

## Self guided Tour

---

### Reaxys Medicinal Chemistry

---

**WHICH SUBSTANCES ARE THE MOST ACTIVE ON MY  
TARGET (HUMAN) OF INTEREST ?**

# WHICH SUBSTANCES ARE THE MOST ACTIVE ON MY TARGET (HUMAN) OF INTEREST ?

## 1.1 Scenario (New Project)

New project focused on finding new AKT1 inhibitors with less affinity on AKT2 (minimizing adverse effect)

- Akt is associated with tumor cell survival, proliferation, and invasiveness.
- The activation of Akt is also one of the most frequent alterations observed in human cancer and tumor cells.
  - Akt1 has been implicated as a major factor in many types of cancer
  - Akt2 is an important signaling molecule in the Insulin signaling pathway
  - The role of Akt3 is less clear, though it appears to be predominantly expressed in the brain

Therefore, understanding Akt and its pathways is important for the creation of better therapies to treat cancer and tumor cells.

### Search for active chemotype on AKT1?

## 1.2 Overview

Step no.	Steps and description	Action
1	Search by Bioactivity	Click 'Bioactivity' button
2	Select 'Target Name'	Type 'AKT' in the 'Target Name' field and select akt1, and push 'Search Bioactivities' button
3	Sort compounds by descending bioactivities on Target	Click on AKT1 column and sort descending
4	Filter by 'Target Species'	Filter by 'Target Species', select 'human', then click on 'Limit to'
5	Filter by 'pX'	Filter by 'pX(-log(Affinity)), move the bar to ca > 9, then click on 'Limit to'
6	Click on Substance (grid)	Will display all the most active compounds on AKT1
7	Save results	Click on 'Output'

## 1.3 Step by step

REAXYS®

Anonymous user (145.36.182.120)

Query Results Synthesis Plans History Report My Alerts My Settings Help Register Login

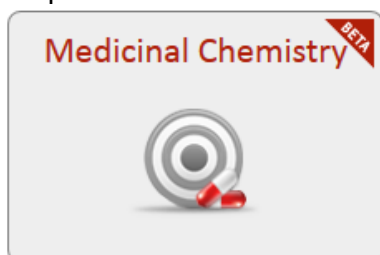
Ask Reaxys Enter a keyword, concept or author Go

Find substances, reactions, bioactivity data, citations, patents, and more from Reaxys, PubChem, and eMolecules

Reactions Substances, Names, Formulas Medicinal Chemistry Literature ReaxysTree

You can also search directly by these common property groups: Physical Spectra Natural Product Advanced

### Step 1 Search Medicinal Chemistry



### Step 2 Select a Target

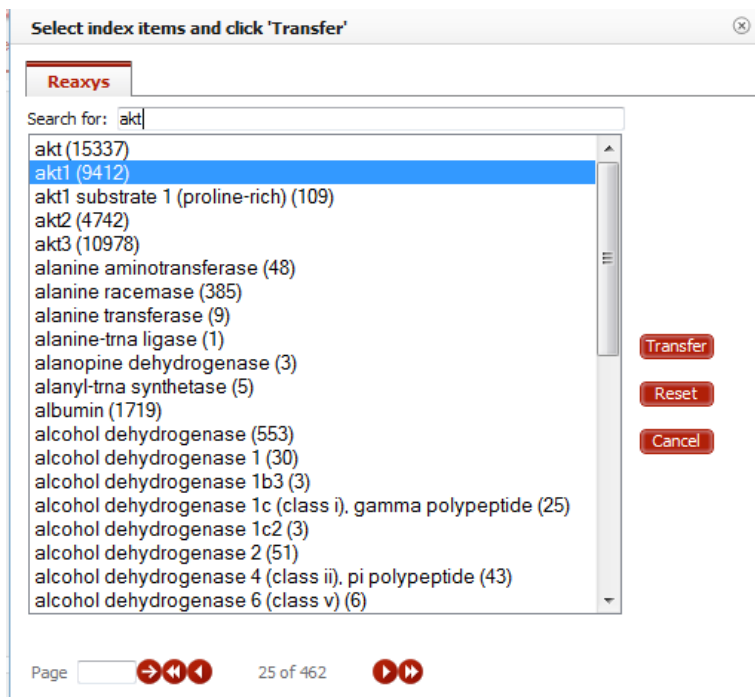
On target Name click on “look up”

