

ExDViewer

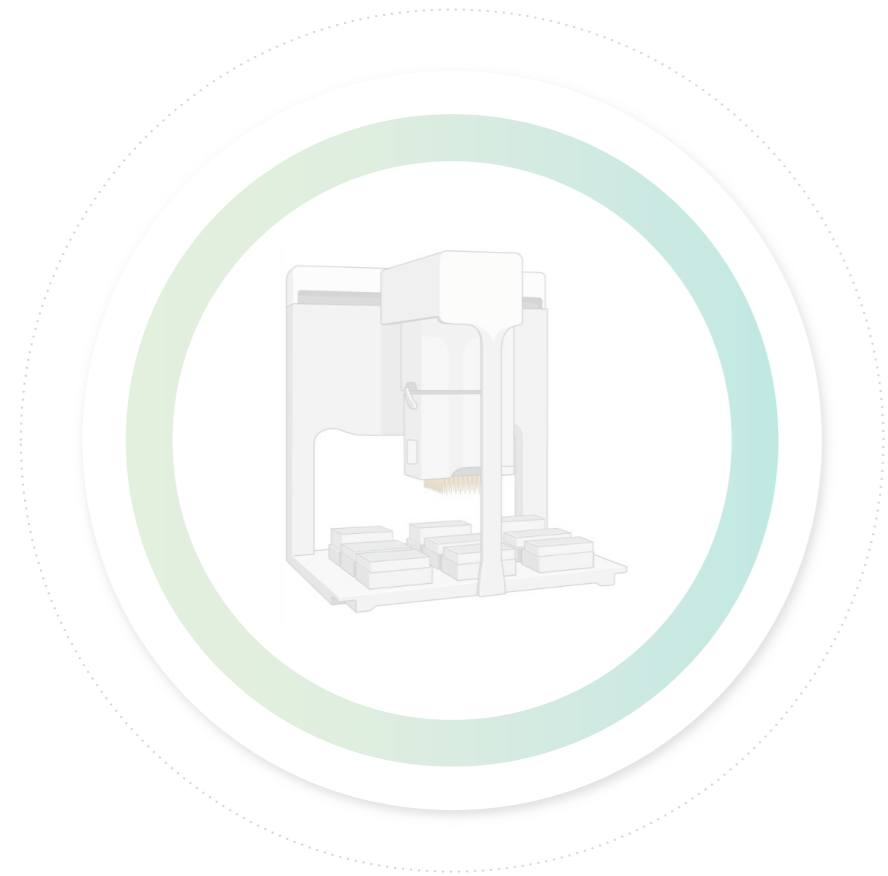


Joseph Meeuwsen, PhD

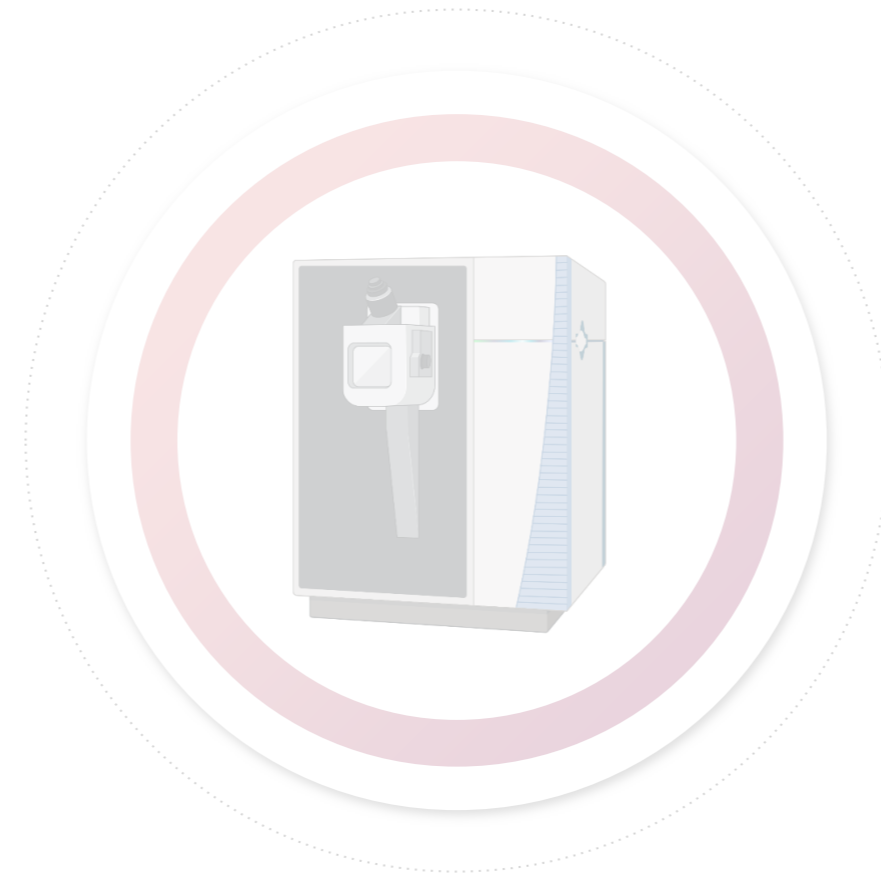
Outline

1. Overview
2. Live demo
