As a standard analytical tool, chromatography requires fast and vendor-independent data processing, and benefits from specialized storage and retrieval tools. The retrieval advantages of application databases using chemical structures for databasing and method development, such as ACD/ChromManager, are discussed.

If your laboratory routinely runs chromatographic separations and develops new applications with a wide array of equipment, then you are likely using different forms of data processing and database software. ACD/ChromManager allows you to process LC and GC data from different vendors within one interface, and to attach chemical structures to peaks before storing the results in fully searchable archives. These databases can be searched by structure, substructure, or chromatographic parameters (1), and they give powerful insights into the elucidation of the chromatographic behavior of novel compounds.

Experimental

For this example we used the ACD/Chromatography Application Database, v.5.0, provided with ACD/ChromManager, to develop a new method for the Quest Structure (Figure 1). We began by searching the database for the Quest Structure to see if this compound was part of another separation developed earlier.

In this case, no hits were found, which replicates a common situation for novel compounds. Next, searching for related compounds by focusing on a characteristic heterocycle in the structure (Fragment A, Figure 1) yielded 93 HPLC separation methods. We refined the search further by performing a subsearch for another distinguishing chemical group (Fragment B, Figure 1). As a result, we found 7 chromatograms of compounds containing both structural Fragments A and B (Figure 2).

Results and conclusions

Using the structural subsearch in ACD/ChromManager, we found 7 well-described chromatograms of compounds whose chromatography should relate to the Quest Structure. These chromatograms provide excellent starting points for method development. Furthermore, if a scientist judges a separation to have suitable characteristics (column, buffer, etc.), he or she can use ACD/LC or GC Simulators to predict the chromatographic behavior and to optimize the operating conditions.

As a result, a separation specialist will have a priori a reasonable column and a method to try—all within minutes!

ACD/ChromManager databases provide easy-to-use interfaces and exceptional search capabilities. They are a logical basis for data storage, retrieval, unification, and exchange, and can be enriched through integration with other ACD packages.

References

(1) A. Williams, E. Kolovanov, American Laboratory 32(6), 22-26 (2000)

Figure 1: Sample structure and substructure search in ACD Chromatography Application Database

Figure 2: Results of the search for Fragments A and B in ACD/Chromatography Application Database v. 5.0