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Biomarkers of the cardiometabolic risk and system inflammation in preobese and obese women

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Understanding *in silico* characterization of cancer gene is an important aspect in bioinformatics, a lot of research work is in progress. It has been known that KRAS gene is associated with risk and outcome of various types of cancers that's why KRAS gene was selected among all other cancer causing genes. Development of different tools in bioinformatics made the cancer research more precise and accurate. In current planned study, SNPs and its effect in KRAS gene was predicted by using number of bioinformatics tools, moreover possible inhibitors and their toxicity effects were identified and analyzed. The research plan was divided in to five steps: 1. Complete mutational analysis was done by different tools (SAAP, SIFT, I-MUTANT, PolymiRTS, poly-phen2, GeneMANIA), 2. Mutant 3D-structures of KRAS gene was modeled by DS-visualizer, 3. Virtual screening against 11600 compounds was performed using idock on line server (based on Auto Dock algorithm) 4. Protein-ligand interactions of docked compounds were studied using ligplot and DS-visualizer. 5. Toxicity of the compounds was predicted using lazar tool. The identified SNPs in KRAS gene which can cause structural instability and functional damage are (K5E, K5N, V14I, P34L, P34R, T58I, A59T, G60R, G60S, A146T, K147E and G12R) apart from these one of the SNPs G12R in KRAS is known to be more prevalent in majority of the cancer. So G12R mutant structure was selected for docking studies and toxicity prediction. From the result of idock server the top 5 inhibitors from ZINC database having lowest energy score was selected (94016294, 67732740, 19235389, 14541999 and 21187043 ids and their energy scores are -11.389, -11.104, -10.939, -10.696 and -10.644 respectively) for knowing the hydrophobic interaction and hydrogen bonding of top 5 inhibitors with G12R mutant structure ligplot was used. According to toxicity prediction, the compound ids (Unk1, Unk2, Unk3, Unk4 and Unk5) can be predicted as finest inhibitor against G12R KRAS gene.

Biography

Fareha Masood received Bachelor's degree in Bioinformatics. Her expertise lies in Docking, Virtual screening, Programming languages (C/C++, C#), (HTML and asp.net) Framework, DBMS, Sql (oracle 11g) and Microsoft Office. She works on various biological tools (NCBI, Uniprot, i-mutant, SAAP, SIFT, POLYMIRT, Gene Mania, Discovery Studio Visualizer, Chimera, Modeler, ProtParam server, PSIPRED server, SBASE server, STRING v10.0, ProSa server, SAVES, iPBA server and PMDB database).

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