



## Release notes for September 2020

### New database: Reaxys Commercial Substances

To support experimental planning and improve productivity, Reaxys now contains essential information on commercially available substances. Reaxys Commercial Substances is a fully integrated chemical supplier database that contains essential data on approximately 35 million unique molecules and 95 million associated products, including screening compounds and building blocks.

These data are drawn from important, high-quality aggregators, including eMolecules and LabNetwork, as well as being obtained directly from a growing pool of over 330 relevant suppliers located worldwide. The content is intended to ideally inform synthesis-or-purchase decisions. The database is updated monthly to ensure accuracy.

Customers' preferred suppliers can be integrated upon request. Simply ask your suppliers to register their interest [here](#). Our partner Innodata will contact them to discuss their addition.

Users can search directly for information on commercial substances using Quick Search; using *Commercial Substances* querylets in Query Builder; or via the shopping cart icon in the results for any substance, reaction or literature queries. It is possible to export the data to ELNs or purchasing systems.

Reaxys Commercial Substances results include the following information:


- CAS number and catalog-specific product ID
- Price and package size
- Purity, structure and supplier specific details (address, telephone, email address etc)
- Stock availability, shipment time and supplier country

## Search using Quick Search or Query Builder

For Quick Search: enter the chemical's CAS number, name or structure in the appropriate field (A).

For Query Builder: choose one of the appropriate querylets in the *Commercial Substances* section (B). This supports the addition of search parameters such as catalog identifiers, package size and usage classification.

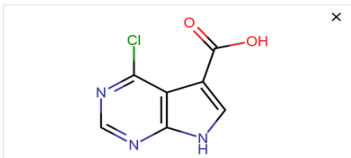
Quick search Query builder Results Synthesis planner History Alerts

**A** Search for 

Search Reaxys  Find >

Documents, e.g. published by Schrock

AND



As drawn

Search in: Reactions Targets Substances Documents

Import Save Reset form Delete all

Structure Molecular Formula CAS RN TI, AB & KW

Field	Operator	Value	Remove
Supplier	is	Supplier	X
Product Name	is	Product Name	X
Purity %	=	Purity %	X
Package Size (Text)	is	Package Size (Text)	X
Price	=	Price	X
Shipment Time	is	Shipment Time	X

**B** Search fields

Fields Forms History

Commercial Substances

- Suppliers
- Supplier
- Supplier Geolocation
- Usage Classification
- Product Name
- Supplier Product Number
- Catalog Identification Number
- Supplier SKU
- Purity %
- Package Size (Text)
- Price
- Currency
- Stock Availability

## Access commercial information from multiple locations

Commercial substances information can be accessed directly from the *Results Preview* for Quick Search (C), from the shopping cart icon for individual substance results (D), or using the database selection menu in the top right corner of the interface (E). Note that option D only accesses information for that substance. The selection menu E can access purchasing information on multiple substances. To filter results in Reaxys to only show commercial available substances, the filter selection (F) can be used

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Alerts Combined ...

Results for 186519-92-6 New Edit

Icon	Count	Category	Details	Actions
	1	Substances	CAS# : 186519-92-6 Edit in Query Builder Create Alert	Preview Results View Results
	0	Documents	Titles, Abstracts, Keywords : "186519-92-6" Edit in Query Builder Create Alert	
	2	Commercial Substances	CAS# : 186519-92-6 Edit in Query Builder Create Alert	Preview Results View Results

Reaxys<sup>®</sup> Quick search Query builder Results Synthesis planner History Alerts Combined ...

