

# ▶ HOW TO

Use the New Features



SciFinder®

September 2009

SciFinder® offers many new reaction, substance, and collaboration features. See also [SciFinder: Overview of Enhancements](#) (WebEx, 49 minutes), or click the Help link within SciFinder.

## Reactions

### Get Similar Reactions\*

#### 1. Retrieve similar reactions.

The search algorithm looks for single-step reactions with identical reaction centers and related structural characteristics.

82. Reaction Detail [Link](#) **Similar Reactions**

Get Similar Reactions

Retrieve similar reactions from:

- All reactions
- Current answer set

Include this level of similarity:

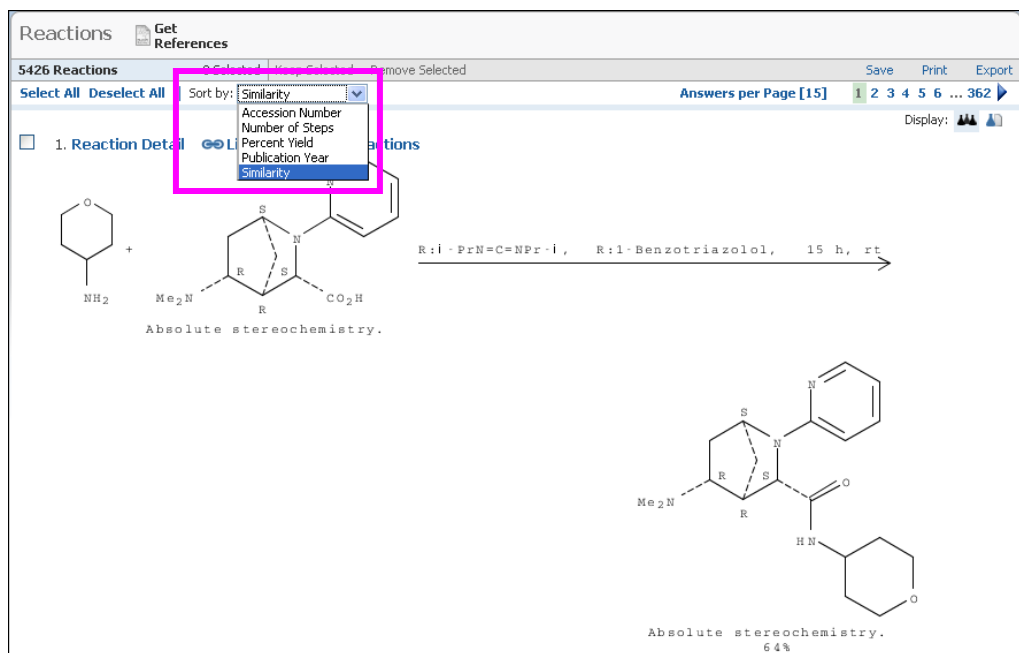
- Broad - Reaction centers only (214107)
- Medium - Reaction centers plus adjacent atoms and bonds (40243)
- Narrow - Reaction centers plus extended atoms and bonds (5426)

Get Reactions Cancel

\* Unique to the web version.

## Sort Reactions

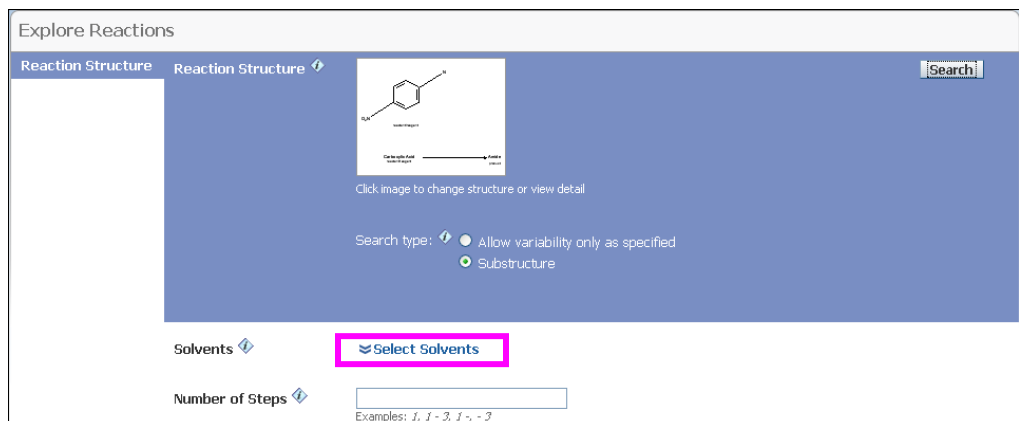
- Sort reaction answers by various criteria, including similarity.



The screenshot shows a web interface for "Reactions" with 5426 results. A dropdown menu is open, showing sorting options: Similarity (selected), Accession Number, Number of Steps, Percent Yield, Publication Year, and Similarity. Below the menu, a chemical reaction is displayed. The reactants are a piperidine ring with an amino group and a benzotriazole derivative. The reaction conditions are "R:1-PrN=C=NPr-i, R:1-Benzotriazolol, 15 h, rt". The product is a complex bicyclic structure with a benzotriazole ring and a piperidine ring, with a 64% yield. The text "Absolute stereochemistry." is present below the reactants and product.

## Limit Reactions by Solvents\*

- On the Explore Reactions page, click the double arrow next to **Select Solvents** to display the solvent list or hierarchy.



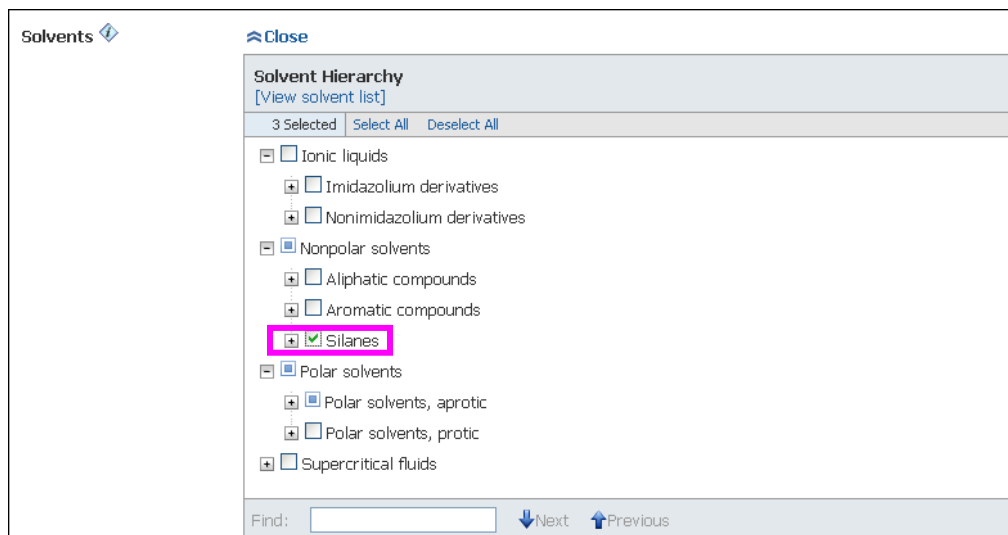
The screenshot shows the "Explore Reactions" interface. It features a "Reaction Structure" section with a chemical structure and a "Search" button. Below the structure, there are search options: "Allow variability only as specified" (selected) and "Substructure". At the bottom, there is a "Solvents" section with a "Select Solvents" button highlighted by a pink box. Below this, there is a "Number of Steps" section with a text input field and examples: "Examples: 1, 1-3, 1-3".

