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Advanced Searching Tips

Substructure Searching

Retrieval possibilities

- Exact matches, including stereoisomers, radiolabeled matches, and charged matches.
- Matches of the structural skeleton, with substitution at open positions.
- Matches of the structural skeleton, with the skeleton embedded within a larger ring system.
- Closely related matches resulting from hydrogen migration, double-bond rearrangement, and charge migration, including tautomers and zwitterions.

Tools for Controlling Substitution & Ring Formation

- **Variables Menu** – list of predefined variable symbols -e.g., X = all halogen atoms.
- **R-group Tool** – create customized variable groups containing combinations of atoms, shortcuts, and variables.
- **Lock Tool** – prevents retrieval of structures having a bond to a non-hydrogen atom at an open position.
- **Drawing Hydrogen Attachments** – not assumed in a substructure search.
- **Terminal Shortcuts** – such as Me - are locked from substitution by default. To allow substitution at a terminal position, draw the open position explicitly.
- **Lock Out Rings tool** – controls ring formation.

Synthetic Pathway Searching

- **Full Reaction Sequence**.
  - Locate organic synthetic pathways with specific structural transformations.
- **Preparation**
  - Locate preparations for any type of chemical compound, without regard for the reactants and reagents used or the transformation involved.
- **Functional Group**
  - Locate methods used to carry out a broadly defined transformation.
- **Reaction Mechanism**
  - Reactions for any type of chemical compound, without regard to specific reactants or products.

When you want	For these reactions	And you know	Use this strategy
Precise Matches	Organic	Structures on both sides of the arrow Reactant structure(s) only	Full Reaction
	Organic, inorganic, biochemical	Product structure	Full Reaction Preparation
General Matches	Organic	Names of functional groups of reaction participants on either/both sides of the reaction arrow	Functional Group
Very General Matches	Organic, inorganic, biochemical	Name of the reaction mechanism	Reaction Mechanism

Similarity Searching

- Compares your query structure with all substances in the database and determines which are the most similar (based on the Tanimoto algorithm).
- Results grouped by similarity score (60 ≥ 99% similar).
- Complementary to the other structure searches because it returns many answers that are neither exact nor substructure answers.

Polymer Searching

- **Name or RN** – Use Substance Identifier Search.
- **Formula** – Use Molecular Formula Search and follow directions below.
- **Structure** – Use the Structure Search for one monomer and refine results based on additional monomer units.
- **Class** – Use the Research Topic Search with keywords describing general classes of polymers.

Polymer Formula Searching

1. Write the chemical formula for the monomer as it is known (for monomer salts see below).
   - **CH3CO-O-CH=CH2**
   - **H2C=CH-Cl**
   - **H2C=CH-F**
2. Determine element counts for each monomer. No count is used for element counts of 1.
   - **4 C, 6 H, 2 O**
   - **2 C, 3 H, Cl**
   - **2 C, 2 H, F**
3. List monomer formulas in any order, separating each formula by a period.
   - **C4H6O2**
   - **C2H3Cl**
   - **C2H2F**
4. Enclose the copolymer formula in parentheses, followed by X.
   - **(C4H6O2.C2H3Cl.C2H3F)X**

Formulae for Monomer Salts

- Salts of Acids – Remove the metal from the formula to create two fragments and add H to the non-metal fragment to create the formula for the neutral acid.
- Salts of Amines – Move the H from the N to the anion to create two fragments.

Biosequence Searching (Proteins, Nucleic Acids, Enzymes)

- **Biosequence Families** – Use the Research Topic Search with keywords to specify sequence type and family group:
  protein sequences for epidermal growth factor (egf)
- **Specific Biosequences** – Use the Substance Identifier Search with the biomolecule name (protein, nucleic acid or enzyme), including variations:
  heat shock protein 70 Anopheles albimanus
  protein hsp 70 Anopheles albimanus
  hsp70 Anopheles albimanus

Other Resources

- **SciFinder Scholar 2006 Overview Handout**
- **CAS SciFinder Scholar Solutions** - www.cas.org/SCIFINDER/SCHOLAR/resources.html

If you need further assistance with SciFinder Scholar, please contact a reference librarian at the Physical Sciences Library (pslref@cornell.edu, 255-4016).

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