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Research Article

Mapping of Literature in the Field of Chemo-informatics

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Abstract: Chemo-informatics is a recent development in the field of chemistry. It has helped scientists develop various chemical structures using computers, leading to the solution of some intricate problems in chemistry, including in medical chemistry.

Objective: The mapping of literature in chemo-informatics was performed to reveal publication trends, authorship trends, core journals, and collaborative authors at the national, international, and institutional levels. The annual growth rate revealed the growth pattern of publications. The data of collaboration was visualized using the VOS Viewer tool.

Methodology: The methodology used for this study was citation analysis of the publications downloaded from the SCOPUS database for the years 2017 to 2022. A total of 1425 data items were downloaded based on the keywords used for searching. Out of these 1425 after cleaning the data, only 1,413 citations were used for further study. Out of these 1,413 citations, 13 citations were anonymous so they were also ignored for authorship analysis.

Findings: The findings of the study were that the annual growth rate of publications as shown by the highest number of publications (276) was in 2021 and the lowest 195 (13.80%) in 2018. Articles (65.46%) were the preferred publications by the authors. Multiple author (5 or more) publications show the prevalence of teamwork, which was further substantiated by the Av.

Collaboration Index of 4.48; Av. Degree of collaboration was .0926 and Av. collaboration coefficient was .0179. J. Medina-Franco of Universidad Nacional Autónoma de México was the most prolific author with 53 publications during the 5 years of the study period. The Journal of Chemical Information and Modeling headed the list of publications with 48 publications while the Journal of Chemical Education received the highest number of citations (1052). In the list of countries with maximum contribution, the USA headed the list with 327 publications receiving 7735 citations. The international link strength was 211, which iswas revealed by the International Cooperation Index (ICI) of 64.52. China was placed in second place in international collaboration.

All these papers could be only b possible through the use of computers, as the 21st century has allowed the use of computers in general studies which have become precursors to develop various models and theories based on computers. The present study reveals the collaborative nature of research which is very much prevalent nowadays and which can also be seen in the visualization report. The study also reveals that authors are adopting team research and have a wider perspective of their research.

1. Introduction

Chemo-informatics, with its modest origins in 1978 as chemical informatics, is the study of chemical information with the help of computers. It involves the use of computers and information technologies to solve chemistry problems. All sorts of methodologies used in information science, like Image processing, data mining, signal processing, modelling and simulation, computational theory, software engineering, etc., are used in chemo-informatics to generate new knowledge in chemistry. This recent field of study had its modest origin in 1998 when Frank K. Brown defined "chemical informatics as the mixing of information resources to transform data into information and information into knowledge". D. Mendeleev is supposed to be the father of chemo-informatics because he created a visualization tool called a 'Periodic table of the elements.' chem-informatics, chemo-informatics, or chemical informatics, used synonymously, helped scientists develop various chemical structures with the help of computers. Chemo-informatics is storage, indexing, searching and retrieving chemical compounds' information (Brown, 1998).

In this study mapping of literature was performed to reveal the extent of the spread of roots of a discipline into other disciplines. Mapping is a vital strategy to represent knowledge of a field while conducting literature reviews, to know the evolutionary stages of primary specialties in disciplines and intellectual milestones in developing critical things in the domain (Chen, 2017). Mapping has been described variously as a 'graphic blueprint' by Heinrich (2001), 'a geographical metaphor' by Kamler & Thomson (2006) or 'Diagrammatic representation' (Hart, 1998)

and helps in understanding the discipline and its characteristics. It allows researchers to know the various hidden patterns and identify the gaps in studies. It will enable students to identify potential research areas in a discipline that has been untouched 'till now (Heinrich, 2001; Kamler & Thomson, 2006). Mapping is done either through deduction or through induction (Heinrich, 2001) or by using descriptors (using keywords) or authors who are experts in the field, by referencing and citing, using their quotations (Machi & McEvoy, 2008).

Various ways of mapping, as given by Hart (1998), include-

Feature Map represents specific features of the entity.

Subject Tree Map showing different levels of subject development.

Content Map showing the organization of content through hierarchical classification.

Taxonomic Map showing classes of standards taxonomies.

