CALIFORNIA STATE SCIENCE FAIR
2014 PROJECT SUMMARY

Name(s)

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Project Number

34628

Project Title

3D Structure of Powerful Antimicrobial and Potential Cancer Treatment Naegleriapore A

Abstract

Objectives/Goals

The objective of my project was to find an accurate homology model of the powerful antimicrobial and potential cancer treatment naegleriapore A.

Methods/Materials

Materials: Computer, Protein sequence, Modeller software, Access to modweb homology modeling servers, Jmol and Protein Workshop, Uniprot.org, Pfam, Rosetta protein docking

Methods: Naegleriapore A sequence copied from uniprot and searched on Pfam database for subunit. Then saposin B subunit was extracted and sent to the homology modeling servers of Modweb. The best two models where then submitted to Rosetta protein docking to be turned into pores (Mod1 and Mod2). For Mod3 and Mod4, Modeller was used to create homology models for the subunits. Template molecules 1N69 or 2QYP were used for Modeller's homology modeling. The best results from each template were sent to Rosetta to be made into pores. The final resulting pores were analyzed with molecular viewing programs such as Jmol and Protein Workshop.

Results

Results show that mod1 and mod2 were both incorrect and didn't fit my criteria. Criteria included: expressing the correct lengths to pass through the cell membrane (at least 3.5 nanometers), a pore radius of 3.6-5.2 nanometers wide, a molecular weight of 66 kDa, low energy score indicating spontaneous formation, a clear hydrophobic charge on the outside and a clear polar charge inside. Mod3 produced a perfect pore, but statistically poor subunits. Mod4 had statistically correct subunits but made a pore that didn't fit the size criteria.

Conclusions/Discussion

The subunit that was statistically incorrect, mod3, produced a better resulting pore than that of the statistically correct subunit, mod4. Mod3 fit the hypothesized criteria and is accepted as the final model. The model of naegleriapore A can be used to estimate its interactions as well as be used for ligand docking, which could lead to its development as an antimicrobial and anticancer drug.

Summary Statement

Modeling an accurate 3D structure is the first step to understanding and utilizing naegleriapore A as an effective antimicrobial and cancer treatment.

Help Received

Dr. Peter Rose, Scientific Lead, RCSB Protein Data Bank, UCSD showed me how to use the homology modeling software and various databases.