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SCIFINDER® AS A LATEST TOOL IN INNOVATIVE RESEARCH WITHIN A NEW DIMENSION FOR INTEGRATING SCIENTIFIC CHEMICAL DATABASES

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ABSTRACT: *SciFinder® is a research discovery application that provides integrated access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences. SciFinder® is a database of chemical and bibliographic information. Originally a client application, a web version was released in 2008. It has a graphics interface and can be searched for chemical structures and reactions. The client version is for chemists in commercial organizations. Versions for both the Windows and Macintosh exist. SciFinder® Scholar is for universities and other academic institutions and lacks some supplementary features for multi-database searching.*

SciFinder® offers a one-stop shop experience with flexible search and discovers options based on user input and workflow. You can search for substances, reactions and patent and journal references anytime, anywhere. Make better, more confident decisions knowing that you have access to the largest collection of substances, reactions and patent and journal references produced, compiled and updated daily by CAS scientists around the world. Save time with an array of powerful tools to search, filter, analyze and plan that allow you to quickly find the most relevant answers to your research questions. Don't worry about missing vital research - if it's publically disclosed, high quality and from a reliable source, SciFinder® has it! Industry experts rely on SciFinder® as their only source for high-quality content combined with ease-of-use features that help complete their research project from start to finish and now with PatentPak™, a robust, new patent workflow solution which offers instant access to hard-to-find chemistry in full-text patents directly in SciFinder®.

KEYWORDS: CAS, CAPLUS, CAS REGISTRY, CASREACT, CHEMCATS, CHEMLIST, SSM, CHEMPORT, MEDLINE, MARPAT, SCIFINDER®SCHOLAR.

INTRODUCTION

SciFinder®, produced by Chemical Abstracts Service (CAS), is the most comprehensive database for the chemical literature, indexing journal articles and patent records (and other document types), as well as chemical substances and reactions. You can search by topic, author and substances by name or CAS Registry Number, OR use the editor to draw chemical structures, substructures or reactions.

It's a core research tool for chemistry, biochemistry, chemical engineering, materials science, nanotechnology, physics, environmental science and other science and engineering disciplines. Depending on your research, SciFinder®'s is complementary to other databases like Reaxys, Web of Science, PubMed, Compendex and INSPEC. What sets SciFinder® apart? CONTENT! Did you know that SciFinder®is the only research tool with access to the world's most reliable and largest collection of substances, reactions and references (from both journals and patents)? A global network of scientists update content daily to ensure you have access to the most timely and accurate information available.

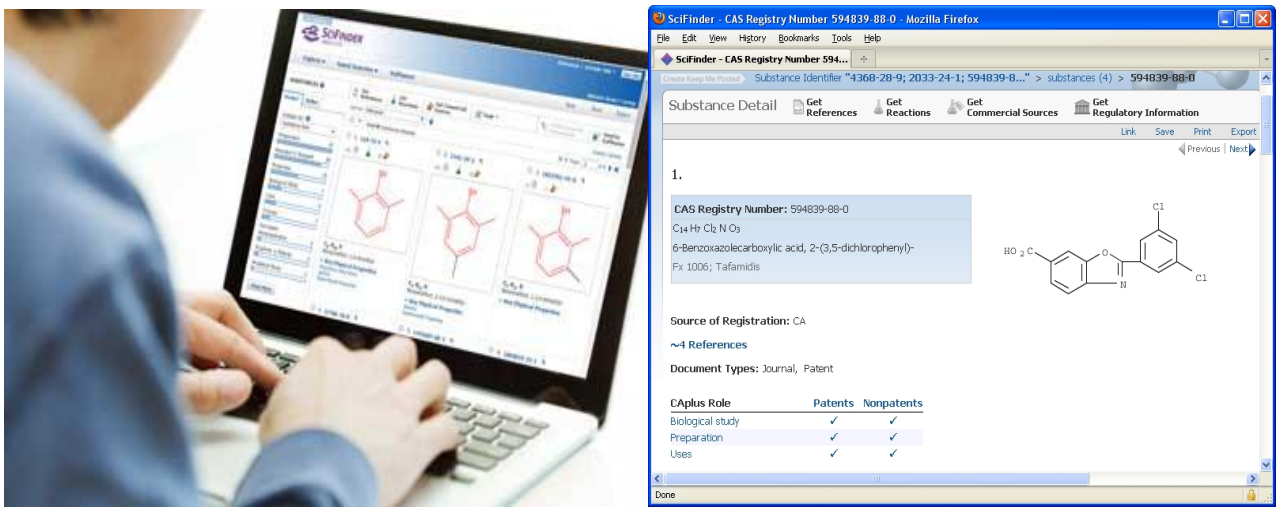


Figure-1: SciFinder® database

It's a core research tool for chemistry, biochemistry, chemical engineering, materials science, nanotechnology, physics, environmental science and other science and engineering disciplines. Depending on your research, SciFinder®'s is complementary to other databases like Reaxys, Web of Science, PubMed, Compendex and INSPEC. What sets SciFinder® apart? CONTENT! Did you know that SciFinder®is the only research tool with access to the world's most reliable and largest collection of substances, reactions and references (from both journals and patents)? A global network of scientists update content daily to ensure you have access to the most timely and accurate information available.

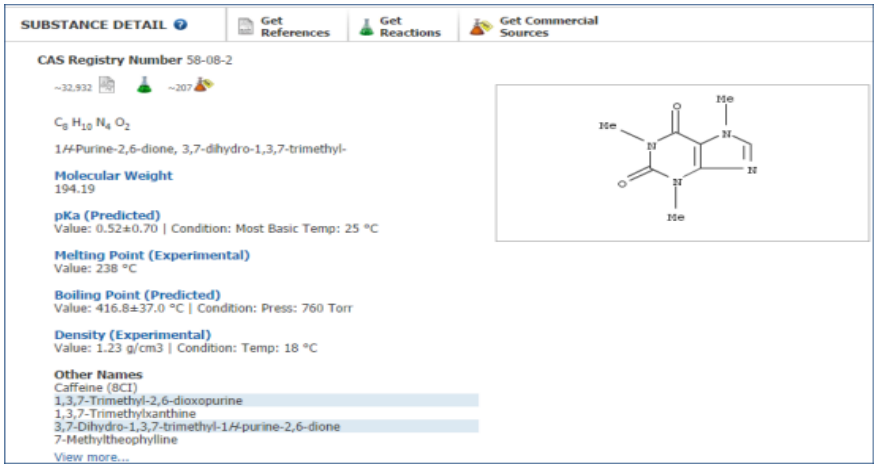


Figure-2: Get substances

Get substances – access the world's most trusted resource for substance information including chemical structures, chemical names, CAS Registry Numbers®, properties, commercial availability and regulatory information. **Substances –** SciFinder® provides easy, instant access to CAS REGISTRYSM, the gold standard for substance information, offering more substances than any other single-source tool including organic and inorganic molecules, DNA, RNA, proteins, polymers and Markush structures. SciFinder® saves you time with convenient access to: >120 million organic and inorganic substances, >66 million DNA and protein sequences, millions of experimental properties and billions of properties predicted by state-of-the-art technology, millions of ^{13}C and ^{1}H NMR spectra and mass spectra, bioactivity and target indicator (protein, enzyme, glycoprotein, etc.) information, commercial availability and pricing information with purchasing options all within your SciFinder® session, regulatory information, substances found in patents, journals and reputable web sources from around the world, ~15,000 new substances added daily.

