Artificial Intelligence in Predictive Toxicology: Identifying influential topics based on science mapping

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Abstract
This research paper delves into the transformative landscape of Predictive Toxicology, marked by the integration of Artificial Intelligence (AI) and cutting-edge technologies. The emergence of Predictive Toxicology, driven by computational models leveraging machine learning, signifies a departure from traditional methods, promising accelerated risk assessment and enhanced comprehension of chemical-biological interactions. Through science mapping, this study explores the interconnected web of literature in this dynamic field, aiming to trace its historical evolution, identify influential research hubs, and discern collaborative networks. The dataset analysis spanning 1993 to 2023 unveils trends, emphasizing the surge in AI's prominence and the sustained relevance of foundational topics. This study not only offers a comprehensive overview but also provides a roadmap for future research in the intersection of AI and Predictive Toxicology.

Keywords: Predictive Toxicology, Artificial Intelligence (AI), Science Mapping

Introduction:
Artificial Intelligence (AI) is one of the most innovative technologies that has revolutionized the world of toxicology in recent years. The intersection of artificial intelligence and toxicology has led to the development of a revolutionary method called Predictive Toxicology(1). In this method, computer models use data analytics and machine learning to predict the possible negative effects of chemicals. This convergence of modern technologies has enormous promise in accelerating the risk assessment process, reducing dependency on traditional experimental approaches, and expanding our understanding of the complicated link between chemical exposure and biological reactions(1,2).

With an emphasis on artificial intelligence, this paper undertakes a thorough investigation of the field of predictive toxicology. Study aims to disentangle the complex network of scientific literature in this dynamic and quickly developing topic via the lens of science mapping(1).

With the introduction of AI in Predictive Toxicology, researchers can now leverage extensive datasets, apply advanced algorithms, and obtain previously unattainable levels of accuracy in toxicity prediction. This marks a significant shift from conventional methods. The more we get into the nuances of this symbiotic relationship between toxicology and AI, the more important it is to understand the field's historical development, pinpoint key research centers, and uncover the networks of collaboration that spur innovation(3).

This paper intends to give a thorough assessment of the state of artificial intelligence in predictive toxicology as well as a research roadmap for future approaches.

Objectives:

1. **Examine Artificial Intelligence's (AI) Impact on Research:** Examine how traditional models gave way to AI between 2003 and 2022, highlighting changes in research methodology as well as an increasing reliance on technology for data analysis in the fields of biology and chemistry.

2. **Explore Interdisciplinary Trends:** Examine the spike in interdisciplinary inquiries around 2020, notably in domains like humans, neural networks, and computational biology, demonstrating joint efforts affecting the developing landscape of scientific inquiry.

3. **Determine a Topic's Long-Term Relevance**: Determine a topic's long-term relevance, taking into account factors like social demands or technology improvements that may have an impact on research trends. Examples of such topics are "models, biological," "toxicology," and sustained attention.

Literature Review:

The aforementioned research offer a thorough summary of all the different facets of predictive toxicology. A gap analysis indicates the necessity for a more concentrated investigation of Artificial Intelligence (AI) applications within the predictive toxicology landscape in order to integrate AI into predictive toxicology and identify important issues based on science mapping. Although the research discusses advances in computer models, liver-chip technology, and in vitro profiling, a focused analysis of the role AI approaches play in predictive toxicology would improve our comprehension of the possible implications.

The research by Lorna Ewart et al. (2022) and Giorgini et al. (2023) illustrate the usefulness of liver-chip technology and in silico approaches in prediction toxicology. The incorporation of artificial intelligence (AI) into these frameworks holds significant potential for enhancing the precision and efficacy of drug-induced liver injury prediction and chemical compound cytotoxicity assessment.

The significance of novel approach methodologies (NAMs) for assessing chemical toxicity in developmental and reproductive contexts is emphasized in the workshop report by Knudsen et al. (2021). Nonetheless, a more thorough investigation of the ways in which AI might improve NAMs and support predictive toxicology in these particular domains would offer insightful information.

