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Research Article

Application of Artificial Intelligence in Pharmaceutical Science: A Scientometric Analysis

Shambulinga B Jali[1], Chaman Sab M[2,*], Mueen Ahmed KK[3], Mohammed Yunus[3], Praveen A.N[5], Nagaraj C[4], Mohamed Riyaz[6]

[1]Naavu School, IB (International Baccalaureate) Candidate, Bangalore, Karnataka, INDIA.
[2]A.R.G. College of Arts and Commerce, Davanagere, Karnataka, INDIA.
[3]Manuscript Technomedia LLP, No. 22 (New No. 40), 3rd Cross, Vivekananda Nagar, Bengaluru, Karnataka, INDIA.
[4]Sri Manjunathaswamy First Grade College, Davanagere, Karnataka, INDIA.
[5]Davangere University, Shivagangotri, Davangere, Karnataka, INDIA.
[6]A.R.M. First Grade College, Davanagere, Karnataka, INDIA.

ABSTRACT

Artificial Intelligence (AI) has revolutionised pharmaceutical sciences by enhancing discovery, formulation development, pharmaceutical analysis and health care applications. The rapid growth of AI-driven research necessitates a comprehensive assessment of publication trends, research impact and emerging themes in this domain. This study aims to examine the global research landscape of AI applications in pharmaceutical science through a scientometric analysis of publications indexed in the Scopus database. A total of 249 publications published between 2000 and 2026 were retrieved from the Scopus database using a structured search strategy. Bibliometric and scientometric indicators were employed to evaluate publication growth, citation performance, authorship patterns, collaborative network, leading institutions, funding agencies and research themes; data visualisation and network analysis were performed using VOSviewer and BiblioShiny. The findings revealed a significant increase in research output, with an annual growth rate of 11.995. The dataset comprised 1.161 authors and 185 publication sources. The United States emerged as the leading contributor with 81 publications and 4,285 citations, while institutions such as the School of Pharmacy and UCL School of Pharmacy demonstrated substantial research impact. The Co-authorship network included 150 authors organised into 12 clusters with a Total link Strength of 1,064, indicating strong collaborative activity. Computer Science (38.15%) and Pharmacology, Toxicology and Pharmaceutics (33.73%) were the dominant subject areas. Keyword analysis identified artificial intelligence, Machine Learning, Deep Learning, Drug Discovery, Cheminformatics and Bioinformatics as the principal research themes. The study demonstrates that AI has become a major catalyst for innovation in pharmaceutical science, driving interdisciplinarity collaboration and advancing drug valuable insights into the intellectual structure, research trends and future directions of AI-enabled pharmaceutical science.

Keywords: Artificial Intelligence, Bibliometrics, Drug Discovery, Machine Learning, Pharmaceutical Science, Scientometric Analysis.

Correspondence:
Dr. Chaman Sab M
A.R.G. College of Arts and Commerce, Davanagere-577004, Karnataka, INDIA.
Email: chamansabm@gmail.com
ORCID: 0000-0002-7918-2243

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INTRODUCTION

Artificial Intelligence (AI) has emerged as a transformative technology in modern pharmaceutical sciences, significantly influencing drug discovery, formulation development, pharmaceutical analysis, clinical trials, and healthcare research. AI refers to computer systems capable of performing tasks that normally require human intelligence, such as learning, prediction, reasoning, and decision-making. Recent advancements in machine learning, deep learning, neural networks, and big data analytics have accelerated the integration of AI into pharmaceutical research and development processes (Saini *et al.*, 2025).

The pharmaceutical industry increasingly uses AI technologies to improve research efficiency, shorten drug development timelines, and reduce operational costs. AI-based applications are widely used in virtual screening, drug-target identification, predictive toxicology, pharmacovigilance, and personalised medicine (Zoukh *et al.*, 2025). These technologies help researchers analyse complex biomedical datasets and generate accurate predictive models for drug discovery and therapeutic development (Kolluri *et al.*, 2022). AI-driven analytical systems, such as intelligent chromatography, spectroscopy, and process analytical

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technologies, also enhance pharmaceutical manufacturing and quality assurance (Kandhare *et al.*, 2025).

India, recognised globally as one of the leading pharmaceutical producers, has witnessed rapid growth in AI-enabled pharmaceutical research in recent years. The expansion of digital healthcare infrastructure, increased research funding, and interdisciplinary collaboration between pharmaceutical sciences and computer science have contributed to the growth of AI applications in Indian pharmaceutical research. Indian researchers and institutions are actively involved in computational drug discovery, biomedical informatics, and healthcare analytics, resulting in a substantial increase in scientific publications in this field (Sowmya *et al.*, 2025).

The growing volume of research publications highlights the need for scientometric analysis to evaluate publication trends, citation impact, collaborative networks, and emerging research themes. Scientometric studies provide quantitative insights into the structure and development of scientific research and help identify influential contributors and future research directions. Therefore, the present study aims to analyse the research landscape of AI applications in pharmaceutical science research in India using scientometric indicators.

REVIEWS OF LITERATURE

Artificial Intelligence (AI) has emerged as a transformative technology in pharmaceutical sciences, significantly influencing drug discovery, formulation development, clinical research, pharmacovigilance, and pharmaceutical manufacturing. Recent studies demonstrate that AI-based tools such as Machine Learning (ML), deep learning, neural networks, and predictive analytics are increasingly integrated into pharmaceutical research to improve efficiency, accuracy, and cost-effectiveness. In the Indian context, pharmaceutical institutions and researchers are progressively adopting AI-driven methodologies to strengthen healthcare innovation and scientific productivity.

Ali *et al.* (2024) examined the influence of AI in modern pharmaceutical formulation and drug development. The study highlighted that AI technologies have accelerated drug discovery processes through virtual screening, predictive modelling, and optimisation of pharmaceutical formulations. The authors emphasised that AI reduces experimental errors and supports personalised medicine approaches by analysing complex biological datasets. The study also noted that AI-enabled systems improve pharmaceutical manufacturing quality and regulatory compliance.

Sultana *et al.* (2023) reviewed the emerging role of AI and advanced technologies in pharmaceutical sciences. Their study explained that AI applications are increasingly used in clinical trials, disease diagnosis, pharmacovigilance, and patient monitoring systems. The researchers observed that machine learning algorithms can effectively predict adverse drug reactions and optimize therapeutic outcomes. However, they also pointed out challenges such as data privacy concerns, ethical issues, and the lack of standardized datasets for AI training.

