Reaxys®

Reaxys® Medicinal Chemistry

Usage Statistics

A guide to the usage statistics available to customers

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Available statistics

The Reaxys system generates three types of usage statistics, which provide information about the amount of stations, users, sessions, searches and exports per month.

Typically, the statistics are provided as a Microsoft® Excel® workbook with three worksheets:

- An overview sheet showing the overall usage per account and month
- User-based statistics showing the sessions, searches and exports per user
- IP-based statistics showing the sessions, searches and exports per identified public IP address

This document explains the details of the Reaxys and Reaxys Medicinal Chemistry statistics provided by Elsevier from 2022 onwards.

General account statistics

These statistics provide a general overview of usage of a given account. The general account provides monthly summary statistics for the current year for the information shown below.

Note: The statistics also contain information about batch and link-in searches and Retrosynthesis projects.

> **Batch search** is a special feature of Reaxys and Reaxys Medicinal Chemistry. It allows users to upload files containing multiple reaction, substance or citation queries. Each reaction, substance or citation query of such a batch file is counted as a single query. The numbers in the columns below provide additional information helping to differentiate searches performed in batch mode from regular searches. The searches are automatically added to the corresponding search columns.
>
> **Link-in searches** are searches that are triggered through a parametrized URL of Reaxys. Please refer to our support center for more details about this feature

Retrosynthesis can be started from each displayed structure in any result set by clicking the **Synthesize** hyperlink/icon. A click on **Create Retrosynthesis Plans** in the dropdown is counted as one single reaction search. Retrosynthesis can also be started from the Retrosynthesis page in Reaxys: draw a target molecule and click Synthesize will start a retrosynthesis project which is counted as a reaction search. (see also “Reaction searches via Retrosynthesis” for more details)

Department/Group Name = Elsevier internal customer identifier

Customer Name = Customer name

SISID = Elsevier internal customer ID

Total unique named users = total number of logged in users

Total unique anonymous users = total number of anonymous users

Year = 4-digit number, current year

Month = number for the counted month

Total Users = number of different users

Total Named Users = number of logged in users

Total Anonymous Users = number of anonymous users

Search Sessions = number of different sessions

Search Stations = number of different station IDs counted

All searches = number of all searches including reactions, substances, documents, bioactivity, and all batch searches

Searches Reactions = number of reaction searches (Reaxys)

R-Batch Searches = number of reaction searches performed in batch mode (Reaxys)

SynthesisPlan (published) = number of synthesis plans requested using published data (Reaxys)

SynthesisPlan (predicted) = number of predicted synthesis plans requested (Reaxys predictive Retrosynthesis)

Bioactivity Searches = number of bioactivity searches (Reaxys Medicinal Chemistry)

B-Batch Searches = number of bioactivity searches performed in batch mode (Reaxys Medicinal Chemistry)

Searches Substances = number of substance searches

S-Batch Searches = number of substance searches performed in batch mode

Searches Citations = number of document searches

C-Batch Searches = number of document searches performed in batch mode

Link-in Searches = number of searches triggered by the Reaxys/Reaxys Medicinal Chemistry Link-in feature (via URL)

Alert Searches = number of searches triggered by an Alert

History R/B/S/C searches = 0
Combined history searches are now performed using the Query Builder and therefore are counted as a reaction, substance, document or bioactivity search. The history searches field is kept for compatibility with older Reaxys usage reports.

R-Exports = number of times reaction data was exported

R-Exported = total number of reaction data exported

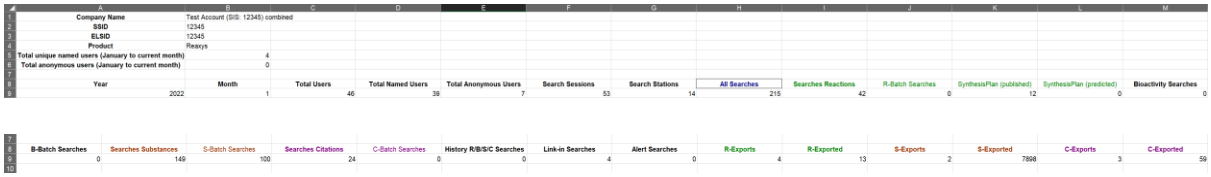
S-Exports = number of times substance data was exported