 - Basic concepts
 - Native NISTmAb
3. Summary & Q&A

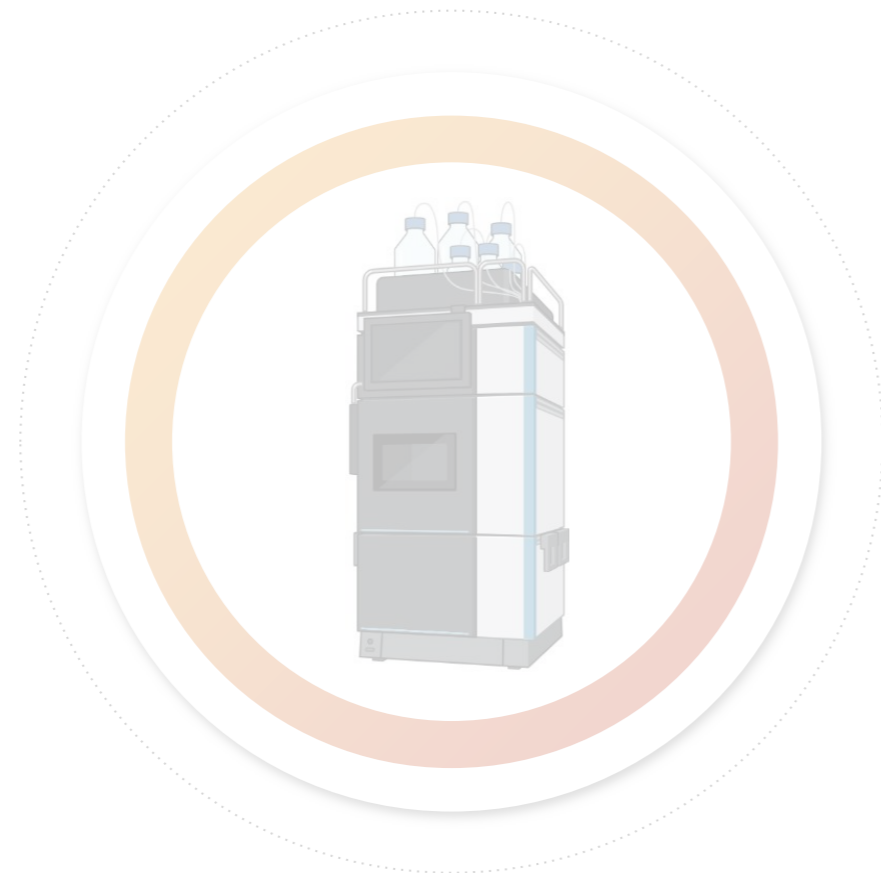
Areas of Advancement in Protein Mass Spectrometry



