Open data transparency with example datasets on the Orbitrap Exploris 240 mass spectrometer

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Your trusted resources for large- and small-molecule analysis

The Thermo Scientific™ Orbitrap Exploris™ 240 mass spectrometer (MS) (Figure 1) provides leading quantitative performance, sensitivity, and versatility, designed to meet your needs for proteomic, metabolomic, and lipidomic analyses. Add the Thermo Scientific™ FAIMS Pro interface to experience the power of differential ion mobility technology that provides orthogonal gas-phase separation and increased selectivity for the highest-quality quantitation and proteome depth. Thermo Scientific™ Example Datasets were created to assist scientists in confidently deploying the correct choice of powerful quantitative methods when utilizing Thermo Scientific™ Orbitrap™ technology in combination with the FAIMS Pro interface, ensuring data transparency with the highest workflow performance.

Here we describe applications on the Orbitrap Exploris 240 mass spectrometer demonstrating the high performance for proteomic workflows that include targeted protein quantitation using Parallel Reaction Monitoring (PRM), or proteome-wide quantitation with label-free quantitation (LFQ) using data-dependent acquisition (DDA) or high-resolution (HR) data-independent acquisition (DIA), and Thermo Scientific™ Tandem Mass Tags (TMT) multiplexing. The experimental versatility and benefits for small-molecule applications are also highlighted for metabolomics and lipidomics on the Orbitrap Exploris 240 mass spectrometer.

Figure 1. Orbitrap Exploris 240 mass spectrometer with the FAIMS Pro interface.
Providing leading quantitative performance, sensitivity, and versatility, for proteomic, metabolomic, and lipidomic analyses.

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For customers interested in Example Datasets on other high-resolution, accurate-mass (HRAM) instrumentation, resources are available for:

- Thermo Scientific™ Orbitrap Eclipse™ Tribrid™ mass spectrometer for TMT-based single-cell proteomic analysis.
- Thermo Scientific™ Orbitrap Exploris™ 480 mass spectrometer, covering targeted protein quantitation using the Thermo Scientific™ SureQuant™ method, or proteome-wide quantitation using TMT multiplexing, LFQ with DDA or HR-DIA, and LFQ single-cell proteomic analysis (1).

Additional datasets may be available in the future.

In addition to describing the proteomic, metabolomic, and lipidomic approaches that can be deployed, the Example Datasets demonstrate the quality of quantitative data obtained and the efficient processing strategies to accelerate your path to certainty in results, allowing you to spend less time on method optimization and more time on biologically relevant work. The full documentation provided by the Example Datasets exemplifies Thermo Fisher Scientific's commitment to data transparency.

For each application, the Example Datasets contain:

- Raw data files acquired on an Orbitrap Exploris 240 mass spectrometer.
- Complete experimental methods, along with flexible method templates, to enable users to reproduce data and results, while allowing further customization to meet user requirements. The methods include LC-MS instrument parameters.
- Post-acquisition data processing methods using Thermo Scientific™ Proteome Discoverer™ software for proteomics, Thermo Scientific™ Compound Discoverer™ software for metabolomics, or Thermo Scientific™ LipidSearch™ software for lipidomics.
- A presentation explaining method use and capabilities for a variety of applications and experiments.
- Other supplemental information to facilitate successful method deployment, including details on sample type, preparation, and commercial availability.

The Orbitrap Exploris 240 mass spectrometer with the FAIMS Pro interface is the platform for highest-quality quantitation. Go faster and dig deeper into your samples while enjoying the benefits of robust, precise, and accurate quantification using your preferred methods.

All of the following Example Datasets are available to download after registering for a free account at **https://thermo.flexnetoperations.com/**. Detailed instructions follow in Figures 2-4.

