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Research Article

Scientometric Analysis of the Combined Application of Molecular Docking Technique and CRISPR Genome Editing Technology

Tingting Jiang[1,*], Jorge Gulín-González[2], Yunwei Chen[1,3]

[1]National Science Library (Chengdu), Chinese Academy of Sciences, Chengdu, CHINA.
[2]Centro de Estudios de Matemática Computacional (CEMC), Universidad de las Ciencias Informáticas (UCI), La Habana, CUBA.
[3]Department of Information Resources Management, School of Economics and Management, University of Chinese Academy of Sciences, Beijing, CHINA.

ABSTRACT

Molecular Docking (MD), a computational technique that examines the conformation and orientation of molecules (mainly ligands) into the binding site of a protein target, has emerged as a pivotal strategy for modeling biomolecular interactions. It has significantly contributed to the advancement of Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) genome editing technologies. Despite the impact of these technologies on drug development, medicine, and other applied fields, a comprehensive scientometric analysis of the integration of MD and CRISPR genome editing iscurrently lacking in the literature. Based on 5165 publications sourced from the Web of Science Core Collection (2005–2024), this study implemented a scientometric analysis to chart the development trajectory and collaborative landscape of CRISPR-MD research. To achieve this, we employed longitudinal bibliometric techniques to track the thematic evolution through keywords and to analyze the structure of co-authorship and institutional collaboration networks over time. The analysis reveals remarkable growth in publications over the past two decades, marking the transition of CRISPR-MD from an emerging technique to a prominent research frontier. The evolution of keywords and collaboration networks delineates the field's expanding scope and intensifying interdisciplinary integration. This study provides critical insights into the convergence of computational biology and genome engineering. The findings highlight the maturation of CRISPR-MD research and underscore its future potential in driving innovation for precision medicine and other interdisciplinary applications.

Keywords: Molecular docking, CRISPR, CRISPR-Cas, Genome editing, Scientometrics.

Correspondence:
Tingting Jiang
National Science Library, (Chengdu),
Chinese Academy of Sciences, Chengdu,
CHINA.
Email: jiangtt@clas.ac.cn

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INTRODUCTION

The advent of CRISPR genome editing technologies has revolutionized molecular biology. It allows for exact changes to genetic material with unprecedented efficiency (Jiang *et al.*, 2024; An *et al.*, 2024). Concurrently, MD, a cornerstone of computational biology, is widely used to predict the binding modes and affinities between biomolecular entities, including proteins, nucleic acids, and small molecules (Liu *et al.*, 2018). In recent years, MD has also been applied to identify active site amino acids in proteins, providing critical insights into protein function and ligand binding (Liu *et al.*, 2024). MD has rapidly gained prominence in genome editing research, particularly for optimizing CRISPR-Cas systems (Bhattacharya & Satpati, 2022). MD simulations facilitate the prediction of binding interactions between CRISPR components and their targets, aiding in the identification of key residues for mutagenesis, the design of anti-CRISPR proteins, and the discovery of small-molecule enhancers or inhibitors (Hwang *et al.*, 2023; Fu *et al.*, 2024). Jinek *et al.* (2012) demonstrated that Cas9 could be programmed by a dual-RNA complex to cleave target DNA with sequence specificity, thereby laying the molecular foundation for programmable genome editing. Cong *et al.* (2013) and Mali *et al.* (2013) adapted CRISPR-Cas9 for genome engineering in mammalian cells. They introduced the concept of multiplexed editing and enabled the targeting of multiple genomic loci with high efficiency and specificity. CRISPR systems have since evolved into powerful tools for precise gene manipulation, culminating in the awarding of the 2020 Nobel Prize in Chemistry (The Nobel Prize, 2020).

Recent advancements have expanded CRISPR's capabilities beyond gene knockout to include base editing, prime editing, and RNA targeting (Komor *et al.*, 2016; Anzalone *et al.*, 2019;

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Yang & Patel, 2024). These innovations enable precise nucleotide modifications and RNA-level interventions without inducing double-stranded DNA breaks, significantly enhancing the safety and versatility of genome engineering. CRISPR genome editing technology has also achieved notable progress in clinical applications, such as drug delivery and cancer therapy (Halmi *et al*., 2023). For example, Gillmore *et al*. (2021) demonstrated the feasibility of *in vivo* CRISPR-Cas9 editing to treat transthyretin amyloidosis, providing compelling evidence for the therapeutic potential of CRISPR-based interventions in monogenic disorders. These breakthroughs highlight CRISPR's increasing importance in translational medicine.

Subsequent developments have further expanded the scope of CRISPR genome editing technologies. Shalem *et al*. (2014) pioneered genome-wide CRISPR-Cas9 knockout screening in human cells, facilitating high-throughput functional genomics. Behan *et al*. (2019) employed large-scale CRISPR screens to prioritize therapeutic targets in cancer, marking a critical step toward precision oncology. Technological diversification has also played a key role. Unlike Cas9, Cas12a does not require a tracrRNA for activation, enabling efficient multiplexed genome editing *in vivo* (Breinig & Schweitzer, 2019). Moreover, in contrast to the DNA-targeting activities of Cas9 and Cas12a, Cas13 exhibits RNA-activated RNase activity, making it uniquely suited for RNA-centric applications (Yang & Patel, 2024).

CRISPR genome editing technology's potential extends across basic science, biotechnology, agriculture, and medicine (Nature, 2020; Zhu *et al*., 2020). In December 2023, the U.S. Food and Drug Administration (FDA) approved the first CRISPR-based gene therapy for sickle cell disease (FDA, 2023), marking a significant milestone for clinical applications. Concurrently, MD simulations have advanced to support the rational engineering of Cas proteins, screening of CRISPR inhibitors, design of synthetic guide RNAs (gRNA), and modeling of RNA-protein interactions using tools such as CRISPR-Cas-Docker (Park & Won, 2023).

A comprehensive scientometric analysis of the integration of MD and CRISPR genome editing technologies has not been found in the existing literature. Current studies primarily focus on individual applications, such as gRNA optimization (Ke *et al*., 2022), anti-CRISPR protein discovery (Figueroa *et al*., 2023), or small-molecule screening (Sun *et al*., 2021), without synthesizing broader trends, collaborative networks, or emerging research hotspots. To address this gap, the present study conducts a scientometric analysis of MD applications in CRISPR genome editing over the past two decades (2005-2024). Our study aims to bridge the gap between current scientometric studies and the desired state with a more comprehensive characterization of the use of these technologies. Developing this type of study can be very useful for identifying current and future trends in the combined use of both technologies, their applications, and impact. Here, we examine the publication growth trends, collaboration networks at the country, institution, and author levels, as well as reference and journal analyses to identify influential works. Additionally, keywords co-occurrence and clustering analyses are employed to reveal thematic shifts. By visualizing the knowledge landscape and pinpointing emerging hotspots and key challenges, this study provides valuable insights for researchers and policymakers aiming to understand the trajectory and future directions of computational approaches in genome editing. The research questions guiding our study are as follows: How can we characterize the state of the art about the combined use of molecular docking technologies and CRISPR genome editing technology? What are the key publication trends, influential journals and authors, collaborative networks, and thematic hotspots in this field? What are the recent advances and methodology in this field?

METHODOLOGY

Data Collection

We conducted a comprehensive scientometric analysis using the Web of Science Core Collection (WoSCC) database, spanning publications from 2005 to 2024. Our systematic search strategy employed a carefully designed query to capture all relevant studies at the intersection of molecular docking and CRISPR technologies. The retrieval strategy used in this study was set to TS=(("Virtual Screening" OR "Docking" OR "Molecular Docking" OR "Computational Molecular Docking" OR "Molecular Dynamics" OR "Empirical Scoring Function*" OR "Force-Field Scoring Function*" OR "Mean-Field Scoring Function*" OR "Machine Learning Scoring Function*" OR "Computational Molecular Docking" OR "Protein-Ligand Docking" OR "Protein-Protein Docking" OR "Protein-DNA Docking" OR "Drug*" OR "Drug Design" OR "Rational Drug Design" OR "Computer-Aided Drug Design") AND ("CRISPR*" OR "CRISPR-Cas*" OR "Clustered Regularly Interspaced Short Palindromic Repeat*"OR "CRISPR gene editing" OR "CRISPR-Cas-Docker" OR "CRISPR-Cas9" OR "CRISPR-Cas12a" OR "CRISPR-Cas13" OR "CRISPRa" OR "CRISPRi" OR "Base Edit*" OR "Prime Edit*" OR "dCas9" OR "Cas protein*" OR "sgRNA" OR "gRNA" OR "Anti-CRISPR" OR "Acr protein*" OR "CRISPR Inhibitor*" OR "CRISPR Enhancer*" OR “*CRISPR” OR “Anti-CRISPR” OR "Cas protein*")) AND PY=(2005-2024)[1]. A total of 5391 records were retrieved from the WoSCC. The document types were limited to articles and review articles, with no restriction on language. After excluding 226 records based on predefined criteria, 5165 records remained (Reviews: n=1289; Articles: n=3876), which served as the foundation for our scientometric analysis. This dataset comprehensively captures research integrating molecular docking approaches with CRISPR genome editing technologies,

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[1] https://webofscience.clarivate.cn/wos/woscc/summary/ce9c4b7d-0575-465c-9245-c2765f3b8cce-0166b3ac99/relevance/1

providing a robust basis for bibliometric evaluation and network visualization.

Data Analysis

In accordance with our inclusion criteria, all pertinent bibliographic records were methodically collected from the WoSCC. The raw bibliometric data were imported into Microsoft Excel and InCites for preliminary organization. To guarantee consistency, standard data cleaning techniques were used, such as deduplication and normalization of institutional and country names. Co-author analysis and cooperation network visualization were done using CiteSpace and VOSviewer. In the context of molecular docking applications in CRISPR research, this multi-method analytical framework allowed for a thorough evaluation of publication dynamics, research collaboration patterns, and the evolution of knowledge structures. The analytical workflow shown in Figure 1 was used to process the retrieved dataset.

