

Agilent Instrument platforms and total workflow for analyte quantification

Seminar Sample
Preparation 2011

Dr. Manfred Bergmann

Agilent Technologies



TECHNOLOGIEN UND LÖSUNGEN

Separations Technology



- 1290 Infinity UHPLC
- 12x0 Infinity HPLC
- 7100 Capillary Electrophoresis
- HPLC Chip Cube System
- 7890 GC



MS Detector Technology



- 6000 Series LC/MS/MS
- 7000 Series GC/MS/MS
- 597X GC/MSD
- Agilent Ion Trap LC/MS and GC/MS

Data Analysis / Application Software



- MassHunter MS Software Family
- Mass Profiler Professional w/ Pathway Analysis
- Personal Compound AMRT Databases and Libraries
- Pharma Workflows; ADME, Bioanalysis, Confirmation

Solutions



- Fast Track Solution Kits for LC, GC, LC/MS & GC/MS
- Analyzer
- Clinical Application Offer
- More to come



AGILENT 40 JAHRE MASSENSPEKTROMETRIE

HP GC/MS-5930A

5930A 1971

5992A 1976

5970B MSD 1986

5971 - 5975 1988 - heute

LC/MSD Series 1997-2005

Ion Trap Series 2000-heute

ESI-TOF Series 2003-heute

6100 Single Quad 2006, 2007

6000 Series 2006-heute

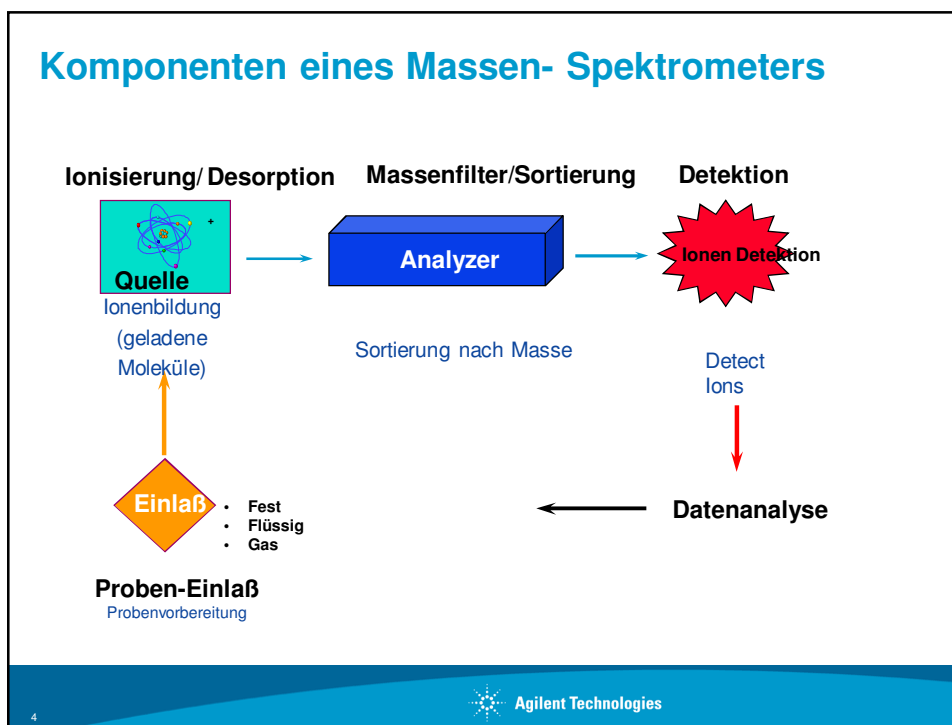
4500, 7500 Series ICP/MS 1994-Present

6410 Triple Quad 2006, 2007

6510, 6520 Q-TOF 2006, 2007

Page 3

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Ionisierung

GC-MS

Analyt ist bereits gasförmig
Ionisierung im Vakuum

Elektronen(stoß) Ionisierung (EI)
Chemische Ionisierung (CI)

LC-MS

Analyt ist gelöst (flüssig)
Ionisierung unter Normaldruck

Electrospray Ionisierung (ESI)
Chemische Ionisierung (APCI)
Weitere Methoden....



Analyt muss:

- in die Gasphase gebracht werden
- ionisiert werden
- ins Hochvakuum des MS überführt werden

5

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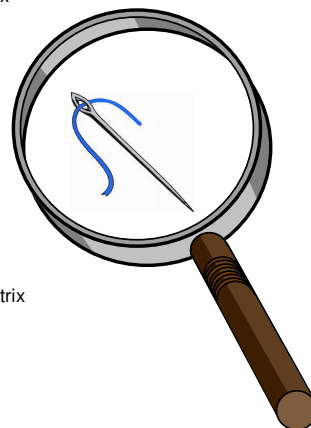
Warum MS/MS ?



Einfache Matrix



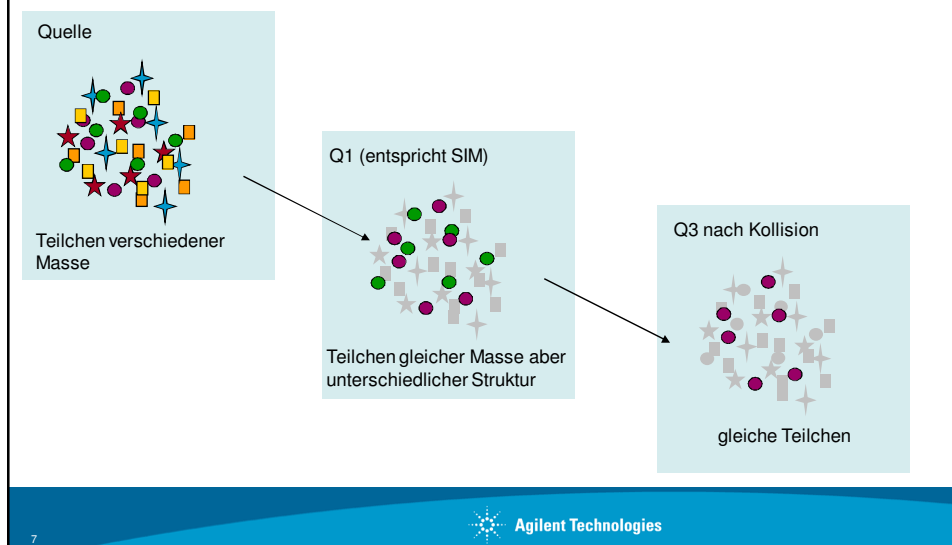
Komplexe Matrix



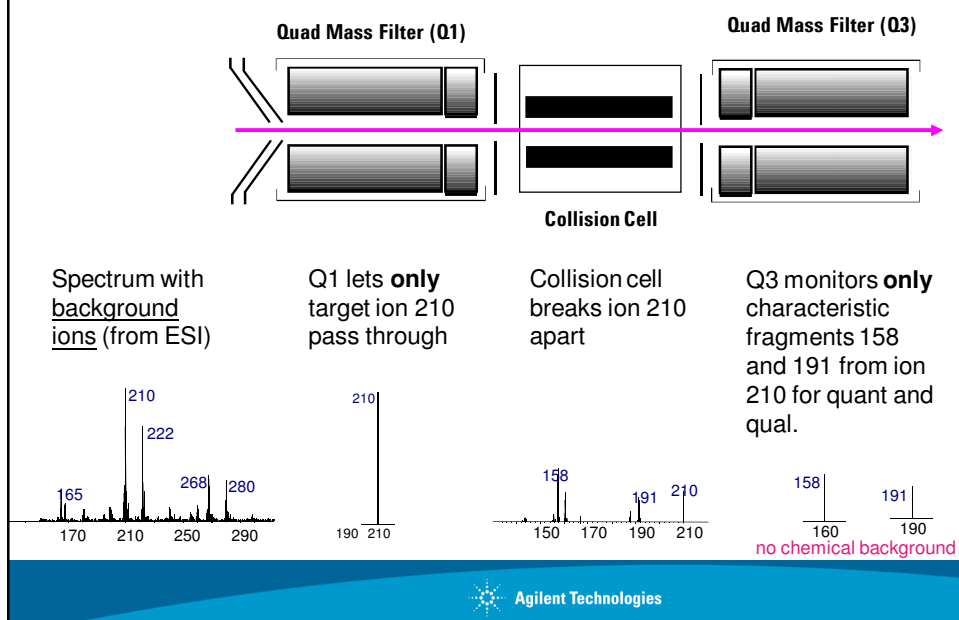
6

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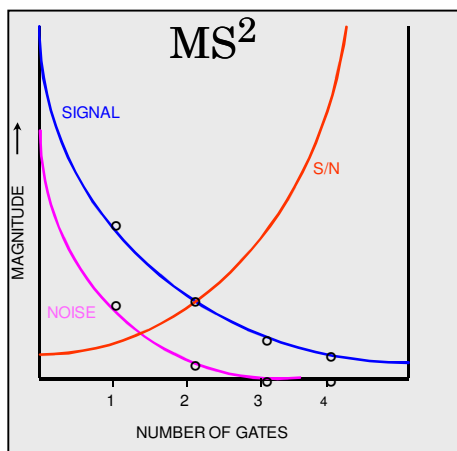
Verbesserung des Signal/Rausch-Verhältnisses → Steigerung der Empfindlichkeit



TRIPLE QUAD FUNKTION MRM (MULTIPLE REACTION MONITORING)



MS/MS: starke Zunahme des Signal/Rausch Verhältnis



Graham Cooks

-Verhältnis Signal/Rauschen:
Anstieg mit Anzahl der
analytischen "Schritte"

z.B.:

1=GC, 2=GC/MS, 3= GC/MS/MS

-Signal und Rauschen
(chemisches Rauschen der Matrix)
Abnahme mit Anzahl der "Schritte"

-Rauschen erfährt stärkere
Abnahme als Signal

-Resultat: Exponentielle Zunahme
vom Signal/Rauschen-Verhältnis

From: Busch K.L., Cooks G. in "Tandem Mass Spectrometry"
Ed. Mc Lafferty Wiley, N.Y. 1983, 11-39

9

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Warum wechseln von MS zu MS/MS?

