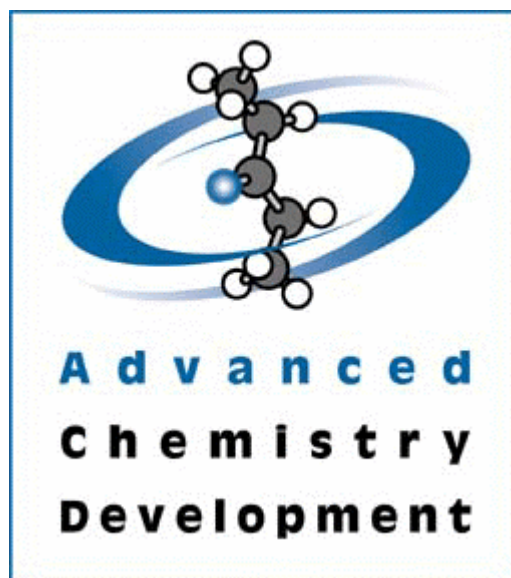


ACD/ChromManager

Version 5.0 for Windows

Technical Note

Structured Method Development with ACD/LC Simulator and ACD/ChromManager



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Structured Method Development with ACD/LC Simulator and ACD/ChromManager

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ACD/ChromManager and LC Simulator link to form a unique system for chromatographic method development. The software utilizes archived methods, structure-based predictions, and experimental optimization to streamline method development considerably.

The first step in the system is substructure search through applications databases in ChromManager. Both the ACD/Labs and user databases can be searched at the same time to retrieve the archived separations based on functionality. The retrieved data consists of the complete chromatographic parameters including column, pH, mobile phase component, gradient if present, etc., chromatogram, and structures with retention times.

