

Custom calculation and filtering packages for SCIEX OS software based on EU guidelines

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This technical note describes the use of pre-built custom calculation and flagging packages to simplify and streamline SCIEX OS software data processing. These calculation packages are uploaded directly into SCIEX OS software 2.2 and higher versions (depending on the available features), and they contain the custom calculations and flagging rules needed to process data for commonly used applications and guidelines.¹

Several European guidelines for different industries—such as guidelines from the Directorate-General for Health and Food Safety (SANTE) and the International Council for Harmonisation of Technical Requirements for Registration of Pharmaceuticals for Human Use (ICH)—provide recommendations for the validation and evaluation of acquired data to ensure quality and consistency. These recommendations often require additional calculations to meet the needs of the validation plan.²⁻⁵

SCIEX OS software is a powerful tool for LC-MS/MS data acquisition and processing. The Analytics module within SCIEX OS software allows the customization of quantitative results via the addition of bespoke calculations and columns to a results table, which eliminates the need for external software and reduces transcription errors and compliance risks.

Key benefits of custom calculation packages in SCIEX OS software

- **Fast, simple data review:** Custom calculations streamline data review and reporting, reducing time spent on data processing
- **Maintain data integrity:** The packages contain importable files for calculated columns, flagging rules, layouts and documentation to facilitate compliance with EU guidelines without the need for additional software such as Microsoft Excel
- **Plug-and-play approach:** The files can be imported directly into an existing method and applied to any results table
- **Customizable to any data set:** Calculations can be tailored to fit any collected data set, lending flexibility to processing and reporting
- **Powerful combination of tools:** Custom calculations can be combined with batch decision rules and report templates to add increased flexibility and useability⁶



SCIEX OS SOFTWARE SUITE

Take advantage of the custom calculation feature in SCIEX OS software



CUSTOM PACKAGES

Download curated packages of calculations to speed up data processing and review



REGULATIONS

Tailor your data set to meet method criteria stipulated in commonly followed regulations

Examples of custom calculation and filtering implementation

Example 1: Calculating carry-over according to ICH M10 2022 guidelines (section 3.2.6)

Figures 1–5 show how custom calculations are implemented seamlessly into SCIEX OS software. This example highlights calculations for carry-over according to the ICH M10 2022 guidelines (section 3.2.6): “Carry-over in the blank samples following the highest calibration standard should not be greater than 20% of the analyte response at the LLOQ and 5% of the response for the IS.”

Index	Sample Name	Component Name	Area	Calculated Concentration	Outlier Reasons
170	Double Blank	Ametryn 1	1.209e5	N/A	
174	Double Blank	Prometon 1	7.907e4	N/A	
178	Double Blank	Simazine 1	1.786e4	4.982e-3	

Figure 1. Filtered results table without calculated columns and flagging applied. The image above shows a results table in SCIEX OS software without custom calculations applied.

