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ACD/LogD Suite Selected by Degussa as (Q)SAR Tool for Registering Chemicals Under EU REACH Mandate

Toronto, Canada, August 1, 2005 - Advanced Chemistry Development, Inc., (ACD/Labs) is pleased to announce that the Services Environment, Safety Health Chemicals Safety Management Department of Degussa AG at Hanau, Germany, will use ACD/LogD Suite software as a (Q)SAR tool to evaluate the structure-activity relationships of many existing chemical substances on the European Union (EU) market. Under a new regulatory framework for chemicals proposed by the European Commission to improve health and environmental protection, chemicals require re-evaluation to gain better knowledge of their potential risks on human health and the environment.

Under the future REACH (Registration, Evaluation, and Authorization of CHemicals) system proposed by the Commission's Future Chemicals Policy, enterprises that manufacture or import more than one tonne of a chemical substance per year will be required to register data for that substance with a central authority. This authority will then evaluate the data and apply authorization requirements to substances of high concern. This system will apply to new substances, along with over 30,000 existing substances that are marketed in high volumes, including a number of substances manufactured by Degussa.

The use of (Q)SARs is currently limited within EU legislation, however, under the REACH system, they will be used more extensively in the interests of time- and cost-effectiveness. ACD/LogD Suite will provide Degussa with a full array of tools for evaluating the structure-activity relationships of their compounds, among those logD (as a pH-dependent measure of hydrophobicity), pKa, and logP. The logPow value as a criterion for hydrophobicity plays a crucial role for the prediction of the partition behavior of chemical substances between environmental compartments (water, soil, sediment) and the assessment of the tendency to bioaccumulate.

Dr. Wilfred Mayr, Head of Toxicology of the department of Environment, Safety, Health - Chemicals Safety Management from Degussa AG, states, "The prediction of the dependence of the hydrophobicity on pH is of particular importance in cases where the logPow value of dissociable substances was experimentally determined at pH ranges that are not environmentally relevant. For these cases the logD program is a valuable tool allowing for the calculation of logPow for the complete dissociation range of a substance. This allows us to use the logPow at environmentally relevant pH values for further modeling of the behavior of a substance in the environment and for risk assessment purposes without extended and time consuming experimental determination of the logPow at different pH values. pKa values on the other hand are an important determinant for the prediction of the toxicokinetic behavior of a substance, for example the absorption along the gastrointestinal tract."

Dr. Antony Williams, Vice President and Chief Science Officer at ACD/Labs, adds, "ACD/Labs has delivered PhysChem prediction software to chemical and pharmaceutical companies for over 10 years. In multiple head-to-head comparisons with other physicochemical prediction software ACD/Labs has been chosen as the standard by multiple companies. When Degussa utilize the ACD/PhysChem software they



will take advantage of the highest accuracy of predictions available today. We look forward to supporting the efforts of Degussa as they work to meet their goals of REACH compliance."

Details on the European Commission's REACH program and the use of (Q)SARs in regulatory processes can be found at the European Chemicals Bureau Web site, <http://ecb.jrc.it/>.

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