



Computational Toxicology: Chapter 13. Future Directions for Computational Toxicology for Risk Assessment

Bruce A. Fowler

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As in many fields of scientific endeavor, computational toxicology represents a broad and expanding group of activities. This chapter attempts to summarize ongoing efforts for a number of computational approaches and suggest ways in which these methods could be applied effectively for improving risk assessment practice going forward in time. Generic issues include QA/QC of data used for computational modeling, graduate education programs for training the next generation of computational modelers with a common language among themselves, and the training in translation of computational toxicology terms for scientists in other related fields and the lay public so that effective communication of modeling data is achieved.

Communication with scientists involved in systems biology approaches will be of particular importance. In this regard, it will also be essential to integrate artificial intelligence (AI) programs into future risk assessment programs for the evolution of this field in order to more fully integrate systems biology into mode of action risk analysis. Expanded use of data mining programs for development of testable hypotheses and to facilitate the incorporation of “green chemistry” approaches will reduce the number of chemicals in need of post-manufacture toxicology testing and risk assessment. In summary, it is hoped that the key elements identified in this chapter will help this field to continue to develop in a robust manner and provide the risk assessment community with a much needed set of modern scientific tools.

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