B4, Advanced use of Custom Fields in Empower

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NORDIC USER TRAINING 2013
September 3-5 • Jurmala, Latvia
www.waters.com/nut
Agenda

- Introduction to custom fields

- Custom field and report example 1
  - Using CF and reports to evaluate method scouting runs during method development

- Custom field and report example 2
  - Using CF and reports in an Impurity analysis
What is a Custom Field?

- A **field** is a column of information in a table.
- A **custom field** is a user-defined field in a table.
- Custom fields can be descriptors or formulae.
Why Use a Custom Field?

- To store information about samples in the Empower database.
- To report information about your sample in an Empower report.
- To sort data by custom sample information.
- To set Empower to perform calculations, and avoid using additional software that needs to be validated.
Custom Fields

- Custom fields are created in a Project.
- To create a custom field, you need the Alter Any Project and the Create Custom Fields privileges.
- These privileges are specific to custom fields:
  - Create
  - Alter
  - Delete
  - Lock
  - Unlock.
- You can include custom fields in reports.
Creating Custom Fields

General Approach

- Plan your custom fields on paper.
- Work in a test project.
- Ensure the custom field performs as expected.
- Copy your custom field to other projects after you verify its usability.
What Type of Field to Create?

- Sample
- Result
- Peak
- Sample Set
- Component
- Distribution
What Data Type is Your Field?

- Integer (0)
- Real (0.0)
- Text
- Date
- Bool
- Enum
Data Types

- **Integer (0):** Whole number (without fractional parts).

- **Real (0.0):** Floating-point number entry

- **Text:** Alphanumeric entry.

- **Date:** Date entry by the user or from an external source.
Data Types

- **Boolean**: On processing, Boolean fields translate a mathematical formula into a specific value or answer.

- **Operator (Field, Value)**
  - Two possible answers: Yes/No, Pass/Fail
  - May define a user-selectable choice
Data Types

- **Enumerated**: Enumerated fields have two possible uses:
  - Provide a user with a list of possible answers
  - Translate multiple Boolean expressions into a value or answer

```
ENUM(Operator(Field,Value),Operator(Field,Value),Operator(Field,Value))
```
## Operations/ Functions

### Mathematical Operators

<table>
<thead>
<tr>
<th>Operator</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>-</code></td>
<td>Subtraction</td>
</tr>
<tr>
<td><code>+</code></td>
<td>Addition</td>
</tr>
<tr>
<td><code>*</code></td>
<td>Multiplication</td>
</tr>
<tr>
<td><code>/</code></td>
<td>Division</td>
</tr>
<tr>
<td><code>(</code></td>
<td>Open Parenthesis</td>
</tr>
<tr>
<td><code>)</code></td>
<td>Close Parenthesis</td>
</tr>
<tr>
<td><code>**</code></td>
<td>Exponent</td>
</tr>
</tbody>
</table>

### Mathematical Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>ABS()</code></td>
<td>Absolute Value</td>
</tr>
<tr>
<td><code>COS()</code></td>
<td>Cosine</td>
</tr>
<tr>
<td><code>LN()</code></td>
<td>Natural Log</td>
</tr>
<tr>
<td><code>LOG()</code></td>
<td>Regular Log</td>
</tr>
<tr>
<td><code>SIN()</code></td>
<td>Sine</td>
</tr>
<tr>
<td><code>SQRT()</code></td>
<td>Square Root</td>
</tr>
</tbody>
</table>

### Summary Functions

<table>
<thead>
<tr>
<th>Function</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>AVE()</code></td>
<td>Average</td>
</tr>
<tr>
<td><code>MAX()</code></td>
<td>Maximum Value</td>
</tr>
<tr>
<td><code>MIN()</code></td>
<td>Minimum Value</td>
</tr>
<tr>
<td><code>SUM()</code></td>
<td>Summation</td>
</tr>
<tr>
<td><code>%RSD</code></td>
<td>Percent Relative Standard Deviation</td>
</tr>
</tbody>
</table>
Custom Field/Report Example 1
Some Concerns in Method Development

- Method development takes too much time

- Complex samples
  - Many components at disparate levels

- No common approach
  - Many times serial iterative process
  - Too many experiments

- Data evaluation is difficult
  - Information is complicated
  - Large volume for manual review
  - Not quantitative
A Quality by Design Approach to Method Development

