Moroccan Journal of Chemistry
ISSN: 2351-812X
http://revues.imist.ma/?journal=morjchem&page=login
Saputra & al. / Mor. J. Chem. 10 N°1 (2022) 037-049
DOI: https://doi.org/10.48317/IMIST.PRSM/morjchem-v10i1.31723

Bibliometric Analysis of Computational Chemistry Research and Its Correlation with Covid-19 Pandemic

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Received 30 0ct 2021,
Revised 03 Nov 2021,
Accepted 02 April 2022

Abstract

Computational Chemistry is a branch of chemistry that employs computer simulations to assist in resolving problems regarding chemistry. The goal of this research is to combine mapping analysis from VOSviewer software to analyze bibliometrics in Computational Chemistry field. The data were obtained through the use of a reference manager application with "Computational Chemistry" as the keyword. We collected 1000 articles published between 2017 - 2021 in the search results. According to the findings, research in the field of Computational Chemistry decreased from 2018 to 2020, but increased since 2021. The primary reason for this is that the pandemic has had a significant impact on Computational Chemistry, which is related to laboratory engineering and molecular modeling. This study demonstrates the value of bibliometric analysis in providing analytical data about a phenomenon. The findings of this study are beneficial for future research to find potential areas of Computational Chemistry that can be studied further, due to the discovery of less-researched areas.

Keywords: *Computational Chemistry, Bibliometric, VOSviewer, Data Analysis, Database.*

1. Introduction

Chemistry has long been recognized as a science based on various experiments, as all scientific explanations described are always based on experimental results. After observing experimental results, a new understanding or theory regarding chemistry emerges [1]. Since the discovery of quantum mechanical chemistry, the concept of Computational Chemistry has emerged. Computational Chemistry is a branch of chemistry that discusses the meaning and scope of computation in chemistry, molecular modeling (describing molecular structures, calculating molecular reactivity, and constants), and examples of molecular modeling applications to explain chemical phenomena [2-4]. The application of Computational Chemistry in the pharmaceutical field through the use of software, such as Hyperchem, aids in determining the relationship between a drug compound's structure and activity [5,6]. VOSviewer is bibliometric data mapping software or a data collection that visually represents bibliographic fields (title, author, author, journal, etc.) [7-9]. You can get an overview and various information about the development of the field of science and the performance of the research that has been done using bibliometric mapping software [10-12]. The term bibliography is derived from the Greek words "bilio" (book) and "graphy" (writing). As a result, a bibliography can be defined as a list of books or articles that cover specific topics [13-16]. According to Van Eck [11], not all bibliometric database sources support all types of data analysis, including co-authorship, co-occurence, citation, bibliographic coupling, and co-citation. Web of Science and Scopus are the primary database sources that support almost all types of analysis. Because of the differences in data structure and policies between the databases, only certain types of analysis are available for each. VOSviewer can map different types of bibliometric analysis. It supports several major bibliographic databases, it can analyze large amounts of data, it can use layout and cluster techniques, and it has many other benefits. One of the critical subjects that must be studied is Computational Chemistry. Many reports on chemical engineering have been published, including research by Barbiric et al. on the energy content of food required to support daily activities [17]. Paredes-Doig et al. used Computational Chemistry software to investigate the interaction of metal ions on the surface of activated carbon [18]. Gobato and Heidari conducted research in performing quantum chemistry calculations in the simulation of inorganic molecules BeLi2SeSi to obtain a stable molecular structure that can be accepted by quantum chemistry [19]. In Esselman and Hill's [20] study, they attempted to integrate Computational Chemistry into the organic chemistry laboratory curriculum for University of Wisconsin-Madison students through WebMO. There have been many previous studies that discuss bibliometric analysis using VOSviewer, including Digital learning [21]; Computer science [22]; Vocational school [23]; High school [24]; Covid-19 research [25]; Scientific publications [26]; Chemical engineering [27]; Materials research [28]; Special Needs Education [29]; Publication of Techno-Economic Education [30]; Engine performance [31]; Dataset portrays decreasing number of scientific publication [32]; Application in robotic hand systems [33]; Research effectiveness in a subject area among top class universities [34]; Educational Research [35]; Management bioenergy [36]; Magnetite Nanoparticle [37]; Nanocrystalline Cellulose Production Research [38]; Nano Metal-Organic Frameworks Synthesis [39]; Titanium Dioxide Nanoparticle Synthesis [40]; Nanocrystalline Cellulose [41]; Carbon Nanotubes [42]; and Nano-Sized Agricultural Waste Brake Pads [43]. However, there has been a few research on bibliometric analysis in the field of Computational Chemistry research. Therefore, to close the gap, we conducted bibliometric analysis of the topic Computational Chemistry. The goal of this study is to conduct bibliometric engineering research in the field of Computational Chemistry. This research is expected to aid and serve as a resource for other researchers in conducting and determining research topics, particularly in the field of Computational Chemistry. This analysis is necessary to determine the quantity and timeliness of a term

