



Elsevier Life Science Solution

Reaxys案例分享，药学院适用，基础化学信息检索，
以及药学专利检索技巧



吴鹏 16621600327
p.wu.1@elsevier.com
爱思唯尔生命科学客户顾问





今天的内容

- 文献检索的原理简介
- Reaxys数据库药物核心信息，合成方法检索技巧
- Reaxys数据库专利检索技巧
- Reaxys Medicinal Chemistry数据检索技巧

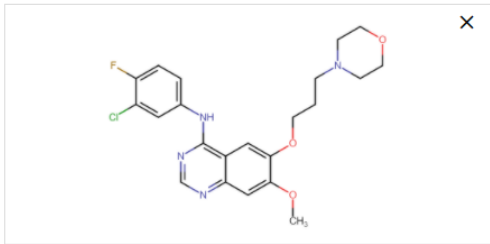
如何有效的检索某个药物的信息

Reaxys® [Quick search](#) [Query builder](#) [Results](#) [Synthesis planner](#) [History](#) [Alerts](#) Peng Wu  

Search for  [Import](#) 

Search Reaxys [Find >](#)

Substance ADME, e.g. [Pharmacokinetic of Imatinib](#)
AND







As drawn


1. 物化性质, 生物活性
2. 合成方法, 分析方法
3. 细节研究文献, 如金型
4. 合成路线涉及

将药物的结构式画入, 直接检索即可

Content Overview | Latest update: 07. May 2021 >

148M	54M	61M	40M
 Substances	 Reactions	 Documents	 Bioactivities

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Reaxys-化合物核心信息的整理特点

362 Substances out of 6,573 Documents, containing 172 Reactions, 1,093 Targets

0 selected Limit To Exclude Export

Sort by No of References ↓ Grid Heatmap

Reaxys - 362

362 Preview

Filters

- Limit to >
- Exclude >
- 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 gefitinib
C₂₂H₂₄N₄ClFO₃ 446.909 8949523 184475-35-2

Identification
Druglikeness

Bioactivity (All)
Physical Data - 94

Spectra - 69
Other Data - 3,110

Preparations - 77 >
Reactions - 120 >
Targets - 1,072 >
Documents - 6,548 >

2 Gefitinib hydrochloride
C₂₂H₂₄ClFN₄O₃*ClH 483.37 14998854 184475-55-6

Identification

Bioactivity (All) 药物生物活性

- In vitro: Efficacy - 10
- In vivo: Animal Model - 634
- Metabolism - 311
- Pharmacokinetic - 672
- Toxicity/Safety Pharmacology - 1404

Spectra - 60 分析鉴定

- NMR Spectroscopy - 36
- IR Spectroscopy - 8
- Mass Spectrometry - 11
- UV/VIS Spectroscopy - 4
- Raman Spectroscopy - 1

Physical Data - 79 物化信息

- Melting Point - 23
- Association (MCS) - 1
- Chromatographic Data - 4
- Conformation - 1
- Crystal Phase - 7
- Crystal Property Description - 18
- Crystal System - 1
- Dissociation Exponent - 2

Reaxys-合成方法

495 Substances out of 10,262 Documents, containing 200 Reactions, 1,188 Targets

0 selected

Limit To Exclude Export Preparations

Reaxys - 495

Sort by No of References ↓

Grid Heatmap

By Structure Measurement pX Highest Clinical Phases Targets Parameters Substance Classes

gefitinib
C22H24N4ClFO3 446,909 8949523 184475-35-2

Identification Druglikeness

Bioactivity (All) Physical Data - 117

Spectra - 81 Other Data - 4,169

Preparations - 83 Reactions - 148 Targets - 1,151 Documents - 10,228

最后一步合成方法

Synthesis Planner Edit

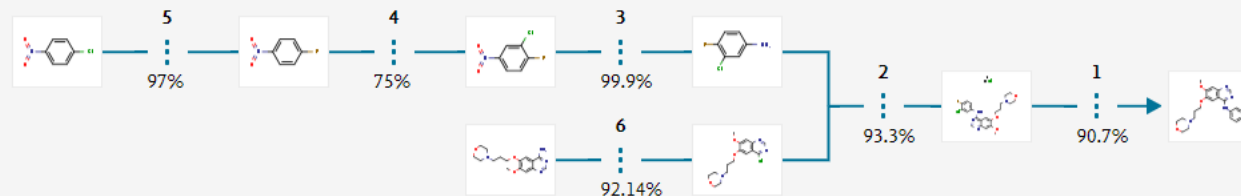
Autoplan 1 5

Plan 1

Import Save Export

Undo Redo

1. 一键获取合成路线
2. 多种不同合成选择



Reaxys-药物相关文献获取

495 Substances out of 10,262 Documents, containing 200 Reactions, 1,188 Targets

0 selected

Limit To Exclude Export Preparations

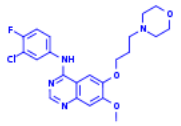
Sort by No of References

Grid Heatmap

By Structure Measurement pX Highest Clinical Phases Targets Parameters Substance Classes

gefitinib
C₂₂H₂₄N₄ClFO₃ 446.909 8949523 184475-35-2

Identification Bioactivity (All) Spectra - 81 Preparations - 83
Druglikeness Physical Data - 117 Other Data - 4,169 Reactions - 148
Targets - 1,151
Documents - 10,228



10,228 Documents with 62,061 Substances, 73,219 Reactions, 2,303 Targets

0 selected

Limit To Exclude Export

Sort by Publication Year

Heatmap

Index Terms (List)

Index Terms (ReaxysTree)

- physico chemical properties 4,870
- chemical transformations 4,684
- physico chemical analysis ... 1,702
- quantum chemical calculatio... 205

View more

Publication Year Document Type Authors Patent Assignee

1 Current progress and future perspectives of polypharmacology: From the view of non-small cell lung cancer
Karuppasamy, Ramanathan; Veerappapillai, Shanthi; Maiti, Sayoni; Shin, Woong-Hee; Kihara, Daisuke [Seminars in Cancer Biology, 2021, vol. 68, p. 84 - 91]
Abstract Index Terms Substances 48 Full Text Hit Substances 1

2 Repurposing of plant alkaloids for cancer therapy: Pharmacology and toxicology
Efferth, Thomas; Oesch, Franz [Seminars in Cancer Biology, 2021, vol. 68, p. 143 - 163]
Abstract Index Terms Substances 43 Full Text Hit Substances 1

3 Repurposing old drugs as new inhibitors of the ubiquitin-proteasome pathway for cancer treatment
Yang, Huanjie; Chen, Xin; Li, Kai; Cheaito, Hassan; Yang, Qianqian; Wu, Guojun; Liu, Jinbao; Dou, Q. Ping [Seminars in Cancer Biology, 2021, vol. 68, p. 105 - 122]
Abstract Index Terms Substances 64 Full Text Hit Substances 1

Index Terms (ReaxysTree) 60

- Index Terms (ReaxysTree) 10,228
 - physico chemical properties 4,870
 - chemical transformations 4,684
 - physico chemical analysis methods 1,702
 - separation method 803
 - spectroscopical analysis 777
 - microscopy 379
 - quantitative analysis 82
 - thermal analysis 79
 - elemental analysis 61
 - crystal structure determination 60
 - X-ray diffraction 52
 - neutron diffraction 2

晶型鉴定

Selected search items:
crystal structure de...