RESULTS

The Number of Publications

The articles were arranged by publication year in order to examine the trends in MD research within CRISPR genome editing technologies. Over the past 20 years, original research in this area has grown significantly (see Figure 2). Less than ten papers were published annually during the first phase, which ran from 2005 to 2013. The field's conceptual and methodological underpinnings

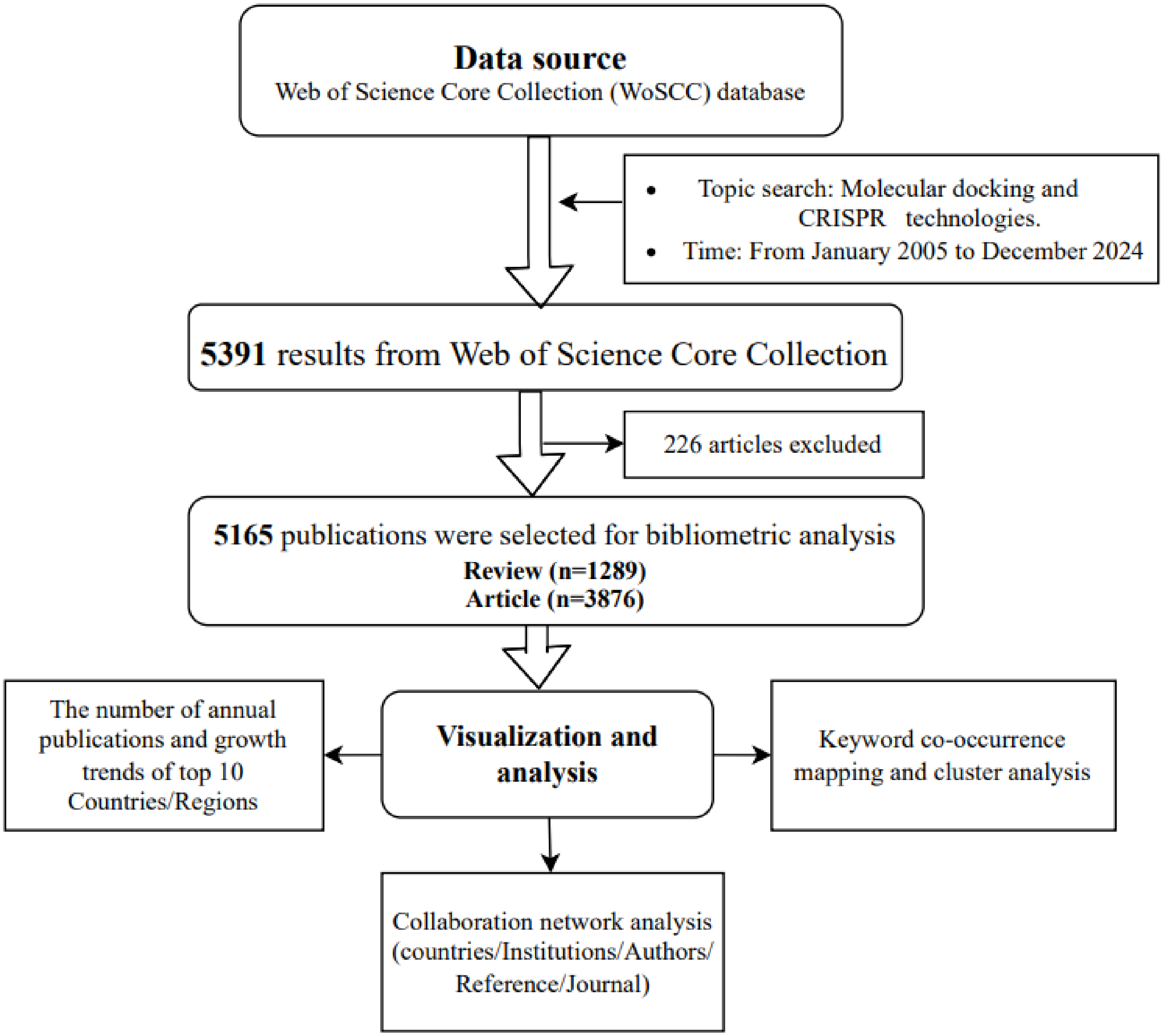


Figure 1: Workflow used for the study; the source used, the literature selection, and the data analysis are specified.

were laid by these early research, which were essential to its development. Around 2014, there was a discernible change as the number of publications increased to 23 annually, signaling the start of faster growth. Research production grew significantly between 2015 and 2022, with a sharp increase in publications from 69 in 2015 to 825 in 2022. This growth reflects the expanding interest and rapid advancements in MD applications for CRISPR technologies. Notably, the trend continued into 2023 and 2024, with 761 and 871 publications, respectively, indicating sustained scholarly engagement despite minor fluctuations.

According to the quadratic fitting curve ($y = 4.3599x^2 - 33.446x + 39.512$, $R^2 = 0.9653$), the quadratic model strongly supports the explosive growth of research in MD for CRISPR applications, particularly after 2014. The exceptionally high coefficient of determination indicates that this model accurately captures developmental dynamics of the field, while the positive quadratic term suggests continued acceleration in research output, at least in the near term. However, as with all rapidly emerging technologies, eventual stabilization is expected as the field matures.

These findings demonstrate that the integration of CRISPR-MD has evolved from a novel technique into a prominent area of research. The rapid increase in publications underscores its potential in precision genome engineering. Although significant research has been conducted, there remains a need to translate theoretical advances into practical, real-world applications. This transition is essential for advancing the field toward clinical implementation and the development of mature technologies. After 2020, numerous studies began focusing on leveraging CRISPR and molecular docking to combat COVID-19. For instance, Fasching *et al.* (2022) developed a rapid test for COVID-19 variants that utilized LAMP and CRISPR-Cas12 to detect mutations in the virus's spike gene. Similarly, Iryanto *et al.* (2022) proposed a CRISPR-Cas13a-based approach as a potential treatment against SARS-CoV-2. These examples demonstrate how researchers rapidly applied CRISPR-MD to address pressing public health challenges. The COVID-19 pandemic likely contributed to the sharp increase in research during this period. The pressing demand for fast and accurate diagnostic and therapeutic tools propelled the combination of CRISPR and molecular docking into the spotlight, accelerating the field's growth and bringing it closer to clinical application.

Growth Trends of Top 10 Countries/Regions

To analyze the development trends in CRISPR-MD research, countries were ranked based on their total number of publications from 2005 to 2024. The results are presented in Figure 3. Figure 3A depicts the global cooperation network among leading countries in this field. The size of each node corresponds to the total number of publications from the respective country or region, while the thickness of the edges indicates the strength of bilateral collaborations. The United States and China stand out as central hubs in the network, each demonstrating extensive collaborative links with multiple countries, highlighting their pivotal roles in international research partnerships. The network is further divided into six clusters, organized by thematic or geographical

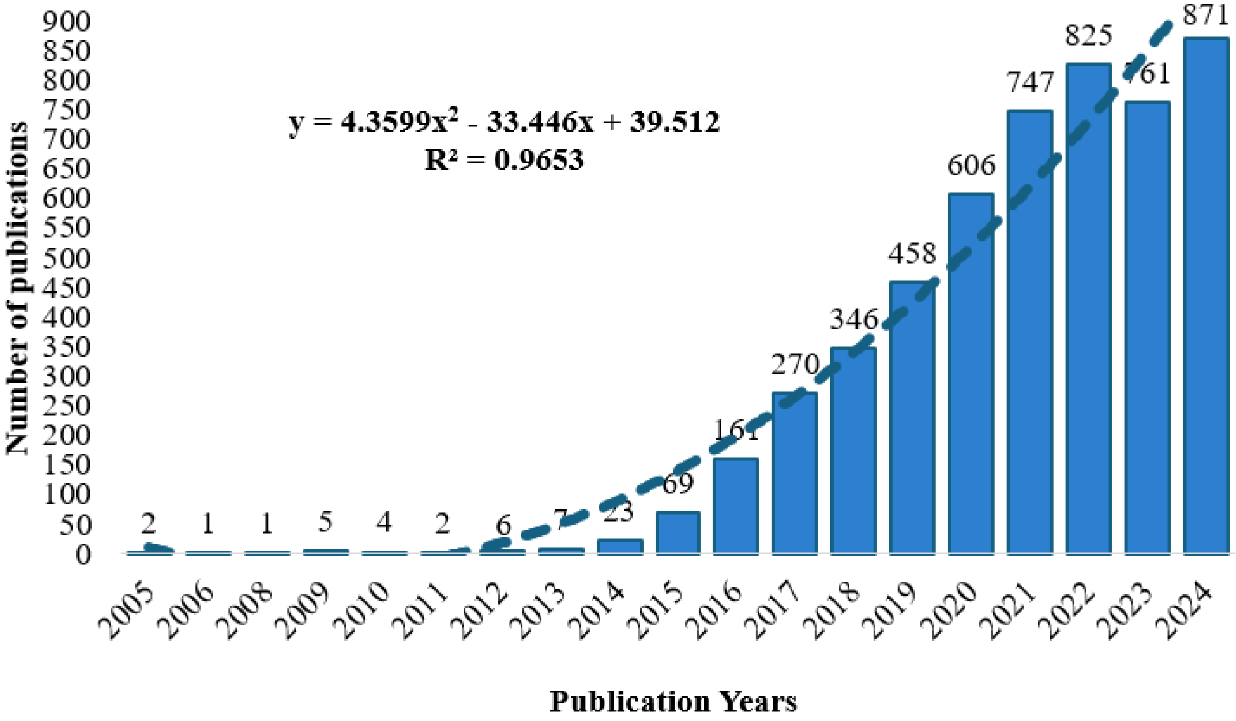


Figure 2: Annual publication trend from 2005 to 2024.

proximity, with different colors representing distinct cooperation groups, thereby emphasizing patterns of regional collaboration.

