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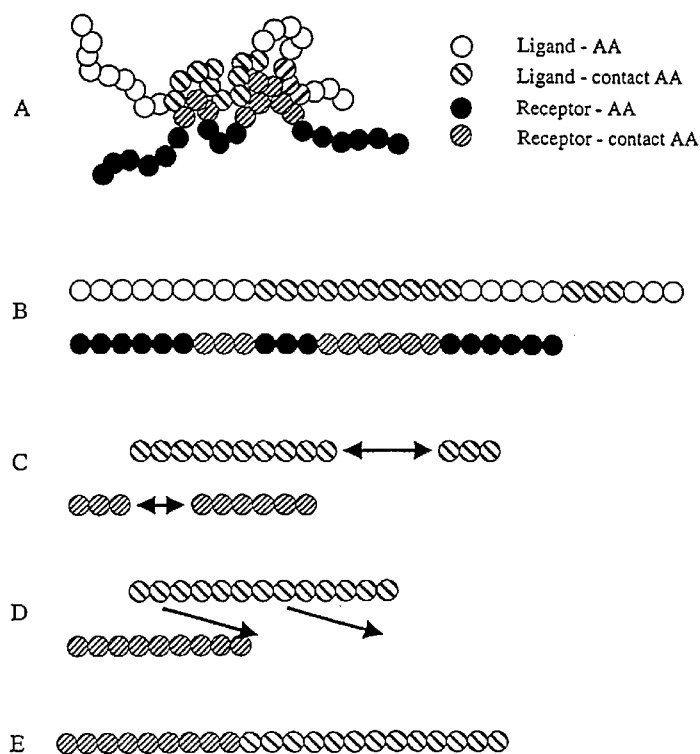
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(54) Title: SYSTEM AND METHOD FOR SYSTEMATIC PREDICTION OF LIGAND/RECEPTOR ACTIVITY



Building a representation of the ligand-receptor interaction.

(57) Abstract: Disclosed is a general system and method, for prediction of binding of peptide-like ligands (peptides) to peptide-like receptors (receptors). Specifically this invention uses non-linear prediction models (including, but not limited to, artificial neural networks), sequence data from ligands and their respective receptors, and known ligand-receptor binding affinities. The representation of ligand-receptor interaction used along with the binding affinity of said interaction is used to train a determining means in a form of a predictive model. Prediction of binding affinity of a novel (not used for training of a predictive model) ligand-receptor interaction, involving a peptide and a particular receptor, involves the combining of representations of both peptide and receptor and presenting that representation to a previously trained predictive model. The system and method can be used as a single predictive model for determination of ligand binding to an individual receptor, or to a group of related receptors. This system and method was validated using data on peptide binding to major histocompatibility complex molecules (MHC) and artificial neural networks (ANN).



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