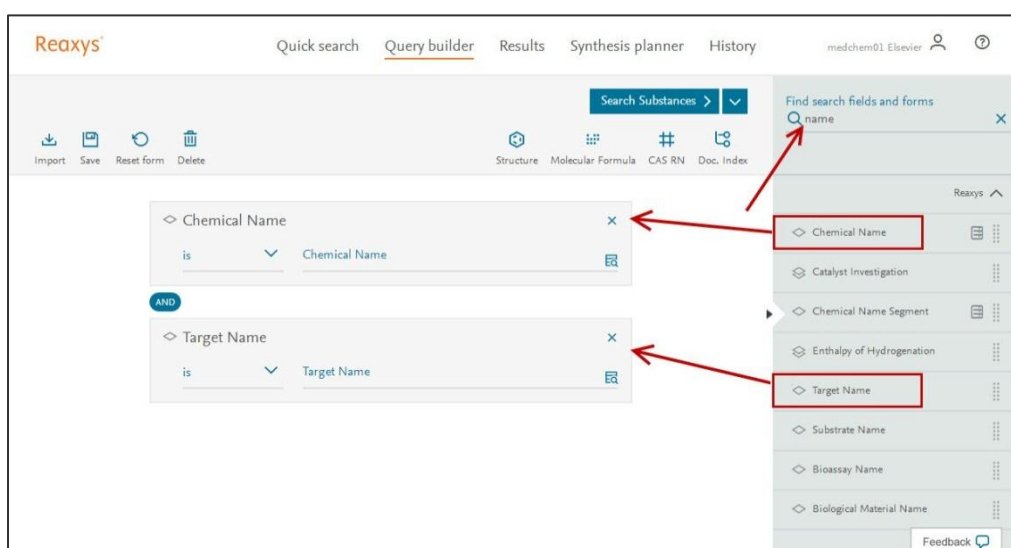


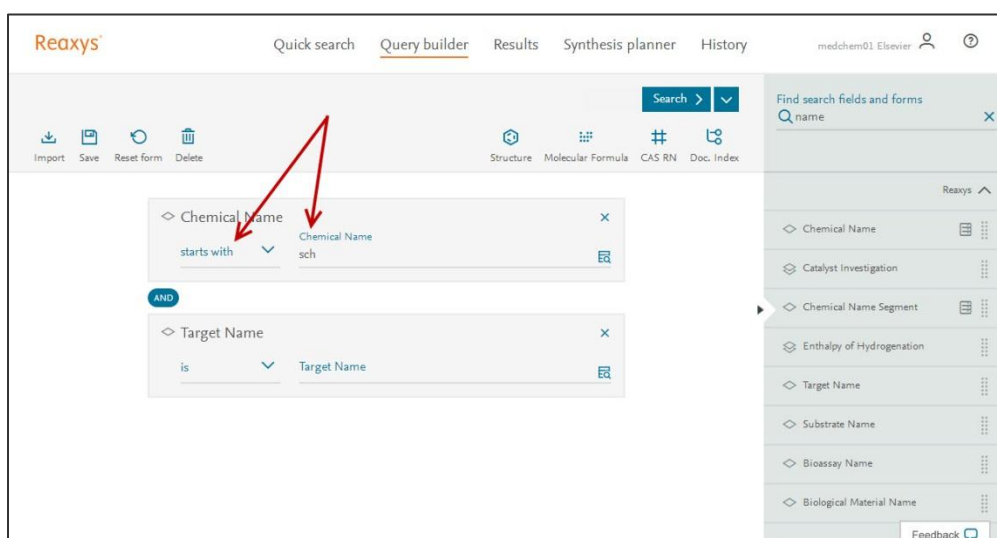
How do I find molecules having a code number like “SCH” that have been tested as ligands of the Dopamine receptors?

