Software

# BioPharma Compass

## Accelerate Routine BioPharma Characterization

Innovation with Integrity

# Faster insights in your BioPharma data

**BioPharma Compass®** increases the productivity of biologics characterization labs with integrated workflows that take full advantage of the benefits of high isotopic fidelity data, complementary ionization modes and trapped ion mobility.

Workflows for multi attribute peptide and protein screening, peptide mapping, oligonucleotide sequence verification as well as top-down sequencing and critical reagent QC are available. This empowers users with the tools to rapidly turn MS data into actionable insights.

---

### Simple interface to get productive quickly

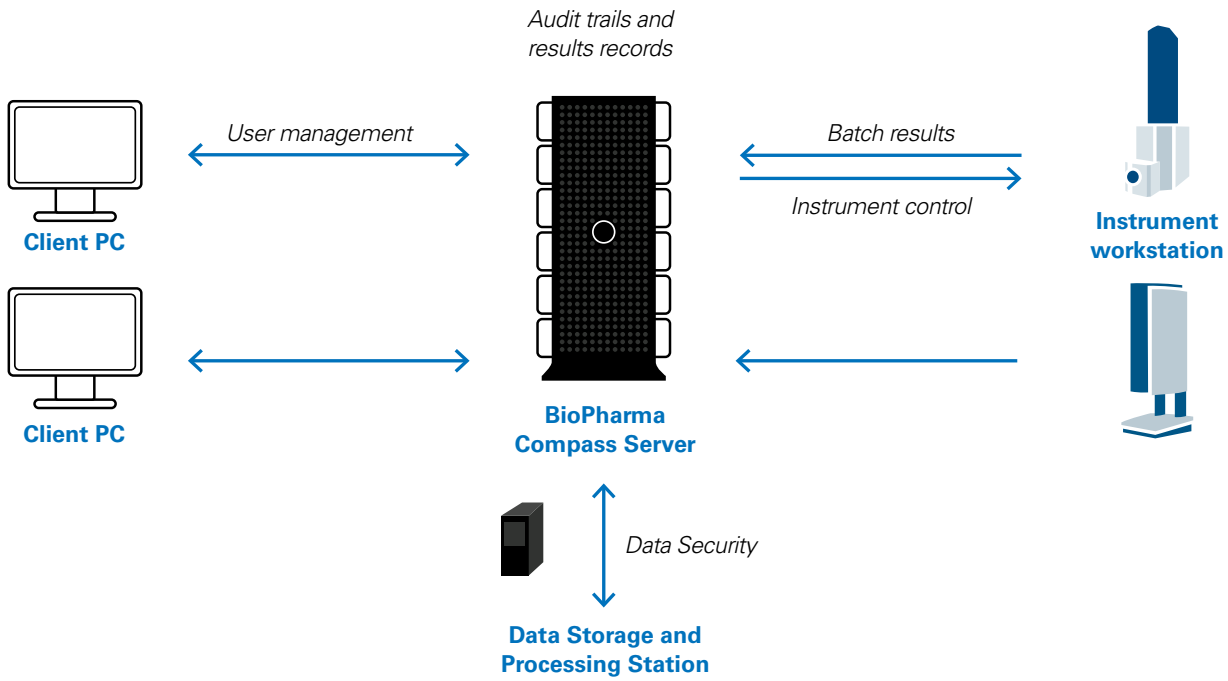
- Single GUI for acquisition and processing
- Entire process contained in a single workflow

