Report customization

- **How it works**
  - Overview
  - Data organization
  - Excel add-in
- **Preparations for report customization**
  - Excel configuration
  - Intermediate XML files
- **Report customization**
  - Report editing rules
  - Width adjustment and table formatting
  - Header and footer
  - Association, ISTD and Formula
  - Graphics
  - Transposed, wrapped and combined tables
  - VLOOKUP
  - TotalRows
- **Creating faster reports**
Overview
Data organization
XML Schema, XML dataset and Composite keys

- **XML Schema**
  - Dictates how XML dataset data is organized
  - Maps where to put information
    - .xds extension
    - Located along with report template

- **XML datasets**
  - MH adds results as when reports called
  - Holds batch data and points to picture files
    - Quant: report.results.xml
    - Qual:
      - ICP-MS:

- **Composite keys (ID)**
  - Uniquely points to relevant data in XML dataset
  - Used in finding and filtering of data
Excel add-in

- **VBA (Visual Basic for Applications) project**
  - Adds excel functionality used in report design and generation
  - .xla (2007) or .xlam (2010/2013) extension
  - Designer Add-in menu
    - Quant/Qual (2010/2013): MASSHUNTER REPORTING
    - Quant/Qual (2007), ICP-MS (2010): Add-in

- **Main functions**
  - Creates Add-in menu
  - Support for report template design
  - Import data
  - Filter tables that contain data for report
  - Final formatting of report
Excel configuration

- **VBA xla/xlam files in correct location and enabled**
  - Install Quant reporting from installation media
    - .\setup.quantreport.exe
  - Install Qual/ICP-MS or copy needed files
    - C:\Program Files (x86)\Microsoft Office\...
      - Excel 2007: ...office12\library
      - Excel 2010: ...office14\library
      - Excel 2013: ...office15\library

- **Enable test mode**
  - Open Notepad in administration mode
  - Open corresponding config file
  - Change Testmode from False to True and save
    - Note extension

- **Enable developer tab**

- **Disable autorecover option**
  - May corrupt template if left enabled
Intermediate XML files

- **XML datasets and image files**
  - XML dataset has all results and image paths
  - Quickly generate different reports
  - Test report templates

- **Quant & ICP-MS**
  - Files remain at report folder
    - Report.results.xml

- **Qual**
  - Intermediate files deleted after report generation
  - Deletion disabled via Qual software
    - Report.xml
    - Configuration>Intermediate Report Files...
Report editing rules

- **Save frequently**
  - Template might corrupt during edit

- **Use XML result file**
  - Don’t save untested report

- **After testing always clear results**
  - Prevents template corruption

- **Don’t try to fix error**
  - Always select end
  - Close excel, MassHunter and check task manager

- **Add table columns from correct source map**
  - Different for each table

- **Delete table columns correctly**
  - Do: Right click: Delete > Table Columns
  - Do: Excel Ribbon: Home > Delete
  - Do: Keyboard: Control + Minus key
  - Don’t: Press Del key
Width adjustment and table formatting

- **Width adjustment**
  - Option page: Auto fit column TRUE > Adjust column width through add-in
    - Comments are error prone and not recommended
    - Transposed tables: Width setting applies only to data. Headers always adjusted to fit
  - Option page: Auto fit column FALSE > Adjust column width as regular spreadsheet
    - FAST reports, tune and acquisition reports
    - Note correct column because of hidden concent > process/clear results

- **Table formatting**
  - Use excel formatting tools > Font / Alignment / Number
    - Text for strings
    - Number for numbers, when you want to set significant digits
    - General for formulas
    - Custom for special date formatting
  - Table header row height can be changed and height for other rows are automatically adjusted
  - Filter data through add-in or use excel custom filter
    - Not found: PeakID= / Found: PeakID=0
  - Use excel conditional formatting
    - Easily change font color and/or change cell color
Header and footer

- **Header/Footer**
  - Divided in three sections
  - Only one picture per section
  - Manual height adjustment can generate errors
    - Edit margins instead

- **Company logo**
  - Try to fit logo to default height limits
    - Tested to fit: 375 x 72 pixels at 300 pixels/inch / 1.25 x 0.24 inch / 3.18 x 0.61 cm
Association, ISTD, Formula

- **Association**
  - Associates item to be printed on same page as associated table/graphic
    - Click header>Advanced properties>Cell-tab>Associate with the following table or graphics
    - Doesn’t work if table contains graphics

- **ISTD columns**
  - Added from add-in
    - Table must contain SampleID, CompoundID, ISTDCompoundID
    - Table must contain corresponding column for target compound

