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Improving the Quality of Lead Candidates by Equipping Chemists with Predictive Tools

Molecular property prediction enables chemists to design lead compounds with optimal physical properties, thereby reducing the likelihood of failure later in the discovery pipeline.

Toronto, Canada (October 10, 2007)—Advanced Chemistry Development, Inc., (ACD/Labs), a leader in providing **molecular physicochemical property predictors** such as **pK_a, logP, logD,** and **aqueous solubility** to Pharmaceutical and Life Sciences, is now making it easier for corporations to provide these tools to all of their scientists in R&D with new corporate packages.

While property data can be gathered through experimental determination, this requires a physical sample (which may not be available in plentiful supply, if at all), and is a time and labor intensive undertaking. **Predictive software** can be used—in the absence of a physical sample or to conserve material for **screening compound libraries**—to build property profiles of compounds; help modify and **optimize properties** in a focused manner; and aid in **property measurement** experiments. The software, however, may only be available to a select few individuals, resulting in a bottleneck in productivity.

Arming more scientists with tools that provide relevant property data means time-savings and research advantages because the information needed is always available *when* it is needed. Some companies in pharmaceutical and biotech R&D have already employed this strategy. Pfizer provides their scientists with unlimited desktop access to our full range of PhysChem predictions, worldwide. At GSK, specialists use full desktop versions, while worldwide accessibility to ACD/Labs' algorithms for other scientists is available through GSK's own graphical user interface.

"Providing discovery chemists with physical prediction tools enables them to design lead compounds that have appropriate physical characteristics," comments Greg Pearl, ACD/Labs' Product Manager for the PhysChem product line. "The new corporate package makes it more affordable for companies to provide tools to their entire R&D division as opposed to a few selected individuals within these organizations."

ACD/LogD Sol Suite, the complete package of our physicochemical predictors, provides solubility, logP, logD, and pK_a predictions for almost any organic compound based on chemical structure, along with a plethora of other **molecular property data** such as **polar surface area, Rule-of-5 parameters,** and more. Users simply put in a structure and get a set of property values that allow chemists to make educated decisions about their work, more quickly and efficiently.

Visit our website to read more about ACD/Labs PhysChem tools for chemists, and flexible deployment options. www.acdlabs.com/propertyprediction/

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