

# Chapter 30

## Informatics and Data Analytics to Support Exposome- Based Discovery: Part 2 – Computational Exposure Biology

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### ABSTRACT

*This chapter aims at outlining the current state of science in the field of computational exposure biology and in particular at demonstrating how the bioinformatics techniques and algorithms can be used to support the association between environmental exposures and human health and the deciphering of the molecular and metabolic pathways of induced toxicity related to environmental chemical stressors. Examples of the integrated bioinformatics analyses outlined herein are given concerning exposure to airborne chemical mixtures, to organic compounds frequently found in consumer goods, and to mixtures of organic chemicals and metals through multiple exposure pathways. Advanced bioinformatics are coupled with big data analytics to perform studies of exposome-wide associations with putative adverse health outcomes. In conclusion, the chapter gives the reader an outline of the available computational tools and paves the way towards the development of future comprehensive applications that are expected to support efficiently exposome research in the 21st century.*

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## **INTRODUCTION**

The advent of new high throughput analytical and multi-sensing methods supports current advances in life and environmental sciences supporting their coming together in the quest to create the premise for delivering precision medicine. Even though this is a true revolution for the promotion of good health and cost-effective healthcare on the individual level, public health promotion warrants paying equal attention to prevention and avoidance/reduction of human exposure to the stressors that contribute to ill health. The exposome, the totality of exposures over one's lifetime, and the genome are the two main determinants of human health. Effectively coupling genetic information with environmental and exposure-related data, as well as capturing epigenetic perturbations and linking them with mechanisms of toxicity and adverse outcome pathways maybe the solution towards the development of efficient environmental policies that protect both the quality of the environment, ecosystem function and human health. Thus, the term exposure biology is introduced to denote the system view of exposure to health stressors considering not only environmental and behavioral dimensions but rather capturing the whole network of interactions between environment and human biology and the corresponding dynamics. Development of exposure biology requires the use of a large array of analytical, biological and computational tools that are put together seamlessly to permit the representation of the complexity of interactions and its interpretation.

This chapter gives a comprehensive overview of the computational tools required focusing on their utility in articulating the mechanistic pathways that link environmental exposures to adverse health outcomes on the individual and population level. Such tools comprise data analytics and machine learning methods for pattern recognition and identification of the most important biological pathways perturbed from human exposure to putative health stressors from the molecular to the metabolic level. They also include advanced statistical bioinformatics algorithms used to explore the association space between the exposome and human health precluding any bias and discarding the use of the term confounders. Unlike the traditional environmental epidemiology paradigm, computational exposure biology and exposome-wide association studies embrace all factors that determine or modulate human health and its interaction with the exposome. Thus, issues such as pre-existing health conditions, prior exposures or deleterious habits such as smoking, but also age, gender, socio-economic status are considered part of an individual's exposome. As such they are included in the high-dimension analysis of multiple -omics data derived from human sampling and phenotypic data stemming from clinical examination or biochemical markers.

## **Background**

The scope of the currently available statistical methods is to understand biological functions comprising toxicity pathways and their interactions in relation to external/internal exposure, to confirm the causative effect between exposure and disease endpoint through theoretical (computational) models, to combine mixed data, resulted from various sources, through the utilization of advanced data mining analysis techniques, to provide the methodological tools for integrating multiple biomarkers into a mechanistic description and to derive the systems biology exposome model.

Gene expression data can be a valuable tool for understanding gene regulation, biological networks, and cellular states. One goal in analyzing expression data is to try to determine how the expression of any particular gene might affect the expression of other genes; the genes involved in this case could belong to the same gene network. By a gene network, we mean a set of genes being expressed together in a non-random pattern. Another goal of expression data analysis is to try to determine what genes are

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