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## Advanced Chemistry Development and BioByte extend relationship to include pKa data.

**Toronto, Ontario and Claremont, California - March 1, 2001** - As part of an ongoing effort to improve the scope and predictive accuracy of ACD/pKa DB, Advanced Chemistry Development, Inc. today announced that it has extended its strategic partnership with BioByte Corp. Under the terms of a new agreement, ACD will be able to use pKa data from BioByte's Masterfile database of measured pKa values to improve the accuracy and scope of its prediction of pKa and related properties. Additionally, the pKa related content of the Masterfile will be added to the internal database of ACD/pKa DB, with primary literature citation and credit to BioByte.

This extends an agreement announced on February 2, 2001 wherein ACD gained access to BioByte's Star List of measured logP data.

The prediction of pKa is paramount to understanding the behavior and characteristics of a compound in solutions of varying acidity. In physiological phenomena, compounds encounter ambient solutions ranging from strong acid in the stomach to weak base in the later intestines. In environmental phenomena, compounds are found at pH near 7, which for some implies a predominance of cation, others a predominance of anion, and still others are predominantly neutral.

"ACD has established itself as the clear leader in the world of pKa prediction, and BioByte have been the most diligent in collecting pKa data," said Robert DeWitte, Ph.D., Scientific Product Manager, Advanced Chemistry Development. "By combining the rich treasury of pKa data in the MasterFile with the predictive expertise already embodied in ACD/pKa DB, we will be able to produce a tool of inscrutable accuracy."

"Our cooperation with ACD is proving to be a very satisfying relationship, and we are pleased to support their progress in pKa prediction," said Dr. Albert Leo, President of BioByte. "ACD's success in bringing consideration of molecular physical properties to the practicing medicinal chemist has created a wonderful opportunity for BioByte to distribute this valuable pKa information in an intelligent package for chemists."

The Masterfile currently contains 13,382 pKa values for 10,910 structures. ACD/pKa DB 4.5 contains an internal database of 8,800 structures with over 23,000 experimental pKa values. The new data will substantially improve the quality of ACD's predictions of pKa, logD, solubility, bioconcentration factor, and adsorption coefficient. This addition to the data already in use at ACD will bring the knowledge base within ACD/pKa DB to an unprecedented size. It will also enable ACD to add many new reaction centers and equations to its algorithms.

ACD's LogP, pKa and LogD predictions are becoming ever more popular in the chemistry research community, and ACD continues to strive to improve our offering. This is one of several steps being taken to maintain this leadership position.



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