

- Failed Reactions—those that did not proceed as expected
- Metabolism—developed in conjunction with the Royal Society of Chemistry
- Methods in Organic Synthesis—33,000 reactions, Protecting Groups—functional group protection with region/stereoselectivity
- Solid Phase Synthesis—with emphasis on small-molecule and combinatorial chemistry

The chemical information programs provided by Accelrys include several database systems.

- Accord for Excel and Access—relational chemical storage for Microsoft programs
- Accord for Oracle—a chemical data cartridge (see Glossary)
- Accord Database Explorer—to access Accelrys reaction databases
- RS<sup>3</sup> Discovery System—with programs for chemical structure, data management, high-throughput screening, and inventory

Accelrys also provides programs for descriptor calculation, QSAR, and data mining (93).

*The Beilstein Database.* The Beilstein Database, with over 8 million structures, is the oldest in existence, based on the Beilstein Handbook of Organic Chemistry, and contains data that extend back to 1771. The database is produced by the independent Beilstein Institute (94). Access to the database is either through Beilstein Online, available through STN and Dialog, or through the Web using Crossfire Beilstein, which is marketed by MDL GmbH—formerly Beilstein Inc. (95). Data that are stored include the structure, Beilstein and CAS Registry Numbers, names, formula, preparations, reactions, natural product isolations, and chemical derivatives. Physical properties, if available, are also stored, including optical data, mechanical properties, multi-component system data, spectral and thermodynamic properties, as well as biological function, ecological data, toxicity, and common uses. Citation data, including author, journal,

CODENs, and patent information, are also stored. The data are organized into substance, reaction, and citation contexts, and a user can easily switch from one context to the other. An ACS symposium volume devoted to the Beilstein database has been published (96).

*Chemical Abstracts Service.* As a division of the American Chemical Society, CAS develops and manages the world's largest databases of chemical structures and reactions.

- CAS Registry—35 million structures—19.5 million distinct structures—13 million bio-sequences
- CASREACT—4 million reactions
- CHEMCATS—2.5 million commercially available chemicals
- MARPAT—500,000 searchable Markush structures

The CAS databases are maintained online, with searching allowed on a subscription basis. *SciFinder* is a client/server application to search CAS databases by author, keyword, exact, and substructure. It includes a "keep me posted" update feature, reaction information back to 1974, nucleotide and protein sequence searching, browsing of 1600 journals, and integration of structure, data, and citation information. STN International is a collection of 200 databases covering chemistry, life sciences, engineering, patents, etc. STN Express provides wizard-assisted searching, and STN on the Web serves as a web client for STN. The *ChemPort* program provides web access to journals (97).

*Daylight Chemical Information Systems, Inc.* This company provides numerous third-party databases in the Thor format. These include the following:

- Databases of organic structures: Available Chemicals Directory—250,000 structures, *Asinex* catalog—115,000 structures, *Maybridge* catalog—62,000 structures, *InfoChem SPRESI'95*—2.5 million structures
- Drug and biological databases: *BioScreen* NP and SC—about 52,000 structures including natural products, *Pomona College Medchem*—36,000 structures with measured *LogP*, *National Cancer Institute*—