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美国化学文摘社北京代表处

SciFinderⁿ专题培训

---药理/药代信息检索

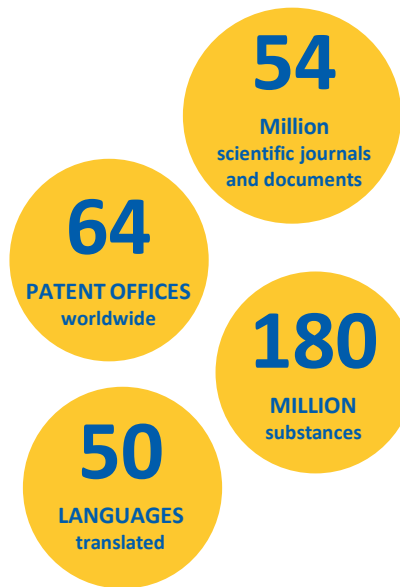


SciFinderⁿ登陆平台

<https://scifinder-n.cas.org>



SciFinderⁿ涵盖内容的独特性



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SciFinder Discovery平台涵盖内容的独特性

- 化学物质数量全球领先。目前收录的化学物质数量已超过1.80亿个，是进行新化合物确认的唯一可用资源。
- 生物大分子数量全球领先。目前收录来自期刊和专利中的约5.8亿条序列（包括蛋白、核酸）
- 由CAS创建的CAS登记号是化学物质的黄金标准；是对物质进行确认的唯一身份识别号；是在进行化学品进出口交易时，必须向相关国家管控机构提供的身份识别号；是在申报课题项目时，需向评议组提供的身份识别号
- CAS几乎收录了从高分子聚合物到纳米颗粒的所有类别的物质，包括有机物、无机物、聚合物、合金、矿物质、配合物、混合物、生物序列等

Sources: <https://www.cas.org/about/cas-content>

SciFinder Discovery平台涵盖内容的独特性

- CAS不但收录专利中报道的确定结构的物质，还收录专利中的通式结构（马库什结构），帮助用户在使用CAS的数据后能够最大程度的避免专利法律风险
- 化学反应数量全球领先，目前收录的化学反应数量超过1.34亿条，是确认新的化学反应、工艺和方法时必不可缺的资源
- 近千名科学家每天阅读来自全球的科技文献，并根据CAS制定的规则 and 标准、从信息专家和科学家的角度对原文中重要的信息进行改写和标引，从而节省CAS的用户花在阅读、理解、总结科技原文文献所需的时间，将更多的时间投入到其他的工作中



大纲

- 疾病模型研究信息
- 药物与受体的相互作用研究
- 药代动力学研究
- 副作用研究



人类疾病动物模型研究信息

用于研究发病机制、药物筛选、药效评价等。



信息的检索方法

构建检索主题

关联文献和物质信息



人类疾病动物模型研究信息

The screenshot shows the SciFinder interface with the search query 'cataract and animal model'. The left sidebar contains a 'Filter by' section with a highlighted 'Publication Year' filter showing a bar chart from 1909 to 2020. The main results area displays three references. Reference 1 is titled 'Deletion mutation in an eye lens beta-crystallin. An animal model for inherited cataracts.' and includes a full-text button. Reference 2 is titled 'An animal model for cataract research: cataract formation in developing chick embryo by glucocorticoid.' and includes a full-text button. Reference 3 is titled 'Age-related nuclear cataract-oxidation is the key.' and includes a full-text button. The interface also shows options for sorting by relevance and viewing partial abstracts.

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References ▾ cataract and animal model

Return to Home

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)
Load More Results

References (7,432) Sort: Relevance ▾ View: Partial Abstract ▾

☐ Substances ▾ ☐ Reactions ▾ ☐ Cited By ▾ ☐ Save

☐ 1

Deletion mutation in an eye lens beta-crystallin. An animal model for inherited cataracts.
By: Chambers, C; Russell, P
The journal of biological chemistry (1991), 266(11), 6742-6 | Language: English, Database: MEDLINE

The most prevalent proteins in the lens of the eye are called crystallins, and it is thought that aberrant crystallins may cause opacification of lens tissue. The Philly mouse, a strain with an inherited cataract, has an abnormal beta B2-crystallin, the principal beta-crystallin in the mouse. The cDNA that codes for the beta B2-crystallin protein has been cloned and sequenced from both the normal and the cataractous Philly mouse. The normal mouse beta B2 cDNA is 756 nucleotides in length with 618 nucleotides of open reading frame. An in-frame deletion of 12 nucleotides has occurred in the Phil...

[View More ▾](#)

☐ 2

An animal model for cataract research: cataract formation in developing chick embryo by glucocorticoid.
By: Nishigori, H; Lee, J W; Iwatsuru, M
Experimental eye research (1983), 36(4), 617-21 | Language: English, Database: MEDLINE

There is no abstract available for this document.

☐ 3

Age-related nuclear cataract-oxidation is the key.
By: Truscott, Roger J W
Experimental eye research (2005), 80(5), 709-25 | Language: English, Database: MEDLINE

cataract and animal model



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广泛的覆盖范围确保尽可能全面地获取文献研究信息

▼ Author

▼ Organization

^ Publication Name

- ☐ World Intellectual Property Organization (597)
- ☐ Experimental Eye Research (278)
- ☐ Molecular Vision (262)
- ☐ United States (196)
- ☐ PLoS One (111)
- [View All](#)

▼ Concept

▼ CAS Solutions

▼ Formulation Purpose

^ Database

- ☒ CAplus (4,913)
- ☐ MEDLINE (2,442)
- ☐ CHEMZENT (77)

▼ Search Within Results

Assessment of oxidative stress to eye in animal model for cataract

By: Bhuyan, Durga K.; Bhuyan, Kallash C.
Methods in Enzymology (1994), 233(OXYGEN RADICALS IN BIOLOGICAL SYSTEMS), 630-9 | Language: English, Database: CAplus

An exptl. procedure is described for induction of cataracts by reactive O species generated in a rabbit's eye by diquat in vivo, as well as spectrophotometric methods for measurement of superoxide anion, hydroxyl radical, and hydrogen peroxide in eye tissues.

Full Text ▼

Substances (5)

Reactions (0)

Cited By (19)

Citation Map

3

Modulation of selenite cataract by the flavonoid fraction of Emilia sonchifolia in experimental animal models

By: Lija, Y.; Biju, P. G.; Reeni, A.; Cibi, T. R.; Sahasranamam, V.; Abraham, Annie
Phytotherapy Research (2006), 20(12), 1091-1095 | Language: English, Database: CAplus

The purpose of the study was to investigate the role of flavonoids from Emilia sonchifolia (ES) on the progression of selenite-induced cataract. The antioxidant property of the flavonoids isolated from ES was assessed by measuring its capacity to inhibit superoxide production and serum oxidation in vitro in comparison with quercetin. Based on these experiments, an in vivo study was conducted to evaluate the modulatory effects of the flavonoids against selenite cataract. Cataract was induced by a single s.c. injection of sodium selenite (4 mg/kg body weight). The treatment group received flavon...

View More ▼

Full Text ▼

Substances (5)

Reactions (0)

Cited By (44)

Citation Map

4

Anticataractogenic property of γ-glutamylcysteine ethyl ester in an animal model of cataract

By: Ohtsu, A.; Kitahara, S.; Fujii, K.
Ophthalmic Research (1991), 23(1), 51-8 | Language: English, Database: CAplus

The anticataractogenic potential of γ-glutamylcysteine Et ester was investigated in model cataracts induced by L-butathione

CAPLUS是CAS核心文献库，同时SciFinder-n中也收录了1946年以来的，来自Medline的文献。

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9

通过Concept标准概念词库，细化模型中涉及的研究点

Concept

Top Count Alphanumeric Search

8 Selected

<input type="checkbox"/> Cataract (6,018)	<input type="checkbox"/> Inflammation (357)	<input type="checkbox"/> Cell proliferation (213)
<input type="checkbox"/> Homo sapiens (2,582)	<input type="checkbox"/> Antidiabetic agents (353)	<input type="checkbox"/> Antiatherosclerotics (212)
<input type="checkbox"/> Human (2,582)	<input type="checkbox"/> Atherosclerosis (337)	<input type="checkbox"/> Cataract, diabetic (212)
<input type="checkbox"/> Animals (1,743)	<input type="checkbox"/> Eye lens, lens epithelium (329)	<input checked="" type="checkbox"/> Diabetes mellitus, diabetic cataract (212)
<input type="checkbox"/> Animal gene (1,499)	<input checked="" type="checkbox"/> Parkinson disease (329)	<input type="checkbox"/> Amyotrophic lateral sclerosis (209)
<input type="checkbox"/> Humans (1,203)	<input type="checkbox"/> Crystallins (327)	<input type="checkbox"/> Rats, Sprague-Dawley (206)
<input checked="" type="checkbox"/> Aging, animal (1,036)	<input type="checkbox"/> Missense mutation (316)	<input type="checkbox"/> Alleles (204)
<input type="checkbox"/> Lens, Crystalline (965)	<input type="checkbox"/> Genotypes (312)	<input type="checkbox"/> Heterozygosity (203)
<input checked="" type="checkbox"/> Male (906)	<input type="checkbox"/> Diabetic retinopathy (308)	<input type="checkbox"/> Arthritis (201)
<input type="checkbox"/> Eye lens (883)	<input checked="" type="checkbox"/> Type 2 diabetes (298)	<input type="checkbox"/> Risk Factors (199)
<input checked="" type="checkbox"/> Disease Models, Animal (827)	<input type="checkbox"/> Apoptosis (296)	<input checked="" type="checkbox"/> Aging (198)
<input type="checkbox"/> Female (796)	<input type="checkbox"/> Stroke (289)	<input checked="" type="checkbox"/> Macular degeneration (276)
<input type="checkbox"/> Proteins (784)	<input checked="" type="checkbox"/> Macular degeneration (276)	<input type="checkbox"/> Huntington disease (197)

Apply Cancel

年龄、并发症影响、
老化、不同发病机制
等

Concept

Top Count Alphanumeric Search

Concept Name

rat

Search

☐ Select All on Page

<input type="checkbox"/> Apba2 protein, rat (1)	<input type="checkbox"/> Ptgs1 protein, rat (1)	<input type="checkbox"/> Rats, Mutant Strains (21)
<input type="checkbox"/> Casp3 protein, rat (1)	<input type="checkbox"/> Ptgs2 protein, rat (1)	<input type="checkbox"/> Rats, Sprague-Dawley (206)
<input type="checkbox"/> Casp9 protein, rat (1)	<input type="checkbox"/> Rat (38)	<input type="checkbox"/> Rats, Transgenic (3)
<input type="checkbox"/> Ccl11 protein, rat (1)	<input type="checkbox"/> Rat cell line PC12 (3)	<input type="checkbox"/> Rats, Wistar (145)
<input type="checkbox"/> Cntnap1 protein, rat (1)	<input type="checkbox"/> Rats (617)	<input type="checkbox"/> Rats, Zucker (2)
<input type="checkbox"/> cryaB protein, rat (2)	<input type="checkbox"/> Rats, Inbred ACI (1)	<input type="checkbox"/> Sand rat (1)
<input type="checkbox"/> Cyp1a2 protein, rat (1)	<input type="checkbox"/> Rats, Inbred BN (25)	<input type="checkbox"/> Slc2a1 protein, rat (1)
<input type="checkbox"/> Egr1 protein, rat (1)	<input type="checkbox"/> Rats, Inbred F344 (6)	<input type="checkbox"/> smooth muscle actin, rat (2)
<input type="checkbox"/> Gja3 protein, rat (1)	<input type="checkbox"/> Rats, Inbred LEC (1)	<input type="checkbox"/> Snai2 protein, rat (1)
<input type="checkbox"/> MsrA protein, rat (1)	<input type="checkbox"/> Rats, Inbred Lew (4)	<input type="checkbox"/> Sprague-Dawley rat (2)

Apply Cancel

集中浏览/选择涉及
大鼠的研究点



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通过Concept标准概念词库，细化模型中涉及的研究点

Concept

Top Count

Alphanumeric

Search

查看药物筛选
相关的研究点

Concept Name

screening

Search

☐ 4 Selected

☐ Disease screening (2)

☒ Drug screening (126)

☒ Drug screening, virtual (2)

☒ High-throughput drug screening (4)

☒ High-throughput screening (11)

Apply

Cancel



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References ▾ cataract and animal model

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)

Load More Results

Filter by

- Document Type
- Language
- Publication Year
 

1997 to 2020

No Min to No Max **Apply**

[View Larger](#)
- Author
- Organization
- Publication Name
- Concept
 - ☐ Cataract (4,025)
 - ☐ Homo sapiens (2,570)
 - ☐ Human (2,570)
 - ☐ Animal gene (1,499)
 - ☐ Aging, animal (1,036)
 - ☒ Drug screening (126)

References (139)

☐ Substances ▾ ☐ Reactions

Sort: Relevance ▾ View: Partial Abstract ▾

☐ 1

Non-human animal for eye disease model with Vav2 and/or Vav3 gene knockout
By: Fujikawa, Keiko; Inoue, Kaoru
World Intellectual Property Organization, WO2008090742 A1 2008-07-31 | Language: Japanese, Database: CAPlus

It is intended to provide an **animal model** which shows a naturally occurring eye disease symptom, particularly ocular hypertension and/or retinal degeneration. The invention relates to a non-human **animal** for eye disease **model** in which the function of Vav2 gene and/or Vav3 gene have/has been impaired. Because the **animal** shows a naturally occurring eye disease symptom, such as ocular hypertension and/or retinal degeneration without administering a drug or placing it in a special growth environment, it can be used as a **model** useful for elucidation of onset mechanism of eye disease or evaluation fo...

