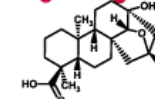
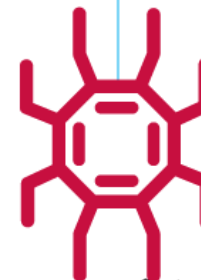
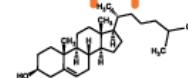
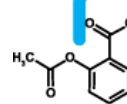
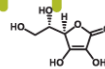
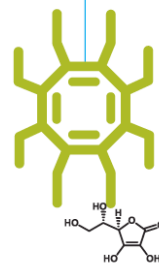


# ChemSpider: Building A Community Platform to Support Chemistry

RSC | Advancing the Chemical Sciences



**ChemSpider**  
Building community for chemists



Some background and history

Searching ChemSpider

# What is ChemSpider?

- ChemSpider is:
  - Building Community for Chemists
  - >25 million compounds from >300 data sources
  - A deposition and curation platform
  - A publishing platform for the community
  - Grows daily – more depositions, more links, more data
- ChemSpider SyntheticPages
  - An online database of synthetic procedures

# Aggregating Data – Who to Trust???

- Encyclopedic articles (Wikipedia)
- Chemical vendor databases
- Metabolic pathway databases
- Property databases
- Patents with chemical structures
- Drug Discovery data
- Scientific publications
- Compound aggregators
- Blogs/Wikis and Open Notebook Science

# Just “Public Compound” Databases

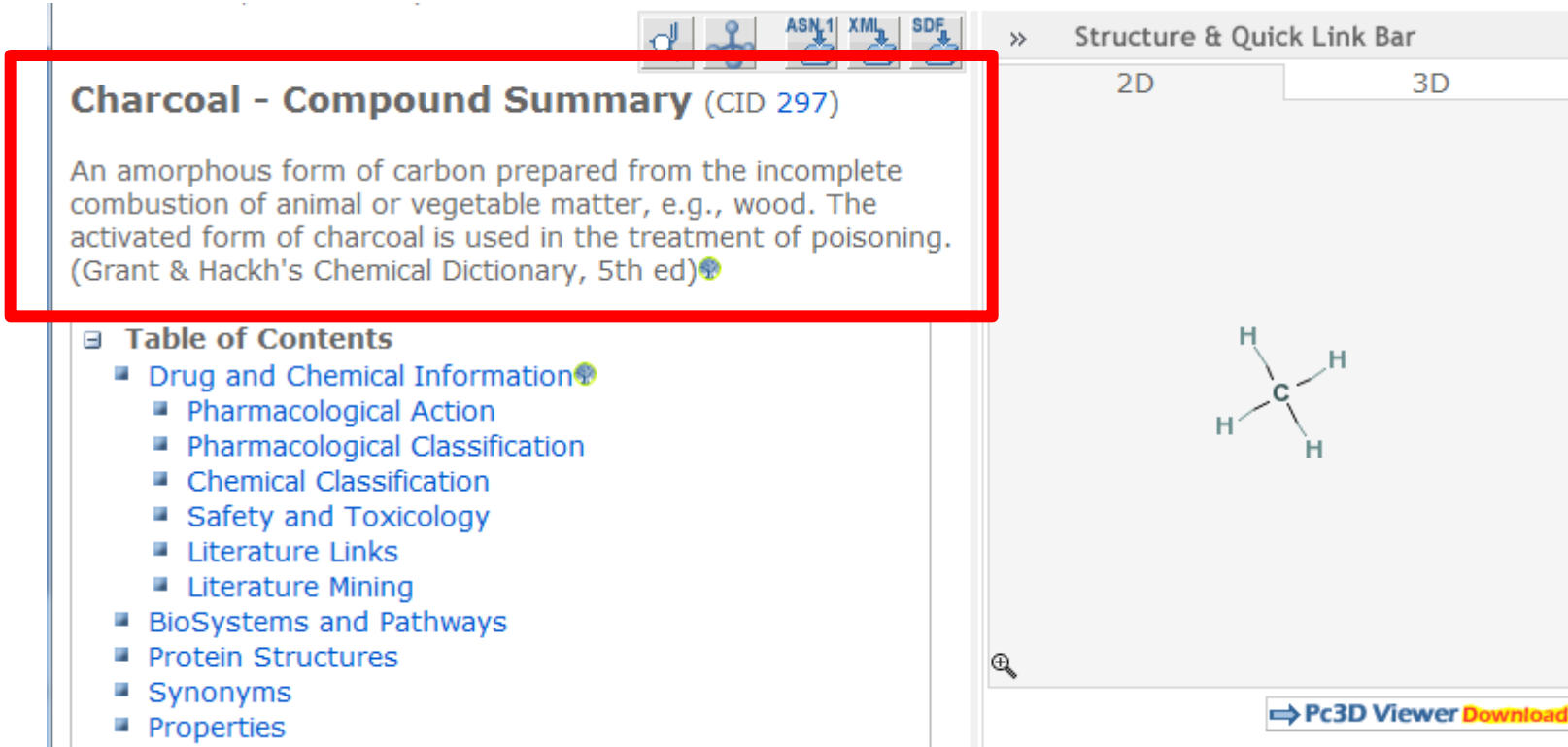
- PubChem
- Drugbank
- ChEBI/ChEMBL
- KEGG
- LipidMAPs
- ChemIDPlus
- eMolecules
- ZINC
- Lots of chemical vendors

