Protein Nano-Object Software for Biomolecular Modeling (2013-020)

Allows for modeling nano-objects with biological macromolecules

Market Overview

This Protein Nano-Object Integrator (ProNOI) software allows for researchers to generate atomic-style geometrical objects in the desired shape and dimensions either from cryelectron photography or user-specified shape. Biomolecular modeling is important to address biological problems at the molecular level and to understand the interactions between molecules to predict behavior. This is especially useful for pharmaceutical development and within the general research community. Biological macromolecules must frequently be modeled in conjunction with nano-objects in order to understand their interactions. However, nano-objects are typically unavailable in commonly used modeling systems and the customization of these objects can be limited. Clemson University researchers have developed the versatile Protein Nano-Object Integrator (ProNOI) software which allows for modeling of nano-objects with biological macromolecules. An unlimited number of customizable objects can be created and combined with biological macromolecules. The objects can be tailored in regards to their position, size, shape, distributed charge, and surface or volumetric parameters depending on the user's needs.

Technical Summary

The ProNOI software provides a convenient and user-friendly method for simulating surfaces and regular objects. An unlimited number of objects can be created and combined with biological macromolecules in the Protein Data Bank (PDB) format file. Once the objects are generated, the user can use sliders to manipulate their shape, dimension and absolute position. In addition, the software offers the option to charge the objects with either specified surface or volumetric charge density and to model them with user-desired dielectric constants. According to the user's preference, the biological macromolecule atoms can be assigned charges and radii with four force fields, including Amber, Charmm, OPLS and PARSE. Furthermore, the output file is compatible with most biophysical software.

Application

Pharmaceutical development; institutional research

Development Stage

Working Prototype

Advantages

- Enables customizable object property parameters, allowing for various scenarios of modeling and multiple object manipulation
- Is compatible with commercially available bimolecular modeling software packages, enabling easy integration into existing research
- Allows creation of atomic-style objects from Cryo-electron photography

App Type	Country	Serial No.	Patent No.	CURF Ref. No.	Inventors
Copyright	United States	NA	NA	2013-020	Dr. Emil Alexov Dr. Nicholas Smith

About the Inventor

Dr. Emil Alexov

Professor of Biophysics and Bioinformatics at Clemson University

Prior to joining Clemson, Dr. Emil Alexov earned his B.S., M.S., and Ph.D. in Physics at Sofia University in Sofia, Bulgaria. Dr. Alexov was involved with co-developing the Multi Conformation Continuum Electrostatics (MCCE) method, one of the most popular methods for calculating pKa's accounting for alternative positions of the side chains, structured waters and ligands. Currently, his research lab is maintaining and developing DelPhi package for modeling electrostatics in proteins, RNAs and DNAs.

For more information on this technology contact:

A. Chris Gesswein
Director of Licensing for Technology Transfer
E: agesswe@clemson.edu
P: (864) 656-0797