

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

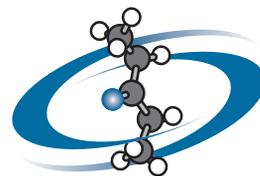
rings, with atoms from among only H, C, N, P, O, S, F, Cl, Br, I, Li, Na, and K. Presently, this service generates about 100 IUPAC names per day.

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



**A d v a n c e d
C h e m i s t r y
D e v e l o p m e n t**

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