

patsnap

Getting Started with PatSnap Chemical



Welcome to PatSnap Chemical

Innovation in chemistry is required in all sectors of industry, whether it be life science, or material science, or indeed many other branches of science. These innovations are the foundation of our modern society and lead the way for businesses to develop.

PatSnap Chemical is a platform that has been created using direct feedback and ideas from both leading academics and multinational companies in the chemical industry. The result is a solution that enables researchers to instantly jump from chemical structure searches to related patents and back again in one seamless workflow.

PatSnap Chemical, with over 120 million patents, 114 million chemical structures, plus regulatory and clinical trial information, allows users to capture all the most important information on a chemical of interest and the patents associated with it.

The platform streamlines the workflow of your new projects and ideas as well as providing ways of searching for research material.

Search | locate the chemical of interest

Results | refine further the data behind your search

Chemical Information | obtain all the important data about the chemical

Analysis | put patents related to the structure into a statistical context

Chemscape | gain a strategic perspective of your chemical of interest

Patents | obtain a detailed view of any innovation

Extract | extract all chemicals from one or multiple patents

Search

The image shows a screenshot of the Marvin JS search interface. The interface is divided into several sections: a top navigation bar with 'Search', 'LabBench', and 'Alert'; a main search area with tabs for 'Structure', 'Multi-Structure', 'Polymer', 'Keyword', 'Properties', and 'Bulk'; a central workspace with the Marvin JS logo; a right-hand panel with a 'Draw Helper' section and a 'History' list; and a bottom search bar with options like 'Search Across All Databases', 'Title/Abstract/Claims/Desc.', '+ Add Keyword', and 'Preferences'. Annotations with green arrows point to various parts of the interface:

- List of searches available in PatSnap Chemical:** Points to the 'Original Search Style' dropdown menu.
- Build or edit the structure being searched:** Points to the central workspace.
- Select specific jurisdictions, search area and other options:** Points to the 'Search Across All Databases' and 'Title/Abstract/Claims/Desc.' options.
- Enter Chemical name or Identifier:** Points to the 'Name to structure' input field in the Draw Helper.
- Search by uploading an image of a structure:** Points to the image upload icon in the Draw Helper.
- Previous searches will appear here:** Points to the 'History' list in the Draw Helper.
- Choose the type of search:** Points to the 'Exact Structure' and 'Search Similar Structure' buttons.

Results

Refine results using different criteria such as Simple Legal Status, Publication year and much more

Refine further with bespoke properties

Transform search results into an Analysis dashboard

The screenshot shows the PatSnap 'Similarity Search - Structure Results' interface. The search results are displayed in a table-like format with columns for chemical structure, name, similarity score, patent count, and assignee. The results are: 1. Aspirin (Similarity Score: 1, Patents: 869,474 (100%) / 869,474, Top Std. Assignee: ZENEFILM), 2. 2-acetyloxybenzoate (Similarity Score: 1, Patents: 3,000 (100%) / 3,000, Top Std. Assignee: ELI LILLY AND COMPANY), and 3. hypyirin (Similarity Score: 1, Patents: 5,284 (100%) / 5,284, Top Std. Assignee: PHARMACIA). On the right side, there is a 'View Patents' section showing a list of relevant patents with buttons to view each. The interface includes a 'Refine by Structure' sidebar on the left and a 'Similarity' filter on the top right.

Adjust results settings to change what information is displayed and what order and format

View the patents associated with the structure with a click of a button

View the results in a Chemical Landscape

Chemical Information

Mouse over the structure for more zoomed in look at the structure

Under the Overview tab the following data are available
Structural properties
identifiers
and external references

The screenshot shows the 'Overview' tab for Aspirin. On the left, there is a chemical structure of Aspirin. Below it are sections for 'Identifiers', 'Cross-References', and 'Structure Properties'. The 'Structure Properties' section is expanded, showing a list of various chemical and physical properties.

