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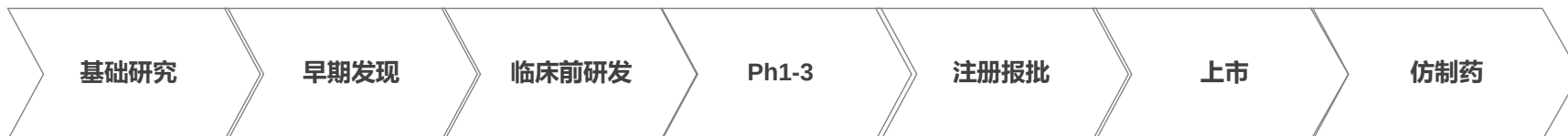
张慧

产品与方案解决专家，生命科学事业部

2014年11月



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Thomson Reuters Integrity可以减小全校师生对SciFinder数据库的依赖。

Thomson Reuters Integrity 是专业的医药信息数据库, 能够为药物研发一线的人员提供可靠、及时、连续和深度的前沿科研信息, 帮助研发人员在研发早期做出正确的决策、加速“药物发现”阶段向“临床应用阶段”的转化过程, 避免医药研发机构和企业研发经费与时间的浪费, 最终降低研发风险。可以满足药物研发一线人员的信息需求、包括化学家、药物学家、生物学家、临床学家、医学家等。

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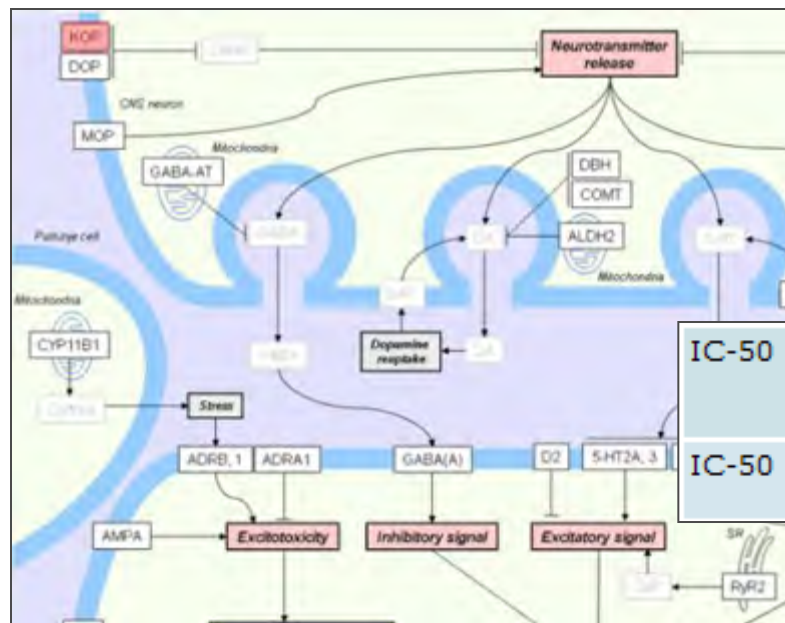
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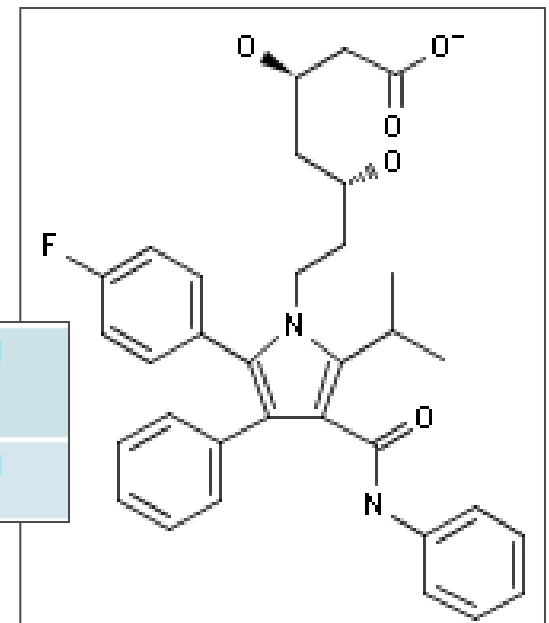
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IC-50	2.80 nM
IC-50	8.60 nM



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- 每天更新
- 信息准确
- 专家意见
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Thomson Reuters Integrity 数据库主要内容

药物（包括化药与生物药）	441,834(404,723化学结构式数据)
药物靶标以及发病通路图	2,564 药物靶标
药物/疾病相关的基因组学信息	34,325 相关基因
化学合成	26,851合成路线
药理/毒理试验数据	1,671,149药理/毒理
药代动力学/药物代谢试验数据	661,051药代/药动
疾病相关的综合性评述	149疾病综述
临床试验方案/结果	237,779临床试验
研发单位	15,134家企业或研发机构
文献期刊及会议	1,841,482个记录
专利文献	276,019个专利家族
实验模型	29,758实验模型

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Drug Name	Target	Phase	Company	Indication	Status
Drug A	Target A	Phase 1	Company A	Indication A	Active
Drug B	Target B	Phase 2	Company B	Indication B	Active
Drug C	Target C	Phase 3	Company C	Indication C	Active
Drug D	Target D	Phase 1	Company D	Indication D	Active
Drug E	Target E	Phase 2	Company E	Indication E	Active

- 药理学实验数据比较

- 寻找具有某药理学特性的相关药物
- 比较同一领域/类似结构等药物之间的药理学活性

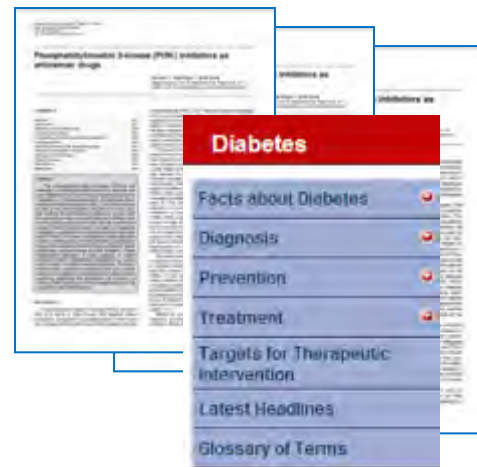


- 靶标进展报告和通路图

- 了解某一靶标的研发进展、研究领域、作用机理等
- 促进药物设计及基础机理的研究

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- RegeneRx receives orphan drug designation for thymosin beta-4

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- RadioMedix receives orphan drug designation for GalioMedix

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- FDA grants orphan drug status to DiaVacs' immunotherapy product for type 1 diabetes
- FDA accepts for filing Aeterna Zentaris' NDA for macimorelin acetate for AGHD
- NPS Pharmaceuticals receives European orphan drug designation for Natpara

Cancer

- FDA grants fast track designation to Peregrine's immunotherapy bavituximab for second-line NSCLC

Today's Features

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52nd Annual Meeting (ACNP) (December 8-12, 2013)

HEP DART (December 8-12, Kohala Coast, Hawaii) 2013

Annual Meeting of the American Society of Hematology (December 7-10, New Orleans) 2013

Winter Meeting of the British Thoracic Society (December 4-6, London) 2013

18th International Symposium on Cancer Chemotherapy, JFCC-ISCC (December 4-5, Tokyo) 2013

99th Annual Meeting of the Radiological Society of North America (RSNA) (December 1-6, Chicago) 2013

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A selection of new molecular entities and targets ready to enter the R&D arena.

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Today's Featured Patents

Click here to display today's featured patent family entries in Integrity

Conferences

52nd Annual Meeting of the American College of Neuropsychopharmacology (ACNP) (December 8-12, Hollywood) 2013

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HEP DART (December 8-12, Kohala Coast, Hawaii) 2013

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收到孤儿药物认定

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- RegeneRx receives orphan drug designation for thymosin beta4

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FDA授予Bavituximab二线治疗非小细胞肺癌快速审批通道

Cancer

- FDA grants fast track designation to Peregrine's immunotherapy bavituximab for second-line NSCLC

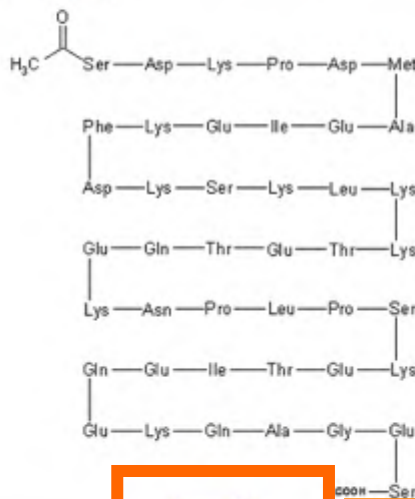
雷根内克斯生物制药公司已收到FDA的孤儿药认定：胸腺肽beta4对于神经营养角膜病的治疗

Today's News - Mozilla Firefox

integrity.thomson-pharma.com/integrity/xmbst/pk_home.show_todaynews?p_id=128015

RegeneRx receives orphan drug designation for thymosin beta4

RegeneRx Biopharmaceuticals has received FDA orphan drug designation for **thymosin beta4** for the treatment of neurotrophic keratopathy, a preservative-free, sterile, ophthalmic eye drop whose active ingredient is thymosin beta4, stimulated healing within 4 to 8 weeks in minimum of 6 weeks to over 1 year (RegeneRx Biopharmaceuticals News Release; FDA Web site).



Thymosin B4

Close

Integrity Drug & Biologics interface showing the chemical structure of Thymosin B4 and associated clinical trial data.

Product Name	Status	Date
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14
Thymosin B4	Approved	2014-03-14

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Today's Patents

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- HEP DART (December 8-12, Kohala Coast, Hawaii 2013)
- Annual Meeting of the American Society for Cell Biology (ASCB) (December 1-5, New Orleans 2013)
- Winter Meeting of the American Society for Cell Biology (ASCB) (December 1-5, 2013)
- 18th International Symposium on Cancer Chemotherapy, JFCC-ISCC (December 4-5, Tokyo) 2013
- 99th Annual Meeting of the Radiological Society of North America (RSNA) (December 1-6, Chicago) 2013

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一周具有潜在治疗前景基因相关研究

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一周在生物学医学论文与会议中被引用的临床试验研究

加速发现：最近新公布的具有活性的新分子实体



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The Starting Line - Mozilla Firefox

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The Starting Line

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The Starting Line

January 06 - 12, 2014

Company	Product	Condition	Comments
Amgen	AMG-3969	Diabetes type 2	Glucose Lowering Agents
Korea Research Institute Chem Technol Korea University	KR-67105	Diabetes type 2 Metabolic syndrome	11-beta-Hydroxysteroid Dehydrogenase Type 1 (11beta-HSD1) Inhibitors
University North Carolina, Chapel Hill	UNC-2250 UNC-2250B	Cancer	Mer Receptor Inhibitors Signal Transduction Modulators

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99th Annual Meeting of the Radiological Society of North America (RSNA) (December 1-6, Chicago) 2013
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紧密跟踪：汇总药物研发阶段的改变



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Options

Pipeline on the Move (December 30 - 5, 2014)

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Organization	Main Name	Condition	Milestone	Country/Area	Notes
Heat Biologics	HS-410	Cancer, bladder	Phase I/II	United States	Treatment of patients with high-risk non-muscle invasive bladder cancer who have undergone transurethral resection of bladder tumor and received prior treatment with BCG; Injections; Parenteral
NPS Pharmaceuticals	Teduglutide	Short-bowel syndrome	Phase III	United States	Treatment of short-bowel syndrome in pediatric patients aged 1 year through 17 years, who are dependent on parenteral support; Subcutaneous
Cell Therapeutics	Tosedostat	Hematologic/blood cancer	On Hold lifted	United States	Partial Clinical Hold lifted in US by Cell Therapeutics for the treatment of hematologic/blood cancer
Peregrine Pharmaceuticals	Bavituximab	Cancer, lung (non-small cell) (NSCLC)	Phase III		In combination with docetaxel in patients with second line stage IIIb/IV non-squamous non small-cell lung cancer; Infusion; Intravenous
Serodus Evolve	EV-077	Nephropathy, diabetic	Licensed		Licensed to Serodus by Evolve for the treatment of diabetic nephropathy
Genzyme	Alemtuzumab	Multiple sclerosis, relapsing-remitting	Complete Response Letter	United States	Infusion; Intravenous
Veloxis Pharmaceuticals	Tacrolimus	Transplant rejection, kidney	NDA Filed	United States	Prevention of transplant rejection in kidney transplant patients; Tablets, once-daily; Using MeltDose technology

99th Annual Meeting of the Radiological Society of North America (RSNA)
(December 1-6, Chicago) 2013

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Infections

- Affinium obtains QIDP designation for AFN-1252, completes dosing in study of new prodrug
- FDA grants QIDP designation to oritavancin
- Preclinical antiviral efficacy seen in Tekmira's TKM-Ebola and TKM-Marburg programs

Respiratory Disorders

- Boehringer Ingelheim seeks European approval of tiotropium Respimat for asthma

Today's Featured Patents

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Conferences

Annual Meeting of the American Association of Pharmaceutical Scientists (AAPS) (November 10-14, San Antonio, TX) 2013
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43rd Annual Meeting of the Society for Neuroscience (November 9-13, San Diego) 2013
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28th Society for Immunotherapy of Cancer (SITC) Annual Meeting (November 8-10, National Harbor) 2013
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ASCO-EORTC-NCI Annual Meeting on Markers in Cancer (November 7-9, Brussels) 2013
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Annual Meeting of the American Association for the Study of Liver Diseases (November 1-5, Washington, D.C.) 2013
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64th AALAS National Meeting (October 27-31, Baltimore) 2013

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- Recorded Training
- Quick Guides



THOMSON REUTERS

IntegritySM



Quick Search

90

Reports

Start

Targetscapes

[Index](#) AND ▶

关联药物数量较少的的则为目的研究不多的较新靶标

Records Retrieved

Records 1 to 25 of 141 retrieved

Options

Targets & Pathways Search Results

Query > Available Since = from 20130401

Target Name	Type	Major Condition & Status	Links												
☐ Acylglycerol kinase, mitochondrial precursor	Protein	<table><tr><td>Major Condition</td><td>V</td><td>C</td><td>E</td></tr><tr><td>Cancer</td><td></td><td></td><td>1</td></tr></table>	Major Condition	V	C	E	Cancer			1	UniProtKB: Q53H12				
Major Condition	V	C	E												
Cancer			1												
☐ Adrenomedullin	Protein	<table><tr><td>Major Condition</td><td>V</td><td>C</td><td>E</td></tr><tr><td>Critical care medicine</td><td></td><td></td><td>3</td></tr><tr><td>Renal Disorders</td><td></td><td></td><td>1</td></tr></table>	Major Condition	V	C	E	Critical care medicine			3	Renal Disorders			1	UniProtKB: P35318
Major Condition	V	C	E												
Critical care medicine			3												
Renal Disorders			1												

Records Retrieved

1 Record retrieved

Options

Targets & Pathways Search Results

☐ **CDK2/Cyclin E**

Type	Protein
Related Names	CCNE; CCNE1; CDK2 variant 1; Cyclin E1; Cyclin-dependent kinase 2, transcript variant 1; p33(CDK2)
Description/Function	CDK2/Cyclin E is a complex that mediates cell cycle progression. The enzymes are also involved in regulation of transcription. CDK1 is activated by association with cyclin E which results in formation of a cyclin-dependent kinase complex. Inhibition of CDKs selectively interrupts the cell cycle in cancer cells.
Scientific Animations	 Cell Cycle: Schematic Diagram  Retinoblastoma: Role in G1 Phase Progression
Condition (Status)	☐ Collapse All ☒ Expand All ☒ Cancer ☐ E ☐ (View Drugs) V 1 Conditions C 0 Conditions E 1 Conditions
Related Mechanisms	CDK2/Cyclin E Inhibitors
Products Under Development and Launched	Cancer

Related Information

Drugs & Biologics 198

Biomarkers 11

Targets & Pathways 3

Genomics 2

Experimental Pharmacology 597

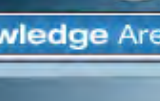
提纲

- Thomson Reuters Integrity数据库简介
- Integrity解决如下问题
 - 动态监测新分子实体和新靶标
 - 快速概览特定领域的研发进展和布局
 - 选题立项评估药物品种的综合状况
 - 比较药理学活性进行结构式优化
 - 一站式概览疾病综述和主流药物
 - 设置专属Email跟踪获取更新内容
- Q &A

快速概览特定领域的研发进展和布局

- 肝癌领域的当前在研药物研发进展和布局
- 结构式检索举例

选择相应的检索限制条件：Condition
可根据需要设定多个条件，如天然产物来源等



THOMSON REUTERS

IntegritySM

Drugs & Biologics

Knowledge Areas

Quick Search

go

Home

Support/Help

Query Manager/Alert Center

Reports

398603 Records in Drugs & Biologics

368015 Records with chemical structure

Advanced Search

Session History

Clear Form

Start

Product

Structure Search

Active Development

Cancer, liver"

Index AND

Index AND

Index AND

Index AND

Index AND

Index AND

Index AND

Index AND

Index AND

Condition

Natural Source (Y/N)

The Starting Line

A selection of new molecular ent targets ready to enter the R&D an

Pipeline on the Move

Milestones for drugs under active development.

