Reaxys®

Workflow example

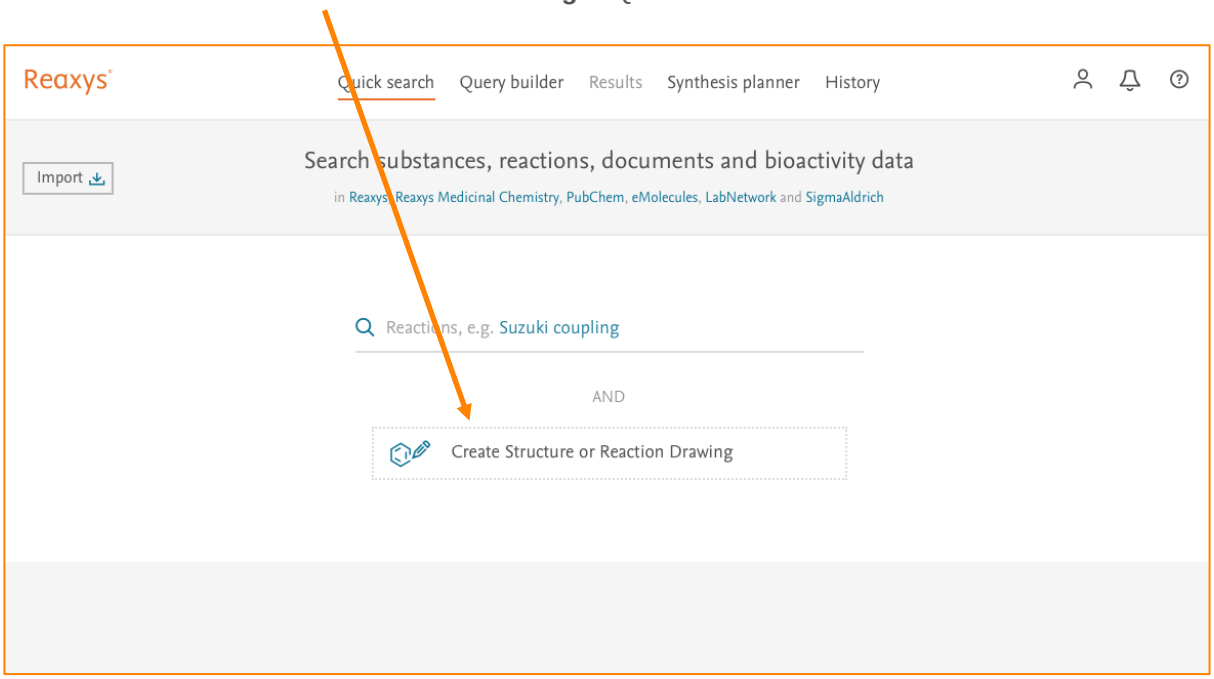
Finding reactions of substituted anilines with aryl boronic acids and finding experimental preparations with optimal yields

