

Reaxys®

# Reaxys Link-In

User Guide



**Description:** The Link-In feature allows you to link to Reaxys from other applications and documents. It can be used to configure in-house applications to call Reaxys (i.e., open the relevant Results page in the default browser) when the user clicks on Reaxys-enabled hyperlinks.

**Function:** When an active hyperlink is clicked in an IP-authenticated environment, Reaxys opens in the default browser and after a short loading time, displays the corresponding Results page.

If the user does not have IP access, the login page displays. When the user logs in, the search automatically begins and the results are displayed.

**Notes on authentication:** Authentication through Link-In using clear text user name/password pairs is not supported for security reasons. However, Reaxys allows Shibboleth/Institutional Login using Link-In URLs as the return URL. This is the recommended approach.

**Note on search context:** It is important to specify the target search context (substance, reaction, citation) in the Link-In statement to ensure that the desired result is found. If no context is specified, then all queries are performed in the default reaction context.

**Note on reserved characters:** It is possible that the URL may contain characters typically reserved for other purposes, e.g., the character "#". To use those characters in queries, e.g., SMILES strings, where # is representative of a triple bond, the characters must be 'masked' with the corresponding ASCII Hexcode.

**Example:** Adding a SMILES string to a Reaxys command URL containing a triple bond marker (prop-1-ynyl-cyclopentane = CC#CC1CCCC1)

The character "#" is ASCII 35 (Hex = 23). Therefore, a URL could be generated as follows:

<https://www.reaxys.com/reaxys/secured/hopinto.do?context=S&query=SMILES='CC%23CC1CCCC1'&qname=pk%20of%20sarcosinamide&ln=>

Other characters requiring coding are:

Space	=	Hex 20	/	=	Hex 47
!	=	Hex 33	:	=	Hex 58
\$	=	Hex 36	;	=	Hex 59
%	=	Hex 37	<	=	Hex 60
&	=	Hex 38	=	=	Hex 61
'	=	Hex 39	>	=	Hex 62
(	=	Hex 40	?	=	Hex 63
)	=	Hex 41	@	=	Hex 64
*	=	Hex 42	[	=	Hex 91
+	=	Hex 43	]	=	Hex 93)
,	=	Hex 44			

**Syntax:** The following Syntax is required to construct a link to Reaxys. Not all syntax fields are mandatory to create a link to Reaxys.

`<Reaxys-link-in-URL>?context=<context>&query=<query>&options=<options>&qname=<query name>&origin=<your name or institution name or application name>&ln=`

You can construct the link to Reaxys using HTTP or HTTPS. The link will automatically redirect to the HTTPS URL. Queries in string fields require quotes around the query terms, e.g. IDE.RN='102625-70-7' has to be set for CAS# searches

#### Definitions for syntax fields:

`<Reaxys-link-in-URL>`: <https://www.reaxys.com/reaxys/secured/hopinto.do>

`<context>`: R, S or C (reaction, structure, or citation); default = R

`<query>`: `<field name><operator><field content>`

Text example for a melting point search: MP.MP=80-100

Structure example: SMILES='N1C=CC2=C1C=CC=C2'

Please refer to "Searching property data" for a list of available search fields and their syntax. Structures can be either MOLFILES or SMILES. Their operator is =. Their field content is enclosed in single quotes

MOLFILE='<molfile as string, new line indicated as \n>'

SMILES='<smiles string>'

`<options>`: Contains the reaction or structure search options, as listed below; field is optional

**starting\_material:** This must be a substance structure that is searched in reaction context. The resulting hitset is all reactions where an reactant matches the structure searched for.

**product:** Same restriction as starting\_material with the condition applying to the product.

**all\_reactions:** Same restriction and same condition as previous two options, but searching both the reactant and the product side, i.e., effectively merging the results of the 2 restrictions.

**reagent:** This must be a substance structure that is searched in reaction context. This option searches for all reactions where one of the substances found originally occurs as a reagent.

**catalyst:** This must be a substance structure that is searched in reaction context. This option searches for all reactions where one of the substances found originally occurs as a catalyst.

**solvent:** This must be a substance structure that is searched in reaction context. This option searches for all reactions where one of the substances found originally occurs as a solvent.

**reagent\_or\_catalyst:** This must be a substance structure that is searched in reaction context. This option searches for all reactions where one of the substances found originally occurs as a reagent or a catalyst.

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**exact:** The hit structure should contain as many heavy atoms, bonds, fragments, rings, charges and radicals as the query structure. For reactions, the restriction on the fragment count is lifted. This is the default structure search.

**substructure:** The query structure can be embedded into the hit structure, with none of the previous restrictions. This option is mutually exclusive to 'exact', which is the default.

**sub\_hetero:** Exact search, but free substitution allowed on all non-C atoms.

**isotopes:** If unset, the hit may only contain isotopes if the query does. Valid for both exact and substructure.

**tautomers:** If specified, tautomers of original hits are also found.

**stereo\_absolute:** All stereo centers in the query match the mapped centers in the hit.

**stereo\_relative:** All stereo centers in the query match the mapped centers in the hit or its mirror image (all centers synchronously inverted). This is mutually exclusive to stereo\_absolute. The default is a non-steric search.

**separate\_fragments:** Request that non-interconnected fragments of the query structure are mapped onto different fragments in the hit.

**ignore\_mappings:** Ignore requests of the query to specifically find reactant atoms mapped to product atoms.

**salts:** If set, allow more fragments, charges and radical dots to be present in the hit than in the query.

**no\_extra\_rings:** If set, don't allow rings in the hit that are connecting two atoms in the query but are not yet present in the query.

