

药物信息免费资源推介

疫情无情，服务有情！图书馆为更好满足我校师生“停课不停学”的需求，继续为大家寻找免费的电子资源，本期着重推荐药物信息免费资源。资源使用过程中如遇问题，请拨打电话 029-（84）774758。

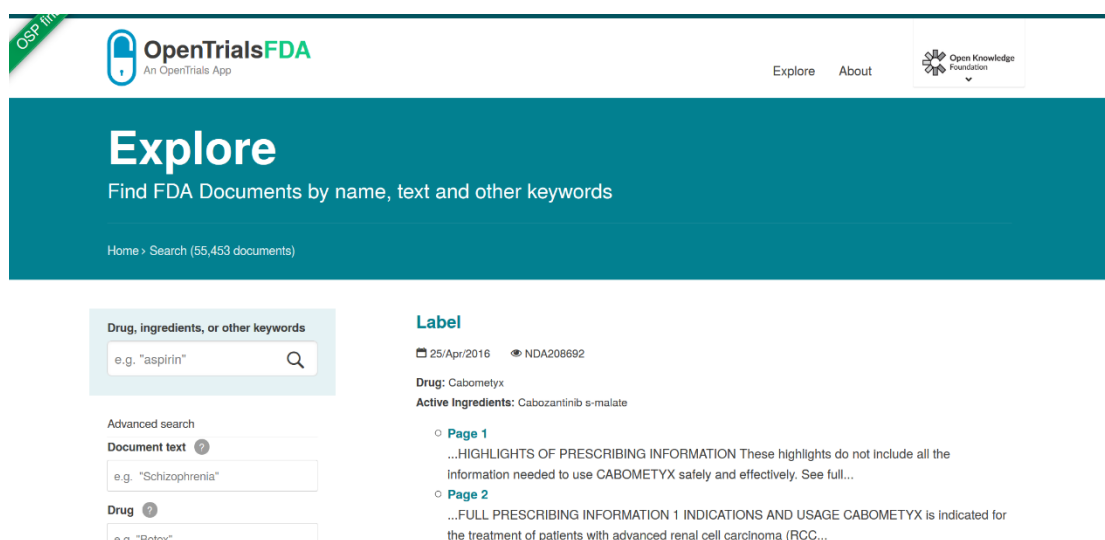
一. 国外药物信息平台

1. 美国食品和药物管理局(FDA)药物信息平台

(1) OpenTrialsFDA

OpenTrialsFDA 致力于使来自美国食品和药物管理局(The US Food and Drug Administration, FDA)的临床试验数据更容易获取和搜索。OpenTrialsFDA 从 FDA 发布的药品批准包 (Drug Approval Packages) 中提取相关数据，并可链接到其他临床试验数据，任何用户都可以输入药物名称，查看 FDA 文档中提到该药物的所有文档。目前，该平台提供 55,453 份文档可供查阅。

网址: <https://fda.opentrials.net/search>

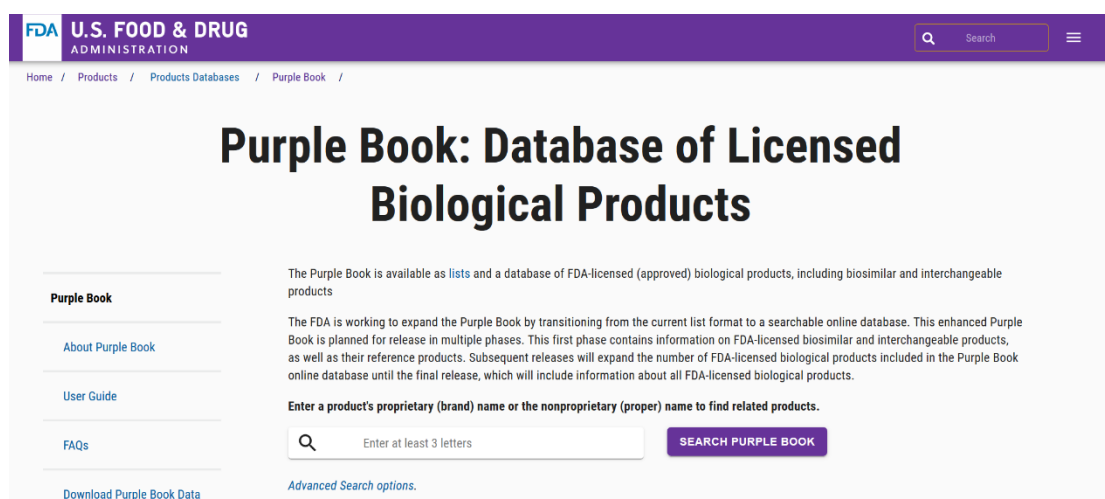


(2) 《FDA 批准的生物制品数据库》(Purple Book 紫皮书)

2020 年 2 月 24 日，美国食品和药物管理局 (FDA) 发布《FDA 批准的生物制品数据库》(Purple Book 紫皮书)，其目的是为进一步改善生物类似药的透

明度，促进生物类似药的使用和开发。紫皮书扩展和数字化目的是使人们更容易获得有关 FDA 许可生物制品的更多信息，为患者和消费者提供简单搜索，为处方者提供高级检索，为研究人员和企业代表提供更多的技术信息。进一步促进现有生物类似药的接受和使用，以及新生物类似药的开发，从而降低患者的治疗费用，并且更容易获得安全、有效、高质量的药物。（生物类似是指生物制品与参比制剂高度相似，尽管在临床非活性成分方面存在微小差异，但其与参比制剂在安全性、纯度和有效性方面在临床上无显著差异）

网址：<https://purplebooksearch.fda.gov/>



（3）《经过治疗等效性评价批准的药品》（FDA Orange Book 橙皮书）

《经过治疗等效性评价批准的药品》（Approved Drug Products with Therapeutic Equivalence Evaluations），简称 Orange Book 橙皮书，收录的是美国 FDA 根据《联邦食品药品化妆品法案》，基于安全性与有效性原则而批准上市的药物，其中明确列出新药所涉及的所有专利以及市场专营保护信息。通过该数据库，可查询 FDA 批准的药品审批注册信息及相关文件、专利数据、市场保护等。从药品批准到列入橙皮书，一般有三周的滞后时间。

网址：<https://www.accessdata.fda.gov/scripts/cder/ob/index.cfm>

U.S. FOOD & DRUG ADMINISTRATION

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Search FDA

Home > Drug Databases > Orange Book Home

Orange Book: Approved Drug Products with Therapeutic Equivalence Evaluations

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On March 23, 2020, FDA removed from the Orange Book the listings for "biological products" that have been approved in applications under section 505 of the FD&C Act because these products are no longer "listed drugs" (see section 7002(e)(4) of the Biologics Price Competition and Innovation Act of 2009).

