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ACD/Labs Raises the Standard for NMR Prediction Accuracy with the Release of Version 8.0

Asilomar, CA, April 18, 2004 - Advanced Chemistry Development, Inc., (ACD/Labs) improves the prediction accuracy of their industry leading 1H and 13C NMR prediction software with the release of version 8.0.

The quality of ACD/Labs' NMR prediction algorithms are the foundation of all ACD/NMR predictor modules. These algorithms have continued to be optimized over the past decade and have undergone major enhancements in version 8.0 to provide noticeably improved prediction accuracy.

Along with the enhanced algorithms, the HNMR and CNMR Predictors are integrated with their respective NMR content database that contains critically evaluated shifts and coupling constants derived from the literature. In version 8.0, both the 1H and 13C databases were expanded to include an additional 10,000 entries, resulting in over 165,000 organic structures with reference information and assigned chemical shifts for each of the HNMR and CNMR Predictors.

A new capability in version 8.0 of the HNMR and CNMR Predictors is solvent-dependent prediction, which enables users to predict spectra using selected database entries from different solvents in order to make closer comparisons with experimental spectra. Several common NMR solvents can be utilized.

Brent Lefebvre , B.Sc., NMR Product Manager for ACD/Labs, states, "The improved accuracy of NMR prediction with version 8.0 shows this company's commitment to innovation and pushing the limits of software capabilities. The improved performance of the NMR predictors directly impacts our ability to perform verification of structure-spectra pairs for both 1D and 2D NMR. This accuracy is what makes 2DNMR structure-based verification possible. ACD/Labs continues to be the sole provider of this technology."

ACD/Labs made additions to other NMR databases in version 8.0 as well, including those containing 15N, 19F, and 31P chemical shifts and coupling constants. These databases, which can be searched using the same powerful searching tools as described for ACD/HNMR and CNMR DB, have been expanded to contain data from approximately 8000, 13,800, and 22,600 structures respectively for each of the 15N, 19F, and 31P nuclei. ACD/2D NMR Predictor makes it possible to predict spectra for a variety of 2D NMR experiments using 1H, 13C, and 15N NMR responses.

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