

The logo for SciFinder SCHOLAR 2002 is centered on a vertical rectangular background with a purple-to-pink gradient and a diagonal light streak. The text "SciFinder" is in a large, blue, serif font with a registered trademark symbol. Below it, "SCHOLAR" is in a smaller, blue, sans-serif font, and "2002" is in a large, blue, sans-serif font. Two horizontal lines separate the three text elements.

SciFinder®
SCHOLAR
2002



HBZ



HBZ

Stereochemie und
Substanzeigenschaften

Strukturen in SciFinder

- CAS Registry enthält über 21 Mio. "kleine Moleküle" oder kurze Sequenzen
- Z.Zt. haben 4.8 Mio. Strukturen eine definierte Stereochemie
- Stereochemische Informationen sind für folgende Klassen nicht verfügbar:
 - Koordinationsverbindungen, Allene und Cumulene, Atropisomerie zwischen zwei Ringsystemen

Struktursuche in SF Scholar

- SciFinder Scholar nutzt eine breitere Struktursuche die Tautomere und verwandte Verbindungen mit aufgreift
 - Die Doppelbindungsgeometrie kann durch Tautomerie beeinflußt werden
 - Kohlenhydrate und Hemiacetale können zusätzliche Stereozentren bilden, die ebenfalls als Hits angezeigt werden

The logo for SciFinder Scholar 2002 is located in the bottom right corner. It features the text "SciFinder" in a blue serif font, "SCHOLAR" in a blue sans-serif font below it, and "2002" in a larger blue sans-serif font at the bottom. The logo is set against a vertical gradient bar that transitions from purple at the top to blue at the bottom.

Suche nach einem Stereoisomer

The screenshot shows the ChemDraw software interface. The main window displays a chemical structure of (S)-1-(pyridin-2-yl)propan-1-ol. The structure consists of a pyridine ring connected via an oxygen atom to a propan-1-ol chain, where the hydroxyl group is shown with a wedge bond, indicating its stereochemistry. The interface includes a menu bar (File, Edit, View, Tools, Template, Help), a toolbar with various drawing tools, and a bottom toolbar with buttons for 'Preview', 'Get Substances', 'Get Reactions', and 'Cancel'. The bottom toolbar also features a row of buttons for stereochemistry: a red box highlights the 'Wedge' button, followed by 'Dash', 'E', and 'Z' buttons. The 'Scale' is set to 100. The status bar at the bottom indicates 'Formula not available'.

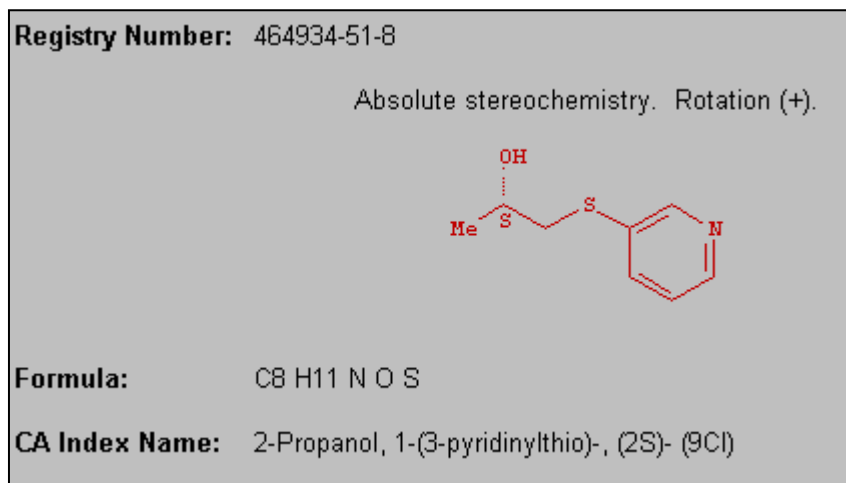
Automatische Stereoanalyse

The screenshot shows a software window titled "Stereo Analysis" with a menu bar (File, Edit, Task, Tools, Help). The main area is titled "Select Histogram Entries of interest:" and contains a list of five entries, each with a checkbox, a blue bar representing its count, and the count value. The entries are:

Entry	Count
<input type="checkbox"/> Absolute stereo match	142
<input type="checkbox"/> Absolute stereo mirror image	49
<input type="checkbox"/> Relative stereo match	5
<input type="checkbox"/> Stereo that doesn't match query	51
<input type="checkbox"/> No stereo in answer structure	414

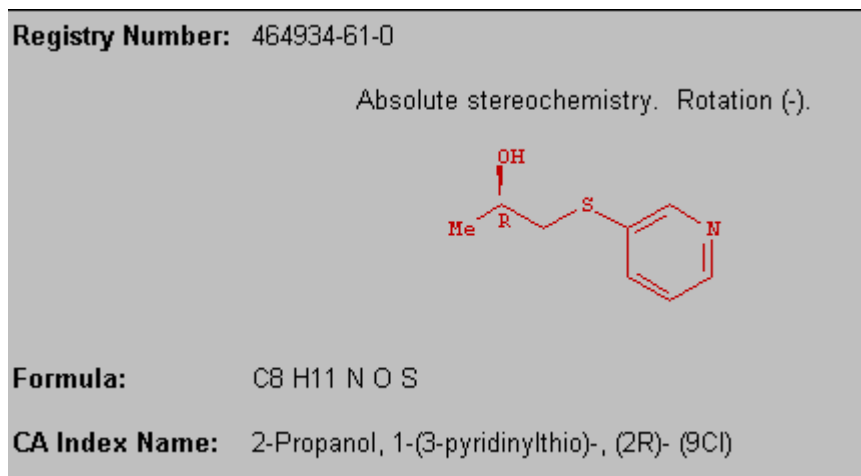
At the bottom of the window, there are two buttons: "Get Substances" and "Back". The status bar at the very bottom indicates "Histogram Entries 1-5 of 5".