[Additional information and resources for the Orange Book](#)

We've updated our mobile app! Download Orange Book Express 2.0

Find Approved Drugs

▼ Search by Proprietary Name, Active Ingredient or Application Number

Enter at least 3 characters Search

► Search by Applicant (Company)

► Search by Dosage Form (for example: TABLET)

► Search by Route of Administration (for example: ORAL)

Find Patent Information

► Search by Patent Number

► View Newly Added Patents or Delisted Patents

（4）美国 FDA《特定药物的生物等效性指导原则》数据库

美国食品和药物管理局（FDA）建立的《特定药物的生物等效性指导原则》数据库，对于生物等效性试验需要确定的受试者、试验设计方法、药品规格选择和给药剂量选择中不易确定的相关问题，指导原则给出具体研究方案，包括研究类型、试验设计、给药剂量和受试者，还包含体内试验豁免要求和溶出度试验方法和采样次数，对开展生物等效性试验具有重要意义。

网址：<https://www.fda.gov/regulatory-information/search-fda-guidance-documents>

U.S. FOOD & DRUG ADMINISTRATION

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Advisory Committee Guidance Documents

Clinical Trials Guidance Documents

Combination Products Guidance Documents

Import and Export Guidance Documents

The table below lists all official FDA Guidance Documents and other regulatory guidance. You can search for documents using key words, and you can narrow or filter your results by product, date issued, FDA organizational unit, type of document, subject, draft or final status, and comment period.

This feature is provided to give a convenient way to search for all FDA guidance documents from a single location.

If you cannot find the document you're looking for here, you can browse separate collections of guidance documents by topic.

[Go to Guidance Document Search](#)

Browse Guidance Documents By Topic

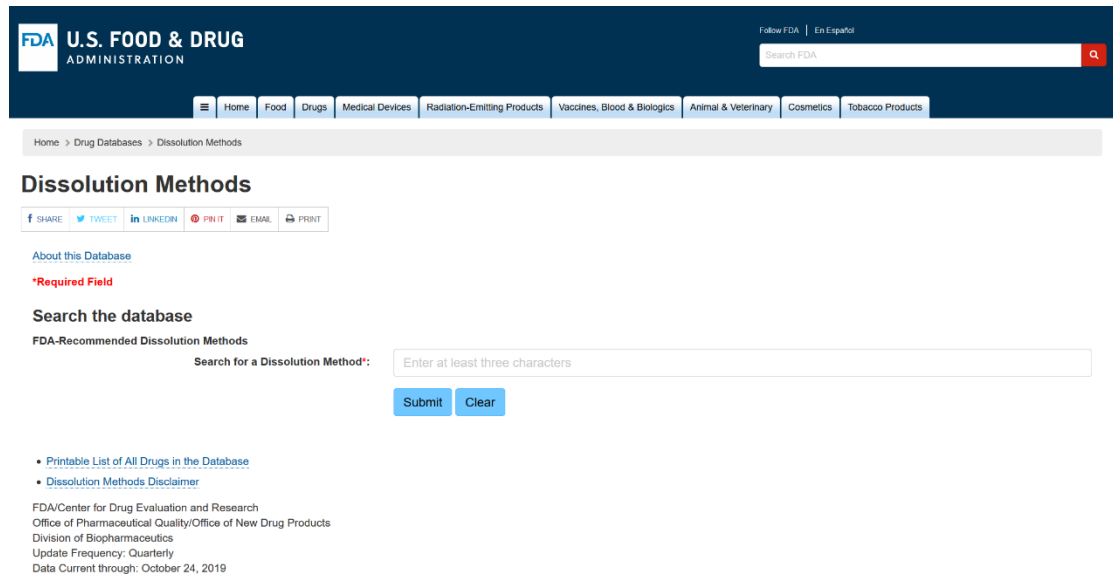
About FDA Guidance Documents

Content current as of: 03/28/2020

（5）美国 FDA 溶出度方法数据库（Dissolution Methods Database）

美国食品和药物管理局（FDA）建立的溶出度方法数据库（Dissolution Methods Database），包含了 1331 种化合物的各类溶出度方法信息，如药品名称、剂型、USP 溶解方法、转速、溶出介质、容积、推荐采样时间和更新时间等。

网址: <https://www.accessdata.fda.gov/scripts/cder/dissolution/index.cfm>



U.S. FOOD & DRUG ADMINISTRATION

Home Food Drugs Medical Devices Radiation-Emitting Products Vaccines, Blood & Biologics Animal & Veterinary Cosmetics Tobacco Products

Home > Drug Databases > Dissolution Methods

Dissolution Methods

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About this Database

*Required Field

Search the database

FDA-Recommended Dissolution Methods

Search for a Dissolution Method*: Enter at least three characters

Submit Clear

- Printable List of All Drugs in the Database
- Dissolution Methods Disclaimer

FDA/Center for Drug Evaluation and Research
Office of Pharmaceutical Quality/Office of New Drug Products
Division of Biopharmaceutics
Update Frequency: Quarterly
Data Current through: October 24, 2019

2. 欧盟《特定药物的生物等效性指导原则》数据库

欧盟药品管理局（EMA）建立的《特定药物的生物等效性指导原则》数据库，该指导原则仅适用于仿制化学药品的普通制剂，不包括调释制剂、透皮制剂、经口吸入制剂以及无法用药物浓度证明生物等效性，需要药效动力学或临床终点试验证明等效的药物制剂。

