

Symyx Cheshire Cheminformatics

Symyx Cheshire dramatically improves an organization's ability to interpret the growing volume of chemical information by automatically calculating properties and changing structures based on custom cheminformatics business rules.

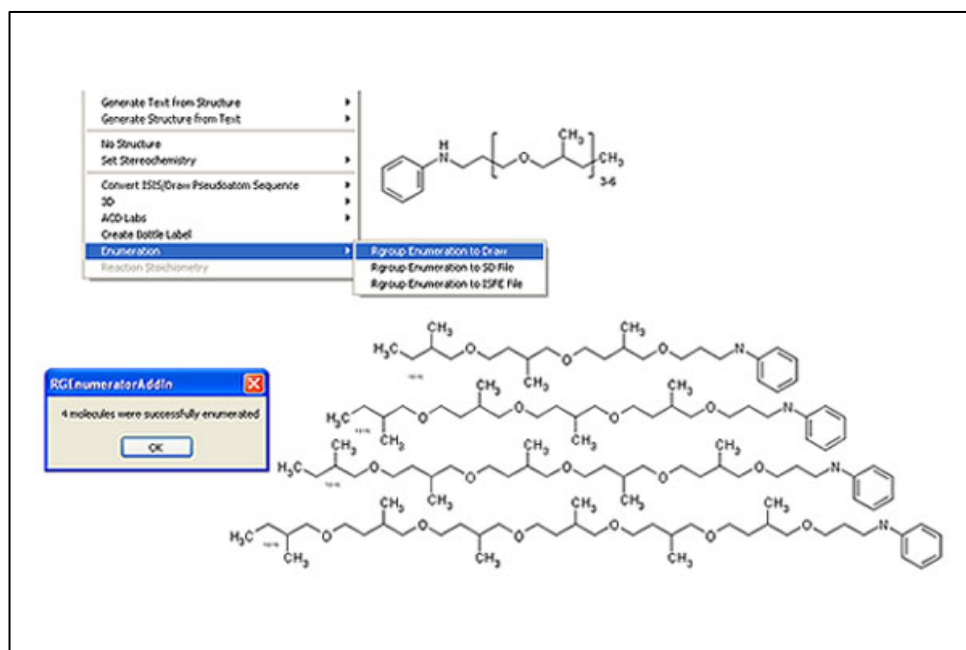


Figure 1: **Enumeration of Markush structures.** Symyx Cheshire is incorporated in a Symyx Draw add-in that enumerates Markush structures. A wide range of custom chemistry functionality can be incorporated into applications.

The need for consistency

The ultimate value of chemical information in a structure database depends on the consistency of data representation. Chemical information systems that use different conventions to represent chemical structures and reactions make it difficult to interpret chemical information when it is exchanged between scientists in different laboratories. In recent years, company mergers, database acquisitions, and the proliferation of data have amplified the problem.

A simple, automated solution

Symyx Cheshire uses a simple scripting interface to automate the analysis, interpretation, and manipulation of large volumes of heterogeneous chemical information based on a company's custom cheminformatics rules and calculations. By standardizing chemistry information conventions, Symyx Cheshire ensures that search and registration operations are accurate and complete, allowing trouble-free use of chemical intellectual property.

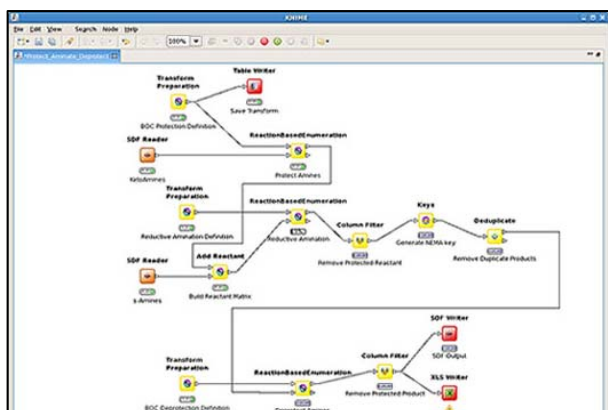


Figure 2: **Three-step, reaction-based enumeration within KNIME.** This workflow shows a multi-step, reaction-based enumeration of a reductive amination investigation. Before reactants can be enumerated, they must be BOC-protected. The products are de-duplicated and then the BOC-protecting group is removed. Finally, the list of structures is written to an SDfile, and exported to a Microsoft Excel spreadsheet.

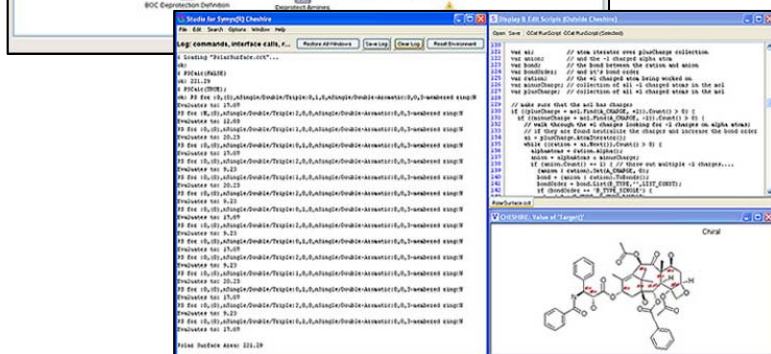


Figure 3: **A development environment that supports scripting.** In this example, a script that calculates polar surface area is being developed. An output window, a script writing and execution window, and a window containing the target structure – taxol – are shown.

Extensive chemical intelligence

Symyx Cheshire builds, validates, and applies “rules” that analyze and standardize chemical representation. Using familiar programming constructs, developers script business rules that are used in different applications to perform particular operations across all chemistry objects, including structures and reactions. With Symyx Cheshire, you can:

- Automatically check structures and reactions for consistency with corporate standards and adjust structures as needed
- Validate or create structure abbreviations, or fully expand them
- Define chemical environments such as ring clusters, polarity, and aromaticity
- Calculate the properties of structures and reactions

Intuitive Programming

Programmable interfaces in the Symyx Cheshire user environment expose structure analysis and manipulation functions. High-level abstraction makes the language intuitive and easy to program, while also enabling researchers to perform high-level operations such as exploring reactions, individual atoms and bonds, and collections of atoms and bonds as chemotypes.

Interactive prototyping

An interactive prototyping environment is included with Symyx Cheshire for building, editing, and running scripts. Developers can use this environment to test functions and syntax and execute single functions or entire scripts.

Convenient Utilities

Symyx Cheshire also includes example utilities and scripts that are used within other applications to scan databases, filter libraries, calculate chemical properties, and more. The scripts can be executed over local or remote databases, SDfiles, and RFiles.

Clean migration to new technologies

Symyx Cheshire works with Symyx Isentris to provide a common application programming interface. As a result, existing business rules are transferable to new Symyx Isentris solutions.