

Self guided Tour

Reaxys Medicinal Chemistry

IS MY COMPOUND OF INTEREST ACTING ON HERG CHANNEL?

<http://beta.reaxys.com>

 **REAXYS**[®]
Medicinal Chemistry

IS MY COMPOUND OF INTEREST ACTING ON HERG CHANNEL?

1.1 Scenario

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).

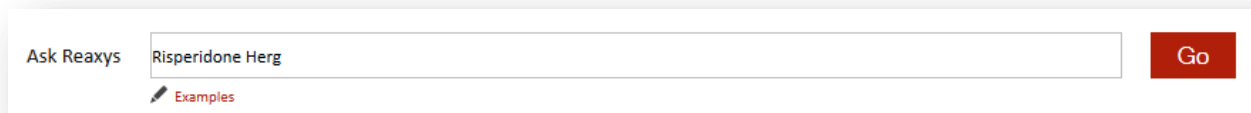
Search whether risperidone was tested on Herg (Kv11.1)?

1.2 Step by step

The screenshot displays the Reaxys search interface. At the top, there is a navigation bar with tabs: Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, Help, Live Chat, and Logout. Below the navigation bar, there is a search bar with the placeholder text "Enter a keyword, concept or author" and a "Go" button. Below the search bar, there is a section titled "Find substances, reactions, bioactivity data, citations, patents, and more from Reaxys, PubChem, and eMolecules". Below this section, there are five category buttons: Reactions (with a flask icon), Substances, Names, Formulas (with a molecular structure icon), Medicinal Chemistry (with a target icon), Literature (with a book icon), and ReaxysTree (with a tree icon). Below these buttons, there is a section titled "You can also search directly by these common property groups:" with four buttons: Physical (with a cube icon), Spectra (with a spectrum icon), Natural Product (with a globe icon), and Advanced (with a magnifying glass icon).

Step 1 Search using Ask Reaxys

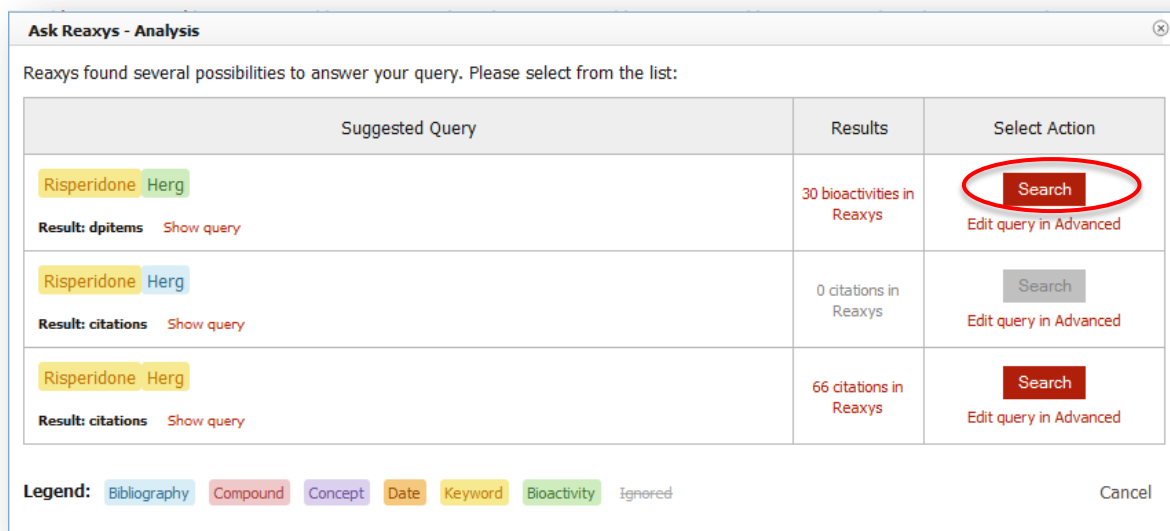
Type in Risperidone Herg and click on Go



Ask Reaxys recognize 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 Subto retrieve substance tested on the corresponding target.

