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Using Reaxys for Searching Chemistry in Patents

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Chemistry from Patents (a short history)

- The role of patents in chemical information has changed dramatically over the last 20 years
- Today more relevant chemistry information published in patents than in journals

Prestigious Crossfire Databases containing Patent Chemistry

- Beilstein Database for organic chemistry from journals and patents (patents until 1980)
- Gmelin Database for inorganic and organometallic chemistry from journals and patents (patents until 1980)
- Patent Chemistry Database for both areas from patents (WO, EP and US since 1980)

→ Combined into Reaxys



Reaxys – Content extracted from:

- Selected core chemistry journals from 1771 – present (organic, inorganic, organometallic chemistry)
- Selected organic chemistry patent publications (1889 - 1980)
- English-language organic chemistry patent publications (WO, US, EP 1976-Present) from the primary International Patent Class (IPC)
 - C07 Organic Chemistry
 - A61K Medicinal Preparations (with C07 as sec. IPC)
 - A01N Biocides, Agrochemicals
 - C09B Dyes

➔ Not only Information, but **Knowledge!**



Reaxys – Content extracted from:

The collage features several documents related to the asymmetric epoxidation of α,β -unsaturated ketones. On the left, a document from Tetrahedron (2006, 31, 10165) describes the use of diaryl-2-pyrrolidinemethanol ethers as chiral organocatalysts. The central document is US Patent 6,900,191 B1 (May 31, 2005), which details a method for the asymmetric epoxidation of α,β -unsaturated ketones using a chiral organocatalyst. The patent includes a list of references (12-60), a list of other publications (61-65), and a list of inventors (66-68). A chemical structure of a chiral organocatalyst is shown, with substituents R1, R2, R3, and R4. The patent also includes a list of physical data, spectra, bioactivity data, and natural product data. A large red cylinder labeled "Reaxys" is overlaid on the central part of the collage.

Physical Data

Spectra

Bioactivity Data

Natural Product

Abstract—Catalytic enantioselective epoxidation of α,β -unsaturated ketones promoted by diaryl-2-pyrrolidinemethanol ether and *tert*-butyl hydroperoxide (TBHP) is described. Investigation on structural modifications of the diaryl-2-pyrrolidinemethanol ether showed that fine tuning of the stereoelectronics of the substituents on the aryl moiety is important to achieve high efficiency. By employing an structurally optimized organocatalyst, significantly reduced loading (10 mol %) can be used to produce the epoxides in high yield and up to 90% ee at room temperature. © 2006 Elsevier Ltd. All rights reserved.

1. Introduction

Enantiomerically enriched α,β -epoxy ketones are versatile intermediates in organic synthesis and important synthetic pharmaceuticals.¹ Efficient asymmetric epoxidation reactions of α,β -unsaturated ketones, mainly chalcones, have been reported using chiral metal allyl hydroperoxide systems.² Moreover, polyaminocatalysts³ and cinchona alkaloids⁴ have been used in the presence of hydrogen peroxide as an oxygen source under basic conditions. The development of simple, catalytic and environmentally benign methodologies to access optically pure compounds is a fundamental goal of current organic synthesis. Asymmetric organocatalysis⁵ satisfies most of these requirements; low cost and easily accessible chiral organic molecules are able to catalyze an ever-increasing number of reactions under operational simplicity and mild conditions. In order to achieve good yields of products and satisfactory level of enantioselectivity, in most of the reactions, e.g., those promoted by proline-based compounds, 20–30 mol % of catalyst loading is generally employed. Thus, one of the most challenging goals in organocatalysis is to reduce catalyst loading to the level used in metal-catalyzed asymmetric synthesis (≤ 10 mol %).

Chiral diaryl-2-pyrrolidinemethanol ethers have been successfully employed as organocatalysts in different transformations such as C–C bond forming reactions,⁶ functionalizations of carbonyl compounds⁷ and epoxidation of α,β -unsaturated aldehydes.⁸ On the other hand, the OH-free proline-like have met with poor success as promoters because of the formation of unreactive cyclic *N,O*-acetals with carbonyl compounds.⁹ Very recently, the asymmetric vinylogous Michael addition reaction has been promoted by diaryl-2-pyrrolidinemethanol ether through the formation of iminium intermediates.¹⁰ We have recently reported that chiral organocatalysts can be used to promote the asymmetric epoxidation of α,β -unsaturated ketones using TBHP as oxidant. In this paper, we report on the use of chiral organocatalysts to promote the asymmetric epoxidation of α,β -unsaturated ketones using TBHP as oxidant. The results are discussed in terms of the effect of the substituents on the aryl moiety on the efficiency of the reaction.

Keywords: Epoxidation; α,β -ketones; Asymmetric organocatalysis; Epoxidation

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0940-4035/\$ - see front matter © 2006 Elsevier Ltd. All rights reserved. doi:10.1016/j.tet.2006.10.005

