The DART Forum

American Society for Mass Spectrometry
Annual Conference

June 7, 2011
Denver, CO

Presented by

ionSense®
Your source for open-air mass spectrometry

Agenda

6:45 – 7:15 AM **Registration and Breakfast Buffet**

7:15 – 8:15 **The State of DART - Presentations**

Advances in DART Instrumentation: Transmission Mode, Laser Ablation and Mobility Separations

Facundo Fernandez, Georgia Institute of Technology, Athens, GA

Dietary Supplements at Lightning Speed: From Identity Requirements to Contaminant Screens

James Neal-Kababick, Flora Research Laboratories, Grants Pass, OR

The Latest Developments in DART Applications

John Dane, JEOL USA, Peabody, MA

What's New from IonSense:

DART in a Flash - A New Approach to Getting your Questions Answered

Joseph Tice, Engineering Manager, IonSense, Inc.

Going Vertical for High Throughput DART

Liz Crawford, Applications Manager, IonSense, Inc.

Service in a Box - Keeping Your DART Up and Running

Douglas Simmons, Manager, IonSense, Inc.

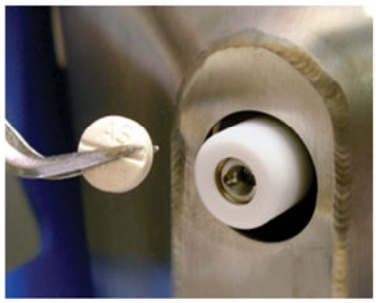
Program Concludes **8:15**

Networking **8:15 – 8:30**

Advances in DART Instrumentation: Transmission Mode, Laser Ablation and Mobility Separations

Facundo M. Fernández
Georgia Institute of Technology, Atlanta, Georgia, USA

Ambient MS in the Real World: DART



JEOL

FINGERING FAKES DART can identify counterfeit pharmaceuticals, such as those purporting to be the antimalarial drug artesunate.

Advantages include:

- **No sample preparation required.**
- **Sample is not placed in vacuum.**
- **Sizeable objects can be directly examined in the open air.**
- **Very high sample throughput.**
- **Can be coupled to any mass spectrometer with an atmospheric pressure interface for accurate mass or MS/MS experiments.**
- **No memory effects**

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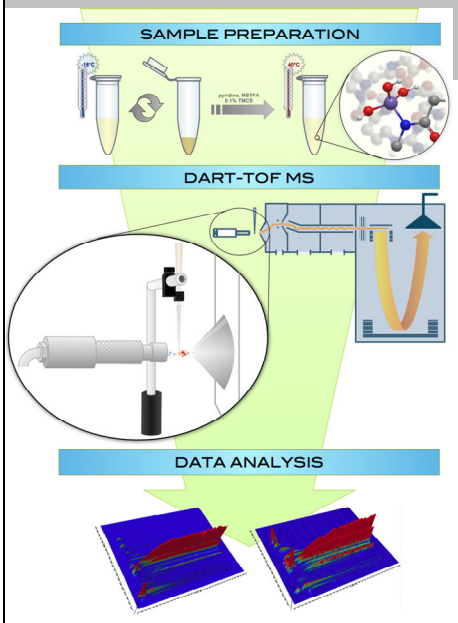
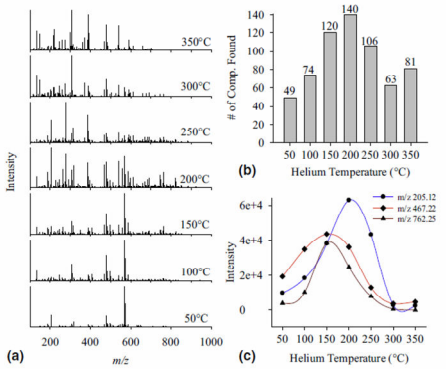
DART Metabolomic Discovery Workflow





Effect of helium gas temperature on DART-TOF MS sensitivity for metabolomic profiling of derivatized serum: (a) background corrected mass spectra at various helium temperatures, (b) number of metabolites matched to HMDB database, and (c) change in S/N of three mass spectrometric signals at m/z 205.12, 467.22, and 762.25 versus helium temperature.