Concept Map indicates the evolution of concepts and processes of their development.

Also relevant are rhetorical mapping and citation mapping.

The present mapping study used descriptors and attempted to map the well-known authors, journals and institutions in the field and the country at the top of the list of international collaborations based on the data downloaded from the SCOPUS database.

The study addressed the following research questions.

1. What is the growth rate of publication and also who is the most prolific author in the field of chemoinformatics?
2. Which country and institutions are the highest contributors in the field of chemoinformatics?
3. Which are the highest contributing journals and the publication type publishing the chemoinformatics research output?

2. Literature Review

A literature review is a comprehensive, systematic analysis of literature in a field to identify and evaluate the work of researchers, scientists and practitioners to reveal some trend or pattern or to provide an understanding of the field. It provides a solid starting point to start a work in a particular area or topic (Mulrow, 1987). Mapping techniques are used to understand the trend of development of the subject and its concepts (Concept Mapping) as well as to clarify critical arguments or issues. Mapping collects data on kinds of activity, locations where it occurs, and media where it is published (Cooper, 2016).

Mapping studies has been carried out in almost all disciplines ranging from medicine (Potter, 2010; Venable *et al.*, 2014; Gautam & Mishra, 2020) nursing (Guenther, 2006), health care management (Taylor, Gebremichael, & Wagner, 2007), social sciences and is very much used in library & information science too.

Various areas of mapping study include individual journals to identify core topics (Lamba & Madhusudhan, 2019), core journals in the field, coverage in various indexes as well as databases (Taylor, Gebremichael, & Wagner, 2007; Potter, 2010), various research methods used in the discipline (Ngulube, 2010) or the emergence of new field of study or paradigm shift like the discipline (Janssens, Glänzel, & De Moor, 2008). These types of studies are known as bibliographic mapping, which aims to reveal intellectual connections with the continuously changing system of scientific knowledge (Small, 1999). Hung has also used the bibliographic mapping method in 2012, Hsu, Hung, & Ching (2013) in 2013 and Bond (2018) in 2018 with different subjects and analysis methods. Donthu *et al.* (2021) opined that bibliometric analysis helps decipher and map the cumulative scientific knowledge and evolutionary nuances of well-established fields by making sense of large volumes of unstructured data in rigorous ways.

Analysis of large amounts of data on complex research topics becomes very difficult for literature review. However, visualization techniques using bibliographic data can give a clear literature overview. They also show the current trends of literature and its properties. Rodrigues *et al.* (2013) used visualization techniques to map 'patient safety'. A study was also carried out in Information science using a hybrid method of the linear combination of distance metrics, revealing three large traditional sub-disciplines. - information retrieval, bibliometrics/scientometrics & patent analysis and webometrics (Janssens, Leta, Glänzel, & De Moor, 2006; Janssens, Glänzel, & De Moor, 2008).

Mapping studies have been abundantly performed in various disciplines like medicine, nursing, health, educational technology, and social science although there have been few such studies in chemoinformatics, which is why this topic has been chosen for the current study. Although there are several bibliometric studies based on a single journal, "chemoinformatics", using WoS as the database (Willett, 2020; Willett, 2022), the present mapping of chemo-informatics literature is a citation mapping of the publications available in the field of chemoinformatics based on SCOPUS database (not on a single journal) trying to find the growth of publications, core journals, well-known authors and their affiliations both at national and international levels, the country with the highest production of literature in chemoinformatics and visualization of the result using VOSviewer. Using a bibliographic mapping tool enables the researchers to save time and cost as it makes fewer efforts to systematically filter large amounts of text data, select the most related articles, and cluster them with a specified criterion (Bardakci *et al.*, 2021).

3. Objectives and Methodology

The current mapping study identified the number and types of publications, growth trend of the publication, core journals in the field, and collaboration of authors with national

and international authors and institutions in chemo-informatics.

The comprehensive SCOPUS database was used for downloading the literature on chemo-Informatics since it includes data that are part of the other databases like WoS, Medline, Google Scholar, etc., side by side SCOPUS rigorous selection process of the publications by the team of experts, to include in the database differentiates from other databases in quality resources (Zyoud *et al.*, 2023). For bibliometric analysis, data was downloaded and interpreted at a fixed time (2017-2022) to present a static field picture.