# ChemSpider - A Pragmatic Vision

## “Build a Structure Centric Community to Serve Chemists”

- Aggregate and integrate chemical structure data on the web – **names, structures, links**
- Create a “structure-based hub” to information, data and algorithmic predictions
- Let chemists contribute their own data
- Allow the community to curate/correct data

# What's Methane?



**Charcoal - Compound Summary** (CID 297)

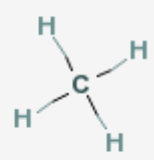
An amorphous form of carbon prepared from the incomplete combustion of animal or vegetable matter, e.g., wood. The activated form of charcoal is used in the treatment of poisoning. (Grant & Hackh's Chemical Dictionary, 5th ed)

**Table of Contents**

- Drug and Chemical Information
  - Pharmacological Action
  - Pharmacological Classification
  - Chemical Classification
  - Safety and Toxicology
  - Literature Links
  - Literature Mining
- BioSystems and Pathways
- Protein Structures
- Synonyms
- Properties

Structure & Quick Link Bar

2D 3D



[Pc3D Viewer](#) [Download](#)

# What **ELSE** is Methane???

Charcoal activated  
Animal bone charcoal  
Carbon, activated  
Plumbago (graphite)  
Carbon-12  
Philblack N 550  
Philblack N 765  
**CHARCOAL**   
**DIAMOND**   
Monarch 700  
Witcarb 940  
Graphite (synthetic)  
Irgalite 1104

# Semantic Markup: Project Prospect

## 6,7-Dimethylumazine as a potential ligand for selective recognition of adenine opposite an abasic site in DNA duplexes†

Zhiqiang Ye†<sup>a</sup>, Burki Rajendar†§<sup>a</sup>, Dai Qing<sup>a</sup>, Seiichi Nishizawa<sup>ab</sup> and Norio Teramae<sup>\*ab</sup>

<sup>a</sup>Department of Chemistry, Graduate School of Science, Tohoku University, Aoba-ku, Sendai, 980-8578, Japan. [E-mail: teramae@mail.tains.tohoku.ac.jp](mailto:teramae@mail.tains.tohoku.ac.jp); Fax: +81 22 7956552; Tel: +81 22 7956549

<sup>b</sup>CREST, Japan Science and Technology Agency (JST), Aoba-ku, Sendai, 980-8578, Japan

Received (in Cambridge, UK) 26th September 2008, Accepted 20th October 2008

First published

6,7-Dimethylumazine  
X = AP site (S  
the binding affi

Single nucleoti  
Thus, simple a  
research effort  
have recently s  
and they succe  
other hand, we  
fluorescence li  
binders or inter  
intrahelical nuc  
containing DN  
amiloride,<sup>3</sup> and  
developing an  
1.21 × 10<sup>6</sup> M  
adenine. Sever  
stabilization of  
increase the sta

Manuscript DOI 10.1039/b816876h Compound information for 2-amino-6,7-dimethyl-4-hydroxypteridine ...

http://www.rsc.org/delivery/\_articlelinking/cheminfo.asp?XMLID=3&compoundtext=2-amino-6,7-dimethyl-4-hydroxypteridine&MSID

RSC Publishing

Compound information '2-amino-6,7-dimethyl-4-hydroxypteridine'

Synonyms:

