

TIMS-MS

timsOmni™ Σ

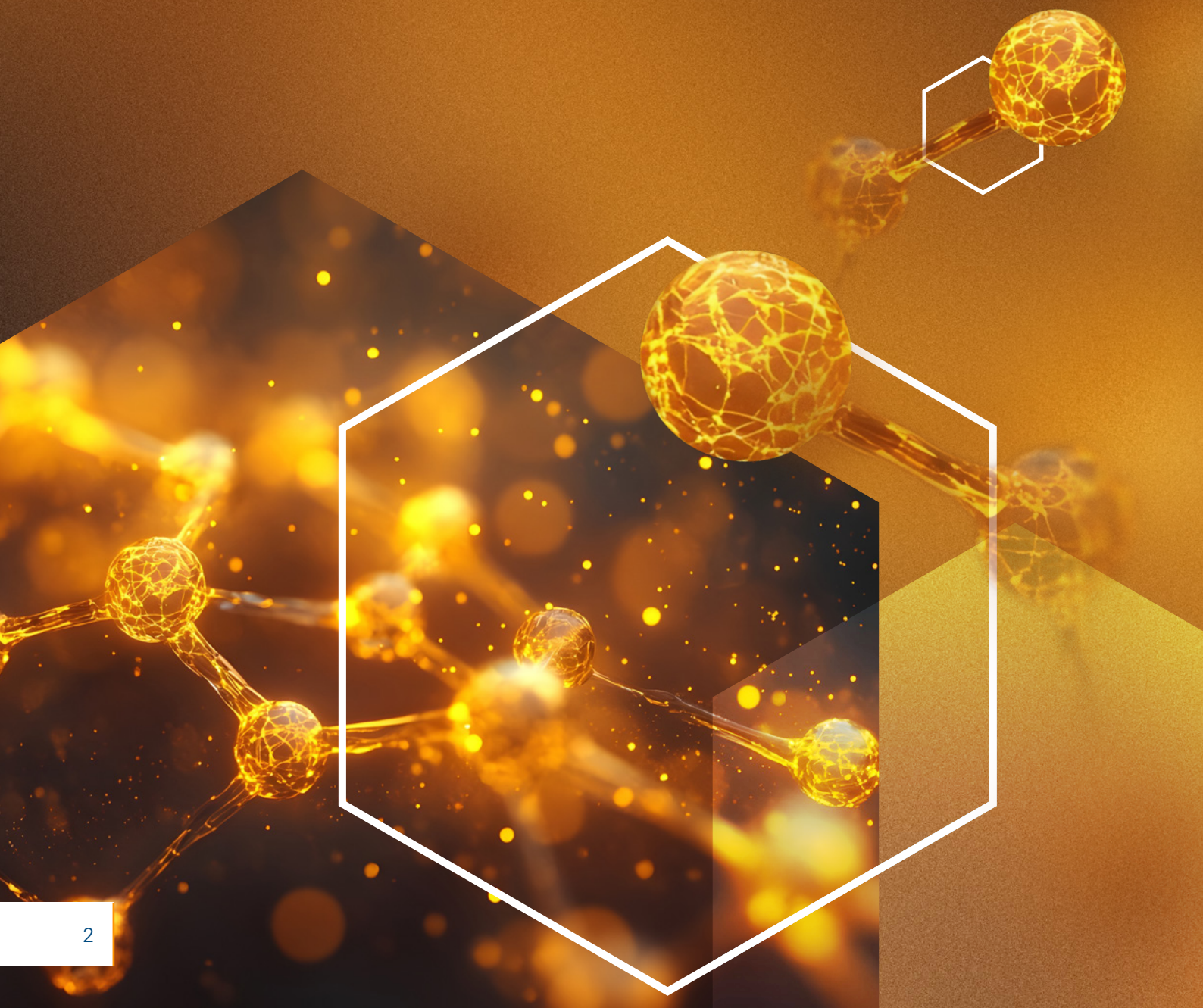
High sensitivity multiOmics powered by PASEF-EXD
for advanced structural elucidation

Innovation with Integrity

A transformative advance for electron-based fragmentation techniques

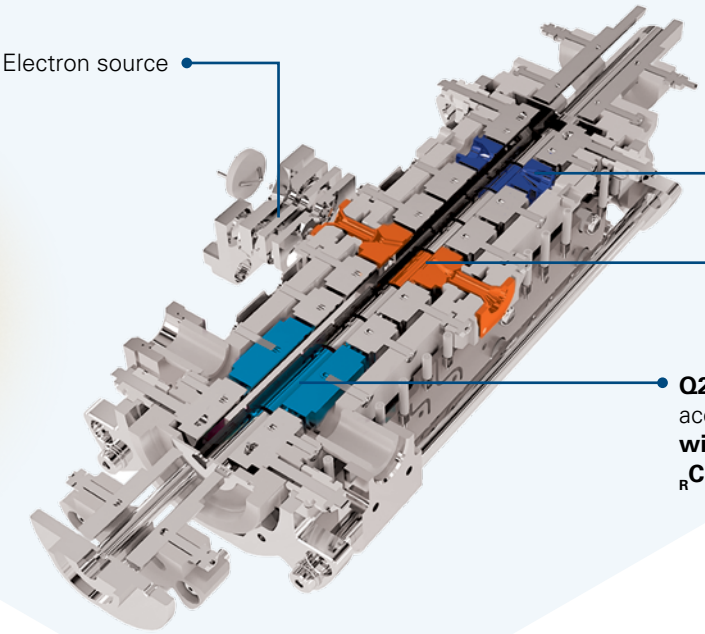
Welcome to the timsOmni™ Σ, a transformative instrument poised to revolutionize mass spectrometry in systems biology. Designed to push the boundaries of scientific discovery, the timsOmni ∑ achieves extraordinary sensitivity and delivers unprecedented precision in structural elucidation. The timsOmni ∑ enables detailed structural insights of potential mutagenic impurities, revealing how subtle chemical modifications can transform benign small molecules into carcinogenic threats, corroborating the superior versatility of this groundbreaking technology.

Empowered by advanced MS" eXd and ion enrichment methods, this innovative platform detects labile post-translational modifications (PTMs), produces complementary fragment ions to resolve ambiguous spectra, delivering biology- and chemically relevant insights with unmatched depth and accuracy.

