SciFinder®
SCHOLAR
2002

Stereochemie und Substanzeigenschaften

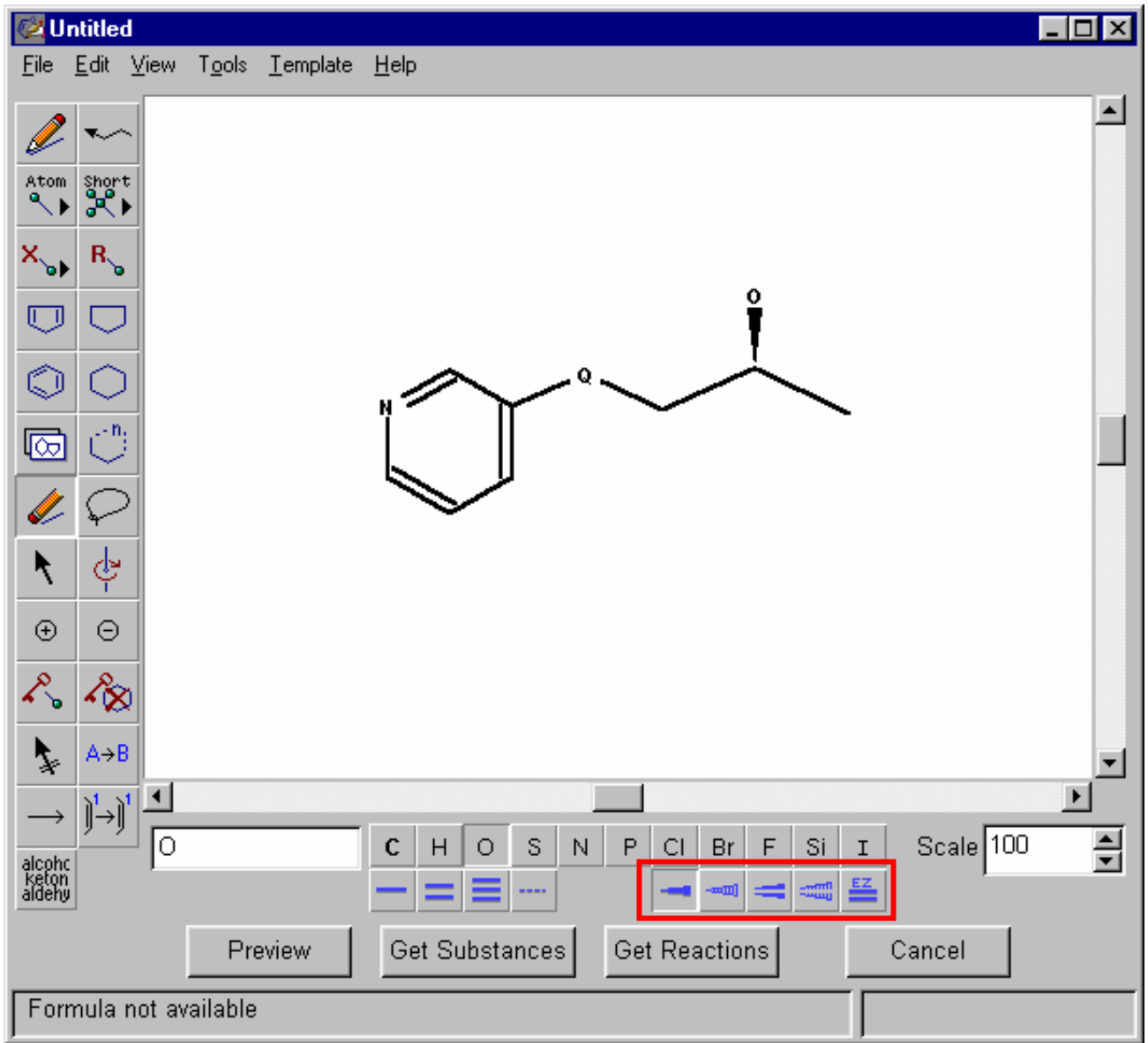
Strukturen in SciFinder

- 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 zusatzliche Stereozentren bilden, die ebenfalls als Hits angezeigt werden

Suche nach einem Stereoisomer



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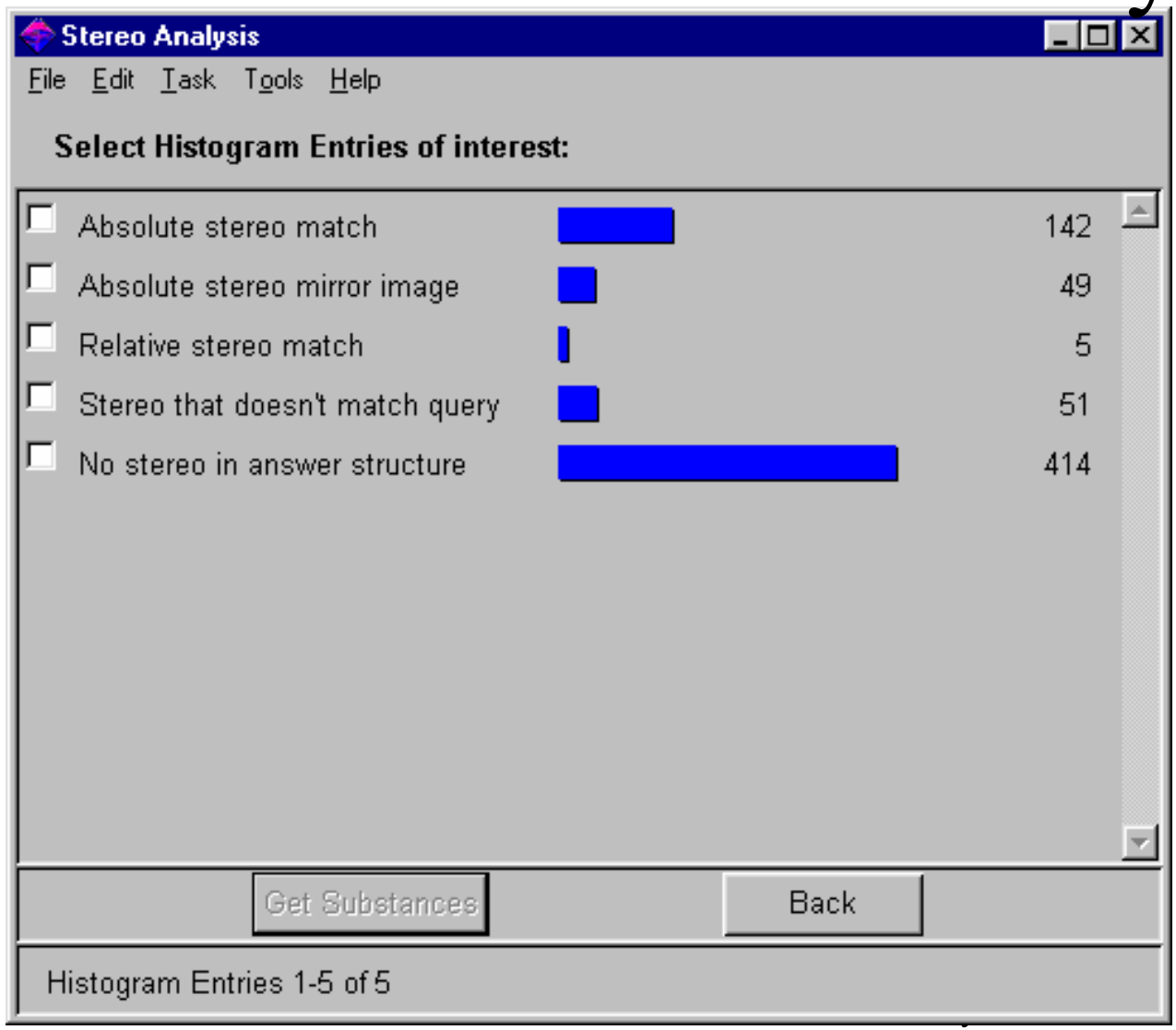
Automatische Stereoanalyse



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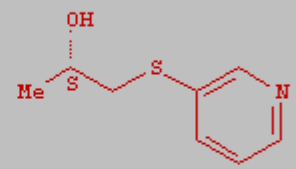
"Absolute stereo" Hits

Registry Number: 464934-51-8

Absolute stereochemistry. Rotation (+).



Formula: C8 H11 N O S

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

- 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.

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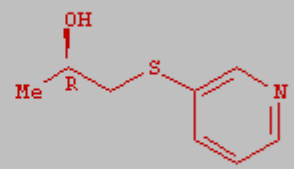
"Absolute stereo mirror image"

Registry Number: 464934-61-0

Absolute stereochemistry. Rotation (-).



