CALIFORNIA STATE SCIENCE FAIR
2017 PROJECT SUMMARY

Name(s)

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Project Number

S0514

Project Title

A Comparative Study on the Effectiveness of Plant Based AChE Inhibitors and Drug AChE Inhibitors for Treatment of AD

Abstract

Objectives/Goals

The purpose of this study was to investigate the binding affinities of Ferulic acid, Safranal and Curcumin derived from spices, Asafoetida, Saffron and Turmeric, for the inhibition of Acetylcholinesterase (AChE) and compare them to the binding affinities of the current AChEI medications, Rivastigmine, Galantamine and Donepezil. If these spices have similar binding affinities then they have the potential to be effective treatments for memory related symptoms of Alzheimer's Disease.

Methods/Materials

Laptop computer with molecular building & docking programs, Avogadro 1.1.1, & AutoDockTools 1.5.6. Ligands were built & optimized using Avogadro 1.1.1, & docked into AChE using AutoDockTools 1.5.6 to get binding affinities of each molecule.

Results

Among the 3 plant based inhibitors tested, Curcumin had the strongest binding affinity to AChE with -12.1 kcal/mol. Ferulic Acid and Safranal both had a binding affinity of -7.1 kcal/mol to AChE.

Of the 3 drug molecules tested, Donepezil displayed a binding affinity of -10.5 kcal/mol & Rivastigmine & Galantamine had binding affinities of -9.3 kcal/mol & -8.1 kcal/mol.

These results show that the binding affinities of each molecule tested are within a close range of each other.

Conclusions/Discussion

I compared the binding affinities of current medications (Rivastigmine, Galantamine, and Donepezil) to that of known plant-based AChE inhibitors (Ferulic Acid, Safranal, and Curcumin) for the inhibition of AChE. Curcumin was found to have the strongest binding affinity to AChE, out of all the molecules tested, with a binding affinity of -12.1 kcal/mol followed by Ferulic Acid and Safranal, each with a binding affinity of -7.1 kcal/mol. The 3 drugs molecules included Donepezil, Galantamine and Rivastigmine. Donepezil displayed a binding affinity of -10.5 kcal/mol followed by Rivastigmine and Galantamine with binding affinities of -9.3 kcal/mol and -8.1 kcal/mol.

The hypothesis that the binding affinities of Ferulic acid, Safranal and Curcumin derived from spices, Asafoetida, Saffron and Turmeric for AChE inhibition are very similar to the binding affinities of current medications, Rivastigmine, Galantamine and Donepezil was proven to be correct by the results of my study. Therefore, these plant-based AChE inhibitors have the potential to treat memory related symptoms of Alzheimer's Disease.

Summary Statement

My study investigated the effectiveness of plant-based AChE inhibitors compared to drug AChE inhibitors for the treatment of symptoms of Alzheimer's Disease.

Help Received

I attended a Computational Modeling workshop at UCR under the guidance of my teacher, where I got the programs used to conduct the study. In addition, I received feedback throughout my study from Dr. Christopher C. Roberts, P.h.D.