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# Mapping of Global Research Performance on Molecular Docking: A Bibliometric Study

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**Abstract**

The paper examines the global scientific literature on Molecular Docking (MD). MDis a keyapproachusedinbioinformatics to identify and developnovel compounds towards drug discovery.This study uses the bibliometric method to analyze scientific data covered in the Scopus database from 2013 to 2022 using MS Excel,R Studio, andVOS Viewer software.A total of 12173 documents on Molecular Docking were retrieved and considered for the study. The paper provides an in-depth evaluation of the research output of MD. The research found that MuthuS.was a most prolific author in MD scientific research, with 98 publications that received 1481 global citations. The most productivecountries in this field areIndia (4020 publications), followedbyChina (2675 publications), Saudi Arabia (1362 publications) and Egypt (1071 publications). The hot keywords in MD research are molecular modelling, molecular docking simulation, unclassified drug and controlled study, but Molecular Docking is the burning author keyword. The finding also shows that the publications are increasing consistently from 2013onwards.Most articles have been published in the 'Journal of Molecular Structure'. As it is an emerging and a trending topic, it has scope for further studies. This studywillbenefit future researchers and practitioners worldwide in understanding the research pattern on MD and identifying the other key areas related to the topic.

**Keywords:**Molecular Docking, Bibliometrics, Bibliometrix,Protein-Ligand Interaction, Drug design.

## Introduction

Molecular Docking is a computer-assisted drug design model and a vital tool for drug discovery towards predicting the binding affinity between receptors and ligands1,2. During docking"lock and key model" (Figure 1A), which refers to the internal geometry of the receptor and the ligand to find the correct orientation for the "key" to open up the "lock" kept fixed3. The real flexible docking process (Figure 1B) in which the receptor and ligands change their conformation to fit each other is called an"induced fit model"(1,4).

Molecular docking simulations are generally used for reproducing the experimental data through docking validations algorithms, where protein-protein or protein-ligand conformations are obtained by using in silico method (5). Docking is one of the main toolsfor virtual screening procedures. By using this method a library of several compounds is "docked" alongside one drug target and proceeds to the best hit (6).

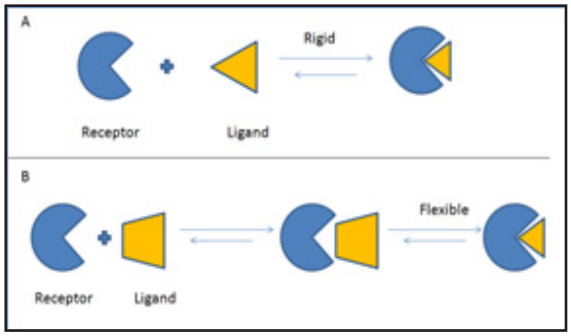



Figure 1:MolecularDockingModels: (A) A lock-and-key model (B) Induced fit model

It is a structure-based drug-designing method that generally stimulates molecular interaction for predicting the binding modeusingshape and electrostatic interactions like van der Waals &Coulombic interactions (1, 7, 8). The sum of all these interactions is calculated by a docking score (9). Various MD software is available to find the best orientation and optimal conformation according to pre-organization and specific complementarity with a definite algorithm, followed by a scoring function to calculate the binding affinity (10,11). The most widely used MD software is Flex X: fragmentation algorithm, Gold: genetic algorithm, Glide: Exhaustive Systematic search, AutoDock: genetic algorithm & Lamarckian genetic algorithm, ZDOCK: Geometric complementarity & molecular dynamics, RDOCK: genetic algorithm, MC (monte carlo) & MIN (Simplex minimization, LeDOCK: Simulated annealing (SA) & Genetic algorithm (GA) followed by AutodockVina: GA genetic algorithm (9). The three main distinct forms of MD are Rigid Docking, Flexible-rigid Docking, and Flexible (soft) Docking. The most widely used software is Flexible-rigid Docking because of its accuracy1. We can analyze the interactive mode of protein-DNA docking with the help of AutodockVina, which is displayed in PyMOL (1, 12, 13) Figure 2 shows the flow chart of the Process of Molecular Docking (14).