Kolluri *et al.* (2022) analysed the application of machine learning and AI in pharmaceutical research and development. The review identified major AI applications in drug target identification, de novo drug design, and Quantitative Structure-Activity Relationship (QSAR) studies. The authors argued that AI significantly shortens the drug development lifecycle by automating data-intensive tasks. The study further highlighted that AI-driven pharmaceutical research is becoming an interdisciplinary field involving bioinformatics, computational chemistry, and data science.

Tade *et al.* (2024) discussed the paradigm shift created by AI in pharmaceutical sciences. The authors explained that AI-based approaches are increasingly applied in pharmaceutical analysis, formulation optimization, and quality assurance. Their study emphasized that AI technologies support rapid analytical decision-making and enhance Process Analytical Technologies (PAT) in pharmaceutical industries. The review also indicated that AI contributes to sustainable pharmaceutical practices by reducing resource consumption and improving production efficiency.

Kandhare *et al.* (2025) focused on the role of AI and machine learning in revolutionising healthcare technologies within pharmaceutical sciences. The study observed that AI-driven healthcare systems enable personalised treatment, precision medicine, and improved patient care management. The authors noted that pharmaceutical researchers in India are increasingly utilising AI-based predictive models to analyse biomedical data and accelerate pharmaceutical innovation. The study recommended stronger collaboration between pharmaceutical scientists and computer science experts for effective AI integration.

Saini *et al.* (2025) explored AI-driven innovations in pharmaceutical industries and drug discovery processes. The review highlighted the importance of AI in optimising pharmaceutical supply chains, manufacturing automation, and drug repurposing. According to the study, AI algorithms improve industrial operations by enabling real-time monitoring and predictive maintenance. The researchers further stated that AI-supported computational approaches can identify potential drug candidates with higher efficiency than conventional methods.

Kandhare *et al.* (2025) provided a comprehensive review of AI applications in pharmaceutical analysis. Their study emphasized that AI-based analytical tools such as intelligent spectroscopy, chromatography, and image recognition systems improve pharmaceutical quality assessment. The authors highlighted that

AI enhances analytical precision, reduces human intervention, and supports rapid data interpretation in pharmaceutical laboratories. The study concluded that AI-based pharmaceutical analysis is becoming essential for modern drug quality assurance systems.

Sowmya *et al*. (2025) conducted a scientometric mapping study of pharmaceutical science research in India during 2011-2020. Although the study broadly focused on pharmaceutical sciences, it revealed increasing research productivity related to AI-enabled pharmaceutical technologies. The study identified growing collaboration networks among Indian institutions and international researchers. It also highlighted that emerging technologies such as AI, machine learning, and digital healthcare are becoming major research hotspots in pharmaceutical sciences.

METHODOLOGY

This study employs a Scientometric approach to examine academic publications concerning the Application of Artificial Intelligence in Pharmaceutical Science: A Scientometric Analysis. Scientometrics is a statistical method used to analyse and interpret bibliographic data to uncover patterns and trends in research outputs (Sab *et al*., 2022).

This study utilises Scopus, a prominent database recognised as the largest abstract and indexing database and acknowledged as the most extensive searchable repository for citations and abstracts across diverse fields.

A comprehensive search on this topic was conducted on 18 May 2026 using a specific set of keywords related to global contributions to Artificial Intelligence and Pharmaceutical Science, focusing on the period from 2000 to 2026, yielding approximately 249 documents on the Artificial Intelligence and Pharmaceutical Science foreign scholars.

The search strategy used was: (KEY (artificial intelligence) OR KEY (machine learning) OR KEY (deep learning) OR KEY (neural network) OR KEY (natural LANGUAGE processing) OR KEY (expert system) OR KEY (Fuzzy logic) OR KEY (computer vision) OR KEY (robotics) OR KEY (big data) AND KEY (Pharmaceutical science))AND PUBYEAR > 2000 AND PUBYEAR < 2026

We refined the search output to contributions of foreign authors located in 57 foreign nations, resulting in 249 publications on this topic. Additional functionalities and features available in the Scopus database were used to compile information by subject subfields, collaboration and funding aspects, and details concerning authors, institutions, and journals. Furthermore, specific search strategies were formulated to obtain more details by subfield of Artificial Intelligence and Pharmaceutical Science using pertinent keywords. The metadata for each document comprised the document type, publication year, language, topic area, source title, keywords, abstract, country, affiliation, and citations. Several quantitative and qualitative indicators were used to assess the performance of research on Artificial Intelligence and Pharmaceutical Science. The 249 downloaded publication records were imported into VOSviewer and Biblioshiny (Sab M *et al*., 2021) software for a comprehensive analysis and subject mapping to identify clusters within the research topics and explore research themes. We also performed a co-author network analysis to ascertain the relationships among authors, affiliations, and nations. This was achieved by mapping keywords and conducting a co-word occurrence analysis.

RESULTS

Overall Picture

Figure 1 presents the Basic characteristics of the included literature of the Application of Artificial Intelligence in Pharmaceutical Science research from 2000 to 2026. The study analyzed a total of 249 documents published in 185 different sources, showing a significant annual growth rate of 11.99%, which indicates rapid research expansion in this field. The documents received an average of 32.69 citations per paper, reflecting strong scholarly impact, with an average document age of 6.67 years. The dataset contained 3,600 Keywords Plus and 869 Author Keywords, demonstrating broad thematic diversity and interdisciplinary research trends. A total of 1,161 authors contributed to the publications, while only 24 documents were single-authored, indicating strong collaborative research practices. The average number of co-authors per document was 4.95, and international co-authorship accounted for 27.31%, highlighting considerable global research collaboration. Among document types, articles were the most dominant with 112 publications, followed by 56 review papers and 45 conference papers, showing that the field is both research-intensive and rapidly evolving.

