Using Citation Indexes, Citation Searching, and Bibliometrics To Improve Chemistry Scholarship, Research, and Administration

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ABSTRACT: Citation searching and bibliometrics are terms foreign to many chemists and educators, yet well-known and used by librarians and information specialists. This article aims to help chemistry students, educators, and other readers of this *Journal* to better appreciate and use these powerful and profound methods. Although these subjects have been described previously, several developments in the methods and new alternative metrics have occurred in the intervening 16 years, so the field is being reviewed again. Citation practices have also contributed to the study of bibliometrics which is used to evaluate publications, authors, and journals.

KEYWORDS: *First-Year Undergraduate/General, Second-Year Undergraduate, Upper-Division Undergraduate, Graduate Education/Research, Chemoinformatics, Computer-Based Learning*

INTRODUCTION

Over the past few decades, several articles have been published in this *Journal* and elsewhere about resources for and teaching methods and pedagogy of chemical information (ref 1 and references cited therein). However, most have covered reference works and indexed and abstracted databases both in print and online. Citation indexes and citation searching have been described previously in this *Journal*[2] as well as several additional articles reporting the pedagogical use of these methods, including the most recent[3] (fittingly on research articles on chemical education). Several developments in the methods have occurred in the intervening 16 years; thus, the field is being reviewed again to complement other articles in this special issue of the *Journal of Chemical Education*. In addition, the emerging field of bibliometrics, based on the general principles of citations of the literature, is being used to evaluate publications, authors, and journals, as well as individuals for performance and promotion.

HISTORY

Although searches for information have evolved considerably over the last several decades, an examination of the history of the resources involved and the genius of their creators should be described and acknowledged. In some cases, chemists and teachers may have encountered the previous resources and may not be aware of the improvements and additional opportunities currently available. For example, some readers may only know of the Chemical Abstracts database in its currently most available format: the end-user oriented SciFinder collection of databases. However, the database goes back to 1907 and before and has evolved from print format to computer readable portions to online availability within the STN family of databases, which are still produced and in use in many organizations including some in academia. In the case of citation searching, knowledge of the history and functioning of the SCI database, nee Science Citation Index, is essential to the understanding of the effective use and worth of citation

searching as well as the additional metrics which have evolved from it.

Everyone who has performed research, either "library" or laboratory, has searched for information by reading, by searching for key terms using text-based electronic resources, or by using abstracted and indexed reference works in print or electronic formats. For chemists, the latter resources have included Chemical Abstracts, both in print and as an electronic database (either on STN or on SciFinder), and Beilstein, both in print and currently as the electronic resource Reaxys from Elsevier. Once key references are found, most researchers have used the reference bibliography listed at the end of the article to search for prior information on the subjects and concepts in the key article.

In the 1950s, Eugene Garfield, educated as a chemist, including laboratory experience and as an indexer, was working on a research project at Johns Hopkins investigating computer-based processing of information. Those experiences led to his development of several novel chemical and scientific information resources. One of them, also inspired by Shepard's Citations that cited prior case law or statutes to establish legal precedence, was his proposal of citation indexes[4] and eventually the Science Citation Index (SCI).[5,6] The SCI, along with a number of related information resources and products, was produced and vended by ISI (the Institute for Scientific Information, founded in 1955). In 1922, ISI was sold to the Thompson Corporation, which became Thompson Reuters.

An excellent review of the history of ISI, its products and services, and Eugene Garfield himself can be found in the chapter by Bonnie Lawlor,[7] a long-term ISI employee, in a recent ACS Symposium Series book. An interesting fact is that in addition to the several, often revolutionary products and services spawned by ISI and Eugene Garfield, is that some consider Garfield to be the "Grandfather of Google" in that he

is cited as an inspiration for PageRank, the Google search algorithm.

Although machine-produced, the SCI first appeared as a reference in print but digital databases eventually were mounted on database producers and vendors, including Dialog and STN International (the SciSearch database) as well as the SCI database on the Web of Science (WoS) from Thomson Reuters.[8] The Web Of Science, formerly the Web of knowledge, contains the SCI in the subset titled the Web of Science Core collection. Of course, these online resources allow easier and more rapid searching.