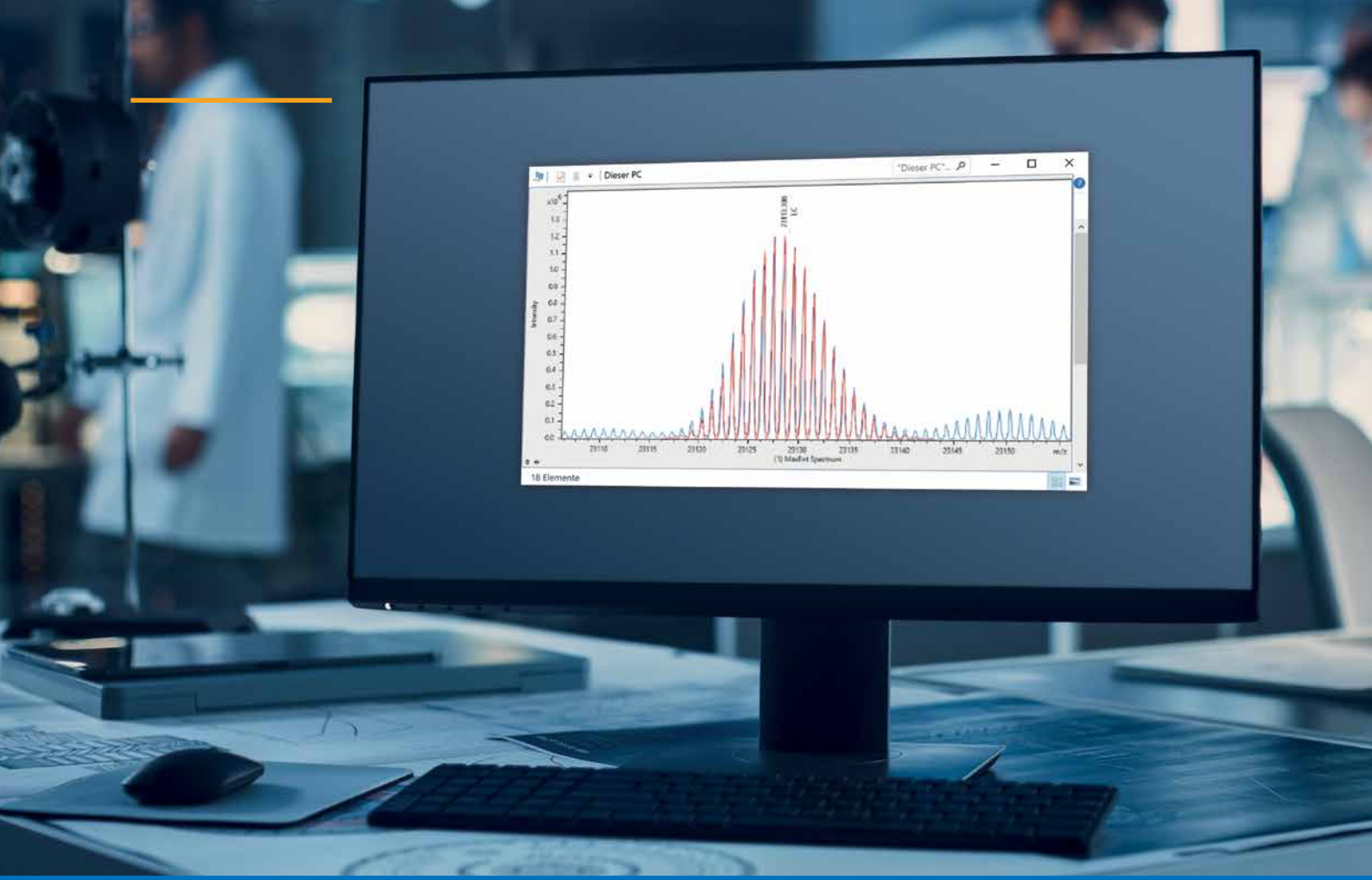
### Powerful algorithms

- Optimized for high isotopic fidelity data
- Multi attribute screening with collisional cross section (CCS)
- Fast PASEF® peptide maps with CCS-enabled selectivity

### Easier implementation of GLP guidelines

- State-of-the-art data security
- Version tracking for all editable items
- User management and audit trails






Algorithms built for instruments with **high isotopic fidelity** deliver sub-ppm mass accuracy.

Support for timsTOF, QTOF and MALDI-TOF offers users a comprehensive range of options to optimize **resolution, speed and selectivity** for their application and budget.

