Dotmatics
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PRODUCT FEATURE OVERVIEW

Analytical Studio Expressions

Turning Raw Data and Metadata into Actionable Decisions and Information

Modern labs need software that thinks like a scientist

Modern analytical laboratories are driven by an increasing need for automation and workflows that integrate seamlessly with orchestration software, master schedulers, ELNs, LIMS, and other informatics systems. While instrumentation has evolved at a fast pace, software to deal with the instrumental data and transform this into what we might call “Actionable Decisions” that mimic a scientists’ manual interpretation has, until Analytical Studio, been lacking.

Analytical Studio’s Expressions, built by analytical scientists, turn chromatography and MS data into actionable decisions. They combine processed results with metadata to produce the outputs that mimic scientist interpretations: review by exception, pass/fail flags, method scores, and color-coded results that can drive automated experimentation.

Expressions enhance Analytical Studio’s core capabilities: user-defined formulas, logic, and business rules that calculate derived metrics (e.g., percent conversion, purity) and apply evaluation criteria (e.g., fraction usability, best chromatography method). Expressions were designed to address persistent issues in chromatography and MS workflows, including:

01 **Every lab interprets data differently;** HTE groups, AS-MS teams, and purification labs care about different metrics and use different thresholds, making hardcoded logic unworkable

02 **Labs often run instruments** and their respective software from multiple vendors which can lead to different interpretations of the same sample

03 **Chromatographic peak data** (peaks, masses, intensities) lacks the type of analytical insight that chemists want from their experiments

04 When logic lives in a spreadsheet or someone’s head, it can’t scale, transfer between teams, or be centrally updated

Expressions summarize critical experiment information by referencing metadata, experimental results, derived calculations, and Boolean logic. Examples include:

TYPE	EXAMPLE
Metadata	Sample Name
	Method Name
	Column Name
Experimental Data	Target Peak Area
	Target Retention Time
	Internal Standard Retention Time
Calculations	Percent Purity or Percent Conversion
	AS-MS Hit Rates
	Kd values
Boolean Logic	Does sample pass purity criteria?
	Which is the best detector for fraction trigger?
	Is this the best chromatography method?

Together, these customizable expressions give teams a consistent rulebook across instruments and sites, so the same sample yields the same interpretation, day-to-day and lab-to-lab.

Why Expressions Matter

In practice, expressions bring clarity, consistency, and control to high-throughput data processing. They:

- Standardize interpretation across methods, instruments, and locations
- Automate pass/fail assessments and method comparisons using your thresholds (not hardcoded defaults)
- Make decisions traceable, showing exactly which criteria were met or violated
- Adapt flexibly to evolving scientific needs without rebuilding workflows

With that foundation, the examples below show how expressions drive plate-level visual triage, explain flags, and link results across experiments.

Visualizing Expressions in Action

Consider a high-throughput purification (HTP) experiment in which samples are analyzed using both an acidic (PreQC-TFA) and a basic method (PreQC-Amm). Analytical Studio displays the results as two virtual well plates, one per method, so outcomes can be reviewed at a glance. In Figure 1, each well is summarized with a color indicator: green (purifiable with good confidence), purple (probable coeluting impurities that will compromise fraction purity), teal (possible isomers detected), or a black slash (review recommended). Note, these review indicators and expressions continue to evolve. These colors are driven by expressions. For each sample, Analytical Studio combines raw chromatography/MS data and metadata, performs calculations, and applies lab-specific criteria to flag exceptions consistently across plates, methods, and labs.

Digging Deeper

If you wanted to further investigate why Analytical Studio's expressions indicated a particular sample was likely to have a problem, that can be easily done by reviewing the expression results. For the sample in well B5, the expression results are shown in Figure 2 where we see that if the method referred to in the bottom panel were used, there's a risk that an impurity would elute in what's called the "target peak zone," a customizable retention time window, around the compound of interest. The method referenced in the top panel is labeled as PreQC-PrepOK meaning that there shouldn't be issues collecting the wrong compound using this method.

