

DECEMBER 2014

REAXYS R203

**ADVANCED REACTION
QUERIES**

NOTES ON REAXYS R203

REAXYS R203

- ◆ Outlines:
 - ◆ How to search for preparations of single substances or groups of substances
 - ◆ How to *narrow* reactions by marking bonds and matching atoms involved in the reactions
 - ◆ How to *expand* your answers through finding similar reactions and through Similarity search (reactions)
 - ◆ How to develop Synthesis Plans
- ◆ For an outline of further presentations in this series, go [here](#)

NOTES

- ◆ Reaxys R104 gives an *introduction* to searching for chemical reactions, e.g. :
 - ◆ Outlines how to search for chemical reaction information through:
 - ◆ AskReaxys
 - ◆ ReaxysTree
 - ◆ Search Forms
 - ◆ Introduces the concept of searching for reactions by structure queries
 - ◆ Illustrates some of the post-processing options that may be applied to reaction answers

CONTENTS

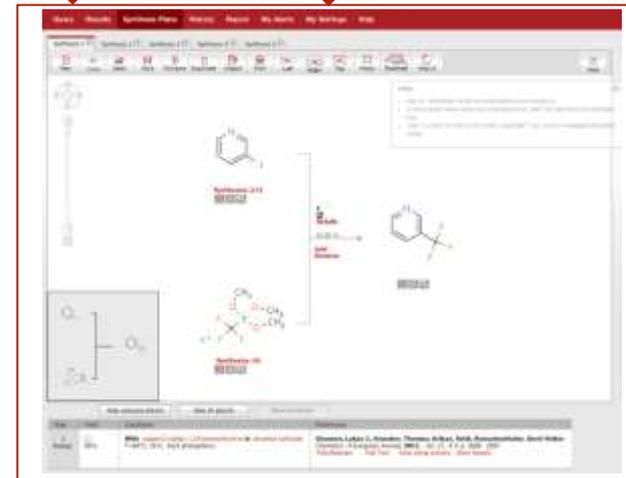
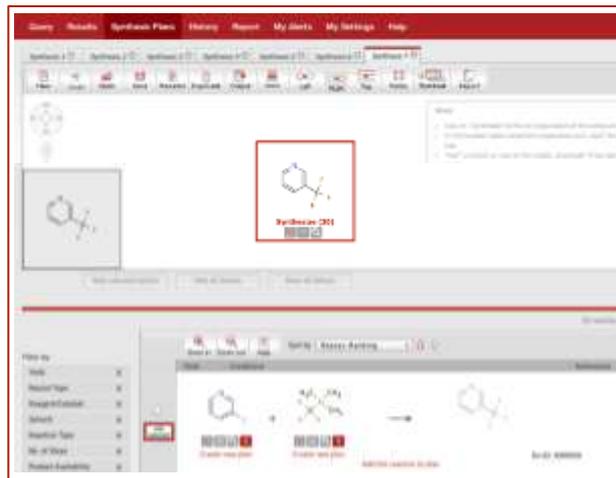
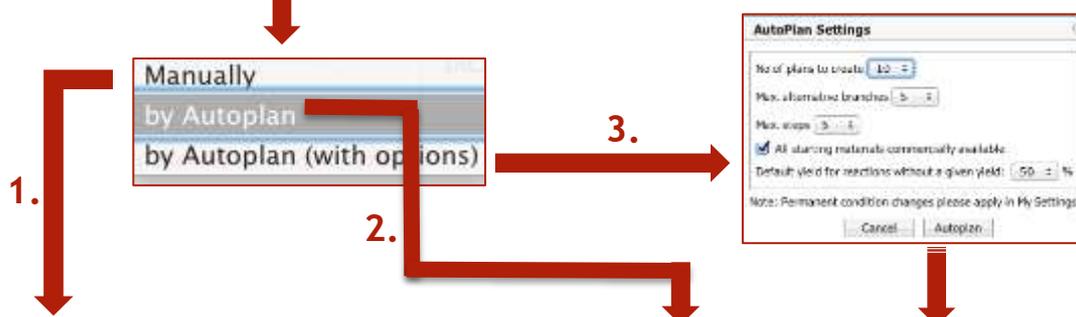
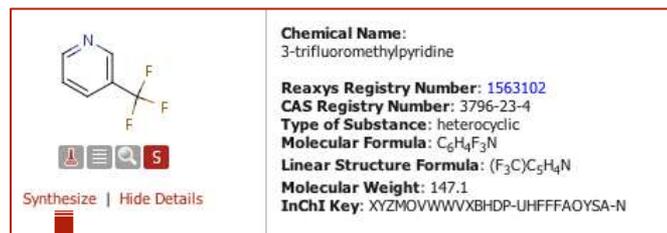
- ◆ The “Synthesize” link
- ◆ Structure search for substances => look for preparations and reactions
 - ◆ Structure search with reaction diagrams
- ◆ Specifying reacting centres through marking bonds
 - ◆ Retrosynthetic analysis through marking bonds
 - ◆ Atom mapping
 - ◆ The “Find similar reactions” link
- ◆ Similarity search with reaction diagrams
 - ◆ Stereochemistry
 - ◆ Synthesis Plans