As shown in the publication statistics, the United States ranked first with 2253 publications, followed by China (1297) and the United Kingdom (719). Among the top ten contributing countries, five are located in Europe (United Kingdom, Germany,

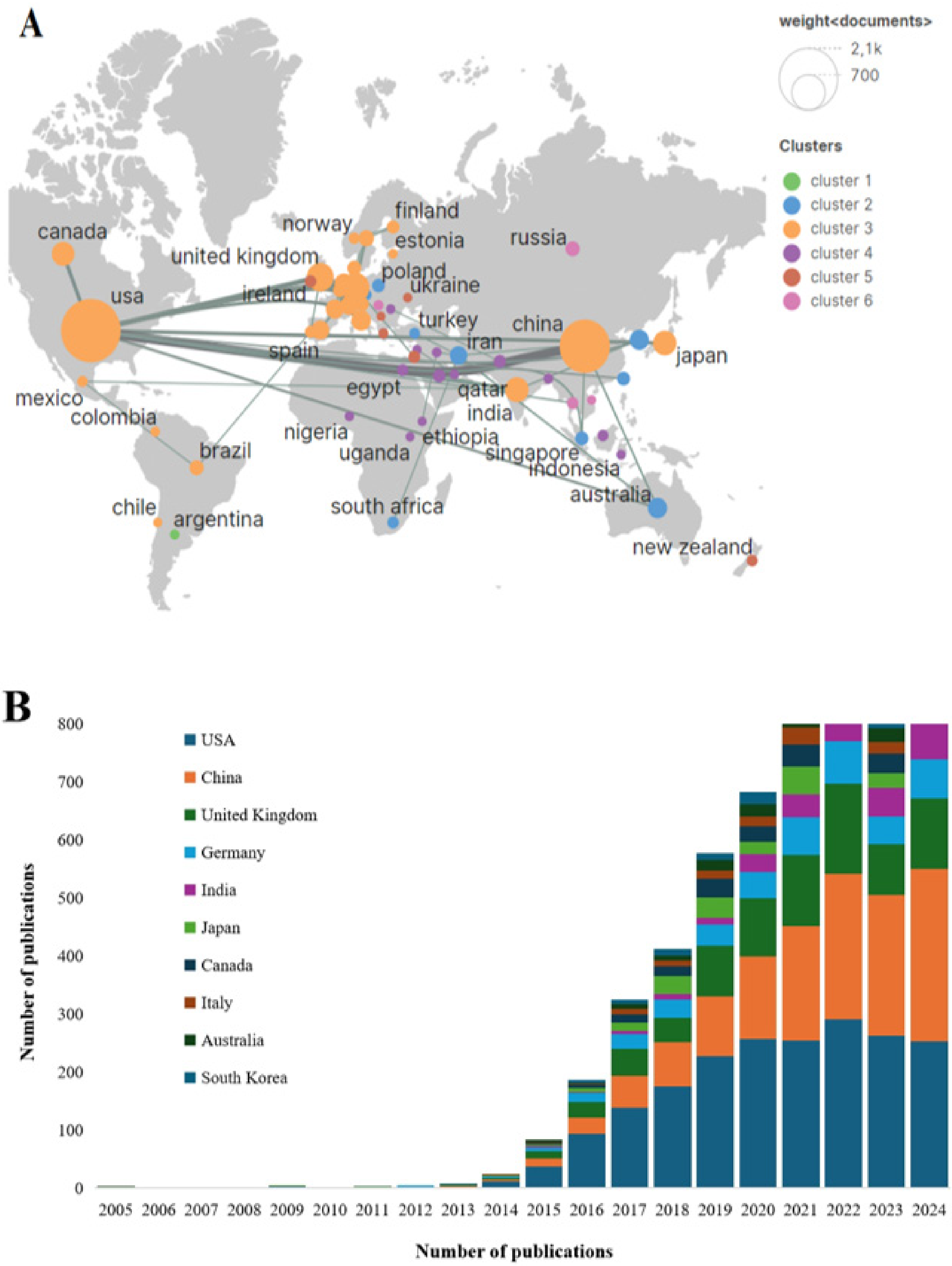


Figure 3: (A) Global cooperation network map among major countries worldwide in the field of CRISPR-MD research. (B) Annual publication trends of the top ten countries or regions.

Italy, France, and Spain), two in North America (United States and Canada), two are in Asia (China and Japan), and one is in Oceania (Australia), reflecting the global distribution of research efforts.

Figure 3B presents the annual publication trends of the top ten countries or regions over the past two decades. The United States maintained a leading position throughout the study period, peaking around 2021, followed by a slight decline in subsequent years. China showed a marked upward trajectory, especially after 2020, reflecting its rapidly increasing productivity in this research domain. The United Kingdom consistently ranked third, with relatively stable output and notable peaks in 2020 and 2023. Germany maintained a steady publication volume, while Japan contributed fewer publications among the top five but sustained consistent engagement. India, Canada, Australia, and South Korea demonstrated significant growth in publication output, indicating an expanding and diversifying global research landscape in this emerging interdisciplinary field.

Collaboration Network Analysis of Institutions

Based on publication counts in the fields of MD and CRISPR technology, the top 10 contributing institutions are listed in Table 1. These include the University of California System (270), Harvard University (265), Chinese Academy of Sciences (219), Harvard University Medical Affiliates (186), Harvard Medical School (168), Massachusetts Institute of Technology (MIT) (151), University of Texas System (132), National Institutes of Health (NIH) – USA (113), Broad Institute (112), and the Helmholtz Association (108). These institutions serve as major research hubs, primarily in the United States and China, and play pivotal roles in driving innovation and fostering collaboration.

To strong international collaboration, significant institutional partnerships are evident within individual countries. As shown in Figure 4A, each node represents an institution, with the node size proportional to publication volume, thereby indicating research activity. Notably, institutions such as Chinese Academy of Sciences, Shanghai Jiao Tong University, and Sun Yat-sen University have developed dense collaborative networks. Figure 4B illustrates the publication timeline by institution, revealing that Chinese institutions such as Shenzhen university have markedly increased their presence in this field since 2021.

Analysis of Author and Co-author

Top 10 Authors by Publication

The analysis of publication output reveals key contributors to molecular docking applications in CRISPR genome editing. As shown in Table 2, Giulia Palermo (University of California System) leads with 30 publications, demonstrating substantial

Table 1: Top 20 institutions with the number of publications.

Rank	Institution	Publications	County/Regions
1	University of California System	270	USA
2	Harvard University	265	USA
3	Chinese Academy of Sciences	219	China
4	Harvard University Medical Affiliates	186	USA
5	Harvard Medical School	168	USA
6	Massachusetts Institute of Technology (MIT)	151	USA
7	University of Texas System	132	USA
8	National Institutes of Health (NIH) - USA	113	USA
9	Broad Institute	112	USA
10	Helmholtz Association	108	Germany
11	University of Chinese Academy of Sciences, CAS	96	China
12	Shanghai Jiao Tong University	95	China
13	University of London	95	UK
14	Howard Hughes Medical Institute	94	USA
15	Dana-Farber Cancer Institute	94	USA
16	Stanford University	92	USA
17	University of California San Francisco	89	UAS
18	Fudan University	86	China
19	Institut National de la Sante et de la Recherche Medicale (Inserm)	85	France
20	Sun Yat Sen University	82	China

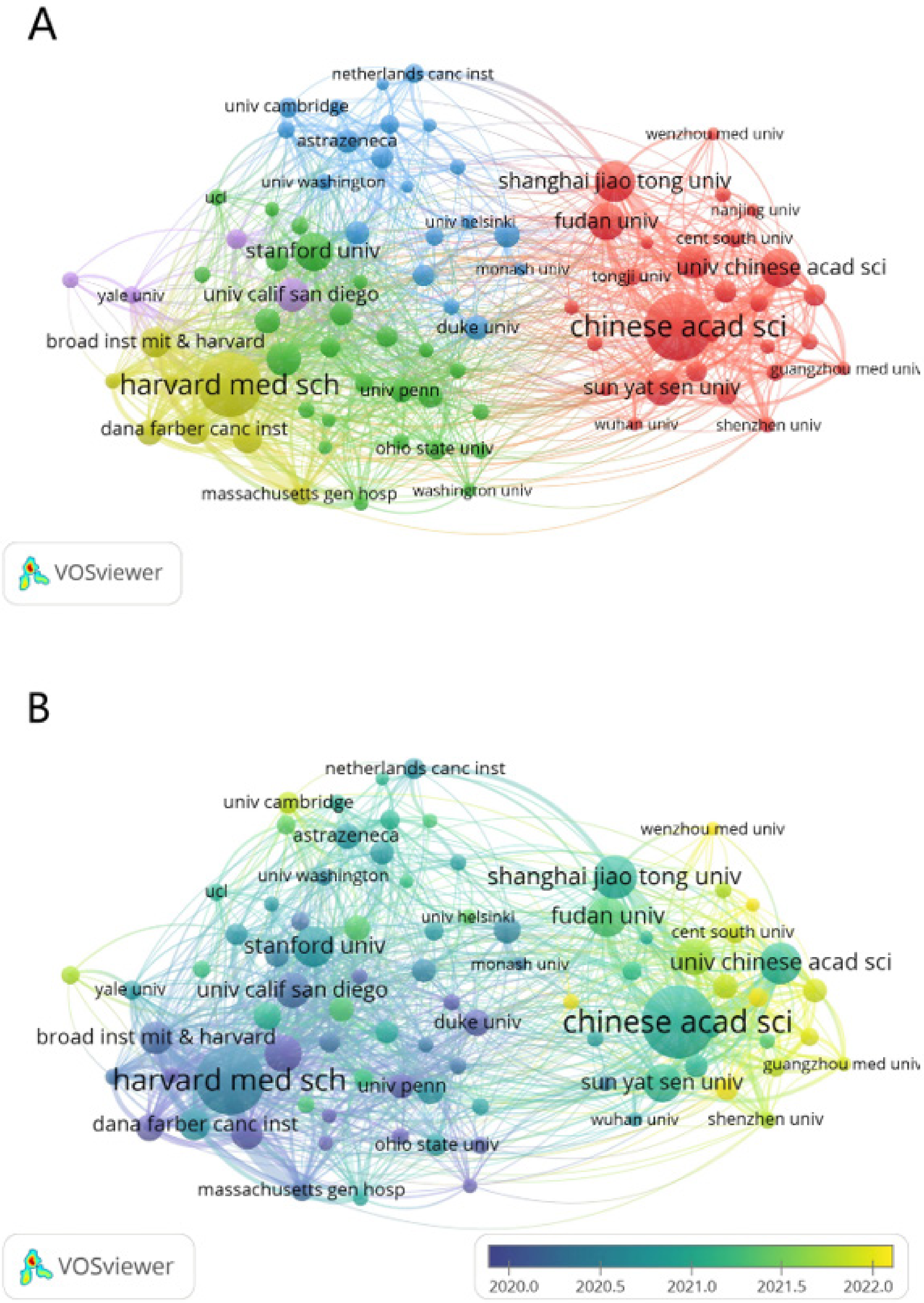


Figure 4: (A) The institutional clusters and co-occurrence network. (B) The institutional co-occurrence density map.

scholarly output and influence in this interdisciplinary field. European institutions are prominently represented, with Mathew J. Garnett (Wellcome Trust Sanger Institute, UK; 17 publications) and Roderick L. Beijersbergen (Netherlands Cancer Institute; 16 publications) ranking second and third, respectively.

A notable institutional clustering effect is evident. Harvard University and its affiliated Broad Institute account for five of the top ten authors, including Kimberly Stegmaier, William Hahn, and David E. Root, underscoring Harvard's collaborative and resource-rich research environment in CRISPR-related applications. Importantly, Navid Rabiee from the Saveetha Institute of Medical and Technical Sciences (India) stands

Table 2: The top 10 productive authors related to CRISPR-MD research.

