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Toxicology unveiled: Navigating the complex web of chemical threats

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DESCRIPTION

Toxicology is the scientific discipline that investigates the adverse effects of chemicals on living organisms. It encompasses a broad range of substances, including pharmaceutical drugs, environmental pollutants, industrial chemicals, and naturally occurring toxins. The primary goal of toxicology is to understand the mechanisms, by which these substances exert their toxic effects, as well as to assess and manage the risks they pose to human health and the environment.

Principles of toxicology

Toxicologists study the toxic properties of substances by examining their absorption, distribution, metabolism, and excretion within the body. These processes are collectively known as ADME. The effects of toxic substances can manifest at various levels, from molecular and cellular to organ systems and the whole organism.

Types of toxicity

Toxicity can be acute or chronic. Acute toxicity refers to the adverse effects that occur shortly after exposure to a high dose of a substance, while chronic toxicity involves long-term exposure to lower doses, leading to cumulative effects over time. Additionally, toxicologists distinguish between local toxicity (effects at the site of exposure) and systemic toxicity (effects throughout the body).

Testing methods of toxicity

Toxicity experiments may be conducted *in vivo* (using the whole animal) or *in vitro* (testing on isolated cells or tissues), or *in silico* (in a computer simulation).

In vivo model organism

The classic experimental tool of toxicology is testing on non-human animals. Examples of model organisms are *Galleria mellonella*, which can replace small mammals, Zebrafish (*Danio rerio*), which allow for the study of toxicology in a lower order vertebrate *in vivo* and Caenorhabditis elegans. As of 2014, such animal testing provides information that is not available by other means about how substances function in a living organism. The use of non-human animals for toxicology testing is opposed by some organisations for reasons of animal welfare, and it has been restricted or banned under some circumstances in certain regions, such

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as the testing of cosmetics in the European Union.

In vitro methods

While testing in animal models remains as a method of estimating human effects, there are both ethical and technical concerns with animal testing.

Since the late 1950's, the field of toxicology has sought to reduce or eliminate animal testing under the rubric of "Three Rs" – reduce the number of experiments with animals to the minimum necessary; refine experiments to cause less suffering, and replace *in vivo* experiments with other types, or use more simple forms of life when possible. The historical development of alternative testing methods in toxicology has been published by Balls.

Computer modeling is an example of an alternative *in vitro* toxicology testing method; using computer models of chemicals and proteins, structure-activity relationships can be determined, and chemical structures that are likely to bind to, and interfere with, proteins with essential functions, can be identified. This work requires expert knowledge in molecular modeling and statistics together with expert judgment in chemistry, biology and toxicology.

In 2007 the American NGO national academy of sciences published a report called "toxicity testing in the 21st century: A vision and a strategy" which opened with a statement: "Change often involves a pivotal event that builds on previous history and opens the door to a new era. Pivotal events in science include the discovery of penicillin, the elucidation of the DNA double helix, and the development of computers. Toxicity testing is approaching such a scientific pivot point. It is poised to take advantage of the revolutions in biology and biotechnology. Advances in toxicogenomics, bioinformatics, systems biology, epigenetics, and computational toxicology could transform toxicity testing from a system based on whole-animal testing to one founded primarily on *in vitro* methods that evaluate changes in biologic processes using cells, cell lines, or cellular components, preferably of human origin."As of 2014 that vision was still unrealized.

The United States environmental protection agency studied 1,065 chemical and drug substances in their ToxCast program (part of the CompTox Chemicals Dashboard) using in silica modelling and a human pluripotent stem cell-based assay to predict *in vivo* developmental intoxicants based on changes in cellular metabolism following chemical exposure. Major findings from the analysis of this ToxCast_STM dataset published in 2020 include: 19% of 1065 chemicals yielded a prediction of developmental toxicity, assay performance reached 79%–82% accuracy with high specificity (>84%) but modest sensitivity (<67%) when compared with *in vivo* animal models of human prenatal developmental toxicity, sensitivity improved as more stringent weights of evidence requirements were applied to the animal studies, and statistical analysis of the most potent chemical hits on specific biochemical targets in ToxCast revealed positive and negative associations with the STM response, providing insights into the mechanistic underpinnings of the targeted endpoint and its biological domain.

In some cases shifts away from animal studies have been mandated by law or regulation; the European Union (EU) prohibited use of animal testing for cosmetics in 2013.

Routes of exposure

Toxic substances can enter the body through different routes, including ingestion, inhalation, dermal contact, and injection. The route of exposure significantly influences the toxicokinetics (movement within the body) and toxicodynamics (mechanisms of toxicity) of a substance.

Risk assessment

One of the key applications of toxicology is in risk assessment, which involves evaluating the potential harm posed by a substance and determining safe exposure levels. This process considers factors such as the toxicity of the substance, the level and duration of exposure, and the characteristics of the exposed population.

Environmental toxicology

Beyond human health, toxicology extends to the study of the impact of chemicals on the environment. Environmental toxicologists assess how pollutants affect ecosystems, wildlife, and aquatic systems, contributing to the development of strategies for environmental protection and conservation.

Analytical techniques

Toxicologists employ various analytical techniques to detect and quantify toxic substances in biological samples and environmental matrices. These techniques include chromatography, mass spectrometry, immunoassays, and molecular biology methods. Advanced technologies have enhanced the sensitivity and specificity of these analyses.

Regulatory toxicology

Regulatory toxicology involves the application of toxicological principles to develop regulations and guidelines for the safe use of chemicals. Government agencies, such as the U.S. Environmental Protection Agency (EPA) and the Food and Drug Administration (FDA), rely on toxicological data to establish permissible exposure limits, set safety standards, and make regulatory decisions.

Toxicogenomics

Recent advances in molecular biology have given rise to the field of toxicogenomics, which explores how genes respond to toxic exposures. This interdisciplinary approach integrates genomics, transcriptomics, proteomics, and bioinformatics to gain insights into the molecular mechanisms of toxicity and individual susceptibility.

Emerging issues

Toxicology is continuously evolving to address emerging challenges, such as the assessment of nanotoxicology (toxicity of nanomaterials), endocrine disruptors (chemicals that interfere with the endocrine system), and the effects of mixtures of chemicals commonly encountered in the environment.

In summary, toxicology plays a pivotal role in safeguarding human health and the environment by unraveling the complexities of chemical exposures. From understanding the mechanisms of toxicity to informing regulatory decisions, toxicologists contribute to enhancing our knowledge of the potential risks associated with a wide array of substances. As the field continues to advance, toxicology remains instrumental in shaping policies and practices that promote safety and sustainability.