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

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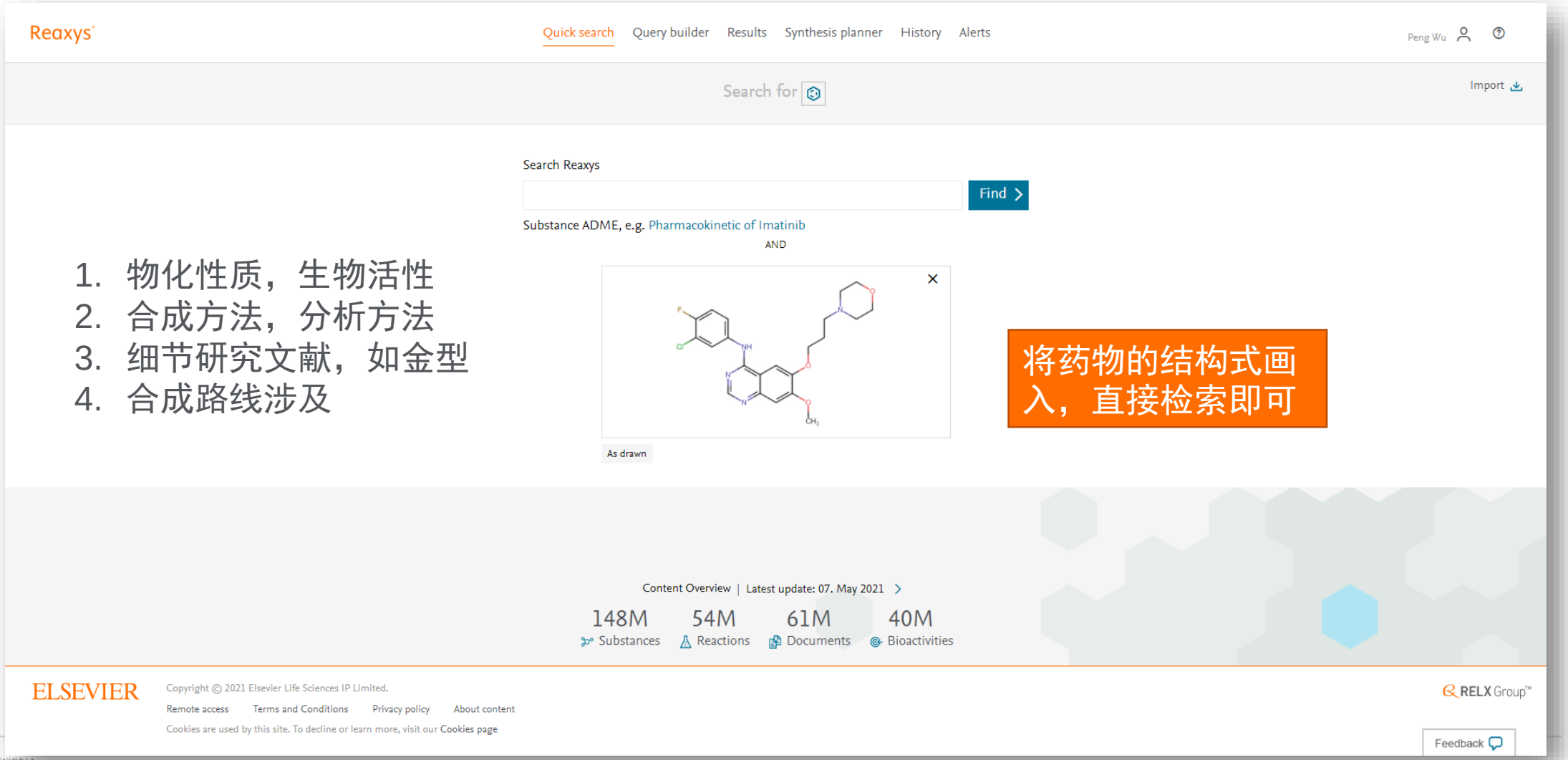
爱思唯尔生命科学客户顾问

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

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

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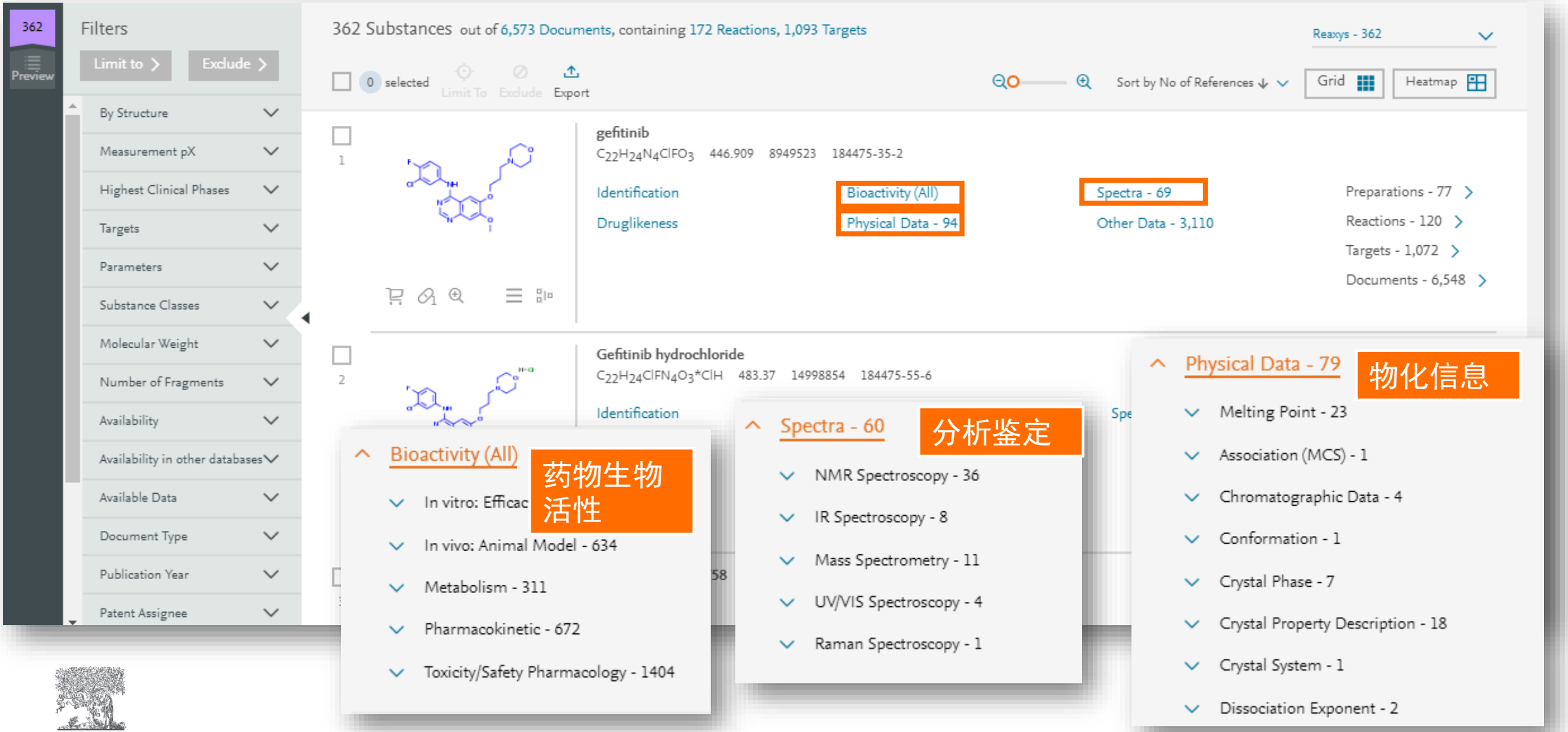
Reaxys-化合物核心信息的整理特点



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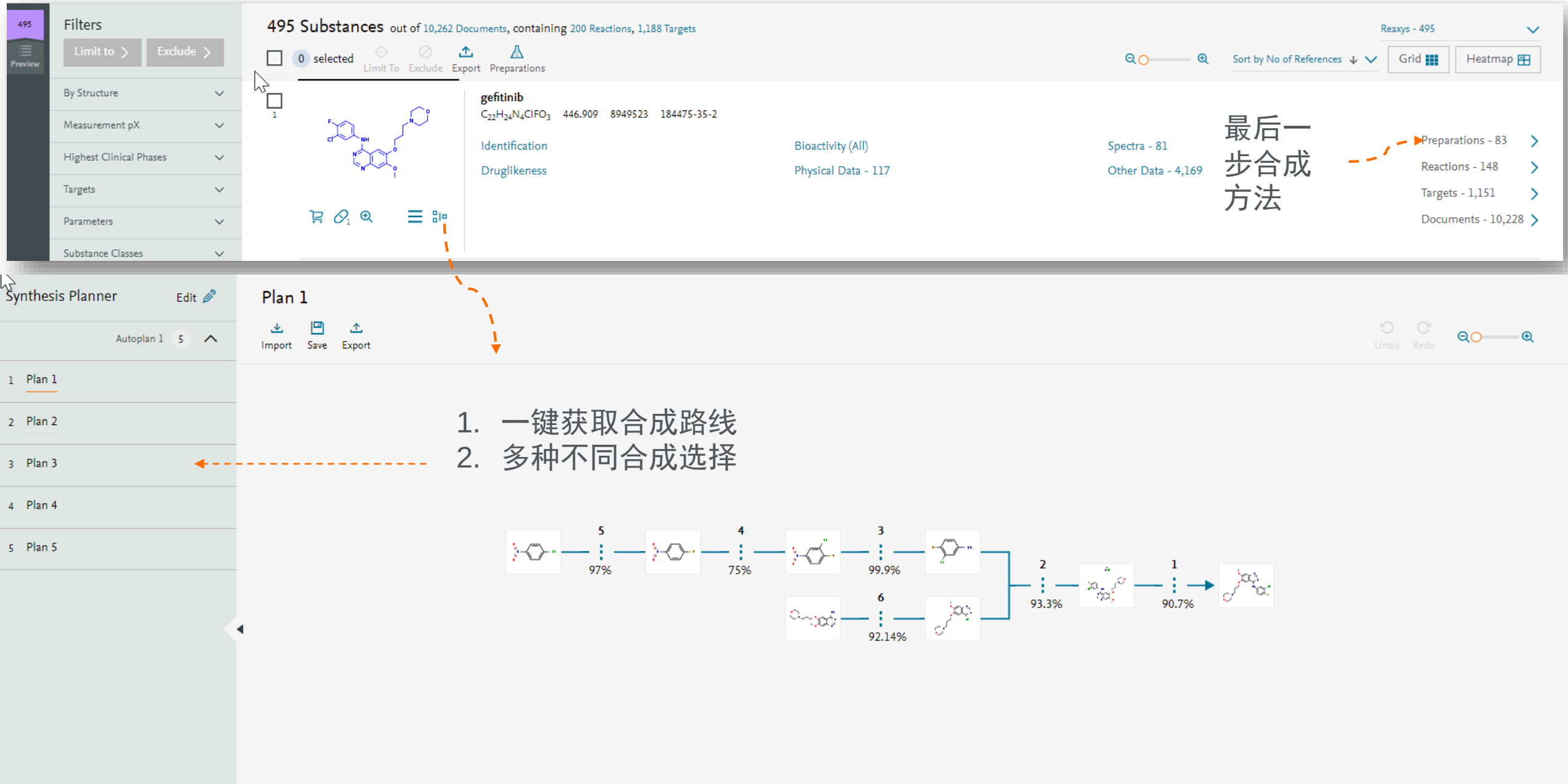
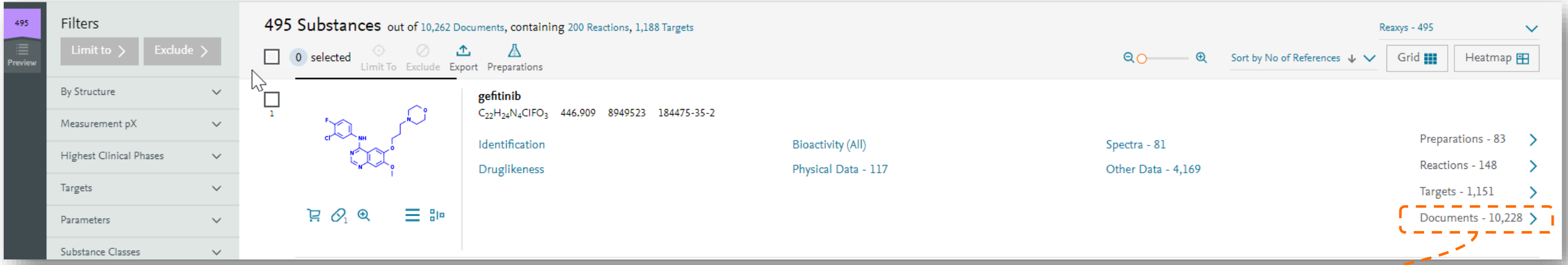
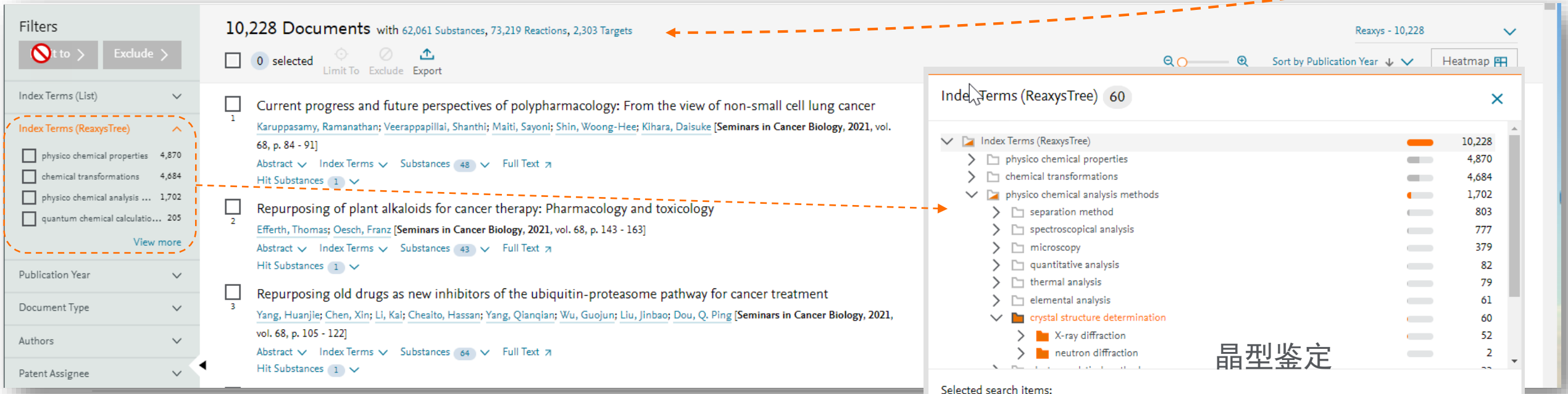
Reaxys-合成方法


