

Acetylcholin binding proteins are playing an essential role in the comprehension of the features of the cholinergic synapse. They are in the focus of the development of new therapy strategies against diseases like Alzheimer's dementia. New contributions to the knowledge about AChE, nAChR and β -amyloid have been made through combination of synthesis, biochemistry, docking, molecular dynamics and pharmacophore search.

With the synthesis of photogalanthamin a probe for identification of the APL binding site has been developed. Different tracer techniques have been evaluated for the isotopic labelling of APL. The location of the APL binding site was narrowed down using to a small area on the α -subunit of the nAChR mass spectroscopic methods.

Models of the nAChR were constructed to study the dynamic behaviour in MD simulations. The binding properties of agonists and APL and the resulting conformational changes of the receptor were studied with them. The simulation of sodium ion permeation through the pore succeeded with steered MD.

The LIE method was implemented for the prediction of binding affinities on the basis of inhibitors of the AChE. Hereby an efficient support has been established for the evaluation of inhibitor properties of new lead structures.

The dissociation behaviour of β -amyloids was studied by MD, hence multiple residues were localized, which are playing a part in the stabilisation of the aggregates. The allocation of suitable substrates to these residues would enable a causal therapy of Alzheimer's dementia.