

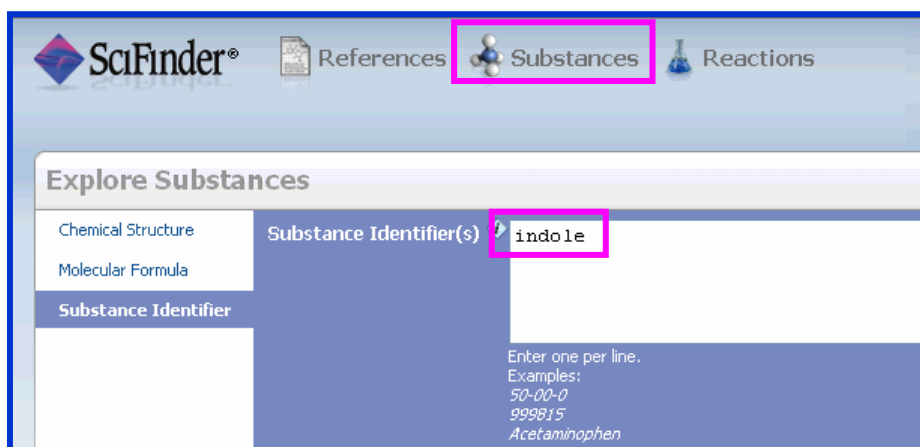
# ▶ HOW TO

## Explore Reactions with Built-in Links

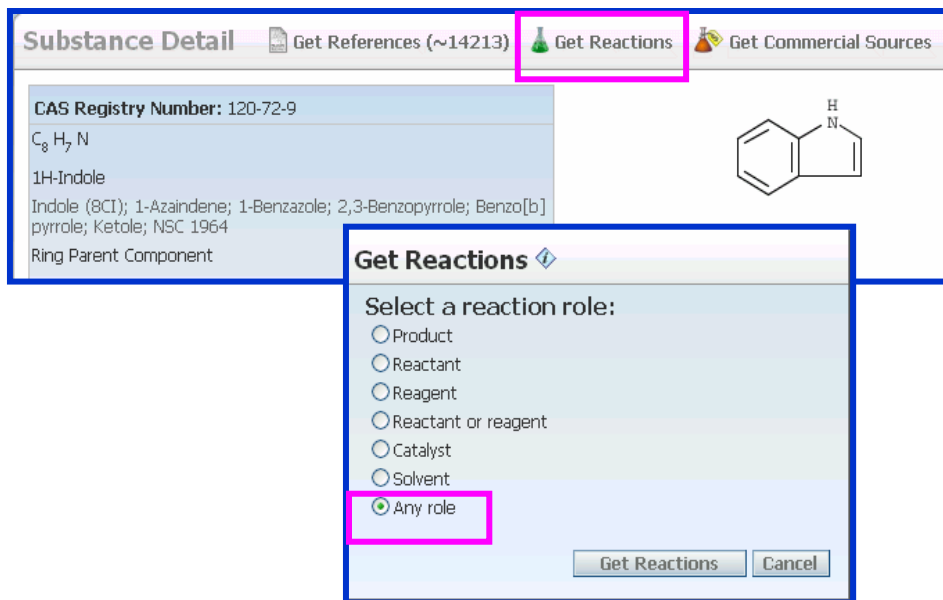


CASREACT<sup>®</sup> offers more than 15 million single- and multi-step reactions making it the largest collection of reaction information in the world. Providing information on synthetic organic research, CASREACT is also rich in organometallics, natural products, and biocatalyzed reactions. SciFinder has many built-in links to help you locate reaction information from any point in your explorations. These links will quickly connect you to the information you need.

1. Suppose you are interested in the antitumor properties of natural products from marine sponges. Most of these products are alkaloids containing indole molecules. Let's begin by exploring with *Substances* using *Substance Identifier*. Enter the chemical name *indole*.



2. SciFinder locates the CAS Registry<sup>SM</sup> record for *indole*. Click *Get Reactions* at the top of the record and then choose *Any role*.



