

HOW TO ChemisTwin®

Episode 7:
Verify & quantify
your primary
compound
Targeted
quantitation

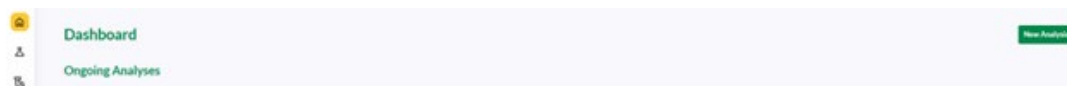


How to Verify & Quantify your Primary Compound

Targeted quantitation

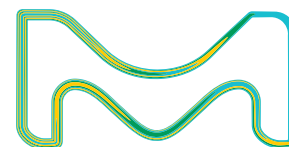
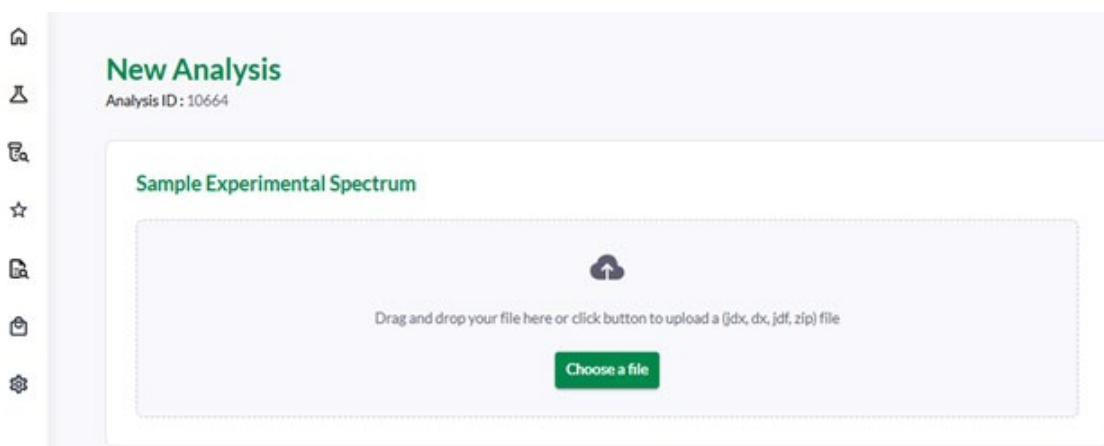
Step 1: Start a New Analysis.

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.

Type of Analysis*

☐ Qualitative

Identification or Verification of your compound.

☒ Quantitative - Targeted

Calculation of the concentration of your selected compound.

☐ Quantitative - Non-Targeted

Calculation of the concentration of your non-specified compound.

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.

Quantitative Analysis Details

Measurement ID	PH89074 0.025 mg/mL 520Proton_publical_10-DMSO-D6 (Bruker) 300MHz3.4.21 no 17	Measurement Details	Instrument
Analysis Title*	Sample 1: PH89074 MW: 192.25 SW: 3.04 Solv: W096.96	Product and Batch Number	Product and Batch Number
Calibration*	Select a calibration	Project ID	Project ID
Measurement Date	23/06/2023	Measurement Executor ID	Measurement Executor ID
Solvent*	DMSO	Additional Details	Type Additional Notes Here
Sample Weight (mg)	[mg]		
Solvent Weight (mg)	[mg]		

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 2: Add Reference Load from Favorites

What are we quantifying?

Search for a substance that corresponds your sample substance

PH89074

Latest Used Substances All Substances

 **2,2-Dimethyl-4-(1-methylethyl)-1,3-benzodioxole**

CAS Number 201166-22-5
Molecular Formula C12H16O2
Molecular Weight 192.25 g/mol
Synonyms 201166-22-5 4-(prop-1-yn-2-yl)-2,2-dimethylbenzo[d][1,3]dioxole 2,2-DIMETHYL...

Reference Code	Quality Grade	Solvent	Frequency (MHz)
PH89074 430MHz DMSO-D6	Good	DMSO	400

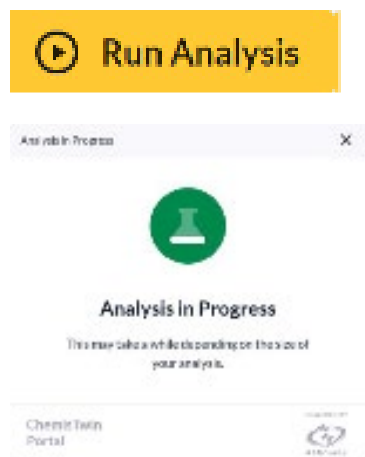
View Details Add to Analysis

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

