

## Researchers discover a new anticancer compound using accelerated drug screening process

## May 21 2014, by Olli Ernvall

A team of research scientists from VTT Technical Research Centre of Finland, the University of Turku and the University of Eastern Finland has discovered a previously unknown Cent-1 molecule that kills cancer cells. Their research also shows that new cancer drug candidates can be identified faster and at lower cost by using computer-assisted and cell-based screening of compounds.

The objective of the research project led by Marko Kallio, Principal Scientist at VTT, was to accelerate the <u>drug development</u> process by identifying new compounds that would possess similar binding properties and cellular phenotype, but a different chemical structure, as the selected drugs in clinical use or investigational compounds in development.

The scientists combined computer-based screening and cell-based assays to create a method that can significantly accelerate drug discovery and thereby lower development costs. It is highly likely that the new compounds identified using this method have not yet been patented.

The research team conducted a computer-assisted screening of 65,000 compounds and cell-based assays on the 150 highest scoring hit compounds, before identifying the Cent-1 molecule. The Cent-1 molecule kills <u>cancer cells</u> through a mechanism similar to that of the template drug Rigosertib that is currently under commercial



development. However, since the <u>chemical structure</u> of the Cent-1 compound differs from Rigosertib, there are no major obstacles to further development.

What makes the study also significant is evidence that Rigosertib did not inhibit its reported target genes; there is reason to believe that the drug has a different mechanism of action at molecular level than anticipated. This <u>drug discovery</u> related study was published in the *Molecular Cancer Therapeutics* in April 2014.

Development of new drugs is an expensive and time-consuming process. It usually takes around 10–15 years to complete and costs several hundreds of millions of euros. In addition, risks associated with the usability, therapeutic efficacy and market share of medicinal substances are usually realised only in the final stages of drug development.

## Provided by VTT Technical Research Centre of Finland

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