

### Reaxys and Reaxys Medicinal Chemistry

A How To Guide For Commonly Used Searches - CONFIDENTIAL



### Contents

- 1. How to do literature search by author name?
- 2. How to do a topic search on "nanomedicine in lung cancer"?
- 3. How to do a topic search on "jak2 inhibitor"?
- 4. How to find all substances that blocks my target of interest "EGFR"?
- 5. How to search for a patent using patent number?
- 6. How to search for patent by a particular assignee?
- 7. How to do a reaction search where the substance of interest is a product?
- 8. How to do a reaction search where the substance of interest is a starting material?
- 9. How to do a reaction search where the substance of interest is a reagent?
- 10. How to define specific conditions for a reaction?
- 11. How to do define specific conditions for a reaction?
- 12. How to use advanced query forms in Reaxys MedChem?
- 13. How to do retrosynthesis in Reaxys?
- 14. How can I export the list of substances which were claimed in a patent as SD-file or SMILES?
- 15. How do I export bioactivity data for my target or substance results?
- 16. How do I quickly draw a functional group like nitrate, acetate or BOC?
- 17. How do I view citing articles?
- 18. How do I look for documents associated to a particular association/author affiliation?
- 19. How to search for patents using structure editor? (documents as entering point)



#### 1) How to do literature search by author name?

1.	Go to query	Reaxys'	Quick search Query builder Results Synthesis planner	History	Abhinav Kumar 😤 📮 💿
2.	In "search			Search in: Reactions > Targets > Substances > Documents	Find search fields and forms Q Author X
	fields and forms' enter	出 四 つ 音 Import Save Reset form Delete all		③ III 井 년 Structure Molecular Formula CAS RN TI, AB	ž KW 3 Rezora A
			*		· · · · · · · · · · · · · · · · · · ·
	Author	♦ Authors is ♥ Authors		<u>E</u> ×	◇ Authors
3.	Select the				😞 Keywords
	field author				

4. Enter author name in the following format "last\_name\* first\_name\*; first\_name\*last\_name\*" for example for author Stephen Buchwald you would enter the query as shown below

5. Click on documents to find literature associated with author Stephen Buchwald

Reaxys	Quick search	Query builder	Results	Synthesis planner	History			5		Abhinav Kumar 🛛 🞗	ΟĴ (Ĵ
					Search in:	Reactions >	Targets >	Substances >	Documents >	Find search fields and forms	Q
出 回 り 前 Jacob San Default							0		# 4	Fields Forms History	
import save reset form Delete all		<b>A</b>					Structure	e Molecular Formula CA	I, AD & KW		Reaxys 🔨
4	1									<b>T</b> 1 1 <b>K</b> 1	
◇ Authors is ∨ Buchwald*stephen*; stephen*Buchwald*									R ×	Topics and Keywords	$\sim$
										Identification	$\sim$



#### 2) How to do a topic search on "nanomedicine in lung cancer"?

							<u> </u>											
	Reaxy	ys <sup>°</sup>					Quick search	Query builder	Results	Synthesis planner	History					Abhinav Kumar	ΥĻ	. @
											Search in:	Reactions >	Targets >	Substances 🖒	Documents >	Find search fields and	forms	Q
	· 보   Import S	Save Reset form Delete all											Structure	Molecular Formula	CAS RN TI, AB & KW	Fields Forms	History	
		3				-									(2)		Rea	20/5 ^
4		Titles, Abstracts & K	is	➤ nan	nomedicine*; nanoparticle*										a ×	Topics and Keywords		^
Τ	NEAR 3	→ Titles, Abstracts & K	is	✓ lung	ig* NEXT cancer*	1									a ×	<ul> <li>Substance Proper</li> <li>Comments</li> </ul>	ies δχ [	8
																Reaction Data & C	onditions	
						5										Titles, Abstracts &	Keywords	
																All Keywords		
																Identification		~

- 1. Go to query builder
- 2. Click on "Title, Abstracts & Keywords" ("TI, AB & KW" shortcut key). This field can be added multiple times (x2 in this example)
- 3. In the first box, enter the search query using synonyms for nanomedicine such as nanoparticle and use wild card operator "\*" to account for plurality of terms as shown above
- 4. Change the operator from "AND" to "NEAR" (use your preferred number to indicate how near you want the terms)
- 5. In the second box, enter the search term for lung cancer as shown above i.e. lung\* NEXT cancer\* the use of the operator NEXT ensures that the terms lung & cancer appear next to each other making the results more specific
- 6. Click on documents to find literature associated with nanomedicine in lung cancer



