

"Our aim is to identify and develop antiviral drugs against dengue, hepatitis C, West Nile, and yellow fever viruses"

06 November 2007 | News

image not found or type unknown



"Our aim is to identify and develop antiviral drugs against dengue, hepatitis C, West Nile, and yellow fever viruses"

-Dr Daniel Dias, Director, IBM Indian Research Laboratory

In an interview with BioSpectrum, Dr Daniel Dias, Director, IBM Indian Research Laboratory, gives an insight into the Discovering Dengue Drugs "Together" project, IBM's initiatives towards healthcare and the World Community Grid.

When was the project Discovering Dengue Drugs "Together" launched?

Phase 1 of the project began in August 2007 and will finish in early 2008. Phase 2 will start Fall 2007 and complete by the end of 2008.

How does it work?

"Discovering Dengue" project is distributed using the BOINC client, which is available for download on the IBM site for computers with Windows, Macintosh, or Linux operating systems. The calculations done on World Community Grid will predict which small molecule compounds, out of the millions contained in our library database, will inhibit the flavivirus protease.

Phase 1 of this project will predict how each small molecule might bind to the active site of the viral protease. This phase also produces preliminary "energies" that coarsely rank the strength of the intermolecular interactions between the compound and viral protease.

Phase 2 will accurately predict free energies of binding between each compound and the viral protease. This calculation utilizes the binding orientations calculated in phase 1. Due to computation time required for each free energy of binding calculation, only compounds with "good" scores from phase1 will be selected for Phase 2 calculations.

How far has the vast computational research power been successful in identifying drug molecules for HIV and AIDS?

Thanks to the volunteer power of World Community Grid, researchers completed five years of research for the FightAIDS@Home project in just six months, and IBM was able to send the best anti-HIV protease drug compounds to synthetic chemists so they could incorporate them into the design of even better inhibitors than the clinically-approved drugs. This work required quadrillions of computations of 270 protease mutants against a set of 2,000 chemicals that the National Cancer Institute has identified as a "diversity sample," e.g. representing the full variety of chemicals.

The initial results from FightAIDS@Home were published in the ACS Journal of Chemical Information and Modeling in a paper entitled "Analysis of HIV wild-type and mutant structures via in silico docking against diverse ligand libraries." Two additional scientific papers are also in preparation. This project was launched in November 2005 and is expected to run through 2008.

How has the World Community Grid impacted research?

World Community Grid has a significant impact on research because it can help hasten the progress of projects into further phases of development. For example, on this project, researchers estimate that they would need 50,000 years of compute time on traditional computing devices. Using World Community Grid, research will only take approximately a year.

Researchers on the Dengue Fever project credit World Community Grid with allowing them to do more correct science because they don't have to make as many assumptions to conduct the calculations in a reasonable timeframe. As a result, they will have less "false positive" results, be able to study a smaller group of drug molecules that have a better odds of actually working, and thus speed drug development.

How does IBM see the future of healthcare and what are some of the initiatives that the company has taken to address the issue?

IBM recently announced that it has made available an advanced software technology that can help predict the transmission of diseases across countries and around the globe to the open source community. The tool will aid scientists and public health officials in understanding and planning more efficient responses to health crises, ultimately providing new tools for protecting population health. The software, known as Spatio-Temporal Epidemiological Modeler (STEM), is now available for use through the Eclipse Open Healthcare Framework Project (OHF), hosted at the Eclipse Foundation, the non-profit foundation that guides the Eclipse open source community.

Shalini Gupta