



ELSEVIER

Elsevier Life Science Solution 获取药物研发信息系列主题培训

Jul 2020



Elsevier Life Science 用户群



该二维码7天内(7月21日前)有效, 重新进入将更新

Agenda

- 7月8日
 - 15: 00-15: 10: Elsevier Life Science整体解决方案介绍
 - 15: 10-16: 30: 物质结构/合成信息的获取与精炼
- 7月15日
 - 15: 00-16: 00: 生物活性数据与文献的获取与提炼
- 7月22日
 - 15: 00-16: 00: 化合物毒理药理学文献的获取
- 7月29日
 - 15: 00-16: 00: Elsevier Life Science整体解决方案数据库使用答疑
- 8月5日
 - 15: 00-16: 00: 如何将Elsevier Life Science整体解决方案贯穿药物研发的全流程



ELSEVIER

生物活性数据与文献的获取与提炼

涉及：RMC, PharmaPendium



Agenda

- 化合物活性数据的获取
- 文献与专利中活性数据的获取与提炼
- FDA/EMA审评文档中活性数据的获取与提炼

RMC (Reaxys Medicinal Chemistry)

- RMC是建立在Reaxys平台上的，和药物化学数据有关的数据库。
 - 包含真实的，实验确证的，小分子化合物在不同生物体系中的相关实验数据
 - 是市场上最全的，最广泛的小分子生物活性数据库
 - 实验数据源自对学术全文，专利中的相关数据的摘取，以及来自GOSTAR数据库的相关数据，并将二者在底层数据上进行整合。
 - RMC中所提供的文献，包含所有摘录的相关信息和数据，可靠，可信

Patents Origin and starting date

- **>126 600 Patents**
- US : 1971-present
- EP : 1979-present
- WO : 1978-present (English only)
- Patents are coming from the A61K class mainly but not only.

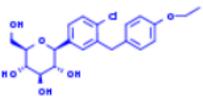
Articles and Journals

- **>5000 Journals Covered**
- **>353 400 Articles**
- From 1980 to Present

Drugable Targets

- **>12 700 Drugable Targets**

Case 1: 单一化合物生物活性数据的获取



1

dapagliflozin
C₂₁H₂₅ClO₆ 408.879 11966426 461432-26-8

Identification
Druglikeness
Bioactivity (All)

Physical Data - 52
Spectra - 54
Other Data - 351

Preparations - 81 >
Reactions - 398 >
Targets - 24 >
Documents - 217 >

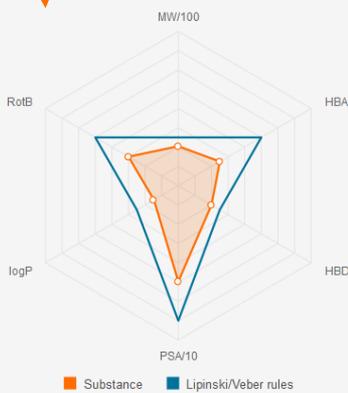
Druglikeness

Lipinski rules component

Molecular Weight	408.879
logP	2.937
HBA	5
HBD	4
Matching Lipinski Rules	4

Veber rules component

Polar Surface Area (PSA)	99.38
Rotatable Bond (RotB)	6
Matching Veber Rules	2



Legend: Substance (orange), Lipinski/Veber rules (blue)

Bioactivity (All)

- ✓ In vitro: Efficacy - 261
- ✓ In vivo: Animal Model - 208
- ✓ Metabolism - 67
- ✓ Pharmacokinetic - 229
- ✓ Toxicity/Safety Pharmacology - 114

具体化合物的生物活性数据

^ Bioactivity (All)

- v In vitro: Efficacy - 261
- v In vivo: Animal Model - 208
- v Metabolism - 67
- v Pharmacokinetic - 229
- v Toxicity/Safety Pharmacology - 114

RMC将全文中的数据
全部提炼出来，同时
对于用Mol为单位的数
据进行标准化处理：
 $pX = -\lg(\sim\text{mol})$

Show/Hide columns v

pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Tissue/Organ	Cell	Dose	Effect	Concomitants	Reference
9.91	amount (Glycogen)		50 - 175	pg/ml	Sprague Dawley rat			pancreas		20 μmol/l	antidiabetic agent		Wang, May-Yun; Yu, Xinxi; Lee, Young; McCorkle, Sara Kay; Chen, Shihwei; Li, Jianping; Wang, Zhao V.; (...) Unger, Roger H.; Roth, Michael G [Proceedings of the National Academy of Sciences of the United States of America, 2017, vol. 114, # 25, p. 6611 - 6616] Full Text ↗ Cited 10 times ↗ Details > Abstract >
9.84	pIC50 ([14C]Methyl-Alpha-D-Glucopyranoside Uptake)		9.84		human		Sodium/glucose cotransporter 2 [human]Wild		COS-7 cell line			Radioligand: [14C]AMG	Ho, Low-Tone; Kulkarni, Suvarn S.; Lee, Jinq-Chyi [Current Topics in Medicinal Chemistry, 2011, vol. 11, # 12, p. 1476 - 1512] Full Text ↗ Cited 9 times ↗ Details > Abstract >
9.84	pIC50		9.84		human		Sodium/glucose cotransporter 2 [human]Wild		COS-7 cell line			Radioligand: ALPHA-D-(U-14C)-GLUCOPYRANOSIDE; Other compound: NACL;	Zhou, Huiqiang; Danger, Dana P.; Dock, Steven T.; Hawley, Lora; Roller, Shane G.; Smith, Chari D.; Handlon, Anthony L [ACS Medicinal Chemistry Letters, 2010, vol. 1, # 1, p. 19 - 23] Full Text ↗ Cited 35 times ↗ Details > Abstract >
9.31	IC50	=	0.49	nM	human	Inhibitor	Sodium/glucose cotransporter 2 [human]Wild		CHO cell line				Lee, Suk Ho; Song, Kwang-Seop; Kim, Jong Yoo; Kang, Misuk; Lee, Jun Sung; Cho, Seung-Hwan; Park, Hyun-Ju; Kim, Jeongmin; Lee, Jinhwa [Bioorganic and Medicinal Chemistry, 2011, vol. 19, # 19, p. 5813 - 5832] Full Text ↗ Cited 17 times ↗ Details > Abstract >
9.31	IC50	=	0.49	nM	human	Inhibitor	Sodium/glucose cotransporter 2 [human]Wild						Lee, Jinhwa; Kang, Suk Youn; Song, Kwang-Seop; Lee, Junwon; Lee, Sung-Han [Bioorganic and Medicinal Chemistry, 2010, vol. 18, # 16, p. 6069 - 6079] Full Text ↗ Cited 30 times ↗ Details > Abstract >
9.31	IC50 ([14C]Methyl-Alpha-D-Glucopyranoside Uptake)		0.49	nM	human		Sodium/glucose cotransporter 2 [human]Wild		CHO cell line			Radioligand: [14C]AMG	Ho, Low-Tone; Kulkarni, Suvarn S.; Lee, Jinq-Chyi [Current Topics in Medicinal Chemistry, 2011, vol. 11, # 12, p. 1476 - 1512] Full Text ↗ Cited 9 times ↗ Details > Abstract >
9.31	IC50	=	0.49	nM	human		Sodium/glucose cotransporter 2 [human]Wild		CHO cell line			Substrate: [14C]AMG	Park, Eun-Jung; Kong, Younggyu; Lee, Jun Sung; Lee, Sung-Han; Lee, Jinhwa [Bioorganic and Medicinal Chemistry Letters, 2011, vol. 21, # 2, p. 742 - 746] Full Text ↗ Cited 10 times ↗ Details > Abstract >

