

Mass Media

JEOL

Mass Spectrometry News and Applications
JEOL USA, Inc. May - June 2008

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JEOL and DART Papers and Posters at ASMS 2008
Printable Schedule
Link to Abstracts

DART User Forum - You're Invited!

New Mass Spec Applications Specialist Joins JEOL

ACS Molecule of the Week Analysis with AccuTOF-DART

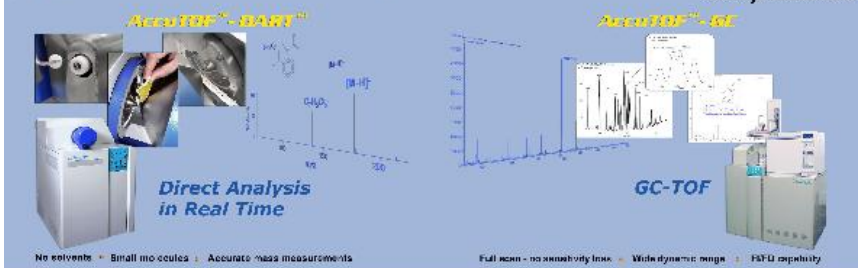
Challenges in the Analysis of Soft Drinks Using GC-MS-TOF and DART-MS-TOF (as printed in LCGC Europe May 2008)

4th Edition of Application Notes Available

Visitor's Field Guide to ASMS - Identifying Elemental Composition with JEOL!

High Resolution Mass Spectrometers

JEOL
www.jeolusa.com



Looking for answers and an easier way to get them? Visit with us in the [JEOL booth \(#125\)](#) and we'll answer your questions about JEOL mass spectrometry solutions, including the flexibility of open air ionization with [AccuTOF-DART](#) and rapid sampling with the [AccuTOF-GC/MS](#).

This year we are pleased to note that there are thirteen posters and two presentations on the popular DART technique for atmospheric ionization. There are also several other-JEOL-related posters. Here is a guide to help you find them:

Monday

Session: Direct Ionization I - Poster Hall

Poster 024

Comparison of Mass Spectrometric Methods for the Detection of Phosphodiesterase-5 Inhibitor Prescription Drugs in Dietary Supplements

Martha L. Gay; John A.G. Roach; Gregory O. Noonan - FDA, College Park, MD

Poster 026

Identification of fluorochemical paper coatings and characterization of packaging by LC-MS/MS and DART-MS

Gregory O. Noonan; Timothy H. Begley; Luke K. Ackerman; Gregory W.

Upcoming Events

Visit JEOL at

ASMS

June 1-5, 2008
Denver, CO
Booth #125

Fall ACS

August 18-20, 2008
Philadelphia, PA
Booth 1126/1128

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Diachenko; John A.G. Roach - US Food & Drug Administration, College Park, MD

Poster 029

Field Optimization of Data Collection using DART/DESI Mass Spectrometry

Ronny C Robbins ; William M. Lagna - US Army, Gunpowder, MD

Poster 039

Optimizing DART-MS Sampling for Quadrupole MS/MS Analysis of Food Contaminants

Luke K. Ackerman; Gregory O. Noonan; Timothy H. Begley - FDA Center for Food Safety &, College Park, MD

Poster 041

DART-TOF Validation and Applications in Forensic Science

Yongyi Jiang; Stephen Houck; Mark Dixon; Ashraf Mozayani - Harris County MEO, Houston, TX

Poster 042

Rapid, Automated Determination of Elemental Compositions of Ions in Mass Spectra Obtained with an Open-Air Ion Source

Andrew H. Grange ; G. Wayne Sovocool - U.S EPA, Environmental Chemistry Branch, Las Vegas, NV

Session: APPI - Poster Hall

Poster 072

Ionization mechanism of NI-DART (negative ion-direct analysis in real time): a comparative study with NI-APPI (negative ion-atmospheric pressure photoionization)

Liguo Song; ANDREW DYKSTRA; Huifang Yao; John Bartmess - University of Tennessee, Knoxville, TN

Tuesday

Session: Direct Ionization II - Poster Hall

Poster 021

A Comparative Study of DESI and DART on a Mobile Lab Atmospheric Pressure Ionization Ion Trap MS

Michael Roth, Mitch Wells - Griffin Analytical Technologies, W. Lafayette, IN

Poster 023

Heat Transfer and Fluid Dynamic Simulations of a DART-type Ambient Mass Spectrometry Ion Source

Facundo Fernandez ; Glenn A Harris - Georgia Institute of Technology, Atlanta, GA

