

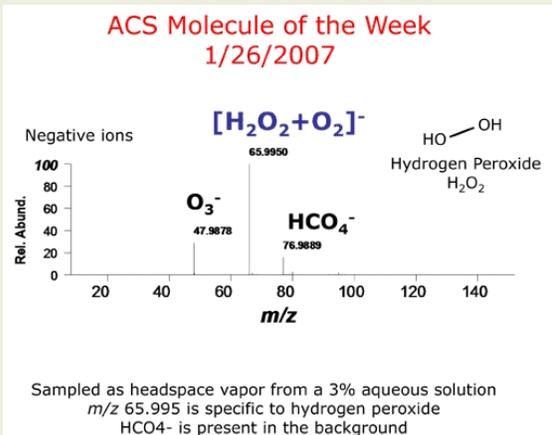
# Mass Media

# JEOL

Mass Spectrometry News and Applications  
JEOL USA, Inc. August-September 2008

## ACS Molecule of the Week

### Hydrogen Peroxide Analyzed with AccuTOF-DART



Hydrogen peroxide decomposes easily into water and oxygen:



This elusive molecule is not easily detected intact with traditional mass spectrometry techniques

DART™ (Direct Analysis in Real Time), when coupled with the AccuTOF Time-of-Flight Mass Spectrometer, detects hydrogen

## Streamline your synthetic workflow with DART and NMR

Visit JEOL at ICMRBS and SMASH

High Performance NMR

JEOL

Cyber-enabled

Expandable

Open Access

50 Years of NMR

Powerful, easy-to-use Delta™ Software

Run Mass Spec from NMR Samples™ - AccuTOF-DART™

NMR Mass Spec

Stability Performance Productivity

www.jeolusa.com

JEOL has the solution for streamlining the NMR workflow with the open air analysis directly from the NMR tubes. Using the [AccuTOF-DART™ mass spectrometer](#) at each step, you can check starting materials, monitor reaction progress, and validate your pure products or product formulations. JEOL offers a wide range of [NMR spectrometers](#) for liquids, solids, small molecules, and proteins. With 50 years of expertise in producing high-performance NMR systems, we have a winning mass spec-NMR spectrometer duo!

Visit us at the International Conference on Magnetic Resonance in Biological Systems (ICMRBS) in San Diego, or the Small Molecule NMR Conference (SMASH) in Santa Fe, New Mexico this summer. Or contact us directly at

peroxide as an oxygen adduct in negative-ion mode. Vapor from a 3% solution of hydrogen peroxide produces a good, strong  $[M+O_2]^-$  peak. The DART ion source operates in real time, so it detects the molecule before the  $H_2O_2$  has a chance to decompose.

Join us as we analyze selected samples in parallel with the American Chemical Society's "molecule of the week" using the DART ion source. Visit our website to see all the molecules of the week that we have analyzed so far, and check back when the new one is posted on the ACS website.

This week's molecule: [capsaicin](#)—the "hot stuff" in chili peppers.

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## Reaction Monitoring with Open Air Analysis of TLC Slides

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LETTERS

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Vol. 10, No. 16  
3493–3496

### HRMS Directly From TLC Slides. A Powerful Tool for Rapid Analysis of Organic Mixtures

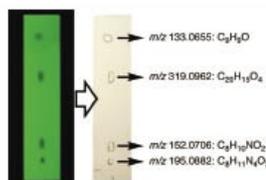
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#### ABSTRACT



High-resolution mass spectra (HRMS) of individual spots on thin-layer chromatography (TLC) slides can now be obtained quickly and easily at atmospheric pressure, with zero sample preparation, using commercially available instrumentation. The method is complementary to GC–mass spectrometry but is not limited to compounds of high volatility and high thermal stability. TLC–HRMS can be used to monitor chemical reactions in real time and has the capacity thereby to accelerate significantly the pace of synthetic organic chemistry.

Thin-layer chromatography (TLC) continues to enjoy widespread popularity as one of the fastest and simplest methods for monitoring the progress of reactions in synthetic organic chemistry.<sup>1</sup> Disappearance of the spot corresponding to starting material on consecutive TLC slides is generally accompanied by the appearance of one or more new spots corresponding to the product(s). Assigning chemical structures to the products that give rise to each new spot typically entails preparative TLC, HPLC, or column chromatography for isolation of the various components, which are then analyzed individually by NMR and/or other spectroscopic methods. By using the new open air

ionization sources recently developed for mass spectrometry,<sup>2</sup> however, it is now a simple matter to obtain high-resolution mass spectra (HRMS) of compounds directly from standard TLC slides, routinely, even while monitoring the course of a chemical reaction, without the need for preparative-scale chromatography or time-consuming sample preparation. Herein we illustrate the simplicity and power of this new tool by describing the TLC separation and direct HRMS analysis of the components in an artificial mixture of four familiar organic compounds: cinnamaldehyde, phenolphthalein, acetaminophen, and caffeine (see abstract graphic and Figure 1).<sup>3</sup>

The four spectra pictured in Figure 1 show base peaks for the individual compounds as their protonated molecular ions

(1) (a) Sherma, *J. Anal. Chem.* 2000, 72, 9R–25R. (b) Calimonte, D. S.; Strand, S. M.; Chang, S.; Lewis, D. E. *J. Chem. Educ.* 1999, 76, 82–83. (c) Jones, T. B.; Jones, T. H. *J. Chem. Educ.* 1985, 62, 813–814. (d) *Introduction to Organic Laboratory Techniques: A Microscale Approach*, 3rd ed.; Pavia, D. L., Lampman, G. M., Kriz, G. S., Engel, R. G., Eds.; Brooks/Cole-Thomson Learning: Pacific Grove, CA, 1999; pp 115–119.

