



STN[®]: Revisiting the Basics of Structure Searching

Goals for this e-seminar include

- Revisit basic to intermediate structure searching tips
- Focus on things that we get many questions about
- Remind you of tools you may not use everyday
- Increase confidence in structure building skills

Agenda

- Closed Substructure Search
- Ring Isolation and Variable Points of Attachment
- Building G-groups with user defined fragments
- Subset Searching
- Searching with text terms-Ring Identifiers

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Structure preparation checklist

- | | |
|--|---|
| <input type="checkbox"/> Search type | <input type="checkbox"/> G-Group |
| <input type="checkbox"/> Ring System –
Fused/Isolated
Variable Nodes | <input type="checkbox"/> Orientation |
| <input type="checkbox"/> Variable Points of
Attachment | <input type="checkbox"/> Block Substitution |
| <input type="checkbox"/> Generic Groups | <input type="checkbox"/> Valency |
| <input type="checkbox"/> Subset Searches | <input type="checkbox"/> Ring Systems –
Specific/Generic |
| <input type="checkbox"/> Text Terms | <input type="checkbox"/> Chain Nodes |
| <input type="checkbox"/> Open Positions | <input type="checkbox"/> Chain Bonds |
| | <input type="checkbox"/> Ring Bonds |

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Don't forget about previously recorded
e-Seminars for additional information



SCIENTISTS SERVING SCIENCE



STN: Advanced Structure Search Techniques, Ring Information	Structure Techniques
STN: Advanced Structure Searching with Filters/Screens	Structure Techniques
STN: Organometallics and Coordination Compounds	Structure Techniques
STN: Stereochemistry in the CAS Registry File	Structure Techniques
STN: Structure and Substructure Searching Tips	Structure Techniques

<http://casevents.webex.com>

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Agenda

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Closed Substructure Search (CSS)

- Substructure search (SSS) is broadest type of search
 - Allows for substitution at any open valent positions
- CSS is a special type of SSS
 - Isolates all rings
 - Automatically puts H's at open nodes, UNLESS the position is OPENED for substitution
- Use CSS when
 - You want to build a query with variable nodes such as G-groups or generic variables
 - Only want substitution in a FEW places

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Features of CSS

- Automatically
 - Blocks substitution at all open sites
 - Isolates any rings in the structure
- Allows for
 - STN-defined variable groups
 - Variable points of attachment
 - Repeating groups
 - Excluded atoms
 - Variable bonds

A CSS search requires planning at the query construction stage, as you draw the structure.

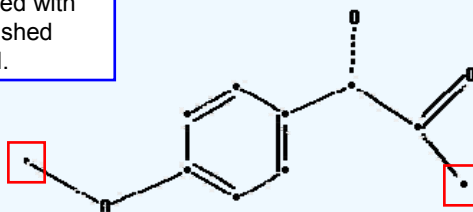
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CSS search

Search Question: Locate substances that meet the following requirements:

Substitution is desired only at the terminal carbon atoms marked with red boxes. The O on the dashed bond can be carbonyl or OH.



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Search Strategy

For creating and searching a CSS query

- Step 1. Build the structure in STN Express®
- Step 2. Open sites for substitution by setting Non-Hydrogen attachments to **Minimum 1**
- Step 3. Logon to STN and enter CAS REGISTRYSM
- Step 4. Search the structure as a closed substructure search (CSS)

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Open sites for substitution by using Non-H attachments

The unspecified bond is used to pick up any bond variation in the answers.

To open a site for substitution:
Right mouse click on the node.
Choose Non-H attachments from the pop-up menu.

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Set Non Hydrogen Attachments to MINIMUM 1

Non Hydrogen Attachments (Connectivity)

Specific Any

Exact Chain

Minimum Ring

Maximum Ring/Chain

Mixture

Count (0 to 16):

Cancel OK

Set Non-H attachments to MINIMUM 1.
The selected node is *already* attached to 1 other atom, so it is open to accept any other substitution.
Repeat for any additional atom nodes.

Run the CSS search

```
=> FILE REG
Uploading C:\Program Files\...
L1      STRUCTURE UPLOADED

=> S L1 CSS SAM
L2 ...
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**

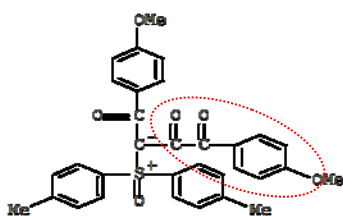
=> S L1 CSS FULL
L3      83 SEA CSS FUL L1
```

As a comparison, an SSS search of the same structure retrieved 246 answers.

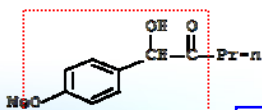
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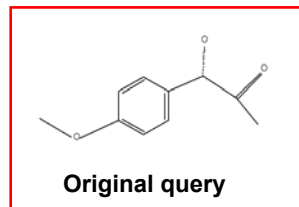
Answers from the CSS search are only substituted at the terminal ends of the query



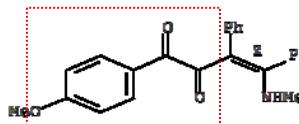
42888-20-0



856339-78-1



Original query



68114-52-3

Use CSS when:
Flexibility is desired i.e., variable nodes, bonds,
or G-groups, but substitution is limited.

