

REAXYS - 2010

<http://www.reaxys.com>

Beilstein / Gmelin / (Organic) Patents

| | |
|--|---------|
| Introduction / Registration | 1 - 2 |
| Reaxys Options | 3 |
| Reactions Searching | 4 |
| Reactions Search Results | 5 - 6 |
| Substances and Property Searching | 7 |
| Substances and Property Search Results | 8 - 9 |
| Text, Authors and more Searching | 10 |
| Text, Authors and more Search Results | 11 - 12 |
| References | 13 - 15 |

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Introduction:

Reaxys (1) is a web accessible chemical compound database that combines the online versions of the Beilstein, Gmelin and a new English language (organic) Patent Chemistry Database.

Reaxys runs on PC or MAC with Internet Explorer (6.0 or higher), Firefox (1.5 or higher), or Safari (2 or higher). A Java plug-in (1.5 or higher) is a prerequisite. With an institutional subscription, users have unlimited access with IP authentication.

Beilstein is based on Beilstein's Handbuch der Organischen Chemie (1771-1980) and selected organic chemistry journal articles beginning in 1981. A listing of journals excerpted is at:

<http://www.info.crossfirebeilstein.com/bsjournals.pdf>

Gmelin is based on Gmelin's Handbuch der Anorganischen Chemie (1771-1994) and selected inorganic/organometallic chemistry journal articles since 1995. A listing of journals excerpted is at:

<http://info.crossfiregmelin.com/GMJournals.pdf>

The Patent Chemistry Database (2) <http://www.info.patentchemistrydatabase.com/> is limited to English-language US(1976+), WO(1978+) & EP(1978+) patents, with IPC codes:

C07-Organic Chemistry / Organometallics (including named polymers and bio-sequences);
A61K-Medicinal, Dental and Toilet Preparations (with C07 as secondary IPC)
A01N-Biocides, Pesticides, Herbicides (Agrochemicals);
C09B-Dyes

Additional patent coverage (1869-1980) comes from Beilstein and Gmelin Handbuch records. Please note that foreign patents may have US and/or UK equivalents in SciFinder.

Reaxys Registration:

Click 'Register' to access Reaxys Registration in order to: choose a PC structure editor, select reaction and substance search options, etc. and save histories or create alerts (from search results).

reaxys®

Welcome to Reaxys

Query Results Synthesis Plans History My Alerts My Settings Help Register Login

Welcome to Reaxys Registration

Registration allows you to personalize Reaxys, save History and create Alerts. [Privacy Policy](#)

User Name *

Title Mr *

First Name *

Last Name *

Email *

Job title

Institution

Location

Password *

Confirm password *

I wish to receive special offers and promotions from Elsevier B.V. and its Elsevier group affiliates about Reaxys and other products and services related to my subject area(s) of interest.

Register

Figure 1. Welcome to Reaxys Registration

After 'Registration' and 'Login', click 'My Settings' .

Figure 2. 'My Settings' options.

Click 'Modify Application Settings' to replace the default structure editor ... Marvin Sketch (2a) with: Crossfire (PC only), Symyx (PC only), or ChemDraw (PC) structure editors.

Installing the Crossfire Structure Editor (2b) first requires installation of the Crossfire client <http://www.info.crossfirecommander.com/>

Installation of the ChemDraw (Version 11 or higher) requires an additional plug-in (2c).

Reaction ... and Substance search options can also be pre-set.

Figure 3. Reaxys – Modify Application Settings

Reaxys Search Options:

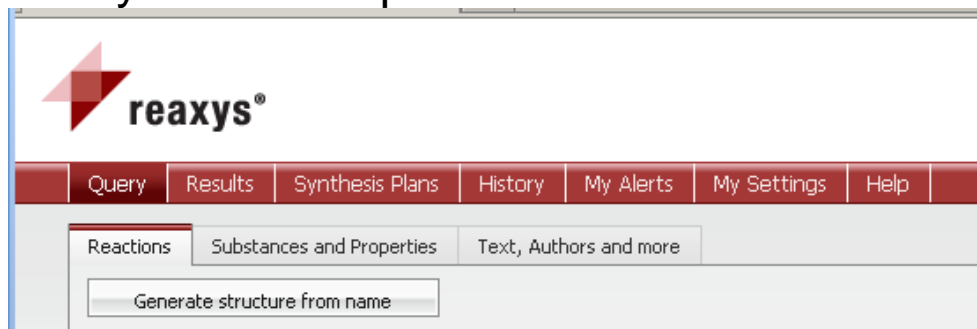


Figure 4. Reaxys Options

The 'Query', 'Results', and 'Synthesis Plans' tabs allow moving back and forth between these options during a search session.