具体化合物的生物活性数据

^ Bioactivity (All)

- ✓ [In vitro: Efficacy - 261](#)
- ✓ [In vivo: Animal Model - 208](#)
- ✓ [Metabolism - 67](#)
- ✓ [Pharmacokinetic - 229](#)
- ✓ [Toxicity/Safety Pharmacology - 114](#)

^ Metabolism - 67

Quantitative Results

pK	Parameter	Value (range)	Unit	Biological Species	Action target	Target	Tissue/Organ	Cell	Substrate / Carried Molecule	Dose	Concomitants
8.1	IC50	0.0008	µM		Inhibitor	Sodium/glucose cotransporter 2 (human)/Wild		HEK293 cell line		0.1 mM - 200 µM	Other compound: 2-DG, 2-thiophosphorylidine nucleoside
7.9	IC50	1	nM		Inhibitor	Sodium/glucose cotransporter 2 (human)/Wild		CHO-K1 cell line	[14C]-alpha-Methyl-glucopyranoside		Other compound: OMTG; [14C]-alpha-Methyl-glucopyranoside;
8.32	IC50	3	nM		Inhibitor	Sodium/glucose cotransporter 1 (human)/Wild		Fig-in-CHO cell line	Methyl-alpha-D-glucopyranoside		Marker: [14C]-methyl-alpha-D-glucopyranoside; Other compound: Phlorizin; Substrate: Methyl-alpha-D-glucopyranoside;
8.59	IC50	3	nM		Inhibitor	Sodium/glucose cotransporter 2 (human)/Wild + Sodium/glucose cotransporter 1 (human)/Wild		Fig-in-CHO cell line	[14C]-methyl-alpha-D-glucopyranoside		Substrate: [14C]-methyl-alpha-D-glucopyranoside; Other compound: Phlorizin;
8.46	IC50	3.2	nM		Inhibitor	Sodium/glucose cotransporter 2 (human)/Wild		CHO-K1 cell line	[14C]-methyl-alpha-D-glucopyranoside		Marker: [14C]-methyl-alpha-D-glucopyranoside; Substrate: [14C]-methyl-alpha-D-glucopyranoside;
8	concentration (parameter)	10 - 20	nM	human				plasma cell			Xu, Ge, Lu, Erhuxia, Robarge, Jacques Y, Xu, Baihua, Du, Jiyun, Dong, Jiaqi, Chen, Yueshen, L., J. Wirthwein, Appl. Syn. J. <i>Journal of Medicinal Chemistry</i> , 2014, vol. 57, # 4, p. 1238 - 1251 Full Text > Cited 38 times > Details > Abstract >
8	plasma protein-bound fraction	97.2	%	rat				plasma		3 µM	LIU, JIANG, LI, LEE, TAN/IN/Annual Reports in Medicinal Chemistry, 2011, vol. 46, p. 103 - 115 Full Text > Cited 9 times > Details > Abstract >
								plasma		3 µM	NATIONAL INSTITUTE OF BIOLOGICAL SCIENCES, BEIJING, ZHANG, Zhiyuan, HUANG, Shaoping, ZHANG, Zhaolin, SU, Yanning, REN, Yan - WO201541470, 2016, 41 Full Text > Details > Abstract >

^ Pharmacokinetic - 229

Quantitative Results

Parameter	Value (range)	Unit	Biological Species	(Clinical) Findings / Disease	Route of administration	Dose	Dosing regimen	Reference
Cmax	551	ng/mL	human African, human Asian, Human Caucasian	Healthy; Healthy;	oral administration	50 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >
AUC (0-inf)	2303	ng h/mL	human African, human Asian, Human Caucasian	Healthy; Healthy;	oral administration	50 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >
AUC (0-t) (to the last detectable concentration)	2236	ng h/mL	human African, human Asian, Human Caucasian	Healthy; Healthy;	oral administration	50 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >
Cmax	551	ng/mL	human African, human Asian, Human Caucasian	Healthy; Healthy;	oral administration	50 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >
AUC (0-inf)	2303	ng h/mL	human African, human Asian, Human Caucasian	Healthy; Healthy;	oral administration	50 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >
AUC (0-t) (to the last detectable concentration)	2236	ng h/mL	human African, human Asian, Human Caucasian	Healthy; Healthy;	oral administration	50 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >
Cmax	134	ng/mL	human African, Human Caucasian	Healthy; Healthy;	oral administration	20 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >
AUC (0-inf)	947	ng h/mL	human African, Human Caucasian	Healthy; Healthy;	oral administration	20 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >
AUC (0-t) (to the last detectable concentration)	903	ng h/mL	human African, Human Caucasian	Healthy; Healthy;	oral administration	20 mg	Single	Courtney, Pfeifer, Al-Hasani, Gemes, Vieira, Ben-Ohman, Colombari/Diabetes, obesity and metabolism, 2011, vol. 13, # SUPPL. 1, p. 47 - 52 Full Text > Cited 23 times > Details > Abstract >

所有数据都提供原文链接，以保证数据的真实性。

Agenda

- 化合物活性数据的获取
- 文献与专利中活性数据的获取与提炼
- FDA/EMA审评文档中活性数据的获取与提炼

Case 2: 如何用Reaxys快速筛选对“冠状病毒”有活性的化合物

- 获取文献中报道的对“RNA依赖的RNA聚合酶（RdRp）”有活性报道的化合物
- 希望这些化合物的IC50在um级别

The screenshot displays the Reaxys Query Builder interface. At the top, the 'Substances' tab is selected and highlighted with an orange box. The search criteria are defined in a query builder panel:

- Target Name: is rdrp
- Measurement Parameter: is ic50
- Measurement pX: >= 6

Navigation and utility icons are visible at the top, including 'Import', 'Save', 'Reset form', 'Delete all', 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. A 'Tips' box on the right side of the interface contains the following text:

Tips:
利用Query Builder构建靶点，检测参数，以及参数大小的检索式

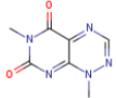
Reaxys中的结果

Reaxys[®] Quick search Query builder **Results** Synthesis planner History Register > Sign in ?

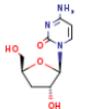
1.20 K Filters

Limit to > Exclude > 0 Limit To Exclude Export Preparations No of References ↓ Grid Heatmap

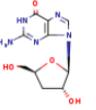
1,204 Substances out of 33 Documents, containing 2,896 Reactions, 6 Targets

1  **toxoflavin**
C₇H₇N₅O₂ 193.165 21014 84-82-2

Identification	Physical Data - 22	Preparations - 19 >
Druglikeness	Spectra - 29	Reactions - 23 >
Bioactivity (Hit Data)	Other Data - 3	Targets - 27 >
Bioactivity (All)		Documents - 124 >

2  **3'-deoxycytidine**
C₉H₁₃N₃O₄ 227.22 616742 7057-33-2

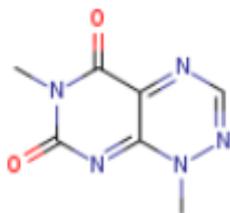
Identification	Bioactivity (All)	Preparations - 54 >
Druglikeness	Physical Data - 15	Reactions - 92 >
Bioactivity (Hit Data)	Spectra - 31	Targets - 10 >
		Documents - 44 >

3  **3'-deoxyguanosine**
C₁₀H₁₃N₅O₄ 267.244 561508 3608-58-0

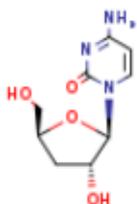
Identification	Bioactivity (All)	Preparations - 20 >
Druglikeness	Physical Data - 12	Reactions - 55 >

