Applications of Bioinformatics

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- Technologies that measure some characteristic of a large family of cellular molecules, such as genes, proteins, or small metabolites, have been named by appending the suffix "-omics," as in "genomics."
- Omics refers to the collective technologies used to explore the roles, relationships, and actions of the various types of molecules that make up the cells of an organism.

• Genomics, "the study of genes and their function" (Human Genome Project (HGP), 2003)

- Proteomics, the study of proteins
- Metabolomics, the study of molecules involved in cellular metabolism
- Transcriptomics, the study of the mRNA
- Glycomics, the study of cellular carbohydrates
- Lipomics, the study of cellular lipids

- Omics technologies provide the tools needed to look at the differences in DNA, RNA, proteins, and other cellular molecules between species and among individuals of a species.
- These types of molecular profiles can vary with cell or tissue exposure to chemicals or drugs and thus have potential use in toxicological assessments.

• Omics experiments can often be conducted in high-throughput assays that produce tremendous amounts of data on the functional and/or structural alterations within the cell.

• "These new methods have already facilitated significant advances in our understanding of the molecular responses to cell and tissue damage, and of perturbations in functional cellular systems"

Bioinformatics

• Bioinformatics is used to abstract knowledge and principles from large-scale data, to present a complete representation of the cell and the organism, and to predict computationally systems of higher complexity, such as the interaction networks in cellular processes and the phenotypes of whole organisms

Genomics

- The first of the -omics technologies to be developed, genomics has resulted in massive amounts of DNA sequence data requiring great amounts of computer capacity.
- Genomics has progressed beyond sequencing of organisms (structural genomics) to identifying the function of the encoded genes (functional genomics).

Genomics

- It was originally thought that obtaining the sequence of the human genome would immediately tell us the identity of the human genes
- Although the sequencing of the human genome was completed in 2003 (HGP, 2003), the identification of all of the genes within the human DNA sequence is not complete

Genomics

• Gene annotation is "adding pertinent information such as gene coded for, amino acid sequence or other commentary to the database entry of raw sequence of DNA bases".

• This involves describing different regions of the code, identifying which regions can be called genes, and identifying other features such as exons and introns, start and stop codons, and so

Proteomics

• Proteins are the primary structural and functional molecules in the cell, and are made up of a linear arrangement of amino acids.

• Unlike the static nature of the cell's genes, proteins are constantly changing to meet the needs of the cell.

Proteomics

- Characterizing the identity, function, regulation, and interaction of all of the cellular proteins of an organism, the proteome, will be a major achievement.
- Studies of changes in the proteome of cells and tissues exposed to toxic materials, compared to normal cells, is being used to develop an understanding of the mechanisms of toxicity

Proteomics

• As proteomics tools become more powerful and widely used, protein and proteome changes in response to exposures to toxic substances (fingerprints or response profiles) will be developed into databases that can be used to classify exposure responses at various levels of organization of the organism, thus providing a predictive in silico toxicology tool.

Metabolomics

- Metabolomics refers to the comprehensive evaluation of the metabolic state of a cell, organ or organism, in order to identify biochemical changes that are characteristic of specific disease states or toxic insults.
- Typical metabolomics experiments involve the identification and quantitation of large numbers of endogenous molecules in a biological sample (e.g., urine or blood) using chemical techniques such as chromatography and mass spectrometry

Metabolomics

- The output from these techniques is compared to computerized libraries of mass spectrometry tracings to facilitate identification of the compounds that are present.
- Environmental stresses such as exposure to chemicals or drugs alter the metabolic pathways in cells, and metabolite profiling can be used to assess toxic responses/exposures.

Toxicogenomics

- Compares the genes expressed in organisms that have been exposed to a drug, chemical, or toxin to those of unexposed organisms (negative controls).
- The up or down regulation of certain genes or groups of genes may be linked to toxic responses occurring in the organism, and to particular organs or cell types in that organism.