The bibliographic and citation data was downloaded and curetted for the required parameters, using the following search string-

(TITLE-ABS-KEY (chemical AND informatics) OR TITLE-ABS-KEY (Chemoinformatics) OR TITLE-ABS-KEY (Chem-informatics)) AND (LIMIT-TO (PUBYEAR, 2022) OR LIMIT-TO (PUBYEAR, 2021) OR LIMIT-TO (PUBYEAR, 2020) OR LIMIT-TO (PUBYEAR, 2019) OR LIMIT-TO (PUBYEAR, 2018) OR LIMITTO (PUBYEAR, 2017))

Data was downloaded on April 5, 2023. A total of 1,425 citations were downloaded. After cleaning the data (whose source, publisher, and affiliation were unavailable), 1,413 were suitable for study. Of these 1,413 citations, 13 were anonymous, so they were also ignored in the authorship study.

Analysis of data was performed to find the annual growth rate of the publications (Sweileh *et al.*, 2017) using formula-

$$AGR = \frac{end\ value\ - first\ value}{first\ value} x100$$

Compound annual Growth Rate has been calculated using formula given at www.investopedia.com/calculator/cagr.aspx.

Types of publication and author count were made on the basis of simple mathematical calculations and percentage calculations. Authorship pattern based on collaboration between authors was calculated using the formula of Collaboration Index suggested by Lawani (1980) and Elango & Rajendran (2012) for Degree of collaboration (formula by Subramanyam (1983)) and Collaboration Coefficient (using formula of Ajiferuke, Burell, & Tague (1988)). Data was also analysed for the top 10 authors in the field with their affiliated institutions and publications. Top productive journal were identified by the name of the journal with highest number of publications and the citations received by them. Countries which were at the top in chemoinformatics research were also studied and the International Collaboration Index of the countries has been calculated using formula given by Frame & Carpenter (1979).

$$ICI = \frac{Number\ of\ international\ links}{Total\ number\ of\ papers\ published\ by\ country} x100$$

In the last data has been visualized using the VOS Viewer Tool.

4. Result Analysis and Interpretation

4.1 Annual growth of publications

During 2017-2022, a total of 1,413 publications were published on chemo-informatics research (Table 1 and Figure 1). The highest number of publications was 276 (19.53%) published in 2021, while the lowest number of publications, (195, 13.80%) was in 2018. The average number of publications per year was 235.50. Years 2017, 2018 and 2019 had less than average papers published, while more than the average number of articles were published in 2020, 2021 and 2022. It is clear from the given Table 1 that there was a consistently increasing growth trend of literature except in 2018. Annual Growth Rate (AGR) is defined as the percentage change in the number of publications in a year (Sweileh *et al.* 2017) which is calculated using the formula-

$$AGR = \frac{end\ value\ - first\ value}{first\ value} x100$$

For the years 2019, 20 and 2021, AGR was positive, while it was negative for the years 2018 and 2022. Table 1 provides the Yearly Growth of the documents for 2017-2022 globally. Figure 1 presents the growth and dissemination of publications in chemo-informatics. The compound annual growth rate or CAGR calculated using the given formula (www.investopedia.com/calculator/cagr.aspx) was 26.46 % for the duration of 2017-2022. There were also some fluctuations during the entire period of study (Figure). The changes can be attributed to the absence of constant publication growth. The annual growth rate was either declining or increasing.

Table 1. Year-wise Growth of Publication and % Annual Growth

Year	TNP	TNP (%)	Cumulative	AGR (%)
2017	206	14.57%	206	00
2018	195	13.80%	401	-5.34%
2019	224	15.85%	625	14.87%
2020	250	17.69%	875	11.60%
2021	276	19.53%	1151	10.40%
2022	262	18.54%	1413	-5.07%
Total	**1413**	**Av 16.63%**	**4671**	**Av. 4.41%**