2. Materials and Methods

This study used research data from articles published in journals indexed by Google Scholar. We chose Google Scholar over Scopus because it is free to use. In contrast to Scopus, which cannot be accessed for free by general readers.

However, in future research, we will use the Scopus database. To collect research data, reference manager software was used, namely Publish or Perish. Each article must be indexed by Google Scholar, formatted as a journal article, in accordance with the theme, and saved into *.ris file to be made into the network map in VOSviewer. In this study, the articles were filtered to include only articles about chemistry using the criteria of title, abstract, and keyword. Firstly, we chose Google Scholar as the database in Publish or Perish software. Next, we input the "Computational Chemistry" keyword, "2017-2021" as the Year period, and "Journal" as the Publication name. As a result, 1000 articles were obtained and evaluated on the basis of the topic chosen. This study's articles were published between 2017 and 2021. The collected articles were then saved in *.ris format. Next, using VOSviewer, trends are visualized and analyzed in the form of a bibliometric map. Data mapping articles were produced using ready-to-use database sources. Furthermore, we examined the difference in the number of publications each year and classify the 20 articles with the highest number of citations for each publisher from a total of 1000 articles.

3. Results and Discussion

3.1. Research developments in Computational Chemistry field

Figure 1 shows the research on Computational Chemistry, which experienced a decrease in the period of 2017-2021 with 2020 as the lowest point. As shown in Figure 4, 2018 had a decrease of 42 papers from previously 254 articles in 2017. 2019 also experienced a decrease of 29 articles from the previous 212. Lastly, 2020 had a decrease of 48 articles from the previous 183. Therefore, the decrease was as many as 119 articles from 2017 to 2020. In contrast, the field also experienced an increase of 78 articles between the year of 2020 and 2021, making the total number of articles published in 2021 to be 213 articles.

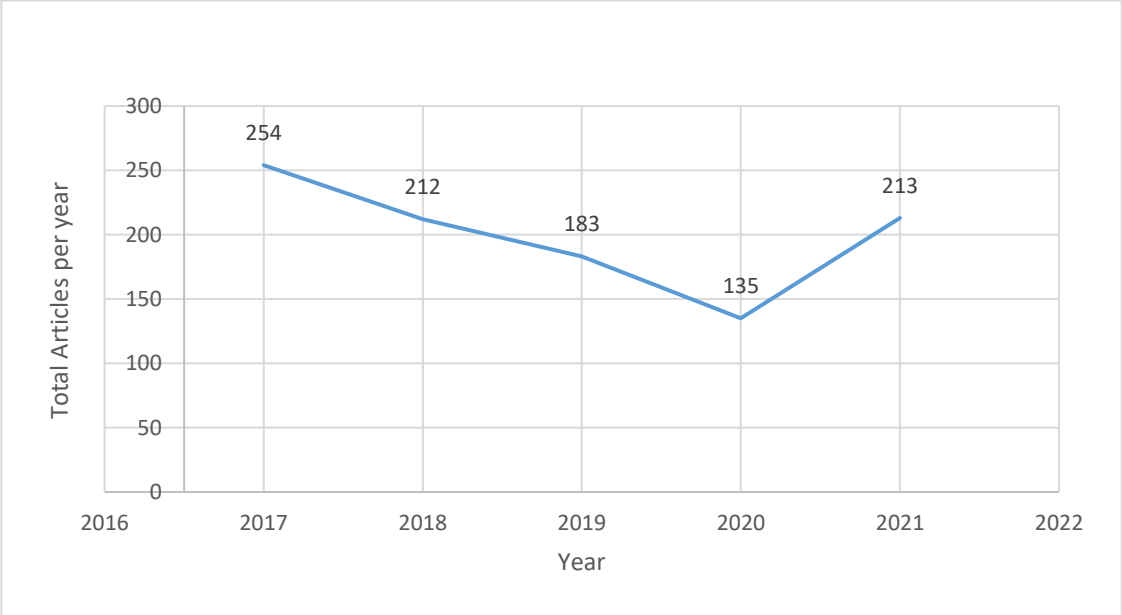

Figure 1. Level of development of research on Computational Chemistry.