[View More ▾](#)

PATENTPAK ▾ Full Text ▾ ☒ Substances (2) ☐ Reactions (0) ☐ Cited By (0) ☐ Citation Map

☐ 2

DLAD (DNase II like acid DNase) gene knockout animals as models for screening of drugs for prevention and treatment of cataract
By: Nagata, Shigekazu
Japan, JP2004357652 A 2004-12-24 | Language: Japanese, Database: CAPlus

DLAD (DNase II like acid DNase) gene knockout **animals**, including mice and other laboratory **animals** with chromosome deficiency, are claimed as **models** for screening of drugs for prevention and treatment of **cataract**.

PATENTPAK ▾ Full Text ▾ ☒ Substance (1) ☐ Reactions (0) ☐ Cited By (1) ☐ Citation Map

☐ 3

Means and methods for treating a pruritus-like skin-disease comprising 4-1BB antagonists
By: Loser, Karin; Kupas, Verena
World Intellectual Property Organization, WO2015091653 A2 2015-06-25 | Language: English, Database: CAPlus

一键获取文献中的关键物质结果

通过文献获取关联的物质结果



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分析文献中的物质结果

研究角色

生物活性

靶点信息

物质类型

属性

谱图

等等

Filter by

Commercial Availability

Reaction Role

Reference Role

Adverse Effect (1,481)

Analytical Study (1,283)

Biological Study (3,597)

Combinatorial Study (410)

Formation (801)

View All

Stereochemistry

Number of Components

Substance Class

Isotopes

Metals

Molecular Weight

Experimental Property

Experimental Spectrum

Regulatory Information

Bioactivity Indicator

Antitumor agents (1,725)

Anti-inflammatory agents (1,533)

Nervous system agents (1,327)

Cardiovascular agents (1,020)

Enzyme inhibitors (975)

View All

Target Indicator

Enzymes (1,808)

Secreted proteins (1,390)

Signaling proteins (1,251)

Membrane proteins (960)

Proteinaceous antigens (950)

View All

Search Within Results

Substances (5,644)

Sort: Relevance View: Partial

References

Reactions

Suppliers

1

1041491-63-7

Image Not Available

Unspecified

DNA, d(G-T-T-G-C-C-T-G-T-T-C-T-A-T-T-A-C-C-C-C-T-T-G-T-C-C-A-G-C-T-G-G-C-T-G-T...

Nucleic Acid Sequence

Sequence Length: 45

1 Reference

0 Reactions

0 Suppliers

2

1041491-62-6

Image Not Available

Unspecified

DNA, d(A-G-C-T-G-G-A-G-A-C-C-G-G-C-T-T-G-A-G-G-C-C-C-T-G-T-G-T-G-T-G-T-T-C-G-C...

Nucleic Acid Sequence

Sequence Length: 45

1 Reference

0 Reactions

0 Suppliers

3

9025-64-3

Image Not Available

Unspecified

Deoxyribonuclease II

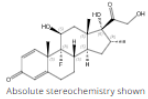
929 References

0 Reactions

9 Suppliers

4

50-02-2



Absolute stereochemistry shown

C₂₂H₂₈O₅

Dexameasone

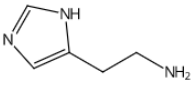
100K References

318 Reactions

147 Suppliers

5

51-45-6



C₆H₉N₃

Histamine

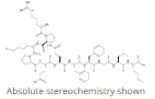
89K References

2,045 Reactions

77 Suppliers

6

33507-63-0



Absolute stereochemistry shown

C₆₃H₉₈N₁₈O₁₃S

Substance P

Protein/Peptide Sequence

Sequence Length: 11

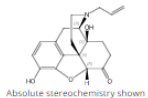
35K References

99 Reactions

68 Suppliers

7

465-65-6



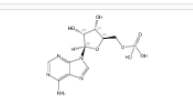
Absolute stereochemistry shown

C₁₉H₂₁NO₄

Naloxone

8

24937-83-5



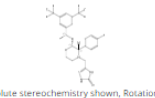
Absolute stereochemistry shown

(C₁₀H₁₄N₅O₇P)_x

Poly(A)

9

170729-80-3



Absolute stereochemistry shown, Rotation (+)

C₂₃H₂₇F₃N₄O₃

Aprepitant

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大纲

- 疾病模型研究信息
- 药物与受体的相互作用研究
- DMPK药代药动学研究
- 副作用研究



例1: PTP1B和小分子抑制剂的作用研究

The screenshot displays the SciFinder database interface. The search query is 'inhibitors and PTP1B'. The left sidebar shows filter options under 'Document Type', with 'Substance Role' selected. The main results area shows two entries:

- Entry 1:** **PTP1B inhibitors for type 2 diabetes treatment: a patent review (2011 - 2014)**
By: Tamrakar, Akhilesh Kumar; Maurya, Chandan K.; Rai, Amit K.
Expert Opinion on Therapeutic Patents (2014), 24(10), 1101-1115 | Language: English, Database: CPlus
A review. Introduction: Protein tyrosine phosphatase 1B (PTP1B) plays an important role in the neg. regulation of insulin signal transduction pathway and has emerged as novel therapeutic strategy for the treatment of type 2 diabetes. PTP1B inhibitors enhance the sensibility of insulin receptor (IR) and have favorable curing effect for insulin resistance-related diseases. A large number of PTP1B inhibitors, either synthetic or isolated as bioactive agents from natural products, have developed and investigated for their ability to stimulate insulin signaling. Areas covered: This review includes...
View More
- Entry 2:** **5-Arylidene-2-phenylimino-4-thiazolidinones as PTP1B and LMW-PTP inhibitors**
By: Ottana, Rosaria; Maccari, Rosanna; Ciarleo, Rosella; Paoli, Paolo; Jacomelli, Michela; Manao, Giampaolo; Camici, Guido; Laggner, Christian; Langer, Thierry
Bioorganic & Medicinal Chemistry (2009), 17(5), 1928-1937 | Language: English, Database: CPlus
As part of a project aimed at identifying effective low mol. weight nonphosphorus monoanionic inhibitors of PTPs, we have synthesized 4-[(5-arylidene-4-oxo-2-phenyliminothiazolidin-3-yl)methyl]benzoic acids (4) and evaluated their inhibitory activity against human PTP1B and LMW-PTP enzymes. The introduction of a 2-phenylimino moiety onto the 4-thiazolidinone ring was designed to enhance the inhibitor/enzyme affinity by means of further favorable interactions with residues of the active site and the surrounding loops. Some of the compounds (4a-d, f) showed interesting inhibition levels in the 1...
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The bottom of the interface shows the start of a third entry: 'The design strategy of selective PTP1B inhibitors over TCPTP'.

inhibitors and PTP1B



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通过Concept概念词库，细化具体的研究点

药物靶点、药物设计、前药、
构效关系、分子对接等

Concept

Top Count Alphanumeric Search

<input type="checkbox"/> Signal transduction (331)	<input type="checkbox"/> Antioxidants (103)	<input type="checkbox"/> Platelet aggregation inhibitors (60)
<input type="checkbox"/> Antitumor agents (226)	<input checked="" type="checkbox"/> Drug design (101)	<input type="checkbox"/> β 3-Adrenoceptor agonists (59)
<input type="checkbox"/> Protein phosphorylation (185)	<input type="checkbox"/> Glucagon receptors (101)	<input type="checkbox"/> New natural products (59)
<input type="checkbox"/> Anti-inflammatory agents (183)	<input type="checkbox"/> High-density lipoproteins (101)	<input type="checkbox"/> Vascular restenosis (59)
<input type="checkbox"/> Neoplasm (167)	<input type="checkbox"/> Phosphorylation (101)	<input type="checkbox"/> Insulin receptor substrate 1 (58)
<input type="checkbox"/> Hypolipemic agents (166)	<input type="checkbox"/> Pharmaceutical carriers (92)	<input type="checkbox"/> Type 1 diabetes (58)
<input type="checkbox"/> Proteins (165)	<input type="checkbox"/> Protein tyrosine phosphatase PTP1B inhibitors (91)	<input type="checkbox"/> Crohn disease (57)
<input type="checkbox"/> Sulfonylureas (165)	<input type="checkbox"/> Animal gene (84)	<input type="checkbox"/> Interleukin 6 (57)
<input type="checkbox"/> Combination chemotherapy (163)	<input type="checkbox"/> Crystal structure (80)	<input checked="" type="checkbox"/> Prodrugs (57)
<input checked="" type="checkbox"/> Drug targets (148)	<input type="checkbox"/> Molecular association (79)	<input type="checkbox"/> Calcium channel blockers (56)
<input type="checkbox"/> Enzyme inhibitors (148)	<input type="checkbox"/> Prophylaxis (78)	<input type="checkbox"/> Irritable bowel syndrome (56)
<input type="checkbox"/> Peroxisome proliferator-activated receptor δ (143)	<input type="checkbox"/> Cardiovascular agents (76)	<input type="checkbox"/> Body weight (55)
<input type="checkbox"/> Antifolate agents (139)	<input type="checkbox"/> Sodium-dependent glucose transporter SGLT2 (76)	<input type="checkbox"/> Pancreatitis (55)

Apply Cancel

Concept

Top Count Alphanumeric Search

<input type="checkbox"/> Hyperlipidemia (139)	(76)	<input type="checkbox"/> Low-density lipoprotein receptors (54)
<input checked="" type="checkbox"/> Structure-activity relationship (138)	<input type="checkbox"/> Cholesteryl ester transfer proteins (75)	<input checked="" type="checkbox"/> Molecular structure, natural product (54)
<input type="checkbox"/> Insulin receptors (137)	<input type="checkbox"/> Molecular modeling (72)	<input type="checkbox"/> Inflammatory bowel disease (53)
<input type="checkbox"/> Inflammation (134)	<input type="checkbox"/> Low-density lipoproteins (71)	<input type="checkbox"/> Retinal disease (53)
<input type="checkbox"/> Peroxisome proliferator-activated receptor α (133)	<input type="checkbox"/> Neurodegenerative disease (71)	<input type="checkbox"/> Fatty acids (52)
<input type="checkbox"/> Hyperglycemia (131)	<input type="checkbox"/> Alzheimer disease (70)	<input type="checkbox"/> Microsomal triglyceride transfer protein (52)
<input type="checkbox"/> Metabolic syndrome X (131)	<input type="checkbox"/> Peroxisome proliferator-activated receptors (69)	<input type="checkbox"/> Hydrogen bond (50)
<input type="checkbox"/> Atherosclerosis (130)	<input type="checkbox"/> Bile acids (68)	<input type="checkbox"/> Kidney disease (50)
<input type="checkbox"/> Hypertension (127)	<input type="checkbox"/> Epidermal growth factor receptors (68)	<input type="checkbox"/> Lipids (50)
<input checked="" type="checkbox"/> Structure-activity relationship, enzyme-inhibiting (125)	<input type="checkbox"/> Apoptosis (67)	<input type="checkbox"/> Nervous system agents (50)
<input checked="" type="checkbox"/> Molecular docking (122)	<input type="checkbox"/> Cell proliferation (67)	<input type="checkbox"/> Ulcerative colitis (50)
<input type="checkbox"/> Anticholesteremic agents (121)	<input type="checkbox"/> Disease, animal (67)	

Apply Cancel



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References | Inhibitors and PTP1B

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
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 - Miscellaneous (1)
 - Preparation (4)
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- Publication Year
- Author
- Organization
- Publication Name
- Concept
 - Homo sapiens (801)
 - Human (801)
 - Antidiabetic agents (722)
 - Type 2 diabetes (444)
 - Obesity (427)
 - Drug targets (148)
 - Structure-activity relationship (138)
 - Structure-activity relationship, enzyme-inhibiting (125)
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 - Molecular structure, natural product (54)

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Substances

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1

5-Arylidene-2-phenylimino-4-thiazolidinones as PTP1B and LMW-PTP inhibitors
By: Ottana, Rosaria; Maccari, Rosanna; Curleo, Rosella; Paoli, Paolo; Jacomelli, Michela; Manao, Giampaolo; Camici, Guido; Langer, Thierry
Bioorganic & Medicinal Chemistry (2009), 17(5), 1928-1937 | Language: English, Database: C.Aplis

As part of a project aimed at identifying effective low mol. weight nonphosphorus monoanionic inhibitors of PTPs, we have synthesized 4-[(5-arylidene-4-oxo-2-phenyliminothiazolidin-3-yl)methyl]benzoic acids (4) and evaluated their inhibitory activity against human PTP1B and LMW-PTP enzymes. The introduction of a 2-phenylimino moiety onto the 4-thiazolidinone ring was designed to enhance the inhibitor/enzyme affinity by means of further favorable interactions with residues of the active site and the 5-oxo imine lone pair. Some of the compounds (3a-4, 6) showed interactive inhibition levels in the I

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Substances (29) Reactions (39) Cited By (54) Citation Map

2

The design strategy of selective PTP1B inhibitors over TCPTP
By: Li, XiangQian; Wang, Lijun; Shi, DaYong
Bioorganic & Medicinal Chemistry (2016), 24(16), 3343-3352 | Language: English, Database: C.Aplis

A review. Protein tyrosine phosphatase 1B (PTP1B) has already been well studied as a highly validated therapeutic target for diabetes and obesity. However, the lack of selectivity limited further studies and clin. applications of PTP1B inhibitors, especially over T-cell protein tyrosine phosphatase (TCPTP). In this review, we enumerate the published specific inhibitors of PTP1B, discuss the structure-activity relationships by anal. of their X-ray structures or docking results, and summarize the characteristic of selectivity related residues and groups. Furthermore, the design strategy of select

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3

Targeting Inactive Enzyme Conformation: Aryl Diketoacid Derivatives as a New Class of PTP1B Inhibitors
By: Liu, Sijiu; Zeng, Li-Fan; Wu, Li; Yu, Xiao; Xue, Ting; Gunawan, Andrea M.; Long, Ya-Qiu; Zhang, Zhong-Yin
Journal of the American Chemical Society (2008), 130(50), 17075-17084 | Language: English, Database: C.Aplis

There has been considerable interest in protein tyrosine phosphatase 1B (PTP1B) as a therapeutic target for diabetes, obesity, as well as cancer. Identifying inhibitory compounds with good bioavailability is a major challenge of drug discovery programs targeted toward PTPs. Most current PTP active site-directed pharmacophores are neg. charged pTyr mimetics which cannot readily enter the cell. This lack of cell permeability limits the utility of such compounds in signaling studies and further therapeutic development. Aryl diketoacids were

Identified as novel αTyr mimetic and neutral acids.

