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## Contact:

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

## Advanced Chemistry Development, Inc., Provides Medicinal Chemists with Tools for Drug Discovery with the Release of Version 7.0

**Toronto, Canada, February 24, 2003** - Advanced Chemistry Development, Inc., (ACD/Labs) announces the release of ACD/PhysChem version 7.0, the prediction software package that assists medicinal chemists in the crucial decision making process that accompanies drug design/discovery.

Developed for chemists involved in the innovation of new potential therapeutics, ACD/PhysChem version 7.0 provides predictive tools which help chemists select potential compounds for pharmaceutical screening purposes. By maximizing the information content in experiments, scientists are able to recognize the trends in molecular physical properties pertaining to their specific chemical class, therefore avoiding problematic molecules. This approach can drastically reduce the number of molecules that do not meet the requirements for passive human absorption, saving weeks of work for a medicinal chemist.

With the help of ACD/PhysChem version 7.0, scientists gain key insight into molecular ADME properties. This software provides the industry's most accurate prediction of critical physical organic properties such as logP, pKa, aqueous solubility, logD, and polar surface area. These molecular parameters form the basis for passive absorption, protein binding, tissue binding, food effect, clearance, half-life, and excretion. As a result, medicinal chemists are equipped with the appropriate knowledge to enhance the potency and efficacy of their compounds.

Aqueous solubility has become increasingly important to ensure successful oral absorption of candidate bio-organic compounds. Since the various compartments of the gastrointestinal tract have different pHs, ACD/PhysChem places great emphasis on enabling medicinal chemists to calculate solubility at specified pH values.

In the art and science of prediction, measurement is critical. "This year, we've worked hard to ensure our clients can use every logD, logP, and pKa measurement they make to enhance the accuracy of the ACD/PhysChem predictions. We believe that a systematic combination of targeted measurement and ACD/PhysChem can provide high throughput and high accuracy. The upshot is that timely data will be in the hands of medicinal chemists when they are actively considering alternative compounds for synthesis," stated Robert S. DeWitte, Ph.D., Director, Medicinal Chemistry Solutions, ACD/Labs.

New to ACD/PhysChem version 7.0 is ACD/LogP Accuracy Extender. This advanced training tool helps users extract fragments from their own data to calculate new increments for the ACD/LogP additive algorithm, resulting in improved accuracy of logP prediction and increased speed of calculation for the required classes of organic compounds.

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