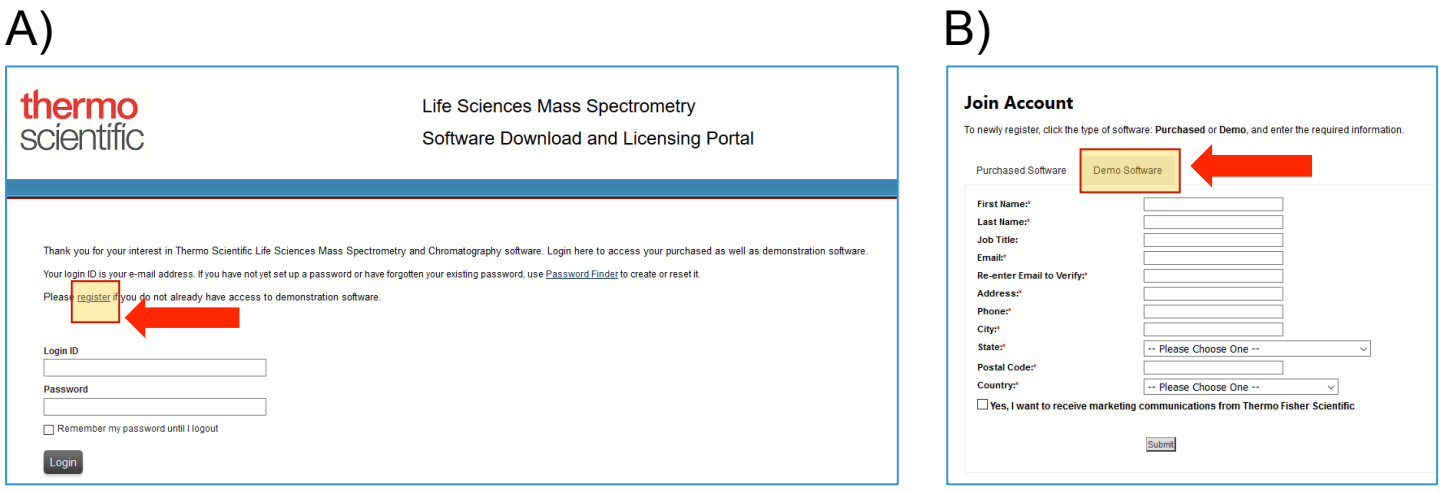

Figure 2. How to register for a Thermo Scientific™ Flexera Account.
(A) If you don't already have a Thermo Scientific Flexera account, then go to thermo.flexnetoperations.com and click on "Register". (B) On the registration page, click the "Demo Software" tab and fill out the required information. Then click on "Submit".

