



## FOR IMMEDIATE RELEASE

## Contact:

ACD/Labs  
(416) 368-3435 ext 297  
[media@acdlabs.com](mailto:media@acdlabs.com)

## ACD/Labs Improves the Support of Virtual Screening with Increased Speed of Calculation in Version 8.0

**Toronto, Canada, February 12, 2004** - Advanced Chemistry Development, Inc., (ACD/Labs) extends the application of its industry standard PhysChem prediction software by significantly increasing the speed of property calculation in version 8.0.

ACD/PhysChem provides the industry's most accurate prediction of critical drug-related properties, including logP, pKa, aqueous solubility, logD, and polar surface area. ACD/PhysChem Batch applies these leading algorithms to large databases with tens of thousands of compounds at a time, allowing the rapid and automatic screening of compound libraries to filter out compounds that will not meet the criteria of potential drug candidates.

Developments in version 8.0 of ACD/PhysChem Batch have led to property calculation speeds up to ten times faster than in the preceding version for pKa, logP, logD, solubility, and all four properties combined. Version 8.0 makes it possible to predict the entire range of required physicochemical properties for hundreds of compounds each minute, and provides the accuracy necessary to filter compounds across numerous classes, thus leading to enriched screening sets for further stages of drug discovery research.

Robert S. DeWitte, Ph.D., Director of Medicinal Chemistry Solutions for ACD/Labs, comments, "We are very pleased with this first step of progress toward ultra-high throughput physical property prediction without compromising our renowned standards of accuracy and quality. With this in hand, computational chemists will be more able to focus downstream screening applications on pharmaceutically viable molecules, producing high quality hits. We are motivated by enabling our customers to avoid the enormous potential costs of trying to optimize 'red-herring' compounds. With higher compute speed and accuracy, these cost savings can begin earlier."

Also new to ACD/PhysChem and PhysChem Batch, version 8.0, is ACD/pKa Accuracy Extender, which enables the expert chemist to train the system with his own experimental data in order to calculate more accurate pKa values for novel chemical classes. This program, along with the existing ACD/LogP Accuracy Extender, facilitates the overall increase in prediction accuracy and speed amongst the range of ACD/PhysChem version 8.0 products.

ACD/PhysChem, version 8.0, is estimated to be available for shipping in May 2004.

###

