

# NOVEDADES EN CROMATOGRAFÍA Y ESPECTROMETRÍA DE MASAS

# Gama de productos



- Cromatografía de gases (GC)
- Cromatografía de líquidos (HPLC)
- Cromatografía de gases acoplada a espectrometría de masas (GCMS & GCMSMS)
- Cromatografía de líquidos acoplada a espectrometría de masas (LCMS & LCMSMS)
- Extracción y cromatografía de fluidos supercríticos
- Espectrómetros de masas tipo MALDI



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2

# Gama de productos

FTIR



UV



RF



GC



HPLC



AAS / ICP



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# Gama de productos

LC-MS



LC-MS/MS



GC-MS



GC-MS/MS



LCMS-IT-TOF



MS imaging



MALDI



ICP-MS



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# Novedades

- GC –Tracera – Detector BID
- HPLC – Method Scouting – Desarrollo de método
- HPLC – UFPLC – Purificación de fracciones
- SFE-SFC – Extracción & Separación por fluidos supercríticos online
- LCMS – Nueva tecnología en triples cuadrupolos
- CLAM – Preparación de muestra online automatizada
- iMScope TRIO – Imagen óptica + MS

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# Cromatografía de gases (GC) TRACERA

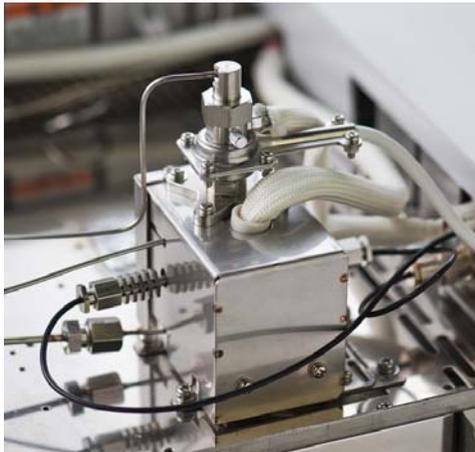
## Tracera

GC-2010 Plus +

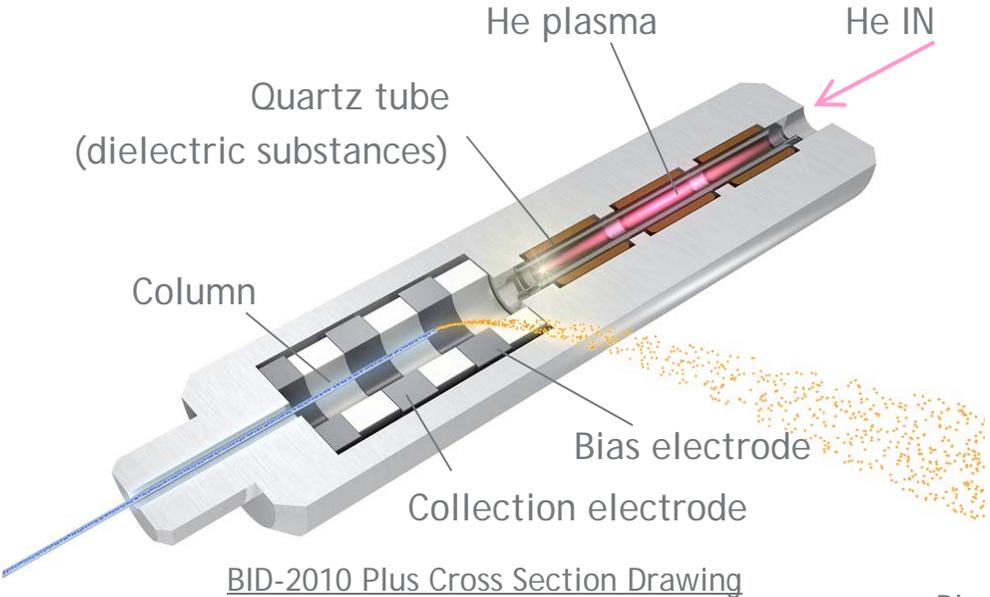
+ detector BID-2010 Plus

## BID

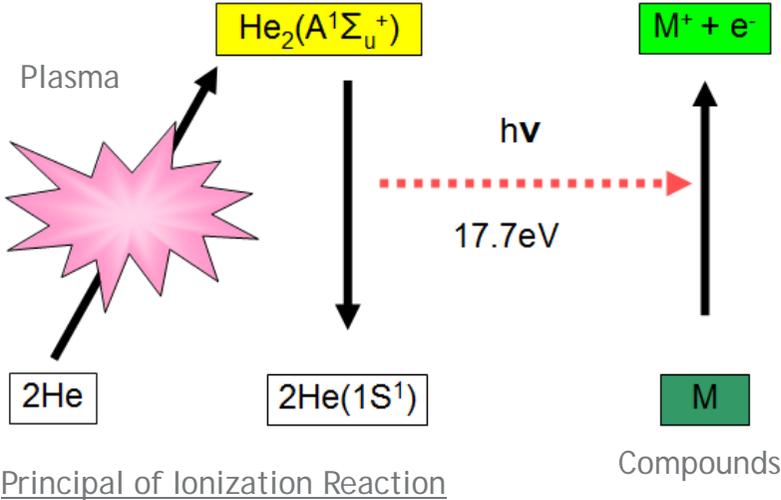
Barrier discharge Ionization Detector



# Cromatografía de gases (GC) TRACERA



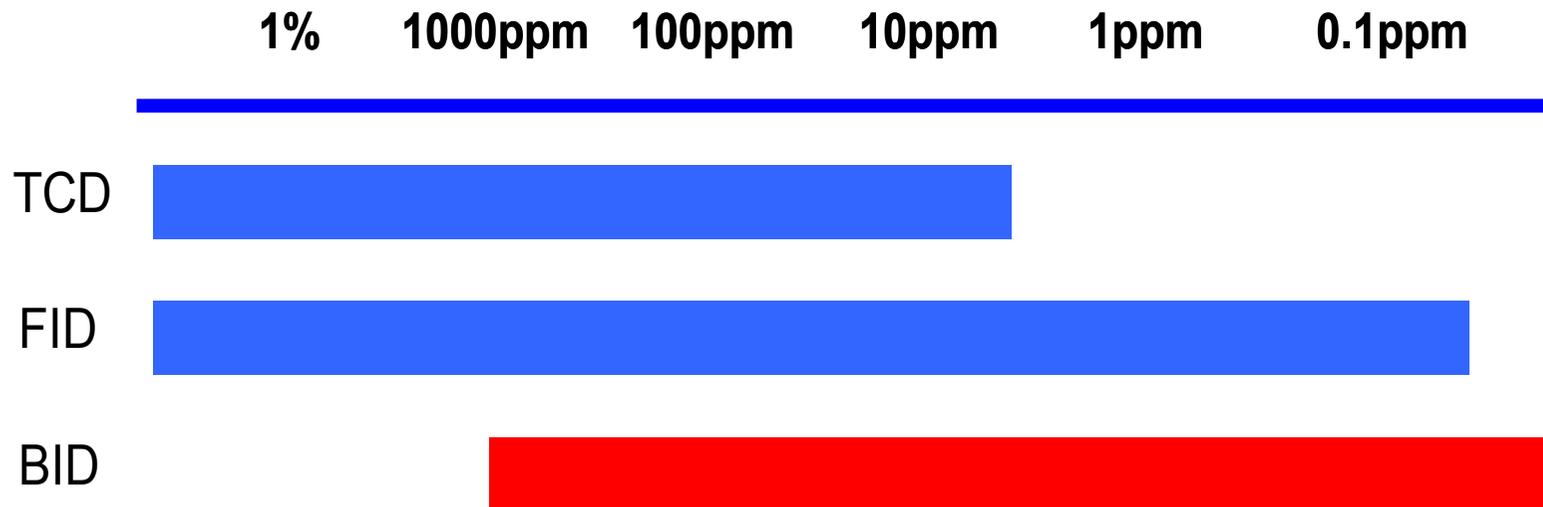
Low-temperature plasma



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# Cromatografía de gases (GC) TRACERA

## Sensibilidad de detectores clásicos vs BID

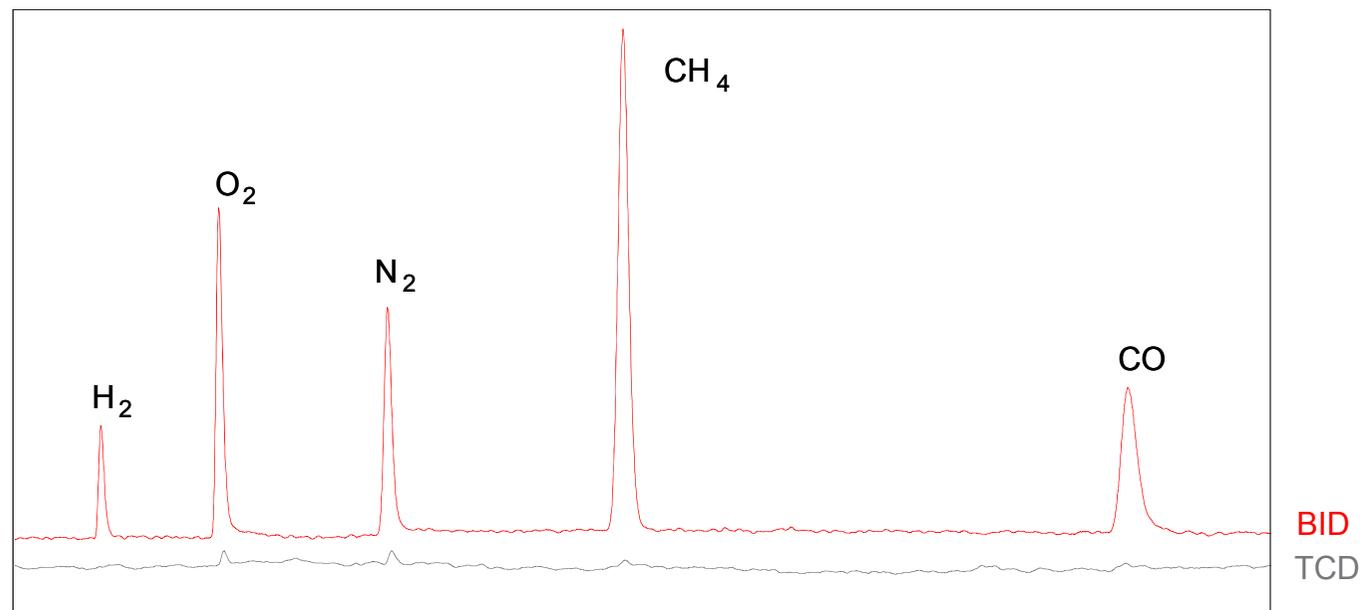


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# Cromatografía de gases (GC) TRACERA

## TCD vs BID en muestras gaseosas

El detector BID es más de 200 veces más sensible que el TCD para compuestos orgánicos y varias decenas más sensible para gases permanentes.