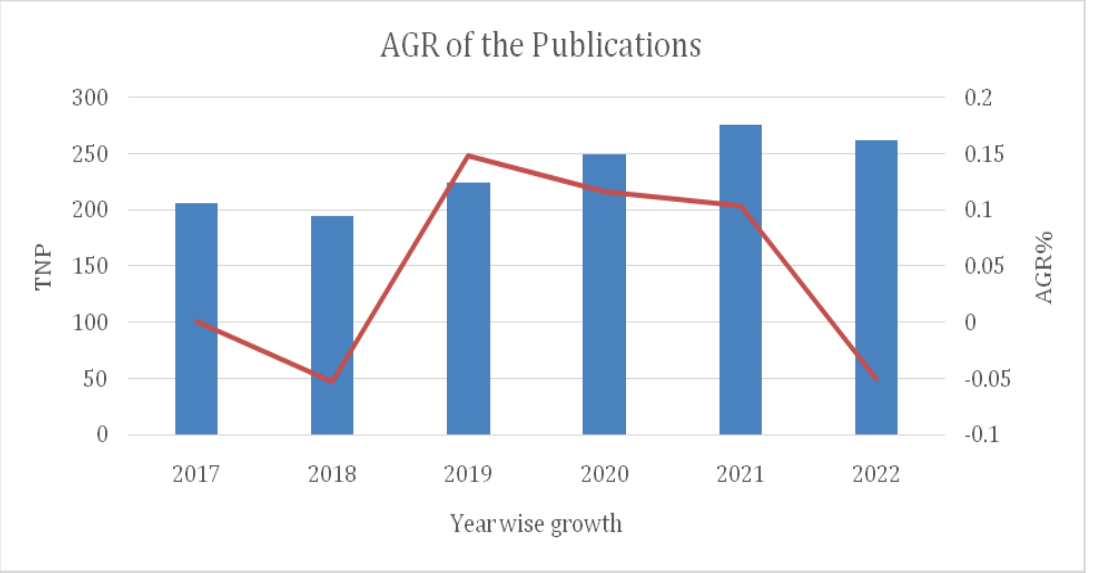

Figure 1 Bar chart showing AGR of the publications

Table 2. Publication type (Number and Percentage of Publications by Type)

S. No.	Type of Publication	Total No. of Publications	Publication (%)
1	Article	926	65.46
2	Review	181	12.74
3	Conference Paper	143	10.04
4	Book Chapter	96	7.28
5	Editorial Material	27	1.69
6	Book	16	1.13
7	Conference Review	7	0.49
8	Note	5	0.35
9	Erratum	4	0.21
10	Data Paper	3	0.21
11	Short Survey	3	0.35
Total		**1413**	**100.00**

4.2 Publication type

Table 2 shows the significant publication types available in the Scopus database on chemo-informatics research, with the number of journal articles being 926 (65.46%) and review 181 (12.74%) publications. Conference papers, with 143 (10.04%) publications, ranked third, Book chapters with 96 (7.28%) publications was in fourth place with editorial material and books, with 27 and

16 (1.69 & 1.13 %) publications, respectively, while other publication types were below 1%. Significant research output was in the form of journal articles for the entire study period. This data is represented through in a pie chart as shown in Figure 2.

4.3 Authorship pattern in chemo-informatics publications

To measure the authorship trend of the literature, the entire publication was categorized into single, double, multi and mega-authored. Table 3 presents that of the total 1,413 Chemo-informatics publications, 13 publications were anonymous, 103 (7.25%) were single-authored, 232 (16.34%) joint-authored, 456 (32.13%) were multi-authored and 609 (42.91%) mega-authored papers. The authorship analysis revealed that 75.04 % of papers were contributed by multiple authors, while 23.59% of publications were by single and joint two authors. The study indicates the dominance of multi and mega-authored publications for the entire study period.