S-Exported = total number of substance data exported

C-Exports = number of times citation data was exported

C-Exported = total number of citation data exported

Figure 1. Example of general account statistics



	A	B	C	D	E	F	G	H	I	J	K	L	M
1	Company Name	Test Account (SIS: 12345) combined											
2	SSID	12345											
3	ELSID	12345											
4	Product	Reaxys											
5	Total unique named users (January to current month)	4											
6	Total anonymous users (January to current month)	0											
7													
8	Year	Month	Total Users	Total Named Users	Total Anonymous Users	Search Sessions	Search Stations	All Searches	Searches Reactions	R-Batch Searches	SynthesisPlan (published)	SynthesisPlan (predicted)	Bioactivity Searches
9	2022	1	46	39	7	53	14	215	42	0	12	0	0

	B-Batch Searches	Searches Substances	S-Batch Searches	Searches Citations	C-Batch Searches	History R/B/S/C Searches	Link-in Searches	Alert Searches	R-Exports	R-Exported	S-Exports	S-Exported	C-Exports	C-Exported
9	0	149	100	24	0	0	4	0	4	13	2	7898	3	59

User-specific statistics

These statistics provide an overview of the usage per user.

Anonymous users are counted as one if they access Reaxys or Reaxys Medicinal Chemistry with the same station ID. If anonymous users come in from different station IDs, then they are separated by sequential numbers. If a user logs into Reaxys or Reaxys Medicinal Chemistry during an anonymous session, then all searches performed after login are counted for that user ID.

Since the station ID is an arbitrary number stored in a cookie, it can be deleted at any time. This generates a new anonymous user ID, which is counted separately.

The following information is given:

Year = as for general account statistics

Month = as for general account statistics

User = user name (see note for general account statistics about anonymous users)

Search Sessions = as for general account statistics

Search Stations = as for general account statistics

All searches = as for general account statistics

Searches Reactions = as for general account statistics

R-Batch Searches = as for general account statistics

SynthesisPlan (published) = as for general account statistics

SynthesisPlan (predicted) = as for general account statistics

Bioactivity Searches = as for general account statistics

B-Batch Searches = as for general account statistics

Searches Substances = as for general account statistics

S-Batch Searches = as for general account statistics

Searches Citations = as for general account statistics

C-Batch Searches = as for general account statistics

Link-in Searches = as for general account statistics

Alert Searches = as for general account statistics

R-Exports = number of times reaction data was exported

R-Exported = total number of reaction data exported

S-Exports = number of times substance data was exported

S-Exported = total number of substance data exported

C-Exports = number of times citation data was exported

C-Exported = total number of citation data exported

Please see comment about batch searches under general account statistics.

Figure 2. Example of user-specific statistics

	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Year	Month	User	Search Sessions	Search Stations	All Searches	Searches Reactions	R-Batch Searches	SynthesisPlan (published)	SynthesisPlan (predicted)	Bioactivity Searches	B-Batch Searches	Searches Substances	S-Batch Searches
2	2022	1	83612fd6434300cb481	8	4	14	4	0	0	0	0	0	3	0
3	2022	1	9a007dbd30481e44d7f	4	4	14	2	0	0	0	0	0	6	0
4	2022	1	b82ad37210dd58cf0c9	8	2	33	3	0	0	0	0	0	23	0
5	2022	1	fee4ba3aea5754cd852	5	4	125	0	0	0	0	0	0	117	100

	O	P	Q	R	S	T	U	V	W	X	Y
1	Searches Citations	C-Batch Searches	History R/B/S/C Searches	Link-in Searches	Alert Searches	R-Exports	R-Exported	S-Exports	S-Exported	C-Exports	C-Exported
2	3	0	0	4	0	0	0	0	0	0	0
3	6	0	0	0	0	0	0	0	0	0	0
4	7	0	0	0	0	4	13	0	0	3	59
5	8	0	0	0	0	0	0	2	7898	0	0

IP address-specific statistics

Reaxys and Reaxys Medicinal Chemistry typically use IP authentication to identify a given account. However, several IP ranges may have been entered for a customer to reflect a license situation covering multiple sites or departments with different firewalls. Reaxys and Reaxys Medicinal Chemistry log the public IP address of incoming calls and usage statistics based on the IP addresses provided in this section.

