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# 2D-SIFt – a matrix describing ligand-receptor interactions

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Structural Interaction Fingerprints (SIFts), as defined in [1], encode a ligand-receptor complex in form of a bit string depicting the detailed interactions of the receptor. The lack of recognition of pharmacophore features of the ligand is one of the major disadvantages of this methods. To address this issue, a modification of original SIFt methodology has been done, encapsulating interactions between the features of ligand and receptor in form of 6x9xN matrix (6 standard pharmacophore features, 9 types of interactions with amino acid [2], N – number of residues in described receptor). Matrix fields can take values greater than 1, there can be more than one separate pharmacophore feature of one type within ligand interacting with one residue (for instance three phenyl groups surrounding a phenylalanine).

Analogously to the previously demonstrated methodology, such matrices can be averaged to create profiles showing the most important interactions, thus being a hybrid between structure-based pharmacophore model and classical interaction fingerprint.

[1] Deng Z, Chuaqui C, Singh J. Structural interaction fingerprint (SIFt): a novel method for analyzing three-dimensional protein-ligand binding interactions. *J Med Chem.* (2004) 47(2):337-44.
[2] Mordalski S, Kosciolek T, Kristiansen K, Sylte I, Bojarski AJ, Protein binding site analysis by means of Structural Interaction Fingerprint patterns, *Bioorg Med Chem Lett* (2011) 21(22):6816-9.

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