BRUKER

timsTOF™

- Flexibility to Empower Your Ideas

TIMS-QTOF MS

Innovation with Integrity

timsTOF™

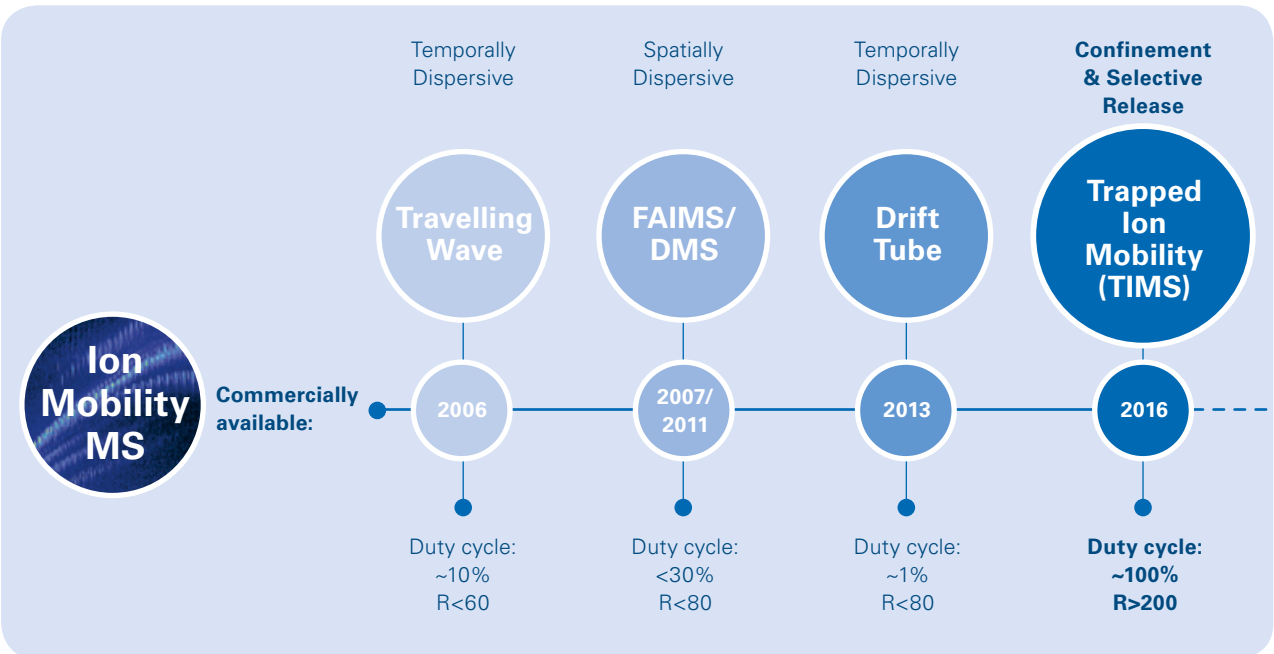
Flexibility to Empower Your Ideas

With timsTOF™, Bruker introduces the next generation of ion mobility mass spectrometry

Unlock an additional dimension using the power of trapped ion mobility spectrometry (TIMS) mass spectrometry. This unique capability strengthens confidence in your structures through adding to the information derived from retention time, m/z, and MS/MS, enabling a leap forward in the characterization of molecules.

The highly unique TIMS design enables unmatched duty cycle (up to 100%), significant improvement in IMS resolution (R>200), unprecedented CCS reproducibility and high sensitivity.

