Titolo del Progetto di Ricerca:

Rational design of curcumin-based bifunctional ligands for early diagnosis and therapy of Alzheimer's disease

Elenco WP

ERC	TITOLO WP	RESPONSABILE WP
PE	Computational simulation of ligands interacting with amyloid-beta aggregates	Maria Cristina Menziani
PE	Synthesis and characterization of curcumin-based ligands and their metal-complexes	Erika Ferrari
LS	Biological activity of selected molecules in neuronal cells	Carol Imbriano

Abstract

Alzheimer's disease (AD) affects approximately 10% of the world's population with 65 years of age, and the number of patients is expected to double in the next 20 years, leading to a huge cost for the society. AD is characterized by the formation of amyloid plaques and neurofibrillary tangles bringing the patient to a neurological disorder accompanied by the loss of cortical and subcortical neurons. Plaques are mainly made by amyloid-beta (Aβ) fibrils that interact each other forming extended structures. To date, the only way to assess definitively the presence of AD is post-mortem and there is no valuable cure for the disease. Only a few drugs for AD are available, and they are at best only able to offer some relief of symptoms. Besides, these are effective only for the first 6-12 months of the therapy, and only for the half of patients with a milder form of AD.

The aim of this project is to design, in a rational way, new multifunctional Curcumin-Derived agents for the treatment of the AD disease in order to provide both second-generation potential drugs with improved efficacy and safety, and early diagnostic tools of the disease.

The project involves multi-disciplinary and multi-methodological approaches, and it will be carried out by a group of researchers with complementary competences in the field of computational chemistry, synthesis, coordination chemistry, radiochemistry, molecular and cellular biology.

The use of computational simulations as a pervasive tool throughout the design cycle will allow us to shed some light on the determinants for fibril-ligand interactions, the topologies of fibril aggregation and the mechanisms of fibril destabilization upon ligand binding. We expect that this knowledge will accelerate the design of a) more effective molecule for early diagnosis and therapy of AD, and b) new experiments to aid in more accurate and efficient characterization of these agents.

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Firma del Responsabile scientifico

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