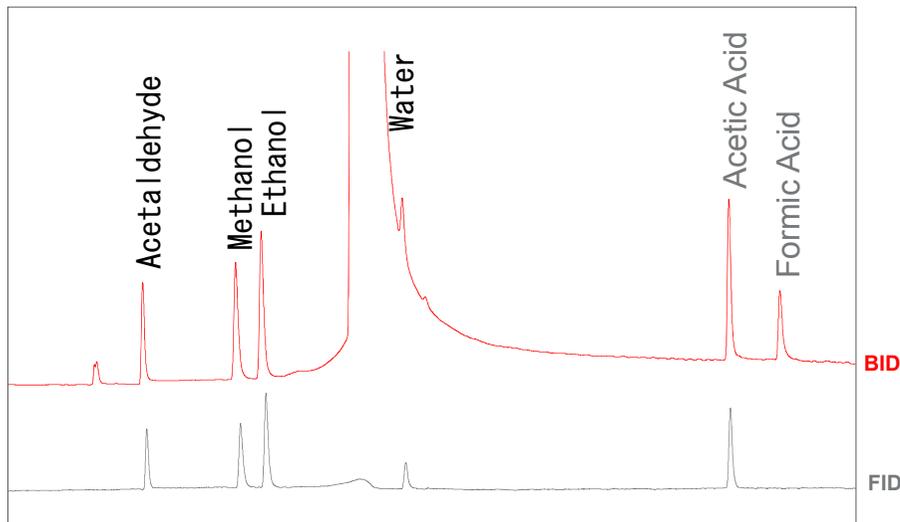


10 ppm concentration each component in He,  
1:30 split analysis, 500  $\mu$ L sample volume

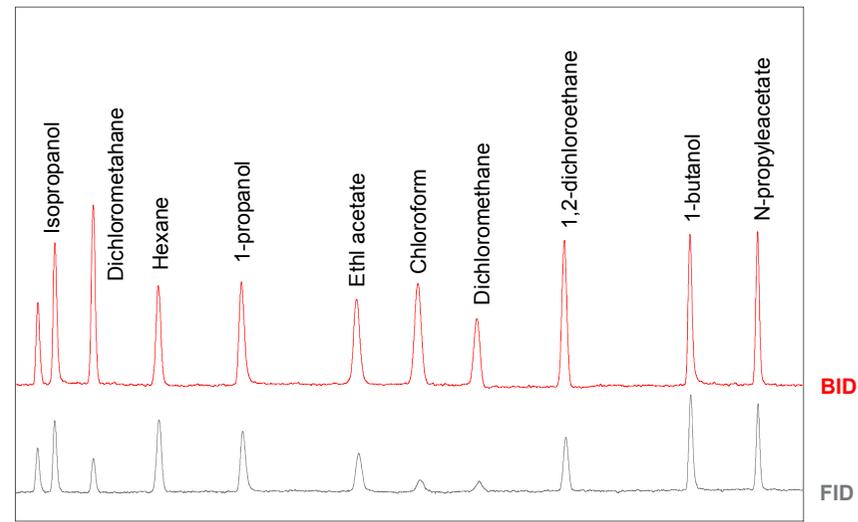
# Cromatografía de gases (GC) TRACERA

## FID vs BID en muestras gaseosas

El FID ofrece muy mala respuesta para ácido fórmico o formaldehído. Para compuestos que contienen grupos hidroxilo (-OH), aldehído (-CHO) o halógenos (F, Cl,...) ofrece una respuesta menor que para otros analitos con hidrocarburos. El detector BID ofrece buena sensibilidad para todos ellos y poca variación en su respuesta relative.



100 ppm concentration each component in water, 1:24 split analysis, 0.5  $\mu$ L sample volume



10 ppm concentration each component in n-C6, 1:29 split analysis, 1  $\mu$ L sample volume

# Cromatografía de gases (GC) TRACERA

“Greatest Innovation Award 2013”  
of the Analytical Scientist Magazine

Tracera/BID has made 4. place in the  
ranking of most innovative products 2013

Followed by:

7. LCMS 8050

13. MDGC configuration



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# Cromatografía de líquidos (HPLC)

## From HPLC to UHPLC – Extensive Lineup of Shimadzu LCs –

Shimadzu's extensive LC lineup fulfills a wide range of analytical needs, from conventional to ultra-high speed analysis. With scalable column size and packing material particle size, Shimadzu can provide an LC system most appropriate for your applications.

Packing material particle size (µm)	Conventional		Ultra-high speed/High-separation	
	10 – 3	3 – 2	– 75	– 150
Column size (mm)	~ 250	– 75	– 150	Shim-pack XR II
Typical column	Shim-pack VP	Shim-pack XR	Shim-pack XR II	Shim-pack XR III
Prominence / Prominence-i	[Bar chart showing range]			
Nexera XR / Nexera-i	[Bar chart showing range]			
Nexera X2	[Bar chart showing range]			

Shimadzu LC lineup according to column categories

Routine Analysis  
Easy Operation



### Prominence-i

The HPLC system perfect for checking synthetic compounds, quantitative testing with standard operative procedures, etc. This system is suitable for a wide range of industries, such as pharmaceuticals, chemicals, foods and the environment. It can be operated as a single-use system or a shared system. Its small footprint facilitates the management and relocation of systems.

### Nexera-i

The UHPLC system perfect for multi-analyte processing such as drug dissolution testing. Autosampler accommodates a total of 216 standard vials and features a direct access mechanism that allows the user to place the sample even during analysis.



### Nexera X2

The flagship UHPLC system supporting columns with sub-2 µm micro-particle packing materials, realizing both ultra-high speed and ultra-high separation. Excellent reproducibility of low injection volume and ultra-low carryover ensures reliable data, even with ultra-sensitive LC/MS/MS methods.

≤ 1300 Bar



### Nexera XR

The UHPLC system supporting most commercial UHPLC and HPLC columns. Superior gradient performance and minimized delay volume enable ultra-high speed analyses with excellent reproducibility. The Method Scouting System can be constituted to support more efficient method development.

≤ 660 Bar

All-round LC  
Expandability



### Prominence

The standard HPLC system with excellent expandability. It can be configured to meet a variety of analytical conditions. This system offers reduced maintenance costs while still enabling high-speed analysis by using short columns with 2 µm particles.

≤ 400 Bar

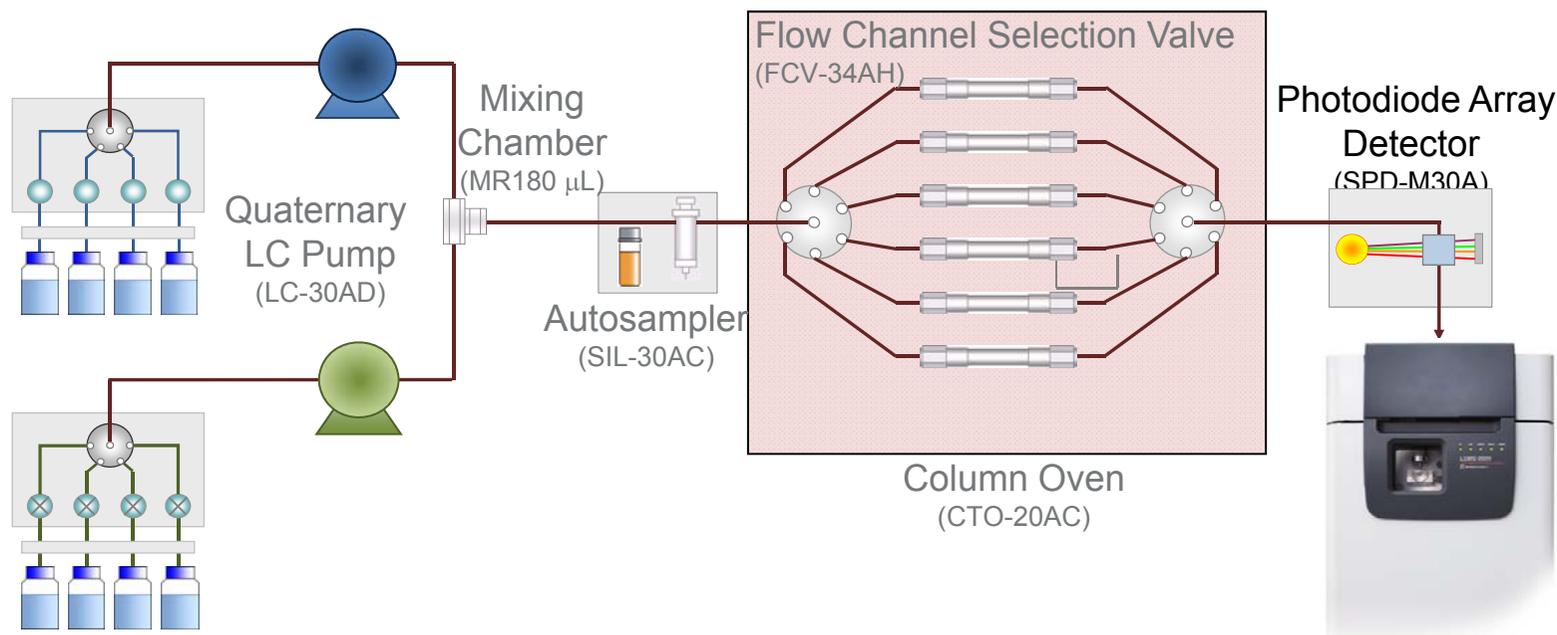
i-Series  
LC Systems

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# Cromatografía de líquidos (HPLC)

