

CrossFire Commander V6. MDL Information Systems, Inc. 14600 Catalina Street, San Leandro, CA 94577. www.mdl.com. See Web Site for Pricing Information

Although the *Beilstein Handbook of Organic Chemistry* and the *Gmelin Handbook of Inorganic and Organometallic Chemistry* have both ceased publication in printed form, these invaluable databases continue to thrive in their electronic incarnations: CrossFire Beilstein and CrossFire Gmelin, using the CrossFire client/server platform. CrossFire Beilstein contains 8.5 million compounds and 9 million reactions. CrossFire Gmelin contains 1.8 million compounds and 1.4 million reactions. Both databases are updated quarterly at over 500 worldwide server sites. Introduced in 1994 by Beilstein Information Systems (now a part of MDL Information Systems), CrossFire Commander (the client) provides the interface to search, retrieve, and capture information from Beilstein and Gmelin databases. It is designed to search not only bibliographic information, but also information concerning structures, substructures, and reactions. It can also perform searches for specific values or ranges of values in the more than 350 data fields associated with compounds. The Commander interface continues to be improved by added features and ease of use. This software (and the reasonable pricing scheme for access to the databases) has returned Beilstein and Gmelin from near extinction to their proper importance as valuable information resources for chemists. CrossFire Commander V.6 is the newest edition of the client for searching these databases.

PC or Macintosh computer users can download the client from the MDL Web site (<http://www.mdl.com/downloads/knowledge.html>). The file sizes are 10.9 MB and 21.1 MB, respectively. A Quick Reference Guide in PDF format (37 pages) is also available from this site. It provides easy-to-follow explanations for beginners on how to start searching the databases. A CD-ROM containing CrossFire Commander and other applications, such as LitLink and AutoNom, is available to purchasers upon request.

CrossFire Commander V.6 has several new features: (1) the Beilstein and Gmelin databases can now be searched simultaneously; (2) a new "Text Search" feature that allows the user to perform a keyword search in all text fields, that is, Structure Index, Reaction Index, and Citation Index, or in the bibliographic field, that is, Citation Index, has been added to the search interface; (3) common structure search options are now displayed beside the Structure Editor on the main Commander search screen; (4) the new "AutoSearch" feature automatically broadens the query and searches again when a search results in no hits; and (5) in the "Display Results" window, the new "Tree View" feature can maintain an overview of all of the search results, thus enabling users to navigate easily through current and previous search results down to the fact field level (Note: this feature is not available for Mac OS X users).

In addition to the Quick Reference Guide mentioned above, Commander has a detailed, context-sensitive online help file,

which can be accessed via the Help menu. From there, users can find more thorough explanations on using any particular application. The MDL Web site also has more general documentation on CrossFire Commander. Once users familiarize themselves with the program, they can see the potential in Commander to build very powerful searches.

There are three ways to search the databases in Commander. Besides the new "Text Search" feature, users can begin a search using either the Fact Editor or the Structure Editor. The Fact Editor allows the user to input field-delimited factual queries to search the databases. There are over 350 searchable fact fields in the Beilstein and Gmelin databases, and every field has a field name: for example, the field name for molecular formula is MF. There are also several predefined query forms for easy input of queries. In Beilstein, the forms include Bibliographic Data, Bioactivity, Physical Data, and so on. To search data fields that are not in the predefined query forms, the user can use the generic tabular form. Users can employ Boolean and proximity operators (and, or, not, near, next, and proximity) and nesting parentheses to compose complex search statements in the tabular form. Truncation and wildcard usage are also possible in the query. Advanced users who know the field names and how to build a nested search can type queries directly in the "EDS" (Easy Data Search) window.

