

**FOR IMMEDIATE RELEASE****Contact:**

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ACD/Labs Software Integrated into ChemSpider Service

Partnership brings predicted $\log P$ property values and systematic nomenclature identifiers to over 10 million chemical structures online, to support ChemZoo's vision of creating a chemical community.

RALEIGH, North Carolina, and TORONTO, Canada, April 10, 2007—ChemZoo and Advanced Chemistry Development, Inc., (ACD/Labs) announced a collaboration that will allow integration of a number of ACD/Labs software tools to the ChemSpider service, a new online chemistry database and property prediction service provider. ACD/Labs properties will be generated and published for over 10 million chemical structures using some components of the ACD/Labs PhysChem and Nomenclature software suites.

“By collaborating with novel chemistry information sources such as ChemSpider, we strive to make chemically intelligent web resources available to researchers and chemistry students, to help them navigate their way through the publicly available annals of chemistry knowledge, and be able to find useful information quickly,” comments Daria Thorp, ACD/Labs' Director of Marketing Communications. “ACD/Labs' commercial chemistry software is about bringing scientists within a department or across an organization together into a network that facilitates collaboration and knowledge sharing to achieve a fast breakthrough in their proprietary research, discovery, or development efforts. We are pleased to be able to contribute to the public chemistry community as well, to help educate future scientists, and enable knowledge exchange between researchers via the Internet.”

This collaboration is a part of the continuous efforts by ACD/Labs to deliver access to chemistry software to the fingertips of chemists, students, and researchers. Since 1998, ACD/Labs has offered a comprehensive freeware version of their chemistry drawing software, ACD/ChemSketch [<http://www.acdlabs.com/download/>], that also includes IUPAC naming conversion, to the research community. Now enhanced with free $\log P$ prediction, ACD/ChemSketch freeware has just celebrated its $\frac{3}{4}$ millionth download. ACD/Labs' recent collaborative efforts have included the integration of physicochemical properties into the online chemistry database provided at www.emolecules.com. Joint efforts with the Selected Organic Reactions Database (SORD) [www.sord.nl] is tapping into the vast reserves of chemical reaction information from academic research, making it searchable by a variety of parameters and accessible over the internet to users worldwide. The collaboration with ChemSpider brings together some of the industry's premier prediction algorithms to provide added value to chemists for the purpose of data mining.

The ChemSpider service offers chemists access to an enormous collection of chemical structures and associated properties. Currently, ChemSpider allows access to a database of over 10 million compounds with text and structure/substructure searching capabilities. The addition of ACD/Labs' physicochemical parameters offers the benefits of filtering the data using an abundance of molecular physical properties (ACD/Log P , polar surface area, boiling point, number of freely rotatable bonds, and more) to further refine data mining, and to quickly identify chemical structures of interest. The ChemSpider service strives to become the foundation of an online community for chemists. Future development will enable chemists



around the world to add their own structures and reactions to the database for public review and access. The intention is for ChemSpider to provide an environment where chemists will feel comfortable annotating an already existing database of chemical structures, adding to the dataset, and exposing their research in a structure-centric environment.

About ChemZoo

ChemZoo, Inc., was founded with the intention of providing online chemistry software and services to help build a chemical structure centric community for chemists. Their first offering, ChemSpider [www.chemspider.com], is a chemistry search engine built with the intention of aggregating and indexing chemical structures and their associated information into a single searchable repository and making it available to everybody, at no charge. Founded in 2007 and located in Raleigh, North Carolina, ChemSpider intends to become a facilitator in the exchange of structure-based information between chemists worldwide.

About Advanced Chemistry Development

Advanced Chemistry Development, Inc., (ACD/Labs) is a chemistry software company offering solutions that truly integrate chemical structures with analytical chemistry information. ACD/Labs creates innovative software packages that aid chemical research scientists worldwide with spectroscopic validation of structures, elucidation of unknown substances, chromatographic separation, medicinal chemistry, preformulation of novel drug agents, and chemical patenting and publication. Combined, ACD/Labs solutions create an analytical informatics system that provides dramatic feed-forward effects on the chemical research process. Founded in 1994, and headquartered in Toronto, Canada, ACD/Labs employs a team of over 145 dedicated individuals whose continual efforts carry ACD/Labs innovative technologies into pharmaceutical, biotech, chemical, and materials companies throughout the world. Information about Advanced Chemistry Development and its products can be found at www.acdlabs.com.

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