The 'History' tab displays the session history, which includes an option to combine hit sets (3).

'My Alerts' shows all saved Alerts (4).

'Query' search options include:

- Reactions;
- Substances and Properties;
- Text, Authors and more.

'Generate Structure from name' accepts both chemical names (5) and textual identifiers (6):

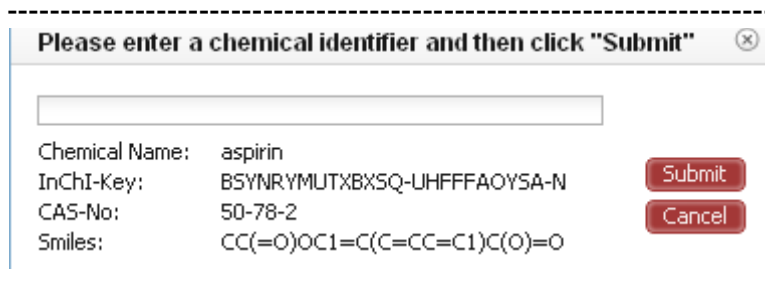


Figure 5. Generate Structure from Name

'Generate Structure from name' allows both full and right-truncated names. However, only one structure can be generated on the screen.

For example, entering brasilinolide* only retrieves the first compound listed in the Compound Name dictionary... brasilinolide A. To view the CN dictionary, click 'Substances and Properties, ... then Properties (Advanced), ... then Show Fields and Operators, then open Identification, and open Substance Identification and click on Chemical Name, and click on [...] and type brasilinoide.

Ctrl/Click the compounds of interest, click Transfer and click Search.

This is equivalent to typing: IDE.CN = Brasilinolide* which retrieves 5 compound records. The three records for Brasilinolide A are a result of authors giving the same name to slightly different structures.

Generate Structure from Name does not recognize (+/-) and (R/S) descriptors. Bonds may be manually edited to designate stereochemistry.

Reactions searching: (structure generated from name=aspirin)

Figure 6. Reactions search screen

Double clicking the structure frame opens the structure editor ... which allows drawing complete or partial reactions, modifying generated structures (6a) and atom mapping (6b). Use the lasso tool and the Edit menu for copy/paste, etc.

Please note that organometallic compounds with unusual bonding (e.g. Ferrocene) will generate a structure that requires 'cleaning' (6c) and checking off 'ignore stereo' to be searchable.

'Reactions' structure searching allows limiting to: product, starting material, any role or reagent/catalyst, and either 'as drawn' or 'substructure'. It also provides options to restrict: stereo, isotopes, charges, radicals, etc. It is not possible to restrict salts or mixtures from the reaction results.

Conditions (Form-based) + Reaction Data allows searching or refining with: reactants or products (NOTE: the 1st compound name listed (7a), must be used); a reagent/catalyst; range of yields, etc.) or Bibliographic Data (e.g., an author, patent assignee, journal title, etc.)

Conditions (Advanced) + Show Fields and Operators ... offers additional Reaction Data options: (number of steps, solvent, temperature, etc.)

Use any of the 'Conditions' fields will limit the reaction to substances with these constraints.

If an 'As drawn' search results in no hits, Reaxys will automatically search for 'substructure on heteroatoms' and then, if necessary, 'substructure on all atoms', unless disabled (7b)

Please use the 'Copy to Substances' tab since switching will erase the structure displayed.

Please note the presence of a large number of half-reactions (e.g., product only)

Reactions search results:

The screenshot shows the Reaxys interface with a search query for Aspirin. The results are displayed in a table with columns for Yield, Conditions, and References. The top reaction is highlighted, showing the chemical structures of Acetic Anhydride, Salicylic Acid, and Aspirin. The table lists three reactions with yields of 99%, 95%, and 93%.