495
Preview
Filters
Limit to
Exclude
By Structure
Measurement pX
Highest Clinical Phases
Targets
Parameters
Substance Classes
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
gefitinib
C22H24N4ClFO3 446.909 8949523 184475-35-2
Identification
Bioactivity (All)
Spectra - 81
Druglikeness
Physical Data - 117
Other Data - 4,169
最后一步合成方法
Preparations - 83
Reactions - 148
Targets - 1,151
Documents - 10,228
Synthesis Planner
Edit
Autoplan 1 5
1 Plan 1
2 Plan 2
3 Plan 3
4 Plan 4
5 Plan 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
5
97%
4
75%
3
99.9%
2
93.3%
1
90.7%
6
92.14%

Reaxys-药物相关文献获取





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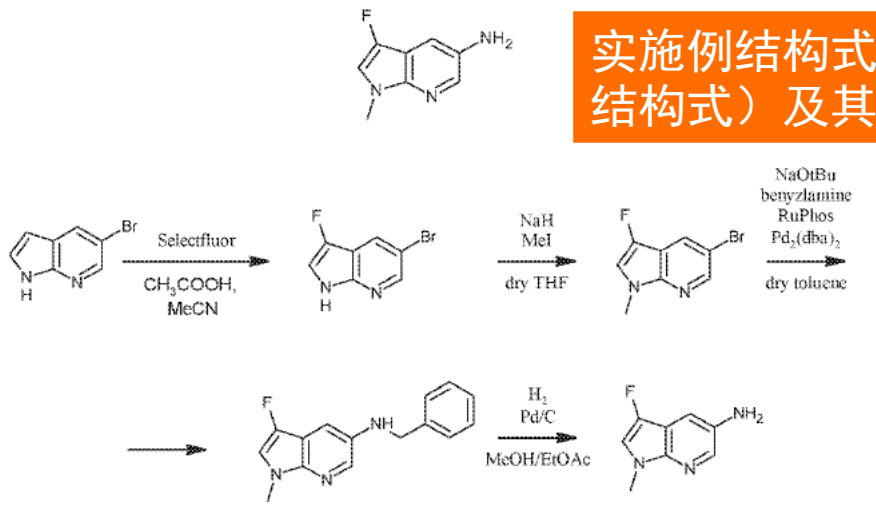
专利信息检索的挑战

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？

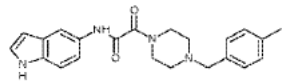
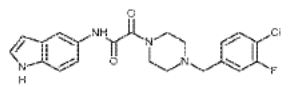
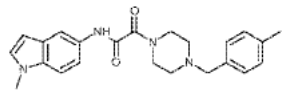
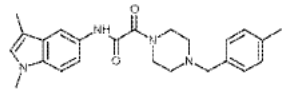
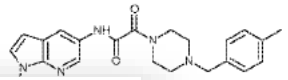
1. 理解：专利中的化合物结构式与Markush结构关系
2. 在专利结构式被提炼到数据库前，快速跟踪专利
3. 拆分专利细节，靶点，晶型，剂型，工艺等

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 EC_{50} values in the $[Ca^{2+}]_i$ 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

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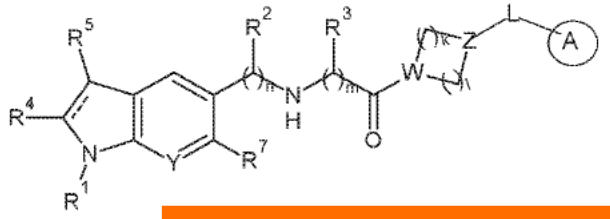
专利基础信息简介-人工抓取内容-claim

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

wherein

R¹ is hydrogen or C1-6alkyl;

R² is hydrogen or C1-6alkyl, or R^2 is absent when n is 0;

R³ is hydrogen or O; or R^3 is absent when m is 0;

R⁴ and **R⁵** are independently hydrogen, C1-6alkyl, halogen, haloC1-6alkyl, C1-6alkoxy, 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(R^6);

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 α7 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

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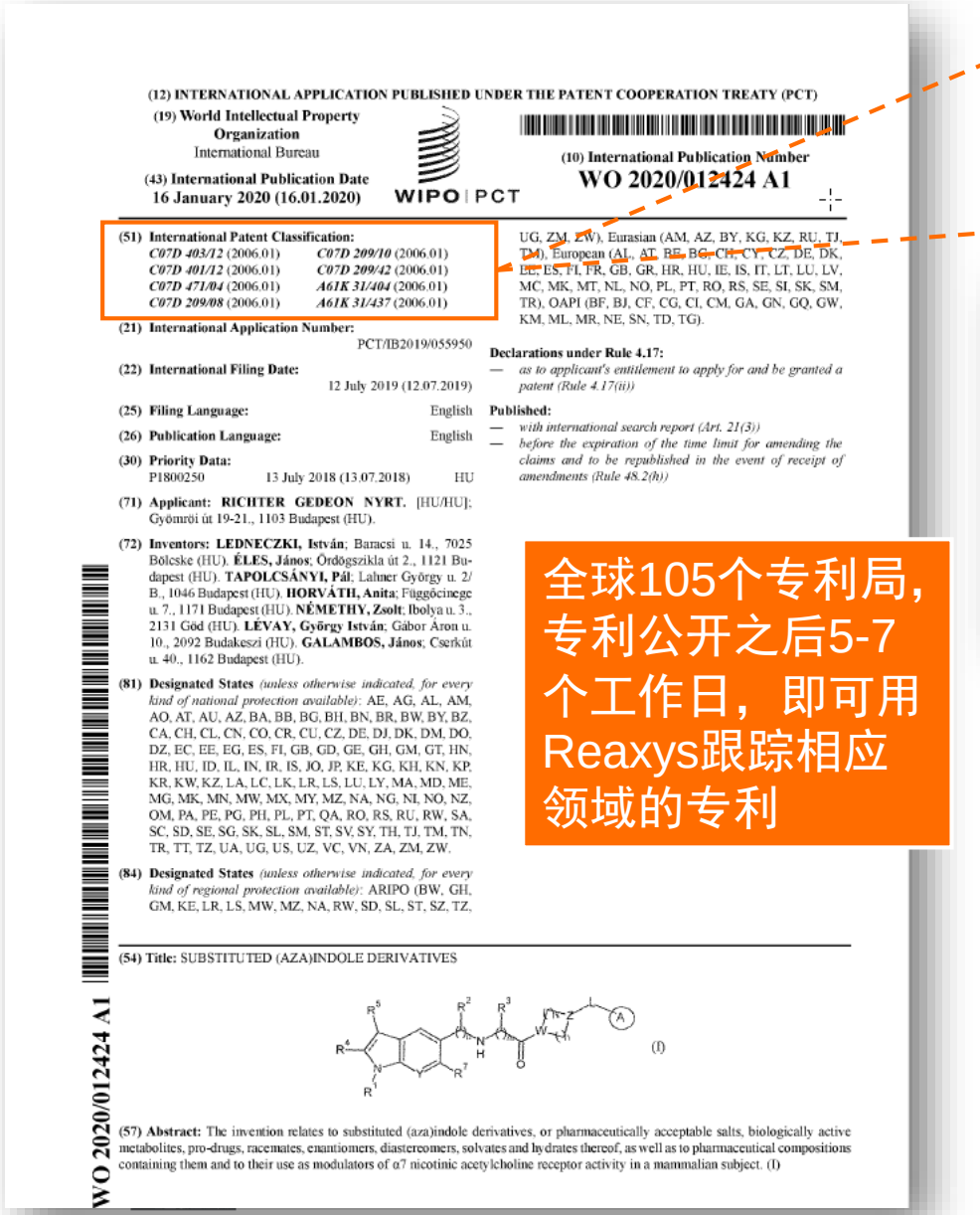
专利基础信息简介-专利标记



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C07D 471/04 (2006.01) *A61K 31/404* (2006.01)
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(71) Applicant: **RICHTER GEDEON NYRT.** [HU/HU]; Gyömröi út 19-21., 1103 Budapest (HU).

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(I)

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WO 2020/012424 A1

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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

Main IPC

Secondary IPC

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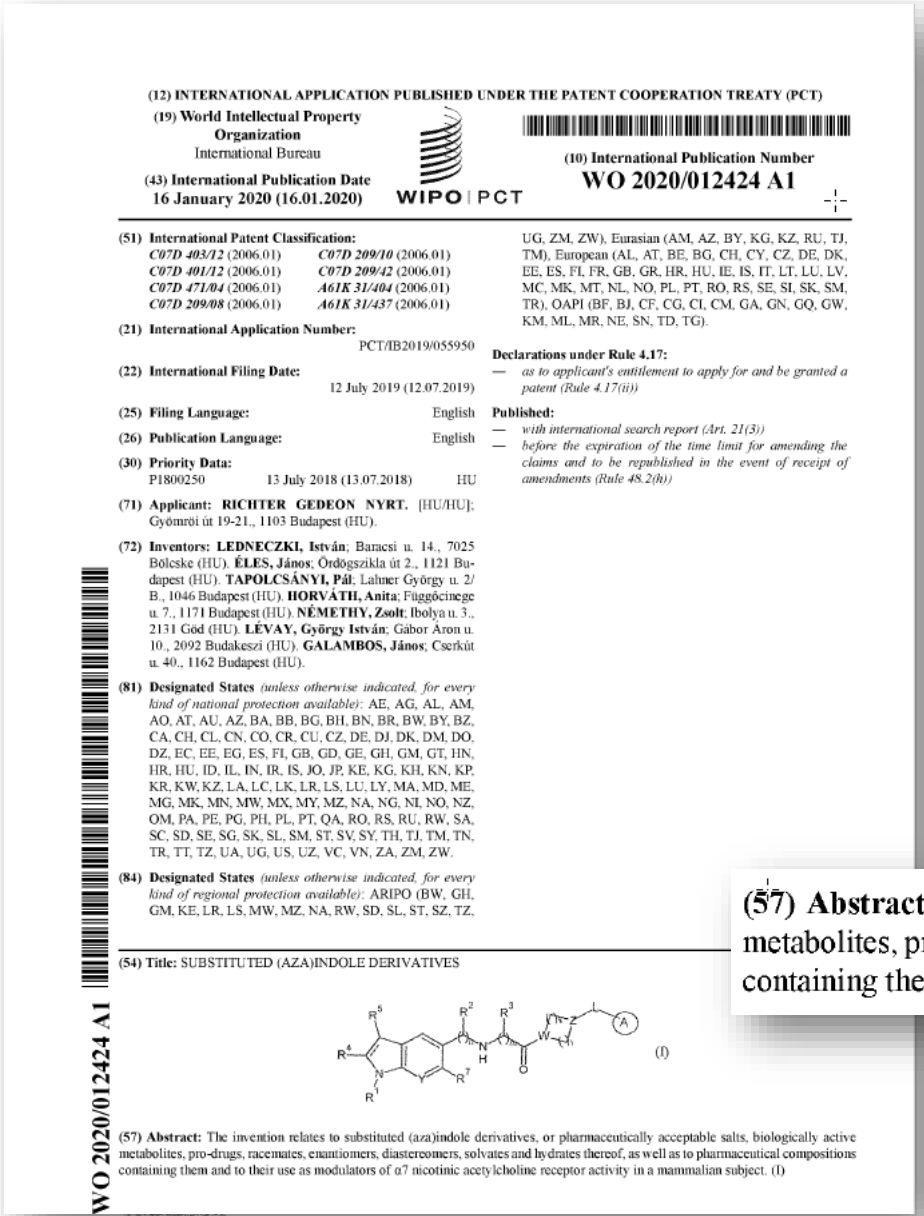
C07D 401/12 (2006.01)	*C07D 209/42* (200
C07D 471/04 (2006.01)	*A61K 31/404* (200
C07D 209/08 (2006.01)	*A61K 31/437* (2006.01)

分类号	含义		
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	中国专利	世界专利
403/02	.含两个杂环	中国专利	世界专利
403/12	..被含有杂原子的链作为键链连接		世界专利

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		
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	中国专利	世界专利
31/33	.杂环化合物	中国专利	世界专利
31/395	..有氮作为环杂原子的，例如胍乙啶、利福霉素	中国专利	世界专利
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	中国专利	世界专利
31/403	....与碳环稠合的，例如咔唑	中国专利	世界专利
31/404	.....吲哚类，例如吲哚洛尔	中国专利	世界专利



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Patent assignee
（专利受让人）

(72) **Inventors: LEDNECZKI, István**; Baracsi u. 14., 7025 Bölcske (HU). **ÉLES, János**; Ördögszikla út 2., 1121 Budapest (HU). **TAPOLCSÁNYI, Pál**; Lahner György u. 2/B., 1046 Budapest (HU). **HORVÁTH, Anita**; Függőcinege 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）

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专利的标题摘要

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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