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Agenda

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Ring Isolation and Variable Points of Attachment on Rings

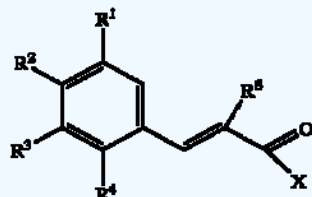
- Ring Isolation controls whether a ring can have additional rings fused to the ring structure drawn
- Variable Points of Attachment (VPA) allows for substituents to “float” on a ring system instead of being attached at a fixed position

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Search Question: Search for preparations of a polyhalogenated cinnamic acid (or its derivatives) having the structure shown below

R1, R2, R3 and R4 are identical or different and represent H, F, Cl, or Br, at least two of them are not H.



Note: For the purpose of this next section, we will ignore the R⁵ and X variables in the structure.

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The strategy

- The ring should be isolated to prevent retrieval of polycyclic rings on the C6 ring
- Use the X (halogen) variable group to represent F, Cl, or Br
 - I and At will also be possible answers
- Use two X variables
- Use the Variable Point of Attachment – (VPA) feature to specify that they are attached to the ring

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Isolate the ring by right-clicking on a node in the ring

The screenshot shows the 'Structure Drawing' software interface. A benzene ring is highlighted in pink. A right-click context menu is open over one of the ring nodes, listing options: 'Ring Isolation...', 'Markush Attributes...', 'Node Characteristics...', 'Hydrogen Attachments...', 'Non-H Attachments...', and 'Other Attributes...'. A text box on the left contains the instruction: 'Select Ring Isolation from the pop-up menu. Only one node needs to be changed to isolate the entire ring system.'

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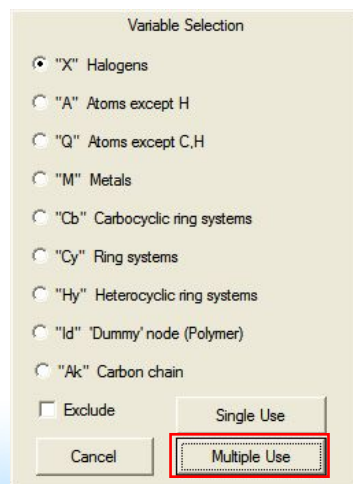
Variables are found under the Draw menu

The screenshot shows the 'Structure Drawing' software interface. The 'Draw' menu is open, and 'Variables...' is selected. Other menu items include 'Bond...', 'Atom...', 'Shortcut...', 'Variable Points of Attachment', 'G-groups... (Ctrl+G)', 'Repeating Group...', 'Delete Repeating Group', 'Chain Superatoms...', 'Ring Superatoms...', 'Other Superatoms...', 'Square Brackets...', and 'Euse Fragment'. The benzene ring in the background is highlighted in pink.

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Select the X variable from the menu

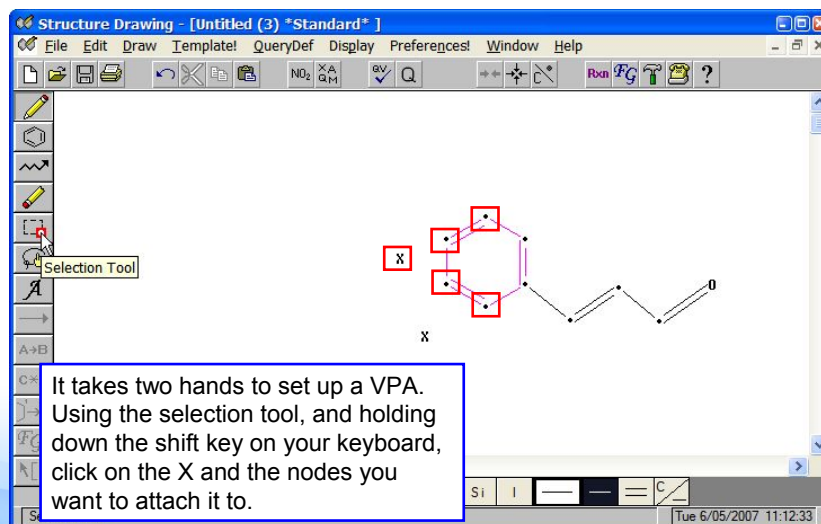


Variables allow you to build generic character into a structure query. The multiple use button will make **X** the default atom until you change it again.

