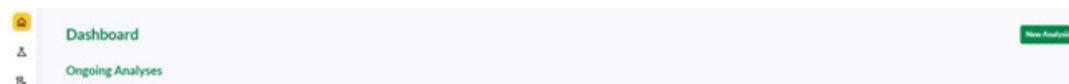


How to Quantify all your Compounds by ^1H NMR

Non-targeted quantitation

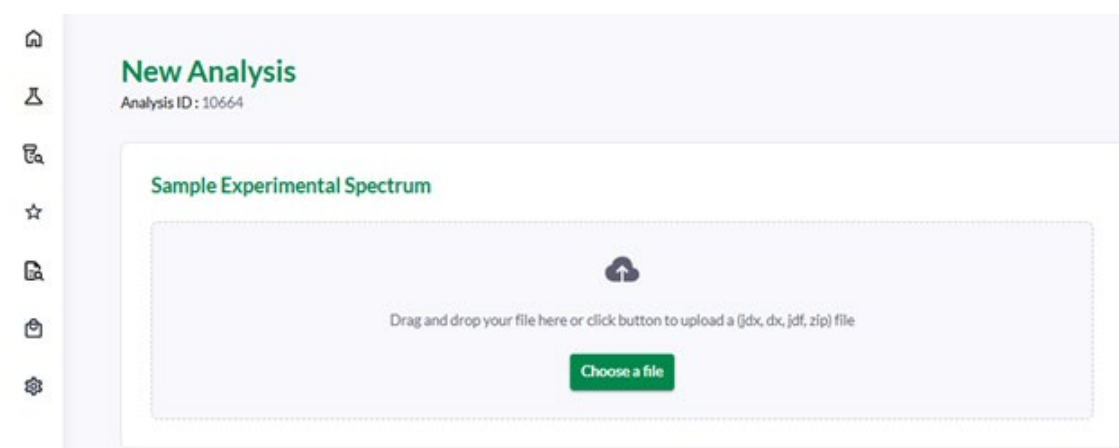
Step 1: Start a New Analysis.

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



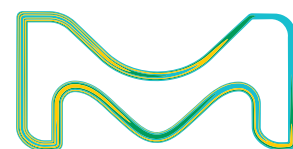
Step 2: Upload your Spectra

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!](#))



HOW TO ChemisTwin®

Episode 6:
Quantify your
compounds
Non-Targeted
Quantitation



Step 3: Choose Your Analysis Type

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

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

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.)

Quantitative Analysis Details

Measurement ID

PHR9074 0,015 mg/mL S2qProton_pulsecal_10 DMSO [D:\Bruker\TopSpin3.6.2] ep 17

Measurement Device

Bruker

Analysis Title*

Sample 1 PHR9074 MW:192.25 SW:3.04 SolvW:996.96

Product and Batch Number

Product and Batch Number

Calibration*

Select a calibration

Project ID

Project ID

Measurement Date

23/08/2023

Measurement Executor ID

Measurement Executor ID

Solvent*

DMSO

Additional Details

Type Additional Notes Here

Sample Weight [mg]

[mg]

Solvent Weight [mg]

[mg]

Step 5: 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 2: Add Compound

+ Add Compound

Min 1 compound is required

Compound 1

Compound Name*

Compound 1

Molecular Weight [g/mol]

260.09

Compound 2

Compound Name*

Compound 2

Molecular Weight [g/mol]

168.19

Step 3: Integrated Peak Table

Enter the number of protons for each peak you would like to select to enable concentration calculation. The number of protons must be a positive integer.

Entry	Compound Name	Chemical Shift [ppm]	Multiplicity	Coupling Constant [Hz]	Number of Protons	Relative Integral	Absolute Integral
<input type="checkbox"/> 1	<input type="checkbox"/> 100% to select name	6.720	m	-	<input type="checkbox"/> 100% to select value	0.947	54308558.629
<input type="checkbox"/> 2	<input type="checkbox"/> 100% to select name	6.680	m	-	<input type="checkbox"/> 100% to select value	0.967	554753898.458
<input checked="" type="checkbox"/> 3	<input type="checkbox"/> Compound 1	6.643	dd	7.46, 1.41	<input type="checkbox"/> 1	1.026	594079311.556
<input checked="" type="checkbox"/> 4	<input type="checkbox"/> Compound 2	2.925	dt	13.87, 6.93, 6.93	<input type="checkbox"/> 1	1.002	574869532.899

Step 6: Assign Protons to Peaks

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

Add

×

Add Compound and Protons

Compound*

Compound 1

Number of Protons*

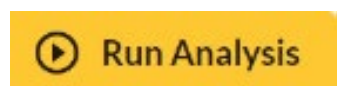
1

Cancel

Save

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.



Analysis Results				
Quantitative, Non-Targeted				
Your sample User case PR01663 MW: 178.27, SW: 19.74 (Solvent: 990.24) was quantified.				
Molecular Weight [g/mol]	Sample Weight [mg]	Solvent Weight [mg]	Mass Fraction [g/g]	Concentration [mg/g]
178.27	19.74	990.24	1.05	19.84



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

