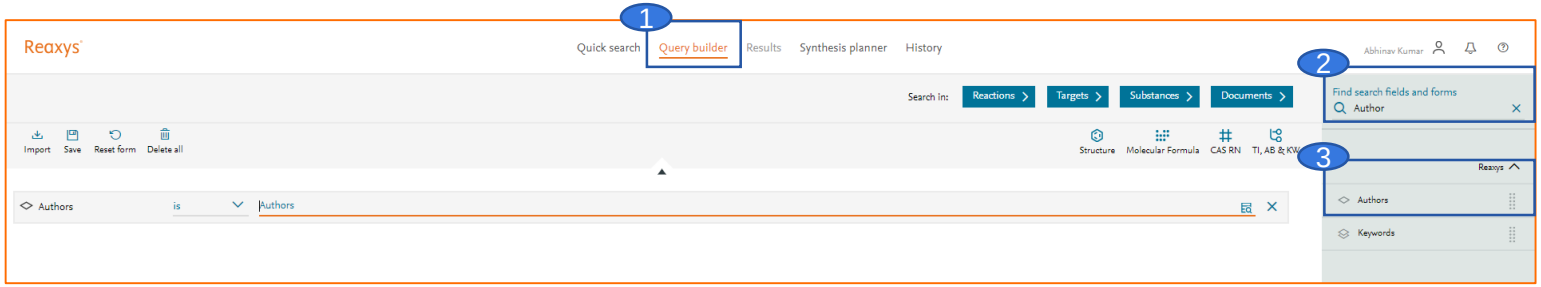
Reaxys and Reaxys Medicinal Chemistry

A How To Guide For Commonly Used Searches - CONFIDENTIAL

Contents

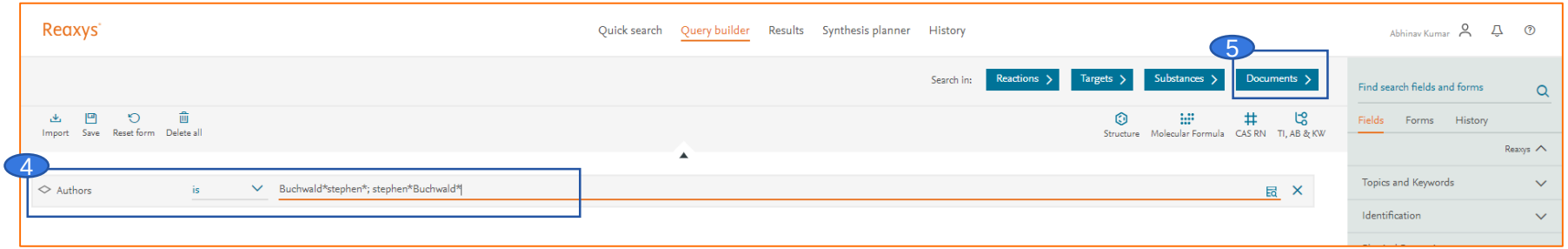
1) How to do literature search by author name?

1. Go to query builder
2. In “search fields and forms’ enter Author
3. Select the field author



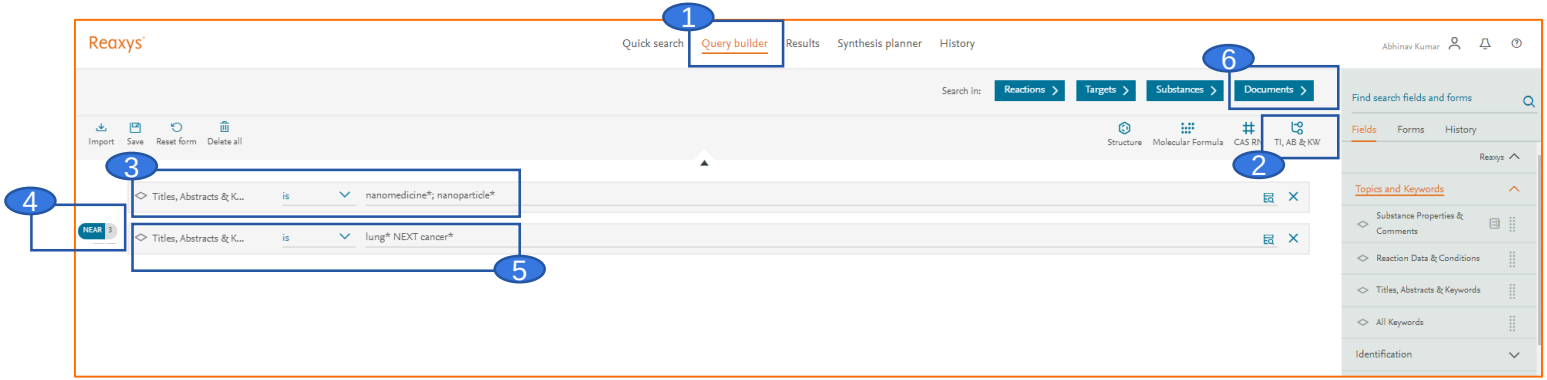
4. Enter author name in the following format “last_name* first_name*;first_name*last_name*” for example for author Stephen Buchwald you would enter the query as shown below

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



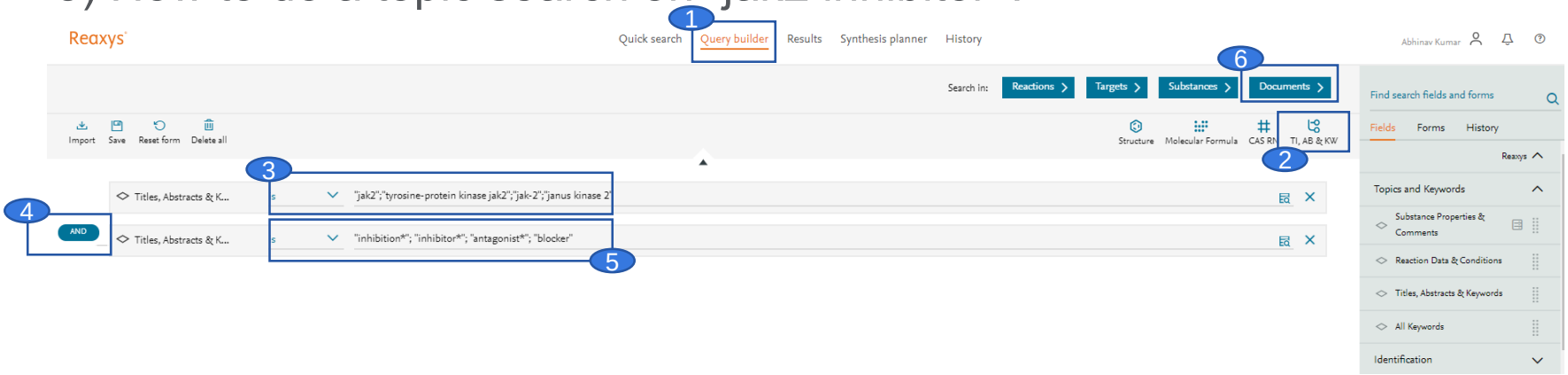
ELSEVIER

2) How to do a topic search on “nanomedicine in lung cancer”?



