

23-04-2019



Reaxys – a structure based search and retrieval chemistry information

Mohammad Ghanbari

t.me/chemistry_uk



1. About Reaxys

- 🔬 Concept of design
- 🔬 Coverage
- 🔬 Who is it for
- 🔬 Community's response

2. Using Reaxys to...

- 🔬 Find properties, reactions, patent information, citations...
- 🔬 Plan a synthetic scheme
- 🔬 Create your own report, library of compounds...

3. Demonstration

- 🔬 www.reaxys.com
- 🔬 Tips and tricks

4. Summary

- 🔬 Trial duration and access model
- 🔬 Online training centre
- 🔬 Customer support

1. 1 - Concept of Design

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What does a Chemist want to know?

1. What is this?

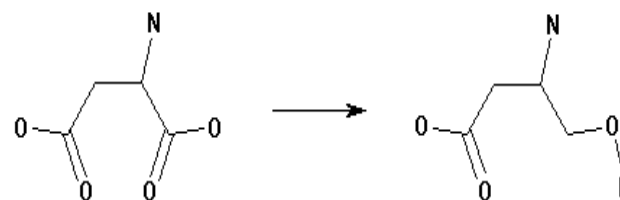
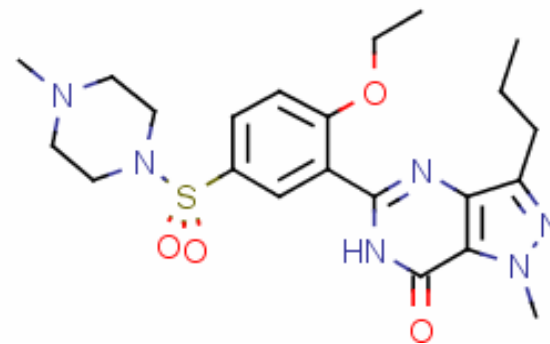
- Is it novel? Patented?
- What are its physical characteristics (weight, melting point, etc)?

2. What does it do?

- Is it a reagent? Solvent?
- What is its bioactivity? Pharmacology?
- Is it toxic?

3. How can I make it?

- How can I change it?
- How can I make it better?



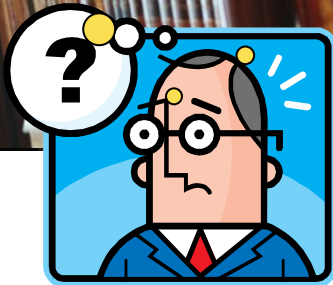
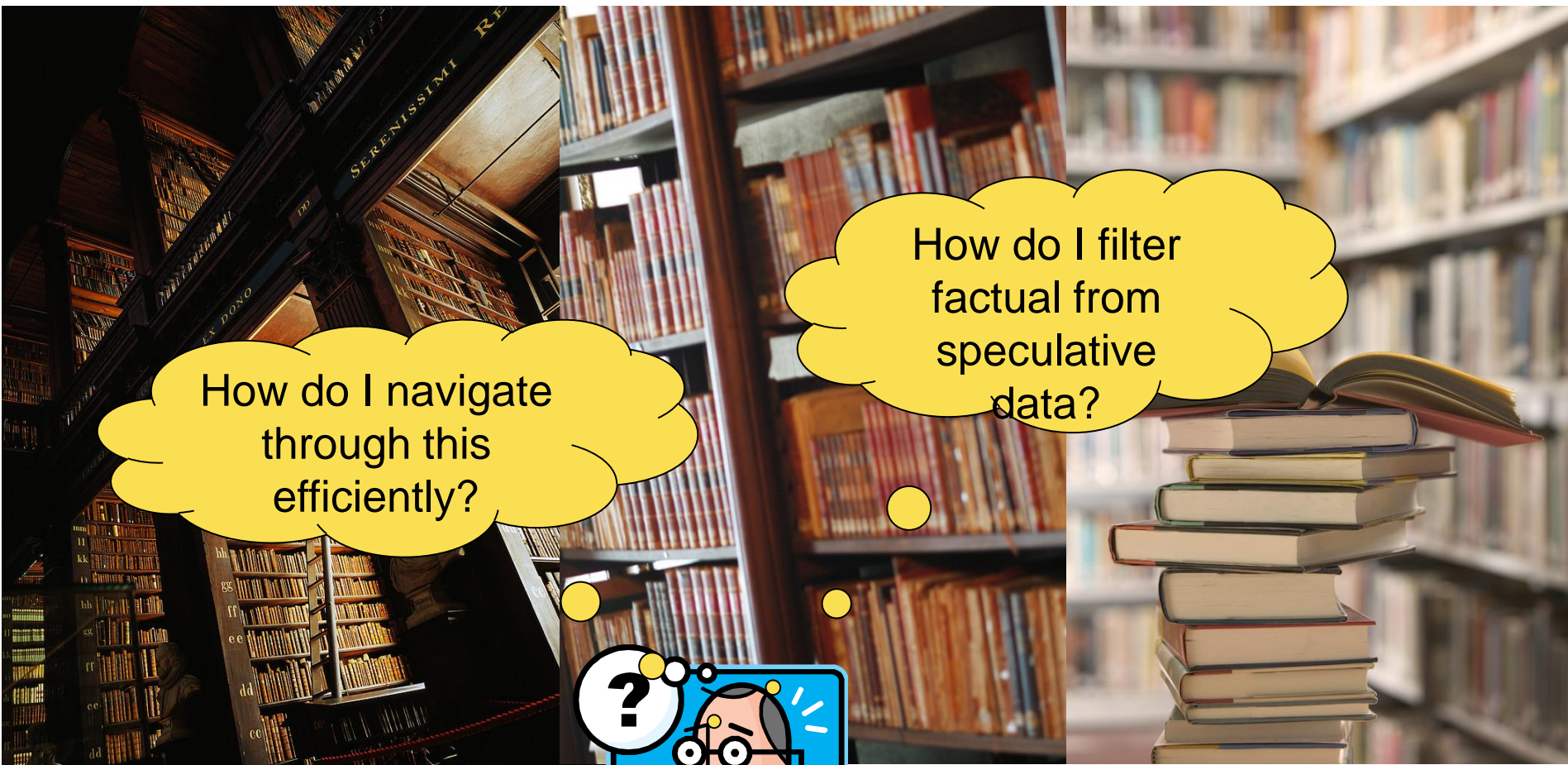
1. 1 - Concept of Design

