

Mapping the Landscape of Drug Delivery Research with a Focus on Artificial Intelligence

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ABSTRACT

Aim: This study analyzed the landscape of drug delivery research with a bibliometric approach, focusing on Artificial Intelligence (AI) using data from the Web of Science. **Materials and Methods:** The analysis included 20 years from 1992 to 2023, using R Studio and VOS Viewer for data analysis. **Results:** Findings reveal a surge in interest post-2012, with 254 articles published in 182 journals, and the average age of articles remarkably low at 2.04 years, indicating the dynamism of the field. The study identified China as the leading contributor, followed by notable contributions from the United States of America and India. The National University of Singapore emerged as the most productive institution. The International Journal of Pharmaceutics was highlighted as the most impactful journal. The co-word analysis revealed thematic clusters such as AI in fabrication, formulation design, nanoparticles, and prediction of *in vivo* drug delivery, with niche themes like targeted delivery and toxicity prediction. The thematic map showcases 17 clusters, providing a nuanced understanding of the evolution of research themes over time. The hierarchical clustering dendrogram reveals that AI has been primarily applied in modeling nanoparticulate drug delivery for cancer. As a result, AI-based models for predicting drug delivery for other diseases remain lacking. **Conclusion:** This bibliometric study provides a holistic view of AI in drug delivery research, identifying trends, collaborations, and emerging themes. The remarkable growth observed in recent years indicates the promising future of AI-driven drug delivery research.

Keywords: Artificial intelligence, Bibliometric, Cancer, Drug delivery, Nanoparticles, Targeted delivery.

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INTRODUCTION

Integrating Artificial Intelligence (AI) in drug delivery research has revolutionized traditional approaches. The convergence of AI and drug delivery has redefined how therapeutic agents are transported to their intended targets in the body, allowing for unprecedented accuracy, efficiency, and personalized treatments.^[1] In the past, drug delivery systems relied on trial-and-error methods, which required extensive experimentation

and optimization. However, AI has enabled researchers to use machine learning and computational models to accelerate the development of novel drug delivery platforms.

AI can analyze vast amounts of data, extract valuable insights, and identify optimal drug formulations and delivery mechanisms, leading to the discovery of innovative strategies for targeted drug delivery. AI technology can predict and model drug behavior inside the human body. This allows scientists to simulate and optimize drug release profiles, absorption rates, and distribution patterns. The ability to make accurate predictions has far-reaching implications for improving therapeutic efficacy while also reducing adverse effects. AI algorithms can forecast drug behavior under various physiological conditions and determine the best

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parameters for efficient drug delivery. Furthermore, AI-driven approaches enable real-time patient data and feedback integration, enabling personalized and adaptive drug delivery strategies.^[2] AI has immense potential to reshape drug delivery and improve healthcare outcomes worldwide.

Bibliometric analysis is a powerful mathematical method that allows researchers to explore and visualize scientific literature quantitatively.^[3] R studio-Bibliometrix is a robust software that facilitates quantitative literature analysis in its “Biblioshiny” platform by specialized statistical techniques.^[4] VOS Viewer is another program that generates better visual representations of bibliographic data, including keywords co-occurrence and thematic maps.^[5] Integrating R Studio and VOS Viewer enables systematic exploration of scholarly publications and thematic clusters, facilitating evidence-based decision-making and strategic planning by identifying research gaps and emerging subtopics.^[6] No bibliometric study on the role of AI in drug delivery is available. We conducted a comprehensive bibliometric assessment of drug delivery research with a specific focus on artificial intelligence, combining the analytical power of R Studio with the visual capabilities of VOS Viewer. The bibliometric analysis aims to critically examine the existing research on AI in drug delivery and identify trends and gaps in the current literature to guide future research efforts. The quantitative bibliometric study also aims to gain insights into the trends, collaboration patterns, and keyword usage in drug delivery research that involves artificial intelligence. By analyzing the data, we seek to understand the current state of this interdisciplinary field.

MATERIALS AND METHODS

Extraction of bibliographic data and processing

On October 1, 2023, we accessed the Web of Science (WoS). With our licensed access to WoS, we could use all search features and filters on the platform. We searched WoS using Medical Subject Headings (MeSH) terms obtained from the database. The search criteria are compiled as follows: (“artificial intelligence” OR (“artificial”[All Fields] AND “intelligence”[All Fields]) OR “artificial intelligence”[All Fields]) OR (“machine learning”) OR (“machine”[All Fields] AND “learning”[All Fields]) OR “machine learning”[All Fields])) AND (“drug delivery systems” OR (“drug”[All Fields] AND “delivery”[All Fields] AND “systems”[All Fields]) OR “drug delivery systems”[All Fields] OR (“drug”[All Fields] AND “delivery”[All Fields]) OR “drug delivery”[All Fields]) AND (“author manuscript”[Filter]

AND “1992/10/01”[PDat]: “2023/10/01”[PDat]). We ensured accuracy by using appropriate filters to retrieve the data. We extracted the information from research and review articles published in the last ten years, from 1 October 1992 to 1 October 2023. We checked the “all field” options during the download process to retrieve information related to authors, titles, journals, language, article type, author keywords, keywords plus, abstract, addresses, affiliations, funding organizations, cited reference count, times cited (WoS score), times cited (all databases), 180-day usage count, since 1992 usage count, highly cited paper, hot paper status, article DOI, publisher, and ISSN number.

The data was downloaded as a raw file from WoS and then converted to an Excel file using R Studio. We checked the file for missing documents, authors, titles, and duplications. After these checks, we confirmed that the Excel file is clean and ready for further quantitative assessment.

