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Advanced Chemistry Development, Inc., Provides Powerful Tools for the Elucidation of Unknown Structures with the Release of Version 7.0

Toronto, Canada, February 24, 2003 - Advanced Chemistry Development, Inc., (ACD/Labs) is pleased to announce the release of version 7.0 of their spectroscopy software that provides solutions for elucidating unknown structures. Advanced tools enable scientists to discover the structure of unknown organic molecules in less time and with more confidence. Never before has a scientist been able to determine a structure from a minimal amount of experimental data with such ease.

ACD/Labs' solution for the elucidation of unknown structures is built on the combined strength of our NMR prediction software (ACD/HNMR, ACD/CNMR, and ACD/NNMR) and spectral data processing software (ACD/MS Manager, ACD/NMR Manager, and ACD/2D NMR Manager). These tools allow scientists to import and process data, attach one or more chemical structures to the spectrum, and assign MS or NMR signals to molecular fragments or nuclei accordingly.

ACD/Structure Elucidator allows scientists to determine the chemical structure for an unknown compound from nearly any combination of experimental input data such as ¹H and ¹³C 1D NMR, 2D NMR, MS, and IR, as well as information from Elemental Analysis. Typically, the type of input data available for a particular unknown can vary widely. This is why ACD/Structure Elucidator has been designed to utilize nearly any combination of input data available. Days spent on manually elucidating an unknown can be reduced to a few hours or minutes through the use of ACD/Structure Elucidator. Also, this software is capable of producing a range of possible structures that may have otherwise been overlooked by an NMR spectroscopist. This kind of intelligence and flexibility is common in ACD/Structure Elucidator and is what makes this software package so powerful.

New to ACD/Structure Elucidator in version 7.0 is the Elucidation Wizard. Scientists are now able to elucidate their structure with step-by-step instructions. As a result, ACD/Structure Elucidator's easy-to-use interface enables users to navigate with confidence through the elucidation process. "Continuing efforts have further refined the already robust and mature ACD/Structure Elucidator package that will be released as version 7.0," said Dr. Gary Martin, Senior Fellow, Rapid Structural Characterization Group at Pharmacia.

Together, version 7.0 of ACD/Labs' suite of elucidation tools provide the knowledge, automation, and structure correlation that is vital in the identification of unknown structures. Dr. Gary Martin from Pharmacia also stated, "When dealing with NDRI's (Non Drug-Related Impurities), ACD/Structure Elucidator provides a means of objectively determining structures consistent with the available data for the NDRI that can serve as a point of departure for the spectroscopist's elucidation efforts, allowing him/her to more effectively multitask. NDRI's are considerably more challenging than drug-related impurities and the structural characterization of them can be particularly time consuming and the time savings that can accrue by having reasonable starting points for the data analysis can result in considerable cost savings. Using ACD/Structure Elucidator we were also recently able to solve an academic problem that had remained frustratingly unsolved for a dozen years due to extensive resonance



overlap in both the proton and carbon frequency domains that led to extensive ambiguities that initially prevented the determination of the structure."

Antony Williams, Ph.D., VP of Scientific Development and Marketing, comments that, "ACD/Structure Elucidator is being applied on a daily basis to the solution of problems which have challenged even the best NMR spectroscopists in the world. The computer offers an unbiased approach to elucidation which can elude even the most skilled NMR scientist."

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