

## Reaxys and Reaxys Medicinal Chemistry

A How To Guide For Commonly Used Searches - CONFIDENTIAL



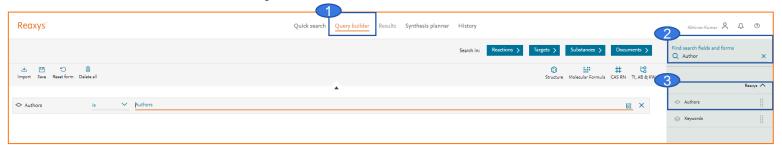
## Contents

- 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)

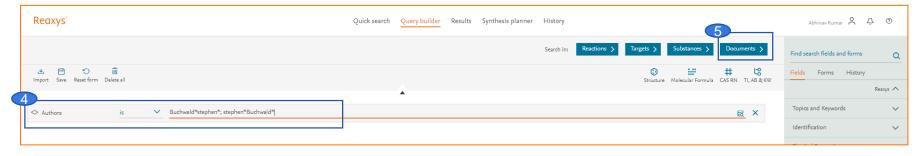


#### 1) How to do literature search by author name?

- Go to query builder
- 2. In "search fields and forms' enter Author
- Select the field author

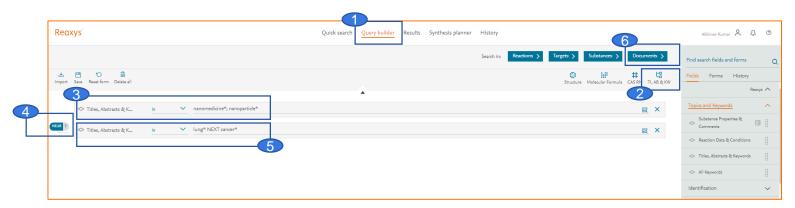


- 4. Enter author name in the following format "last\_name\* first\_name\*; first\_name\*last\_name\*" for example for author Stephen Buchwald you would enter the query as shown below
- 5. Click on documents to find literature associated with author Stephen Buchwald





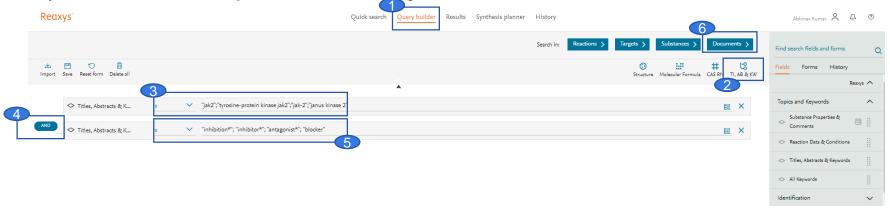
#### 2) How to do a topic search on "nanomedicine in lung cancer"?



- 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



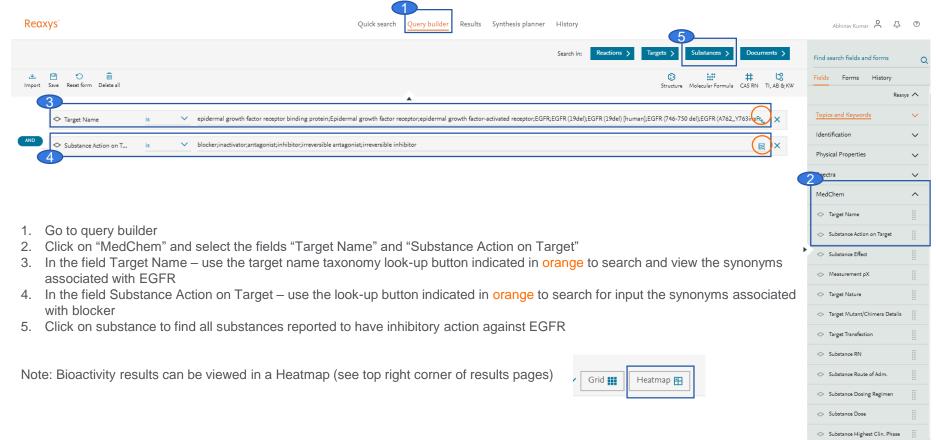
3) How to do a topic search on "jak2 inhibitor"?