❖ Define Search Query

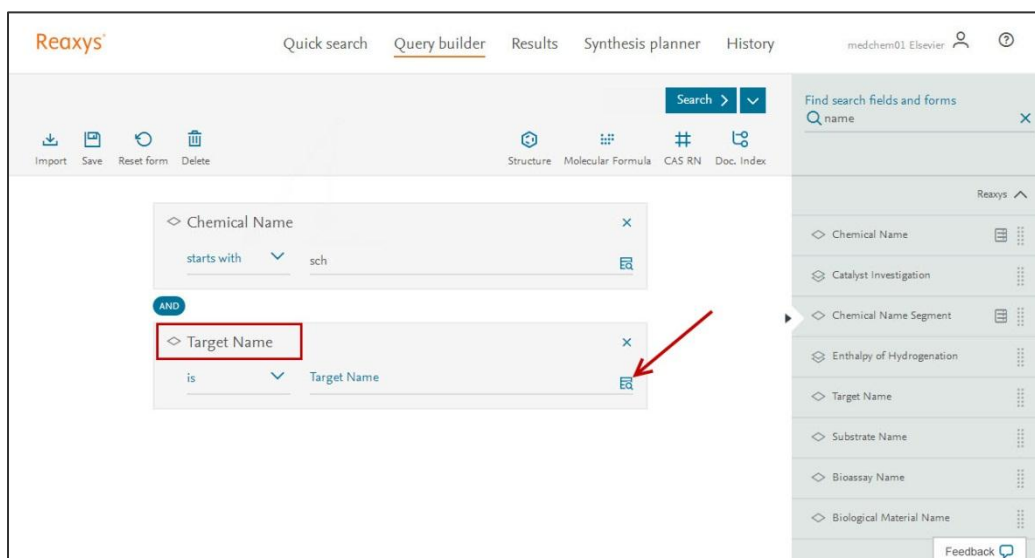
1. Click **Query builder**
2. In the **Find search fields and forms** field, type **name** – the list is filtered to include fields and forms that include the word **name**.
 - a. Drag and drop **Chemical Name** onto the Query builder
 - b. Drag and drop **Target name** onto the Query builder



3. Change the Chemical Name fields to **starts with sch**



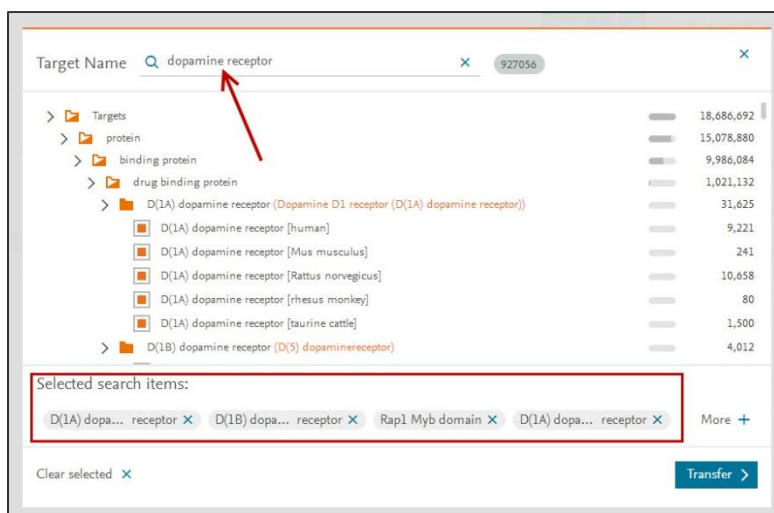
4. Click the **Lookup** tool for *Target Name*



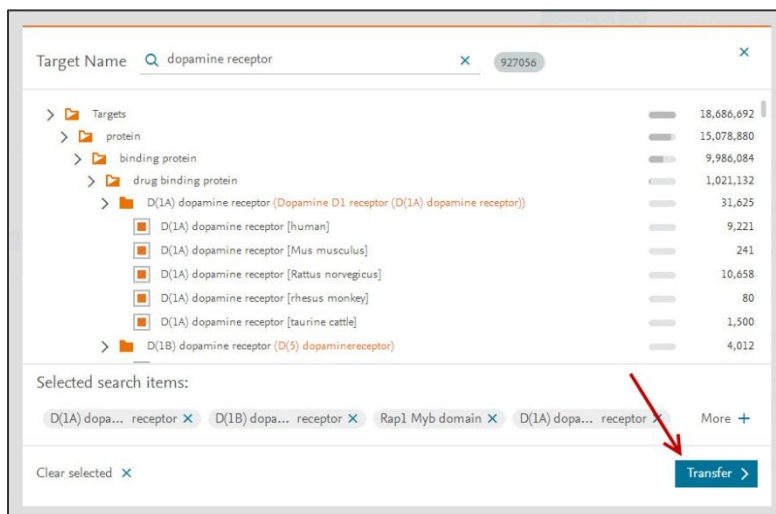
5. Search for **dopamine receptor** and press the **Enter key**

Note: The search in the Taxonomy is performed using a substring within the full name and the associated synonyms of the target. The searched term is highlighted in orange when found in synonyms and corresponding main terms are displayed as a flat list at the bottom of the page.

