

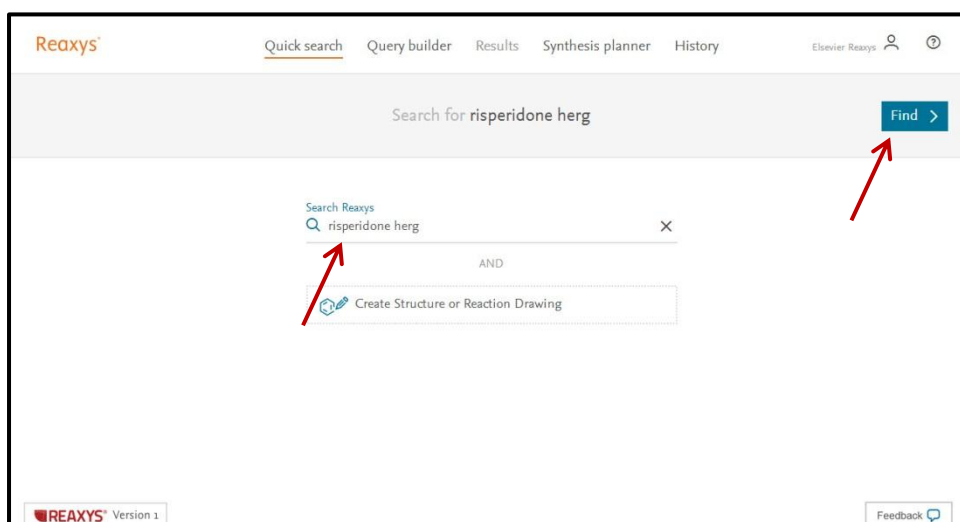
## Is my Compound of Interest Acting on hERG Channel?

Risperidone (trade name Risperdal, and generics) is an atypical antipsychotic drug which is mainly used to treat schizophrenia (including adolescent schizophrenia), schizoaffective disorder, the mixed and manic states associated with bipolar disorder, and irritability in people with autism.

Adverse effects of risperidone include significant weight gain and metabolic problems such as type 2 diabetes mellitus, as well as tardive dyskinesia and neuroleptic malignant syndrome. Risperidone and other antipsychotics also increase the risk of death in patients with dementia. Risperidone prolongs the QT interval (hERG related).

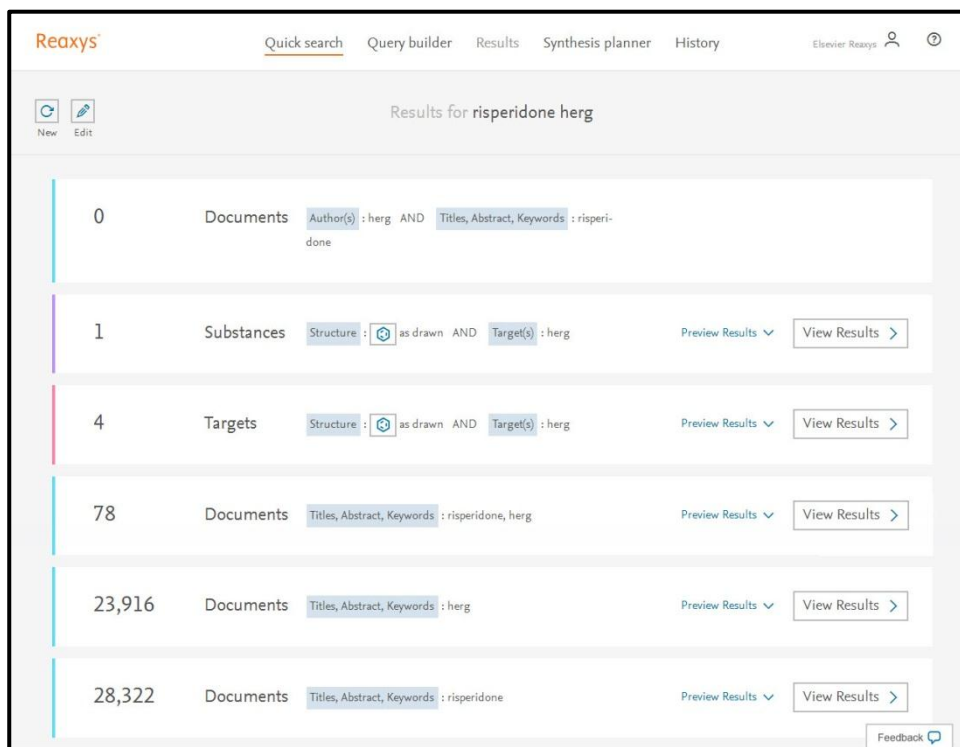
### ❖ Search using Quick search

1. On the Reaxys home page click the **Search Reaxys** field and type **risperidone hERG**
  - a. Click **Find** (or press **Enter** on your keyboard)



The Results Preview is displayed.