10.1021/ol8012759 CCC: \$40.75 © 2008 American Chemical Society  
Published on Web 07/16/2008

(2) (a) McEwen, C.; Guttridge, S. *J. Am. Soc. Mass Spectrom.* 2007, 18, 1274–1278. (b) Takats, Z.; Wiseman, J. M.; Gologan, E.; Cooks, R. G. *Science* 2004, 306, 471–473. (c) Cotte-Rodriguez, I.; Takats, Z.; Talaty, N.; Chen, H.; Cooks, R. G. *Anal. Chem.* 2005, 77, 6755–6764.

## Upcoming Events

### Visit JEOL at

### ICMRBS

Int'l. Conf. on Magnetic Resonance  
in Biological Systems  
Aug 25-29, 2008  
San Diego, CA

### SMASH

Small Molecule NMR Conference  
Sept 7-10, 2008  
Santa Fe, NM

### EAS

Nov 17-19, 2008  
Somerset, NJ

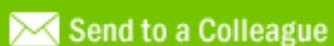
A new paper describes direct analysis of TLC slides to monitor the course of chemical reactions. The paper, written by Natalie J. Smith, Marek A. Domin, and Lawrence T. Scott in the Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, Massachusetts, was published in July 2008 in *Organic Letters*, 2008, Vol. 10, No. 16, 3493–3496.

Thin-layer chromatography (TLC) is one of the most widely accepted methods for monitoring reactions in synthetic organic chemistry. To analyze the resulting products that appear as spots on the TLC slide typically requires preparative TLC, HPLC, or column chromatography, followed

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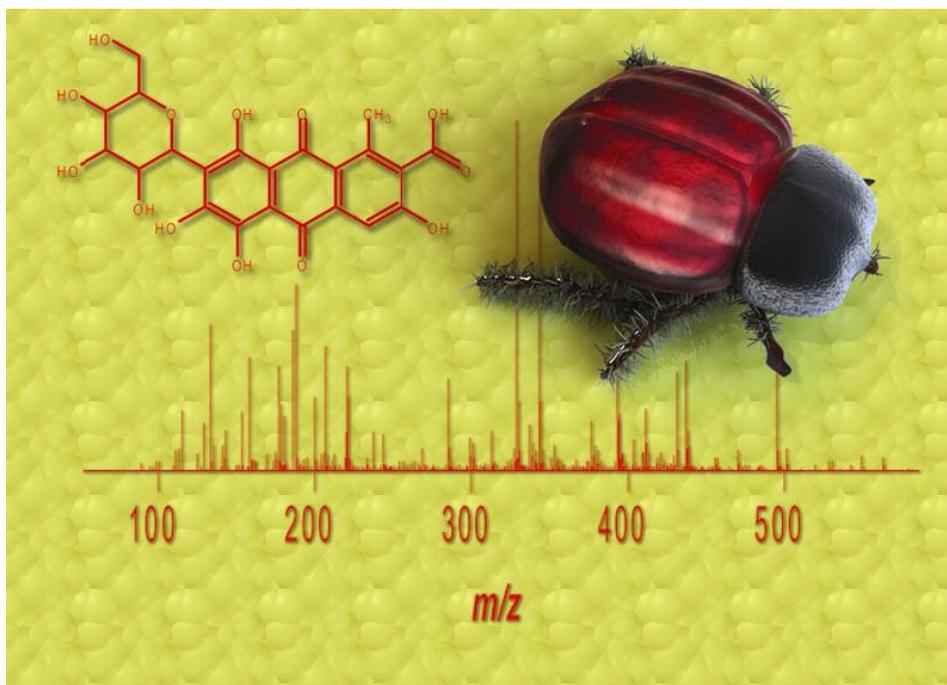
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**Service:**  
Bill Miller

by NMR spectroscopy and/or other spectroscopic methods. The DART ion source makes it easy to directly and routinely obtain high-resolution mass spectra (HRMS) of the compounds directly from standard TLC slides routinely without the need for sample preparation.