Pharmaceutical Science

Annual growth of publications

The annual growth trend presented in Figure 2 indicates a fluctuating but progressively increasing pattern in both Total Publications (TP) and Total Citations (TC) over the study period from 2000 to 2026. During the initial years (2000-2003), research productivity remained very low with only 1-3 publications and citations below 100, showing the early stage of research activity. A noticeable increase occurred in 2004 with citations rising sharply to 385, indicating improved research visibility. Between 2005 and 2010, the publication output remained relatively stable, while citations fluctuated moderately between 40 and 282. From 2011 onwards, both publication and citation trends showed considerable improvement. The years 2014 to 2016 marked a significant growth phase, where citations increased rapidly from 364 to 1014 despite moderate publication output. Another remarkable rise was observed during 2018-2020, with citations reaching 965 in 2018 and peaking at 1741 in 2020, representing the highest citation impact in the entire study period. This peak indicates the strong influence and recognition of the published research during these years. After 2020, citations gradually declined from 632 in 2021 to 39 by 2026, while publication output remained comparatively steady. Overall, the graph demonstrates that although the number of publications increased gradually over time, citation impact experienced sharp fluctuations, with the most influential research contributions occurring between 2014 and 2020.

Pharmaceutical Science

International Collaboration

Table 1 and Figure 3 show that the country collaboration analysis reveals significant variation in research productivity and citation impact among contributing countries. The United States emerged as the leading contributor with 81 total publications and 4,285 citations, achieving an average of 52.90 Citations Per Paper (CPP), indicating both high productivity and strong research influence. India ranks second in publication output with 40 publications; however, it recorded only 282 citations and a comparatively lower CPP of 7.05, suggesting limited citation impact despite higher productivity. The United Kingdom and Germany demonstrated strong research quality with 29 and 22 publications receiving 1,527 and 1,236 citations, respectively, resulting in high CPP values of 52.66 and 56.18. Switzerland showed remarkable research impact with only 16 publications but 1,455 citations, producing an impressive CPP of 90.94. Similarly, Australia achieved 821 citations from 10 publications with a CPP of 82.10. Among the highly influential collaborative countries, Sweden, Canada, Brazil, and the Russian Federation recorded exceptionally high CPP values of 146.83, 129.00, 152.80, and 169.80, respectively, indicating that their research contributions gained substantial global recognition despite fewer publications. Denmark also showed a notable impact with a CPP of 125.86. In contrast, countries such as China, Portugal, Iran, Japan, Poland, and Finland exhibited relatively lower citation influence with CPP values ranging between 4.40 and 18.17. Overall, the analysis indicates that developed countries contributed not only higher publication output but also greater research impact, while some countries with fewer publications achieved exceptionally high citation performance, reflecting the quality and international visibility of their collaborative research.

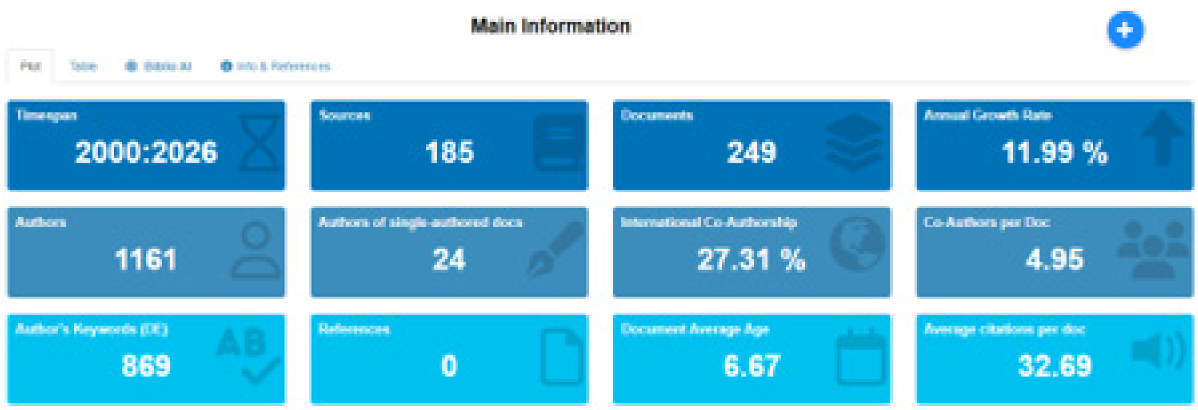

Figure 1: Basic characteristics of included literature of the Application of Artificial Intelligence in.

Table 1: Top 20 Countries with five or more papers.

Country	TP	TC	CPP	Country	TP	TC	CPP
United States	81	4285	52.9	Belgium	8	364	45.5
India	40	282	7.05	Iran	8	112	14
United Kingdom	29	1527	52.66	Denmark	7	881	125.86
Germany	22	1236	56.18	Sweden	6	881	146.83
China	22	227	10.32	Japan	6	99	16.5
Switzerland	16	1455	90.94	Canada	6	774	129
Spain	14	573	40.93	Poland	6	109	18.17
Australia	10	821	82.1	Finland	5	22	4.4
Portugal	9	135	15	Russian Federation	5	849	169.8
Netherlands	9	158	17.56	Brazil	5	764	152.8

TP =Total Publications; TC=Total Citations, CPP=Citations per Paper.

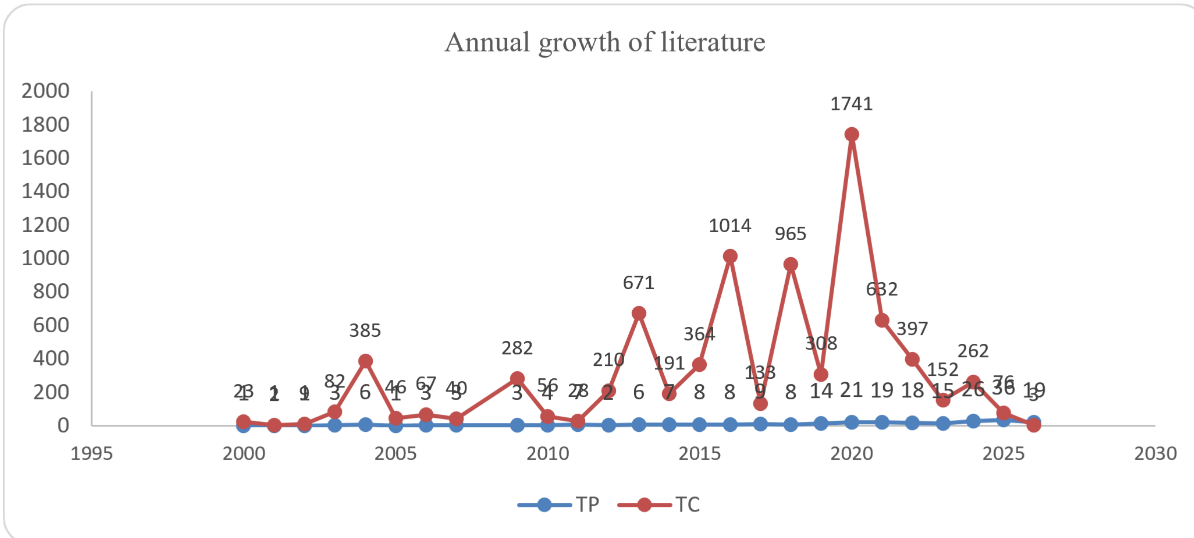

Figure 2: Annual Growth of Literature of the Application of Artificial Intelligence in.