US PATENT 6,900,191 B1
May 31, 2005

Physical Data

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Bioactivity Data

Natural Product

Abstract

1. Introduction

Chemical Structure

References

Other Publications

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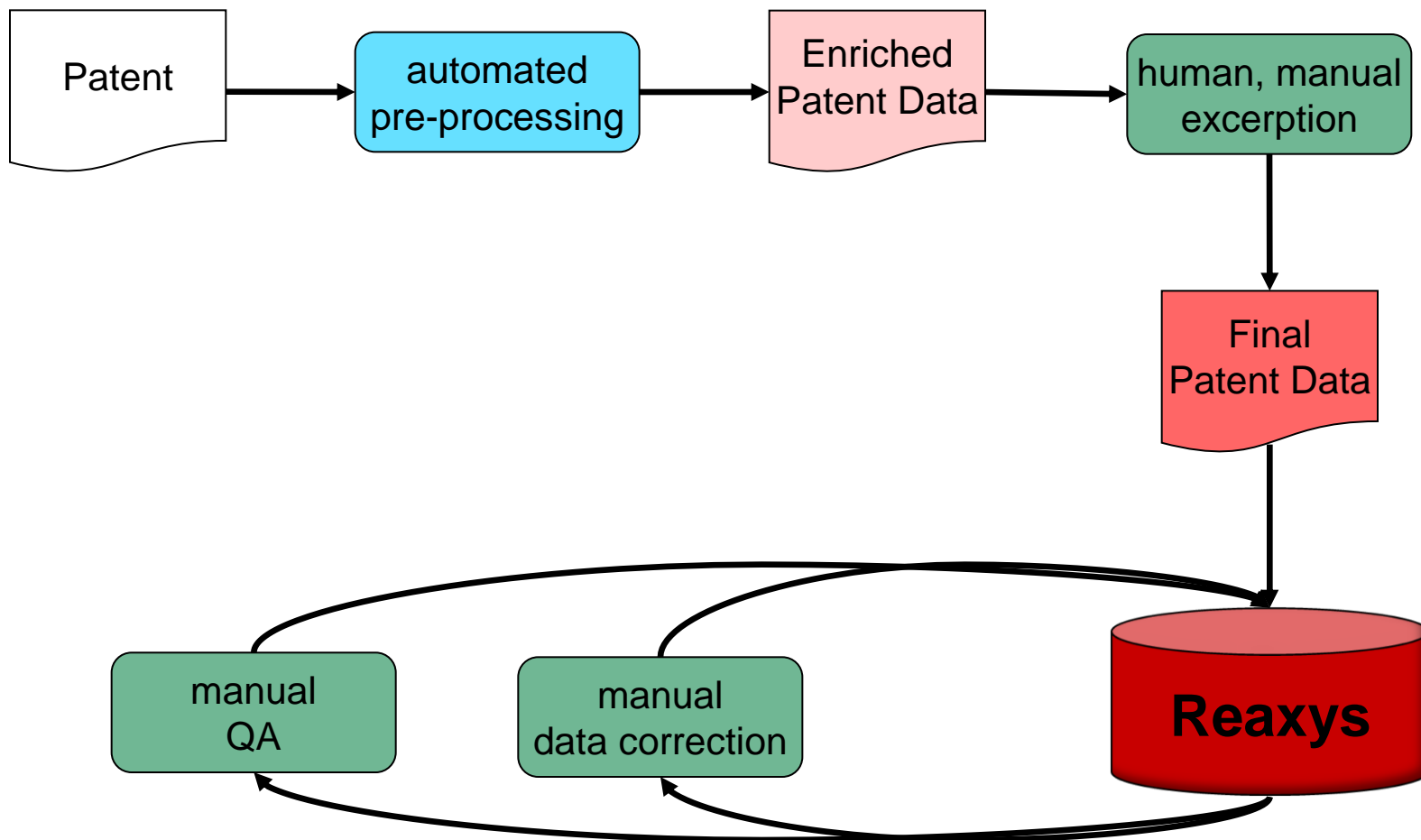
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Reaxys – Patent Features

- Markush structures and references to example structures
- Prophetic substances
- Chemical reactions
 - all substances (starting materials, products, catalysts, reagents) as references to the substances
 - including example text (preparations)
- Commercial Availability
- Detailed physical and chemical properties for substances
 - as dedicated searchable values
 - but also original data (e.g. NMR and IR data)
- Support of InChi keys
 - 1.02 beta
 - 1.02 final



Reaxys – Excerption Workflow for Patents



Reaxys – Automated Pre-processing

3.2.1

2,2-Dimethyl-5-(4-pentenyl)-1,3-dioxane-4,6-dione (**10**)

Ethylene diammonium diacetate (EDDA) (248 mg, 1.4 mmol) was added to a solution of Meldrum's acid (1.188 g, 8.5 mmol) and 4-pentenal (460 mg, 5.5 mmol) in absolute EtOH (6.6 mL) at rt and the resulting solution was stirred for 1 h. $\text{BH}_3 \cdot \text{NH}(\text{CH}_3)_2$ (326 mg, 5.5 mmol) was added to the reaction, which was stirred for 17.5 h. Water (35 mL) and 5% aqueous HCl solution (3 mL) were added to the reaction, which was extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried (MgSO_4) and concentrated to give 1.47 g of crude product. Flash chromatography (9:1 hexanes/EtOAc containing 0.5% HOAc) gave 805 mg (69%) of pure **10** as a white solid: mp 48-50°C; ^1H NMR 5.80 (ddt, 1, $J=17.1, 10.4, 6.1$ Hz), 5.04 (d, 1, $J=17.1$ Hz), 4.99 (d, 1, $J=10.4$ Hz), 3.52 (t, 1, $J=4.9$ Hz), 2.17-2.10 (m, 4), 1.79 (s, 3), 1.76 (s, 3), 1.61-1.53 (m, 2); ^{13}C NMR 165.5 (2C), 137.7, 115.2, 104.8, 46.1, 33.5, 28.4, 26.9, 26.1, 25.6.



Reaxys – Automated Pre-processing

3.2.1

2,2-Dimethyl-5-(4-pentenyl)-1,3-dioxane-4,6-dione (10)

Ethylene diammonium diacetate (EDDA) (248 mg, 1.4 mmol) was added to a solution of Meldrum's acid (1.188 g, 8.5 mmol) and 4-pentenal (460 mg, 5.5 mmol) in absolute EtOH (6.6 mL) at rt and the resulting solution was stirred for 1 h. $\text{BH}_3 \cdot \text{NH}(\text{CH}_3)_2$ (326 mg, 5.5 mmol) was added to the reaction, which was stirred for 17.5 h. Water (35 mL) and 5% aqueous HCl solution (3 mL) were added to the reaction, which was extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried (MgSO_4) and concentrated to give 1.47 g of crude product. Flash chromatography (9:1 hexanes/EtOAc containing 0.5% HOAc) gave 805 mg (69%) of pure **10** as a white solid: mp 48-50°C; ^1H NMR 5.80 (ddt, 1, $J=17.1, 10.4, 6.1$ Hz), 5.04 (d, 1, $J=17.1$ Hz), 4.99 (d, 1, $J=10.4$ Hz), 3.52 (t, 1, $J=4.9$ Hz), 2.17-2.10 (m, 4), 1.79 (s, 3), 1.76 (s, 3), 1.61-1.53 (m, 2); ^{13}C NMR 165.5 (2C), 137.7, 115.2, 104.8, 46.1, 33.5, 28.4, 26.9, 26.1, 25.6.

