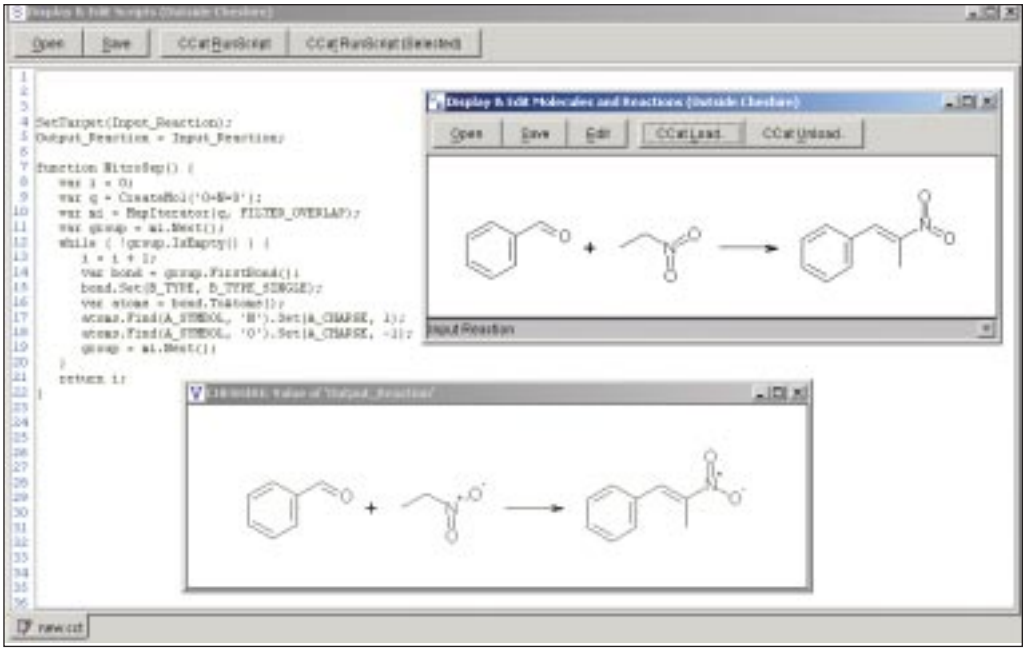
MDL® Cheshire®

MDL® 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.



MDL Cheshire automates the conversion between two mesomeric forms of a nitro-group. The code converts to or from the localized charge-separated species and the form where the nitrogen is doubly bonded to each oxygen atom.

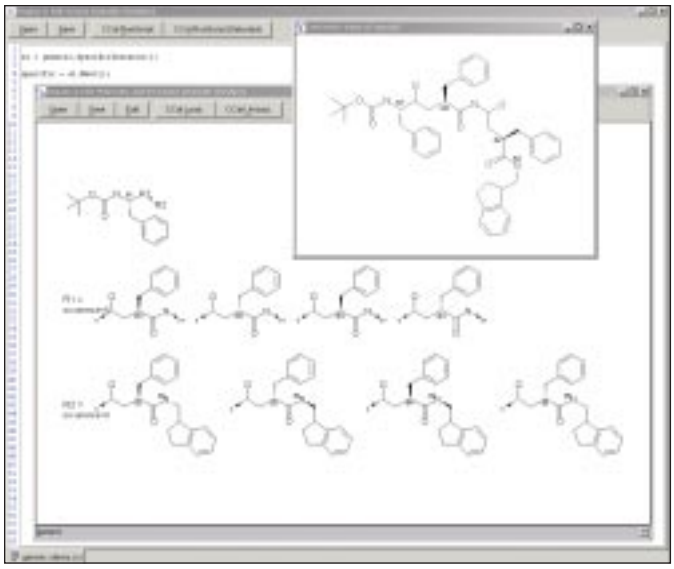
The need for consistency

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

MDL 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, MDL Cheshire ensures that search and registration operations are accurate and complete, allowing trouble-free use of chemical intellectual property.

MDL®



MDL Cheshire provides sophisticated methods for analyzing and interpreting chemistry, including stereochemical representation.

Extensive chemical intelligence

MDL 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 MDL 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 MDL 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 MDL 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

MDL 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 RDfiles.

Clean migration to new technologies

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

For more information about MDL Cheshire, please contact an Elsevier Account Manager or visit www.MDL.com.

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