Poster 026

Enabling More Efficient Ion Collection in Surface Ionization Experiments

Elizabeth A. Crawford; Brian D. Musselman; Joseph Tice - IonSense, Inc., Saugus, MA

Poster 030

Utility of Reactions in the Source of a Helium Metastable-Beam Open-Air-Ion-Source Mass Spectrometer

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GC-TOF-MS and DART-TOF-MS: Challenges in the Analysis of Soft Drinks

Tomas Cajka, Lukas Vaclavik, Katerina Riddellova and Jana Hajslova,
Institute of Chemical Technology, Faculty of Food and Biochemical Technology,
Department of Food Chemistry and Analysis, Prague, Czech Republic

The potential of the time-of-flight mass spectrometry (TOF-MS) to innovate the analysis of soft drinks is described using gas chromatography (GC) hyphenated to TOF-MS and a new type of ion source, direct analysis in real time (DART), coupled to high-resolution TOF-MS. High-speed solid-phase extraction (HS-SPE) was used to simultaneously isolate compounds related to GC-TOF-MS to identify natural components in contaminated soft drinks. Direct analysis in real time-time-of-flight mass spectrometry (DART-TOF-MS) was also used to obtain negative and positive ion profiles of different soft drinks to determine the presence of various compounds, including antimicrobial preservatives, artificial sweeteners, oxidants and saccharides, without any sample preparation and chromatographic separation.

Techniques involving mass spectrometry (MS) as a detection tool in food analysis have evolved substantially. Gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-mass spectrometry (LC-MS) are commonly used to detect, identify, quantify and confirm both natural and synthetic substances in the food production chain. One of the major challenges faced in MS-based analysis is the set of two or eight

mass spectrometry (TOF-MS) for both target and non-target analysis of a wide range of organic compounds that occur in keto matrices. High-speed solid solution TOF-MS instruments can be combined with fast one-dimensional GC and/or conventional two-dimensional GC (GC²) set-up with "fast" separation in the second dimension to identify and quantify wide range of

LC600 Sample May 2000

GC-TOF-MS and DART-TOF-MS: Challenges in the Analysis of Soft Drinks

Tomas Cajka, Lukas Vaclavik,
Katerina Riddellova and Jana Hajslova,
Institute of Chemical Technology,
Faculty of Food and Biochemical
Technology,
Department of Food Chemistry and
Analysis, Prague, Czech Republic.

Matthew Curtis; Patrick R. Jones; O. David Sparkman - University of the Pacific, Stockton, CA

Session: *Metabolomics II - Poster Hall*

Poster 371

Defining Instrument Performance and Assessing the Reproducibility of Mass Spectromic Analyses of Complex Samples

Paolo Lecchi, Jean Zhao, Wes Wiggins, Greg Bertenshaw, Tzong-Hao Chen, Brian Mansfield, John M. Peltier - Correlologic Systems, Inc., Rockville, MD

Wednesday

Session: *LC/MS I - Poster Hall*

Poster 285

Comparison of different ionization techniques (ESI, DART, APGD) for coupling of mass spectrometry with planar chromatography (HPTLC/MS)

Gertrud E. Morlock, University of Hohenheim, Stuttgart, GERMANY

Poster 288

Polymer-coated C18 stationary phase designed for high-sensitivity and high-throughput analyses in LC-MS

Osamu Shirota, Hiroko Arai, Miho Ebata - Shiseido, Yokohama, Japan

Poster 293

Qualitative Analysis of Tea by Ion Chromatography - Time-of-flight Mass Spectrometry with High Sensitivity and Resolution

Kazuko Tanaka, Kazutetsu Nojima, Toshinobu Hondo - JEOL Ltd., Akishima, Tokyo Japan

Session: *Quantitation of Small Molecules - Poster Hall*

Poster 345

Methods for Quantitative Measurements Using a Helium Metastable-Beam Open-Air-Ion-Source Mass Spectrometer

O.David Sparkman, Patrick R. Jones, Matthew Curtis, Teresa Vail
University of the Pacific, Stockton, CA

Thursday

Session: *Increasing Throughput for Pharmacokinetic Assays Through Mass Spectrometry - Four Seasons Ballroom 3-4*

8:50 am

Improving the Reproducibility and Practicability of DART for the Direct Quantification of Drugs in Biological Fluids

Shaoxia Yu¹; Elizabeth Crawford²; Joe Tice²; Brian Musselman²; Jing-Tao Wu¹ - 1Millennium Pharmaceuticals, Cambridge, MA; 2IonSense, Inc., Saugus, MA

