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Homology modeling of PAG 7 and a comparative interaction analysis of different PAG isoforms in buffalo (*Bubalus bubalis*)

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Pregnancy associated glycoproteins (PAG) are inactive aspartic proteinases found variably expressed in ruminant placenta at different stages of gestation. In buffalo although sequence information of 21 PAG isoforms are available, the structural information of only PAG1 and 2 are reported. Studies have shown that PAG7 (GenBank: KP233844.1) is predominantly expressed in buffalo placental cotyledon during early to mid-pregnancy. To have a better insight into the sequence a 3D protein model of buPAG7 was developed from the derived amino acid sequence. To understand the functional significance of different buPAG isoforms, interactions with other proteins have also been studied. The buPAG7 open reading frame is comprised of 380 amino acids of which 1-15 residues constitute the secretory signal peptide, 16-53 the propeptide and 70-379 the conserved aspartic peptidase family domain. There are four potential N-glycosylation sites and 24 phosphorylation sites but no O-glycosylation sites in the sequence. The catalytic motif lies between residues 89-92 and 270-273 within which the catalytic Asp is located at positions 89 and 270. Mutations are noticed at residues 92 (Pro instead of Ser) and 273 (Ser instead of Thr), which might render it as an inactive protease. A homology model developed from porcine pepsinogen (2psg) template showed a reliable quality score of 90.4%. *In silico* interaction with other proteins revealed that all the buffalo PAG isoforms interact with placenta specific subtilisin like proprotein convertase family proteins that are involved in trafficking of protein and peptide precursors through regulated or constitutive branches of the secretory pathway. Also, many proteins interact with specific PAG isoforms indicating different functional significance of each isoform.

Biography

Shree Vidhya S has completed her Master's degree in Biotechnology from Macquarie University, Sydney, Australia and she is currently a PhD scholar at the National Institute of Animal Nutrition and Physiology (NIANP), Bangalore in MoU with Jain University, Bangalore.

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