# Reaxys<sup>®</sup> 快速使用指南



# 化学数据与文献的最简路径

为了支持全方位化学研究,包括药物开发、环境健康与安全以 及材料科学研究,Reaxys为从新手到专家的每一位科学家,提 供解决问题的最简路径。化学查询经由高度直观的搜索界面, 迅速检索相关文献和专利信息,以及有效的物质属性和实验操 作流程。寻找答案从未如此简易。



# 1. Quick search-自然语言检索

Quick search	Query builder	Results	Synthesis planner	History							
Search substances, reactions, documents and bioactivity data in Reaxys, Reaxys Medicinal Chemistry, PubChem, eMolecules, LabNetwork and SigmaAldrich											
Q Substance Properties, e.g. ferroelectric materials											
	AND										
Create Structure or Reaction Drawing											

 文本搜索选项支持输入自然语言术语,既可以直接用关键词 检索文献,也可以检索化合物具体性质数据,反应等 (例如: melting point of xylitol, Pharmacokinetic of imatinib; Pt(PPh3)4; lapatinib; 102605-70-7 etc.)。

### 1.1.1 Quick search-文献检索

Quick search	Query builder	Results	Synthesis planner	History
	Search for	polymer	nanofiber	
Search Rea Q polyr	axys ner nanofiber			×
()¢				

### 1 例如:检索检索 '聚合纳米纤维相关的文献'

Quick scarch       Query builder       Results       Synthesis planner       History         Results for polymer nanofiber       Results for polymer nanofiber       Preview Results < View Results >         265       Substances       Results @ a draw builder & Cours for @       Preview Results < View Results >         9,804       Documents       This, Abstracts, Krywerdi: polymer       2       Preview Results < View Results >         43,682       Documents       This, Abstracts, Krywerdi: ranofiber       Preview Results < View Results >							
Results for polymer nanofiber         265       Substances       Section (Section (Sect		Quick	search Query builder	Results	Synthesis planner	History	
265     Substances     Structure : (i) is drawn Edit in Query Builds (i) Cruss Res.)     Preview Res./ls 、     View Res.ills >       9,804     Documents     Titles, Abstructs, Keywords : polymer, nanofiler     Q     Preview Res./ls 、     View Res.ills >       833,826     Documents     Titles, Abstructs, Keywords : polymer     Preview Res./ls 、     View Res.ills >       43,682     Documents     Titles, Abstructs, Keywords : sanofiber     Preview Res./ls 、     View Res.ills >			Results for	polymer n	anofiber		
265     Substances     Structure : (i) in drawn     Preview Results ∨     View Results >       9,804     Documents     Tifes, Abstracts, Keywords : polymer, nanofiler     2     Preview Results ∨     View Results >       833,826     Documents     Tifes, Abstracts, Keywords : polymer     Preview Results ∨     View Results >       43,682     Documents     Tifes, Abstracts, Keywords : nanofiler     Preview Results ∨     View Results >							
9,804     Documents     Titles, Abstracts, Keywoods     : polymer     Q     Preview Results <     View Results        833,826     Documents     Titles, Abstracts, Keywoods     : polymer     Preview Results      View Results        43,682     Documents     Titles, Abstracts, Keywoods     : nanofiber     Preview Results      View Results	265	Substances	Structure : 🔯 as drawn Edit in Query Builder 🔗 Create A	lert 🗛		Preview Results 🗸	View Results 🗲
9,804     Documents     Titles, Abstracts, Keywords     : polymer     ? </td <td>I</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	I						
833,826     Documents     Title, Abstracts, Keywords : polymer     Preview Results >       43,682     Documents     Titles, Abstracts, Keywords : nanofiber     Preview Results >	9,804	Documents	Titles, Abstracts, Keywords : p	olymer, nanofibe	· 2	Preview Results 🗸	View Results >
833,826     Documents     This, Abstracts, Keywords : polymer     Preview Results ∨     View Results >       43,682     Documents     This, Abstracts, Keywords : randilier     Preview Results ∨     View Results >							
43,682 Documents Thiles, Abstracts, Keywords : nanofiber Preview Results View Results >	833,82	5 Documents	Titles, Abstracts, Keywords : p	olymer		Preview Results 🗸	View Results >
43,682 Documents Titles, Abstracts, Keywords : nanofiber Preview Results > View Results >							
	43,682	Documents	Titles, Abstracts, Keywords : n	anofiber		Preview Results 🗸	View Results 🗲

2 预览界面不但给出'polymer nanofiber相关文献',还给出了 相关化合物供参

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- 3 导航栏
- 4 Filter(筛选器),对文献集进一步筛选,如:
- 5 结果集总结,可以直接查看这些文献中的,化合物,反应, 以及靶点信息
- 6 结果导出
- 7 这些文献中,涉及到的,化合物靶点生物活性构效关系图
- 🔒 检索词高亮
- 🧐 问题反馈

### 1.1.2 Quick search-化合物性质检索

Quick search	Query builder	Results	Synthesis planner	History
	Search for <b>m</b>	elting po	int of xylitol	
Search Rei Q melti	axys ng point of xylitol	1		×
L		AND		
	Create Structure or	Reaction Dr	awing	

1 检索化合物的具体性质,能够直击结果

O	e De Colt		Results for melting point of xylite	ı
	4	Substances	Structure : D as drawn AND Property : melting point	t Preview Result 2 View Results >
	138	Documents	Titles, Abstracts, Keywords : melting point, xylitol	Preview Results >
	637,245	Documents	Titles, Abstracts, Keywords : melting point	Proview Results  View Results
Jine	6,362	Documents	Titles, Abstracts, Keywords : xylitol	Preview Results >

