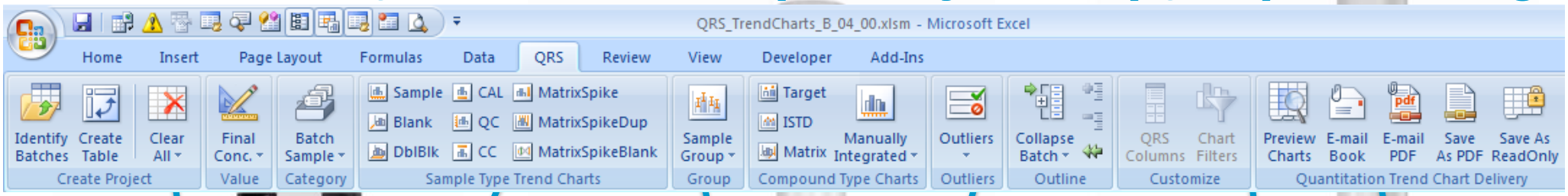
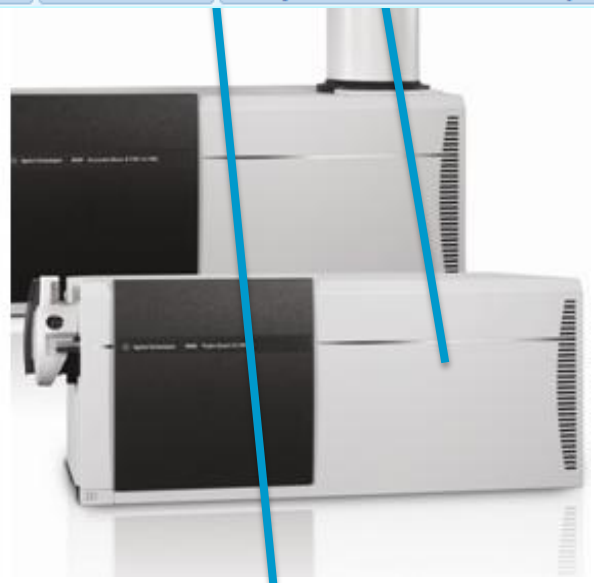
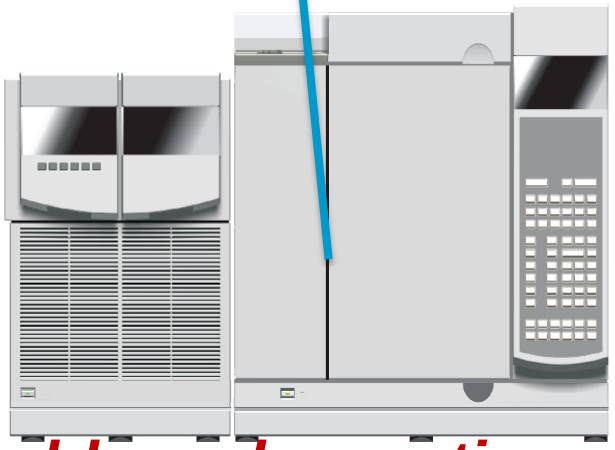
Excel-based Quantitation Report System (QRS) Trending

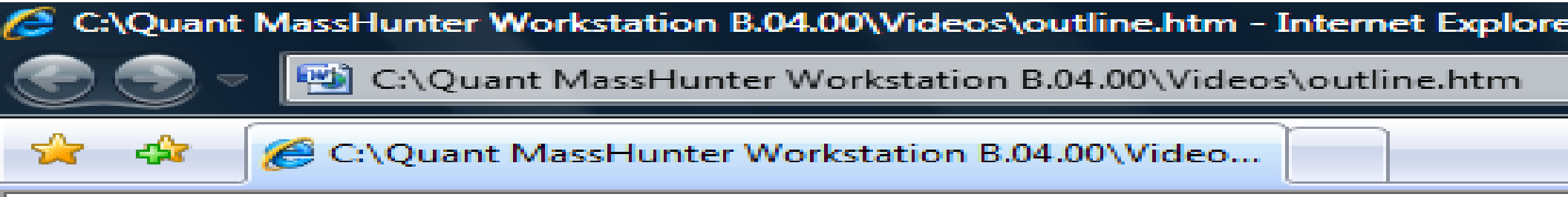






- ***Extension of MassHunter integrated Excel-based reporting***

Excel-based Quantitation Report System (QRS) Videos



Excel-based QRS Trending

Quantitation Report System
- Introduction (Background)
- Scenarios (Background)

Quick Demo
- Calibration (Advanced)
- Target Compounds (Advanced)
- Qualifiers (Advanced)
-

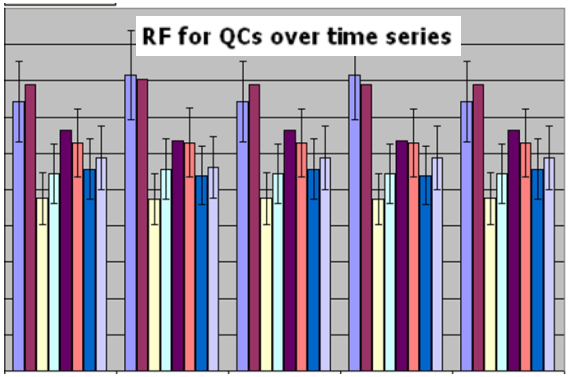
Advanced Demo
- Calibration (Expert)
- Target Compounds (Expert)
- Qualifiers (Expert)

Technical Design
- Design explanation (Wizard)
- Error Recovery Advice (Wizard)

Videos on shipping Quant DVD

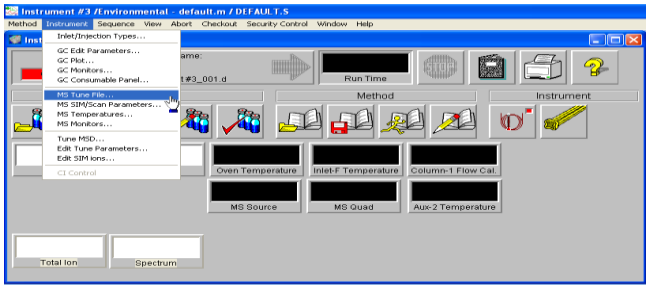
QRS Excel-based Trend Report Value Proposition

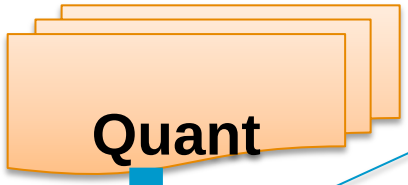
- Address trend reporting needs across batches or date/time
  - Monitor samples types
    - Trend by Samples, CALs, QCs, Blanks, Spikes
  - Monitor target compounds or qualifiers results
    - Trend metrics grouped by sample/compound/group
    - Trend organized by time series { before/after, treated/untreated }
  - Monitor outliers results
    - Trend by quality metrics



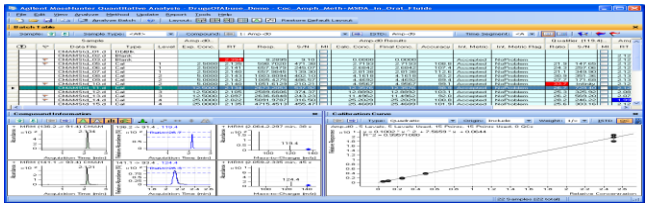
Quantitation Pipeline software architecture

