

# Mass Media

**JEOL**

Mass Spectrometry News

December 1999

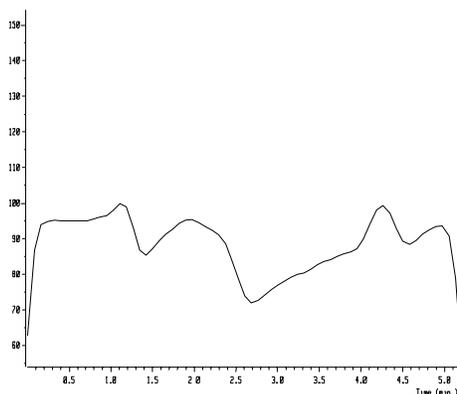
## *LCmate up and running at Eastern Analytical Symposium*

The JEOL LCmate was on display at the Eastern Analytical Symposium held on Nov. 15-18 at the Garden State Convention and Exhibit Center in Somerset, NJ. The benchtop high-resolution mass spectrometer system was fully operational and able to demonstrate more than 5000 resolving power. Onlookers were invited to operate the LCmate themselves. By using electrospray ionization with an autosampler and flow injections, visitors were invited to pick one of several vials and use the Open Access software to find out which of several common drugs the vial contained.

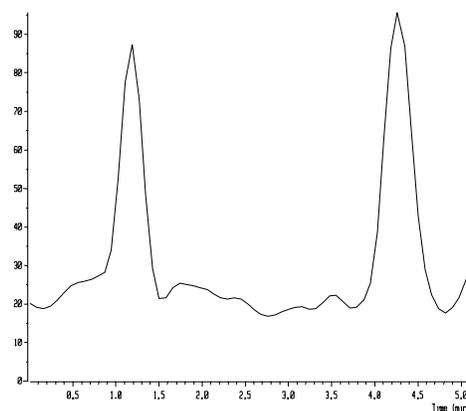
## *Chromatographic Enhancement Software*

The *Shrader System for Windows*<sup>TM</sup> software<sup>1</sup> provided with the data systems for the JEOL LCmate, *GCmate*, and *RSVP* mass spectrometers offers a component detection algorithm (CODA)<sup>2</sup> for identifying compounds that may be difficult to detect in the presence of a high chemical background during GC/MS or LC/MS analysis. This capability is discussed in application note MS-111999A, available in PDF format on our website at <http://www.jeol.com>.

A function of the XMS data system for the MStation, and AX505, SX102, and HX110 mass spectrometers can also be used to find components in the presence of a high chemical background. This function is active whenever mass chromatograms are created for the "fractional m/z" data type using the "Exact" option.



*ESI Flow injections with high chemical background*



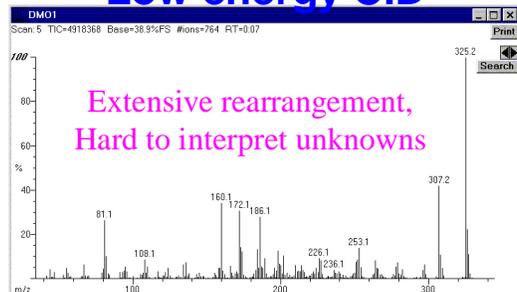
*XMS: Reconstructed ion chromatogram using "Exact" option*

## *Not all MS/MS is alike!*

With the exception of the JEOL *LCmate* and *GCmate* systems, all benchtop MS/MS systems offer low-energy collision-induced dissociation (CID). Low-energy CID (occurring at translational energies in the range of tens to hundreds of electron volts) is believed to work by vibrational excitation, and activated precursor ions have a narrow internal energy distribution. This means that the resulting product-ion mass spectra are strongly dependent on experimental conditions such as collision gas pressure and composition, collision energy, and temperature. Low-energy collisions can also favor rearrangement reactions, which can sometimes be hard to interpret.

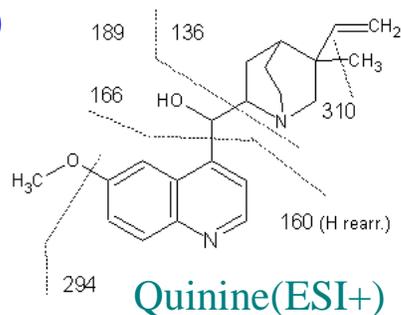
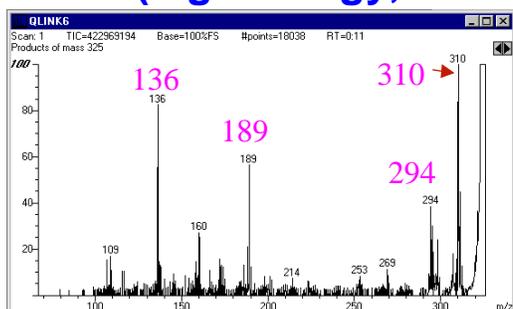
In contrast, high-energy CID (occurring at kilovolt translational energies) is believed to operate by electronic excitation. The mass spectra show a broader range of fragmentation reactions and are relatively insensitive to collision conditions. These advantages can be very valuable if one has to interpret the MS/MS spectra of unknown compounds. All JEOL mass spectrometers offer high-energy CID with the easily installed linked-scan MS/MS option. The benefits of high-energy CID are clearly illustrated by comparing the low-energy CID and high-energy CID production mass spectra for the  $[M+H]^+$  species from electrospray ionization of quinine.

### Low energy CID



**High-energy CID  
mass spectrum is  
more reproducible,  
shows less  
rearrangement, and  
is easier to interpret**

### MS/MS (high energy, 2.5 kV)



### References

<sup>1</sup> Shrader Analytical & Consulting Laboratories Inc., 3814 Vinewood, Detroit, MI 48208

<sup>2</sup> W. Windig, J.M. Phalp and A.W. Payne, *Analytical Chemistry*, 68(20), p. 3602.