Workflow concept

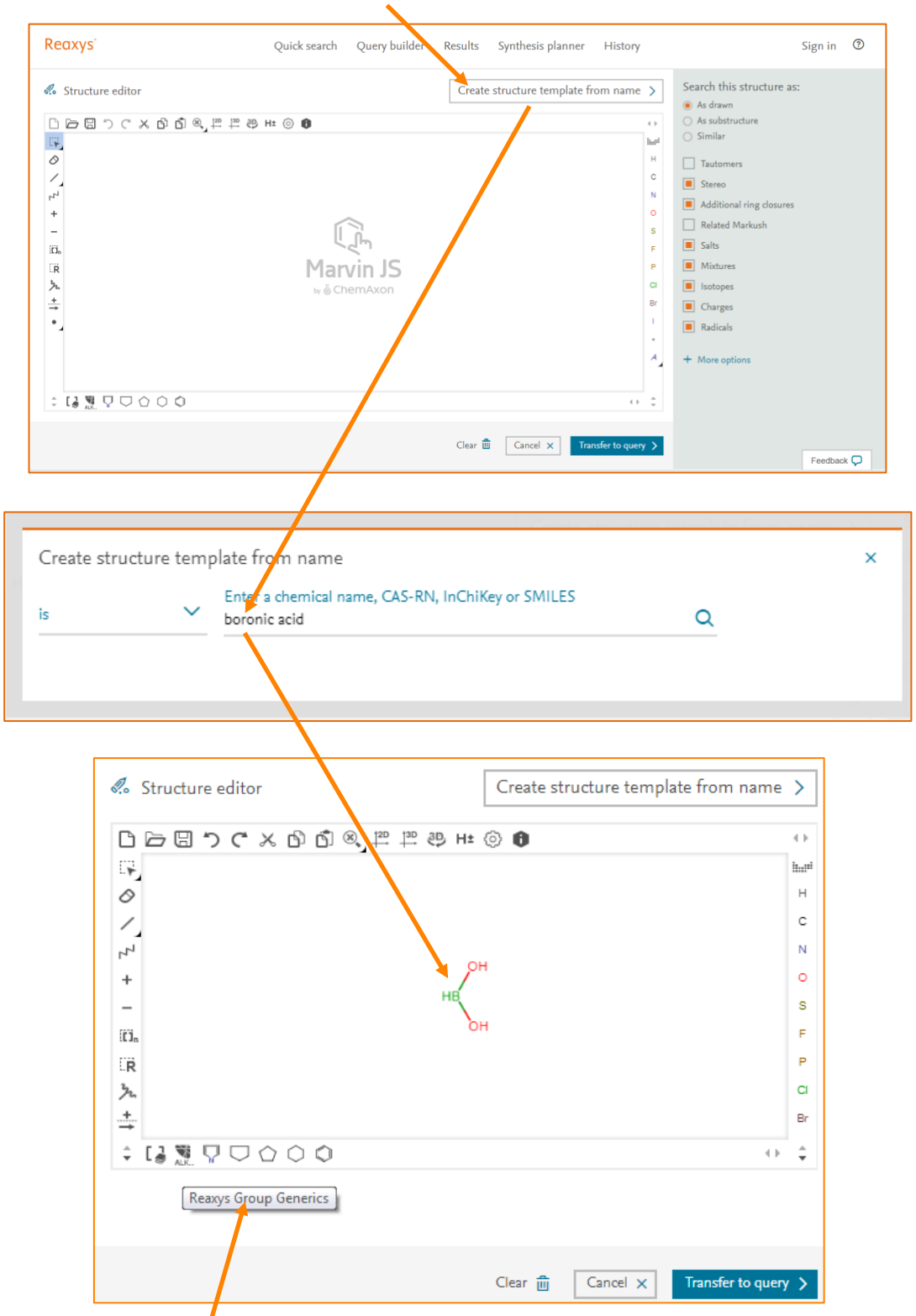
Using Reaxys, the scientist wishes to explore the reactions of substituted anilines with aryl boronic acids. They will be looking at experimental preparations to find catalysts and conditions that give the optimal yield.

1. Use the drawing tool in Quick Search to create the reaction

Click on **Create Structure or Reaction Drawing** in Quick Search.