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Use the "red dot" Selection Tool to choose the floating attachments



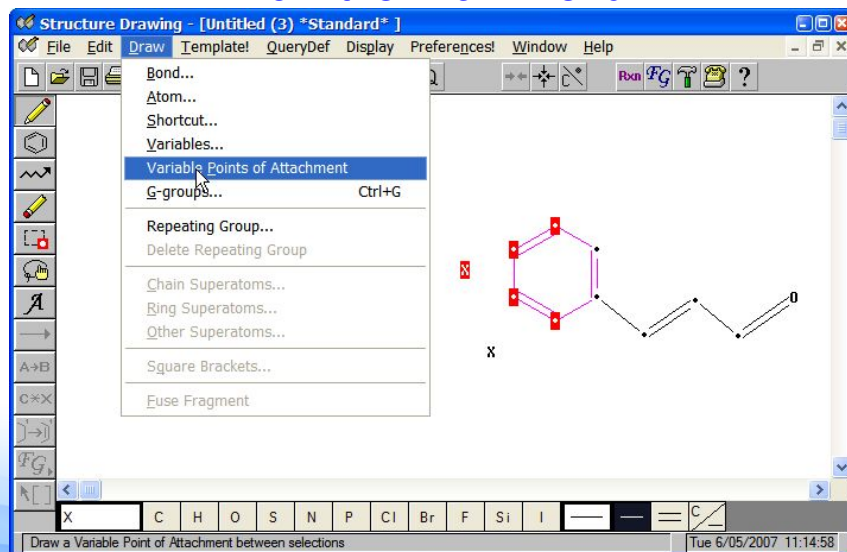
The image shows a screenshot of the 'Structure Drawing' software interface. The main window displays a chemical structure with a variable 'X' and several nodes highlighted with red boxes. A 'Selection Tool' is shown in the toolbar, pointing to one of the red boxes. A text box at the bottom left explains the process of setting up a VPA.

It takes two hands to set up a VPA. Using the selection tool, and holding down the shift key on your keyboard, click on the X and the nodes you want to attach it to.

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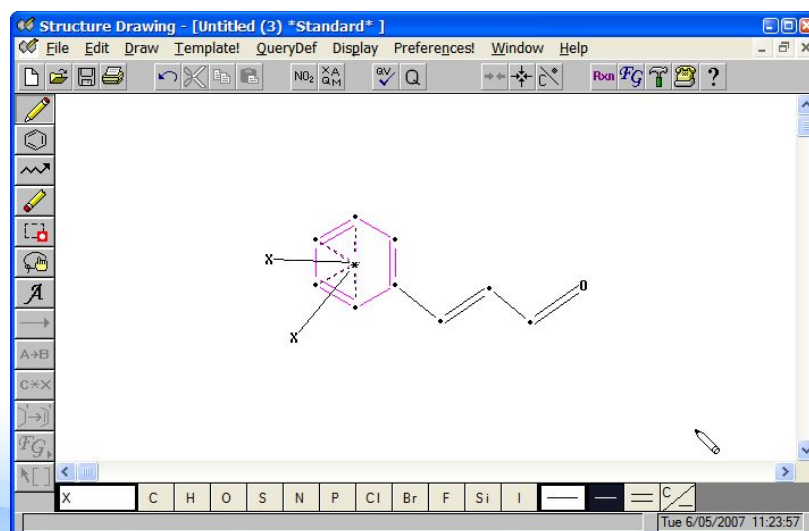
Choose Variable Points of Attachment from the Draw menu



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Repeat for the second X variable

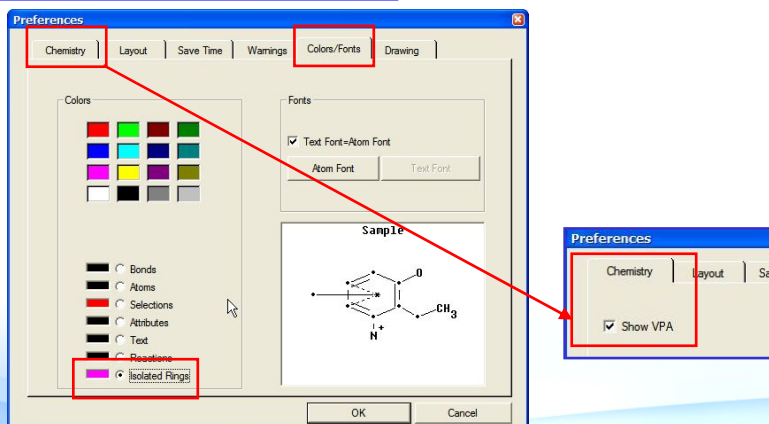


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Set Preferences to see dashed VPA lines or highlight isolated rings in your structure

From the structure drawing window menu, choose **Preferences**.



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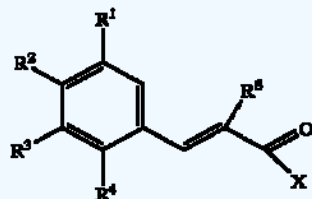
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Revisit the Search Question

Search Question: Search for preparations of a polyhalogenated cinnamic acid (or its derivatives) having the structure shown below

X represents OR^5 or $N(R^6)(R^7)$. R^5 is H or optionally substituted C_1-C_{10} alkyl, phenyl, or benzyl; R^6 and R^7 are identical or different and represent optionally substituted C_1-C_{10} alkyl.



Note: We still are ignoring R8 in this teaching example.

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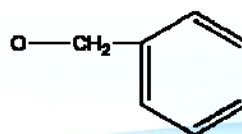
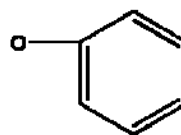
R^5 is defined as

- H
- C_1-C_{10} alkyl (optionally substituted)
- phenyl
- benzyl

What does OR^5 look like structurally?

OH

O-Ak

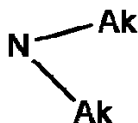


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What does $N(R^6)(R^7)$ look like?

