Jun Xu
Sun Yat-Sen University, China

Chinese herbal medicine innovation through chemoinformatics

Chemoinformatics has been applied in Chinese herbal medicine studies for decades. These studies mainly focus on creating databases, mining the active components, or classifying the Chinese herbal medicines into hot or cold according to the theory of Chinese Medicine. Conceptually, however, Chinese herbal medicine is significantly different from western medicine. From the view point of modern pharmacology, a drug acts against at least one disease, while a Chinese herbal medicine is taken against at least one symptom that can be caused by many diseases. In this talk, the relationship between the drug targets and the Chinese medical concepts is articulated through herb-chemome-MOA network (HCMN). Based upon the privileged chemotypes (chemome) in HCMN, the knowledge intrinsic to Chinese medicine can be translated into new agents against the targets through the steps in this protocol: (1) elucidate herbal compatibilities, (2) identify active constituents, (3) derive privileged chemotypes, (4) select targets by referencing HCMN, (5) enumerate a virtual library by connecting the privileged chemotypes with chemical linkers, (6) generate conformations for the compounds in the virtual library, (7) virtually screen this library against the selected targets from step 4, and (8) confirm the hits by biological assays. The approach can offer a bridge between Chinese herb treatments and the search for molecular targets thus helping to discover new chemotherapies for other systemic diseases.

Biography

Jun Xu received his PhD from University of Science & Technology of China, and Postdoctoral studies from Australian National University and McGill University. He is the Professor of School of Pharmaceutical Sciences and the Founding Director of Research Center for Drug Discovery at Sun Yat-Sen University (SYSU). Prior to joining SYSU, he worked in US pharmaceutical industry, practicing chemoinformatics and computer-aided drug design (CADD) for over 20 years. He was a Principle Scientist at Boehringer Ingelheim Pharmaceuticals, Inc., and Research Director for BIO-RAD Sadtler Labs, Biofocus/DPI and other firms. He has published more than 90 papers in reputed journals.

junxu@biochemomes.com