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A Method for Predicting Antiviral Drug or Vaccine Targets

New Rochelle, NY, April xx, 2020–A novel method to predict the most promising targets for antiviral drugs or vaccines is based on the conformational changes viral glycoproteins go through during the process of recognition and binding to the host cell. This prediction method, which targets backbone hydrogen bonds with the highest free energy, is published in ***Journal of Computational Biology,*** a peer-reviewed journal from Mary Ann Liebert, Inc., publishers. Click here to read the full-text article free on the ***Journal of Computational Biology*** website through XXX date.

Robert Penner, Institut des Haute Etudes Scientifiques (Bures-sur-Yveette, France) and University of California at Los Angeles is the author of the article entitled "Backbone Free Energy Estimator Applied to Viral Glycoproteins."

During viral entry and absorption into a host cell, the virus typically undergoes dramatic reconformation to form fusion/penetration motifs. Penner presents a general method to predict the residues of high conformational activity from the three-dimensional structure of viral glycoproteins. The method involves analyzing the hydrogen bonds of a protein and computing the free energy differences of corresponding features to identify regions where conformational change is most likely.

"It is nothing short of miraculous for a mathematical idea to directly lead to a practical implication, but the pay-off can be enormous, as it happened to the Maxwell's theory of electromagnetic fields -- this brought radio and television -- and with Turing's and von Neumann's ideas on the theory of computation which opened the portal to our digital world," says Misha Gromov, Institut des Hautes Études Scientifiques (Paris, France) and New York University. "Such an idea may have a chance to work, only when its author, besides being a brilliant mathematician, has a broad scientific vision, which is rare among even the best mathematicians of our time. Robert Penner is this kind of a rare mathematician, and his method of detection of patterns in the protein structures, a fruit of purely mathematical thinking, is different from everybody else's in the world. There is a positive chance this method will work and accelerate the development of antiviral drugs or vaccines. Only an experiment can tell if this is so."

About the Journal

Journal of Computational Biology is the leading peer-reviewed journal in computational biology and bioinformatics, publishing in-depth statistical, mathematical, and computational analysis of methods, as well as their practical impact. Published online only with open access options, this is an essential journal for scientists and students who want to keep abreast of developments in bioinformatics. Complete tables of content and a sample issue may be viewed on the ***Journal of Computational Biology*** website.

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