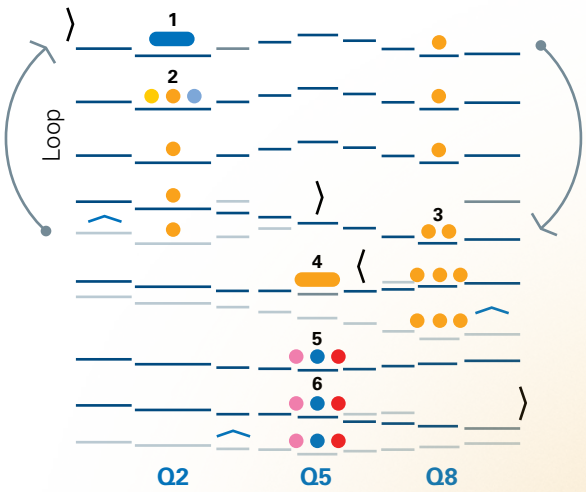


Experience unmatched MS and MS^n sensitivity

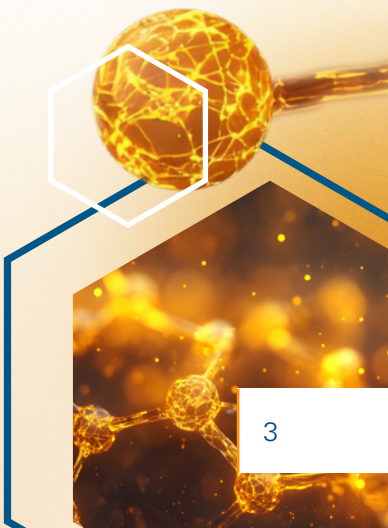
Powered by proprietary omni-directional lossless transfer and ion enrichment, signals for even the lowest-abundance ions are drastically amplified. Through precise modulation of selected ion packets, any ion, regardless of its intensity, can be selectively targeted for electron-based fragmentation.



Omni-directional MS^n eXd with ion enrichment



1) Quad isolation and direct omni-accumulation of precursor ions in section Q2.
2) Resonance excitation Collision Induced Dissociation ($_R$CID) and isolation of target fragments for further interrogation.
3) Signal amplification via ion enrichment of selected MS^2 CID fragments in Q8.
4) Transfer of the accumulated MS^2 CID ion population in section Q5.
5) MS^3 trapped eXd fragmentation of the enriched ion population
6) Ejection of MS^3 product ions to TOF.

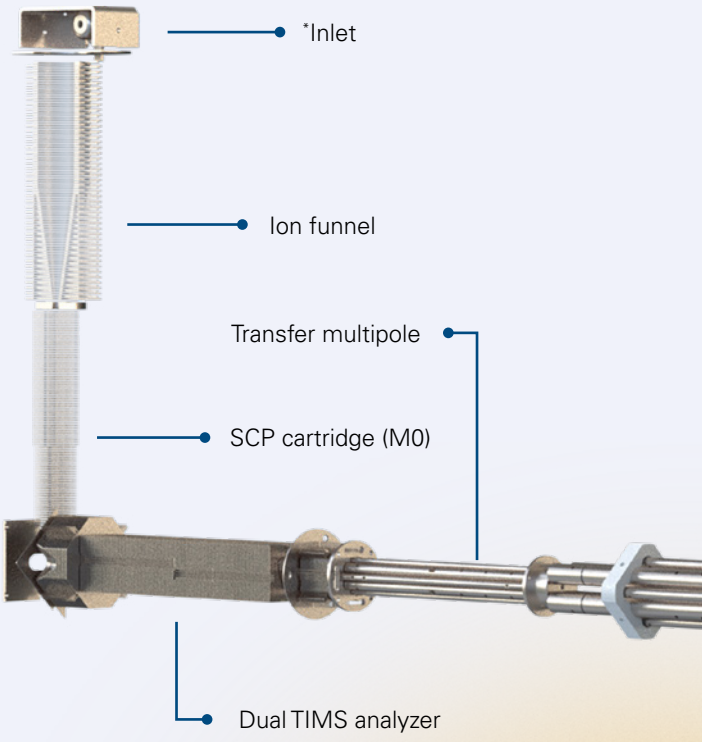


Introducing the timsOmni Σ

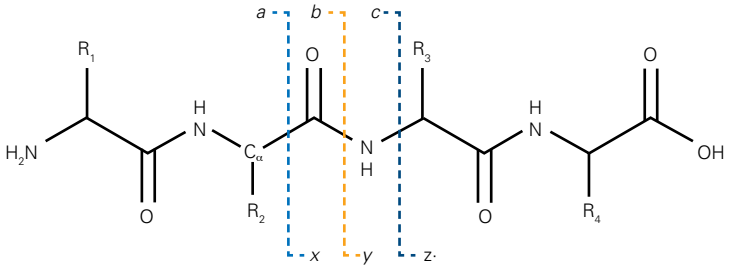
Advanced structural elucidation and deep proteoform sequencing by **MS^n eXd** coupled to the power of TIMS.



- TIMS separation to determine conformational heterogeneity and CCS to reveal structure
- Trapped eXd for optimal precursor utilization boosting fragment ion yield
- Precise control of electron-based fragmentation for detailed molecular profiling
- Omni-directional MS^n and trapped eXd with ion enrichment for unmatched sensitivity
- Utilization of all PASEF modes for bottom-up proteomics and multiomics



*Incompatible with NEOS source

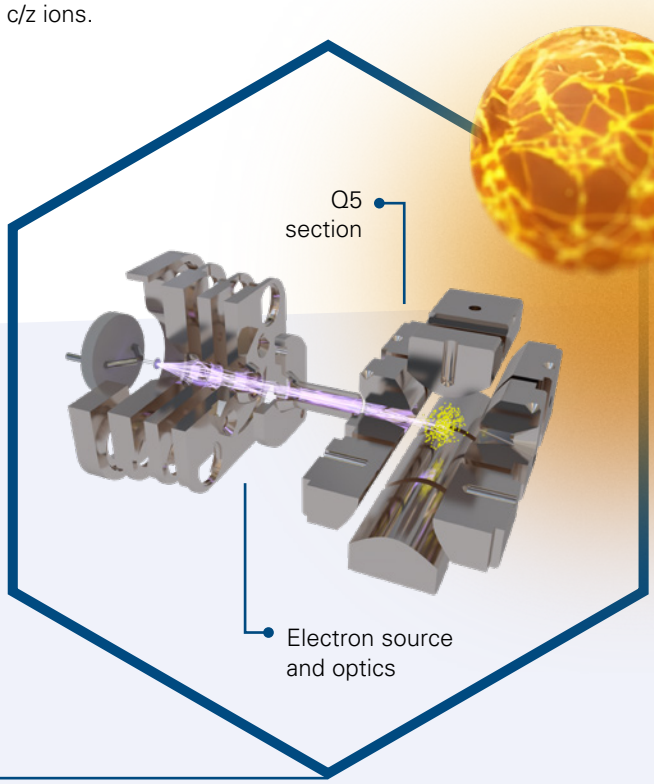


Nomenclature for the primary fragment ions types observed for peptides and proteins in tandem mass spectrometry.