Zhou et al., *J. Am. Soc. Mass Spectrom.*, **2010**, 21, 68-75

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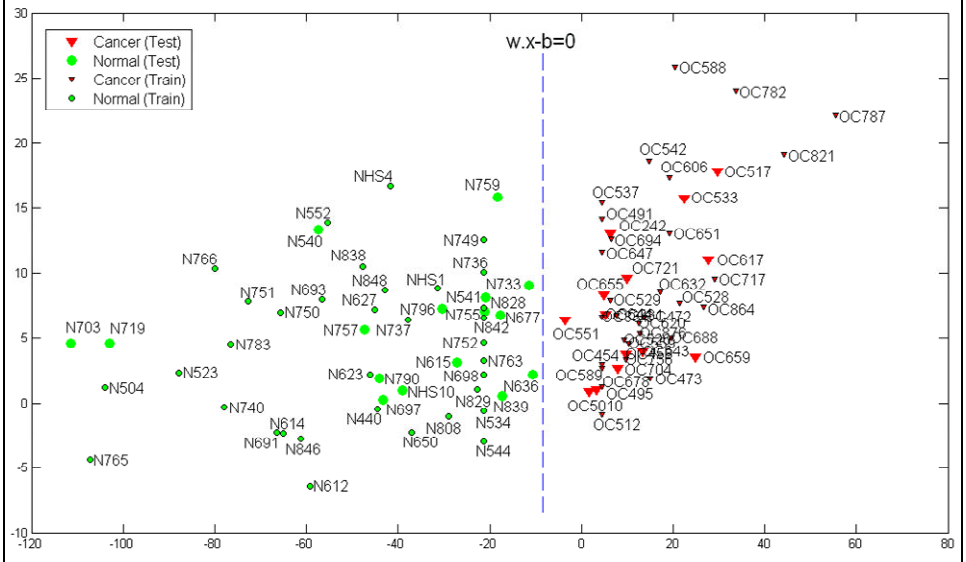
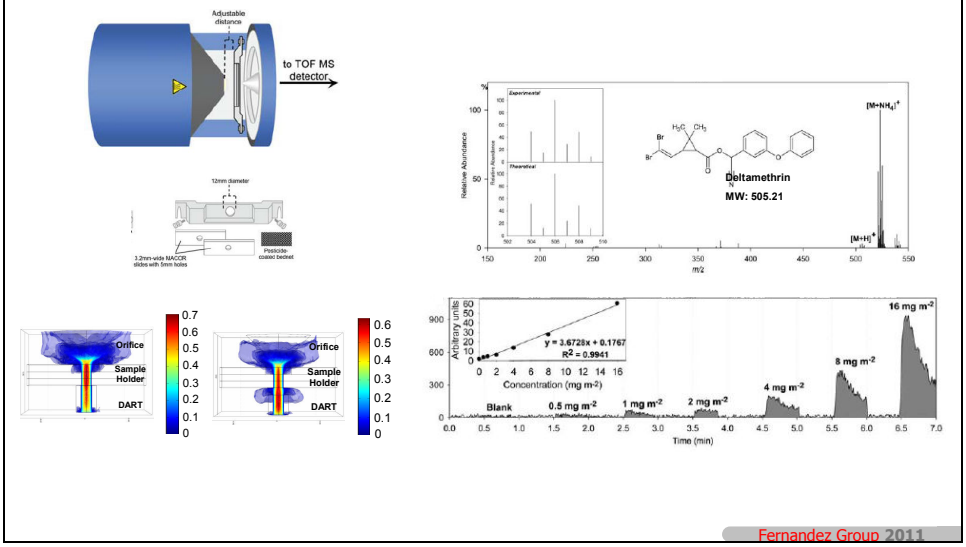
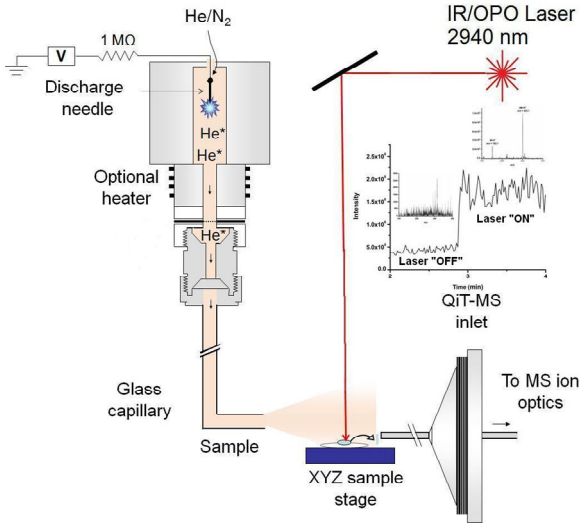
DART Diagnostics Results



TM-DART



IR-DART



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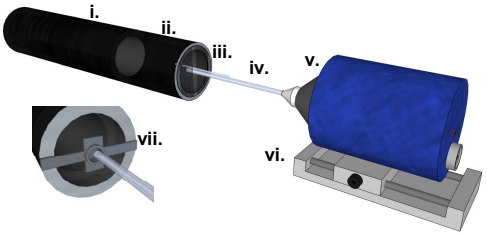
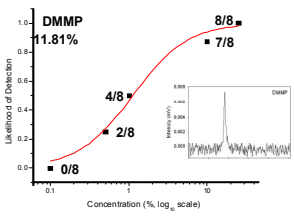
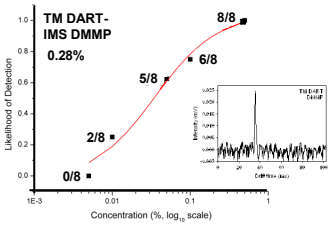
DART-IMS







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Dietary Supplements at Lightning Speed: From Identity Requirements to Contaminant Screens

James Neal-Kababick
Flora Research Laboratories, Grants Pass, OR

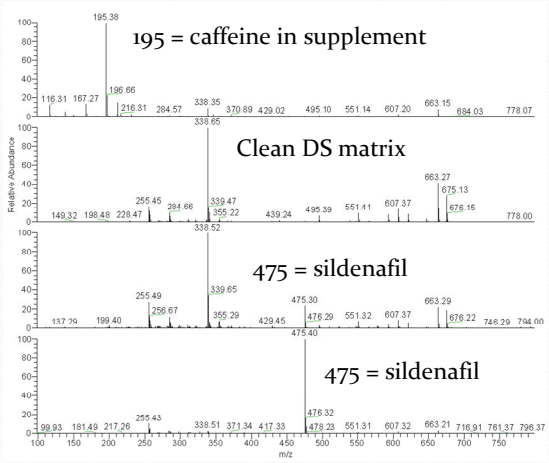
Issues Facing DS Industry

- Now under new cGMP's (21 CFR part 111)
- FDA FSMA gives FDA direct recall authority/expanded detention authority
- FDA expanding staff and intensifying enforcement
- Companies need new and faster ways to test product lots
- Scientifically valid lot sampling plans required meaning many samples per lot need analysis
- API Contaminants and identity main concerns at FDA