Quantitative assessment of bibliographic data

We employed R Studio and VOS Viewer to evaluate bibliographic data quantitatively.^[7] To do this, we used command lines to run Biblioshiny and accessed it through the R Studio platform. The Biblioshiny interface was then used to analyze the data, including performance metrics related to publications and citations. For science mapping associated with the conceptual structure, such as keyword co-occurrence network, thematic map, and enrichment metrics like factorial analysis, we used VOS Viewer and visualized the graphs and networks. Finally, we interpreted the results of the established metrics to understand the research landscape of artificial intelligence in drug delivery.

RESULTS

Summary of Information

The study used data obtained from WoS to conduct a bibliometric analysis of research on AI in drug delivery. WoS is one of the world’s most essential and updated platforms for academic and research information and scientific citation discovery. Tens of millions of bibliographic records made up of billions of citation connections and other metadata fields are already in WoS.^[8] R Studio and VOS Viewer were utilized for quantitative academic data analysis. A rigorous protocol was applied to scan, sense, and substantiate the data to obtain meaningful interpretations.^[9] The following text summarizes the primary information related to using AI in drug delivery research, categorized by the source of the articles, their contents, authors, author

collaborations, and article types. The data was retrieved from WoS and is presented in Table 1.

Table 1: Summary of information on AI in drug delivery research retrieved from Web of Science.

Description	Results
Timespan	1992:2023
Sources (Journals)	182
Documents	254
Annual Growth Rate %	14.53
Document Average Age	2.04
Average citations per doc	20.92
Keywords Plus	1170
Author's Keywords	1008
Authors	1212
Authors of single-authored docs	6
Co-Authors per Document	5.41
International co-authorships %	34.25
Research articles	132
Review articles	122

Performance metrics

Performance metrics are a tool for assessing the contributions of various research components to a specific field.^[4] Figure 1 shows the annual scientific output of AI in drug delivery research. Between 2021 and 2023, there was a substantial rise in publications related to AI-driven drug delivery, accounting for 74% of total publications in this field.

It is crucial to evaluate the contributions made by different nations in a particular field of research. Bibliometric analysis has revealed that 44 countries

have published at least one paper on AI-driven drug delivery research. China ranks first in the number of publications, while Egypt and Saudi Arabia are in the ninth and tenth positions, respectively. Table 2 shows the top 10 countries that have actively participated in drug delivery research using AI. It is worth noting that the top three countries maintained their positions regarding their individual contributions. At the same time, Egypt made a significant leap and secured the fifth position based on single-country publications. When considering the corresponding author country or single-country publication, Saudi Arabia was placed 13th. Figure 2 illustrates the rankings of different countries based on whether the publication comes from a research group with the corresponding author credit of the same country or an international collaboration.

The WoS database facilitates the analysis of the most reliable and productive affiliations of authors involved in AI applications in drug delivery research. A threshold of at least 2 documents and 1 citation was set to retrieve the most productive author affiliations list. Figure 3 presents a comprehensive list of the most productive affiliations of authors in drug delivery research utilizing AI. We observed that all 32 articles from Egypt extracted by WoS are listed under the Egyptian Knowledge Bank (EKB) affiliation in the Biblioshiny report, even though the publications are from different universities in Egypt, such as Cairo University, Future University, and Ain Shams University. Therefore, we present the data as retrieved from WoS without segregating the publications from Egypt universities. The National University of Singapore is the most productive institution in this research area, accounting for 14.96% of publications.

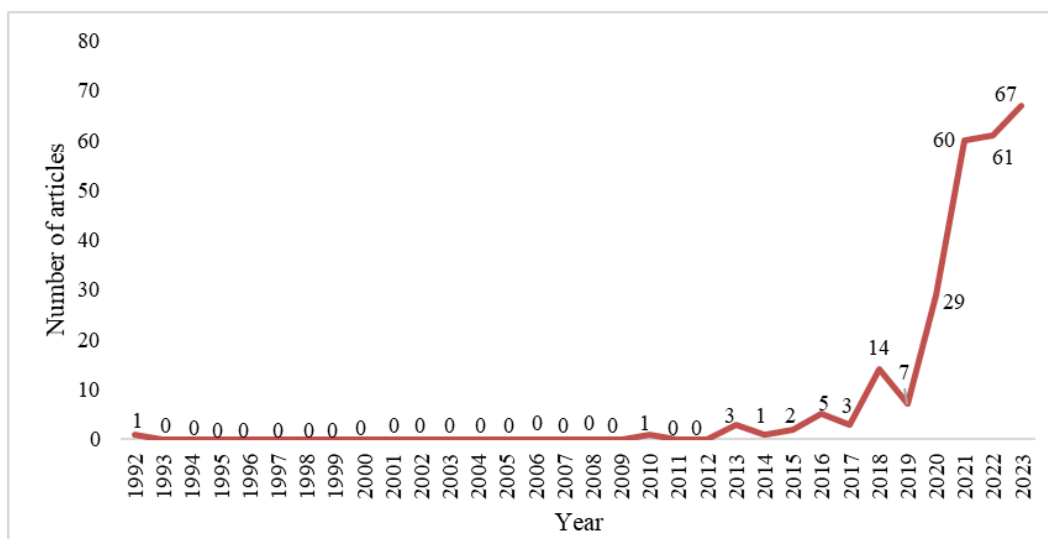


Figure 1: Annual scientific output of AI in drug delivery research.

Table 2: Top 10 countries that contributed to AI-driven drug delivery research.

Country	Number of publications
China	164
USA	149
India	76
UK	64
Singapore	46
Iran	45
Spain	43
Canada	37
Egypt	32
Saudi arabia	27

To analyze the performance of research on AI in drug delivery, it is essential to examine relevant journal sources, citation rates, and the journal's impact. The list of most relevant journal sources that have published at least 3 papers on AI in drug delivery research can be seen in Figure 4, retrieved from the Biblioshiny report. It is evident from the list that several journals in the field of pharmaceuticals have published drug delivery models predicted using AI. The mean total citations per article are displayed in Figure 5. Interestingly, the citation rate experienced a surge in 2017 but has surprisingly declined in recent years. The impact of the journal is measured by its h index. Figure 6 displays the journals with an h index of at least 2. The International Journal of Pharmaceutics was ranked the most productive and high-impact journal.

