

# Industry Application



## Screening Method Simulation at NLS

The National Laboratory Service (NLS), a branch of the UK's Environment Agency, is a leading provider of high quality environmental testing and analysis. Melanie Schumacher, a Development Chemist at the NLS, had a project to develop a new chromatography method for screening environmental samples of unknown composition. One of her challenges was to develop a suitable method encompassing screening hundreds of compounds. In response to this challenge, Schumacher used ACD/ChromGenius software to predict retention times, simulate chromatograms, and speed the development of the new methods.

ACD/ChromGenius simulates the results of separation experiments using existing methods, and previously collected experimental data. Simulations are drawn from a database of experimental retention times and peak widths associated with chemical structures for each method. This information, together with built-in advanced physicochemical property prediction, is used to generate simulated separations. The result is a table of predicted retention times and a simulated chromatogram for each method, ranked in terms of suitability for the project at hand.

The accuracy of ACD/ChromGenius predictions depends upon the size of the reference database, and the similarity of compounds

within it to the compounds of interest. In her work, Schumacher was able to show that even with a limited database of 200 compounds, retention times accurate to +/- 1.5 minutes, well within the limits of what she would expect for a screening method, could be achieved.

ACD/ChromGenius becomes smarter over time by facilitating the integration of new experimental data into the prediction database as it becomes available. This additional data then becomes part of the data set, increasing the accuracy and reliability of future predictions.

*"What I particularly liked was the prediction plot of theoretical values against experimental which could be used to easily decide the best model to use. The ability to be able to search for structurally similar molecules was also helpful."*

Melanie Schumacher,  
Development Chemist,  
National Laboratory Service



To learn more about how ACD/ChromGenius can work in your organization, visit [www.acdlabs.com/chromgenius/](http://www.acdlabs.com/chromgenius/) or email [info@acdlabs.com](mailto:info@acdlabs.com)

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