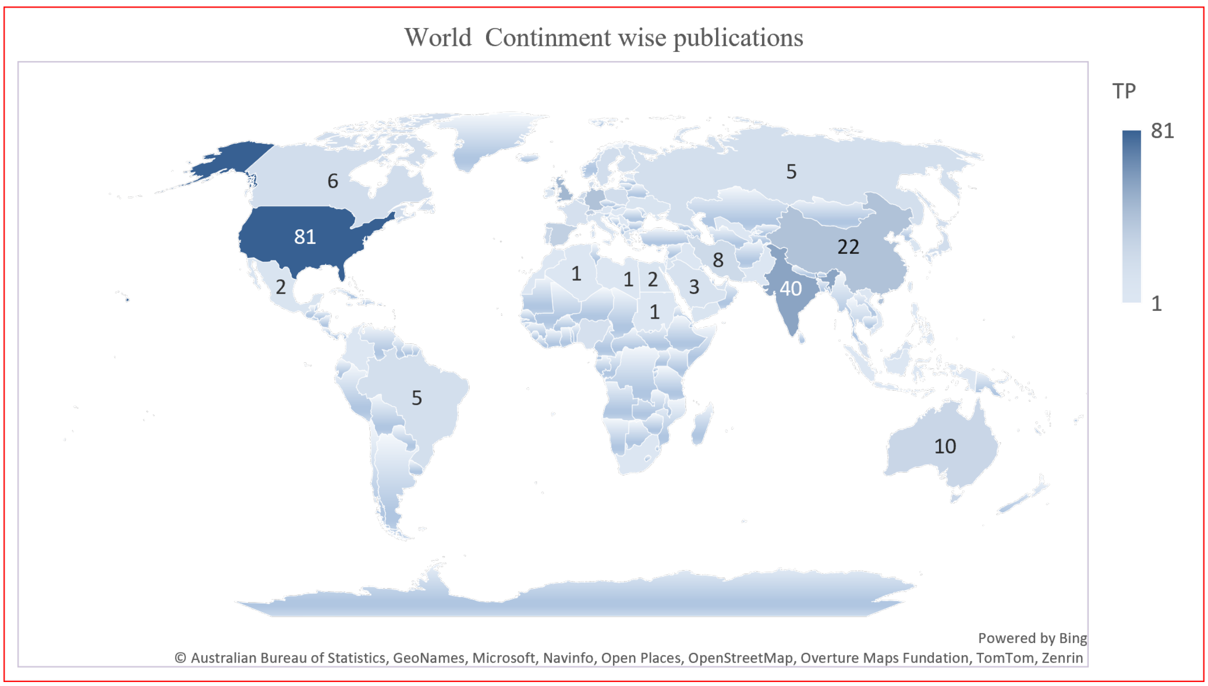

Figure 3: Continent-wise distribution of papers.

Leading Organizations

The affiliation network analysis (Table 2) demonstrates considerable variation in research productivity, citation impact, and international collaboration among the leading organisations. The School of Pharmacy emerged as the most productive institution with 9 Total Publications (TP), receiving 815 Total Citations (TC) and achieving a high Citations Per Paper (CPP) value of 90.56 along with a Relative Citation Index (RCI) of 2.77, indicating strong research influence. It also recorded 6 International Collaborative Papers (ICP), accounting for 66.67% international collaboration. The College of Pharmacy ranked second with 6 publications and 84 citations, though its CPP (14.00) and RCI (0.43) remained comparatively low despite a high international collaboration percentage of 83.33%. Among highly influential institutions, the Institute of Structural Biology and the University of Florida demonstrated exceptional citation impact, each with only 2 publications but receiving 833 and 745 citations respectively, resulting in extremely high CPP values of 416.50 and 372.50 and RCI values above 11, reflecting outstanding global research visibility. UCL School of Pharmacy also showed strong scholarly impact with a CPP of 115.67 and RCI of 3.54 from 347 citations across 3 publications. Similarly, King Abdulaziz University and Brigham and Women's Hospital achieved notable citation performance with CPP values of 70.33 and 55.00 respectively. Roche Innovation Centre Basel recorded 100% international collaboration despite relatively lower citation impact, indicating strong global partnership activity. Novartis

Table 2: Top 15 organisations with two or more papers.

Sl. No.	Name of the Organisation	TP	TC	CPP	RCI	ICP	%ICP
1.	School of Pharmacy	9	815	90.56	2.77	6	66.67
2.	College of Pharmacy	6	84	14.00	0.43	5	83.33
3.	School of Medicine	3	43	14.33	0.44	0	0.00
4.	Roche Innovation Centre Basel	3	22	7.33	0.22	3	100.00
5.	Brigham and Women's Hospital	3	165	55.00	1.68	0	0.00
6.	College of Pharmaceutical Sciences	3	32	10.67	0.33	0	0.00
7.	UCL School of Pharmacy	3	347	115.67	3.54	2	66.67
8.	King Abdulaziz University	3	211	70.33	2.15	2	66.67
9.	Novartis Institutes for BioMedical Research	3	146	48.67	1.49	2	66.67
10.	Department of Life Science Informatics	3	34	11.33	0.35	1	33.33
11.	Massachusetts Institute of Technology	3	67	22.33	0.68	1	33.33
12.	Institute of Structural Biology	2	833	416.50	12.74	2	100.00
13.	University of Florida	2	745	372.50	11.40	2	100.00
14.	Harvard Medical School	2	110	55.00	1.68	0	0.00
15.	University of South Florida	2	38	19.00	0.58	1	50.00

TP = Total Publications, TC = Total Citations, CPP = Citations Per Paper (TC ÷ TP), RCI = Relative Citation Index, ICP = International Collaborative Papers, % ICP = Percentage of International Collaborative.