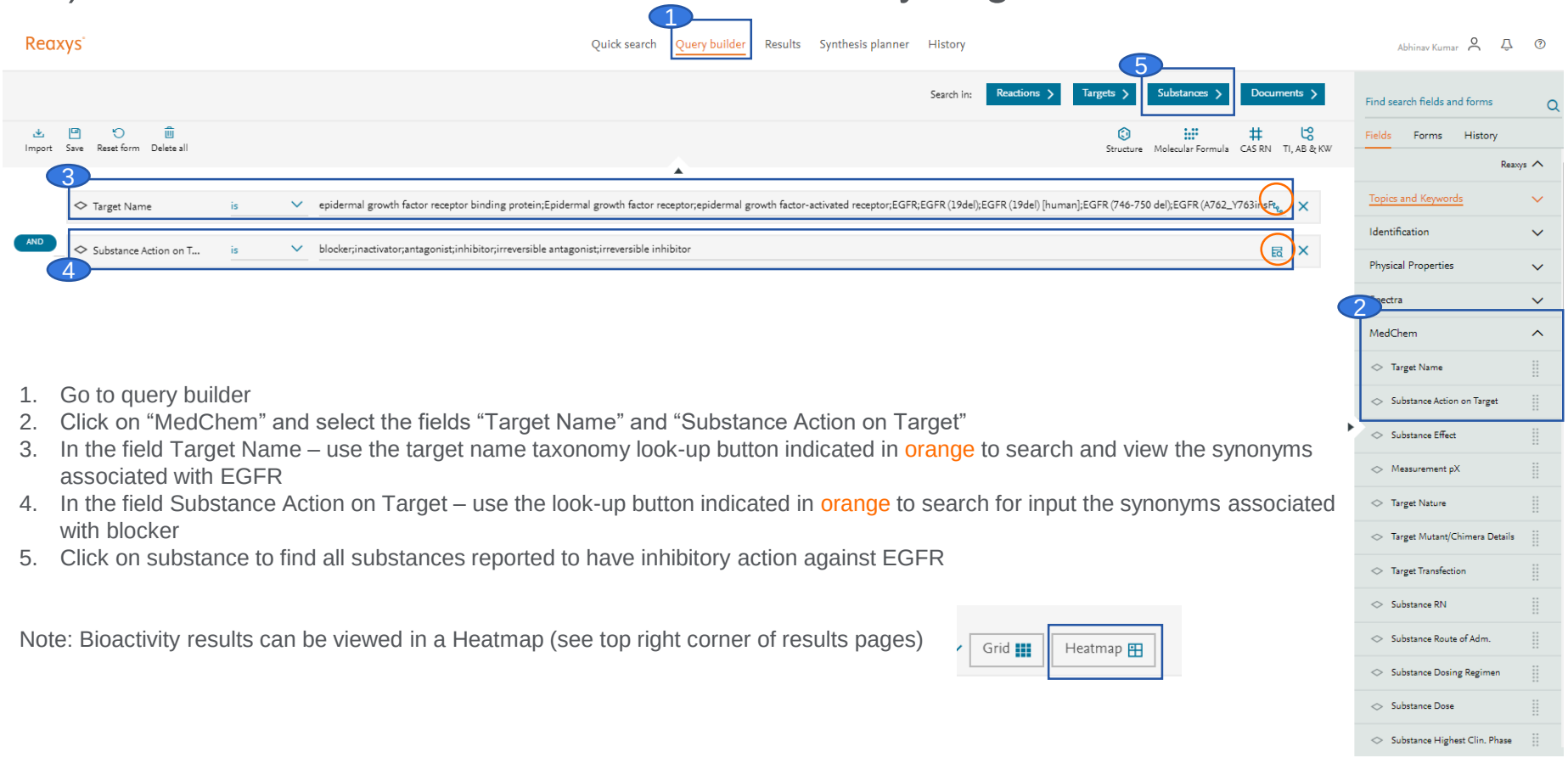
1. Go to query builder
2. Click on “Title, Abstracts & Keywords” (“TI, AB & KW” shortcut key). This field can be added multiple times (x2 in this example)
3. In the first box, enter the search query using synonyms for nanomedicine such as nanoparticle and use wild card operator “*” to account for plurality 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”?



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”?

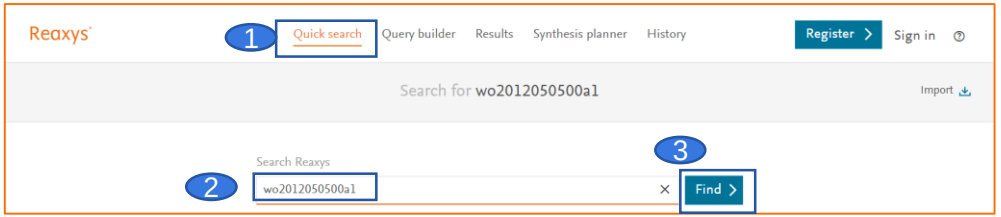


1. Go to query builder
2. Click on “MedChem” and select the fields “Target Name” and “Substance Action on Target”
3. In the field Target Name – use the target name taxonomy look-up button indicated in orange to search and view the synonyms associated with EGFR
4. In the field Substance Action on Target – use the look-up button indicated in orange to search for input the synonyms associated with blocker
5. Click on substance to find all substances reported to have inhibitory action against EGFR

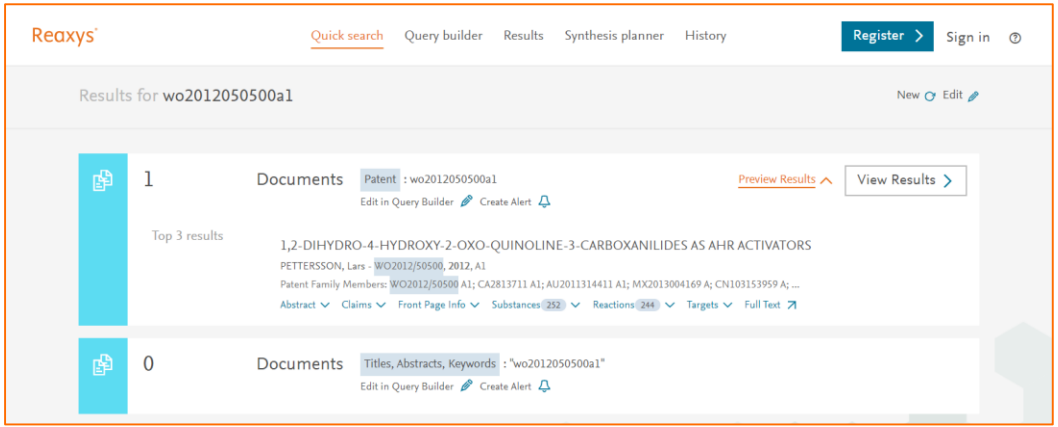
Note: Bioactivity results can be viewed in a Heatmap (see top right corner of results pages)

