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ACD's Version 6.0 Helps Medicinal Chemists Battle the Challenges of Passive Human Absorption

Toronto, Canada, March 18, 2002 - Advanced Chemistry Development (ACD) announces the release of ACD/PhysChem version 6.0, the suite of prediction products that provides key insights into the passive human absorption challenges faced by medicinal chemists involved in drug discovery projects. The emphasis on solubility and increased database functionality in version 6.0 makes it easier for medicinal chemists to acquire appropriate compounds for screening purposes and to maximize information content in experiments while avoiding problematic molecules. Version 6.0 also helps medicinal chemists to recognize the influence of trends in molecular physical properties on activity.

Within the suite of PhysChem 6.0 products, chemists are able to predict values for the properties most pertinent to medicinal chemistry, including LogD, LogP, pKa and solubility. Version 6.0 uses improved prediction algorithms that can be trained by multiple databases, both internal and external, to increase the accuracy of the calculations.

The internal ACD/pKa DB has been expanded in version 6.0 to almost double its size due to the addition of data provided by BioByte Corporation under an agreement that grants ACD access to BioByte's Masterfile database of measured pKa values.

"By combining the rich treasury of pKa data in BioByte's Masterfile with the predictive expertise already embodied in ACD/pKa DB, we have produced a tool of inscrutable accuracy," said Robert DeWitte, Ph.D., Director of Marketing at ACD. ACD has also expanded their ACD/LogP database with data from the BioByte Star List of LogP values.

ACD/PhysChem version 6.0 places great emphasis on solubility, as it is the largest single factor driving passive human absorption. New features allow medicinal chemists to calculate intrinsic solubility, solubility at specified pH values, and solubility in unbuffered water with a corresponding pH value. This, combined with the increased database and prediction capabilities of version 6.0, makes it possible for medicinal chemists involved in combinatorial chemistry and parallel synthesis to design effective high throughput chemistry experiments, where insoluble compounds are easily eliminated from acquisition plans, and where the diversity of physical properties within their screening collections is balanced.

"Medicinal chemists will be pleasantly surprised with the revolutionary advancements that version 6.0 will bring to their drug discovery projects," said Robert DeWitte, Ph.D., Director of Marketing. "We are committed to helping them battle the challenges faced with passive human absorption through our software."

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