Year = as for general account statistics

Month = as for general account statistics

User = user name (see note for general account statistics about anonymous users)

Search Sessions = as for general account statistics

Search Stations = as for general account statistics

All searches = as for general account statistics

Searches Reactions = as for general account statistics

R-Batch Searches = as for general account statistics

SynthesisPlan (published) = as for general account statistics

SynthesisPlan (predicted) = as for general account statistics

Bioactivity Searches = as for general account statistics

B-Batch Searches = as for general account statistics

Searches Substances = as for general account statistics

S-Batch Searches = as for general account statistics

Searches Citations = as for general account statistics

C-Batch Searches = as for general account statistics

Link-in Searches = as for general account statistics

Alert Searches = as for general account statistics

R-Exports = number of times reaction data was exported

R-Exported = total number of reaction data exported

S-Exports = number of times substance data was exported

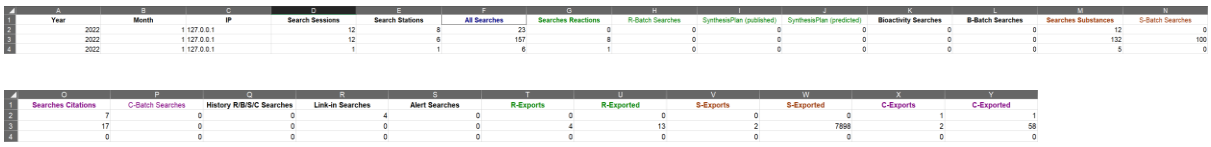
S-Exported = total number of substance data exported

C-Exports = number of times citation data was exported

C-Exported = total number of citation data exported

Please see comment about batch searches under general account statistics.

Figure 3. Example of IP address-specific statistics



	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Year	Month	IP	Search Sessions	Search Stations	All Searches	Searches Reactions	R-Batch Searches	SynthesisPlan (published)	SynthesisPlan (predicted)	Bioactivity Searches	B-Batch Searches	Searches Substances	S-Batch Searches
2	2022	1	127.0.0.1	12	8	23	0	0	0	0	0	0	12	0
3	2022	1	127.0.0.1	12	6	157	8	0	0	0	0	0	132	100
4	2022	1	127.0.0.1	1	1	6	1	0	0	0	0	0	5	0

	O	P	Q	R	S	T	U	V	W	X	Y
1	Searches Citations	C-Batch Searches	History R/B/S/C Searches	Link-in Searches	Alert Searches	R-Exports	R-Exported	S-Exports	S-Exported	C-Exports	C-Exported
2	7	0	0	4	0	0	0	0	0	1	1
3	17	0	0	0	0	4	13	2	7898	2	58
4	0	0	0	0	0	0	0	0	0	0	0

Definitions

1.1 Session definition

Reaxys and Reaxys Medicinal Chemistry count a session if an IP authentication is successful and the now anonymous user can see the query page directly after entering the Reaxys or Reaxys Medicinal Chemistry URL in a web browser OR after the user has logged into the system via user name and password. If an anonymous user logs into Reaxys or Reaxys Medicinal Chemistry after already using the system, then this is also counted as a new session until the user logs out or closes the browser.

1.2 Station definition

On first use, Reaxys and Reaxys Medicinal Chemistry generate an arbitrary station ID number that is stored in a cookie on the local workstation. The algorithm used ensures that there is a high probability that this number is always unique on a global basis. This station ID is sent to the Reaxys/Reaxys Medicinal Chemistry server with each successful session and enables Reaxys/Reaxys Medicinal Chemistry to distinguish different anonymous users. However, it cannot be used to identify anonymous users and if the cookie is deleted during normal browser hygiene operations, then a new station ID and new anonymous user are generated. For an IP authenticated environment, this is the only method possible to attain some level of insight into how many different users are using Reaxys and/or Reaxys Medicinal Chemistry.

1.3 Search definition

The core of the Reaxys and Reaxys Medicinal Chemistry usage statistics is the number of different searches counted by the system. In contrast to other systems, Reaxys and Reaxys Medicinal Chemistry have several ways of triggering an event that is counted as search and can therefore provide statistics for the different types of searches as outlined in the table below, in the **Object** column. Several of these objects will be counted together in different categories as outlined in the column **Count as**.

The following list shows the operation types counted as one search.

