

## Tokyo Institute of Technology and Astellas Launch Collaborative Research for New Anti-Dengue Virus Drugs for Neglected Tropical Diseases

### - IT drug-discovery research through use of Tokyo Tech's Supercomputer TSUBAME2.0 -

**Tokyo, Japan, March 21, 2012** – Tokyo Institute of Technology (“Tokyo Tech”; Tokyo, Japan; President: Yoshinao Mishima) and Astellas Pharma Inc. (“Astellas”;Tokyo:4503; President and CEO: Yoshihiko Hatanaka) today announced that they have signed a joint research agreement for drug discovery research utilizing Tokyo Tech’s TSUBAME2.0 supercomputer to efficiently discover candidates for the treatment of neglected tropical diseases (“NTDs”)<sup>(1)</sup> caused by dengue virus.

NTDs, prevalent mainly among the poor in tropical areas of developing countries, are infectious diseases spread by parasites or bacteria. As it is estimated that approximately one billion people are affected with NTDs worldwide, NTDs are a serious healthcare issue that is being addressed on a global scale. Among them, diseases caused by dengue virus, such as dengue fever/dengue hemorrhagic fever<sup>(2)</sup> are with high unmet medical needs for treatment and development of new therapeutic drugs. There is no existing drug to treat dengue fever/dengue hemorrhagic fever in the market as well as under development, and the effectiveness of some vaccines to prevent dengue virus currently under development is unclear at this time.

Under the collaborative agreement, Tokyo Tech which has cutting-edge computation technique, and Astellas will cooperate on an IT drug-discovery research project for the treatment of NTDs caused by dengue virus. The research will be conducted in collaboration with a research group led by Professor Yutaka Akiyama, Dr.Eng., at the Department of Computer Science in the Graduate School of Information Science and Engineering, with a proven track record in the field of bioinformatics<sup>(3)</sup> research, and Associate Professor Masakazu Sekijima, Ph.D., at the Global Scientific Information and Computing Center, with a proven track record in the field of computational chemistry research.

The collaborative research is largely divided into two phases. In the first step, data mining<sup>(4)</sup> of public information such as patents and published articles will be carried out to obtain useful and effective knowledge about the drug discovery for the treatments for diseases caused by dengue virus. In the second step, *in-silico* screening<sup>(5)</sup> will be performed to identify compounds which are predicted to have anti-dengue virus activities. Tokyo Tech boasts Japan’s first petaflop class supercomputer TSUBAME2.0, and will assume responsibility for data mining and for *in-silico* screening calculations of commercially available compounds. Astellas will be responsible for preparing input data for data mining, selecting, and listing of hit compounds to be evaluated based on the *in-silico* screening calculations, thereby implementing efficient drug discovery in a short time period.

Tokyo Tech and Astellas will work together to accelerate the discovery of new drugs for patients suffering

from dengue fever/dengue hemorrhagic fever in the world, through their collaborative research aiming to contribute to improve global public health problems.

Also, Tokyo Tech and Astellas signed a joint research agreement for drug discovery research utilizing Tokyo Tech's TSUBAME2.0 supercomputer to efficiently discover candidates for the treatment of NTDs caused by protozoan parasites on July 30, 2012.

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### **Tokyo Institute of Technology (Tokyo Tech)**

Tokyo Institute of Technology established as Tokyo Technical School in 1881, became Tokyo Technical High School in 1929, and then acquired the university status in 1929. Tokyo Tech is the largest national university of science and technology in Japan with a 130 year history. The creative education at Tokyo Tech has resulted in fostering a great number of excellent alumni, including Dr. Hideki Shirakawa, Nobel laureate in chemistry, and in sending them to science fields and Japanese major companies which have helped support Japan's economy. Tokyo Tech has three schools (Science, Engineering, and Bioscience and Biotechnology), six graduate schools (Science and Engineering, Bioscience and Biotechnology, Interdisciplinary Graduate School of Science and Engineering, Information Science and Engineering, Decision Science and Technology and Innovation Management), five research laboratories under the Integrated Research Institute, and numerous other Research and Service Centers. For further information on Tokyo Tech please see the university website at [www.titech.ac.jp/english/index.html](http://www.titech.ac.jp/english/index.html).