Formula: C8 H11 N O S

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

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

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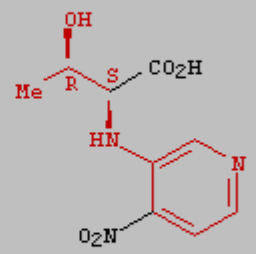
"Relative stereo answers"

Registry Number: 13505-15-2

Relative stereochemistry.



Formula: C9 H11 N3 O5

CA Index Name: Threonine, N-(4-nitro-3-pyridyl)-, DL- (8CI)

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

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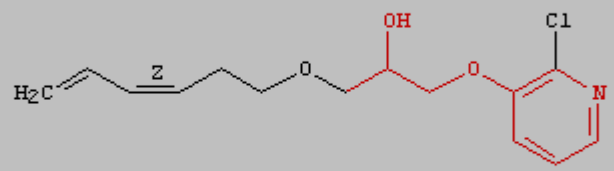
"Stereo answers not matching"

Registry Number: 383901-31-3

Double bond geometry as shown.



Formula: C14 H18 Cl N O3

CA Index Name: 2-Propanol, 1-[(2-chloro-3-pyridinyl)oxy]-3-[(3Z)-3,5-hexadienyloxy]- (9CI)

- 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.

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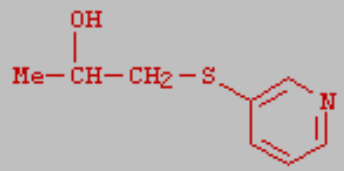
"No stereo in answer structure"

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.

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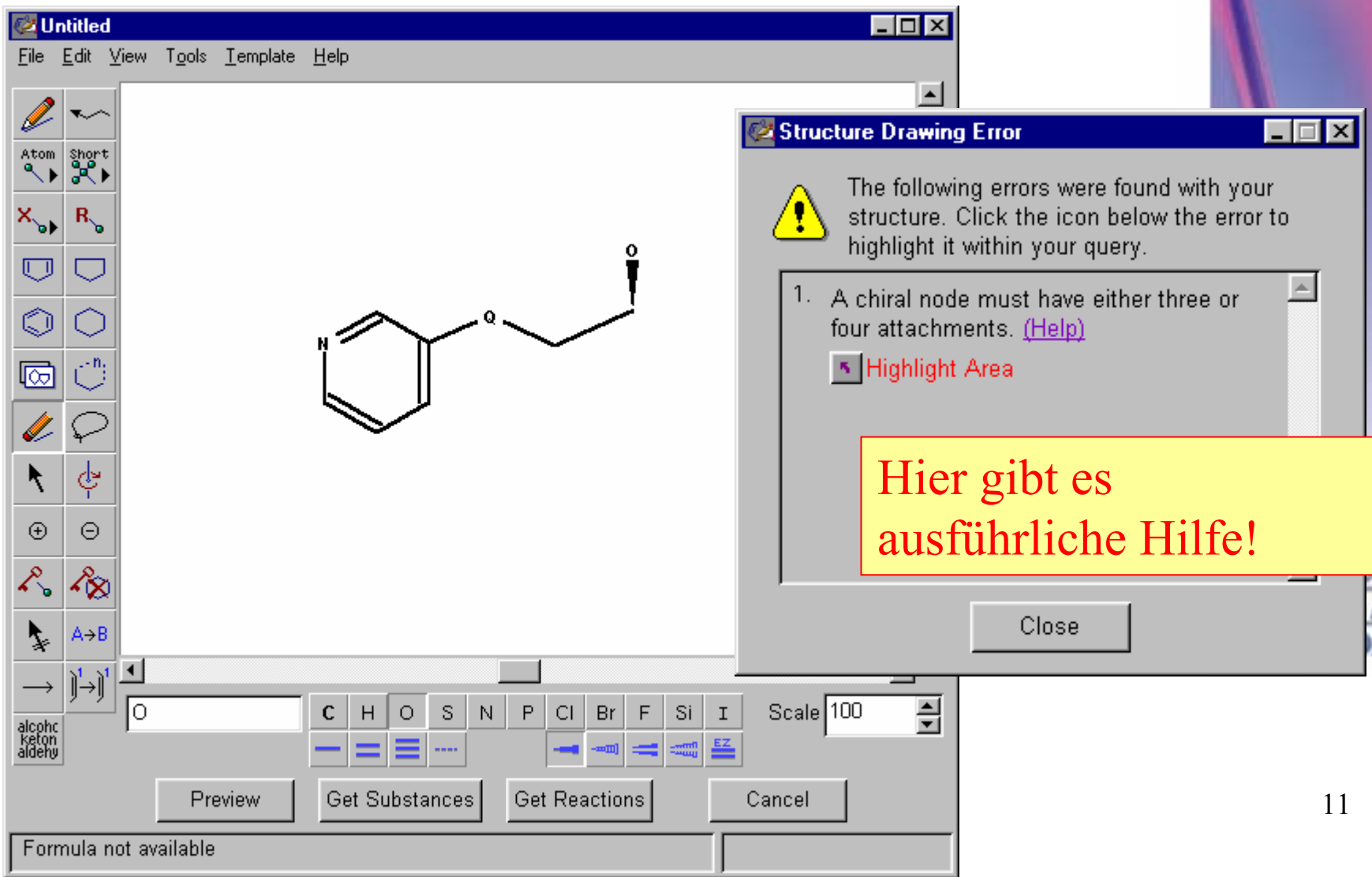
Zeichnen der Stereochemie

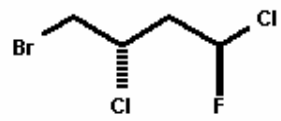
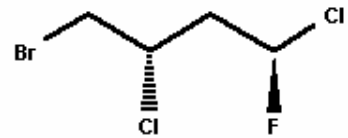
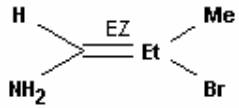
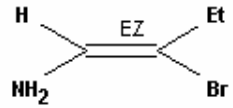
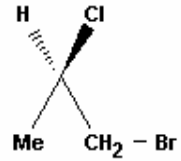
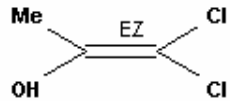
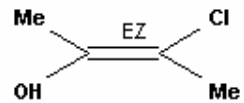