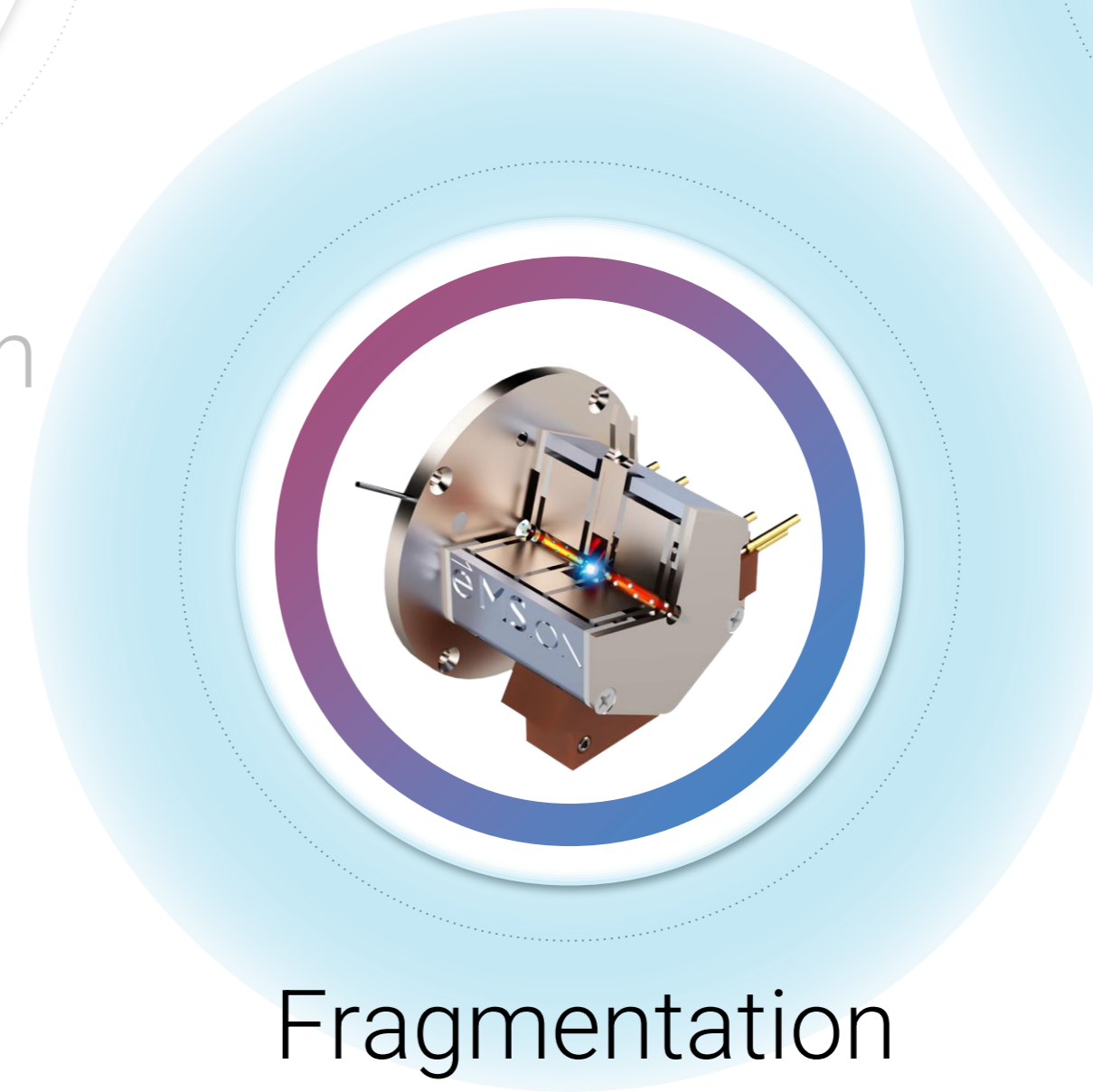
Throughput



Instrumentation



Separation



Fragmentation



Data Analysis

Overview

What is ExDViewer?

MS/MS data analysis software from e-MSion.

What does it do?

Matches m/z data to a target sequence, producing an interactive annotated spectrum.

Why use ExDViewer?

Validate methods & tuning.
Browse evidence supporting structural hypotheses.
Interpret top-down spectra.
Generate figures.

How do I access it?

Currently in beta.
Email betateesting@e-msion.com for access.