Method Screening
Select column & solvent using quantitative Trend Responses

Formal Method Development & Optimization
Characterize and model ALL study parameter effects on ALL critical method performance attributes

Mean Method Performance Models
- Establish ICH Design Space
- Identify Optimal Method
- Establish Operating Space

Method Robustness Models

Method Validation
Formal experiments to demonstrate method robustness
Up to 5 impurities published in literature

Difficulty due to many isomeric forms
  — Cis-, Meta-, and Ortho-

Methods can range from:
  — Normal phase to reversed phase
  — Up to 90 minutes in run time

Glimepiride: \( \text{C}_{24}\text{H}_{34}\text{N}_4\text{O}_5\text{S} \)
FW: 490.615

Brand Name: Amaryl®

Treatment: Type 2 Diabetes (non-insulin dependent), administered orally

Intended Use of the Method

Impurity Profile

Scope of Methodology
  • Forced degradation
  • Semi-quantitative
  • Resolution over speed

Candidate Properties

\( \lambda \text{ max: 228 nm} \)

Solubility: MeOH

Mass: 490.6
Identify Available Tools

- **Data Acquisition**
  - Columns & instrumentation
    - Short columns with different selectivities
    - ACQUITY UPLC® System
      - Column Manager to hold and switch 4 columns
      - PDA for peak purity
      - MS for peak tracking
  - Empower™ Software
    - Acquisition template

- **Data Management**
  - Informatics solutions
    - Empower
      - Calculation template
      - Reporting template
Method Scouting Protocol for Glimepiride Method Development

- **Methodology**
  - Four ACQUITY UPLC chemistries 2.1 x 50 mm, 1.7 µm
    - ACQUITY UPLC BEH C18
    - ACQUITY UPLC BEH Phenyl
    - ACQUITY UPLC BEH Shield RP18
    - ACQUITY UPLC HSS T3 (Silica based column, cannot run at pH 10)
  - **Solvents**
    - Acetonitrile
    - Methanol
  - **Buffers**
    - Low pH (pH 3 Ammonium Formate)
    - High pH (pH 10 Ammonium Bicarbonate)

Number of Scouting runs: \((2 \times 2 \times 3) + (2 \times 1 \times 1) = 14\)
ACQUITY UPLC® H-Class: Ideal for Method Development

Column Manager
- Stack to support up to 6 columns
- Independent heating/cooling zones

Sample Manager—FTN
- Direct injection simplifies mode of injection selection
- Injection volume flexibility without reconfiguring injector

Quaternary Solvent Manager with Optional Solvent Select Valve
- Up to 9 solvents with integrated solvent selection valve on the D line (1-6 solvents)
PDA Peak Purity Plot

Spectrally Pure Peak

Glimepiride

Empower automatically identifies potentially impure peaks

Questionable peak

Unknown @ 1.482 minutes

The “M” denotes the point of maximum difference
Why Use Mass Spectrometry?

- Ability to track peaks
- Assists as orthogonal analysis
- Confirm identity of knowns
- Verify purity of the peak(s) of interest
- Help to identify unknowns
ACQUITY SQD Featuring the SQ MS Detector

- IntelliStart™
  - Enables simplified set up
- Robustness and sensitivity
  - ZSpray™
- Fast data acquisition
  - 10,000 amu/sec
  - Rapid polarity switching 20 msec
- Richer information
  - ESCi®, ESI, APCI, APPI
  - Positive/negative ionization
UV Peak Tracking

Tracking peaks by UV during the method development process may be difficult as the spectra of related substances can be similar.
Mass Spectra Peak Tracking

...with MS data, the peaks can now be easily tracked as well as any additional peaks invisible to UV detection
ACQUITY SQD MS Peak Tracking: pH 3 vs. pH 10

Column - ACQUITY UPLC® BEH C\textsubscript{18} Solvents - Acetonitrile

**pH 3.0**

Glimepiride – 491.3
Peak 2 – 497.5
Peak 3 – 352.3
Peak 4 – 383.1
Peak 5 – 410.1
Peak 6 – 398.1
Peak 7 – 505.2, 561.3

