

Edition

14

SEARCH GUIDE

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The Merck Index 14<sup>th</sup> Edition Web

The Merck Index

# The Merck Index Search Screen Help Guide

## Compound Names searches:

Monograph Title (Bisotrizole)  
CAS Name (5-butylpicolinic acid)  
Additional Names (betulic acid)  
Trademark (Coumadin)  
Manufacturer Code (H-168)  
Derivative Type (hydrochloride)

## Literature References and Notes

Search by keywords (inhibitor, antioxidant, herb), author, journal title, reference type (prepn, isoln, determ, clinical, pharmacology, review), caution statement (carcinogen, overexposure)

## Manufacturer (BASF)

Consult Company Register in the Supplemental Tables section of the book for company abbreviations

## Properties (Full Text)

Search by keywords (solid, yellow, vapor pressure)

## Molecular Formula searches:

Line Formula  
Molecular Formula  
Derivative Molecular Formula  
Extra Formula

Use Hill Convention (C, then H, then other elements in alphabetical order)

## Molecular Weight

Search parent and derivative molecular weights as numerical ranges

## TEXT SEARCH [Help](#)

Compound Names   
CAS Registry Number   
Literature References and Notes   
Manufacturers   
Full Text

Monograph Title  <  
Non-Medical Uses  <  
Human Therapeutic Use  <  
Veterinary Therapeutic Use  <

## PROPERTIES SEARCH [Help](#)

Properties (Full Text)   
Mol Formula   
Mol Weight  g/mol  
Boiling Point  °C  
Melting Point  °C  
pKa   
Log P   
Atom Count

Density   
Index of Refraction   
Optical Rotation   
Flash Point  °F  °C  
Absorption Max  nm  
Toxicity   
Monograph #

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### Monograph Title

(Entecavir, Mepact, Noviflumuron)  
Searches only the monograph title as it appears in the book

### Non-Medical Uses

Search by keywords (solvent, catalyst, herbicide)

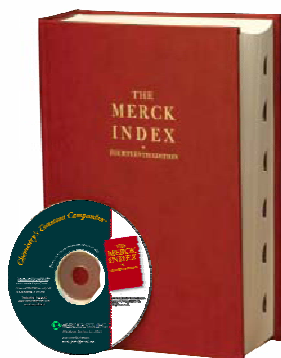
### Human Therapeutic Use (vasodilator)

Searches the therapeutic categories and associated index terms  
Consult Therapeutic Category and Biological Activity Index in the back of book

### Veterinary Therapeutic Use (antibacterial, anthelmintic)

### Notes

- Properties are range searchable except for Molecular Formula
- Temperatures are given in °C unless otherwise noted
- Examples are included in parenthesis following the field name



Welcome to *The Merck Index* 14<sup>th</sup> Edition internet product! The same valuable information found in *The Merck Index* 14<sup>th</sup> Edition book is also at your fingertips through this fully searchable website. The information is divided into three primary areas: Compound Search, Organic Name Reactions, and Supplemental Tables. Compound Search provides access to the compound monographs through text, numerical, and structure searching. Organic Name Reactions (ONRs) provide searchable access to organic chemical reactions referred to by name in the chemistry community. The Supplemental Tables cover a range of supporting information in the chemical, biomedical, and pharmaceutical sciences.

## Getting Started

To access Compound Search, Organic Name Reactions, or Supplemental Tables, click on the link provided.

### Main Menu

The main menu provides access to the search interface as well as links to the supplemental tables, user help guides, technical support, and content information.

*The Merck Index* is an encyclopedia of chemicals, drugs, and biologicals that contains more than 10,000 monographs. Each monograph in this authoritative reference source is a concise description of a single substance or a small group of closely related compounds.

- Compound Search**  
Basic   Structure (Plug-in required; Download Now)
- Organic Name Reactions**
- Supplemental Tables**
- User Help Guides**
- Technical Support**
- About *The Merck Index***
- Purchase *The Merck Index* Book**

*Chemistry's Constant Companion™*

**MERCK & CO., INC.**  
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Navigate between the different features by selecting the tabs at the top of the page.



