

HOW TO

Combine Answer Sets - Reactions



The SciFinder 2007 feature **Combine Answer Sets** offers you many techniques to use with saved answer sets to cut time and effort when deadlines are tight. For example, if you know that certain reactants or products are undesirable for your projects, you can save answer sets of references to such substances for future use.

Suppose your project involves synthesizing the anti-depressant drug duloxetine. An exploration with SciFinder yields an answer set that includes references featuring 1-fluoro-naphthalene as a reactant for this process. You are reluctant to employ this substance given the unhealthy side effects associated with the use of fluoro compounds and have already saved an answer set of reactions in which 1-fluoro-naphthalene functions as a reactant. By using the Combine Answer Sets feature, you can expedite your literature search for duloxetine.

1. Click on Locate to begin exploring references associated with duloxetine. Type the trade name duloxetine as the substance identifier. SciFinder provides you with the CAS REGISTRYSM record. Note: This example shows 387 references associated with this substance.
2. Since you are interested in only those reactions where duloxetine is a product, you can specify that your answers include these reactions. To accomplish this, take advantage of the new shortcut available with SciFinder 2007 by clicking the substance's structure diagram. Select **Reactions** and then **Product** to view only those reactions where duloxetine is the product.

Locate by Substance Identifier

Enter Substance Identifiers, one per line. Read from file ...

duloxetine

A Substance Identifier is a substance.

Examples:
50-00-0
999815
Acetaminophen
1,4-dichlorobenzene

OK

116539-59-4

~387 References
REGISTRY

SciFinder

File Edit View Task T

Explore by Chemical Structure
Refine by Chemical Structure

Reactions

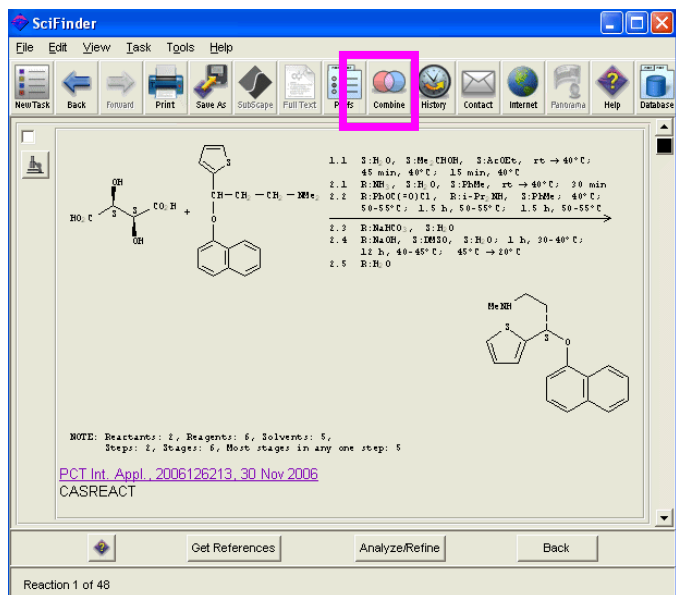
Product

Reactant
Reagent
Reactant or Reagent
Catalyst
Solvent
Any role

116539-59-4

~387 References
REGISTRY

3. In this example, SciFinder provides you with 48 reaction answers in which duloxetine is a product. Now use the **Combine Answer Sets** feature as a quick way to eliminate reactions that use the undesirable reactant 1-fluoro-naphthalene.



4. First activate the answer set containing 184 reactions that you purposely saved in your project file, anticipating that you might need to eliminate 1-fluoro-naphthalene from a reaction.

