



Constructing Dynamic Knowledge Mapping Graph of Quantitative Measures of Research Contributions of David Macmillan from the Chemistry Domain

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Abstract

This study aims to explore the measures of 216 research contributions of Nobel Laureate David MacMillan through a dynamic knowledge mapping graph in a quantitative way in the field of Chemistry domain. We have used Web of Science database to extract Scientific research articles that are relevant to David Macmillan for a period of 20 years from 2006 to 2022 and 216 research publications have been retrieved. The obtained primary data was exported to Microsoft Excel for further analysis to meet the study's objectives. The level of collaboration, journal collaborative distribution, disciplinary collaborative distribution and country collaboration, inter and intra subject collaboration have been scrutinised. Major findings from the above perspectives have been noted that David MacMillan's majority of papers were written in collaboration, as evidenced by the 0.90 collaboration rate across all publications and 71.30 % are journal articles. Le, Chi Chip co-authored 10.8% of David MacMillan's 216 publications, making her the most prolific co-author. Between 2013 and 2022 his recent work mainly focused on Catalysis (55.95%), Combinatorial chemistry (33.76%), Photoredox catalysis (16.40%), etc. Future graduate students in library and information science as well as other domain researchers and students will find it valuable to investigate David MacMillan's Scientometric profile in Chemistry domain.

Keywords: David MacMillan, Knowledge mapping, Nobel laureate, Relative growth rate, Scientometric study

1. Introduction

Large-scale domain knowledge graphs have been used in numerous fields since Google first suggested the idea of a knowledge graph in 2012. The construction of a dynamic knowledge graph of research contributions of Nobel Laureates through quantitative measures is explored in this work which is also related to "Scientometric portrait" analysis which is a study of a particular scientist or author who is renowned

in a certain field or specialty, with a group of related scholars collaborating throughout his or her career. Scientometrics primarily focuses on the quantitative traits and properties of science and scientific inquiry. Measurement of the influence of academic journals and research publications, comprehension of scientific citations, and application of such measurements in management and policy contexts are major research concerns. A Nobel laureate, scientist, or subject matter expert in any discipline is



well renowned for his or her contributions to that field or society. Scientific articles could be produced to contribute to this. Quantitative markers are used in scientometric analysis which may be quite helpful in examining a person's scholarly accomplishments and the numerous social contributions he has made.

2. Author profile

Sir David William Cross MacMillan, a Scottish chemist and Professor of Chemistry at Princeton University, shared the 2021 Nobel Prize in Chemistry with Benjamin List for the development of asymmetric organocatalysis. He obtained his Ph.D. in 1996 and focused on enantioselective catalysis, particularly the creation of Sn(II) boxes. MacMillan's research interests include organic chemistry, catalysis, enantioselective synthesis, organocatalysis, and iminium.

Between 2010 to 2014, MacMillan served as the journal's first editor-in-chief of *Chemical Science*, the Royal Society of Chemistry's premier general chemistry publication. As of 2021, Google Scholar and Scopus both give MacMillan an h-index of 110 and 100, respectively. Sir David MacMillan has published his research work in different categories such as Chemistry Multi-disciplinary (158), Multi-disciplinary Sciences (34), Organic Chemistry (9), Marine Freshwater Biology (5), Biochemistry and Molecular Biology (3), etc. in various forms of the document i.e. research article (161), patents (30), meeting abstract (48), review article (8), early access (5), editorial material (5), correction (3), proceeding paper (3), biographical-item (2), etc.

3. Significance of the study

In the present paper, the investigators have attempted to study the authorship pattern, domain wise preferred medium of scientific communication, authors' production over time, growth in publica-

tions, the rates of collaboration, the impact governing successful scientific careers and to explore the measures of research contributions of Nobel Laureate David Macmillan through dynamic knowledge mapping graph both in a quantitative way in the field of Chemistry domain.

