Rupam. Dutta et al., J Proteomics Bioinform 2013, 6:7
http://dx.doi.org/10.4172/0974-276X.S1.069

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Proteomics & Bioinformatics
July 15-17, 2013 Courtyard by Marriott Philadelphia Downtown, USA

In silico prediction of GDF9 encoded protein in goat

Rupam. Dutta, Nabajyoti Goswami, Dhrubajyoti Kalita and Probodh Borah
Assam Agricultural University, India

Growth differentiation factor 9 (GDF9) belongs to the transforming growth factor-b superfamily. It plays a critical role as a growth and differentiation factor during early folliculogenesis in female reproduction in mammals. Different mutations of GDF9 gene may cause either an increased ovulation rate or infertility in sheep and goat. Genomic DNA from goat was extracted and pcr was performed. The purified pcr product was send for sequencing. Modelling of GDF9 was carried out initially by using I-TASSER (#ref) web server (http://zhanglab.ccmb.med.umich.edu/I-TASSER/) to generate a complete template of the sequence which was further used for homology modelling performed by MODELLER 9.10 using multiple template modules. Another template, namely 3EVS was selected by performing NCBI BLAST against Protein Databank (PDB). A Multiple Sequence Analysis was generated by using ClastalW (http://www.ebi.ac.uk/Tools/msa/clustalw2/) to recognize the structural alignments of the templates with GDF9 sequence. Models generated by the MODELLER were validated by PROCHECK and evaluated by the discrete optimized potential energy (DOPE) profiles of MODELLER. Structural modifications and visualizations were done by using UCSF Chimera.

NCBI protein BLAST of the amino acid sequence of *GDF9* gene against protein data bank (PDB) shows 99% sequence identity and 66% query coverage with the A chain of PDB entry 3MDY-–the crystal structure of the cytoplasmic domain of the Bone Morp Protein Receptor Type-1b (Bmpr1b) in complex with Fkbp12 and Ldn-193189. From this result it is clear that structure of the protein can be well predicted by homology modelling. Because of the low percentages of query coverage among the templates, initially, the sequence has been submitted to I-TASSER server (http://zhanglab.ccmb.med.umich.edu/I-TASSER) to generate an automated *ab initio* model of the entire sequence. The server shows top ten templates, top ten structural analogs, and top five enzyme homolog's in the PDB and generates five models for the submitted sequence by predicting secondary structure and solvent accessibility. Residues from 1 to 113 in the model selected from the server have not been modelled properly, whereas the structural homolog, C chain of PDB entry 3EVS, clearly aligned from residue 29 to 113. In order to introduce this region in to the I-TASSER model, 3EVS has been considered as another template along with the I-TASSER one. Salign module of MODELLER has been used to generate the same pair wise sequence alignment of two templates which has been used to generate the query sequence–templates' structural alignment. Loop refinement has been performed by using loop refine module of Modeller for the disordered loops and 100 loop-refined models have been generated. Of the 100s, the best model has 96.8% residues in the most favoured region.

Finally, all the selected models have been evaluated by the discrete optimized potential energy (DOPE) profiles generated by the evaluate model module which shows that the model selected from the loop refinement is the accurate homology model of the amino acid sequence encoded by the *GDF9* gene.

drrupamdutta@gmail.com