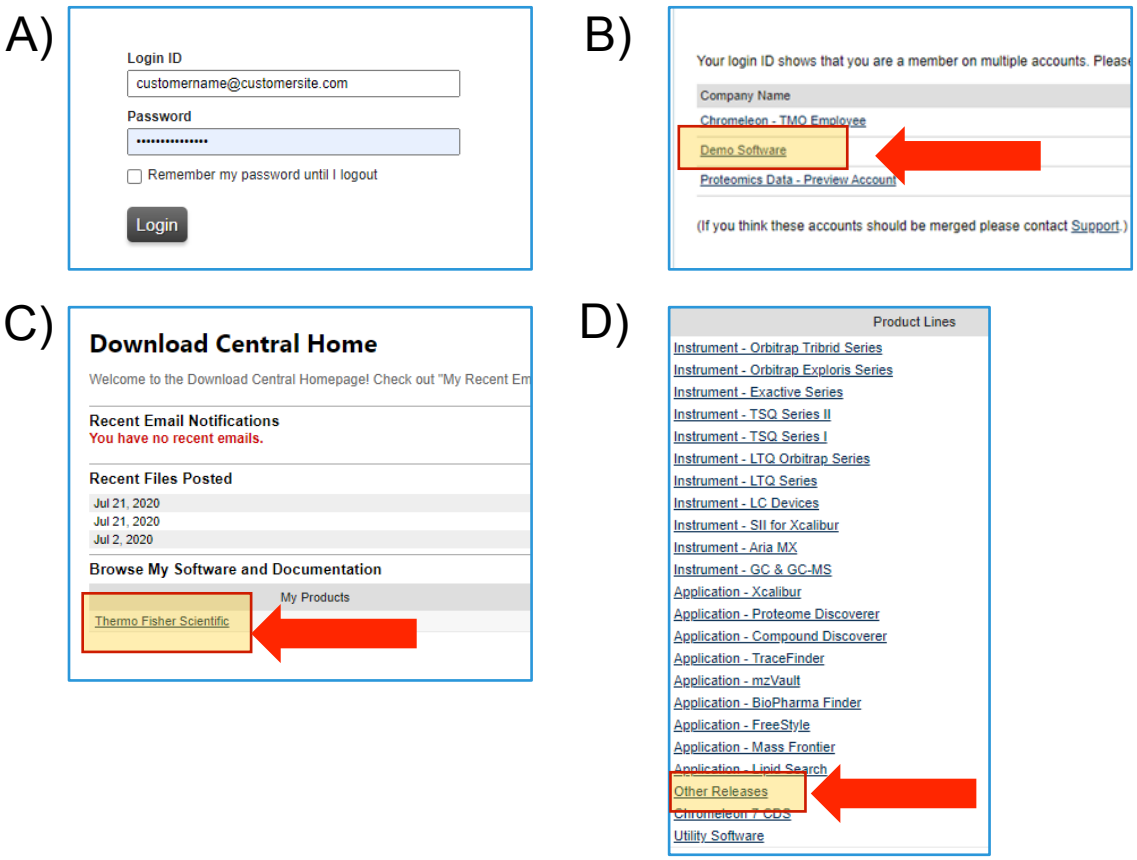

Figure 3. How to navigate to the Example Datasets within Flexera.
(A) Once you have registered, enter your login information and click on "Login". (B) Navigate to "Demo Software". (C) Then under "My Products," click "Thermo Fisher Scientific". (D) Then under "Product Lines," click "Other Releases".