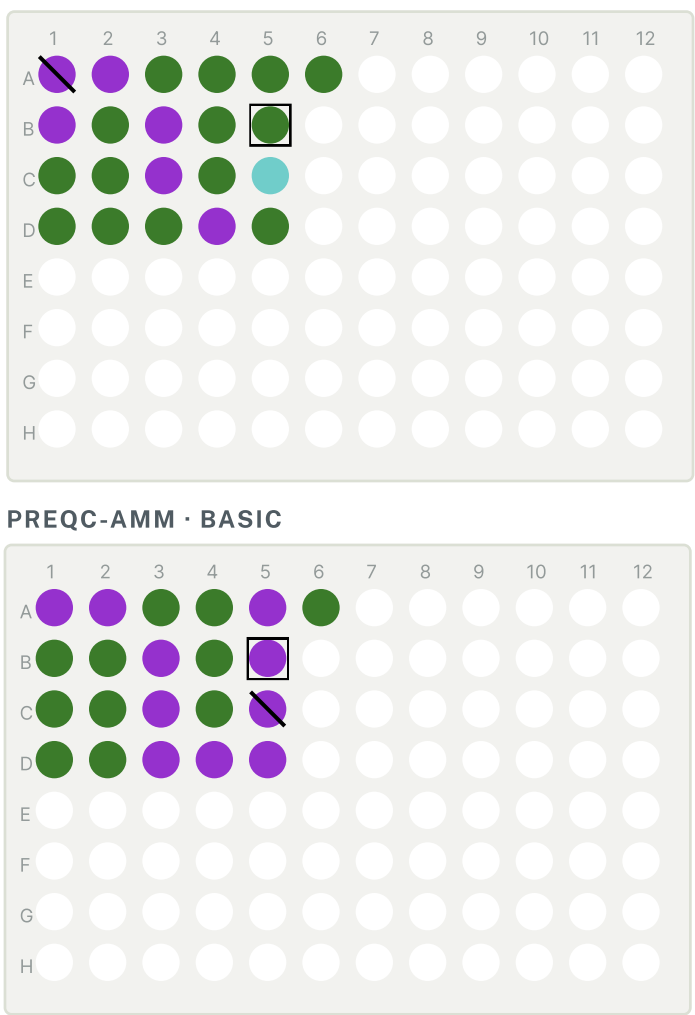

Figure 1: *Color-coded 96-well plate views from an HTP experiment, using two different methods. Green indicates samples suitable for purification; purple indicates potential impurities; teal denotes isomers; black slashes mark samples flagged for review.*