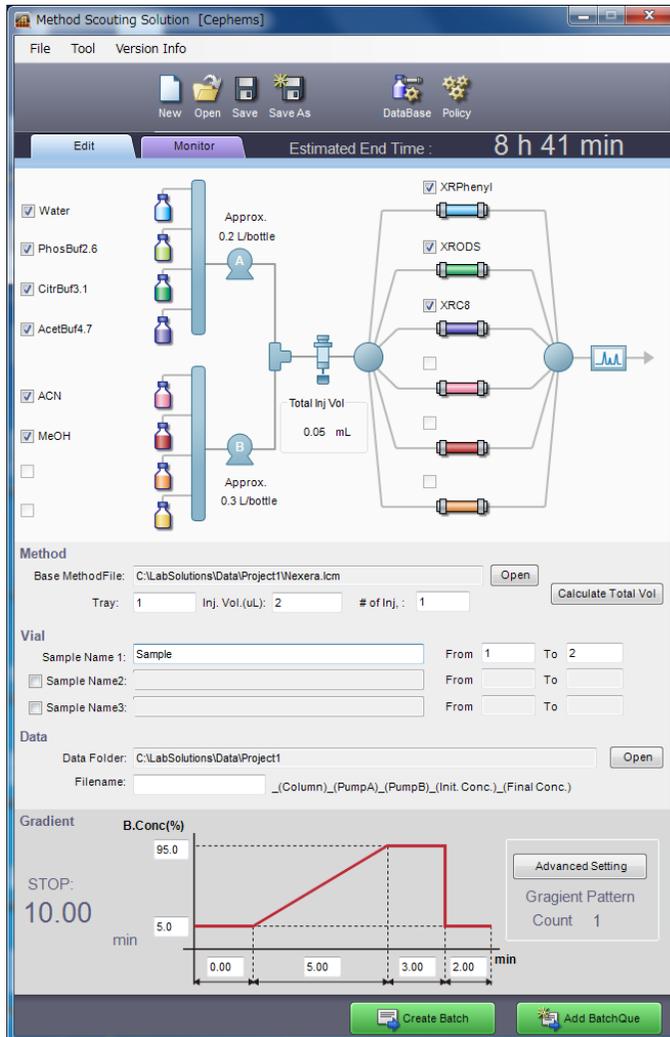
## Versatilidad / Personalización

### Method Scouting



- ▶ Capaz de manejar 6 columnas y 8 fases móviles diferentes
- ▶ Compatible con columnas de UHPLC columns (100 MPa)
- ▶ El software para Method scouting permite una fácil configuración
- ▶ Posibilidad de interactuar con el LCMS para seguimiento fiable de los picos

# Cromatografía de líquidos (HPLC) Versatilidad / Personalización



## Method Scouting

- La configuración de columnas, fases móviles, gradients y demás parámetros en un software dedicado y en una sola pantalla.
- Integrado en el software cromatográfico de tal manera que las secuencias se crean automáticamente.

# Novedades

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# Cromatografía de líquidos (HPLC) Versatilidad / Personalización



## Prominence UFPLC (Ultra Fast Preparative and Purification Liquid Chromatography)

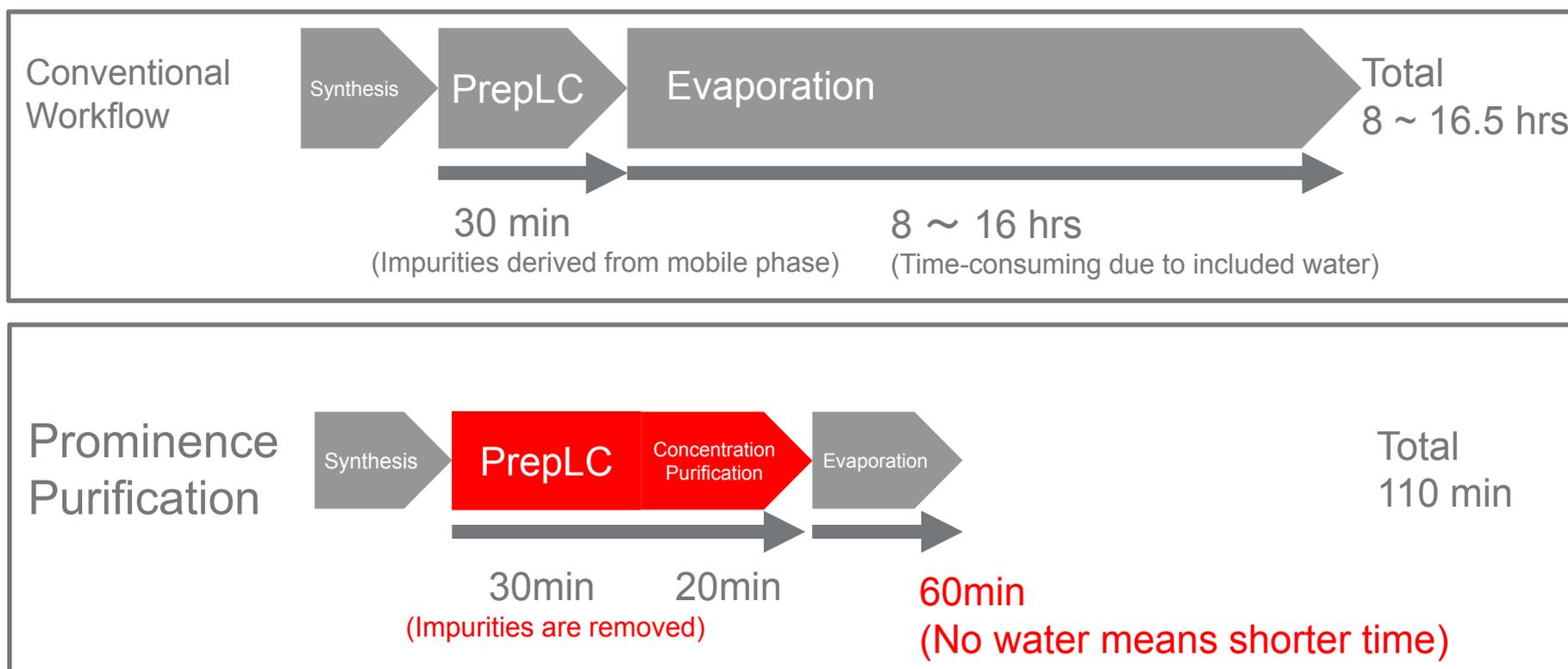


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# Cromatografía de líquidos (HPLC)

## Versatilidad / Personalización

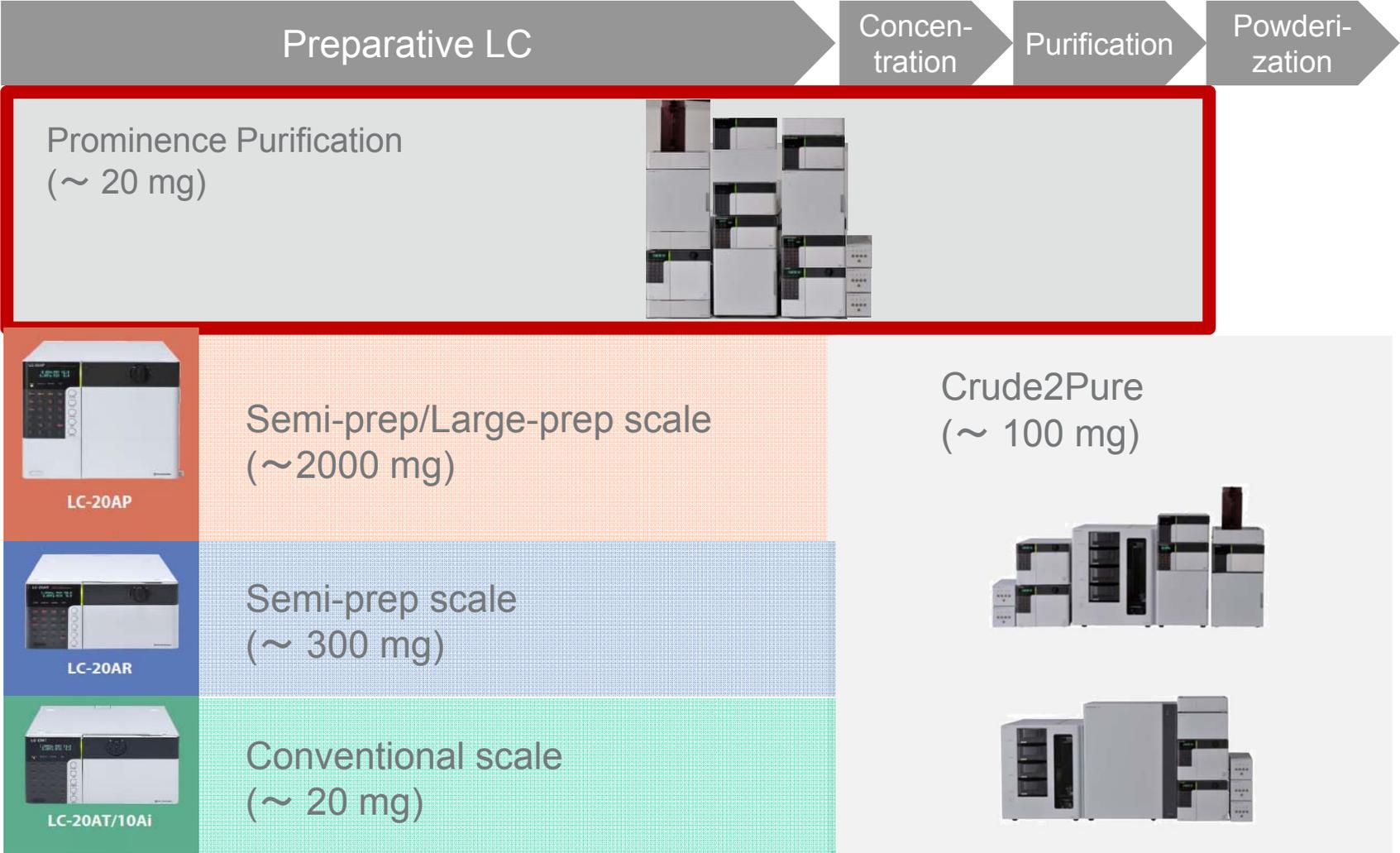
### Prominence UFPLC (Ultra Fast Preparative and Purification Liquid Chromatography)



