

International Conference and Exhibition on **VIROLOGY** 5-7 September 2011 Baltimore, USA

Structural Bioinformatics and Chinese Traditional Medicine Database For Drug Design and Personalized Medicine

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 \mathbf{S} tructural bioinformatics tools and databases have been developed and applied to study diversified biological problems. Molecular modeling tools were developed to generate 3D structure from sequences of novel gene. It allows us pursue structure based drug design. Applications were made to drug design for SARS, H5N1 and HIV. A octapeptide AVLQSGFR designed by us was synthesized and its antiviral potential against SARS coronavirus (BJ-01) was assessed, which demonstrates that AVLQSGFR is the most active in inhibiting replication of the SARS coronavirus compared with other compounds reported so far(EC50 is 2.7×10-2mg/L, and its selectivity index is more than 3704). We have built an effective component Database of the Traditional Chinese Medicine(TCMD), which contains 3-D structures of 10000 different compounds from various sources of traditional Chinese medicines. The database is screened with various cheminformatics tools, many promising molecules were obtained, for example, agaritine and gx-50 was singled out through similarity search, molecular docking and molecular dynamics simulations. Experimental studies were carried out to test the effectiveness of these molecules. In our structural bioinformatics studies, the three-dimensional (3D) structures of selected enzymes were built, for example, 2C19, 2E1. By a series of docking studies and MD simulations, the binding affinities of existing drugs with various CYP enzymes were analyzed to understand role of SNPs, which accord well with the results obtained from photo-affinity labeling studies, and will be very useful for conducting mutagenesis studies, providing useful information for drug metabolism and personalization of drug treatments, as well as stimulating novel strategies for finding desired personalized drugs.

Biography

Prof. Dong-Qing Wei, obtained his Ph.D. at the age 24, is the deputy director at the Luc Montagnier BioMedical Research Institute and acting head, Department of Bioinformatics and Biostatistics, College of Life Science and Biotechnology, Shanghai Jiaotong University, Shanghai, China, editor-in-Chief, "Interdisciplinary Sciences-Computational Life Sciences", chairman, International Association of Scientists in the Interdisciplinary Areas(IASIA). Prof. Wei's research is in the general area of structural bioinformatics and computational physics. He has made many important contributions to sciences. With more than 100 journal papers and SCI 2700 citations, he is becoming a leading figure in the area of structural bioinformatics and computational physics.