



**reaxys**

Innovation from CrossFire Beilstein

## Reaxys – Onemli ve One Cikan Noktalar

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## Reaxys Nedir?

- > Organik ve inorganik kimya ve ilgili disiplinlerdeki bilimadamları için **Web-tabanlı çözümdür.**
- > **CrossFire Beilstein, Gmelin ve Patent Chemistry** Veritaban'larının birleştirilmiş içeriğine dayanır.
- > Doğru ve geçerliliği denetlenmiş **deneysel reaksiyon & madde özellik verisi**
- > Hedef bileşim sentezini planlamada kimyagerlere yardım etmek için analize ve araç planlamayla **Kullanımı kolay bir ara birimdir.**
- > En ilgili hitleri bulmak için **Akıllı sıralama, filtreleme ve araçları analiz etme**
- > **Uygun Sonuç Görüntüleme**
- > **Kampüs / Kurumsal geniş erişim** (IP-tanıma: kullanıcı ismi/ Şifre gerekmez)
- > **Web-uygulamaları**, kullanıcı yönetimi ve kurulum gerektirmez
- > MAC'I destekler ve URL'ye açıktır



**Sentez Planlama, reaksiyon arařtırmaları ve madde verisi bulmak için** eđer sentetik kimya, ilaç arařtırması , katalizör, veya madde bilimi çalışıyorsanız problem yok: **Reaxys yardım eder.**

## Reaxys – Önemli ve Öne Çıkan Noktalar

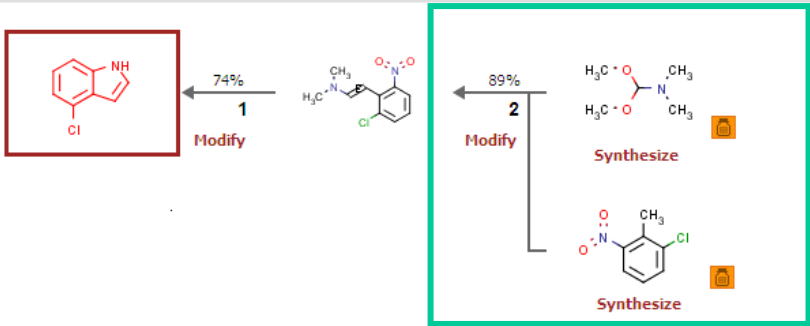
- > **Dünyanın her yerinde En büyük birleştirilmiş reaksiyon kaynağı** (tekli- ve çoklu adım reaksiyonları)
- > **Sentez Planlayıcı Aracı:** Sentez stratejisi oluşturmak için reaksiyonları seçme
- > Patent yayınlarından **reaksiyon prosedür metinleri**
- > **Büyük deneysel** (hesaplanmış değil!) madde veri **havuzu**
  - > ör. maddeyi tespit için **ölçülmüş spektral doruklar**
- > Sadece esas özellikler değil, **Farklı özelliklerin geniş çeşitliliği,**
- > **Madde&Reaksiyon Dosyaları:**
  - > **bir** madde kaydına dahil olan farklı yayınlardan madde verisi
  - > **bir** reaksiyon kaydına dahil olan farklı yayınlardan reaksiyon verisi
- > Akıllı hit analizleri, **daha bağlantılı** hitler almak için **sınıflandırma** ve görüntüleme araçları
- > **Verileriyle birlikte reaksiyonları ve yapıları export etmek için, yüksek esneklik** ör. reaksiyon-veri-**tabloları**. Formatlar: WORD, EXCEL, PDF, **XML, SD/RD** (Yapı-/Reaksiyon-Veri-Dosya), RIS (Endnote, Referans Yönetimi)
- > **Diğer Elsevier sistemleriyle entegrasyon**, ör. Scopus'la iki yönlü bağlantı, especially **“aktarılan”-bilgi**
- > **Kampüs / Kurumsal geniş erişim lisans modelleri** (IP lisansı için tam destek)

## Sentez Planlayıcı

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

Synthesis 1

Undo Open Save Output Copy plan to new page representation Horizontal tree Hide Hints



Hints

- Click on "Synthesize" to find all preparations of the compound.
- In the browser below review the preparations and „Add“ the best one to the synthesis tree.
- Click on „Modify“ if you want to select different starting materials.
- Click on the button „Copy plan to new page“ if you want to investigate alternative routes.