**Substance Detail** Get References (~14213) Get Reactions Get Commercial Sources

**CAS Registry Number:** 120-72-9

$C_8H_7N$

1H-Indole

Indole (BCI); 1-Azaindene; 1-Benzazole; 2,3-Benzopyrrole; Benzo[b]pyrrole; Ketole; NSC 1964

Ring Parent Component

**Get Reactions**

Select a reaction role:

- Product
- Reactant
- Reagent
- Reactant or reagent
- Catalyst
- Solvent
- Any role

Get Reactions Cancel

3. SciFinder retrieves an answer set of 12,824 reactions in which *indole* appears in *Any role*. We can use SciFinder's powerful *Refine* tool to limit this answer set to *single-step reactions* only.

The screenshot shows the SciFinder interface with 12,824 reactions listed. A pink box highlights the '12824 Reactions' count and the 'Get References' button. Below the list, a chemical reaction is shown: a nitro olefin (Ph-CH=CH-NO<sub>2</sub>) reacts with indole and a substituted olefin (Me-CH=CH-NO<sub>2</sub>) in two steps. The conditions for both steps are R:EDAP, C:H<sub>2</sub>SO<sub>4</sub>, S:ClCH<sub>2</sub>CH<sub>2</sub>Cl, 2.2-4 h, rt. A 'Refine by' panel on the right is open, with 'Number of Steps' set to 1. The 'Refine' button is highlighted with a pink box.

**Refine by**

- Reaction Structure
- Product Yield
- Number of Steps
- Reaction Classification

**Number of Steps:** 1  
Examples: 1, 1-3, 1-, -4

**Refine**

NOTE: 1) Friedel-Crafts alkylation, solid-supported catalyst, 2) Friedel-Crafts alkylation, solid-supported catalyst, Reactants: 3, Reagents: 1, Catalysts: 1, Solvents: 1, Steps: 2, Stages: 2

Silica sulfuric acid-catalyzed Friedel-Crafts alkylation of indoles with nitro olefins

4. SciFinder locates 6088 single-step reactions with *indole* in *Any role*. Let's click *Get References* to view a list of the document references linked to these 6088 reactions. SciFinder locates 2171 document references. Since we are interested in substances found in marine animals, let's refine our answers once again—by *marine*.

The screenshot shows the SciFinder interface with 6088 reactions listed. A pink box highlights the '6088 Reactions' count and the 'Get References' button. Below the list, a chemical reaction is shown: a nitro olefin (MeO-CH=CH-NO<sub>2</sub>) reacts with indole under conditions R:EDAP, C:H<sub>2</sub>SO<sub>4</sub>, S:ClCH<sub>2</sub>CH<sub>2</sub>Cl, 2.2-4 h, rt. A 'References' panel is open, showing three references. A 'Refine by' panel on the right is open, with 'Research Topic' set to 'marine'. The 'Refine' button is highlighted with a pink box.

**References**

- 1. Process for preparation of 1-pyridin-4-yl-indoles from 4-halopyridines and indoles in the presence of base.**  
By Aoki, Hidenori; Tsujiyama, Shinichiro; Ishikawa, Yuji; Harada, Susumu  
From Eur. Pat. Appl. (2008) English CAPLUS  
Title compds. (I; R1, R4 = H, alkyl, alkenyl, alkynyl, aryl, aryloxy, arylcarbonyloxy, CO<sub>2</sub>H, etc; alkynyl, alkylcarbonyl, alkoxy, CO<sub>2</sub>H, etc.; R5 = alkyl, alkenyl, alkynyl, aryl, alkoxy, arylcarbonyloxy, alkylsulfonyl, arylsulfonyl, carbamoyl, etc.; n = 0-6), were prepd. by reaction of Cl, Br, iodo, R1-R4 as above) with indoles (III; R5, n as above) in the presence of base. The hydrochloride, and NaOCMe<sub>3</sub> were heated together in dimethylacetamide at 110° to give 90% yield of I.
- 2. Preparation of 3-selenoindole derivatives as plant growth regulator and selenocyanatoindole.**  
By Li, Zhong; Qian, Xuhong; Ma, Yanming; Huang, Qingchun; Song, Gonghua  
From Faming Zhuanli Shengqing Gongsi Shuomingshu (2008) Chinese CAPLUS  
The invention provided a series of 3-selenoindole deriv. I [R1 = alkyl, substituted alkyl; R2 = alkyl, etc.; R3 = H, alkylsulfonyl, arylsulfonyl, alkyl, substituted alkyl; X = Se, Se(O), SeO<sub>2</sub>] as selenium-enrichment agent and the method for prepg. For example, stirring malononitrile with indole in DMF, 78% 3-selenocyanatoindole.
- 3. Iron-copper cocatalyzed process for carbon-carbon or carbon-heteroatom bond formation.**  
By Taillefer, Marc; Xia, Ning; Ouali, Armelle  
From PCT Int. Appl. (2008) English CAPLUS  
Claimed is a process for creating a Carbon-Carbon bond (C-C) or a Carbon-Heteroatom bond (C-X) between a nucleophilic compd. carrying a carbon atom or a substitute for the leaving group, creating a C-C or C-X bond, wherein the reaction takes effective quantity of a catalytic system comprising iron and copper. Addnl. claims give the nucleophilic compd.; for example, the nucleophilic compd. is of formula HNR1R2 (R1, R2 = H, alkyl, aryl, etc.).