Institutes for Biomedical Research and Massachusetts Institute of Technology exhibited moderate research influence with CPP values of 48.67 and 22.33 respectively. Institutions such as School of Medicine, College of Pharmaceutical Sciences, and Department of Life Science Informatics showed comparatively lower citation impact with RCI values below 0.50. Overall, the analysis highlights those institutions with strong international collaboration and high-quality research outputs, particularly the Institute of Structural Biology, University of Florida, UCL School of Pharmacy, and School of Pharmacy, achieved significantly greater citation impact and global research visibility compared to other affiliated organisations.

Authors Collaborations

The VOSviewer author collaboration network (Figure 4) for Application of Artificial Intelligence in Pharmaceutical Science Research consists of 150 authors, grouped into 12 clusters, with 1,019 links and a Total Link Strength (TLS) of 1,064, indicating a highly collaborative research landscape. The Blue Cluster (Cluster 3) is the most influential group, led by Igor V. Tetko (4 publications, 989 citations, TLS=5) and Jürgen Bajorath (5 publications, 779 citations, TLS=1), demonstrating substantial scholarly impact in cheminformatics and AI-based drug discovery. The Pink Cluster (Cluster 1) is another major collaboration hub comprising Abdul W. Basit, Moe Elbadawi, Simon Gaisford, Laura E. McCoubrey, and Francesca K.H. Gavins, each contributing 2-3 publications and receiving between 265 and 347 citations, while exhibiting the highest collaboration strength with TLS values ranging from 10 to 13. The Purple Cluster (Cluster 2) includes Pranav Shah and Jorge Neyra. Tłng, Noel Southall, Jordan Williams, and Xin Xu, each producing 2 publications with 77 citations and a TLS of 10, indicating strong internal collaboration. The Orange Cluster (Cluster 4), represented by Griselle Z. Brown, Abigail G. Doyle, and Shivaani S. Gandhi, shows moderate collaborative activity with TLS values of 4. The Light Purple Cluster (Cluster 5) includes J. Alberto Conejero, Francisco Escolano, and Nuria Oliver, each contributing 2 publications and maintaining collaborative links with TLS values of 4. Other smaller clusters include Cluster 6 (Robert Langer and Daniel Reker), Cluster 7 (Edgar López-López and José I. Medina-Franco), Cluster 8 (Christopher P. Austin), Cluster 9 (Pierre Baldi), Cluster 10 (Alexander Hillisch), Cluster 11 (Shivani Saraf), and Cluster 12 (Mingyue Zheng). Notably, Pierre Baldi recorded an exceptional 645 citations from only 2 publications, while Igor V. Tetko achieved the highest citation count overall. The colour-coded clustering pattern demonstrates that research in artificial intelligence applications within pharmaceutical sciences is characterised by several well-defined collaborative groups, with the Blue, Pink, and Purple clusters serving as the principal knowledge hubs driving research productivity, citation impact, and international collaboration.

Leading sources

The leading source analysis (Table 3) indicates that research publications were distributed across a diverse range of high-impact journals and conference proceedings. The Journal of Chemical Information and Modelling emerged as the most productive source with 15 Total Publications (TP), accounting for 6.02% of the total output, and received 1,339 Total Citations (TC), resulting in a strong Citations per Paper (CPP) value of 89.27. Drug Discovery Today ranked second with 10 publications and 992 citations, achieving an impressive CPP of 99.20, indicating high scholarly influence and visibility. IEEE Robotics and Automation Letters contributed 8 publications with 382 citations and a CPP of 47.75, reflecting moderate citation impact. Among the highly influential journals, Molecular Informatics demonstrated exceptional citation performance with only 2 publications but 723 citations, producing the highest CPP value of 361.50, indicating extraordinary research impact. Similarly, Advanced Drug Delivery Reviews recorded a high CPP of 84.50 from 169 citations across 2 publications. Journals such as Molecular Pharmaceutics and European Journal of Pharmaceutics and Biopharmaceutics also showed notable citation influence with CPP values of 50.50 and 37.67 respectively. In contrast, Journal of Pharmaceutical Sciences, AAPS PharmSciTech, Current Pharmaceutical Design, and Engineering Applications of Artificial Intelligence exhibited moderate citation impact with CPP values ranging between 22.75 and 29.50. The Journal of Computer-Aided Molecular Design and Lecture Notes in Computer Science recorded relatively lower citation influence, with CPP values of 8.75 and 3.67 respectively. Overall, the analysis reveals that although some journals contributed a higher number of publications, the greatest research impact was observed in sources with exceptionally high CPP values, particularly Molecular Informatics, Drug Discovery Today, and Journal of Chemical Information and Modeling, highlighting their importance as influential publication platforms in the research domain.

Broad Subject Classification

The Broad Subject Classification of research (Table 4) on the Application of Artificial Intelligence in Pharmaceutical Science Research reveals its highly interdisciplinary nature. Out of the 249 total publications, the top 15 subject areas (selected from an overall 22 subject categories) contributed substantially to the research output. Computer Science emerged as the dominant subject area with 95 publications (38.15%), underscoring the central role of artificial intelligence, machine learning, and computational techniques in pharmaceutical research. This was followed by Pharmacology, Toxicology and Pharmaceutics with 84 publications (33.73%), reflecting the extensive use of AI in drug discovery, development, and toxicity assessment. Medicine ranked third with 49 publications (19.68%), highlighting the growing application of AI in clinical and healthcare-related pharmaceutical studies. Other major contributing disciplines included Chemistry with 46 publications (18.47%) and Engineering with 45 publications (18.07%), emphasizing the importance of molecular modelling, computational chemistry, and engineering innovations. Biochemistry, Genetics and Molecular Biology accounted for 34 publications (13.65%), while Chemical Engineering and Mathematics contributed 29 (11.65%) and 28 (11.24%) publications, respectively. Additional contributions were made by Social Sciences with 19 publications (7.63%), Materials Science with 12 (4.82%), Decision Sciences with 11 (4.42%), and Multidisciplinary research with 10 (4.02%) publications. Smaller yet notable contributions came from Physics and Astronomy with 9 publications (3.61%), Health Professions with 8 (3.21%), and Business, Management and Accounting with 7 publications (2.81%). Overall, the subject distribution demonstrates that