Molecular Weight	180.159 g/mol
XLogP3	1.3101
Hydrogen Bond Donor Count	1
Hydrogen Bond Acceptor Count	3
Rotatable Bond Count	3
Exact Mass	180.042258738 g/mol
Monoisotopic Mass	180.042 g/mol
Topological Polar Surface Area	63.60000000000001
Heavy Atom Count	13
Formal Charge	0
Complexity	212
Isotope Atom Count	0
Defined Atom Stereocenter Count	
Undefined Atom Stereocenter Count	
Defined Bond Stereocenter Count	
Undefined Bond Stereocenter Count	
Covalently-Bonded Unit Count	
Molecular Species	
#Ro5 Violations	
ACD Acidic pKa	
ACD LogP	
ACD LogD pH7.4	
OED Weighted	
Color/Form	
Taste	
Viscosity	

Tab through other available information on the chemical including Regulatory Approval and Clinical Trial

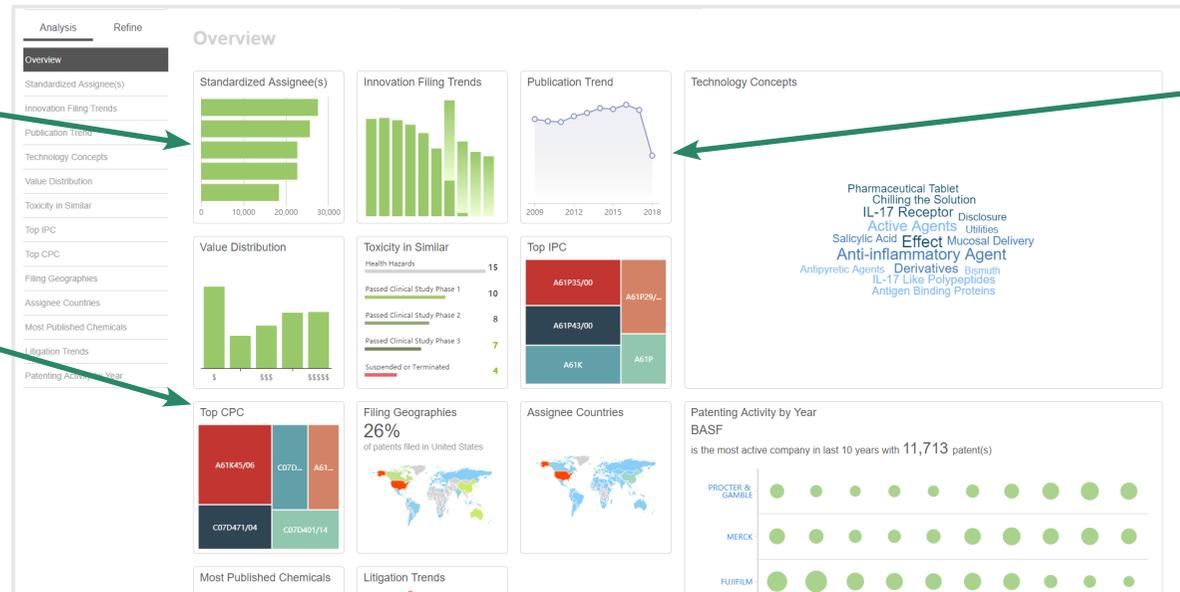
The screenshot shows the 'Human Approvals' tab for Aspirin. It features a navigation bar with tabs for 'FDA (USA)', 'EMA (Europe)', 'CFDA (China)', 'ECHA REACH', 'NLM HSDB', 'SPC (Europe)', and 'EHS (Canada)'. The main content area displays the 'United States of America Food and Drug Administration' section, listing approvals for 'PLX PHARMA INC' and 'ARALEZ PHARMACEUTICALS TRADING DAC'. The 'PLX PHARMA INC' section includes an 'Approved' status and a table of patents.