#### 3) How to do a topic search on "jak2 inhibitor"?

	Reaxys	·	Quick search	Query builder	Results	Synthesis planner	History	6		Abhinav Kumar 👌	Ô Ũ
							Search in: Rez	sactions > Targets > Substances >	Documents 🖒	Find search fields and forms	۹
	速 🖻 🏷 🛍 Import Save Resetform Delete all							Structure Molecular Formula CA	# С 5 RN ТІ, АВ & КW	Fields Forms History	Reaxys 🔨
		s v "jak2";"tyrosine-protein kinase jak2";"jak-2";"janus kinase 2							R ×	Topics and Keywords	^
Ľ	AND 🗢 Titles, Abstracts & K	s 🗸 "inhibition*"; "inhibitor*"; "antagonist*"; "blocker"							R ×	Substance Properties & Comments	₿ !!
										<ul> <li>Reaction Data &amp; Conditions</li> <li>Titles, Abstracts &amp; Keywords</li> </ul>	
										All Keywords	
										Identification	~

- 1. Go to query builder
- 2. Click on "Title, Abstracts & Keywords" ("TI, AB & KW" shortcut key). This field can be added multiple times (x2 in this example)
- 3. In the first box, enter the search query using synonyms for JAK2 such jak-2; janus kinase 2; tyrosine-protein kinase jak2 as shown above
- 4. Change the operator from "AND" to "NEAR" (use your preferred number to indicate how near you want the terms) or leave the operator as "AND"
- 5. In the second box, enter the search term for inhibitor as shown above i.e. inhibition\*; inhibitor\*; antagonist\*; blocker\* use wild card operator "\*" to account for plurality of terms
- 6. Click on documents to find literature associated with jak2 inhibitors



### 4) How to find all substances that blocks my target of interest "EGFR"?

Re	JXYS     Quick search     Query builder     Results     Synthesis planner     History	Abhinav Kumar 📍 🗘	1 ()
	Search In: Reactions > Targets > Substances > Documents >	Find search fields and forms	Q
یک Impo	E Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW	Fields Forms History	
	3	Re	axys 🔨
	Target Name is vepidermal growth factor receptor binding protein; Epidermal growth factor receptor; epidermal growth factor-activated receptor; EGFR (19del); EGFR (19del) [human]; EGFR (746-750 del); EGFR (A762_Y763in EPi, 2)	Topics and Keywords	~
AND	Substance Action on T is V blocker;inactivator;antagonist;inhibitor;irreversible antagonist;irreversible inhibitor	Identification	~
	4	Physical Properties	~
		2 ectra	$\sim$
		MedChem	^
		🗇 Target Name	
1.	Go to query builder Click on "ModCham" and colort the fields "Target Name" and "Substance Action on Target"	Substance Action on Target	
∠. 3	In the field Target Name – use the target name taxonomy look-up button indicated in orange to search and view the synonyms	Substance Effect	
0.	associated with EGFR	⊘ Measurement pX	
4.	In the field Substance Action on Target – use the look-up button indicated in orange to search for input the synonyms associated	Target Nature	
_	with blocker	Target Mutant/Chimera Details	ls
5.	Click on substance to find all substances reported to have inhibitory action against EGFR	Target Transfection	
		Substance RN	
No	te: Bioactivity results can be viewed in a Heatmap (see top right corner of results pages)	Substance Route of Adm.	
		Substance Dosing Regimen	

Substance Dose
 Substance Highest Clin. Phase

#### 5) How to search for a patent using patent number?

- 1. Go to quick search
- 2. Enter the patent number
- 3. Click Find



This then adapts the input so that it fits best into the Reaxys search engine

Reax	sys"		Quick search Query builder Results Synthesis planner History	Register > Sign in ③
	Result	s for <b>wo201205</b> (	0500al	New 🍞 Edit 🤌
	4	1 Top 3 results	Documents         Patent         : wo2012050500a1         Preview           Edit in Query Builder         Create Alert         Image: Creat	Results View Results > TORS A:
	¢	0	Documents Titles, Abstracts, Keywords : "wo2012050500a1" Edit in Query Builder 🖋 Create Alert 🗘	



#### 6) How to search for patent by a particular assignee?

Reaxys	Quick search Query builder Res	esults Synthes	is planner Hist	ory				Abhinav Kumar  💍	Ϋ́ (	3
			Sear	ch in: Reactions >	Targets 🗲	Substances >	Documents >	Find search fields and forms Q patent		×
نٹ 🖻 🏷 🌐 Import Save Reset form Delete all					Structure M	Aolecular Formula Ci	# <b>않</b> AS RN TI, AB & KW			
3	<b>A</b>								Reaxys 🖌	<u>`</u>
◇ Patent Assignee contains ∨ basf							R ×	Patents: Location in Patent		
								Patents: Prophetic Compound	und	
								Patents: Related Markush Structure		
								Patent Specific Data exists/	any	
								Patent Assignee	-	
								Common Patent Number		
1. Go to query builder								Patent Country Code		
2. In "search fields and forms' enter "Patent Assig	nee" and select the field	d					,	◇ Patent Number		
<ol> <li>Change the field to contains and enter assigned</li> <li>Click on documents to get all patents with the result of the second second</li></ol>	e name in the field							Patent Kind Code		
								◇ Patent Year		
								Patents: Application number	er	
								◇ Patents: Date of filing		
								Patents: Date of publication	n	
								Patents: Family member: D filing	Date of	
								Patents: Family member: Application number		
								Patents: Family member: D	ate of	