Clear selected

Limit to Exclude



今天的内容

- 文献检索的原理简介
- Reaxys数据库药物核心信息，合成方法检索技巧
- Reaxys数据库专利检索技巧
- Reaxys Medicinal Chemistry数据检索技巧

专利信息检索的挑战



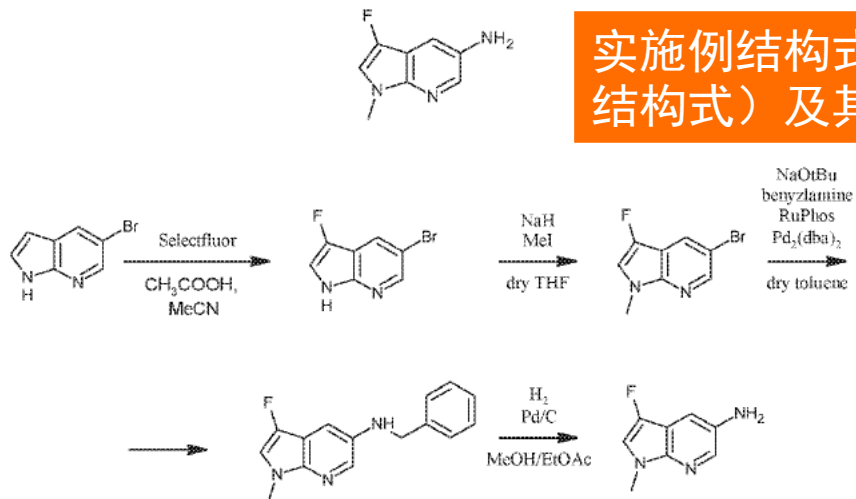
1. 如何进行结构式检索？如何解读Markus
2. 如何不用结构式，追踪最新的专属领域的专利？
3. 如何用关键词细分，专利细节？



1. 理解：专利中的化合物结构式与Markush结构关系
2. 在专利结构式被提炼到数据库前，快速跟踪专利
3. 拆分专利细节，靶点，晶型，剂型，工艺等

专利基础信息简介-人工抓取内容-结构式生物活性收录

Intermediate 11



实施例结构式（具体化合物结构式）及其生物活性

Example	Structure	Method Starting intermediate	LC-MS (ESI) [M+H] ⁺
1		A 1 and 48	377.2
2		A 1 and 49	415.1
3		A 2 and 48	391.2
4		A 10 and 48	405.2
5		E 3 and 48	392.2

20 Table 16 shows the PAM EC₅₀ values in the [Ca²⁺]_i assay:

Table 16

Example	EC ₅₀ (nM)	Example	EC ₅₀ (nM)
1	500	86	590
2	760	88	2800
3	90	90	85
4	920	92	55
5	400	108	2200
6	100	109	900

Tips:

1. 实施例结构决定化合物的‘新颖性’
2. 目前WO的英文版+US/EP/CN/TW/JR/KR
非英文版会摘取结构式
3. WO/US/EP会摘取靶点，生物活性等

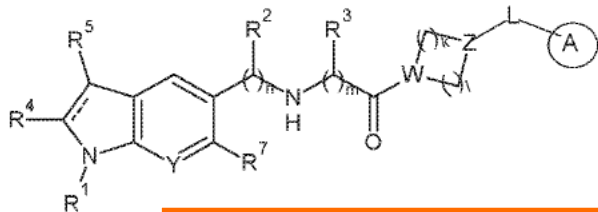
专利基础信息简介-人工抓取内容-claim



CLAIMS

1. A compound of formula (I),

Markus结构
(专利中具体结构式的通式)



Markus结构包含了，专利中的具体实施例结构，以及由实施例方法同理可推的结构式

5 wherein

R¹ is hydrogen or C₁₋₆alkyl;

R² is hydrogen or C₁₋₆alkyl, or R² is absent when n is 0;

R³ is hydrogen or O; or R³ is absent when m is 0;

R⁴ and R⁵ are independently hydrogen, C₁₋₆alkyl, halogen, haloC₁₋₆alkyl, C₁₋₆alkoxy,

10 or CN;

n and m are independently 0 or 1, with the proviso that, n and m cannot be 0 at the same time;

k and l are independently 1, 2 or 3;

Y is N or C(R⁶);

15 R⁶ is hydrogen, C₁₋₆alkyl, halogen, or haloC₁₋₆alkyl;

R⁷ is hydrogen, C₁₋₆alkyl, or halogen;

W is CH or N;

专利claim是对专利的核心发明内容的具体描述

prevention of a disease associated with $\alpha 7$ nicotinic acetylcholine receptor activity.

A compound according to claim 5, wherein the disease is selected from the group of psychotic disorders, including, but not limited to, schizophrenia, schizophreniform disorder, schizoaffective disorder, delusional disorder, brief psychotic disorder, psychotic disorder due to a general medical condition, substance-induced psychotic disorder or psychotic disorder not otherwise specified, cognitive impairment, including, but not limited to, cognitive impairment as a result of stroke, Alzheimer's disease, Huntington's disease, Pick disease, HIV associated dementia, frontotemporal dementia, Lewy body dementia, vascular dementia, cerebrovascular disease or other dementia states and dementia associated to other degenerative disorders, including, but not limited to, amyotrophic lateral sclerosis, other acute or sub-acute conditions that may cause cognitive decline, including, but not limited to, delirium, traumatic brain injury, senile dementia, mild cognitive impairment, Down's syndrome, depression and cognitive deficit related to other diseases, and dyskinetic disorders including, but not limited to, Parkinson's disease, neuroleptic-induced parkinsonism, or tardive dyskinesias, depression and mood disorders, including, but not limited to, depressive disorders and episodes, bipolar disorders, cyclothymic disorder, and bipolar disorder not otherwise specified, other mood disorders, substance-induced mood disorder and mood disorder not otherwise specified, anxiety disorders, panic disorder and panic attacks, obsessive compulsive disorder, posttraumatic stress disorder, acute stress disorder, generalized anxiety disorder, anxiety disorder due to a

同类型数据库，只有Rx对claim进行全文抓取，并索引可检索，且全球专利，统一翻译为英文

专利基础信息简介-专利标记

Main IPC

International Patent Classification:

C07D 403/12 (2006.01) C07D 209/10 (2006.01)
 C07D 401/12 (2006.01) C07D 209/42 (2006.01)
 C07D 471/04 (2006.01) A61K 31/404 (2006.01)
 C07D 209/08 (2006.01) A61K 31/437 (2006.01)

Secondary IPC

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)
 (19) World Intellectual Property Organization
 International Bureau
 (43) International Publication Date
 16 January 2020 (16.01.2020) **WIPO | PCT**



(10) International Publication Number
WO 2020/012424 A1

(51) International Patent Classification:
 C07D 403/12 (2006.01) C07D 209/10 (2006.01)
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 C07D 471/04 (2006.01) A61K 31/404 (2006.01)
 C07D 209/08 (2006.01) A61K 31/437 (2006.01)

UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU, TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK, SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, KM, ML, MR, NE, SN, TD, TG).

(21) International Application Number: PCT/IB2019/055950

(22) International Filing Date: 12 July 2019 (12.07.2019)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data: P1800250 13 July 2018 (13.07.2018) HU

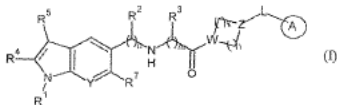
(71) Applicant: RICHTER GEDEON NYRT. [HU/HU]; Gyömrői út 19-21., 1103 Budapest (HU).

(72) Inventors: LEDNECZKI, István, Baracsi u. 14., 7025 Böleske (HU); ELES, János, Ördögszikla út 2., 1121 Budapest (HU); TAPOLCSÁNYI, Pál, Lahner György u. 2/B., 1046 Budapest (HU); HORVÁTHI, Anita, Fügöcinegy u. 7., 1171 Budapest (HU); NEMETHY, Zsolt, Ibolya u. 3., 2151 Göd (HU); LEVAY, György István, Gábor Áron u. 10., 2092 Budakeszi (HU); GALAMBOS, János, Cserkút u. 40., 1162 Budapest (HU).

