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The Concept of the *Imploded Boolean Search*: A Case Study with Undergraduate Chemistry Students

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Ⓢ *Supporting Information*

ABSTRACT: Critical thinking and analytical problem-solving skills in research involves using different search strategies. A proposed concept for an "Imploded Boolean Search" combines three unique identifiable field types to perform a search: keyword(s), numerical value(s), and a chemical structure or reaction. The object of this type of search is to help refine, narrow, and speed the searching process for finding relevant information, which would otherwise yield humanly unmanageable result sets. This search strategy is introduced to third year chemistry students in an information literacy workshop using SciFinder, Reaxys, and Web of Science Structure Search. The aim of the workshop is to help students develop hands-on familiarity on the use of chemistry databases and search strategies for scientific information retrieval. The "Imploded Boolean Search" adds a new skill set to a student's arsenal of search strategies. A survey and training exercise are used to assess the workshop.

KEYWORDS: *Upper-Division Undergraduate, Graduate Education/Research, Chemoinformatics, Internet/Web-Based Learning, Problem Solving/Decision Making, Testing/Assessment, Applications of Chemistry, Student-Centered Learning, Undergraduate Research*

■ INTRODUCTION

The Chemistry Department at University College London (UCL) is the oldest in England and ranked as one of the best in the country.[1] It has an undergraduate intake of about 100 students per year and a low student/staff ratio.[2] Chemistry is offered either as a three-year BSc or as a four-year MSci where students take more advanced courses and research projects. Each year, the library offers an hour and a half workshop on literature searching techniques for third year chemistry students utilizing three different databases of chemical information (i.e., SciFinder, Reaxys, Web of Science Structure Search), thereby enabling students to see the strengths and weaknesses of each. The focus on the workshop is on chemical structure and reaction searching and introduces the concept of an "Imploded Boolean Search." The unique fields in chemistry allow for combining text and nontext searching. The proposed idea of an "Imploded Boolean Search" combines three unique identifiable field types: keyword(s), numerical value(s), and chemical structure or reaction (Figure 1a). Numerical values may include data such as melting point and viscosity range. Chemical structure or reaction may also allow for assigning stereochemistry, geometry and bond order; incorporating selective R-groups, system- or user-defined generics, atoms, ligands; and determining the topology of the atoms and connections in the structure. In an "Imploded Boolean Search," the search is compressed (i.e., collapses inward) by combining these three unique search fields in order to extract relevant information. This can be compared to a normal search were researchers combine keywords and/or numerical values when searching for information[3] (Figure 1b). The object of an "Imploded Boolean Search" is to allow for greater precision in finding relevant information by refining and narrowing down data, which would otherwise yield humanly unmanageable result sets. The search process would end up saving researchers' time. This combined type search is in contrast to the explode search option (i.e., automatic explosion) in databases like PubMed, which allows a searcher to include more specific subheadings beneath the broader subheading and thereby broadening the search. Jiang et al. recently published a paper that describes a combined search for a heterogeneous chemistry database by combining structure and compound property search results.[4]

The jungle of chemical information and data is overwhelming and continuously increasing as evident from the content of different scientific databases (Table 1). The size and complexity of chemistry databases make it essential for users to use a combination search involving a structure or reaction, numerical value(s), and keyword(s). This is particularly important to academic and industrial chemists who search the literature for specific or structurally similar molecules and reactions. For example, a search for cisplatin (CASRN 15663-27-1) in SciFinder yields 84,072 references from which there are 3596 on reactions and preparations, 1748 on property data, 499 on spectra, and 67,597 on use/applications,[5] while Reaxys yields 3368 references from which there are 545 on reactions and preparations, 73 on property data, 76 on spectra, and 3000 on use/applications.[6]

■ BACKGROUND

George Boole (1815−1864), the British born mathematician and philosopher, was the inventor of Boolean algebra from which he proposed three operations, AND, OR, NOT and used these operators to analyze and compare mathematical functions termed as "Process of Analysis."[7] Many databases perform searches with these three main Boolean operators directly with