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Citation Map

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Journal

Source
Bioorganic & Medicinal Chemistry
Volume: 17
Issue: 5
Pages: 1928-1937
Journal
2009
DOI:
[10.1016/j.bmc.2009.01.044](https://doi.org/10.1016/j.bmc.2009.01.044)

Database Information

AN: 2009:264073
CAN: 150:506193
CAplus

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Company/Organization

Dipartimento Farmaco-chimico,
Polo Universitario dell'Annunziata
University of Messina
Messina, VI. SS. Annunziata 98168
Italy

5-Arylidene-2-phenylimino-4-thiazolidinones as PTP1B and LMW-PTP inhibitors

By: Ottana, Rosaria; Maccari, Rosanna; Ciurleo, Rosella; Paoli, Paolo; Jacomelli, Michela; Manao, Giampaolo; Camici, Guido; Laggner, Christian; Langer, Thierry

Abstract: As part of a project aimed at identifying effective low mol. weight nonphosphorus monoanionic inhibitors of PTPs, we have synthesized 4-[(5-arylidene-4-oxo-2-phenyliminothiazolidin-3-yl)methyl]benzoic acids (4) and evaluated their inhibitory activity against human PTP1B and LMW-PTP enzymes. The introduction of a 2-phenylimino moiety onto the 4-thiazolidinone ring was designed to enhance the inhibitor/enzyme affinity by means of further favorable interactions with residues of the active site and the surrounding loops. Some of the compounds (4a-d, f) showed interesting inhibition levels in the low micromolar range. The 5-arylidene moiety of acids 4 proved to markedly improve the potency of these inhibitors. Mol. modeling experiments inside the binding sites of both enzymes were performed.

Full Text

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Concepts

Enzyme inhibitors	Human
Homo sapiens	Molecular association
	Structure-activity relationship

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18

Substances

Substances (29)

300865-11-6

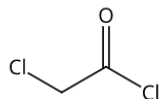
Image Not Available

Unspecified

PTP1B

Role: Biological Study, Unclassified, Biological Study

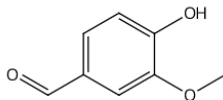
79-04-9



$C_2H_2Cl_2O$
Chloroacetyl chloride

Role: Reactant, Reactant or Reagent

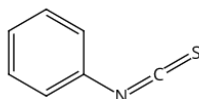
121-33-5



$C_8H_8O_3$
Vanillin

Role: Reactant, Reactant or Reagent

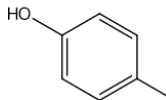
103-72-0



C_7H_5NS
Phenyl isothiocyanate

Role: Reactant, Reactant or Reagent

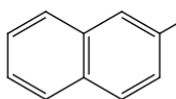
123-08-0



$C_7H_6O_2$
4-Hydroxybenzaldehyde

Role: Reactant, Reactant or Reagent

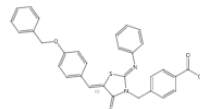
66-99-9



$C_{11}H_8O$
2-Naphthalenecarboxaldehyde

Role: Reactant, Reactant or Reagent

1148126-96-8

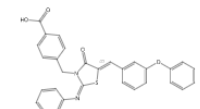


E/Z labels describe double bond geometry

$C_{31}H_{24}N_2O_4S$
Benzoic acid, 4-[[[(5Z)-4-oxo-2-(phenylimino)-5-[[4-(phenylmethoxy)phenyl]methylene]-3-thiazolidinyl]methyl]-

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

1148126-91-3

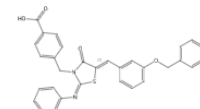


E/Z labels describe double bond geometry

$C_{30}H_{22}N_2O_4S$
Benzoic acid, 4-[[[(5Z)-4-oxo-5-[[3-phenoxyphenyl]methylene]-2-(phenylimino)-3-thiazolidinyl]methyl]-

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

1148126-95-7

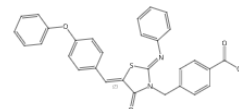


E/Z labels describe double bond geometry

$C_{31}H_{24}N_2O_4S$
Benzoic acid, 4-[[[(5Z)-4-oxo-2-(phenylimino)-5-[[3-(phenylmethoxy)phenyl]methylene]-3-thiazolidinyl]methyl]-

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

1148126-93-5



E/Z labels describe double bond geometry

$C_{30}H_{22}N_2O_4S$
Benzoic acid, 4-[[[(5Z)-4-oxo-5-[[4-(phenoxyphenyl)methylene]-2-(phenylimino)-3-thiazolidinyl]methyl]-

Role: Pharmacological Activity, Synthetic Preparation, Therapeutic Use, Biological Study, Preparation, Uses

352548-19-7

Image Not Available

Unspecified

Low-mol.-wt. protein tyrosine phosphatase

Role: Biological Study, Unclassified, Biological Study

文献中重要物质列表及研究角色



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 ☐ Not Available (6,569)

Reaction Role

Reference Role

☒ Adverse Effect (744)
 ☐ Analytical Study (498)
 ☒ Biological Study (8,034)
 ☐ Combinatorial Study (279)
 ☐ Formation (348)
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Stereochemistry

Number of Components

Substance Class

☐ Organic/Inorganic Small Molecule (7,167)
 ☐ Salt and Compound With (465)
 ☐ Manual Registration (350)
 ☐ Nucleic Acid Sequence (259)
 ☐ Protein/Peptide Sequence (55)
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Isotopes

Metals

Molecular Weight

Experimental Property

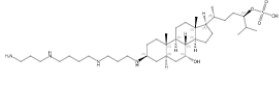
Substances (8,034)

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 ☐ 3
 ☐ 4
 ☐ 5
 ☐ 6

186139-09-3



Absolute stereochemistry shown

$C_{37}H_{72}N_4O_5S$
 Trodusquemine

84

4

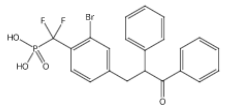
15

References

Reactions

Suppliers

345953-08-4



Absolute stereochemistry shown

$C_{22}H_{18}BrF_2O_4P$
 P-[[[2-Bromo-4-(3-oxo-2,3-diphenylpropyl)phenyl]di fluoromethyl] phosphonic acid

7

11

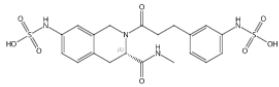
2

References

Reactions

Suppliers

875662-69-4



Absolute stereochemistry shown

$C_{20}H_{24}N_4O_8S_2$
 N-[3-[3-[(3S)-3,4-Dihydro-3-[(methylamino)carbonyl]-7-(sulfoamino)-2(1H)-isoquinolin-6-yl]propyl]phenyl]methanesulfonamide

3

1

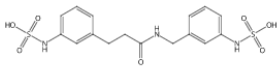
5

References

Reaction

Suppliers

875662-71-8



Absolute stereochemistry shown

$C_{16}H_{19}N_3O_7S_2$
 Sulfamic acid, 3-[3-oxo-3-[[[3-(sulfoamino)phenyl]methyl]amino]propyl]phenyl est...

2

1

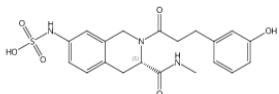
0

References

Reactions

Suppliers

875662-68-3



Absolute stereochemistry shown

$C_{20}H_{23}N_3O_6S$
 N-[[3-(3S)-1,2,3,4-Tetrahydro-2-[3-(3-hydroxyphenyl)-1-oxopropyl]-3-[(methylamino)car...

2

1

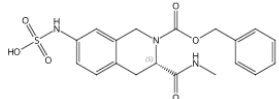
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References

Reactions

Suppliers

875662-52-5



Absolute stereochemistry shown

$C_{19}H_{21}N_3O_6S$
 2(1H)-Isoquinolinecarboxylic acid, 3,4-dihydro-3-[(methylamino)carbonyl]-7-(sulf...

2

1

0

References

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20

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References ▾ inhibitors and PTP1B

Document Type

- ☐ Journal (486)
- ☒ Patent (93)
- ☐ Review (48)
- ☐ Conference (2)
- ☐ Dissertation (1)

Substance Role

- ☐ Adverse Effect (11)
- ☐ Analytical Study (3)
- ☒ Biological Study (93)
- ☐ Miscellaneous (1)
- ☐ Properties (1)
- ☐ Uses (4)

Language

Publication Year

Author

Organization

Publication Name

Concept

- ☐ Antidiabetic agents (415)
- ☐ Homo sapiens (354)
- ☐ Human (354)
- ☐ Antiobesity agents (294)
- ☐ Obesity (261)
- ☒ Prodrugs (52)
- ☒ Drug targets (24)

China, CN107555205 A 2017-11-17 | Language: Chinese, Database: CAPLUS

The title preparation method includes: (a) pulverizing *Nigella glandulifera* seeds, cold soaking with petroleum ether for defatting for 5 times, fully drying defatted residue, performing cold soaking, percolation extraction or heating reflux extraction with ethanol, methanol or acetone, concentrating to obtain total extract, ultrasonically dissolving with acetone for 5-10 times, filtering off insoluble substance, and collecting and concentrating acetone part; (b) subjecting the acetone part to normal-phase silica gel column chromatog. to obtain a fraction containing the title ester compound; an...

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Substances (2) Reactions (0) Cited By (0) Citation Map

2

C-aryl glucoside SGLT2 inhibitors and method for the treatment of diabetes and related diseases

By: Washburn, William; Meng, Wei
United States, US20060063722 A1 2006-03-23 | Language: English, Database: CAPLUS

The invention discloses a compound I, (preparation described) as well as a method for treating diabetes and related diseases employing I alone or in combination with another therapeutic agent.

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Substances (74) Reactions (8) Cited By (12) Citation Map

Patent	Language	Kind Code	PatentPak Options
US20060063722	English	A1	PDF PDF+ Viewer
AU2005286608	English	A1	PDF
CN101065391	Chinese	A	PDF
CN101065391	Chinese	B	PDF
JP4945450	Japanese	B2	PDF

fused heterocycle as SGLT inhibitors

hara, Hiroaki; Teranishi, Hiroataka; Shimizu, Kazuo; Ito, Fumiaki;

0-14 | Language: Japanese, Database: CAPLUS

, etc.; Y = O, S, (un)substituted NH with alkyl, haloalkyl; Q =

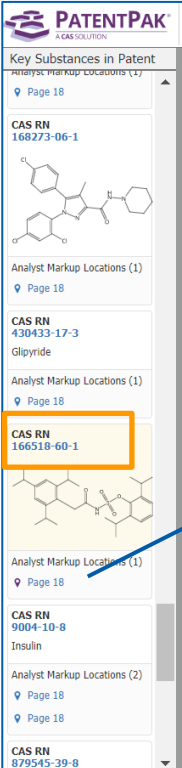
alkylene, etc.; A = aryl, heteroaryl; G = n, m) were prepared For example, glycosidation of 6-benzyloxy-4-hydroxy-3-(2-phenylethyl)benzofuran with 2,3,4,6-tetra-O-acetyl-1-O-trichloroacetimidoyl- α -D-glucopyranose in the presence of $\text{BF}_3 \cdot \text{OEt}_2$ followed by debenzoylation, deacetylation afforded compound IV. In SGLT1 (sodium/glucose cotransporter 1) inhibition assays, the IC_{50} value

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CAS RN 168273-06-1

Analyst Markup Locations (1)

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CAS RN 430433-17-3

Glipizide

Analyst Markup Locations (1)

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CAS RN 166518-60-1

Analyst Markup Locations (1)

Page 18

CAS RN 9004-10-8

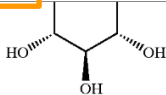
Insulin

Analyst Markup Locations (2)

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Page 18

CAS RN 879545-39-8



or a pharmaceutically acceptable salt, complex, stereoisomer, or prodrug ester thereof.

2. A pharmaceutical composition comprising a compound of formula I and a pharmaceutically acceptable carrier therefore.

3. A pharmaceutical combination comprising a compound of formula I and at least one therapeutic agent selected from the group consisting of an antidiabetic agent, an anti-obesity agent, a anti-hypertensive agent, an anti-atherosclerotic agent and a lipid-lowering agent.

4. The pharmaceutical combination as defined in claim 3 comprising the compound of formula I and at least one antidiabetic agent.