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ, TZ,

(54) Title: SUBSTITUTED (AZA)INDOLE DERIVATIVES



(57) Abstract: The invention relates to substituted (aza)indole derivatives, or pharmaceutically acceptable salts, biologically active metabolites, pro-drugs, racemates, enantiomers, diastereomers, solvates and hydrates thereof, as well as to pharmaceutical compositions containing them and to their use as modulators of $\alpha 7$ nicotinic acetylcholine receptor activity in a mammalian subject. (1)

全球105个专利局，
 专利公开之后5-7
 个工作日，即可用
 Reaxys跟踪相应
 领域的专利

分类号	含义	中国专利	世界专利
C	化学; 冶金		
C07	有机化学		
C07D	杂环化合物		
403/00	杂环化合物，含有两个或更多的杂环，以氮原子作为仅有的杂环原子，C07D 401/00 组不包含的	<input type="checkbox"/>	<input type="checkbox"/>
403/02	含两个杂环	<input type="checkbox"/>	<input type="checkbox"/>
403/12	...被含有杂原子的链作为键链连接	<input type="checkbox"/>	<input type="checkbox"/>

IPC可以大致描述结构概况，
 快速跟踪同类型结构专利

分类号	含义	中国专利	世界专利
A	农业		
A61	医学或兽医学; 卫生学		
A61K	医用、牙科用或梳妆用的配制品		
31/00	含有机有效成分的医药配制品	<input type="checkbox"/>	<input type="checkbox"/>
31/33	杂环化合物	<input type="checkbox"/>	<input type="checkbox"/>
31/395	...有氮作为环杂原子的，例如胍乙啶、利福霉素	<input type="checkbox"/>	<input type="checkbox"/>
31/40	...有仅以1个氮作为环杂原子的五元环的，例如舒必利、琥珀酰亚胺、托尔米丁、甲氧吡丁苯	<input type="checkbox"/>	<input type="checkbox"/>
31/403	...与碳环稠合的，例如咪唑	<input type="checkbox"/>	<input type="checkbox"/>
31/404	...咪唑类，例如咪唑洛尔	<input type="checkbox"/>	<input type="checkbox"/>

WO 2020/012424 A1

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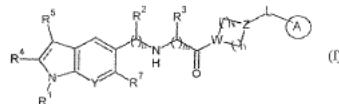
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(71) Applicant: RICHTER GEDEON NYRT. [HU/HU] Gyömrői út 19-21., 1103 Budapest (HU).

Patent assignee
(专利受让人)

(72) Inventors: LEDNECZKI, István; Baracsi u. 14., 7025 Bölske (HU). ÉLES, János; Ördögcsikla út 2., 1121 Budapest (HU). TAPOLCSÁNYI, Pál; Lahner György u. B., 1046 Budapest (HU). HORVÁTH, Anita; Fügöcinege u. 7., 1171 Budapest (HU). NÉMETHY, Zsolt; Ibolya u. 3., 2131 Göd (HU). LÉVAY, György István; Gábor Áron u. 10., 2092 Budakeszi (HU). GALAMBOS, János; Cserkút u. 40., 1162 Budapest (HU).

Patent inventors
(专利发明人)

(54) Title: SUBSTITUTED (AZA)INDOLE DERIVATIVES

专利的标题摘要

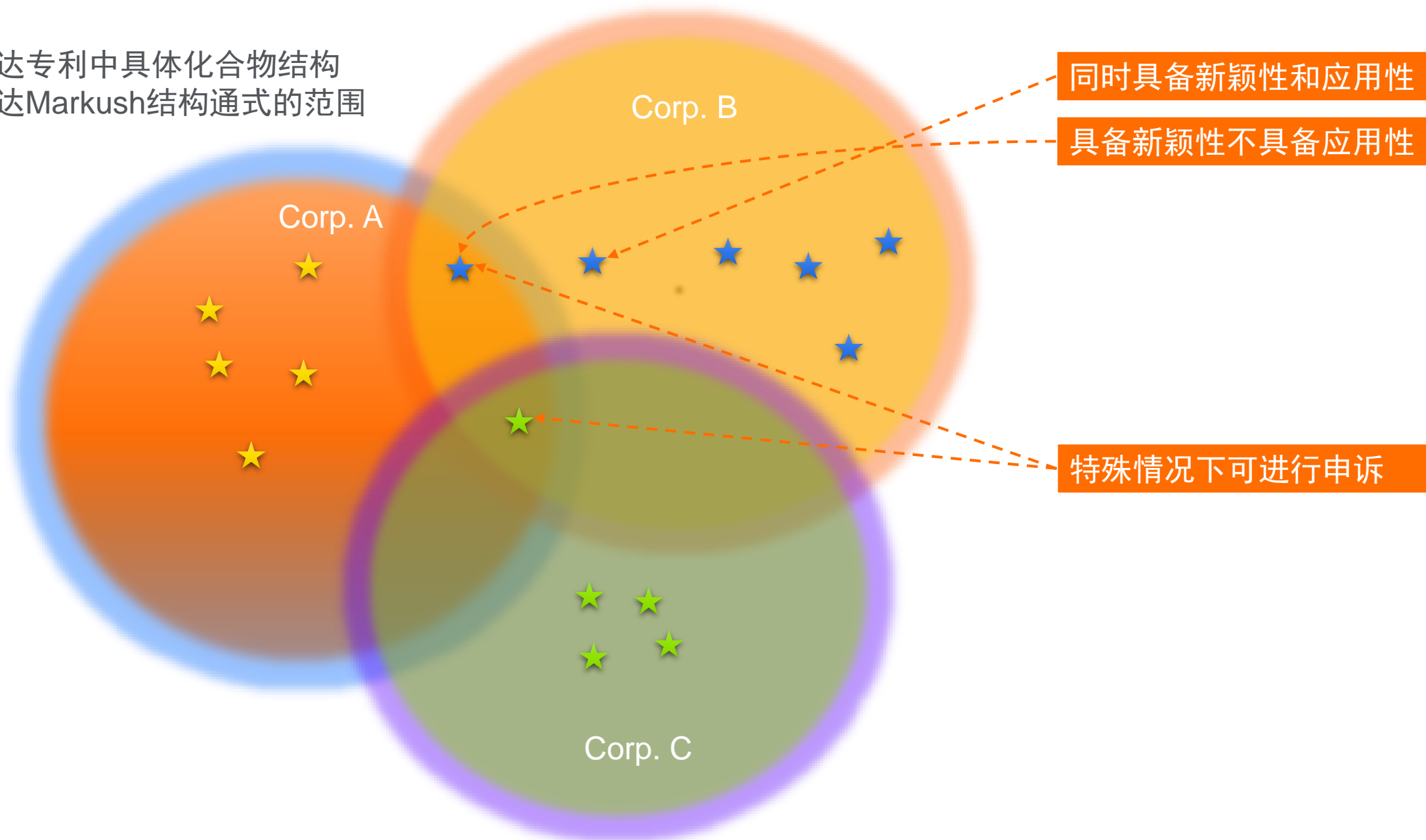
(57) Abstract: The invention relates to substituted (aza)indole derivatives, or pharmaceutically acceptable salts, biologically active metabolites, pro-drugs, racemates, enantiomers, diastereomers, solvates and hydrates thereof, as well as to pharmaceutical compositions containing them and to their use as modulators of $\alpha 7$ nicotinic acetylcholine receptor activity in a mammalian subject. (I)

Tips:

1. 专利标记机器收录
2. 收录时间快, 收到专利局数据后约7个工作日内
3. 无论何种语言, 只要属于rx专利收录范围, 都会收录

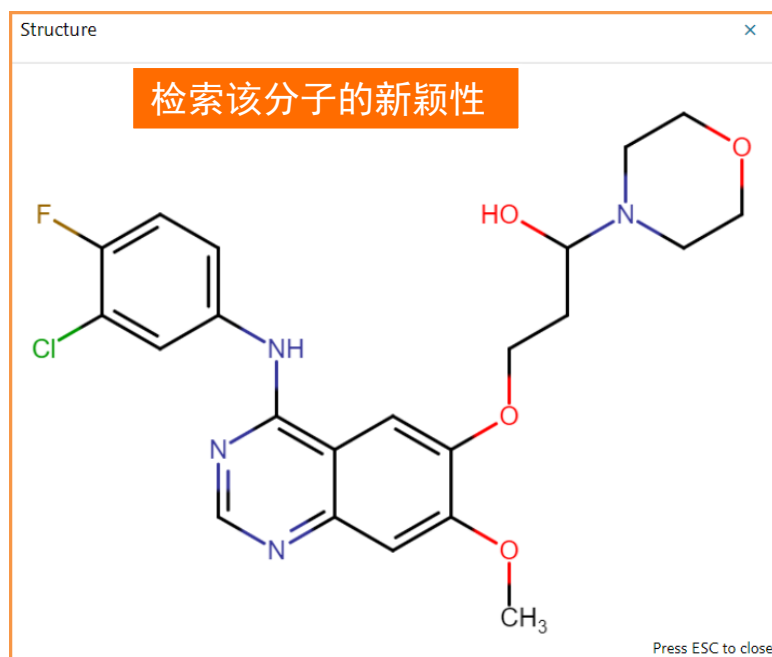
专利布局概览（应用性/新颖性研究）

1. 星星表达专利中具体化合物结构
2. 圆圈表达Markush结构通式的范围



Case 1 小分子药物新颖性检索--Markush检索的基本模式

- 是否有专利的实施例结构跟新设计的分子一致？
- 是否有专利的Markush结构已经覆盖了该新颖分子？
- 如何设计分子能绕开Markush覆盖范围？

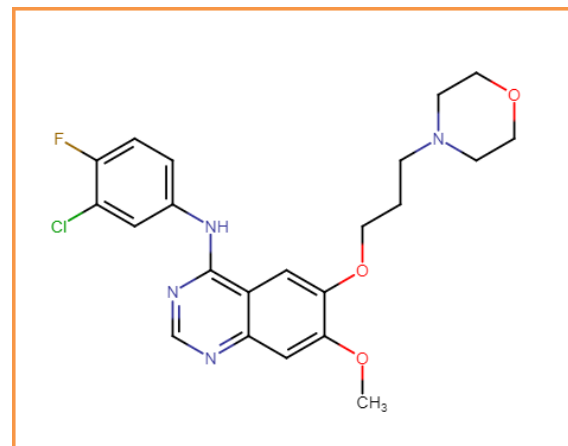
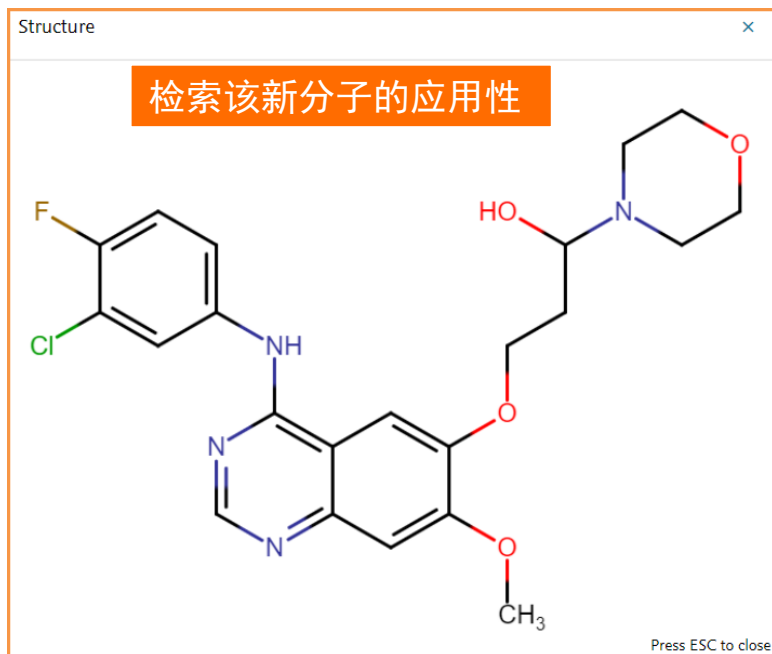


	0	Substances	Structure : as drawn Edit in Query Builder	直接检索结果为零
	0	Targets	Structure : as drawn Edit in Query Builder Create Alert	
	0	Substances	Structure : average similarity; included: only absolute stereo, additional ring closures allowed, salts, mixtures, isotopes, charges, radicals Edit in Query Builder Create Alert	
	0	Reactions	Reaction Query : as drawn Edit in Query Builder Create Alert	

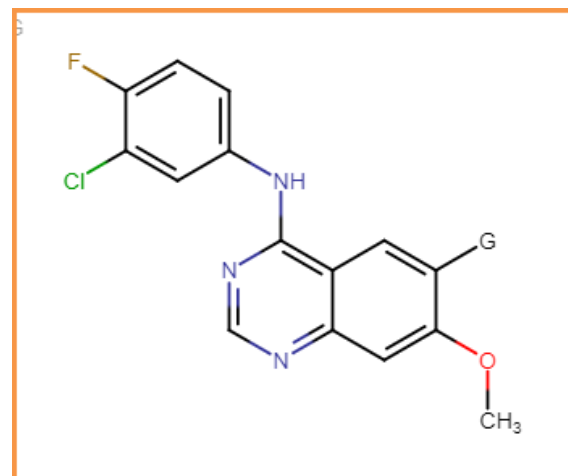
Tip: 具体化合物检索, 检索为0, 即可大致确认其为新颖的, 新颖性需要不同数据库重复多检索几次, 以保证不漏检

Markush检索的基本模式

➤ 通过分析之后，可以通过相似已存在结构的markush锁定结果



方法1：通过一直的分子，对应的Markush，研究该Markush是否包含新分子



方法2：限定一定范围的检索，总览在‘G’为点做改构，一系列专利中Markush是否包含新分子

Tip: Rx Markush规则：所检索的结构必须是实施例或者实施例的一部分

Markush检索的基本模式-方法1：最相关结构检索

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

Structure editor ChemAxon's MarvinJS Create structure template from name >

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes
- Charges
- Radicals

+ More options

Clear Cancel Transfer to query > Feedback

Markush检索，会把‘结构式’中确切的部分去匹配专利中的‘实施例结构’命中相关专利

整个分子都是确切结构

注意关联Markush其余的‘异构体’选项请关闭以避免干扰

Markush检索的基本模式-检索结果

Reaxys

Quick search Query builder Results Synthesis planner History

Register > Sign in

11 Substances out of 6,211 Documents, containing 116 Reactions, 1,069 Targets

1 selected Limit To Exclude Export

Sort by No of References ↓ Grid Heatmap

1 gefitinib
C22H24N4ClF3 44

Bioactivity (All) Spectra - 65
Druglikeness Physical Data - 88 Other Data - 2,972

Preparations - 76 >
Reactions - 116 >
Targets - 1,069 >
Documents - 6,211 >

2

Reaxys ID: 11329531
11329531

Identification Documents - 1 >
Other Data - 3

3

Reaxys ID: 18419582
18419582

Identification Documents - 1 >
Other Data - 42

4

Reaxys ID: 20784707
20784707

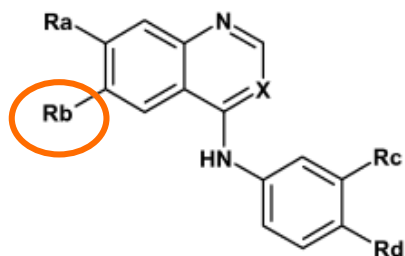
Identification Documents - 1 >

Feedback

排除第一个结构所包含的文献，即为10个Markush结构及其对应的专利

方法1：通过最相关结构，检索到‘最相关’Markush，解读Markush结构，理解新分子的‘应用性’，并获取最相关专利

Markush结构解读



原文中的markush结构，
Rb到底是什么结构？

- 20 wherein each Ra, Rb, Rc and Rd is independently selected from hydrogen, halo, amino, hydroxyamino, carboxy, C₁₋₈alkoxycarbonyl, nitro, guanidino, ureido, carbamoyl, cyano, trifluoromethyl, (R⁶)₂N-carbonyl and phenyl-W-alkyl wherein W is selected from a single bond, O, S and NH;
- 25 or each Ra or Rb is independently selected from cyano-C₁₋₈alkyl and R9 wherein R9 is from the group consisting of R5, R5O, (R5)₂N, R7C(=O), R5ONH, A and R5Y; wherein R5 is C₁₋₈alkyl; R6 is hydrogen or R5 wherein the R5s if more than one is present are the same or

