PRESS RELEASE
EMBARGOED UNTIL 9:00 AM EDT ON TUESDAY, SEPTEMBER 10, 2024

For more information, contact:
Estrid Jakobsen at estrid.jakobsen@conscience.ca
Preeti Singh at psingh@burness.com

Conscience Announces Top Performers in Open Science Challenge to Design Promising Pan-Coronavirus Drugs

Highest-Performing Team Hailed from Regional Universities in Brazil and Used Combination of Open Source Tools and Artificial Intelligence to Design Molecules

TORONTO (10 September 2024) — To help address the need for improved treatments against future coronavirus pandemic threats, the nonprofit drug discovery biotech Conscience today released seven newly discovered promising early-stage molecules that could lead to a new treatment effective against all coronaviruses, not just SARS-CoV-2. These molecules were identified by research teams from around the world as part of Conscience's "open science" competition. The top-scoring team, led by Karina dos Santos Machado, hailed from two lesser-known universities in Brazil.

This edition of the CACHE (Critical Assessment of Computational Hit-Finding Experiments) Challenges, governed by Conscience, along with pharmaceutical companies Bayer and Boehringer Ingelheim, was sponsored by the U.S. National Institutes of Health and tapped into small molecule design expertise across continents. The top-scoring Brazilian team submitted the highest number of confirmed predictions using a combination of open source and internally developed artificial intelligence (AI) tools to design the molecules that could treat coronaviruses. Other top participants were from universities in Canada, the U.K. and U.S. — including a group using a citizen science gaming interface called Drug-It to design molecules — and from biotech companies in Canada and Ukraine.

The dataset generated from the competition, including the promising new molecules, is now available publicly on the CACHE Challenges website for researchers anywhere to advance upon the research, including for training AI drug-design algorithms.

"While the market incentives for research and development in coronavirus has waned, the need for new treatments has not," said Ryan Merkley, CEO of Conscience. "The CACHE Challenge uses collaboration where competition falls behind, bringing talented researchers from anywhere — both well-funded pharma companies and under-resourced institutions — to drive new discovery in areas of unmet need."

For this second CACHE Challenge, participants were asked to design molecules that bind to the most conserved site in coronavirus proteins, located on the NSP13 helicase, a protein that is critical for viral replication. Targeting helicases as an antiviral strategy has proven effective against viruses like herpes, shingles and hepatitis C, but is underexplored for coronaviruses, with no drug candidates having targeted this site so far. The goal is to create a coronavirus treatment that complements existing therapies like Paxlovid and that would be resilient to new coronavirus strains, helping to address future coronavirus outbreaks.

All the submitted molecules were tested in the lab for their ability to bind to the target.

“The molecules discovered by CACHE participants and experimentally confirmed by the biophysics team at the Structural Genomics Consortium are promising chemical starting points to investigate an entirely novel therapeutic strategy against coronavirus,” said Dr. Matthieu Schapira, from the Structural Genomics Consortium at the University of Toronto and the lead scientist for the CACHE program. “If one of these molecules is eventually developed into a drug, the drug should be effective in treating any coronavirus, not just SARS-CoV-2, and therefore useful in future pandemic threats.”

“Addressing gaps in the development of drugs and therapeutics is an important part of the spectrum of biomanufacturing solutions for Canadians. We’re looking forward to seeing the results from this new round of Conscience’s challenges and adding them to the list of Canadian innovation successes,” said the Honourable François-Philippe Champagne, Canada’s Minister of Innovation, Science and Industry. Canada announced CA $49 million in funding for Conscience in October 2023.

Twenty-two teams from across academia and industry using different computational methods competed in the challenge, submitting a total of 2,576 molecules, which were then tested in the lab. According to Merkley, this dataset, which is now openly available to researchers worldwide, helps to lay the foundation for the development of effective AI methods to accelerate the early-stages of drug discovery.

“The value of the CACHE Challenges lies not only in the scientific outcomes but also in the opportunity to compare competing methods and their results, backed by unbiased, high-quality experimental feedback on methods and designs from AI experts and computational chemists around the world,” said Merkley.

The most successful teams of this CACHE Challenge in ranked order, based on the number and strength of the molecules they identified, were:

1. **Karina dos Santos Machado, Adriano Velasque Werhli** (Universidade Federal do Rio Grande - FURG, Rio Grande, Brazil), **Frederico Schmitt Kremer** (OmixLab, Universidade Federal de Pelotas, Capão do Leão, Brazil)
2. **David Koes, Ian Dunn** (University of Pittsburgh, Pittsburgh, U.S.)

3. **Dmitri Kireev** (University of Missouri, Columbia, U.S.)
4. **Rocco Moretti, Thomas Scott** (Vanderbilt University, Nashville, U.S.), **Jens Meiler** (Vanderbilt University, U.S. & Leipzig University, Germany)
5. **Yurii Moroz, Olga Tarkhanova, Mykola Protopopov** (Chemspace, Kyiv, Ukraine)

While these five teams had the highest aggregated scores across all of the molecules they identified, four additional teams also identified one promising molecule each: **Gennady Poda** and **Laurent Hoffer** (Ontario Institute for Cancer Research and University of Toronto, Canada), a team led by **Douglas Houston** and **Vincent Blay** (University of Edinburgh, Scotland), a team led by **Daniel Cole** (Newcastle University, U.K.) and another team from Canada. Collectively, the challenge participants identified seven promising hits and an additional six potential chemical starting points that may turn into promising molecules with additional research.

The results from this second competition in Conscience's CACHE Challenge series follows the results of the first challenge in January, for finding more effective drugs for familial Parkinson's disease. Four more challenges are underway — focusing on developing treatments to address COVID-19, multiple forms of cancer, and obesity — and a fifth will be announced in early 2025.

###

About Conscience
Conscience is a nonprofit biotech focused on changing the game on drug development, by enabling new discoveries for diseases that have received limited attention from the pharmaceutical industry. Using collaborative approaches and artificial intelligence, it breaks down barriers and inefficiencies imposed on profit-driven models. Powered by a network that includes academics, industry, technologists, and public support, a key initiative is the CACHE Challenge. It empowers scientists worldwide to unlock promising drug targets, accelerating the path to treatments for those who need them most. For more information, visit www.conscience.ca