Patent	Expiration Date	Time until Expiry	Use Codes
US9101637	23 Mar 2022	43 MONTHS	U-1732 , U-1733 , U-1731
US9216150	29 Sep 2032	170 MONTHS	- Drug Product
US9351984	19 Dec 2021	40 MONTHS	- Drug Product
US8865187	23 Mar 2022	43 MONTHS	- Drug Product
US9226892	29 Sep 2032	170 MONTHS	U-1733 , U-1731 , U-1732

Analysis

Click into any chart to analyse data relating to the chart topic

Further refine your search directly from the graphs



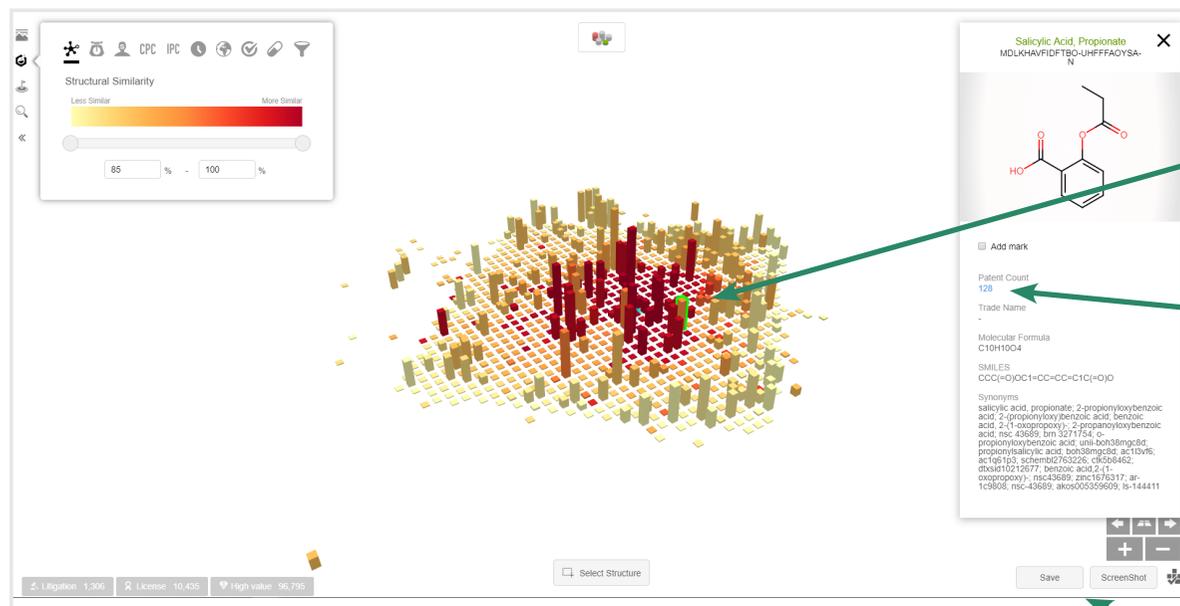
Hover over a chart to get quick information

Chemscape

Manage and view your saved Chemscape

Group and Refine your Chemscape to show key information

Further refinement by Keywords, dates and other patent properties



Click on any bars to view structures and number of patents associated to it

Hyperlink directs straight to the associated patents

Save and Screenshot your Chemscape

Patents

Use Structure field option to see most mentioned structure

Assignee	Title	Assignee Name	Current Assignee	Application Date	Publication Date	Structure
FUJIFILM PHOTO FILM CO., LTD.	1958					
FUJIFILM CORPORATION	1606					
EASTMAN KODAK COMPANY	1563					
BASF AKTIENGESELLSCHAFT	1519					
BASF SE	1301					
ORAL DRUG TECHNOLOGY OPER.	1224					
THE FROCTER & GAMBLE COMP.	1051					
CANON KABUSHIKI KAISHA	813					
GENERAL ELECTRIC COMPANY	802					
BRISTOL-MYERS SQUIBB COMPANY	More					
IPC						
Application Year						
Standardized Assignee						
Grouped Assignee Name						
Std. Assignee Type						
Authority						
Patent Type						
CPC						
LOC						
IPC						
Publication Year						
Simple Legal Status						
Legal Status						
Legal Events						
Inventor						
Agency						
Patent Value						
SEP Source						

Spot the Chemicals with Chemical highlighter and navigate through the patent to see where they appear

US20060153935A1 Stabilizing Salicylate Compositions And Method Of Preparation For Oral And Topical Use

Overview Dual View Citation Patent Family Legal Information

Abstract

Claims

Description

1. A compound comprising a salicylic acid or acetylsalicylic acid, citric acid, and potassium hydroxide for topical or oral use.