- 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

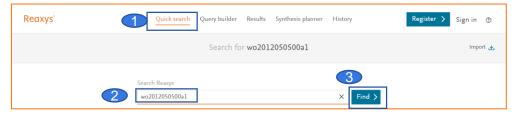


### 4) How to find all substances that blocks my target of interest "EGFR"?

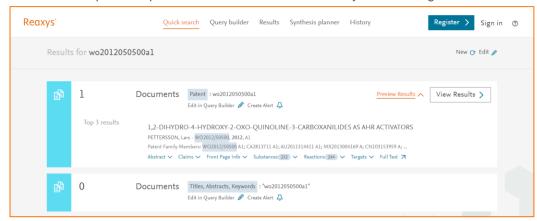


#### 5) How to search for a patent using patent number?

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

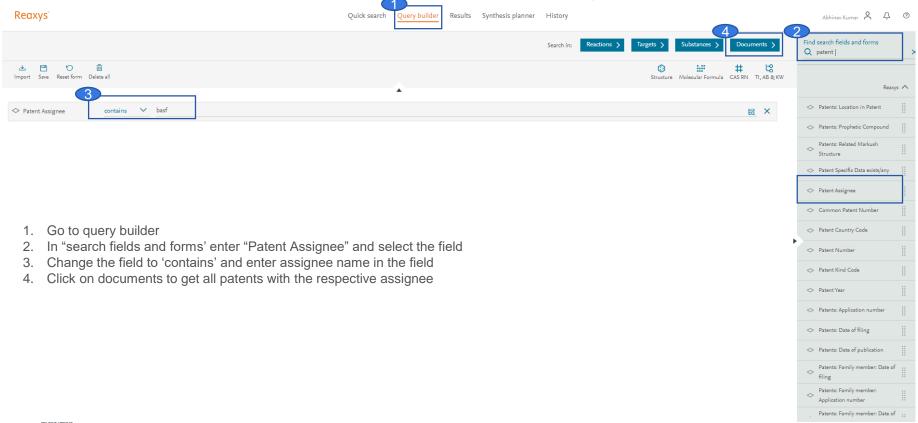


#### This then adapts the input so that it fits best into the Reaxys search engine



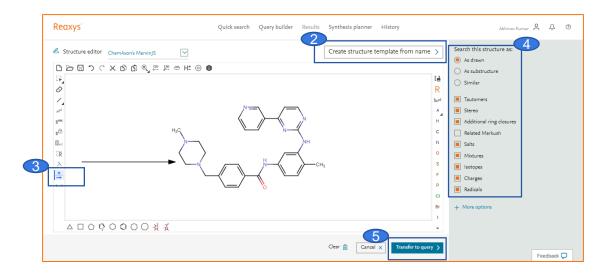


6) How to search for patent by a particular assignee?



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

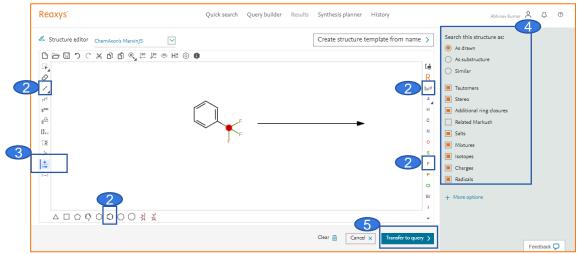
product?



- 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?

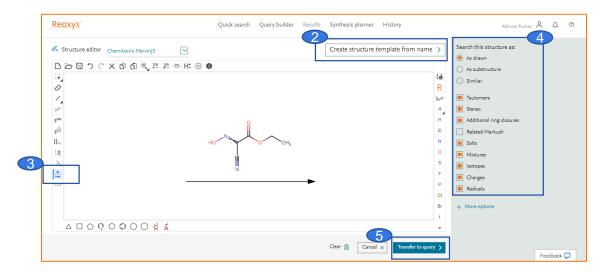


- 1. Click on "DRAW" on the landing page
- 2. Either draw the structure using the drawing tools available (MarvinJS and ChemDraw) or use create structure from template option. Here the structure was drawn using the tools
- 3. Use reaction arrow button to indicate that this structure is desired as a starting 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

