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Veli-Pekka Hyttinen

ACS International Ltd., Central and Eastern Europe

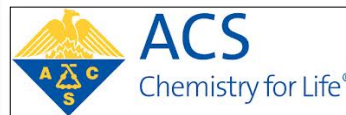


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ACS Mission

To improve people's lives through the transforming power of chemistry.



CAS Mission

To provide the world's best digital research environment to search, retrieve, analyze and link chemical information.



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Document Indexing



RXN, Methods Formulations



Markush Indexing



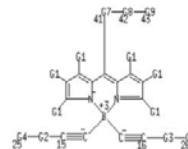
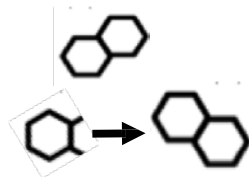
Authority Processing



Data pre-repository



1990
Smith, M.
anthracene



Androst-4-en- 3-one, 17- hydroxy-17- methyl-, (17β)-



CAS®

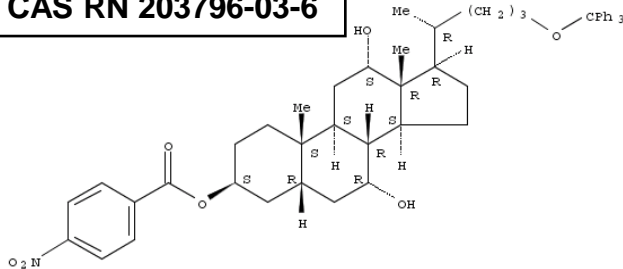
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AMERICAN CHEMICAL SOCIETY

CAS scientists find the chemistry, and save you time!

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C, and was stirred for half an hour during which time the yellow solution became a paste.

- 5 Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding NaHCO₃ solution followed by extraction with EtOAc (3x50 mL). The combined extracts were washed with brine once and dried over anhydrous Na₂SO₄. The desired product (2.72 g, 85% yield) was obtained as white powder after
- 10 SiO₂ chromatography (Et₂O/hexanes 1:2). m.p. 207-209 °C.; IR (KBr) 3434, 3056, 2940, 2868, 1722, 1608, 1529, 1489, 1448, 1345 cm⁻¹; ¹H NMR (CDCl₃, 300 MHz) δ 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.46-7.42 (m, 6 H), 7.31-7.18 (m, 9 H) 5.33 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.09-2.97 (m, 2 H), 2.68 (td, J=14.95, 2.56 Hz, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.06 (series of multiplets, 24 H), 1.01 (s, 3 H), 0.98 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H). ¹³C NMR (CDCl₃, 75 MHz) δ 164.21, 150.56,
- 15 144.70, 136.79, 130.77, 64.22, 47.79, 46.79, 42.18, 28.74, 27.71, 26.85, 26.3 (thioglycerol+Na⁺ matrix)