Reaxys直接给出符合条件的化合物，大量节省了科研人员阅读文献的时间，可以通过各自的Hit Data查看具体数据

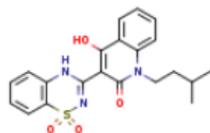
Reaxys中的结果



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Concomitants	Reference
6.22	IC50	=	0.6	μM	Hepatitis C virus	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild	Other compound: ATP; Radioligand: [3H]UTP;	Middleton; Lim; Montgomery; Rockway; Liu; Klein; Qin; Harlan; Kati; Molla [Letters in drug design and discovery , 2007, vol. 4, # 1, p. 1 - 8] Full Text ↗ Cited 3 times ↗ Details > Abstract >



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Concomitants	Reference
7.1	IC50		0.08 - 1.2	μM	Hepatitis C virus		RNA-dependent RNA polymerase [Hepatitis C virus]:Wild		Mayhoub, Abdelrahman S. [Bioorganic and Medicinal Chemistry , 2012, vol. 20, # 10, p. 3150 - 3161] Full Text ↗ Cited 35 times ↗ Details > Abstract >



pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Action on target	Target	Concomitants	Reference
7.1	IC50	=	0.08	μM	Hepatitis C virus (strain DELTA 21)	Inhibitor	RNA-dependent RNA polymerase [Hepatitis C virus]:Wild		Dhanak, Dashyant; Duffy, Kevin J.; Johnston, Victor K.; Lin-Goerke, Juili; Darcy, Michael; Shaw, Antony N.; Gu, Baohua; (...) Keenan, Richard M.; Sarisky, Robert T. [Journal of Biological Chemistry , 2002, vol. 277, # 41 p. 38322 - 38327] Full Text ↗ Cited 172 times ↗ Details > Abstract

利用HeatMap看结构与靶点关系

Reaxys

Quick search Query builder Results Synthesis planner History Register > Sign in

1,20 K Filters

Limit to > Exclude >

1,204 Substances out of 33 Documents, containing 2,896 Reactions, 6 Targets

Limit To Exclude Export Preparations No of References Grid Heatmap

By Structure Measurement pX Highest Clinical Phases Targets Parameters Substance Classes Molecular Weight Number of Fragments Availability Availability in other databases Available Data Document Type Publication Year Patent Assignee

toxoflavin
C₁₁H₇N₅O₂ 193 165 21014 84-82-2
Identification Physical Data - 22 Preparations - 19 >
Druglikeness Spectra - 29 Reactions - 23 >
Bioactivity (Hit Data) Other Data - 3 Targets - 27 >
Bioactivity (All) Documents - 124 >

3'-deoxycytidine
C₉H₁₃N₃O₄ 227.22 616742 7057-33-2
Identification Bioactivity (All) Preparations - 54 >
Druglikeness Physical Data - 15 Reactions - 92 >
Bioactivity (Hit Data) Spectra - 31 Targets - 10 >
Documents - 44 >

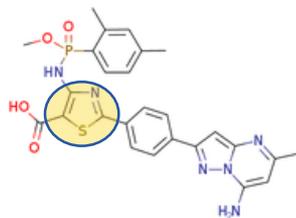
3'-deoxyguanosine
C₁₀H₁₃N₅O₄ 267.244 561508 3608-58-0
Identification Bioactivity (All) Preparations - 20 >
Druglikeness Physical Data - 12 Reactions - 55 >



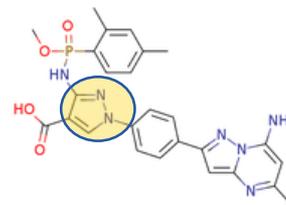
利用Reaxys中的Heat Map，直接进行查看，靶点，结构，活性数据之间的关系，并可将活性从高到低进行排序。

一些非常有意思的结构

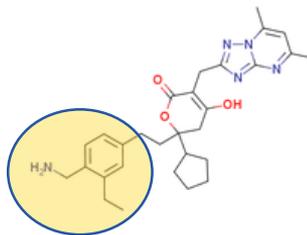
Substances	Targets
	RNA-dependent RNA polymerase
5-thiazolec... ylamine]	9.5
(E)-N-(4-(... fonamide	9.5
IDX17119	9.4
20673525	9.3
5-thiazolec... l-amine]	9.1
20673509	9.1
20673487	9.1
29885944	9
27259279	9
6-cyclope... an-2-one	9
(6R)-6-cy... an-2-one	9
6-cyclope... an-2-one	9
6-cyclope... an-2-one	9
6-cyclope... an-2-one	9
N-(4-(3-(t... fonamide	8.9
5-[2-(4-flu... boxamide	8.7
(1aR,12b... boxamide	8.7
20673500	8.7
N-(4-(2-(2... cetamide	8.7
6-cyclope... an-2-one	8.7
6-cyclope... an-2-one	8.7
N-(2-[4-(2... cetamide	8.7
6-cyclope... an-2-one	8.7



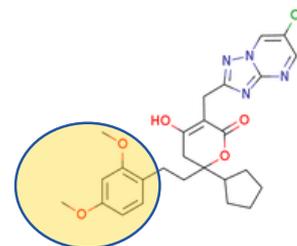
PX=9.5



PX=9.4



PX=8.0



PX=7.7

Case 3: 双靶点活性化合物的获取

- PI3K和mTOR双抑制剂，且活性都在nM级别化合物

The screenshot displays the Reaxys Query Builder interface. At the top, there are navigation tabs: Quick search, Query builder (selected), Results, Synthesis planner, and History. On the right, there are buttons for Register and Sign in. Below the navigation, there is a search bar with the text "Search in:" and four dropdown menus: Reactions, Targets, Substances, and Documents. Underneath the search bar, there are icons for Import, Save, Reset form, and Delete all. To the right of these icons are icons for Structure, Molecular Formula, CAS RN, and TI, AB & KW. The main area shows a "Selectivity Profile" window with two target profiles. The first profile is for PI3K, with the condition "Target Name is PI3K" and "Measurement pX >= 9". The second profile is for mTOR, with the condition "Target Name is mTOR" and "Measurement pX >= 9". On the right side of the interface, there is a sidebar with "Search fields and forms" and a list of search criteria: Reaxys Forms, Reaxys MedChem Forms, Affinity on target, Cell proliferation: inhibition, Selectivity Profile, Animal models: Tumor xenografts, Bioavailability, Volume of distribution, and Absorption (Cmax, Cavg).