- 2-amino-6,7-dimethyl-4-hydroxypteridine

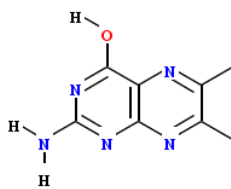
SMILES: OC1=NC(=NC2=NC(=C(N=C12)C)C)N

InChI: InChI=1/C8H9N5O/c1-3-4(2)11-6-5(10-3)7(14)13-8(9)12-6/h1-2H3,(H3,9,11,12,13,14)/ffh14H,9H2

InChIKey: InChIKey=ZKWZUPPXTCQQJL-JPLXFSROCR

CML (Chemical Markup Language) Representation: [Download File](#)

2-D Representation:



Other resources:

- Search for this compound in PubChem
- Search for this compound in SureChem patents

Toolbox

Tools and Resources

- Print this article
- Download PDF
- Email a friend
- Supplementary information
- Prospect View FAQ
- Normal View
- Advanced features
- Find citing articles

GO

Navigation

GX GCA AC-3'/3'-AGG TCN CGT TG-5',  
1.0 μM; substituted methyl groups enhance  
[highlight terms](#)

[Hide compounds](#)

[Show Gold Book](#)

nes and detection of genetic mutations.<sup>1,2</sup>  
nacogenomics.<sup>3</sup> Consequently, considerable  
by fluorescent molecules.<sup>4</sup> Nakatani *et al.*<sup>5</sup>  
sine,<sup>6</sup> and guanine-adenine<sup>7</sup> mismatches,  
plasmon resonance (SPR) assay. On the  
have discovered a series of small  
typical DNA-drug binding ligands (groove  
pseudo-base pairing of ligands with  
AP site. In combination with AP site-  
<sup>6</sup> 2-amino-6,7-dimethyl-4-hydroxypteridine,<sup>2</sup>  
among these base-selective ligands,  
mate A (the 1 : 1 binding constant,  $K_{11}$  =  
selective detection of SNPs related to  
ve the binding affinity of ligands and  
s in a DNA strand has been known to

# Depends on Validated Dictionaries

## Food Interactions

with [clofibrate](#), [fenofibrate](#), [gemfibrozil](#), which are fibrates used in accessory therapy in many forms of hypercholesterolemia, usually in combination with [atorvastatin](#).<sup>[23][24][25]</sup>

Co-administration of Atorvastatin with one of CYP3A4 inhibitors like itraconazole<sup>[26]</sup>, telithromycin, and voriconazole, may increase serum concentrations of [atorvastatin](#). This may also happen with other CYP3A4 inhibitors like diltiazem, erythromycin, fluconazole, ketoconazole, clarithromycin, cyclosporine, protease inhibitors, verapamil, amiodarone, and aprepitant<sup>[6]</sup>. Often [bosentan](#), [fosphenytoin](#), and [phenytoin](#) which are CYP3A4 inducers can decrease the plasma concentrations of [atorvastatin](#). Similarly, [efavirenz](#), [nevirapine](#), [oxcarbazepine](#), [nifedipine](#), and [nifedipine](#)<sup>[28]</sup>, which are CYP3A4 inducers can decrease the plasma concentrations of [atorvastatin](#).<sup>[29]</sup> And [ethinyl estradiol](#), these increases should be considered when selecting an oral contraceptive for a woman taking [atorvastatin](#).<sup>[29]</sup>

They may also slightly decrease the plasma concentrations of [atorvastatin](#) but do not affect the LDL-C lowering efficacy.

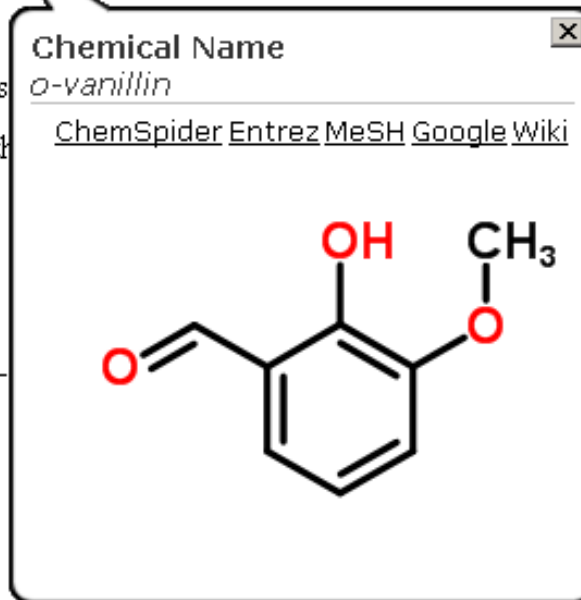
## Link to a Structure or the Right Structure?

