GCmate, LCmate, *RSVP*

Chromatographic Enhancement Software

Component Detection for GC/MS and LC/MS

Introduction

A high chemical background or the continuous introduction of a reference compound can make it difficult to locate and identify trace components in a total ion current chromatogram in a GC/MS or LC/MS experiment. The *Shrader System for Windows*^{TM} software[1] available with the **JEOL** *GCmate, LCmate,* and *RSVP* mass spectrometers provides a solution to this problem based on the *Component Detection Algorithm* (***CODA***), developed by Windig *et. al.*[2] The *CODA* algorithm identifies significant peaks by comparing a smoothed, mean-subtracted reconstructed ion chromatogram (RIC) with the original RIC.

Figure 1 shows the data processing screen when CODA is applied to a GC/MS chromatogram where a high chemical background is present. Note the improvement in signal-to-noise for the CODA-enhanced chromatogram. This enhancement can be dramatic and can often reveal "hidden" features in a chromatogram (see *Figure 4*).

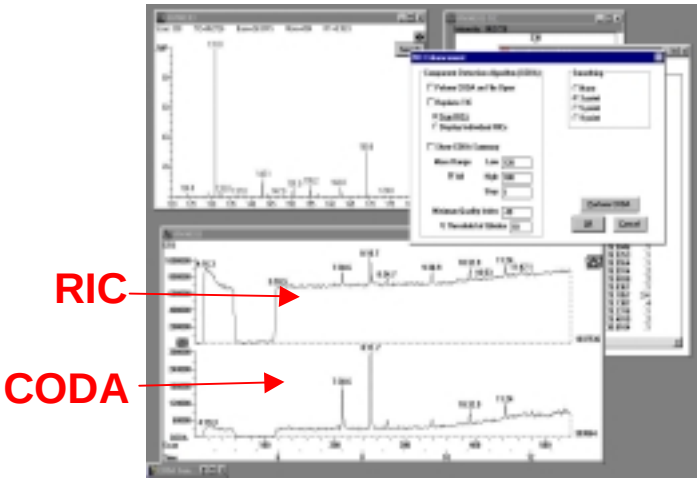

*Figure 1. CODA is used to enhance the signal-to-noise for a GC/MS reconstructed ion chromatogram (JEOL **GCmate**).*

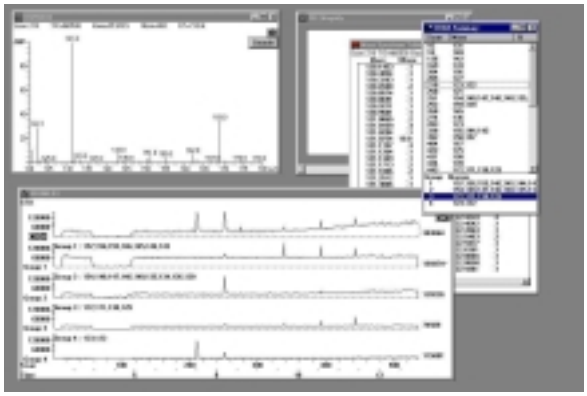

Figure 2. CODA is used to find series of related compounds in the mixture shown in Figure 1.

CODA can identify groups of mass-to-charge ratios whose mass chromatograms have similar elution times. This can be helpful in identifying related compounds. Figure 2 shows how the CODA-reconstructed chromatogram in Figure 1 can be decomposed into components.

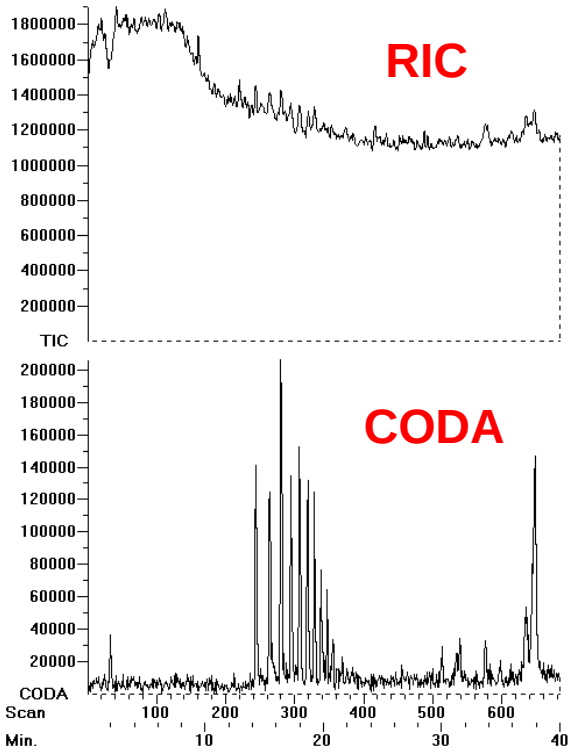

*Figure 3. Component detection for tea analyzed by electrospray ionization LC/MS (JEOL **LCmate**).*

Figure 4 shows the result of applying CODA to a GC/MS exact-mass measurement where the reference compound (PFK) is continuously introduced, producing a high chemical background that makes it difficult to find the analyte peak.

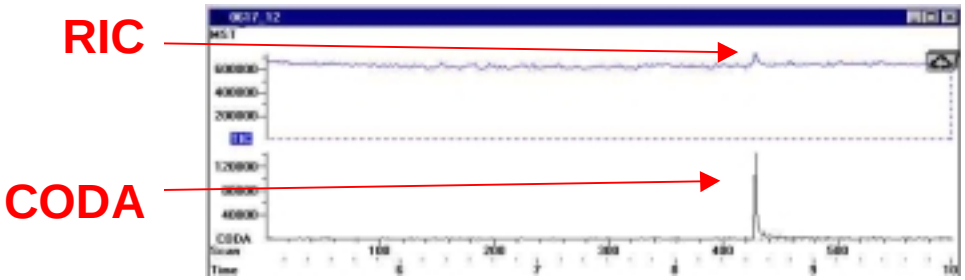

*Figure 4. CODA is used to eliminate background from continuous introduction of a reference compound (PFK) during an exact mass measurement with the JEOL **GCmate**.*

References

[1] Shrader Analytical & Consulting Laboratories Inc., 3814 Vinewood, Detroit, MI 48208
[2]W. Windig, J.M. Phalp and A.W. Payne, **Analytical Chemistry**, *68*(20), p. 3602.

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