4. Review of related literature

Numerous quantitative research studies about Nobel Laureates and other people have been published. Maurya, A. examined the academic legacy of MIT's Chemistry Nobel Laureates in 2020 and concluded that the university creates extraordinarily prolific scientists. The most accurate measurement of research output that is currently available appears to be found in scientific publications. Nobel Laureate William Shockley was among the first authors to propose the number of research papers as a scientific indicator of research productivity (1957). Lehman (1958) talked about the ages at which scientists in various areas and nations reached their peak productivity as well as scientific inventiveness. He obtained data by counting the publications of scientists at a given age and found chemists' maximum production rate at ages 30 through 34. The publications of Nobel Laureate Jeffrey C. Hall during his 46-year productive life, which began in 1972 and ended in 2017, have been examined by Kumar, Ruhela, and Kumar (2018). Although the author has authored 201 publications, the years 1990-1999 saw a rise in his productivity. The author has 22 single-authored publications and 179 collaboratively published papers. His computed collaboration coefficient is 0.89. Jeffrey C. Hall published his works in 50 esteemed publications with a high impact factor; one of his 1999 studies was cited in 632 distinct papers. M. Rosbash was the most productive author he had worked with out of all the others. A reference curve for an Indian role model scientist has recently been established (Kalyane, Madan, & Kumar,



2001). According to the results of this pilot study, it is feasible to create a model that directly influences the identification of promising scientists and the development of human resources in developing nations by analysing the performance of a nation's role model scientist. Studies on individual scientists, including Nobel Laureates, are the present focus of science metrics. The Nobel Prize is thought to be the highest accolade bestowed upon scientific achievement. Because of the Nobel Prize's immense status, countries, institutions, and its laureates' reputations are all improved (Zuckerman, 1977).

5. Objective of the study

To achieve the goal, the study will precisely attempt:

- To analyse the distribution of research output of David MacMillan by year
- To find out the growth in publications
- To find out the rates of collaboration
- To analyse the domain-wise authorship patterns
- To find out the channels of communication
- To find authors' production over Time
- To find out the citation network
- To find out research article productivity.

6. Methodology

One of the most comprehensive and extensively utilised databases for

bibliometric analyses and literature reviews was the Web of Science database, which was employed for this study. We utilised End Note X4 as a bibliographic manager to organise the downloaded data. The articles and reviews were exported from the Web of Science using this application. The information that was looked for to fulfill the goal of this quantitative analysis included the following: author(s), addresses, editor(s), keywords, times cited, source, title, language, and Web of Science category.

First, articles and reviews were selected within the period taken from David MacMillan's 20 year social science citation index from 2006 to 2022, corresponding to the category "Author" of the Web of Science. Nearly 216 articles in the category "Author" were located overall throughout the previous seventeen years when utilising the search parameters (downloaded in February 2023). The degree of collaboration, co-distribution of journals, co-distribution of specialties, and cross-border co-operation between and within subject collaborations have been tested. Transformations in knowledge development, knowledge recency, knowledge refinement, or knowledge enrichment are also considered.

7. Results and discussions

7.1 *Distribution of research output by year*

Table 1 displays the distribution of Sir David MacMillan's whole body of research outputs as taken from the Web of Science databases between 2006-2022. A total of 216 research papers over 18 years were found, with an average of roughly 10 publications each year. According to Web of Science, his first publication came out in the year 2006, when he was 38 years old.

**Table 1: Distribution of research output of David MacMillan**

Actual age of David MacMillan (1968)	Year of Publication	Number of Publications under several authorships			Cumulative Total	Collaboration rate	Publishing age
		Single Authored	Multi-Authored	Total			
38	2006	1	6	7	1	0.85	1
39	2007	1	9	10	11	0.90	2
40	2008	4	5	9	20	0.55	3
41	2009	2	12	14	34	0.85	4
42	2010	0	14	14	48	1.00	5
43	2011	0	21	21	69	1.00	6
44	2012	2	6	8	77	0.75	7
45	2013	1	12	13	90	0.92	8
46	2014	0	18	18	108	1.00	9
47	2015	1	13	14	122	0.92	10
48	2016	1	10	11	133	0.90	11
49	2017	2	12	14	147	0.55	12
50	2018	0	12	12	159	0.85	13
51	2019	3	8	11	170	1.00	14
52	2020	0	11	11	181	1.00	15
53	2021	0	11	11	192	0.92	17
54	2022	1	17	18	208	1.00	18
	Total	19	197	216			

