IBBR Researchers Develop Web Platform for Modeling Structure of Immune System Proteins

Submitted by Timna Wyckoff on August 9, 2018 - 13:40

Immune system proteins called T cell receptors (TCRs) are involved in fighting infectious disease and are implicated in a number of autoimmune diseases, such as diabetes and multiple sclerosis. In addition, T cells are an important part of the body’s defense against cancer, and T cell receptors have major potential as a platform for the development of cancer drugs.

In the age of genomics, the DNA sequence of many TCRs are available, but determining the 3-D structure is labor intensive. Accurate prediction of 3-D structure from DNA sequence could facilitate development of new therapeutics.

IBBR Fellow Dr. Brian Pierce (Assistant Professor, Department of Cell Biology and Molecular Genetics, University of Maryland) and postdoctoral associate Dr. Ragul Gowthaman recently published an article describing their development of TCRModel, a web server and interface that allows researchers around the world to input TCR sequences and retrieve high-resolution structure predictions in a matter of minutes.

Dr. Pierce shares, “We’re very excited to provide this server to the community, enabling those in the field to readily gain structural insights into their TCR sequence data. This represents an ongoing effort in my laboratory to model and design this therapeutically important class of molecules. The work was made possible with start-up funding from the University of Maryland and IBBR, as well as the support of the RosettaCommons community, in which my

Summary of the TCRmodel server, where TCR sequences input by users proceed through steps of template-based modeling and refinement, resulting in 3D structural models.

In the age of genomics, the DNA sequence of many TCRs are available, but determining the 3-D structure is labor intensive. Accurate prediction of 3-D structure from DNA sequence could facilitate development of new therapeutics.

IBBR Fellow Dr. Brian Pierce (Assistant Professor, Department of Cell Biology and Molecular Genetics, University of Maryland) and postdoctoral associate Dr. Ragul Gowthaman recently published an article describing their development of TCRModel, a web server and interface that allows researchers around the world to input TCR sequences and retrieve high-resolution structure predictions in a matter of minutes.

Dr. Pierce shares, “We’re very excited to provide this server to the community, enabling those in the field to readily gain structural insights into their TCR sequence data. This represents an ongoing effort in my laboratory to model and design this therapeutically important class of molecules. The work was made possible with start-up funding from the University of Maryland and IBBR, as well as the support of the RosettaCommons community, in which my
laboratory recently became a member, as we developed the underlying method in the Rosetta framework."

The TCRmodel server is available at: https://tcrmodel.ibbr.umd.edu

The article describing this server appears in *Nucleic Acids Research*: https://doi.org/10.1093/nar/gky432