

Direct Analysis in Real Time: Changing the Course of Mass Spectrometry

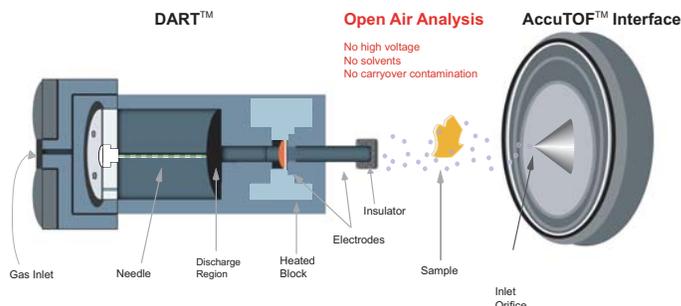
Since its development in 2003, the DART™ direct analysis ion source has been used in applications that, prior to this new technology, would have been virtually impossible.

The ability to analyze samples in open air, and preserve them in their native state while obtaining exact mass information has made mass analysis both simple and fast for chemists, scientists, and researchers in a wide range of fields.

DART can reveal chemical information that might otherwise only be done through extensive sample preparation, and by permanently destroying the sample materials. For example:

- ✓ DART can detect and identify the chemical components of fingerprints, often providing information about specific substances a subject has been handling while keeping the fingerprint intact on its original surface.
- ✓ Rapid screening of bodily fluids for impurities, amino acids, lipids, or metabolites is easily done without time-consuming sample preparation.
- ✓ New synthetic products can be rapidly analyzed to detect new compounds and chemical reactions.
- ✓ Drugs can be directly analyzed in tablet or capsule form by simply passing the tablet between the ion source and the mass spectrometer.
- ✓ DART can pinpoint pesticide residue and analyze compounds on foods directly from the surface of the food item or from a drop of liquid.

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DART Ion Source

Contact JEOL USA

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978-536-2310

For direct access to JEOL mass spectrometry and NMR spectrometry information, visit our website at www.jeolusa.com/ai.html

DART was awarded the U.S. Patent # 6,949,741 in 2005 after capturing the Editor's Gold Award at Pittcon in March 2005. DART was also the winner of the R&D 100 Award as one of the 100 most technologically significant new products of 2005.

How DART Works

DART is a dry, open-air, ion source that uses no exposed high voltages, solvents, or x-rays. Gas flow can be directed toward a liquid or solid sample, or it can interact with vapor-phase samples.

DART Analysis of 43 Writing Inks *in Situ*
 Published in *J. Forensic Science*

Analysis of writing inks to authenticate documents is described in the *Journal of Forensic Science*, July 2006, Vol. 51, No. 4, pages 915-918 in "Differentiating Writing Inks Using Direct Analysis in Real Time Mass Spectrometry." Authored by Drs. Roger Jones and John McClelland of the Institute for Physical Research and Technology, Iowa State University, and Dr. Robert Cody of JEOL USA, Inc., the paper describes methods for rapid, non-invasive, *in-situ* analysis of forty-three writing inks on paper without visible alteration of the documents.

Identification of inks provides information that is helpful in identifying whether a document is real or fraudulent. In contrast with traditional mass spectrometric methods of ink analysis that require removal of material from the document, DART™ analysis can be carried out on the intact document. In addition, the DART technique characterizes inks by detecting dyes as well as additives and carriers, providing more complete information about the ink composition than techniques that detect only dyes. The article shows that individual ink compositions produce "fingerprint" DART mass spectra that can be rapidly identified by searching against a user-generated library database.



Direct analysis of writing inks.

2006 Events

You can see JEOL at any of the upcoming events. Please check our website for more current listings.

Sept 11-13

ACS
 San Francisco, CA
 Booth 411/413

Oct 3-7

SOFT Meeting
 Austin, TX

Nov 13-15

EAS
 Somerset, NJ

Spectroscopy Audio Seminar on DART

Spectroscopy magazine offers audio seminars, a unique online learning opportunity for anyone working in the separations sciences. Recently, DART was the subject of an audio seminar presented by Dr. O. David Sparkman, Adjunct Professor of Chemistry at the University of the Pacific, author, and consultant who has been active in the field of analytical chemistry since the mid-1960s. In the seminar, he discussed the theory of DART, how desorption/ionization work, Penning ionization, negative ion formation, and calibrating the m/z scale. Sparkman answered questions posed to him online. The DART CD and other audio seminar CDs are available at www.spectroscopymag.com

DART Appeals to Crime TV Audiences

Forensic science is a fascinating topic and the subject of popular television programs. *CSI NY* offers the forensic enthusiast a realistic view of a crime lab (shown in photo), right down to the mass spectrometer. *CSI NY* borrowed an AccuTOF-DART for their 2005-2006 season, and plans to show it in use again in upcoming episodes.