Since the 1980s, the molecular docking approach has been widely used to predict the interaction between two proteins, identify the

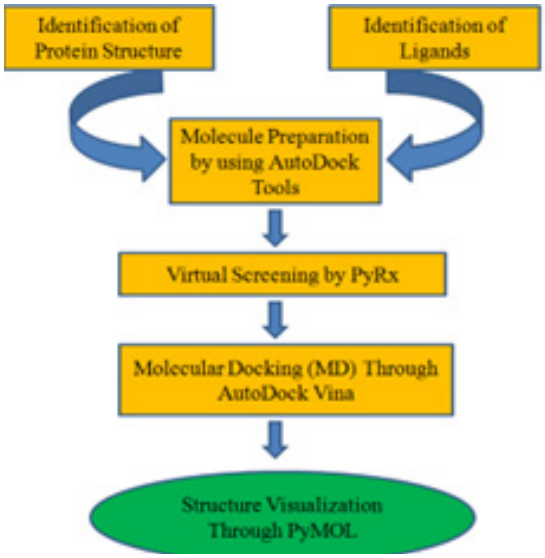



Figure 2: Process of Molecular Docking

ligand binding pocket, and predict the interaction(s) between a protein and a small molecule (15). Now a day's, the development of drug discovery computational docking simulation is the need of today's research (16,17). The impact of molecular Docking is well recognized and established in pharmaceutical industries. Day by day, molecular docking-based virtual screening is growing and significantly enhanced towards the recognition of new lead candidates (18). This paper analyzed the global literature on Molecular Docking (MD) conducted in the last ten years, from 2013 to 2022, using bibliometric methods. Review of Literature

MD research started in the early 1980's, with the establishment of the Molecular Graphics Society in 1982. The major role of Society is to support anddevelop research towards designing bioactive molecules (Willett, 2007). In 2016, Agarwal and Mehrotra reported thatMD helps to form a stable complex by predicting the preferred binding orientation of the ligand to the receptor using novel computational tools and techniques.It aims to attain an optimized docked conformer for ligand and receptor molecules (15,19) in their study discussedthecommonly applied methods in computational biolo-

gy, drug design, computational chemistry, and material science. Computer-aided drug design and discovery (CADDD) plays a major role towards drug discovery and development (19). The use and application of computational methods have facilitated the proliferation of biological databases and become an early driving force for developing MD techniques towards drug designing (20). Molecular Docking is the future of medicinal research as reported recently (21).

This study tries to assess global works of literature on MD using bibliometrics methods based on data retrieved from the Scopes. In 1963, Pritchard stated that bibliometrics is the application of mathematical and statistical methods for quantitative data analysis that extracts patterns from publications such as the growth of publication, journal impact, citations patterns, authorship in the literature, and so on (22,23,24). Bibliometrics comprises a set of methods to examine or measure books, articles and other publications. In recent decades, Bibliometrics has been considered a standard science policy and research management tool (25) It is generally applied to scientific fields to quantitatively measure the various aspects of literature like subject, author, citations, affiliation, country, etc. (26). The study identifies the prominent and impactful(a)authors, (b)geographic regions, (c)research institutions, (d) scholarly documents, (e)significant keywords and research topics, (f) highly cited countries, (g)most publishing sources that have been highly influential in the field over the last ten years. Bibliometric indicators like authorship patterns, citation statistics, and bibliometric techniques are useful for decision-making and tracking the evolution of science and technology (27,28). For specific scientific research, bibliometric studies comprehensively assess and help to identify the number and distribution of publications related to authorship, co-authorship, most cited articles etc.Overthe past few decades, several bibliometric and scientometric approaches have been adopted by researchers to study computational researchin different areas (29). But there isno bibliometric studies have been conducted on Molecular Docking yet. This paper is entirely new and innovative.The main objectives of this study are to provide a systematic overview of MD by employing the bibliometrics methods based on information retrieved from the Scopes database.