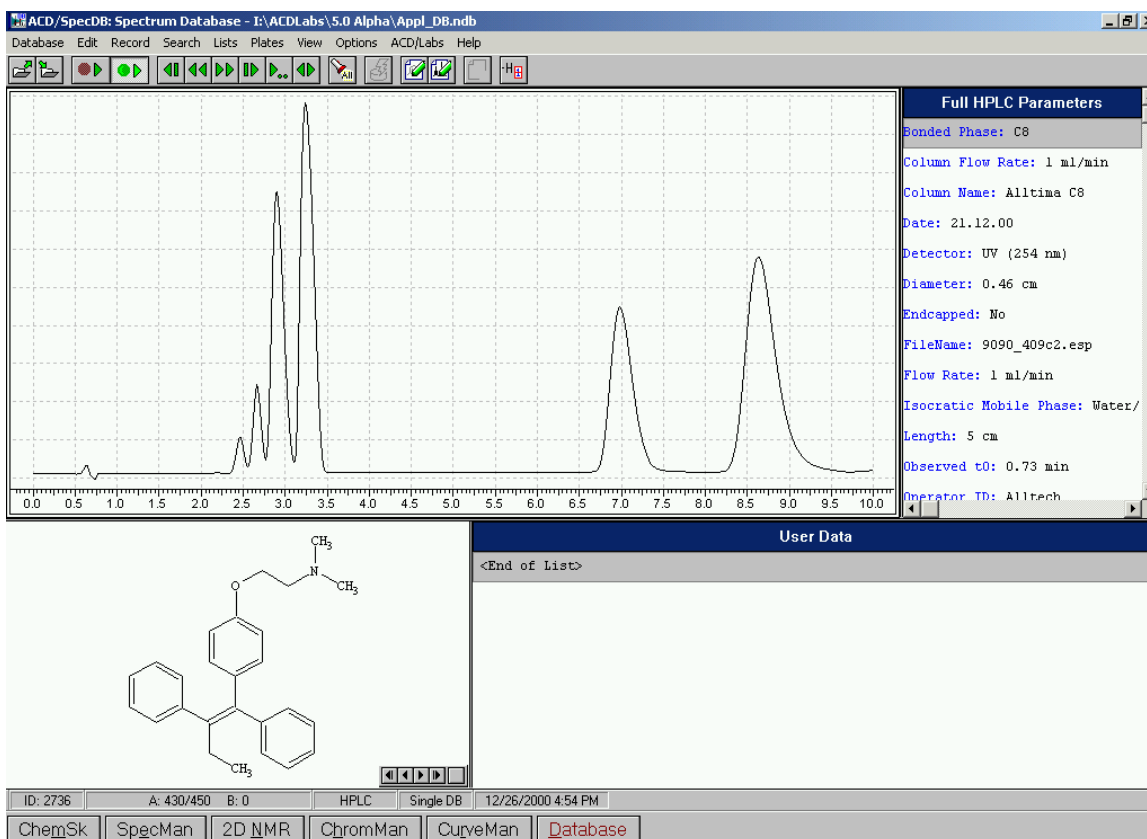


Figure 1. ACD/ChromManager links structures to chromatograms and methods in a fully searchable fashion. Substructure search yields methods for systems related to the one at hand.

The second step is to predict retention times for the compounds at hand under the conditions retrieved. This is done in LC Simulator. LC Simulator works by predicting the pKa, LogP, and LogD values for the compounds. It forms an expression for structure versus retention time for the system using the archived structures, and then predicts retention times for the new compounds. Once the retention times have been predicted, the user can reject the method and try another from the database, or modify mobile phase components (strength or pH) based on the predictions.

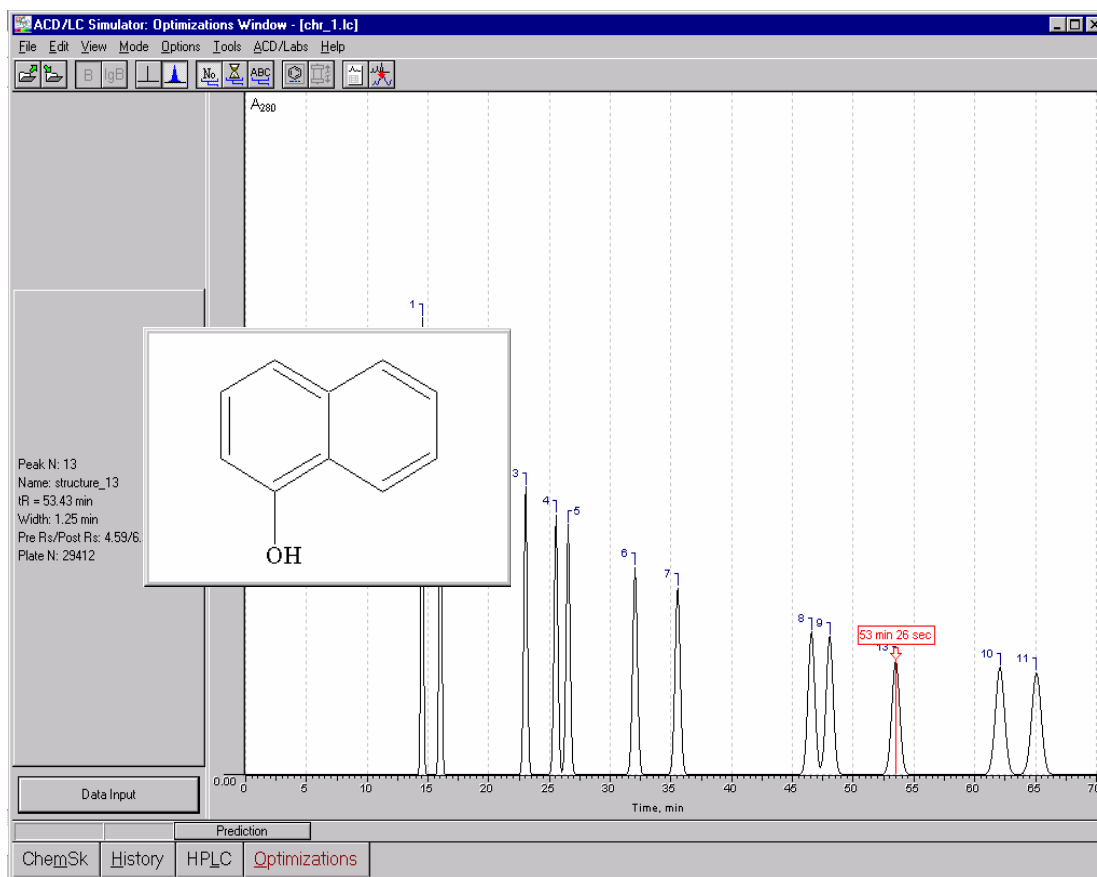


Figure 2. ACD/LC Simulator evaluates retrieved methods by predicting retention times for new compounds. Mobile phase modifications can be made prior to the first injection.

