

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.

The screenshot shows the 'Explore Substances' interface. On the left, a sidebar contains options: 'Chemical Structure', 'Markush', 'Molecular Formula', and 'Substance Identifier'. The 'Markush' option is highlighted with a pink box. The main area displays a chemical structure of a substituted indazole. Below the structure, there is a 'Search type:' section with two radio buttons: 'Substructure' (selected) and 'Allow variability only as specified'. A 'Search' button is located in the top right corner.

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.

The screenshot shows the 'Combine Answer Sets' dialog box. At the top, it says 'Select saved answer set(s) to combine with your current answer set (156):'. Below this, a table lists available answer sets. One set is selected and highlighted with a pink box:

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

Below the table, there are three options 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)

Buttons for 'Combine Answer Sets' and 'Cancel' are at the bottom right.

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.

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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

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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 CAPUSSM and MEDLINE[®] and how many duplicates have been removed.

The screenshot shows the SciFinder interface with a search for "osteoporosis in children". A yellow banner at the top states "91 duplicates were automatically removed." A pink box highlights a summary of the automatic duplicate removal process: "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, the search results are displayed, with the first result highlighted: "1. Administration of the Bisphosphonate Zoledronic Acid During Tooth Development Inhibits Tooth Eruption and Formation and Induces Dental Abnormalities in Rats".

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 displays "40 Reactions" and "0 Selected". A pink box highlights the "Similar Reactions" link. Below this, two reaction schemes are shown. The first reaction shows the conversion of 4-hydroxybenzoic acid to 4-mercaptobenzoic acid using the reagent $R: H_2NC(=S)Cl$. The second reaction shows the conversion of 2-naphthol to 2-mercaptanaphthalene using the reagent $R: H_2NC(=S)Cl$ and solvent $S: (CH_2OH)_2$. The transformation center highlighting is visible on the reactant and product molecules in both reactions.

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
Select All Deselect All Sort by: Similarity Save Print Export
Answers per Page [15] 1 2
Display: [Icons]

1. Reaction Detail Link Similar Reactions

O=C(O)c1ccc(O)cc1 $\xrightarrow{R: Me_2NC(=S)Cl}$ O=C(N)c1ccc(O)cc1

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 displays a web interface for a chemical database. At the top, there are navigation tabs: "Substances", "Get References", "Get Reactions", "Get Commercial Sources", and "Combine Answer Sets". Below these, a status bar shows "4851 Substances", "0 Selected", and "Keep Selected" and "Remove Selected" buttons. A "Sort by:" dropdown menu is open, showing options: "CAS Registry Number", "Molecular Weight", and "Molecular Formula". The "Remove Selected" button and the dropdown menu are highlighted with pink boxes. The main content area shows three substance detail cards. Each card includes a chemical structure, a molecular formula, and the full name of the substance.

Substance ID	Molecular Formula	Substance Name
1225190-35-1	C ₁₈ H ₁₉ N ₃ O ₆	Butanamide, 4-[3-[[[(2-aminobenzoyl)oxy]methyl]-4-nitrophenoxy]-
1224954-12-4	C ₁₈ H ₁₇ N ₁ O ₄	9-Phenanthrenecarboxylic acid, 10-amino-2,7-dimethoxy-, methyl ester
1224954-11-3	C ₁₇ H ₁₅ N ₁ O ₃	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 visible at the bottom.

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 visible at the bottom.



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