THE “SYNTHESIZE” LINK

A SIMPLE OPTION TO PLAN SYNTHETIC ROUTES TO A SINGLE SUBSTANCE

Synthesize

- ◆ Below substances are links: **Synthesize**
- ◆ Click this when you want to find preparations of a single substance
- ◆ This link opens up a menu with 3 options:
 1. **Manually** opens a screen that shows the substance and a number of synthetic routes
 - ◆ The routes are shown underneath the screen - click those of interest, and then click Add
 - ◆ You then build your own synthetic routes to the substance
 2. **by Autoplan** opens up a number of plans:
 - ◆ You scroll through the different tabs and develop your own synthesis tree
 3. **by Autoplan (with options)** allows you to choose options for how many plans you wish to see, and your requirements for the plans
- ◆ **Synthesize** offers a simple and straight forward way to help you choose the syntheses of interest, and then to explore details further
 - ◆ For example, you may then create a Report, e.g., to share with colleagues



PREPARATION OF SUBSTANCES

STRUCTURE SEARCH IN THE SEARCH SUBSTANCES CONTEXT;
CLICK LINKS TO PREPARATIONS AND REACTIONS

STRUCTURE SEARCH FOR SUBSTANCES

- To find preparations for a group of substances related by structure, you may:
 - Perform a (sub)structure search under the Substances Icon (i.e., in the Search Substances Context)
 - Click links to preparations in the column: N° of preparations
- You may also click the Reactions Tab to view reaction information directly

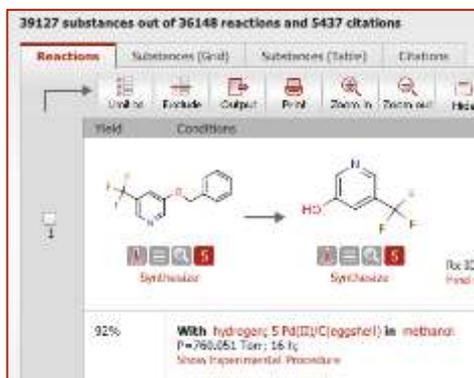


39127 substances out of 36148 reactions and 5437 citations

Filter by:

- Sub-structure
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Biocatalysis
- Biological Data
- Natural Product
- Availability
- Availability in other DBs

Structure	Structure/Compound Data	# of preparations out of # Reactions
	Chemical Name: 2-chloro-5-(trifluoromethyl)pyridine Reaxys Registry Number: 3648688 CAS Registry Number: 52334-81-3 Type of Substance: heterocyclic Molecular Formula: C ₇ H ₄ ClF ₃ N Linear Structure Formula: C7C1H4ClF3N1 Molecular Weight: 181.545 InChI Key: JFZMS0000AGV-GHFFADYSA-N	13 prep out of 679 reactions.
	Chemical Name: 2,3-dichloro-5-(trifluoromethyl)pyridine Reaxys Registry Number: 4992810 CAS Registry Number: 69045-84-7 Type of Substance: heterocyclic Molecular Formula: C ₇ H ₂ Cl ₂ F ₃ N Linear Structure Formula: C7H2Cl2F3N1 Molecular Weight: 215.99 InChI Key: MWBOMWGLQJG-GHFFADYSA-N	11 prep out of 412 reactions.
	Chemical Name: 2-chloro-3-(trifluoromethyl)pyridine Reaxys Registry Number: 4179716 CAS Registry Number: 52733-42-1 Type of Substance: heterocyclic Molecular Formula: C ₇ H ₄ ClF ₃ N Linear Structure Formula: ClC7H4ClF3N1 Molecular Weight: 181.545 InChI Key: 8XWZPCOM9ME-GHFFADYSA-N	4 prep out of 272 reactions.



PREPARATION OF SUBSTANCES

STRUCTURE SEARCH IN THE SEARCH REACTIONS CONTEXT

SUBSTRUCTURE SEARCH FOR REACTIONS

- ◆ To find preparations for a group of substances related by structure, you may also search in the Search Reactions Context:

1. Click the Reactions Icon
2. Draw the structure and transfer it to the reaction query screen
3. Click Please select role Product
4. Click Search Reactions

Reaxys displays reactions. Remember each reaction is displayed separately (with different conditions and references under each reaction)

- ◆ Depending on the reaction query, you may get a large number of substances, which you may narrow through **Filter by:** (e.g., by substance or reaction filters) and/or **Analysis View**
- ◆ This process (and the process described in the previous slide) give answer sets for the preparations of substances, but it does not specify starting materials or the type of reaction involved
- ◆ Suggestions on how to search for specific conversions are shown on the next slides

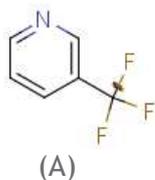
The screenshot shows the Reaxys search interface. At the top, there are navigation icons for Reactions, Substances, Literature, PolicyTree, Physical, Spectra, and Natural Prod. Below these, the 'Reactions' icon is highlighted. In the center, a chemical structure of a pyridine ring with a trifluoromethyl group is being drawn. To the right of the structure, there are several checkboxes for search criteria: 'As drawn', 'Substructure', 'as heteroatoms', 'as all atoms', 'Stereo', 'Exclude isotopes', 'Ignore stereo', 'No isotopes', 'No charges', 'No radicals', 'No ring closures', 'Ignore atom mappings', 'Align results with query', 'Keep fragments', 'Advanced', and 'Regular'. At the bottom, there are radio buttons for 'Please select role' with 'Product' selected, and other options like 'Starting material', 'Reagent / Catalyst', and 'Any role'. A red 'Search Reactions' button is at the bottom right.

