日本学術振興会に紙媒体で提出する必要はありません。

様　式　Ｆ－７－１

科学研究費助成事業（学術研究助成基金助成金）実施状況報告書（研究実施状況報告書）（令和２年度）

機関番号	１４６０３

所属研究機関名称		奈良先端科学技術大学院大学
研究代表者	部局	先端科学技術研究科
	職	准教授
	氏名	AMIN　MD. ALTAFUL

１．研究種目名　基盤研究(C)(一般)　　２．課題番号　20K12043

３．研究課題名　On searching antimicrobial agents among natural products:Fighting against Superbug

４．補助事業期間　令和２年度～令和４年度

５．研究実績の概要

Chemoinformatics has become greatly involved with modern drug discovery processes. Antimicrobial agents are drugs that can kill microorganisms or stop their growth. Massive imprudent usage of antibiotics in clinical practice for both human and livestock has resulted in resistance of bacteria to antimicrobial agents. Such multidrug-resistant (MDR) bacteria are recently called as Superbugs. MDR bacteria poses global threats to human health and economy. Antimicrobials work based on multiple mechanisms and multiple drugs are necessary to treat microbial infections effectively. But multiple drugs cause lots of side effects. Traditional medicines are known to have no or less side effects. Therefore, good combination of multiple antibiotic drugs derived from natural products might be a good solution to combat superbug. Because of the covid pandemic we are focusing on finding natural antibiotics effective against virus and bacteria that cause respiratory diseases. We have collected around 10000 Traditional Chinese Medicine (TCM) Formulas. We developed an approach to construct and validate TCM dataset effective against bacterial pneumonia and published a conference paper. Currently we are working on Identification of Antibacterial Natural Products based on appropriate TCM formulas and computational techniques using on machine learning algorithms. We will apply Lasso regression, Random Forest and XGBoost algorithms and utilize the best classification/regression results to identify natural product antibiotics.

６．キーワード

Antimicrobial　Natural products　Traditional Medicines　Lasso regression　Random Forest　Machine Learning

７．現在までの進捗状況

区分　(2) おおむね順調に進展している。

理由

I have been conducting research on traditional medicibes for a decade. Previously I worked on Indonesian Jamu and sub-continental traditional medicines such as Ayurvedic and Unani. My experience is helping to conduct the research of the current project. Also, a graduate student of our lab is working with me. With his help we are conducting our research and experiments smoothly. We have collected around 10000 Traditional Chinese Medicine (TCM) Formulas. We developed an approach to construct and validate TCM dataset effective against bacterial pneumonia and published a conference paper. Currently we are working on Identification of Antibacterial Natural Products based on the selected TCM formulas by applying computational techniques. We have already done part of the work and will write a paper soon.

８．今後の研究の推進方策

Our next work is Identification of Antibacterial Natural Products based on appropriate TCM formulas using computational approaches based on machine learning algorithms. We will apply Lasso regression:, Random Forest and XGBoost algorithms and utilize the best classification/regression results to identify natural product antibiotics.

９．次年度使用が生じた理由と使用計画

This year we could not attend a conference because of the pandemic. This year we hope in the second part we will be able to attend some conferences domestic or overseas. By attending conferences we can gather feedback on our work and new research ideas.

１０．研究発表（令和２年度の研究成果）

〔雑誌論文〕　計1件（うち査読付論文　1件／うち国際共著　1件／うちオープンアクセス　1件）

１．著者名 Hossain, Shaikh Farhad, Ming Huang, Naoaki Ono, Aki Morita, Shigehiko Kanaya, and Md Altaf-Ul-Amin	４．巻 2021
２．論文標題 Development of a biomarker database toward performing disease classification and finding disease interrelations	５．発行年 2021年
３．雑誌名 Database	６．最初と最後の頁 1-17
掲載論文のDOI（デジタルオブジェクト識別子） 10.1093/database/baab011	査読の有無 有
オープンアクセス オープンアクセスとしている（また、その予定である）	国際共著 該当する

〔学会発表〕　計1件（うち招待講演　0件／うち国際学会　1件）

１．発表者名 3.G. Pei, C. Zheng, H. Ming, O. Naoaki, K. Shigehiko, and M. Altaf-Ul-Amin
２．発表標題 An approach to construct and validate TCM dataset effective against bacterial pneumonia
３．学会等名 2021 IEEE 3nd Global Conference on Life Sciences and Technologies (LifeTech)（国際学会）
４．発表年 2021年

〔図書〕　計1件

１．著者名 Altaf-Ul-Amin, M., & Kanaya, S.	４．発行年 2020年
２．出版社 Elsevier	５．総ページ数 32
３．書名 Comprehensive Natural Products III: Chemistry and Biology.	

１１．研究成果による産業財産権の出願・取得状況

計0件（うち出願0件／うち取得0件）

１２．科研費を使用して開催した国際研究集会

計0件

１３．本研究に関連して実施した国際共同研究の実施状況

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１４．備考

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