In silico prediction of skin sensitization: Quo vadis?

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Abstract

Direct skin contact with chemical or physical substances is predisposed to allergic contact dermatitis (ACD), in which the skin contact area develops various allergic reactions. ACD can be triggered by extremely complicated adverse outcome pathways. A variety of non-animal in vitro tests such as direct peptide reactivity assay (DPRA), KeratinoSens, human cell line activation test (h-CLAT), U-SENSTM, and SENS-IS based on different mechanisms have been developed to identify the sensitizers. Additionally, a broad spectrum of in silico models to predict skin sensitization have emerged based on various animal and non-animal data using assorted modeling schemes.

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