Deliverables:
Acquisition data

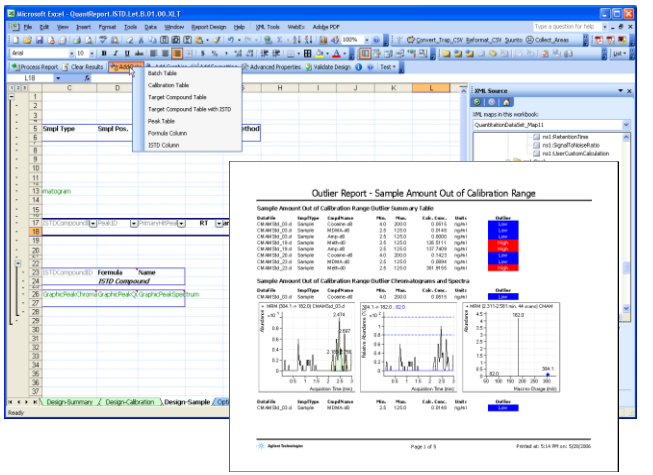




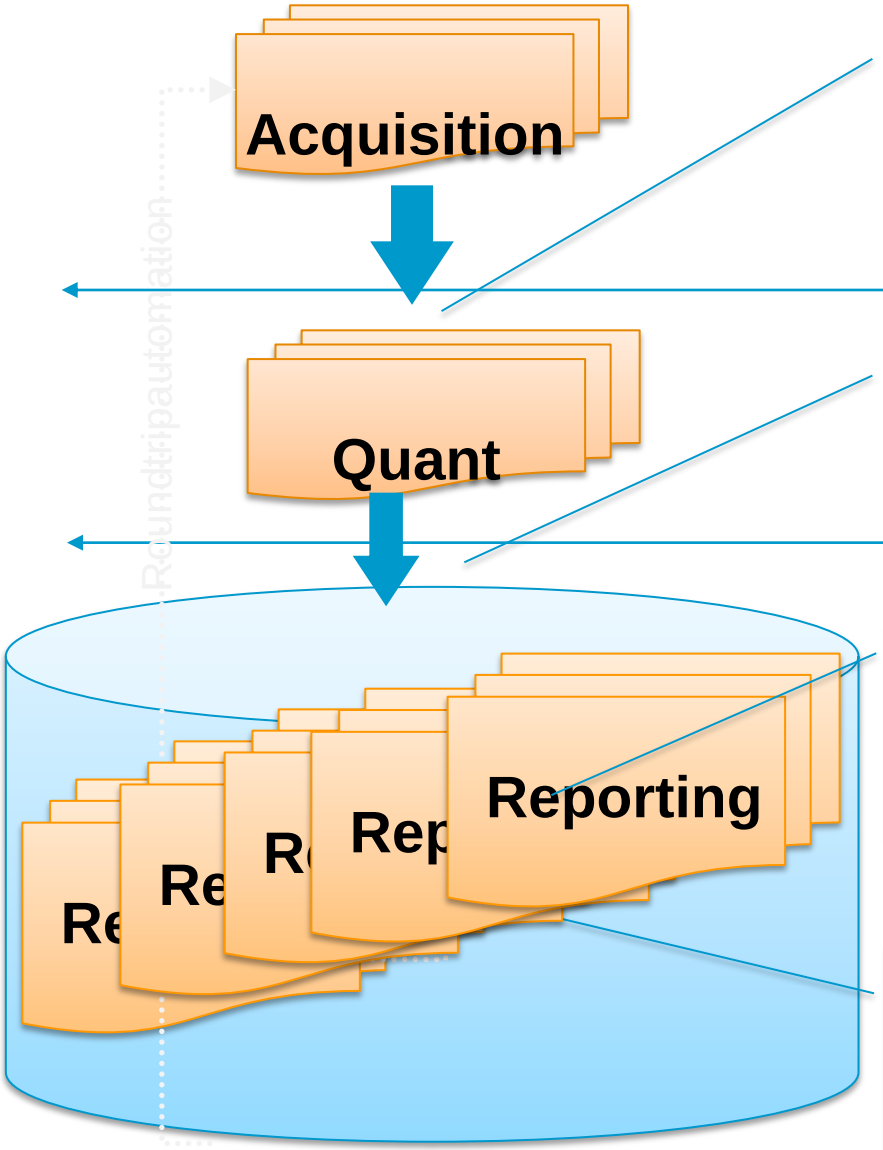
Deliverables:
Reporting results



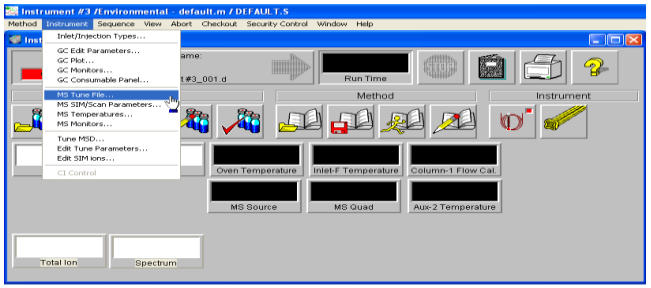
Deliverables:
Batch based
Excel-based Reports



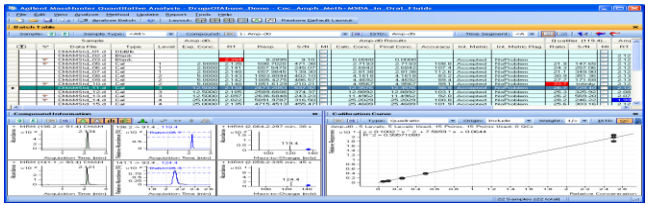
Quantitation Pipeline software architecture



