Yersinia enterocolitica O:3 (Ye O:3) is a human pathogen, which causes a diarrheal disease (yersiniosis). It expresses lipopolysaccharide (LPS), which has a hexasaccharide branch called outer core (OC). OC is important for the resistance of Ye to cationic antimicrobial peptides and functions as a receptor for bacteriophage and enterocoliticin. The biosynthesis of the hexasaccharide is directed by the OC gene cluster with 9 genes (wzx wbcKLMNOPQ gne). The six genes wbcKLMNOQ putatively encode six glycosyltransferases (GTs) that are essential to form the six glycosidic linkages of the OC hexasaccharide. Based on sequence information, WbcK and WbcL are categorized into the GT2 family and WbcM, WbcN and WbcQ belong to the GT4 family.

The Wbc proteins characterizing the GT4 family were studied by making homology based 3D models. The sequence identities of the model sequences with their respective template were in the range of twilight zone. Therefore, extensive structure based multiple sequence alignments were made prior to modeling. In addition, the docking of donor sugars into the active site of the proteins assisted in predicting the catalytically important residues.

The UDP sugars bind within the deep fissure that lies between the N- and C-terminal domains of these Wbc proteins. The catalytically important residues as well as the residues involved in stabilizing the donor sugar into the binding sites are highly similar if not identical. The findings from this thesis provide enough support to conduct further experimental studies on these proteins.

Keywords

Yersinia enterocolitica, glycosyltransferases, lipopolysaccharide, Wbc, substrate-binding site