Supelco®
Analytical Products

MERCK

HOW TO
ChemisTwin®

Episode 6:
Quantify your compounds Non-Targeted Quantitation

How to Quantify all your Compounds by ^{1}H NMR

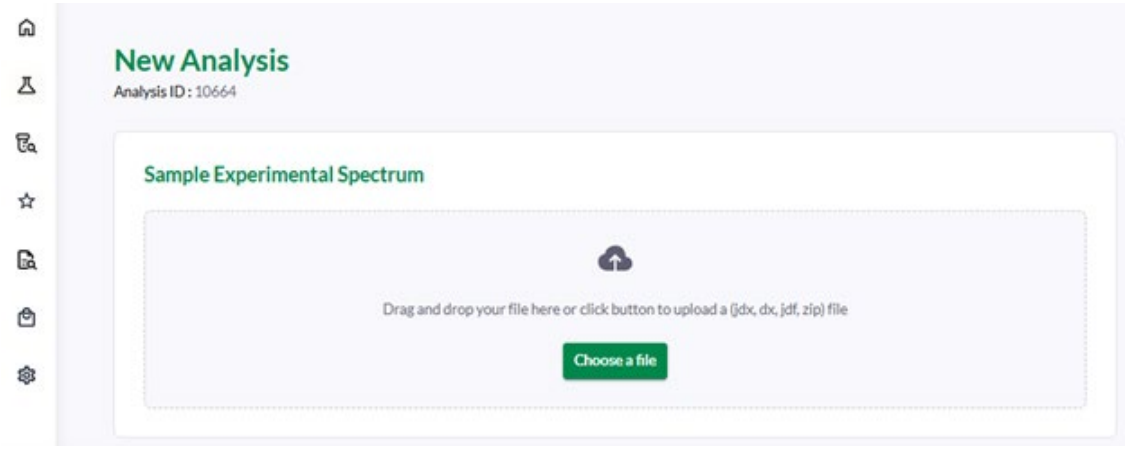
Non-targeted quantitation

Step 1: Start a New Analysis.

First things first—head over to the dashboard (1) and click “New Analysis” to get started.

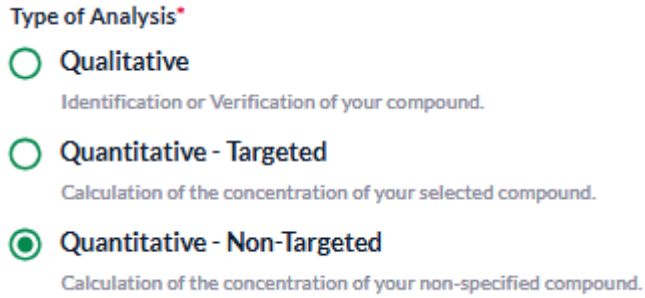
Step 2: Upload your Spectra

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 on capturing high-quality spectra? Check out ChemisTwin® Episode 1!)



Step 3: Choose Your Analysis Type

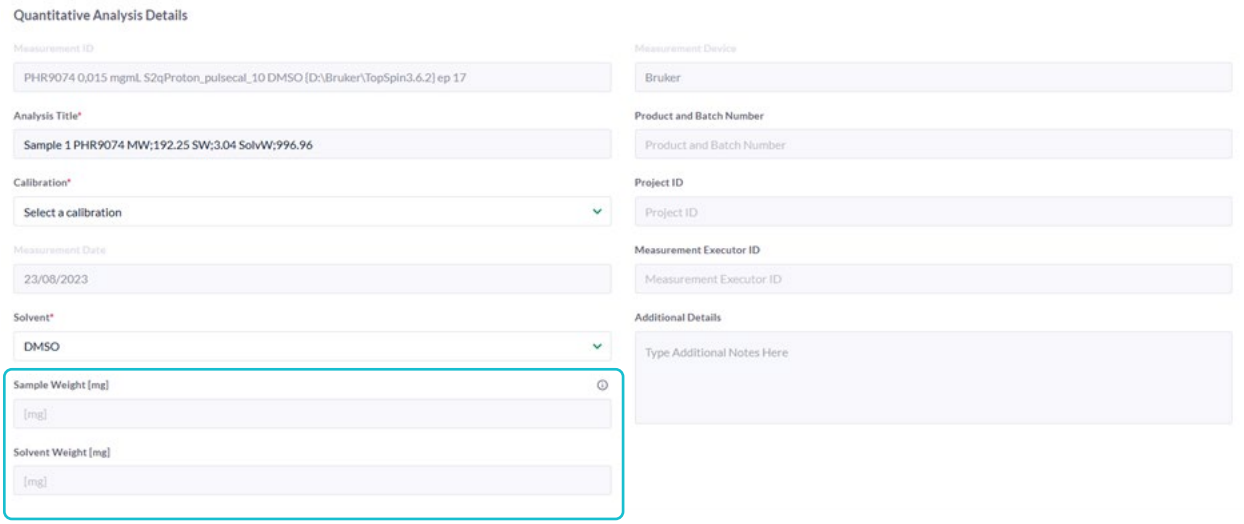
Select “Quantitative – Non-Targeted” to define your analysis approach.