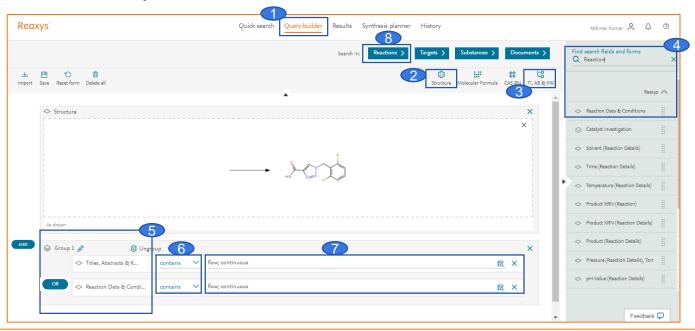
reagent?



- 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"



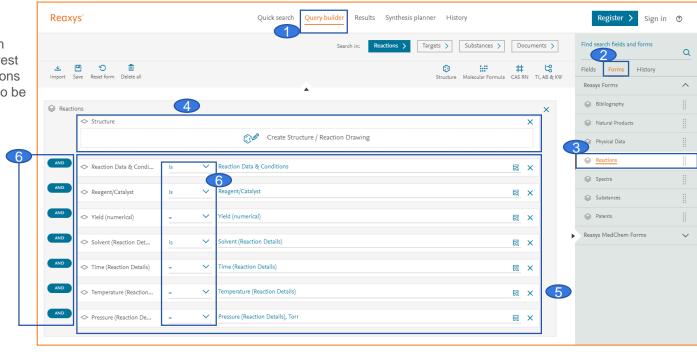
#### 10) How to define specific conditions for a reaction?



- 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 guery 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?

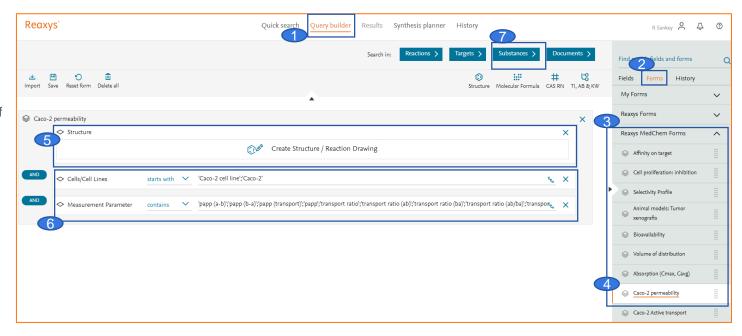
- 1. Go to query builder
- 2. Go to Reaxys Forms
- 3. Select the Reactions form
- Draw the reaction of interest
- Enter the relevant conditions (note: not all fields need to be filled)
- Change the operator as required to match your search criteria





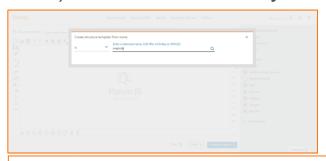
#### 12) How to use advanced query forms in Reaxys MedChem

- 1. Go to query builder
- 2. Go to Reaxys Forms
- Review Reaxys MedChem forms
- 4. Add the form of interest e,g, Caco-2 permeability
- 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

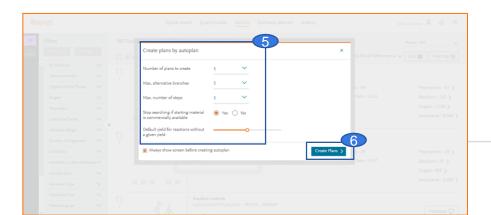


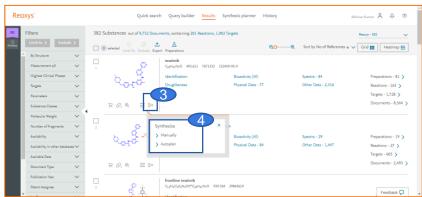


#### 13) How to do retrosynthesis in Reaxys?



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





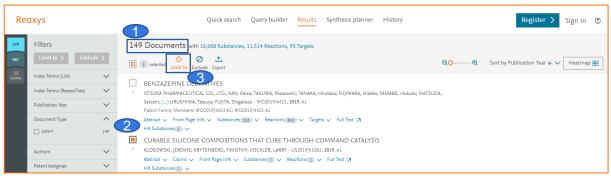
- 3. Click on icon for synthesis
- 4. Select either "autoplan" where Reaxys automatically creates multiple synthesis plans for you or "manually" letting you manually create synthesis plans
- 5. Select the parameters for the synthesis plan
- 6. Click on create plans to obtain the results

