



Reaxys®

Workflow example

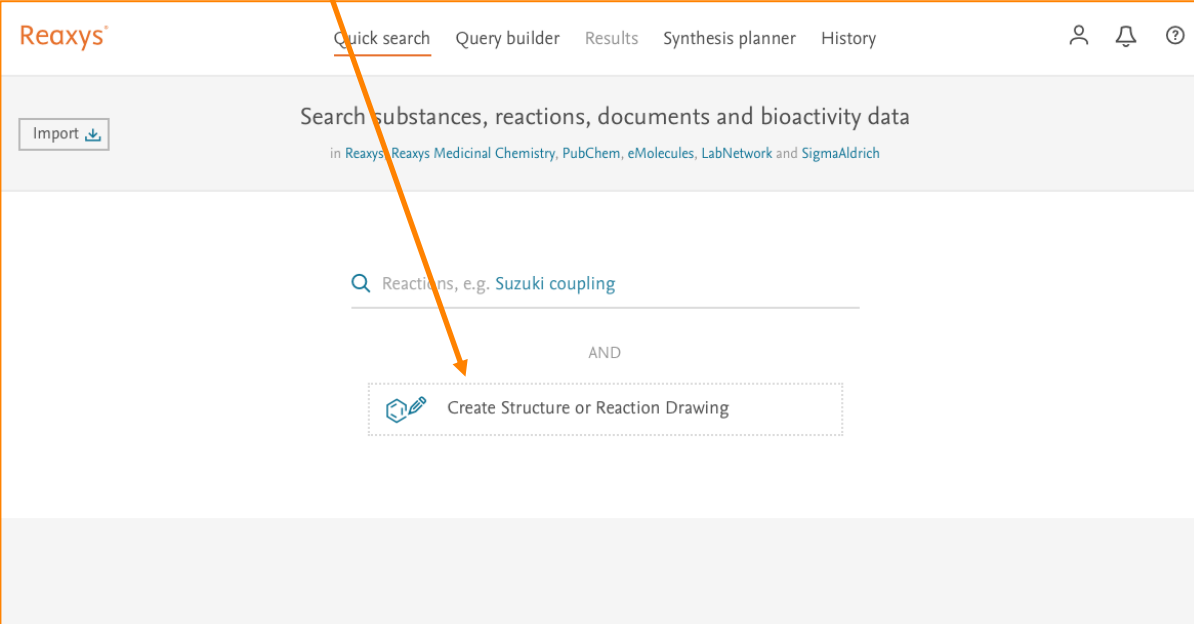
Finding reactions of substituted anilines with aryl boronic acids
and finding experimental preparations with optimal yields

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.



The screenshot displays the Reaxys Quick Search interface. At the top, the Reaxys logo is on the left, and navigation links for 'Quick search', 'Query builder', 'Results', 'Synthesis planner', and 'History' are in the center. On the right, there are icons for user profile, notifications, and help. Below the navigation bar, a search bar contains the text 'Reactions, e.g. Suzuki coupling'. To the left of the search bar is an 'Import' button with a download icon. Below the search bar, the word 'AND' is centered. A button labeled 'Create Structure or Reaction Drawing' with a drawing tool icon is highlighted with a dashed border and an orange arrow pointing to it from the text above.

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

Reaxys' Quick search Query builder Results Synthesis planner History Sign in

Structure editor Create structure template from name

Marvin JS by ChemAxon

Search this structure as:
 As drawn
 As substructure
 Similar

Tautomers
 Stereo
 Additional ring closures
 Related Markush
 Salts
 Mixtures
 Isotopes
 Charges
 Radicals
+ More options

