Evaluation of ACD/Autochrom Software for LC Method Development

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Background

Goal: Minimize time needed to optimize methods
- Ensure selectivity, robustness, minimum measurement time attained by optimizing more than one method per project
- Compare Advanced Chemistry Development’s Autochrom software to offline optimization software
- LC Simulator (method optimization) alone with manual importing of data
- Autochrom includes instrument control, automated peak identification, and method optimization
- Evaluated using agricultural chemicals
- Agilent 1290 Instrument
- Development system to allow choosing 6 different columns, 10 different A or B mobile phases
- Binary pump/DAD/6130 single quad MS

Experimental Design

Screening Data

- Data collected with three columns and three solvents
- Example data comparing three columns using acetonitrile

Optimization

- Mass Spec Data used for Automatic Peak Identification
- Automatic peak identification was accurate for all components
- Most operator time was spent confirming peak identifications
- Important to examine peak identifications for compounds that are not well characterized
- Resolution upon optimization: It is possible that a column that gave lower resolution during screening will give superior resolution during optimization.

Screening output: Chose conditions to optimize

- Manual adjustment of Gradient
- Comparison of predicted and actual chromatograms

Optimization Data

- Advantages of Autochrom versus manual methods
- Documentation of all phases of development
- Facile navigation of data sets
- Enables use of multiple samples and signals to perform optimization
- If multiple samples and signals are to be used, manually identifying each component
- For each condition, time required
- Software optimization of method contains a tremendous advantage

Conclusions

- Use of Autochrom saves time and costs
- Documentation of all phases of development
- Facile navigation of data sets
- Enables use of multiple samples and signals to perform optimization
- If multiple samples and signals are to be used, manually identifying each component
- For each condition, time required
- Software optimization of method contains a tremendous advantage

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