Contents | Index | Search

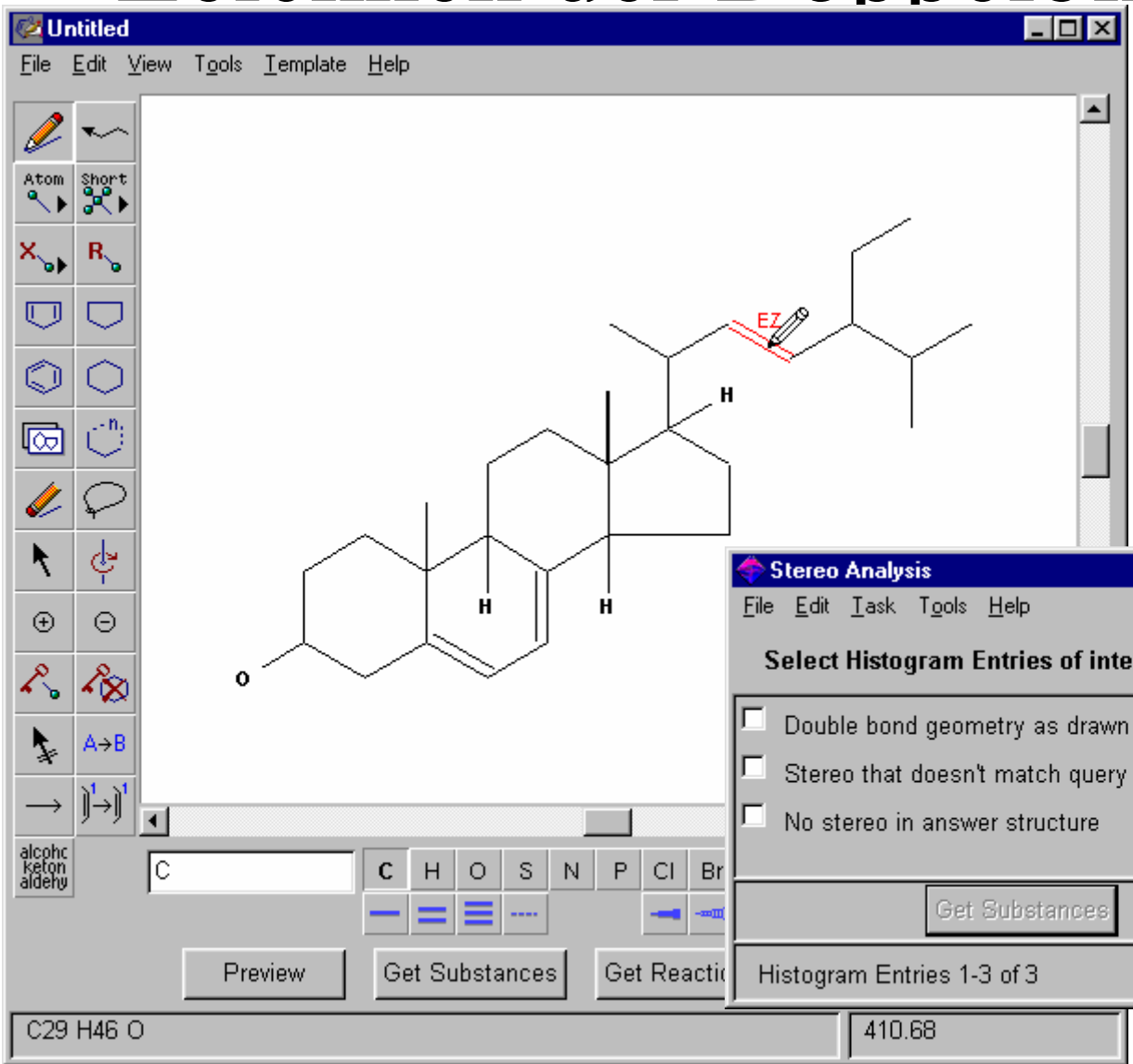
- USING SCIFINDER
- PERFORMING TASKS
  - Begin a Search
  - Set the Display Format for Your Curren
  - Understanding Your Explore Results
  - Explore by Chemical Substance or Rea
    - Explore by Chemical Substance or R
    - Explore by Chemical Structure
      - Access Explore by Chemical Struc
      - Exact vs. Substructure Searching
      - How Explore by Chemical Structur
      - 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
        - Import a Structure Query
        - Moving Structures or Structure Fr
        - Prohibiting Substitution or Fusio
        - Check for Overlapping Nodes
        - Check Valencies in Your Structu
        - Tips for Modifying a Structure
        - Draw a Reaction
        - Explore by Functional Group
    - Previewing Structures
    - Searching Structures
  - Explore by Substance Identifier

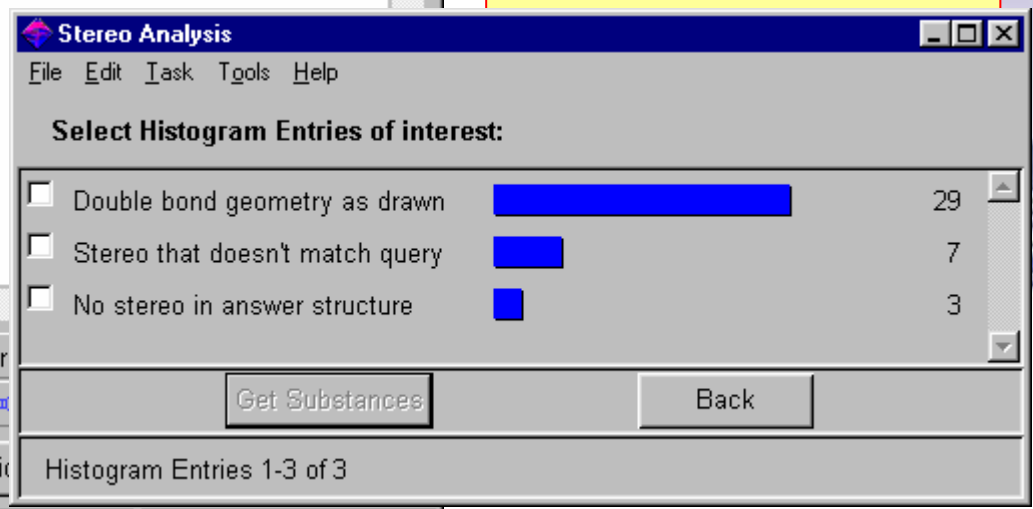
Structure Drawing Errors

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.	 R_1 = C, N, Si	
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

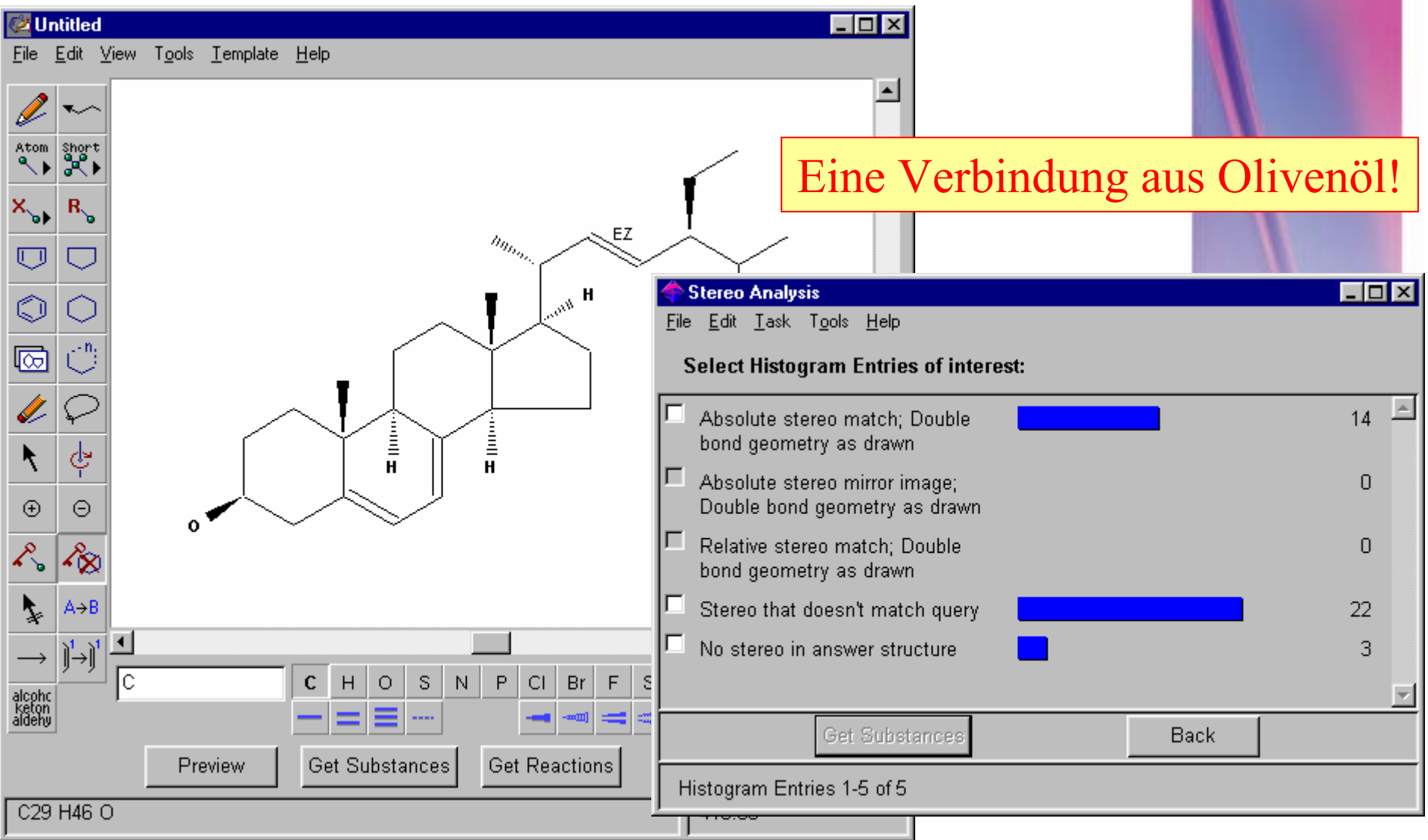
Zeichnen der Doppelbindung





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

Mehrere Stereozentren



Eine Verbindung aus Olivenöl!