A key inspiration for the need of the SCI was the perception that searching for text was virtually nonexistent and indexing was often rudimentary and insufficient to retrieve all of the relevant information. For the sciences, Chemical Abstracts and Biological Abstracts were key abstracting and indexing resources. Once found, the bibliographies of key articles could be consulted to provide prior relevant information of which the current author was aware. Once published, an article is not only a citing reference but a citable reference for future articles. The SCI can then be searched "forward" to find subsequent articles citing the key article of interest.

A valuable reference and resource for a number of chemical information topics and resources, including the Science Citation Index, is The Chemical Information Sources Wikibook.[9] It began as the digital update of the book *Chemical Information Sources* by Gary Wiggins.[10] Chapters are being updated by the original or other authors and experts.

Novel or otherwise unfamiliar concepts are difficult to search with either indexed or text-based resources. As described in the Chemical Information Sources Wikibook chapter on Author and Citation searches,[11] the print SCI was actually composed of three indexes: (i) the Source Index, organized alphabetically by author; (ii) the Citation Index, which lists articles in the stated time frame citing previous references; and (iii) a Subject Index, based on keywords in the titles of articles. Along with other resources, the Source Index and the Subject Index can be used to find key articles to process with the Citation Index. All three indexes are incorporated in the online databases.

The chapter on Author and Citation Searches[11] also describes the difficulties and pitfalls encountered in searching for authors (including corporate authors) in general in any database. Examples are presented for searching authors in the printed Chemical Abstracts, the CA databases on both STN and SciFinder, Beilstein in print and on Reaxys, Derwent World Patents Index, and PubMed. Examples of cited reference searching are presented for the SCI on WoS and the SciSearch database on STN. This chapter, like all of the chapters on the Wikibook, is in the process of being updated.

■ USE OF CITATION INDEXES

Use of the SCI, although featuring many advantages for searching, also has some disadvantages and deficiencies. Originally limited to about 3000 journals, including a plurality of chemistry journals, the source list on the WoS has been expanded to more than 8500 journals, deemed to be the most important in their fields. Journals covering sciences other than chemistry are included, but the latter constitute the majority (see the WoS Web site[8] for current coverage). This does represent the "cream of the crop", but even with the expanded journal list other resources, including Chemical Abstracts and Reaxys, they are significantly more comprehensive.

Also, as pointed out previously[8] and in other sources, documentation of author names is notorious for errors. Because the SCI is organized by the names of the authors of articles, the producers of the SCI try to systematize author names as much as possible. However, unlike the Chemical Abstracts and Reaxys databases which list the entire name when available (or initials when not), author names in the SCI are limited to last name and first initial (or first two initials if available). In all of these databases, it is possible to browse author names. In addition, in the early days of the SCI, only the first named author of multiauthored articles was listed and used for citation searching, which complicated author searches in the SCI. All authors are listed in the digital databases. For unusual names like Robert E. Buntrock (searching **Buntrock R or Buntrock RE** will suffice) or Paul von Rague Schleyer (searching **Schleyer P** works), there is little or no problem with accuracy. However, searching author names such as John Smith or Mary Jones by initials only will most likely yield a large number of erroneous results. Other problems with author names include varying surname/first name formats for Asian authors, midcareer name changes, and so forth. This problem of inaccurate attribution was described in a recent article.[12] "Super authors", actually composites of many authors with similar Chinese or Korean names, are described as each publishing more than 1000 articles per year garnering on the average of 1350 citations. Processes for systemizing author names—"author registry numbers"—are appearing, but not all authors are enrolled as yet. Thompson Reuters introduced ResearcherID[13] in 2008. ORCID, Open Researcher and Contributor,[14,15] was established in 2010 as a subset of ISNI, International Standard Name Identifier.[16] Data exchange between ORCID and ResearcherID has been established.

