Alzheimer's disease (AD), discovered in 1906, is the main source of dementia, affecting mainly the elder people of the age of over 60 year old. Despite intense theoretical and experimental researches the etiology of AD remains largely unknown. Consequently, there exist several drugs that can be used for symptom treatment but no efficient drugs have been found to cure this disease. Nowadays, there are about 20 different hypotheses about the cause behind pathological progress of AD. One of the most promising is the so called amyloid cascade hypothesis which posits that the neuron death is caused by progressive accumulation of amyloid beta (Aβ) peptides of 40 and 42 residues. Importantly, soluble Aβ oligomers but not mature fibrils are the culprit of the mental degeneration. Therefore, one possible ways to treat AD is to find drugs that can inhibit the activity of oligomers. To solve this problem one need to know oligomers' structures, but due to their transient nature, they cannot be experimentally resolved. In this situation, computer simulation is a good choice.

In this project, we propose using multi-scale molecular dynamics simulation to obtain oligomers' structure. Oligomers of different sizes ranging from dimer to 12-mer will be simulated first by replica exchange molecular dynamics with UNRES course-grained model. Then most representative structures followed from course-grained simulation will be refined and validated by conventional all-atom simulation. Final structures will be recommended as target for AD drug design as well as for designing markers to detect oligomer *in vitro*. The second goal of our project is that by simulating oligomers of different weights we will be able to theoretically verify the recent experimental observation that the minimal number of peptides to form a stable oligomer is 5 or 6.