## 7) How to do a reaction search where the substance of interest is a product?



- 1. Click on "DRAW" on the landing page
- 2. Either draw the structure using the drawing tools available (MarvinJS and ChemDraw) or use create structure from template option e.g. here imatinib was entered
- 3. Use reaction arrow button to indicate that this structure is desired as a product
- 4. Select the search options from right hand side by checking or un-checking boxes
- 5. Click on transfer to query and then click "find"



## 8) How to do a reaction search where the substance of interest is a starting material?



- 1. Click on "DRAW" on the landing page
- 2. Either draw the structure using the drawing tools available (MarvinJS and ChemDraw) or use create structure from template option. Here the structure was drawn using the tools
- 3. Use reaction arrow button to indicate that this structure is desired as a starting material
- 4. Select the search options from right hand side by checking or un-checking boxes
- 5. Click on transfer to query and then click "find"



## 9) How to do a reaction search where the substance of interest is a reagent?



- 1. Click on "DRAW" on the landing page
- 2. Either draw the structure using the drawing tools available (MarvinJS and ChemDraw) or use create structure from template option e.g here the CAS number 3849-21-6 was entered
- 3. Use reaction arrow button to indicate that this structure is desired as a reagent
- 4. Select the search options from right hand side by checking or un-checking boxes
- 5. Click on transfer to query and then click "find"



#### 10) How to define specific conditions for a reaction?



- 1. Go to Query Builder
- 2. Click on "Structure" and either draw structure or choose create structure from template and the appropriate "Reaction Arrow"
- 3. Click on "Title, Abstracts & Keywords" ("TI, AB & KW" shortcut key)
- 4. In "search fields and forms" enter "Reaction" and select the field "Reaction data & conditions"
- 5. Drag and drop to "Group" the query and change the operator to "OR"
- 6. Change the operator to "contains"
- 7. Enter desired condition e.g. here researcher may be interested in flow or continuous reaction to avoid organic-azide intermediate
- 8. Click on "Reactions" to obtain results matching the search criteria

### 11) How to do define specific conditions for a reaction?

- 1. Go to query builder
- 2. Go to Reaxys Forms
- 3. Select the Reactions form
- 4. Draw the reaction of interest
- 5. Enter the relevant conditions (note: not all fields need to be filled)
- 6. Change the operator as required to match your search criteria





#### 12) How to use advanced query forms in Reaxys MedChem

- 1. Go to query builder
- 2. Go to Reaxys Forms
- 3. Review Reaxys MedChem forms
- 4. Add the form of interest e,g, Caco-2 permeability
- 5. Add the (sub)structure of interest
- Querylets have been pre-filled with required parameters. Review and amend if desired
- Click on "Substances" to obtain results matching the search criteria





#### 13) How to do retrosynthesis in Reaxys?

 e structure template from name Enter a chemical name, C imatinitj	KS-RN, InChiKey or SMILES	٩	<ul> <li>period</li> <li>destructions</li> <li>period</li> </ul>

- 1. Click on "DRAW" on the landing page
- 2. Draw your substance of interest or create structure from template, transfer query and click "find"

	5	Reanys - 382
	Create plans by autoplan	🗙 by No of References 4 🗸 Grid 🎹 Heatma
	Number of plans to create 5 V	
	Max. alternative branches 5 V	
	Max. number of steps 5 🗸	
	is commercially available	
~ *	Default yield for reactions without	
	a given yield	6
	Always show screen before creating autoplan	Create Plans > 2 - 29 Preparations - 1
		Data - 1,447 Reactions - 27



#### 3. Click on icon for synthesis

4. Select either "autoplan" where Reaxys automatically creates multiple synthesis plans for you or "manually" - letting you manually create synthesis plans

- 5. Select the parameters for the synthesis plan
- 6. Click on create plans to obtain the results

#### Generate retrosynthesis plans for any known molecule

# 14) How can I export the list of substances which were claimed in a patent as SD-file or SMILES?

- 1. Go to the document results page
- 2. Select the patent of interest
- 3. Limit the results to this patent
- 4. Switch from document results to substance results
- 5. Export the substances in "SMILES" or "SD/Molfile" format

