

Symyx ISENTRIS Synthesis Package

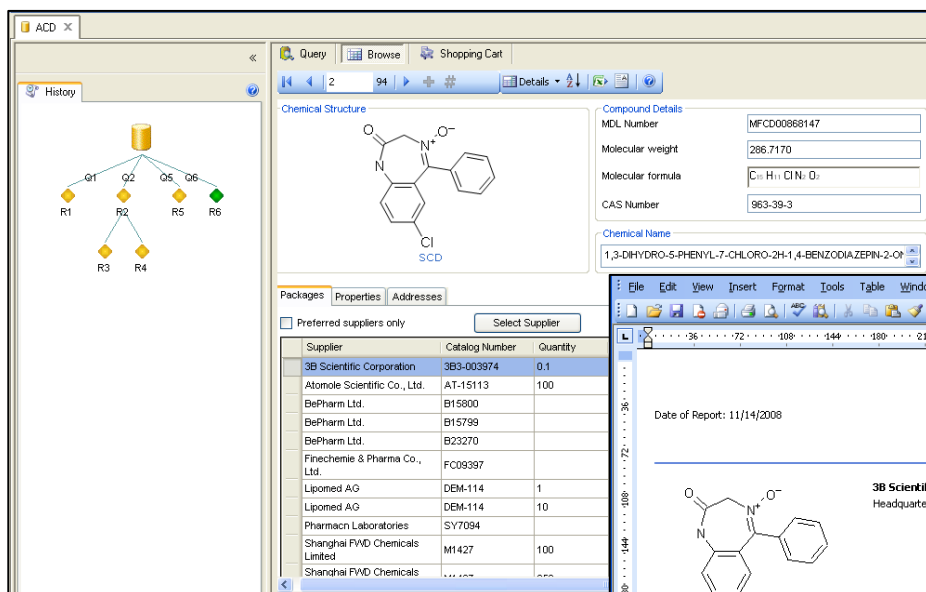
Better, faster synthesis of novel compounds

Reduce time and costs while improving the success of compound synthesis by accessing Symyx's Synthesis Package with ISENTRIS. Design optimal synthesis plans by exploring known reactions, transformations, and reaction schemes. Simple-to-use compound and transformation searches make it easy for the scientist to pick and report the reactions and transformations that will best deliver results. Integration with commercially available compounds offering supplier, packaging, and pricing availability information enables scientists to pick the cheapest and most readily available compounds for synthesis execution.

ISENTRIS provides rich functionality to access the Synthesis databases:

ISENTRIS enables R&D organizations to search in-house and Symyx reaction databases together. An automatic availability flag enables the scientist to see instantly if any component of a reaction is commercially available or available from internal inventories. The novel reaction planner provides multi-step reaction pathways to the desired product based on known reaction transformations, citation information, and reagent availability.

- Search for reactions based on reaction centers, transformation, and components
- Cluster reactions for easy viewing
- Instantly determine if a component of a reaction is available in-house or commercially
- Build, report, and share multi-step reaction plans
- Build a shopping list of compounds for selected multi-step reaction pathways
- Create reports of suppliers, compounds, and packages
- Compile lists of literature citations relevant to the synthesis plan
- Link to online citation details for instant citation access
- Customize forms for searching, browsing, and reporting reaction data

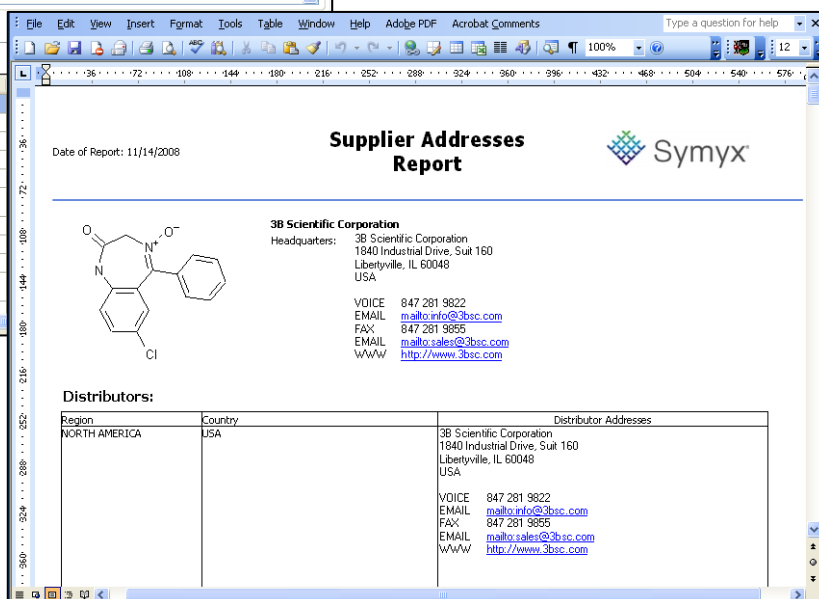


The screenshot shows the Symyx ACD software interface. On the left, a 'History' tree displays a reaction pathway with nodes Q1-Q6 and R1-R6. The main window shows a chemical structure of a benzodiazepine derivative. To the right, 'Compound Details' are listed: MDL Number (MFCD00868147), Molecular weight (286.7170), Molecular formula (C₁₇H₁₄ClN₂O), and CAS Number (963-39-3). Below this, a table lists suppliers and their quantities:

Supplier	Catalog Number	Quantity
3B Scientific Corporation	3B3-003974	0.1
Atomole Scientific Co., Ltd.	AT-15113	100
BePharm Ltd.	B15800	
BePharm Ltd.	B15799	
BePharm Ltd.	B23270	
Finchemie & Pharma Co., Ltd.	FC09397	
Lipomed AG	DEM-114	1
Lipomed AG	DEM-114	10
Pharmach Laboratories	SY7094	
Shanghai FWD Chemicals Limited	M1427	100
Shanghai FWD Chemicals		

Symyx ACD: Quickly find compounds, suppliers, packages, and prices from over 850 suppliers.

