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RESEARCH ARTICLE

Diş Hekimliğinde Moleküler Yerleştirme (Molecular Docking) Araştırmalarının Bilimsel Haritalandırılması: Bibliyometrik Bir Çalışma

Scientific Mapping of Molecular Docking Research in Dentistry: A Bibliometric Study

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ÖZET

Amaç: Moleküler docking, ligandların hedef biyomakromoleküllerle etkileşimlerini öngörmeye yönelik kullanılan bilgisayar destekli bir yöntem olup, son yıllarda diş hekimliği alanında da giderek yaygınlaşmaktadır. Bu bibliyometrik çalışma, diş hekimliğinde moleküler docking uygulamalarına yönelik bilimsel literatürü kapsamlı biçimde değerlendirmeyi amaçlamaktadır; bildiğimiz kadarıyla bu, alandaki ilk bibliyometrik analizdir.

Materyal-Metot: Web of Science (WoS) Core Collection veri tabanında "Dentistry, Oral Surgery & Medicine" alanı ile sınırlandırılan taramada "Molecular Docking", "Docking", "In Silico" ile "Dental", "Dentistry" anahtar kelimeleri kullanılmıştır. Veriler 17 Mart 2026 tarihinde toplanmış; 1981-2025 yılları arasındaki 34 yayın (2026 verileri hariç) analize dahil edilmiştir. Bibliometrix/Biblioshiny (R) ve VOSviewer yazılımlarıyla yayın, atıf, iş birliği ve anahtar kelime ağları incelenmiştir.

Bulgular: İlk yayın 2002'de bir konferans özeti olarak ortaya çıkmış, 2021 sonrasında belirgin bir artış gözlenmiş; 2025 yılı tek başına yayınların yaklaşık %32'sini oluşturmuştur. Endonezya ve Hindistan en üretken ülkeler olarak öne çıkmakta, Kharisma VD ve Nugraha AP en üretken yazarlar olarak (altışar yayınla) dikkat çekmektedir. En aktif dergi Journal of Pharmacy & Pharmacognosy Research (5 yayın) olup, yayınlar toplam 19 farklı dergiye dağılmıştır. Dental biyomateryal optimizasyonuna odaklanan çalışmalar en yüksek atıf etkisini yaratmıştır.

Tartışma ve Sonuç: Diş hekimliğinde moleküler docking literatürü, özellikle 2021 sonrasında hızlı bir büyüme ve olgunlaşma sürecine girmiştir. Alan; biyomateryal optimizasyonu, antibakteriyel ajan taraması ve doğal bileşiklerin değerlendirilmesi gibi konularda giderek merkezi bir araştırma temeli oluşturmakta, gelecekte yapay zekâ destekli docking yaklaşımlarının bu etkiyi daha da artırması beklenmektedir.

Anahtar Kelimeler: Moleküler docking, Diş hekimliği, Bibliyometrik analiz, In silico, Dental biyomateryaller

ABSTRACT

Objective: Molecular docking is a computer-aided computational method used to predict the interactions of ligands with target biomacromolecules, and its application in dentistry has grown considerably in recent years. This bibliometric study aims to comprehensively evaluate the scientific literature on molecular docking applications in dentistry; to the best of our knowledge, it represents the first bibliometric analysis in this field.

Materials and Methods: A search was conducted in the Web of Science (WoS) Core Collection database, restricted to the "Dentistry, Oral Surgery & Medicine" category, using the keywords "Molecular Docking," "Docking," "In Silico," combined with "Dental" and "Dentistry." Data were collected on 17 March 2026, and 34 publications from 1981–2025 (excluding 2026 due to incomplete indexing) were included in the analysis. Publication, citation, collaboration, and keyword networks were examined using Bibliometrix/Biblioshiny (R) and VOSviewer software.

Results: The first publication appeared in 2002 as a conference abstract, with a marked increase observed after 2021; 2025 alone accounted for approximately 32% of all publications. Indonesia and India emerged as the most productive countries, while Kharisma VD and Nugraha AP were the most prolific authors (six publications each). The most active journal was the Journal of Pharmacy & Pharmacognosy Research (5 publications), with the literature spread across 19 different journals in total. Studies focusing on the optimization of dental biomaterials generated the highest citation impact.

