Structural Insights in Inflammatory Bowel Disease (IBD)

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Abstract

Despite recent advances, the majority of the susceptibility genes for Inflammatory Bowel Disease (IBD), a chronic inflammatory disorder that affects the gastrointestinal tract and is commonly diagnosed as Crohn's disease and ulcerative colitis, are still unknown. Empirical data indicates that the human IL10RA mutation could impact the regulation of the gut inflammatory response, with IRF5 being a key player in controlling mucosal inflammation in IBD. Notably compounds such as *Aloin, Andrographolide, Incensole,* and *Curcumin* show up as leading contenders that are significantly contributing to anti-inflammation and a natural adjuvant therapy for IBD. Nevertheless, the exact chemical process by which these substances block IL10RA and IRF5 is still unknown. In order to close this gap, we carried out molecular interaction and MD Simulation experiments to understand how synthetic and herbal drugs interact with IL10RA and IRF5 variants. The molecular docking experimental results have demonstrated that *Aloin* (-9.0268 kcal/mol) has the highest binding affinities when compared to *Mesalazine* (-7.215 kcal/mol), a synthetic drug. These findings suggest that *Aloin* as a promising inhibitors of IL10RA and IRF5 variants. Additional insights from 10 ns molecular dynamics simulations that include structural studies and RMSD analysis shows that *Aloin* is more stable than synthesized drugs and it could be a potential drug candidate for IBD treatment in the future.