In ECD, when a protein or peptide ion captures a free electron, bond cleavage occurs rapidly and locally at the N–Cα bond, producing primarily c/z fragments. This non-ergodic process preserves labile post translational modifications like phosphorylation, glycosylation, sulfonation, etc.

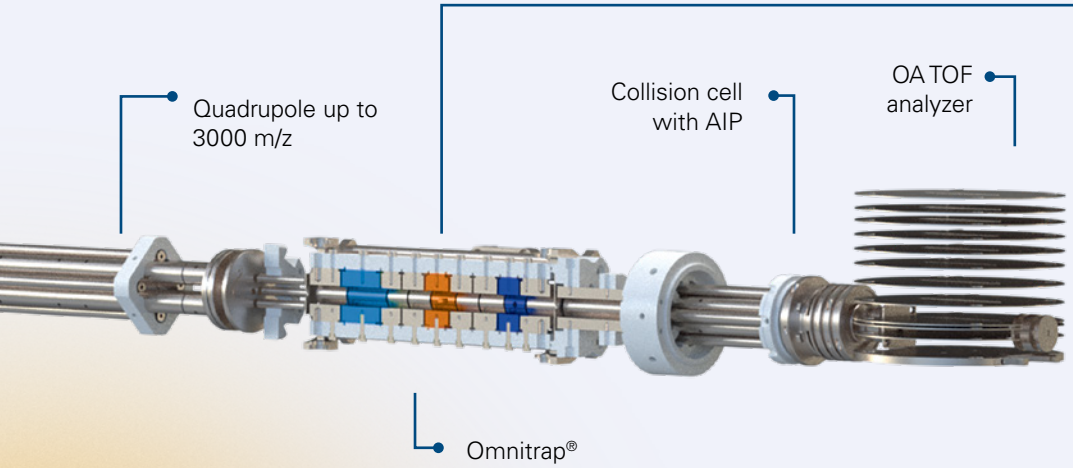
In CID, ions are gradually heated through multiple collisions, spreading energy throughout the molecule (ergodic). This causes only the lowest-energy bonds to break, mainly producing b/y fragments with limited sequence coverage and often poor PTM characterization.

Combinations of ECD and CID using **MS^n eXd** can be used to further enhance protein sequence coverage through formation of a/x, b/y and c/z ions.



A small detail with a big impact

A hot cathode produces a high-density electron beam, guided by a lens system into section Q5 for high efficiency eXd reactions with trapped ions, increasing product ion yield compared to other soft fragmentation methods.

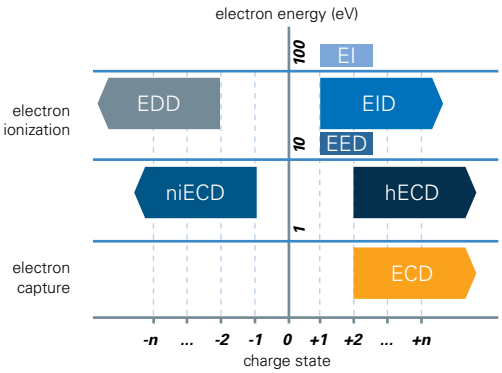


Why AIP is a game changer?

The AIP addresses mass discrimination effects in transferring ions to the TOF and results in a much broader mass range of ions being observed in the mass spectrum.

Precise modulation of electron kinetic energy and reaction time

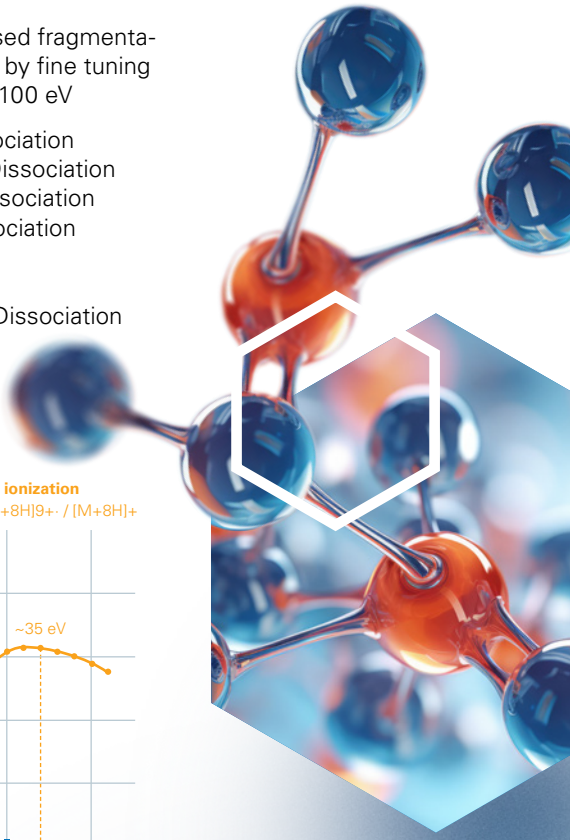
Precisely tune electron energy to access diverse fragmentation regimes. Adjust eXd reaction times and explore uncharted electron energy levels for different classes of analytes to achieve optimal product ion coverage.



eXd Landscape

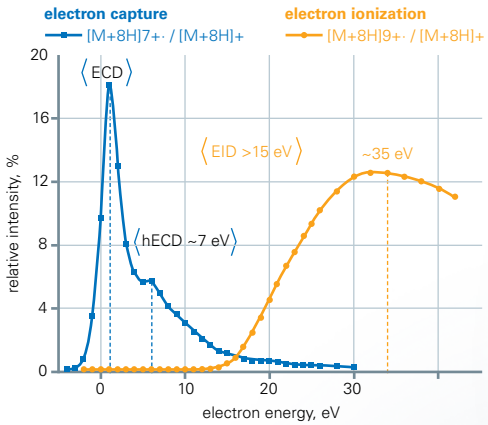
Access to different electron-based fragmentation regimes becomes available by fine tuning electron energy from 0.1eV to >100 eV