- dialkylamino, with Ak set to C_1-C_{10}



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Using fragments in G-groups is a 3 step process

- Build the fragments
- Label them as fragments (using the point of attachment @ symbol)
- Add the fragments to the G-group definition

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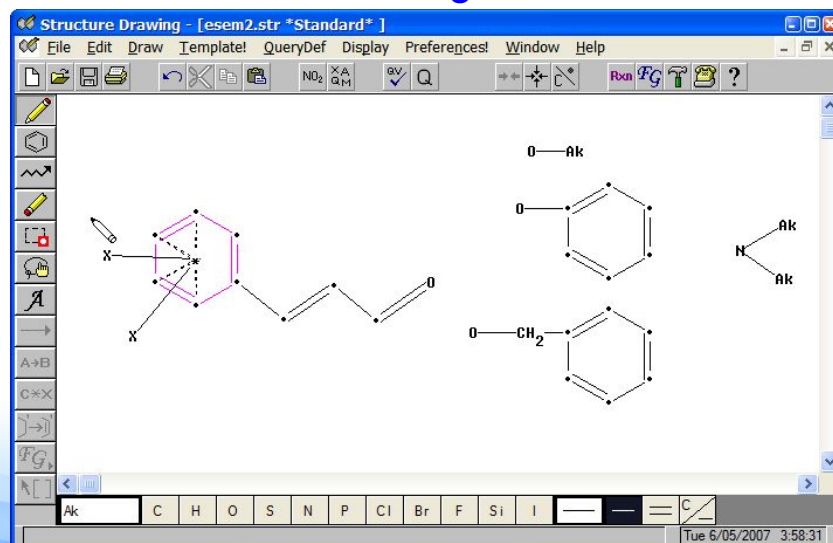
Step 1- Build fragments

- C₁-C₁₀ alkoxy: Build an O-Ak fragment; assign element count attributes to Ak
- O-phenyl: Build phenyl fragment
 - Note: Ph shortcut is not used because it searches **un-substituted** phenyl
- O-benzyl: Build benzyl fragment
- Build dialkylamino fragment: Assign attributes

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Fragments are drawn separately in the drawing window



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Add Element Count to a Variable

The screenshot illustrates the steps to add an element count to a variable. It shows a context menu (1) with 'Element Count...' selected, a main 'Element Count' dialog (2) with 'Range' selected and '1' to '10' entered, and a secondary 'Element Count' dialog (3) with 'Range, 1-10' selected and 'OK' button highlighted.

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Step 2- label fragments with points of attachments

- Choose *Draw... G-groups* from the menu
- Choose the @ attachment
- Click on the point of attachment atom node in the structure to label it with the @ symbol

The @ point of attachment is found under Draw...G-groups

The screenshot shows the 'Structure Drawing' software interface. The 'Draw' menu is open, and the 'G-groups...' option is highlighted with a red arrow. The 'G-Group Definitions' dialog box is open, showing the '@ point of attachment' field and the 'Multiple Use' button, which is also highlighted with a red box. The main window displays several chemical structures with 'Ak' labels and '@' symbols indicating attachment points.

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Points of attachment must be in the structure before creating a New G-group

The screenshot shows the 'Structure Drawing' software interface. The main window displays several chemical structures with attachment points highlighted in red boxes. The structures include a benzene ring with an 'Ak' label, a benzene ring with an '@' symbol, a benzene ring with a 'CH2' group and an '@' symbol, and a benzene ring with an 'N' atom and an 'Ak' label. The bottom status bar shows the date and time: 'Tue 6/05/2007 4:44:45'.

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Step 3- Add the fragments to the G-group definition

- Choose *Draw... G-groups* from the menu
- Choose New
- Select fragments in the G-group definition window

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Adding fragments to a G-group

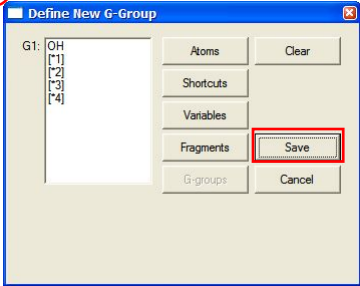
The screenshot displays the 'Structure Drawing - [esem2.str *Standard*]' application window. The 'Define New G-Group' dialog is open, with the 'Fragments' tab selected. The 'G-group Fragments' sub-dialog is also open, showing a chemical structure and the 'Include All Fragments' button. The main window shows a chemical structure with a G-group definition 'G1: OH'.

