Graduate School of Science and Technology Master's Thesis Abstract

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Abstract

Novel kinds of antibiotics are needed to combat the emergence of antimicrobial resistance. Meanwhile, in silico approaches to antibiotic discovery can improve the detection rates of candidates and reduce the early costs. In this study, a relevant network was constructed by mapping the correspondence between bacteria, antibiotics, Traditional Chinese Medicine (TCM) syndromes, TCM formulae, herbs, and natural products (NP). After searching the network, TCM formulae with the efficacy against various groups of bacterial infectious were screened out. By taking into consideration the NP existing in herbs used as TCM formulae ingredients, a sizable dataset consisting of the NP-efficacy relationship was constructed. A supervised learning model (Random Forest) was carried out as a single filter to verify the validity of the dataset. Three classifiers were then trained on the filtered dataset. According to cross-validation results, the mean accuracy of multilayer perceptron was slightly better than XGboost and Lasso. The NP features significant for the classification of each label of the antibacterial group were extracted from the multilayer perceptron models. The selected NP were validated on their antibacterial potential by searching the published literature and calculating the structural similarity to existing antibiotics. The remaining NP that we predicted novel associations with antimicrobial efficacy can be considered as candidates in the early step of the new antibiotics discovery cycle.