Gateways to Development Status

Select a condition to generate program status list for compou launched or under active deve for that condition.

AIDS

Anesthesia

Cancer

Cardiovascular Disor

Congenital defects

Critical care medicin

Dermatological Disor

THOMSON RE

汤森路透

从标准词表索引选择检索词，让检索更全面准确

The screenshot displays the Thomson Reuters Integrity web application interface. The main window is titled "List of Values - Selection - Mozilla Firefox" and shows a hierarchical tree of medical terms. The tree is expanded to show the "Cancer" category, which includes "Benign neoplasms", "Cancer associated disorders", "Cancer therapy associated disorders", "Cyst", "Hyperplasia", and "Malignant neoplasms". Under "Malignant neoplasms", the "Digestive/gastrointestinal cancer" category is expanded, showing "Cancer, gastroenteropancreatic", "Cancer, hepatobiliary", and "Cancer, liver (hepatocellular carcinoma)". The "Cancer, liver" term is highlighted in red. To the left of the tree, there is a search box containing the text "Cancer, liver" and a "Lookup" button. Below the search box, there are navigation links: "<<First", "<Prev", "Next>", and "Last>>". The result number "Result number: 1 of 6" is displayed. On the right side of the interface, there is a "Start" button and a "Structure Search" section with multiple "Index AND" buttons.

THOMSON REUTERS
Integrity

Knowledge

398603 Records in Drug
368015 Records with ch

The Starting Line
A selection of new molecule
targets ready to enter the f

Pipeline on the Mo
Milestones for drugs under
development.

Gateways
Development
Select a condition to get
program status list for c
launched or under active
for that condition.

▶ AIDS
▶ Anesthesia
▶ Cancer
▶ Cardiovascular I
▶ Congenital defec
▶ Critical care med
▶ Dermatological I

Click the plus sign next to a term to display subclasses and make your selection.
Alternatively, enter a word or part of a word in the box below and click Lookup. Then use the scroll bar in combination with the First, Previous, Next and Last buttons to locate terms within the hierarchy.

Cancer, liver

Lookup

Click the button below to change between Hierarchical and Alphabetical lists.

Order Alphabetically

<<First <Prev Next> Last>>

Result number: 1 of 6

Select a Value:

- ⊕ AIDS
- ⊕ Anesthesia
- ⊖ Cancer
 - ⊕ Benign neoplasms
 - ⊕ Cancer associated disorders
 - ⊕ Cancer therapy associated disorders
 - ⊕ Cyst
 - ⊕ Hyperplasia
 - ⊖ Malignant neoplasms
 - ⊕ Cancer of unspecified body location/system
 - ⊕ Cancer, breast
 - ⊕ Cancer, eye
 - ⊕ Cancer, head and neck
 - ⊕ Cancer, peritoneum
 - ⊕ Cancer, skin
 - ⊖ Digestive/gastrointestinal cancer
 - ⊕ Cancer, gastroenteropancreatic
 - ⊖ Cancer, hepatobiliary
 - ⊕ Cancer, bile duct
 - ⊕ Cancer, biliary
 - ⊕ Cancer, gallbladder
 - ⊖ Cancer, liver (hepatocellular carcinoma)
 - Carcinosarcoma, liver
 - Hepatoblastoma
 - Hepatobiliary carcinoma in situ

431个肝癌相关的药物记录

Records Retrieved 431 in Drugs & Biologics Search Results Options								
Drugs & Biologics Search Results								
Query > Condition = "Cancer, liver"								
1 2 3 4 5 6 7 8 9 10 (Next>)(Last>>)								
Entry Number	Highest Phase	Code Name	Generic Name	Brand Name	Product Category	Therapeutic Group	Mechanism of Action	Organization
☐ 170011 *	Launched-1956	MMc	Mitomycin (USAN) Mitomycin C (JAN)	Ametycine Mito-medac Mitosol Mutamycin		Antibiotics Lung Cancer Therapy Oncolytic Drugs Bladder Cancer Therapy Digestive/Gastrointestinal Cancer Therapy Colorectal Cancer Therapy Liver Cancer Therapy	DNA Alkylating Drugs Apoptosis Inducers	EORTC National Cancer Institute Bristol-Myers Squibb (Originator) Mobius Therapeutics Medac Ohio State University Sangfi Medical Research Council Halozyme
☐ 190434 *	Phase III	E-5166 K-333 NIK-333 NK-333	Acyclic retinoid Peretinoin (Prop INN) Polyprenoic acid		Retinoids	Chemopreventive Agents Oncolytic Drugs	Retinoid RARbeta Ligands Retinoid RXRalpha Ligands Apoptosis Inducers	Kowa Pharmaceutical Eisai (Originator)
☐ 190725 *	Launched-1995	NSC-296961 SAPEP WR-2721 YM-08310	Amifostine hydrate (BANM; Rec INN); (USAN) Gammaphos Ethiofos (former USAN)	Ethiol		Myelodysplastic Syndrome Therapy Treatment of Mucositis Radioprotectants/Radiomitigators Chemoprotective Agents Cancer Associated Disorders, Treatment of		National Cancer Institute Pinnacle Pharmaceuticals MedImmune Oncology (Originator)

Filter by Statistics

- Development Status
- Organization
- Major Therapeutic Groups
- Therapeutic Group
- Major Condition Groups
- Condition
- Mechanistic Scope
 - Molecular Mechanisms
 - Cellular Mechanisms
- Major Product Categories
- Product Category
- Launch Year
- Target
- Under Active Development / No Development Reported
- Filter Only Lead Compounds
- Natural Source Categories
- Natural Source Scientific Name
- Prescription/ Indication Type
- Administration Route

概览药物的研发状态：Filter by Statistics

Records Retrieved431 in Drugs & Biologics Search ResultsOptions

Drugs & Biologics Search Results

12345678910 (Next>)(Last>>)

Query > Condition = "Cancer, liver"

Entry Number	Highest Phase	Code Name	Generic Name	Br Na	Mechanism of Action	Organization
☐ 070011 *	Launched-1956	MMc	Mitomycin (USAN) Mitomycin C (JAN)	Am Mit Mit	Alkylating Agents Apoptosis Inducers	NCI National Cancer Institute Bristol-Myers Squibb (Originator) Mobiu Therapeutics Medac Ohio State University Sanofi Medical Research Council Halozyme
☐ 090434 *	Phase III	E-5166 K-333 NIK-333 NK-333	Acyclic retinoid Peretinoin (Prop INN) Polyprenoic acid		Retinoids	Chemopreventive Agents Oncolytic Drugs
☐ 090725 *	Launched-1995	NSC-296961 SAPEP WR-2721 YM-08310	Amifostine hydrate (BANM; Rec INN); USAN) Gammaphos Ethiofos (former USAN)	Ethiol	Myelodysplastic Syndrome Therapy Treatment of Mucositis Radioprotectants/Radiomitigators Chemoprotective Agents Cancer Associated Disorders, Treatment of	National Cancer Institute Pinnacle Pharmaceuticals MedImmune Oncology (Originator)

检索结果进行分析：药物技术类型；药物来源；治疗领域；作用机制；研发机构；研发阶段；药物靶标;给药途径等等

Filter by Statistics

Development Status

Organization

Major Therapeutic Groups

Therapeutic Group

Major Condition Groups

Condition

Mechanistic Scope

Molecular Mechanisms

Cellular Mechanisms

Major Product Categories

Product Category

Launch Year

Target

Under Active Development / No Development Reported

Filter Only Lead Compounds

Natural Source Categories

Natural Source Scientific Name

Prescription/ Indication Type

Administration Route

检索结果进行分析：药物技术类型；药物来源；治疗领域；作用机制；研发机构；研发阶段；药物靶标;给药途径等等



研发阶段分析：概览领域内最新进展

可进一步过滤感兴趣的内容

Development Status

Condition = "Cancer, liver"



Export to Excel



Snapshot Tool

Display Options



Horizontal
Display



Vertical
Display



Pie Chart
Display



View Subset(s)



Print Chart

Records Retrieved

112 in Drugs & Biologics Search Results

Options

Drugs & Biologics Search Results

1 2 3 4 5 6 7 8 9 10 [Next>] [Last>>]

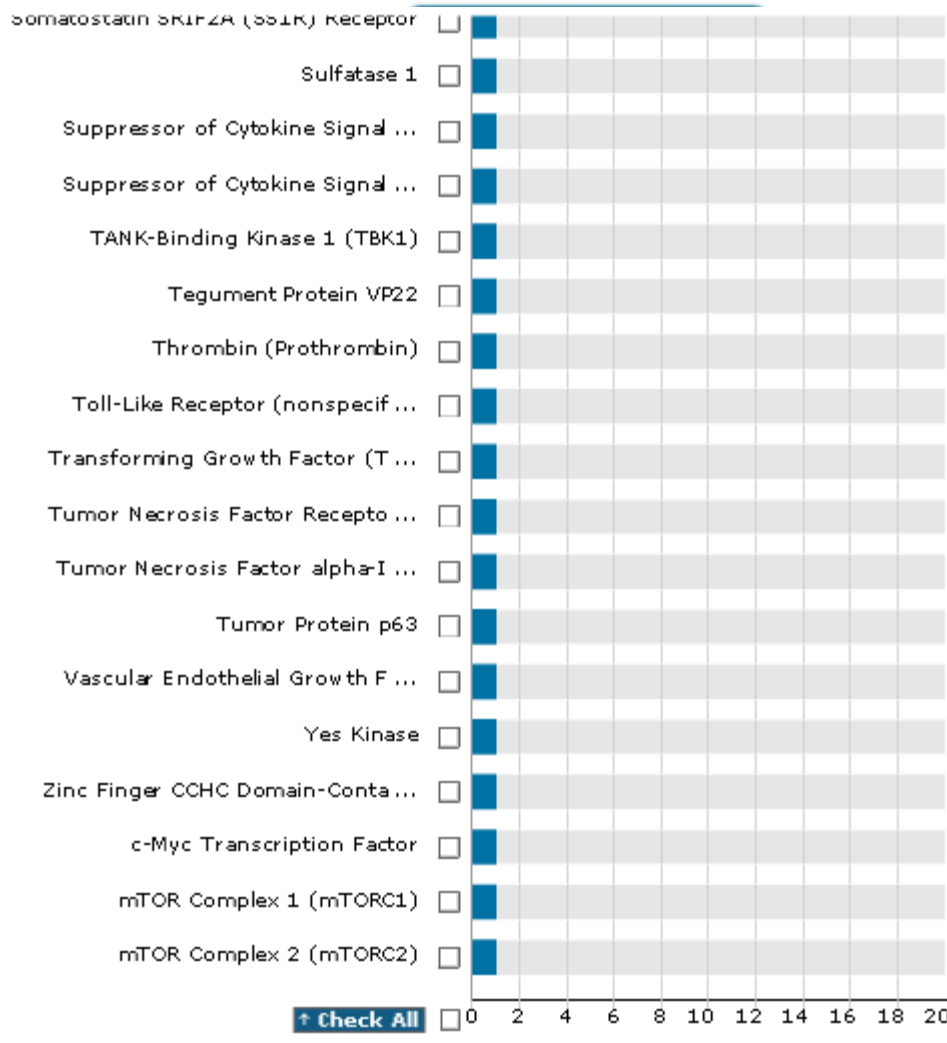
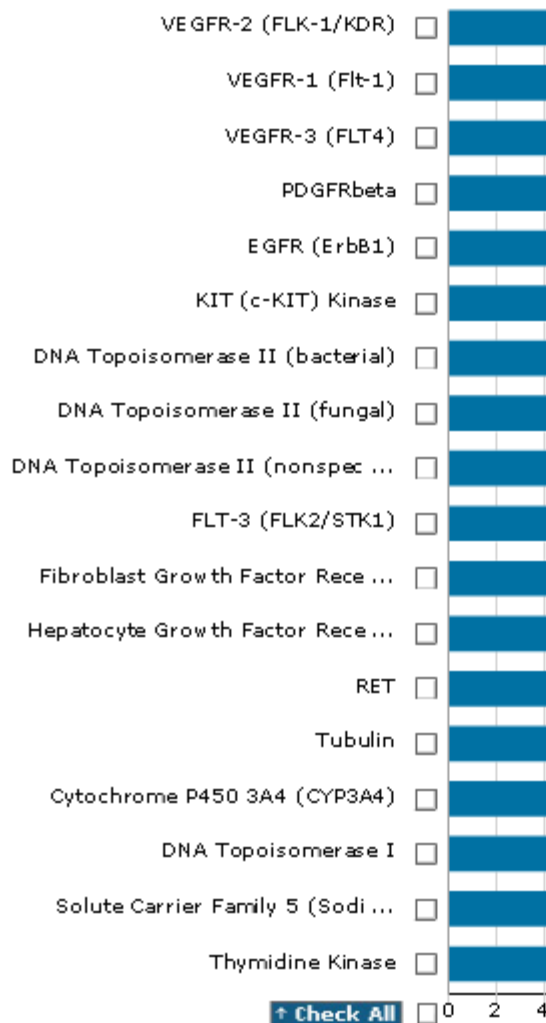
Entry Number	Highest Phase	Code Name	Generic Name	Brand Name	Product Category	Therapeutic Group	Mechanism of Action	Organization
☐ 090434	Phase III	E-5166 K-333 NIK-333 NK-333	Acyclic retinoid Peretinoin (Prop INN) Polyprenoic acid		Retinoids	Chemopreventive Agents Oncolytic Drugs	Retinoid RARbeta Ligands Retinoid RXRalpha Ligands Apoptosis Inducers	Kowa Pharmaceutical Eisai (Originator)
☐ 103954	Phase II	CB-1954	Tretazicar (Rec INN)		Radiosensitizers	Liver Cancer Therapy	DNA-Damaging Drugs	Cancer Research UK Morvus Technology Institute of Cancer Research (ICR) (Originator) PTC

靶标分析：431个药物对应222个靶标

概览本领域热门和悄然兴起的靶标

Target

Condition = "Cancer, liver"