Identify:

- **Formal structure**



Reaxys – Automated Pre-processing

3.2.1

2,2-Dimethyl-5-(4-pentenyl)-1,3-dioxane-4,6-dione (10)

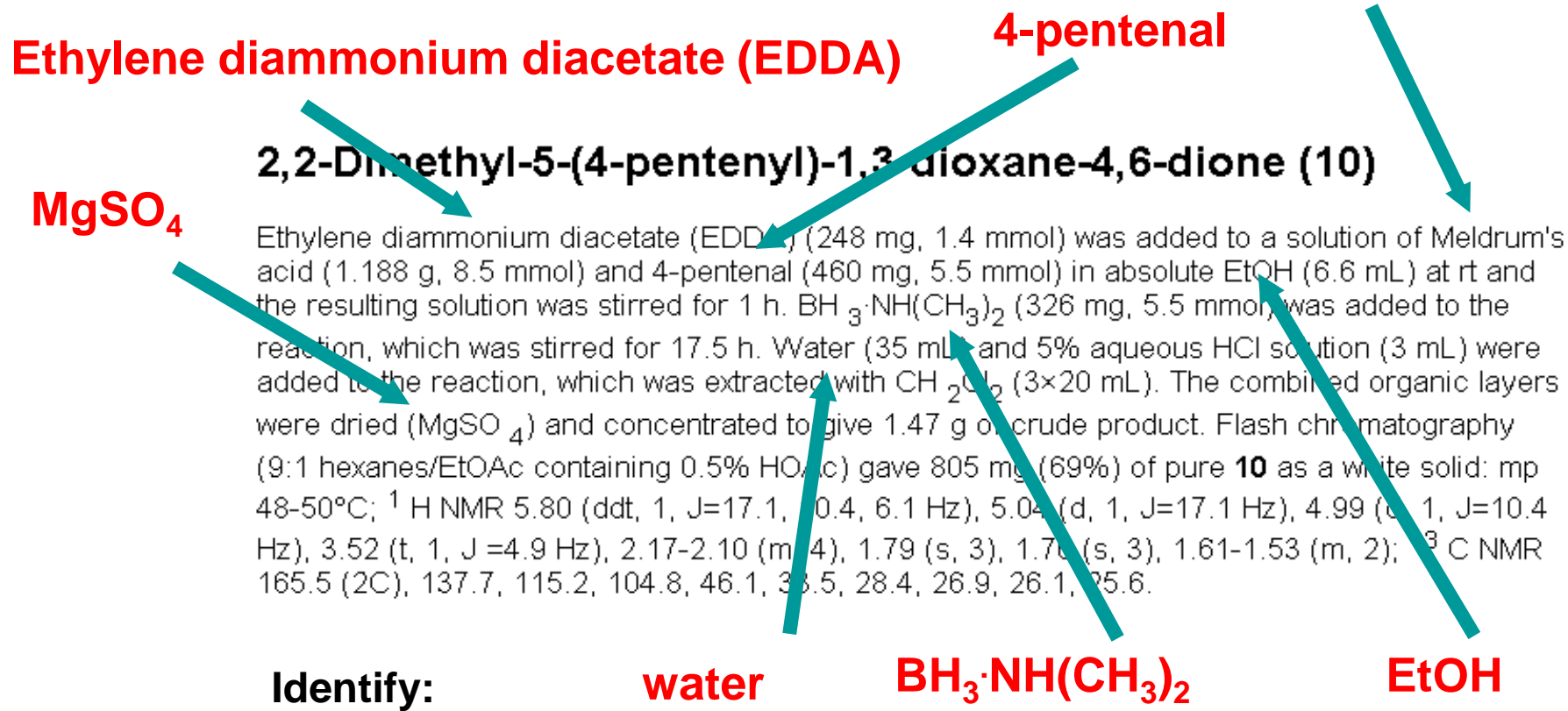
Ethylene diammonium diacetate (EDDA) (248 mg, 1.4 mmol) was added to a solution of Meldrum's acid (1.188 g, 8.5 mmol) and 4-pentenal (460 mg, 5.5 mmol) in absolute EtOH (6.6 mL) at rt and the resulting solution was stirred for 1 h. $\text{BH}_3 \cdot \text{NH}(\text{CH}_3)_2$ (326 mg, 5.5 mmol) was added to the reaction, which was stirred for 17.5 h. Water (35 mL) and 5% aqueous HCl solution (3 mL) were added to the reaction, which was extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried (MgSO_4) and concentrated to give 1.47 g of crude product. Flash chromatography (9:1 hexanes/EtOAc containing 0.5% HOAc) gave 805 mg (69%) of pure **10** as a white solid: mp 48-50°C; ^1H NMR 5.80 (ddt, 1, $J=17.1, 10.4, 6.1$ Hz), 5.04 (d, 1, $J=17.1$ Hz), 4.99 (d, 1, $J=10.4$ Hz), 3.52 (t, 1, $J=4.9$ Hz), 2.17-2.10 (m, 4), 1.79 (s, 3), 1.76 (s, 3), 1.61-1.53 (m, 2); ^{13}C NMR 165.5 (2C), 137.7, 115.2, 104.8, 46.1, 33.5, 28.4, 26.9, 26.1, 25.6.

Identify:

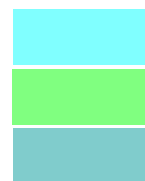
- Formal structure
- Physical properties



Reaxys – Automated Pre-processing Meldrum's acid



- **Formal structure**
- **Physical properties**
- **Name Candidates**



Reaxys – Automated Pre-processing

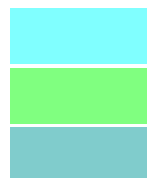
3.2.1

2,2-Dimethyl-5-(4-pentenyl)-1,3-dioxane-4,6-dione (10)

