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Editorial

The future of toxicology research in the era of artificial intelligence: the vision of 1H-TOXRUN Hub

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Abstract

Toxicology, the great science of understanding the toxic effects of chemical substances on living organisms, is increasingly being integrated within the One Health framework – the holistic approach that recognizes the interconnectedness of human, animal, and ecosystem health [1,2]. The One Health concept advocates interdisciplinary collaboration among veterinarians, physicians, environmental scientists, and other professionals to address complex health challenges that transcend species and ecological boundaries. This vision gives legitimacy and uniqueness to 1H-TOXRUN, the research Hub for One Health Toxicology. Integrating toxicology into the One Health paradigm encourages collaboration across disciplines to investigate the mechanisms, sources, and impacts of toxic exposures. This includes studying xenobiotics' cellular and molecular mechanisms, assessing environmental contamination, and evaluating the health outcomes in both animals and humans. Ecotoxicology, as a subfield, emphasizes the effects of pollutants on ecosystems, including plants, animals, and microbial communities, further reinforcing the need for a unified approach [3]. Adopting a One Health perspective in toxicology leads to more comprehensive risk assessments that account for the complexities of real-world exposure scenarios. Therefore, policies and interventions must be designed to address the interconnected nature of these risks, promoting sustainable practices and preventive measures at the ecosystem level.

However, the world is changing, and the massive availability of artificial intelligence (AI) will shape the future of toxicology as a mother science, just as it is already transforming forensic science, as previously highlighted [4]. Integrating AI into toxicology is poised to redefine the discipline, transitioning it from relying on empirical observation to a data-driven, predictive science. By leveraging machine learning, deep neural networks, and generative AI, toxicology will enhance chemical risk assessment, reduce animal testing, and enable personalized toxicity predictions [5]. Indeed, AI models, such as quantitative structure-activity relationship (QSAR) frameworks and read-across-based structure-activity relationships (RASAR), now achieve high accuracy in predicting chemical toxicity, outperforming traditional animal test reproducibility [6]. For example, deep learning algorithms analyze chemical structures, biological activity, and omics data to forecast mutagenicity, streamlining drug development and reducing reliance on *in vivo* experiments [6]. Tools like eToxPred prioritize compounds for testing, minimizing costs and ethical concerns [7]. In addition, AI can decipher complex molecular pathways by integrating transcriptomic, proteomic, and metabolomic datasets [8]. Moreover, neural networks process high-content imaging from high-throughput screens to identify biomarkers for hepatotoxicity, nephrotoxicity, cardiotoxicity, and neurotoxicity, linking genetic susceptibility to chemical exposure [9]. This capability enables precision toxicology, where AI tailors risk assessments using individual genetic, microbiome, and exposure profiles [10]. AI platforms are also already simulating biological systems to predict human responses. For instance, virtual organ models replicate chemical interactions, enabling dose-response extrapolations and antidote efficacy testing. These systems support probabilistic risk assessments, quantifying uncertainties in exposure scenarios. Toxicology education is also a target of reshaping with AI, enabling personalized learning, and bridging gaps between theoretical knowledge and real-world

applications [11]. This transformation, driven by AI's capacity, makes it possible to analyze complex datasets, simulate experiments, and predict toxicological outcomes, offering educators and students unprecedented tools to enhance understanding and engagement. AI-driven toxicology education will offer safer virtual labs for students to conduct impractical experiments in physical settings. Therefore, by embedding AI tools into curricula, educators prepare students to innovate in chemical safety, drug development, and public health crises, ensuring the next generation of toxicologists excels in both computational and experimental realms. But future directions are even more disruptive and revolutionary. Indeed, quantum computing will make it possible to solve complex systems, such as toxicology models, including multi-organ interactions, beyond classical computational limits, and cloud-based platforms will democratize access to predictive tools, empowering low-resource regions in chemical safety management. Moreover, quantum annealing optimizes the prioritization of 10,000+ chemicals for regulatory review, focusing resources on high-risk compounds [12].

The IV 1H-TOXRUN International Congress, held in Porto, Portugal, on May 8–9, 2025, promises to be a dynamic and enriching event for professionals across toxicology, biomedical, and environmental sciences, exploring the new expected world for toxicology. Under the visionary theme "EMPOWERING THE FUTURE GENERATIONS: THE SYNERGY OF SCIENCE, EDUCATION, AND SOCIETY", this congress is set to foster interdisciplinary debate, knowledge exchange, and collaborative reflection within the One Health framework. Four carefully curated sessions anchor the scientific program this year: the i) **Session I: Pioneering the Future – Bridging Science and Entrepreneurship** is the spotlight of the intersection of research and innovation, exploring how scientific advances translate into entrepreneurial ventures and societal benefits. By merging cutting-edge science with commercial agility, academic institutions and startups are translating mechanistic insights into scalable solutions, from AI-driven risk assessment platforms to targeted therapeutics; the ii) **Session II: Shaping the Future of Education – Innovation, Impact and Digital Transformation** focus on transformative educational strategies, digital tools, and the impact of innovation on the training of tomorrow's scientists and health professionals. Integrating digital innovation into toxicology education is driving a paradigm shift, equipping future scientists with skills to address global chemical safety challenges through data-driven, ethical, and interdisciplinary approaches; the iii) **Session III: Global Challenges on Migration and Health** addresses the pressing health implications of global migration, emphasizing the need for integrated, cross-sectoral responses to emerging public health challenges. Global migration is one of the defining challenges of the 21st century, with more people than ever crossing borders due to conflict, economic hardship, environmental change, and opportunity. This movement brings significant health implications for both migrants and host populations [13], and toxicology plays a critical but often underappreciated role in this context. While infectious diseases often receive the most attention, non-communicable diseases (NCDs) and environmental exposures, including toxicological hazards, are major contributors to morbidity and mortality in these populations [14]. Moreover, continued use of traditional medicines, cosmetics, or imported foods may involve substances banned or regulated in the host country, leading to unintentional poisonings or adverse drug interactions; and the iv) **Session IV: Innovation for Sustainability and Environmental Transformation** is intertwined with advances in toxicology, particularly through the emergence of "green toxicology". This discipline reshapes how chemicals and materials are designed, produced, and regulated, prioritizing human and environmental health alongside economic and functional considerations. In other words, green toxicology offers a proactive, preventive approach to chemical safety [15]. Unlike traditional toxicology, which often assesses risks after products are already used, green toxicology integrates toxicological principles early in the design and development. This strategy enables identifying and mitigating potential hazards before chemicals reach the market, minimizing adverse impacts across global supply chains, and supporting the broader goals of sustainability and environmental stewardship [16]. Participants explore the cutting-edge research and initiatives aimed at environmental sustainability, resilience, and mitigating health risks from environmental pressures.

Altogether, the congress underscores the importance of safety, health risk prevention, and promoting resilient communities and circular economy models. By integrating cross-cutting issues aligned with the Sustainable Development Goals, the event aims to advance a unified approach to optimizing people, animals, and environmental health. All authors with relevant work in the aforementioned areas are presenting their oral and poster presentations, both representing fundamental components of scientific congresses, each playing a distinct and complementary role in the dissemination of research, fostering collaboration, and advancing scientific dialogue, and contributing to the success and vibrancy of the 1H-TOXRUN International Congress brand of credibility.

Cordial greetings
Ricardo Jorge Dinis-Oliveira

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