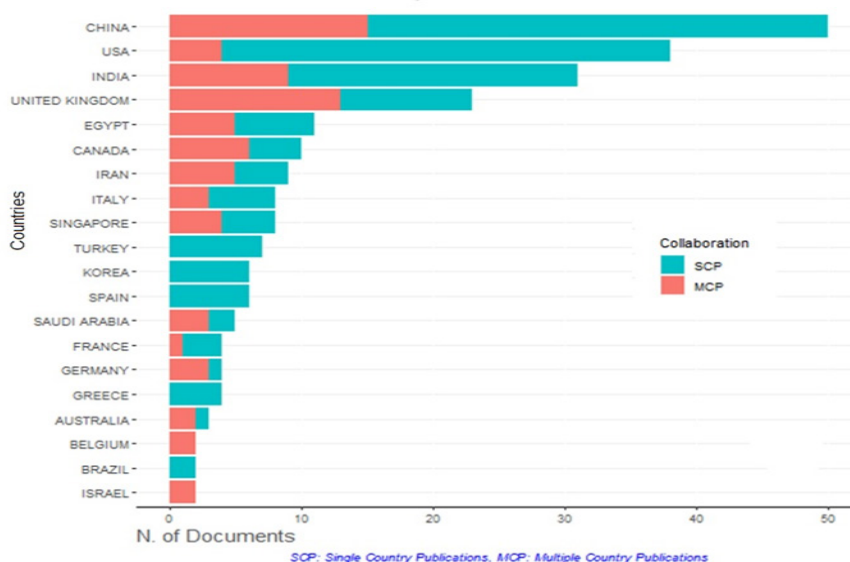


Figure 2: Country rankings by corresponding author.

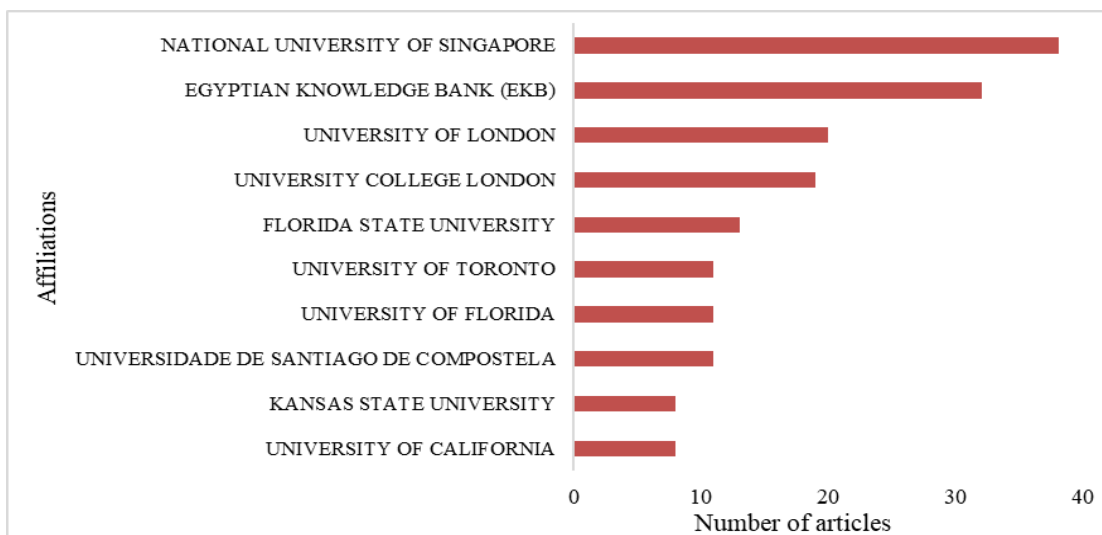


Figure 3: Most productive affiliations of authors in AI-driven drug delivery research.

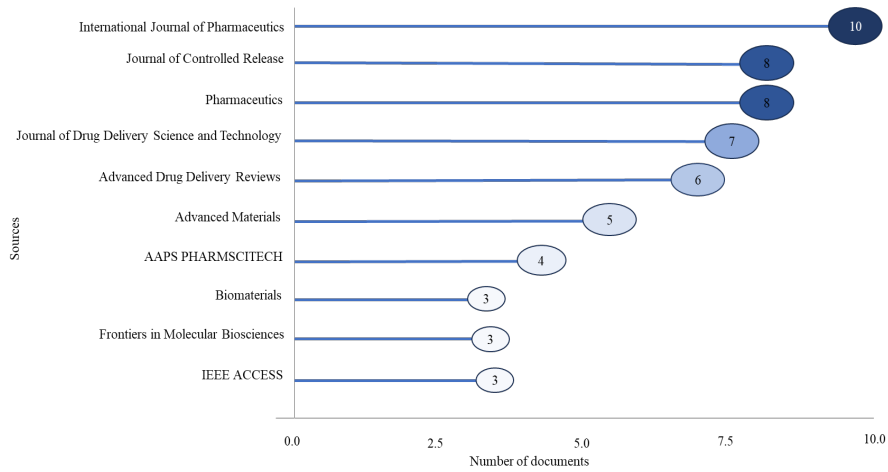


Figure 4: Most relevant journal sources for AI in drug delivery research.