网址：

<https://www.ema.europa.eu/en/human-regulatory/research-development/scientific-guidelines/clinical-pharmacology-pharmacokinetics/product-specific-bioequivalence-guidance>



The screenshot shows the EMA website with the 'Human regulatory' section selected. The main heading is 'Human regulatory'. Below it, there are links for 'Overview', 'Research and development', 'Marketing authorisation', 'Post-authorisation', and 'Herbal products'. The 'Research and development' link is highlighted. On the left, there is a sidebar with links: 'Adaptive pathways', 'Advanced therapies', 'Clinical trials', 'Compassionate use', 'Compliance', 'Data on medicines (ISO IDMP standards)', 'Ethical use of animals', and 'Innovation in medicines'. The main content area is titled 'Product-specific bioequivalence guidance' with a 'Share' button. The text states: 'This section includes the European Medicines Agency's (EMA) product-specific bioequivalence guidance, which summarises in a standardised format the relevant study design principles for demonstration of bioequivalence.' It then explains that product-specific guidance helps applicants meet the expectations of regulators in the European Union, particularly for generic applications, across all regulatory submission routes, i.e. via the centralised, decentralised, mutual recognition or national procedures. For more information about product-specific guidance, see:

- [Concept paper on development of product-specific guidance on demonstration of bioequivalence \(EMA/CHMP/423137/2013\)](#).

 It also mentions that EMA publishes finalised guidance documents for individual products on a regular basis, once the [Committee for Medicinal Products for Human Use](#) has adopted them following a **public consultation**.

3. 日本《医疗用药品品质情报集》（日本橙皮书）

日本厚生省药品管理机构每年出版的《医疗用药品品质情报集》（日本橙皮书），并上线数据库，详细收录口服固体制剂的溶出度研究与评价信息（如：不同溶出介质下的标准溶出曲线信息）。

根据日本《医疗用药品品质情报集》收录的制剂信息，中国国家药品监督管理局药品审评中心（CDE），组织相关专家编译并构建了“日本厚生省药品体外溶出试验信息库”。收录日本橙皮书收录的已完成评价的部分品种（666个），主要包括药品有效成分、制剂类型、制剂规格、溶出度试验条件、4条标准溶出曲线、该制剂的溶出度试验质量标准、该原料药的理化性质等信息，并整理构建数据库。

网址：

http://www.jp-orangebook.gr.jp/cgi-bin/search_h/search_e.cgi（英文版）

Quality Reevaluation

Please select any Option.

☐ :Therapeutic Classification
 ☐ :Notified No
 ☒ :Nonproprietary Name:
 ☐ :Company

Please input keyword.

KeyWord:

Japanese Orange Book

[HOME](#)

[Japanese Orange Book English Version](#)

[Orange Book Search](#)

[Dissolution mediums](#)

[Nonproprietary name]

[A](#)
[B](#)
[C](#)
[D](#)

[E](#)
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[K](#)
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[P](#)

[Q](#)
[R](#)
[S](#)
[T](#)

[U](#)
[V](#)
[W](#)
[X](#)

[Y](#)
[Z](#)
[Other](#)

T.C.	Nonproprietary Name	Dosage Forms	Product Characteristics	Content	Brand Name	Company	Notified No.	Dissolution Test
112	Alprazolam	Tablets	Immediate-release	0.4mg 0.8mg	Solanax Tab. 0.4mg	Pfizer Japan Inc.	15	●
112	Estazolam	Powder	Immediate-release	10mg/g 1mg 2mg	EURODIN Powder 1%	Takeda Pharmaceutical Co., Ltd.	14	●
112	Flurazepam Hydrochloride	Capsules	Immediate-release	10mg 15mg	BENOZIL Cap. 10	Kyowa Hakkō Kirin Co., Ltd.	17	●
112	Rilmazafone Hydrochloride Hydrate	Tablets	Immediate-release	1mg 2mg	Rhythmy Tab. 1mg	Shionogi & Co., Ltd.	14	●
112	Oxazolam	Powder	Immediate-release	100mg/g 5mg 10mg 20mg	SERENAL Powder 10%	Daiichi Sankyo Co., Ltd.	15	●
112	Tandospirone Citrate	Tablets	Immediate-release	5mg 10mg	Sediel Tab. 5mg	Dainippon Sumitomo Pharma Co., Ltd.	24	●
112	Cloxazolam	Powder	Immediate-release	10mg/g 1mg 2mg	SEPAZON Powder 1%	Daiichi Sankyo Co., Ltd.	15	●
112	Clorazepate Dipotassium	Capsules	Immediate-release	7.5mg	Mendon Cap. 7.5mg	Abbott Japan Co., Ltd.	13	●
112	Diazepam	Powder	Immediate-release	10mg/g 1mg 2mg 3mg 5mg	Horizon Powder 1%	Astellas Pharma Inc.	33	●

<http://www.jp-orangebook.gr.jp/> (日文版)

オレンジブック総合版ホームページ

<http://www.jp-orangebook.gr.jp/>

公開開始日：2002年9月9日 最終更新日：2019年10月29日 396704

[ENGLISH](#)

■ [添付文書情報](#)

■ [ジェネリック医薬品品質情報検討会](#)

薬事日報社

JiP 株式会社じほう

中和印刷株式会社

再評価資料集

品質再評価の通知等
技術情報のページ

Quality Reevaluation

注意事項・お問い合わせ
本ホームページご利用上の
注意事項・お問い合わせ先

新着情報

○令和1年10月29日付 医療関係の方へ（品目情報等）を削除致しました。
品目情報は、「ジェネリック医薬品品質情報検討会」ホームページ ブルーブック一覧を参照ください。

網址：<http://www.cde.org.cn/drugInfo.do?method=init&frameStr=3> (CDE 编译版)



国家药品监督管理局药品审评中心
CENTER FOR DRUG EVALUATION, NMPA
СЕНТРЪ ЛОВ ДВНО ЕЛУВРАЦИОН, ИМБВ

