Graphs are natural way of representing molecules. However, graph representations and algorithms are not being used for finding similarity of molecules in virtual screening. In this work we test the graph-based methods in ligand-based virtual screening. The similarity of molecular graphs is determined by maximum common subgraph and graph edit distance. We use implementations `fmcs` from chemoinformatic library RDKit for maximum common subgraph and GraphMatchingToolkit from K.Riesen to determine graph edit distance. We have found suitable combinations of parameters for aplication in ligand-based virtual screening. The results suggest that performance of graph based methods is comparable to the state-of-the-art methods.