



SciFinder[®]

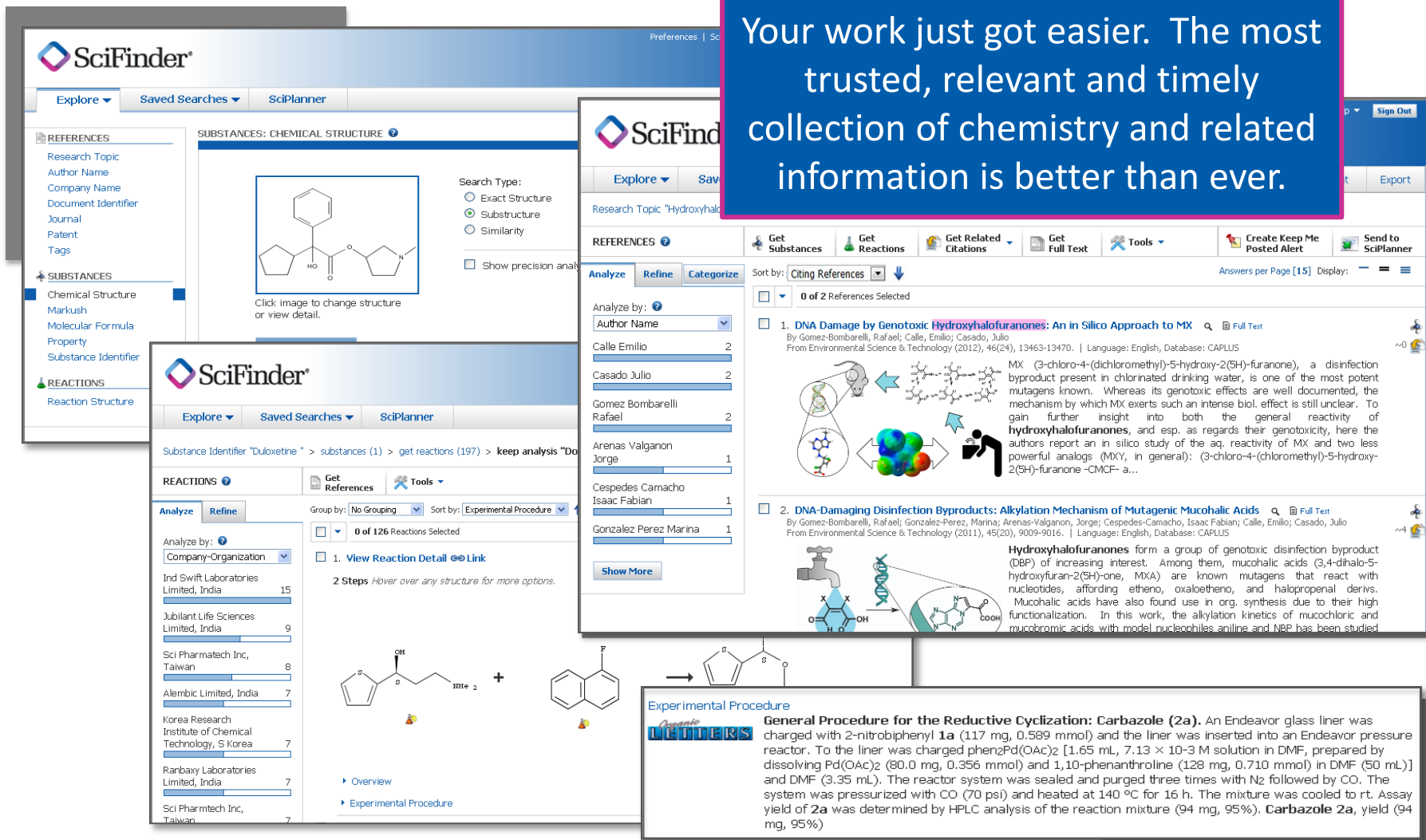
The choice for chemistry research.[™]

Introducing the New SciFinder

*Overview of the latest release and examples of how
SciFinder can help you with your research*

Welcome to SciFinder

Your work just got easier. The most trusted, relevant and timely collection of chemistry and related information is better than ever.



The image displays several overlapping screenshots of the SciFinder web interface. The top-left screenshot shows the 'REFERENCES' section with a search for 'SUBSTANCES: CHEMICAL STRUCTURE' and a chemical structure of Duloxetine. The top-right screenshot shows a search for 'Research Topic Hydroxyhalo' with a list of authors and their counts. The middle-left screenshot shows the 'REACTIONS' section for 'Duloxetine' with a list of companies and their counts. The middle-right screenshot shows a list of references, including 'DNA Damage by Genotoxic Hydroxyhalofuranones: An In Silico Approach to MX' and 'DNA-Damaging Disinfection Byproducts: Alkylation Mechanism of Mutagenic Mucohalic Acids'. The bottom-left screenshot shows a chemical reaction scheme for the synthesis of Carbazole (2a). The bottom-right screenshot shows the 'Experimental Procedure' for the reductive cyclization of Carbazole (2a).

Company-Organization

Ind Swift Laboratories Limited, India	15
Jubilant Life Sciences Limited, India	9
Sci Pharmatech Inc, Taiwan	8
Alembic Limited, India	7
Korea Research Institute of Chemical Technology, S Korea	7
Ranbaxy Laboratories Limited, India	7
Sci Pharmtech Inc, Taiwan	7

Author Name

Calle Emilio	2
Casado Julio	2
Gomez Bombarelli Rafael	2
Arenas Valganon Jorge	1
Céspedes Camacho Isaac Fabian	1
Gonzalez Perez Marina	1

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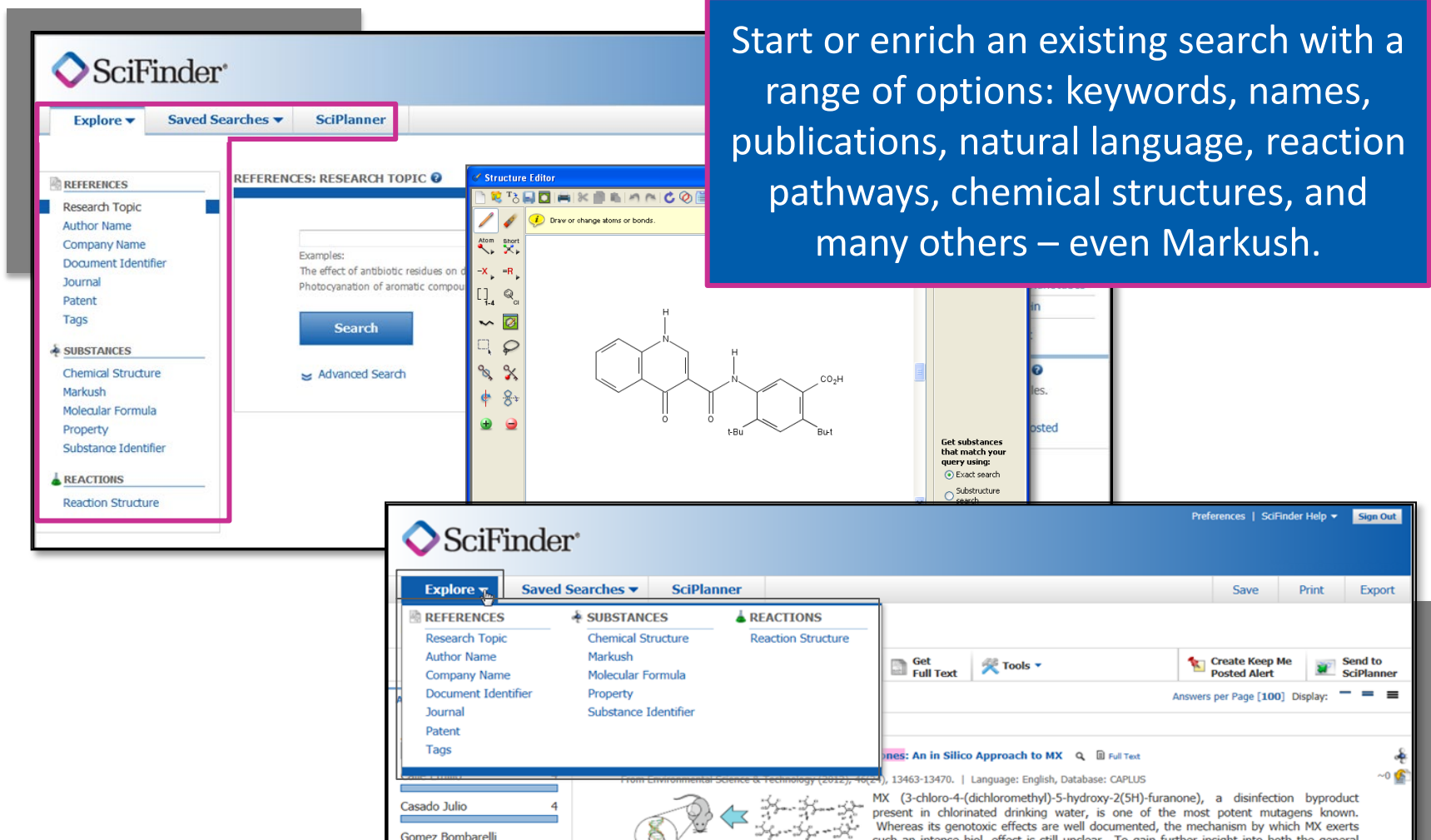
Calle Emilio	2
Casado Julio	2
Gomez Bombarelli Rafael	2
Arenas Valganon Jorge	1
Céspedes Camacho Isaac Fabian	1
Gonzalez Perez Marina	1