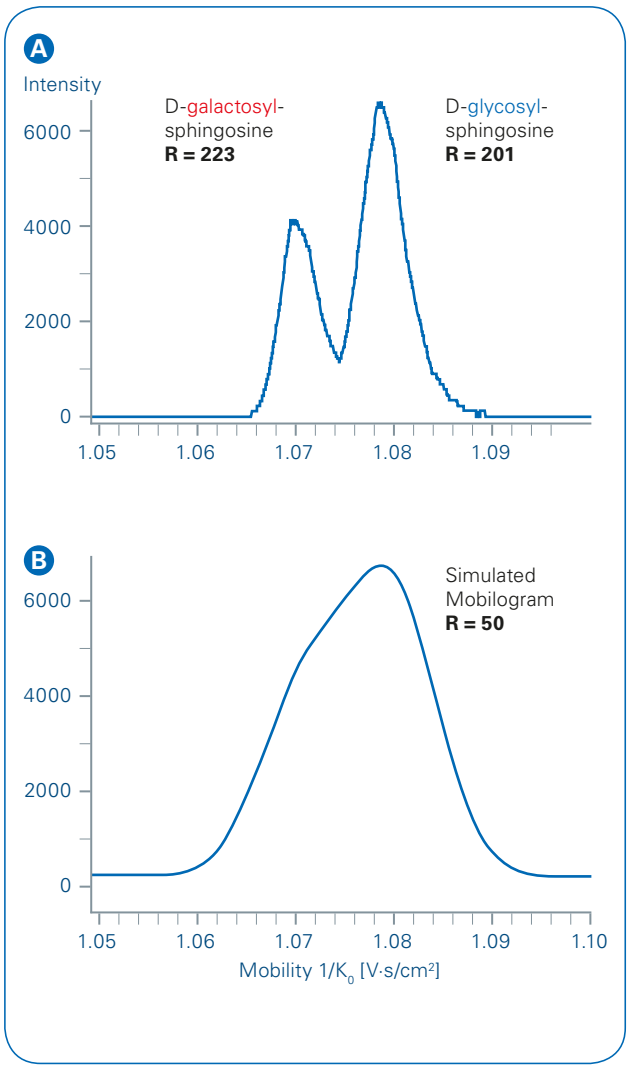
timsTOF was engineered by Bruker experts as an open platform to accelerate the adoption of ion mobility mass spectrometry analysis across all applications.



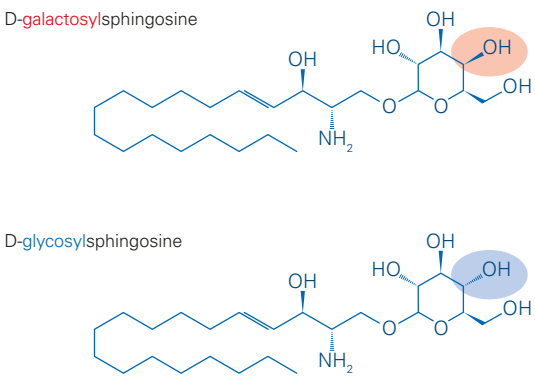
Resolution of 200 achieved by a unique design

Providing consistently high ion mobility resolution, timsTOF unravels the complexity of samples and unlocks insights that remain hidden in standard mass spectrometry.

With high resolution ion mobility separation, timsTOF adds an orthogonal dimension that increases peak capacity beyond the resolving power achieved by chromatography and time-of-flight. Whereas unresolved precursor ions can yield inconclusive structural assignment, timsTOF enables more confident and specific identification. Even isomeric and isobaric compounds become accessible.



> ***Dr. Carlos Afonso, University of Rouen:***
> *We are already using ion mobility in our lab, but with the much higher ion mobility resolution that timsTOF provides now, there is a lot of room for different applications based on this technology.*