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# Cromatografía de líquidos (HPLC)

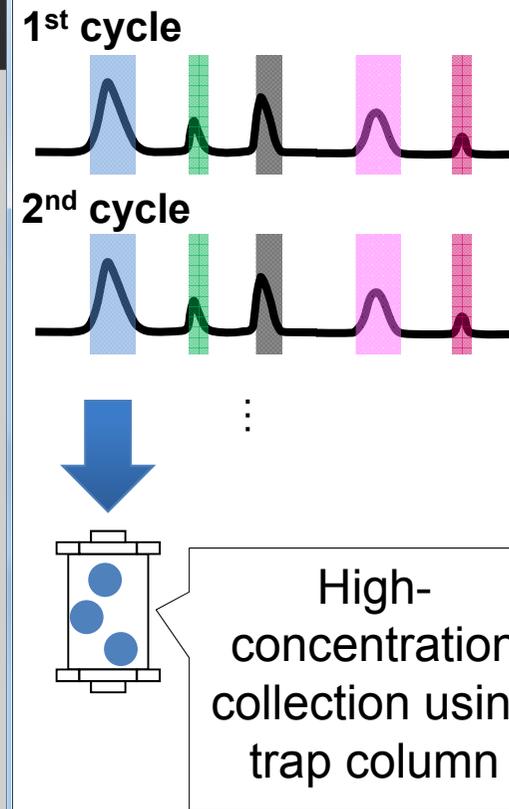
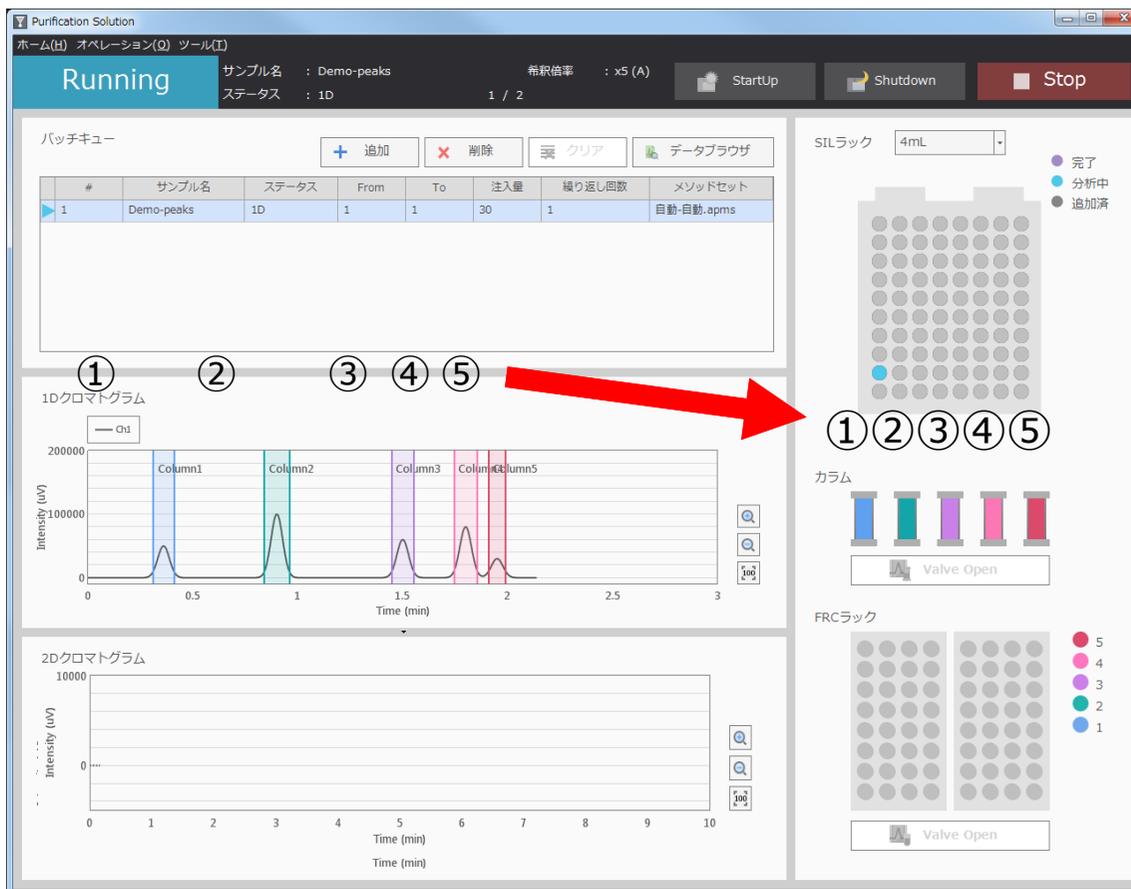
## Versatilidad / Personalización



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# Cromatografía de líquidos (HPLC) Versatilidad / Personalización

## Prominence UFPLC (Ultra Fast Preparative and Purification Liquid Chromatography)



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# Fluidos supercríticos (SFC) Extracción + Separación

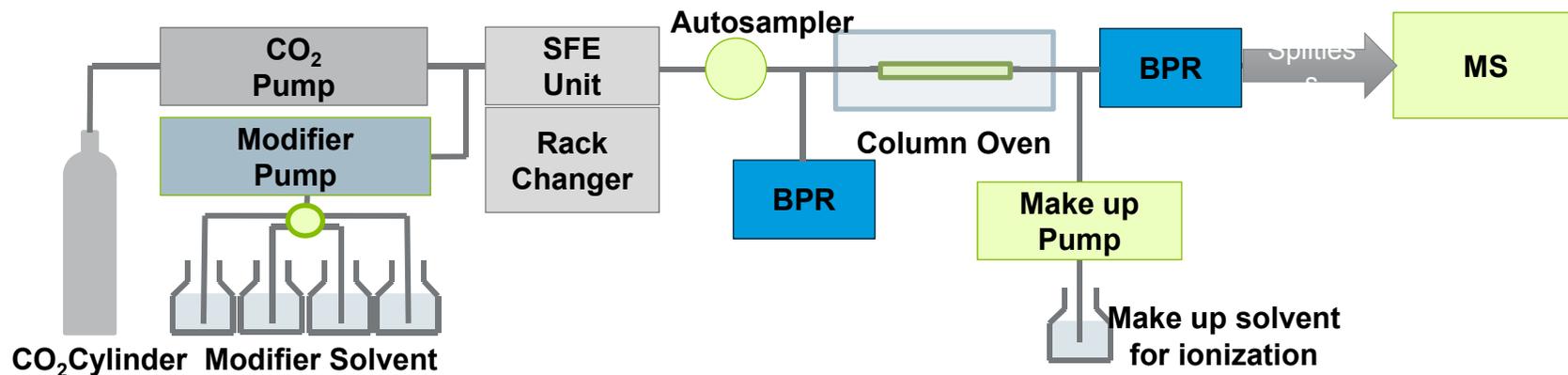
**Nexera UC – Unified Chromatography**  
**Sistema online capaz de hacer SFE-SFC**



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# Fluidos supercríticos (SFC) Extracción + Separación

## Sistema online SFE-SFC-MS



- El modulo SFC unifica la cromatografía de gases y de líquidos, combinando algunas de las mejores características de ambas técnicas
- El Nexera UC puede usarse en modo SFC o LC
- La plataforma online SFE-SFC-MS unifica una preparación de muestra rápida y sencilla, con un potente sistema de separación y alta sensibilidad de detección

# Novedades

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# Espectrometría de masas

## Triples cuadrupolos (LC-MS/MS)

### LCMS-8060

A new vision in sensitivity.  
It simply changes everything.  
Increased sensitivity by 90  
times compared to LCMS-8030

### LCMS-8050

scan speed of 30,000 u/sec  
5 msec polarity switching time  
Increased sensitivity