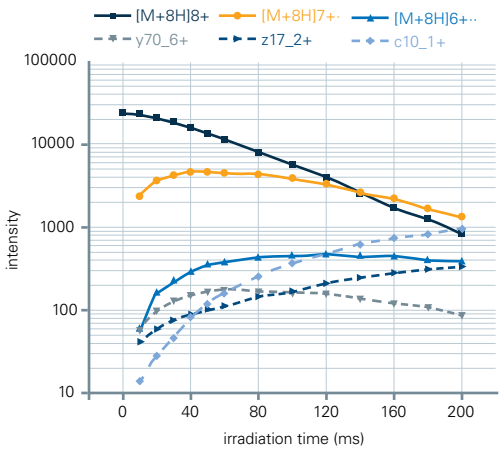
ECD – Electron Capture Dissociation
hECD – hot Electron Capture Dissociation
EED – Electron Excitation Dissociation
EID – Electron Induced Dissociation
EI – Electron Ionization
niECD – Negative-Ion ECD
EDD – Electron Detachment Dissociation



Electron energy optimization

Optimized electron energies allow controlled access to distinct eXd regions affecting fragmentation patterns leading to advanced structural insight for the target molecule.





Trapped ion eXd

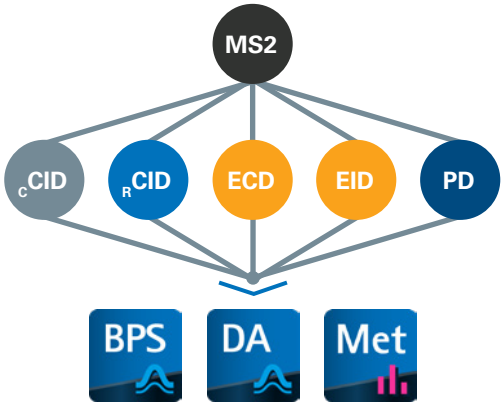
In trapped ion eXd, precursor ions are confined and rapidly fragment upon electron irradiation. Adapting the trapping time enables it to boost the fragment yield and reach optimal precursor consumption (>90%). This unique capability differs from traditional in-line electron-based fragmentation techniques.

Unlocking deep-sequencing in multimodal and MS^n modes

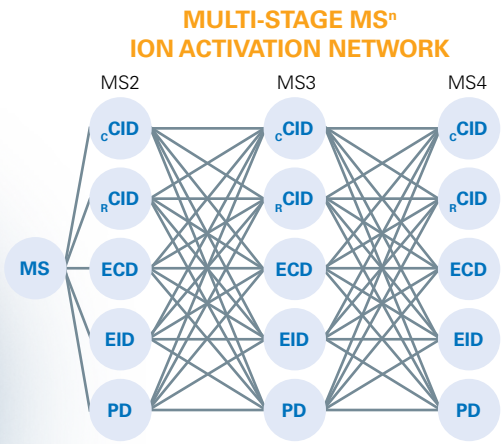


Online multimodal fragmentation

Multimodal fragmentation relies on combining information from first-generation fragment ion types produced by complementary ion dissociation methods to drastically increase sequence coverage.

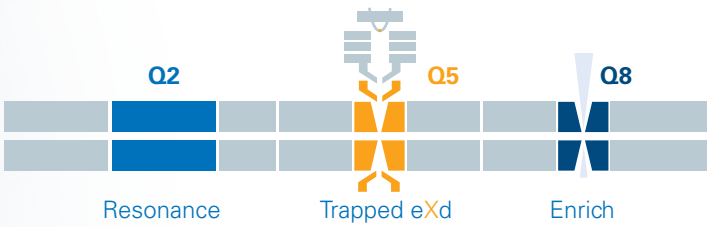


cCID – Collision-cell Collision Induced Dissociation
rCID – Resonant-excitation Collision Induced Dissociation
ECD – Electron Capture Dissociation
EID – Electron Induced Dissociation
PD – Photo-dissociation



Successive stages of ion activation enable first- and second-generation fragments to be selected for subsequent analysis. Distinct dissociation techniques can be employed at each MS^n stage, allowing for highly customizable workflows. These tailored MS^n strategies are well-suited to explore a broad range of analytes with diverse structural and chemical characteristics.

Ion enrichment provides unprecedented levels of sequence and structural interrogation through signal amplification, leveraging the high-capacity trapping sections across the Omnitrap platform.



Let's break it down!

cCID occurs by axial acceleration of ions into the collision cell

rCID occurs by resonant excitation in section Q2 of the Omnitrap platform

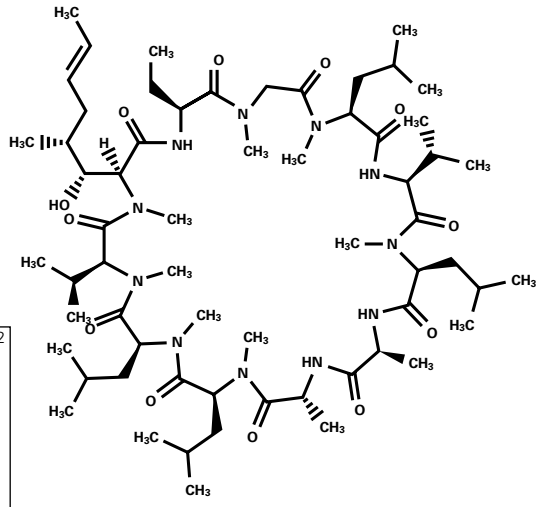
eXd occurs in section Q5, receiving variable energy electrons from an external hot cathode