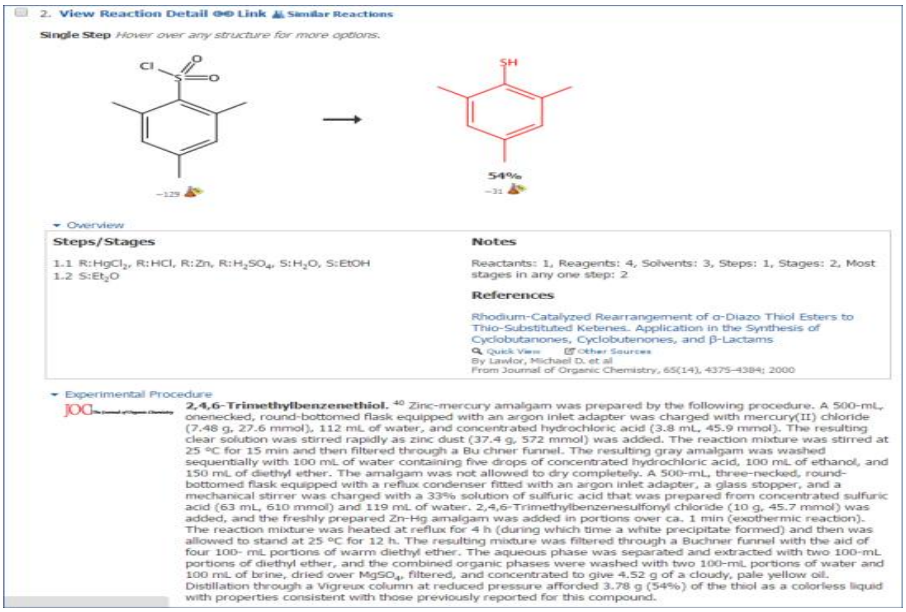
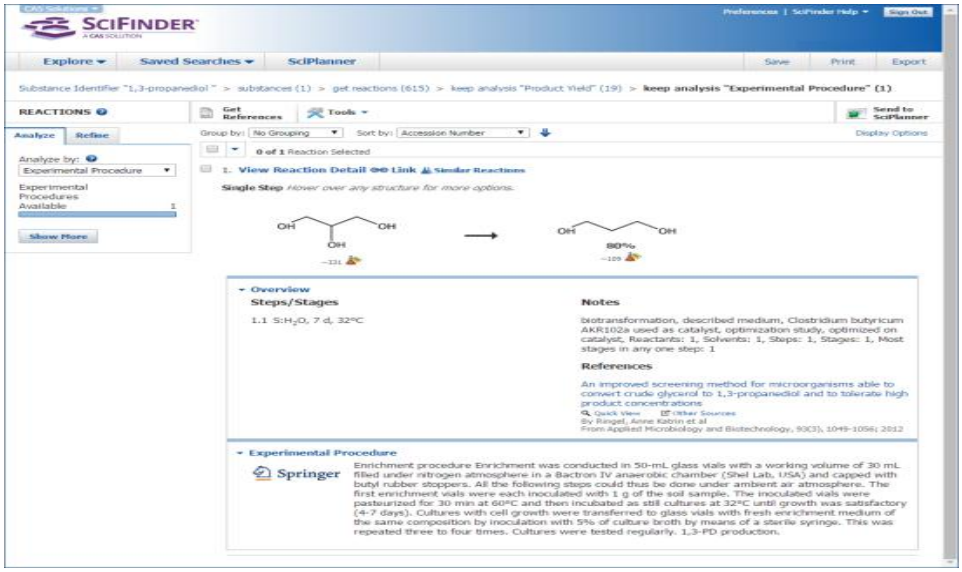


Figure-3: Get reactions

Get reactions – find dependable and current chemical reaction information from our extensive databases including reaction schemes, experimental procedures, conditions, yields, solvents, catalysts, as well as commercial availability of substances with direct links to leading producer and supplier sites.

Reactions – Reduce time and effort searching the most current chemical reaction information on SciFinder® for synthetic organic and organometallic reactions, natural product syntheses and biotransformation reactions.



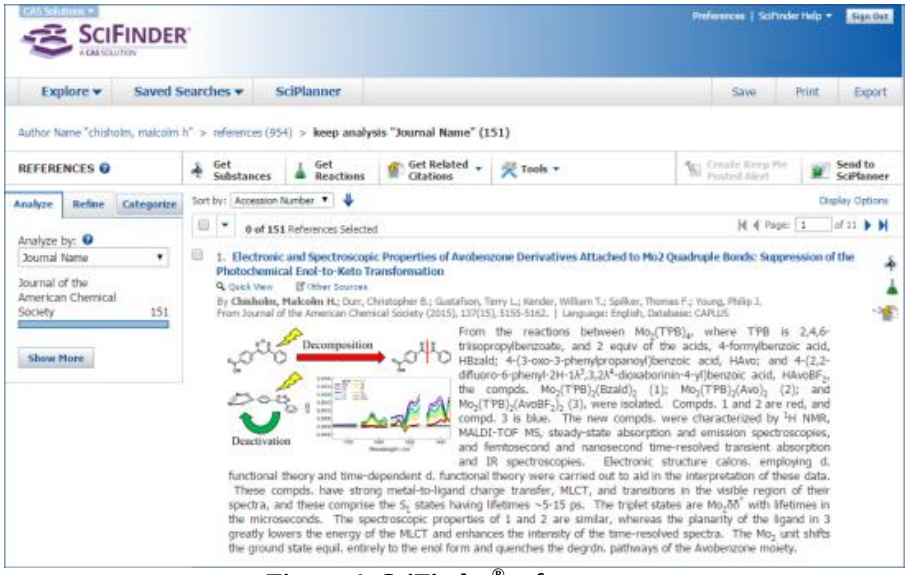


Figure-4: SciFinder® references

Get references – get the information you need when you need it with the unrivaled collection of the world's most up-to-date chemistry and related science information found in journals, patents, dissertations and more. SciFinder® is the only source that brings you information from early discovery through clinical trials with the combined coverage of CAplusSM and MEDLINE® and full-text is just a click away*. **References** – Save time with instant access to the world's most up-to-date and comprehensive source for chemistry, biomedical, patent coverage and related science information. SciFinder® is the only source that brings you information from early discovery through clinical trials with combined CaplusSM and MEDLINE® access in a single tool and now PatentPak™, a robust new patent workflow solution, offers instant access to hard-to-find chemistry in full-text patents directly in SciFinder®.

Rely on SciFinder® for convenient access to: Thousands of active journals from Caplus and MEDLINE, 63 patent authorities with the most expansive Asian coverage, >486 million citing references beginning in 1997, Combined information from patents, journals, dissertations, abstracts, reviews, books, reputable web sources and more, Information covering organic and inorganic chemistry, biochemistry, applied and physical chemistry, biology, medicine, engineering, material science, agricultural science and more, References from 1800s-present, More than 5,000 references added daily.

SciFinder® is a relation between objects in which one object designates, or acts as a means by which to connect to or link to, another object. The first object in this relation is said to refer to the second object. The second object, the one to which the first object refers, is called the referent of the first object. SciFinder®'s easy-to-use search features offer fast and convenient access to the most comprehensive source for substance, reaction and reference information in a single tool designed for a more efficient workflow. SciFinder® offers convenient access to: >77.5 million single- and multi-step reactions from journals and patents, experimental procedures with content from all ACS publication journals, Springer, Taylor and Francis publications and English, German and Japanese (translated to English) language patents from authorities such as USPTO, EPO, JPO and WIPO, reaction conditions (time, temperature, pressure, yields, etc.), catalysts, solvents and more, descriptions of catalysts, solvents and yields, comprehensive commercial availability and pricing information for reactants, reagents, catalysts and solvents covering hundreds of catalogs and suppliers, reactions from 1840-present, ~30,000 new single- and multi-step reactions added daily, a new generation of research tool.[1]

By the mid-1990s, electronic information services were already proliferating; CAS realized that no matter how innovative SciFinder®'s search interface would be, another dimension was needed to differentiate the product (i.e., content, the collection of information) that scientists would access through SciFinder®. Providing access to CAS databases became a key factor in distinguishing SciFinder® from competitive search tools.

SciFinder® classification

1. CAplus: SciFinder® provides access to several CAS databases, including the comprehensive file of bibliographic records, CAplus. CAplus contains records for all the documents selected for coverage and indexing by CAS. Like the familiar publication Chemical Abstracts, the database covers worldwide literature from all areas of chemistry, biochemistry, chemical engineering and related sciences from 1967 to the present. Documents include journal articles from more than 8000 journals, conference proceedings, technical reports, books, dissertations and reviews. Unlike any other database, CAplus contains scientific literature and patent documents from more than 30 national and international patent offices. CAplus also includes references to documents not indexed by CAS for

coverage in the printed CA. These additional references are derived from cover-to-cover analysis of more than 1300 scientific journals. Some of the additional references are to journal articles; others are for items not covered in CA— biographical items, book reviews, editorials, errata, letters to the editor, news announcements and product reviews. To make CAplus current, CAS includes fully indexed records, as well as records in progress. The latter includes bibliographic information, even if an abstract is not yet available. The abstracts are added as soon as they become available. CAplus, produced by CAS, contains more than 43 million chemistry and chemistry related research records categorized in 80 sections, with references in:

All areas of biochemistry: Agrochemical regulators, Biochemical genetics, Fermentation, Immunochemistry, Pharmacology.

All areas of organic chemistry: Amino acids, Biomolecules, Carbohydrates, Organometallic compounds, Steroids.

All areas of macromolecular chemistry: Cellulose, lignin, paper, Coatings, inks, Dyes, organic pigments, Synthetic elastomers, Textiles, fibers.

All areas of applied chemistry: Air pollution, Ceramics, Essential oils, cosmetics, Fossil fuels, Ferrous metals, Alloys.

All areas of physical, inorganic, analytical chemistry Surface chemistry, Catalysts, Phase equilibrium, Nuclear phenomena, Electrochemistry.

