



# UNLOCK R&D PRODUCTIVITY

# COST OF MISSING SCIENTIFIC INFORMATION IS HIGH



**>\$1B** Lost Market Leadership  
MARKET SHARE LAG: >6% <sup>1</sup>

**>\$31M** R&D Spend Inefficiency  
TIME LOSS: >3 MOS <sup>2</sup>

**>\$4B** Reputational Risk  
LOSS OF EXCLUSIVITY: >6 YRS <sup>3</sup>

# POORLY MANAGED SCIENTIFIC INFORMATION AFFECTS R&D EFFICIENCY



**18% Time Spent**  
IN SEARCH VS. RESEARCH <sup>4</sup>

**\$15K-\$20K**  
COST PER YEAR, PER SCIENTIST <sup>5</sup>

**R&D cycles are too long and costly**



# COST TO MANAGE SCIENTIFIC INFORMATION CONTINUES TO ESCALATE

## Scientific Information Trends <sup>6</sup>

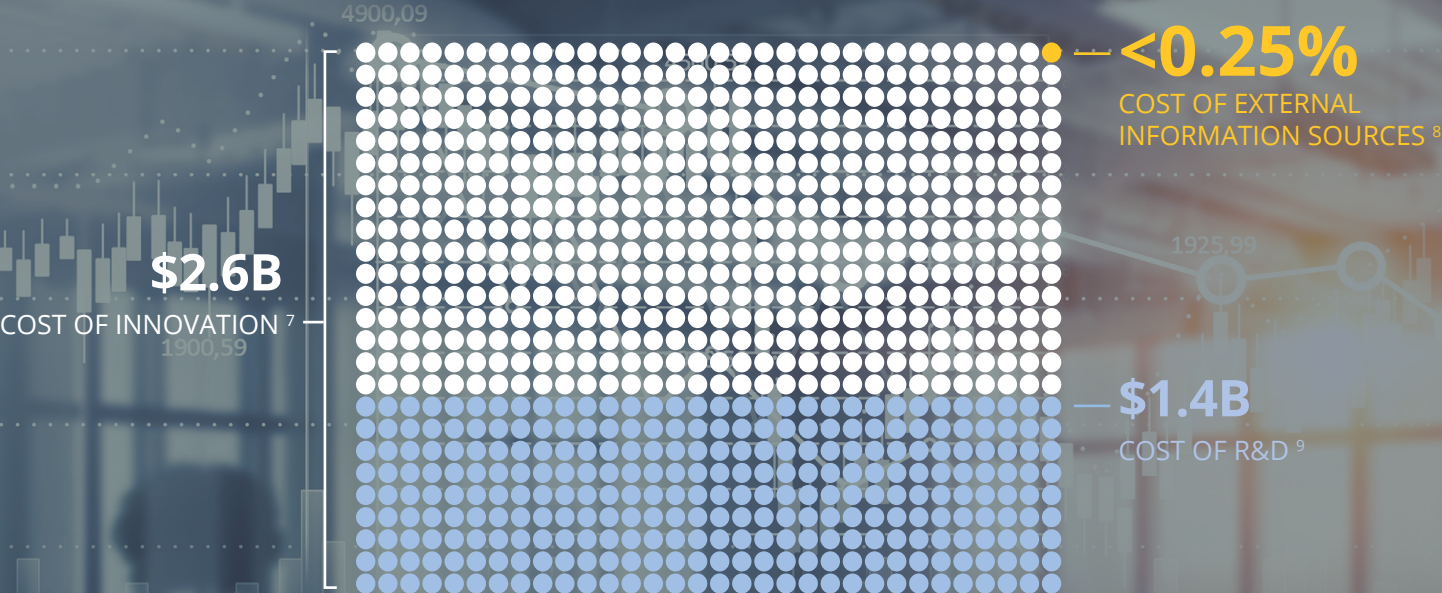


Volume

Complexity

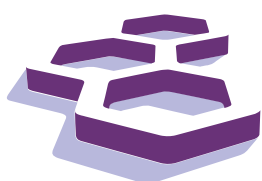
Interconnectedness

# YET, INVESTMENT IN EXTERNAL SCIENTIFIC INFORMATION SOURCES REMAINS LOW



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

INTRODUCING A NEW CALIBER  
OF CHEMICAL INTELLIGENCE



**SCIFINDER<sup>n</sup>**  
A CAS SOLUTION

NOW WITH A NEW  
**SYNTHESIS PLANNER**

**63%**

of researchers say SciFinder<sup>n</sup> allows them to **work more quickly**<sup>10</sup>

**63%**

of researchers say SciFinder<sup>n</sup> allows them to **be more innovative**<sup>10</sup>

**62%**

of researchers say SciFinder<sup>n</sup> allows them to **be more confident**<sup>10</sup>

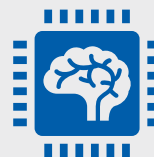
## The blueprint of chemical intelligence



**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

## SciFinder<sup>n</sup> halves the time taken to perform literature reviews<sup>10</sup>

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 SciFinder<sup>n</sup> with the most chemistry-aware relevance engine in the industry. It doesn't just search faster, it helps you search smarter, anticipates your information needs and accelerates your work.