Object	Action	Counts as (type of search)
Reaction	Search Query Builder	Reaction Search (A)
Target	Search Query Builder	Bioactivity Search (A)
Substance	Search Query Builder	Substance Search (A)
Document	Search Query Builder	Document Search (A)
Reaction	Click “View Results” on results preview	Reaction Search (A1)
Target	Click “View Results” on results preview	Bioactivity Search (A1)
Substance	Click “View Results” on results preview	Substance Search (A1)
Documents	Click “View Results” on results preview	Document Search (A1)

Object	Action	Counts as (type of search)
Reaction	SearchBatch	Reaction Search (B)
Target	SearchBatch	Bioactivity Search (B)
Substance	SearchBatch	Substance Search (B)
Document	SearchBatch	Document Search (B)
ReactionDisplay	Apply Filter (Limit to, Exclude)	Reaction Search (C)
ReactionDisplay	Selection Filter (Limit to, Exclude)	Reaction Search (D)
TargetDisplay	Apply Filter (Limit to, Exclude)	Bioactivity Search (K1)
TargetDisplay	Selection Filter (Limit to, Exclude)	Bioactivity Search (K2)
SubstanceDisplay	Apply Filter (Limit to, Exclude)	Substance Search (C)
SubstanceDisplay	Selection Filter (Limit to, Exclude)	Substance Search (D)
DocumentDisplay	Apply Filter (Limit to, Exclude)	Document Search (C)
DocumentDisplay	Selection Filter (Limit to, Exclude)	Document Search (D)
SynthesisPlan (published)	Create Plan with option Published enabled	Reaction Search (E1)
SynthesisPlan (predicted)	Create Plan with option Predicted enabled	Reaction Search (F1)
Synthesize	Find Preparations	Reaction Search (A2)
Heatmap	Apply Filter (Limit to, Exclude)	Bioactivity Search (G)
Heatmap	Selection Filter (Limit to, Exclude)	Bioactivity Search (H)
Link-In	Open URL	Link-in
Alert	Scheduled Alert search	Alert

Number of reaction searches = reaction search (A) + reaction search (A1) + reaction search (A2) + reaction search (B) + reaction search (C) + reaction search (D) + reaction search (E1) + reaction search (F1)

Number of bioactivity searches = bioactivity search (A) + bioactivity search (A1) + bioactivity search (K1) + bioactivity search (K2) + bioactivity search (G) + bioactivity search (H)

Number of substance searches = substance search (A) + substance search (A1) + substance search (B) + substance search (C) + substance search (D)

Number of citation searches = document search (A) + document search (A1) + document search (B) + document search (C) + document search (D)

Number of all searches = number of reaction searches + number of bioactivity searches + number of substance searches + number of citation searches + Link-in searches + Alert searches

Note: Link-in and alert searches values are not discriminated by reaction, substance or citation mode of search. They are simply added to all the searches.

1.4 Export definition

Reaxys and Reaxys Medicinal Chemistry counts an export if the data is successful downloaded by a user from the Results page. User can download multiple result set in the desired format from the application.

Per result context system provide two export counts. First one is the number of times export is invoked and the second is the total number of rows that have been exported in a month.

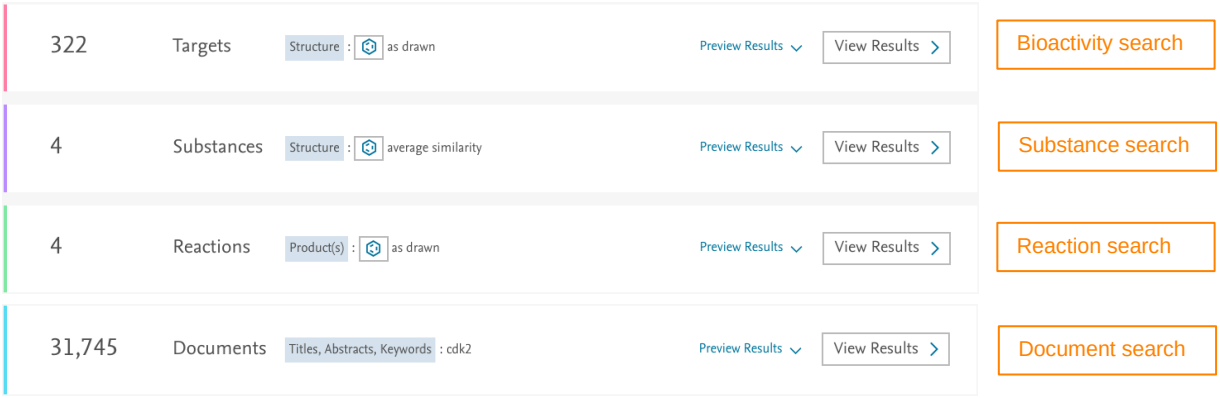
Note: Any export from the target and bioactivity page are accounted as substance exports in the statistics.

