

CRACK THE CODE

ON RETROSYNTHESIS PLANNING

SCIFINDERⁿ CUTS TIME SPENT IN RETROSYNTHESIS
PLANNING FROM HOURS TO MINUTES!

COMING SOON:

Predictive Routes for Novel Functional Design

For any known molecule, SciFinderⁿ will perform a full retrosynthetic analysis utilizing the renowned CAS collection of reactions, presenting results in a highly intuitive retrosynthesis plan.

SciFinderⁿ Retrosynthesis Planner interface showing a retrosynthetic plan. The plan includes steps A through F, with associated suppliers and maximum yields. Plan Information: Estimated Yield: 82%, Overall Price: \$558.10 (USD per 100 grams), Commercially Available: A, B, C, D, E, F.

Use SciFinderⁿ's Retrosynthesis Planner to:

- Automatically generate plans to known molecules and intermediates
- Easily organize and navigate alternative routes
- Quickly identify material suppliers
- Conveniently share plans with key stakeholders
- And more...

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ON RETROSYNTHESIS PLANNING

SYNTHESIS PLANNING HAS NEVER BEEN EASIER

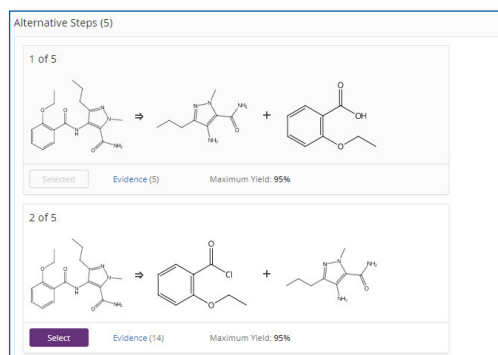
COMING SOON:
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Alternative Route Selector

The route recommendation is offered based on a number of criteria including:

- simplicity of synthesis
- expected yield
- availability and cost of needed materials

Additionally SciFinder[®] allows you to intuitively navigate available alternative routes and upon selection will regenerate the entire plan in seconds.



Convenient Plan Summary

SciFinder[®] offers a recommended retrosynthetic route from a full analysis of the authoritative collection of reactions from CAS. The synthetic plan provides an estimate of the yield, cost and a summary of the available synthetic alternatives at each step along the way.

Overview Steps

Plan Information

Estimated Yield: 82%
Overall Price: \$558.10
(USD per 100 grams)

Commercially Available:
A, B, C, D, E, F

Overview Steps

A → B
Maximum Yield: 100%
Evidence (9)
Alternative Steps (36)

B → C + D
Maximum Yield: 86%
Evidence (1)
Alternative Steps (8)

D → E + F
Maximum Yield: 95%

Access to Material Suppliers

The success of your plan rests on the availability of the proper materials to perform the synthesis. You can directly access comprehensive and up-to-date sourcing information for all commercially available substrates, reagents, solvents and catalysts described in the plan.

Supplier	Substance	Purity	Purchasing Details	Availability
<input type="checkbox"/> Merck KGaA ALDRICH United States	134-11-2 2-Ethoxybenzoic acid	95-98%	Order From Supplier 10 g 100 g Bulk	Maintained in stock
<input type="checkbox"/> Alfa Aesar United States	134-11-2 2-Ethoxybenzoic acid	95-98%	Order From Supplier 25g USD 20.30 100g USD 33.40 500g USD 190.00 Bulk Screening	Typically in stock Ships within 1 week
<input type="checkbox"/> CarboSynth Carbosynth Product List United Kingdom	134-11-2 2-Ethoxybenzoic acid	≥99%	Order From Supplier 250 g USD 70.00 500 g USD 115.00 1 kg USD 180.00	Maintained in stock Ships within 1 week