The screenshot shows the Reaxys search results page. At the top, there is a search bar and an 'Open Analysis View' button. Below the search bar, there is a summary: '35069 reactions out of 30622 substances and 3256 citations'. On the left, there is a 'Filter by:' section with various filters like Sub-structure, Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type, No. of Steps, Product Availability, Reactant Availability, and Availability in other DBs. Below these are more filters like Molecular Weight, Number of Fragments, Physical Data, Spectroscopic Data, Reactivity, Ecological Data, Natural Product, Availability, and Availability in other DBs. The main content area shows a list of reactions. The first reaction is highlighted, showing a chemical structure of a pyridine derivative and its conditions: 'With hydrogen; 5 PdCl₂(C(eggshell) in methanol; P=760.051 Torr; 16 h; Show Experimental Procedure'. The second reaction is '69.9% With hydrogen; palladium on activated charcoal in methanol; water; T=50°C; P=2844.36 Torr; 48 h; Show Experimental Procedure'. The third reaction is 'With palladium monochloride in methanol; Show Experimental Procedure'. The page also includes a 'Reactions' tab and a 'Sort by' dropdown menu set to 'Reaxys-Ranking'.

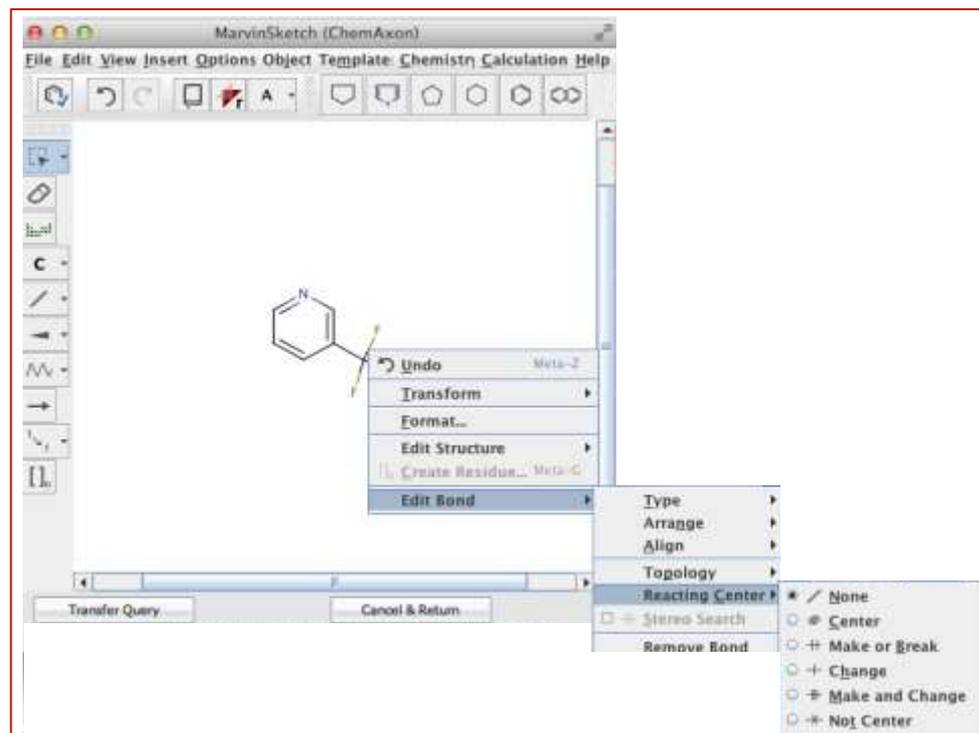
SPECIFYING REACTING CENTERS

REACTING CENTERS => MARK BONDS

- ◆ The reaction query on the previous slide may be modified to require that specific bonds take part in the reaction
- ◆ A simple way to do this is to “right click” on the bond of interest, then choose **Edit Bond => Reacting Center**
- ◆ The default is None, but this may be overridden by any one of the 5 options shown
- ◆ The most general option is # Center and if this is chosen then that bond will be involved in the reaction; the query structure (A) has cross lines at an *angle* to the bond. If + Make or Break is chosen, the query structure (B) has cross lines at *right angles* to the bond



- ◆ In many cases very similar answer sets are obtained from queries (A)/(B)



SPECIFYING REACTING CENTERS

Center versus + Make or Break

- ◆ The different options to specify reacting centers may give different answer sets, and the differences depend on the query involved
 - None
 - # Center
 - + Make or Break
 - Change
 - # Make and Change
 - Not Center
- ◆ The approach, if you are not getting the types of answers expected, is simply to try a few different options
- ◆ In the case of queries (A) and (B) (previous slide), query (A) gives two additional answers that involve the replacement of ^{19}F with ^{18}F

For a comment on Answer #1, go [here](#)

RETROSYNTHETIC ANALYSIS THROUGH SPECIFYING REACTING CENTERS

RETROSYNTHETIC ANALYSIS

- ◆ If a substance is known then the first steps are to find whether the substance is commercially available or whether there is a known, efficient synthesis
- ◆ **Reaxys** provides information on both of these and most easily through the links  and **Synthesize** respectively
- ◆ If the substance is not known, or if alternative synthetic methods are required, then the synthetic chemist may undertake a retrosynthetic analysis
- ◆ One way to do this is to use the functions in Reacting Centers, and in particular through marking bonds to be formed
- ◆ For example the query (right) does a “retrosynthetic analysis” of starting materials where the bond indicated is formed
- ◆ An even more general query is shown below (CHC = any heterocyclic ring)
 - ◆ This search gives > 4,000 answers, and one is shown



95% **With** copper(I) iodide; fluoroacetyl(2-fluoroacetic acid methyl ester) in N,N-dimethyl-formamide
T=120°C; 5 h; Sealed tube;
Show Experimental Procedure

97.3% **Stage #1:** (trifluoromethyl)-trimethylsilane **With** potassium fluoride; copper(I) iodide in tetrahydrofuran; N,N-dimethyl-formamide
T=20 - 50°C; 21 h;
Stage #2: 3-iodo-2,6-dichloropyridine in tetrahydrofuran; N,N-dimethyl-formamide
T=50°C;
Show Experimental Procedure