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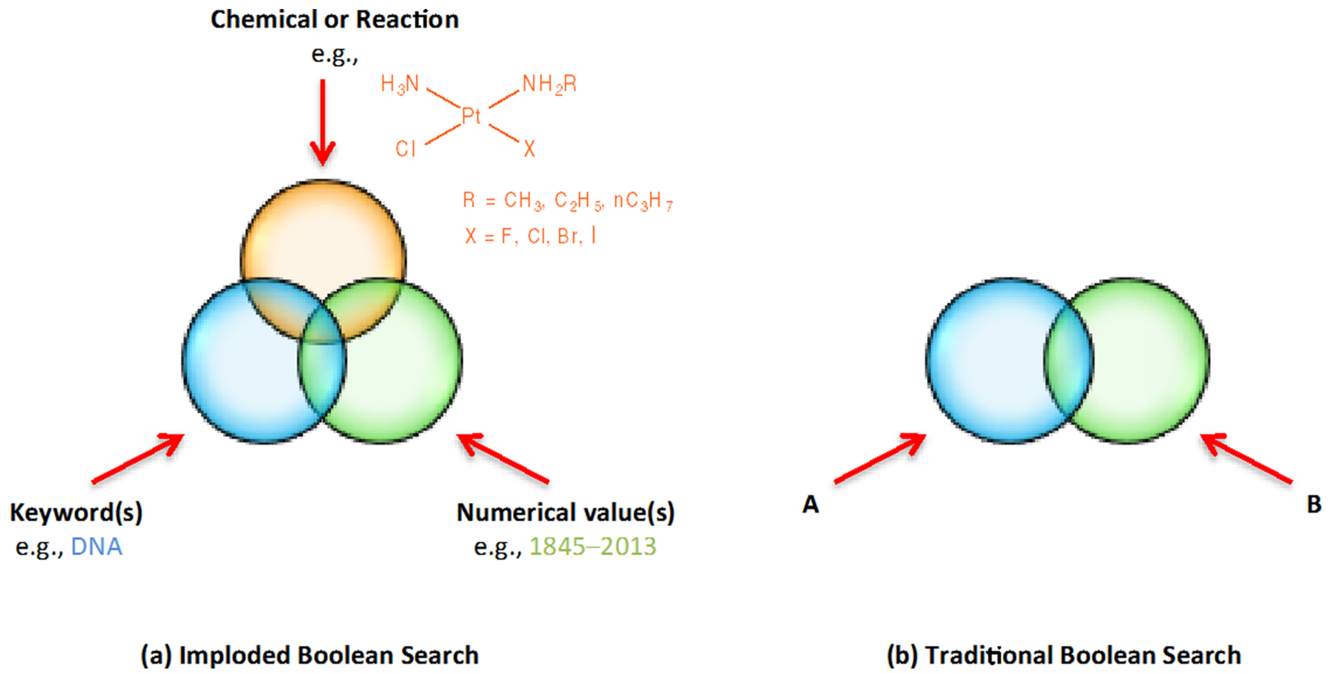

Figure 1. Venn diagrams showing the "Imploded" and "Traditional" Boolean search.

terms (i.e., keywords or numericals) or combine hit sets. A search that uses AND yields results that contain *all* the entered terms appearing together, while a search that uses OR yields results which contain *at least one* of the terms in the search. The OR operator searches simultaneously for *any one* of the synonyms such as "DNA OR deoxyribonucleic acid." The NOT operator *excludes all* results that contain the term(s) entered. Hence, the AND and NOT operators narrow a search, while the OR operator broadens a search. Many databases further allow for phrase searching, proximity searching, stemming, and other forms of lemmatization techniques.[3,8] Academic librarians often use the concept of Boolean operators during database instruction to show students how to narrow and broaden a search.