Author	Count	Institution (Current)	Country/Region
Palermo, Giulia	30	University of California System,University of California Riverside	USA
Garnett, Mathew J.	17	Wellcome Trust Sanger Institute	UK
Beijersbergen, Roderick L	16	Netherlands Cancer Institute	Netherlands
Stegmaier, Kimberly	15	Harvard University, Harvard University Medical Affiliates;Boston Children's Hospital	USA
Lieftink, Cor	14	Netherlands Cancer Institute	Netherlands
Rabiee, Navid	14	Saveetha Institute of Medical & Technical Science, Saveetha Dental College & Hospital	India
Hahn, Willliam	14	Harvard University, Harvard University Medical Affiliates Brigham & Women's Hospital	USA
Root, David E.	13	Harvard University, Massachusetts Institute of Technology (MIT), Broad Institute	USA
Tsherniak, Aviad	13	Harvard University, Massachusetts Institute of Technology (MIT), Broad Institute	USA
Vazquez, Francisca	13	Harvard University, Massachusetts Institute of Technology (MIT), Broad Institute	USA

Table 3: Top 10 most cited authors in molecular docking and CRISPR genome editing research.

Rank	Cited Authors	Count	Centrality	Institution (Current)	Country/ Region
1	Jinek, Martin	776	0.16	University of Zurich Faculty of Medicine, Department of Biochemistry	Switzerland
2	Cong, Le	674	0.07	Stanford University School of Medicine, Department of Pathology	USA
3	F Ann Ran	577	0.09	Harvard University, Massachusetts Institute of Technology (MIT), Broad Institute	USA
4	Mali, Prashant	529	0.04	University of California San Diego Department of Bioengineering	USA
5	Shalem, Ophir	490	0.04	University of Pennsylvania Department of Genetics, Childrens Hospital of Philadelphia	USA
6	Hsu, Patrick D.	456	0	Ecole Polytechnique Federale de Lausanne, University of California Berkeley	Switzerland USA
7	Wang Ting	367	0.1	Washington University (WUSTL)	USA
8	Doudna, Jennifer A.	360	0.02	University of California Berkeley	USA
9	Barrangou, Rodolphe	351	0.06	North Carolina State University	USA
10	Doench, John G	338	0.02	Harvard University, Massachusetts Institute of Technology (MIT), Broad Institute	USA

out as the only scholar from a developing country among the top contributors, reflecting ongoing geographic disparities in research capacity and resource distribution.

Top Cited Authors

Co-citation analysis identifies key figures whose foundational studies have had a lasting impact on the field. As illustrated in Table 3, Martin Jinek (University of Zurich) leads with 776 citations, largely due to his groundbreaking work elucidating the CRISPR-Cas9 mechanism. He is followed by Le Cong (Stanford University; 674 citations) and F. Ann Ran (Harvard/MIT/Broad Institute; 577 citations), indicating the central role of USA institutions in foundational and technical advancements. Although Jennifer A. Doudna (University of California, Berkeley), a Nobel laureate in CRISPR research, ranks eighth with 360 citations, her influence extends far beyond citation metrics. Other frequently cited scholars, such as Prashant Mali, Patrick D. Hsu, and John G. Doench, represent key figures in genome editing tool development and functional genomic screening, reflecting the methodological integration of molecular docking within CRISPR-based applications.

Journal Co-Citation Analysis

Journal co-citation analysis serves as a powerful tool for mapping the intellectual structure and interdisciplinary connectivity of a research field. In the context of molecular docking in CRISPR genome editing, CiteSpace was employed to identify the most frequently co-cited journals, thereby revealing the foundational sources that shape scholarly discourse in this domain. As presented in Table 4, the top ten co-cited journals comprise high-impact, authoritative sources that collectively represent the core knowledge base of the field.

Nature emerged as the most frequently co-cited journal (3690), followed closely by the Proceedings of the National Academy of Sciences of the United States of America (3515), Science (3425), and *Cell* (3275). These premier journals are globally recognized for their scientific rigor and interdisciplinary scope, and they dominate the citation landscape in life sciences, biomedical research, and biotechnology. Notably, *Cell* exhibited the highest betweenness centrality (0.42), signifying its pivotal role in bridging various subfields within the research network.

Multidisciplinary journals such as Nature Communications (2925), Scientific Reports (2442), and Plos One (2546) also featured prominently, underscoring the integrative and collaborative nature of research at the intersection of gene editing and computational modeling. Furthermore, the inclusion of more specialized outlets such as Nucleic Acids Research (2470) and Nature Biotechnology (2436) emphasizes the critical roles played by structural genomics, nucleic acid chemistry, and molecular engineering in advancing the precision and functionality of CRISPR systems.

Importantly, all ten journals are indexed in the Q1 quartile of the Journal Citation Reports (JCR), affirming their academic prestige and influence. Among them, *Nature* (IF=50.5), *Science* (IF=44.8), and Nature Biotechnology (IF=33.1) demonstrated particularly high impact, reinforcing their status as primary vehicles for publishing groundbreaking research in CRISPR-MD. The high centrality of Cell further reflects its role as a hub for interdisciplinary exchange, particularly between experimental biology and emerging biotechnologies.

Figure 5 presents a journal co-citation network generated by CiteSpace, offering a comprehensive visualization of the disciplinary structure and knowledge diffusion within the field of CRISPR-based molecular docking from 2005 to 2024. Each node represents a distinct scholarly journal, with node size proportional to citation frequency and color gradient indicating the year of the strongest citation burst. Edges denote co-citation relationships, and their density reflects the degree of scholarly interconnectedness. The network highlights a well-defined cluster of journals that serve as the intellectual backbone of the field. High-impact, generalist journals such as Nature, Science,

Table 4: Top 10 co-cited journals in molecular docking and CRISPR genome editing research.

Rank	Cited Journal	Count	Centrality	Years	IF（2023）	JCR
1	Nature	3690	0.03	2009	50.5	Q1
2	Proceedings of the National Academy of Sciences of the United States of America (PNAS)	3515	0.05	2005	9.4	Q1
3	Science	3425	0.03	2005	44.8	Q1
4	Cell	3275	0.42	2006	5.1	Q1
5	Nature Communications	2925	0	2014	14.7	Q1
6	Plos One	2546	0.06	2011	2.9	Q1
7	Nucleic Acids Research	2470	0.38	2012	16.7	Q1
8	Scientific Reports	2442	0.01	2015	3.8	Q1
9	Nature Biotechnology	2436	0.03	2013	33.1	Q1
10	Journal of Biological Chemistry	2013	0.04	2005	4	Q1

Cell, and PNAS form a central core, both in terms of frequency and structural centrality. These high-impact journals exhibit strong citation bursts and centrality, indicating their foundational influence. The network also includes specialized journals like Nature Biotechnology and Nucleic Acids Research, reflecting the field's methodological diversity. A high silhouette score (0.9353) and strong modularity further suggest a coherent and robust disciplinary structure, shaped by both generalist and specialist publications. This structure reflects the maturity of the field and its continued evolution toward a highly integrated scientific ecosystem.

Co-Cited References and Citation Bursts

Co-citation analysis offers a lens into the intellectual structure and thematic development of literature at the intersection of and CRISPR-MD. As presented in Table 5, the top 10 co-cited references were identified by citation frequency. Among these, the most highly cited work is Le Cong *et al.* (2013), published in Science, with 220 citations-highlighting its foundational role in demonstrating multiplex genome engineering using CRISPR/Cas systems. Notably, three of the top five co-cited papers appeared in *Science* between 2013 and 2014, emphasizing the journal's pivotal role during the early phase of CRISPR research. Other prominent venues include Nature, Nature Biotechnology, and Cell, all of which contributed landmark publications that collectively constitute the field's core knowledge base.

Citation burst analysis further captures the dynamic influence of these publications over time. As shown in Figure 6, the strongest burst was observed in Cong *et al.* (2013) with a strength of 81.23, spanning from 2013 to 2018, indicating sustained scholarly attention. Similarly, works by Mali *et al.* (2013) and Jinek *et al.* (2012) exhibit high burst intensity, reflecting their critical role in the foundational development of CRISPR/Cas technologies. More recent bursts, such as those from Sung *et al.* (2021) and Frangoul *et al.* (2021), suggest an emerging shift toward translational and clinical applications.

Co-citation and burst analyses chart a clear trajectory in the field's evolution. Early influential studies concentrated on mechanism elucidation, sgRNA design, and the enhancement of genome editing fidelity (Jinek *et al.*, 2012; Cong *et al.*, 2013; Mali *et al.*, 2013). This laid a robust technical groundwork for subsequent large-scale functional screening and drug target discovery (Shalem *et al.*, 2014; Behan *et al.*, 2019), marking a pivotal shift toward translational research.