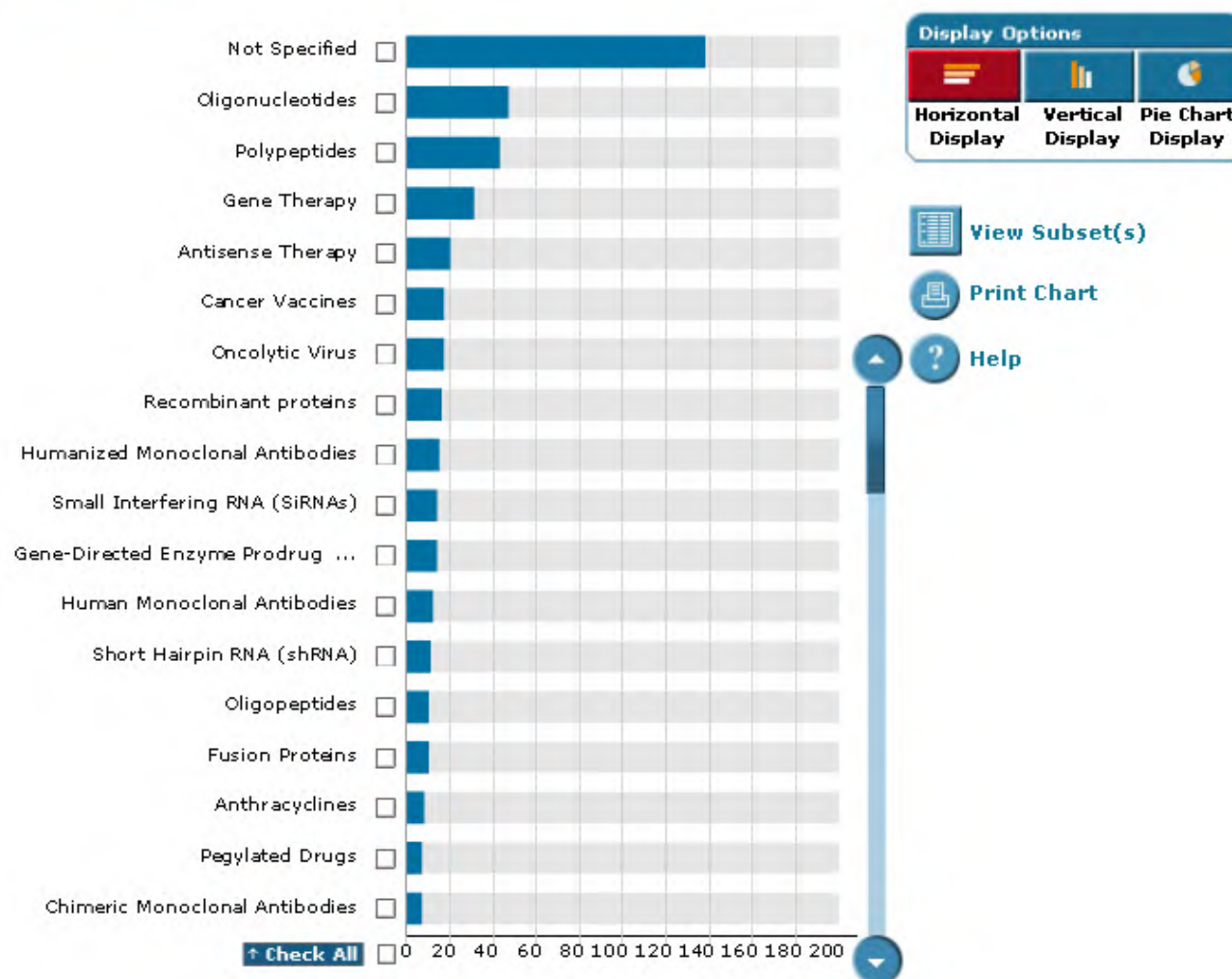


药物类别分析：洞悉热门和新兴技术及各类药物目前的状态

寡核苷酸，多肽，基因治疗，反义治疗，癌症疫苗，溶瘤病毒，重组蛋白，人源化单克隆抗体，siRNAs，基因定向酶前药治疗等

Product Category

Condition = "Cancer, liver"

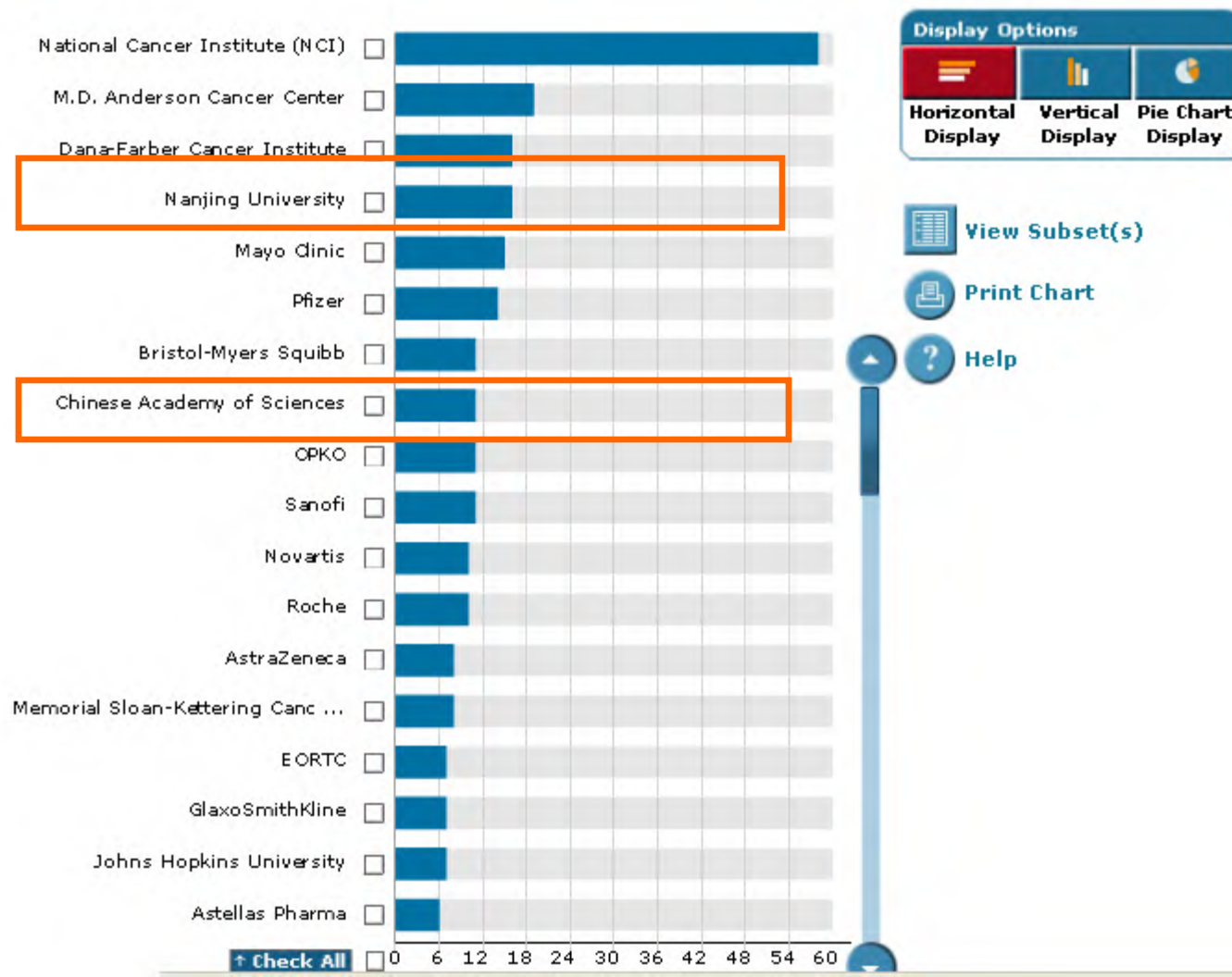


研究机构分析：了解同行和竞争者的目前状态

美国国家癌症研究所，安德森癌症研究中心，法伯癌症研究所，
南京大学，梅约医学中心，辉瑞，百时美施贵宝，中科院等

Organization

Condition = "Cancer, liver"

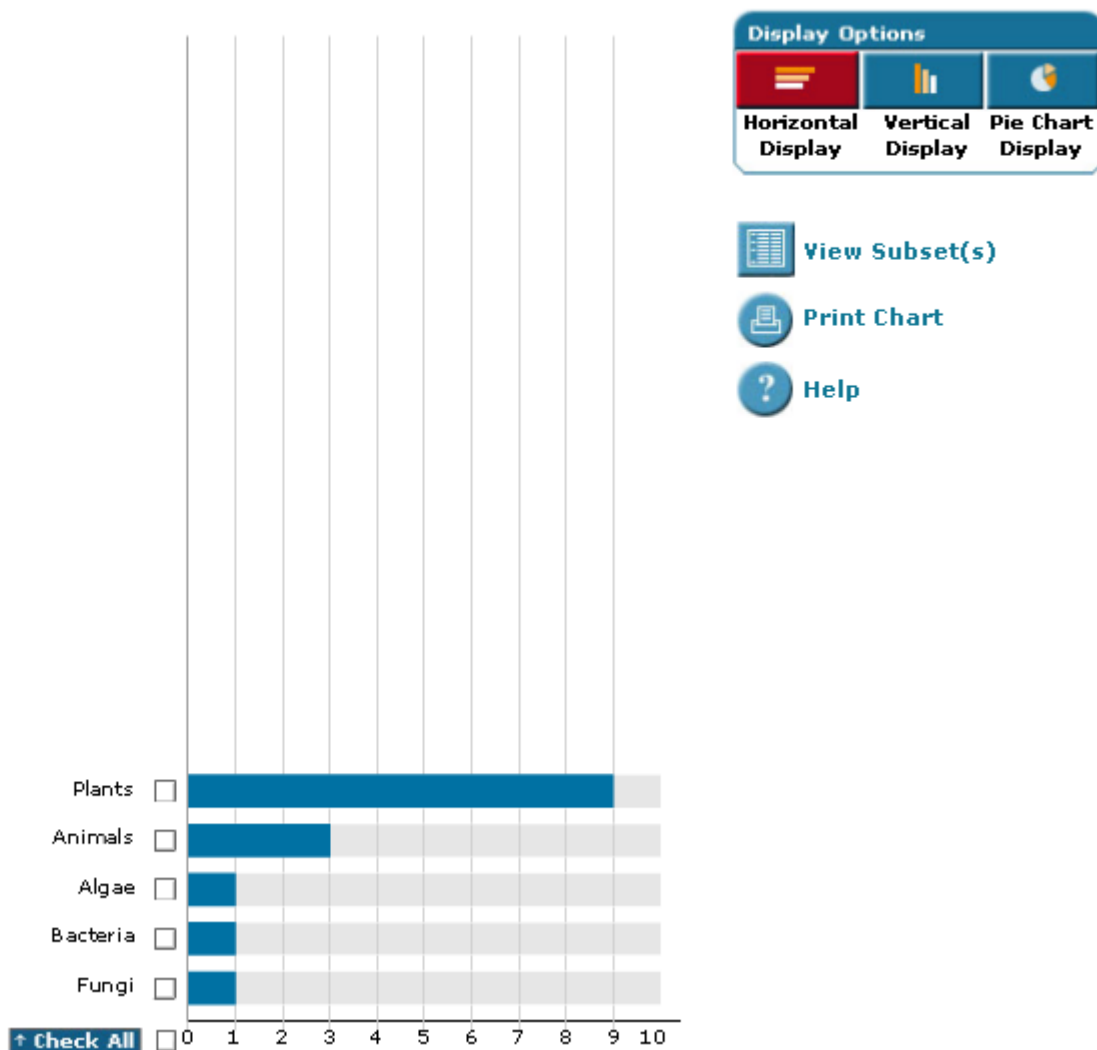


天然产物药物来源分析：

植物类；动物类；海藻类；细菌类；真菌类药物

Natural Source Categories

.. Condition = "Cancer, liver" ...



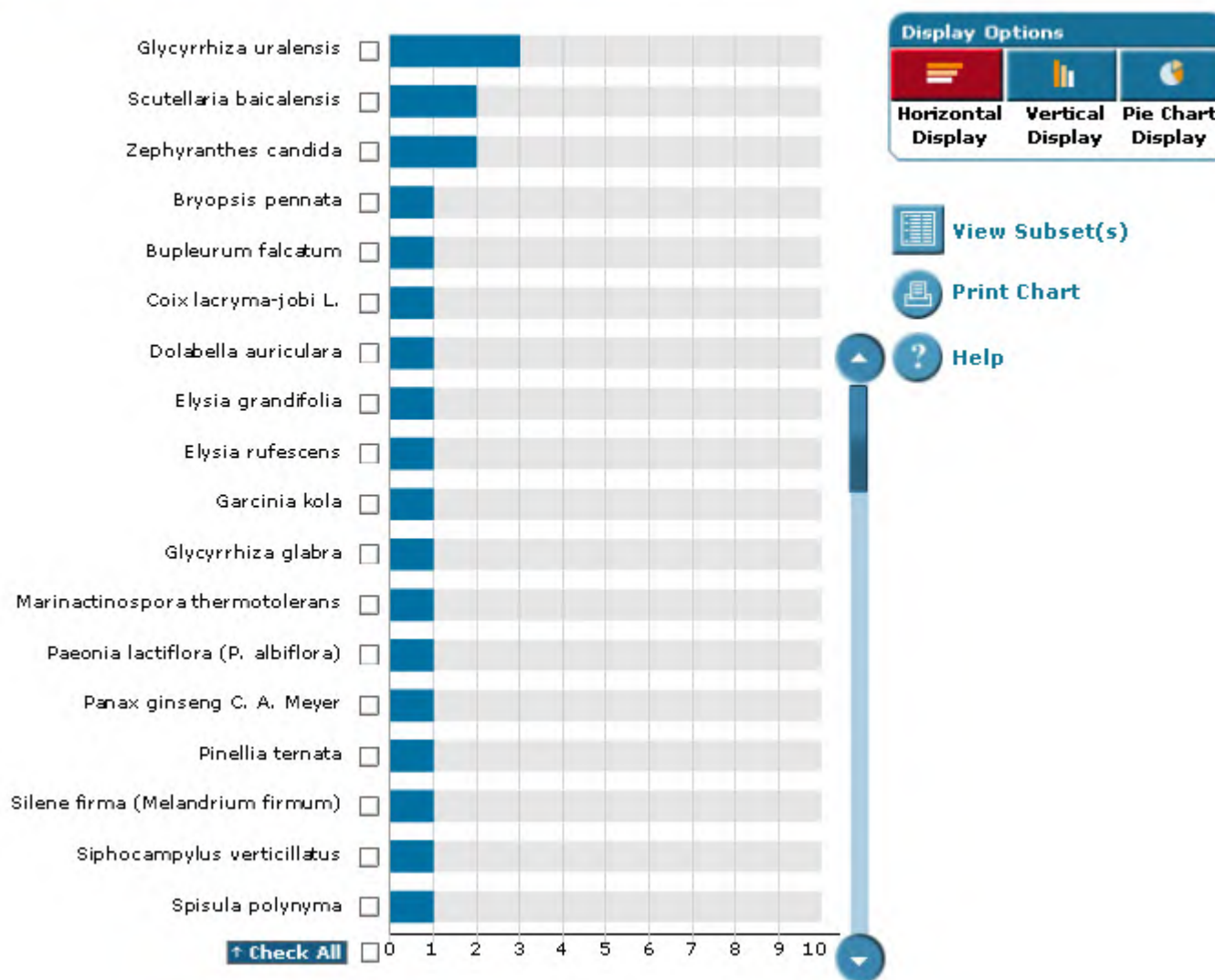
药物的天然产物来源名称分析：

甘草、黄芩、柴胡、薏苡、芍药、人参、半夏，金丝小枣等

Natural Source Scientific Name

.. Condition = "Cancer, liver"

....



按照结构式查看药物列表

Records Retrieved 431 in Drugs & Biologics Search Results

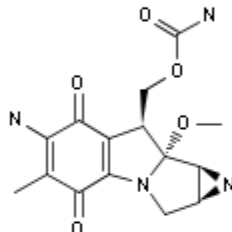
Options ▾

Drugs & Biologics
 Query > Condition :

Records Retrieved 431 Record(s) Retrieved Options ▾

Drugs & Biologics Search Results

1 2 3 4 5 6 7 8 9 10 [Next>] [Last>>]

Entry Number	Highest Phase	Drug Name	Category	Therapeutic Group	Mechanism of Action	Organization
☐ 070011 *	Launcher	Peritoinin		Antibiotics Lung Cancer Therapy Oncolytic Drugs Bladder Cancer Therapy Digestive/Gastrointestinal Inducers Cancer Therapy Colorectal Cancer Therapy Liver Cancer Therapy	DNA Alkylating Drugs Apoptosis 	EORTC National Cancer Institute Bristol-Myers Squibb (Originator) MobiUS Therapeutics Medac Ohio State University Sanofi Medical Research Council Halozyne
			 Structure Feature Options			
			Standard InChI	1S/C15H18N4O5 /c1-5-9(16)12(21)8-6(4-24-14(17)22)15(23-2)13-7(18-13)3-19(15)/h6-7,13,18H,3-4,16H2,1-2H3,(H2,17,22)/t6-,7+,13+,15-/m1/s1		
			Standard InChIKey	NWIBSHFKIJFRCO-WUDYKRTCSEA-N		
☐ 090434 *	Phase II	Peretinoin		Product Category: Retinoids	Therapeutic Group: Chemopreventive Agents	Mechanism of Action: Retinoid RARbeta
			Organization: Kowa Pharmaceutical			
☐ 090725 *	Launcher					

点击查看药物报告



以Erlotinib为例查看药物报告

Records Retrieved 1 in Drugs & Biologics Options

Drug Metabolites - Mozilla Firefox

integrity.thomson-pharma.com/integrity/xmlsl/PK_MET_LIST.met_popup?p_entry_number=250837&p_a

Thomson Reuters Integrity
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<http://integrity.thomson-pharma.com>

Metabolism

The diagram illustrates the metabolic pathways of Erlotinib (CP-394356). The central molecule is Erlotinib, which can be converted into several metabolites:

- M9**: A metabolite with a sulfonic acid group ($\text{O SO}_3\text{H}$) on the phenyl ring.
- M17**: A metabolite with a hydroxyl group (OH) on the phenyl ring.
- M3**: A metabolite with a glucuronide conjugate (O Gluc) on the phenyl ring.
- M10**: A metabolite with a glucuronide conjugate (Gluc O) on the ethoxy side chain.
- M7**: A metabolite with a hydroxyl group (OH) on the phenyl ring and a hydroxymethyl group (CH_2OH) on the quinoline ring.
- M16**: A metabolite with a hydroxyl group (OH) on the phenyl ring and a hydroxymethyl group (CH_2OH) on the quinoline ring.
- M12**: A metabolite with a hydroxyl group (OH) on the phenyl ring and a hydroxymethyl group (CH_2OH) on the quinoline ring.