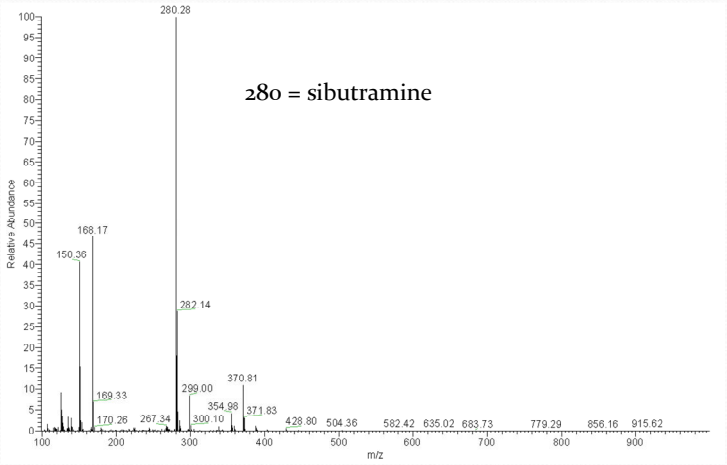
API Adulteration

- Active Pharmaceutical Ingredients (API)
- Many drugs are novel analogues not previously known
- Emergence of old abandoned pharmaceuticals
- Often multiple complex mixtures of pharmaceuticals buried in botanical matrix
- Industry needs rapid methods for pass/fail testing of targeted compounds
- Ability to run many replicates from one lot quickly vital to industry survival

Analysis of ED Drugs by DART



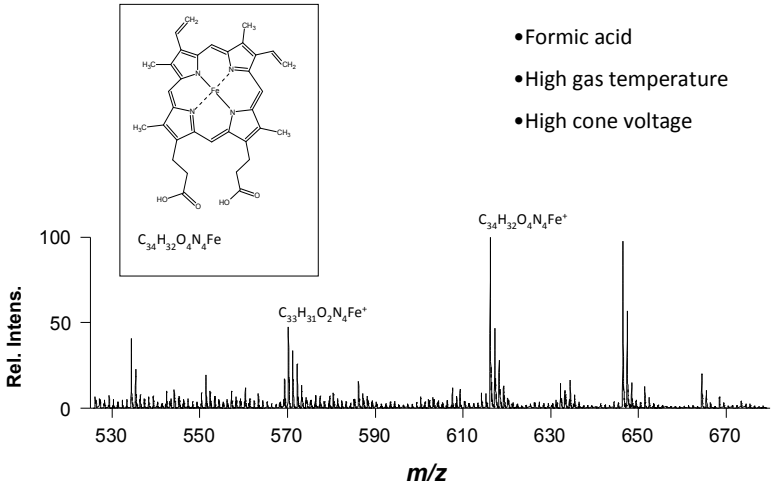
Sibutramine in DS by DART



The Latest Developments in DART Applications

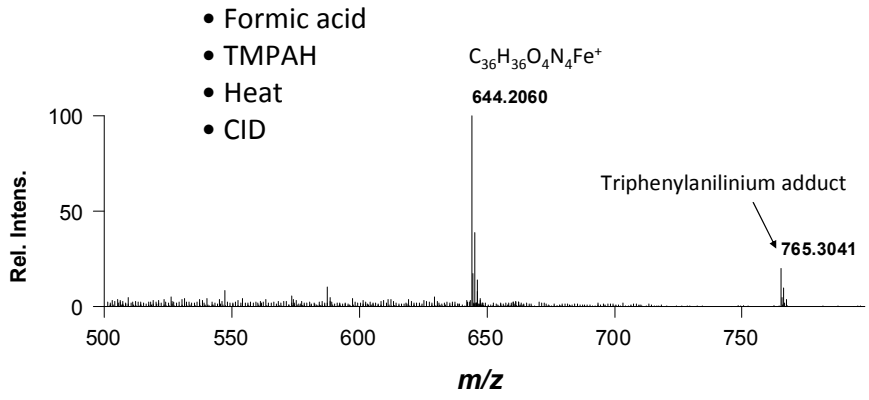
John Dane
JEOL USA, Peabody, MA

DART: Heme from Myoglobin



Work done with Prof. Ruth Ann Armitage (Eastern Michigan U.)

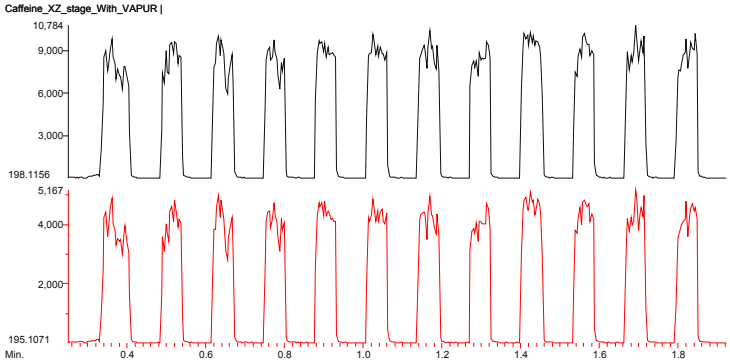
Permethylation of Acid Groups with TMPAH Improves S/N



Work done with Prof. Ruth Ann Armitage (Eastern Michigan U.)

