Supporting Information

Anomer-Specific Recognition and Dynamics in a Fucose-binding Lectin

Paweł M. Antonik,[a,b,#] Alexander N. Volkov,[c,d,#] Ursula N. Broder,[a] Daniele Lo Re,[a] Nico A. J. van Nuland,[c,d] and Peter B. Crowley[a,]*

[a]School of Chemistry, National University of Ireland Galway, University Road, Galway, Ireland.

[b]Department of Food BioSciences, Teagasc Food Research Centre Ashtown, Dublin 15, Ireland.

[c]Jean Jeener NMR Centre, Structural Biology Brussels, Vrije Universiteit Brussel, Pleinlaan 2, 1050 Brussels, Belgium.

[d]Structural Biology Research Centre, VIB, Pleinlaan 2, 1050 Brussels, Belgium.

[#]These authors contributed equally

*Correspondence to: peter.crowley@nuigalway.ie, +353 91 49 24 80

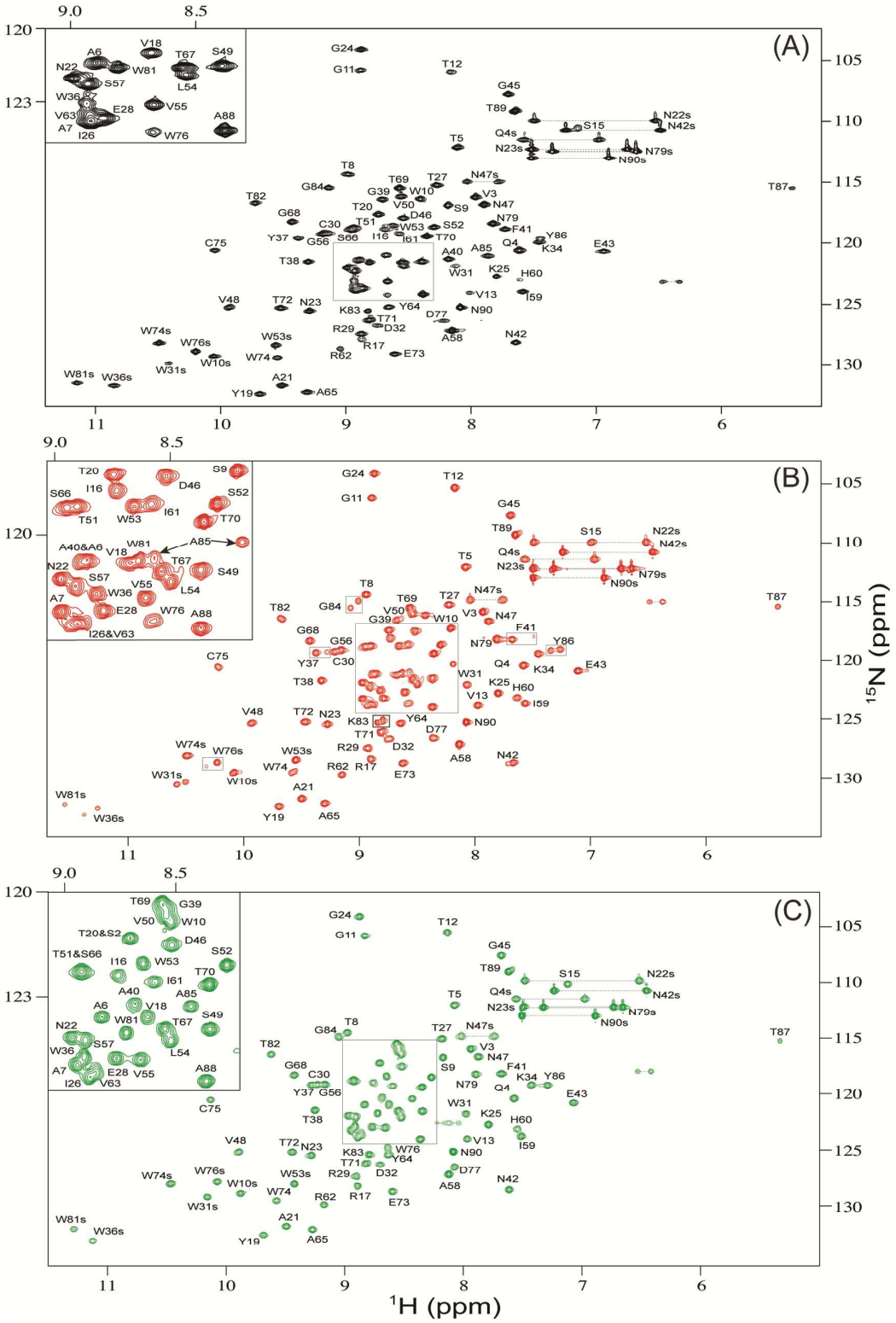

Figure S1. Assigned ^{1}H-^{15}N HSQC spectra of RSL in (A) sugar-free, (B) L-fucose-bound and (C) D-mannose-bound forms. Split resonances due to α or β-L-fucose are boxed; Y37, F41, W76s, K83 and G84. Sample conditions were 0.25 mM protein in 20 mM potassium phosphate, 50 mM NaCl, pH 6.0 at 303 K.