# Confident characterization of oligonucleotides and RNA

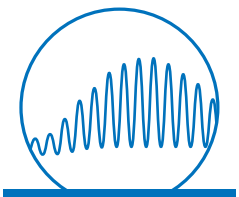
**RNA and oligonucleotides** are an increasingly important class of molecules. Whether an RNA molecule is used directly as API or as a tool for gene editing, it is necessary to comprehensively characterize its primary sequence, modifications and impurities.

In particular the MS2 analysis of these compounds raises unique interpretation challenges due to the complexity of the fragmentation pattern and the limited number of nucleic acids building blocks. Embedded in BioPharma Compass, **OligoQuest™** provides BioPharma scientists with the tools to comprehensively verify oligonucleotides and related impurities by accurate mass and CID fragmentation.

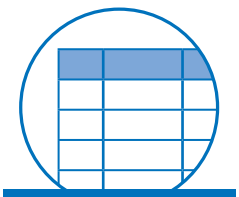
## Comprehensive tools for RNA and oligonucleotide sequence verification

- Flexible definition of building blocks nomenclature and nucleotides modifications
- Deconvolution and peak picking optimized for high isotopic fidelity data
- Interpretation of termini and internal MS2 fragments enabled by high mass accuracy and fidelity, and resolution of fragment ions.

Oligonucleotide LC-MS analysis



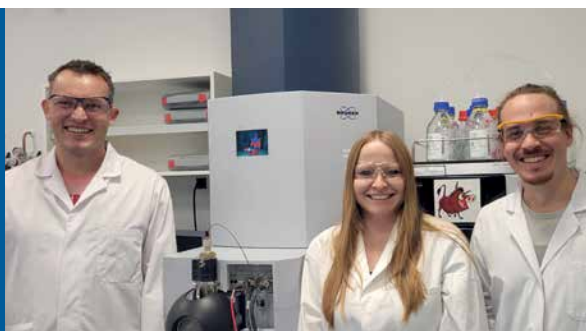
Deconvolution and monoisotopic annotations



MS2 based impurities confirmation

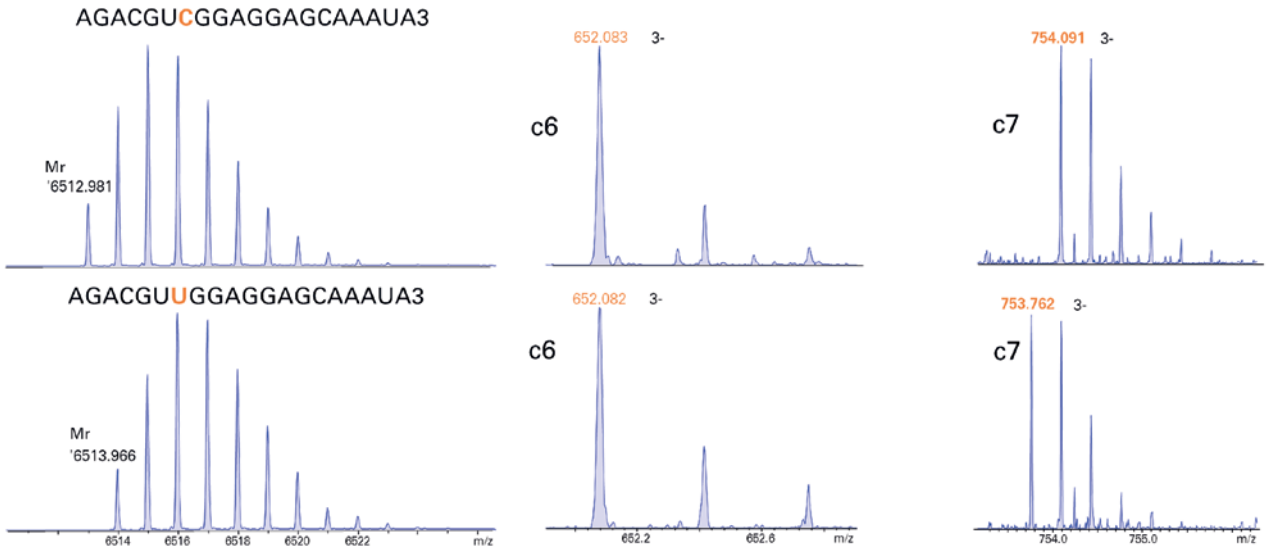
» "Isomeric Oligonucleotides can be analyzed with OligoQuest™ allowing to identify base exchanges. Already the first version could be included in our day-to-day workflow."