Session: *Analyte "Fingerprinting" With No Sample Prep - Rooms 601-607*

8:50 am

Identifying Materials, Formulations, and Other Complex Substances by Direct Analysis and Exact Mass Measurements

Robert B. Cody - JEOL USA, Inc., Peabody, MA

Session: *LC/MS II - Poster Hall*

The potential of the time-of-flight mass spectrometry (TOF-MS) to innovate the analysis of soft drinks is described using gas chromatography (GC) hyphenated to TOF-MS and a new type of ion source, direct analysis in real time (DART), coupled to high-resolution TOF-MS. Head-space solid-phase microextraction (SPME) was used to isolate/extract volatile compounds followed by GC-TOF-MS to identify tainted compound in contaminated soft drinks. Direct analysis in real time-time-of-flight mass spectrometry (DART-TOF-MS) was also used to obtain negative and positive ion profiles of different soft drinks to determine the presence of various compounds, including antimicrobial preservatives, artificial sweeteners, acidulants and saccharides, without any sample preparation and chromatographic separation.

Read the [full article](#) published in LCGC Europe May 2008.

New Website Feature: ACS Molecule of the Week Analysis

Join us as we analyze selected samples in parallel with the American Chemical Society's "molecule of the week". Using the DART ion source, we plan to produce timely, interesting mass spectra for our DART database. 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](#).

JEOL Publishes 4th Ed. Applications Notebook for AccuTOF-DART™ Open Air Mass Spectrometry

JEOL USA has published the fourth edition of its popular collection of applications notes for open air mass spectrometry. The AccuTOF-

Poster 276

A comparison of LC/MS mass analyzers for screening, confirmation and quantification of drugs in blood

JOHN M. HUGHES¹; Greg Kilby¹; Michael C. Zumwalt¹; Jeri D. Roper-Miller²; Peter R. Stout²; H. Chip Walls³

¹Agilent Technologies, Pleasanton, CA; ²RTI International, Research Triangle Park, NC; ³U. of Miami Medical School, Miami, FL

Session: GC/MS - Poster Hall

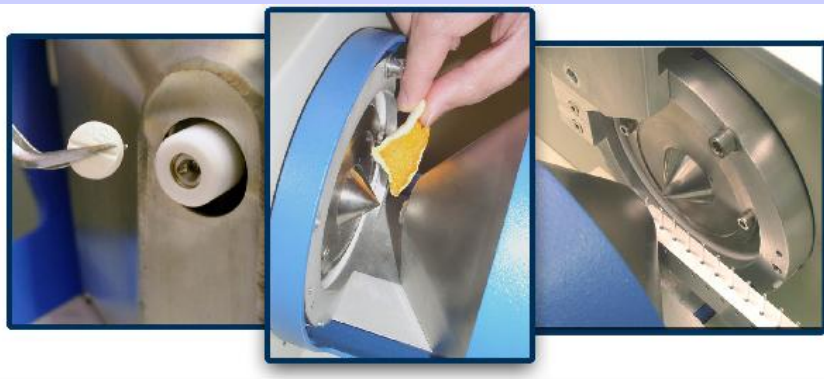
Poster 193

Development of a New EI/FI Ion Source for a GC/TOFMS

Susumu Fujimaki, Kanji Miyamoto, Kazuo Tanaka, Yoshihisa Ueda, Doug Meinhart - JEOL Ltd, Tokyo Japan and JEOL USA, Peabody, MA

To read the abstracts, click [here](#).

To download a printable schedule of JEOL and DART posters and presentations at ASMS, click [here](#) for the pdf file.



You're Invited to a DART User Forum and Reception at ASMS

Please join us on Sunday afternoon, June 1st, for a Reception and brief Forum discussing the DART and its applications.

DATE: Sunday June 1, 2008
TIME: 1:00 to 3:00pm
LOCATION: Marriott Denver City Center

Light Refreshments will be served
Registration 12:30 - 1:00 PM

Short Presentations 1:00 - 2:30PM

EXCITING TIMES FOR AMBIENT IONIZATION

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

ENABLING BIOANALYSIS WITHOUT SAMPLE CLEANUP

DART Applications Notebook 4th edition is updated to include several new applications notes covering topics as diverse as real-time analysis of deoxynivalenol in beer to GC/MS using the DARTTM ion source. The new book includes 58 pages of real-time analysis of pharmaceuticals, drugs in dose form or in bodily fluids, synthetic organic or organometallics compounds, inks on paper, explosives and arson accelerants, chemical weapons agents, foods, oils, rubber, adhesives, and more. All analysis was performed in ambient conditions directly from surfaces and liquids, including TLC plates, paper, melting point tubes, and unaltered samples such as pieces of rubber, basil leaves, and currency.

