



## FOR IMMEDIATE RELEASE

### Contact:

Tara Sinclair  
ACD/Labs  
(416) 368-3435 ext 297  
[media@acdlabs.com](mailto:media@acdlabs.com)

## How Natural Product Research Benefits from Computer Assisted Structure Elucidation

**Unigen Pharmaceuticals reaps the rewards of a software product that enables CASE, better data management, and reporting.**

**Toronto, Canada (July 26, 2007)**—Leading **natural product research** and development company and proprietary ingredients supplier, Unigen Pharmaceuticals, found a solution to the challenges of managing multiple analytical techniques and data formats to effectively carry out structure elucidation for lead compounds. Implementing an innovative software product, [ACD/Structure Elucidator](#), eases the burden of structure elucidation with **computer assisted structure elucidation (CASE)** and provides a platform to process, analyze, and store all analytical data in one place.

**Structure elucidation** is a critical task in natural product research. It usually involves the use of many different analytical techniques ranging from **NMR, mass spectrometry, IR, and chromatography**. Various vendor formats further complicate the issue, rendering it difficult to collect and store all of this data, and even more difficult to interpret the data in order to elucidate a compound's structure.

What Unigen needed was a product that could combine the NMR spectroscopist's expert knowledge with data from other analytical techniques, integrating, predicting, processing, and databasing the available information. ACD/Structure Elucidator from Advanced Chemistry Development, Inc., (ACD/Labs) includes processing and databasing tools for 1D and 2D NMR, MS, UV-IR, and Chromatography. Once all of this information has been coherently brought together, ACD/Structure Elucidator, using its industry leading **CASE** capabilities, helps determine the structure of unknown compounds.

To work with ACD/Labs, using their state-of-art structure elucidation software, is one of the key technology initiatives at Unigen in 2007. ACD/Structure Elucidator has significantly enhanced the structure elucidation competency in the novel natural ingredient discovery process through the screening of tens of thousands of medicinal plants in the PhytoLogix™ library at UNIGEN® USA.

“At present, Unigen has five on-going discovery screening projects with each project yielding hundreds of purified natural compounds after bioassay guided isolation. How to



improve our accuracy and efficiency in structure identification is a huge technology challenge to our chemists,” commented Dr. Qi Jia, Chief Scientific Officer at Unigen. “ACD/Labs software, the database and the experience of the company in natural products offer a perfect solution to our needs.”

The ability to create a comprehensive database opens up the opportunity for a company to build a library of experimental data that can serve as a valuable resource for [compound identification](#) in the future. In addition, ACD/Structure Elucidator includes ACD/Labs'  $^1\text{H}$ ,  $^{13}\text{C}$ , and 2D NMR prediction packages which can also be used independently for other challenging NMR projects.

Dr. Jia forecasts that the extensive use of ACD/Structure Elucidator will help Unigen to bring more novel natural products into its discovery and development pipeline. The success of the collaboration with ACD/Labs has led to a decision from Unigen's board to bring in new NMR equipment to its Lacey, WA, facility in the third quarter of this year.

For more information about ACD/Structure Elucidator, visit our website [www.acdlabs.com](http://www.acdlabs.com)

#### **About Advanced Chemistry Development, Inc.**

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 Unigen Pharmaceuticals, Inc.**

Unigen Pharmaceuticals, Inc. ([www.unigenpharma.com](http://www.unigenpharma.com)) is a leading natural products research and development company and proprietary ingredients supplier. The company is dedicated to the discovery of botanically derived therapeutic compounds that address consumer health needs and help improve the quality of human life. Its research and discovery process includes extensive work at both the human cell and gene level. Unigen focuses on identifying and studying the unique ingredients of medicinal botanicals and then formulating proprietary raw materials for use in cosmeceutical, nutraceutical, functional food and pharmaceutical products. Unigen is part of the

ECONET global family of health and natural product companies which have operations in the United States, Canada, Korea, Mexico, Russia and China.

###