The American Chemical Society (ACS) has laid out the importance of information literacy for undergraduate degree programs stating that "Both library and online exercises should be a part of such instruction on information retrieval."[9] The Special Libraries Association (SLA), Chemistry Division (DCHE), working with the ACS Division of Chemical Information (CINF) outline a comprehensive document of resources recommended for chemistry undergraduate students, which includes SciFinder, Reaxys, and Web of Science.[10] The Association of College and Research Libraries (ACRL), a division of the American Librarian Association, further outlines information literacy standards for science, engineering, and technology disciplines to which performance indicators in "Standard Two" emphasize the importance of designing effective search strategies.[11] Many science departments have integrated information literacy components into courses. Incorporating chemistry databases in introductory and advanced information literacy training workshops has been detailed and predominately applied for SciFinder,[12−28] Reaxys,[14−16,20,23,29,30] and Web of Science.[14−16,18,19,26,31] Few studies have been able to evaluate the use of Web of Science Structure Search in the past due to subscription costs, however this has changed in the past year with a bundled discounted pricing offered by Thomson Reuters. Unlimited simultaneous access to chemistry resources such as SciFinder has opened up opportunities for librarians to conduct instruction workshops for all course levels. Due to time limitations, few workshops reported in the literature have incorporated three or more databases into one session. However, it is important to teach students not to solely rely on one database or on one search strategy. A thorough literature search will always require the use of more than one database and more than one search strategy.

For many workshops, in-class exercises are essential learning tools for helping students understand concepts, while experimenting with different search strategies for finding information. In-class exercises also provide an opportunity for students to ask questions during a workshop in the presence of a library instructor. Obtrusive and interactive face-to-face assessment of students' performance on an exercise during the class helps students understand the database functionality using search strategies, and at the same time provide feedback on how well concepts are grasped. In addition, assessing students' answers to problem sets after class provides information for possible modifications to exercise questions and presentation material for better learning outcomes in future workshops. According to Ferrer-Vinent,[25]

These exercises provided the students some individual, hands-on practice with available instructor help and allowed them to ask questions based on what they did. In addition, the instructor used immediate review of the exercises to highlight some points and introduce new ones.

Moreover, incorporating course credit to exercises adds legitimate weight to the value of using search strategies with databases for finding information. Surveys from workshops are also important as they provide new ideas and suggestions for helping librarians improve the workshop. Swoger and Helms state that, "Assessment results and student comments have helped librarians and faculty clarify confusing concepts and improve their presentation of material during the session."[28] Workshops dealing with search strategies and databases should also be introduced for training postgraduate students and postdoctoral scholars since research is the most essential

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Table 1. Comparison of SciFinder, Reaxys, and Web of Science Structure Search

	SciFinder	Reaxys	Web of Science (WoS) Structure Search
Database Coverage	CAS REGISTRY (Chemical substances, 1957–present) CAplus (References, 1907–present) CASREACT (Reactions, 1840–present) CHEMLIST (Regulated chemicals, 1980–present) CHEMCATS (Chemical suppliers, 2013–present) CIN (Chemical Industry Notes, 1974–present) MARPAT (Markush, 1961–present) Also searches, MEDLINE (1946–present)	Crossfire Beilstein (Organic chemistry, 1771–present) Crossfire Gmelin (Inorganic/Organometallic chemistry, 1772–present) Patent Chemistry Database (1976–present) Also searches, PubChem	Current Chemical Reactions (Organic chemistry, 1985–present, includes Institut National de la Propriété Industrielle (NPI) structure data, 1840–1985) Index Chemicus (Organic chemistry, 1993–present)
Content	>**101 million** organic and inorganic compounds >**5.8 billion** property values >**66 million** DNA and protein sequences >**41 million** records >**80 million** single and multistep reactions, and synthetic preparations >**344,000** inventoried/regulated substances >**102 million** commercial chemicals >**1.7 million** record industry notes >**1 million** Markush structures >**448,000** patent records (MEDLINE >**22 million** references)	>**26 million** compounds >**39 million** reactions >**50 million** citations (PubChem >**68 million** compounds. >**198 million** records)	>**1 million** reactions >**140,000** reactions from NPI >**4.8 million** compounds
Indexing	>50,000 journals >1,500 core journals[a] 63 patent authorities (Also, conference proceedings, technical reports, books, dissertations, review meeting abstracts, Web preprints)	>16,000 journals >400 core journals[b] WO, US, EP patents	>200 core organic chemistry journals[c] 39 patent authorities
Searchable Information	Structures, reactions, numeric data, property data, text searchable	Structures, reactions, numeric data, >500 chemical and physical data fields, text searchable	Structures, reactions, numeric data, cited references via WoS, text searchable
Updates	CAS REGISTRY (~15,000 new substances added daily), CAplus, CASREACT (~150,000 single- and multistep reactions added weekly), MARPAT, MEDLINE – **Daily** CHEMCATS, CHEMLIST (>50 new substances/additions added weekly), CIN – **Weekly**	**Biweekly**	**Weekly**