How do we count

CAplus covers international journals, patents, patent families, technical reports, books, conference proceedings and dissertations from all areas of chemistry, biochemistry, chemical engineering and related sciences from 1907 to the present. In addition, over 180,000 records for pre-1907 patent and journal references are available, from sources such as the American Chemical Society (ACS), the Royal Society of Chemistry (RSC) and Chemisches Zentralblatt. Chemisches Zentralblatt is the first and oldest abstracts journal published in the field of chemistry. It covers the chemical literature from 1830 to 1969 and describes therefore the "birth" of chemistry as science, in contrast to alchemy. The information contained in this German journal is comparable with the content of the leading source of chemical information Chemical Abstracts Service (CAS), which started publishing abstracts in English in 1907. Chemisches Zentralblatt was originally founded as Pharmaceutisches Centralblatt by Gustav Theodor Fechner and published by Leopold Voß in Leipzig in 1830. In the first year, 544 pages containing 400 abstracts were published, reporting all relevant research results in pharmaceutical chemistry. In the following 20 years the relevance of chemistry grew so much that in 1850 the title changed in Chemisch-Pharmazeutisch Zentralblatt and in 1856 it became Chemisches Zentralblatt. In 1969, after 140 years the expenses for the collection of primary literature in many languages and the production of abstracts were too high and the publication of Chemisches Zentralblatt ceased. In these 140 years, scientific editors reported research progresses in chemistry with approximately 2 million abstracts, publishing over 650,000 pages. Additional 180,000 pages contain indexes such as index of authors, subject indexes, general indexes, register of patents and formula register. Chemisches Zentralblatt was completely digitized by FIZ Chemie in Berlin. FIZ Chemie scanned the entire work and developed a full text searchable database for the web. In addition the database can be purchased and integrated in Intranets. The chemical software company InfoChem, based in Munich, developed an Internet-based database, the Chemisches Zentralblatt Structural Database. This database provides access to the chemical content within the Chemisches Zentralblatt by performing chemical structure and substructure searches. Electronic-only journals and web preprints are also covered. Since October 1994, records for all articles from more than 1,500 key chemical journals are added, including records for document types not covered in Chemical Abstracts (CA): biographical items, book reviews, editorials, errata, letters to the editor, news announcements, product reviews, meeting abstracts and miscellaneous items. Cited references are included for journals, conference proceedings, and basic patents from the USPTO, EPO, WIPO and German patent office's added to the CAS databases from 1997 to the present. Also included are patent examiner citations from British and French basic patents (2003 to the present), Canadian patents (2005 to the present) and Japanese patents (2011 to the present). In addition, nearly 300,000 existing patent records from 1982-2008 have been supplemented with information for cited patents. As of August 2016, CAplus contains over 486 million cited references. Legal status information is available for U.S. patents since 1980. Coverage: Early 1800's.

Patent (and patent family) references from 63 patent authorities around the world. Chemistry indexed from more than 50,000 scientific journals worldwide, with thousands of active titles currently covered. From 1907 to present, CAS has indexed chemistry from more than 50,000 journal titles. In that time, publishers have discontinued, merged, split, revised and changed the focus of many titles. For more information about journal titles and abbreviations for publications indexed by CAS since 1907 please consult the CAS Source Index (CASSI) search tool: Conference proceedings, Technical reports, Books, Dissertations and Reviews. Meeting abstracts, Electronic-only journals, Web preprints.

Cover-to-cover coverage for more than 1,500 key chemical journals (since October 1994), including records for document types not covered in Chemical

Abstracts (CA): Biographical items, Books reviews, Editorials, Errata. Letters to the editor, News announcements, Product reviews, Meeting abstracts.

Update frequency: Updated daily, Patent references from nine major issuing authorities available within two days from the time the patent was issued.

2. CAS Registry

Complementing the bibliographic information in CAplus is the CAS Registry database, the world's largest substance identification system. The substances in this file are derived from the chemical literature and patents indexed in CAplus and other sources, such as regulatory lists. All kinds of substances are recorded in the Registry: inorganic and organic compounds, alloys, biosequences, coordination compounds, minerals, mixtures, polymers and salts. Registry records contain chemical structures for more than 24 million substances, along with the systematic CA index names, CAS Registry number, synonyms, molecular formulas, alloy composition tables, nucleic acid or protein sequences and ring analysis data. More than 43 million references (citations and abstracts) to journal articles and patents, as well as conference proceedings, technical reports, books, dissertations and meeting abstracts. Substances and reactions indexed with links to the corresponding CAS Registry and CASREACT records. Currently indexes 10,000+ journals (1,500 journals indexed cover-to-cover) and patents from 63 patent authorities. Mostly 1907 to present, with some pre-1907 content: including ACS (1879-1906) and RSC (1841-1906) journals, Chemisches Zentralblatt 1897-1906 (machine translations) and 38,000 US patents. CAS REGISTRY^{SM} contains more than 120 million unique organic and inorganic chemical substances, such as alloys, coordination compounds, minerals, mixtures, polymers and salts and more than 66 million sequences—more than any other database of its kind. When you need to positively identify a chemical substance, you can rely on the authoritative source for chemical names and structures of CAS REGISTRY. You can also identify your substance of interest by its CAS Registry Number®, which is universally used to provide a unique, unmistakable identifier for chemical substances. Records for more than 117 million organic and inorganic substances (including alloys, coordination compounds, minerals, mixtures, polymers and salts) and 66 million DNA and protein sequences. Substance information includes: synonyms, molecular formulas, structure diagrams and experimental & calculated property data. 15,000 new substances are added daily. 6.8 billion predicted properties for 102 million substances; 4.5 million experimental properties for 3 million substances. 1.4 million experimental spectra (MS, IR, ^{1}H-NMR) for 983,000 substances and 200 million predicted spectra (^{13}C-NMR and ^{1}H-NMR spectra). Complete coverage from 1957 to date, with additional substances going back to early 1900's. CAS Registry records link to the other SciFinder® databases: CAplus, CASREACT, CHEMCATS and CHEMLIST.

You can also use CAS REGISTRY to locate: literature references to the substance, experimental and predicted property data (boiling and melting points, etc.), CA Index Names and synonyms, commercial availability, preparative methods spectra, regulatory information from international sources. You can obtain the information you need for millions of substances from the most current and reliable collection of chemical substance information in the world, CAS REGISTRY.

Content: Substances reported in the literature back to the early 1800s, Updated daily with about 15,000 substances. Substance information enriched with experimental and predicted property data, including more than 6.9 billion property values, data tags and spectra.

How do we count: The CAS REGISTRY database contains records for specific substances identified by the Chemical Abstracts Service (CAS) REGISTRY system. All substance records contain a unique CAS Registry Number. Records may also have CA index names, synonyms, structure diagrams, stereochemistry, molecular formulas, ring data, alloy composition tables, protein and nucleic acid sequences, classes for polymers and the number of references in the CA/CAplus databases. All of this information is displayable and searchable on STN, but some of it is only displayable in SciFinder®. In addition to substance information, REGISTRY records contain super roles and document type information from CAplus, experimental and predicted (calculated) property data and tags pointing to references containing experimental property data.

3. CASREACT

SciFinder® access includes a specialized chemical reaction database of substance information called CASREACT. This database offers reaction information derived from documents covered in the organic sections of Chemical Abstracts—journals from 1985 to the present and patents from January 1991. Single- and multistep reactions are included. The records contain reaction information consisting of structure diagrams for reactants and products; CAS Registry numbers for all reactants, products, reagents, solvents, and catalysts; yields for many products; and textual reaction information. The reactants, reagents and products can be searched by structure with a single reaction query. Roles, reaction sites and mapping of atoms between reactants and products are also structure-searchable. 91 million single and multi-step reactions, and 14 million synthetic preparations, with additional information about the reactions.

Indexed from journal articles, patents and evaluated reference sources, 1840 to date. Reactions link to CAplus and CAS Registry.

Benefit to you: Access precise, dependable and timely information on synthetic organic research, including organometallics, total syntheses of natural products and

biotransformation reactions, find information concerning reaction conditions, yields and catalysts, answer questions such as: different reactions producing the same product, uses or applications of a particular catalyst, various ways to carry out specific functional group transformations.

Content: CASREACT®, produced by CAS, contains: >77.5 million single- and multi-step reactions available with SciFinder® and on STN, >14 million additional synthetic preparations available with SciFinder®.

How do we count: CASREACT consists of single- (A->B, B->C, C->D) and multi-step (A->C, A->D, B->D) reactions, plus synthetic preparations. Single- and multi-step reactions can be found in all CAS and STN products. Synthetic preparations are accessible through the SciFinder® Explore Reactions function or by applying a product role limiter on a CAS Registry Number search in STN.