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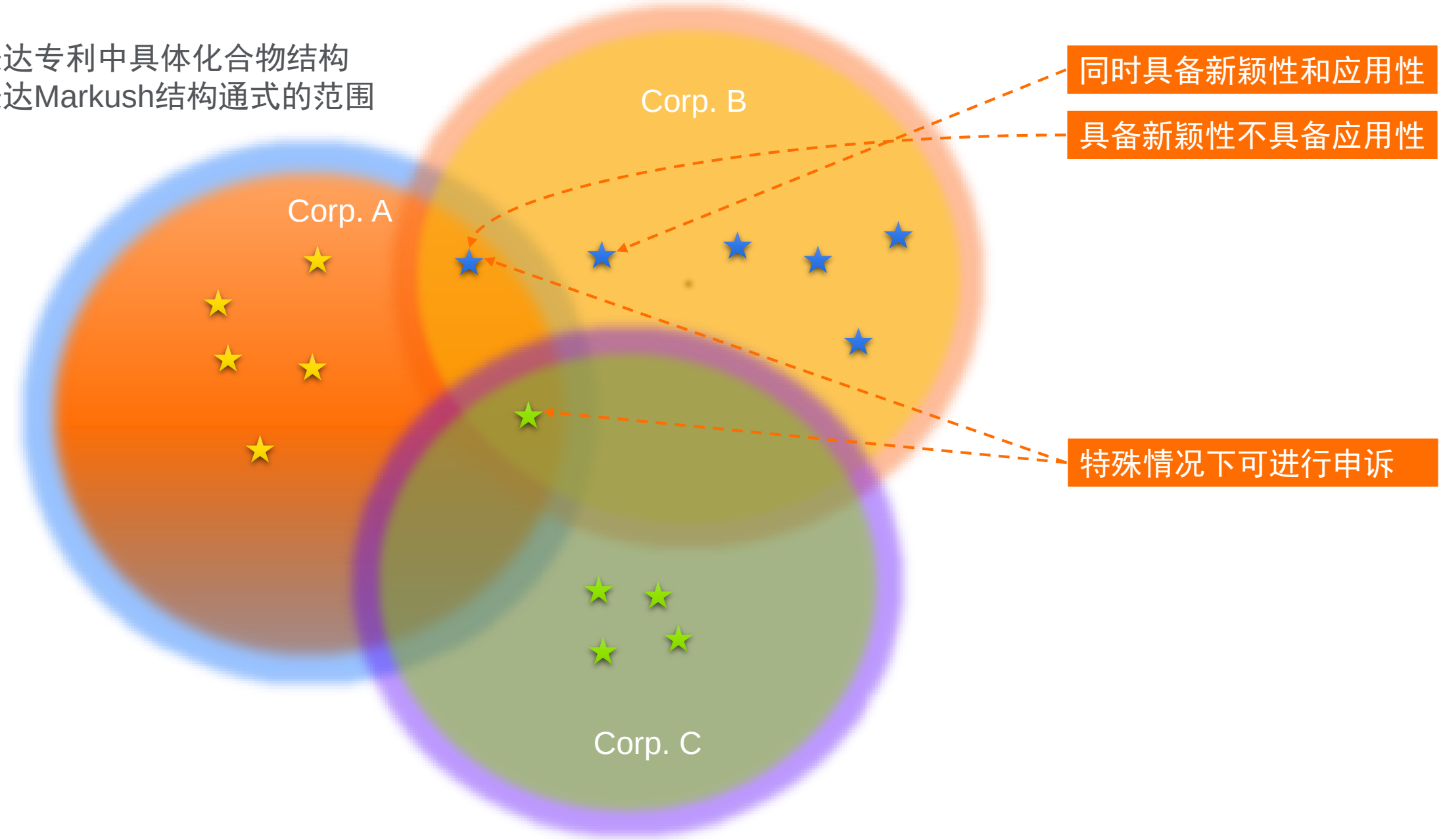
专利布局概览（应用性/新颖性研究）

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



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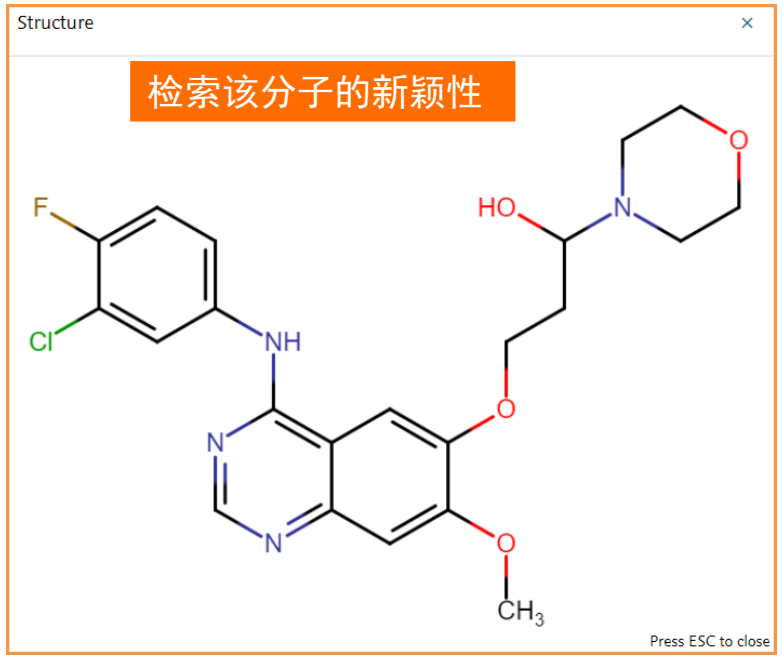
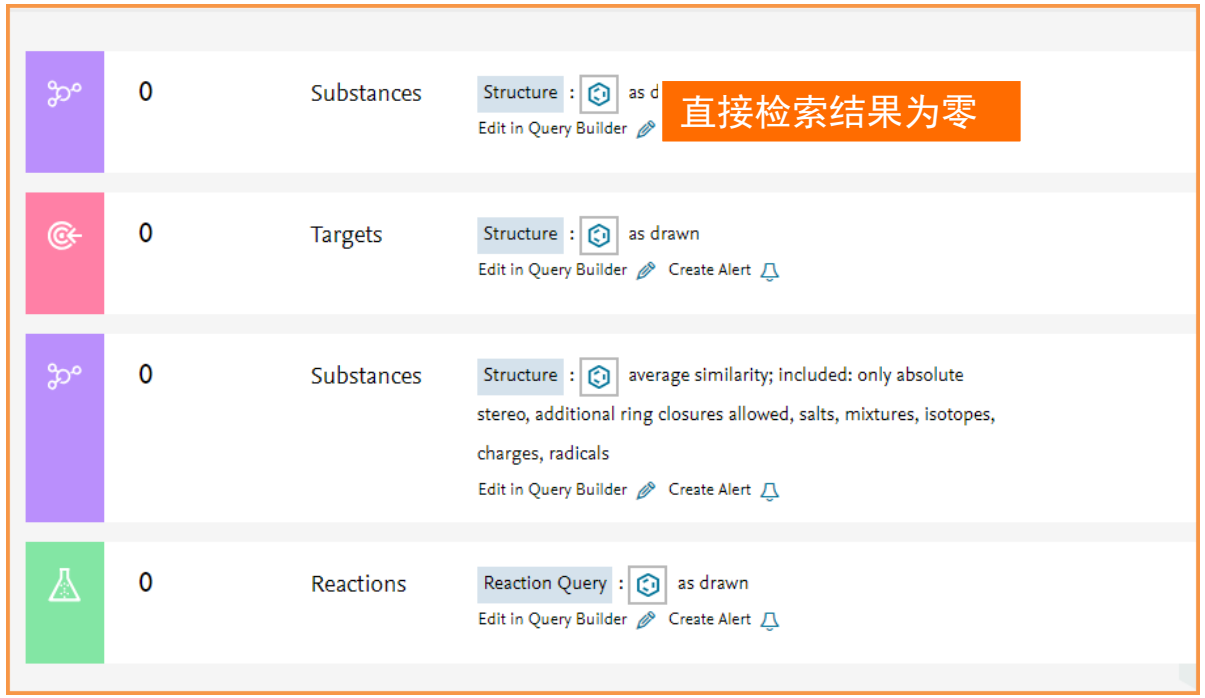
Case 1 小分子药物新颖性检索--Markush检索的基本模式

- 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？



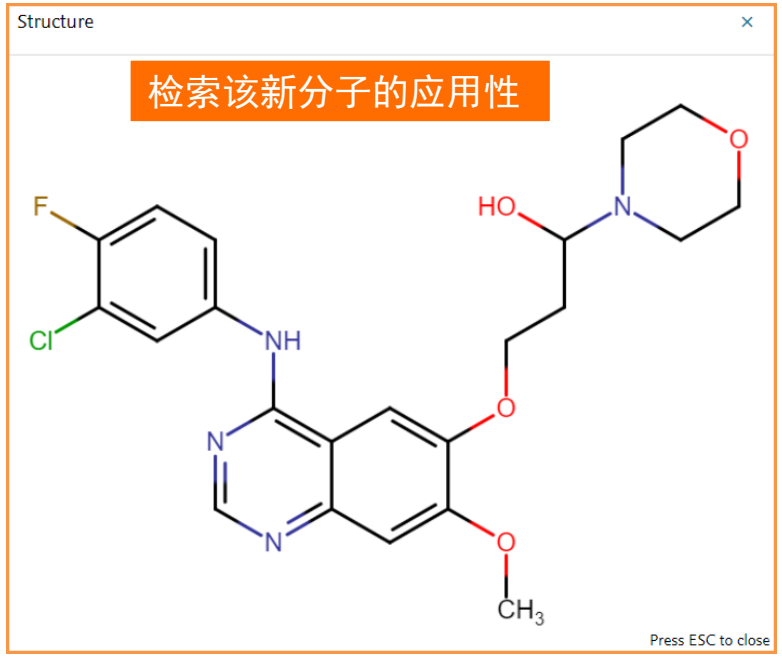


Tip：具体化合物检索，检索为0，即可大致确认其为新颖的，**新颖性需要不同数据库重复多检索几次，以保证不漏检**

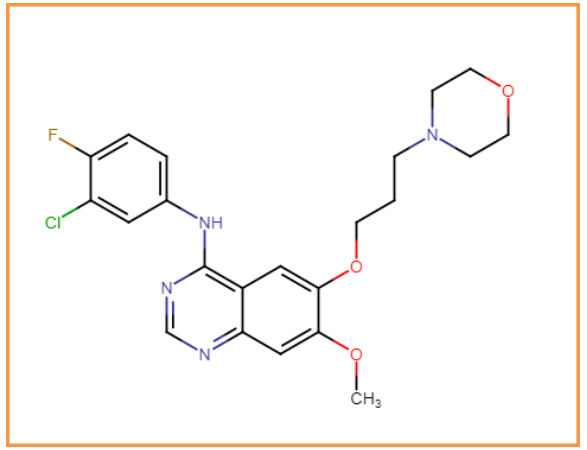
ELSEVIER

Markush检索的基本模式

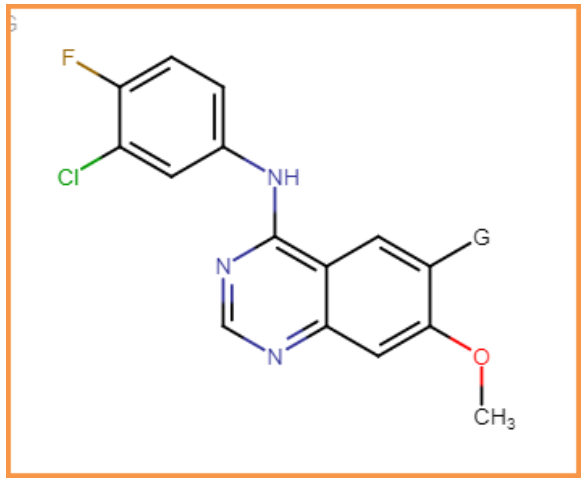
- 通过分析之后，可以通过相似已存在结构的markush锁定结果



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



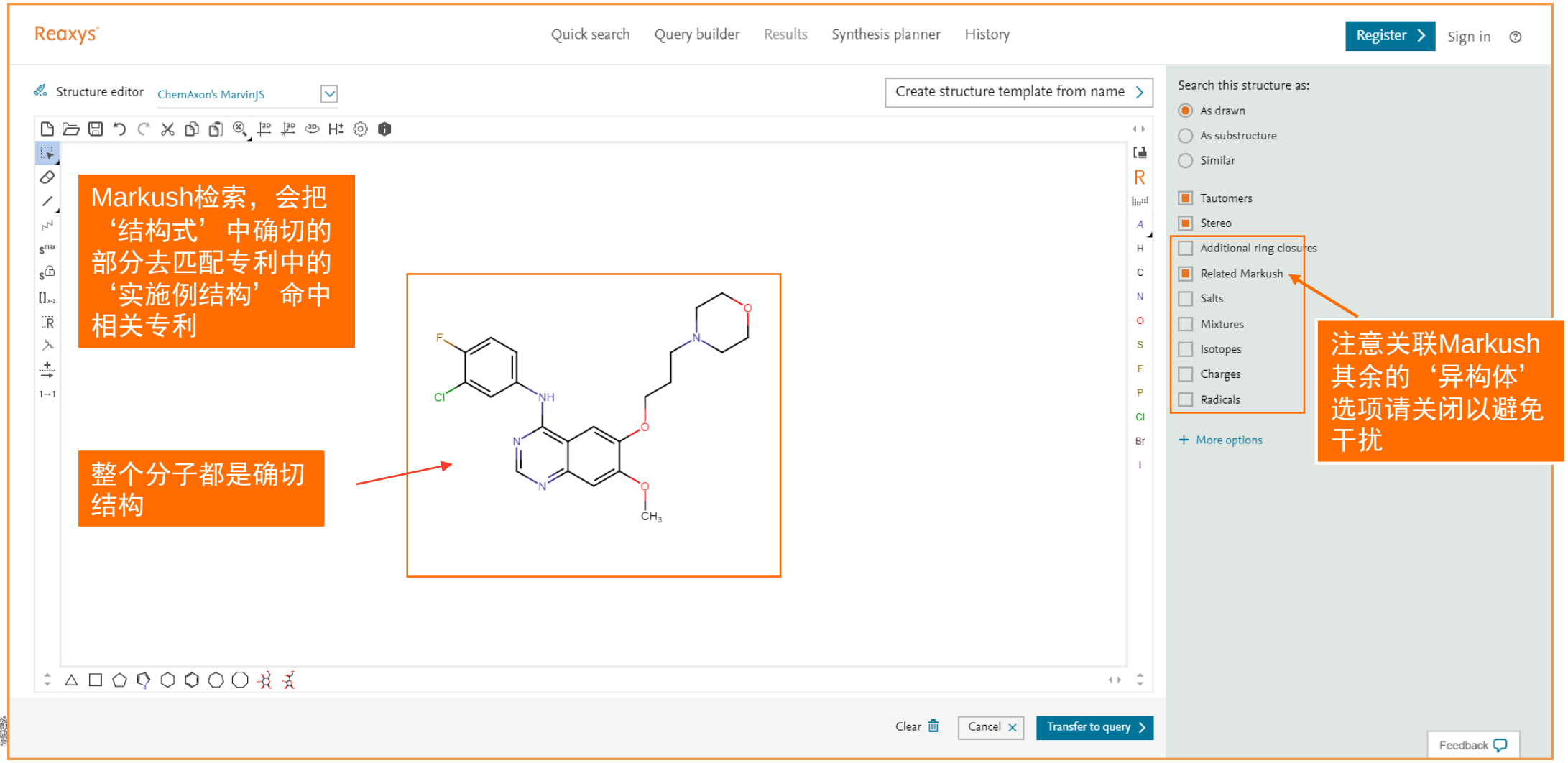
方法1：通过一直的分子，对应的Markush，研究该Markush是否包含新分子