Experimental Procedure

General Procedure for the Reductive Cyclization: Carbazole (2a). An Endeavor glass liner was charged with 2-nitrophenyl **1a** (117 mg, 0.589 mmol) and the liner was inserted into an Endeavor pressure reactor. To the liner was charged phen₂Pd(OAc)₂ [1.65 mL, 7.13 × 10⁻³ M solution in DMF, prepared by dissolving Pd(OAc)₂ (80.0 mg, 0.356 mmol) and 1,10-phenanthroline (128 mg, 0.710 mmol) in DMF (50 mL)] and DMF (3.35 mL). The reactor system was sealed and purged three times with N₂ followed by CO. The system was pressurized with CO (70 psi) and heated at 140 °C for 16 h. The mixture was cooled to rt. Assay yield of **2a** was determined by HPLC analysis of the reaction mixture (94 mg, 95%). **Carbazole 2a**, yield (94 mg, 95%)

Search options match your research needs

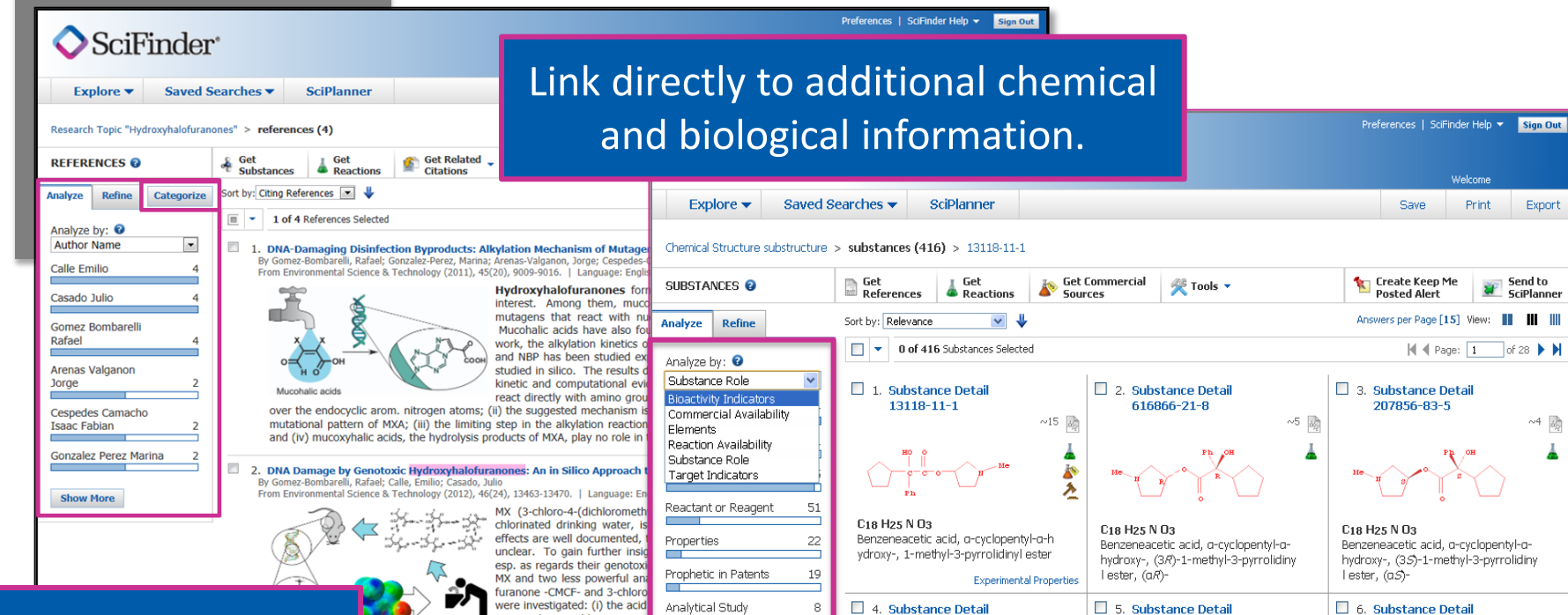
Start or enrich an existing search with a range of options: keywords, names, publications, natural language, reaction pathways, chemical structures, and many others – even Markush.



The image displays two screenshots of the SciFinder web interface. The top screenshot shows the 'SciFinder' search page with a sidebar menu on the left. The menu is divided into three main sections: REFERENCES, SUBSTANCES, and REACTIONS. The REFERENCES section includes options like Research Topic, Author Name, and Company Name. The SUBSTANCES section includes Chemical Structure, Markush, and Molecular Formula. The REACTIONS section includes Reaction Structure. A 'Structure Editor' window is open in the center, showing a chemical structure of a complex organic molecule with a benzene ring fused to a pyridine-like ring, and a side chain with a carboxylic acid group and two tert-butyl groups. The bottom screenshot shows a search results page with a similar sidebar menu. The SUBSTANCES section is expanded, showing options like Chemical Structure, Markush, Molecular Formula, Property, and Substance Identifier. The main content area shows search results for a query, including a snippet of text and a chemical structure diagram.

Results are accurate, relevant and actionable

Link directly to additional chemical and biological information.



The screenshot displays the SciFinder interface with search results for 'Hydroxyhalofuranones'. The interface includes a navigation bar with 'Explore', 'Saved Searches', and 'SciPlanner'. The main content area shows a list of references, with the first one highlighted: 'DNA-Damaging Disinfection Byproducts: Alkylation Mechanism of Mutagenesis'. The interface also features a 'REFERENCES' sidebar with an 'Analyze' section containing a list of authors and their counts. A central 'SUBSTANCES' sidebar provides a detailed analysis of the selected substance, including 'Substance Role', 'Bioactivity Indicators', 'Commercial Availability', 'Elements', 'Reaction Availability', 'Substance Role', and 'Target Indicators'. The main results area shows a grid of substance details, each with a chemical structure and a brief description.

Graphical content and interface make review easy.

Experimental procedures and properties streamline your work.

Experimental Procedure



General Procedure for the Reductive Cyclization: Carbazole (2a). An Endeavor glass liner was charged with 2-nitrophenyl **1a** (117 mg, 0.589 mmol) and the liner was inserted into an Endeavor pressure reactor. To the liner was charged phenylPd(OAc)₂ [1.65 mL, 7.13 × 10⁻³ M solution in DMF, prepared by dissolving Pd(OAc)₂ (80.0 mg, 0.356 mmol) and 1,10-phenanthroline (128 mg, 0.710 mmol) in DMF (50 mL)] and DMF (3.35 mL). The reactor system was sealed and purged three times with N₂ followed by CO. The system was pressurized with CO (70 psi) and heated at 140 °C for 16 h. The mixture was cooled to rt. Assay yield of **2a** was determined by HPLC analysis of the reaction mixture (94 mg, 95%). **Carbazole 2a**, yield (94 mg, 95%)

hydroxy-, (3*R*)-1-methyl-3-pyrrolidiny l ester, (a*S*)-

Example 1:

SciFinder answers critical research questions

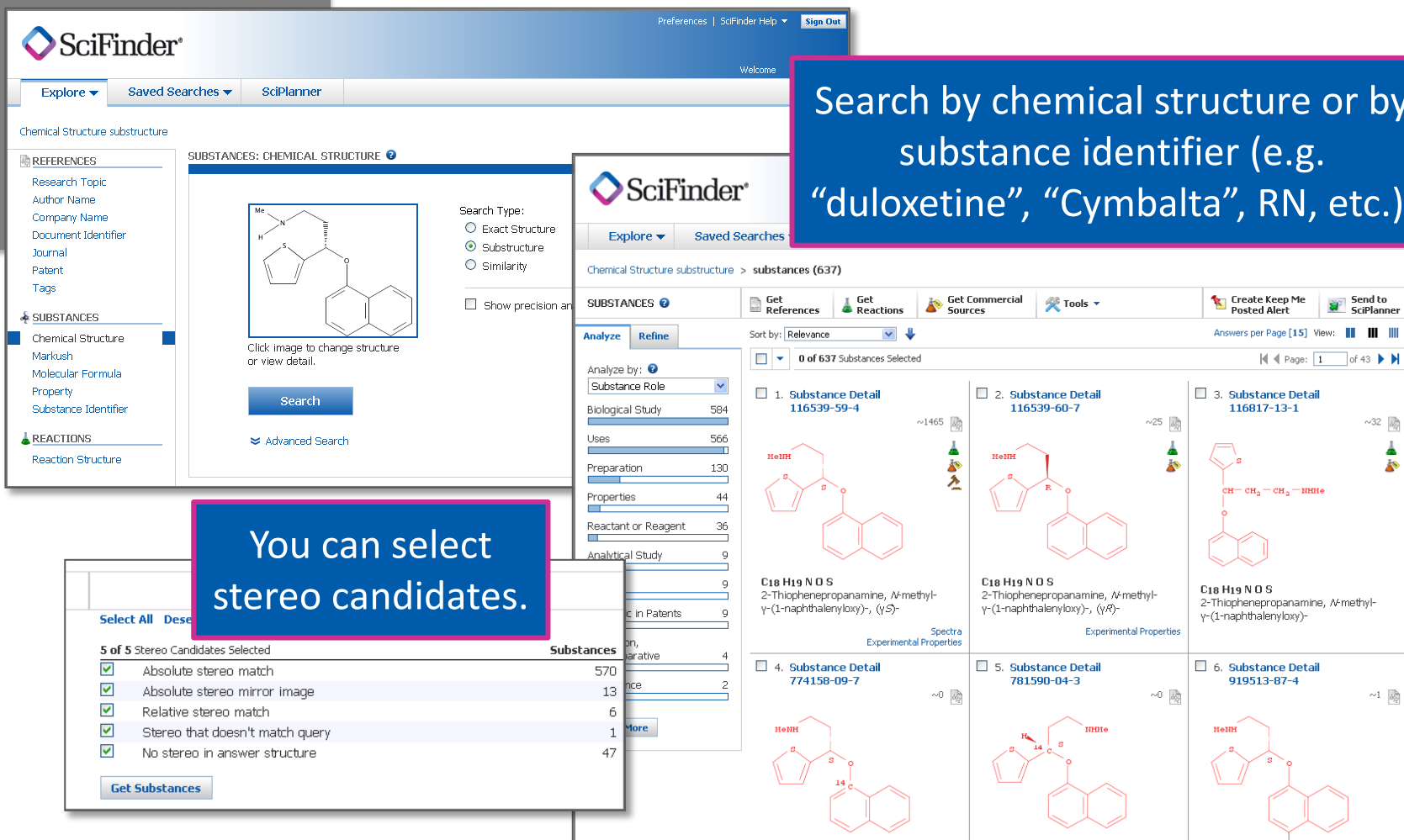
The patent for Cymbalta® is scheduled to expire and you want to learn more about the parent compound, duloxetine

- Where can I find important property information?
- How can it be made efficiently?
- What patent protection exists?
- Are there related regulatory restrictions?
- Where can you buy commercially available starting materials?
- Are there potential collaborators or competitors?
- How do you keep aware of developments and share information?