***Objective of the study***

The study aims to analyze the global research output on MDbetween 2013 and 2022. Several parameters, such as year-wise growth of publications, authorship patterns, author's keywords and citations, are assessed (30). Th following are the main objectives:

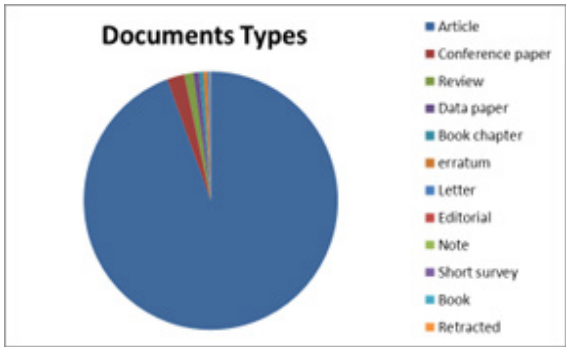
To study the type of research publications and their year-wise growth, To analyze the research trends of MD geographically, To identify the most prolific authors,productivesourcesandtitlesin MD research, To state the mostwidely used keywords in MD research, To assess the worldwide collaborations and institutions in MD research output, and, To visualize the co-authorship, co-citation and co-occurrence networks and map the relationships among the bibliographic entities.

**Methodology**

The sample dataset for the study was collected from the Scopus database in the third week of February 2023. The database Scopus was chosen because it is the oldest and most comprehensive database of records of citation indexes that itself uses an inbuilt analysis tool. The keyword "Molecular Docking"was used as the search string and qualified with the 'title' tag. The instant result was then restricted and downloaded from 2013 to 2022, as the authors felt that the ten years of data were sufficient for viewing the results appropriately and justice to the present study. Subsequently, the data are analyzed using MS Excel and Bibliometrix (R package) to understand the research performance. For science mapping or network visualization, we usedVOSViewer (31, 32).The stage-wise methodologies are shown in figure 3

## Result and Discussions

The result discussed in part: (a) performance analysis and (b) science mapping. The performance analysis examines the characteristics of the publications and the perception of quality using different tools and techniques. The performance analysis accounts for the publication patterns, contribution and productivity of the research in the given field of study. In contrast, science mapping focuses on the relationship between research constituents(Chen et al., 2022; Cobo et al., 2015). It identifies how authors, disciplines, and studies are related to one another and their evolutionary significance. The mapping analysis illustrates the thematic links by examining the co-occurrences of keywords, co-authorship, co-citation etc.(Cobo et al., 2015; Moral-muñoz et al., 2020; Rojas-Sánchez et al., 2022)



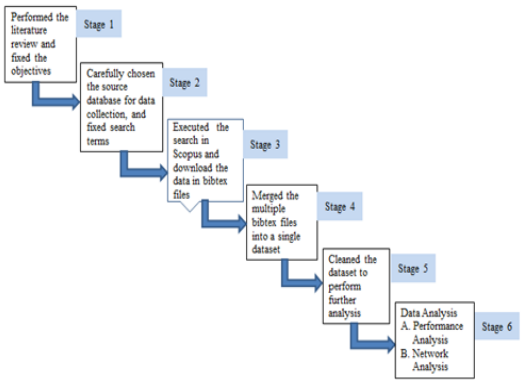




Figure 3: Flowchart of Methods applied to conduct the bibliometric study

### *Performance analysis*

Performance analysis is the easiest way to conduct a bibliometric study. It presents the performance of different research constituents, such as authors, institutes, countries, journals and citations (33). In Performance analysis, we aim to evaluate the different parameters' productivity and popularity based on bibliographic data considered for this study using the metrics such as publication count, citation rates and their impacts as the key performance indicators (34).

### *Distribution of document type, annual scientific production and country-wise scientific production*

A total of 12172 publications on Molecular Docking were identified from the Scopus database between 2013 and 2022. The summary of the findings shows that these articles were published in 1501 journals and had a total of 20629 keywords, followed by 33466 authors who authored these documents. The type of documents included 11493 (94.41%) research articles, 269 (2.21 %) conference papers, 140 (1.15 %) review articles, 114 (0.94%) other forms of publications, including the book, book chapter, data papers, editorial papers, erratum, letter and short review as shown in Figure 3.