Discussion and Conclusion: The molecular docking literature in dentistry has entered a phase of rapid growth and maturation, particularly since 2021. The field is increasingly forming a central research foundation around topics such as biomaterial optimization, antibacterial agent screening, and the evaluation of natural compounds, with AI-assisted docking approaches expected to further enhance its impact in the future.

Keywords: Molecular docking, Dentistry, Bibliometric analysis, In silico, Dental biomaterials

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INTRODUCTION

Molecular docking is a computer-aided computational modeling method used to predict the interactions, binding modes, and binding energies of small molecules (ligands) with target biomacromolecules. This approach enables the understanding of interactions at the molecular level and plays an important role, particularly in drug discovery and development processes (1, 2). Molecular docking methods, which are widely used in pharmaceutical chemistry, molecular biology, and biomaterial research, have in recent years also begun to be applied in dentistry as a result of increasing computational power and advances in algorithms, gaining a notable place in research in this field.

Applications of molecular docking in dentistry range from the evaluation of the molecular interactions of dental biomaterials, restorative materials, and adhesive systems (3) to the screening of potential antibacterial agents against oral pathogens (4). The biocompatibility and binding properties of resin composites, nanomaterials, and natural compounds can be assessed at the molecular level through molecular docking analyses. In addition, docking studies conducted on target proteins associated with periodontal disease, dental caries, and endodontic infections contribute to the development of new treatment strategies (5). This indicates that molecular docking has become a complementary tool supporting experimental and clinical studies in dentistry.

Bibliometric analysis is recognized as an important method for evaluating the scientific development, trends, and production dynamics of a research field (6). Bibliometric analyses reveal the quantitative and structural characteristics of a given field through indicators such as the number of publications, citation structures, countries, institutions, authors, and keyword networks (7). This method enables the systematic examination of the increasingly extensive and interdisciplinary docking literature. A review of the existing literature reveals that no bibliometric study has comprehensively addressed the use of molecular docking methods in the field of dentistry.

The aim of this study is to comprehensively evaluate, through bibliometric analysis methods, the scientific literature published on molecular docking applications in dentistry. To the best of our knowledge, this study represents the first bibliometric analysis addressing the use of molecular docking in dentistry. In this context, the distribution of publications by year, the most productive countries, institutions, and authors were identified, and citation relationships and keyword networks were analyzed to reveal research trends in this field. The findings obtained are expected to systematize the existing body of knowledge on molecular docking in dentistry and to guide future research.

MATERIALS AND METHODS

In this bibliometric analysis, the Web of Science (WoS) Core Collection database, which provides comprehensive access to international scientific publications (https://www.webofscience.com/wos/woscc/basic-search), was used. Because the WoS database is updated on a daily basis, in order to minimize potential data bias, all data were collected within a single day (17 March 2026). The research area was restricted to "Dentistry, Oral Surgery & Medicine". In order to comprehensively reveal the scientific development and publication diversity of molecular docking-based studies in dentistry, the search was conducted in the Topic field using the keywords "Molecular Docking" OR "Docking" OR "In Silico" AND "Dental" OR "Dentistry". Among the results obtained, the researchers selected eligible publications by carefully examining the titles and abstracts of studies directly addressing the use of molecular docking in dentistry. Since the study did not involve any human or animal experimentation, ethics committee approval was not required.

In order to broaden the bibliometric scope of the study and to evaluate the methodological, theoretical, and applied dimensions of the field together, no restriction was applied with respect to document type. Accordingly, the analysis included original research articles, review articles, case reports, editorial materials, notes, meeting abstracts, proceedings papers, letters, and book chapters. This approach allows for a holistic evaluation not only of the quantitative productivity of the molecular docking literature in dentistry but also of the forms of scientific communication and knowledge dissemination.

The exclusion criteria comprised publications that did not involve molecular docking methods or were not directly related to the field of dentistry. During the preliminary screening process, only studies with no methodological or thematic connection to dentistry were excluded from the analysis.

The research was conducted in March 2026, and publications concerning the use of molecular docking in dentistry from 1981–2026 were considered for evaluation. However, as publications from 2026 had not yet completed their data integrity and indexing processes, studies from this year were excluded from the scope of the bibliometric analysis.

The publication year, language, country distribution, total citation counts, institutional affiliations, research areas, journals, authors, and keywords of the publications included in the analysis were examined within the scope of bibliometric indicators. The WoS output files were saved in TXT format and transferred to Microsoft Excel. In presenting the obtained data, descriptive statistical methods were used.