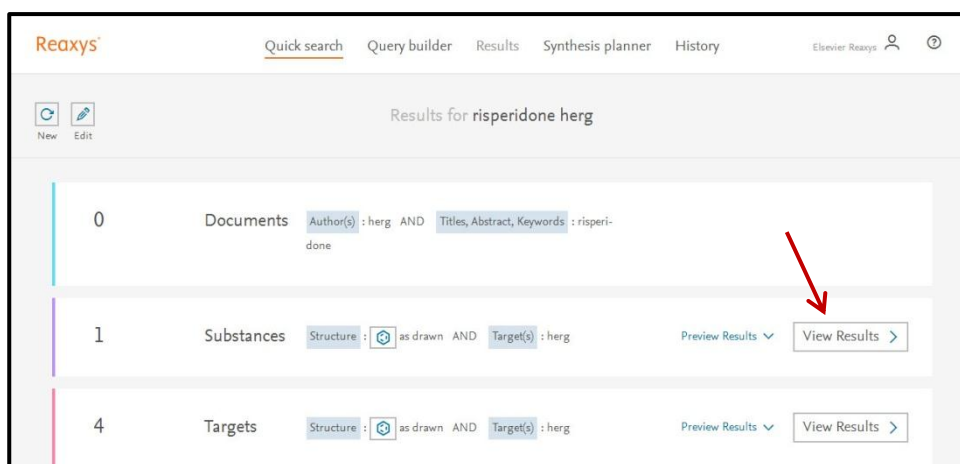
- In this case, Reaxys presents a Results Preview showing different variations of the entered query to provide you with options, which you may not have thought of at query formulation time.
- Quick search recognizes the abbreviated term *hERG* as a target by using the target taxonomy (main terms as well as synonyms are searched) and *Risperidone* is recognized as a Substance to retrieve substances tested on the corresponding target.



The screenshot shows the Reaxys interface with the search results for 'risperidone hERG'. The results are displayed in a list format with the following entries:

Count	Category	Query	Preview Results	View Results
0	Documents	Author(s) : hERG AND Titles, Abstract, Keywords : risperidone		
1	Substances	Structure : as drawn AND Target(s) : hERG	Preview Results	View Results
4	Targets	Structure : as drawn AND Target(s) : hERG	Preview Results	View Results
78	Documents	Titles, Abstract, Keywords : risperidone, hERG	Preview Results	View Results
23,916	Documents	Titles, Abstract, Keywords : hERG	Preview Results	View Results
28,322	Documents	Titles, Abstract, Keywords : risperidone	Preview Results	View Results

2. Click **View Results** for the *Substances* set to retrieve hERG results for Risperidone.



This screenshot is identical to the previous one, but with a red arrow pointing to the 'View Results' button for the 'Substances' category (the second row in the results list).

The Substances Results Page is displayed showing Risperidone.

The screenshot shows the Reaxys interface with the 'Results' tab selected. The main content area displays '1 Substances out of 37 Documents, containing 22 Reactions, 4 Targets'. The substance 'Risperidone' is listed with its chemical structure and CAS number. A red box highlights the 'Bioactivity (Hit Data)' link in the list of categories.

3. Click **Bioactivity (Hit Data)** for Risperidone to view the Bioactivities.

This screenshot shows the 'Bioactivity (Hit Data)' page for Risperidone. A red arrow points to the 'Bioactivity (Hit Data)' link in the list of categories, which is now expanded to show sub-categories.

The Bioactivity Categories are displayed:

The screenshot shows the expanded 'Bioactivity (Hit Data)' section. The categories are listed as follows:

- ^ Bioactivity (Hit Data)
  - ∨ In vitro: Efficacy - 58
  - ∨ Toxicity/Safety Pharmacology - 2
- ∨ Bioactivity (All)
- ∨ Physical Data - 26
- ∨ Spectra - 20
- ∨ Other Data - 761

The 'Bioactivity (Hit Data)' category is highlighted with a red box.

- Click a category, such as **In vitro: Efficacy** to display the corresponding bioactivities affinity on hERG (Potassium voltage gated channel subfamily H Member 2).

The screenshot shows the Reaxys 'Results' page. On the left is a 'Filters and Analysis' sidebar. The main content area shows a tree view under 'Bioactivity (Hit Data)' with 'In vitro: Efficacy - 58' selected. Other categories include 'Toxicity/Safety Pharmacology - 2', 'Bioactivity (All)', 'Physical Data - 26', 'Spectra - 20', and 'Other Data - 761'. The footer contains Elsevier and RELX Group logos and copyright information.

