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Advanced Chemistry Development Provides Solutions to Method Development with the Release of Version 6.0

Toronto, Canada, March 18, 2002 - Advanced Chemistry Development (ACD) is pleased to announce the release of version 6.0, which offers chromatography software packages that enable separation scientists to go from chemical structure to a viable separation method in minutes. While the definition of suitability changes at each stage in the chemical product life cycle, ACD software can reduce the time it takes to arrive at suitable methods at any stage, and can help to unite data and knowledge within the laboratory setting so that efficiency is increased with each new compound being studied.

ACD allows separation scientists to use previously developed methods, or to develop new chromatographic methods for their sample using ACD/ChromManager, ACD/LC Simulator, and ACD/GC Simulator. ACD/ChromManager contains the ACD/Chromatography Applications DB, which contains complete information for 3000 separations in version 6.0, including full method details and assigned chemical structures for each chromatogram. Each application is searchable by structure, sub-structure, or similar structure using the new Similarity Search feature in version 6.0, which allows users to retrieve suitable separation conditions for compounds structurally related to their own.

ACD/ChromManager version 6.0 also contains the Chromatographic Smart Search feature, which enables separation scientists to predict retention times for new compounds based on the similarity search results and prediction equations stored within the ACD/Chrom Applications DB. Separation scientists doing method development and structure elucidation are able to instantly choose the most suitable methods available for their compound in the Applications Database, dramatically reducing the number of trials that must be performed to find the optimal method.

Once the separation scientist captures which methods are most favorable for their compound, they can use ACD/LC Simulator or ACD/GC Simulator to refine the conditions for their separation with respect to composition of elution buffer, gradient, temperature, salt concentration, and column characteristics. Optimization on custom parameters is available in version 6.0, enabling the separation scientist to define functional dependence of retention time on one or two parameters of their choice. A suitability map has also been added in version 6.0, allowing the separation scientist to optimize run time and robustness in addition to resolution. "This visualization of suitability rather than resolution is a fantastic improvement in the experimental design step. As every chromatographer knows, resolution is not the only important parameter in chromatographic design," said Michael McBrien , M.Sc., Chromatography Product Manager at ACD.

Along with the major improvements in method development, ACD now offers separation scientists the Advanced Structures Package for Waters Millennium32. This package significantly enhances the ACD/MolX technology that is embedded in Millennium32 chromatography software, enabling users to perform structure and sub-structure searches within Millennium32. Michael McBrien of ACD also stated, "The ability to utilize chromatographic prediction and accumulate chromatographic knowledge enables ACD users to drastically streamline their method development process."