

Reaxys Alerting and History

Reaxys Alerting and History: how to save hitsets

reaxys.com



Introduction

Reaxys allows users who have logged into the system with their user name and password to create Alerts from queries and to store result sets via the History. Both Alerts and History Hitsets are stored on the Reaxys server and both contain the original source queries, which can be edited and retrieved via the Reaxys interface.

How to back-up and restore your created Reaxys Alerts?

All your saved Alerts are available from the My Alerts tab.

To create a new Alert perform a new search and click the 'Create Alert' link on the results page

Name	Query	Description	Date created	Last run	Frequency
23456_project Modify alert	 Edit query	Substances: As drawn Comment: Annelated Pyridine	2010-01-14	2012-02-13 hits: 1057 View results	Monthly
addex Modify alert	 Edit query	Substances: As drawn, Effect="anticancer" Comment: iryozeozopezo	2010-08-26	2010-08-26 hits: 26 View results	After each update
annearie Modify alert	 Edit query	Substances: As drawn	2010-09-24	2012-02-10 hits: 1 View results	After each update

A local back-up of your Alert can be obtained simply by storing the original query for the Alert on your local hard drive. Please follow these steps:

- Click the tab "My Alerts" and Reaxys will display a table listing your available Alerts together with the Query and the given result sets.
- Click on the *Edit Query* link displayed in the Query Column (second column). This will transfer the Alert query into the Query tab:

- Click the **Save query** button and enter the name of your Alert in the upcoming file save dialog box.
- Repeat this sequence for all Alerts.

If you want to restore the Alerts from the stored queries simply load the query via the Reaxys query tab and click the Search button. On the result page click the “Create Alert” hyperlink below the query breadcrumb and follow the dialog boxes


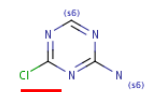

Your Alert will be active and available again in My Alerts.

How to back-up and restore permanent History entries?

When you are logged in, you can access both current and saved queries and hitsets from the History page.

The lower part of the table shows the hitsets, which you have stored manually so far, the 'Saved' hitsets. Please note: you may have stored hitsets from queries or from linking/filtering operations. The latter typically do not show any entry in the Query column and both require different procedures for a backup.

- Procedure for hitsets with a Query
 - Open the History tab and click the "Edit" hyperlink below the query shown in the query tab.

Query	Temporary result description	Date
4	123 reactions 59 citations	2012-02-29 13:41
2 1	 31924 substances Substances: As drawn 8947 citations	2012-02-29 13:37
5	 Markush 7692 substances	2009-04-15:03:58:16.047
6	 Christanetest 12485899 reactions	2010-03-26 11:24

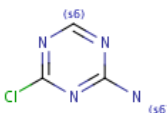
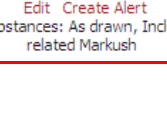
- Reaxys will load the query in the Query Tab and allows you to save it from there. Please do this for each query of permanent hitsets in your history.
-
- Procedures for hitsets without a query
 - For each of those saved hitsets, click on the **View** link; the hits are then displayed in the Result tab.

- Click on Output to export your hits as SDF file or as RDF file (do not forget that Export limits are set to 5000 for XML, SD, RD and SMILES formats, and 1000 for other file types; the Fact export limit is at 10000 occurrences: so it can be necessary to execute various batches).

- Save your SD or RD file with a name corresponding to the hitset name. Please note: it will not be possible to restore the history from those files.

To restore your history for saved queries login to Reaxys with your userID and password, and go to the Query tab. Click on the **Load Query/Batch** button, and open one of the previously saved hitset queries. Run the search (click on the **Search** button), view your results and change to the history tab. There click on the corresponding *Store* link, to save the hitset. Repeat this procedure for each stores hitset query.

The screenshot shows the Reaxys interface with the 'History' tab selected. At the top, there is a navigation bar with tabs: Query, Results, Synthesis Plans, History, My Alerts, My Settings, Help, Forum, and Info. Below the navigation bar, there is a 'Combine hitsets' section with a dropdown menu and the text 'Select at least two hitsets for combining'. The main content area is a table with the following columns: Query, Temporary result description, and Date. The table contains two rows of data. The first row shows a query with a chemical structure of 2-chloro-4,6-diazopyrimidine (SMILES: Clc1ncnc2ncc12) and a date of 2012-02-29 13:41. The second row shows a query with a chemical structure of 2-chloro-4,6-diazopyrimidine (SMILES: Clc1ncnc2ncc12) and a date of 2012-02-29 13:41. The 'Store' button for the second row is highlighted with a red box.

Query	Temporary result description	Date
<input type="checkbox"/> 4  Edit Create Alert Substances: As drawn, Include related Markush	123 reactions View	2012-02-29 13:41
<input type="checkbox"/> 3  Edit Create Alert Substances: As drawn, Include related Markush	59 citations View	

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