ComptoxAI is a revolutionary data platform for computational and artificial intelligence research in predictive toxicology, presented by Romano et al. (2022). To fully grasp the state-of-the-art in this field, a more thorough examination of the particular AI methods used in ComptoxAI, as well as their uses and effects on predictive toxicology, is necessary.

Presumably, even though the aforementioned studies make a substantial contribution to various aspects of predictive toxicology, a focused study on the incorporation of AI techniques and their impact on toxicological outcome prediction could offer a more nuanced and thorough picture of the current situation. Such an analysis would assist discover influential issues and gaps in knowledge within the framework of AI applications in predictive toxicology.

Methodology:
Using a combination of free-text terms and Medical Subject Headings (MeSH), PubMed was used in this investigation. The search query looks for journal articles related to "artificial intelligence" and "predictive toxicology." It includes a range of expressions, such as MeSH phrases for "artificial intelligence" and a synthesis of distinct terminology for artificial and intelligence in diverse domains. The query further refines the results by stating that the publications must be published in English, have the term "predictive toxicology" stated in the title or abstract, and fall within the publishing type of "journal article(4)."

The temporal scope is restricted to articles published between January 1, 1993, and December 31, 2023. This refined search strategy aims to yield articles that align with the intersection of artificial intelligence and predictive toxicology within the specified linguistic, publication, and temporal criteria.

The study utilized the R base biblioshiny package to perform data cleaning and processing, taking advantage of its features to simplify and prepare the dataset. The statistical studies were then carried out with Python programming. The Python software effectively calculated a number of statistical measures, giving the data analysis procedure more depth and accuracy. This cooperative strategy, which combined the advantages of R and Python, guaranteed a thorough and reliable analysis of the dataset, enabling efficient data cleaning, manipulation, and statistical computations(5).

Data Analysis and Interpretation:
This study provides a thorough examination of a dataset that spans the years 1993 to 2023. The dataset is made up of 43 documents, mostly journal articles, and was gathered from 27 publications.

Table 1: Study Information

Description	Results
MAIN INFORMATION ABOUT DATA	
Timespan	1993:2023
Sources (Journals, Books, etc)	27
Documents	43
Annual Growth Rate %	6.15
Document Average Age	9.19
Average citations per doc	0
References	0
DOCUMENT CONTENTS	
Keywords Plus (ID)	161
Author's Keywords (DE)	77
AUTHORS	
Authors	236
Authors of single-authored docs	4
AUTHORS COLLABORATION	

Single-authored docs	5
Co-Authors per Doc	5.86
International co-authorships %	0
DOCUMENT TYPES	
comparative study	8
evaluation study	2
journal article	33

This study provides a thorough examination of a dataset that spans the years 1993 to 2023. The dataset is made up of 43 documents, mostly journal articles, and was gathered from 27 publications. With an average document age of 9.19 years, the dataset shows an annual growth rate of 6.15%, suggesting a consistent increase in document production over time. The dataset includes 236 writers, demonstrating collaborative efforts with an average of 5.86 co-authors per document. However, insights into the influence and external sources mentioned are limited by the lack of information on average citations per document and references.

Verifying the stated 0% of foreign co-authorships is important. Eight comparison studies, two assessment studies, and thirty-three journal articles are among the document categories that make up the dataset; they represent a wide range of study focuses and approaches. This study offers insightful information about the dynamics and patterns of research in the area in question.

Table 2: Trend Topics

item	**freq**	**year_q1**	**year_med**	**year_q3**
models, biological	8	2003	2003	2008
structure-activity relationship	8	2003	2003	2005
rats	7	2003	2003	2008
models, chemical	5	2005	2005	2009
artificial intelligence	12	2003	2006	2015
reproducibility of results	10	2003	2006	2014
algorithms	13	2003	2007	2022
databases, factual	11	2003	2007	2020
toxicology	14	2003	2008	2013
animals	20	2004	2012	2020
drug-related side effects and adverse reactions	6	2008	2014	2022
quantitative structure-activity relationship	15	2010	2018	2021
computer simulation	7	2008	2018	2020
toxicity tests	7	2008	2018	2020
humans	18	2015	2020	2021
neural networks, computer	9	2006	2020	2021
computational biology	7	2016	2020	2020
machine learning	11	2020	2021	2022
drug discovery	5	2022	2022	2023