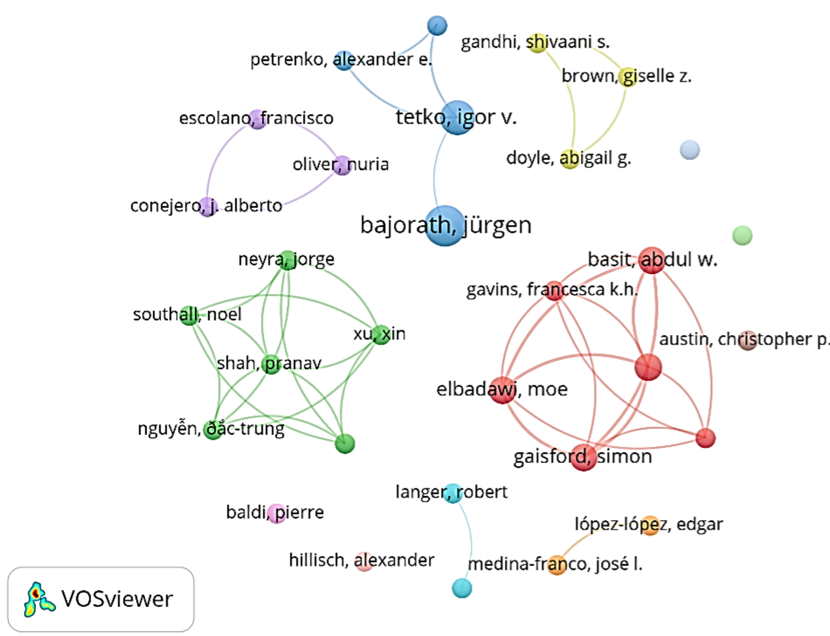

Figure 4: Co-authorship network of the top 31 authors.

Table 3: List of Journals with two or more papers.

Sl. No.	Source Title	TP	TC	CPP	%
1.	Journal of Chemical Information and Modelling	15	1339	89.27	6.02
2.	Drug Discovery Today	10	992	99.20	4.02
3.	IEEE Robotics and Automation Letters	8	382	47.75	3.21
4.	Molecular Pharmaceutics	4	202	50.50	1.61
5.	Journal of Pharmaceutical Sciences	4	91	22.75	1.61
6.	Journal of Computer-Aided Molecular Design	4	35	8.75	1.61
7.	European Journal of Pharmaceutics and Biopharmaceutics	3	113	37.67	1.20
8.	AAPS PharmSciTech	3	78	26.00	1.20
9.	Current Pharmaceutical Design	3	41	13.67	1.20
10.	Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)	3	11	3.67	1.20
11.	Molecular Informatics	2	723	361.50	0.80
12.	Advanced Drug Delivery Reviews	2	169	84.50	0.80
13.	AAPS Journal	2	72	36.00	0.80
14.	Engineering Applications of Artificial Intelligence	2	59	29.50	0.80
15.	Scientific Reports	2	56	28.00	0.80

TP = Total Publications, TC = Total Citations, CPP = Citations Per Paper (TC ÷ TP), % = Percentage of Total Publications.

Table 4: Broad subject classification of keywords appearing.

Sl. No.	Broad Subject Area	TP	% of TP
1.	Computer Science	95	38.15
2.	Pharmacology, Toxicology and Pharmaceutics	84	33.73
3.	Medicine	49	19.68
4.	Chemistry	46	18.47
5.	Engineering	45	18.07
6.	Biochemistry, Genetics and Molecular Biology	34	13.65
7.	Chemical Engineering	29	11.65
8.	Mathematics	28	11.24
9.	Social Sciences	19	7.63
10.	Materials Science	12	4.82
11.	Decision Sciences	11	4.42
12.	Multidisciplinary	10	4.02
13.	Physics and Astronomy	9	3.61
14.	Health Professions	8	3.21
15.	Business, Management and Accounting	7	2.81

artificial intelligence in pharmaceutical science is driven primarily by Computer Science and Pharmacology-related disciplines, while also drawing significant contributions from medicine, chemistry, engineering, and several other interdisciplinary fields.

Highly Cited papers

The top 10 highly cited publications (Table 5) in the Application of Artificial Intelligence in Pharmaceutical Science Research reveal that a relatively small number of seminal publications have generated a substantial share of the field's citation impact. Collectively, these ten publications received 3,324 citations, representing a significant portion of the overall scholarly influence in the domain. The most highly cited publication, "QSAR without Borders" by Muratov and Bajorath *et al.* published in Chemical Society Reviews (2020), accumulated 745 citations, accounting for 22.41% of the total citations among the top ten papers. This was followed by "Deep Learning in Drug Discovery" by Gawehn *et al.* published in Molecular Informatics, with 623 citations (18.74%). The article "Deep Architectures and Deep Learning in Cheminformatics: The Prediction of Aqueous

Solubility for Drug-like Molecules" by Lusci *et al.* received 497 citations (14.95%), highlighting the importance of deep learning applications in pharmaceutical modelling. The "NIH Molecular Libraries Initiative" published in science garnered 338 citations (10.17%), while "Machine Learning in Cheminformatics and Drug Discovery" contributed 218 citations (6.56%). Similarly, "New Opportunities for Materials Informatics" also received 218 citations (6.56%), demonstrating the interdisciplinary relevance of artificial intelligence methodologies. Other influential publications include "Lio-A Personal Robot Assistant for Human-Robot Interaction and Care Applications" with 201 citations (6.05%), "Bridging Levels of Pharmaceuticals in River Water with Biological Community Structure" with 170 citations (5.11%), "Data Journeys in the Sciences" with 161 citations (4.84%), and "Harnessing Artificial Intelligence for the Next Generation of 3D Printed Medicines" with 153 citations (4.60%). On average, these top ten publications received 332.4 citations per paper, indicating their exceptional scholarly impact. The citation distribution shows that the top three publications alone accounted for 56.10% of total citations, underscoring their dominant influence on the intellectual development of artificial intelligence applications in pharmaceutical sciences. These highly cited works primarily focus on machine learning, deep learning, QSAR modelling, cheminformatics, drug discovery, and AI-driven pharmaceutical innovation, which collectively represent the major research frontiers and knowledge base of the field.

