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Screening of proteins targeting circulating miRNAs for improved diagnosis of multiple myeloma using computational methods

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Multiple myeloma is a B-cell malignancy, which is characterized by the expansion of clonal plasma cells in the bone marrow, thereby leading to abnormal accumulation of monoclonal antibodies in circulation. The condition arises from an asymptomatic multiplication of plasma cells, called MGUS (Monoclonal gammopathy of undetermined significance) which eventually progresses to Myeloma. Till date, there are no explicit assays that can discriminate between the premalignant and malignant stages. Circulating miRNAs are deregulated in MM cells and bone marrow. Their differential expression profiles in various body fluids can be quantified and used for the diagnosis of MM. The study focuses on identification of such a protein which would show exclusive affinity for a selected panel of circulating miRNAs reported to be deregulated in MM. A few human RNA binding proteins were selected based on their RNA binding domains and their interacting probabilities with the panel of miRNAs. The 3D structure of miRNAs and proteins were modelled and validated. Molecular Docking was performed for determining the protein-miRNA interaction using AutoDock Vina. Out of the selected proteins, DKC1 showed good binding affinity values of -17.4 kcal/mol with miRNA-720, -16 kcal/mol with miRNA-1246 and -16.9 kcal/mol with miRNA-1308. It also showed some significant hydrogen bonding. miRNA 26 was used as an internal control for docking as it is a circulating miRNA without any significant relation to MM. This protein-miRNA interaction could be used as an economical and reliable ELISA based method for the improved diagnosis of Multiple Myeloma patients.

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