4

Where do you go to find answers?

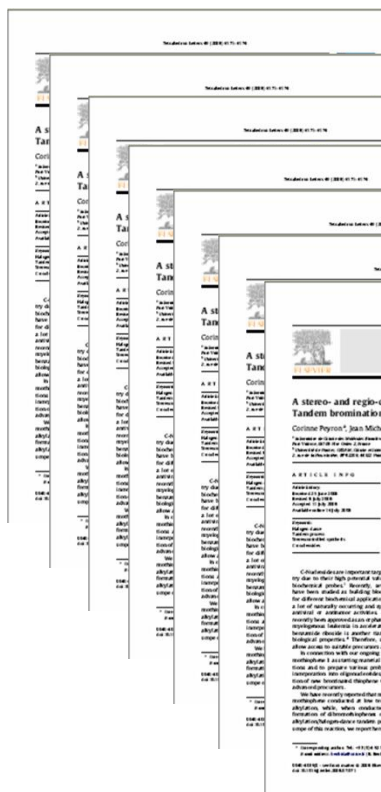


Information Explosion



Information explosion

How much time will it take to filter through all these to find the relevant information?



1. 1 - Concept of Design

7

Designed with **chemistry as the organising principle** to **reduce your time** to get to the **relevant results**

- 🔬 Reaxys is an extensive repository of experimentally validated structural, chemical, and physical data
- 🔬 **Designed** around chemists workflows **to improve efficiency**;
- 🔬 **Simple web-based interface** makes it easy to work with, and easily accessible;
- 🔬 Functionality that **allow chemists to query and filter by property data, design the optimum synthesis route, and view multi-step reactions.**
- 🔬 **A synthesis planner** lets chemists plan the synthesis of compounds and to compare alternative synthetic routes. Identify the shortest potential path, generate a list of reagents, et cetera.

Reaxys extracts valuable chemical properties and reaction details from journals and patents.....

reaxys

Query Results Synthesis Plans History My Alerts My Settings Help Logout

Query 78 reactions 35 reactions filtered by Journal Title

Create Alert

35 reactions out of 15 citations

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

Limit to Selection Output Sort by Reaxys-Ranking Hide Details

Yield Conditions References

Synthesize Rx-ID: 8768344

35 % Chromat. With SnCl₄·2H₂O; RuCl₃·3H₂O/Ph₃ in dioxane; H₂O T=180°C; 20 h;

Cho, Chan Sik; Kim, Jin Hwang; Kim, Tae-Jeong; Shim, Sang Chul
 Tetrahedron, 2001, vol. 57, # 16, p. 3321-3330
 Title/Abstract Full Text View citing articles

A: 45%
 B: 14%
 C: 36%

Stage #1: With sec-BuLi; sparteine in diethyl ether; hexane; cyclohexane
 T=78°C;Metalation; 1 h; 1-(2,2-diethylbutanyloxy)indole; Metalation;
 Stage #2: With MeCO T=78°C;Substitution; 0.5 h; Substitution;

Fukuda, Tsutomu; Maeda, Ryoichi; Iwao, Masatomo
 Tetrahedron, 1999, vol. 55, # 30, p. 9151-9162
 Title/Abstract Full Text View citing articles

Structure	Chemical Name	Nº of preparations	Available Data	Nº of ref.	Boiling Point
	1-(2,2-diethylbutanyloxy)indole	1 prep out of 19 reactions.	Identification Spectra (3)	2	