### LCMS-8040

Increased sensitivity

### LCMS-8030

scan speed of 15,000 u/sec  
15 msec polarity switching time

New  
LCMS-  
8045



>  
2013  
AUGUST

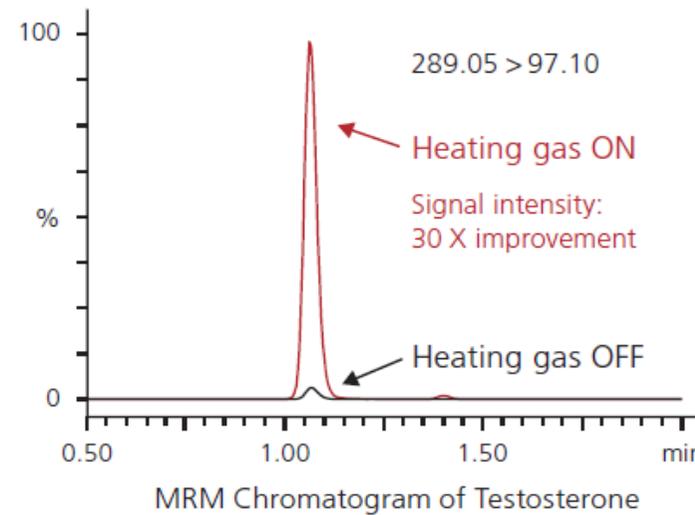
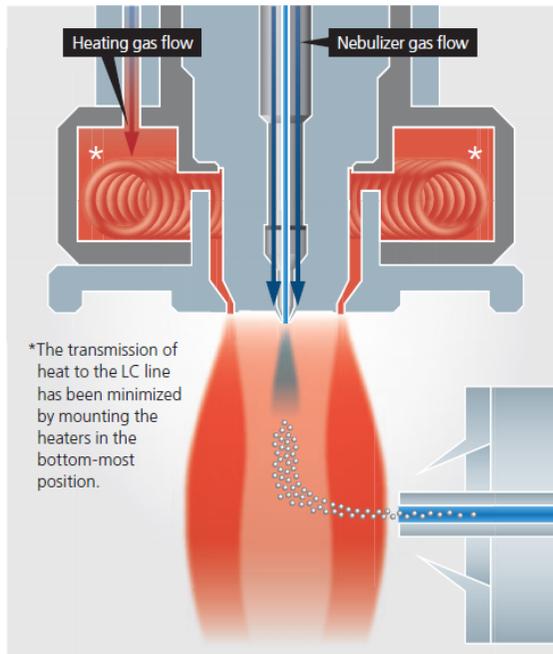
>  
2015  
ASMS 2015  
MAY

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# Espectrometría de masas

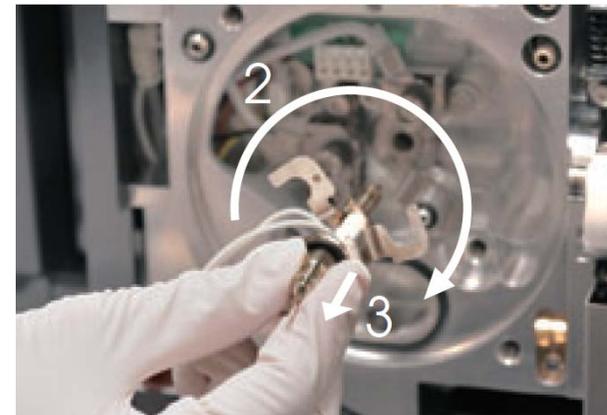
## Triples cuadrupolos (LC-MS/MS)

### Fuente de ionización ESI con calentamiento



# Espectrometría de masas Triples cuadrupolos (LC-MS/MS)

Fácil mantenimiento sin romper el vacío

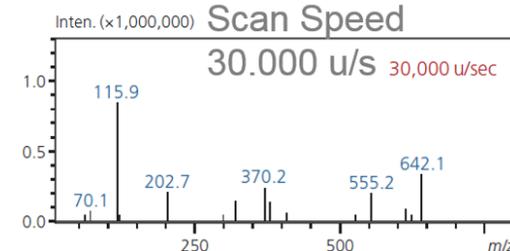
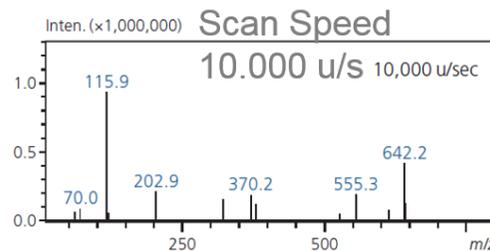
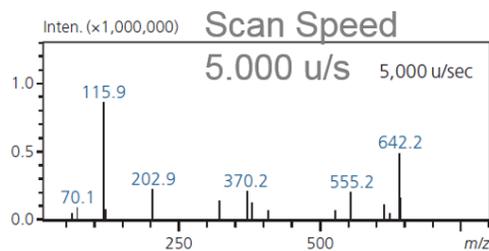
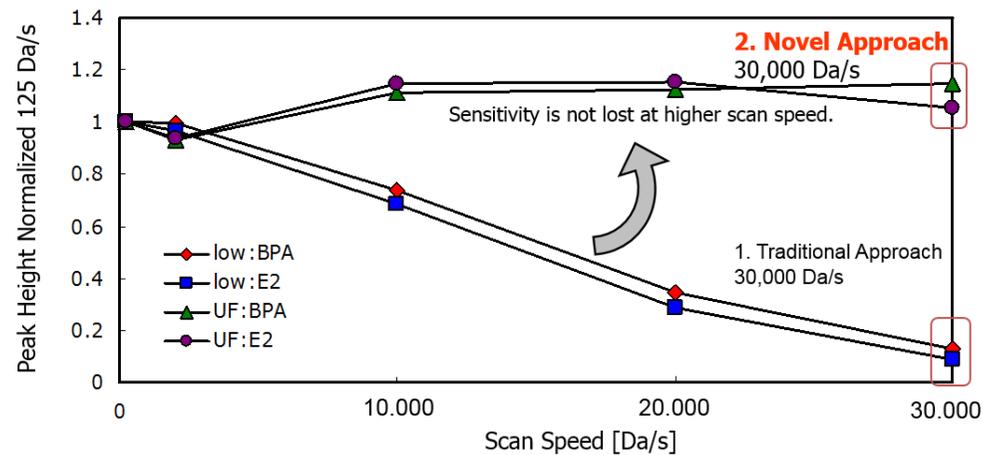


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# Espectrometría de masas

## Triples cuadrupolos (LC-MS/MS)

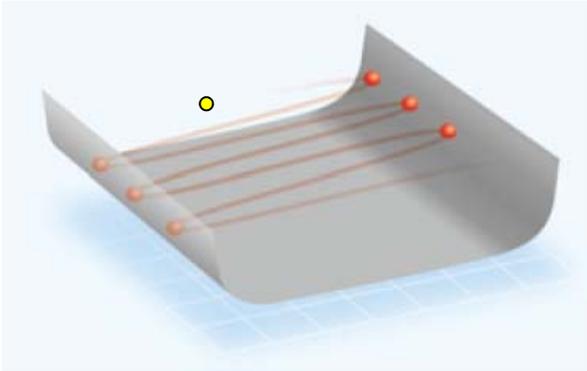
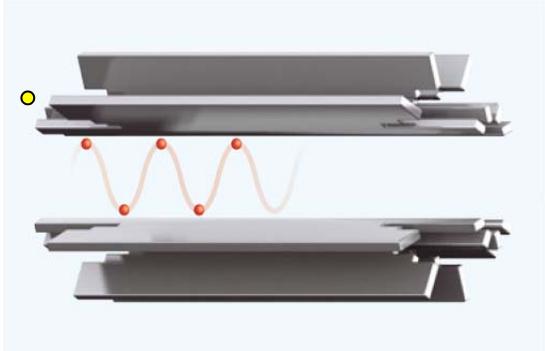
Scan de alta velocidad: 30.000 Da/s en pasos de 0,1 Da



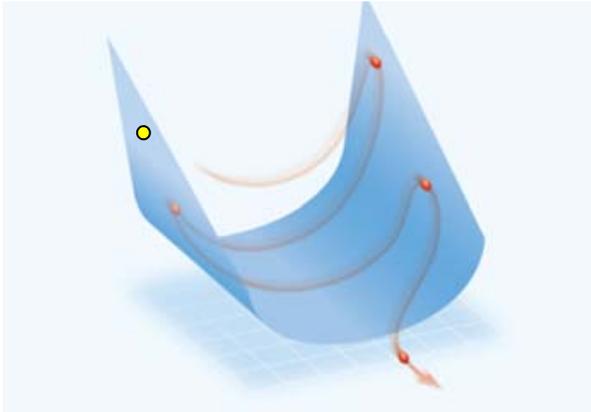
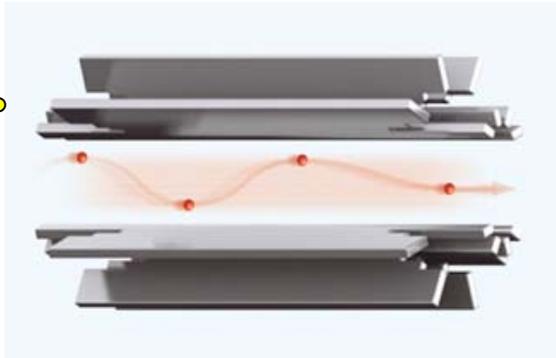
# Espectrometría de masas