At this stage, we are ready to attempt the separation. If the separation is not successful, the chromatographic data can be directly transferred to LC Simulator for optimization based on experimental retention time changes; a kind of “directed trial and error”.

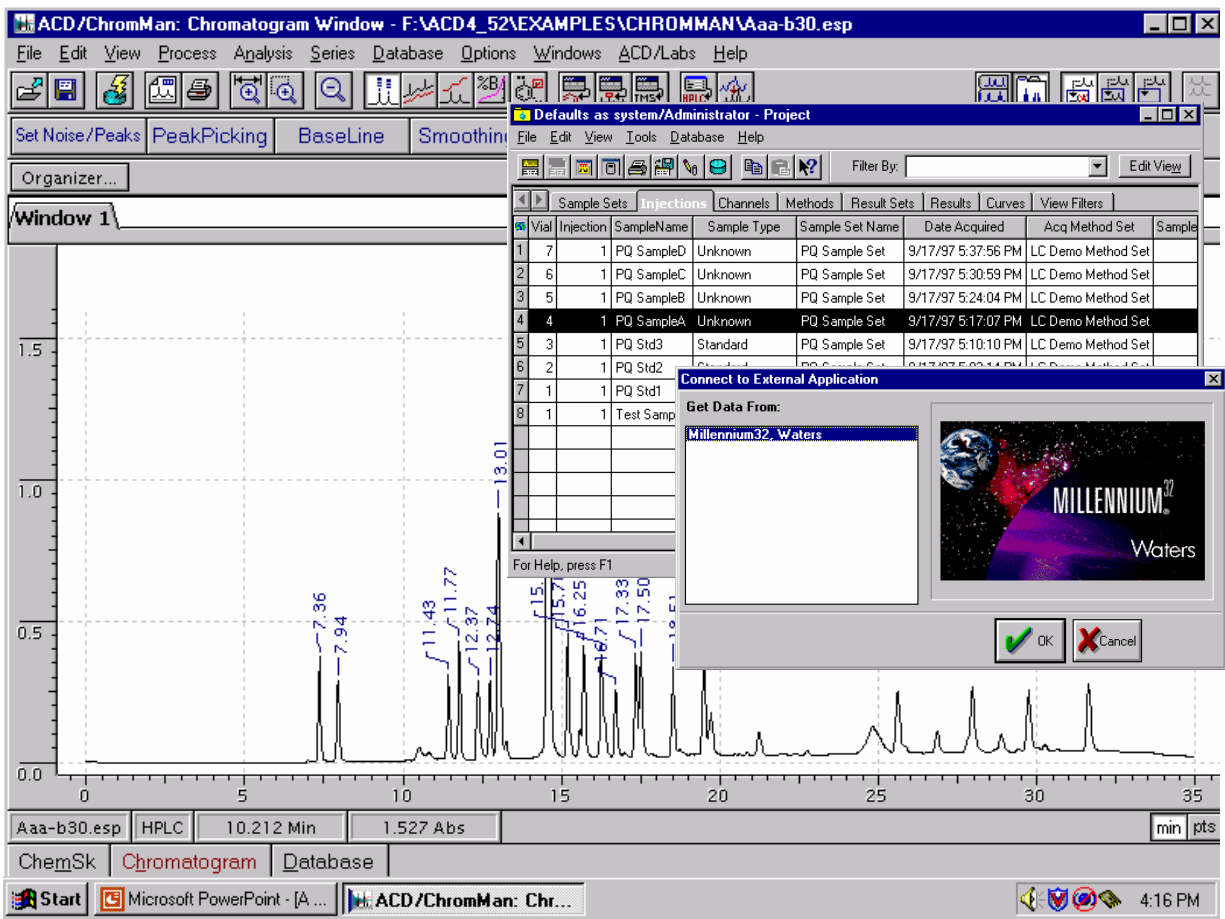


Figure 3. Both LC Simulator and ChromManager link directly to Waters Millennium32 in order to transfer experimental data. Most other chromatographic formats are also supported.

Once an adequate separation has been obtained, all that remains is to transfer the chromatogram to ACD/ChromManager, and archive the application so that it can be used as part of the knowledge base of the software. This database can be searched concurrently with the ACD/Chromatography Applications Database.