Team at Axolabs GmbH Kulmbach, Germany



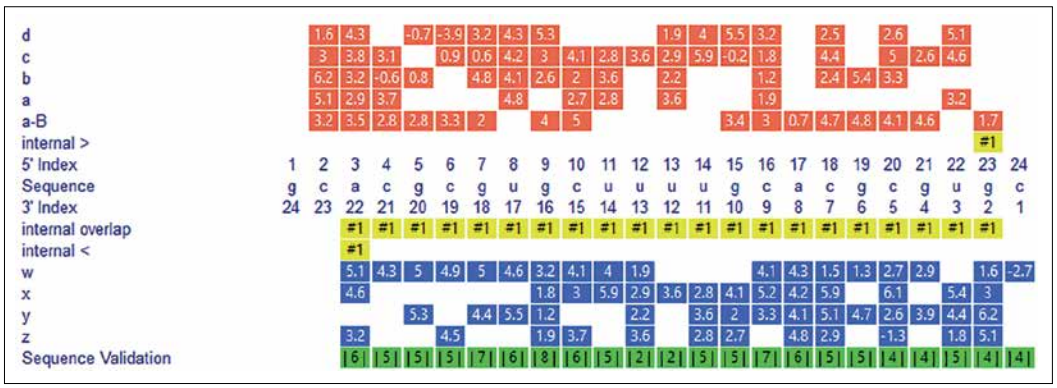
## OligoQuest workflow

Confident annotation of 1 Da C>U variants
using high isotopic fidelity data




**Deconvoluted MS spectrum**

**Confirmatory MS2 fragments (CID, 30 ev)**



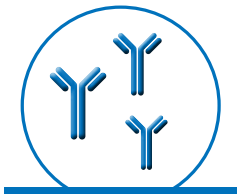

# Routine characterization of protein therapeutics

**In recent years**, monoclonal antibody-based therapeutics have been highly represented in both new drug approvals and clinical pipelines. For the related development projects it is essential to characterize the molecule's primary sequence as well as identify and track modifications that are identified as critical quality attributes. The intact analysis of mAbs or related domains requires high mass accuracy in order to confidently confirm the molecule's identity.

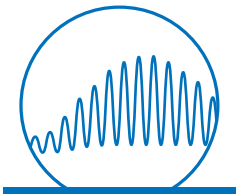
BioPharma Compass is optimized to take advantage of high isotopic fidelity data for intact mass analysis.
Heterogeneities of interest can be further characterized by top-down analysis or peptide mapping.

## Confident mAb characterization

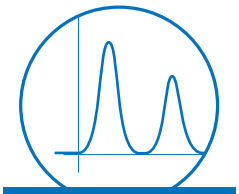
- Deconvolution and deisotoping optimized for high isotopic fidelity data
- Simulation of theoretical isotopes and butterfly views for visual comparison
- Full automation from sample submission to report