[a]In SciFinder, bibliographic information and abstracts are added for the 1,500 "core" journals to the CAPlus file within 7 days (https://www.cas.org/content/references/corejournals). [b]In Reaxys, the 400 "core" journals are used to index structures, reactions, and properties (http://www.elsevier.com/__data/assets/pdf_file/0005/91616/R_D-Solutions_RX_Fact-Sheet_DIGITAL1.pdf). [c]In WoS Structure Search, the 200 "core" journals are "world's leading organic chemistry journals" (http://wokinfo.com/media/pdf/wos-core-coll-brochure.pdf).

academic component with these researchers. This study outlines an advanced chemistry workshop, directed toward critical thinking and analytical problem-solving skills.

■ OBJECTIVES OF WORKSHOP

This case study introduces the concept of an "Imploded Boolean Search" as an additional search skill set to encourage and enable creative thinking with a focus on structure and reaction searching. In addition, the class was aimed to raise students' confidence level via hands-on familiarity in the use of search strategies with chemistry databases for conducting a thorough literature review on a research question or topic statement. The workshop objectives are in line with information literacy standards set by the ACS Committee on Professional Training[9] and the ACRL in "Standard Two" for effective search strategies.[11] The effectiveness of the workshop was assessed by a training exercise and survey.

■ METHODOLOGY OF WORKSHOP

A literature searching techniques workshop was conducted for third year chemistry students at the start of the Fall semester. To accommodate all students, the workshop was offered four consecutive times, each lasting an hour and a half for up to 25 students. Students were asked to register on SciFinder before class by going to the chemistry support guide for directions to the registration process. Upon arrival, students were asked to sign-in with their name and e-mail address. Each session included a 60 min PowerPoint presentation blended with demos of Web of Science Core Collection, Web of Science Structure Search (accessed from Web of Science Core Collection via Index Chemicus and Current Chemical Reactions), SciFinder, and Reaxys. The presentation started by describing the importance of planning a search strategy and worked toward structure and reaction searching using caffeine as the example in the demos (Supporting Information, Appendix I). Following the demos, students were given 30

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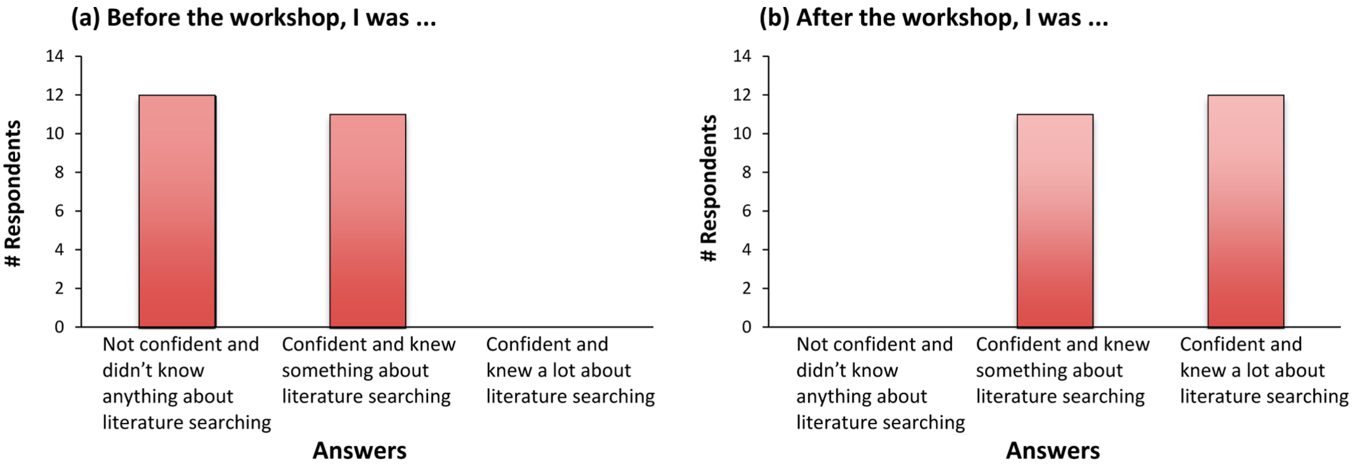

