IONTOF

2	9

New Hybrid SIMS

Surface analysis meets organic mass spectrometry

SIMS is well suited to acquire organic and inorganic chemical information from submicron sample areas. This capability is especially intriguing for researchers in life science applications. The vision to image and unambiguously identify molecules on a sub-cellular level has been driving instrumental and application development over the last years.

While new cluster ion sources expanded the usability of SIMS instruments for biological applications, the mass spectrometers in use had a lack of mass resolution, mass accuracy and MS/MS capabilities.

With the new Q Exactive™ Extension for its current product line IONTOF introduces the first commercial SIMS instrument which combines highest mass resolution (> 250,000) and highest mass accuracy (< 1 ppm) with high resolution cluster SIMS imaging.

The new instrument extension also provides field-proven and advanced MS/MS capabilities and sets a new benchmark for high resolution molecular SIMS applications.

Ultra-high mass resolution in imaging mode

The latest generation gas cluster ion source allows for sub-micron imaging in combination with ultra-high mass resolution, thus enabling the distinction of different features even in extremely complex organic systems such as tissue or cells.
In this example mass intervals representing the collagenous fibres within the bone marrow are shown in red. In blue, the distribution of $C_5H_{15}NPO_4^+$ is shown, corresponding to the phosphatidylcholine head group.
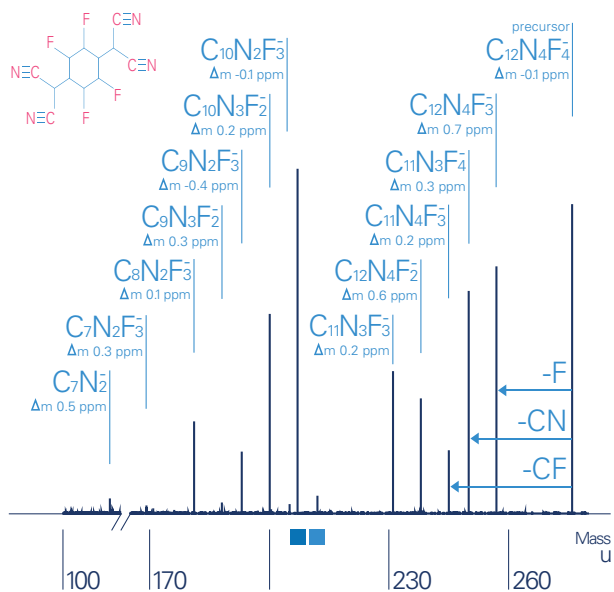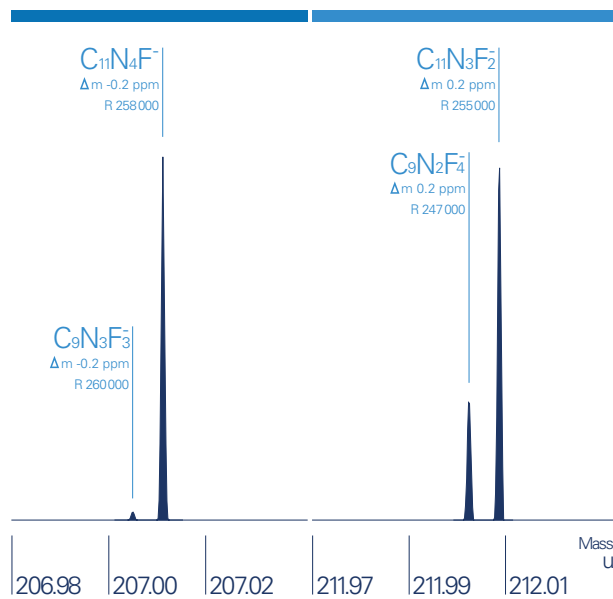
The example shows a cutout of a human bone section. Mineralized bone is shown in green, two different components in the bone marrow region are shown in red and blue.

Sample provided by Kaija Schäpe and Dr. Marcus Rohnke (University of Giessen, Germany)

JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN
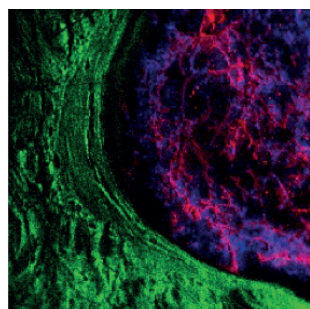
480µm

Structural analysis with high resolution MS/MS

The second example shows a high resolution structural analysis of a molecule used for OLED devices. The overview spectrum displays the full MS/MS information for the precursor ion $C_{12}N_4F_4^-$. The two detail spectra show plots of different fragment ions. Please note that even for the MS/MS spectrum the same level of mass resolution and mass accuracy is reached. Both are a prerequisite for unambiguous peak identification.

$C_{10}N_2F_3^-$
Δm -0.1 ppm

$C_{10}N_3F_2^-$
Δm 0.2 ppm

$C_9N_2F_3^-$
Δm -0.4 ppm

$C_9N_3F_2^-$
Δm 0.3 ppm

$C_8N_2F_3^-$
Δm 0.1 ppm

$C_7N_2F_3^-$
Δm 0.3 ppm

$C_7N_2^-$
Δm 0.5 ppm

precursor
$C_{12}N_4F_4^-$
Δm -0.1 ppm

$C_{12}N_4F_3^-$
Δm 0.7 ppm

$C_{11}N_3F_4^-$
Δm 0.3 ppm

$C_{11}N_4F_3^-$
Δm 0.2 ppm

$C_{12}N_4F_2^-$
Δm 0.6 ppm

$C_{11}N_3F_3^-$
Δm 0.2 ppm

-F

-CN

-CF

Mass u

100   170   230   260

Full MS/MS spectrum of the precursor ion $C_{12}N_4F_4^-$

$C_{11}N_4F^-$
Δm -0.2 ppm
R 258 000

$C_9N_3F_3^-$
Δm -0.2 ppm
R 260 000

$C_{11}N_3F_2^-$
Δm 0.2 ppm
R 255 000

$C_9N_2F_4^-$
Δm 0.2 ppm
R 247 000

Mass u

206.98   207.00   207.02   211.97   211.99   212.01

Detail plot of different fragment ions at mass 207 u and 212 u