Examples

The following screenshots illustrate the events which trigger certain usage counts. They have been created from a product license for the combined Reaxys and Reaxys Medicinal Chemistry, which display together through a single interface to the user.

1.1 Reaction, substance, document and target search: basics

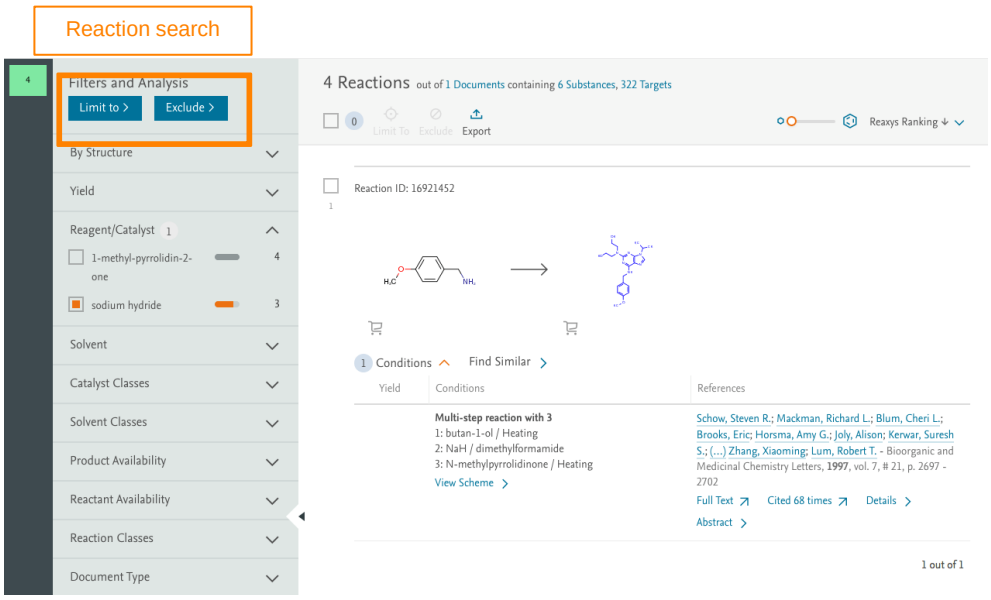
If the user starts from Quick Search, a Results Preview screen appears. Clicking on **View Results** in each case counts as the search type shown to the right of the screenshot. Clicking on **Preview Results** does not affect the search count.



1.2 Reaction, substance, document and target search: filters and Limit to/Exclude selection

On any given **Results** page, the user can define various filters by opening the desired topic in the **Filters** column and selecting from the presented values. As soon as the button **Limit to** or **Exclude** is clicked, a search is triggered and counted for the statistics. Depending on the result context, this filter application is either counted as substance, reaction, bioactivity or document search.

In this example, clicking **Limit to** or **Exclude** would add a new reaction search count because this is the results page for reaction searches

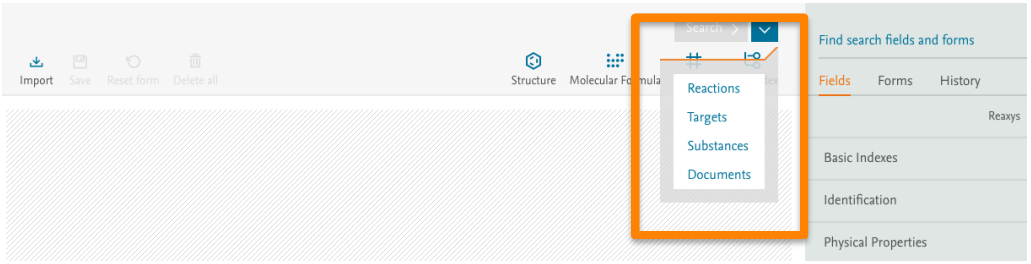


If the user browses through the hitset and selects several items in the **Filters** column, they can use the **Limit to** or **Exclude** option each time. Each application of this operation adds a new breadcrumb and is counted as a search in the respective context.

