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S2SNET Model for prediction of epitopes in vaccine design

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The prediction of immunogenic peptides that can be used for production of antipeptide antibodies is of great importance for design of vaccines however a problem in immunology is the impact on the immunological response after of a perturbation or variation in the sequence of a known peptide and/or other boundary conditions. Methods that establish mathematical models to identify the structure-Activity/Property (QSAR/QSPR) relationships have been developed in the past. On the other hand, Epitope Data- base (IEDB) http://www.iedb.org/, released public data useful for these studies. Specifically, Perturbation Theory QSAR method (PT-QSAR) has been used to predict B-epitopes from IEDB database. This method adds variation terms to a known experimental solution of one problem to approach a solution for a related problem without known exact solution. In this specific case, the method predicts the epitope activity $E_q(c_j)$ of one query peptide (q) in a set of experimental conditions (c_j). In so doing, the method uses as input the epitope activity $E_r('c_j)$ of one similar peptide already known that is used as peptide of reference (r); which have been assayed on the same or a different set of experimental conditions ($'c_j$). The method also uses as input the information about the sequences and conditions of assay of both peptides in the pair. In the present study we developed a model able to classify 500000 cases of perturbations with accuracy, sensitivity to 99%, and specificity 100% for training validation series. The perturbations include structural changes in 83683 peptides determined in experimental assays with boundary conditions involving 1448 epitope organism name, 2283 host organisms, 15 biological process, 28 experimental techniques and 505 possible adjuvants. The model may be useful for the prediction and optimization in silico of new epitopes under different boundary conditions for vaccine development [1–4].

Keywords: Vaccine design, QSAR, Cheminformatics

References and Notes

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