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

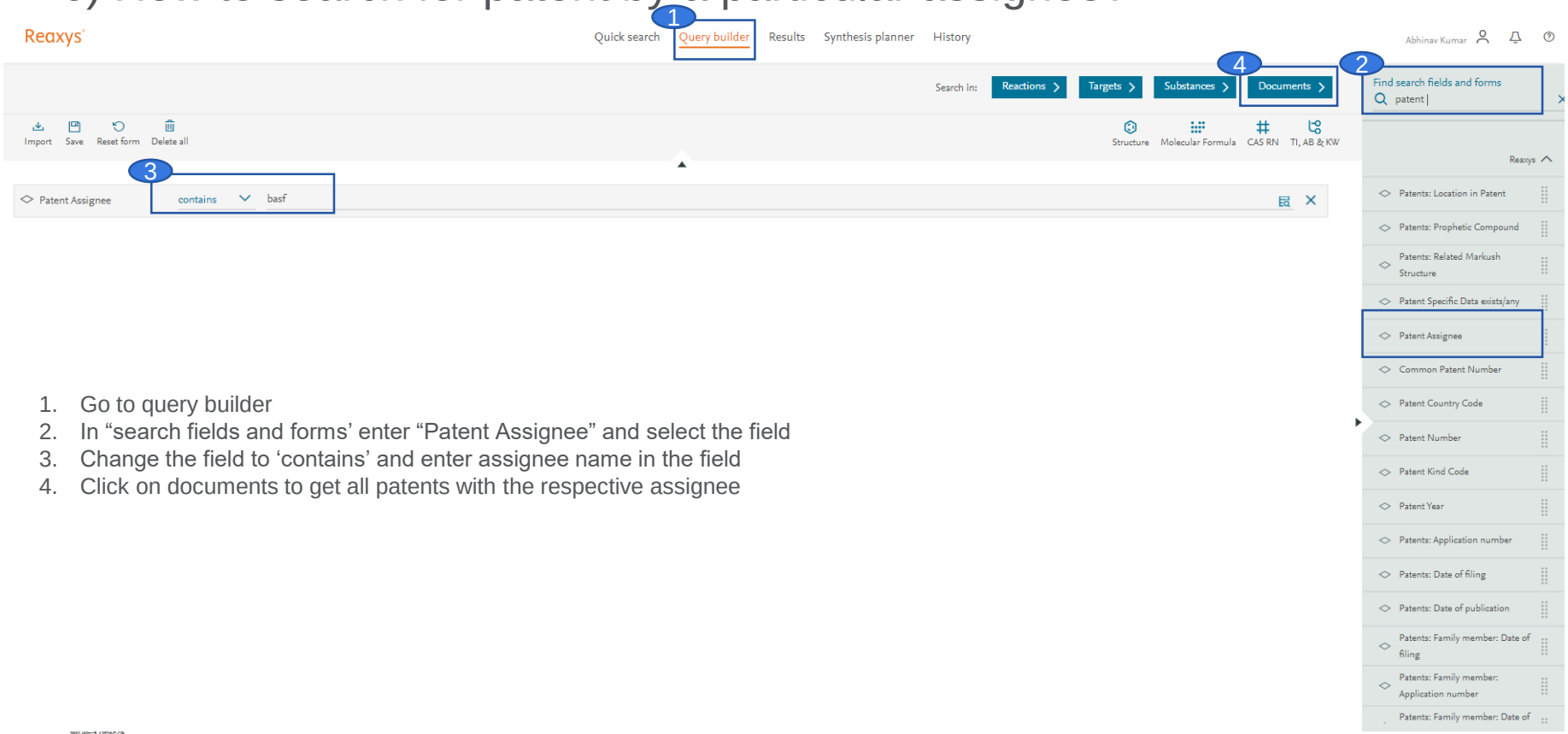
1. Go to quick search
2. Enter the patent number
3. Click Find



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



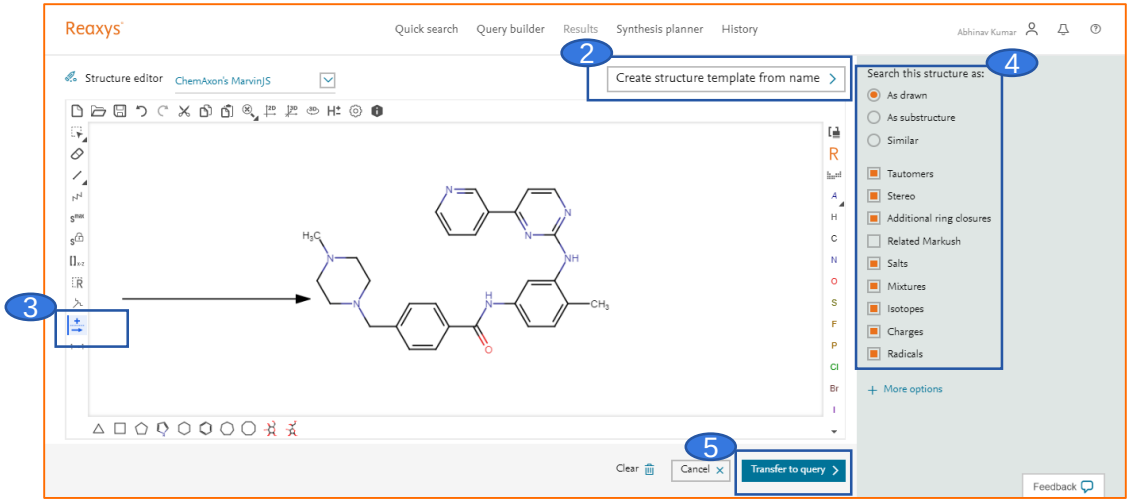
6) How to search for patent by a particular assignee?



1. Go to query builder
2. In “search fields and forms’ enter “Patent Assignee” and select the field
3. Change the field to ‘contains’ and enter assignee name in the field
4. Click on documents to get all patents with the respective assignee

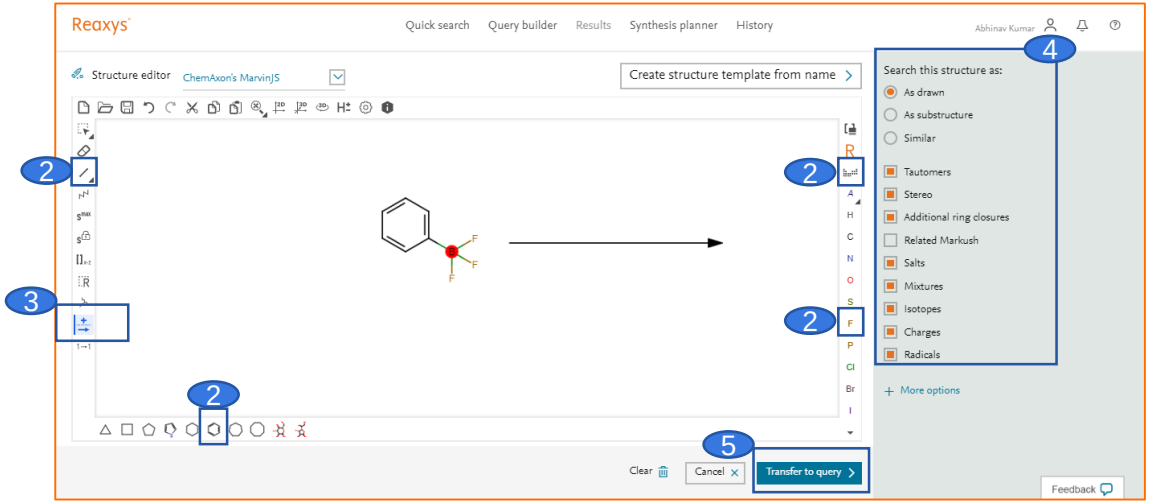
ELSEVIER

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



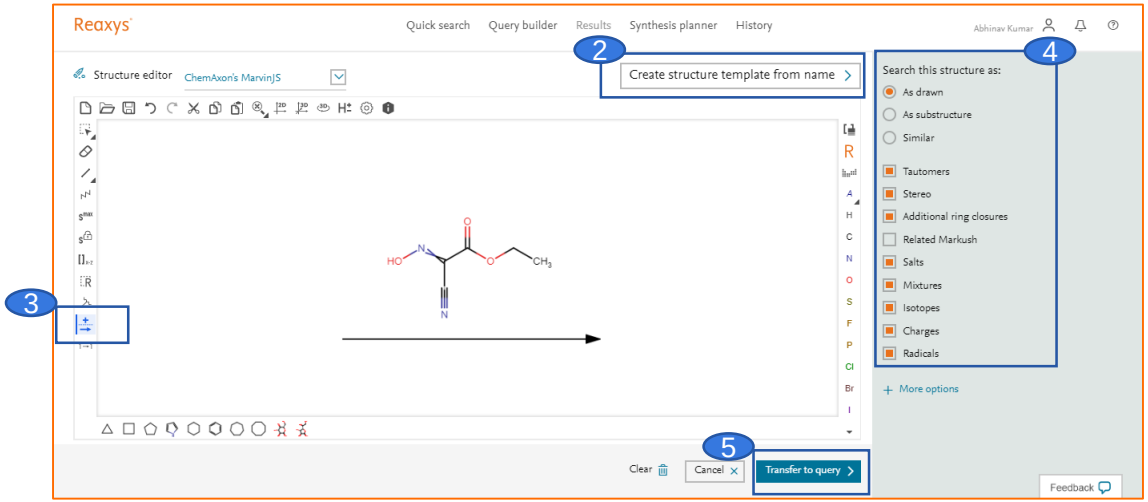
1. Click on “DRAW” on the landing page
2. Either draw the structure using the drawing tools available (MarvinJS and ChemDraw) or use create structure from template option e.g. here imatinib was entered
3. Use reaction arrow button to indicate that this structure is desired as a product
4. Select the 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?



