

Enclosed is the latest newsletter from [Advanced Chemistry Development, Inc. \(ACD/Labs\)](http://www.acdlabs.com). This edition highlights the latest advances in molecular property prediction, as well as its application to ADME and medicinal chemistry.

If you are interested in learning more about ACD/Labs Products, visit <http://www.acdlabs.com/products>. Also, don't forget about our freeware offerings (<http://www.acdlabs.com/download/>) including ACD/ChemSketch version 5, with over 300,000 downloaders!

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Enhancements to Compute Speed of ACD/Labs' Molecular Property Predictors

ACD/Labs provides the industry's most accurate prediction of physicochemical properties, including $\log P$, pK_a , aqueous solubility, $\log D$, and polar surface area. Developments in our latest software release have led to property calculation speeds of up to ten times faster.

In our recent test, pK_a , $\log P$, $\log D$ at 3 pH values, and solubility at 3 pH values for 10,000 compounds of pharmaceutical significance were predicted within one hour on a standard Windows Pentium IV 2.0 computer.

Read more about this exciting new development in ACD/Labs PhysChem version 8.0 software in our press release: [ACD/Labs Improves the Support of Virtual Screening with Increased Speed of Calculation in Version 8.0](#).

[Review the new features of the latest software and compare the speed of calculation of the current and previous versions.](#)

Measurement and Prediction—Which is More Relevant?

We say: Measurement; but you do not always want to measure many physicochemical properties for numerous compounds from the same class, especially if quality prediction tools for $\log P$, pK_a , aqueous solubility, and other physicochemical properties are readily available.

Version 8.0 of ACD/PhysChem software contains unsurpassed capabilities for tuning predictions with your own experimental data.

New modules, such as pK_a Accuracy Extender and LogP Accuracy Extender, help scientists incorporate their targeted measurements into the ACD/Labs prediction tools to enhance the prediction quality for novel and rare chemical classes.

Please review our application note: [Using Measurement to Improve the Accuracy of PhysChem Predictions](#).

Read more about this improvement in ACD/Labs PhysChem version 8.0 software in our press release: [ACD/Labs Tightens the Coupling Between Measurement and Prediction with the Release of ACD/PhysChem Version 8.0](#).

First Annual PhysChem Symposium

ACD/Labs is excited to introduce our 1st Annual PhysChem Symposium to be held on Thursday, Oct. 21, 2004, in Obernai, France.

The focus of the Symposium is Early ADME and Medicinal Chemistry, including presentations from Bernard Faller (Novartis Institute for Biomedical Research), Mike Abraham (University College London), and Klara Valko (GlaxoSmithKline).

View the [Symposium agenda](#).

This event is presented in conjunction with our [5th Annual European Users' Meeting](#) which takes place on Oct. 19-20.

Upcoming Conferences

ACD/Labs would like to invite you to learn more about new developments in our version 8.0 PhysChem software at these upcoming conferences.

28th National Medicinal Chemistry Symposium

June 27-30, 2004
Madison, WI, USA

Drug Discovery Technology

August 8-13, 2004
Boston, MA, USA

International Symposium on Medicinal Chemistry

Copenhagen, Denmark
August 15-19, 2004

QSAR

September 5-10, 2004
Istanbul, Turkey