**Refine by**

- Research Topic
- Author Name
- Company Name
- Document Type
- Publication Year
- Language
- Database

**Research Topic:** marine  
Examples: The effect of antibiotic residues on dairy products; Photocyanation of aromatic compounds

**Refine**

5. SciFinder now locates 13 document references discussing substances containing indoles produced by marine animals that display antitumor properties. Let's select reference #5 for closer inspection. Click the hyperlinked title of the reference.

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

13 References 0 Selected Keep Selected Remove Selected

Select All Deselect All

1. 3,5-Bis(3'-indolyl)pyrazoles, analogues of marine alkaloid nortopsentin: Synthesis and antitumor properties  
By Diana, Patrizia; Carbone, Anna; Barraja, Paola; Martorana, Annamaria; Gia, Ornella; Dalla Via, Lisa; Cirrincione, Girolamo  
From *Bioorganic & Medicinal Chemistry Letters* (2007) English CAPLUS

5. **Synthesis and antitumor properties of 2,5-bis(3'-indolyl)thiophenes: Analogues of marine alkaloid nortopsentin**  
By Diana, Patrizia; Carbone, Anna; Barraja, Paola; Montalbano, Alessandra; Martorana, Annamaria; Dattolo, Gaetano; Gia, Ornella; Dalla Via, Lisa; Cirrincione, Girolamo  
From *Bioorganic & Medicinal Chemistry Letters* (2007) English CAPLUS  
A series of 11 bis-indolylthiophenes of formula I were obtained by cyclization of bis-indole 1,4-diketones using Lawesson's reagent. Derivs. I (R = OMe, R1 = SO2Ph), I (R = OMe, R1 = Me), I (R = Cl, R1 = Me), and I (R = OMe, R1 = H) were selected to be evaluated in the full panel of about 60 human tumor cell lines derived from nine human cancer cell types and showed antiproliferative activity generally in the micromolar range. The most sensitive cell lines were: CCRF-CEM, MOLT-4, HL60 (TB), and RPMI-8226 of the leukemia subpanel, HT29 and HCC-2998 cell lines of the colon sub-panel, NCI-H522 ...  
[Substances](#) [Reactions](#) [Citing](#) [Full Text](#)

6. **New routes to 3-(arythio)indoles: application to the synthesis of the 3,3'-bis(indolyl)sulfone core of the marine alkaloid echinosulfone A**  
By Shirani, Hamid; Stensland, Birgitta; Bergman, Jan; Janosik, Tomasz  
From *Synlett* (2006) English CAPLUS  
A new approach to 3-(arythio)indoles and related compds. was developed, based on the reactions of aryl Grignard reagents or lithiated heteroaroms. with a phenylsulfonyl-protected 3,3'-bis(indolyl)disulfide I (R = H, R1 = R2 = SO2Ph, X = S-S). In addn., a rational approach to the 3,3'-bis(indolyl)sulfone core I (R = R1 = R2 = H, X = SO2) of the alkaloid echinosulfone A I (R = Br, R1 = CO2H, R2 = H, X = SO2) was accomplished and involved the treatment of 3-bromo-1-(tert-butylidimethylsilyl)indole with BuLi and subsequent reaction of the in situ formed 3-lithioindole deriv. with (PhSO2)2S to for...  
[Substances](#) [Reactions](#) [Citing](#) [Full Text](#)