Step 4: Review and Edit Meta Data

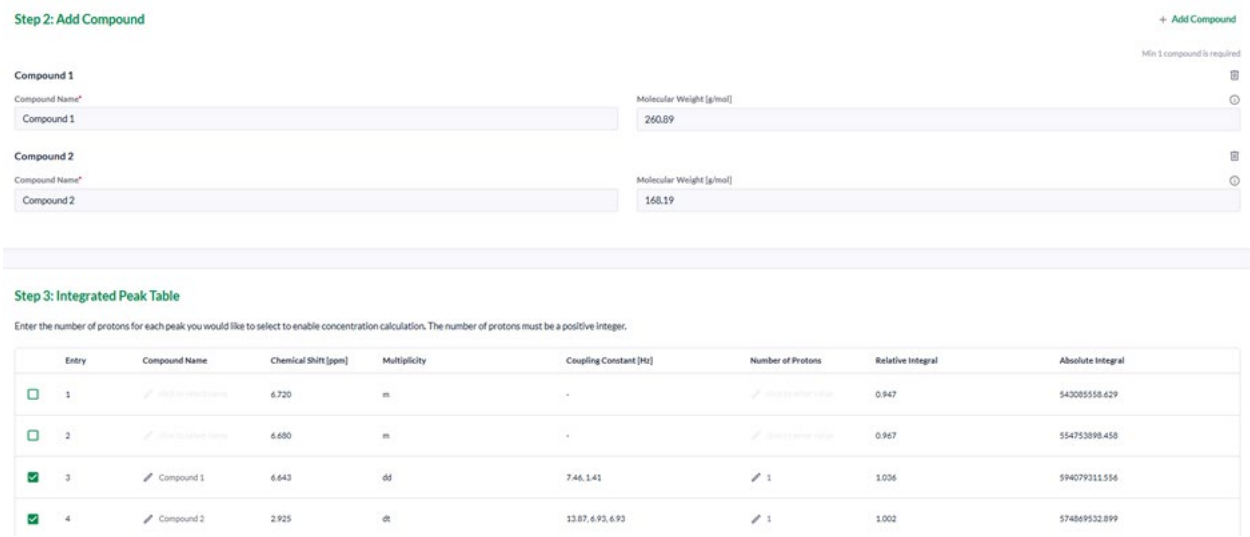
We’ve got you covered—certain details will be auto-extracted from your file. Just scroll down to verify and fine-tune any additional info, like product and batch numbers, project ID, or measurement executor ID.

To calculate the mass fraction, don’t forget to input sample and solvent weights in this section (blue square.)



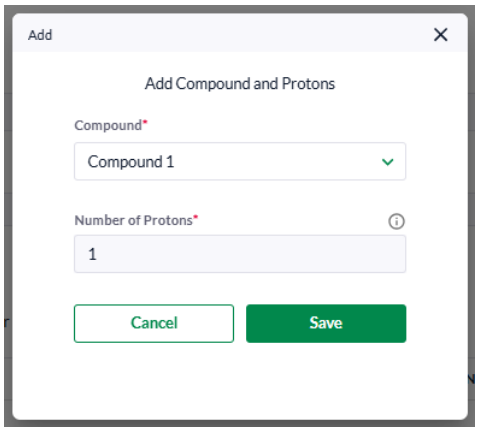
Step 5: Select Components and Peaks

Add the components you want to quantify and choose peaks from your spectra. You’ll get access to relative and absolute integral values to guide your selections - pick as many peaks as you need!



Step 6: Assign Protons to Peaks

Time to put those protons in their place! Enter the number of protons assigned to each peak.



Step 7: Run the Analysis and Check Out your Results

Click Run Analysis and let ChemisTwin® do its thing. 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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