## Carminic Acid Molecule

*Beetle Juice Once Considered More Valuable than Gold*

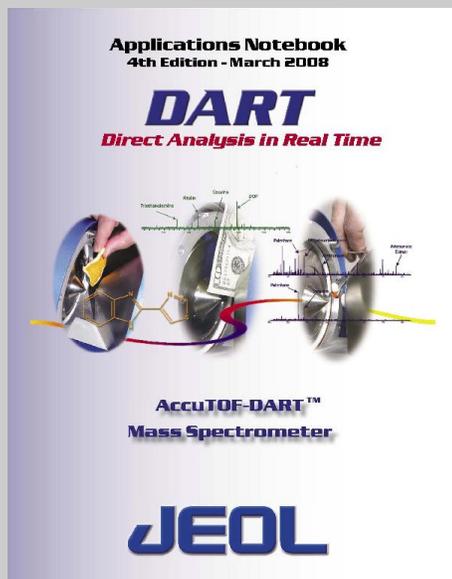


Keeping pace with the American Chemical Society's "Molecule of the Week" has demonstrated the AccuTOF-DART's ability to make quick work of analyzing substances in liquid, solid or gaseous form, without preparation. So it's no surprise when our applications chemists acquire some of the more exotic samples to analyze, like dried insects.

Reconstituted with a little water, the cochineal produced a burgundy wine-colored liquid that is known to have been used since ancient times to dye fabrics, food, and skin. This "beetle juice," or carminic acid, was once more valuable than gold in some cultures. Even now it shows up in some commercial fruit juices and yogurt as the ingredient carmine.

Using the AccuTOF mass spectrometer with the DART ion source, chemists identified the carminic acid molecule in mere seconds. It was just one of a series added to the AccuTOF-DART library of molecules analyzed in open air.

## Applications Notebook for AccuTOF-DART™ Open Air Mass Spectrometry



The 4th Edition of Applications Notes for the AccuTOF-DART is now available. To download, click on the image.

## GCMate II



JEOL's GCMate II, a compact, double-focusing, reverse geometry magnetic sector mass spectrometer is explained [here](#).

## Forensic Workshop on AccuTOF-DART

The [NFSTC](#) (National Forensic Science Technology Center, a program of the Justice Department's NIJ), hosted a two-day workshop on AccuTOF-DART at the [Ames Lab](#) in Ames, Iowa on August 12-13. Instructors were Roger Jones (Ames Lab), Robert Steiner (Virginia Department of Forensic services), Peter Stout (RTI) and Chip Cody (JEOL). Twelve people attended, mostly from various state forensic laboratories. The workshop consisted of lectures and labs, and the entire session was professionally videotaped.



## DART User Forum and Reception at ASMS 2008

Over 75 people attended the DART User Forum in Denver to hear the talks on applications of DART ranging from quantitation in PK studies to postmortem toxicology to detection of API's in drug tablets. We would especially like to thank the speakers who shared their latest research with us.

### EXCITING TIMES FOR AMBIENT IONIZATION

Robert "Chip" Cody, Ph.D., JEOL USA, Peabody, MA

### ENABLING BIOANALYSIS WITHOUT SAMPLE CLEANUP

## Fast GC-TOF



The AccuTOF-GC satisfies both demands for high speed responding to the fast GC method, and for obtaining accurate mass easily.

Read the comprehensive article in [JEOL News](#).

## AccuTOF-DART



See [videos](#) of the AccuTOF-DART as it analyzes samples in open air.

Shaoxia Yu, Ph.D., Millennium Pharmaceuticals, Inc, Cambridge

### DART-TOF VALIDATION AND APPLICATIONS IN CONTROLLED SUBSTANCE CASEWORK

Yongyi Julia Jiang, Ph.D., Harris County Medical Examiner's Office, Houston, TX

### EVALUATION OF DART-TOF FOR POSTMORTEM SCREENING

Peter Stout, Ph.D., Center for Forensic Sciences, RTI International (RTI), RTP, NC

### DART AT ULTRAHIGH MASS RESOLUTION (FTMS)

Laszlo Prokai, Ph.D., Dept. of Molecular Biology & Immunology, University of North Texas Health Science Center, Fort Worth, TX

### DART IN PROCESS RESEARCH; ENABLING HIGH-THROUGHPUT DECISIONS

Roy Helmy, Ph.D., Merck Co, Inc, Linden, NJ

### COMING SOON FOR A DART NEAR YOU!

Brian Musselman, Ph.D., IonSense, Inc, Saugus, MA

Contact [jeolink@jeol.com](mailto:jeolink@jeol.com) for a copy of the handout.

## DART Training Class Inspires Students

Nine very enthusiastic students attended the AccuTOF-DART training class in July, held at JEOL in Peabody, Massachusetts.



This inspired group included forensics investigators, a neuropsychology scientist, and an explosives analyst. The class was taught by Drs. John Dane and Chip Cody. Our applications team never tires of helping people learn the DART technology. The next course will be held in the fall.



## MStation



The [MStation™](#) is a fully-automated, high-performance, double-focusing magnetic sector mass spectrometer designed for both high-resolution GC/MS and LC/MS analyses. The MStation is capable of achieving a resolving power of 60,000 or greater at 10% valley.



## Tutorials & Application Notes

Bookmark [www.jeolusa.com](http://www.jeolusa.com) for complete access to useful mass spec [Tutorials](#) , [NMR Tutorials](#), and [application notes](#).

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