"Absolute stereo" Hits



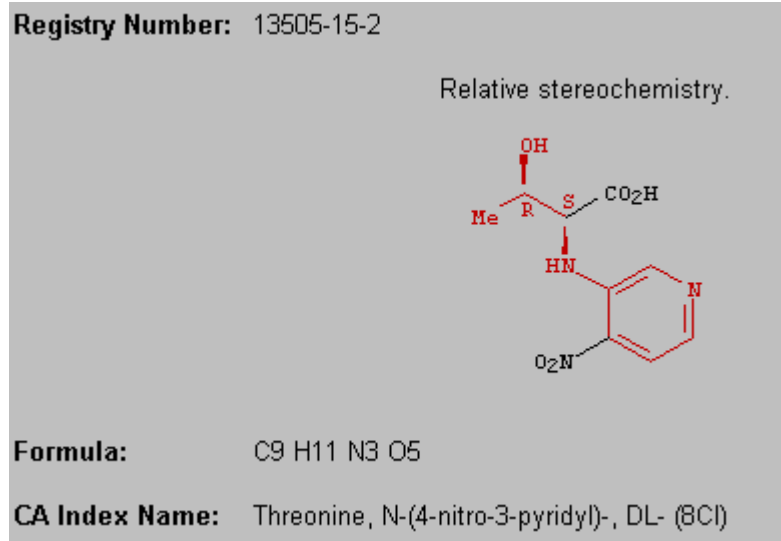
- Diese Antworten haben auf jeden Fall die S-Konfiguration am gesuchten Zentrum. Die graph. Darstellung kann aber aus der Zeichenebene heraus oder hinein deuten. Der Autor muss explizit die absolute Konfiguration angegeben haben.

"Absolute stereo mirror image"



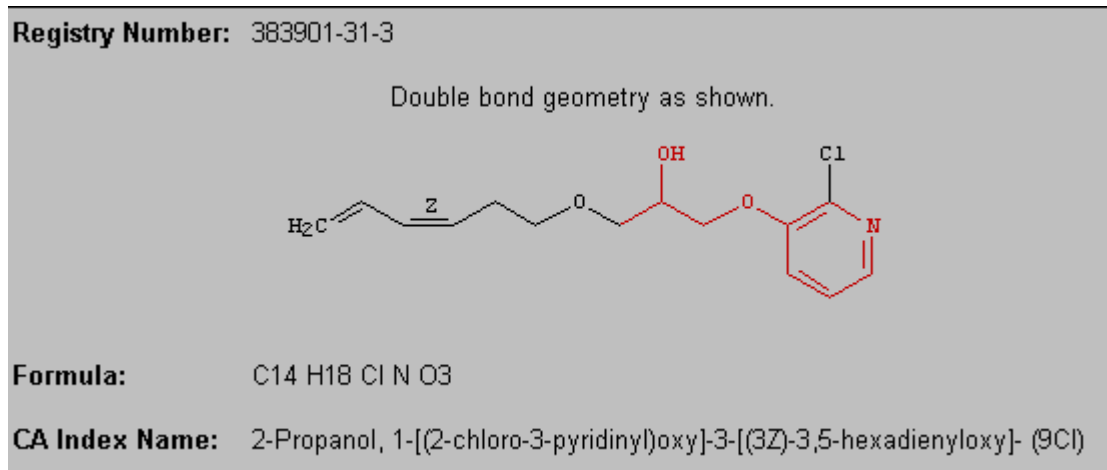
- Hier ist das Stereozentrum R konfiguriert. Es handelt sich um das Spiegelbild der gesuchten Verbindung.

"Relative stereo answers"



- Bei diesen Antworten ist nur die relative Stereochemie bekannt. Die graphische Darstellung kann von der tatsächlichen Konfiguration abweichen.

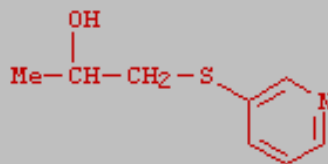
"Stereo answers not matching"



- Diese Verbindungen haben zwar nicht die gewünschte Stereochemie an dem chiralen Zentrum, aber es gibt eine definierte Stereochemie an einem anderen Zentrum im Molekül. Hier die Z Konfiguration der Doppelbindung.

"No stereo in answer structure"

Registry Number: 464934-46-1



Formula: C8 H11 N O S

CA Index Name: 2-Propanol, 1-(3-pyridinylthio)- (9CI)

- Hier hat der Autor keine Stereochemie angegeben oder es handelt sich um die Racemate oder um undefinierte Gemische der Stereoisomere. Keine Stereoinformation – die Grafik ist flach.

Zeichnen der Stereochemie

Untitled

File Edit View Tools Template Help

Atom Short

Structure Drawing Error

The following errors were found with your structure. Click the icon below the error to highlight it within your query.

1. A chiral node must have either three or four attachments. [\(Help\)](#)
 Highlight Area

Hier gibt es ausführliche Hilfe!