Bibliometric analyses were performed using R-Studio (R version 4.2.2) software, through the Biblioshiny (version 2.0) web-based interface. The open-source Bibliometrix and Biblioshiny packages were used to analyze publication productivity, citation distributions, author and country collaborations, and keyword trends. In addition, graphs and maps were created to visualize the evolution of research themes and publication dynamics over time. For a detailed examination of bibliometric network structures, VOSviewer (version 1.6.18, Windows) software was used to visualize and evaluate author, country, keyword, and citation networks.

RESULTS

This study examined the developmental trends of publications in the field of molecular docking and dentistry over the 2002–2025 period. The first record appeared in 2002 as a conference abstract, followed by fairly sparse publications in 2008, 2010, 2011, 2015, and 2018. This indicates that the field initially attracted limited research interest.

However, a marked increase in the number of publications has been observed since 2021: 2 publications in 2021, 5 in 2022, 4 in 2023, 6 in 2024, and 11 in 2025. In particular, 2025 alone accounts for approximately 32% of the entire dataset, indicating that the field has entered a period of rapid growth. This trend shows that an interdisciplinary field that could be termed computational dentistry or "in silico dental research" has been gaining momentum since the early 2020s.

The possible reasons for this increase include the growing accessibility of bioinformatics tools, the wider adoption of molecular modeling and simulation techniques, and the increasing use of these methods as complementary approaches to traditional experimental methods. Moreover, in recent years the effectiveness of in silico methods in biomaterial optimization, antimicrobial agent development, and pharmacological effect prediction in dentistry has accelerated researchers' interest in this field (Figure 1).

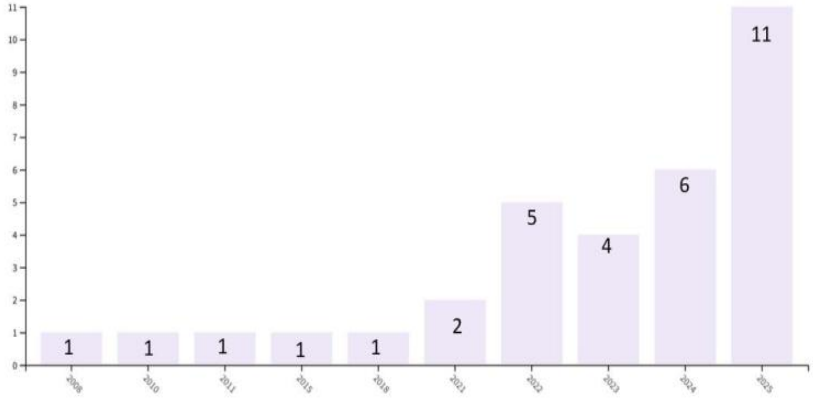

Figure 1. Distribution of publications by year

The bibliometric analysis reveals a pronounced geographic concentration in the distribution of publications in the field of molecular docking and dentistry. India, Indonesia, and Malaysia stand out by far as the leading contributing countries, together accounting for more than two-thirds of the dataset. In terms of publication volume, India ranks first with 9 records (26.5% of the dataset), followed jointly by Indonesia and Malaysia with 7 records each (20.6%). Although India therefore leads quantitatively, Indonesia shows a distinct qualitative concentration within the collaboration network, owing to the high productivity of a closely connected group of authors such as Nugraha, Kharisma, and Noor. This indicates that Indonesia occupies a central, cluster-defining position in the field's intellectual structure even though it does not hold the single largest publication count (Table 1).

Table 1. Number of publications by country

Countries/Regions	Record Count	% of 34
INDIA	9	26.471
INDONESIA	7	20.588
MALAYSIA	7	20.588
SAUDI ARABIA	6	17.647
PEOPLES R CHINA	5	14.706
IRAN	4	11.765
ARMENIA	3	8.824
SCOTLAND	3	8.824
USA	3	8.824
CYPRUS	2	5.882

Other active countries include Malaysia, Saudi Arabia, Iran, Türkiye, and Egypt; these countries contribute at varying levels, thereby strengthening the international character of the field. The data indicate the existence of a strong Indonesia-centered collaboration network. The same group of authors (e.g., Nugraha, Alexander Patera; Kharisma, Viol Dhea; Nugraha, Albertus Putera) has co-authored numerous articles, reflecting the intensity of domestic and regional collaboration. In addition, partnerships established with researchers from Saudi Arabia, India, Türkiye, and the USA support the global-scale integration of the field.