Chemical structures are shown for each metabolite, highlighting the specific modifications to the parent molecule. The parent molecule is labeled **M16** with the identifier **OSI-356** and **CP-394356**.

以埃罗替尼为例查看药物报告，销售额数据

Records Retrieved 1 in Drugs & Biologics **Options**

Product Sales Results - Mozilla Firefox

integrity.thomson-pharma.com/integrity/xmlsl/pk_com_list.showProductSalesResults?p_entryNumber=250837

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http://integrity.thomson-pharma.com

Astellas Pharma (www.astellas.com)

Brand Name	Drug Name	Conditions
Tarceva	Erlotinib hydrochloride	Cancer, lung (non-small cell) (NSCLC)

Geographic Area	Year	Q1 (M)	Q2 (M)	Q3 (M)	Q4 (M)	Annual Sales (M)
Worldwide	2012	JPY 8000	JPY 8600	JPY 8700	JPY 8400	JPY 33700 (USD 427)
Worldwide	2013	JPY 9100	JPY 8300	JPY 8900		

Fiscal Year Ends: Mar 31

Roche (www.roche.com)

Brand Name	Drug Name	Conditions
Tarceva	Erlotinib hydrochloride	Cancer, pancreas Cancer, lung (non-small cell) (NSCLC) Cancer, pancreas metastatic

Geographic Area	Year	Q1 (M)	Q2 (M)	Q3 (M)	Q4 (M)	Annual Sales (M)
Japan	2007				CHF 2	CHF 2 (USD 2)
Japan	2008	CHF 8	CHF 12	CHF 11	CHF 16	CHF 47 (USD 44)
Japan	2009	CHF 15	CHF 17	CHF 16	CHF 19	CHF 67 (USD 62)

Molecular Mechanism EGFR (HER1; erbB1) Inhibitors

Cellular Mechanism Inhibitors of Signal Transduction Pathways

易于打印的药物综述报告

Molecular Mechanism	Cellular Mechanism	
EGFR (HER1; erbB1) Inhibitors	Inhibitors of Signal Transduction Pathways	
Product Category	Therapeutic Group	Prescription/ Indication Type
Tyrosinase Inhibitors	Prostate Cancer Therapies	

Tyrosinase Inhibitors

Organization

[National Cancer Institute](#)
[Genentech](#)
[EORTC](#)
[Roche](#)
[Astellas Pharma](#)
[Pfizer \(Originator\)](#)
[Chugai Pharmaceutical](#)
[M.D. Anderson Cancer Center](#)
[University of California, San Francisco](#)
[Sanofi](#)
[Astellas Pharma](#)
[Schwarz Pharma](#)
[National Cancer Research Institute](#)
[Mayo Clinic](#)
[Dana-Farber Cancer Institute](#)
[University of California, Davis](#)
[Canadian Cancer Society Research Inst](#)

Product Summary

REPORT

Erlotinib hydrochloride is an EGFR (erbB1) inhibitor used for the oral treatment of locally advanced or

Product Summary Details - Mozilla Firefox

integrity.thomson-pharma.com/integrity/xmls/pk_prod_list_productSummaryDetails?p_entryNumber=250837

Phase I/II	National Cancer Institute (NCI)	Oligodendroglioma
Phase I	National Cancer Institute (NCI)	Barrett's esophagus
Phase I	Mayo Clinic	Cholangitis, sclerosing

Development Status - Launched, Registered or Under Active Development							
Country/Area	Phase	Organization	Brand Name	Condition	Indication	Admin. Route	Formulation
	Phase III	Genentech		Cancer, pancreas metastatic	First-line treatment in combination with bevacizumab		
Canada	Registered - 2005	Astellas Pharma	Tarceva	Cancer, lung (non-small cell) (NSCLC)	In patients with advanced or metastatic disease following failure of first or second-line chemotherapy	oral	Tablets
Europe	Phase III	Roche		Cancer, lung (non-small cell) (NSCLC)	Adjuvant treatment; in first-line treatment in combination with Avastin; as first-line maintenance therapy for unresectable NSCLC		
European Union	Registered - 2005	Roche	Tarceva	Cancer, lung (non-small cell) (NSCLC)	Stage IIIB/IV disease after failure of at least one prior chemotherapy regimen	oral	Tablets, once-daily
European Union	Registered - 2007	Roche	Tarceva	Cancer, pancreas metastatic	First line treatment of advanced pancreatic cancer, in combination with gemcitabine	oral	Tablets, once-daily
European Union	Registered - 2010	Roche	Tarceva	Cancer, lung (non-small cell) (NSCLC)	First-line maintenance treatment after platinum-based first-line chemotherapy in patients with advanced non-small cell	oral	Tablets, once-daily



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更多药物相关的详尽信息，点击即可获取

Phase 1

Records Retrieved 784 in Experimental Pharmacology

Options

Phase 1

Experimental Pharmacology Search Results

1 2 3 4 5 6 7 8 9 10 (Next>) (Last>>)

Drug Name	Biomarker	Mechanism of Action	Experimental Activity	Pharmacological Activity	Material / Experimental Model	Method	Parameter	Value	Details
Erlotinib			Cancer, vulvar (squamous cell) remission/reduction, IN VITRO	Cytotoxicity @ 72 h	A431 human vulvar epidermoid carcinoma cells (EGFR-overexpressing)	Dye assay (XTT)	CC-50	1.27 μ M	Pat. 1
Erlotinib			Cancer, lung (non-small cell) (NSCLC) remission/reduction, IN VITRO	Cytotoxicity @ 72 h	H1975 human non-small-cell lung cancer cells	Dye assay (XTT)	CC-50	3.99 μ M	Pat. 1
Erlotinib			Cancer, ovary (adenocarcinoma) remission/reduction, IN VITRO	Cytotoxicity @ 72 h	SKOV3 human ovary adenocarcinoma cells	Dye assay (XTT)	CC-50	> 10 μ M	Pat. 1
Erlotinib			EGFR (erbB1) inhibition, IN VITRO	Protein-tyrosine kinase (EGF receptor), inhibition		Fluorescent assay	IC-50	1.30 nM	Pat. 1
Erlotinib			Cancer remission/reduction, IN VITRO	Mitogenesis, inhibition	A16-F10 human cancer cells	Dye assay (MTT)	IC-50	20 nM	Ref. 1
Erlotinib			EGFR (erbB1) inhibition, IN VITRO	Protein-tyrosine kinase (EGF receptor), inhibition			IC-50	24.6 $\pm$ 1.70 nM	Ref. 2
Erlotinib			EGFR (erbB1) inhibition, IN VITRO	Protein-tyrosine kinase (EGF receptor) autophosphorylation, inhibition	Purified enzyme	Fluorescent assay	IC-50	30 nM	Ref. 1
Erlotinib			Melanoma remission/reduction, IN VITRO	Mitogenesis, inhibition	G361 human melanoma cells	Dye assay (MTT)	IC-50	30.4 nM	Pat. 2
Erlotinib			Cancer, prostate (adenocarcinoma)	Mitogenesis, inhibition	PC3 human prostate adenocarcinoma cells	Dye assay (MTT)	IC-50	35.3 nM	Pat. 2

Filter by Statistics

Biomarker

Experimental Activity

System

Activity/Effect

Target/Condition/Toxicity

Pharmacological Activity

Parameter

Material

Method

Reference Type

Product in Studies

Drug Mechanism of Action

Administration Route

Dose Regimen

Experimental Model

Species

Strain

Filter by Value Range

Related Information

Drugs & Biologics 8	Biomarkers 1088	Targets & Pathways 1	Literature 3171	Patents 209	Organic Synthesis 1	Experimental Pharmacology 784
Experimental Models 16	Pharmacokinetics / Metabolism 1261	Clinical Studies 1438	Companies & Research Institutions 15	Disease Briefings 9		



The screenshot displays the 'Structure Feature Options' dialog box in a Mozilla Firefox browser window. The dialog is titled 'Structure Feature Options - Mozilla Firefox' and shows the URL 'integrity.thomson-pharma.com/integrity/xmlxsl/pk_prod_utils.show'. The main content of the dialog includes a description of structure feature options and several interactive elements:

- Copy structure to the Marvin applet structure editor.**
- Copy structure to the Marvin structure editor inside Integrity.**
- Export Molfile**
- Export SMILES**
- Display structurally similar compounds (80% default value can be modified manually).** This section is highlighted with an orange box, and the value '80' is entered in the adjacent input field.

The background application interface includes a sidebar with filters such as 'Entry Number', 'Record Creation', 'Last Updated Date', 'CAS Registry Number', 'Molecular Formula', 'Molecular Weight', 'Highest Phase', 'Under Active Development', 'Chemical Name', and 'Code Name'. The main area displays a chemical structure and various labels including 'STRUCTURE FEATURES', 'METABOLITES', and 'SALES'.

查看类似结构药物，调阅比较药理学活性数据

Records Retrieved 55 Record(s) Retrieved

Drugs & Biologics Search Results

Entry Number: [404449](#) Drug Name: Highest Phase: Biological Testing

Product Category: Therapeutic Group: Mechanism of Action: EGFR (HER1; erbB1) Inhibitors

Asthma Therapy Oncolytic Drugs Inhibitors of Signal Transduction Pathways

Standard InChI: 1S/C27H30N4O4/c1-6-16-8-7-9-19(14-18)30-25-21-/h1,7-9,14-17,20H,10-13H2,2-5H3,(O)C

Standard InChIKey: QJQCSXAKSADYBA-UHFFFAOYSA-N

Structure Feature Options

Entry Number: [446953](#) Drug Name: Highest Phase: Biological Testing

Product Category: Therapeutic Group: Mechanism of Action: EGFR (HER1; erbB1) Inhibitors

Asthma Therapy Oncolytic Drugs Inhibitors of Signal Transduction Pathways

Standard InChI: 1S/C26H28N4O4/c1-3-18-6-4-7-19(14-18)29-26-21-15-24(23(33-2)16-22(21)27-17-28-26)34-20-9-11-30(12-10-20)25(32)8-5-13-31/h1,4,6-7,14-17,20,31H,5,8-13H2,2H3,(H,27,28,29)

Standard InChIKey: VCCZA0HJZAECHL-UHFFFAOYSA-N

Structure Feature Options

Entry Number: [790203](#) Drug Name: Highest Phase: Biological Testing

Product Category: Therapeutic Group: Mechanism of Action: EGFR (HER1; erbB1) Inhibitors

Asthma Therapy Oncolytic Drugs Inhibitors of Signal Transduction Pathways

Standard InChI: 1S/C26H28N4O4/c1-3-18-6-4-7-19(14-18)29-26-21-15-24(23(33-2)16-22(21)27-17-28-26)34-20-9-11-30(12-10-20)25(32)8-5-13-31/h1,4,6-7,14-17,20,31H,5,8-13H2,2H3,(H,27,28,29)

Standard InChIKey: VCCZA0HJZAECHL-UHFFFAOYSA-N

Structure Feature Options

Options

- Keep Me Posted
- Export Center
- Integrity Reports
- Product List
- Display Milestones
- Gateways to Product Development Status
- Full Records
- References
- Patents
- All Related Information via Quick Search
- Printer Friendly Format

Filter by Statistics

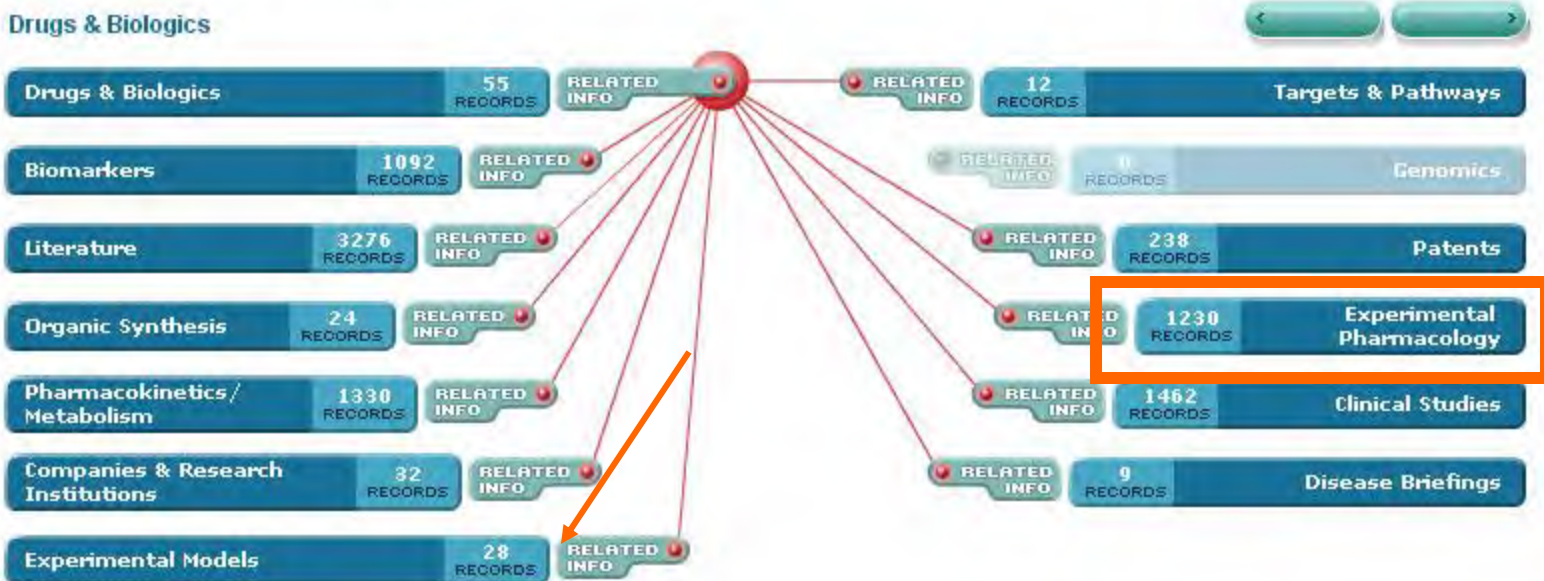
- Development Status
- Organization
- Major Therapeutic Groups
- Therapeutic Group
- Major Condition Groups
- Condition
- Mechanistic Scope
 - Molecular Mechanisms
 - Cellular Mechanisms
- Major Product Categories
- Product Category
- Launch Year
- Target
- Under Active Development / No Development Reported
- Filter Only Lead Compounds
- Natural Source Categories
- Natural Source Scientific Name
- Prescription/ Indication Type
- Administration Route

链接到相关信息，专利，文献，靶标，药理，药代，临床试验等信息。

所有与上页药物相关的信息经过归类整理如下



You have entered the Quick Search feature. Click one of the Knowledge Areas containing results to access a list of the records retrieved by your Quick Search. To be shown which Knowledge Areas contain information related to the Knowledge Area you are in, click the adjacent Related Information icon.