2. A method of forming the compound as claimed in claim 1 comprising a first step of mixing said acetylsalicylic acid/citric acid mixture.

3. The method as claimed in claim 2 comprising said salicylic acid/citric acid mixture or said acetylsalicylic acid solution or a stabilized potassium acetylsalicylic acid solution.

4. The method as claimed in claim 3 comprising said stabilized potassium salicylic acid or said acetylsalicylic acid solution or a stabilized potassium acetylsalicylic acid solution.

5. The method as claimed in claim 4 wherein said enhancements are selected from a group of calcium and cherry juice.

6. A compound as claimed in claim 1 where said citric acid is present in amount to make said preservative.

7. A compound as claimed in claim 1 comprising said citric acid being present in amount to elicit preservative.

8. A compound as claimed in claim 1 comprising said stabilized potassium salicylic acid or stabilized potassium acetylsalicylic acid produced in oral forms selected from health drinks, soups, puddings, powders, and tablets.

9. A compound as claimed in claim 1 comprising said stabilized potassium salicylic acid or stabilized potassium acetylsalicylic acid is prepared as a topical formulation consisting of gels, lotions, ointments, and poultices.

10. A compound as claimed in claim 1 comprising said stabilized potassium salicylic acid or said stabilized potassium acetylsalicylic acid is used for hydration, flea and tick control, dental malodors, pain relief, earaches, headaches, tension pain, arthritis, shingles, microbioocides, spermaticocides, reduces stress, pesticide, deodorants, washes, lubricants, anti-burn, anti-itch, muscle spasms, and muscle cramps.

11. A method of dehydrating said stabilized potassium salicylic acid or said stabilized potassium acetylsalicylic acid for use topically or orally comprising pouring a thin layer of said stabilized potassium salicylic acid or said stabilized potassium acetylsalicylic acid onto preheated plates where said preheated plates are allowed to dry, said preheated plates are then scraped to removed the powdered potassium salicylic acid or powdered potassium acetylsalicylic acid.

12. A method of dehydrating as claimed in claim 12 wherein said preheated plates are heated to about 170.degree. F.

13. A method of dehydrating as claimed in claim 11 wherein said dehydrating systems include fluid bed dryers, airstream systems, flash dryers, spray drier absorbers or granulators.

14. A method of blending topical formulation as claimed in claim 1 comprising diluting said stabilized potassium salicylic acid solution or said stabilized potassium acetylsalicylic acid solution with water to cool said salicylic acid solution and blending with cold pressed aloe vera.

Structure Highlighter

210,762 Patents

2 US20060153935A1

Stabilizing salicylate compositions and method of preparation for oral and topical use

1 US5723453

Stabilized, water-soluble aspirin composition

3 US20110263526A1

Nitric Oxide Releasing Prodrugs of Therapeutic Agents

4 EP023459A1

Medicament containing a magnesium-urea complex of acetylsalicylic acid and process for the preparation of this complex

5 GB993682A

Salts of acetylsalicylic acid, their production and pharmaceutical preparations containing them