#### 2 具体信息结果集

3 相关信息结果集,关键词相关文献



Re	axys	Quid	ck search	Query builder	Results Synth	esis planner History	Peng Wu	Ŷ	(
4	Filters and Analysis		4 Sub	ostances out of 1,4	661 Documents, containing 4	69 Reactions, 6 Targets	Reaxys - 4		~
	By Structure	~		⊡ ⊘ Limit To Exclude E	企 ixport	•••	No of References 🖗 🤝	Heatmap	E
	Measurement pX	~	_						
	Highest Clinical Phases	~	1	10	C3H12O3 152.147	1720523 87-99-0			
	Targets	~		HO arrest H	Hit Data - 23	Physical Data - 313	Prepara	tions - 107	>
					Identification	Spectra - 52	Read	tions - 469	>
	Parameters	~		ъ	Druglikeness	Other Data - 542		Targets - 6	>
	Substance Classes	~		24	Bioactivity (All)		Docume	nts - 1,661	>
	Molecular Weight	~	[	∧ Hit Data - 2	3 4				
	Availability	~		✓ Melting P	oint - 23 hits out of 23	5			

④ Hit data 显示希望检索的具体数据

### 5 点击展开结果

^ Melti	ng Point - 23	hits out of 2	23	
				Show/Hide columns 🗸
Melting Point, °C	Solvent (Melting Point)	Location	Comment (Melting Point)	Reference
92 - 96		Paragraph 0126		Yonsei University Industry-Academic Cooperation Foundation,; wooshin medics co. ltd; Hwang, Sung Joo; Kang, Han; Song, In Ho; Kwon, Min Jun; Seon, Bo Kyung - KR2016/79954, 2016, A
		7	8	Full Text 🛪 Details > Abstract >
107.2				Fujii, Kahori; Izutsu, Ken-Ichi; Kurne, Migiwa; Yoshino, Takeshi; Yoshihashi, Yasuo; Sugano, Kiyohiko; Terada, Katsuhide - Chemical and Pharmaceutical Bulletin, 2015, vol. 63, # 5, p. 311 - 317
				Full Text 🏹 Details > Abstract >
93 6				Gowda, Jayant I.; Nandibewoor, Sharanappa T Synthesis and Reactivity in Inorganic, Metal-Organic and Nano- Metal Chemistry, 2012, vol. 42, # 8, p. 1183 - 1191,9
•				Full Text 🛪 Details > Abstract >
94.49	H2O		Decomposition	Wang, Shui; Li, Qun-Sheng; Li, Zhao; Su, Ming-Gao - Journal of Chemical and Engineering Data, 2007, vol. 52, 8 1, p. 186 - 188
				Full Text 🛪 Cited 12 times 🛪 Details > Abstract >

6 具体数据

7 文献中位置

\rm ⑧文出处

## 1.1.3 Quick search-用词汇进行反应检索

Quick search	Query builder	Results	Synthesis planner	History
	Search fo	r suzuki o	coupling	
Search Rea Q suzul	xys ki coupling			×
		AND		
¢¢	Create Structure	e or Reactior	n Drawing	

 输入反应名称: Suzuki coupling, Wittig reaction等,或者 输入反应类型'substitution, oxidation reaction'等

			Results for suzuki coupling	
127,608 Reactions Condition : suruki coupling Preview Results View Results >	127,608	Reactions	Condition : suzuki coupling	Preview Results >
15,369 Documents Titles, Abstracts, Keywords : saraki coupling Preview Results >	15,369	Documents	Titles, Abstracts, Keywords : suzuki coupling	Preview Results >

2 一次性获得相关反应及其相关文献

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Re	axys'		Quick search Query builder Results Synthesis planner History	reg™r Å Æ ®
127,600	Filters and Analysis		127,608 Reactions out of 30,928 Documents containing 191,418 Substances, 7,166 Targets	i
	By Structure	~	Contraction Contraction Compared	0 🔿 — — 🟮 Sort by Roomy Ranking o
	Yield	~		
	Reagent/Catalyst	~	Baadior ID: M520866	
	Solvert	~	No. 1 0.	
	Catalyst Classes	~	$ \neg \neg$	
	Solvent Classes	~	4 x a, 5 x a, x a,	
	Product Availability	~	Hits      CandSizes      Find Similar	
	Reactant Anailability	~ 4	Hit Details	
	Reaction Classes	~	1910         Step: R1: p-tert-but/phery/Boranic acid, antho-Irranobenaldehyde With         Werts, Scientins: Leffert, Dric Studey, Armido - Organic Latters, 2015, vol. 13.	
	Document Type	~	solum columnia la varier. N.N.4 inertial formanide for 6.0333335; 84, p. 521 - 931 Blage 83: Web partial un diamétric la varier. N.N. obverby/domanide at Full Yes. 29 Citad 81 times 29 Details > Alatast > 2022	
	Publication Year	~	10% With Intellity intersplotagenced particulars <sup>10</sup> , potenciere phosphate Chosen, Gaubeth, Robeit, Christopher, Legay, Revit, Gauter, Java Saphere	
	Single step reactions only		Sauki Hypers over modeling. Microsovi indiator: English Hypers over modeling. Microsovi indiator: English Hypers over modeling. Microsovi indiator: English Hypers over Hypers A. Status S. Abstract S.	
			38/9         With Intrinsity patron particular particular and the T_A volume or at BOX;         One, Designs L.; Endry, Brandury J; Link, Addry MJ, Klowan, Byan A.	
			Glassinas, Organic Letters, 20(2), vol. 29, 47, p. (37) - (373) Full Text 29 Databa > Abrana: >	
			6 + Show all likes + Show all conditions	2 hits out of 8
				Context D

- 3 各种反应相关筛选器
- ④ 高亮检索词条,和相关试剂,与检索词条相关条件结果集
- 该反应全部反应条件,包含'非检索词条 (Suzuki coupling)'
- 6 增加显示更多反应条件

#### 1.2 Quick search-结构检索

Reaxys'	Quick search Query builder Results Synthesis planner History Program Query Builder Q	
Import 🛓	Search substances, reactions, documents and bioactivity data in Rawy, Reary Medical Overnov, Publicker, Mateulas, Labiteurer ind SignaMatch	
	Q Substance CAS Registry Number, e.g. 102625-70-7 AND € Create Structure or Reaction Drawing	
REAXYS' Version 1	Techas Q	

 Java-Free结构编辑器,点击打开,可以在智能手机,平板 电脑等任意移动设备上直接画图。

Reaxys	Quick search Query	builder Results	Synthesis planner	History	Peng Wu	2	Ŷ	0
	R, E E & H ⊗ ● Marvin ⊮åchemAv	2 Create str	ucture template from	name > → hate H c N C Br I A → C C Br I A → C C C C C C C C C C C C C	Search this str A drawn A substructur Smilar Tautomers Storeo Additional rin Related Mark Salts Mixtures Mixtures Charges Reliciols + More options	e e e	s 7	)
https://www.com/defaultion.org		Clear 💼	Canoel X Transfer	to query 🗲			Feedba	* O

