Web-based Fragment Library

Junjie Wang, Pradeep Kumar Gurunathan, Lyudmila Slipchenko
Department of Chemistry, Purdue University

ABSTRACT

A new polarized force field BioEFP for modeling process in biology is far superior in accuracy to the common classical force fields. One of the main shortcomings of BioEFP is that the parameters are not readily available, thus it will take a lot of time to be calculated.

Developing an online repository of pre-computed fragment parameters and a similarity algorithm will allow ascribing each fragment of a biological macromolecule to a pre-defined fragment.

This study incorporates three parts to create the online repository. First, the visual design for the website using the Hypertext Markup Language and the Cascading Style Sheets to create the format for each part on the web page. Secondly, the Hypertext Preprocessor is used for the server side to run certain functions and building dynamic websites. Lastly, an online database is created by MySQL to sort and organize all the data file. The results from the project is allowing us to upload our own file with xyz coordinates and get the result as the efp file.

KEYWORDS

Web development, Fragment library