QSPR-Perturbation Models for the Prediction of B-Epitopes from Immune Epitope Database: A Potentially Valuable Route for Predicting ?In Silico? New Optimal Peptide Sequences and/or Boundary Conditions for Vaccine Development

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In the present study, three different physicochemical molecular properties for peptides were calculated using the program MARCH-INSIDE: atomic polarizability, partition coefficient, and polarity. These measures were used as input parameters of a linear discriminant analysis (LDA) in order to develop three different quantitative structure?property relationship (QSPR)-perturbation models for the prediction of B-epitopes reported in the immune epitope database (IEDB) given perturbations in peptide sequence, in vivo process, experimental techniques, and source or host organisms. The accuracy, sensitivity and specificity of the models were >90 % for both training and cross-validation series. The statistical parameters of the models were compared to the results achieved with the electronegativity QSPR-perturbation model previously reported by González-Díaz et al. (J Immunol Res. doi:10.1155/2014/768515, 2014). The results indicate that this type of approach may constitute a potentially valuable route for predicting ?in silico? new optimal peptide sequences and/or boundary conditions for vaccine development.

Epitopes

Markov chains

Perturbation theory

QSAR/QSPR models

Vaccine design

epitope

amino acid sequence

Article

atomic polarizability

computer model

controlled study

in vivo study

Markov chain

partition coefficient

physical chemistry

polarity

prediction

quantitative structure property relation

vaccine production