

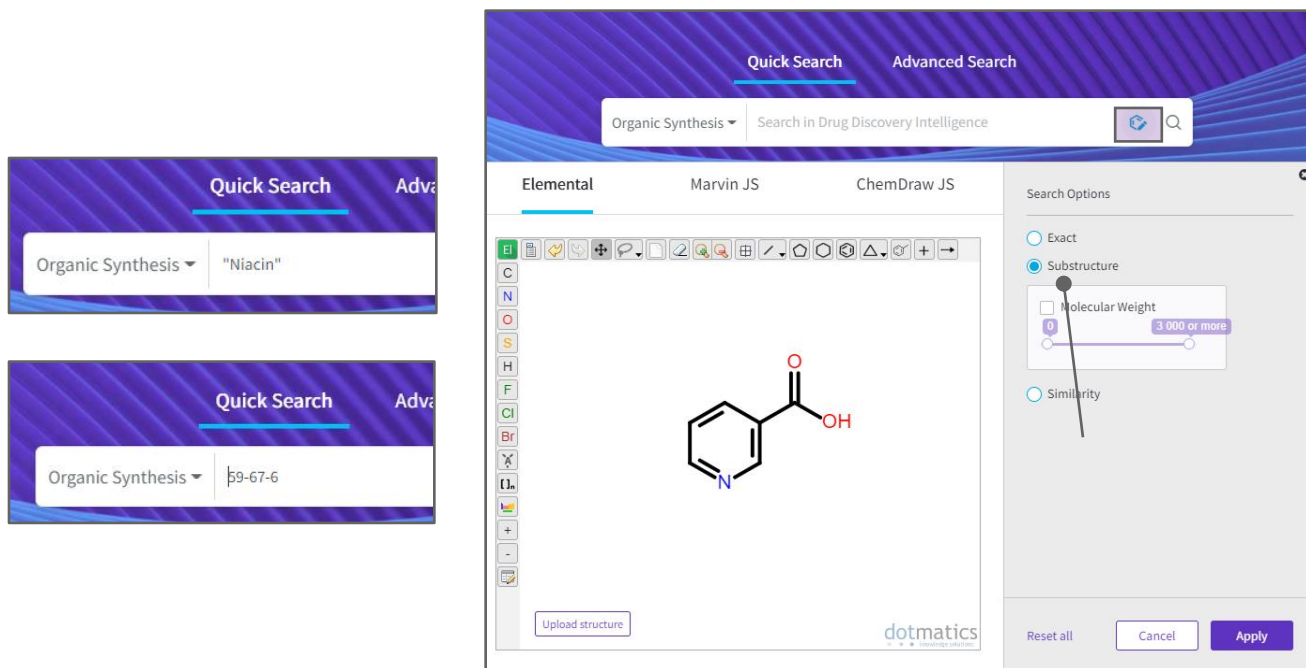
# Find promising APIs for your intermediates

## Cortellis Drug Discovery Intelligence

In this guide you'll learn how to:

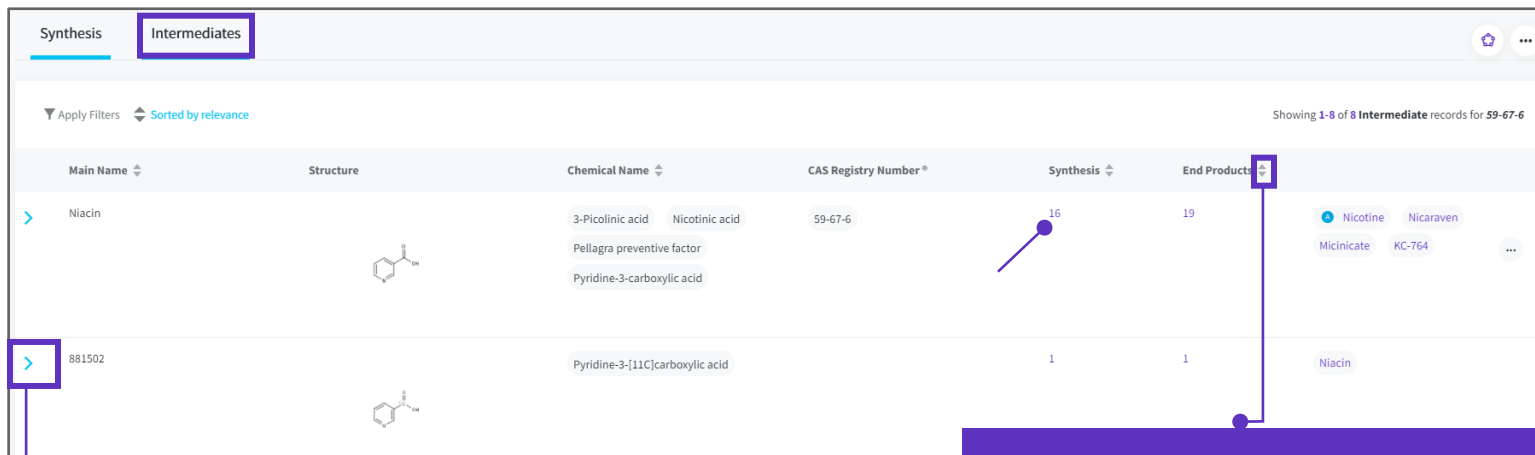
- Use Quick Search to find your intermediate
- Review the associated routes of synthesis and determine your freedom to operate
- Find associated end-products and organizations that are developing/marketing them



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.



The screenshot displays the 'Quick Search' interface of the Cortellis Drug Discovery Intelligence platform. At the top, there are tabs for 'Quick Search' and 'Advanced Search'. Below these, a search bar is shown with 'Organic Synthesis' selected from a dropdown menu and 'Niacin' entered in the search input field. A chemical structure of Niacin (pyridine-3-carboxylic acid) is displayed in the center. To the right, a 'Search Options' panel is visible, showing radio buttons for 'Exact', 'Substructure', and 'Similarity'. The 'Substructure' option is selected. Below this, a 'Molecular Weight' filter is shown with a range from 0 to 3,000 or more. At the bottom right, there are buttons for 'Reset all', 'Cancel', and 'Apply'. The interface is branded with 'dotmatics' at the bottom right.

- 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.