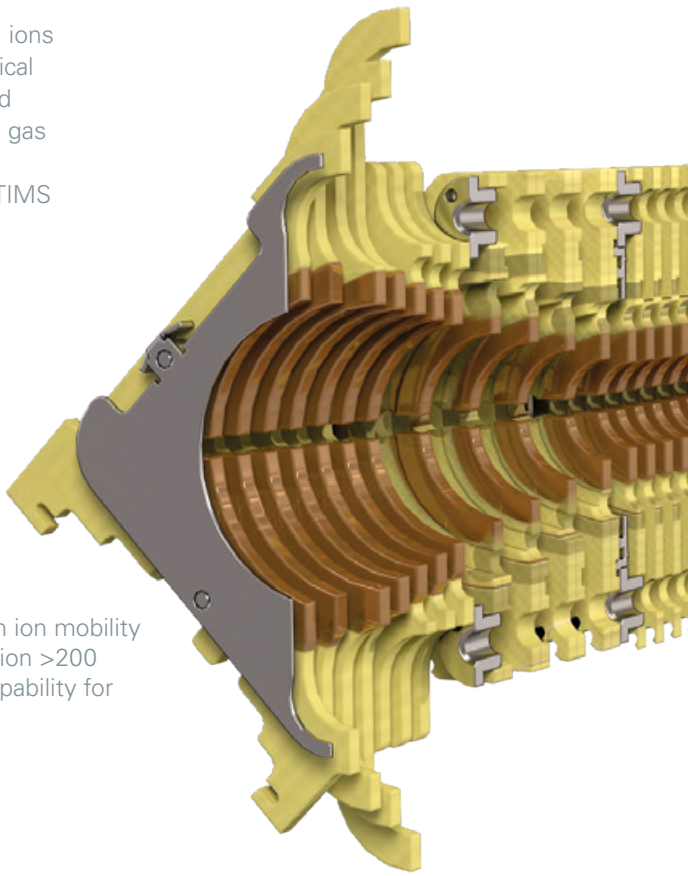


The two isomeric compounds D-galactosylsphingosine and D-glycosylsphingosine differ only by orientation of one OH group in the sugar moiety (above/below the ring system).

Figure 1. Trapped ion mobility separates isomeric compounds. **A** Measured mobilograms of D-galactosylsphingosine and D-glycosylsphingosine. The peaks give a resolution of 223 and 201 respectively. **B** Simulated mobilograms with resolution of 60 for both compounds

Flexibility to view samples the way you want

What is TIMS? In Trapped Ion Mobility Spectrometry (TIMS), ions are propelled through the TIMS tunnel by a gas flow. An electrical field controls each ion from moving beyond a position defined by the ion's mobility, where the push it experiences from the gas flow matches the force of the electrical field. Ramping down the electrical field allows selectively releasing ions from the TIMS tunnel according to their mobility.



TIMS tunnel: High resolution ion mobility separation capable of resolution >200 with parallel accumulation capability for up to a 100% duty cycle.

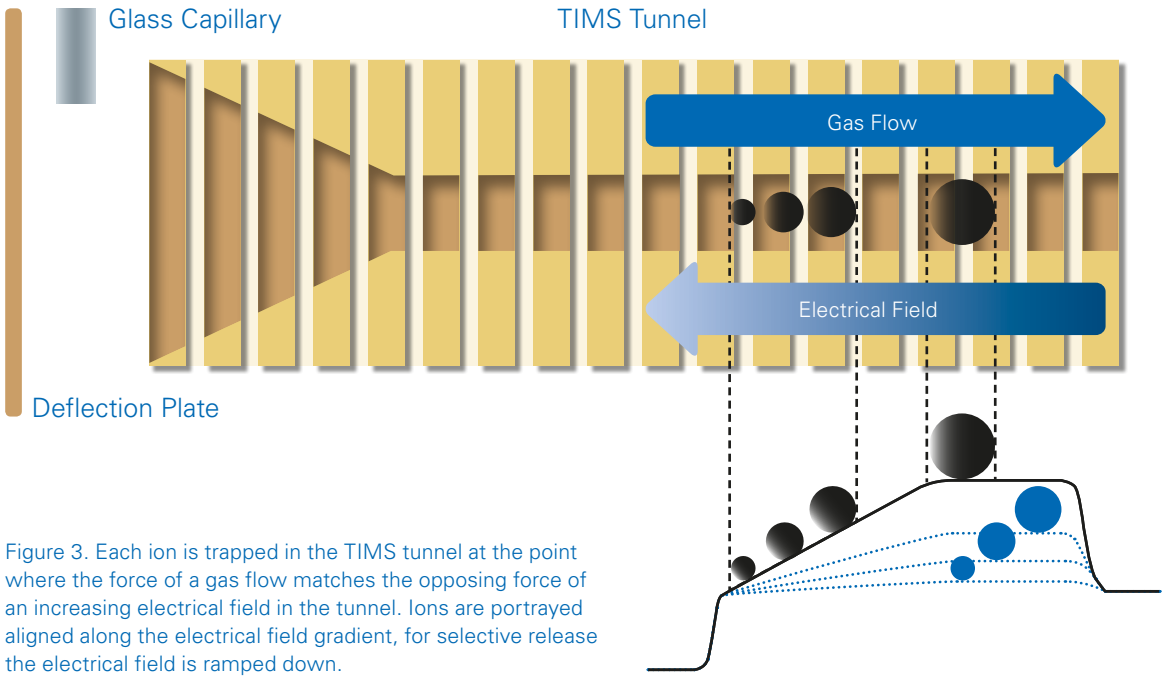


Figure 3. Each ion is trapped in the TIMS tunnel at the point where the force of a gas flow matches the opposing force of an increasing electrical field in the tunnel. Ions are portrayed aligned along the electrical field gradient, for selective release the electrical field is ramped down.