Synthesize Hide Details

Structure/Compound Data

Reaxys Registry Number: 8318639
 CAS Registry Number: 242805-86-3
 Chemical Name: 1-(2,2-diethylbutanyloxy)indole
 Type of Substance: heterocyclic

Molecular Formula: C₁₇H₂₇NO
 Linear Structure Formula: C₁₇H₂₇NO
 Molecular Weight: 243.349
 InChI Key: CBDJPHJZJQZMAK-UHFFFAOYSA-N

NMR Spectroscopy (2)

Description	Nucleus	Solvents	Frequency	Reference
Spectrum	¹ H	CDCl ₃	300MHz	Fukuda, Tsutomu; Maeda, Ryoichi; Iwao, Masatomo Tetrahedron, 1999, vol. 55, # 30, p. 9151-9162 Title/Abstract Full Text View citing articles

TETRAHEDRON

1999, 9151-9162

TETRAHEDRON

TETRAHEDRON

1999, 9151-9162

Directed C-7 Alkylation of 1-(2,2-Diethylbutanyloxy)indoles

Tsutomu Fukuda, Ryoichi Maeda, and Masatomo Iwao

Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, 1-8 Bunkyo-2-1, Nagasaki 852-8581, Japan

Received 16 April 1999; accepted 26 May 1999

Abstract: Introduction of a hydroxyl derivative was investigated. It was discovered that a bulky indole nucleus is more suitable for C-7 alkylation than a cyclic indole nucleus. Especially in the case of 1-(2,2-diethylbutanyloxy)indole, C-7 alkylation was achieved in a synthetically useful level. The bulky group was easily removed by H₂O. The reaction system also allowed the functionalization of C-7. This study provides a new method for the synthesis of 7-substituted indoles which are not readily available by conventional methods. © 1999 John Wiley & Sons, Inc. *J Heterocyclic Chem.* 36: 1999, 1999

Some biologically significant natural products and synthetic drugs comprise 7-substituted indole nucleus as a key structural unit. For the synthesis of 7-substituted indoles, de novo ring construction of the whole nucleus from appropriately substituted benzene precursors has been utilized as a major approach. This includes Longmire-Bassett's¹ sequence, Ito-Suzuki's² method, and Kambe-Sakamoto's³ procedure. Another ring construction route has been cyclic precursor is also useful, especially for the synthesis of complex natural products such as tryptamine.⁴ Compared to these ring construction methods, Tsuboi⁵ and Iwao⁶ utilized 1-protected indoles (2,3-dihydroindoles) as stable equivalents for 7-selective alkylation and bromination, respectively. Reported direct general benzene-alkene exchange route to the benzamide ring-substituted indole including 7-substituted ones.⁷ This approach, however, requires the synthesis of benzamide derivatives from efficient reagents. Nucleophilic alkylation⁸ and lithiation⁹ routes via indole-CHCl₃ complexes have also been reported. Since we felt these procedures are lengthy and tedious for the synthesis of rather simple 7-substituted indole derivatives, we decided to explore more straightforward routes.

It is well known that the lithiation of 7-substituted indoles occurs at C-2 position preferentially.¹⁰ Although a variety of blocking groups (R₁) have been utilized so far, none of them could prevent C-7 alkylation. This is due to the inordinately strong directing group was found toward H-7. Hence, alkylation at C-7 could be blocked by a bulky indole directing group (R₂) (Scheme 1).

Scheme 1

T. Fukuda et al. / Tetrahedron 55 (1999) 9151-9162

Table 3. Deprotection of DEB Group

Entry	Conditions	Yield (%)	Time (h)	Temp (°C)	Yield (%)
1	K ₂ CO ₃ , MeOH	100	1	40	100
2	NaOH, EtOH	100	1	40	100
3	NaOH, EtOH	100	1	40	100
4	tert-BuOK, H ₂ O, THF	100	1	17(40)	100
5	tert-BuOK, H ₂ O, THF	100	1	5(mn)	100
6	tert-BuOK, H ₂ O, THF	50	30(mn)	10	100

In conclusion, we discovered the first example of the directed C-7 alkylation of indole ring which was substituted 1-(DEB)indoles were employed as the indoles. Since DEB group was easily removed by H₂O after BuOK in THF, this method allows easy conversion of a variety of 7-substituted indoles derivatives which are not readily available by using conventional methods.