Note: If the user switches to the Documents results view from this **Reactions** screen and then applies a filter using the **Limit to** or **Exclude** option, this is counted as a document search, although the overall number of searches is the same.

1.3 Query Builder searches

The **Query Builder** provides users with the ability to flexibly create complex queries and search them in the desired context (Reactions, Targets, Substances or Documents, see the dropdown in the image below). A click on a search context adds a search count to the respective context search statistics.



Reaction search

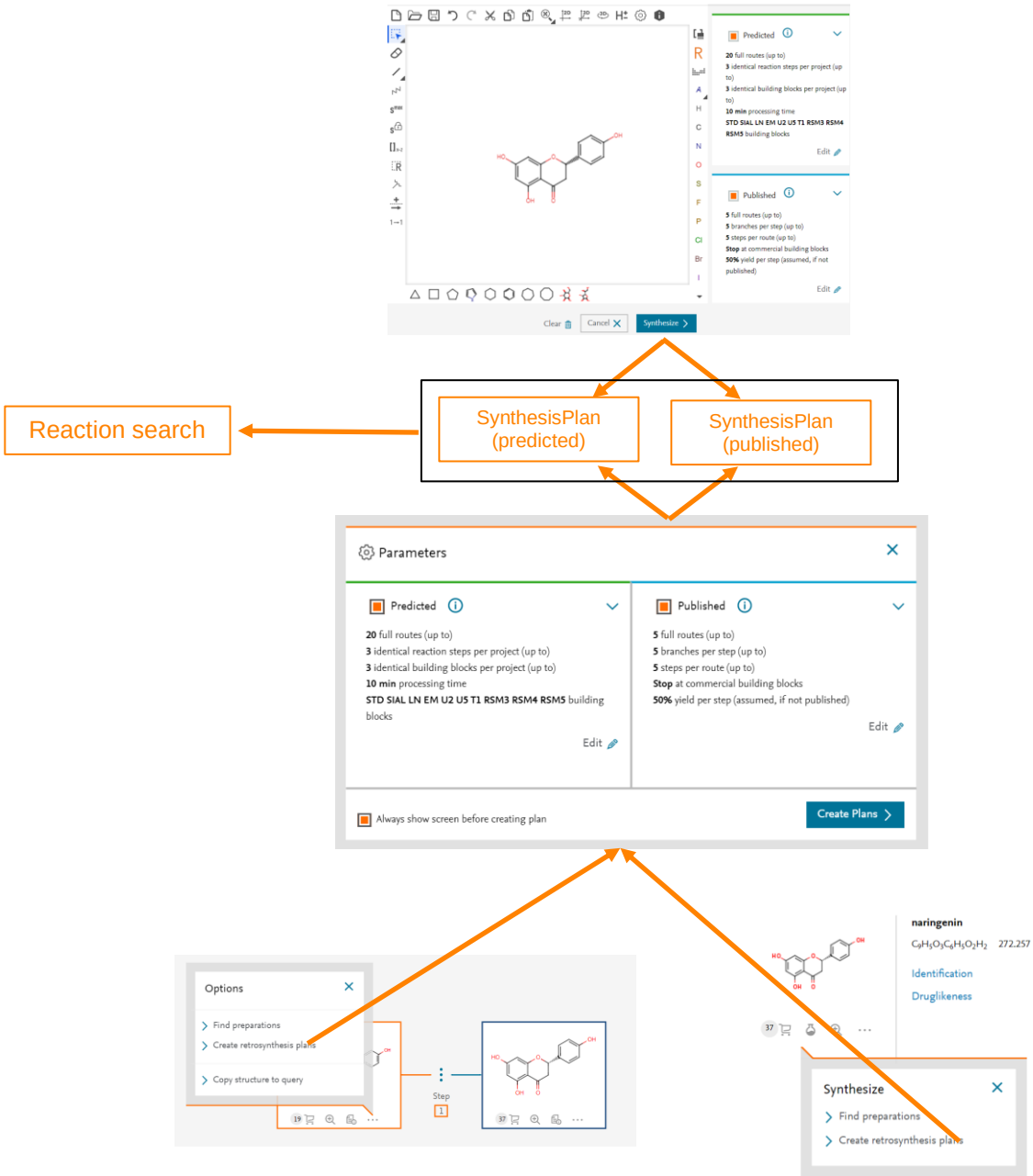
