

GEMINI: an integrated structure and AI based approach for new vaccine identification

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Abstract

Vaccines have proven pivotal against an array of infectious viral and bacterial diseases. However, there are still no effective vaccines against many pathogens as antigen identification and development of vaccine is a time-consuming process. In this context, finding the most optimal antigen is the bottleneck to make a vaccine accessible to patients everywhere in an accelerated manner.

Several vaccines on the market are composed by antigens expressed on the surface of the microorganism. Identification of these proteins, characterization of their structural insights as well as, their conformation and their antigenic epitopes can accelerate the timeline for the identification and thereafter, the design of novel vaccine(s).

Towards this, GEMINI, an integrated visual proteomic- based (Cryo-EM, HDxMS, X-ray crystallography) approach in combination with a structure-based similarity search tool for protein screening based on a Structure Similarity Algorithm has been recently developed to allow a rapid identification of new antigens based on their 3D structure. This allows the tool to generate score similarity between a new protein and the entire dataset in a fast and antigen focused approach.

Once identified, the novel antigen needs to be evaluated and screened for its functionality and antigenicity before being considered as potential vaccine candidate. An additional GEMINI prediction module tool will allow a structure-based antigenicity scoring where protein structural context as well as physio-chemical protein characteristics are considered to derive the antigenicity-dominant region. GEMINI will be also enriched by ProtLM, a protein functional characterization tool capable to predict protein functionality from their sequence.

Finally, GEMINI, based on advanced structural approaches and important contribution of AI/ML approaches enable a new era of rational structure-based identification of new antigens as potential vaccine candidates.

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