A dialogue box is displayed because Ask Reaxys found several possibilities to answer to your query Choose the most relevant one.

In our case we will select the first one where Herg was recognized as part of the bioactivity concept.

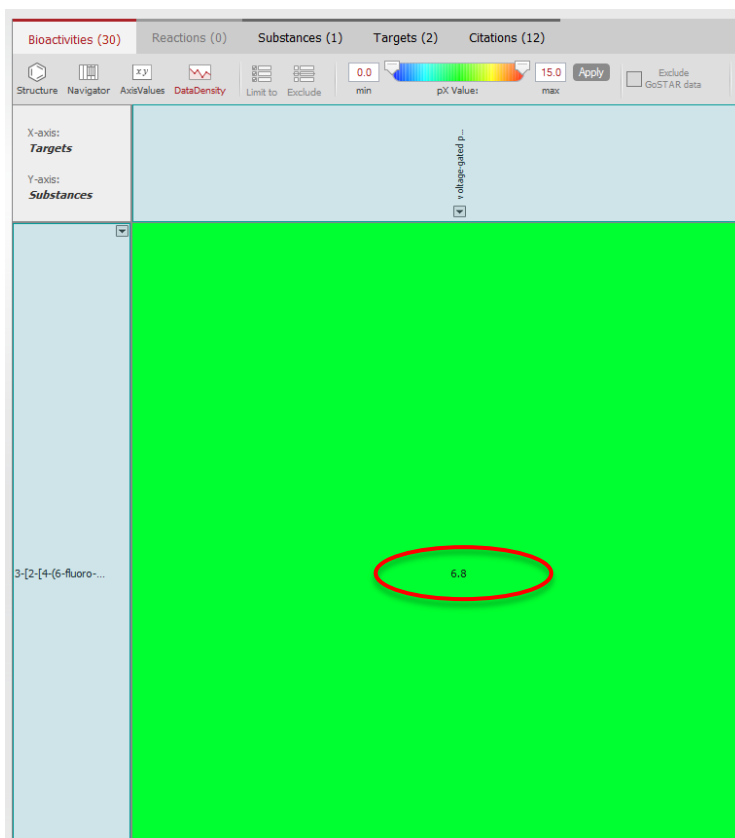


Suggested Query	Results	Select Action
Risperidone Herg Result: dpitems Show query	30 bioactivities in Reaxys	Search Edit query in Advanced
Risperidone Herg Result: citations Show query	0 citations in Reaxys	Search Edit query in Advanced
Risperidone Herg Result: citations Show query	66 citations in Reaxys	Search Edit query in Advanced

Legend: Bibliography Compound Concept Date Keyword Bioactivity Ignored

Cancel

Heatmap is displayed showing Risperidone activity on Herg Voltage gate potassium Channel (Kv11.1)

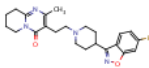


Step 2 : Click on the cell to access Risperidone Bioactivities on Herg

Heatmap Cell Details Page 1 of 1

6.80 X-axis: Targets Y-axis: Substances Select value type: MAX 1 substances and 30 bioactivities

Structure



Hide Details

Chemical Names and Synonyms
 3-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-6,7,8,9-tetrahydro-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one, [3H]-Risperidone, Risperidone, RISPERDAL®, risperidone, Risperdal, RIS

Drug likeness

Bioactivity

In vitro: Efficacy (30)

Quantitative Results

Parameter	Value (qual)	Value (quant)	Unit	Target	Target subunit	Target Species	Tissue/Organ	Cell	Bioassay	Dose	Effect	Reference
IC50		167	nM	Voltage-gated potassium channel	Kv11.1	Human		CHO	Electrophysiology	1.00000E-10 M		European Title/Abstract

Substance View Close

For more information please Contact

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