Prediction of Structures and Binding sites for V2R and V1AR vasopressin receptors

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Using the MembStruk we predicted the 3D structure of V2R and used HeierDock to predict the binding site of three antagonists, OPC321260, SR121463A and SR49059. OPC321260 and SR121463A bind well to V2R with Ki = 14 nM and 4.1 nM, respectively, and SR49059 with Ki more than 100-fold weaker. The results of HeirDock show that good antagonist OPC321260 and SR121463A bind to the hydrophobic cavity built by TM3, 4, 5, and 6, burying deep into the middle of TM regions. However, the bad antagonist SR49059 binds on the top of the TM regions interacting with TM3, 5, 6, and 7. The binding modes of antagonists into the predicted binding sites will be explained and compared with the experimental results of mutations.

We also present the preliminary results for the structure of V1AR.