

Alzheimer's disease is an illness which affects the brain, leading to disabling memory loss, and the loss of other important cognitive function. Though the disease is not hereditary, there are genetic factors that can make people more likely to develop it. Until this decade it was widely believed that the damage from the disease that causes dementia was a result of the accumulation of Amyloid β peptide (a building block of protein, AB) in the brain, forming structures called plagues. This was believed as plagues have been found in the brain of every patient who has died of Alzheimer's. It is now becoming apparent however, that other toxic forms of these AB peptides (oligomers of the Aß peptide) may be responsible for the damage caused to neurons in the brain.



In Hungary, Gábor Paragi and colleagues of MTA-SZTE Biomimetic Systems Research Group (the Hungarian Academy of Sciences at the University of Szeged) and the Institute of Physics (at the University of Pecs) are probing the processes that lead to plaque formation, hunting for clues about, and causes of Alzheimer's disease. Many previous studies neglected the earlier activities of AB peptides as the final products - the plaques - which were thought to be critical, were most closely scrutinised. However, whilst investigating Aß peptide formation, it became apparent to Gábor Paragi and colleagues that mutations in the components (monomers) that form AB peptides can lead to

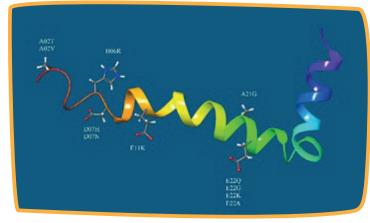
toxic effects.

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The research group has been using Replica Exchange Molecular Dynamics (REMD) techniques, utilising the computational resources and power of the Debrecen2 (Leo) GPU cluster to analyse the molecular dynamics at play during this process. They have discovered connections between the presence of certain structures and mutated toxic peptides. This will hopefully increase the understanding, and ultimately the treatability of this disease, reducing the burden of suffering endured by those affected and their families worldwide.



Project name: FEHERJEK Project Leader: Gábor Paragi

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