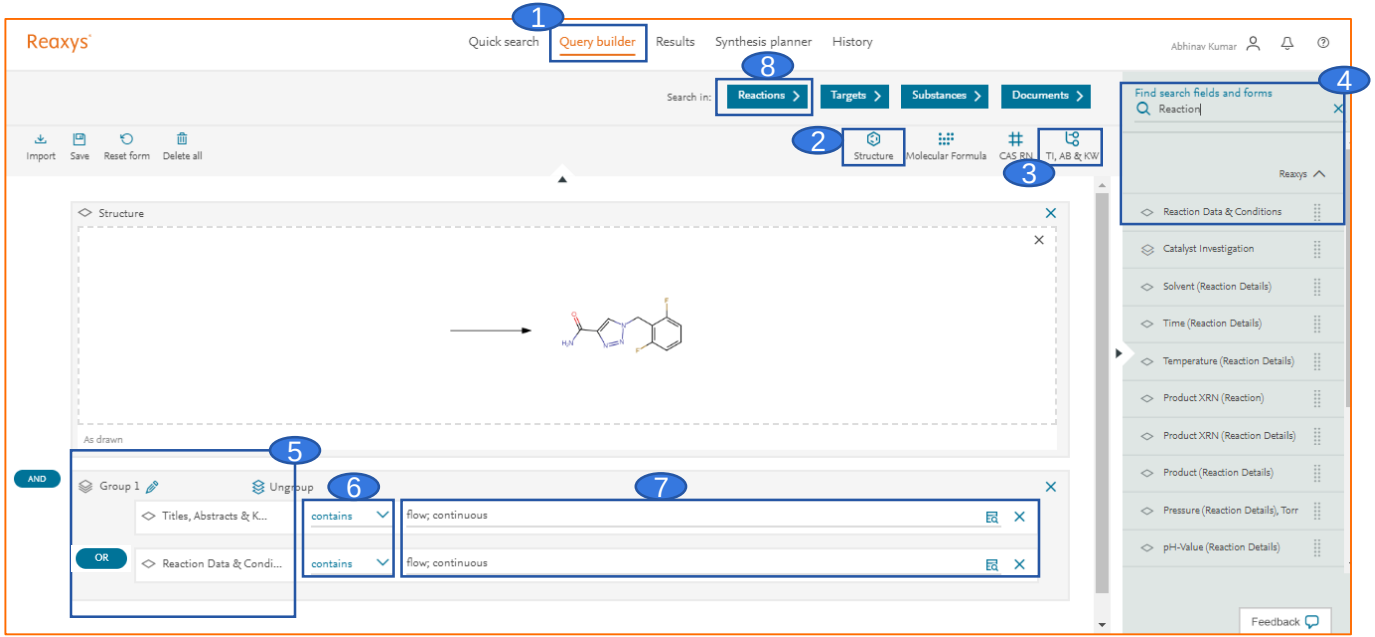
1. Click on “DRAW” on the landing page
2. Either draw the structure using the drawing tools available (MarvinJS and ChemDraw) or use create structure from template option. Here the structure was drawn using the tools
3. Use reaction arrow button to indicate that this structure is desired as a starting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

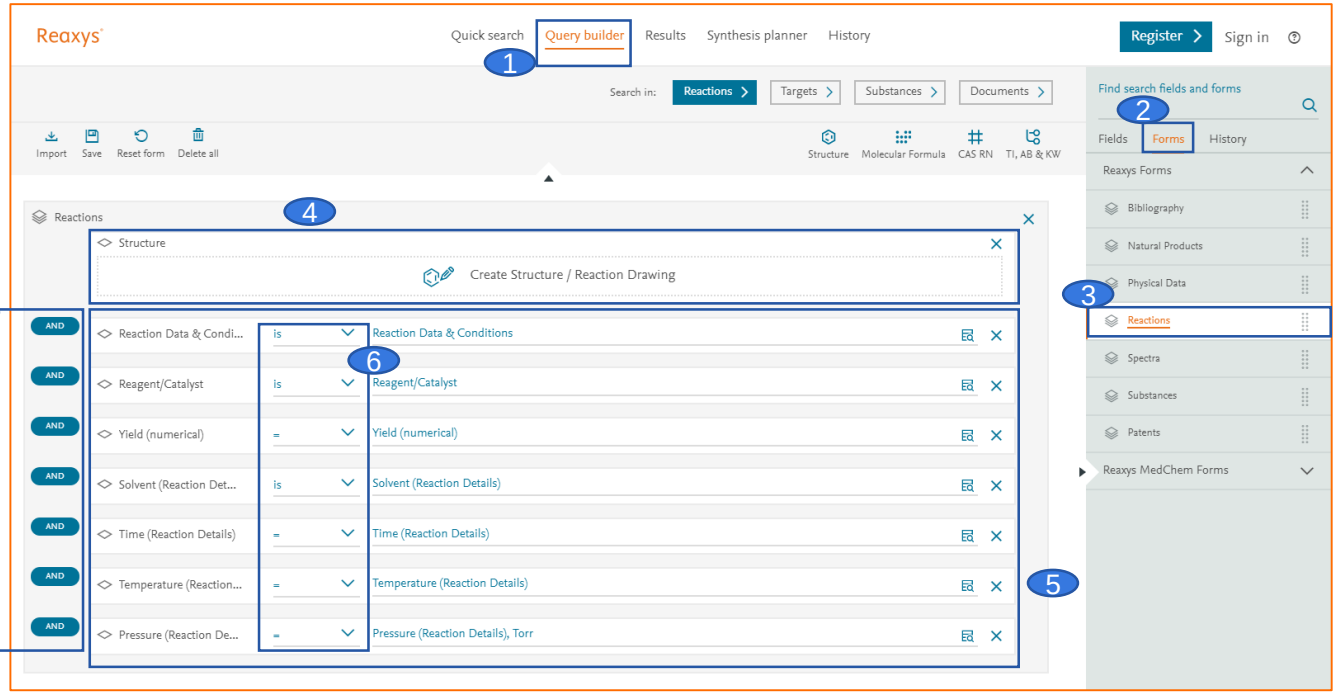
10) How to define specific conditions for a reaction?



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?

