



# Structure Searching in the CAS Registry<sup>SM</sup> File on STN<sup>®</sup>

Presentation

---

# Structure building tools

- Draw carbon chains and rings with the Pencil Tool
- Create rings with the Ring Tool
- Create chains with the Chain Tool
- Select Common Atoms
- Select atoms or shortcuts from the Draw Menu
- Select Common Bonds



# Types of structure searches

<i>Type of substance retrieved</i>	<i>EXACT</i>	<i>FAMILY</i>	<i>SSS</i>
Structure with no additional substitution	X	X	X
Radiolabeled forms of the substance with no additional substitution	X	X	X
Stereoisomers with no additional substitution	X	X	X
Homopolymers with no additional substitution	X	X	X
Free radicals with no additional substitution	X	X	X
Charged compounds with no additional substitution	X	X	X
Salts and mixtures of unsubstituted compounds		X	X
Molecular addition compounds of unsubstituted compounds		X	X
Copolymers of unsubstituted compounds		X	X
Structures with additional substitution			X



# Refining substructure search queries to increase precision

- Isolate one or more rings
- Block substitution
- Add more nodes



# Refining substructure search queries to broaden retrieval

- Allow some bonds to be ring or chain
- Allow some nodes to be ring or chain
- Allow bonds to be of any value
- Use variable nodes or variable groups



# Variable nodes

X = any halogen

A = anything, except hydrogen

Q = anything, except carbon or hydrogen

M = any metal

Cb = any carbocycle

Cy = any ring system

Hy = any heterocycle

Ak = any carbon chain



# Variable groups

- Specific elements
- Shortcuts, e.g., Me, COOH
- System-defined variable nodes, e.g., X, M
- Structural fragments
- Other G-groups



# Substructure search worksheet

1. Do I want rings in my answers to be fused to other ring systems, spiro-attached to other ring systems, or isolated from other ring systems?

Use ring isolation: Isolated/Embedded (default) or Isolated

2. Do I want atoms in my structure to be part of a ring or chain in my answers?

Change node characteristics: Ring (default for atoms in rings),  
Chain (default for atoms in chains),  
or Ring/Chain

3. Do I want bonds in my structure to be part of a ring or chain in my answers?

Change bond characteristics: Ring (default for bonds in rings),  
Chain (default for bonds in chains),  
or Ring/Chain



# Substructure search worksheet (cont.)

4. Do I want to allow a bond in my structure to take on value (single, double, or triple) in my answers?

Use unspecified bond.

5. Do I want to block substitution at a position?

Draw in hydrogen atoms.

6. Do I want to define substitution options at a position?

Use variable nodes or G-groups.

