



**Advanced
Chemistry
Development**

ACD/Labs

Dear ,

ACD/Labs is pleased to present our latest NMR newsletter which highlights what some of our users are saying about NMR processors and predictors, a structure elucidation challenge, details of a recently published article, and more.

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In this issue:

- New **Corporate Packages** available for Large Groups
- Can **ACD/Structure Elucidator** solve your toughest problem?
- The **latest publication** co-authored by ACD/Labs employees
- Updates from **Ryan's Blog**

Corporate Packages Mean Affordable NMR for Everyone

More and more organizations are turning to ACD/Labs to help with their **open-access NMR processing and analysis** needs. Read what some of our customers are saying about their recent deployments:



"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 the server resident, multi-seat [ACD/Labs] license provided the best available facilities with exceptional value for the money."



Dr. Roger Speak of Manchester University



"When SCYNEXIS was formed in 2000, we initially had no NMR software other than at the workstations on the instruments. SCYNEXIS management's decision to provide desktop NMR processing and analysis tools for all our chemists in 2001 resulted in a huge boost in efficiency."



Dr. Darryl Leblanc of Scynexis, Inc.

After reading about how ACD/Labs has helped several organizations with their open-access bottlenecks, you should investigate whether or not a similar solution can help out in your own environment.

A new ACD/Labs corporate package will make the same tools that are used by spectroscopists available to broader groups of scientists, including synthetic chemists, and account for the fact that they will only use part of the functionality at a fraction of the time compared to a power user. In addition, ACD/Labs continues to offer competitively priced site-wide licensing for academic institutions.

Go to our website for more information

Latest Research Papers Published by ACD/Labs Authors

Mag. Res. Chem.
Application of unsymmetrical indirect covariance NMR methods to the computation of the ^{13}C - ^{15}N HSQC-IMPEACH and ^{13}C - ^{15}N HMBC-IMPEACH correlation spectra

Mag. Res. Chem.
Automated structure verification based on a combination of 1D ^1H NMR and 2D ^1H - ^{13}C HSQC spectra

Upcoming NMR Seminars

RTP Seminar
October 3, 2007
North Carolina
Biotechnology Center
Research Triangle Park,
NC

Agenda Register

**New Jersey NMR
Seminar**
October 11, 2007
Hyatt Regency
New Brunswick, NJ

Agenda Register

**Do You Use
MDL® Draw?**

Is Computer Assisted Structure Elucidation an Option for You?

Does your job or research require you to **elucidate several chemical unknowns**? Do some of these unknowns take days, weeks, or even months to elucidate?



ACD/Structure Elucidator has provided crucial assistance to spectroscopists who spend a considerable amount of time on structure elucidation. In fact, some of its greatest challenges have been focused on in articles from many peer-reviewed chemistry journals. See a list of [peer-reviewed articles](#)

If you are interested in finding out if this software can help with some of your elucidation endeavors, why not try out the **Elucidator Challenge**? This trial service is available to any company or institution that has structural elucidation problems and is interested in evaluating the performance of ACD/Structure Elucidator.

NEW Article on Automated Structure Verification Using ^1H NMR and ^1H - ^{13}C HSQC Spectra Now Available

A recent publication on **automated structure verification** is now available for early viewing on the Magnetic Resonance in Chemistry website. This study outlines the performance of a combined approach that uses both 1D ^1H and 2D ^1H - ^{13}C HSQC NMR data to automatically identify correct and incorrect chemical structures without human intervention. It directly compares this new process to the one previously published that used only ^1H NMR data for structure confirmation.



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

Ryan's Blog on NMR Software

In our last broadcast we announced that our own employee Ryan Sasaki, Technical Specialist for ACD/Labs, had created a blog to provide the NMR community with up-to-date information on the world of NMR software. A few months, and a hundreds of subscribers later, the blog is going strong and attracting more and more readers by the day. Check out what Ryan has to say about:

[The 10 Best Kept Secrets in ACD/Labs NMR Software](#)
[The Price of NMR Software](#)
[The Curse of Knowledge](#)
[Neural Network vs. HOSE Code Algorithms](#)
[Electronic Lab Notebook Integration](#)

And much, much more.

Be sure to [subscribe](#) to Ryan's blog (via RSS or e-mail) and be automatically notified of new postings.

Integrate the powerful ACD/Labs tools you already use with MDL Draw:

[ACD/HNMR Predictor](#)
[ACD/CNMR Predictor](#)
[ACD/2D NMR Predictor](#)
[ACD/Labs PhysChem Software](#)

Get accurate, reliable predictions and chemical naming from within the familiar MDL Draw interface.

Go to our website for more information and to request the [free add-in](#).

News & Events

News

Helping Chemists Get Access to the NMR Tools They Need—September 18, 2007 [Read](#)

Upcoming Events

RTP NMR Seminar
Research Triangle Park, NC, USA
October 3, 2007

Visit us at
www.acdlabs.com
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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](#)



New Jersey NMR Seminar

New Brunswick, NJ
October 11, 2007



8th International ISSX Meeting

Sendai, Japan
October 9–12, 2007

Toll free (USA and Canada):

 1-800-304-3988 

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