- 2 名字, CAS RN 导入结构
- 3 工具栏
- 4 模板栏
- 5 原子相关设定
- 6 检索逻辑: 1. 如图所画; 2. 亚结构检索; 3. 相似检索
- 7 结构相关异构体

# 1.2.1 结构检索—化合物检索

Reaxys'	Quick search Query builder Results Synthesis planner History Peng Wu	2	¢	0
Import 💩	Search for 🔕		Find	4 >
	Q. Substance Molecular Formula, e.g. P((PPh3)3			
	AND X			
REAXYS* Version 1	As drewn		Feedba	* 🖓

Reaxys'		Quie	k search Query builder	Results Synthesis	planner History	Pe	A	¢	٢
	226	Substances	Structure : as drawn; in additional ring docume allower radicals, no separate fragments	cludes) only absolute stereo, i, salts, mixtures, isotopes, ch	Preview Results 🗸	View Results >			
	1,039	Targets	Structure : () as drawn; in additional ring closures allower radicals, no separate fragments	cluded: only absolute stereo, i, salts, mbitures, isotopes, ch :	Preview Results 🗸	View Results >	2		
	198	Substances	Structure 1 😰 average sim stereo, additional ring closures charges, radicals, no separate fi	llarity; included: only absolute allowed, salts, mixtures, isoto sagments	: Preview Results 🗸	View Results >	3		
	117	Reactions	Product(t) : (b) as drawn; in additional ring closures allower radicals, no separate fragments	ncludect: only absolute stereo, d, salts, mòtures, isotopes, ch i	Preview Results 🗸	View Results >	•		
FLOENTED									_

- ① 如图所画化合物,及其相关盐类异构体
- 2 化合物测试过的靶点信息,及其对应生物活性数据
- 3 相似结构衍生物
- 4 相关反应

Rec	ixys'	Qui	ck search	Query builder	Results	Synthesis planner	History	Peng Wu	2	Ŷ	0	
226	Filters and Analysis		226	Substances out of 2,5	978 Documents,	, containing 137 Reactions,	1,039 Targets	6	Reaxys - 226		$\sim$	-
	By Structure	~		O O A Limit To Exclude Expo	et		•••	No of Reference	• <b>7</b> [	Heatmap	-	
	Measurement pX	~			_							
	Highest Clinical Phases	~	1	Q Options \	<ul> <li>gefitinib</li> <li>C<sub>22</sub>H<sub>24</sub>CIFP</li> </ul>	N <sub>4</sub> O3 446.909 8949523	184475-35-2	9			_	1
	Targets	~		- <u>æ</u>	Identificat	tion	Physical Data - 54		Preparatio	ons - 56	>	
	Parameters	~		~ ~ ~	Bioactivity	v (All)	Spectra - 47 Other Data - 2,469	10	Targets	ons - 86 i - 1,028	>	
	Substance Classes	~		Synthesize	<u>ч</u>			- [	Documents	- 2,958	>	
	Molecular Weight	~	2		Gefitinib C <sub>22</sub> H <sub>24</sub> CIFP	hydrochloride N <sub>4</sub> O3 <sup>A</sup> CIH 483.37 14991	8854 184475-55-6					
	Availability	~		jag	Identificat	tion	Physical Data - 1		Preparat	tions - 1	>	
	Availability in other databases	~		o u	Drugliken	iess . (AID	Spectra - 1		React	tions - 1	2	
	Available Data	~		Ъ.	Bioactivity	y (All)			Docum	rgets - 3 ients - 5	>	
	Document Type	~		8	18F-Iress C <sub>22</sub> H <sub>24</sub> CIF	a N <sub>4</sub> O3 445.911 9525414				Feedbac	k 🖓	

- 6 各种筛选器,结构,临床阶段等
- 6 结果来源数据库
- 7 构效关系图
- 8 自动设计合成路线
- 0 化合物相关性质信息,点击查看具体数据
- 🕕 相关反应, 文献, 靶点信息

### 快速设计合成路线,直观清晰

Reaxys	Quick search Query builder Results Synthesis planner History	Peng Wu 🔍 💭 🕐
Synthesis plan 1		⊙ Urado Redo
		- 1 + Formation () Reference ()

- 1 导出结果(多种文件格式)
- 2 鼠标点击图片,能查看该化合物其他详细信息,添加合成步骤等
- 3 点击查看反应操作
- 4 购物车,化合物供应商信息
- 互 放大缩小,便于查看

### 1.2.2 结构检索-化学反应检索

Reaxys	Quick search Query builder Results Synthesis planner History Pre	ing Wu	¢	Ŷ	0		
Import 🛃	Search for			Find	$\left \right\rangle$		
	Q Substance CIS Registry Number, e.g. 102625-70-7						
	AND						
	$\bigcirc_n \rightarrow \bigcirc_{\gamma^m}$						
	On al atoms						
REAXYS® Version 1				Feedbar	* 🖓		



 各种反应筛选器,如:结构筛选,反应试剂筛选,催化剂筛 选,反应类型筛选等

- 😢 包含反应相关文献,化合物,靶点信息等
- 3 反应条件,操作步骤,以及不同文章的相同反应归纳在一起
- 4 反应来源

### 2. Query builder-自定义检索

Reaxys	Quick se 1 Query builder Result	s Synthesis planner	History	Perg Wa	O
📩 🖻 O 🛢 Import Save Restform Debte sil	(	2 Structure Molecular For	Search > V # C3 mula CAS RN Doc. Index	Find search fields and Fields Forms	forms Q History
			Reavys 🔨		
		Basic Indexes	~		
				Identification	~
				Physical Properties	~
			4	Spectra	~
	Drag & Drop to build a new query	Drag & Drop to build a new query	MedChem	~	
				Other	~
				Reactions	~
				Bibliography	~
					PubChem 🧹
					Feedback 🖵