English Page 搜索

首页 新闻中心 法规与规章 信息公开 科学研究 数据查询 申请人之窗 交流与反馈 临床试验登记 BE试验备案平台

当前位置: 数据查询>>药品体外溶出试验信息库

药品名称: 信息来源: 检索

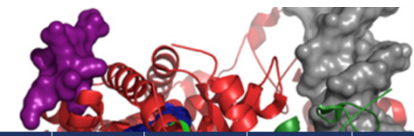
共有 666 条新闻

序号	药品名称	信息来源
1	盐酸洛美利嗪	日本医疗用医药品品质情报集2011-11-21
2	盐酸米诺环素	日本医疗用医药品品质情报集2011-11-21
3	盐酸卡普地尔	日本医疗用医药品品质情报集2011-11-21
4	盐酸异丙嗪	日本医疗用医药品品质情报集2011-11-21
5	盐酸羟嗪	日本医疗用医药品品质情报集2011-11-21
6	盐酸罂粟碱	日本医疗用医药品品质情报集2011-11-21
7	盐酸尼卡地平	日本医疗用医药品品质情报集2011-11-21
8	盐酸托烷司琼	日本医疗用医药品品质情报集2011-11-21
9	盐酸曲唑酮	日本医疗用医药品品质情报集2011-11-21
10	盐酸酞氨西林	日本医疗用医药品品质情报集2011-11-21

4. 药理学指南数据库 (Guide to Pharmacology)

药理学指南数据库 (Guide to Pharmacology) 是由英国药理学学会(The British Pharmacological Society,BPS)和国际基础与临床药理学联合会(the International Union of Basic and Clinical Pharmacology ,IUPHAR)合作建立, 目的是成为获取药理学信息的“一站式”门户网站。通过该网站, 用户可以获取关于药物分子靶点的大量信息, 同时这些信息也将指导研究人员建立更多遗传学、治疗、分子生物学、免疫学及化学特性的在线数据库, 帮助科学家从事相关研究工作。该数据库不仅适合药理学家, 也适用于生理学家、健康科学家、细胞生物学家和在生命科学和化学领域工作的人员。

网址: <http://guidetopharmacology.org/>



IUPHAR/BPS
Guide to PHARMACOLOGY

Home About Targets Ligands Diseases Resources Advanced search Immuno Portal Malaria Portal

An expert-driven guide to pharmacological targets and the substances that act on them.

Quick links

Targets

- G protein-coupled receptors
- Ion channels
- Nuclear hormone receptors
- Kinases
- Catalytic receptors
- Transporters
- Enzymes
- Other protein targets

Ligands

- Approved drugs
- Synthetic organics
- Metabolites
- Natural products
- Endogenous peptides
- Other peptides
- Inorganics
- Antibodies
- Labelled ligands

What's new to Guide to PHARMACOLOGY

Coronavirus (Covid-19) - view our information page

New database version 2020.1 (12 Mar 2020) - full details in our blog post

- Ligand Activity Charts**
 - GtoPdb provides a useful visualisation tool that displays ligand activities against different targets, and across different species - see the [blog post](#) for more info. Now includes data from ChEMBL 26
- New publication on [IUPHAR Guide to Immunopharmacology: connecting immunology and pharmacology](#)
- Updated target data in ~30 different target families
- Incorporated ChEMBL 26 data into our ligand activity charts and pharmacology search.
- New download for [approved drugs and their primary targets](#)
- P. falciparum* (3D7) targets [PiCLK3](#), [PiPMV](#) and [PiNCR1](#) have been added to Antimalarial targets family

Latest News and Hot Topics in Pharmacology

GtoMPdb

IUPHAR/MMV Guide to Malaria Pharmacology



Visit the [IUPHAR/MMV Guide to MALARIA PHARMACOLOGY portal](#) Launched in September 2019 to provide optimised access to GtoPdb data for the malaria research community

The Concise Guide to PHARMACOLOGY 2019/20

5. 免疫药理学指南数据库（Guide to ImmunoPharmacology）

免疫药理学指南数据库（Guide to ImmunoPharmacology）是由英国药理学学会(The British Pharmacological Society,BPS)和国际基础与临床药理学联合会(the International Union of Basic and Clinical Pharmacology ,IUPHAR)合作建立，旨在加大免疫学专家和药理学专家之间的信息交流，能够更好地支持免疫、炎症或传染性相关药物的研究和开发。

网址：<http://www.guidetoimmunopharmacology.org/immuno/>



IUPHAR Guide to IMMUNOPHARMACOLOGY

Search Database

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Diseases
Resources ▾
Guide to PHARMACOLOGY

Processes ?



- Antigen presentation
- Barrier integrity
- B cell (activation)
- Cellular signalling
- Chemotaxis & migration
- Cytokine production & signalling
- Immune regulation
- Immune system development
- Inflammation
- T cell (activation)
- Tissue repair

[View immuno processes home page](#)

Cell Types ?



- B-cells
- Dendritic cells
- Granulocytes
- Innate lymphoid cells
- Macrophages & monocytes
- Mast cells
- Natural killer (NK) cells
- T-cells (alpha/beta)
- Other T-cells (NKT, MAIT, TRM etc.)
- Stromal cells

[View immuno cell types home page](#)

Latest Updates & Links

CVR Onlife Interview

Prof. Alberto Mantovani and Prof. Michael Spedding introduce the Guide to Immunopharmacology in this CVR Onlife interview

[Read the Cardiovascular Research article](#)

Immunopaedia



immunopaedia.org

Immunopaedia promotes education, knowledge and research in immunology globally. We are establishing valuable links between GtoImmuPdb and Immunopaedia.

Targets ?



- G protein-coupled receptors
- Ion channels
- Nuclear hormone receptors
- Kinases
- Catalytic receptors
- Transporters
- Enzymes
- Other protein targets

[Search for targets](#)

Ligands ?