## Triples cuadrupolos (LC-MS/MS)

### Conventional collision cell



### UFsweeper® collision cell

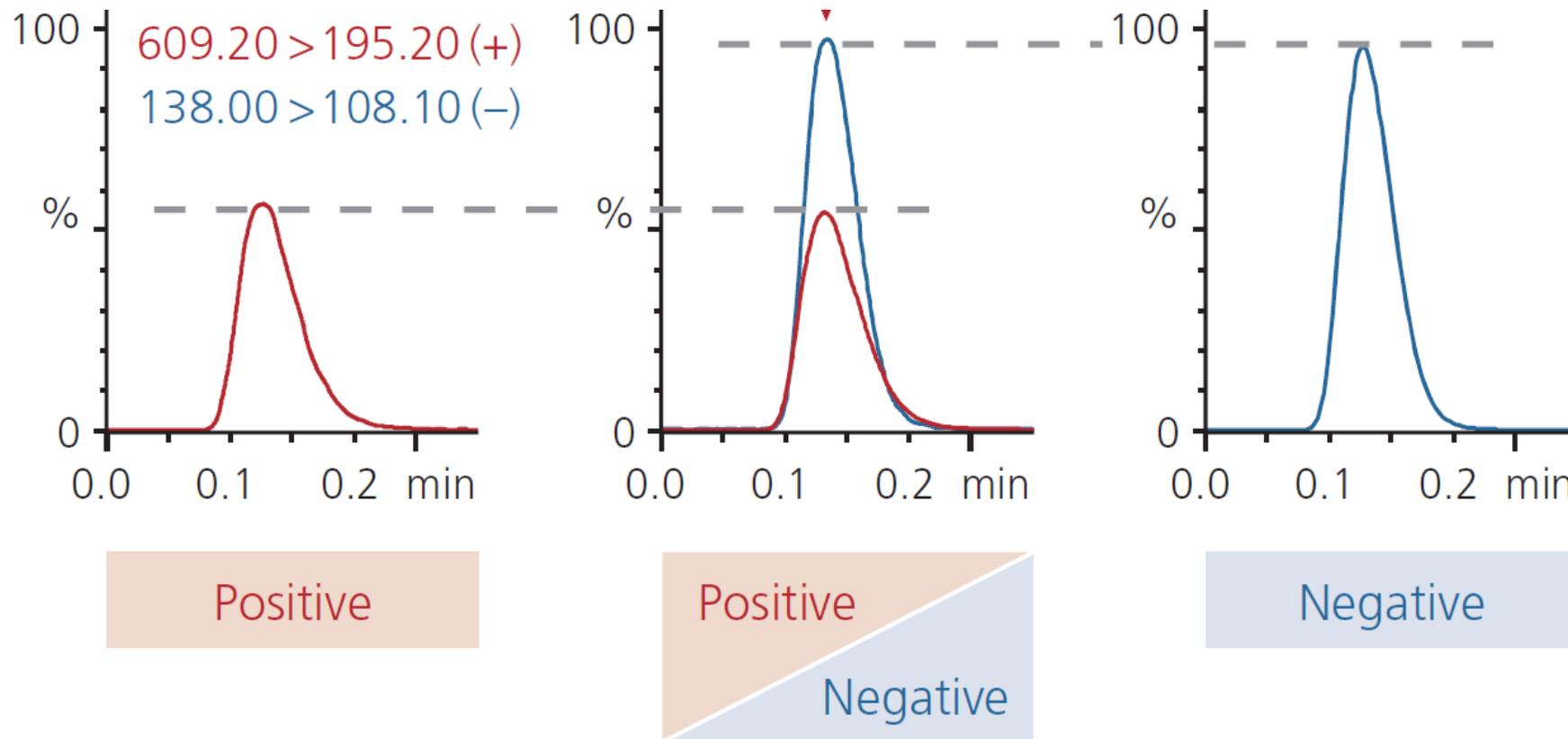


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# Espectrometría de masas

## Triples cuadrupolos (LC-MS/MS)

Cambio de polaridad ultra-rápido (5ms): No afecta a la sensibilidad



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# Espectrometría de masas

## Triples cuadrupolos (LC-MS/MS)

Librerías de transiciones. Generación automática de métodos.

<u>LC/MS/MS Method Packages</u>	<u>Número de compuestos</u>
LC/MS/MS Method Package for Drugs of Abuse	286
LC/MS/MS Method Package for Lipid Mediators Ver. 2	158
LC/MS/MS Method Package for Primary Metabolites Ver. 2	55 en método 1 97 en método 2
LC/MS/MS Rapid Toxicology Screening System Ver. 2	161
LC/MS/MS Method Package for Residual Pesticides Vers. 2	766 167 en método 1 646 en método 2
LC/MS/MS Method Package for Veterinary Drugs	42 compounds
LC/MS/MS Method Package for Water Quality Analysis	44 en campos de golf 32 en calidad de aguas
LC/MS/MS Method Package for Progranulin and Granulin Peptides	4
LC/MS/MS Method Package for Cell Culture Profiling	96

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# Espectrometría de masas

## Triples cuadrupolos (LC-MS/MS)

 **SHIMADZU**

**Quantitative analysis of 646 pesticides (1,919 MRMs) by LC-MS/MS with a fast 10.5 minute gradient**

David Baker<sup>1</sup>; Neil Loftus<sup>1</sup>; Laetitia Fages<sup>2</sup>; Eric Capodanno<sup>2</sup>;

<sup>1</sup>Shimadzu Corporation, Manchester, UK; <sup>2</sup>Phytocontrol, Nimes, France

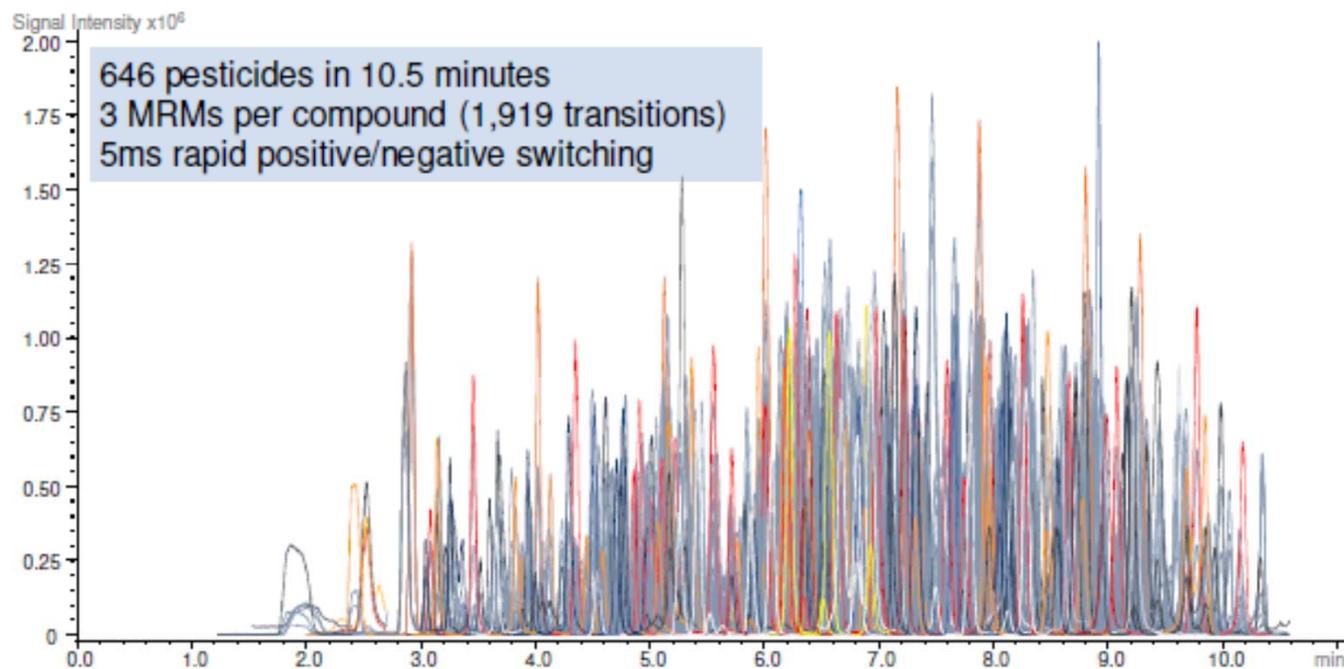


Figure 1. Chromatogram of 646 pesticides spiked into a mint extract at 0.010 mg/kg. (3 MRMs per compound and a 5 msec polarity switching time).

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# Preparación de muestra online CLAM

¿Qué es el CLAM-2000?



# Preparación de muestra online CLAM

CLAM (Clinical Laboratory Automated sample preparation Module)

*Módulo de preparación de muestra  
completamente automatizado para LC-MS*



CLAM-2000 + Shimadzu LC-MS/MS

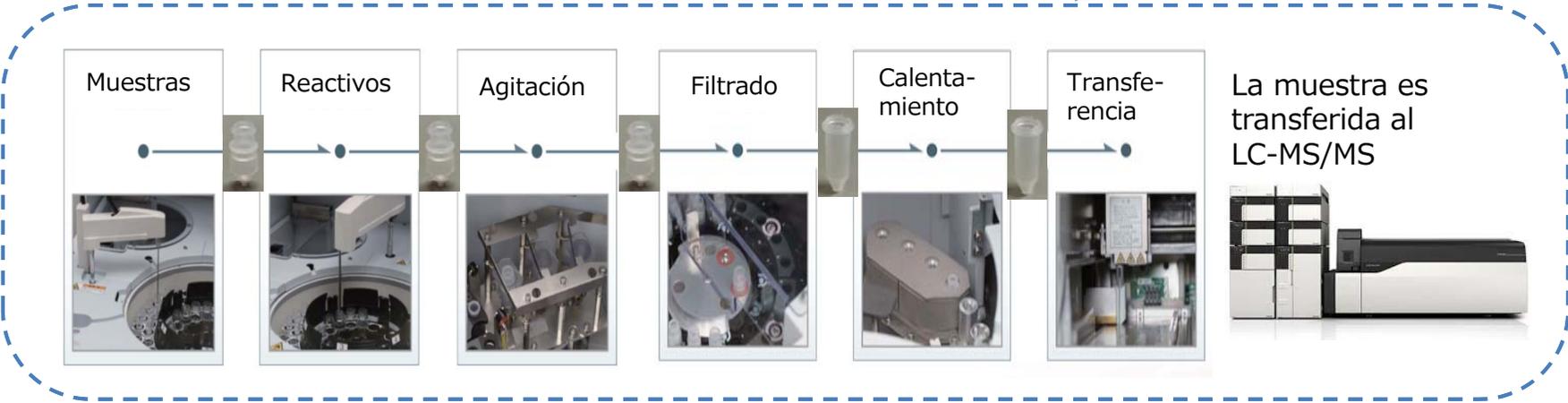
# Preparación de muestra online CLAM



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# Preparación de muestra online CLAM