Hide text

Hide selected details Hide all details Show all details

Step	Yield	Conditions	References
1	243.3 g	With aq. hydrazine hydrate in tetrahydrofuran; methanol T=10 - 20°C ;	<b>Katayama, Masato</b> Biosci., Biotechnol., Biochem., <b>2000</b> , vol. 64, # 4 p. 808 - 815 Abstract Full Text <a href="#">SCOPUS</a>
	74%	With Zn; AcOH in methanol; CH <sub>2</sub> Cl <sub>2</sub>	<b>Siu, Jason; Baxendale, Ian R.; Ley, Steven V.</b> Org. Biomol. Chem., <b>2004</b> , vol. 2, # 2 p. 160 - 167 Abstract Full Text <a href="#">SCOPUS</a>
		In benzene Experimental Procedure	<b>Patent: Hoffmann-La Roche Inc.</b> US3976639 A1 (1976/08/24) Abstract Full Text
2	89%	With CuI; DMF T=180°C ; P=6000.6 - 7500.75 Torr;	<b>Siu, Jason; Baxendale, Ian R.; Ley, Steven V.</b> Org. Biomol. Chem., <b>2004</b> , vol. 2, # 2 p. 160 - 167 Abstract Full Text <a href="#">SCOPUS</a>

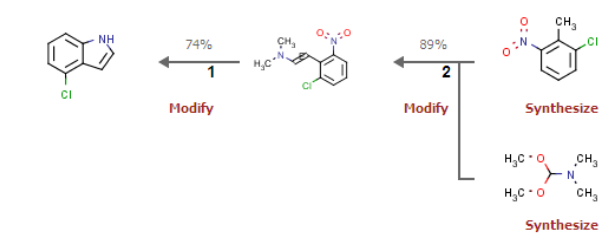
Scopus:  
"Aktarılan"-Bilgi !  
ve fazlası

## Reaksiyon Prosedür Metni

Query Results Synthesis Plans My Settings Help Login

Synthesis 1

Undo Open Save Copy plan to new page Synthesis representation Horizontal tree Hide Hints



Hints

- Click on "Synthesize" to find all preparations of the compound.
- In the browser below review the preparations and "Add" the best one to the synthesis tree.
- Click on "Modify" if you want to select different starting materials.
- Click on the button "Copy plan to new page" if you want to investigate.

**“Reaksiyon Dosyası“: Bir kayda dahil olan patent ve yazılardan veri**

Step	Yield	Conditions	References
1	243.3 g	With aq. hydrazine hydrate in tetrahydrofuran; methanol T=10 - 20°C; Reduction cyclization; 2007/12/10;	<b>Katayama, Masato</b> Bioscience, Biotechnology, and Biochemistry, <b>2000</b> , vol. 64, # 4 p. 808 - 815 Abstract Full Text Scopus
	74%	With Zn; AcOH in methanol; CH <sub>2</sub> Cl <sub>2</sub> Heating; 2007/12/27;	<b>Siu, Jason; Baxendale, Ian R.; Ley, Steven V.</b> Organic and Biomolecular Chemistry, <b>2004</b> , vol. 2, # 2 p. 160 - 167 Abstract Full Text Scopus
		in benzene 969212; 2008/07/04; <a href="#">Hide Experimental Procedure</a>	<b>Hoffmann-La Roche Inc.</b> Patent: US3976639, 1976 Abstract Full Text

EXAMPLE 20  
Preparation of 4-chloroindole  
To a solution containing 10.40 g. of trans-6-chloro-β-dimethylamino-2-nitrostyrene in 250 ml. of benzene in a 500-ml. Parr bottle was added a half teaspoon of Raney nickel.  
The suspension was shaken under an initial hydrogen pressure of 3.5 atm.  
Until the absorption of hydrogen ceased.  
The catalyst was removed by filtration and was washed several times with benzene.  
The benzene filtrate was then extracted with 3 \* 75 ml. of 1M sulfuric acid and 2 \* 100 ml. of water.  
The aqueous phases were back-washed with 125 ml. of benzene in a counter-current manner.  
The combined benzene phases were dried (K<sub>2</sub>CO<sub>3</sub>), filtered, and evaporated to give 5.4 g. of dark green oil which, on distillation, yielded 4.75 g. of a yellow liquid having a boiling point of 116.deg./2 mm.