| Yield | Conditions | References |
|-------|--|---|
| 99% | With erbium(III) chloride 0.2 h; Heating; | Dalpozzo, Renato; Nino, Antonio De; Maiuolo, Loredana; Oliverio, Manuela; Procopio, Antonio; Russo, Beatrice; Tocci, Amedeo Australian Journal of Chemistry, 2007, vol. 60, # 1 p. 75 - 79 Title/Abstract Full Text View citing articles Show Details |
| 95% | With nano-crystalline sulfated zirconia T=120°C; 0.5 h; | Tyagi, Beena; Mishra, Manish Kumar; Jasra, Raksh Vir 2010, vol. 317, # 1-2 p. 41 - 45 Title/Abstract Full Text View citing articles Show Details |
| 93% | With anhydrous magnesium perchlorate T=20°C; 2 h; | Chakraborti, Asit K.; Sharma, Lalima; Gulhane, Rajesh; Shivani Tetrahedron, 2003, vol. 59, # 39 p. 7661 - 7668 Title/Abstract Full Text View citing articles Show Details |

Figure 7: 'Reactions' search results for Aspirin as a product and Acetic Anhydride as a reactant

'Reactions' search results screen (note 'Show Next ...')

A listing of reactions (Show Next for more) ranked by yield with reagents, and references

'Filter by' options

Tabs for: 'Commercial availability' from eMolecules and Symyx ACD

'Display further options ...' (e.g. Compound Data, Copy/View Structure options)

'Enlarge Structure & rotate in 3D'

'Synthesize' links for both reactants and products to display 'Synthesis Plans'.

References have links to: Title/Abstract; Full Text; View citing articles (in Scopus) and Show Details(links to 'All reactions' and 'All substances' in that article).

'Citations' search results screen has:

Title of the Document / Authors / Year / Source / Times cited

Links to: Full Text and View citing articles

Links to: Title/Abstract or FrontPage Information (if available for patents); Show all Reactions; Hit Reactions in this article; Show all Substances.

Additional display options include:

Limit to Selection (check off specific reactions/click) / Output / Quick Print / Sort by

Output ... offers:

reaxys®

Output Reaction Results

Output Reactions Table Reactions Citation Table

to PDF/Print XML Microsoft Word Microsoft Excel

Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File

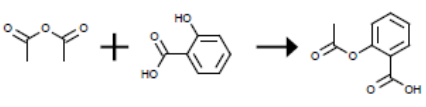
Include the following headline

Output range All Hits Range:
e.g. 1, 2-5, 10

Output contains include Structures include Experimental Procedure All available data Identification data only Hit data only

Quick Print display:

reaxys® Acetic Acid -> Aspirin



Rx-ID: 572028

| Yield | Conditions & References |
|-------|--|
| 99 % | With erbium(III) chloride, Time= 0.2h, Heating Dalpozzo, Renato; Nino, Antonio De; Maiuolo, Loredana; Oliverio, Manuela; Procopio, Antonio; Russo, Beatrice; Tocci, Amedeo; Australian Journal of Chemistry; vol. 60; nb. 1; (2007); p. 75 - 79 |
| 93 % | With Mg(ClO ₄) ₂ , Time= 2h, T= 20 °C Chakraborti, Asit K.; Sharma, Lalima; Gulhane, Rajesh; Shivani; Tetrahedron; vol. 59; nb. 39; (2003); p. 7661 - 7668 |
| 93 % | Example Name 15 0.0072 moles of salicylic acid and 0.029 moles acetic anhydride (molar ratio of 1:4) were taken in a 20 ml reaction tube of reaction station. Nano-crystalline sulfated zirconia catalyst (SZ-2), activated at 450.deg. C. in static air with salicylic acid to catalyst weight ratio 10:1, was added and the mixture was heated at 120.deg. C. for 30 minutes. The reaction mixture was filtered to separate the catalyst. The acetyl salicylic acid was crystallized from the reaction mixture. The crude yield of acetyl salicylic acid was 93percent. |

Substances and Properties searching: (structure generated from name=aspirin)

reaxys®

Query Results Synthesis Plans History My Alerts My Settings Help

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw structure query

As drawn
Substructure:
on heteroatoms
on all atoms

Ignore stereo
No salts
No mixtures
No isotopes
No additional rings
Further options

Search

Properties (Form-based) Properties (Advanced)

Substance Data
Bibliographic Data

Clear Query Load Query/Batch Save Query

Figure 8: 'Substances and Properties' Search Interface

Please note that organometallic compounds with unusual bonding (e.g. Ferrocene) will Generate a structure from name that requires cleaning (6c) and checking off 'ignore stereo' to be searchable.

Structure searches will retrieve all stereochemical variants, salts, mixtures, isotopic variants, etc. (unless checked-off). Further Options include Markush structures and options for ions, radicals.

Checking off: Ignore Stereo, No salts, No mixtures, No isotopes, No charges, No radicals reduces the retrieval from over 350 'aspirin' substances to only 1 (aspirin).