# Name-Structure Pairs

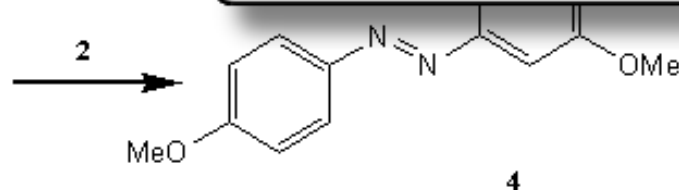
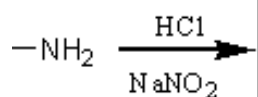
Accepted: 20 February 2004 / Published: 24 February 2004

nisidine, **o-vanillin**, Schiff bases, biological activity.

interesting biological  
the methoxy groups  
an azoaldehyde with



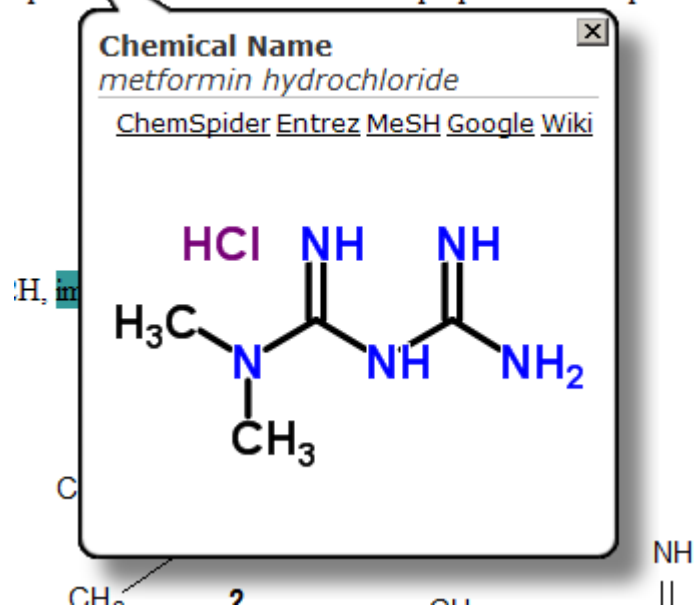
presence of an **azo** functionality in n  
activities [6]. As such, we sy  
corresponding Schiff bases. Their :



# Semantic Linking of Structures

- What would you want to link off a structure?
  - Chemical suppliers
  - Other publications
  - Analytical Data
  - Related Reactions
  - Wikipedia
  - Patents
  - “Everything”
  - **Through ChemSpider!**

subjected to MWI intermittently at an interval of 40 s at 540  
: product was scratched from the preparative TLC plate an



# ChemSpider SyntheticPages – An Online Database of Synthetic Reactions

The screenshot shows the ChemSpider SyntheticPages website. At the top left is the ChemSpider logo, a stylized spider, and the text "ChemSpider SyntheticPages beta". To the right is a search bar with the word "Search" inside. Below the logo is a navigation bar with links for "Home", "About", "Browse", "Leaderboard", and "Login". The main content area is titled "About ChemSpider SyntheticPages" and contains a paragraph describing the database as a freely available interactive resource for synthetic chemistry. Below this is a link to the "Editorial board". To the right of the main content is a blue box with the text "Submit your SyntheticPage online" and a note stating that submissions are currently disabled as the site is in read-only mode. Below this is a "Publication Alert" section with an input field for an email address and a "GO" button. The main content area also features a section for "Recent Publications" with two entries. The first entry is "Nickel chloride catalyzed Biginelli reactions" by Sirin Gülten, published on Sep 22 2009. The second entry is "One-pot synthesis of terpyridine derivatives" by Jérôme Husson, published on Jul 15 2009. To the right of each entry are three icons: a thumbnail, a structure, and full text.

**ChemSpider SyntheticPages beta**

Search

Building Community for Chemist

Home About Browse Leaderboard Login

## About ChemSpider SyntheticPages

ChemSpider SyntheticPages is a freely available interactive database of synthetic chemistry. We publish practical and reliable organic, organometallic and inorganic chemical synthesis, reactions and procedures deposited by synthetic chemists. Synthetic methods on the site are updated continuously by chemists working in academic and industrial research laboratories.

ChemSpider SyntheticPages encourages submissions from graduate students, postdocs, industrialists and academics.