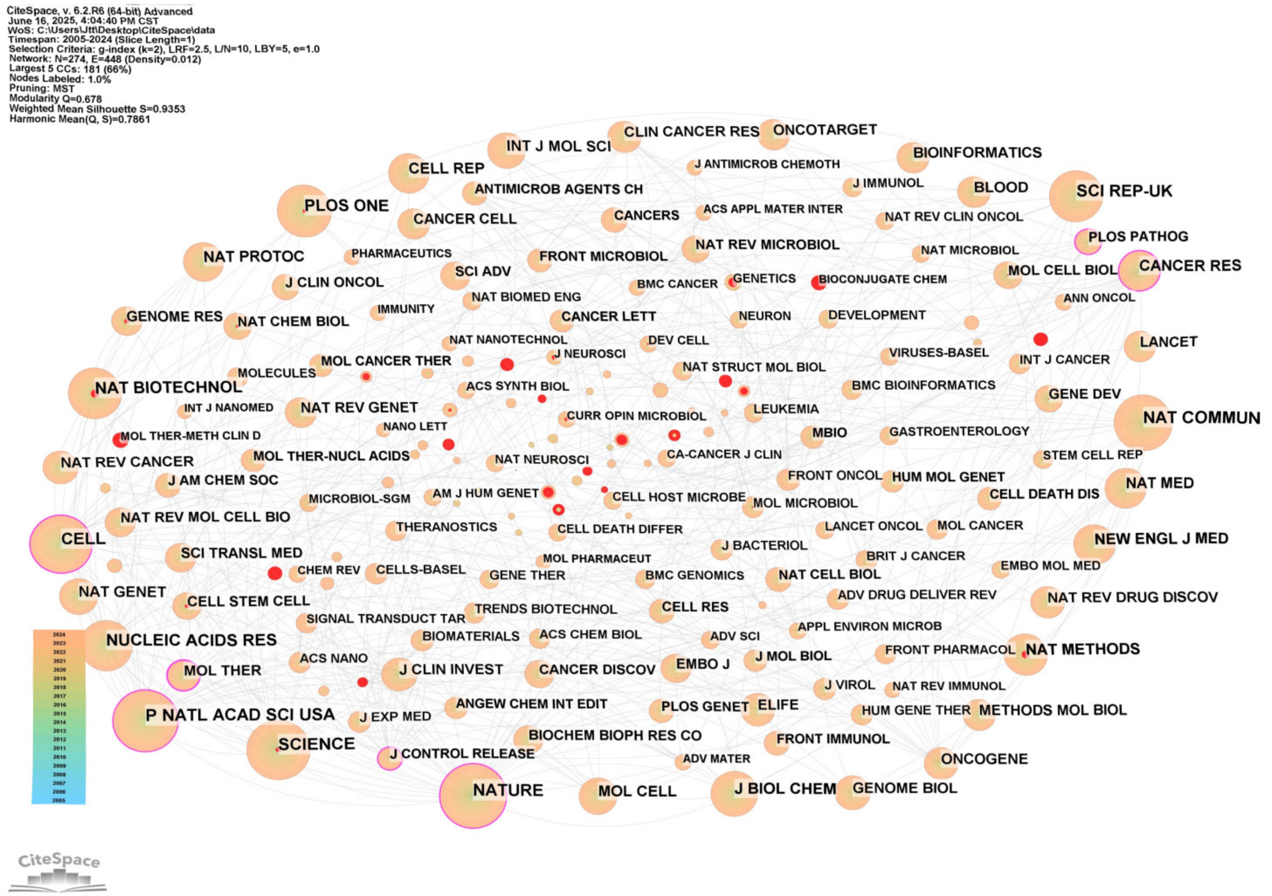
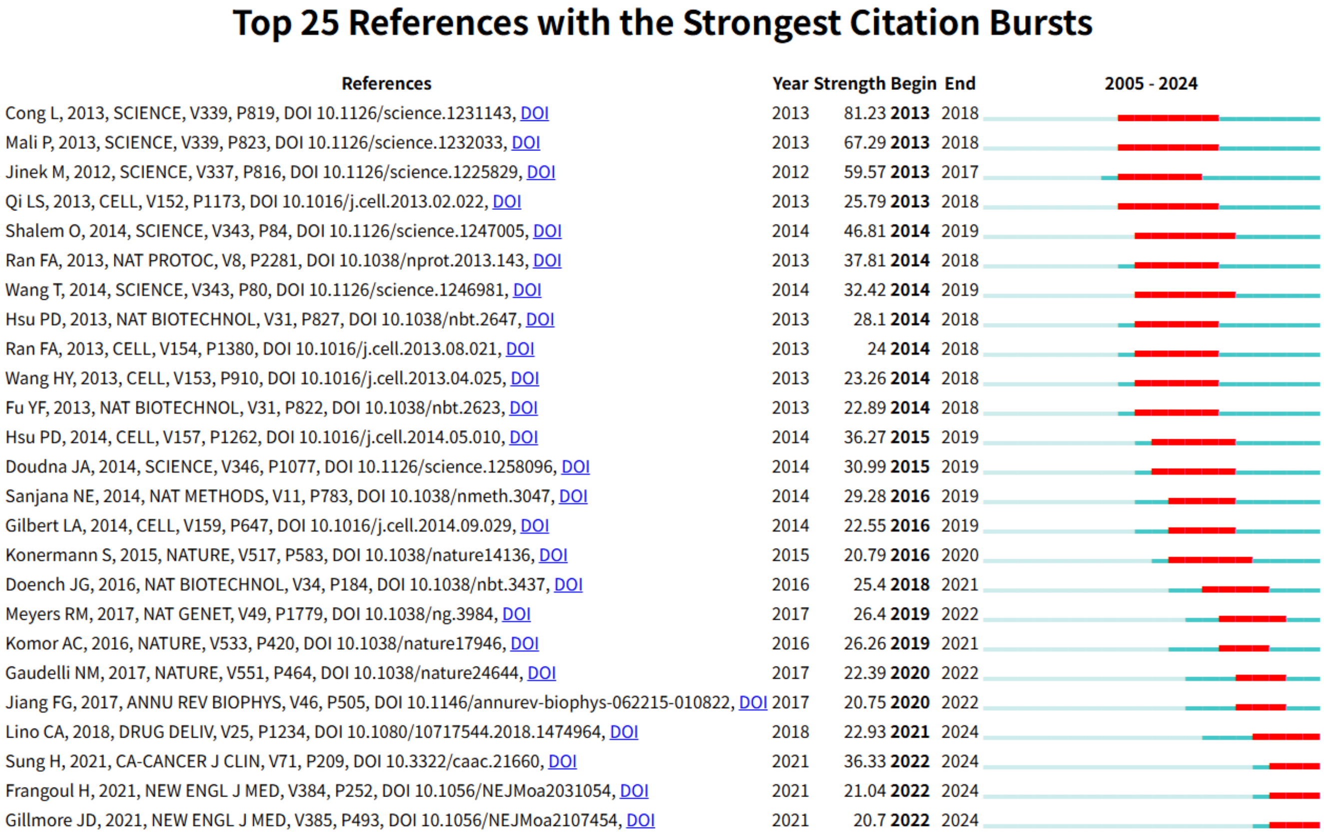


Figure 5: Network map of cited journals generated by CiteSpace. Each node represents a distinct journal, with node size proportional to citation frequency. Red indicates citation burst periods; denser edges reflect stronger co-citation ties.



Top 25 References with the Strongest Citation Bursts

References	Year	Strength	Begin	End	2005 - 2024
Cong L, 2013, SCIENCE, V339, P819, DOI 10.1126/science.1231143, DOI	2013	81.23	**2013**	2018	
Mali P, 2013, SCIENCE, V339, P823, DOI 10.1126/science.1232033, DOI	2013	67.29	**2013**	2018	
Jinek M, 2012, SCIENCE, V337, P816, DOI 10.1126/science.1225829, DOI	2012	59.57	**2013**	2017	
Qi LS, 2013, CELL, V152, P1173, DOI 10.1016/j.cell.2013.02.022, DOI	2013	25.79	**2013**	2018	
Shalem O, 2014, SCIENCE, V343, P84, DOI 10.1126/science.1247005, DOI	2014	46.81	**2014**	2019	
Ran FA, 2013, NAT PROTOC, V8, P2281, DOI 10.1038/nprot.2013.143, DOI	2013	37.81	**2014**	2018	
Wang T, 2014, SCIENCE, V343, P80, DOI 10.1126/science.1246981, DOI	2014	32.42	**2014**	2019	
Hsu PD, 2013, NAT BIOTECHNOL, V31, P827, DOI 10.1038/nbt.2647, DOI	2013	28.1	**2014**	2018	
Ran FA, 2013, CELL, V154, P1380, DOI 10.1016/j.cell.2013.08.021, DOI	2013	24	**2014**	2018	
Wang HY, 2013, CELL, V153, P910, DOI 10.1016/j.cell.2013.04.025, DOI	2013	23.26	**2014**	2018	
Fu YF, 2013, NAT BIOTECHNOL, V31, P822, DOI 10.1038/nbt.2623, DOI	2013	22.89	**2014**	2018	
Hsu PD, 2014, CELL, V157, P1262, DOI 10.1016/j.cell.2014.05.010, DOI	2014	36.27	**2015**	2019	
Doudna JA, 2014, SCIENCE, V346, P1077, DOI 10.1126/science.1258096, DOI	2014	30.99	**2015**	2019	
Sanjana NE, 2014, NAT METHODS, V11, P783, DOI 10.1038/nmeth.3047, DOI	2014	29.28	**2016**	2019	
Gilbert LA, 2014, CELL, V159, P647, DOI 10.1016/j.cell.2014.09.029, DOI	2014	22.55	**2016**	2019	
Konermann S, 2015, NATURE, V517, P583, DOI 10.1038/nature14136, DOI	2015	20.79	**2016**	2020	
Doench JG, 2016, NAT BIOTECHNOL, V34, P184, DOI 10.1038/nbt.3437, DOI	2016	25.4	**2018**	2021	
Meyers RM, 2017, NAT GENET, V49, P1779, DOI 10.1038/ng.3984, DOI	2017	26.4	**2019**	2022	
Komor AC, 2016, NATURE, V533, P420, DOI 10.1038/nature17946, DOI	2016	26.26	**2019**	2021	
Gaudelli NM, 2017, NATURE, V551, P464, DOI 10.1038/nature24644, DOI	2017	22.39	**2020**	2022	
Jiang FG, 2017, ANNU REV BIOPHYS, V46, P505, DOI 10.1146/annurev-biophys-062215-010822, DOI	2017	20.75	**2020**	2022	
Lino CA, 2018, DRUG DELIV, V25, P1234, DOI 10.1080/10717544.2018.1474964, DOI	2018	22.93	**2021**	2024	
Sung H, 2021, CA-CANCER J CLIN, V71, P209, DOI 10.3322/caac.21660, DOI	2021	36.33	**2022**	2024	
Frangoul H, 2021, NEW ENGL J MED, V384, P252, DOI 10.1056/NEJMoa2031054, DOI	2021	21.04	**2022**	2024	
Gillmore JD, 2021, NEW ENGL J MED, V385, P493, DOI 10.1056/NEJMoa2107454, DOI	2021	20.7	**2022**	2024	

Figure 6: Top 25 references with the strongest citation bursts. Blue bars denote the publication timeline, while red bars represent periods of citation bursts.

Recent citation bursts underscore the growing importance of next-generation editing modalities, such as base editing and prime editing, which bypass double-stranded breaks and improve precision (Komor *et al.*, 2016; Anzalone *et al.*, 2019). At the same time, clinical milestone studies, especially in oncology and hematology (Frangoul *et al.*, 2021; Gillmore *et al.*, 2021), reflect the field's increasing focus on real-world therapeutic application.

DISCUSSION

Emerging Trends and Challenges

From the VOSviewer keywords cluster analysis (Figure 7), MD predominantly appears in the context of drug discovery and bioinformatics (blue clusters), indicating its strong integration into *in silico* screening strategies. Although it has already demonstrated promising results in preclinical modeling, the field still requires further refinement in accuracy and predictive reliability. Meanwhile, CRISPR technologies such as CRISPR-Cas9, CRISPR-Cas12a, and CRISPR, are clustered separately (mainly in green and yellow clusters), with high publication and citation counts, reflecting their rapid expansion and maturity as gene-editing platforms across various biomedical domains.