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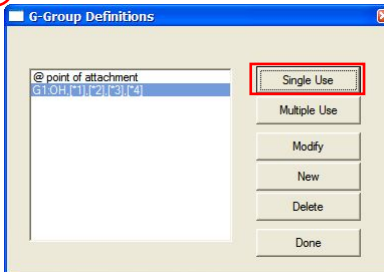
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Save the G-group definition to use in the structure

①



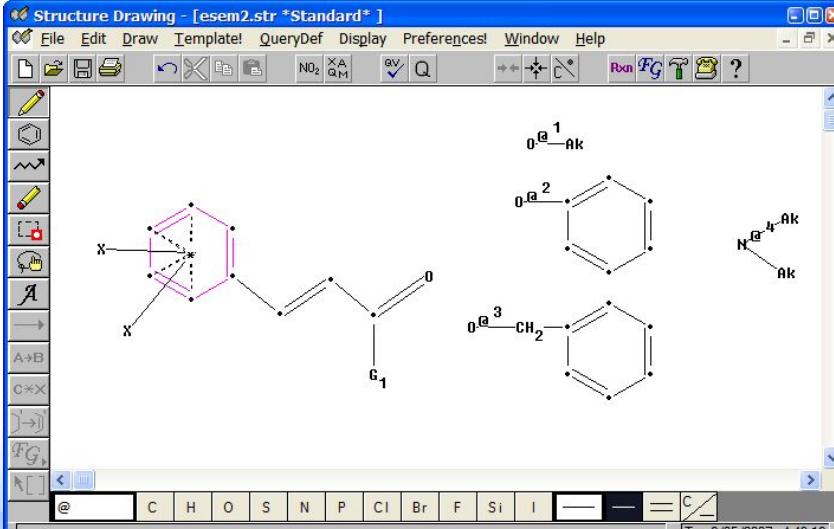
②



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Final query



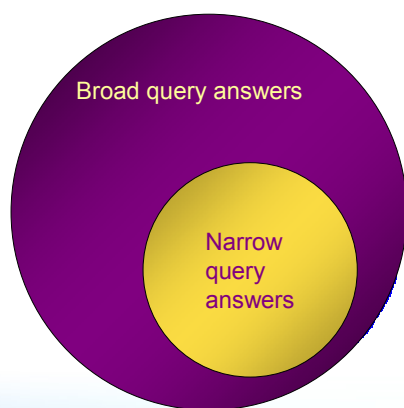
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Agenda

- Closed Substructure Search
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- **Subset Searching**
- Searching with text terms - Ring Identifiers

Subset Searching



An answer set of a narrower, more specific search will always lie within the answer set of a broader query search.
The broader query may be *any L-number* built from:

- Text terms
- A broader structure query

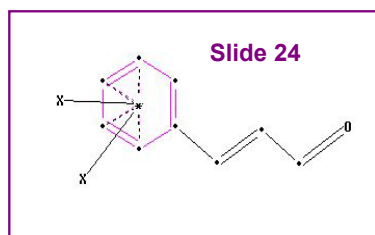
SUBSET searches of structure queries can be cost effective

- Start with broader, more general query
- Run subset searches of more specific, narrow queries against the answers from the broad search
- Cost advantage- multiple subset structure searches can be run for the cost of a full search
- There is no cost advantage to subset searching L-numbers from text searches

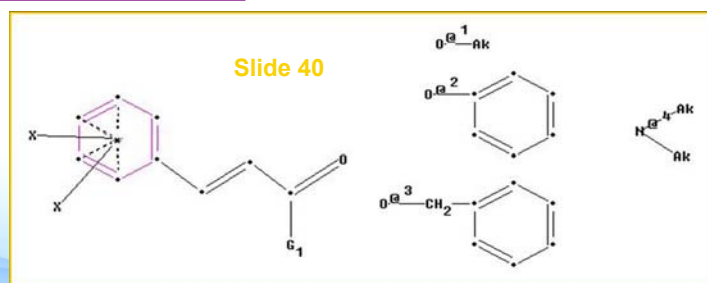
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A structure subset search of a structure answer set is cost effective



The query from slide 24 is more general than the query on slide 40, where more specific criteria in G1 were added. All of the answers to the query on slide 40 will be in the answer set of slide 24, i.e. 40 is a subset of 24.



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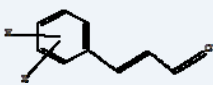
Run initial broad structure search

```

=> FILE REGISTRY
Uploading C:\Program Files\STN Express...
=> D L1;S L1 SSS SAM
L1 HAS NO ANSWERS
L1          STR

```

The broad query from slide 24 is run first.



```

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**

=> S L1 SSS FULL
FULL SEARCH INITIATED 15:44:24
FULL SCREEN SEARCH COMPLETED - 97633 TO ITERATE
100.0% PROCESSED      97633 ITERATIONS      18181 ANSWERS

L3          18181 SEA SSS FUL L1

```

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Run narrower query as a subset search

```

=>
Uploading C:\Program Files\

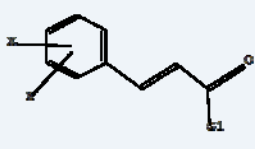
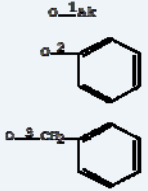


```

The narrower query from slide 40 is run second, as a subset of L3.

```

=> D L4
L4 HAS NO ANSWERS
L4          STR

```

```

01 CH, [01], [02], [03], [04]

=> S L4 SSS SAM SUBSET=L3
PROJECTIONS (WITHIN SPECIFIED SUBSET):  ONLINE  **COMPLETE**

=> S L4 SSS FULL SUBSET=L3

L6          3581 SEA SUB=L3 SSS FUL L4

```

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Save answers for later subset searches

=> **SAVE L3 BROAD24/A**

ANSWER SET L3 HAS BEEN SAVED AS 'BROAD24/A'

Don't forget to save answer sets from structure searches, in case you want to do subset searches against the answers at a later date. Answers can be saved indefinitely or temporarily.

