

# ▶ HOW TO

Use the New Features



SciFinder®

Summer 2010

This release of SciFinder® provides a pathway to finding additional patent information via Markush searching. Other search and usability enhancements include automatic duplicate removal of references via a one-time preference setting, the ability to set weekly or monthly KMP profiles, and search by digital object identifier (DOI).

## Finding Information

### Markush Search

1. This feature allows users to retrieve patent documents containing generic Markush structures relevant to the query structure. Search results are presented as a reference answer set.

Markush searches are run against the MARPAT® database with a predefined set of search parameters that differ in some cases from SciFinder defaults (for example, rings are isolated in Markush searches).

Searches are intended to provide focused answers that can be helpful in a preliminary assessment of the patent landscape.

Structure Editor

Draw or change atoms or bonds.

Shortcut Keys

Atom Short

-X =R

1-4

Cl

+

Structure Editor:

Structure

Reaction

Markush

Get Markush patents that match your query using:

Variable only at the specified positions

Substructure search

OK

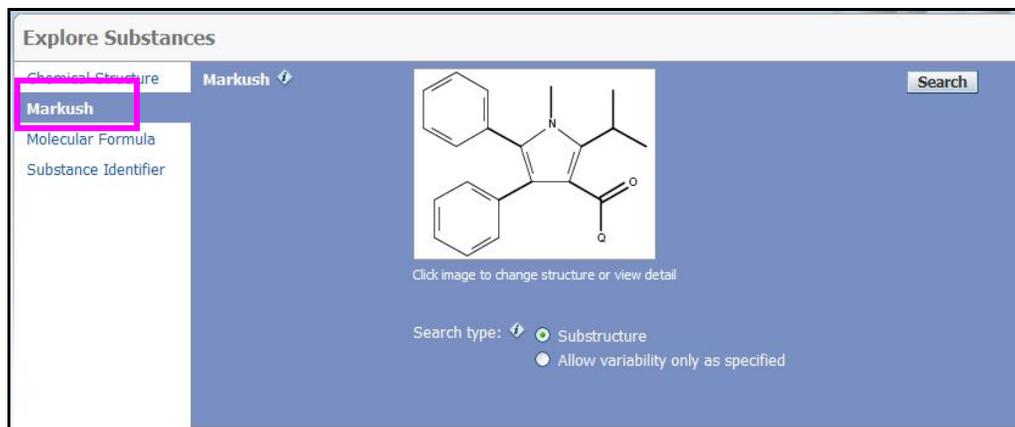
Cancel

Formula not available

Scale 100

## Markush Search - continued

1. Markush search is an option in **Explore Substances** and is available to all customers who have the Substructure Search Module (SSM).
2. This feature provides additional access to patent information and is complementary to structure searching in REGISTRY.



Explore Substances

Chemical Structure | Markush | Search

Molecular Formula

Substance Identifier

Click image to change structure or view detail

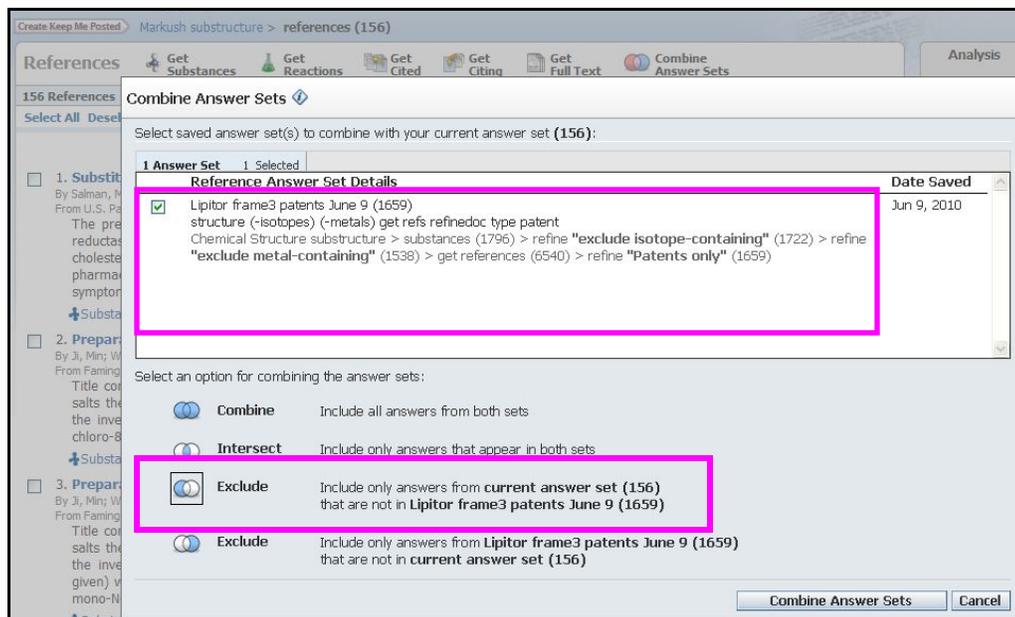
Search type:  Substructure  Allow variability only as specified