Search for duloxetine

Search by chemical structure or by substance identifier (e.g. "duloxetine", "Cymbalta", RN, etc.).

You can select stereo candidates.



REFERENCES

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

SUBSTANCES

- Chemical Structure
- Markush
- Molecular Formula
- Property
- Substance Identifier

REACTIONS

- Reaction Structure

SUBSTANCES: CHEMICAL STRUCTURE

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis

Click image to change structure or view detail.

Search

[Advanced Search](#)

Chemical Structure substructure > substances (637)

Get References | Get Reactions | Get Commercial Sources | Tools

Create Keep Me Posted Alert | Send to SciPlanner

Analyze | Refine

Sort by: Relevance

0 of 637 Substances Selected

Answers per Page [15] View: [List Icon]

Page: 1 of 43

1. Substance Detail 116539-59-4 ~1465

2. Substance Detail 116539-60-7 ~25

3. Substance Detail 116817-13-1 ~32

4. Substance Detail 774158-09-7 ~0

5. Substance Detail 781590-04-3 ~0

6. Substance Detail 919513-87-4 ~1

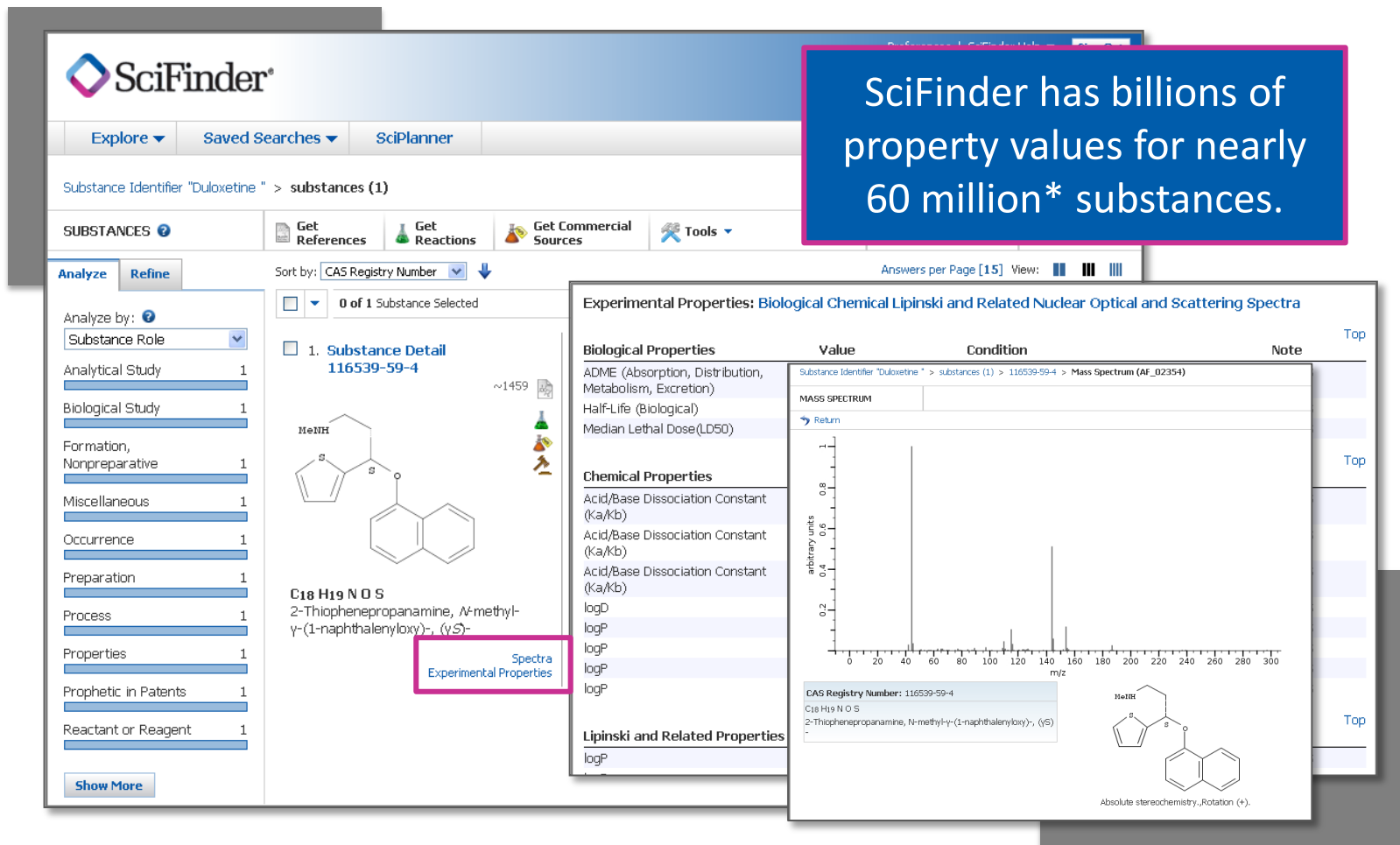
5 of 5 Stereo Candidates Selected

Option	Count
<input checked="" type="checkbox"/> Absolute stereo match	570
<input checked="" type="checkbox"/> Absolute stereo mirror image	13
<input checked="" type="checkbox"/> Relative stereo match	6
<input checked="" type="checkbox"/> Stereo that doesn't match query	1
<input checked="" type="checkbox"/> No stereo in answer structure	47

Get Substances

Experimental and predicted properties highlight substance characteristics

SciFinder has billions of property values for nearly 60 million* substances.



Substance Identifier "Duloxetine" > substances (1)

Get References | Get Reactions | Get Commercial Sources | Tools

Sort by: CAS Registry Number

0 of 1 Substance Selected

1. Substance Detail
 116539-59-4

Chemical Structure: CN(C)CCc1ccoc1Oc2ccc3ccccc32

C₁₈ H₁₉ N O S
 2-Thiophenepropanamine, N-methyl-γ-(1-naphthalenyloxy)-, (γS)-

Experimental Properties: Biological Chemical Lipinski and Related Nuclear Optical and Scattering Spectra

Biological Properties	Value	Condition	Note
ADME (Absorption, Distribution, Metabolism, Excretion)			
Half-Life (Biological)			
Median Lethal Dose(LD50)			

Chemical Properties

Acid/Base Dissociation Constant (Ka/Kb)			
Acid/Base Dissociation Constant (Ka/Kb)			
Acid/Base Dissociation Constant (Ka/Kb)			
logD			
logP			
logP			
logP			
logP			

Lipinski and Related Properties

logP			
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Mass Spectrum: Substances (1) > 116539-59-4 > Mass Spectrum (AF_02354)