=> **SAVE TEMP L6**

ENTER NAME OR (END): **NARROW40/A**

ANSWER SET L6 HAS BEEN SAVED AS 'NARROW40/A'

Use the **ACT**ivate command to reuse the answers.

=> **ACTIVATE NARROW40/A**

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Ring Identifiers (RID)

- Ring Identifiers
 - Numbers assigned to rings in structures in REGISTRY
 - The number has no chemical meaning
 - There is a 3-part structure to the number, separated by periods

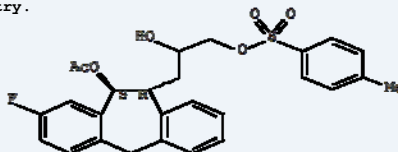
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D IDE RSD format will display the Ring System Data Table

```
RN 501666-02-0 REGISTRY
ED Entered STN: 04 Apr 2003
CN Benzenesulfonic acid, 4-methyl-, 3-[(10R,11S)-11-(acetyloxy)-2-fluoro-
10,11-dihydro-5H-dibenzo[a,d]cyclohepten-10-yl]-2-hydroxypropyl ester,
rel- (CA INDEX NAME)
```

• • •
Relative stereochemistry.





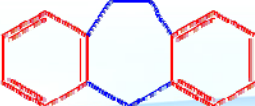
Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C6	C6	6	C6	46.150.18	1
C6-C6-C7	C6-C6-C7	6-6-7	C15	3068.4.16	1

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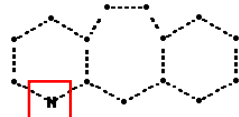
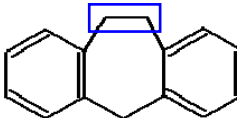
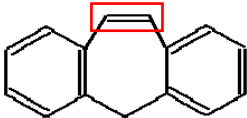
A RID breakdown

First group of digits represents the ring skeleton, e.g. 3068 means this 6-7-6 fused ring arrangement:	3068.4.16	
First and second groups together represent the atom arrangement around the ring skeleton.	3068.4.16 3068.4 has all carbons	
All three groups of digits together represent skeleton, atom arrangement and exact bonding pattern in the ring system.	3068.4.16 3068.4.16 has all carbons, joined with a combination of exact and normalized bonds	

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To emphasize subtle differences in RIDs

Atom differences	3068.4 has all carbon atoms (represented by dots)	3068.10 has a N at this precise location
		
Bonding differences	3068.4.16	3068.4.17
		

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Search Tips

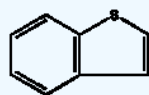
- **In general**, search the first two groups of digits
 - Full RID search may be too limiting, as ring bonding patterns may be influenced by substituents on the ring
- RID simply requires at least one instance of the ring to be present
 - Multiple occurrences can be searched e.g.,
 - => `S 2 3068.4/RID`
 - => `S >=3 46.383/RID`
- RID does not include information about how rings are connected to each other, or anything about substituents on the rings

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Search Question: Find compounds in REGISTRY which contain at least:

1 benzothiophene ring



1 cyclopropane ring



and either 1 piperidine or 1 pyridine ring



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RID Search Strategy

- Step 1. Enter REGISTRY
- Step 2. Search to find ring containing substances
- Step 3. **D IDE RSD** to see ring system data
- Step 4. Search using Ring Identifiers
- Step 5. Find references in CAplusSM

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Enter REGISTRY and locate Ring Identifiers

```
=> FILE REG
```

```
=> E BENZOTHIOPHENE/CN
```

```
E1      1      BENZOTHIOPHEN-7-OL/CN
E2      1      BENZOTHIOPHEN-7-YL/CN
E3      1  -->  BENZOTHIOPHENE/CN
E4      1      BENZOTHIOPHENE 1,1-DIOXIDE/CN
E5      1      BENZOTHIOPHENE 5,5-DIOXIDE HYDROXYLASE/CN
E6      1      BENZOTHIOPHENE 5,5-DIOXIDE MONOOXYGENASE/CN
E7      1      BENZOTHIOPHENE DICARBOXYLIC ANHYDRIDE/CN
```

```
• • •
```

```
=> S E3
```

```
L1      1      BENZOTHIOPHENE/CN
```

Try searching the parent ring name.
Even a truncated form of the name
will often work.

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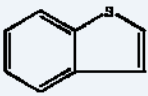
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Enter REGISTRY and locate Ring Identifiers

```

=> D IDE RSD
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 95-15-8 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzo[b]thiophene (CA INDEX NAME)
OTHER NAMES:
. . .
CN Benzothiophene
. . .