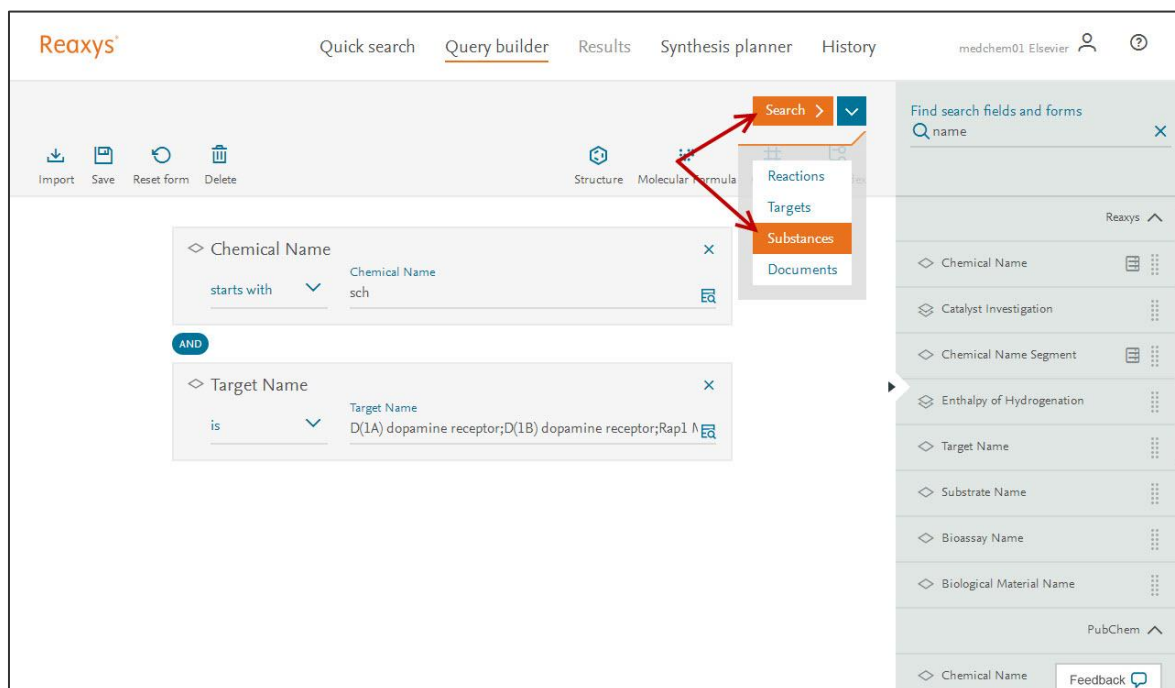
In the *Selected search items* section the term(s) can be deleted by clicking the blue 'X'. Numbers on the right hand side of the windows are counting bioactivities (data points) on the corresponding target or family of target.



6. Click **Transfer**



7. Click **Search** on the top of the screen and click the desired content (Reactions, Targets, Substances or Documents), in this case **Substances**.



You will retrieve substances having a name starting with “sch” and tested on the above-mentioned targets.

Reaxys® Quick search Query builder Results Synthesis planner History medchem01 Elsevier

29 Filters and Analysis

29 Substances out of 275 Documents, containing 114 Reactions, 100 Targets

By Structure Measurement pX Highest Clinical Phases Targets Parameters Substance Classes Molecular Weight Availability Availability in other databases Available Data Document Type

SCH 23390
C12H18ClNO 287.789 3620147 73445-63-3, 84384-04-3, 87075-17-0, 95191-55-2

8-chloro-3-methyl-5-phenyl-1,2,4,5-tetrahydro-3-benzepin-7-ol
C12H18ClNO 287.789 4323128 95191-55-2

Heatmap

❖ View the Heatmap

1. Click Heatmap
 - a. Review **Settings** and Click **Apply**.

Reaxys® Quick search Query builder Results Synthesis planner History medchem01 Elsevier

29 Filters and Analysis

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SCH 23390
C12H18ClNO 287.789 3620147 73445-63-3, 84384-04-3, 87075-17-0, 95191-55-2

8-chloro-3-methyl-5-phenyl-1,2,4,5-tetrahydro-3-benzepin-7-ol
C12H18ClNO 287.789 4323128 95191-55-2

Heatmap settings

Value of X-axis: Targets

Value of Y-axis: Substances

Value of Cells: Maximum of pX

Show substances: Names Structure drawing

Display mode: Normal Full Screen

Always show settings

Apply

The heatmap view will give you a visual display of selective substances.