双靶点活性化合物

利用Heat Map查看活性数据

96 Substances out of 47 Documents, containing 148 Reactions, 17 Targets

0 selected Limit To Exclude Export Preparations

1

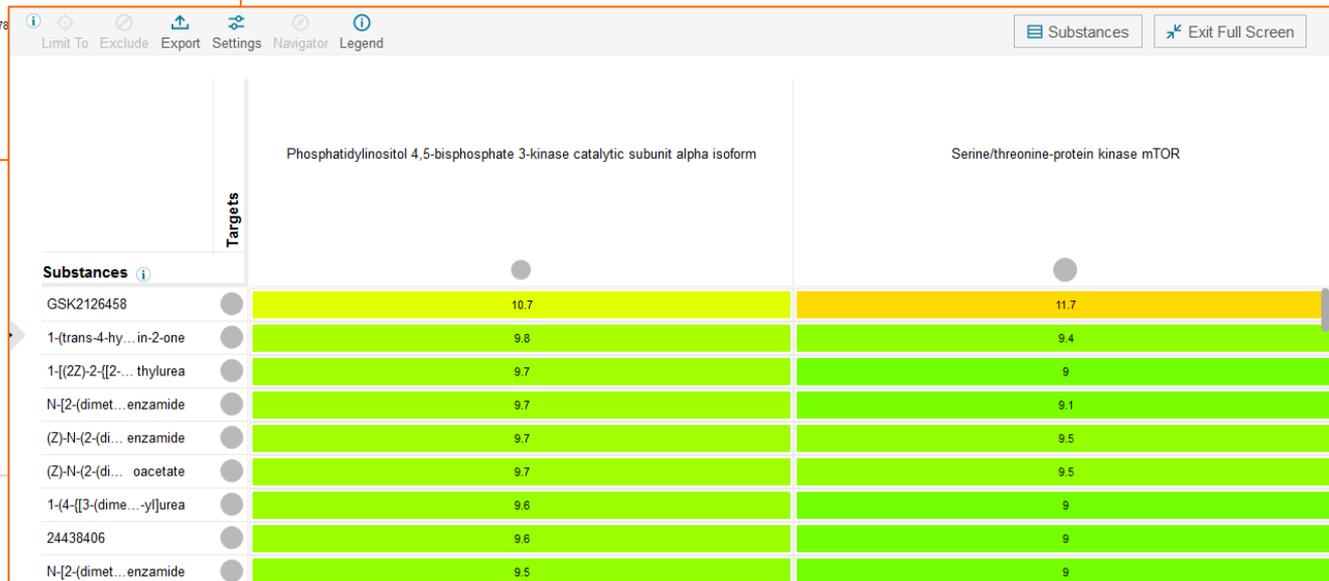
GSK2126458
C28H17F2N4O3S 505.504 20875369 1086062-66-9

Identification Bioactivity (All)
Druglikeness Physical Data - 3
Bioactivity (Hit Data) Spectra - 3

2

PKI-587
C22H41N5O4 615.735 19641026 1197160-78

Identification
Druglikeness
Bioactivity (Hit Data)



Case 4: 通过效用找化合物

- 看一下近3年内文献/专利中报道过的，有抗生素效用的化合物，且IC50在uM级别的化合物

The screenshot displays the Reaxys Query Builder interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History' are in the center. On the right, there are 'Register >' and 'Sign in' buttons. Below the navigation, a 'Search in:' section includes buttons for 'Reactions >', 'Targets >', 'Substances >', and 'Documents >'. A toolbar contains icons for 'Import', 'Save', 'Reset form', and 'Delete all'. The main search area features a 'Structure' icon and buttons for 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. A search criteria panel is open, showing a query with the following conditions:

- Publication Year \geq 2018
- Group 1 (AND):
 - Measurement Parameter is ic50
 - Substance Effect contains antibiotic agent
 - Measurement pX \geq 6

On the right side, a 'Search fields' sidebar is visible, listing various search categories: Fields, Forms, History, Reaxys, Topics and Keywords, Identification, Physical Properties, Spectra, MedChem, Other, Reactions, and Bibliographv. A 'Feedback' button is located at the bottom right of the sidebar.

最后的结果

Filters

1,988 Substances out of 129 Documents, containing 6,692 Reactions, 142 Targets

Limit to > Exclude >

0 selected Limit To Exclude Export Preparations

Sort by No of References ↑

Grid Heatmap

By Structure

Measurement pX

Highest Clinical Phases

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Availability in other databases

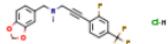
Available Data

Document Type

Publication Year

Patent Assignee

1



N-(benzo[d][1,3]dioxol-5-ylmethyl)-3-(2-fluoro-4-(trifluoromethyl)phenyl)-N-methylprop-2-yn-1-amine hydrochloride
C₁₉H₁₅F₄NO₂*ClH 401.788 32162844

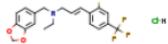
Hit Data - 7 Bioactivity (Hit Data) Spectra - 3 Preparations - 6 >

Identification Bioactivity (All) Reactions - 6 >

Druglikeness Physical Data - 3 Documents - 1 >

Hit Data - 7

2



(E)-N-(benzo[d][1,3]dioxol-5-ylmethyl)-Nethyl-3-(2-fluoro-4-(trifluoromethyl)phenyl)prop-2-en-1-amine hydrochloride
C₂₀H₁₉F₄NO₂*ClH 417.831 32162857

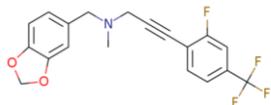
Hit Data - 7 Bioactivity (Hit Data) Spectra - 3 Preparations - 6 >

Identification Bioactivity (All) Reactions - 6 >

Druglikeness Physical Data - 3 Documents - 1 >

Hit Data - 7

一些比较有意思的数据



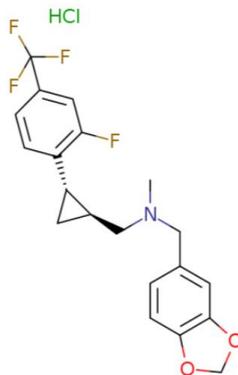
Cl-H

^ In vitro: Efficacy - 1

Quantitative Results

Show/Hide columns

pX	Parameter	Value (quant)	Unit	Biological Species	Effect	Reference
7.75	IC50	17.9	nM	Staphylococcus aureus Newman	antibiotic agent	Wei, Hanwen; Mao, Fei; Ni, Shuaishuai; Chen, Feifei; Li, Baoli; Qiu, Xiaoxia; Hu, Linghao; (...) Lan, Lefu; Li, Jian[European Journal of Medicinal Chemistry, 2018, vol. 145, p. 235 - 251] Full Text Cited 4 times Details Abstract



HCl

^ In vitro: Efficacy - 1

Quantitative Results

Show/Hide columns

pX	Parameter	Value (qual)	Value (quant)	Unit	Biological Species	Effect	Reference
6	IC50	>	1000	nM	Staphylococcus aureus Newman	antibiotic agent	Wei, Hanwen; Mao, Fei; Ni, Shuaishuai; Chen, Feifei; Li, Baoli; Qiu, Xiaoxia; Hu, Linghao; (...) Lan, Lefu; Li, Jian[European Journal of Medicinal Chemistry, 2018, vol. 145, p. 235 - 251] Full Text Cited 4 times Details Abstract

Agenda

- 化合物活性数据的获取
- 文献与专利中活性数据的获取与提炼
- FDA/EMA审评文档中活性数据的获取与提炼

PharmaPendium(www.pharmapendium.com)

- PharmaPendium是唯一提供上市药物，临床前与临床，药效，药物安全与药代动力学、药物代谢与转运酶，药物不良反应报告等数据的一站式平台；同时还收录此领域的权威期刊书籍内容，如Meyler副反应大全和Mosby用药参考等，助力药物筛选和研发进程。