File name:

Files of type:

Preview:

File:

Create Date: February 12, 2007 16:24:32

Title:

Content: 184 reaction answers

Description: Substance Identifier task started on Mon Feb 12, 2007 at 4:22 PM Explored by Substance Identifier

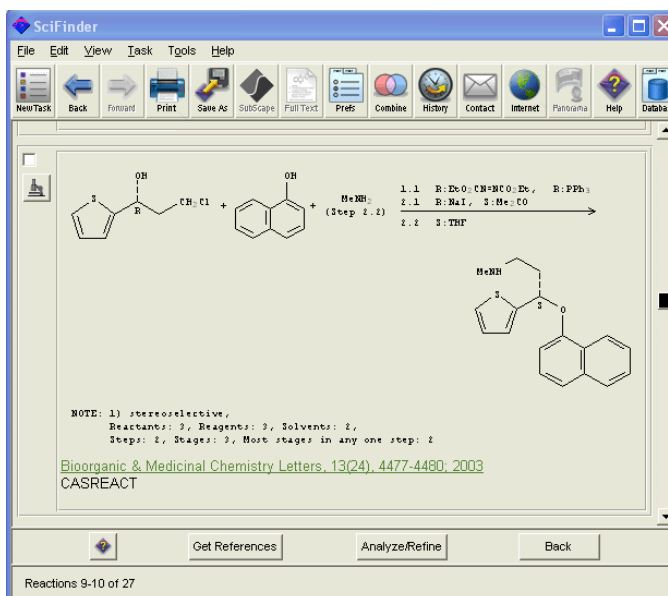
5. When you click the **Estimate** button of the Combine Answer Sets feature, you will see all options available to you along with the number of reactions that will result from each option. Select the “remove saved set from current set” option to eliminate all reactions in which 1-fluoro-naphthalene is a reactant.

Combine Answer Sets

Reactions Current: 48 Saved: 184

<input type="radio"/>	Combine sets	211
<input type="radio"/>	Intersect sets	21
<input checked="" type="radio"/>	Remove saved set from current set	27
<input type="radio"/>	Remove current set from saved set	163

6. You can now explore 27 reactions containing duloxetine as a product that do not use 1-fluoro-naphthalene as a reactant—meeting your original research goal.



7. View the abstract, structure image, and bibliographic details concerning any of the 27 reactions by clicking the **Reference hyperlink**.

Detail of Reference for Reaction 10

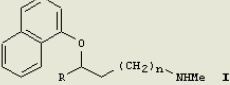
File Edit Help

Bibliographic Information

Duloxetine (Cymbalta), a dual inhibitor of serotonin and norepinephrine reuptake. Bymaster, F. P.; Beedle, E. E.; Findlay, J.; Gallagher, P. T.; Krushinski, J. H.; Mitchell, S.; Robertson, D. W.; Thompson, D. C.; Wallace, L.; Wong, D. T. Eli Lilly and Company, Lilly Research Laboratories, Lilly Corporate Center, Indianapolis, IN, USA. Bioorganic & Medicinal Chemistry Letters (2003), 13(24), 4477-4480. Publisher: Elsevier Science B.V., CODEN: BMCLE8 ISSN: 0960-894X. Journal written in English. CAN 140:145679 AN 2003:926695 CAPLUS

Abstract

A series of naphthalenyloxy-substituted amines I ($n = 2 - 4$, $R = H$; $n = 1$, $R = H, Ph, 4-FC_6H_4, 2-MeOC_6H_4, 2-furyl, 2-thienyl, 2-thiazolyl$, etc.) has been prepd., and these compds. are demonstrated to be inhibitors of both serotonin and norepinephrine reuptake. One member of this series, duloxetine (Cymbalta), (S)-I ($n = 1$; $R = 2-thienyl$), has proven to be effective in clin. trials for the treatment of depression.



Indexing -- Section 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

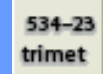
Get Related... Close

When you want to . . .

Click



Locate a reference or a substance



Use a substance identifier to locate a substance



Combine answer sets

- Create an answer set that contains all answers from both the saved and current sets
- Create an answer set that contains only answers common to both sets
- Create an answer set in which answers common to both the saved and current are removed along with answers from the saved set
- Create an answer set in which answers common to both the saved and current are removed along with answers from the current answer set



View details concerning a reference of interest

Contact CAS Customer Care at help@cas.org or call 800-753-4227 (North America) or 614-447-3700 (worldwide).