

The 7th Conference on Bioinformatics, 3-5 January 2018

Faculty of Biological Sciences, Tarbiat Modares University, Tehran, Iran



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Vision and Mission of Bioinformatics in Toxicology

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Abstract: Growing knowledge based on informatics affect all fields of science and toxicology is not the exception. So predicting toxicity, metabolism, kinetic models and even antidote designing have become the most intrest of today's toxicology. Among the broad scope of informatics, chemoinformatics and bioinformatics two main levers of informatics play the pivot role not only in the future toxicology methods but also in the momentous setting of computational drug design. Although incomparable in cost, consumed time, even ethic problems and the most important of all, deficity of obtained results of in vivo, in vitro and ex vivo, now the in silico studies of computational designed pharmacophores or even metabolized toxicophores play the main role in selecting of hit and lead compounds. In this article after introducing of recent advances in the area of computer aided toxicity prediction, we will discuss the importance of in silico studies in toxicology as an aproach in toxicity modeling. Even more the role of data mining based on next-generation sequencing (NGS) will be considered as a more reliable tool for implementation of personalized medicine, the most recent topic in the cal sciences. The other indication in this article is the application of biological networks and pathway analysis for extrapolation of results as close as the reality of system biology against only one cell line or one target organ testing. This paper is part of a comprehensive study program planned to identify visions and missions of bioinformatics in the biological sciences especially in toxicology to address the challenges ahead and the need for change.

Keywords: in silico studies; predictive toxicology; chemoinformatics; bioinformatics

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