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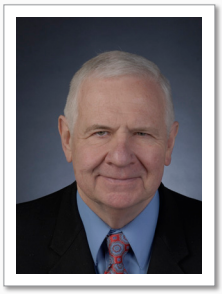

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Roles of computational toxicology in risk assessment

In recent years, computer-based modeling techniques have gained increasing acceptance as powerful tools for informing risk assessment decisions regarding the toxic potential of a variety of chemicals and pharmaceutical agents on an individual or mixture basis. These methods generally identified as computational toxicology offer a number of advantages, rapid and relatively inexpensive evaluations of chemical or pharmaceutical agents both during development and once they are in commercial use. Data mining techniques for rapidly evaluating the published toxicology literature have proven extremely useful for assessing available knowledge. Incorporation of computational toxicology approaches for extrapolating omic-biomarker data from *in vitro* studies and experimental animal studies for human risk assessment has grown rapidly as an approach for expediting initial chemical evaluations on new chemicals or those for which there are relatively few available published data (eg: III-V semiconductors). Incorporating chemical structure information into QSAR models has permitted rapid and inexpensive preliminary assessments of new chemicals or drugs or chemical mixtures for which there are few or no published toxicology data. Reverse dosimetry applications of computer models such as Berkeley-Madonna have permitted evaluation of data from the NHANES data for identifying subpopulations at special risk for toxicity from agents such as cadmium. Computer modeling of molecular pathways or networks has also permitted development of testable hypotheses for evaluating the putative mechanistic roles of persistent organic pollutants (POPs) as underlying causes of important metabolic diseases such as diabetes. In summary, the application of computational toxicology techniques for safety evaluations has proven to be a valuable asset to the field of toxicology which is growing more robust every year. These tools can be expected to make further contributions to chemical risk assessments of chemicals and pharmaceuticals in the future as computational artificial intelligence programs (AI) continue to evolve.

Biography

Bruce A. Fowler obtained his B.S. degree in Fisheries (Marine Biology) from the University of Washington in 1968 and a Ph.D. in Pathology from the University of Oregon Medical School in 1972. He was a staff scientist at the National Institute of Environmental Health Sciences from 1972 until 1987 when he became director of the University of Maryland System-wide Program in Toxicology and Professor at the University of Maryland School of Medicine. He was a senior research advisor to the Agency for Toxic Substances and Diseases Registry (ATSDR) in the Division of Toxicology 2002-2003 and associate director for Science in the Division of Toxicology and Environmental Medicine at ATSDR 2003-2011. He joined ICF International in 2011 as a senior fellow. Dr. Fowler is an internationally recognized expert on the toxicology of metals and chemical mixtures including persistent organic pollutants such as the dioxins. He has served on a number of state, national and international committees in his areas of expertise including those of the NAS/NRC, WHO and IARC and has been a fellow of the Japanese Society for the Promotion of Science, a Fulbright Scholar and Swedish Medical Research Council Visiting Professor at the Karolinska Institute, Stockholm, Sweden. He is a fellow of the Academy of Toxicological Sciences and a member of the AAAS Recruitment and Screening Committee for the Court Appointed Scientific Experts (CASE) Demonstration Project. He is the author of over 200 research papers/book chapters and editor/co-editor of 7 books dealing with molecular mechanisms of toxicity and molecular biomarkers for early detection of chemical-induced cell injury and cell death. Most recently, he has focused on the application of computational toxicology methods for risk assessment.

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