\* Unique to the web version.

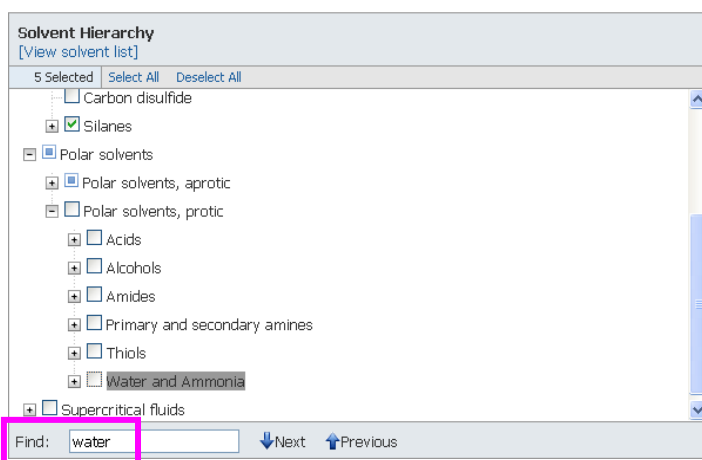
## Limit Reactions by Solvents\* (cont.)

2. Select  solvents to limit your reaction results to those using specific solvents.

**Note:** When you make solvent selections, other solvents and solvent categories may become selected by association ()



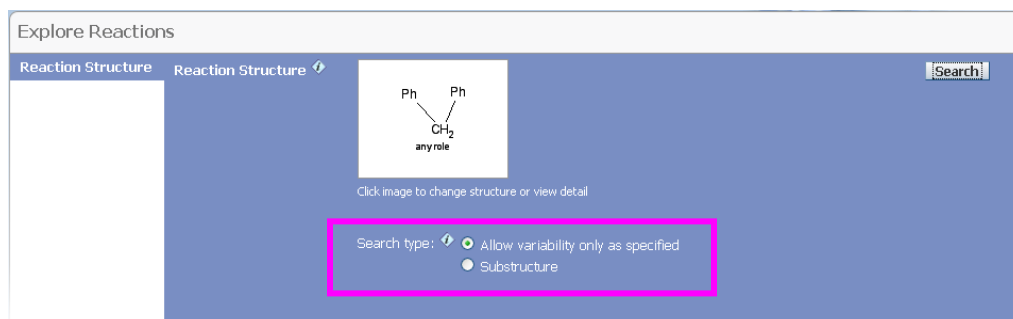
3. Use the **Find** field to search for solvents within the solvent list or hierarchy.



## Specify Reaction Search Type More Easily

1. Specify a reaction search type from the Explore Reactions page.

(Previously, this feature was available only within the Reaction Editor.)



\* Unique to the web version.

## Quick or "Shortcut" Search from Reactions

1. Click any reaction participant to perform various quick or "shortcut" searches.

(Previously, this feature was available only from the Reaction Detail.)

The screenshot shows the 'Reactions' search results page. At the top, it indicates '5426 Reactions' and '0 Selected'. A dropdown menu is open over a reaction participant, showing options: 'Reactions', 'References', 'Substance Detail', 'Commercial Sources', 'Regulatory Information', 'Explore by Chemical Structure', and 'Explore Reactions'. The 'Product' dropdown is also open, showing options: 'Reactant', 'Reagent', 'Reactant or Reagent', 'Catalyst', 'Solvent', and 'Any role'. The reaction shown is between a cyclohexane derivative and a benzotriazole derivative, with conditions 'R:i-PrN=C=NPr-i, R:1-Benzotriazolol, 15 h, rt'. The product is a complex molecule with absolute stereochemistry. The text 'Absolute stereochemistry. 64%' is visible at the bottom of the reaction diagram.

## Substances

### Refine by Property Value

1. To refine substance answer sets by specific property value(s), choose **Property Value** and click **Select Properties**.

The screenshot shows the 'Substances' search results page. It displays a list of three substances with their chemical structures and names. The first substance is '2-Cyclohexen-1-one, 2-[2-chloro-4-(methylsulfonyl)-3-(1H-tetrazol-1-ylmethyl)benzoyl]-3-(2-methyl-1H-pyrrol-1-yl)'. The second is '2-Cyclohexen-1-one, 3-(3-bromo-1H-pyrrol-1-yl)-2-[2-chloro-4-(methylsulfonyl)-3-(1H-tetrazol-1-ylmethyl)benzoyl]'. The third is '2-Cyclohexen-1-one, 3-(3-bromo-1H-pyrrol-1-yl)-2-[2-chloro-4-(methylsulfonyl)-3-(1H-tetrazol-1-ylmethyl)benzoyl]'. On the right side, there is a 'Refine by' sidebar with a list of properties: 'Chemical Structure', 'Isotope-Containing', 'Metal-Containing', 'Commercial Availability', 'Property Availability', 'Property Value', 'Reference Availability', and 'Atom Attachment'. The 'Property Value' option is selected and highlighted with a pink box. Below the list, there is a 'Select Properties' button, also highlighted with a pink box.

## Refine by Property Value (cont'd)

- Specify the values for the selected properties.

**Note:** You can also select  **Include substances with no value for the specified properties** to include substances for which the specified property is either not present or present but without a reported value.

- Click **Refine**.

Refine by Property Value

1. Select one or more properties. Click each property to display value options.

2. Specify values and limits.

Properties - 3 selected

Experimental

- Boiling Point
- Melting Point

Predicted

- H Acceptors
- H Donors
- Molecular Weight
- logP
- Freely Rotatable Bonds
- Bioconcentration Factor
- Boiling Point
- Density
- Enthalpy of Vaporization
- Flash Point
- H Donor/Acceptor Sum
- Koc
- logD
- Mass Intrinsic Solubility
- Mass Solubility
- Molar Intrinsic Solubility
- Molar Solubility

Values - Experimental Boiling Point

Specify range (degrees C):

30 to 120

Min: -273.0 Max:

Pressure (Torr):

0.0 to 760.0

Min: 0.0 Max:

Reset

Include substances with no value for the specified properties

Refine Cancel

## Export Properties to Microsoft® Excel\*

- To create a spreadsheet of substance properties associated with one or more substance answers, click **Export**.