An additional problem that often occurs with citation searching is that the authors of citing articles may be interested in articles in their cited bibliography for reasons other than concepts of interest to the searcher. As with other modes of literature searching, citation searching can lead to "false drops". This inevitable problem of inaccuracy was encountered several times throughout the author's 44-year career as a chemical information specialist. At the large petrochemical company at which the author worked, it was discovered that a compound prepared by one of the chemists might not be new or novel after all. It was "mentioned" in the abstract of an English language journal of Japanese origin (*Bulletin of the Chemical Society of Japan*) but not described anywhere else in the article, and not even an experimental procedure was given. The patent attorney processing the disclosure asked the author to perform a search on the article in the Science Citation Index. More than a dozen citing articles were retrieved, but all of them cited the key article only for the novel NMR spectroscopy, not the key or related compounds. The attorney decided to err on the side of caution anyway and did not file a composition of matter patent (for a novel compound).

In addition to the SCI, the WoS includes additional citation databases originally created at ISI.[8]

- Conference proceedings Citation Index, covering 160,000 conference titles, an otherwise segment of "gray literature" not adequately covered by several other databases
- Social Sciences Citation Index, covering 3000 journals in the social sciences

- Arts and Humanities Citation Index, covering 1700 arts and humanities journals
- Book Citation Index, covering 60,000 selected books since 2005

The WoS also includes two additional databases: Index Chemicus, with 2.6 million compounds; and Current Chemical Reactions, with 1 million reactions. If one is searching for chemical compounds or reactions, searching these databases can yield key articles for further searching in the SCI.

PATENTS AND PATENT CITATIONS

Garfield also discussed the extension of citation searching to patents.[6] In contrast to the nonpatent literature, the patent literature is considerably more complicated, especially to the noninitiated. Before one delves into citation practices, it is advisable to consult one of the excellent resources on patents in general to act as a primer.[17,18] The one by Edlyn Simmons[17] describes citations in patents and also compares searching patents by searching with citations and by index terms, classification systems, and text. Citation of patents in the nonpatent literature is straightforward, treating patents like any other form of literature. This capability is available in databases including the CA database on both STN and SciFinder, IFI Claims Citations (U.S. Patents), WoS, and Google Scholar. However, citations included in patent documents come from two sources, the inventor and the patent examiner, and are included for different reasons. Although comprehensive searches for "prior art" are not required for submission of an application for a patent, the erstwhile inventor must submit any possible prior art they may be aware of, including any on which they are making novel extensions of the technology. The patent examiner also does not do a comprehensive search, but if any references are found that would reject the claims of the patent application, they are cited for the inventor to refute if the inventor is really entitled to be issued a patent. The examiner may cite general references in the area of the technology described. All such references become part of the patent record. Because examiner references can indicate where the examiner's search was done, they become fodder for those in the future who would try to find information to invalidate an issued patent by searching where the examiner did not. If all of this resembles, to an outsider, a jousting match or a duel with challenge and parry, it probably is. No wonder there are patent attorneys, agents, and expert patent searchers.

In her conclusions,[17] Simmons points out that if the area of technology, like chemistry, is well indexed, searching the indexed database provides the most rewarding results. However, even in these areas, citation searching can provide an excellent supplement to provide prior art with inadequate indexing or nomenclature. Of course, for those technological areas not very well indexed, typically mechanical or electrical, citation searching becomes more important.

BIBLIOMETRICS

Another area where literature citations have been extended is citation metrics—also known as bibliometrics, alternative metrics, or altimetrics—where data from citations is used to evaluate articles, patents, journals, research laboratories, and even individuals.[19,20] The evaluation of journals was key to the establishment and development of the SCI, as it was used to form the list of journals that were indexed. To be considered, typically a journal had to have both a significant number of references within its published articles as well as have its articles cited a significant number of times. Impact factors were determined and complied for both journals and articles and later extended to research laboratories.