- **Formula columns**
  - Add through add-in
  - Add column directly to table
    - Right-click table header to add column
    - Must be set as formula through add-in advanced properties
Graphics (1)

- **MassHunter report settings**
  - Picture formatting through analysis software
  - X-/Y-axis settings

- **Multiple graphics in row**
  - Excel add-in advanced properties
    - Relative to page width

- **Graphics row height**
  - Add-in automatically adjusts height by default
  - Can be adjusted manually
    - Program uses largest height adjustment found in table
    - Must be correct or else graphics overlap
    - Faster reporting
Graphics (2)
Transposed, wrapped and combined tables

- **Transposed**
  - Changes headers from side-by-side to stacked format

- **Wrap columns**
  - Tables continue as side-by-side table
  - Saves space in report when tables narrower than ½ page width

- **Combine table rows**
  - Starting from varying information data is side-by-side
  - Super header adds additional header row

```
<table>
<thead>
<tr>
<th>Name</th>
<th>Comp</th>
<th>Level</th>
<th>Height</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name 1</td>
<td>C1</td>
<td>L1-1</td>
<td>H1-1</td>
<td>R1-1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>L1-2</td>
<td>H1-2</td>
<td>R1-2</td>
</tr>
<tr>
<td>Name 1</td>
<td>C1</td>
<td>L1-3</td>
<td>H1-3</td>
<td>R1-3</td>
</tr>
<tr>
<td>Name 2</td>
<td>C2</td>
<td>L2-1</td>
<td>H2-1</td>
<td>R2-1</td>
</tr>
<tr>
<td>Name 2</td>
<td>C2</td>
<td>L2-2</td>
<td>H2-2</td>
<td>R2-2</td>
</tr>
</tbody>
</table>
```

```
<table>
<thead>
<tr>
<th>Name</th>
<th>Comp</th>
<th>Level</th>
<th>Height</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name 1</td>
<td>C1</td>
<td>L1-1</td>
<td>H1-1</td>
<td>R1-1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>L1-3</td>
<td>H1-3</td>
<td>R1-3</td>
</tr>
<tr>
<td>Name 2</td>
<td>C2</td>
<td>L2-1</td>
<td>H2-1</td>
<td>R2-1</td>
</tr>
<tr>
<td></td>
<td></td>
<td>L2-2</td>
<td>H2-2</td>
<td>R2-2</td>
</tr>
</tbody>
</table>
```

```
<table>
<thead>
<tr>
<th>L1</th>
<th>L2</th>
<th>L3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Name</td>
<td>Comp</td>
<td>Conc</td>
</tr>
<tr>
<td>Name 1</td>
<td>C1</td>
<td>0.2</td>
</tr>
<tr>
<td>Name 2</td>
<td>C2</td>
<td>0.3</td>
</tr>
</tbody>
</table>
VLOOKUP

- **Useful for getting data from other branches to one table**
  - Add qualifier ratios to sample table

- **Only works with one lookup value**
  - Use composite keys to pinpoint data
  - Glue keys together with an Excel text concatenation
  - Qualifier page: =SampleID"-"&CompoundID"-"&QualifierID"-"&PeakID
  - Table item: =SampleID"-"&CompoundID"-0-"&PeakID
  - QualifierID = 0 for Qualifier1
  - QualifierID = 1 for Qualifier2
  - Etc...

- **Reminders**
  - Makes report slower
VLOOKUP – XML Branches...

- Global Attributes
  - Batch (1)
    - TargetCompound (1 to n)
      - Peak (1 to n)
        - PeakQualifier (1 to n)
      - TargetQualifier (1 to n)
      - Calibration (1)
    - Sample Attributes
    - Method Attributes
    - Result Attributes
Total Row

- **Total row**
  - Useful for adding different calculations
    - Average/sum/count etc.
  - Additional information can be added

```excel
fx = "Average factor=\&TEXT(SUBTOTAL(101,[ResponseRatio]), ",.0000")"
```

0.481950706  
0.713812136  
0.610733832  
1.994909207  
1.229336884  
1.454008294  
1.515036732

Average RR = 2.8922
Creating faster reports

- **Manually format Excel**
  - Column width
    - Report template options > Adjust columns to fit data = False
    - Graphic row height

- **Avoid graphics when possible**
  - Needs most resources

- **Run report in single sample mode if possible**
  - Repeats and sheetbreaks per sample/data file?
  - Summary sheets and sample sheets in different reports

- **Delete unused XML maps**

- **Limit VLOOKUP function ranges to minimum**