CAS RN 203796-03-6



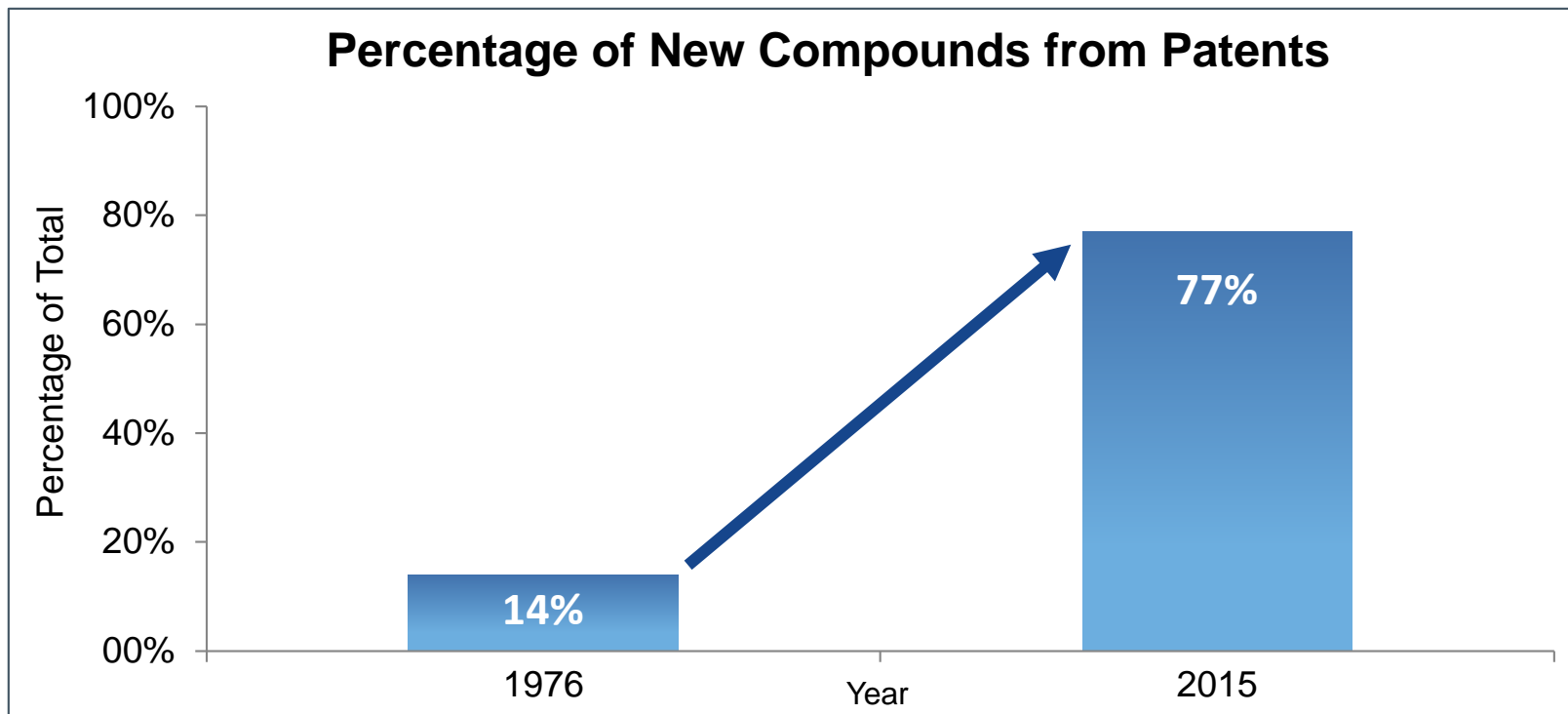
Absolute stereochemistry.



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Increasingly, new compounds in the literature are first disclosed in patents



CAlplus coverage of patents from Asia is unmatched



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CAS coverage includes publications scientists read daily across the spectrum of biomedical disciplines

Molecular Biology and Genetics

- *Annual Review of Genetics*
- *Cell*
- *Developmental Cell*
- *Genome Research*
- *Journal of Cell Biology*
- *Molecular Genetics and Genomics*
- *Nature*
- *New England Journal of Medicine*
- *Proceedings of the National Academy of Sciences*
- *Science*