69

Rb is di-(C₁₋₈alkyl)-amino-C₁₋₈alkoxy, pyrrolidin-1-yl-C₁₋₈alkoxy, piperidino-C₁₋₈alkoxy, morpholino-C₁₋₈alkoxy, piperazin-1-yl-C₁₋₈alkoxy, 4-C₁₋₈alkylpiperazin-1-yl-C₁₋₈alkoxy, imidazol-1-yl-C₁₋₈alkoxy, di-(C₁₋₈alkoxy-C₁₋₈alkyl)-amino-C₁₋₈alkoxy, thiomorpholino-C₁₋₈alkoxy, 1-oxothiomorpholino-C₁₋₈alkoxy or 1,1-dioxothiomorpholino-C₁₋₈alkoxy, and wherein any of the above-mentioned Rb substituents comprising a CH₂ (methylene) group which is not attached to a N or O atom optionally bears on said CH₂ group a hydroxy substituent;

wherein

X is N,

Ra is -D-E-F and Rb is -SR^{4*}, halo, -OR^{4*}, -NHR^{3*} or hydrogen, or

Rb is -D-E-F and Ra is -SR^{4*}, halo, -OR^{4*}, -NHR^{3*} or hydrogen,

wherein X is C-CN;

Ra is C₁₋₈alkoxy;

20 Rb is amino- or N-[N'-mono- or N',N'-di(C₁₋₈alkyl)]amino-C₄₋₈alkenoyl)-amino;

Rc is halo or R₂^{**}-(CH₂)_n-R₃^{**};

wherein R₂^{**} is a pyridyl, thiophenyl, pyrimidinyl, thiazolyl or phenyl, each optionally substituted with up to three substituents selected from C₁₋₈alkyl, C₁₋₈alkoxy and halogen, R₃^{**} is -O- or -S- and n^{**} is 0 to 8, preferably 0 or 1;

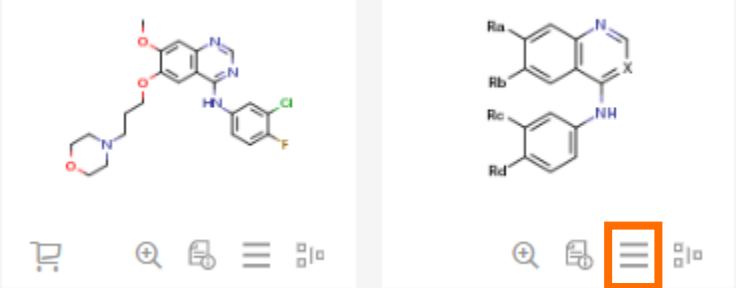
25 and Rd is halo;

or a pharmaceutically acceptable salt or prodrug thereof;

and an antibody inhibiting EGFR;

Markush结构解读

Hit Substances

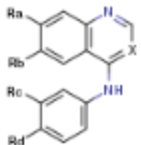


0 selected Limit To Exclude Export

Options

- > Find Similar
- > View details
- > Copy structure to query

1



Reaxys ID: 23992506
23992506

Identification

Other Data - 5

Identification

Reaxys ID: 23992506

Chemical Names:

CAS Registry Number(s):

Molecular Formula:

Molecular Weight:

InChIKey:

Patent-Specific Data - 1

Markush Details

Substance type:

Linear Structure

Formula:

No of references:

Label	什么基团	Value	具体官能团	Size	Attributes	Substituted by	Frequency
Rb		Ra		官能团大小		有无取代基	取代基频次
Ra		hydrogen					
		halogen					
		hydroxy	OH			\$s1	
		amino				\$s1	
		hydroxyamino				\$s1	
		carboxy				\$s1	
		alkoxycarbonyl		1-8C	or cyclic	\$s1	
		nitro					
		guanidino				\$s1	
		ureido				\$s1	
		carbamoyl				\$s1	
		cyano					
		trifluoromethyl					
		(R6)2N-\$carbonyl				\$s1	0-2
		Sphenyl-W-\$alkyl				\$s1	0-2

\$s1	halogen
	R9

R9	R5
	R5O
	(R5)2N
	R7C(=O)
	R5ONH
	A
	R5Y

Markush检索的基本模式-方法2：评估某侧链结构的新颖性

Structure editor ChemAxon's MarvinJS

Create structure template from name >

Search this structure as:

- As drawn
- As substructure
- Similar
- Tautomers
- Stereo
- Additional ring closures
- Related Markush
- Salts
- Mixtures
- Isotopes

charges
radicals
more options

指定原子取代
全开放S6

G为任意官能团

任意非氢原子A

原子取代全开放
S6

评估某侧链结构的新颖性—筛选Markush结构

1,359 Substances out of 6,552 Documents, containing 2,819 Reactions, 1,123 Targets

0 selected Limit To Exclude Export

Sort by No of References ↓ Grid Heatmap

Reaxys - 1,359

1.36 K Preview

Filters

- 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
- LogP

Molecular Weight 1

Clear selected × ↓ ↑ Sort by Occurrence ×

<input type="checkbox"/>	>816 - 828	1
<input type="checkbox"/>	>780 - 792	1
<input type="checkbox"/>	>768 - 780	1
<input type="checkbox"/>	>744 - 756	1
<input type="checkbox"/>	>720 - 732	1
<input type="checkbox"/>	>708 - 720	1
<input type="checkbox"/>	>672 - 684	1
<input type="checkbox"/>	>660 - 672	1
<input type="checkbox"/>	>336 - 348	1
<input checked="" type="checkbox"/>	(no entry given)	90

1 2 3 Limit to Exclude

Preparations - 76 >
Reactions - 116 >
Targets - 1,068 >
Documents - 6,334 >

Preparations - 41 >
Reactions - 254 >
Targets - 7 >
Documents - 72 >

Preparations - 3 >
Reactions - 3 >
T: Feedback

Identification Bioactivity (All) Other Data - 116
Druglikeness Physical Data - 1

筛选后的Markush结构

Reaxys[®] TotalPatent One[®] Quick search Query builder Results Synthesis planner History Alerts Peng Wu

From history Filters

Limit to > Exclude >

0 selected Limit To Exclude Export Preparations

97 Substances out of 69 Documents, containing 19 Reactions, 1 Targets

Sort by No of References ↓ List Heatmap

Markush及其对应的专利

1 2 3 4 5

6 7 8 9 10

11 12 13 14 15

Feedback



Tip: 当‘新分子’涉及项目非常重要是，需要对很多Markush进行解读，确保新分子的应用性

Case2: IPC快速索引专利

1. 用该结构检索的专利，是否会由遗漏？如何，快速检查？

The screenshot displays the Reaxys TotalPatent One web interface. At the top, the navigation bar includes the Reaxys logo, 'TotalPatent One', and menu items for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', 'History', and 'Alerts'. The user 'Peng Wu' is logged in. Below the navigation bar, a 'Search in:' section offers filters for 'Reactions', 'Targets', 'Substances', and 'Documents'. A toolbar provides actions like 'Import', 'Save', 'Reset form', and 'Delete all', along with search field options: 'Structure', 'Molecular Formula', 'CAS RN', and 'TI, AB & KW'. The main workspace shows a chemical structure of a complex molecule with a fluorinated and chlorinated benzene ring, a bicyclic amine, a pyridine ring with a methoxy group, and a tetrahydrofuran ring. The structure is labeled 'Absolute'. On the right, a 'Search fields' sidebar lists various search categories such as 'Fields', 'Forms', 'History', 'Topics and Keywords', 'Identification', 'Physical Properties', 'Spectra', 'MedChem', 'Other', 'Reactions', and 'Bibliography'. A 'Feedback' button is located at the bottom right of the sidebar.

Reaxys[®] | TotalPatent One[®] Quick search Query builder Results Synthesis planner History Alerts Peng Wu

Search in: **Reactions** > **Targets** > **Substances** > **Documents** >

Import Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW

◇ Structure Absolute

As drawn
ELSEVIER

Search fields

Fields Forms History

Reaxys ^

Topics and Keywords v

Identification v

Physical Properties v

Spectra v

MedChem v

Other v

Reactions v

Bibliography v

Feedback

1 Documents with 72 Substances, 122 Reactions, 4 Targets

该结构检索到专利1篇

0 Limit To Exclude Export

Publication Year ↓

Heatmap

AZABICYCLO-SUBSTITUTED TRIAZOLE DERIVATIVE, PREPARATION METHOD THEREOF, AND APPLICATION

1 OF SAME IN MEDICINE

Jiangsu Hengrui Medicine Co., Ltd.; Shanghai Hengrui Pharmaceutical Co., Ltd.; LI, Xin; CHEN, Yang; LIU, Tao; HE, Feng; TAO, Weikang - EP3564231, 2019, A1

Patent Family Members: TW2018/23231 A; CA3047641 A1; WO2018/121551 A1; CN109071492 A; AU2017389819 A1; ...