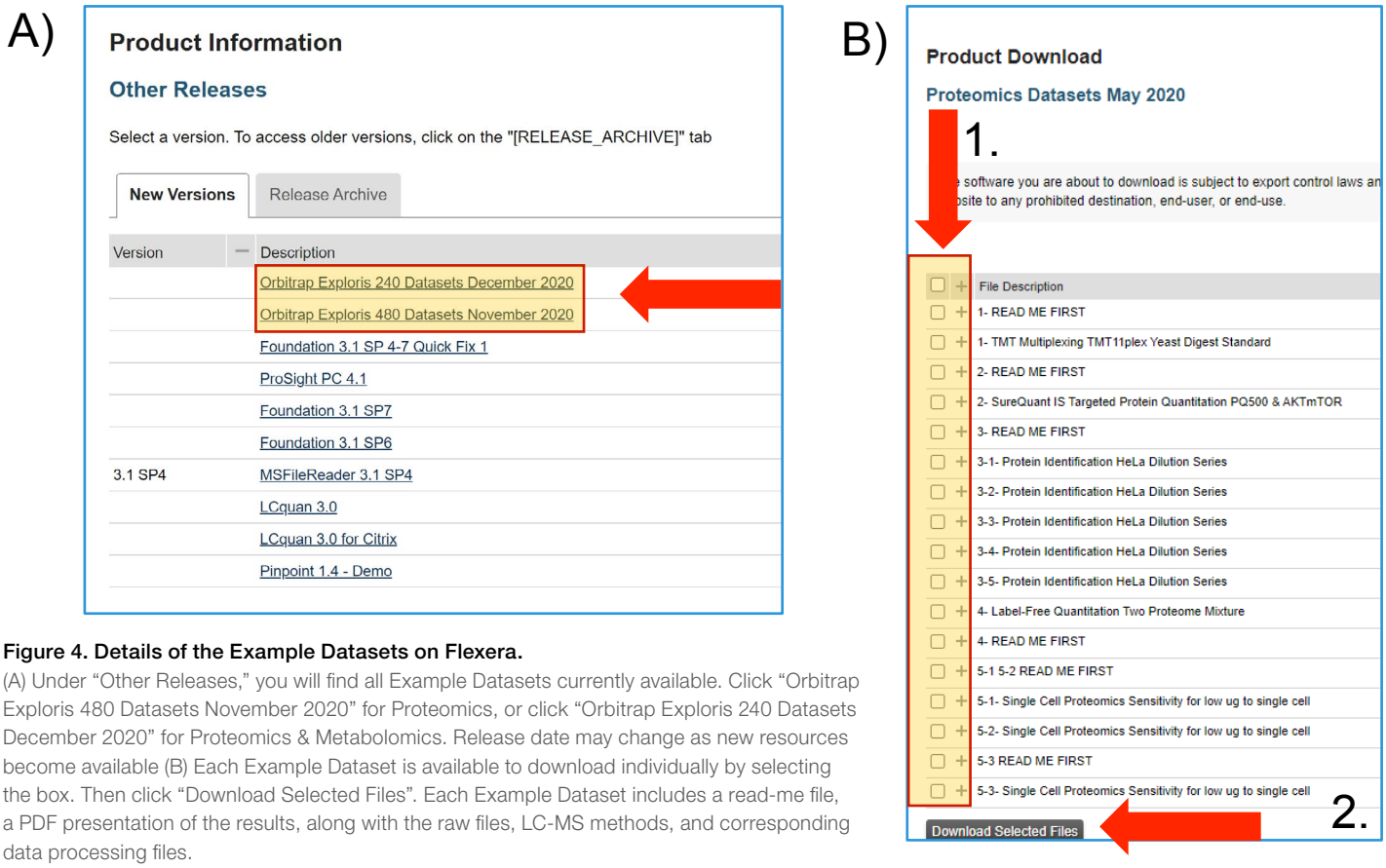

Figure 4. Details of the Example Datasets on Flexera.
(A) Under "Other Releases," you will find all Example Datasets currently available. Click "Orbitrap Exploris 480 Datasets November 2020" for Proteomics, or click "Orbitrap Exploris 240 Datasets December 2020" for Proteomics & Metabolomics. Release date may change as new resources become available (B) Each Example Dataset is available to download individually by selecting the box. Then click "Download Selected Files". Each Example Dataset includes a read-me file, a PDF presentation of the results, along with the raw files, LC-MS methods, and corresponding data processing files.

Additional applications and grant writing resources

To discover additional applications and the Top 10 reasons to choose the Orbitrap Exploris 240 mass spectrometer over Q-TOF instrumentation, check out these proofs of performance at: **https://www.thermofisher.com/OrbitrapExploris240Proof**

For grant writing resources highlighting specific instrumentation, new benefits, features, and reasons to upgrade, including how to accelerate high-confidence insights for small- and large-molecule research using the Orbitrap Exploris 240 mass spectrometer (2), check out: **https://www.thermofisher.com/grantcentral**

Summary

For laboratories considering the Orbitrap Exploris 240 mass spectrometer, the Example Datasets provide increased confidence in three important ways. The Example Datasets:

- Empower prospective users to make informed decisions when considering the Orbitrap Exploris mass spectrometer platform for their proteomic, metabolomic, or lipidomic workflows including higher performance and improved confidence for identification and quantitation.
- Provide full documentation to support new and current Orbitrap Exploris 240 mass spectrometer users in reproducing the results presented and achieving success.
- Ensure data transparency while enabling users to obtain the highest workflow performance. The Orbitrap Exploris mass spectrometer platform delivers HRAM performance that can be combined with the next-generation differential ion mobility device—the FAIMS Pro interface—to achieve the highest performance proteome coverage, quantitation accuracy, and precision, all with exceptional data quality.

References

1. Example Datasets for Choosing the Optimal Data Acquisition Method. Aaron Robitaille. Thermo Fisher Scientific AN-65932
2. Accelerate High-Confidence Insights for Small- and Large-Molecule Research using the Orbitrap Exploris 240 Mass Spectrometer. Maciej Bromirski and Aaron Robitaille. Thermo Fisher Scientific WP-65937

Find out more at **thermofisher.com/OrbitrapExploris**

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