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ACD/Labs
(416) 368-3435 ext 297
media@acdlabs.com

Advanced Chemistry Development Simplifies the Elucidation of Unknown Substances with the Release of Version 6.0

Toronto, Canada, March 18, 2002 - Advanced Chemistry Development (ACD/Labs) is pleased to announce the release of version 6.0, which offers tools that enable scientists to discover the structure of unknown metabolites, process impurities, or degradants, in less time and with more confidence than ever before. ACD/Labs' solution for the elucidation of unknown substances is, for the most part, comprised of three tools: ACD/MS Manager, ACD/NMR Manager, and ACD/Structure Elucidator.

ACD/MS Manager and ACD/NMR Manager are branches of the overall spectroscopic processing and data management software, ACD/SpecManager. Both ACD/MS Manager and ACD/NMR Manager enable scientists to import and process raw spectra data, attach one or more chemical structures to the spectrum, and assign MS or NMR signals to molecular fragments or nuclei accordingly. ACD/MS Manager is also able to read experimental LC(GC)/MS data into the program. New to the ACD/NMR Manager in version 6.0 are the ability to perform automated multiplet analysis as well as auto-assign ¹³C NMR spectra. The version 6.0 software also adds the ability to predict ¹⁵N NMR spectra to its present series of NMR nuclei that includes ¹H, ¹³C, ¹⁹F, and ³¹P.

One key to ACD/MS Manager's capabilities is the Component Detection Algorithm, CODA, which enables users to reduce noise and background in their chromatography/MS data, enabling recovery of mass spectra from even minor components from LC-MS and GC-MS. ACD/MS Manager also contains COMPARE LCMS, an extension of the CODA algorithm that allows scientists to find small differences between two or more similar samples within seconds. Scientists can use this feature to find and identify both metabolites and degradants. Both CODA and COMPARE are proprietary to ACD/Labs under license from Kodak, offering scientists a shortcut to solving their elucidation problems.

ACD/Structure Elucidator enables scientists to generate the chemical structure for an unknown compound based on its experimental spectra. Typical inputs are ¹H and ¹³C 1D spectra, 2D NMR, Mass, Elemental Formula, and optical spectra. It is also able to generate structural fragments in cases where complete structures cannot be found.

When ACD/Structure Elucidator is only able to generate fragments for a spectrum, the scientist can draw a candidate structure containing those fragments in ACD/ChemSketch, and then use the Match Factor capability within ACD/MS Manager or ACD/NMR Manager to determine if the drawn structure fits the spectrum. The Match Factor capability enables scientists to determine with what probability a candidate structure fits an assigned spectrum. Scientists can verify in one click the spectrum structure correlation for their candidate. This enables scientists to validate with confidence that the candidate structure for the experiment is accurate. The match factor is derived using the prediction algorithms based on over 100,000 assigned molecules and can be enhanced to include user databases to cover diverse chemistry.



ACD/Structure Elucidator is fully integrated with ACD/SpecManager, enabling smooth and automatic import of spectral data from ACD/MS Manager and ACD/NMR Manager into the elucidator. Version 6.0 of ACD/SpecManager also incorporates a new interface to view properties along with structures, as well as similarity search capabilities, which enable scientists to retrieve data for compounds structurally related to their own.

Together, version 6.0 of ACD/Labs' suite of elucidation tools provide the chemical knowledge, automation, and structure correlation know-how that is vital to sample identification. "The use of computer-assisted structure elucidation programs from ACD/Labs in conjunction with new probe and experimental methodology can lead to significant improvements in the time required to determine complex molecular structures," says Gary Martin from Pharmacia

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