5. The combination as defined in claim 4 wherein the antidiabetic agent is at least one agent selected from the group consisting of a biguanide, a sulfonyl urea, a glucosidase inhibitor, a PPAR gamma agonist, a PPAR alpha/gamma dual agonist, an α 2 inhibitor, a DPP4 inhibitor, an insulin sensitizer, a glucagon-like peptide-1 (GLP-1), a PPAR γ inhibitor, a glycogen phosphorylase inhibitor, a glucos-6-phosphatase inhibitor, insulin and a meglitinide.

6. The combination as defined in claim 4 wherein the antidiabetic agent is at least one agent selected from the group consisting of metformin, glyburide, glimepiride, glycyride, glipizide, chlorpropamide, glizalazide, acarbose, nifedipine, pioglitazone, troglitazone, rosiglitazone, insulin, isaglitazone, repaglinide, nateglinide, muraglitazir and

lipid lowering agent, at least one agent selected from the group consisting of pravastatin, lovastatin, simvastatin, atorvastatin, cerivastatin, fluvastatin, nisvastatin, visvastatin, atorvastatin, rosuvastatin, fenofibrate, gemfibrozil, clofibrate and avasimibe.

12. The combination as defined in claim 10 wherein the compound of formula I is present in a weight ratio to the lipid-lowering agent within the range from about 0.01 to about 300:1.

13. A method for treating or delaying the progression or onset of diabetes, diabetic retinopathy, diabetic neuropathy, diabetic nephropathy, delayed wound healing, insulin resistance, hyperglycemia, hyperinsulinemia, elevated blood levels of fatty acids or glycerol, hyperlipidemia, obesity, hypertriglyceridemia, Syndrome X, diabetic complications, atherosclerosis or hypertension, or for increasing high density lipoprotein levels, comprising administering a therapeutically effective amount of a compound of formula I.

14. The method of claim 13 further comprising administering, concurrently or sequentially, a therapeutically effective amount of at least one additional therapeutic agent selected from the group consisting of an antidiabetic agent, an anti-obesity agent, a anti-hypertensive agent, an anti-atherosclerotic agent and a lipid-lowering agent.

15. A method for treating type II diabetes comprising administering a therapeutically effective amount of a compound of formula I, alone or in combination with at least one other therapeutic agent selected from the group consisting of antidiabetic agent, an agent for treating the complications of

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- 药代动力学研究
- 副作用研究

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References - pharmacokinetics of clopidogrel

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 - Miscellaneous (5)
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- Language
- Publication Year
- Author
- Organization
- Publication Name
- Concept
 - Pharmacokinetics (96K)
 - Homo sapiens (60K)
 - Human (60K)
 - Blood plasma (16K)
 - Pharmacodynamics (15K)
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- CAS Solutions
- Formulation Purpose
- Database
- Search Within Results

References (117,236)

Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

1

Pharmacokinetics of clopidogrel

By: Caplain, Henri; Donat, Francois; Gaud, C.; Necciari, Jose
Seminars in Thrombosis and Hemostasis (1999), 25(Suppl. 2), 25-28 | Language: English, Database: CPlus

Single- and multiple-dose **pharmacokinetics** of SR26334, the inactive carboxylic acid metabolite of **clopidogrel**, were investigated following oral doses of **clopidogrel** to healthy men. The mean maximum plasma concentrations (C_{max}) of SR26334 following single doses of 50, 75, 100, and 150 mg **clopidogrel** were 1.6, 2.9, 3.1, and 4.9 mg/L, resp. This demonstrated a dose-proportional increase of C_{max} in this range of **clopidogrel** doses. The urinary excretion of SR26334 was low (2.2-2.4% of the dose administered), and renal clearance remained virtually constant for 2-24 h after all 4 doses. Median times

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Full Text Substances (2) Reactions (0) Cited By (144) Citation Map

2

Pharmacokinetics of clopidogrel.

By: Caplain, H; Donat, F; Gaud, C; Necciari, J
Seminars in thrombosis and hemostasis (1999), 25 Suppl 2, 25-8 | Language: English, Database: MEDLINE

Clopidogrel is extensively metabolized, as evidenced by the absence of detectable amounts of unchanged **clopidogrel** in plasma samples in most clinical trials. The major circulating compound is the inactive carboxylic acid derivative SR26334, and information on the absorption and elimination of **clopidogrel** after oral administration is derived from the **pharmacokinetics** of this metabolite. Single-dose **pharmacokinetics** of SR26334 were investigated in a randomized, dose-proportionality study comparing single 50, 75, 100, and 150 mg oral doses of **clopidogrel** administered to 12 subjects. Multiple dose

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Full Text Substances (2) Reactions (0) Cited By (152) Citation Map

3

The Influence of Smoking Status on the Pharmacokinetics and Pharmacodynamics of Clopidogrel and Prasugrel

By: Gurbel, Paul A.; Blieden, Kevin P.; Logan, Douglas K.; Kereiakes, Dean J.; Lasseter, Kenneth C.; White, Alex; Angiolillo, Dominick J.; Nolin, Thomas D.; Maa, Jen-Fue; Bailey, William L.; et al
Journal of the American College of Cardiology (2013), 62(6), 505-512 | Language: English, Database: CPlus

The goal of this study was to evaluate the effect of smoking on the **pharmacokinetics** and pharmacodynamics (PD) of **clopidogrel** and prasugrel therapy. Major randomized trial data demonstrated that nonsmokers experience less or no benefit from **clopidogrel** treatment compared with smokers (i.e., the "smokers' paradox"). PARADOX was a prospective, randomized, double-blind, double-dummy, placebo-controlled, crossover study of objectively assessed nonsmokers (n = 56) and smokers (n = 54) with stable coronary artery disease receiving aspirin therapy. Patients were randomized to receive **prasugrel** (75

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方法一：通过主题词进行文献检索

Pharmacokinetics and clopidogrel
Pharmacokinetics not clopidogrel



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通过Substance Role可筛选相关研究方向的文献，如Biological Study

The screenshot displays the SciFinder web interface. At the top, the search bar contains the query 'pharmacokinetics of clopidogrel'. The left sidebar shows filter options under 'Document Type' and 'Substance Role'. The 'Substance Role' filter 'Biological Study' is selected and highlighted with a yellow box. The main content area shows two search results. The first result, 'Pharmacokinetics of clopidogrel', is highlighted with a blue box. The second result, 'The Influence of Smoking Status on the Pharmacokinetics and Pharmacodynamics of Clopidogrel and Prasugrel', is also highlighted with a blue box. The interface includes buttons for 'Full Text', 'Substances', 'Reactions', 'Cited By', and 'Citation Map'.

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
[Learn about result relevance.](#)
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Filter by

- Document Type
 - ☐ Journal (6,566)
 - ☐ Patent (958)
 - ☐ Review (1,553)
 - ☐ Book (4)
 - ☐ Conference (55)
 - [View All](#)
- Substance Role
 - ☐ Adverse Effect (877)
 - ☐ Analytical Study (213)
 - ☒ **Biological Study (7,632)**
 - ☐ Formation (4)
 - ☐ Miscellaneous (5)
 - [View All](#)

References (7,632) Sort: Relevance View: Partial Abstract

☐ Substances ☐ Reactions ☐ Cited By ☐ Save

1

Pharmacokinetics of clopidogrel
By: Caplain, Henri; Donat, Francois; Gaud, C.; Necciari, Jose
Seminars in Thrombosis and Hemostasis (1999), 25(Suppl. 2), 25-28 | Language: English, Database: CPlus

Single- and multiple-dose **pharmacokinetics** of SR26334, the inactive carboxylic acid metabolite of **clopidogrel**, were investigated following oral doses of **clopidogrel** to healthy men. The mean maximum plasma concentrations (C_{max}) of SR26334 following single doses of 50, 75, 100, and 150 mg **clopidogrel** were 1.6, 2.9, 3.1, and 4.9 mg/L, resp. This demonstrated a dose-proportional increase of C_{max} in this range of **clopidogrel** doses. The urinary excretion of SR26334 was low (2.2-2.4% of the dose administered), and renal clearance remained virtually constant for 2-24 h after all 4 doses. Median times ...
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2

The Influence of Smoking Status on the Pharmacokinetics and Pharmacodynamics of Clopidogrel and Prasugrel
By: Gurbel, Paul A.; Bliden, Kevin P.; Logan, Douglas K.; Kereiakes, Dean J.; Lasseter, Kenneth C.; White, Alex; Angiolillo, Dominick J.; Nolin, Thomas D.; Maa, Jen-Fue; Bailey, William L.; et al
Journal of the American College of Cardiology (2013), 62(6), 505-512 | Language: English, Database: CPlus

The goal of this study was to evaluate the effect of smoking on the **pharmacokinetics** and pharmacodynamics (PD) of **clopidogrel** and prasugrel therapy. Major randomized trial data demonstrated that nonsmokers experience less or no benefit

通过Concept标准概念词库，筛选感兴趣的研究点

Publication Year



1890 to 2020

No Min to No Max Apply

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Author

Organization

Publication Name

Concept

☐ Pharmacokinetics (96K)

☐ Homo sapiens (60K)

☐ Human (60K)

☐ Blood plasma (16K)

☐ Pharmacodynamics (15K)

View All

CAS Solutions

Formulation Purpose

By: Gurbel, Paul A.; Bliden, Kevin P.; Logan, Douglas K.; Kereiakes, Dean J.; Lasseter, Kenneth C.; White, Alex; Angiolillo, Dominick J.; Nolin, Thomas D.; Maa, Jen-Fue; Bailey, William L.; et al
Journal of the American College of Cardiology (2013), 62(6), 505-512 | Language: English, Database: CAPlus

The goal of this study was to evaluate the effect of smoking on the **pharmacokinetics** and pharmacodynamics (PD) of **clopidogrel** and prasugrel therapy. Major randomized trial data demonstrated that nonsmokers experience less or no benefit from **clopidogrel** treatment compared with smokers (i.e., the "smokers' paradox"). PARADOX was a prospective, randomized, double-blind, double-dummy, placebo-controlled, crossover study of objectively assessed nonsmokers (n = 56) and smokers (n = 54) with stable coronary artery disease receiving aspirin therapy. Patients were randomized to receive **clopidogrel** (75 ...

View More

Full Text Substances (4) Reactions (0) Cited By (66) Citation Map

☐ 4

Clinical Pharmacokinetics and Pharmacodynamics of Clopidogrel
By: Jiang, Xi-Ling; Samant, Snehal; Lesko, Lawrence J.; Schmidt, Stephan
Clinical Pharmacokinetics (2015), 54(2), 147-166 | Language: English, Database: CAPlus

A review. Acute coronary syndromes (ACS) remain life-threatening disorders, which are associated with high morbidity and mortality. Dual antiplatelet therapy with aspirin and **clopidogrel** has been shown to reduce cardiovascular events in patients with ACS. However, there is substantial inter-individual variability in the response to **clopidogrel** treatment, in addition to prolonged recovery of platelet reactivity as a result of irreversible binding to P2Y₁₂ receptors. This high inter-individual variability in treatment response has primarily been associated with genetic polymorphisms in the genes...

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Full Text Substances (2) Reactions (0) Cited By (36) Citation Map



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如，药代动力学、药物传递系统，药物相互作用等

Concept

Top Count Alphanumeric Search

7 Selected

<input checked="" type="checkbox"/> Pharmacokinetics (96K)	<input type="checkbox"/> Anticoagulants (2,905)	<input type="checkbox"/> Human immunodeficiency virus 1 (1,868)
<input type="checkbox"/> Homo sapiens (60K)	<input type="checkbox"/> HPLC (2,876)	<input type="checkbox"/> Solubility (1,831)
<input type="checkbox"/> Human (60K)	<input type="checkbox"/> Human groups (2,864)	<input type="checkbox"/> Analgesics (1,805)
<input type="checkbox"/> Blood plasma (16K)	<input type="checkbox"/> Neoplasm (2,823)	<input type="checkbox"/> Anti-inflammatory agents (1,804)
<input checked="" type="checkbox"/> Pharmacodynamics (15K)	<input type="checkbox"/> Biological uptake (2,812)	<input type="checkbox"/> P-glycoproteins (1,800)
<input type="checkbox"/> Drug bioavailability (12K)	<input type="checkbox"/> Stability (2,796)	<input type="checkbox"/> Anti-HIV agents (1,775)
<input type="checkbox"/> Antitumor agents (10K)	<input type="checkbox"/> Antibiotics (2,761)	<input type="checkbox"/> Drug discovery (1,771)
<input type="checkbox"/> Platelet aggregation inhibitors (9,598)	<input type="checkbox"/> Middle Aged (2,569)	<input type="checkbox"/> Immunosuppressants (1,760)
<input checked="" type="checkbox"/> Oral drug delivery systems (8,979)	<input type="checkbox"/> Bioavailability (2,564)	<input type="checkbox"/> Diabetes mellitus (1,729)
<input type="checkbox"/> Drug toxicity (7,772)	<input type="checkbox"/> Genetic polymorphism (2,505)	<input type="checkbox"/> Coronary artery disease (1,713)
	<input type="checkbox"/> Pharmaceutical natural products (2,484)	

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Concept

Top Count

Alphanumeric

Search

Concept Name

pharmacokinetics

Search

☒ 5 Selected

☒ Drug interactions, pharmacokinetic (6,311)

☒ Pharmacokinetic-pharmacodynamic modeling (13)

☒ Pharmacokinetics (96K)

☒ Pharmacokinetics, chronopharmacokinetics (62)

☒ Structure-activity relationship, pharmacokinetic (597)

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Filter by

- Document Type
 - Substance Role
 - ☐ Adverse Effect (37)
 - ☒ Analytical Study (22)
 - ☐ Biological Study (510)
 - ☐ Process (1)
 - ☐ Properties (13)
 - [View All](#)
 - Language
 - Publication Year
 - Author
 - Organization
 - Publication Name
 - Concept
 - ☐ Homo sapiens (72)
 - ☐ Human (72)
 - ☐ Blood analysis (40)
 - ☐ Pharmaceutical tablets (40)
 - ☐ Reversed-phase HPLC (39)
 - ☒ Pharmacokinetics (20)
 - ☒ Drug interactions, pharmacokinetic (2)
 - ☒ Structure-activity relationship, pharmacokinetic (0)
 - ☒ Pharmacokinetics, chronopharmacokinetics (0)
 - ☒ Pharmacokinetic-pharmacodynamic modeling

References (22) Sort: Relevance View: Partial Abstract

☐ Substances ☐ Reactions ☐ Cited By ☐ Save

☐ 1

Interaction study of aspirin or clopidogrel on pharmacokinetics of donepezil hydrochloride in rats by HPLC-fluorescence detection
 By: Wada, Mitsuhiro; Nishiwaki, Junichiro; Yamane, Tomoko; Ohwaki, Yuichi; Aboul-Enein, Hassan Y.; Nakashima, Kenichiro
 Biomedical Chromatography (2007), 21(6), 616-620 | Language: English, Database: CAPLUS

The present study aims to investigate the possibility of interaction of aspirin (Asp) or **clopidogrel** (CG) on donepezil (DP) hydrochloride in rats by HPLC-fluorescence detection. The separation of DP was achieved in ca. 13 min without interference of Asp and CG on the chromatogram. DP levels in rat blood plasma with a single administration of DP (5 mg/kg, i.p., group I) and those with a co-administration of Asp (200 mg/kg, p.o., group II or 200 mg/kg, i.p., group III) or CG (5 mg/kg, p.o., group IV) were monitored. The DP concentrations determined in rat plasma ranged from 25.0 to 336.1 ng/mL.