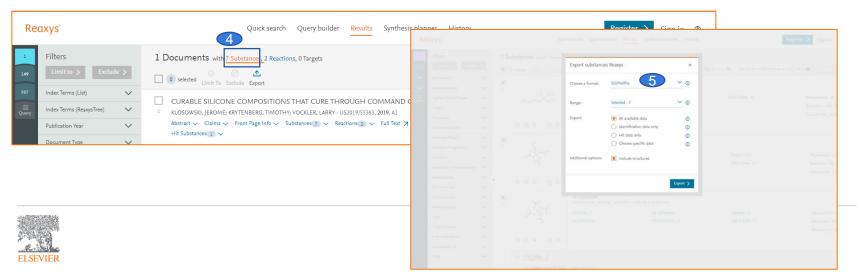
#### Generate retrosynthesis plans for any known molecule

More details and video tutorial can be found here: https://service.elsevier.com/app/answers/detail/a\_id/12233/suppo\_rthub/reaxys/kw/synthesis+planner/

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

- 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
- Export the substances in "SMILES" or "SD/Molfile" format





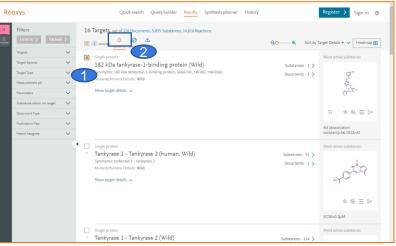
15) How do I export bioactivity data for my target or substance

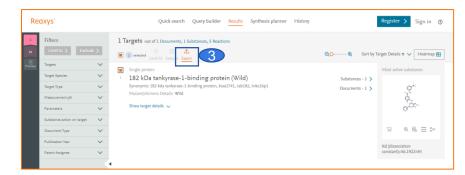
results?

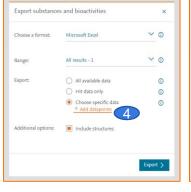
 On target/substance results page select the target/substance of interest

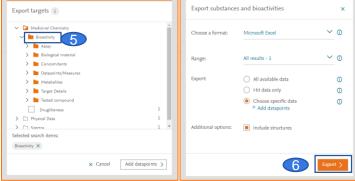
- 2. Limit to the particular target/substance result (optional step)
- Click on Export
- 4. Choose specific data points and click 'Add datapoints'
- 5. Click on 'Bioactivity' (or select the required datapoints under it)
- Click export

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









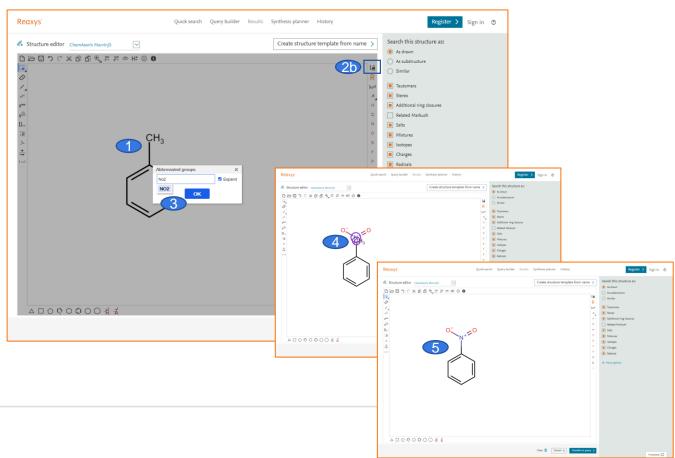


16) How do I quickly draw a functional group like nitrate, acetate or

BOC?

