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ACD/Labs Accelerates Method Development with Analyte pKa Prediction

Toronto, Ontario, March 8, 2004 - Advanced Chemistry Development, Inc., (ACD/Labs) introduces the ability to predict analyte pKa values prior to method development with version 8.0 of ACD/LC Simulator. This capability will enable chromatographers to better select the mobile phase pH for new experiments based on the chemical structures or substructures of their ionizable compounds.

Mobile phase pH has a powerful influence on the retention times of ionizable compounds, but can also greatly affect the robustness of a separation due to secondary equilibria effects that occur close to the pKa. Predicting pKa values prior to developing a method will enable chromatographers to avoid working in pH ranges where secondary equilibria effects may occur, allowing them to select mobile phase pH values that will lead to high resolution, robustness, and short run times.

"Chromatographers have always been conscious of the importance of pKa to effective chromatographic method design. The problem has been that pKa measurements are not easy to perform, and that even when an organization has measured the pKa of a species, the data may not be readily available to the method development lab. With MDS 8.0, chromatographers can have access to an accurate pKa in just seconds," states Michael McBrien, M.Sc., Chromatography Product Manager at ACD/Labs.

ACD/LC Simulator is part of ACD/Method Development Suite, which provides all the tools necessary to retrieve starting methods, predict retention times, and model the separation of new compounds starting from their chemical structures. Within the ChromManager module of Method Development Suite, users can search the ACD/Chromatography Applications Database to recover methods for structures similar to their own, and then use LC Simulator to predict the retention times for their compounds using each recovered method. Once a viable starting method is selected, optimal conditions can be determined for the user's specific compounds with respect to pH, elution buffer composition, gradient, temperature, salt concentration, and column characteristics.

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