Impact factors (IF) for journals[21,22] are also discussed extensively in Garfield's book in the book's longest chapter[6] and in two recent books.[23,24] The latter[24] is a compendium of previous articles on the subject of bibliometrics. IFs are calculated annually and listed in the Journal Citation Reports (JCR)[21] and represent the average number of citations to recent articles published in that journal. The IF for a given year (the year of publication of the JCR) is the ratio of the number of citations received for all articles published in that journal in the previous two years divided by the number of "citable items" that journal published in those same two previous years. The JCR publishes ranked lists, including breakdowns by discipline and by publisher.

Lists of highly cited articles are also published in Garfield's book and elsewhere.[6] Highly cited papers have been used to predict Nobel Prize winners for decades, beginning with Garfield. Highly cited papers tend to be papers on methodology and experimental procedures or review articles. Of course, citation counts are dependent on the elapsed time from publication, the field of research, and other factors. The phenomenon of "Sleeping Beauty" articles has been discussed recently.[25−29] These are articles that were poorly cited or even relatively ignored for years or even decades after their publication, but changing circumstances, often developments in fields other than that described in the original paper, caused the dormant research to become relevant. Even one of Einstein's papers falls into this category.[25]

Further extension of citation impact from journals and articles to organizations and authors is inevitable as discussed in books,[6,16,19,23,24] articles,[4,5,30] and even a dedicated journal, *Scientometrics*.[31] Raw counts of citations can provide hard data on both the use of the articles by subsequent authors and the impact of the work on further research.[6,30] This raw data, for a number of reasons, may not provide fair quantification of impact for individuals, so other measures have been proposed and used. One is the *h*-index or Hirsch index[14,32] (cited more than 1000 times), which can also be applied to the other subjects of bibliometrics, including journals and research departments. The *h* number is the number of an author's publications that have been cited *h* times, which is compared to all the other papers by that author that have been cited less than *h* times.[33] Therefore, the *h*-index represents the mean number of citations that an author's opus of publications has received. Several databases, including Google Scholar, Google Scholar Citations, Web of Science Core Collection (WOS), and Scopus, provide calculations of *h*-indexes.

The *g*-index[34] is based the distribution of citations to an author's publications, which depends more on the citation counts for highly cited papers. The *h*-index is described as being insensitive to both lowly cited articles (including uncited articles) and highly cited articles. Evidence is given for the use of the *g*-index to correct those oversights.[35] The i10-index was created in the development of Google Scholar[36] as a method of correcting deficiencies in use of the *h*-index. It is a measure of the number of an author's publications that have received 10 or more citations in other publications. Calculations of both the *h*- and i10-indexes are performed in the summary of the results of a citation search in Google Scholar Citations.

The use of both *h*- and *g*-indexes has limitations, several of which are discussed.[19,23,24,33,37,38] The indexes provide more appropriate data for comparisons of scientists within the same fields or disciplines. Eminent chemists have been ranked by *h*-number.[39] Authors who publish in a number of disciplines (interdisciplinary) can be improperly evaluated. The value of published research of an interdisciplinary nature may be either enhanced or devalued. Self-citations can enhance one's *h*-index. Both highly cited and poorly cited articles may not be properly recognized. The index tends to favor career longevity but can also penalize authors with a small number of highly cited articles. The *h*-index can vary significantly, depending on the database used and which publications are covered, both by genre and by source journal. Discussion of a recent article with more than 1000 authors pointed out that the *h*-factors of the authors may be distorted.[40]

These extensions of citation impact to individuals are not without controversy. Although it has become common practice for organizations, especially universities and colleges, to place extensive value of citation impact on the employability (or tenure suitability) of individuals, such extensive contributions to personnel evaluations has come under fire from many quarters. Misuse of citation metrics for evaluation of individuals has been debated and discussed for decades, even before the advent of the *h*-index (ref 6, Ch. 10). As Garfield succinctly stated, "Citation data is subtle stuff" (ref 6, p 241). An additional in-depth and statistical analysis of citation metrics ranging from the significance of citations through impact factors and *h*-indexes and their misuse has been published.[22,41] The interest continues as described in recent articles[42,43] and references cited therein.