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

ELSEVIER

Markush检索的基本模式-方法1：最相关结构检索



ELSEVIER

Markush检索的基本模式-检索结果

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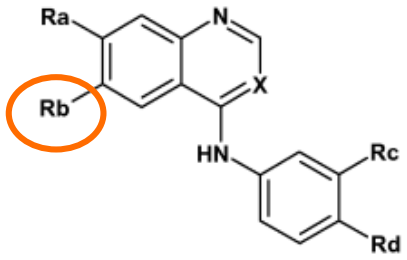
Markush结构解读



原文中的的markush结构，Rb到底是什么结构？

wherein each Ra, Rb, Rc and Rd is independently selected from hydrogen, halo, h
amino,
hydroxyamino, carboxy, C_{1-8}alkoxycarbonyl, nitro, guanidino, ureido, carbamoyl,
cyano, trifluoromethyl, $(R^6)_2$N-carbonyl and phenyl-W-alkyl wherein W is selected f
a single bond, O, S and NH;
or each Ra or Rb is independently selected from cyano-C_{1-8}alkyl and R9 wherein R
from the group consisting of R5, R5O, $(R5)_2$N, R7C(=O), R5ONH, A and R5Y; whe
R5 is C_{1-8}alkyl;
R6 is hydrogen or R5 wherein the R5s if more than one is present are the same or

69

Rb is di-(C_{1-8}alkyl)-amino-C_{1-8}alkoxy, pyrrolidin-1-yl-C_{1-8}alkoxy, piperidino-C_{1-8}alkoxy, morpholino-C_{1-8}alkoxy, piperazin-1-yl-C_{1-8}alkoxy, 4-C_{1-8}alkylpiperazin-1-yl-C_{1-8}alkoxy, imidazol-1-yl-C_{1-8}alkoxy, di-(C_{1-8}alkoxy-C_{1-8}alkyl)-amino-C_{1-8}alkoxy, thiomorpholino-C_{1-8}alkoxy, 1-oxothiomorpholino-C_{1-8}alkoxy or 1,1-dioxothiomorpholino-C_{1-8}alkoxy, and wherein any of the above-mentioned Rb substituents comprising a CH_2 (methylene) group which is not attached to a N or 0 atom optionally bears on said CH_2 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 C_{1-8}alkoxy;

Rb is amino- or N-[N'-mono- or N',N'-di(C_{1-8}alkyl)]amino}-C_{4-8}alkenoyl)-amino;

Rc is halo or R_2**-$(CH_2)_n$--R_3**-

wherein R_2** is a pyridyl, thiophenyl, pyrimidinyl, thiazolyl or phenyl, each optionally substituted with up to three substituents selected from C_{1-8}alkyl, C_{1-8}alkoxy and halogen, R_3** is –O- or –S- and n** is 0 to 8, preferably 0 or 1;

and Rd is halo;

or a pharmaceutically acceptable salt or prodrug thereof;

and an antibody inhibiting EGFR;

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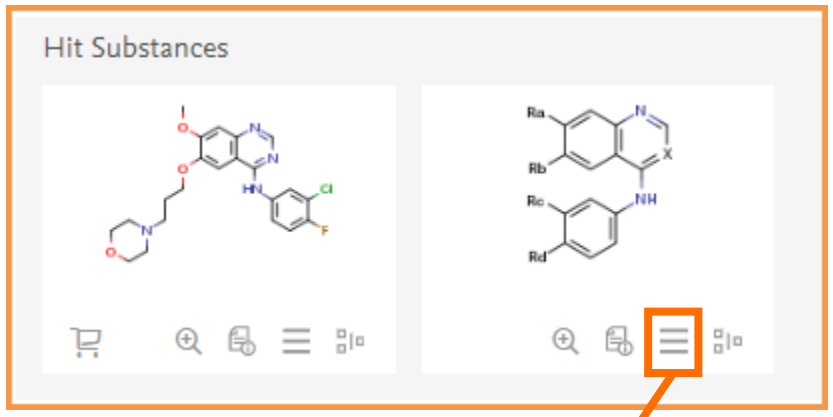
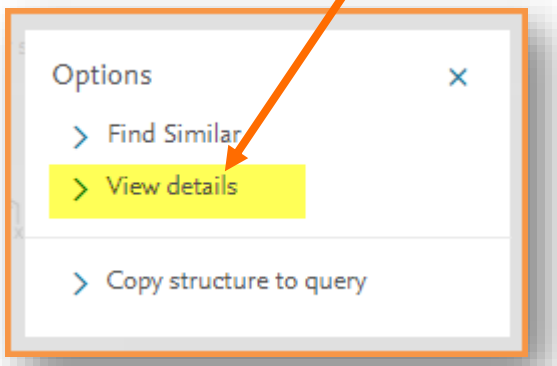
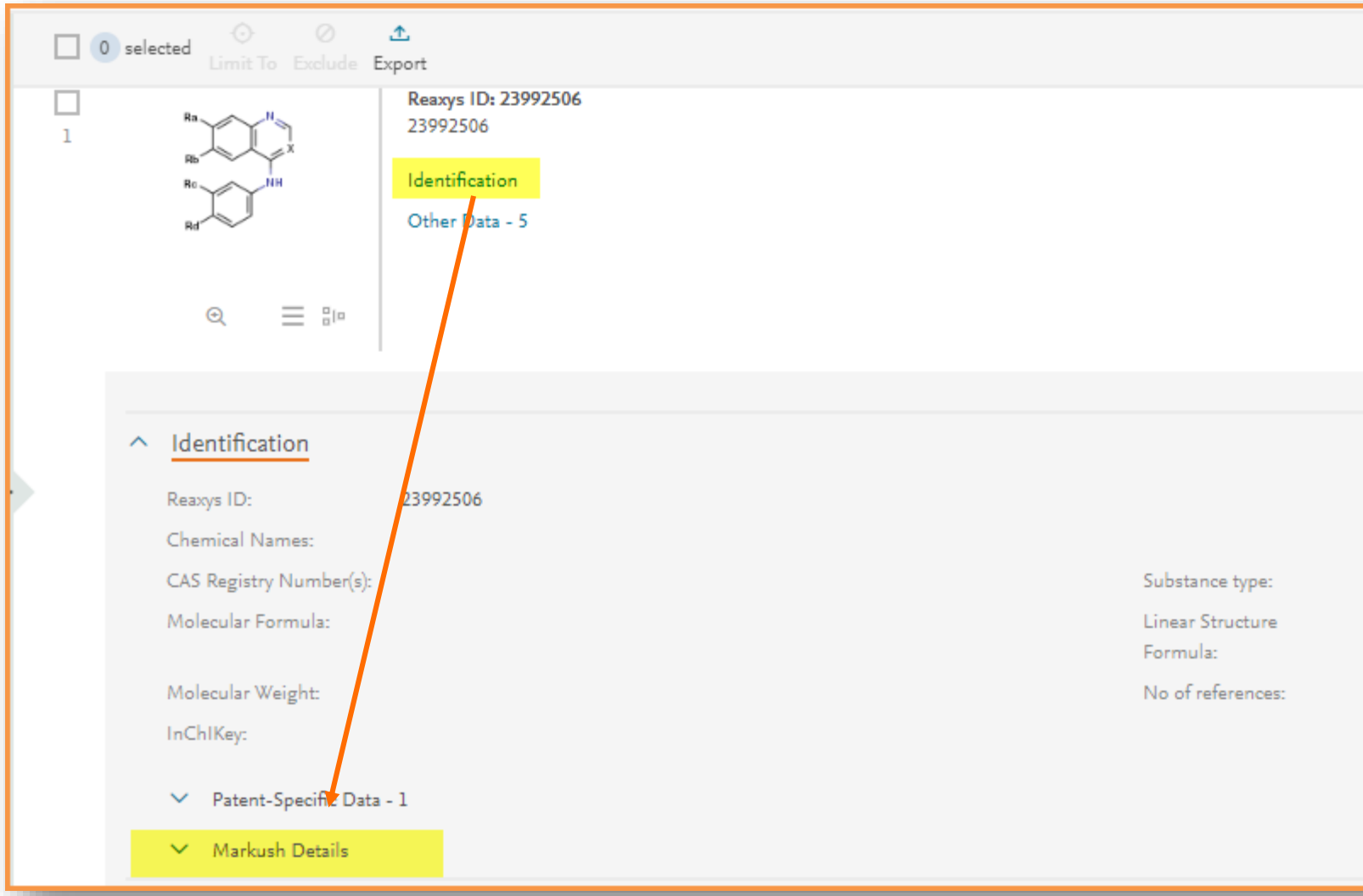
Markush结构解读







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什么基团

具体官能团

官能团大小

有无取代基

取代基频次

Label	Value	Size	Attributes	Substituted by	Frequency
Rb	Ra				
Ra	hydrogen				
	halogen				
	hydroxy			$s1	
	amino			$s1	
	hydroxyamino			$s1	
	carboxy			$s1	0-?
	alkoxycarbonyl	1-8C	or cyclic	$s1	
	nitro				
	guanidino			$s1	
	ureido			$s1	
	carbamoyl			$s1	
	cyano				
	trifluoromethyl				
	(R6)2N-$carbonyl			$s1	0-?
	$phenyl-W-$alkyl			$s1	0-?

OH

OH上取代基为

$s1	halogen
	R9

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

Feedback

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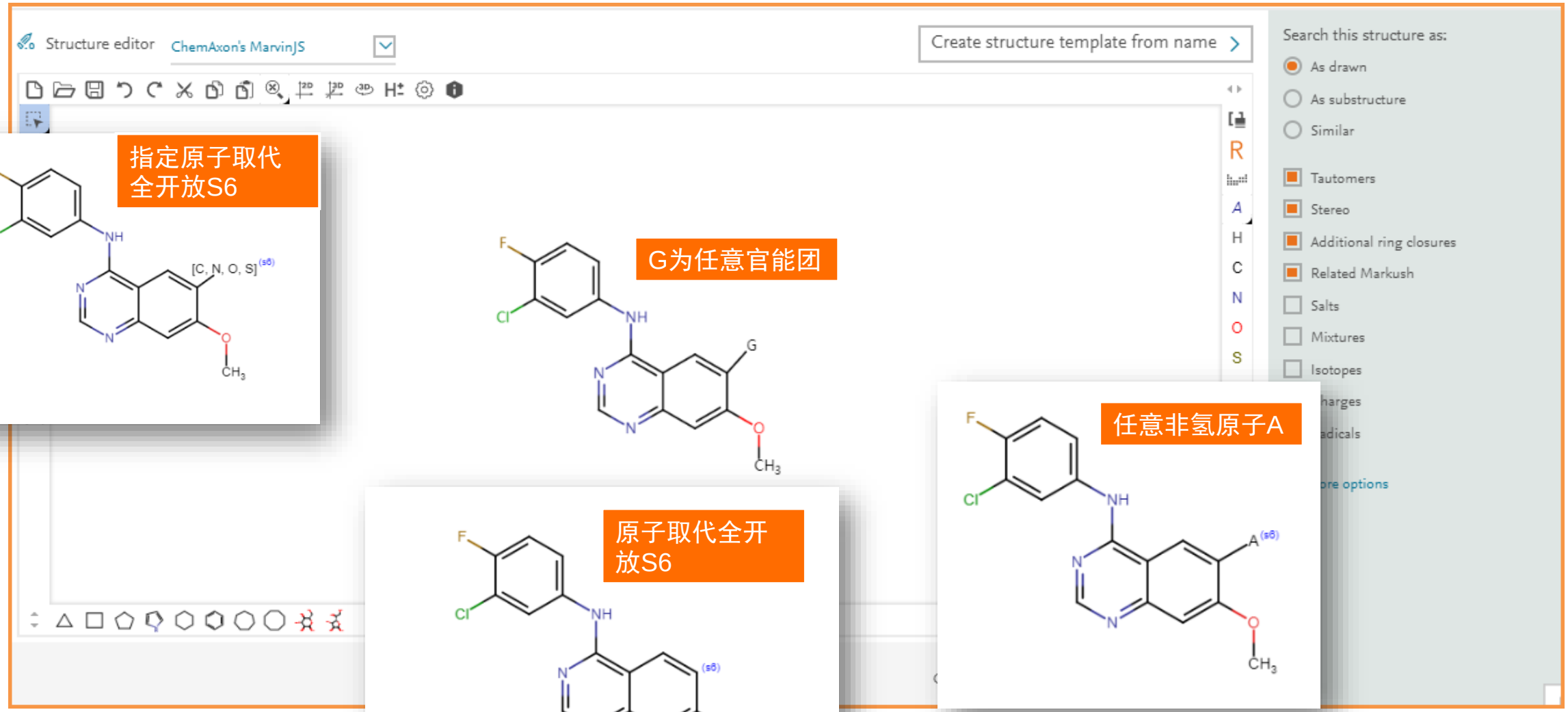
Markush检索的基本模式-方法2：评估某侧链结构的新颖性



