

TREN PEMANFAATAN LC-MS DALAM BIDANG ILMU FORENSIK

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TREN PEMANFAATAN LC-MS DALAM BIDANG ILMU FORENSIK

oleh

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Jurusan Farmasi – FMIPA - Udayana

Liquid Chromatography – Mass Spectroscopy sejak dikenalkan pada bidang analisis 25 tahun yang lalu, berkembang menjadi alat yang sangat penting untuk uji indentifikasi senyawa anorganik, organik, dan senyawa biologis. LC-MS adalah kombinasi dari HPLC dan MS, sehingga dapat digunakan untuk mengidentifikasi molekul dengan berat molekul besar dan susah menguap, seperti: metabolit senyawa aktif, oligosakarida dan protein. Kegunaan LC-MS ini dapat dimanfaatkan dalam bidang: Kedokteran Forensik, Toksikologi Forensik, Forensik Lingkungan, balistik forensik, dan DNA-Forensik.

Kata kunci: LC-MS, Ilmu Forensik

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Presented to :

I Made Agus Gelgel Wirasuta

(as Participant / Speaker / Moderator)

Tren Pemanfaatan LC-MS dalam bidang Ilmu Forensik

**in the 5th National Congress of Indonesian Forensic Medicine and Medicolegal (PDFI)
in conjunction with the 1st National Congress of Indonesian Association of Forensic Sciences (AIFI)**

Clarion Hotel Makassar, October 16-18, 2010

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Tren Pemanfaatan LC-MS dalam bidang Ilmu Forensik

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LC-MS



Agilent Accurate-Mass Time-of-Flight (TOF) and Quadrupole Time-of-Flight (Q-TOF) LC/MS systems combine Ultra High Definition UHDEF technology with advanced MassHunter Workstation software—plus the superior HPLC and UHPLC performance and flexibility of the new 1290 Infinity LC.

Instrumentation

- Two key components in this process are
 - the ion source, which generates the ions, and
 - the mass analyzer, which sorts the ions.

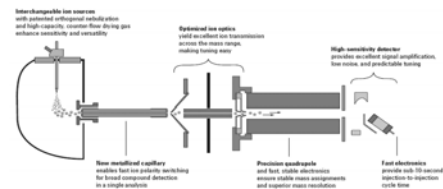
Ion Sources

- The introduction of atmospheric pressure ionization (API) techniques greatly expanded the number of compounds that can be successfully analyzed by LC/MS.
 - In atmospheric pressure ionization, the analyte molecules are ionized first, at atmospheric pressure. The analyte ions are then mechanically and electrostatically separated from neutral molecules.
 - Common atmospheric pressure ionization techniques are:
 - Electrospray ionization (ESI)
 - Atmospheric pressure chemical ionization (APCI)
 - Atmospheric pressure photoionization (APPI)
- Static sample primarily use Matrix-assisted laser desorption/ionization (MALDI)

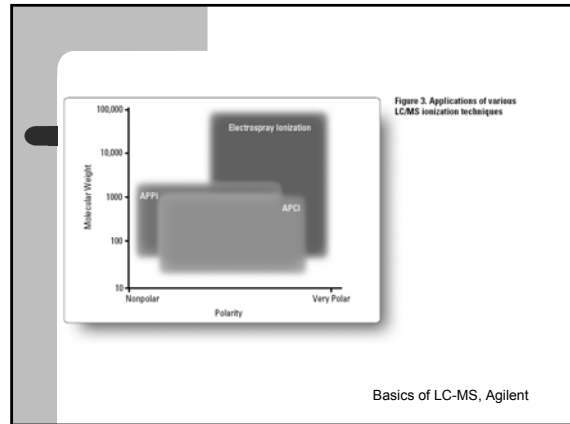
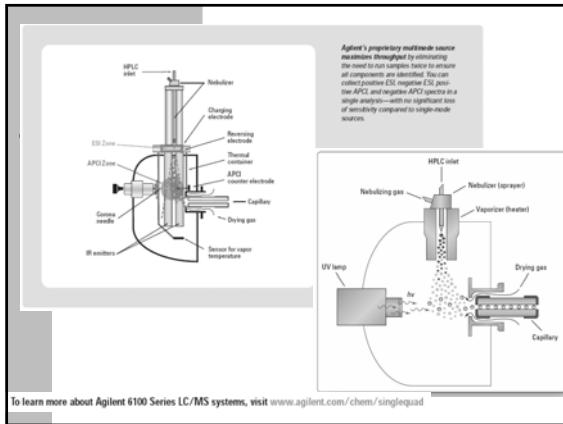
History of Electron spray