Table 1 provides year-wise scientific production and citation impact from 2013 to 2022. There was a consistent rise in publications from 2013 to 2022. The highest 3315 (27.23%) number of papers were published in 2022, followed by 2219 (18.22%) papers in 2021, 1669 (13.71%) papers in 2020 and 1186 (9.74%) papers in 2019. The data indicates that most of the articles were published in the last four years, from 2019 to 2022. The average annual growth rate is 29.70%. The citations increased significantly over the study period, and the highest number of citations was received in 2022. In contrast, an average citation per year (ACPP) was the maximum in 2015 (22.79), followed by 2022 (20.41), 2013 (19.51) and lowest in 2021 (6.85). However, the citation rate (CR)

was highest reported in 2015 (95.59) and the lowest in 2022 (51.89).

Figure 4 shows the top ten countries in terms of scientific research publications on MD. The data reflects that India has published the highest number of 4029 papers, which is 33% of total publications in the MD domain under the study, followed by China with 2675 papers, Saudi Arabia with 1368 papers and Egypt with 1075 papers. At the same time, developing countries like the USA have ranked eighth position in the row.

### *Distribution of most prolific authors and author's productive life*

Table 1: Year-wise Publications and citation impact

| Year | TP | TC | h-Index | CR |
|---|---|---|---|---|
| 2013 | 328 | 6399 | 41 | 93.9 |
| 2014 | 401 | 7792 | 44 | 94.51 |
| 2015 | 544 | 12400 | 52 | 95.59 |
| 2016 | 695 | 12245 | 46 | 94.24 |
| 2017 | 840 | 15059 | 47 | 94.64 |
| 2018 | 975 | 15345 | 45 | 95.28 |
| 2019 | 1186 | 15989 | 46 | 91.99 |
| 2020 | 1669 | 19564 | 49 | 91.31 |
| 2021 | 2219 | 15195 | 63 | 83.42 |
| 2022 | 3315 | 67663 | 38 | 51.89 |

Table 2 indicates the top ten most productive authors on MD Research. It is observed that the highest number of papers are published by 'Muthu, S.' from India and are associated with Arignar Anna Government Arts College. He authored 98 articles with an h-index of 22, 15.11 g-index and received 1481 citations. The second prominent author, ' Taha, M', from Imam Abdulrahman Bin Faisal University, Saudi Arabia, published 83 articles with 28 h-index, 27.33 ACPP and has received the highest 2269 citations. 'Wadood, A.' and 'Rahim, F.' both from Pakistan, secured third and fourth positions with 76 and 75 papers. The table aslo shows that four authors from Pakistan secured positions in the top 10 most prolific authors table in the field of MD.

Table 3 discusses the highly productive institutions in terms of publications, total citations, h-Index, average citation per publication, and their geographic locations. The data shows that the King Saud University of South Arabia was leading in the domain, followed by the Ministry of Education China and the National Research Centre from Egypt in 2nd and 3rd positions, respectively. Regarding citations, King Saud University also received the highest 6437 citations, with an average citation per paper of 15.47, followed by Cairo University (4203 TC, 17.23 ACPP) and Chinese Al-Azhar University (4135 TC, 17.23 ACPP) in the top three positions. It has also been observed that the most productive institutions in molecular docking research belong to Egypt and Saudi Arabia.

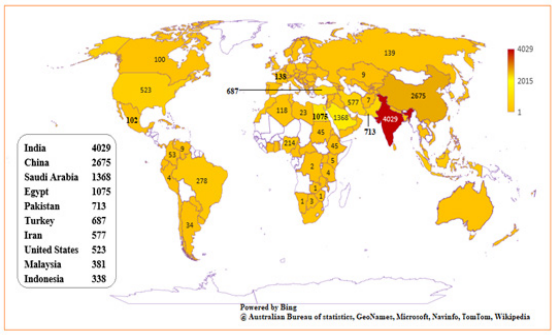



Figure 4: Most productive countries

Table 4 provides the highly productive sources in the MD research with theirPublisher and Scimago ranking. Data exposed that the journal entitled 'Journal of Molecular Structure' (855 total publications, 10111 total citations) was the most productive journal in Molecular Docking research, followed by the 'Journal of Biomolecular Structure and Dynamics' (496 total publications, 4998 total citations), and 'Bioorganic Chemistry' (335 total pub., 7688 total citations). The analysis also discovered that the journal "Molecules" ranked fourth in terms of total publications and total citations (4409 total citations, 7.5 average citations) with an SJR rank