Re	axys		Quick search Query builder Results Synthesis planner History Register > Sign in O
149 987	Filters Limit to > Exclude	• >	149 Documents       with 16,068 Substances, 11,514 Reactions, 93 Targets         □ 1 selected
	Index Terms (List) Index Terms (ReaxysTree)	~ ~	BENZAZEPINE DENTICAL CO., LTD; KAIN, Keizo; TAKUWA, Massitoshi; TANAKA, Hirotaka; FUJWARA, Hideto; YAMABE, Hokuto; MATSUDA,
	Publication Year	$\sim$	Satoshi, () URUSHIMA, Tatsuya; FUJITA, Shigekazu - WO2019/4421, <b>2019</b> , A1 Patent Family Members: W02019/3433 A1; W02019/4421 A1
	Document Type	149	Abstract v Front Page Info v Substances 225 v Reactions 242 v Targets v Full Text 7 Hit Substances 1 v
			CURABLE SILICONE COMPOSITIONS THAT CURE THROUGH COMMAND CATALYSIS
	Authors	$\sim$	<sup>2</sup> KLOSOWSKI, JEROME; KRYTENBERG, TIMOTHY; VOCKLER, LARRY - US2019/55863, 2019, AL
	Patent Assignee	$\sim$	Abstract v Claims v Front Page Into v Substances 7 v Reactions 2 v Full lext 7 Hit Substances 1 v



## 15) How do I export bioactivity data for my target or substance results?

- 1. On target/substance results page select the target/substance of interest
- 2. Limit to the particular target/substance result (optional step)
- 3. Click on Export
- 4. Choose specific data points and click 'Add datapoints'
- 5. Click on 'Bioactivity' (or select the required datapoints under it)
- 6. Click export

(note: export is limited to 1000 substances for anonymous users and 5000 substances for registered users)







### 16) How do I quickly draw a functional group like nitrate, acetate or BOC?

- Draw the structure of interest (with the atom to be replaced by functional group already in place)
- 2. (a) press key board 'enter' button to open abbreviated groups or (b) open from the toolbar
- type the functional group (expand, if needed) and press OK
- Move the attachment atom on the atom to be replaced by functional group
- 5. Attach the functional group





#### 17) How do I view citing articles?

Search

3

1

Top of page

- 1. If a reference or document in Reaxys has corresponding data available in Scopus, the hyperlink 'Cited ...' is available
- 2. To view the cited articles for the given document, click 'Cited [a number] times'

Scopus

Society of Internal Medicine

Search within results.

Refine results

Access type ①

Other

Year

2018

Author name

Set feed

(2019) Anaesthesist, 68 , pp. 25-39.

1 document have cited:

3. This will open the Scopus document page in a new tab with the documents that cite this article.

00 Analyze search results

Document title

Display: 20 results per page

of emergent evidence and international guidelines

View abstract v Full Text View at Publisher Related documents

 $\sim$ 

~ \*

(1) >

 $\sim$ 



#### 18) How do I look for documents associated to a particular association/author

### affiliation?

Reaxys does not contain an affiliation field for journal articles. For these cases please use Scopus which is a multidisciplinary bibliographic database produced by Elsevier.For this

- 1. You can access Scopus with the URL: http://www.scopus.com
- 2. Go to affiliation search
- 3. Click 'Search for documents by affiliation'
- 4. Enter the name of affiliation name (and other details as required
- 5. Click Search
- 6. You can also search for author affiliation from Authors tab

Scopus	Search	Sources	Alerts	Lists	Help 🗸	SciVal »	Register >	Login 🗸	=
Author search									
O Documents  Atthors O Attiliations Advanced								Sear	ch tips 🕞
Author last name		Author	first name						
eg Smith Affiliation eg Uneesty of Sevents		eg↓L — □ Show	v exact match	nes only				Se	arch Q
ORCID     #g 1111 2020 3133 4466		Search	Q						
Brought to you by The Sempus Team							<u>ې</u>	) Help impi	ove Scopus
FISEVIER									



#### 19) How to search for patents using structure editor? Reaxvs Query builder Quick search Results Synthesis planner History Ryan Huang 👌 🗘 🕐 Go to query 1. builder Search in: Reactions Targets Substances Documents > 2. Click on Find search fields and forms 0 Structure 2 ٢ 俞 .... LS Э # 坐 Fields Forms History Edit your 3. Import Save Reset form Delete all Structure Molecular Formula CAS RN TI, AB & KW Reaxys 🔨 Structure Topics and Keywords > Structure х $\sim$ () Create Structure / Reaction Drawing Identification $\sim$

4. Click related Markush to broaden your search

Reaxys

Filters

patent

letter

chapter

T report

Authors

- 5. Click on documents or substances
- 6. Limit the document type to patent



Query builder Results Synthesis planner History

Quick search

Ryan Huang 😤 📮 💿





# Thank you

