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ACD and CAS Announce the Publication of Predicted Molecular Properties for Over 12 Million Chemical Structures

Toronto, Ontario, June 4, 2002 - Advanced Chemistry Development, Inc. (ACD) and Chemical Abstracts Service (CAS) are proud to announce the publication of predicted molecular properties for over 12 million chemical structures. This is a significant milestone in ACD's collaboration with CAS, which was announced on August 26th, 2001, at the American Chemical Society meeting in Chicago. As part of their ongoing work to enrich the CAS Registry with new data, CAS successfully computed and published calculated physical properties for 11.5 million chemical substances by the end of 2001, and is currently calculating properties for more than 20,000 new substances each week.

Researchers seeking candidate substances for new drugs will especially benefit from the addition of calculated property data to the CAS Registry. The calculated properties from ACD, now available in the CAS Registry, include number of hydrogen donors, number of hydrogen acceptors, number of rotatable bonds, molecular weight, logD, logP, pKa, and solubility in water. These calculated properties, created by using CAS substance connection tables and software developed by ACD, will enable researchers to quickly and easily focus on the more "drug-like" molecules identified in the Registry file.

"Adding the calculated properties from ACD to substance information in the CAS Registry has created a uniquely powerful resource," said Matthew J. Toussant, CAS Editorial Operations Director. "This collaboration strengthens our ability to give researchers the insights they need for more efficient drug discovery."

"This collaboration has been of wonderful value to ACD as it has allowed us to exercise our predictive methodologies over a range of compound classes never experienced before," said Robert DeWitte, Director of Marketing at ACD. "Because of this implementation, our PhysChem Batch product is now more efficient, more stable and more accurate than ever, and it is able to compute a significantly broader range of compound classes. It continues to be a personal delight to collaborate with all of the staff at CAS who are involved in this project."

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