Türkiye's position is noteworthy. Turkish researchers (e.g., Ucuncu, Musa Kazim; Erdag, Emine; Namsoy, Ege) have contributed to at least 3–4 publications and have become integrated into international collaborations. This indicates that Türkiye plays an active role in this emerging field and has become part of global research networks (Table 2).

Table 2. Number of publications by author

Author	Record Count	% of 34
Kharisma VD	6	17.647
Nugraha AP	6	17.647
Noor TNEBTA	5	14.706
Ramadhani NF	4	11.765
Ardani IGAW	3	8.824
Heboyan A	3	8.824
Kurunyan MS	3	8.824
Puspitaningrum MS	3	8.824
Rizqianti Y	3	8.824
Saini RS	3	8.824

A clear productivity gap is evident among authors publishing in the field of molecular docking and dentistry. Kharisma, Viol Dhea and Nugraha, Alexander Patera stand out as the most productive authors, each with six publications. These two researchers have played a pioneering role in the development of the field and have produced a substantial portion of its research output. Ranked third, Noor, Tengku Natasha Eleena Binti Tengku Ahmad draws attention with five publications. In addition, Ramadhani, Nabila Fitri is another key contributor to this core group, with four publications.

These authors are mostly affiliated with Indonesia and form a central research core that works in close collaboration and determines the direction of the field. This core shapes the intellectual structure of the field in terms of both publication volume and topic diversity.

Other influential authors include Saini, Ravinder S. and Heboyan, Artak, each of whom stands out in terms of both productivity and citation level with three publications each. These researchers have contributed particularly to biomaterial optimization and molecular simulation topics and have taken part in international collaborations (Figure 2).

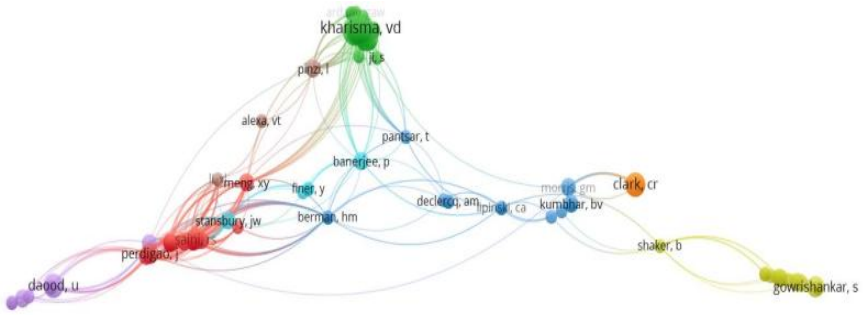

Figure 2. Author collaboration network

The most active journal, with five publications, is Journal of Pharmacy & Pharmacognosy Research, which serves as an important platform for applying pharmaceutical and phytochemical research to dentistry. This reflects the integration of the field between pharmacology and dental sciences.

The publications are distributed across 19 different journals in total. This diversity reflects the multidisciplinary nature of the field. These journals span different categories, including dentistry (European Journal of Dentistry), general science (Scientific Reports), materials science (Polymers), bioinformatics (Bioinformation), and molecular sciences (International Journal of Molecular Sciences). This distribution shows that the research encompasses both clinical and basic science perspectives.

As an indicator of quality, publication in Scientific Reports and International Journal of Molecular Sciences, high-volume journals with moderate-to-high impact factors, demonstrates that the field is recognized by mainstream scientific journals and holds a methodologically strong position. This indicates the growing acceptance of computational dentistry and in silico approaches within the scientific community (Figure 3).