## Compound Search

To conduct a query over *The Merck Index* content, click on Compound Search from the main menu. When the search form opens, place your cursor in any of the fields. Enter a keyword, numerical value, or a combination thereof. Keywords should be used for the fields in the Text Search portion of the search form. Numerical values should be used for the fields in Properties Search portion of the search form with the exception of the Properties (Full text). The Search Screen Help Guide, located at the front of this document, provides a quick overview of the types of information that are ideal for each search field.

There are two search interfaces both with the same search fields. The primary difference is that the Structure Search option allows substructure searches to be conducted over *The Merck Index* data using the ChemDraw plug-in.

### Basic Search Screen

## Structure Search Screen


LOG OFF

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[HOMEPAGE](#)

[BASIC SEARCH](#)

[STRUCTURE SEARCH](#)

[ORGANIC NAME REACTIONS](#)

[SUPPLEMENTAL TABLES](#)


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**Total Records**  
11189

[File](#) [Queries](#) [Hit Lists](#) [Marked Hits](#) [Help](#) [Home](#)

Search Active Monographs
  Search Active + Retired Monographs

**Tools**




**STRUCTURE SEARCH** [Help](#)

Substructure

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**Tools**




**TEXT SEARCH** [Help](#)

Compound Names	<input type="text"/>	Monograph Title	<input type="text"/>
CAS Registry Number	<input type="text"/>	Non-Medical Uses	<input type="text"/>
Literature References and Notes	<input type="text"/>	Human Therapeutic Use	<input type="text"/>
Manufacturer	<input type="text"/>	Veterinary Therapeutic Use	<input type="text"/>
Full Text	<input type="text"/>		

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**Tools**



**PROPERTIES SEARCH** [Help](#)

Properties (Full Text)	<input type="text"/>	Density	<input type="text"/>
Mol Formula	<input type="text"/>	Index of Refraction	<input type="text"/>
Mol Weight	<input type="text"/> g/mol	Optical Rotation	<input type="text"/>
Boiling Point	<input type="text"/> °C	Flash Point	<input type="text"/> F <input type="text"/> C
Melting Point	<input type="text"/> °C	Absorption Max	<input type="text"/> nm
pKa	<input type="text"/>	Toxicity	<input type="text"/>
Log P	<input type="text"/>	Monograph #	<input type="text"/>
Atom Count	<input type="text"/>		

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## Search Options

With each edition of *The Merck Index* monographs must be retired to make room for new information. Monographs that have been removed from the 12<sup>th</sup> and 13<sup>th</sup> editions are available in the 14<sup>th</sup> edition web version. Each retired monograph contains a statement at the bottom and has not been subject to updates.

- The default is to conduct searches over all active and retired monographs.
- If a search over only active monographs is preferred, select Search Active Monographs.
- After each search the default is restored and searches will be conducted over active and retired monographs unless the box next to Search Active Monographs is checked again.

Searches are executed by selecting Search or hitting Enter on the keyboard.

### Search Examples

A molecular formula search would be conducted as follows:

- Click in the Molecular Formula field.
- Type: C12 AND O4
  - This will retrieve records with molecular formulas containing 12 carbon atoms and 4 oxygen atoms.

**Mol Formula**

C12 AND O4

- Hit Enter on the keyboard or Search at the top of the screen to execute the search.
- Acifran is the first monograph that will appear

A search for a compound by name can be conducted in two ways. If the name of interest is the title of a monograph, use the Monograph Title field. If uncertain whether the name of interest is the title of a monograph, then use the Compound Names field. The Compound Names field searches the following: monograph title, CAS Name, additional names, trademarks, manufacturer codes, and derivative types.

- Click in the Compound Names field.
- Type benz
  - Records containing fragment benz in the monograph title, CAS Name, additional names, trademarks, manufacturer codes, or derivative type are retrieved
- Hit Enter on the keyboard or Search at the top of the screen.

