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Natural products as Novel Therapeutic molecules against Alzheimer's Disease

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Abstract

Alzheimer's disease (AD) is considered the most devastating neurodegenerative disorder that affects more than 50 million people worldwide. AD is a complex and multifactorial disease where endogenous and exogenous factors can be involved in the triggering of this illness, whose hallmark is amyloid-β (Aβ), formed by cleavage of amyloid precursor protein by β- and γ-secretase. While there is no definitive cure for AD to date, drug discovery based on nutraceutical molecules for prevention and treatment of AD is a growing topic. As well as helping to delay disease development, natural products such as carotenoid and polyphenol compounds have demonstrated positive preventive efficacy.. We are focus on carotenoids by their chemical structure and their neuroprotective activity against Aβ aggregation using molecular docking analysis. In our computational analysis, lutein showed the most prevalent anti-amyloidogenic followed by cryptocapsin, astaxanthin, fucoxanthin, and the apocarotenoid bixin where important interactions between carotenoids and Aβ via hydrogen bonding and van der Waals interactions were involved. Curcumin is another interesting natural product that revealed to be a potential compound for treating of AD following different neuroprotective mechanisms, such as inhibition of aggregation and decrease in brain inflammation. But, the low bioavailability, and susceptibility to degradation in biological systems and poor solubility in plasma avoid converting this compound a medicine, but curcumin derivatives can be a potential alternative. We synthesised new derivatives of curcumin in order to have strong anti-aggregation ability but also enhanced anti-inflammatory behaviour. One curcumin derivatives exhibited a strong anti-aggregation effect higher than curcumin. Better bioactivity than difunctionalized compounds was demonstrated by monofunctionalized curcumin derivatives. Analysis of molecular docking showed that carotenoids and curcumin derivatives might adopt two pathways to inhibit Aβ aggregation: one by preventing fibril formation and the second by disruption Our studies thus illuminate mechanistic insights on how carotenoids and curcumin derivatives can inhibit Aβ aggregation.

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Biography

Johant Lakey Beitia currently works at the Center For Biodiversity and Drug Discovery, Instituto de Investigaciones Cientificas y Servicios de Alta Tecnologia. Johant does research in Neuroscience, Biotechnology and Chemical Biology. Their current project is 'carotenoids as anti-alzheimer's'. Her skills and expertise are Organic Synthesis, Alzheimer's Disease, Organometallics and Nuclear Magnetic Resonance.

Publications

1. Polyphenols as Potential Metal Chelation Compounds Against Alzheimer's Disease
2. Reproducible molecular networking of untargeted mass spectrometry data using GNPS
3. Isolation and identification of sapotexanthin 5,6-epoxide and 5,8-epoxide from red mamey (Pouteria sapota)
4. Carotenoids as Novel Therapeutic Molecules Against Neurodegenerative Disorders: Chemistry and Molecular Docking Analysis
5. Reproducible Molecular Networking Of Untargeted Mass Spectrometry Data Using GNPS

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