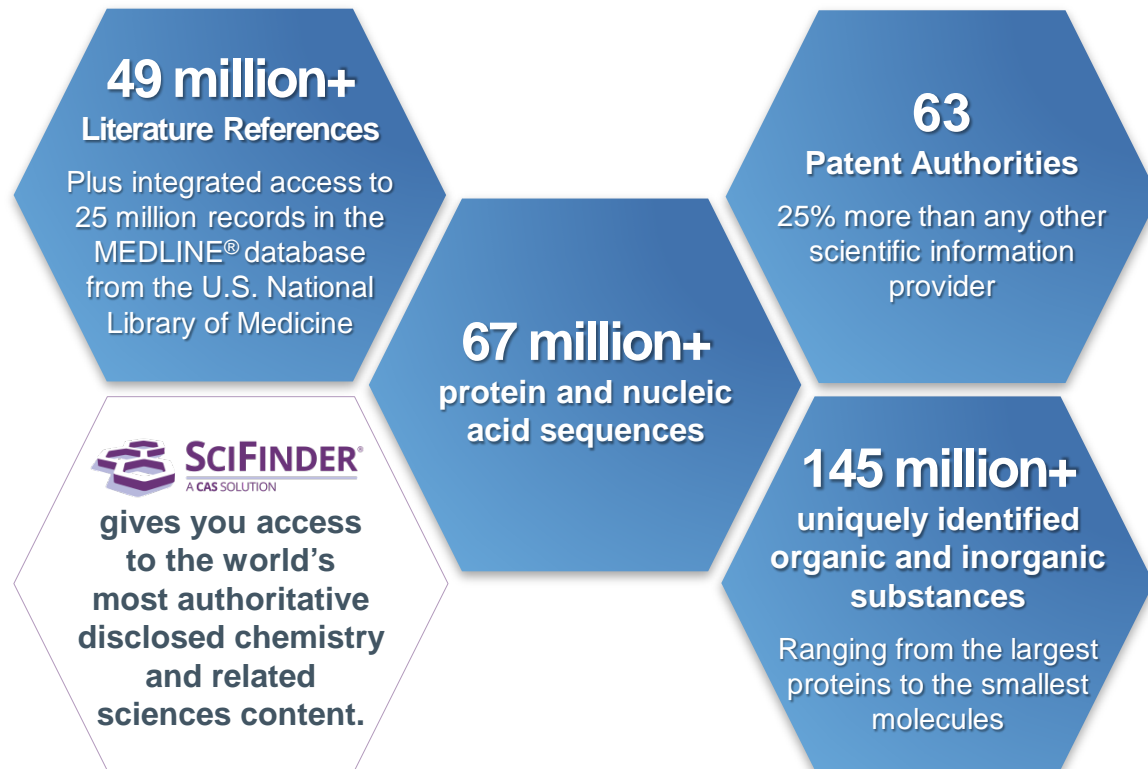
Biochemistry

- *ACS Chemical Biology*
- *ACS Synthetic Biology*
- *Annual Review of Biochemistry*
- *Biochemistry and Cell Biology*
- *Cellular Physiology and Biochemistry*
- *Journal of Biological Chemistry*
- *Journal of Cellular Biochemistry*
- *Molecular and Cellular Biochemistry*
- *Preparative Biochemistry and Biotechnology*

Pharmaceuticals and Medicinal Chemistry

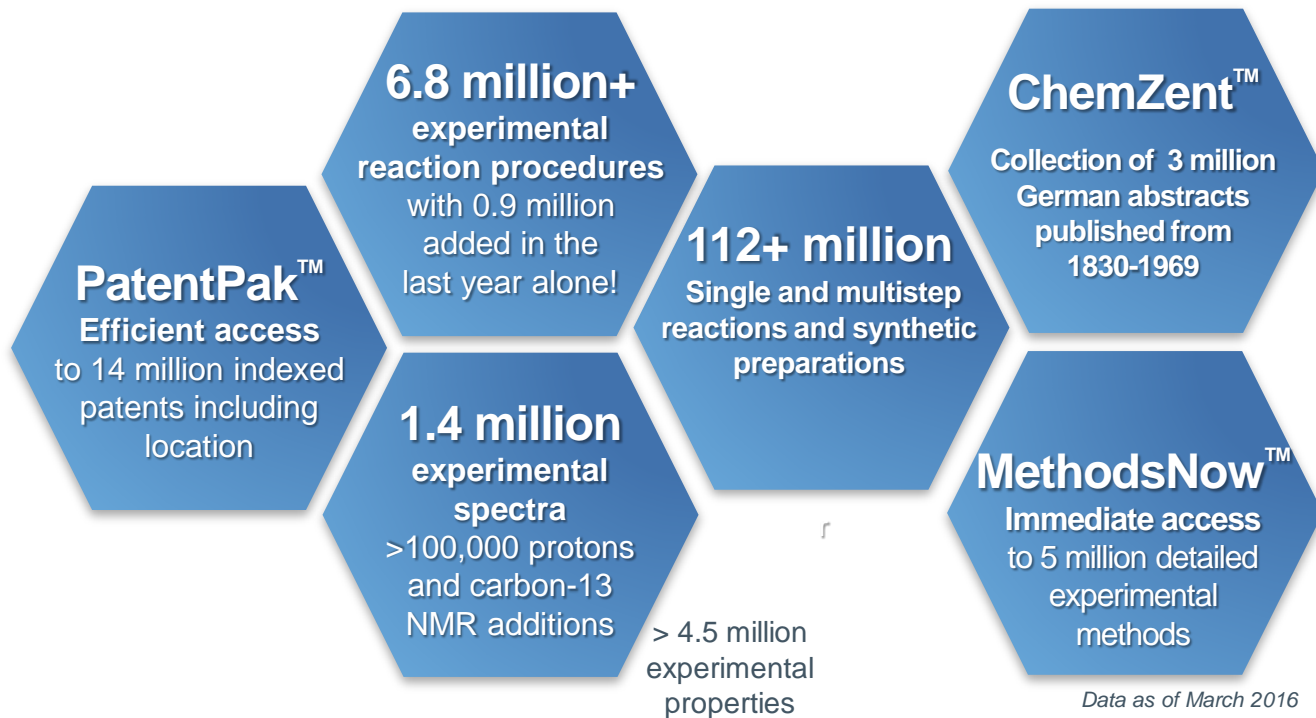
- *Advanced Drug Delivery Reviews*
- *Annual Review of Pathology: Mechanisms of Disease*
- *Anti-Inflammatory Anti-Allergy Agents in Medicinal Chemistry*
- *Circulation Research*
- *Immunity*
- *Journal of the American Medical Association*
- *Journal of Experimental Medicine*
- *Nature Reviews Drug Discovery*

