

Abstract ID:- 180

Abstract Topic:- Genetic, genome and epigenome databases and resources

Abstract Title:- Network pharmacology and Molecular Docking of diet-derived phytonutrients to manage the collagen family gene expression in LGMD R12

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Aims:-Human civilizations on the globe have acquired genetic alteration/s that cataclysmic to genetic Oddities may be due to niche nature by man. One of these is Muscular Dystrophies (MDs), Limb-Girdle Muscular Dystrophy (LGMD) type has been at the forefront for the recent span with its associated group of more than 30 genes. Limited research has been conducted on LGMD in the past due to the diverse phenotypic variations, which necessitates more in-depth exploration. The aim of the current study is to investigate the differentially expressed genes and network pharmacology in a microarray dataset of 84 LGMD R12 patients and manage the disease condition by molecular docking with 'Diet-derived' phytonutrients.

Methods:- The present research seeks to identify differentially expressed genes in LGMD R12 using the GSE202745 Illumina NovaSeq 6000 (Homo sapiens) analyzed microarray dataset with an 84-sample size. Using network pharmacological analysis, the PPI network was generated to check the interconnectivity of the sister genes. Hub gene analysis through 12 different methods in the cytoHubba plugin. Molecular docking of >65 diet-derived phytonutrients with collagen proteins for a management strategy MM-GBSA evaluation and ADMET analysis provide an in-silico manifesto to analyze the ΔG free energy change and toxicity of the natural compound with highly upregulated genes in the ANO5 mutation.

Results:- Analysis of 84 samples shows the misexpression of 220 genes, out of which 215 are up-regulated and 5 are down-regulated. 220 DEGs are interconnected by 200 nodes and 240 edges in a network pharmacological study, including COL9A1, COL22A1, COL1A2, COL17A1, COL25A1, and COL3A1. Collagens are found in at least 09 of the 12 techniques in the cytoHubba plugin that indicate their function as superior hub genes. Molecular Docking (MD) of >65 diet-derived phytonutrients with collagen proteins and associated transcription factors gives the list of greater than -7.0 Kcal/mol. ADMET and MM-GBSA evaluations further filter the compounds by their toxicity level and binding energy, providing conclusive evidence for management strategy.

Conclusions:- Here, a combination of computational analysis and molecular profiling clears the picture of LGMD spectra by finding up and down-regulated genes. Our 'Satvik' cultural dietary phytonutrients offer a broad range for managing LGMDR12 disorders by suppressing collagen hub genes. > -7.0 docking-scored phytonutrients have the potential to manage the whole condition through restrictive action on hub genes. It may be possible in the future to create specific management procedures for the same by employing our cultural 'Satvik' dietary elements as management molecules.

Keywords:- LGMD R12, Collagen family genes, Dietary phytonutrients, Molecular Docking (MD)