Substance Detail

Get References Get Reactions Get Commercial Sources Get Regulatory Information

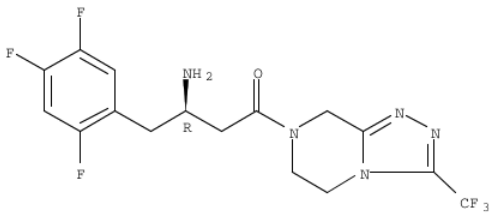
Link Save Print **Export**

1.

CAS Registry Number: 486460-32-6

C<sub>16</sub> H<sub>15</sub> F<sub>8</sub> N<sub>6</sub> O

1-Butanone, 3-amino-1-[5,6-dihydro-3-(trifluoromethyl)-1,2,4-triazolo[4,3-a]pyrazin-7(8H)-yl]-4-(2,4,5-trifluorophenyl)-, (3R)-1,2,4-Triazolo[4,3-a]pyrazine, 7-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-(trifluoromethyl)-(9CI); (2R)-4-Oxo-4-[3-(trifluoromethyl)-5,6-dihydro-[1,2,4]triazolo[4,3-a]pyrazin-7(8H)-yl]-1-(2,4,5-trifluorophenyl)butan-2-amine; Sitagliptin



Absolute stereochemistry.

\* Unique to the web version.

## Export Properties to Microsoft® Excel\* (cont.)

2. Select a file type of **Microsoft Excel Worksheet (\*.xls)**.
3. Specify whether to export all property values or only selected values. Then click **Continue**.

Export

\* Required

File Name: \*  
butanone

File Type:  
Microsoft Excel Worksheet (\*.xls)

Properties to Export:

All property values  
 Only experimental property values  
 Only predicted property values  
 Select property values..

Continue Cancel

4. If you chose to export selected values, select the properties to export, and then click **Export**.

Export Selected Property Values

Properties to Export:

Select: All All Experimental All Predicted Deselect All

Experimental	Predicted	
<input checked="" type="checkbox"/> Boiling Point	<input type="checkbox"/> Bioconcentration Factor	<input type="checkbox"/> LogP
<input checked="" type="checkbox"/> Density	<input checked="" type="checkbox"/> Boiling Point	<input type="checkbox"/> Mass Intrinsic Solubility
<input type="checkbox"/> Electric Conductance	<input checked="" type="checkbox"/> Density	<input type="checkbox"/> Mass Solubility
<input type="checkbox"/> Electric Conductivity	<input checked="" type="checkbox"/> Enthalpy of Vaporization	<input type="checkbox"/> Molar Intrinsic Solubility
<input type="checkbox"/> Electric Resistance	<input type="checkbox"/> Flash Point	<input type="checkbox"/> Molar Solubility
<input type="checkbox"/> Electric Resistivity	<input type="checkbox"/> Freely Rotatable Bonds	<input type="checkbox"/> Molar Volume
<input type="checkbox"/> Glass Transition Temperature	<input type="checkbox"/> H Acceptor/Donor Sum	<input type="checkbox"/> Molecular Weight
<input type="checkbox"/> Magnetic Moment	<input type="checkbox"/> H Acceptors	<input type="checkbox"/> pKa
<input type="checkbox"/> Median Lethal Dose	<input type="checkbox"/> H Donors	<input type="checkbox"/> Polar Surface Area
<input type="checkbox"/> Melting Point	<input type="checkbox"/> Koc	<input type="checkbox"/> Vapor Pressure
<input type="checkbox"/> Optical Rotatory Power	<input type="checkbox"/> LogD	
<input type="checkbox"/> Refractive Index		
<input type="checkbox"/> Tensile Strength		

Export Cancel

\* Unique to the web version.

## Specify Substance Search Type More Easily

1. Specify a substance search type from the Explore Substances page.

(Previously, this feature was available only within the Reaction Editor.)

Explore Substances

Chemical Structure  Molecular Formula  Substance Identifier

Search

Click image to change structure or view detail

Search type:  Exact Structure  Substructure  Similarity

Show precision analysis

## Quick or "Shortcut" Search from Substances

1. Click one of the options to perform a quick or "shortcut" search.

(Previously, this feature was available only from the Substance Detail.)

Substances

307 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [20] 1 2 3 4 5 6 ... 16 View: [Icons]

1. Substance Detail 1024999-62-9

2. Substance Detail 1013653-86-5

3. Substance Detail 1013409-32-9

Explore by Chemical Structure  
Explore Reactions

Absolute stereochemistry.

**C<sub>18</sub> H<sub>21</sub> N<sub>2</sub> O<sub>5</sub> Tl**

Thallium, [1-[5'-deoxy-3-methyl-2',3'-O-(1-methylethylidene)uridin-5'-yl]-2,4-cyclopentadien-1-yl]-

~1 References  
Reactions  
Commercial Sources  
Regulatory Information  
Link

**C<sub>5</sub> H<sub>5</sub> B Tl**

Thallium(1+), (boron)[μ-(η<sup>5</sup>:η<sup>5</sup>-2,4-cyclopentadien-1-yl)]-

**C<sub>5</sub> H<sub>5</sub> Tl<sub>2</sub>**

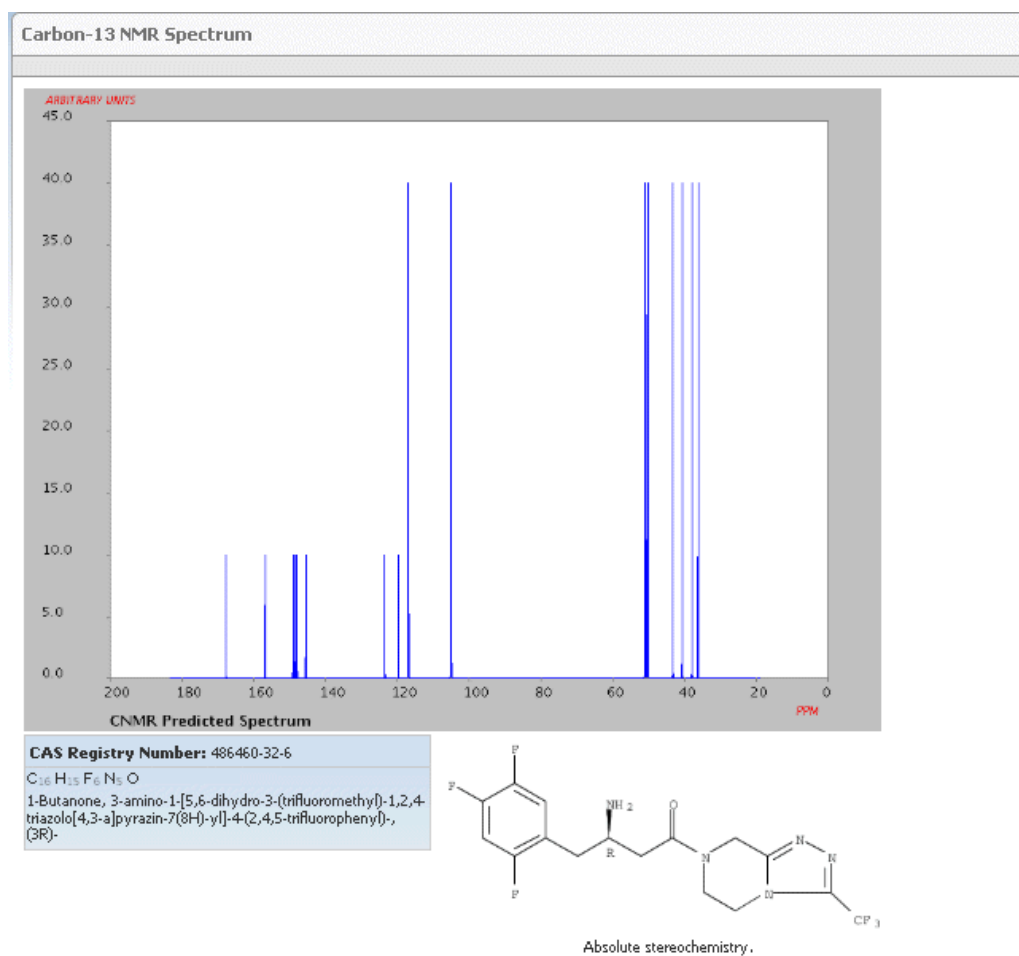
Thallium(1+), [μ-(η<sup>5</sup>:η<sup>5</sup>-2,4-cyclopentadien-1-yl)]di-