■ SEARCHES

Comparisons are made between the similarities and differences between searches run on Google Scholar and the Web of Science (WoS) as well as citations to similar searches on other databases.

Previously, when searching for cited references in the print SCI, one had to search for the first named author, although author searches for source references could be done regardless of author name order. However, this limitation is eliminated when searching the digital version of the SCI. Cited references can be found for the chosen author regardless of name order on the publication. There exist examples in the literature of searches in the print SCI on SciSearch,[6,11] on STN,[2,11] and on the WoS.[11,44] Instructions for searching Elsevier's Scopus[45,46] are given in the Scopus Tutorials Menu.[47] Cited reference data can be found for references retrieved in SciFinder.[48,49] Displays of citation information from a variety of databases are also shown.[49] Unlike searching SciSearch on STN, cited reference searches cannot be performed directly in SciFinder, but citing references to articles retrieved by keyword and other search methods in SciFinder can be displayed.

If the same cited references search is performed in different databases, the results will most likely be different for a number of reasons, including source publications covered, the date range of the database, and differences in author citation. As one is probably most familiar with one's own publications, searching oneself will probably make possible the best comparisons.

To illustrate comparisons of the various databases, the author updated searches run in 2011 for a publication comparing Google Scholar (GS)[36,50] and SCI on WOS for both publication coverage and citations.[50] In that study, variability

in coverage of publications led to differences in retrieval (Table 1). The overlap in retrieval was 47, and 57 publications

Table 1. Results of Searches for Citations to Publications of R. E. Buntrock

Database Searched	Publications Retrieved	Total Citations	*h*-Index	i10 Index
GS 2011	81	ND[a]	ND[a]	ND[a]
WOS 2011	90	ND[a]	ND[a]	ND[a]
GS 2015	51	ND[a]	ND[a]	ND[a]
GSC 2015	140	199	8	7
GSC 2010+	ND[a]	46	3	1
WOS 2015	95	144	7	ND[a]

[a]Not determined.

retrieved from WOS were not found in GS. Citation data results were more erratic in the GS retrieval, and other comparisons were described, including the observation that entries in GS were more prone to errors possibly because they were scanned into the database.

The original intent was to compare Google Scholar Citations (GSC)[50,52] with WoS. Google Scholar Citations allows users to better manage citations to their publications. However, the beta test of GSC was nearing completion, and the full version of the database was not available. An update search on GS (using the recommended strategy **author:"r buntrock" or author:"re buntrock" or author:"robert e buntrock"**) yielded only 51 references. Not all of the author's publications in the last four years were included, and several of those previously retrieved were missing for unknown reasons. Recent "publications" that were included were letters to the editor for both *Nature* and *Chemical and Engineering News*. Publications from the 1980s and 1990s in the magazines *ONLINE* and *DATABASE* are erratic, some are there, some are not. Out of three patents, only the most recent is included (with 3 citations). None of the author's several dozen book reviews in *Choice* from the ALA (American Library Association)[53] are included.

Searching GSC for the first time yielded some surprises. The search strategy is much simpler: **author:"Robert E Buntrock"**. More publications were retrieved, 140, with 199 total citations, an *h*-index of 8, and an i10 index[38] of 7. For more recent publications, since 2010, 46 citations were found with an *h*-index of 3, and an i10-index of 1. Eight articles have 9 or more citations and 100 have no citations. This shows how misleading the *h*-index can be. Of the 29 references with 2 or more citations, all 5 of the author's chemistry publications, including three patents, are included. The remainder are on various aspects of chemical information, including book reviews. The two coauthored papers on end-user searcher training are in third and seventh place, with 17 and 10 citations. As in the GS search, letters to the editors of *Nature* and *Chemical and Engineering News* were included. The discrepancies between the search results from GS and GSC are yet to be explained.

