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Advanced Chemistry Development, Inc., Provides Powerful Mass Spectral Fragmentation Prediction Tools with the Release of ACD/MS Fragmenter

Toronto, Canada, February 24, 2003 - Advanced Chemistry Development, Inc., (ACD/Labs) is pleased to announce the release of ACD/MS Fragmenter. This powerful software application predicts mass spectral fragmentation patterns, which accelerates the identification of unknown molecular structures in mass spectral data sets.

ACD/Labs has automated the rule-based task of determining possible fragmentation for organic molecules in an easy-to-use interface. ACD/MS Fragmenter's prediction capability complements the powerful verification capabilities of autoassignment in ACD/MS Manager enabling scientists to reduce the time consuming, expert knowledge-based task of identifying unknown compounds.

Fully integrated with ACD/ChemSketch, this sophisticated tool is able to predict the likely mass spectral fragmentation for any organic chemically drawn or imported structure. "ACD/MS Fragmenter is designed for visualization of predicted structure fragments in mass spectrometry built on the proven and widely used fragmentation engine that is integrated into our ACD/MS Manager product line," said Mark Bayliss, Ph.D., Mass Spectrometry Product Manager at ACD/Labs. "Early discussions with a number of mass spectrometrists indicate that ACD/MS Fragmenter will have wide applicability for anyone interested in structural elucidation studies and the fragmentation routes of the individual fragments within a spectrum."

Advanced features enable scientists to select fragmentation-rule parameters to mimic different ionization techniques that range from classical electron ionization to low energy protonation techniques such as electrospray (ESI) and atmospheric pressure ionization (APCI). Fragmentation is presented in an organized fashion through a genealogical tree that establishes the parent child relationship of fragment ions in a natural manner. ACD/MS Fragmenter allows easy navigation along the fragmentation scheme with a smart graph tree structure. As a result, the normally tedious, manual, expert-requiring task of fragment prediction is reduced from countless hours to mere seconds.

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