Bioactivity search

Substance search

Document search

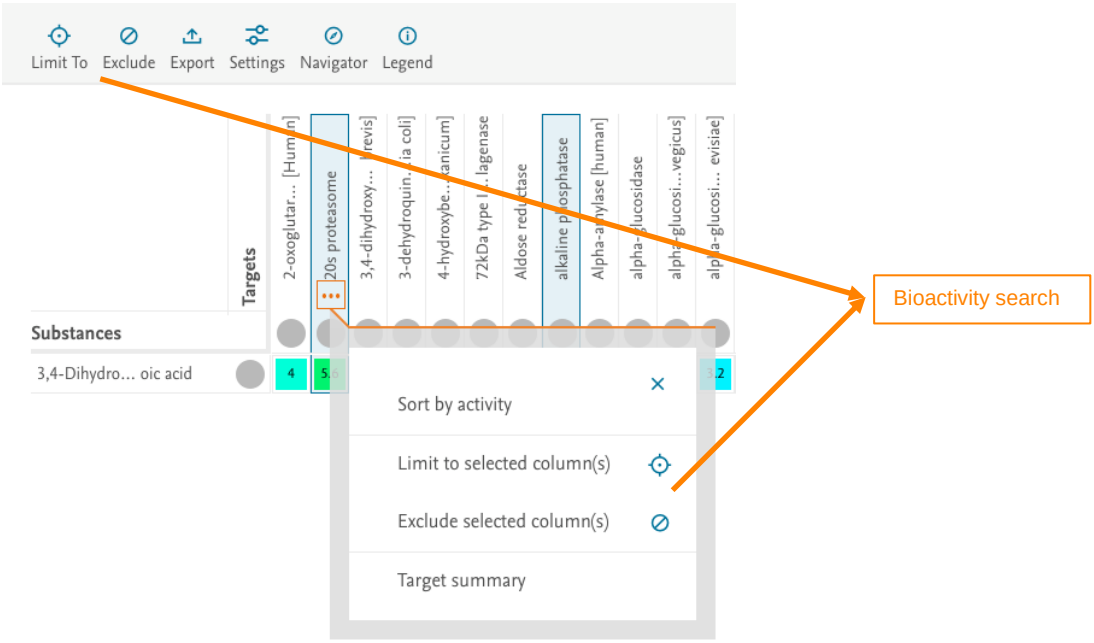
1.4 Reaction searches via Retrosynthesis

Retrosynthesis plan generation can be started from a results page using the **Synthesize Icon**, a **Synthesis Plan**, or from the **Sketcher**. Independent from from the starting point, creating a plan using published data will count as SynthesisPlan (published), creating a plan using predictive Retrosynthesis will count as SynthesisPlan (predicted). Each published and predicted plan creation will count as a reaction search. Each click on **Find Preparations** will count as reaction search.