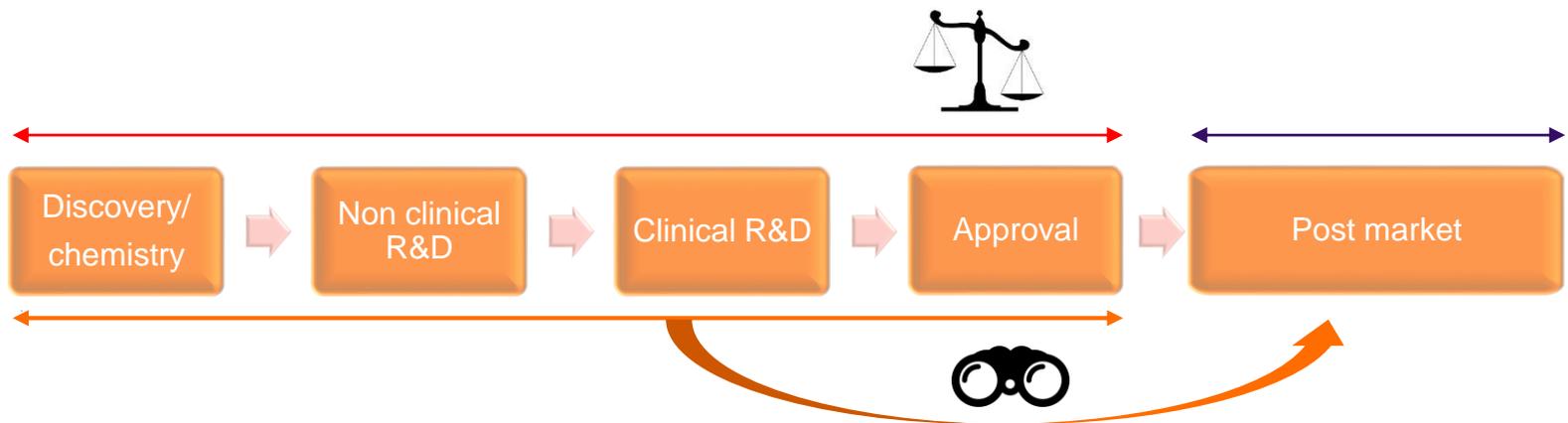
FDA & EMA所有的approval package (FDA: 1938年- 今，EMA: 1995年— 今)



PharmaPendium的主要用途

报批：监管机构将安全性、有效性和可交付性与已上市药品进行比较（风险/效益分析）

只有当药物的性能优于市场上已经上市的药物时，才会批准使用



因此，在开发和批准过程中，您需要充分了解已上市药品的监管数据！！

Case 5: FDA/EMA中获批药物活性数据的获取

- 案例要求与背景：
 - 正在开发一个用于治疗克罗恩病的单抗
 - 竞争产品的Cmax数据有哪些？什么情况下做出来的这个数据？
 - 数据影响：评估竞争定位并优化实验设计

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Browse ▾ Search ▾ My tools ▾ | IP-authorized

Quick Search

All These Sources ▾ e.g. Coronar* artery disorders

Include synonyms

Find adverse effect/toxicity data across preclinical, clinical, post-market reports and more

- Pharmacokinetic Data
- Metabolizing Enz. & Trans. Data
- Drug Safety Data
- FAERS Data ^{new}
- Chemistry Search
- Efficacy Data
- Activity Data
- DDI risk calculator

ELSEVIER

- Drugs
- Adverse Effects/Toxicity
- Targets
- Indications

获取所有FDA/EMA中用于治疗克罗恩疾病的药物

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Browse Search My tools | IP-authorized

Browse indications > Gastrointestinal disorders > Gastrointestinal inflammatory conditions > Gastrointestinal inflammatory disorders NEC > Crohn's disease > Crohn's disease

Crohn's disease

Drugs related to indication
Showing 6 out of 29 items

Drugs	Sources where Indication - Drug association is found							
	FDA Label	EMA ANNEX	FDA Classic	Efficacy (FDA)	Efficacy (EMA)	DESI	MOSBY'S	Meyler
Adalimumab	FDA Label	EMA ANNEX		Efficacy (FDA)	Efficacy (EMA)			
Betamethasone							MOSBY'S	
Betamethasone Acetate; Betamethasone Sodium Phosphate							MOSBY'S	
Betamethasone Sodium Phosphate							MOSBY'S	
Budesonide	FDA Label			Efficacy (FDA)			MOSBY'S	
Certolizumab Pegol	FDA Label			Efficacy (FDA)	Efficacy (EMA)			

▼ Show all 29

Biology data:
Crohn's disease

- View Pharmacokinetic Data
- View Metabolizing ENZ. & Trans. Data
- View Drug Safety Data
- View FAERS Data
- View Efficacy Data
- View All Activity Data (Primary/Non-Primary) for Drugs approved for Crohn's disease

通过疾病检索，获取所有获批药物

其中所有的PK数据

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Browse Search My tools | IP-authorized

Pharmacokinetic data search results

Show/hide columns Show drugs in... Alert Save Share Export

18640 records from PK Data: [Budesonide (3483) OR Methylprednisolone Acetate (1075) OR Dexamethasone (674) OR Certolizumab Pegol (1071) OR Natalizumab (1032) OR Methylprednisolone Sodium Succinate (168) OR Ustekinumab (875) OR Secukinumab (705) OR Prednisone (515) OR Methylprednisolone (287) OR Hydrocortisone (144) OR Triamcinolone Acetonide (2097) OR Dexamethasone Sodium Phosphate (24) OR Dexamethasone Sodium Phosphate (30) OR Cortisone Acetate (1) OR Infliximab (1773) OR Vedolizumab (462) OR Prednisolone Sodium Phosphate ...

Filters Clear all Apply

Preclinical Data Clinical Data All Data

Parameter ranges	ID	Drug	Species	Study Group	Dose	Route	Parameter	Parameter Value
	1	Adalimumab	Human		160 mg loading dose followed by 80 mg on Week 2	Subcutaneous	Cavg	12.0 ug/mL
Drugs	2	Adalimumab	Cynomolgus monkey		157 mg/kg	Intravenous	AUC(0-168h)	632786.0 ug*h/mL
Routes of Administration	3	Adalimumab	Human	healthy, anti-drug antibodies (ADA) - negative	40 mg	Subcutaneous	AUC(0-inf)(geometric mean)	2627.0 ug*h/mL
Sources	4	Adalimumab	Human	rheumatoid arthritis	0.5 mg/kg	Intravenous	AUC(0-inf)	3189.0 ug*h/mL
Species	5	Adalimumab	Cynomolgus monkey		157 mg/kg	Subcutaneous	AUC(0-168h)	589000.0 ug*h/mL
Study Group	6	Adalimumab	Human	rheumatoid arthritis	40 mg	Subcutaneous	Tmax	5.0 d
Radiolabelled	7	Adalimumab	Human	moderate-severe Crohn's disease	80-160 mg	Subcutaneous	Cmin(serum)	12.3 ug/mL (6.3ug/mL - 23.5ug/mL)
Metabolites/Enantiomers	8	Adalimumab	Human	moderate to severe	40 mg	Subcutaneous	Cmin(serum)(geometric mean)	6139.12 ng/mL

Default Settings or Save Filter Settings

利用筛选工具进行筛选

Parameter ranges

Type parameter ranges to search

- Absorption (9668)
 - %absorbed (56)
 - Bioavailability (423)
- Concentrations (7450)
 - C (1925)
 - Cavg (237)
 - Cmax (3124)
 - Cmin (2138)
 - LCmax (26)
- Fa (17)
- FaFg (2)
- Fh (1)

Drugs

Type drug or drug class to search

- Antipsoriatics (217)
- Biologics (1264)
 - Monoclonal antibodies (1264)
 - Recombinant DNA Origin (548)
- Corticosteroids (1683)
- Dermatologics (811)
- Disease modifying antirheumatic drugs (...)
- Gastrointestinals (609)
- Immunomodulators (715)
- Immunosuppressives (217)
- Ophthalmics (216)

Sources

- FDA approval packages (861)
- EMA approval documents (395)
- PharmaPendium Published PK (8)

多种筛选工具，进行筛选，Cmax，单抗，FDA

最后的结果

PharmaPendium[®] Browse Search My tools | IP-authorized

Pharmacokinetic data search results

861 records from PK Data: [Budesonide (0) OR Methylprednisolone Acetate (0) OR Dexamethasone (0) OR Certolizumab Pegol (0) OR Natalizumab (229) OR Methylprednisolone Sodium Succinate (0) OR Ustekinumab (78) OR Secukinumab (78) OR Prednisone (0) OR Methylprednisolone (0) OR Hydrocortisone (0) OR Triamcinolone Acetonide (0) OR Betamethasone Sodium Phosphate (0) OR Dexamethasone Sodium Phosphate (0) OR Cortisone Acetate (0) OR Infliximab (206) OR Vedolizumab (68) OR Prednisolone Sodium Phosphate (0) OR Betamethasone (0) OR Triamcinolone (0) OR Adalimumab (202) OR Prednisolone (0)] AND [Natalizumab (229) OR Infliximab (206) OR Ustekinumab (78) OR ...]

