

3rd International Conference on Medicinal Chemistry & Computer Aided Drug Designing

December 08-10, 2014 DoubleTree by Hilton Hotel San Francisco Airport, USA

Chemomics and systems biology for traditional Chinese medicine

Guoan Luo

Tsinghua University, China

The advance of systems biology has enabled us to characterize the response of biological system to the disturbance of a single entity drug via multi-omics approaches such as genomics, proteomics and metabolomics. But there were some problems for its application in Traditional Chinese Medicine (TCM). How to characterize and optimize the compatibility between/among multi-component combination of the TCM formula is one of key issues. We have proposed an approach, chemomics, to characterize the complex system of TCM formulas which represents a complex mixture consisting of multi-herbs and multi-compounds. The hierarchical strategy based on chemomics enables the optimization of formularization in three levels, combination of raw herbs, combination of fractional components, and combination of definite compositions. The original TCM formula, combination of raw herbs, can be simplified successively through holistic bioactivity-guided screening to achieve an optimized combination of fractional components, and eventually combination of minimal phytochemical compositions for further drug development of "Modernized Composite Medicine" (MCM), while maintaining its curative effect for a specific disease. Holistic bioactivity of TCM can be characterized well by systems biology. Therefore the integration of chemomics and systems biology, so-called integrative systems biology, provides a new paradigm for the modern research on TCM by characterizing the interaction of TCM system to body system (system to system, S2S). As demonstrative studies, TCM SLF which consisted of two raw herbs with 83 known compounds was managed to simplified and achieve an optimal combination of two fractional components with ten known compounds while exhibiting superior efficacy where systems biology and "genes - protein - metabolism" network regulation mode were adopted for the characterization of efficacy and the synergic effects. S2S model was also applied in study of the early diagnosis and treatment assessment of diabetic nephropathy; we proposed an Integrated Biomarker System (IBS) for the characterization of disease and syndrome which consisted of quantitative syndrome indicators, proper clinical pathological and biochemical indicators and systems biological indicators at levels of genes, proteins and metabolites. Chemomics and IBS can also be applied in other aspects, for example, we have had good outcome in the research on tea chemome.

luoga@mail.tsinghua.edu.cn