7.2 Collaboration rate

It is the ratio between multi authored papers and total papers published in a particular year or for a specific period. Sir David MacMillan published 11 single-authored papers throughout his 18-year publishing career, with the highest

collaboration rates being in the years 2010, 2011, 2014, 2021, 2019, 2020 and 2022 (1.00), while the lowest rates were in 1993, 2008 & 2017 (0.55). Additionally, table 1 shows that David MacMillan collaborated with others to publish the majority of his works. Out of 216 publications, only 19 (9%) were single-authored studies.

7.3 Growth of publications

Table 2: Block wise Relative Growth Rate and Doubling Time(Dt) of publications

Blocks	Year Range	Publications	Cumulative Total	Log _e N1	Log _e N2	Log _e N2-Log _e N1	RGR= Log _e N2 - Log _e N1 / T2-T1	Mean RGR	Dt= 0.693/ RGR	Mean Dt	Received Citations	Avg. Citations/ Publications	
1	2006-2008	26	26	-	3.258	-	-	0.016	-	44.134	2,456	94.46	
2	2009-2011	49	75	3.258	4.317	1.059	0.041		16.902		3,926	80.12	
3	2012-2014	39	114	4.317	4.736	0.419	0.006		115.5		6,187	158.64	
4	2015-2017	39	153	4.736	5.030	0.294	0.003	0.002	231	539	9,291	238.23	
5	2018-2020	34	187	5.030	5.231	0.201	0.001				693	13,228	389.05
6	2021-2023	29	216	5.231	5.375	0.144	0.001				693	11,309	389.96
		216									46,397	225.08	



Table 2 shows the rise of publications over 18 years, divided into six segments. The most publications were from 2009-2011(49 in total). The relative growth rate from 2009-2011 was 0.041, the highest of all the other blocks. Later, from 2015 to 2023, the mean RGR (Relative Growth Rate) was 0.002 with a doubling time of 539 and from 2014 to 2014, it was 0.016 with the value of the doubling

time being 44.134. A total of 216 documents received a total of 50,467 citations, averaging 234 citations per document. Table 2 also presents the citation patterns of the documents published in each block. 2005 to 2007 noted the highest number of citations for three years duration with 13,228 citations for 34 documents published at an average of 390 citations for each document.

7.4 Authorship pattern and most productive authors

Table 3: Authorship patterns of works by David MacMillan

Sl. No	Authorship Patterns	Number of publications	% of publications	Degree of collaboration
1.	Single authored	19	8.80	(as suggested by Subramanyam, 1983) $C = Nm/Nm+Ns = 197/197+19 = 0.91$ Where, C = Degree of collaboration Nm = Number of multi-authored papers Ns = Number of single authored papers
2.	Multiple authored	197	91.20	
	Total	216	100	

According to Wikipedia (dated 18.07.2022), collaborative papers refer to a distributed process of labor involving writing, resulting in the co-authorship of a text by more than one writer. A total of 216 publications have been published by David MacMillan, out of which he published only 19 (8.80%) publications under single authorship and 197 (91.20%) under multiple authorship. The overall collaboration rate has been found 0.91 which signifies most of the publications of David MacMillan were written in collaboration (Table 3).

7.5 Most productive and cited publications by David MacMillan

Table 4 represents the 10 most cited works of David MacMillan which all have more than 900 citations each since its publication. The most significant number of citations received by the work 'Visible light photoredox catalysis with transition metal complexes' which was a multi-authored contribution from David MacMillan and the documents published in Chemical Reviews in 2013 with 6313 citations till the time of data collection for this study which was in July, 2022. Others are listed below.