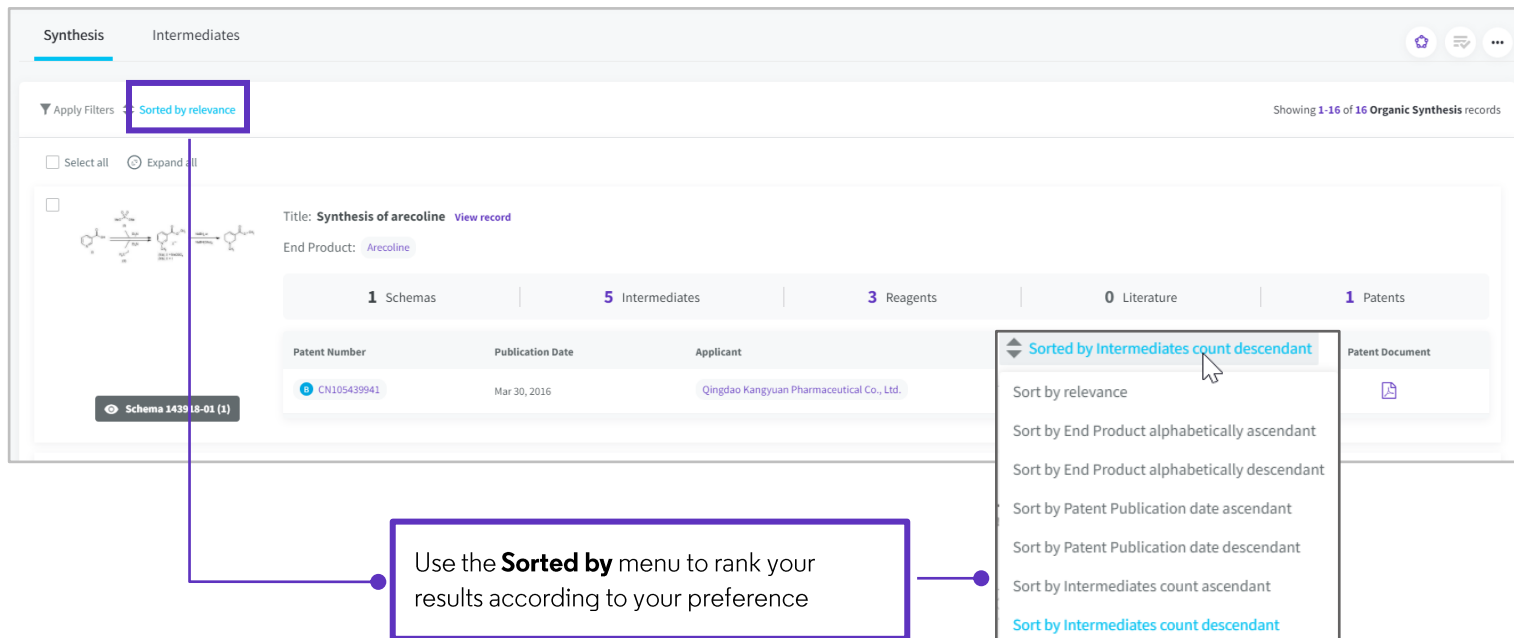


Main Name	Structure	Chemical Name	CAS Registry Number	Synthesis	End Products
Niacin		3-Picolinic acid Nicotinic acid Pellagra preventive factor Pyridine-3-carboxylic acid	59-67-6	16	19 Nicotine Nicaraven Micinicate KC-764 ...
881502		Pyridine-3-[11C]carboxylic acid		1	1 Niacin

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.



Sorted by relevance

Showing 1-16 of 16 Organic Synthesis records

Select all Expand all

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

End Product: [Arecoline](#)

Patent Number	Publication Date	Applicant
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

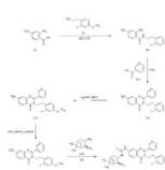
Use the **Sorted by** menu to rank your results according to your preference

- 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-1718 (Originator)** [View record](#)  
End Product: **GSK-1718**

2 Schemas	16 Intermediates	15 Reagents	0 Literature	2 Patents
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Patent Number	Publication Date	Applicant	Patent Document
WO2005051391	Jun 09, 2005	GlaxoSmithKline Inc. (US) <b>Novartis Vaccines and Diagnostics Inc. (Originator)</b>	
WO2004112793	Dec 29, 2004	GlaxoSmithKline Inc. (US) <b>Novartis Vaccines and Diagnostics Inc. (Originator)</b>	

[Show less](#)

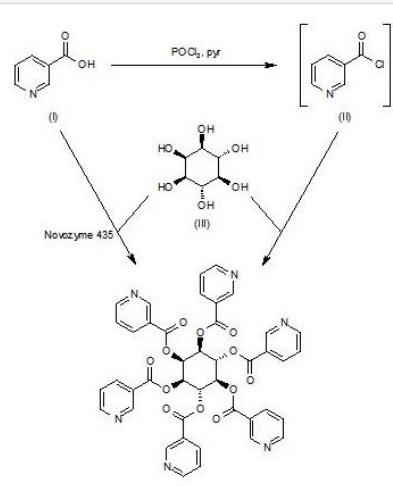
☐  Title: **Synthesis of 310418** [View record](#)  
End Product: **310418**

1 Schemas	12 Intermediates	11 Reagents	1 Literature	0 Patents
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- 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.