Strukturen und Eigenschaften

- In CAS Registry finden Sie berechnete Eigenschaften für 13 Mio. einfache organ. Verbindungen. (ACD Labs)
- In CAS Registry finden Sie experi-mentell 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

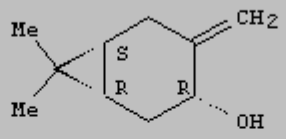
Registry ist inzwischen auch eine grosse Quelle für phys. Eigenschaften

	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	-	-	-

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-, (

Other Names: 3(10)-Caren-4-ol, (1S,4R,6R)-(-)- (8CI); Bicyclo[4.1.0]h
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

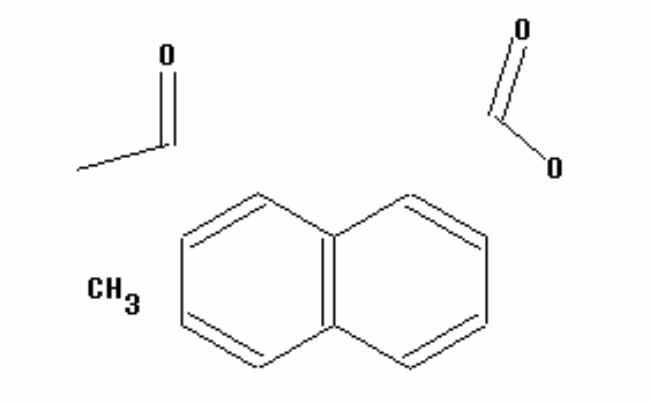
Property	Experimental Value	Condition	Note
Boiling Point	40-50 °C	Press: 0.5 Torr	(2) IC
Melting Point	53-54 °C		(2) IC
Optical Rotatory Power	-119.8°	Conc: 2.47 g/mL Solv: chloroform (67-66-3) Temp: 20 °C	(2) IC

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

SciFinder is
the Ameri

Ein Suchbeispiel:

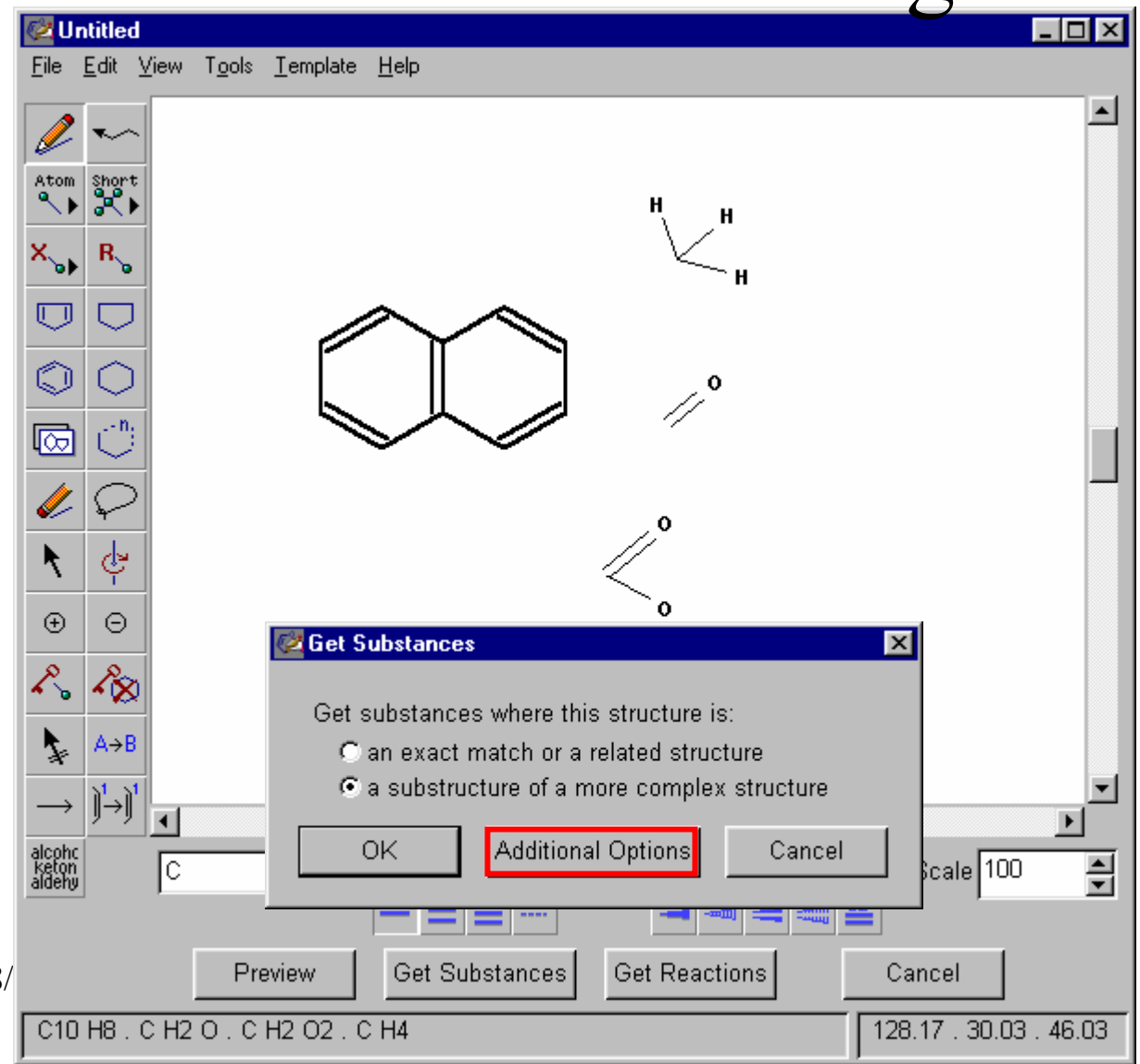
Die Analyse einer Verbindung hat ergeben, dass sie folgende Stukturelemete enthält:



Die Verbindung schmilzt bei 165-170ºC. Das Semicarbazon schmilzt bei 212ºC.

Was ist die Struktur der Verbindung?

Substruktursuche mit Fragmenten



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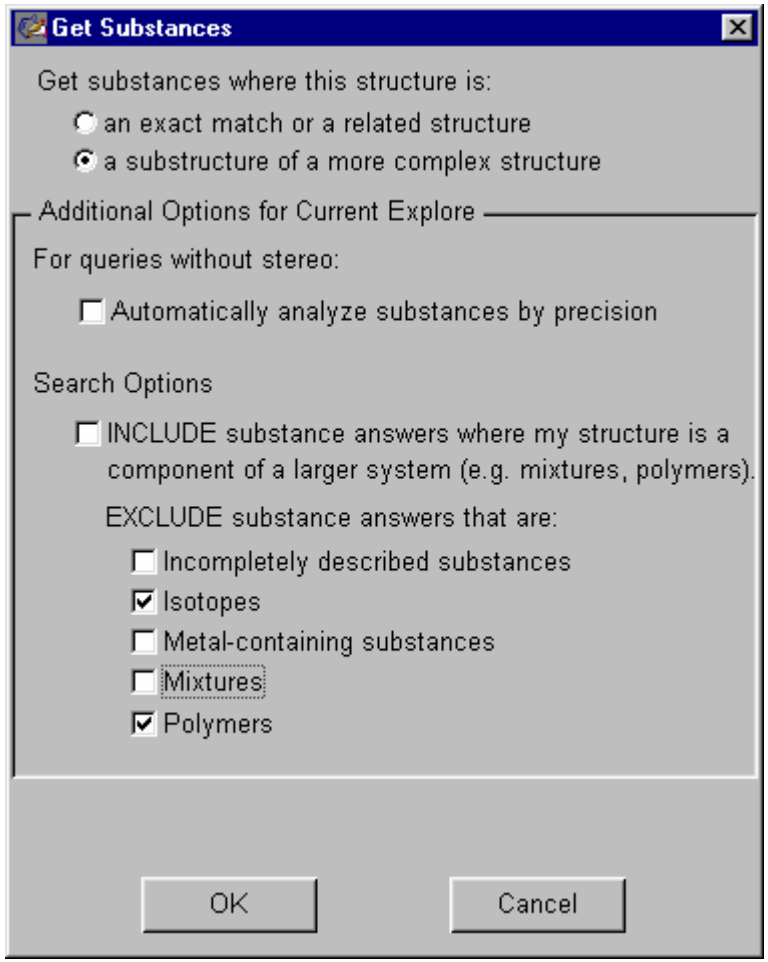
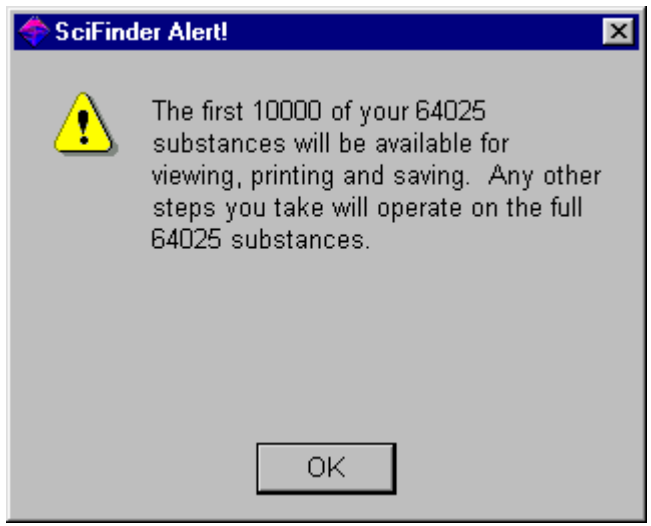
Unerwünschte Substanzen ausschließen:



Die Einstellungen gelten nur für die aktuelle Suche!



