

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

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**eMolecules Announces Integration of ACD/Labs LogP Predictions for Chemical Structures**

Partnership brings predicted LogP and related property values to more than 5 million chemical structures online.

**DEL MAR, California and TORONTO, Canada, March 29, 2007** – eMolecules, Inc., the provider of the world's largest online chemistry database, and Advanced Chemistry Development, Inc. (ACD/Labs), today announced a collaboration that will allow predicted logP data to be displayed in [eMolecules](#) freely accessible online database of 5.6 million unique chemical structures.

By integrating [ACD/Labs' logP Batch](#) into its state-of-the-art chemical structure search platform eMolecules extends the power and relevance of its high-performance search engine with the ability to preload predicted logP values for small molecule structures. The addition of logP— a measure of a molecule's **lipophilicity**—enables more efficient selection and procurement of chemical structures from the eMolecules data set of more than 3.5 million commercially available chemicals. Application of this property spans many industries and areas of research from **drug discovery**, **agrochemicals research**, and **flavors and fragrances**, to monitoring pollutants and their progress through our **environment**. As such, this physicochemical property is of importance to a broad audience.

For each available structure, search users will be presented with a predicted value for logP in the basic search results, and additional Lipinski Rule-of-5 predicted properties in a 'Details' page, including the number of **proton donors and acceptors**, number of **freely rotatable bonds** and **polar surface area**.

"At eMolecules, our primary focus is on delivering tools and information that enable chemistry professionals and biotech researchers to do their jobs more efficiently. Free access to valuable chemistry information forms the essential starting point for this. The integration of the ACD/Labs LogP batch calculator demonstrates our commitment to provide our users with a modern chemical information platform that provides unsurpassed value and accessibility," said Klaus Gubernator, Founder and CEO of eMolecules. "Future partnerships will enable eMolecules to present additional sources of high-value reference content in the coming months."

"Through this partnership with eMolecules, we continue our tradition of advancing chemical research by making critical physicochemical properties freely available to scientists. By adding value to the eMolecules service in this fashion, users get more of the information they need, quickly and without resorting to the use of secondary tools", said Greg Pearl, PhysChem Product Manger, ACD/Labs. "The ACD/LogP algorithm has been in existence since 1994 and has been continuously developed and refined. As a result, eMolecules users can be sure that the values it produces are accurate and reliable."

**About eMolecules**

eMolecules, Inc. has created the world's leading open-access chemistry search engine. The company's mission is to discover, curate and index all of the public chemical information in the world, and make it available to scientists everywhere, free of charge. eMolecules distinguishes itself by extremely fast



searches, an appealing presentation of results, high-quality chemical drawings, valuable reference information and cheminformatics tools. Founded in 2005 and located in San Diego, California with offices in London, it has rapidly become the world's most popular public chemical structure search engine. eMolecules also provides custom web search solutions for databases and catalogs of chemical structures, including hosted eCommerce solutions for chemical suppliers of any size.

**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](http://www.acdlabs.com).

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