Computationally Augmented Intelligence for Predictive Toxicology

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The field of computational toxicology has enjoyed rapid growth over the last decade, with the maturation of cognitive algorithmic tools and software to mine, process, and model data to facilitate robust and reliable predictions of chemical property, activity, and toxicity endpoints. Success lies in iterative and mutually informative approaches along a continuum of FAIR data resources, predictive analyses, experimentation, and mechanistic models, with the goal of generating insights into human disease processes and their susceptibility to environmental perturbations. Underpinning this “CompTox continuum” is augmented intelligence, a field that leverages big data and computational tools to join techniques of machine learning, artificial intelligence, natural language processing, mathematical modeling, and data analytics to enhance and support human intellect. Applications of augmented intelligence to predictive toxicology will be discussed, with examples ranging from model development for specific toxicity endpoints, to automation of data curation and annotation, to computational workflows enabling hypothesis generation and testing, to establishing scientific confidence in novel approach methodologies.