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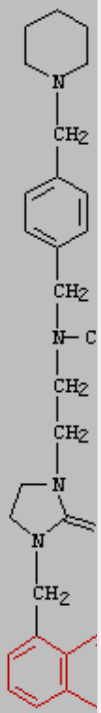
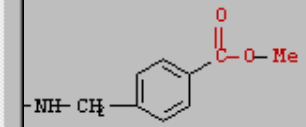
New Task | Back | Forward | Print | Save As | Full Text | Prefs | Database | History | Message | Internet | Panorama | Help | Exit

471929-48-3

Component Number 1



Component Number 2



Untitled

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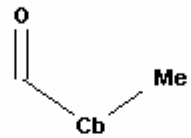
Atom | Short | R | A→B | alcohc keton aldehy



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

O | C | H | O | S | N | P | Cl | Br | F | Si | I | Scale 100

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Formula not available

Get References | Analyze or Refine Substances | Back

Substances 1-3 of 64025

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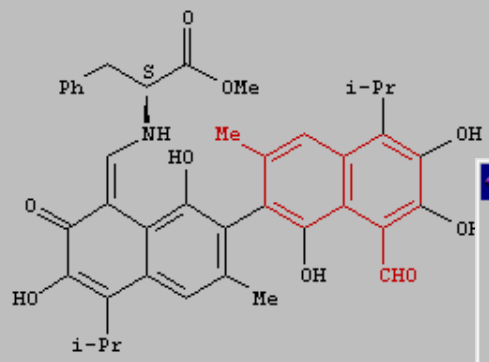
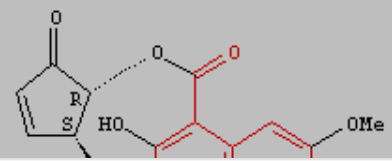
471925-55-0

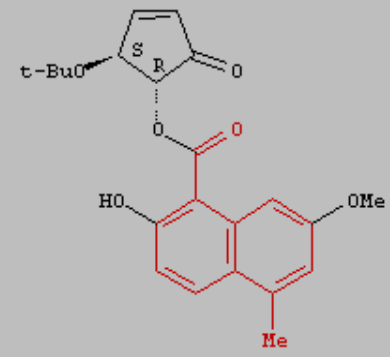


~1 Reference
REGISTRY

471254-33-8

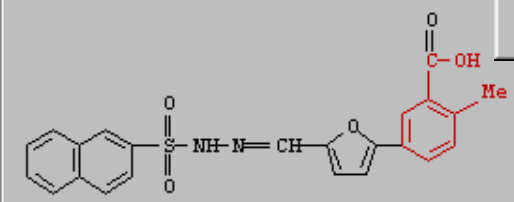


471254-32-7

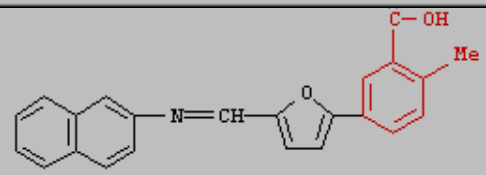


-1 Reference
REGISTRY

470673-82-6



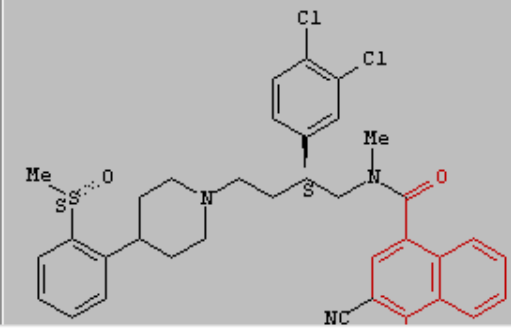
No References
REGISTRY



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.

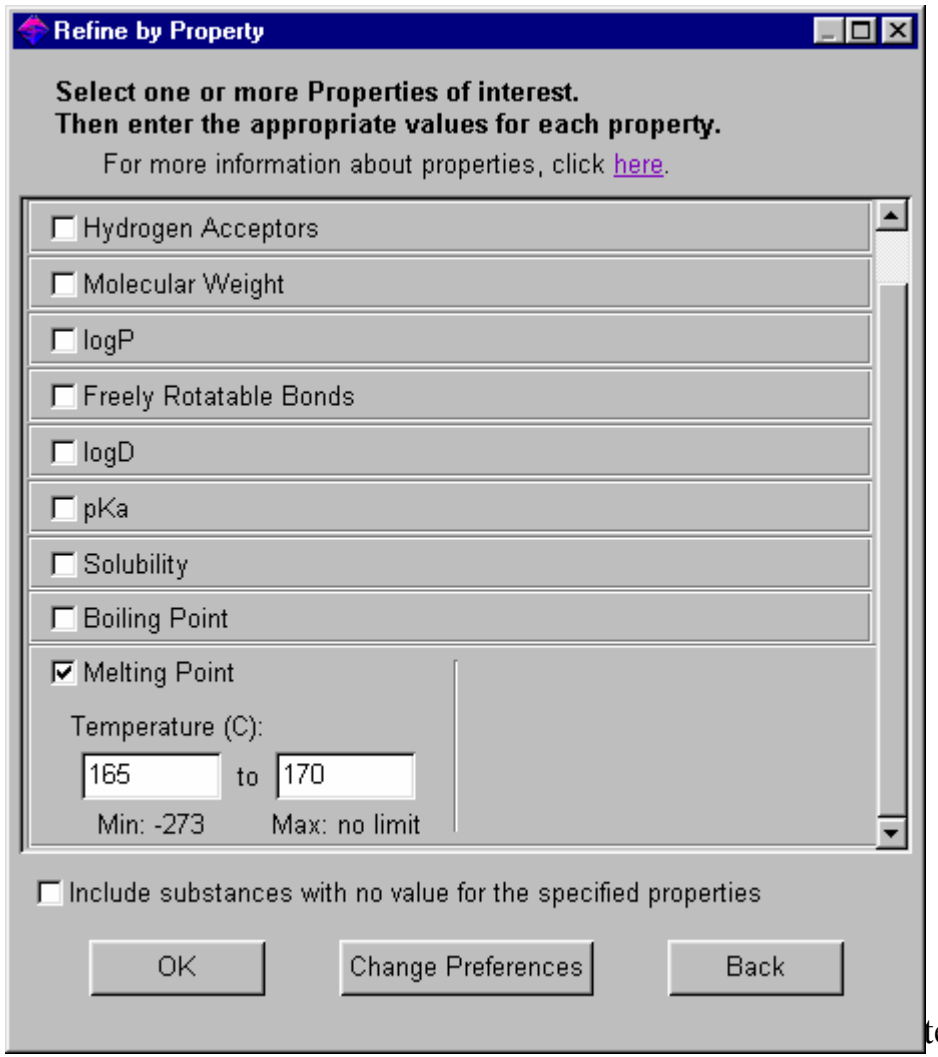
Property Data
Limit results by property values.

