Supelco®
Analytical Products

MERCK

HOW TO
ChemisTwin®

Episode 7:
Verify & quantify your primary compound

Targeted quantitation

How to Verify & Quantify your Primary Compound

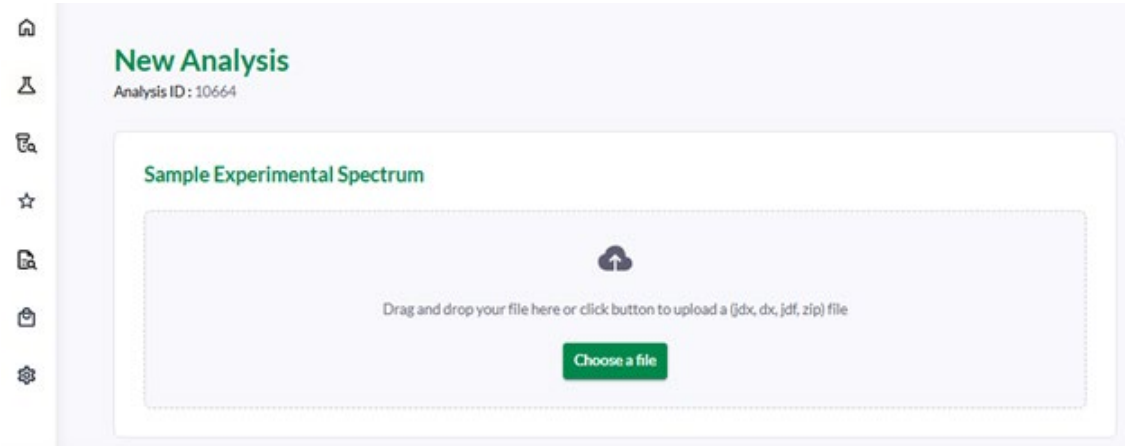
Targeted quantitation

Step 1: Start a New Analysis.

Head over to the dashboard (1) and click “New Analysis” to begin.

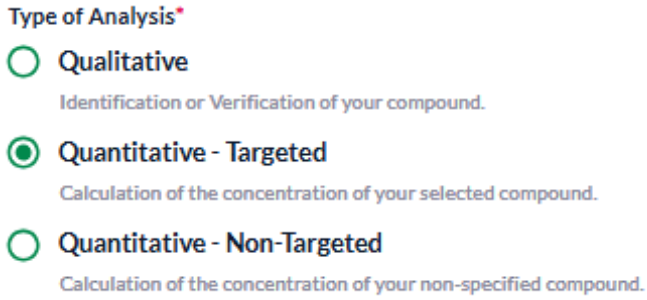
Step 2: Upload your Spectra

Drag and drop your file into the portal or browse your computer to select it. We support jdx, dx, jdf, and zip formats.*(Need tips for high-quality spectra? Check out ChemisTwin® Episode 1.)



Step 3: Choose Your Analysis Type

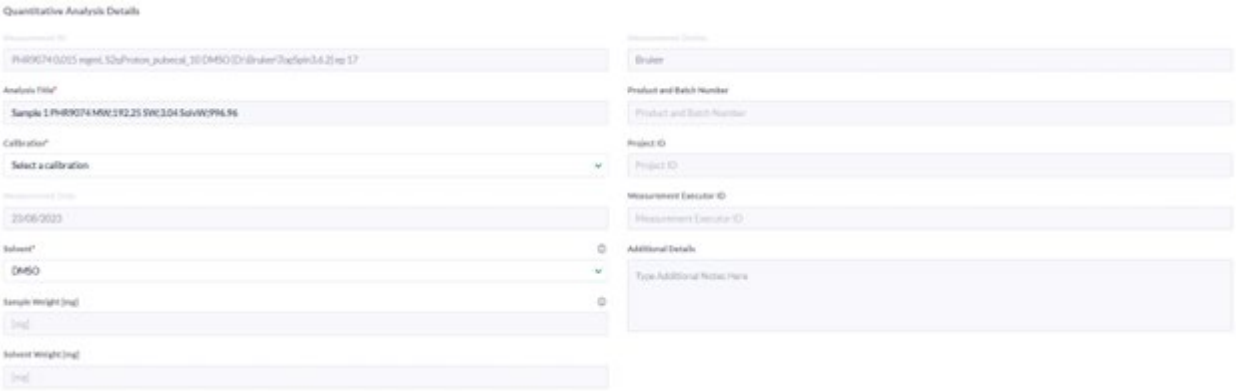
Select “Quantitative – Targeted” to focus your analysis on specific compounds.



Step 4: Review and Edit Meta Data

ChemisTwin® does the heavy lifting - certain data points are auto-extracted from your file. Just double-check the details and add any extras, like product and batch number, project ID, or measurement executor ID.

To calculate the mass fraction, be sure to enter your sample and solvent weights in this section.



Step 5: Add Digital References

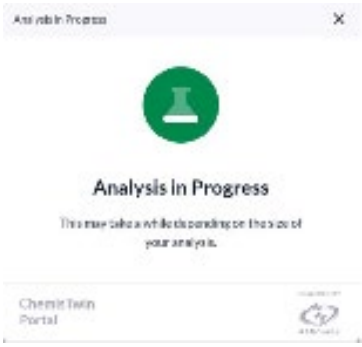
Let’s make sure your compound is correctly identified! Scroll down to select digital reference materials (dRMs), theoretical spectra, or your own user references to verify your sample before quantification.

Step 6: (Optional): Request a New dRM

Can’t find the reference you need? Click “Request dRM” and fill out the form. Just provide the CAS number, chemical name, and your email, and we’ll notify you once it’s available.

Step 7: Run the Analysis and Check your Results.

Click “Run Analysis” and let ChemisTwin® work its magic. Your results will be ready in no time!



Enjoying ChemisTwin®? We’d love to hear from you! Drop in your thoughts and feedback at: **ChemisTwin@merckgroup.com**

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