We discovered the cause of the increase in the number of publications between 2020 and 2021. The COVID-19 pandemic was responsible for this condition. Computational Chemistry, as we know, is linked to experiments [44]. This encourages researchers to keep innovating in their search for drugs to combat the COVID-19 outbreak.

Table 1. Articles with the highest number of citations in the field of Computational Chemistry

No	Citation Number	Authors	Title	Publisher	Year	Ref
1	845	R. M. Parrish, et al.	Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability	ACS Publications	2017	[51]
2	453	G. B. Goh, N. O. Hodas, A. Vishnu	Deep learning for computational chemistry	Wiley Online Library	2017	[52]
3	350	A. J. Williams, et al.	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry	Springer	2017	[53]
4	338	D. Sharma, S. Kanchi, K. Bisetty	Biogenic synthesis of nanoparticles: a review	Elsevier	2019	[54]
5	317	N. Muralidharan, et al.	Computational studies of drug repurposing and synergism of lopinavir, oseltamivir and ritonavir binding with SARS-CoV-2 protease against COVID-19	Taylor & Francis	2021	[55]
6	289	F. Neese, et al.	The ORCA quantum chemistry program package	aip.scitation.org	2020	[56]
7	266	H. Moriwaki, et al.	Mordred: a molecular descriptor calculator	jcheminf.biomedcentral.com	2018	[57]
8	111	R. Gobato, A. Heidari	Calculations Using Quantum Chemistry for Inorganic Molecule Simulation BeLi2SeSi	researchgate.net	2017	[58]
9	111	S. J. Gershman	The successor representation: its computational logic and neural substrates	Soc Neuroscience	2018	[59]
10	96	S. Ji, Z. Wang, J. Zhao	A boron-interstitial doped C 2 N layer as a metal-free electrocatalyst for N 2 fixation: a computational study	pubs.rsc.org	2019	[60]
11	82	L. Goerigk, N. Mehta	A trip to the density functional theory zoo: warnings and recommendations for the user	CSIRO Publishing	2019	[61]
12	82	Y. Wu, G. Wang	Machine learning based toxicity prediction: from chemical structural description to transcriptome analysis	mdpi.com	2018	[62]
13	71	H. Lee, et al.	Caveolin-1 selectively regulates microRNA sorting into microvesicles after noxious stimuli	rupress.org	2019	[63]
14	63	M. Amanlou, S. M. Mostafavi	In sillico screening to aim computational efficient inhibitors of caspase-9 by ligand-based pharmacophore modeling	medbiotech.net	2017	[64]
15	62	A. Broom, et al.	Computational tools help improve protein stability but with a solubility tradeoff	ASBMB	2017	[65]
16	62	E. P. Alsaç, et al.	Tuning the electronic properties of prussian blue analogues for efficient water oxidation electrocatalysis: experimental and computational studies	repository.bilkent.edu.tr	2018	[66]
17	60	Y. Wu, et al.	Properties of C4F7N–CO2 thermal plasmas: thermodynamic properties, transport coefficients and emission coefficients	iopscience.iop.org	2018	[67]
18	50	S. Hussain, et al.	Zinc-doped boron phosphide nanocluster as efficient sensor for SO2	hindawi.com	2020	[68]
19	48	I. Qaddir, Net al.	Computer-aided analysis of phytochemicals as potential dengue virus inhibitors based on molecular docking, ADMET and DFT studies	jvbd.org	2017	[69]
20	47	J. C. Bardin, et al.	Design and characterization of a 28-nm bulk-CMOS cryogenic quantum controller dissipating less than 2 mW at 3 K	ieeexplore.ieee.org	2019	[70]

Molecular engineering and screening, nanotechnology approaches, and computational studies of COVID-19 are all part of the research [45-49]. On the other hand, as a result of the Covid-19 pandemic, the chemical, pharmaceutical, and traditional medicine industry groups experienced annual growth of 9.39%, an increase from 8.48% in 2019 [50]. Based on articles published between 2017 and 2021, we categorized the articles with the most citations. Table 1 displays the top 20 most cited articles in Computational Chemistry from various publishers.From Table 1, the highest citated article was Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and

