

Supporting

Figure S1. ^1H -STD-NMR spectra of the interaction of Gal8N

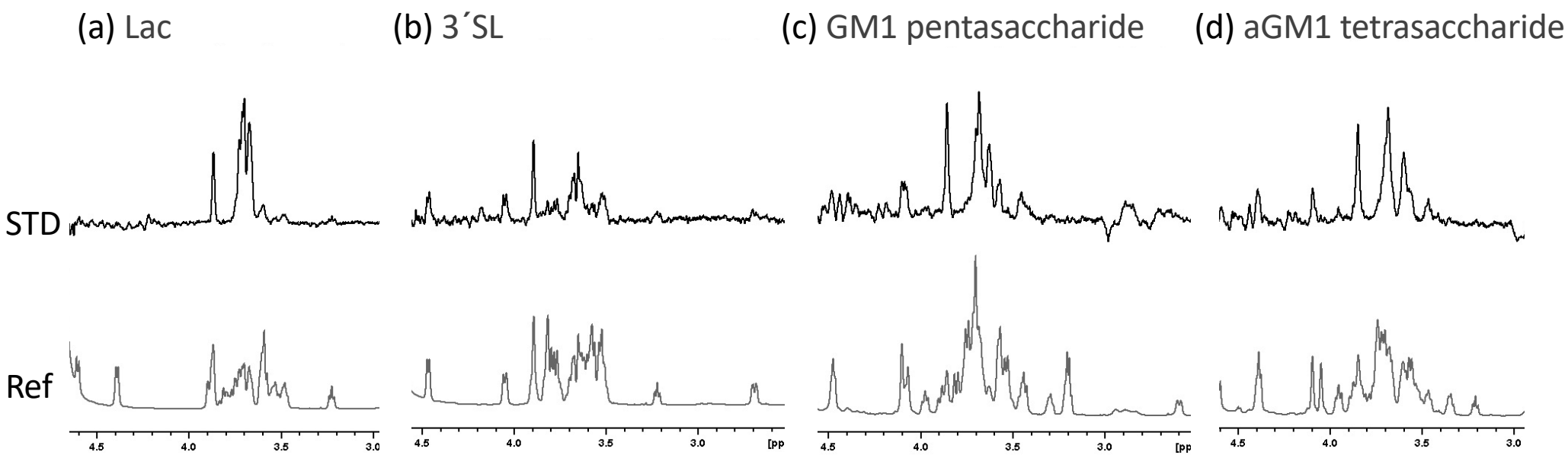


Figure S2. ^1H - ^{15}N HSCQ-NMR spectra showing the CSP of Gal3 (50 μM) upon addition of increasing concentration of the saccharide moiety of (A) GM3 (B) asialo-GM1(C) GM1, and of Gal8N (50 μM) (D) GM3 (E) asialo-GM1(F) GM1. All titrations were done with at least 7 different ligand concentrations. In this panel 4 different titration points are shown: blue protein alone, red 1 eq, yellow 5 eq, and green 10 eq of ligand. Except for panel D: blue protein alone, red 0.5 eq, yellow 1 eq, and green 1.5 eq of ligand.

