FOR IMMEDIATE RELEASE

ACD/Labs' Collaborating with GlaxoSmithKline to Provide New and Enhanced Prediction Algorithms for Their Scientists

Toronto, Canada (August 14, 2006)—Advanced Chemistry Development, Inc., (ACD/Labs) today announced an exciting collaboration with GlaxoSmithKline (GSK) (one of the world’s leading research-based pharmaceutical and healthcare companies), that is focused on the creation of a specially adapted algorithm for predicting solubility in aqueous DMSO solution as well as related enhancements to ACD/Labs’ pKa and aqueous solubility prediction algorithms.

Complementing the collaboration, GSK’s recent purchase of ACD/Solubility DB, following their previous purchase of ACD/Labs’ logD, logP, and pKa predictors, now provides the full range of ACD/Labs’ physicochemical predictors to GSK scientists worldwide. The deployment provides GSK scientists with access to ACD/Labs’ predictors through their corporate intranet.

In response to the request by GSK to anticipate specific characteristics of compounds relating to their workflow, ACD/Labs is working on new customized algorithms for the prediction of solubility in aqueous DMSO solution. The algorithms will be derived from tens of thousands of experimentally determined data points provided by GSK, likely one of the largest such data sets measured under uniform and controlled experimental conditions.

In addition, the collaboration is also focused on the facilitation of training the pKa algorithm for the out-of-the-box solution, using ACD/Labs’ Accuracy Extender module and GSK’s own experimental measurements. The outcome of this work in particular will provide augmented automation and speed of introducing new pKa data into ACD/pKa DB. ACD/Labs’ customers will benefit from features being developed for pKa Accuracy Extender that have been influenced by discussions with scientists at GSK.

Antony Williams , VP and Chief Science Officer for ACD/Labs, adds, "It is a privilege to collaborate with GSK scientists, using their insights and experience in experimental solubility determinations, to deliver a unique prediction platform for DMSO solubility to the scientific community. The meshing of our scientific intellect in physicochemical prediction algorithm development with their skills in high quality data acquisition is a model for collaborative science. We believe that the results will deliver an innovative example of our ongoing mission to provide visionary software for scientists."

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