Experimental

Melting points were determined with a Yamaguchi micro melting point apparatus and an infrared (IR) spectra were obtained with a Perkin Elmer Spectrum 2000 instrument. ¹H NMR spectra were recorded on 200 MHz on a Varian Gemini-200 instrument. differential NOE measurements were carried out on a Bruker Avance DPX-200 spectrometer. Mass spectra were recorded on a Bruker Avance DPX-200 spectrometer. All measurements were performed at the microanalytical laboratory in Nagasaki University. Elemental analyses were performed on a Perkin Elmer 2400 instrument. All reagents were purchased from Aldrich Chemical Co., Inc. All solvents were dried according to the standard procedure. 2,5-Diisobutylbenzyl alcohol, 3-Thiavaldehyde (I) was synthesized according to the literature.¹¹

1-(2,2-Diethylbutanyloxy)indole (2). Indole (1.00 g, 9.16 mmol) was added to a solution of NaH (50% dispersion in mineral oil, 540 mg, ca. 13.7 mmol) prepared with caution in 20 mL of THF. After stirring at the same temperature for 1 h, 2,2-diethylbutanyloxy chloride¹² (1.00 g, 9.16 mmol) was added dropwise at 0 °C and the whole mixture was gradually warmed to room temperature. The reaction mixture was quenched with saturated aqueous NH₄Cl and extracted with ether. The ether extract was washed successively with water and brine, dried over Na₂SO₄, and concentrated in vacuo. The residue was purified by Kugelrohr distillation (30 °C/2 mmHg) as colorless oil: IR (neat) 1555 (C=C), 1510, 1495, 1485, 1480, 1475, 1470, 1465, 1382, 1346, 1306, 1294, 1225, 1206, 1186, 1176, 1155 (C-H), 1076, 1065, 1060, 1055, 1050, 1045, 1040, 1035, 1030, 1025, 1020, 1015, 1010, 1005, 1000, 995, 990, 985, 980, 975, 970, 965, 960, 955, 950, 945, 940, 935, 930, 925, 920, 915, 910, 905, 900, 895, 890, 885, 880, 875, 870, 865, 860, 855, 850, 845, 840, 835, 830, 825, 820, 815, 810, 805, 800, 795, 790, 785, 780, 775, 770, 765, 760, 755, 750, 745, 740, 735, 730, 725, 720, 715, 710, 705, 700, 695, 690, 685, 680, 675, 670, 665, 660, 655, 650, 645, 640, 635, 630, 625, 620, 615, 610, 605, 600, 595, 590, 585, 580, 575, 570, 565, 560, 555, 550, 545, 540, 535, 530, 525, 520, 515, 510, 505, 500, 495, 490, 485, 480, 475, 470, 465, 460, 455, 450, 445, 440, 435, 430, 425, 420, 415, 410, 405, 400, 395, 390, 385, 380, 375, 370, 365, 360, 355, 350, 345, 340, 335, 330, 325, 320, 315, 310, 305, 300, 295, 290, 285, 280, 275, 270, 265, 260, 255, 250, 245, 240, 235, 230, 225, 220, 215, 210, 205, 200, 195, 190, 185, 180, 175, 170, 165, 160, 155, 150, 145, 140, 135, 130, 125, 120, 115, 110, 105, 100, 95, 90, 85, 80, 75, 70, 65, 60, 55, 50, 45, 40, 35, 30, 25, 20, 15, 10, 5, 0.

Hundreds of searchable fields

Boiling Point

218 - 222°C

Solubility	Saturation	Temperature	Solvent
0.000341568g/l-1	in pure solvent	25°C	H2O

Use Pattern

Antitumor drug

Effect	cell growth; inhibition of
Species or Test-System	acute promyelocytic leukemia NB4 cells of human
Concentration	0.01 - 50 µmol/l

- ⊕ Mutarotation exists
- ⊕ Circular Dichroism exists
- ⊕ Optical Rotatory Dispersion exists
- ⊕ Magnetic Susceptibility exists
- ⊕ Magnetic Data exists
- ⊕ Static Dielectric Constant exists
- ⊕ Dielectric Constant exists
- ⊕ Electrical Data exists
- ⊕ Electrochemical Behaviour exists
- ⊕ Dissociation Exponent exists
- ⊕ Isoelectric Point pH exists
- ⊕ Electrochemical Characteristics exists
- ⊕ Flash Point exists
- ⊕ Autoignition exists
- ⊕ Explosion Limits exists
- ⊕ Further Information exists
- ⊕ Solubility (MCS) exists
- ⊕ Solubility Product (MCS) exists
- ⊕ Solution Behaviour (MCS) exists
- ⊕ Critical Micelle Concentration (MCS) exists
- ⊕ Henry Constant (MCS) exists
- ⊕ Partition octan-1-ol/water (MCS) exists
- ⊕ Liquid/Vapour Systems (MCS) exists
- ⊕ Azeotropes (MCS) exists
- ⊕ Complex Phase Equilibria (MCS) exists
- ⊕ Liquid/Liquid Systems (MCS) exists
- ⊕ Liquid/Solid Systems (MCS) exists
- ⊕ Mechanical & Physical Properties (MCS) exists
- ⊕ Transport Phenomena (MCS) exists
- ⊕ Energy Data (MCS) exists
- ⊕ Electrical Data (MCS) exists
- ⊕ Optical Data (MCS) exists
- ⊕ Boundary Surface Phenomena (MCS) exists
- ⊕ Adsorption (MCS) exists
- ⊕ Association (MCS) exists
- ☒ Spectra exists
 - ⊕ NMR Spectroscopy exists
 - ⊕ IR Spectroscopy exists
 - ⊕ Mass Spectrometry exists