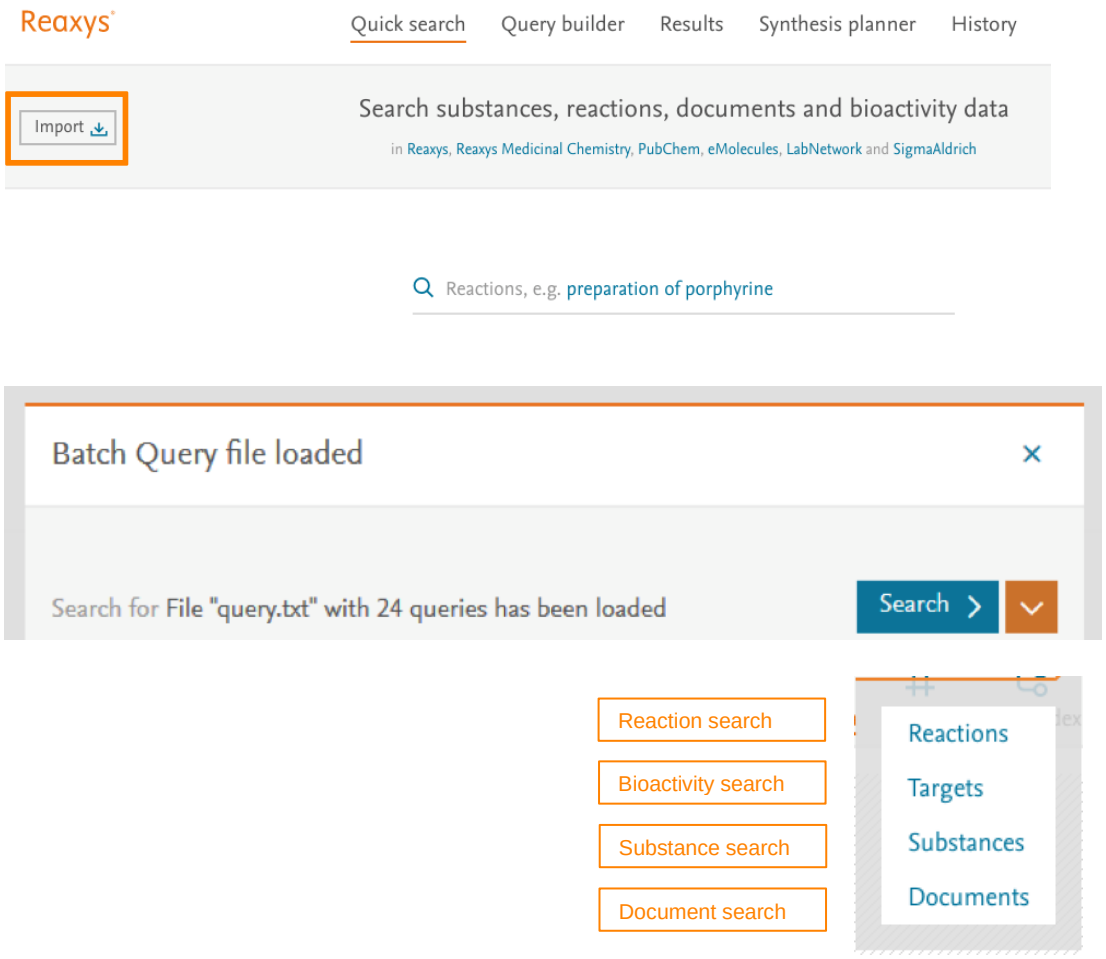
1.5 Filters and limits to the Heatmap selection

Heatmap is a powerful tool for visualizing bioactivity data. Users can define various filters by opening the desired topic on the left side and selecting the presented values. When **Limit to** or **Exclude** is clicked, a search is triggered and counted as a bioactivity search. A user also can select single or multiple columns or rows and use the **Limit to** or **Exclude** options. Again, this counts as a bioactivity search.



1.6 Batch queries

Users have the option of loading SD files containing multiple substance queries in Molfile format or factual queries as text files. When loaded, Reaxys presents the file analysis, together with the count of searches included in the batch file. Clicking **Search** start the batch process. Each query in the loaded batch file is counted as a batch reaction, batch substance, batch document or batch bioactivity search, depending on the context selected by the user.



1.7 Link-in searches

The **Link-in** feature allows customers to create links into Reaxys and Reaxys Medicinal Chemistry from external sources, such as Microsoft Word® documents, Microsoft Excel sheets or Intranet sites. In addition, some of the supported export formats, such as PDF or Microsoft Excel, yield documents enriched with hyperlinks pointing back to Reaxys and Reaxys Medicinal Chemistry.

In terms of usage reporting, it means that when a user clicks on a hyperlink in such a document, the relevant search is run and counted in the usage statistics as one search. It is added to the All Searches column of the usage report.

1.8 Alert searches

Registered users can schedule searches to be run automatically at a defined time (e.g., after each update, weekly, monthly) based on previously defined queries. Each automatic run of an alert generates a search counted in the usage statistics under Alert Searches and All Searches.

1.9 History combine searches

Combining searches from the **History** is performed using Query Builder, so the search is counted as a reaction, substance, document or bioactivity search, depending on the context chosen by the user. The count for History R/B/S/C Searches is reported as 0. This column is kept for compatibility with the former Reaxys usage reports.

1.10 Reaction, substance and document download: Export selection

On any given **Results** page, the user can select various result items from the presented values. As soon as the button Export is clicked, system presents a screen to select the format and the range of the data to be exported. On click of the **Export**, the download event is triggered and counted for the statistics. Depending on the result context, this Export is either counted as substance, reaction, or document export.

Note: Any export from the Target and Bioactivity page are accounted as substance exports in the statistics.

In this example, clicking on **Export** would add a reaction export count because export is triggered for the reaction results. Hence R-Export = 1 and R-Exported = 2 indicating that 2 reaction rows were downloaded by a single export. Subsequent exports will increment these metrics.