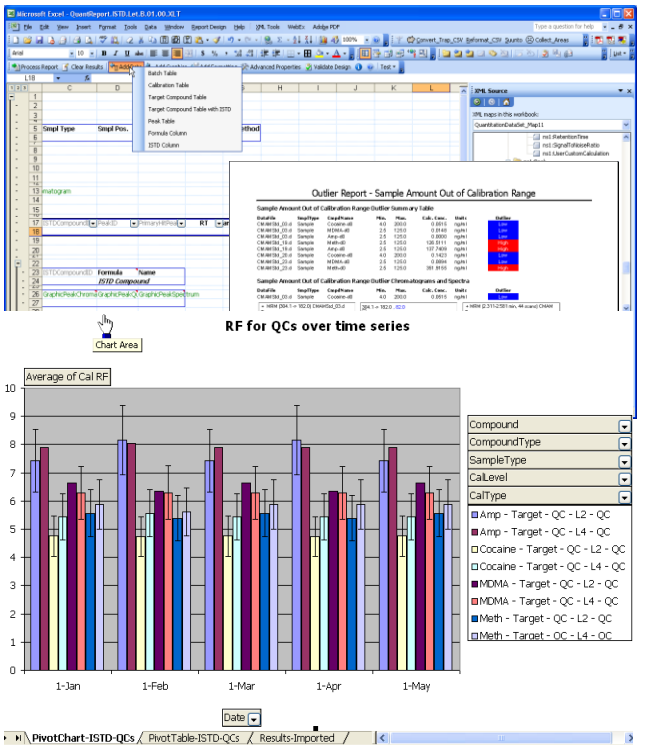
Deliverables:
Acquisition data



Deliverables:
Reporting results

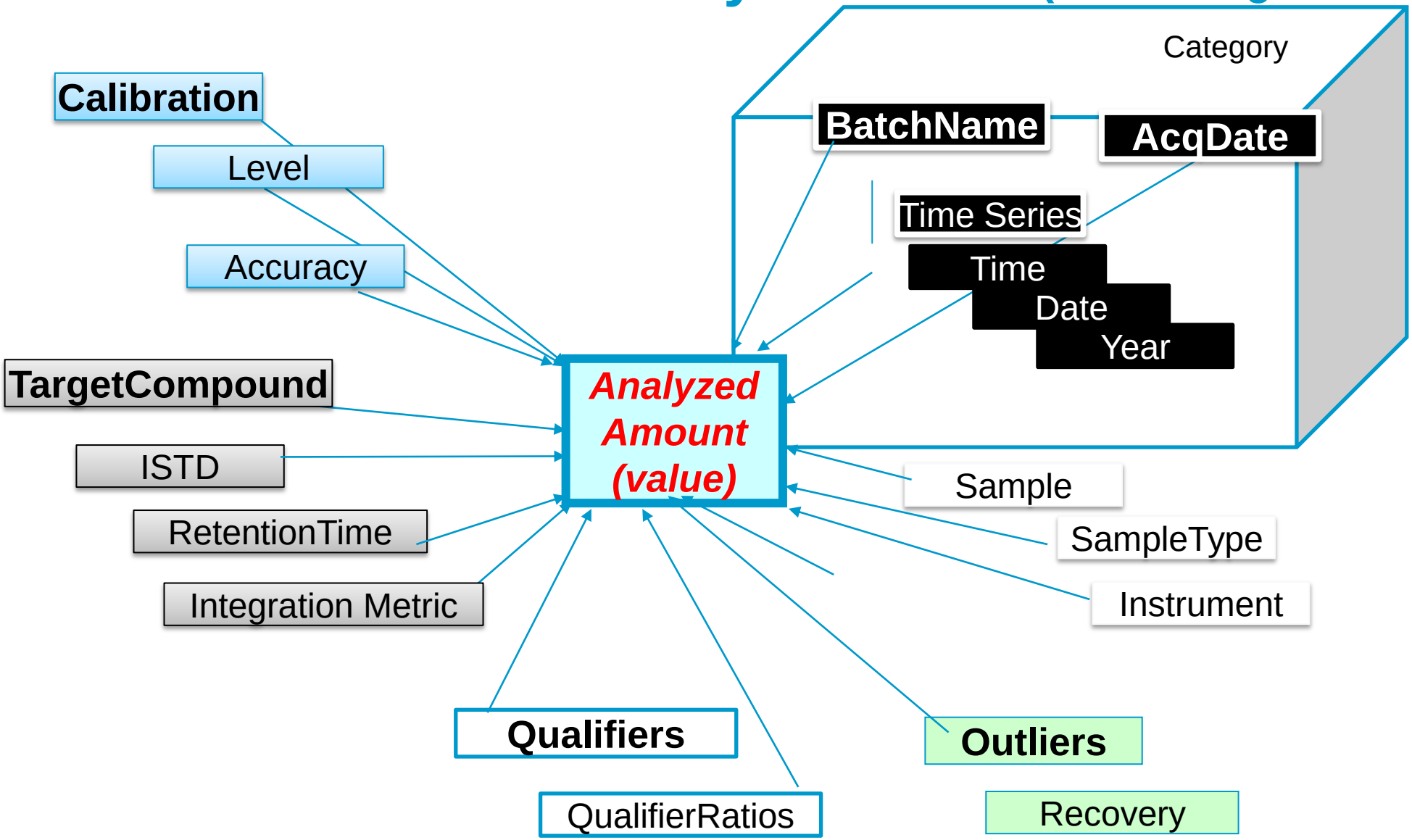


Deliverables:
Batch based
Excel-based Reports

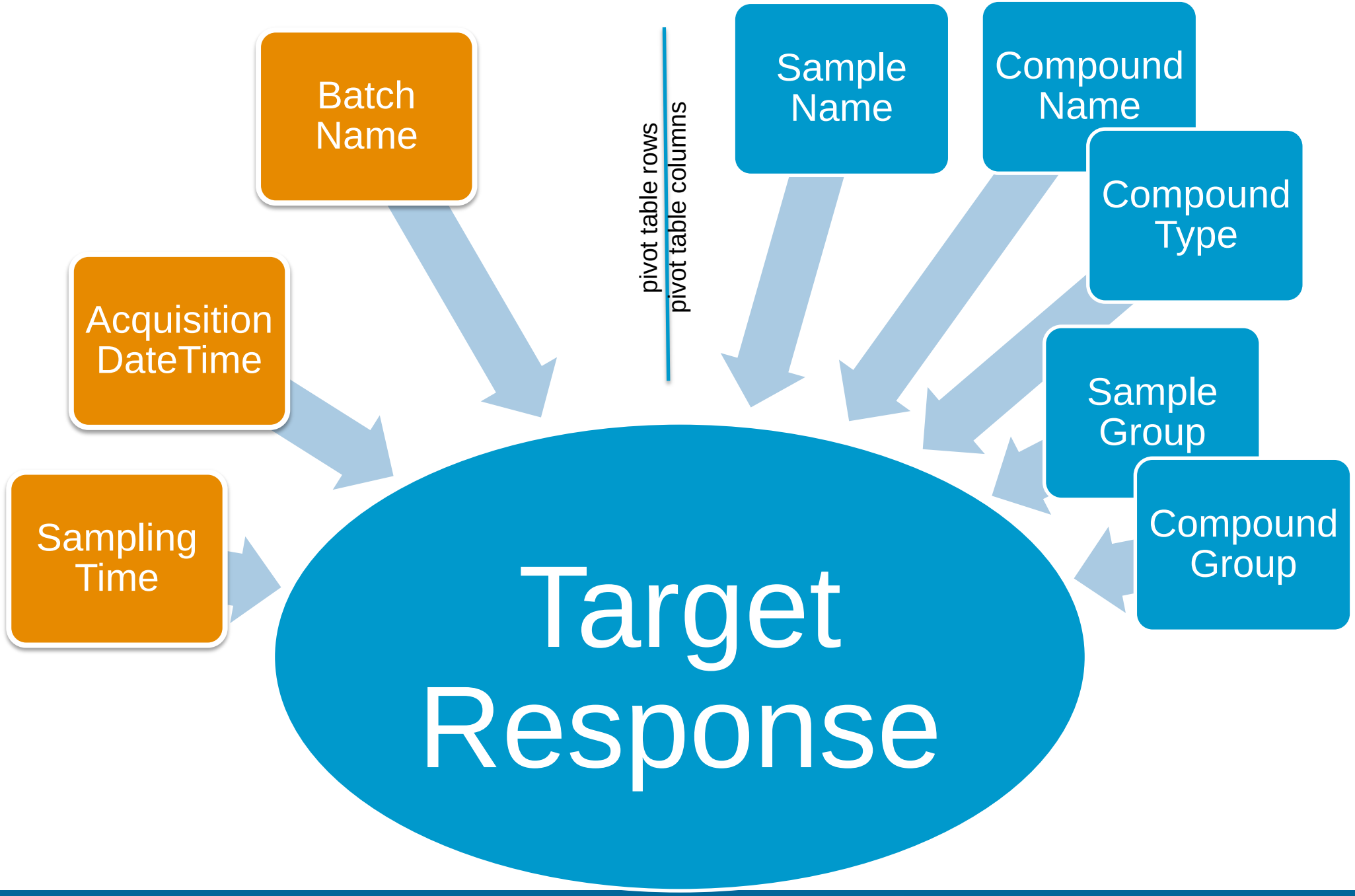


Deliverables:
Trend Reporting
Cross-batch
QA trend metrics

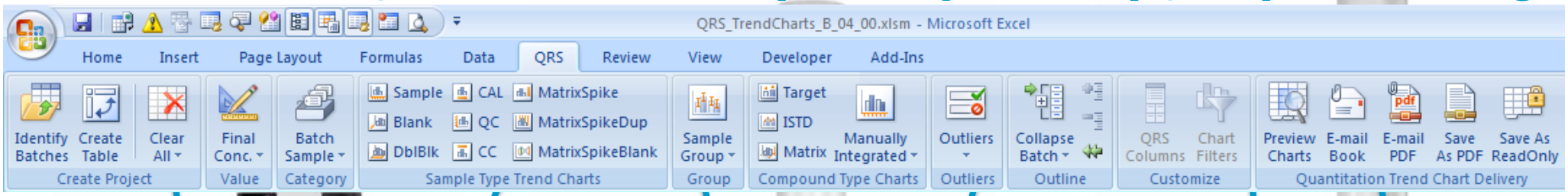
Data Warehouse and Analysis Cube (star configuration)



QRS Star Configuration (MultiDimensional Analysis)



Excel-based Quantitation Report System (QRS) Trending



- ***Extension of MassHunter integrated Excel-based reporting***

Quantitation Report System Trend Report

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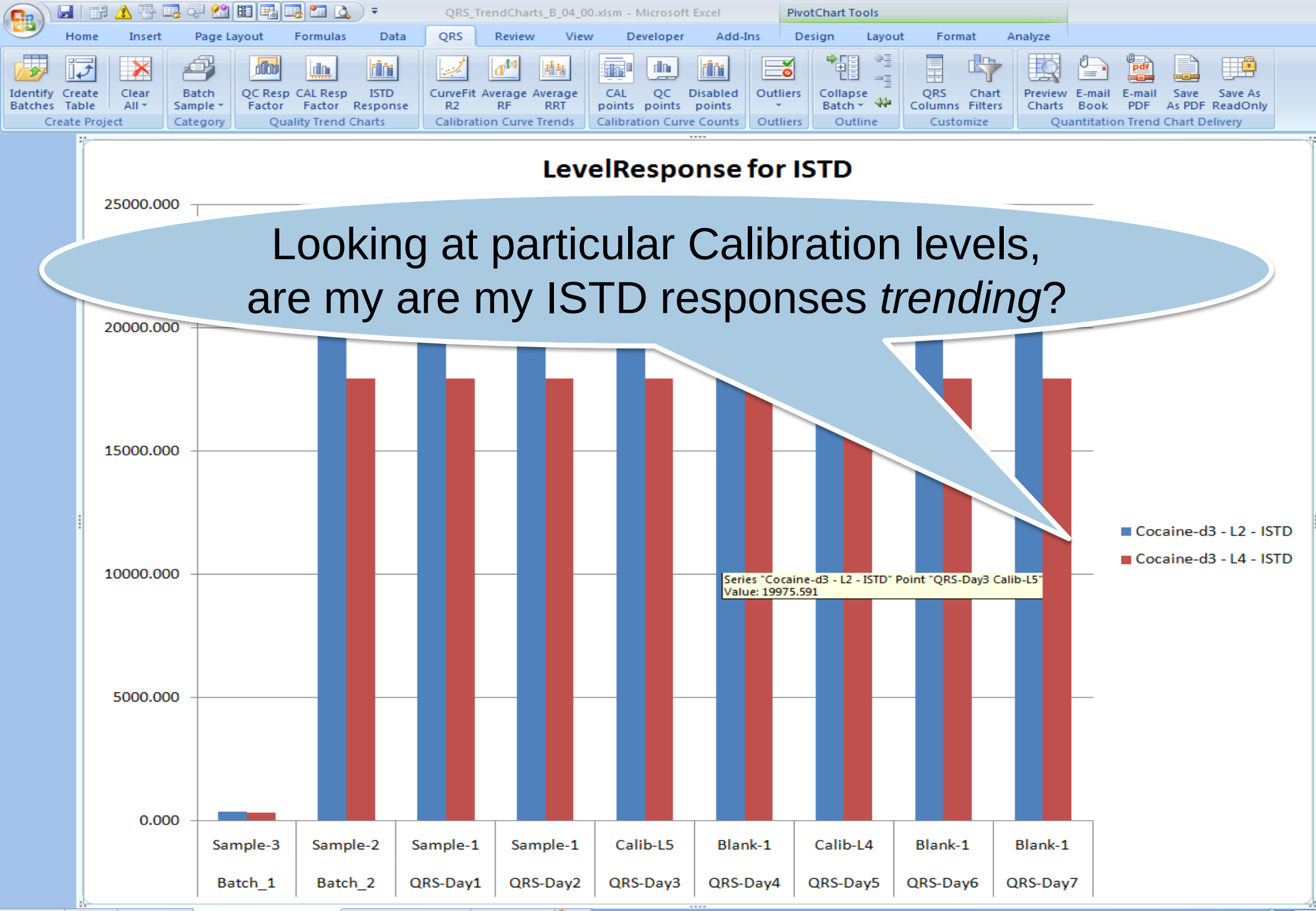
QRS offers an interactive stepwise process to building your charts:

1. QRS creates an XML Table from importing multiple XML quantitation reporting results files.
2. QRS creates a PivotTable Cache which organizes the combined cross-batch quantitated results.
3. QRS creates a PivotTable with appropriate measures and filters from the shared PivotTable Cache.
4. QRS creates a PivotTable Chart which displays the trend report graphically.