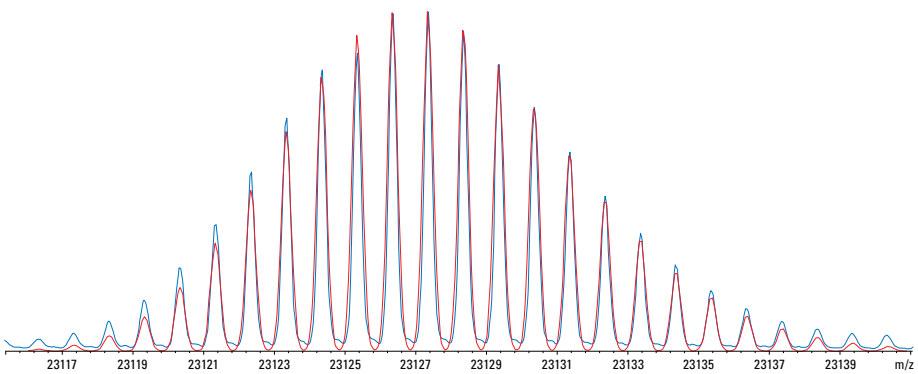
Clone Screening



Intact, reduced and subunit analysis

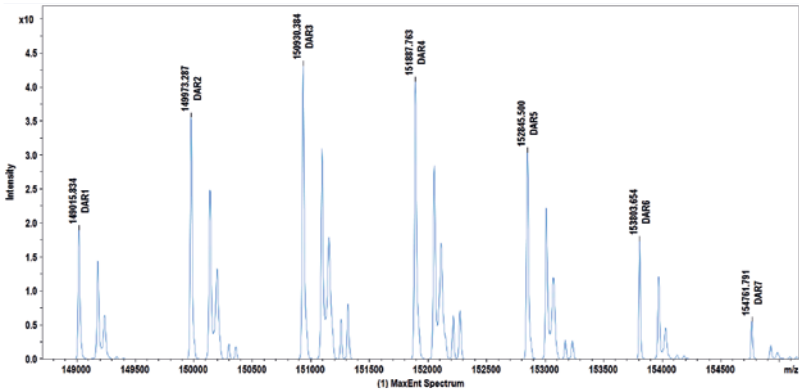


Peptide mapping




mAb light chain measured wirh high isotopic fidelity for sub-ppm mass accuracy

## Intact protein and drug distribution analysis



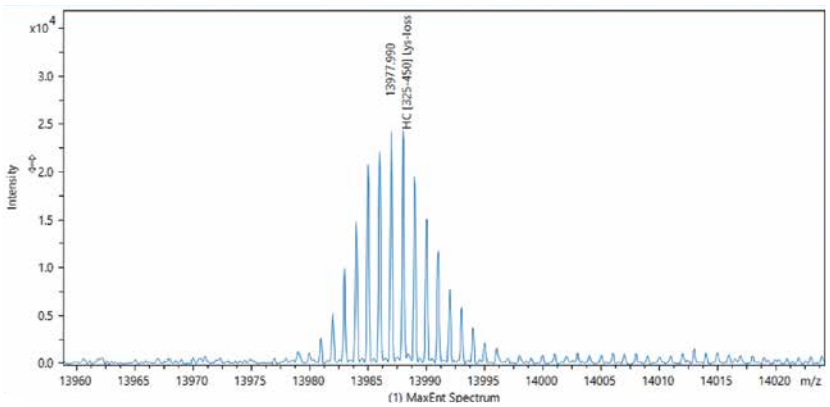

Tools optimized to gain the most insights in your intact and subunit analysis for characterization or clone screening. Carry out multiple attribute method (MAM) analysis at the intact level with speed and confidence.

- **Algorithms designed to take advantage of data with high isotopic fidelity.**
- Flexible peak annotation system
- Support for top-down analysis the investigation of unknown peaks

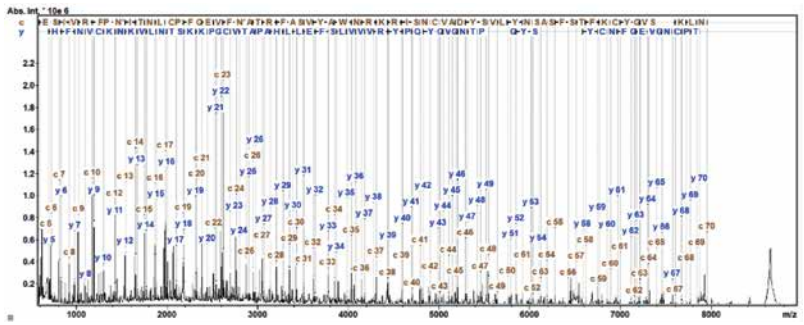
**MAM Protein screening** ↔ **Top-down/ Middle down**

