MedicalXpress

Supercomputers join cancer fight

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Edmonton-A University of Alberta physicist will lead the fight against cancer, armed with a supercomputer and the will to make Alberta one of the world's top innovation centres.

Jack Tuszynski, who is the Allard chair, Division of Experimental Oncology at the Cross Cancer Institute and professor in the Department of Physics, will lead the three-year $5.6 million collaborative project that will take the fight against cancer to the molecular level in order to determine what drug compounds will work best when they interact with affected cells.

"Instead of trial and error, we'll employ sophisticated predictive software and bioinformatic algorithms to select drugs that can be moved more quickly from the laboratory to the trials process and perhaps into production and the clinic," said Tuszynski.

This is done, he says, by whittling down the body's vast inventory of chemical compounds in hopes of finding the one that is paramount in either restricting the division of cancer cells, or promoting the division of cells that need to be active in the fight against the disease.

"We have a pretty good idea of what the biological players are in cell division," said Tuszynski. "You either activate those players that are supposed to be active and are not, or you inhibit the players that are overactive.

"That's what the biology gives us. The chemistry gives us these huge

catalogues of millions of compounds and now we have to find the matches."

Tuszynski says "millions of billions of calculations" are needed to screen all of the human body's 40 million compound combinations in hopes of possibly identifying the one cancer-fighting compound.

To achieve this monumental task in a conceivable time frame, Tuszynski says the first step is to cast a wide net and do a "quick and dirty" analysis using between 3,000 and 5,000 computer processors. This six-month process will filter that long list of compounds down to the 1,000 or so cancer-fighting hopefuls, which are then put through a more thorough screening. This final test involves a single processor with a specific target and takes about a day to complete the analysis of each compound.

However, Tuszynski says the first results will start trickling in sooner than later.

"The first approach is just a computational screen where we identify the potential hits," he said. "Then we have to find which ones really works, and that requires taking them to the lab.

"As soon as we get some promising compounds from the computational search we will start doing the experiments."

Of the $5.6 million in funding, the Alberta Government came up with a total of $3.1 million as part of its action plan, "Bringing Technology to Market." The $178 million, three-year initiative has been created to strengthen the technology commercialization space in Alberta's priority technology areas: clean energy, life sciences, information and communications technology, and nanotechnology. The project is partnered by the Ministry of Advanced Education and Technology, Hewlett Packard Canada, Alberta Health Services, the Alberta Cancer

Board, and an international partnership of pharmaceutical and computing firms.

The Tuszynski-led agreement was reached during a trade mission to California led by Premier Ed Stelmach, designed to introduce market players along the west coast to the Alberta government's action plan.

Source: University of Alberta