Table 2. Top ten authors the relationship between author, country and institution

| Author Name | TP | TC | h-index | ACPP | Institution | Country |
|---|---|---|---|---|---|---|
| Muthu, S. | 98 | 1481 | 22 | 15.11 | Arignar Anna Government Arts College | India |
| Taha, M. | 83 | 2269 | 28 | 27.34 | Imam Abdulrahman Bin Faisal university, | Saudi Arabia |
| Wadood, A. | 76 | 1828 | 25 | 24.05 | Abdul Wali Khan University Mardan, | Pakistan |
| Rahim, F. | 75 | 1833 | 26 | 24.44 | Hazara University Pakistan | Pakistan |
| Bouachrine, M. | 54 | 306 | 10 | 5.67 | UniversitéMoulay Ismail | Morocco |
| Khan, K.M. | 52 | 1754 | 24 | 33.73 | University of Karachi | Pakistan |
| Saeed, A. | 52 | 826 | 18 | 15.88 | Quaid-i-Azam University, Department of Chemistry | Pakistan |
| Iqbal, J. | 47 | 701 | 17 | 14.91 | COMSATS University Islamabad | Pakistan |
| Hassan, M. | 44 | 693 | 17 | 15.75 | Research Institute at Nationwide Childrens Hospital | USA |
| Khedkar, V.M. | 43 | 662 | 15 | 15.40 | Vishwakarma University | India |

Table 3: Top ten productive institutions

| Affiliation | Country | TP | TC | h-Index | CR | ACPP |
|---|---|---|---|---|---|---|
| King Saud University | Saudi Arabia | 416 | 6437 | 41 | 88.70 | 15.47 |
| Ministry of Education China | China | 279 | 2539 | 25 | 81.72 | 9.10 |
| National Research Centre | Egypt | 279 | 3589 | 32 | 83.15 | 12.86 |
| Cairo University | Egypt | 244 | 4203 | 31 | 90.16 | 17.23 |
| Al-Azhar University | Egypt | 240 | 4135 | 33 | 91.25 | 17.23 |
| College of Pharmacy | Saudi Arabia | 228 | 3995 | 36 | 89.91 | 17.52 |
| College of Sciences | Saudi Arabia | 206 | 2773 | 30 | 86.89 | 13.46 |
| Faculty of Pharmacy | Egypt | 161 | 2801 | 31 | 91.30 | 17.40 |
| University of Karachi | Pakistan | 157 | 2933 | 29 | 89.81 | 18.68 |
| King Abdulaziz University | Saudi Arabia | 151 | 1546 | 21 | 82.78 | 10.24 |

Table 4: Distribution of highly cited sources, their Scimago rank, and Country

| Name of Source Title | Publisher | TP | TC | SJR_2021 | h_index | ACPP |
|---|---|---|---|---|---|---|
| Journal of Molecular Structure | Elsevier | 855 | 10111 | 0.48 | 39 | 15.47 |
| Journal of Biomolecular Structure and Dynamics | Taylor & Francis | 496 | 4998 | 0.561 | 32 | 9.10 |
| Bioorganic Chemistry | Elsevier | 335 | 7688 | 0.728 | 42 | 12.86 |
| Molecules | MDPI | 334 | 4409 | 0.705 | 29 | 17.23 |
| Medicinal Chemistry Research | Springer Nature | 212 | 2146 | 0.357 | 22 | 17.23 |
| Chemistryselect | Wiley-Blackwell | 158 | 838 | 0.407 | 15 | 17.52 |
| SpectrochimicaActa Part a Molecular and Biomolecular Spectroscopy | Elsevier | 154 | 3405 | 0.59 | 32 | 13.46 |
| RSC Advances | Royal Society of Chemistry | 154 | 2681 | 0.667 | 31 | 17.40 |
| Polycyclic Aromatic Compounds | Taylor & Francis | 145 | 227 | 0.228 | 7 | 18.68 |
| Evidence Based Complementary and Alternative Medicine | Hindawi | 141 | 383 | 0.461 | 10 | 10.24 |

