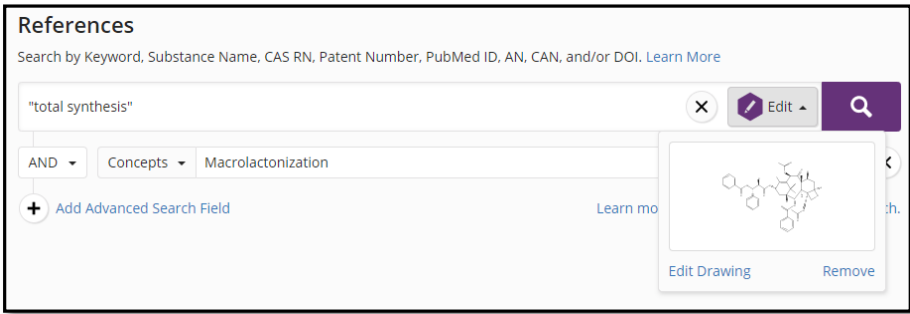


SciFinder-n is the premium new solution of Chemical Abstracts Service CAS, which provides access to the most comprehensive and reliable collection of chemistry and life science information. The scientific research information is curated by CAS editorial scientists who speak 50 languages and index and maintain the content from scientific publications and patents worldwide every day. **SciFinder-n** is the only chemistry database search engine that hosts Structure, Text, Graph/Semantic and Machine learning technologies, and works quickly and smoothly without system limits with highly advanced *Relevance ranking* algorithms. SciFinder-n saves time compared to classic SciFinder, and works also on smartphones and tablets.

SciFinder-n is new generation search platform with the following new features

- **Search history** is saved automatically as a script
- **Autosuggest** helps to browse key words, terms and author, inventor, organization names
- **Exact, Substructure** and **Similarity structure** results are presented simultaneously
- **Markush structure** includes assembled structures with claims and examples in patent
- Interactive **Filtering** new **Exclude** behavior option, and **Sorting** by Relevance, Cited and Publication date help to work with very large answers sets without limits
- Opening **new Tab / Window** allow working with multiple searches simultaneously
- **Alerts** can be easily created to monitor today also Reactions and Markush structures
- **Boolean operators** (AND, OR, NOT) – "cancer therap*" **AND** target* nano*
- **Combine text search with a structure** – "quinoline structure" with previous search
- **Reaction Schemes** include answers grouped with identical reactants and products
- **Asterisk (*)** can be used to truncate key words, substance, author and company names, i.e. cancer therap* search will include i.e. phytotherapy of cancer, Mu*ller search will bring i.e. Muller, Mueller, Müller, Miller
- **Relevance Ranking algorithms** bring the best answers first and save a lot of time
- **Citation Map** shows a dendrogram visualization on the document level with cited and onward citations helps to connect records and to find "hidden" literature and research
- **Advanced Reference** search allows today to add advanced search fields i.e. Concepts including Boolean operator with General text search and Structure:



The screenshot displays the SciFinder-n search interface. At the top, it says "References" and "Search by Keyword, Substance Name, CAS RN, Patent Number, PubMed ID, AN, CAN, and/or DOI. Learn More". The search bar contains the text "total synthesis". Below the search bar, there are filters for "AND", "Concepts", and "Macrolactonization". A button labeled "Add Advanced Search Field" is visible. On the right side, there is a preview window showing a chemical structure drawing with "Edit Drawing" and "Remove" buttons below it.

SciFinder-n gives access to CAS Content Collection, the World's Largest Collection of Chemistry Insights and human-curated scientific data

- **CAS REGISTRY®** - the CAS substance collection, is the premier accurate and authoritative source for chemical names, structures, and CAS Registry Numbers® substance data. REGISTRY covers 184 million organic and inorganic substances, including alloys, coordination compounds, minerals, mixtures, polymers, and salts disclosed in publications since the early 1800s, 70 million protein and nucleic acid sequences, and 8 billion experimental and predicted property data points and spectra. REGISTRY is updated daily with thousands of new substances to alert you to the most recent discoveries names, structures, and CAS Registry Numbers® linked to relevant publications, reactions, chemical suppliers, formulations, and more.
- **CAS REACTIONS** - The CAS reactions collection provides detailed and scientist-curated dependable data on more than 137 million single- and multi-step reactions including organic and organometallic reactions, total syntheses of natural products, and biotransformation reactions. It covers yield data, detailed reaction conditions, defined substance roles, and experimental procedures which are scientist-curated and enhanced with yield data, detailed reaction conditions, defined substance roles, and experimental procedures. Reaction data is updated daily and searchable by structure, reaction role, functional group, reaction site, atom mapping, and more.
- **CAS REFERENCES** - The CAS Reference Collection aggregates and connects scientific knowledge from 50,000 scientific journal titles worldwide over the years, with thousands of current titles actively covered from international journals, books, conference proceedings, and dissertations since 1907, with some earlier coverage back to the early 1800s. English language titles and summaries are updated daily and translated by CAS scientists from publications in more than 50 different languages from more than 180 different countries. Searchable details include standardized concept keywords, substances, reactions, and more indexed by scientists and connected to other relevant data enhanced with cited and citing references and direct links to the full-text publications (where available).
- **CAS PATENTS** - The CAS patent collection published in 50 languages by 64 issuing authorities covering more than 35,000 unique IPC codes in areas including chemistry, pharmaceuticals, consumer goods, processes, materials, engineering, agriculture, and more. Daily updated collection is augmented with English titles and abstracts and