**pH 10.0**

Glimepiride

ACQUITY SQD MS Peak Tracking:

pH 3 vs. pH 10
## Setting Up Method Scouting Experiments with Empower Templates

### Essential for streamlining sequential workflow

<table>
<thead>
<tr>
<th>Plate/Mayl</th>
<th>SampleName</th>
<th>Inj Vol (uL)</th>
<th># of Injs</th>
<th>Function</th>
<th>Run Time (Minutes)</th>
<th>Next Inj. Delay (Minutes)</th>
<th>Column Position</th>
</tr>
</thead>
<tbody>
<tr>
<td>1:A,1</td>
<td>Blank</td>
<td>2.0</td>
<td>1</td>
<td>Condition Column</td>
<td>5.00</td>
<td>1.00</td>
<td>Position 1</td>
</tr>
<tr>
<td>1:A,2</td>
<td>Glimepiride MS</td>
<td>2.0</td>
<td>1</td>
<td>Inject Samples</td>
<td>5.00</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>1:A,1</td>
<td>Blank</td>
<td>2.0</td>
<td>1</td>
<td>Condition Column</td>
<td>5.00</td>
<td>1.00</td>
<td>Position 2</td>
</tr>
<tr>
<td>1:A,2</td>
<td>Glimepiride MS</td>
<td>2.0</td>
<td>1</td>
<td>Inject Samples</td>
<td>5.00</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>1:A,1</td>
<td>Blank</td>
<td>2.0</td>
<td>1</td>
<td>Condition Column</td>
<td>5.00</td>
<td>1.00</td>
<td>Position 3</td>
</tr>
<tr>
<td>1:A,2</td>
<td>Glimepiride MS</td>
<td>2.0</td>
<td>1</td>
<td>Inject Samples</td>
<td>5.00</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>1:A,1</td>
<td>Blank</td>
<td>2.0</td>
<td>1</td>
<td>Condition Column</td>
<td>5.00</td>
<td>1.00</td>
<td>Position 4</td>
</tr>
<tr>
<td>1:A,2</td>
<td>Glimepiride MS</td>
<td>2.0</td>
<td>1</td>
<td>Inject Samples</td>
<td>5.00</td>
<td>1.00</td>
<td></td>
</tr>
</tbody>
</table>

### Key to data visualization

<table>
<thead>
<tr>
<th>Buffer_type</th>
<th>Column_Type</th>
<th>Solvent_Type</th>
<th>pH</th>
</tr>
</thead>
<tbody>
<tr>
<td>10mM Ammonium Formate</td>
<td>ACQUITY BEH C18</td>
<td>ACN</td>
<td>pH=3.00</td>
</tr>
<tr>
<td>10mM Ammonium Formate</td>
<td>ACQUITY BEH C18</td>
<td>ACN</td>
<td>pH=3.00</td>
</tr>
<tr>
<td>10mM Ammonium Formate</td>
<td>ACQUITY BEH Phenyl</td>
<td>ACN</td>
<td>pH=3.00</td>
</tr>
<tr>
<td>10mM Ammonium Formate</td>
<td>ACQUITY BEH Phenyl</td>
<td>ACN</td>
<td>pH=3.00</td>
</tr>
<tr>
<td>10mM Ammonium Formate</td>
<td>ACQUITY BEH Shield RP18</td>
<td>ACN</td>
<td>pH=3.00</td>
</tr>
<tr>
<td>10mM Ammonium Formate</td>
<td>ACQUITY BEH Shield RP18</td>
<td>ACN</td>
<td>pH=3.00</td>
</tr>
<tr>
<td>10mM Ammonium Formate</td>
<td>ACQUITY HSS T3</td>
<td>ACN</td>
<td>pH=3.00</td>
</tr>
<tr>
<td>10mM Ammonium Formate</td>
<td>ACQUITY HSS T3</td>
<td>ACN</td>
<td>pH=3.00</td>
</tr>
</tbody>
</table>

### User Defined
- Template Defined
- Custom Fields
Importance of Scouting with Various Selectivity Tools

Manually tracking and labeling known peaks of interest peaks (approx. 4 hours).