**Clone screening (ESI/MALDI)**

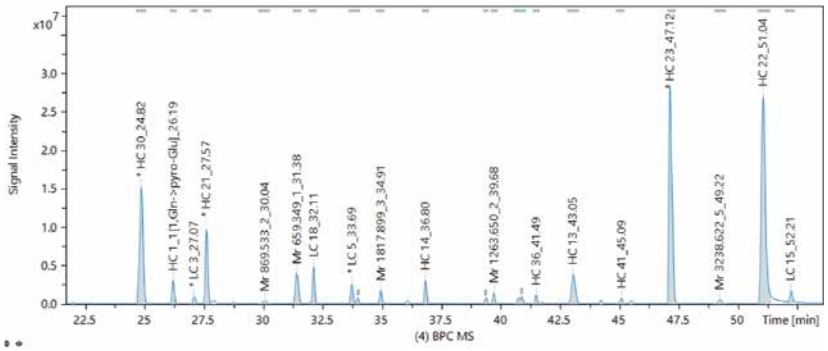
## Automated annotation of clipped fragments

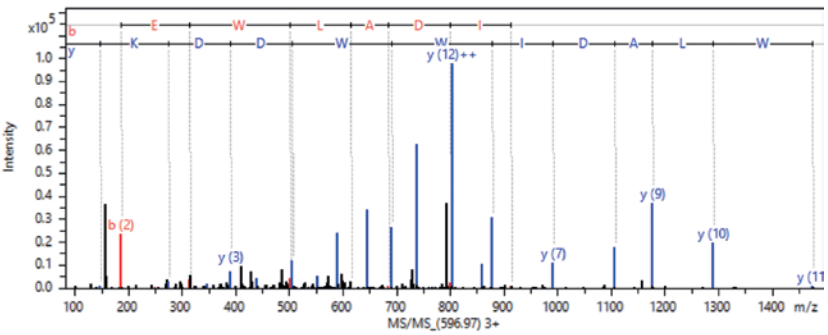


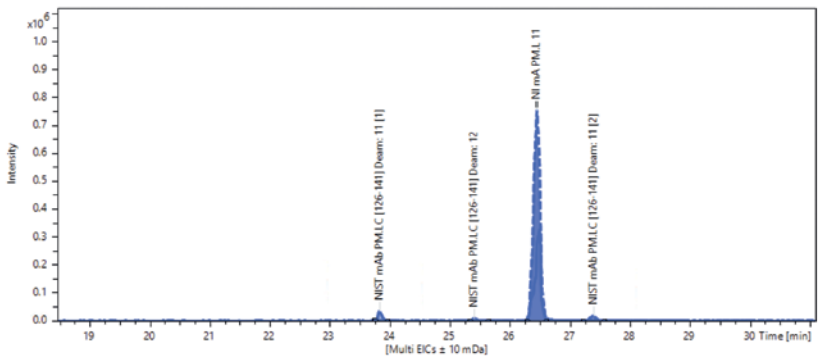

## Top-down sequencing by ESI or MALDI



## Peptide level analysis




From database search for HCP analysis to in-silico digest for peptide mapping and development of multiple attribute monitoring methods, fully characterize and quantify your molecule's impurities and heterogeneities.

- Interactive sequence coverage maps simplify data review
- Annotated chromatograms and MS2 spectra to verify primary sequence and identify modifications
- Easy conversion of peptide map data into MAM screening methods for EIC based quantitation
- Easy conversion of peptide map data into MAM screening methods