- Immuno ligands
- Antibodies
- Approved drugs
- Synthetic organics
- Metabolites
- Natural products
- Endogenous peptides
- Other peptides
- Inorganics

6. 毒理学文献目录库 (TOXLINE)

毒理学文献目录库 (TOXNET) 是美国国立医学图书馆 (NLM) 旗下数据库, 它提供 1840 年至今有关药物和其它化学品的生化、药理、生理和毒理作用的文献目录信息。它收录 500 多万篇参考文献, 大多有文摘、标引词和 CAS 登记号。网址: <https://www.nlm.nih.gov/toxnet/index.html>

NIH National Library of Medicine

Search NLM

PRODUCTS AND SERVICES RESOURCES FOR YOU EXPLORE NLM GRANTS AND FUNDING

COVID-19 is an emerging, rapidly evolving situation.
Get the latest public health information from CDC: <https://www.coronavirus.gov>
Get the latest research information from NIH: <https://www.nih.gov/coronavirus>

TOXNET HAS MOVED
As part of a broader NLM reorganization, most of NLM's toxicology information services have been integrated into other NLM products and services.

How to access TOXNET information

COMPREHENSIVE TOXICOLOGY INFORMATION

- HSDB in PubChem
- Help for HSDB Users in PubChem (PDF)
- Help for HSDB Users in PubChem (Web Page)
- Video Tutorial

TOXICOLOGY LITERATURE

- TOXLINE in PubMed
- Help for TOXLINE Users in PubMed (PDF)
- Help for TOXLINE Users in PubMed (Web Page)

7. 药物及哺乳数据库 (LactMed)

药物及哺乳数据库 (LactMed) 是美国国立卫生研究院 (NIH) 资助的在线哺乳数据库, 提供哺乳期妇女可能接触的药物及其他化学物品相关信息, 包括: 药物在乳汁、婴儿血液中的分布水平; 受乳婴儿的潜在风险; 可替换药物等。数据库信息均基于系统检索并经同行评议, 数据每月更新, 可为药师, 特别是妇产科专业药师, 提供专业的药学信息。

网址: <https://toxnet.nlm.nih.gov/newtoxnet/lactmed.htm>

NCBI Resources How To Sign in to NCBI

Bookshelf Books Search Browse Titles Advanced Help

Drugs and Lactation Database (LactMed)

Bethesda (MD): National Library of Medicine (US); 2006-.

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Search this book

The LactMed® database contains information on drugs and other chemicals to which breastfeeding mothers may be exposed. It includes information on the levels of such substances in breast milk and infant blood, and the possible adverse effects in the nursing infant. Suggested therapeutic alternatives to those drugs are provided, where appropriate. All data are derived from the scientific literature and fully referenced. A peer review panel reviews the data to assure scientific validity and currency.

Views

- PubReader
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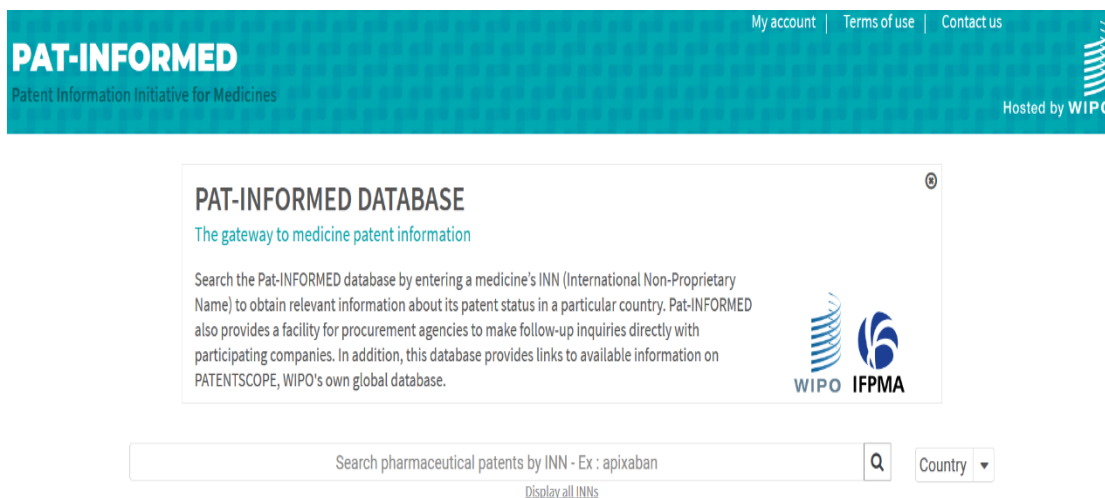
LactMed Support Resources

- User and Medical Advice Disclaimer
- LactMed App
- Drugs and Lactation Database (LactMed) - Record Format
- LactMed - Database Creation and Peer Review Process
- Fact Sheet, Drugs and Lactation Database (LactMed)

8. 在线药品专利检索资源 (Pat-INFORMED)

在线药品专利检索资源 (Pat-INFORMED) 是世界知识产权组织 (WIPO) 联合制药业共同推出了一种新的在线工具, 旨在帮助公共卫生采购部门更好地了解药品的全球专利状况。该平台涵盖超过 1.4 万件个人专利, 600 个专利家族和 169 个国际非专利药品名称的信息。平台包含艾滋病、心血管疾病、糖尿病、丙型肝炎、肿瘤疾病、呼吸系统疾病治疗药品的专利信息, 以及《世界卫生组织基本药物标准清单》上其他产品信息。

网址: <https://www.wipo.int/patinformed/>



9. 靶点与生物活性数据库 (ChEMBL)

靶点与生物活性数据库 (ChEMBL) 是欧洲生物信息研究所 (European Bioinformatics Institute, EBI) 开发的免费数据库, 它通过从大量文献中收集各种靶点及化合物的生物活性数据, 为药物化学家们提供查询靶点和化合物的生物活性数据的平台。截至 2020 年 4 月 4 日, 该数据库共收集了 13377 个靶点, 195 万个化合物, 共有 15996 万条生物活性信息。

通过该数据库, 用户可以快速获取某个靶点已报道的化合物及其活性信息, 也可以查询某个化合物在哪些靶点做的生物活性测试及其数据。这些数据均来源于已报道的文献, 数据可靠, 且能够溯源。