## View New Predicted – <sup>13</sup>C-NMR Spectra

1. Within the Predicted Properties section of the Substance Detail, click [See spectrum](#) next to *Carbon-13 NMR Spectrum*.

Lipinski and Related Properties	Value	Conditions	Notes	Top
Freely Rotatable Bonds	5		(8)	
H Acceptors	6		(8)	
H Donors	2		(8)	
H Donor/Acceptor Sum	8		(8)	
logP	1.298±1.178	Temp: 25 °C	(8)	
Molecular Weight	407.31		(8)	
Spectra Properties	Value	Conditions	Notes	Top
Carbon-13 NMR Spectrum	<a href="#">See spectrum</a>		(9)	
Proton NMR Spectrum	<a href="#">See spectrum</a>		(9)	
Structure-related Properties	Value	Conditions	Notes	Top
Polar Surface Area	77.0 A2		(8)	
Thermal Properties	Value	Conditions	Notes	Top
Boiling Point	529.9±60.0 °C	Press: 760 Torr	(8)	
Enthalpy of Vaporization	80.51±3.0 kJ/mol	Press: 760 Torr	(8)	
Flash Point	274.3±32.9 °C		(8)	

2. View the predicted <sup>13</sup>C-NMR spectrum.



# Collaboration

## Comment on References\*

1. Add comments – thoughts, remarks, project information – to individual references. Optionally, share the comments with My Connections colleagues within your research site.

The box. A lab. expt. that involves the synthesis of CdSe quantum dot nanocrystals is described as an example of green chem., where relatively safe materials are used. The CdSe nanocrystals are synthesized from CdO, elemental Se, oleic acid, and trioctylphosphine using a

2. **Micelle-mediated extraction of heavy metals from environmental samples: an environmental green chemistry laboratory experiment**  
By Giokas, Dimosthenis L.; Paleok  
From Journal of Chemical Education  
An expt. utilizing the cloud as Cd<sup>2+</sup>, Pd<sup>2+</sup>, Cu<sup>2+</sup>, and using ammonium pyrrolid and reproducibly ext. the wastewater from water t

3. **Going green: lecture assignments and laboratory experiences for the college curriculum**  
By Haack, Julie A.; Hutchison, James E.; Kirchoff, Mary M.; Levy, Irvin J.  
From Journal of Chemical Education  
Green chem., the design environment, provides unique opportunities for innovation in the chem. curriculum and for engaging a broad spectrum of students in the study of chem. A symposium held at the ACS national meeting in San Diego in Mar. 2005 illustrated the creative

4. **Green chemistry education: Preparing the next generation reaching out to those with non-scientists. A major program and materials future of Green Chem. A**  
By Beach, Evan S.; Eghball, Nicolas; Karayannis, Miltiades I.  
From Abstracts of Papers, 239th

**Comments**  
Micelle-mediated extraction of heavy metals from environmental samples: an environmental green chemistry laboratory experiment

3 Comments Sort by: **Newer First** | Older First

supports findings of diomed study!  
Anthony Machosky Posted June 12, 2009 9:57 AM  
Last Modified June 12, 2009 9:57 AM

uses heavy metals - great experiment  
Marie Sparks Posted May 22, 2009 12:20 PM  
Last Modified June 11, 2009 10:24 AM

Your comment has been added.

**Add Comment:** Maximum of 1024 characters per comment; 50 comments per user.  
Reminder: Your comments and tags can be viewed by your connected colleagues.

Save Characters Remaining: 1024 Close

Beach Evan S 1  
Boatman Elizabeth M 1  
Eghball Nicolas 1  
Giokas Dimosthenis L 1  
Haack Julie A 1  
Hutchison James E 1  
Karayannis Miltiades I 1  
Kirchoff Mary M 1  
Levy Irvin J 1

Show More

**Categorize**  
More detailed analysis based on CAS indexing  
Categorize

## Tag References\*

1. Use tags to label references with descriptive terms or keywords to facilitate grouping and recall. Optionally, share the tags with My Connections colleagues within your research site.

References Get Substances Get Reactions Get Cited Get Citing

4 References 2 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [20] View: [icon]

1. **A safer, easier, faster synthesis for CdSe quantum dot nanocrystals**  
By Boatman, Elizabeth M.; Lisensky, George C.; Nordell, Karen J.  
From Journal of Chemical Education (2005), 82(11), 1697-1699. Language: English, Database: CAPLUS  
Cadmium selenide quantum dot nanocrystals are a visually engaging way to demonstrate quantum effects in chem., since their transition energies can be explained as a "particle in a box", where a delocalized electron is the particle and the nanocrystal is the box. A lab. expt. that involves the synthesis of CdSe quantum dot nanocrystals is described as an example of green chem., where relatively safe materials are used. The CdSe nanocrystals are synthesized from CdO, elemental Se, oleic acid, and trioctylphosphine using a

2. **Micelle-mediated extraction of heavy metals from environmental samples: an environmental green chemistry laboratory experiment**  
By Giokas, Dimosthenis L.; Paleok  
From Journal of Chemical Education  
An expt. utilizing the cloud as Cd<sup>2+</sup>, Pd<sup>2+</sup>, Cu<sup>2+</sup>, and using ammonium pyrrolid and reproducibly ext. the wastewater from water fr

