



Dear ,

ACD/Labs is pleased to present our latest newsletter for the academic community highlighting recent publications from ACD/Labs, examples of how customers are putting our software to use, and interesting presentations from recent meetings in North America and Europe.

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In this issue;

- How UCB Uses **Predictive Data** to Complement Experimental Findings
- **Manchester University** Offers NMR for Everyone...Anywhere
- Science Behind the Software—**Recent Publications** by ACD/Labs Authors
- How a Fellow Educator is Using a **Virtual Laboratory** to Teach Chromatography
- The Impact of PhysChem Properties on **Medicinal Chemistry**
- The Results Are In...How Did You Rate on the **PhysChem Quiz**?

UCB's Predictions Complement Experimental Determination

Emily Freeman is a member of the PhysChem Measurements group at UCB (Slough, UK) that measures permeability, solubility, and lipophilicity for new



chemical entities in early drug discovery. At the **3rd Annual PhysChem Forum Symposium** earlier this summer, Emily presented the high-throughput method used in her group for determination of aqueous solubility and approximation of pK_a , and methods for measurement of $\log D$. She also shared the PhysChem reports that provide chemists with at-a-glance summaries, including predicted values for pK_a , polar surface area, and number of hydrogen bond donors and acceptors using **ACD/Labs software**. ACD/Labs

predictions are used to support the efforts of the PhysChem group and allows them to provide other scientists with additional property data that is not experimentally determined in-house.

[View Emily's presentation](#)

Read other interesting presentations from the Symposium—visit the PhysChem Forum

The speaker list included scientists from **Novartis**, **GSK**, **AstraZeneca**, **Bayer**, and **Organon**. Topics varied from practical methods for the measurement of physical properties to the use of computational methods to extend property knowledge from known compounds to related analogs.

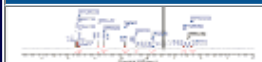
NMR For Everyone...Everywhere

After a year of using **ACD/2D NMR Processor** on a site-wide license,

More Solutions from ACD/Labs



Agricultural Chemistry



NMR Laboratory



Open-Access Laboratory

Manchester University's School of Chemistry noticed that using the software lead to more available instrument time, and less burden on expert's time. So, when the time came to decided whether retain the software and continue making NMR processing available to its students and faculty, both on and off-campus, the decision was simple.

"The volume and range of the School NMR services continues to expand, with more than 50,000 spectra being produced by our autosampler based spectrometers last year," said Roger Speak, Analytical Services Manager, Manchester University School of Chemistry. "We looked at several packages; however, [ACD/Labs'] server resident multi-seat license provided the best available facilities with exceptional value for the money."



Manchester's license package allows authorized faculty and students to use the software at home, in the office, or from anywhere the school's network can be accessed. [Read the full story](#)

For more information about what ACD/Labs has to offer Academia, e-mail us at education@acdlabs.com.

The Science Behind the Software—New Articles Now Available

The Rule-of-5 Revisited

The majority of chemistry graduates leaving school are familiar with the **Rule-of-5** (Ro5). It has been widely adopted in drug discovery and continues to be refined and adapted, yielding several variants. This rule of thumb is used as a first step filter to quickly eliminate lead candidates with poor physicochemical properties for oral bioavailability. One of the key parameters, **logP**, is a useful descriptor but one that fails to take into account the impact on lipophilicity of varying concentrations of different ionic species in the changing pH environments of biological systems. At ACD/Labs we compared application of the Ro5 using **logD** in place of **logP** on 9 commercial compound libraries. See the results of our study in *J. Mol. Pharm.*, 4, 556–560, 2007.

[Read the abstract](#)

Automated Structure Verification Using ¹H NMR and ¹H–¹³C HSQC Spectra

A recent publication on automated structure verification in **Magnetic Resonance in Chemistry** is now available for early view that outlines the performance of the combined verification algorithms available in **ACD/2D NMR Expert**. This article outlines the performance of a combined approach that uses both 1D ¹H and 2D ¹H–¹³C HSQC NMR data to automatically identify correct and incorrect chemical structures without human intervention. In the publication, we directly compare this new process to the one previously published that used only ¹H NMR data for structure confirmation.

[Read the abstract](#)

Virtually Teaching—Lessons in Chromatography

In the September issue of *J. Chem. Ed.* (Vol. 84, No. 9, 2007, 1488–1496), Dr. David Stone discusses a project undertaken at the **University of Toronto** (Canada) to help teach GC and HPLC **method development** and optimization to undergraduates. With the help of colleagues, David used **ACD/LC Simulator** to set up virtual laboratory exercises to teach, among other concepts, the effects of



operating parameters on run-time and resolution in chromatography. These exercises were used to supplement and extend undergraduate laboratory experiments and provided “an alternative means of delivering course content [while students still had] first-hand involvement with the subject material”. In the publication, David provides details of the exercises along with students’ comments about their virtual experience.

[Read the abstract](#)

PhysChem Properties & Medicinal Chemistry

Medicinal chemists are required to be mindful of the physicochemical properties of compounds they produce. In smaller biotech’s and research laboratories this can be an informal process, while in large Pharma, a list of set requirements is often provided per project/target. Although the work of Lipinski and others in the field has contributed greatly to our awareness of **physicochemical properties** and their influence on physiological endpoints, our mastery of this subject remains incomplete. At the ACS Spring meeting we discussed topics in this area, with relevant pharmaceutical case studies:

- The importance of physicochemical properties in **medicinal chemistry**
- The commonly misunderstood concepts of **logP** and **logD**
- Effective application of PhysChem data in **lead optimization**

[View the presentation](#)

Results of the PhysChem Challenge Are In...

After having the quiz posted on our website for a year, we decided to analyze the results to see what could be learned about our understanding of PhysChem concepts.



If you want to try it and haven’t done so already, now’s your chance! [Try the quiz](#).

Of the **572 people** who took the quiz, the average score was **3/6 (50%)**. Duplicate and triplicate results of those who tried over and over again for the perfect score were removed...you know who you are.

- Top two correct answers were #4 and #5—It seems the majority of us know the **difference between logP and logD** (fantastic); and since aqueous solubility is a common problem, especially in drug discovery, it was gratifying that most of us know that ionization and lipophilicity both influence this property.
- Top two wrong answers were #1 and #2—‘logP’ and ‘lipophilicity’ are terms learned in undergraduate studies but knowing the theoretical definitions and understanding how a property can influence the final product and its action is different altogether. Apparently this connection of theory to practical use is missing in our repertoire.

Ranking compounds for any property is a challenge when structures differ significantly, this is much more easily done for analogous substances. The problem is magnified when ionizable groups are added into the mix especially since logP pertains to neutral species. Question 2

was a perfect example of $\log P$ vs. $\log D$.

- Only 7 people got a **perfect score** of 6/6 (1%).

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News & Events

News

Biochemical Profiling Research Group Implements New Software for Metabolomics—August 31, 2007 [Read](#)

NMR for Everyone—Manchester University Provides Access to Industry-Leading Software—August 8, 2007 [Read](#)

How Natural Product Research Benefits from Computer Assisted Structure Elucidation—July 26, 2007 [Read](#)

Upcoming Events

SMASH 2007

Chamonix, France
September 16–19, 2007

ACD/Labs Mass Spectrometry and Chromatography Seminar 2007

New Brunswick, NJ, USA
September 25, 2007

ILMAC

Basel, Switzerland
September 25–28, 2007

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