



WHERE SCIENCE &
STRATEGY CONVERGE

SCIENTIFIC INFORMATION

THE KEY TO R&D EFFICIENCY
& PRODUCTIVITY



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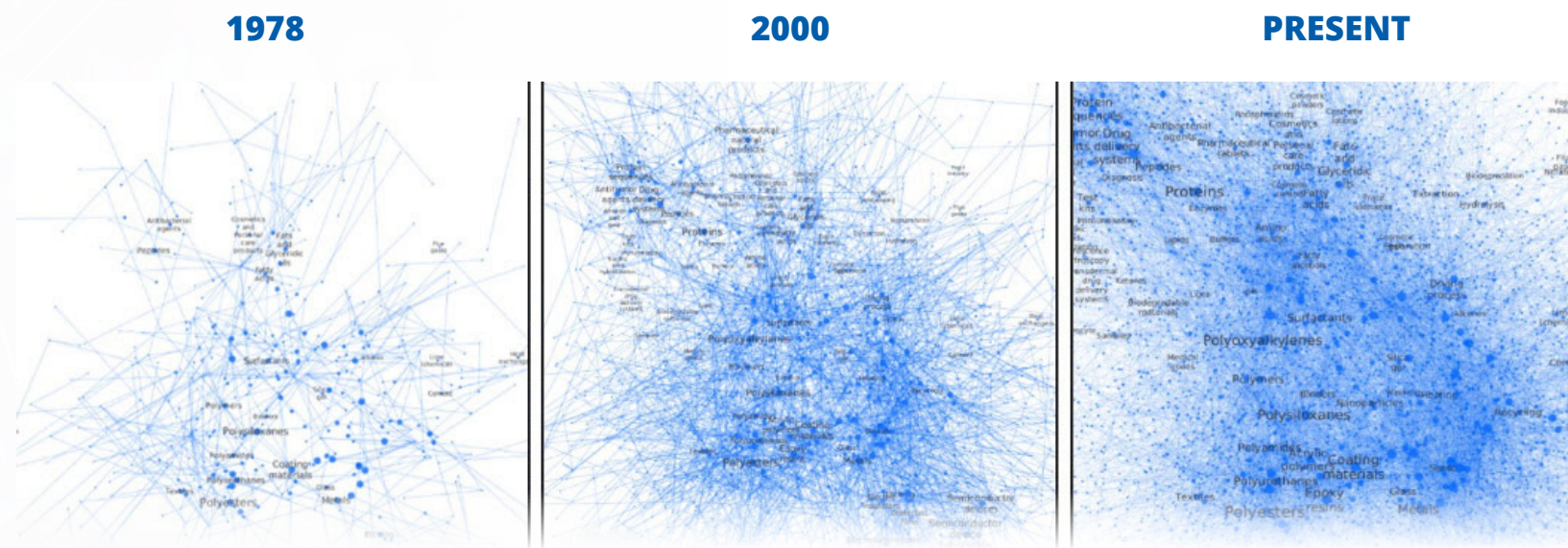