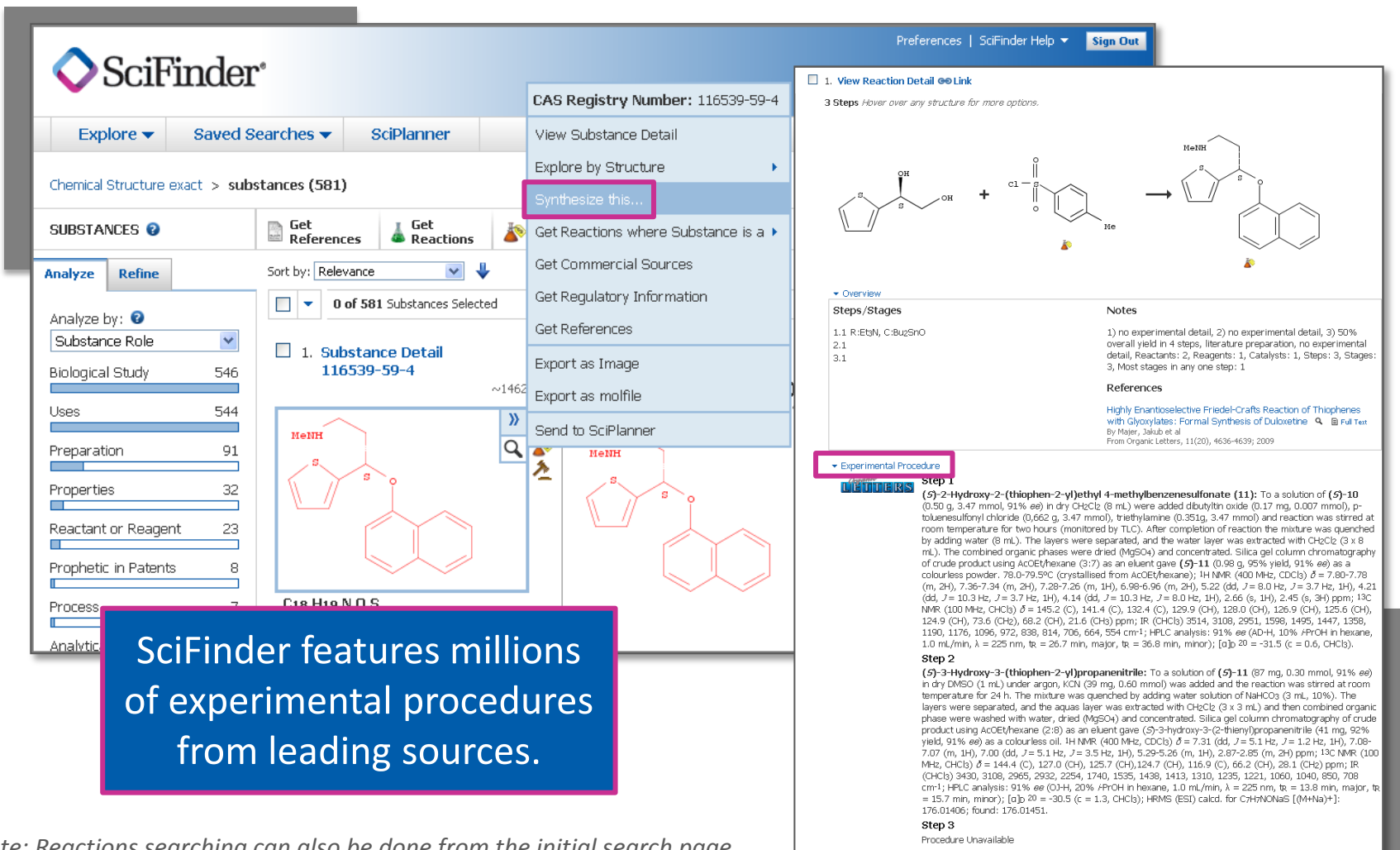
Arbitrary units vs m/z

CAS Registry Number: 116539-59-4
C₁₈ H₁₉ N O S
 2-Thiophenepropanamine, N-methyl-γ-(1-naphthalenyloxy)-, (γS)-

Absolute stereochemistry, Rotation (+).

* SciFinder gives you access to over 71 million unique substance records.

Experimental procedures allow you to start planning your synthesis work immediately



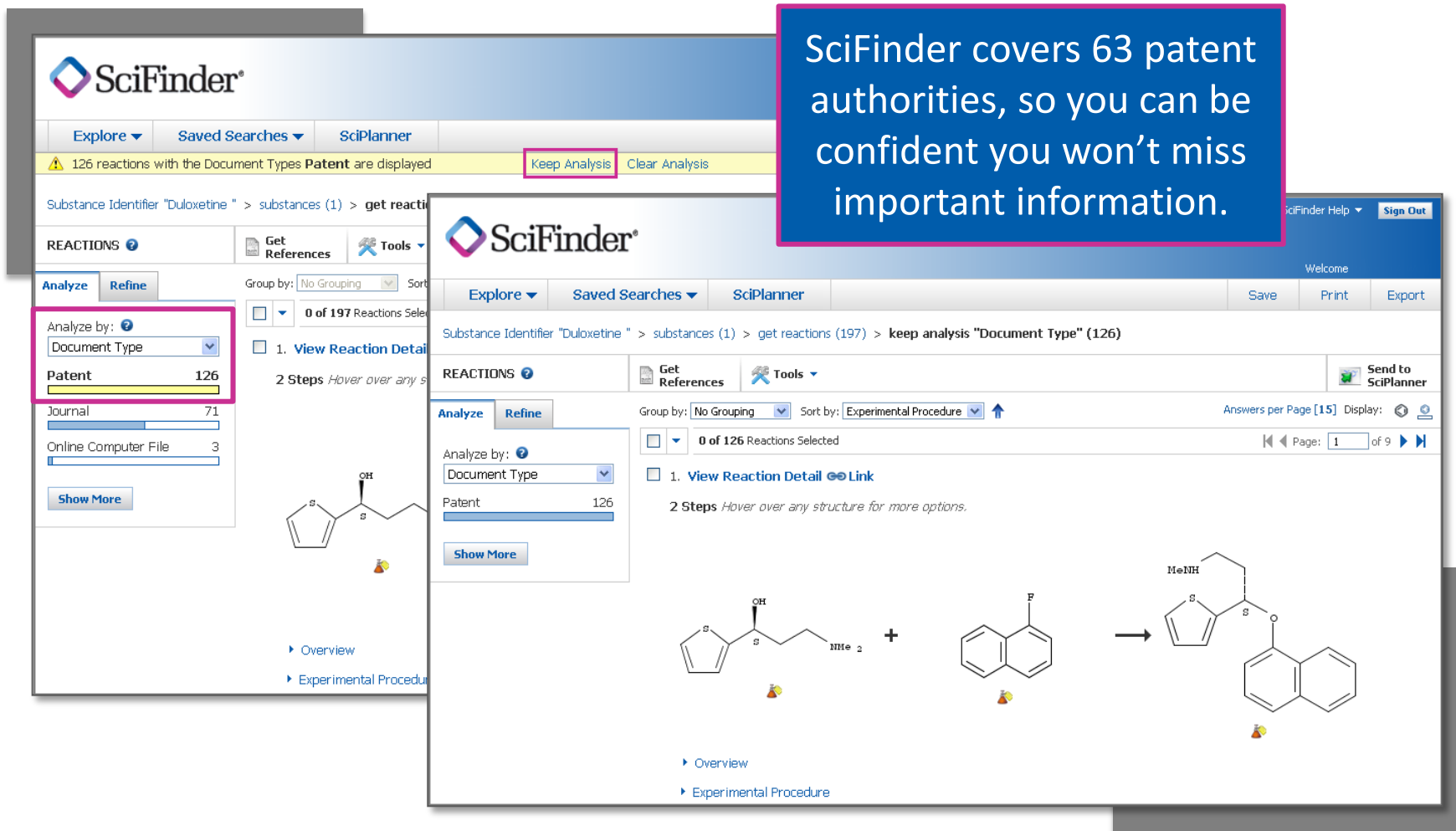
The screenshot displays the SciFinder interface. On the left, the 'Substances' search results are shown, with a list of categories and counts. The main area shows a search for '1. Substance Detail 116539-59-4'. A dropdown menu is open over the search results, with 'Synthesize this...' highlighted. The right panel shows the 'View Reaction Detail' for the selected substance, including a chemical reaction scheme and a detailed experimental procedure.

SciFinder features millions of experimental procedures from leading sources.

Note: Reactions searching can also be done from the initial search page.

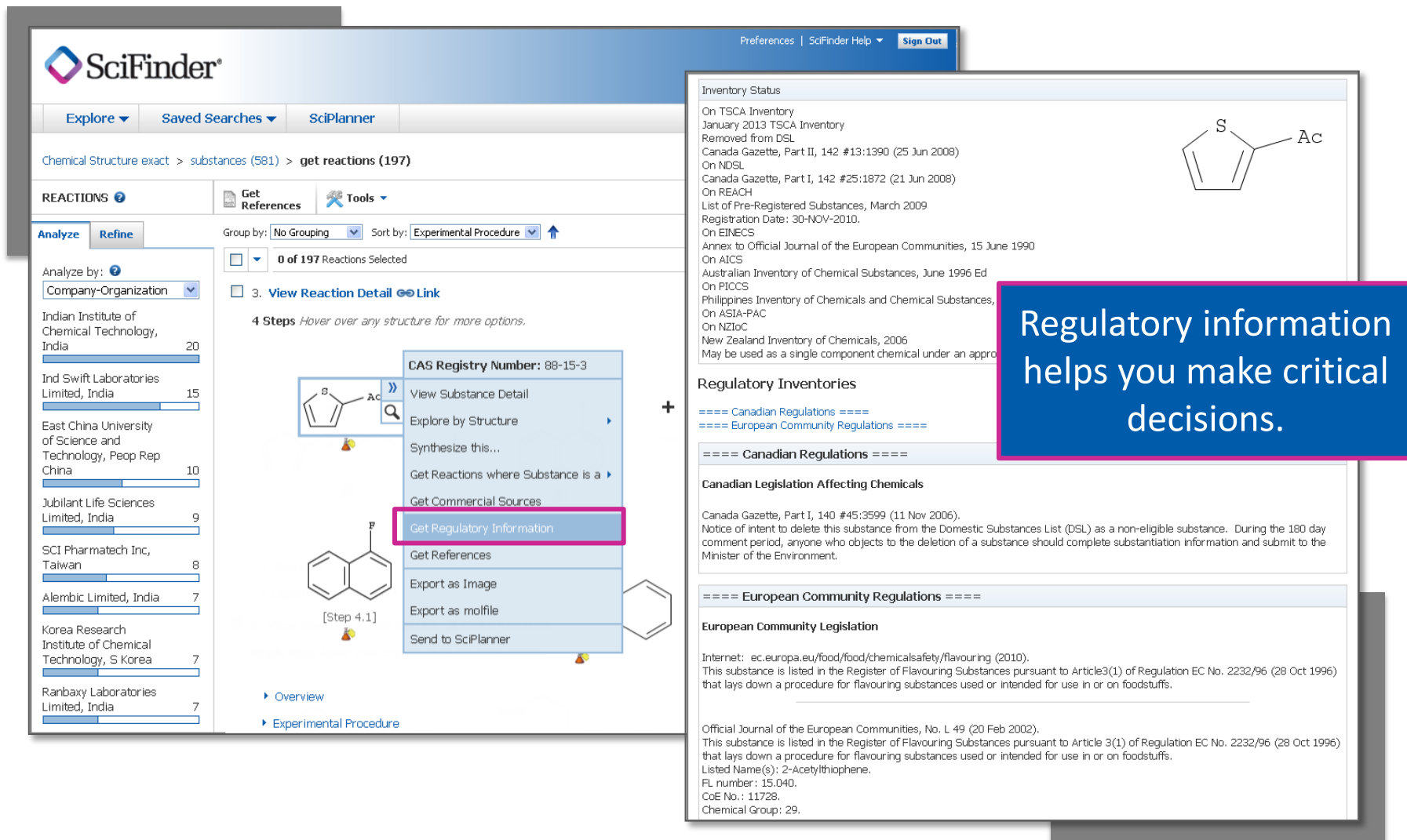
Patents are important to research

SciFinder covers 63 patent authorities, so you can be confident you won't miss important information.