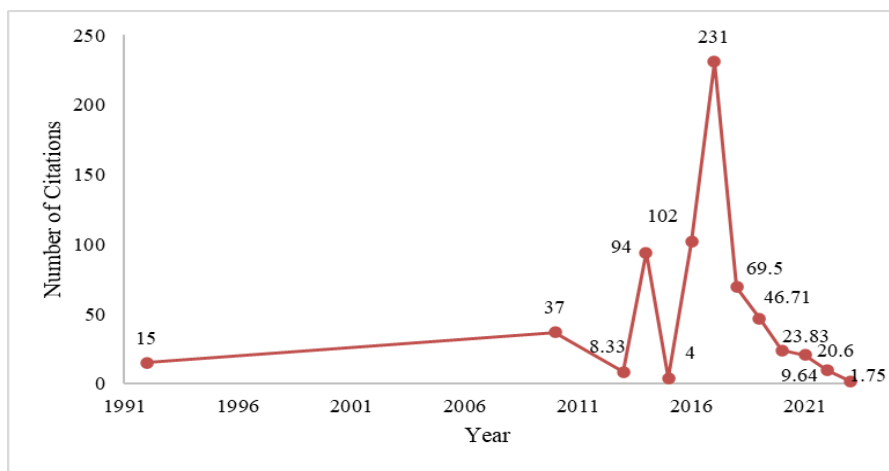


Figure 5: Mean total citations per article on AI-driven drug delivery research.

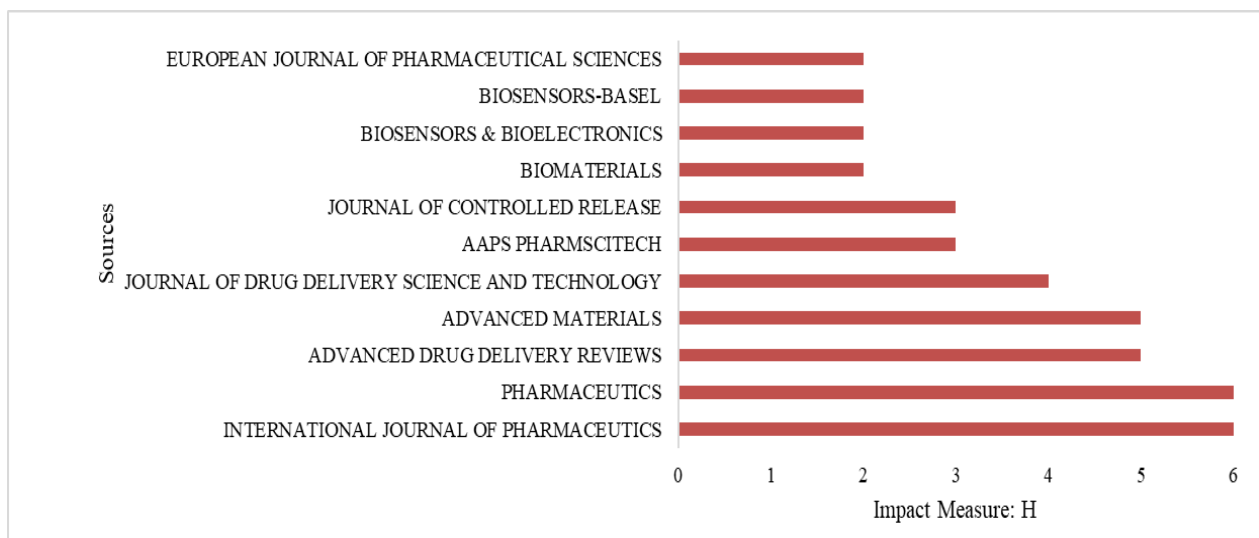


Figure 6: AI-driven drug delivery research's relevant source's local impact by H index.

Science mapping

Science mapping visually represents the relationships between scientific publications, authors, and research topics to identify patterns and gaps within a specific

field.^[10] Bibliometric techniques such as citation analysis, co-authorship analysis, and keyword analysis were used to analyze the data obtained from the WoS. The results are visualized in the form of maps, graphs, or

diagrams, which help researchers gain a comprehensive understanding of the structure and dynamics of AI-driven drug delivery research.

Based on citation analysis, we have identified the most frequently cited document in the last twenty

years. Figure 7 illustrates the six most cited articles globally, each with a minimum of 90 citations. Our study has focused on these six articles to explore the conceptual framework around the role of AI in drug delivery.

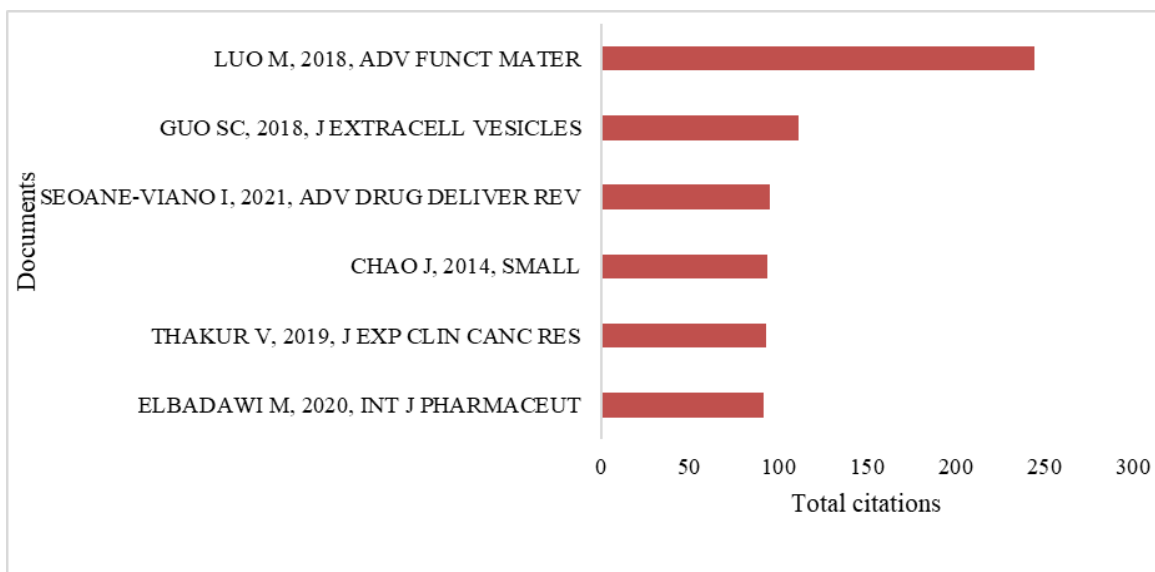


Figure 7: Most globally cited documents in AI-driven drug delivery.