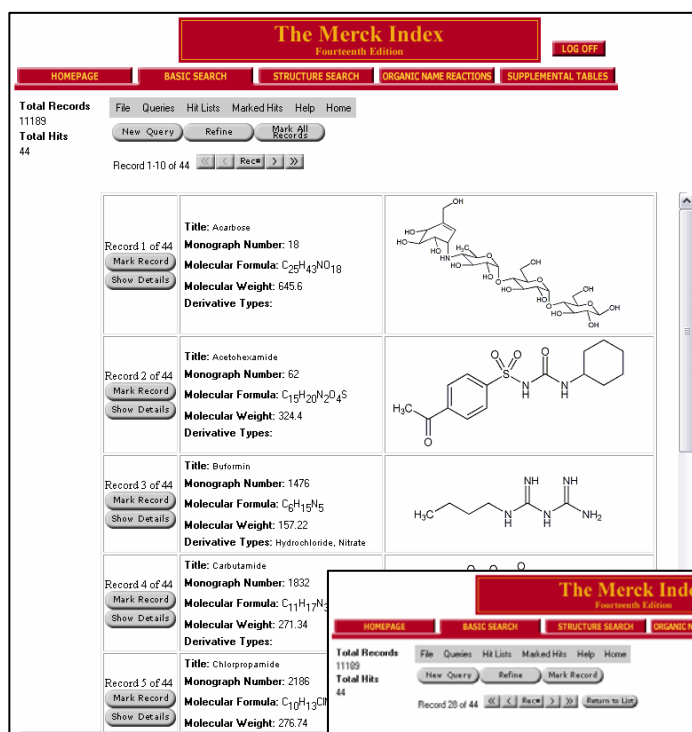
### Search Screen Help Guide

The Search Screen Help Guide, located at the front of this document, provides a quick overview of the types of information ideal for each search field.

A numerical search can be performed using either an exact value or a range of values. One example is to search by molecular weight. Clicking in the Molecular Weight and entering 90-100 will retrieve monographs with a molecular weight ranging between 90 and 100.

### View of Result

After each search is conducted the list view is compiled providing an easy and quick way to review the results from a search. If a particular monograph is of interest, select Show Details and the full monograph can be viewed.

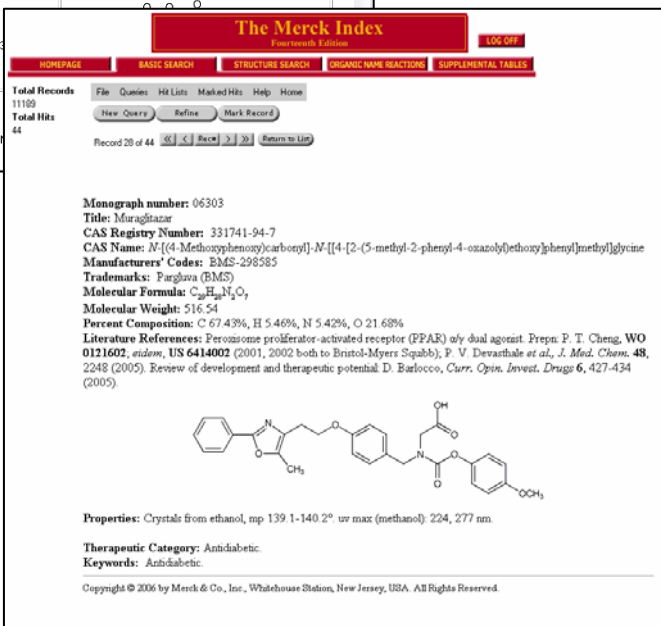


The screenshot shows a list of search results for 'The Merck Index'. The interface includes a navigation bar with 'HOME PAGE', 'BASIC SEARCH', 'STRUCTURE SEARCH', 'ORGANIC NAME REACTIONS', and 'SUPPLEMENTAL TABLES'. Below the navigation bar, there are options for 'File', 'Queries', 'Hit Lists', 'Marked Hits', 'Help', and 'Home'. The search results are displayed in a table with columns for 'Record', 'Title', 'Monograph Number', 'Molecular Formula', 'Molecular Weight', and 'Derivative Types'. The first five records are:

Record	Title	Monograph Number	Molecular Formula	Molecular Weight	Derivative Types
Record 1 of 44	Acarbose	18	$C_{25}H_{43}NO_{18}$	645.6	
Record 2 of 44	Acetohexamide	62	$C_{15}H_{20}N_2O_4S$	324.4	
Record 3 of 44	Bufomemin	1476	$C_8H_{15}N_5$	157.22	Hydrochloride, Nitrate
Record 4 of 44	Carbutamide	1832	$C_{11}H_{17}N_3$	271.34	
Record 5 of 44	Chlorpropamide	2186	$C_{17}H_{17}ClN_2O_2$	276.74	

▶ List View  
Provides a brief overview of the search results and enables quick browsing.