The screenshot displays the SciFinder interface for a search on 'Duloxetine'. The top navigation bar includes 'Explore', 'Saved Searches', and 'SciPlanner'. A yellow banner indicates '126 reactions with the Document Types Patent are displayed', with 'Keep Analysis' and 'Clear Analysis' buttons. The breadcrumb trail shows 'Substance Identifier "Duloxetine" > substances (1) > get reactions (197) > keep analysis "Document Type" (126)'. The 'Analyze' panel on the left shows a bar chart for 'Document Type' with 'Patent' at 126, 'Journal' at 71, and 'Online Computer File' at 3. The main results area shows '0 of 126 Reactions Selected' and a list item '1. View Reaction Detail' with '2 Steps'. Below the list is a chemical reaction scheme showing the synthesis of a duloxetine derivative from a thienothiopyran intermediate and a fluorinated benzene derivative.

Chemical inventories detail relevant regulations



The screenshot displays the SciFinder interface for a chemical search. The main search results show 197 reactions. A specific reaction is highlighted, showing the chemical structure of 2-acetylthiophene and its synthesis from thiophene and acetyl chloride. A context menu is open over the structure, with the 'Get Regulatory Information' option highlighted in pink. This menu includes options like 'View Substance Detail', 'Explore by Structure', 'Synthesize this...', 'Get Reactions where Substance is a...', 'Get Commercial Sources', 'Get Regulatory Information', 'Get References', 'Export as Image', 'Export as molfile', and 'Send to SciPlanner'.

On the right side, a detailed view of the 'Inventory Status' is shown, listing various regulatory inventories such as TSCA, NDSL, REACH, EINECS, AICS, PICCS, and NZIoC. Below this, a section titled 'Regulatory Inventories' provides details for Canadian and European Community regulations. A blue callout box with a pink border contains the text: 'Regulatory information helps you make critical decisions.'

Inventory Status

- On TSCA Inventory
- January 2013 TSCA Inventory
- Removed from DSL
- Canada Gazette, Part II, 142 #13:1390 (25 Jun 2008)
- On NDSL
- Canada Gazette, Part I, 142 #25:1872 (21 Jun 2008)
- On REACH
- List of Pre-Registered Substances, March 2009
- Registration Date: 30-NOV-2010.
- On EINECS
- Annex to Official Journal of the European Communities, 15 June 1990
- On AICS
- Australian Inventory of Chemical Substances, June 1996 Ed
- On PICCS
- Philippines Inventory of Chemicals and Chemical Substances,
- On ASIA-PAC
- On NZIoC
- New Zealand Inventory of Chemicals, 2006
- May be used as a single component chemical under an approval

Regulatory Inventories

==== Canadian Regulations ====

==== European Community Regulations ====

==== Canadian Regulations ====

Canadian Legislation Affecting Chemicals

Canada Gazette, Part I, 140 #45:3599 (11 Nov 2006).
 Notice of intent to delete this substance from the Domestic Substances List (DSL) as a non-eligible substance. During the 180 day comment period, anyone who objects to the deletion of a substance should complete substantiation information and submit to the Minister of the Environment.

==== European Community Regulations ====

European Community Legislation

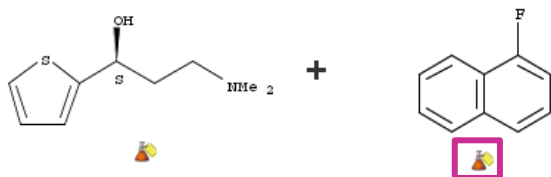
Internet: ec.europa.eu/food/food/chemicalsafety/flavouring (2010).
 This substance is listed in the Register of Flavouring Substances pursuant to Article3(1) of Regulation EC No. 2232/96 (28 Oct 1996) that lays down a procedure for flavouring substances used or intended for use in or on foodstuffs.

Official Journal of the European Communities, No. L 49 (20 Feb 2002).
 This substance is listed in the Register of Flavouring Substances pursuant to Article 3(1) of Regulation EC No. 2232/96 (28 Oct 1996) that lays down a procedure for flavouring substances used or intended for use in or on foodstuffs.
 Listed Name(s): 2-Acetylthiophene.
 FL number: 15.040.
 CoE No.: 11728.
 Chemical Group: 29.

Quickly identify and order commercially available starting materials

1. **View Reaction Detail**  Link

2 Steps *Hover over any structure for more options.*



Commercially available substances are linked to suppliers.

1. **ALDRICH**  **Catalog is associated with a preferred supplier(s)**

Supplier Name: Sigma-Aldrich, Catalog Publication Date: 9 May 2013

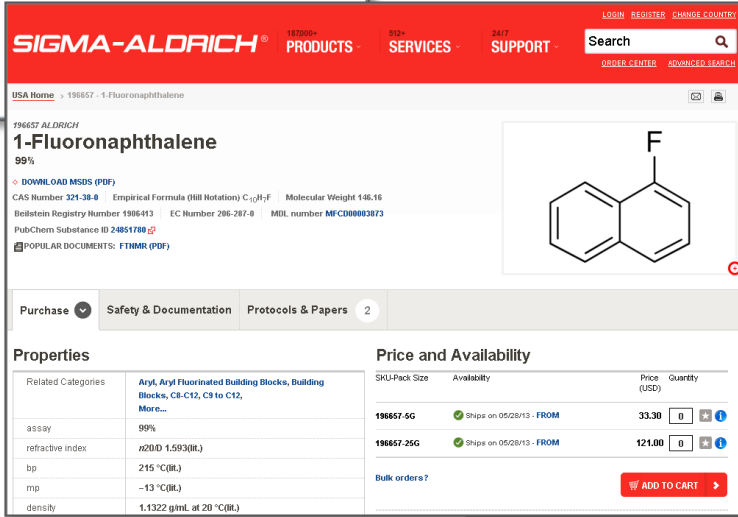
Order Number: 196657

Quantity: 5 g, 25 g






321-38-0 1-Fluoronaphthalene 99%

 Link  Pricing & Availability

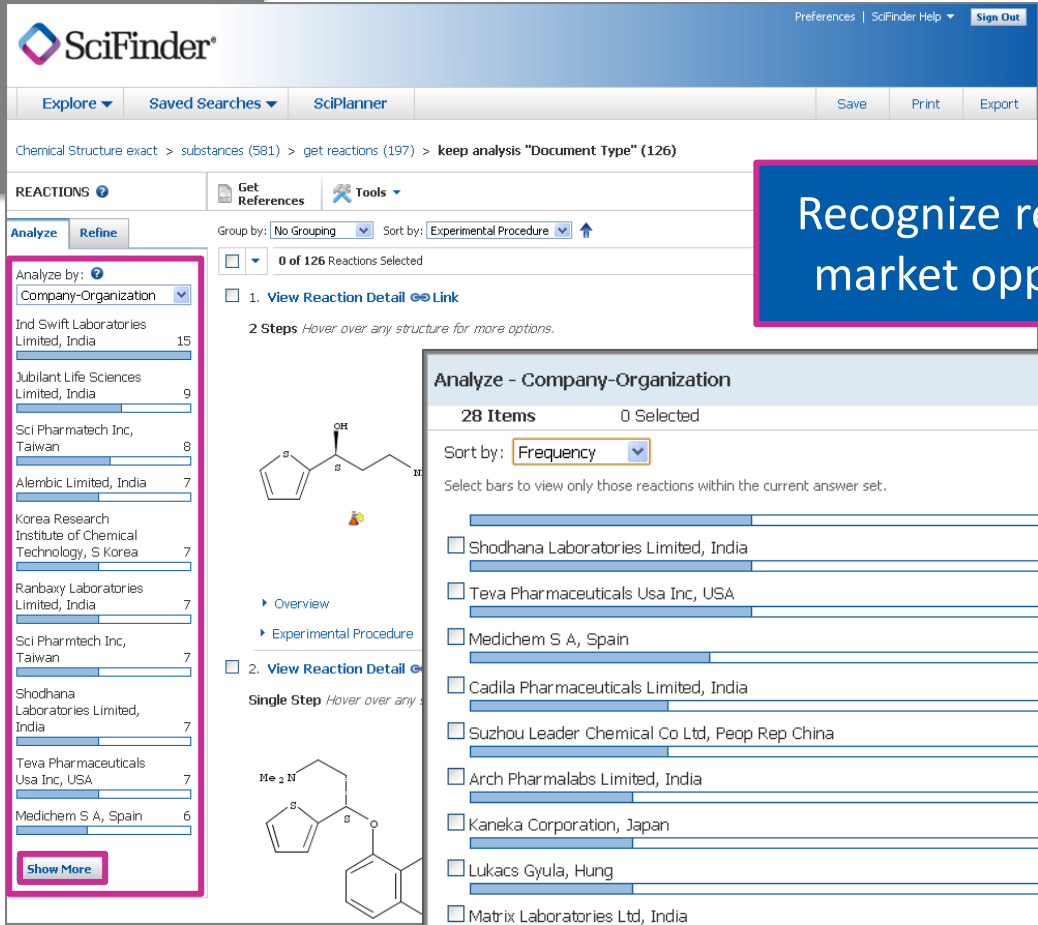
Ordering is easy and convenient.