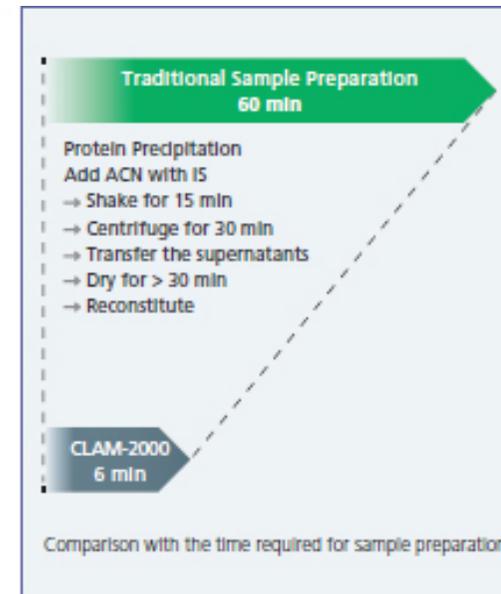
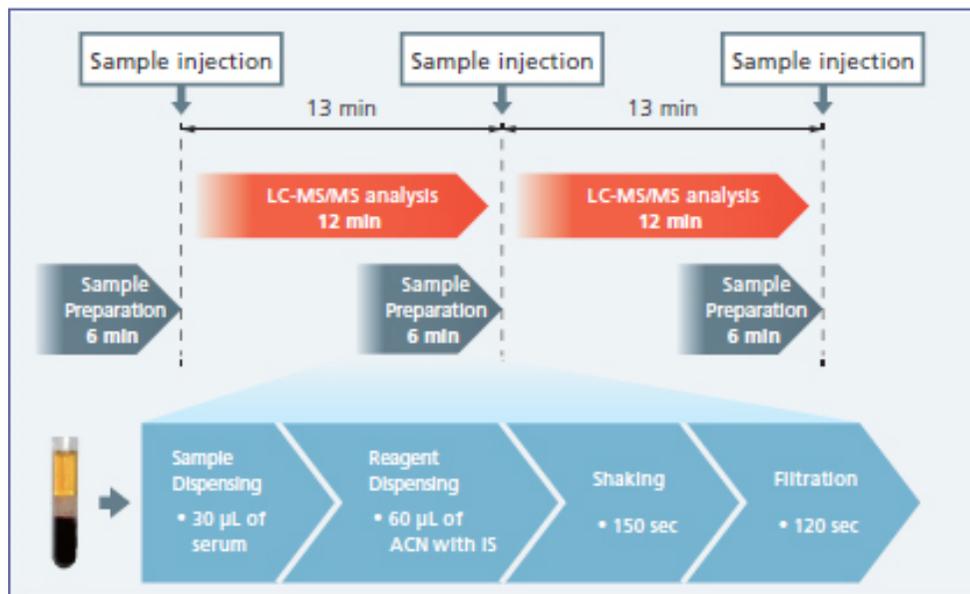
Preparación de muestra completamente automatizada



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# Preparación de muestra online CLAM

- Elimina el error humano
- Mejora exactitud de los datos
- Reduce tiempos de análisis
- Integrado en un mismo software



# Preparación de muestra online CLAM

<p><b>SHIMADZU</b> Excellence in Science</p>	<p><b>SHIMADZU</b> Excellence in Science</p>	<p><b>SHIMADZU</b> Excellence in Science</p>	<p><b>SHIMADZU</b> Excellence in Science</p>	<p><b>SHIMADZU</b> Excellence in Science</p> <p>PO-CON1663E</p>
<p>Integration serum using full-automated</p>	<p><b>Application News</b></p> <p><b>No. C123</b></p> <p>Liquid Chromatography High Molecular Weight LC/MS/MS</p> <p>Therapeutic drug monitoring (TDM) processes where the blood concentration of a patient is measured to determine the optimal method of administration for an individual. Pharmacokinetic and pharmacodynamic data is used during drug treatment with drug administration management difficulties, with a narrow therapeutic range or wide range and toxic range that are close to the performance liquid chromatography (HPLC) the main analytical method used with TDM. Liquid chromatography-mass spectrometry is being used to improve analytical precision based on its superior selectivity. LC/MS/MS normally requires sample preparation such as deproteinization and dilution to serum or blood plasma sample. These steps increase the risk of error or variability occur operator skill. The volume of work per operator also increases in accordance with the number of samples. Therefore, the sample preparation can become the bottleneck of an analysis when analyzing a large number of samples.</p> <p>■ <b>High-Throughput Analytical Workflow for Antiepileptic Drug Analysis</b></p> <p>We introduce an example simultaneous analysis of seven antiepileptic drugs and drug active ingredients in blood serum using a fully automated sample preparation LC/MS/MS system. Preparation of blood serum sample normally requires deproteinization by organic solvent, and then centrifugal separation of components followed by supernatant recovery and automated sample preparation LC/MS/MS.</p> <div data-bbox="548 1117 728 1292"> </div> <p>Fig. 1 Workflow for Simultaneous Analysis of Antiepileptic Drugs</p>	<p>The Novel LC/MS/MS System for Drugs Analysis</p>	<p>High throughput analysis of anticoagulant drugs integrated with sample preparation</p>	<p>Fully automated platform for determination of immunosuppressant drugs in whole blood</p> <p><b>ASMS 2016</b> TP 412</p> <p>Davide Vecchiotti<sup>1</sup>, Brambilla M.<sup>2</sup>, Kawakami D.<sup>2</sup>, Tsukamoto T.<sup>2</sup>, Brambilla P.<sup>3</sup>  <sup>1</sup> Shimadzu Corporation, Milan, Italy  <sup>2</sup> Shimadzu Corporation, Kyoto, Japan  <sup>3</sup> Desio Hospital, University Department of laboratory medicine, Desio, Italy</p>

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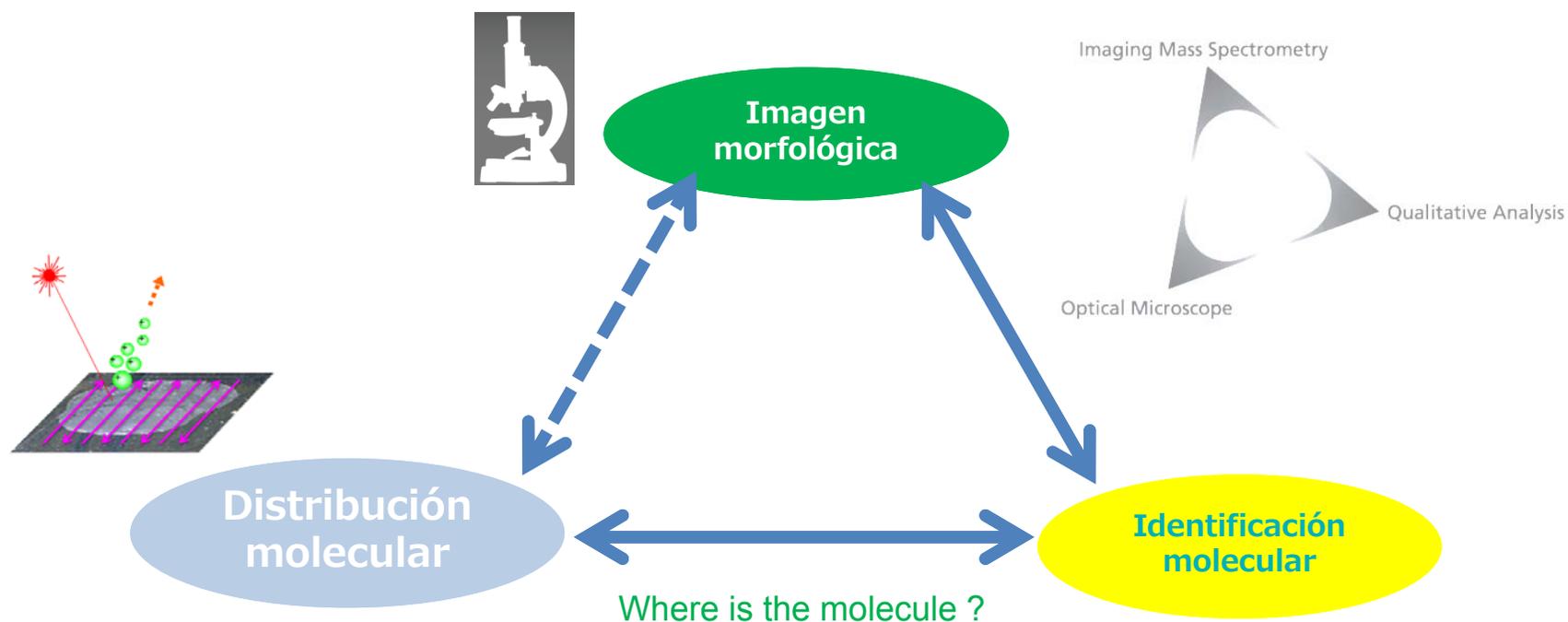
# Imagen por MS - iMScope