Peak Performance: Convert LC to Nano-LC

Nano-LC/MS has demonstrated many advantages, including lower sample consumption, higher mass sensitivity and less matrix effect. Here, we introduce a very simple method to convert an AccuTOF™LC system into a nano-LC/MS system very inexpensively.

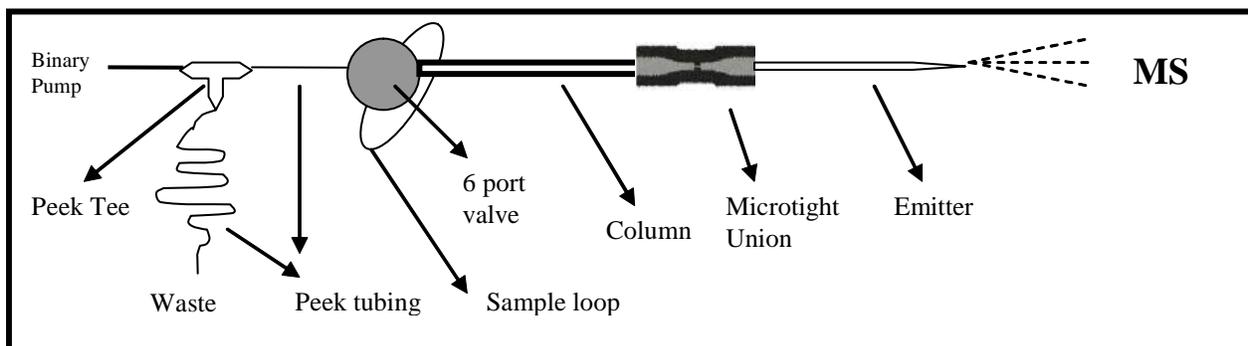
What you need

- ◆ AccuTOF time-of-flight mass spectrometer (JEOL)
- ◆ Agilent 1100 or 1200 HPLC with binary pump (JEOL or Agilent)
- ◆ NanoESI source (JEOL)
- ◆ 6 port external loop sample injector (Valco, part number C2-0006)
- ◆ Peek tee (Upchurch, part number P-727)
- ◆ Peek tubing, 1/16" OD x .0025" ID (Upchurch, part number 1560)
- ◆ Microtight sleeve, .0155 x .025 (Upchurch, part number F-185X)
- ◆ Microtight union (Upchurch, part number P-720)
- ◆ SilicaTip™Emitter (New Objective, part number FS360-50-30-CE-5-C15 for the flow rate of 300 – 1000 nL/min; part number FS360-75-15-CE-5-C15 for the flow rate of 200 – 500 nL/min)
- ◆ Integragrit column (Recommend New Objective Proteopep II™C₁₈ column, part number IFC75-PP2-10)

How to connect

1. Cut Peek tubing to an appropriate length for waste line.
2. Cut Peek tubing to an appropriate length to make a sample loop with a desired volume.
3. Choose a nano-LC column and an emitter based on your desired flow rate.
4. Connect all parts according to the diagram.

An application of peptide analysis was used as an example to test the nano-LC/MS system. The RSD of retention time for gradient elution is less than 1 %. For the full applications note, visit our on-line papers at www.jeolusa.com/ms/docs/convert_nano-LC.pdf.



Changing the Course of Mass Spectrometry

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DART is a near-universal source for small molecule analysis, exact mass measurements, accurate quantitative analysis of intensities and isotopic abundances. It is simple to use and allows easy, open access for lab personnel and for a multitude of unprepared samples in open air.

DART has gained acceptance and recognition in major pharmaceutical companies, forensics labs, universities, and homeland security operations.