How much time is now needed to evaluate each of the other 7 chromatogram’s various separation attributes?
Managing the Specifics of the Data

Need to monitor selectivity changes
- Up to 14 or more injections

Data to evaluate
- Resolution values per peak
- Retention of API
- Various peak widths
- Tailing
- Area%

Information can lead up to a matrix of results essential to making the proper method development decision

- 14 runs, 7 separate decision factors, up to 20 peaks, 2 modes of detection

Data to evaluate:
- 1 run = 280 resulting values
- 14 runs = 3920 resulting values

Then COMPARE to each other!!
Challenges with Manual Review

- **SUBJECTIVE** decision making
- Level of **EXPERIENCE** of analyst
- **COMPLEXITY** of information
- **VOLUME** of Data
- **TIME-CONSUMING** process
Data Processing and Interpretation with Empower 2

- Sorting and visualization to evaluate:
  - Peak attributes
    - Area, RT, width, number of peaks
    - System suitability results
      - Resolution, tailing, k’
  - Purity
    - Flags impure peaks

- Decision Making Tools
  - Appropriate calculation and reporting templates
Obtaining Separation Attributes

System Suitability is used to obtain information related to quality of separation criteria.

- Resolution
- Tailing
- Efficiency
- Symmetry
- Retention Factor ($k'$)

*Scouting injection of Glimepiride on ACQUITY Phenyl, ACN, pH 3.0
Labeled only major peaks of interest
Using Separation Attributes to Evaluate and Interpret Separation Conditions

Identify the Method Intent

Resolution?
- Impurity profile, stability indicating, forced degradation evaluation?
  - Plot greatest number of separated peaks
    - How many peaks meet your resolution criteria?
    - How many critical pairs of peaks are present?
    - Average Peak width?

Speed?
- API assay identification, content uniformity intent?
  - Least amount of tailing for the API?
  - Which has a suitable k’ for API?
  - Which exhibits the best peak width?
Determining Number of Peaks

One of the fastest ways to roughly mine the method scouting data is to determine the conditions that separated the **most number of peaks of interest > x%**

Required Custom Fields:

Peaks_GT_1pct : GT(%Area,1.0)
Boolean field

<table>
<thead>
<tr>
<th>Value</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>N/S</td>
</tr>
<tr>
<td>2</td>
<td>Significant</td>
</tr>
</tbody>
</table>

Use as position all peaks with %Area>1.0 results in a 1=Significant. In subsequent CF calculations the value 1 will be used.

Total_Peaks_GT_1pct : SUM(Peaks_GT_1pct)
This will give the total number of peaks with %Area>1.0
Required Custom Fields:

**PurityFactor**: Purity Threshold – Purity Angle
If peaks is pure Threshold > Angle and then PurityFactor > 0

**Flag_Purity**: GT(PurityFactor, 0)
Boolean field
If peak is NOT pure Flag_Purity = 1

**Impure_Peaks**: SUM(Flag_Purity)
This will give the total number of impure peaks
How many peaks meet the Resolution Criteria?

Task: Find the number of peaks with Rs ≥ 1.5

Required Custom Fields:

**Flag_Critical_Rs_GTE_1o5**: GTE(USP Resolution, 1.5)
Boolean field

<table>
<thead>
<tr>
<th>Value</th>
<th>Translation</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Use as position: all peaks with USP Rs ≥ 1.5 results in a 1=Yes. In subsequent CF calculations the value 1 will be used.

**Total_Peaks_with_Rs_GT_1o5**: SUM(Flag_Critical_Rs_GTE_1o5)
This will give the total number of peaks with Rs ≥ 1.5
How many critical pairs?

Task: Find the number of peaks with Rs<1.5

Required Custom Fields:

**Flag_Critical_Rs_LT_1o5**: LT(USP Resolution, 1.5)
Boolean field

Use as position for all peaks with USP R<1.5 results in a 1=Yes. In subsequent CF calculations the value 1 will be used.

**Total_Peaks_with_Rs_LT_1o5**: SUM(Flag_Critical_Rs_LT_1o5)
This will give the total number of peaks with Rs<1.5
Using Peak Width as Criteria

Task: Find the Separation with the most narrow peaks

Required Custom Field:

**Avg_PeakWidth_Total_Peaks**: AVE(Width)

System Suitability Summary Bar plot
Average Peak Width
Peak Capacity

Task: Find the Separation with Highest Peak Capacity

Required Custom Field:

**Peak_Capacity**: \[ \frac{\text{Runtime}}{\text{AVE(Width@60.7\%)} + 1} \]
API Specific Plots

Tailing Factor
Lowest is Best

Retention Factor
Define a range (i.e: \( k' = 4-9 \))

Peak Width
Lowest is Best

Identify the Method Intent

Speed
API Tailing?
Which has a suitable \( k' \) for API?
Best peak width?
The “Injection Score” is an estimation of which conditions are suitable to explore for further optimization.

