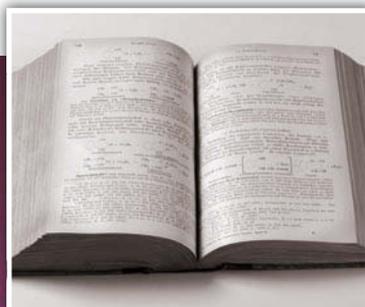


Science of Synthesis

Houben–Weyl Methods of Molecular Transformations®

The Electronic Version



Some things age – others simply get better.

http://www.science-of-synthesis.com/prod/curr/index.html?app=sos

Science of Synthesis

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31.21.1.30.2 Variation 2:
Using Hydrogen Peroxide

Aitken, K. M.; Aitken, R. A., in *Science of Synthesis*, 31 (2007), p.1228

Information on Science of Synthesis Volume 31
Feedback

Coumarin (2H-1-benzopyran-2-one) reacts with ammonium cerium(IV) nitrate in acetic acid to give 6-nitrocoumarin in 9%. Changing the solvent to water and the addition of aqueous hydrogen peroxide allows substituted coumarins to be nitrated with good selectivity at the 6-position, e.g. to give **87** (Scheme 59).^[181]

Scheme 59 Nitration of Coumarins Using Ammonium Cerium(IV) Nitrate–Hydrogen Peroxide^[181]

87 88-78%



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A truly authoritative online resource, **Science of Synthesis** offers comprehensive and in-depth coverage of synthetic organic chemistry. This work is designed to be the first point of reference for chemists searching for reliable synthetic methods.

Science of Synthesis focuses on the most effective and reliable methods for functional group transformations, and imparts essential reviews as well as detailed experimental procedures. Under the guidance of an international Editorial Board composed of distinguished chemists with unparalleled experience, over 1000 authors are contributing to **Science of Synthesis**. The volume editors and authors, who are leading experts in their respective fields, evaluate all the literature of relevance including the vast amount of primary literature available to modern researchers.

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All of the information contained within **Science of Synthesis** is presented in a logical, clear and didactic format with the methods being organized in a hierarchical system based on the compound or functional group to be synthesized. This system permits efficient and easy navigation through the series.

Electronic Interface

The electronic version of **Science of Synthesis** has been developed under the guidance of an international advisory board, each of whom is a leading expert in electronic information provision.



Co-operation with InfoChem has ensured the use

of the latest developments in information technology and the availability of a powerful and user-friendly information-retrieval system for searching.

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- Pyridopyrimidines

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Scheme 4 Tautomerism of Pyridazinones^[47-53,55,56]

4A 4B

5A 5B

6A 6B 6C

The spectroscopic properties of pyridazine and many of its derivatives are discussed in some detail in *Houben-Weyl*, Vol. E 9a, pp 559-563, and they have been extensively reviewed elsewhere.^[7,8,16] ¹H NMR and ¹³C NMR spectroscopic data are available for a very large number of pyridazines; the proton chemical shifts and coupling constants for a selection of simple representatives are presented in Table 2.^[58] The ¹³C NMR spectroscopic properties of the parent heterene are given in Scheme 5; chemical shifts for some 3- and 4-substituted derivatives are listed in Table 3 in order to illustrate the influence of various functional groups on the shift values of the ring carbon atoms.^[58] A systematic collection of ¹³C NMR chemical shift data for 3,6-disubstituted pyridazines has also been published.^[57]

Table 2 ¹H NMR Data of Some Pyridazines^[58]

| Substituent | Chemical Shift ^a (δ) | Coupling Constants ^a (Hz) |
|-------------|---------------------------------|--------------------------------------|
|-------------|---------------------------------|--------------------------------------|

Intuitive Navigation

Users may browse through **Science of Synthesis** using the hierarchical table of contents in the left hand frame. The frame tiling buttons allow the user to view both the table of contents and the full text side-by-side, or either frame in full screen for comfortable reading. Further exploration is facilitated by the browse command, which downloads successive documents as if the user were leafing through the pages of a book.

Extensive cross-linking allows smooth navigation between **Science of Synthesis** and related content in the Houben-Weyl archive. In addition links from each citation enable fast access to the original research literature.

Printing

Science of Synthesis offers high quality printing to deliver a hard copy for convenience in the lab. The print-out contains high resolution graphics embedded in the document. Users can print individual documents using the print command in the document frame. Printing of multiple documents is possible with a single click of the mouse directly from the table of contents.