3. **Going green: lecture assignments and laboratory experiences for the college curriculum**  
By Haack, Julie A.; Hutchison, James E.; Kirchoff, Mary M.; Levy, Irvin J.  
From Journal of Chemical Education (2005), 82(7), 974-976. Language: English, Database: CAPLUS  
Green chem., the design (and redesign) of chem. products and processes to eliminate hazards to human health and the environment, provides unique opportunities for innovation in the chem. curriculum and for engaging a broad spectrum of students in the study of chem. A symposium held at the ACS national meeting in San Diego in Mar. 2005 illustrated the creative

**Add Tags**

Add tags to:  
 All answers  
 Only selected answers

**Add Tags:** Separate multiple tags with semicolons, max. of 100 characters per tag, 50 tags max. per user.  
Reminder: Any colleague you connect with will be able to view your comments and tags.

green  
green chemistry

Save Cancel

Analyze by: Author Name  
Click bar to view only those references within the current answer set

Anastas Paul T 1  
Beach Evan S 1  
Boatman Elizabeth M 1  
Eghball Nicolas 1  
Giokas Dimosthenis L 1  
Haack Julie A 1  
Hutchison James E 1  
Karayannis Miltiades I 1  
Kirchoff Mary M 1  
Levy Irvin J 1

\* Unique to the web version.

## Explore by Tag\*

1. Once tagged, references can be searched for by tag.
2. Your My Connections colleagues can also use your tags to find references, and can add their own tags to the same or related references.

Explore References

Research Topic: Tags are shared between you and your connected colleagues. Click a tag to retrieve references associated with that tag.

Author Name	0 - 9 (and Special Characters)	P
Company Name	#####	pig
Document Identifier	##oxygen	piglets
Journal	123456	pollen related
Patent	2,2,2-trifluoro	polymorphic
Tags	9,9,9-hex	polyvinylpyrrolidone
	@new tag	prevention
	A	primitive

## Connect with SciFinder Colleagues\*

1. If you choose to, you can link to other SciFinder users within your research site for the purpose of sharing project information via the Comments and Tags features.

**Note:** Only your connections – colleagues with whom you have chosen to connect – can view and interact with your reference information.

SciFinder®

Welcome | Sign Out

Substance Identifier "486460-32-6" > substances (1) > 486460-32-6

Explore References | Explore Substances | Explore Reactions

Keep Me Posted | My Connections | History | References

Explore References

Research Topic: Research Topic

Author Name

Company Name

Document Identifier

Journal

Patent

Tags

Publication Year(s): Examples: 1995, 1995-1998, 1995-, ~1995

Document Type(s):  
 Biography  Dissertation  Patent  
 Book  Editorial  Preprint  
 Clinical Trial  Historical  Report  
 Commentary  Journal  Review  
 Conference  Letter

Language(s):  
 Chinese  German  Polish  
 English  Italian  Russian  
 French  Japanese  Spanish

Author Name: Last, First, Middle

Company Name

Saved Answer Sets: medical marijuana, hypoxia apnea, sleep disorder apnea, central apnea, urea-d4, diphenhydramine, thallium, life on Mars, aureomycin

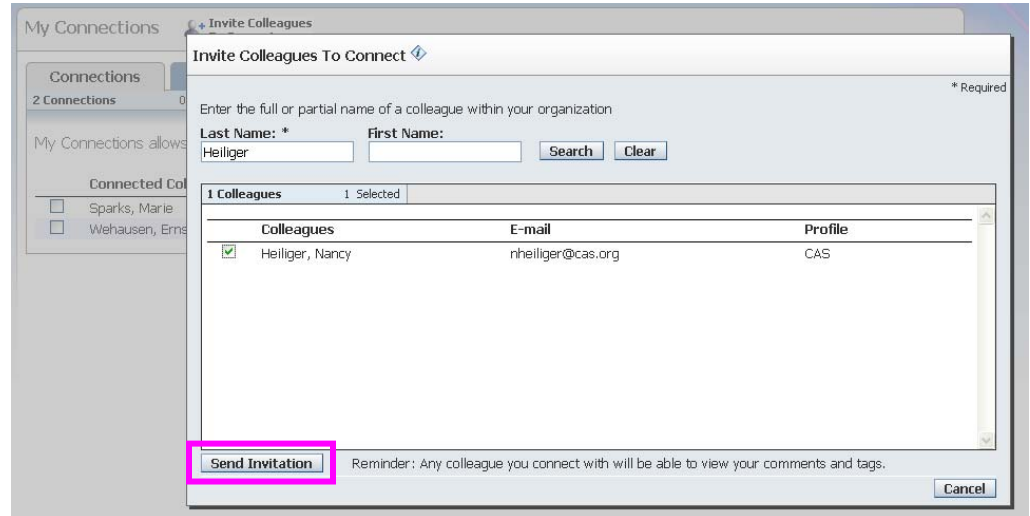
Keep Me Posted Results: intra hydro amino (Sep 05, 2009 (1)), atenolol and cardura (Aug 29, 2009 (1)), opiate (May 23, 2009 (1)), No results

My Connections: No invitations to connect, No outstanding sent invitations, You have 4 connections

\* Unique to the web version.

## Connect with SciFinder Colleagues\* (cont'd)

- To connect to SciFinder colleagues, they must be part of your research site and you must invite them or accept their invitation to connect.



## Usability Enhancements

### Combine Keep Me Posted (KMP) Results

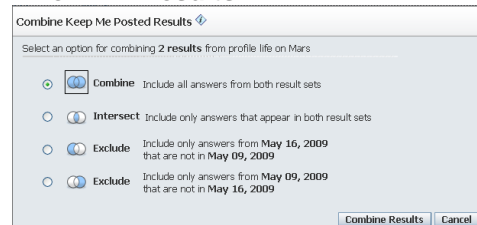
- Select  two or more Keep Me Posted (KMP) results and combine them into a single saved answer set.

Only results within the same KMP profile can be combined.

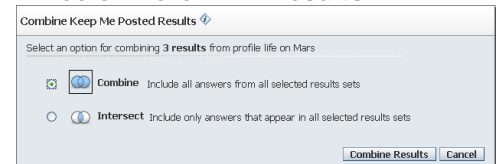


- Select a combine option.

#### Two KMP Results



#### Three or More KMP Results



## Change Number of Answers per Page

1. Within any type of answer set, click **Answers per Page** to change how many answers display per page.

**Note:** Each type of answer set – references, substances, reactions, commercial sources – has its own answers-per-page setting.

The screenshot shows the 'Substances' interface with 307 substances listed. The 'Answers per Page' dropdown menu is open, showing options: 15, 20, 25, and 50. The current selection is 15. Below the dropdown, there are two substance detail cards. The first card shows a chemical structure of a nucleotide derivative with the label '1. Substance Detail 1024999-62-9' and the text 'Absolute stereochemistry.' The second card shows a chemical structure of a boron complex with the label '2. Substance Detail 1013653-86-5'.

## Customize View of Substances

1. Click one of the **View** buttons to change the number of columns (1–4) for displaying substance answers.

Three columns is the default.