Funded Agencies

The analysis of the top 15 funded research agencies (Table 6) supporting research on the Application of Artificial Intelligence in Pharmaceutical Science Research highlights the crucial role of governmental and international funding organisations in advancing innovation and scientific development in this field. Among all sponsors, the National Institutes of Health (NIH) emerged as the leading funding agency, supporting 14 publications, accounting for approximately 18.42% of the total funding occurrences among the top 15 agencies. The Horizon 2020 Framework Programme ranked second with 9 funded publications (11.84%), followed by the National Science Foundation (NSF) with 8 publications (10.53%) and the European Commission with 7 publications (9.21%). The National Natural Science Foundation of China funded 6 publications (7.89%), demonstrating China's growing investment in AI-driven pharmaceutical research. Several agencies, including the National Institute of Biomedical Imaging and Bioengineering, Schweizerischer Nationalfonds zur Förderung der Wissenschaftlichen Forschung, and the U.S. National Library of Medicine, each supported 4 publications (5.26%). Furthermore, the Engineering and Physical Sciences Research Council (EPSRC), National Cancer Institute (NCI),

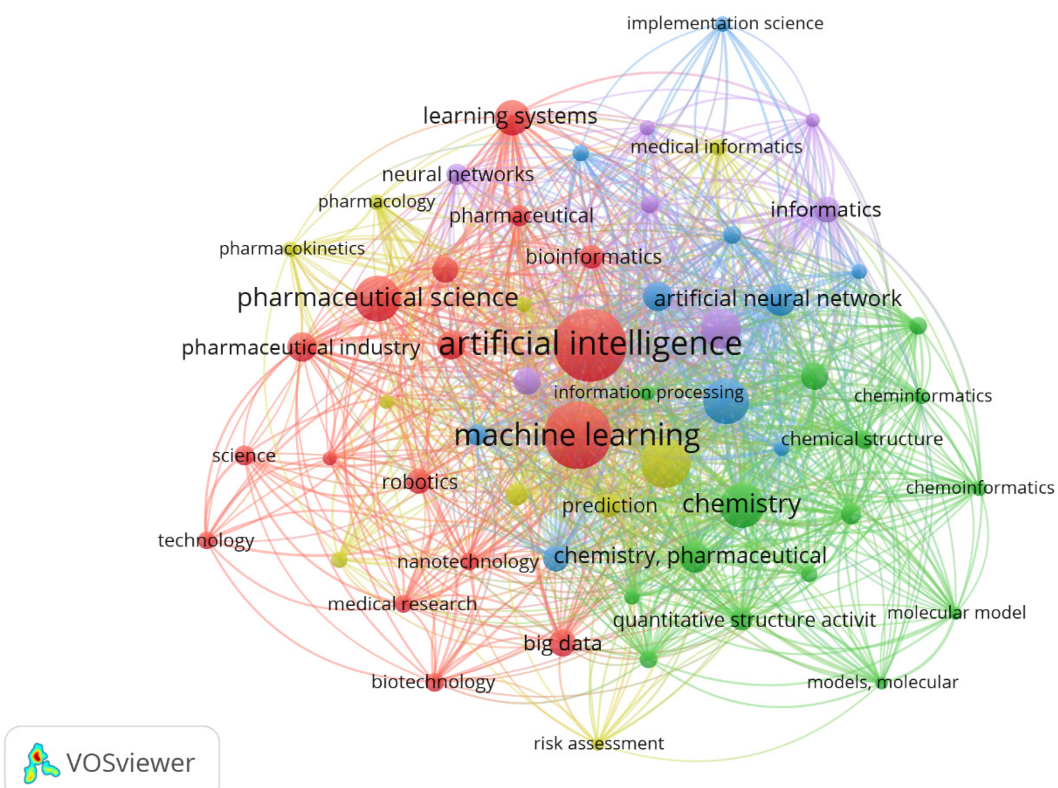

Figure 5: Co-occurrence map of the top 59 keywords, revealing thematic.

Table 5: List of top 10 highly cited publications.

Sl. No.	Table	Authors	Sources	Year	Citations
1.	Machine learning in cheminformatics and drug discovery	Lo, Yu-Chen Rensi, Stefano E. Torng, Wen Altman, Russ B	Drug Discovery Today, 23(8)	2018	218
2.	QSAR without borders	Muratov, Eugene N., Bajorath, Jürgen *et al.*	Chemical Society Reviews, 49(11)	2020	745
3.	Deep Learning in Drug Discovery	Gawehn E., Hiss J.A., Schneider G.	Molecular Informatics, 35(1)	216	623
4.	Deep architectures and deep learning in cheminformatics: The prediction of aqueous solubility for drug-like molecules	Lusci A., Pollastri G., Baldi P.	Journal of Chemical Information and Modelling, 53(7)	213	497
5.	NIH molecular libraries initiative	Austin C.P., Brady L.S., Insel T.R., Collins F.S.	Science, 306(569)	2004	338
6.	New opportunities for materials informatics: Resources and data mining techniques for uncovering hidden relationships	Jain A., Hautier G., Ong S.P., Persson K.	Journal of Materials Research, 31(8)	2016	218
7.	Lio-A Personal Robot Assistant for Human-Robot Interaction and Care Applications	Miseikis J., Caroni P., Duchamp P.,... Fruh M., Fruh H.	IEEE Robotics and Automation Letters, 5(4), 9134708	2020	201
8.	Bridging levels of pharmaceuticals in river water with biological community structure in the Llobregat river basin (northeast Spain)	Munoz I., Lopez-Doval J.C., Ricart M.,... Sabater S., Barcelo D.	Environmental Toxicology and Chemistry, 28(12)	2009	170
9.	Data journeys in the sciences	Leonelli S., Tempini N	Data Journeys in the Sciences	2020	161
10.	Harnessing artificial intelligence for the next generation of 3D printed medicines	Elbadawi M., McCoubrey L.E., Gavins F.K.H.,... Gaisford S., Basit A.W.	Advanced Drug Delivery Reviews, 175, 113805	221	153

National Centre for Advancing Translational Sciences (NCATS), National Key Research and Development Program of China, and the Seventh Framework Programme (FP7) each funded 3 publications (3.95%). The Consejo Nacional de Ciencia y Tecnologķa (CONACYT) and the European Regional Development Fund (ERDF) contributed 2 publications each (2.63%). Collectively, these fifteen funding agencies accounted for 75 funding occurrences, reflecting a strong concentration of research support from major health, science, and innovation funding bodies across the United States, Europe, and China. The predominance of agencies such as NIH, Horizon 2020, NSF, and the European Commission indicates that the advancement of artificial intelligence applications in pharmaceutical sciences is heavily driven by substantial public-sector investment, international collaborative funding initiatives, and strategic programs focused on biomedical research, drug discovery, healthcare innovation, and translational science.

