



**Supplementary Figure 1. Each CS tetrasaccharide favors a distinct set of torsion**

**angles: torsion plots for  $\psi_1$  and  $\phi_1$ .** The blue circles represent the torsion angles sampled by each CS tetrasaccharide during the Boltzmann jump analysis. The red squares represent the torsion angles of the lowest energy MD conformations. Torsion angles were defined as  $\phi = \text{O1-C1-O-C}(x)$ ,  $\psi = \text{C1-O-C}(x)\text{-C}(x+1)$ .