

Symyx Notebook: More than just a chemistry notebook

To maximize return on investment, an electronic lab notebook (ELN) must enable scientists to re-use and combine knowledge captured from in-house and public sources to accelerate experimental design, document experiment workflows, and improve the success of experiments.

Built on the industry-leading Symyx chemistry foundation, Symyx Notebook supports synthetic chemists in designing experiments, capturing and sharing results, and then combining these results with public sources of information in the context of laboratory workflows.

Execute successful workflows

Symyx delivers more than just an ELN. Symyx supports chemistry workflows by providing commercial sourcing and synthetic methodology databases along with the tools to explore, combine, and report synthesis information. Chemists can search over 6 million reactions and methodologies in the public literature and use these references to design optimal syntheses. As chemists design experiments they are informed of key molecular properties and the commercial availability of compounds, their suppliers, and costs via Symyx Available Chemicals Directory (ACD).

Support effective synthesis planning

Combining Symyx Notebook, Symyx ISENTRIS, and Symyx databases further reduces time and costs while improving the success of compound synthesis. The Symyx Synthesis Package for ISENTRIS provides access to 6 million reactions, methodologies, and links to literature citations. Combine these reactions with reactions captured in Symyx Notebook to create a combined reaction set for use in designing future synthesis steps.

Design synthesis plans with the right information

Symyx ISENTRIS provides unparalleled information and functionality for selecting the right reaction or set of reaction steps. Search by structure to locate starting materials and intermediates. Design solution-phase and solid-phase combinatorial libraries. Develop plans for novel syntheses. Simple-to-use compound and transformation searches with ISENTRIS make it easy for scientists to select and report the reactions and transformations that deliver the best results.

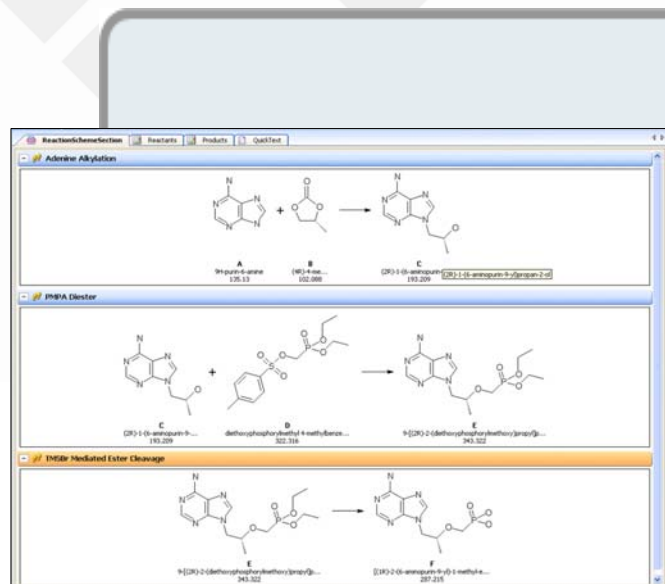
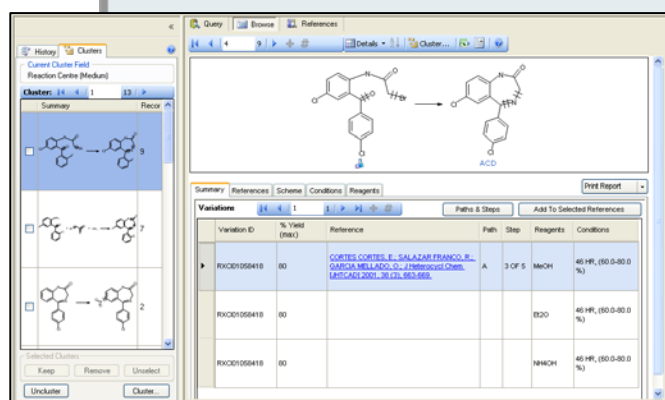


Figure 1: With Symyx Notebook, easily design and capture single- and multi-step linear and convergent reactions into searchable databases for re-use later in planning.



Variation ID	% Yield (max)	Reference	Path	Step	Reagents	Conditions
RXC01050418	80	CORTES CORTES, E.; SALAZAR FRANCO, R.; GARCIA HERRERO, D. // <i>International Chem. Medicines</i> 2002, 30 (1), 403-405.	A	3 OF 5	MeOH	40 HR, (80.0-80.0 %)
RXC01050418	80				EtOAc	40 HR, (80.0-80.0 %)
RXC01050418	80				NHCOH	40 HR, (80.0-80.0 %)

Figure 2: With Symyx ISENTRIS, quickly search and browse over 6 million commercially available reactions as well as in-house reactions.

Lower synthesis costs and accelerate syntheses

While designing a reaction in Symyx Notebook or selecting a reaction from within Symyx Isestris, chemists are automatically informed if compounds of interest are commercially available. Instantly chemists can decide if it is easier to buy or synthesize the compound, or if they should choose a different reaction. Chemists can drill down to commercial suppliers, availability, and compound cost with access to over 800,000 compounds supplied by over 850 suppliers. With instant access to commercial availability and reaction information, synthetic chemists can choose the cheapest and fastest paths to synthesis.

Develop multi-step, retro-synthetic plans in minutes

The Isestris reaction planner enables chemists to navigate through known reactions while assembling multi-step reactions on-the-fly based on reactants and products. Multi-step plans are assembled automatically from Notebook-captured reactions and over 16 million reactions from commercial sources. Based on methodology, reagents, and commercial availability, chemists can select a desired synthesis plan and create reports that include the scheme and conditions, citations supporting the synthesis, and a shopping cart of compounds required to complete the synthesis plan.

Supporting databases

Symyx Available Chemicals Directory (ACD): Symyx ACD provides complete chemical supplier catalogs for 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 access via Isestris, other options for deploying ACD content include online access through DiscoveryGate and access via Symyx Logistics.

Symyx Synthesis Databases: Symyx offers reaction databases that provide broad, in-depth coverage of synthetic chemistry, unsurpassed by any other combination of content products on the market. These databases are available via Symyx Isestris and DiscoveryGate.

Region	Country	Distributor Addresses
North America	USA	3B Scientific Corporation 1840 Industrial Drive, Suit 160 Libertyville, IL 60048 USA VOICE 847 291 9822 EMAIL marketing@3b.com FAX 847 291 9895 EMAIL marketing@3b.com Website http://www.3b.com

Figure 3: With Symyx ACD, explore the commercial availability and costs of compounds with access to over 800,000 compounds and 850 suppliers.

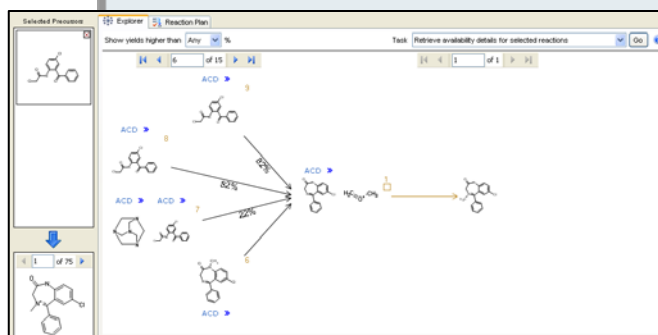


Figure 4: With the Isestris reaction planner, navigate through automatically generated, multi-step reaction plans assembled from reactions captured in Symyx Notebook and the Symyx synthesis databases.