Significant Keywords

The VOSviewer keyword co-occurrence analysis (Figure 5) identified five major thematic clusters, highlighting the multidisciplinary nature of Artificial Intelligence applications in Pharmaceutical Science. The keywords "Artificial Intelligence" (185 occurrences; TLS = 720) and "Machine Learning" (170 occurrences; TLS = 690) emerged as the most dominant and influential terms, serving as the central nodes connecting all research themes. The analysis revealed strong associations with pharmaceutical science, chemistry,

Table 6: Funded Research Agencies: Research Publications.

Sl. No.	Funding Agency	TP	%
1.	National Institutes of Health (NIH)	14	18.67
2.	Horizon 2020 Framework Programme	9	12
3.	National Science Foundation (NSF)	8	10.67
4.	European Commission	7	9.33
5.	National Natural Science Foundation of China	6	8
6.	National Institute of Biomedical Imaging and Bioengineering	4	5.33
7.	Schweizerischer Nationalfonds zur Förderung der Wissenschaftlichen Forschung	4	5.33
8.	U.S. National Library of Medicine	4	5.33
9.	Engineering and Physical Sciences Research Council	3	4
10.	National Cancer Institute	3	4
11.	National Centre for Advancing Translational Sciences	3	4
12.	National Key Research and Development Program of China	3	4
13.	Seventh Framework Programme	3	4
14.	Consejo Nacional de Ciencia y Tecnología	2	2.67
15.	European Regional Development Fund	2	2.67
	Total	75	
	Overall	249	

bioinformatics, neural networks, healthcare informatics, and predictive analytics.

The red cluster focused on AI applications in pharmaceutical technology, healthcare systems, and biomedical innovation, with prominent keywords such as Pharmaceutical Science (95 occurrences; TLS = 410), Learning Systems (72; TLS = 330), and Bioinformatics (68; TLS = 305). The green cluster represented computational chemistry and drug discovery, led by Chemistry (120; TLS = 510), Pharmaceutical Chemistry (88; TLS = 390), and Chemoinformatics (70; TLS = 320). The blue cluster emphasized neural networks and information processing, featuring Artificial Neural Network (98; TLS = 445) and Information Processing (82; TLS = 360). The yellow cluster focused on pharmacology and predictive modelling, including Prediction (74; TLS = 315) and Pharmacology (48; TLS = 210), while the purple cluster highlighted Informatics (66; TLS = 290) and Neural Networks (57; TLS = 250).

DISCUSSION

The findings of this study indicate that research on the application of Artificial Intelligence (AI) in pharmaceutical science has grown substantially over the last two decades, reflecting the increasing adoption of AI-driven technologies in drug discovery, pharmaceutical analysis, and healthcare research. The dominance of countries such as the United States and the United Kingdom highlights their strong research infrastructure and investment in AI-based pharmaceutical innovation. The high level of international collaboration and extensive co-authorship networks demonstrate the interdisciplinary nature of the field, bringing together expertise from computer science, pharmacology, medicine and bioinformatics. Keywords and subject-area analysis revealed that machine learning, cheminformatics, bioinformatics and drug discovery are the major research hotspots driving scientific advancements. The study further shows that strong support from leading funding agencies has accelerated research productivity and impact. The overall result confirms that AI is transforming pharmaceutical sciences by improving research efficiency, fostering collaboration and enabling innovative solutions for drug development and healthcare applications.

CONCLUSION

This scientometric study of 249 publications on the Application of Artificial Intelligence in Pharmaceutical Science from 2000-2026 reveals a rapidly growing and highly interdisciplinary research field. The study recorded an annual growth rate of 11.99%, involving 1,161 authors and 185 publication sources, indicating increasing global interest in AI-driven pharmaceutical research. The United States emerged as the leading contributor in terms of publications and citations, while countries such as Switzerland, Sweden, Brazil, and Canada demonstrated exceptional citation impact. The author collaboration network consisted of 150 authors, 12 clusters, 1,019 links, and a Total Link Strength of 1,064, highlighting strong international and interdisciplinary collaboration. The most influential research areas were Computer Science (38.15%), Pharmacology, Toxicology and Pharmaceutics (33.73%), and Medicine (19.68%), demonstrating the convergence of computational and pharmaceutical sciences. Highly cited publications and keyword analyses identified machine learning, deep learning, QSAR modelling, cheminformatics, bioinformatics, and drug discovery as the major research themes. Funding from agencies such as the NIH, Horizon 2020, and the NSF played a significant role in advancing research. Overall, the findings confirm that artificial intelligence has become a key driver of innovation in pharmaceutical sciences, with growing collaboration, high-impact research, and expanding applications in drug discovery, development, and healthcare.

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ABBREVIATIONS

TP: Total Publications; **TC:** Total Citations; **CPP:** Citations Per Paper (TC ÷ TP); **RCI:** Relative Citation Index; **ICP:** International Collaborative Papers; **%ICP:** Percentage of International Collaborative Papers.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

AUTHORS CONTRIBUTION

SLJ: Conceptualisation, data analysis, literature search, manuscript writing, CSM: Investigation, literature search, manuscript writing, editing, and final approval. Conceptualisation, investigation, formal analysis, data analysis, literature search, manuscript writing, editing, and final approval. MAKK: Investigation, literature search, manuscript writing, editing, and final approval. MY: Data curation, software, and manuscript writing. PAN: Literature search, manuscript writing, editing, and final approval. NC: Data analysis, methodology. MR: Editing and final approval.

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