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Computational Oxalate-Curcumin Based Probe Molecules for Functionality in Alzheimer's Disease

Elizabeth Phillips* Yin Shao, PhD†

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†University of Oklahoma

Computational Oxalate-Curcumin Based Probe Molecules for Functionality in Alzheimer's Disease*

Elizabeth Phillips and Yin Shao, PhD

Abstract

Alzheimer's Disease (AD), is a progressive neurodegenerative disease that is fatal. Amyloid ? (A?) aggregates are produced in the relation between AD and its later stages. While AD is not necessarily present because of the A? aggregates, they are however a cohesive sublimate of each other within the later stages of the disease. Currently there are no drug preventative measures that have been successful in bringing treatment to the A? aggregates. It has been shown that AD had been most closely associated with the production of A? aggregates in relation to the progression of the disease. However, in regards to the lack of preventative measures in A? aggregates it is suggested that reactive oxygen species (ROS) should be taken into consideration when taking drug related measures. Specifically speaking it has been found that ROS levels are significantly higher in brains with AD than in brains that are healthy. Taking into consideration both the ROS levels, as well as the A? aggregates, it can be beneficial in detecting AD early on in order to take preventative measures.

CRANAD-X is a family of curcumin analogue molecules which have previously been used in NIRF (Near Infra-Red Fluorescence spectroscopy) imaging. This study is to show the computational values of each prospective system for an experimental value such as excitation, emission, and wavelength emission. Experimental values found in this computational study will help to further a close approximation to other molecules that are similar in structure in other experimental investigations. Similar molecules found in this study could be used for probes to detect A? aggregates, and ROS levels.

KEYWORDS: Alzheimer's Disease; ROS; CRANAD-X; Amyloid? aggregates

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School of Public Health
University of Nevada, Las Vegas

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Elizabeth Phillips
Yin Shao, PhD in Chemistry, University of Oklahoma
Coordinating Center: University of Nevada, Las Vegas

ABSTRACT

Alzheimer's Disease (AD), is a progressive neurodegenerative disease that is fatal. Amyloid β (Aβ) aggregates are produced in the relation between AD and its later stages. While AD is not necessarily present because of the Aβ aggregates, they are however a cohesive sublimate of each other within the later stages of the disease. Currently there are no drug preventative measures that have been successful in bringing treatment to the Aβ aggregates. It has been shown that AD had been most closely associated with the production of Aβ aggregates in relation to the progression of the disease. However, in regards to the lack of preventative measures in Aβ aggregates it is suggested that reactive oxygen species (ROS) should be taken into consideration when taking drug related measures. Specifically speaking it has been found that ROS levels are significantly higher in brains with AD than in brains that are healthy. Taking into consideration both the ROS levels, as well as the Aβ aggregates, it can be beneficial in detecting AD early on in order to take preventative measures.

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Keywords: Alzheimer's Disease, ROS, CRANAD-X, Amyloidβ aggregates

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