The screenshot shows the Sigma-Aldrich website interface for the product 1-Fluoronaphthalene. The page includes a search bar, navigation tabs (PRODUCTS, SERVICES, SUPPORT), and a detailed product page. The product name is 1-Fluoronaphthalene (99%), with CAS number 321-38-0 and molecular weight 146.16. The page also features a 'Purchase' dropdown menu, 'Safety & Documentation' and 'Protocols & Papers' tabs, and a 'Properties' table. The 'Price and Availability' section shows two options: 5g for \$33.30 and 25g for \$121.00, both with a 'Ships on 05/28/13 - FROM' status. An 'ADD TO CART' button is visible at the bottom right.

Related Categories	Price and Availability
Aryl, Aryl Fluorinated Building Blocks, Building Blocks, C8-C12, C8 to C12, More...	SKU-Pack Size Availability Price Quantity (USD)
99%	196657-5G  Ships on 05/28/13 - FROM 33.30 0 
refractive index n _D 20/D 1.5930(L)	196657-25G  Ships on 05/28/13 - FROM 121.00 0 
bp 215 °C(B/L)	Bulk orders?
mp -13 °C(B/L)	
density 1.1322 g/mL at 20 °C(B/L)	

Identify potential collaborators or competitors with analysis capabilities



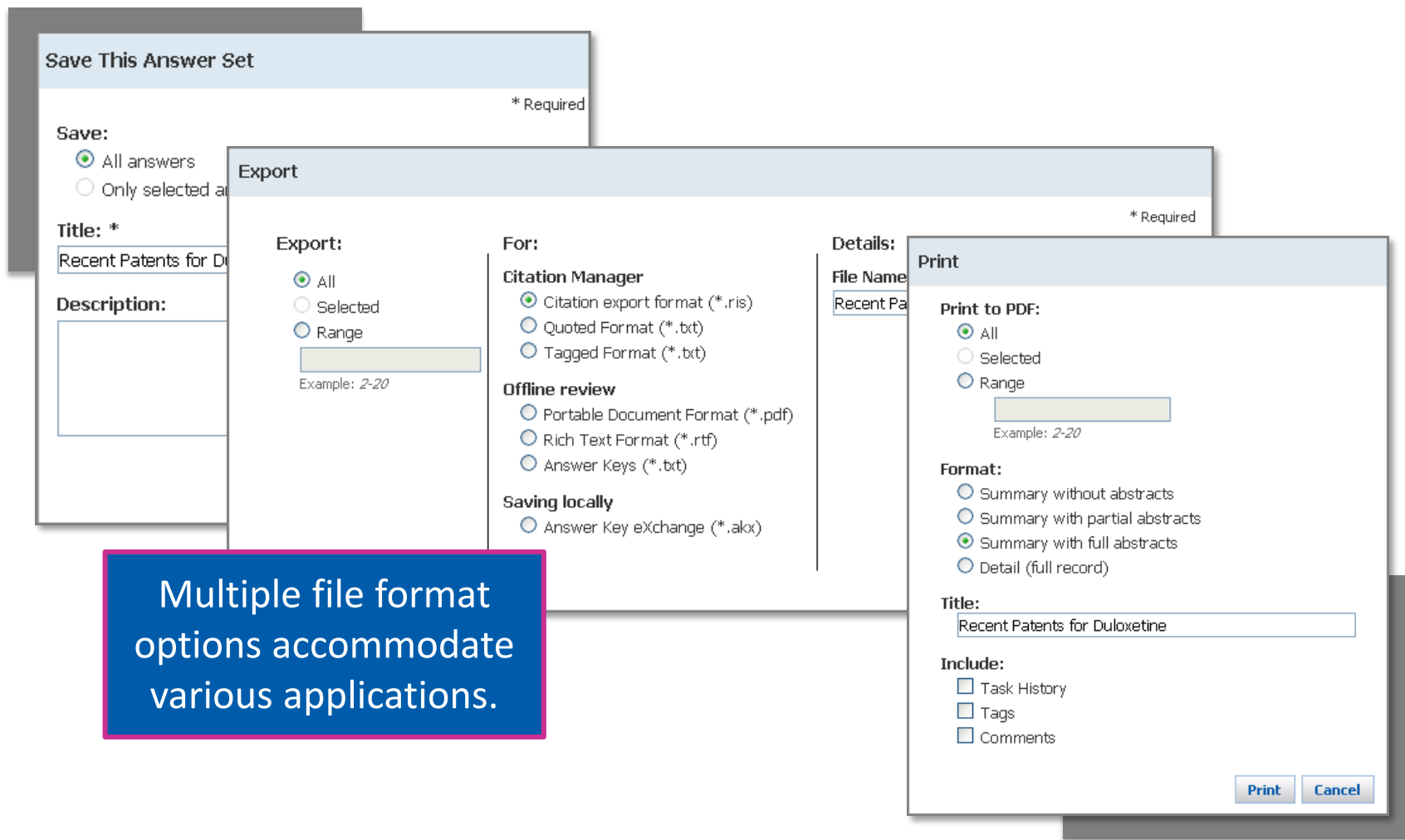
The screenshot displays the SciFinder interface for a search query: "Chemical Structure exact > substances (581) > get reactions (197) > keep analysis 'Document Type' (126)". The "REACTIONS" section is active, showing 0 of 126 reactions selected. The "Analyze" tab is selected, and the "Analyze by:" dropdown is set to "Company-Organization". A list of companies is shown with their respective counts, such as "Ind Swift Laboratories Limited, India" with 15 and "Jubilant Life Sciences Limited, India" with 9. A "Show More" button is visible at the bottom of this list.

A callout box on the right states: "Recognize research and market opportunities." This box highlights the analytical capabilities of the interface.

An "Analyze - Company-Organization" dialog box is open, showing 28 items and 0 selected. The "Sort by:" dropdown is set to "Frequency". The dialog lists various companies and their counts, such as "Shodhana Laboratories Limited, India" with 7, "Teva Pharmaceuticals Usa Inc, USA" with 7, and "Medichem S A, Spain" with 6. The dialog also includes an "Export" button and "Apply" and "Cancel" buttons at the bottom.

Chemical structures are visible in the background, including a thiazole ring system and a substituted benzene ring.

Save, print or export answers for future analysis and collaboration



Save This Answer Set * Required

Save:

- All answers
- Only selected answers

Title: *

Recent Patents for Duloxetine

Description:

Export * Required

Export:

- All
- Selected
- Range

Example: 2-20

For:

Citation Manager

- Citation export format (*.ris)
- Quoted Format (*.txt)
- Tagged Format (*.txt)

Offline review

- Portable Document Format (*.pdf)
- Rich Text Format (*.rtf)
- Answer Keys (*.txt)

Saving locally

- Answer Key eXchange (*.akx)

Details: * Required

File Name:

Recent Patents for Duloxetine

Print

Print to PDF:

- All
- Selected
- Range

Example: 2-20

Format:

- Summary without abstracts
- Summary with partial abstracts
- Summary with full abstracts
- Detail (full record)

Title:

Recent Patents for Duloxetine

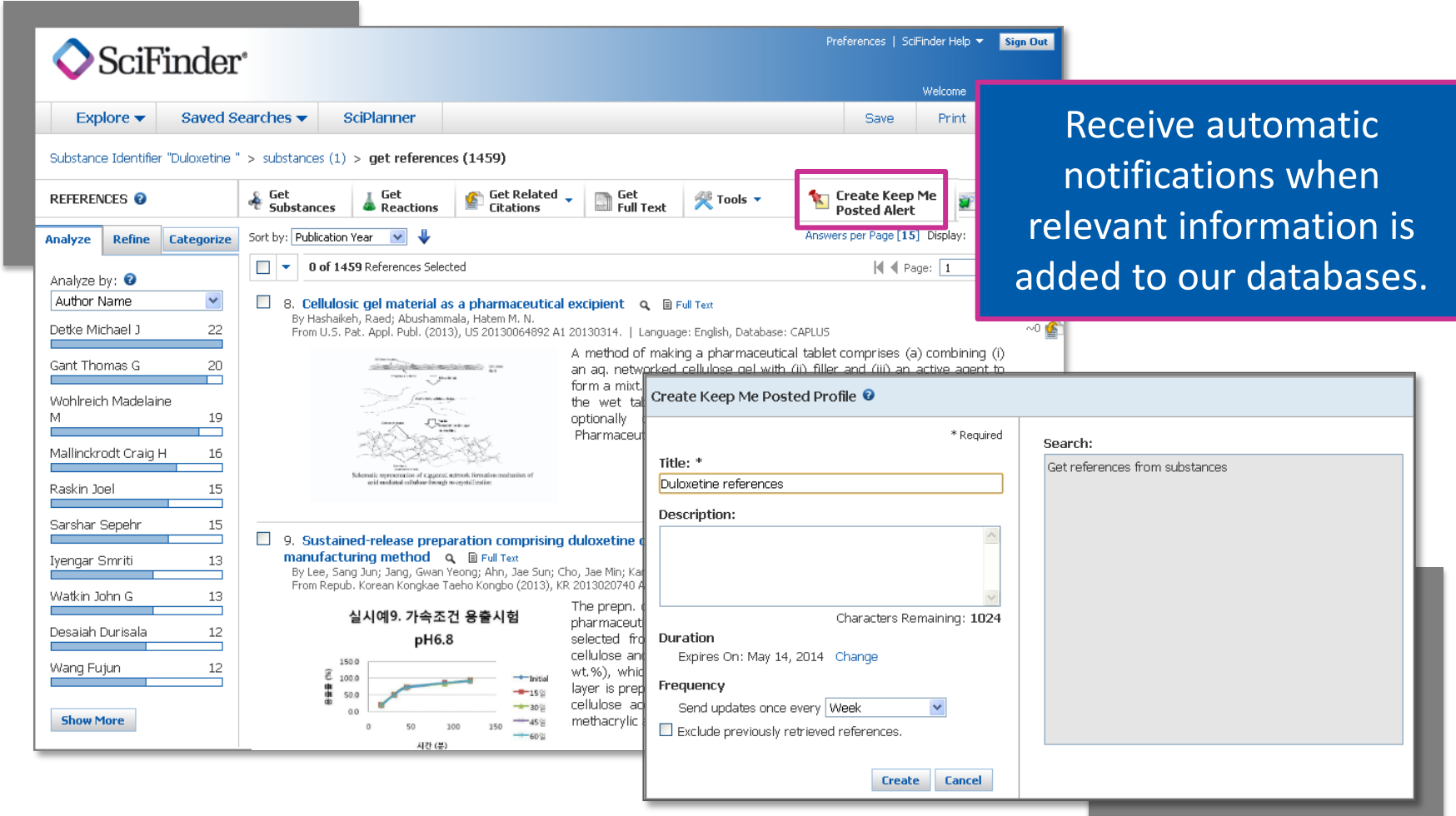
Include:

