Communiqués de presse

# Grâce au World Community Grid d'IBM, une nouvelle avancée dans la lutte contre le sida

**Paris - 02 mars 2010:** Une équipe de chercheurs a découvert deux composés du virus HIV prouvant l'existence d'un enzyme créateur de nouvelles particules infectieuses. Cette découverte permettra le développement de médicaments aux nouvelles capacités thérapeutiques capables de contrer les résistances développées par le virus. L'équipe s'est appuyée sur les capacités de calcul du World Community Grid(1) d'IBM via le projet FightAIDS@Home**.**

*(1)***Le World Community Grid** est une grille d'internautes solidaires mettant la puissance de calcul inexploitée (en moyenne 80%) de leur ordinateur, au service de la recherche, dans le cadre des projets de leur choix. Ils traitent simultanément des calculs complexes que les chercheurs ont divisés en petits morceaux. Ce «calcul distribué» permet ainsi de réduire considérablement les délais de traitement. Le WCG est la plus importante grille de calcul publique à but non lucratif avec 500 000 membres dans 200 pays et 1,7 million d'ordinateurs inscrits à ce programme. Depuis son lancement, il a permis de réaliser l'équivalent de 235 000 années de calculs et de renvoyer 266 millions de résultats, à savoir près de 2 résultats par seconde.

A team of researchers at the renowned Scripps Research Institute has discovered two new compounds that prove the existence of new binding sites on HIV protease. Associate Professor C. David Stout, senior author of the study, explained "These results open the door to a whole new approach to drug design against HIV protease," which is an enzyme used by HIV to create new, infectious viral particles.

According to the World Health Organization, about 33 million people currently live with HIV infections. Several drugs used to treat AIDS inhibit this HIV protease target, but drug-resistant mutants that impede the effectiveness of these drugs keep appearing and getting worse.

Two members of the FightAIDS@Home team, Research Associate Alex L. Perryman, Ph.D., and Professor Arthur J. Olson, were part of this innovative research and are now working to extend it. This experimental breakthrough will serve as the basis for new drug development to combat the increasing number of drug-resistant HIV strains and to improve the potency of current drug therapies. The results form the groundwork for a new class of more powerful treatments to fight HIV/AIDS. The findings appear as the March cover story in the journal *Chemical Biology and Drug Design*.

Utilizing computing power from 1.5 million devices networked through IBM'sWorld Community Grid, the new sites on the HIV protease are being used as docking targets for virtual screening experiments, in order to guide the development of these chemical compounds into a new class of potent HIV inhibitors. Using the massive computational resources of the World Community Grid, the FightAIDS@Home team has already docked over 500,000 compounds against these newly characterized binding sites.

By aggregating the unused cycle time of 1.5 million personal computers donated by volunteers in over 80 countries, World

Community Grid is now the world's largest public humanitarian grid, equivalent in power to a Top 10 supercomputer, and crunched more than 107,000 years of computational time in just 5 years for the Scripps Research Institute project, providing more than 104 million calculations.

"IBM's World Community Grid and its volunteers help us run millions of computations to evaluate the potential interactions between compounds and mutant viral proteins," said Dr. Arthur J. Olson, Anderson Research Chair Professor, Department of Molecular Biology at The Scripps Research Institute. "Through this effort we were able to significantly speed up our investigation. Without the computational power of World Community Grid, it would have taken us many more years to get to this important step in our research."

Once the HIV virus enters a human cell, it uses a small set of proteins called enzymes to force the cell to produce many new copies of itself, which then go on to infect other cells. Most HIV drugs work by blocking the operation of one or more of these enzymes. In the current work, the Scripps researchers are looking for new compounds that will stabilize the inhibited conformation, or shape, of the HIV protease enzyme, and thus help stop the virus from replicating. Because HIV mutates so frequently, some drugs that inhibit the enzyme from replicating are no longer working, or are not working as effectively. By running calculations on the World Community Grid FightAIDS@Home project, the team at Scripps is trying to develop new drugs that bind to more parts of the mutant enzyme, thereby shutting it down more effectively.

World Community Grid speeds up humanitarian research by providing scientists with millions of dollars of supercomputer power, for free, that would otherwise not be available to them.

In a second paper recently published in the *Journal of Molecular Biology*, the Scripps team has used computational modeling to improve understanding of another HIV enzyme and key drug target - integrase. Integrase, along with protease and a third enzyme, reverse-transcriptase, is one of three key proteins that allow the HIV virus to take over the cellular machinery of the host cell and replicate itself. By producing a more accurate model of integrase, the research allows further searches for new drug molecules that will inhibit the mutant drug resistant forms of this enzyme, as well. The Scripps team was recently awarded government stimulus funding as part of the American Recovery and Reinvestment Act to advance their new project against HIV integrase.

"The volunteers around the world who donate their computer time have helped usher in a potentially new class of drugs that may save lives and increase the quality of life for people living with HIV," said Dr. Joesph Jasinski, Distinguished Engineer and Program Director of IBM's Healthcare and Lifesciences Institute. "World Community Grid enables a smarter way to conduct promising research by providing unprecedented computing power to projects that might not be positioned to make a difference in the world without access to a free supercomputer."

The FightAIDS@home project will continue to run calculations to further this research against drug-resistant mutant "superbugs" of HIV.

"In the fight against HIV/AIDS it is important to remind people that HIV has not gone away, and that there are many things still to be done," said Joe Solmonese, President of the Human Rights Campaign. "World Community Grid is one way to get involved and makes it easy to contribute to this important research in a meaningful and effective way."

To donate your computer cycle time to humanitarian research covering areas from cancer to more nutritious rice to more efficient energy sources, please visit: www.worldcommunitygrid.org. From this site you can install a small, safe, and secure program that will connect you to the grid. When your computer is idle, data is requested from World Community Grid's server to

perform a computation.  Once finished, the result is sent back to the server, prompting it for a new piece of work.  It is not necessary to leave a computer on more than usual and we encourage members to continue their normal routines.  We can harvest substantial computational power during a normal work day just by taking advantage of the time when someone is on the phone, talking with colleagues, taking a coffee break or doing simple tasks that don't require the full power of the computer.

Other projects running on World Community Grid have produced results including:

· The Help Defeat Cancer project proved their more accurate technique for identifying cancer and received a $2.5 million grant from NIH to further deploy its system.

· Discovering Dengue Drugs Together project has identified potential antiviral compounds and is continuing with laboratory work on those.

· Nutritious Rice for the World project has already returned 12 million transactions and 11,000 years of compute time.

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