In this talk, I would like to share our ongoing efforts toward computational (structural) glycobiology in terms of (1) glycan structure and dynamics in glycoproteins, (2) roles of glycans as ligands in protein-glycan and protein-protein interactions, (3) glycolipid structure and dynamics, and (4) bacterial outer membranes containing lipopolysaccharides and their interactions with membrane proteins. We have developed various tools available at http://www.glycanstructure.org: Glycan Reader for automatic detection and annotation of carbohydrates and glycosidic linkages in PDB files, Glycan Fragment DB for carbohydrate fragment structures in the PDB and torsion angle distributions of specific glycosidic linkages of searched structures, GS-align for glycan structure alignment and similarity measurement. A PDB survey study of N-glycan structures in PDB is also presented and a potential way to model a glycan structure from its sequence is discussed.