OMICS Group Conferences
Accelerating Scientific Discovery

2nd International Conference on
Proteomics & Bioinformatics

July 2-4, 2012 Embassy Suites Las Vegas, USA

Mining the structural details of human wnt-crd (fzd) complex for computational drug repurposing

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The observed genetic alterations of various extracellular and intracellular WNT signaling components can result in increase or decrease of gene expression and hence can be obstructed proficiently. These target sites may include the prevention of WNT-FZD binding, destruction of β-catenin and formation of Axin, APC and GSK-3β complex. Hence, the localized targeting of these interacting partners can help in devising novel inhibitors against WNT signaling. In order to computationally target the initiating components of this pathway, we need to know the tertiary structures of WNT ligands and their Frizzled (FZD) receptors. At present, no crystallographic experimental data is available for human WNT and FZD proteins.

In our study, we constructed three dimensional structure models for WNT proteins including, WNT-1, WNT-6, WNT-10A, and WNT-10B and Cysteine rich domain (CRD) of human Frizzled-1 protein. Furthermore, the docking studies were performed to predict the binding interfaces of WNT and FZD CRD. Altogether, structural prediction analysis of WNT proteins was performed to reveal newer details about post-translational modification sites and mapping the novel interaction sites.

Biography

Ms. Qurrat-ul-Ain (Corresponding author) has completed her M.Phil Bioinformatics from National Center for Bioinformatics, Quaid-i-Azam University Islamabad Pakistan. She is currently serving COMSATS Institute of Information Technology Pakistan as a Lecturer for Bioinformatics. Her research interests include structural bioinformatics, protein-protein interactions, Drug-DNA interactions and Pharmaco-genomics studies.

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