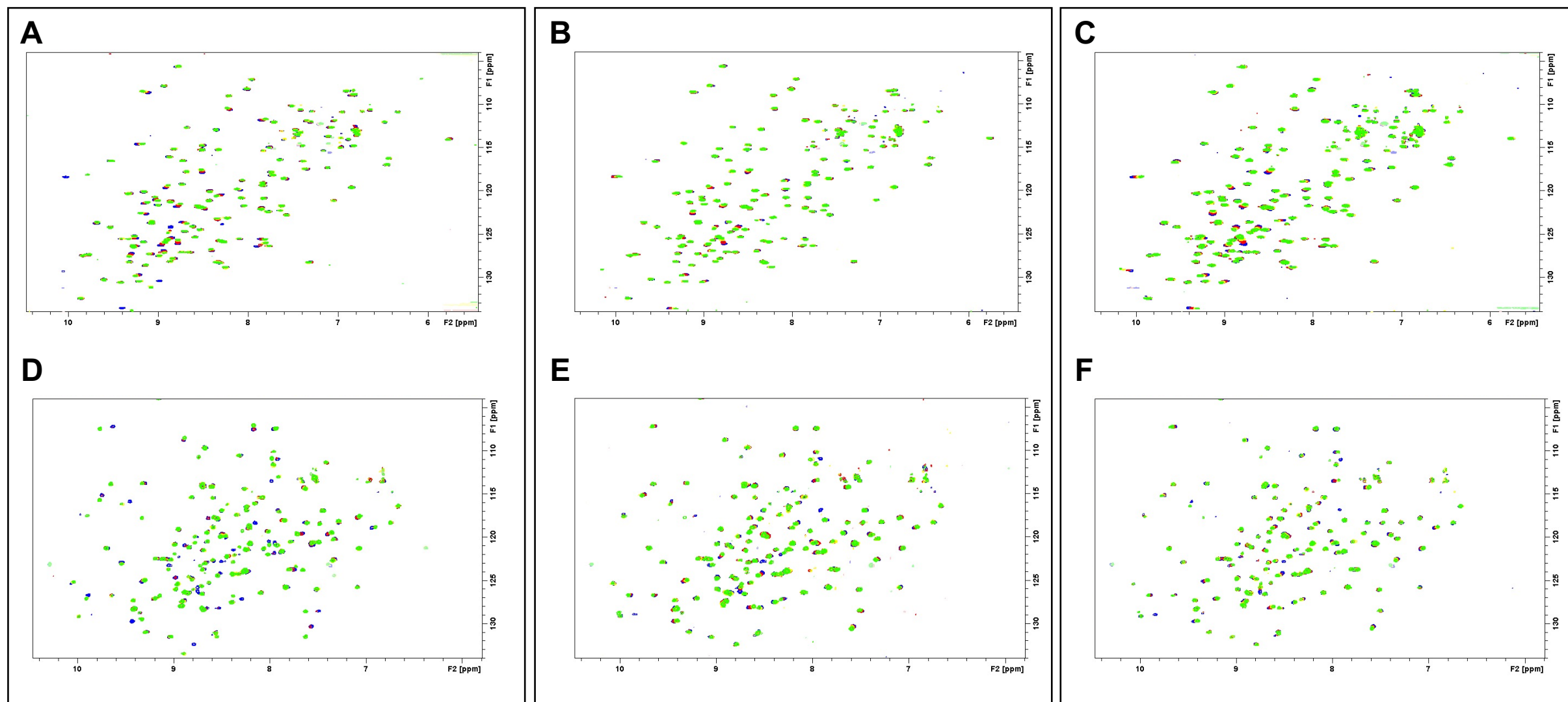


Figure S3. Surface charge of Gal3 and Gal8N

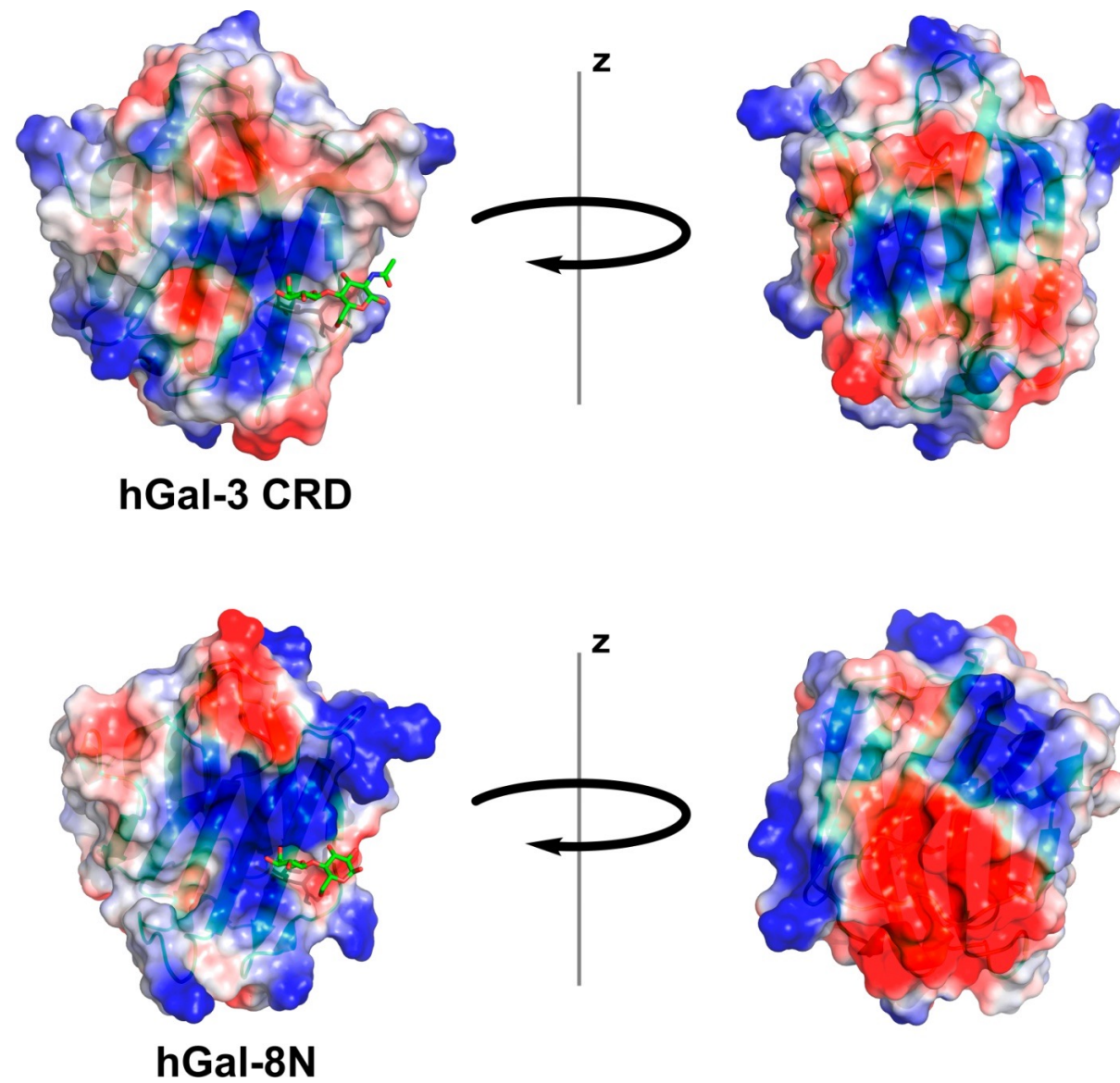


Figure S4. RMSD plots for **(A)** POPC:LacCer bilayer; **(B)** POPC:GM3; **(C)** POPC:aGM1; **(D)** POPC:GM1 and **(E)** Recognition of POPC:aGM1 bilayer by hGal3.