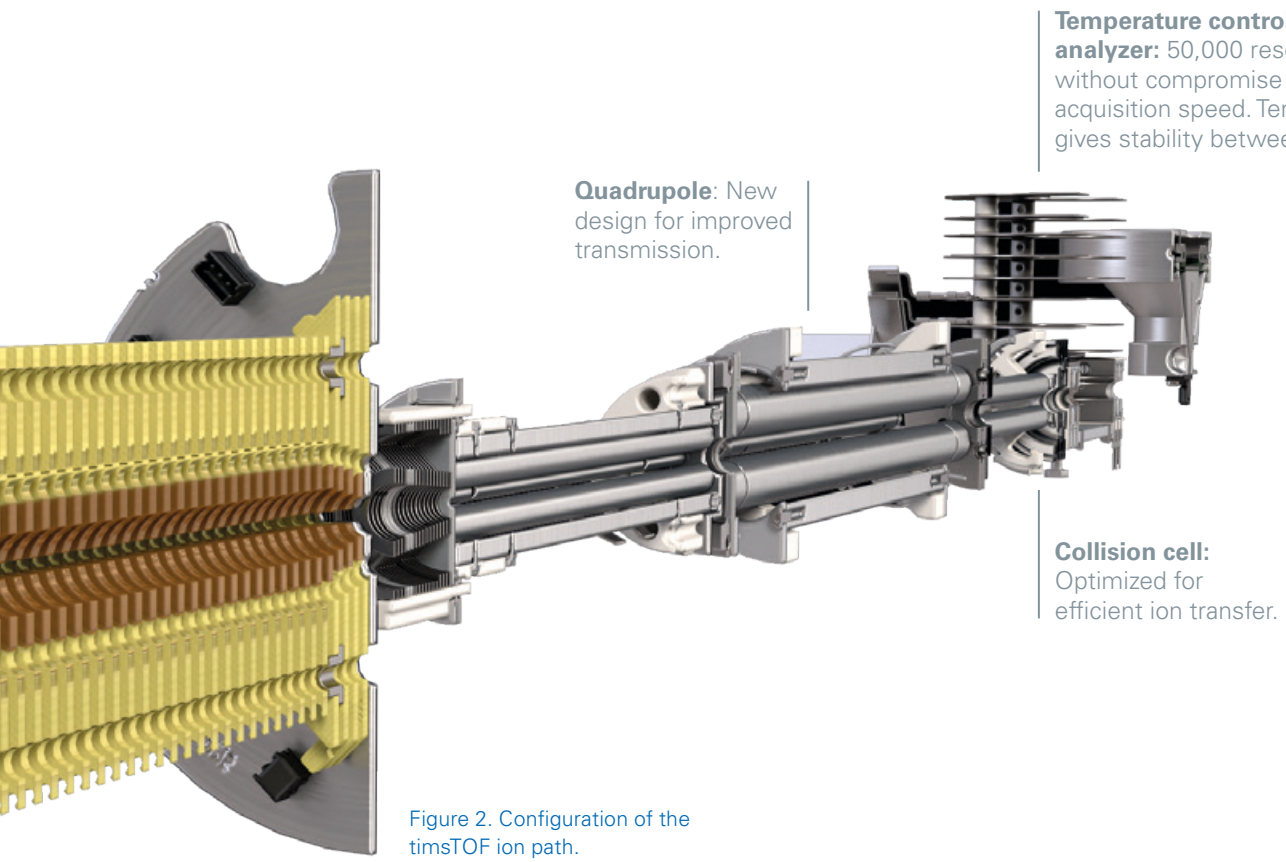
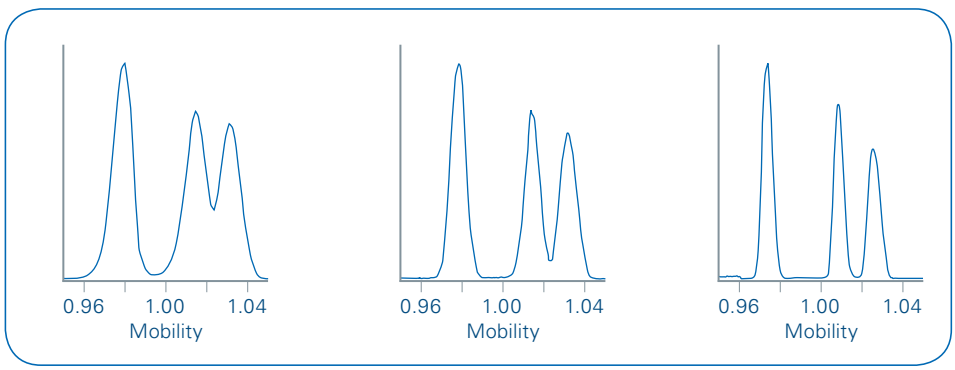