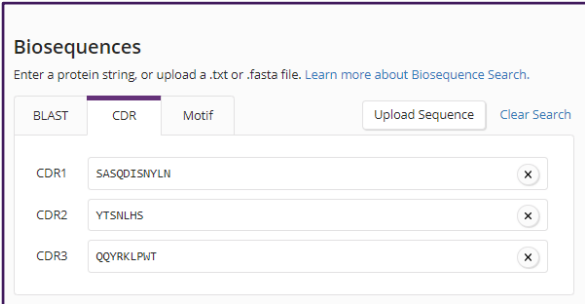
detailed indexing by CAS scientists, making complex aspects of patent documents, including chemical substances, biosequences, Markush structures, assignees, and classification codes, searchable and accessible. It includes consolidated patent family summaries and convenient connections to global full-text patent documents, claims text, legal status information, cited references, examiner citations (for select authorities) and key invention details including substances, reactions, Markush representations, and more.

- CAS COMMERCIAL SOURCES** – The CAS Commercial Sources connects researchers with chemical suppliers by providing an aggregated source of current global chemical catalog data. Consolidated listings for millions of chemical products including hundreds of up-to-date catalogues of global suppliers. CAS Commercial Sources connects researchers with chemical suppliers including verified product details include catalog name, product number, chemical and trade names, CAS Registry Number®, chemical structure, quantity, price, and contact information.

SciFinder-n gives access to the following CAS solutions

CAS SciFinderⁿ speeds the process of finding relevant, actionable insights and produces better research in less time to perform literature reviews, to mine substances and reactions, to devise synthetic plans, to conduct comprehensive biologics research, to inform IP strategy and to visualize search results.

- Biosequences** – access to 500+ million biosequences from patents to search proteins, nucleotides using the most powerful sequence search engine including **BLAST**, antibody and t-cell receptors by **CDR**, and short DNA, RNA or protein strings with **Motif algorithms**.
- Bioscape Analysis** – to visualize the similarity and patent landscape for a set of sequence results. The location of the sequence bar corresponds to the similarity of the sequence to the query, and the height of the sequence bar corresponds to the number of patents published.



Biosequences

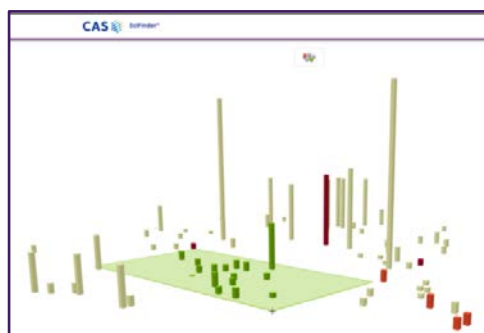
Enter a protein string, or upload a .txt or .fasta file. [Learn more about Biosequence Search.](#)

BLAST CDR Motif Upload Sequence Clear Search

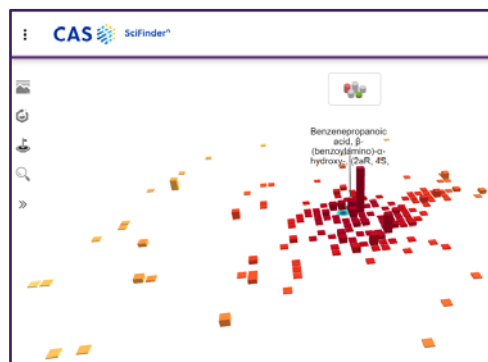
CDR1 SASQDISNYLN

CDR2 YTSNLHS

CDR3 QQYRKLPIVT



- Chemscape Analysis** – to visualize the similarity and patent landscape for a set of substance results. The location of the substance bar corresponds to the similarity of the substance to the query and the height of the substance in the visualization corresponds to the number of patents in which the substance has been published.



- Formulation purpose** – SciFinder-n includes basic information about Formulation purpose, agent and a link to new CAS Formulus[®] the largest collection of millions of agrochemical, pharmaceutical, flavors and fragrances related formulations indexed from patents, journals and product inserts.

Paclitaxel Nanoparticles: Pharmaceutical Formulation

View CAS Formulus[®] Detail [↗](#)

Location: Article page 2
 Purpose: Pharmaceutical formulations
 Target: paclitaxel

Component	Function	Amount Reported
PLGA	additives	20 mg
Paclitaxel	antiproliferative agent	2.5 mg
Dichloromethane	Solvents	1 mL
poly(vinyl alcohol) solution	solutions	4 mL

- MethodsNow-Synthesis** – millions of CAS indexed *Synthetic method protocols* which include step-by-step recipes in combination with the collection of millions of *Experimental protocols* indexed reaction details.