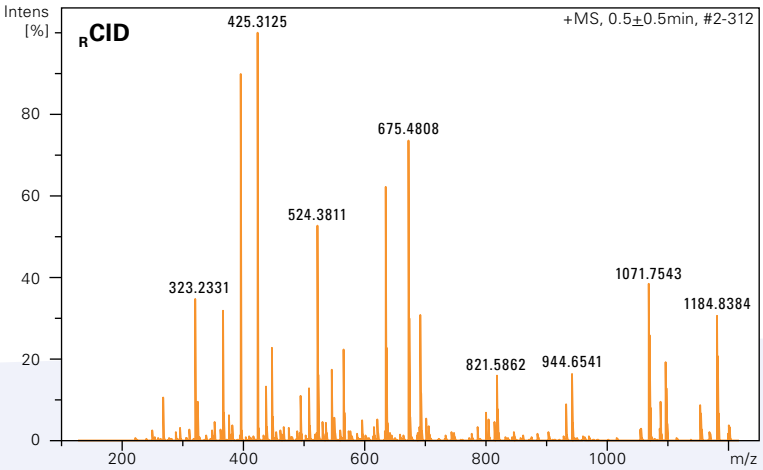
Signal amplification via ion enrichment and also optical access is provided in section Q8

Breaking the cycle: A dedicated workflow for characterizing cyclic peptides

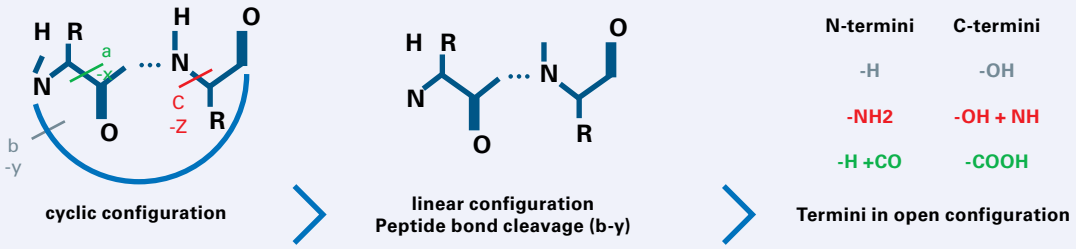
Non-linear peptides

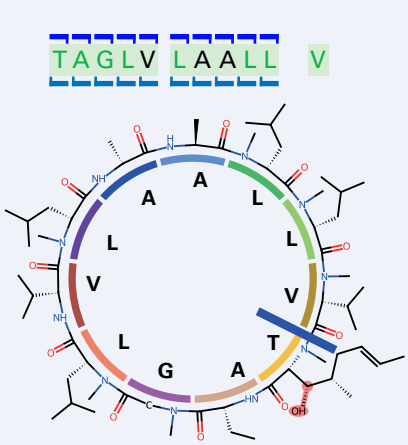
Cyclic peptides are modular polypeptide chains composed of canonical and non-canonical amino acids that are connected at distant positions to form macrocyclic structures. Large libraries can be easily created for biological screening.

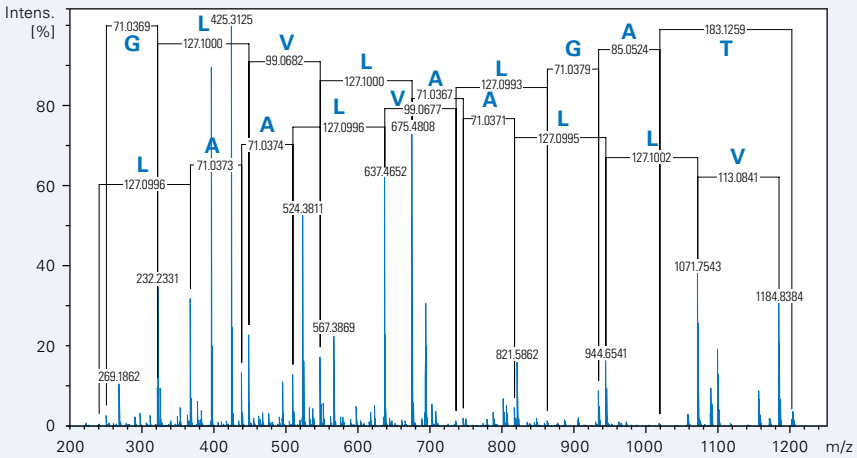




The timsOmni ∑ collision-based and electron-based fragmentation techniques are used to linearize and sequence cyclic peptides. The exquisite control on the collision-based and electron-based activation as well as the ability to combine multiple activation steps allows to generate easy-to-read fragment ion ladders for unambiguous characterization.