Searching the SCI in the WOS database yielded 95 references with 144 citations, 117 citing articles, and an *h*-index of 7. The strategy used was searching Buntrock R* in the author field, the "*" being the truncation symbol. The data for citations minus self-citations was 123 and that for citing articles minus self-citations was 109. The average number of citations per article is 1.52, and bar graphs are provided for published items per year and citations in each year. The publication and citation histories are interesting. Seven papers have been cited

more than the *h*-index of 8. With a few exceptions, citation figures are similar to but not always identical to the figures from the GSC search. Coverage of the author's articles in *ONLINE* and *DATABASE* magazines seems comprehensive, as well as the author's letters to the editors, but all of the author's book reviews since 2007 are absent. The *Journal of Chemical Education* is covered by the Web of Science Core Collection, but book reviews since 1984 are not covered. The only book reviews covered are from the journals *Science*, *Nature*, and *The Scientist*.[54]

Bottom line: from an information science perspective, in citation searching both recall (number of relevant resources retrieved) and comprehension (proportion of known relevant references retrieved) are dependent on the resource used. As with using all resources on the Web, the date of the use should be documented because the content of the resource and the retrieval can vary. In addition, not all relevant resources may be available to all students and educators, especially those in schools with less funding available for such resources.

CONCLUSIONS

Citation searching is an often-neglected but powerful searching method. Its extension to evaluating articles, journals, organizations, countries, and individuals—virtually all predicted and practiced by Garfield, ISI, and now Thomson Reuters—has helped create the field of bibliometrics. Users must be aware of the limitations of citation searching because there are several reasons to cite a prior paper. Acknowledging prior research is a primary reason, but that attention can be positive (agreement with the significance and accuracy) or negative (disagreement with the significance or accuracy, or citing a portion of the prior article for reasons not of interest to the searcher). Journal coverage and timing are very important to all aspects of citation searching and analysis. Additional pitfalls are encountered when the bibliometrics are extended to evaluations in all categories, especially for evaluating individuals for hiring, firing, and promotion. The data derived is also dependent on the field or fields of study as well as the other limitations already described.

Many veteran searchers, especially those in chemical information, prefer searching indexed databases as primary sources for accuracy, efficiency, and comprehension instead of citation searching or text searching using Google and similar resources. However, citation searching can be a powerful supplement to the primary sources to provide additional information and insight. Instruction in and training for searching for information, including citation searching, should be part of the chemistry curriculum for both undergraduate and graduate students. Bibliometrics are also important to scientists and the organizations in which they work.

Hopefully, readers are inspired to utilize citation searching and bibliometrics in their acquisition and evaluation of information as well as to gain awareness of the expanding use of bibliometrics to evaluate people and organizations.

SOURCES

Google Scholar and Google Scholar Citations are no-cost (Open) services available on the Web. STN and SciFinder are fee-based services of collections of databases available from the Chemical Abstracts Service (CAS). WoS and Scopus are fee-based services available from Thomson Reuters and Elsevier, respectively. However, WoS allows users to limit search results to open access (OA) articles. The WoS also has links to the Google Scholar version of a citation as well links to the OA version of the article in the PebMedCentral database. The author does not have access to Scopus but has library proxy or on-site university access to WoS and *Nature*. Wikipedia articles are cited in addition to key references cited therein or elsewhere because several of the sources cited may be not readily available to independent scholars and those in smaller schools with fewer library and information resources. In addition, some of the Wikipedia articles cited provide an excellent history of developments in the programs or services cited. Owing to an expert volunteer editorial board, the chemistry articles in Wikipedia, especially the data, are accurate and excellent.[55] An ACS symposium on chemistry in Wikipedia and a workshop on authoring and editing Wikipedia articles were recently described in *Chemical and Engineering News*.[56] For more on chemical information in Wikipedia, see "Improving Information Literacy Skills through Learning To Use and Edit Wikipedia: A Chemistry Perspective"[57] in this issue of the *Journal*. It would appear that the relevant information and bibliometric articles in Wikipedia are also accurate and excellent, although it is not known if a similar editorial board exists.

Those using citation searching and bibliometrics should work with science librarians at their schools for advice, and resources such as the Research Impacts Using Citation Metrics site at the University of California Irvine.[58]

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Notes

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