Die Analyten sind dieselben (MS oder MS/MS)

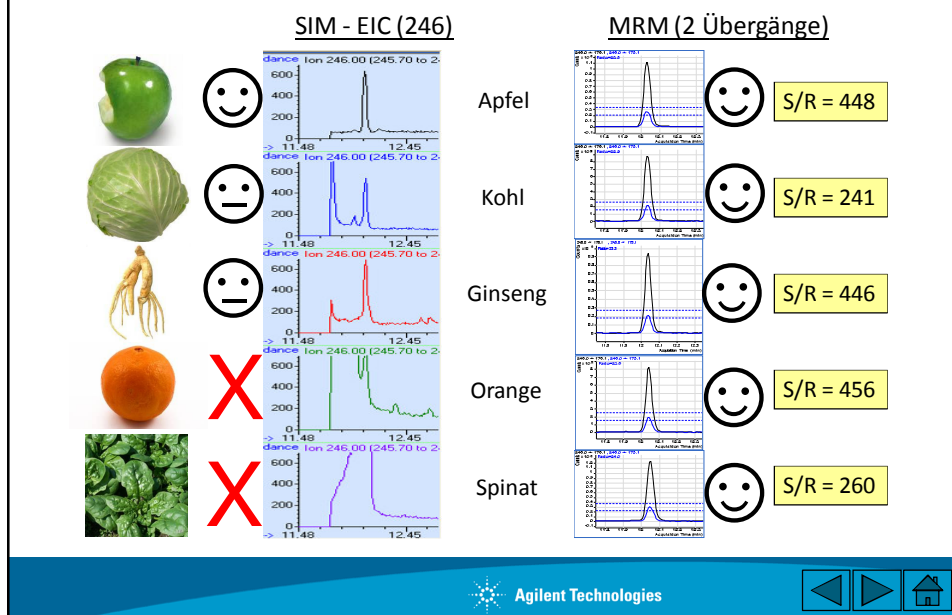
**Der Wechsel wird veranlasst durch
DIE MATRIX**

Die MS/MS-Selektivität ermöglicht den
konsistenten NACHWEIS von SPUREN
in einem weiten Bereich von Matrices

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Der gleiche Analyt, aber sehr unterschiedliche Matrices Vergleich zwischen SIM und MS/MS: Nahrungsmittel-Sicherheit



MS/MS ermöglicht den Nachweis kleinster Mengen in auch in komplexer Matrix.

Die Triple-Quadrupol Technologie ermöglicht den parallelen Nachweis einer Vielzahl von Analyten.

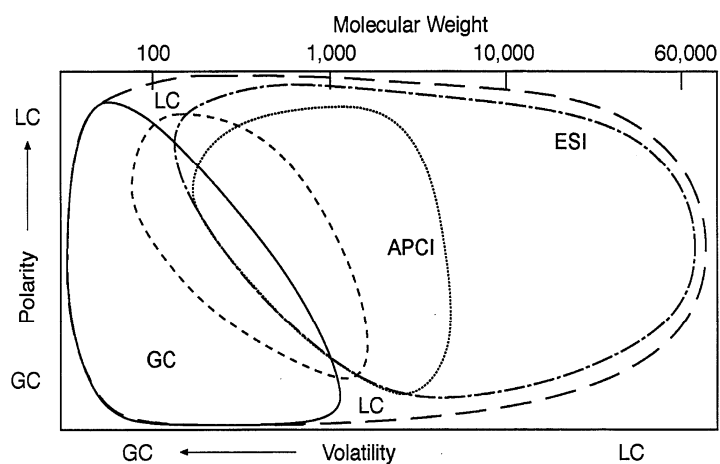
Die Entscheidung, ob GC/MS/MS oder LC/MS/MS die bessere Methode darstellt hängt von neben der chemischen Struktur der Analyten auch von der gewünschten Art der Probenvorbereitung sowie der Matrix ab.

Anwendungsbereiche GC/MS und GC/MS/MS im Vergleich zu LC/MS and LC/MS/MS?

13

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MS Applikationen: Einfluss von Polarität, Molekulargewicht und Flüchtigkeit



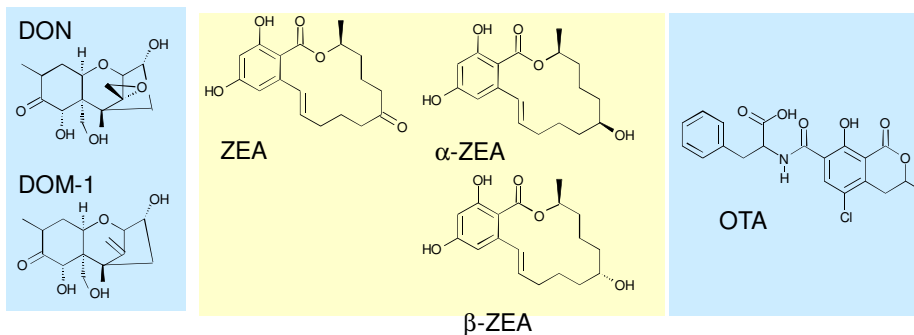
O.D. Sparkman and F.E. Klink, "Chromatography/Mass Spectrometry: Principles and Practice", American Chemical Society Continuing Education Courses, 2001.

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14

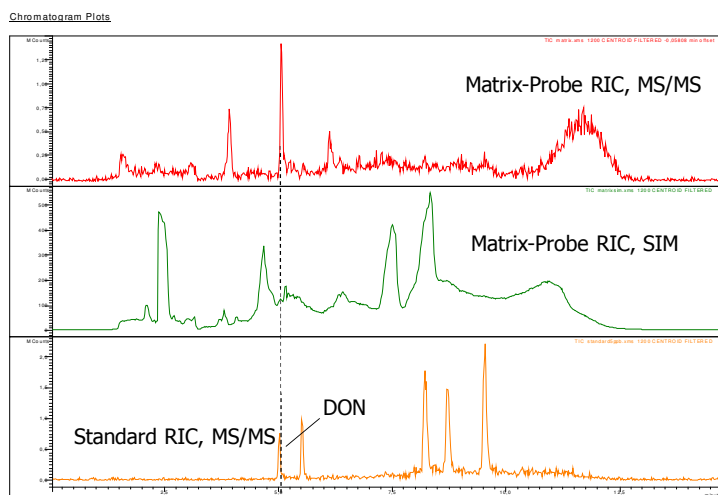
Mycotoxine

- Mycotoxine sind Sekundärstoffwechselprodukte von (Schimmel)-Pilzen.
- Häufig betroffen sind Getreide und Mais (aber auch Nüsse, Kaffee und andere Früchte).
- Einige dieser Gifte entstehen bereits auf dem Feld wie Deoxynivalenol (DON) oder Zearaleon (ZEA), andere hingegen, wie z.B. Ochratoxin A (OTA), erst bei der Lagerhaltung.
- Sie stellen ein starkes Problem in der Nahrung sowie in Futtermitteln dar.



15

Vergleich SIM : MS/MS Matrix: Schweineurin



16

Probenvorbereitung GC/MS

Amphetamine im Urin mit GC/MS

- Aliquot samples.
- Adjust pH with KOH and add KHP buffer solution.
- Heat 15 minutes @ 50-60C with 0.15M Na₂IO₄.
- Clean up samples via SPE.
- Derivatize samples ~1 hr.
- Transfer samples to vials.
- Inject samples onto GC, runtime 9.0 minutes.
- Linear Range 100-5000 ng/mL.
- Initial cut-off level 500 ng/mL, confirm 250 ng/mL.

