

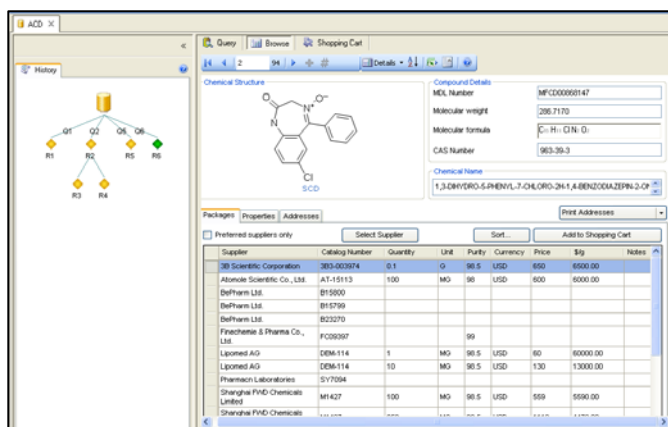
Symyx Isestris Discovery Package

Making fully informed research decisions

Whether a scientist is designing a library for screening, optimizing leads, or selecting the best leads to move forward to the next stage of testing, access to high-quality databases can improve hypothesis and decision confidence. The Isestris Discovery Package helps scientists to better understand drug properties, toxicology, and metabolism on a structural basis. The databases can help in the optimization of library design, synthesis, and selection, while ensuring that scientists take the best candidate leads forward for further experimentation.

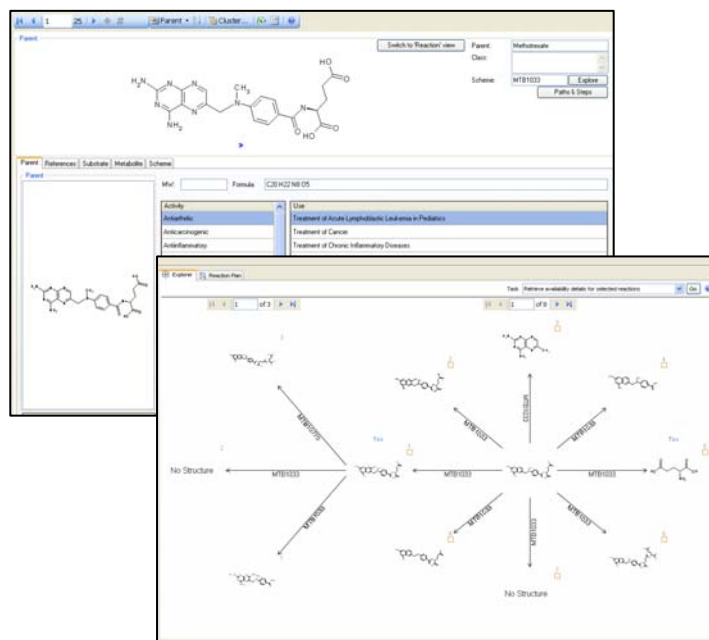
Isestris provides rich functionality to access the Discovery databases:

- Reaction planner enabling rapid exploration of the cheapest, fastest and most productive synthesis procedures
- Citation hyper-linking to source literature information so scientists can obtain literature information without delay
- Customizable search, display, and report forms
- Automatic links from displayed structures to commercial availability of compounds
- Support for integration of in-house and Symyx databases so information can be searched as a single source.
- Metabolite explorer enabling researchers to explore known metabolite routes quickly.
- Automatic links in metabolic pathways to toxicity data indicating toxic metabolic intermediates
- Support for integration of content into existing scientific applications

