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Amyloid β-peptide: secondary structure analysis by Molecular Dynamics simulation

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Alzheimer's disease (AD) is a neurodegenerative disorder that is the sixth leading cause of death and the most common cause of brain dementia worldwide. Over the last years, representative advancements have been made in our understanding of AD by studying the molecular mechanisms underlying amyloid-β(Aβ) and tau proteins pathology.
In general, AD is characterized by the deposition of β-sheet–rich, insoluble Aβ plaques. Here, we investigated Aβ peptide settled in lipid structure, to understand their interaction using Molecular Dynamics(MD) simulation. We hope that in future these investigations could provide an opportunity for translating our understanding of the pathogenesis and physiological mechanisms underlying disease and related disorders into new diagnostic approaches and disease-modifying therapies to prevent disease or restore brain function for symptomatic individuals.

Primary authors: Mr ARYNBEK, Yersultan (JINR, INP, KazNU); SHUTIKOV, Artem (Department of Raman Spectroscopy, FLNP, JINR); Ms DEMINA, Ekaterina (Department of Raman Spectroscopy, FLNP, JINR); ZAKRYTNAYA, Darya (Department of Raman Spectroscopy, FLNP, JINR); Mr MAMATKULOV, Kakhramon (Department of Raman Spectroscopy, FLNP, JINR); Mr ARZUMANYAN, Grigory (Department of Raman Spectroscopy, FLNP, JINR)

Presenter: Mr ARYNBEK, Yersultan (JINR, INP, KazNU)

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