Figure 2. Students confidence with literature searching. The survey was conducted in Fall 2014.

min to work on the databases using a training exercise (Supporting Information, Appendix II). The exercise was collected after class, while the answer key, PowerPoint slides, and a quick guide to ACS citation style were e-mailed to all students the following week. Students were also free to collect their assignment from the librarian's office. An online survey (eSurv.org) was delivered three times during the following 3 weeks via e-mail to all workshop attendees. The survey consisted of 9 questions (6 close-ended and 2 open-ended questions; Supporting Information, Appendix III).

■ EXERCISE EVALUATION

The in-class exercise consisted of three questions with parts to each question. Students were asked to use ACS citation style. A total of 67 students submitted the exercise after class. Question one required students to create a search strategy in Web of Science for finding a review article within five years on a given topic. Most students were able to successfully provide some citation data. A few students just gave the search strategy using Boolean operators, as discussed in-class, without a reference to the review article. Knowing the elements of a citation is a concept that merits a higher level of understanding and would require further instruction.

Question two consisted of four parts and required students to use either SciFinder or Reaxys for each part. The first and second parts asked students to retrieve the CAS registry number and structure of L-Tyrosine, respectively. All students were able to successfully answers both parts correctly (100%) and most used SciFinder. SciFinder now has a "handbook" format in the Substance Details which improves readability and user-friendliness through a menu that highlights important scientific content areas including experimental properties and experimental spectra. The third part (2c) asked for one literature reference that supports the melting point of L-Tyrosine to which all students except five (93%) were able to answer correctly using Reaxys. One student just stated the DOI number, one student gave a different reference source, and three students left the question blank. The fourth part (2d) required students to find a reference to a spectrum for L-Tyrosine from which 61 out of 67 students (91%) answered correctly, while 6 students left it blank. Interestingly, those students who left question 2c blank also left question 2d blank, and this could have been attributed to time constraints. A few students did not include page numbers with their reference source and most just cited the source as they saw it in the database. No student was able to successfully supply a correct ACS citation format to any of the references. Evidently, this suggests a need of bibliographic management workshops designed specifically for scientists. A quick guide to ACS citation style was e-mailed to the students after assessing the training exercise. The high scores for correct answers are partly attributed to the high calibre of students, but also and more likely, it is a reflection of the clear instruction provided by the science librarian.

The third question asked students to find the number of reference hits by carrying out an "Imploded Boolean Search" using SciFinder, Reaxys, and Web of Science Structure Search. This question involved a search for the DNA binding of L-Tyrosine, between the years 1900 and 2013, and resulted in SciFinder yielding the highest number of references, while Web of Science Structure Search yielding the lowest number of references. SciFinder's capability with searching CAS and MEDLINE simultaneously often explains the high number of hits. A total of 40 students attempted this question, while 18 students obtained at least one answer in agreement with the key. Depending on the search term(s) used, the answers may vary. The question also asked students to provide reasons why different databases give different numbers of search hits using the same search strategy. Student referred to journal selection, subject coverage, number of journal articles, and other documents, as well as to indexing of terms:

Different sources, different access to resources, slightly different search engine processes.
Each search engines searches with different parameters.
Different search algorithms in each database.
The search spans different areas of research.

Table 1 illustrates why different databases yield different results and includes factors such as the size of the database, scope of coverage, number of sources indexed, and update frequency.

■ SURVEY ASSESSMENT

A total of 76 students attended the workshops. Twenty-three students responded to the survey (30%). There were 52% male and 48% female students. The majority of students had *never* used any of the databases: Web of Science (64%), Web of Science Structure Search (82%), Reaxys (86%), and SciFinder (86%). Students rated the workshop as either good or excellent (96%).