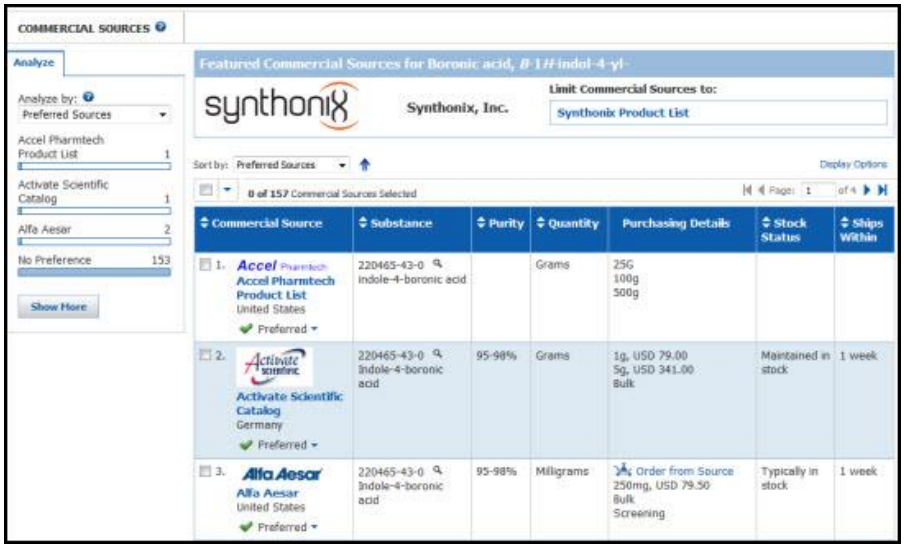
Coverage: 1840 to the present, CASREACT contains reaction information from the millions of published journal articles and patent documents selected for inclusion in *Chemical Abstracts*™ (CA).

Update frequency: Updated daily, more than 150,000 single- and multi-step reactions are added each week.

4. CHEMCATS

Recognizing that scientific interests and business-related tasks often go hand-in-hand, CAS added a data base to the SciFinder® array to help clients identify commercial sources of chemicals. CHEMCATS (Chemical Catalogs Online) is a catalog file containing listings of commercially available chemicals and their suppliers worldwide. Each record includes the supplier's information (e.g., name, pricing terms, products and services and packaging), the catalog name, chemical and trade names, grade information, CAS Registry number, structure diagram, properties, regulatory information and prices. Catalog database of commercially available products from chemical suppliers, often with information about pricing and availability. You can customize the view to prioritize preferred vendors.[2]

Product improvement has been continuous. In 1996, CAS released SciFinder® 2.0. In a review of that release, co- authors Carmen Nitsche and Robert Buntrock confirmed that the product fulfilled its essential purpose: "With SciFinder®, chemists can help themselves, exploring the literature as they wish, rediscovering the serendipity that comes with browsing. Information professionals take on the role of trainer and coach, guiding end-users to finding the best answers and advising them on when to seek more complete information through other means".



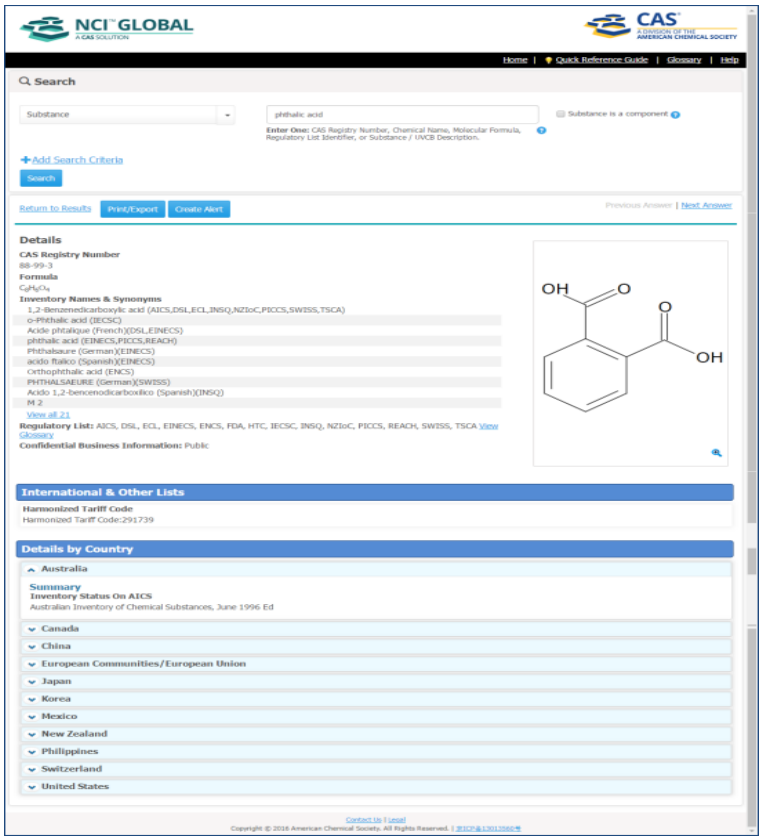


Figure-5: Chemical catalogs

Benefit to you
The next time you have to order chemicals, you can quickly find the substances you need thanks to CHEMCATS®. You will find the following information (depending on the supplier): Catalog name, Order number, Chemical and trade names, CAS Registry Number®, Chemical structure, Pricing terms. Supplier contact information: Company name and address, Phone and fax number, E-mail, Web address.

Content
CHEMCATS (Chemical Catalogs Online), produced by CAS, is a catalog database containing information about commercially available chemicals and their worldwide suppliers.

How do we count
CHEMCATS consists of commercially available products. Products listed by vendors as different catalog items may reflect various factors, such as purity, grade or quantity.

Coverage: Current catalogs and chemical libraries.

Update frequency: Updated at least two times per week with new and revised catalog information.

5. CHEMLIST
Database of 346,000 substances that are regulated by state, federal and international agencies, including EINECS (European Inventory of Existing Commercial Chemical Substances) and TSCA (Toxic Substances Control Act (TSCA) Inventory. Covers inventories and lists from 1980 to date.

Benefit to you
You can quickly locate the regulatory information you need because each substance reference provides all the agencies - international, national and state - that regulate the substance.

Content
CHEMLIST® (Regulated Chemicals Listing), produced by CAS, is an electronic collection of thousands of chemical substances that are regulated in key markets across the globe. CHEMLIST contains more than 346,000 substances.

How do we count
The CHEMLIST database began with national chemical inventories such as Toxic Substances Control Act (TSCA), European Inventory of Existing Commercial Chemical Substances (EINECS), Existing and New Chemical Substances (ENCS), and Inventory of Existing Chemical Substances in China (IECSC). Today, it includes international lists for high production volume (HPV) chemicals, priority chemicals, dangerous chemicals with transportation restrictions, as well as pollutant release inventories. CHEMLIST offers the convenience of identifying--in one place--the regulatory requirements for a specific substance from many of the world's most significant regulated substances lists.

Coverage: Inventors and lists from 1980 to the present.

Update frequency: More than 50 new substances or additions to existing substances are added to the database each week.

6. SSM

In 1997, CAS upgraded SciFinder®'s capabilities with the SciFinder® Substructure Module (SSM). The user defines rings, chains, substituents and R-groups. A Substructure Explore presents a set of candidate substances that match the substructure. They then can retrieve all the references or just those relating to specific topics, such as adverse effects, biological activity, and preparation. SSM allows researchers to generate new ideas for research as well as to identify derivatives of existing chemicals that exhibit more desirable properties.

7. CHEMPORT

Whenever possible, SciFinder® provides a set of references in response to the user's questions and a link to the full text of the identified journal article or patent. The ChemPort Connection feature works automatically when the user clicks on the PC icon that appears to signal the availability of electronic full text. A ChemPort options page may show a number of choices for accessing the full-text document. For example, "Subscribers view e-article" is available for subscription holders. Other options appear for accessing the full text through a subscription agent or the user's in-house library, or even for purchasing the article for a one-time additional fee.

8. MEDLINE

Skipping ahead a few versions, SciFinder® 5.0 was released in mid-1999, and a new biomedical component became available—the U.S. National Library of Medicine's MEDLINE database. MEDLINE can be searched with CAplus during the Research Topic and Author exploration. Users also can execute a substance identification search and choose to get references from CAplus and MEDLINE. 22 million references to articles from more than 5,600 biomedical and related health sciences journals (including chemistry and biochemistry), 1946 to date. Medline is searched alongside CAplus in reference searching, and you can remove the duplicate Medline references. If you want to search Medline only, use PubMed.

9. MARPAT

More than 1 million searchable Markush structures from 468,000 patents covered by CAS from 1988 to date (with structures derived from INPI records from 1961-1987). Markush structures use R groups to identify a set of molecules with common features. More about Markush and its limitations from these presentations: Cresset, ACS and RSC. Markush structures (-R) are chemical symbols used to indicate a collection of chemicals with similar structures. They are commonly used in chemistry texts and also in patent claims. Markush structures are depicted with R groups, in which the side chain can be a structure type, e.g. 'cyclohexyl'. This more general depiction of the molecule, versus detailing every atom in the molecule, is used to protect intellectual property. The company which files the patent makes a general claim for the usage of the molecule without revealing to their competitors the exact molecule for which they are declaring a useful application. Markush - MARPAT - Database containing the keys to substances in patents.