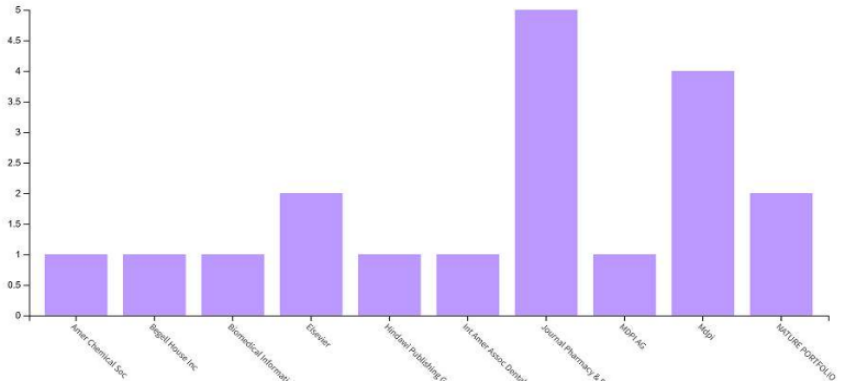

Figure 3. Number of publications by journal

The citation distribution of the studies examined shows that publications focusing on the optimization of dental biomaterials through molecular docking and molecular dynamics simulations have generated the highest impact in the literature. In this context, studies conducted on graphene and its derivatives, SiO2–TRIS systems, resin-based composites, and adhesive materials have been published in high-impact-factor journals such as Scientific Reports, BMC Oral Health, International Journal of Molecular Sciences and Journal of Dental Research and have received extensive citations. In the citation-based author analysis, researchers such as Ravinder S. Saini, Seyed Ali Mosaddad, Artak Heboyan, Alexander Patera Nugraha and Emine Erdag stand out, and the works of these authors have been found to form

central nodes in citation networks. A common feature of these authors' work is their holistic approach, combining molecular docking analyses with molecular dynamics simulations and either biomaterial mechanics or bioactivity assessments. At the country level, India and Saudi Arabia stand out in terms of publication numbers, while China and the United States, despite a more limited publication volume, are notable for their high average citation values. This finding indicates that methodological depth, a multidisciplinary approach, and publication in high-impact-factor journals — rather than sheer quantitative output — are the key factors determining scientific impact. In addition, institutions such as Saveetha University, King Khalid University, Airlangga University, and Sichuan University appear to have formed strong collaboration networks through highly cited authors and to have played a guiding role on a global scale in molecular docking-based dental research. Overall, the findings show that the molecular docking literature in dentistry is not only growing quantitatively but is also maturing by concentrating around specific authors, institutions, and thematic foci, and that AI-assisted docking approaches are expected to further increase citation impact in the future (Figure 4).

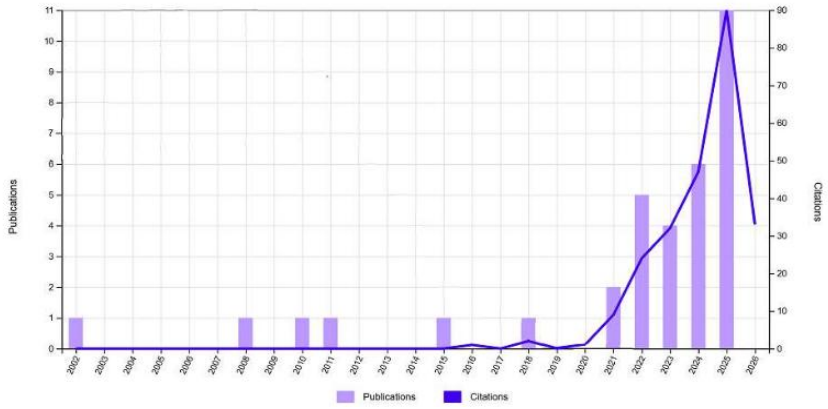

Figure 4. Distribution of citation counts of publications on molecular docking in dentistry by year

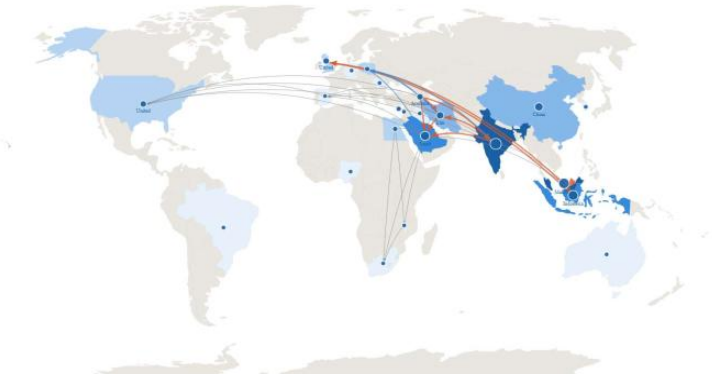

Figure 5. Collaboration network among countries publishing on the use of molecular docking in dentistry

