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Molecular modeling of the binding characteristics of some natural flavonoid compounds to amyloid β -peptide-42**Awwad Abdoh Radwan Salama***King Saud University, Saudi Arabia*

The accumulation of amyloid beta peptide A β 1-42 in the brain is a critical early event in the progression of Alzheimer's disease. Four flavonoid compounds isolated from Psoralea fruits (PF) were found to have anti-Alzheimer properties in vitro and in vivo in recent research. These natural compounds inhibited A β 1-42 aggregation in a promising way. Docking studies and molecular dynamics (MD) simulations were used in our work to conduct a molecular modeling study on the substances as potential A β 1-42 aggregation inhibitors. A molecular mechanics calculation was performed to determine the binding free energy, gain insight into the binding modes of the ligands, and pinpoint the key interacting residues.

Biography

Awwad Salama received his B.S. in pharmaceutical sciences from Assiut-Egypt, Assiut University 1988, where he named as administrator member and got his MD in Pharmaceutical Organic chemistry in 1995. He got his Ph.D. in computer-aided drug discovery from Tokyo-Japan, Kitasato University in 2002. 2002-until now, he named as lecture, associate professor and professor at Faculty of Pharmacy, Assiut University, Egypt. In 2008-until now, he moved to College of Pharmacy, King Saud University, KSA. Awwad's work has led to 65 publications, 2 patents and several conferences' participations. He got two awards From 'ACDIMA Award as a co-author for best research from ACDIMA drug company (Oman, Jordanian' years 2008 and 2012) and he got Silver Medal from Geneva Innovation Salon (Switzerland, 2-6 April 2014).