Symyx Notebook for Synthetic Chemists
Lab Notebooks

A single, enterprise electronic laboratory notebook (ELN) that is adaptable to meet the needs of many scientific disciplines, enabling synthetic and medicinal chemists to collaborate effectively with analytical chemists and biologists in regulated and non-regulated R&D environments.

Built on the industry-leading Symyx chemistry foundation, Symyx Notebook accelerates the designing, documenting, storing, and secure sharing of synthesis experiments with proven chemical representation, molecule/reaction searching, small-molecule library enumeration and compound registration capabilities. Chemists can use the Symyx Registration service to register purchased or synthesized compounds while also quickly capturing information from document management and laboratory information management systems.

Handling of single- and multi-step reactions

Symyx Notebook offers capabilities for handling text, data, and forms required to plan, record, analyze, and report synthesis plans—including capturing reaction transformation details and handling single- and multi-step, linear and convergent reaction schemes. The Notebook automatically populates the materials section from the reaction scheme and calculates the stoichiometry. Reactants, reagents, and products are automatically named. Easy look-ups in Symyx ACD via the DiscoveryGate® Web Service provide information about key properties like molecular formula, molecular weight, density, purity, etc., which speeds stoichiometry calculations.

Enumerate compound libraries

Out-of-the-box Symyx Notebook includes a best-in-class enumeration tool, Symyx Cheshire, enabling medicinal chemists to enumerate both single- and multi-step libraries directly in a Notebook document. Chemists can define a plate representing the physical layout of the reaction library and generate a reaction list with the amounts of each building block required in each enumerated reaction.

Full reaction capture

The Notebook stores reactions with all reaction transformation and mapping information, enabling chemists to search all reactions captured in their notebook for specific transformations. Chemists can perform single searches over both in-house Notebook reactions and up to 6 million commercially available reactions and methodologies provided by Symyx.

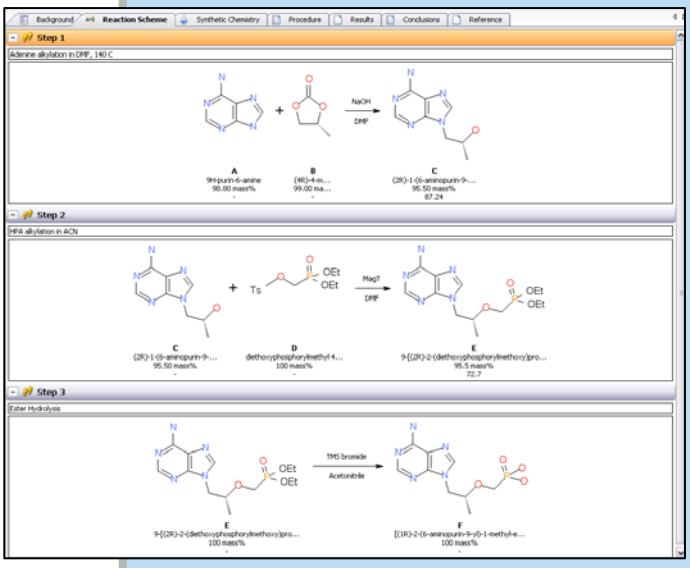


Figure 1: Easily design and share single- and multi-step, linear, and convergent reactions.

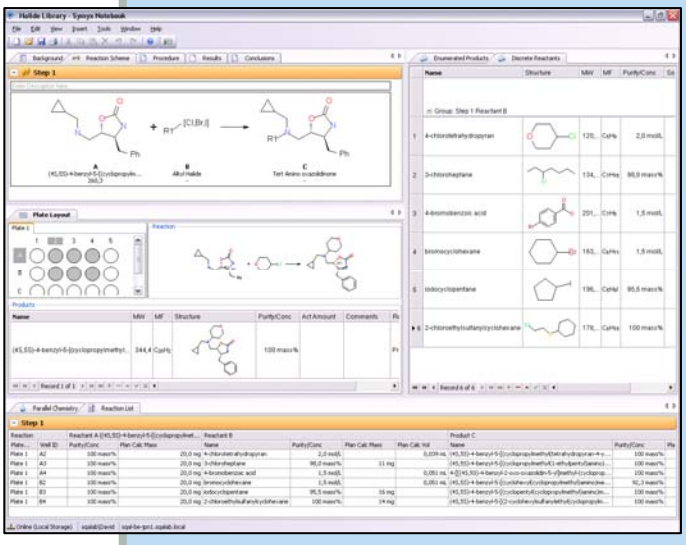


Figure 2: Use the integrated enumeration tool to create compound libraries; for example, you can use a series of alkyl halides as building blocks. Define a plate layout and view product details such as purity, actual amount, and Sample ID.