```



Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C4S-C6	SC4-C6	5-6	C8S	333.246.11	1

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Locate Ring Identifiers for other rings

```

=> E CYCLOPROPANE/CN
. . .
=> S CYCLOPROPANE/CN
L2          1 CYCLOPROPANE/CN
=> D IDE RSD
L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2007 ACS on STN
RN 75-19-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Cyclopropane (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Trimethylene (6CI)
Ring System Data

```



Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C3	C3	3	C3	1.13.1	1

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Locate Ring Identifiers for other rings

=> S PIPERIDINE/CN

• • •

=> S PYRIDINE/CN

• • •

=> D IDE RSD L3; D IDE RSD L4

Ring System Data

Elemental Analysis	Elemental Sequence	Elemental Size of the Rings	Elemental Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C5N	NC5	6	C5N	46.156.1	1



Ring System Data

Elemental Analysis	Elemental Sequence	Elemental Size of the Rings	Elemental Ring System Formula	Ring Identifier	RID Occurrence
EA	ES	SZ	RF	RID	Count
C5N	NC5	6	C5N	46.156.30	1



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Search broadly using the RING IDs

=> S (333.246 AND 1.13 AND 46.156)/RID

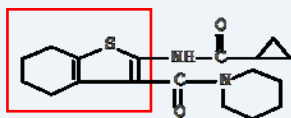
L5 246 (333.246 AND 1.13 AND 46.156)/RID

=> D SCAN

L5 246 ANSWERS REGISTRY COPYRIGHT 2007 ACS on

IN Cyclopropanecarboxamide, N-[4,5,6,7-tetrahydro-3-(1-piperidinylcarbonyl)benzo[b]thien-2-yl]-

MF C18 H24 N2 O2 S



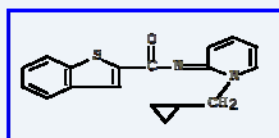
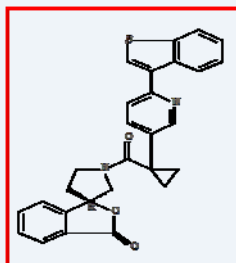
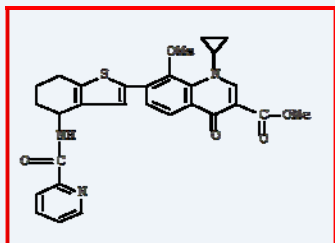
This broader search (333.246) includes the tetrahydro-benzothiophene form- it is up to the searcher/client to decide if these may be relevant.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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Pure RID searches are not limited to only the rings searched



For additional information on searching compound information by text terms, refer to the Quick Reference Card "How to Search for CAS Registry Numbers in the CAS Registry File" at <http://www.cas.org/support/stngen/qrc/index.html>

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Narrower search using the RING IDs

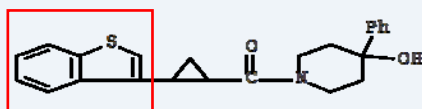
=> S (333.246.11 AND 1.13 AND 46.156)/RID

L6 205 (333.246 AND 1.13 AND 46.156)/RID

=> D SCAN

L6 205 ANSWERS REGISTRY COPYRIGHT 2007 ACS on

IN Piperidinol, 1-[(2-benzo[b]thien-3-ylcyclopropyl)carbonyl]-4-phenyl-
(9CI) (CA INDEX NAME)



Adding the third set of digits to the benzothiophene RID eliminates the tetrahydro form.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

STN

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Find references in CPlus

```
=> FILE CAPLUS  
  
=> S L5  
L7          39 L5  
  
=> S L6  
L8          34 L5  
  
=> S L7 NOT L8  
L9          5 L7 NOT L8  
  
=> D L8 TI 1-  
  
=> D L9 TI 1-
```

L5 is the broadest query answer set of 246 compounds from REGISTRY. With only 39 references in L7 to view, perhaps no further refinements need to be made.

L6 is the narrower, more restricted set of compounds which appear in 34 of the references (L8).

The difference in the reference sets is placed in L9 so they can be viewed separately.

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Display references in CPlus

```
=> D L7 IBIB ABS HITSTR 1-
```

```
L7 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2007:257347 CAPLUS Full-text  
DOCUMENT NUMBER: 146:316939  
TITLE: Preparation of benzo[b]thiophen-4-yl-piperazine and  
related compounds as antipsychotic agents for the  
treatment of mental disorders  
INVENTOR(S): Yamashita, Hiroshi; Matsubara, Jun; Oshima, Kunio;  
Kuroda, Hideaki; Ito, Nobuaki; Miyamura, Shin;  
Shimizu, Satoshi; Tanaka, Tatsuyoshi; Taira, Shinichi;  
Kondo, Kazumi; Itotani, Motohiro; Bando, Masahiko;  
Fukushima, Tae; Oshiro, Yasuo; Takahashi, Haruka;  
Sakurai, Yohji; Kuroda, Takeshi; Shimada, Jun; Maeda,  
Kenji; Tadori, Yoshihiro; Amada, Naoki; Akazawa,  
Hitomi; Yamashita, Junko; Mori, Atsushi; Uwahodo,  
Yasufumi; Masumoto, Takumi; Sugino, Haruhiko; Kikuchi,  
Tetsuro; Hashimoto, Kazuya  
PATENT ASSIGNEE(S): Otsuka Pharmaceutical Co., Ltd., Japan  
• • •
```

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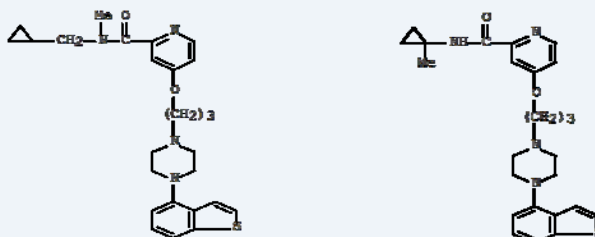
Abstract and hit structures

AB Title compds. I [R1 = cycloalkyl, (un)substituted aryl, heterocyclyl; R2 = H or lower alkyl; A = lower alkylene or lower alkenylene], and their pharmaceutically acceptable salts, are prepared and disclosed as antipsychotic agents for the treatment of mental disorders.