相关的：药物；专利，药理 / 毒理试验数据；药代动力学试验数据；临床试验；相关靶标及路径；合成路线；代谢途径；公司相关信息；疾病总结；生物标志物



药理学活性数据，可以按照多种条件过滤比较

Records Retrieved1230 in Experimental PharmacologyOptions

Experimental Pharmacology Search Results12345678910[Next>][Last>>]

Drug Name	Biomarker	Mechanism of Action	Experimental Activity	Pharmacological Activity	Material / Experimental	Method	Parameter	Value	Details
☐ 298493		EGFR (HER1; erbB1) Inhibitors	EGFR (erbB1) inhibition, IN VITRO	Protein-tyr kinase (EGF receptor), inhibition				£ 5.00 nM	Ref. 142
☐ 298493		EGFR (HER1; erbB1) Inhibitors	Fructose-Biphosphatase (Fructose-1,6-Bisphosphate; FBPase) inhibition, IN VITRO	Fructose-bisphosphatase inhibition				0.250 µM	Ref. 142
☐ 298493		EGFR (HER1; erbB1) Inhibitors	Fructose-Biphosphatase (Fructose-1,6-Bisphosphate; FBPase) inhibition, IN VITRO	Fructose-bisphosphatase, inhibition	Kidney, pig		IC-50	0.770 µM	Ref. 142
☐ 298493		EGFR (HER1; erbB1) Inhibitors	Fructose-Biphosphatase (Fructose-1,6-Bisphosphate; FBPase) inhibition, IN VITRO	Fructose-bisphosphatase, inhibition	Liver, rabbit		IC-50	> 10 µM	Ref. 142
☐ 298493		EGFR (HER1; erbB1) Inhibitors	Fructose-Biphosphatase (Fructose-1,6-Bisphosphate; FBPase) inhibition, IN VITRO	Fructose-bisphosphatase, inhibition	Liver, rat		IC-50	> 10 µM	Ref. 142
☐ 475319		EGFR (HER1; erbB1) Inhibitors	EGFR (erbB1) inhibition, IN VITRO	Protein-tyrosine kinase (EGF receptor), inhibition	Human enzyme	Fluorescent assay	IC-50	£ 0.100 µM	Pat. 22
☐ 475319		EGFR (HER1; erbB1) Inhibitors	HER2 (erbB2; HER2/neu) inhibition, IN VITRO	Protein-tyrosine kinase (ErbB2/HER2),			IC-50	0.100 - 1.00 µM	Pat. 22

检索结果进行分析：可以按照实验活性、药理学活性、参数、实验材料、实验方法等等

检索结果进行分析：可以按照实验活性、药理学活性、参数、实验材料、实验方法等等

Filter by Statistics

- ▶ **Biomarker**
- ▶ **Experimental Activity**
 - System
 - Activity/Effect
 - Target/Condition/Toxicity
- ▶ **Pharmacological Activity**
- ▶ **Parameter**
- ▶ **Material**
- ▶ **Method**
- ▶ **Reference Type**
- ▶ **Product in Studies**
- ▶ **Drug Mechanism of Action**
- ▶ **Administration Route**
- ▶ **Dose Regimen**
- ▶ **Experimental Model**
 - Species
 - Strain

Filter by Value Range

比较不同化学结构的药理学活性

THOMSON REUTERS
IntegritySM Experimental Pharmacology

Knowledge Areas Quick Search 90 Home Support/Help Query Manager/Alert Center Reports

Records Retrieved 9708 in Experimental Pharmacology

Experimental Pharmacology Search Results

Query > Include Literature Results = Y AND Include Patent Results = Y AND Pharmacological Activity = "Cytotoxicity"

1 2 3 4 5 6 7 8 9 10 [Next>] [Last>>]

Drug Name	Biomarker	Mechanism of Action	Experimental Activity	Pharmacological Activity	Parameter	Value	Details
☐ (+)-2,3,9-Trimethoxypterocarpan		Caspase 3 Activators	Leukemia, acute promyelocytic (M3) remission/reduction, IN VITRO	Cytotoxicity @ 24 h	CC-50	0.100 mM	Ref. 1
☐ (+)-2,3,9-Trimethoxypterocarpan		Caspase 3 Activators	Leukemia, T-cell acute lymphocytic remission/reduction, IN VITRO	Cytotoxicity @ 24 h	CC-50	0.600 mM	Ref. 1
☐ (+)-2,3,9-Trimethoxypterocarpan		Caspase 3 Activators	Digestive/gastrointestinal cancer remission/reduction, IN VITRO	Cytotoxicity @ 24 h	CC-50	0.600 mM	Ref. 1
☐ (+)-2,3,9-Trimethoxypterocarpan		Caspase 3 Activators	Cancer, breast (adenocarcinoma) remission/reduction, IN VITRO	Cytotoxicity @ 24 h	CC-50	0.700 mM	Ref. 1
☐ (+)-2,3,9-Trimethoxypterocarpan		Caspase 3 Activators	Melanoma remission/reduction, IN VITRO	Cytotoxicity @ 24 h	CC-50	2.90 mM	Ref. 1
☐ (+)-9-Isovaleroxylaricresinol			Digestive/gastrointestinal cancer remission/reduction, IN VITRO	Cytotoxicity @ 24 h	CC-50	5.30 µM	Ref. 2
☐ (+)-9-Isovaleroxylaricresinol			Cancer, prostate (adenocarcinoma) remission/reduction, IN VITRO	Cytotoxicity @ 24 h	CC-50	8.10 µM	Ref. 2
☐ (+)-Catechin	Fatty Acid Synthase Inhibitors LDL Antioxidants Nav1.5			Cytotoxicity @ 120 h	CC-50	> 75 µM	Ref. 4

Options

- Export Center
- Integrity Reports
- Structure Activity**
- Information via Quick Search
- Calculate Mean/Median Values
- Unify Parameter to Non-Log Form
- Unify Parameter to Log Form
- Convert Molar Units to Grams
- Convert Grams to Molar Units
- References
- Patents
- Printer Friendly Format

Filter by Statistics

- Biomarker
- Experimental Activity
 - System
 - Activity/Effect
 - Target/Condition/Toxicity
- Pharmacological Activity
- Parameter
- Material
- Method
- Reference Type
- Product in Studies
- Drug Mechanism of Action
- Administration Route
- Dose Regimen

Filter by Value Range

查看SAR及具体的活性数据，指导结构式优化

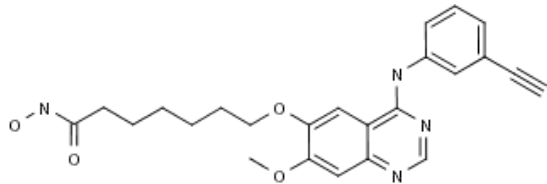
Records Retrieved 1230 in Experimental Pharmacology

Experimental Pharmacology Search Results

Experimental Activity: 5-Hydroxytryptamine Receptors affinity, IN VITRO

Pharmacological Activity: Serotonin 5-HT receptors affinity

Parameter: IC-50

Drug Name & Structure	Mechanism of Action	Material	Value	Details
☐ CUDC-101 	EGFR (HER1; erbB1) Inhibitors Apoptosis Inducers Histone Deacetylase (HDAC) Inhibitors HER2 (erbB2) Inhibitors		> 10 μM	Ref. 2

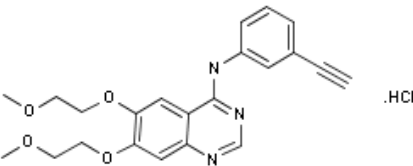
Options

- Export Center
- Experimental Pharmacology Data
- References
- All Related Information via Quick Search
- Printer Friendly Format

Experimental Activity: ABCB1 (P-Glycoprotein, MDR-1) inhibition, IN VITRO

Pharmacological Activity: P-Glycoprotein [MDR1], inhibition

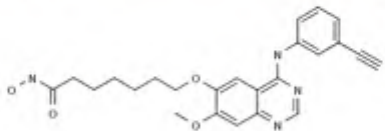
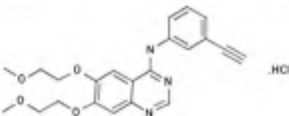
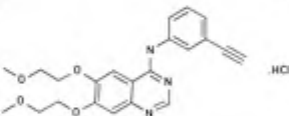
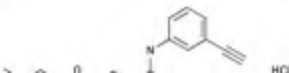
Parameter: IC-50

Drug Name & Structure	Mechanism of Action	Material	Method	Value	Details
☐ Erlotinib hydrochloride 	EGFR (HER1; erbB1) Inhibitors Inhibitors of Signal Transduction Pathways	MDCK Madin-Darby canine kidney epithelial cells (MDR1-overexpressing)	Calcein-AM uptake assay	19.1 $\pm$ 7.22 μM	Ref. 9

Parameter: MIC

方便导出整理好的表格，比较更容易

export(15) - Microsoft Excel

	C	E	F	H	I	L	V
	Parameter	Drug Name	Structure	Mechanism of	Material	String Value	Target/Condition/Toxicity
1	IC-50	CUDC-101		(HER1; erbB1) Inhibitors; osis Inducers; ne Deacetylase) Inhibitors; (erbB2) Inhibitors		> 10 μ M	5-Hydroxytryptamine Receptors
2	IC-50	Erlotinib hydrochloride		EGFR (HER1; erbB1) Inhibitors; Inhibitors of Signal Transduction Pathways	MDCK Madin-Darby canine kidney epithelial cells (MDR1-overexpressing)	19.1 $\pm$ 7.22 μ M	ABCBI (MDR-1)
3	MIC	Erlotinib hydrochloride		EGFR (HER1; erbB1) Inhibitors; Inhibitors of Signal Transduction Pathways	A549 human non-small-cell lung carcinoma cells (paclitaxel-resistant)	1.00 μ M	ADCB1 (MDR-1)
4	MIC	Erlotinib hydrochloride		EGFR (HER1; erbB1) Inhibitors; Inhibitors of Signal Transduction Pathways	DLKP human metastatic lung carcinoma	5.00 μ M	ADCB1 (MDR-1)



快速概览特定领域的研发进展和布局

- 肝癌领域的当前在研药物研发进展和布局
- 结构式检索举例



Integrity结构式检索

The screenshot displays the Thomson Reuters Integrity web interface. On the left, a 'Knowledge Area' sidebar lists various categories: Drugs & Biologics, Targets & Pathways (highlighted), Genomics, Biomarkers, Organic Synthesis, Experimental Pharmacology, Experimental Models, Pharmacokinetics/Metabolism, Clinical Studies, Disease Briefings, Companies & Research Institutions, Literature, and Patents. Below these are specific medical areas like Cardiovascular Disorders, Congenital defects, Critical care medicine, and Dermatological Disorders. The main content area features a 'Quick Search' bar and an 'Advanced Search' section. The 'Advanced Search' section includes a 'Product' section with checkboxes for 'Lead Compounds' and 'Under Active Development', followed by input fields for 'Select Value', 'Optional Value', and 'Optional Value'. Below this is a 'Reference' section with similar input fields. The 'Targets & Pathways' section also has input fields. At the bottom is a 'Patent' section with input fields. On the right side of the 'Advanced Search' section, there is a 'Structure Search' button (highlighted) and a 'Start' button. A red box highlights the text: '除了Genomics/Targets & Pathways 和 Biomarker模块之外，均可结构式检索。点击Structure Search打开结构式检索框'.

除了Genomics/Targets & Pathways 和 Biomarker模块之外，均可结构式检索。点击Structure Search打开结构式检索框

Integrity结构式检索

Knowledge Areas QuickSearch Home Support/Help Query Manager/Alert Center Reports

126618 Records in Patents

Click below to display the most recent patent information for each Condition, updated each Monday

Conditions

- Pain
- Psychiatric Disorders
- Neurological Disorders
- Respiratory Disorders
- Cardiovascular Disorders
- Hematologic Diseases
- Genitourinary Disorders
- Gastrointestinal Disorders
- Nutrition disorders
- Endocrine Disorders
- Infections
- AIDS
- Musculoskeletal and Connective Tissue Disorders
- Immunological Disorders
- Metabolic Diseases
- Cancer
- Other disorders (Systemic disorders)
- All Conditions

► Click here to display today's featured patent family entries in Integrity

Learning center

Combining Chemical Structure and Patent Criteria for Drugs and Biologics

Advanced Search Session History Clear Form Start

Structure Search Options Structure Search

Search Type

- ☒ Substructure
- ☐ Exact Structure
- ☐ Similarity (0-100%) 80

Structure Representation

- ☒ Normal
- ☐ Stereoisomerized

Search Options

- ☐ Match Stereochemistry

[Guide to Structure Search Options](#)

File Edit View Insert Help

H C N O F React Select Erase Paste Undo Redo Zoom

- + P S Cl →

More Br I

ChemAxon Marvin Applet structure drawing tool

You are using the ChemAxon Marvin Applet structure drawing tool.

[Click here to change to another structure editor.](#)

Patent



结构式检索指南



Searches run in *Integrity* on structures drawn with
Symyx Draw, Symyx MDL ISIS/Draw + Symyx MDL Chime, ChemAxon
Marvin Applet, CambridgeSoft CS ChemDraw Plugin

Structure search types

Exact Structure Search

- In the case of exact structure searching, all molecules that are isomorphic with the query are returned.
- Includes exact topology matching: the whole molecular graph must match (Implicit and explicit hydrogens are treated equally.)
- Ignores exact stereo matching: queries allowed.
- Ignores exact atom matching:
 - ExactChargeMatching
 - ExactIsotopeMatching
 - ExactQueryAtomMatching
 - ExactRadicalMatching
- Ignores exact bond matching: queries allowed.

Substructure Search

- Substructure search finds all molecules that contain the query structure as a portion in the molecule.
- Query structures may contain query atoms and bonds.

Similarity Search

- Similarity searching finds molecules that are similar to the query structure.
- The calculation applies the Tanimoto coefficient that has two arguments:
 - the fingerprint (a bit string that contains structural information on the molecule) of the query structure
 - the fingerprint of the molecule in the database

切换结构式检索插件

The screenshot displays the ChemAxon Marvin Applet interface. On the left, a sidebar shows '126618 Records in Patents' and a list of medical conditions including Pain, Psychiatric Disorders, Neurological Disorders, Respiratory Disorders, Cardiovascular Disorders, Hematologic Diseases, Genitourinary Disorders, Gastrointestinal Disorders, Nutrition disorders, Endocrine Disorders, Infections, AIDS, Musculoskeletal and Connective Tissue Disorders, Immunological Disorders, Metabolic Diseases, Cancer, and Other disorders (Systemic disorders). Below this is a 'Learning center' section with a link to 'Combining Chemical Structure and Patent Criteria for Drugs and Biologics'.

The main area is titled 'Advanced Search' and 'Session History'. It features a 'Structure Search Options' panel with the following settings:

- Search Type:** Substructure (selected), Exact Structure, Similarity (0-100%) [80]
- Structure Representation:** Normal (selected), Standardized
- Search Options:** Match (checked), Stereochemistry (unchecked)

A link 'Guide to Structure Search Options' is provided. Below the options is a chemical structure drawing toolbar with menus for File, Edit, View, Insert, and Help. The toolbar includes buttons for H, C, N, O, F, React, Select, Erase, Paste, Undo, Redo, Zoom, and various chemical symbols like P, S, Cl, Br, I, and rings (pentagon, hexagon, benzene, naphthalene). A message box at the bottom states: 'You are using the ChemAxon Marvin Applet structure drawing tool. Click here to change to another structure editor.'