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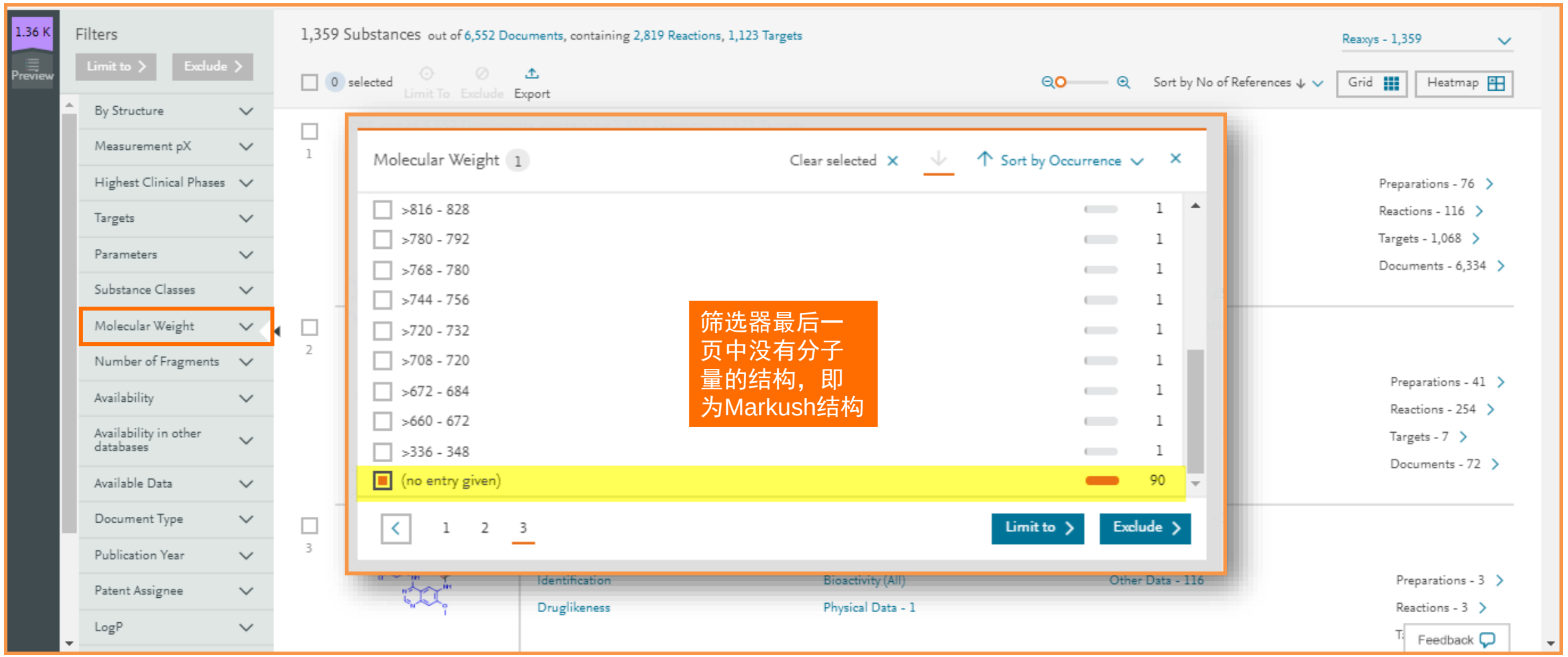
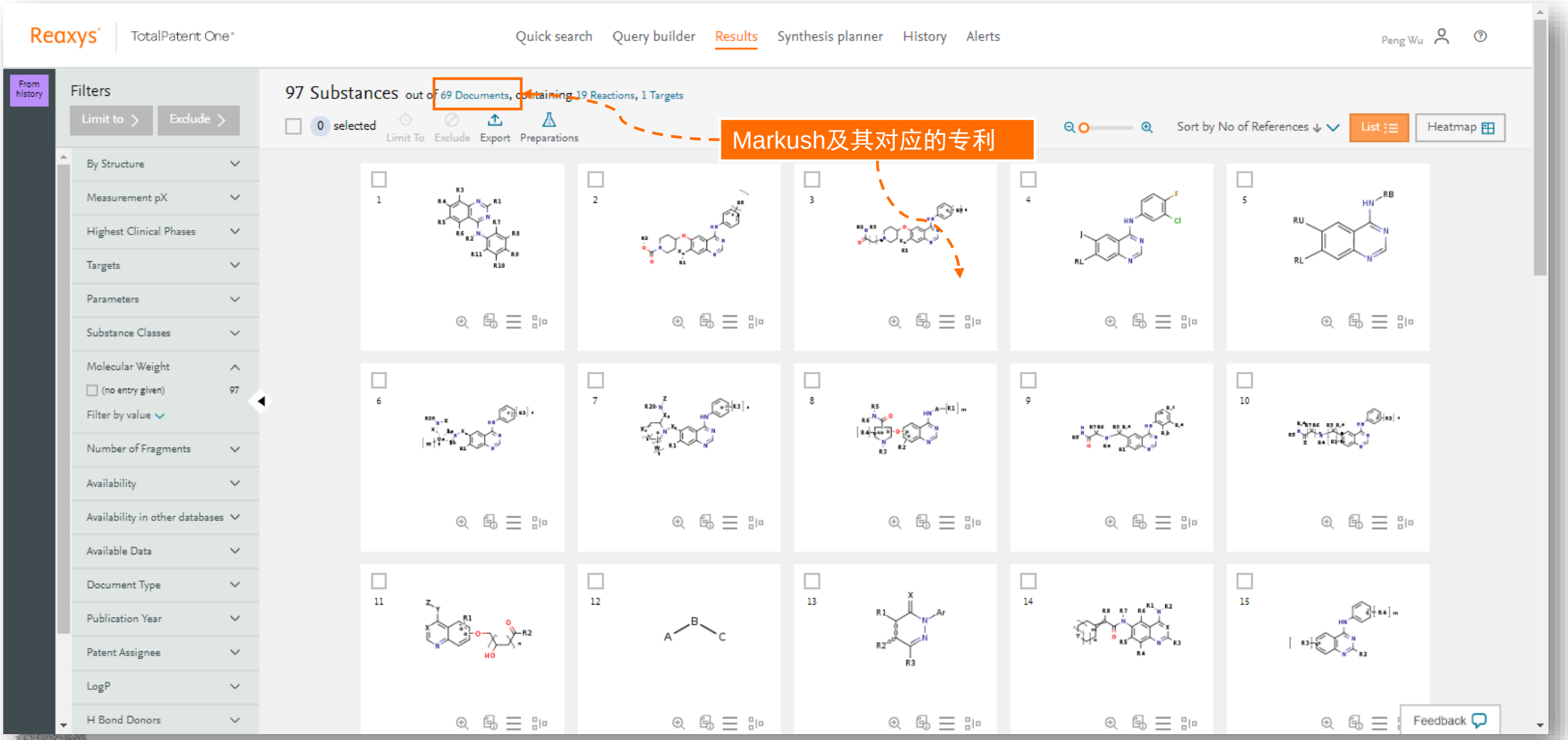
评估某侧链结构的新颖性—筛选Markush结构



