

# Reaxys – Content at a Glance

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# Reaxys – what is the content?

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A resource for validated measured data you can trust combining the content of the three prestigious databases CrossFire Beilstein, CrossFire Gmelin and Patent Chemistry Database extracting

- chemical reactions
- chemical substances
- measured substance property data
  - Physical, biochemical, application data

from

- selected core chemistry journals (1771 -) (organic, metallorganic, inorganic chemistry)
- selected organic chemistry patent publications (1869 -)



# Patent coverage in detail

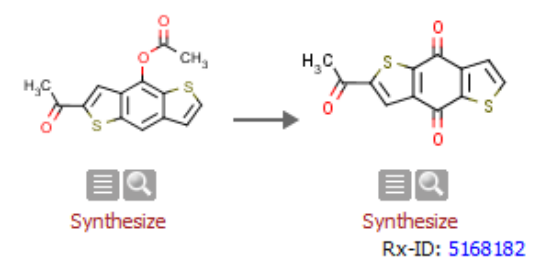
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- Selected organic chemistry patent publications (1869 -1980)
- Selected English-language patent publications (WO, US, EP; 1976 -) from the primary International Patent Class IPC [\* with C07 as sec. IPC]
  - C07           Organic Chemistry
  - A61K        Medicinal Preparations\*
  - A01N        Biocides, Agrochemicals
  - C09B        Dyes

# A typical reaction record: a reaction profile merging data from different sources

Reactions Citations go to Page  Page 1 of 1

Limit to Selection  Sort by Reaxys-Ranking

Yield	Conditions	References
 <p>Synthesize <input type="button" value="Synthesize"/> Rx-ID: 5168182</p>	<p><b>With</b> HOAc, CrO<sub>3</sub> 1 h; Yield given;</p> <p>45% <b>With</b> chromium(VI) oxide in acetic acid 1 h; <a href="#">Hide Experimental Procedure</a></p>	<p><b>Chao, Yu-Hua; Kuo, Sheng-Chu; Wu, Chun-Hsiung; Lee, Chun-Yann; Mauger, Anthony; et al.</b> Journal of Medicinal Chemistry, <b>1998</b>, vol. 41, # 23 p. 4658 - 4661 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a></p> <p><b>University of North Carolina at Chapel Hill</b> <b>Patent:</b> US6337346, 2002 <a href="#">Title/Abstract</a> <a href="#">Full Text</a></p>

**Example 1**  
2-Acetyl-4,8-dihydrobenzo[1,2-b:4,5-b']dithiophene-4,8-dione (9)  
To a stirring mixture of acetyl chloride (5.1 g, 65 mmol) and AlCl<sub>3</sub> (8.7 g, 65 mmol) in 1,2-dichloroethane (200 ML) under N<sub>2</sub> was added dropwise a solution of 4-acetoxybenzo[1,2-b:4,5-b']dithiophene (7)7a (8 g, 32.3 mmol) in 1,2-dichloroethane (90 ML)..  
After stirring for 4 h, this solution was poured into dilute HCl and the aqueous layer was extracted with CHCl<sub>3</sub> three times..  
The combined extracts were washed with saturated NaHCO<sub>3</sub> and water, dried over anhydrous MgSO<sub>4</sub>, and concentrated under reduced pressure to give 7.5 g of the crude intermediate 4-acetoxy-2-acetylbenzo[1,2-b:4,5-b']dithiophene (8).  
To a suspension of crude 8 (7.5 g) in HOAc (30 ML) was added CrO<sub>3</sub> (5.7 g, 57 mmol)..  
After stirring for 1 h, i-PrOH (20 ML) and CHCl<sub>3</sub> (300 ML) were added and stirred for 30 min..  
The resulting solution was poured into ice water, and the aqueous layer was extracted with CHCl<sub>3</sub> three times..  
The combined extracts were dried over anhydrous MgSO<sub>4</sub> and concentrated under reduced pressure..  
The residue was purified by column chromatography (silica gel, CHCl<sub>3</sub>) to give 9 (mp 223-225 .deg. C.) in a 45percent yield. IR (KBr) 1650, 1670 (C=O) cm<sup>-1</sup>; <sup>1</sup>H NMR (CDCl<sub>3</sub>) δ 2.67 (s, 3H, CH<sub>3</sub>), 7.68 (d, J=5.1 Hz, 1H, H-7), 7.74 (d, J=5.1 Hz, 1H, H-6), 8.12 (s, 1H, H-3); <sup>13</sup>C NMR (CDCl<sub>3</sub>): δ 26.9 (C-2-CH<sub>3</sub>), 126.9 (C-7), 129.4 (C-3), 134.3 (C-6), 170.0 (C-4), 174.4 (C-8), 190.7 (C-2-C=O); MS m/z 262 (M<sup>+</sup>); Anal. (C<sub>12</sub>H<sub>6</sub>O<sub>3</sub>S<sub>2</sub>) C, H.

