



Computational Toxicology: Chapter 1.

Introduction

Bruce A. Fowler

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This book is intended to be an introduction to various applications of computational toxicology and to show how these approaches are currently being used effectively for risk assessment purposes in the near term. It is important to note that the field of computational toxicology is rapidly evolving and that subsequent editions of this book will take up new methods that are currently under development, such as high-throughput screening, and others that are still in a conceptual stage. There are many advantages for including computational toxicology approaches in the risk assessment process. Among these are reducing costs, minimizing use of animals in toxicology testing, improving speed in providing answers regarding chemicals in emergency situations such as the Gulf Oil spill, and dealing with the common problem of decision making for chemical mixtures. In addition, computational methods may be used for extrapolating or translating data from both in vitro and in vivo experimental animal test systems for human risk assessments of chemicals and drugs. In addition, computational methods may be used for focusing laboratory studies into productive areas by data mining the published literature and developing testable hypotheses by application of systems biology approaches to identify chemical interactions with functional molecular pathways to generate a more comprehensive picture of likely primary and secondary modes of chemical or drug activity. In summary, there is much that computational toxicology is now contributing to helping make better societal risk assessment decisions about chemicals and drugs. The future for these approaches is optimistic and limited only by human ingenuity and availability of resources.



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