Properties (Form-based) + Substance Data ... for limiting results to ranges of physical properties or with spectra or pharmacological data . + Bibliographic data could be used for specific authors, journals or article title words.

Properties (Advanced) + Show Fields and Operators ... offers a 'Search for Field' option. Clicking 'exists' adds that field to the search ... e.g., Spectra exists, NMR Spectra exists ...

Clicking Identification offers options to search: name segments (8), molecular formula, etc.

If a compound (7c) or segment name cannot be found, try searching in 'Text, Authors and more', as a name or segment may be included in an article title, along with an un-named structure.

If an 'As drawn' search results in no hits, Reaxys will automatically start searching for 'substructure on heteroatoms' and then, if necessary, 'substructure on all atoms', unless disabled (7b)

Substances and Properties search results:

reaxys®

Welcome to Reaxys
Dana Roth (dzrlb) is logged in

Query Results Synthesis Plans History My Alerts My Settings Help Logout

Query 368 substances

Create Alert

368 substances out of 2528 citations

Filter by:

- Sub-structure
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Natural Product
- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

Substances (Grid) Substances (Table) Citations

go to Page Page 1 of 13

Limit to Output Print Zoom in Zoom out Hide Sort by No of References

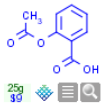
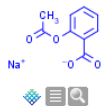
| Structure | Chemical Name | N° of preparations All Preps All Reactions | Available Data | N° of ref. | Boiling Point |
|--|--|---|---|------------|---------------|
|  Synthesize Show Details | acetylsalicylic acid O-acetyl salicylic acid 2-(acetyloxy)-benzoic acid 2-(acetyloxy)benzoic acid 2-(acetoxy)benzoic acid 2-acetoxy-benzoic acid 2-acetoxybenzoic acid | 88 prep out of 575 reactions. | Identification Physical Data (444) Spectra (100) Bioactivity/ECotox (2105) Use/Application (3131) | 2337 | |
|  Synthesize Show Details | sodium salt of acetylsalicylic acid acetyl salicylic acid sodium salt acetylsalicylic acid, sodium salt sodium acetylsalicylate sodium salt of aspirin Aspirin sodium salt sodium salicylate | 4 prep out of 41 reactions. | Identification Physical Data (9) Spectra (5) Bioactivity/ECotox (12) Use/Application (54) | 39 | |

Figure 9. Substances and Properties search results – Substances (Table)

1. 'Substances (Table)' results screen has:

'Filter by' options

Tabs for: 'Commercial availability' from eMolecules

'Display further options ...' (e.g. Compound Data, Copy/View Structure options)

'Enlarge Structure & rotate in 3D'

'Synthesize' link to Synthesis Plans ... Show Details (links to properties)

A listing of Structures; Chemical Names; number of preparations (with links to All Preps or All Reactions, links to available property data and the number of (and link to) literature references.

2. 'Substances(Grid)' search results screen omits: Chemical Names, numbers of preparations & refs

3. 'Citations' search results screen has:

Title of the Document / Authors / Year / Source / Times cited

Links to: Title/Abstract & FrontPage Information (if available); Show all Reactions; Show all Substances; and Hit Substances in this article).

Additional display options include:

Limit to Selection ... specific reactions can be checked-off / Output / Quick Print / Sort by

Output ... offers:

reaxys®

Output Substance Results

Output Substance Grid Substance Details Table Substance Citations Table

to PDF/Print XML Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File

Microsoft Word Microsoft Excel SD/Molfile Smiles

Include the following headline

Output range All Hits Range: e.g. 1, 2-5, 10

Output contains include Structures All available data Identification data only Hit data only Select data

OK **Cancel**

Which gives a display similar to Quick Print:

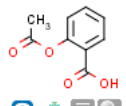
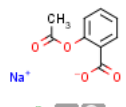
http://test02-www.reaxys.com/reaxys/secured/printpreview.jsp

Print

3 substances out of 2350 citations

Substances (Table)

