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ACD/Labs Naming Software Celebrates Support of Worldwide Repository of Protein Structures for Over Five Years

Piscataway, NJ, and Toronto, Canada (March 2, 2007)—Advanced Chemistry Development, Inc., (ACD/Labs) and the Worldwide Protein Data Bank (wwPDB) are proud to announce the extension of a collaboration in which ACD/Labs will continue to provide molecular nomenclature software support to wwPDB for use in its data processing and annotation operations. Their mutually beneficial relationship has recently celebrated its five year anniversary.

During the past five years, ongoing feedback from the wwPDB management team to the ACD/Labs nomenclature specialists has supported the enhancement and extension of the nomenclature algorithms. These algorithms allow rapid systematic chemical naming according to the International Union of Pure and Applied Chemistry (IUPAC) Recommendations on Nomenclature of Organic Chemistry (1979 and 1993), and during this collaboration has included enhancements to the naming of biochemical, organometallic, and inorganic structures.

The wwPDB is the authoritative worldwide data repository for the processing and distribution of 3D biological macromolecular structure data, and protein crystal structures dating back to the very first structures ever solved by x-ray diffraction. It is a vital resource for all aspects of structural biology and modern techniques in drug discovery. Currently, the Data Bank has over 41,000 protein structures and adds new structures every year. The wwPDB has been adding systematic names of small molecules to the Data Bank using ACD/Name, aiding researchers by providing unequivocal names for the co-factors and ligands bound to macromolecules in the database.

"ACD/Labs has been happy to support the efforts of the wwPDB and we look forward to continuing our relationship. Our collaboration with the Worldwide Protein Data Bank has challenged us to continue to enhance and extend our nomenclature algorithms. As a result of this work, all of our users have benefited from the extensions to our software," said Antony Williams, Vice President and Chief Science Officer, ACD/Labs. "Our hope is that our joint efforts will continue to deliver value to all of our users as well as users of the wwPDB database. Nomenclature will continue to give researchers added clarity about the nature of small molecule ligands in the wwPDB and offer a rich source of information for those who study and employ techniques in Structure Based Drug Design."

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