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Reaxys[®]

新しいRetrosynthesisの使い方

カスタマーコンサルタント
今田泰史, PhD
y.Imada@elsevier.com

October 2021



Retrosynthesisによる合成経路の策定 ～その1～①

～「Retrosynthesis」画面から自分で構造描画して経路策定をする方法～

The screenshot shows the Reaxys website navigation bar with the following items: [Quick search](#), [Query builder](#), [Results](#), **[Retrosynthesis](#)**, [History](#), and [Alerts](#). Below the navigation bar is a search area with the text "Search substances, reactions and documents in Reaxys, PubChem, SigmaAldrich and Commercial Substances". A search input field contains the text "Substance Properties, e.g. ferroelectric materials" and a "Find >" button. Below the search field is an "AND" operator and a "Draw" button with a chemical structure icon. A callout box with a black border and white background contains the text "「Synthesis Planner」→「Retrosynthesis」に名称が変更". An orange arrow points from the callout box to the "Retrosynthesis" menu item.



※通常契約の範囲内ではReaxysに収録のある化合物のみ解析可能(得られる経路もReaxysに収録のある反応を組み合わせたもの)
新規化合物の解析も可能なAIによる逆合成予測ツールの利用はオプション契約となります。

Retrosynthesisによる合成経路の策定 ～その1～②

Structure editor selected: MarvinJS ChemDrawJS

Insert structure from name >

Parameters

Published ⓘ

Create upto 5 full routes.

Branches per step: 3

Max. number of steps: 5

Stop searching if building block is commercially available Yes No

Assumed yield for reactions without a given yield

0% 100%

Clear Cancel Synthesize >

- ・ 生成する最大経路数
- ・ 経路中の最大分岐数
- ・ 最大ステップ数
- ・ 市販化合物に帰着した時点で解析を止める
→ 「No」を推奨
(大きな分子も販売されているため)
- ・ 各反応の許容収率の設定

構造描画は通常のReaxysでの描画と同じ

解析

Retrosynthesisによる合成経路の策定 ～その2～

～化合物検索結果の中から気になる化合物の経路策定をする方法～

The screenshot shows a chemical structure of a complex molecule with a cyanide group and a benzimidazole ring system. A 'Synthesize' menu is overlaid on the structure, containing two options: 'Find preparations' and 'Create synthesis plans'. The 'Create synthesis plans' option is highlighted with an orange box. Below the structure, there are several icons: a shopping cart, a magnifying glass, and a flask icon which is also highlighted with an orange box. The number '18' is visible in the top left corner of the interface.

The 'Parameters' dialog box is shown with the following settings:

- Published** (with an information icon)
- Create upto: 5 full routes.
- Branches per step: 3
- Max. number of steps: 5
- Stop searching if building block is commercially available: Yes No
- Assumed yield for reactions without a given yield: A slider bar ranging from 0% to 100%, currently set at approximately 50%.
- Always show screen before creating plan:
- Create Plans >

解析

Retrosynthesisによる合成経路の策定

～合成経路策定のプロジェクト管理画面～

No.	Date/Time	Project name	No. of routes
9850	06 Oct 2021 05:09	Project #9850	Published 5

Buttons: Delete Edit View

Text: 生成経路を確認

削除

新たに構造を描画して解析したい場合

この構造を基に構造を編集して解析したい場合

> Parameters

- 5 full routes (up to)
- 5 steps per route (up to)
- 3 branches per step (up to)
- Don't Stop at commercial building blocks
- 40% yield per step (assumed, if not published)



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Retrosynthesisによる合成経路の策定

～生成された合成経路の一覧表示画面～

Project #9577
0 selected
Limit to

No. of steps ^^^
Route topology
Get to routes

Building blocks to target

Published Route #1

13 steps

Tree view >
Table view >

Published Route #2

16 steps

Tree view >
Table view >

Preview

この経路の出発基質が表示されている

経路のステップ数や枝分かれの様子を把握できるので他経路との比較が容易

各経路のステップ数で並び替えが可能

経路の詳細
「Tree View」: 枝分かれの形で表示
「Table View」: 経路中の各反応を表の形で表示

Retrosynthesisによる合成経路の策定

～合成経路のTree View画面～

経路中の各Stepの参照文献の表示切替

経路の出力

他の経路への表示切替

反応情報の表示方法の変更

プロジェクト
管理画面などへ戻る

Export Legend

Hide conditions Tree view Table view

Published route #1

Step 1 Step 2 Step 3 Step 4 Step 5

Rotate

経路の拡大縮小
(マウスホイールでも可能)