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# Imagen por MS - iMScope

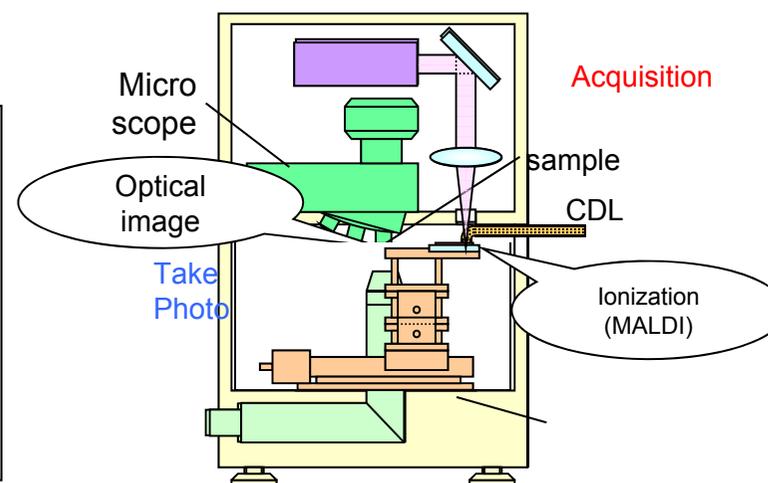
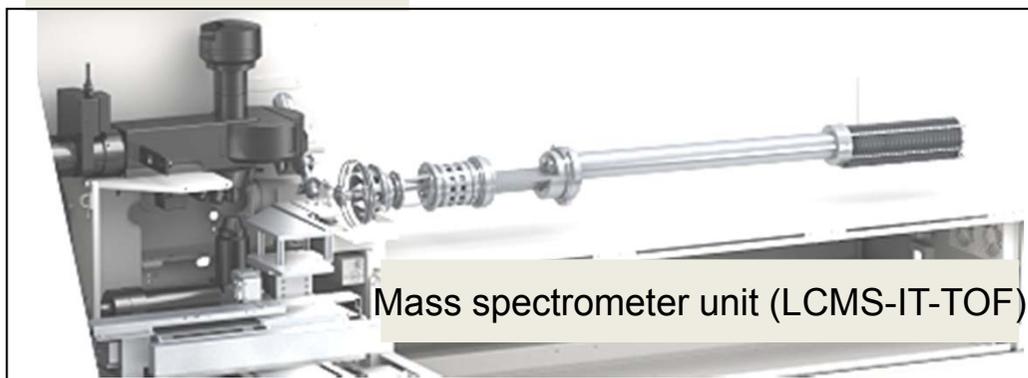
iMScope TRIO sirve para identificar directamente sustancias por espectrometría de masas después de la adquisición de una imagen óptica a través del microscopio integrado



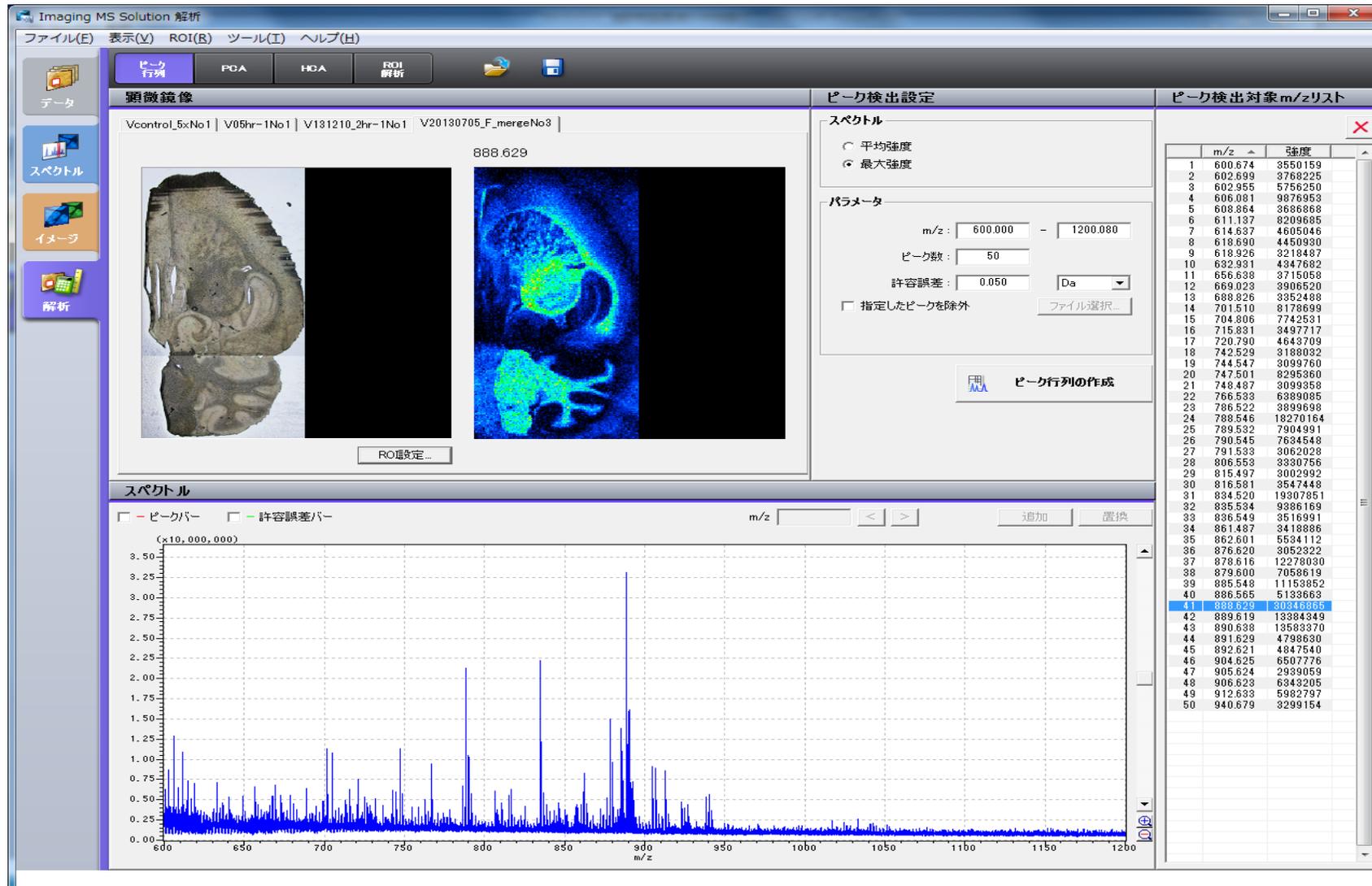
# Imagen por MS - iMScope

- Fuente de ionización MALDI a presión atmosférica
- Integra imágenes ópticas y de masas
- Alta resolución espacial (ND:YAG laser 5-200  $\mu\text{m}$ )
- Alta velocidad de adquisición (6 píxeles/s)
- Posibilidad de análisis estructural por fragmentación MSn

Microscope MALDI unit



# Imagen por MS - iMScope



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# Imagen por MS - iMScope

The screenshot displays the iMScope software interface for mass spectrometry data analysis. The main window is titled 'Imaging MS Solution 解析' and contains several key sections:

- 各種データ・解析条件 (Data Analysis Conditions):** Shows sample names (Vcontrol\_5xNo1, V05hr-1No1, V131210\_2hr-1No1, V201307), data scaling options (バレットスケーリング), and PCA execution settings.
- 寄与率 (Contribution Rate):** A bar chart showing the relative contribution of different m/z values to the total signal.
- イメージング指定m/zリスト (Imaging Specified m/z List):** A table listing m/z values and their corresponding color-coded imaging channels.
- 解析結果 (Analysis Results):** A grid of four main components (第1主成分 to 第4主成分). Each component includes a heatmap, a mass spectrum plot, and four smaller heatmaps corresponding to specific m/z values.
- 解析結果テーブル (Analysis Results Table):** A detailed table of the first component's data, listing m/z, factor loadings, and intensities.

m/z	因子負荷...	強度	
1	888.629	0.530	33162752
2	890.638	0.418	16185856
3	889.619	0.362	15925248
4	891.629	0.256	7106560
5	862.601	0.236	8293376
6	806.553	0.232	6054912
7	816.581	0.208	6290944
8	786.522	0.109	6712320
9	815.497	0.087	5580800
10	602.955	0.075	8687616
11	878.616	0.073	15004160
12	701.510	0.072	11319296
13	747.501	0.069	11316224
14	859.023	0.066	5845440
15	632.931	0.058	7107584
16	906.623	0.055	8949248
17	618.926	0.053	5735424
18	879.600	0.050	9609216
19	608.864	0.048	6504448
20	788.546	0.048	21320704
21	832.621	0.046	7237632
22	748.487	0.037	5792768
23	876.620	0.032	5265920
24	789.532	0.022	10528768
25	835.534	0.022	12108288
26	749.590	0.018	6193760

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# Imagen por MS - iMScope

Fields	Item Analyzed	Purposes
Medical	Analyze cancers and other diseased tissues or micro areas.	Identify substances causing illnesses or analyze tissue characteristics.
Pharmaceuticals	<b>Analyze pharmacokinetics</b> or metabolites in biological tissues.	Applications in <b>pharmacokinetics</b> or safety testing, or for <b>drug discovery screening</b> .
Engineering	Analyze micro defects or micro organic contaminants in synthetic materials.	Applications in materials development and degradation analysis
Agriculture	Analyze the content or distribution of components in food.	Developing improved varieties
<b>Analytical center</b>	<b>Wide variety field (from biological to industrial )</b>	<b>Multi user and multi form</b>

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# Novedades - Conclusiones

- Tracera – El detector para GC más universal y sensible
- Method Scouting – Desarrollo métodos de forma sencilla y ahorrando tiempo
- UFPLC – Rápida separación, purificación y elución de fracciones
- SFE-SFC – Extracción & Separación por SF en un instrumento y online
- LCMS – Más rápidos y sensibles
- CLAM – Preparación de muestra online automatizada
- iMScope TRIO – Distribución e identificación en molecular en imágenes

# Gracias



**Envío de un sistema Shimadzu a la estación polar del Polo Sur**