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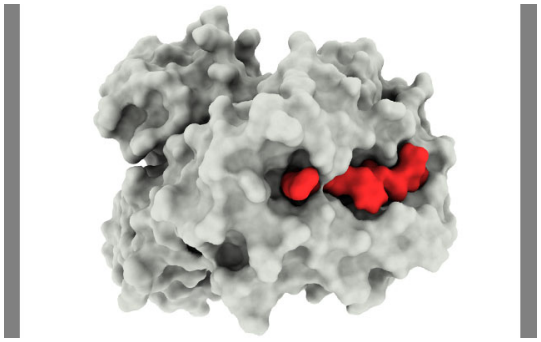
SDSC's Comet Supercomputer Helps Benchmark Cancer Immunotherapy Tool

Rice University study advances research on individualized patient treatment

With the American Cancer Society estimating 1.76 million new cases and more than 600,000 deaths during 2019 in the U.S. alone, cancer remains a critical healthcare challenge. In efforts to help mitigate these numbers, researchers at Rice University used the *Comet* supercomputer at the San Diego Supercomputer Center (SDSC) to evaluate their new molecular docking tool, called Docking INCrementally or DINC, which aims to improve immunotherapy outcomes by identifying more effective personalized treatments.



The Comet supercomputer at the San Diego Supercomputer Center was used to test interactions between thousands of pairs of molecules to advance immunotherapy research aimed at combating cancer. This image depicts a Human Leucocyte Antigen (HLA) receptor (in grey) that displays a small protein fragment or peptide (in red) at the surface of a cell. If this peptide is recognized as "suspicious" by the immune system, the cell will be destroyed. Credit: D. Devaurs, Rice University

Led by postdoctoral researcher Didier Devaurs, the Rice researchers recently published their evaluation of DINC in the *BMC Molecular and Cell Biology* journal. The most significant result is that their molecular docking approach can make predictions of molecular interactions that other docking tools would miss. This has strong implications in cases where these predictions are notoriously difficult to make, and especially in the context of immunotherapy, which leverages the immune system to combat cancer.

"Immunotherapy is an innovative cancer treatment that has shown promising results," said Devaurs. "It consists of 'training' a patient's cells by recognizing specific tumor-derived peptides, which are fragments of proteins within a cell." He further explained that each cancer patient displays a unique set of tumor-derived proteins and requires a fully personalized treatment.

The goal of their DINC tool is to assist with identifying these peptides for cancer immunotherapy, which required significant high-performance computing resources.

“The computational challenge here is that thousands of tumor-derived peptides were tested, and each test required exhaustive computing on *Comet*,” said Devaurs. “Our study showed that *Comet* has the computational power to make predictions that could be useful to immunotherapy. We will next assess how to rank the numerous predictions it makes to provide only the most realistic ones to our clinician colleagues working on novel cancer treatments.”

Access to *Comet* was done via the National Science Foundation’s Extreme Science and Engineering Discovery Environment (XSEDE) program, under NSF grant ACI-1548562. Additional funding came from the National Institutes of Health (1R21CA209941-01), the Informatics Technology for Cancer Research (ITCR) initiative of the National Cancer Institute (NCI), and the Cancer Prevention & Research Institute of Texas (RP170508). This work was also supported by a training fellowship from the Gulf Coast Consortia through the Computational Cancer Biology Training Program (RP170593).

Molecular structures are depicted by images produced with the PyMOL Molecular Graphics System, Version 1.8 Schrödinger, LLC. The funding bodies had no role in the design of the study and collection, analysis, and interpretation of data, or in writing the manuscript.

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