Sort by **No of References** ↓

| | Structure | Chemical Name | N° of preparations | Available Data | N° of |
|---|--|--|-------------------------------------|--|-------|
| 1 |  Synthesize Show Details | acetylsalicylic acid O-acetyl salicylic acid 2-(acetyloxy)-benzoic acid 2-(acetoxy)benzoic acid 2-(acetoxy)-benzoic acid 2-acetoxybenzoic acid | 88 prep out of 566 reactions. | Identification Physical Data (443) Spectra (97) Bioactivity/Ecotox (1981) Use/Application (3125) | 2298 |
| 2 |  Synthesize Show Details | sodium salt of acetylsalicylic acid acetyl salicylic acid sodium salt acetylsalicylic acid, sodium salt sodium acetylsalicylate sodium salt of aspirin Aspirin sodium salt sodium salicylate | 4 prep out of 41 reactions. | Identification Physical Data (9) Spectra (5) Bioactivity/Ecotox (12) Use/Application (54) | 39 |

Text, Authors and more searching

The screenshot shows the Reaxys search interface. At the top is the Reaxys logo. Below it is a navigation bar with tabs: Query, Results, Synthesis Plans, History, My Alerts, My Settings, and Help. The main content area has three tabs: Reactions, Substances and Properties, and Text, Authors and more. The 'Text, Authors and more' tab is active. It contains two sub-tabs: Form-based and Advanced. The 'Form-based' sub-tab is selected. The search form includes the following fields and options:

- Quick Search:** A large text input box with a dropdown arrow. Example text: e.g. Stereoselective AND reduction, e.g. Stereo*
- Author(s) Assignee(s):** A text input box with a dropdown arrow. Example text: e.g. Snyder, Peter A. or e.g. Sny*
- Journal Title:** A text input box with a dropdown arrow. Example text: e.g. Journal of Organic Chemistry, e.g. *organic*
- Patent Number:** A text input box with a dropdown arrow. Example text: e.g. US12345678
- Patent Country:** A text input box with a dropdown arrow. Example text: e.g. EP
- Publication Year:** A radio button for a year range (e.g. 2005, e.g. 2000-2008) and a radio button for 'All years'.

At the bottom of the form are four buttons: Clear Query, Load Query/Batch, Save Query, and Search (highlighted with a red box). Below the form is a footer with links: Contact Us | Support | About Reaxys | Terms and Conditions | Privacy Policy. Copyright © 2009 Elsevier Properties SA. All rights reserved. Reaxys® is owned and protected by Elsevier Properties SA and used under license.

Figure 10: Text, Authors and more [Form-based] search interface

'Form-based' searching for:

Text words; Author(s)/Assignee(s); Journal Title; Patent Number/Country; Publication Year

[...] Displays a dictionary ... listing entries ... including personal name variations.

Author name entries are not uniform: marcus r. a.; marcus, r. a.; marcus, rudolph a.

'Advanced' search interface / 'Show Fields and Operators' allows additional search options:

Expanding 'Bibliographic Data/Citation' offers searching with DOIs or ISSNs

Expanding 'Bibliographic Data/Patent Bibliography' offers searching with IPC codes

Expanding 'Physical Data', etc. offers searching with a wide variety of properties.

Text, Authors and more search results:

A search for 'stereoselective reduction' limited to publication year = 2010

reaxys®

Welcome to Reaxys
Anonymous user (131.215.226.152)

Query Results Synthesis Plans History My Alerts My Settings Help Register Login

Query citations 48 citations No structure

Create Alert

48 citations out of 1133 reactions and 1650 substances

Filter by:

- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year
- Yield
- Record Type
- Reagent/Catalyst
- Solvent
- Reaction Type
- No. of Steps
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Natural Product

Citations Reactions Substances (Grid) Substances (Table)

Limit to Output Print Zoom in Zoom out Hide Sort by Publication Year

| | Title of the Document | Authors | Year | Source | Times cited |
|---|---|---|------|---|-------------|
| <input type="checkbox"/> | Cyclisation of 1,2-dioxines containing tethered hydroxyl and carboxylic acid functionality: synthesis of tetrahydrofurans and dihydrofuran-2(3H)-ones | Taylor, Dennis K.; Zvarec, Ondrej; Avery, Thomas D.; Tiekink, Edward R. T. | 2010 | Tetrahedron, 2010, vol. 66, # 4 p. 1007 - 1013 Full Text View citing articles | |
| Title/Abstract Herein we outline cyclisations of tethered hydroxyl and carboxylic acid moieties onto the olefinic motif of 1,2-dioxines to generate tetrahydrofurans and dihydrofuran-2(3H)-ones, whilst maintaining the peroxide linkage intact. This work demonstrates the first examples of intramolecular cyclisation of tethered hydroxyl groupings onto 1,2-dioxines generating functionalised THFs in a highly stereoselective manner and includes improved methods for previously reported carboxylic acid tether cyclisations. Additionally, improved methods for the oxidation of 1,2-dioxines containing tethered alcohols to furnish tethered carboxylic acids are also detailed. Subsequent reduction of the peroxide linkage enables the generation of functionalised tetrahydrofurans and dihydrofuran-2(3H)-ones, which are useful building blocks for the construction of natural products. Show All Reactions (32) Show All Substances (36) | | | | | |
| <input type="checkbox"/> | Reduction of alkynyl α -hydroxy esters: Stereoselective α -ketol rearrangement | Hameury, Thomas; Bellosta, Ve; Cossy, Janine; Guillemont, Jerome; Van Hijfte, Luc | 2010 | European Journal of Organic Chemistry, 2010, # 4 p. 607 - 610 Full Text View citing articles | |