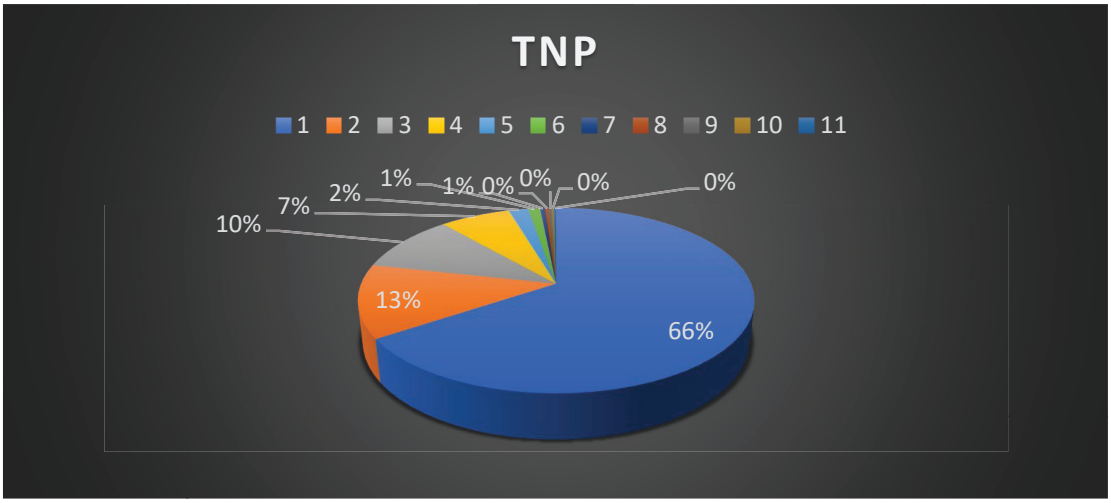

Figure 2. Types of publication (Percentage-wise Differentiation)

Table 3. Total number, %age and type of authorship

S. No.	Authors	Value	%age
1	Single Author	103	7.29
2	Joint Author	232	16.42
3	Multi Author	456	32.27
4	Mega Author	609	43.09
5	No Author	13	.92
Total		**1413**	**100**

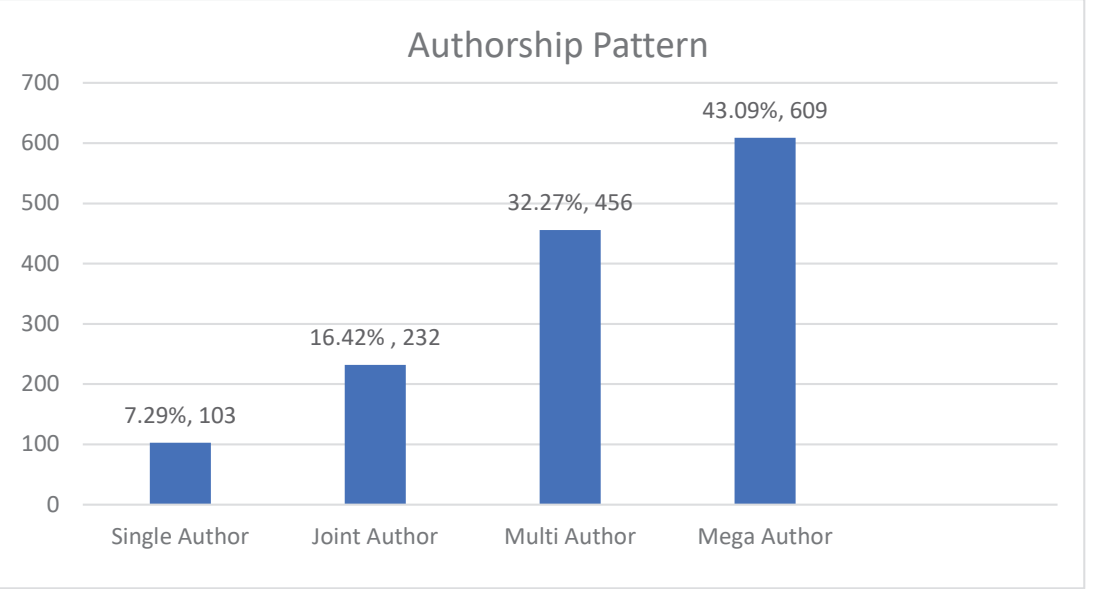

Figure 3. Authorship Pattern (%Age, Number and Type of Authorship)

4.4 Measures of authorship pattern

The advent of ICTs in the 21st Century facilitated collaboration of authors with their peers not only at the institutional level but within different disciplines at a global level. Applying ICTs has paved the way for the fast dissemination of innovative information, boosting information production and utilization.

