**Abstract:** Chosen molecular representation is one of the key parameters of virtual screening campaigns where one is searching in-silico for active molecules with respect to given macromolecular target. Most campaigns employ a molecular representation in which a molecule is represented by the presence or absence of a predefined set of topological fragments. Often, this information is enriched by physiochemical features of these fragments: i.e. the representation distinguishes fragments with identical topology, but different features. Given molecular representation, however, most approaches always use the same static set of features irrespective of the specific target. The goal of this thesis is, given a set of known active and inactive molecules with respect to a target, to study the possibilities of parameterization of a fragment-based molecular representation with feature weights dependent on the given target. In this setting, we are given a very general molecular representation, with targets represented by sets of known active and inactive molecules. We subsequently propose a machine-learning approach that would identify which of the features are relevant for the given target. This will be done using a multi-stage pipeline that includes data preprocessing using statistical imputation and dimensionality reduction, application of subspace clustering in the molecular feature space, and finally analysis and scoring of the results. This information will then be fed into the molecular representation and used in further virtual screening campaigns.