ACD/Labs' Free Naming Software Service Generates 200 000 IUPAC Names via the Web

Advanced Chemistry Development, Inc., (ACD/Labs), the premier supplier of quality systematic nomenclature generation for the past five years, recently generated its 200 000th free IUPAC name on its Web site.

New synthetic structures are constantly being developed, making it increasingly important for scientists to adopt a definitive systematic nomenclature and use a software tool that can ensure accuracy and organizational homogeneity in generating chemical names. ACD/Name has grown to support the nomenclature rules agreed upon by IUPAC, the International Union of Biochemistry and Molecular Biology (IUBMB), and the Chemical Abstracts Service (CAS). ACD/Name systematic nomenclature software is the current industry standard used by nomenclature specialists worldwide and by a multitude of corporations in the chemical and pharmaceutical industries. The software is used to quickly and accurately name compounds for reports, databases, and publications.

The ACD/Labs Online Service enables chemists to generate IUPAC names at no extra cost by using the online portal.[1] Free chemical names can be generated according to the systematic application of a preferred set of IUPAC nomenclature rules for molecules containing no more than 50 atoms, and no more than three rings, with atoms from among only H, C, N, P, O, S, F, Cl, Br, I, Li, Na, and K. Presently, this service generates about 100 IUPAC names per day.

As well as generating IUPAC names online, the ACD/ChemSketch freeware available also includes the free naming algorithms. There have now been more than 520 000 downloads of ACD/ChemSketch, and scientists around the world are benefiting from instant access to ACD nomenclature tools. ACD/Name is now compatible with the InChI™ chemical nomenclature protocol, making it possible to produce unique alphanumeric string representations for chemical compounds that facilitate the communication of molecular structures electronically.[2] ACD/Labs' commercial products also offer the unique "reverse" InChI-to-structure conversion that enables convenient decoding of InChI strings.

ACD's new software product, ACD/Name Chemist Version, which was introduced in August 2005, made ACD/Labs' quality IUPAC nomenclature generation algorithms more affordable for chemists.

www.acdlabs.com

1. One can also access the ACD/Labs Online Service from IUPAC: <www.iupac.org/nomenclature>
2. <www.iupac.org/inchi>

Chmoogle Search Engine Integrates ChemSketch

Advanced Chemistry Development, Inc. (ACD/Labs), has integrated both its commercial and freeware ChemSketch application to the Chmoogle® Web site <www.chmoogle.com> created by eMolecules, Inc. Chmoogle is the world's leading open-access chemistry search engine. Its mission is to discover, curate, and index all of the public chemical information in the world and make it available to the public for free. Chmoogle distinguishes itself with extremely fast searches, an appealing presentation of results, high-quality chemical drawings, and powerful advanced search capabilities such as persistent hit lists and hit list logic operations. ACD/Labs has integrated Chmoogle into the commercial ChemSketch software and freeware. This integration gives ChemSketch users direct access to Chmoogle's structure and substructure searches.

Antony Williams, vice president and chief science officer for ACD/Labs, notes that "the mission of

Chmoogle—to discover, curate, and index all public chemical information in the world and make it available for free—is a worthy mission. ACD/Labs' intention to provide a chemical structure drawing package to every chemist in the world at no charge via our freeware ChemSketch downloads is just as worthy. We are happy to provide an integrated solution between ChemSketch and Chmoogle to allow users to sketch molecules at their desktop and view their results via a Web browser. It is our hope that sketching and Chmoogling will deliver value to chemists around the world."

Chmoogle is created by continuously indexing all of the public chemical information in the world. Chmoogle is attracting a large amount of the chemistry-related Internet traffic by industrial and academic decision-makers.

www.chmoogle.com

In Memorium—Dale B. Baker

Dale B. Baker, director emeritus of Chemical Abstracts Service (CAS), died 11 December 2005 in Columbus, Ohio. He had served as director of CAS from 1958 until his retirement in 1986. Under Baker's leadership over those years, CAS invented database publishing by developing databases from which any form of output, printed or electronic, could be produced.

Baker started with CAS as a part-time office boy in 1939 while attending Ohio State University. After graduating with a degree in chemical engineering, he spent four years working as a supervisory chemist at E.I. du Pont de Nemours & Co., before returning to CAS as an assistant editor in 1946. He rose steadily up the editorial ladder, succeeding E.J. Crane as director in 1958. During Baker's tenure as a director, CAS faced many challenges, including a difficult transition from a subsidized operation of the ACS to a financially self-sufficient division.

When Baker joined CAS, the organization had for decades been identified as the publisher of the printed Chemical Abstracts (CA), the leading reference work for keeping chemists and other scientists in touch with the latest chemistry-related publications. But keeping up with the explosion in scientific research required the adaptation of new technology. Starting in the 1960s, under Baker's direction, CAS moved from the conventional, print-oriented abstracting and indexing cottage industry to become a highly automated operation of international stature. In the course of that evolution, CAS developed one of the world's premier automated information processing and retrieval systems, which served as the model for those in other scientific disciplines.

www.cas.org/dalebaker.html