Bioactivities

Substance Route	is		Lookup X
Bioassay Category	is		Lookup X
Putative action on target	is		Lookup X
Effect	is		Lookup X
Cells/Cell lines	is		Lookup X
Organs/Tissues	is		Lookup X
Target Name	is		Lookup X
Target Subunit Name	is		Lookup X
Target Nature	is		Lookup X
Species	is		Lookup X
pX	=		Lookup X

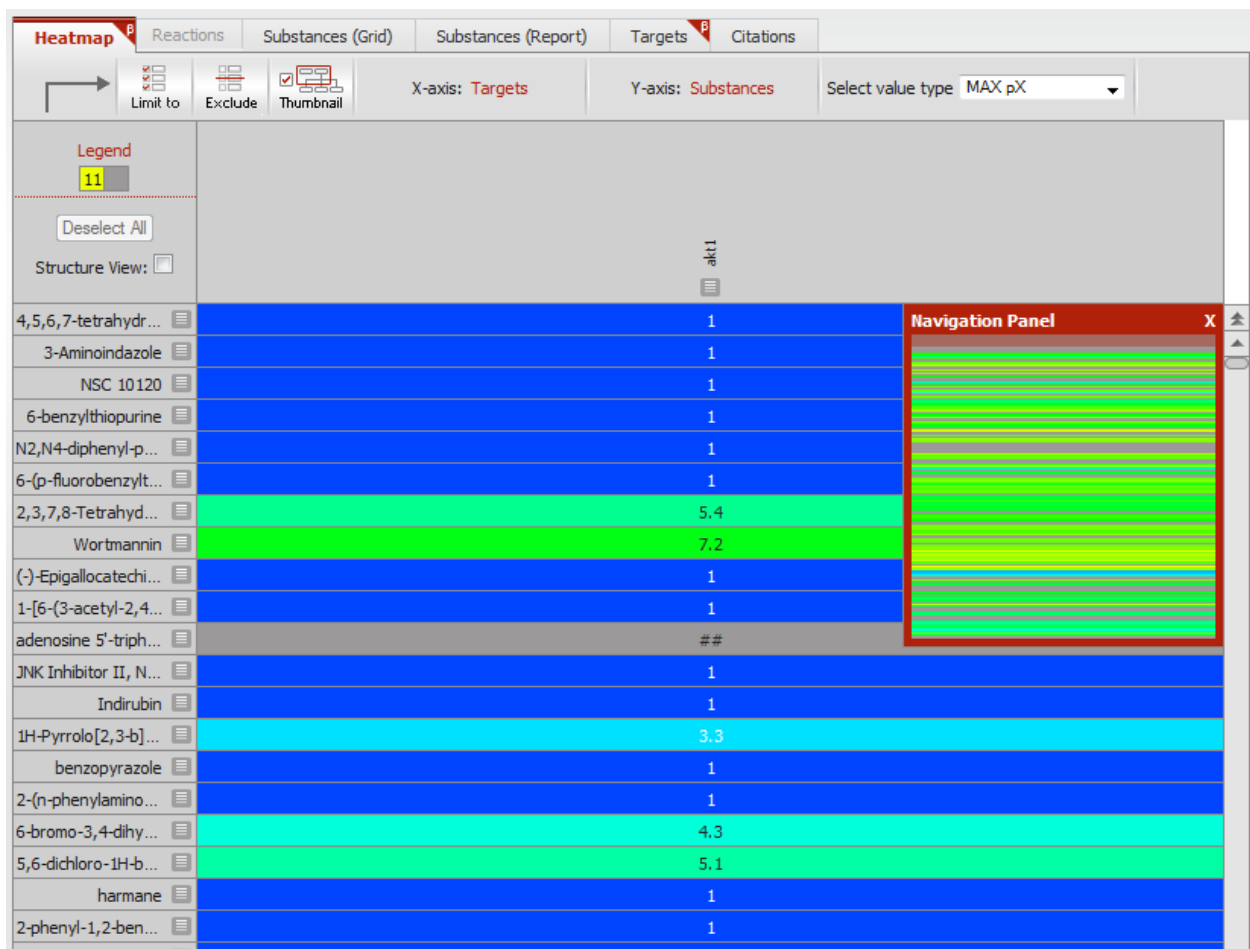
Show AND Buttons

A new popup appear and Search for AKT  
Select AKT1 and Click on transfer




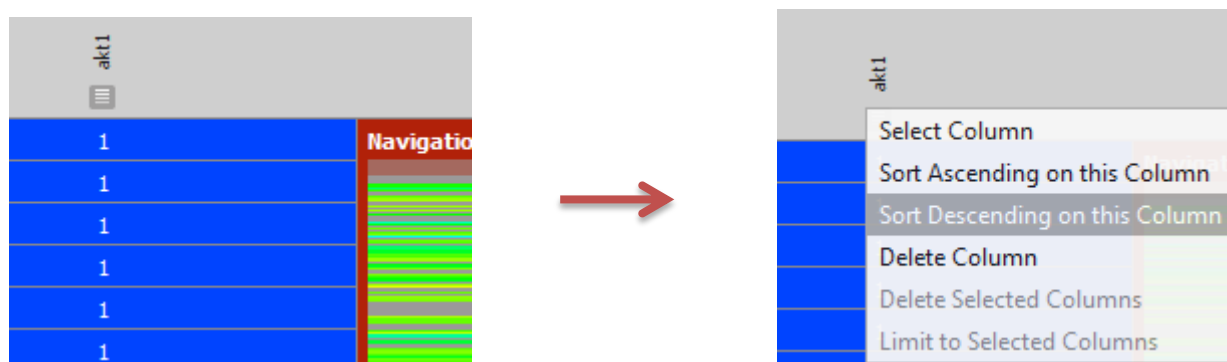
Step 3 Search for bioactivities

Step 4 : A full heatmap will appear with compounds tested on AKT1

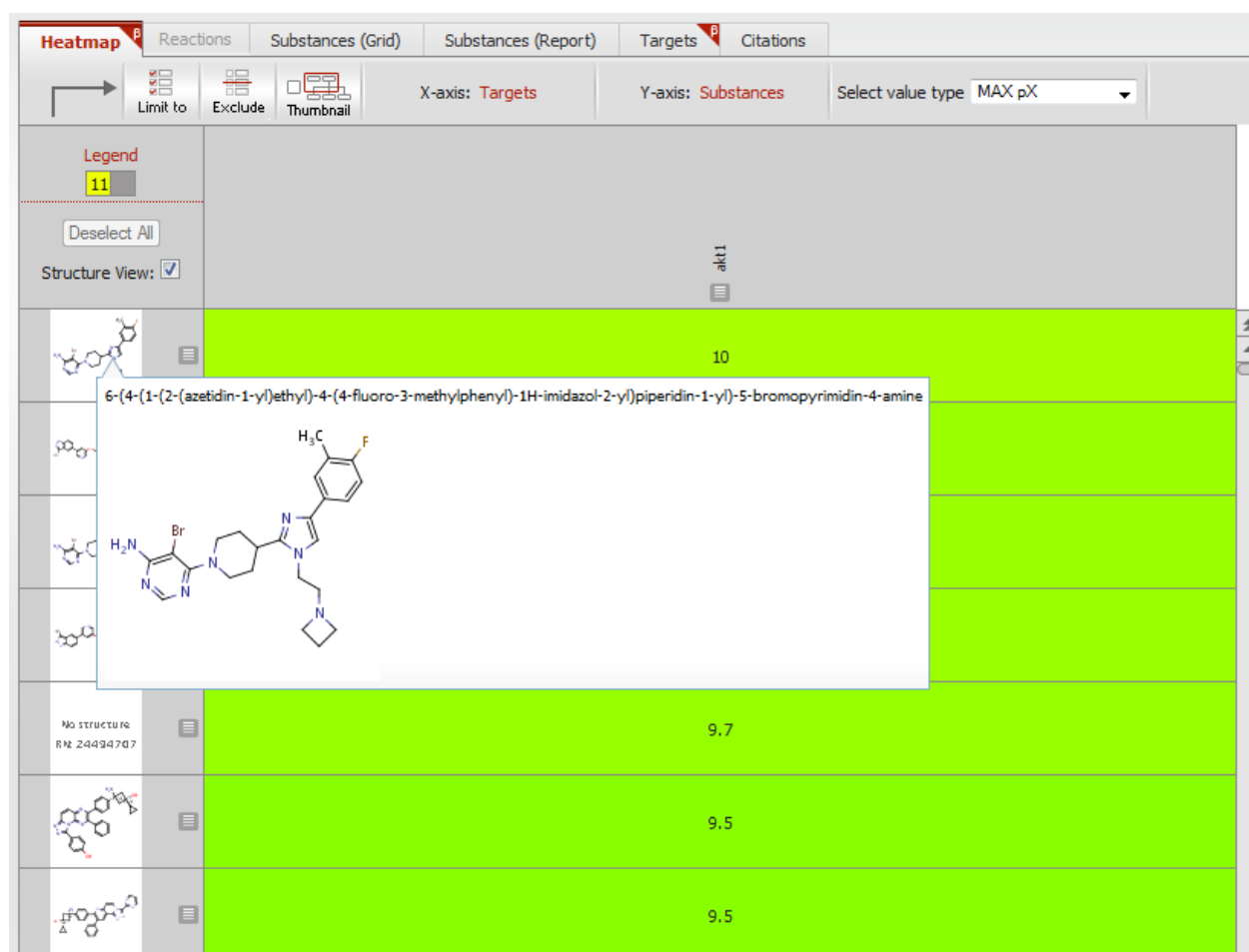


Step 5 : Sort compounds by descending bioactivities on AKT1