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☐ 2

Clopidogrel: review of bioanalytical methods, pharmacokinetics/pharmacodynamics, and update on recent trends in drug-drug interaction studies
 By: Mullangi, Ramesh; Srinivas, Nuggehalli R.
 Biomedical Chromatography (2009), 23(1), 26-41 | Language: English, Database: CAPLUS

A review. **Clopidogrel**, owing to its excellent inhibitory property of platelet aggregation, is used to reduce the cardiovascular risks in patients with multiple co-morbid conditions such as stroke, myocardial infarction and atherosclerosis. The current review focuses distinctly on 3 aspects: (a) an in-depth coverage on the bioanal. methods for the quantification of **clopidogrel** and its inactive carboxylic acid metabolite as well as the active metabolite in pre-clin. and clin. samples; (b) an overview of the pharmacokinetic/pharmacodynamic aspects of **clopidogrel**; and (c) enumerating the key findi...

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☐ 3

通过Substance Role，可继续选择 Analytical Study 获取分析相关信息



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方法二：先获取物质，再获取相关研究文献

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation links for 'Saved', 'History', and 'Account' are on the right. The main section is titled 'Search' and includes a sidebar with filters: 'All', 'Substances' (selected), 'Reactions', 'References', and 'Suppliers'. The search bar contains the text 'clopidogrel'. Below the search bar, a dropdown menu lists several results: 'Clopidogrel', 'Clopidogrel bisulfate', 'Clopidogrel hemisulfate', 'Clopidogrel hydrogen sulfate', 'Clopidogrel sulfate', 'Clopidogrel hydrochloride', 'Clopidogrel benzenesulfonate', 'Clopidogrel benzenesulfonic acid salt', 'Clopidogrel besylate', and 'Clopidogrel (-)-(1R)-camphor-10 sulfonate'. The 'Recent Search History' section is visible at the bottom left.

方法二：先获取物质，再获取相关研究文献

Filter by

^ Commercial Availability

☐ Available (1)

^ Reaction Role

^ Reference Role

^ Stereochemistry

^ Number of Components

^ Substance Class

^ Isotopes

^ Metals

^ Molecular Weight

^ Experimental Property

^ Experimental Spectrum

^ Regulatory Information

^ Bioactivity Indicator

^ Target Indicator

^ Search Within Results

Substances (1)

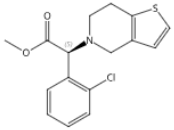
☐ References

☐ Reactions

☐ Suppliers

☐ 113665-84-2

[View Detail](#)



Absolute stereochemistry shown, Rotation (+)

C₁₆H₁₆ClNO₂S

Clopidogrel

☐ 8,063

References

☐ 758


Reactions

☐ 63

Suppliers

点击物质结构下方的文本图标，获取其对应的研究文献

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32

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References ▾ Enter a query...

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Filter by

- Document Type
- Substance Role
- Language
- Publication Year
- Author
- Organization
- Publication Name
- Concept**
 - ☐ Homo sapiens (6,380)
 - ☐ Human (6,380)
 - ☐ Platelet aggregation inhibitors (4,249)
 - ☐ Myocardial infarction (2,520)
 - ☐ Anticoagulants (1,574)
 - [View All](#)
- CAS Solutions
- Database
- Search Within Results

References (8,058) Sort: Relevance ▾ View: Partial Abstract ▾

☐ Substances ▾ ☐ Reactions ▾ ☐ Cited By ▾ ☐ Save

☐ **Effects of clopidogrel in addition to aspirin in patients with acute coronary syndromes without ST-segment elevation**

By: Yusuf, Salim; Zhao, Feng; Mehta, Shamir R.; Chrolavicius, Susan; Tognoni, Gianni; Fox, Keith K.
New England Journal of Medicine (2001), 345(7), 494-502 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: Despite current treatments, patients who have acute coronary syndromes without ST-segment elevation have high rates of major vascular events. We evaluated the efficacy and safety of the antiplatelet agent clopidogrel when given with aspirin in such patients. We randomly assigned 12,562 patients who had presented within 24 h after the onset of symptoms to receive clopidogrel (300 mg immediately, followed by 75 mg once daily) (6259 patients) or placebo (6303 patients) in addition to aspirin for 3 to 12 mo. The first primary outcome - a composite of death from cardiovascular causes, nonfatal myoc...

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Full Text ▾ Substances (2) Reactions (0) Cited By (2,250) Citation Map

☐ **Early and sustained dual oral antiplatelet therapy following percutaneous coronary interventions a randomized controlled trial**

By: Steinhubl, Steven R.; Berger, Peter B.; Mann, J. Tift III; Fry, Edward T. A.; DeLago, Augustin; Wilmer, Charles; Topol, Eric J.; Smallwood, Tanya; Edmunds, Kim; Green, Jane; et al
JAMA, the Journal of the American Medical Association (2002), 288(19), 2411-2420 | Language: English, Database: CAplus
[View Reference Detail](#)

Abstract: Following percutaneous coronary intervention (PCI), short-term clopidogrel therapy in addition to aspirin leads to greater protection from thrombotic complications than aspirin alone. However, the optimal duration of combination oral

如，药物代谢

Concept ×

Top Count

Alphanumeric

Find

<input type="checkbox"/> Homo sapiens (6,380)	<input type="checkbox"/> Genotypes (419)	<input type="checkbox"/> Angina pectoris, unstable (232)
<input type="checkbox"/> Human (6,380)	<input type="checkbox"/> Heart failure (404)	<input type="checkbox"/> Death (232)
<input type="checkbox"/> Platelet aggregation inhibitors (4,249)	<input type="checkbox"/> Angiotensin II receptor antagonists (401)	<input type="checkbox"/> Single nucleotide polymorphism (231)
<input type="checkbox"/> Myocardial infarction (2,520)	<input type="checkbox"/> Atherosclerosis (389)	<input checked="" type="checkbox"/> Drug metabolism (221)
<input type="checkbox"/> Anticoagulants (1,574)	<input type="checkbox"/> Atrial fibrillation (378)	<input type="checkbox"/> Hyperlipidemia (217)
<input type="checkbox"/> Blood platelet (1,348)	<input type="checkbox"/> Angina pectoris (367)	<input type="checkbox"/> Hypolipemic agents (215)
<input type="checkbox"/> Combination chemotherapy (1,329)	<input type="checkbox"/> C-reactive protein (339)	<input type="checkbox"/> Smoking behavior (210)
<input type="checkbox"/> Stroke (1,222)	<input type="checkbox"/> Prognosis (330)	<input type="checkbox"/> Fibrinogens (208)
<input type="checkbox"/> Platelet aggregation (1,094)	<input type="checkbox"/> Pharmacodynamics (328)	<input type="checkbox"/> Prophylaxis (205)
<input type="checkbox"/> Coronary artery disease (1,018)	<input type="checkbox"/> Low-density lipoproteins (325)	<input type="checkbox"/> Leukocyte (200)
<input type="checkbox"/> Thrombosis (951)	<input type="checkbox"/> Cardiovascular agents (316)	<input type="checkbox"/> Blood coagulation (195)
<input type="checkbox"/> Diabetes mellitus (904)	<input type="checkbox"/> Anti-inflammatory agents (310)	<input type="checkbox"/> Triglycerides (195)

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(4,249)

☐ Myocardial infarction (2,520)

☐ Anticoagulants (1,574)

☒ Drug metabolism (221)

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▼ CAS Solutions

▼ Database

^ Search Within Results

metabolite

☐ **The metabolism of clopidogrel is catalyzed by human cytochrome P450 3a and is inhibited by atorvastatin**

By: Clarke, Thomas A.; Waskell, Lucy A.
Drug Metabolism and Disposition (2003), 31(1), 53-59 | Language: English, Database: CAPlus
[View Reference Detail](#)

Abstract: The prodrug clopidogrel (Plavix) is activated by cytochrome P 450 (P 450) to a metabolite that inhibits ADP-induced platelet aggregation. Clopidogrel is frequently administered to patients in conjunction with the CYP3A4 substrate atorvastatin (Lipitor). Since clin. studies indicate that atorvastatin inhibits the antiplatelet activity of clopidogrel, we investigated whether CYP3A4 metabolized clopidogrel in vitro. Microsomes prepared from dexamethasone-pretreated rats metabolized clopidogrel at a rate of 3.8 pmol min⁻¹ pmol of P 450⁻¹ which is 65 and 1270% faster than the rate of metabolism by...

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Full Text ▼

☐ **CYP2C19 genotype, clopidogrel metabolism, platelet function, and cardiovascular revents. A systematic review and meta-analysis**

By: Holmes, Michael V.; Perel, Pablo; Shah, Tina; Hingorani, Aroon D.; Casas, Juan P.
JAMA, the Journal of the American Medical Association (2011), 306(24), 2704-2714 | Language: English, Database: CAPlus
[View Reference Detail](#)

Abstract: A review. The US Food and Drug Administration recently recommended that CYP2C19 genotyping be considered prior to prescribing clopidogrel, but the American Heart Association and American College of Cardiologists have argued evidence is insufficient to support CYP2C19 genotype testing. To appraise evidence on the association of CYP2C19 genotype and clopidogrel response through systematic review and meta-anal. PubMed and EMBASE from their inception to Oct. 2011. Studies that reported clopidogrel metabolism, platelet reactivity or clin. relevant outcomes (cardiovascular disease [CVD] events and b...

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点击文献标题，获取文献详情

The screenshot displays the SciFinder web interface. On the left is a sidebar with various filters: Document Type, Substance Role, Language, Publication Year, Author, Organization, Publication Name, Concept (with checkboxes for Homo sapiens, Human, Platelet aggregation inhibitors, Pharmacokinetics, Platelet aggregation, and Drug metabolism), CAS Solutions, Database, and Search Within Results. The 'Drug metabolism' filter is selected. The main area is titled 'References (90)' and shows a list of search results. The first result, 'Identification and biological activity of the active metabolite of clopidogrel', is highlighted with a yellow box. Below it is another result, 'The metabolism of clopidogrel is catalyzed by human cytochrome P450 3a and is inhibited by atorvastatin'. Each result includes the authors, publication details, and an abstract snippet. The interface also features a top navigation bar with 'References', a search bar, and icons for drawing, saving, and user profile.