Table 3. Number of publications by publisher

Publishers	Record Count	% of 34
Journal Pharmacy & Pharmacognosy Research-Jppres	5	14.706
Mdpi	4	11.765
Springer Nature	4	11.765
Wiley	3	8.824
Elsevier	2	5.882
Nature Portfolio	2	5.882
Thieme Medical and Scientific Publishers Pvt Ltd	2	5.882
Amer Chemical Soc	1	2.941
Begell House Inc	1	2.941
Biomedical Informatics	1	2.941

In addition, recent studies with high annual citation rates are noteworthy. The article published by Chikowe et al. in 2024 is one of the most rapidly impactful publications in the field, with an average of 15 citations per year. Similarly, the 2024 study by Saini et al. stands out with an average of 12.5 citations per year. These two studies have attracted considerable attention because they focus on current and clinically critical topics such as analgesic agent screening and dental resin composite optimization.

Most of the 11 articles published in 2025 have not yet received citations. This is due to the recency of these publications, and time is needed to assess their impact. Nevertheless, the diversity of content and topics covered by these articles offers important clues regarding the future directions of the field.

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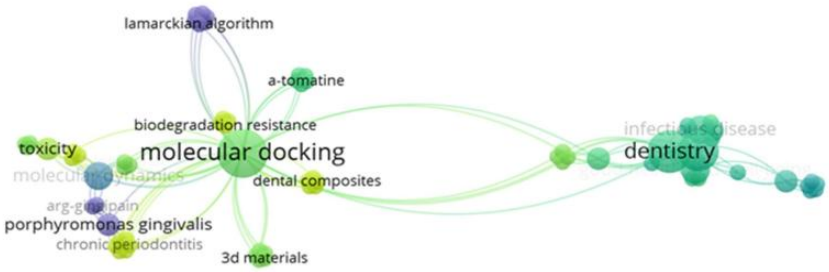

Figure 6. Most frequently used keywords. Bubble size increases with the frequency of keyword usage.

DISCUSSION

The findings of this bibliometric study reveal that the integration of molecular docking techniques into dental research has gained marked momentum over the past decade, particularly after 2021. The sparse publication activity observed during 2002–2018 suggests that this methodology was still regarded as a niche area, whereas the exponential increase in publications observed since the early 2020s is a strong indicator that the field has entered a phase of "maturation and widespread adoption" (7). This transformation has largely been made possible by the increasing availability of user-friendly bioinformatics software and access to high computational power; in silico methods have gained a legitimate place within the dental research ecosystem as a complementary and predictive approach to costly and time-consuming experimental procedures (2).

One of the most striking findings of this study is the shift in the geographic center of knowledge production. In bioinformatics research traditionally dominated by Western countries, the fact that India and Indonesia emerge as the clear leading countries — India by publication volume and Indonesia by network centrality — indicates that scientific capacity and interest have spread at the global level (8). A distinct, Indonesia-centered core research team composed of Nugraha, Kharisma, and Noor appears to shape the intellectual structure of the field through numerous co-authored publications and a dense collaboration network, even though India records the highest overall publication count. This indicates that Southeast Asia has become a global hub for an interdisciplinary research model that combines dentistry and traditional herbal pharmacology with computational methods (9). The active participation of countries such as Türkiye, Egypt, Saudi Arabia, and Iran further broadens the inclusiveness of this global network and offers an opportunity for strategic collaborations, particularly for countries with expertise in fields such as dental materials science.

The analysis of author productivity and collaboration networks confirms that the field has a distinct social structure. The fact that most of the highly productive authors co-author the same articles suggests that the flow of knowledge and methodological approaches spreads outward from a few influential groups (10). This represents a typical consolidation pattern in a still-young field. At the same time, the fact that researchers from different geographic regions, such as Saini and Heboyan, are connected to these core networks shows that collaborations exhibit a dynamic that transcends national boundaries.

The distribution of publications across journals confirms the inherently interdisciplinary nature of the field. Journal of Pharmacy & Pharmacognosy Research being the most active platform indicates that research focus has shifted toward the exploration of natural products for dental

applications. At the same time, Scientific Reports and International Journal of Molecular Sciences, high-impact-factor journals with broad readerships, demonstrates that molecular docking-based dental research is increasingly recognized and valued by the mainstream scientific community. This indicates that the field is not confined to dentistry alone but also builds bridges with fields such as materials science, pharmacology, and microbiology.