Click on the caspase 3 button  and select “sort descending on this column” See Below.

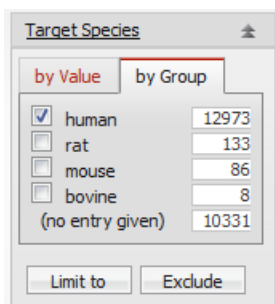


The most active compounds will be on the top of the Heatmap



Step 6 : Filter by Target Species

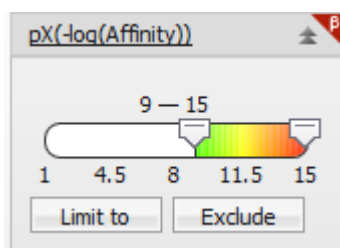
On the left had side click on “Target species” select human and click on “Limit to”



A new heat map will appear with the AKT1 target

Step 6 : Retrieve Active compounds by filtering by pX value >9

Move the cursor to the right without releasing the mouse button and click on “Limit to”



Heat map will appear with the most active compounds on AKT1

Step 9: Retrieve all the compounds active on AKT1 family by clicking on the “Substances grid”

The screenshot shows a software interface with a 'Substances (Grid)' tab. The grid contains six cards, each representing a different compound. Card 2 is highlighted with a blue border and labeled 'Chemotype 1'. Below the grid, a large chemical structure of Chemotype 1 is displayed. The structure consists of a central piperidine ring connected to a benzimidazole ring on the left and a pyrroloindole ring on the right. The piperidine ring has a methyl group at the 2-position and a propyl chain at the 4-position. The propyl chain has an amino group at the end.

For more information please Contact

**E-Customer Service**

Theodor-Heuss-Allee 108  
60486 Frankfurt/Main, Germany  
Tel: +49-69-5050 4268

Email: [pharmabiotechEH@elsevier.com](mailto:pharmabiotechEH@elsevier.com)