The screenshot displays the SciFinder interface for a search query: "Novel Nonpeptide Inhibitors of coronavirus". The interface is divided into several sections:

- References (2,031):** The top section shows search results. The first result is titled "Structure-Based Drug Design and Structural Biology Study of Novel Nonpeptide Inhibitors of Severe Acute Respiratory Syndrome Coronavirus Main Protease". It includes a chemical structure diagram and a brief abstract. Below the abstract, there are buttons for "Full Text", "Substances (25)", "Reactions (0)", "Cited By (55)", and "Citation Map".
- Substances (222):** The middle section displays a grid of chemical structures. Each structure is accompanied by a "View Detail" link and a set of buttons for "Reference", "Reactions", and "Suppliers". For example, the first structure (1190882-42-8) has 1 reference, 2 reactions, and 0 suppliers.
- Reactions (14):** The bottom section shows chemical reaction schemes. "Scheme 1" and "Scheme 2" are visible, each showing a single reaction step with a 94% yield. Below each scheme, there are "Suppliers" buttons with counts (e.g., 2 suppliers for Scheme 1, 15 for Scheme 2).



# Synthetic Planning

## SciFinder<sup>n</sup> halves the time required for synthetic planning<sup>10</sup>

Being successful in the lab requires a great synthetic plan. Your chemists are juggling many variables especially when devising routes to novel compounds with no literature based precedent. For both known and unknown molecules, SciFinder<sup>n</sup> will perform a full retrosynthetic analysis fueled by the renowned CAS collection of reactions. The best potential synthetic routes are determined based on steps from both the literature and predicted steps generated by our synthetic chemistry engine. The algorithm can be customized to fit the specific requirements of the synthesis and the plan is easily navigated to evaluate alternative routes and also offers quick access to information on material suppliers, step-by-step methods curated by experts, product yields, and more.

The image shows two screenshots from the SciFinder interface. The top screenshot displays 'Experimental Protocols' for a synthesis. It lists the following details:

- Products:** p-Terphenyl, Yield: 100%
- Reactants:** Iodobenzene, 4-Biphenylboronic acid
- Reagents:** Potassium carbonate
- Catalysts:** Palladium, Graphene
- Solvents:** Dimethylformamide, Water
- Procedure:**
  - Mix a DMF solution of iodobenzene (0.25 M) and arylboronic acid (0.30 M) with isopycnic aqueous solution of K<sub>2</sub>CO<sub>3</sub> (0.75 M).
  - Pump the mixture into the reactor with a controllable flow velocity.
  - Integrate the reactor with Pd/GN catalysts pre-heated to 90 °C for 6 min in an oil bath.
  - Extract the products of the reaction with ethyl acetate.
  - Purify the product by a microcolumn filled with silica gel to obtain the product.

The bottom screenshot shows the 'Retrosynthesis' interface. It features a central reaction network with nodes A through G. Node A is the target molecule. Node B is a precursor with a 'Max. Yield: 76%' and 'Suppliers (14)'. Node C is another precursor with a 'Max. Yield: 92%' and 'Suppliers (74)'. Nodes E, F, and G are further precursors with their respective yields and supplier counts. The interface includes a 'Scoring Profiles' sidebar with sliders for 'Complexity Reduction', 'Convergence', 'Evidence', 'Yield', and 'Atom Efficiency'. A 'Create Retrosynthesis Plan' button is visible at the bottom left of the sidebar.

# IP Strategy

## SciFinder<sup>n</sup> reduces the time taken to analyze the IP landscape by nearly 10%<sup>10</sup>

In order to successfully manage your research portfolio and bring your innovation to market, it's essential to first understand the technology landscape. SciFinder<sup>n</sup> 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<sup>n</sup> 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 image shows a screenshot of the 'Patent Markush' search results in SciFinder. The interface includes a 'Patent Markush Match' sidebar with filters for 'As Drawn (6)', 'Substructure (151)', and 'Patent Office' (World Intellectual Property Organization (5), Korea, Republic of (1)). The main area displays search results for 'KR2010125109'. It shows a chemical structure with Markush groups (G1, G2, G3) and a 'Patent claim 1' section with a dropdown menu set to 'PATENTPAK' and 'Full Text'. The text of the patent claim is visible, including '54: alkyl <containing 1-10 C> (opt. subst. by G2)' and '119: alkyl <containing 1-10 C> (opt. subst. by G2)'. Below the search results, there is a 'Key Substances in Patent' section listing three CAS RNs: 67928-57-3, 501007-24-5, and 501007-25-6, each with a chemical structure and 'Analyst Markup Locations (1)'. The bottom right of the screenshot shows a snippet of the patent text with 'Step-2:' and 'Step-3:' sections, detailing synthesis procedures for various compounds.

## Sources

1. <https://www.mckinsey.com/industries/pharmaceuticals-and-medical-products/our-insights/pharmas-first-to-market-advantage>
2. Drug Discovery World Fall 2004, Failure rates in drug discovery and development: will we ever get any better?
3. <https://www.hhrjournal.org/2017/11/patent-fighters-taking-on-big-pharma>
4. SciFinder user survey of top discovery research organizations
5. Average hourly cost for fully-loaded, full-time researcher
6. CAS Proprietary data, CAS Analytics & Insights
7. Tufts Center for the Study of Drug Development
8. CAS Market Analysis
9. Tufts Center for the Study of Drug Development
10. Research Report, "SciFinder<sup>®</sup> Improves Productivity"
11. Pharm Exec's Top 50 Companies 2020
12. Genetic Engineering & Biotechnology News Top 25 Biotech Companies of 2019
13. C&EN's Global Top 50 for 2020
14. WIPO IP Facts and Figures 2019
15. ShanghaiRanking's Global Ranking of Academic Subjects 2020 – Chemistry

# INDUSTRY LEADERS ACROSS ORGANIZATIONS RELY ON CAS SOLUTIONS

## Pharma

49 of the top 50 <sup>11</sup>

## Biotech

24 of the top 25 <sup>12</sup>

## Chemical

46 of the top 50 <sup>13</sup>

## Government

10 of the top 10  
global patent offices <sup>14</sup>

## Academic

100 of the top 100 <sup>15</sup>



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