**Table 4: Most cited publications received by David MacMillan**

Sl. No.	Work Details	Total Citations Received (Till 25.07.2022)
1.	Prier, C. K., Rankic, D. A., & MacMillan, D. W. (2013). Visible light photoredox catalysis with transition metal complexes: applications in organic synthesis. <i>Chemical reviews</i> , 113(7), 5322-5363.	6313
2.	MacMillan, D. W. (2008). The advent and development of organocatalysis. <i>Nature</i> , 455(7211), 304-308.	2377
3.	Ahrendt, K. A., Borths, C. J., & MacMillan, D. W. (2000). New strategies for organic catalysis: the first highly enantioselective organocatalytic Diels–Alder reaction. <i>Journal of the American Chemical Society</i> , 122(17), 4243-4244.	2100
4.	Nicewicz, D. A., & MacMillan, D. W. (2008). Merging photoredox catalysis with organocatalysis: the direct asymmetric alkylation of aldehydes. <i>Science</i> , 322(5898), 77-80.	1993
5.	Shaw, M. H., Twilton, J., & MacMillan, D. W. (2016). Photoredox catalysis in organic chemistry. <i>The Journal of organic chemistry</i> , 81(16), 6898-6926.	1772
6.	Twilton, J., Le, C. C., Zhang, P., Shaw, M. H., Evans, R. W., & MacMillan, D. W. (2017). The merger of transition metal and photocatalysis. <i>Nature Reviews Chemistry</i> , 1(7), 1-19.	1249
7.	Zuo, Z., Ahneman, D. T., Chu, L., Terrett, J. A., Doyle, A. G., & MacMillan, D. W. (2014). Merging photoredox with nickel catalysis: Coupling of α -carboxyl sp^3 -carbons with aryl halides. <i>Science</i> , 345(6195), 437-440.	1174
8.	Nagib, D. A., & MacMillan, D. W. (2011). Trifluoromethylation of arenes and heteroarenes by means of photoredox catalysis. <i>Nature</i> , 480(7376), 224-228.	1106
9.	Nagib, D. A., Scott, M. E., & MacMillan, D. W. (2009). Enantioselective α -trifluoromethylation of aldehydes via photoredoxorganocatalysis. <i>Journal of the American Chemical Society</i> , 131(31), 10875-10877.	969
10.	Allen, A. E., & MacMillan, D. W. (2012). Synergistic catalysis: a powerful synthetic strategy for new reaction development. <i>Chemical science</i> , 3(3), 633-658.	945

7.6 Most cited article by David MacMillan

Out of 216 total papers from the Web of Science database, David MacMillan cited 71 papers from Journal of the American Chemical Society as his top choice, followed by 47 from Science and 15 from abstracts of

papers of the American Chemical Society. With 10 publications, US publishers were chosen over UK publishers in these top channels of communication for the publication of journal papers by David MacMillan.

**Table 5: Top communication outlets, according to David Macmillan**

Sl. No	Journal Name	Country	Published by	No. of Articles
1.	Journal of the American Chemical Society	United States	American Chemical Society	71
2.	Abstracts of Papers of the American Chemical Society	Washington, USA, DC, 20036	American Chemical Society	47
3.	Science	It is based in Washington, D. C., United States, with a second office in Cambridge, UK.	American Association for the Advancement of Science (United States).	15
4.	Angewandte Chemie International Edition	Weinheim, Germany	Wiley-VCH on behalf of the German Chemical Society (Gesellschaft Deutscher Chemiker).	14
5.	Nature	London, England	<u>Nature Research</u> (subsidiary of <u>Springer Nature</u>) (United Kindom)	13
6.	Chemical Science	United Kingdom	<u>Royal Society of Chemistry</u> (United Kingdom)	10
7.	Others			46
	Total			216

7.7 Imparting evolutionary recent research trends by bibliographic coupling network

Current research targets may be better reflected through the bibliographical coupling network years which is analysed

(Figure 1). Bibliographical coupling networks use bibliographical data sets as nodes, differing in co-authors and co-cited reference lists. From deep blue to light green, the nodes representing the articles have been published from 2006 to 2022.