DART X-Z Stage

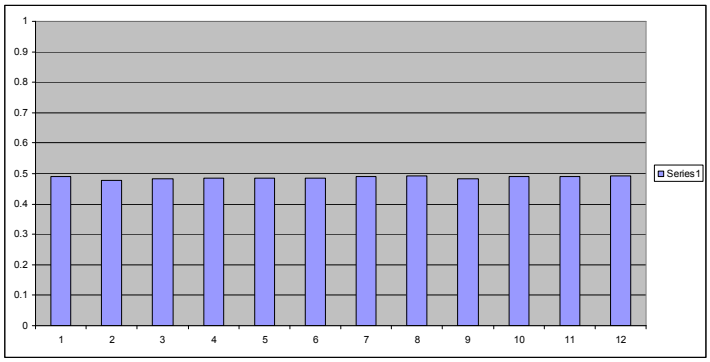
- 2 trials on **JEOL AccuTOF-DART** of 12 replicates caffeine + internal standard



Good Reproducibility with X-Z Stage

Results on **JEOL AccuTOF-DART** system:

With I.S.	**Without I.S.**
Trial 1 CV% = 0.9	*m/z* 195: CV% = 7.2
Trial 2 CV% = 1.1	*m/z* 198: CV% = 6.9

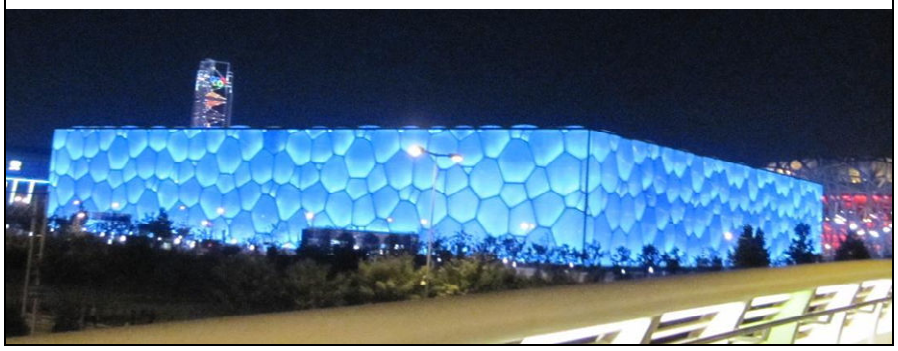


DART in a Flash - A New Approach to Getting your Questions Answered

Joseph Tice
IonSense, Inc., Saugus, MA

ID-CUBE™

Providing Near-Instantaneous Characterization of Chemicals using DART Technology



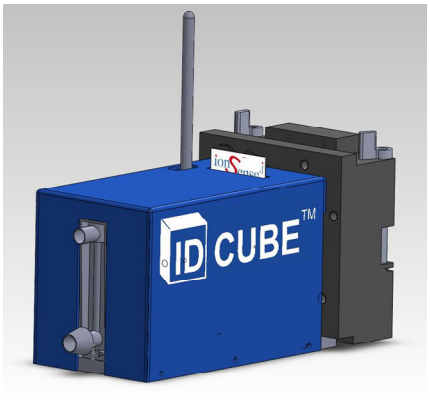
ID-CUBE™ Source with OpenSpot ™ Sample Card

- Transmission" DART stainless steel screens offers high throughput capacity:
  - Improvement in precision of the measurement
  - Automated sample handling devices enabled
- Near instant vaporization of sample and subsequent ionization without solvent
  - NO wait for answers
  - Analyze liquids or powders
  - High resolution support system for MS

OpenSpot™ Sample Card

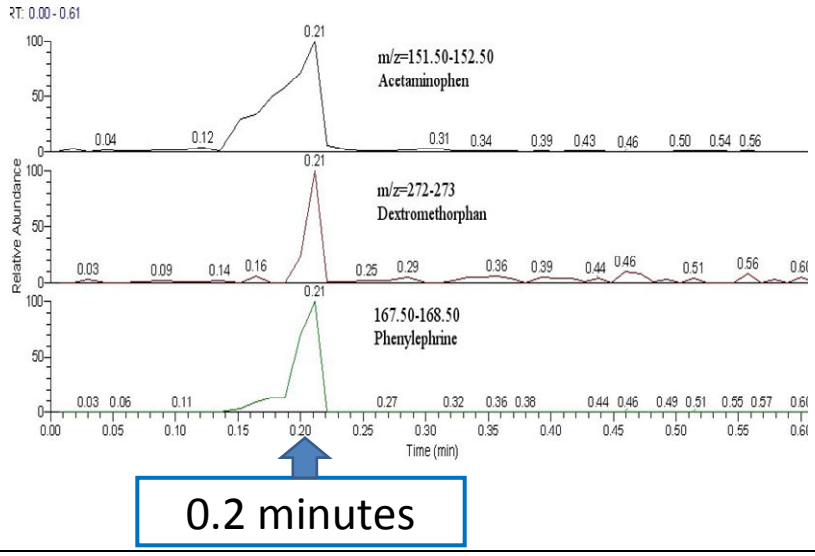
- Business Card shape and size
- Sample applied to metal screen incorporated in cutout zone
- Sample information can be written on the card
- Integral part of the thermal desorption process

The ID-CUBE™ Source



- Compact unit mounts via VAPUR
- Implementation required external HV and gas connections from LC/MS instrument
- Mounts in seconds
- Contact closure
- Manual gas control