Preclinical Data Clinical Data All Data

ID	Drug	Species	Study Group	Dose	Route	Parameter	Parameter Value	SD	t	Concomitants	Source	Year
1	Adalimumab	Human	healthy	40 mg	Subcutaneous	C _{max} (geometric mean)	3,901 ug/mL				FDA approval package document: Approval Package (Page:11) View Full Study PDF 440k	2019
2	Adalimumab	Human	healthy	40 mg	Subcutaneous	C _{max}	4.7 ug/mL	1.6			FDA approval package document: Clinical Pharmacology and Biopharmaceutics Review (Page:27) View Full Study PDF 844k	2017
3	Adalimumab	Human	healthy, anti-drug antibodies (ADA) - negative	40 mg	Subcutaneous	C _{max} (geometric mean)	3172.0 ng/mL				FDA approval package document: Clinical Pharmacology and Biopharmaceutics Review (Page:15) View Full Study PDF 7359k	2016
4	Adalimumab	Human	healthy	40 mg	Subcutaneous	C _{min} (geometric mean)	4.7 ng/mL	1.6			FDA approval package document: Approval Package (Page:23) View Full Study PDF 4141k	2007
5	Adalimumab	Human	healthy	40 mg	Subcutaneous	C _{min}					FDA approval package document: Approval Package (Page:30) View Full Study PDF 4973k	2010
6	Adalimumab	Cynomolgus monkey		32 mg/kg	Subcutaneous	C _{min}					FDA approval package document: Approval Package (Page:42) View Full Study PDF 4358k	2019
7	Adalimumab	Cynomolgus monkey		157 mg/kg	Subcutaneous	C _{min}					FDA approval package document: Approval Package (Page:19) View Full Study PDF 3010k	2019
8	Adalimumab	Human	healthy	40 mg	Subcutaneous	C _{min}					FDA approval package document: Label (Page:15) View Full Study PDF 2933k	2007
9	Adalimumab	Cynomolgus monkey		157 mg/kg	Intravenous	C _{min}					FDA approval package document: Review (Page:16) View Full Study PDF 1743k	2017
10	Adalimumab	Human	healthy	40 mg/0.8 mL	Subcutaneous	C _{min}					FDA approval package document: Clinical Pharmacology and Biopharmaceutics Review (Page:6) View Full Study PDF 733k	2016
11	Adalimumab	Cynomolgus monkey		157 mg/kg	Subcutaneous	C _{min}					FDA approval package document: Approval Package (Page:18)	2019

Biosimilar Multi-disciplinary Evaluation and Review (BMER)
BLA 761118
PF-06410293 a proposed biosimilar to Humira

06410293 and US-Humira.

Table 6. Summary of statistical analyses for assessment of PK similarity (Study B5381007)

Parameter	Statistic	PF-06410293 (n=106)		US-HUMIRA (n=101)	EU-HUMIRA (n=104)	Geometric Mean Ratio* (90% CI)		
		PF-06410293 vs US-HUMIRA	PF-06410293 vs EU-HUMIRA	PF-06410293 vs US-HUMIRA	PF-06410293 vs EU-HUMIRA			
Primary								
AUC ₀₋₂₄ (µg·h/mL)	Geometric Mean	2910	2534	2757	112.00 (102.39, 122.50)	104.3 (91.3, 114.62)	106.81 (97.62, 116.85)	
AUC ₀₋₄₈ (µg·h/mL)	Geometric Mean	2569	2275	2414	112.90 (103.60, 123.63)	106.42 (97.72, 115.90)	106.09 (97.31, 115.65)	
C _{min} (µg/mL)	Geometric Mean	4.344	3.891	3.901	111.64 (104.18, 119.64)	111.36 (103.97, 119.27)	100.25 (93.52, 107.46)	

*Presented as percent. Source: FDA analysis

Overall, from a clinical pharmacology perspective, the submitted clinical pharmacology studies [1] support a demonstration that there are no clinically meaningful differences between PF-06410293 and US-Humira and [2] establish the PK component of the scientific bridge that justifies the relevance of comparative data generated using EU-Humira to the assessment of biosimilarity.

ELSEVIER

Case 6: 如何利用FDA/EMA中的数据评估竞争地位

- 案例要求与背景:

- 想评估我的新药对Histone deacetylases (HDAC) 的血清蛋白结合率
- 其他药物的血清蛋白结合值有哪些?
- 数据影响: 评估竞争定位和优化实验设计, 避免监管问题



PharmaPendium®

Browse Search My tools

Pharmacokinetic data search Clinical & preclinical data

Reset all Search

Drugs

- + Add drugs by drug class or drug name
- + Add drugs by primary target or primary target class
- + Add drugs by indication

Parameter ranges

- + Add parameter ranges

Species

- + Add species

Sources

- + Add sources

Add drugs by primary target or primary target class

Search on: Histone Deacetylases

By SuperFamily

- Enzymes
- Deacetylases
- Histone Deacetylases

Add parameter ranges

Search on: Serum protein binding

Binding

- Protein binding
- Serum protein binding

Search on: Serum protein binding

Above Below %

最后的检索策略

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Pharmacokinetic data search Clinical & preclinical data Reset all Search

Drugs

Belinostat Panobinostat Lactate Romidepsin

Parameter ranges

Serum protein binding

Above Below %

- + Add drugs by drug class or drug name
- + Add drugs by primary target or primary target class
- + Add drugs by indication

Pharmapendium将
FDA/EMA中的数据
全部提炼，并做了
结构化处理

PharmaPendium®

Pharmacokinetic data search results

24 records from PK Data: [Belinostat (0) OR Panobinostat Lactate (0) OR Romidepsin (24)] AND [Serum protein binding (24)]