Figure 11: Text, Authors and more [Citation] search results

Citations results screen has:

Title of Document; Authors; (Publication) Year; Source; Times cited (link to Scopus)

Links to: Title/Abstract & FrontPage Information (patents); Show all Reactions ... Substances.

Filter by options.

Additional display options: Reactions; Substances (Grid); Substances (Table)

Limit to Selection: Specific citations can be checked-off / Output / Quick Print /

Sort by: Publication Year (default) or Document Type, Author, Journal Title.

Note: British English spelling

Output offers:



Output Citation Results

Output to

Citations Table Citation Reactions Table Citation Substances Grid Citation Substances Table

PDF/Print XML Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File

Microsoft Word

Microsoft Excel

Include the following headline

Output range

All Hits Range: e.g. 1, 2-5, 10

Output contains

include Abstracts

include Structures

include Reactions

All available data

Hit data only

Which gives a display similar to Quick Print:



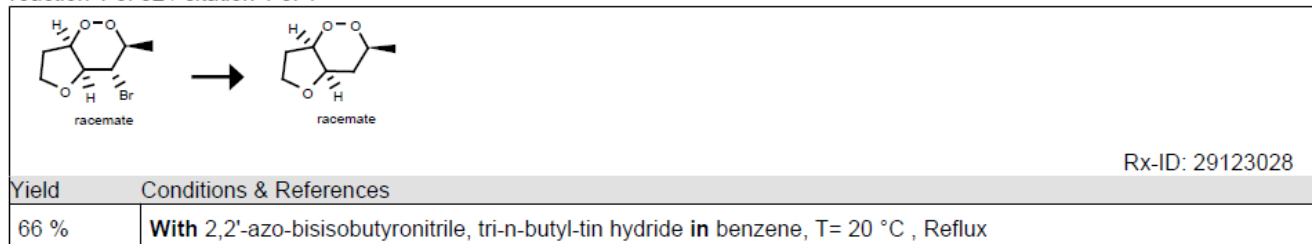
Taylor, Dennis K.; Zvarec, Ondrej; Avery, Thomas D.; Tiekink, Edward R. T.

Cyclisation of 1,2-dioxines containing tethered hydroxyl and carboxylic acid functionality: synthesis of tetrahydrofurans and dihydrofuran-2(3H)-ones

Tetrahedron; vol. 66; nb. 4; (2010); p. 1007 - 1013

Abstract: Herein we outline cyclisations of tethered hydroxyl and carboxylic acid moieties onto the olefinic motif of 1,2-dioxines to generate tetrahydrofurans and dihydrofuran-2(3H)-ones, whilst maintaining the peroxide linkage intact. This work demonstrates the first examples of intramolecular cyclisation of tethered hydroxyl groupings onto 1,2-dioxines generating functionalised THFs in a highly **stereoselective** manner and includes improved methods for previously reported carboxylic acid tether cyclisations. Additionally, improved methods for the oxidation of 1,2-dioxines containing tethered alcohols to furnish tethered carboxylic acids are also detailed. Subsequent **reduction** of the peroxide linkage enables the generation of functionalised tetrahydrofurans and dihydrofuran-2(3H)-ones, which are useful building blocks for the construction of natural products.

reaction 1 of 32 / citation 1 of 1



reaction 2 of 32 / citation 1 of 1

References:

1. Reaxys

What is Reaxys?