6 EP1684725A1

NOVEL NIMESULIDE COMPOSITIONS

7 EP1094819A1

INJECTABLE SODIUM ACETYLSALICYLATE COMPOSITION AND METHOD

8 US20090312433A1

TREATMENT OF VRI1-ANTAGONIST-INDUCED INCREASE IN BODY TEMPERATURE WITH AN ANTIPYRETIC AGENT

9 US4783551

Potassium acetylsalicylate addition compound and process of preparing

Hover over the highlighted chemical to get a preview of the structure

Extract

Extract all chemicals within selected patents to PatSnap Chemical

The screenshot shows the PatSnap interface with a search query: (INCHI_TITLE:(9557105 OR 12882120 OR 80437066 OR 721011 OR 79646970 OR 142419305 OR 117332813 OR 21600061 OR 86262648 OR 15430928 OR 1...)). The interface displays a table of patent results with columns for Assignee, Publication Number, Title, Assignee Name, Current Assignee, Application Date, and Publication Date. A context menu is open over the third row, showing options: Export, Save to Workspace, Extract Chemical Structures, and Extract Sequences. The menu also indicates '3 Selected' and 'Unselect all'.

#	Publication Number	Title	Assignee Name	Current Assignee	Application Date	Publication Date	Structure
1	US6723453	Stabilized, water-soluble aspirin composition	HEALTH CORPORATION	SOLUPRIN PHARMACEUTICALS, INC.	13 Nov 1995	03 Mar 1998	<chem>CC(=O)OC1=CC=CC=C1</chem>
2	US20060153935A1	Stabilizing salicylate compositions and method of preparation for oral and topical use	BLAHUT NATALIE	BLAHUT NATALIE	09 Jan 2006	13 Jul 2006	<chem>CC(=O)OC1=CC=CC=C1</chem>
3	US20110263526A1	Nitric Oxide-Releasing Prodrugs of Therapeutic Agents	PIRAMAL LIFE SCIENCES LIMITED	PIRAMAL ENTERPRISES LIMITED	22 Apr 2011	27 Oct 2011	<chem>CC(=O)OC1=CC=CC=C1</chem>
4	EP0233459A1	Medicament containing a magnesium-urea derivative of acetylsalicylic acid and process for the preparation of the complex	ARTIKA INTERNATIONAL (HONG-KONG) LIMITED	ARTIKA INTERNATIONAL (HONG-KONG) LIMITED	09 Jan 1987	26 Aug 1987	<chem>CC(=O)OC1=CC=CC=C1</chem>
5	GB993682A	Salts of acetylsalicylic acid, their production and pharmaceutical preparations containing them	AKTIEBOLAGET HASSLE APOTEKARE PAUL NORDSTROMS FABRIKER	AKTIEBOLAGET HASSLE APOTEKARE PAUL NORDSTROMS FABRIKER	04 Jul 1963	02 Jun 1965	<chem>CC(=O)OC1=CC=CC=C1</chem>
6	EP1684725A1	NOVEL NIMESULIDE COMPOSITIONS	ELAN PHARMA INTERNATIONAL LIMITED	ELAN PHARMA INTERNATIONAL LIMITED	31 Oct 2003	02 Aug 2006	<chem>CC(=O)OC1=CC=CC=C1</chem>
7	EP1094819A1	INJECTABLE SODIUM ACETYLSALICYLATE COMPOSITION AND METHOD	GALAT, ALEXANDER	GALAT, ALEXANDER	09 Jul 1999	02 Aug 2006	<chem>CC(=O)OC1=CC=CC=C1</chem>
8	US20090312433A1	TREATMENT OF VRI-ANTAGONIST-INDUCED INCREASE IN BODY TEMPERATURE WITH AN ANTIPIRETYC AGENT	AMGEN INC.	AMGEN INC.	28 Aug 2009	02 Aug 2006	<chem>CC(=O)OC1=CC=CC=C1</chem>
9	US4783551	Potassium acetylsalicylate addition compound and process of preparing	GALAT, ALEXANDER	GALAT, ALEXANDER	20 May 1986	08 Aug 1987	<chem>CC(=O)OC1=CC=CC=C1</chem>

Innovators ask. PatSnap answers.

PatSnap answers the hardest questions encountered throughout the innovation life cycle—from creating new inventions to commercializing them.

The tool stores in one place all the information typically consulted by R&D and intellectual property teams—including millions of patents, scientific journals, litigation data, as well as company technology and financial profiles.

Our deep learning algorithms find patterns across these billions of data points, so you get game-changing insights in the blink of an eye.

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