- 1 点击进入自定义检索界面
- 2 常用检索模块,结构,分子式,CAS RN,索引词
- ④ 通过词汇搜索相关检索模块,如:patent,target等
- 4 其他检索模块,包含Reaxys,RMC以及其他数据库

#### 2.1 Query builder-组合信息检索

(检索某母核相关化合物,制剂信息)



- 1 选择检索文献
- 2 结构编辑器
- 3 关键词索引
- 4 组合成综合信息检索组
- ⑤ 逻辑连接符,确定不同模块之间逻辑关系

#### 检索结果 - 检索某母核相关化合物 , 制剂信息

Reaxys'	Quick search Query builder Results Synthesis planner History	Peng Wu A	Ą	٢						
78 Filters and Analysis	78 Documents with 4,302 Substances, 4,303 Reactions, 118 Targets	2								
Index Terms (List)	V O Selected Carlot Export	Sort by Relevance + 🗸	Heatmap	8						
Index Terms (ReaxysTree)	×									
Publication Year	CRYSTALLINE FORMS OF IBRUTINIB     SUN PHARMACEUTICAL INDUSTRIES LIMITED; SANTRA, Ramkinkar; BHOGALA, Bala Kristma Redg; KHANDUR, Chandra Ha									
Document Type	WC/2017/29586, 2017, A1 Patent Family Members: WC/2017/29586 A1	66, 8917, A1 Membersi, WO2017/29586 A1								
Authors	Adstract   Front Page Info   Substances   Full Text 71  Hit Substances   V									
Patent Assignee	PROCESS FOR THE PREPARATION OF THE AMORPHOUS FORM OF IBRUTINIB AND NOVEL     CRYSTALLINE FORM									
Journal Title	OLON S.R.A.; BERTOLIN, Gorgio; FELKIANI, Lazzaro; FERRANDO, Ilaria; SADA, Mara - WO2017/85628, 2017, A1.      Distant Section: Manahaman WY2007/85629, A1.									
Substance Classes	Abstract      Front Page Info      Substance:     Abstract      Front Page Info      Substance:     Abstract      The Abstract      Abstr	4								
Reaction Classes	CRYSTALLINE FORM I OF IBRUTINIB									
	<sup>1</sup> CHYSEL PARKINTECH (HLS, SUPERIOR PARKINE) PARKINTECH (CL, UTEL) CHI, Michau ZHANG, Yanding YANG, Chunhu ZHANG, Xinoyau ULi Ang GL, Heng WANG, Anegu J, Pane V 200305(11103), 2015, 41 Pater haniy Antonico MUSHERIA A CONSERVATION A WOOSING1100, ALCONISOR ALI, AUSSI (SISTER ALI,	:								
	BRUTINIB HEMISULPHATE		Feedbac	* 🖓						

- 关于整个检索结果的总结,点击查看,相关化合物,反应以 及靶点信息等
- 😢 关于这个结果集,涉及到的生物活性的构效关系图
- 3 关于单篇文章的总结,摘要,专利标记信息,化合物(事实列),化学反应,原文来源等
- 4 检索关键词,检索结构式高亮,直接表现出与检索条件相关性

### 2.2.1 Query builder – 专利检索 (结构式检索相关专利)



1 画入结构直接检索文献

#### 检索结果

Re	axys'		Quick search Query builder Results Synthesis planner History	Peng Wa 🔍 🗘 🔿
2,094	Filters and Analysis		2,094 Documents with 28,234 Substances, 148,186 Reactions, 3,080 Targets	
	Index Terms (List)	$\sim$	selected     Umit To Exclude Expert	Sort by Relevance + 🗸 Heatmap 🎛
	Index Terms (ReaxysTree)	~		
	Publication Year	$\sim$	The Geigy Corporation - US3948913, 1976, AL	
1	Document Type	~	Patent Family Members: IL392AT D0; 8E782658 A1; IE36312 L; NL7205668 A; DE2218717 A1; Abstract 🗸 Front Page Info 🗸 Substances 😰 🗸 Reactions 😰 🗸 Full Test 🌶	
	Authors	~	Hit Substances (11)  7-Substituted nucleoside compounds	
	Patent Assignee	~ ~ •	<sup>2</sup> The University of Ush - US3952211, 1976, A1 Datent Evenils Manufacture (IS286231), ar OS260720 A1, IS2207234 A1, ISS2105206 A, 74360333 P.	
	Journal Title	~	Abstract $\lor$ Front Page Info $\lor$ Substances (S $\lor$ Reactions (S $\lor$ Full Test 7)	
	Substance Classes	~	Meso-ionic didehydro derivatives of 1,7-dehydro-1-substituted-3H-pyrazolo[4,]-1,2,4-triazolo[4,]	3.
	Reaction Classes	~	3         c]pyrimidine-3-thiones and 3-ones           E. R. Spibb and Sen, Inc1051/2064, 1978, A1           Patter Finity Memorieum US631244, RES20231018, Q DE2213540 A2; RE2146972 A2; US4607423 Ac           Attentianty Memorieum US631244, RES20231018, Q DE2213540 A2; RE2146972 A2; US4607423 Ac           Attentianty Memorieum US631244, RES20231018, Q DE2213540 A2; RE2146972 A2; US4607423 Ac           Attentianty Memorieum US631244, RES20231018, Q DE2213540 A2; RE2146972 A2; US4607423 Ac           Attentianty Memorieum US631244, RES20231018, Q DE2213540 A2; RE2146972 A2; US4607423 Ac           Attentianty Memorieum US631244, RE2146972 A2; US4607423 Ac           Attentianty Memorieum US67444, RE2146972 A2; US4607423 Ac           Attentianty Ac	
			No tell     No tell     Scherberger (NE)	Cited 9 times Feedback 🖓