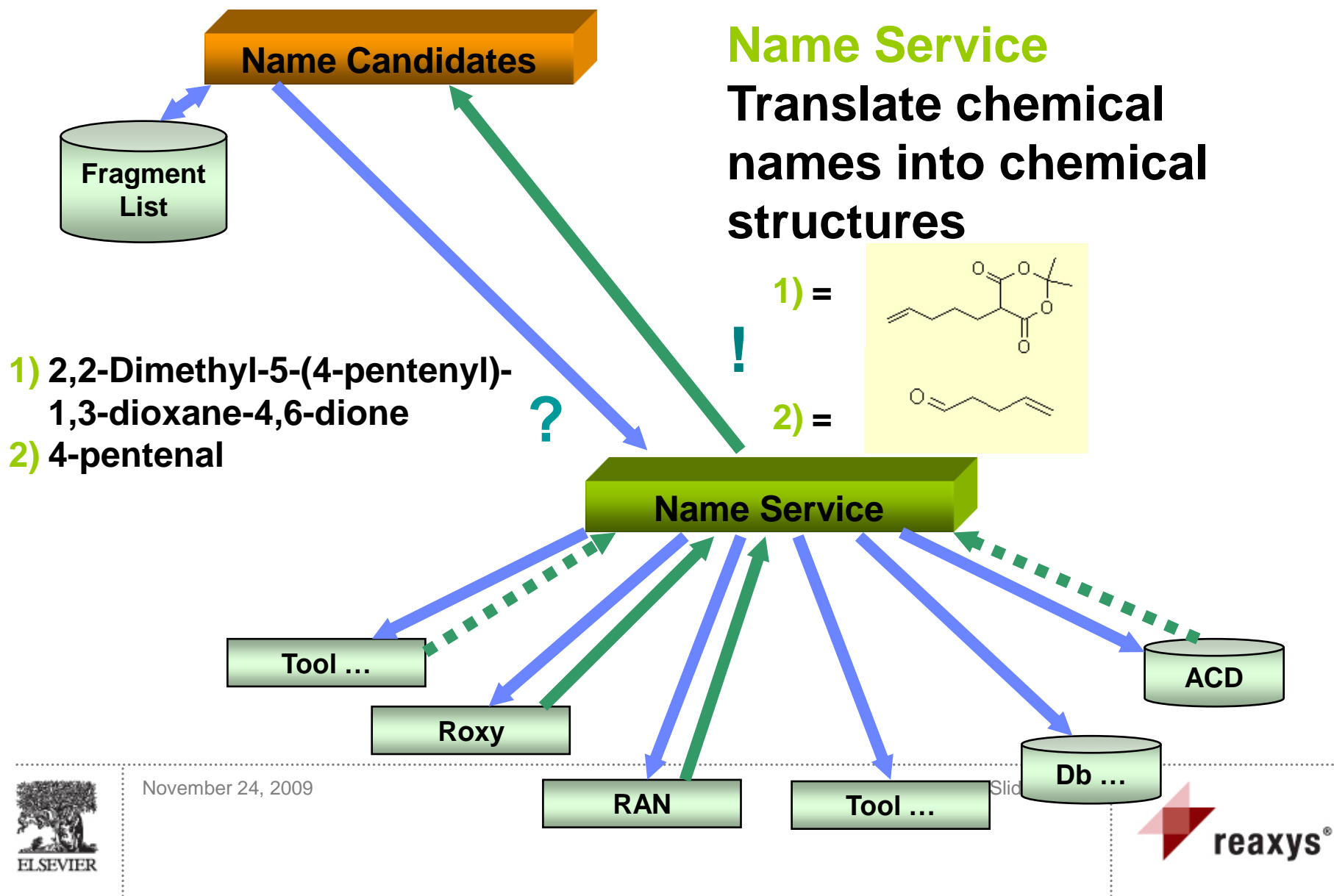
Ethylene diammonium diacetate (EDDA) (248 mg, 1.4 mmol) was added to a solution of Meldrum's acid (1.188 g, 8.5 mmol) and 4-pentenal (460 mg, 5.5 mmol) in absolute EtOH (6.6 mL) at rt and the resulting solution was stirred for 1 h. $\text{BH}_3 \cdot \text{NH}(\text{CH}_3)_2$ (326 mg, 5.5 mmol) was added to the reaction, which was stirred for 17.5 h. Water (35 mL) and 5% aqueous HCl solution (3 mL) were added to the reaction, which was extracted with CH_2Cl_2 (3×20 mL). The combined organic layers were dried (MgSO_4) and concentrated to give 1.47 g of crude product. Flash chromatography (9:1 hexanes/EtOAc containing 0.5% HOAc) gave 805 mg (69%) of pure 10 as a white solid: mp 48-50°C; ^1H NMR 5.80 (ddt, 1, $J=17.1, 10.4, 6.1$ Hz), 5.04 (d, 1, $J=17.1$ Hz), 4.99 (d, 1, $J=10.4$ Hz), 3.52 (t, 1, $J=4.9$ Hz), 2.17-2.10 (m, 4), 1.79 (s, 3), 1.76 (s, 3), 1.61-1.53 (m, 2); ^{13}C NMR 165.5 (2C), 137.7, 115.2, 104.8, 46.1, 33.5, 28.4, 26.9, 26.1, 25.6.

Identify:

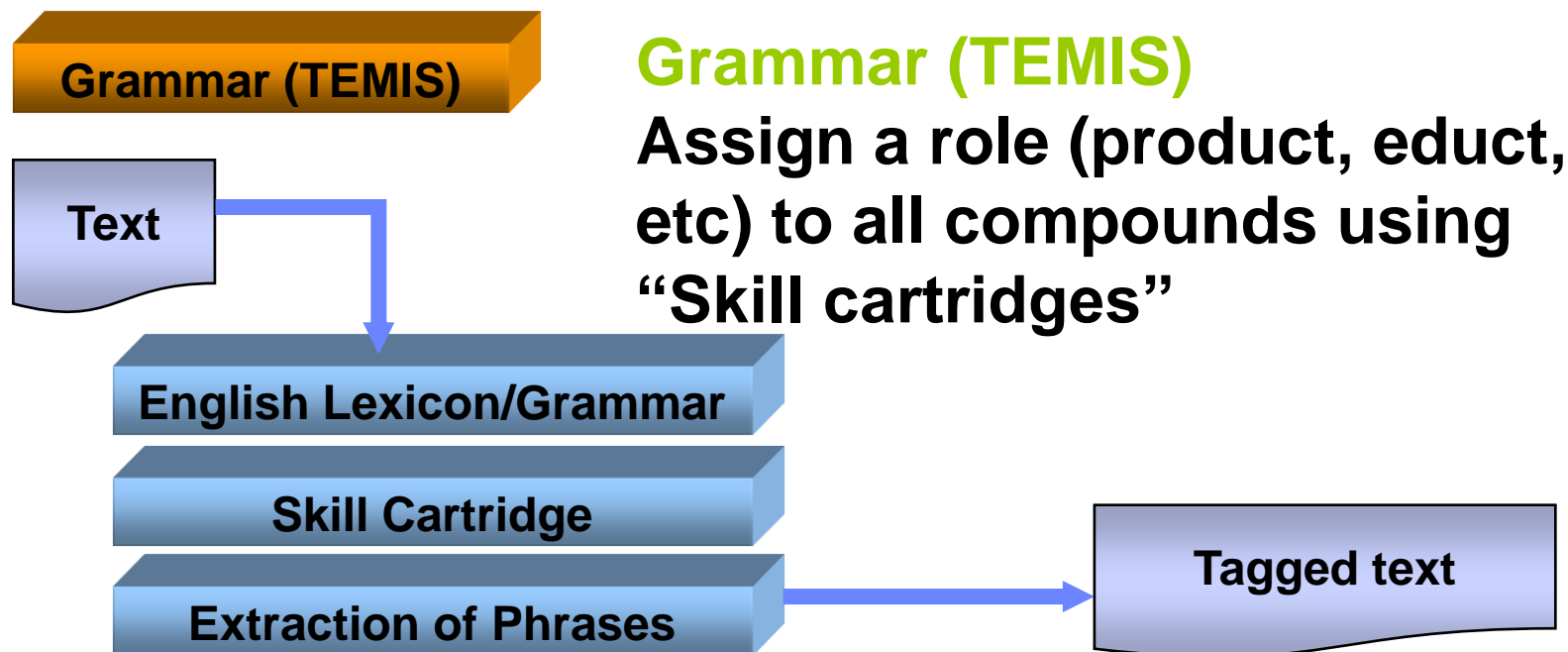
- Formal structure
- Physical properties
- Name Candidates