Close

Scale 100

Preview Get Substances Get Reactions Cancel

Formula not available

USING SCIFINDER

PERFORMING TASKS

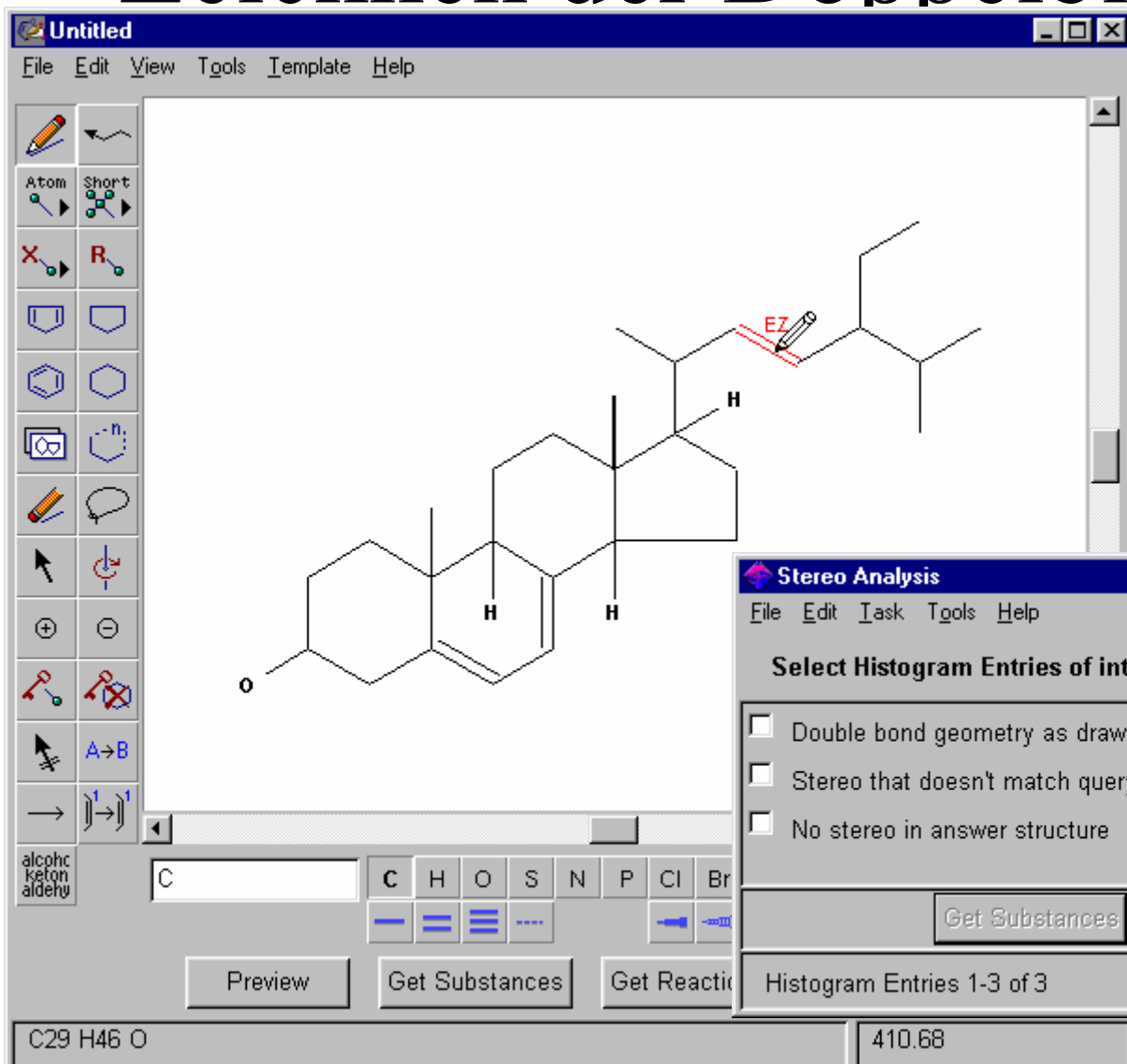
- Begin a Search
- Set the Display Format for Your Current Session
- Understanding Your Explore Results
- Explore by Chemical Substance or Reaction
- Explore by Chemical Substance or Reaction
- Explore by Chemical Structure
- Access Explore by Chemical Structure
- Exact vs. Substructure Searching
- How Explore by Chemical Structure
- Structure Drawing Window
- Drawing Structures and Reactions
 - Draw a Structure
 - Draw Nodes and Bonds
 - Change Nodes and Bonds
 - Display Atoms as Dots
 - Display Position Numbers
 - Use Fixed Angles and Lengths
 - Reverse a Shortcut
 - Drawing Stereo**
 - Use a Structure Template
 - Copy a CAS Registry Number to Clipboard
 - Import a Structure Query
- Moving Structures or Structure Fragments
- Prohibiting Substitution or Fusion
- Check for Overlapping Nodes
- Check Valencies in Your Structure
- Tips for Modifying a Structure
- Draw a Reaction
- Explore by Functional Group
- Previewing Structures
- Searching Structures
- Explore by Substance Identifier

Structure Drawing Errors

This table indicates possible stereo drawing errors:

Error Message	Incorrect	Correct
The stereo in this structure drawing cannot be interpreted. Please redraw the stereo using the Stereo Bond Palette, or replace the highlighted bonds with flat bonds. ¹		
Shortcuts, variables, R-groups, and hydrogen cannot be chiral nodes.		
Shortcuts, variables, R-groups, and hydrogen cannot have a geometric double bond.		
A chiral node cannot have two or more identical attachments.		
A node with a geometric double bond cannot have two or more identical attachments.		
A chiral node must have either three or		P

Zeichnen der Doppelbindung



Zeichnen Sie die Doppelbindung wie gewünscht und klicken Sie dann auf das EZ Tool

Stereo Analysis

File Edit Task Tools Help

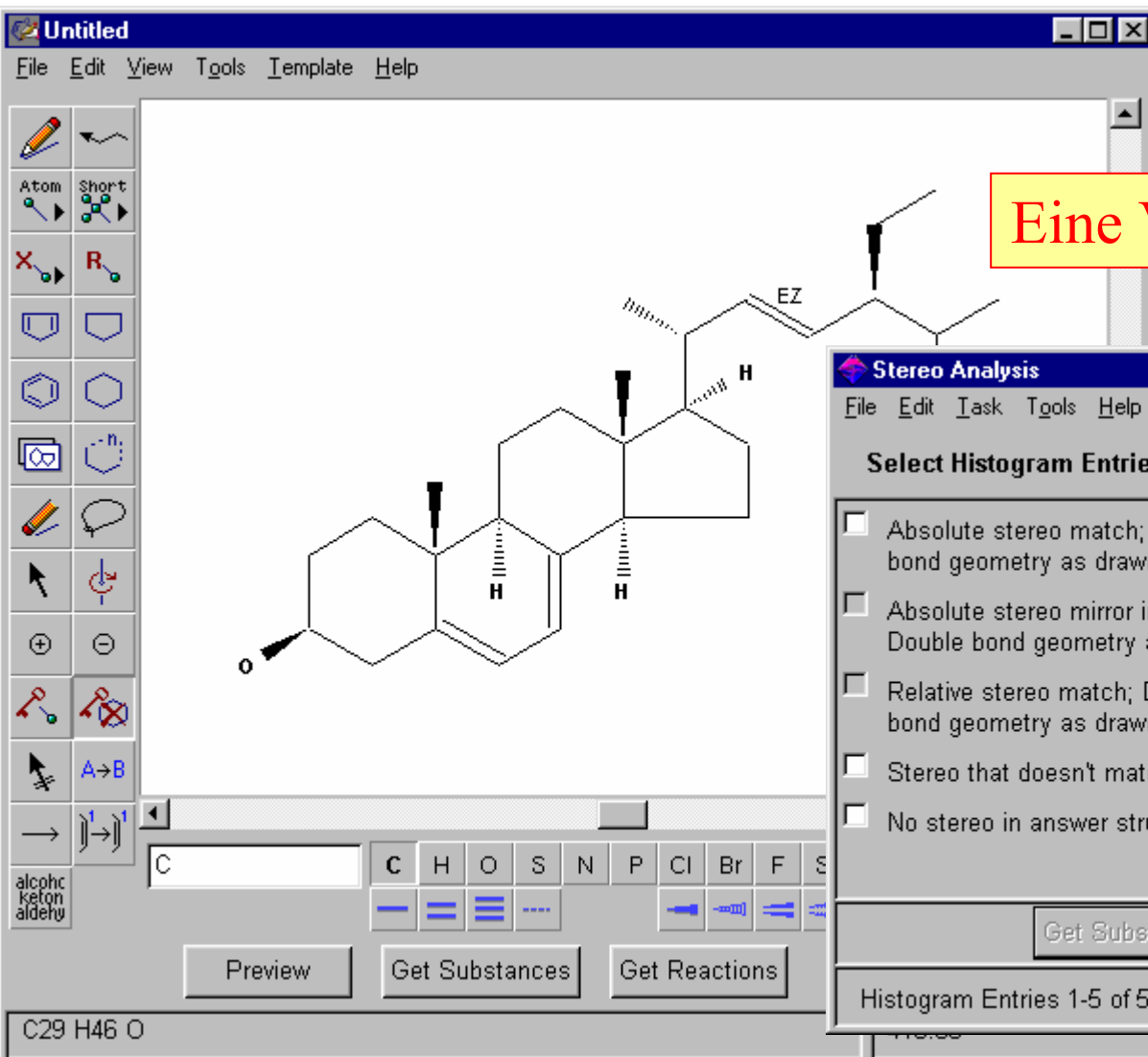
Select Histogram Entries of interest:

<input checked="" type="checkbox"/>	Double bond geometry as drawn	<div style="width: 100%;"></div>	29
<input type="checkbox"/>	Stereo that doesn't match query	<div style="width: 25%;"></div>	7
<input type="checkbox"/>	No stereo in answer structure	<div style="width: 10%;"></div>	3

Get Substances Back

Histogram Entries 1-3 of 3

Mehrere Stereozentren



Eine Verbindung aus Olivenöl!

The "Stereo Analysis" dialog box displays a histogram of stereochemical matches. The "Stereo that doesn't match query" entry is selected and highlighted in blue.

Select Histogram Entries of interest:	Count
<input type="checkbox"/> Absolute stereo match; Double bond geometry as drawn	14
<input type="checkbox"/> Absolute stereo mirror image; Double bond geometry as drawn	0
<input type="checkbox"/> Relative stereo match; Double bond geometry as drawn	0
<input checked="" type="checkbox"/> Stereo that doesn't match query	22
<input type="checkbox"/> No stereo in answer structure	3

Buttons: Get Substances, Back

Footer: Histogram Entries 1-5 of 5

Strukturen und Eigenschaften

- In CAS Registry finden Sie berechnete Eigenschaften für 13 Mio. einfache organ. Verbindungen. (ACD Labs)
- In CAS Registry finden Sie experimentell bestimmte Eigenschaften für 830000 Verbindungen. (Infochem)
- Referenzen die bestimmte Eigenschaften beschreiben können in CAPlus gefunden werden.



Experimentelle Eigenschaften in Registry

- Folgende Daten sind für ca. 800000 Verbindungen erfasst:
 - Schmelzpunkt
 - Siedepunkt
 - Brechungsindex
 - Dichte
 - Optische Rotation
- Informationen zu den Eigenschaften
 - Der Wert
 - Messbedingungen, wenn vom Autor angegeben
 - Quelle
- Ca. 20% der Substanzen in Registry mit physikalischen Eigenschaften haben keine Eigenschaften in anderen STN Datenbanken

Registry ist inzwischen auch eine grosse Quelle für phys. Eigenschaften

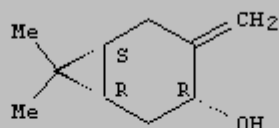
	REGISTRY	BEILSTEIN	HODOC	MRCK	DIPPR	HSDB
Melting Point	687,000	3,950,000	16,000	6,800	1,700	2,900
Boiling Point	123,000	680,000	12,400	2,200	1,700	2,100
Refractive Index	51,500	350,000	7,600	1,200	1,700	-
Optical Rotatory Power	32,800	680,000	1,200	2,100	-	-
Density	19,700	180,000	7,400	-	-	-

The logo for SciFinder SCHOLAR 2002, featuring the text 'SciFinder' in a large serif font, 'SCHOLAR' in a smaller sans-serif font below it, and '2002' in a bold sans-serif font at the bottom. The logo is set against a background of a hand holding a pen, with a blue and purple gradient.

Ein Beispiel

Registry Number: 4017-83-8

Absolute stereochemistry. Rotation (-).



Formula: C₁₀ H₁₆ O

CA Index Name: Bicyclo[4.1.0]heptan-3-ol, 7,7-dimethyl-4-methylene-, [1R-(1α,3α,6α)]-

Other Names: 3(10)-Caren-4-ol, (1S,4R,6R)-(-)- (8Cl); Bicyclo[4.1.0]heptan-3-ol, 7,7-dimethyl-4-methylene-, [1R-(1α,3α,6α)]-

-- Properties --

Property	Calculated Value	Condition	Note
H donors	1		(1) ACD
H acceptors	1		(1) ACD
Molecular Weight	152.23		(1) ACD
logP	2.454±0.249		(1) ACD
logD	2.45	pH 1	(1) ACD
logD	2.45	pH 4	(1) ACD
logD	2.45	pH 7	(1) ACD
logD	2.45	pH 8	(1) ACD
logD	2.45	pH 10	(1) ACD
Molar Solubility	Sparingly Soluble	pH 1	(1) ACD
Molar Solubility	Sparingly Soluble	pH 4	(1) ACD
Molar Solubility	Sparingly Soluble	pH 7	(1) ACD
Molar Solubility	Sparingly Soluble	pH 8	(1) ACD
Molar Solubility	Sparingly Soluble	pH 10	(1) ACD

Property	Experimental Value	Condition	Note
Boiling Point	40-50 °C	Press: 0.5 Torr	(2) IC
Melting Point	53-54 °C		(2) IC
Optical Rotatory Power	-119.8°	Conc: 2.47 g/mL Solv: chloroform (67-66-3) Temp: 20 °C	(2) IC

Notes:

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 (© 1994-2002 ACD)

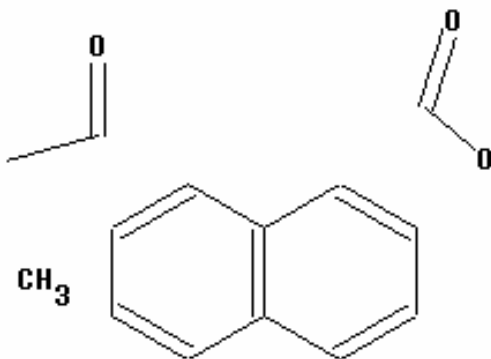
(2) Paquette, Leo A.; Journal of Organic Chemistry 1990, V55(5), P1589-98

3/18/2003

SciFinder is
the Ameri

Ein Suchbeispiel:

Die Analyse einer Verbindung hat ergeben, dass sie folgende Strukturelemente enthält:



Die Verbindung schmilzt bei 165-170°C. Das Semicarbazon schmilzt bei 212°C.