Clear Cancel X Transfer to query Feedback

Create structure template from name

is Enter a chemical name, CAS-RN, InChiKey or SMILES boronic acid

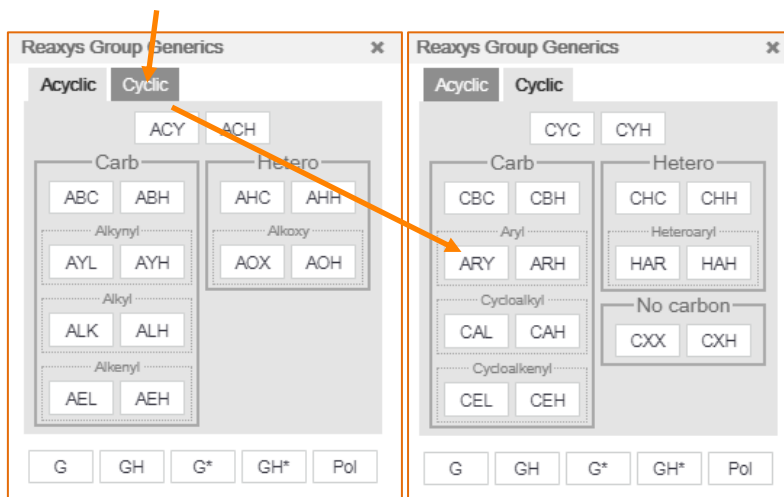
Structure editor Create structure template from name

Reaxys Group Generics

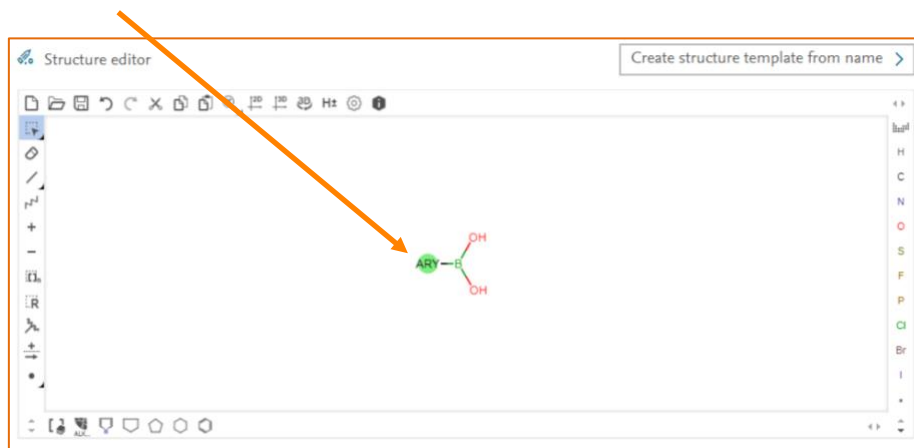
Clear Cancel X Transfer to query

Then click **Reaxys Group Generics**.

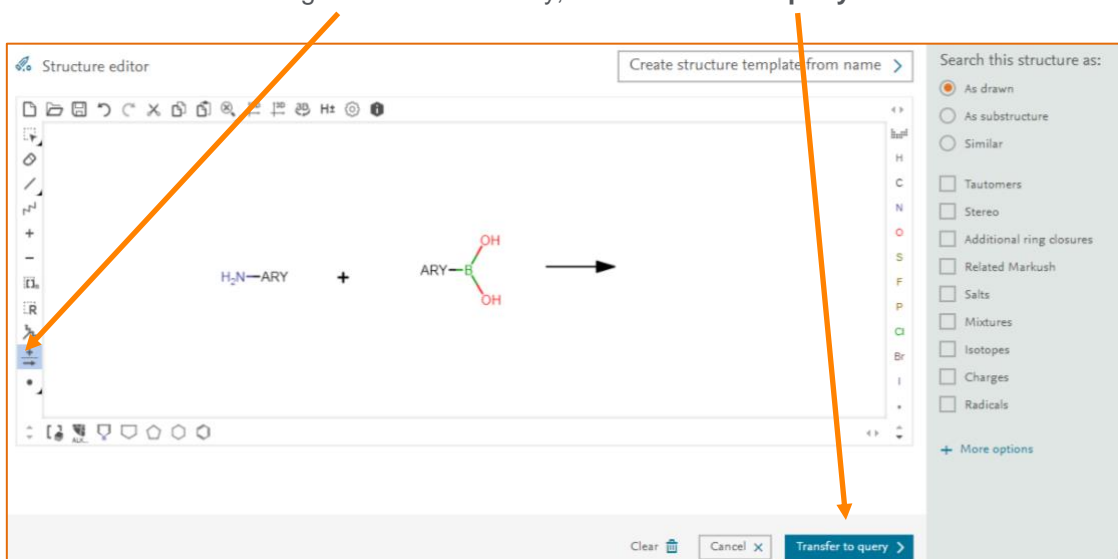
In the dialog boxes, select **Cyclic** and **Aryl**.



