



## Structural Chemogenomics for the Discovery of Novel Antibiotics

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**T**he structural chemoproteomics is the effort to understand structural aspects of recognition between proteins and chemicals. Namely, it aims to identify chemical moieties to recognize specific part of protein structures (e.g. active site) and characterize protein structures to recognize a specific chemical moiety. Such efforts are highly important for the drug discovery because drug molecules, to demonstrate their pharmacological effects, interact with therapeutic target proteins in a three dimensional manner.

To investigate such interactions, we have used computational methods, NMR spectroscopy and X-ray crystallography. Moreover, we construct structural chemoproteomic chemical libraries to accelerate lead discovery process. In these libraries, each library includes chemical compounds that target specific protein families such as kinases, phosphatases, metalloenzymes and nuclear receptors. Thus, if we identify the function of new targets, we just screen the corresponding library for the discovery of new leads.

Currently, the human race is facing serious resistance problems of antibiotics. We believe that our structural chemoproteomic techniques can provide a way to overcome the problem. Thus, we have applied these techniques to genomic targets for antibiotics. In this presentation, I would like to introduce such techniques and discuss the application of them to the researches for the discovery of novel antibacterial drugs.