60% **With** potassium fluoride; Foid Red No. 105 in acetonitrile
T=20°C; 48 h; Irradiation;
Hide Experimental Procedure

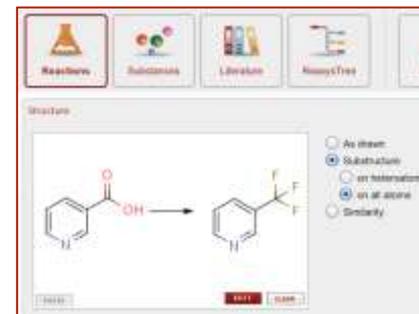
Fu, Weijun; Guo, Wenbo; Xu, Chen; Zou, Guanglong
Journal of Fluorine Chemistry, **2012**, vol. 140, p. 88 - 94
Title/Abstract Full Text View citing articles Show Details

4.2. Typical procedure for trifluoromethylation of tetrahydroisoquinolines
General procedure: RB (0.015 mmol, 5 molpercent) was added to a mixture of 2-phenyl-1,2,3,4-tetrahydroisoquinoline 1a (0.3 mmol), potassium fluoride (1.5 mmol) and trifluoromethyltrimethylsilane (1.5 mmol) in CH₃CN (3 mL). The resulting mixture was stirred at room temperature under green LEDs irradiation. After 1a was completely consumed (monitored by TLC), the solvent was removed in vacuo. The crude product was directly purified by SiO₂ gel column chromatography to give the corresponding product 2a.

ATOM MAPPING

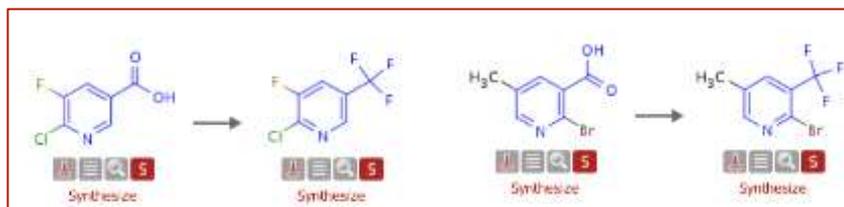
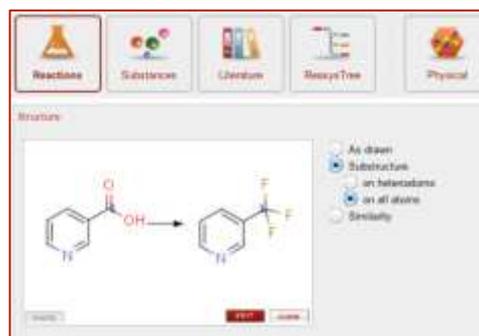
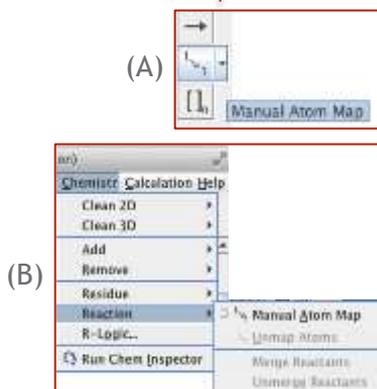
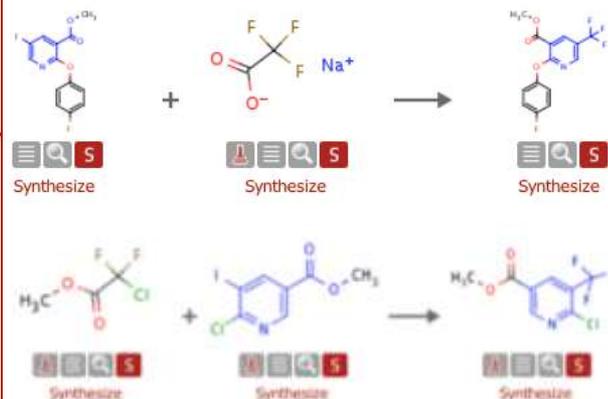
STARTING MATERIALS => PRODUCTS

- ◆ When a reaction query involves the conversion of specific reactants to products, e.g., the query on the right, then **Reaxys** performs a substructure search of the reactants and of the products, and retrieves reactions in which respective substructures are present
- ◆ However, if the intent of the query was to convert nicotinic acid derivatives to 3-trifluoromethylpyridines then some of the answers, e.g. those shown on the right, would not necessarily be of interest
- ◆ The solution is to map atoms in the reactants and products, and in **MarvinSketch** this may be done either through the Manual Atom Map icon in the left panel (A), or through the Chemistry drop-down menu (B)
- ◆ Having clicked either of these, you simply click on the atom in the reactant, drag to the required atom in the product, and then release
- ◆ The process, and outcomes (2 sample answers), are shown below



SOME OF THE ANSWERS

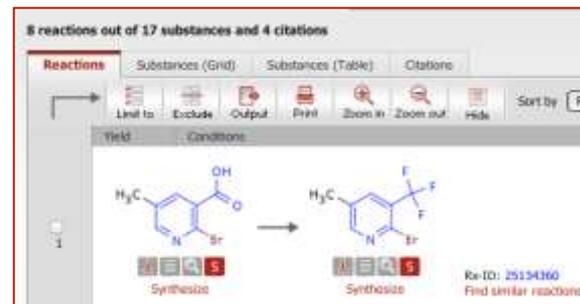
ONE OF THE REACTANTS HAS THE NICOTINIC ACID PART STRUCTURE AND THE PRODUCT HAS THE 3-TRIFLUOROMETHYLPYRIDINE PART STRUCTURE



