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Amyloid β Fibrils Disruption by Oleuropein Aglycone: Investigation of the Mechanism of Action of this Polyphenol from Extra Virgin Olive Oil

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ABSTRACT

In the Central Nervous System (CNS), EVOO produces interesting effects against neurodegenerative disorders including Alzheimer's disease (AD). The valuable properties of EVOO are largely ascribable to oleuropein aglycone (OA), the most abundant phenolic constituent. In particular, it has been demonstrated that in AD, OA produces strong neuroprotective effects being able to reduce amyloid β (Aβ) aggregates, diminishing the related cytotoxicity and inflammation. OA prevents the Aβ aggregation, but more important OA it was proven that is able to disrupt the preformed Aβ fibrils. Herein, we describe for the first time a comprehensive computational investigation about OA mechanism of action as Aβ fibrils disruptor at molecular level. We employed extensive molecular docking calculation and long-time molecular dynamics simulation for mimicking the system OA/Aβ fibrils for an aggregated time of 10 μs. Results showed that OA is able to move in depth within the Aβ fibrils targeting a key motif in Aβ peptide, known to be relevant for stabilizing the assembled fibrils. OA causes a structural instability of Aβ preformed fibrils, determining an effective Aβ fibrils disaggregation. Accordingly, this study highlighted the role of OA as a potent anti-amyloidogenic drug. On the other hand, our work can possess relevant implication for rationally designing potent multifunctional compounds acting as disease modifying anti-Alzheimer drugs for the development of innovative anti-AD therapeutics.

Keywords: Neurodegenerative disorders, Alzheimer's disease, Anti-Alzheimer drugs

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