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Prediction of B-Cell Epitope for 24 Mite Allergens: An in Silico Approach towards Epitope-Based Immune Therapeutics

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Abstract : Immunotherapy with allergy vaccines is of great importance in allergen-specific immunotherapy. In recent years, B-cell epitope-based vaccines have attracted considerable attention and the prediction of epitopes is crucial to design these types of allergy vaccines. B-cell epitopes might be linear or conformational. The prerequisite for the identification of conformational epitopes is the information about allergens' tertiary structures. Bioinformatics approaches have paved the way towards the design of epitope-based allergy vaccines through the prediction of tertiary structures and epitopes. Mite allergens are one of the major allergy contributors. Several mite allergens can elicit allergic reactions; however, their structures and epitopes are not well established. So, B-cell epitopes of various groups of mite allergens (24 allergens in 6 allergen groups) were predicted in the present work. Tertiary structures of 17 allergens with unknown structure were predicted and refined with RaptorX and GalaxyRefine servers, respectively. The predicted structures were further evaluated by Rampage, ProSA-web, ERRAT and Verify 3D servers. Linear and conformational B-cell epitopes were identified with Ellipro, Bcepred, and DiscoTope 2 servers. To improve the accuracy level, consensus epitopes were selected. Fifty-four conformational and 133 linear consensus epitopes were predicted. Furthermore, overlapping epitopes in each allergen group were defined, following the sequence alignment of the allergens in each group. The predicted epitopes were also compared with the experimentally identified epitopes. The presented results provide valuable information for further studies about allergy vaccine design.

Keywords : B-cell epitope, Immunotherapy, In silico prediction, Mite allergens, Tertiary structure
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