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.

5,255 Reactions out of 2,296 Documents containing 7,484 Substances, 1,146 Targets

0 selected Limit To Exclude Export Sort by Reaxys Ranking

Reaction ID: 8894173

1

15 Conditions Find Similar

Yield	Conditions	References
99%	With copper diacetate; potassium carbonate; benzoic acid In ethyl acetate at 20 - 80°C;	Wang, Xi; Jang, Hye-Young - Bulletin of the Korean Chemical Society, 2012, vol. 33, # 5, p. 1785 - 1787 Full Text Cited 5 times Details Abstract
96%	With Fe ₃ O ₄ magnetic nanoparticles-supported EDTA-copper(II) complex In water at 50°C; for 2h; Green chemistry;	Mostafalu, Ramin; Kaboudin, Babak; Kazemi, Foad; Yokomatsu, Tsutomu - RSC Advances, 2014, vol. 4, # 90, p. 49273 - 49279 Full Text Cited 10 times Details Abstract Feedback

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**.

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

The screenshot shows a search interface with a sidebar on the left titled "Filters and Analysis" containing various filter categories like "By Structure", "Yield", "Reagent/Catalyst", "Solvent", etc. The main area displays a chemical reaction scheme and a table of search results. An orange arrow points from the reaction scheme to the "Experimental Procedure" section of the first result.

Yield	Conditions	References
85%	With tetrakis(triphenylphosphine) palladium ⁰ ; potassium carbonate In water; toluene at 100°C; for 24h; Inert atmosphere;	Hee Sung Material Co., Ltd; Kim, Ji Hee; Jang, So Hyun; Kim, Yeong Woo; Kim, Hyun Dong; Uhm, Song Jin; Lee, Ju Dong - KR2016/1508, 2016, A Location in patent: Paragraph 0156-0159 Full Text > Details > Abstract >
80%	With tetrakis(triphenylphosphine) palladium ⁰ ; potassium carbonate In water; toluene for 12h; Reflux;	SFC Ltd.; KIM, TAE IL; YOO, TAE JONG; CHOI, YEONG TAE; KIM, PYEONG CHOS; VARMAN, HATHIYA - KR2015/124677, 2015, A Location in patent: Paragraph 0256; 0261-0264 Full Text > Details > Abstract >
78%	With potassium carbonate; tetrakis(triphenylphosphine) palladium ⁰ In tetrahydrofuran; water at 70°C; for 5h;	Samsung Mobile Display Co., Ltd. - EP2447250, 2012, A1 Location in patent: Page/Page column 42 Full Text > Details > Abstract >

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.

The screenshot shows the "Filters and Analysis" sidebar with the "Yield" filter set to ">90 - 95" (303 results). The "Reagent/Catalyst" and "Solvent" filters are updated with green indicators for the most likely reagents and solvents for this yield range.

Yield	Count
>95 - 100	193
>90 - 95	303
>85 - 90	337
>80 - 85	379
>75 - 80	350
>70 - 75	303
>65 - 70	250

Reagent/Catalyst	Count
tetrakis(triphenylphosphine) palladium ⁰	145
sodium carbonate	125
potassium carbonate	151
palladium diacetate	99
copper diacetate	47
bis-triphenylphosphine-palladium(II) chloride	52
caesium carbonate	343

Solvent	Count
water	244
toluene	176
1,4-dioxane	76
ethanol	101
n,n-dimethyl-formamide	79
dichloromethane	29
tetrahydrofuran	56

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

The screenshot shows the "Filters and Analysis" sidebar with the "Limit to" button highlighted in blue.

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.

Export reactions Reaxys

Choose a format: PDF/Print

Range: Selected - 1

Export:

- All available data
- Identification data only
- Hit data only

Additional options:

- Include structures
- Include experimental procedure
- Include a description in the document

Export >

Further information on using Reaxys can be found in the user guide in the [Reaxys Support Center](#).