▶ Monograph View  
Provides details of a monograph



The screenshot shows the detailed monograph view for Miraglitazar (06303). The interface includes a navigation bar with 'HOME PAGE', 'BASIC SEARCH', 'STRUCTURE SEARCH', 'ORGANIC NAME REACTIONS', and 'SUPPLEMENTAL TABLES'. Below the navigation bar, there are options for 'File', 'Queries', 'Hit Lists', 'Marked Hits', 'Help', and 'Home'. The monograph details are as follows:

**Monograph number:** 06303  
**Title:** Miraglitazar  
**CAS Registry Number:** 331741-94-7  
**CAS Name:** *N*-[[4-(4-Methoxyphenoxy)carbonyl]-*N*'-[[4-[2-(5-methyl-2-phenyl-4-oxazolyl)ethoxy]phenyl]methyl]glycine  
**Manufacturers' Codes:** EMS-298585  
**Trademarks:** Parglona (BMS)  
**Molecular Formula:**  $C_{29}H_{34}N_4O_7$   
**Molecular Weight:** 516.54  
**Percent Composition:** C 67.43%, H 5.46%, N 5.42%, O 21.68%  
**Literature References:** Peroxisome proliferator-activated receptor (PPAR)  $\alpha$ 1 dual agonist. Prepn. P. T. Cheng, WO 0121602, *in situ*, US 6414002 (2001, 2002 both to Bristol-Myers Squibb), P. V. Desvarthale *et al.*, *J. Med. Chem.* **48**, 2248 (2005). Review of development and therapeutic potential. D. Barlocco, *Curr. Opin. Invest. Drugs* **6**, 427-434 (2005).

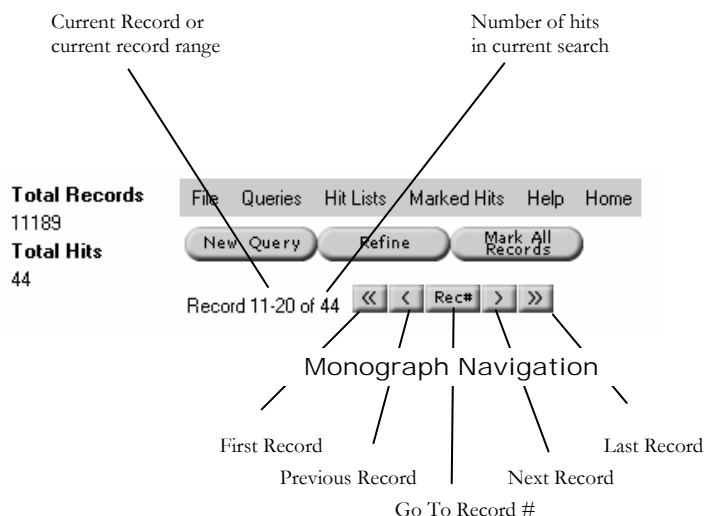
**Properties:** Crystals from ethanol, mp 139-140.2°; *uv* max (methanol): 224, 277 nm.

**Therapeutic Category:** Antidiabetic.  
**Keywords:** Antidiabetic.

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### Navigation Toolbar

The navigation toolbar allows browsing in list view and monograph view. Total Records indicates the number of monographs in *The Merck Index* database. Total Hits indicates the number of hits resulting from the current search. Browse through monographs or monograph lists by using right and left arrows. Go directly to a specific monograph by using Rec #. When the Record Number dialog box appears, enter the desired record number from the current list and click OK.



