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Feature selection for structure based pharmacophore model by means of Structural Interaction Fingerprint and 3D motif.

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Pharmacophore models are a common tool used in experiments of Virtual Screening (VS) aimed for searching active compounds. Among the various methods of developing such molds, the structure based pharmacophore model is of great importance, as it encapsulates the information about the binding site of the target protein.
In this research we present the method of selecting the pharmacophore features of the amino acids forming the binding cleft, which play an important role in accommodating the active compounds. On the basis of Structural Interaction Fingerprints (SIFts) [1], the bitstrings describing ligand – receptor contacts in a formalized manner, the frequently interacting residues are selected, and an ensemble of atoms common for a set of ligand – protein complexes named 3D motif [2] is employed to assign the appropriate pharmacophore features of the binding site.
Such a model of the binding site can be further used in the process of developing the structure based pharmacophore model, or to apply the restrains for the docking experiments.

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