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C h e m i s t r y
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ACD/Labs

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Demo Movie ACD/Structure Design Suite

View a demonstration of how the software quickly suggests structural modifications to the lead compound in order to produce analogs that are expected to overcome the physicochemical property-related PK liabilities—in this case—solubility.

[View Online](#)
(Flash, 4.22MB)
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Dear :

ACD/Labs is pleased to present our latest Physicochemical and Medicinal Chemistry newsletter highlighting recent literature and presentations, along with stories from our users of how they are applying our tools.

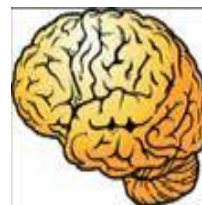
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In this issue;

- Predicting Blood Brain Barrier Permeability
- Test Your PhysChem Savvy
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- Symposium Highlights Applications of ACD/PhysChem Tools in Research
- ACD/Labs at ACS Spring

Predicting Blood Brain Barrier Permeability—Refining Current In-Silico Techniques

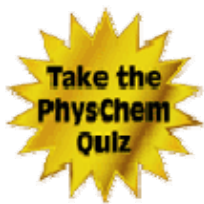
In keeping with the ACD/Labs tradition of collaborating with scientists on the front lines of research, we teamed up with Dr. Gilbert Rishton, Founder and Director of the Channel Island Alzheimer's Institute, at California State University to investigate molecular physical descriptors that would help to predict blood brain barrier (BBB) permeability. The comparative study of known central nervous system drugs versus new secretase inhibitors selected from medicinal chemistry literature lead the team to add a new term—based on the molecule's number of freely rotatable bonds—to a modified Clark Equation, refining current in-silico techniques for the prediction of BBB. Results of this research are published in Current Opinions in Drug Discovery & Development, 2006.



[Read the abstract and access the publication.](#)

How PhysChem Savvy Are You?

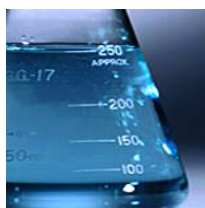
At the 30th National Medicinal Chemistry Symposium in Seattle last year, we challenged conference attendees to complete a short quiz about physical properties ($\log P$, $\log D$, solubility, and pK_a), and how they relate to questions that arise in day-to-day research. These questions apply equally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



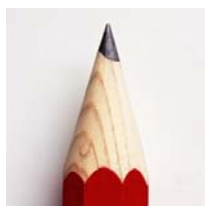
Upon completion, gain free access to the poster we presented at AAPS 2006 outlining how our software can help you address physicochemical property concerns.

Research into Treatments for Cocaine Abuse— PhysChem Tools in Action

Having used our physicochemical property prediction software daily for both research and education, Dr Mark Wentland, currently a Professor at the Rensselaer Polytechnic Institute, recently shared with us how he applied predicted property values to his work, and what he found valuable about the software:



Application in Research—the main goal of Mark's research is to identify isosteres of the phenolic-OH group in cyclazocine (currently in clinical trials for remediation of cocaine addiction) to increase duration of action. The calculation of physicochemical properties such as $\log P$, $\log D$, and polar surface area (PSA) using ACD/Labs software, helped them to understand oral bioavailability and blood brain barrier permeability of alternative groups, so they could select the best analogs for synthesis.



Application in Teaching—Mark used the software to teach physicochemical concepts to students in his classroom, and also expanded this to drug discovery workshops that he took to pharmaceutical companies such as Pfizer and Novartis to teach participants the application of molecular physical properties (including $\log P$, $\log D$, solubility, and pK_a) in drug discovery.

[Read more...](#)

Application of ACD/Labs' PhysChem Tools in Research

At ACD/Labs' third annual European Users' Meeting, the PhysChem Symposium brought together experts from many fields. The one thing they had in common was application of our PhysChem tools in their research. [Read how](#) our physicochemical property predictors are applied in different research environments.

ACD/Labs at ACS Spring Meeting

ACD/Labs will be at the ACS Spring Meeting in Chicago from March 25–29.

**Come to booth# 1065 in the exhibition hall
(Mon–Wed) to discuss how our solutions can aid**

(EXE, 12.2MB)

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your research, and see a demonstration of the software.

See our full [ACS Activities Schedule](#) to also plan time for our oral and poster presentations. We look forward to seeing you there.

News and Events

News

Collaborative Efforts Deepen Understanding in Alzheimer's Research—March 12, 2007 [Read](#)

ACD/Labs Naming Software Celebrates Support of Worldwide Repository of Protein Structures—March 2, 2007 [Read](#)

Wockhardt Equips Drug Discovery Researchers with ACD/Labs Software—February 6, 2007 [Read](#)

Upcoming Events

233rd ACS National Conference & Expo

Chicago, IL, USA
March 25–29, 2007
Booth #1065

MedChem India 2007

Hyderabad, India
April 12–13, 2007
Booth #7

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