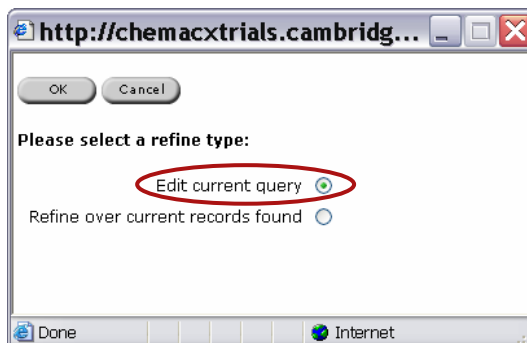
### Broadening or Narrowing Search Retrieval

Search retrieval can be modified in a number of ways. Multiple keywords or numerical values can be entered in the search form when conducting an initial search. Boolean operators “AND” and “OR” can be used to broaden or narrow a given search; the terms must be entered as capital letters, for example: nucleotide AND nucleoside. The Refine feature allows revisions either of the current search query or over the search results of the current search query.

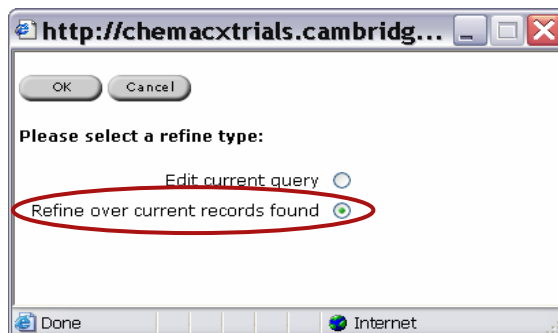
- To refine search results, click on Refine from the Navigation Toolbar.



- Editing the original search query will return to the search form to allow modification. The revised search will be conducted over the entire database.



- Refining over the current records searches only the records that were included in the original answer set.



## Performing a Structure Search

Structure searching is an option through the use of the ChemDraw plugin. This plugin can be downloaded from *The Merck Index* homepage at <http://themerckindex.cambridgesoft.com/>. Structures are drawn using ChemDraw. More information on using ChemDraw can be found at [www.cambridgesoft.com](http://www.cambridgesoft.com).

Structure searches may be used to find compounds which:

- contain the drawn structure as a substructure (the default setting)
- are identical to the drawn structure
- are similar to the drawn structure
- and can be combined with text and properties searching

## Structure Search Preferences

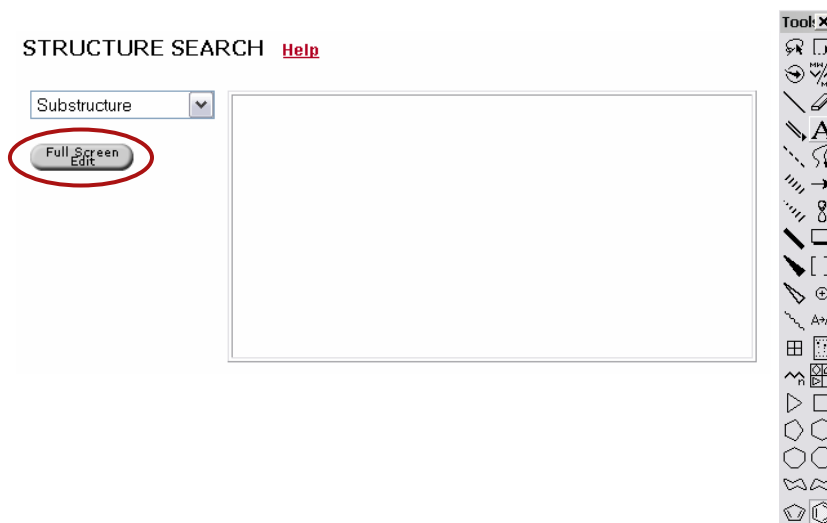
Four different search preferences are available. The default is substructure. Conducting a substructure search yields structures that contain the query and any additional attachments at the open positions. A full structure search identifies structures as drawn, without additional attachments. Isotopes are recognized as hits using the full structure search preference. Exact structure searching yields structures exactly as drawn (taking stereochemistry into account); isotopes are not recognized as hits. Tanimoto structure search identifies structures that have features similar to those in the query structure.

Structure Search Preferences  
Select from Substructure, Full, Exact, or Tanimoto.



