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Docking studies of coconut oil components with amyloid beta peptide fragments

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Virgin coconut oil is composed of group of unique fat molecules called Medium Chain Fatty Acids (MCFAs) which has always shown multiple health benefits like management of inflammatory diseases, cardio-vascular diseases, etc. Moreover, 50% of this oil is Lauric acid which is most important for building and maintaining the body's immune system. There are evidences that show the benefits of coconut oil in reducing the symptoms of Alzheimer's disease (AD) also. The aggregation of the Amyloid beta (A β) peptide fragments is considered as one of the causes for the onset of the pathogenecity observed in AD. This aggregation event starts from the binding of each of these soluble A β peptides with one another and forms an insoluble clumps called Amyloid Plaques which in turn deposit in the neurons and disrupt the cell signaling between them. Binding studies with the MCFAs of coconut oil, shows that these fatty acids bind with A β fragments 1-12, 1-16, 1-28 and 1-42 at similar sites that bind to metals like Al, Zn, Cu, etc. Interestingly, metal binding triggers aggregation events, and their inhibition is solicited from therapeutic point of view. Hence, studies with these fragments and binding of MCTs may be important in design of inhibitors for AD therapy.

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