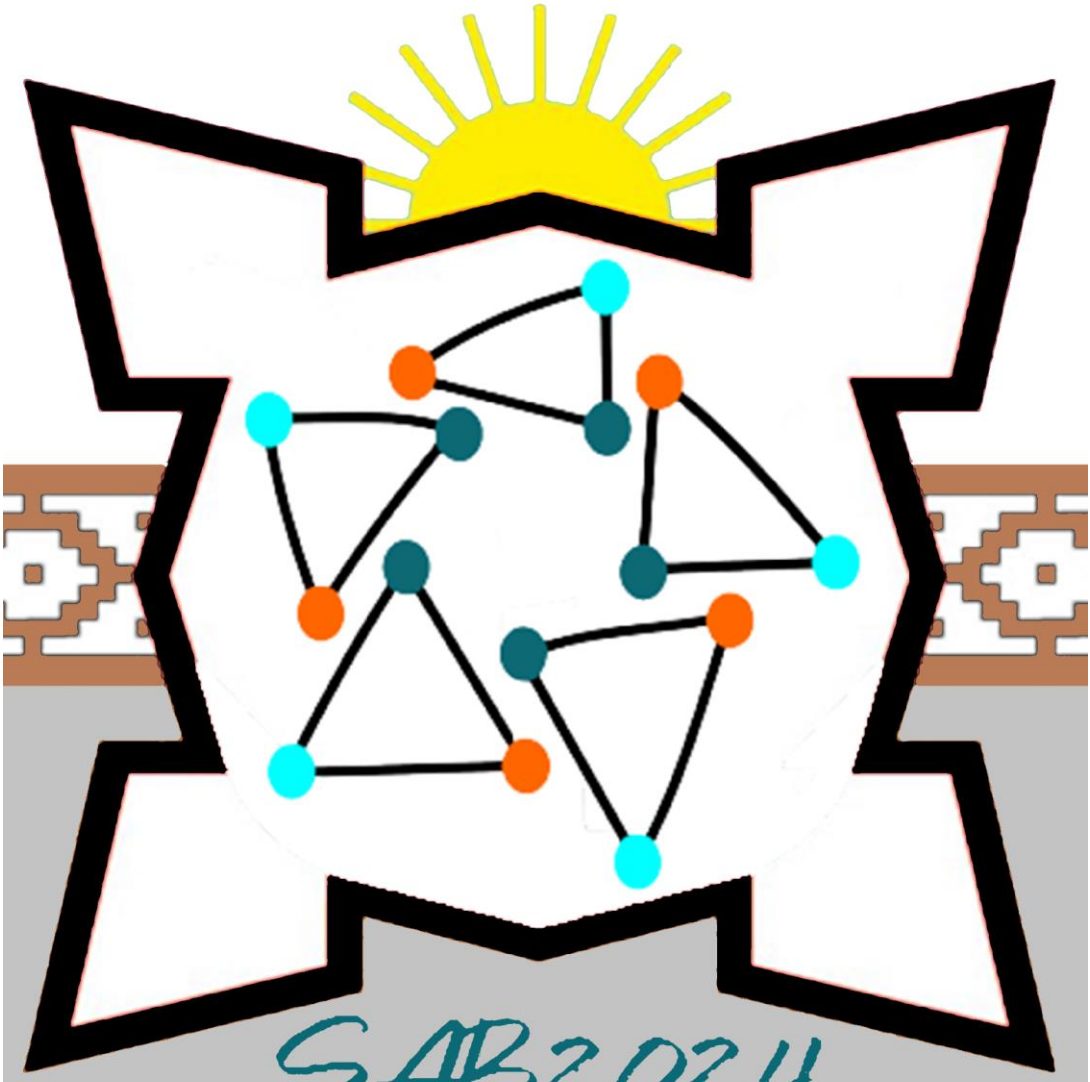
Sociedad Argentina de Biofísica

LII Reunión Anual

27 al 29 de noviembre



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Bahía Blanca, Argentina

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Multi-Target Fatty Acid Compounds for Alzheimer's disease: Modulation of AChE, nAChR, and Aβ Aggregation process

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Alzheimer's disease (AD), the most prevalent neurodegenerative disorder among the elderly, is characterized by progressive cognitive decline. The amyloid hypothesis proposes an exacerbated production of reactive Aβ structures (monomers, oligomers, fibrils). Additionally, the cholinergic hypothesis suggests that increased Aβ production reduces nicotinic acetylcholine receptor (nAChR) density, reflecting neuron loss and cholinergic denervation. Acetylcholinesterase (AChE), responsible for acetylcholine breakdown at its catalytic site (CAS), also promotes Aβ aggregation through its interaction with the peripheral anionic site (PAS). Dual-action AChE inhibitors targeting both CAS and PAS thus enhance cholinergic signaling and reduce Aβ aggregation, offering therapeutic advantages over conventional AChE inhibitors. Here, we investigated the role of natural fatty acids (FA) as potential multi-target compound candidates to manage this complex disease. By combining experimental and *in silico* approaches, we evaluated the effects of FA, focusing on three objectives: 1) assessing their interaction with and inhibition of AChE, 2) attenuating Aβ oligomerization or fibrillation, and 3) modulating nAChR activity. Results revealed a correlation between the evaluated effects and the hydrocarbon chain length and degree of unsaturation of the studied FA. Molecular docking indicated that almost all FA were positioned with the carboxyl group at CAS. However, only oleic acid and DHA formed salt bridges with H447 of the catalytic triad, displaying higher inhibitory capacity in AChE inhibition assays. Based on these findings, we plan to synthesize FA analogs to enhance the evaluated activities by creating hybrids between FA and a series of compounds previously synthesized in our lab with anti-AChE activity and enhanced nAChR potentiation, with the aim of providing new therapeutic strategies for AD.

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