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INTERACTING MECHANISM OF TRANSCRIPTIONAL INHIBITOR PROTEIN ID3 AND TCF4 PROTEIN: MOLECULAR DYNAMICS AND DOCKING APPROACH

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ID3, a member of the ID multigene family of helix loop helix domain can inhibit the regulation of transcription upon protein-protein interaction. DNA binding inhibitor protein has long been characterized as an oncogene that implicates its functional role through its helix–loop–helix (HLH) structure. TCF4 protein which is involved in the transcription regulation is inhibited by ID3 the protein that lacks DNA domain. Our current work aims to identify the functional and physical interaction of this proteins and designing of an aptamer to prevent the interaction of TCF4 and ID3. Network analysis has been performed to predict the inhibitor for ID3. At present there is no three dimensional structure available for these proteins which limits our understanding of its interacting mechanism. We used ***ab initio*** method to build the model from primary sequence. The stability of these proteins and peptide were obtained through MD simulation at 30ns. The integration of PCA and FEL were shown to be a very useful approaches to gain an overall view of the conformational landscape accessible to a protein and helped in the identification of the key residues of TCF4 (Arg 567, Arg 515, Glu 587, Met 590, Gln 519) and ID3 (Glu 36, Asp 43, Cys 47, Arg 50, Arg 60) buried in their HLH motifs which are responsible for dimerization process. All these observations correlate with experimental reports, suggesting that these key residues might play a crucial role in the regulation of transcription and muscle specific genes and cellular signaling pathways controlling proliferation. Thus, the study throws light on the interacting mechanism of ID3-TCF4 and ID3-peptide (ID1/3-PA7) complex and conformational space indicating the key structural changes within the helical regions of the motif.

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