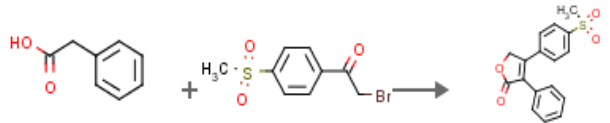
Experimental data and much more at your fingertips

View full experimental details taken directly from the literature

See all related data in a single view

Same transformation with different experimental properties from Patent Chemistry

Full searchable experimental details directly in the database

□ 2	 e e e Rx-ID: 8904422	
54%	Stage #1: With Et₃N in acetonitrile T=25°C; 0.333333 h; 1; 1099647 881861; phenylacetic acid 2-bromo-1-(4-(methylsulfonyl)-phenyl)-ethanone; Stage #2: With DBU in acetonitrile T=0°C; 0.333333 h; 2;	Therien, Michel; Gauthier, Jacques Yves; Leblanc, Yves; Leger, Serge; Perrier, Helene; Prasit, Petpiboon; Wang, Zhaoyin Synthesis, 2001 , # 12 p. 1778 - 1779 Title/Abstract Full Text Scopus
58%	Stage #1: With triethylamine in acetonitrile T=20 - 25°C; 0.333333 h; 1; 1099647 881861; phenylacetic acid 2-bromo-1-(4-(methylsulfonyl)-phenyl)-ethanone; 605283; 741857; Stage #2: With 1,8-diaza-bicyclo[5.4.0]undec-7-ene in acetonitrile T=0°C; 0.333333 h; 2; 508906; 741857; Hide Experimental Procedure	Pfizer Inc. Patent: US2005/65130 , 2005 Title/Abstract Full Text
<p>To a solution of phenylacetic acid (27.4 g, 201 mmol) and 2-bromo-1-(4-(methylsulfonyl) phenyl)ethanone (synthesis set forth in Step 1 below) (60 g, 216 mmol, 1.075 eq.) in acetonitrile (630 mL) at 25.deg. C. was added slowly triethylamine (30.8 mL, 1.1 eq.). The mixture was stirred for 20 min. at room temperature and then cooled in an ice bath. DBU (60.1 mL, 3 eq.) was slowly added. After stirring for 20 min. in the ice bath, the reaction was complete and the mixture was acidified with 1N HCl (color changes from dark brown to yellow). Then 2.4 L of ice and water were added, stirred for a few minutes, then the precipitate was filtered and rinsed with water (giving 64 g of crude wet product). The solid was dissolved in 750 mL of dichloromethane (dried over MgSO₄, filtered) and 300 g of silica gel was added. The solvent was evaporated to near dryness (silica gel a bit sticky) and the residue was applied on top of a silica gel plug (sintered glass funnel) eluted with 10percent EtOAc/CH₂Cl₂, giving after evaporation of the solvent and swish in ethyl acetate, 36.6 g (58percent) of the title compound. Analysis calculated for C₁₇H₁₄O₄S C, 64.95; H, 4.49; S, 10.20 Found: C, 64.63; H, 4.65; S, 10.44</p>		

Interoperability with Scopus and Science Direct

11

SCOPUS
Search Sources And
Quick Search
Scopus: 5 Web Pat
5 Documents that cite:
[Mankad N.P., Peters J.](#)
Diazoalkanes react v
and [Ph2BPTBu2]Cu-
(2008) Chemical Comr
Abstract + Refs View at

ScienceDirect
Home Browse Search My Settings
Quick Search All fields
search tips Journal/book title
Tetrahedron
Synthesis of bicyclo[3.1.0]hexanones via 1,3-
of diazoalkanes to homochiral α -sulfinyl-2-
José Luis García Ruano^{a*}, Marina Alonso^a, David Cruz^b,
M. Teresa Peromingo^a, Amelia Tijo^{a*}, Francisco Yuste^b
^a Facultad de Química, Departamento de Química Orgánica, Universidad Autónoma de Madrid, C
^b Instituto de Química, Universidad Autónoma de Madrid, Cantalejo, 28049 Madrid

The following information is from the Reaxys Database
Sekiya et al.
1976, *Chemical and Pharmaceutical Bulletin*, 24, pp. 369,372,375
2 Chemical Compounds [View reactions \(2\)](#)
1.

Reaxys RN	1912879
Chemical name	ethyl (4-nitrophenyl)carboxylate
CAS number	99-77-4
Mol. formula	C ₉ H ₉ NO ₄
Mol. weight	195.175

For more information access the Reaxys Database:
Related documents found
[View all documents with this compound in Scopus](#)

2.