EXD-PASEF: Ultimate versatility for deep PTM characterization

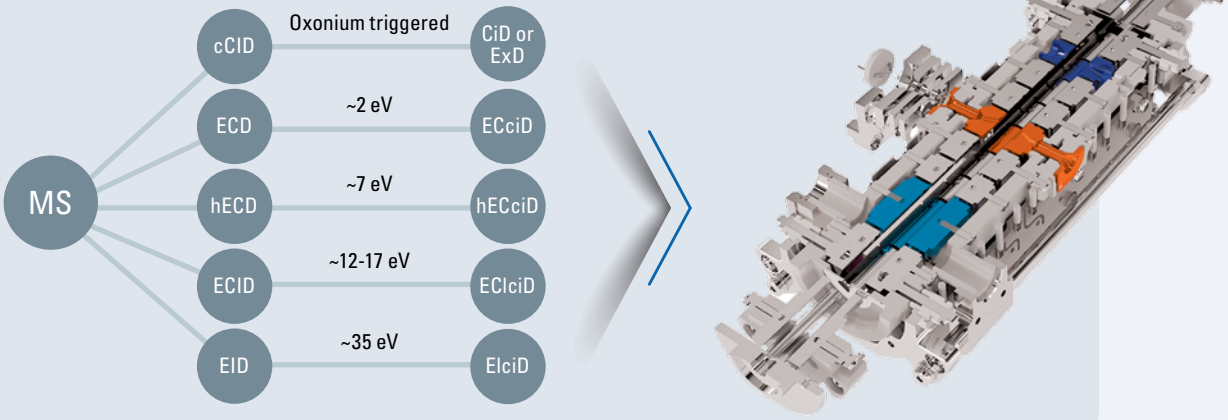
Online multimodal fragmentation

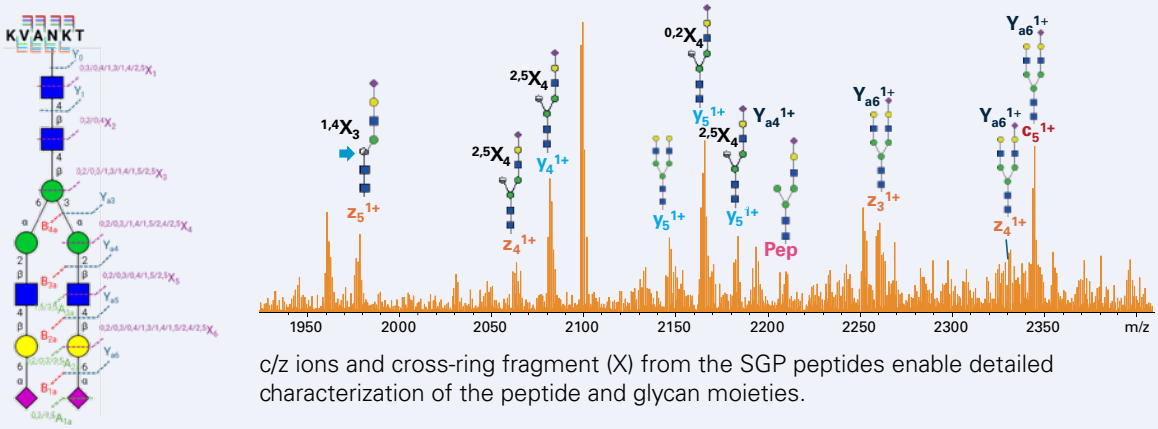
Multimodal fragmentation relies on combining information from first-generation fragment ion types produced by complementary ion dissociation methods to drastically increase sequence coverage.

Fit-for-purpose workflows for glycoproteomics

The timsOmni platform offer an unprecedented control for the fragmentation of PASEF selected precursor ions. Electron fragmentation takes place in the Omnitrap region, trapped ions are confined in the electron beam before travelling through the collision cell where product ions can be further activated (denoted with ci in graph below), giving researchers the opportunity to adjust conditions for their analytical objectives.

- Low electron energy (ECD: 0-2 eV) promotes peptide fragments with intact glycans, ideal for O-glycan localization
- Higher electron energy (ECID 12-17 eV and EID 35 eV) favors the fragmentation of the glycan and enables structural insights



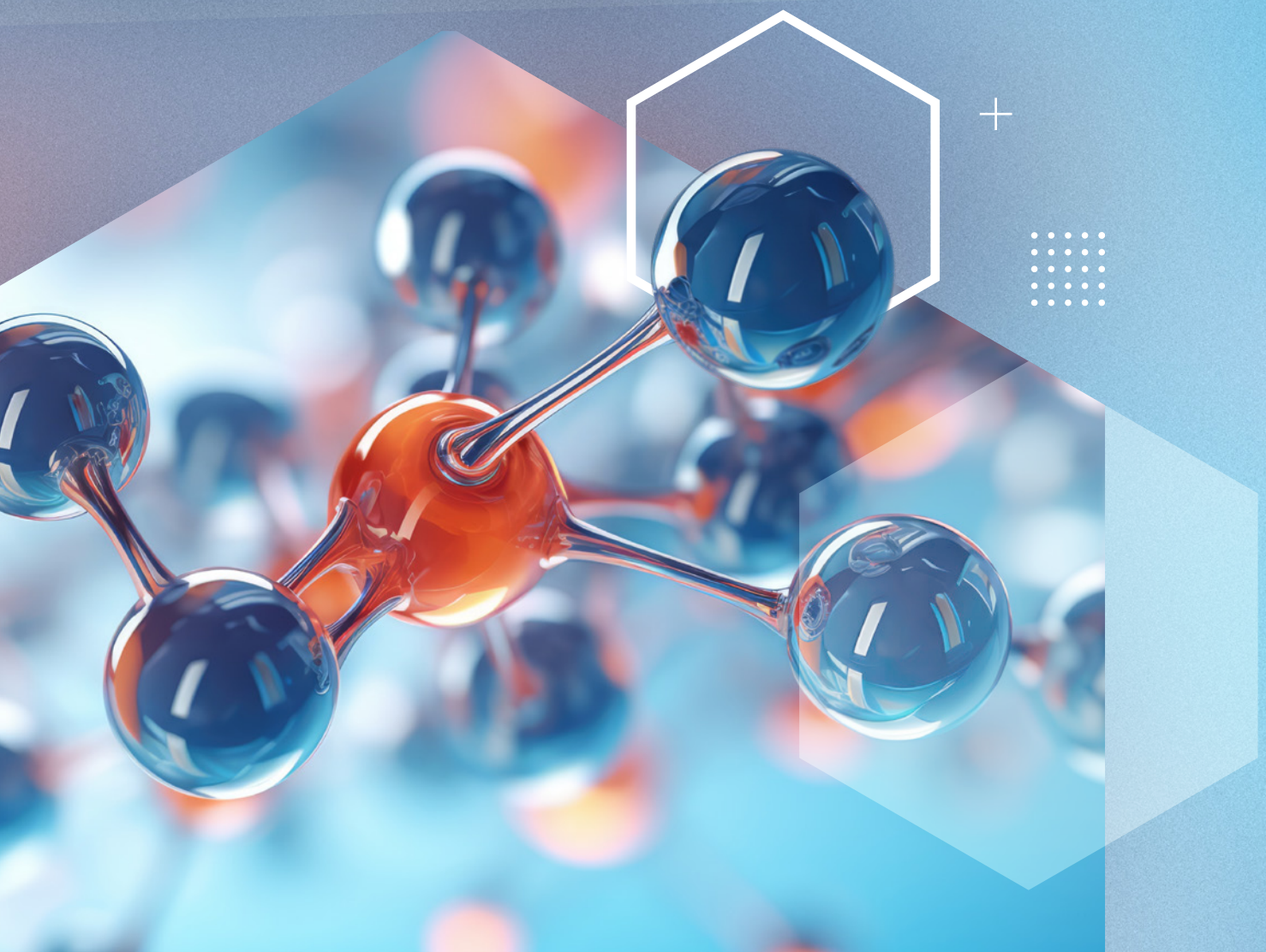


c/z ions and cross-ring fragment (X) from the SGP peptides enable detailed characterization of the peptide and glycan moieties.