**charges:** Allow the hit to contain more charges than the query.

**radicals:** Allow the hit to contain more radical dots than the query.

**mixtures:** After a search for substances, add those substances to the result, which references a substance in the initial result as a mixture component.

**markush:** After a search for substances, add those substances that are referenced from an initial hit as a Markush structure scheme to the result.

**atoms=:** Restrict the number of atoms in the hit to a (range of) positive integer(s). Ranges look like lower-hyphen-upper, e.g., 10-20.

**fragments=:** Restrict the number of fragments (interconnected atoms) in the hit to a (range of) positive integer(s).

**rings=:** Restrict the number of rings in the hit to a (range of) non-negative integer(s).

**<query name>:** This is the name for the user display. This field is optional.

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### Notes on syntax

- Adjoining syntax fields are conjoined using standard URL space delimiters, in this case, '&'.
- An origin tag should always be used.
- 'ln=' must be included at the end of each URL to indicate the termination of the URL string.

Example:

```
https://www.reaxys.com/reaxys/secured/hopinto.do?context=S&query=MP.MP=2022&qname=L  
w%20melting%20compounds&origin=my_app&ln=
```

**Shibboleth Link-In with Institutional login:** It is possible to use the Link-In feature together with an institutional login by specifying the corresponding appReturnURL parameter value. The syntax is:

```
<Reaxys-shibboleth-url>?entityID=<URL encoded value of Institutional-federation-  
url>&appReturnURL=<URL encoded value of Reaxys-shibboleth-return-url>
```

```
<Reaxys-shibboleth-url> = https://auth.elsevier.com/ShibAuth/institutionLogin
```

```
<Institutional-federation-url> refers to authentication page of institution
```

```
<Reaxys-shibboleth-return-url> = https://www.reaxys.com/services/oauth/shibboleth-  
sso?_target=<URL encoded value of short-reaxys-link-in-url>
```

```
<short-reaxys-link-in-url> is a shortened version of link-in url, where /hopinto is used for  
reaxys-url, e.g /hopinto?context=S&query=IDE.MW%3C%3D100&ln=
```

It's important that every query-string parameter is properly encoded, according to <https://en.wikipedia.org/wiki/Percent-encoding>. The appReturnURL parameter has an embedded URL with sub-parameters, so some values are double and triple encoded.

This example uses a non-existent IdP

```
https://auth.elsevier.com/ShibAuth/institutionLogin?entityID=https%3A%2F%2Fidp.test.elsevier.com%2Fshib  
boleth&appReturnURL=https%3A%2F%2Fwww.reaxys.com%2Fservices%2Foauth%2Fshibboleth-  
sso%3F_target%3D%252Fhopinto%253Fcontext%253DS%2526query%253DIDE.MW%25253C%25253D1  
00%2526ln%253D
```

**Link-In Syntax Examples:** The following URLs are examples of a properly constructed Reaxys link using the Hop-Into syntax.

Get all reactions of indole

```
https://www.reaxys.com/reaxys/secured/hopinto.do?query=IDE.XRN=107693&qname=1H-  
indole&origin=my_app&ln=
```

Get data for 4 known compounds with the Reaxys registry numbers 281866 ,16002, 281867 and 240646:

<https://www.reaxys.com/reaxys/secured/hopinto.do?context=S&query=IDE.XRN=281866 OR IDE.XRN=16002 OR IDE.XRN=281867 OR IDE.XRN=240646&ln=>

Get all compounds which have a melting point between 20 and 22°C:

[https://www.reaxys.com/reaxys/secured/hopinto.do?context=S&query=MP.MP=20-22&qname=Low%20melting%20compounds&origin=my\\_app &ln=](https://www.reaxys.com/reaxys/secured/hopinto.do?context=S&query=MP.MP=20-22&qname=Low%20melting%20compounds&origin=my_app &ln=)

Perform a reaction product search with a given SMILES string:

[https://www.reaxys.com/reaxys/secured/hopinto.do?context=R&query=SMILES='C\[C%40\]12CC\[C%40%40H\]3\[C%40H\]\(CC\[C%40H\]4CC\(%3DO\)C\(%2DC\[C%40\]34C\)%3DC%2DO\)\[C%40%40H\]1CCC\(%3DO\)O2'&qname=2-Hydroxymethylen-dihydrotestololactones&options=product,substructure&origin=my\\_app &ln=](https://www.reaxys.com/reaxys/secured/hopinto.do?context=R&query=SMILES='C[C%40]12CC[C%40%40H]3[C%40H](CC[C%40H]4CC(%3DO)C(%2DC[C%40]34C)%3DC%2DO)[C%40%40H]1CCC(%3DO)O2'&qname=2-Hydroxymethylen-dihydrotestololactones&options=product,substructure&origin=my_app &ln=)

**Restrictions:** The GET request is constrained by individual browser support requirements for URL construction. The GET request cannot exceed the following limits:

Internet Explorer – 2,083 characters

Firefox – 2,000 characters

Because some characters must be coded (e.g., blank as %20 or the equal sign as %3D), the effective character string limit may be even less.

The GET request provides only for the link from a separate document or web page into Reaxys. The GET request does not provide an alternate user interface. The GET request displays the individual single objects (substances, reactions, citations), or represents a simple query.

Because the browsers' support of GET requests varies by length, we recommended implementing the "length" parameter, so that the server can indicate when a request hasn't been transferred completely by providing an error message, for example:

"Query too long for transmission via GET request."

In addition to other parameters, a password can be added to a link-in request along with the username. This password will have to be encrypted.

In case you need to upload reaction queries that exceed the character limit of the browser, you may use a POST request instead and upload an SD or RD file.