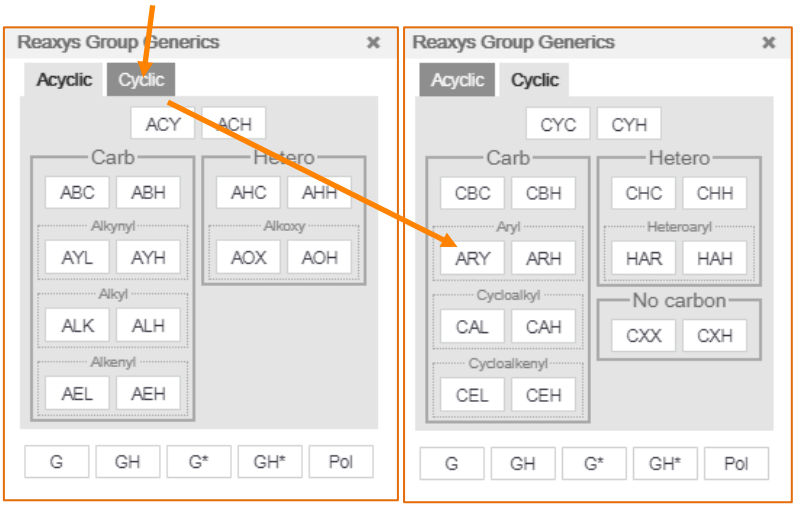


Click **Create structure template from name** and type “boronic acid”. The structure will autopopulate.

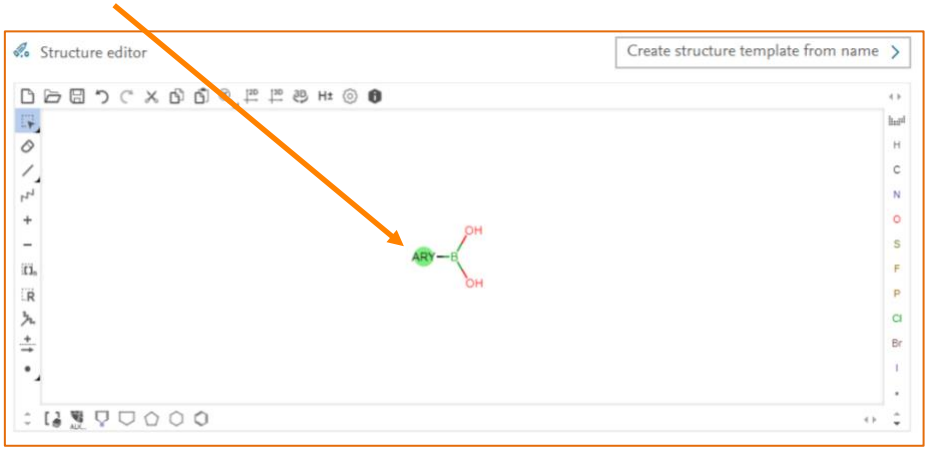


Then click **Reaxys Group Generics**.

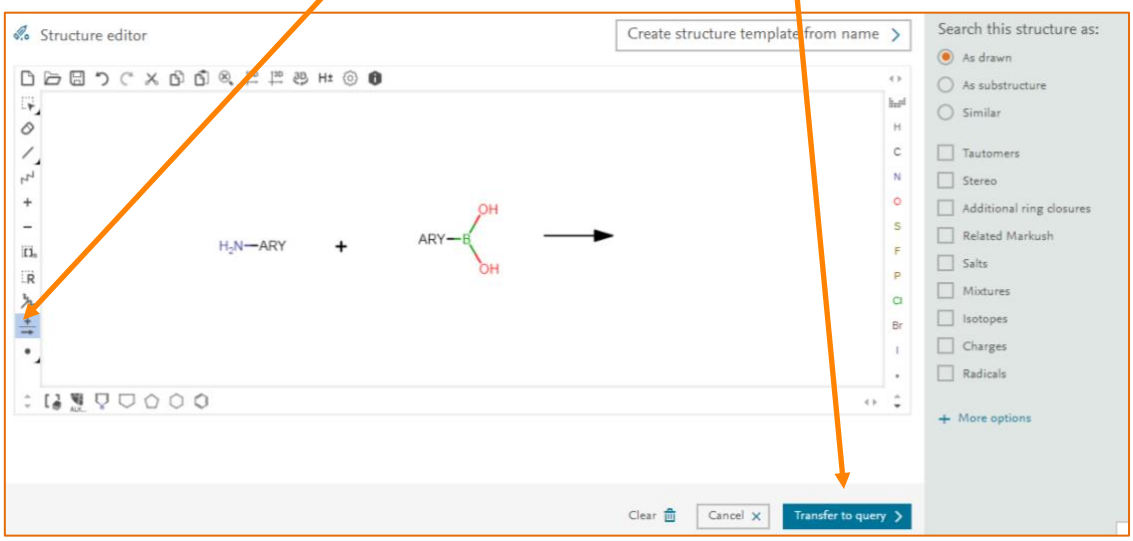
In the dialog boxes, select **Cyclic** and **Aryl**.



