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

## Advanced Chemistry Development, Inc., Provides Advanced Solutions for Method Selection in High-Throughput Chromatography with the Release of ACD/ChromGenius

**Toronto, Canada, February 24, 2003** - Advanced Chemistry Development, Inc., (ACD/Labs) is pleased to announce the release of ACD/ChromGenius. This intuitive software enables scientists to accurately predict retention times from chemical structures and select the optimal standard method to apply in high-throughput chromatography.

Developed for parallel synthesis and chromatographic walk-up laboratories faced with hundreds and even thousands of samples on a routine basis, ACD/ChromGenius accelerates the selection of suitable starting separation methods from a group of candidate standard methods, which helps to eliminate iterative experiments and instrument downtime. Advanced algorithms allow ACD/ChromGenius to learn as it works, utilizing user-specific experimental data to enhance the prediction for subsequent compounds.

ACD/ChromGenius allows scientists to automatically select the best separation method for high-throughput chromatography based on expected chemical structures in the sample, avoiding rerunning samples and wasting materials. In combinatorial chemistry, a group of samples will typically all be analyzed or purified using the same chromatographic method. This "one size fits all" approach has led to sample reruns, acceptance of questionable chromatographic data, and costly instrument down time. Based on the expected structures, ACD/ChromGenius considers each sample individually to advise scientists as to which standard methods are apt to be viable. Sample/method lists can then be imported into the instrument so that each sample is tested appropriately.

ACD/ChromGenius learns as it works by updating its chromatographic knowledge base with each new compound. As the chromatographic knowledge base grows, the accuracy of prediction increases. Automated tools for extraction of this new knowledge are also available. "ACD/ChromGenius is a truly fantastic complement to ACD/ChromManager. The unique nature of ACD/ChromGenius allows scientists to develop in-depth knowledge based on a smaller number of methods, which greatly increases the accuracy of selecting a suitable method," said Michael McBrien, M.Sc., Chromatography Product Manager at ACD/Labs.

The accurate retention time prediction of ACD/ChromGenius is also useful for structure verification purposes. Generally, LCMS verification is done based only on molecular weight. With ACD/ChromGenius, experimental versus predicted retention times can be visualized prior to the first chromatographic run. Large deviations from the expected retention times are highlighted, allowing users to target these samples for HNMR or other added analysis. This approach can drastically reduce the number of incorrect structures in an organization's compound library, and save weeks of work for the synthetic chemist.



ACD/ChromGenius can also be applied on the preparative scale. Methods can be selected based on structures of all expected compounds, targeting resolution of expected product, run time/elution volume, and even peak shape. The end result is fewer runs, faster purification, and purer samples.

ACD/ChromGenius has been developed in collaboration with Specs, the leading supplier of chemistry solutions for drug discovery to the Life Science industry. Included with ACD/ChromGenius is the same database used by Specs to select LCMS methods and assist in the verification of structures-a knowledge base including thousands of retention times for two different methods.

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