FIND SIMILAR REACTIONS

FIND SIMILAR REACTIONS

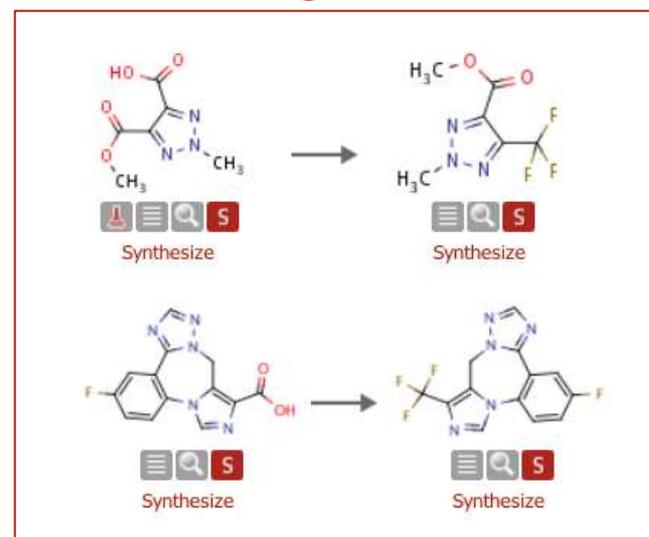
- ◆ Each different reaction in **Reaxys** is given a Reaction ID (Rx-ID), and all references to this reaction are given in a single display
- ◆ Underneath the Rx-ID is a link **Find similar reactions**
- ◆ When this is clicked, **Reaxys** considers the bonds formed/broken in the actual reaction, and then looks at the non-reacting atoms elsewhere in the structure(s)
 - ◆ i.e., **Reaxys** looks for the same conversion, but in different structure(s)
- ◆ The similarities of the non-reacting atoms are then specified as Tight, Near, Medium, Wide, and Widest; the usual process is to look at some of the categories in turn, and choose reactions of interest
- ◆ Further help on **Find similar reactions** is available at http://help.elsevier.com/app/answers/detail/a_id/3911/p/9459/kw/similar%20reactions



Find Similar Reactions by Transition States...

Click on one of the hyperlinks below for getting similar reactions according to the selected scope; the reactions were determined by regarding **similar transition states** based on your reaction query:

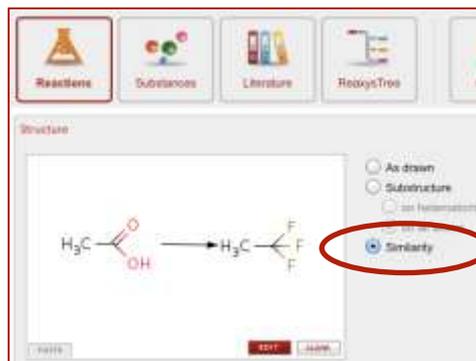
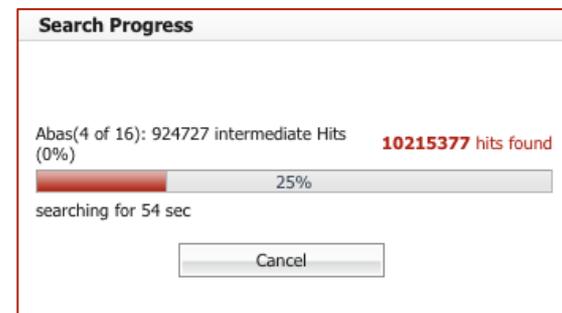
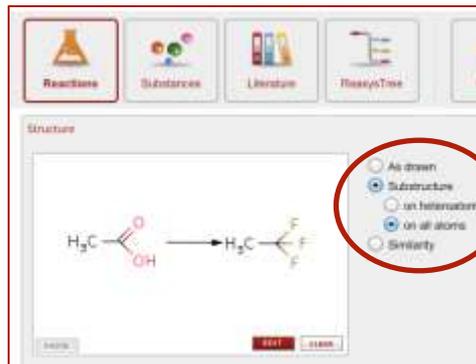
Query Reaction	Tight	Near	Medium	Wide	Widest
	1	3	23	95	95



REACTION SEARCH: SIMILARITY

SIMILARITY SEARCH FOR REACTIONS

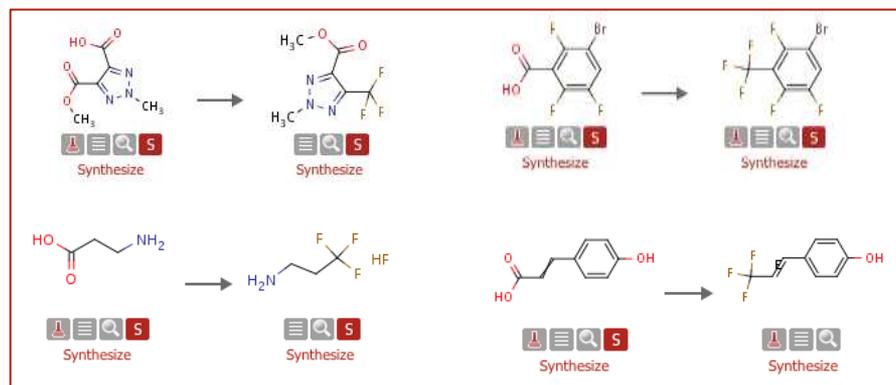
- ◆ There are three main choices for searching reactions by structure in the Reaction Query Context:
 - ◆ **As Drawn** - the precise reaction drawn is searched
 - ◆ **Substructure** - structure queries are searched as substructures, i.e. substituted at allowed positions
 - ◆ **Similarity** - the chemical transformation indicated is searched
- ◆ When very general reaction queries, e.g., the conversion of one functional group (COOH) to another (CF₃) are searched by substructure, the structure search screening process may take several minutes
 - ◆ For example, the screening process for the reaction query (by substructure) on the top right is only 25% complete after almost 1 minute and millions of candidates have past the screening process; all these then will need to be matched atom-by-atom
- ◆ A solution is to use **Similarity**, and in this case similar reactions are identified in less than a second
 - ◆ (Some answers are shown)



Reaxys: Find Similar Reactions by Transition States...