Luo *et al.* discuss the significant progress in micro- and nanorobots and their capability to load, transport, and deliver therapeutic payloads to disease sites.^[11] This improves the effectiveness and reduces the side effects of toxic drugs. The article mentioned above also covers various propulsion methods, biocompatibility, and the advantages and limitations of using these tiny robots in drug delivery. It also discusses future developments in *in vitro* and *in vivo* active drug delivery.

Guo SC explains that extracellular vesicles are crucial in intercellular communication and have gained interest as diagnostic biomarkers or therapeutic drug delivery systems.^[12] Conventional methods have limitations, but microfluidics-based technologies offer advantages like low cost, low sample volumes, high throughput, and precision. This study discusses recent advances in microfluidics-based technologies, their potential clinical applications, and the potential of cloud-based portable disease diagnosis and monitoring systems, possibly with artificial intelligence.

Seoane-Viano I and his authors highlighted that 3D printing revolutionizes pharmaceutical development by producing personalized drug products on demand.^[13] This technology allows for small-batch dose flexible medicines, personalizing them to individual patient needs and expediting drug development timelines. However, the clinical potential is yet to be realized. This review overviews recent investigations in AI-steered 3D

printing pharmaceuticals, additive manufacturing, and early-phase therapeutics development.

Drug delivery carriers can improve drug solubility, stability, and efficacy. Chao J and his team suggest that DNA nanotechnology is a promising approach for drug delivery, thanks to its unique self-recognition properties.^[14] AI-powered DNA nanostructures can be designed with precise structures, controlled movements, and enhanced permeability to cell membranes. Recent advancements in designing and fabricating static and dynamic DNA nanostructures for drug delivery show that they have the potential to release drugs in a controlled manner.

Triple-Negative Breast Cancer (TNBC) is a complex and aggressive disease that lacks hormonal receptors, making chemotherapy the only effective treatment. However, the development of nanomedicine has enabled the targeting of TNBC cells using nano-carriers. Furthermore, applying AI and machine learning in nanotheranostics has enhanced early diagnosis and treatment of TNBC. Thakur V and his group's ideas have highlighted the positive impact of AI in novel nano-therapeutic modalities for TNBC diagnosis and treatment.^[15]

According to Elbadawi M and co-workers, AI can revolutionize pharmaceutical formulation development by analyzing large datasets.^[16] Fused Deposition Modeling (FDM) three-Dimensional Printing (3DP)

significantly improved oral drug delivery. M3DISEEN, a web-based pharmaceutical software, uses AI machine learning techniques to accelerate FDM 3D printing. The software accurately predicts key fabrication parameters, including printability and filament characteristics. The AI models also predict hot melt extrusion and FDM processing temperatures with a mean absolute error of 8.9 °C and 8.3 °C, respectively.

Academic collaboration through co-authorship is crucial in today's research, resulting in richer insights and more clarity. Scholarly cooperation has become the norm, creating a network of «hidden networks» among academics. Such collaborations can help identify research grouped among academics from a specific region and inspire further studies by scholars from underrepresented locations. We conducted a co-authorship analysis to investigate the collaboration network of countries. We applied a filter that required a minimum of 5 articles published by a country and a minimum of 1 citation per document to obtain the most effective author-based countries collaboration network. Figure 8 is the research collaboration network for published AI-driven drug delivery research across eighteen countries. Authors seeking intellectual support for AI-based drug delivery research may approach these countries and their affiliated institutions for productive collaborations.

Co-word analysis is a technique for science mapping that focuses on analyzing the actual content of publications. Unlike other methods, such as citation

analysis and co-citation/author analysis, which use citations or co-cited publications as a focal point, the unit of analysis for co-word analysis is «words.» The words in a co-word analysis are usually derived from “keyword plus” or «author keywords.” This technique assumes that words that frequently appear together have a thematic relationship with one another. Figure 9 displays the keywords obtained from the articles that appeared at a frequency of 15 times or more. This figure illustrates the significance of 10 keywords that describe the relationship of AI in drug delivery, specifically in nanoparticle design and nanomaterial fabrication for drug delivery.

A minimum number of 5 occurrences was used to determine the co-occurrence network of keywords. Out of 1170 keywords, only 54 met the above criteria. These keywords were grouped into 6 clusters by VOS Viewer, and their co-occurrence network is illustrated in Figure 10. The keyword co-occurrences network establishes the relationships between research themes in AI-aided drug delivery. The network consists of circles, with each circle representing a keyword and its size corresponding to its frequency of occurrence. The circles are connected by lines that show the links between themes or keywords, indicating where they co-occur. Different colors represent the different thematic clusters. Therefore, the published research suggests that drug delivery and drug release are closely linked to artificial intelligence, neural networks, mathematical modeling, and prediction.