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References ▾ Enter a query... Draw 🔍 ⭐ ⌚ 👤

Filter by

- Document Type
- Substance Role
- Language
- Publication Year
- Author
- Organization
- Publication Name
- Concept
 - ☐ Homo sapiens (424)
 - ☐ Human (424)
 - ☐ Platelet aggregation inhibitors (275)
 - ☐ Pharmacokinetics (171)
 - ☐ Platelet aggregation (118)
 - ☒ Drug metabolism (90)
- CAS Solutions
- Database
- Search Within Results
 - Find

metabolite

References (90) Sort: Relevance ▾ View: Partial Abstract ▾

☐ Substances ▾ ☐ Reactions ▾ ☐ Cited By ▾ ☐ Save

☐ Identification and biological activity of the active metabolite of clopidogrel

By: Savi, P.; Pereillo, J. M.; Uzabiaga, M. F.; Combalbert, J.; Picard, C.; Maffrand, J. P.; Pascal, M.; Herbert, J. M. Thrombosis and Haemostasis (2000), 84(5), 891-896 | Language: English, Database: CPlus
[View Reference Detail](#)

Abstract: Like ticlopidine, the ADP receptor antagonist clopidogrel is inactive in vitro and must be administered i.v. or orally to exhibit antiaggregatory and antithrombotic activities. We have previously shown that hepatic metabolism is necessary for activity. This study demonstrates that an active metabolite can be generated from human liver microsomes incubated with clopidogrel. Using several anal. methodologies (LC/MS, NMR, chiral supercritical fluid chromatog.), we have identified its structure. In vitro, this highly unstable compound, different from that formed from ticlopidine, exhibited all the ...
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Full Text ▾ Substances (3) Reactions (0) Cited By (523) Citation Map

☐ The metabolism of clopidogrel is catalyzed by human cytochrome P450 3a and is inhibited by atorvastatin

By: Clarke, Thomas A.; Waskell, Lucy A. Drug Metabolism and Disposition (2003), 31(1), 53-59 | Language: English, Database: CPlus
[View Reference Detail](#)

Abstract: The prodrug clopidogrel (Plavix) is activated by cytochrome P 450 (P 450) to a metabolite that inhibits ADP-induced platelet aggregation. Clopidogrel is frequently administered to patients in conjunction with the CYP3A4 substrate atorvastatin (Lipitor). Since clin. studies indicate that atorvastatin inhibits the antiplatelet activity of clopidogrel, we investigated whether CYP3A4 metabolized clopidogrel in vitro. Microsomes prepared from dexamethasone-pretreated rats metabolized clopidogrel at a rate of 3.8 nmol min⁻¹ nmol of P 450⁻¹, which is 65 and 1270% faster than the rate of metabolism by ...
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在物质列表中，通过Substances列表查看文献涉及的物质及角色描述

Journal

Source

Thrombosis and Haemostasis
Volume: 84
Issue: 5
Pages: 891-896
Journal
2000

Database Information

AN: 2000:894035
CAN: 134:80497
CAplus

View MEDLINE Reference

Company/Organization

Sanofi-Synthelabo
Toulouse 31036
France

Publisher

F. K. Schattauer
Verlagsgesellschaft mbH

Language

English

Identification and biological activity of the active metabolite of clopidogrel

By: Savi, P.; Pereillo, J. M.; Uzabiaga, M. F.; Combalbert, J.; Picard, C.; Maffrand, J. P.; Pascal, M.; Herbert, J. M.

Abstract: Like ticlopidine, the ADP receptor antagonist clopidogrel is inactive in vitro and must be administered i.v. or orally to exhibit antiaggregatory and antithrombotic activities. We have previously shown that hepatic metabolism is necessary for activity. This study demonstrates that an active metabolite can be generated from human liver microsomes incubated with clopidogrel. Using several anal. methodologies (LC/MS, NMR, chiral supercritical fluid chromatog.), we have identified its structure. In vitro, this highly unstable compound, different from that formed from ticlopidine, exhibited all the biol. activities of clopidogrel observed ex vivo: Irreversible inhibition of the binding of ^{33}P -2MeS-ADP to washed human platelets ($\text{IC}_{50} = 0.53 \mu\text{M}$), selective inhibition of ADP-induced platelet aggregation ($\text{IC}_{50} = 1.8 \mu\text{M}$) and ADP-induced adenyllyl cyclase down-regulation. The irreversible modification of the ADP-receptor site which is responsible for the biol. activity could be explained by the formation of a disulfide bridge between the reactive thiol group of the active metabolite and a cysteine residue of the platelet ADP receptor.

Full Text ▾


Expand All | Collapse All

▼ Concepts

▲ Substances

Substances (3)

317322-48-8

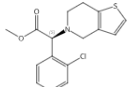


Absolute stereochemistry shown
Double bond geometry shown

$\text{C}_{16}\text{H}_{18}\text{ClNO}_4\text{S}$
1-Methyl (αS,3Z,4R)-3-(carboxymethylene)-α-(2-chlorophenyl)-4-mercapto-1-piperid...

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Biological Study

113665-84-2

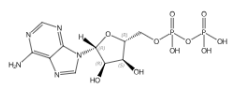


Absolute stereochemistry shown, Rotation (+)

$\text{C}_{16}\text{H}_{16}\text{ClNO}_2\text{S}$
Clopidogrel

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Therapeutic Use, Biological Study, Uses

58-64-0



Absolute stereochemistry shown

$\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$
5'-ADP

Role: Biological Activity or Effector, Except Adverse, Biological Study, Unclassified, Biological Study

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例2：如何获取代谢小分子磷脂(DSPC)的谱图研究信息？

Substances DSPC

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
- Stereochemistry**
 - ☐ Stereo in Answer Structure (1)
 - ☐ No Stereo in Answer Structure (1)
- Number of Components
- Substance Class
- Isotopes
- Metals
- Experimental Property
- Experimental Spectrum**
 - ☐ Mass (1)
 - ☐ Phosphorus-31 NMR (1)
- Regulatory Information
- Search Within Results

Substances (2)

References Reactions Suppliers

1 816-94-4

Absolute stereochemistry shown, Rotation (+)

$C_{44}H_{88}NO_8P$
DSPC

3,902 References 68 Reactions 79 Suppliers

2 4539-70-2

$C_{44}H_{88}NO_8P$
DSPC

2,765 References 28 Reactions 28 Suppliers

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查看物质详情

DSPC为俗名，对应了不同异构体的结构；
通过CAS登记号可以获取准确的物质信息。



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通过物质详情，获取物质属性、谱图和管控等信息

Substance Detail (1 of 2)

References (3,902)

Reactions (68)

Suppliers (79)

← Prev

Next →

📄

✉

★ Save

CAS Registry Number

816-94-4

Absolute stereochemistry shown, Rotation (+)

C₄₄H₈₈NO₈P

3,5,9-Trioxa-4-phosphaheptacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-oxo-7-[(1-oxooctadecyl)oxy]-, inner salt, 4-oxide, (7R)-

Key Physical Properties	Value	Condition
Melting Point (Experimental)	230.5-231.5 °C	-

Experimental Properties | Spectra

Other Names

Expand All

Experimental Properties

Chemical	Interface	Optical and Scattering	Thermal
Property		Value	Condition Source
Melting Point		230.5-231.5 °C	- (1) CAS
Melting Point		55 °C	- (2) CAS
Enthalpy - 1 Source		See Full Text	(3) CAS
Entropy - 1 Source		See Full Text	(4) CAS
Liquid Crystal Transition Temperature - 1 Source		See Full Text	(5) CAS

Sources

(1) Shvets, V. I.; Zhurnal Obshchei Khimii, (1964), 34(6), 1908-11, Capius
(2) Greenough, Kelly P.; Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy, (2009), 71A(5), 2050-2056, Capius
(3) Matsuki, Hitoshi; Chemistry Letters, (2005), 34(2), 270-271, Capius
(4) Matsuki, Hitoshi; Chemistry Letters, (2005), 34(2), 270-271, Capius
(5) Kalmbach, Rolf; Journal of Molecular Biology, (2007), 371(3), 639-648, Capius

Experimental Spectra

Hetero NMR	IR	Mass	Raman	X-Ray	Additional Spectra
					Source
					NMR Spectrum - 1 Source (1) CAS
					Phosphorus-31 NMR Spectrum - 1 Source (2) CAS

Sources

(1) Matsuoka, Shigeru; Biochemistry, (2005), 44(2), 704-710, Capius
(2) Ledo, D. Correia; ECS Transactions, (2009), 19(33), 1-10, Capius

Regulatory Information

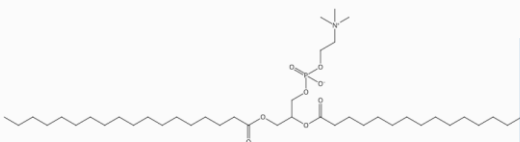
Additional Details

通过物质详情，获取物质属性、谱图和管控等信息

Substance Detail (2 of 2)

References (2,765) Reactions (28) Suppliers (28)

CAS Registry Number
4539-70-2



$C_{44}H_{88}NO_8P$
3,5,9-Trioxa-4-phosphaheptacosan-1-aminium, 4-hydroxy-*N,N,N*-trimethyl-10-oxo-7-[(1-oxooctadecyl)oxy]-, inner salt, 4-oxide

Key Physical Properties	Value
Melting Point (Experimental)	230.5-231.0 °C

Experimental Properties | Spectra

Other Names

Experimental Properties

Interface

Property

Surface Tension - 1 Source

Sources

(1) Bonte, Frederic; EP214055, A1, 1987, CAlplus

Experimental Spectra

Hetero NMR Mass X-Ray

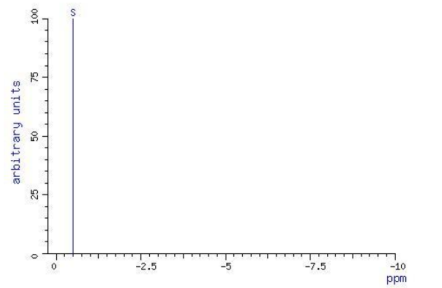
[View Phosphorous-31 NMR Spectrum](#)

Sources

(1) Nifant'ev, E. E.; Zhurnal Organicheskoi Khimii, (1978), 14(1), 63-71, CAlplus

Additional Details

Phosphorous-31 NMR Spectrum Detail (1 of 1)



arbitrary units

ppm

Reset

Spectrum Summary	Conditions
Spectrum ID	CC-01-P-NMR-4359
Spectrometer	JEOL C-60HL
Source	Spectral data were obtained from John Wiley & Sons, Inc.
Solvent	Chloroform (δ7-66-3)
Temperature	25 °C

(1) WSS



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大纲

- 疾病模型研究信息
- 药物与受体的相互作用研究
- 药代动力学研究
- 副作用研究

例：药物毒副作用研究信息的获取

检索方法：

方法一、通过主题词进行检索

方法二、先进行物质检索，再获取其毒性研究方面的信息

Based on your query, we've returned the most relevant results. Would you like to load the entire result set?
Learn about result relevance.

Load More Results

Filter by

Document Type

Substance Role

- ☐ Adverse Effect (465)
- ☐ Analytical Study (35)
- ☐ Biological Study (791)
- ☐ Nanoscale (2)
- ☐ Occurrence (9)

View All

Language

Publication Year

Author

Organization

Publication Name

Concept

- ☐ Drug toxicity (578)
- ☐ Homo sapiens (478)
- ☐ Human (478)
- ☐ Antipsychotics (381)
- ☐ Haloperidol (168)

View All

References (1,080)

Sort: Relevance View: Partial Abstract

Substances Reactions Cited By Save

1

Antagonism of cocaine, amphetamine, and methamphetamine toxicity

By: Derlet, Robert W.; Albertson, Timothy E.; Rice, Pam

Pharmacology, Biochemistry and Behavior (1990), 36(4), 745-9 | Language: English, Database: CAPLUS

The effect of diazepam, haloperidol, MK-801, and propranolol in antagonizing behavioral symptoms induced by LDs of cocaine, amphetamine, and methamphetamine were studied in a rat model. Animals were first pretreated i.p. with potential antagonists, diazepam (2, 5, and 10 mg/kg), haloperidol (5, 10, and 20 mg/kg), propranolol (5, 10, and 20 mg/kg), MK-801 (0.5, 1.0, and 2.5 mg/kg), and then were challenged i.p. with cocaine (70 mg/kg) (LD₅₀), d-amphetamine (75 mg/kg) (LD₁₀₀), and methamphetamine (100 mg/kg) (LD₅₀). Diazepam, at all doses, provided protection against cocaine- and methamphetamine-

View More

Full Text

Substances (8)

Reactions (0)

Cited By (38)

Citation Map

2

Cytotoxic effects of neuroleptic drugs

By: Munyon, William H.; Salo, Richard; Briones, David F.

Psychopharmacology (Berlin, Germany) (1987), 91(2), 182-8 | Language: English, Database: CAPLUS

Agranulocytosis and the release of transaminase enzymes from liver cells are known consequences of neuroleptic drug use. These effects are most common with low potency neuroleptic drugs. It has been hypothesized that these effects are due to the direct toxic action of these drugs on blood and liver cells. The purpose of this study is to compare the cytotoxic effects of 8 neuroleptic drugs in 5 different biol. test systems. In all of the test systems, thioridazine [50-52-2], chlorpromazine [50-53-3], trifluoperazine [117-89-5], fluphenazine [69-23-8], and thiothixene [5591-45-7] (group one...

View More

Full Text

Substances (8)

Reactions (0)

Cited By (20)

Citation Map

3

Influence of haloperidol on the central nervous system

By: Vinogradov, V. V.; Krylov, S. S.; Snegirev, E. A.; Sysoeva, A. F.; Chasabova, V. A.