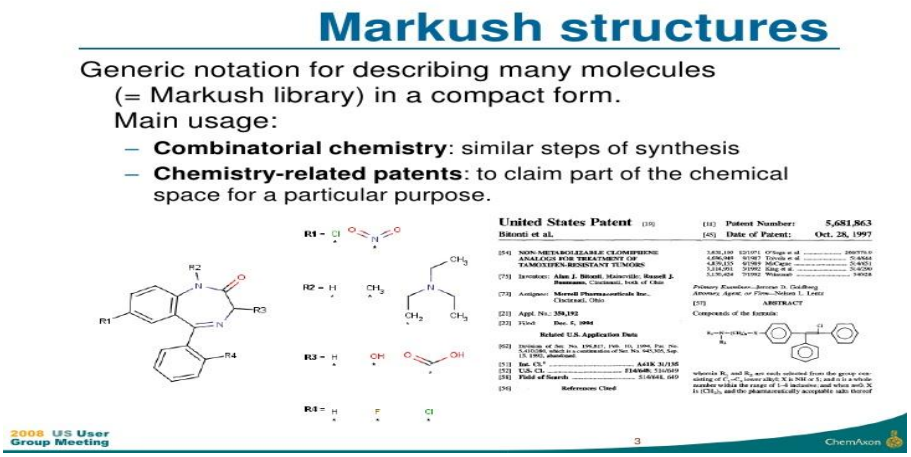


Figure-6: Markush database

MARPAT®, produced by CAS, contains

More than 1,134,000 searchable Markush structures from patents covered by CAS from 1988 to the present with selected coverage of Japanese patents from 1987. In addition, English language patents from 1984-1987 plus French and German patents from 1986-1987 have selective coverage. Other records from 1961-1987 are derived from INPI (Institute National de la Propriete Industrielle) data. Russian patents published after January 10, 2000 and Korean patents from 2008 to the present are also covered - 08/31/16, More than 469,000

displayable citations for the Markush structure-containing patents - 08/31/16.

Coverage: All countries whose patent offices are covered in the CA[SM]/CAplus[SM] file are candidates for MARPAT indexing, Not included**:** Alloys, metal oxides, inorganic salts, intermetallics and polymers.

Update frequency: Updated daily with approximately 60-75 patent citations and 150-200 Markush structures.

How do we count: Contains the Markush structure records for patents found in the CA/CAplus files with their respective patent citation for patent publication years 1988 to the present with selected coverage of Japanese patents from 1987 plus selective coverage of English, French and German patents from 1985-1987. Russian patents published after January 10, 2000 and Korean Patents from 2008 to the present are also covered. Other Markush structures are derived from INPI data from 1961 to 1987.

WebLab ViewerLite. In another enhancement drawing upon resources outside of CAS, SciFinder®5.0 incorporates links from substances in the CAS Registry to WebLab ViewerLite (Molecular Simulations Inc.). WebLab ViewerLite is a high-end molecular visualization application that uses OpenGL graphics for visualizing molecular models. These models can be rotated, scaled, edited, labeled, and analyzed. Of course, the more traditional method of ordering a document copy is not neglected: SciFinder® also gives customers a direct link to the CAS Document Detective Service. Along with the ChemPort feature, SciFinder® strives to ensure the researcher a means of acquiring the full-text document, if desired.

Table-1: SciFinder® Case Study

An evolving product					
1995	**1996**	**1997**	**1998**	**1999**	**2000**
SciFinder® launched	**SciFinder® 2.0**	**SciFinder® 3.0**	**SciFinder® 4.0**	**SciFinder® 5.0**	**SciFinder® 2000**
Explore Caplus	Explore by reaction	SciFinder® Substructure Module (SSM)	ChemPort Connection	MEDLINE Explore	Explore by company
Explore CAS Registry	Explore by patent number	Scholar launched	Links to regulatory information	Full reaction explore	Explore with Panorama
Keep Me Posted		"Refine and save answers" capability		Patent family information	Functional group transformations
Browse journal table of contents	No data available			Substance analysis tools	Browse journal table of contents

SciFinder® Scholar

In 1997, CAS launched SciFinder® Scholar to address the needs of chemistry students and faculty. Although Scholar has the same look, ease of use, and the main search tools as SciFinder®, many of the features that allow SciFinder® to be personalized are not available on SciFinder® Scholar. Because different individuals may use SciFinder® Scholar at different times, pricing is based on the number of simultaneous users, whom the university does not need to identify personally.

The pathways to knowledge

SciFinder® is a new and simple way for researchers to obtain information. Instead of a blinking cursor waiting for the users to enter a command, the opening screen of SciFinder®'s GUI presents several pathways to knowledge that is, obtaining information: Explore, Browse, and Keep Me Posted. The user explores information easily by chemical substance (e.g., exact structure, molecular formula, or substance ID), reaction, substructure, research topic, author, or document identifier. Searches are conducted in a user-friendly, question-and-answer format, using internal dictionaries and a thesaurus to look up key terms in the request phrase and increase the search power. Users can also browse through the tables of contents of 1300 journals, and a Keep Me Posted function monitors new literature on current subjects and alerts users to recent arrivals. SciFinder® is designed to "make it look easy", in spite of its sophisticated algorithms and platforms. Unlike "command line" search systems that expect the user to anticipate the variety of terms a database may contain, SciFinder® automatically considers synonyms. For example, a user wants to find literature on the effects of ACE inhibitors on treating heart disease. Included in the search would be synonymous terms such as cardiovascular disease. The search results display all the literature references that include heart disease and ACE inhibitors, heart disease or ACE inhibitors, and entries that include just heart disease and just ACE inhibitors. Thus, the user can choose a narrowly defined set of documents or a more general set about heart disease or ACE inhibitors. After examining a few of the references, the user wants to narrow the search and identify literature that pertains to the treatment of one kind of heart disease: heart failure. A "Refine" tool makes it possible to select a subset of the answers, limited by any of several criteria: author name, research topic, document type (e.g., journal or patent), language, or publication year. The user may choose to refine by research topic and enter the phrase

"treatment of heart failure". SciFinder® runs this search against the set of existing records found originally and identifies a subset that deals specifically with ACE inhibitors used to treat heart failure.

Table-2: Journey of Chemical Abstract Service (CAS)

Year	Event
1907	William A. Noyes became the first editor of *Chemical Abstracts* (*CA*), which debuted in January 1907. In its first year of publication, *CA* contained fewer than 12,000 abstracts. *CA* was first published at the U.S. Bureau of Standards. Later, the offices moved to the University of Illinois, Urbana.
1909	*CA*'s editorial operation was moved to the campus of the Ohio State University in Columbus, Ohio.
1956	*CA* became Chemical Abstracts Service (CAS) and an operating division of the American Chemical Society.
1965	A new era in scientific research dawned with the introduction of the CAS Chemical Registry System. Using a unique CAS Registry Number® to identify each chemical substance without the ambiguity of chemical nomenclature, the system proved to be a boon to chemical research, health and safety information, and the communication of chemical information in many media.
1966	CAS management and technical teams devised an automated processing system that not only produced printed *CA* issues and indexes more efficiently, but also fed a computer-readable database that could generate new kinds of services. CAS was an early adopter of the new photocomposition technology, and went on to produce services in print, microform and magnetic tape.
1980	CAS ONLINE was launched, making it possible for users (primarily information specialists) to search the CAS REGISTRY database. Users with a specific model of an intelligent graphics terminal could select structure features from a menu and then assemble them on the terminal monitor using a graphics tablet and stylus. These terminals could display answers with well-drawn structure diagrams.
1983	ACS and FIZ Karlsruhe cooperated in forming an international online network. STN®, the scientific and technical information network, was launched the next year. The network made databases accessible through distributed processing on a global scale. At first, only CAS databases and physics briefs were accessible. Over time, STN grew to include many databases from a range of information providers.
1988	STN Express® software provided assisted searching at the desktop and soon became the preferred interface for STN users.
1995	CAS introduced the SciFinder® research tool to give scientists direct access to CAS databases with no need to learn a command language. With its intuitive, graphical interface, SciFinder® simplified the exploration of the world's scientific literature, patents and substance information, making this activity "part of the process" for scientific research.
1997	CAS recognized the possibilities of the Internet to speed and simplify access to source documents. ChemPort® was introduced to CAS and STN electronic services in 1997 to provide links to full-text journal articles and patents identified via online searching.
2005	CAS continued to develop electronic services to make scientific information more accessible and useful. STN® AnaVist™ was introduced by CAS and FIZ Karlsruhe to enable the analysis and visualization of search results from a variety of perspectives.
2007	CAS celebrated its 100-year anniversary and was recognized by the American Chemical Society as an ACS.
2008	The web version of SciFinder® was released, providing users with enhanced search capabilities and instant access to CAS database content from anywhere in the world.
2009	The CAS REGISTRY database registered its 50 millionth substance, marking a significant milestone not only for CAS but for the scientific community as a whole. The scientific knowledge amassed and chronicled in REGISTRY by CAS scientists enables continued discovery by chemists and researchers around the globe.
2010	The United States Patent Office awards CAS a five-year sole source contract for STN, stating in its solicitation letter that "CAS' STN databases offer the largest collection and depth of chemical and related information compared to other commercial web based databases. In addition, CAS is the only company that has a unique, proprietary, chemical structure searching capability using its STN Express software. No other source can successfully meet the USPTO's requirements."
2011	The 60 millionth substance was recorded in CAS REGISTRY for a patent application submitted to the State Intellectual Property Office of the People's Republic of China. CAS observed in 2009 that China surpassed all other nations as the top producer of chemical patent applications. Coming less than two years after CAS REGISTRY crossed the 50 million mark, this major milestone shows the continued acceleration of chemical and scientific output across the globe.
2012	CAS and FIZ Karlsruhe announced Version One of the new STN platform in beta for fixed fee customers. This was the first major milestone in a multi-year initiative to create the next generation of STN, the choice of patent experts™. CAS also registered the 70 millionth substances, a therapeutic patent from Korea. Patents continue to be an important source of chemical information.
2013	CAS registered the 75 millionth substances from a chemical catalog in the CAS REGISTRY. SciFinder®