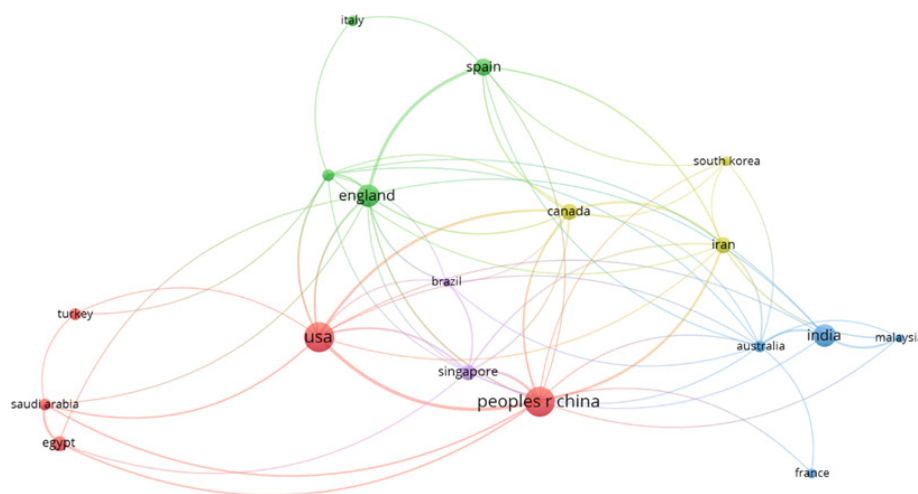


Figure 8: Countries collaboration network for AI-driven drug delivery research.

From the above analysis, it is understood that science mapping is a valuable tool for identifying research trends, locating key researchers and institutions, identifying research gaps, and facilitating knowledge dissemination and collaboration within a field.

Enrichment metrics

The study employed a sophisticated technique known as «network analysis of keywords» to delve into the various research themes that have emerged in AI-driven drug delivery over the past two decades. By examining the

complex networks of research themes, the study aimed to comprehensively understand how these themes have developed and evolved over time.^[4] A thematic map was generated in R Studio, using keywords with a minimum frequency of 2. R Studio calculates closeness and betweenness to centrality and page rank of published research and visualizes the results in a thematic map consisting of spheres in four quadrants. Each sphere represents a thematic cluster, and its size is proportional to the frequency of the keyword's occurrence. The position of the sphere in the quadrants depends on

values of closeness and betweenness of centrality and Page Rank. Closeness to centrality is a concept that describes how effectively spheres (themes) in a network can exchange information by being closer to other spheres. If the sum of distances between spheres is small, it means that these can carry information effectively. On the other hand, betweenness centrality refers to the ability of a thematic cluster to connect to other clusters that are not directly connected to each other. Finally, PageRank analysis is an alternative way to measure the impact of a publication.

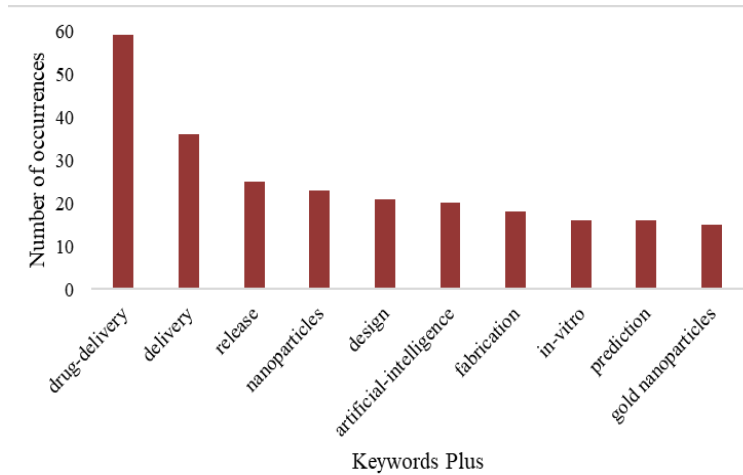


Figure 9: Most frequently used keywords representing AI in drug delivery research.

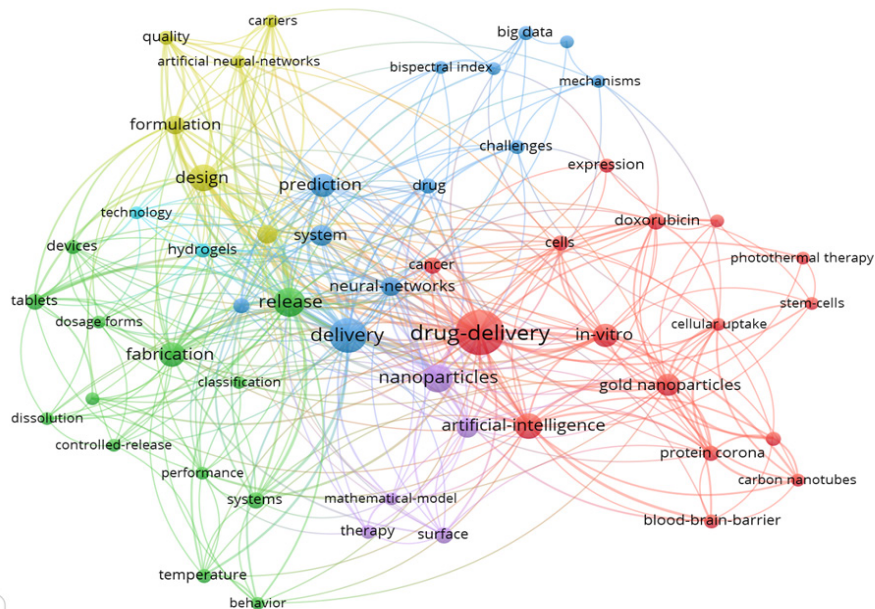


Figure 10: AI-driven drug delivery Keywords Plus co-occurrences network.

Figure 11 displays a thematic map showcasing the evolution of themes related to AI-powered drug delivery over 20 years. The map highlights 17 different thematic clusters categorized as basic, motor, niche, and emerging themes based on their position on the

map. The motor themes indicate that these fields are well-developed and drive research forward, with genetic algorithm-linked gold, iron-oxide, and silver nanoparticle drug delivery gaining momentum in recent years. Basic themes such as using AI in fabrication,

formulation design, nanoparticles, and prediction of *in vivo* drug delivery had a more significant impact than

using big data in health and AI in drug delivery for bacterial infections.