Collaborations by authors were measured using various collaboration measures. The **Collaborative Index (CI)** is the ratio of authors to their collaborated papers (Elango & Rajendran, 2012; Elango, 2018).

In measuring CI, single-author papers have been ignored deliberately and are always taken to be equal to 1. The formula used to measure the CI is -

$$Collaborative\ Index = \frac{Total\ Authors}{Total\ Joint\ Papers}$$

Table 4 shows that CI varied between 4.16 to 4.91, 4.48 being the average, indicating maximum cooperation of researchers to have a CI of 4 to 5, in chemo-informatics research.

Degree of Collaboration (DC), which is the ratio of single authored and joint authored papers, is determined by the formula (Subramanyam,1983) -

$$DC = \frac{Nm}{Ns + Nm}$$

whereas, *DC*= Degree of Collaboration, *Nm* = Number of multiple-authored Papers and *Ns* = Number of single-authored papers.

Table 4 shows the average value of CC was 0.0179 for the study period. During 2017 to 2018, the Collaborative Coefficient (CC) was higher than the average overall

value, while it was below average for the years 2019, 2020, 2021 and 2022, indicating a mixed trend of collaboration.

DC gives 0 weights to single-authored papers and 1 for maximum collaboration.

$$DC = \frac{1297}{1297+103} = 0.926$$

Hence, the degree of collaboration for the chemo-informatics publication was found to be 0.926, which reveals the dominance of team research in the field. Of the total publications, 92.64 % of the contributions were by multiple authors, while only 7.35 % were without collaboration.

The degree of collaboration varies from discipline to discipline. It leaves behind single-authored articles, thereby creating a gap in study. It also does not differentiate levels of multiple authorship. This discrepancy can be removed by another measure called **collaboration-coefficient.** It helps in measuring the collaborative research pattern. Collaboration Co-efficient is the measure of the number of joint research papers during a given time period. CC is calculated using a formula (Ajiferuke, Burell, & Tague, 1988) -

$$CC = 1 - \sum (1/j)\, P(X=j)$$

4.5 Measure of authors' productivity

Table 5 presents the top ten authors in the field. It reveals that Medina-Franco J., with 53 articles, ranks at first place in the list of productive authors, Varnek A. (16) ranks second and Torshin, I. Y. with 14 articles, third place and Bajorath J. & Gromova, O. A. shares the 4th position by publishing 13 articles each.

Table 4. Measures of authorship pattern

Year	No Author	Single	Double	Three	Four	Five	Six	Seven	Eight	Total Authors	Total Articles	CI	DC	CC
2017	2	15	39	41	35	19	16	10	5	873	206	4.16	.93	.0226
2018	1	21	30	33	31	21	21	17	6	882	195	4.52	.89	.0227
2019	4	19	45	37	36	25	19	9	10	935	224	4.17	.92	.0170
2020	4	18	33	49	31	29	30	23	12	1117	250	4.47	.93	.0167
2021	1	15	43	44	45	26	28	21	15	1266	276	4.62	.95	.0123
2022	1	15	42	37	37	26	24	21	24	1286	262	4.91	.94	.0165
Total	**13**	**103**	**232**	**241**	**215**	**146**	**138**	**101**	**72**	**6359**	**1413**	**Av. 4.48**	**Av .926**	**Av. .0179**

Table 5. Top 10 productive authors, institutions and their publications

S.N.	Authors	Institutions	publications
1.	Medina-Franco, J.	Universidad Nacional Autónoma de México	53
2.	Varnek, A.	Professor of Chemistry, University of Strasbourg, France	16
3.	Torshin, I. Y.	Federal Research Center Informatics and Management of the Russian Academy of Sciences, Moscow, Russian Federation	14
4.	Bajorath, J.	Department of Life Science Informatics and Data Science, University of Bonn, Germany	13
5.	Gromova, O. A.	Moscow Institute of Physics and Technology and Ivanovo State Academy of Medicine Ivanovo, Russia	13
6.	Hassan, M.	Institute of Molecular Biology and Biotechnology, The University of Lahore, Lahore, Pakistan	11
7.	Nite-Kang, F.	Faculty of Science, Department of Chemistry, University of Buea, Cameroon	11
8.	Ramprasad, R.	School of Materials Science and Engineering, Georgia Tech, Atlanta, USA	10
9.	Saldivar-Gonzalez, F. I.	Faculty of Chemistry, National Autonomous University of Mexico	10
10.	Schneider, G.	Department of Chemistry and Applied Biosciences, Vladimir-Prelog-Weg 4, Switzerland	10