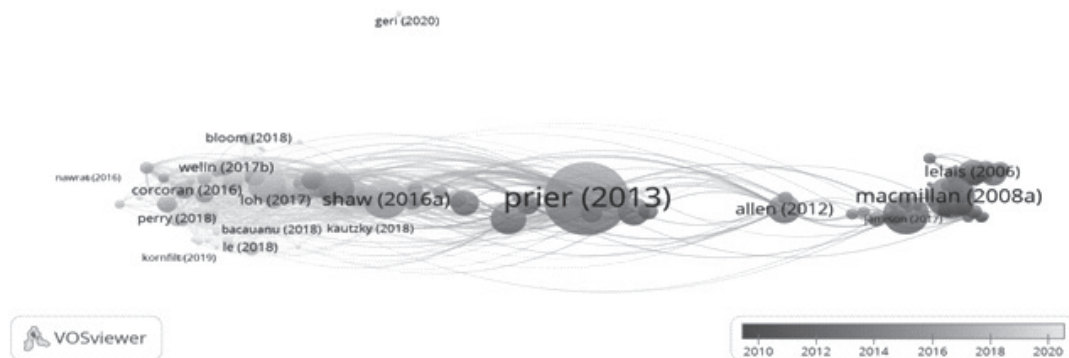


Figure 1: Bibliographical coupling network of the recent years for the articles published by David MacMillan



Many works have been investigated by David MacMillan and it has been noticed some highlighted nodes with big size. On the middle part of figure 1, the work represents "Visible light photoredox catalysis with transition metal complexes: applications in organic synthesis" (Prier et al. 2013). By investigating these representative works, we can notice some highlighted nodes with big

sizes. Some recent works on the topic of "Photoredox Catalysis" are also found.

Figure 2 represents the strongest citation bursts which are an indicator of a most active area of research. Citation burst is a detection of a burst event, which can last for multiple years as well as a single year. Figure 3 also figures out about top 6 keywords which depict strongest citation bursts.