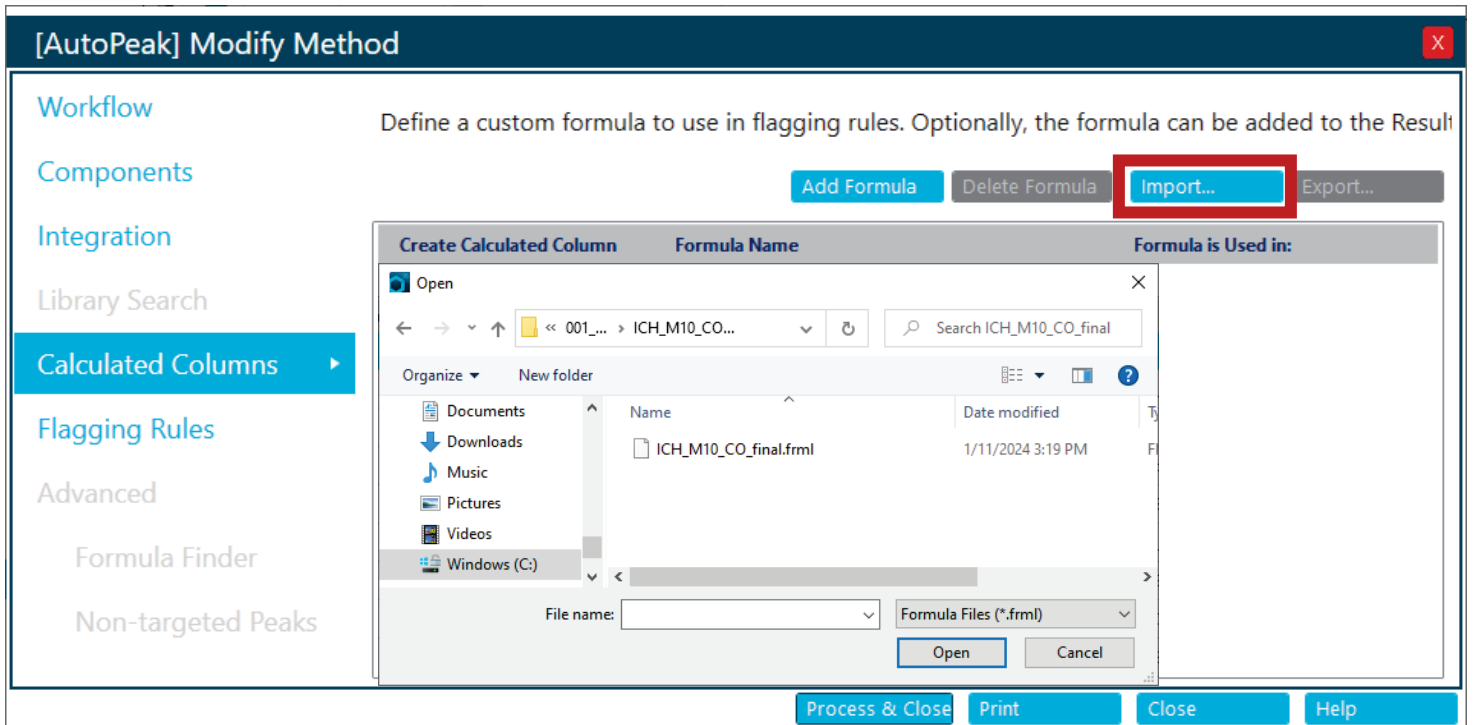


Figure 2. How to import custom calculation packages into a processing method in SCIEX OS software. To import a package into SCIEX OS software, create a processing method, open the calculated columns tab and click on the import button (highlighted in red). This will open the file explorer window, where the package can be chosen and imported.

[MQ4] Modify Method

Workflow Define a custom formula to use in flagging rules. Optionally, the formula can be added to the Results Table as a calculated column.

Components Add Formula Delete Formula Import... Export...

Integration

Library Search

Calculated Columns

Flagging Rules

Advanced

Formula Finder

Non-targeted Peaks

Create Calculated Column	Formula Name	Formula is Used in:
<input checked="" type="checkbox"/>	CO_01_Blank_Area	Rules: none Formulas: CO_04_Percent_CO ;
<input checked="" type="checkbox"/>	CO_02_LLOQ_Area	Rules: none Formulas: CO_03_MEAN_LLOQ_Area;
<input checked="" type="checkbox"/>	CO_03_MEAN_LLOQ_Area	Rules: none Formulas: CO_04_Percent_CO ;
<input checked="" type="checkbox"/>	CO_04_Percent_CO	Rules: Carry Over; Formulas: CO_Area_is_above_20percent_of LLOQ;
<input checked="" type="checkbox"/>	CO_05_Blank_IS_Area	Rules: none Formulas: CO_08_Percent_CO_IS, CO_IS_Area_is_above_5percent_of LLOQ;
<input checked="" type="checkbox"/>	CO_06_LLOQ_IS_Area	Rules: none Formulas: CO_07_MEAN_LLOQ_IS_Area;
<input checked="" type="checkbox"/>	CO_07_MEAN_LLOQ_IS_Area	Rules: none Formulas: CO_08_Percent_CO_IS;
<input checked="" type="checkbox"/>	CO_08_Percent_CO_IS	Rules: CO_Carry_Over_Check_IS; Formulas: CO_IS_Area_is_above_5percent_of LLOQ;
<input checked="" type="checkbox"/>	CO_09_IS_Peak_Name	Rules: none Formulas: CO_08_Percent_CO_IS, CO_IS_Area_is_above_5percent_of LLOQ;
<input checked="" type="checkbox"/>	CO_Area_is_above_20percent_of LLOQ	Rules: none Formulas: none
<input checked="" type="checkbox"/>	CO_IS_Area_is_above_5percent_of LLOQ	Rules: none Formulas: none

Process & Close Print Close Help

Figure 3. The processing method in SCIEX OS software showing the imported custom calculations according to the ICH M10 2022 guidelines (section 3.2.6).

[MQ4] Modify Method

Workflow Define a rule to flag results in the table.

Components Add Rule Delete Rule Import... Export...

Integration

Library Search

Calculated Columns

Flagging Rules

Advanced

Formula Finder

Non-targeted Peaks

Apply Rule	Rule Name	Formulas, Columns and Rules Used
<input type="checkbox"/>	Ion Ratio Acceptance	Columns: Ion Ratio Confidence
<input type="checkbox"/>	Accuracy Acceptance	Columns: Accuracy
<input type="checkbox"/>	Concentration Acceptance	Columns: Calculated Concentration
<input type="checkbox"/>	Integration Acceptance	Columns: Quality, Asymmetry Factor, Total Width, Retention Time Error (%)
<input type="checkbox"/>	Qualitative Rules	Columns:
Custom Rules		
<input checked="" type="checkbox"/>	Carry Over	Formulas: CO_04_Percent_CO
<input checked="" type="checkbox"/>	Carry Over IS	Formulas: CO_08_Percent_CO_IS
Combined Custom Rules		
<input checked="" type="checkbox"/>	CO Check	Rules: Carry Over, Carry Over IS

Process & Close Print Close Help

Figure 4. The applied flagging rules for carry-over calculations according to the ICH M10 2022 guidelines (section 3.2.6). Custom flagging rules can be imported in the same way as custom calculations and appear similarly in the processing method within the flagging rules tab. Data are then processed using both the imported custom calculations and flagging rules.