CAS analyzes the world's disclosed research to keep SciFinder the most valuable tool supporting your organization's research enterprise



Data as of March 2016

SciFinder saves you time by delivering valuable information to advance your research



Key Substances in Patent

CAS RN 7440-38-2D

As

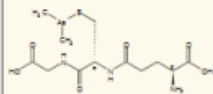
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Analyst Markup Location

- page 2
- page 3

CAS RN 69819-86-9

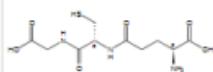


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Analyst Markup Location

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CAS RN 70-18-8

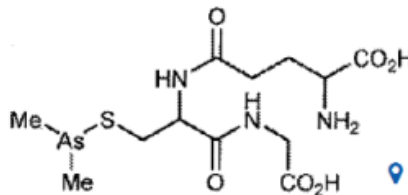


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Analyst Markup Location

- page 19

[0005] The present invention provides novel crystalline forms of organic arsenical compounds having anti-cancer properties. In certain embodiments, the present invention provides a crystalline form of a compound having a structure of formula (I) (darinaparsin)



(I)

[0006] wherein the crystalline form has a melting point greater than or equal to 185 °C. In some embodiments, the crystalline form has a melting point in the range of about 185-200 °C. In some embodiments, the crystalline form has a melting point in the range of about 187-200 °C, e.g., 187-197 °C. In some embodiments, the crystalline form has a melting point in the range of about 190-200 °C. In other embodiments, the invention provides a crystalline form of a compound having a structure of formula (I) (darinaparsin) wherein the crystal form has an X-ray powder diffraction pattern comprising characteristic peaks at one or more of the following angles: about 16.6°, about 17.4°, about 18.4°, about 19.3°, about 20.0°, about 21.0°, about 22.0°, about 23.3° and about 25.0°.

[0007] In some embodiments, the X-ray powder diffraction pattern of a compound having a structure of formula (I) (darinaparsin) expressed in terms of 2θ, at one or more of the following angles: about 14.4°, about 19.3°, about 22.0°, about 23.3° and about 25.0°. In some embodiments, the X-ray powder diffraction pattern of the crystalline form of a compound having a structure of formula (I) (darinaparsin) has



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METHODSNOW™ – Step-by-step experimental protocols

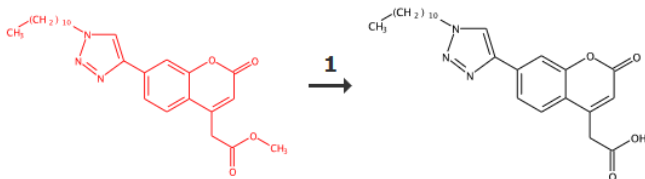
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MethodsNow

7-Triazolylcoumarin-based fluorescent tag system for stepwise, comparative assessment of small molecule mi

By Jeon, Moon-Kook; Kang, Myoung-Ku; Park, Koon Ha
From Tetrahedron, 68(30), 6038-6053; 2012
Published by Elsevier Ltd.

Reaction Steps **1** 2 3 4



Products	2 <i>H</i> -1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1 <i>H</i> -1,2,3-triazol-4-yl)-, 75%, CAS RN 1384966-77-1
Reactants	2 <i>H</i> -1-Benzopyran-4-acetic acid, 2-oxo-7-(1-undecyl-1 <i>H</i> -1,2,3-triazol-4-yl)-, methyl ester, 1384966-75-9
Reagents	Hydrochloric acid, CAS RN: 7647-01-0 Lithium hydroxide, CAS RN: 1310-65-2
Solvents	Water, CAS RN: 7732-18-5 Tetrahydrofuran, CAS RN: 109-99-9

Print

MethodsNow

Procedure

1. Add lithium hydroxide monohydrate(327 mg, 7.80 mmol) to 4-methoxycarbonylmethyl-7-(1-undecyl-1*H*-1,2,3-triazol-4-yl)-2*H*-chromen-2-one (343 mg, 0.780 mmol) in THF/water(25 mL/25 mL) at room temperature.
2. Stir the reaction mixture for 3 hours at room temperature.
3. Adjust pH 3-4 to the reaction mixture by adding 1 N hydrochloric acid.
4. Partition the reaction mixture between ethyl acetate and water.
5. Extract the aqueous layer with ethyl acetate.
6. Dry the combined organic layer over magnesium sulfate.