The 4th edition of the AccuTOF-DART applications notebook and the individual applications notes can be downloaded from the JEOL USA [website](#). A printed, bound, full color edition can be requested by emailing salesinfo@jeol.com.

The AccuTOF-DART, now in production for 3 years, has revolutionized mass spectrometry with its ability to perform elemental composition in real time from unaltered samples. Its range of applications is continually growing and the AccuTOF-DART is now in use in many university and industrial settings. A complete bibliography of published papers on the AccuTOF-DART is also listed in the applications notebook.

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

Reception 2:30 - 3:00 PM

We hope that you will be able to join us at the Forum. Please RSVP to bidgood@ionsense.com

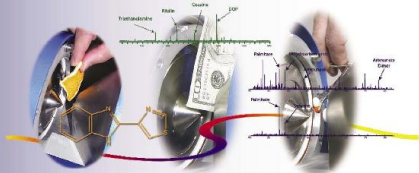
New Applications Specialist Joins JEOL from Colorado School of Mines



Applications Notebook
4th Edition - March 2008

DART

Direct Analysis in Real Time



AccuTOF-DART™
Mass Spectrometer

JEOL

New Applications Notebook

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

Fast GC-TOF



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

JEOL welcomes a new applications specialist to its mass spectrometry group. Dr. John Dane is now located in our Peabody office and will help provide support for all JEOL mass spectrometers, including the AccuTOF-DART and AccuTOF-GC.

While he is new to the TOF and DART products, John already has extensive experience with the JEOL MStation, a double-focusing magnetic sector mass spectrometer designed for both high-resolution GC/MS and LC/MS analyses. Additionally, during his research at Colorado School of Mines (CSM), he worked with Dr. Robert (Chip) Cody, JEOL Mass Spectrometry Product Manager, on the application of the tunable energy electron monochromator (TEEM) that was coupled to the MStation. The TEEM was a previous technology that provided some initial ideas that led to the development of the DART ion source.

John and his colleagues, under the direction of Professor Kent Voorhees, utilized the TEEM MStation to identify the presence of Nitro-Polycyclic Aromatic Hydrocarbons (NPAHs) in tobacco smoke. The project was funded by a tobacco company in their research to develop a safer product. "NPAHs are generally harmful to humans if they are present at any levels," John explains. "The exciting feature of the TEEM source was the ability to analyze complex mixtures containing electronegative compounds that are susceptible to electron capture." The MStation, used in conjunction with this technology, provided a very selective and sensitive device for detecting nitro compounds found in tobacco smoke (which contains over 4800 previously identified compounds), particularly when it was tuned to selectively generate specific ions (i.e. NO_2^- groups and molecular ions).

Despite the selectivity and specificity of the analytical technique, the smoke samples, which were collected onto filters, had to be put through a rigorous multi-step process that included solvent extraction, two solid phase extractions, an acid wash, and LC fractionation - "We tried any number of combinations to eliminate one or two of these cleanup steps, but ultimately all of these steps were necessary to create samples clean enough to generate reproducible results," he says. Each step removed components of the smoke matrix that would contaminate the GC column, thus affecting the reproducibility of subsequent injections. The results of their research surprised them though, because while they found only trace levels of the NPAHs, the carcinogen they were expecting to find, they also identified significant levels of nitro pesticides

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

AccuTOF-DART



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

GCMate II



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

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.

that were applied to the budding tobacco plant in the field. Even more surprising was the fact that every cigarette type and brand tested showed some level of these nitro pesticides present in the tobacco smoke.

In another area of research involving John's expertise, CSM partnered with the National Renewable Energy Laboratory to investigate NPAH levels produced in diesel engine exhaust. Using the TEEM MStation, their research showed large quantities of NPAHs in conventional (petroleum) diesel fuels as compared to ultra-low sulfur/low-aromatic content diesel, Fischer-Tropsch synthetic diesel, and conventional diesel/synthetic diesel blend. The diesel exhaust samples were much simpler to handle than the smoke samples in that they only required a one-step cleanup prior to analysis by the TEEM-MS.

John authored two papers that were published in *Analytical Chemistry* in 2006. He is a native of Texas, where as an undergraduate he attended Angelo State University prior to his graduate work at Colorado School of Mines. He can be reached at jdane@jeol.com, or by calling 978-535-5900.

Tutorials & Application Notes

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

The tutorials have been updated and include useful reference tables for day-to-day DART operation.

We continually add to our application notes. Please check our website for the latest updates.