Cancel

Get References | Analyze or Refine Substances | Back

Substances 1-6 of 1674

Eingrenzen auf den Schmelzpunkt:



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

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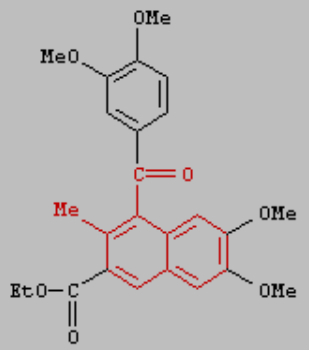
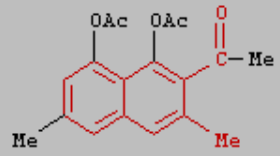
128981-46-4



~1 Reference
REGISTRY

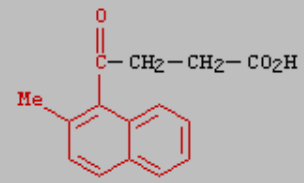
89586-46-9



~1 Reference
REGISTRY

Das Semicarbazon dieser Verbindung hätte folgende Summenformel C19H21N3O5

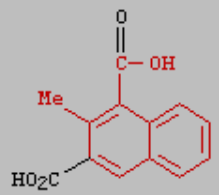
78540-11-1



~1 Reference
REGISTRY

Das Semicarbazon dieser Verbindung hätte folgende Summenformel C16H17N3O3

72391-94-7



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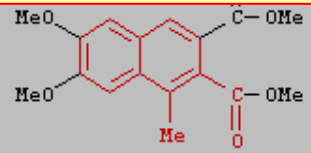

~3 References
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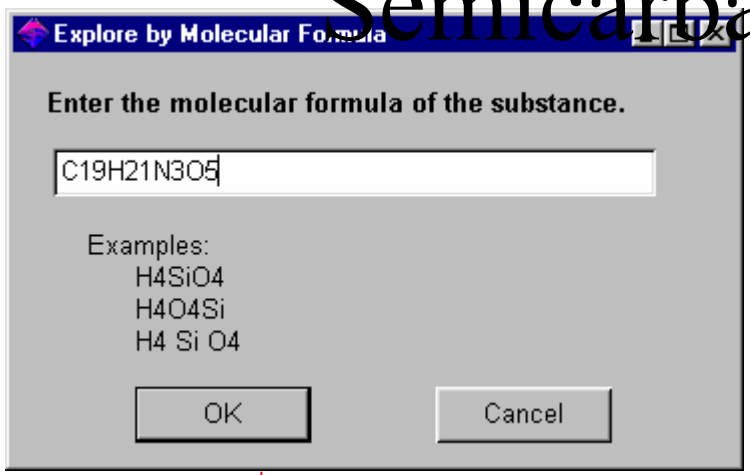
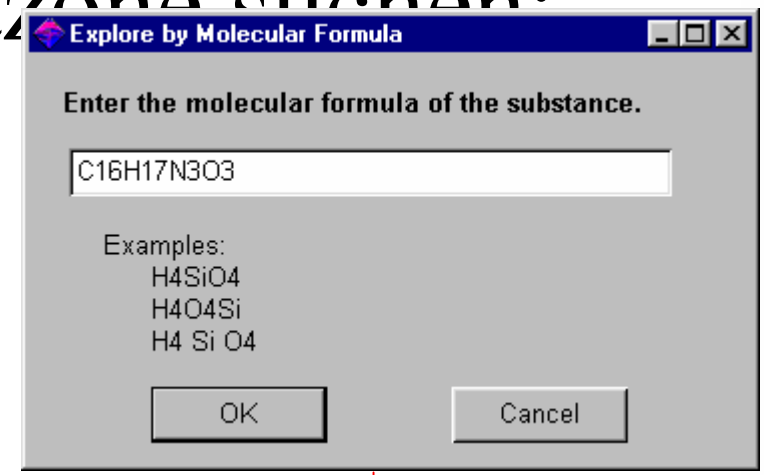
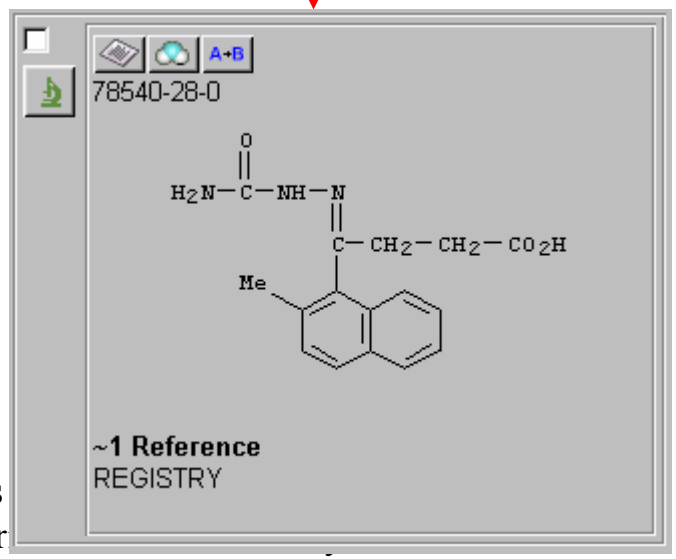
Substances 1-5 of 5

Summenformel der Semicarbazone suchen:



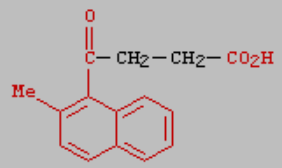


Nicht beschrieben



Die gesuchte Verbindung:

Registry Number: 78540-11-1



Formula: C15 H14 O3

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

-- **Properties** --

Calculated

Property	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

Experimental

Property	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

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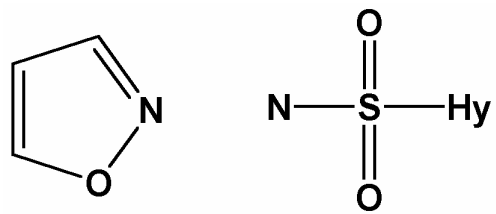
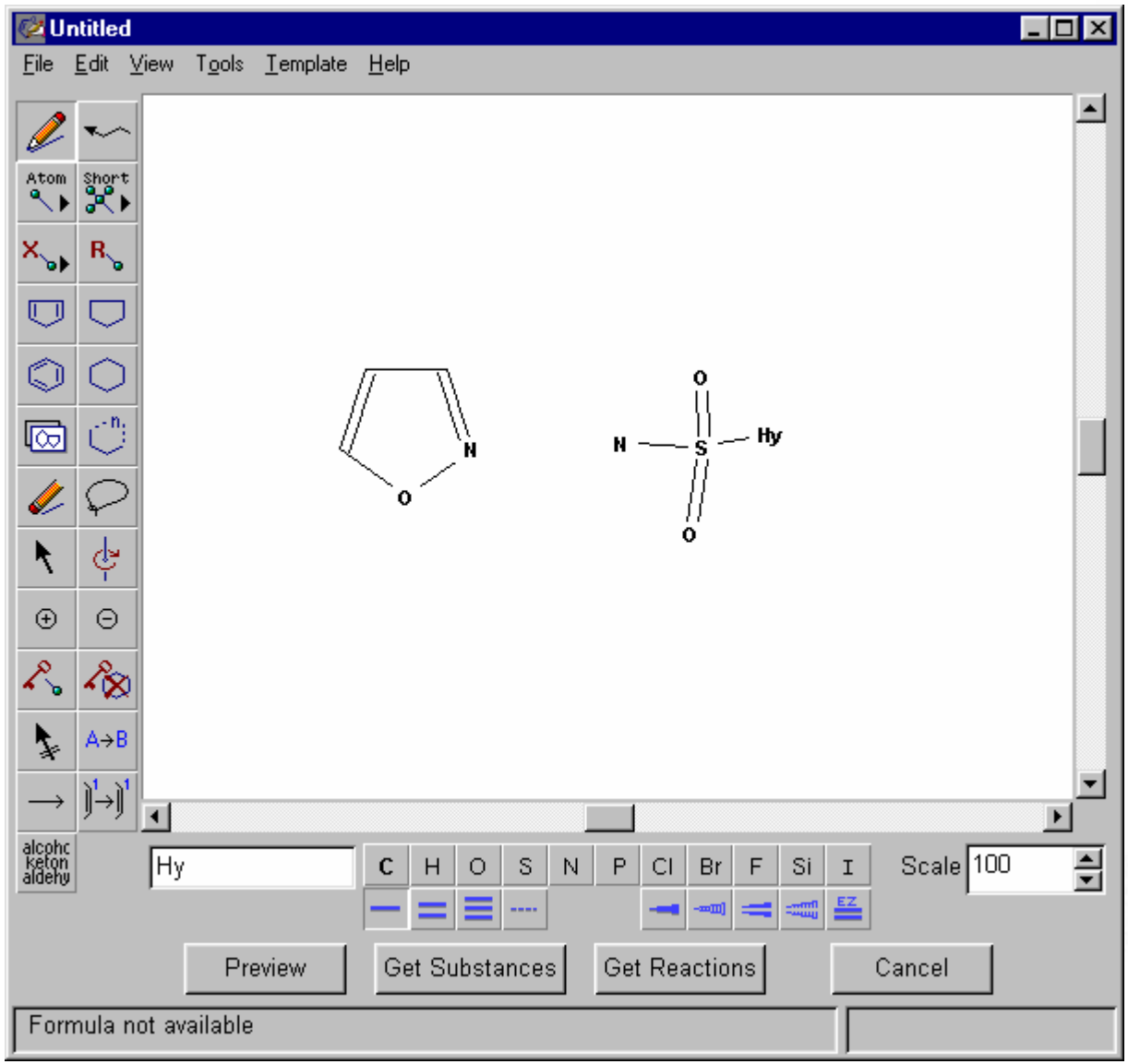
Suchbeispiel 2

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?