#### 1 文献分类,筛选专利

Reax	kys'				Quick search Query builder Results Synthesis planner History Perg Big R							
2,094	Filters and Analysis	>		2,0	94 Documents with 28,234 Substances, 148,186 Reactions, 3,080 Targets @ selected	Sort by Relevance + 🗸	Heatmap	E	Î			
	Index Terms (List) Index Terms (ReaxysTree Ublication Year		~ ~ ~	1	New 5-nitrolling) derivatives           Olle Gege Opposition- UTMRH11, 1076, AL           New 6-lingh Networks 1330 CNR 107204AL           Neutr 5-lingh Networks 1330 CNR 107204AL           Neutron 5-lingh Networks 1330 CNR 107204AL           Net							
	Decument Type 1     patent     article     review     conference paper	- 1,0 - 9	63 4 52 12	2	Hit Salancess ↓ Additional of unclosedia compounds The Universe Virtua - UNIVERZIE INFA L Panel Freinhy Revenue UNIXEZIE CONSTRUCT REPORTED ALL (\$50316/005 ALZ 2020/0113 BL							
	book review / secondary ref. letter short survey More	_	7 2 1	3	Mana-alenk Galahydra derindines d J2 dehydra 1-substituted 3H-pyrastol(4,1-2,4-trianol(4,3- gylynnialine 3 Hones and J Leven E S Soltword Sen sen - USE2004 (J2012) R Man Henry Mennes (J2012) Mennes (J2							
	Authors		~	•	No title <u>Compter R. Toept W.</u> - Chemische Berichte, 1962, vol. 55, p. 2881 - 2884 <u>Contempor R. Toept W.</u> - Services 2000 - 5, p. 2881 - 2884	Cited 9 tim	Feedbac	×Q				

### 2 勾选并筛选得到相关结构化合物的所有专利

Rec	ixys'		Quick search Query builder Results Synthesis planner History	Peng Wu 🔍 🗘 🕚
1,055	Filters and Analysis		1,055 Documents with 23,556 Substances, 104,375 Reactions, 1,564 Targets	i
2,094	Index Terms (List)	~	🗋 🔞 melected 🖉 🔗 📤 Linet To Exclude Export	Sort by Relevance + 🗸 Heatmap 🎛
	Index Terms (ReaxysTree)	~		
	Publication Year	~	View 3- hitroturyi derivatives     Ciba-Geigy Corporation - US3948913, 1976, A1	
	Document Type	^	Patent Family Memberse IL39247 D0; BE782658 AL; IE38312 L; NL7205668 A; DE2218717 AL;     Autract      Front Page Info      Substances 122      Reactions 119      Full Test 7	
	patent	- 1,055	Hit Substances (11) V	
	Authors	~ ~	7-Substituted nucle Oppounds     The University of Utah - US3962211, 1976, A1	
	Patent Assignee	~	Patent Family Members: US3962211 A; DE2600729 A1; FR2297216 A1; pS519/5015 A; ZA7600113 B; Abstract 🗸 Front Page Info 🗸 Substances 🛐 🗸 Reactions 😰 🗸 Full Text 🌶	
	Journal Title	~	Hit Substances 👔 🗸	
	Substance Classes	~	Meso-ionic didehydro derivatives of 1,7-dehydro-1-substituted-3H-pyrazolo[4,j-1,2,4-triazolo[4,3- <sup>3</sup> c]pyrimidine-3-thiones and 3-ones	
	Reaction Classes	~	E. R. Squibb and Sons, Inc US4124764, 1998, A1 Patent Family Members: US4053474 Ac JP5521/28398 Ac DE2717549 A1; FR2348927 A1; US4087423 A;	
			Abstract $\lor$ Front Page Info $\checkmark$ Substances (31) $\lor$ Reactions (33) $\lor$ Full Test (2) Hit Substances (3) $\lor$	
			PREVENTIVES OR REMEDIES FOR MYOCARDITIS, DILATED CARDIOMYOPATHY AND CARDIAC     INSUFFICIENCY CONTAINING NF-KAPPA B INHIBITORS AS THE ACTIVE INGREDIENT     DETORMUNETTE, COLUMN, AL	Feedback 💭 🖕

- ③ 历史导航栏,点击回看历史筛选结果
- 4 该专利结果集包含的生物活性构效关系图
- ⑤ 专利相关信息总结,摘要,家族专利号相关信息,实事例化 合物,反应等
- 6 专利中与检索结构相关化合物

### 2.2.2 Query builder – 专利标记检索专利(专利号)

Reaxys'	Quick search Query builder Res	sults Synthesis planner History	Peng Wu 👌 📮 🕲
🕁 🖻 🏷 🎁 Import Save Reset form Delete all		Starch Documents > Starch Documents > Starch H CAS RN Doc. Index Structure Molecular Formula CAS RN Doc. Index	Pind search fields and forms Q patent
	Common Patent Number     in       in	×	Reary         A           ◇         Patertis Location in Paterti         I           ◇         Patertis Rosphetic Compound         I           ◇         Patertis Rosphetic Compound         I           ◇         Patertis Rosined Merkunk         I           >         Patertis Rosined Merkunk         I           >         Patertis Rosined Merkunk         I
	3		Pritert Anligene     Common Pritert Number     Pritert Country Code     Pritert Number     Pritert Status
			Feedback 💭

1 输入'patent',获得专利相关所有检索模块

2 点击添加,专利号检索模块

3 其他途径获得的专利号需要加工才能在Reaxys数据中检索 专利,如: 'WO2009/020825' 是专利原文中专利号,需 要去掉 '斜线后面的0'变成 'WO2009/20825' 才是 Reaxys中收录的专利号

Re	axys'		Quick search Q	uery builder Resu	lts Synthesis plan	ner History		Peng Wu 🞗	Ą	٢	
1	Filters and Analysis		Process for Synthesiz	ing Compounds Usefu	I for Treating Hepati						
	Index Terms (List)	× 1	Bristol-Myers Squibb Com Patent Family Members: U	pany - US2009/43107, 2009, 5 52009/43107 A1; AU2008284	A] 007 A]; CA2605711 A	20/20825 A1; TW2009/1444	L.A				
	Index Terms (ReaxysTree)	~ 5	latinat v <u>freet Rystelle</u> ∧ Substances ()) v Resclow ()) v ful Test // Front page info								
	Publication Year	~									
	Document Type	~	Amignom	Amigness Inventors (Authon)							
	Authors	~	Bristol-Myers Squibb (	ompany		Pack, Shavin K.; Geng, Peng; Smith, Michael J.; Hamm, Jason					
	Patent Assignee	~ <	Patent No	Kind Code	Publ. Date 2009/02/12	Application No	Filing Date	Indexed Pater			
	Journal Title	~	AU2008284097	AL	2009/02/12	AU2008284097	2008/07/31	10			
	Substance Classes	~ 6	CA2695711	AL	2009/02/12	CA2695711	2008/07/31				
	Reaction Classes		W02009/20825	AL	2009/02/12	WO2008-U571696	2008/07/31				
		~	TW2009/14441	A	2009/04/01	TW2008-97130362	2008/08/08				
			PE06112009	AL	2009/05/16	PE0013252008	2008/08/08				
			AR067896	AL	2009/10/28	ARP080103487	2008/08/08				
			MX2010001415	A	2010/03/01	MX2010001415	2008/07/31				
			EP2178863	Al	2010/04/28	EP2008-796910	2008/07/31		Feedback	0	