Mouse over the “B” and drag left to drag the bond from the atom. Release to drop the “ARY” in place.

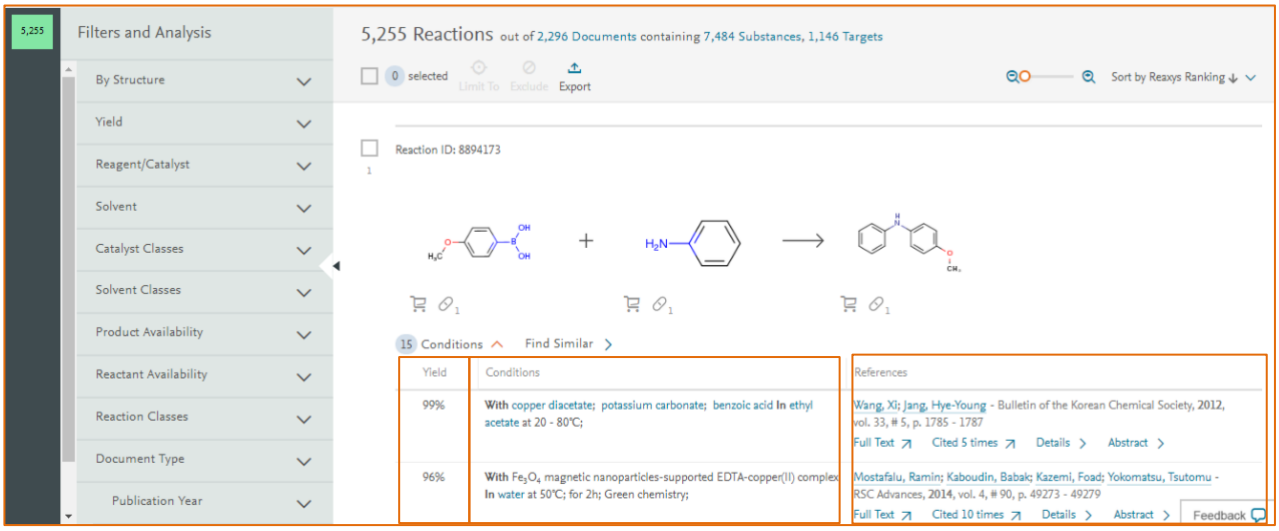


Repeat a similar process for aniline derivatives — create the structure, then add the ARY group. Add the reaction information using this function. Finally, click **Transfer to query** and then **Find.**