Was ist die Struktur der Verbindung?

Substruktursuche mit Fragmenten

The screenshot shows the ChemDraw software interface. The main window, titled 'Untitled', contains a drawing of naphthalene and its fragments: a methyl group (CH3), a carbonyl group (C=O), and a carboxyl group (COOH). A 'Get Substances' dialog box is open in the foreground, with the 'Additional Options' button highlighted in red. The dialog box contains the following text:

Get substances where this structure is:

- an exact match or a related structure
- a substructure of a more complex structure

Buttons: OK, Additional Options, Cancel

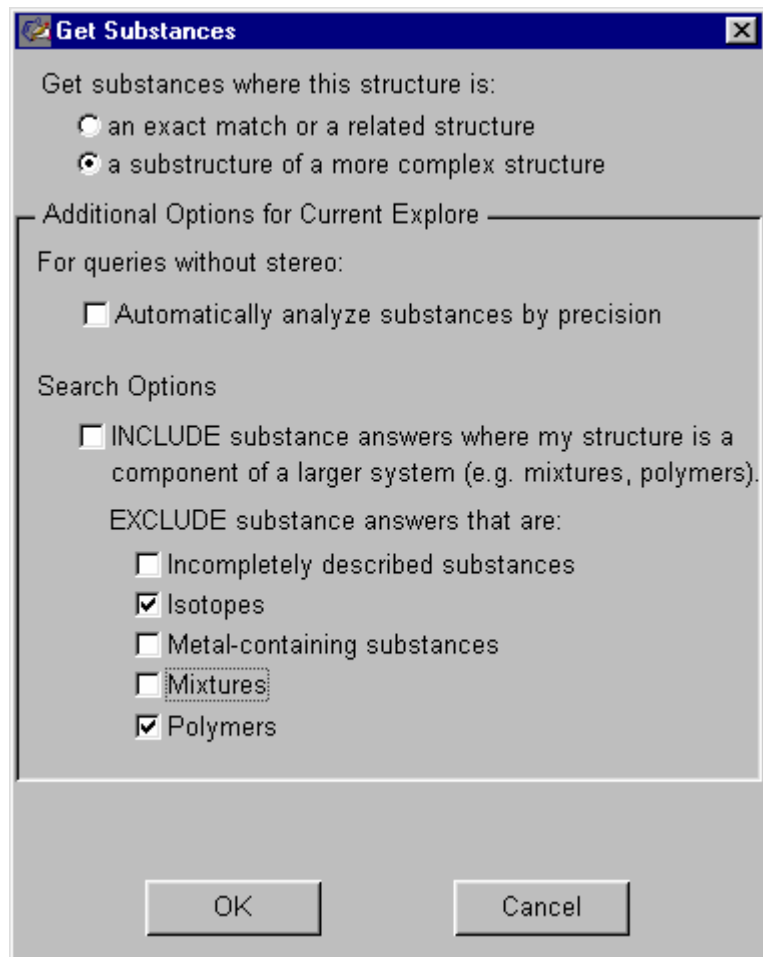
Scale: 100

alcoh keton aldehy C

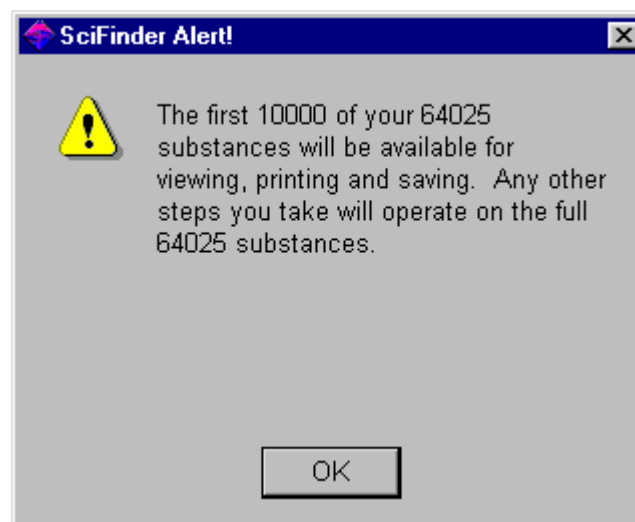
Preview Get Substances Get Reactions Cancel

C10 H8 . C H2 O . C H2 O2 . C H4 128.17 . 30.03 . 46.03

Unerwünschte Substanzen ausschließen:



Die Einstellungen gelten nur für die aktuelle Suche!



SciFinder
SCHOLAR
2002

Navigation icons: NewTask, Back, Forward, Print, Save As, FullText, Prefs, Database, History, Message, Internet, Panorama, Help, Exit.

Untitled

Chemical drawing toolbar with icons for Atom, Short, R, and various ring structures (cyclopentane, cyclohexane, etc.).

Central drawing area showing a chemical structure of a methyl ketone: CC(=O)C1CCCCC1. A yellow text box is overlaid on the structure.

**Verfeinern mit der Bedingung,
daß die Methyl und die Keto
Gruppe direkt am Ring sitzen.**

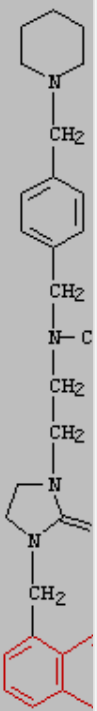
Element selection keyboard: O, C, H, O, S, N, P, Cl, Br, F, Si, I, Scale 100.

Get Substances Cancel

Formula not available

471929-48-3

Component Number 1



Component Number 2



Reference chemical structure: CC(=O)Oc1ccc(NC)cc1

Get References

Analyze or Refine Substances

Back



471925-55-0

~1 Reference
REGISTRY

471254-33-8

471254-32-7

~1 Reference
REGISTRY

470673-82-6

No References
REGISTRY

No References
REGISTRY

65535-92-6

Component Number 1

Refine by Chemical Substance

Refine by:

- Chemical Structure
Limit results using a chemical structure.
- Commercial Availability
Limit to commercially available substances.
- Property Data
Limit results by property values.

