

Ligand based virtual screening can be realised with various molecular representations. Fragment-feature representation represents the molecules as a set of fragments, where each fragment receives a set of descriptors. First goal of this thesis is to find suitable similarity function for such representation. This representation can also be improved by assigning a weight for each descriptor, which gives it a priority in a given similarity function. The second goal of this thesis is to examine simulated annealing as an algorithm used to find the weights. We experimentally analysed the influence of various fragment types, descriptor types, similarity functions, correlated descriptors, fragment noise and parameters of simulated annealing. Because the experiments are computationally demanding, we also created a tool for large scale computations.