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ACD/Labs and Protasis Shatter the High-Throughput Bottleneck for NMR Analysis

Collaboration between ACD/Labs and Protasis/MRM produces the most complete automated high-throughput system available for NMR data production and analysis.

Toronto, Canada and Marlboro, USA (April 16, 2007)—An automated NMR verification system combining Protasis' One-Minute NMR system and ACD/Labs' ACD/Automation Server—effectively automating the entire NMR process, from loading samples to interpretation— has been successfully deployed in three high-profile, high-throughput laboratories.

Traditionally, high-throughput laboratories experience a bottleneck in the interpretation of NMR spectra as the ability to generate more data increases. The combined system from ACD/Labs and Protasis allows users to seamlessly collect samples, and automatically confirm the identity of the synthesized compounds in a matter of minutes. One particular laboratory within a large pharmaceutical company implemented the new system and now automatically confirms the structure-spectrum matches for greater than 50% of their high-throughput samples. This translates directly into a 50% decrease in the workload of spectrum interpretation.

"Routine spectrum interpretation can be made a thing of the past with this system. Now, a user can automatically have their spectrum-structure match confirmed by the software and not have to look at the spectrum at all." commented Brent Lefebvre, NMR Product Manager at ACD/Labs. "In fact, this is what one of our first users is doing with his 1D Proton spectra. Fifty percent of his workload is being handled by this system. Connecting our spectrum analysis software with the instrument automation of One-Minute NMR from Protasis, is enabling a shift back to high-throughput NMR. No longer is the data bottleneck an issue of this system."

Adds Bob Albrecht, One-Minute NMR Product Manager, Protasis, "Our automation system and probe increases the efficiency of sample submission, NMR detection, and throughput on any instrument. By working closely with ACD/Labs we are able to combine the best processing and databasing software, with our front-end to deliver the answers chemists need to do their work more effectively, using existing NMR equipment in the most efficient way possible. Continued work with ACD/Labs will put us in a position to deliver accuracy at least as good as that of human experts for structure verification and possibly elucidation."

For more information on this collaboration and the system that has been created, please refer to the original press release [here](#).

About Advanced Chemistry Development, Inc.

Advanced Chemistry Development, Inc., (ACD/Labs) is a chemistry software company offering solutions that truly integrate chemical structures with analytical chemistry information to produce ChemAnalytics®.



ACD/Labs creates innovative software packages that aid chemical research scientists worldwide with spectroscopic validation of structures, elucidation of unknown substances, chromatographic separation, medicinal chemistry, preformulation of novel drug agents, systematic nomenclature generation, and chemical patenting and publication. Combined, ACD/Labs' solutions create an analytical informatics system that provides dramatic feed-forward effects on the chemical and pharmaceutical research process. Founded in 1994, and headquartered in Toronto, Canada, ACD/Labs employs a team of over 145 dedicated individuals whose continual efforts carry ACD/Labs' innovative technologies into pharmaceutical, biotech, chemical, and materials companies throughout the world. Information about Advanced Chemistry Development and its products is available at www.acdlabs.com.

About Protasis/MRM

Protasis Corporation (Marlboro, MA) is the leading manufacturer and seller of capillary-based, microliter-volume NMR automation systems for NMR spectroscopy. The MRM Division of Protasis (Savoy, IL) was originally founded in 1994 by an interdisciplinary group of chemists, NMR spectroscopists, and engineers from the Beckman Institute at the University of Illinois to develop and bring to market microcoil (microliter-volume) NMR detection technology. Protasis was founded in 1999 as a spinoff of Waters Corporation (Milford, MA) to utilize microfluidics technologies and expertise to address new markets in microchemistry. Since joining forces in 2000, the combination of MRM's microcoil detection technologies with Protasis' microfluidics systems has resulted in systems offerings that target economical use of small volumes of sample to achieve excellent NMR data quality. The ability to collect data from smaller amounts of sample means that NMR can be applied earlier and more economically in the customer's process, resulting in faster decision-making. The intrinsic sensitivity of MicroFlow NMR is complemented by a complete suite of software tools that enable automation of the analysis, from the importing of sample lists at the time of sample submission, to automatic e-mail reporting of results at the end of the run. The addition of structure confirmation to high quality NMR spectra now provides chemists with complete information about their samples. Protasis products are described in greater detail at www.protasis.com.

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