In this particular example, the injection score equation included factors about:

- Total peaks found
- Total peaks above 1% area
- Run time
- Average peak width
- Separation space

Injection score equations are recommended to include a weighted relationship of the user’s goals and criteria.
Selecting the best conditions (Column, Solvent & pH) to optimize further

- Based on total number of peaks and injection score, the conditions to optimize are:

- ACQUITY BEH C18
- pH 3
- Acetonitrile
Custom Field/Report Example 2
Test of API for impurities. 6 known impurities, possibly some unknowns.
Criteria: Each known impurity < 1.0% Area.
Each unknown impurity < 1.0% Area
Sum of all known imp. < 5.0% and Sum of all unknown imp. < 1.0%
No CF and standard % Area summary report

Difficult to get a quick overview over Samples that do not meet criteria
Testing for known impurities
With % Area ≥ 1.0

Formula:

GTE(% Area,1.0)
Testing for unknown impurities
With % Area ≥ 1.0

Formula:

GTE(% Area, 1.0)
Calculating the Sum of % Area known impurities.

Formula:

\[ \text{SUM}(\% \text{ Area} \times \text{NEQ}(\text{Name}, "API")) \]
Calculating the Sum of % Area unknown impurities.

Formula:

\[ \text{SUM}(\% \text{ Area}) \]
Testing if Sum of Known Impurities $< 5\%$ AND if Sum Of unknown impurities $< 1\%$

Formula:

$\text{LT(Total\_known\_impurities,5)} \& \text{LT(Total\_unknown\_impurities,1)}$
Report for known impurities

Easy overview over which samples and which peaks fail the criteria of < 1.0 % Area

<table>
<thead>
<tr>
<th>SampleName</th>
<th>Inj</th>
<th>Vial</th>
<th>Impurity1</th>
<th>Impurity2</th>
<th>Impurity3</th>
<th>Impurity4</th>
<th>Impurity5</th>
<th>Impurity6</th>
</tr>
</thead>
<tbody>
<tr>
<td>SampleA</td>
<td>1</td>
<td>A,7</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleA</td>
<td>2</td>
<td>A,7</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleB</td>
<td>1</td>
<td>A,8</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleB</td>
<td>2</td>
<td>A,8</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleC</td>
<td>1</td>
<td>B,1</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleC</td>
<td>2</td>
<td>B,1</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleD</td>
<td>1</td>
<td>B,2</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleD</td>
<td>2</td>
<td>B,2</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleE</td>
<td>1</td>
<td>B,3</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleE</td>
<td>2</td>
<td>B,3</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleF</td>
<td>1</td>
<td>B,4</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleF</td>
<td>2</td>
<td>B,4</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleG</td>
<td>1</td>
<td>B,5</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleG</td>
<td>2</td>
<td>B,5</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
</tr>
<tr>
<td>SampleH</td>
<td>1</td>
<td>B,6</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
</tr>
<tr>
<td>SampleH</td>
<td>2</td>
<td>B,6</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
<td>Known Impurity&gt;1.0%</td>
</tr>
<tr>
<td>SampleI</td>
<td>1</td>
<td>B,7</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleI</td>
<td>2</td>
<td>B,7</td>
<td>Known Impurity&gt;1.0%</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleJ</td>
<td>1</td>
<td>B,8</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleJ</td>
<td>2</td>
<td>B,8</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleJ</td>
<td>1</td>
<td>C,1</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleJ</td>
<td>2</td>
<td>C,1</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>SampleK</td>
<td>1</td>
<td>C,2</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
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<tr>
<td>SampleK</td>
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<td>C,2</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
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</tr>
</tbody>
</table>
Report Properties

Unknown impurities will not be reported

Results for Standards and Controls will not be included

Results for the main peak = API will not be reported
Report for unknown impurities

Easy overview over which samples and which peaks fail the criteria of < 1.0 % Area