Interoperability written by Parrish et al. in 2017, published by ACS Publication and cited by 845 articles. While the 20th highest was Design and characterization of a 28-nm bulk-CMOS cryogenic quantum controller dissipating less than 2 mW at 3 K written by Bardin et al. in 2019, published by IEEE and cited by 47 articles. On the other hand, the recent articles (published in 2021) did not necessarily position on the bottom of top 20 as shown by Muralidharan et al.'s article entitled Computational studies of drug repurposing and synergism of lopinavir, oseltamivir and ritonavir binding with SARS-CoV-2 protease against COVID-19 positioned on the top 5 highest citated article among publishers. It can be concluded that an article's age has smaller influence than other factors, such as relevancy, in their number of citations.

3.2. Visualization Computational Chemistry topic area using VOSviewer

Two words define the minimal number of linkages between terms in the depiction of mapping analysis in VOSviewer [70, 71]. The application can show bibliometric mappings in three different ways: network visualization, overlay visualization, and density visualization. Colored circles (node) represent keywords, and the circle's size is proportional to how many times the keywords appear in the title and abstract. As a result, the frequency with which the letters and circles appear determines their size. The more frequently the keyword appears, the greater the typeface and circle size.

3.2.1. Network visualization of Computational Chemistry keyword

The network visualization depicted the relationship between the terms that are visualized [9] as shown in Figure 2. In network visualization, relationships were represented as networks or lines connecting two terms. The clusters for each research topic area are depicted in Figure 2.

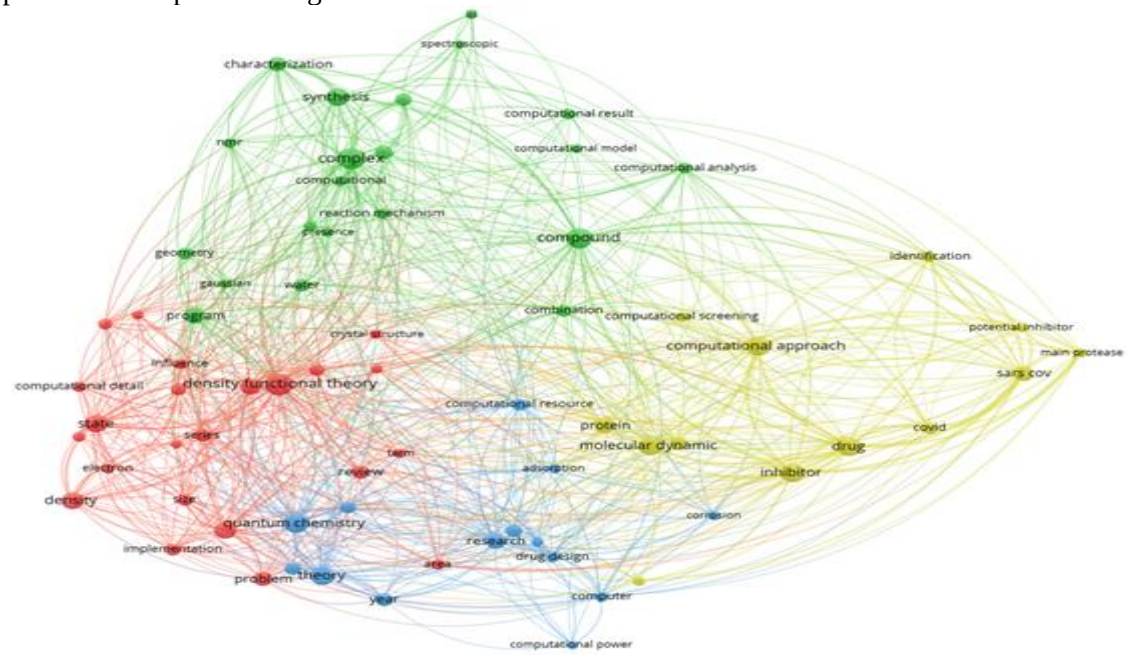

Figure 2. Network visualization of Computational Chemistry keywords.