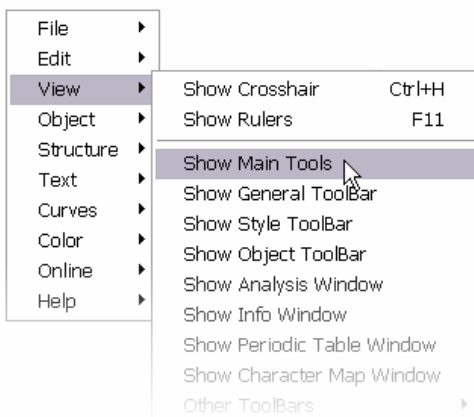
## Full Screen Edit

The Full Screen Edit option opens a new, larger window for easier structure drawing. After a structure is drawn in the full screen, click OK to transfer the structure to the structure search box.

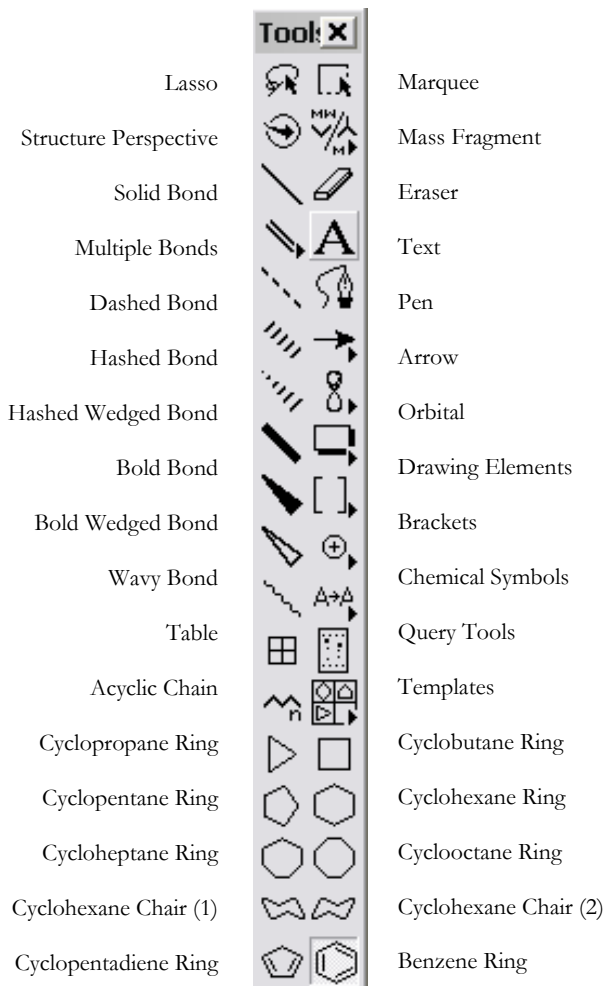


## ChemDraw Toolbar

If the ChemDraw toolbar does not appear, right click in the structure window. Select view → Show Main Tools.



## Features of the ChemDraw Toolbar



## Organic Name Reactions

In general, the description for each Organic Name Reaction provides alternate names for the reaction, original contributors, concise description of the transformation, reaction scheme, and key references. Selecting the Organic Name Reactions link from the main menu provides access to an alphabetical list of reactions, as well as a means to search.

ONRs: Browse

The Browse tab provides an alphabetical list of the reactions.

The Merck Index  
Fourteenth Edition

HOME PAGE BASIC SEARCH STRUCTURE SEARCH ORGANIC NAME REACTIONS SUPPLEMENTAL TABLES

BROWSE SEARCH

**Organic Name Reactions**

The Organic Name Reactions (ONR) section is intended to serve the professional chemist and student by describing organic chemical reactions which have come to be recognized and referred to by name within the chemistry community. A select group has been chosen for addition to this section. Each reaction description is designed to be informative and representative of the pertinent literature; however, it is not meant to be comprehensive. The descriptions are composed of the following: (1) name(s) associated with the reaction, (2) the original and/or primary contributor(s) connected with the discovery and/or development of the reaction, (3) a concise description of the transformation, (4) a reaction scheme, (5) key references, and (6) cross references to other ONR based on commonalities. The index included in this section also lists supplementary terms.