- Jean-Antoine Nollet (1750) observed water flowing from an electrified metal vessel shows a tendency to aerosolize when the vessel is placed near the electrical ground.
- Lord Kelvin (1850s) studied the charging between water dripping from two different liquid nozzles, which leads to electrospray phenomena at nozzles themselves
- 1968 Electrospray became of scientific interest.
- **1984 Yamashita & Fenn brought electrospray in the analytical world and from then an electrospray**
 - Easily couple LC to MS
 - Introduce Nobel Prize in 2002

A. Cappiello, (2007), *advances in LC-MS instrumentation*, Elsevier,



To learn more about Agilent 6100 Series LC/MS systems, visit www.agilent.com/chem/singlequad



Mass Analyzers

- For LC/MS
 - Quadrupole
 - Time of flight
 - Ion trap
 - Fourier transform-ion cyclotron resonance (FT-ICR or FT-MS)

Application

- **Molecular Weight Determination**
 - Differentiation of similar octapeptides
 - Determining the molecular weight of green fluorescent protein
- **Structural Determination**
- **Pharmaceutical Applications**
 - Pharmaceutical chemistry and pharmacology (structural characterization of drugs and their impurities, metabolic and pharmacokinetic investigations, etc.)
- **Biochemical and Clinical Applications**
 - Clinical chemistry and biochemistry (quantitation of endogenous and xenobiotic compounds having diagnostic significance, reference and definitive clinical chemistry analytical methods, etc.)
- **Food Applications**
 - Food chemistry and agriculture (food analysis, devoted to nutritional compounds and residual components determination, characterization and determination of additives, etc.)
- **Environmental Applications**
 - Environmental control (identification, characterization and quantitation of polar water pollutants, determination of pesticides, surfactants and their metabolites or degradation products, etc.)

Application

- Genomics
 - Single nucleotide polymorphisms (SNPs) are the most abundant genetic variation.
 - For medicine propose
 - Pharmaceutical propose
 - **MALDI-TOF MS is emerging as a valuable genotyping tool**
- Proteomic
 - The study of protein structure, function, quantity, and interaction during maturation and progression of disease is referred to as proteomics.
 - Analytical:
 - 2-D gel electrophoresis for separation and MS
 - Extrated peptides from gels are analyzed by **MALDI-TOP MS**

Application in Forensic Field

- Toxicology forensic
 - PubMed (1995 s/d 2010): 207 Pub.
- Medicine forensic
 - PubMed (1995 s/d 2010) 280 Pub
 - Pathology forensic : 21 Pub
 - DNA-Forensic: 1 Pub
- Environmental Forensic:
 - PubMed: (1995 s/d 2010): 28 Pub
- Ballistic forensic:
 - PubMed: 4 Pub.

Dual examinations for identification of urine as being of human origin and for DNA-typing from small stains of human urine.

Nakazono T, Kashimura S, Hayashiba Y, Hara K, Matsusue A, Augustin C.
Forensic Science Laboratory, Fukuoka Prefectural Police Headquarters, Fukuoka, Japan. nakazono@indigo.plala.or.jp

Abstract

Concurrent methods for identification of urine as being of human origin, and for DNA-typing from small stains of human urine were examined. A urine stain was extracted with phosphate-buffered saline (PBS), and the extract was filtered using a Centricon-100 device. The filtrate was subjected to electrospray ionization liquid chromatography-mass spectrometry (ESI-LC-MS) for identification of human urine and a DNA-typing sample was obtained by diafiltration of the residue using a

Anal Bioanal Chem. 2009 Sep;395(2):401-9. Epub 2009 May 31.

