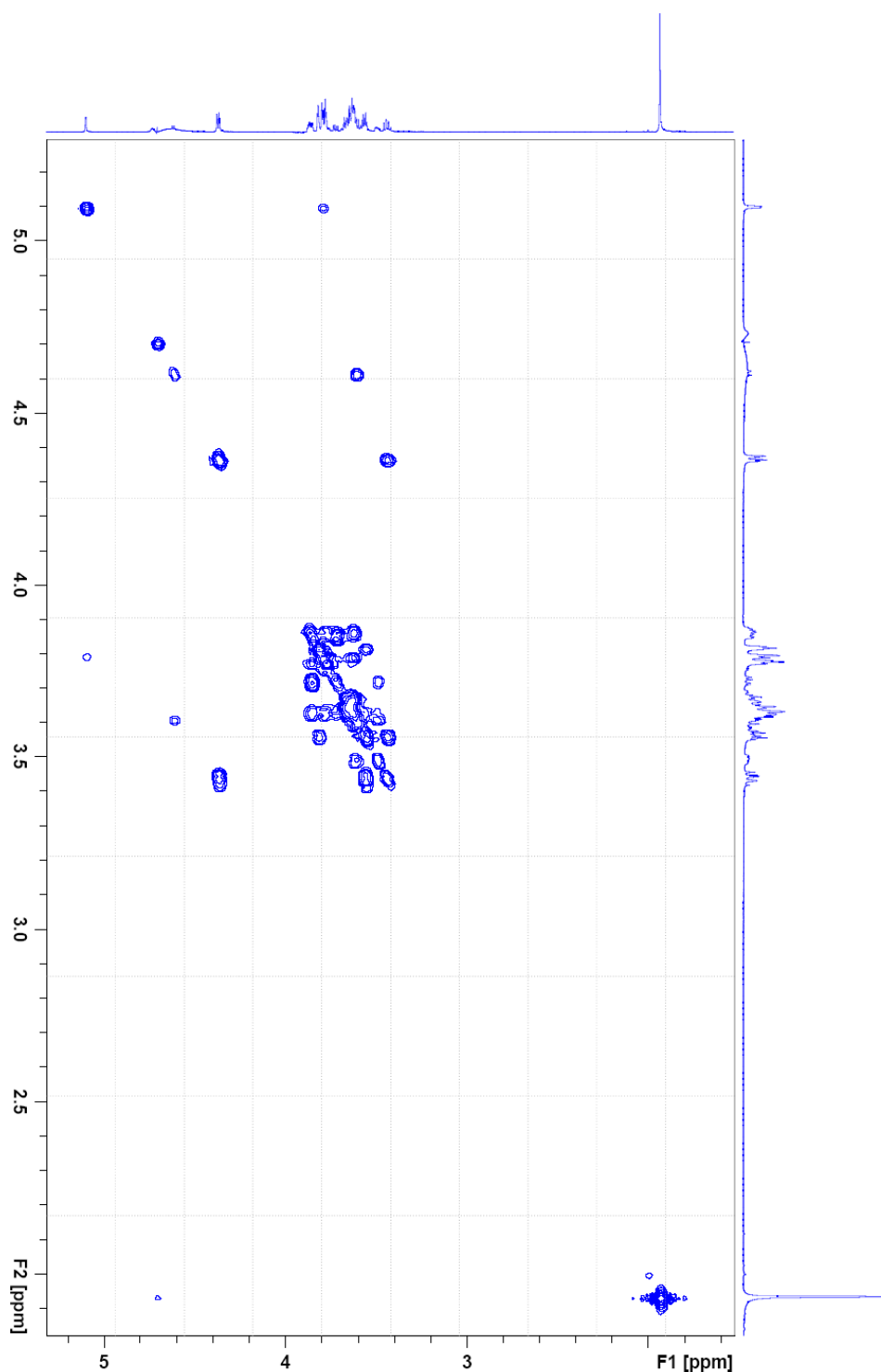


Figure 3: COSY experiment for Gal-(β 1 $\rightarrow$ 4)-GlcNAc

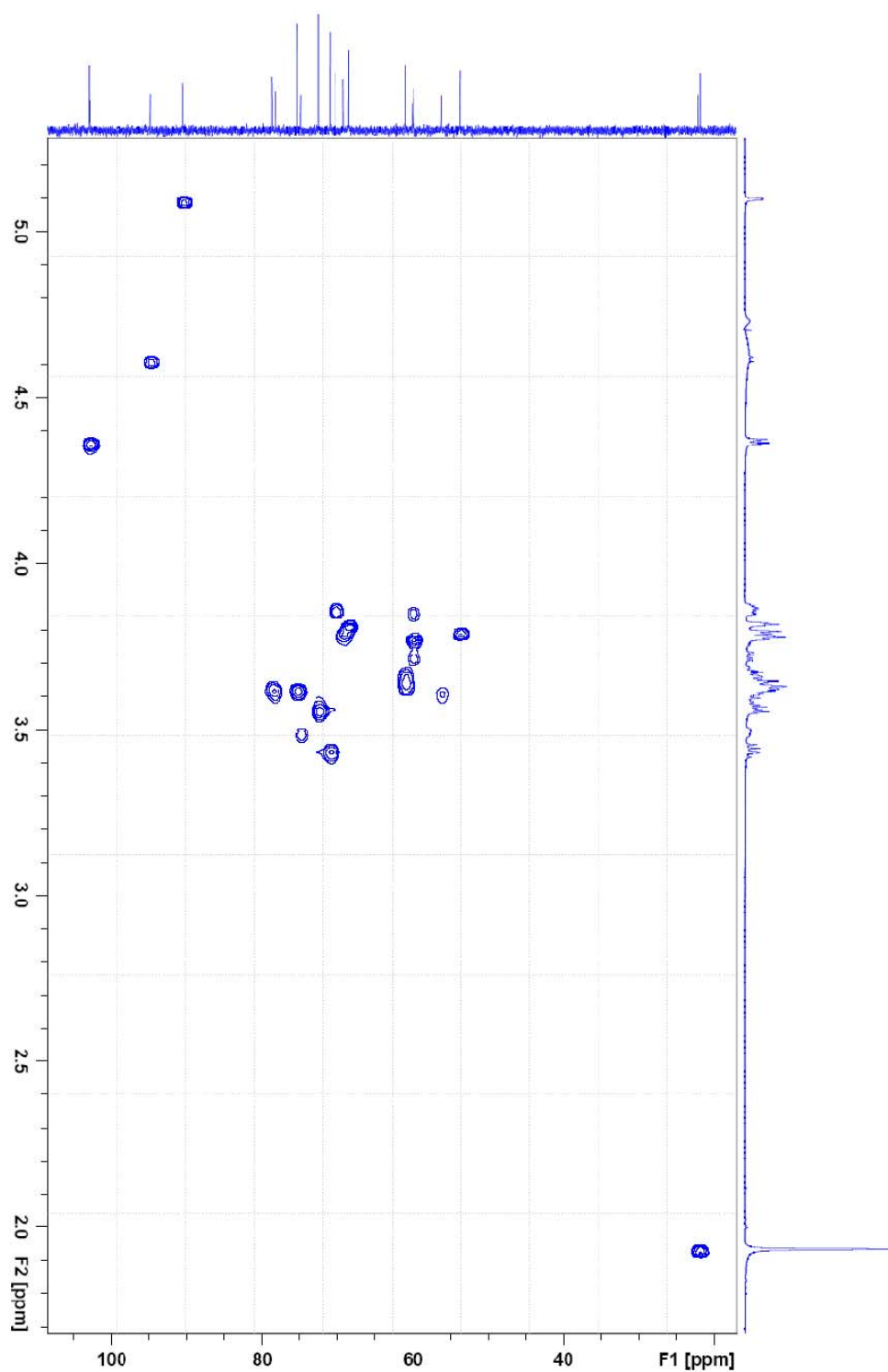


Figure 4: HSQC experiment for Gal-(β 1 $\rightarrow$ 4)-GlcNAc

REFERENCES

- ^a N. Bridiau, and T. Maugard, A comparative study of the regioselectivity of the β -galactosidases from *Kluyveromyces lactis* and *Bacillus circulans* in the enzymatic synthesis of *N*-acetyl-lactosamine in aqueous media. *Biotechnol. Prog.*, 2011, 27(2). 386-394.