7. **Michael reaction of indoles with 3-(2-nitrovinyl)indole under solvent-free conditions and in solution. An efficient synthesis of 2,2-bis(indolyl)nitroethanes and studies on their reduction**  
By Chakrabarty, Manas; Basak, Ramkrishna; Ghosh, Nandita; Harigaya, Yoshihiro  
From *Tetrahedron* (2004) English CAPLUS  
Michael reaction of 3-(2-nitrovinyl)indole with eight 3-substituted indoles on TLC-grade silica gel furnished unsym. bis(indolyl)nitroethanes in 7-12 min under microwave irradiation and in 8-14 h at room temp. In contrast, the p-TsOH-catalyzed reaction of the nitrovinylindole with the 3-unsubstituted and two 3-substituted indoles in solution under reflux furnished both unsym. and sym. bis(indolyl)nitroethanes; the latter resulting from novel tandem Michael addition-elimination-Michael addition...

6. The abstract of reference #5 is right on target. Let's click *Get Reactions* to see how many reactions are associated with this journal article.

Reference Detail [Get Substances](#) [Get Reactions](#) [Get Cited](#) [Get Citing](#) [Get Full Text](#)

**Synthesis and antitumor properties of 2,5-bis(3'-indolyl)thiophenes: Analogues of marine alkaloid nortopsentin**

Diana, Patrizia; Carbone, Anna; Barraja, Paola; Montalbano, Alessandra; Martorana, Annamaria; Dattolo, Gaetano; Gia, Ornella; Dalla Via, Lisa; Cirrincione, Girolamo

A series of 11 bis-indolylthiophenes of formula I were obtained by cyclization of bis-indole 1,4-diketones using Lawesson's reagent. Derivs. I (R = OMe, R1 = SO2Ph), I (R = OMe, R1 = Me), I (R = Cl, R1 = Me), and I (R = OMe, R1 = H) were selected to be evaluated in the full panel of about 60 human tumor cell lines derived from nine human cancer cell types and showed antiproliferative activity generally in the micromolar range. The most sensitive cell lines were: CCRF-CEM, MOLT-4, HL60 (TB), and RPMI-8226 of the leukemia subpanel, HT29 and HCC-2998 cell lines of the colon sub-panel, NCI-H522 of the non-small cell lung cancer sub-panel, LOX 1MVI of the melanoma sub-panel, and UO-31 of the renal cancer sub-panel.

**Indexing**

Alkaloids (Section 31-5) [↕](#)

Section cross-reference(s): 1

**Concepts** [↕](#)

Alkaloids, preparation

**Substances** [↕](#)

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Universita degli Studi di Palermo  
Palermo, Italy 90123

**Accession Number**

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CAN 147:10084  
CAPLUS

**Publisher**

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**Language**

English

7. A total of 75 different reactions indexed from reference #5 are available for perusal.

**Reactions** Get References

75 Reactions 0 Selected Keep Selected Remove Selected

Select All Deselect All

1. Click for detail

1 R:NaOH, R:POCl<sub>3</sub>  
 2 R:NaH, S:THF  
 3 C:693794-24-0, C:AcONa, S:EtOH, reflux  
 4 R:Lawesson's reagent, S:PhMe  
 5 R:KOH, S:EtOH, reflux

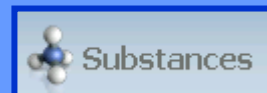
NOTE: Reactants: 4, Reagents: 5, Catalysts: 2, Solvents: 3,  
 Steps: 5, Stages: 5

Synthesis and antitumor properties of 2,5-bis(3'-indolyl)thiophenes: Analogues of marine alkaloid nortopsentin  
 By Diana, Patrizia et al  
 From Bioorganic & Medicinal Chemistry Letters, 17(8), 2342-2346; 2007

When you want to...

Click

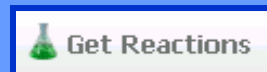
Locate a specific substance



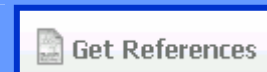
Locate a substance by chemical name or CAS Registry Number

Substance Identifier(s)

Explore reaction information linked to a given substance



Explore document references linked to a given substance



Refine an answer set

Refine by

Contact CAS Customer Care at [help@cas.org](mailto:help@cas.org) or call 800-753-4227 (North America) or 614-447-3700 (worldwide).