Reaxys – Automated Pre-processing



Reaxys – Automated Pre-processing



{-}[EX_]3.2.1

{-}[P#STR60-normal] 2,2-Dimethyl-5-(4-pentenyl)-1,3-dioxane-4,6-dione {-}[C60] (10)

{-}[E#STR61-REACTANT] ethylene diammonium diacetate {-}[C61] (EDDA) (248 mg, 1.4 mmol) was added to a solution of {-}[E#STR20-REACTANT] meldrum's acid (1.188 g, 8.5 mmol) and {-}[E#STR23-REACTANT] 4-pentenal (460 mg, 5.5 mmol) in absolute {-}[S#STR17-SOLVENT] EtOH (6.6 mL) at rt and the resulting solution was stirred for 1 h. {-}[E-REACTANT] BH₃-NH(CH₃)₂ (326 mg, 5.5 mmol) was added to the reaction, which was stirred for 17.5 h. {-}[S#STR62-REACTANT] water (35 mL) and 5% {-}[A-REACTANT] aqueous HCl solution (3 mL) were added to the reaction, which was extracted with {-}[X] CH₂Cl₂ (3*20 mL). The combined organic layers were dried ({-}[X] MgSO₄) and concentrated to give {-}[YIELD_VALm] 1.47 g of crude {-}

[ANAPHORIC_PRODUCT] product . Flash chromatography (9:1 {-}[X-class] hexanes / {-}[X-normal] EtOAc containing 0.5% HOAc) gave {-}[YIELD_VALm] 805 mg (69%) of pure {-}[COMP-PRODUCT] 10 as a white {-}[ANAPHORIC_PRODUCT] solid : mp 48-50°C; {-}[NMR_NUC] 1H NMR 5.80 (ddt, 1, J=17.1, 10.4, 6.1 Hz), 5.04 (d, 1, J=17.1 Hz), 4.99 (d, 1, J=10.4 Hz), 3.52 (t, 1, J=4.9 Hz), 2.17-2.10 (m, 4), 1.79 (s, 3), 1.76 (s, 3), 1.61-1.53 (m, 2); {-}[NMR_NUC] 13C NMR 165.5 (2C), 137.7, 115.2, 104.8, 46.1, 33.5, 28.4, 26.9, 26.1, 25.6.

Reaxys – Manual Excerption & Curation

{JEX_13.2.1
{P#STR60.normal} 2,2-Dimethyl-5-(4-pentenyl)-1,3-dioxane-4,6-dione {C61}(10)
{E#STR61-REACTANT} ethylene diammonium diacetate {C61}(EDDA) (248 mg, 1.4 mmol) was added to a solution of {E#STR20-REACTANT} meldrum's acid (1.188 g, 8.5 mmol) and {E#STR23-REACTANT} 4-pentenal (460 mg, 5.5 mmol) in absolute {S#STR17-SOLVENT} EtOH (6.6 mL) at it and the resulting solution was stirred for 1 h. {E-REACTANT} BH₃NH(CH₂)₂ (326 mg, 5.5 mmol) was added to the reaction, which was stirred for 17.5 h. {S#STR62-REACTANT} water (35 mL) and 5% {A-REACTANT} aqueous HCl solution (3 mL) were added to the reaction, which was extracted with {X} CH₂Cl₂ (3*20 mL). The combined organic layers were dried ({X} MgSO₄) and concentrated to give {YIELD_VAL} 1.47 g of crude {
{ANAPHORIC_PRODUCT} product. Flash chromatography (9:1 {X-class} hexanes : {X-normal} EtOAc containing 0.5% HOAc) gave {YIELD_VAL} 805 mg (69%) of pure {COMP_PRODUCT} 10 as a white {
{ANAPHORIC_PRODUCT} solid : mp 48-50°C, {NMR_NUC} 1H NMR 6.80 (ddt, 1, J=17.1, 10.4, 6.1 Hz), 5.04 (d, 1, J=17.1 Hz), 4.99 (d, 1, J=10.4 Hz), 3.52 (t, 1, J=4.9 Hz), 2.17-2.10 (m, 4), 1.79 (s, 3), 1.76 (s, 3), 1.61-1.53 (m, 2); {NMR_NUC} 13C NMR 165.5 (2C), 137.7, 116.2, 104.8, 46.1, 33.5, 28.4, 26.9, 26.1, 26.6.

Manual excerption
& curation

Manual qa
& correction

{JEX_13.2.1
{P#STR60.normal} 2,2-Dimethyl-5-(4-pentenyl)-1,3-dioxane-4,6-dione {C61}(10)
{E#STR61-REACTANT} ethylene diammonium diacetate {C61}(EDDA) (248 mg, 1.4 mmol) was added to a solution of {E#STR20-REACTANT} meldrum's acid (1.188 g, 8.5 mmol) and {E#STR23-REACTANT} 4-pentenal (460 mg, 5.5 mmol) in absolute {S#STR17-SOLVENT} EtOH (6.6 mL) at it and the resulting solution was stirred for 1 h. {E-REACTANT} BH₃NH(CH₂)₂ (326 mg, 5.5 mmol) was added to the reaction, which was stirred for 17.5 h. {S#STR62-REACTANT} water (35 mL) and 5% {A-REACTANT} aqueous HCl solution (3 mL) were added to the reaction, which was extracted with {X} CH₂Cl₂ (3*20 mL). The combined organic layers were dried ({X} MgSO₄) and concentrated to give {YIELD_VAL} 1.47 g of crude {
{ANAPHORIC_PRODUCT} product. Flash chromatography (9:1 {X-class} hexanes : {X-normal} EtOAc containing 0.5% HOAc) gave {YIELD_VAL} 805 mg (69%) of pure {COMP_PRODUCT} 10 as a white {
{ANAPHORIC_PRODUCT} solid : mp 48-50°C, {NMR_NUC} 1H NMR 6.80 (ddt, 1, J=17.1, 10.4, 6.1 Hz), 5.04 (d, 1, J=17.1 Hz), 4.99 (d, 1, J=10.4 Hz), 3.52 (t, 1, J=4.9 Hz), 2.17-2.10 (m, 4), 1.79 (s, 3), 1.76 (s, 3), 1.61-1.53 (m, 2); {NMR_NUC} 13C NMR 165.5 (2C), 137.7, 116.2, 104.8, 46.1, 33.5, 28.4, 26.9, 26.1, 26.6.