Click on one of the hyperlinks below for getting similar reactions according to the selected scope; the reactions were determined by regarding similar transition states based on your reaction query:

Query Reaction	Tight	Near	Medium	Wide	Wildcard
<chem>CC(=O)O >> CC(F)(F)F</chem>	1	151	191	191	255



SEARCHING STEREOCHEMISTRY IN REACTION QUERIES

SEARCHING STEREOCHEMISTRY

- ◆ Stereochemical features may be built into reaction queries, and may be searched in **Reaxys**
- ◆ For example, if you wished to find reactions for α -hydroxycarboxylic acids (and derivatives) in which the stereochemistry was inverted at the α -C then you could build the reaction query on the left (below)
- ◆ One of the answers is shown
- ◆ If required, reactions may be narrowed through **Filter by: Reaction Type** gives further information about the types of reactions involved (note: mitsunobu reaction)
- ◆ You may also wish to search for Mitsunobu Reactions through **ReaxysTree**!

Navigation icons: Reactions, Substances, Literature, ReaxysTree, Physical.

Search:

Filter by: Sub-structure, Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type

Reaction Type Filter:

Reaction Type	Count
<input type="checkbox"/> mitsunobu reaction	11
<input type="checkbox"/> esterification	5
<input type="checkbox"/> ester-ester reaction	5
<input type="checkbox"/> mitsunobu coupling	4
<input type="checkbox"/> methylation	1
<input type="checkbox"/> alkylation	1
<input type="checkbox"/> dealkylcarbonylation	1

ReaxysTree:

- chemical transformations
 - named reaction
 - Mitsunobu Reaction

Structure:

C[C@H](O)C(=O)O >> C[C@@H](O)C(=O)O

Filter by:

- As drawn
- Substructure
 - on heteroatoms
 - on all atoms
- Similarity

Include options:

- Include tautomers
- Ignore stereo
- No isotopes
- No charges
- No radicals
- No ring closures
- Ignore atom mappings
- Align results with query
- Keep fragments
 - separate
 - together

256 reactions out of 364 substances and 95 citations

Filter by: Sub-structure, Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type

Reaction Type Filter:

Reaction Type	Count
<input type="checkbox"/> mitsunobu reaction	11
<input type="checkbox"/> esterification	5
<input type="checkbox"/> ester-ester reaction	5
<input type="checkbox"/> mitsunobu coupling	4
<input type="checkbox"/> methylation	1
<input type="checkbox"/> alkylation	1
<input type="checkbox"/> dealkylcarbonylation	1

Reaction Example:

CC(O)C1=CC=C(Cl)C=C1 + O=C(O)C1=CC=C(N)C=C1 >> CC(O)C1=CC=C(C1)C=C1

Yield: 88%
With: triphenylphosphine; diethylazodicarboxylate in tetrahydrofuran
T=0 - 20°C; Inert atmosphere;
Show Experimental Procedure

Reference: Davis, Gary C.; Hansen, Todd; Brown, Milton L.; Cordova, Antoinette; Dakshnamurthy, Shvanesan; Davis, Gary C.; Hansen, Todd; Kong, Yali; Li, Zhang; Paige, Mikell; Su, Siwen; Wang, Kan; Merrick, Ellen C.; Patel, Manoj K.; Williams, Brande S.; Chruszcz, Maksymilian; Minor, Wlodek; McManus, Owen B. *Inorganic and Medicinal Chemistry*, 2012, vol. 20, # 6 p. 2180 - 2188
Title/Abstract Full Text View citing articles Show Details