Select Quantitation Report System Trend Report:

Calibration | TargetCompound | TargetQualifier


QRS_TrendCharts_B_04_00.xlsm - Microsoft Excel
PivotChart Tools
Home
Insert
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Formulas
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Developer
Add-Ins
Design
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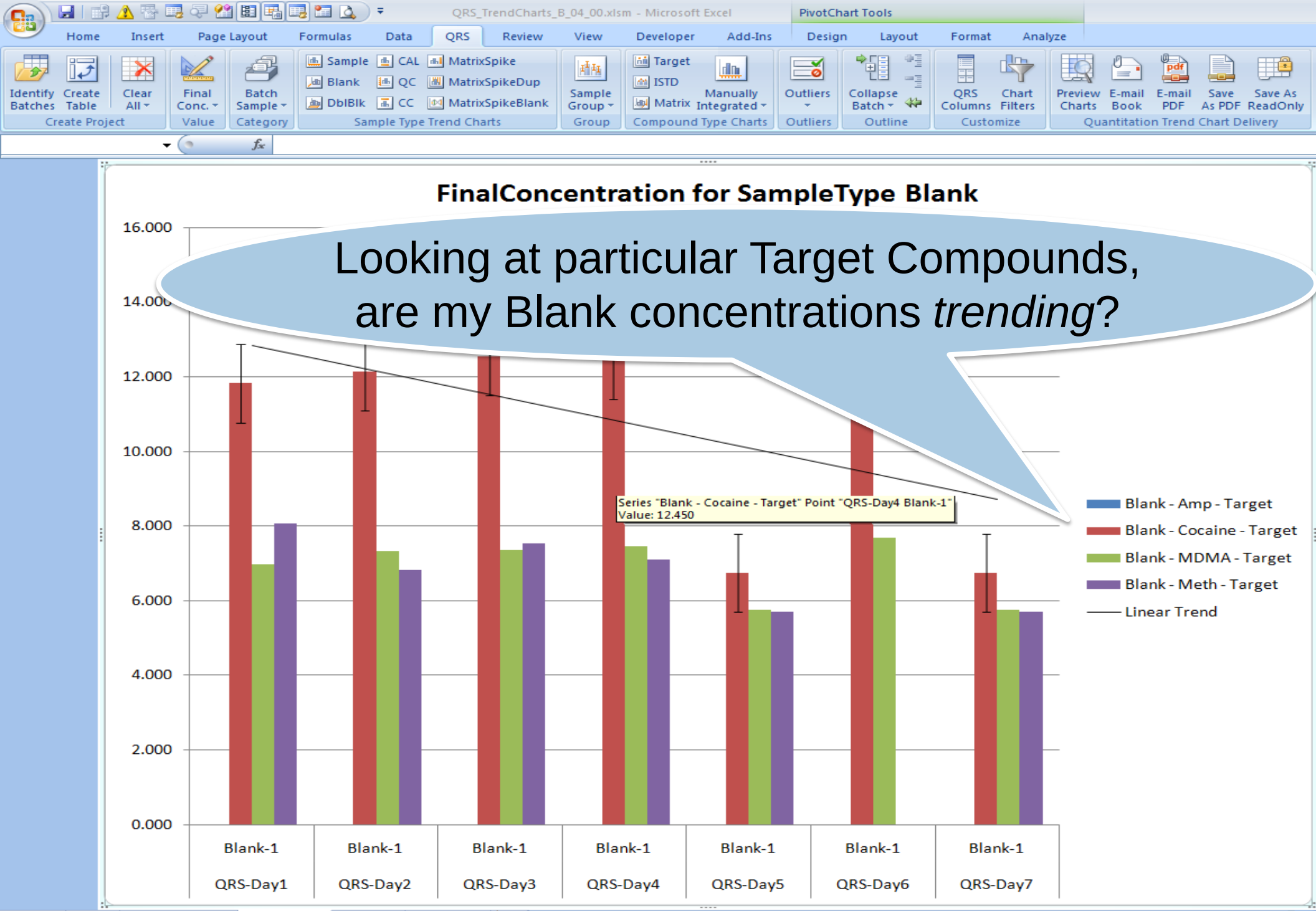
Format
Analyze
Identify Batches
Create Table
Clear All
Create Project
Batch Sample
Category
QC Resp Factor
CAL Resp Factor
ISTD Response
Quality Trend Charts
CurveFit R2
Average RF
Average RRT
Calibration Curve Trends
CAL points
QC points
Disabled points
Calibration Curve Counts
Outliers
Outliers
Collapse Batch
Outline
QRS Columns
Chart Filters
Customize
Preview Charts
E-mail Book
E-mail PDF
Save As PDF
Save As ReadOnly
Quantitation Trend Chart Delivery
LevelResponse for ISTD
Looking at particular Calibration levels,
are my are my ISTD responses *trending*?
25000.000
20000.000
15000.000
10000.000
5000.000
0.000
Series "Cocaine-d3 - L2 - ISTD" Point "QRS-Day3 Calib-L5"
Value: 19975.591
Cocaine-d3 - L2 - ISTD
Cocaine-d3 - L4 - ISTD
Sample-3
Batch_1
Sample-2
Batch_2
Sample-1
QRS-Day1
Sample-1
QRS-Day2
Calib-L5
QRS-Day3
Blank-1
QRS-Day4
Calib-L4
QRS-Day5
Blank-1
QRS-Day6
Blank-1
QRS-Day7
QRS
Calibration
CRT-ISTDResponse
PT-ISTDResponse
PivotTable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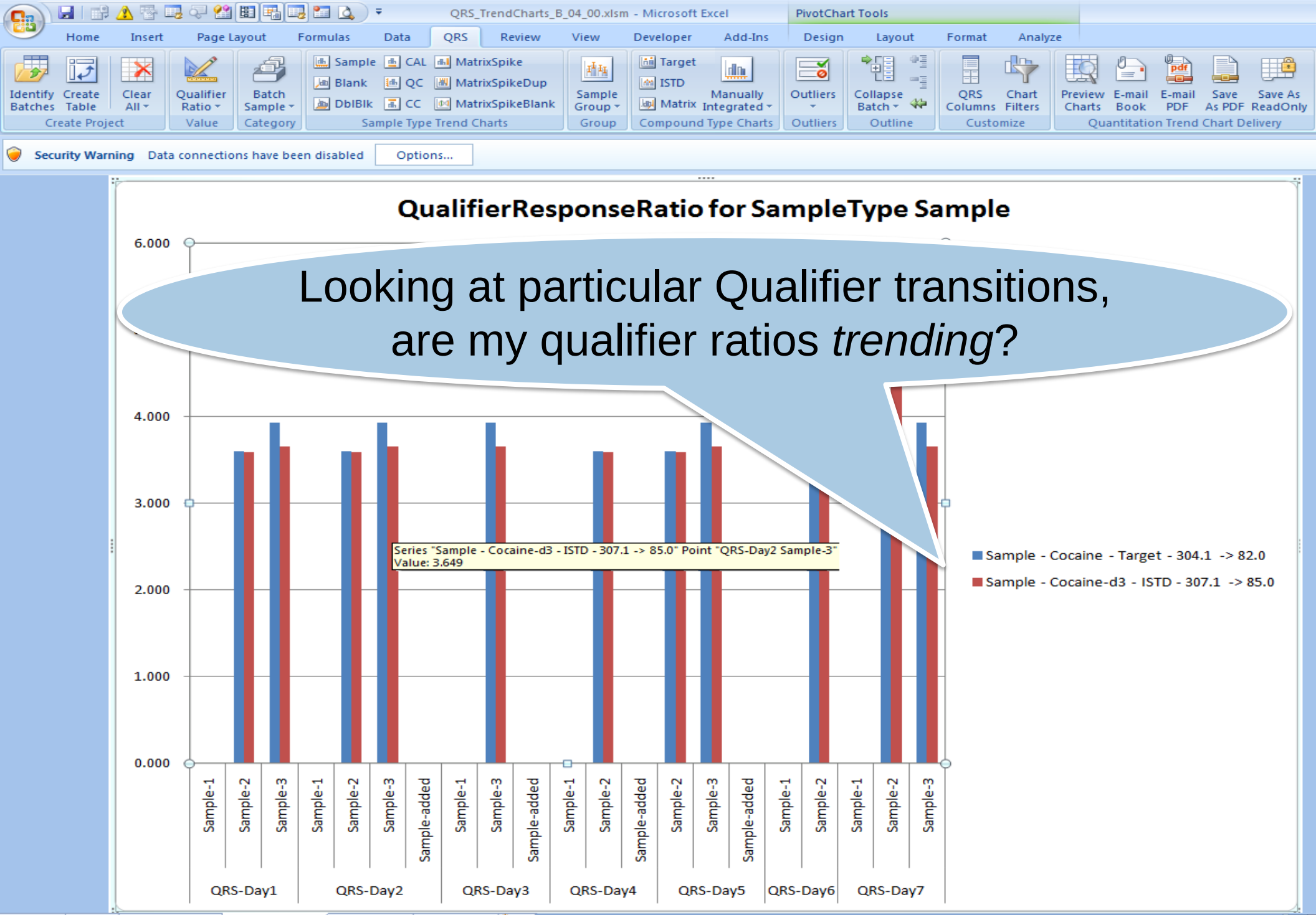
MatrixSpike
MatrixSpikeDup
MatrixSpikeBlank
Sample Type Trend Charts
Sample Group
Group
Target
ISTD
Matrix
Manually Integrated
Compound Type Charts
Outliers
Outliers
Collapse Batch
Outline
QRS Columns
Chart Filters
Customize
Preview Charts
E-mail Book
E-mail PDF
Save As PDF
Save As ReadOnly
Quantitation Trend Chart Delivery
FinalConcentration for SampleType Blank
Looking at particular Target Compounds, are my Blank concentrations trending?
16.000
14.000
12.000
10.000
8.000
6.000
4.000
2.000
0.000
Series "Blank - Cocaine - Target" Point "QRS-Day4 Blank-1"
Value: 12.450
Blank - Amp - Target
Blank - Cocaine - Target
Blank - MDMA - Target
Blank - Meth - Target
Linear Trend
Blank-1 QRS-Day1
Blank-1 QRS-Day2
Blank-1 QRS-Day3
Blank-1 QRS-Day4
Blank-1 QRS-Day5
Blank-1 QRS-Day6
Blank-1 QRS-Day7
QRS
TargetCompound
CRT-Blank
PT-Blank
PivotTable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Clear All
Create Project
Qualifier Ratio
Value
Batch Sample
Category
Sample
Blank
DblBlk
CAL
QC
CC
MatrixSpike
MatrixSpikeDup
MatrixSpikeBlank
Sample Type Trend Charts
Sample Group
Group
Target
ISTD
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Outliers
Collapse Batch
Outline
QRS Columns
Chart Filters
Customize
Preview Charts
E-mail Book
E-mail PDF
Save As PDF
Save As ReadOnly
Quantitation Trend Chart Delivery
Security Warning
Data connections have been disabled
Options...
QualifierResponseRatio for SampleType Sample
Looking at particular Qualifier transitions, are my qualifier ratios *trending*?
6.000
4.000
3.000
2.000
1.000
0.000
Series "Sample - Cocaine-d3 - ISTD - 307.1 -> 85.0" Point "QRS-Day2 Sample-3"
Value: 3.649
Sample - Cocaine - Target - 304.1 -> 82.0
Sample - Cocaine-d3 - ISTD - 307.1 -> 85.0
Sample-1
Sample-2
Sample-3
Sample-added
QRS-Day1
QRS-Day2
QRS-Day3
QRS-Day4
QRS-Day5
QRS-Day6
QRS-Day7
QRS
TargetQualifier
CRT-Sample
PT-Sample
PivotTable