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The Query form, Hitlist, and Full text can be viewed in parallel for ease of use and quick cross-checking of search results and hit documents.

Synthesis

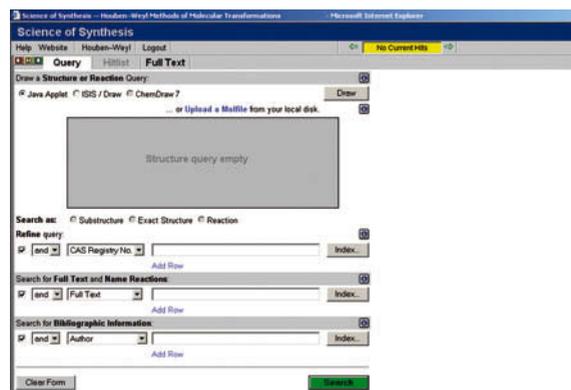
Searching in Science of Synthesis

Today's chemists need reference works to be readily available, practical and reliable. **Science of Synthesis: Houben-Weyl Methods of Molecular Transformations**, offers the user access to a vast quantity of evaluated information all on an electronic platform. This 21st century reference work combines new developments with established and proven methods, making it truly the most comprehensive database in terms of coverage available today.

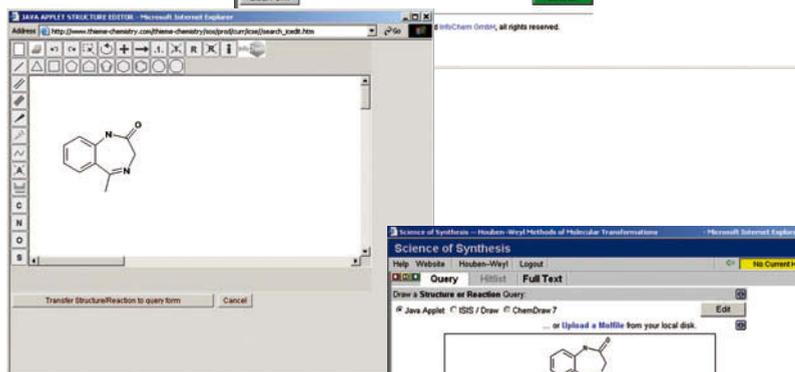
Searching for a synthesis of Valium

The search demonstrated on the right hand side highlights some of the key features and functions available when using **Science of Synthesis**.

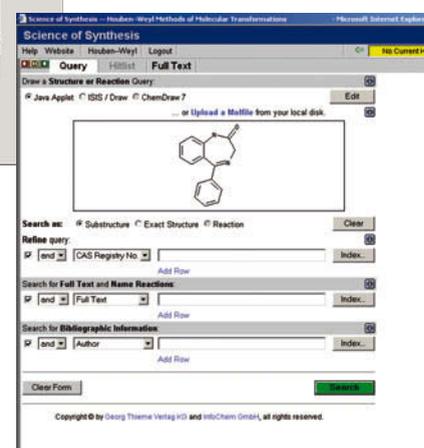
1 Open the draw window by clicking on the Draw button in the Search interface.



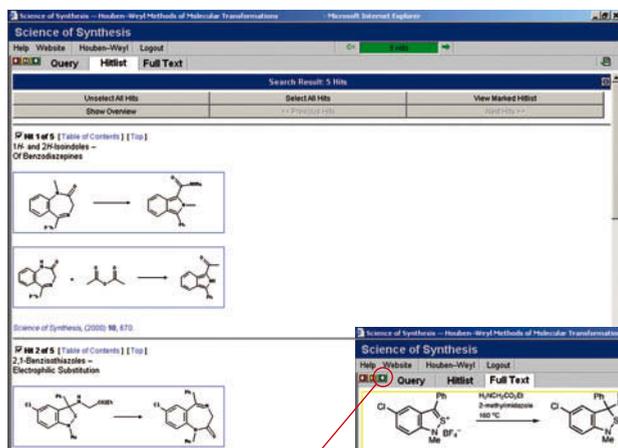
2 Use the drawing tools to draw the structure of interest.



3 Transfer the structure back to the Search interface using the transfer button and begin the search using the Search button.