Gustaf Hulthe, Pharmaceutical Technology & Development, AstraZeneca R&D, Gothenburg, Sweden

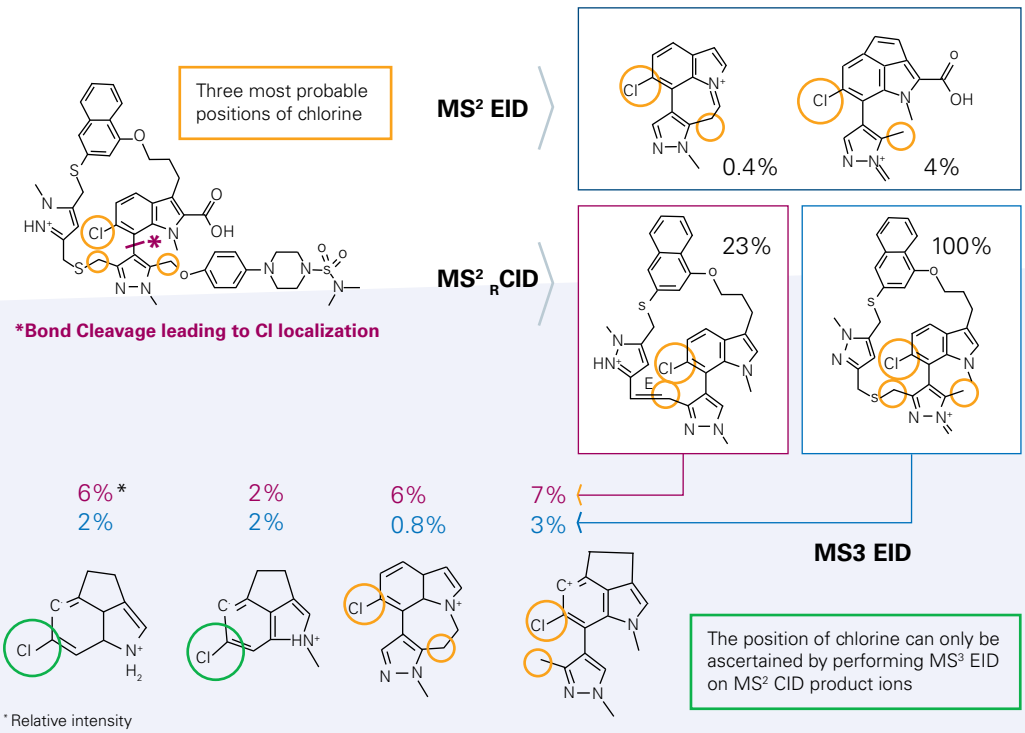
"In many cases MSn CID or EID cannot resolve the structure of observed impurities. The extremely versatile possibilities the timsOmi provides is a gamechanger and so far has solved every structural problem we have challenged it with, without performing synthesis."

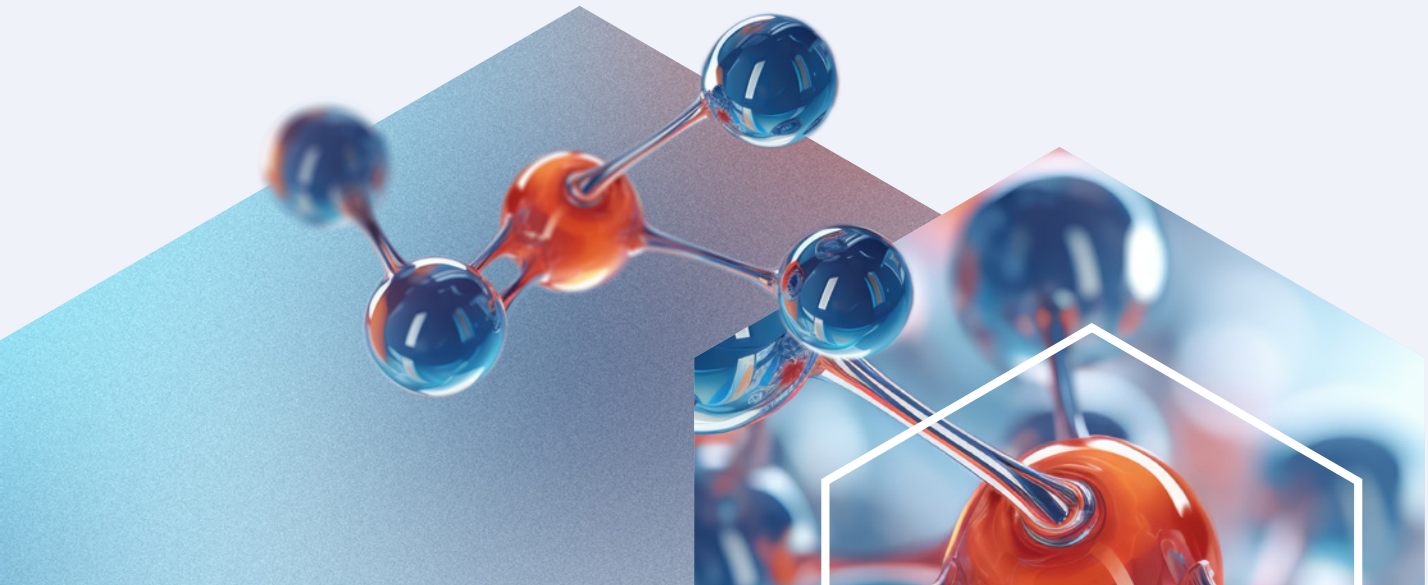


Advanced Structural Elucidation of Small Molecules with MSn eXd

In pharmaceutical development, detailed information on chemical structures is crucial to assess toxicity of impurities often produced during degradation or synthesis. New analytical workflows providing detailed structural elucidation eliminate the need to synthesize impurity standards, considerably accelerating drug development.

Where is the chlorine? Aromatic chlorines are not reactive and are found in many drugs, while benzylic chlorines are potent alkylating reagents for DNA and proteins, rendering them carcinogenic. Locating the position of chlorination in trace impurities is critical as benzylic chlorines must be strictly controlled to minimize mutagenicity. The timsOmni ∑ goes beyond currently available MSn CID and MS2 EID activation methods, addressing such questions by accessing previously unreachable molecular bonds with MS**n** e**X**d.





Connecting PTMs and Biology:
Advance glycobiology with timsOmni Σ

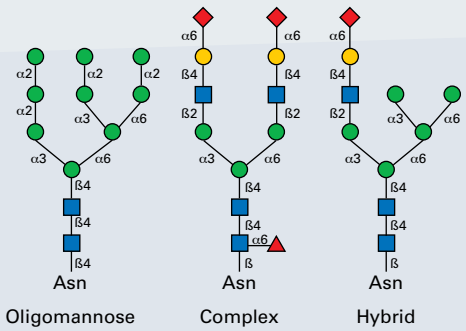
Glycoproteomics presents unique analytical hurdles: labile glycan structures, high heterogeneity and isomeric species raise the need for tools beyond traditional bottom-up.

timsOmni Σ was designed to tackle these challenges head-on, combining Trapped Ion Mobility Spectrometry (TIMS) with multimodal fragmentation to deliver both high-throughput discovery and deep structural characterization of glycopeptides. With PASEF-EXD, researchers can identify more glycopeptides with greater confidence and decipher glycan structures in unprecedented detail using a single instrument platform.