The screenshot shows the 'Substances' interface with 307 substances listed. The 'View' buttons are visible, showing a grid of three columns. The 'Answers per Page' dropdown menu is also visible, showing options: 1, 2, 3, 4, 5, 6, 21. Below the dropdown, there are three substance detail cards. The first card shows a chemical structure of a nucleotide derivative with the label '1. Substance Detail 1024999-62-9' and the text 'Absolute stereochemistry.' The second card shows a chemical structure of a boron complex with the label '2. Substance Detail 1013653-86-5'. The third card shows a chemical structure of a boron complex with the label '3. Substance Detail 1013409-32-9'.

## Customize View of Substances (cont'd)

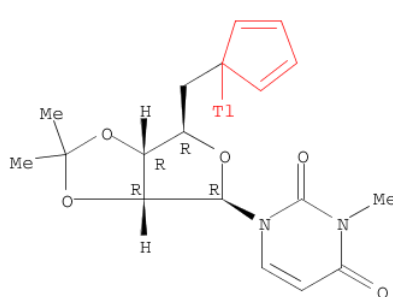
- As you change the number of display columns, the structure drawings resize accordingly.

Substances [Get References](#) [Get Reactions](#) [Get Commercial Sources](#)

307 Substances 0 Selected Keep Selected Remove Selected Save Print Export

Select All Deselect All Sort by: CAS Registry Number Answers per Page [15] 1 2 3 4 5 6 21 View: [dropdown]

1. Substance Detail  
1024999-62-9



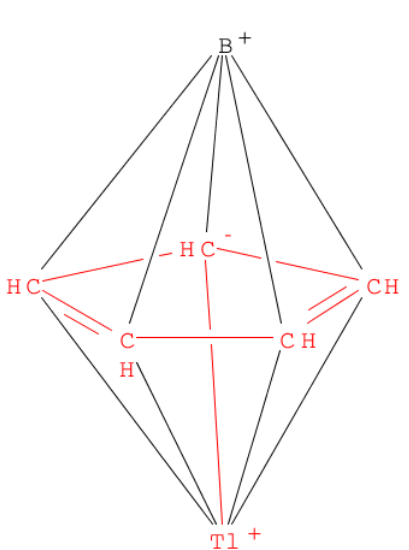
Absolute stereochemistry.

$C_{18} H_{21} N_2 O_5 Tl$

Thallium, [1-[5'-deoxy-3-methyl-2',3'-O-(1-methylethylidene)uridin-5'-yl]-2,4-cyclopentadien-1-yl]-

[~1 References](#)  
[Reactions](#)  
[Commercial Sources](#)  
[Regulatory Information](#)

2. Substance Detail  
1013653-86-5



$B^+$

$H C^-$

$Tl^+$

## Customize View of References

- Click one of the **View** buttons to change the amount of abstract information (none, partial, full) that displays as part of your answers.

Partial abstract information is the default.

References [Get Substances](#) [Get Reactions](#) [Get Cited](#) [Get Citing](#)

4509 References 0 Selected Keep Selected Remove Selected Remove Duplicates Add Tags Save Print Export

Select All Deselect All Sort by: Accession Number Answers per Page [50] 1 2 3 4 5 6 21 View: [dropdown]

1. **Effect of subtherapeutic administration of antibiotics on the prevalence of antibiotic-resistant Escherichia coli bacteria in feedlot cattle**  
By Alexander, T. W.; Yanke, L. J.; Topp, E.; Olson, M. E.; Read, R. R.; Morck, D. W.; McAllister, T. A.  
From Applied and Environmental Microbiology (2008), 74(14), 4405-4416. Language: English, Database: CAPLUS  
Antibiotic-resistant Escherichia coli presence was studied in 300 feedlot steers (initial body wt. 198 ± 20 kg) receiving subtherapeutic levels of antibiotics in feed. Fecal samples (n = 3300) were collected over 314-day period. The antibiotics were selected based on their common use in cattle industry and included chlortetracycline + sulfamethazine (TET-SUL; Aureo S-700G), chlortetracycline (TET; Aureomycin 100G), virginiamycin (V-max), monensin (Rumensin), and tylosin phosphate (Tylan); no antibiotic use served as control. The steers were initially fed barley silage-based diet, followed b...

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)

2. **Competitive detection for antibiotics in dairy products based on surface plasmon resonance (SPR)**  
By Xu, Kexin; Liu, Jin; Zhang, Zengfu  
From Faming Zhuanli Shengqing Gongkai Shuomingshu (2008), CN 101216423 A 20080709. Language: Chinese, Database: CAPLUS  
The invention relates to competitive detection for antibiotics in dairy products based on surface plasmon resonance (SPR). The method comprises resp. mixing certain amt. of specific antibody and dairy products with different known antibiotic contents to obtain a series of std. samples; utilizing SPR optical method to measure refractive indexes of the std. samples; corresponding the refractive indexes to antibiotic contents in the dairy products to build prediction model; prepg. sample from dairy product to be detected and measuring its refractive index with the same method; and calcg. antibio...

[Substances](#) [Reactions](#) [Citing](#) [Full Text](#) [Link](#) [0 Comments](#) [0 Tags](#)

## Customize Print of References

1. Select how much abstract information to include in your printout.

Your current View option is the default for print.

**Print**

**Print:**

All

Only selected

**Format:**

Summary without abstracts

Summary with partial abstracts

Summary with full abstracts

Detail (full record)

**Title:**

**Include:**

Task History

Tags

Comments

## Search for References by Linked CAS Roles\*

1. Within a Substance Detail, search for references related to a substance by clicking a CAS role, one of the reference categories (patents, nonpatents, or derivatives), or an intersection (✓) of the two.

Substance Detail

Link Save Print Export

◀ Previous | Next ▶

1.

**CAS Registry Number:** 486460-32-6

C<sub>16</sub> H<sub>15</sub> F<sub>6</sub> N<sub>5</sub> O

1-Butanone, 3-amino-1-[5,6-dihydro-3-(trifluoromethyl)-1,2,4-triazolo[4,3-a]pyrazin-7(8H)-yl]-4-(2,4,5-trifluorophenyl)-, (3R)-1,2,4-Triazolo[4,3-a]pyrazine, 7-[(3R)-3-amino-1-oxo-4-(2,4,5-trifluorophenyl)butyl]-5,6,7,8-tetrahydro-3-(trifluoromethyl)-(9CI); (2R)-4-Oxo-4-[3-(trifluoromethyl)-5,6-dihydro-[1,2,4]triazolo[4,3-a]pyrazin-7(8H)-yl]-1-(2,4,5-trifluorophenyl)butan-2-amine; Sitagliptin

Absolute stereochemistry.