Symyx ACD: Generate compound, supplier, and address reports.



The screenshot shows a 'Supplier Addresses Report' generated by Symyx ACD. The report includes the date (11/14/2008) and the Symyx logo. It features a chemical structure of the same compound as in the previous screenshot. The report details the following information for 3B Scientific Corporation:

3B Scientific Corporation
 Headquarters: 3B Scientific Corporation
 1840 Industrial Drive, Suit 160
 Libertyville, IL 60048
 USA

VOICE 847 281 9822
 EMAIL m.alloinfo@3bssc.com
 FAX 847 281 9855
 EMAIL m.allo.sales@3bssc.com
 WWW <http://www.3bssc.com>

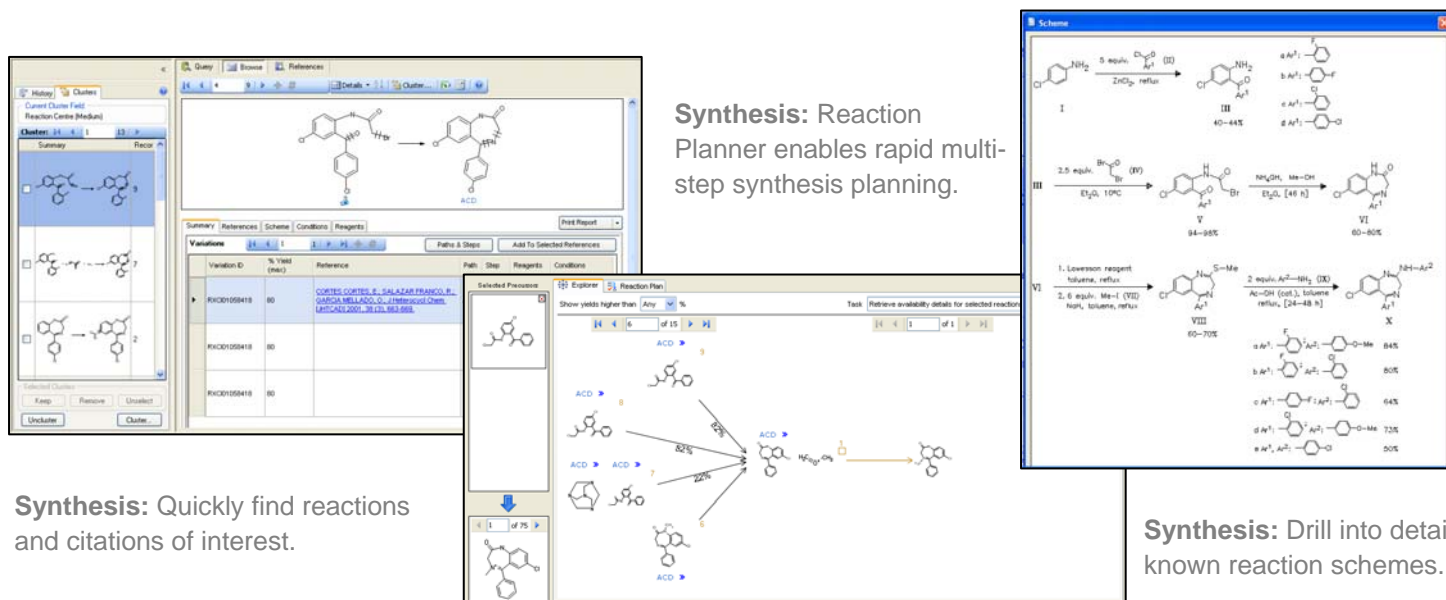
Distributors:

Region	Country	Distributor Addresses
NORTH AMERICA	USA	3B Scientific Corporation 1840 Industrial Drive, Suit 160 Libertyville, IL 60048 USA VOICE 847 281 9822 EMAIL m.alloinfo@3bssc.com FAX 847 281 9855 EMAIL m.allo.sales@3bssc.com WWW http://www.3bssc.com

Included Databases:

Chemical sourcing information

Symyx Available Chemicals Directory (ACD) provides complete chemical supplier catalogs from over 850 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 the DiscoveryGate Web Service.



The image displays three screenshots of Symyx software. The left screenshot shows the 'Current Clusters Field' and 'Reaction Centre (Medium)' with a list of variations and a table of results. The middle screenshot shows a 'Synthesis: Reaction Planner' interface with a reaction scheme and a 'Selected Processes' window. The right screenshot shows a 'Scheme' window with a detailed multi-step reaction scheme.

Synthesis: Reaction Planner enables rapid multi-step synthesis planning.

Synthesis: Quickly find reactions and citations of interest.

Synthesis: Drill into details for known reaction schemes.

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. Current Synthetic Methodology database is a subset of CIRX. RefLib database is included with CIRX.

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*.

SPRESI Database improves decision support in synthesis planning by providing access to over 6 million structures, 3.8 million reactions, and 28 million factual data entries extracted from 636,000 references and 164,000 patents. The data collection includes chemical structures, reactions, chemical/ physical properties, keywords, and factual data abstracted from the most important journals in the field of organic chemistry from 1974 forward. InfoChem GmbH has maintained and distributed SPRESI since 1991.

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. SPORE is produced by FIZ Chemie Berlin.