

DiscoveryGate® Synthesis Package

Better, faster synthesis of novel compounds

Search by structure to locate starting materials and intermediates, design solution-phase and solid-phase combinatorial libraries and develop plans for entirely novel syntheses. Search over multiple databases with a single query and integrate in-house data.

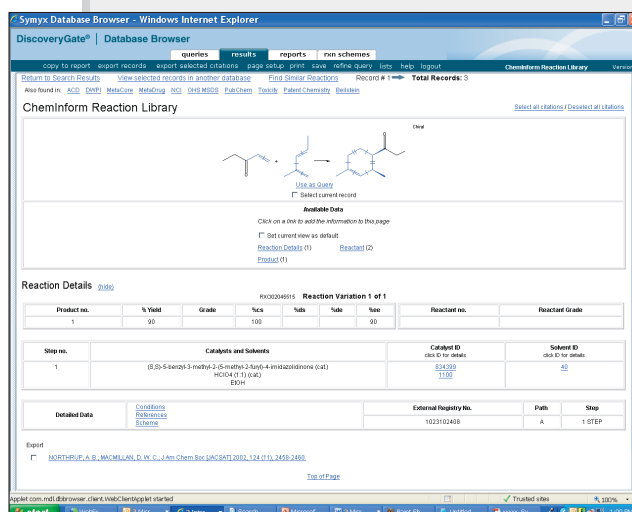
Chemical sourcing information

- **Symyx Available Chemicals Directory (ACD)** provides complete chemical supplier catalogs from over 700 suppliers consolidated into a single, easy-to-access, structure-searchable database providing product purities, forms, grades, available quantities, prices and ordering information for over 800,000 unique compounds representing approximately 2.5 million products. In addition to online access via DiscoveryGate, other options for deploying ACD content include in-house installation and access via Symyx Logistics or Symyx ACD Web Service.

Synthetic methodology databases

- **ChemInform Reaction Library (CIRX)** provides reactions of interest to synthetic chemists from 1990 to the present and, in combination with RefLib, over one hundred years of chemical literature citations supporting synthetic methodologies. CIRX is the best source for the synthesis of novel organic compounds, providing scope and limitations of reactions and targeted, highly relevant hit sets. CIRX also contains information on chemo- and regioselective reactions. The Current Synthetic Methodology database, containing the most innovative and significant reactions since 1992, is a subset of CIRX. The RefLib database is included with CIRX. CIRX is produced by FIZ Chemie Berlin.
- **Derwent Journal of Synthetic Methods (DJSM)** includes new synthetic methods, applications of known methods, novel functional group and ring chemistry, protecting group chemistry, high-yield functional group transformations, improvements to existing methodologies and reactions representing the most significant new patents. The database is produced by Thomson Reuters.
- **ORGSYN Database** presents general synthetic methods and proven compound preparations, information on product purity, yield and hazards, as well as references to original procedures and journal sources, as published in the print series, *Organic Syntheses*.
- **Symyx Reference Library of Synthetic Methodology (RefLib)** provides novel organic synthetic methodologies covering functional group transformations, metal-mediated chemistry and asymmetric syntheses, as well as reactions abstracted from Theilheimer's *Synthetic Methods of Organic Chemistry* (1900-1991).
- **Symyx Solid-Phase Organic Reactions (SPORE)** offers information on the scope and limitations of reactions as well as new and novel methodologies on solid support including data on polymeric materials, linkers, solid supports and protecting groups, designed to meet the needs of combinatorial chemists. SPORE is produced by FIZ Chemie Berlin.

With a single search for a target molecule, retrieve synthesis information with related supplier, molecular pathway, toxicity and patent information.

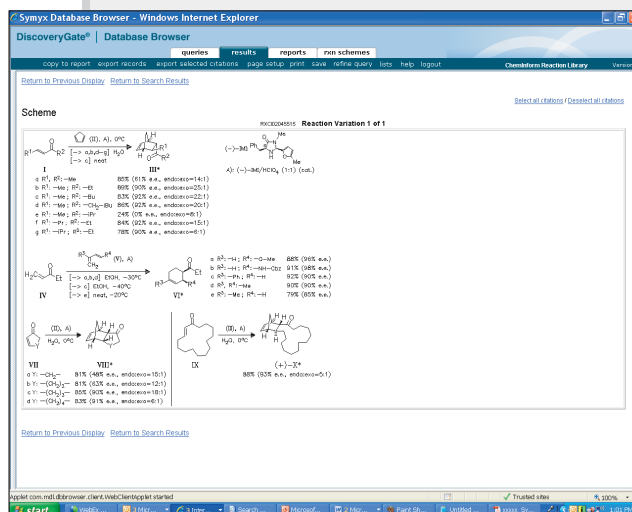


Product no.	% Yield	Grade	Size	Units	Unit	Reactant no.	Reactant Grade
1	90		100		g		

Step no.	Catalysts and Solvents	Catalyst ID	Solvent ID
1	(S)-5-benzyl-3-methyl-2-(S)-methyl-2-allyl-4-imidazolidinone (sulf) HODAP (10 mg)	834399	45

Database	External Registry No.	Path	Step
ChemInform	162202499	A	1 STEP

Search across CIRX, JSM, ORGSYN and SPORE to retrieve reaction pathways to a target molecule.



The screenshot displays a complex reaction scheme with multiple steps (I through IX) and various reagents and conditions. The scheme includes chemical structures and associated reaction conditions such as reagents (e.g., H₂, Pd/C, CuI, CuBr), solvents, and temperatures. The interface also shows a search bar and navigation options.