Experimental Protocols

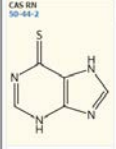
Synthetic Methods	Experimental Procedure
Products	Paclitaxel, Yield: 100%
Reactants	Benzenepropanoic acid, β-(benzylamino)-α-hydroxy-, (2aR,4S)-4-(5-(6R,6S,11S,12S,12aR,12bD)-6,12b-bis(acetyloxy)-12-(benzoyloxy)-2a,3,4,4a,5,6,9,10,11,12,12a,12b-dodecacyclo-11-hydroxy-4a,8,13,13-tetramethyl-5-oxo-4-(trithylsilyloxy)-7,11-methano-14-cyclodeca[3,4]benz[1,2-b]oxole-9-yl ester, (αR, βS)-
Reagents	Hydrochloric acid
Solvents	Ethanol Water
Procedure	1. Add HCl (2 M, 2 mL) to a solution of 7-O-(triethylsilyl)paclitaxel (7 mg) in ethanol (2 mL) at 0 °C. 2. Stir the reaction for 2h and 25 minutes from 0 °C to room temperature. 3. Add EtOAc and aqueous sodium hydrogencarbonate at 0 °C. 4. Extract the mixture with dichloromethane. 5. Dry the organic layer over sodium sulfate. 6. Filter the mixture and evaporate the solvent. 7. Purify by silica gel column chromatography to obtain paclitaxel.
Transformation	Formation of Alkyl Halides/ Alcohols from Ethers /Silyl Ethers

- CAS PatentPak[®]** – integrated workflow solution designed to radically reduce time spent acquiring and searching through 18 million searchable, full-text patents from 46 major patent offices across the globe. CAS scientists have annotated the important chemistry to interactive patent chemistry viewer to quickly pinpoint the examples, claims, including intermediates and starting materials which could not be identified by algorithms.

CAS PatentPak PAGE 13 ZOOM DOWNLOAD PDF PDF+

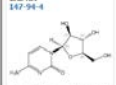
Key Substances in Patent

CAS RN 50-44-2



Analyt Markup Locations (2)
 Page 8
 Page 12

CAS RN 147-94-4



Analyt Markup Locations (2)
 Page 6
 Page 10

20 **Glaxal Water (tradename)**
 The above-mentioned antitumor antimetabolites are commercially available, as exemplified by the following: methotrexate from Takeda Pharmaceutical Co., Ltd. as **Methotrexate (tradename)**; 6-mercaptopurine riboside from Aventis Corp. as **Thioguanine (tradename)**; thiopurine from Takeda Pharmaceutical Co., Ltd. as **Lodatin (tradename)**; 5-fluorouracil from Kyowa Hakko Kogyo Co., Ltd. as **5-FU (tradename)**; tegafur from Taiho Pharmaceutical Co., Ltd. as **Futafur (tradename)**; doxifluridine from Nippon Roche Co., Ltd. as **Furston (tradename)**; capecitabine from Yamanouchi Pharmaceutical Co., Ltd. as **Yamafur (tradename)**; cytarabine from Nippon Sharyaku Co., Ltd. as **Cytocide (tradename)**; cytarabine octofate from Nippon Kayaku Co., Ltd. as **Straid (tradename)**; encicidine from Aashi Kasei Corp. as **Sarabine (tradename)**; 5-1 from Taiho Pharmaceutical Co., Ltd. as **TS-1 (tradename)**; gemcitabine from Eli Lilly & Co. as **Gemzar (tradename)**; Edoxarabine from Nippon Schering Co., Ltd. as **Fluders (tradename)**; and pentostereon disodium from Eli Lilly & Co. as **Alanta (tradename)**.

25 The above-mentioned antitumor antibiotics are commercially available, as exemplified by the following: actinomycin D from Iriyo Pharmaceutical Co., Ltd. as **Caromycin (tradename)**; doxorubicin from Kyowa Hakko Kogyo Co., Ltd. as **adriatic (tradename)**; idarubicin from Meiji Seika Kaisha Ltd. as **Duoistone**; teniposide from Yamanouchi Pharmaceutical Co., Ltd. as **Nocarcinostatin (tradename)**; teniposin from Nippon Kayaku Co., Ltd. as **Elivo (tradename)**; piroperonyl from Nippon

- 10 -

WO 2006/046728 PCT/JP2005/01958

- Retrosynthesis Analysis** – Experimental and predictive retrosynthetic analysis for known and novel substances in SciFinder-n is based on “Computer-Aided Synthetic Design” AI software which includes synthesizing intermediates, updating and optimizing production synthesis, evaluating alternative synthetic routes and competitor IP differentiation for synthetic pathways. It speeds up the navigation of alternative routes or evaluation of expected yields and finding estimated overall costs and commercially available starting materials and cuts time spent in retrosynthetic planning from days or hours to minutes!