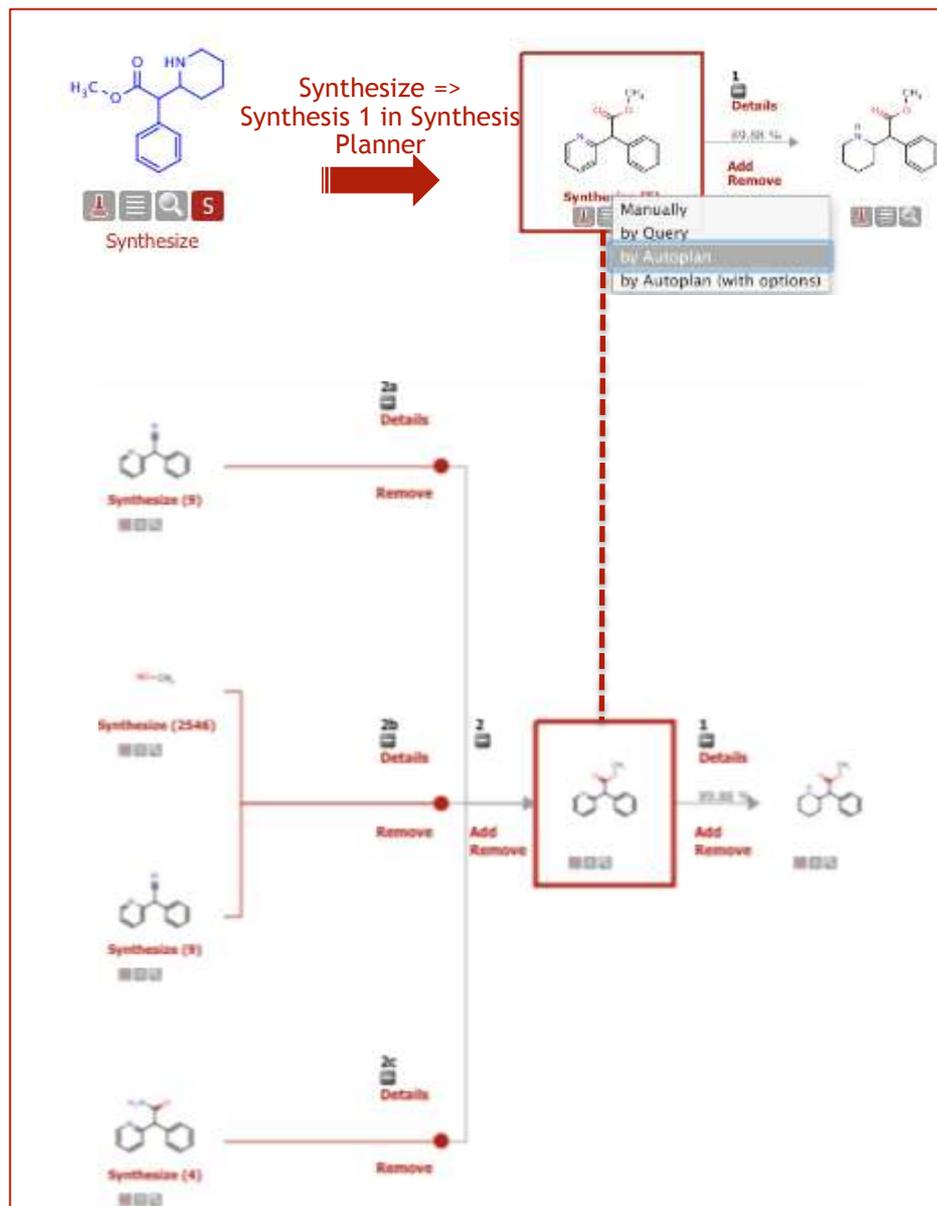
Synthesize opens SYNTHESIS PLANNER

- ◆ One way to open the Synthesis Planner is to click on the **Synthesize** link below the structure
- ◆ You choose the option required (e.g., by **Autoplan**) and the first (of a number of plans) is displayed
- ◆ If you need to go back further, simply click the **Synthesize** link under the starting material (e.g., on the pyridine precursor) and earlier steps are displayed
- ◆ Click **Remove** if you are not interested in a particular method
- ◆ Click **Add** to add another branch to the preparation of the compound
- ◆ Notes:
 - ◆ you may set your own Autoplan requirements through **My Settings**



- ◆ algorithms behind Autoplan choose highest yielding routes and ...

this is very convenient since when there are a large number of preparative options, **Reaxys** ranks displays in the Synthesis Planner so preferred methods are shown first



A FULL SYNTHESIS PLAN

Synthesize (97)
[Icons]

Synthesize (303)
[Icons]

Synthesize (65)
[Icons]

Synthesize (4)
[Icons]

Synthesize (2568)
[Icons]

Synthesize (9)
[Icons]

2a
[Icon]
Details

Remove

3a
[Icon]
Details

90.00 %

Remove

3
[Icon]

Add Remove

2b
[Icon]

Remove

2
[Icon]

Remove

1
[Icon]

Remove

- ◆ Your full plan may look like this
- ◆ Click Details to display reaction conditions ([click here now](#))

Step	Yield	Conditions	References
1 Reacts	89.88%	Stage #1: With perchloric acid; hydrogen; acetic acid; palladium on activated carbon in methanol; water T=45 - 50°C; P=8826.87 - 11033.6 Torr; 15 - 18 h; Stage #2: With sodium hydroxide in water Show Experimental Procedure	IPCA Laboratories Limited Patent: EP1807388 A3, 2005 Location in patent: Page/Page column 4 Title/Abstract Full Text Show Details
	89.88%	Stage #1: With perchloric acid; hydrogen; palladium on activated carbon in methanol; acetic acid Stage #2: With sodium hydroxide in water Show Experimental Procedure	Kumar, Ashok; Singh, Dharmendra; Patil, Swapnil Hemant; Mahale, Devdatta; Sawant, Uttamrao Arjunrao Patent: US2005/277667 A1, 2005 Location in patent: Page/Page column 3 Title/Abstract Full Text Show Details
2a Reacts		With hydrogenchloride; methanol	Kloss Archiv der Pharmazie (Weinheim, Germany), 1953 , vol. 266, p. 433,436 Full Text Show Details
2b Reacts		Stage #1: With hydrogenchloride T=0°C; 0.333333 h; Stage #2: T=23°C; 18 h; Show Experimental Procedure	Pfizer Inc. Patent: US6407120 B1, 2002 Location in patent: Page column 26 US 6407120 B1 Title/Abstract Full Text Show Details
2c Reacts		With hydrogenchloride; sodium hydroxide in methanol; hexane; ethyl acetate Show Experimental Procedure	Hoffmann-La Roche Inc. Patent: US548522 B1, 2003 US 6548522 B1 Title/Abstract Full Text Show Details
2a Reacts	90%	With sodium amide in toluene T=0 - 30°C; 17 h;	Celgene Corporation Patent: US5359139 B1, 2002 Location in patent: Example 1 Title/Abstract Full Text Show Details
	68%	With potassium tert-butoxide in 1-methyl-pyrrolidin-2-one T=110°C; 0.0166667 h; microwave irradiation;	Cheng, Yin-Jia Tetrahedron, 2002 , vol. 58, # 24 p. 4931 - 4925 Title/Abstract Full Text View citing articles Show Details
		With sodium amide; toluene	Parizzon Helvetica Chimica Acta, 1944 , vol. 27, p. 1748,1753 Full Text Show Details Kloss Archiv der Pharmazie (Weinheim, Germany), 1953 , vol. 266, p. 433,436 Full Text Show Details