[Editorial board](#)

Recent Publications Most Popular

**Nickel chloride catalyzed Biginelli reactions**

Sirin Gülten

Published: Sep 22 2009

Thumbnails Structures Full Text

**One-pot synthesis of terpyridine derivatives**

Jérôme Husson

Published: Jul 15 2009

Thumbnails Structures Full Text

Submit your SyntheticPage online

Note: submissions to ChemSpider SyntheticPages are currently disabled as the site is in read only mode.

Publication Alert

Your e-mail here... GO

# SyntheticPages Online Publishing

- Deposit synthetic procedures on SyntheticPages and share your chemistry
- Replicate syntheses that can't be done via publications
- Cite the syntheses in your resume
- Contribute to adding quality chemistry syntheses to a growing database of reactions

# Other system enhancements?

- What ChemSpider doesn't deal with yet...
  - Markush structures and other “non-defineds”
  - Materials
  - Minerals
  - Polymers
  - Biological macromolecules

# What's Next?

- Continue the curation effort and keep cleaning
- Enhanced integration with RSC publishing workflows and databases
- Tighter integration to RSC databases
  - Natural Product Updates
  - Methods of Organic Synthesis
- Use ChemSpider dictionaries to enhance markup precision and recall

# What's Next?

- Use entity extraction approaches and ChemSpider dictionaries to analyze the entire RSC archive
- Deposit structures into ChemSpider from the backfile
- Use crowdsourced curation approaches to optimize the results

# Pragmatic Vision Delivered...

- Aggregate, integrate and link data from across the internet
- Almost **25 million** structures from **>300 data sources**
- Linked to vendors, literature, online databases (open and commercial), open notebook science, patents and.....
- Robotic and **Crowdsourced** Curation

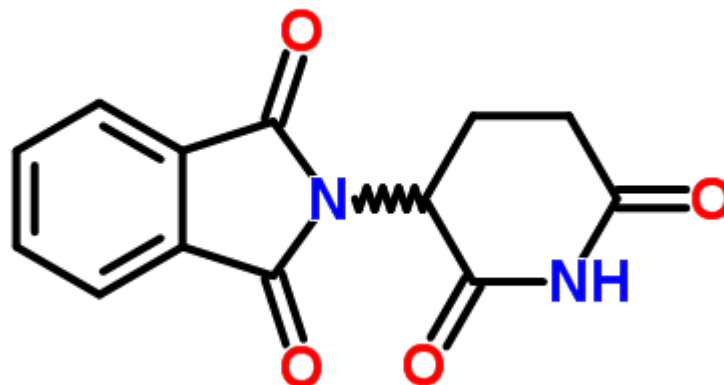




# Searching ChemSpider for Thalidomide

- I want...
  - The structure
  - Any patent information
  - Related publications
  - Where can I buy it?
  - Metabolic pathway info
  - What else is easy to find...

# What is a compound?



Thalidomide – Distaval

CAS RN = 50-35-1

CSID = 5233

Systematic name: 2-(2,6-dioxopiperidin-3-yl)-1H-isoindole-1,3(2H)-dione

SMILES: O=C3NC(=O)CCC3N1C(=O)C2C=CC=CC=C2C1=O

Std. InChIKey: UEJJHQNACJXSKW-UHFFFAOYSA-N

# The InChI Identifier

## International Chemical Identifier

---

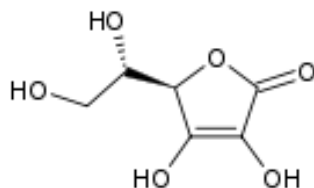
From Wikipedia, the free encyclopedia

(Redirected from [InChI](#))

The **IUPAC International Chemical Identifier (InChI)**, pronounced "INchee") is a textual [identifier](#) for [chemical substances](#), designed to provide a standard and human-readable way to encode molecular information and to facilitate the search for such information in databases and on the web. Developed by [IUPAC](#) and [NIST](#) during 2000-2005, the format and algorithms are non-proprietary and the software is freely available under the [open source LGPL](#) license (though the term "InChI" is a [trademark](#) of IUPAC).<sup>[1]</sup>

CH<sub>3</sub>CH<sub>2</sub>OH  
[ethanol](#)


InChI=1/C2H6O/c1-2-3/h3H,2H2,1H3



InChI=1/C6H8O6/c7-1-2(8)5-3(9)4(10)6(11)12-5/h2,5,7-10H,1H2/t2-,5+/m0/s1

[L-ascorbic acid](#)