of0.705, following the journal 'Bioorganic Chemistry with the highest SJR of 0.728.Elsevier and Taylor &Francisare leading publishers of MD research. Table 5 describes the ten most highly cited papers. The paper, 'Molecular docking and structure-based drug design strategies' by 'Ferreira et al., published in the journal 'Molecules', in 2015, has received the highest number of 864 citations. The second most cited paper 'Software for molecular docking: a review' by 'Pagadala et al., published in 'Biophysical Review', in 2017, has 624 citations,followed by 'Ribavirin, Remdesivir, Sofosbuvir, Galidesivir, and Tenofovir against SARS-CoV-2 RNA dependent RNA polymerase (RdRp): A molecular docking study 'by 'Elfiky A. A., published in 'Life Sciences' has a total of 577 citations and ranked the third position.

Table 5. Highly Cited Documents

| Name of Source Title | TP | TC | SJR_2021 | h_index |
|---|---|---|---|---|
| Journal of Molecular Structure | 855 | 10111 | 0.48 | 39 |
| Journal of Biomolecular Structure and Dynamics | 496 | 4998 | 0.561 | 32 |
| Bioorganic Chemistry | 335 | 7688 | 0.728 | 42 |
| Molecules | 334 | 4409 | 0.705 | 29 |
| Medicinal Chemistry Research | 212 | 2146 | 0.357 | 22 |
| Chemistryselect | 158 | 838 | 0.407 | 15 |
| SpectrochimicaActa Part a Molecular and Biomolecular Spectroscopy | 154 | 3405 | 0.59 | 32 |
| RSC Advances | 154 | 2681 | 0.667 | 31 |
| Polycyclic Aromatic Compounds | 145 | 227 | 0.228 | 7 |
| Evidence Based Complementary and Alternative Medicine | 141 | 383 | 0.461 | 10 |

### *Science mapping*

It is a highly critical method used in bibliometrics analysis to map the scientific output (35). This methodology uses computational techniquestoanalyze the bibliographic objects quantitatively& qualitatively and then visualize their interrelationships. To perform this analysis, we choseVOSviewer software, a highly used-science mapping tool, in order todraw the overarching structure, evolution of research themes and research fronts, and geographic spread of the MD research (36). The VOS Viewer software is mainly used for networking and visualization to understand the research pattern. Further, it exploresthe relationshipofthe authors with countries, the keywords frequently appearing in the papers, and the documents and their citations in terms of total network links, clusters and network strength.

