

[Academic Research](#)[NMR Solutions](#)[Reporting and Publishing](#)ACD/Labs
Web Poll

Where do you see the value of physical property predictions in teaching?

- To illustrate the connection between property values and structural elements of a compound
- In explanation of chemical behavior and complex macro properties
- To create interesting examples that help retain the interest of my students
- I don't see any value in them

[Click Here to Vote](#)[Free Web Surveys](#)

Application Note:
Improving Predictions for Novel and Proprietary Compounds

It can sometimes be challenging to get accurate physicochemical property predictions for novel compounds from 'out-of-the-box' software solutions. ACD/Labs software tools facilitate the use of experimental measurements of proprietary/novel compounds to train predictor algorithms—allowing you to expand the 'vendor database' to reflect the

As the Academic Account Manager for ACD/Labs, I am happy to announce a new freeware offering for physical chemistry—ACD/LogP Freeware (see details below). In this newsletter you can read about the extensive applications of logP in industry, and see how our PhysChem prediction tools can help you interactively teach physicochemical property concepts. Feel free to contact me directly to discuss how our software can help in teaching and research.

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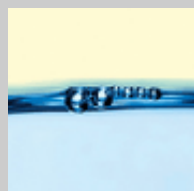
In this issue:

- Download New **LogP Freeware**
- What is **LogP** and Why Should You Care?
- **Interactive Tools** for Educators
- How **PhysChem Savvy** Are You?

ACD/LogP Freeware—Fast & Accurate Predictions at Your Desktop

ACD/Labs is delighted to announce the release of
ACD/LogP Freeware.

This **add-on** to our drawing package, **ACD/ChemSketch**, will give you easy access to predictions of the octanol/water partition coefficient, also referred to as logP or K_{ow} .



Continually enhanced since its introduction in 1995, our calculations are based on an experimental data set of over 18,000 reliable logP measurements, and are used by scientists worldwide through CAS's SciFinder service, and at companies like Pfizer and GSK.

[Read More & Download ACD/LogP Freeware](#)

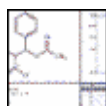
The Significance of LogP

The partition coefficient (logP) describes solvation of a compound between two immiscible layers (oil and water). The phenomenon of compounds partitioning between immiscible layers (octanol/water being the most avidly studied and applied), has far-reaching consequences in biology and chemistry—for estimating the fate of compounds in the environment; their ability to permeate biological membranes; and even partitioning in a liquid chromatography column.

Read our recent application note, [LogP—Making Sense of the Value](#), to learn how this property impacts research in different industries, and the significance of the value.

Interactive Tools for Educators

One of the common complaints we hear from educators attempting to teach physical chemistry is that it takes a long time for students, both undergraduate and graduate, to get a feeling for a compound's physicochemical parameters.



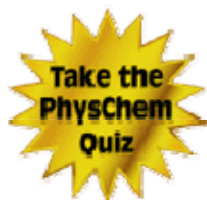
The next gap in understanding comes with students attempting to apply this knowledge in a "common sense" manner for problem solving, and finally for rational chemical design.

See how you can use our **property prediction tools** to help your students get a sense of the importance of **molecular physical properties**, and teach them how to apply multiple physicochemical parameters to problem solving.

[Using Pharmaceuticals to Teach Chemistry: Educational Innovations for Majors and Non-Majors](#)

How PhysChem Savvy Are You?

At the 30th National Medicinal Chemistry Symposium in Seattle last year, we challenged conference attendees to complete a short quiz about physical properties ($\log P$, $\log D$, solubility, and pK_a), and how they relate to questions that arise in day-to-day research. These questions apply equally to wider chemical research, though structures and property value targets differ.



Upon completion, gain free access to the poster we presented at AAPS 2006 outlining how our software can help you address physicochemical property concerns.

chemistry space being investigated in-house.
[Download PDF](#)

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Events and News

News

ACD/Labs and Protasis Shatter the High-Throughput Bottleneck for NMR Analysis—April 16, 2007 [Read](#)

ACD/Labs Software Integrated into ChemSpider Service—April 10, 2007 [Read](#)

Scientists at ACD/Labs Co-Author 'Most Accessed' Paper in MRC—April 9, 2007 [Read](#)

Upcoming Events

[5th Annual UK Users' Meeting and PhysChem Symposium](#)

Old Windsor, UK
May 15–17, 2007

[234th ACS National Conference & Expo](#)

Boston, MA, USA
August 19–23, 2007