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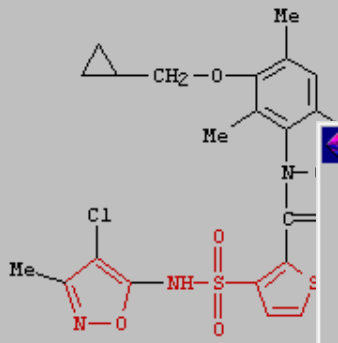

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REGISTRY

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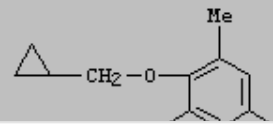

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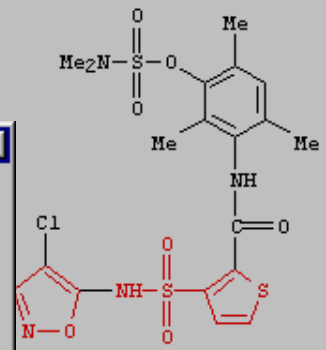

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Data.

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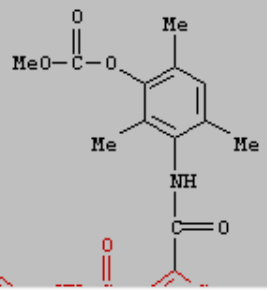
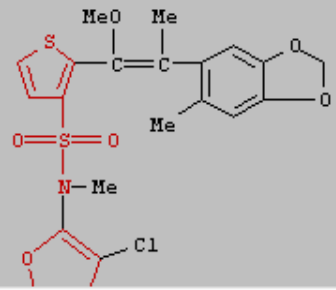
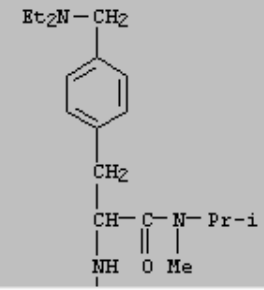
469911-82-8







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8.91 LogP pKa
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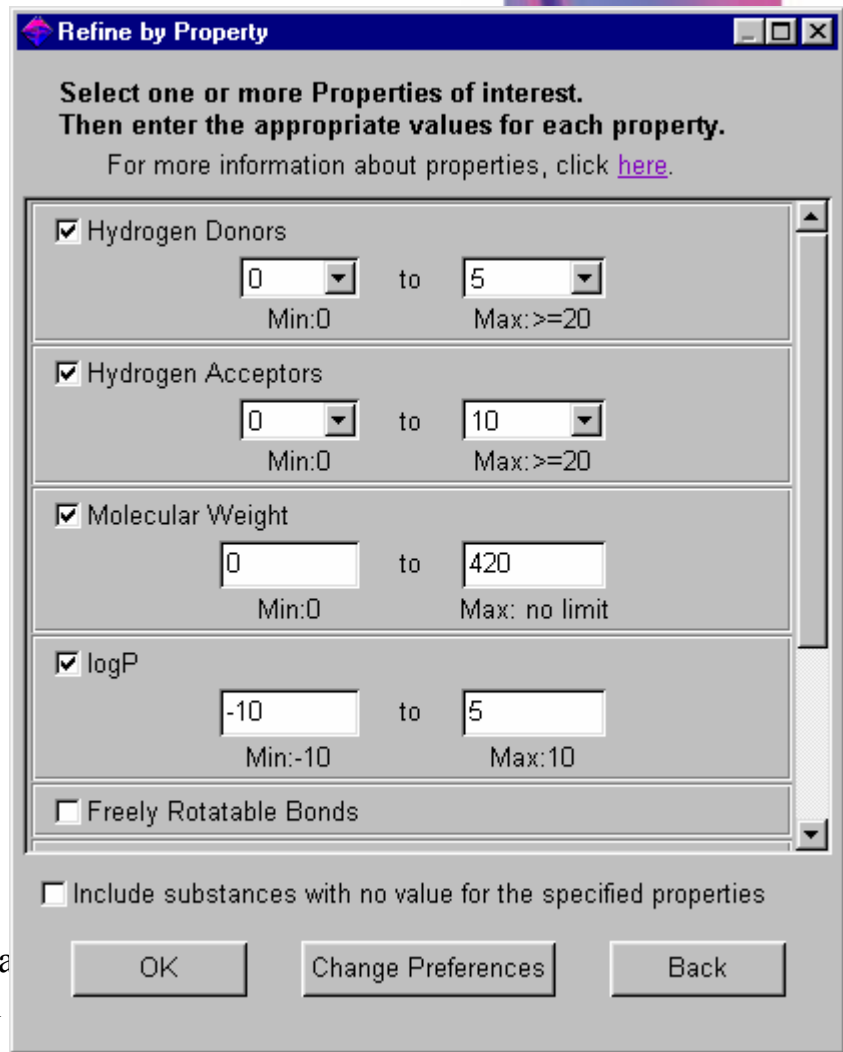
Substances 1-6 of 1922

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



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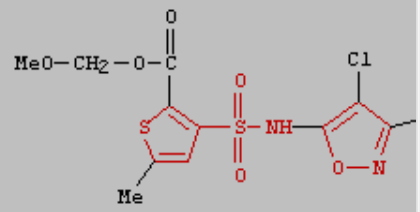

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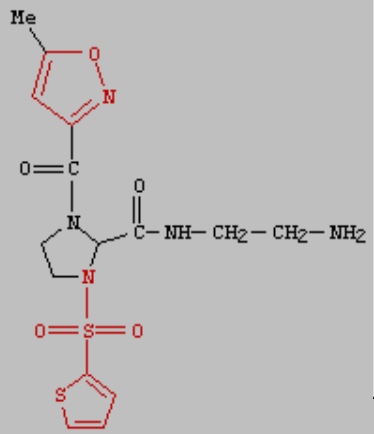

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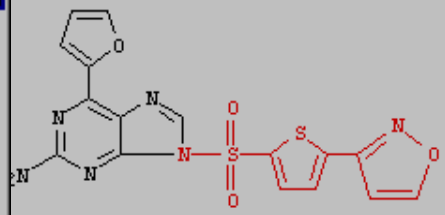
84-35-7



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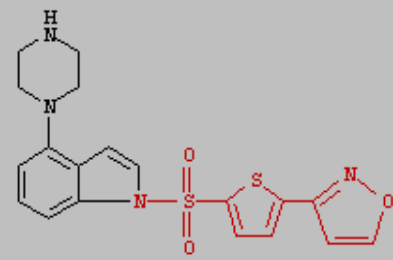

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- [x] Biological Study
- [ ] Combinatorial Study
- [ ] Crystal Structure
- [ ] Formation, nonpreparative
- [ ] Miscellaneous
- [ ] Occurrence
- [ ] Preparation
- [ ] Process
- [ ] Properties
- [ ] Reactant or Reagent
- [ ] Spectral Properties
- [ ] Uses

