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Structural modeling and docking studies of cloned *Bacillus subtilis* keratinase with psoriasis drugs

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Keratinases are unique group of proteolytic enzymes adept to hydrolyze different keratin substrates viz. α- keratins (hair, hooves, nail etc) and β- keratins (Feather and silk fibrions, β-amyloid) into simple polypeptides and amino acids. Since the skin and nails composed of keratins, keratinase are thought to be alternative ungual enhancers in hyperkeratosis (psoriasis, nail disorders) conditions which hydrolyze the keratin and thus can enhance the permeability and efficacy of topical drugs. Psoriasis is a common inflammatory skin disease personified by keratinocyte, hyperproliferation, dedifferentiation, neoangiogenesis and inflammation affecting 2-3% of the world population. Presently a broad range of treatment modalities are available for psoriasis viz. topical treatments, light therapy and systemic medications. A range of ointments, gels, pastes, creams and scalp solutions containing anthralin, calcipotriene, calcitriol, tazarotene and salicylic acid etc. were used as medication. But skin morphology leads to variability in drug permeation and their systemic absorption. Present study demonstrated the expression of *Bacillus subtilis* RSE163 keratinase gene and it's *in silico* binding affinities with psoriasis topical drugs for systemic absorption and permeation through skin. The *ker* gene expressed in *E. coli* showed significantly higher keratinase activity 450 ±10.43 U representing 1,342 bp nucleotides encoding 447 amino acids with molecular weight of 46 kDa. The crystallographic structure obtained from PDB database (PDB ID: 1SCJ) was validated using ramachandran's plot showing 322 residues (84.3%) in most favoured region. Docking studies using extra precision (XP) method showed optimum binding affinities with the drugs Acitretin (-39.62 Kcal/mol), Clobetasol propionate (-37.90 Kcal/mol), Fluticasone (-38.53 Kcal/mol), Desonide (-32.23 Kcal/mol), Anthraline (-38.04 Kcal/mol), Calcipotreine (-21.55 Kcal/mol) and Mometasone (-28.40 Kcal/mol) in comparison to other psoriasis drugs. The results can further be correlated with *in vitro* enzymatic experiments using keratinase as an effective drug mediator through skin to serve the unmet need of industries.

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