Figure 2. Configuration of the timsTOF ion path.

Maximize insights

Analyze samples in survey mode for an overview and investigate a resulting heatmap interactively. Then, select an **imeX mode** to magnify a specific mobility range. Focusing on a target set of peaks, you can perform an accurate analysis of collisional cross sections or resolve overlapping ions with ultra-high ion mobility resolution.



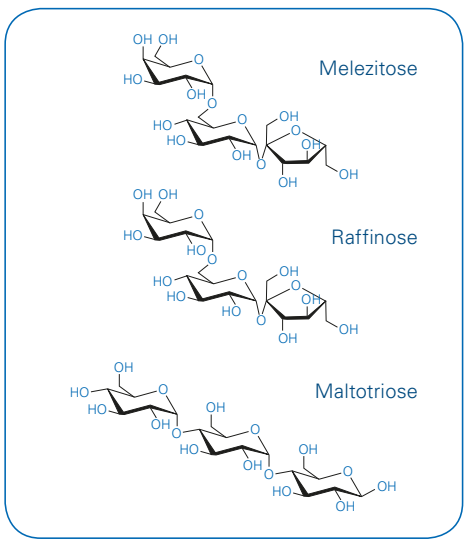


Figure 4. Raffinose, Melezitose and Maltotriose have the same elemental composition $C_{18}H_{32}O_{16}$, but differ in their structure. imeX technology allows adjusting ion mobility resolution in three steps. Here, ion mobility resolution up to RP 80 (left), up to RP 120 (middle) and baseline separation with up to RP 185 in imeX Ultra mode (right) was achieved.

Confidence through unprecedented detail and clarity

timsTOF boosts confidence and specificity of compound identification with an expanded set of orthogonal qualifiers that are measured with great accuracy.

timsTOF increases the depth of your LC-MS/MS workflow by adding high resolution ion mobility separation. Keep your established chromatography settings and investigate data in the usual way, e.g. create a Base Peak Chromatogram (BPC) of a compound of interest.

Clean fragmentation spectra that are easily correlated with their precursor ion support conclusive compound identification. Ultimately, this expanded set of orthogonal characteristics for every ion grants greater analytical flexibility and confidence.