Abstract ▾ Claims ▾ Front Page Info ▾ Substances 72 ▾ Reactions 122 ▾ Targets ▾ Full Text ↗

Hit Substances 1 ▾

1. 打开Front Page，找到IPC
2. 全部复制IPC，或者部分复制IPC

Patent Classification

Main IPC

C07D 401/14

Secondary IPC

C07D 405/14; A61K 31/44; A61K 31/4196; A61P 15/00

Main IPC: 表达专利化合物种类核心结构
其余 IPC: 表达专利化合物种类细节结构, 表达治疗疾病细节 'A61P 12/00'



ELSEVIER

查找IPC模块方法

Reaxys[®] Quick search [Query builder](#) Results Synthesis planner History

Search in: Reactions > Targets > Substances > Documents >

Search fields: ipc

Import Save Reset form Delete all

Patent Assignee Structure Molecular Formula CAS RN TI, AB & KW

Patents: Main IPC is c07d 401/14

AND Patents: Secondary IPC is a61p 15/00

C07D 401/14 前一页专利的核心结构

A61P 15/00 前一页专利的治疗领域

Feedback

1. 在query builder页面建立IPC模块
2. 将之前检索的专利的IPC 全部拷贝，或依次拷贝，进行检索
3. 注意：全拷贝IPC可能检索不出新结果，需要对IPC号进行简单解读，并选择进行扩展检索
4. IPC解读网页 <http://www.soopat.com/IPC/Parent/A61K>

由于化合物结构专利，因为各种原因，会没抓取结构式，通过IPC能有效扩展追踪同领域专利

37 Documents with 3,857 Substances, 5,483 Reactions, 28 Targets
















0 selected Limit To Exclude Export

- 1 Condensed ring group azacyclobutyl triazole derivative, preparation method therefor and use thereof in medicine
Jiangsu Hengrui Medicine Co., Ltd.; Shanghai Hengrui Pharmaceutical Co., Ltd. - US10889569, 2021, B2
Patent Family Members: AU2017379024 A1; BR112019011758 A2; BRP11911758 A2; CA3047643 A1; CN108884071 A; ...
[Abstract](#) [Index Terms](#) [Claims](#) [Front Page Info](#) [Full Text](#)
- 2 Condensed ring group azacyclobutyl triazole derivative, preparation method therefor and use thereof in medicine
Jiangsu Hengrui Medicine Co., Ltd.; Shanghai Hengrui Pharmaceutical Co., Ltd. - AU2017379024, 2021, B2
Patent Family Members: AU2017379024 A1; AU2017379024 B2; BR112019011758 A2; BRP11911758 A2; CA3047643 A1; ...
[Abstract](#) [Claims](#) [Front Page Info](#) [Full Text](#)
- 3 PDGFR kinase inhibitors and uses thereof
No author - CN112442014, 2021, A
Patent Family Members: CN112442014 A; WO2021/35788 A1; WO2021/36814 A1
[Abstract](#) [Index Terms](#) [Claims](#) [Front Page Info](#) [Substances](#) 69 [Reactions](#) 64 [Full Text](#)
- 4 Novel quinoline derivative inhibitor
Nanjing Transthera Biosciences Co., Ltd. - AU2019323455, 2021, A1
Patent Family Members: AR116008 A1; AU2019323455 A1; CA3109891 A1; CN110857293 A; TW2020/21589 A; ...
[Abstract](#) [Claims](#) [Front Page Info](#) [Full Text](#)
- 5 Heterocyclic derivatives and uses thereof
No author - CN112625027, 2021, A
Patent Family Members: CN112625027 A; WO2021/57782 A1; TW2021/15028 A
[Abstract](#) [Index Terms](#) [Claims](#) [Front Page Info](#) [Full Text](#)
- 6 Substituted amino triazole [hitokichinaze] useful as inhibitors
No author - JP6859325, 2021, B2
Patent Family Members: AU2016314345 A1; AU2016314345 B2; BRP1804193 A2; CA2997382 A1; CL2018000564 A1; ...
[Abstract](#) [Index Terms](#) [Claims](#) [Front Page Info](#) [Full Text](#)
- 7 NOVEL QUINOLINE DERIVATIVE INHIBITOR
NANJING TRANSTHERA BIOSCIENCES CO LTD - SG11202101622V, 2021, A
Patent Family Members: AR116008 A1; AU2019323455 A1; CA3109891 A1; CN110857293 A; SG11202101622V A; ...
[Abstract](#) [Front Page Info](#) [Full Text](#)
- 8 PHARMACEUTICALLY ACCEPTABLE SALT, CRYSTAL FORM OF AZABICYCLO SUBSTITUTED TRIAZOLE DERIVATIVE AND PREPARATION METHOD
JIANGSU HENGRUI MEDICINE CO., LTD.; SHANGHAI HENGRUI PHARMACEUTICAL CO., LTD.; WANG, Lin; SHAO, Qiyun; FENG, Jun; HE, Feng; CAO, Xiaoli; DU, Zhenxing - WO2020/1460, 2020, A1
Patent Family Members: WO2020/1460 A1; TW2020/19908 A; CN111902406 A
[Abstract](#) [Front Page Info](#) [Full Text](#)


History


Recent Saved

Reaxys


37 Documents	Today 13:42	Query Builder: in documents - Main IPC "c07d 401/14" AND Secc	Edit Query  Save  Alert  View >
37 Documents	Today 13:37	Query Builder: in documents - Main IPC "c07d 401/14" AND Secc	Edit Query  Save  Ale
3 Documents	Today 13:37	Query Builder: in documents - Main IPC "c07d 401/14" AND Secc	Edit Query  Save  Ale
1 Documents	Today 13:36	Quick Search: "WO2020001460"	Edit Query  Save  Ale
8 Documents	Today 13:35	Query Builder: in documents - Main IPC "c07d 405/14" AND Secc	Edit Query  Save  Ale
0 Documents	Today 13:35	Query Builder: in documents - Main IPC "c07d 405/14"	Edit Query  Save  Ale
0 Documents	Today 13:35	Query Builder: in documents - Main IPC "c07d 405/14" AND Secc	Edit Query  Save  Ale



1. 选择检索历史
2. 登陆个人账号
3. 设置检索方法提醒, 可以定时推送同领域新专利到邮箱



Create Alert 


Query: Query Builder: in documents - Main IPC "c07d 401/14"... [Show Query](#) 


Alert name:

Send alerts to: 

Frequency:  on: 


Send alert:  

Do not send alerts with zero results 

ADVANCED ALERT CONTENT: 

From databases: Reaxys

Include in email: Title and bibliographic information
 Abstract
 Full abstract
 Partial abstract
 Hit details (keywords, substances, reactions or targets)

Email alerts will produce an email with a maximum of 99 records. 

Case 3: 检索2019年2月，与CD137相关的，人用药，含抗原或抗体的医药配置品（生物药类专利）

The screenshot shows the Reaxys Query Builder interface. The search criteria are as follows:

- Patents: Main IPC** contains **a61k 39/00**
- Patents: Secondary IPC** contains **a61k 39/00**
- Document Basic Index** contains **cd137**
- Patents: Date of publication** contains **2019/02**

The search terms are connected by **AND** logic. The IPC codes are connected by **OR** logic within their respective groups.