## Markush Search - continued

1. **Search Tip:** To compare the results of a Substructure and Markush search do the following:

a. Run a substructure search for the structure of interest. **Get References** for the substance answer set and **Refine** that answer set by document type to find only patents. **Save** the resulting reference answer set.

b. Run a Markush substructure search of the same structure and then use the **Combine Answer Sets** feature with the **Exclude** option to find additional patents found only by the Markush search.



References | Markush substructure > references (156) | Analysis

156 References | Select All | Deselect

Combine Answer Sets

Select saved answer set(s) to combine with your current answer set (156):

Reference Answer Set Details	Date Saved
<input checked="" type="checkbox"/> Lipitor frame3 patents June 9 (1659) structure (-isotopes) (-metals) get refs refinedoc type patent Chemical Structure substructure > substances (1796) > refine "exclude isotope-containing" (1722) > refine "exclude metal-containing" (1538) > get references (6540) > refine "Patents only" (1659)	Jun 9, 2010

Select an option for combining the answer sets:

- Combine: Include all answers from both sets
- Intersect: Include only answers that appear in both sets
- Exclude: Include only answers from current answer set (156) that are not in Lipitor frame3 patents June 9 (1659)
- Exclude: Include only answers from Lipitor frame3 patents June 9 (1659) that are not in current answer set (156)

Combine Answer Sets | Cancel

## DOI Search and Display

1. A Digital Object Identifier (DOI) can now be searched directly via the **Document Identifier** option in **Explore References**.

**Explore References**

Research Topic  
Author Name  
Company Name

**Document Identifier(s)**

Search

**Document Identifier**

Journal  
Patent  
Tags

Enter one per line.  
Examples:  
1983:4296  
107:12935  
10.1021/np050327j

2. If CAS has a DOI for a reference it will be displayed in the bibliographic information for that record.

As a component of the bibliographic detail, DOI information can be saved and exported.

Create Keep Me Posted | Document ID "10.1021/ol1007907; 10.1021/jo1..." > references (3) > Synthesis and Evaluation of 2,...

**Reference Detail** | Get Substances | Get Reactions | Get Cited | Get Citing | Get Full Text

Link | Save | Print | Export

Return | Previous | Next

**1. Synthesis and Evaluation of 2,5-Linked Alternating Pyridine-Thiophene Oligomers**

By: Rocha, Silvia V.; Finney, Nathaniel S.

[image omitted] The first iterative access to alternating 2,5-linked pyridine-thiophene (Py-Th) oligomers is presented. These oligomers exhibit strong absorption and emission, even in the solid state (picture of the longest oligomer, above). Protonation leads to large red shifts in emission and, unlike most known thiophene-contg. oligomers, they are readily reduced but not oxidized. These species represent a promising new class of materials for further study and potential application.

**Quick Links**  
0 Tags, 0 Comments

**Source**  
Organic Letters  
Volume 12  
Issue 11  
Pages 2598-2601  
Journal  
2010  
CODEN: ORLEF7  
ISSN: 1523-7060  
**DOI: 10.1021/ol1007907**

## User Preference Setting

### Automatic Duplicate Removal

1. A new **Preferences** setting allows users to automatically remove duplicate references from answer sets of up to 10,000 answers.