4.6 Journals' productivity measures

Table 6 lists prolific journals in chemo-informatics literature. The highest productivity (48, 3.39%) of total chemo-informatics literature was published in the Journal of Chemical Information and Modeling, followed by the Journal of Chemical Education with 45 (3.18%), Molecular Informatics with 44 (3.11%), and the remaining journals had less than 2 per cent publications.

4.7 Most collaborating countries

Table 7 reveals that the USA is the most prolific country with a share of 327 (23.14%) papers, followed by the People's Republic of China with 134 (9.48%) papers, Japan with 117 (8.28%) papers, Germany and India with 95 (6.72%), UK with 81 (5.73%) papers and Mexico with of 59 (4.17%) papers stood at 7th position. At the same time, France, Russia and Spain have 50, 49 and 39 publications, respectively. Yet France, with 1044 citations, had link strength = 87 (more than India), showing a robust international collaboration Index.

Table 6. Most productive journals and citations received

S. no.	Title of the Periodicals	TNP	%	Citations	ACP
1	Journal of Chemical Information and Modeling	48	3.39	997	30.29
2	Journal of Chemical Education	45	3.18	1052	31.96
3	Molecular Informatics	44	3.11	347	10.54
4	Molecules	25	1.77	130	3.95
5	Journal of Chem-informatics	21	1.49	331	10.06
6	Wiley Interdisciplinary Reviews: Computational Molecular Science	21	1.49	24	0.73
7	Studies in Health Technology and Informatics	18	1.27	36	1.09
8	Scientific Reports	18	1.27	23	.70
9	Methods in Molecular Biology	13	.92	184	5.59
10	Biomolecules	12	.85	167	5.07

Table 7. Top collaborating countries citations received and ICI

Countries	TNP	TNP (%)	Citations	International link strength	ICI
USA	327	23.14	7735	211	64.52
PEOPLES R CHINA	134	9.48	2124	69	51.49
JAPAN	117	8.28	1153	54	46.15
GERMANY	95	6.72	2001	147	154.73
INDIA	95	6.72	678	35	36.84
UNITED KINGDOM	81	5.73	1359	119	146.91
MEXICO	59	4.17	907	32	54.23
FRANCE	50	3.53	1044	87	174
RUSSIA	49	3.47	634	49	100
SPAIN	39	2.76	457	70	179.48