- ④ 高亮检索的专利号
- 5 专利相关总结
- ⑤ 家族号,以及其他专利标记的总结,可以通过任意的专利标记,检索到该篇专利

#### 2.2.3 Query builder - 组合信息检索

#### (母核结构相关在中国发表过的专利)



- Query builder允许进行,多重逻辑关系的组合检索
- 2 检索时从上往下, '组内'逻辑关系会先满足,再满足组间 逻辑关系
- ③ 首发专利号或者家族专利号,含有CN标记的专利,优先匹配,再与结构交集匹配

Re	axys'	Quick search Query builder <u>Results</u> Synthesis planner History Pergrav A	Q C	)
40	Filters and Analysis	450 Documents with 58,663 Substances, 57,866 Reactions, 672 Targets		Î
	Index Terms (List)	V Det by Releance V Set by Releance V	Hestrop 🎛	
	Index Terms (RearysTree)	×		
	Publication Year	<ul> <li>PREVENTIVES OR REMEDIES FOR MYOCARDITIS, DILATED CARDIOMYOPATHY AND CARDIAC</li> <li>INSUFFICIENCY CONTAINING INF-KAPPA B INHIBITORS AS THE ACTIVE INGREDIENT</li> </ul>		
	Document Type	SUNTORY LIMITED - EP1352095, 2001, A1 Patent Family Members: CK255999 2 A1; W002001,02200 A1; AU7335400 A; EP1352099 A1; CK1355977 k;		
	Authors	Abstract v Print Page Info v Substances (20) v Pail Test 7/ Hit Substances (1) A		
	Patent Assignee	V Hit Substances	×	
	Journal Title	× •		
	Substance Classes	× Ro		
	Reaction Classes	· · · · · · · · · · · · · · · · · · ·		
		Agent for pupphylasis and treatment of internitial provincesis and pulmosary fillipoid     Well-Corporation COMMINS (COMMINS ALL ADDAMES, ACTIVATION (COMMINS ALL     Monte holy house COMMINS (COMMINS ALL ADDAMES, ACTIVATION (COMMINS ALL     Montes)     Well-Communication (COMMINS ALL ADDAMES, ACTIVATION (COMMINS A		
		PREVENTIVES/REMEDIES FOR ANGIOSTENOSIS	Feedback 💭	۰.



### 3. Reaxys Medicinal Chemistry - 药化信息检索

当购买了Reaxys完整版,及包含了RMC模块的Reaxys以后,在 Quick search和Query builder界面可以方便的检索各种生物活性

### 3.1 检索吉非替尼药代动力学生物活性数据

Quick search Query builder Results	Synthesis planner	History	Peng Wu	Š	Ŷ	0
Search for Pharmacokir	netic of gefitinib				Finc	>
Search Reaxys Q Pharmacokinetic of gefitinib		×				
AND	Drawing					
					Easter	
	Current Search for Pharmacokin Search for Pharmacokin Q Pharmacokinetic of gefitinb A10 Create Structure or Reaction (	Construction of the series of synthesis plantice Search for Pharmacokinetic of geftinib Construction of geftinib ANO Construction of Reaction Drawing	Contraction of the series of sprintices plantine in the series of sprintices plantine is a series of sprintice of sprintices plantine is a series plantine is a series plantine is a seri	Carlos Series     Carlos Series     Page 10       Search for Pharmacokinetic of gefitinib     Search for Pharmacokinetic of gefitinib     X       Q     Pharmacokinetic of gefitinib     X       AD     Crede Structure or Reaction Drawing	Carlos Series     Carlos Synthesis publicity     Program     Program </th <th>Carlos Search for Pharmacokinetic of gefitinib     Image: Control of the second symptotic symptotic</th>	Carlos Search for Pharmacokinetic of gefitinib     Image: Control of the second symptotic

#### Quick Search中可以使用的方式:

- 1. 靶点,或者基因名称,5-ht1a
- 2. 靶点活性, PIP4K2C Activity
- 3. 靶点抑制性, Inhibitors of CXCR4
- 4. 物质在靶点上的抑制性, PIP4K2C by imatinib
- 5. 靶点作用机制, Agonist of GLP-1
- 6. 物质作用效果, Atenolol Pharmacological effect
- 7. 物质药物代谢动力学研究, Pharmacokinetic of Imatinib
- 8. 结构

### 完整版的Reaxys 在检索'吉非替尼药代动力学' 会出现以下'预览结果'

Reaxy	ýS'	Quic	k search Query builder Results Synthesis planner	History	Peng Wu 🙏 🗘 💿
	1	Targets	Structure : 💽 as drawn AND Bioassay Category : Pharmacakkastic Edit in Query Builder 🔗 Crean Ater 👰	Preview Results 🗸	View Results >
	1	Substances	Structure : 🚱 as drawn AND Bioassay Category : Pharmacokinetic	Preview Results 🗸	View Results > 2
	596	Documents	Titles, Abstracts, Keywords : Pharmacokinetic, gefitinib	Preview Results 🗸	View Results >
	331,586	Documents	Titles, Abstracts, Keywords : Pharmacokinetic	Preview Results 🗸	View Results >