We discovered four clusters in the network, with a total intensity of 432 and occurrence of 63 with "density functional theory" as the major node in Cluster 1, "complex" in Cluster 2, "research" in Cluster 3, and "computational approach" in Cluster 4. In addition, the major nodes in this network were identified based on the links they have to other keywords as well as its frequency of appearance in the 1000 articles. Cluster 1 was related to the term density function theory, Cluster 2 was related to the term compound, and Cluster 3 was related to research terms. Each cluster was marked with a different color. Cluster 1 was marked in red, Cluster 2 was marked in green, Cluster 3 was marked in blue, and Cluster 4 was marked in yellow. Research related to Computational Chemistry based on visualization of mapping analysis is divided into 4 clusters. Cluster 1 has 23 items, which are area, article, atom, computational cost, computational detail,

computational technique, crystal structure, density, detail, electron, electronic structure, example, hydrogen bond, implementation, influence, mean, problem, review, series, size, state and term. Figure 3 shows network visualization of Cluster 1.

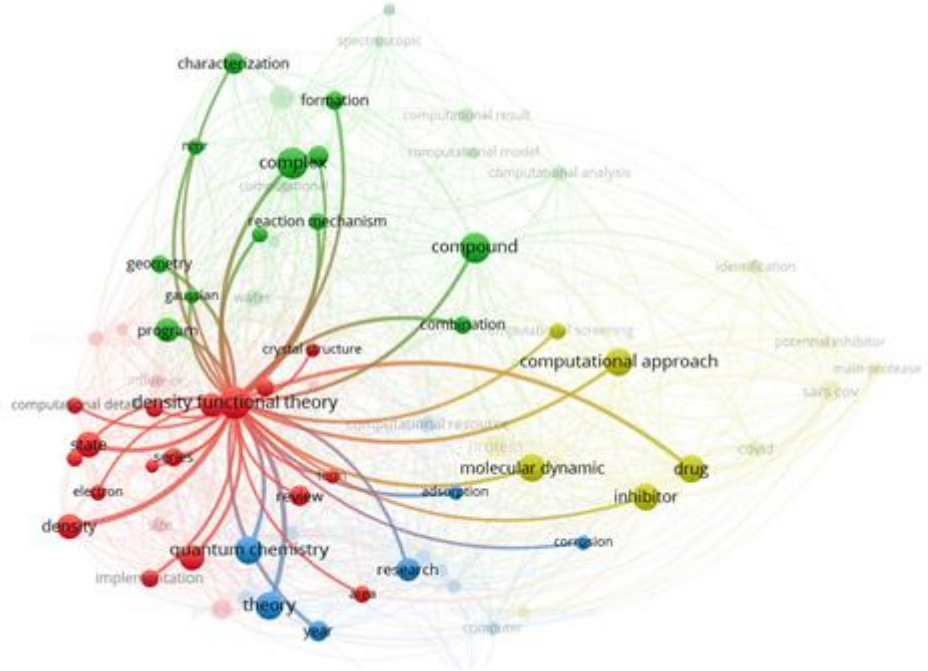

Figure 3. Network visualization of Cluster 1.

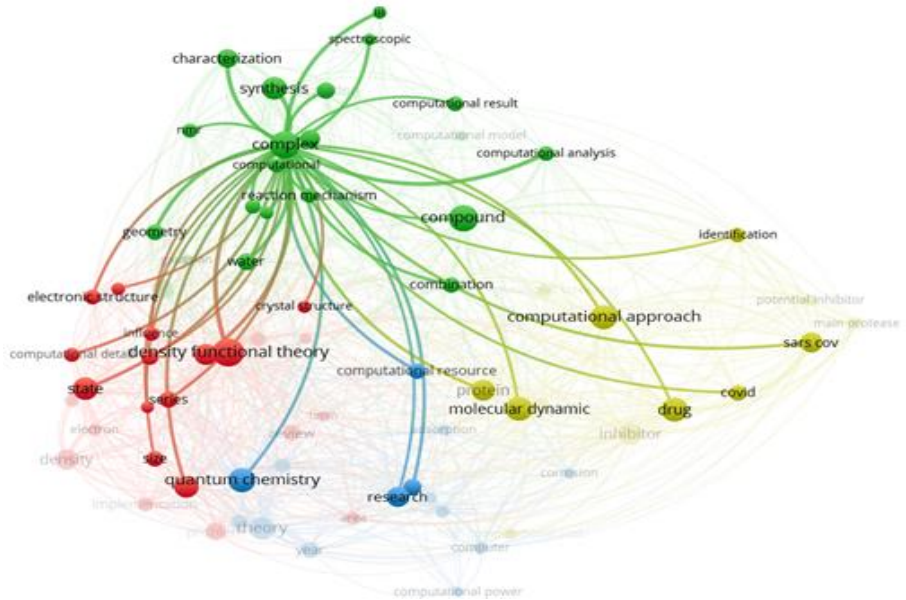

Figure 4. Network visualization of Cluster 2.