Scale

milligram

¹H NMR

¹H NMR (300 MHz, acetone-*d*₆): δ = 7.83 (s, 1H), 8.58 (s, 1H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 6.47 (s, 1H), 4.50 (t, *J* = 7.2 Hz, 2H), 3.99 (s, 2H), 2.00 (quintet, *J* = 7.2 Hz, 2H), 1.32-1.43 (m, 4H), 1.22-1.32 (m, 12H), 0.87 ppm (t, *J* = 6.8 Hz, 3H).

¹³C NMR

¹³C NMR (125 MHz, DMF-*d*₇, 60 °C): δ = 161.0, 155.1, 154.2, 146.5, 136.0, 127.2, 123.7, 122.1, 120.4, 115.3, 113.5, 51.1, 32.8, 29.9, 27.3, 23.5, 18.7, 14.7 ppm (decarboxylation occurred to give the corresponding 4-methyl derivative).

IR

IR (ATR, neat): ν = 3423, 2922, 2851, 1702 (2C=O, overlapped), 1619, 1561, 1375, 1154, 936, 852, 809 cm⁻¹.

HRMS

HRMS (EI): *m/z* calculated for C₂₄H₃₁N₃O₄: 425.2315 [M⁺]; found: 425.2315.

Mass Spec

MS (ESI): *m/z*: 426 [M+H⁺].

MP

235.5±0.8 °C.

CAS Method Number

3-352-CAS-78415

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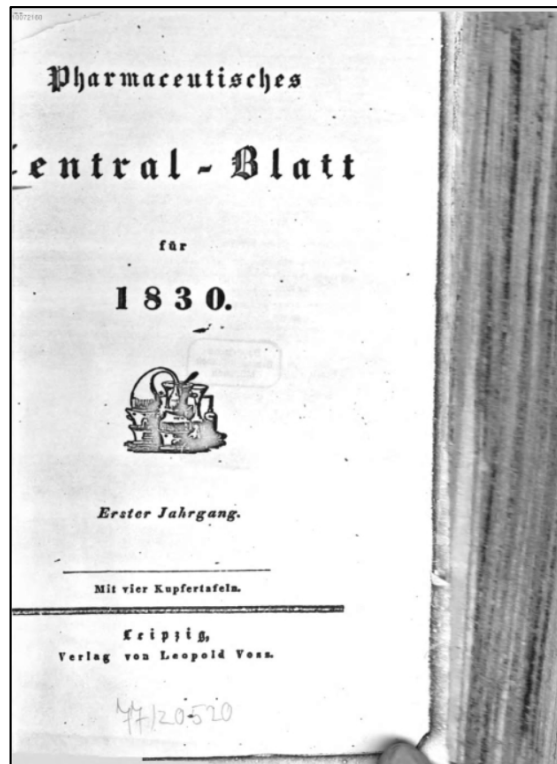


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Chemisches Zentralblatt predates the introduction of Chemical Abstracts by almost 80 years

- Published German language abstracts from 1830-1969
- Chronicles the birth of chemistry as a science
 - Before 1800, chemistry was more alchemy (i.e. how to turn lead into gold) than actual science
- Searchable substance structures in 3 million machine translated abstracts



First Issue:
Note, the name changed several times before 1856

Get to actionable results more quickly with a streamlined new interface

Streamlined search navigation saves you clicks

Immediately run past searches

The screenshot displays the SciFinder search interface. At the top, there is a navigation bar with 'SciFINDER A CAS SOLUTION' logo, 'Saved', 'History', and 'Account' options. Below this is a search bar with the text 'Search by Keyword, Substance Name, CAS RN, Patent Number, etc.' and a search button. The search results are categorized into 'All', 'Substances', 'Reactions', 'References', and 'Suppliers', with 'References' selected. A search for 'treatment of cancer' is shown. Below the search bar, there is a section for 'Recent Searches' with a date filter for 'March 28, 2017'. The recent searches list includes: 'References: high temperature low density plasma (424K)' at 11:55 AM, 'References: Advanced Search (6) Organization: Memorial Sloan-Kettering Cancer Ctr.' at 10:14 AM, and 'Reactions: As Drawn (9), Substructure (39)' at 5:33 PM. A chemical structure drawing tool is visible on the right side of the interface, showing a complex organic molecule with 'Edit Drawing' and 'Remove' buttons.