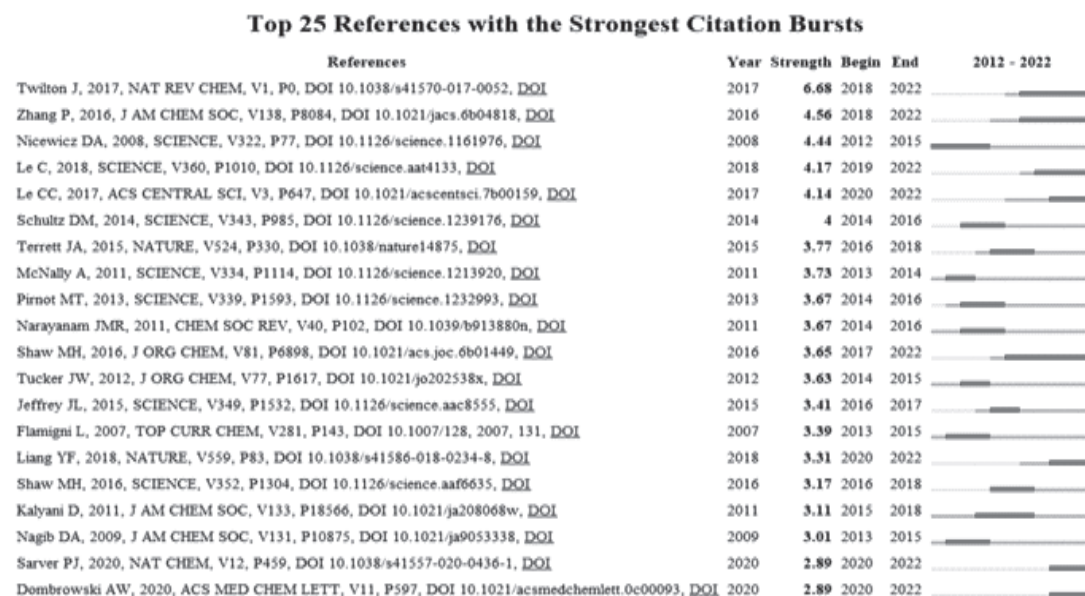


Figure 2: References producing strongest citation bursts

Top 6 Keywords with the Strongest Citation Bursts



Figure 3: Keywords producing strongest citation bursts

**7.8 Most bountiful authors****7.8.1 Authors with most collaboration**

Table 6 shows the list of co-authors who

have written two or more two documents with collaboration with David MacMillan till 2023. There are 10 co-authors listed with five publications at least.

Table 6: Collaboration of authors

Sl. No.	Co-authors Name	Journal Articles	Total	Affiliation	Designation	Research Interests
1.	Le, Chi 'Chip'	11	11	Princeton University, Princeton, New Jersey, United States.	Senior Scientist, Medicinal Chemistry	Chemistry; Microbiology; Gut Microbiome.
2.	C. Conrad, Jacinta	8	35	University of Houston, Houston, Texas, United States.	American soft matter physicist	Soft matter; Complex fluids; Colloids; Polymers; Bacteria
3.	Simonovich, Scott	6	10	Princeton University, Princeton, New Jersey, United States.	Director of Medicinal Chemistry at Princeton University	supramolecular chemistry and catalysis, Medicinal Chemistry
4.	Scholes, Gregory D.	6	621	Princeton University, Princeton, New Jersey, United States.	Professor of Chemistry at Princeton University	Spectroscopy; Physical Chemistry
5.	Zhang, Xiaoheng	6	12	Fudan University, Yangpu District, Shanghai, China	Organic Chemistry, Assistant Professor, Yangpu District, Shanghai, China	Photoredox catalysis. Transition metal catalysis. Total synthesis of structurally and biologically interesting natural glycoconjugates.
6.	Prier, Christopher. K	5	18	Princeton University, Princeton, New Jersey, United States.	Director of Enzyme Catalysis at Debut (a biotechnological research company), San Diego, California & Princeton University.	Applications of photoredox catalysis, in which visible light is employed to promote chemical reactions.
7.	Seath, Ciaran P.	5	6	UF-Scripps Biomedical Institute, Jupiter, FL, USA.	Assistant Professor of Chemical Biology; Department of Chemistry, Wertheim UF-Scripps Biomedical Institute, Jupiter, Florida USA.	Biochemistry and Cell Biology; Clinical and translational science; Pediatric brain tumors.
8.	Terrett, Jack A.	5	31	Genentech Inc, South San Francisco, California, United States of America	Senior Scientist in the Discovery Chemistry group at Genentech	Medicinal chemistry, Oncology, Photoredox catalysis, Organic synthesis
9.	Vander Wal, Mark	5	14	University of California, Berkeley. Department of Chemistry.	Medicinal Chemist/Scientist	Therapeutics, Neurology, Biochemistry & Molecular Biology Science & Technology - Other Topics Education & Educational Research
10.	Jui, Nathan T.	5	59	Loxo Oncology at Lilly; Boulder, Colorado, United States	Principal Scientist at Loxo Oncology at Lilly ; Boulder, Colorado, United States	Chemistry Pharmacology & Pharmacy Biochemistry & Molecular Biology Science & Technology - Other Topics Neurosciences & Neurology



7.10 Growth of publications

From 2006 to 2022, a span of 17 years of research output of Nobel Laureate David MacMillan has been measured. To understand the pattern of growth figure 7 describes the growth of publications with cumulative total of the publications, where the linear line indicates that the growth of publication was below till 2010 but then it was above the line till the end date of the study. Among the 17 years of each block, i.e. the year between 2018 to 2020 has noted the highest number with 28 research publications. This block has also

received the highest number of citations, which accounted for 13,314 citations at an average of 1551 citations per publication. A total of 50,467 citations were received by David MacMillan's 216 publications during the period. The average number of citations received per publication accounted for 234. 2018 to 2020 has been identified as the peak years of received average citations per paper with 749 citations. The graph of average citation noted an increasing ratio which proves that the publications have an impact as much as earlier publications.