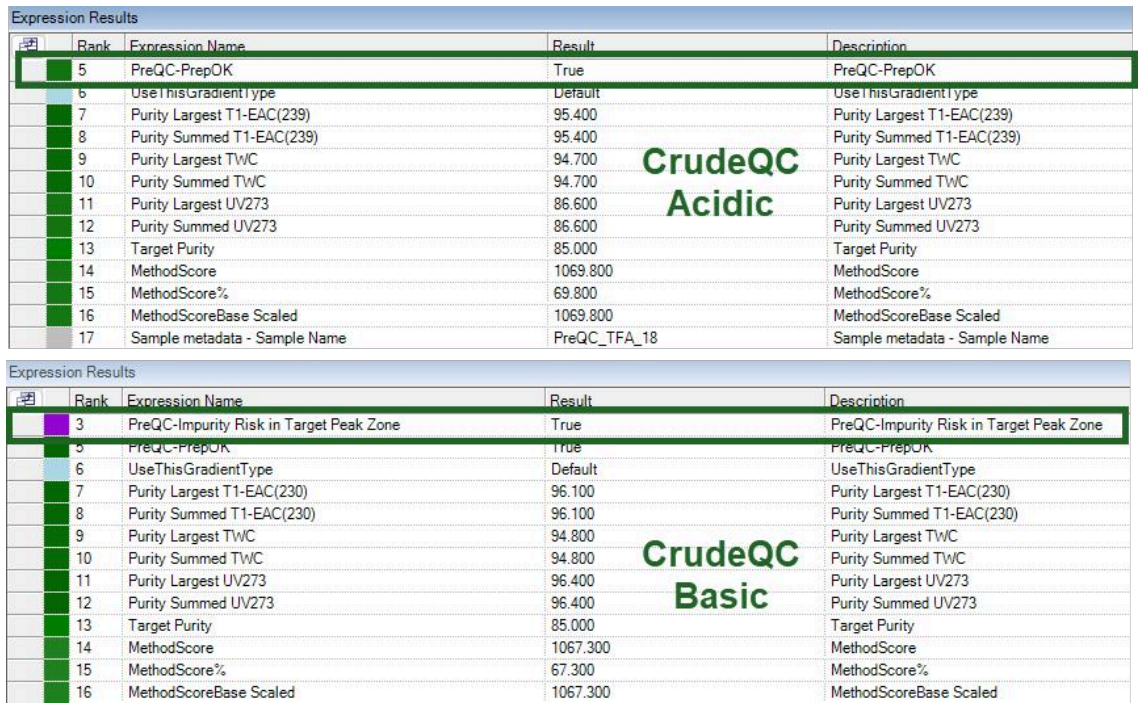

Figure 2: *Expression Results output for sample B5 for the acidic method (top) and the basic method (bottom) highlighting that an adjacent impurity peak in the basic method triggers a review flag due to its proximity to the target compound.*

We've quickly seen from the well plate view that for the sample in well B5, the top method looks better (green coloring). We've seen we can investigate why the bottom method doesn't look as good by reviewing the expression results where we see there's an impurity eluting too close to the compound of interest. If we still want to investigate this possible co-eluting impurity further, we can easily look at the raw data.

The separation between a compound of interest and co-eluting or closely-eluting compounds is defined by specifying minimum acceptable chromatographic peak resolution values (i.e., the separation between peaks before or after the target compound) in the corresponding expressions. Analytical Studio refers to the peak separation using the terms RsPre and RsPost where RsPre is the separation between the specified peak and the peak immediately preceding it. Conversely, RsPost refers to the separation between a specified peak and the peak immediately after. Figure 3 illustrates the difference between the chromatographic peak resolution labels.

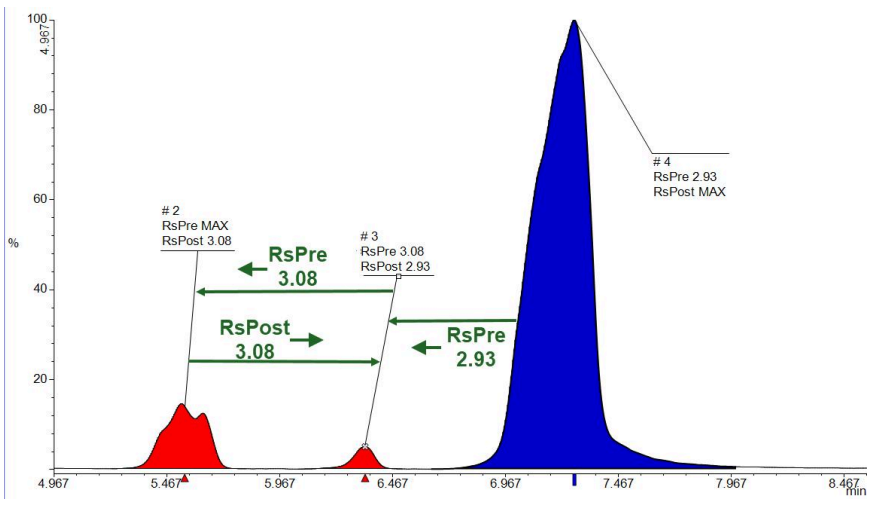

Figure 3. *The RsPost value for a peak is defined as the distance between a given peak and the next eluting peak. Conversely, the RsPre value is the distance between a given peak and the preceding peak.*

If desired, to confirm the plate-level summary and expression outcome, we can review the TWCs for these samples (Figure 4). The peak separation values shown are 4.66 (RsPost for the product peak) for the top method and 3.03 for the bottom method, indicating closer-eluting peaks under the bottom conditions for this sample. The green star on the top method TWC further indicates that, after all calculations are applied, this is the preferred purification method for B5.

No longer do you need to rely on personal preferences or individual methods for reviewing data, nor do you have to worry about a "black box" making decisions for you without allowing you to clearly explore why those decisions were made. Analytical Studio combines expert level rules and expressions with easily accessible decision review to give you the confidence that it is making the right decisions every time.