Reaxys – Patent Workflow Example 1

- Search a certain patent (here EP2055699)

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SAMPLE TEXT FOR CUSTOMERS

Sample text for group els-supp test Stefan Roller (sroller) is logged in

Query Results Synthesis Plans History My Alerts My Settings Help Logout

Query citations 1 citations No structure 10 substances

Create Alert

10 substances out of 1034 citations


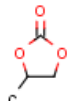
Substances (Grid) Substances (Table) Citations

go to Page Page 1 of 2

Filter by:

- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Natural Product
- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

Sort by No of References


Structure	Chemical Name	N° of preparations	Available Data	N° of ref.	Boiling Point
 <input type="checkbox"/> 1 Synthesize Show Details	2-oxo-1,3-dioxolane [1,3]dioxolan-2-one ethylene carbonate glycol carbonate 1,3-dioxolanone propylene carbonate 1,3-dioxolan-2-one	82 prep out of 772 reactions.	Hit Data (1) Identification Physical Data (244) Spectra (61) Use/Application (8)	634	
 <input type="checkbox"/> 2	4-methyl-1,3-dioxolan-2-one propylene carbonate 1,2-propylene cyclic carbonate 4-methyl-[1,3]-dioxolan-2-one 4-methyl-1,3-dioxolane-2-one 4-methyl-[1,3]dioxolan-2-one 1,2-propanediol carbonate	72 prep out of 247 reactions.	Hit Data (1) Identification Physical Data (736) Spectra (65) Bioactivity/ECotox (1) Use/Application (114)	439	

November 24, 2009

Slide 15

Reaxys – Patent Workflow Example 2

- Refine an interesting substance on patents



Output Substance Results

Output to

Substance Grid

PDF/Print

Include the following headline Derivatives of

Output range

All Hits

Output contains

include Structure

All available data


Identification data

Hit data only

Select data

OK Cancel


Show 99 results



Derivatives of ...

Reaxys ID	14420221	12
Chemical Name	ethyl (2R,3R)-2-(2-benzoyloxyphenyl)-2,3-dihydroxy-2-methylpropanoate 2,3-carbonate, ethyl (2R,3R)-2-(2-benzoyloxyphenyl)-2,3-dihydroxy-2-methylpropanoate 2,3-carbonate, ethyl (2R,3R)-2-(2-benzoyloxyphenyl)-2,3-dihydroxy-2-methylpropanoate 2,3-carbonate	
Molecular Formula	C ₂₄ H ₂₈ O ₈	
Molecular Weight	398.375	
Linear Structure Formula	C ₂₄ H ₂₈ O ₈	
InChI Key	JKWWOPUCBVPJE-YLJYHZDQSA-N	
External Identifiers (2)		
InChI Code		
JKWWOPUCBVPJE-YLJYHZDQSA-N		
JKWWOPUCBVPJE-YLJYHZDQBN		

Reaxys ID	12691991	22
Molecular Formula	C ₂₄ H ₂₈ Cl ₂ N ₂ O ₂	
Molecular Weight	578.489	
Linear Structure Formula	C ₂₄ H ₂₈ Cl ₂ N ₂ O ₂	
InChI Key	FXWWOPKAPZECX-DMJUDRBSA-N	
Substance Label (1)		
Label	References	
Compound No. 24	Patent, SCHERING CORPORATION; PHARMACOPEIA DRUG DISCOVERY, INC., WO200908921, (2009), (A2) English	
Patent-Specifics Data (1)		
References	Patent, SCHERING CORPORATION; PHARMACOPEIA DRUG DISCOVERY, INC., WO200908921, (2009), (A2) English	
External Identifiers (2)		
InChI Code		
FXWWOPKAPZECX-DMJUDRBSA-N		
FXWWOPKAPZECX-CBHXKXRDV		
Pharmacological Data (1)		
1 of 1	Effect	CXCR3 (N-delta 4) receptor; binding to
	Species or Test-System	CXCR3 (N-delta 4) receptor of human
	Method	Biological Examples The inventive compounds can readily be evaluated to determine activity at the CXCR3 receptors by known methods, such as, for example, development of a human CXCR3 (N-delta 4) binding assay. Cloning and expression of human CXCR3 (N-delta 4) The DNA encoding human CXCR3 was cloned by PCR using human genomic DNA (Promega, Madison, WI) as a template. The PCR primers were designed based on the published sequence of human orphan receptor GPR5 (1) with incorporated restriction sites, a Kozak consensus sequence, CD8 leader and Flag tag. The PCR product was subcloned into the mammalian expression vector pME103neo, a derivative of the SP-alpha expression vector (designated as pME103neo-CXCR3 (N-delta 4))-IL-3-dependent mouse pre-B cell BaP3 were transfected by electroporation in 0.4 ml Dureco's PBS containing 4 x 10 ⁶ cells with 20 µg of pME103neo-CXCR3 (N-delta 4) plasmid DNA. Cells were pulsed at 400 Volts, 100 nA, 300 µF. The transfected cells were under selection with 1 mg/ml G418 (Life Technologies, Gaithersburg, MD). G418-resistant BaP3 EPO clones were screened for CXCR3 expression by specific binding of [¹²⁵ I]-IP-10 (INB Life Science Products, Boston, MA). Preparation of BaP3-CXCR3 (N-delta 4) membrane: BaP3 cells expressing human CXCR3 (N-delta 4) were pelleted and resuspended in the lysis buffer containing 10 mM



Derivatives of ...

HEPES, pH 7.5 and CompleteTM protease inhibitors (1 tablet per 100 ml) (Boehringer Mannheim, Indianapolis, IN) at a cell density of 20 x 10⁶ cells per ml. After 5 minute incubation on ice, cells were transferred to 4000 cell disruption bowls (Parr Instrument, Moline, IL) and applied with 1,500 psi of nitrogen for 30 minutes on ice. Large cellular debris was removed by centrifugation at 1,200 x g. Cell membrane in the supernatant was sedimented at 100,000 x g. The membrane was resuspended in the lysis buffer supplemented with 10 percent sucrose and stored at -80 °C. Total protein concentration of the membrane was determined by BCA method from Pierce (Rockford, IL). Human CXCR3 (N-delta 4) scintillation proximity assay (SPA). For each assay point, 2 µg of membrane was preincubated for 1 hr with 200 µg wheat germ agglutinin (WGA) coated SPA beads (Amersham, Arlington Heights, IL) in the binding buffer (50 mM HEPES, 1 mM CaCl₂, 5 mM MgCl₂, 125 mM NaCl, 0.02 percent Na₂S₂O₈, 1.0 percent BSA) at room temperature. The beads were spun down, washed once, resuspended in the binding buffer and transferred to a 96-well ligature (Nalco, Gaithersburg, MD), 25 µM of [¹²⁵I]-IP-10 with tested compounds in a series of titration were added to start the reaction. After 3 hr reaction at room temperature, the amount of [¹²⁵I]-IP-10 bound to the SPA beads was determined with a Wallac 1450 Microbeta counter. The Ki ratings for the various compounds of the present invention are given in the afore-mentioned Table 1. From these ratings and value ranges, it would be apparent to the skilled artisan that the compounds of the invention have excellent utility as CXCR3 receptor antagonists.

