

This work is based on the Molpher SW project, which is client-server application aiding exploration of chemical space between two input molecules. Aim of master thesis was modify the current version of program to manage scaffold hopping technique. This technique represents molecule in a simplified way. The simpler molecule is called scaffold. First of all there was need to define several levels of granularity and for each level define morphing operators. Server was modified with respect for parallelization. Experimental exploration of chemical space with and without the new feature is part of this work too.