Pivot Chart

Pivot Table

Pivot Cache

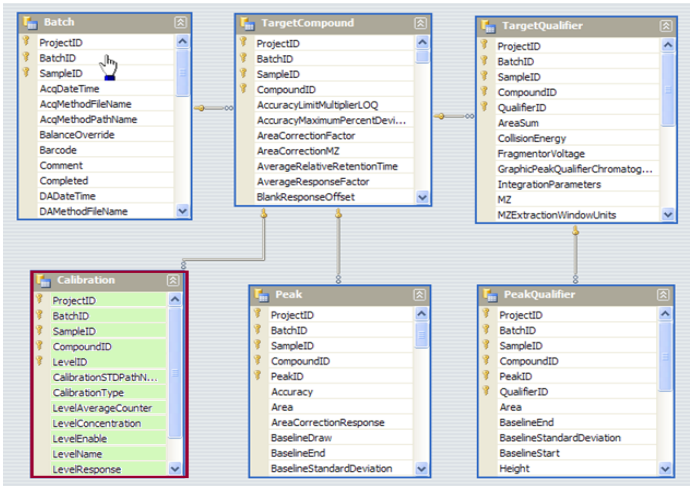
Excel Table

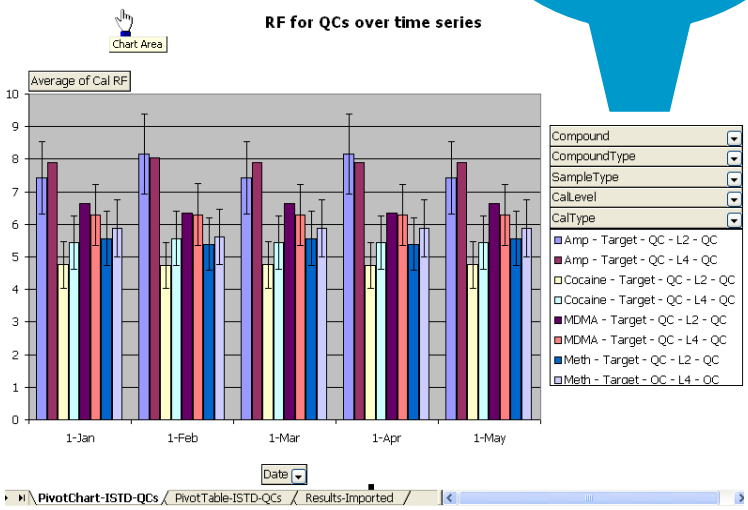
Import

Quant

XML

results





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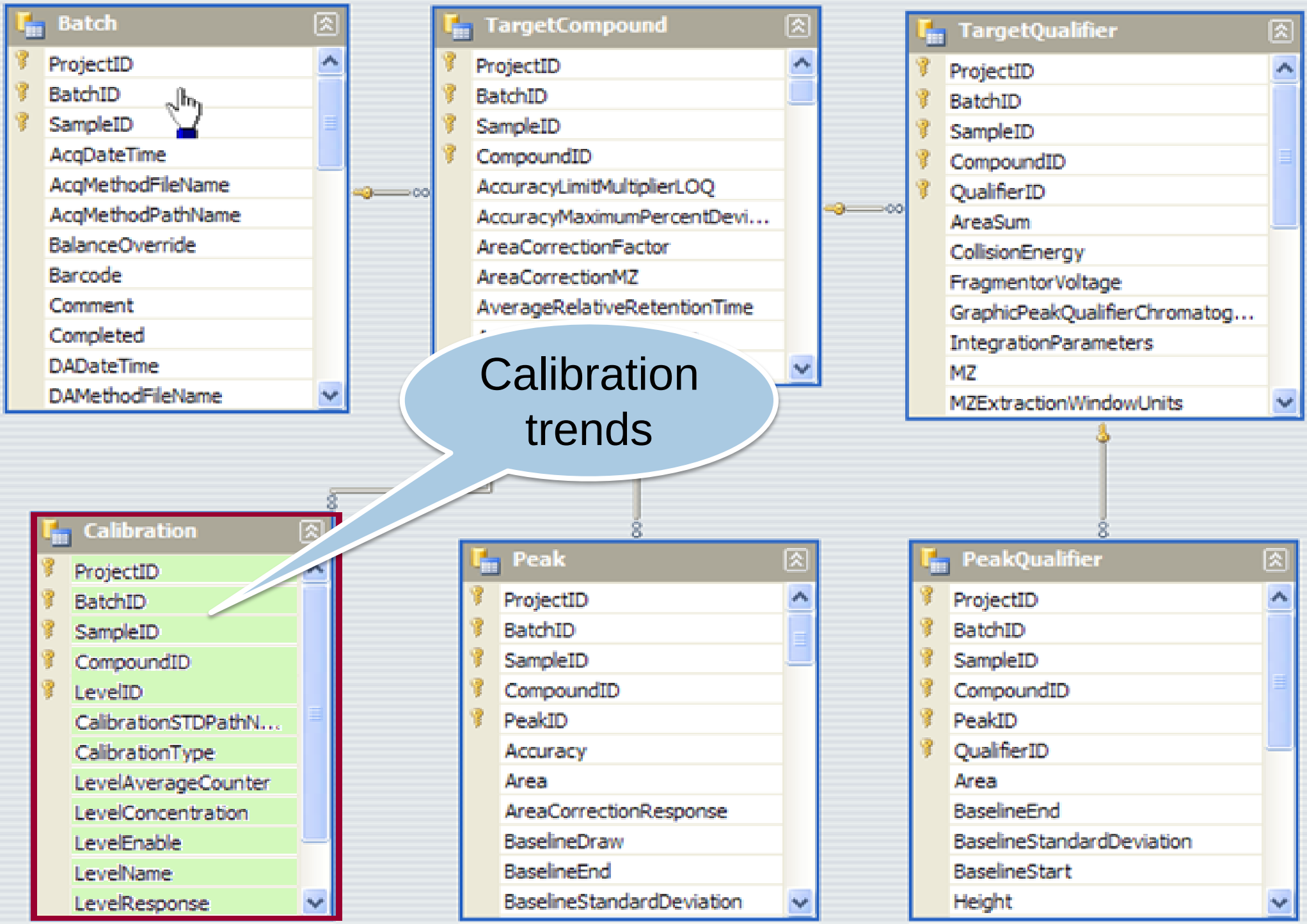
Calibration | TargetCompound | TargetQualifier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SampleID
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AcqMethodFileName
AcqMethodPathName
BalanceOverride
Barcode
Comment
Completed
DADateTime
DAMethodFileName
TargetCompound
ProjectID
BatchID
SampleID
CompoundID
AccuracyLimitMultiplierLOQ
AccuracyMaximumPercentDevi...
AreaCorrectionFactor
AreaCorrectionMZ
AverageRelativeRetentionTime
TargetQualifier
ProjectID
BatchID
SampleID
CompoundID
QualifierID
AreaSum
CollisionEnergy
FragmentorVoltage
GraphicPeakQualifierChromatog...
IntegrationParameters
MZ
MZExtractionWindowUnits
Calibration trends
Calibration
ProjectID
BatchID
SampleID
CompoundID
LevelID
CalibrationSTDPathN...
CalibrationType
LevelAverageCounter
LevelConcentration
LevelEnable
LevelName
LevelResponse
Peak
ProjectID
BatchID
SampleID
CompoundID
PeakID
Accuracy
Area
AreaCorrectionResponse
BaselineDraw
BaselineEnd
BaselineStandardDeviation
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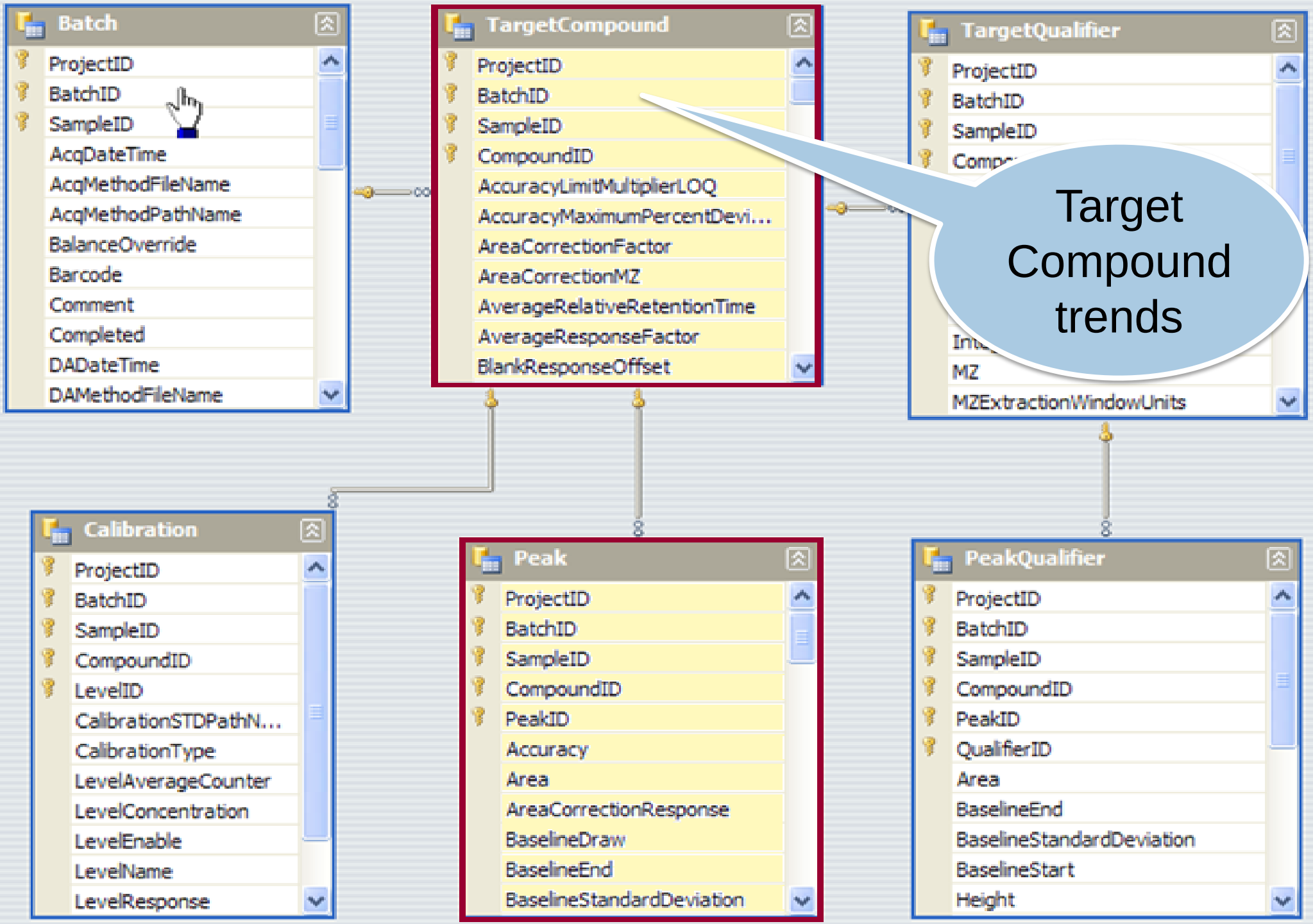
Area
BaselineEnd
BaselineStandardDeviation
BaselineStart
Height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AreaCorrectionMZ
AverageRelativeRetentionTime