**Patent yayınlarından Reaksiyon Prosedür Metni**

# Akıllı Hit Ayarı Sıralaması



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Query Results Synthesis Plans My Settings Help Logout

Query 10 reactions

Sınıflandırma „Reaxys-Sıralaması“:  
Ticari Kullanılabilirlik > Yüksek Verim (Yield)

Filter by:  
Yield  
Record Type  
Reagent/Catalyst  
Solvent  
Reaction Type  
No. of Steps  
Document Type  
Authors  
Patent Assignee  
Journal Title  
Publication Year

Reactions Citations

Limit to Selection Output Sort by Reaxys-Ranking

10 reactions out of 13 citations go to No. Page 1

Yield	Conditions	References
60%	 Rx-ID: 23742625	<b>HERBEX, PRODUTOS QUIMICOS, SA; SARAGGA, Jose, Manuel</b> <b>Patent:</b> WO2003/97606 , 2003 Abstract Full Text
	 Rx-ID: 24127082	<b>Whittle, Robert R.; Sancilio, Frederick D.; Stowell, Grayson Walker; Jenkins, Douglas John; Whittall, Linda B.</b> <b>Patent:</b> US6369087 , 2002 Abstract Full Text

Birinci hit: Ürün/ reaktant ticari olarak kullanılır; tedarikçi bilgiye bağlantı

# Deneysel Madde Verisi Yüksek Çeşitliliği



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Substances (Grid) Substances (Table) Citations 1 substances out of 480 citations go to No.  Page 1

Filter by: Molecular Weight, Number of Fragments, Physical Data, Spectroscopic Data, Bioactivity, Document Type, Authors, Patent Assignee, Journal Title, Publication Year

Limit to Selection Output Sort by Molweight Hide Details

Structure	Chemical Name	Available Data	N° of ref.	N° of prep.	Boiling Point
	5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)-methyl]sulphonyl]-1H-benzimidazole (-)-5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-pyridin-2-yl)-methylsulfinyl]benzimidazole 2-[[[3,5-dimethyl-4-methoxypyridin-2-yl)methylsulfinyl]-5-methoxybenzimidazole rac-omeprazole	Identification (70) Physical Data (41) Spectra (26) Bioactivity/ECOTOX (658) Use/Application (746)	480	15 prep out of 79 reactions.	

**Structure/Compound Data**

Reaxys Registry Number: 3628192  
CAS Registry Number: 73590-58-6 119141-88-7 119141-89-8 131959-78-9 326602-80-6  
Chemical Name: 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)-methyl]sulphonyl]-1H-benzimidazole, (-)-5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole, 2-[[[3,5-dimethyl-4-methoxypyridin-2-yl)methylsulfinyl]-5-methoxybenzimidazole, rac-omeprazole  
Type of Substance: heterocyclic

Molecular Formula: C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>S  
Linear Structure Formula: C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>S  
Molecular Weight: 345.422

- Solubility (MCS) (2)
- Partition octan-1-ol/water (MCS) (3)
- Energy Data (MCS) (3)
- Adsorption (MCS) (1)
- Association (MCS) (6)
- Spectra
- Bioactivity/ECOTOX
- Use/Application

**Identification**

**Physical Data**

- Melting Point (4)
- Conformation (2)
- Crystal Property Description (1)
- Crystal Phase (1)
- Crystal System (1)
- Space Group (1)
- Density of the Crystal (1)
- Optics (1)
- Optical Rotatory Power (3)
- Electrochemical Behaviour (2)
- Dissociation Exponent (7)
- Electrochemical Characteristics (2)
- Solubility (MCS) (2)