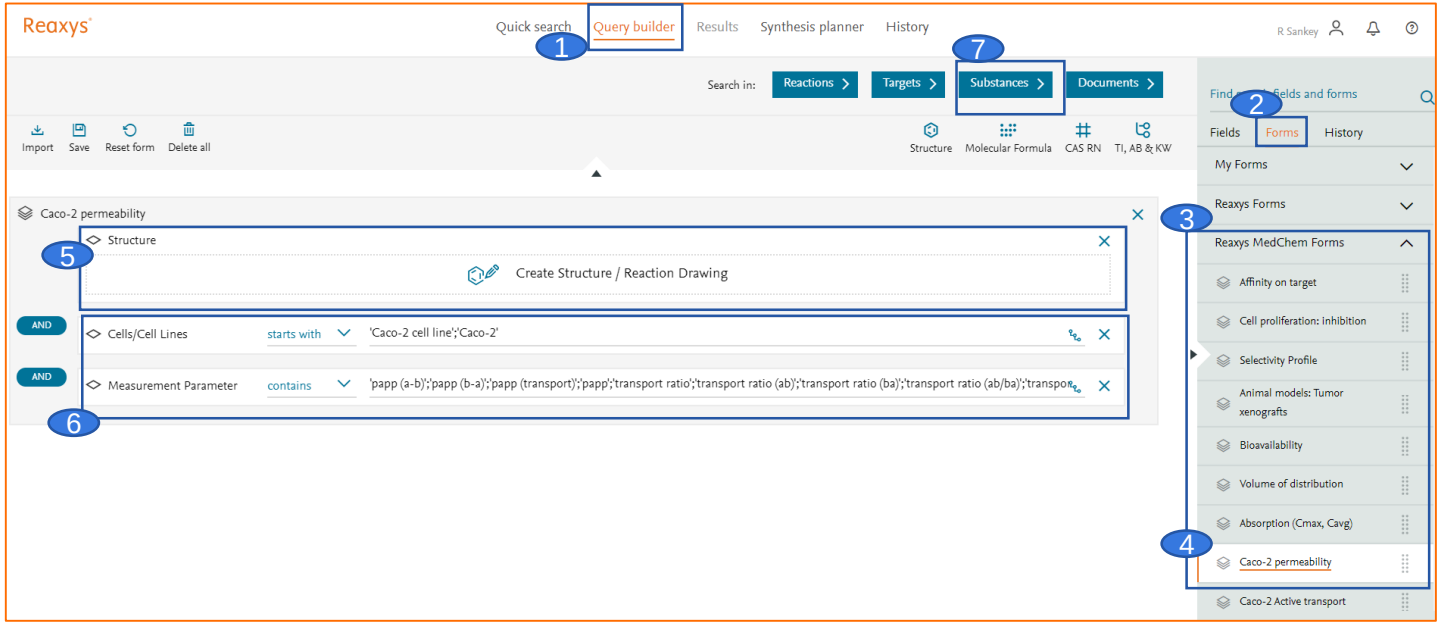
1. Go to query builder
2. Go to Reaxys Forms
3. Select the Reactions form
4. Draw the reaction of interest
5. Enter the relevant conditions (note: not all fields need to be filled)
6. Change the operator as required to match your search criteria



ELSEVIER

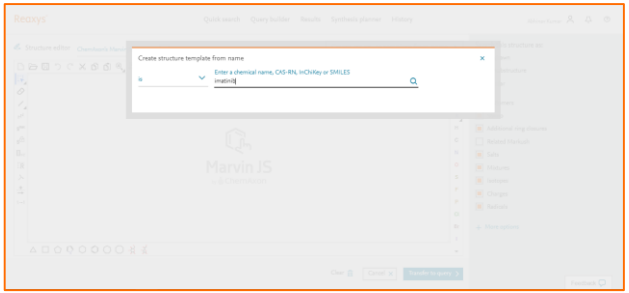
12) How to use advanced query forms in Reaxys MedChem

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
6. Querylets have been pre-filled with required parameters. Review and amend if desired
7. Click on “Substances” to obtain results matching the search criteria

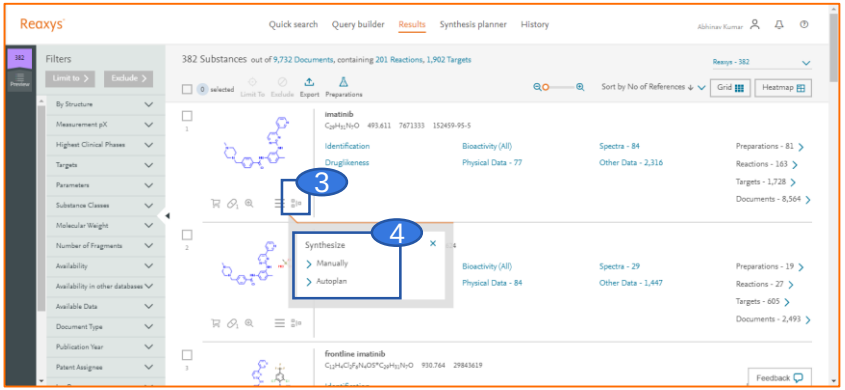


ELSEVIER

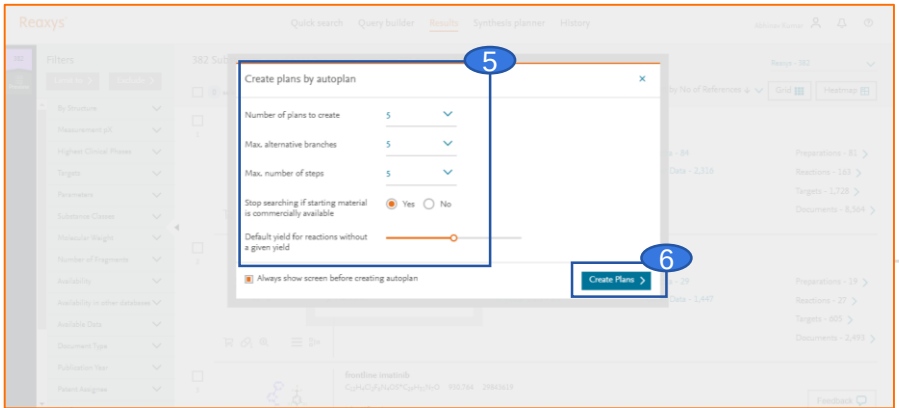
13) How to do retrosynthesis in Reaxys?



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



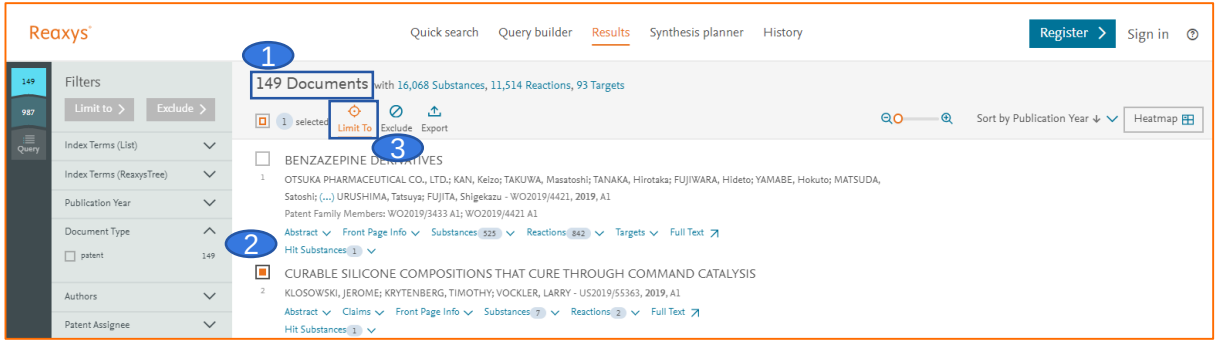
5. Select the parameters for the synthesis plan
6. Click on create plans to obtain the results