1 Substances out of 5 Documents, containing 11 Reactions, 0 Targets

1

4-chloro-7H-pyrrolo[2,3-d]pyrimidine-5-carboxylic acid  
C<sub>7</sub>H<sub>4</sub>ClN<sub>3</sub>O<sub>2</sub> 197.581 14006617 186519-92-6

Identification  
Druglikeness  
Physical Data - 1  
Spectra - 2

Substance Availability

- Commercial Substances
- Accelrys' ACD
- CambridgeSoft ACX
- Sigma Aldrich
- eMolecules

Filters

Limit to Exclude

Substance Classes  
Molecular Weight  
Number of Fragments  
Availability  
Availability in other databases  
Available Data  
Document Type  
Publication Year  
Patent Assignee  
LogP

1  
Commercial Substances  
eMolecules  
PubChem

Reaxys - 1

- Commercial Substances - 2
- eMolecules - 2
- LabNetwork - 0
- PubChem - 1
- SigmaAldrich - 1

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Get a detailed view of what is available from different suppliers

Reaxys Commercial Substances provides a detailed view of all suppliers (G) of each individual substance, making purchasing decisions easier. Information given includes purity, pricing, package size and delivery time. Supplier information can be refined further with specific filters (H), limiting the need to find, refine and compare supplier details outside of Reaxys.

The screenshot displays the Reaxys Commercial Substances interface. On the left, a 'Filters' sidebar allows refinement by structure, molecular weight, number of fragments, and availability. The main area shows the chemical structure of 5-Methoxy-6-nitro-pyridine-2-carboxylic acid methyl ester. Below the structure, a table lists suppliers with columns for Supplier, Product, Purity, Package size & price, and Availability. An orange box labeled 'G' highlights the 'Identification' tab, and another orange box labeled 'H' highlights the 'Supplier Information - 94' tab. A third orange box labeled 'I' highlights a direct link to the supplier website (Activate Scientific Germany) in the table.

Supplier	Product	Purity	Package size & price	Availability
Abayon Chemicals Inc.	Methyl 5-methoxy-6-nitropicolinate 390816-44-1 61-9369	95percent	1g 520 USD	Tier Time: not specified Last updated: 2020-01-12
Abayon Chemicals Inc.	Methyl 5-methoxy-6-nitropicolinate 390816-44-1 61-9369	95%	1g 520 USD	Tier Time: not specified Last updated: 2020-01-12
Abayon Chemicals Inc.	Methyl 5-methoxy-6-nitropicolinate 390816-44-1 61-9369	95%		Tier Time: not specified Last updated: 2020-01-12
AbayChem	Methyl 5-methoxy-6-nitropicolinate 390816-44-1 ACS12880	98%	1g	Tier Time: not specified Last updated: 2020-01-28
Activate Scientific Germany	Methyl 5-methoxy-6-nitropicolinate 390816-44-1 ACS12880 AS37949	95%	250 mg 230 USD	Stock availability: in stock Shipment time: 4-5 days Tier Time: not specified Last updated: 2019-10-30
Activate Scientific Germany	Methyl 5-methoxy-6-nitropicolinate 390816-44-1 AS37949	95%	1 g 476 USD	Stock availability: in stock Shipment time: 4-5 days Tier Time: not specified Last updated: 2019-10-30
AEchem Scientific Corp. USA	Methyl 5-methoxy-6-nitro-2-pyridinecarboxylate 390816-44-1	95-percent	1g	Shipment time: 1 week Tier Time: not specified

Directly access product webpages on supplier websites

If a direct link to the supplier website is available, an arrow is shown beside the catalog identifier (I). Click this to go directly to the source for further supplier-specific information on that product.

## Changes to the data export and concurrent login policy

### Data export policy change:

Freedom of data export is a unique feature of Reaxys. However, excessive numbers of concurrent export operations can impact the solution's performance for all users. To ensure consistent and fast performance for everyone using the solution, we've implemented a cap on the number of export operations per user in a 24-hour period.

**Registered users** can export data from Reaxys a maximum of 10 times in 24 hours. Each export operation can contain 5,000 items. This means a cap of 50,000 exported items in 24 hours.

**Anonymous users** cannot export any data. They will be prompted to register and/or sign in.

If you require a higher data export capability, please [contact us](#).



### Concurrent login policy change:

Changes to the policy for concurrent logins with the same user name: in the past there was no limit and a user could open Reaxys many times simultaneously. However, this is not supported by our current licensing policy and we have changed this, to **only allow a maximum number of 3 simultaneous logins per user name**.

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