AverageResponseFactor
BlankResponseOffset
TargetQualifier
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MZExtractionWindowUnits
Target Compound trends
Calibration
ProjectID
BatchID
SampleID
CompoundID
LevelID
CalibrationSTDPathN...
CalibrationType
LevelAverageCounter
LevelConcentration
LevelEnable
LevelName
LevelResponse
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ProjectID
BatchID
SampleID
CompoundID
PeakID
Accuracy
Area
AreaCorrectionResponse
BaselineDraw
BaselineEnd
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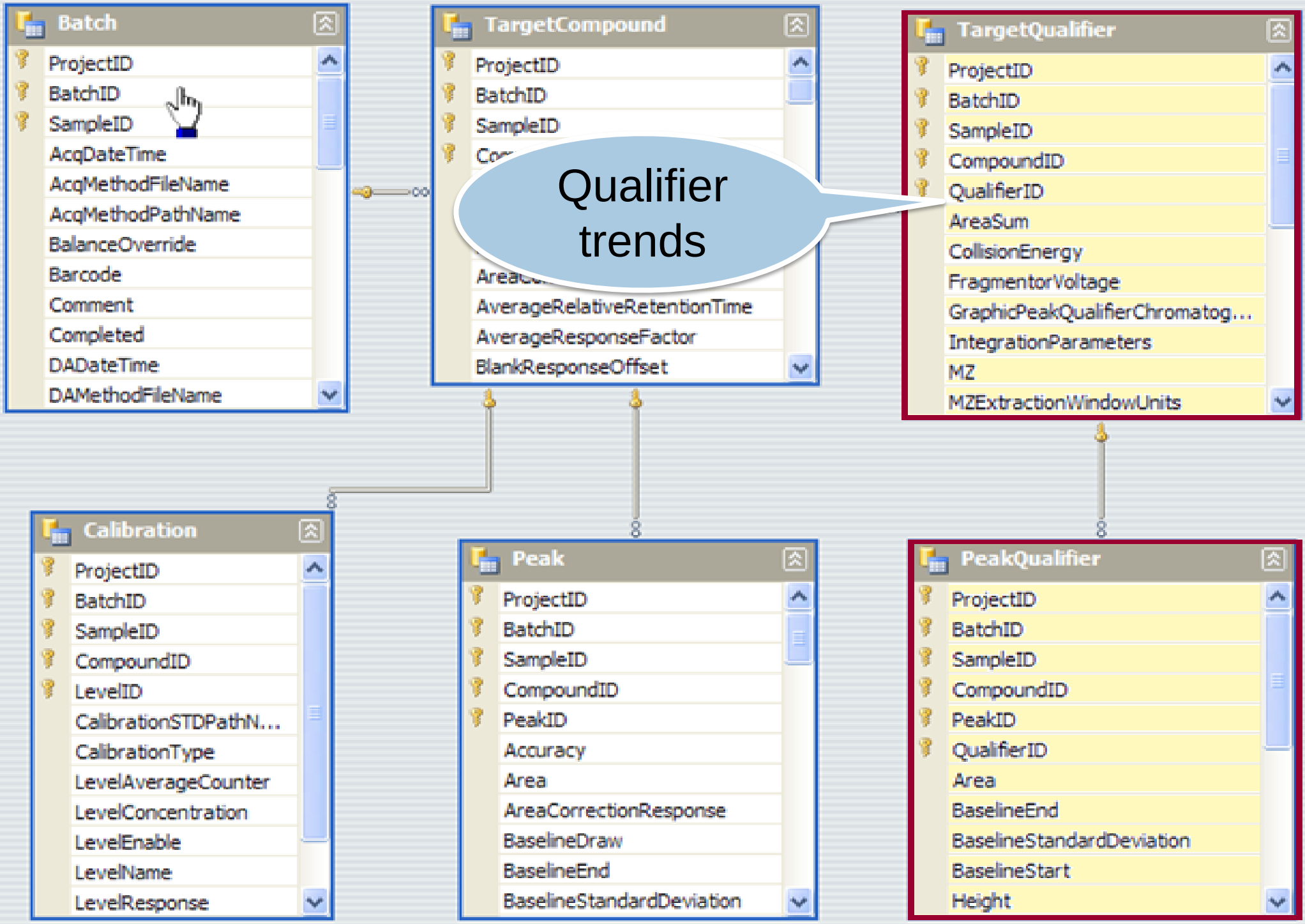
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DAMethodFileName
TargetCompound
ProjectID
BatchID
SampleID
AverageRelativeRetentionTime
AverageResponseFactor
BlankResponseOffset
Qualifier trends
TargetQualifier
ProjectID
BatchID
SampleID
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GraphicPeakQualifierChromatog...
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CompoundID
LevelID
CalibrationSTDPathN...
CalibrationType
LevelAverageCounter
LevelConcentration
LevelEnable
LevelName
LevelResponse
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BatchID
SampleID
CompoundID
PeakID
Accuracy
Area
AreaCorrectionResponse
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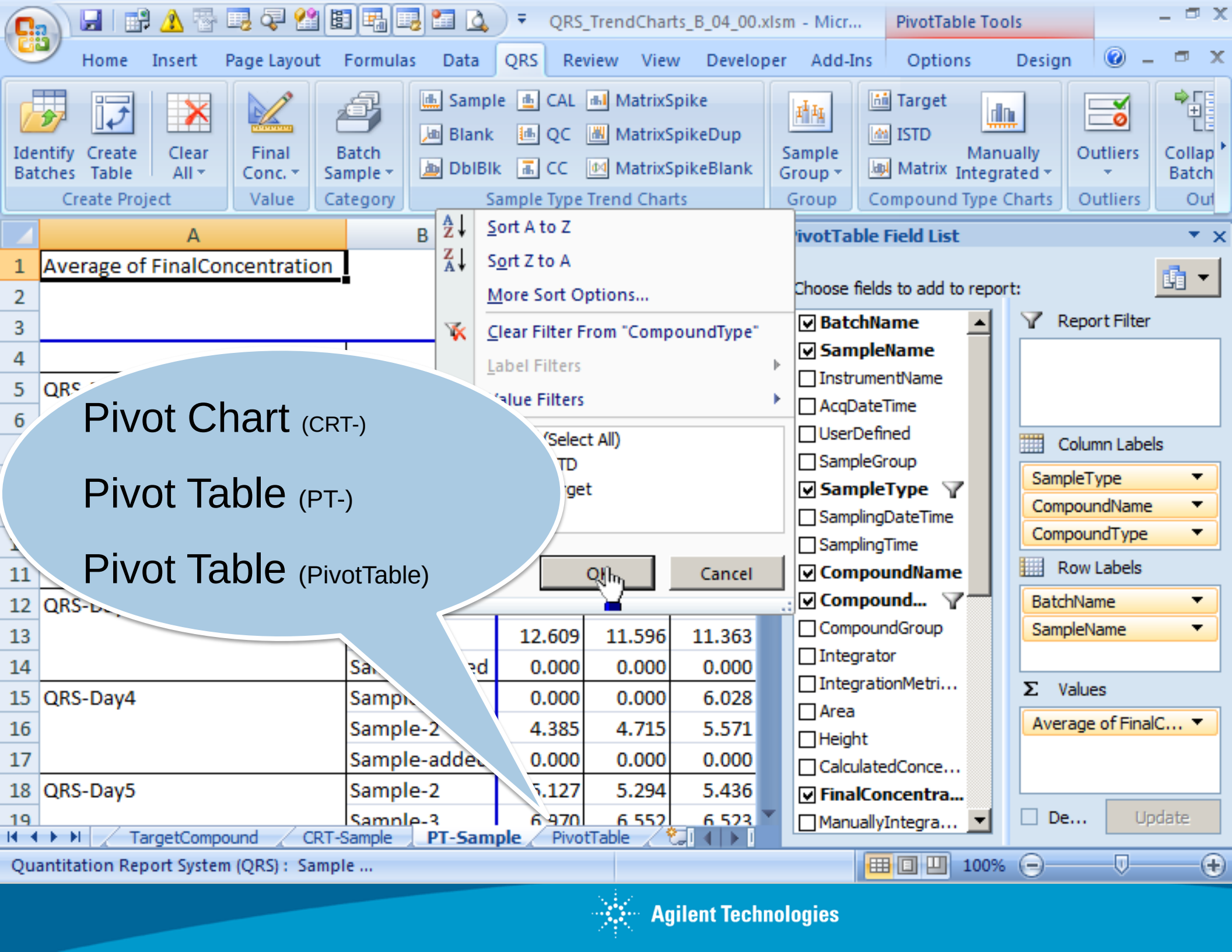
BaselineEnd
BaselineStandardDeviation
PeakQualifier
ProjectID
BatchID
SampleID
CompoundID
PeakID
QualifierID
Area
BaselineEnd
BaselineStandardDeviation
BaselineStart
Height