8.91
LogP
pKa

Cancel

Get References

Analyze or Refine Substances

Back



Eingrenzen auf den Schmelzpunkt:

Refine by Property

Select one or more Properties of interest.
Then enter the appropriate values for each property.
For more information about properties, click [here](#).

Hydrogen Acceptors

Molecular Weight

logP

Freely Rotatable Bonds

logD

pKa

Solubility

Boiling Point

Melting Point

Temperature (C):

165 to 170

Min: -273 Max: no limit

Include substances with no value for the specified properties

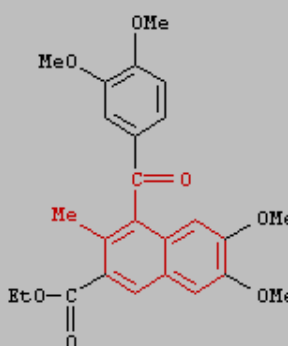
OK Change Preferences Back

Nicht relevante
Eigenschaften
ausgrenzen und
Schmelzpunktsbereich
eingeben.
Antworten ohne
Schmelzpunkt
ebenfalls ausgrenzen.

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SCHOLAR
2002

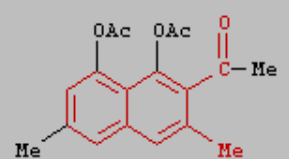
[New Task](#)
[Back](#)
[Forward](#)
[Print](#)
[Save As](#)
[Full Text](#)
[Prefs](#)
[Database](#)
[History](#)
[Message](#)
[Internet](#)
[Panorama](#)
[Help](#)
[Exit](#)

128981-46-4



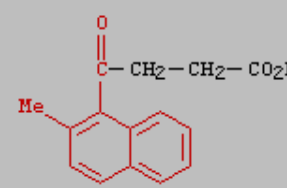
~1 Reference
REGISTRY

89586-46-9



~1 Reference
REGISTRY

78540-11-1

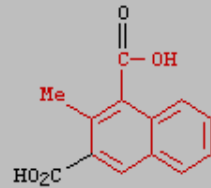


~1 Reference
REGISTRY

Das Semicarbazon dieser Verbindung hätte folgende Summenformel $C_{19}H_{21}N_3O_5$

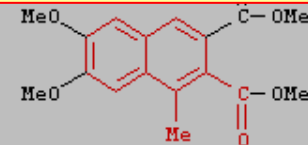
Das Semicarbazon dieser Verbindung hätte folgende Summenformel $C_{16}H_{17}N_3O_3$

72391-94-7



~1 Reference
REGISTRY

89586-46-9



~3 References
REGISTRY

Get References

Analyze or Refine Substances

Back



Summenformel der Semicarbazone suchen:

Explore by Molecular Formula

Enter the molecular formula of the substance.

Examples:
H4SiO4
H4O4Si
H4 Si O4

OK Cancel

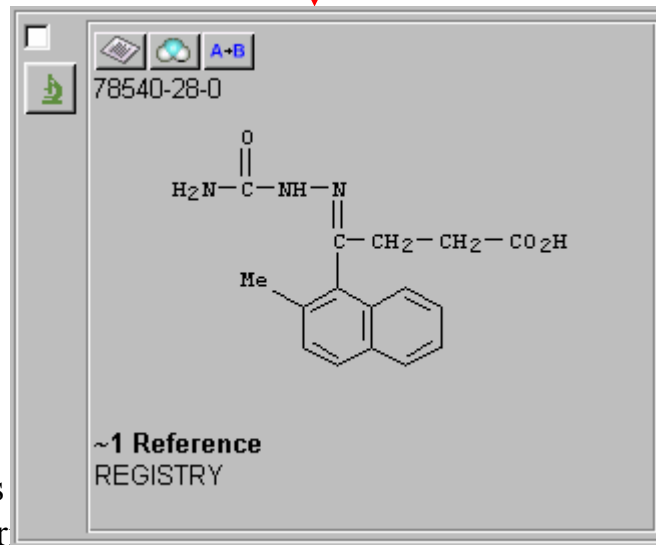
Explore by Molecular Formula

Enter the molecular formula of the substance.

Examples:
H4SiO4
H4O4Si
H4 Si O4

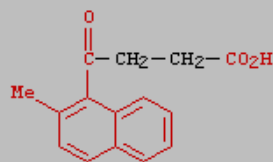
OK Cancel

Nicht beschrieben



Die gesuchte Verbindung:

Registry Number: 78540-11-1



Formula: C15 H14 O3

CA Index Name: 1-Naphthalenebutanoic acid, 2-methyl-γ-oxo- (9CI)

-- Properties --

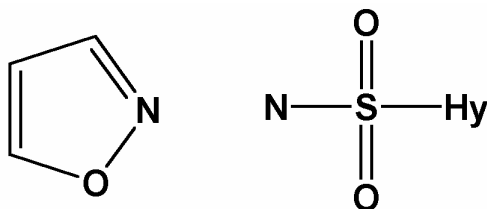
Property	Calculated Value	Condition	Note
H donors	1		(1) ACD
H acceptors	3		(1) ACD
Molecular Weight	242.27		(1) ACD
logP	2.977±0.363		(1) ACD
logD	2.98	pH 1	(1) ACD
logD	2.87	pH 4	(1) ACD
logD	0.53	pH 7	(1) ACD
logD	-0.39	pH 8	(1) ACD
logD	-1.10	pH 10	(1) ACD
pKa	4.54±0.20	Most Acidic	(1) ACD
Molar Solubility	Sparingly Soluble	pH 1	(1) ACD
Molar Solubility	Sparingly Soluble	pH 4	(1) ACD
Molar Solubility	Slightly Soluble	pH 7	(1) ACD
Molar Solubility	Soluble	pH 8	(1) ACD
Molar Solubility	Very Soluble	pH 10	(1) ACD

Property	Experimental Value	Condition	Note
Melting Point	168 °C	Solv: benzene (71-43-2)	(2) IC

Die
Schmelzpunkte
dieser
Verbindung und
ihres
Semicarbazons
sind nirgendwo
sonst zu finden