The Structure Editor allows searching by exact structure, substructure, or reaction. For drawing structures, users can choose between the MDL CrossFire Structure Editor and MDL ISIS/Draw (the latter requires a free download for academic and personal use). In the MDL CrossFire Structure Editor, the structures or reactions are entered using a drawing board similar to other chemical drawing programs. For drawing exact structures, users can choose atoms and bond orders from the function bars or pick a structure from predefined template files of about 500 structures and modify it. For drawing substructures, users can specify free sites in a structure to allow for further substitution. There are also predefined atom groups (X for any halogen, M for any metals) or generic groups (ACY for acyclic, AHC for heterocyclic). Users can create user-defined atom groups and generic groups for their substructure searches. In the reaction drawing board, reaction roles (reactant or product) can be assigned to each structure. For every atom and bond in the reaction, users can designate reaction centers and assign stereochemical and bond changes (bond order, bond topology, bond breaking or making, etc.) during the reaction. Finally, users can map corresponding atoms in reactants and products to indicate that these atoms must be the same.

Searches can also combine queries in the Fact Editor and Structure Editor by using the default AND operator. For example, one can draw methylbenzene as a reaction product in the Structure Editor and input "py>1995" (publication year after 1995) in the Fact Editor. This query will retrieve results in which methylbenzene is a reaction product from literature published after 1995. Every search along with its hit set is saved in

Commander. Users can select a particular search and narrow it by adding further queries regarding structure or fact.

The response time for a search in both of the databases is normally very short. Based on the search, there are three kinds of formats for displaying the results: substance, reaction, or citation. Once a search is completed, the results are displayed in a separate "Display Hits" window with the Tree View window on the left and one or several display windows on the right. There are five hierarchical levels in the Tree View: (1) databases (Beilstein and Gmelin); (2) folders (saved hit sets and session hit sets); (3) list of hit sets; (4) list of substances/reactions/citations; and (5) list of facts/reaction details/citation details. By clicking on the "+" before every expandable level, users can select an item in (3), (4), or (5) and view the corresponding fact in the display window on the right. To have the structure/reaction always visible while navigating the hit sets, users can also activate a Structure/Reaction display window by clicking the "Structure on/off" button from the tool bar. The "Copy structure to editor" button will transfer the current structure or reaction to the Structure Editor so that users can make modifications for further searching.

The ability to save and export search results in a variety of formats is one of the best new features of CrossFire Commander V6. An easy and intuitive interface with Microsoft Office applications gives searchers the option of saving results to tables in Excel or Word, or as HTML reports. Citations can be exported to reference management software, such as EndNote and ProCite. As with many of the other commands in V6, the Export feature has many levels of complexity, which most users can happily forego. Several of the most common tabular and report formats are available as default settings, and more detailed user-defined formats are easily generated using a five-step Export Wizard. A particularly useful feature of the report generator is the "save link" capability, which creates a hot link from report data to the original site in Commander.

There are several other MDL products, free of charge to CrossFire Commander V6 users, that can be downloaded and installed to enhance database searching and linking to full text citations:

(1) LitLink is client server software implemented in CrossFire Commander that provides a direct link from the citation to full text journal articles, patents, and other types of primary literature (third party agreement required). The LitLink client for PC users is 1.22 MB. Unfortunately, a version of LitLink for Mac users is not yet available. More information can be found at <http://www.mdl.com/products/litlink.html>.

(2) AutoNom (Automatic Nomenclature) is a program that generates systematic IUPAC chemical names for drawn structures. AutoNom Standard is available at no cost to CrossFire Commander users. See <http://www.mdl.com/products/autonom.html>.

(3) ISIS/Draw is a package that enables drawing of chemical structures. It is free for academic and personal home use. Users can draw structures and reactions in ISIS/Draw and transfer them into the Structure Editor by clicking on the CrossFire button in ISIS/Draw. See <http://www.mdl.com/products/isisdraw.html>.

In summary, CrossFire Commander is a very sophisticated tool for searching chemical information in the Beilstein and Gmelin databases. Despite its complexity, novice users can quickly learn how to perform simple searches. If they want to use the retrieval power of the Commander V6 software more fully, they can refer to several types of documentation. The newest version of Commander has added a number of features to aid users in conducting searches and has greatly expanded and improved the ability to export and save search results.

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