结构式检索插件切换及下载

注：第三种ChemAxon 是基于在线的插件，无需另行下载安装



342725 Records
319553 Records
304895 Records in Drugs & Biologics

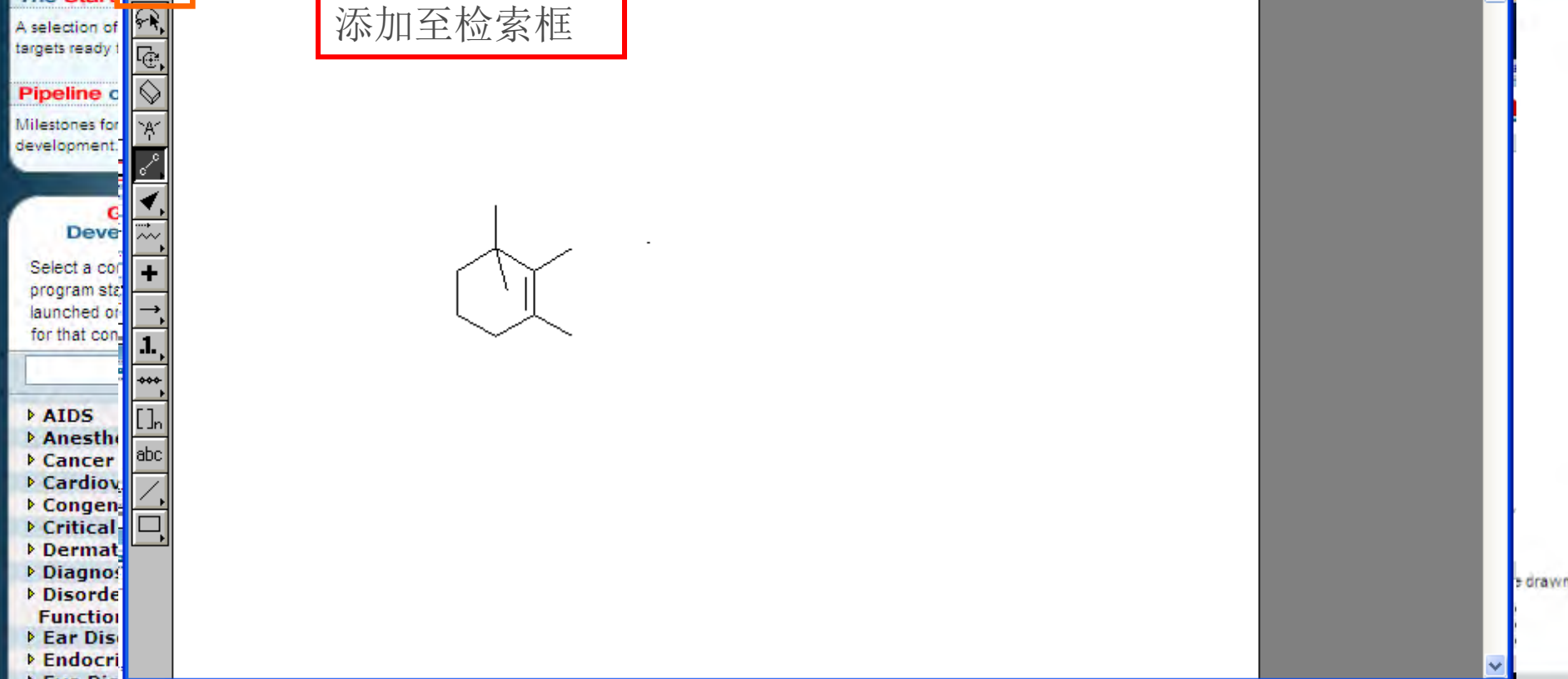
Advanced Search Session History Clear Form Start

ISIS/Draw - [Manual Transfer: Chime, 6 Integrity B.../Plugin]

File Edit Options Object Text Templates Chemistry Window Help



添加至检索框



- AIDS
- Anesthetics
- Cancer
- Cardiovascular
- Congenital
- Critical Care
- Dermatological
- Diagnostic
- Disorders
- Function
- Ear Disorders
- Endocrine
- Eye Disorders
- Gastrointestinal
- Genetic Disorders
- Genitourinary
- Hematological
- Immunological
- Musculoskeletal and Connective Tissue Disorders
- Immunological Disorders
- Metabolic Diseases
- Cancer
- Ear Disorders
- Eye Disorders
- Mouth and Salivary Glands

Product

☐ Lead Compounds ☐ Under Active Development

Select Value

Optional Value

Optional Value

Reference

Index AND

Index AND

Index AND



342725 Records in Drugs & Biologics
319553 Records with chemical structure

The Starting Line

A selection of new molecular entities and targets ready to enter the R&D arena.

Pipeline on the Move

Milestones for drugs under active development.

Gateways to Development Status

Select a condition to generate a program status list for compounds launched or under active development for that condition.

- ▶ AIDS
- ▶ Anesthesia
- ▶ Cancer
- ▶ Cardiovascular Disorders
- ▶ Congenital defects
- ▶ Critical care medicine
- ▶ Dermatological Disorders
- ▶ Diagnostics
- ▶ Disorders of Sexual Function and Reproduction
- ▶ Ear Disorders
- ▶ Endocrine Disorders
- ▶ Eye Disorders
- ▶ Gastrointestinal Disorders
- ▶ Genetic Disorders
- ▶ Genitourinary Disorders
- ▶ Hematologic Diseases
- ▶ Immunological Disorders
- ▶ Infections
- ▶ Metabolic Diseases
- ▶ Mouth and Salivary Glands Disease
- ▶ Musculoskeletal and

Advanced Search

Session History

Structure Search Options

Structure Search

Search Type

☒ Substructure☐ Exact Structure

Structure Representation

☒ Normal☐ Standardized

Search Options

☐ Match☐ Stereochemistry[Guide to Structure Search Options](#)

Select Value

Entry Number
Drug Name
Chemical Name / Description
Standard InChI
Standard InChIKey
CAS Registry No.
Molecular Formula
Molecular Weight
Highest Phase
Year Launched / Registered
Organization
Organization (+ Related Orgs.)
Condition
Therapeutic Group
Mechanism of Action
Product Category
Prescription/Indication Type
New Molecular Entity (Y/N)
Metabolites (Y/N)
Natural Source (Y/N)

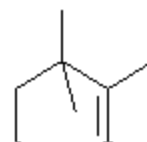
+ Development Status

+ Milestone

+ Natural Source

Last Updated

Available Since



可以与其他条件一起组合检索式

可以是最终产物，也可以是中间体

Double-click in the structure drawing window above to launch Symyx MDL ISIS/Draw. When you have drawn ure, click Transfer to copy the structure into the Integrity Structure Drawing Window.

[Click here to change to another structure editor.](#)

Active Development

Index AND


```

graph LR
    B --> C
    C --> A
    A --> B

```

打开结构式检索

画出结构式，或插入以前保存的结构式，以萆为例

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IntegritySM
Organic Synthesis

Knowledge Areas Quick Search Home Support/Help Query Manager/Alert Center Reports

THOMSON REUTERS
IntegritySM
Organic Synthesis

Knowledge Areas Quick Search go Home Support/Help Query Manager/Alert Center Reports

24033 Records in Organic Synthesis

Advanced Search Session History Clear Form **Start**

Structure Search Options Structure Search

Search Type

- ☒ Substructure
- ☐ Exact Structure
- ☐ Similarity (0-100%)

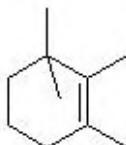
Structure Representation

- ☒ Normal
- ☐ Standardized

Search Options

- ☐ Match Stereochemistry

[Guide to Structure Search Options](#)

CC1=CCCC(C)C1

包含赅子结构为中间体的合成路线298条，调阅终端药物

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Organic Synthesis

Knowledge Areas QuickSearch go Home Support/Help Query Manager / Alert Center Reports

Records Retrieved 1 Record retrieved Options

Schemes Results List: 298 Schemes

Query > Structure Search =

Schemes		
☐	1	(-)-2-(2
☐	1	
☐	1	
☐	2	
☐	1	
☐	1	
☐	2	
☐	2	
☐	1	
☐	1	
☐	1	
☐	1	

☐ Scheme Number 301519-01-a
End Product [\(-\)-2-\(2-Bromohexadecanoyloxy\)acetyl](#)

(I)

DCC

(II)

Filter by Statistics

- Drug Name
- Development Status
- Organization
- Major Therapeutic Group
- Therapeutic Group
- Major Condition
- Condition
- Mechanistic Scope
 - Molecular Mechanism
 - Cellular Mechanism
- Under Active Development / No Development Reported
- Natural Product Y/N

包含帖子结构为中间体的合成路线298条，调阅终端药物

THOMSON REUTERS
IntegritySM Organic Synthesis

Knowledge Areas Quick Search go Home Support/Help Query Manager / Alert Center Reports

Records Retrieved Records 1 to 25 of 113 retrieved

Schemes Results List: 298 Schemes relating to 113 End Products

Query > Structure Search =

Options

- Save Query
- Export Center
- Integrity Reports
- Scheme Full Records
- Intermediate List
- Reagent List
- All Related Information via Quick Search
- Printer Friendly Format

Filter by Statistics

- Drug Name
- Development Status
- Organization
- Major Therapeutic Group
- Therapeutic Group
- Major Condition
- Condition
- Mechanistic Scope
 - Molecular Mechanism
 - Cellular Mechanism
- Under Active Development / No Development Reported
- Natural Product Y/N

	Schemes	End Product	Intermediates	Reagent		
☐	1	(-)-2-(2-Bromohexadecanovl)paclitaxel	2	1		
☐	1	2'-Palmitoylpaclitaxel	2	1		
☐	1		1	2		
☐	2		2	2		
☐	1		3	4		
☐	1	270079	7	4	0	1
☐	2	275579	10	12	0	1
☐	2	275580	9	8	0	1
☐	1	279796	8	8	0	1
☐	1	281066	6	3	0	2
☐	1	286137	4	7	1	1
☐	1	299805	12	18	0	2

2013 APR 10 PM 3:22

查看终端药物

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Organic Synthesis



Knowledge Areas Quick Search go Home Support/Help Query Manager / Alert Center Reports

You have entered the Quick Search feature. Click one of the Knowledge Areas containing results to access a list of the records retrieved by your Quick Search. To be shown which Knowledge Areas contain information related to the Knowledge Area you are in, click the adjacent Related Information icon.

Organic Synthesis

Drugs & Biologics 104 RECORDS 

Biomarkers 0 RECORDS 

Literature 140 RECORDS 

Organic Synthesis 298 RECORDS 

Pharmacokinetics/
Metabolism 0 RECORDS 

Companies & Research
Institutions 0 RECORDS 

Experimental Models 0 RECORDS 

 0 RECORDS **Targets & Pathways**

 0 RECORDS **Genomics**

 **122 RECORDS** **Patents**

 0 RECORDS **Experimental Pharmacology**

 0 RECORDS **Clinical Studies**

 0 RECORDS **Disease Briefings**



使用Filter by查看终端药物所处阶段和所属公司

 **THOMSON REUTERS**
IntegritySM

Drugs & Biologics

Knowledge AreasQuick SearchgoHomeSupport/HelpQuery Manager / Alert CenterReports

Records Retrieved104 in Drugs & Biologics Search ResultsOptions

Drugs & Biologics Search Results12345678910[Next>][Last>>]

Entry Number	Highest Phase	Code Name	Generic Name	Brand Name	Mechanism of Action	Organization
☐ 070003	Launched-1955		Methylprednisolone	Medrol Urbason		Imperial College Jiangsu Province Hospital of TCM Pfizer (Originator) Sanofi Vilnius University
☐ 090214	Phase III	KM-2210	Atrimustine Bestrabucil Busramustine	Kregan	Steroids	Oncolytic Drugs DNA-Damaging Drugs
☐ 090412	Phase III	Win-32729	Epostane			Progesterone Receptor Antagonists Kureha (Originator) Sanofi (Originator)
☐ 090670	Phase II	4-HPR HPR McN-R-1967 NSC-374551 ST-602 SYT-101	Fenretinide		Retinoids	Apoptosis Inducers Retinoid RARbeta Agonists Retinoid RARgamma Agonists Cancer Research UK CerRx Department of Veterans Affairs Janssen Research & Development (Originator) M.D. Anderson Cancer Center National Cancer Institute (NCI) (Originator)

按照终端药物所处阶段进行分析

Filter by Statistics

- Development Status
- Organization
- Major Therapeutic Groups
- Therapeutic Group
- Major Condition Groups
- Condition
- Mechanistic Scope
 - Molecular Mechanisms
 - Cellular Mechanisms
- Major Product Categories
- Product Category
- Launch Year
- Therapeutic Impact and Organization (3D chart)
- Target
- Under Active Development / No Development Reported
- Condition and Phase (3D chart)
- Filter Only Lead Compounds
- Natural Source Categories
- Natural Source Scientific Name
- Prescription/ Indication Type

终端药物所处阶段分析



Export to Excel

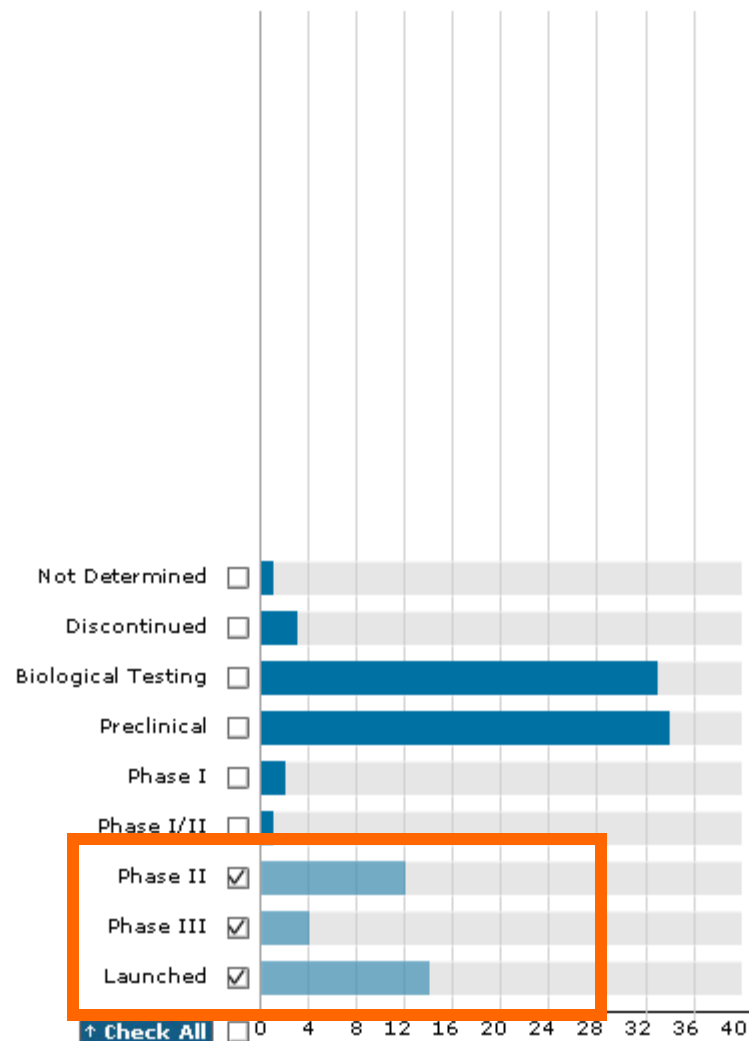


Snapshot Tool

Development Status

Query definition not available for this operation.

...



Display Options



Horizontal Display



Vertical Display



Pie Chart Display



View Subset(s)



Print Chart



Help

分析拥有II期以上临床药物的公司和机构

Records Retrieved

30 in Drugs & Biologics Search Results

Options

Drugs & Biologics Search Results

1 2 3

Entry Number	Highest Phase	Code Name	Generic Name	Brand Name	Mechanism of Action	Organization
☐ 070003	Launched-1955		Methylprednisolone	Medrol Urbason		Imperial College
						Jiangsu Province Hospital of TCM
						Pfizer (Originator)
						Sanofi
						Vilnius University
☐ 090214	Phase III	KM-2210	Atrimustine Bestrabucil Busramustine	Kregan	Steroids	Oncolytic Drugs
☐ 090412	Phase III	Win-32729	Epostane			DNA-Damaging Drugs
☐ 090670	Phase II	4-HPR HPR McN-R-1967 NSC-374551 ST-602 SYT-101	Fenretinide		Retinoids	Apoptosis Inducers Retinoid RARbeta Agonists Retinoid RARgamma Agonists

按照终端药物所属机构进行分析

Filter by Statistics

Development Status

Organization

Major Therapeutic Groups

Therapeutic Group

Major Condition Groups

Condition

Mechanistic Scope

Molecular Mechanisms

Cellular Mechanisms

Major Product Categories

Product Category

Launch Year

Therapeutic Impact and Organization (3D chart)

Target

Under Active Development / No Development Reported

Condition and Phase (3D chart)

Filter Only Lead Compounds

Natural Source Categories

Natural Source Scientific Name

Prescription/ Indication

机构组织分析:

台湾长庚大学; 中科院; 浸会大学
医学技术学院.....



