

Handbook Of Systems Toxicology

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the network approaches of systems pharmacology and toxicology serve as early predictors of the most relevant screening approach to pursue both in drug discovery and development and ecotoxicological assessments computational approaches have the potential to improve toxicological experimental design enable more rapid drug efficacy and safety testing and also reduce the number of animals used in experimentation rapid advances in availability of computing technology hold tremendous promise for advancing applied and basic science and increasing the efficiency of risk assessment this book provides an understanding of the basic principles of computational toxicology and the current methods of predictive toxicology using chemical structures toxicity related databases in silico chemical protein docking and biological pathway tools the book begins with an introduction to systems pharmacology and toxicology and computational tools followed by a section exploring modelling adverse outcomes and events the second part of the book covers the discovery of protein targets and the characterisation of toxicant protein interactions final chapters include case studies and additionally discuss interactions between phytochemicals and western therapeutics this book will be useful for scientists involved in environmental research and risk assessment it will be a valuable resource for postgraduate students and researchers wishing to learn about key methods used in studying biological targets both from a toxicity and pharmacological activity standpoint

this detailed volume explores key state of the art computational applications that are crucial in systems toxicology the recent technological developments in experimental

biology and multi omics measurements that enable systems biology and systems toxicology can only be fully leveraged by the application of a broad range of computational approaches ranging from data management to mathematical modeling taking this into account chapters in this book cover data management and processing data analysis biological network building and analysis as well as the application of computational methods to toxicological assessment written for the methods in pharmacology and toxicology series computational systems toxicology includes the kind of key practical advice that will aid readers in furthering our knowledge of toxic substances and reactions to them

an indexed directory of current research project abstracts in toxicology and related fields

systems toxicology a branch of toxicology that studies chemical effects on biological systems presents exciting knowledge discovery challenges for the information researcher the exponential increase in availability of genomic and proteomic data in this domain needs to be matched with increasingly sophisticated network analysis approaches improved ability to mine complex gene and protein interaction networks may eventually lead to discovery of drugs that target biological sub networks network medicine instead of individual proteins in this thesis we have proposed and investigated the use of a maximal edge centrality criterion to discover drug toxicity signaling paths inside a human protein interaction network the signaling path detection approach utilizes drug and toxicity information along with two novel edge weighting measures one based on edge centrality for detected paths and another using differential gene expression between tissues treated with toxicity inducing drugs and a control set drugs known to induce non immune neutropenia were analyzed as a test case and common path proteins on discovered signaling paths were evaluated for toxicological significance in addition to investigating the value of topological connectivity for identification of toxicity biomarkers the gene expression based measure led to identification of a proposed biomarker panel for screening new drug candidates comparative evaluation of findings from the dtsp approach with standard microarray analysis method showed clear improvements in various performance measures including true positive rate positive predictive value negative predictive value and overall accuracy comparison of non immune neutropenia signaling paths with those discovered for a control set showed increased transcript level activation of discovered signaling paths for toxicity inducing drugs we have demonstrated the scientific value from a systems based approach for identifying toxicity related proteins inside complex biological networks the algorithm should be useful for biomarker identification for any toxicity assuming availability of relevant drug and drug induced toxicity information

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