<https://www.lib.utexas.edu/chem/info/reaxys.html>

Versions (including statistics), Tested Environments, Release Notes:

https://www.reaxys.com/documentation/about_query.htm

Reaxys Quick Reference Guide

http://www.info.reaxys.com/userfiles/Reaxys_QRG_Feb2010.pdf

2. Patent Chemistry Database (updated bi-weekly) <http://www.info.patentchemistrydatabase.com/>

The Patent Chemistry Database (PCD) indexes reactions, experimental reaction text and substance related information from English language organic chemistry and life science patent documents published since 1976.

PCD complements CrossFire Beilstein, which covers patent literature from 1876 until 1980. PCD indexes one million prophetic compounds, and offers an easy-to-read, expanded Markush structure display and claims text.

Highlights:

- * excerpts not only specific ("real") substances with data, but also "prophetic compounds"
- * contains substances with their experimental bioactivity data*(since 12/2003+) ... e.g., IC/EC50-, Ki / Kd –values and allows exporting them to create structure activity relationship tables using CrossFire Commander.
- * displays the claims' text together with the Markush* structures and reactions (since 12/2003+)

2a. Tips for using ChemAxon MarvinSketch (and Crossfire, Symyx, ChemDraw editors)

https://www.reaxys.com/reaxys/WebHelp/All_Files/Tips_for_using_ChemAxon_MarvinSketch.htm

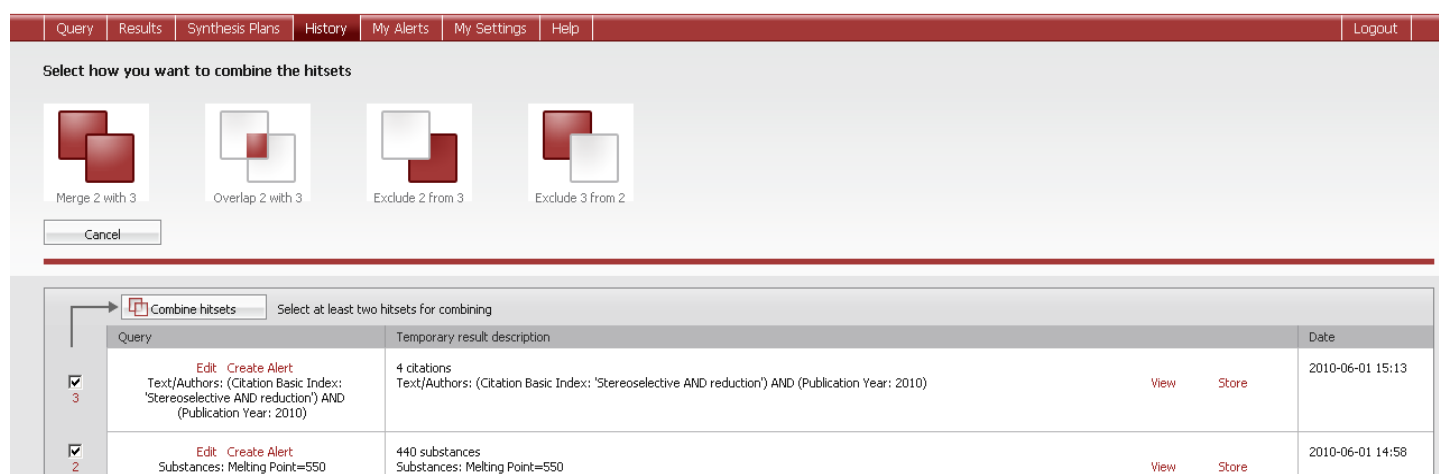
2b. Reaxys does NOT recommend long term use the Crossfire Structure Editor, since its search features will not be developed in the future, it will be simply continue to be compatible.

2c. CambridgeSoft ChemDraw - (Version 11 or higher). The connection software is Not included in the Reaxys Structure Editor plug-in and requires an additional plug-in. Please install CambridgeSoft ChemDraw **before** installing the Reaxys Structure Editor Plug-in. After installing both, please install the ChemDraw for Reaxys plug-in:

<http://scistore.cambridgesoft.com/ScistoreProductPage.aspx?ItemID=5943>

3. The History tab displays a listing of search queries and their 'temporary result descriptions'

These Queries can be combined



The screenshot shows a web application interface with a navigation bar at the top containing tabs: Query, Results, Synthesis Plans, History, My Alerts, My Settings, Help, and Logout. Below the navigation bar, there is a section titled "Select how you want to combine the hitsets" with four options: Merge 2 with 3, Overlap 2 with 3, Exclude 2 from 3, and Exclude 3 from 2. A "Cancel" button is located below these options. Below this section is a "Combine hitsets" dialog box with a "Select at least two hitsets for combining" prompt. The dialog box contains a table with the following data:

| Query | Temporary result description | Date |
|--|---|------------------|
| <input checked="" type="checkbox"/> 3 Edit Create Alert Text/Authors: (Citation Basic Index: 'Stereoselective AND reduction') AND (Publication Year: 2010) | 4 citations Text/Authors: (Citation Basic Index: 'Stereoselective AND reduction') AND (Publication Year: 2010) | 2010-06-01 15:13 |
| <input checked="" type="checkbox"/> 2 Edit Create Alert Substances: Melting Point=550 | 440 substances Substances: Melting Point=550 | 2010-06-01 14:58 |