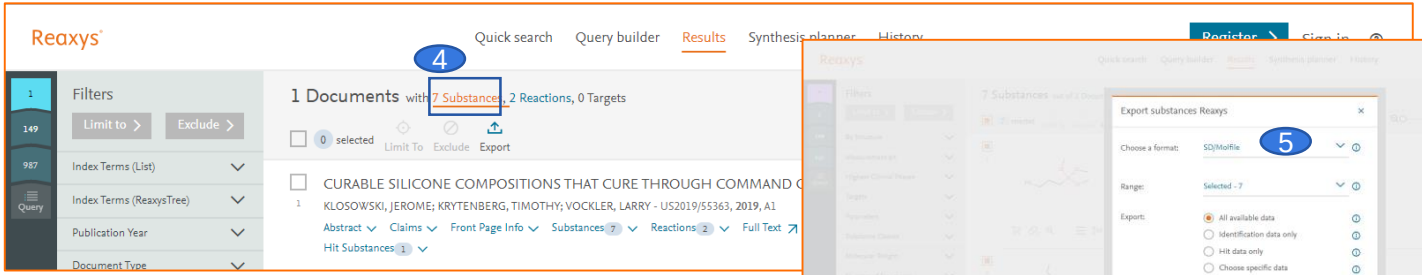
Generate retrosynthesis plans for any known molecule

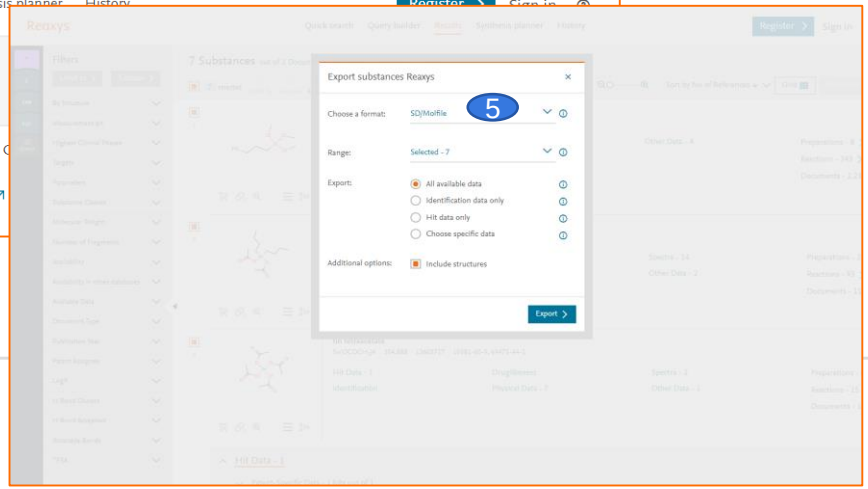
More details and video tutorial can be found here: https://service.elsevier.com/app/answers/detail/a_id/12233/supporthub/reaxys/kw/synthesis+planner/

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



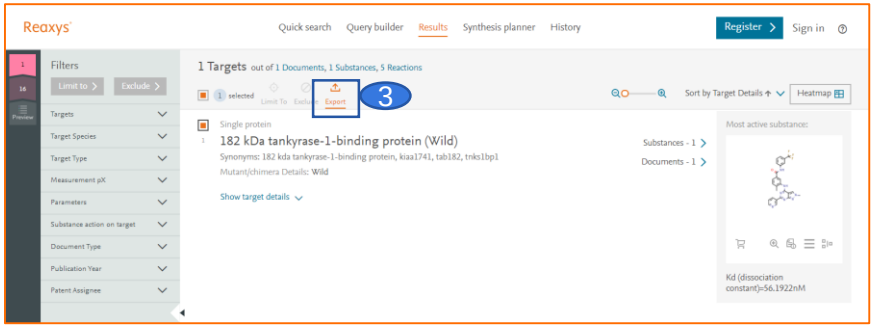


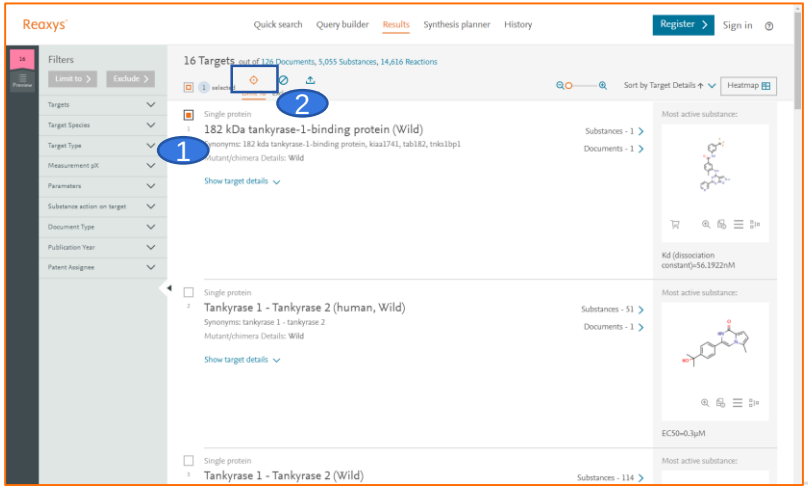


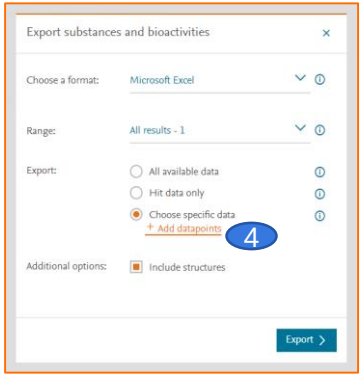
15) How do I export bioactivity data for my target or substance results?

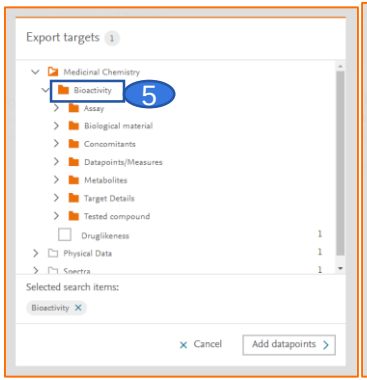
1. On target/substance results page select the target/substance of interest
2. Limit to the particular target/substance result (optional step)
3. Click on Export
4. Choose specific data points and click ‘Add datapoints’
5. Click on ‘Bioactivity’ (or select the required datapoints under it)
6. Click export

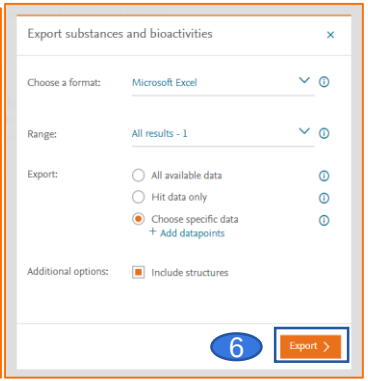
(note: export is limited to 1000 substances for anonymous users and 5000 substances for registered users)







