Contribution ID: **4** Type: **特邀报告**

Predicting Metalloproteomes by Machine Learning

Metal ions play various important biological functions in proteins, including structural maintenance, molecular recognition, and catalysis1. Attracted by numbers and essential function of metalloproteins, many computational methods have been developed to predict metalloproteins and their metal binding sites. However, those methods were based on homology from either 1D sequence or 3D structural motifs2. Here, we explored a 2D coevolution-based approach named "MetalNet" to systematically predict metal-binding sites in proteomes. Our method used a powerful machine learning model to differentiate metal-binding coevolved residue pairs from non-liganding ones, and employed graph theory to assemble these pairs into a high-order metal-binding coevolved residue network. MetalNet exhibited an impressive performance on a benchmark set. When the method was applied to survey proteomes from four representative prokaryotic species, it identified a large number of novel metal-binding sites with high confidence, a large portion of which can be supported by interring knowledge from existing literature or database. We biochemically validated a novel prediction without any structural or sequence homology to known metalloproteins. Our computational method will provide a unique and enabling tool for interrogating the hidden metalloproteome.

Primary author: Prof. WANG, Chu (Peking University)

Presenter: Prof. WANG, Chu (Peking University)