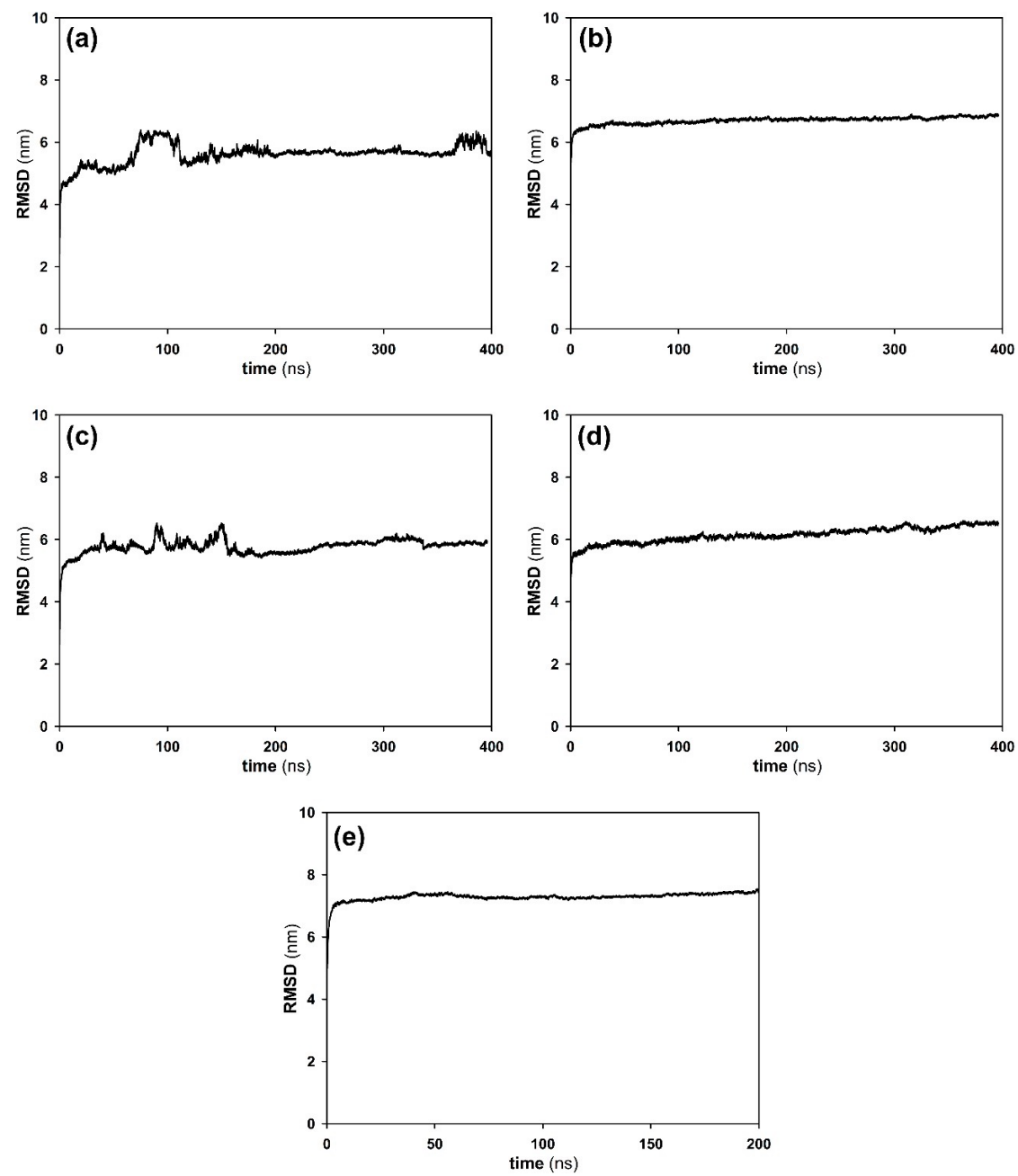


Figure S5. Initial ($t = 0$ ns) and final ($t = 400$ ns) snapshots of **(A)** POPC:LacCer bilayer; **(B)** POPC:GM3 bilayer; **(C)** POPC:aGM1 and **(D)** POPC:GM1 bilayer.

