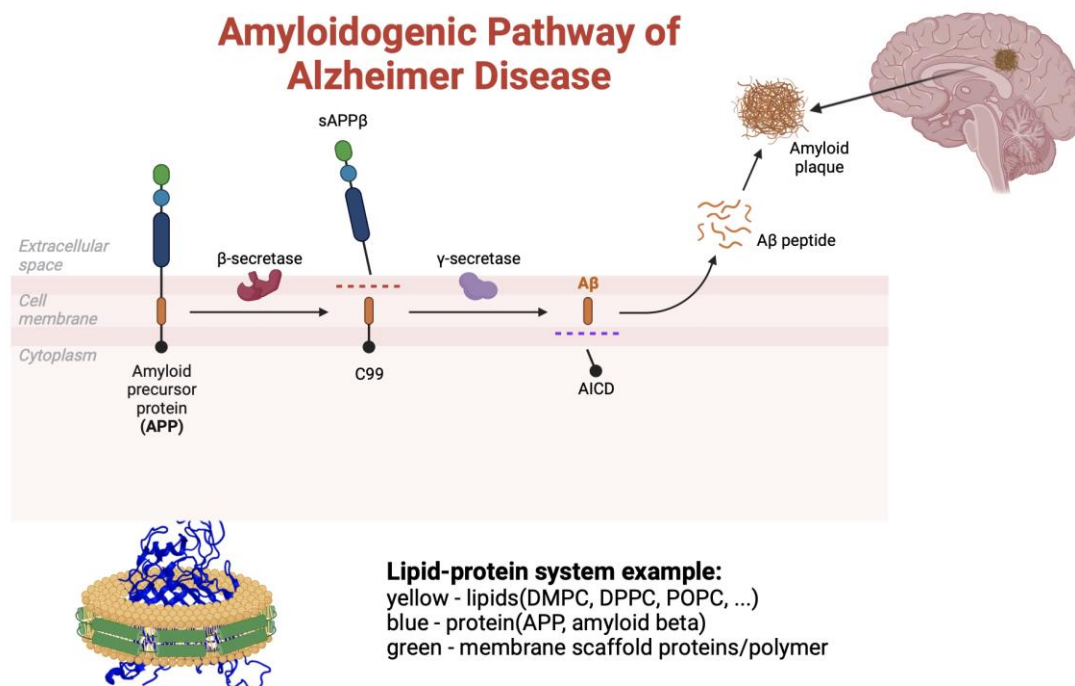# Investigation of lipid-protein system by Raman Spectroscopy and Molecular Dynamics

Yersultan Arynbek
Department of Raman Spectroscopy, Frank Laboratory of Neutron Physics

Introduction

At the present stage of development of experimental and theoretical methods for the analysis of molecular systems, the development of complex approaches to establish the patterns of their interaction with cell membranes and study the conformational changes in the structure and composition of molecules that occur in this case is becoming increasingly in demand. One of the most intriguing objects of such research is the peptides of the beta-amyloid group, which are formed from a transmembrane protein called the beta-amyloid precursor. As a rule, these peptides include about 40/42 amino acid residues. At the moment, it is generally accepted that the Aβ40 peptide does not have a negative effect on the human body, since it does not contain a number of amino acid residues that have pathogenic properties. In contrast, Aβ42 peptides are extremely dangerous and are thought to be the cause of Alzheimer's disease, which affects the brain, where they accumulate and fold into beta folds to form amyloid plaques (Fig. 1.).

Amyloidogenic Pathway of Alzheimer Disease

Lipid-protein system example:
yellow - lipids(DMPC, DPPC, POPC, ...)
blue - protein(APP, amyloid beta)
green - membrane scaffold proteins/polymer

Experimental:

Students will be introduced to the whole range of the measurement procedure, consisting of: calibration, alignment of laser lines, selection of optical filters and microlens, sample preparation, scanning of samples on a multimodal optical platform (CARS microscope http://flnph.jinr.ru /en/facilities/cars).

Simulation:

All molecular dynamics calculations will be performed using the GROMACS 5.1.3 software package (GROningen MAchine for Chemical Simulations), which is installed on the Hybrilit heterogeneous platform at JINR.

Requirements for the level of student training:

Students should know the basic principles of spectroscopy and condensed matter physics, should have basic skills of working with typical scientific software. Experience in computer simulation, spectral analysis will be advantageous.

Recommended literatures:

1. http://flnph.jinr.ru/en/facilities/cars
2. https://www.horiba.com/rus/scientific/technologies/raman-imaging-and-spectroscopy/raman-spectroscopy
3. http://solinstruments.com
4. https://www.gromacs.org
5. http://www.mdtutorials.com/gmx/

Number of students: 1

The project supervisor:

Yersultan Arynbek, researcher, Group of Nonlinear microspectroscopy, Department of Raman Spectroscopy, Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research