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Evaluating bovine beta-lactoglobulin as a potential drug carrier for and γ-amino butyric acid (GABA) and prostaglandin, using computational approaches

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Background and Aims: Beta-lactoglobulin (BLG) is the main whey protein in bovine milk and belongs to the lipocalin superfamily. The three-dimensional structure of monomeric bovine BLG is based on 9 strands of anti-parallel β-sheets that eight of them create calyx with a binding site for hydrophobic ligands. The features such as availability, easy purification and peculiar resistance to acid and proteolytic environments could make BLG a vehicle for hydrophobic and/or acid sensitive drugs for oral intake. In this study the potential of Bovine Beta-lactoglobulin as a carrier for GABA and Prostaglandin were evaluated.
Methods: Crystallographic structure of BLG obtained from the Protein Data Bank. Docking analysis performed by using Molegro software to indicate the binding affinity GABA and Prostaglandin. For confirmation in silico results, experimental study on bovine BLG will be done.
Results: MolDok Scores indicated BLG could be appropriate carrier for GABA and prostaglandin. Amino acids such as Ala86, Glu 89, Asp 85, Pro 38, Asn 88, Lys 69 and Lys 60 in BLG structure are relevant for ligand binding.
Conclusions: Due to BLG, naturally, binds fatty acids, vitamins, cholestrol and several other hydrophobic compounds, it could be a carrier for GABA and Prostaglandin with hydrophobic essence. Application of this protein as a drug carrier is proven in many studies. In these studies some amino acids involved in binding are above-mentioned amino acids. So it seems BLG could be suitable carrier for acid-sensitive or hydrophobic drugs could pass through the stomach and ultimately release the ligand further down the gut.

Keywords: Beta-lactoglobulin; GABA; Prostaglandin; Comutational approaches