

**FOR IMMEDIATE RELEASE****Contact:**ACD/Labs
(416) 368-3435 ext 297
media@acdlabs.com

CAS Will Enrich Databases with Calculated Properties and Reactions Back to 1975

STN®, SciFinder® and SciFinder Scholar Will Give Researchers More Powerful Content for Scientific Discovery

Columbus, OH, August 26, 2001 - Chemical Abstracts Service (CAS) is extending the reach and content of its databases, already recognized as the world's most comprehensive for chemistry-related research and substance information. Researchers seeking candidate substances for new drugs will benefit especially by CAS's addition of calculated property data from Advanced Chemistry Development, Inc. (ACD) and another ten years of reaction information back to 1975 provided by InfoChem GmbH in the CASREACT® file. These additions are planned for Fall 2001 and will be accessible through STN services, SciFinder and SciFinder Scholar. CAS made these announcements during the ACS National Meeting in Chicago this week.

"Our new enhancements will dramatically enrich the content and value of CAS databases for pharmaceutical research and many other avenues of exploration," said CAS Editorial Operations Director, Matthew J. Toussant. "The property data created using ACD software and CAS substance connection tables, along with the InfoChem/ZIC reactions added to CASREACT, open new possibilities for an entire range of substance investigation. In sum, scientists can find more answers to a broader range of questions."

CAS is strengthening its offering in two complementary areas of substance information, accessible to users of CAS databases through SciFinder, SciFinder Scholar or STN search services:

- CAS is adding eight calculated property values to several million substance records in the CAS Registry: number of hydrogen donors, number of hydrogen acceptors, number of rotatable bonds, molecular weight, logD, logP, pKa, and solubility in water. These calculated properties are provided using CAS substance connection tables and software developed by ACD and will enable researchers to quickly and easily focus on the more "drug-like" molecules identified in the Registry file. The same types of property data will gradually be supplied for a wider set of substances in Registry.
- The CASREACT file will be extended back to 1975, with the addition of more than 750,000 single- and multi-step reactions from the German software company, InfoChem. For this collection of reactions, jointly built by the All-Union Institute of Scientific and Technical Information of the Academy of Sciences of the USSR (VINITI) and the German Zentrale Informationsverarbeitung Chemie, Berlin (ZIC), CAS Registry Numbers® will be assigned to reaction participants and each reaction will be linked to its corresponding CAPLUS document record. These reactions from journal and patent literature will be seamlessly integrated with those previously existing in CASREACT, giving chemists insights in the synthetic information reported during the past quarter of a century.

###

