

## **Abstract**

### **English**

Drug development suffers from high failure rates. Apart from adverse side effects the limited efficacy of a drug under study in the entire disease population is often a reason for stopping development. Specifically, single nucleotide polymorphisms (SNPs) occurring in the drug targets binding site region may hamper the efficacy of a drug.

In the course of this thesis a computational workflow for evaluating drug efficacy in the context of mutation status of drug targets was developed. The implemented workflow was exemplarily applied to drugs used in breast cancer therapy. Relevant drugs, drug targets, and SNPs were retrieved from the following publicly accessible biological databases: ClinicalTrials.gov, ChEMBL, DrugBank and COSMIC. A major part of the in-silico workflow deals with the integration of such heterogeneous data from different sources and making them accessible for common processing. The identified set of drugs and their targets were analysed in greater detail including a target relevance ranking.

A significant difference in the mutation ratios between targets of the identified breast cancer drug set and other human proteins was observed. Drug targets of the identified set reveal lower mutation ratios. In addition, they show a higher number of associated breast cancer publications.

Furthermore, SNPs occurring in drug-targets were evaluated. For some of them, evidence of the influence on the drug binding efficacy and consequently on the therapy outcome was found in literature.

**Keywords:** breast cancer, drug efficacy, data integration, in-silico workflow, clinical trials, drug-target interactions, SNPs