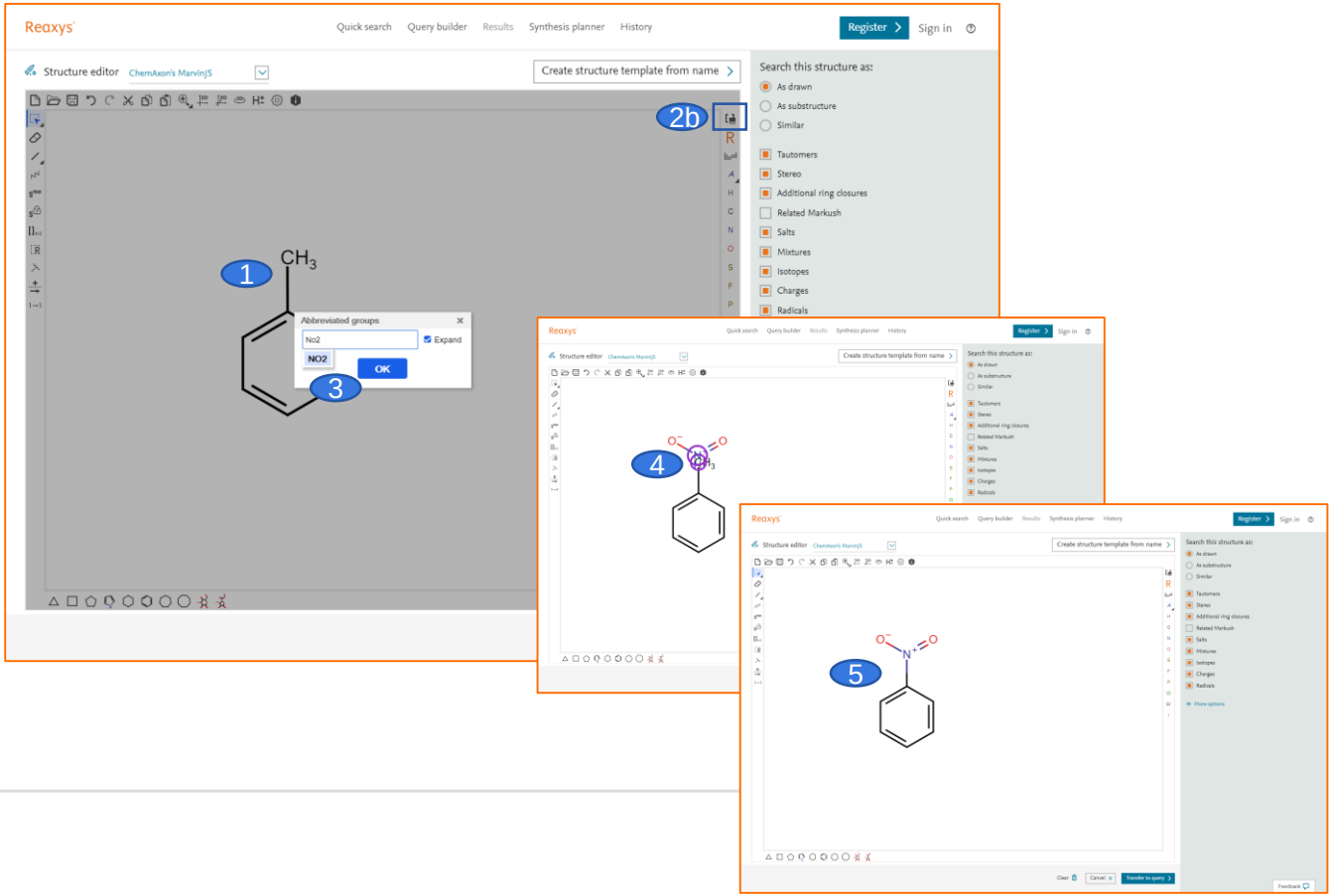




ELSEVIER

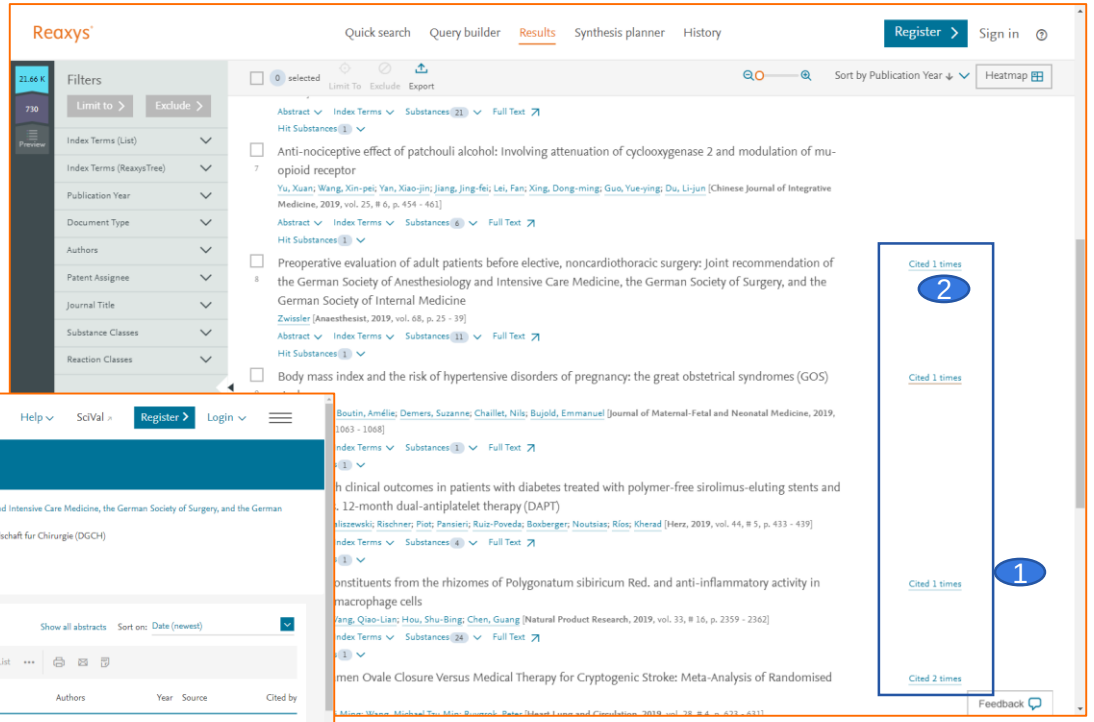
16) How do I quickly draw a functional group like nitrate, acetate or BOC?

1. 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
3. type the functional group (expand, if needed) and press OK
4. 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?

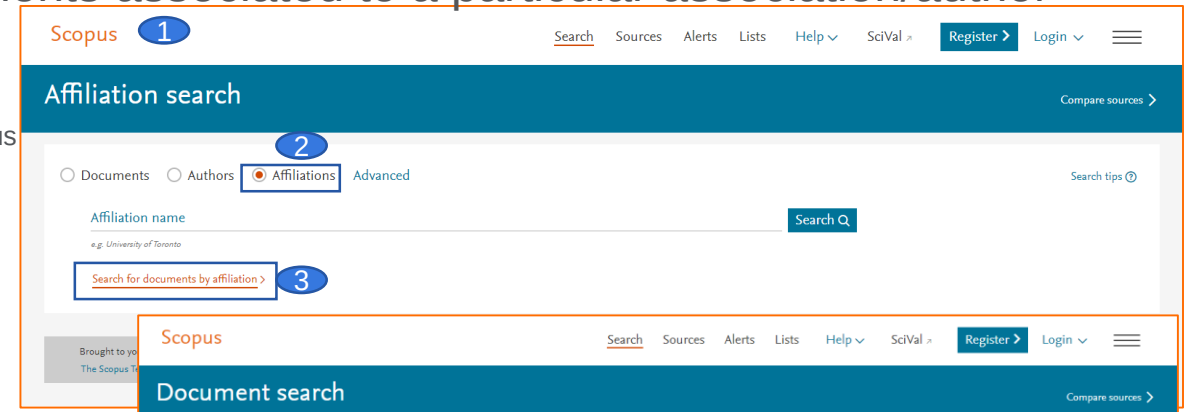
1. If a reference or document in Reaxys has corresponding data available in Scopus, the hyperlink ‘Cited …’ is available
2. To view the cited articles for the given document, click ‘Cited [a number] times’
3. This will open the Scopus document page in a new tab with the documents that cite this article.

