

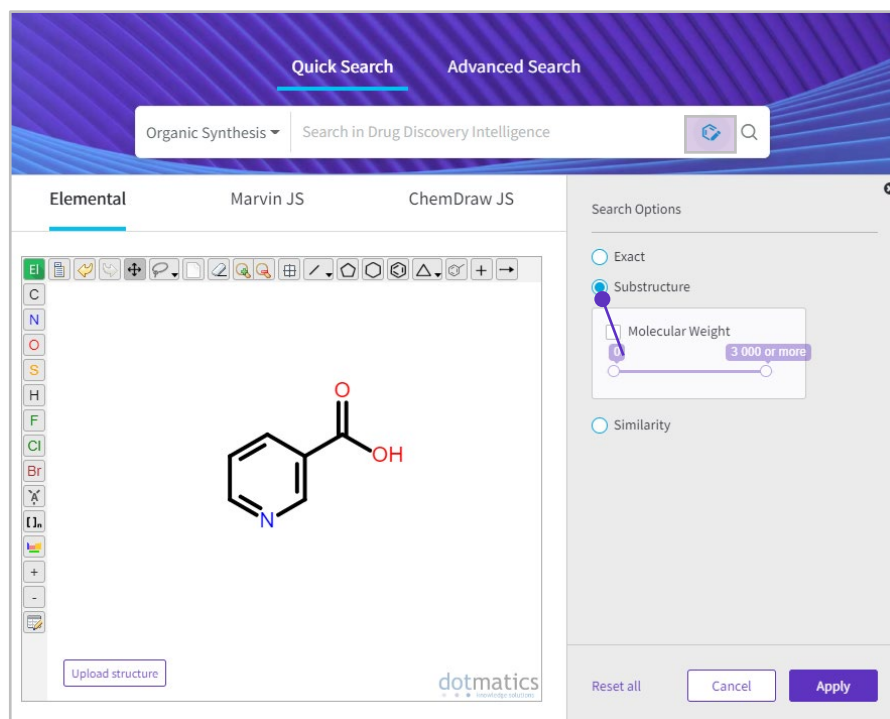
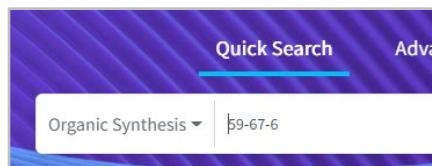
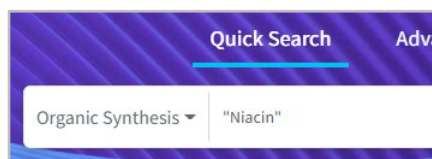
Find promising APIs for your intermediates

Cortellis Drug Discovery Intelligence

In this guide you'll learn how to:

- Use Quick Search to find your intermediate
- Review the associated routes of synthesis and determine your freedom to operate
- Find associated end-products and organizations that are developing/marketing them

1. Use **Quick Search** to find your intermediate within the Organic Synthesis knowledge area. You can search by **keyword**, **CAS number**, or by **Substructure** using the structure editors.



Quick Search Advanced Search

Organic Synthesis Search in Drug Discovery Intelligence

Elemental Marvin JS ChemDraw JS

Search Options

- Exact
- Substructure
 - Molecular Weight: 3,000 or more
- Similarity

Reset all Cancel Apply

dotmatics
knowledge solutions

- On your results page, go to the **Intermediates** tab to find those associated with your search. Click on the **Synthesis** number to navigate to all schema associated with your intermediate.

Main Name	Structure	Chemical Name	CAS Registry Number	Synthesis	End Products
Niacin		3-Picolinic acid Nicotinic acid Pellagra preventive factor Pyridine-3-carboxylic acid	59-67-6	16	19 Nicotine, Nicaraven, Micinicate, KC-764, ...
881502		Pyridine-3-[[11C]carboxylic acid		1	1 Niacin

Click on the arrow heads to see full details on the intermediates, such as **InChI** and **Suppliers**

Use the arrows at the top of the columns to rank your results as you need, for example by number of associated **End Products**

- By default, synthesis results show a miniature drawing of the schema, a hyperlink to the **End product**, and the most relevant patent info.