Pivot Table Data Crunching for Microsoft Office Excel 2007 consolidates all the best functionality of pivot tables including Using VBA to Create Pivot Tables


QRS_TrendCharts_B_04_00.xlsm - Micr...
PivotTable Tools
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Developer
Add-Ins
Options
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Identify Batches
Create Table
Clear All
Create Project
Final Conc.
Value
Batch Sample
Category
Sample
CAL
MatrixSpike
Blank
QC
MatrixSpikeDup
DblBlk
CC
MatrixSpikeBlank
Sample Type Trend Charts
Sample Group
Group
Target
ISTD
Matrix
Manually Integrated
Compound Type Charts
Outliers
Outliers
Collap Batch
Sort A to Z
Sort Z to A
More Sort Options...
Clear Filter From "CompoundType"
Label Filters
Value Filters
(Select All)
TD
get
OK
Cancel
PivotTable Field List
Choose fields to add to report:
BatchName
SampleName
InstrumentName
AcqDateTime
UserDefined
SampleGroup
SampleType
SamplingDateTime
SamplingTime
CompoundName
Compound...
CompoundGroup
Integrator
IntegrationMetri...
Area
Height
CalculatedConce...
FinalConcentra...
ManuallyIntegra...
Report Filter
Column Labels
SampleType
CompoundName
CompoundType
Row Labels
BatchName
SampleName
Values
Average of FinalC...
De...
Update
Average of FinalConcentration
QRS-Day4
QRS-Day5
Sample-2
Sample-added
12.609
11.596
11.363
0.000
0.000
0.000
0.000
6.028
4.385
4.715
5.571
0.000
0.000
0.000
5.127
5.294
5.436
6.970
6.552
6.523
TargetCompound
CRT-Sample
PT-Sample
PivotTable
Quantitation Report System (QRS) : Sample ...
100%
Pivot Chart (CRT-)
Pivot Table (PT-)
Pivot Table (PivotTable)
Agilent Technologies

Sharing the Pivot Cache

Many times, you may have to analyze the same dataset in multiple ways. In most cases, this process requires you to create se… rate pivot tables from the same data source. You might remember that each time you crea… pivot table, you are storing a snapshot of your entire dataset in a pivot cache. Every pivo… he that is created increases your memory usage and file size. Because of this increase in fi… you should consider sharing your pivot cache. That is, in those situations in which yo… to create multiple pivot tables from the same data source, use the same pivot cache to … ltiple pivot tables. By using the same pivot cache for multiple pivot tables, you gain a … el of efficiency when it comes to memory usage and files size.

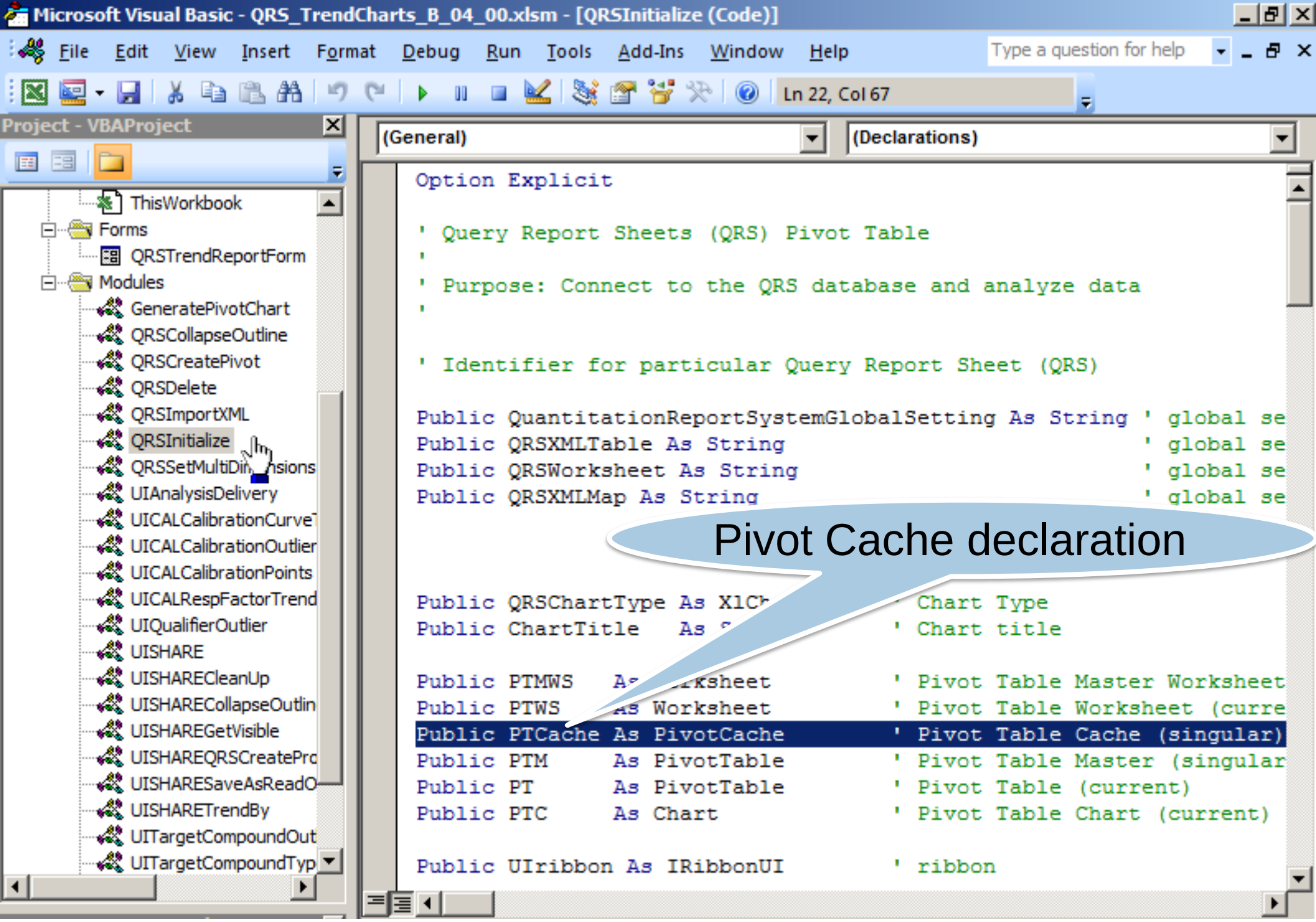
In previous versions of Excel, when you create… ly being used in another pivot table, Excel actually ga… cache. In Excel 2007, Excel gives you no … table in Excel 2007, a new pivot cache is … exist for the dataset being used. The si… bloats with redundant data each time y…