**Peptide mapping (PASEF)** ↔ **MAM Peptide screening**

**Advanced analysis:**
**Database search, glycan MS2 annotation**

## Fast sample screening

Info | Result

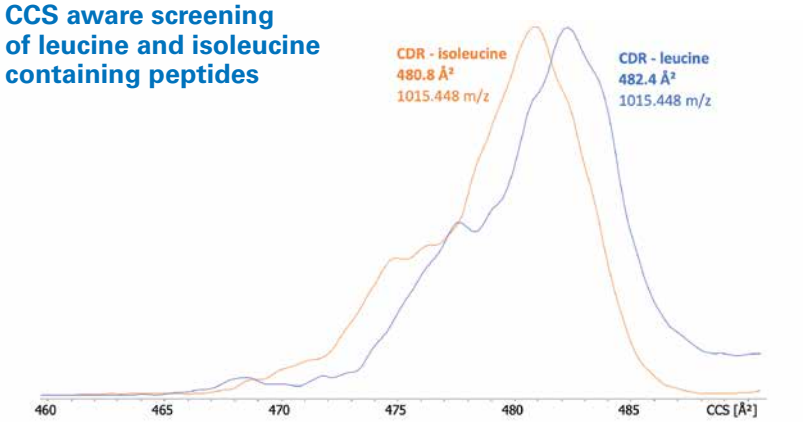
| Row | Result | Position | Base Peak Mr [Da] | ΔBase Peak Mr [Da] | Sample Name | Matrix | Operator |
|---|---|---|---|---|---|---|---|
| 1 | | B3 | 555.2642 | -0.0051 | Leu-Enkephalin | CCA | AR |
| 2 | | C3 | 756.3875 | -0.0043 | Bradikinin fragment | CCA | AR |
| 3 | | D3 | 898.4560 | -0.0101 | Angiotensin III | CCA | AR |
| 4 | | E3 | 1045.5256 | -0.0090 | Angiotensin II | CCA | AR |
| 5 | | F4 | 1295.6731 | -0.0044 | Angiotensin I | CCA | AR |
| 6 | | G3 | 1362.7093 | 15.9811 | Substance P | CCA | AR |
| 7 | | H3 | 1551.6370 | -18.0325 | Glu-Fib B | CCA | AR |
| 8 | | I3 | 1618.7885 | -0.0266 | Bombesin | CCA | AR |
| 9 | | J3 | 1757.8914 | -0.0339 | Renin Substrate | CCA | AR |
| 10 | | K3 | 2092.0380 | -0.0409 | ACTH clip 1-17 | CCA | AR |
| 11 | | L3 | 2464.1436 | -0.0475 | ACTH clip 18-39 | CCA | AR |

**Confident detection of analytes based on accurate mass, collisional cross section and retention time.**

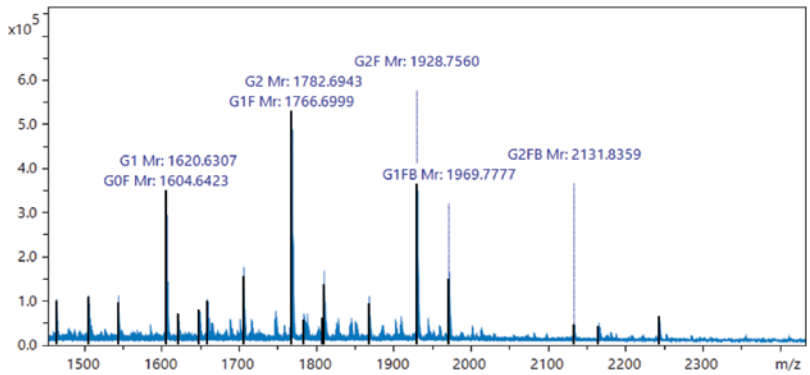
**Flexible workflow can be applied to the QC of oligonucleotides, synthetic peptides, glycan mixtures or raw materials.**

**Rapidly analyze large sample batches with automated analysis and data processing. Results are easily visualized with traffic light based attributes reporting.**

## CCS aware screening of leucine and isoleucine containing peptides




## Released glycan profiling with MALDI




**Peptides and oligonucleotides screening (ESI/MALDI)**

**Accelerate your routine BioPharma assays**

BioPharma Compass simplifies data acquisition and processing for users of Bruker QTOF, timsTOF and MALDI instruments with an interface optimized for the routine characterization of therapeutics proteins and oligonucleotides.

- Automation of routine characterization tasks from acquisition to report from a single interface
- Integrated tools assist with data integrity requirements
- Workflows supporting major analytical tasks for proteins and oligonucleotides analysis



For Research Use Only. Not for use in clinical diagnostic procedures.

**Bruker Switzerland AG**

Fällanden · Switzerland
Phone +41 44 825 91 11

**Bruker Scientific LLC**

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

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

**Online information**
bruker.com