Overview

Visualize

Process

Share

Process

Share

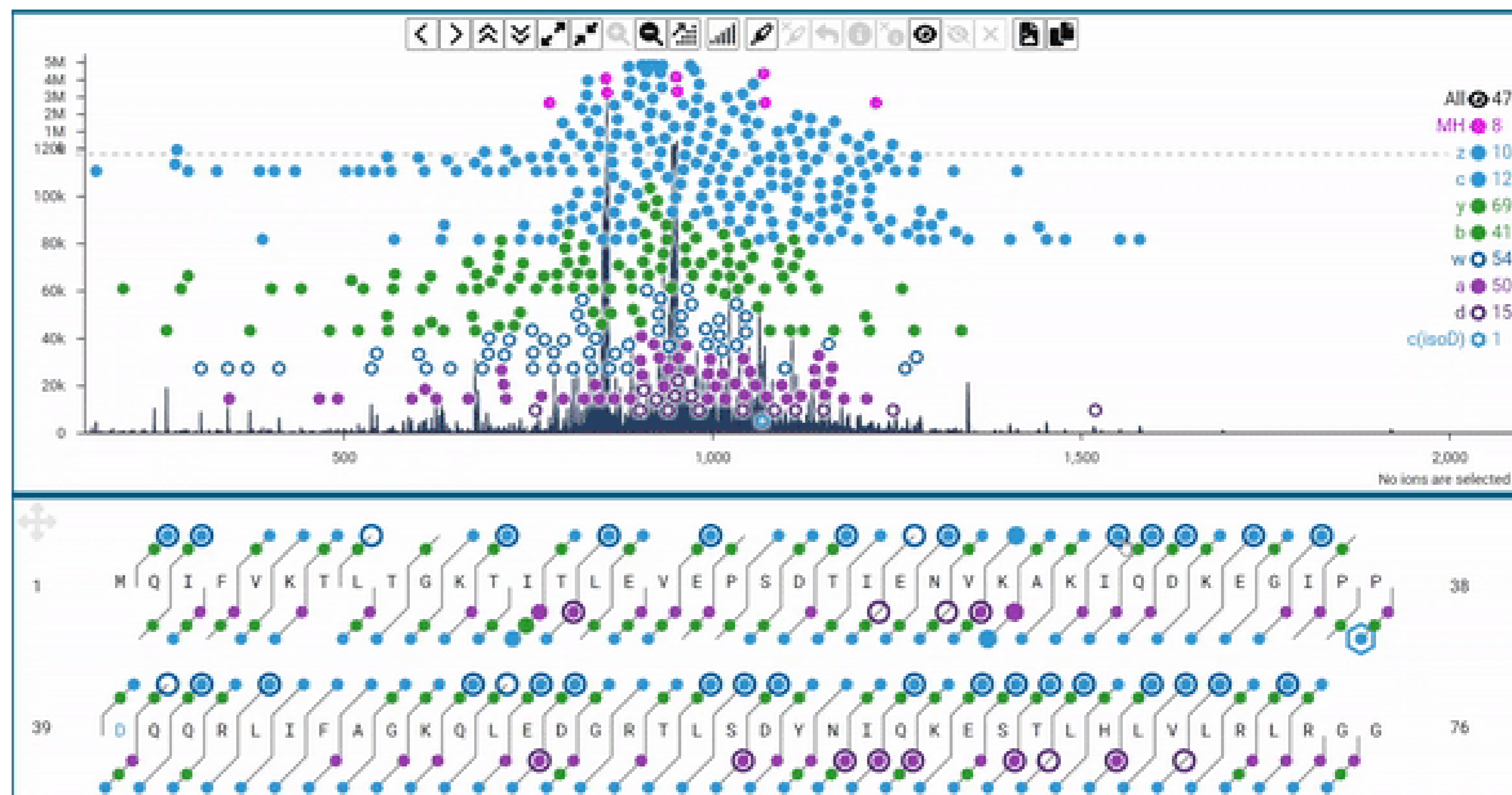
Overview

Visualize

- Match MS/MS data to a target sequence
- Browse the annotated m/z or decharged mass spectrum
- Use the interactive sequence coverage map to quickly zoom to peaks of interest

Process

Share



Overview

Visualize

Process

- Convert between common data types while maintaining informative metadata
- Merge spectra by m/z or retention time
- Use the output in third-party software

Share

The screenshot displays a software interface with a progress bar at the top showing three steps: 'Input Files', 'Convert Options', and 'Peak Picking'. The 'Convert Options' step is currently active. Below the progress bar, there are navigation buttons: 'Previous', 'Next', 'Run Now', and 'Cancel'. The 'Input File:' field contains the path 'C:\Users\Manufact Comp\1\Downloads\Carbonic_Native_HCD50eV_IsCID60V_Slens70_Temp150C_140KRes_10-27-2020_1.RAW'. To the right of this field are buttons for file formats: '.d', '.raw, .mzML, .mgf, .bt', and '.raw (dir)'. A note below states: 'Agilent, and Waters vendor formats are supported along with open-source and text-based formats.' The 'Output File:' field contains 'carbonic anhydrase.mzML', with a button for '.mzML, .mzXML, .mgf' to its right. Under 'Output data type:', there are radio buttons for 'profile' and 'centroid', with 'centroid' selected. Below this are four checkboxes: 'Average Spectrum', 'Relabel MS1 as MS2', 'Use centroids from input file', and 'Run baseline filter'. At the bottom right, there are another set of navigation buttons: 'Previous', 'Next', 'Run Now', and 'Cancel'.