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From the survey, the majority of students stated that at the start of the workshop they were either "not confident and didn't know anything about literature searching" (52%) or "confident and knew something about literature searching" (48%), while no student (0%) stated that they were "confident and knew a lot about literature searching." After the workshop, *all* students (100%) stated that they were either "confident and knew something or a lot about literature searching after the workshop" (Figure 2). Clearly, the workshop has an impact on students' confidence with their information literacy skills.

The first open-ended question asked students what they liked most about the workshop to which several positive aspects and opinions were emphasized:

Advice given on literature searching and how to find chemistry reactions.

Learning about new ways to track down information.

Unlocked a vault of information I didn't know existed.

One student mentioned the usefulness of the training exercise stating, "*The practice problems were a good example of how to use the databases and search functions,*" while another student suggested, "*Given practice problems with immediately available 'answers' to show the search has been done correctly.*"

The second open-ended question asked for possible workshop improvements to which students commented on the benefits for offering such workshops earlier in the degree program as well as other suggestions:

Should be offered in first or second year.

Research techniques should be taught in years 1 and 2. At year 3 it is a little late.

Should be offered from first year, particularly for organic chemistry.

Smaller group sizes.

Leaving more time to complete the exercises for practice.

From the survey and classroom interactions, it was discovered that students would have preferred such database and structure searching workshops earlier in the degree program. The lack of advanced structure searching workshops at the University is attributed to a serious failure by senior library management with hiring permanent qualified science librarians who are knowledgeable in the use of sophisticated scientific resources and have an understanding in the fine arts of the subject area. Further, given the high subscription costs and usefulness of chemistry databases for quickly finding spectral, chemical, and physical properties, it makes it all the more important for libraries to inform, make aware, and train students in the use of these resources. The comments for smaller group sizes, more time spent on the in-class exercise, and providing an answer key to the exercise toward the end of class are planned for improving this workshop in the future. Some students mentioned that they would have liked to see more example searches. One student mentioned that the workshop "*Should be done after we got our titles so that we can practice with searching our literature project.*" It is recommended that an exercise could be started in class and completed as an outside assignment for course credit. Adding course credit to a workshop exercise reaffirms to students the legitimate importance on the use of search strategies and databases for a thorough literature search. It was evident from the survey responses and classroom interactions that students recognized the value of introducing scientific databases, applying different searching skills, and the importance of the science librarian for help and guidance.

THE "IMPLODED BOOLEAN SEARCH"

Survey question 6 revealed that the majority of students (57%) plan on using an "Imploded Boolean Search" as a search strategy for finding information (Figure 3). There are different ways of approaching an "Imploded Boolean Search" from a database. The substances and reactions icons in Reaxys contain the structure editor as well as an option for adding fields on an form-based page. Specific field types can be added from different categories (e.g., identification, physical data, spectra, ecological data, use/applications, natural product, quantum chemical data, reaction data, bibliographic data). These fields can then be combined using the AND or NOT operators. The Web of Science Structure Search also contains a form-based page for data entry that uses an implicit AND operator, but it is somewhat clunky for adding functional groups in the structure editor and keyword insertion. The Web of Science Structure Search searches mainly for organic compounds and does not yet allow for effective functional group variations in compounds, however, atom and bond modification can be performed by right-clicking on the mouse. As database structure capability and functionality tools evolve, the searching for molecules or reactions, keywords and numerical values is likely to improve. In SciFinder, a search can be performed stepwise from an initial structure or reaction search, followed by filtering by keyword(s) and various numerical data. Reaxys also allows for a stepwise filtering search approach. SciFinder,[8,32] uses natural language processing algorithms, which does not allow for Boolean operations in the standard way, but instead uses parentheses (e.g., "DNA (deoxyribonucleic acid)" rather than "DNA OR deoxyribonucleic acid"). In addition, SciFinder retrieves variant forms of search terms via an automatic truncation process at various positions within the term.[8]

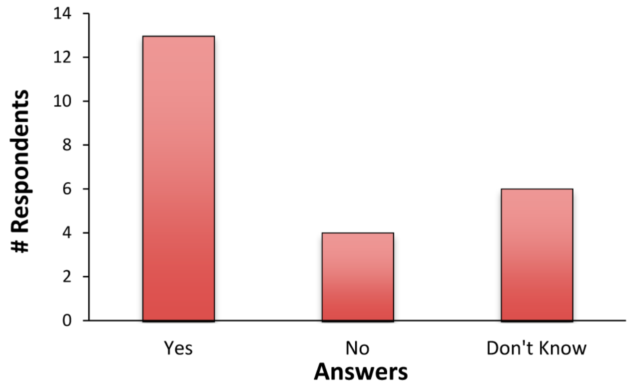

Figure 3. Number of students who plan to use the "Imploded Boolean Search". The survey was conducted in Fall 2014.