- 1 结构对应的药代动力学'靶点信息'
- 2 结构对应的药代动力学信息
- 3 关键词相关文献

当查看'吉非替尼药代动力学信息'时,会看到具体的药 代动力学数据

Reaxys	Quick search Query builder Results Synthesis planner History Perg Wa & D O	
1	gefine.         G_2S_2CPU(A_2 46.00)         0.00221         214073/52           G_2S_2CPU(A_2 46.00)         0.0021         0.0011         0.0011           Degliness         Proved Dirk - 55         0.0011         0.0011           T         Degliness         Spectra - 07         Torpet-12012           T         Disaminary (HD Dirk)         Spectra - 07         Torpet-12012	
	gefitinib ×	
Recoys'	✓ Identification	ł
	Druglikeness	
	Sicactivity (Hit Data) <sup>A</sup> Enumeratures: epi <sup>A</sup>	
	Purameter         Wite         Unit         Biological power         Populations         Dose         Dosing regimes         Reference         Simulative columna         <	
	Concentration 8.03 yapint, Mus Interpretational 25 Performatives Agareus, Sperg Serve, Randus Galanda, Jook J. Officer, John H. Dhegala, William F Journal of Remaining and Experiment Part State (2014), 110-1135 Experimentation of the serve of the se	

- 1 具体的'药代'生物活性
- 2 全部生物活性
- 3 点击查看具体数据
- 4 完成版Reaxys才能查看具体数,并且得到详细出处

#### 3.2 RMC-靶点相关生物活性检索(如:EGFR)

	South Toronto A	
	© # #	Find search fields and forms Q
	Sincure molecular formular GLS AVE D	Razon A
Zarget Name	3 R	Basic Indexes
		Physical Properties
		► Spectra V
	2	A Target Name
		<ul> <li>Substance Action on Target</li> </ul>
		Substance Effect     Measurement aX
	V Target Name	Shuther Meesuin Formula Coll 94 D

- 靶点转换器帮助科研人员,把靶点'缩写', '同义词'等 转化为标准索引词,以尽可能确保不会漏检相关信息
- 2 完整版Query builder会增加药化模块
- 3 点击靶点模块,从靶点出发检索生物活性

Target Name 3577084 Q EGFR 4		××	1
> 🖾 largets	-	18,873,531	
> 🔁 protein		15,228,090	
> 🔁 binding protein		10,095,021	
> 🔁 heterocyclic compound binding protein	•	3,265,935	
> 🔁 nucleic acid binding protein	-	1,267,137	41
> 🔁 DNA binding protein	-	1,066,408	1
Structure-specific DNA binding protein	-	148,051	1
> 🎽 double-stranded DNA binding protein		147,382	1
> 🔁 Epidermal growth factor receptor (EGFR (Epidermal growth factor receptor))		62,947	2
Epidermal growth factor receptor [human] (EGFR)	-	59,057	T
Epidermal growth factor receptor [dog] (EGFR)	_	2	1
Epidermal growth factor recentor (Mus musculus) (Fofr)		3 723	1
Selected search items:		More +	1
Epidermal gro [human] × Epidermal groor [dog] × Epidermal grousculus] × Epidermal gro	egicus] 🗙	I	ļ
- Clear sele	cted × 8	Transfer 🗲	

- 6 靶点便准索引词
- 7 可以在这些区域内,增加或删减想要检索的靶点相关信息
- 8 选择好后点击转换即可

Reaxys <sup>-</sup>	Quick search Query builder Results	Synthesis planner History
소 🖻 🌍 💼 Import Save Reset form Delete all		Structure Molecular Formula CAS RN Doc. Index
	○ Target Name is Yest Name Epidermal growth factor receptor (human).Epider	× mal grow 🛃

1 选择检索靶点

Fil	ters and Analysis			157 Targets out of 6,547 Documents, 187,342 Substances, 207,812 Reactions		4
lî [	Targets		^	selected     Limit To Enclude Expert	Sort	by Target Details 🕈 🧹 🛛 Heatmap 🔛
	vascular endothelial growth factor receptor 2	_	5,858	Single protein 1-aminocyclopropane-1-carboxylate synthase 4 (Wild)	Substances - 1	Example structure
	epidermal growth factor-activated receptor	-	5,034	Synorymic Laminocyclopropane L carbonylate synthase 4, acc synthase 4, acc 4, ac-4, as (L-aminocyclopropane-L-carbonylate synthase 4), a2g22810, bas4, le-acs4, <u>+3 more</u> Show target details $\checkmark$	cs <sup>4</sup> Documents - 1 >	~~~~
	epidermal growth factor receptor	-	3,946			
	vascular endothelial growth factor receptor 1		1,661			R No quantitative value reported

2 Filter中可以看到,具体每个靶点生物活性数量,并且可以进 一步筛选关注的主要信息

8 EGFR相关靶点结果集,包含,EGFR家族所有靶点,以及相 关的脱靶靶点和适应症靶点

🔮 一键拿到,靶点相关生物活性构效关系图

Rec	axys'		Quick search	Que	ry bu	ilder	Res	ults	Sy	nthe	sis pla	innei		Histo	эry						Pe	ng Wi	. ^			٢	
757	Filters and Analysis		757 Target 5	57 Target 5 / ( 6) coursents, 167,342 Substances, 207,812 Reactions																							
	Measurement pX	~	Contraction Contraction	CTO Exclude Export Settings Navigator Legend																Targ	sts E	1	Fullson	en 27			
	Parameters	~		Шſ	8	R.	X	202	tor A	(659)	(sec.	ter C	Q as	ter 1	otein	ter 2	ter 3	-007	option	[umu]						nsel	-
	Targets	~		6	e ptor	rol. tri	r nine	e e ZA	nd fac	0VPa	nVEG	nd fo	nd fad	rd cep	rd pr	ar cop	rd cep	rd hd	nd reo	rd[hu		(human)	~			44 m	oidase
	Target Species	~			rosine-p	notice p	rotire-p	costee p	soular et	scular er	soular e	soular er	scular et	soular er	ricular er	fuery a	scular et	scular er	rioular er	south er	EGF 165	EGF 165	EGF-A16	89	EGR/2	inge ga	rthine o
	Target Type	~		Targe	F 6		F F		3	3	\$ \$	3	3	3	9 5		3	2	9	g	2	>	>	>	5 3	: 9	2
	Substance action on target	~~	Substances				• •		•					•	- 0	2	*		•	Ē	Na	dant	hor				ĥ
	Molecular Weight	~	6-(6-acetyla]-arriide	-		Name and Address of						1		*		2				1		Bar			1.6	-	
	Highest Clinical Phases	~	7-(6-acetylal)-amide 6-(6-aminoyl)amide	-		p <sup>1</sup> q	5			Mart allog	1483	-		1 11 K								1				1	ŀ
	Effect	~ (	8 1-(2-fluororyf)urea		X considered Sector Sector S						7.4	1	3				0										
	Document Type	~	11010957	-	viburanda produnet - deritate - Deplement						1	2										-	H				
	Publication Year	~	6-(6-hydroxyl]amide			- Sude (Nay 1 - Next Next )						5.9			1				2-								
	Patent Assignee	~	5-[2-(3R-h nylamide sunitinib	-			2	5	41			5.2	<b>9</b>	4		1			9.5	ľ							
			Gentendensid	_									-											- F	redbad	* <b>Ç</b>	-