Index	Sample Name	Component Name	Area	Calculated Concentration	Outlier Reasons	*CO Check
170	Double Blank	Ametryn 1	1.209e5	N/A	Carry Over	●
174	Double Blank	Prometon 1	7.907e4	N/A	Carry Over	●
178	Double Blank	Simazine 1	1.786e4	4.982e-3	Carry Over	●

Figure 5. Example results table containing custom calculations for carry-over according to the ICH M10 2022 guidelines (section 3.2.6). The double blank, which was acquired directly after the highest standard sample, shows carry-over greater than the acceptable limit and therefore is highlighted both with an outlier reason and an easily identifiable red circle to indicate that the sample needs further investigation.

Example 2: Calculating acceptance criteria for an analytical run according to the ICH M10 2022 guidelines (section 3.3.2)

Figures 6 and 7 show an excerpt from a results table before and after applying the custom calculations for acceptance criteria for an analytical run according to the ICH M10 2022 guidelines (section 3.3.2): “The back-calculated concentrations of the calibration standards should be within $\pm 15\%$ of the nominal value, except for the LLOQ for which it should be within $\pm 20\%$. At least 75% of the calibration standard concentrations, which should include a minimum of six concentration levels, should fulfil these criteria.”

Index	Sample Name	Component Name	Used	Accuracy	Outlier Reasons
118	STD_6	Ametryn 1	<input checked="" type="checkbox"/>	115.63	
120	STD_6	Atrazine 1	<input checked="" type="checkbox"/>	103.97	

Figure 6. Filtered results table without calculated columns and flagging applied.

Index	Sample Name	Component Name	Used	Accuracy	Outlier Reasons	*Number_calibrant_levels	*Percent_STDs_ok
118	STD_6	Ametryn 1	<input checked="" type="checkbox"/>	115.63	Accuracy, Less than 75% of STDs are ok	9.000	66.667
120	STD_6	Atrazine 1	<input checked="" type="checkbox"/>	103.97	Less than 6 STD levels	5.000	100.000

Figure 7. Example results table containing a version of the custom calculations of acceptance criteria for an analytical run according to the ICH M10 2022 guidelines (section 3.3.2). For both components, at least one of the acceptance criteria is not met. This is made visible in the Outlier Reasons columns and in colored cells that show the failing values.

SCIEX offers packages for several guidelines

- **SANTE/11312/2021**
 - ✓ C15: The determination system has been shown to be free from significant drift
 - ✓ C16: The unknowns should lie within the range of the calibration curve
 - ✓ C18: Response factor check
 - ✓ D2: Retention time check
- **SANTE/2020/12830**
 - ✓ 3.2: Residual plot
- **ICH M10 (May 2022)**
 - ✓ 3.2.1: Selectivity
 - ✓ 3.2.2: Specificity
 - ✓ 3.2.3: Matrix effect
 - ✓ 3.2.4: Calibration curve and range
 - ✓ 3.2.6: Carry-over
 - ✓ 3.2.7: Dilution integrity
 - ✓ 3.3.2: Acceptance criteria for an analytical run
- **Directive EU 2020/2184**
 - ✓ Sum of 20 PFAS
 - ✓ Sum of 4 PFAS
- **Additional packages coming soon – contact SCIEXNow@sciex.com for more information**

How to obtain custom calculation packages

To obtain custom calculation packages, or to explore further options for custom calculations, please open a case with SCIEX Now via sciex.com or contact SCIEXNow@sciex.com. Please note that while the custom calculation packages provide a plug-and-play approach, customers must evaluate and adjust the calculations to meet their specific needs. More details are available in SCIEX Now knowledgebase articles.⁷

References

1. Calculated columns, flagging rules, and filtering, RUO-MKT-18-10566-A, [SCIEX.com](https://sciex.com)
2. International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use (ICH). ICH harmonised guideline. Bioanalytical method validation and study sample analysis, [24 May 2022](#).
3. European Commission, Directorate-General for Health and Food Safety (SANTE). Analytical quality control and method validation procedures for pesticide residues analysis in food and feed, SANTE/11312/2021, [implemented 1 January 2024](#)
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5. Directive (EU) 2020/2184 of the European parliament and of the council of 16 December 2020 on the quality of water intended for human consumption, [23 December 2020](#)
6. SCIEX OS software: decision rules, RUO-MKT-11-13239-A, [April 2021](#)
7. SCIEX Now knowledge base articles, [SCIEX.com](https://sciex.com)

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