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COST OF MISSING SCIENTIFIC INFORMATION IS HIGH



COST TO MANAGE SCIENTIFIC INFORMATION CONTINUES TO ESCALATE



SCIENTIFIC INFORMATION TRENDS⁶ VOLUME COMPLEXITY INTERCONNECTEDNESS

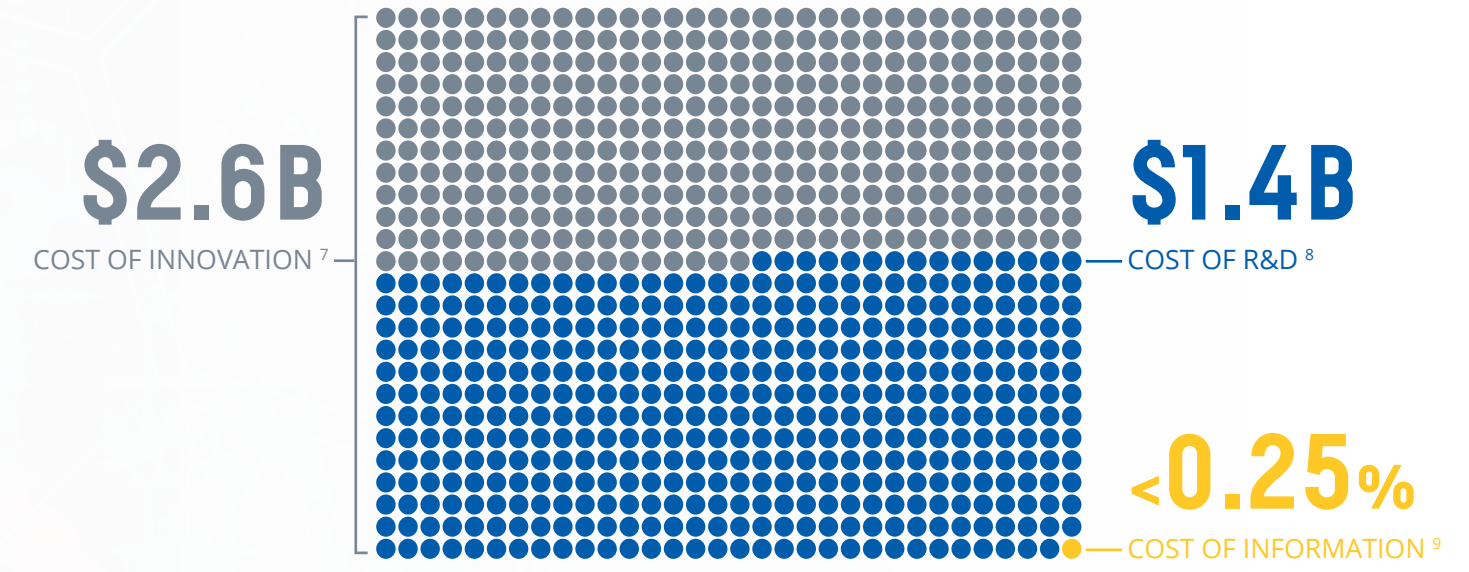
POORLY MANAGED SCIENTIFIC INFORMATION AFFECTS R&D EFFICIENCY

YET, INVESTMENT IN EXTERNAL SCIENTIFIC INFORMATION SOURCES REMAINS LOW



18% TIME LOST
 IN SEARCH VS. RESEARCH⁴

COST \$15K-\$20K
 PER YEAR, PER SCIENTIST⁵



CAS HAS INVESTED > \$1B IN SCIENTIFIC INFORMATION SOLUTIONS OVER THE LAST 5 YEARS. INTRODUCING A NEW CALIBER IN CHEMICAL INTELLIGENCE...



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DIRECT ACCESS to the unmatched CAS content collection, patent documents and step-by-step synthetic procedures and methods



The most advanced Chemical **RELEVANCE SEARCH ENGINE** shows you where to start and what to focus on



Platform for machine learning & **AI, COMPUTER-AIDED SYNTHETIC DESIGN**, patent search and workflow enhancement

INSIGHTS

In today's competitive landscape, your research team needs to quickly gain knowledge and insights from relevant discoveries. You can't afford to spend hours sifting through extraneous content in patents and journals. That's why we designed SciFinderⁿ with the most chemistry-aware relevance engine in the industry. It doesn't just search faster—it helps you search smarter, anticipating your information needs and accelerating your work.

The screenshot displays the SciFinder interface for a search on "Sirtuin 2 inhibitors and cancer".

- References (37):** Shows a list of search results. The top result is "Chroman-4-one- and Chromone-Based Sirtuin 2 Inhibitors with Antiproliferative Properties in Cancer Cells". The abstract mentions that Sirtuins (SIRT2) catalyze the NAD⁺-dependent deacetylation of N^ε-acetyl lysines and that the authors report novel chroman-4-one and chromone-based SIRT2 inhibitors.
- Substances (222):** Displays a grid of chemical structures with their corresponding IDs (e.g., 1190882-42-8, 1057649-28-1, 1089662-03-2) and buttons for "View Detail", "Reference", "Reactions", and "Suppliers".
- Reactions (14):** Shows reaction schemes. "Scheme 1" and "Scheme 2" are visible, each showing a chemical transformation with a yield of 94% and a single step.

SYNTHETIC PLANNING

Being efficient in the lab requires a great synthetic plan. Your chemists are juggling many variables in their synthetic planning, from the cost of materials, to the complexity of the procedure and the final yield. SciFinder[®] helps your team locate the right reactions quickly and maximizes productivity with direct access to chemical sourcing information as well as step-by-step synthetic procedures curated by experts.

The screenshot displays the SciFinder interface for a synthetic planning task. At the top, there's a search bar and navigation options. Below, a table lists suppliers for various substances, including Succinic anhydride and Terfenadine. The main section is titled 'Experimental Protocols' and includes a detailed procedure for the synthesis of Butanedioic acid, 1-[1-[4-(1,1-dimethylethyl)phenyl]-4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]butyl] ester. The procedure involves adding terfenadine to a solution of succinic anhydride and 4-dimethylaminopyridine in dimethylformamide, followed by pyridine addition, evaporation, and purification.