The user must select this setting. It is off by default.

**Preferences**

**Keep Me Posted Notification**

Receive e-mail notification of Keep Me Posted results  
Please ensure that CAS has your current e-mail address. Visit [myCAS](#) to add or change your address.

**My Suppliers**

You have 3 preferred suppliers and 0 non-preferred suppliers. [Edit supplier preferences.](#)

**Remove Duplicate References**

Automatically remove duplicate MEDLINE answers  
If selected, response time may be impacted.

**Starting Page**

Select the default starting page:

Explore References  
 Explore Substances  
 Explore Reactions

OK Cancel

Contact Us | Copyrights and Trademarks  
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## Automatic Duplicate Removal - continued

2. If automatic duplicate removal has been set, SciFinder will show you how many answers come from CAPUS<sup>SM</sup> and MEDLINE<sup>®</sup> and how many duplicates have been removed.

The screenshot shows the SciFinder interface for a search on "osteoporosis in children". A yellow banner at the top states "91 duplicates were automatically removed." A pink box highlights a summary box on the right that reads: "Candidates Selected: 754 references were found containing the two concepts 'osteoporosis' and 'children' closely associated with one another. Automatically removed 91 duplicate MEDLINE answer(s). Answer set 1 created with 287 answers from CAPLUS and 376 answers from MEDLINE." Below the banner, there are buttons for "Select All", "Deselect All", and "Sort by: Accession Number". The main content area shows a list of references, with the first one highlighted: "1. Administration of the Bisphosphonate Zoledronic Acid During Tooth Development Inhibits Tooth Eruption and Formation and Induces Dental Abnormalities in Rats". The right sidebar shows an "Analyze by:" section with a dropdown for "Author Name" and a list of authors with their respective counts.

## Results Display

### Transformation Center Highlighting in Reactions

1. Transformation center highlighting shows the reaction centers of the reactants and products for the get **Similar Reactions** feature.
2. Once a reaction of interest has been identified, click on the **Similar Reactions** link.

The screenshot shows the SciFinder "Reactions" interface. At the top, it says "40 Reactions" and "0 Selected". There are buttons for "Select All", "Deselect All", and "Sort by: Similarity". A pink box highlights the "Similar Reactions" link in the reaction list. The first reaction is highlighted: "1. Reaction Detail Link Similar Reactions". It shows a chemical reaction where a reactant (a benzene ring with a hydroxyl group and a carboxylic acid group) reacts with  $R: H_2NC(=S)Cl$  to form a product (a benzene ring with a thiol group and a carboxylic acid group). Below the reaction, there is a "NOTE: prophetic reaction, Reactants: 1, Reagents: 1, Steps: 1, Stages: 1" and a description: "Preparation and purification of synthetic DNA via alkynes cyclization with azides and homolytic acrylamide polymerization reactions". The second reaction is also shown: "2. Reaction Detail Link Similar Reactions". It shows a reactant (a naphthalene ring with a hydroxyl group) reacting with  $R: H_2NC(=S)Cl$ ,  $R: KOH$ ,  $R: HCl$ ,  $S: H_2O$ ,  $S: THF$ , and  $S: (CH_2OH)_2$  to form a product (a naphthalene ring with a thiol group) in 59% yield.

## Transformation Center Highlighting in Reactions - continued

1. Specify the level of similarity you are interested in. For example, Medium, which shows the reaction center and adjacent atoms and bonds. Then click **Get Reactions**.

Reactions 1 Reaction 0 Selected Keep Selected  
Select All Deselect All Sort by: Access

Get Similar Reactions

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

- Broad - Reaction centers only (40)
- Medium - Reaction centers plus adjacent atoms and bonds (18)
- Narrow - Reaction centers plus extended atoms and bonds (9)

Get Reactions Cancel

## Transformation center highlighting in Reactions - continued

2. The reaction answer set shows the reaction center and the immediately adjacent atoms and bonds.

Reactions 18 Reactions 0 Selected Keep Selected Remove Selected Save Print Export  
Select All Deselect All Sort by: Similarity Answers per Page [15] 1 2 Display: [Icons]