Citation analysis reflects the development of the field in two stages. In the first stage, early methodological articles such as that of Iman et al. (11) laid the foundations of the field by accumulating citations steadily over an extended period. In the second and current stage, studies published in 2024 and 2025, focusing on urgent and current research needs such as dental biomaterial optimization and the discovery of naturally derived therapeutic agents, have achieved high citation rates within a very short time (12,13). This is clear evidence that the field has evolved from being merely a "method" into an active research front generating concrete and innovative clinical solutions.

This bibliometric study has certain limitations. First, the analysis was restricted to publications indexed in the Web of Science (WoS) Core Collection database. This may have resulted in the exclusion of relevant publications indexed in other databases such as Scopus, PubMed, or Google Scholar but not in WoS. Consequently, the findings obtained may not fully reflect the entire body of molecular docking literature in dentistry.

Second, although the keywords used ("Molecular Docking", "Docking", "In Silico", "Dental", "Dentistry") were comprehensive, some studies published using different terminology may have been overlooked. In particular, publications that employed molecular docking as a method but did not explicitly state the term in their title or abstract may have been excluded from the analysis.

A third limitation is that citation analyses are time-sensitive. The research was conducted in March 2026, and publications from 2026 were not included in the analysis because their data integrity had not yet been completed (14, 15). This may lead to the citation impact of recently published studies not being fully reflected. In addition, older publications are likely to show relatively higher impact due to citation accumulation over time.

In addition, all document types (articles, reviews, case reports, editorial materials, meeting abstracts, proceedings papers, letters, and book chapters) were evaluated together in this study. Although this approach allows for a holistic examination of the literature, the differing citation dynamics of the various document types may partially affect the overall citation analysis.

Finally, bibliometric analyses focus on the quantitative indicators of publications (number of publications, citation counts, collaboration networks, and keywords) and do not directly assess

the scientific quality, methodological rigor, or clinical validity of the studies. Therefore, the results obtained reflect the numerical and structural trends of molecular docking studies and should be interpreted with caution with respect to clinical efficacy or experimental validation.

CONCLUSION

This bibliometric analysis has comprehensively revealed the development of the scientific literature, publication trends, and research dynamics related to molecular docking applications in dentistry. The findings show that molecular docking has received growing interest in dental research, particularly in recent years, and is widely used as an interdisciplinary method for evaluating dental biomaterials, antibacterial agents, and natural compounds. The increase in the number of publications demonstrates that computational methods have become an important tool supporting experimental and clinical studies in dentistry.

Country-, institution-, and author-based analyses have shown that molecular docking-based dental research is concentrated around specific academic centers, while increasingly being adopted by a broader research community at the global level. Notably, the productivity of developing countries in this field is remarkable — with India leading in publication volume and Indonesia forming the field's most densely collaborating research core — and studies published in high-impact-factor journals were found to occupy a central position within citation networks. Keyword and citation analyses further revealed that biomaterial optimization, antibacterial effects, natural products, and molecular interaction mechanisms are the leading research themes in the literature.

The results of this study indicate that molecular docking methods are not merely a theoretical tool in dentistry but also hold strategic importance for the development of new treatment approaches and the design of biocompatible materials. The bibliometric data suggest that future research directions in this field will be shaped by AI-assisted docking algorithms, multi-target ligand analyses, and computational models integrated with clinical data.

In conclusion, this bibliometric analysis presents the current state of the molecular docking field in dentistry from both quantitative and structural perspectives, offering a guiding resource for researchers. The findings obtained are expected to contribute to the planning of future studies and to enhance the scientific impact of molecular docking-based approaches in the dental literature.

Scientific Responsibility Statement

The authors declare that they are responsible for the article’s scientific content including study design, data collection, analysis and interpretation, writing, some of the main line, or all of the preparation and scientific review of the contents and approval of the final version of the article.

Ethics Approval and Consent

This study is a bibliometric analysis based on data obtained from publicly available databases and does not involve human participants, animals, patient data, or biological materials. Therefore, ethics committee approval and informed consent were not required.

Conflict of Interest

The author(s) declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

Author Contributions

Conceived and designed the study: MVK, MSD.

Collected the data, performed the analysis: MSD

Interpreted the results: MVK, MSD.

Wrote and approved the final manuscript: MVK, MSD.

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This study did not involve patients, patient data, or human participants.

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