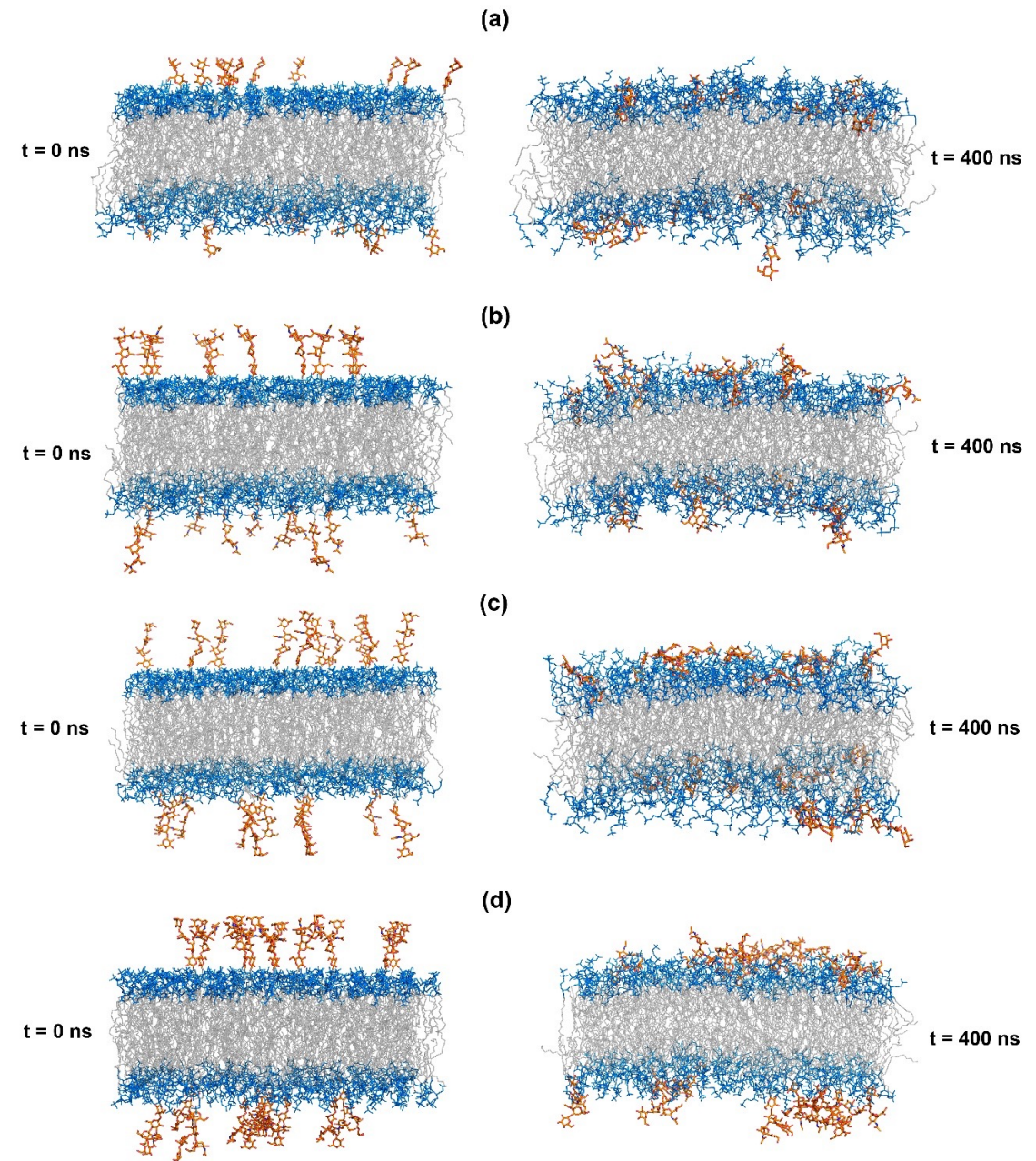


Figure S6. ^1H assignment of asialo-GM1 (A) and GM1 (B) of internal galactose residue (Gal_int) and of external galactose (Gal_ex) residues.