网址: <https://www.ebi.ac.uk/chembl/>

The image shows the ChEMBL website interface. At the top, there is a search bar with the text "Search in ChEMBL" and a magnifying glass icon. Below the search bar, there are examples of search terms: "Imatinib", "erbB2", "brain", "MDCK", "c10000c1N". To the right of the search bar, there are links for "Draw a Structure" and "Enter a Sequence". Below the search bar, there is a navigation menu with links for "UniChem", "ChEMBL-NTD", "SureChEMBL", "Downloads", "Web Services", and "More". Below the navigation menu, there is a message about planned maintenance: "As a result of planned maintenance that is due to end on 4th April 2020, there may be unexpected disruption caused to some of the services we host. If you experience any issues, please contact the relevant help desk directly for support." Below the message, there is a description of ChEMBL: "ChEMBL is a manually curated database of bioactive molecules with drug-like properties. It brings together chemical, bioactivity and genomic data to aid the translation of genomic information into effective new drugs." Below the description, there is a bubble chart showing the following data: 1.8K Cells, 4.8K Macromolecules, 1.2M Assays, 76K Documents, 707 Tissues, and 33K Indications. To the right of the bubble chart, there is a section titled "Explore ChEMBL" with a description: "Description: Shows a summary of the ChEMBL entities and quantities of data for each of them." and instructions: "Instructions: Click on a bubble to explore a specific ChEMBL entity in more detail." Below the instructions, there is a right-pointing arrow.

10. 抗癌药物敏感性基因组学数据库（GDSC）

抗癌药物敏感性基因组学数据库（GDSC）是由英国桑格研究院开发，收集肿瘤细胞对药物的敏感度和反应。GDSC的数据来自 75000 个实验，描述约 200 个抗癌药物在 1000 多种肿瘤细胞中的反应。该数据库中的癌基因组突变信息来自 COSMIC 数据库，包括癌基因点突变、基因扩增与丢失、组织类型以及表达谱等。用户可以从化合物、癌基因和细胞系对数据库进行检索，癌基因或细胞系对不同药物的反应会被详细列出，并且结果会以图形化的界面加以展示，包括统计分析，火山图及相关文献等。检索结果以及整个数据库都可由用户下载以进行后续分析。

网址：<https://www.cancerrxgene.org/>



Genomics of Drug Sensitivity in Cancer

We have characterised **1000 human cancer cell lines** and screened them with **100s of compounds**.
On this website, you will find **drug response data** and **genomic markers** of sensitivity.

Search by drug, gene or cell line name
e.g. Docetaxel, RP-56976, BRAF, COLO-829

Overview

Coverage
518 compounds targeting 24 pathways

Other, kinases: 61
Other: 60

What's new?
Release 8.2 (Feb 2020)
Release 8.2 adds 47 compounds to the GDSC1 dataset and 23 compounds to the GDSC2 dataset. In total there are 60434 new IC50s, 15% more than in release 8.1. Two datasets are available: GDSC1 updates our previous screening results; and GDSC2 uses the latest improved screening technology.

Datasets

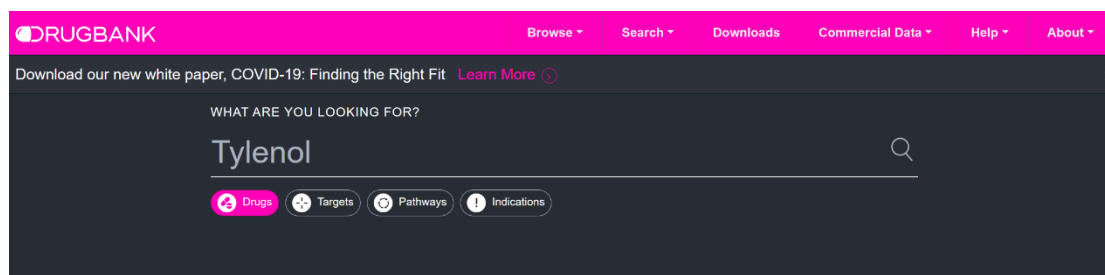
	GDSC1	GDSC2
Age	from 2010 to 2015	✓ NEW
Size	987 Cell lines	809 Cell lines
	367 Compounds	198 Compounds
	310904 IC50s	135242 IC50s
Assay	Resazurin or Syto60	CellTiterGlo
Duration	72 hours	72 hours

Key Publications
Genomics of Drug Sensitivity in Cancer

11. DrugBank 数据库

DrugBank 是由加拿大国立卫生研究院资助，多个医学非营利组织及商业公司合作建立，将详细的药品数据(即化学、药理学和制药)与综合药物靶点信息(即序列、结构和作用通路)相结合的“生物信息学和化学信息学”资源。它包含 13540 种药物条目，其中包括 2630 种经批准的小分子药物、1372 种经批准的生物技术(蛋白质/肽)药物、131 种药物和 6358 种实验药物。此外，5212 个非冗余蛋白(即药物靶标/酶/转运体/载体)序列与这些药物条目相关联。DrugBank 最大的特色是它支持全面而复杂的搜索，结合 DrugBank 可视化软件，这些工具能让科学家们非常容易的检索到新的药物靶目标、比较药物结构、研究药物机制以及探索新型药物。

网址: <https://www.drugbank.ca/>



DRUGBANK

The DrugBank database is a unique bioinformatics and cheminformatics resource that combines detailed drug data with comprehensive drug target information.

The latest release of DrugBank (version 5.1.5, released 2020-01-03) contains 13,534 drug entries including 2,629 approved small molecule drugs, 1,372 approved biologics (proteins, peptides, vaccines, and allergens), 131 nutraceuticals and over 6,356 experimental (discovery-phase) drugs. Additionally, 5,212 non-redundant protein (i.e. drug target/enzyme/transporter/carrier) sequences are linked to these drug entries. Each entry contains more than 200 data fields with half of the information being devoted to drug/chemical data and the other half devoted to drug target or protein data.