Examples of imploded searches using a chemical substance and reaction as well as a comparison to a strictly keyword approach are shown in Table 2. The imploded search yields smaller and more manageable result sets. The imploded search also provides a visual overview of the chemical structures and reactions from the result set, allowing the user to quickly scan and identify relevant information. From Table 2, it is clear that different databases yield different numbers of search results with various degrees of overlap. This reinforces the fact that relying solely on one database is not recommended.

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Table 2. Normal and Imploded Boolean Searches[a]

Database	No. References: Normal Keyword Search[b]	Imploded Substance Search[c]	Imploded Reaction Search[d]	Comparison Search in WoS[e]
SciFinder	219	39	12	N/A
Reaxys	133	12	16	N/A
WoS Structure Search	N/A	N/A	0	3
WoS Core Collection	342	N/A	N/A	11
Overlapping References	49	0	1	0

[a]N/A denotes not applicable. Searches were conducted in July 2015. [b]The topic is cisplatin analogues and binding to DNA. In SciFinder, the keyword search, "cisplatin analogues and binding to DNA' is placed in the "Reasearch Topic" search box. Duplicate references should be removed as SciFinder searches simultaneously in the Chemical Abstracts database and MEDLINE. In Reaxys, the same keyword search is used in the "Ask Reaxys" single-click search option. In WoS Core Collection, the same keyword search is used in the search box and the "Topic" field is selected. [c]The information needed is cisplatin analogues that bind to DNA, between the years 1845−2013 (Figure 1a). The platinum complex is drawn with the variable functional groups in the structure editors of each database. SciFinder retrieves substances from which all references can be filtered from the "Refine" tab using "DNA" in the "Research Topic" search box and then by publication year range. In Reaxys, the search is conducted with the drawn substructure and the variable functional groups AND "DNA" in the abstract field AND date range, from the Bibliographic Data form. Fields in Reaxys can be added by clicking on the Add/Remove fields tab. Reaxys also allows for information to be filtered from the results list. [d]The query is to find references that contain an one step photochemical reaction for converting methane to ethene. The reaction is drawn in the structure editors of each database. In SciFinder, the reaction is searched to retrieve all references which are then filtered from the "Refine" tab by selecting "photochemical" in reaction classification, and then by selecting number of steps as "1". In Reaxys, the reaction is drawn AND "photo" is used as the term in the "Reaction Basic Index" field (i.e., searches for words found in titles, abstracts, and indexing terms) and the resulting references can be filtered by number of reaction steps. In WoS Structure Search, the reaction is drawn AND "Photochemical OR sunlight" is selected from the term list link into the "Other" search box. [e]The question is to find phenanthrene containing compounds that bind to DNA. In WoS Core Collection, the keywords, "phenanthrene AND analog* AND bind* AND DNA" are added to the search box and the "Topic" field is selected. In WoS Structure Search, a substructures search is carried out by drawing phenanthrene in the structure editor AND "DNA Binding Activity" (Compound Biol. Act. field) AND "<500" (Molecular Weight field as product).

CONCLUSION

Information literacy workshops using search strategies with databases are essential to critical thinking and analytical problem-solving skills of scientists for finding clearly defined research information. The size and complexity of chemistry databases make it essential for users to apply different combination searches in order to refine search results. The concept of an "Imploded Boolean Search" (i.e., a combined search using keyword(s), numerical value(s), and a chemical structure or reaction) adds a new search skill to a student's arsenal of search strategies for finding relevant and specific refined information.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00255.

Presentation slides, training exercise, and survey for the workshop (PDF)

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Notes

The author declares no competing financial interest.

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