Annotations in the image:

- Contains 便于快速模糊检索** (Contains facilitates quick fuzzy search) points to the 'contains' dropdown menus.
- 4个模块同时组合，并设定需要逻辑** (4 modules combined simultaneously, and logic is set) points to the overall query structure.
- IPC分类:人用药类A61K, 含抗体类39/00** (IPC classification: human drugs A61K, containing antibodies 39/00)
- 关键索引: CD137** (Key index: CD137)
- 公开日期: 2019年2月** (Publication date: February 2019) with a note: (注: 该公开日期为专利的最后一个公开日期, 不一定是首发。可能是族号, 可能是不同版本的最新公开日期, 如, A1, A2, B)

4个模块同时组合，
并设定需要逻辑

组合模块构建

Reaxys[®] Quick search Query builder Results Synthesis planner History

Search in: Reactions > Targets > Substances > **关键词模块**

Import Save Reset form Delete all

Structure Molecular Formula CAS RN **Doc. Index**

在Query Builder中只需要点击所需模块即可进行组合检索

Drag & Drop to build a new query

查询特定模块

Find search fields and forms
Q ipc

Reaxys ^

- ◇ Patents: Main IPC
- ◇ Patents: Secondary IPC

Feedback

检索结果

METHODS AND COMPOSITIONS FOR PREPARING GENETICALLY ENGINEERED CELLS

2 JUNO THERAPEUTICS, INC.; BONYHADI, Mark L. WO2019/32929, 2019, A1

Patent Family Members: WO2019/32929 A1

Abstract Claims **Front Page Info** Full Text [↗](#)

Claims hit: {...of CD28, CD137 (4-1-BB), OX40, or ICOS.42. The method of claim 41, wherein...}

Assignees		Inventors (Authors)	
JUNO THERAPEUTICS, INC.; BONYHADI, Mark L.		BONYHADI, Mark L.	
Patent No	Kind Code	Publ. Date	Application No
WO2019/32929	A1	2019/02/14	WO2018-US46151
Priority No	公开日期 授权状况		Priority Date
US2017-543359P			2017/08/09
Patent Classification			
Main IPC	A61K 39/00	IPC 分类	
Secondary IPC	C12N 5/0783		

Claims

CLAIMS

WHAT IS CLAIMED:

1. A method for genetically engineering (a) incubating an input composition, under stimulating conditions, a population of T cells, wherein the stimulating conditions comprise one or more intracellular signaling domains; (b) introducing a nucleic acid encoding a genetically engineered recombinant receptor, wherein the method thereby generates cells expressing the genetically engineered recombinant receptor.

2. A method for genetically engineering a population of T cells comprising naive-like T cells, wherein the stimulating conditions comprise one or more intracellular signaling domains; (b) introducing into the stimulated cell composition a nucleic acid encoding a genetically engineered recombinant receptor, wherein the method thereby generates cells expressing the genetically engineered recombinant receptor.

the incubating the input composition under stimulating conditions is performed prior to, during and/or subsequent to introducing a nucleic acid encoding a genetically engineered recombinant receptor.

3. The method of claim 1 or claim 2, wherein the incubating is carried out for at least 3 days.

4. The method of claim 1 or claim 2, wherein the incubating is carried out for at least 4 days.

5. The method of claim 1 or claim 2, wherein the incubating is carried out for at least 5 days.

6. The method of claim 1 or claim 2, wherein the incubating is carried out for at least 6 days.

7. A method for stimulating T cells, the method comprising:

(a) incubating, under stimulating conditions, an input composition comprising T cells comprising a culture-initiating amount of naive-like T cells or a CD8+ stimulated composition, wherein the stimulating conditions comprise the presence of a stimulatory reagent capable of activating one or more intracellular signaling components of a TCR complex and/or one or more intracellular signaling domains of one or more costimulatory molecules, thereby generating a stimulated cell composition;

(b) introducing into the stimulated cell composition a nucleic acid encoding a genetically engineered recombinant receptor, wherein the method thereby generates cells expressing the genetically engineered recombinant receptor.

专利‘Claim’部分的摘取和可索引，对于生物药类专利的检索非常有利。

通常生物药类的专利，不具有结构式，且专利标题和摘要一般会撰写得比较简单，造成了生物药类专利检索的困难



ELSEVIER

今天的内容

- 文献检索的原理简介
- Reaxys数据库药物核心信息，合成方法检索技巧
- Reaxys数据库专利检索技巧
- Reaxys Medicinal Chemistry数据检索技巧

Case 5: 如何通过靶点筛选小分子抑制剂

Reaxys Quick search Query builder Results Synthesis planner History Peng Wu

Search in: Reactions > Targets > Substances > Documents >

Import Save Reset form Delete all

Structure Molecular Formula CAS RN

Find search fields and forms

Fields Forms History

Target Name is epidermal growth factor receptor binding protein;Epidermal growth factor receptor;epidermal growth factor-activated receptor

AND Substance Action on T... is inhibitor

Details information selection (highlighted)

Drug chemistry information search module (highlighted)

缩写快速转化相关靶点

is EGFR

- Targets 20,141,813
 - protein 17,245,173
 - binding protein 3,108,588
 - protein binding protein 1,666,788
 - signaling receptor binding protein 67,023
 - growth factor receptor binding protein 271
 - epidermal growth factor receptor binding protein 7
- enzyme 9,455,640
 - catalytic acting on a protein 6,861,203
 - protein kinase 4,811,620
 - Protein kinase domain 3,631,410

Selected search items: epidermal gro... protein Epidermal gro...receptor epidermal gro... receptor EGFR EGFR (19del)

Clear selected Transfer

化合物作用效果

Su inhibitor

<input type="checkbox"/> activator	82,778
<input type="checkbox"/> agonist	849,420
<input type="checkbox"/> allosteric modulator	120,497
<input type="checkbox"/> antagonist	886,505
<input type="checkbox"/> blocker	156,879
<input type="checkbox"/> inactivator	2,044
<input checked="" type="checkbox"/> inhibitor	10,653,338
<input type="checkbox"/> inverse agonist	13,675
<input type="checkbox"/> irreversible antagonist	3
<input type="checkbox"/> irreversible inhibitor	83
<input type="checkbox"/> modulator	306,408
<input type="checkbox"/> opener	18,294
<input type="checkbox"/> partial agonist	707

1 of 2 Go to page

Clear selected Transfer

71.40 K

Filters

Limit to > Exclude >

By Structure

Measurement pX

Highest Clinical Phases

Targets

Parameters

Substance Classes

Molecular Weight

Number of Fragments

Availability

Availability in other databases

Available Data

Do

Pu

Patent Assignee

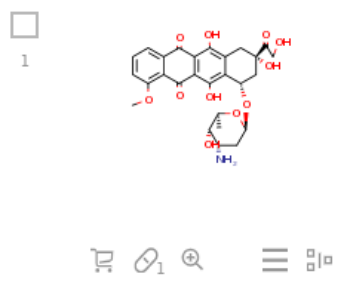
LogP

H Bond Donors

71,403 Substances out of 2,922 Documents, containing 102,517 Reactions, 375 Targets

0 selected

Sort by No of References



doxorubicin

C₂₇H₂₉NO₁₁ 543.527 1445814 23214-92-8

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Physical Data - 164

Spectra - 239

Other Data - 6,037

Preparations - 68 >

Reactions - 364 >

Targets - 393 >

Documents - 27,491 >

doxorubicin

Identification

Druglikeness

Bioactivity (Hit Data)

Bioactivity (All)

Physical Data - 164

Spectra - 239

Bioactivity (All)

In vitro: Efficacy - 12410

In vivo: Animal Model - 2116

Metabolism - 756

Pharmacokinetic - 995

Toxicity/Safety Pharmacology - 12536

生物活性数据

pX	Parameter	Value (qual)	Value (quant)	Unit	Action on target	Cell	Bioassay	Effect
14.9	IC50	=	1.3E-09	μM	Inhibitor	MMA cell line		
13.2	IC50		6.19E-08	μM		OVCAR-3 cell line	In Vitro (others)	antiproliferative agent
12.3	GI50	=	3E-07	μg/mL		NCI-H460 cell line		

建立构效关系

27,166 Substances out of 1,749 Documents, containing 57,983 Reactions, 222 Targets