17



Probenvorbereitung LC/MS

Amphetamine im Urin mit LC/MS

- Aliquot samples.
- ~~Adjust pH with KOH and add KHP buffer solution.~~
- ~~Heat 15 minutes @ 50-60C with 0.15M Na₂IO₄.~~
- Clean up samples via SPE.
- ~~Derivatize samples ~1 hr.~~
- ~~Transfer samples to vials*.~~
- ~~Inject samples onto GC, runtime 9.0 minutes.~~
- Inject samples onto LC, runtime 6.0 minutes
- Linear Range 5-1000 ng/mL

Time Savings ~1.5 hours of sample prep, plus 3 minutes/sample! *If collecting SPE eluant directly into vials.

18



Vorteile der GC-MS(/MS)

- ◆ EI-Spektren sind sehr aussagekräftig
- ◆ große Bibliotheken von EI-Spektren vorhanden
- ◆ exzellente Reproduzierbarkeit von Retentionszeiten, hohe Trennleistung der Säulen

Vorteile der LC-MS/MS

- ◆ minimale Probenvorbereitung
- ◆ "kalte" ESI-Ionisierung für thermolabile Verbindungen
- ◆ Ionisierung auch von großen, hochpolaren Molekülen

19

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Page 20

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ÜBERSICHT DER AGILENT LC-MS SYSTEME

	SQ	TOF	QQQ	Q-TOF
Anwendung	Synthesekontrolle Reinheitskontrolle Massenbasierte Fraktionierung Quantifizierung UV inaktiver Substanzen Studium und Ausbildung	General Unknown Screening Synthesekontrolle Biomarker Discovery Forensik Strukturaufklärung	Quantifizierung	Strukturaufklärung General Unknown Screening Biomarker Discovery Metabolomics Forensik
Vorteile	Einfach Preis	einfache Methodenentwicklung (generischer Gradient) alle Informationen sind in den Daten (Forensik / Doping / Pharmaforschung)	Empfindlichkeit einfach in der Routine	einfache Methodenentwicklung alle Informationen sind in den Daten (Forensik / Doping / Pharmaforschung) umfassende Softwarepakete (Profiler / Metlin / Metabolid ID)
Nachteile		geringere Empfindlichkeit als QQQ große Datenmengen	Methodenentwicklung aufwendig Nur Targetanalyse	geringere Empfindlichkeit als QQQ große Datenmengen

NEU: 6490 TRIPLE QUADRUPOLE LC/MS

Zeptomole Empfindlichkeit!

iFunnel Technology

- A new paradigm for atmospheric ion sampling
-  10X sensitivity breakthrough for ESI
- Improves assay robustness; simplifies sample prep

Curved, Tapered Collision Cell

- Efficient ion transmission; Reduced noise
-  Compact design

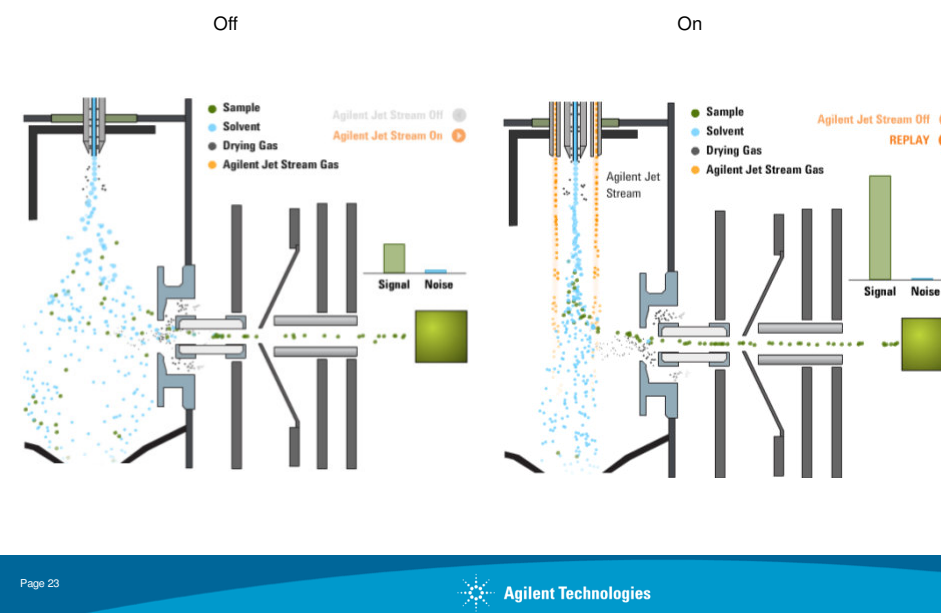
New scanning capabilities

- 0.4 m/z precursor isolation reduces interference
-  Dynamic MRM
- Data dependent scanning



6490 Triple Quadrupole LC/MS System
with iFunnel Technology

AGILENT JET STREAM



NEW iFUNNEL TECHNOLOGY

iFunnel Technology nutzt 10fach mehr Ionen

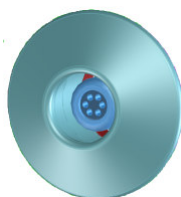
Agilent Jet Stream

- Thermische Fokussierung des Elektrospray
- Effektivere Desolvatisierung der Ionen in der Gasphase
- Erzeugt Zone mit vielen Ionen



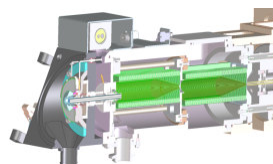
Hexabore Capillary

- 6 capillary inlets
- 10fache Anzahl der Ionen können transferiert werden



Dual Ion Funnel

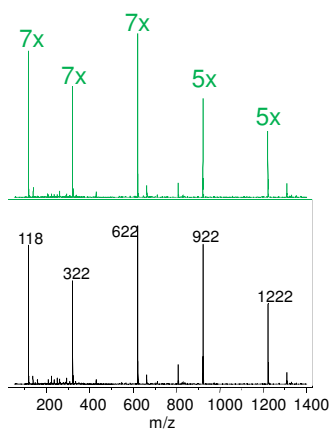
- Ionen werden gehalten, Restgas abgepumpt
- Reduktion des Rauschens
- Schont die Turbopumpe



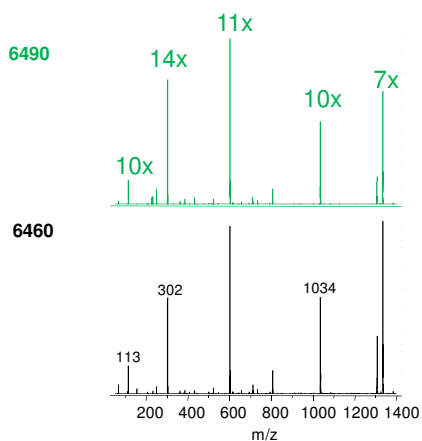
Shortcut to iFunnel_Technology_xvid.aviLink

BEISPIEL DER VERBESSERUNG

Agilent Jet Stream
positive ion



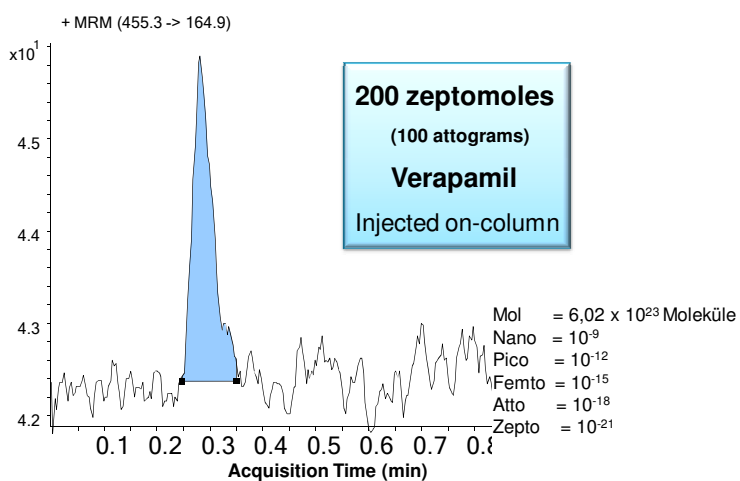
Agilent Jet Stream
negative ion



25

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6490 ERREICHT ZEPTOMOLAR DETEKTIONS LIMITS

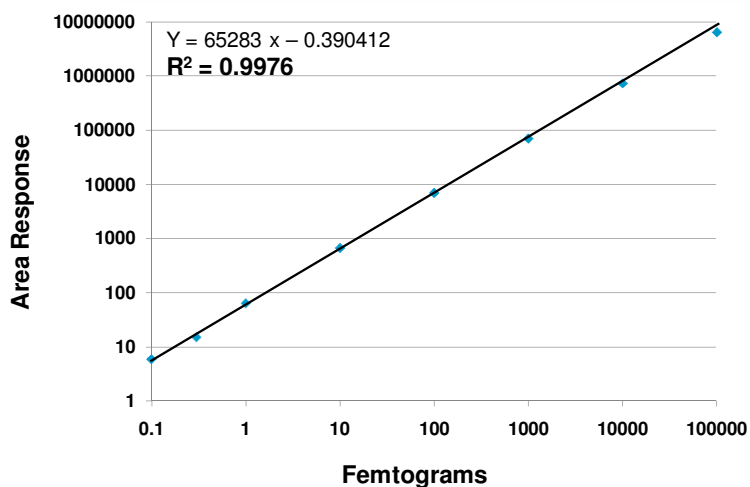


Ein Zeptomol (zmol = 10^{-21}) sind 602 Moleküle.