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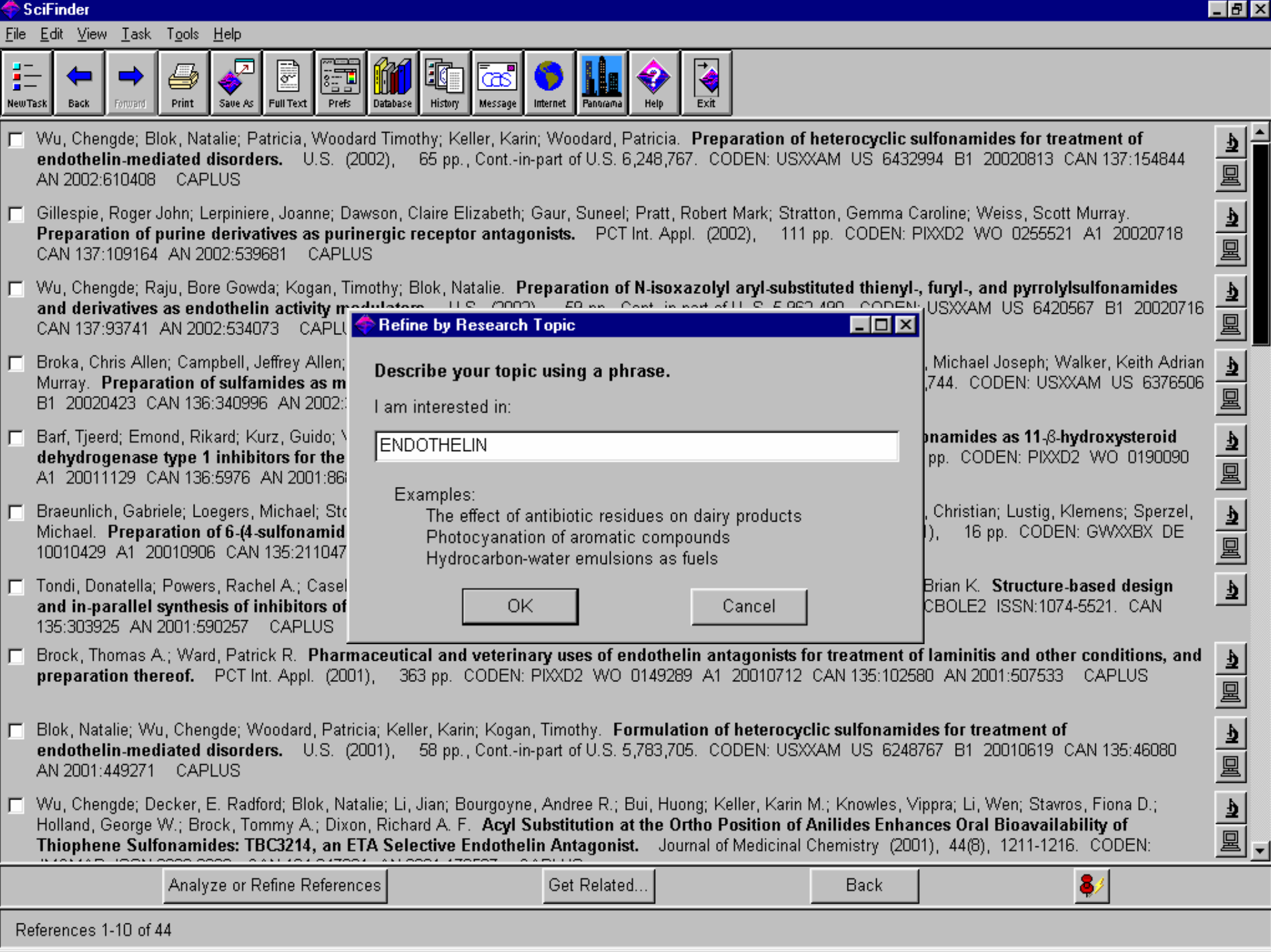
Substances 1-6 of 261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Wu, Chengde; Blok, Natalie; Patricia, Woodard Timothy; Keller, Karin; Woodard, Patricia. Preparation of heterocyclic sulfonamides for treatment of endothelin-mediated disorders. U.S. (2002), 65 pp., Cont.-in-part of U.S. 6,248,767. CODEN: USXXAM US 6432994 B1 20020813 CAN 137:154844 AN 2002:610408 CAPLUS
Gillespie, Roger John; Lerpiniere, Joanne; Dawson, Claire Elizabeth; Gaur, Suneel; Pratt, Robert Mark; Stratton, Gemma Caroline; Weiss, Scott Murray. Preparation of purine derivatives as purinergic receptor antagonists. PCT Int. Appl. (2002), 111 pp. CODEN: PIXXD2 WO 0255521 A1 20020718 CAN 137:109164 AN 2002:539681 CAPLUS
Wu, Chengde; Raju, Bore Gowda; Kogan, Timothy; Blok, Natalie. Preparation of N-isoxazolyl aryl-substituted thienyl-, furyl-, and pyrrolylsulfonamides and derivatives as endothelin activity
USXXAM US 6420567 B1 20020716 CAN 137:93741 AN 2002:534073 CAPL
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Hydrocarbon-water emulsions as fuels
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onamides as 11-β-hydroxysteroid
pp. CODEN: PIXXD2 WO 0190090
Christian; Lustig, Klemens; Sperzel,
16 pp. CODEN: GWXXBX DE
Brian K. Structure-based design
CBOLE2 ISSN:1074-5521. CAN
Brock, Thomas A.; Ward, Patrick R. Pharmaceutical and veterinary uses of endothelin antagonists for treatment of laminitis and other conditions, and preparation thereof. PCT Int. Appl. (2001), 363 pp. CODEN: PIXXD2 WO 0149289 A1 20010712 CAN 135:102580 AN 2001:507533 CAPLUS
Blok, Natalie; Wu, Chengde; Woodard, Patricia; Keller, Karin; Kogan, Timothy. Formulation of heterocyclic sulfonamides for treatment of endothelin-mediated disorders. U.S. (2001), 58 pp., Cont.-in-part of U.S. 5,783,705. CODEN: USXXAM US 6248767 B1 20010619 CAN 135:46080 AN 2001:449271 CAPLUS
Wu, Chengde; Decker, E. Radford; Blok, Natalie; Li, Jian; Bourgoyne, Andree R.; Bui, Huong; Keller, Karin M.; Knowles, Vippra; Li, Wen; Stavros, Fiona D.; Holland, George W.; Brock, Tommy A.; Dixon, Richard A. F. Acyl Substitution at the Ortho Position of Anilides Enhances Oral Bioavailability of Thiophene Sulfonamides: TBC3214, an ETA Selective Endothelin Antagonist. Journal of Medicinal Chemistry (2001), 44(8), 1211-1216. CODEN:
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Um alle Verbindungen zu erhalten, die mit Endothelin erwähnt sind, benutzten Sie "get related substances" mit der entsprechenden Role
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References 1-10 of 23

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441786-94-3

~1 Reference
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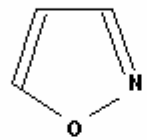
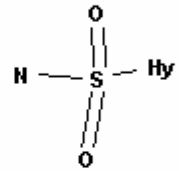
Noch einmal mit der ursprünglichen Anforderung verfeinern:





Atom | Short | alcohc keton aldehy | A→B

C | H | O | S | N | P | Cl | Br | F | Si | I

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Substances 1-6 of 1756

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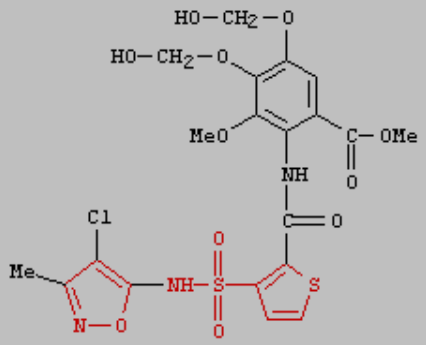

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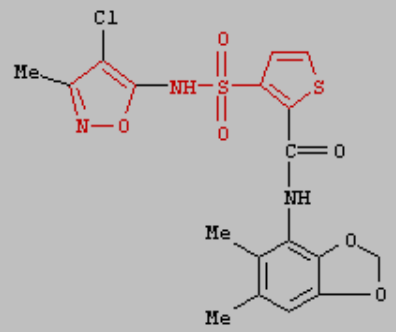

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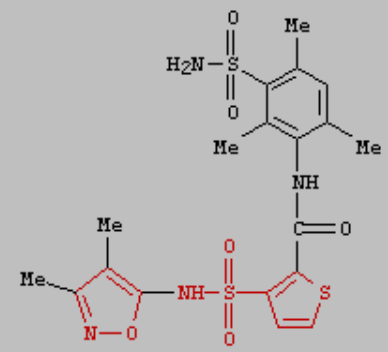

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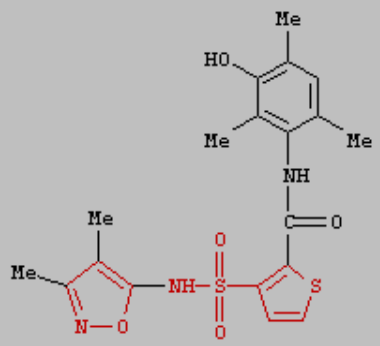

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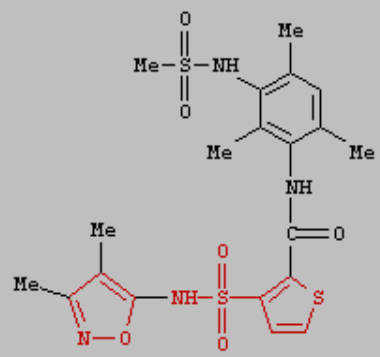

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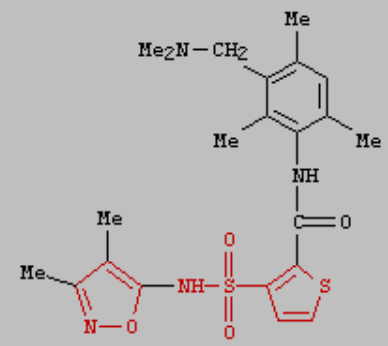

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Substances 1-6 of 1484

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