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## Biochemical Profiling Research Group Implements New Software for Metabolomics

**Virginia Bioinformatics Institute uses innovative software from ACD/Labs to tackle biomedical and agricultural research.**

**Blacksburg, VA** (August 30, 2007)—Researchers at the **Virginia Bioinformatics Institute** (VBI) at Virginia Tech are examining ways in which **metabolomics** can be applied to the study of **systems biology**. Recently, they invested in new technology, [ACD/IntelliXtract](#), to further enhance their ability to handle the data obtained by liquid chromatography/mass spectrometry (LC/MS).

Metabolomics involves the systematic study of the metabolic processes of living cells and requires the **high-throughput analysis** of a large number of **small-molecule cellular metabolites**. While current instrument technology enables samples to be analyzed more and more quickly, the resulting avalanche of data must then be managed—often an overwhelming task.

ACD/IntelliXtract quickly and accurately **extracts all chromatographic components**, assigning adducts and **interpreting mass spectra** for each component. Components of interest can then be labeled and isolated from other components for identification, helping researchers to gain a quicker understanding of their results. Moreover, this process can be carried out as part of manual data interpretation for a few samples, or can be automated for large numbers of samples.

“We were looking for software that could help alleviate the pressure of data interpretation we were experiencing. There is an inevitable backlog of information that occurs with high-throughput analysis and ACD/IntelliXtract is able to automate some of that work,” said Dr. Vladimir Shulaev, Associate Professor at VBI and the head of the Biochemical Profiling Research Group. “Having already used [ACD/MS Manager](#) extensively, we were familiar with ACD/Labs software and their customer service, and confident about the quality of the results IntelliXtract would generate.”

One application—especially useful to VBI’s metabolomics studies—uses ACD/IntelliXtract to assist with **related fragment screening**, taking advantage of the fact that many intermediates in a metabolic pathway have similar structures. Exploiting this knowledge in identifying and elucidating metabolites seems intuitive; however, in practice, organizing the data and visualizing relationships is much more difficult. With the help of ACD/IntelliXtract, LC/MS data is automatically analyzed and organized, presenting the relevant data for related metabolites in a clear and concise report. Read more about related fragment screening in an [application note](#) downloadable from the ACD/Labs website

For more information about IntelliXtract visit our website [www.acdlabs.com](http://www.acdlabs.com).

### 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 to produce ChemAnalytics®. 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, systematic nomenclature generation, and chemical patenting and publication. Combined, ACD/Labs' solutions create an analytical informatics system that provides dramatic feed-forward effects on the chemical and pharmaceutical 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 is available at [www.acdlabs.com](http://www.acdlabs.com).

#### **About VBI**

The Virginia Bioinformatics Institute (VBI) at Virginia Tech has a research platform centered on understanding the "disease triangle" of host-pathogen-environment interactions in plants, humans and other animals. By successfully channeling innovation into transdisciplinary approaches that combine information technology and biology, researchers at VBI are addressing some of today's key challenges in the biomedical, environmental and plant sciences. Visit [www.vbi.vt.edu](http://www.vbi.vt.edu) for more information.

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