- Task History
- Tags
- Comments

Print **Cancel**

Multiple file format options accommodate various applications.

Stay current with Keep Me Posted alerts



The screenshot displays the SciFinder web interface. At the top, there are navigation options like 'Explore', 'Saved Searches', and 'SciPlanner'. The main search area shows 'Substance Identifier "Duloxetine" > substances (1) > get references (1459)'. A 'Create Keep Me Posted Alert' button is highlighted with a red box. A blue callout box on the right contains the text: 'Receive automatic notifications when relevant information is added to our databases.'

The 'Create Keep Me Posted Profile' dialog box is open, showing the following fields and options:

- Title:** * Required, containing 'Duloxetine references'
- Description:** A text area for additional details.
- Duration:** Expires On: May 14, 2014 (Change)
- Frequency:** Send updates once every (Week)
- Exclude previously retrieved references.
- Search:** A dropdown menu currently set to 'Get references from substances'.
- Buttons:** Create, Cancel

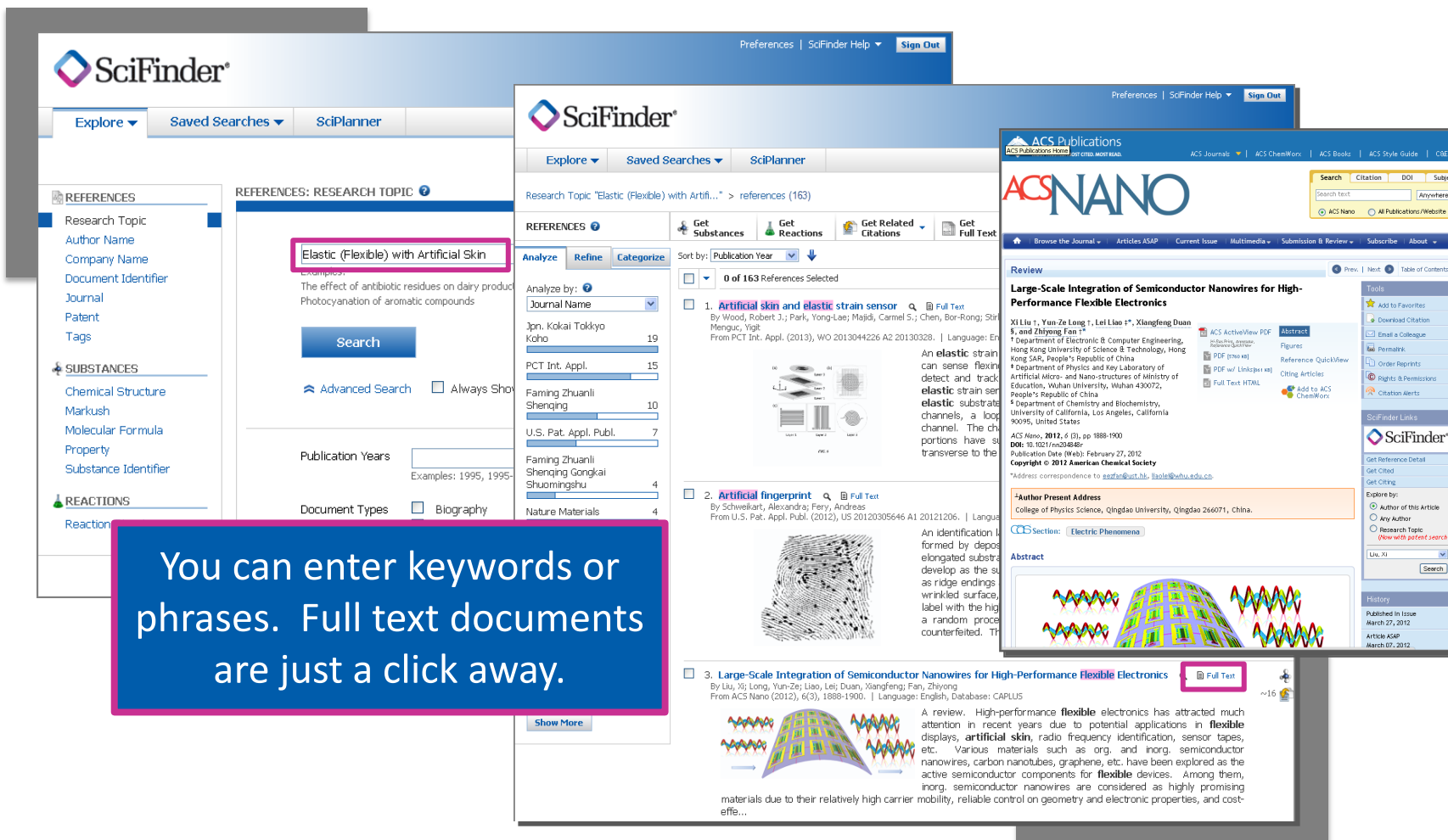
The background interface shows a list of references. Reference 8 is 'Cellulosic gel material as a pharmaceutical excipient' by Hashaikeh, Raed; Abushammala, Hatem M. N. Reference 9 is 'Sustained-release preparation comprising duloxetine and a manufacturing method' by Lee, Sang Jun; Jang, Gwan Yeong; Ahn, Jae Sun; Cho, Jae Min; Kang, Young Hyeon. A graph titled '실시예9. 가속조건 용출시험 pH6.8' is also visible, showing release percentage over time for different conditions.

Example 2: SciFinder helps you get started

You are beginning a research project and need to learn more about the elasticity of artificial skin

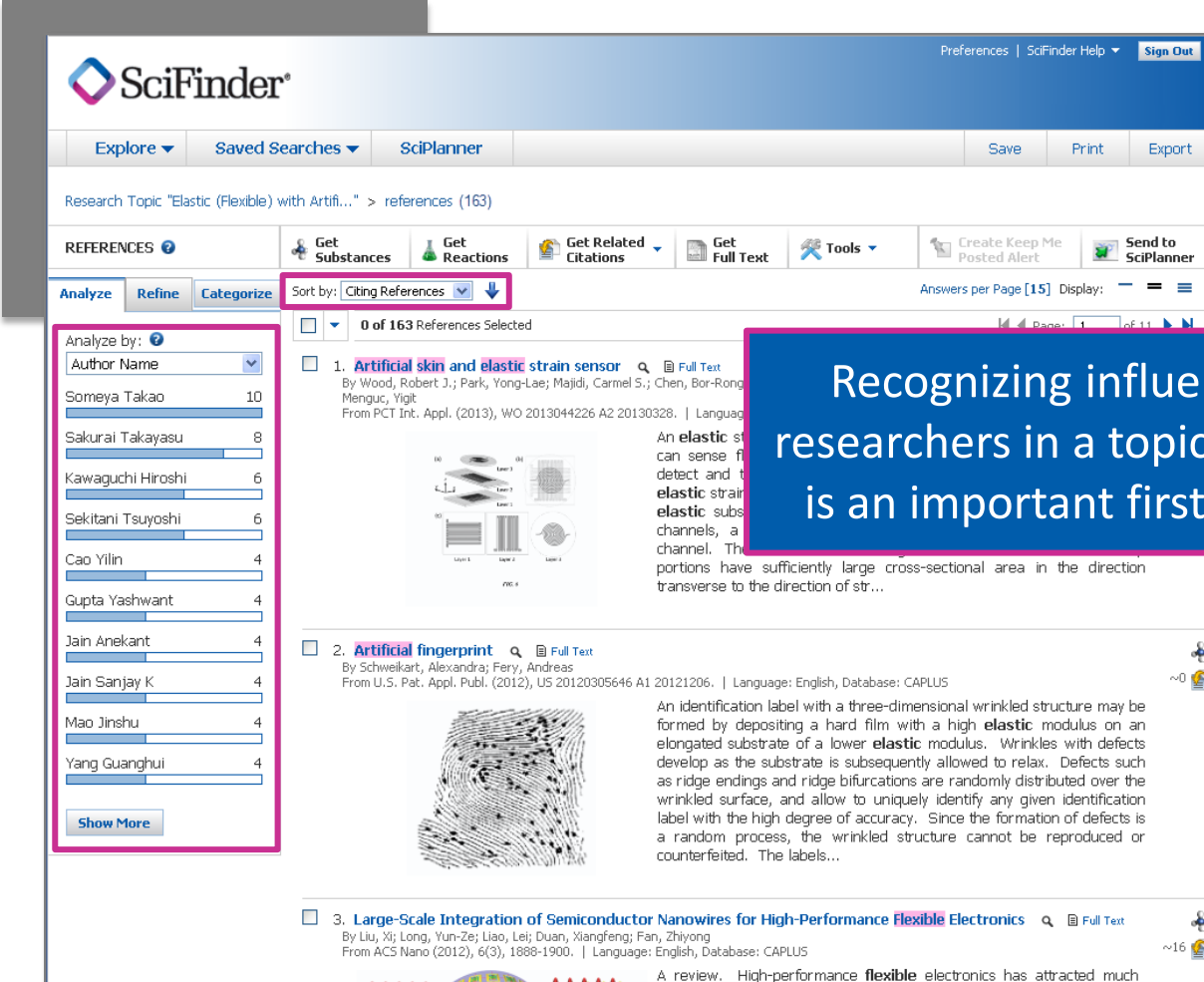
- Which documents should you review?
- Who are the key researchers in this area?
- What substance information is relevant to your research?