Hurdles to comprehensive glycopeptides characterizaations

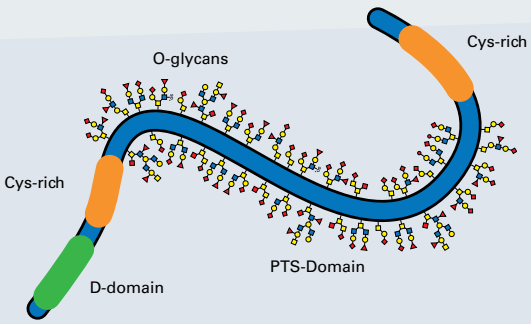
N-linked glycans

Complex multiantennary structures require orthogonal fragmentation methods to confidently identify the glycan topology.



O-linked glycans

While simpler in structure, their close proximity on the protein backbone requires methods to fragment peptides while keeping the glycans intact.

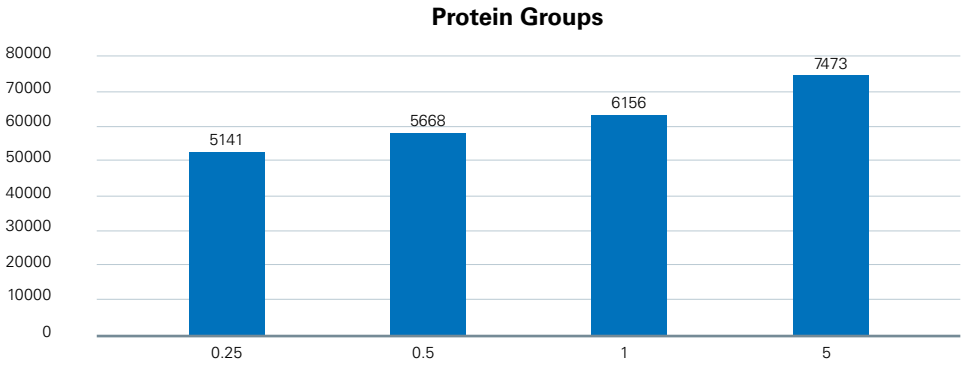


High performance technology stack for glycoproteomics

Ultra sensitivity	TIMS	CID	Omnitrap technology	Bioinformatics
Optimized for low sample input	Proteomics at scale with PASEF	Oxonium triggered modes maximize duty cycle	O-linked Glycan localization with ECciD	Real time search with ProteoScape
High dynamic range	Reduced chimeric spectra with CCS based separation	Stepped collision energy improves IDs	N-linked Glycan topology with EXciD and ElciD	Open data format supports innovation
			Enrichment capabilities for maximum sensitivity	

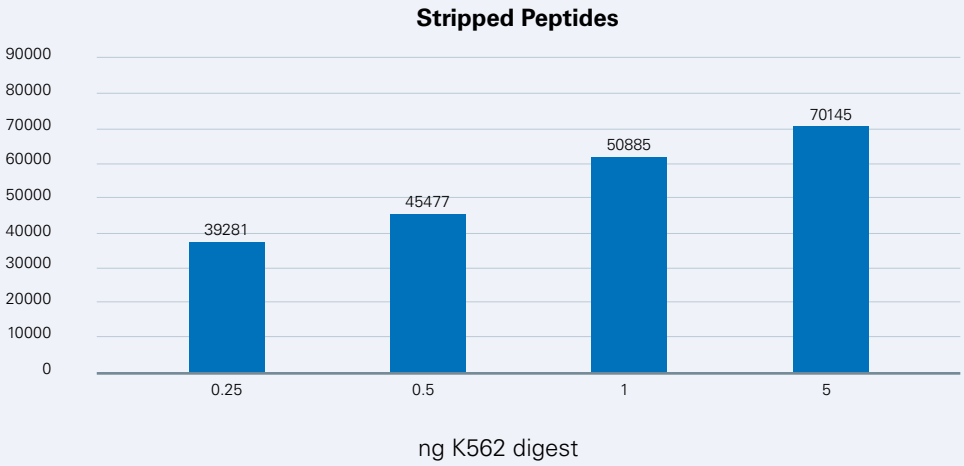
timsOmni Σ: Exceptional Sensitivity for High-Confidence Bottom-Up Proteomics

timsOmni ∑ is an evolution of the timsTOF Ultra 2 system developed with improved bottom-up proteomics and a focus on glyco-peptides, small molecules structural identification with EXD capabilities and AIP.



A single fact

The timsOmni Σ delivers the entire range of PASEF modes from the timsTOF platform family



Peptides and protein groups in a Promega K562 digest measured by DIA-PASEF. A 22min gradient was used with an Aurora Ultimate column at 250 nl/min flow rate. Results were searched against the Swissprot human database.

Fit-for-purpose workflows for glycoproteomics

- **Dual excellence:** exceptional sensitivity for bottom-up proteomics and industry-leading structural-analysis capabilities.
- **Switch seamlessly** between advanced MS**n** e**X**d fragmentation and standard PASEF workflows.
- **Unlock a versatile ion-activation network** for deep structural insight across a broad range of biomolecules

The timsOmni Σ - High sensitivity multiOmics powered by PASEF-EXD for advanced structural elucidation

Feature	
Compatible Ion Sources*:	• CaptiveSpray • VIP-HESI (with built-in APCI) • Apollo II
MS^n eXd for multiple stages of ion activation and dissociation:	Multi-stage trapped eXd fragmentation with charge state dependent reaction times and precise modulation of electron energy to access diverse fragmentation schemes.
Ion enrichment technology for structural elucidation:	Signal amplification via ion enrichment and MS^n eXd using omni-directional ion transfer for advanced ion processing workflows.
Athena Ion Processor (AIP) for broader m/z range detection:	Optimized release of ions depending on the application, addressing mass discrimination effects across a very wide m/z range and boosting sensitivity.



*Incompatible with NEOS source

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