



FOR IMMEDIATE RELEASE

Contact:

ACD/Labs
(416) 368-3435 ext 297
media@acdlabs.com

Advanced Chemistry Development, Inc., Delivers 2D NMR Verification Capabilities

Pittcon, Orlando, March 10, 2003 - Advanced Chemistry Development, Inc., (ACD/Labs) is the first software company to deliver 2D NMR verification capabilities to scientists worldwide.

ACD/Labs has been at the forefront of chemical structure verification using 1D NMR prediction for the past 8 years. Presently, ACD/Labs provides NMR prediction for a number of nuclei. The verification and automated assignment of chemical structures using ¹H, ¹³C, and ¹⁵N NMR prediction has now been extended to include 2D NMR.

"ACD/Labs continues to innovate and develop both structure verification and elucidation technologies for spectroscopy. At this time we are uniquely placed in supporting structure verification using IR, MS, 1D and 2D NMR spectroscopies," comments Antony Williams, Ph.D., VP of Scientific Development and Marketing for ACD/Labs.

Verification produces three values that quantify the degree of agreement of a structure to a spectrum. These are the Match Factor, a total measure of spectrum-structure correspondence; the RMS of Assignment, a measure of chemical shifts matching predicted values; and the Structure Purity, an estimate of the percentage of pure substance under question in the sample. These time-tested algorithms of NMR auto-assignment and verification have been enhanced to allow, for the first time, verification of chemical structures using predicted 2D NMR spectra. Both homonuclear and heteronuclear 2D NMR verification are possible and will be in Version 7.0 of ACD/2D NMR Manager available in late Spring 2003.

Brent Lefebvre, B.Sc., NMR Product Manager comments, "Advanced Chemistry Development's innovative 2D Verification will extend the utility of our 2D NMR Processing software to new heights. No other software product makes the preparation of 2D NMR data so intuitive and easy while still wielding the advanced tools necessary for challenging spectral manipulations."

###