☐ Synthesis of inositol hexanicotinate - 824292-01

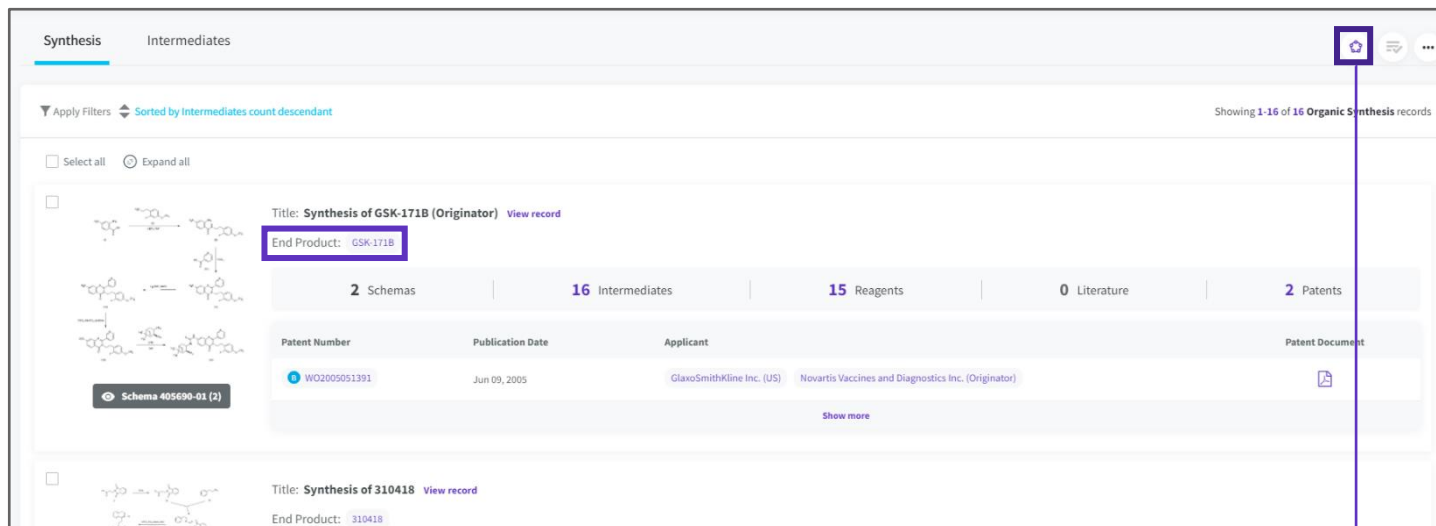
**824292-01-a**



**Summary**

Chlorination of nicotinic acid (I) with POCl<sub>3</sub> 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.



Synthesis Intermediates

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

Select all Expand all

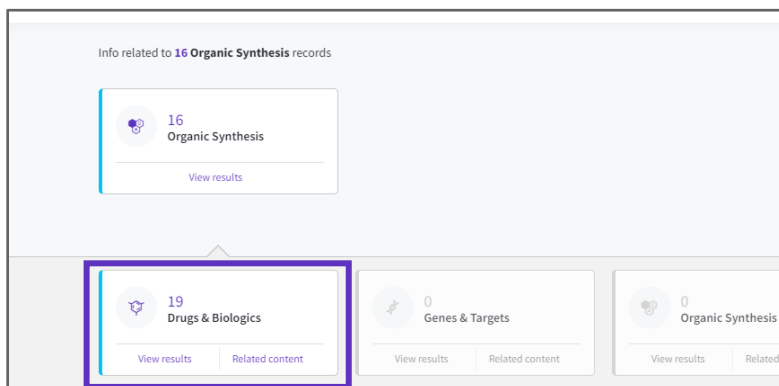
Title: **Synthesis of GSK-1718 (Originator)** View record  
End Product: **GSK-1718**

2 Schemas 16 Intermediates 15 Reagents 0 Literature 2 Patents

Patent Number	Publication Date	Applicant	Patent Document
WO2005051393	Jun 09, 2005	GlaxoSmithKline Inc. (US) Novartis Vaccines and Diagnostics Inc. (Originator)	

Show more

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



Info related to 16 Organic Synthesis records

16 Organic Synthesis  
View results

19 Drugs & Biologics  
View results Related content

0 Genes & Targets  
View results Related content

0 Organic Synthesis  
View results Related content

For more information contact Customer Service at **LS Product Support**.