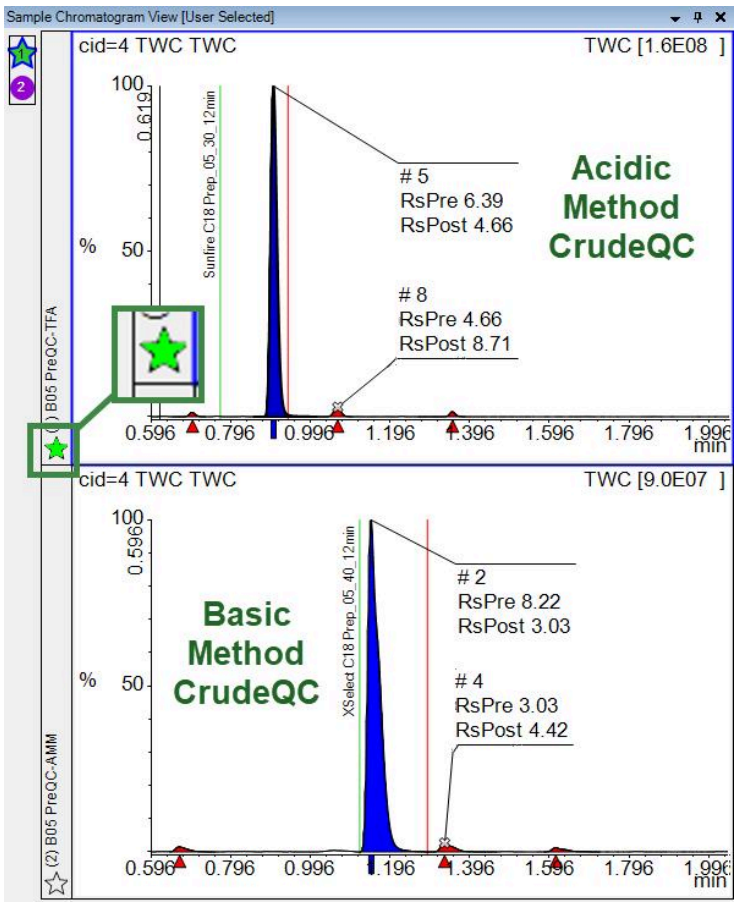

Figure 4. *Overlay of Total Wavelength Chromatograms (TWCs) for sample B5 under both methods. The basic method shows a lower resolution (RsPost = 3.03) between product and impurity peaks, compared to the acidic method (RsPost = 4.66), supporting the review flag.*

Expressions can be used for more than just identifying closely eluting possible impurity peaks. Expressions can be used to measure and evaluate a whole range of experimental results, and you can easily dig into the results to understand why a particular decision was made. For example, in Figure 4, we are looking at the TWC for the same compound analyzed with two different methods.

Now instead, let's look at two different samples that were analyzed using the same basic method, wells B5 and C5 shown on the bottom (basic) plate. in Figure 1. Here, we see that the sample in well C5 was flagged for review while the sample in B5 had no review flags. As we did above, we can dig into the expression results and data to better understand why C5 was flagged for review. For C5, the expression logic flags strong peak tailing (Figure 5a). By eye, the TWCs for B5 (no review flag) and C5 (review flag) appear to have similar tailing (5b). In situations such as this, some chemists might discard one or both fractions based on tailing while another might accept both. This inconsistency in data review criteria and reliance on “eyeballing it” can lead to irreproducible decisions.

Expressions eliminate this subjectivity by applying explicit, quantitative criteria. In this case, an asymmetry threshold is used to flag strong peak tailing. Figure 6a shows the method settings: strong tailing is defined here as asymmetry > 3 for detector D1 (the TWC). In Figure 6b, peak labels show asymmetry values of 2.794 for B5 (not flagged) and 3.087 for C5 (flagged). By relying on calculated metrics rather than visual judgment alone, Analytical Studio enables transparent and consistent interpretation of nuanced differences.