Abbreviations

Ac	acetyl	E	electrophile
Ar	aryl	ee	enantiomeric excess
aq	aqueous	Et	ethyl
B	base	EtOH	ethanol
BEN	borabicyclo[3.3.1]nonane	EWG	electron withdrawing group
BDAP	2,2'-bis(diphenylphosphino)-1,1'-binaphthyl	HA	protic acid
BOC	<i>t</i> -butyloxycarbonyl	HMPA	hexamethylphosphoric triamide
Bu	butyl	LDA	lithium diisopropylamide
cat	catalytic	LHMDS	lithium hexamethyldisilazide
Cp	cyclopentadienide	Me	methyl
Δ	heat	NuH	nucleophile
dba	dibenzylideneacetone	Ph	phenyl
DCC	dicyclohexylcarbodiimide	Pr	propyl
DEAD	diethylazodicarboxylate	salen	<i>N,N'</i> -ethylenebis

Search

To search the list of ONRs, click on the Search tab. Searching a reaction name will retrieve all reactions that contain that keyword.

The Merck Index  
Fourteenth Edition

HOME PAGE BASIC SEARCH STRUCTURE SEARCH ORGANIC NAME REACTIONS SUPPLEMENTAL TABLES

BROWSE SEARCH

Enter your query below:  
indole  
Search Tips for searching

Found 11 matches

- Bartoli Indole Synthesis
- Bischler-Mislow Indole Synthesis
- Borsche-Drechsel Cyclization
- Fischer Indole Synthesis
- Knoevenagel Condensation
- Madelung Synthesis
- Neritzescu Indole Synthesis
- Pitoy-Robinson Synthesis
- Pummerer Rearrangement
- Reissert Indole Synthesis
- Stoll Synthesis

**020. Bartoli Indole Synthesis**

G. Bartoli *et al.*, *Tetrahedron Lett.* **30**, 2129 (1989).

One-step reaction of *ortho*-substituted nitroarenes with vinyl Grignard reagents to yield 7-substituted indoles:

Mechanistic studies: M. Bosco *et al.*, *J. Chem. Soc. Perkin Trans.* **2** **1991**, 657.  
Improved protocols: A. Dobbs, *J. Org. Chem.* **66**, 638 (2001), M. C. Pirrung *et al.*, *Synlett* **2002**, 143. Indole synthesis on solid supports: K. Knepper, S. Bräse, *Org. Lett.* **5**, 2829 (2003). Review: R. Dalpozzo, G. Bartoli, *Curr. Org. Synth.* **9**, 163-178 (2005).

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## Supplemental Tables

All of the tables provided in the Supplemental Tables section of *The Merck Index* are available on the electronic products. To access the tables select Supplemental Tables from the homepage or from the tab at the top of the page. To view a particular table, click on the link provided. All tables are in PDF format and, therefore, require the Adobe Acrobat Reader to view. If you do not have Adobe Acrobat Reader installed, click on the link provided to obtain a free copy.

The screenshot shows the website interface for The Merck Index, Fourteenth Edition. At the top, there is a red navigation bar with the following tabs: HOMEPAGE, BASIC SEARCH, STRUCTURE SEARCH, ORGANIC NAME REACTIONS, and SUPPLEMENTAL TABLES. The SUPPLEMENTAL TABLES tab is currently selected. In the top right corner, there is a "LOG OFF" button. The main content area displays a list of 20 supplemental tables, organized into two columns. The tables listed are:

- Abbreviations
- Acronyms
- Alchemical Symbols Used in Biology and Botany
- Amino Acids Found in Proteins
- Atomic Weights
- Chemical Terms Translator
- Code Letters Used By Companies for Experimental Substances
- Common Heterocyclic Ring Systems
- Company Register
- Fundamental Physical and Mathematical Constants
- Glossary
- Greek Alphabet
- International Patent Country Codes
- International System of Units
- Latin Terms
- Numerical Prefixes Commonly Used in Forming Chemical Names
- Periodic Chart of the Elements
- Prescription Notation
- Radioactive Isotopes Used in Medical Diagnosis and Therapy
- Roman Numerals
- Russian Alphabet
- Selected Hexoses and Pentoses
- Table of Minerals
- Terms for Radicals and Groups Used for Nonproprietary Names
- Thermometric Equivalents
- Universal Conversion Factors
- Vaccines

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