<table>
<thead>
<tr>
<th>SampleName</th>
<th>Inj</th>
<th>Vial</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>SampleA</td>
<td>1</td>
<td>1:A,7</td>
<td>OK</td>
</tr>
<tr>
<td>SampleA</td>
<td>2</td>
<td>1:A,7</td>
<td>OK</td>
</tr>
<tr>
<td>SampleB</td>
<td>1</td>
<td>1:A,8</td>
<td>OK</td>
</tr>
<tr>
<td>SampleB</td>
<td>2</td>
<td>1:A,8</td>
<td>OK</td>
</tr>
<tr>
<td>SampleC</td>
<td>1</td>
<td>1:B,1</td>
<td>OK</td>
</tr>
<tr>
<td>SampleC</td>
<td>2</td>
<td>1:B,1</td>
<td>OK</td>
</tr>
<tr>
<td>SampleD</td>
<td>1</td>
<td>1:B,2</td>
<td>OK</td>
</tr>
<tr>
<td>SampleD</td>
<td>2</td>
<td>1:B,2</td>
<td>OK</td>
</tr>
<tr>
<td>SampleE</td>
<td>1</td>
<td>1:B,3</td>
<td>OK</td>
</tr>
<tr>
<td>SampleE</td>
<td>2</td>
<td>1:B,3</td>
<td>OK</td>
</tr>
<tr>
<td>SampleF</td>
<td>1</td>
<td>1:B,4</td>
<td>OK</td>
</tr>
<tr>
<td>SampleF</td>
<td>2</td>
<td>1:B,4</td>
<td>OK</td>
</tr>
<tr>
<td>SampleG</td>
<td>1</td>
<td>1:B,5</td>
<td>OK</td>
</tr>
<tr>
<td>SampleG</td>
<td>2</td>
<td>1:B,5</td>
<td>OK</td>
</tr>
<tr>
<td>SampleI</td>
<td>1</td>
<td>1:B,7</td>
<td>OK</td>
</tr>
<tr>
<td>SampleI</td>
<td>2</td>
<td>1:B,7</td>
<td>OK</td>
</tr>
<tr>
<td>SampleJ</td>
<td>1</td>
<td>1:B,8</td>
<td>OK</td>
</tr>
<tr>
<td>SampleJ</td>
<td>2</td>
<td>1:B,8</td>
<td>OK</td>
</tr>
<tr>
<td>SampleK</td>
<td>1</td>
<td>1:C,1</td>
<td>OK</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Report Properties

Only Unknown impurities will not be reported

Results for Standards and Controls will not be included

Results for the main peak = API will not be reported
# Report for total known and unknown impurities with pass/fail criteria

Easy overview over which samples that fails.

<table>
<thead>
<tr>
<th>SampleName</th>
<th>Vial</th>
<th>Injection</th>
<th>Total_known_impurities</th>
<th>Total_unknown_impurities</th>
<th>Test_impurities</th>
</tr>
</thead>
<tbody>
<tr>
<td>SampleA</td>
<td>1:A,7</td>
<td>1</td>
<td>3.73</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleA</td>
<td>1:A,7</td>
<td>2</td>
<td>3.72</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleB</td>
<td>1:A,8</td>
<td>1</td>
<td>3.29</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleB</td>
<td>1:A,8</td>
<td>2</td>
<td>3.29</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleC</td>
<td>1:B,1</td>
<td>1</td>
<td>3.61</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleC</td>
<td>1:B,1</td>
<td>2</td>
<td>3.61</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleD</td>
<td>1:B,2</td>
<td>1</td>
<td>3.99</td>
<td>1.76</td>
<td>Imp. to high</td>
</tr>
<tr>
<td>SampleD</td>
<td>1:B,2</td>
<td>2</td>
<td>3.99</td>
<td>1.76</td>
<td>Imp. to high</td>
</tr>
<tr>
<td>SampleE</td>
<td>1:B,3</td>
<td>1</td>
<td>3.16</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleE</td>
<td>1:B,3</td>
<td>2</td>
<td>3.16</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleF</td>
<td>1:B,4</td>
<td>1</td>
<td>3.59</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleF</td>
<td>1:B,4</td>
<td>2</td>
<td>3.58</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleG</td>
<td>1:B,5</td>
<td>1</td>
<td>4.54</td>
<td>0.02</td>
<td>OK</td>
</tr>
<tr>
<td>SampleG</td>
<td>1:B,5</td>
<td>2</td>
<td>4.55</td>
<td>0.02</td>
<td>OK</td>
</tr>
</tbody>
</table>
Results for Standards and Controls will not be included.
Conclusion

- By combining Custom Fields and appropriate report formats, interpretation of results will be much easier