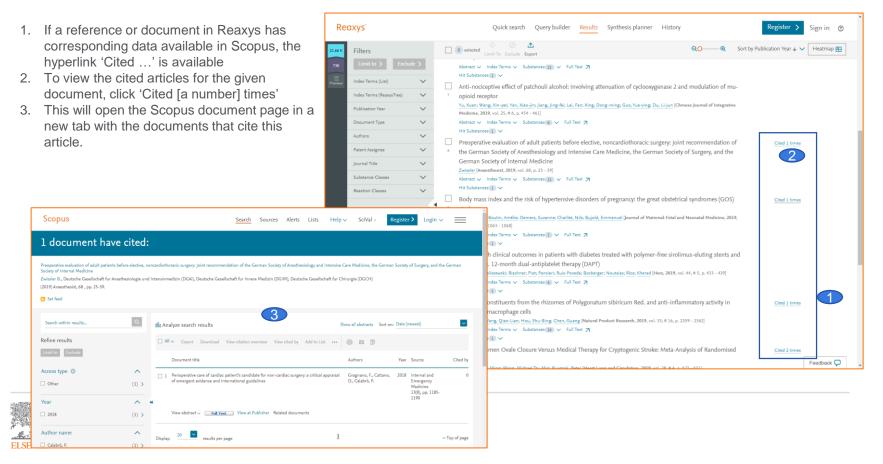
 Draw the structure of interest (with the atom to be replaced by functional group already in place)

- (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?

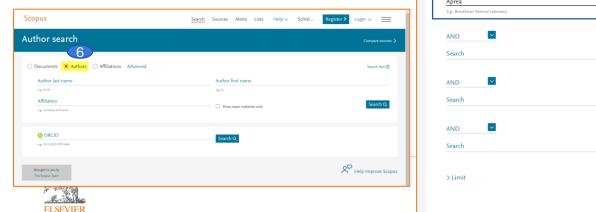


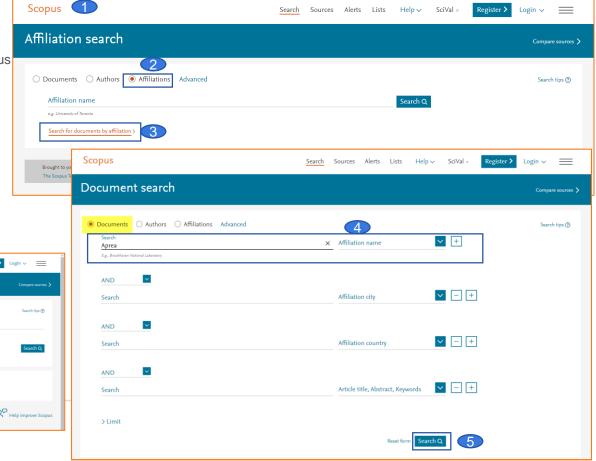
18) How do I look for documents associated to a particular association/author

affiliation?

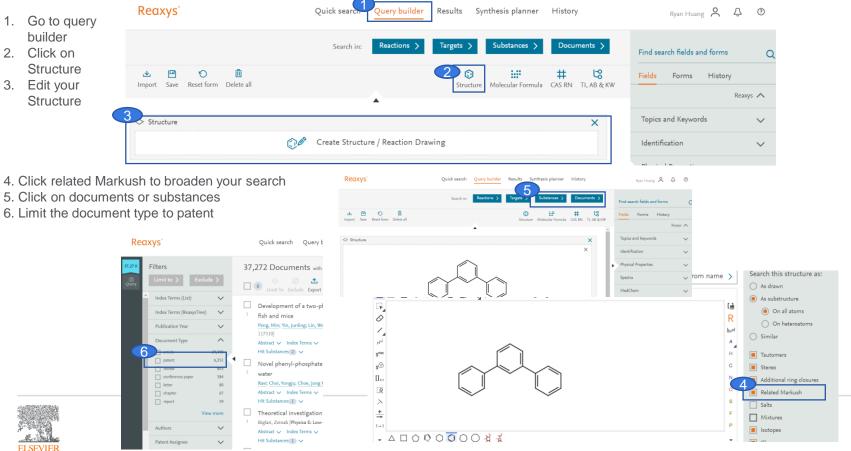
Reaxys does not contain an affiliation field for journal articles. For these cases please use Scopus which is a multidisciplinary bibliographic database produced by Elsevier.For this

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





19) How to search for patents using structure editor?





# Thank you

