

3D motion of common cold virus offers hope for improved drugs

July 16 2012, By Rebecca Scott

Melbourne researchers are now simulating in 3D, the motion of the complete human rhinovirus, the most frequent cause of the common cold, on Australia's fastest supercomputer, paving the way for new drug development.

Rhinovirus infection is linked to about 70 per cent of all asthma exacerbations with more than 50 per cent of these patients requiring hospitalization. Furthermore, over 35 per cent of patients with acute chronic obstructive pulmonary disease (COPD) are hospitalised each year due to respiratory viruses including rhinovirus.

A new antiviral [drug](#) to treat rhinovirus infections is being developed by [Melbourne](#) company Biota Holdings Ltd, targeted for those with these existing conditions where the [common cold](#) is a serious threat to their health and could prove fatal.

A team of researchers led by Professor Michael Parker from St Vincent's Institute of Medical Research (SVI) and the University of Melbourne is now using information on how the new drug works to create a 3D simulation of the complete rhinovirus using Australia's fastest supercomputer.

“Our recently published work with Biota shows that the drug binds to the shell that surrounds the virus, called the capsid. But that work doesn't explain in precise detail how the drug and other similar acting compounds work,” Professor Parker said.

Professor Parker and his team are working on the newly installed IBM Blue Gene/Q at the University of Melbourne with computational biologists from IBM and the Victorian [Life Sciences](#) Computation Initiative (VLSCI).

In production from 1 July 2012, the IBM Blue Gene/Q is the most powerful supercomputer dedicated to life sciences research in the Southern Hemisphere and currently ranked the fastest in [Australia](#).

“The IBM Blue Gene/Q will provide us with extraordinary 3D computer simulations of the whole virus in a time frame not even dreamt of before,” Professor Parker said.

“Supercomputer technology enables us to delve deeper in the mechanisms at play inside a human cell, particularly how drugs work at a molecular level.

“This work offers exciting opportunities for speeding up the discovery and development of new antiviral treatments and hopefully save many lives around the world,” he said.

Professor Parker said that previously we have only been able to run smaller simulations on just parts of the virus. Professor James McCluskey Deputy Vice-Chancellor (Research) at the University of Melbourne said:

“The [work](#) on rhinovirus is an example of how new approaches to treat disease will become possible with the capacity of the IBM Blue Gene Q, exactly how we hoped this extraordinary asset would be utilised by the Victorian research community in collaboration with IBM.”

“This is a terrific facility for Victorian life science researchers, further strengthening Victoria’s reputation as a leading biotechnology centre,” he

said.

Dr. John Wagner, Manager, IBM Research Collaboratory for Life Sciences-Melbourne, co located at VLSCI, said these types of simulations are the way of the future for drug discovery.

“This is the way we do biology in the 21st Century,” he said. The newly operational IBM Blue Gene/Q hosted by the University of Melbourne at the VLSCI is ranked 31st on the prestigious global TOP500 list.

The TOP500 table nominates the 500 most powerful computer systems in the world.

The VLSCI is an initiative of the Victorian Government in partnership with the University of Melbourne and the IBM Life Sciences Research Collaboratory, Melbourne.

Provided by University of Melbourne

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