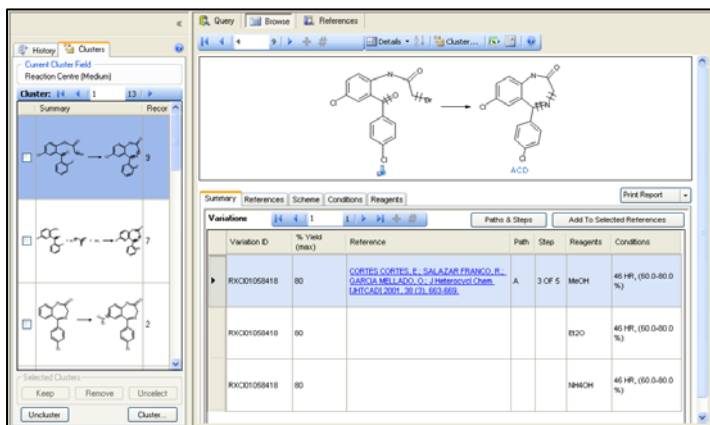


Supplier	Catalog Number	Quantity	Unit	Purity	Currency	Price	Sg	Notes
3B Scientific Corporation	3B3-003974	0.1	G	99.5	USD	650	6500.00	
Abcr Scientific Co., Ltd.	AT-15113	100	MG	98	USD	800	8000.00	
DePharm Ltd.	D15500							
DePharm Ltd.	915759							
DePharm Ltd.	B23270							
Fincohen & Pharma Co., Ltd.	FC03207			99				
Lipomed AG	DEM-114	1	MG	99.5	USD	60	60000.00	
Lipomed AG	DEM-114	10	MG	99.5	USD	130	13000.00	
Pharmaco Laboratories	SV7204							
Shanghai FMD Chemicals Limited	M1427	100	MG	99.5	USD	559	5590.00	
Shanghai FMD Chemicals								

Sourcing: Quickly find compounds, suppliers, packages, and prices



Bioactivity: Explore metabolic pathways and toxicity together



Variation ID	% Yield (max)	Reference	Path	Step	Reagents	Conditions
RXC01058418	80	CORTES-CORTES, E.; SALAZAR-FRANCO, R.; GARCIA-MELLADO, O.; J. Heterocycl. Chem. Lett. 2001, 30(7), 863-869.	A	3 OF 5	MeOH	46 HR, (90.0-90.0 %)
RXC01058418	80				EtOAc	46 HR, (90.0-90.0 %)
RXC01058418	80				NaNH2	46 HR, (90.0-90.0 %)

Synthesis: Choose the right reactions and reaction pathways

Chemical sourcing information - *Easy, cost-effective compound acquisition*

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, available quantities, and prices and ordering information for over 800,000 unique compounds.

Synthetic methodology databases - *Better, faster synthesis of novel compounds*

ChemInform Reaction Library (CIRX) provides reactions of interest to synthetic chemists from 1990 to the present. 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 is produced by FIZ Chemie Berlin.

Current Synthetic Methodology offers the most innovative and significant reactions since 1992, emphasizing new synthetic methodologies, reactions that use new reagents or an important modification of known reagents, and regio-, chemo- and stereoselective reactions carried out on multi-functional substrates. The database is produced by FIZ Chemie Berlin.

Derwent Journal of Synthetic Methods 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

Bioactivity information - *Smarter lead generation*

MDDR provides current bioactivity findings for newly launched and developmental drugs including calculated properties based on chemical structures. The database is produced by Symyx and Thomson Reuters.

National Cancer Institute Databases including CAS Registry (127,000 structures), Plated Compounds, AIDS, and Cancer databases are offered as a public service to Symyx customers.

Symyx Comprehensive Medicinal Chemistry (CMC) offers information on marketed and clinically studied drugs including biochemical properties, drug class, measured logP and pKa, and searchable 3D models. CMC is derived from the Drug Compendium in Elsevier's *Comprehensive Medicinal Chemistry*.

Symyx Screening Compounds Directory (SCD) provides consolidated supplier data from vendors offering diverse, drug-like compounds, product lines and sample collections specifically designed for high-throughput screening programs—over 5.5 million unique compounds in an electronic, structure-searchable format.

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, asymmetric syntheses, chiral and heterocyclic chemistry, 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.

Symyx Metabolite is the world's most comprehensive collection of xenobiotic compounds and biotransformations (primarily medicinal drugs), which also indexes path and scheme information and experimental data from *in vivo* and *in vitro* studies.

Symyx Toxicity is a structure-searchable bioactivity database of toxic chemical substances containing data from *in vivo* and *in vitro* studies of acute toxicity, mutagenicity, skin and eye irritation, tumorigenicity and carcinogenicity, reproductive effects, and multiple dose effects. Toxicity Database includes the complete contents of the Registry of Toxic Effects of Chemical Substances database, the GENE-TOX database (US Environmental Protection Agency) and the Chemical Carcinogenesis Research Information System database (National Cancer Institute).