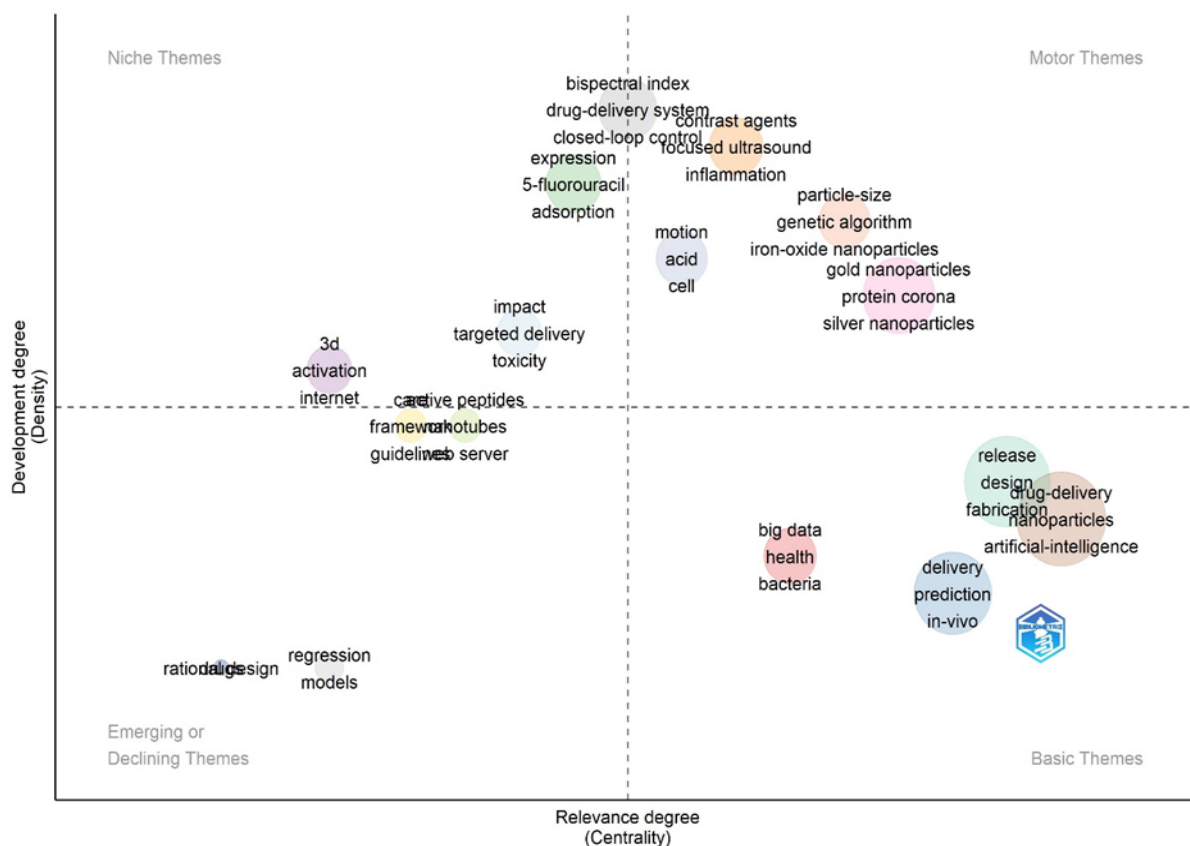


Figure 11: Thematic map revealing the evolution of themes in AI-driven drug delivery.

The map also reveals niche themes, including AI-powered drug delivery systems that use bispectral index to measure the brain delivery of drugs and 5-fluorouracil for cancer drug delivery on the central line, indicating the field's potential to develop tremendously. Targeted delivery and toxicity prediction using AI may also significantly impact future drug development. The keywords active peptides, care, framework, guidelines, nanotubes, and web server are closely related but have not developed much in the past 20 years. However, as these themes lie adjacent to the central line, it suggests that they may progress in the future, significantly impacting the use of AI in drug delivery. No emerging or declining themes were observed, indicating that the field has seen unprecedented growth recently.

The dendrogram is a method of hierarchical clustering that helps identify relationships in a large set of publications. It provides a comprehensive view of the relationships between various entities by dividing them into different levels of clustering.^[17] The thematic cluster dendrogram explores the relationship between the evolved themes in AI-driven drug delivery research in the past two decades. This also clarifies in detail the

keywords co-occurrences network. In Figure 12, the thematic cluster dendrogram shows that all themes have been clustered under one color (Red), indicating the existence of only one line of research in AI-powered drug delivery. The height of the vertical lines represents the distance between the research theme clusters, while the horizontal lines display the position at which the thematic clusters merge. The maximum height between the whole group is 4, indicating that the themes are well related. The central theme can be divided into five sub-domains: i) nanoparticles related to protein corona and cellular uptake, ii) artificial neural networks in carriers, formulation, and quality, iii) AI-involved prediction, design, fabrication, drug delivery, optimization of tablets and hydrogel formulations, iv) Use of big data, artificial neural networks, mathematical models in controlled or targeted (bispectral index for brain delivery) drug delivery, modeling nanoparticle surface, therapy, *in vivo* performance, expression, devices, and health v) AI in photothermal therapy for breast cancer, design of Doxorubicin loaded gold nanoparticles for *in vitro* release, modeling nanoparticles to cross the blood-brain barrier, and stem cell therapy.