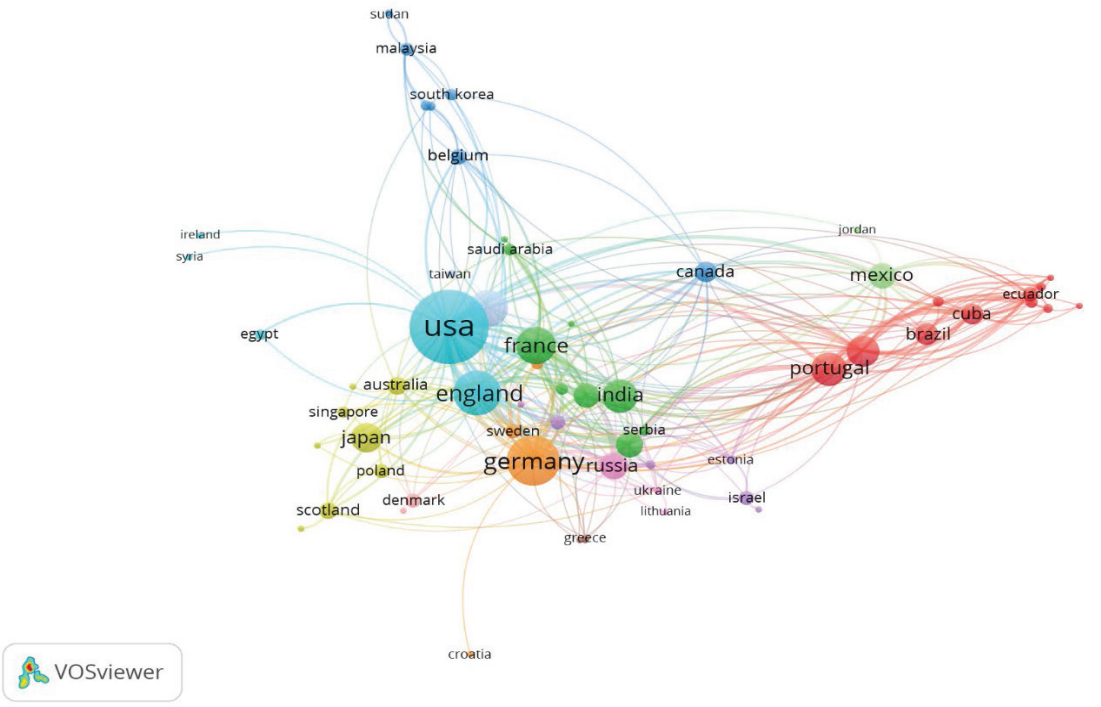

Figure 4. The VOS viewer that visualization map of the collaborating countries

4.8 International cooperation index (ICI)

The International Cooperation Index (ICI), also called the Internationalization Index, was suggested by Frame and Carpenter (1979) and measures the international links between countries for a specific publication. According to the formula, ICI is calculated in percentage of the total as follows. -

$$ICI = \frac{Number\ of\ international\ links}{Total\ number\ of\ papers\ published\ by\ country} x100$$

The USA had the highest number of citations, followed by China, Germany and the UK. India, with 678 citations, is in 8th position. Here, it can be seen that both Germany and India had an equal number of publications, but Germany had higher citations (2001) than India. The figure shows that the USA was the central point regarding collaboration links. Spain's International Cooperation Index (ICI) was the highest at 179.48, followed by France at 174.00, Germany at 154.73, UK at 146. 91, USA with 64.52, Mexico with 54.23 and the lowest 36.84 ICI was for India. A visualization map of the collaborating countries is given below (Figure 4).

5. Conclusion

This study of literature mapping in chemo-informatics revealed that periodicals are the significant source for publications in the field, followed by Reviews. The annual growth rate for the publication was found to be 26.46%. In the area of authorship, multi and mega-authorship patterns were

found to be prevalent (75.04 %), which was clear from the Collaborative Index (4.48 av.), and the degree of collaboration which was was found to be 0.926. The Collaboration Coefficient was 0.179 on average for the entire study period, showed the prevalence of team research. Medina-Franco J. of the University of México was the most prolific author, followed by Varnek A. Professor of Chemistry, University of Strasbourg, France, and Torshin, I. Y. of the Federal Research Center Informatics and Management of the Russian Academy of Sciences, Moscow, Russian Federation. The core journal was shown to be the Journal of Chemical Information and Modeling, with 48 publications (although the Journal of Chemoinformatics also featured), followed by the Journal of Chemical Education and Molecular Informatics. In the collaborative countries section, the USA ranked at the top with 327 papers, followed by the People's Republic of China with 134 papers and Japan with 117 papers. India was in the 5th rank 95 papers. Spain's International Cooperation Index (ICI) was the highest at 179.48, followed by Germany and the United Kingdom at 154.73 and 146.91, respectively, while India had the lowest ICI (36.84). This shows that Indian contribution needs improvement in terms of internationally collaborative papers.

Some **suggestions** inferred from the study are as follows. Co-citation and co-occurrence analysis, could be carried out to find the more comprehensive result of bibliographic mapping as bibliographic mapping tools can search concepts, subjects, and approaches inside the chosen texts that have been left accidentally by the authors of the text. A further study taking the top 5 journals identified in this study can be analyzed with a wider time span and dataset, using co-word analysis to achieve a comprehensive result.

A **limitation** of this study was the data collection as SCOPUS, although being a very comprehensive database, is not subscribed to by every library.

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