More conveniently search structures and text

Information presented to facilitate rapid understanding

Powerful filtering capabilities allow rapid focus

The screenshot displays the SciFinder interface for a reaction search. On the left, a sidebar contains various filters: Structure Match (As Drawn (5), Substructure (18)), Filter by Substance Role (Product (13), Reactant (5)), Yield (90-100% (4), 80-89% (2), 70-79% (4), 50-69% (1), 30-49% (2)), Number of Steps (1 (13)), Experimental Protocols (MethodsNow Available (2), Procedure Available (6)), Reaction Type (Reagent, Catalyst, Solvent, Commercial Availability, Reaction Notes), and Source Reference (Publication Year, Document Type, Language). The main area shows 'Reactions (13)' with a 'Scheme 1 (2 Reactions) View' of a chemical reaction. The reaction involves a complex starting material and furfural, yielding a product. Below the reaction, there are two identical 'Reaction Summary' blocks. Each block lists Reagents: Sodium acetate, Acetic acid, manganese(3+) salt (3:1); Steps: 1; Yield: 92%; Catalysts: -; Solvents: Acetic acid; Conditions: -. To the right of each summary is a reference: 'Carbon-carbon bond-forming reactions promoted by trivalent manganese', 'View Reference Detail', 'By: Melikyan, Gagik G.', 'Organic Reactions (Hoboken, NJ, United States) (1997)', 'No pp. given', and a 'Full Text' button. The interface also includes 'Suppliers (3)' and 'Suppliers (6)' buttons, and a 'View 2 Reactions' link at the bottom.

Intuitive information layouts fosters quick comprehension

One idea can lead you to another - SciFinderⁿ has you covered!

The screenshot displays the SciFinder web application in a browser window. The browser's tab bar at the top shows five open tabs, all labeled 'SciFinder', which are circled in purple. An arrow points from this circle to the search bar on the right side of the page. The main content area shows search results for 'treatment of cancer'. On the left, there are filters for 'Structure Match' (As Drawn: 3,103; Substructure: 3,290) and 'Filter by' (Document Type, Language, Publication Year). The main results list includes two entries: 'Multikinase inhibitors: a new option for the treatment of thyroid cancer' and 'sorafenib for the treatment of renal cancer'. Each entry shows the author, journal, abstract, and options for 'Full Text', 'Substances', 'Reactions', 'Cited By', and 'Citation Map'.

Simultaneous searches can be performed in new browser/windows

Citation Mapping helps you understand where to go next in your literature review

The screenshot shows the SciFinder Citation Map interface. At the top, there is a search bar with the SciFinder logo and a search icon. Below the search bar, the title "Citation Map" is displayed. The main content area is divided into two columns: "References This Document Cites" and "References Citing This Document".

References This Document Cites:

- Basic local alignment search tool. 34K Citations.
- DNA sequencing with chain-terminating inhibitors. 16K Citations.
- A simple method for displaying the hydrophobic character of a protein. 16K Citations.

References Citing This Document:

- The commercial production of chemicals using pathway engineering. 155 Citations.
- The biochemistry, physiology and genetics of PQQ and PQQ-containing enzymes. 131 Citations.
- Glucanase oxidase: its biotechnological applications. 62 Citations.
- Immune evasion of the human pathogenic yeast *Candida albicans*: Pra1 is a Factor H, FHL-1 and plasminogen binding surface protein. 40 Citations.
- The periplasmic serine protease inhibitor ecotin protects bacteria against neutrophil elastase. 123 Citations.
- Multigene editing in the *Escherichia coli* genome via the CRISPR-Cas9 system. 39 Citations.
- Quinoprotein ethanol dehydrogenase of *Pseudomonas aeruginosa* is a homodimer. Sequence of the gene and deduced structural properties of the enzyme. 26 Citations.
- Genetic and biochemical characterization of the pathway in *Pantoea citrea* leading to pink disease of pineapple. 18 Citations.
- The epidemiology and management of seedborne bacterial disease... 18 Citations.
- Mathematical modeling of in vitro enzymatic...

Interactive map allows speedy identification of important research (maybe even that one paper you wouldn't otherwise find!)