MOL2NET, International Conference Series on Multidisciplinary Sciences
http://sciforum.net/conference/mol2net-03

Alignment-Free Model for Prediction of B-cell Epitopes

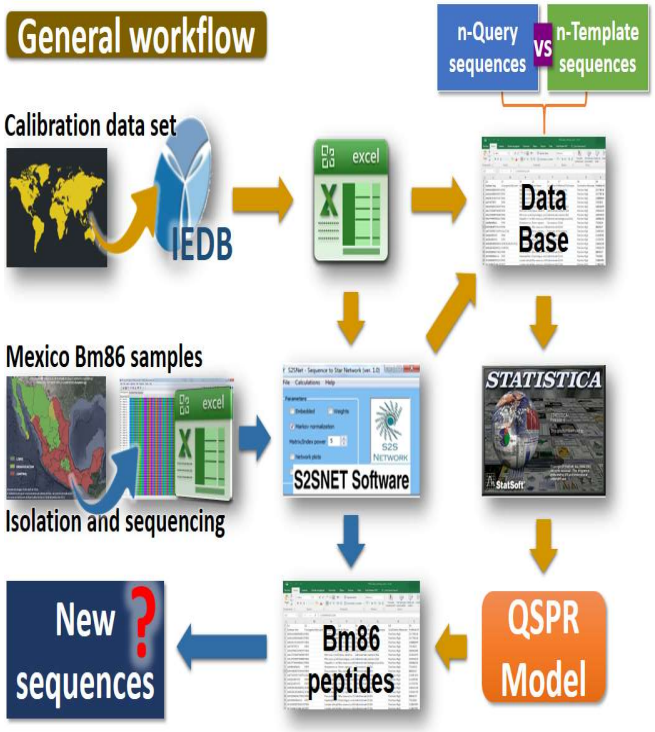
Saúl G. Martínez-Arzate[§], [*] *Esvieta Tenorio-Borroto*[§], *Alberto Barbabosa Pliego*[§], *Héctor M. Díaz-Albiter*[#,Δ], *and Juan C. Vázquez-Chagoyán* [§,*]

[§] Molecular Biology Laboratory, CIESA, FMVZ, Autonomous University of The State of Mexico (UAEM), 50200 Mexico State, Mexico.

[#] Laboratory of Biochemistry and Physiology of Insects, Oswaldo Cruz Institute, FIOCRUZ, 4365, Rio de Janeiro, Brazil.

[Δ] Wellcome Trust Centre for Molecular Parasitology, University of Glasgow, University Place, Glasgow G12 8TA, United Kingdom.

Graphical Abstract



Abstract. In this work, we developed a general Perturbation Theory model for prediction of B-cell epitopes in vaccine design. The method predicts the epitope activity $\varepsilon_q(c_{qj})$ of one query peptide (q-peptide) in a set of experimental query conditions (c_{qj}). The model proposed here is able to classify 1,048,190 pairs of query and reference peptide sequences reported on IEDB database with perturbations in sequence or assay conditions. The model has accuracy, sensitivity, and specificity between 71% and 80% for training and external validation series. The model may become a useful tool for epitope selection towards vaccine design. The theoretic-experimental results on Bm86 protein may help on the future design of a new vaccine based on this protein. **Ref:** J Proteome Res. 2017 Sep 18. doi: 10.1021/acs.jproteome.7b00477**.**

References

1. Vita, R.; Overton, J. A.; Greenbaum, J. A.; Ponomarenko, J.; Clark, J. D.; Cantrell, J. R.; Wheeler, D. K.; Gabbard, J. L.; Hix, D.; Sette, A.; Peters, B., The immune epitope database (IEDB) 3.0. Nucleic acids research 2015, 43 (Database issue), D405-12.
2. Vázquez-Prieto, S.; Paniagua, E.; Ubeira, F. M.; González-Díaz, H., 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. International Journal of Peptide Research and Therapeutics 2016, 1-6.

3. Gonzalez-Diaz, H.; Perez-Montoto, L. G.; Ubeira, F. M., Model for vaccine design by prediction of B-epitopes of IEDB given perturbations in peptide sequence, in vivo process, experimental techniques, and source or host organisms. Journal of immunology research 2014, 2014, 768515.
4. Peters, B.; Sidney, J.; Bourne, P.; Bui, H. H.; Buus, S.; Doh, G.; Fleri, W.; Kronenberg, M.; Kubo, R.; Lund, O.; Nemazee, D.; Ponomarenko, J. V.; Sathiamurthy, M.; Schoenberger, S.; Stewart, S.; Surko, P.; Way, S.; Wilson, S.; Sette, A., The immune epitope database and analysis resource: from vision to blueprint. PLoS biology 2005, 3.