No manual data accumulation anymore – comparative easy-to-read tabular overviews: reactions with the same reaction scheme, but different conditions extracted from different publications are merged to one reaction profile:

- From journal publication

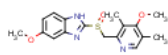
- From patent publication

From patent publications the reaction procedure text is provided to immediately validate conditions. Spectral peaks of product often also given.

# A typical substance record: a substance profile merging measured data from different sources

Substances (Grid) Substances (Table) Citations go to Page 1 Page 1 of 1

Limit to Selection Output Sort by No of References

Structure	Chemical Name	N° of preparations	Available Data	N° of ref.	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]sulphonyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulphonyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulphonyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridin-2-yl)methyl]sulphonyl]benzimidazole 2-[[[(3,5-dimethyl-4-methoxypyridin-2-yl)methyl]sulphonyl]-5-methoxybenzimidazole rac-omeprazole	16 prep out of 91 reactions.	Identification Physical Data (42) Spectra (26) Bioactivity/ECotox (723) Use/Application (1044)	548	

Synthesize Hide Details

**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, 0073590-58-6  
**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]sulphonyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulphonyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulphonyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridin-2-yl)methyl]sulphonyl]benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridin-2-yl)methyl]sulphonyl]benzimidazole, 2-[[[(3,5-dimethyl-4-methoxypyridin-2-yl)methyl]sulphonyl]-5-methoxybenzimidazole, rac-omeprazole  
**Type of Substance:** heterocyclic

**Molecular Formula:** C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>  
**Linear Structure Formula:** C<sub>17</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>  
**Molecular Weight:** 345.422

- 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)
- Partition octan-1-ol/water (MCS) (3)
- Energy Data (MCS) (3)
- Adsorption (MCS) (1)
- Association (MCS) (7)
- Spectra
  - NMR Spectroscopy (8)
  - IR Spectroscopy (7)
  - Mass Spectrometry (1)
  - UV/VIS Spectroscopy (10)
- Bioactivity/ECotox
- Pharmacological Data (714)

**Partition octan-1-ol/water (MCS) (3)**

log POW	Reference
2.23	Riley, R. J.; Parker, A. J.; Trigg, S.; Manners, C. N. <i>Pharmaceutical Research</i> , 2001, vol. 18, # 5 p. 652 - 655 <a href="#">Title/Abstract</a> <a href="#">Full Text</a> <a href="#">View citing articles</a>

**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)

Measured Spectral Peaks e.g. NMR Shifts

# A typical citation record

Reactions Citations go to Page  Page 1 of 1

Limit to Selection Output Sort by Publication Year Hide Details

Title of the Document	Authors	Year	Source	Times cited
<input type="checkbox"/> 1 Synthesis of the DE-ring of goniiodomin A and prediction of its natural relative stereochemistry	Katagiri, Takahiro; Fujiwara, Kenshu; Kawai, Hidetoshi; Suzuki, Takanori	2008	Tetrahedron Letters, <b>2008</b> , vol. 49, # 2 p. 233 - 237 <a href="#">Full Text</a> <a href="#">View citing articles</a>	

**▲ Title/Abstract**  
**Synthesis of the DE-ring of goniiodomin A and prediction of its natural relative stereochemistry**  
Goniiodomin A (1) was first isolated from *Alexandrium hiranoi* as a stereochemically unidentified antifungal agent in 1987 by Murakami. In this study, two stereoisomeric series of non-macrocyclic and macrocyclic DE-ring model compounds of 1 were synthesized, and the natural relative stereochemistry of the DE-ring was predicted by NMR comparison of 1 with these model compounds.

▼ **Show All Reactions (86)**  
**▲ Hit Reactions in this article (1 out of 86)**

Yield	Conditions
91%	<b>With</b> t-BuOOH; 4 Angstrom molecular sieves; titanium(IV) isopropoxide; D-(-)-diethyl tartate in CH <sub>2</sub> Cl <sub>2</sub> T=-25°C; Sharpless epoxidation;

▼ **Show All Substances (101)**

Not only bibliographic data, but additionally the option to view the hit reaction/substance or all reactions/ substances in the article