Construction of human ghrelin receptor (hGHS-R1a) and

analysis of its binding mode by molecular docking

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A peptide hormone, ghrelin, exerts various physiological effects through a G protein-coupled receptor (GPCR), called the ghrelin receptor, including pancreatic exocrine secretion, cardiovascular function, motility, prolactin release and inflammation. To simulate ghrelin's bioactivity, a homology modeling of human ghrelin receptor was built with three types of receptors as templates, including Nociceptin, Beta-1 adrenergic, and two opioid receptors. The built model was validated through molecular docking on a set of 50 ghrelin-mimetic compounds with their biological activities available in literature. The significant correlation between the reported biological activity and docking score of these compounds was found. This indicates our homology model of ghrelin receptor and the docking scheme can provide a reliable platform in molecular design of ghrelin-related compounds.