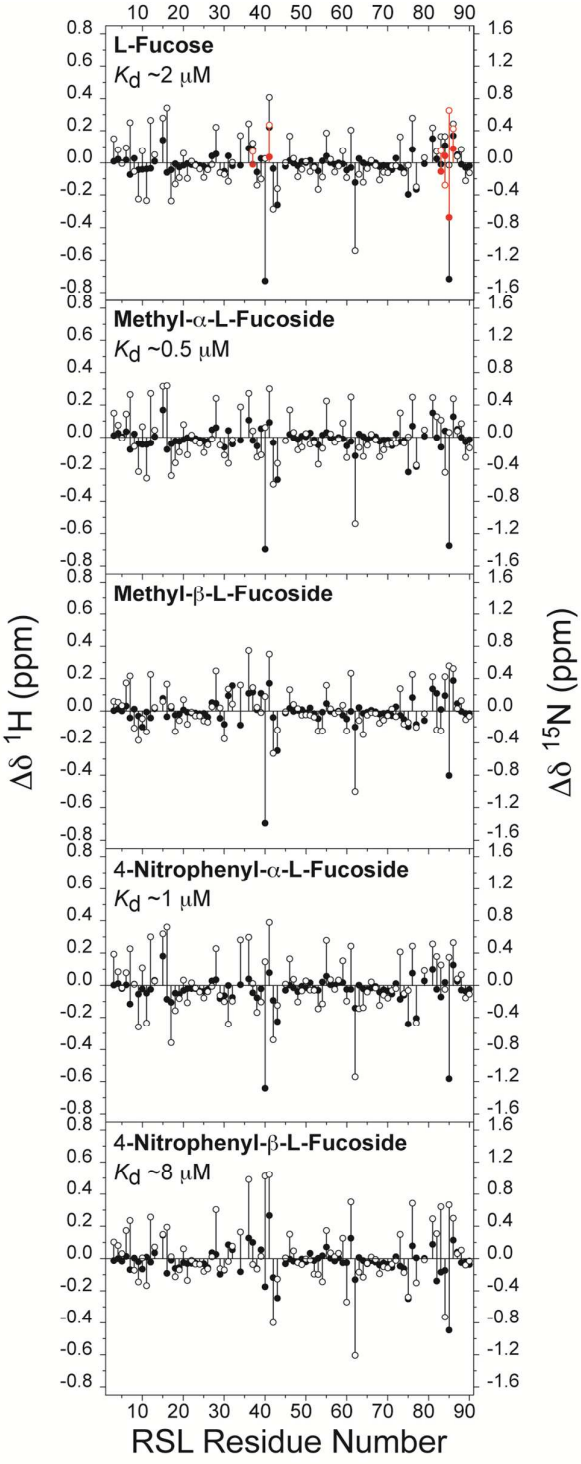

Figure S2. Plot of chemical shift perturbations for RSL backbone resonances in the presence of L-fucose, methyl-α-L-fucoside, methyl-β-L-fucoside, nitrophenyl-α-L-fucoside or nitrophenyl-β-L-fucoside. In the L-fucose complex some resonances were split in two (red data points) due to the presence of the α- and β-monomers.

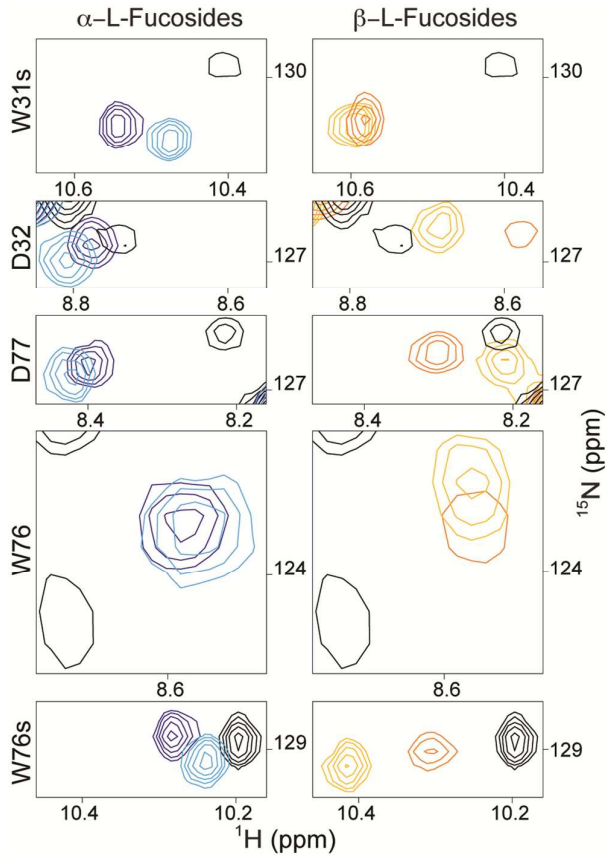

Figure S3. Regions from the overlaid ^{1}H-^{15}N HSQC spectra of pure RSL (black contours) and RSL bound to methyl-α-L-fucoside (navy), methyl-β-L-fucoside (dark orange), nitrophenyl-α-L-fucoside (light blue) or nitrophenyl-β-L-fucoside (light orange). See Figure 5 in the main text.

Figure S4. The RSL monomer (PDB 2bt9) coloured by R_{2ex} values (see scale bar) in the sugar-free (upper), D-mannose-bound (middle) and L-fucose-bound (lower panel) forms. The residues for which R_{2ex} data could not be obtained are grey. The intra-monomeric binding site residues are shown as sticks, with the backbone nitrogen shown as spheres. Methyl-α-L-fucoside is shown as sticks.