[About DrugBank](#)

[Cite DrugBank](#)

[DrugBank for Commercial Use](#)

12. 遗传药理学和药物基因组学数据库（PharmGKB）

遗传药理学和药物基因组学数据库（PharmGKB）是由美国国立卫生研究院（NIH）支持，主要收录与药物基因组学相关的基因型、表型信息，并将这些信息整理归类，方便研究人员和工作查询。PharmGKB 提供药物的 PK 和 PD 相关通路，挑选对药物基因组学非常重要的基因，并对这些基因进行详细的注释。PharmGKB 根据数据的种类将所有信息划分为临床结局（CO）、药物效应动力学（PD）、药物代谢动力学（PK）、分子及细胞功能分析（FA）和基因型（GN）五大类。PharmGKB 还收录了由各国政府或国际组织颁布的某些特定药物个体化用药指南，指导医生根据个体的基因型合理用药。

网址：<https://www.pharmgkb.org/>

New to the site? Take a short tour of the home page. ✕

 PHARMGKB

[Publications](#) [News](#) [Downloads](#) [Contact](#) [Help](#)

Search PharmGKB... Q

Search for a molecule, gene, variant, or combination

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Category	Count
Annotated Drugs	684
Curated Pathways	149
Clinical Guideline Annotations	143
Drug Label Annotations	753

 WHAT IS PHARMACOGENOMICS? PHARMACOGENOMICS. KNOWLEDGE.



二、国内药物信息平台

1. 国家药品监督管理局药品审评中心

国家药品监督管理局药品审评中心，负责药物临床试验、药品上市许可申请的受理和技术审评。《药品审评中心技术审评报告》记录提交上市申请新药的基本信息、审评经过、现场检查及样品检验等基本信息，其核心内容是药品审评中心（CDE）对该药品的综合审评意见，披露内容包括支持该新药上市申请的关键有效性和安全性临床试验数据（尤其是国内临床数据），以及药品审评中心（CDE）在审评过程中发现的问题及处理，这些信息对业内有重要的参考意义。

网址：<http://www.cde.org.cn/index.jsp>



2. 中药系统药理学数据库与分析平台 (TCMSP)

中药系统药理学数据库与分析平台(TCMSP)是西北农林科技大学王永华教授课题组历时两年,构建的中药系统药理学数据库,是一个融合了药物化学、药代动力学、药物-靶标-疾病网络的药理学平台。它能捕捉药物、靶标和疾病之间的关系。该数据库包括化学物质、靶点和药物靶点网络,以及相关的药物靶点网络,涉及口服生物利用度、药物相似度、肠上皮通透性、血脑屏障、水溶性等天然化合物的药代动力学特性。

网址: <http://tcmsp.w.com/index.php>

Lab of Systems Pharmacology 计算系统生物学实验室

首页 软件 发表文章 引用查询 专利展示 团队动态 工具 联系我们

NEWS

《系统药理学》专著出版了！
TCMSP database has upgraded to Version 2.3
2016年系统药理学原理、方法及应用研讨班(第4期)开课了！
Research Finds Herbal Medicines Can Inhibit Influenza

SERVICE

TCMSP Analysis Platform

JOURNALS

Molecular Systems Biology
Nature
Nature Communications
Nature Medicine
Nature China
PLOS Computational Biology
CPT: Pharmacometrics & Systems Pharmacology
Briefings in Bioinformatics
Journal of Ethnopharmacology

HOT LINKS

Drugbank

Latest Research Highlights:

TCMSP
TCMSP: a database of systems pharmacology for drug discovery from herbal medicines

Results and Applications
Drug Discovery, Mechanism of Action, Disease Association, Toxicology Analysis, Functional Characterization, Hypothesis-driven Analysis, Potential Targets, Network Analysis

Journal of Cheminformatics 2014
Evidence based complementary and alternative medicine 2013
Journal of Ethnopharmacology 2013
Briefings in Bioinformatics 2013

Introduction:

Recently, computational systems biology, as new emerging discipline, has brought a new combination of computational and experimental tools to bear on the discovery and investigation of drugs. System-level understanding of pharmacological effects will help to understand how drugs work on specific pathways, on different cell types and in individual patients, thus facilitating drug discovery and development of combination therapies.

Using a variety of mathematical approaches combining with experimental validations, the current research topics of Systems Pharmacology Group led by Prof. Yonghua Wang focus on but not limit to:

(1) Computational systems biology theory and methods
(2) Study of Traditional Chinese Medicine by computational systems biology
(3) Cardiovascular computational systems biology

3. 中药分子机制的生物信息学分析工具（BATMAN-TCM）

北京蛋白组研究中心开发的中药分子机制生物信息学在线分析工具（BATMAN-TCM），是专门为研究中药分子机制而设计的在线生物信息学分析工具。主要功能包括：中药组成成分的靶标预测；潜在靶标的功能分析；成分-靶标-通路/疾病关联网络的可视化；中药不同组分的比较分析。

网址：<http://bionet.ncpsb.org/batman-tcm/>

BATMAN-TCM
A Bioinformatics Analysis Tool for Molecular Mechanism of Traditional Chinese Medicine

Brief Introduction

This web server is built and free for academics. For commercial use, please contact us!
For better user experience, Chrome is recommended to navigate BATMAN-TCM.

Traditional Chinese Medicine (TCM), with a history of thousands of years of clinical practice, plays an important role in maintaining the health of peoples of Asia, and is gaining more and more application all over the world. However, owing to the diversity of TCM's ingredients and the complexity of TCM's interaction with human body, it is still quite difficult to uncover the underlying molecular mechanism of TCM. The clarification of the TCM's molecular mechanism has become a bottleneck in TCM modernization and internationalization. **BATMAN-TCM** (a Bioinformatics Analysis Tool for Molecular Mechanism of Traditional Chinese Medicine) is the first online bioinformatics analysis tool specially designed for the research of molecular mechanism of TCM.

1. Please input the interested TCM

Example 1 Example 2 Example 3 Example 4

Cluster name: Cluster1 (default) **Cluster1**

Select input type: Formula (Pinyin name)

*Formula (Pinyin name): e.g. WU MEI GAO, case insensitive.

+ Add one cluster

*** Required Field.**

Annotation

Three alternative input types: TCM formula (Pinyin name) (e.g. JIA WEI CAN XIA TANG), Herb or Herb list (Pinyin, English or Latin name) (e.g. ren shen, Ginseng or Panax ginseng) or User defined composite compound list of the TCM (compounds are denoted by PubChem_CIDs or chemical structures of InChI format). For the second and third input types, multiple herbs/compounds are supported, one herb/compound per line.