	content and functionality were enhanced with a streamlined design, a new non-Java CAS Structure Editor, API integration, and collaborations with Springer, Thieme Publishing Group and PerkinElmer, among others. The new STN platform had two version releases that included core STN content, global patent content and new functionality. The 2013 Inventory of Existing Chemical Substances in China was added to CHEMLIST®, the CAS database containing international regulatory information for chemical substances.
2014	CAS and PerkinElmer released their shared research solution, pairing SciFinder® with ChemDraw® software, the drawing tool of choice for chemists. Global value pricing options were introduced for STN. CAS expanded coverage of reactions from dissertations in CASREACT®.
2015	CAS registered the 100 millionth chemical substances in CAS REGISTRY, in its 50th anniversary year of the world's largest database of unique chemical substances. CAS released three new solutions during the year: PatentPak™, a patent workflow solution that is available in SciFinder® and classic STN; NCI™ Global a regulatory solution; and the CHEMCATS® Chemical Supplier Program. CAS continued its commitment to global research and business development, adding dedicated sales and support representatives around the world.

The cost of knowledge: Pricing is always a crucial factor in the acceptance of an electronic information service. CAS speculated that novices would be intimidated by the "ticking meter" effect of the connect-time pricing model. It was important that researchers be given the time to do need, thorough searches without financial limitations. So SciFinder® was priced to encourage companies and their research scientists to make the product a daily research tool. SciFinder® is available principally through flat-rate annual subscriptions that allow unlimited use for a given number of "seats"; however, CAS also offers an option to purchase a certain number of "tasks" (a task means one search question and the resulting answers). Pricing arrangements are prepared for each organization and determined according to the requirements of its research groups, the number of SciFinder® users, and the installation options. CAS plans to release SciFinder® 2000 in the fall of 2000. The exact release date has not been finalized; access www.cas.org for more updated information. SciFinder® 2000 will introduce a range of new capabilities for desktop research. The new capabilities include the following: company or organization name exploration, expanded access to full-text documents in the customer's corporate library, citation linking, and reaction exploration enhancements. These state-of-the art exploration tools for data mining and visualization will provide multidimensional graphing and navigation capabilities. SciFinder® 2000's new visualization tools incorporate a set of capabilities. Rather than simply searching for references on a specific topic, a scientist can use these tools to see at a glance how various research interests are represented in the databases and how they relate to one another in the scientific literature. Today's electronic research environment is a whole new ballgame. To remain a winner in this exciting competition, CAS is committed to making SciFinder® increasingly versatile and responsive to the needs of scientists. And like the fielder who makes even the most difficult catches in stride, SciFinder® will always try to make it look easy.[3]

CONCLUSION

SciFinder® is a research discovery application that provides unlimited access to the world's most comprehensive and authoritative source of references, substances and reactions in chemistry and related sciences. SciFinder® offers a one-stop shop experience with flexible search and discovers options based on user input and workflow. You can search for substances, reactions and patent and journal references anytime, anywhere. Make better, more confident decisions knowing that you have access to the largest collection of substances, reactions and patent and journal references produced, compiled and updated daily by CAS scientists around the world. Save time with an array of powerful tools to search, filter, analyze and plan that allow you to quickly find the most relevant answers to your research questions. Don't worry about missing vital research – if it's publically disclosed, high quality and from a reliable source, SciFinder® has it! See why industry experts rely on SciFinder® as their only source for high-quality content combined with ease-of-use features that help complete their research project from start to finish and now with PatentPak™, a robust, new patent workflow solution which offers instant access to hard-to-find chemistry in full-text patents directly in SciFinder®.

What is PatentPak?

PatentPak is a robust patent workflow solution available in SciFinder®. Designed to radically reduce time spent acquiring and searching through multiple patents to find vital chemistry. PatentPak saves users up to half the time they spend researching patents by providing instant access to hard-to-find chemistry in patents and patent families in languages users know. The only patent workflow solution of its kind! Only PatentPak offers all of the following: Instant access to searchable full-text patents from major patent offices around the world: Patent family coverage in multiple languages, substance location mapping, secure and confidential patent research. PatentPak is an add-on workflow tool within SciFinder® that is intended to enhance access to and analysis of full text patent documents. PatentPak is not included in our base SciFinder® subscription and at present we have no plans to add it, due to its cost. All user accounts receive five free uses as a trial. PatentPak is an add-on workflow tool within SciFinder® that is intended to enhance access to and analysis of full text patent documents. PatentPak is not included in our base SciFinder® subscription, and at present we have no

plans to add it, due to its cost. All user accounts receive five free uses as a trial.

How does it work?
Once you have located a patent of interest, use the PatentPak option to immediately view available full-text documents, often available in a variety of source languages depending on the patent family. CAS analysts have annotated the important chemistry in many patents available in PatentPak. You can view the annotated patent in our unique interactive patent chemistry viewer to quickly pinpoint the locations in the document that you need to see.

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How does full text linking work?
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Can I view patent documents via SciFinder®?
Most patent documents (including applications) that are indexed in CAPLUS can be viewed via the "Link to Other Sources" button in the detailed record display. The PatentPak button in the brief display is not active for UT Austin users. CAS links to U.S. patents via the USPTO web site. Foreign patent documents are accessed via the Espacenet site of the European Patent Office. Be sure to examine the Patent Family information in SciFinder®'s full record display: this will list equivalent patents and applications from other agencies. SciFinder® links to the "parent" document as indexed in CAPLUS. To retrieve others in the family, copy the number and search it directly in the USPTO or Espacenet sites.

How can I translate journal abbreviations to full titles, or vice-versa?
Most journal titles now appear in full form in SciFinder®. For those that don't, you can translate them to full titles – or find official abbreviations for use in your references – in CASSI, the Chemical Abstracts Service Source Index, which lists all publications indexed by CAS since 1907. The printed CASSI (1907-2004) is located behind the Circulation Desk in the Chemistry Library.

Who can use SciFinder®?
Table-3: SciFinder® usability

Yes	No
Currently enrolled students, including extension and distance-learning students with necessary EID permissions	Alumni and former students, Students not enrolled for current semester
Currently appointed faculty and staff	Former faculty/staff/postdocs
Retired and emeritus faculty	Unofficial visitors**
Currently appointed postdocs	Library Courtesy Borrowers
Official visiting scholars*	TexShare cardholders
*Official Visitors include visiting scholars paid by their home institutions who have UT ID cards and appropriately authorized EIDs. Visiting scholars should continue using SciFinder® remotely via their home institutions if it is available to them. Otherwise, a working email address ending in utexas.edu is required for SciFinder® registration. Visitor EIDs do not have permission to use licensed resources from off campus, and may not be permitted to enter the SciFinder® registration area. **Unofficial visitors do not have UT IDs, and are not eligible to use SciFinder®.	

Yes: Currently enrolled students, including extension and distance-learning students with necessary EID permissions.

Currently appointed faculty and staff, Retired and emeritus faculty, Currently appointed postdocs, Official visiting scholars*.

No: Alumni and former students, Students not enrolled for current semester, Former faculty/staff/postdocs, Unofficial visitors**, Library Courtesy Borrowers, TexShare cardholders.

*Official Visitors include visiting scholars paid by their home institutions who have UT ID cards and appropriately authorized EIDs. Visiting scholars should continue using SciFinder® remotely via their home institutions if it is available to them. Otherwise, a working email address ending in utexas.edu is required for SciFinder® registration. Visitor EIDs do not have permission to use licensed resources from off campus and may not be permitted to enter the SciFinder® registration area.

