

Reaxys Xcelerate - Less Searching. More Discovery.

Does your Research workflow

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Introduction

Reaxys Xcelerate is a new premium version of Reaxys. Reaxys is a web based workflow tool for synthetic chemists. It is designed to support the optimization of synthetic processes and offers a valuable resource for accurate & validated experimental reaction & substance data.

Reaxys & Reaxys Xcelerate

Greater productivity throughout the chemistry research workflow. Immediate insights and ability to make correlations between the results for informed decision making. **Reaxys Xcelerate** is about bringing greater conveyance to complex searches and enabling more insights earlier in the research process.

- Organic, inorganic, organometallic chemistry from 400 journals
- Coverage from 1771 - present
- English language World, EU and US Patent Office patent from the major chemistry patent classes

Workflows

Some typical workflow scenarios (from agrochemicals, medical chemistry and general organic chemistry) demonstrate the usefulness of **Reaxys Xcelerate** to your every day chemistry research:

- Reduced data analysis complexity** when faced with large amounts of data
- Automated synthesis plans** to view and analyze numerous potential routes
- Instant information exchange** possibilities: global terms and diverse research groups can share ideas and information instantly

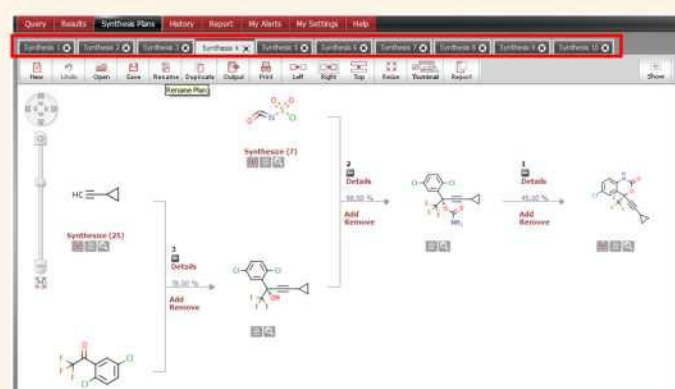
LAB TO PILOT SCALE UP: SYNTHETIC METHODOLOGIES

Sustiva (Efavirenz) for the treatment of HIV type 1

Efavirenz (EFV, brand names **Sustiva** and **Stocrin**) is a non-nucleoside reverse transcriptase inhibitor (NNRTI) and is used as part of highly active antiretroviral therapy (HAART) for the treatment of a human immunodeficiency virus (HIV) type 1. Efavirenz was approved by the FDA on September 21, 1998, making it the 14th approved antiretroviral drug

1: Efficient and Reproducible Synthetic Methods
2: Transfer of technology to Production plants
3: Use of least hazardous Reagents and solvents
4: Commercially available reagents

Create 10 synthetic plans simultaneously for the query



Report Research or Substance to your supervisor or colleague

Create the query by using "Generate structure from name" or draw in structure editor of your choice

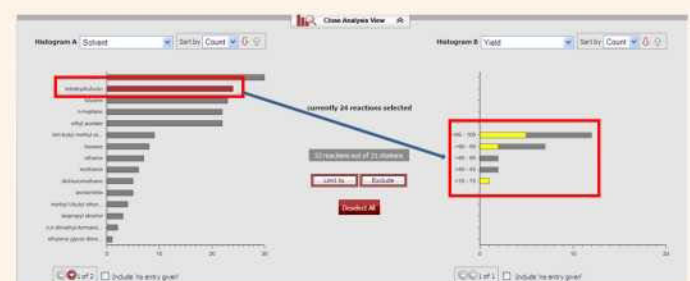
Create a report of the synthetic plan in format of your choice

Annotate for a reaction or substance

Generic name converted to a chemical structure

View the full experimental process exactly reported in Patent or Article

Do an analysis of the reaction or substance e.g. based on Solvent or Yield



34 substances for the query with 52 preparations methods for first substance
Click synthesis to create a synthetic plan manually or automatically

View the spectral information like NMR data for a substance

Chemical Name and Synonyms	Structure	SMILES	Pubchem ID	Pubchem Name
2-((4-chlorophenyl)amino)-2-methylpropan-1-ol		CC(C)(C)Nc1ccc(Cl)cc1	10100	2-((4-chlorophenyl)amino)-2-methylpropan-1-ol
2-((4-chlorophenyl)amino)-2-methylpropan-1-ol		CC(C)(C)Nc1ccc(Cl)cc1	10100	2-((4-chlorophenyl)amino)-2-methylpropan-1-ol
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2-((4-chlorophenyl)amino)-2-methylpropan-1-ol		CC(C)(C)Nc1ccc(Cl)cc1	10100	2-((4-chlorophenyl)amino)-2-methylpropan-1-ol
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