- 5 结果导出
- 6 改变X,Y轴的参数值等设置工具
- ♂ X轴以EGFR为基础的,家族靶点,家族突变靶点,适应症靶 点,脱靶靶点
- 8 Y轴, 靶点做过生物活性的化合物
- 9 具体信息点击可以查看详细数据
- 10 导航栏显示数据总量概况

### 3.3 RMC-药化信息预设模块专项检索 (化合靶点检索靶点选择性)

Reaxys'	Quick search Query builder Results	Synthesi	is planner History		Perg Wa 🞗 🗘 👁
💩 📴 🌑 👸 Import Save Resat form Delete all			Search Substances > Search Substances > Substances + Search Substances > Malexalar Formula CAS RV Data Index		Find search fields and forms Q
	Selectivity Profile	×		2	Reaxys Forms V
	Target Name     In Y Torret Name			2	Affeity on target     Out problemation: Inhibition
		8		ļ	Salectivity Profile     Animal models: Tumor sanografia
	Measurement pX     Measurement pX	R			Biomelability     Solume of distribution
	(trans				Absorption (Onex, Cavg)
	© Target Name				Case-2 permeability Case-2 Active transport
	is V Target Name	R			Blood-Brain Barrier Penetration     (005)
					Feedback

- 1 Query builder中已经预设好了各种专项检索模块
- 2 点击直接得到组合信息模块,填入相关数据即可检索
- 3 如: 靶点选择性, hERG阻断,血脑屏蔽等

检索,对COX-1抑制能力高于uM级别,对COX-2抑制能力低于nM级别

$\otimes$				
<	> Target Name			
	is V	Target Name	1	R
AN				
<	> Measurement pX	(		
	>= ~	Measurement pX	2	EQ
омы	NE			
<	> Target Name			
	is 🗸	Target Name		EQ
AN	)			
<	> Measurement pX	(		
	<=	Measurement pX		R
N 9	Aeasurement pX	(	2	EQ
Ta	irget Name ox-1			EQ
c				

2 量级数值,9为10<sup>-9</sup>次方



Rec	axys'		Quick sea	rch Query builder	Results	Synthesis planner	History	Peng Wu	Š	Ŷ	0		
62	Filters and Analysis		1 62 Su	ubstances out of 478 Do	cuments, containing	g 395 Reactions, 11 Targets			Reavys	62	~	Î	
	By Structure	$\sim$		O ⊘ ▲ Limit To Exclude Export			• <b>o</b> — ©	No of References	2	Heatmap	88		
	Measurement pX	~										1	
	Highest Clinical Phases 🗸 🗸				[1-(4-chloroben C <sub>15</sub> H <sub>10</sub> CINO <sub>4</sub> 3	zoyl)-5-methoxy-2-meth 57.793 497341 53-86-1							
	Targets	$\sim$			Identification	PI	rysical Data - 495		Preparati	ons - 61	>		
	Deseminations			~	Druglikeness	S	oectra - 156		ns - 871	>			
	Parameters	× .	4	20	Bioactivity (Hit I	Data) O	ther Data - 1,666		Targets - 708				
	Substance Classes	$\sim$		6	Bioactivity (AJI)			D	s - 7,358	>			
	Molecular Weight	~	2	~	[2-(2,6-dichloro C14H11Cl2NO2	anilino)phenyljacetic acie 196.153 2146636 15307-	I 86-5						
	Availability	$\sim$		the second	Identification	PI	rysical Data - 162		Preparati	ons - 29	>		
	Availability in other databases 🔍	~		5	Druglikeness	S	pectra - 68		Reactio	ns - 424	>		
					Bioactivity (Hit I	Data) O	ther Data - 2,424		Targo	ets - 343	>		
	Available Data			H	Bioactivity (AJI)	D	Documents - 4,823 🔉						
	Document Type	V								Feedbac	* 🖓		

已报到过的做过双靶点选择性的化合,都被检索出来

### 2 直接点击获得构效关系图

Re	axys'		Quick search Query builder Results Synthesis planner History			
6	Filters and Analysis 62 Substances out of 478 Documents containing 395 Readiens, 11 Targets					Range - 62 🗸 🗸
	Measurement pX	~	O Depart Se	gi Navigator Legend		Substances 🖽 🛛 Fullecreen 🖉
	Parameters	~				Prostantancin C/H synthese 2
	Targets	~			Prostandardin Civil surfaces 1	
	Target Species	~				
	Target Type	~				
	Substance action on target	~	Substances		•	•
	Molan dis Walakt	~	melosiam (			124
	notcour regit		· 2 (+ (avail		-	112
	Highest Clinical Phases	~	a the design of the second sec			
	Effect	~	н-тир-тус-мар-Он		42	127
	Document Type	~	3-(4-faoro H-Indole (	Navigator ×	51	107 4
			3-(4-meth., H-indole (		1	117
	Publication Year	~	2-(4-methylylindole (		1	13.6
	Patent Assignee	~	2 (4-aminus fjindole (		1	12.2
			2-(4-Methylyindole (		1	35.2
			N-cyclope2-amine (		1	30
			2-(4-aminosyindole (		1	30
			2-(4-methylaJ)indole (		1	×

- 直接导出具有对比性的构效关系图数据
- 2 COX-1标准名称
- COX-2标准名称
- 2 点击查看具体数据









ELSEVIER官方微博

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