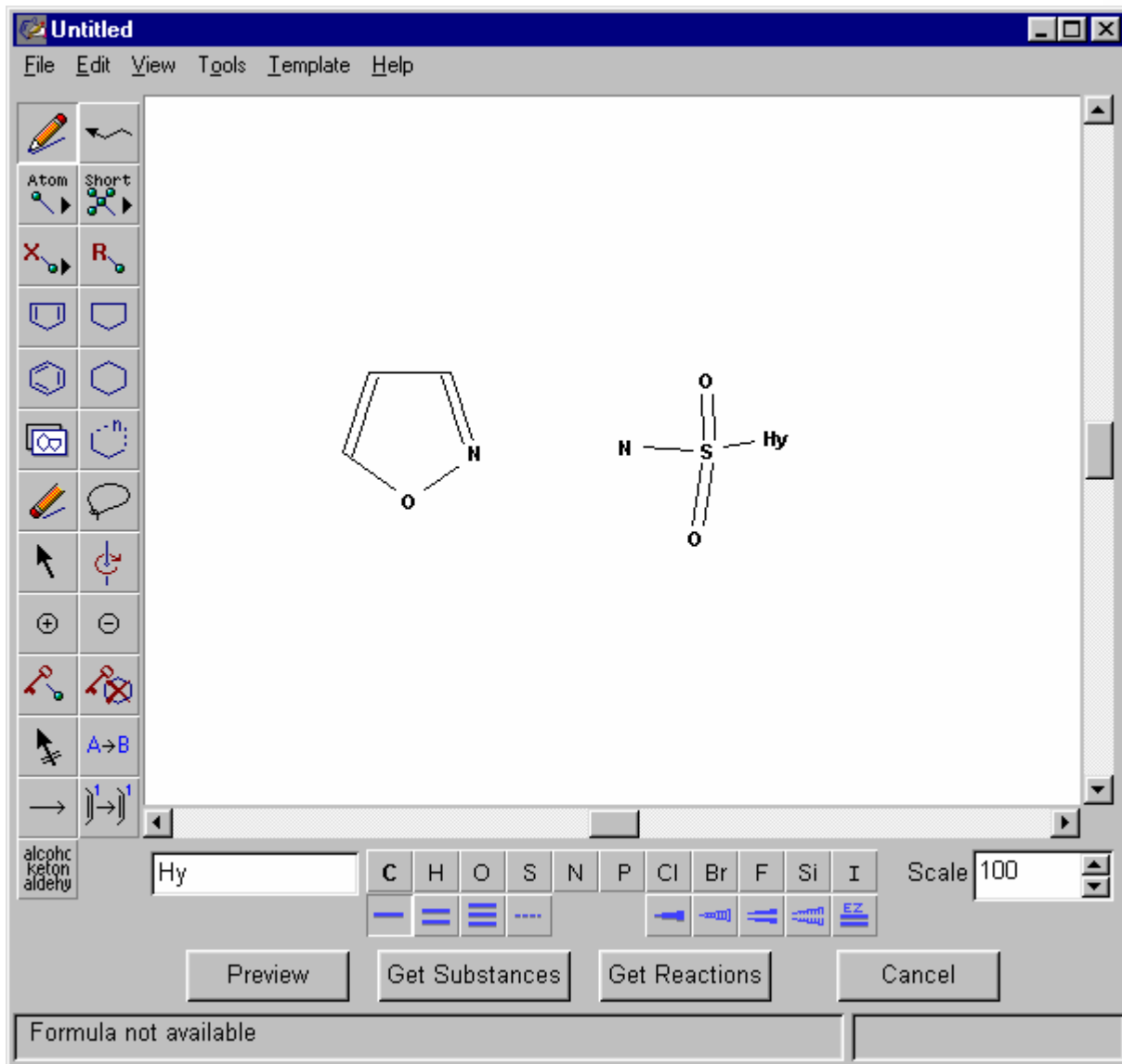
Suchbeispiel 2

Verbindungen mit folgenden Strukturfragmenten



sind in vielen Endothelin Receptor-A Antagonisten vorhanden.

Welche Verbindung aus Registry hat diese Strukturfragmente und passende Eigenschaften um als Wirkstoff verwendet zu werden?





469911-85-1

• Na

~1 Reference
REGISTRY

469911-84-0

469911-83-9

• Na

Analyze or Refine

Refine by Chemical Substance

Select

Refine by:

- Chemical Structure
Limit results using a chemical structure.
- Commercial Availability
Limit to commercially available substances.
- Property Data
Limit results by property values.

8.91
LogP
pKa

Cancel

469911-82-8

Get References

Analyze or Refine Substances

Back



Eingrenzen mit den phys. Eigenschaften

- Voreinstellung Lipinski
“rule of 5”
- Bereich der Eigenschaft
eingeben
- Substanzen die keine phys.
Eigenschaften in Registry
haben können
aufgenommen oder
ausgegrenzt werden

Refine by Property

Select one or more Properties of interest.
Then enter the appropriate values for each property.
For more information about properties, click [here](#).

Hydrogen Donors
0 to 5
Min:0 Max:>=20

Hydrogen Acceptors
0 to 10
Min:0 Max:>=20

Molecular Weight
0 to 420
Min:0 Max: no limit

logP
-10 to 5
Min:-10 Max:10

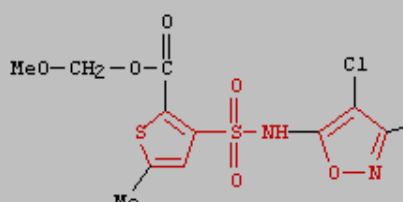
Freely Rotatable Bonds

Include substances with no value for the specified properties

OK Change Preferences Back

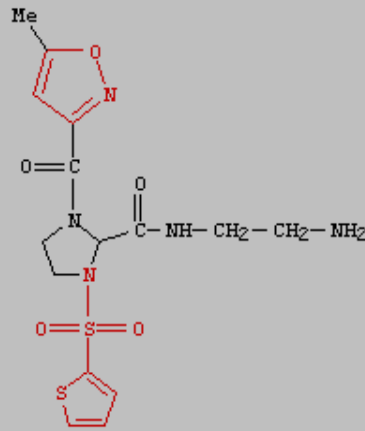


446063-95-2



~1 Reference
REGISTRY

441324-53-4



No References

Get References

Retrieve references for:

All substances Selected substances

For each substance, retrieve:

All references References associated with:

