



When performing liquid chromatography–mass spectrometry (LC–MS) analyses to identify new or unknown compounds, such as for impurity and degradant analysis or for metabolism studies, the analyst is searching for trace compounds in an often noisy and complex dataset. A number of noise-reduction and peak-extraction algorithms are available, notably CODA (1), which can help the analyst focus in on the relevant peaks. However, the analyst must still interpret the mass spectrum associated with each peak in order to identify or confirm the molecular ion.

ACD/IntelliXtract is new LC–MS software for component extraction and molecular ion identification. The software combines sensitive peak-extraction algorithms with MS knowledge in order to quickly and easily identify the relevant information in the dataset.

### Experimental

Bupirone was incubated with rat liver S9 fractions in the presence of phase II cofactors. Capillary LC was performed with an Agilent 1100 Series system (Agilent Technologies, Palo Alto, California) consisting of a capillary pump, a vacuum degasser, and a micro well-plate sampler coupled to an Agilent 1100 Series LC/MSD Trap XCT. The column was a prototype ZORBAX SB-Aq 0.3 3 150 mm, 3.5 mm. Solvent A consisted of water containing 0.1% formic acid and solvent B consisted of acetonitrile containing 0.1% formic acid. The gradient started with 0% B, reached 15% B after 65 min, 90% B after 70 min, and ended at 80 min with a post run time of 10 min. The mass spectrometer was operated in positive ESI mode. Full experimental details are reported by Fandino and colleagues (2).

Data processing and reporting were performed using ACD/IntelliXtract software, release version 9.0, and ACD/MS Manager, release version 9.0.

### Summary of the Data Reduction

Number of individual mass chromatogram peaks in the dataset: 1285

Number of  $^{12}\text{C}$  identified ions in the dataset: 122

Number of molecular ions in the dataset: 61

Number of components which pass  $^{12}\text{C}/^{13}\text{C}$  ratio test: 43

Number of components identified as possible metabolites: 19

In 5 min, the software was able to find trace components, even if they were overlapping with other components.

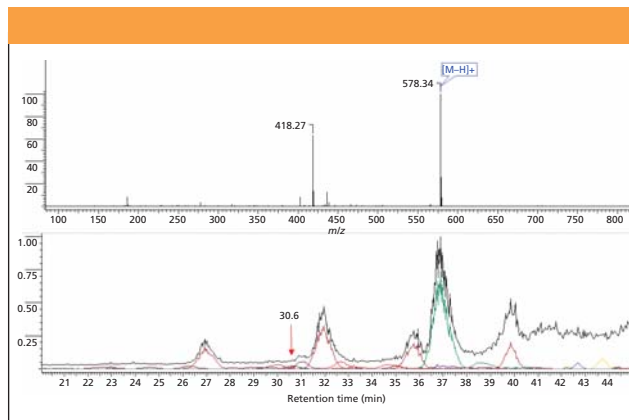
### Conclusions

ACD/IntelliXtract is able to quickly and easily extract the most relevant information from LC–MS datasets. The software confirms that trace components are real by checking

## Advanced Data-Reduction Strategies for LC–MS

Margaret Antler, Vitaly Lashin, and Mark Bayliss

Advanced Chemistry Development, Inc.



**Figure 1:** The lower window shows the extracted components. The upper window shows the mass spectrum for the trace component at 30.6 min, with the molecular ion automatically assigned in the spectrum.

that the  $^{12}\text{C}/^{13}\text{C}$  ratio is within the expected range. Components are extracted from the dataset in an unbiased fashion, so no prior knowledge of the sample is necessary.

### References

- (1) W. Windig, J.M. Phalp, A.W. Payne, *Anal. Chem.* **68**, 3602–3606 (1996).
- (2) A.S. Fandino, E. Nagele, P.D. Perkins, *J. Mass Spectrom.* **41**, 248–255 (2006).

### Advanced Chemistry Development, Inc. (ACD/Labs)

110 Yonge St. 14th floor  
Toronto ON M5C 1T4, Canada  
Tel. (416) 368-3435; (800) 304-3988,  
Fax. (416) 368-5596  
[www.acdlabs.com/IntelliXtract/](http://www.acdlabs.com/IntelliXtract/)