The keyword analysis, generated using CiteSpace, reveals prominent research trends at the intersection of CRISPR-MD. The top 20 keywords, ranked by frequency and centrality in CRISPR genome editing research incorporating MD approaches, are presented in Table 6. The five most frequently occurring keywords were expression (count=769), cells (count=368), activation (count=356), cancer (count=346), and identification (count=342). Notably, activation demonstrated the highest centrality (0.16), indicating its pivotal role as a bridging concept across studies. Figure 8 displays the keyword co-occurrence network, where node size corresponds to keyword frequency, illustrating conceptual connections between MD applications and CRISPR technology development.

Figure 9 shows the timeline visualization of keyword evolution in molecular docking-assisted CRISPR genome editing research from 2005 to 2024. The temporal analysis reveals distinct research phases and paradigm shifts, organized by CiteSpace-generated clusters (a silhouette score > 0.7 indicates high homogeneity). As shown in Figure 8, most keywords are clustered after 2008. We found that "focal adhesion kinase" (cluster 4) and "gene therapy" (cluster 6) were relatively early research hotspots. The emergence of "synthetic lethality" (cluster 8) and "protein degradation" (cluster 9) in 2020 marks the mature application of CRISPR docking in precision medicine. Interestingly, the clustering topics of "drug discovery" (cluster 5) and "prostate cancer" (cluster 8) are currently new hotspots and directions in this field. From early structural analysis (before 2015) to therapeutic applications (after

Table 5: Top 10 Co-cited references in molecular docking and CRISPR genome editing research.

Rank	Title	Author	Publication Year	Source	Citation
1	Multiplex Genome Engineering Using CRISPR/Cas Systems	Le Cong *et al.*	2013	Science	220
2	RNA-Guided Human Genome Engineering via Cas9	Prashant Mali *et al.*	2013	Science	183
3	Genome-Scale CRISPR-Cas9 Knockout Screening in Human Cells	Ophir Shalem *et al.*	2014	Science	168
4	Search-and-replace genome editing without double-strand breaks or donor DNA	Andrew V Anzalone *et al.*	2019	Nature	159
5	Prioritization of cancer therapeutic targets using CRISPR–Cas9 screens	Fiona M Behan *et al.*	2019	Nature	136
6	Optimized sgRNA design to maximize activity and minimize off-target effects of CRISPR-Cas9	John G Doench *et al.*	2016	Nature Biotechnology	134
7	Development and Applications of CRISPR-Cas9 for Genome Engineering	Patrick D Hsu *et al.*	2014	Cell	125
8	Programmable editing of a target base in genomic DNA without double-stranded DNA cleavage	Alexis C Komor *et al.*	2016	Nature	124
9	A Programmable Dual-RNA–Guided DNA Endonuclease in Adaptive Bacterial Immunity	Martin Jinek *et al.*	2012	Science	122
10	Genetic Screens in Human Cells Using the CRISPR-Cas9 System	Tim Wang *et al.*	2014	Science	117

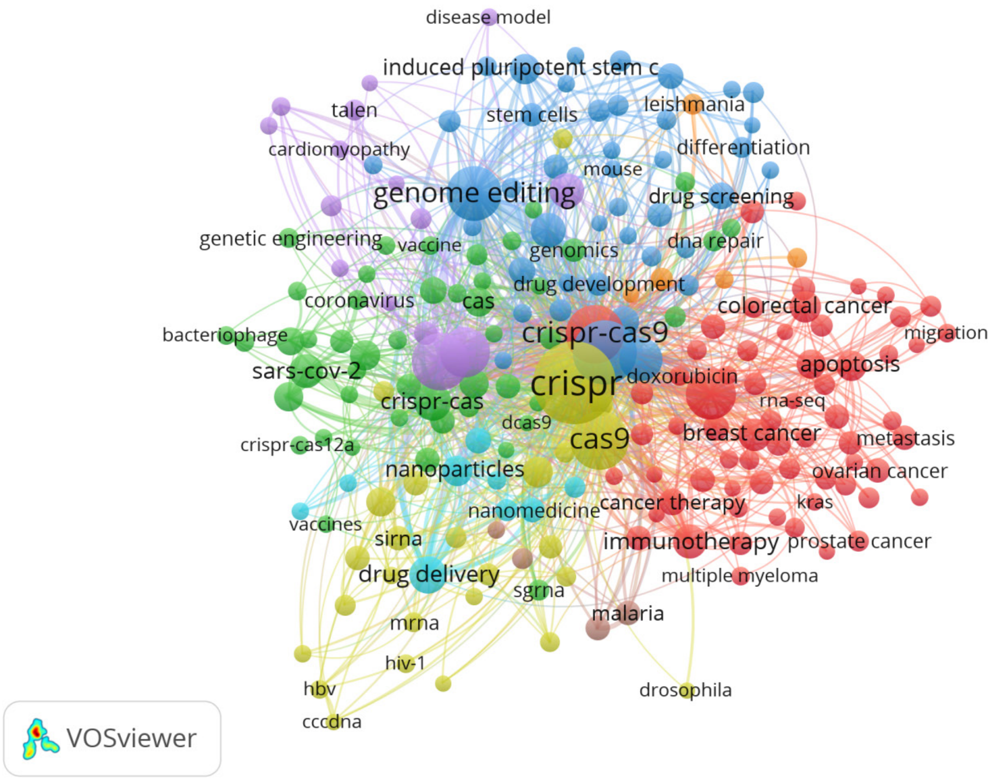


Figure 7: The co-occurrence network and clusters of keywords related to CRISPR-MD research. Minimum number of occurrences of keywords≥10.

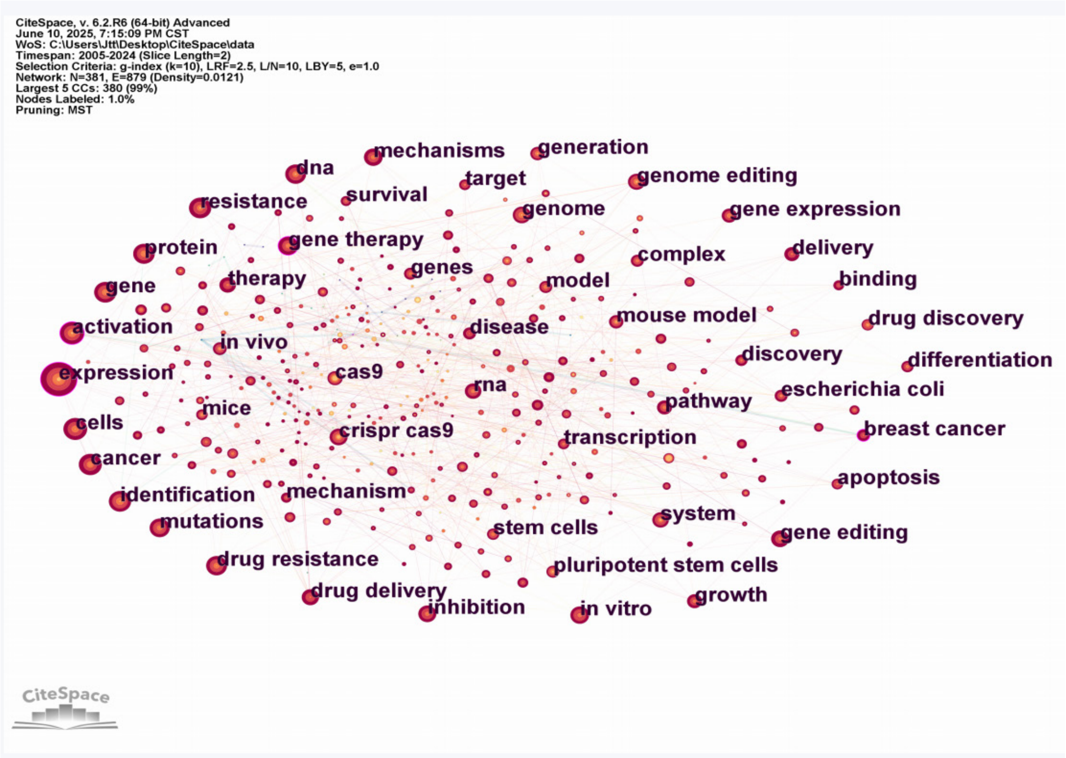


Figure 8: Network map of keywords from CiteSpace. Each node represents a distinct keyword, with node size proportional to the keyword's frequency.