Type	IC50
Value of Type	25 - 102 nmol/l
Patent, SCHERING CORPORATION; PHARMACOPEIA DRUG DISCOVERY, INC., WO200908921, (2009), (A2) English	

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November 24, 2009

Reaxys – Patent Workflow Example 3

- Synthesize a substance taken from the report

The screenshot displays the Reaxys software interface for a synthesis plan. The main workspace shows a 5-step synthesis starting from methyl bromide and methyl bromoacetate, proceeding through various intermediates to a final complex product. Each step is labeled with a number and a yield percentage. The interface includes buttons for 'Synthesize', 'Modify', 'Undo', 'Open', 'Save', 'Copy plan to new page', 'Output', and 'Show Hints'. A table at the bottom provides detailed information for each step.

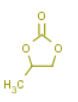
Step	Yield	Conditions	References
1	100%	in toluene T=60°C; 1 h; Show Experimental Procedure	MERCK and CO., INC. Patent: WO2005/70905, 2005 Title/Abstract Full Text
2	85%	in tetrahydrofuran T=20°C; 2 h; Product distribution / selectivity; Show Experimental Procedure	Hologaya Chemical Co., Ltd. Patent: EP1731510, 2006 Title/Abstract Full Text
3		With potassium hexacyanidoferrate(III); potassium osmate (VI); potassium carbonate; (DHQD)2-PHAL in water; tert-butyl alcohol T=4°C; 48 h; Show Experimental Procedure	MERCK and CO., INC. Patent: WO2005/70905, 2005 Title/Abstract Full Text
		With AD-mix- α in water; tert-butyl alcohol T=4°C; 48 h; Show Experimental Procedure	MERCK and CO., INC. Patent: WO2007/18956, 2007 Title/Abstract Full Text
4		With 1.) NaH 1.) THF, 35 min, 2.) RT, 2 h; Yield given. Multistep reaction;	Galemmo, Robert A.; Johnson, William H.; Learn, Keith S.; Lee, Thomas D. Y.; Huang, Fu-Chih; et al. <i>Journal of Medicinal Chemistry</i> , 1990, vol. 33, # 10 p. 2828 - 2841 Title/Abstract Full Text View citing articles
5	74%	With phosphorous acid triethyl ester Show Experimental Procedure	Ethyl Corporation Patent: US5302752, 1994 Title/Abstract Full Text

Reaxys – Further Patent Examples

- Searches for sub-structures with facts

Substances (Grid) Substances (Table) Citations go to Page: Page 1 of 2

Limit to Selection Output Sort by No of References

Structure	Chemical Name	N° of preparations	Available Data	N° of ref.	Boiling Point
	4-methyl-1,3-dioxolan-2-one propylene carbonate 1,2-propylene cyclic carbonate 4-methyl-[1,3]-dioxolan-2-one 4-methyl-1,3-dioxolane-2-one 4-methyl-[1,3]dioxolan-2-one 1,2-propanediol carbonate	72 prep out of 247 reactions.	Hit Data (50) Identification Physical Data (736) Spectra (65) Bio Use	439	48 °C (0.00150015 Torr)

Structure/Compound Data

Reaxys Registry Number: 107913
CAS Registry Number: 108-32-7, 16606-55-6, 51260-39-0, 127128-76-1
Chemical Name: 4-methyl-1,3-dioxolan-2-one, propylene carbonate, 1,2-propylene cyclic carbonate, 4-methyl-[1,3]-dioxolan-2-one, 4-methyl-1,3-dioxolane-2-one, 4-methyl-[1,3]dioxolan-2-one, 1,2-propanediol carbonate
Type of Substance: heterocyclic

Molecular Formula
Linear Structure
Molecular Weight
InChi Key: RUOJZ

Hit Data

Boiling Point (1 Hits out of 28 view all)

NMR Spectroscopy (15 Hits out of 35 view all)

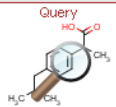
Description	Nucleus	Solvents	Temperature	Frequency	Original Text	Reference
	¹³ C	chloroform-d3	20°C		δ _c 154.5,73.7, 70.9, 19.7;	UNIVERSITY OF NEWCASTLE UPON TYNE Patent: WO2008/132474 , 2008 Title/Abstract Full Text
Chemical shifts	¹³ C	CDCl3		100.4MHz		Dou, Xiao-Yong; Wang, Jin-Quan; Du, Ya; Wang, Er; He, Liang-Nian Syrlett, 2007 , # 19 p. 3058 - 3062 Title/Abstract Full Text View citing articles
Spectrum	¹³ C			100MHz		Du, Ya; Wang, Jin-Quan; Chen, Jian-Yu; Cai, Fei; Tian, Jie-Sheng; Kong, De-Lin; He, Liang-Nian Tetrahedron Letters, 2006 , vol. 47, # 8 p. 1271 - 1275 Title/Abstract Full Text View citing articles
Spectrum	¹³ C	various solvent(s) CDCl3	30.84°C	100.6MHz		Ziani, L.; Courtieu, J.; Merlet, D. Journal of Magnetic Resonance, 2006 , vol. 183, # 1 p. 60 - 67 Title/Abstract Full Text View citing articles
Spectrum	¹³ C	solution		75MHz		Jiang, Jia-Li; Gao, Feixue; Hua, Ruimao; Qiu, Xiangqing Journal of Organic Chemistry, 2005 , vol. 70, # 1 p. 381 - 383 Title/Abstract Full Text View citing articles
Chemical shifts	¹³ C	solution		75MHz		Jiang, Jia-Li; Gao, Feixue; Hua, Ruimao; Qiu, Xiangqing Journal of Organic Chemistry, 2005 , vol. 70, # 1 p. 381 - 383 Title/Abstract Full Text View citing articles
Spectrum	¹³ C	dimethylsulfoxide-d6				Kim, Yong Jin; Varma, Rajender S. Journal of Organic Chemistry, 2005 , vol. 70, # 20 p. 7882 - 7891 Title/Abstract Full Text View citing articles
Chemical shifts	¹³ C	CDCl3		75MHz		Shen, Yu-Mei; Duan, Wei-Liang; Shi, Min