Bioassays for bomb-makers: proof of concept.

Bell SC, Gayton-Ely M, Nida CM.
Forensic Science & Chemistry, West Virginia University, 1600 University Avenue, Oglebay Hall, Room 208, Box 6121, Morgantown, WV 26505-6121, USA. Suzanne.Bell@mail.wvu.edu

Abstract

Clandestine bomb-makers are exposed to significant amounts of explosives and allied materials. As with any ingested xenobiotic substance, these compounds are subject to biotransformation. As such, the potential exists that characteristic suites of biomarkers may be produced and deposited in matrices that can be exploited for forensic and investigative purposes. However, before such assays can be developed, foundational data must be gathered regarding the toxicokinetics, fate, and transport of the resulting biomarkers within the body and in matrices such as urine, hair, nails, sweat, feces, and saliva. This report presents an in vitro method for simulation of human metabolic transformations using human liver microsomes and an assay applicable to representative nitro-explosives. Control and metabolized samples of TNT, RDX, HMX, and tetryl were analyzed using high-performance liquid chromatography coupled to tandem mass spectrometry (LC/MS/MS) and biomarkers identified for each. The challenges associated with this method arise from solubility issues and limitations imposed by instrumentation, specifically, modes of ionization.

Use of porous graphitic carbon for the analysis of nitrate ester, nitramine and nitroaromatic explosives and by-products by liquid chromatography-atmospheric pressure chemical ionisation-mass spectrometry.

Tachon R, Pichon V, Le Borgne MB, Minet JJ.
Laboratoire Central de la Prefecture de Police, 39 bis rue de Dantzig, 75015 Paris, France.

J. Forensic Sci. 2008 Mar;53(2):303-7.

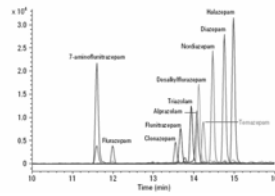
The identification of the emulsifier component of emulsion explosives by liquid chromatography-mass spectrometry.

De Tata D, Collins P, Campbell N.
Forensic Science Laboratory, Chemistry Centre (WA), 125 Hay Street, East Perth, WA 6004, Australia. Ddetata@ccwa.wa.gov.au

Abstract

The widespread availability of emulsion explosives for commercial blasting has inevitably lead to their diversion for criminal misuse. Present techniques for the characterization of emulsion explosives and their residues is generally based on the detection and identification of the oxidizer and the hydrocarbon components. Use of these components

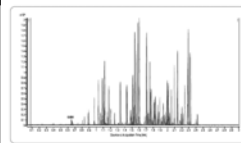
Toxicology forensic



Analysis of benzodiazepines in scan mode. Extracted ion chromatograms can be used to question target analysis. Confirming ions increase confidence in results.

Powerful, easy-to-use solutions for food safety and environmental analysis

Ultra-fast screening and identification of pesticides



D-TOF identification of 180 pesticides in less than three minutes. Superior peak capacity and fast MS acquisition lets you resolve large numbers of pesticides and ensure high confidence in compound identification. The fast acquisition capability of the D-TOF allows considerably shorter run times while still acquiring full spectral data. (120 Infinity LC using a ZORBAX RHD column and 660 Accurate-Mass D-TOF)

High resolution MS, sub 1 ppm mass accuracy, and isotope peak fidelity at 10 scans per second



Screening for thousands of pesticides in three minutes. In this example, 10 data points are collected across each one-second wide LC peak, allowing thousands of pesticides to be screened in the three-minute timeframe.

Conclusion

- LC-MS offer an analytical tool for the un-volatile, thermo labile, very polar, and bigger molecule/substance
 - Create open opportunity for use in forensic field.