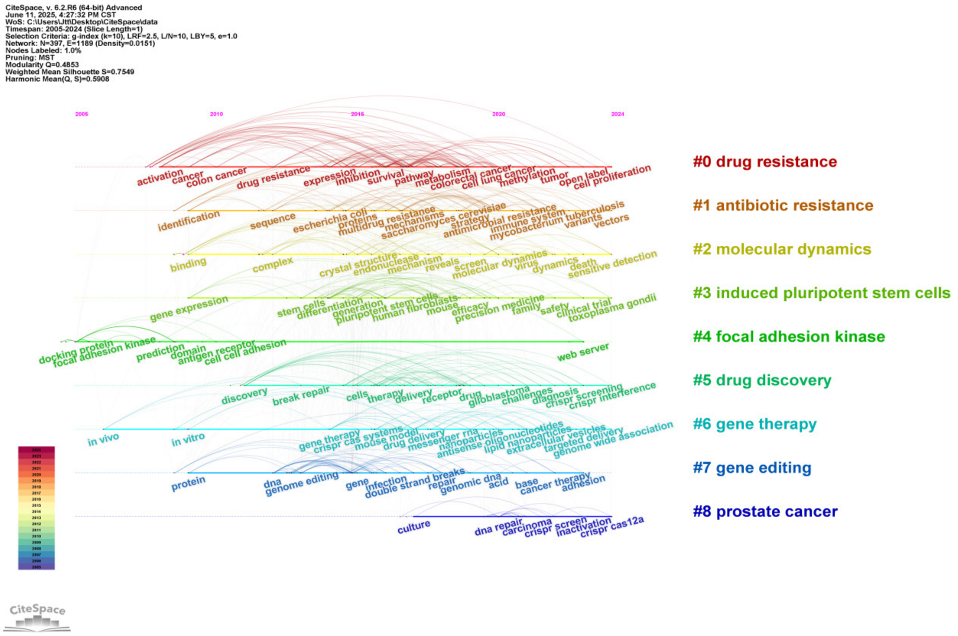
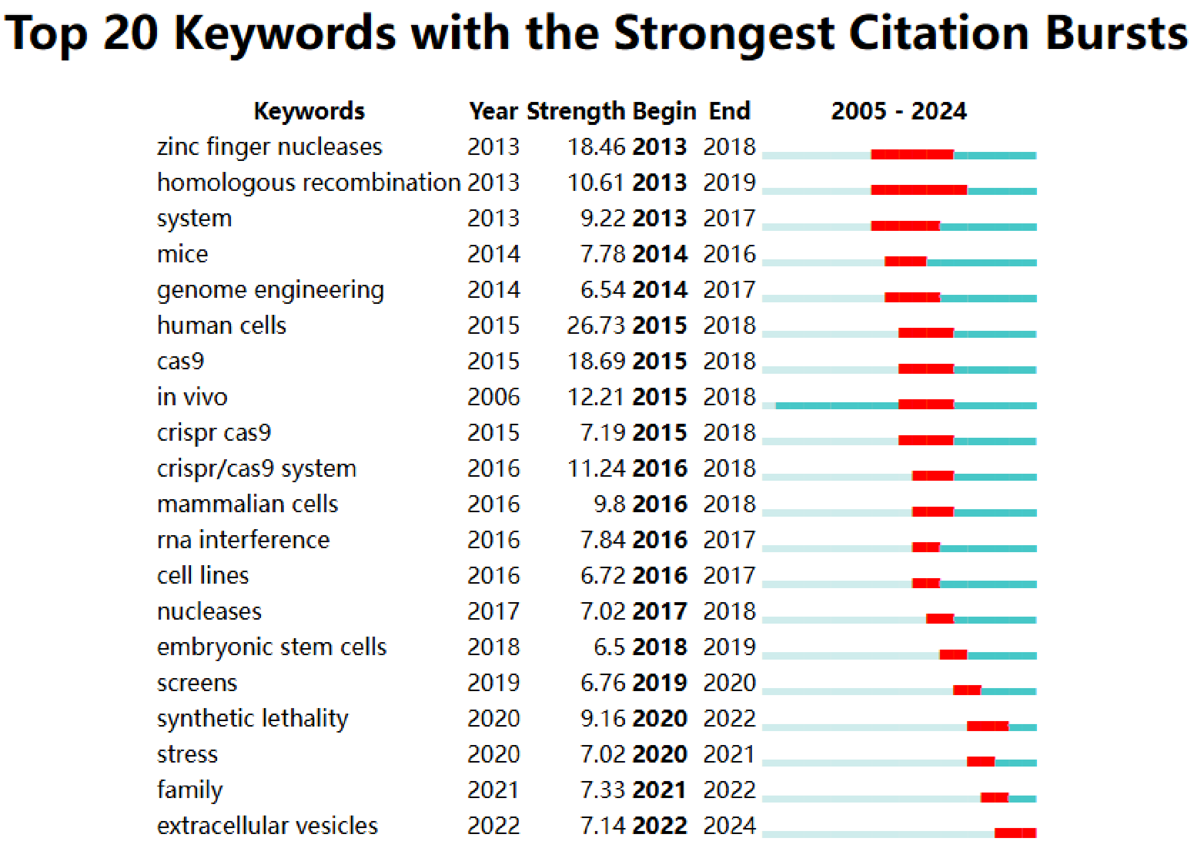


Figure 9: Timeline view of keywords related to molecular docking in CRISPR genome editing research.

2016), molecular docking has gradually become a core tool for CRISPR off-target evaluation and delivery vector optimization.

Figure 10 illustrates the keyword burst detection results for research on CRISPR-MD. The burst detection analysis reveals the evolving research hotspots at the intersection of molecular docking and CRISPR gene editing from 2005 to 2024. Burst strength reflects the intensity of a sudden increase in a keyword's influence, while the time span (Begin-End) indicates the active period of the keyword. Notably, cas9 emerged as a keyword in 2015 with a burst strength of 18.69, active from 2015 to 2018, indicating the rapid development of this technology. The CRISPR/Cas9 system reached a high burst strength of 11.24 in 2016, with an active period from 2016 to 2018, highlighting the



Top 20 Keywords with the Strongest Citation Bursts

Keywords	Year	Strength	Begin	End	2005 - 2024
zinc finger nucleases	2013	18.46	**2013**	2018	
homologous recombination	2013	10.61	**2013**	2019	
system	2013	9.22	**2013**	2017	
mice	2014	7.78	**2014**	2016	
genome engineering	2014	6.54	**2014**	2017	
human cells	2015	26.73	**2015**	2018	
cas9	2015	18.69	**2015**	2018	
in vivo	2006	12.21	**2015**	2018	
crispr cas9	2015	7.19	**2015**	2018	
crispr/cas9 system	2016	11.24	**2016**	2018	
mammalian cells	2016	9.8	**2016**	2018	
rna interference	2016	7.84	**2016**	2017	
cell lines	2016	6.72	**2016**	2017	
nucleases	2017	7.02	**2017**	2018	
embryonic stem cells	2018	6.5	**2018**	2019	
screens	2019	6.76	**2019**	2020	
synthetic lethality	2020	9.16	**2020**	2022	
stress	2020	7.02	**2020**	2021	
family	2021	7.33	**2021**	2022	
extracellular vesicles	2022	7.14	**2022**	2024	

Figure 10: Keywords burst detection for the study.

swift progress of the CRISPR technology system. Additionally, CRISPR Cas9 was developed in 2015 with a burst strength of 7.19, underscoring the significance of CRISPR in the field of gene editing.

Keywords such as "zinc finger nucleases" and "homologous recombination" emerged in 2013 with burst strengths of 18.46 and 10.61, respectively, and remained active from 2013 to 2018. These represent early technologies and innovations in gene editing, laying the foundation for the subsequent development of CRISPR technology. The keyword "nucleases" also emerged in 2017 with a burst strength of 7.02, reflecting the application of enzymes in gene editing. In summary, research interest in MD and CRISPR technology gradually increased from 2013 to 2024, with notable growth between 2015 and 2016. During this period, CRISPR-related keywords and gene editing technologies received widespread attention, with MD playing a significant role in this process.

Challenges of the CRISPR Technologies

Despite significant advancements, several persistent challenges continue to hinder the full translational potential of CRISPR genome editing, including off-target effects, variable editing efficiency, and limitations in delivery and specificity (Hwang *et al.*, 2023). To address these issues, enhanced and sophisticated computational support is as crucial as experimental innovation. Through structural and thermodynamic modeling, molecular docking has become a viable method for optimizing CRISPR components, including Cas proteins, guide RNAs, and regulatory inhibitors.

This strategy has been demonstrated by recent research. Li *et al.* (2020) used dynamics simulations and molecular docking to find tiny compounds that might stabilize the Cas12a-crRNA complex and increase the effectiveness of genome editing. Similarly, using docking analysis, Ke *et al.* (2022) showed that 2′-O-methyl modifications in gRNAs greatly increased CRISPR-Cas12a specificity by changing binding affinity. Furthermore, docking models have been used to structurally characterize anti-CRISPR proteins like AcrIIC5 in order to clarify their inhibitory processes (Hwang *et al.*, 2023), indicating therapeutic promise for gene-editing regulation. The development of quantum computing algorithms, like the quantum approximate optimization algorithm (QAOA), offers the possibility of overcoming constraints in high-dimensional search spaces, enabling more precise and effective prediction of CRISPR component interactions.

Nevertheless, current research remains fragmented, often focusing on isolated applications such as gRNA optimization or small-molecule screening, without a comprehensive synthesis of the field's intellectual structure or its emerging interdisciplinary connections. To accelerate translational impact, future

Table 6: Top 20 keywords ranked by frequency and centrality.

Rank	Keywords	Count	Centrality	Rank	Keywords	Count	Centrality
1	expression	769	0.15	11	drug resistance	280	0.07
2	cells	368	0.04	12	gene therapy	253	0.1
3	activation	356	0.16	13	*in vitro*	251	0.07
4	cancer	346	0.06	14	genome	239	0.03
5	identification	342	0.07	15	gene editing	230	0.03
6	gene	332	0.03	16	inhibition	220	0.03
7	resistance	317	0.06	17	rna	220	0.05
8	protein	302	0.01	18	genome editing	215	0.03
9	dna	287	0.08	19	mechanisms	215	0.04
10	mutations	283	0.03	20	drug delivery	214	0.07

research should strategically integrate advanced computational methodologies, such as QAOA with high-throughput screening and synthetic biology platforms. This study provides a thorough overview of how molecular docking is being utilized to enhance CRISPR technologies and offers strategic insights for future research and policy development aimed at harnessing these tools for biomedical innovation and translational impact.

CONCLUSION

The integration of MD with CRISPR genome editing represents a transformative shift from tool development toward application-oriented, interdisciplinary convergence. This study employs scientometric analysis to map the intellectual landscape of this evolving field, which highlights key publication trends, influential journals and authors, collaborative networks, and topic hotspots.

There is a noticeable change in the keywords and citation burst analysis. The research focus from foundational studies on Cas9 mechanisms and sgRNA design to advanced topics such as drug discovery, synthetic lethality, and precision medicine. Journals with high centrality, including Cell, Nature, and Science, highlight the foundational role of structural biology and computational modeling in the development of genome editing techniques.

Despite its growing significance, systematic scientometric studies investigating the convergence of CRISPR-MD remain limited. Future research should prioritize the development of integrative databases and knowledge graphs that connect the structural features of CRISPR systems with docking-based computational outputs, thereby enabling meta-analyses and predictive modeling. Furthermore, AI-enhanced MD has great potential to further personalized genome editing techniques, optimize sgRNA design, and improve off-target risk assessment.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interest.