Conditions	Yield	Reference
With bis-triphenylphosphine-palladium(II) chloride; potassium hydrogencarbonate; triphenylphosphine In water; N,N-dimethyl-formamide at 95 - 100°C; Reagent/catalyst; Solvent; Suzuki Coupling; Inert atmosphere; Large scale;	88%	Baenziger, Markus; Pachinger, Werner; Stauffer, Frédéric; Zaugg, Werner [Organic Process Research and Development, 2019, 23, # 9, p. 1908 - 1917] Full Text ↗ Cited 2 times ↗ Details > Abstr
With potassium phosphate; tetrakis(triphenylphosphine) palladium(0) In water; N,N-dimethyl-formamide at 150°C; for 0.166667h; Suzuki Coupling; Microwave irradiation; Inert atmosphere;	85%	Lu, Xiao; Kim, Myunghoon; Orr, Meghan J.; Li, Hao; Huang, Wenwei [European Journal of Organic Chemistry, 2018, vol. 2018, # 13, p. 1572 - 1580] Full Text ↗ Cited 1 times ↗ Details > Abstr
With potassium phosphate; tetrakis(triphenylphosphine) palladium(0) In water; N,N-dimethyl-formamide at 150°C; for 0.166667h; Suzuki Coupling; Microwave irradiation;	85%	THE UNITED STATES OF AMERICA, AS REPRESENTED BY THE SECRETARY, DEPARTMENT OF HEALTH AND HUMAN SERVICES; LOYOLA UNIVERSITY OF CHICAGO; HUANG, Wenwei; LI, Hao; SUN, Wei; HUANG, Xiuli; PATEL, Paresma R.; (...); TAWA, Greg; WILLIAMSON, Kim C. WO2018/71836, 2018, A1 Location in patent: Paragraph 0073 Full Text ↗ Details > A



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Retrosynthesisによる合成経路の策定

～合成経路のTable View画面～

Table中の各行に各ステップの反応が表示される

Published Route #1

Project #9850

My Synthesis Projects

Draw

Export Legend

Hide conditions Tree view Table view

Steps	Reaction	Yield
1		88 %
2		78 %

Step 1 Step 2 Step 3 Step 4 Step 5 Step 6 Step 7 Step 8 Step 9 Step 10 Step 11 Step 12 Step 13

Conditions

With bis-triphenylphosphine-palladium(II) chloride; potassium hydrogencarbonate; triphenylphosphine In water; N,N-dimethyl-formamide at 95 - 100°C; Reagent/catalyst; Solvent; Suzuki Coupling; Inert atmosphere; Large scale;

Yield

Reference

88% Baenziger, Markus; Pachinger, Werner; Stauffer, Frédéric; Zaugg, Werner [Organic Process Research and Development, 2019, vol. 23, # 9, p. 1908 - 1917] Full Text ↗ Cited 2 times ↗ Details > Abstract >

Feedback



Retrosynthesisによる合成経路の策定

～合成経路が得られなかった場合～

① 解析対象の化合物に類似した構造の化合物で経路が出せる場合

Published Route #1	No.	Date/Time	Project name	No. of routes
Project #9877				
My Synthesis Projects	10137	06 Oct 2021 07:43	Project #10137 Delete	

② 類似した構造含め解析ができなかった場合

→ 「No Results」と表示

→ この場合は、通常の化合物検索をSimilarityで検索を行い、検索結果から自分の目的に近い化合物を探してページ4の方法で解析することを推奨

Please select a substance for synthesis planning

Structure (1)	% Similarity	Chemical Name	No of Ref	No of preparations
	88.7	2-(((4-methoxy-3,5-dimethylpyridin-2-yl)methyl)sulfinyl)benzo[d]oxazole	1	3

[Submit >](#)

類似度合いを確認して、この代替化合物でも良ければ「Submit」をクリック