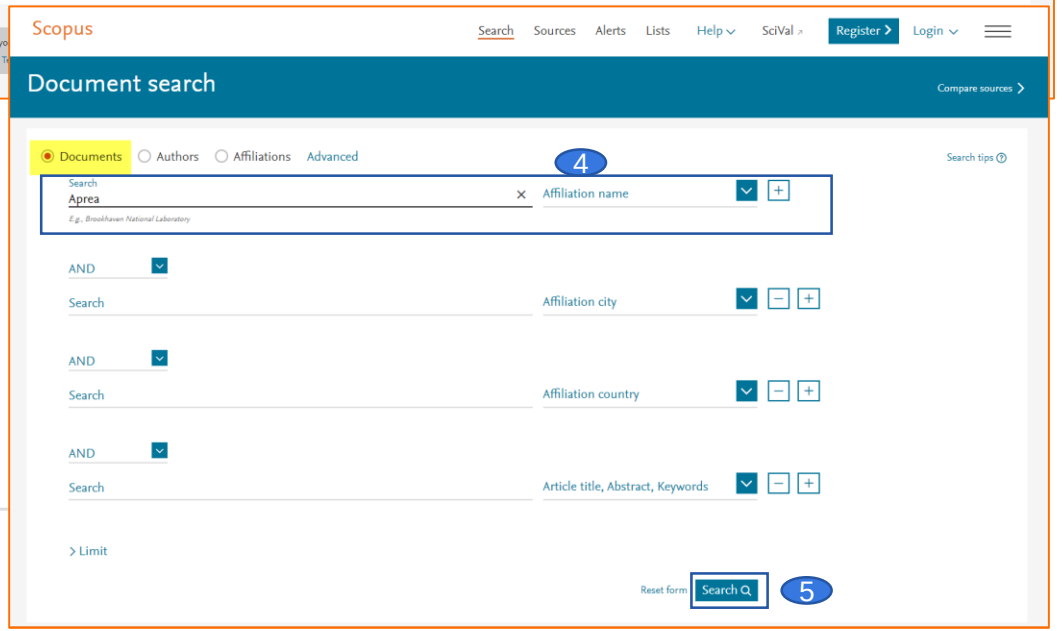


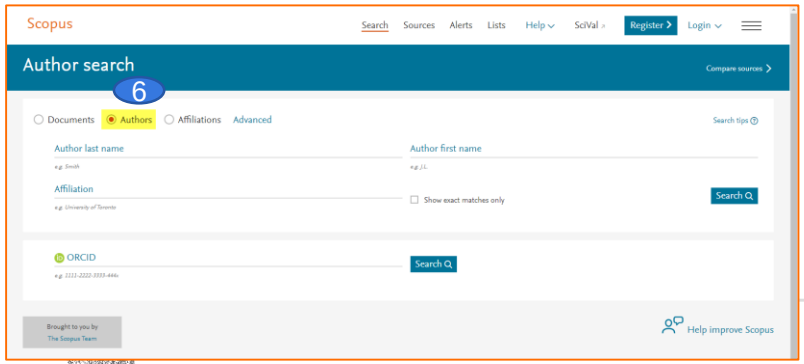
18) How do I look for documents associated to a particular association/author affiliation?

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



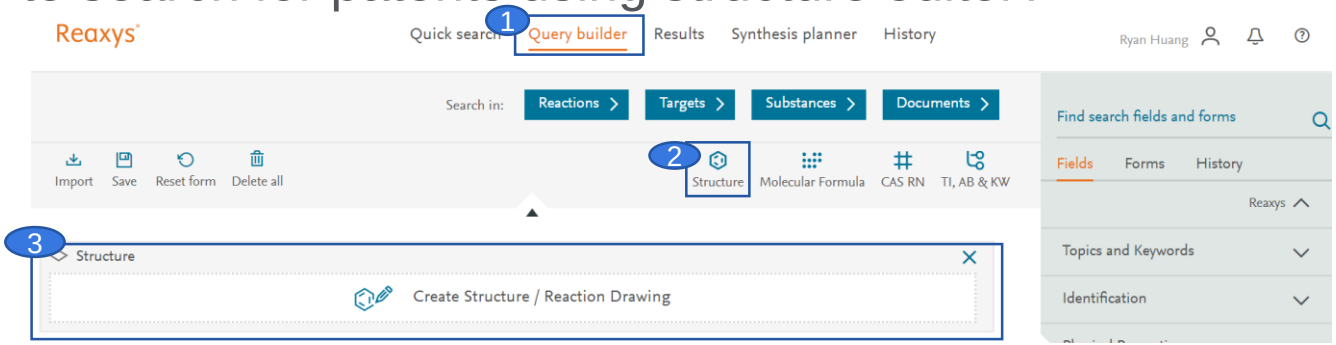




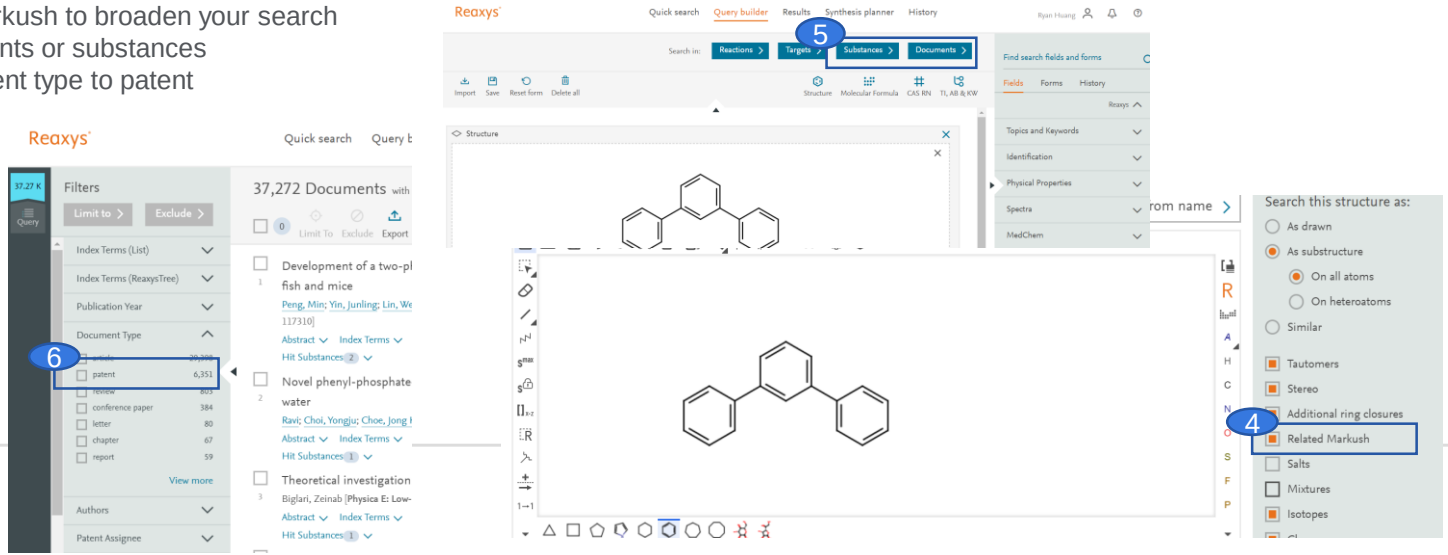
ELSEVIER

19) How to search for patents using structure editor?

1. Go to query builder
2. Click on Structure
3. Edit your Structure



4. Click related Markush to broaden your search
5. Click on documents or substances
6. Limit the document type to patent



ELSEVIER

ELSEVIER

Thank you