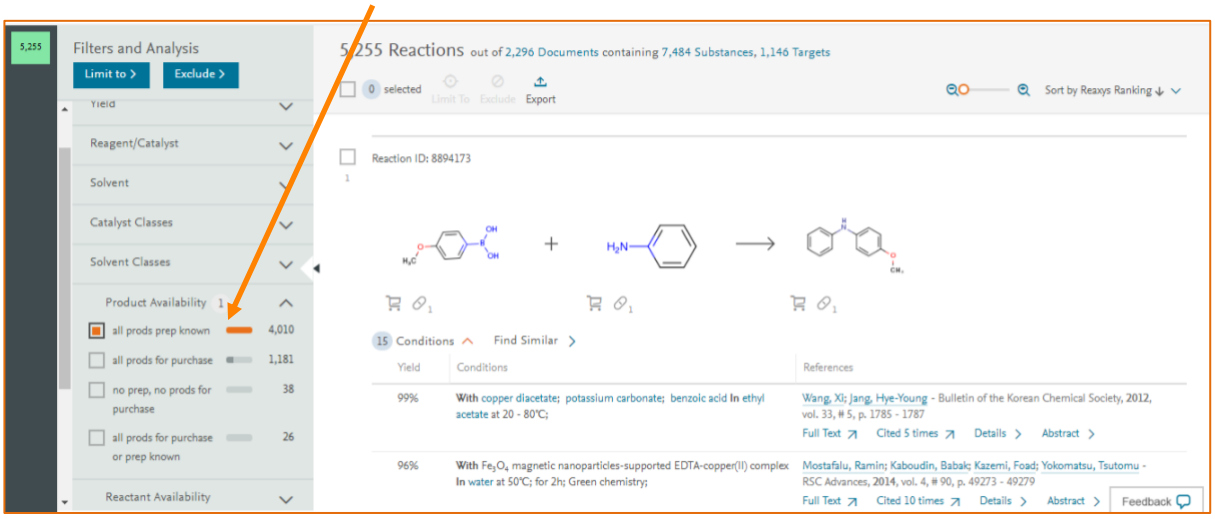


2. Filter and review the results

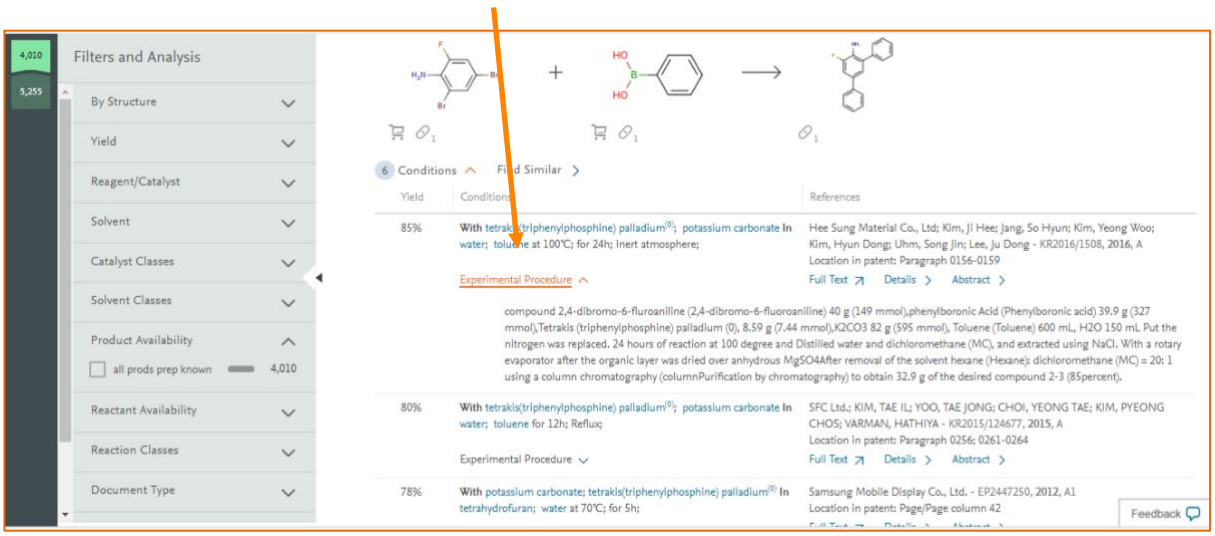
Reaxys will return over 5,000 results in response to this query. The reaction information includes yields, conditions and references.



To narrow the search down to reactions associated with experimental procedures, use the **Filter and Analysis** panel. Click on **Product availability** and choose **all prods prep known**.