方法一、通过主题词进行检索

主题词 (toxicity and haloperidol) not ecotoxicity

通过Substance role分析研究方向，concept分析具体的研究点



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可以直接选择Top Count中涉及toxicity的概念词，或者通过Find在Concept词库中检索toxicity

Concept

Top Count Alphanumeric Search

5 Selected

<input checked="" type="checkbox"/> Drug toxicity (578)	<input type="checkbox"/> Tranquillizers (48)	<input type="checkbox"/> Aging, animal (29)
<input type="checkbox"/> Homo sapiens (478)	<input checked="" type="checkbox"/> Neurotoxicity (45)	<input type="checkbox"/> Diabetes mellitus (29)
<input type="checkbox"/> Human (478)	<input type="checkbox"/> Tardive dyskinesia (45)	<input type="checkbox"/> Kidney (29)
<input type="checkbox"/> Antipsychotics (381)	<input type="checkbox"/> Behavior (43)	<input type="checkbox"/> Antiarrhythmics (28)
<input type="checkbox"/> Haloperidol (168)	<input checked="" type="checkbox"/> Oral drug delivery systems (43)	<input type="checkbox"/> Antibiotics (28)
<input type="checkbox"/> Schizophrenia (163)	<input type="checkbox"/> Anxiolytics (42)	<input type="checkbox"/> Antioxidants (28)
<input type="checkbox"/> Animals (120)	<input type="checkbox"/> Drug delivery systems (42)	<input type="checkbox"/> Cardiac arrhythmia (28)
<input type="checkbox"/> Male (119)	<input type="checkbox"/> Animal gene (40)	<input type="checkbox"/> Central nervous system (28)
<input type="checkbox"/> Antidepressants (111)	<input type="checkbox"/> Antiparkinsonian agents (40)	<input type="checkbox"/> 5-HT reuptake inhibitors (27)
<input type="checkbox"/> Combination chemotherapy (99)	<input type="checkbox"/> Brain corpus striatum (40)	<input type="checkbox"/> Antiemetics (27)
<input type="checkbox"/> Humans (90)	<input type="checkbox"/> Drug metabolism (40)	<input type="checkbox"/> Anti-inflammatory agents (27)
<input type="checkbox"/> Psychosis (85)	<input checked="" type="checkbox"/> Hepatotoxicity (40)	<input type="checkbox"/> Anxiety (27)
<input type="checkbox"/> Brain (83)	<input type="checkbox"/> Mice (40)	<input type="checkbox"/> Cardiovascular agents (27)
<input type="checkbox"/> Liver (73)	<input type="checkbox"/> Long QT syndrome (39)	<input checked="" type="checkbox"/> Cognitive disorders (27)
		<input type="checkbox"/> Disease, animal (27)

Apply Cancel

Concept

Top Count Alphanumeric Search

Concept Name

toxicity

Search

17 Selected

<input checked="" type="checkbox"/> Aquatic toxicity (1)	<input checked="" type="checkbox"/> Pulmonary toxicity (7)	<input checked="" type="checkbox"/> Toxicity Tests (10)
<input checked="" type="checkbox"/> Chronic toxicity (1)	<input checked="" type="checkbox"/> Reproductive toxicity (7)	<input checked="" type="checkbox"/> Toxicity Tests, Acute (2)
<input checked="" type="checkbox"/> Drug toxicity (578)	<input checked="" type="checkbox"/> Toxicity (70)	<input checked="" type="checkbox"/> Toxicity Tests, Subacute (1)
<input checked="" type="checkbox"/> Gastrointestinal toxicity (8)	<input checked="" type="checkbox"/> Toxicity, acute (9)	
<input checked="" type="checkbox"/> Inhalation toxicity (1)	<input checked="" type="checkbox"/> Toxicity test (7)	

Apply Cancel



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References ▾ (toxicity and haloperidol) not ecotoxicity

Draw 🔍 ★ ⌚ 👤

☐ Analytical Study (2)
☐ Biological Study (61)
☐ Properties (5)
☐ Uses (48)

^ Language
☐ English (71)

^ Publication Year

1970 2018

No Min to No Max Apply

View Larger

^ Author
 ^ Organization
 ^ Publication Name
 ^ Concept
 ^ CAS Solutions
 ^ Formulation Purpose
 ^ Database

^ Search Within Results

drug metabolism

2

Haloperidol-induced changes in glutathione and energy metabolism: effect of nicergoline
 By: Vairetti, Mariapia; Feletti, Fausto; Battaglia, Angelo; Pamparana, Franco; Canonico, Pier Luigi; Richelmi, Plinio; Berte, Francantonio
 European Journal of Pharmacology (1999), 367(1), 67-72 | Language: English, Database: CPlus

The aim of this study was to evaluate the possible effects of nicergoline, a semisynthetic ergot derivative, on the biochem. changes observed during chronic treatment with **haloperidol** in male Sprague-Dawley rats. Chronic treatment with **haloperidol** induced a significant decrease in the cellular glutathione (GSH) content in selected areas of the brain (cerebellum, striatum and cortex) and in the liver. Prolonged nicergoline administration was able to antagonize the **haloperidol**-induced GSH decrease, maintaining the GSH concentration at levels comparable to those observed in the control group. Ana...

View More ▾

Full Text ▾ Substances (4) Reactions (0) Cited By (21) Citation Map

3

Metabolism of haloperidol and its tetrahydropyridine dehydration product HPTP
 By: Usuki, Etsuko; Van Der Schyf, Cornelis J.; Castagnoli, Neal Jr.
 Drug Metabolism Reviews (1998), 30(4), 809-826 | Language: English, Database: CPlus

A review with 106 references on the **metabolism** of **haloperidol** and its tetrahydropyridine dehydration product HPTP in relation to its neurotoxic potential.

Full Text ▾ Substances (2) Reactions (0) Cited By (15) Citation Map

4

The possible role of an active metabolite derived from the neuroleptic agent haloperidol in drug-induced parkinsonism
 By: Igarashi, Kazuo
 Journal of Toxicology, Toxin Reviews (1998), 17(1), 27-38 | Language: English, Database: CPlus

A review with many references This report summarizes the case for development of extrapyramidal side-effects associated with chronic **haloperidol** (HP) use, such as **drug**-induced parkinsonism and tardive dyskinesia. The involvement of neurotoxic metabolites has been proposed as an idea. The results from metabolic studies have demonstrated that HP is oxidatively converted to the pyridinium metabolite, 4-(4-chlorophenyl)-1-[4-(4-fluorophenyl)-4-oxobutyl] pyridinium species (HPP⁺), which

也可在Search Within Results中输入关键词, 比如drug metabolism, 进一步精炼所需信

点击标题, 查看文献详情



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Reference Detail (2 of 71)

Substances (4) Reactions (0) Cited By (21) Citation Map

Journal
Source
European Journal of Pharmacology
Volume: 367
Issue: 1
Pages: 67-72
Journal
1999
DOI:
10.1016/s0014-2999(98)00925-x

Database Information
AN: 1999-96789
CAN: 130:320708
CAplus

View MEDLINE Reference

Company/Organization
Institute of Pharmacology II
University of Pavia
Pavia 27100
Italy

Publisher
Elsevier Science B.V.

Language
English

Haloperidol-induced changes in glutathione and energy metabolism: effect of nicergoline
By: Vairetti, Mariapia; Feletti, Fausto; Battaglia, Angelo; Pamparana, Franco; Canonico, Pier Luigi; Richelmi, Plinio; Berte, Francantonio

Abstract: The aim of this study was to evaluate the possible effects of nicergoline, a semisynthetic ergot derivative, on the biochem. changes observed during chronic treatment with **haloperidol** in male Sprague-Dawley rats. Chronic treatment with **haloperidol** induced a significant decrease in the cellular glutathione (GSH) content in selected areas of the brain (cerebellum, striatum and cortex) and in the liver. Prolonged nicergoline administration was able to antagonize the **haloperidol**-induced GSH decrease, maintaining the GSH concentration at levels comparable to those observed in the control group. Anal. of the energy charge revealed changes similar to those observed for GSH: **haloperidol** induced a significant decrease in ATP and energy charge that was completely reversed by repeated nicergoline administration. In conclusion, chronic treatment with the classical antipsychotic **haloperidol** induces profound biochem. changes in the brain and in the liver. Nicergoline treatment is able to counteract the **haloperidol**-induced decrease in GSH levels and energy charge, suggesting a potential role of the **drug** in the treatment of neuroleptic-induced side effects.

Full Text

Expand All | Collapse All

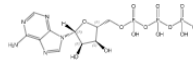
Concepts

Antipsychotics	Drug toxicity
Brain	Energy metabolism
Liver	

Substances

Substances (4)

56-65-5

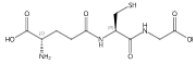


Absolute stereochemistry shown

$C_{10}H_{16}N_5O_{13}P_3$
5'-ATP

Role: Biological Study, Unclassified, Biological Study

70-18-8

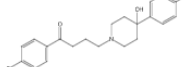


Absolute stereochemistry shown

$C_{10}H_{17}N_2O_6S$
Glutathione

Role: Biological Study, Unclassified, Biological Study

52-86-8



$C_{21}H_{23}ClFNO_2$
Haloperidol

Role: Adverse Effect, Including Toxicity, Therapeutic Use, Biological Study, Uses

27848-84-6

文献详情：可以查看摘要及CAS科学家人工标引信息，如Concepts（概念词库）及Substances（物质列表）等

Concepts、Substances及其Role（研究角色）有助于快速判断文献的研究主旨



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方法二、先进行物质检索，再获取其毒性研究方面的信息

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Substances haloperidol

Filter by

- Commercial Availability
- Reaction Role
- Reference Role
 - ☐ Adverse Effect (1)
 - ☐ Analytical Study (1)
 - ☐ Biological Study (1)
 - ☐ Formation (1)
 - ☐ Miscellaneous (1)
 - [View All](#)
- Number of Components
- Substance Class
- Isotopes
- Metals
- Molecular Weight
- Experimental Property
- Experimental Spectrum
- Regulatory Information
- Bioactivity Indicator
- Target Indicator
- Search Within Results

Substances (1)

☐ References ☐ Reactions ☐ Suppliers

52-86-8
[View Detail](#)

C21H23ClFNO2
Haloperidol

29K References 195 Reactions 76 Suppliers

物质详情中的标引信息

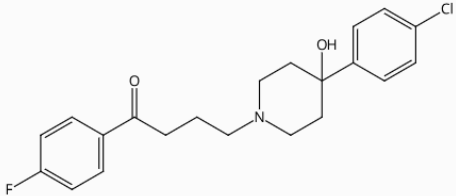
Substance Detail (1 of 4)

References (29K) Reactions (195) Suppliers (81)

← Prev Next →

📄 📧 ★ Save

CAS Registry Number
52-86-8



C₂₁H₂₃ClFNO₂
1-Butanone, 4-[4-(4-chlorophenyl)-4-hydroxy-1-piperidinyl]-1-(4-fluorophenyl)-

Key Physical Properties	Value	Condition
Molecular Weight	375.86	-
Melting Point (Experimental)	151.5 °C	-
Boiling Point (Predicted)	529.0±50.0 °C	Press: 760 Torr
Density (Predicted)	1.239±0.06 g/cm ³	Temp: 20 °C; Press: 760 Torr
pKa (Predicted)	13.86±0.20	Most Acidic Temp: 25 °C

Experimental Properties | Spectra

Expand All | Collapse All

Other Names

结构式、理化属性、名称等



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物质详情中的标引信息

^ Experimental Properties

Biological	Chemical	Lipinski	Thermal
Property	Value	Condition	Source
Median Lethal Dose	600-1200 mg/kg	Organism: mouse; Route: subcutaneous	(1) CAS
Median Lethal Dose	165 mg/kg	Organism: rat; Route: oral	(2) APC
Median Lethal Dose	60 mg/kg	Organism: mouse; Route: intraperitoneal	(2) APC
Median Lethal Dose	>20 mg/kg	Organism: monkey; Route: oral	(3) CAS
ADME (Absorption, Distribution, Metabolism, Excretion) - 12 Sources	See Full Text		(4-15) CAS
Half-Life (Biological) - 4 Sources	See Full Text		(16-19) CAS

Sources

(1) Yamamoto, Hisao; DE2065311, A1, 1973, CAplus

(2) (2000), 1280 pages, CAplus

(3) Oberst, Fred W.; Archives Internationales de Pharmacodynamie et de Therapie, (1967), 167(2), 450-64, CAplus

(4) Yan, Zhixia; Rapid Communications in Mass Spectrometry, (2005), 19(9), 1191-1199, CAplus

(5) Poulin, Patrick; Journal of Pharmaceutical Sciences, (2009), 98(12), 4941-4961, CAplus

(6) Beaumont, Kevin; Journal of Pharmaceutical Sciences, (2011), 100(10), 4518-4535, CAplus

(7) Obach, R. Scott; Drug Metabolism and Disposition, (2008), 36(7), 1385-1405, CAplus

(8) Zhang, Liying; Pharmaceutical Research, (2008), 25(8), 1902-1914, CAplus

(9) Di, Li; Journal of Pharmaceutical Sciences, (2009), 98(6), 1980-1991, CAplus

(10) Zhang, Guodong; Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, (2007), 856(1-2), 20-28, CAplus

View All v

实验属性、实验谱图、
预测属性、预测谱图、
生物活性、靶点信息、
管控信息等

v Experimental Spectra
v Predicted Properties
v Predicted Spectra
v Bioactivity Indicators
v Target Indicators
v Regulatory Information
v Additional Details



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在文献结果的基础上，通过Substance Role，获取物质在文献中的研究角色

The screenshot displays the SciFinder web interface. At the top, there is a search bar with the text 'Enter a query...' and a 'References' dropdown menu. Below the search bar, the 'References' section is active, showing a list of 24,402 references. The interface includes a left sidebar with filters for 'Document Type' and 'Substance Role'. The 'Substance Role' filter is highlighted with a blue box, showing options like 'Adverse Effect (1,353)', 'Analytical Study (834)', 'Biological Study (11K)', 'Formation (6)', and 'Miscellaneous (3)'. The main content area displays a list of references, including 'A rating scale for extrapyramidal side effects' and 'Dopamine receptor binding predicts clinical and pharmacological potencies of antischizophrenic drugs'. Each reference entry includes the author, title, journal information, and an abstract snippet. The interface also features a 'Full Text' dropdown and buttons for 'Substance', 'Reactions', 'Cited By', and 'Citation Map' for each reference.