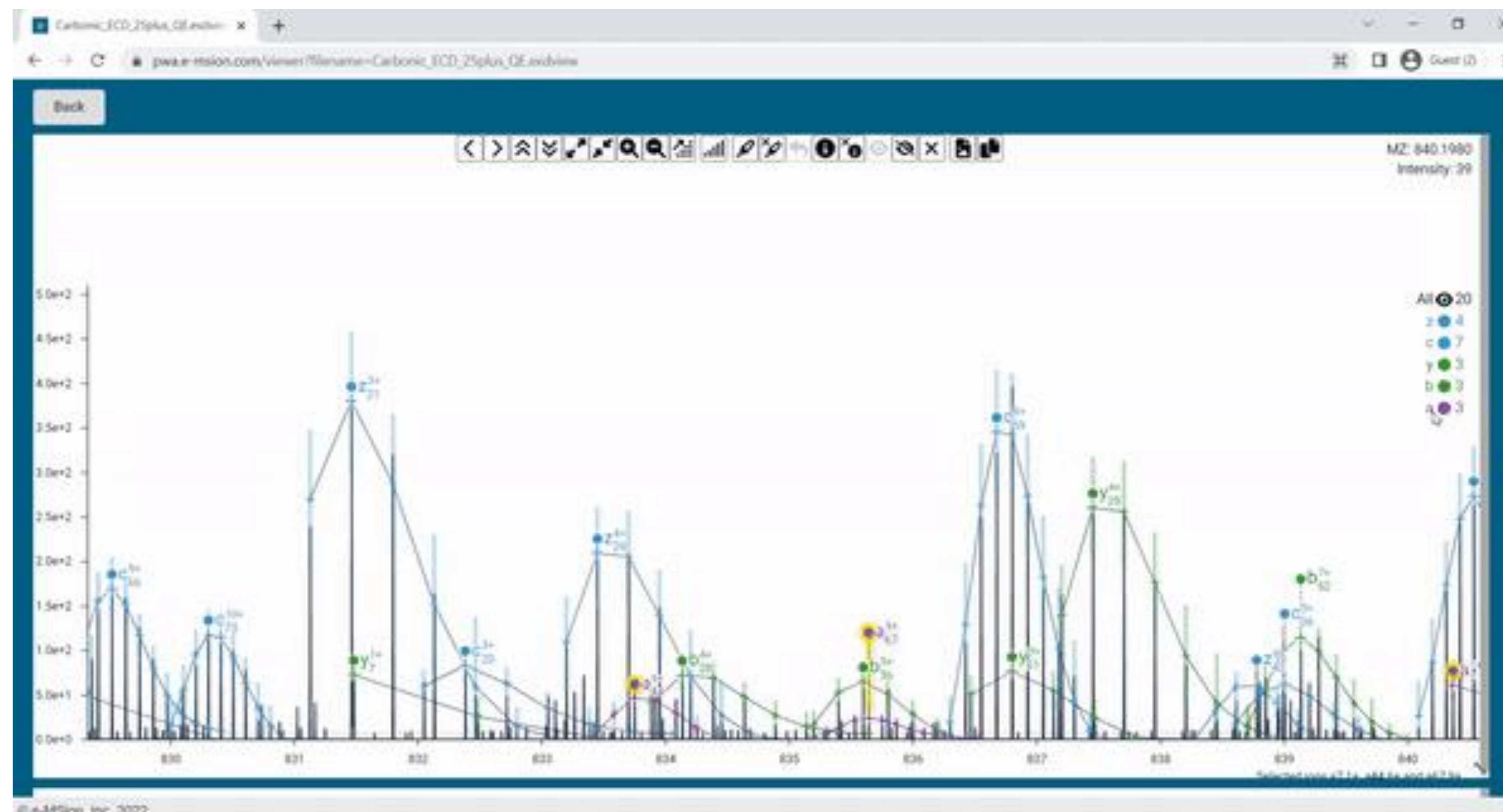
Overview

Visualize

Process

Share

- Export publication-quality figures
- Curate and export a table of peaks including fragment type, charge, match score, sequence position, etc.
- Share web URL to your analysis, no download required to view



Come back here to summarize after the demo

- Match m/z data to a target sequence
- Interactively browse spectrum & coverage map
- View m/z or decharged spectrum
- Filter & sort peaks table
- Make summary figures

Future directions

- Web-based app, shareable links
- Better PTM, internal fragment, multi-target support
- Lots of polish!

Email betatesting@e-msion.com for access

<https://e-msion.com/exdviewer>