Other Syntheses of Ritalin

- ◆ The previous set of slides developed a plan from “Synthesis 1”
- ◆ However, **Reaxys** generated other plans, e.g. “Synthesis 6” (second tool bar)
- ◆ Note the various functions in the third tool bar: Save, Resize, Report...
- ◆ Note also you can click **Help** (click [Help](#) now)

- ◆ Reaxys contains numerous Help messages
- ◆ Once you enter Help, type in the search box

The screenshot displays the Reaxys Synthesis Planner interface. At the top, there are tabs for 'Query', 'Results', and 'Synthesis Plans'. Below the tabs is a search bar containing 'synthesis planner' and a 'Contact Us' link. The main content area is titled 'Synthesis Planner' and contains a description of the tool's capabilities. Below the description is a list of actions: 'AutoPlan', 'Select a substance and begin a new synthesis plan', 'Open a saved synthesis plan', 'Begin a Synthesis Plan from the Synthesis Planner', and 'Export or print a synthesis plan'. At the bottom, there is a table of results with columns for 'Step', 'Reaxys', 'Description', and 'References'. The first result shows a reaction scheme for the synthesis of Ritalin (methylphenidate) from a precursor, with a yield of 45.00%. The second result is a patent entry for Merrell Pharmaceuticals Inc. (US5519048 A, 1996).

REAXYS

synthesis planner

Contact Us

Back to List

Synthesis Planner

The Synthesis Planner can be used to create a pathway of reactions starting from compounds, which are commercially available, up to a target compound, which has previously been found during a reaction or substance search. The Synthesis Planner can be started from any compound visible in the result view: simply click the **Synthesize** link below a structure. You can manually create a synthesis plan or use the **AutoPlan** feature.

AutoPlan - The quickest way to create a retrosynthetic plan is to use the **AutoPlan** feature. AutoPlan lets you preselect certain criteria and automatically creates up to 10 unique synthesis plans when you click the synthesize link below a substance.

- [AutoPlan](#)
- [Select a substance and begin a new synthesis plan](#)
- [Open a saved synthesis plan](#)
- [Begin a Synthesis Plan from the Synthesis Planner](#)
- [Export or print a synthesis plan](#)

Step	1	Reaxys	Stage #1: C ₁₀ H ₁₂ N ₂ O ₂ With C ₁₀ H ₁₂ ClNO ₂ in dichloromethane; Mannich reaction; 0.166667%; Inert atmosphere;	Notte, Gregory T.; Baxter Vu, Jenny M.; Leighton, James L. <i>Organic Letters</i> , 2011 , vol. 13, # 4 p. 816 - 818 Title/Abstract Full Text View citing articles Show Details
	2	Reaxys	Stage #2: 1-methoxy-2-phenyl-1-(trimethylsilyloxy)ethylene in dichloromethane; T=0°C; Mannich reaction; 1.5%; Inert atmosphere; optical yield given as percent enantioselective reaction;	
	4	Reaxys	With triethylsilyl trifluoromethanesulfonate; triethylamine in dichloromethane; Show Experimental Procedure	Merrell Pharmaceuticals Inc. Patent: US5519048 A, 1996 ; US 5519048 A Title/Abstract Full Text Show Details

Supplementary Slides

FURTHER PRESENTATIONS IN THIS SERIES

REAXYS R101

A QUICK GUIDE

An overview of the functions of Reaxys 2014

REAXYS R102

TIPS FOR LITERATURE SEARCHING

A quick guide to searching literature

REAXYS R103

BASIC SUBSTANCE QUERIES

A quick guide to searching for specific substances by name, formula and structure

REAXYS R104

BASIC REACTION QUERIES

A quick guide to searching for chemical reactions

REAXYS R105

SEARCHING PROPERTIES

A quick guide to searching for properties

REAXYS R201

ADVANCED STRUCTURE SEARCHING

Searching by substructure

REAXYS R202

ADVANCED NAME AND FORMULA SEARCHING

Searching for Substances by Names and Formulas

REAXYS R203

ADVANCED REACTION QUERIES

Additional ways to search for reactions

INCONSISTENT DATA?

- ◆ At times data may appear “inconsistent” and this may be because of a variety of reasons including apparent errors/inconsistencies:
 1. In the original documents
 2. In the input of data into the database
 3. In the way the search engine interprets the query and in the way the data is presented in answers
- ◆ For example:
 - ◆ the answer on the right (above) mentions the reactant 5-fluoromethyl-2-mercaptopyridine in the Experimental Procedure and shows this substance in the reaction diagram but the starting material should be 5-trifluoromethyl-2-mercaptopyridine
 - ◆ the answer on the right (below) describes a phenyl tetrahydroisoquinoline whereas the diagram shows the reaction of the benzyl derivative (in this case the issue is the reporting of a general procedure, whereas the actual reaction describes a specific example)
- ◆ The addition of millions of records annually is challenging, and databases endeavour to maintain data quality
- ◆ However “inconsistencies” arise and, when detected, users are encouraged to report them to the database producer
- ◆ Additionally, authors and referees (unfortunately data in patents is not refereed) need to be vigilant to ensure the quality of the original data

