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"ACD/Labs pK_a predictions are the Most Accurate"



That is the claim of a study, published in December 2007, by a research group at the University of Pardubice. The study was carried out by M. Meloun and S. Bordovska, and is entitled "**Benchmarking and validating algorithms that estimate pK_a values of drugs based on their molecular structure**" (*Anal. Bioanal. Chem.*, **389**, 1267–1291, 2007). It compares predicted values in four software packages (PALLAS, MARVIN, ACD/pK_a DB, and

SPARC), to experimental results for three sets of compounds.

Using a linear regression analysis technique (fully defined in the paper) they concluded that **ACD/pK_a provided the most accurate predicted values** compared to the other packages, showing the best results in six different statistical characteristics.

[Read the abstract and access the paper](#)

Property Profiles at a Glance with Quick Report

Earlier this year we introduced a new functionality in version 11 of the PhysChem modules that can provide a snapshot of the property profile one compound at a time. The **ACD/Quick Report** interface was designed to allow you to **customize the display of pertinent data**. It provides the option to add color bins and text flags for at-a-glance review. Furthermore this simplified interface allows you to make structural changes on the fly, re-calculating the parameters at the click of a button. Property profiles compiled in-house can help guide the day-to-day efforts of scientists without getting entangled in exhaustive property information and calculation protocols.



See this feature in action in a short 3 minute [demo movie](#).



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PhysChem Predictions in Applied Preformulations Research

In the November 2007 issue of **Chemistry World**, Jeff Botts (a senior scientist at Aptuit) discussed how he uses ACD/Labs' predicted property data to aid his research, and reviewed the software.

Jeff's group carry out experimental measurements of pK_a , partition coefficient, and solubility. The majority of their work involves novel compounds so the starting point can be something of a mystery, involving some trial-and-error investigative studies before accurate measurements can be obtained. This pre-formulations group uses ACD/Labs property predictions to guide their work. For example, to get an idea of whether a compound is likely to be highly soluble or insoluble, or to verify that experimental measurements are consistent with literature values. "The software has been a huge time-saving for me," says Botts. Previously he spent hours in the library searching through reference books for relevant information. If the information was not available in the published literature, he would resort to calculating expected values by hand—a tiresome and time-consuming activity.

[Read Jeff's review of ACD/Structure Design Suite](#)

How Discontent Bred a New Scientific Community

The PhysChem Forum came about as a result of grumblings about the state of affairs at a European solubility conference in 2004. Barbara Mason and John Comer* discussed poor turn-out at the meeting, and the travel-expense difficulties faced by, in particular, less well-established scientists. How to enable everybody interested in the PhysChem arena to participate and discuss their challenges? Instead of crying into their beer, they decided to do something about it. And so came about the PhysChem Forum, an online community aimed at providing scientists with better access to information, and a forum to discuss problems and share their experience.

**PhysChem
FORUM**

The Forum is a volunteer-run organization open to everyone who measures, predicts, or applies PhysChem data (including medicinal chemists and biologists). Scientists come to the Web and email-based forum with questions on experimental techniques, predictive software, and the best way to interpret and use data.

The first free symposium, hosted by Perkin Elmer (UK) in 2005, attracted 40 scientists. Meetings are now regularly attended by more than 70 delegates from across the UK, Europe, and the US; and cover the entire span of PhysChem topics. The 5th PhysChem Forum Symposium (sponsored and hosted by GSK, Stevenage, UK) will cover topics such as polymorphism, pK_a measurements, formulation and dosing, and physical chemistry from a chemist's perspective. The keynote presentation will be given by Professor Robert Glen (The Unilever Centre for Molecular Sciences Informatics, University of Cambridge), and will focus on solubility.



For more information, visit the PhysChem Forum at <http://physchem.org.uk>

*Barbara Mason previously worked for UCB and recently started her own consultancy business (PhysChem Consulting Ltd.), John Comer is with Sirius Analytical Instruments.



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The Conference Circuit

As usual, ACD/Labs will be attending the Spring ACS meeting, which is fast approaching (April 6–10 in New Orleans). We will be presenting our Rule-of-5 study—published last year in the Journal *Molecular Pharmaceutics*—in both the COMP and MEDI divisions.

For a sneak peek at the data to be presented, [read the poster](#) from AAPS earlier this winter.

News & Events

News

Study Finds ACD/Labs pK_a Predictions to be Most Accurate—March 11, 2008 [Read](#)

Agilent Technologies and ACD/Labs Sign Collaborative Marketing Agreement—March 5, 2008 [Read](#)

ACD/Labs Introduces ACD/AutoChrom at PITTCON 2008—March 3, 2008 [Read](#)

Upcoming Events

ANALYTICA

Munich, Germany
April 1–3, 2008
Hall A2, Booth #116

235th ACS National Conference & Expo

New Orleans, LA, USA
April 6–10, 2008
Booth #1338

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