Reaxys RN	1912198
Chemical name	methyl (4-nitrophenyl)carboxylate
CAS number	619-50-1
Mol. formula	C ₈ H ₇ NO ₄
Mol. weight	181.148

For more information access the Reaxys Database:

1.2 - COVERAGE

12

Beilstein

- 📖 Beilstein handbook (since 1771)
- 📖 Small molecular organic chemistry
- 📖 Key journals
- 📖 Patent publications 1889 – 1990 (Select)

Gmelin

- 📖 Gmelin handbook (since 1772)
- 📖 Ceramics, glass, alloys, catalysts, minerals, coordination compounds...
- 📖 Physical data, electric, mechanical, magnetic, thermodynamic properties.

Patent Chemistry

- 📖 1976 till present: World Patent Office (1978 <), USPTO (1976 <), & EPO (1978 <)
- 📖 English language patents
- 📖 IPC C07, A61K, A01N and C09B

1.2 - COVERAGE

13

Organic
Chemists

Reaxys

Organic
Chemistry

- 📖 **Experimentally validated** content built upon more than 100 years tradition with Beilstein and Gmelin.
- 📖 An **extensive repository** of experimentally validated **structural, chemical, and physical** data
- 📖 Abstract sources and extracting data **relevant** to synthetic chemists
- 📖 Excerpted by trained chemists, Quality checked by trained chemists, process managed and overseen by PhD chemists

.....And gives you what no other database has.....

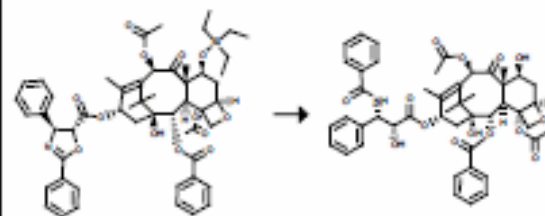
14

28.6 million Reactions

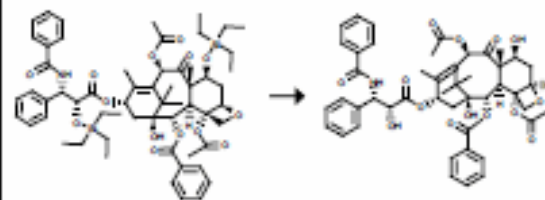
18.017.396 Substances

4.118.881 Citations

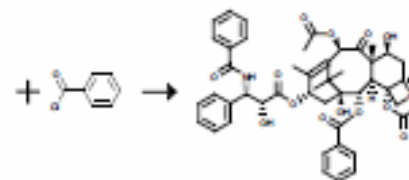
 reaxys™



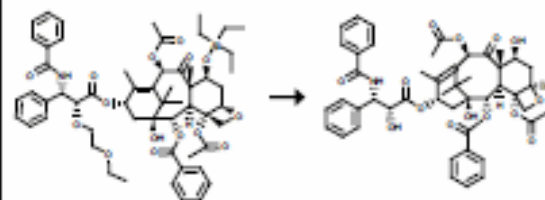
Rx-ID: 3716879



Rx-ID: 3691173



Rx-ID: 231-0548








Rx-ID: 3690700

 reaxys®

1.3 Who is it for?

Anyone who needs accurate and instant information on chemical synthesis, structural, spectroscopic, biological, chemical & physical property data

-  Medicinal Chemists
-  Synthetic Chemists
-  Process Engineers
-  Chemical Engineers
-  Material Scientists

Note: Reaxys may not be very intuitive for chemistry specialties that are not listed here, however, it may still contain very valuable data.

1.4 Reaxys users feedback



“I welcome Reaxys to the chemistry information world, so do my users. If you have not tried it, please give yourself a chance, and I hope, and I know, you will like it”

Norah Xiao – University of Southern California
(2/2010 Library Connect Article)



“Reaxys is a powerful tool in the armory of structure-based literature searching. It will be very **useful both for teaching and research and deserves to be widely used.**”

Prof Jonathan Goodman – University of Cambridge
(12/2009 article in Journal of Chemical Information & Computing)

“You guys should be proud to be involved in something that will change the chemistry world”

Prof Xue Chen Li – Hong Kong University
(letter to Elsevier)



“Having had access to Reaxys this past few months have been such a boon to our efforts. We are now even more enthralled with this program. To say that this is a **powerful tool for getting information quickly and reliably** is an understatement.

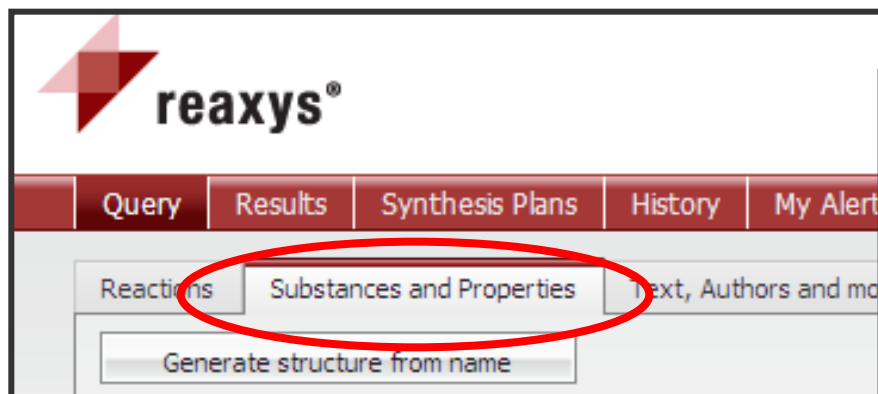
Dr. Aileen Bongat – National Institutes of Health

2.1. Finding physical properties

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Example: Search for substances with...