• • •

IT 928244-55-7P 928244-78-4P 928245-05-0P 928254-86-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of benzo[b]thiophen-4-yl-piperazine and related compds. as antipsychotic agents for the treatment of mental disorders)



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RID Summary

- RID - numeric identifiers for rings
- Useful when you have 1 or more unique rings
 - Can be used to build subset of REGISTRY for structure searches
- Can be very cost efficient
- Less precise than structure searching

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Summary

- Closed Substructure Search
- Ring Isolation and Variable Points of Attachment
- Building G-groups with user defined fragments
- Subset Searching
- Searching with text terms-Ring Identifiers

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Date & Time	Event
June 2007	
June 26, 2007 10:00- 11:00 PDT	STN: Revisiting the Basics of Structure Searching
June 28, 2007 6:00- 7:00 PDT	STN: STN® Viewer™ – A New Workflow Productivity Tool for Engineering Information
June 28, 2007 8:00- 9:00 PDT	STN: STN® Viewer™ – A New Workflow Productivity Tool for Engineering Information
June 28, 2007 10:00- 11:30 PDT	STN Continuing Education – STN: What's New?
June 28, 2007 13:00- 14:00 PDT	STN: STN® Viewer™ – A New Workflow Productivity Tool for Engineering Information
June 28, 2007 15:00- 16:00 PDT	STN: STN® Viewer™ – A New Workflow Productivity Tool for Engineering Information
July 2007	
July 12, 2007 6:00- 7:00 PDT	STN: Revisiting the Basics of Structure Searching
July 31, 2007 10:00- 11:00 PDT	STN Case Study: Adhesives
August 2007	
August 9, 2007 6:00- 7:00 PDT	STN Case Study: Adhesives
August 28, 2007 10:00- 11:00 PDT	STN: Text-Based Techniques for Engineering Information

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Structure Preparation Checklist

You are preparing to draw a structure to search on STN. The following is a list of things you may want to consider when building your query.

- Search type:** What kind of answers do you want to retrieve? Exact matches, stereoisomers, homopolymers, isotopically labeled structures, ions, copolymers, free radicals, charged compounds, salts, addition compounds, mixtures, additional substitutions on open sites?
- Ring Systems: Allow Ring Fusion or Change Ring Nodes to Isolated?**
By default, rings are designated as isolated/embedded. Isolation prevents retrieval of substances containing the isolated ring embedded in larger ring systems. Isolating the rings results in both fewer iterations and fewer answers. It does **NOT** affect ring substitution.
- Variable Points of Attachment: Allow an Atom or Group to Attach at Multiple Sites of a Ring System?** Does the substituent have to be in a specific position or can it be attached at other sites on a ring? Can it be attached at more than one site on the ring?
- Generic Groups: Create One or More Generic Groups for the Structure?** A generic group (G-group) allows for more than one substituent at a position in the structure. A G-group may contain up to 20 variables, and up to 20 G-groups can be created. A G-group may include specific elements, shortcuts, variable nodes, fragments, and other G-groups.
- Variable Nodes: Change One or More Specific Atoms to a Variable Node?**
Do you need to have that exact atom at a particular node or would equivalent atoms be acceptable? Substituting a variable atom will enlarge your answer set, e.g., X will retrieve At, Br, Cl, F or I; Q will retrieve any atoms except C and H.
- Ring Systems: Specific, Generic or In Between?**
Do I need a phenyl ring, a carbocyclic ring with at least one unsaturated bond, any carbocyclic ring, any heterocyclic ring or any ring system?
- Chain Nodes: Allow Chain Nodes to Retrieve Only Chains or Change Chain Nodes to Ring or Chain?**
By default, if in your query structure a node is part of a chain, you will only retrieve answers that have that atom as part of a chain. Do you want any nodes, especially terminal nodes, to be *ring/chain*? Node designations **do not** affect the bonds connecting the nodes.
- Chain Bonds: Change Chain Bonds to Ring or Chain?**
By default, if in your query structure a bond is part of a chain, you will only retrieve answers that have that bond as part of a chain. Do you want any bonds, especially those connecting terminal nodes, to be *ring/chain*? Bond designations **do** affect the nodes they connect.
- G-Group Orientation: Attach G-group to core structure at different nodes on the G-group?**
Can the G-group structure be attached to the core structure in more than one way?
- Limit substitution by using Closed Substructure Search (CSS)?** Sites can be opened for substitution by using Non-H attachments.
- Open Positions in Substructure SSS Searches:** Allow substitution at open positions or block substitution with hydrogen?
- Valency:** Allow non-standard valency or do you have a drawing error?
- Is my query a candidate for a subset search?**