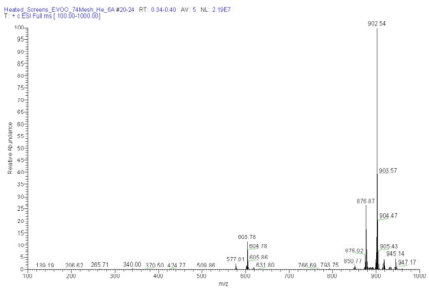
Analysis of Tylenol Tablet



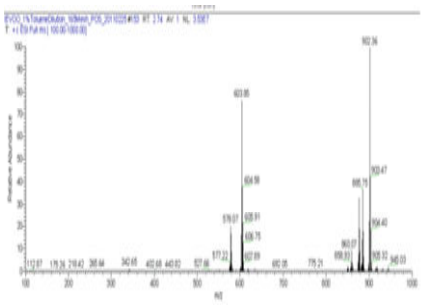
0.2 minutes

Effect on Thermal Degredation

ID-CUBE Technology

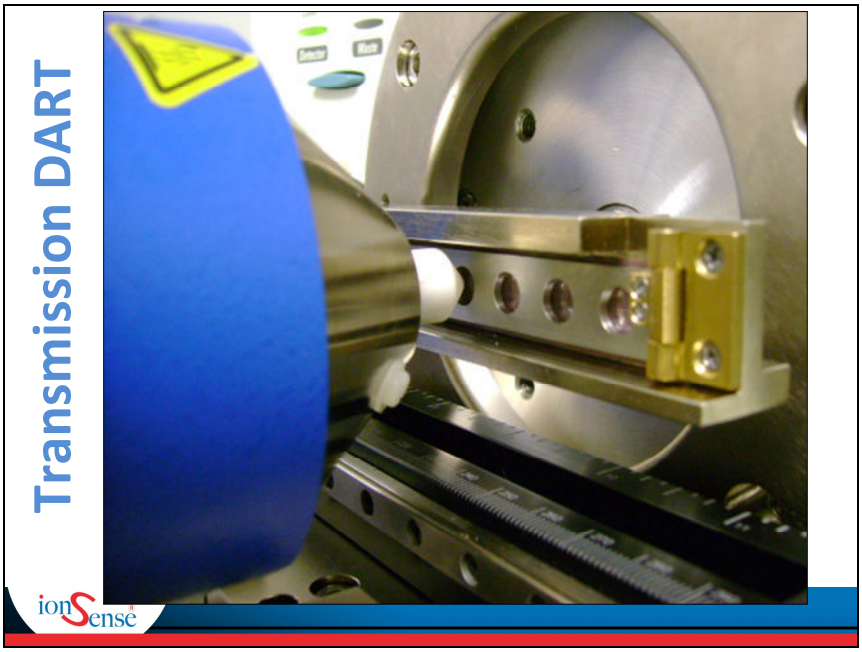


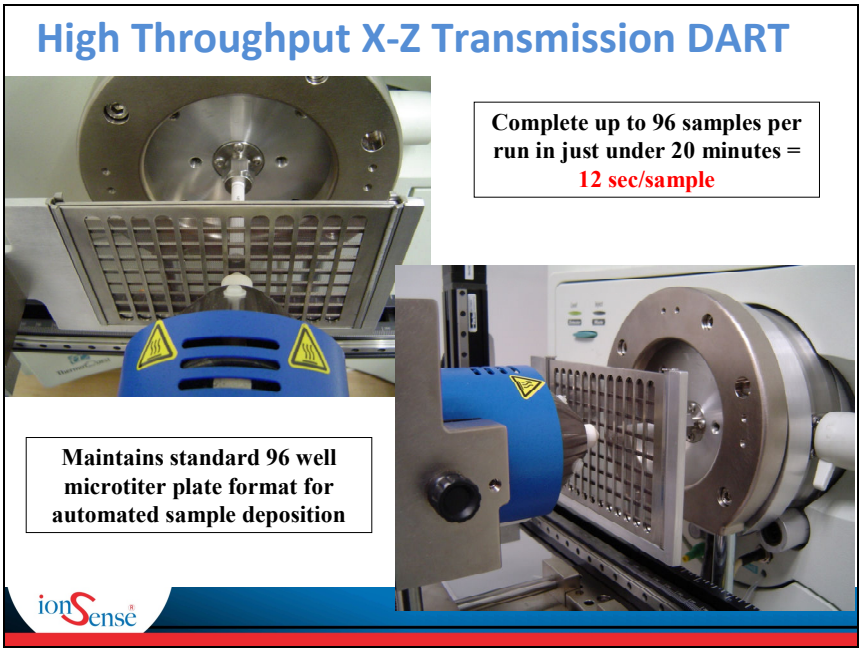
Conventional DART 450C

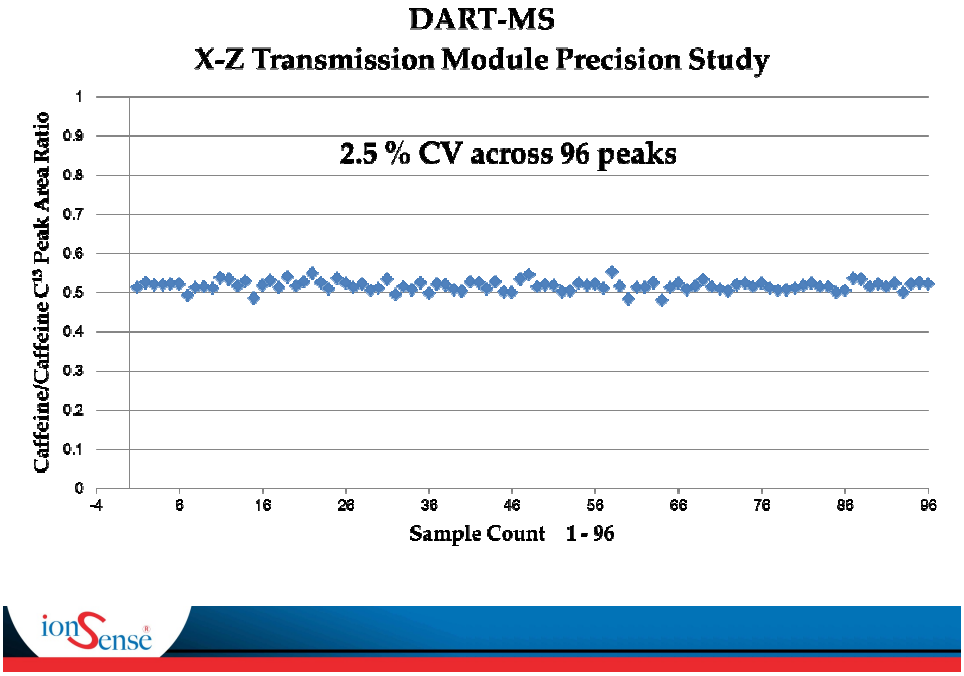


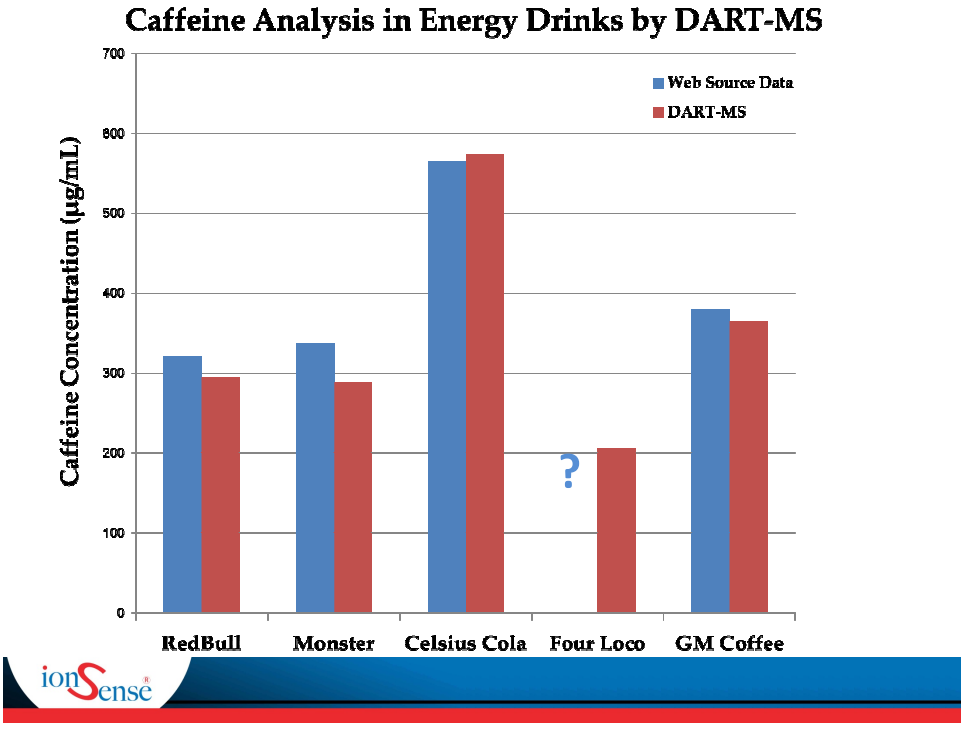
Going Vertical for High Throughput DART

Liz Crawford
IonSense, Inc., Saugus, MA






DART-MS
X-Z Transmission Module Precision Study
2.5 % CV across 96 peaks
Caffeine/Caffeine C13 Peak Area Ratio
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-4
8
16
26
36
46
56
66
76
86
96
Sample Count 1 - 96
ionSense


Caffeine Analysis in Energy Drinks by DART-MS
Caffeine Concentration (µg/mL)
700
600
500
400
300
200
100
0
Web Source Data
DART-MS
?
RedBull
Monster
Celsius Cola
Four Loco
GM Coffee
ionSense

Selected DART Presentations and Posters
ASMS 2011

Booth 133

Booth 51

Monday

Poster: MP22 - Homeland Security, poster number: 400, Monday, Poster Hall

Capabilities of molecular imaging by high resolution mass spectrometry with DESI and DART sources

Olivier Vigneau; Xavier MACHURON-MANDARD;
CEA, DAM, DIF, Arpajon, FRANCE
View poster/extended abstract PDF

Tuesday

Poster: TP01 - Ionization Mechanisms, poster number: 021, Tuesday, Poster Hall

Ion Yield and Ion Suppression "Hot-Spots" in Direct Analysis In Real Time Mass Spectrometry

Glenn A Harris; Caitlin E. Falcone; Facundo Fernandez;
Georgia Institute of Technology, Atlanta, GA
View poster/extended abstract PDF

Poster: TP02 - Direct Ionization: Instrumentation, poster number: 025, Tuesday, Poster Hall

Improving DART Sample Introduction Via Induction Based Fluidics

Drew Sauter[1]; Andrew Grange[2];
[1]Nanoliter, LLC, Henderson, NV; [2]U.S. EPA, Las Vegas, NV
View poster/extended abstract PDF