1. Reaction Detail Link Similar Reactions

OC1=CC=C(C(=O)O)C=C1  $\xrightarrow{R: Me_2NC(=S)Cl}$  OC1=CC=C(C(=O)O)C=C1

NOTE: prophetic reaction,  
Reactants: 1, Reagents: 1,  
Steps: 1, Stages: 1

Preparation and purification of synthetic DNA via alkynes cyclization with azides and homolytic acrylamide polymerization reactions  
By Fang, Shiyue  
From U.S. Pat. Appl. Publ., 2008081902, 03 Apr 2008

2. Reaction Detail Link Similar Reactions

Oc1ccc2ccccc2c1  $\xrightarrow{R: Me_2NC(=S)Cl, R: KOH, R: HCl, S: H_2O, S: THF, S: (CH_2OH)_2}$  Oc1ccc2ccccc2c1 59%

# Working With Answer Sets

## Options for Sorting Substance Answer Sets

1. Substance answer sets can also be sorted by Molecular Weight or Molecular Formula, and in ascending or descending order.

The screenshot shows a web interface for a chemical database. At the top, there are navigation buttons: "Substances", "Get References", "Get Reactions", "Get Commercial Sources", and "Combine Answer Sets". Below this, a status bar indicates "4851 Substances", "0 Selected", and "Remove Selected" (highlighted with a pink box). A "Sort by:" dropdown menu is open, showing options: "CAS Registry Number", "Molecular Weight", and "Molecular Formula" (the latter two are highlighted with a pink box). The interface displays three substance detail cards:

- 1. Substance Detail 1225190-35-1**  
Chemical structure: CCCC(=O)Oc1ccc(N)cc1COc2ccc([N+](=O)[O-])cc2  
Molecular Formula:  $C_{18}H_{19}N_3O_6$   
Name: Butanamide, 4-[3-[[[(2-aminobenzoyl)oxy]methyl]-4-nitrophenoxy]-
- 2. Substance Detail 1224954-12-4**  
Chemical structure: COc1ccc2c(c1)c(N)cc(C(=O)OC)c2  
Molecular Formula:  $C_{18}H_{17}N O_4$   
Name: 9-Phenanthrenecarboxylic acid, 10-amino-2,7-dimethoxy-, methyl ester
- 3. Substance Detail 1224954-11-3**  
Chemical structure: COc1ccc2c(c1)c(N)cc(C(=O)OC)c2  
Molecular Formula:  $C_{17}H_{15}N O_3$   
Name: 9-Phenanthrenecarboxylic acid, 10-amino-2-methoxy-, methyl ester

# Post-Processing

## Setting and Managing KMP Profiles

1. The frequency of KMP updates can be set to weekly or monthly.

The screenshot shows the 'Create Keep Me Posted Profile' dialog box. The 'Title' field contains 'Osteoporosis in Children'. The 'Description' field is empty. The 'Duration' section shows 'Expires On: May 26, 2011'. The 'Frequency' dropdown menu is highlighted with a pink box, showing options for 'Month', 'Week', and 'Month'. The 'Send updates once every' dropdown is set to 'Month'. The 'Exclude previously retrieved' checkbox is unchecked. The 'Create' and 'Cancel' buttons are at the bottom right.

2. The duration of a KMP profile can also be set. The default is one year from the date the profile is established.

3. Users can renew expiring profiles from the e-mail notification, with options allowing renewal of a single profile or all profiles.

4. KMP alert e-mail messages are more informative and contain hyperlinks for up to the first five new hits for titles and/or substances.

The screenshot shows the 'Create Keep Me Posted Profile' dialog box. The 'Title' field contains 'Osteoporosis in Children'. The 'Description' field is empty. The 'Duration' section shows 'Expires On: Nov 26, 2010' and 'Expires In: 6 Months'. The 'Frequency' dropdown menu is highlighted with a pink box, showing options for '6 Months', '3 Months', and '1 Month'. The 'Send updates' dropdown is set to '3 Months'. The 'Exclude previously retrieved references' checkbox is unchecked. The 'Create' and 'Cancel' buttons are at the bottom right.



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