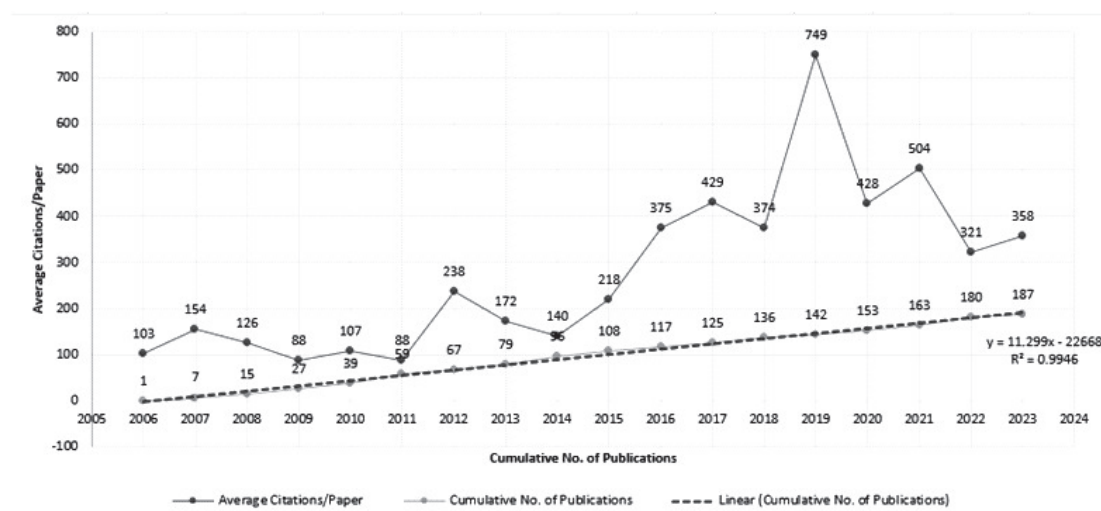


Figure 4: Growth of publications and average citation pattern

8. Major findings

Major findings of this research paper are listed below: -

- Out of 216 publications, 71.30 percent are journal articles indexed in Web of Science.
- From 2015 to 2022, the relative growth rate declined to 0.002 and the time for doubling climbed to 539, respectively, from 2015 to 2014 when the mean relative growth rate of his articles was 0.016 and the

doubling time was 44.134.

- Le, Chi Chip co-authored 10.8% of David MacMillan's 216 publications, making her the most prolific co-author.

The majority of his papers were written in collaboration, as evidenced by the 0.90 collaboration rate across all publications and published much of his studies were published in the United States based journal. Most of his top-cited



journals came from the US, UK and Netherlands with medium to high impact factor Journals.

- According to Web of Science citation counts, in May 2023, the h-index counted 107 due to the large number of papers he created that earned a lot of citations.

9. Conclusion

David MacMillan's first publication productivity was discovered in 2006, when he was 38 years old, and up to 2022 he had produced 216 works according to Web of Science database; the majority of which were journal articles. Many of his works have received a significant number of citations, and as of the time the data for this study were collected (June 2023), his h-index was 109. The mean relative growth rate was strong up until 2014, then in comparison, it started to decline. As a result, it took longer for publications to double later in the study period. David MacMillan has published most of his documents in collaboration with other authors, with only 19 documents published as single authored. He pioneered and specialized in the domain of Organic Synthesis and Catalysis. He received innumerable awards and honors including the Nobel Prize in 2021 at the age of 53 years. This pattern suggests that honours and awards a scientist receives may attract more collaborators resulting in accelerating publication productivity.

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