Title: **Synthesis of arecoline** [View record](#)

End Product: [Arecoline](#)

1 Schemas | 5 Intermediates | 3 Reagents | 0 Literature | 1 Patents

Patent Number	Publication Date	Applicant	Patent Document
CN105439941	Mar 30, 2016	Qingdao Kangyuan Pharmaceutical Co., Ltd.	

Sorted by Intermediates count descendant

- Sort by relevance
- Sort by End Product alphabetically ascendant
- Sort by End Product alphabetically descendant
- Sort by Patent Publication date ascendant
- Sort by Patent Publication date descendant
- Sort by Intermediates count ascendant
- Sort by Intermediates count descendant**

Use the **Sorted by** menu to rank your results according to your preference

- Click on **Expand all** at the top of the table to see the full list of associated patents to your schemas. Note that synthesis from **Originator** companies are indicated in the title. Use the patent info to get a quick view of freedom to operate and potential competitors / collaborators.

Synthesis Intermediates

Apply Filters Sorted by Intermediates count descendant Showing 1-16 of 16 Organic Synthesis records

Select all Collapse all

Title: **Synthesis of GSK-171B (Originator)** View record
End Product: GSK-171B

2 Schemas | 16 Intermediates | 15 Reagents | 0 Literature | 2 Patents

Patent Number	Publication Date	Applicant	Patent Document
WO2005051391	Jun 09, 2005	GlaxoSmithKline Inc. (US)	Novartis Vaccines and Diagnostics Inc. (Originator)
WO2004112793	Dec 29, 2004	GlaxoSmithKline Inc. (US)	Novartis Vaccines and Diagnostics Inc. (Originator)

Show less

Title: **Synthesis of 310418** View record
End Product: 310418

1 Schemas | 12 Intermediates | 11 Reagents | 1 Literature | 0 Patents

- Click on any of the schemas to see them full screen and read the related **Summary**. Navigate all the schemas in your results using the arrows on the top right of the pop-up.

824292-01-a

Summary

Chlorination of nicotinic acid (I) with POCl₃ in the presence of pyr at 60 °C, followed by esterification of the resulting acid chloride (II) with inositol (III) at 80 °C affords the target inositol hexanicotinate (1,5). Alternatively, this compound is obtained directly by enzymatic esterification of carboxylic acid (I) with inositol (III) by means of Novozyme 435 in t-BuOH (previously dehydrated by treatment with activated molecular sieves) (3).

- Review the end products individually by clicking on the **End product** link; or go to an overview of all end products by clicking on the **Related Content** icon. From there you can navigate to the list of drugs to understand the status of the drugs' development programs; and then on to the related organizations.

The screenshot shows the 'Synthesis' tab in a software interface. At the top right, there is a 'Related Content' icon (a gear with a plus sign) highlighted by a red box. Below the header, there are filter options and a sorting dropdown set to 'Sorted by Intermediates count descendant'. The main content area displays a record for 'Synthesis of GSK-171B (Originator)'. The 'End Product: GSK-171B' is highlighted with a red box. Below this, there are statistics: 2 Schemas, 16 Intermediates, 15 Reagents, 0 Literature, and 2 Patents. A table lists patent information:

Patent Number	Publication Date	Applicant	Patent Document
WO2005051391	Jun 09, 2005	GlaxoSmithKline Inc. (US)	Novartis Vaccines and Diagnostics Inc. (Originator)

At the bottom of the record, there is a 'Show more' link. Below the record, another record for 'Synthesis of 310418' is partially visible.

The screenshot shows a dashboard titled 'Info related to 16 Organic Synthesis records'. It features several cards with icons and counts:

- 16 Organic Synthesis**: View results
- 19 Drugs & Biologics**: View results, Related content (highlighted with a red box)
- 0 Genes & Targets**: View results, Related content
- 0 Organic Synthesis**: View results, Related content

A red line connects the 'Related Content' icon from the top screenshot to the '19 Drugs & Biologics' card in this dashboard.

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