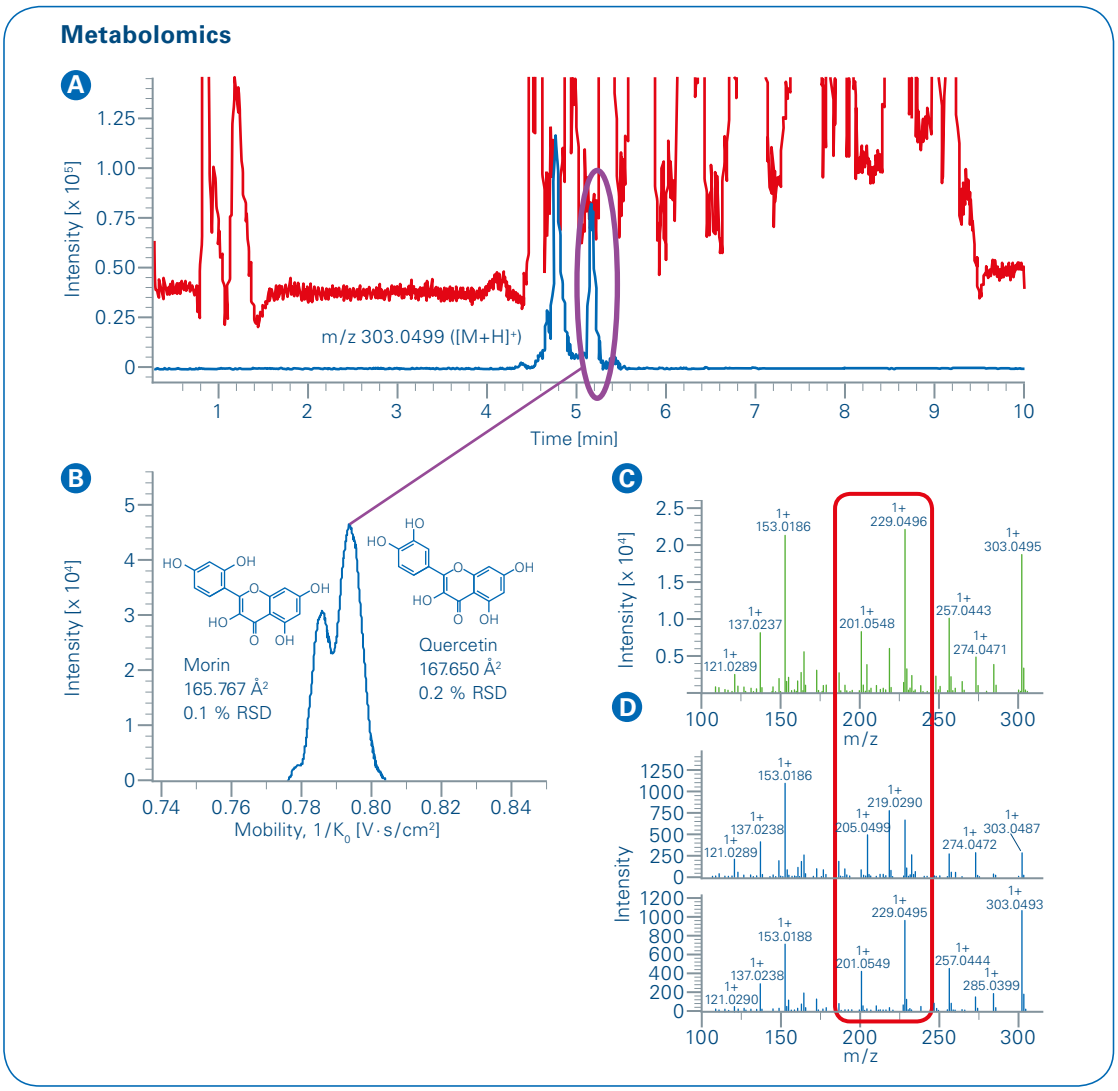
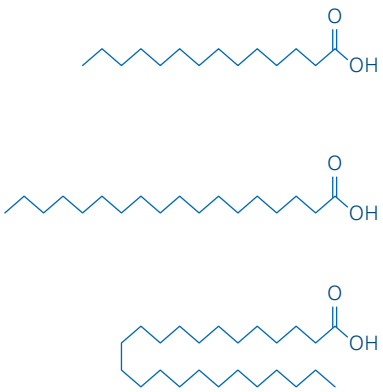


Figure 5. The timsTOF mass spectrometer separates isomers in real-life complex samples. **A** The two pentahydroxyflavone isomers Quercetin and Morin cannot be distinguished by mass spectrometry alone as they co-elute from column. The data show the base peak chromatogram of a propolis extract (red trace) and an extracted ion chromatogram of m/z 303.0499 (blue trace). **B** But their different substitution patterns facilitate the separation in the additional dimension of mobility. **C**/**D** A subsequent fragmentation gives clean MS/MS spectra of the compounds. **C** Mixed MS/MS on top, **D** clean MS/MS below.

Expand what you know about a compound

With timsTOF, you can construct enhanced libraries of compounds, where each entry is characterized by ppm accurate mass, collisional cross section (CCS) with a precision of < 0.5%, and Bruker's unique isotopic pattern fidelity (True Isotopic Pattern or TIP).

