

PROJECT INTRODUCTION

Objectives

To construct better ligands against targets involved in diabetes.

Project Investigator / Manager

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Period of Project

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Abstract

Several ligands have been designed against steroid receptors for treatment in diabetes and atherosclerosis. We are now trying to dock novel compounds found to interact against several of these receptors. We will next design compounds with higher efficacy.

PROJECT DETAILS

Description

Several compounds have been designed against many known steroid receptors as treatment in many diseases from diabetes to atherosclerosis. We are working with several novel compounds which appear to have synergistic response and could greatly increase the efficacy of treatment in diabetes. Binding and functional assays are being carried out and our lab is in the process of virtual docking of these compounds to predict the mechanism of binding. We will next carry our structure determination using X-ray crystallography. Real experimental information will be used in conjunction with computational modeling to increase the prediction quality. Better prediction will lead to more efficient methods of ligand design.

We have already carried out predictions of several of these compounds but would like to extend this study to a large library. This information will make possible design of more suitable compounds in the future. Better prediction will also help to minimize the number of wet lab experiments which are quite expensive. Thus better computation will lead to cheaper experimentation as well as better ligands.

Collaborating Organizations:

- National University of Singapore
- Nanyang Polytechnic