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REFERENCES

An, X., Zhang, S., Jiang, Y., Liu, X., Fang, C., Wang, J., Zhao, L., Hou, Q., Zhang, J., & Wan, X. (2024). CRISPR/Cas9-based genome editing of 14 lipid metabolic genes reveals a sporopollenin metabolon ZmPKSB-ZmTKPR1-1/-2 required for pollen exine formation in maize. Plant Biotechnology Journal, 22(1), 216–232. https://doi.org/10.1111/pbi.14181

Anzalone, A. V., Randolph, P. B., Davis, J. R., Sousa, A. A., Koblan, L. W., Levy, J. M., Chen, P. J., Wilson, C., Newby, G. A., Raguram, A., & Liu, D. R. (2019). Search-and-replace genome editing without double-strand breaks or donor DNA. Nature, 576(7785), 149–157. https://doi.org/10.1038/s41586-019-1711-4

Behan, F. M., Iorio, F., Picco, G., Gonçalves, E., Beaver, C. M., Migliardi, G., Santos, R., Rao, Y., Sassi, F., Pinnelli, M., Ansari, R., Harper, S., Jackson, D. A., McRae, R., Pooley, R., Wilkinson, P., van der Meer, D., Dow, D., Buser-Doepner, C., Garnett, M. J. (2019). Prioritization of cancer therapeutic targets using CRISPR–Cas9 screens. Nature, 568(7753), 511–516. https://doi.org/10.1038/s41586-019-1103-9

Bhattacharya, S., & Satpati, P. (2022). Insights into the mechanism of CRISPR/Cas9-based genome editing from molecular dynamics simulations. ACS Omega, 8(2), 1817–1837. https://doi.org/10.1021/acsomega.2c05583

Breinig, M., Schweitzer, A. Y., Herianto, A. M., Revia, S., Schaefer, L., Wendler, L., Cobos Galvez, A., & Tschaharganeh, D. F. (2019). Multiplexed orthogonal genome editing and transcriptional activation by Cas12a. Nature Methods, 16(1), 51–54. https://doi.org/10.1038/s41592-018-0262-1

Cong, L., Ran, F. A., Cox, D., Lin, S., Barretto, R., Habib, N., Hsu, P. D., Wu, X., Jiang, W., Marraffini, L. A., & Zhang, F. (2013). Multiplex genome engineering using CRISPR/Cas systems. Science, 339(6121), 819–823. https://doi.org/10.1126/science.1231143

Fasching, C. L., Servellita, V., McKay, B., Nagesh, V., Broughton, J. P., Sotomayor-Gonzalez, A., Wang, B., Brazer, N., Reyes, K., Streithorst, J., Deraney, R. N., Stanfield, E., Hendriks, C. G., Fung, B., Miller, S., Ching, J., Chen, J. S., & Chiu, C. Y. (2022). COVID-19 variant detection with a high-fidelity CRISPR-Cas12 enzyme. Journal of Clinical Microbiology, 60(7), Article e0026122. https://doi.org/10.1128/jcm.00261-22

Figueroa, W., Cazares, A., Cazares, D., Wu, Y., de la Cruz, A., Welch, M., Kameyama, L., Nobrega, F. L., & Guarneros, G. (2023). Distribution and molecular evolution of the anti-CRISPR family AcrIF7. PLOS Biology, 21(4), Article e3002072. https://doi.org/10.1371/journal.pbio.3002072

Frangoul, H., Altshuler, D., Cappellini, M. D., Chen, Y.-S., Domm, J., Eustace, B. K., Foell, J., de la Fuente, J., Grupp, S., Handgretinger, R., Ho, T. W., Kattamis, A., Kernytsky, A., Lekstrom-Himes, J., Li, A. M., Locatelli, F., Mapara, M. Y., de Montalembert, M., Rondelli, D., Corbacioglu, S. (2021). CRISPR-Cas9 gene editing for sickle cell disease and β-thalassemia. The New England Journal of Medicine, 384(3), 252–260. https://doi.org/10.1056/NEJMoa2031054

Fu, B., Chen, M., Bao, X., Lu, J., Zhu, Z., Guan, F., Yan, C., Wang, P., Fu, L., & Yu, P. (2024). Site-directed mutagenesis of bifunctional riboflavin kinase/FMN adenylyltransferase via CRISPR/Cas9 to enhance riboflavin production. Synthetic and Systems Biotechnology, 9(3), 503–512. https://doi.org/10.1016/j.synbio.2024.04.011

Gillmore, J. D., Gane, E., Taubel, J., Kao, J., Fontana, M., Maitland, M. L., Seitzer, J., O'Connell, D., Walsh, K. R., Wood, K., Phillips, J., Xu, Y., Amaral, A., Boyd, A. P., Cehelsky, J. E., McKee, M. D., Schiermeier, A., Harari, O., Murphy, A., Lebwohl, D. (2021). CRISPR-Cas9 *in vivo* gene editing for transthyretin amyloidosis. The New England Journal of Medicine, 385(6), 493–502. https://doi.org/10.1056/NEJMoa2107454

Halmi, M. F. A., Zulkifli, M. A. F., & Zaman, K. H. K. (2023). CRISPR-Cas9 genome editing: A brief scientometric insight on scientific production and knowledge structure. Journal of Scientometric Research, 12(2), 395–402. https://doi.org/10.5530/jscires.12.2.035

Hwang, S., Shah, M., Garcia, B., Hashem, N., Davidson, A. R., Moraes, T. F., & Maxwell, K. L. (2023). Anti-CRISPR protein AcrIIC5 inhibits CRISPR-Cas9 by occupying the target DNA binding pocket. Journal of Molecular Biology, 435(7), Article 167991. https://doi.org/10.1016/j.jmb.2023.167991

Iryanto, A. P., Christy, C., Ewaldo, M. F., Prasetyoputri, A., Ningrum, R. A., Putranto, R. A., & Atikana, A. (2022). *In silico* design and validation of CRISPR-Cas13a system as a potential antiviral for SARS-CoV-2 in Indonesia. Nusantara Science and Technology Proceedings, 44–51. https://doi.org/10.11594/nstp.2022.2107

Jiang, C., Zou, D., Jiang, X., Han, W., Chen, K., Ma, A., & Wei, X. (2024). Enhancement of green production of heme by deleting odor-related genes from Bacillus amyloliquefaciens based on CRISPR/Cas9n. Journal of Agricultural and Food Chemistry, 72(29), 16412–16422. https://doi.org/10.1021/acs.jafc.4c04521

Jinek, M., Chylinski, K., Fonfara, I., Hauer, M., Doudna, J. A., & Charpentier, E. (2012). A programmable dual-RNA–guided DNA endonuclease in adaptive bacterial immunity. Science, 337(6096), 816–821. https://doi.org/10.1126/science.1225829

Ke, Y., Ghalandari, B., Huang, S., Li, S., Huang, C., Zhi, X., Cui, D., & Ding, X. (2022). 2′-O-methyl modified guide RNA promotes the single nucleotide polymorphism (SNP) discrimination ability of CRISPR–Cas12a systems. Chemical Science, 13(7), 2050–2061. https://doi.org/10.1039/D1SC06832F

Komor, A. C., Kim, Y. B., Packer, M. S., Zuris, J. A., & Liu, D. R. (2016). Programmable editing of a target base in genomic DNA without double-stranded DNA cleavage. Nature, 533(7603), 420–424. https://doi.org/10.1038/nature17946

Li, W., Chan, C., Zeng, C., Turk, R., Behlke, M. A., Cheng, X., & Dong, Y. (2020). Rational design of small molecules to enhance genome editing efficiency by selectively targeting distinct functional states of CRISPR-Cas12a. Bioconjugate Chemistry, 31(3), 542–546. https://doi.org/10.1021/acs.bioconjchem.0c00062

Liu, X.-L., Xie, J., Xie, Z.-N., Zhong, C., Liu, H., Zhang, S.-H., & Jin, J. (2024). Identification of squalene epoxidase in triterpenes biosynthesis in Poria cocos by molecular docking and CRISPR-Cas9 gene editing. Microbial Cell Factories, 23(1), Article 34. https://doi.org/10.1186/s12934-024-02306-3

Liu, Z., Liu, Y., Zeng, G., Shao, B., Chen, M., Li, Z., Jiang, Y., Liu, Y., Zhang, Y., & Zhong, H. (2018). Application of molecular docking for the degradation of organic pollutants in the environmental remediation: A review. Chemosphere, 203, 139–150. https://doi.org/10.1016/j.chemosphere.2018.03.179

Mali, P., Yang, L., Esvelt, K. M., Aach, J., Guell, M., DiCarlo, J. E., Norville, J. E., & Church, G. M. (2013). RNA-guided human genome engineering via Cas9. Science, 339(6121), 823–826. https://doi.org/10.1126/science.1232033

The Nobel Prize. (2020)[OL]. Nobel Prize in Chemistry. Retrieved 2025/6/18, https://www.nobelprize.org/prizes/chemistry/2020/prize-announcement/

Park, H.-M., Won, J., Park, Y., Anzaku, E. T., Vankerschaver, J., Van Messem, A., De Neve, W., & Shim, H. (2023). CRISPR-Cas-Docker: Web-based *in silico* docking and machine learning-based classification of crRNAs with Cas proteins. BMC Bioinformatics, 24(1), Article 167. https://doi.org/10.1186/s12859-023-05296-y

Shalem, O., Sanjana, N. E., Hartenian, E., Shi, X., Scott, D. A., Mikkelson, T., Heckl, D., Ebert, B. L., Root, D. E., Doench, J. G., & Zhang, F. (2014). Genome-scale CRISPR-Cas9 knockout screening in human cells. Science, 343(6166), 84–87. https://doi.org/10.1126/science.1247005

Strzyz P. CRISPR–Cas9 wins nobel. (2020). Nature Reviews Molecular Cell Biology, 21(12), 714–714

Sun, Y., Lu, H., Fang, X., Xiao, S., Yang, F., Chen, Y., Wang, H., Li, X., Lu, J., Lin, H., Luo, C., Zhao, K., & Chen, S. (2021). Discovery of a novel 53BP1 inhibitor through AlphaScreen-based high-throughput screening. Bioorganic and Medicinal Chemistry, 34, Article 116054. https://doi.org/10.1016/j.bmc.2021.116054

Sung, H., Ferlay, J., Siegel, R. L., Laversanne, M., Soerjomataram, I., Jemal, A., & Bray, F. (2021). Global cancer statistics 2020: GLOBOCAN estimates of incidence and mortality worldwide for 36 cancers in 185 countries. CA: A Cancer Journal for Clinicians, 71(3), 209–249. https://doi.org/10.3322/caac.21660

United States Food and Drug Administration. (2023/08/12). FDA approves first gene therapies to treat patients with sickle cell disease. Retrieved 2025/6/18, https://www.fda.gov/news-events/press-announcements/fda-approves-first-gene-therapies-treat-patients-sickle-cell-disease

Yang, H., & Patel, D. J. (2024). Structures, mechanisms and applications of RNA-centric CRISPR–Cas13. Nature Chemical Biology, 20(6), 673–688. https://doi.org/10.1038/s41589-024-01593-6

Zhu, H., Li, C., & Gao, C. (2020). Applications of CRISPR–Cas in agriculture and plant biotechnology. Nature Reviews. Molecular Cell Biology, 21(11), 661–677. https://doi.org/10.1038/s41580-020-00288-9.

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