ELSEVIER

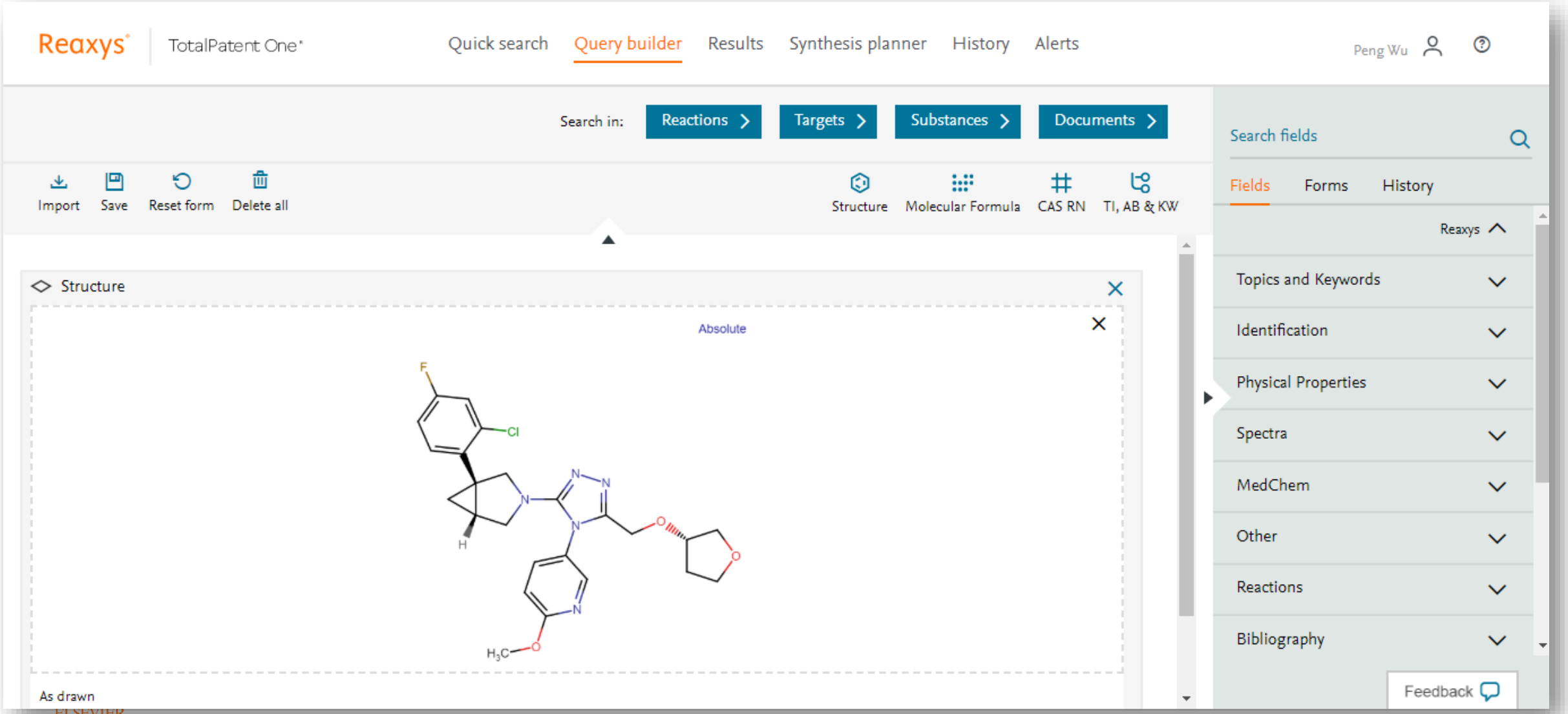
筛选后的Markush结构

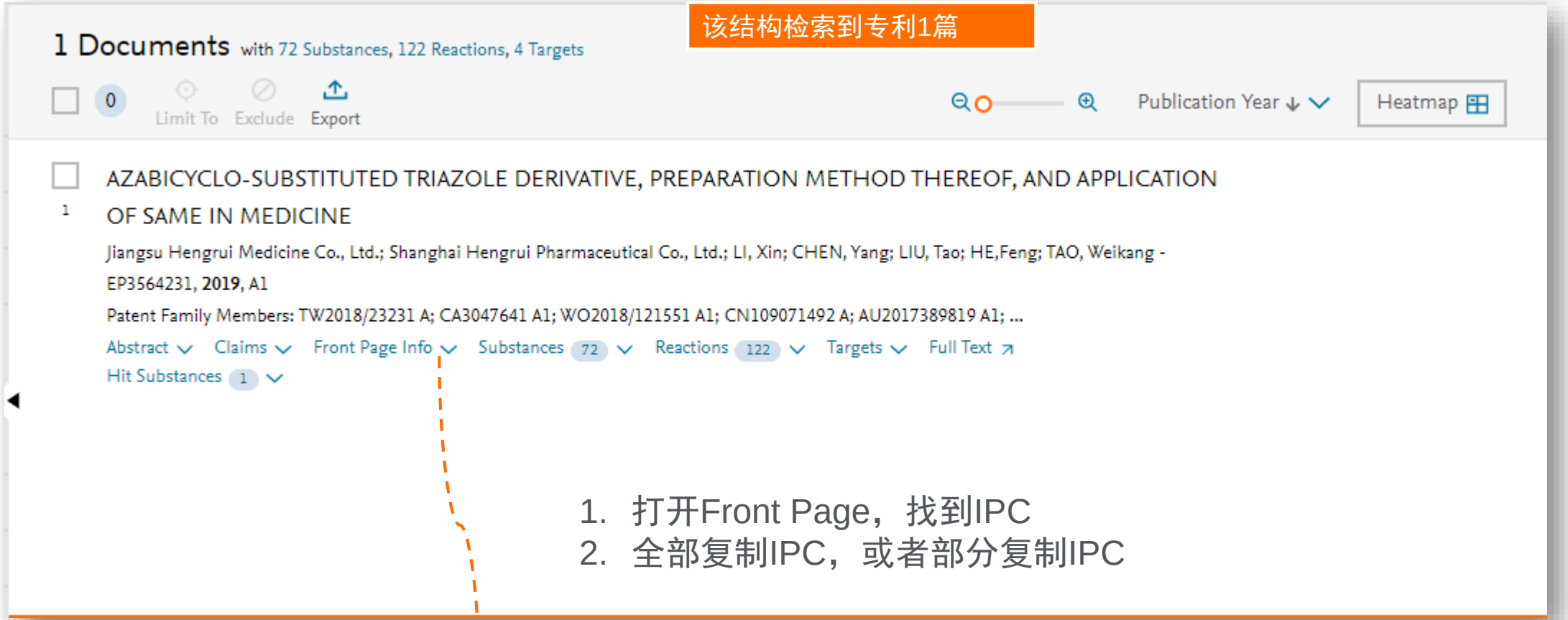


Tip：当‘新分子’涉及项目非常重要是，需要对很多Markush进行解读，确保新分子的应用性

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？





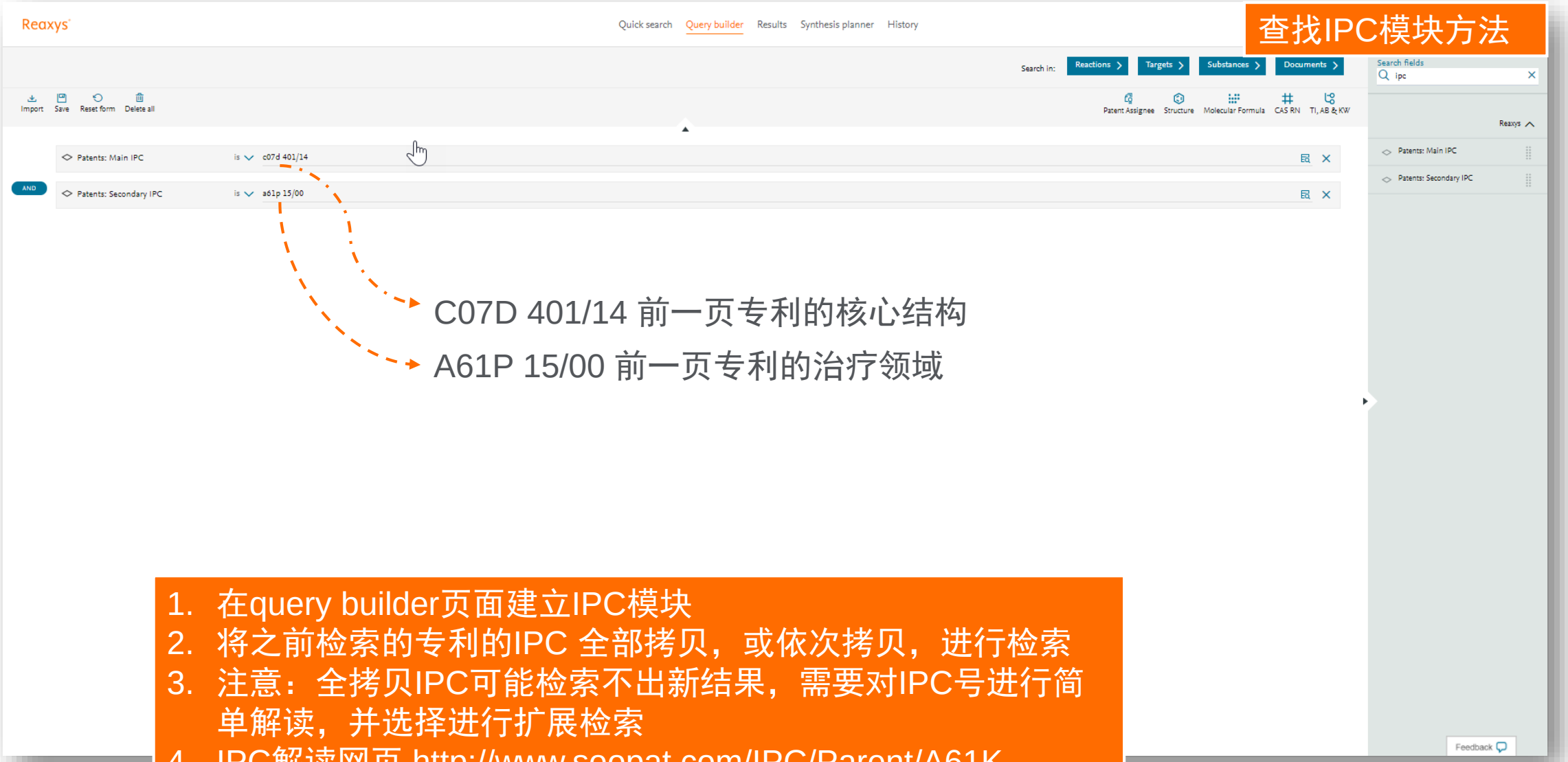
Patent Classification	
Main IPC	C07D 401/14
Secondary IPC	C07D 405/14; A61K 31/44; A61K 31/4196; A61P 15/00

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



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

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

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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; BRPI1911758 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; BRPI1911758 A2; CA3047643 A1; ...
Abstract Claims Front Page Info Full Text

3 PDGGFR 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[hitokichinaze] useful as inhibitors
No author - JP6859325, 2021, B2
Patent Family Members: AU2016314345 A1; AU2016314345 B2; BRPI1804193 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

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Reaxys

Quick search | Query builder | Results | Synthesis planner | History | Alerts

Peng Wu

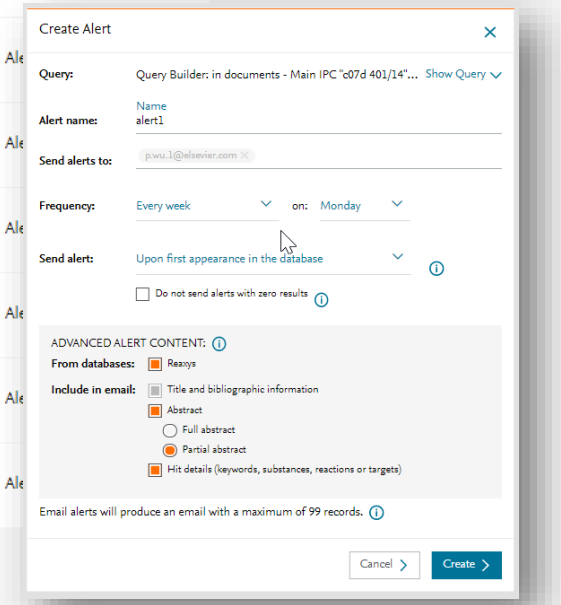
1. 选择检索历史
2. 登陆个人账号
3. 设置检索方法提醒，可以定时推送同领域新专利到邮箱

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	



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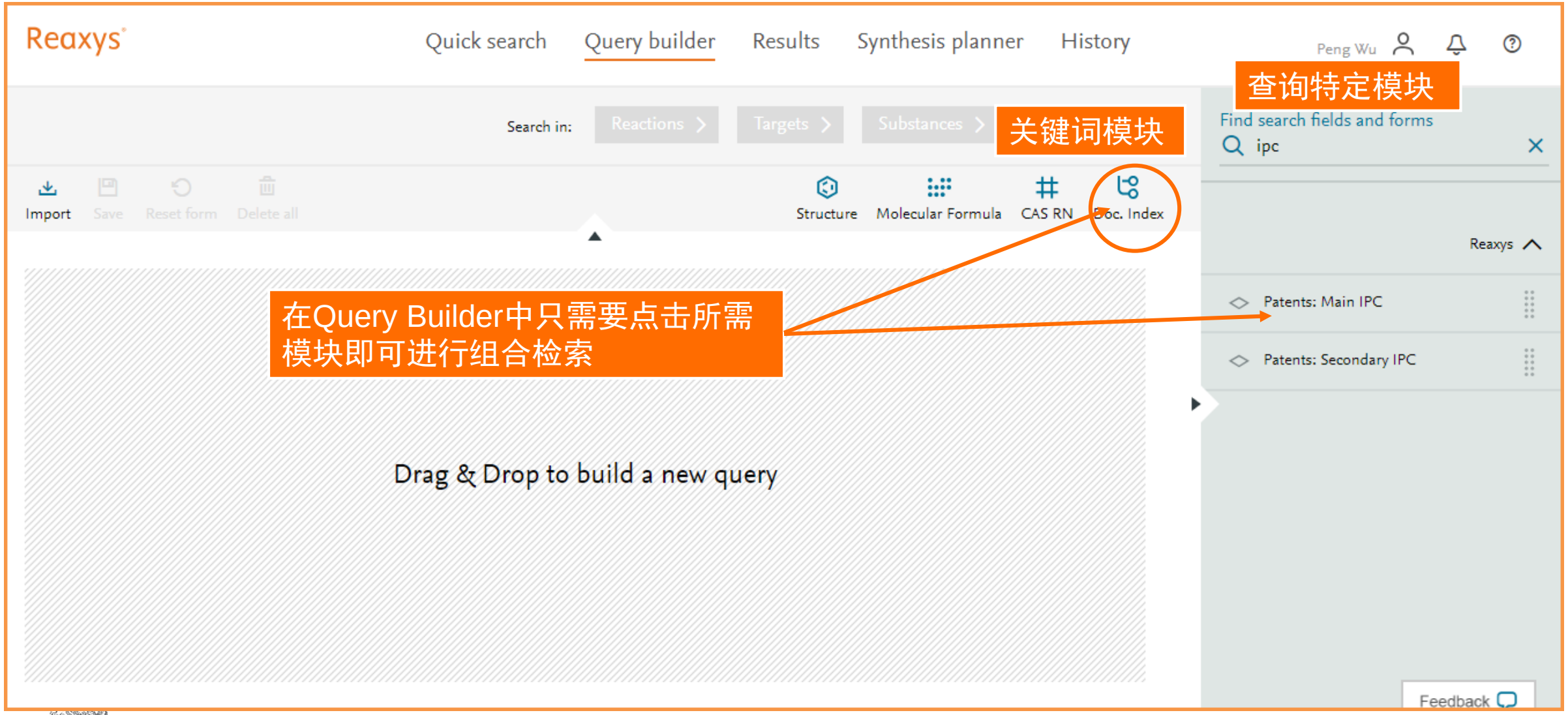
Case 3：检索2019年2月，与CD137相关的，人用药，含抗原或抗体的医药配置品（生物药类专利）

组合模块构建



ELSEVIER

检索结果

2 METHODS AND COMPOSITIONS FOR PREPARING GENETICALLY ENGINEERED CELLS

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			Priority Date
US2017-543359P			2017/08/09
Patent Classification			
Main IPC	A61K 39/00		
Secondary IPC	C12N 5/0783		

公开日期
授权状况

IPC
分类

Claims

CLAIMS

WHAT IS CLAIMED:

1. A method for genetically engineering
(a) incubating an input composition, ur
T cells, wherein the stimulating conditi
or more intracellular signaling domains
(b) introducing a nucleic acid encoding
incubating.
2. A method for genetically engineering
population of T cells comprising naive-
the stimulating conditions comprises th
or more intracellular signaling domains
the incubating the input composition under stimulating conditions is performed prior to, during and/or subsequent to introducing a nucleic acid encoding a
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 si
components of a TCR complex and/or one or more intracellular signaling domains of one or more costimulatory molecules, thereby generating a stimulated
(b) introducing into the stimulated cell composition a nucleic acid encoding a genetically engineered recombinant receptor, wherein the method thereby gen
cells expressing the genetically engineered recombinant receptor.

ation of T cells com
ains of one or more
the introducing is
for between 2 and 6
ains of one or more

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

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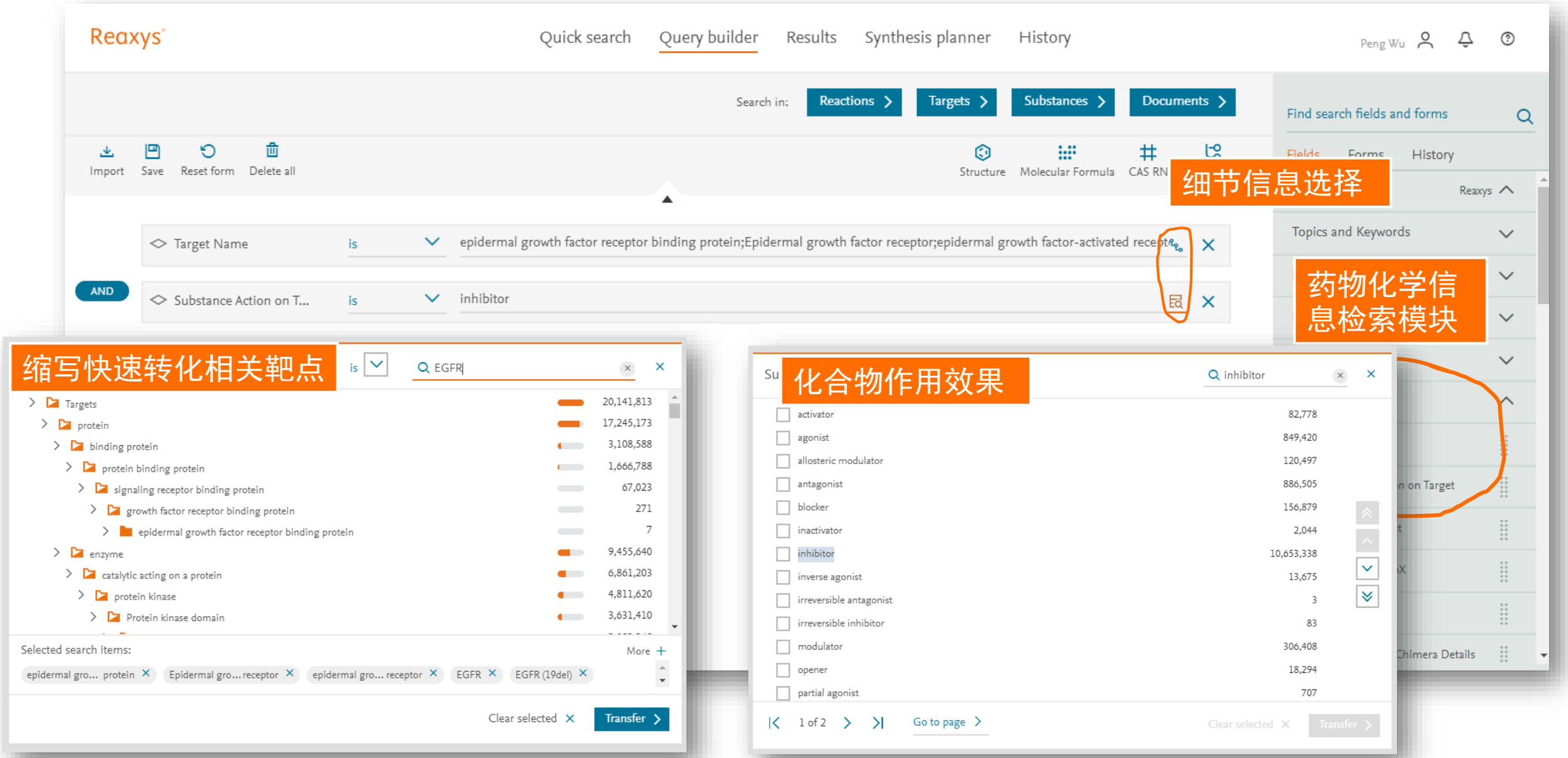
今天的内容