The dataset offers insightful information about how scientific research has evolved over time, showing how old models and experimental methods have given way to a landscape that is more driven by technology(6). A paradigm shift in research methodology is suggested by the steady rise of artificial intelligence and machine learning from 2003 to 2022, which points to an increasing reliance on computational tools for modeling and data analysis. Moreover, there is a persistent interest in learning about the safety profiles of substances, as seen by the temporal patterns in themes pertaining to toxicology and drug-related side effects(7). The rise in popularity of neural networks and computational biology corresponds with the growing adoption of cutting-edge technologies in chemical and biological research(8).

Topics like databases and algorithms have been around for a long time and are still relevant, which highlights their fundamental role in scientific research. The focus of research efforts around 2020, particularly in the fields of computational biology, neural networks, and humans, points to a recent upsurge in multidisciplinary studies, which may be the result of technological breakthroughs and a more comprehensive approach to scientific problem-solving.

The landscape of research in biological and chemical sciences has witnessed dynamic shifts, as indicated by the trends. While biological models, rats, and structure-activity relationships held steady attention from 2003 to 2008, artificial intelligence (AI) emerged as a dominant force, experiencing a significant surge from 2003 to 2015(6). This period also saw a growing emphasis on the reproducibility of results, accompanied by a persistent reliance on algorithms and factual databases. Toxicology topics, particularly toxicity tests, displayed a declining trend post-2013, whereas machine learning and drug-related side effects gained prominence from 2020 onwards. Human-centric research became increasingly relevant from 2015 to 2021, aligning with the rising importance of neural networks and computational biology(3). The latter half of the provided data points to an accelerating interest in machine learning applications and drug discovery, emphasizing the ongoing evolution and diversification of research themes within the biological and chemical sciences(7).

Correlation analysis

The correlation analysis unveils a captivating narrative about the intricate relationship between topic frequency and temporal distribution.

Table 3: Correlation analysis

Correlation analysis				
Variable	**Freq**	**Year_Q1**	**Year_Med**	**Year_Q3**
Freq	1	-0.645	-0.679	-0.595
Year_Q1	-0.645	1	0.959	0.955
Year_Med	-0.679	0.959	1	0.975
Year_Q3	-0.595	0.955	0.975	1

The negative associations highlight an interesting pattern that implies highly debated subjects have historical origins, reiterating the idea that scientific discourse frequently has historical foundations. Interestingly, several subjects, such as "biological models," "structure-activity relationship," and "artificial intelligence," are consistently present in all quartiles, indicating their ongoing importance. The rise of contemporary technologies is interesting since terms like "artificial intelligence," "algorithms," and "machine learning" become more prominent throughout time. The intricate interplay between frequency and quartile years adds dimension, illustrating a dynamic landscape where highly talked issues tend to be connected with earlier times(9). The themes' temporal growth, such as the rise of "machine learning" and the advent of "models, chemical," adds a level of curiosity and reflects how scientific research is always changing. The persistent focus on "toxicology" and "drug discovery" attests to ongoing research dedication, while the prominence of "animals" and "humans" signifies enduring significance across diverse research realms(10).

Conclusion:

To sum up, the thorough examination of a dataset covering the years 1993 to 2023 offers insightful information on how biological and chemical research is developing. With a consistent increase in the use of computer tools for data analysis, the apparent paradigm shift towards artificial intelligence (AI) and machine learning demonstrates a revolutionary influence on methodology. The wave of transdisciplinary research that began to emerge around 2020 showcases cooperative endeavors in a variety of fields, including computational biology, neural networks, and people, which are influencing the state of science today. The persistence and longevity of particular topics highlight their lasting importance, and the relationships between topic frequency and historical distribution show complex patterns in the development of scientific discourse. This study emphasizes the importance of technology, teamwork, and the eternal relevance of fundamental subjects, adding to a more nuanced knowledge of the trends and dynamics within the biological and chemical sciences.

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