- Density 0.9 – 1.1 g/cc at 20 degree celsius
- Viscosity 0.02 – 0.12P at 20 degree celsius
- Surface tension 55 – 65 dyn/cm

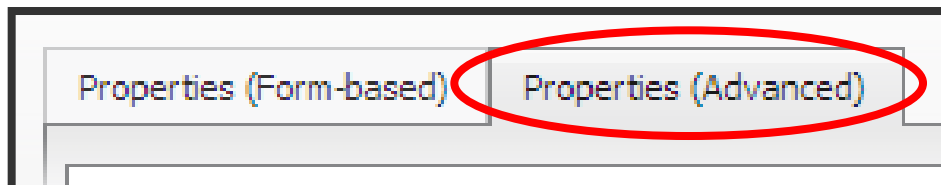


reaxys®

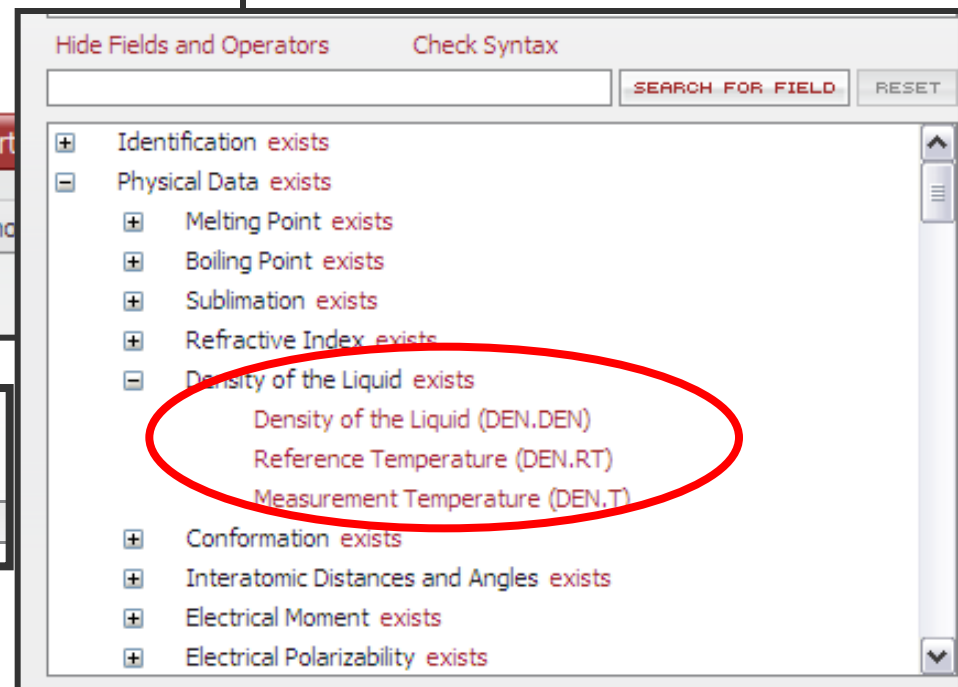
Query Results Synthesis Plans History My Alerts

Reactions **Substances and Properties** Text, Authors and more

Generate structure from name



Properties (Form-based) **Properties (Advanced)**



Hide Fields and Operators Check Syntax

SEARCH FOR FIELD RESET

- Identification exists
- Physical Data exists
 - Melting Point exists
 - Boiling Point exists
 - Sublimation exists
 - Refractive Index exists
 - Density of the Liquid exists**
 - Density of the Liquid (DEN.DEN)
 - Reference Temperature (DEN.RT)
 - Measurement Temperature (DEN.T)
 - Conformation exists
 - Interatomic Distances and Angles exists
 - Electrical Moment exists
 - Electrical Polarizability exists

2.2. Finding reactions

The screenshot shows the 'Reactions' tab selected in the top navigation bar. Below it is a 'Generate structure from name' button. A large text area contains the instruction 'Double click this frame and draw reaction query'. To the right, a 'Search as / by' section is circled in red, containing the following options:

- Product
- Starting material
- Any role
- Reagent/ Catalyst
- As drawn
- Substructure:
 - on heteroatoms
 - on all atoms

At the bottom of the search area are two buttons: 'COPY TO SUBSTANCES TAB' and 'CLEAR'.