Poster: TP02 - Direct Ionization: Instrumentation, poster number: 026, Tuesday, Poster Hall

Integration of Automated Methods for Improved Qualitative and Quantitative Analysis in DART-MS

Michael Festa; Elizabeth Crawford; Joseph Tice;
IonSense, Inc., Saugus, MA
View poster/extended abstract PDF

Poster: TP02 - Direct Ionization: Instrumentation, poster number: 031, Tuesday, Poster Hall

Direct Ambient Analysis using Atmospheric Pressure Photoionization (APPI)

Kaveh Jorabchi; Sheng-Suan (Victor) Cai ; Brian J. Nies; Jack A. Syage;
Syagen Technology, Inc., Tustin, CA
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 037, Tuesday, Poster Hall

Rapid screening of synthetic antidiabetic drugs adulterated in herbal dietary supplements using DART MS

Zhigui Zhou; Jialing Zhang; Yu Bai; Huwei Liu;
College of Chemistry, Peking University, Beijing, CHINA
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 038, Tuesday, Poster Hall

Determination of Ginsenosides in Ginseng Roots and Commercial Products by using In-situ Derivatization Direct Analysis in Real Time

Rachel N Liu[1]; Hao Yue[2]; Jordan Krechmer[3]; Lili Jiao[2]; Charles C Liu [1]; Brian Musselman[3]; Shuying Liu[2];
[1]ASPEC Technologies, Beijing, CHINA; [2]Jilin Ginseng Academy, Changchun University of TCM, Changchun, China; [3]IonSense, Inc., 999 Broadway, Suite 404, Saugus, MA 01906
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 039, Tuesday, Poster Hall

Transmission-Mode Direct Analysis in Real Time (DART) Quadrupole Time-of-Flight Mass Spectrometry for Fast Untargeted Metabolomic Profiling of Human Serum

Christina Jones; Manshui Zhou; Facundo Fernandez;
Georgia Institute of Technology, Atlanta, GA
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 040, Tuesday, Poster Hall

Quantitative Capabilities of DART-Orbitrap MS for Determination of Pesticides on Fruits and Vegetables

Lenin Parrales[2]; Peter T. Palmer[1]; Adam Leung[1];
[1]San Francisco State University, San Francisco, CA; [2]Food & Drug Administration, Alameda, CA
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 041, Tuesday, Poster Hall

Ionization and Sequence of Peptides Bound to Solid Supports without Deprotection or Cleavage Prior to Analysis by DART TOF MS

Matthew Curtis[1]; Laura Sanchez[2]; Bianca Bracamonte[2]; Roger Linington[2]; Patrick R. Jones[1]; O. David Sparkman[1];
[1]University of the Pacific, Stockton, CA; [2]University of California Santa Cruz, Santa Cruz, CA
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 042, Tuesday, Poster Hall

Ambient Ionization High Resolution Mass Spectrometry to determine non-visible set-off in food contact materials

Karim Bentayeb; Luke Ackerman; John H. Callahan; Timothy Begley;
FDA Center for Food Safety, College Park, MD
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 043, Tuesday, Poster Hall

Enabling High Throughput Bioanalysis by Transmission Mode DART: In-line Desorption Ionization of Small Molecules from an Array of Samples

Elizabeth Crawford; Joseph Tice; Michael Festa; Brian D. Musselman ;
IonSense, Inc., Saugus, MA
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 044, Tuesday, Poster Hall

Rapid sample cleanup procedure using Disposable Pipette eXtraction (DPX) for detection of drugs in urine by DART

Robert B. Cody[1]; John Dane [1]; William E. Brewer[2];
[1]JEOL USA, Inc., Peabody, MA; [2]DPX Laboratories, Columbia, SC
View poster/extended abstract PDF

Poster: TP03 - Direct Ionization: Applications II, poster number: 045, Tuesday, Poster Hall

Mass Spectrometric Fragmentation Behavior of Chalcone Derivatives Employing Direct Analysis in Real Time (DART) Technique

Adnan Kadi; Mohamed Attwa; A. F. M. Motiur Rahman;
King Saud University, College of Pharmacy, Riyadh, SAUDI ARABIA
View poster/extended abstract PDF

Poster: TP04 - New Developments in Ionization II, poster number: 078, Tuesday, Poster Hall

A Novel Method for Rapid Vaporization of Samples for Higher Throughput Direct Analysis in Real Time (DART) Mass Spectrometry

Jordan Krechmer; Joseph Tice; Elizabeth Crawford; Brian D. Musselman ;
IonSense, Inc., Saugus, MA
View poster/extended abstract PDF

Wednesday

Poster: WP08 - Small Molecule - Qualitative Analysis, poster number: 114, Wednesday, Poster Hall

Confirmation of the Identity of a Previously Unknown Alkaloid of Commercial Significance by EI and Other Mass Spectral Techniques

O. David Sparkman[1]; Patrick R. Jones[1]; Matthew Curtis[1]; Manali Aggrawal [1]; Liang Xue[1]; Christine Vandervoort[2];
[1]University of the Pacific, Stockton, CA; [2]Michigan State University, East Lansing, MI
View poster/extended abstract PDF

Poster: WP11 - Nucleic Acids II, poster number: 186, Wednesday, Poster Hall

Study of Fragmentation of RNA Nucleotides and DNA Oligonucleotides in a Direct Analysis in Real Time Mass Spectrometer

Liang Xue; Matthew Curtis; Manali Aggrawal; Priyanka Chitranshi; O. David Sparkman; Patrick R. Jones;
University of the Pacific, Stockton, CA