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根据检索需要，选择Substance Role

The screenshot displays the SciFinder web interface. At the top, the SciFinder logo is on the left, and navigation tools like 'References', 'Enter a query...', 'Draw', and search icons are on the right. Below the header, a 'Return to Home' link is visible. On the left side, there is a 'Filter by' section with two main categories: 'Document Type' and 'Substance Role'. The 'Substance Role' section is highlighted with a blue border and contains several checked items: 'Adverse Effect (1,353)', 'Analytical Study (834)', and 'Biological Study (11K)'. Other unchecked items include 'Journal (10K)', 'Patent (1,350)', 'Review (304)', 'Conference (246)', 'Dissertation (49)', 'Formation (6)', 'Miscellaneous (3)', 'Nanoscale (3)', 'Occurrence (59)', 'Preparation (109)', 'Process (175)', 'Properties (621)', 'Prophetic in Patents (7)', 'Reactant or Reagent (80)', and 'Uses (5,111)'. A 'View All' link is at the bottom of the filter list. The main content area is titled 'References (11,678)' and includes sorting and viewing options. Below this, there are two search result entries. The first entry is titled 'Neuroleptics increase c-fos expression in the forebrain: contrasting effects of haloperidol and clozapine' by Robertson, G. S.; Fibiger, H. C. The second entry is titled 'Antipsychotic dosing in preclinical models is often unrepresentative of the clinical condition: A suggested solution based on in vivo occupancy' by Kapur, Shitij; Vanderspek, Susan C.; Brownlee, Barbara A.; Nobrega, Jose N. Both entries include an abstract and a 'View Reference Detail' link. At the bottom of the results, there are buttons for 'Full Text', 'Substances (2)', 'Reactions (0)', 'Cited By (285)', and 'Citation Map'.

SciFinderⁿ
A CAS SOLUTION

References ▾ Enter a query... Draw 🔍 ⭐ ⌚ 👤

← Return to Home

Filter by

Document Type

- ☐ Journal (10K)
- ☐ Patent (1,350)
- ☐ Review (304)
- ☐ Conference (246)
- ☐ Dissertation (49)

View All

Substance Role

- ☒ Adverse Effect (1,353)
- ☒ Analytical Study (834)
- ☒ Biological Study (11K)
- ☐ Formation (6)
- ☐ Miscellaneous (3)
- ☐ Nanoscale (3)
- ☐ Occurrence (59)
- ☐ Preparation (109)
- ☐ Process (175)
- ☐ Properties (621)
- ☐ Prophetic in Patents (7)
- ☐ Reactant or Reagent (80)
- ☐ Uses (5,111)

View Fewer

References (11,678) Sort: Relevance ▾ View: Partial Abstract ▾

☐ Substances ▾ ☐ Reactions ▾ ☐ Cited By ▾

📄 📧 ⭐ Save

☐ **Neuroleptics increase c-fos expression in the forebrain: contrasting effects of haloperidol and clozapine**

By: Robertson, G. S.; Fibiger, H. C.
Neuroscience (Oxford, United Kingdom) (1992), 46(2), 315-28 | Language: English, Database: CApus
[View Reference Detail](#)

Abstract: The mechanisms by which the atypical neuroleptic clozapine produces its therapeutic effects in the treatment of schizophrenia without causing the extrapyramidal side effects that are characteristic of most antipsychotic drugs remain unclear. Recently, a single injection of the typical antipsychotic haloperidol has been shown to increase *c-fos* expression in the striatum. *c-fos* is a proto-oncogene that encodes a 55,000 mol. weight phosphoprotein, Fos, which is thought to assist in the regulation of the "target genes" containing an AP-1 binding site. Because a wide variety of physiol. and pharmac...

[View More ▾](#)

Full Text ▾ Substances (2) Reactions (0) Cited By (285) Citation Map

☐ **Antipsychotic dosing in preclinical models is often unrepresentative of the clinical condition: A suggested solution based on in vivo occupancy**

By: Kapur, Shitij; Vanderspek, Susan C.; Brownlee, Barbara A.; Nobrega, Jose N.
Journal of Pharmacology and Experimental Therapeutics (2003), 305(2), 625-631 | Language: English, Database: CApus
[View Reference Detail](#)

Abstract: What is the appropriate dose of an antipsychotic in an animal model. The literature reveals no standard rationale across studies. This study was designed to use in vivo dopamine D₂ receptor occupancy as a cross-species principle for deriving clin. comparable doses for animal models. The relation between dose, plasma levels, and in vivo dopamine D₂ receptor occupancy was established in rats for a range of doses administered as a single dose or multiple doses (daily injections or osmotic minipump infusions) for five of the most commonly used antipsychotics. As a single dose, haloperidol (0.04-0.

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☐ **Antipsychotic dosing in preclinical models is often unrepresentative of the clinical condition: A suggested solution based on in vivo occupancy**

By: Kapur, Shitij; Vanderspek, Susan C.; Brownlee, Barbara A.; Nobrega, Jose N.
Journal of Pharmacology and Experimental Therapeutics (2003), 305(2), 625-631 | Language: English, Database: CAPlus
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Abstract: What is the appropriate dose of an antipsychotic in an animal model. The literature reveals no standard rationale across studies. This study was designed to use in vivo dopamine D₂ receptor occupancy as a cross-species principle for deriving clin. comparable doses for animal models. The relation between dose, plasma levels, and in vivo dopamine D₂ receptor occupancy was established in rats for a range of doses administered as a single dose or multiple doses (daily injections or osmotic minipump infusions) for five of the most commonly used antipsychotics. As a single dose, haloperidol (0.04-0. ...
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☐ **Olanzapine versus placebo and haloperidol acute phase results of the North American double-blind olanzapine trial**

By: Beasley, Charles M.; Tollefson, Gary; Tran, Pierre; Satterlee, Winston; Sanger, Todd; Hamilton, Susan
Neuropsychopharmacology (1996), 14(2), 111-23 | Language: English, Database: CAPlus
[View Reference Detail](#)

Abstract: Olanzapine is a potential new "atypical" antipsychotic agent. The double-blind acute phase of this study compared three dosage ranges of olanzapine (5 mg/day [Olz-L], 10 mg/day [Olz-M], 15 mg/day [Olz-H]) to a dosage range of haloperidol (15 mg/day [Hal]) and to placebo in the treatment of 335 patients who met the DSM-III-R criteria for schizophrenia. In overall symptomatol. improvement (Brief Psychiatric Rating Scale [BPRS]-total), Olz-M, Olz-H, and Hal were significantly superior to placebo. In pos. symptom improvement (BPRS-pos.), Olz-M, Olz-H, and Hal were comparable and significantly sup...
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☐ **Antipsychotic drug effects on brain morphology in first-episode psychosis**
By: Lieberman, Jeffrey A.; Tollefson, Gary D.; Charles, Cecil; Zipursky, Robert; Sharma, Tonmoy; Kahn, Rene S.; Keefe, Richard S. E.; Green, Alan I.; Gur, Raquel E.; McEvoy, Joseph; et al
Archives of General Psychiatry (2005), 62(4), 361-370 | Language: English, Database: CPlus
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Abstract: Pathomorphol. brain changes occurring as early as first-episode schizophrenia have been extensively described. Longitudinal studies have demonstrated that these changes may be progressive and associated with clin. outcome. This raises the possibility that antipsychotics might alter such pathomorphol. progression in early-stage schizophrenia. Objective: To test a priori hypotheses that olanzapine-treated patients have less change over time in whole brain gray matter volumes and lateral ventricle volumes than haloperidol-treated patients and that gray matter and lateral ventricle volume changes ...
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Cited By (274)

Citation Map

☐ **Feasibility, efficacy, and safety of antipsychotics for intensive care unit delirium: the MIND randomized, placebo-controlled trial**
By: Girard, Timothy D.; Pandharipande, Pratik P.; Carson, Shannon S.; Schmidt, Gregory A.; Wright, Patrick E.; Canonico, Angelo E.; Pun, Brenda T.; Thompson, Jennifer L.; Shintani, Ayumi K.; Meltzer, Herbert Y.; et al
Critical Care Medicine (2010), 38(2), 428-437 | Language: English, Database: CPlus
[View Reference Detail](#)
Abstract: Objective: To demonstrate the feasibility of a placebo-controlled trial of antipsychotics for delirium in the intensive care unit and to test the hypothesis that antipsychotics would improve days alive without delirium or coma. Design: Randomized, double-blind, placebo-controlled trial. Setting: Six tertiary care medical centers in the US. Patients: One hundred one mech. ventilated medical and surgical intensive care unit patients. Intervention: Patients were randomly assigned to receive haloperidol or ziprasidone or placebo every 6 h for up to 14 days. Twice each day, frequency of study drug ...
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Volume: 62

Issue: 4

Pages: 361-370

Journal

2005

DOI:

10.1001/archpsyc.62.4.361

Database Information

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Company/Organization

New York State Psychiatric Institute

New York, New York 10032

United States

Publisher

American Medical Association

Language

English

Antipsychotic drug effects on brain morphology in first-episode psychosis

By: Lieberman, Jeffrey A.; Tollefson, Gary D.; Charles, Cecil; Zipursky, Robert; Sharma, Tonmoy; Kahn, Rene S.; Keefe, Richard S. E.; Green, Alan I.; Gur, Raquel E.; McEvoy, Joseph; et al

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Abstract: Pathomorphol. brain changes occurring as early as first-episode schizophrenia have been extensively described. Longitudinal studies have demonstrated that these changes may be progressive and associated with clin. outcome. This raises the possibility that antipsychotics might alter such pathomorphol. progression in early-stage schizophrenia. Objective: To test a priori hypotheses that olanzapine-treated patients have less change over time in whole brain gray matter volumes and lateral ventricle volumes than haloperidol-treated patients and that gray matter and lateral ventricle volume changes are associated with changes in psychopathol. and neurocognition. Design: Longitudinal, randomized, controlled, multisite, double-blind study. Patients treated and followed up for up to 104 wk. Neurocognitive and magnetic resonance imaging (MRI) assessments performed at weeks 0 (baseline), 12, 24, 52, and 104. Mixed-models analyses with time-dependent covariates evaluated treatment effects on MRI end points and explored relationships between MRI, psychopathol., and neurocognitive outcomes. Setting: Fourteen academic medical centers (United States, 11; Canada, 1; Netherlands, 1; England, 1). Participants: Patients with first-episode psychosis (DSM-IV) and healthy volunteers. Interventions: Random allocation to a conventional antipsychotic: haloperidol (2-20 mg/d), or an atypical antipsychotic, olanzapine (5-20 mg/d). Main Outcome Measures: Brain volume changes assessed by MRI. Results: Of 263 randomized patients, 161 had baseline and at least 1 postbaseline MRI evaluation. Haloperidol-treated patients exhibited significant decreases in gray matter volume, whereas olanzapine-treated patients did not. A matched sample of healthy volunteers (n=58) examined contemporaneously showed no change in gray matter volume. Conclusions: Patients with first-episode psychosis exhibited a significant between-treatment difference in MRI volume changes. Haloperidol was associated with significant reductions in gray matter volume, whereas olanzapine was not. Post hoc analyses suggested that treatment effects on brain volume and psychopathol. of schizophrenia may be associated. The differential treatment effects on brain morphol. could be due to haloperidol-associated toxicity or greater therapeutic effects of olanzapine.

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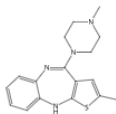
^ Concepts

Antipsychotics	Drug toxicity
Brain gray matter	Homo sapiens
Brain ventricle, lateral ventricle	Human
	Psychosis

^ Substances

Substances (2)

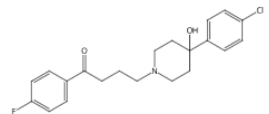
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$C_{17}H_{20}N_4S$
Olanzapine

Role: Adverse Effect, Including Toxicity, Pharmacological Activity, Therapeutic Use, Biological Study, Uses

52-86-8



$C_{21}H_{23}ClFNO_2$
Haloperidol

Role: Adverse Effect, Including Toxicity, Pharmacological Activity, Therapeutic Use, Biological Study, Uses

^ Citations

Citations (49)

- 1) McCarley, R; Biol Psychiatry, 1999, 45, 1099
- 2) Shenton, M; Schizophr Res, 2001, 49, 1
- 3) Lawrie, S; Br J Psychiatry, 1998, 172, 110
- 4) DeLisi, L; Psychiatry Res, 1997, 74, 129
- 6) Lieberman, J; Biol Psychiatry, 2001, 49, 487
- 7) Wood, S; Schizophr Res, 2001, 52, 37
- 8) Cahn, W; Arch Gen Psychiatry, 2002, 59, 1002
- 9) Ho, B; Arch Gen Psychiatry, 2003, 60, 585
- 10) Davis, K; Biol Psychiatry, 1998, 43, 783
- 11) Mathalon, D; Arch Gen Psychiatry, 2001, 58, 148
- 12) Rapoport, J; Arch Gen Psychiatry, 1999, 56, 649
- 13) Gogtay, N; Am J Psychiatry, 2003, 160, 569
- 14) Woods, B; Am J Psychiatry, 1998, 155, 1661
- 15) Lieberman, J; Biol Psychiatry, 1999, 46, 729
- 16) Duncan, G; J Pharmacol Exp Ther, 2000, 293, 8
- 17) Fumagalli, F; J Neurosci Res, 2003, 72, 622
- 18) Bai, O; J Neurosci Res, 2003, 71, 127
- 19) Marx, C; Neuropsychopharmacology, 2003, 28, 1
- 20) Wakade, C; J Neurosci Res, 2002, 69, 72
- 21) Halim, N; Neuropsychopharmacology, 2004, 29, 1063
- 22) Wang, H; Neuropsychopharmacology, 2004, 29, 1230



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