Lipids



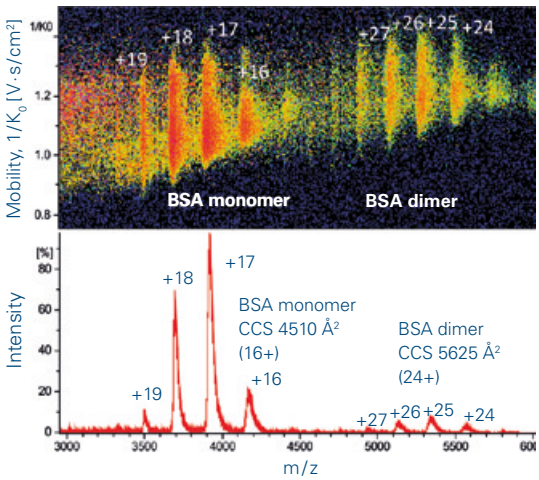
Myristic acid
TIMS CCS 158.2 Å²
Literature value[1] 158.2 Å²
Difference 0 %

Stearic acid
TIMS CCS 173.3 Å²
Literature value[1] 173.2 Å²
Difference 0.1 %

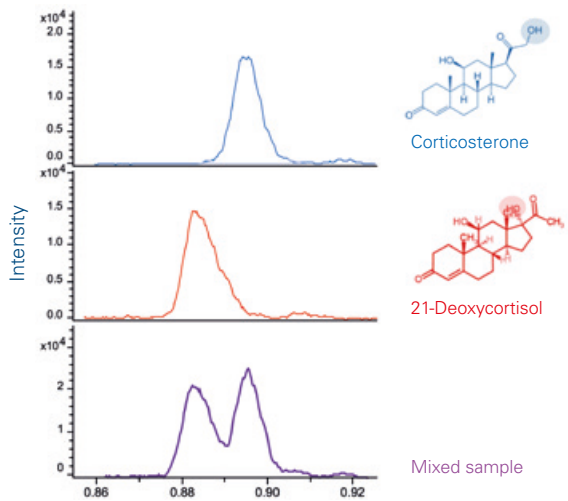
Lignoceric acid
TIMS CCS 196.4 Å²
Literature value[1] 196.3 Å²
Difference 0.2 %

[1] Zhang et al. Journal of The American Society for Mass Spectrometry, 2015, **50**, 7, 906-913

Intact proteins



Steroids



Polymers

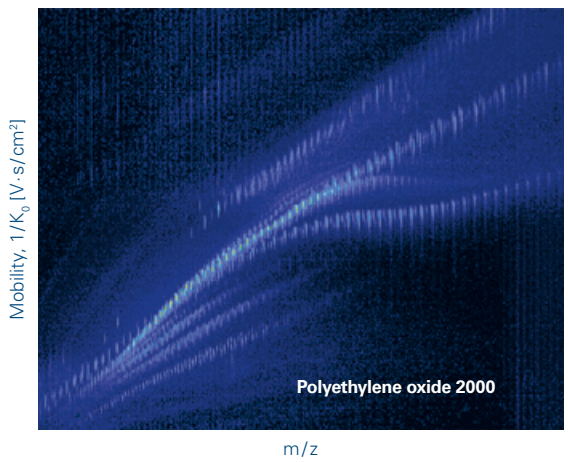


Figure 6: Unlock new information in all your applications. Further investigate the mobilogram and heatmap to discover potentially overlapping compounds. Automatically calculate CCS values with high reproducibility to give you confidence in your structural identifications.

> ***Dr. Jan Jordens, DSM Resolve:*** *timsTOF gave us much more information right from the beginning, even information we did not expect to be in the data. Now the platform really helps us to get new knowledge about processes that are taking place in our samples and also about impurities. It means that with the ion mobility we saw the presence of impurities and phenomena we could not observe before with regular MS and which is thus information we did not expect to be in the samples. It shows things, hidden for the analyst without using TIMS.*

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Flexibility to Empower Your Ideas

Flexibility **Resolution** **Confidence**

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Bruker Daltonik GmbH

Bremen · Germany
Phone +49 (0)421-2205-0

Bruker Scientific LLC

Billerica, MA · USA
Phone +1 (978) 663-3660

ms.sales.bdal@bruker.com - www.bruker.com

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