# Search ChemSpider for Thalidomide

Systematic Name, Synonym, Trade Name,  
Registry Number, SMILES, InChI or CSID 

 **OPTIONS**

Search

Search by chemical name or Trade Name –  
Options to run a structure search

# Search ChemSpider for Thalidomide

- Auto-generate structure from chemical name or SMILES or InChI

The screenshot shows a web browser window with the address <http://www.chemspider.com>. The page title is "Input Chemical Structure". At the top, there are three radio buttons: "Convert" (selected), "Load", and "Draw or Edit". Below this is a section titled "Convert from String (Name, SMILES, InChI, etc)" with a text input field containing "thalidomide" and a "Convert" button. The chemical structure of thalidomide is displayed below the input field. The structure consists of a phthalimide ring system connected to a glutarimide ring system. The nitrogen atom in the glutarimide ring is labeled "HN" in blue. The oxygen atoms in both carbonyl groups are highlighted in red. At the bottom of the browser window, there are "Accept" and "Cancel" buttons.


Chemical Structure Search - <http://www.chemspider.com> - Input Chemical Structure - Microsoft Internet Explorer

File Edit View Favorites Toolbars

Back Forward Stop Refresh

Address <http://www.chemspider.com>

Links Customize Links Internet Options

 **Che**  
Building c

About Login

Simple Search

Structure Search

LASSO Search

Advanced LASSO

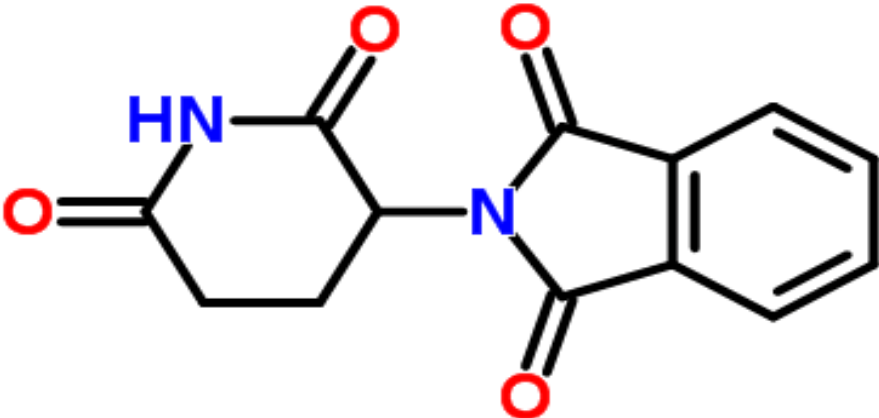
Chemical Elements

Properties Search

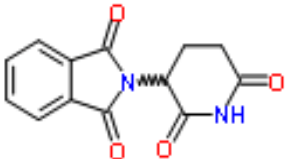
Convert  Load  Draw or Edit

Convert from String (Name, SMILES, InChI, etc)

thalidomide



# Search ChemSpider for Thalidomide

Add:	Description	Identifier	CIF	Spectrum	Image	Comments
<b>INHERENT PROPERTIES, IDENTIFIERS AND REFERENCES</b>						
2D 3D						
	<b>ChemSpider ID:</b>	5233	<b>Quick Links:</b> <a href="#">Permalink</a> <a href="#">Similar</a> <a href="#">Isomers</a> <a href="#">Wikibox</a>			
	<b>Empirical Formula:</b>	C <sub>13</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub>				
	<b>Molecular Weight:</b>	258.2295				
	<b>Nominal Mass:</b>	258 Da				
	<b>Average Mass:</b>	258.2295 Da				
<b>Monoisotopic Mass:</b>	258.064057 Da					
load save zoom						
<b>Systematic Name:</b>	2-(2,6-dioxopiperidin-3-yl)-1H-isindole-1,3(2H)-dione					
<b>SMILES:</b>	<chem>O=C3NC(=O)CCC3N1C(=O)c2ccccc2C1=O</chem> <a href="#">Copy</a>					
<b>InChI:</b>	<u>InChI=1/C13H10N2O4/c16-10-6-5-9(11(17)14-10)15-12(18)7-3-1-2-4-8(7)13(15)19/h1-4,9H,5-6H2,(H,14,16,17)</u> <a href="#">Copy</a>					
<b>InChIKey:</b>	UEJJHQNACJXSKW-UHFFFAOYAZ					
<b>Std. InChI:</b>	<u>InChI=1S/C13H10N2O4/c16-10-6-5-9(11(17)14-10)15-12(18)7-3-1-2-4-8(7)13(15)19/h1-4,9H,5-6H2,(H,14,16,17)</u> <a href="#">Copy</a>					
<b>Std. InChIKey:</b>	UEJJHQNACJXSKW-UHFFFAOYSA-N					