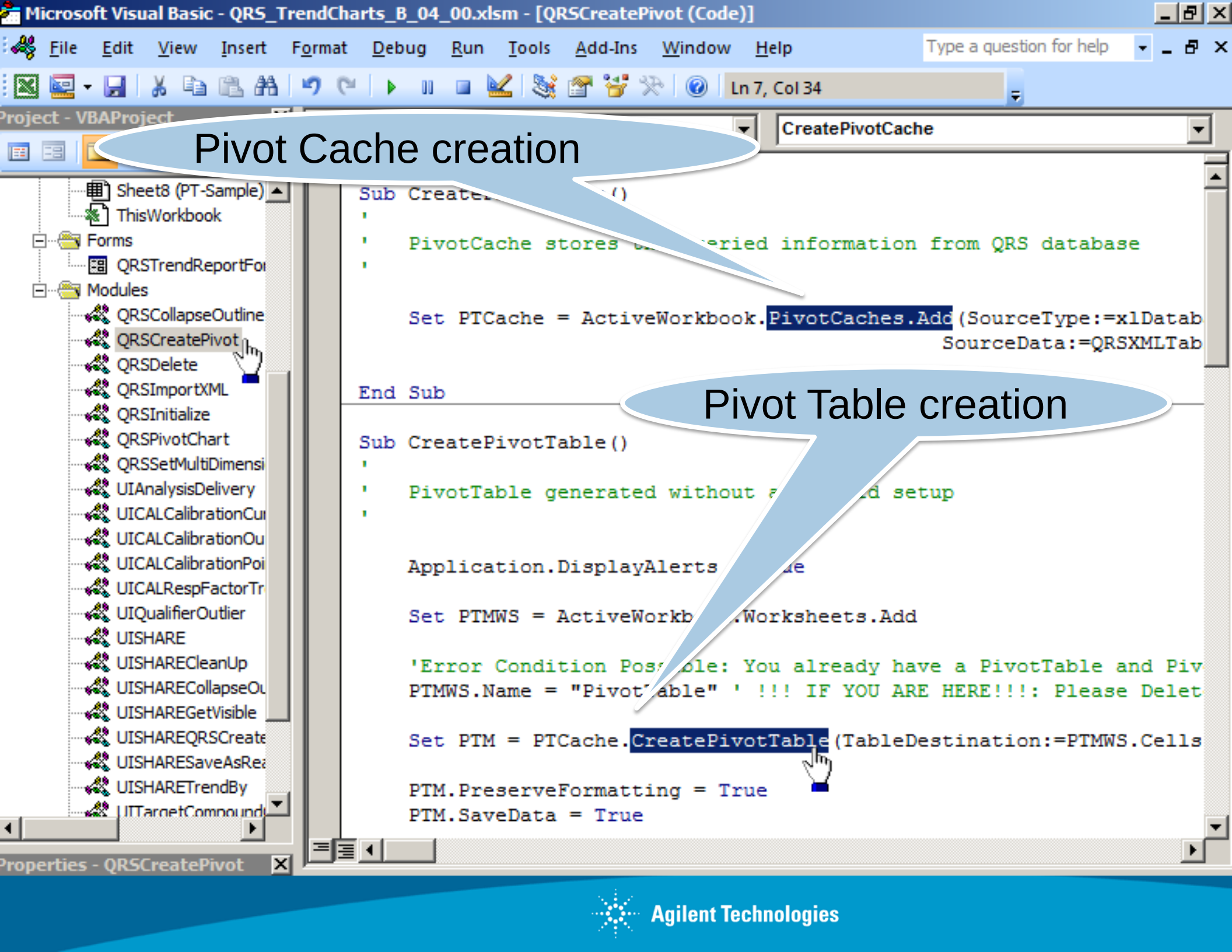
You can easily work around this poten… right. By simply copying a pivot table a… pivot table, *without* duplicating the pivot … es as you want to the same pivot cache, with a…

Pivot Cache shared by Pivot Tables. Different Pivot Caches created for
- Calibration
- TargetCompound
- Qualifier

Side Effects of Sharing a Pivot Cache

It's important to note that there are a few side effects to sharing a pivot cache. For example, suppose you have two pivot tables using the same pivot cache. Certain actions affect both pivot tables. They include


Microsoft Visual Basic - QRS_TrendCharts_B_04_00.xlsm - [QRSInitialize (Code)]
File Edit View Insert Format Debug Run Tools Add-Ins Window Help
Type a question for help
Ln 22, Col 67
Project - VBAProject
ThisWorkbook
Forms
QRSTrendReportForm
Modules
GeneratePivotChart
QRSCollapseOutline
QRSCreatePivot
QRSDelete
QRSImportXML
QRSInitialize
UIAnalysisDelivery
UIQualifierOutlier
UISHARE
UISHARECleanUp
UISHAREGetVisible
UITargetCompoundTyp
(General)
(Declarations)
Option Explicit
' Query Report Sheets (QRS) Pivot Table
' Purpose: Connect to the QRS database and analyze data
' Identifier for particular Query Report Sheet (QRS)
Public QuantitationReportSystemGlobalSetting As String ' global se
Public QRSXMLTable As String ' global se
Public QRSWorksheet As String ' global se
Public QRSXMLMap As String ' global se
Public QRSChartType As XlCh ' Chart Type
Public ChartTitle As ' Chart title
Public PTMWS As Worksheet ' Pivot Table Master Worksheet
Public PTWS As Worksheet ' Pivot Table Worksheet (curre
Public PTCache As PivotCache ' Pivot Table Cache (singular)
Public PTM As PivotTable ' Pivot Table Master (singular
Public PT As PivotTable ' Pivot Table (current)
Public PTC As Chart ' Pivot Table Chart (current)
Public UIribbon As IRibbonUI ' ribbon
Pivot Cache declaration


Microsoft Visual Basic - QRS_TrendCharts_B_04_00.xlsm - [QRSCreatePivot (Code)]
File Edit View Insert Format Debug Run Tools Add-Ins Window Help
Type a question for help
Ln 7, Col 34
Project - VBAProject
Sheet8 (PT-Sample)
ThisWorkbook
Forms
QRSTrendReportFor
Modules
QRSCollapseOutline
QRSCreatePivot
QRSDelete
QRSImportXML
QRSInitialize
QRSPivotChart
QRSSetMultiDimensi
UIAnalysisDelivery
UICALCalibrationCur
UICALCalibrationOu
UICALCalibrationPoi
UICALRespFactorTr
UIQualifierOutlier
UISHARE
UISHARECleanUp
UISHARECollapseOu
UISHAREGetVisible
UISHAREQRSCreate
UISHARESaveAsRea
UISHARETrendBy
Properties - QRSCreatePivot
CreatePivotCache
Pivot Cache creation
Sub Create ()
' PivotCache stores ueried information from QRS database
Set PTCache = ActiveWorkbook.PivotCaches.Add(SourceType:=xlDatab
SourceData:=QRSXMLTab
End Sub
Pivot Table creation
Sub CreatePivotTable()
' PivotTable generated without d setup
Application.DisplayAlerts ue
Set PTMWS = ActiveWorkb .Worksheets.Add
'Error Condition Pos ble: You already have a PivotTable and Piv
PTMWS.Name = "Pivot able" ' !!! IF YOU ARE HERE!!!: Please Delet
Set PTM = PTCache.CreatePivotTable(TableDestination:=PTMWS.Cells
PTM.PreserveFormatting = True
PTM.SaveData = True
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