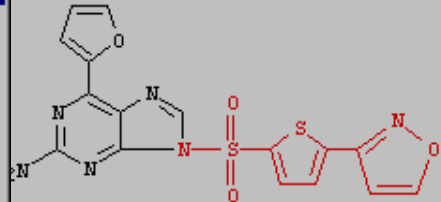
<input type="checkbox"/> Adverse Effect, including Toxicity	<input type="checkbox"/> Occurrence
<input type="checkbox"/> Analytical Study	<input type="checkbox"/> Preparation
<input checked="" type="checkbox"/> Biological Study	<input type="checkbox"/> Process
<input type="checkbox"/> Combinatorial Study	<input type="checkbox"/> Properties
<input type="checkbox"/> Crystal Structure	<input type="checkbox"/> Reactant or Reagent
<input type="checkbox"/> Formation, nonpreparative	<input type="checkbox"/> Spectral Properties
<input type="checkbox"/> Miscellaneous	<input type="checkbox"/> Uses

For each **sequence**, retrieve:

Additional related references, e.g., activity studies, disease studies. For more detail, click [here](#).

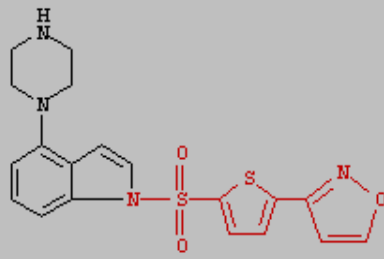
OK Back

442884-35-7



Reference
REGISTRY

444-35-8



References
REGISTRY

Get References

Analyze or Refine Substances

Back





- Wu, Chengde; Blok, Natalie; Patricia, Woodard Timothy; Keller, Karin; Woodard, Patricia. **Preparation of heterocyclic sulfonamides for treatment of endothelin-mediated disorders.** U.S. (2002), 65 pp., Cont.-in-part of U.S. 6,248,767. CODEN: USXXAM US 6432994 B1 20020813 CAN 137:154844 AN 2002:610408 CAPLUS
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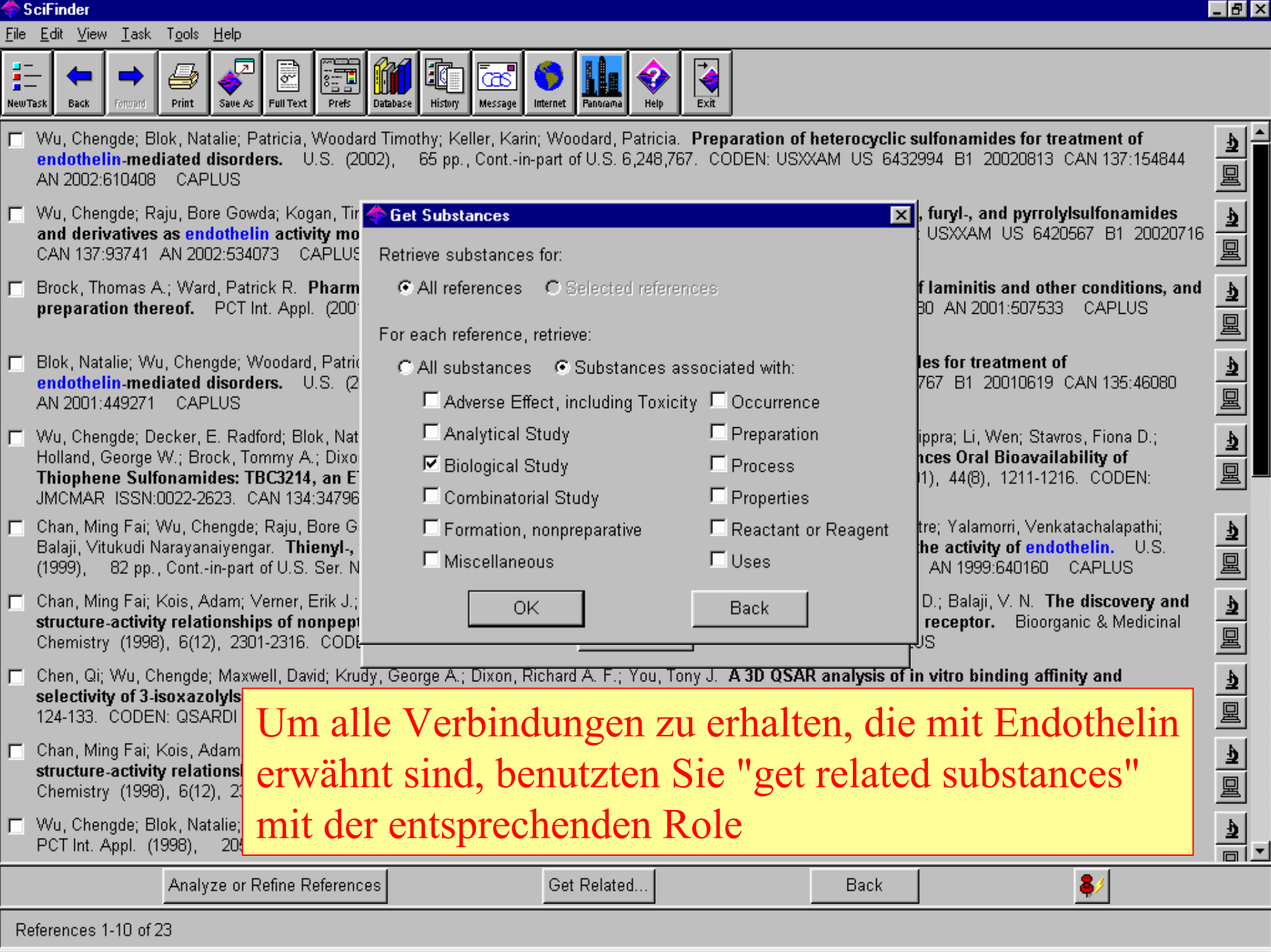
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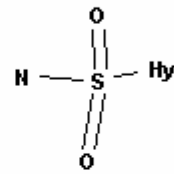
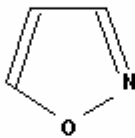


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Zusammenfassung

- SciFinder Scholar kann jetzt stereoselektiv suchen
- Registry enthält viele berechnete und experimentelle phys. Eigenschaften, die sonst nicht zu finden sind
- Die Suche nach Strukturen (Elementen einer Struktur) kann mit einer Textsuche und der Suche nach bestimmten Eigenschaften verknüpft werden

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