Structure, Systematic Name  
and InChIKey

# Search ChemSpider for Thalidomide

IDENTIFIERS

Names and Synonyms Database ID(s)

Validated by Experts, Validated by Users, Non-Validated, Removed by Users, Redirected by Users, Redirect Approved by Experts Edit


(+/-)-2-(2,6-Dioxo-3-piperidiny)-1H-isoindole-1,3(2H)-dione  
(+/-)-THALIDOMIDE  
(±)-Thalidomide  
1H-isoindole-1,3(2H)-dione, 2-(2,3,4,5-tetrahydro-6-hydroxy-2-oxo-3-pyridinyl)-  
1H-isoindole-1,3(2H)-dione, 2-(2,6-dioxo-3-piperidiny)-  
2-(2,6-Dioxopiperidin-3-yl)-1H-isoindol-1,3(2H)-dion  
2-(2,6-Dioxopiperidin-3-yl)-1H-isoindole-1,3(2H)-dione  
2-(2,6-dioxopiperidin-3-yl)-1H-isoindole-1,3(2H)-dione  
200-031-1 [EINECS/ELINCS]  
5-22-13-00224 (Beilstein Handbook Reference) [Beilstein]  
Contergan [Wiki]  
Neosedyn  
Neosydyn  
Neurodyn  
Softenon [Wiki]


Validated names and other Identifiers

# Search ChemSpider for Thalidomide

^ ASSOCIATED DATA SOURCES AND COMMERCIAL SUPPLIERS









FILTER

Chemical Vendors 

Biological Data Syntheses Publishers Metabolism Data Screening Data Phys. Properties 

Theor. Data Tox/Envir. Data Personal Data Web Article Compound Aggreg. Xtal Structures

Natural Products Data Aggregators Safety Data All Data Sources

Data Source	External ID(s)
<a href="#">ChemPacific</a> 	34105, 36151
<a href="#">Microsource</a> 	01503607, 01503607, 01503607
<a href="#">Sigma-Aldrich</a> 	T151_SIGMA, T150_SIGMA, T144_SIGMA
<a href="#">HDH Pharma</a> 	IN1061
<a href="#">Calbiochem</a> 	585970
<a href="#">Rudolf Boehm Institute</a> 	01503607
<a href="#">Tocris Bioscience</a> 	0652
<a href="#">Hangzhou APIChem Technology</a> 	AC-917

Where can I buy it?

# Search ChemSpider for Thalidomide

^ PROPERTIES			
Pred. Prop. (ACD/Labs)	Pred. Prop. (EPISuite)	NMRShiftDB	Exptl. Prop.
<b>ACD/LogP:</b>	0.54	<b># of Rule of 5 Violations:</b>	0
<b>ACD/LogD (pH 5.5):</b>	0.54	<b>ACD/LogD (pH 7.4):</b>	0.54
<b>ACD/BCF (pH 5.5):</b>	1.52	<b>ACD/BCF (pH 7.4):</b>	1.52
<b>ACD/KOC (pH 5.5):</b>	46.9	<b>ACD/KOC (pH 7.4):</b>	46.87
<b>#H bond acceptors:</b>	6	<b>#H bond donors:</b>	1
<b>#Freely Rotating Bonds:</b>	1	<b>Polar Surface Area:</b>	74.76 Å <sup>2</sup>
<b>Index of Refraction:</b>	1.646	<b>Molar Refractivity:</b>	62.35 cm <sup>3</sup>
<b>Molar Volume:</b>	171.7 cm <sup>3</sup>	<b>Polarizability:</b>	24.71 10 <sup>-24</sup> cm <sup>3</sup>
<b>Surface Tension:</b>	69.9 dyne/cm	<b>Density:</b>	
<b>Flash Point:</b>	262.1 °C	<b>Enthalpy:</b>	
<b>Boiling Point:</b>	509.7 °C at 760 mmHg	<b>Vapour:</b>	

Predicted and Experimental Properties are available.  
Also NMRShiftDB

# Search ChemSpider for Thalidomide

^ PATENTS

USPTO (1616)

USPTOA

EPA (415)

EPB

WOPCT

JP

Google Patents

415 patents found in EPA.