Preclinical Data Clinical Data All Data

ID	Drug	Species	Study Group	Dose	Route	Parameter	Parameter Value	SD	t	Concomitants	Source	Year
1	Romidepsin	Human		50-1000 ng/mL	In Vitro	serum protein binding	94.0% - 95.0%				EMA approval document: Assessment Report (Page45) View Full Study PDF 1459k	2012
2	Romidepsin	Human		50-1000 ng/mL	In Vitro	serum protein binding	≥82.0%				FDA approval package document: Pharmacology Review (Page53) View Full Study PDF 5492k	2009
3	Romidepsin	Rat		50-500 ng/mL	In Vitro	serum protein binding	37.0 %				FDA approval package document: Pharmacology Review (Page53) View Full Study PDF 5492k	2009
4	Romidepsin	Rat		50 ng/mL	In Vitro	serum protein binding	40.81 %	0.89			FDA approval package document: Pharmacology Review (Page56) View Full Study PDF 5492k	2009
5	Romidepsin	Human		50 ng/mL	In Vitro	serum protein binding	94.53 %	0.25			FDA approval package document: Pharmacology Review (Page56) View Full Study PDF 5492k	2009
6	Romidepsin	Dog		50 ng/mL	In Vitro	serum protein binding	87.7 %	0.4			FDA approval package document: Pharmacology Review (Page56) View Full Study PDF 5492k	2009
7	Romidepsin	Human	healthy	50-1000 ng/mL	In Vitro	serum protein binding	94.0% - 95.0%				FDA approval package document: Clinical Pharmacology and Biopharmaceutics Review (Page15) View Full Study PDF 4309k	2009
8	Romidepsin	Human		5000 ng/mL	In Vitro	serum protein binding	82.16 %	1.18			FDA approval package document: Pharmacology Review (Page56) View Full Study PDF 5492k	2009
9	Romidepsin	Dog		500 ng/mL	In Vitro	serum protein binding	86.48 %	0.7			FDA approval package document: Pharmacology Review (Page56) View Full Study PDF 5492k	2009
10	Romidepsin	Human		500 ng/mL	In Vitro	serum protein binding(albumin)	19.91 %	0.41			FDA approval package document: Pharmacology Review (Page56) View Full Study PDF 5492k	2009
11	Romidepsin	Rat		5000 ng/mL	In Vitro	serum protein binding	37.98 %	0.27			FDA approval package document: Pharmacology Review (Page56) View Full Study PDF 5492k	2009

导出后的结果

Export date: 14-07-2020
 Pharmacokinetic Data Search Results For: Drugs: [Belinostat (0) OR Panobinostat Lactate (0) OR Romidepsin (24)] AND Parameters
 Total results: 24
 Sort order: Drug (Ascending);

Drug	Species	Study Group	Dose	Route	Parameter	Value	Units	Normalized Value (only standard units are displayed)	SD	t	Concomitants	Source	Source Link
Romidepsin	Human		50-1000 ng/mL	In Vitro	serum protein binding	94 to 95	%	94 to 95	%			EMA approval document: Assessment Re	https://www.pharmapendium.com/b
Romidepsin	Human		50-1000 ng/mL	In Vitro	serum protein binding	>=82	%	>=82	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Rat		50-500 ng/mL	In Vitro	serum protein binding	37	%	37 (37 to 37)	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Rat		50 ng/mL	In Vitro	serum protein binding	40.81	%	40.81 (39.92 to 41.7)	%	0.89		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human		50 ng/mL	In Vitro	serum protein binding	94.53	%	94.53 (94.28 to 94.78)	%	0.25		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Dog		50 ng/mL	In Vitro	serum protein binding	87.7	%	87.7 (87.3 to 88.10000000000001)	%	0.4		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human	healthy	50-1000 ng/mL	In Vitro	serum protein binding	94 to 95	%	94 to 95	%			FDA approval package document: Clinical	https://www.pharmapendium.com/b
Romidepsin	Human		5000 ng/mL	In Vitro	serum protein binding	82.16	%	82.16 (80.97999999999999 to 83.34)	%	1.18		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Dog		500 ng/mL	In Vitro	serum protein binding	86.48	%	86.48 (85.78 to 87.18)	%	0.7		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human		500 ng/mL	In Vitro	serum protein binding (albumin)	19.91	%	19.91 (19.5 to 20.32)	%	0.41		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Rat		5000 ng/mL	In Vitro	serum protein binding	37.98	%	37.98 (37.709999999999994 to 38.25)	%	0.27		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Rat		500 ng/mL	In Vitro	serum protein binding	37	%	37 (37 to 37)	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human	healthy	5000 ng/mL	In Vitro	serum protein binding	82	%	82 (82 to 82)	%			FDA approval package document: Clinical	https://www.pharmapendium.com/b
Romidepsin	Dog		500 ng/mL	In Vitro	serum protein binding	86	%	86 (86 to 86)	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human		500 ng/mL	In Vitro	serum protein binding (alpha1-acid glycoprotein)	93.51	%	93.51 (93 to 94.020000000000001)	%	0.51		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Dog		500 ng/mL	In Vitro	serum protein binding	86	%	86 (86 to 86)	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Rat		500 ng/mL	In Vitro	serum protein binding	37.75	%	37.75 (37.47 to 38.03)	%	0.28		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human		500 ng/mL	In Vitro	serum protein binding	94	%	94 (94 to 94)	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human		500 ng/mL	In Vitro	serum protein binding	94.18	%	94.18 (93.81 to 94.550000000000001)	%	0.37		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human		500 ng/mL	In Vitro	serum protein binding	94	%	94 (94 to 94)	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Human		1000 ng/mL	In Vitro	serum protein binding	93.55	%	93.55 (93.429999999999999 to 93.67)	%	0.12		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Dog		5000 ng/mL	In Vitro	serum protein binding	73.14	%	73.14 (73.02 to 73.26)	%	0.12		FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Rat		500 ng/mL	In Vitro	serum protein binding	37	%	37 (37 to 37)	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b
Romidepsin	Dog		500 ng/mL	In Vitro	serum protein binding	37	%	37 (37 to 37)	%			FDA approval package document: Pharm	https://www.pharmapendium.com/b

2.6.4.4 Distribution

Study title: Non-clinical pharmacokinetics: *in vitro* protein binding of FR901228 in rats, dogs, humans, and human serum proteins

Key study findings:

- Protein binding was independent of romidepsin concentration from 50 ng/mL – 500 ng/mL in rat and dog serum and from 50 ng/mL – 1000 ng/mL in human serum.
- Protein binding decreased at 5000 ng/mL romidepsin in human and dog serum.
- Protein binding was higher in serum from dogs (86%) and humans (94%) than in rats (37%) at 500 ng/mL romidepsin.
- Romidepsin bound better to α_1 -AGP (93%) than to albumin (20%).

Case 7: 如何利用FDA/EMA中的数据进行安全基线评估

- 案例要求与背景:

- 开发PD-1/PD-L1药物
- 作用于这些靶点的药物的上市后常见效应是什么?
- 数据影响: 竞争定位和安全基线的获取



Summary Table and Graphical View ^{new}

Select drugs of interest

Select adverse events (AEs) of interest

[Start](#)

PharmaPendium®

Summary Table with Adverse Effects Tree (FAERS data)

View as [Table](#) [Graph](#) Compare Filters View AEs by [area affected](#) [▼](#) [Exp](#)

Summary Table with Adverse Effects Tree	Add Drugs
+ Blood and lymphatic system disorders	
+ Cardiac disorders	

添加所有的PD-1/PD-L1药物

PharmaPendium®

Browse ▾ Search ▾ My tools ▾ |  IP-authorized   

Add Drugs [Add column\(s\)](#) [Back](#)



[by name or class](#) **[by primary target or target class](#)** [by indication](#)

- By SuperFamily [Add](#)
- Other proteins [Add](#)
- Programmed death ligand-1 (PD-L1) [Add](#)