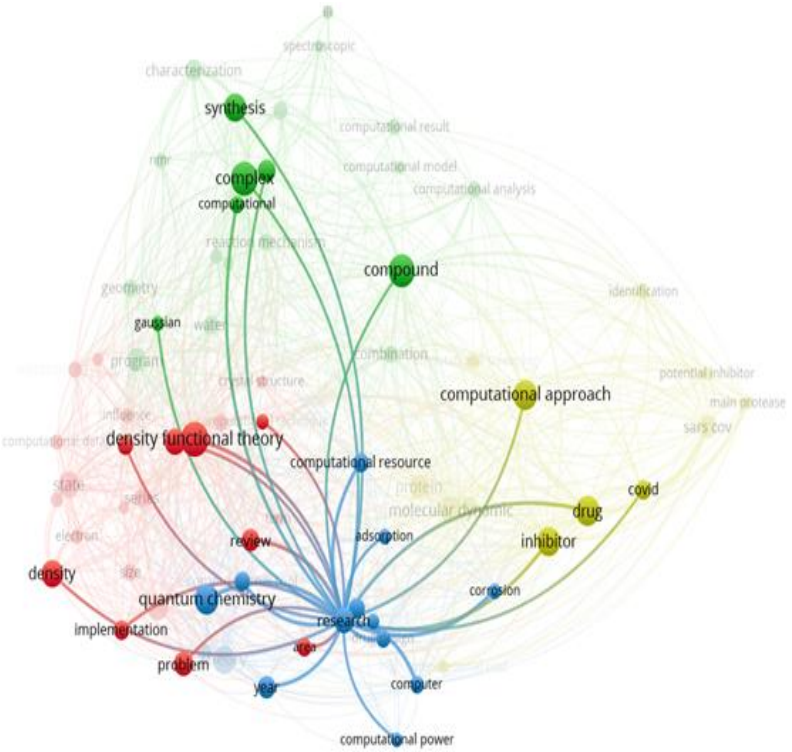

Figure 5. Network visualization of Cluster 3.

On Figure 3, “density functional theory” was the major node in Cluster 1, and it connected to a total of 39 nodes. There were several nodes that did not directly connect to the major nodes such as “protein”, “influence”, and “electron” but they were still included in Cluster 1. It is due to the nodes’ connection ultimately leads to the major node, or to put it simply, had stronger connection to the “density functional theory” as the major node. In addition, the major node not only to the nodes the cluster but also to the other clusters and their major node such as:

- “geometry”, “gaussian”, and “program” in Cluster 2;
- “theory”, “year”, and “research” in Cluster 3; and
- “molecular dynamic”, “inhibitor”, and “drug” in Cluster 4.

Cluster 2 has 19 items, which are addition, characterization, combination, complex, compound, computational, computational analysis, computational model, computational result, formation, gaussian, geometry, presence, program, reaction mechanism, species, spectroscopic, synthesis, and water. Figure 4 shows network visualization of Cluster 2

As shown in Figure 4, “complex” was the major node in Cluster 2, which connected to a total of 41 nodes. In the cluster, “computational model” was connected indirectly to the major node. The major node also connected to other clusters’ nodes such as:

- “state”, “series”, and “crystal structure” in Cluster 1;
- “computational resource”, “research”, and “quantum chemistry” in Cluster 3; and
- “sars cov”, “drug”, and “identification” in Cluster 4

Cluster 3 has 14 items are accuracy, adsorption, computational power, computational resource, computational tool, computer, corrosion, drug design, machine learning, medicinal chemistry, quantum chemistry, research, theory and year. Figure 5 below is a network visualization of Cluster 3.As shown in Figure 5, “research” is the major node in Cluster and

connected to a total of 30 nodes. In the cluster, “theory” connected indirectly to the major node. The major node also connected to nodes in other clusters such as:

- “implementation”, “problem”, and “area” in Cluster 1;
- “gaussian”, “synthesis”, and “computational” in Cluster 2; and
- “inhibitor”, “computational approach”, and “covid” in Cluster 4

Cluster 4 has 13 items are computational approach, computational screening, covid, drug, high computational cost, identification, inhibitor, main protease, molecular dynamic, molecular dynamies simulation, potential inhibitor, protein, and SARS COV. Figure 6 is a network visualization of Cluster 4.