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UNPRECEDENTED SIX LOGS OF LINEARITY WITH 6490

100 Attogram to 100 Picogram verapamil on column



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Page 28

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**Eine Reihe von GC/MS- und GC/MS/MS-
Lösungen; entwickelt für Ihre
Arbeitsabläufe**

Hyperlinks sind
unterstrichen

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7890A/5975C GC/MSD: Die beliebtesten GC/MS-Systeme der Welt



Über 15 000
5975 Systeme seit 2005

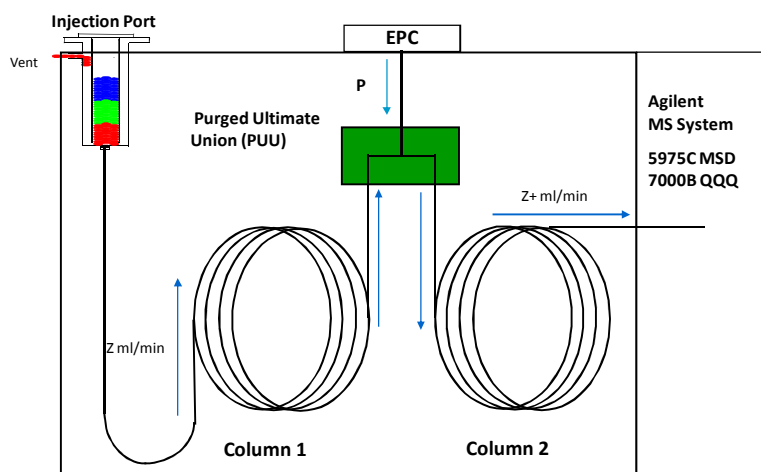
Über 50% aller in den letzten
4 Jahren verkauften GC/MS-
Systeme sind 5975 MSDs

Weltweit über 25 000 Anwender
der MSD/ChemStation

Qualität + Performance + Support = #1

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New GC/MS Backflushing Configurations

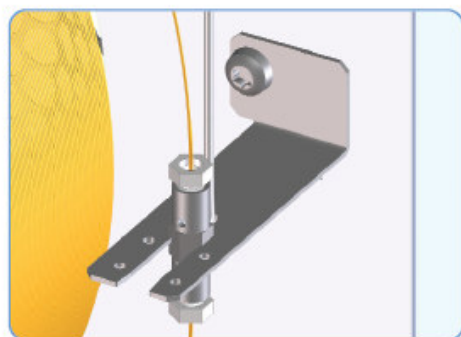


Agilent 7890A GC

Capillary Flow Technology
Research May

Agilent Technologies

Backflush: new Purged Ultimate Union



Backflush with the new Purged Ultimate Union.
This new ultra-inert, low-mass, low-dead volume device guarantees optimal peak shapes and response for the most difficult analytes.

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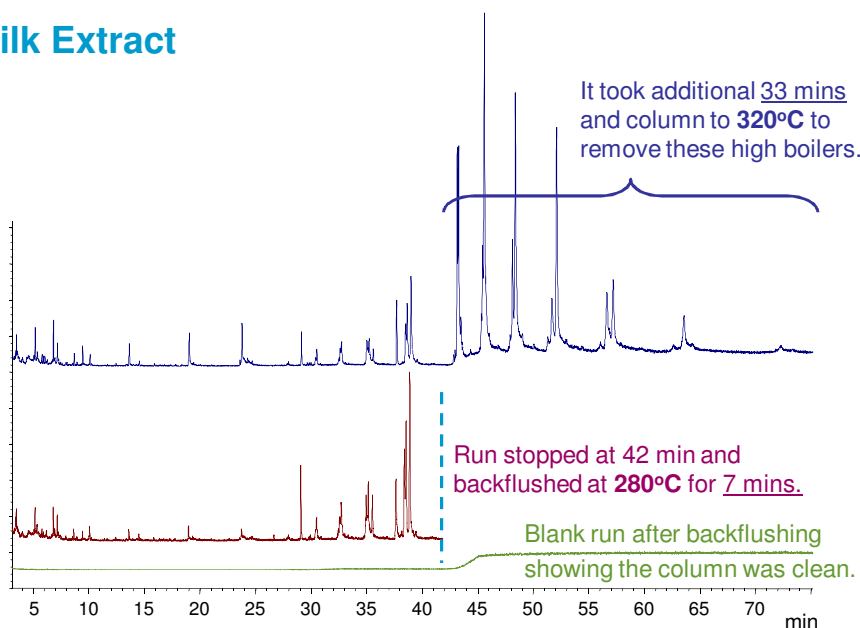
Analytical Reality of GC/MS/MS Methods

- With the selectivity of MS/MS, the **user cannot see the matrix**
 - Hundreds and even thousands of matrix peaks are “invisible” in MS/MS mode
- MS/MS users want the LOWEST detection limits, so they inject even more sample into the GC/MS/MS system with PTV in LVI mode
 - “Invisible” matrix peaks are even **MORE intense**
- Many late eluting peaks are not “chromatographically ideal” and leave a residue throughout the column
 - This residue **increases with each subsequent injection**
 - Matrix carryover increases as more samples are injected
- Heavy matrix contaminates the source faster and **sensitivity is LOST!**

Page 33

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Milk Extract

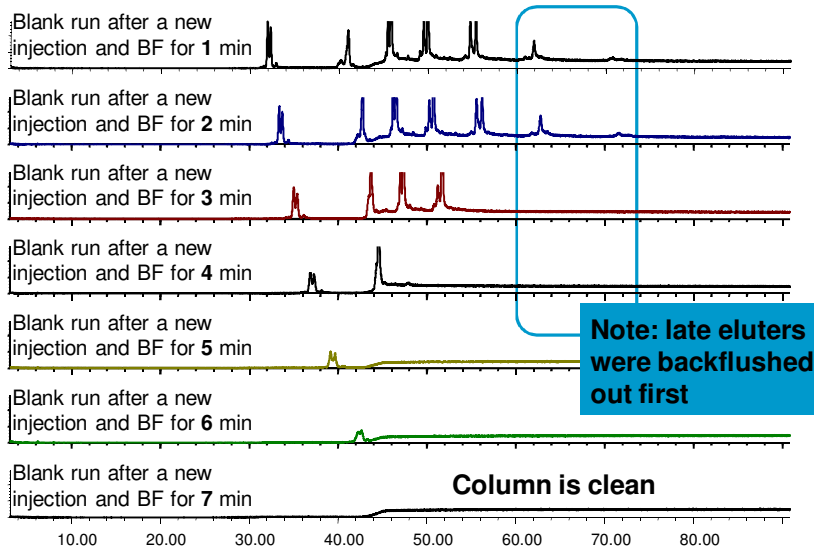


Capillary Flow Technology

Repro-Max

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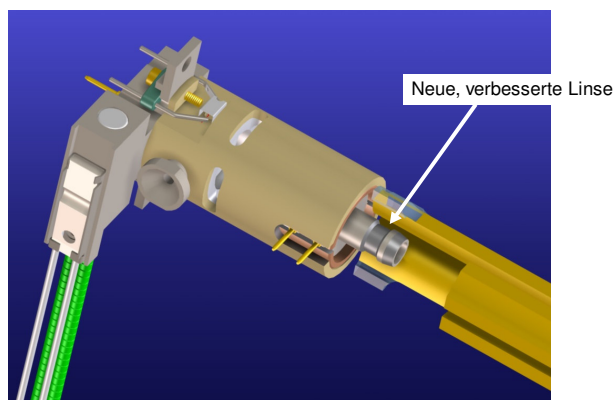
Blank Runs After Backflushing @ 60 psi



Capillary Flow Technology
Reagent-Free

Agilent Technologies

Einzigartige Eingangs-Linse ersetzt den Vorfilter



Die letzte Linse erstreckt sich in den beheizten monolithischen Quadrupol und optimiert die Kopplung der Quelle an den Analysator. Die Spannung an dieser Linse steigt synchron mit der Analysatorspannung dynamisch an. Damit wird das maximale Ionensignal für jede m/z auf das Zentrum des Quadrupol-Feldes fokussiert.

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Quarz – Gold – hyperbolisch und schön!

- Warum Quarz?
- Warum Gold?
- Warum hyperbolisch?

Viel mehr als ein schönes Stück „Glas“!



Hyperbolisch, Gold-beschichtet, aus Quarz und gesetzlich geschützt!

