

# Carbohydrate Ligand Interactions with Genotype Variants of Cholera Toxin B

**Sunil Kumar**

*Institute of Life Sciences, Department of Biotechnology, Nalco Square, Bhubaneswar India*

**Address for correspondence:**

*E-mail: skybiotech@gmail.com*

*Vibrio cholerae* produces cholera toxin (CT) that consists of two subunits, A and B, and is encoded by a filamentous phage CTX $\Phi$ . The A subunit carries enzymatic activity that ribosylates ADP, whereas the B subunit binds to monosialoganglioside (GM1) receptor in epithelial cells. Molecular analysis of toxigenic *V. cholerae* strains indicated the presence of multiple ctxB genotypes. In this study, we employed a comparative modeling approach to define the structural features of all known variants of ctxB found

in O139 serogroup *V. cholerae*. Modeling, molecular dynamics and docking simulations studies suggested subtle variations in the binding ability of ctxB variants to carbohydrate ligands of GM1 (galactose, sialic acid and N-acetyl galactosamine). These findings throw light on the molecular efficiencies of pathogenic isolates of *V. cholerae* harboring natural variants of ctxB in causing the disease, thus suggesting the need to consider ctxB variations when designing vaccines against cholera.