

## 論文内容の要旨

博士論文題目 Natural Antibiotics Prediction based on Traditional Herbal Medicine  
(伝統的な漢方薬に基づいた天然抗生物質の予測)

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(論文内容の要旨)

Antibiotic resistance is a major public health threat and there is an urgent need for new antibiotics. Traditional herbal medicine systems, such as Jamu, Unani, and Traditional Chinese Medicine, have been used for centuries to treat bacterial infections. Machine learning methods have been shown to be effective for predicting potential natural antibiotic candidates in traditional herbal medicine systems. In this study, we used machine learning methods to predict potential natural antibiotic candidates at plant and metabolite levels. We evaluated different machine learning algorithms and preprocessing techniques to obtain the best prediction accuracy. For Jamu, we achieved an accuracy of 91.10% using the Random Forest model. For Unani, we achieved an accuracy of 83% using a multilayer perceptron model with SMOTE preprocessing. In total, we predicted 42 potential plant candidates and 201 candidate metabolites as potential natural antibiotics. Many of these candidates have been validated based on published literature and have demonstrated antibacterial properties or have been structurally similar to known antibiotics. Finally, 201 metabolites were predicted and mapped to eight different types of antibiotics using clustering techniques and matching similarities. Our findings suggest that machine learning methods can be used to effectively predict potential natural antibiotic candidates utilizing traditional herbal medicine. This approach has the potential to accelerate the development of new antibiotics to combat antibiotic-resistant pathogens.

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(論文審査結果の要旨)

令和6年1月12日に開催した公聴会の結果を参考に、令和6年2月5日に本博士論文の審査を実施した。本博士論文は、本学位申請者が、独立した研究者として研究開発活動が続けていくために必要な素養を備えていることを示すものである。本論文は、博士（工学）の学位論文としての価値があるものと認める。