**Unofficial visitors do not have UT IDs and are not eligible to use SciFinder®. Authorized individuals at UT-Austin who have registered for a personal SciFinder® account may use SciFinder® from any computer connected to or proxied through the campus network, including library workstations. Alternative databases that are available to non-affiliated visitors on library workstations include: Web of Science; PubMed; Engineering Index; or Inspec. Printed Chemical Abstracts (1907-2001) is also available in the library. Use of SciFinder® must be for educational and academic research purposes only. Commercial use - including patentability searching - on behalf of any profit-making entity, regardless of one's personal status at UT, is not permitted. Users must agree to these terms when connecting to the resource. CAS actively detects and reports suspect activity and violation of the terms of use may result in loss of access.

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No.

I'm a UT alumnus/a. Can I use SciFinder® after I leave UT?
No. After your EID is updated to reflect your former-student status, you no longer have access to any licensed library content, including SciFinder®. This update usually occurs about one semester (4-6 months) after you leave UT.

How do I register for a search account?
Click on the Register Now button on our SciFinder® page. Read the instructions carefully.

I don't use my utexas.edu email account. Can I still register?
You don't have to actually use your email account ending in utexas.edu, but you have to have one and it has to be functional. You can have it set to forward incoming mail to your active email account, however. You must be able to receive the confirmation email CAS will send to this address in order to complete the registration process.

I'm coming to UT from another institution. Can I use my old login here or do I have to re-register?
If you are relocating permanently, you need to re-register for a new login here at UT. Note: If you had used the "remember me" feature, you need to delete the cookies from your browser so that you can log in with your new ID. Unfortunately, any alerts, saved searches or other account-specific features must be recreated in your new account and can't be brought over from your old one. If you are a temporary visitor, just keep on using your regular login remotely via your home institution's server. (Your login won't work from UT's IP range.).

Can I share an account with someone else?
No. This is a violation of the user agreement and compromises the security of your private information. CAS will disable user accounts it suspects are shared or stolen.

When is the system available?
SciFinder® is available 24 hours a day, EXCEPT Saturday evenings, when database maintenance is done.

Can I use SciFinder® from off campus?
Yes. You can connect via the UT Libraries Proxy Server using the links found on these pages. If you bookmark the link in your browser be sure to include UT's proxy server prefix in the URL:
http://ezproxy.lib.utexas.edu/login?url=https://SciFinder® .cas.org/.

Each time you connect from off campus you'll be asked for your UT EID and password.

Note: If you connect to the campus network using the ITS VPN then go to an external site, you will revert to your original IP address, which SciFinder® will not recognize.

Can I search SciFinder® in the library?
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electronic full text, the menu includes an option to search for the journal in the library catalog. For patents, you should be taken directly to the record in the USPTO or Yes, but it's not an app. Point your device's browser to SciFinder®.cas.org/mobile and log in with your SciFinder®ID and password. You don't need to be on campus or proxied. There is a daily limit of detailed substance or reference displays, structure drawing/searching is not available, and there are no direct links to full text.

What browsers are supported?
Firefox, IE 7+, Safari and Chrome are generally supported. Keep your browser up to date; older versions may have functionality problems. The Java structure editor isn't working. Use the non-Java editor instead. Web browsers (starting with Chrome) are phasing out support for Java-based and other plug-ins.

Are there any alternative structure editors?
SciFinder®'s internal editors are the only options for drawing a structure/reaction query inside SciFinder®. Users of ChemDraw Ultra version 14+ can draw in that software and then click a SciFinder® search button to initiate a search in SciFinder® directly. You can also import .cxf files created in other tools. If you are on campus, are you using an old ID from another institution? If that's a possibility, clear your cookies to delete the old auto-login information. If you are off campus, make sure you are connecting via UT's proxy server (use the link on a library web page) and log in with your UT EID first. If your problem persists, contact the chemistry librarian.

What does a "security certificate" error mean?
Sometimes a browser doesn't trust a site you're trying to get to, and you see a pop-up box that says you are trying to go to an un-trusted site, or words to that effect. Just click the Accept/Continue/Allow button.

What if I forget my password?
Click the "forgot password" link. When you register the first time, you have to answer a secret question. Provide that answer again and CAS will email your password to your registered email address. You will not be allowed to create a duplicate user account.

Where can I get more help?
UT-Austin users can call the Chemistry Library at 512-495-4600 (Monday-Friday, 9am-5pm). Outside of business hours, contact us via email. Persons not affiliated with UT-Austin should contact their home libraries or the CAS Help Desk.

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only for journal articles and patents, and generally won't lead to other types of materials such as books, conferences, dissertations, tech reports, etc., even if they happen to exist digitally somewhere. Furthermore, the *existence* of electronic full text does not guarantee that you (as a UT-Austin patron) will have access to it. In order to view the full text, the document must either be:

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4. Contact the corresponding author and request a copy.
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Where is the full text of ACS meeting papers?

There isn't any. The CAPLUS file has included abstracts of presentations from the ACS national meetings since 1995. But because they're only abstracts, the full text link doesn't lead anywhere. If you've seen the abstract in SciFinder®, you've seen all there is to see. If you want more information about a particular abstract, try to contact the lead author.

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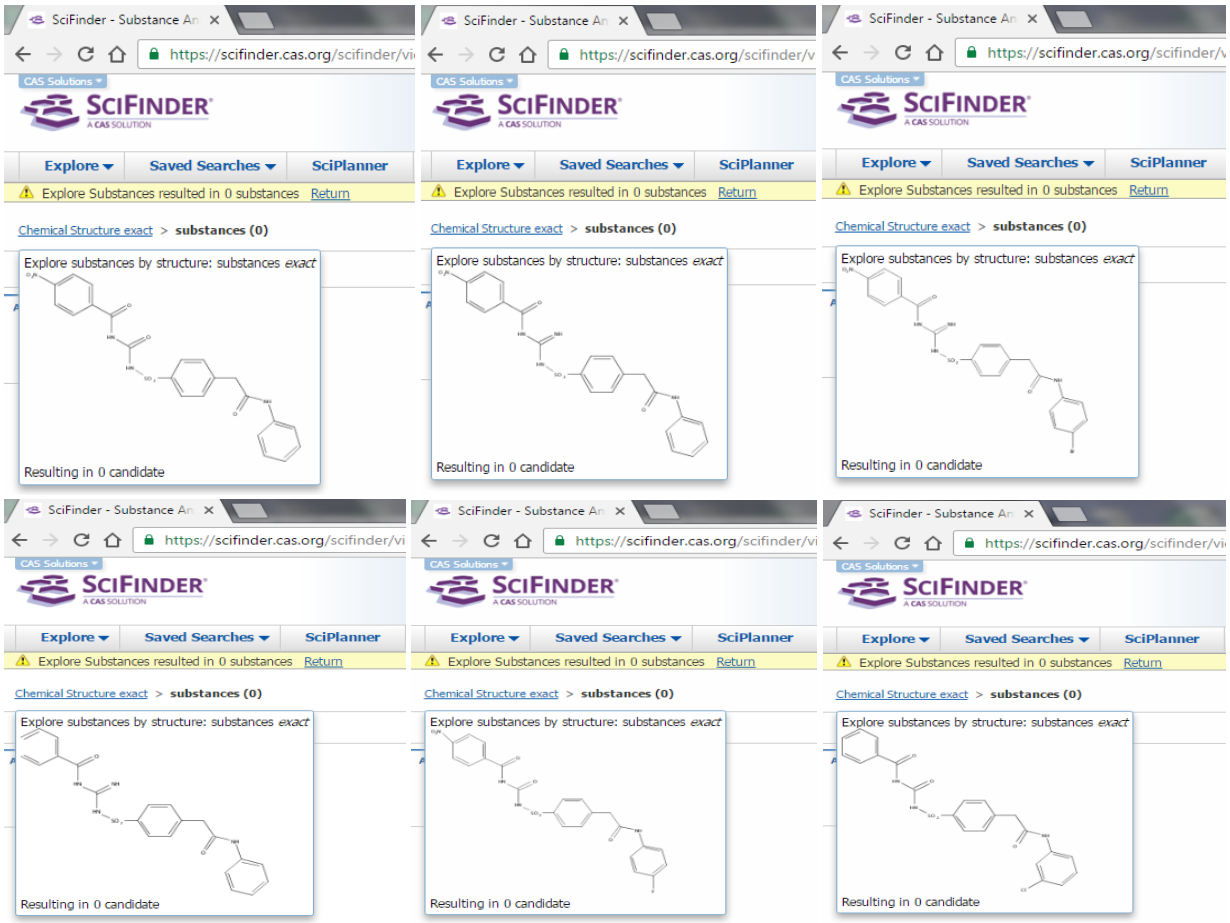