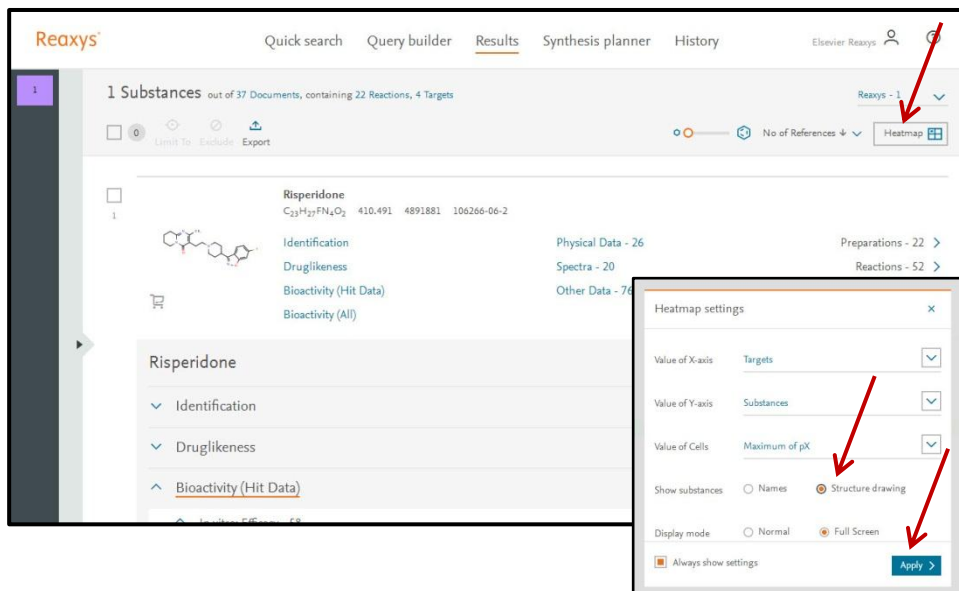
The results are displayed in table view when the results are quantitative (shown below) and in a text view when qualitative.

The screenshot shows the 'Quantitative Results' table for 'In vitro: Efficacy - 58'. The table has columns for pK, Parameter, Value (qual), Value (quant), Unit, Target, and Reference. The pK values are highlighted in green.

pK	Parameter	Value (qual)	Value (quant)	Unit	Target	Reference
8.8	IC50		1.6	nM	Potassium voltage-gated channel subfamily H member 2 [human]:Wild	Mow, Tomas; Frederiksen, Kristen; Thomsen, Morten B - European Journal of Pharmacology, 2015, vol. 748, p. 10 - 17 Full Text <a href="#">↗</a> Cited 2 times <a href="#">↗</a> Show details <a href="#">↗</a>
6.85	IC50		0.14	µM	Potassium voltage-gated channel subfamily H member 2 [human]:Wild	Roche, Olivier; Trube, Gerhard; Zuegge, Jochen; Pflimlin, Pascal; Alanine, Alexander; Schneider, Gisbert - ChemBioChem, 2002, vol. 3, # 5, p. 455 - 459 Full Text <a href="#">↗</a> Cited 146 times <a href="#">↗</a> Show details <a href="#">↗</a>
6.85	pIC50		6.85		Potassium voltage-gated channel subfamily H member 2 [human]:Wild	Choe, Han; Nah, Kwang Hoon; Lee, Soo Nam; Lee, Han Sam; Lee, Hui Sun; Jo, Su Hyeon; Leem, Chae Hun; Jang, Yeon Jin - Biochemical and Biophysical Research Communications, 2006, vol. 344, # 1, p. 72 - 78 Full Text <a href="#">↗</a> Cited 51 times <a href="#">↗</a> Show details <a href="#">↗</a>
6.83	IC50		0.148	µM	Potassium voltage-gated channel subfamily H member 2 [human]:Wild	Elkins, Sean; Crumb, William J.; Dustan Sarazan; Wikel, James H.; Wrighton, Steven A. - Journal of Pharmacology and Experimental Therapeutics, 2002, vol. 301, # 2, p. 427 - 434 Full Text <a href="#">↗</a> Cited 226 times <a href="#">↗</a> Show details <a href="#">↗</a>

## ❖ View the Heatmap

1. Scroll to the top and click **Heatmap**.
  - a. Review the Settings, turn on **Structure drawing** and click **Apply**.



The Heatmap view of Risperidone Bioactivities on hERG is displayed.

- b. Hover over **Potassium voltage-gated channel subfamily E member 1** to display the *Target complex details*.

