

LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN



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M.Sc. Thesis Proposal: Predicting the effect of drug perturbations on the human gut microbiome

*Background:* An increasing body of evidence suggests that many drug-derived compounds influence the abundance of bacterial species in the human gut microbiome. This means that by taking certain medications (e.g. antibiotics), the composition of this bacterial community is perturbed. These alterations can have important consequences for human health, such as drug efficacy, the appearance of opportunistic infections, side-effects, etc. The ability to predict the effect that a drug will have on the gut microbiome is key to rationally design better therapeutic strategies.

*Objective:* The purpose of this M.Sc. thesis project is to create predictive models that can assess a compound's impact on the human gut microbiome. These predictions will be based on a representation of the molecular structure of a compound, as well as information about the microbes for which a representation is made. The predictive model will therefore give information regarding expected changes in microbe abundance in response to chemical treatment. Publicly available data and tools will be used.

*Plan and deliverables:* A successful completion of the M.Sc. thesis requires the following computational and scientific advances. Creating and evaluating predictive models that assess a compound's impact on microbiome composition given the molecular structure and initial composition. A write-up in thesis form and commented code on GitHub are mandatory deliverables at the end of the thesis.