- Search by end product, starting material or catalyst/reagent.
- Search by name or draw a structure

The screenshot shows the 'Conditions (Form-based)' search interface. It features a list of search criteria with dropdown menus and input fields:

Field	Operator	Input
Reactant name	is	[]
Product name	is	[]
Reagent/Catalyst	is	[]
Yield	=	[]
All Reaction fields	is	[]

Below the 'Reaction Data' section is a 'Bibliographic Data' section.

2.3 Synthesis Planner

What you just showed would have taken me a week"

Dr Andy Liepa, CSIRO
Chief Research Scientist and namesake
of Liepa phenanthrenes synthesis

Instant selection of suitable reaction steps from different publications to create your own synthesis strategy.

Step	Yield	Conditions	References
2	<input type="checkbox"/> 94.7%	in CH ₂ Cl ₂	Koul, Surrinder; Koul, Jawahir Lal; Singh, Bud Tetrahedron: Asymmetry, 2005 , vol. 16, # 15, p. 2575-2576 Title/Abstract Full Text Scopus
3	<input type="checkbox"/> 82%	With SOCl ₂ in toluene T=90°C; 4 h;	Bellucci, Giuseppe; Berti, Giancarlo; Bianchini, Roberto; Vecchiani, Sandra Gazzetta Chimica Italiana, 1988 , vol. 118, # 6, p. 451-456 Title/Abstract Full Text
		With thionyl chloride in benzene 3 h; Heating;	Rao, Ch Prasad; Srimannarayana, C Indian Journal of Chemistry, Section B: Organic Chemistry, 1994 , vol. 32, # 1, p. 1-4 Title/Abstract Full Text Scopus
		With SOCl ₂ T=60°C; 3 h;	Gualtieri, Fulvio; Conti, Gabriele; De Journal of Medicinal Chemistry, 1994 , vol. 37, # 1, p. 1-4 Title/Abstract Full Text Scopus

161 reactions out of 117 citations go to Page 1 of 18

Sort by Reaxys-Ranking

Yield	Conditions	References
<input type="checkbox"/>	 Rx-ID: 1062590	

Done Internet

2.4 Creating your own reports

reaxys

Output Substance Results

Output Substance Grid Substance Details Table Substance Citations Table

to PDF/Print XML Microsoft Word Microsoft Excel

Literature Management Systems (e.g. ReferenceManager, EndNote etc.) RD File SD/Molfile Smiles

Include the following headline

Output range All Hits Selected hits Range: e.g. 1, 2-5, 10

Output contains include Structures All available data

SD-/RD-/XML-formats to load structures and data into other systems

... by exporting structures with their data to tables: XLS, WORD, PDF

Structure	Reaxys RegNo	CAS Registry Number	Pharmacological Data: Effect	Species or Test-System	Method	Further Details	Type	Value of Type	References
 <chem>CC(C)C1=CC=C(C=C1)C2=CC=C(C=C2)C(=O)O</chem>	2049713	15687-27-1; 51146-56-6; 51146-57-7; 58560-75-1	enzyme activity; inhibition of	recombinant aldo-keto reductase 1C1	enzyme incubated with title comp.: enzyme activity determined using 9,10-phenanthrene quinone substrate	1C1: 20 α -hydroxysteroid dehydrogenase	IC50	29 μ mol/l	Journal: Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M.; Biochemical Pharmacology; vol. 75; 2; (2008); p. 484 - 493;

3. Live demonstration

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www.reaxys.com

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Reaxys – a workflow tool for chemists

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Validated and Experimental Data only

- Journals – physical properties; bioactivity; natural product; yields, reaction conditions, popular reagents / solvents; catalysts; commercial availability.
- Patents – experimental procedures and spectroscopic data (NMR; IR; MS; UV/VIS).

Synthesis planner:

- Plan multi-step synthesis, compare alternative synthetic routes. Make quick decision on the most appropriate pathway.

Reaxys Ranking, Filtering & Analysis tools:

- It's easy to find, filter and analyze data.

Institutional wide, unlimited access:

- So you can obtain the information you need when you need it.

Trial duration and access model

- Trials are available
- Unlimited access model – anyone can log in at any time when within the institute's IP range.
- Training center to support the trial:
<http://www.info.reaxys.com/training-center>
- <http://china.elsevier.com>

Training Center

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For questions and feedback click [here](#). The videos are in swf-format and require the shockwave plug-in to be installed ([download plug-in](#)).

Topic: Language:

Title	Media Type	Duration	Language
Reaxys - Highlights and values for different user groups	PDF, PPS, Video	10 min	English
Reaxys - Content at a Glance	PDF, PPS	5 min	English
From CrossFire to Reaxys - 10 Reasons why to switch	PDF	2 min	English
Reaxys Quick Reference Guide	PDF		English
Reaxys Quick Reference Guide	PDF		French
Reaxys Quick Reference Guide	PDF		Japanese
Reaxys Quick Reference Guide	PDF		Russian
Structure Editor "ChemAxon MarvinSketch" - Usage Tips			English

Customer Support



helpdesk (Ph.D Chemists answer your questions):



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Questions?

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