Patent No.	Title
<a href="#">1004581</a>	<a href="#">Process for the preparation of thalidomide</a>
<a href="#">2077112</a>	<a href="#">Methods and compositions using thalidomide for the treatment and management of cancers and idiopathic pulmonary fibrosis</a>
<a href="#">0893122</a>	<a href="#">Topical composition comprising thalidomide and their use in cutaneous pathologies</a>
<a href="#">1676577</a>	<a href="#">Compositions for the treatment of cancer comprising a topoisomerase inhibitor and thalidomide</a>
<a href="#">1226824</a>	<a href="#">Use of thalidomide for the treatment of hepatocellular carcinoma</a>
<a href="#">1602654</a>	<a href="#">Process for the synthesis of thalidomide</a>
<a href="#">1607394</a>	<a href="#">WATER-SOLUBLE THALIDOMINE DERIVATIVES</a>
<a href="#">1264597</a>	<a href="#">Methods and compositions for treat</a>
<a href="#">1537870</a>	<a href="#">Methods and compositions for treat</a>
<a href="#">2143444</a>	<a href="#">Compositions for inhibition of anglo</a>

Find patent information –  
click on title to view full text in SureChem

# Search ChemSpider for Thalidomide

ARTICLES

PubMed Links & Reference Google Books Google Scholar RSC Journals RSC Books  
Microsoft Academic Search

Results 1 - 10 of 58

| « previous **1** | 2 | 3 | ... | 5 | 6 | next » |

- Daniella V. Augusti, Rodinei Augusti, Fernando Carazza, R. Graham Cooks. Quantitative determination of the enantiomeric composition of thalidomide solutions by electrospray ionization tandem mass spectrometry, Chem. Commun., 2002, 2242, Issue 19, 2002-09-23, Pages 2242-2243  
*Rapid and simple chiral analysis of thalidomide solutions is demonstrated by using electrospray ionization tandem mass spectrometry and analysis of cluster ion dissociation by the kinetic method. Average deviations of 1% between the actual and experimental enantiomeric compositions are observed.*
- Jenny P. Rosengren, Jesper G. Karlsson, Ian A. Nicholls. Enantioselective synthetic thalidomide receptors based upon DNA binding motifs, Org. Biomol. Chem., 2004, 2, 3374, Pages 3374-3378

Find related publications

# Search ChemSpider for Thalidomide

## ^ RSC DATABASES

Mass Spectrometry Bulletin (1)

Laboratory Hazards Bulletin

Methods in Organic Synthesis (0)

Catalysts & Catalysed Reactions (0)

Natural Product Updates (0)

Analytical Abstracts (28)

Results **1 - 10** of 28

| « previous **1** | 2 | 3 | next » |

- S. Giegold, M. Holzhauser, T. Kiffmeyer, J. Tuerk, T. Teutenberg, M. Rosenhagen, D. Hennies, T. Hoppe-Tichy, B. Wenclawiak. Influence of the stationary phase on the stability of thalidomide and comparison of different methods for the quantification of thalidomide in tablets using high-temperature liquid chromatography., J. Pharm. Biomed. Anal., 2008, 46, 625, Volume 46, Issue 4, 2008-10-01, Pages 625-630

*In this paper, three different HPLC methods for the quantification of thalidomide in tablets were developed and compared. The comparison of a conventional method at 30 °C with two high-temperature methods at 180 °C showed equal results. Using high-temperature HPLC (HT-HPLC), faster analysis times could be achieved. We have also focused on analyte stability and could show that the stationary phase has a pronounced effect on the on-column degradation of thalidomide at high temperatures. Virtually no degradation occurs if a polystyrene divinylbenzene column is used. The stationary phase is not degraded at 180 °C when a carbon clad zirconium dioxide column is used.*

[Search across RSC Databases](#)

# What Do We Know?

- Validated Name-Structure Dictionaries enable “structure-searching” the web.
- Search the structure on ChemSpider and we have integrated many services online
  - NCBI Entrez
  - PubMed
  - Google Scholar, Books, Patents
  - Microsoft Academic Search
  - SureChem Patents
  - .....

# Did we solve this problem now?



[media.obsessable.com](http://media.obsessable.com)

As few interfaces as possible

# Thank you

[support@chemspider.com](mailto:support@chemspider.com)

Twitter: ChemSpiderman

[www.chemspider.com/blog](http://www.chemspider.com/blog)