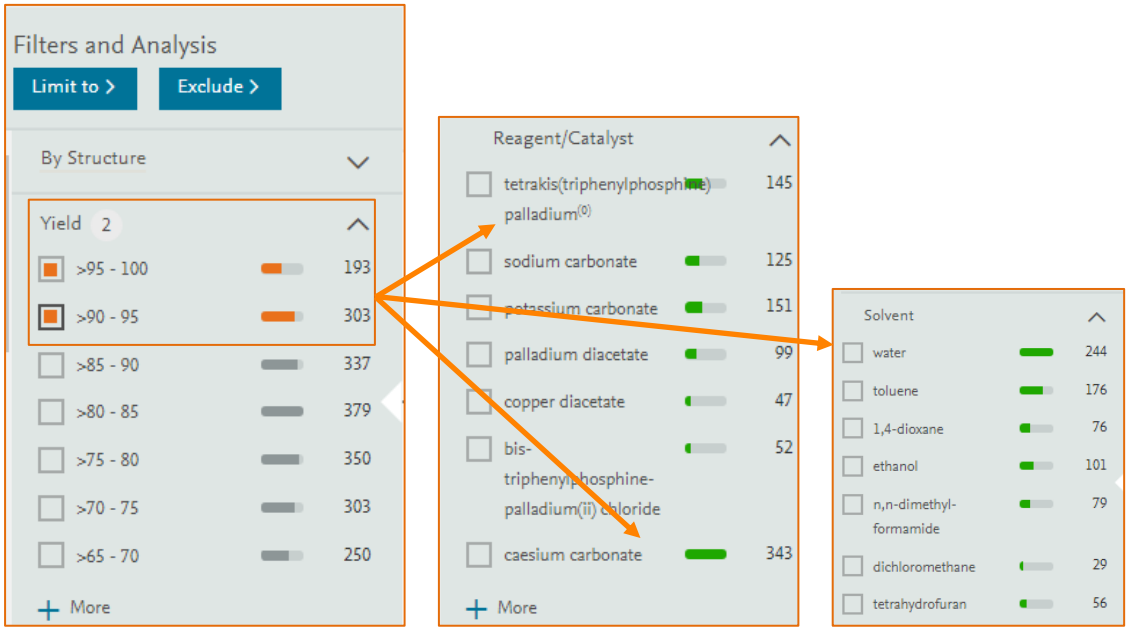


This returns 4,000 results where an experimental procedure is known.

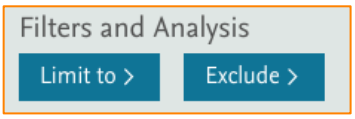


Further filtering is possible using the **Yield**, **Reagent/Catalyst** and **Solvent** filters.

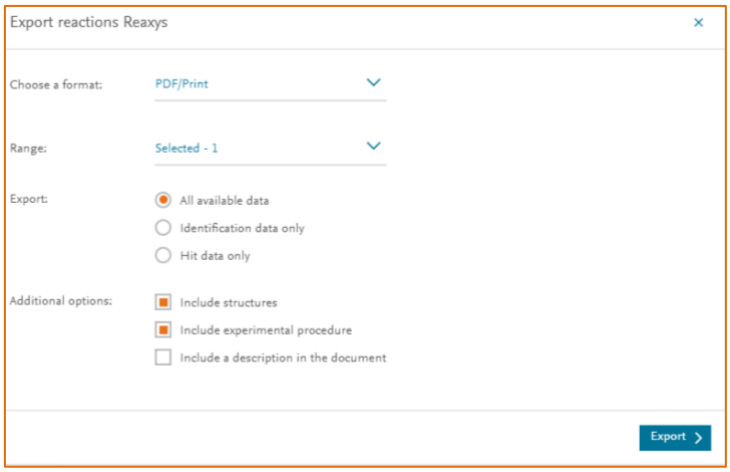
When a yield range is selected in the **Yield** filter (selections become orange), some of the options under **Reagent/Catalyst** and **Solvent** will turn green. This indicates that these are the most likely to give the selected yield.



When the selection is made, click **Limit to** to view the results with the selected conditions.



Note that results can be exported. Select the appropriate format, range and other options to ensure that the exported results are suitable for use in the intended cheminformatics tools.



Further information on using Reaxys can be found in the user guide in the Reaxys Support Center.