Novel Mass Spec Techniques Used to Detect Counterfeit Anti-malarial Drugs

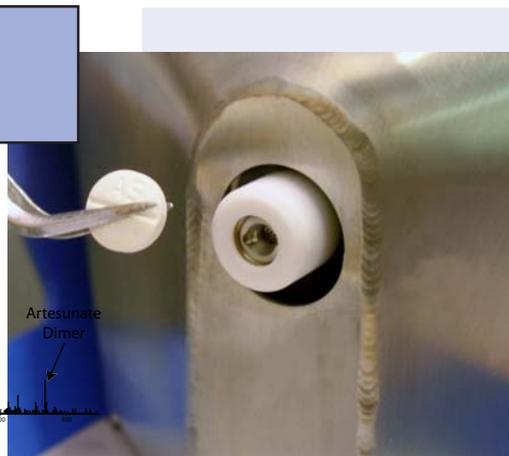
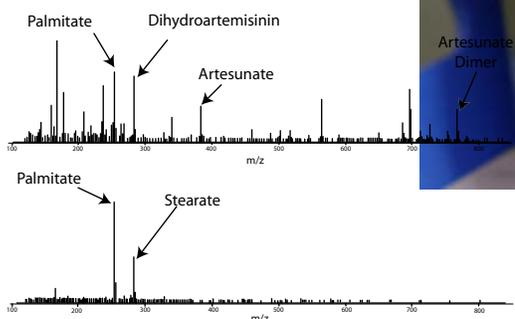
In order to chemically fingerprint counterfeit anti-malarial drugs, Prof. Facundo Fernandez' bioanalytical chemistry lab at Georgia Tech

conducts experiments using novel mass spectrometry techniques. Fernandez, et al., describe the use of ambient mass spectrometry ion sources for open air, high throughput screening of both counterfeit and genuine anti-malarial tablets in

“Characterization of Solid Counterfeit Drug Samples by Desorption Electrospray Ionization and Direct-analysis-in-real-time Coupled to Time-of flight Mass Spectrometry” (*ChemMedChem* 2006, 1, 702-705).

Counterfeiting of an effective but costly anti-malarial drug, artesunate, is a wide-spread health problem. Until now, there have been no satisfactory techniques for rapidly screening large quantities of pills, or for rapidly identifying the components in counterfeit drugs.

Among several techniques described in the paper, Fernandez used a direct analysis, exact-mass time-of-flight mass spectrometer (the JEOL AccuTOF™-DART™) to identify unknown components in counterfeit artesunate tablets. The counterfeit drug tablets were rapidly found to contain a surprising variety of compounds ranging from acetaminophen to antibiotics and antihistamines to older antimalarial drugs that are no longer effective. None of these components are effective against malaria, but may provide temporary relief and false confidence that may prevent the victim from obtaining effective treatment until the disease has progressed to a serious condition. Interestingly, several counterfeit drug tablets were found to contain trace amounts of genuine artesunate, which may have been added to confuse field tests for counterfeit drugs.



Anti-malarial tablet analyzed using DART.

Recent Mass Spec Papers and Posters

“Detection of the Peroxide Explosives TATP and HMTD Using Open Air Analysis”

“The Power of Exact Mass Measurement: Unknown Compound Identification” - *LC/GC Magazine Applications Notebook*, Sept. 2006.

“Out in the Open: Direct Analysis in Real Time One Year Later” - ASMS 2006 Poster

“Analysis of Acrylimide in Food by LC/TOF-MS” - ASMS 2006 Poster.

“Analysis of Drugs of Abuse by AccuTOF Dual ESI LC/TOF Mass Spec” - *LC/GC Magazine Applications Notebook*, June 2006

“Sudan Dyes Analysis by AccuTOF LC/MS System” - *LC/GC Magazine Applications Notebook*, Feb. 2006.

DART Applications Notebook Volume 2 - more than 25 applications notes.

“Determination of Stilbenes in Blueberries” - *LC/GC Magazine*, Nov 2005.

JEOL Mass Spectrometers Selection Guide

Model	Analyzer	Description
AccuTOF-LC	Time-of-Flight	LC/MS; Wide dynamic range; rapid data analysis
AccuTOF-GC	Time-of-Flight	GC/MS; Wide dynamic range; rapid data analysis
AccuTOF-DART	Time-of-Flight	Dry, open air; real time; no sample prep
GCMate II	Magnetic Sector	GC/MS; Benchtop, double-focusing; high res. SIM
MStation	Magnetic Sector	LC/MS & GC/MS; Fully automatic, double-focusing

(All systems include high resolution, exact mass ability)