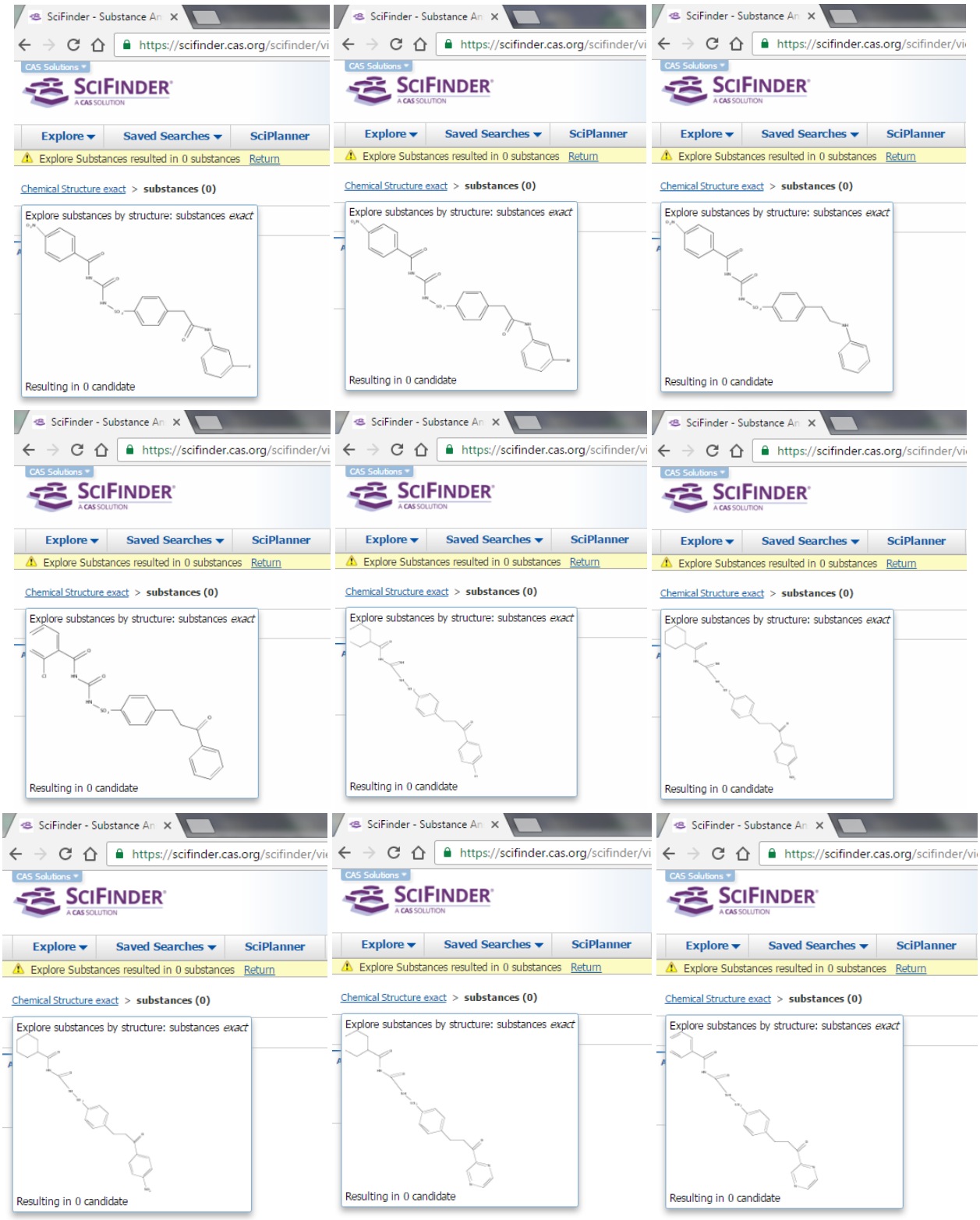
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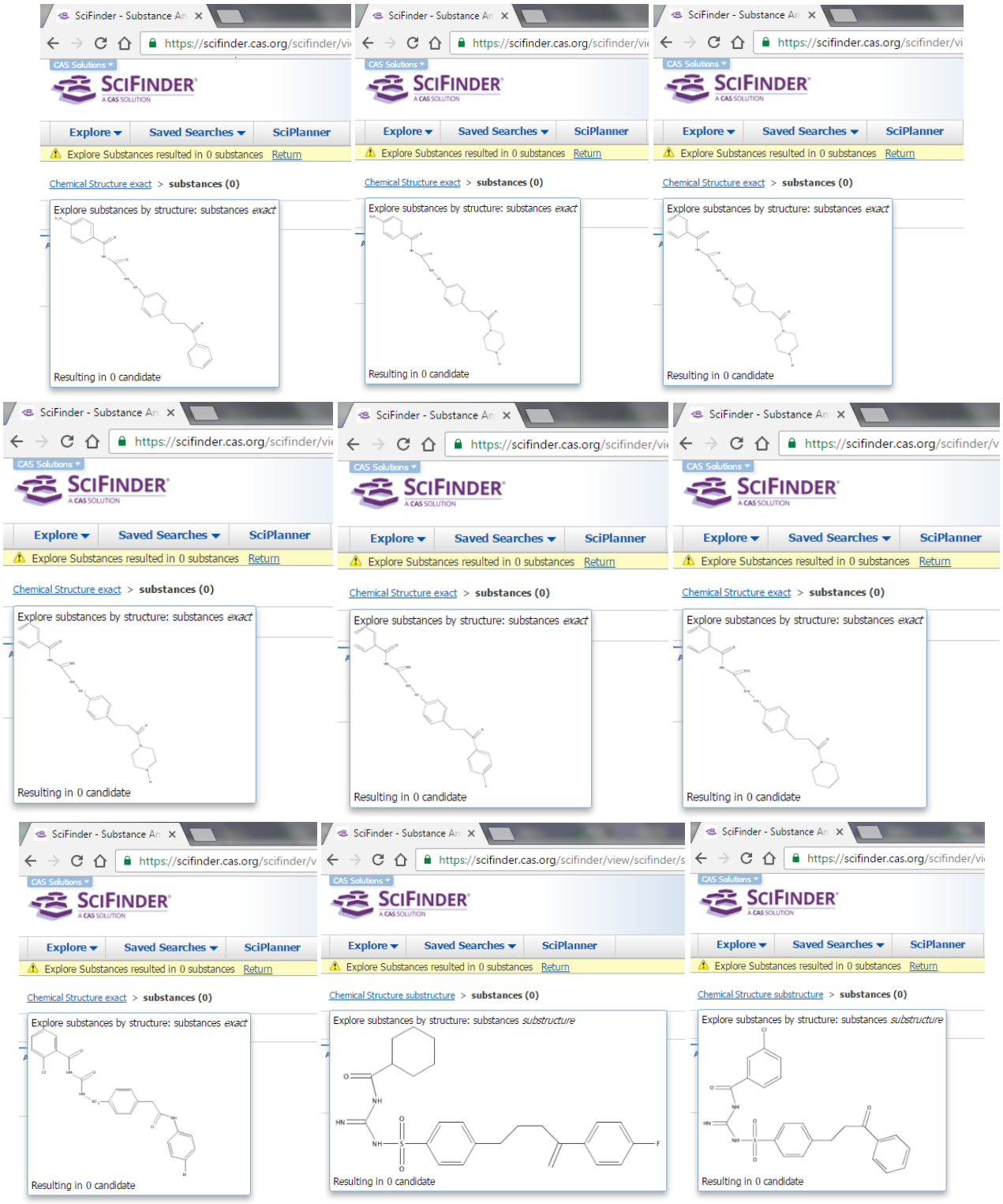

ACKNOWLEDGEMENT

SciFinder® database article has been the fruitful inspiration from my previous three articles on chemical databases: (1) Palakben K. Parikh, Julee P. Soni, Kaumil N. Modi, Urviben Y. Patel, Ravi N. Patel and Prof. Dr. Dhrubo Jyoti Sen; *Chemspider: a magic bullet of chemical database for chemists*: International Journal of Pharmacy and Technology: 2(3), 718-725, 2010. (2) Prof. Dr. Dhrubo Jyoti Sen, Nadim M. R. Chhipa, Deepa P. Patel, Jinal J. Patel, Piyush A. Gediya, Sachin M. Patel, Jaydeep H. Velani, Khushbu P. Patel, Jyoti V. Chaudhary, Sneh N. Patel and Kamlesh R. Prajapati: *SPeicherung und REcherche Struktur chemischer Information: The innovative unscramble scientific literature in chemical world as SPRESI*: Internationale Pharmaceutica Sciencia: 3(4), 22-35, 2013. (3) Prof. Dr. Dhrubo Jyoti Sen; *DrugBank as a recognized bank of drugs having ATM card in database*: World Journal of Pharmaceutical Sciences: 3(1), 1-9, 2015. SciFinder®

database has been implemented by my PhD scholar (Ishan I. Panchal) for his innovative research on *Design, synthesis and biological evaluation of some substituted sulphonyl urea, thiourea and guanidine derivatives as hypoglycemic agents* and all his synthesized derivatives have proved the structural authentification by SciFinder®.

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2. Nitsche CI, Buntrock RE, Database. 1996; 19(6): 51–58.
3. SciFinder® Research Report. CAS, 1998; 1–2.