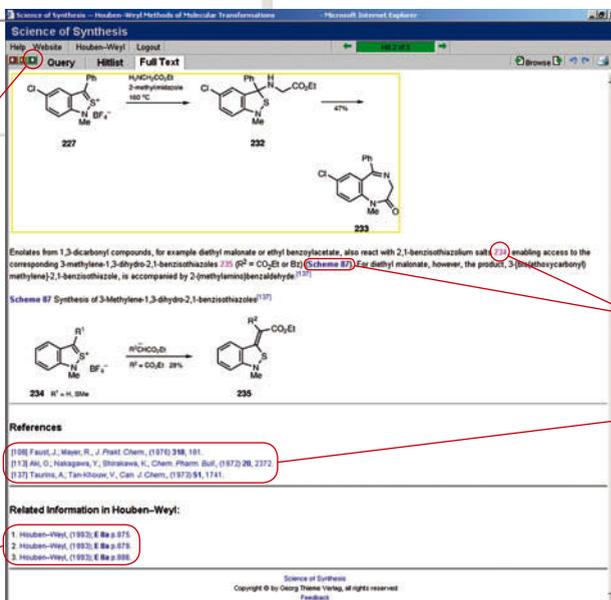
4 The hits are listed as single step reactions. To view a document simply click on the citation or the single step reaction.



The full screen view of the document is available by using the green button in the top left hand corner of each frame.

5 The final search result is displayed with the sections of the document that are pertinent to the search highlighted in yellow.

Links to relevant documents in the electronic backfile are listed at the bottom of the document.



6 Internal cross-referencing within a contribution or volume is fully supported within Science of Synthesis.

Moreover, links to databases and electronic journals are also supported by CrossRef and FIZ AutoDoc.

A Century of Synthetic Organic Chemistry

Back to 1909 ...

The entire Houben–Weyl series, published from 1909 to 2003, is available through the **Science of Synthesis** interface as an electronic backfile. Houben–Weyl documents, available in pdf format, are accessible through links from the latest content in **Science of Synthesis**.

Science of Synthesis documents are linked to related information in the electronic backfile, providing access to the robust and timetested synthetic methods of the past 100 years. References in the electronic backfile go back as far as 1834.

The electronic backfile can also be searched independently from the content of **Science of Synthesis**, via a search of the table of contents or for a name reaction.

In addition, the inclusion of an exclusive structural template facilitates searching in the electronic backfile and permits straightforward information retrieval.

Chemists now have fast access to the **146 000** product specific experimental procedures contained within the electronic backfile, including some **580 000** structures along with **700 000** references relating to the areas covered in each volume.

The screenshot displays the Science of Synthesis interface. On the left, a 'Table of Contents' sidebar lists various categories such as 'Organometallics', 'Monoalkylcopper(I) Compounds', and 'Heterenes'. The main window shows a search result for 'Ethyl (S)-3-(tert-butylidimethylthio)propanoate'. The result includes a chemical structure, a brief description of the synthesis procedure (e.g., 'A 1.0 M soln of CH₂=CHMgBr freshly distilled THF (60 mL) at P(OEt)₃ (10.3 mL, 60 mmol) at iodobutanoate (11.17 g, 30 mmol) before allowing to warm to room temperature, extracted with Et₂O, dried (Mg), hexanes/Et₂O) to give 124 as a colorless oil'), a list of references, and a 'Related information in Houben–Weyl:' section with a link to '1. Houben–Weyl, (1995), E 21b p.2041'. The right side of the interface shows a 'Query' box and a 'Hitlist' with a 'PDF' button. The background shows a preview of a document page with a table of contents and chemical structures.

... and into the Future

From 2010 onwards, the organic chemistry reference series **Science of Synthesis** is going to be continuously updated with high-quality content using clearly defined criteria for method selection as well as established editorial processes. The Editorial Board, in conjunction with the volume editors and authors, is reviewing the whole field of synthetic organic chemistry as presented in **Science of Synthesis** and evaluating significant developments in synthetic methodology.

A list of strict criteria for method selection guides the updating process in order to guarantee that only the best and most reliable synthetic methods are included in **Science of Synthesis**. Authors who are renowned specialists in their respective fields, add new methods and add new (or completely revise existing) product (sub)classes. In addition, the existing series will be complemented by a variety of organic synthesis specialist topic reference works. The first of which is **Stereoselective Synthesis**, which is scheduled to be published in October 2010.

The updating procedure is a continuous one and new content will be added to the electronic version in four releases per year. **Science of Synthesis** continues to be the most up-to-date evaluated electronic reference work available, emphasizing the most significant developments in synthetic methodology. The electronic version's intuitive interface adapts in keeping with the latest technological developments and will enable chemists worldwide in both academia and industry to solve complex synthetic problems.

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