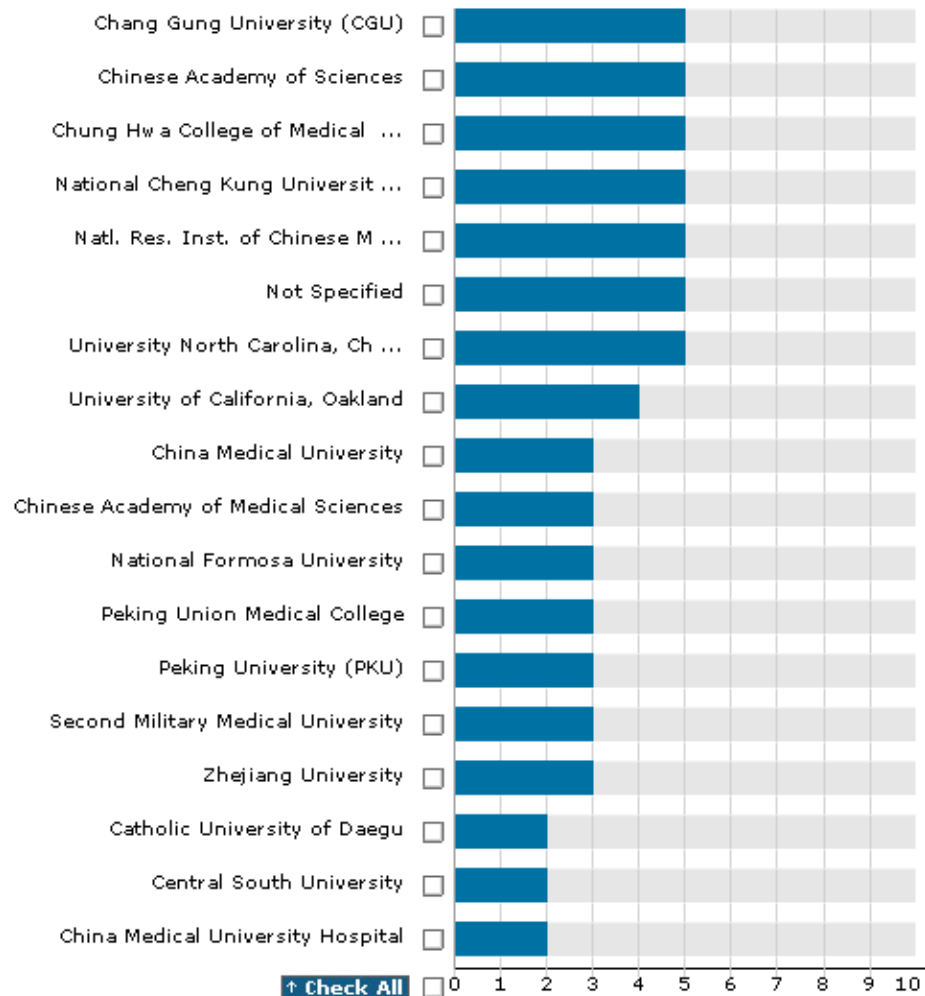
Export to Excel



Snapshot Tool

Organization

Natural Source (Y/N) = Y AND Structure Search =



Display Options



Horizontal
Display



Vertical
Display



Pie Chart
Display



View Subset(s)



Print Chart



Help



提纲

- Thomson Reuters Integrity数据库简介
- Integrity解决如下问题
 - 动态监测新分子实体和新靶标
 - 快速概览特定领域的研发进展和布局
 - 选题立项评估药物品种的综合状况
 - 比较药理学活性进行结构式优化
 - 一站式概览疾病综述和主流药物
 - 设置专属Email跟踪获取更新内容
- Q &A

Disease Briefings 左边直接查看或右边检索

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140 Records in Disease Briefings

Click a specialty below for a list of related Disease Briefings

- ▶ Autoimmune Disorders
- ▶ Biotechnology
- ▶ **Cancer**
- ▶ Cardiovascular Disorders
- ▶ Critical Care Medicine
- ▶ Dermatological Disorders
- ▶ Endocrine Disorders
- ▶ Eye Disorders
- ▶ Gastrointestinal Disorders
- ▶ Genetic Disorders
- ▶ Genitourinary Disorders
- ▶ Hematologic Diseases
- ▶ Immunological Disorders
- ▶ Infections
- ▶ Men's Health
- ▶ Metabolic Diseases
- ▶ Musculoskeletal and
- ▶ Connective Tissue Disorders
- ▶ Neurological Disorders
- ▶ Pain
- ▶ Poisoning
- ▶ Psychiatric Disorders
- ▶ Rare Diseases
- ▶ Reproductive Health
- ▶ Respiratory Disorders
- ▶ Substance Abuse and Dependence
- ▶ Women's Health

Drugs & Biologics

Targets & Pathways

Genomics

Biomarkers

Organic Synthesis

Experimental Pharm

Experimental Mode

Pharmacokinetics/M

Clinical Studies

Disease Briefings

Companies & Rese

Literature

Patents

Advanced Search

Session History

Clear Form

Start

Disease Briefings

Disease Briefing ▶ "Lung Cancer" Index AND ▶

Optional Value ▶ Index AND ▶

Optional Value ▶ Index AND ▶

Product

Structure Search

☐ Lead Compounds ☐ Under Active Development

Select Value ▶ Index AND ▶

Optional Value ▶ Index AND ▶

Optional Value ▶ Index AND ▶

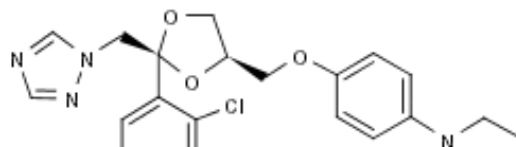
药物报告直接链接查看疾病综述

Records Retrieved	1 in Drugs & Biologics	Options
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Drugs & Biologics Search Results

1

☐ Entry Number	90519	UPDATES	Chemical Structure	STRUCTURE FEATURES
Record Creation Date	Jun 13, 2002			
Last Updated Date	Apr 06, 2013			
CAS Registry No.	84625-61-6			
Molecular Formula	C ₃₅ H ₃₈ Cl ₂ N ₈ O ₄			
Molecular Weight	614.63			
Highest Physicochemical Property	Records Retrieved 7 Record(s) Retrieved			
Physical Properties				



Under Active Development	Disease Briefing	Related Products
	Lung Cancer	Display Related Products (262)
	Current Lung Cancer Pipeline	
	Angiogenesis Inhibitors	
	Agents Targeting Signal Transduction Pathways	
	Prostate Cancer	Display Related Products (230)
	Angiogenesis Inhibitors	
	Signal Transduction Modulators	
	Current Prostate Cancer Pipeline	
	Fungal Infections: Dermatomycoses	Display Related Products (39)
	Treatment	
	Fungal Infections: Candidiasis	Display Related Products (34)
	Treatment	
	Fungal Infections: Aspergillosis	Display Related Products (10)
	Treatment	
	Fungal Infections: Endemic Mycoses	Display Related Products (11)
	Treatment	
	Fungal Infections: Cryptococcosis	Display Related Products (10)
	Treatment	

JK-1211

Itraconazole (BAN; USAN; Rec INN)

Canadiol



了解疾病研发历史、重要靶标、主流药物、治疗方法等，申请基金或课题时作为课题背景信息来源

• 肺癌的流行病学数据

Lung Cancer

Facts about Lung Cancer

- Classification
- Risk Factors
- Epidemiology
- Morbidity and Mortality
- Cost

Diagnosis

Prevention

Epidemiology

According to the International Agency for Research on Cancer's GLOBOCAN 2008 database, lung cancer is the most important cancer in the world today, both in terms of the total number of individuals it affects (1.6 million new cases in 2008) and the total number of resulting deaths (1.4 million in 2008) (Jemal, A. et al., 2011). The mortality-to-incidence ratio for lung cancer is extraordinarily high: 0.87. Lung cancer is the most common type of cancer among men worldwide, with an incidence rate of 35.5 per 100,000. It is less common among women, for whom the global incidence is 12.1 per 100,000.

Cancer Cases by Site and Gender (Animated Chart)

2008年，全球新增160万肺癌病例，140万死亡病例，死亡-发病比率高达0.87。肺癌已经成为当今世界最重要的癌症。2008年，新增病例发展

Cost

According to the U.S. National Institutes of Health, the cumulative national healthcare costs associated with lung cancer care in 2010 totaled USD 12.12 billion. By 2020, this figure is predicted to reach USD 14.73 billion (Mariotto, A.B. et al., 2011).

A study was conducted to more precisely determine the economic burden associated with lung cancer. A database containing financial information on inpatient, outpatient and drug claims for a large number of individuals was analyzed and costs incurred by lung cancer patients were compared to those for controls with no cancer. Lung cancer patients consistently made greater use of health care services and incurred greater costs in concept of outpatient visits, emergency room visits, laboratory and radiology services and pharmaceuticals as compared to controls. The monthly total cost for each lung cancer patient was calculated to be USD 6,520, as compared to USD 339 for controls. Over the study period, which began at time of diagnosis and lasted until time of death or for a maximum of 10 years, total healthcare costs incurred were USD 45,897 per lung cancer patient, as compared to USD 2,907 per healthy control. Treatment costs were significantly higher among patients who failed on initial treatment, underlining the importance of effective first-line therapy (Kutikova, L. et al., 2005). A Spanish study has similarly calculated the per-patient costs associated with non-small cell lung cancer in that country. For patients with advanced or metastatic NSCLC, total cost from start of therapy to death ranged from EUR 11,300 to EUR 32,750, depending upon the treatment regimen employed (Isla, D. et al., 2011).

Related

- Drugs & Biologics (42)
- Literature (390)

common among European men than women, and the highest rates are registered in Hungary, Poland, Czechia, Belgium, the Netherlands, Luxembourg, Italy, Denmark and Greece (O'Connor, S.J., 2011). In the U.K., 40,405 cases of lung cancer were reported in 2010; 86% of these were directly attributable to tobacco smoke (Parkin, D.M., 2011).

深入研究疾病相关靶标通路，指导药物开发和设计

- 与肺癌治疗相关的代谢通路和重要靶点

5-Lipoxygenase

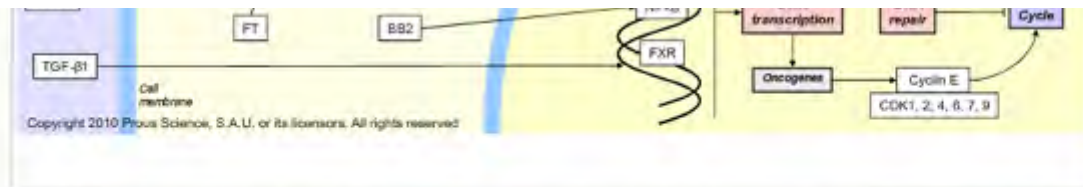
5-Lipoxygenase is an enzyme that catalyzes the first step in the conversion of arachidonic acid (AA) into leukotrienes (LTs), which primarily act as mediators of inflammatory and allergic reactions. 5-Lipoxygenase activity is regulated in a complex manner and involves different signaling pathways. It can be activated by an increase in intracellular Ca^{2+} concentration, diacylglycerols, phosphorylation by MAPKAP kinase-2 and ERK, while protein kinase A and glutathione peroxidase have been found to suppress its function. 5-Lipoxygenase inhibitors, which block the synthesis of hydroperoxide acid, 5-HPETE and subsequent synthesis of leukotrienes, may be effective in the management of COPD, atherosclerosis, cancer and rheumatoid arthritis (Loetzer, K. et al., 2005; Rådmark, O. and Samuelsson, B., 2005; Werz, O. and Steinhilber, D., 2005).

Arachidonic Acid Metabolism: Lipoxygenase/Cyclooxygenase Pathways (Animation + Audio)



[Enlarge](#)

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Lung Cancer targetscape. A diagram showing an overall cellular and molecular landscape or comprehensive network of connections among the current therapeutic targets for the treatment of lung cancer and their biological actions. Arrow: positive effect; dash: negative effect. Gray or lighter symbols are targets that are not validated (i.e., targets not associated with a product that is currently under active development for lung cancer).

治疗肺癌主流药物，主要机构/公司

Records Retrieved 264 in Drugs & Biologics Search Results

Options

Keep Me Posted 9 10 [Next>] [Last>>]

Export Center

Integrity Reports

Products related to Disease Briefing 43 - Lung Cancer

Entry Number	Highest Phase	Code Name	Generic Name	Brand Name	Product Category	Organization
090519	Launched-1988	JK-1211 R-51211	Itraconazole (BAN; USAN; Rec INN)	Canadiol Hyphanox	Triazoles	Janssen (Originator)

Drugs & Biologics

Drugs & Biologics 264 RECORDS RELATED INFO RELATED INFO 201 RECORDS Targets & Pathways

Records Retrieved 450 in Companies & Research Institutions

Options

Companies & Research Institutions Search Results 1 2 3 4 5 6 7 8 9 10 [Next>] [Last>>]

	Organization	Website	Year	Annual Sales (M)
☐	A&G Pharmaceutical	www.agrx.net		
☐	APT Pharmaceuticals	www.aptbio.com		
☐	AVEO Pharma (d/b/a AVEO Oncology)	www.aveooncology.com		
☐	AbbVie	www.abbvie.com	2011	USD 17444
☐	Abbott	www.abbott.com	2011	USD 21407
☐	Ability Pharmaceuticals	www.abilitypharma.com		
☐	Acrostak	www.acrostak.com		
☐	Acusphere	www.acusphere.com		
☐	Aduro BioTech	www.adurobiotech.com		
☐	Advanomics	www.advanomics.com		
☐	Advenschen Laboratories	www.advenschen.com		

Organic Synthesis

Pharmacokinetics Metabolism

Companies & Research Institutions

Experimental

肺癌的各种指南

IntegritySM Disease Briefings

Knowledge Areas Quick Search Home Support/Help Query Manager/Alert Center Reports

Lung Cancer

Links to Guidelines

- Facts about Lung Cancer
- Diagnosis
- Prevention
- Treatment
- Targets for Therapeutic Intervention
- Latest Headlines
- Glossary of Terms

Links

- Links to Related Websites
- Links to Selected Publications
- Links to Guidelines

Related Info

- Drugs & Biologics (290)
- Literature (201)

Print Full Document

Diagnosis and management of lung cancer: American College of Chest Physicians evidence-based clinical practice guidelines (3rd Edition) (American College of Chest Physicians, May 2013)
<http://journal.publications.chestnet.org/issue.aspx?journalid=99&issueid=926876>

American Cancer Society lung cancer screening guidelines (American Cancer Society, 2013)
<http://onlinelibrary.wiley.com/doi/10.3322/caac.21172/pdf>

Cancer screening in the United States, 2013: A review of current American Cancer Society guidelines, current issues in cancer screening, and new guidance on cervical cancer screening and lung cancer screening
<http://onlinelibrary.wiley.com/doi/10.3322/caac.21174/pdf>

Guideline on the evaluation of anticancer medicinal products
http://www.ema.europa.eu/docs/en_GB/document_library/5/uideline/2013/01/WC500137128.pdf

Providing guidance for lung cancer screening: The American Association, April 2012)
<http://www.lung.org/finding-cures/research-news/new-screening-guidelines/lung-cancer-screening.pdf>

Metastatic non-small-cell lung cancer; ESMO clinical practice Medical Oncology, 2012)
http://annonc.oxfordjournals.org/content/23/suppl_7/vii56.full.pdf+html

Guidance for industry: Clinical trial endpoints for the approval of drugs for the treatment of lung cancer (FDA, June 2011)
<http://www.fda.gov/downloads/Drugs/GuidanceComplianceInformation/Guidances/UCM259421.pdf>

Lung cancer: The diagnosis and treatment of lung cancer (NICE, 2011)
<http://www.nice.org.uk/nicemedia/live/13465/54202/54202.pdf>

NCCN clinical practice guidelines in oncology: Small cell lung cancer (National Cancer Institute, 2011)
<http://www.nccn.org/content/9/10/1086.full.pdf+html>

2011 focused update of 2009 American Society of Clinical Oncology non-small-cell lung cancer (American Society of Clinical Oncology, 2011)
<http://jco.ascopubs.org/content/29/28/3825.full>

Early stage and locally advanced (non-metastatic) non-small-cell lung cancer (European Society for Medical Oncology, 2010)
http://annonc.oxfordjournals.org/content/21/suppl_5/v103.full.pdf+html

CHEST JOURNAL
Official Publication of the American College of Chest Physicians

May 2013; 143(5_suppl) Diagnosis and Management of Lung Cancer, 3rd ed: American College of Chest Physicians Evidence-Based Clinical Practice Guidelines

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Diagnosis and Management of Lung Cancer, 3rd ed: American College of Chest Physicians Evidence-Based Clinical Practice Guidelines

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精选的肺癌相关的公开信息

The screenshot displays the Thomson Reuters Integrity website interface. The top navigation bar includes the 'Integrity' logo, 'Disease Briefings' title, and a search bar. Below the navigation bar, the 'Knowledge Areas' section is active, showing a list of topics on the left and a list of links to selected publications on the right. The 'Lung Cancer' topic is selected, and its sub-topics are listed: Facts about Lung Cancer, Diagnosis, Prevention, Treatment, Targets for Therapeutic Intervention, Latest Headlines, and Glossary of Terms. The 'Links' section is expanded, showing 'Links to Related Websites', 'Links to Selected Publications' (highlighted with a red box), and 'Links to Guidelines'. The 'Related Info' section lists 'Drugs & Biologics (290)' and 'Literature (201)'. The 'Print Full Document' button is visible at the bottom left. The right side of the page displays a list of links to selected publications, including 'Breathing in America: Diseases, progress, and hope (American Thoracic Society, 2010)', 'Cancer facts & figures 2010 (American Cancer Society)', 'Cancer facts & figures 2011 (American Cancer Society)', 'Cancer facts & figures 2012 (American Cancer Society)', 'Cancer facts & figures 2013 (American Cancer Society)', 'ecancer (open access cancer journal from the European Institute of Oncology)', 'Estimated prevalence and incidence of lung disease (American Lung Association, April 2013)', 'Food, Nutrition and the Prevention of Cancer: A Global Perspective', 'Global Cancer Facts & Figures 2007 (American Cancer Society, 2007)', 'Lung cancer (PDQ®): Prevention', and 'Lung cancer (PDQ®): Screening'.