### **Astellas Pharma Inc. (Astellas)**

Astellas' raison d'être is to contribute toward improving the health of people around the world through the provision of innovative and reliable pharmaceutical products. Astellas has approximately 17,000 employees worldwide. The organization is committed to becoming a global category leader in Urology, Immunology (including Transplantation) and Infectious Diseases, Oncology, Neuroscience and DM Complications and Kidney Diseases. For more information on Astellas Pharma Inc., please visit the company website at <http://www.astellas.com/en/>

Astellas is committed to improving "Access to Health\*" in developing countries through its partnership initiatives. As part of the contribution to Access to Health, Astellas is committed to undertake an initiative of drug discovery for patients infected with and suffering from NTDs in the world by utilizing its know-how and assets of drug discovery research.

\*: Many therapeutic areas and diseases with high unmet medical needs remain in the world. Furthermore, there are many people who are unable to access adequate medical care due to poverty or weak health systems. Astellas recognized these remaining issues as "Access to Health" and proactively addresses them as responsible corporate citizen.

## **TSUBAME2.0 supercomputer**

TSUBAME2.0 is a production supercomputer operated by Global Scientific Information and Computing Center (GSIC), Tokyo Institute of Technology in corporation with our industrial partners, including NEC, HP, NVIDIA, Microsoft among others. Since Fall 2010, it has been one of the fastest and greenest supercomputers in the world, boasting 2.4 PFlops peak performance by aggressive GPU acceleration, which allows scientists to enjoy significantly faster, larger computing than ever. This is the second instantiation of our TSUBAME-series supercomputers with the first being, as you might guess, TSUBAME1. It also employed various cutting-edge HPC acceleration technologies, such as ClearSpeed and NVIDIA GPUs, where we had learned many important technical lessons that eventually played a crucial role in designing and constructing our latest supercomputer. Compared to its predecessor, TSUBAME2, while keeping its power consumption nearly the same as before, achieves 30x performance boost by inheriting and further enhancing the successful architectural designs.

### **(1) Neglected tropical diseases (NTDs)**

NTDs are infections caused by parasite, bacteria and virus which are mainly endemic in tropical areas of developing countries. It is estimated that over 1 billion people are affected worldwide only with the 17 diseases\*\* of NTDs on which currently WHO is focusing on. Since these patients do not have enough access to needed medicine and healthcare, NTDs are not only a global health challenge but are said to be associated with poverty and affect economic growth in developing countries.

\*\* Group of 17 diseases : Buruli ulcer, Chagas disease (American trypanosomiasis), cysticercosis, dengue fever/dengue hemorrhagic fever, dracunculiasis (guinea-worm disease), echinococcosis, foodborne trematode infections, human African trypanosomiasis, leishmaniasis, leprosy, lymphatic filariasis, onchocerciasis, rabies, schistosomiasis, soil transmitted helminthiasis, trachoma, endemic treponematoses (including yaws)

### **(2) Dengue Fever/Dengue Hemorrhagic Fever**

Dengue fever/dengue hemorrhagic fever are dengue virus infections spreading along with the mosquitoes (mainly, *Aedes aegypti*). Usually, partial of dengue fever which is non-fatal febrile disease can progress to a severe disease called dengue hemorrhagic fever. Dengue virus infections are mosquito-borne disease which spread to tropical/subtropical areas like South-eastern Asia, South Asia, Central and South America and Caribbean countries, also occur in Africa, Australia, China and Taiwan.

### **(3) Bioinformatics**

Bioinformatics is a field that uses computer technology to analyze biological data.

### **(4) Data mining**

Data mining is a technology that applies statistics, artificial intelligence and machine learning technology to massive amounts of data comprehensively to extract useful knowledge.

### **(5) *In-silico* screening**

*In-silico* screening is a technology that identifies the most useful chemical compound that binds to the macromolecular target of interest via high performance computers such as a supercomputer. *In-silico* means "in the silicon chip" or "with computers."

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