- **Warum hyperbolisch?**
 - Hyperbolische (NICHT RUNDE) Oberflächen erzeugen ideale Quad-Felder
 - Manche Systeme nutzen zur Kostensenkung weniger effiziente runde Stäbe
 - Optimale Transmissionseffizienz = Sensitivität (mehr Ionen beim Detektor)
 - Konsistente Massenauflösung = bessere Spektren und Isotopenverhältnisse
 - Hohe Leistung bis zum maximalen Masse/Ladung-Verhältnis (m/z) von 1050 u
- **Warum Gold?**
 - Der Bedampfung folgt die Beschichtung („bridges“ masked)
 - Exzellente elektrische Eigenschaften für Felder mit hoher Spannung (Ionen mit hoher m/z)
 - Chemische Beständigkeit des Goldes (Edelmetall)



Hyperbolisch, Gold-beschichtet, aus Quarz und gesetzlich geschützt!

• Warum Quarz?

- Niedriger linearer Ausdehnungskoeffizient (α)
 - $dL = \alpha L_0 dt$ [t = Temp. ($^{\circ}\text{C}$); dL = Längenänderung (m); L_0 = Länge bei 0°C]
- α ($\text{m/m K} \times 10^{-6}$) unterscheidet sich erheblich für verschiedene Materialien
 - Edelstahl 304: 17,3; Edelstahl 316: 16,0
 - Inconel (Ni-Legierung): 12,6; Monel (Ni/Cu-Legierung): 13,5
 - Pyrex-Glas: 4,0; Quarzglas: 0,59
- *Welches Material dehnt sich zwischen 25 und 150 $^{\circ}\text{C}$ am WENIGSTEN aus?*

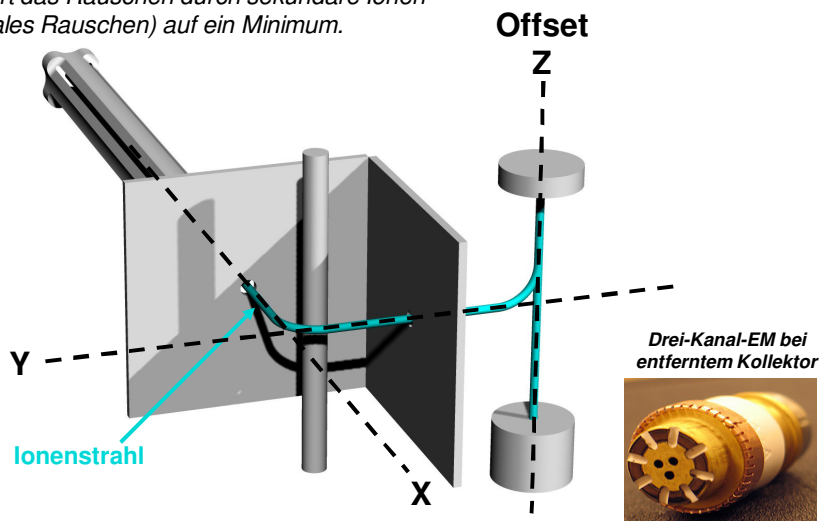
• Aber was ist der „analytische Wert“?

- Die geringe Temperatúrausdehnung hält Maße/Justierungen konstant
- Nach der Wartung kann der Quarz-Quad bei 200 $^{\circ}\text{C}$ ausgeheizt werden
- Der Quarz-Quad kann bei 150, 180 oder sogar 200 $^{\circ}\text{C}$ betrieben werden
- Hitze ist der „Freund“ der GC/MS-Methoden – für Quelle und Analysator!



Triple Axis Detektor

Die Kombination aus drei Achsen mit der entsprechenden Abschirmung reduziert das Rauschen durch sekundäre Ionen (neutrales Rauschen) auf ein Minimum.



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Page 41

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7890A-7000B GC/MS/MS: Die Marke der geprüften Hochleistungs-Funktionen

Neue hoch-empfindliche Extraktionsquelle –
höchste Arbeitstemperaturen (bis 350°C)
und die inertesten Materialien

Der einzige MS/MS der Welt mit zwei
heißen (bis 200°C) hyperbolischen
Quarz-Quadrupol-Analysatoren

Die weltweit einzige lineare
Hochdruck-Stoßkammer für MS/MS
mit „Helium-Quench“-Technik für
ultra-niedriges neutrales Rauschen

Der weltweit einzige MS/MS mit neuer
Ramped-Iris, Triple Axis HED-EM und
„Triple Channel“-EM (Dreikanal)



Sowie alle Vorteile
des 7890 GCs

Hohe Produktivität durch
MassHunter-Software für GC/MS/MS

 Agilent Technologies


7890A-7000B GC/MS/MS: Der populärste Triple-Quadrupol-GC/MS/MS der Welt

Eingeführt im September 2008

Im April 2009 mehr Verkaufs-
abschlüsse pro Monat als
jeder andere Hersteller

Im letzten Jahr über
300 Systeme verkauft

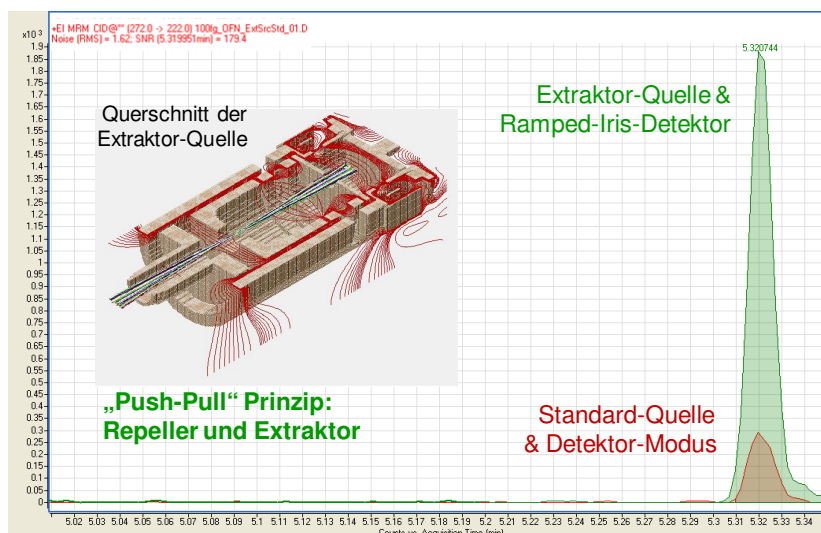


Anwender haben über die Analysen von einigen tausend
Lebensmittelproben auf Pestizid-Rückstände berichtet (viele
Arbeitsmonate) ohne jegliche Wartung an MS oder GC – mit Ausnahme
des Austauschs von Injektor-Liner, Führungssäule und Säule

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7000B: Erhöhtes Signal



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7000B GC/MS Triple-Quad-Applikationen: Typisch



- Mehrfachbestimmung von Pestizid-Rückständen in Umweltproben und Lebensmitteln
- Schnellste MRM erhöht die Genauigkeit bei quantitativen Bestimmungen von Kontaminationen im Spurenbereich
- Robuste Ionenquelle und Quadrupol-Design für maximierte Betriebszeit
- **Andere:** Drogen-, Doping-Kontrolle, PAK, PCB, Dioxine, Tiermedikamente



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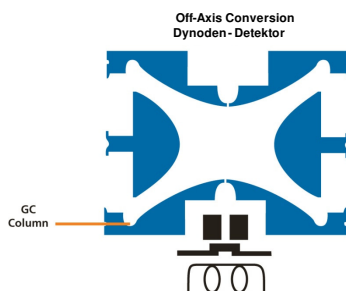
Solutions



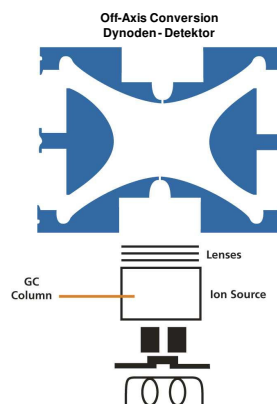
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Interne und externe Ionisierung

Interne Ionisierung



Externe Ionisierung



47



220-MS: Das System

Ein vielseitiges MS für die Routineanalyse im Spurenbereich

450-GC

- Flexibler GC
- Bis zu drei Injektoren
- Bis zu drei Detektoren

MS-Design

- Erprobt, zuverlässig
- Varian 81 L/s Turbo
- Varian DS 42 Vorpumpe
- USB Com
- Breite von 9"
- EI/CI mit 2 Filamenten
- Chrom/SilChrom-Elektroden

Jetzt mit
7890GC



Einzigartige Punkte

- Hohe CI-Empfindlichkeit
- Hohe Vielseitigkeit mit
 - EI/CI/MS/MS
 - FS/SIS/MS/MS,
 im selben Analysenlauf

MS-Eigenschaften

- Massenbereich: 10-650
- Scan-Geschw.: 5560 u/s
- Resonanz-Scan-Funktion
- Rein interne Konfiguration
- Zwei Filamente