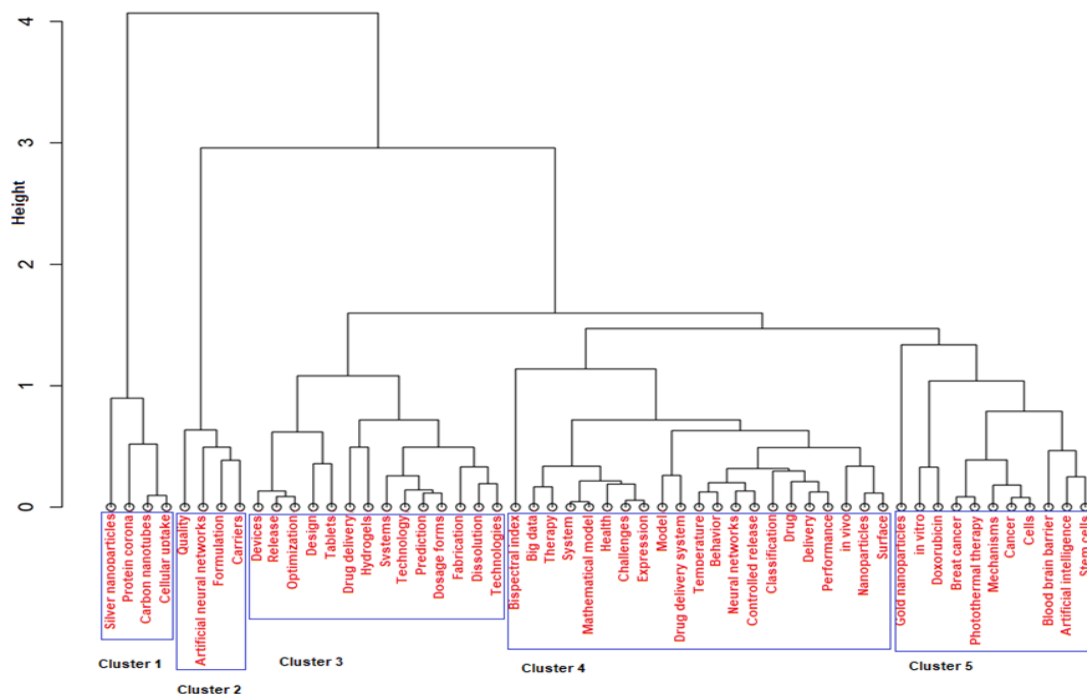


Figure 12: Hierarchical clustering dendrogram revealing the relationship between AI-driven drug delivery research themes.

DISCUSSION

The information related to the source indicates that, in 20 years between 1992 and 2023, 254 articles were published in 182 journals. The search filter was applied exclusively to retrieve articles published in journals, not textbooks, conferences, etc. The study of AI in drug delivery is growing tremendously, and we can use the average age of articles and average citations to understand better the journal sources they come from. Interestingly, the articles we retrieved are recent, with an average age of only 2.04 years. Keywords Plus and the author's keywords pertain to article contents. In contrast, the number of authors, co-authors, single author contributions, and % of international co-authorships define the author contributions and collaboration networks. AI and drug delivery were central in the keywords plus co-occurrence network indicating that the study has retrieved the keywords correctly. China and USA played a central role in collaborations with other countries in conducting the AI-driven drug delivery research. The number of research articles published exceeds the review on AI in drug delivery. Interpreting performance metrics provides insights into the importance of research constituents like authors, journals, countries, and author affiliations. Recent years have seen a significant increase in interest in AI research for drug delivery with almost no publications before 2012. Performance analysis also informs funding decisions, research priorities, and impact evaluation. Benchmarking against peers can

improve research strategies. AI-driven drug delivery research metrics suggest prioritizing the field for impact and funding. Science mapping in bibliometrics provides insights into the landscape of scientific knowledge and facilitates evidence-based decision-making in academia and research. Science mapping results highlight the significance of AI-based drug delivery systems. Enrichment analysis of the keywords revealed the well-developed and underrepresented research domains. This information helped us highlight the hotspots or critical areas of AI application in drug delivery research. Applying network analysis and dendrogram hierarchical clustering for enrichment metrics helped us interpret connections between AI-driven drug delivery research themes.

STRENGTHS AND LIMITATIONS

The study is novel and is a topic of great interest currently. The study revealed the transformative potential of AI in the field of drug delivery. Limitation is that the period between collecting, analyzing, and publishing data can be challenging. Some data might be added to WoS during this time and may not be included in the analysis. Certain keywords can have multiple meanings in different contexts, so reading publications becomes necessary to understand the relationships between words. Moreover, some words are too general (e.g., challenges, expression, health, etc.), making it difficult to assign them to a specific thematic cluster.

CONCLUSION

This bibliometric work analyzes the global trends in AI-powered drug delivery studies conducted in the last two decades. The findings indicate that this interdisciplinary field has grown rapidly and is becoming increasingly significant. China is the leading country in this field, followed by emerging players such as America and India. The National University of Singapore plays a pivotal role in promoting AI-driven drug delivery research. While there has been a decline in citation rates in recent years, the reasons behind this trend are unclear and require further investigation. Thematic map and hierarchical clustering of thematic clusters provided valuable insights into the core and emerging areas of interest in AI-driven drug delivery research. Scientists have used AI to model drug delivery for cancer, but there is a gap in AI's application for drug delivery in other diseases. Future research should design AI models to predict drug delivery for other common diseases. This bibliometric study offers a comprehensive view of the field, serving as a guide for researchers and industry stakeholders.

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CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

SUMMARY

The study used bibliometric analysis to quantify research on drug delivery, with a particular focus on the role of AI. The study found that AI has significantly advanced research on drug delivery for anti-cancer drugs. With further advancements in AI, it is expected that drug formulation design and targeted drug delivery for cancer therapy will improve. However, attention is also needed for other diseases.

ABBREVIATIONS

AI: Artificial intelligence; **FDM:** Fused deposition modeling; **MeSH:** Medical subject headings; **PDat:** Publication date; **3DP:** Three-dimensional printing; **WoS:** Web of Science.

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