**Source of Registration:** CA

**Document Types:** Conference, Journal, Patent

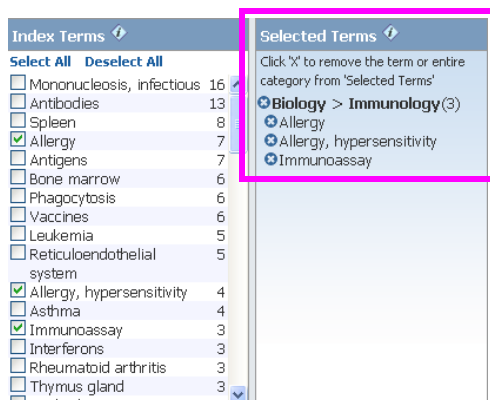
Role	Patents	Nonpatents	Nonspecific
			Derivatives from Patents
Analytical study		✓	
Biological study	✓	✓	✓
Preparation	✓	✓	
Process	✓	✓	
Properties	✓	✓	
Prophetic in patents			✓
Reactant or reagent	✓	✓	
Uses	✓	✓	✓

\* Unique to the web version.

## Select Index Terms within Categorize\*

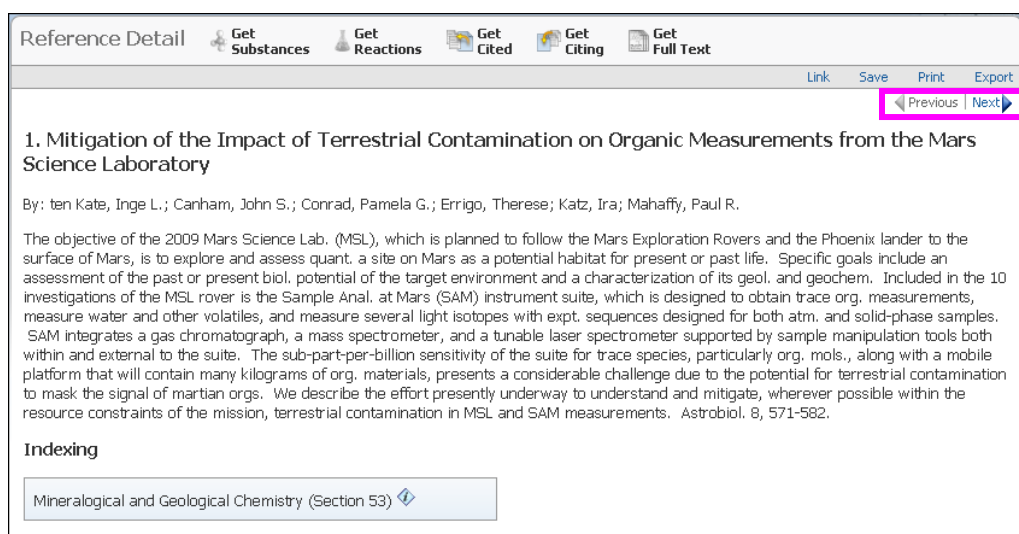
1. To categorize references, make index term selections  on the Categorize dialog box.

The right-hand panel of the Categorize dialog box has been modified to make it easier for you to tailor your list of selected index terms.



## View Previous/Next Answer\*

1. Within an answer detail, click the Previous / Next buttons to move to answers before or after the current answer in the answer set.

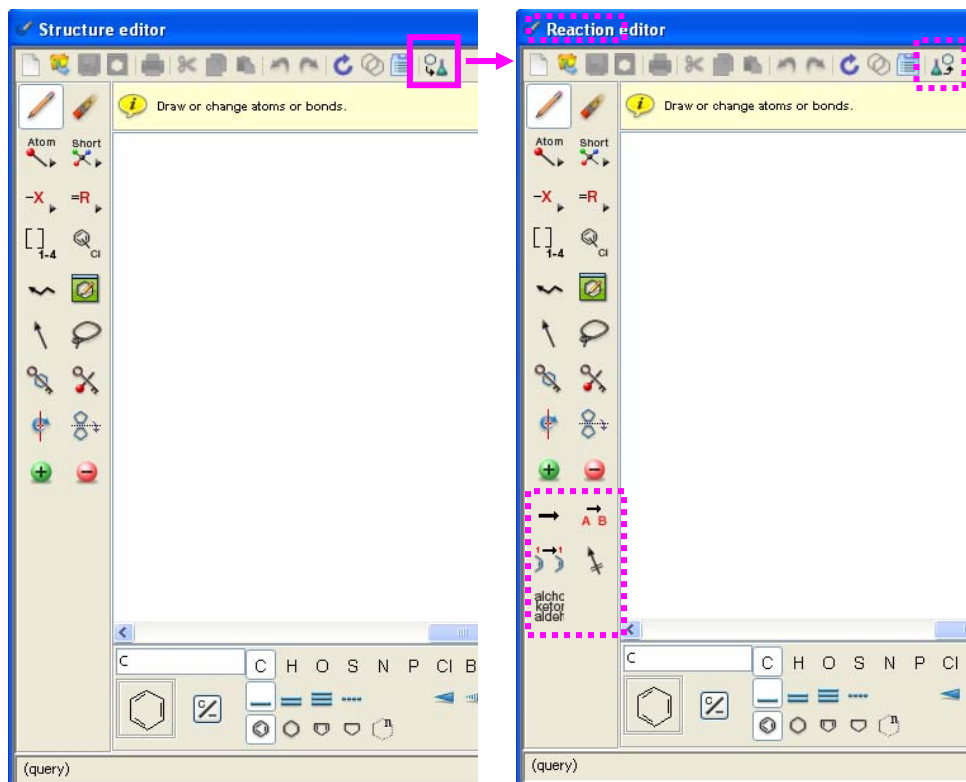


The screenshot shows a 'Reference Detail' page. At the top, there are navigation buttons: 'Get Substances', 'Get Reactions', 'Get Cited', 'Get Citing', and 'Get Full Text'. Below these are 'Link', 'Save', 'Print', and 'Export' buttons. A 'Previous / Next' button is highlighted with a pink border. The main content area displays the title '1. Mitigation of the Impact of Terrestrial Contamination on Organic Measurements from the Mars Science Laboratory', the authors 'By: ten Kate, Inge L.; Canham, John S.; Conrad, Pamela G.; Errigo, Therese; Katz, Ira; Mahaffy, Paul R.', and the abstract text. Below the abstract is an 'Indexing' section with a button for 'Mineralogical and Geological Chemistry (Section 53)'.

\* Unique to the web version.