As shown in Figure 6, “computational approach” is the major node in Cluster 4 and it connected to a total of 41 nodes. In the cluster, “computational screening” is connected indirectly to the major node. The major node also connected to other clusters’ nodes such as:

- “state”, “problem”, and “review” in Cluster 1;
- “program”, “combination”, and “computational analysis” in Cluster 2; and
- “year”, “computational tools”, and “computer” in Cluster 3

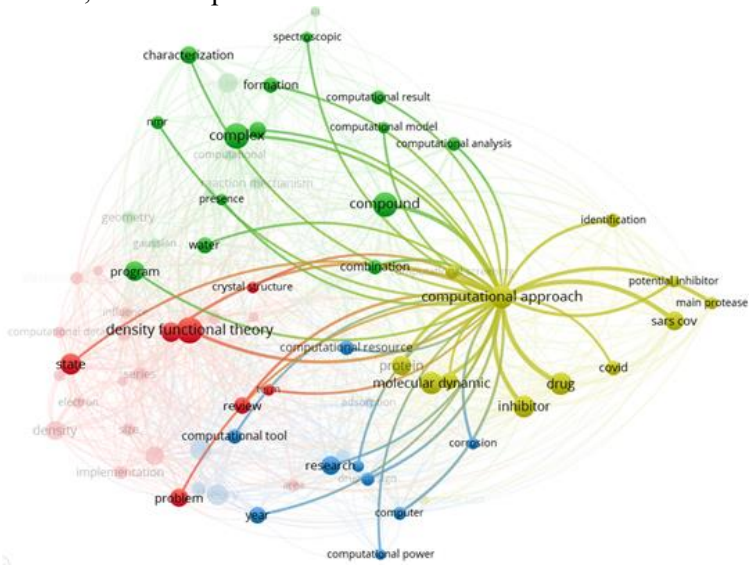

Figure 6. Network visualization of Cluster 4.

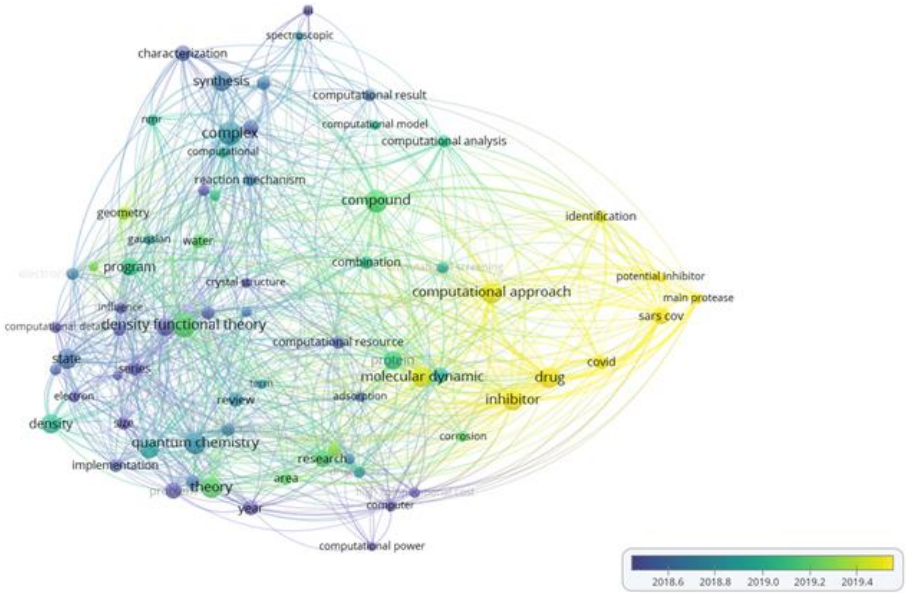

Figure 7. Overlay visualization of computational chemistry Keyword.

3.2.2. Overlay visualization of computational chemistry keyword

Overlay visualization describes the relationship between terms based on the publication time of the article [9]. Figure 7 shows research trends in the 2017 – 2021 range.