0 selected Limit To Exclude Export Preparations

By Structure Measurement pX

Parameters

- ic50 27,166
- (no entry given) 25,029

Filter by value Substance Classes Molecular Weight Number of Fragments Availability Availability in other databases

doxorubicin C27H29NO11 543

Identification Druglikeness Bioactivity (Hit Data)

quercetol (HO)2C6H3C9H2O(

Identification Druglikeness Bioactivity (Hit Data)

Heatmap settings

数据 VS 化合物构效关系

Value of X-axis Parameter

Value of Y-axis Substances

Value of Cells Maximum of pX

Show substances Names Structure drawing

Display mode Normal Full Screen

Always show settings Apply >

Grid Heatmap

Preparations - 68 >
Reactions - 364 >
Targets - 393 >
Documents - 27,491 >

Preparations - 180 >
Reactions - 1,170 >
Targets - 1,079 >
Documents - 26,094 >

快速获取ic50数据



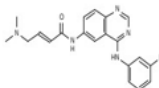
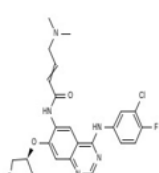
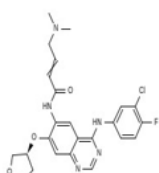
导出结果

ic50

Parameter

Substances

- staurosporine
- 4-[[3-chloro-4... nazoline
- 6,7-dimetho... -4-amine
- 4-Dimethyla... lj-amide
- (1R,5S)-3-(3-((...xan-1-ol
- N-(4-fluorop... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine
- N-(3-chloro-... -4-amine

1	A	B	C	D	E	F	G	H	I	J	K	L	Qu
1	Structure: Image	SMILES	CAS Registry Number	Chemical Name	Molecular Formula	Molecular Weight	Target Name	Target, Subunit, Species	Substance Action on Tar	Bioassay Category	Medchem: Measurement	Unit	Qu
		<chem>CN(C)CC=CC(=O)NC1=C</chem>		4-Dimethylamino-but-2-en-1-ol	C20H20BrN5O	426.316	Epidermal growth factor	Epidermal growth factor Inhibitor		In Vitro (Efficacy)	IC50	nM	=
9		<chem>CN(C)CC=CC(=O)NC1=C</chem>		4-[[3-chloro-4-fluorophenyl]oxy]pyrrolidine	C24H25ClFN5O3	485.946	epidermal growth factor	epidermal growth factor Inhibitor		In Vitro (Efficacy)	IC50	nM	<
16		<chem>CN(C)CC=CC(=O)NC1=C</chem>		4-[[3-chloro-4-fluorophenyl]oxy]pyrrolidine	C24H25ClFN5O3	485.946	epidermal growth factor	epidermal growth factor Inhibitor		In Vitro (Efficacy)	IC50	nM	<



RMC-特定的信息检索方法

◇ Target Name	⋮
◇ Substance Action on Target	⋮
◇ Substance Effect	⋮
◇ Measurement pX	⋮
◇ Target Nature	⋮
◇ Target Mutant/Chimera Details	⋮
◇ Target Transfection	⋮
◇ Substance RN	⋮
◇ Substance Route of Adm.	⋮
◇ Substance Dosing Regimen	⋮

◇ Biological Material Name	⋮
◇ Biological Species	⋮
◇ (Clinical) findings / disease	⋮
◇ Organs/Tissues	⋮
◇ Cells/Cell Lines	⋮
◇ Cell Fraction	⋮
◇ Measurement Parameter	⋮
◇ Measurement Qualitative	⋮
◇ Measurement Unit	⋮

Substance Action on Target Search ×

<input type="checkbox"/> activator		75,140
<input type="checkbox"/> agonist	激动剂	,929
<input type="checkbox"/> allosteric modulator		,961
<input type="checkbox"/> antagonist		,683
<input type="checkbox"/> blocker	阻断剂	160,460
<input type="checkbox"/> inactivator		1,996
<input type="checkbox"/> inhibitor	抑制剂	10,470,915
<input type="checkbox"/> inverse agonist		13,321
<input type="checkbox"/> irreversible antagonist		3
<input type="checkbox"/> irreversible inhibitor		83
<input type="checkbox"/> modulator		313,006

1 of 2 Go to page Clear selected Transfer

检索对靶点作用机制的特点信息时的模块

Measurement Parameter is Enter search term ×

> cellular parameters	94,814
> epidemiological data	120,359
> in-vitro pharmacological parameters	20,175,771
> in-vivo pharmacological parameters	46,741
> mathematical parameters	148,038
> medical parameters	32,006
> metabolic parameters	54,026
> metabolism/transport parameters	110,315
> microbiological parameters	286,015
> pharmacokinetic parameters	835,343
> absorption parameters	59,818
> F (drug bioavailability)	56,062
> kabs	1,550
> MAT (mean absorption time)	7
> t1/2 abs	589
> tlag	1,582

Transfer

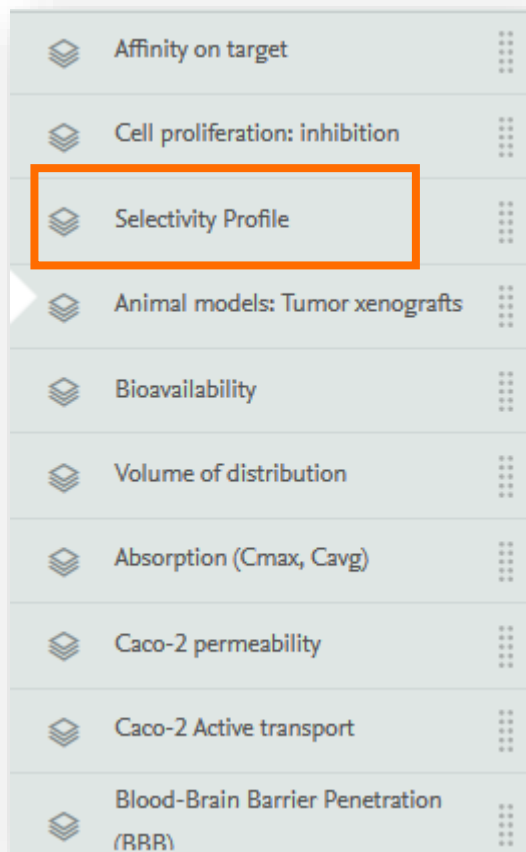
直接检索特定数据时的模块如PK的各种数据

各种分类细致的信息检索模块，快捷锁定对应结果



RMC-组合信息便捷检索

预设的组合检索模块，便捷检索综合信息，如对于不同亚型的同类靶点，差异抑制性



靶点选择性检索

靶点名称

AND

抑制‘数量级’以‘mol’为单位换算，9=10的负9次方

COMBI

AND

Target Name	Operator	Value
Histone deacetylase 2	is	9
Histone deacetylase 8; Histone deacetylase [Neovison vison]; Histone deacetylase 10	is	8

RMC-组合信息便捷检索

- Affinity on target
- Cell proliferation: inhibition
- Selectivity Profile
- Animal models: Tumor xenografts
- Bioavailability
- Volume of distribution
- Absorption (Cmax, Cavg)
- Caco-2 permeability
- Caco-2 Active transport
- Blood-Brain Barrier Penetration (BBB)

- Cytotoxicity
- hERG inhibition
- Cytochrome inhibition (CYP3A4)
- Metabolism by cytochrome (CYP2D6)
- Microsomal stability
- Protein binding (blood, plasma)
- Cardiotoxicity

hERG inhibition

- Structure
Create Structure / Reaction Drawing
- AND
- Target Name
is Target Name 'Potassium voltage-gated channel subfamily H mem'
- AND
- Target Nature
is Target Nature 'wild'
- AND
- Measurement Parameter
is Measurement Parameter '%50';'K';'Kd';'kd'
- AND
- Measurement pX
Measurement pX

Caco-2 permeability

- Structure
Create Structure / Reaction Drawing
- AND
- Cells/Cell Lines
is 'Caco-2 cell line';'Caco-2'
- AND
- Measurement Parameter
is 'papp (a-b)';'papp (b-a)';'papp (transport)';'papp';'transport ratio';'transp'

只需要特定结构即可初步快速检索特殊信息

Thank you