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Disease Briefings

Knowledge Areas QuickSearch

Home Support/Help Query Manager/Alert Center Reports

Lung Cancer

Links to Selected Publications

Facts about Lung Cancer

Diagnosis

Prevention

Treatment

Targets for Therapeutic Intervention

Latest Headlines

Glossary of Terms

Links

- Links to Related Websites
- Links to Selected Publications
- Links to Guidelines

Related Info

- Drugs & Biologics (290)
- Literature (201)

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Breathing in America: Diseases, progress, and hope (American Thoracic Society, 2010)
<http://www.thoracic.org/education/breathing-in-america.pdf>

Cancer facts & figures 2010 (American Cancer Society)
<http://www.cancer.org/acs/groups/content/@epidemiologysurveillance/documents/document/acspc-026238.pdf>

Cancer facts & figures 2011 (American Cancer Society)
<http://www.cancer.org/Research/CancerFactsFigures/CancerFactsFigures/cancer-facts-figures-2011>

Cancer facts & figures 2012 (American Cancer Society)
<http://www.cancer.org/acs/groups/content/@epidemiologysurveillance/documents/document/acspc-031941.pdf>

Cancer facts & figures 2013 (American Cancer Society)
<http://www.cancer.org/acs/groups/content/@epidemiologysurveillance/documents/document/acspc-036845.pdf>

ecancer (open access cancer journal from the European Institute of Oncology)
<http://ecancer.org/>

Estimated prevalence and incidence of lung disease (American Lung Association, April 2013)
<http://www.lung.org/finding-cures/our-research/trend-reports/estimated-prevalence.pdf>

Food, Nutrition and the Prevention of Cancer: A Global Perspective
<http://www.dietandcancerreport.org>

Global Cancer Facts & Figures 2007 (American Cancer Society, 2007)
<http://www.cancer.org/acs/groups/content/@nho/documents/document/globalfactsandfigures2007rev2p.pdf>

Lung cancer (PDQ®): Prevention
<http://www.cancer.gov/cancertopics/pdq/prevention/lung/HealthProfessional>

Lung cancer (PDQ®): Screening
<http://www.cancer.gov/cancertopics/pdq/screening/lung/HealthProfessional>

提纲

- Thomson Reuters Integrity数据库简介
- Integrity解决如下问题
 - 动态监测新分子实体和新靶标
 - 快速概览特定领域的研发进展和布局
 - 选题立项评估药物品种的综合状况
 - 比较药理学活性进行结构式优化
 - 一站式概览疾病综述和主流药物
 - 设置专属Email跟踪获取更新内容
- Q &A

基于检索式的跟踪，跟踪符合条件的新记录

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IntegritySM

Drugs & Biologics

Knowledge Areas

Quick Search

go

Home

Support/Help

Query Manager/Alert Center

Reports

342725 Records in Drugs & Biologics
319553 Records with chemical structure

The Starting Line
A selection of new molecular entities and targets ready to enter the R&D arena.

Pipeline on the Move
Milestones for drugs under active development.

Gateways to Development Status
Select a condition to generate a program status list for compounds launched or under active development for that condition.

- ▶ AIDS
- ▶ Anesthesia
- ▶ Cancer
- ▶ Cardiovascular Disorders
- ▶ Congenital defects
- ▶ Critical care medicine
- ▶ Dermatological Disorders
- ▶ Diagnostics
- ▶ Disorders of Sexual

Advanced Search **Session History**

Product

☐ **Lead Compounds** ☐ **Under Active Development**

Natural Source (Y/N)

Y

Index AND ▶

Condition

"Cardiovascular Disorders"

Index AND ▶

Metabolites (Y/N)

Index AND ▶

Reference

Select Value

Index AND ▶

Optional Value

Index AND ▶

Optional Value

Index AND ▶

Targets & Pathways

Select Value

Index AND ▶

Optional Value

Index AND ▶

Optional Value

Index AND ▶

Patent

Select Value

Index AND ▶

Optional Value

Index AND ▶

Optional Value

Index AND ▶

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345 in Drugs & Biologics Search Results

Query > Natural Source (Y/N) = y AND Condition = "Can"

Save Query

To save your query, enter a Query Name and Description and click Save Query.

A daily, weekly or monthly e-mail alert can be set up to notify you when new records are obtained with this query.

To set up an Alert, enter a Query Name and Description, click the Optional e-mail alert down arrow to choose a daily, weekly or monthly alert frequency, and then click Save Query.

When new records are obtained by this query, you will receive notification by e-mail.

Query Name: Cardiovascular natural drugs

Description: ndition = "Cardiovascular Disorders"

Optional e-mail alert: Never, Daily, Weekly (sent Sat.), Every 4 weeks (sent Sun.)

Save Query

[University of Hong Kong \(Originator\)](#)

[Huazhong University of](#)

- ▶ Development Status
- ▶ Organization
- ▶ Major Therapeutic Groups
- ▶ Therapeutic Group
- ▶ Major Condition Groups
- ▶ Condition
- ▶ Mechanistic Scope
 - ▶ Molecular Mechanisms
 - ▶ Cellular Mechanisms
- ▶ Major Product Categories
- ▶ Product Category
- ▶ Launch Year
- ▶ Therapeutic Impact and Organization (3D chart)
- ▶ Target
- ▶ Under Active Development / No Development Reported
- ▶ Condition and Phase (3D chart)
- ▶ Filter Only Lead Compound
- ▶ Natural Source Categories
- ▶ Natural Source Scientific Name
- ▶ Prescription/ Indication Type
- ▶ Administration Route

基于检索结果的跟踪，跟踪某些记录的最新变化

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Drugs & Biologics

Knowledge Areas

Quick Search

Home Support/Help Query Manager/Alert Center Reports

Records Retrieved345 in Drugs & Biologics Search Results

Drugs & Biologics Search Results

Query > Natural Source (Y/N) = y AND Condition = "Cardiovascular Disorders"

Options

Save Query

Keep Me Posted

Export Center

Integrity Reports

Full Records

Product List with Structures

Display Milestones

Gateways to Product Development Status

References

Patents

All Related Information via Quick Search

Printer Friendly Format

Entry Number	Highest Phase	Code Name	Generic Name	Brand Name	Product Category	Therapeutic Group	Organization
☒ 070266	Biological Testing	RES-1149-2				Antineoplastic Antihypertension, Treatment of	Iowa Hakko
☒ 070274	Launched	MPC-004	Colchicine	Colcrys Colstat		Antibiotics and Anticardiovascular Diseases (Not Specified) Hematologic Disorders, Treatment of Gout	Abbott Laboratories
☒ 090168	Preclinical	BDPH-NSC-325307	Butylidenephthalide Ligusticum lactone			Angina pectoris, Treatment of Smooth Muscle Relaxants	Gamma-Aldrich
☐ 090703	Preclinical	FF-0019 NSC-77037	Hanfangchin A Tetrandrine d-Tetrandrine		Alkaloids	Antidiabetic Drugs Antimalarials Colorectal Cancer Therapy Hypertension, Treatment of Multidrug Resistance Modulators Oncolytic Drugs	Chinese Academy of Medical Sciences (Originator) Shen Hua (Originator) Henia Hope International Cancer Institute
☐ 090892	Preclinical	GFA	Guan-Fu base A Guanfu base A			Antiarrhythmic Drugs	Shanghai Institute of Materia Medica (SIMM) (Originator)
☐	Preclinical		Dehydrosynephrine		Alkaloids	Cognition Disorders Anesthetics	Chinova

Filter by Statistics

Development Status

Organization

Major Therapeutic Groups

Therapeutic Group

Major Condition Groups

Condition

Mechanistic Scope

Molecular Mechanisms

Cellular Mechanisms

Major Product Categories

Product Category

Launch Year

Therapeutic Impact and Organization (3D chart)

Target

Under Active Development / No Development Reported

Condition and Phase (3D chart)

Filter Only Lead Compound

Natural Source Categories

Natural Source Scientific Name

Save Query - Windows Internet Explorer

https://integrity.thomson-pharma.com/integrity/xmlxsl/record_updates_ui_pkg.ne

Use the Keep Me Posted utility of Integrity to be advised by e-mail when changes occur to a set of records.

Enter an Alert Name and Description and select the field or fields to be monitored for change. Optional e-mail alert down arrow to choose a daily, weekly or monthly alert frequency, and then Create Alert.

When a change occurs in a selected field for any record in the set, you will receive notification by e-mail.

Alert Name: Cardiovascular drugs alert

Description:

Changes monitored:

☒ Updated Highest Phase Field	☒ New / Updated Structure
☐ Updated "Under Active Development" Flag	☐ New Chemical Name
☐ New CAS Registry Number	☐ New Product Name
☒ New Mechanism of Action	☐ New Therapeutic Group
☒ New Condition	☐ New Organization
☐ Development Status Table Newly Available	☐ Milestone History Newly Available
☒ New Milestone	☐ New Related Patent Family
☐ New Related Reference	

Optional e-mail alert:

- Never
- Daily
- Weekly (sent Sat.)
- Every 4 weeks (sent Sun.)

Create Alert Cancel

该药物的最新研发状态的改变；新的治疗领域的发现；新的研究机构的介入；新的专利的产生等等



特定报告中设置跟踪：Options-Keep me posted

THOMSON REUTERS Integrity & Biologics

Knowledge Areas

Records Retrieved 1 in Dr

Drugs & Biologics Search Results

☒ Entry Number 162288 UPDA

CAS Registry No. 124750-99-8
114798-26-4

Molecular Formula C22H22ClN6

Molecular Weight 461.001

Highest Phase Launched - 19

Physical Properties White crystals

Under Active Development

Chemical Name/Description
5-[4'-(2-Butyl-4-chloro-5-(hydroxymethyl)-2-Butyl-4-chloro-5-(hydroxymethyl)-

Standard InChI
1S/C22H22ClN6O.K/c1-2-3-8-20-24-21(23)14H2,1H3;/q-1;+1

Standard InChIKey
OXCMYAYHXIHQQA-UHFFFAOYSA-N

Code Name
DuP-753

Generic Name
Losartan potassium

Brand Name
Covance

SALES

Record Update Alert

Use the Keep Me Posted utility of Integrity to be advised by e-mail when changes occur to a record or set of records.

Enter an Alert Name and Description and select the field or fields to be monitored for changes. Click the Optional e-mail alert down arrow to choose a daily, weekly or monthly alert frequency, and then click Create Alert.

When a change occurs in a selected field for any record in the set, you will receive notification by e-mail.

Alert Name

Description

Changes monitored

- ☐ Updated Highest Phase Field
- ☐ Updated "Under Active Development" Flag
- ☐ New CAS Registry Number
- ☐ New Mechanism of Action
- ☐ New Condition
- ☐ Development Status Table Newly Available
- ☐ New Milestone
- ☐ New Related Reference
- ☐ New / Updated Structure
- ☐ New Chemical Name
- ☐ New Product Name
- ☐ New Therapeutic Group
- ☐ New Organization
- ☐ Milestone History Newly Available
- ☐ New Related Patent Family

完成

Internet 100%

Filter by Statistics

- Development Status
- Organization
- Major Therapeutic Groups
- Therapeutic Group
- Major Condition Groups
- Condition
- Mechanistic Scope
 - Molecular Mechanisms
 - Cellular Mechanisms
- Major Product Categories
- Product Category
- Launch Year
- Therapeutic Impact and Organization (3D chart)
- Target
- Under Active Development / No Development Reported
- Condition and Phase (3D chart)
- Filter Only Lead Compound
- Natural Source Categories



Records Retrieved

345 in Drugs & Biologics Search Results

Options

Query Manager - Windows Internet Explorer

https://integrity.thomson-pharma.com/integrity/xmlxsl/alert_center_ui_pkg.alertCenterForm

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IntegritySM Query Manager/Alert Center

Entry Number

07026

07027

09016

09070

09089

09095

09096

Saved Queries Keep Me Posted Controlled Vocabulary Session History Filter VIEW ALL

Alert Set	Query Name	Description	Knowledge Area	Last Performed	
☐	Alzheimer	all	Drugs & Biologics	Sep 27, 2009	options
☐	2-Chlorobenzonitrile	Lianhe Chemical	Organic Synthesis	May 07, 2009	options
☐	0-dichlorobenzonitrile		Drugs & Biologics	Jun 05, 2009	options
☐	Gefitinib(Structure search)		Drugs & Biologics	Jun 09, 2009	options
☐	Structure1		Organic Synthesis	Jun 19, 2009	options
☐	Structure 2		Organic Synthesis	Jun 19, 2009	options
☐	Clinical Search	Condition = "Cardiovascular Disorders" AND Natural Source (Y/N) = y	Clinical Studies	Mar 20, 2011	options
☐	Drug Substances patents	Subject Matters = "Drug Substances" AND Phase = "Launched"	Patents	Mar 20, 2011	options
☐	Pharmacology Search	Include Literature Results = Y AND Include Patent Results = Y AND Experimental Activity = "1-Deoxy-D-Xylulose-5-Phosphat	Experimental Pharmacology	Mar 20, 2011	options
☒	EGFR drugs	Name = "EGFR variant 1" or "EGFR variant c" or "EGFR-RS" or "EGFR2" or "EGFR3" or "EGFR4" Mar 20, 2011 1342	Drugs & Biologics	Mar 20, 2011	Execute Delete Edit View Details

- or by Statistics
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- utic Group
- ndition Groups
- n
- stic Scope
- lar Mechanisms
- or Mechanisms
- oduct Categories
- Category
- Year
- utic Impact and
- ation (3D chart)
- ctive Development
- velopment
- n and Phase
- t)
- ly Lead Compound
- Source Categories
- Source Scientific
- tion/ Indication
- tration Route

Query Manager - Windows Internet Explorer

https://integrity.thomson-pharma.com/integrity/xmlxsl/alert_center_ui_pkg.alertCenterForm?p_pestania=3&p_page=1

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IntegritySM Query Manager/Alert

最近24小时内的检索历史

Session History

Knowledge Area	Query Conditions	Last Performed	Results	
Drugs & Biologics	Natural Source (Y/II) = y AND Condition = "Cardiovascular Disorders"	Mar 20, 2011	345	options ▾
Drugs & Biologics	Structure Search =	Mar 20, 2011	1693	options ▾
Quick Search	304079	Mar 20, 2011	1	options ▾
Quick Search	I036	Mar 20, 2011	533	options ▾
Quick Search	I036	Mar 20, 2011	533	options ▾
Patents	Subject Matters = "Drug Substances" AND Phase = "Launched"	Mar 20, 2011	885	options ▾
Quick Search	EGFR	Mar 20, 2011	8733	options ▾
Drugs & Biologics	Name = "EGFR variant 1" or "EGFR variant c" or "EGFR-RS" or "EGFR2" or "EGFR3" or "EGFR4"	Mar 20, 2011	1342	options ▾
Targets & Pathways	Condition = "Cardiovascular Disorders"	Mar 20, 2011	879	options ▾
Quick Search	caco-2/efflux	Mar 20, 2011	2	options ▾

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提纲

- Thomson Reuters Integrity数据库简介
- Integrity解决如下问题
 - 动态监测新分子实体和新靶标
 - 快速概览特定领域的研发进展和布局
 - 选题立项评估药物品种的综合状况
 - 比较药理学活性进行结构式优化
 - 一站式概览疾病综述和主流药物
 - 设置专属Email跟踪获取更新内容
- Q &A

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The Price of Doing Business – How Will GDUFA Change the API Industry



23 SEP 2013
Michael Glessner

Michael Glessner, Pharmaceutical Research Analyst at Thomson Reuters, discusses how the introduction of the Generic Drug User Fee Act (GDUFA) will influence the API industry and how long these changes are likely to take to come into effect.

One-Time Fee

On Oct. 1, 2012, the U. S. Food and Drug Administration (FDA) implemented the long-discussed GDUFA, authorizing the agency to collect fees from any manufacturers worldwide who wish for their active pharmaceutical ingredients (APIs) to be eligible for use in generic drugs sold in the U. S.

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谢 谢 !

张慧

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