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CloudDD. Cloud computing chemogenomics knowledgebase platform for drug discovery

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Abstract

Chemical genomics (or chemogenomics) is an interdisciplinary research that utilizes chemicals/drugs and genome-wide data to systematically identify and analyze chemicals-protein interactions for the purpose of enhancing new drug design. Computational chemogenomics draws from the cheminformatics and bioinformatics disciplines to produce useful information systems for researchers in pursuit of chemogenomics data, predictive modeling, as well as techniques in ligand- and structure-based drug design. In this regard, there are fast growing andlarge volume of relevant scientific data and information generated, albeit scattered in the literature. It is a challenge for scientists to characterize the molecular interaction networks in chemical genomics scale for pharmacotherapy. Herein, we have established cloud computing chemogenomics knowledgebase drug discovery (CloudDD) platform (www.CBLigand.org/CCGS) with our advanced GPU-accelerated machine learning/cheminformatics/bioinformatics algorithms and tools. These include online programs (TargetHunter, HTDocking, LiCABEDS classifier, ANN-QSAR and BBB predictors, etc) and diseases domain-specific chemogenomics databases (multiple myeloma,liver fibrosis, Alzheimer's disease, etc). It transforms the one-target-one-drug development process to a new multi-target-multi-drug paradigm; as such it is perfect for thestudy of polydrug polypharmacology networks of drugs or chemicals for drug repurposing and new drug discovery.Such a cloud computing serverwill augment our capacity to benefit the broad research community and will help break the knowledge barrier, reduce costs, and accelerate advances in computer-aided drug design by consolidating existing data and computational technology.Ultimately, it will effectively assist medicinal chemists to conduct "virtual to real" translational research for target identification and drug design discovery.

Biography

Xie received his BS degree in Pharmacy in 1982 from the Second Military Medical University in Shanghai, China; his Ph.D. in Medicinal Chemistry in 1993 from the School of Pharmacy, University of Connecticut; and followed by a Biophysics Post-doctoral training at MIT/UCONN. He also received his EMBA degree in 2003. Currently, He is a tenured Professor of Pharmaceutical Sciences/Drug Discovery Institute. He is PI of an integrated research laboratory of CompuGroup, BioGroup and ChemGroup (www.CBLigand.org/XieLab) and Director of Computational Chemical Genomics Screening Center (www.CBLigand.org/CCGS) at University of Pittsburgh. He is a member of the NIH BPNS Study Section, a guest editor for AAPS Journal, and Associate Editor/Editorial Board of BMC Pharmacology and Toxicology. He has over 100 publications of peer-reviewed research articles, book chapters, reviews, abstracts, and patents.