Chemical structure available
NMR available or specify Nuclei is ¹³C
IR available or specify Solvent is

Reaxys – Further Patent Examples

- Searches for a certain substance with a pharmacological effect

Query Results Synthesis Plans History My Alerts My Settings Help

Query  1 substances

Create Alert

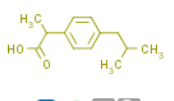
1 substances out of 1708 citations

Filter by:

- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Natural Product
- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

Substances (Grid) Substances (Table) Citations

Limit to Selection Output Sort by No of i

Structure	Chemical Name
	ibuprofen 2-(4-isobutylphenyl)propionic acid α-methyl-4-(2-methylpropyl)benzeneacetic acid α-(p-isobutylphenyl)propionic acid (+/-)-2-(4-isobutylphenyl)propionic acid alpha-(4-isobutylphenyl)propionic acid α-(p-isobutylphenyl)-propionic acid

Synthesize Hide Details

Structure/Compound Data

Reaxys Registry Number: 2049713
CAS Registry Number: 15687-27-1, 51146-56-6, 51146-57-7, 58560-75-

Chemical Name: ibuprofen, 2-(4-isobutylphenyl)propionic acid, α-methyl-4-(2-methylpropyl)benzeneacetic acid, α-(p-isobutylphenyl)propionic acid, (+/-)-2-(4-isobutylphenyl)propionic acid, alpha-(4-isobutylphenyl)propionic acid, α-(p-isobutylphenyl)-propionic acid
Type of Substance: isocyclic

▲ Hit Data

▲ Pharmacological Data (8 Hits out of 865 view all)

Effect	Species or Test-System	Sex	Concentration	Kind of Dosing	Method	Further Details	Type	Value of Type	Comment	Reference
enzyme activity; inhibition of	liver microsomal fraction of Wistar rat	male	<= 1 mmol/l			inhibition of choly-adenylate (CA-AMP) formation studied	Ki	1.46 mmol/l		Ikegawa, Shigeo; Ito, Hiromi; Ohshima, Motohiro; Mitamura, Kuniko; Maeda, Masako; Hofmann, Alan F. Steroids, 2009, vol. 74, # 9 p. 751 - 757 Title/Abstract Full Text
enzyme activity; inhibition of	liver microsomal fraction of Wistar rat	male	<= 1 mmol/l			inhibition of choly-adenylate (CA-AMP) formation studied	inhibition	6 percent		Ikegawa, Shigeo; Ito, Hiromi; Ohshima, Motohiro; Mitamura, Kuniko; Maeda, Masako; Hofmann, Alan F. Steroids, 2009, vol. 74, # 9 p. 751 - 757 Title/Abstract Full Text
enzyme activity; inhibition of	recombinant aldol-keto reductase 1C1				enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C1: 20α-hydroxysteroid dehydrogenase	IC50	29 μmol/l		Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M. Biochemical Pharmacology, 2008, vol. 75, # 2 p. 484 - 493 Title/Abstract Full Text View citing articles
enzyme activity; inhibition of	recombinant aldol-keto reductase 1C2				enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C2: type 3 3α-hydroxysteroid dehydrogenase	IC50	1.9 μmol/l		Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M. Biochemical Pharmacology, 2008, vol. 75, # 2 p. 484 - 493 Title/Abstract Full Text View citing articles
enzyme activity; inhibition of	recombinant aldol-keto reductase 1C3				enzyme incubated with title comp.; enzyme activity	1C3: type 2 3α-hydroxysteroid dehydrogenase	IC50	9.9 μmol/l		Byrns, Michael C.; Steckelbroeck, Stephan;

▲ Pharmacological Data (8 Hits out of 865 view all)

Effect	Species or Test-System	Sex	Concentration	Kind of Dosing	Method	Further Details	Type	Value of Type	Comment	Reference
enzyme activity; inhibition of	liver microsomal fraction of Wistar rat	male	<= 1 mmol/l			inhibition of choly-adenylate (CA-AMP) formation studied	Ki	1.46 mmol/l		Ikegawa, Shigeo; Ito, Hiromi; Ohshima, Motohiro; Mitamura, Kuniko; Maeda, Masako; Hofmann, Alan F. Steroids, 2009, vol. 74, # 9 p. 751 - 757 Title/Abstract Full Text
enzyme activity; inhibition of	liver microsomal fraction of Wistar rat	male	<= 1 mmol/l			inhibition of choly-adenylate (CA-AMP) formation studied	inhibition	6 percent		Ikegawa, Shigeo; Ito, Hiromi; Ohshima, Motohiro; Mitamura, Kuniko; Maeda, Masako; Hofmann, Alan F. Steroids, 2009, vol. 74, # 9 p. 751 - 757 Title/Abstract Full Text
enzyme activity; inhibition of	recombinant aldol-keto reductase 1C1				enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C1: 20α-hydroxysteroid dehydrogenase	IC50	29 μmol/l		Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M. Biochemical Pharmacology, 2008, vol. 75, # 2 p. 484 - 493 Title/Abstract Full Text View citing articles
enzyme activity; inhibition of	recombinant aldol-keto reductase 1C2				enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C2: type 3 3α-hydroxysteroid dehydrogenase	IC50	1.9 μmol/l		Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M. Biochemical Pharmacology, 2008, vol. 75, # 2 p. 484 - 493 Title/Abstract Full Text View citing articles
enzyme activity; inhibition of	recombinant aldol-keto reductase 1C3				enzyme incubated with title comp.; enzyme activity	1C3: type 2 3α-hydroxysteroid dehydrogenase	IC50	9.9 μmol/l		Byrns, Michael C.; Steckelbroeck, Stephan;

Reaxys – Coming Soon ...

- Support of full patent family information
- Increasing the number of multi-step reactions
- Similarity searches and grouping for substances and reactions
- “Quick Search” for novice users
- Analysis tools
- ... and much more ...

Reaxys - Summary

- **Reaxys is**
 - **Chemistry**
 - From patents and journal articles
 - Covering more than 200 years of organic, organometallic and inorganic chemistry
 - Based on CrossFire Beilstein, CrossFire Gmelin and Patent Chemistry Database
 - **Intuitive**
 - Easy to use web-interface, available anytime and anywhere without limits and without installation needs
 - Created from scientist for scientist
 - **The Workflow Solution**
 - Supporting scientists in life science and chemistry in industry and academia in their daily work
 - Providing decision support in finding relevant and validated chemical information
 - Helping to reduce time and efforts in building synthesis plans

Thank you for your attention!