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ACD/Labs Tightens the Coupling Between Measurement and Prediction with the Release of ACD/PhysChem Version 8.0

Toronto, Canada, February 12, 2004 - Advanced Chemistry Development, Inc., (ACD/Labs) tightens the coupling between measurement and prediction with the release of ACD/PhysChem, version 8.0. Providing the industry's most accurate prediction algorithms for logP, pKa, aqueous solubility, and other physicochemical properties, version 8.0 of ACD/PhysChem software contains unsurpassed capabilities for tuning predictions with experimental data. These advances ensure that medicinal chemists can base their molecular design decisions on accurately predicted properties within novel proprietary classes of compounds. Specialists in the measurement lab also benefit from these advances because they identify which subset of compounds need to be measured.

ACD/PhysChem version 8.0 contains ACD/LogP Accuracy Extender (AE), a data analysis tool designed to calculate new increments for the ACD/LogP algorithms based on in-house measurements. ACD/LogP AE also helps you select the best compounds to measure from your corporate back-file and emerging lead series, and enables you to incorporate these measurements back into the calculation procedure, thus improving the accuracy of logP prediction for all molecules within each of these classes. ACD/LogP AE makes it possible to use both experimental logP and logD values as sources of data for improving the accuracy of logP prediction.

Also new to ACD/PhysChem, version 8.0, is ACD/pKa Accuracy Extender, which enables you to overcome any of the sources of error common in ACD/pKa prediction, in particular, ring breaking approximation, strong Hammett equation, and unknown Ortho substituent. With ACD/pKa AE, the expert chemist is able to add new Hammett equations for their novel chemical classes, and automatically incorporate these into the algorithms of every ACD/Labs product that references ACD/pKa predictions.

The ability to measure a smaller number of compounds makes it possible to employ more time consuming analytical methods in order to ensure the best possible measurements. This combination of highly accurate measurements feeding into highly accurate predictions is likely to simultaneously provide the highest throughput and accuracy for new chemical classes.

"Getting accuracy across the board is critical for the application of property-based design methodologies. In our view, this requires a tight cooperation between measurement scientists, computational chemists, and medicinal chemists. For our part, we continue to evolve the capabilities to support the tight integration of measurements into design decisions," states Robert S. DeWitte, Ph.D., Director of Medicinal Chemistry Solutions at ACD/Labs. "In our simulation of the operation of LogP Accuracy Extender, we've demonstrated that measuring 2% of a diverse set of compounds is sufficient to gain near maximal predictive accuracy over the remaining 98%. This means that critical insight can be gained much earlier." Regarding pKa Accuracy Extender, Robert adds, "Getting pKa right is a critical step to enable Medicinal chemists to explicitly manipulate the degree of ionization in order to improve solubility, permeability, protein binding, and blood-brain permeation."

ACD/PhysChem, version 8.0, is estimated to be available for shipping in May 2004.

