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Deep Learning-Based Approach to Accelerate T cell Receptor Design

Tech ID: 32568 / UC Case 2021-679-0

ABSTRACT

Researchers at the University of California, Davis have developed a deep learning simulation model to predict mutated T-cell receptor affinity and avidity for immunotherapy applications.

FULL DESCRIPTION

T-cells are responsible for identifying and eliminating pathogens and triggering immune system responses. T-cell receptors (TCRs) on the surface of each cell bind to antigens as part of the process of identifying foreign materials. TCR avidity is a measure of how sensitive a T-cell is to such antigens - and thus is used to determine how well a TCR is likely to perform in immunotherapy or other applications.

The current method of testing mutated T-cell systems all have various limitations. Costly, low throughput experimental methodologies (e.g. cytokine release, FACS, DNA barcode pMHC multimers, or microfluidic-based assays) are insufficient to sample the vast number of TCR mutants - limiting the acceleration of TCR design. Utilizing deep learning technologies to predict functional TCR mutant biophysical parameters can accelerate the discovery rate of effective TCRs for a given application. However, using randomly generated training groups to train a machine-learning algorithm capable of predicting factors such as mutated TCR affinity and avidity is laborious and often inefficient. The number of possible mutations is so large that this approach is experimentally inefficient, costly, and has a relatively poor record of success. Advancements in a computational model to predict TCR avidity would lower research costs and lead to advancements in hyper-mutated TCR research and development.

Researchers at the University of California, Davis have developed a deep learning computer model that can calculate TCR binding parameters and thus be used to design TCRs for immunotherapy applications. The algorithm begins with a physics-based simulation in full atomistic detail under a wide range of conditions. Factors such as binding duration, mean force, surface area, and other qualities are computed, providing an indication of a mutant TCR's avidity. The results are used as a training set to create a deep learning algorithm based on viable TCR mutants found in humans. This refined, dataset can more accurately train the deep learning model and thus provide higher quality predictions. The deep learning prediction of TCR mutant qualities (that determine TCR avidity) from primary amino acid sequence can then be used for rapid testing to determine which TCR mutants are potentially viable for therapeutic uses.

APPLICATIONS

- T-cell receptor (TCR) discovery and other immunotherapy-based research
- Rapid development of potential TCR mutants for immunotherapy applications

FEATURES/BENEFITS

- A smaller, more refined set of training data allows for more productive results produced by the machine learning model
- Better accuracy, lower cost, and increased efficiency compared to existing methods

PATENT STATUS

| Country | Type | Number | Dated | Case |
|---------------------------|-----------------------|--------------------------------|------------|----------|
| Patent Cooperation Treaty | Published Application | WO 2023/028595 | 03/02/2023 | 2021-679 |

Additional Patent Pending

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OTHER INFORMATION

KEYWORDS

deep learning, artificial intelligence,
immunotherapy, machine-learning algorithm,
molecular dynamics/simulations, T-cell receptor design

CATEGORIZED AS

- **Biotechnology**
 - Bioinformatics
 - Health
 - Other
- **Computer**
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