Projects and assignments often start by locating the latest research



The screenshot displays the SciFinder search results page for the query "Elastic (Flexible) with Artificial Skin". The interface includes a navigation bar with "Explore", "Saved Searches", and "SciPlanner". On the left, there are tabs for "REFERENCES", "SUBSTANCES", and "REACTIONS". The main content area shows a list of search results, with the first result highlighted: "Artificial skin and elastic strain sensor" by Wood, Robert J.; Park, Yong-Lee; Maida, Carmel S.; Chen, Bor-Rong; and Stru Menguc, Yigit. The abstract for this article is visible, describing an elastic strain sensor that can sense and track elastic strain on flexible substrates. A second result, "Artificial fingerprint", is also visible. A third result, "Large-Scale Integration of Semiconductor Nanowires for High-Performance Flexible Electronics", is highlighted with a pink box. The abstract for this article is also visible, discussing the use of semiconductor nanowires in flexible electronics. A blue callout box with white text is overlaid on the bottom left of the screenshot, stating: "You can enter keywords or phrases. Full text documents are just a click away." The SciFinder logo is visible in the top left corner of the interface.

Author research identifies thought-leaders, important papers and potential collaborators



SciFinder®

Explore ▾ Saved Searches ▾ SciPlanner Save Print Export

Research Topic "Elastic (Flexible) with Arti..." > references (163)

REFERENCES ⓘ

Get Substances Get Reactions Get Related Citations Get Full Text Tools Create Keep Me Posted Alert Send to SciPlanner

Analyze Refine Categorize Sort by: Citing References ↓

Answers per Page [15] Display: ▾ ▹ ▸ ▹ ▸ ▹ ▸

0 of 163 References Selected

Analyze by: ⓘ

Author Name	Citation Count
Someya Takao	10
Sakurai Takayasu	8
Kawaguchi Hiroshi	6
Sekitani Tsuyoshi	6
Cao Yilin	4
Gupta Yashwant	4
Jain Anekant	4
Jain Sanjay K	4
Mao Jinshu	4
Yang Guanghui	4

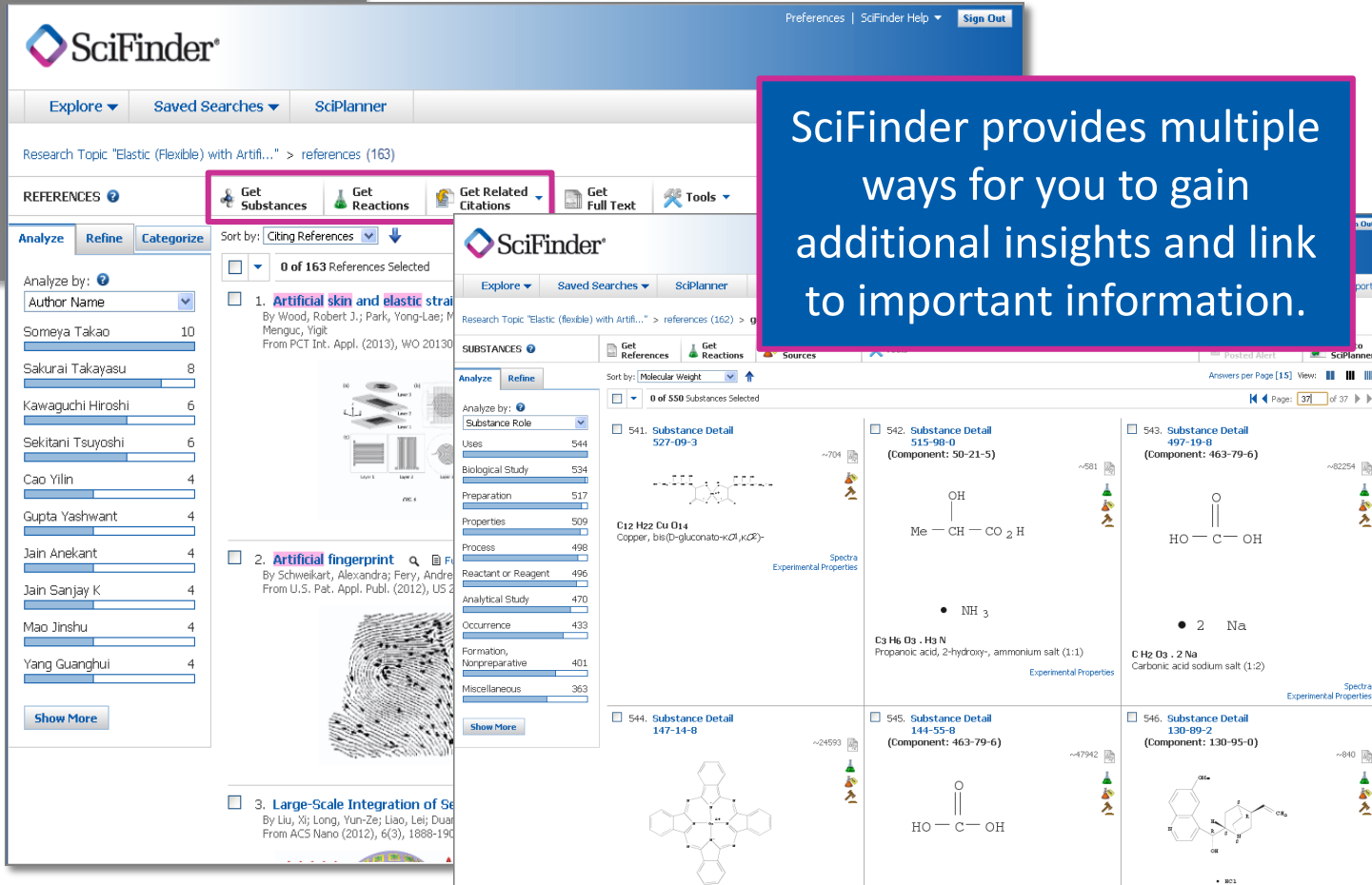
Show More

1. **Artificial skin and elastic strain sensor** Full Text
 By Wood, Robert J.; Park, Yong-Lae; Majidi, Carmel S.; Chen, Bor-Rong; Menguc, Yigit
 From PCT Int. Appl. (2013), WO 2013044226 A2 20130328. | Language: English, Database: CAPLUS

2. **Artificial fingerprint** Full Text
 By Schweikart, Alexandra; Fery, Andreas
 From U.S. Pat. Appl. Publ. (2012), US 20120305646 A1 20121206. | Language: English, Database: CAPLUS

3. **Large-Scale Integration of Semiconductor Nanowires for High-Performance Flexible Electronics** Full Text
 By Liu, Xi; Long, Yun-Ze; Liao, Lei; Duan, Xiangfeng; Fan, Zhiyong
 From ACS Nano (2012), 6(3), 1888-1900. | Language: English, Database: CAPLUS

Retrieve related information, such as substances, reactions and citations



The screenshot displays the SciFinder web interface. At the top, there are navigation tabs: "Explore", "Saved Searches", and "SciPlanner". Below this, a search topic is shown: "Elastic (Flexible) with Artifi..." with 163 references. A toolbar contains buttons for "Get Substances", "Get Reactions", "Get Related Citations", "Get Full Text", and "Tools".

The main content area is divided into two panels. The left panel, titled "REFERENCES", shows a list of search results with an "Analyze by:" dropdown set to "Author Name". A bar chart displays author counts: Someya Takao (10), Sakurai Takayasu (8), Kawaguchi Hiroshi (6), Sekitani Tsuyoshi (6), Cao Yilin (4), Gupta Yashwant (4), Jain Anekant (4), Jain Sanjay K (4), Mao Jinshu (4), and Yang Guanghui (4). A "Show More" button is at the bottom.

The right panel, titled "SUBSTANCES", shows a list of substances with an "Analyze by:" dropdown set to "Substance Role". A bar chart displays various categories: Uses (544), Biological Study (534), Preparation (517), Properties (509), Process (498), Reactant or Reagent (496), Analytical Study (470), Occurrence (433), Formation, Nonpreparative (401), and Miscellaneous (363). A "Show More" button is at the bottom.

Below the substance list, several substance detail cards are visible, each showing a chemical structure and experimental properties. For example, one card shows the structure of Copper, bis(D-gluconato-kCl, kO2)- with the formula $C_{12}H_{22}CuO_{14}$. Another card shows the structure of Propanoic acid, 2-hydroxy-, ammonium salt (1:1) with the formula $C_3H_6O_3 \cdot H_3N$. A third card shows the structure of Carbonic acid sodium salt (1:2) with the formula $C_2H_2O_3 \cdot 2Na$.

A blue callout box on the right side of the interface contains the text: "SciFinder provides multiple ways for you to gain additional insights and link to important information."



Access SciFinder at:

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