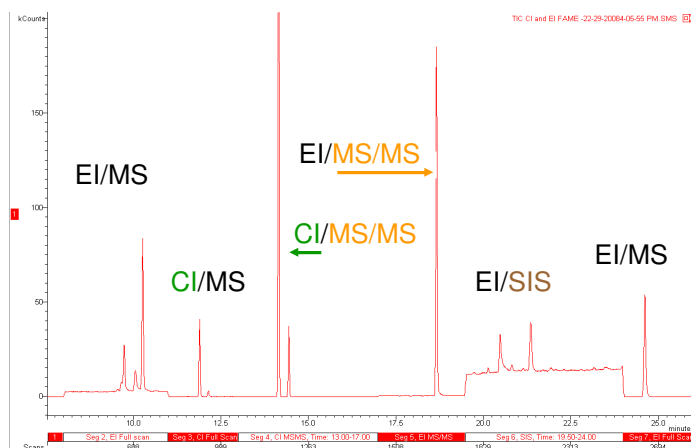
Applikationen

- VOCs und SVOCs
- Nitrosamine
- Pestizid-Rückstände
- PCBs, PAKs

48



Flexibilität – hochempfindliche CI, EI, MS/MS Alles in einem Analysenlauf



Verschiedene Ionisierungs- (EI und CI) und Scan-Optionen (Full-Scan, MS/MS und SIS) können sogar im selben Analysenlauf verwendet werden (220-MS). Dadurch wird sowohl der qualitative als auch quantitative Informationsgehalt der Ergebnisse vergrößert.

49



Agilent GC/MS-Portfolio – Zusammenfassung

Industry-leading analytical performance. Agilent confidence.



Varian GC/MS[®] Ion Trap
Information-rich detection,
unambiguous qualitative
results

- Broadest range of ionization and scanning techniques—on-the-fly EI, CI, MS/MS, MSⁿ
- Highest EI and CI full scan sensitivity
- Robust operation and extended uptime



Agilent 7000 Series Triple Quadrupole GC/MS

The only Triple Quad designed specifically for GC analyses

- High temperature inert ion source and quadrupole analyzers
- Routine femtogram-level sensitivity and superior selectivity
- Industry-leading acquisition speed up to 500 MRM transitions per second
- Integrated backflush for high throughput multi-compound applications in complex matrices



Agilent 5975 Series GC/MSD

The most successful GC/MS of all time

- Lowest limits of detection and quantitation of any Single Quad GC/MS
- Highest mass calibration stability
- Most comprehensive automation features for superior routine analyses and faster results

50



TECHNOLOGIEN UND LÖSUNGEN

Separations Technology



- 1290 Infinity UHPLC
- 12x0 Infinity HPLC
- 7100 Capillary Electrophoresis
- HPLC Chip Cube System



MS Detector Technology



- 6000 Series LC/MS/MS
- 7000 Series GC/MS/MS
- 597X GC/MSD
- Agilent Ion Trap LC/MS and GC/MS

Data Analysis / Application Software



- **MassHunter MS Software Family**
- Mass Profiler Professional w/ Pathway Analysis
- Personal Compound AMRT Databases and Libraries
- Pharma Workflows; ADME, Bioanalysis, Confirmation

Solutions



- Fast Track Solution Kits for LC, GC, LC/MS & GC/MS
- Clinical Application Offer
- More to come

Page 51

Agilent Technologies

MASSHUNTER WORKSTATION

Eine Softwareplattform für alle Agilent Massenspektrometer

- Control of Agilent 6000 Series QQQ, TOF and Q-TOF
- Control of most 1100, 1200 and 1290 HPLC modules incl. Chip-LCMS
- LC/MS Data Processing for QQQ, TOF, Q-TOF, SQ and Trap
- Control for GC/MS/MS & data processing for GC/MS and GC/MS/MS
- Control & data processing for ICP/MS



LC/MS



GC/MS



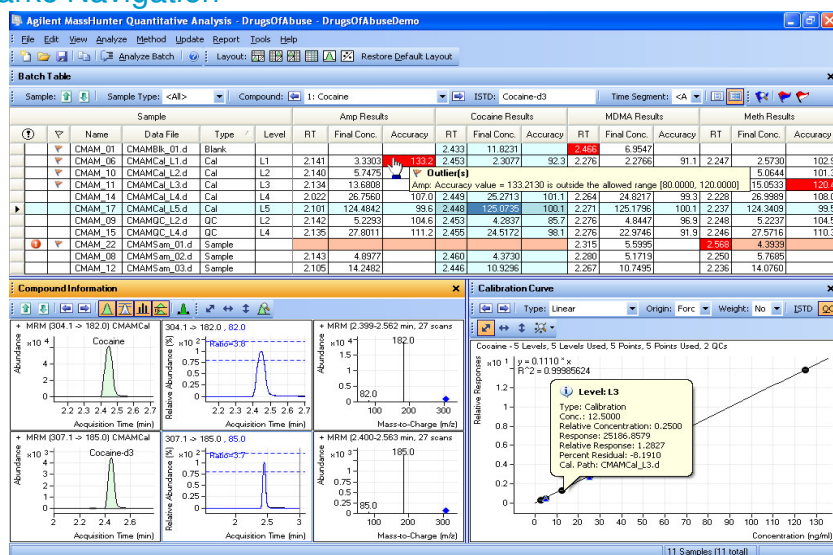
ICP-MS

Page 52

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Batchdaten auf einen Blick

Starke Navigation



Batchdaten auf einen Blick

Batchtabelle: Einzelne Komponente/mehrere Komponenten

Einzelne Komponente, Qualifier, ISTD, ISTD Qualifier

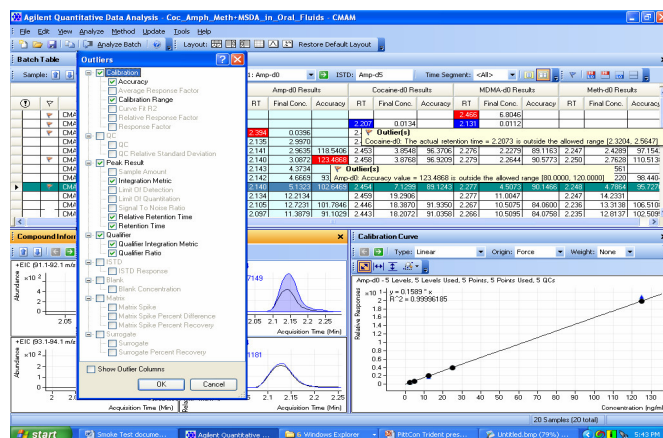
This screenshot shows a 'Batch Table' for a single component, 'Amp'. The table includes columns for Sample, Name, Type, Level, Acq. Date-Time, Exp. Conc., RT, Resp., S/N, MI, Calc. Conc., Final Conc., Accuracy, Ratio, S/N, MI, Resp., Ratio, S/N, MI, and Qualifier (119.4). The table lists several samples, including Blank, Calib-L1, Calib-L2, Calib-L3, Calib-L4, Calib-L5, QC-L2, QC-L4, and QC-L5, with their respective results.

Mehrere Komponenten

This screenshot shows a 'Batch Table' for multiple components: Amp, Cocaine, MDMA, and Meth. The table includes columns for Sample, Name, Type, Level, Acq. Date-Time, Exp. Conc., RT, Final Conc., Accuracy, RT, Final Conc., Accuracy, RT, Final Conc., Accuracy, and Meth Results. The table lists several samples, including Blank, Calib-L1, Calib-L2, Calib-L3, Calib-L4, Calib-L5, QC-L2, QC-L4, and QC-L5, with their respective results for each component.

Ausreißererkennung

- Über 20 Kriterien
- Limits in der Methode
- Flag-Marken & Filterung
- Ausreißer-Report



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MassHunter – gewinnende Vorteile zusammengefasst

- **Weniger Zeit auf die Durchsicht der Daten zu verwenden, bedeutet höheren Probendurchsatz**
 - Batchdaten auf einen Blick
 - Ausreißererkennung und -markierung
 - Parameterlose Integration geschaffen für MS Daten
- **Flexible Report-Funktionen bedeuten: „Ihre Daten, Ihr Weg“**
- **Vereinheitlichung Ihrer Agilent MS-Software**
 - Sie verwenden die MassHunter Datenverarbeitung für alle MS-Produktlinien: GC/MS, LC/MS und ICP-MS
- **MassHunter: erhöhte Produktivität für Ihre MS-Arbeitsabläufe**

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TECHNOLOGIEN UND LÖSUNGEN

Separations Technology



- 1290 Infinity UHPLC
- 12x0 Infinity HPLC
- 7100 Capillary Electrophoresis
- HPLC Chip Cube System
- 7890 GC



MS Detector Technology



- 6000 Series LC/MS/MS
- 7000 Series GC/MS/MS
- 597X GC/MSD
- Agilent Ion Trap LC/MS and GC/MS

Data Analysis / Application Software



- MassHunter MS Software Family
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- More to come

Page 57



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Additional Application Notes and Technical Overviews on Pesticide Analysis