Supplier	Substance	Purity	Purchasing Details	Availability
Alfa Aesar United States	108-30-5 Succinic anhydride	≥99%	Order From Supplier ☑ 250g, USD 16.40 500g, USD 27.60 1000g, USD 43.90 5000g, USD 166.00	Typically in stock Ships within 1 week
	Bulk Screening		Order From Supplier ☑ 0.1 G, USD 452	Maintained in stock Ships within 1 week
	Bulk		Order From Supplier ☑ 0.25 G, USD 705	Maintained in stock Ships within 1 week
	Bulk		Order From Supplier ☑ 5 G, USD 300	Maintained in stock Ships within 1 week

Experimental Protocols

MethodsNow™ Experimental Procedure

Products Butanedioic acid, 1-[1-[4-(1,1-dimethylethyl)phenyl]-4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]butyl] ester, Yield: 91%

Reactants Succinic anhydride
Terfenadine

Reagents Pyridine

Catalysts 4-(Dimethylamino)pyridine

Solvents Dimethylformamide

Procedure

1. Add terfenadine (471.7 mg) to a solution of succinic anhydride (200 mg) and 4-dimethylaminopyridine (12.2 mg, 0.1 mmol) (previously dried under vacuum for 2 hours) in dimethylformamide (4 mL).
2. Add dry pyridine (0.8 mL) to the solution.
3. Stir the solution overnight at room temperature.
4. Evaporate dimethylformamide under vacuum.
5. Wash the residue with petroleum ether.
6. Purify the product by silica gel column chromatography, eluting with chloroform:methanol (90:10).

Transformation Alcoholysis of Anhydrides

Scale milligram

Characterization Data

Butanedioic acid, 1-[1-[4-(1,1-dimethylethyl)phenyl]-4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]butyl] ester

IP STRATEGY

In order to successfully manage your research portfolio and bring your innovation to market, it's essential to first understand the technology landscape. SciFinder[®] can help answer a host of IP-related questions such as: Where are the opportunities for innovation? Are there infringement risks? Who else is working in this space? SciFinder[®] gives you access to industry leading capabilities like patent Markush searching and content such as chemically annotated patents, so you can stay on top of the technological landscape.

The screenshot shows the Patent Markush search interface. It displays a list of patent entries with their respective CAS RN numbers and analyst markup locations. The main view shows a detailed patent entry for KR2010125109, including a chemical structure and the full text of the patent claim. The claim describes a compound with an alkyl group containing 1-10 carbon atoms, substituted by a G2 group.

Patent Markush Match As Drawn (6)

Substructure (151)

Filter by

Patent Office

World Intellectual Property Organization (5)

Korea, Republic of (1)

Patent Markush (6)

References

KR2010125109
View Reference Detail

Patent claim 1

PATENTPAK Full Text

54: alkyl <containing 1-10 C> (opt. subst. by G2)

119: alkyl <containing 1-10 C> (opt. subst. by G2)

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Key Substances in Patent

CAS RN 67828-57-3
Analyst Markup Locations (1)
Page 21

CAS RN 501007-24-5
Analyst Markup Locations (1)
Page 21

CAS RN 501007-25-6
Analyst Markup Locations (1)

Step-2:

5 [0078] Dry K₂CO₃ (10 g, 0.072 mol) in NMP (60 mL, 0.626 mol) was heated to 165°C for 1 hr under nitrogen. N-(2-Methoxy-4-nitrophenyl)pyrrolidine (20 g, 0.090 mol) and thiophenol (28 mL, 0.272 mol) were added with stirring at 165°C. Stirring was continued for 2 hr at 150°C. The mixture was cooled to room temperature, neutralized with 1.5 N HCl and extracted with ether. The ether layer was washed with water, brine, dried over Na₂SO₄ and concentrated. The dark red product obtained was purified by column chromatography using petroleum ether-ethylacetate (9:1) as eluent. Yield: 11.5 g, 61 %.

Step-3:

15 [0079] N-(2-Hydroxy-4-nitrophenyl)pyrrolidine (5 g, 0.024 mol), racemic-epichlorohydrin (40 mL) and catalytic amount of tetrabutylammonium bromide (60 mg) in 100 mL 3N flask was heated at 50 °C with stirring for 30 min. NaOH (2.3 g, 0.058 mol) in water (5 mL) was added slowly over 15 min. Stirring was continued at 50°C for 15 hr. Water (100 mL) was added, extracted with chloroform, washed with water, dried over Na₂SO₄ and concentrated. The crude epoxide was purified by column chromatography using 9.5:0.5 petroleum ether:ethylacetate as eluent. Yield: 2.7 g, 43 %.

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Sources

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2. Drug Discovery World Fall 2004, Failure rates in drug discovery and development: will we ever get any better?
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13. Shanghai Ranking's Global Ranking of Academic Subjects 2017 — Chemistry
14. WIPO IP Facts and Figures 2018

INDUSTRY LEADERS ACROSS R&D ORGANIZATIONS RELY ON CAS SOLUTIONS

PHARMA

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Business Card