Based on Figure 7, Cluster 4 has more recent studies than the other cluster. However, the clusters cannot be considered as an indicator of publication time. It is because the major node of Cluster 1, the "density functional theory" keyword, is more recent than the other nodes in the cluster, the same goes with Cluster 2. Also, there are plenty of nodes that have different coloring with the rest of the nodes in their respective cluster, such as "density" node in Cluster 1, "nmr" node in Cluster 2, and "computational power" node in Cluster 3.

3.2.3. Density visualization of computational chemistry keyword

Density visualization is shown in Figure 8. The level of density is indicated by its color and area which means that the nodes with intense color and wider area have more research conducted on the keyword. In addition, if the color is a bit weak or it did not stand out, the amount of research done on the keyword is not that plenty compared to the more intense and wider color [9, 47].

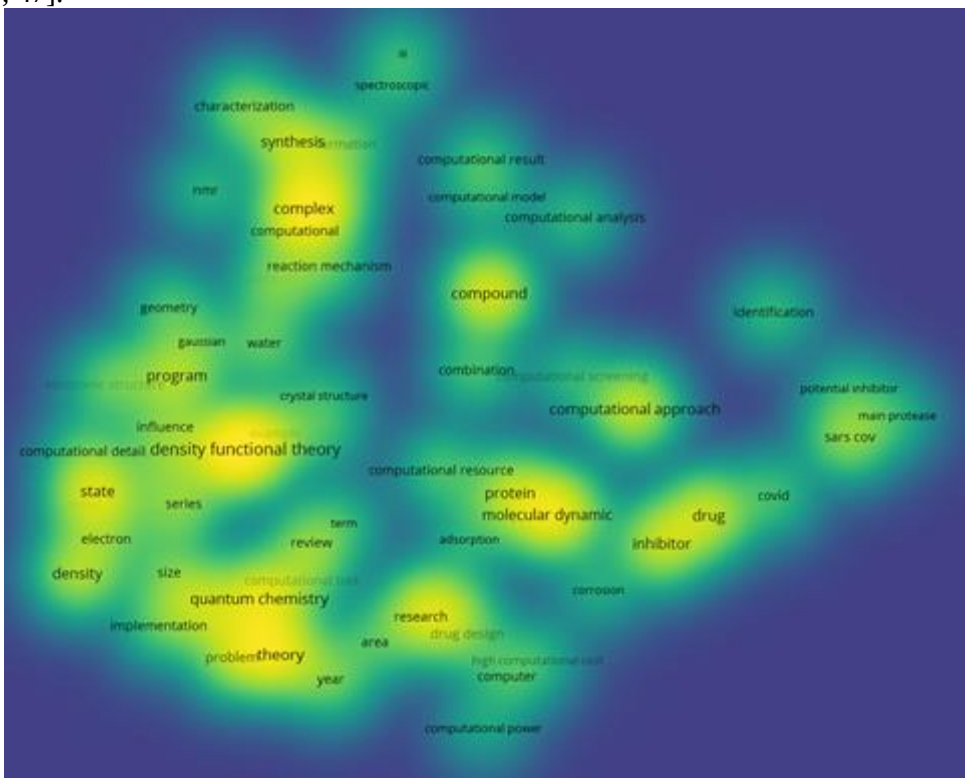

Figure 8. Density visualization of computational chemistry keyword.

Figure 8 shows that the materials that have the greatest number of research conducted. Here, it is shown that "density functional theory"," molecular dynamics", and" complex" have higher frequency to be used as a keyword among the collected data. This information can be used to determine the least researched field in Computational Chemistry to further develop and open up new opportunities and breakthroughs in advancement of the fields.

Conclusion

This study aims to conduct bibliometric research in the field of Computational Chemistry by combining mapping analysis using VOSviewer software, as well as reference management software, Publish or Perish. Search data using the keyword "Computational Chemistry", which is based on the topic area with the title, abstract, and keywords. Based on

the search results, 1000 relevant articles were obtained that were published ranging from 2017-2021. After that, the mapping process is carried out using VOSviewer. Vosviewer mapped with three different types of visualization, namely network visualization, overlay visualization, and density visualization. From the results of the mapping, it can be concluded that research on Computational Chemistry experienced a decline in 2017 - 2020. While the increase occurred since 2020 along with the pandemic, this happened because Computational Chemistry was related to the analysis of chemical aspects of the covid-19 outbreak. In addition, Cluster 4 with the keyword "Computational Approach" showed the most improvement in research in 2019. Lastly, the findings of this study are beneficial for future research to find potential areas of Computational Chemistry that can be studied further, due to the discovery of less-researched areas.

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