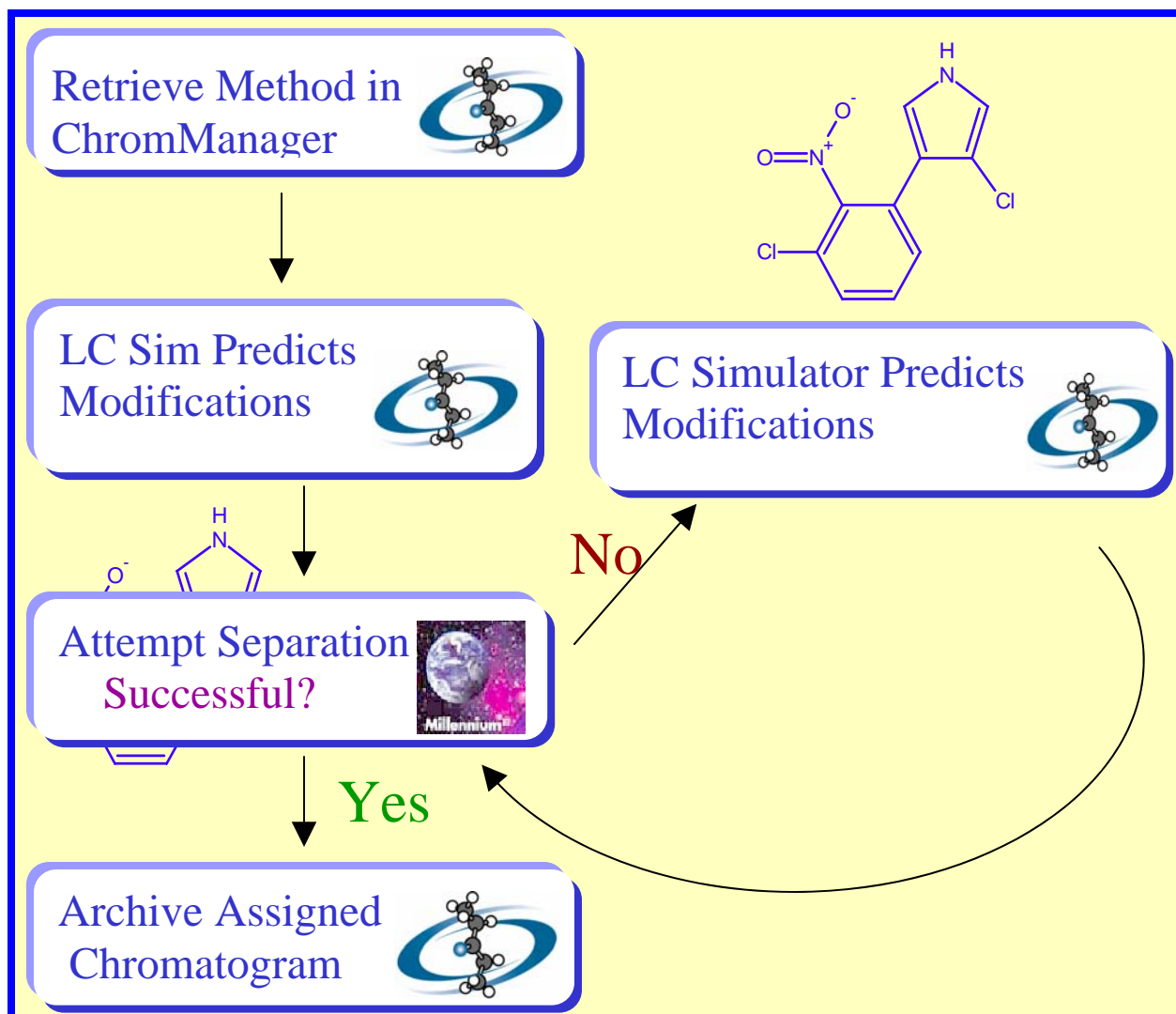


Figure 4. The ACD/Labs method development system integrates structures at each stage of the process, resulting in increased speed and efficiency.

ACD/Labs software provides a unique method development system. It complements data collection software by providing a convenient interface between predicted and experimental data. Perhaps the greatest advantage of this system is that it starts working to find an optimal solution *prior to the first injection*.