Rapid experiment editing and display

Easily drag and drop materials and pre-defined phrases into text sections to quickly build procedures and document experiments. Add files and images into experiments: edit files in native applications and annotate images. Depending on your needs, scroll through an experiment in a single, continuous view, or select tabbed views in floating, docking windows.

Access to essential chemistry information

Integration with Symyx ACD and Symyx Isentris assists with synthesis planning by enabling chemists to access current chemical sourcing, molecular property, synthetic methodology, bioactivity, and toxicology information in the context of laboratory workflows.

Superior searching and browsing

Experience the advantage of the Symyx chemistry engine through advanced molecule and reaction searching. Chemists can map the reacting centers in reaction substructure queries to find the reactions that are truly of interest. Create your own data-entry forms or tables and collect data that is indexed and searchable. Full-text searching of documents, embedded files, and image annotations facilitates the retrieval and re-use of experimental data. Create custom indexing and search/browse capabilities using the Software Developer Kit.

Improved consistency across experiments

Standard document templates drive experiment consistency by facilitating the "cloning" of all or part of an experiment, with or without related data. The ability to reuse successful document procedures and capture data consistently across research domains improves efficiency, productivity, and decision making.

Support for regulated and non-regulated environments

Symyx Notebook consolidates project data into fully versioned, shareable, and searchable documents controlled by customizable workflows. Secure versioning, electronic signatures, and audit trails support work in 21 CFR 11 and Good Practice (GxP) environments.

Configurable tables

Capture data in easily configurable tables by entering data manually, capturing data directly from lab instrumentation, or using Symyx Notebook's auto-fill capability. Easily customize data views (e.g., filter, group, sort, etc.) and integrate useful calculations into tables.

Enhanced collaboration

Improve experimental design with easy access to colleagues' work. Augment experimental write-ups with hyperlinks to related experiments. Track material usage from one experiment to the next.

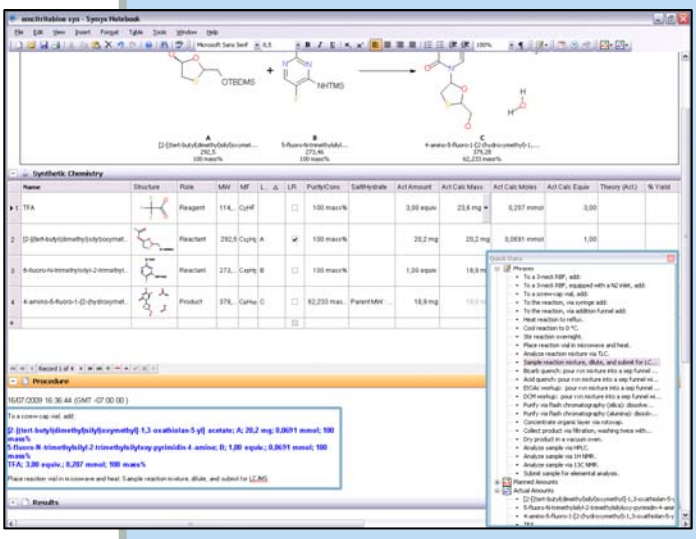
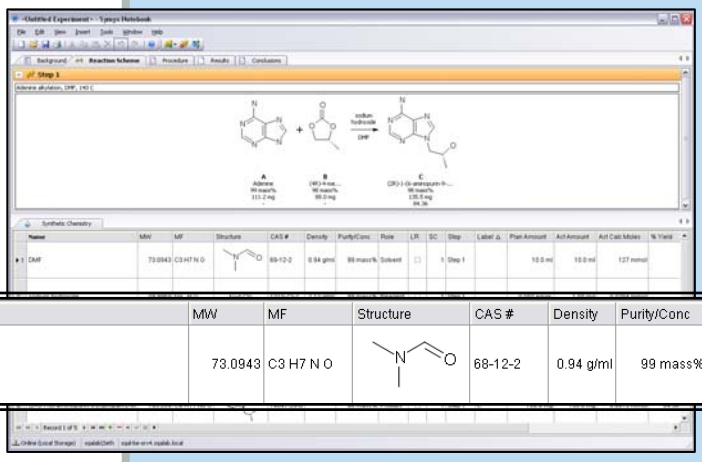


Figure 3: QuickData – drag and drop materials and pre-defined text phrases from the floating, docking tool window into any text section. Create, clone, edit, and reorder your own procedure phrases.



Name	MW	MF	Structure	CAS #	Density	Purity/Conc
DMF	73.0943	C3 H7 N O		68-12-2	0.94 g/ml	99 mass%

Figure 4: Material properties can be retrieved for reagents and solvents from Symyx ACD (e.g., density, CAS #, etc.).

Symyx

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