- 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

71.40 K Query

Filters

Limit to > Exclude >

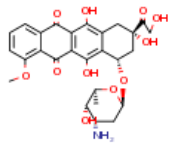
- By Structure
- Measurement pX
- Highest Clinical Phases
- Targets
- Parameters
- Substance Classes
- Molecular Weight
- Number of Fragments
- Availability
- Availability in other databases
- Available Data
- Do
- Pu
- Patent Assignee
- LogP
- H Bond Donors

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

0 selected | Limit To | Exclude | Export | Preparations

Sort by No of References | Grid | Heatmap

1



doxorubicin

$C_{27}H_{29}NO_{11}$ 543.527 1445814 23214-92-8

Identification | Bioactivity (All) | Other Data - 6,037

Druglikeness | Physical Data - 164

Bioactivity (Hit Data) | Spectra - 239

Preparations - 68 >

Reactions - 364 >

Targets - 393 >

Documents - 27,491 >

doxorubicin

- Identification
- Druglikeness
- Bioactivity (Hit Data)
- Bioactivity (All)
- Physical Data - 164
- Spectra - 239

生物活性数据

Bioactivity (All)

- In vitro: Efficacy - 12410
- In vivo: Animal Model - 2116
- Metabolism - 756
- Pharmacokinetic - 995
- Toxicity/Safety Pharmacology - 12536

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)	antiprolifera agent
12.3	GI50	=	3E-07	µg/mL		NCI-H460 cell line		

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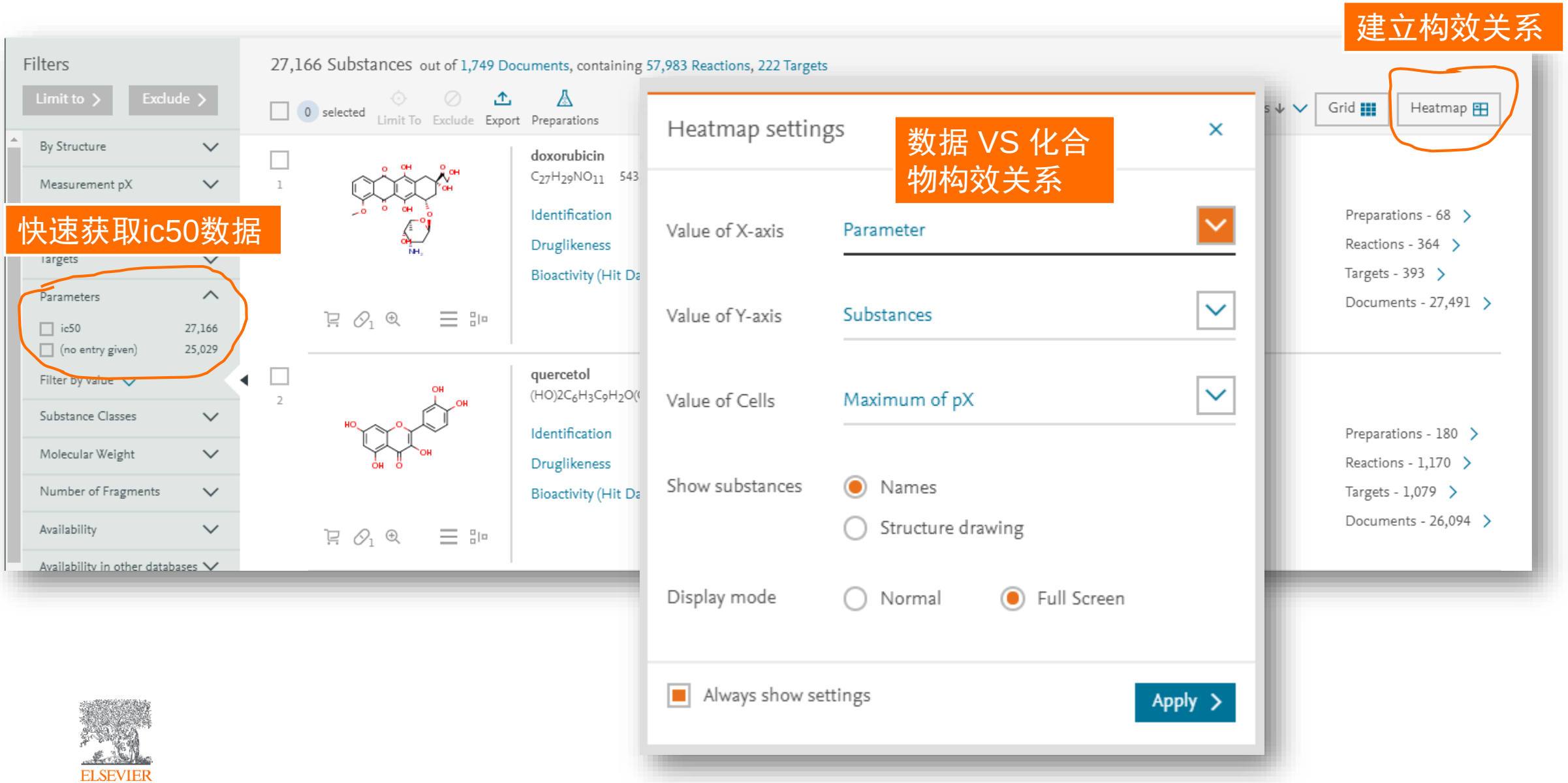
建立构效关系

快速获取ic50数据

数据 VS 化合物构效关系



ELSEVIER

Limit To | Exclude | Export | Settings | Navigator | Legend

Substances | Exit Full Screen

导出结果

ic50

Parameter

Substances

staurosporine — 12.8

4-[(3-chloro-4... nazoline — 12.7

6,7-dimetho... -4-amine

4-Dimethyla... l]-amide

(1R,5S)-3-(3-((...xan-1-ol

N-(4-fluorop... -4-amine

N-(3-chloro-... -4-amine

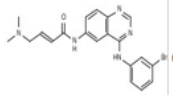
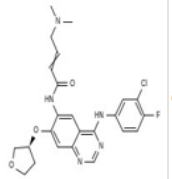
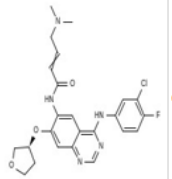
N-(3-chloro-... -4-amine

N-(3-chloro-... -4-amine

N-(3-chloro-... -4-amine

N-(3-chloro-... -4-amine

N-(3-chloro-... -4-amine

	A	B	C	D	E	F	G	H	I	J	K	L
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: Measuremen	Unit
9		CN(C)C\C=C\C(=O)NC1=		4-Dimethylamino-but-2	C20H20BrN5O	426.316	Epidermal growth factor	Epidermal growth factor	Inhibitor	In Vitro (Efficacy)	IC50	nM
16		CN(C)CC=CC(=O)NC1=(		4-[(3-chloro-4-fluoroph	C24H25ClFN5O3	485.946	epidermal growth factor	epidermal growth factor	Inhibitor	In Vitro (Efficacy)	IC50	nM
17		CN(C)CC=CC(=O)NC1=(		4-[(3-chloro-4-fluoroph	C24H25ClFN5O3	485.946	epidermal growth factor	epidermal growth factor	Inhibitor	In Vitro (Efficacy)	IC50	nM

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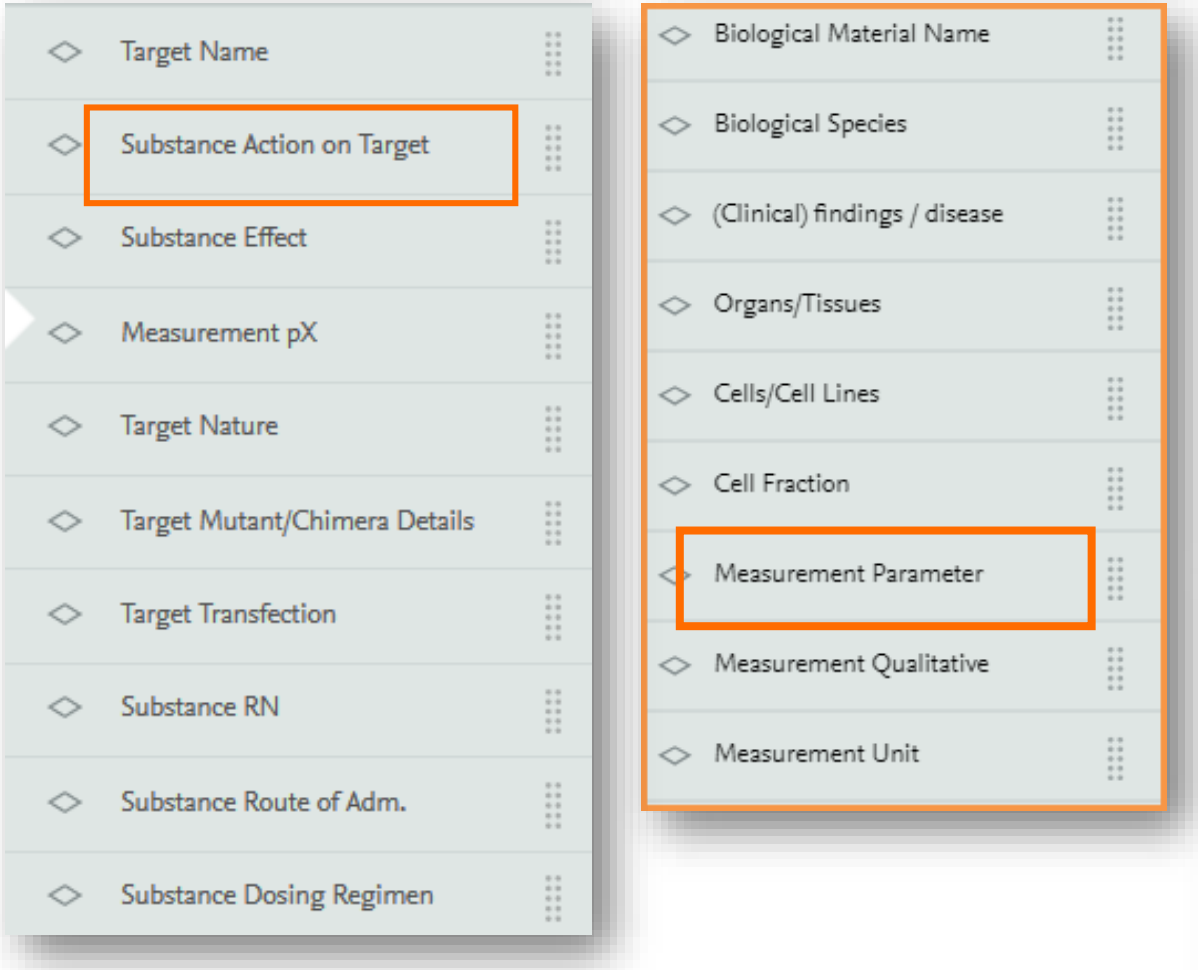
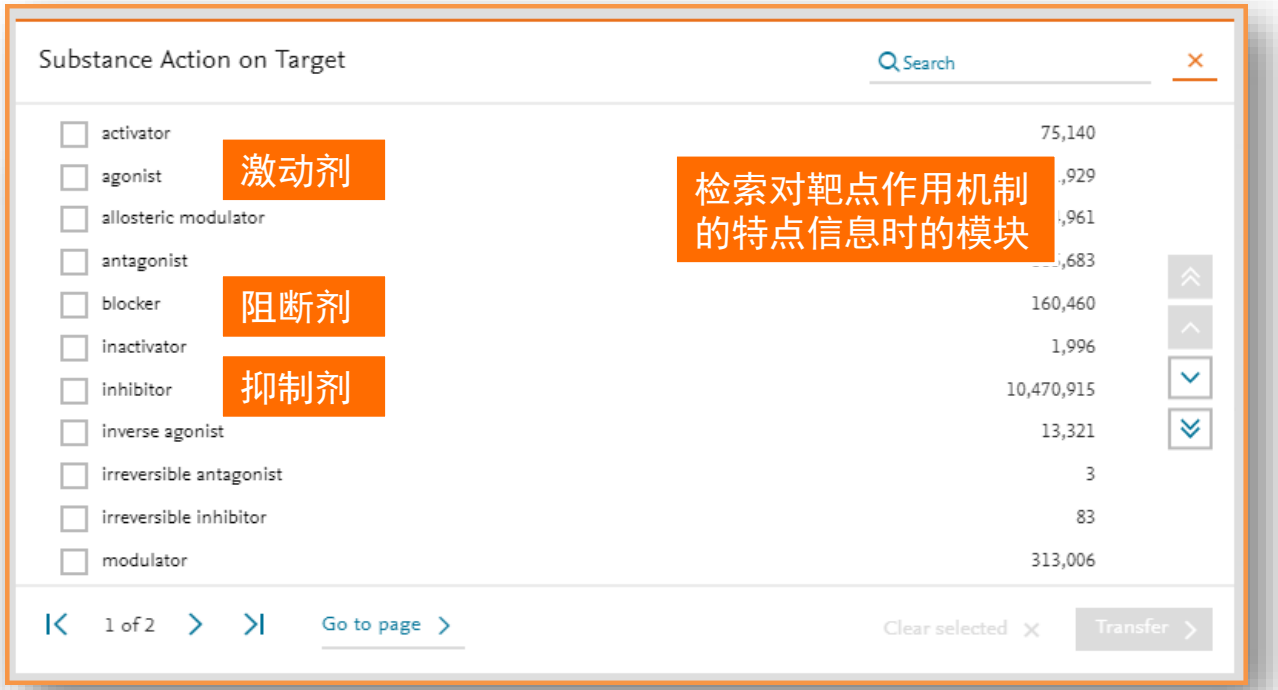
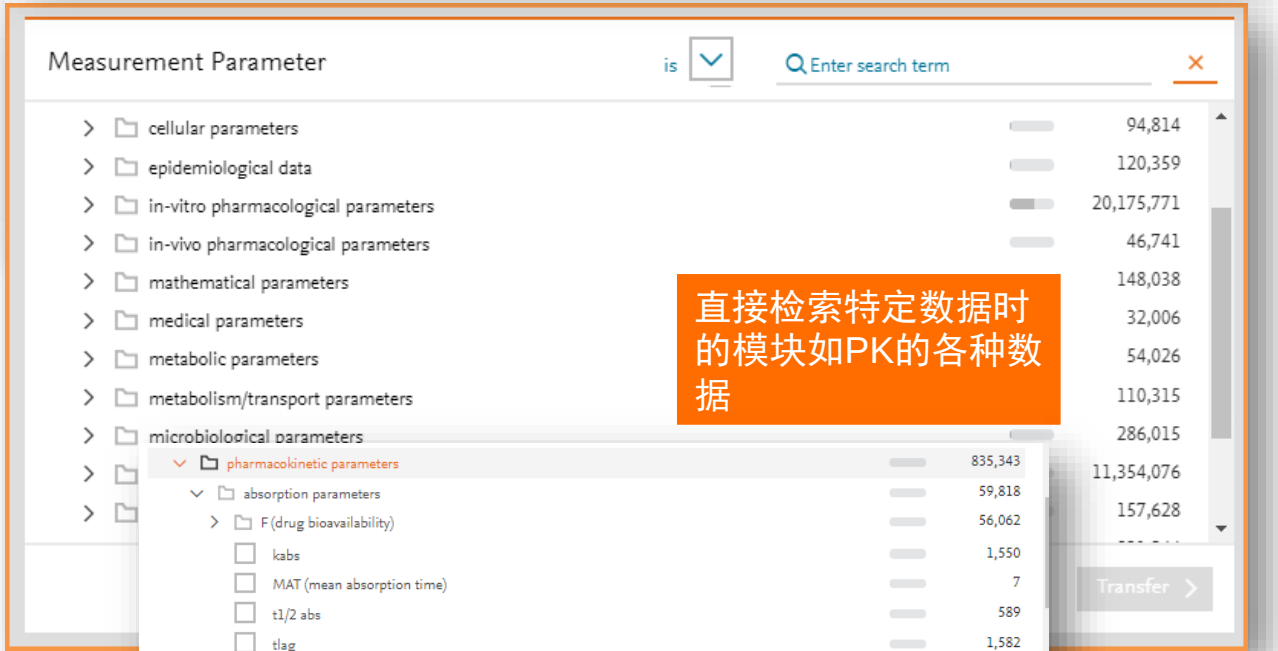
RMC-特定的信息检索方法