DBMMJDZJVOS-LILDFLRNCA

**Burada: Ölçülmüş Spektral Ust Degerler**

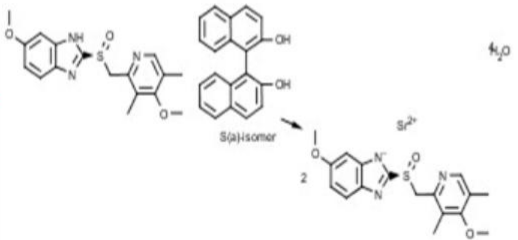
1H	chloroform-d3	300MHz	1H NMR (300 MHz, CDCl <sub>3</sub> ): δ 8.24 (1H, s), 7.58 (1H, mbroad), 7.08 (1H, mbroad), 6.96 (1H, dd), 4.78 and 4.60 (2*1H, system AB), 3.87 (3H, s), 3.72 (3H, s), 2.25 (3H, s), 2.23 (3H, s)
1H	chloroform-d3	300MHz	1H NMR (300 MHz, CDCl <sub>3</sub> ): δ 8.24 (1H, s), 7.58 (1H, mbroad), 7.08 (1H, mbroad), 6.96 (1H, dd), 4.78 and 4.60 (2x1H, system AB), 3.87 (3H, s), 3.72 (3H, s), 2.25 (3H, s), 2.23 (3H, s)



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## Esnek Dönüşüm Fonksiyonu

A	H	J	L	R	S	AC	AG	AI	AJ
reaxys	Reaction	Example label	Fulltext of reaction	Time [h]	Temp. [°C]	Yield	Reagent	Solvent	References
1									
25698679		7	Example 7 Preparation of S-Omeprazole Strontium Tetrahydrate An inclusion complex of (S)-(-)-binol and S-omeprazole (optical purity: 97.0percent ee) prepared according to Examples 1 to 14 of Korean Patent Application No. 2005-68761 (80 g, 126.6 mmol) was dissolved in 400 ml of methanol, and strontium hydroxide octahydrate (20 g, 75.3 mmol) was added thereto, followed by stirring the resulting mixture at room temperature for 3 hours. The precipitate formed was filtered, washed with 150 ml of methanol and dried at 45.deg. C. for 12 hours, to obtain 49.0 g of the title compound (yield: 91percent) as	3	20	91 percent	strontium hydroxide octahydrate	methanol	Patent; HANMI PHARM.CO., LTD.; US2007/93533; A (2007);
2									



EXCEL'e dönüştürülmüş Reaksiyon Tablosu:

- Örnek Etiket (burada Örnek 7)
- Örnek Metin





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## Akıllı Hit Görüntüleme

Abstract  
Show All Reactions (2)  
Hit Reactions in this article (1 out of 2)  
Show All Substances (4)

<input type="checkbox"/> 9	NEW METHOD FOR THE PREPARATION OF THE ANTI-ULCER COMPOUNDS OMEPRAZOLE, LANSOPRAZOLE AND PANTOPRAZOLE	HERBEX, PRODUCTOS QUIMICOS, SA; SARAGGA, Jose, Manuel	2003	Patent: WO2003/97606; A1 Full Text
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Abstract  
NEW METHOD FOR THE PREPARATION OF THE ANTI-ULCER COMPOUNDS OMEPRAZOLE, LANSOPRAZOLE AND PANTOPRAZOLE  
The present invention describes a new process for the preparation of omeprazole, lansoprazole and pantoprazole of formula (XXI), (XXXIII), and which involves the formation of pyridines N-oxide using a rhenum compound as a catalyst, followed by nitration of the 4-position with nitric acid fuming in presence of a claycop. The chlorination of the 2-methyl group of pyridine was achieved by using the POCl<sub>2</sub>/Et<sub>3</sub>N, which allowed the preparation of the derivatives 2-chloromethylpyridines in only one step. These derivatives reacted with the mercaptobenzimidazolic derivatives in presence of ultra-sonic radiation, giving the thioethers. The oxidation of these thioethers was done with several oxidizing agents and the required anti-ulcer compounds were obtained after the substitution of nitro group by the corresponding OR groups.

Show All Reactions (6)  
Hit Reactions in this article (1 out of 6)

Rx-ID: 23742625

Hit Reaksiyon artı özet

Yield	Conditions
60%	With tri-n-butylhexadecylphosphonium bromide in methanol; dichloromethane 4 h; 4167404; 1098229 1730800; Heating / reflux;

Show All Substances (18)

Show 9 results per page

14 reactions out of 13 citations go to No. [ ] Page 1



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> Sizin reaksiyonunuz nedir ?