### *Co-authorship network*

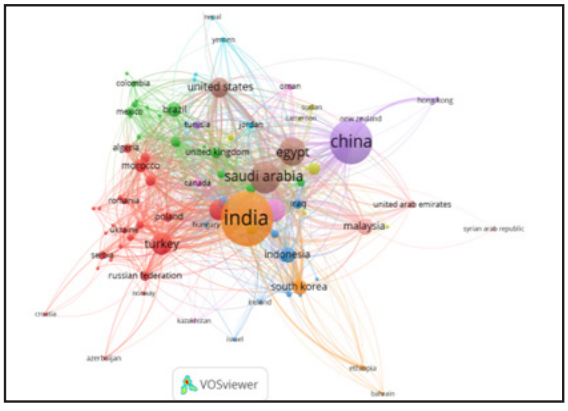



Figure 5: Visualization of co-authorship analysis versus countries

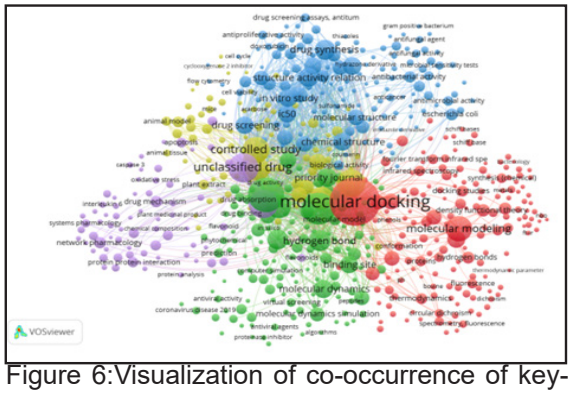


Figure 6:Visualization of co-occurrence of keywords

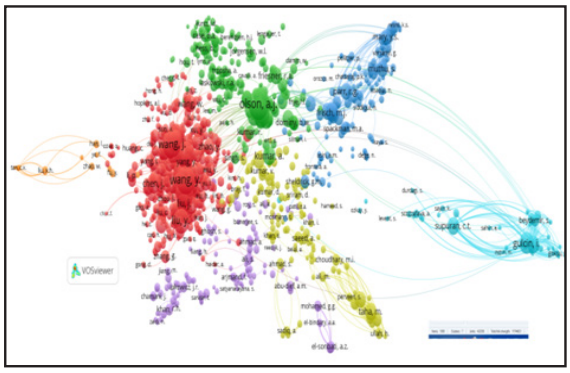


Figure 7: Visualization of co-citation network

Figure 5 plots the co-authorship network versus countries. The circles signify the countries or regions, and the size of the circle symbolizes the number of publications. The links between circles represent the cooperative relationship between two countries/regions. The study considered the criteria of a minimum of 5 papers from the country with 10 citations.Saudi Arabia hasthe highest link strength(2260), followed by India(1665) and Egypt (1098).India secured the firstposition for publishing the most documents, followed by Saudi Arabia and Egypt. Egypt placed in third position receiving 14732 citations after India and Saudi Arabia.

### *Network visualization of co-occurrence of keywords*

Figure6 depicts a network map of all keywords within the research papersselected for the study. The minimum number of occurrences of a keyword is considered to be75. The results show out of a total of 20629 keywords,only 587 keywords met the threshold.The width of the network lines reflects the intra-relationship among the keywords, i.e., the thicker the network line, the stronger the association.The keywords that appeared most were 'Molecular Dockingwith total link strength of 170879,followed by 'unclassified drug' (112155),MD simulation (95466) and 'controlled study'(80694). There are 187 number of clusters of keywords, out of which the most frequently used keywords are Metabolism, Human, Structure activity relation, Molecular dynamics, in vitrostudy, ic50, Neutralizing, binding site, drug screening, structure activity relationship, enzyme inhibition, Drug effects, ligands, Computer model, Molecular dynamic simulation and Drug protein binding.  2.3 Co-citation Network Visualization

Figure 7 shows the network map of co-citation among cited authors. The circle size represents the number of citations in which each author collaborates with another based on the number of co-authors. In general, the larger size of a circle, the more often vital co-citation seems. The author' Olson, A.J.' received the highest number of citations (4464) with top link strength 205881, followed by Wang Y., having 3697  citations with 218016 link strength. Author Wang J and Zhangh Y secured 3rdand 4th positions in co-citation network analysis, having 355 and 3332 citations with 208445 and 190655 link strength, respectively.

## Conclusion

This study performedaquantitative and qualitative analysis of Molecular Dockingresearchovera period of ten years, from 2013 to 2022,to understand the research trends and the contributionsanddistributionsof authors, organizations, countries and journals in the domain. For this study theexperimental data was collected from the Scopus database.Atotalof12172 scientific productions were retrievedduring the study period. The study reveals that most of the MD researchwaspublished in English.Devel-

oped and developing countries like India, China, Saudi Arabia, and Egypt contributed significant researchinMD.Accordingto the study,an author Muthu, S. fromIndia,affiliated with Arignar Anna Government Arts College, dominated the list of publications by publishing 98 documents. The study also finds that most prolific authors belong to India and Saudi Arabia. The article by Ferreira et al., 2015 from the journal MOLECULES has received the highest 864 citations. The authored keyword' Molecular Docking' appeared most, followed by 'Molecular modelling simulation', 'Unclassified Drug' 'Controlled Study', and 'Drug synthesis. The study also discovers that research on MD is increasingexponentially worldwide and collaboratively.The bibliometric study is the most preferred way to measure the productivity of a subject, organization, authors, and source.Still, there is enough scope for further studies on MD because it is an emerging areathat will significantly affect today's Society regarding drug discovery. This study will aid future researchers who wish to undertake bibliometric studies on related domains.

**Conflict of Interest:** There is no conflict of interestrelated to the works in the manuscript.

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