Poster: WP12 - Forensics: General, poster number: 200, Wednesday, Poster Hall

International Effort to Monitor Toy Safety Using Inexpensive Dual Use Military/Civilian Wear Sensors Incorporating DART Mass Spectral Dyes

Ronny Robbins [1]; James McCarty M.D.[2];
[1]US Army, Gunpowder, MD; [2]Springs of Grace Church, Mogoñé, Mexico

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Poster: WP18 - Organic and Organometalic Supramolecular Complexes, poster number: 340, Wednesday, Poster Hall

***DART*-MS, ^{51}VNMR and X–ray crystallographic studies on novel oxo-bridged polyvanadates $[H_2V_{10}O_{28}]$•4[LH] (L = 2-methyl imidazole or 4-picoline): 3D supramolecular assembly**

Zafar A. Siddiqi;
Aligarh Muslim University, Aligarh, INDIA

Thursday

Poster: ThP03 - Instrumentation: New Concepts, poster number: 066, Thursday, Poster Hall

Development of a multi-turn time-of-flight mass spectrometer with an Atrompheric ionization.

Masanobu Nakasono[1]; Hiroki Andoh[1]; Hirofumi Nagao[1]; Shinichi Miki[2]; Michisato Toyoda[1];
[1]Osaka university, Toyonaka, JAPAN; [2]MSI. TOKYO, Chofu, Japan

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Poster: ThP16 - Agriculture, poster number: 299, Thursday, Poster Hall

Analysis Of Switchgrass Biomass By Direct Analysis In Real Time (DART) For Biofuel Production

Sushma Dendukuri[1]; Darrin Smith[1]; Gary Selby[2]; Don Llewellyn[2];
[1]Eastern Kentucky University, Chemistry Department, Richmond, KY; [2]Eastern Kentucky University, Agriculture, Richmond, KY

Poster: ThP19 - Energy: Biofuels and Algae, poster number: 351, Thursday, Poster Hall

Sugar Quantitation by Direct Analysis in Real Time Mass Spectrometry (DART-MS) for Biofuels Production

Daudi Saang'onyo; Darrin Smith;
Eastern Kentucky University, Chemistry Department, Richmond, KY

Poster: ThP21 - Forensics: Toxicological Analysis, poster number: 382, Thursday, Poster Hall

Porous Gold Substrates for Rapid Extraction of Drugs Prior to MS Analysis

Kenyon Evans-Nguyen; Tiffanie Hargraves; Amanda Quinto; Jennifer Devorak;
University of Tampa, Tampa, FL

DART Publications 2010-2011

2010

81. Bajpai, V.; Sharma, D.; Kumar, B.; Madhusudanan, K. P. *Profiling of Piper betle Linn. cultivars by direct analysis in real time mass spectrometric technique.* Biomedical Chromatography, 2010, 24(12), 1283-1286.

82. Bevilacqua, V.L.H.; Nilles, J.M.; Rice, J.S.; Connell, T.R.; Schenning, A.M.; Reilly, L.M.; Durst, H.D. *Ricin Activity Assay by Direct Analysis in Real Time Mass Spectrometry Detection of Adenine Release.* Anal. Chem., 2010, 82(3): 798–800.

83. Block, E.; Cody, R.B.; Dane, A.J.; Sheridan, R.; Vattekkatte, A.; and Wang, K. *Allium chemistry: Use of new instrumental techniques to "see" reactive organosulfur species formed upon crushing garlic and onion*. Pure Appl. Chem., 2010, 82(3): 535–539.

84. Block, E.; Dane, A.J.; Thomas, S.; Cody, R.B. *Applications of Direct Analysis in Real Time Mass Spectrometry (DART-MS) in Allium Chemistry. 2-Propenesulfenic and 2-Propenesulfinic Acids, Diallyl Trisulfane S-Oxide, and Other Reactive Sulfur Compounds from Crushed Garlic and Other Alliums.* J. Agric. Food Chem., 2010, 58(8): 4617–4625.

85. Cajka, T.; Riddellova, K.; Tomaniova, M.; Hajslova, J., *Ambient mass spectrometry employing a DART ion source for metabolomic fingerprinting/profiling: A powerful tool for beer origin recognition.* Metabolomics, 2010, Publication Date (Web): 9 December 2010.

86. Cajka, T.; Riddellova, K.; Tomaniova, M.; Hajslova, J., *Recognition of beer brand based on multivariate analysis of volatile fingerprint.* Journal of Chromatography A, 2010, 1217(25): 4195-4203.

87. Chernetsova, E.; Bochkov, P. O.; Ovcharov, M. V.; Zhokhov, S. S.; Abramovich, R. A. *DART mass spectrometry: a fast screening of solid pharmaceuticals for the presence of an active ingredient, as an alternative for IR spectroscopy.* Drug Testing and Analysis, 2010, 2: 292-294.

88. Chernetsova, E. S.; Khomyakov, Y. Y.; Goryainov, S. V.; Ovcharov, M. V.; Bochkov, P. O.; Zatonsky, G. V.; Zhokhov, S. S.; Abramovich, R. A. *Capabilities of direct analysis in real time mass spectrometry and gas chromatography-mass spectrometry in the mint oil test*. Mendeleev Communications, 2010, 20(5): 299-300.

89. Cody, R. B. and Dane, A. J. *Direct Analysis in Real Time Ion Source*. In Encyclopedia of Analytical Chemistry, Meyers, R. A., Ed. John Wiley & Sons, Ltd.: Publication Date (Web): 15 December 2010.

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