Distinct interactions between the human adrenergic β_2 receptor and Gα_s – an in silico study

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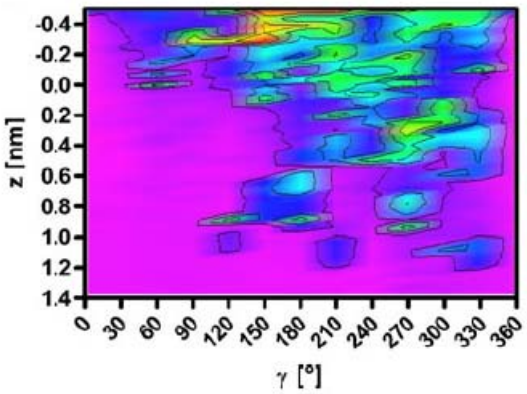
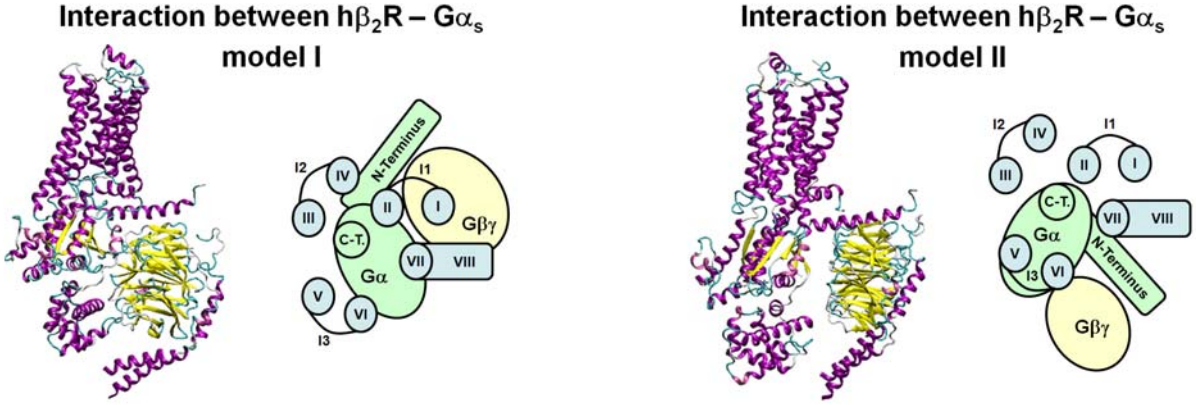
The aim of this study was to perform an in silico analysis of the interaction of the human β_2 adrenergic receptor with Gα_s. In a first step, a systematic surface-interaction-scan between the inactive or active human β_2 adrenergic receptor and Gα_s was performed in order to gain knowledge about energetically preferred areas on the potential energy surface.



Subsequently, two energetically favored regions for the active human β_2 adrenergic receptor – Gα_s – complex were identified. Two representative complex structures were put into a POPC bilayer and solvated in order to perform molecular dynamic simulations. The simulations revealed that both conformations, which have comparable potential energy, are stable. A mean number of about 14 hydrogen bonds was observed between the active receptor and Gα_s for both conformations. Based on these results, two energetically favored β_2-Gα_s-complexes can be proposed.



[1] A. Strasser, H.-J. Wittmann, *J Mol Model*, **2010**, *16*, 1307-1318.