各种分类细致的信息检索模块，快捷锁定对应结果

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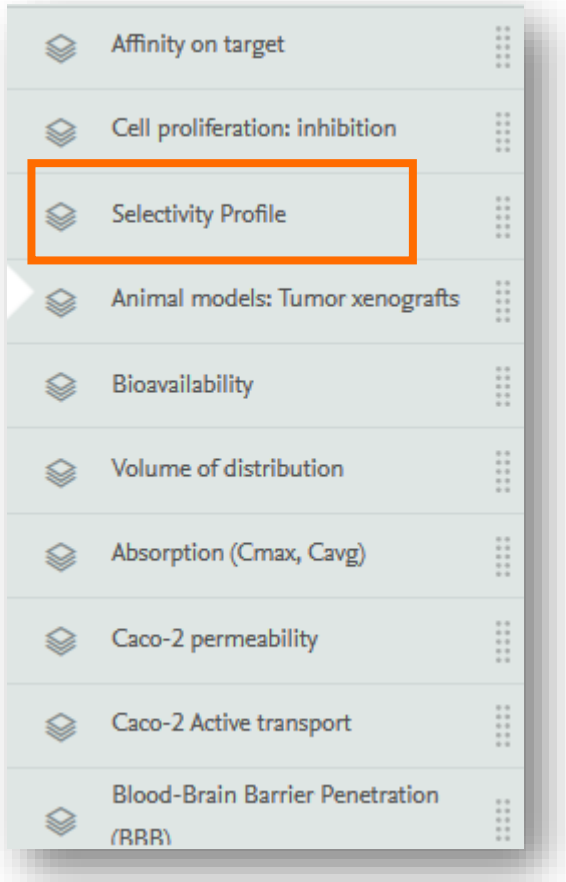
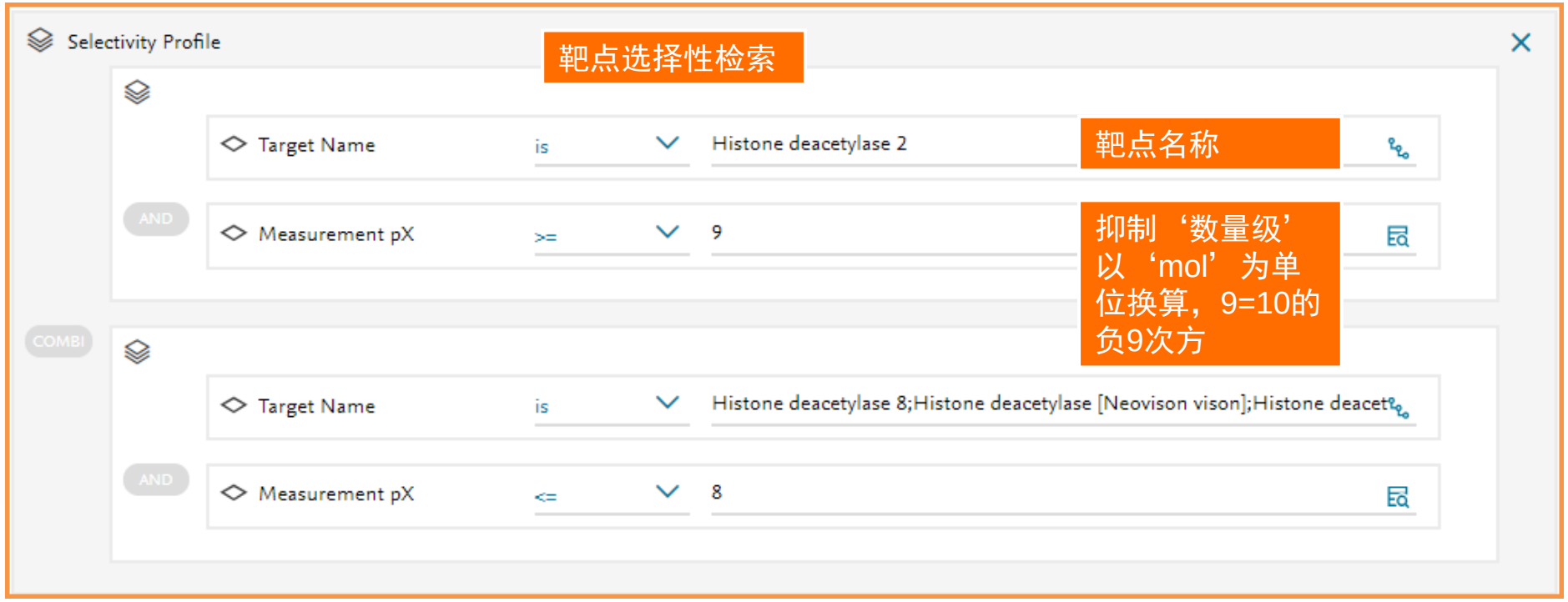
RMC-组合信息便捷检索



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



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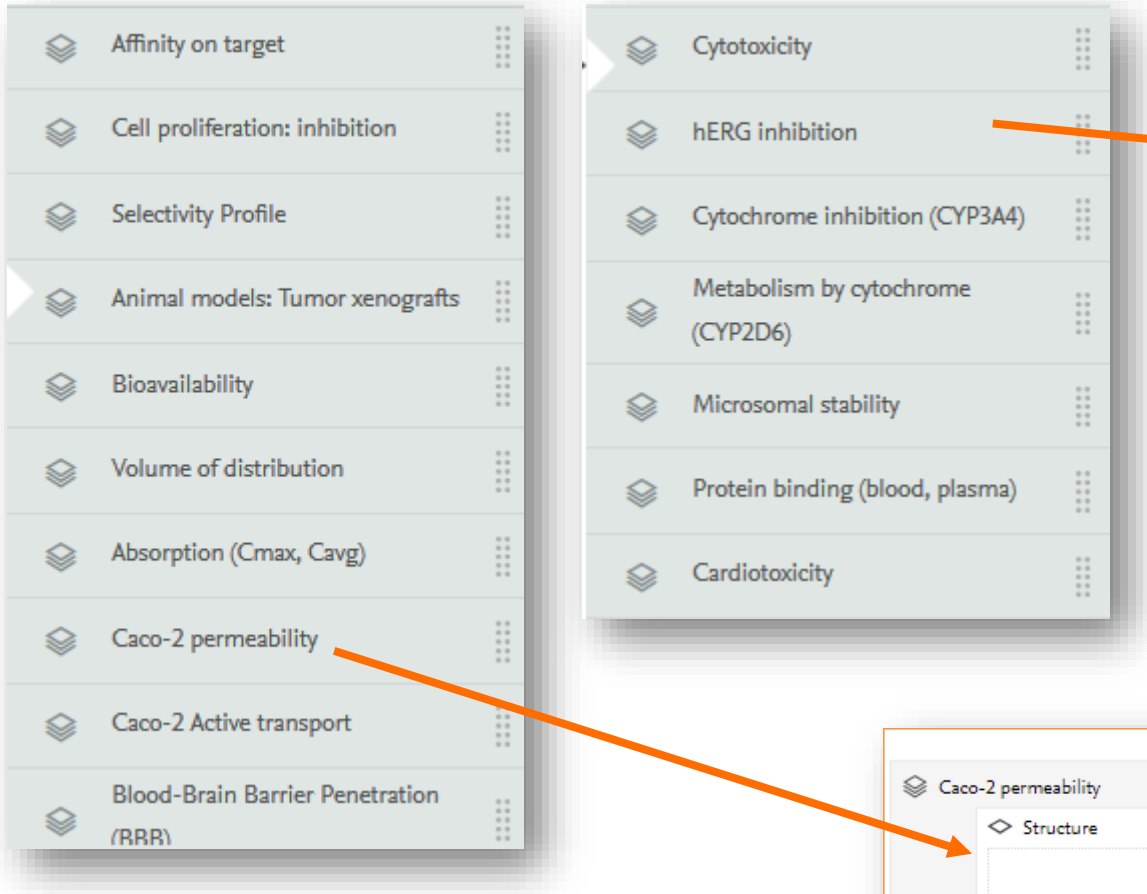
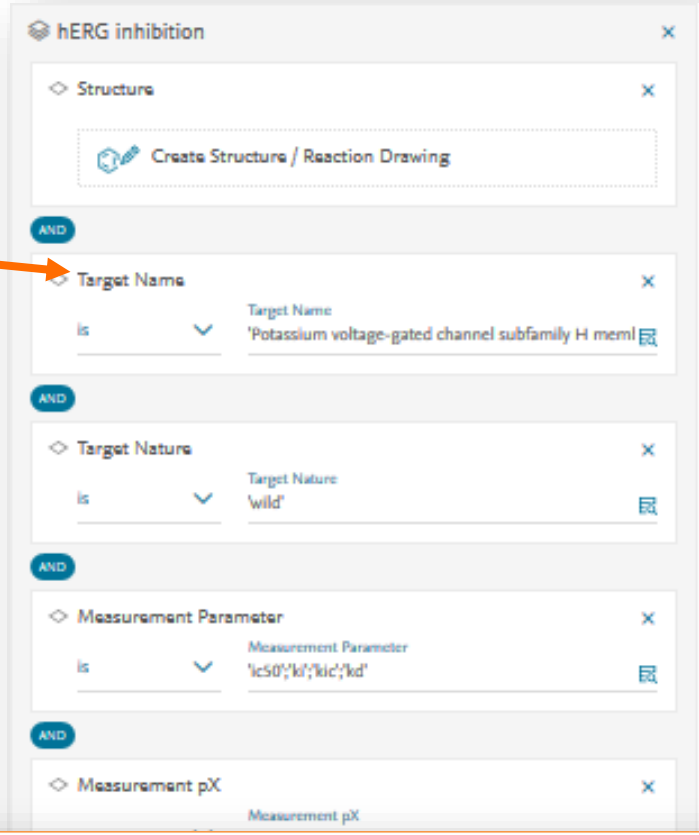
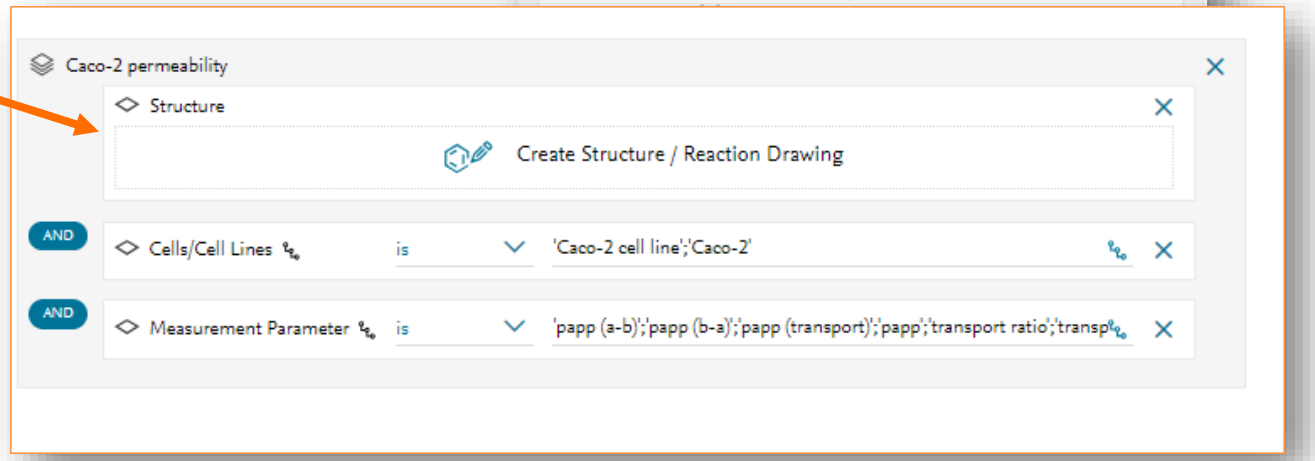
RMC-组合信息便捷检索







只需要特定结构即可初步快速检索特殊信息

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Thank you