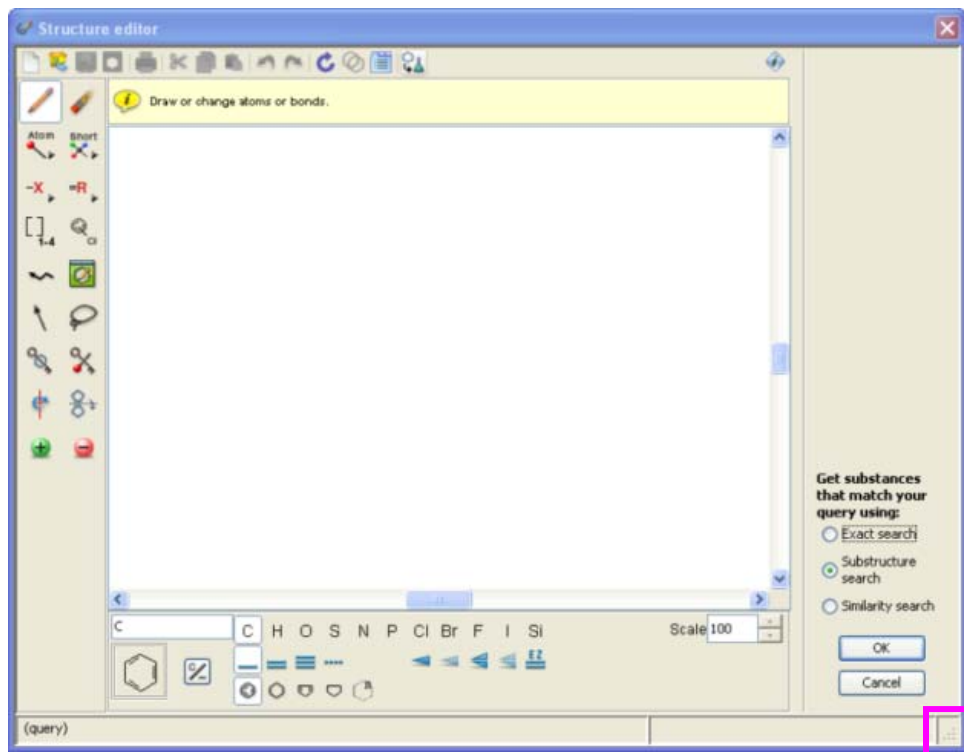
## Switch Easily between Structure and Reaction Editors

1. Without leaving the editor, click the new toolbar button to switch between "Structure" and "Reaction" drawing modes.



## Resize the Structure and Reaction Editors

1. Resize the Structure and Reaction editors by clicking-and-dragging the lower-right corner of the window.

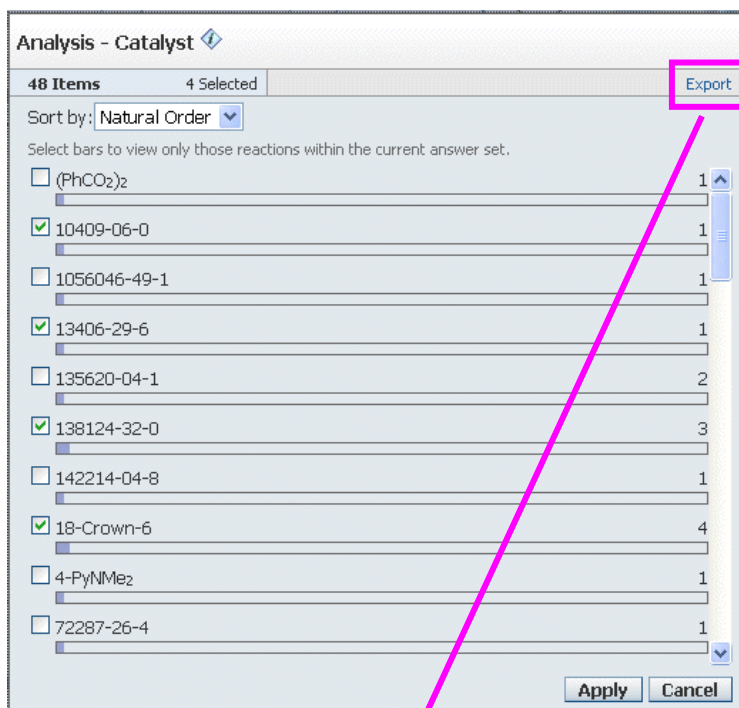


## Export Analysis Data\*

\* Unique to the web version.

## Export Analysis Data\*

1. Click **Export** to create a .pdf or .xls file and save it to a local or shared file location.



Analysis - Catalyst

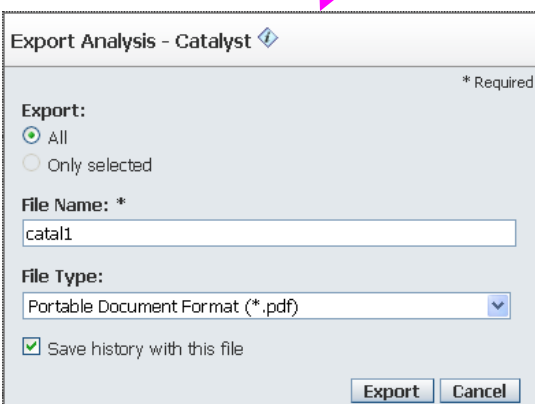
48 Items 4 Selected

Sort by: Natural Order

Select bars to view only those reactions within the current answer set.

<input type="checkbox"/>	(PhCO <sub>2</sub> ) <sub>2</sub>	1
<input checked="" type="checkbox"/>	10409-06-0	1
<input type="checkbox"/>	1056046-49-1	1
<input checked="" type="checkbox"/>	13406-29-6	1
<input type="checkbox"/>	135620-04-1	2
<input checked="" type="checkbox"/>	138124-32-0	3
<input type="checkbox"/>	142214-04-8	1
<input checked="" type="checkbox"/>	18-Crown-6	4
<input type="checkbox"/>	4-PyNMe <sub>2</sub>	1
<input type="checkbox"/>	72287-26-4	1

Apply Cancel



Export Analysis - Catalyst

\* Required

Export:

All

Only selected

File Name: \*

catal1

File Type:

Portable Document Format (\*.pdf)

Save history with this file

Export Cancel

## Export Analysis Data\* (cont'd)

2. View analysis data or use it to report findings to colleagues.

SciFinder® Page 2  
Catalyst  
Jun 11, 2009  
Sorted by Natural Order  
4 Selected terms of 48

<input type="checkbox"/> (PhCO <sub>2</sub> ) <sub>2</sub>	1	<input type="checkbox"/> F <sub>3</sub> CCO <sub>2</sub> H	3
<input checked="" type="checkbox"/> 10409-06-0	1	<input type="checkbox"/> Fe(CO) <sub>5</sub>	1
<input type="checkbox"/> 1056046-49-1	1	<input type="checkbox"/> Fe <sub>3</sub> (CO) <sub>12</sub>	1
<input checked="" type="checkbox"/> 13406-29-6	1	<input type="checkbox"/> FeCl <sub>3</sub>	3
<input type="checkbox"/> 135620-04-1	2	<input type="checkbox"/> HSiCl <sub>3</sub>	1
<input checked="" type="checkbox"/> 138124-32-0	3	<input type="checkbox"/> I <sub>2</sub>	1
<input type="checkbox"/> 142214-04-8	1	<input type="checkbox"/> InCl <sub>3</sub>	1
<input checked="" type="checkbox"/> 18-Crown-6	4	<input type="checkbox"/> KOH	1



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