4. 'Create Alerts' (Reaction, Substance, Author or Text) that are sent out each time the database is updated. The 'Create Alert' tab is located on the Results page underneath the 'Query' breadcrumb.

5. Chemical name [http://en.wikipedia.org/wiki/IUPAC_nomenclature]

6. Textual Identifiers:

InChI-Key [<http://www.chemspider.com/blog/?p=125>]

**CAS-No [http://en.wikipedia.org/wiki/CAS_registry_number]

Smiles string [http://en.wikipedia.org/wiki/Simplified_molecular_input_line_entry_specification]

**CAS Registry Numbers (December 19, 2008)

CAS is helping Elsevier identify additional CAS Registry Numbers through an automated, first level, "machine comparison", which is neither comprehensive nor detailed, so this addition of Registry numbers does not represent a complete comparison of Elsevier resources with the CAS Registry.

6a. MarvinSketch – Modifying Structures

https://www.reaxys.com/reaxys/WebHelp/All_Files/Tips_for_using_ChemAxon_MarvinSketch.htm

Move-Rotate-Zoom ... Allow Substitution ... Block Substitution ... Substitution Count ...
Create an Atom List ... R groups ... R groups shortcuts ... Right click Features
Reaxys Predefined Generic Groups

Query tab (now labeled Periodic Table-Advanced) offers a variety of Generic atoms, Atom query properties and Periodic Table Groups and R-Groups.

6b. MarvinSketch - Atom Mapping:

Draw a reaction arrow between the structures, which turns on the 'add atom maps' button. Then draw a line between the appropriate atoms and click 'Transfer Query'.

NOT all reactions are mapped, so it is important to also search with 'Ignore Atom Mappings', and for compounds as Products. The data for 7/01/10 (expanding on RX.RTYP (record type):

full reaction - 23.424.112 half reaction - 5.216.670 has multi-step - 11.567.223

has preparation - 16.263.841 no reaction scheme - 275.721

6c. MarvinSketch – After a 'Generate structure from name' for Ferrocene, transfer the structure to the structure editor and under the 'Object' tab, click on 'Clean Molecule'.

7a. The 1st name listed

Each compound in the database may have a list of synonymous names. For example:

Chemical Name: acetic anhydride; acetic acid anhydride; acetanhydride; acetic acid anhydride; Ac2O; anhydride acetique; Acetanhydrid

When searching with a compound name, in 'Conditions' (Form-based), the first chemical name listed must be used, i.e., acetic anhydride.

7b. My Settings/Modify application settings has an option to disable automatic search expansion ...

7c. Substances are named according to what is given in the article, which results in same name being listed for different structures (e.g. (+)-discodermolide)

8. Chemical name segments or molecular formulas (instead of structures) can be searched by first clicking 'Properties (Advanced)', then 'Show Fields and Operators', then expanding both 'Identification' and 'Substance Identification', and clicking, for example, on either 'Chemical Name Segment' or 'Molecular Formula' and the [...] box. Then type a name segment or molecular formula, and if found, 'click' to highlight and then click 'Transfer' ... and click 'Search'.

Selecting the chemical name segment '1763', results in a search for: 'IDE.CNS = 1763' and retrieves all compounds with this name segment (e.g., AH-1763 IIa; (14R,16R)-AH-1763 IIA; (14S,16R)-AH-1763 IIA; and ENMD-1763), without generating a structure query. To generate a structure, that can be searched or modified, from these results, click on 'Show further options and data' [=] / 'Copy Structure to Query'. Double clicking in the 'frame' opens the Structure Editor for changes, if desired.

Selecting the molecular formula 'MgO' (caps are essential), results in a search for: IDE.MF = MgO For additional searches on other molecular formulas, simply highlight MgO and replace (for example) with Cr2MgO4 (must search with MF in alphabetical order).