The following is a partial library of Agilent application notes related to pesticide analysis. For a complete listing, please visit: www.agilent.com/chem

GC and GC/MS

- 5989-1335 Analysis of Organophosphorus Pesticides with Agilent 6820 Gas Chromatograph/Nitrogen Phosphorus Detector
- 5989-1334 Analysis of Carbamate Pesticides Using Agilent 6820 Gas Chromatograph/Nitrogen Phosphorus Detector
- 5989-7436 Screening for Pesticides in Food Using the Japanese Positive List Pesticide Method: Benefits of Using GC/MS with Deconvolution Reporting Software and a Retention Time Locked Mass Spectral Database
- 5989-1716 New Tools for Rapid Pesticide Analysis in High Matrix Samples
- 5989-1100 Validated Multi-Residue Method for Extraction and Analysis of Trace-Level Pesticides in Surface Water

Application Notes and Technical Overviews on Pesticide Analysis

5989-8652EN

LC and LC/MS

- 5988-5445 Creating and Using a Performance-Based LC/MSD Mass Spectral Library with NIST MS Search Software
- 5988-8595 Validated Method for the Determination of Phenyl Urea and Triazine Herbicides in Portable and Groundwater by LC/MS Using Selective Ion Monitoring
- 5988-6085 Analysis of Components, Contaminants, and Impurities in Fungicide Formulations by GC/MS and LC/MS
- 5989-5320 Determination of Pesticides in Water by SPE and LC/MS/MS in Both Positive and Negative Ion Modes
- 5989-5459 Determination of 44 Pesticides in Foodstuffs by LC/MS/MS
- 5989-7409 Superior Molecular Formula Generation from Accurate-Mass Data

58



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Webinar and Workshop



Sensitive determination of dioxins and PCBs in food and feed with the Agilent 7890/7000 GC-MS/MS



05

Speaker:
Prof. Dr. PETER FÜRST
Chemical and Veterinary
Analysis Institute
Humboldt University, Germany

[Register now](#)

Dioxins and PCBs are ubiquitous organic contaminants that are primarily present in food and feed. Because of the toxicological adverse effects on humans and animals, the determination of these compounds is required by legislation in the European Union. The LC and a number of other coupling GC/MS systems are currently being tested for the determination of dioxins and PCBs. The results demonstrate good linearity and excellent reproducibility. The results demonstrate good linearity and excellent reproducibility. The results demonstrate good linearity and excellent reproducibility.



Free webinar from Agilent Technologies. Get further details about this webinar.

[More information](#)

The results of this study indicate that the Agilent 7890/7000 GC-MS/MS system is the preferred method for the determination of dioxins and PCBs in food and feed. The results demonstrate good linearity and excellent reproducibility. The results demonstrate good linearity and excellent reproducibility.

Don't miss the date to meet with Prof. Dr. PETER FÜRST at your desktop!



Detection and Identification of Anabolic Steroids by Gas Chromatography Coupled to Tandem Mass Spectrometry



05

Speaker:
Prof. Dr. BRUNO LE BIZEC
LABERCA
Lyon, France

[Register now](#)

During this 1-hour seminar, Professor Bruno LE BIZEC presents the use of the Agilent 7890/7000 GC-MS/MS system for the detection and identification of anabolic steroids. The results demonstrate good linearity and excellent reproducibility. The results demonstrate good linearity and excellent reproducibility.



Free webinar from Agilent Technologies. Get further details about this webinar.

[More information](#)

LABERCA uses the 7890/7000 GC-MS/MS system with Agilent's unique GC/MS/MS technology for a robust detection and identification of anabolic steroids. The results demonstrate good linearity and excellent reproducibility. The results demonstrate good linearity and excellent reproducibility.

Don't miss the date to meet with Prof. BRUNO LE BIZEC at your desktop!

Session will be broadcast live on Thursday, February 17th, 2011 at 14:00 GMT (United Kingdom) 15:00 CET (Central Europe)

[Register Now >>>](#)



Follow Up Workshop
LC/MS/MS Determination of
Marine Toxins in Seaweed
European Dairy Center, Wageningen
February 22nd - 23rd

05

Speaker:
John LE
THOMAS-BAKER
ANALYTICAL
February 22nd - 23rd

[Register now](#)

Many thanks again for attending the Webinar "Determination of Anabolic Steroids in Seaweed with LC/MS/MS". One of the main reasons for your presence at this webinar is the opportunity to meet with John LE THOMAS-BAKER in person at the European Dairy Center in Wageningen, Germany, on February 22nd - 23rd.

You will have the opportunity to meet with John LE THOMAS-BAKER in person at the European Dairy Center in Wageningen, Germany, on February 22nd - 23rd. The results demonstrate good linearity and excellent reproducibility. The results demonstrate good linearity and excellent reproducibility.

Agenda:

9:00-10:00 Welcome

10:00-10:15 John LE THOMAS-BAKER

10:15-10:30 Determination of LC/MS/MS with HPLC and general

10:30-10:45 Determination of LC/MS/MS with HPLC and general

10:45-11:00 Determination of LC/MS/MS with HPLC and general

11:00-11:15 Determination of LC/MS/MS with HPLC and general

11:15-11:30 Determination of LC/MS/MS with HPLC and general

11:30-11:45 Determination of LC/MS/MS with HPLC and general

11:45-12:00 Determination of LC/MS/MS with HPLC and general

We are looking forward to welcoming you in Wageningen to share our experiences and knowledge for the next few days.

Dioxins

Steroids

Marine Toxins

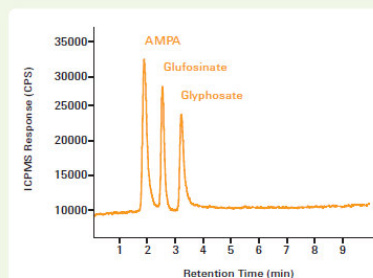
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„Roundup“ by LC ICP-MS

Glyphosate, Glufosinate and AMPA— Rapid detection without derivatization

Glyphosate (Roundup®) and the related compound Glufosinate are among the most widely used of non-selective herbicides.

When coupled with ion-pairing HPLC, the Agilent 7500cx ICP-MS with Octapole Reaction System (ORS) technology offers superior detection capability—without the need for derivatization—for phosphorus-containing herbicides and their metabolites.



	AMPA	Glufosinate	Glyphosate
Regression coefficient	0.999	0.998	0.999
LOD (concentration)	25 ppt	27 ppt	32 ppt
LOD (amount)	2.5 pg	2.7 pg	3.2 pg
RSD, retention time, n=8	1.1 %	0.8 %	1.2 %

5899-8652EN



**Roundup-Einsatz als Alternative zur
Mahd in einer Apfelplantage in Südtirol**

Quelle:
<http://de.wikipedia.org/wiki/Roundup>

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GC/MSD Pesticide Analyzer	Triple Quadrupole GC/MS Pesticide Analyzer	Triple Quadrupole LC/MS Pesticide Application Kit	TOF and QTOF LC/MS Pesticide Application Kit
Workflow Solution	Technologies	Tools	Application Notes
		Ordering Information	Contact Us

Triple Quadrupole LC/MS Pesticide Application Kit

Quickly and efficiently implement target screening methods

Minimize the need for tedious manual method development with pretested methods and a Dynamic MRM database
Analyzing pesticide residues in food and environmental samples is challenging. Large numbers of compounds, many at low concentrations, must be monitored and quantitated. To complicate matters, method development is labor-intensive and time-consuming, due to compound-dependent parameters that must be optimized.

A faster, easier way to develop customized screening methods
Agilent's Pesticide Screening Dynamic MRM Application Kit is truly unique, because much of the development work has already been completed. The kit features easy-to-use examples that show you how to set up screening methods and quickly adapt them to your specific needs. It also includes:

- A more than 750-Pesticide Dynamic MRM database that includes compound names, MRM transitions, fragmentor voltages, collision energies, and retention times for each database compound for reliable pesticide screening.
- Pretested analysis methods, using the Dynamic MRM database, are provided for target screening of pesticides that are routinely monitored around the world.

The following components are included – saving you time and money

- Pesticide Dynamic MRM database
- Positive and negative ion pesticide test mixes
- Agilent ZORBAX Eclipse Plus C18 column (2.1 mm × 50 mm × 1.8 μm)
- Promotional QuEChERS sample preparation kit
- Quick-start guide and Application Note that show you how to run the test mixes and create dynamic MRM methods
- CD-ROM with examples of screening methods, data files, and reports



61

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What is included in the GC/MS Pesticide Analyzer



Instrument (HW, SW, Database ordered separately)



Factory pre-configured + pretested on customer instrument

Column, consumables, checkout mix
Sample prep QuEChERS Trial pack
DVD with method parameters and factory checkout data
Document Set
Advanced features video tutorials

Duplicate factory checkout on customer site by advanced, solution trained customer engineer (CE).