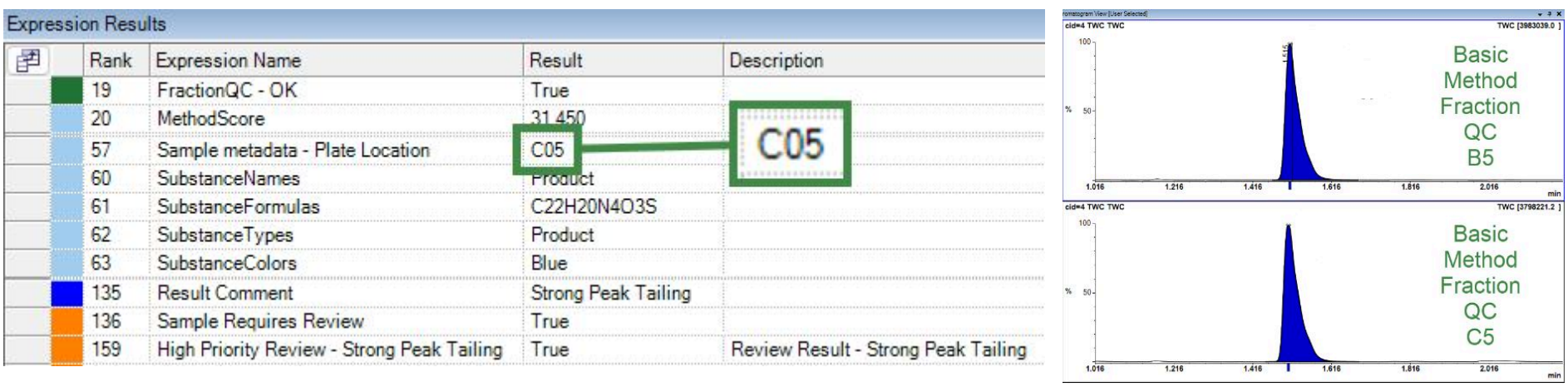

Figure 5a, b. *(a). Expression Results for well C5, indicating the Fraction QC results are ok but there is strong peak tailing. (b). TWC comparison for samples B5 and C5. While tailing appears similar visually, only C5 exceeds the asymmetry threshold defined in method settings, triggering a review flag.*

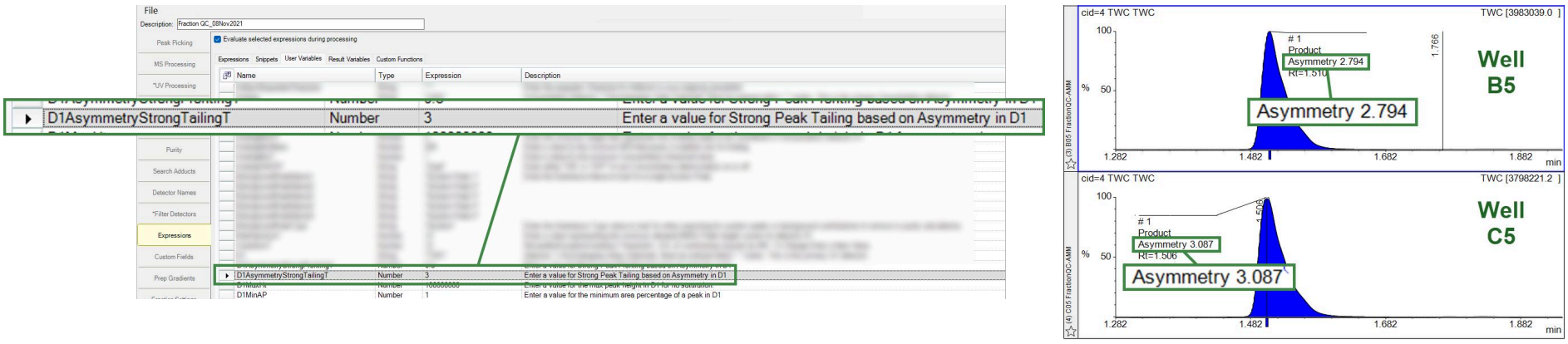

Figure 6a, b. *(a). Method settings showing the user-defined threshold for strong peak tailing (asymmetry >3 in detector D1). (b). Peak labels in the TWC show asymmetry values for B5 (2.794) and C5 (3.087), illustrating how expressions apply quantitative thresholds consistently.*

Expressions Turn Analysis into a Consistent Rulebook

Across the examples above, expressions convert raw chromatography/MS outputs plus metadata into transparent, repeatable decision-edge cases (e.g., co-elution proximity, tailing/asymmetry thresholds) and keeps interpretation consistent across methods, instruments, and reviewers. The result is faster triage, better reproducibility, and clearer justification for every decision made from the data.

Key Takeaways

- ✓ Encode your lab's criteria once; apply them consistently at scale
- ✓ Replace subjective "eyeballing" with quantitative, reviewable thresholds
- ✓ Keep decisions traceable by showing which criteria were met or violated
- ✓ Maintain flexibility as methods and definitions of success evolve

Next Step

If you'd like to see how expressions map to your current calculations (e.g., purity/conversion, peak proximity, tailing/asymmetry, fraction suitability), we can walk through a concrete example using your existing thresholds and workflows. Contact us anytime at info@virscidian.com.

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