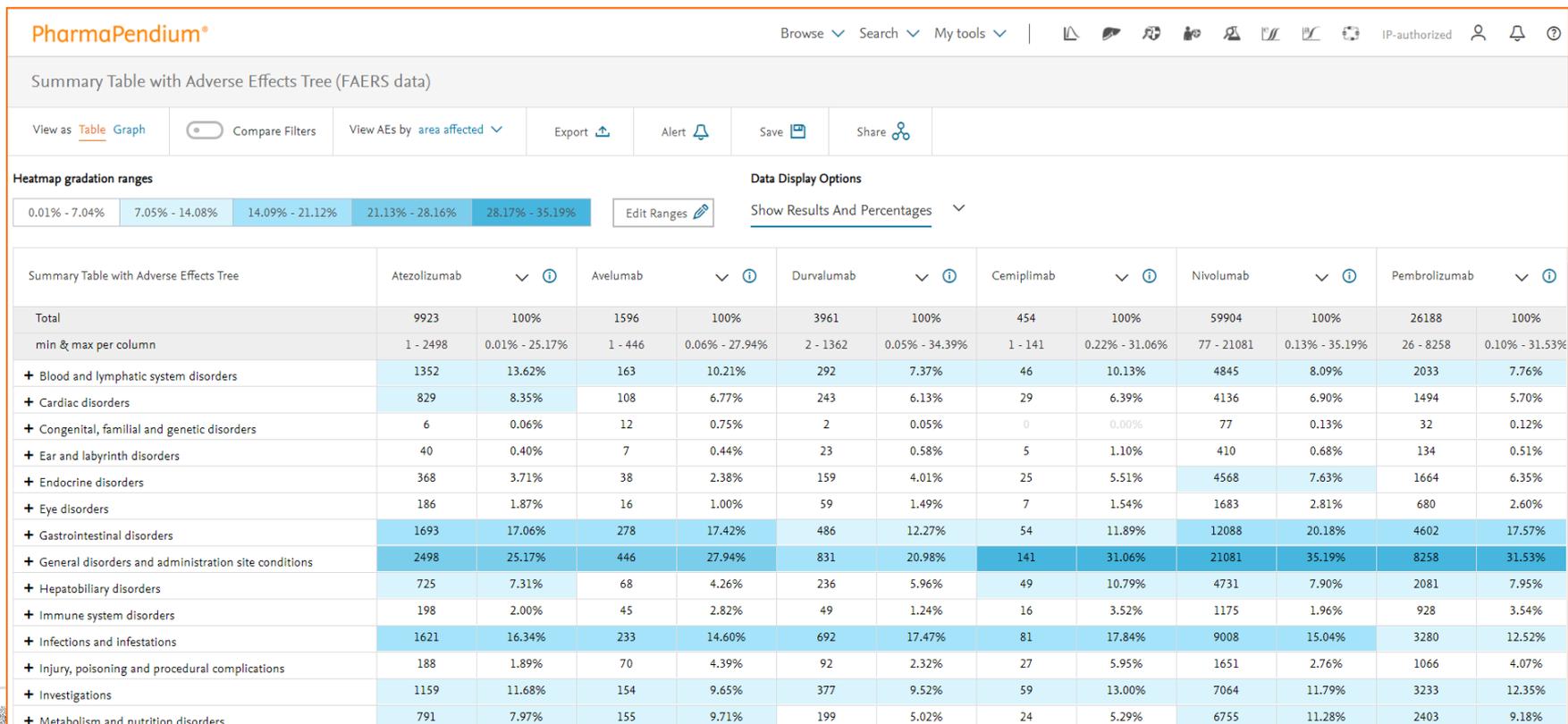
Logic operators

Each element from the following selection will be added as separate column:

× Atezolizumab	Any role ▾
× Avelumab	Any role ▾
× Durvalumab	Any role ▾
× Cemiplimab	Any role ▾
× Nivolumab	Any role ▾
× Pembrolizumab	Any role ▾

通过靶点添加PD-1, PD-L1药物

一键生成数据热图

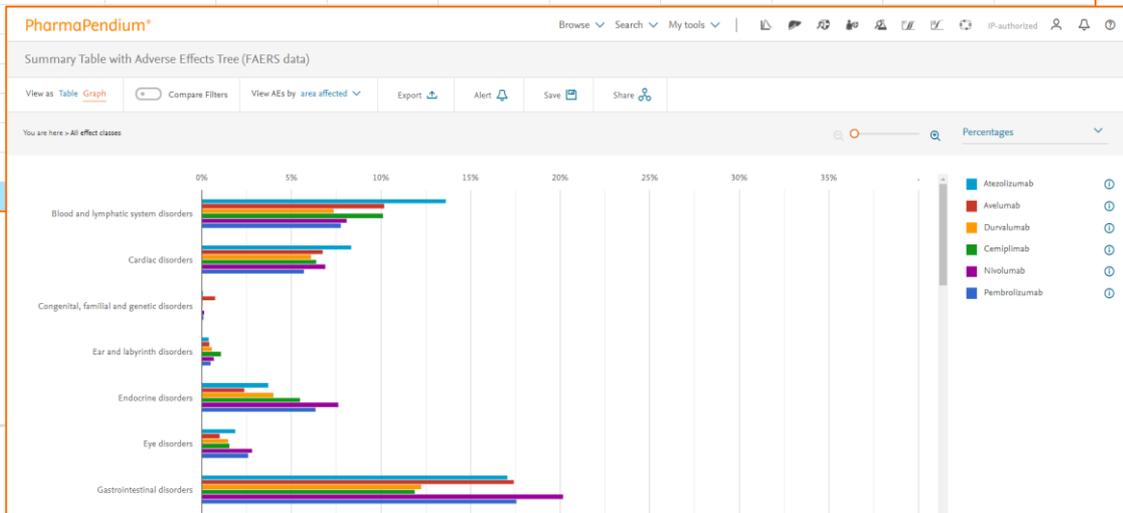


更多具体细节信息

Summary Table with Adverse Effects Tree	Atezolizumab	▼ ⓘ	Avelumab	▼ ⓘ	Durvalumab	▼ ⓘ	Cemiplimab	▼ ⓘ	Nivolumab	▼ ⓘ	Pembrolizumab	▼ ⓘ
- General disorders and administration site conditions	2498	25.17%	446	27.94%	831	20.98%	141	31.06%	21081	35.19%	8258	31.53%
+ Administration site reactions	6	0.06%	2	0.13%	19	0.48%	6	1.32%	88	0.15%	118	0.45%
+ Body temperature conditions	589	5.94%	81	5.08%	199	5.02%	30	6.61%	3120	5.21%	1321	5.04%
+ Complications associated with device	3	0.03%	0	0.00%	5	0.13%	0	0.00%	43	0.07%	10	0.04%
- Fatal outcomes	609	6.14%	95	5.95%	233	5.88%	22	4.85%	8468	14.14%	2085	7.96%
- Death and sudden death	609	6.14%	95	5.95%	233	5.88%	22	4.85%	8468	14.14%	2085	7.96%
Accidental death	0	0.00%	0	0.00%	0	0.00%	0	0.00%	2	0.00%	0	0.00%
Brain death	2	0.02%	0	0.00%	0	0.00%	0	0.00%	2	0.00%	3	0.01%
Cardiac death	2	0.02%	0	0.00%	1	0.03%	0	0.00%	2	0.00%	3	0.01%
Death	587	5.92%										
Death neonatal	0	0.00%										
Drowning	0	0.00%										
Euthanasia	0	0.00%										
Sudden cardiac death	0	0.00%										
Sudden death	18	0.18%										
+ General system disorders NEC	1442	14.53%										



查看不同领域的效应



生物活性数据与文献的获取与提炼

- RMC从大量文献和专利中摘取和物质生物活性相关的数据，帮助科研人员获得标准化，规范化，格式化的数据列表及参考文献
- PharmaPendium帮助全面获取上市药物的监管数据，可以为实验方案的设计，产品定位提供全方位的数据支持
- Elsevier Life Science培训中心
 - <https://www.elsevier.com/zh-cn/rd-solutions/pharma-and-life-sciences-solutions/life-sciences-online-training-center>



扫码进群，获取视频，PPT以及最新资料。





Thank you