Pesticide Analyzer	Pesticide Analyzer	Pesticide Application Kit	Pesticide Application Kit
Workflow Solution	Technologies	Tools	Application Notes
			Ordering Information
			Contact Us

Triple Quadrupole GC/MS Pesticide Analyzer

A ready-to-use system for multiresidue pesticide analysis

Fully configured and factory chemically-tested analyzers make it easy to perform sensitive, multiresidue GC/MS analyses in complex matrices

Based on Agilent's 7890A GC and 7000 Series Triple Quadrupole GC/MS, these GC/MS/MS Pesticide Analyzers feature excellent sensitivity and exceptional area precision even at a dwell time of 1 millisecond, and an acquisition speed of 500 transitions per second, all with zero crosstalk between transitions. They also include Capillary Flow Technology (CFT) backflush for superior selectivity, trace sensitivity, and robustness during routine operation.



Two ready-to-use GC/MS/MS Pesticide Analyzers give you ultimate performance and flexibility

The SP1 07890-0501 GC/MS/MS Analyzer lets you add GC detectors, and is easily scaled for shorter runtimes. It includes a method based on Agilent's Retention Time Locked (RTL) GC/MS/MS MRM database (500+ pesticides), set at constant pressure mode with post-column backflush.

The SP1 07890-0502 GC/MS/MS Analyzer delivers top performance, shorter analysis cycle times, and reduced carrier gas consumption. It features a method based on the USA Targeted Pesticide List RTL GC/MS/MS MRM database (200+ pesticides), set at constant flow mode with mid-column backflush.

The following components are included – saving you time and money

- Pesticide checkout samples
- Retention Time Locked HP-5MS Ultra Inert column for reliable peak identification and quantitation
- Promotional QuEChERS sample preparation kit
- Quick-start guide and Application Note that show you how to set up the identification and quantitation method provided with the Analyzer
- Acquisition method and MRM pesticide database
- CD-ROM with examples of screening methods, data files, and reports

http://www.chem.agilent.com/en-US/Products/Instruments/ms/Pages/pesticide_triplequad_gcms_ws.aspx

63  Agilent Technologies

Agilent Analyzers and Application Kits



GC/MSD Pesticide Analyzer

Simplify and accelerate your pesticide screening

The following components are included with Agilent's Pesticide Analyzer – saving you time and money.

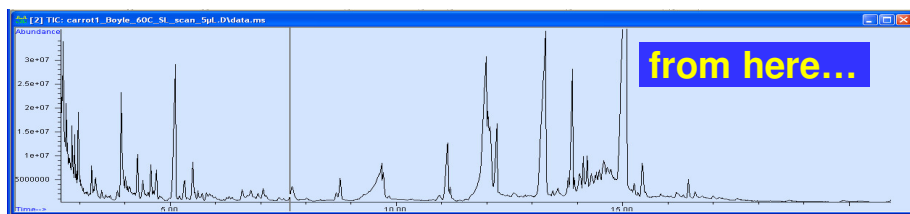
- Pesticide checkout samples
- Retention Time locked HP-5MS column ensuring reliable database matching
- Free-trial QuEChERS sample preparation kit
- Video training tutorials for easy learning of more advanced Analyzer features
- Quick-start guide and Application Note that show you how to run the screening method provided with the Analyzer
- CD-ROM with analysis methods, data files, and report

Ordering information: Order an Agilent 5975C Series GC/MSD along with an Agilent 7890A GC system with one of the following options:

- SP1 7890-0456: Pesticide DRS Screening GC/MSD Analyzer
- SP1 7890-0457: Japanese Positive List DRS Screening GC/MSD Analyzer

64  Agilent Technologies

Agilent Pesticide Analyzer:



Screen for 926
pesticides in
one 21-minute
GC/MS run

MSD Deconvolution
Sample Name: carrot
Data File:
Date/Time: 2:45:59 PM Thursday, February 19, 2009

...to here in 2 - 3 min

Sensitivity = medium
Shape Requirements = Medium

The NIST library was searched for the components that

R.T.	Cas #	Compound Name	Chem station	Amount (ng)	AMDIS Match	R.T. Diff sec.	Reverse Match	Hit Num.
4.4196	33704619	Cashmeran		13.59	60	13.1	67	35
6.9401	1517222	Phenanthrene-d10		35.96	24.68	92	9.2	79
8.0245	84695	Diisobutyl phthalate		16.19	9.88	83	9.2	81
9.27	84742	Di-n-butylphthalate		61.5	23.38	95	7.5	92
12.138	72559	p,p'-DDE		6.15	3.52	87	15	82
12.9476	72548	p,p'-DDD		2.6	1.55	69	12.5	77
12.954	789026	p,p'-DDT		2.6				
13.5916	50293	p,p'-DDT		2.85	1.33	70	12	71
13.9963	115866	Triphenyl phosphate		15.11	9.18	95	16.1	84
14.9048	117817	Bis(2-ethylhexyl)phthalate			4.46	56	9.6	64
14.99	2385855	Mirex		1.38				
6.943		Phenanthrene-d10		10				

Page 65



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Analyzers and Application Kits

Supply Modified 7890-0468 for Headspace Sampler

Supply modified 7890-0467 Greenhouse Gas Analyzer with Oxygen/Nitrogen Separation

Supply Greenhouse Gas Analyzer with the Detection of 0.4 PPM to 20% Carbon Dioxide , 0.2 PPM

Supply Greenhouse Gas Analyzer with the Detection of 0.4 PPM to 0.2% Carbon Dioxide , 0.2 PPM

Supply Fast Greenhouse Gas Analyzer

Semivolatle Compounds DRS Screening GC-MS Analyzer

Pesticide DRS Screening GC-FPD-uECD-MS Analyzer

Pesticide DRS Screening GC/MSD Analyzer

GC/MS/MS Pesticide Analyzer w. Const. Press, Post Col. BF Method

GC/MS/MS Pesticide Analyzer w. Const. Flow, Mid Col. BF Method

GC/MS/MS PAH Analyzer w. Const. Flow, Post Col. BF Method

MassHunter Pesticide Personal Compound Database Kit.

MassHunter Pesticide DMRM Database Kit.

66



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Pesticides Analysis Compendium, Free

http://www.chem.agilent.com/en-US/Products/Instruments/ms/Pages/pesticide_gcmsd_contact.aspx

Identify and confirm pesticides in difficult matrices

Literature Library

Technical Support

Education & Events

GO.

Identify and confirm pesticides in difficult matrices

The pressure to meet stringent safety standards, regulations, and expectations for pesticide analysis has never been greater. As an industry leader with over 40 years of experience, Agilent is uniquely positioned to help you increase analysis speed, improve sensitivity in food and environmental matrices, and simplify data review.

With Agilent Analyzers and Application Kits, you can spend less time on method set-up and instrument configuration, and *more time* identifying pesticides in water, soil, and food.

FREE Compendium



Order your DVD now!

Get our **Pesticides Analysis Compendium**, FREE. A comprehensive collection of over 80 Application Notes and resources specific to pesticides analysis.

**GC/MSD
Pesticide Analyzer**

Triple Quadrupole GC/MS
Pesticide Analyzer

Triple Quadrupole LC/MS
Pesticide Application Kit

TOF and QTOF LC/MS
Pesticide Application Kit

Workflow
Solution

Technologies

Tools

Application
Notes

Ordering
Information

Contact Us

* required field

☐ Please send me the new pesticides analysis compendium DVD (5990-6506EN)

67

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Pesticides Workflow

Sample Prep	Instrument Options	Screening	Confirmation	Quantification
QuEChERS  Extraction  Clean-up	GC/MS <i>Target and non-target, volatile and semi-volatile compounds</i> 	- Backflushing improves retention time precision, eliminates ghost peaks, shortens cycle time - Rapid screening for 927 pesticides in a single injection without oven bakeout	- Automated Deconvolution Reporting Software (DRS) saves hours of data analysis time with fully integrated deconvolution results - Raw, deconvoluted and full spectra displayed for easy review and more confidence	- SIM/Scan capability allows spectral acquisition and high sensitivity quantification in a single injection - Trace Ion Detection (TID) lowers detection limits in complex matrices
	LC/QQQ <i>Target polar or moderately polar compounds</i> 	- Highly selective, sensitive detection of hundreds of compounds in a single injection - Low detection limits in complex matrices	- MRM provides positive confirmation and low detection limits to meet all regulatory requirements - One-run screening and confirmation	- Routine high accuracy MS/MS quantification - Batch-at-a-Glance for fast review of quantification results
	LC/Q-TOF or LC/TOF <i>Non-target polar or moderately polar compounds</i> 	- High resolution reduces noise and matrix interference - Accurate mass provides added compound selectivity and unlimited screening using exact mass databases	- Automated accurate-mass searches against public and private databases - Molecular Formula Generator feature reduces data interpretation time	- Very narrow mass window extracted ion chromatograms provide accurate MS and MS/MS quantification - High dynamic range to quantify wide range of concentrations

68

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Vielen Dank für Ihre Aufmerksamkeit