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A brief overview to systems biology in toxicology: The journey from in to vivo, in-vitro and –omics

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Abstract

Toxicology aims to comprehend and envisage the adverse outcomes of chemicals and xenobiotics on the biological system. Predicting toxicity on the biological system is a complex and immense process. *In-vivo, in-vitro*, pre-, clinical and –omics level experimental approaches have been utilized to describe the toxicological impact of these chemicals and this has generated a vast wealth of data. Hence, there now exist a need for a system that can interrelate and provide accurate and robust extrapolation of these data across various systems. Therefore, it is essential to re-shift our notion from empirical, animal-based testing to a mechanistic understanding. Systems biology is one such system that can extrapolate and interrelate these vast biological system data. Systems biology is a computational and mathematical modelling approach developed to understand interrelationships between networks of biological systems. The use of systems biology to answer toxicology-related questions is termed as systems toxicology. In this review we will look at the standard and classical toxicology experimentations and how we can use mechanistic data (systems biology) to answer toxicology-related questions using systems toxicology and what are the future opportunities in systems toxicology. The advancement of systems toxicology heralds new dawn of technologies that will aid in our quest to better comprehend and envisage the adverse outcomes of chemicals and xenobiotics on the biological system.

Keywords: *In-vivo* and *in-vitro*; Network; biology –Omics; Systems biology; Systems toxicology; Toxicology

Description

Toxicity is demarcated as the adverse sequence of events that are triggered by exposure towards biological, physical or chemical agents and is manifested in various forms; from mild malfunctions to serious organ impairment and even death These reversible or irreversible events are influenced by the poison's absorption, distribution, metabolism and excretion (ADME) properties, as well as the interactions of the toxicant or its metabolites with cellular macromolecules [1].

Toxicology encompasses the study of these events at entire biological system, ranging from molecules to complex ecosystems and requires extensive inter-disciplinary approaches. The question is whether such complex interaction(s) can be studied and mapped. The answer may lie in systems toxicology, where principles and methods of other disciplines; biology, chemistry, molecular biology, computer science and informatics are employed to better understand the resilience of biological system towards toxicants insults. The progressive advancement in genomics and systems-orientated perspective on biology has herald the shifting from empirical testing to a mechanistic understanding of toxicants perturbation. Understanding this systems-orientated perspective in biology involves gathering large sets of high-content technologies data and/or data from mining related literature, articles and databases, followed by recommending possible mathematical models that might be associated to this data set. Thereafter, numerical predictions are obtained from accurate computer simulation generated from these mathematical models and finally, the quality assessment of the models and numerical prediction with actual experimental data [2].

Hence, this review article aims to provide a guide and framework to new and novice researchers that are interested in applying systems biology in toxicological perspective. It provides an overview of the progression in the field of toxicology; from the *in-vivo* and *in-vitro* studies to vast ranges of tools such as the –omics as well as high data and information content screening, bioinformatics and systems biology to determine the changes on cells, tissues, and organisms upon chemical or xenobiotic exposure. Extra emphasis will be given on the latter portion.

Search strategies utilising the following bibliographic databases; Scopus, PubMed, Science Direct and EBSCOHost (Medline, Cumulative Index to Nursing and Allied Health Literature; CINAHL and Academic Search Complete) were developed using the selected keywords such as *in vivo*, *in vitro*, animal testing, network biology, systems biology, mechanistic data, systems toxicology, -omics, toxicogenomics, transcriptomics, proteomic, metabolomic and synthetic biology. Boolean operators, wildcards, exact, truncation and other commands were utilised whenever appropriate. The electronic databases searching across all databases was conducted on October 2019 and no limit was set for the evaluated time. Manual searches of reference lists of relevant articles was also performed and partial grey literature search was conducted using Google Scholar [3].

Systems toxicology

Systems biology unifies studies of biological system at the molecular level It involves and encompasses perturbing system, monitoring molecular expression, integrating response data and modelling and displaying the molecular structure and network function of the system. When this concept is applied into toxicology context, it is then known as systems toxicology Systems toxicology describe the -omics as well as 'classical' endpoints evaluation of a biological system, including perturbation by toxicants and stressors, monitoring molecular expression and toxicological parameters and repetitively integrating

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response data to model and represent the archetypically toxicological system [4].

The wealth of *in-vivo*, *in-vitro* and –omics data is still not fully utilized as it does not lead to an accurate predictive power on the biological system and the robustness of these systems may be questionable. The understanding of the effects are usually done in a single system and broader perspective are merely determined by extrapolation. An accurate prediction and comprehensive integration capabilities are therefore required and systems toxicology aims to address this gap by incorporating computational approaches used in system biology in addressing toxicology-related problems. The computational approaches ranges from relational databases (repository of curated information and screening tools) and even potential digital organism [5].

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Conflict of Interest

None

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