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Chemometric Analysis of LC/MS Electrospray Data

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Introduction

The data analyzed in this study resulted from LC/MS, with electrospray as an interface. The first example is the analysis of a sample of a proprietary surfactant mixture containing at least 15 components. The resulting chromatographic data are heavily dominated by the mobile phase.
The second example is the analysis of three batches of a proprietary material: a good batch, a bad batch and a problematic batch.
The goals of the analyses are:
a) Improve the quality of the chromatographic data by a variable selection algorithm.
b) Extract the mass chromatograms that are different for the three batches.

Results and Discussion

Example 1: Proprietary Surfactant Mixture

The CODA_DW (Component Detection Algorithm approach based on the Durbin Watson criterion) selects high quality chromatograms from the data. In Figure 1a we see the total ion chromatogram (TIC) of the surfactant mixture. The solvent signals dominate the TIC. The CODA_DW selection of high-quality chromatograms results in the reduced TIC in Figure 1b. An overlay plot of all the selected mass chromatograms is shown in Figure 1c. Another step reduced the selected chromatograms in Figure 1c to a single mass chromatogram per component, (see Figure 1d).

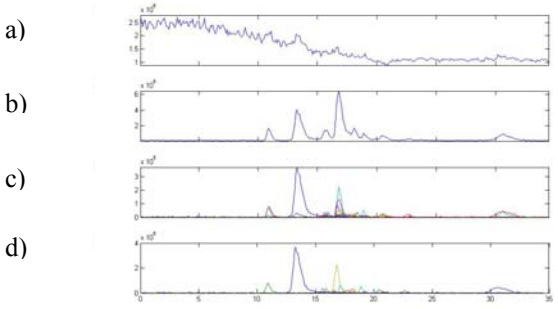

Figure 1. (a) shows the TIC of the original data; (b) is the reduced TIC of the CODA_DW selection of chromatograms; (c) is an overlay plot of the CODA_DW selection and (d) is a further reduction of the CODA_DW selection to a single mass chromatogram per component.

A manual selection of high quality mass chromatograms takes up to 4 hours. The CODA_DW approach achieves the same result in seconds. Due to the fast analysis, LC/MS can be used to monitor processes more efficiently.

Example 2: Different Batches of a Proprietary Material

Data from the three different batches of the proprietary material result in the CODA_DW reduced chromatograms in Figure 2. The differences between the batches cannot be observed easily.

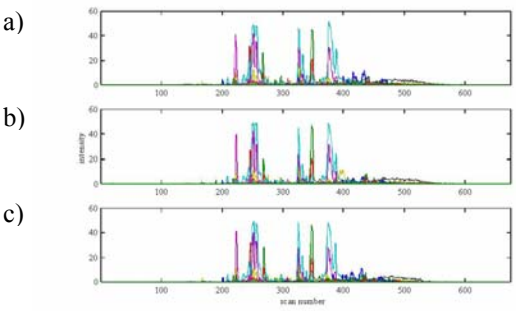

Figure 2. CODA_DW chromatogram selection of three batches of same material. Batch (a) is good, batch (b) is bad, batch (c) is problematic.

The program COMPARELCMS_SIM deletes the mass chromatograms that are similar, resulting in a limited series of mass chromatograms that show the differences between the samples of the batches (Figure 3).

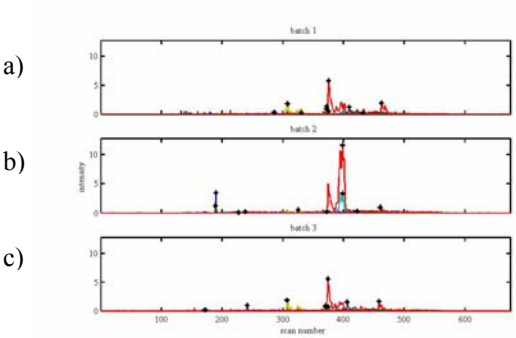

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Figure 3. The selection of COMPARELCMS_SIM, which only shows chromatograms that are different.

Please note the differences in intensity scales between Figure 2 and Figure 3. It is interesting to note that the bad batch (Figure 3b) clearly shows larger differences that the other two samples.
This example shows that the techniques discussed here are powerful quality control tools. The manual analysis of three sample like these takes days. With CODA_DW and COMPARELCMS_SIM the task is done in a matter of seconds and greatly improves productivity.

Conclusion

The tools developed for the analysis for hyphenated MS data result in a very significant reduction in analysis time. These programs can also be applied to other types of hyphenated MS data and are powerful tools for process monitoring and quality control.

Literature

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