For the third input type, currently only PubChem_CID or InChI format is supported. If you have compound lists represented by other types of format, you can use [OpenBabel](#) to transfer the format. By clicking on "Add one cluster", BATMAN-TCM also supports users to simultaneously input multiple TCM formulas/herbs/Compound lists. Please click on "Example 4" to obtain an example (4 clusters maximum).

4. 《中国上市药品目录集》数据库

国家药品监督管理局组织制定《中国上市药品目录集》，收录国家药品监督管理局历年批准上市的药品信息，包括创新药、改良型新药、化学药品新注册分类的仿制药以及通过质量和疗效一致性评价药品的具体信息；指定仿制药的参比制剂和标准制剂，标示可以替代原研药品（过专利保护期的进口药）的具体仿制药品，供制药行业和医学界人员及社会公众了解和查询。现发布的《中国上市药品目录集》收录 131 个品种，203 个品种规格。通过仿制药质量和疗效一致性评价的 13 个品种，17 个品种规格。

网址：<http://202.96.26.102/index/lists>

5. 国家人口与健康科学数据共享服务平台—药学科学数据中心

国家人口与健康科学数据共享服务平台—药学科学数据中心，是国家生命科学数据共享体系的组成部分，负责我国药学及相关学科科学数据实现共享的管理和技术服务，为促进我国的药学科学的发展提供数据和信息支持。药学科学数据共享中心在医学科学数据共享体系的整体框架下，收集、整合全国药学科学及相关数据，实现数据共享。

网址：<http://pharmdata.ncmi.cn/>

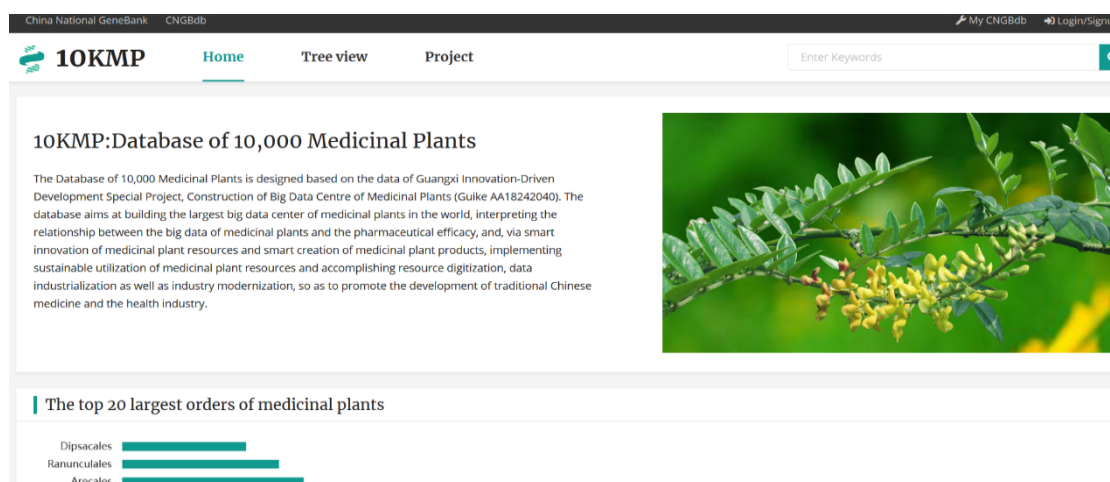


6. 万种药用植物数据库（10KMP）

万种药用植物数据库（10KMP）是广西药用植物园和国家基因库共建的药用植物资源数据库。该平台基于药效高通量筛选及药用植物生物大数据，通过药用植物数据的跨组学研究，解读药用植物形态、生态、组学与药效，以及药效与疾病间的关系，使药用植物研究实现标准化、精准化。万种药用植物数据库（10KMP）中所有药用植物信息为公开状态，可直接搜索获取相关信息。目前，数据信息为受控状态，需先申请，获得授权后即可查看和下载。

网址：<https://db.cngb.org/10kmp/homepage>

申请流程详见：国家基因库数据受控中心 https://db.cngb.org/data_access/



7. 药物临床试验登记与信息公示平台

国家药品监督管理局药品审评中心（CDE）建立的药物临床试验登记与信息

公示平台，是基于国家“药物临床试验数据库”而搭建，对获准在我国开展的所有药物临床试验实行登记与社会公示的信息平台。其主要目的和用途是：保障公众知情权；发挥社会监督作用；促进试验质量和效率的提高；以及服务于技术审评和监督检查等药品监管工作。

网址：<http://www.chinadrugtrials.org.cn/eap/main>

The screenshot shows the homepage of the China Drug Trials Registration and Information Disclosure Platform. The header features the title '药物临床试验登记与信息公示平台' and the URL 'WWW.CHINADRUGTRIALS.ORG.CN'. A navigation bar includes links for '首页', '试验公示和查询', '试验登记', '帮助和链接', '信息统计', '化学药BE试验备案信息平台', and '关于平台'. A search bar with a magnifying glass icon and a '查询' button is present. Below the search bar, there are links for '高级查询' and '查询帮助'. A '问题解答' (FAQ) section is visible at the bottom, with a '更多' (More) link. The FAQ section lists several questions related to drug clinical trials, such as '什么是药物临床试验?' and '为什么要登记药物临床试验信息并对公众公示?'.

药物临床试验登记与信息公示平台

WWW.CHINADRUGTRIALS.ORG.CN

本平台是基于国家药品监督管理局的药物临床试验申请数据，对获准在我国开展的所有药物临床试验实行登记与社会公示的信息平台。其主要目的和用途是：保障公众知情权；发挥社会监督作用；促进试验质量和效率的提高；以及服务于技术审评和监督检查等药品监管工作。更多内容请进入“帮助和链接”和“关于平台”。

郑重声明 重要提示

首页 试验公示和查询 试验登记 帮助和链接 信息统计 化学药BE试验备案信息平台 关于平台

查询药物试验，如输入“糖尿病”

查询

高级查询 查询帮助

问题解答 更多

什么是药物临床试验？
本平台涵盖哪些药物临床试验？
我想参加某项试验，如何做？

为什么要登记药物临床试验信息并对公众公示？
如何查询药物临床试验？
如何登记药物临床试验？登记的所有信息都在平台公示吗？

（编辑：李华）